Full wwPDB EM Validation Report (i)

Jan 1, 2025 – 06:11 PM EST

PDB ID	:	8WA2
EMDB ID	:	EMD-37389
Title	:	cryo-EM structure of native mastigonemes isolated from Chlamydomonas reinhardtii at 3.0 angstrom resolution
Authors	:	Huang, J.; Tao, H.; Chen, J.; Pan, J.; Yan, C.; Yan, N.
Deposited on	:	2023-09-06
Resolution	:	3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

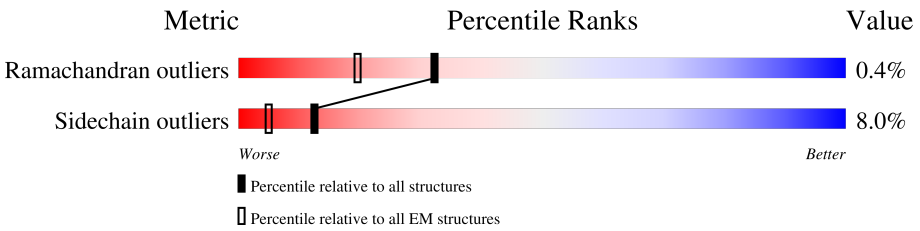
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1987	86% 10% •
1	B	1987	87% 9% •
1	C	1987	18% 69% 6% 25%
1	D	1987	23% 71% 7% 21%
1	E	1987	36% 66% 7% 27%
1	F	1987	35% 66% 7% 27%
2	G	64	8% 38% 62%
2	H	64	8% 20% 27% 53%
2	I	64	9% 19% 33% • 47%

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Mol	Chain	Length	Quality of chain
3	0	3	67% 33%
3	0A	3	67% 33%
3	1	3	67% 33%
3	2	3	100%
3	8C	3	100%
3	9C	3	33% 67%
3	BC	3	67% 33%
3	CC	3	33% 67%
3	DD	3	67% 33%
3	EB	3	100% 67% 33%
3	ED	3	67% 33%
3	FD	3	67% 33%
3	GC	3	67% 33%
3	HA	3	67% 33%
3	HC	3	67% 33%
3	IA	3	100%
3	IC	3	67% 33%
3	ID	3	67% 33%
3	J	3	100%
3	K	3	100%
3	KD	3	67% 33%
3	LB	3	100%
3	LC	3	100%
3	MA	3	100%
3	NA	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	NC	3	100%
3	O	3	67% 33%
3	OA	3	67% 33%
3	OB	3	100% 100%
3	P	3	67% 33%
3	PB	3	33% 100%
3	Q	3	67% 33%
3	QB	3	33% 67% 33%
3	QD	3	100%
3	RA	3	67% 33%
3	RB	3	67% 67% 33%
3	SB	3	33% 67%
3	T	3	67% 33%
3	TA	3	33% 67%
3	TB	3	67% 33%
3	TC	3	100%
3	TD	3	100%
3	UB	3	67% 33%
3	V	3	67% 33%
3	WC	3	33% 67%
3	XA	3	33% 67% 33%
3	ZA	3	67% 33%
3	aD	3	33% 100%
3	b	3	67% 33%
3	bD	3	100%

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Mol	Chain	Length	Quality of chain
3	cA	3	33% 67%
3	dC	3	67% 33%
3	e	3	67% 33%
3	eC	3	100%
3	hB	3	100% 100%
3	iD	3	100%
3	jA	3	33% 67%
3	kA	3	100%
3	l	3	100%
3	lC	3	100%
3	lD	3	67% 100%
3	m	3	100%
3	mD	3	33% 67% 33%
3	nD	3	33% 100%
3	oB	3	67% 33% 67%
3	oC	3	33% 100%
3	oD	3	33% 67% 33%
3	pC	3	67% 33%
3	pD	3	67% 67% 33%
3	qC	3	100%
3	qD	3	67% 100%
3	rA	3	100%
3	rB	3	67% 67% 33%
3	rC	3	100% 67% 33%
3	rD	3	67% 67% 33%

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Mol	Chain	Length	Quality of chain
3	sB	3	33% 100%
3	sC	3	100% 67% 33%
3	t	3	100%
3	tB	3	33% 100%
3	tC	3	33% 67% 33%
3	uA	3	67% 33%
3	uB	3	100%
3	uC	3	67% 67% 33%
3	vA	3	67% 33%
3	vB	3	33% 67% 33%
3	w	3	67% 33%
3	wA	3	67% 33%
3	wB	3	100%
3	x	3	67% 33%
3	xA	3	100%
3	xB	3	67% 33%
3	y	3	100%
3	yA	3	67% 33%
3	z	3	67% 33%
3	zA	3	100%
4	AD	4	50% 50%
4	DC	4	50% 50%
4	JA	4	75% 25%
4	JB	4	50% 100%
4	L	4	75% 25%

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Mol	Chain	Length	Quality of chain
4	LD	4	50% 50%
4	MD	4	100%
4	NB	4	50% 50% 50%
4	OC	4	75% 25%
4	OD	4	75% 25%
4	PC	4	75% 25%
4	RC	4	75% 25%
4	RD	4	50% 50%
4	SD	4	50% 50%
4	UA	4	75% 25%
4	UC	4	100%
4	VA	4	75% 25%
4	VC	4	75% 25%
4	VD	4	50% 50%
4	W	4	75% 25%
4	X	4	100%
4	YC	4	50% 50%
4	Z	4	50% 50%
4	ZD	4	25% 75% 25%
4	aA	4	100%
4	bA	4	100%
4	c	4	75% 25%
4	cC	4	50% 50% 50%
4	d	4	50% 50%
4	eA	4	100%

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Mol	Chain	Length	Quality of chain
4	g	4	75% 25%
4	gD	4	25% 75% 25%
4	iA	4	50% 50%
4	jC	4	75% 25%
4	k	4	100%
4	kD	4	25% 100%
4	mB	4	75% 50% 50%
4	nC	4	25% 50% 50%
4	pA	4	100%
4	qB	4	75% 25% 75%
4	r	4	100%
4	tA	4	50% 50%
4	v	4	75% 25%
5	BD	5	60% 40%
5	EC	5	60% 40%
5	KA	5	40% 60%
5	M	5	20% 80%
6	0B	3	33% 33% 33% 33%
6	0C	3	100% 33% 67%
6	1C	3	100% 67% 33%
6	2C	3	100% 33% 67%
6	3A	3	67% 33%
6	3B	3	33% 67%
6	3D	3	100% 100%
6	4B	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	5	3	67% 33%
6	5B	3	33% 67%
6	6A	3	33% 67%
6	6C	3	100% 33% 67%
6	6D	3	33% 67%
6	7A	3	33% 67%
6	7D	3	33% 67%
6	8	3	33% 67%
6	8A	3	100%
6	8D	3	67% 33%
6	9	3	33% 67%
6	9B	3	33% 67%
6	AA	3	33% 67%
6	CB	3	33% 67%
6	CD	3	33% 33% 33%
6	EA	3	67% 33%
6	FC	3	100%
6	GD	3	33% 67%
6	JC	3	33% 67%
6	LA	3	33% 33% 33%
6	ME	3	67% 33%
6	N	3	33% 33% 33%
6	OE	3	67% 33%
6	PA	3	67% 33%
6	R	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	XB	3	33% / 33% / 33% / 33%
6	ZE	3	33% / 67%
6	aB	3	33% / 67%
6	bB	3	33% / 67%
6	bE	3	67% / 33%
6	cB	3	100%
6	gB	3	67% / 33%
6	mE	3	67% / 33%
6	nE	3	33% / 67%
6	oE	3	33% / 67%
6	uD	3	100% / 33% / 33% / 33%
6	xC	3	100% / 33% / 33% / 33%
6	xD	3	100% / 33% / 67%
6	yD	3	100% / 100%
6	zD	3	100% / 33% / 67%
7	HD	4	50% / 50%
7	KC	4	50% / 50%
7	QA	4	50% / 50%
7	S	4	25% / 75%
7	UD	4	75% / 25%
7	WD	4	75% / 25%
7	XC	4	75% / 25%
7	ZC	4	75% / 25%
7	dA	4	50% / 50%
7	f	4	50% / 50%

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Mol	Chain	Length	Quality of chain
7	fA	4	100%
7	h	4	75% 25%
8	JD	5	80% 20%
8	MC	5	40% 60%
8	SA	5	100%
8	U	5	60% 40%
9	ND	2	50% 50%
9	QC	2	100%
9	WA	2	100%
9	Y	2	50% 50%
9	YD	2	100%
9	bC	2	100%
9	hA	2	50% 50%
9	j	2	50% 50%
10	1A	5	20% 80%
10	3	5	40% 60%
10	MB	5	80% 60% 40%
10	PD	5	60% 40%
10	SC	5	80% 20%
10	VB	5	20% 60% 40%
10	YA	5	80% 20%
10	a	5	40% 60%
10	jD	5	20% 60% 40%
10	mC	5	40% 40% 60%
10	pB	5	100% 60% 40%

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Mol	Chain	Length	Quality of chain
10	sA	5	60% 40%
10	sD	5	60% 80% 20%
10	u	5	60% 40%
10	vC	5	40% 40% 60%
10	yB	5	80% 20%
11	XD	3	33% 67%
11	aC	3	67% 33%
11	gA	3	33% 67%
11	i	3	100%
12	FB	5	100% 60% 20% 20%
12	IB	5	80% 20% 60% 20%
12	cD	5	20% 60% 20% 20%
12	fC	5	20% 60% 20% 20%
12	fD	5	20% 60% 20%
12	iB	5	100% 80% 20%
12	iC	5	20% 80% 20%
12	lA	5	40% 40% 20%
12	lB	5	80% 60% 20% 20%
12	n	5	40% 40% 20%
12	oA	5	60% 20% 20%
12	q	5	20% 60% 20%
13	0D	4	100% 75% 25%
13	1B	4	75% 25%
13	2A	4	75% 25%
13	2B	4	50% 50%

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Mol	Chain	Length	Quality of chain
13	3C	4	100%, 50%, 50%
13	4	4	25%, 50%, 25%
13	4A	4	50%, 50%
13	5A	4	50%, 50%
13	6	4	50%, 50%
13	6B	4	50%, 50%
13	7	4	50%, 50%
13	9A	4	50%, 50%
13	BA	4	50%, 50%
13	GB	4	100%, 75%, 25%
13	WB	4	25%, 25%, 50%, 25%
13	YB	4	50%, 50%
13	ZB	4	75%, 25%
13	dB	4	50%, 50%
13	dD	4	25%, 75%, 25%
13	gC	4	25%, 50%, 25%, 25%
13	jB	4	100%, 50%, 25%, 25%
13	mA	4	50%, 25%, 25%
13	o	4	50%, 25%, 25%
13	tD	4	75%, 25%, 50%, 25%
13	vD	4	75%, 50%, 50%
13	wC	4	75%, 25%, 50%, 25%
13	wD	4	50%, 25%, 75%
13	yC	4	50%, 50%, 50%
13	zB	4	25%, 25%, 50%, 25%

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Mol	Chain	Length	Quality of chain
13	zC	4	100%; 50%; 50%
14	HB	4	100%; 50%; 25%; 25%
14	KB	4	100%; 50%; 25%; 25%
14	eD	4	75%; 25%
14	hC	4	50%; 25%; 25%
14	hD	4	75%; 25%
14	kB	4	100%; 25%; 50%; 25%
14	kC	4	75%; 25%
14	nA	4	75%; 25%
14	nB	4	75%; 50%; 25%; 25%
14	p	4	50%; 25%; 25%
14	qA	4	75%; 25%
14	s	4	75%; 25%
15	1D	5	100%; 40%; 60%
15	2D	5	100%; 40%; 60%
15	4C	5	100%; 60%; 40%
15	5C	5	100%; 20%; 80%
15	7B	5	60%; 40%
15	8B	5	40%; 60%
15	AB	5	20%; 80%
15	BB	5	40%; 60%
15	CA	5	60%; 40%
15	DA	5	40%; 60%
15	eB	5	40%; 60%
15	fB	5	40%; 60%

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Mol	Chain	Length	Quality of chain
16	4D	2	50% / 50% / 50%
16	AC	2	100% / 100%
16	FA	2	50% / 50%
17	5D	6	50% / 50%
17	7C	6	50% / 50%
17	DB	6	17% / 83%
17	GA	6	67% / 33%
18	0E	5	60% / 40%
18	9D	5	20% / 80%
18	BE	5	20% / 40% / 60%
18	DE	5	20% / 40% / 60%
18	IE	5	20% / 80%
18	JE	5	60% / 40%
18	KE	5	60% / 40%
18	PE	5	60% / 40%
18	SE	5	60% / 40%
18	cE	5	60% / 40%
18	fE	5	60% / 40%
18	pE	5	40% / 60%
18	rE	5	20% / 40% / 60%
18	tE	5	40% / 60%
18	yE	5	20% / 40% / 60%
18	zE	5	20% / 60% / 40%
19	1E	4	50% / 100%
19	AE	4	50% / 50%

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Mol	Chain	Length	Quality of chain
19	LE	4	25% 50% 50%
19	NE	4	75% 25%
19	aE	4	25% 50% 50%
19	qE	4	50% 50%
20	CE	4	75% 25%
20	EE	4	50% 50%
20	HE	4	75% 25%
20	TE	4	50% 50%
20	UE	4	75% 25%
20	WE	4	50% 50%
20	gE	4	75% 25%
20	hE	4	75% 25%
20	jE	4	75% 25%
20	sE	4	25% 75%
20	uE	4	50% 50%
20	xE	4	50% 50%
21	FE	5	40% 60%
21	kE	5	20% 80%
21	vE	5	40% 60%
22	GE	6	33% 67%
22	QE	6	17% 33% 67%
22	RE	6	33% 67%
22	VE	6	33% 67%
22	dE	6	17% 83%
22	eE	6	17% 17% 67% 17%

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Mol	Chain	Length	Quality of chain
22	iE	6	17% 50% 50%
22	wE	6	67% 33%
23	XE	6	50% 50%
24	YE	6	17% 83%
24	lE	6	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	AHR	1A	4	X	-	-	-
10	AHR	3	4	X	-	-	-
10	AHR	VB	4	X	-	-	-
10	AHR	sD	4	X	-	-	-
10	AHR	vC	4	X	-	-	-
10	AHR	yB	4	X	-	-	-
12	GZL	FB	3	X	-	-	-
12	GZL	IB	3	X	-	-	-
12	GZL	cD	3	X	-	-	-
12	GZL	fC	3	X	-	-	-
12	GZL	fD	3	X	-	-	-
12	GZL	iB	3	X	-	-	-
12	GZL	iC	3	X	-	-	-
12	GZL	lA	3	X	-	-	-
12	GZL	lB	3	X	-	-	-
12	GZL	n	3	X	-	-	-
12	GZL	oA	3	X	-	-	-
12	GZL	q	3	X	-	-	-
12	AHR	q	5	X	-	-	-
13	FUB	0D	2	X	-	-	-
13	GZL	1B	3	X	-	-	-
13	GZL	2A	3	X	-	-	-
13	GZL	2B	3	X	-	-	-
13	FUB	3C	2	X	-	-	-
13	GZL	4	3	X	-	-	-
13	GZL	4A	3	X	-	-	-
13	GZL	5A	3	X	-	-	-
13	GZL	6	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	FUB	6B	2	X	-	-	-
13	GZL	7	3	X	-	-	-
13	FUB	9A	2	X	-	-	-
13	FUB	BA	2	X	-	-	-
13	GZL	GB	3	X	-	-	-
13	GZL	WB	3	X	-	-	-
13	GZL	YB	3	X	-	-	-
13	GZL	ZB	3	X	-	-	-
13	FUB	dB	2	X	-	-	-
13	GZL	dD	3	X	-	-	-
13	GZL	gC	3	X	-	-	-
13	GZL	jB	3	X	-	-	-
13	GZL	mA	3	X	-	-	-
13	GZL	o	3	X	-	-	-
13	GZL	tD	3	X	-	-	-
13	GZL	vD	3	X	-	-	-
13	GZL	wC	3	X	-	-	-
13	GZL	wD	3	X	-	-	-
13	GZL	yC	3	X	-	-	-
13	GZL	zB	3	X	-	-	-
13	GZL	zC	3	X	-	-	-
14	GZL	HB	3	X	-	-	-
14	GZL	KB	3	X	-	-	-
14	GZL	eD	3	X	-	-	-
14	GZL	hC	3	X	-	-	-
14	GZL	hD	3	X	-	-	-
14	GZL	kB	3	X	-	-	-
14	GZL	kC	3	X	-	-	-
14	GZL	nA	3	X	-	-	-
14	GZL	nB	3	X	-	-	-
14	GZL	p	3	X	-	-	-
14	GZL	qA	3	X	-	-	-
14	GZL	s	3	X	-	-	-
15	GZL	1D	3	X	-	-	-
15	AHR	1D	5	X	-	-	-
15	GZL	2D	3	X	-	-	-
15	GZL	4C	3	X	-	-	-
15	AHR	4C	5	X	-	-	-
15	GZL	5C	3	X	-	-	-
15	GZL	7B	3	X	-	-	-
15	AHR	7B	5	X	-	-	-
15	GZL	8B	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	GZL	AB	3	X	-	-	-
15	AHR	AB	5	X	-	-	-
15	GZL	BB	3	X	-	-	-
15	GZL	CA	3	X	-	-	-
15	AHR	CA	5	X	-	-	-
15	GZL	DA	3	X	-	-	-
15	GZL	eB	3	X	-	-	-
15	AHR	eB	5	X	-	-	-
15	GZL	fB	3	X	-	-	-
17	MAN	5D	4	X	-	-	-
17	MAN	5D	6	X	-	-	-
17	MAN	7C	4	X	-	-	-
17	MAN	7C	6	X	-	-	-
17	MAN	DB	4	X	-	-	-
17	MAN	DB	6	X	-	-	-
17	MAN	GA	4	X	-	-	-
17	MAN	GA	6	X	-	-	-
18	GZL	0E	3	X	-	-	-
18	AHR	0E	4	X	-	-	-
18	AHR	0E	5	X	-	-	-
18	GZL	9D	3	X	-	-	-
18	AHR	9D	4	X	-	-	-
18	GZL	BE	3	X	-	-	-
18	AHR	BE	4	X	-	-	-
18	AHR	BE	5	X	-	-	-
18	GZL	DE	3	X	-	-	-
18	AHR	DE	5	X	-	-	-
18	GZL	IE	3	X	-	-	-
18	AHR	IE	4	X	-	-	-
18	GZL	JE	3	X	-	-	-
18	AHR	JE	5	X	-	-	-
18	GZL	KE	3	X	-	-	-
18	AHR	KE	4	X	-	-	-
18	AHR	KE	5	X	-	-	-
18	GZL	PE	3	X	-	-	-
18	AHR	PE	4	X	-	-	-
18	AHR	PE	5	X	-	-	-
18	FUB	SE	1	X	-	-	-
18	GZL	SE	3	X	-	-	-
18	AHR	SE	4	X	-	-	-
18	AHR	SE	5	X	-	-	-
18	GZL	cE	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AHR	cE	4	X	-	-	-
18	AHR	cE	5	X	-	-	-
18	FUB	fE	1	X	-	-	-
18	GZL	fE	3	X	-	-	-
18	AHR	fE	4	X	-	-	-
18	AHR	fE	5	X	-	-	-
18	GZL	pE	3	X	-	-	-
18	AHR	pE	4	X	-	-	-
18	GZL	rE	3	X	-	-	-
18	AHR	rE	4	X	-	-	-
18	AHR	rE	5	X	-	-	-
18	GZL	tE	3	X	-	-	-
18	AHR	tE	5	X	-	-	-
18	GZL	yE	3	X	-	-	-
18	AHR	yE	4	X	-	-	-
18	GZL	zE	3	X	-	-	-
18	AHR	zE	5	X	-	-	-
19	GZL	1E	3	X	-	-	-
19	AHR	1E	4	X	-	-	-
19	GZL	AE	3	X	-	-	-
19	GZL	LE	3	X	-	-	-
19	AHR	LE	4	X	-	-	-
19	GZL	NE	3	X	-	-	-
19	AHR	NE	4	X	-	-	-
19	GZL	aE	3	X	-	-	-
19	AHR	aE	4	X	-	-	-
19	GZL	qE	3	X	-	-	-
2	HYP	G	23	X	-	-	-
2	HYP	G	26	X	-	-	-
2	HYP	I	23	X	-	-	-
2	HYP	I	26	X	-	-	-
20	GZL	CE	3	X	-	-	-
20	GZL	EE	3	X	-	-	-
20	GZL	HE	3	X	-	-	-
20	GZL	TE	3	X	-	-	-
20	AHR	TE	4	X	-	-	-
20	GZL	UE	3	X	-	-	-
20	GZL	WE	3	X	-	-	-
20	AHR	WE	4	X	-	-	-
20	GZL	gE	3	X	-	-	-
20	AHR	gE	4	X	-	-	-
20	GZL	hE	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	GZL	jE	3	X	-	-	-
20	AHR	jE	4	X	-	-	-
20	GZL	sE	3	X	-	-	-
20	GZL	uE	3	X	-	-	-
20	GZL	xE	3	X	-	-	-
21	GZL	FE	3	X	-	-	-
21	AHR	FE	4	X	-	-	-
21	AHR	FE	5	X	-	-	-
21	GZL	kE	3	X	-	-	-
21	AHR	kE	4	X	-	-	-
21	GZL	vE	3	X	-	-	-
21	AHR	vE	4	X	-	-	-
21	AHR	vE	5	X	-	-	-
22	GZL	GE	3	X	-	-	-
22	GZL	QE	3	X	-	-	-
22	AHR	QE	4	X	-	-	-
22	AHR	QE	6	X	-	-	-
22	GZL	RE	3	X	-	-	-
22	AHR	RE	4	X	-	-	-
22	GZL	VE	3	X	-	-	-
22	AHR	VE	4	X	-	-	-
22	GZL	dE	3	X	-	-	-
22	AHR	dE	4	X	-	-	-
22	AHR	dE	6	X	-	-	-
22	GZL	eE	3	X	-	-	-
22	AHR	eE	4	X	-	-	-
22	GZL	iE	3	X	-	-	-
22	AHR	iE	4	X	-	-	-
22	GZL	wE	3	X	-	-	-
23	GZL	XE	3	X	-	-	-
23	AHR	XE	4	X	-	-	-
23	AHR	XE	5	X	-	-	-
24	GZL	YE	3	X	-	-	-
24	AHR	YE	4	X	-	-	-
24	GZL	lE	3	X	-	-	-
24	AHR	lE	4	X	-	-	-
27	GLA	A	2007	X	-	-	-
27	GLA	B	2008	X	-	-	-
27	GLA	B	2014	X	-	-	-
27	GLA	E	2007	X	-	-	-
27	GLA	F	2009	X	-	-	-
3	FUB	XA	2	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUB	AD	1	X	-	-	-
4	FUB	DC	1	X	-	-	-
4	FUB	JA	1	X	-	-	-
4	FUB	L	1	X	-	-	-
4	FUB	OD	2	X	-	-	-
4	AHR	PC	4	X	-	-	-
4	FUB	RC	2	X	-	-	-
4	AHR	VA	4	X	-	-	-
4	FUB	Z	2	X	-	-	-
5	AHR	BD	5	X	-	-	-
6	GZL	0B	3	X	-	-	-
6	GZL	1C	3	X	-	-	-
6	FUB	2C	2	X	-	-	-
6	GZL	2C	3	X	-	-	-
6	GZL	3A	3	X	-	-	-
6	GZL	3D	3	X	-	-	-
6	GZL	4B	3	X	-	-	-
6	GZL	5	3	X	-	-	-
6	FUB	5B	2	X	-	-	-
6	GZL	5B	3	X	-	-	-
6	GZL	6C	3	X	-	-	-
6	GZL	6D	3	X	-	-	-
6	GZL	7A	3	X	-	-	-
6	GZL	7D	3	X	-	-	-
6	GZL	8	3	X	-	-	-
6	FUB	8A	2	X	-	-	-
6	GZL	8A	3	X	-	-	-
6	GZL	8D	3	X	-	-	-
6	GZL	9	3	X	-	-	-
6	GZL	9B	3	X	-	-	-
6	FUB	AA	2	X	-	-	-
6	GZL	AA	3	X	-	-	-
6	GZL	CB	3	X	-	-	-
6	GZL	CD	3	X	-	-	-
6	GZL	EA	3	X	-	-	-
6	GZL	FC	3	X	-	-	-
6	GZL	GD	3	X	-	-	-
6	GZL	JC	3	X	-	-	-
6	GZL	LA	3	X	-	-	-
6	GZL	ME	3	X	-	-	-
6	GZL	N	3	X	-	-	-
6	GZL	OE	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GZL	PA	3	X	-	-	-
6	GZL	R	3	X	-	-	-
6	GZL	XB	3	X	-	-	-
6	GZL	ZE	3	X	-	-	-
6	GZL	bB	3	X	-	-	-
6	GZL	bE	3	X	-	-	-
6	FUB	cB	2	X	-	-	-
6	GZL	cB	3	X	-	-	-
6	GZL	gB	3	X	-	-	-
6	GZL	mE	3	X	-	-	-
6	GZL	nE	3	X	-	-	-
6	GZL	oE	3	X	-	-	-
6	GZL	uD	3	X	-	-	-
6	GZL	xC	3	X	-	-	-
6	GZL	yD	3	X	-	-	-
6	FUB	zD	2	X	-	-	-
6	GZL	zD	3	X	-	-	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 85288 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

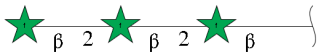
- Molecule 1 is a protein called Mst1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1907	13862	8723	2261	2797	81	0	0
1	B	1907	13862	8723	2261	2797	81	0	0
1	C	1494	10840	6862	1753	2179	46	0	0
1	D	1566	11377	7199	1841	2286	51	0	0
1	E	1449	10491	6595	1712	2105	79	0	0
1	F	1443	10455	6573	1705	2098	79	0	0

- Molecule 2 is a protein called Mstax.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	G	64	438	269	65	104	0	0
2	H	30	201	125	30	46	0	0
2	I	34	238	145	35	58	0	0

- Molecule 3 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	J	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	K	3	27	15	12	0	0
3	O	3	27	15	12	0	0
3	P	3	27	15	12	0	0
3	Q	3	27	15	12	0	0
3	T	3	27	15	12	0	0
3	V	3	27	15	12	0	0
3	b	3	27	15	12	0	0
3	e	3	27	15	12	0	0
3	l	3	27	15	12	0	0
3	m	3	27	15	12	0	0
3	t	3	27	15	12	0	0
3	w	3	27	15	12	0	0
3	x	3	27	15	12	0	0
3	y	3	27	15	12	0	0
3	z	3	27	15	12	0	0
3	0	3	27	15	12	0	0
3	1	3	27	15	12	0	0
3	2	3	27	15	12	0	0
3	HA	3	27	15	12	0	0
3	IA	3	27	15	12	0	0
3	MA	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	NA	3	27	15	12	0	0
3	OA	3	27	15	12	0	0
3	RA	3	27	15	12	0	0
3	TA	3	27	15	12	0	0
3	XA	3	27	15	12	0	0
3	ZA	3	27	15	12	0	0
3	cA	3	27	15	12	0	0
3	jA	3	27	15	12	0	0
3	kA	3	27	15	12	0	0
3	rA	3	27	15	12	0	0
3	uA	3	27	15	12	0	0
3	vA	3	27	15	12	0	0
3	wA	3	27	15	12	0	0
3	xA	3	27	15	12	0	0
3	yA	3	27	15	12	0	0
3	zA	3	27	15	12	0	0
3	0A	3	27	15	12	0	0
3	EB	3	27	15	12	0	0
3	LB	3	27	15	12	0	0
3	OB	3	27	15	12	0	0
3	PB	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	QB	3	27	15	12	0	0
3	RB	3	27	15	12	0	0
3	SB	3	27	15	12	0	0
3	TB	3	27	15	12	0	0
3	UB	3	27	15	12	0	0
3	hB	3	27	15	12	0	0
3	oB	3	27	15	12	0	0
3	rB	3	27	15	12	0	0
3	sB	3	27	15	12	0	0
3	tB	3	27	15	12	0	0
3	uB	3	27	15	12	0	0
3	vB	3	27	15	12	0	0
3	wB	3	27	15	12	0	0
3	xB	3	27	15	12	0	0
3	BC	3	27	15	12	0	0
3	CC	3	27	15	12	0	0
3	GC	3	27	15	12	0	0
3	HC	3	27	15	12	0	0
3	IC	3	27	15	12	0	0
3	LC	3	27	15	12	0	0
3	NC	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	TC	3	27	15	12	0	0
3	WC	3	27	15	12	0	0
3	dC	3	27	15	12	0	0
3	eC	3	27	15	12	0	0
3	lC	3	27	15	12	0	0
3	oC	3	27	15	12	0	0
3	pC	3	27	15	12	0	0
3	qC	3	27	15	12	0	0
3	rC	3	27	15	12	0	0
3	sC	3	27	15	12	0	0
3	tC	3	27	15	12	0	0
3	uC	3	27	15	12	0	0
3	8C	3	27	15	12	0	0
3	9C	3	27	15	12	0	0
3	DD	3	27	15	12	0	0
3	ED	3	27	15	12	0	0
3	FD	3	27	15	12	0	0
3	ID	3	27	15	12	0	0
3	KD	3	27	15	12	0	0
3	QD	3	27	15	12	0	0
3	TD	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	aD	3	27	15	12	0	0
3	bD	3	27	15	12	0	0
3	iD	3	27	15	12	0	0
3	lD	3	27	15	12	0	0
3	mD	3	27	15	12	0	0
3	nD	3	27	15	12	0	0
3	oD	3	27	15	12	0	0
3	pD	3	27	15	12	0	0
3	qD	3	27	15	12	0	0
3	rD	3	27	15	12	0	0

- Molecule 4 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
4	L	4	36	20	16	0	0
4	W	4	36	20	16	0	0
4	X	4	36	20	16	0	0
4	Z	4	36	20	16	0	0
4	c	4	36	20	16	0	0
4	d	4	36	20	16	0	0
4	g	4	36	20	16	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
4	k	4	36	20	16	0	0
4	r	4	36	20	16	0	0
4	v	4	36	20	16	0	0
4	JA	4	36	20	16	0	0
4	UA	4	36	20	16	0	0
4	VA	4	36	20	16	0	0
4	aA	4	36	20	16	0	0
4	bA	4	36	20	16	0	0
4	eA	4	36	20	16	0	0
4	iA	4	36	20	16	0	0
4	pA	4	36	20	16	0	0
4	tA	4	36	20	16	0	0
4	JB	4	36	20	16	0	0
4	NB	4	36	20	16	0	0
4	mB	4	36	20	16	0	0
4	qB	4	36	20	16	0	0
4	DC	4	36	20	16	0	0
4	OC	4	36	20	16	0	0
4	PC	4	36	20	16	0	0
4	RC	4	36	20	16	0	0
4	UC	4	36	20	16	0	0

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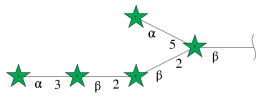
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
4	VC	4	36	20	16	0	0
4	YC	4	36	20	16	0	0
4	cC	4	36	20	16	0	0
4	jC	4	36	20	16	0	0
4	nC	4	36	20	16	0	0
4	AD	4	36	20	16	0	0
4	LD	4	36	20	16	0	0
4	MD	4	36	20	16	0	0
4	OD	4	36	20	16	0	0
4	RD	4	36	20	16	0	0
4	SD	4	36	20	16	0	0
4	VD	4	36	20	16	0	0
4	ZD	4	36	20	16	0	0
4	gD	4	36	20	16	0	0
4	kD	4	36	20	16	0	0

- Molecule 5 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
5	M	5	45	25	20	0	0
5	KA	5	45	25	20	0	0

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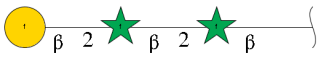
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
5	EC	5	45	25	20	0	0
			Total	C	O		
5	BD	5	45	25	20	0	0

- Molecule 6 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
6	N	3	29	16	13	0	0
			Total	C	O		
6	R	3	29	16	13	0	0
			Total	C	O		
6	5	3	29	16	13	0	0
			Total	C	O		
6	8	3	29	16	13	0	0
			Total	C	O		
6	9	3	29	16	13	0	0
			Total	C	O		
6	AA	3	29	16	13	0	0
			Total	C	O		
6	EA	3	29	16	13	0	0
			Total	C	O		
6	LA	3	29	16	13	0	0
			Total	C	O		
6	PA	3	29	16	13	0	0
			Total	C	O		
6	3A	3	29	16	13	0	0
			Total	C	O		
6	6A	3	29	16	13	0	0
			Total	C	O		
6	7A	3	29	16	13	0	0
			Total	C	O		
6	8A	3	29	16	13	0	0
			Total	C	O		
6	CB	3	29	16	13	0	0
			Total	C	O		
6	XB	3	29	16	13	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
6	aB	3	29	16	13	0	0
6	bB	3	29	16	13	0	0
6	cB	3	29	16	13	0	0
6	gB	3	29	16	13	0	0
6	0B	3	29	16	13	0	0
6	3B	3	29	16	13	0	0
6	4B	3	29	16	13	0	0
6	5B	3	29	16	13	0	0
6	9B	3	29	16	13	0	0
6	FC	3	29	16	13	0	0
6	JC	3	29	16	13	0	0
6	xC	3	29	16	13	0	0
6	0C	3	29	16	13	0	0
6	1C	3	29	16	13	0	0
6	2C	3	29	16	13	0	0
6	6C	3	29	16	13	0	0
6	CD	3	29	16	13	0	0
6	GD	3	29	16	13	0	0
6	uD	3	29	16	13	0	0
6	xD	3	29	16	13	0	0
6	yD	3	29	16	13	0	0

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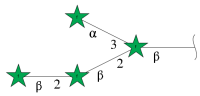
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
6	zD	3	29	16	13	0	0
6	3D	3	29	16	13	0	0
6	6D	3	29	16	13	0	0
6	7D	3	29	16	13	0	0
6	8D	3	29	16	13	0	0
6	ME	3	29	16	13	0	0
6	OE	3	29	16	13	0	0
6	ZE	3	29	16	13	0	0
6	bE	3	29	16	13	0	0
6	mE	3	29	16	13	0	0
6	nE	3	29	16	13	0	0
6	oE	3	29	16	13	0	0

- Molecule 7 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
7	S	4	36	20	16	0	0
7	f	4	36	20	16	0	0
7	h	4	36	20	16	0	0
7	QA	4	36	20	16	0	0
7	dA	4	36	20	16	0	0

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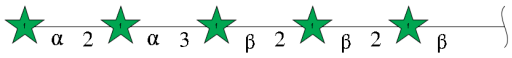
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
7	fA	4	36	20	16	0	0
7	KC	4	36	20	16	0	0
7	XC	4	36	20	16	0	0
7	ZC	4	36	20	16	0	0
7	HD	4	36	20	16	0	0
7	UD	4	36	20	16	0	0
7	WD	4	36	20	16	0	0

- Molecule 8 is an oligosaccharide called alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
8	U	5	45	25	20	0	0
8	SA	5	45	25	20	0	0
8	MC	5	45	25	20	0	0
8	JD	5	45	25	20	0	0

- Molecule 9 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
9	Y	2	18	10	8	0	0

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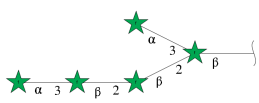
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
9	j	2	18	10	8	0	0
9	WA	2	18	10	8	0	0
9	hA	2	18	10	8	0	0
9	QC	2	18	10	8	0	0
9	bC	2	18	10	8	0	0
9	ND	2	18	10	8	0	0
9	YD	2	18	10	8	0	0

- Molecule 10 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
10	a	5	45	25	20	0	0
10	u	5	45	25	20	0	0
10	3	5	45	25	20	0	0
10	YA	5	45	25	20	0	0
10	sA	5	45	25	20	0	0
10	1A	5	45	25	20	0	0
10	MB	5	45	25	20	0	0
10	VB	5	45	25	20	0	0
10	pB	5	45	25	20	0	0

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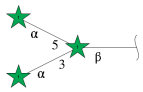
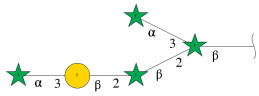
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
10	yB	5	45	25	20	0	0
10	SC	5	45	25	20	0	0
10	mC	5	45	25	20	0	0
10	vC	5	45	25	20	0	0
10	PD	5	45	25	20	0	0
10	jD	5	45	25	20	0	0
10	sD	5	45	25	20	0	0

- Molecule 11 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
11	i	3	27	15	12	0	0
11	gA	3	27	15	12	0	0
11	aC	3	27	15	12	0	0
11	XD	3	27	15	12	0	0

- Molecule 12 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
12	n	5	47	26	21	0	0
12	q	5	47	26	21	0	0
12	lA	5	47	26	21	0	0
12	oA	5	47	26	21	0	0
12	FB	5	47	26	21	0	0
12	IB	5	47	26	21	0	0
12	iB	5	47	26	21	0	0
12	lB	5	47	26	21	0	0
12	fC	5	47	26	21	0	0
12	iC	5	47	26	21	0	0
12	cD	5	47	26	21	0	0
12	fD	5	47	26	21	0	0

- Molecule 13 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
13	o	4	38	21	17	0	0
13	4	4	38	21	17	0	0
13	6	4	38	21	17	0	0
13	7	4	38	21	17	0	0
13	BA	4	38	21	17	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
13	mA	4	38	21	17	0	0
13	2A	4	38	21	17	0	0
13	4A	4	38	21	17	0	0
13	5A	4	38	21	17	0	0
13	9A	4	38	21	17	0	0
13	GB	4	38	21	17	0	0
13	WB	4	38	21	17	0	0
13	YB	4	38	21	17	0	0
13	ZB	4	38	21	17	0	0
13	dB	4	38	21	17	0	0
13	jB	4	38	21	17	0	0
13	zB	4	38	21	17	0	0
13	1B	4	38	21	17	0	0
13	2B	4	38	21	17	0	0
13	6B	4	38	21	17	0	0
13	gC	4	38	21	17	0	0
13	wC	4	38	21	17	0	0
13	yC	4	38	21	17	0	0
13	zC	4	38	21	17	0	0
13	3C	4	38	21	17	0	0
13	dD	4	38	21	17	0	0

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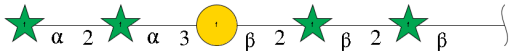
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
13	tD	4	38	21	17	0	0
13	vD	4	38	21	17	0	0
13	wD	4	38	21	17	0	0
13	0D	4	38	21	17	0	0

- Molecule 14 is an oligosaccharide called beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
14	p	4	38	21	17	0	0
14	s	4	38	21	17	0	0
14	nA	4	38	21	17	0	0
14	qA	4	38	21	17	0	0
14	HB	4	38	21	17	0	0
14	KB	4	38	21	17	0	0
14	kB	4	38	21	17	0	0
14	nB	4	38	21	17	0	0
14	hC	4	38	21	17	0	0
14	kC	4	38	21	17	0	0
14	eD	4	38	21	17	0	0
14	hD	4	38	21	17	0	0

- Molecule 15 is an oligosaccharide called alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
15	CA	5	Total	C	O		0	0
			47	26	21			
15	DA	5	Total	C	O		0	0
			47	26	21			
15	AB	5	Total	C	O		0	0
			47	26	21			
15	BB	5	Total	C	O		0	0
			47	26	21			
15	eB	5	Total	C	O		0	0
			47	26	21			
15	fB	5	Total	C	O		0	0
			47	26	21			
15	7B	5	Total	C	O		0	0
			47	26	21			
15	8B	5	Total	C	O		0	0
			47	26	21			
15	4C	5	Total	C	O		0	0
			47	26	21			
15	5C	5	Total	C	O		0	0
			47	26	21			
15	1D	5	Total	C	O		0	0
			47	26	21			
15	2D	5	Total	C	O		0	0
			47	26	21			

- Molecule 16 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	FA	2	Total	C	N	O	0	0
			28	16	2	10		

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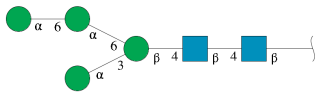
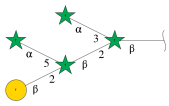
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	AC	2	28	16	2	10	0	0
16	4D	2	28	16	2	10	0	0

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	GA	6	72	40	2	30	0	0
17	DB	6	72	40	2	30	0	0
17	7C	6	72	40	2	30	0	0
17	5D	6	72	40	2	30	0	0

- Molecule 18 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
18	9D	5	47	26	21	0	0
18	BE	5	47	26	21	0	0
18	DE	5	47	26	21	0	0
18	IE	5	47	26	21	0	0
18	JE	5	47	26	21	0	0

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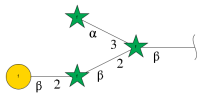
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
18	KE	5	47	26	21	0	0
18	PE	5	47	26	21	0	0
18	SE	5	47	26	21	0	0
18	cE	5	47	26	21	0	0
18	fE	5	47	26	21	0	0
18	pE	5	47	26	21	0	0
18	rE	5	47	26	21	0	0
18	tE	5	47	26	21	0	0
18	yE	5	47	26	21	0	0
18	zE	5	47	26	21	0	0
18	0E	5	47	26	21	0	0

- Molecule 19 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.

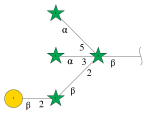


Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
19	AE	4	38	21	17	0	0
19	LE	4	38	21	17	0	0
19	NE	4	38	21	17	0	0
19	aE	4	38	21	17	0	0
19	qE	4	38	21	17	0	0
19	1E	4	38	21	17	0	0

- Molecule 20 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
20	CE	4	38	21	17	0	0
20	EE	4	38	21	17	0	0
20	HE	4	38	21	17	0	0
20	TE	4	38	21	17	0	0
20	UE	4	38	21	17	0	0
20	WE	4	38	21	17	0	0
20	gE	4	38	21	17	0	0
20	hE	4	38	21	17	0	0
20	jE	4	38	21	17	0	0
20	sE	4	38	21	17	0	0
20	uE	4	38	21	17	0	0
20	xE	4	38	21	17	0	0

- Molecule 21 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
21	FE	5	47	26	21	0	0

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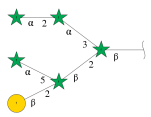
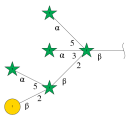
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
21	kE	5	47	26	21	0	0
21	vE	5	47	26	21	0	0

- Molecule 22 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



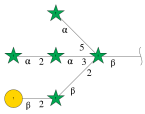
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
22	GE	6	56	31	25	0	0
22	QE	6	56	31	25	0	0
22	RE	6	56	31	25	0	0
22	VE	6	56	31	25	0	0
22	dE	6	56	31	25	0	0
22	eE	6	56	31	25	0	0
22	iE	6	56	31	25	0	0
22	wE	6	56	31	25	0	0

- Molecule 23 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
23	XE	6	56	31	25	0	0

- Molecule 24 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.

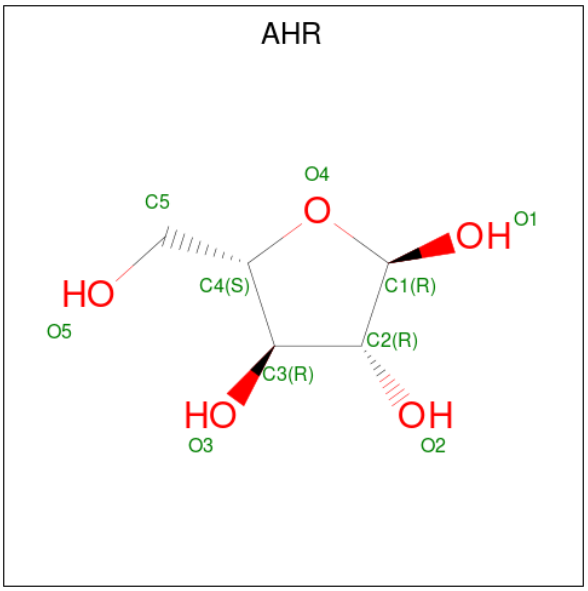


Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
24	YE	6	56	31	25	0	0
			Total	C	O		
24	lE	6	56	31	25	0	0

- Molecule 25 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
25	A	1	1	1	0
			Total	Ca	
25	B	1	1	1	0
			Total	Ca	
25	C	1	1	1	0
			Total	Ca	
25	D	1	1	1	0
			Total	Ca	
25	E	1	1	1	0
			Total	Ca	
25	F	1	1	1	0

- Molecule 26 is alpha-L-arabinofuranose (three-letter code: AHR) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O		0
			9	5	4		
26	A	1	Total	C	O		0
			9	5	4		
26	A	1	Total	C	O		0
			9	5	4		
26	A	1	Total	C	O		0
			9	5	4		
26	B	1	Total	C	O		0
			9	5	4		
26	B	1	Total	C	O		0
			9	5	4		
26	B	1	Total	C	O		0
			9	5	4		
26	B	1	Total	C	O		0
			9	5	4		
26	C	1	Total	C	O		0
			9	5	4		
26	C	1	Total	C	O		0
			9	5	4		
26	D	1	Total	C	O		0
			9	5	4		
26	D	1	Total	C	O		0
			9	5	4		
26	D	1	Total	C	O		0
			9	5	4		
26	E	1	Total	C	O		0
			9	5	4		

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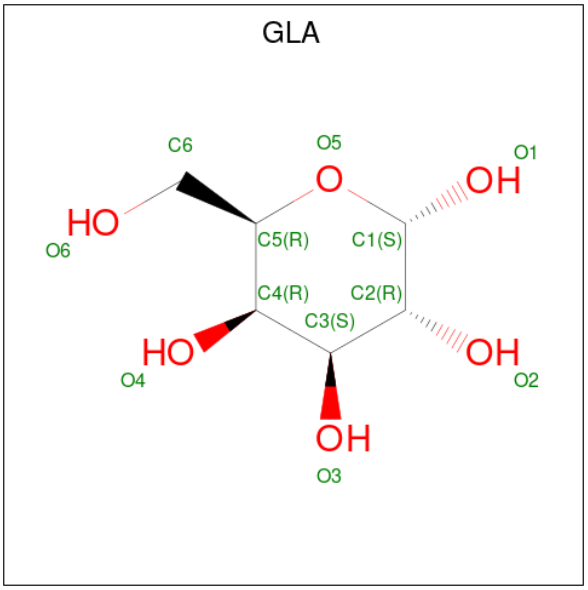
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	E	1	9	5	4	0
26	F	1	9	5	4	0
26	F	1	9	5	4	0
26	F	1	9	5	4	0
26	F	1	9	5	4	0
26	F	1	9	5	4	0

- Molecule 27 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0

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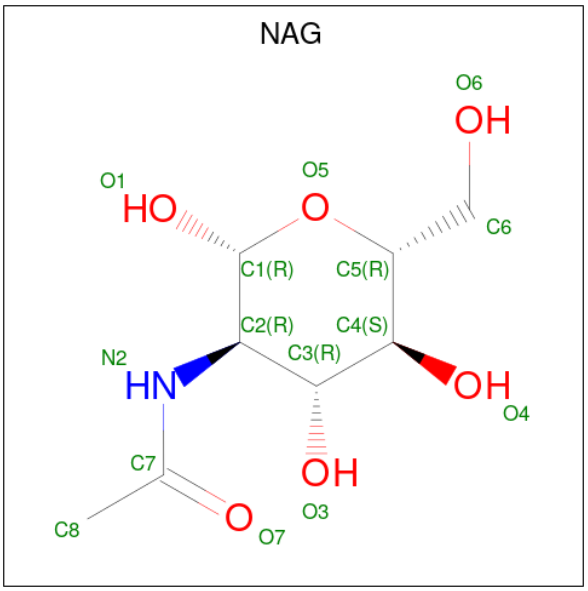
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	E	1	11	6	5	0
			Total	C	O	
27	E	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0
			Total	C	O	
27	F	1	11	6	5	0

- Molecule 28 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



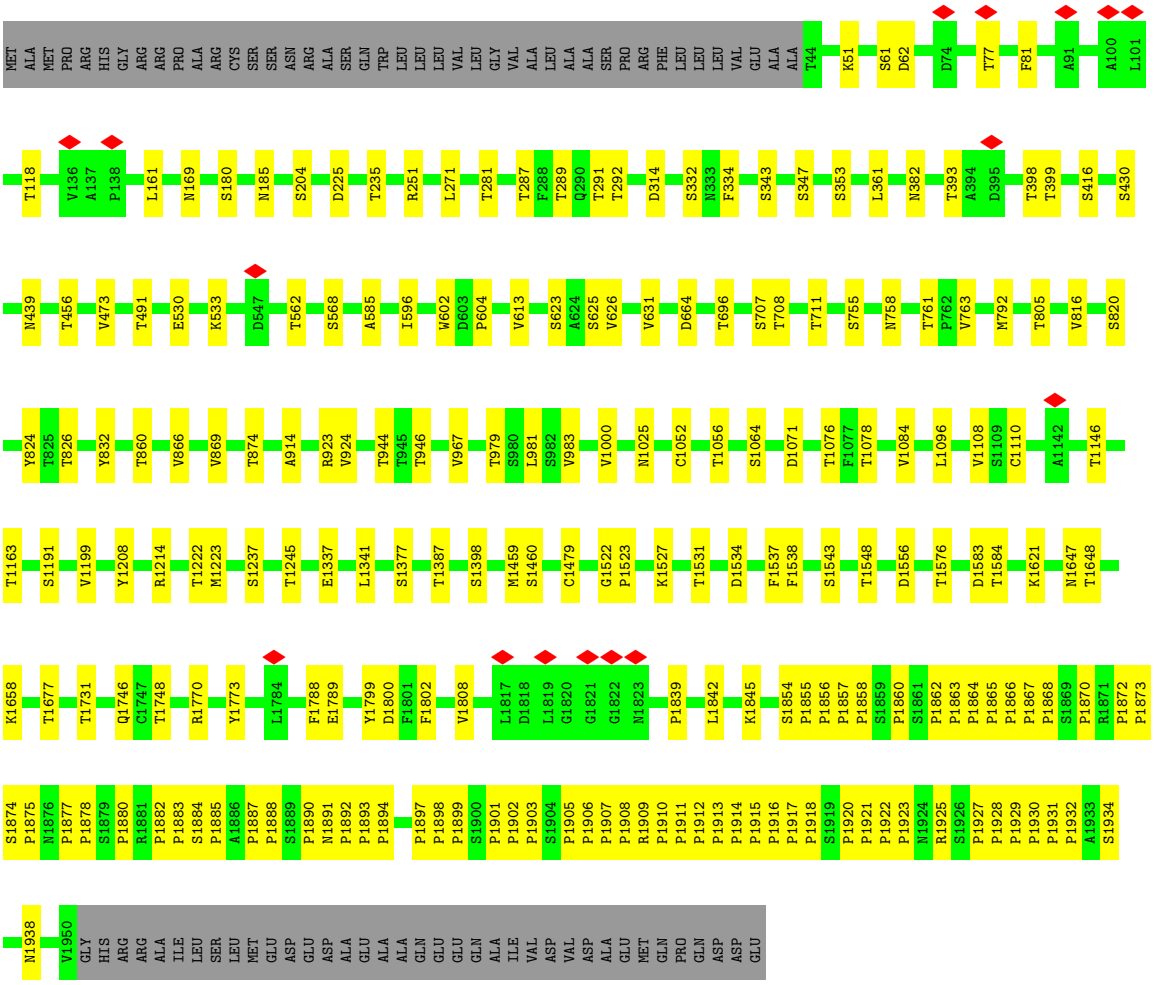
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
28	A	1	14	8	1	5	0
28	B	1	14	8	1	5	0
28	B	1	14	8	1	5	0
28	C	1	14	8	1	5	0
28	C	1	14	8	1	5	0
28	D	1	14	8	1	5	0
28	E	1	14	8	1	5	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

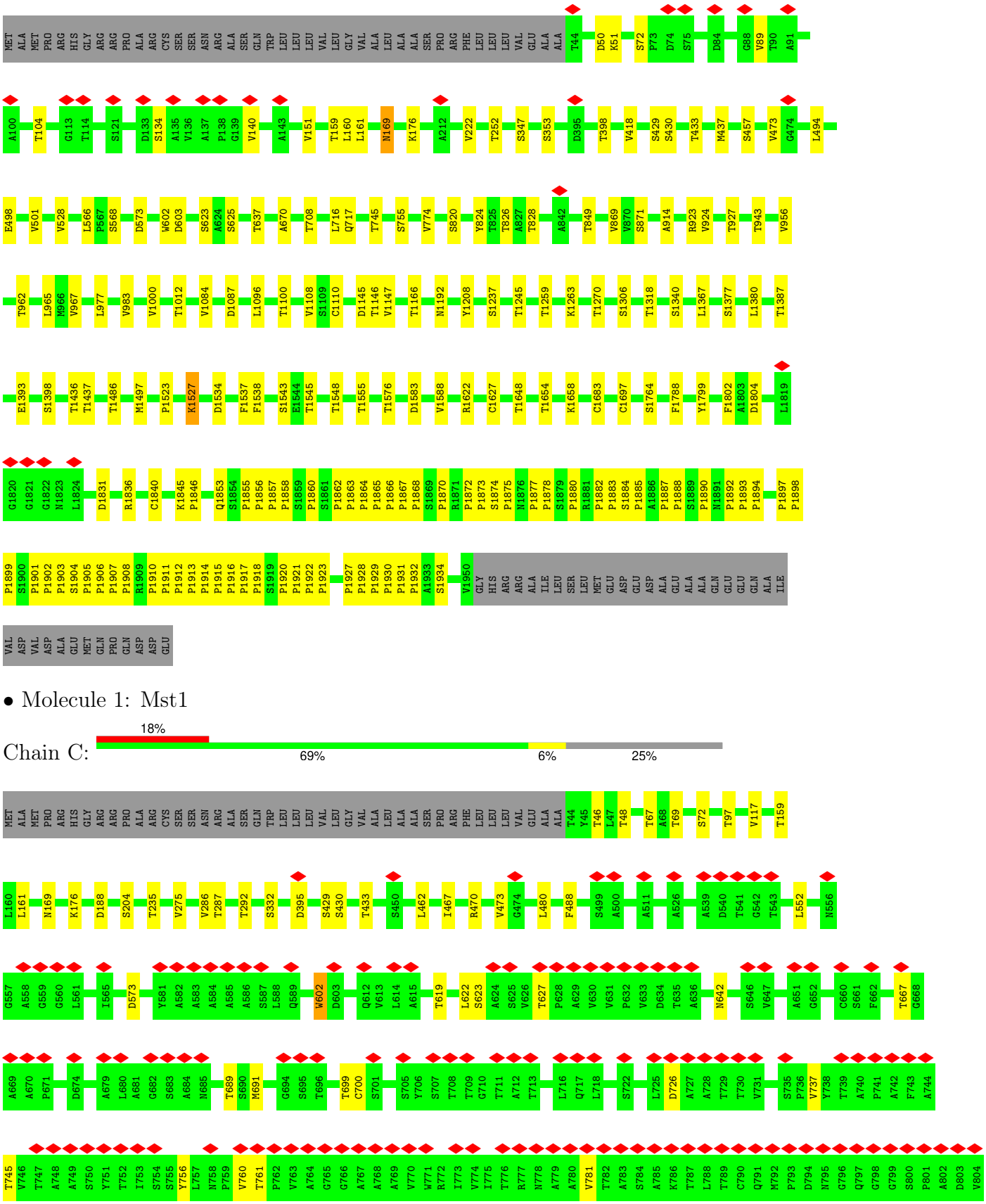
- Molecule 1: Mst1

Chain A:



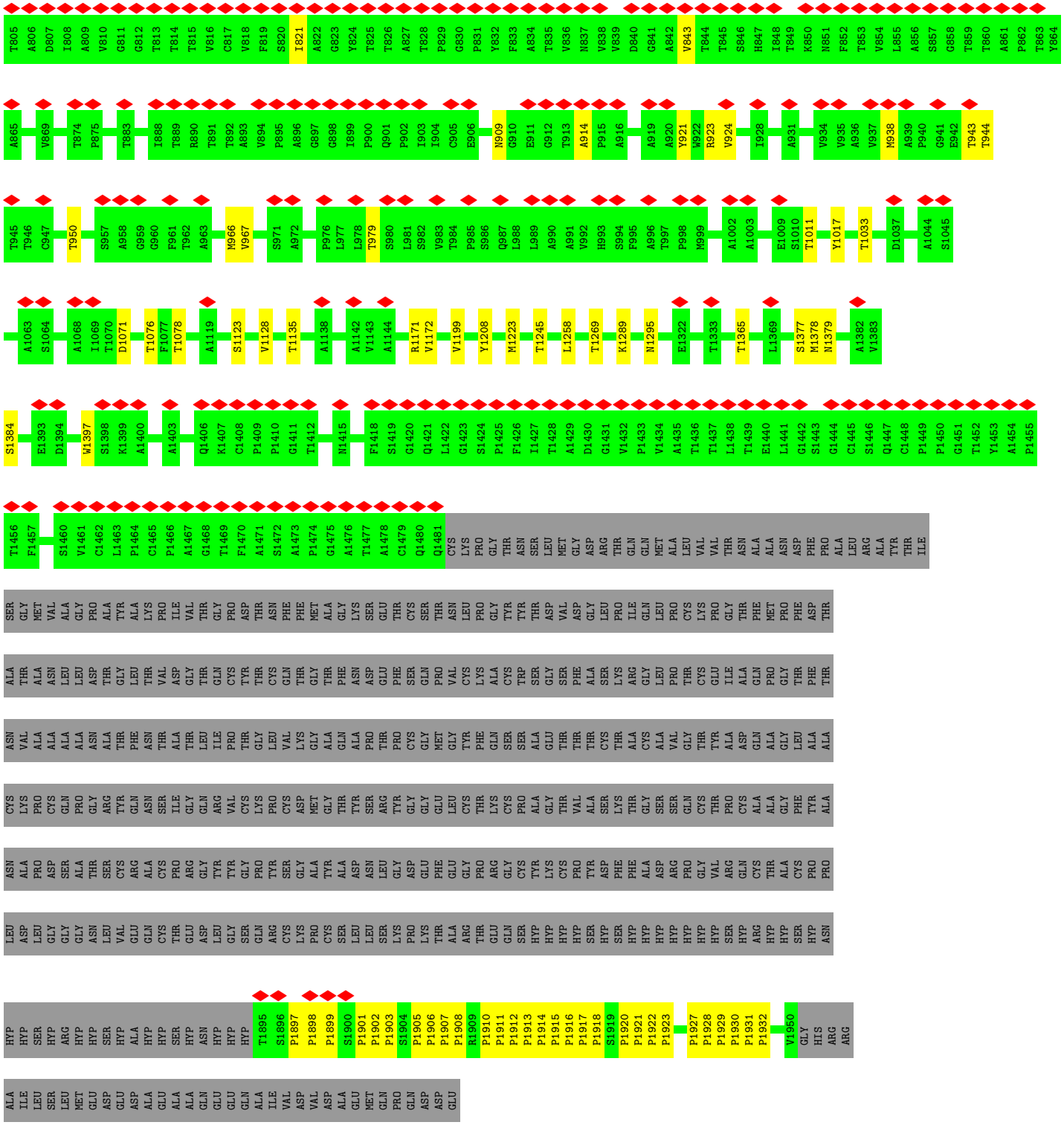
- Molecule 1: Mst1

Chain B:



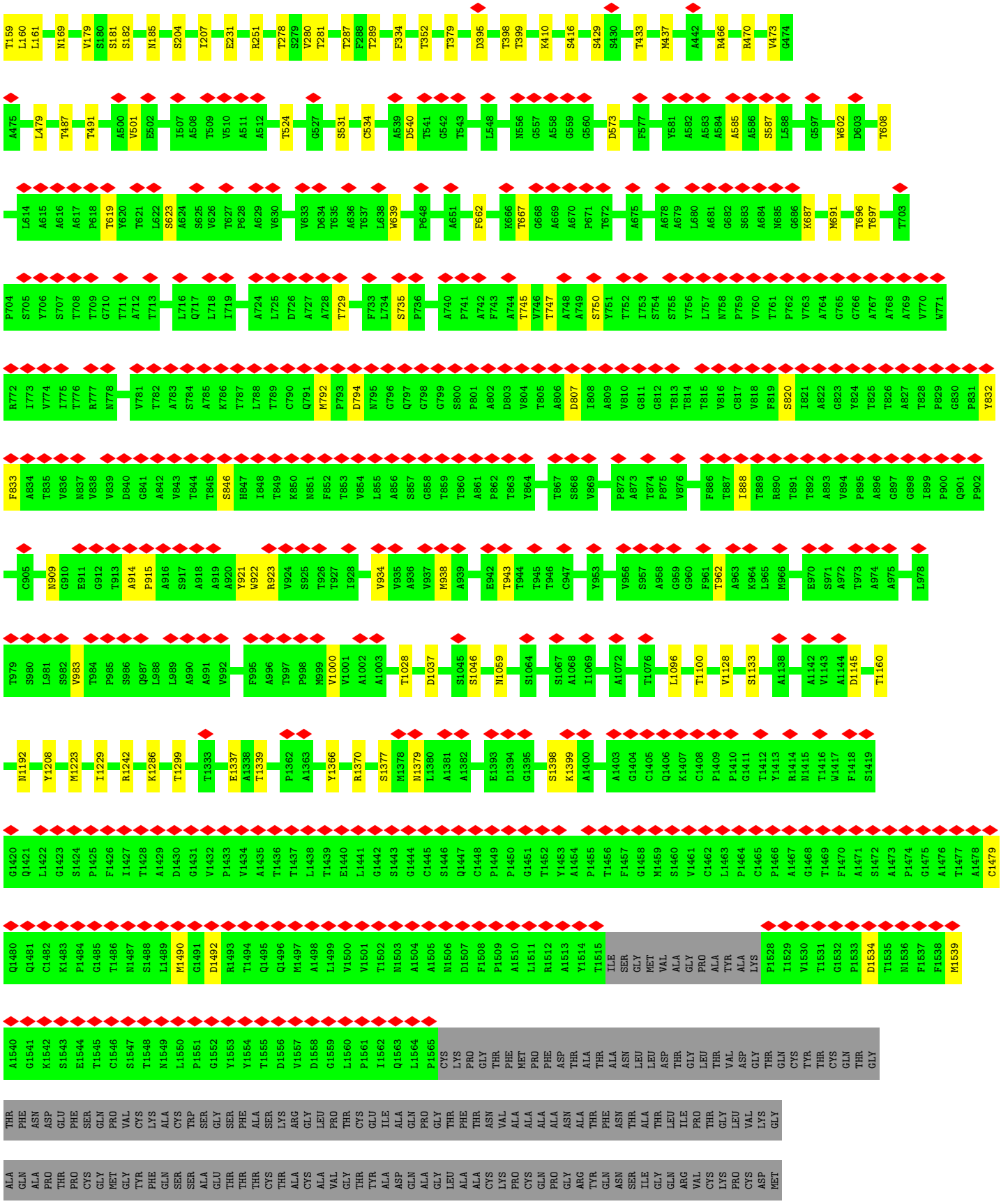
- Molecule 1: Mst1

Chain C:



- Molecule 1: Mst1

Chain D: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A475 L479 T487 T491 A500 V501 E502 I507 A508 T509 V510 A511 A512 T524 G527 S531 C534 A539 D540 T541 G542 T543 L548 N556 G557 A558 G559 G560 D573 F577 Y581 A582 A583 A584 A585 A586 S587 L588 G597 W602 D603 T608
L614 A615 A616 A617 P618 T619 Y620 T621 L622 S623 A624 S625 V626 T627 P628 A629 V630 V633 D634 T635 A636 T637 L638 W639 P648 A651 F662 K666 T667 G668 A669 A670 P671 T672 A675 A678 A679 L680 A681 G682 S683 A684 N685 G686 K687 M691 T696 T697 T703
P704 S705 Y706 S707 T708 T709 G710 T711 A712 T713 L716 Q717 L718 I719 A724 L725 D726 A727 A728 T729 F733 L734 S735 P736 A740 P741 A742 F743 A744 T745 V746 T747 A748 A749 S750 Y751 T752 I753 S754 S755 Y756 L757 N758 P759 V760 T761 P762 V763 A764 G765 G766 A767 A768 A769 V770 W771
R772 I773 V774 I775 T776 R777 N778 V781 T782 A783 S784 A785 K786 T787 L788 T789 C790 Q791 M792 P793 D794 N795 G796 Q797 G798 G799 S800 P801 A802 D803 V804 T805 A806 D807 I808 A809 V810 G811 G812 T813 T814 T815 V816 C817 V818 F819 S820 I821 A822 G823 Y824 T825 T826 A827 T828 P829 G830 P831 Y832
F833 A834 T835 V836 N837 V838 V839 D840 G841 A842 V843 T844 T845 S846 H847 I848 T849 K850 N851 F852 T853 V854 L855 A856 S857 G858 T859 T860 A861 P862 T863 Y864 T867 S868 V869 P872 A873 T874 P875 V876 F886 T887 I888 T889 R890 T891 T892 A893 V894 P895 A896 G897 G898 I899 P900 Q901 P902
C905 N909 G910 E911 G912 T913 A914 P915 A916 S917 A918 A919 A920 Y921 W922 R923 V924 S925 T926 T927 I928 V934 V935 A936 V937 M938 A939 E942 T943 T944 T945 T946 C947 Y953 V956 S957 A958 G959 G960 F961 T962 A963 K964 L965 M966 E970 S971 A972 T973 A974 A975 L978
T979 S980 L981 S982 V983 T984 P985 S986 Q987 L988 L989 A990 A991 V992 F995 A996 T997 P998 M999 V1000 V1001 A1002 A1003 T1028 D1037 S1045 S1046 N1059 S1064 S1067 A1068 I1069 A1072 T1076 L1096 T1100 V1128 S1133 A1138 A1142 V1143 A1144 D1145 T1160
N1192 Y1208 M1223 I1229 R1242 K1286 T1299 T1333 E1337 A1338 T1339 P1362 A1363 Y1366 R1370 S1377 M1378 N1379 L1380 A1381 A1382 E1393 D1394 G1395 S1398 K1399 A1400 A1403 G1404 C1405 Q1406 K1407 C1408 P1409 P1410 G1411 T1412 Y1413 R1414 N1415 T1416 W1417 F1418 S1419
G1420 Q1421 L1422 G1423 S1424 P1425 F1426 I1427 T1428 A1429 D1430 G1431 V1432 P1433 V1434 A1435 T1436 T1437 L1438 T1439 E1440 L1441 G1442 S1443 G1444 C1445 S1446 Q1447 C1448 P1449 P1450 G1451 T1452 Y1453 A1454 P1455 T1456 F1457 G1458 M1459 S1460 V1461 C1462 L1463 P1464 C1465 P1466 A1467 G1468 T1469 F1470 A1471 S1472 A1473 P1474 G1475 F1538 A1476 T1477 A1478 C1479
Q1480 Q1481 C1482 K1483 P1484 G1485 T1486 N1487 S1488 L1489 M1490 G1491 D1492 R1493 T1494 Q1495 Q1496 M1497 A1498 L1499 V1500 V1501 T1502 N1503 A1504 A1505 N1506 D1507 F1508 P1509 A1510 L1511 R1512 A1513 Y1514 T1515 ILE SER GLY MET VAL ALA GLY PRO ALA TYR ALA LYS P1528 I1529 V1530 T1531 G1532 P1533 D1534 T1535 N1536 F1537 F1538 M1539
A1540 G1541 K1542 S1543 E1544 T1545 C1546 S1547 T1548 N1549 L1550 P1551 G1552 Y1553 Y1554 T1555 D1556 V1557 D1558 G1559 L1560 P1561 I1562 Q1563 L1564 P1565 CYS LYS PRO GLY THR PHE MET PRO PHE ASP THR ALA THR ALA ASN LEU LEU ASP THR GLY LEU THR VAL ASP GLY THR GLN CYS TYR THR CYS GLN THR GLY
THR PHE ASN ASP GLU PHE SER GLN PRO VAL CYS LYS ALA CYS TRP SER GLY SER PHE ALA SER LYS ARG GLY LEU PRO THR CYS GLU ILE ALA GLN PRO GLY THR PHE THR ASN VAL ALA ALA ALA ALA ASN ALA THR PHE ASN THR ALA THR LEU ILE PRO THR GLY LEU VAL LYS GLY
ALA GLN ALA PRO THR PRO CYS GLY MET GLY TYR PHE GLN SER SER ALA GLU THR THR THR CYS THR ALA CYS ALA VAL GLY THR TYR ALA ASP GLN ALA GLY LEU ALA ALA CYS LYS PRO CYS GLN PRO GLY ARG TYR GLN ASN SER ILE GLY GLN ARG VAL CYS LYS PRO CYS ASP MET

GLY THR TYR SER ARG TYR GLY GLY GLU LEU CYS THR LYS CYS PRO ALA GLY THR VAL ALA SER LYS THR GLY SER SER GLN CYS THR PRO CYS ALA ALA GLY PHE TYR ALA ASN ALA PRO ASP SER ALA THR SER CYS ARG ALA CYS PRO ARG GLY TYR TYR GLY PRO TYR SER GLY ALA

TYR ALA ASP ASN LEU GLY ASP GLU GLU PHE GLU GLY GLY PRO ARG GLY CYS TYR LYS CYS PRO TYR ASP PHE PHE ALA ASP ARG PRO GLY VAL ARG GLN CYS THR ALA CYS PRO PRO LEU ASP LEU GLY GLY GLY ASN LEU VAL GLU GLN CYS THR GLU ASP LEU GLY SER GLN ARG CYS LYS PRO

CYS SER LEU LEU SER LYS PRO LYS THR ALA ARG THR GLU GLN SER HYP HYP HYP HYP HYP SER HYP SER HYP HYP HYP HYP HYP HYP HYP SER HYP ARG HYP HYP HYP HYP SER HYP HYP HYP HYP HYP SER HYP HYP HYP HYP HYP HYP T1895 S1896 P1897 P1898 P1899

S1900 P1901 P1902 P1903 S1904 P1905 P1906 P1907 P1908 R1909 P1910 P1911 P1912 P1913 P1914 P1915 P1916 P1917 P1918 S1919 P1920 P1921 P1922 P1923 N1924 R1925 S1926 P1927 P1928 P1929 P1930 P1931 P1932 V1950 GLY HIS ARG ARG ALA ILE LEU SER LEU MET GLU GLU ASP GLU ASP ALA GLU GLU ALA ALA GLN GLU GLU GLN ALA ILE VAL

ASP VAL ASP ALA GLU MET GLN PRO GLN ASP ASP GLU

- Molecule 1: Mst1

Chain E: 36% 66% 7% 27%

MET ALA MET PRO ARG HIS GLY ARG ARG PRO ALA ARG CYS SER SER ASN ARG ALA SER GLN TRP LEU LEU LEU VAL LEU GLY VAL ALA LEU ALA ALA SER PRO ARG PHE LEU LEU LEU VAL GLU ALA ALA THR TYR THR LEU THR LEU ASP LYS LEU GLY PRO THR VAL ASN PRO THR THR

SER ASP ALA VAL THR PHE THR ALA THR VAL ALA SER PRO ASP SER THR THR ALA VAL PHE PHE THR LEU ASP TYR GLY ASP GLY VAL THR ALA GLU THR ARG THR THR THR GLY ALA LEU SER THR THR PRO THR ALA ASN LEU VAL SER ALA GLY THR TYR THR VAL THR TYR ALA

SER ILE GLY THR LYS PHE VAL THR LEU ARG LEU TYR ASP SER ALA VAL ALA PRO GLY VAL LEU LEU LEU ALA SER LYS THR VAL PRO ILE TYR VAL GLU ASP SER THR LEU THR ALA THR LEU LEU LEU GLN SER GLY VAL PRO ARG LEU ASN LEU ALA PHE SER GLY PHE LYS GLY ARG VAL SER

SER SER THR ALA ASN ARG ALA ASP MET TRP ALA THR ILE GLN LEU ASP THR ALA PRO GLY VAL PHE GLU SER SER ARG ILE PHE ILE GLY ILE ALA PRO THR ALA SER THR ASN TYR ASP PHE VAL ILE PRO ASP GLN VAL TYR ASN LEU GLU GLY ALA LYS THR THR VAL LEU ARG ILE

TYR ASP ALA PRO VAL GLY GLY THR LEU LEU ARG THR PHE THR PRO ALA ALA ALA ASN ALA VAL TYR VAL VAL ASP PRO SER LYS TYR VAL LEU THR LEU THR VAL GLY PRO THR SER VAL THR THR ALA ASP GLN VAL THR PHE THR GLN THR THR THR GLU VAL SER TYR SER ALA SER

ALA THR SER PRO ILE LEU GLN TRP ARG PHE ASN TRP ASP ASP PRO SER VAL VAL GLU THR PRO LEU ALA TYR PRO ASP ALA LEU THR ALA ALA SER ASN PHE PRO THR THR ALA ALA VAL SER SER ALA ALA ALA SER THR PHE ARG TYR THR SER THR GLY SER LYS ASN ALA ARG

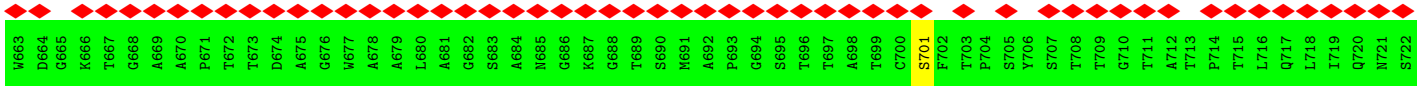
LEU ARG LEU TYR ASP GLY ALA ASN ASN VAL ILE ALA GLU LYS ILE VAL VAL ILE THR VAL SER ASN ALA GLY TYR THR LEU ALA LEU LYS THR THR ALA ASP PRO VAL THR THR THR ASP ASP THR ALA ALA GLY PHE ALA PHE SER ALA GLY ALA LYS HIS LEU SER SER THR SER GLN VAL TRP TRP

THR ILE ASP TYR GLY ALA GLY GLU SER SER PRO ARG THR ALA LEU THR MET THR ASN VAL GLY ALA ALA ALA ALA PRO ASN ALA ILE ALA SER LEU SER ASN GLN TYR THR SER GLY GLY THR LYS LEU ALA THR LEU ARG ILE TYR ASP ARG ASP GLY VAL VAL GLY ALA ASN THR GLY LEU LEU

LEU ALA SER THR THR VAL THR PHE THR VAL THR PRO V493 L494 Y495 A496 L497 E498 S499 A500 V501 E502 P503 F504 S505 P506 I507 A508 T509 V510 A511 A512 K513 W514 S515 F516 R517 I518 Q519 R520 S521 K522 A523 T524 P525 A526 G527 V528 T529 E530 S531 I532 K533 C534 A535 F536 F537 G538 A539 D540

T541 G542 T543 A544 P545 A546 D547 L548 A549 A550 W551 L552 T553 A554 A555 N556 G557 A558 G559 G560 L561 T562 A563 T564 I565 L566 P567 S568 S569 I570 P571 S572 D573 I574 I575 S576 F577 T578 R579 T580 Y581 A582 A583 A584 A585 A586 S587 L588 Q589 G590 G591 L592 Q593 C594 F595 I596 G597 S598 T599 P600

L601 W602 D603 P604 Y605 Y606 P607 T608 P609 V610 F611 Q612 V613 L614 A615 A616 A617 P618 T619 Y620 T621 L622 S623 A624 S625 V626 T627 P628 A629 V630 D634 T635 A636 T637 L638 W639 T640 Y641 N642 I643 I644 R645 S646 V647 P648 V649 P650 A651 G652 G653 P654 S655 L656 P657 I658 L659 C660 S661 F662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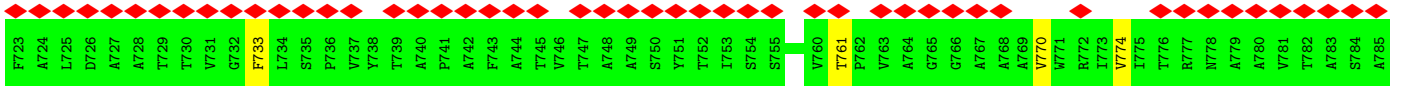
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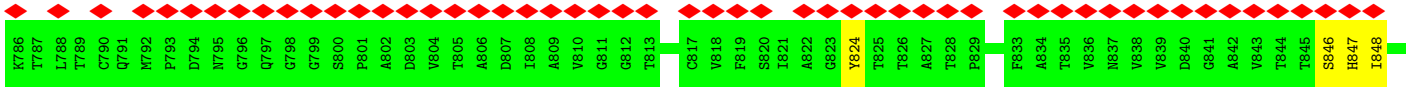
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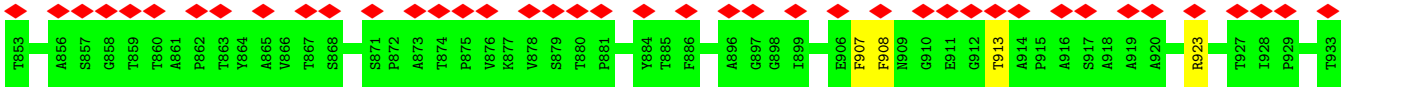
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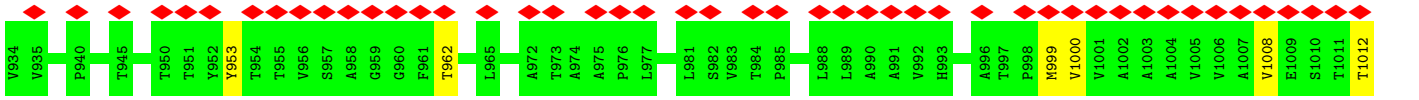
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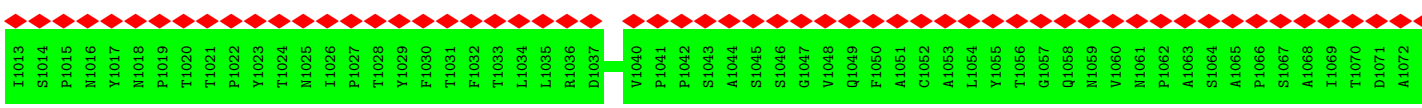
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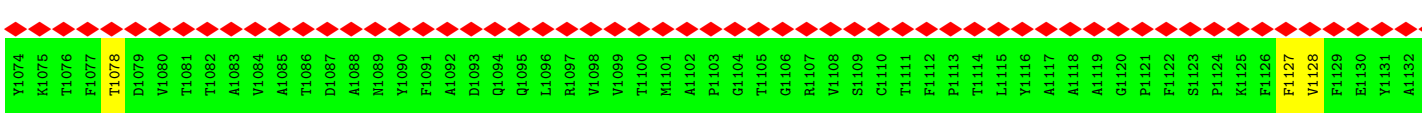
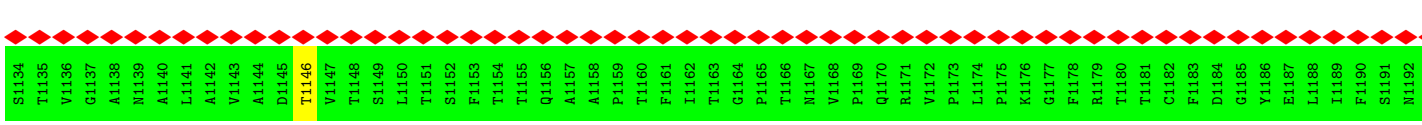

Y1074 K1075 T1076 F1077 T1078 D1079 V1080 T1081 T1082 A1083 V1084 A1085 T1086 D1087 A1088 N1089 Y1090 F1091 A1092 D1093 Q1094 Q1095 L1096 R1097 V1098 V1099 T1100 M1101 A1102 P1103 G1104 T1105 G1106 R1107 V1108 S1109 C1110 T1111 F1112 P1113 T1114 L1115 Y1116 A1117 A1118 A1119 G1120 P1121 F1122 S1123 P1124 K1125 F1126 F1127 V1128 F1129 E1130 Y1131 A1132 S1133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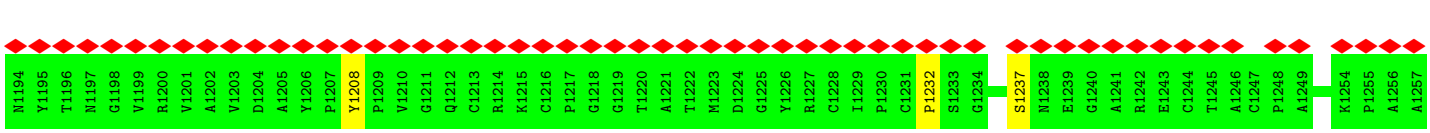
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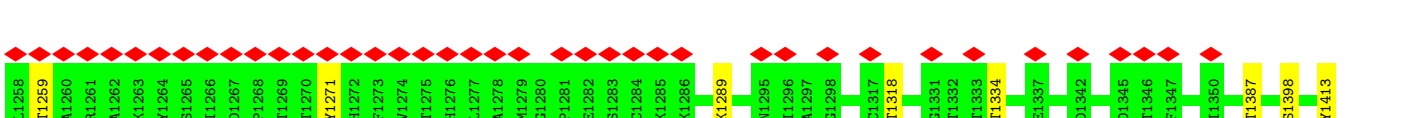
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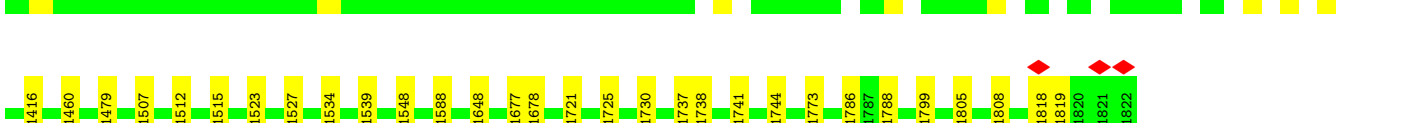
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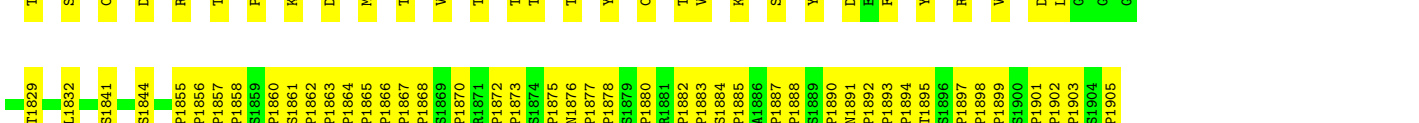
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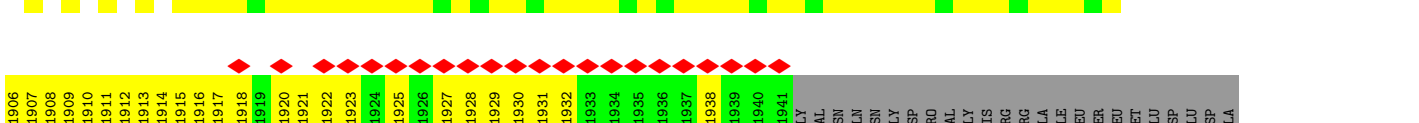

P1906 P1907 P1908 R1909 P1910 P1911 P1912 P1913 P1914 P1915 P1916 P1917 P1918 S1919 P1920 P1921 P1922 P1923 N1924 R1925 S1926 P1927 P1928 P1929 P1930 P1931 P1932 A1933 S1934 S1935 A1936 I1937 N1938 P1939 G1940 G1941 GLY VAL ASN GLN ASN GLY ASP PRO VAL GLY HIS ARG ARG ALA ILE LEU SER LEU MET GLU ASP GLU ASP ALA

GLU ALA ALA GLN GLU GLU GLN ALA ILE VAL ASP VAL ASP ALA GLU MET GLN PRO GLN ASP ASP GLU

- Molecule 1: Mst1

Chain F:

MET ALA MET PRO ARG HIS GLY ARG ARG PRO ALA ARG CYS SER SER ASN ARG ALA SER GLN TRP LEU LEU LEU VAL LEU GLY VAL ALA LEU ALA ALA SER PRO ARG PHE LEU LEU LEU VAL GLU ALA ALA THR TYR THR LEU THR LEU ASP LYS LEU GLY PRO THR VAL ASN PRO THR THR

SER ASP ALA VAL THR PHE THR ALA THR VAL ALA SER PRO ASP SER THR THR ALA VAL PHE PHE THR LEU ASP TYR GLY ASP GLY VAL THR ALA GLU THR THR ARG THR THR THR GLY ALA LEU SER THR THR PRO THR ALA ASN LEU VAL SER ALA GLY THR TYR THR VAL THR TYR ALA

SER ILE GLY THR LYS PHE VAL THR LEU ARG LEU TYR ASP SER ALA VAL ALA PRO GLY VAL LEU LEU ALA SER LYS THR VAL PRO ILE TYR VAL GLU ASP SER THR LEU THR ALA THR LEU LEU LEU GLN SER GLY VAL PRO ARG LEU ASN LEU ALA PHE SER GLY PHE LYS GLY ARG VAL SER

SER SER THR ALA ASN ARG ALA ASP MET TRP ALA THR ILE GLN LEU ASP THR ALA PRO GLY VAL PHE GLU ALA SER SER ARG ILE PHE ILE GLY ILE ALA PRO THR ALA SER THR ASN TYR ASP PHE VAL ILE PRO ASP GLN VAL TYR ASN LEU GLU GLY ALA LYS THR THR VAL LEU ARG ILE

TYR ASP ALA PRO VAL GLY GLY THR LEU LEU ARG THR PHE THR PRO ALA ALA ALA ASN ALA VAL TYR VAL VAL ASP PRO SER LYS TYR VAL LEU THR LEU THR VAL GLY PRO THR SER THR THR THR ALA ASP GLN VAL THR PHE THR GLN THR THR THR GLU VAL SER TYR SER VAL THR SER

ALA THR SER PRO ILE LEU GLN TRP ARG PHE ASN TRP ASP ASP PRO SER VAL VAL GLU THR PRO LEU ALA TYR PRO ASP ALA LEU THR ALA ALA SER ASN PHE PRO THR THR ALA THR ALA VAL SER SER ALA ALA ALA SER THR PHE ARG TYR THR SER THR GLY SER LYS ASN ALA ARG

LEU ARG LEU TYR ASP GLY ALA ASN ASN VAL ILE ALA GLU LYS ILE VAL VAL ILE THR VAL SER ASN ALA GLY TYR THR LEU ALA LEU ALA LYS THR THR ALA ASP PRO VAL THR THR ASP ASP THR ILE ALA PHE SER ALA GLY ALA LYS HIS LEU SER SER THR SER GLN VAL TRP TRP

THR ILE ASP TYR GLY ALA GLY GLU SER SER PRO ARG THR ALA LEU THR MET THR ASN VAL GLY ALA ALA ALA PRO ASN ALA ILE ILE ALA SER LEU SER ASN GLN TYR THR SER GLY GLY THR LYS LEU ALA THR LEU ARG ILE TYR ASP ARG ASP GLY VAL VAL GLY ALA ASN THR GLY LEU LEU

LEU ALA SER THR THR VAL THR PHE THR VAL THR PRO V493 L494 Y495 A496 L497 E498 S499 A500 V501 E502 P503 F504 S505 P506 I507 A508 T509 V510 A511 A512 K513 W514 S515 F516 R517 I518 Q519 R520 S521 K522 A523 T524 P525 A526 G527 V528 T529 E530 S531 I532 K533 C534 A535 F536 F537 G538 A539 D540

T541 G542 T543 A544 P545 A546 D547 L548 A549 A550 W551 L552 T553 A554 A555 N556 G557 A558 G559 G560 L561 T562 A563 T564 I565 L566 P567 S568 S569 I570 P571 S572 D573 I574 I575 S576 F577 T578 R579 T580 Y581 A582 A583 A584 A585 A586 S587 L588 Q589 G590 K591 L592 Q593 C594 F595 I596 G597 S598 T599 P600

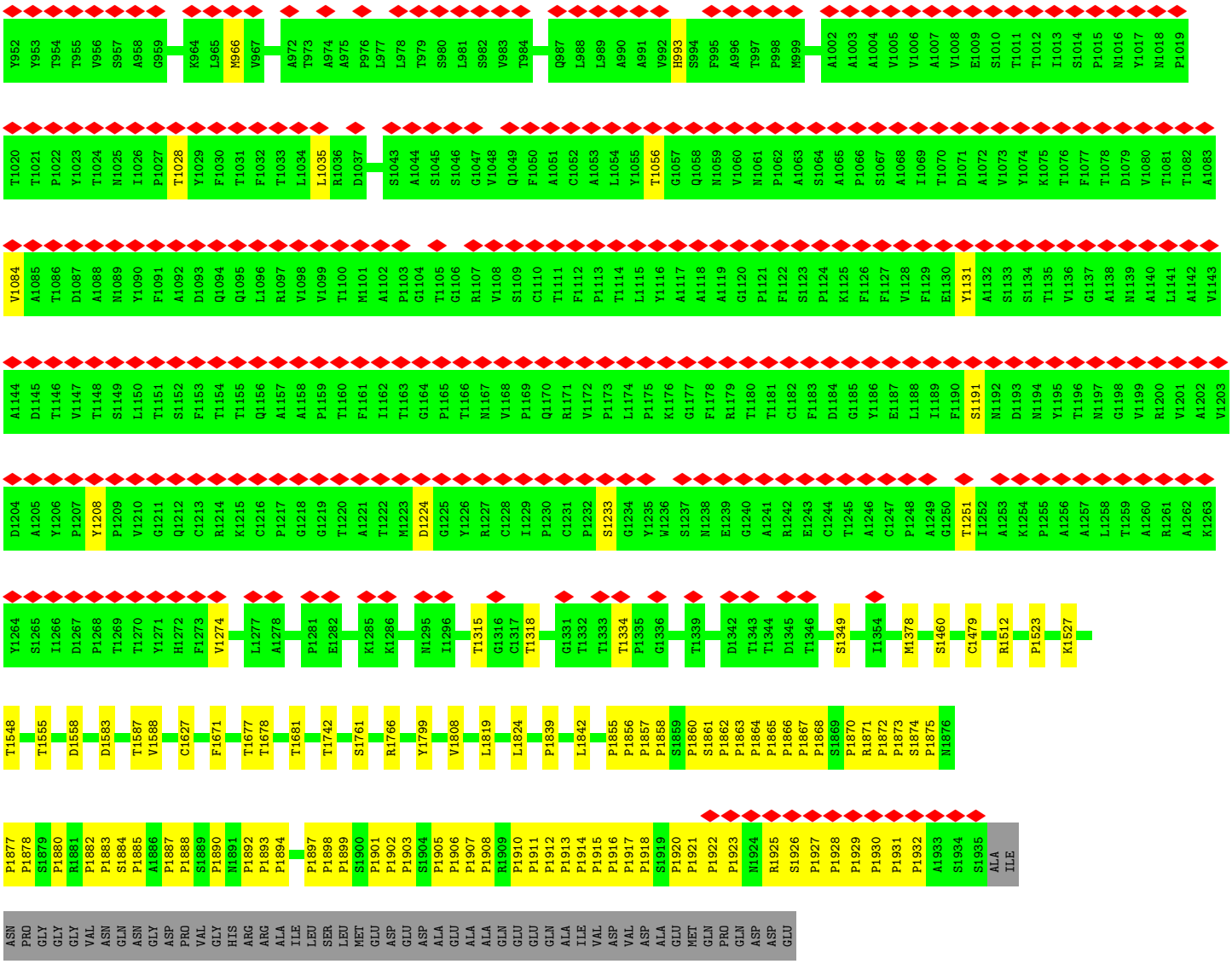
L601 W602 D603 P604 Y605 Y606 P607 T608 P609 V610 F611 Q612 V613 L614 A615 A616 A617 P618 T619 Y620 T621 L622 S623 A624 S625 V626 T627 P628 A629 V630 V631 P632 A636 T637 T640 Y641 N642 I643 I644 R645 S646 V647 P648 V649 P650 A651 G652 G653 P654 S655 L656 P657 I658 L659 C660 S661 F662

G665 K666 T667 G668 A669 A670 P671 T672 T673 D674 A675 G676 W677 A678 A679 L680 A681 G682 S683 A684 N685 G686 K687 G688 T689 S690 M691 A692 P693 G694 S695 T696 T697 A698 T699 C700 S701 F702 T703 P704 S705 Y706 S707 T708 T709 G710 T711 A712 T713 P714 T715 L716 Q717 L718 I719 Q720 N721 S722 F723 A724

L725 D726 A727 A728 T729 T730 V731 G732 F733 L734 S735 P736 V737 Y738 T739 A740 P741 A742 F743 A744 T745 V746 T747 A748 A749 S750 Y751 T752 I753 S754 S755 Y756 L757 N758 P759 V760 T761 P762 V763 A764 G765 G766 A767 A768 W771 R772 I773 N778 A779 A780 V781 T782 A783 S784 A785 K786 T787 L788

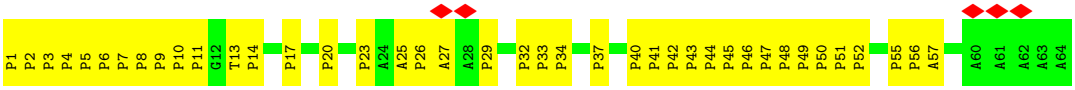
T789 C790 Q791 M792 P793 D794 N795 G798 G799 S800 P801 A802 D803 V804 T805 A806 D807 I808 A809 V810 G811 G812 C817 S820 I821 A822 G823 Y824 T825 T826 A827 T828 P829 G830 P831 Y832 F833 V836 N837 V838 V839 D840 G841 A842 V843 T844 T845 S846 H847 I848 T853 V854 L855 A856 S857

G858 T859 T860 A861 P862 T863 Y864 A865 V866 T867 V870 S871 P872 A873 T874 P875 V876 K877 V878 S879 T880 P881 V882 F886 T891 A896 G897 G898 C905 F908 E911 G912 T913 A914 P915 A916 S917 A918 A919 R923 T926 T927 I928 P929 V937 C947 T950 T951



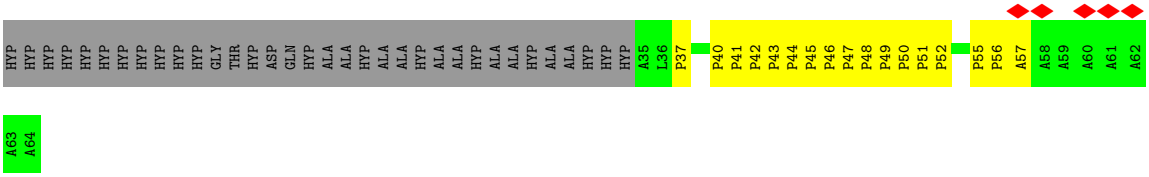
- Molecule 2: Mstax

Chain G:

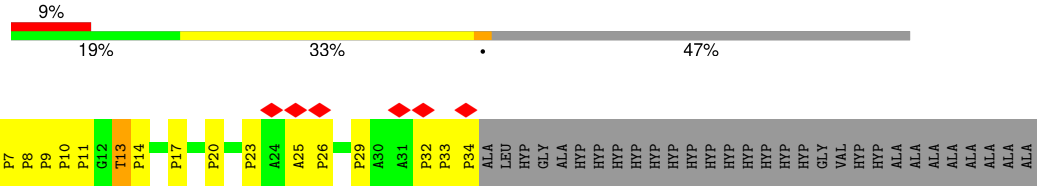


- Molecule 2: Mstax

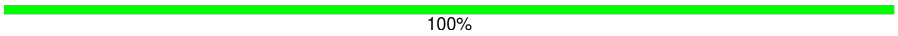
Chain H:



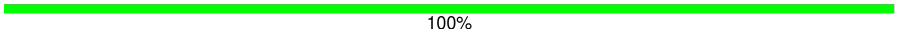
• Molecule 2: Mstax

Chain I: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain J: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain K: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain O:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain P:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain Q:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain T:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain V:

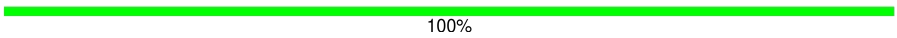
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b:

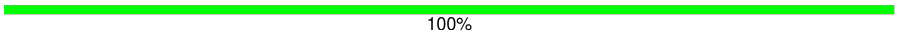
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e:

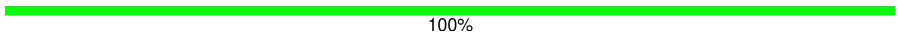
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain l: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain m: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain t: 

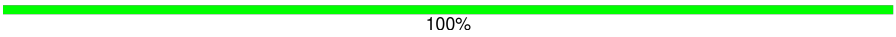
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain w:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain x:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain y: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain z:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2:

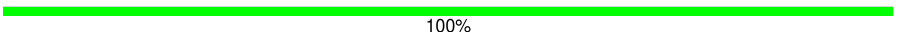
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HA:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain IA:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain MA: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain NA:

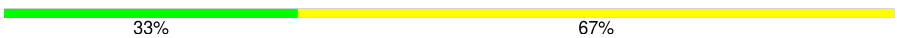
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain OA:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain RA:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TA: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain XA:

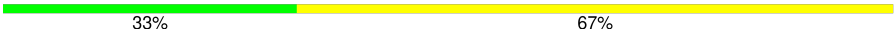
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ZA:

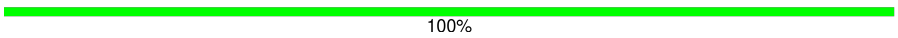
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain cA:

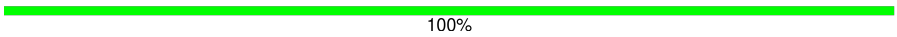
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain jA: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain kA: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain rA: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uA: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain vA: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain wA: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xA: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain yA: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain zA: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0A: 67% 33%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain EB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain LB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain OB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain PB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain QB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain RB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain SB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain UB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain hB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain oB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain rB:

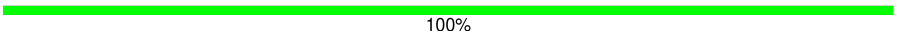
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain sB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain tB:

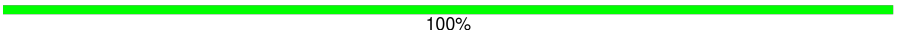
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain vB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain wB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xB:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain BC:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CC:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain GC:

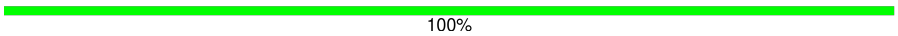
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HC:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain IC:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain LC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain NC: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TC: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WC: 33% 67%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain dC: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain eC: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain lC: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

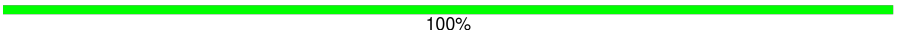
Chain oC: 33% 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain pC:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain qC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain rC:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain sC:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain tC:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uC:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8C: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9C: 33% 67%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain DD: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ED: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain FD: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

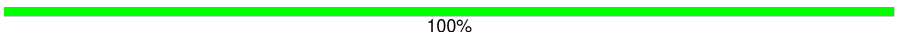
Chain ID: 67% 33%

FUB1 FUB2 FUB3

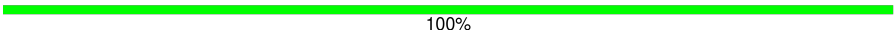
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain KD: 67% 33%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain QD: 

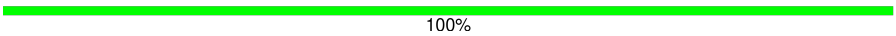
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TD: 

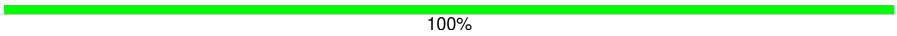
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain aD:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain iD: 

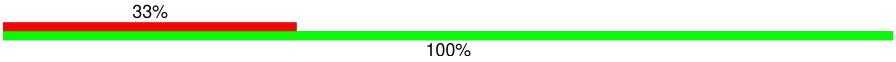
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain lD:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain mD:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain nD: 

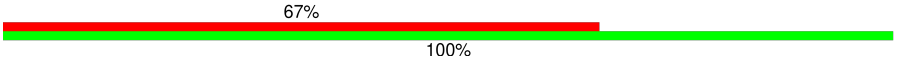
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain oD:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain pD:

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain qD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain rD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain L:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain W:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain X:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain Z:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain c:

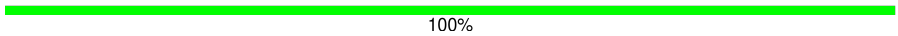
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain d:

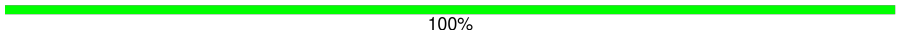
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain g:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain k: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain r: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain v:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain JA:

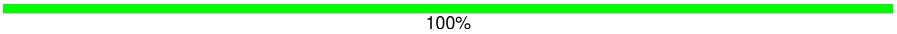
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain UA:

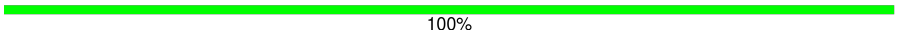
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain VA:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain aA: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain bA: 

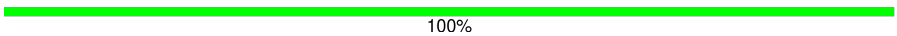
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain eA:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain iA:

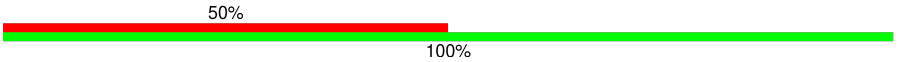
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain pA: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain tA:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain JB: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain NB:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain mB:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain qB:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain DC:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain OC:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain PC:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain RC:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain UC:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain VC:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain YC:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain cC:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain jC:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain nC:

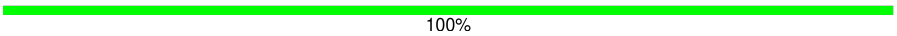
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain AD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain LD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain MD: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain OD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain RD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain SD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain VD:

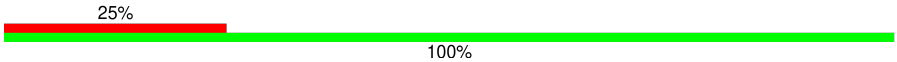
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain ZD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain gD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain kD: 

• Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain M:

• Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain KA:

• Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

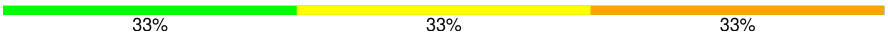
Chain EC:

• Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain BD:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain N:



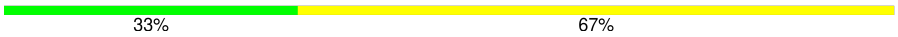
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain R:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain 5:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranos e

Chain 8: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9:

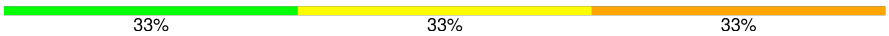
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain AA:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain EA:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain LA: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain PA:

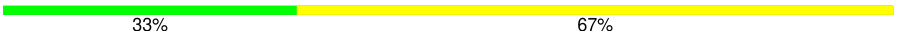
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 3A:

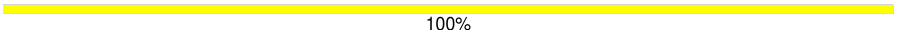
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6A:

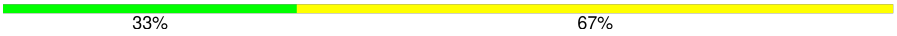
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 7A: 

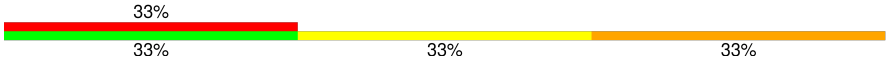
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8A: 

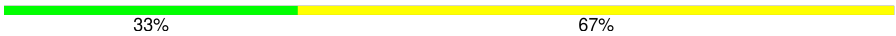
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CB: 

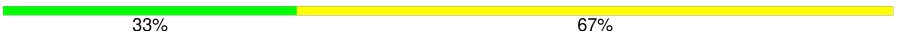
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain XB: 

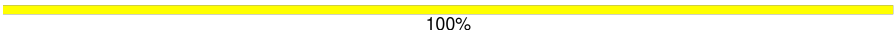
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain aB: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bB: 

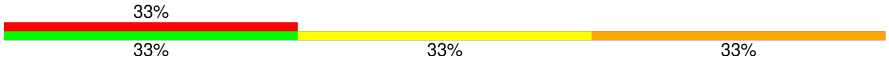
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain cB: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain gB:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0B: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 3B:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4B:

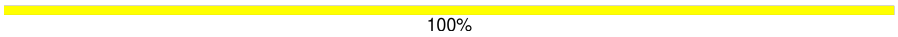
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 5B:

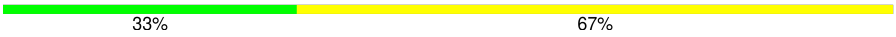
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9B:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain FC: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain JC: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xC:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0C:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1C:

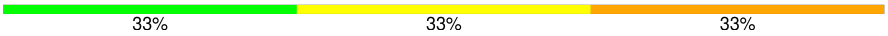
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2C:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6C:

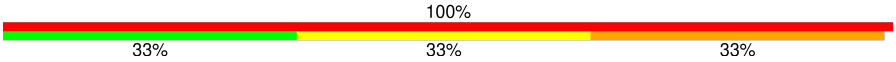
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CD: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain GD:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uD: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xD:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain yD:

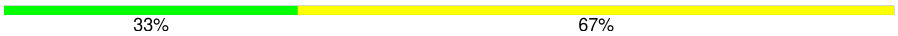
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain zD:

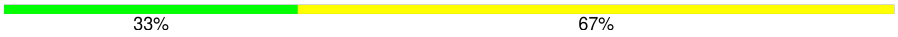
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 3D:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6D: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 7D: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8D:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ME:

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain OE: 67% 33%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ZE: 33% 67%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bE: 67% 33%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain mE: 67% 33%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain nE: 33% 67%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain oE: 33% 67%

FUB1 FUB2 GZL3

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain S: 25% 75%

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain f:

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain h:

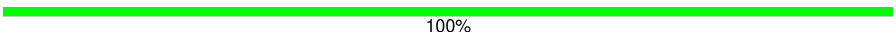
• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain QA:

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain dA:

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain fA: 

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain KC:

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain XC:

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain ZC:

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain HD:

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain UD:

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain WD:

• Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain U:

• Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain SA: 100%

FUB1 FUB2 FUB3 AHR4 AHR5

• Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain MC: 40% 60%

FUB1 FUB2 FUB3 AHR4 AHR5

• Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain JD: 80% 20%

FUB1 FUB2 FUB3 AHR4 AHR5

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain Y: 50% 50%

FUB1 FUB2

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain j: 50% 50%

FUB1 FUB2

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WA: 100%

FUB1 FUB2

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

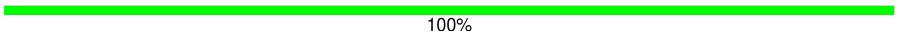
Chain hA: 50% 50%

FUB1 FUB2

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain QC: 100%

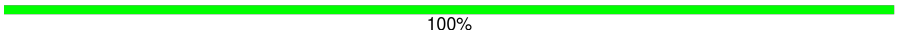
• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bC: 

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ND:

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain YD: 

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain a:

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain u:

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 3:

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain YA:

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

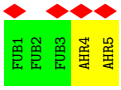
Chain sA:

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 1A:

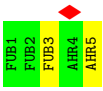
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain MB:



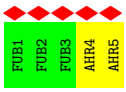
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain VB:



• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain pB:



• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

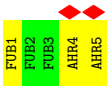
Chain yB:

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain SC:

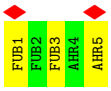
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain mC:



• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain vC:

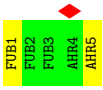


• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain PD:

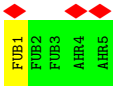
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain jD:



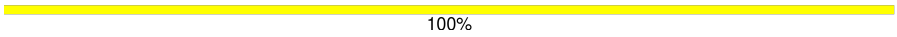
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain sD:



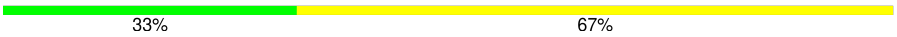
• Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain i:



• Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain gA:



• Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain aC:

• Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

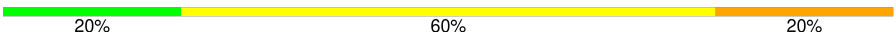
Chain XD:

• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain n:

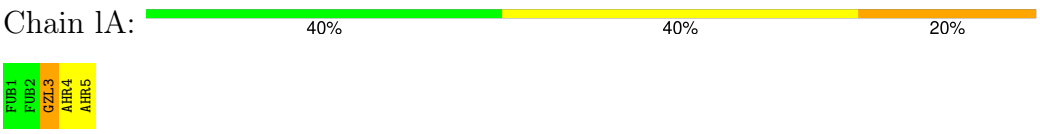
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain q:



• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain lA:

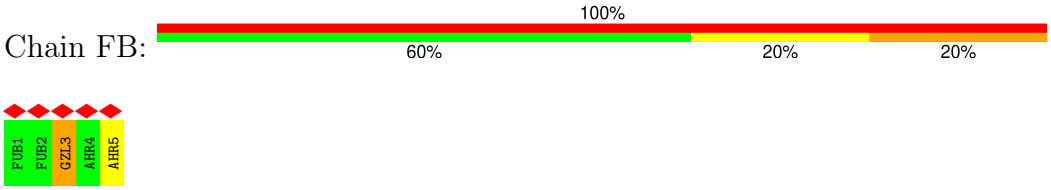


• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain oA:

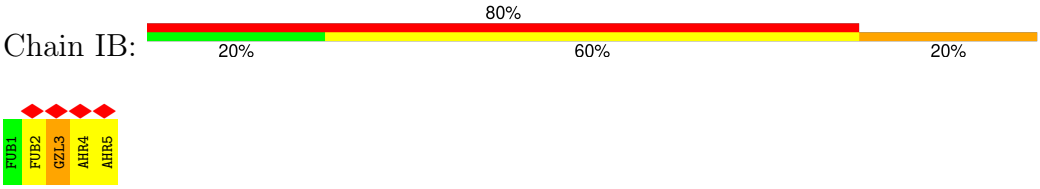
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain FB:



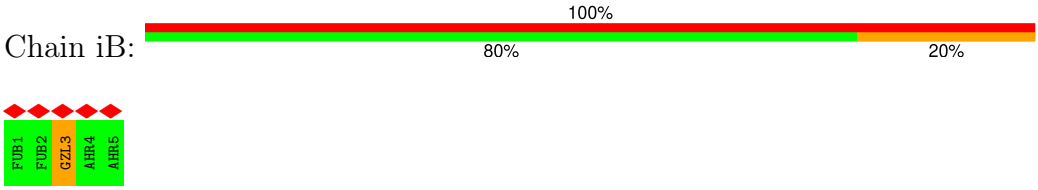
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain IB:



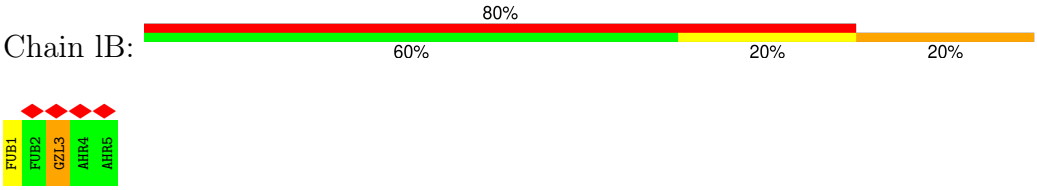
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain iB:



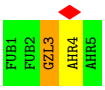
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain lB:



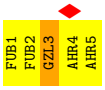
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain fC:



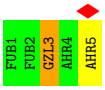
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain iC:

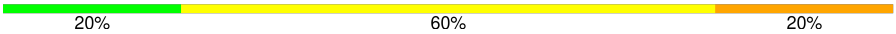


• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain cD:



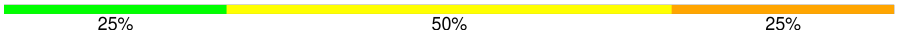
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain fD: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain o:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 7:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain BA:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain mA:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2A:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4A:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

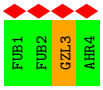
Chain 5A:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

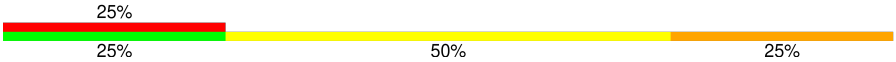
Chain 9A:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain GB:



• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WB: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain YB:

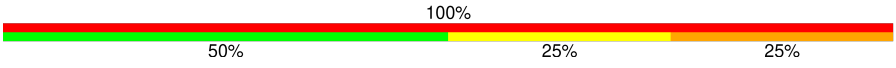
• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

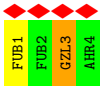
Chain ZB:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

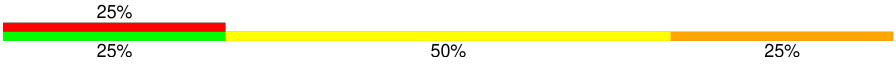
Chain dB:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain jB: 



• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain zB: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1B:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2B:

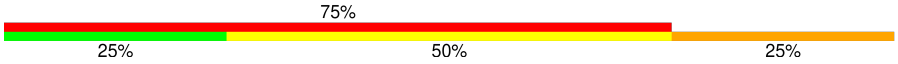
• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6B:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain gC:

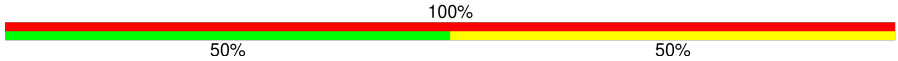
• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

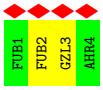
Chain wC: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

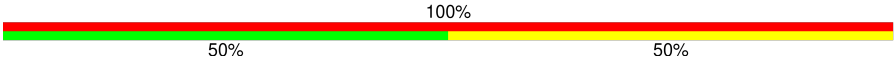
Chain yC:

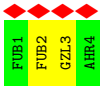
• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain zC: 



• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

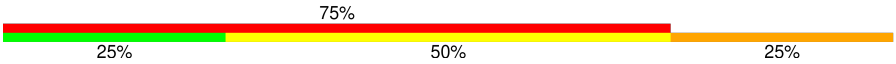
Chain 3C: 



• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain dD:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain tD: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

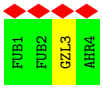
Chain vD:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain wD:

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0D:



• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain p:

• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain s:

• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

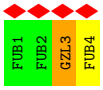
Chain nA:

• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

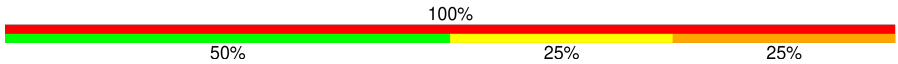
Chain qA:

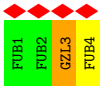
• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain HB:

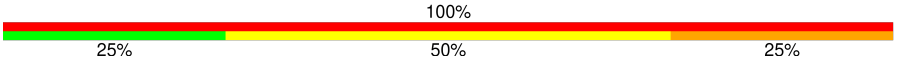


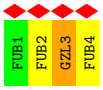
• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain KB: 



• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain kB: 



• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain nB:

• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain hC:

• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain kC:

• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain eD:

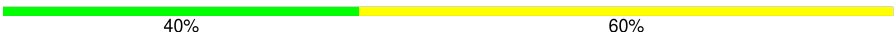
• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain hD:

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CA:

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain DA: 

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain AB:

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain BB: 40% 60%

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain eB: 40% 60%

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain fB: 40% 60%

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

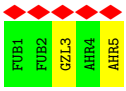
Chain 7B: 60% 40%

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8B: 40% 60%

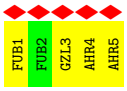
• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4C: 100% 60% 40%



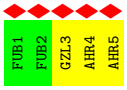
• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 5C:



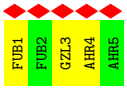
• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1D:



• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2D:



• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:

• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AC:

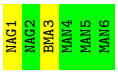
• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4D:

• Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-aceta

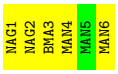
mido-2-deoxy-beta-D-glucopyranose

Chain GA:



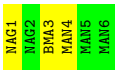
• Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DB:



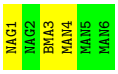
• Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7C:

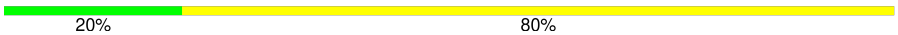


• Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5D:

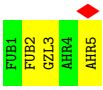


• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 9D: 

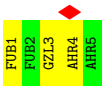
• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain BE:



• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain DE:



• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain IE:

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain JE:

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain KE:

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain PE:

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain SE:

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain cE:

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

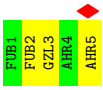
Chain fE:

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

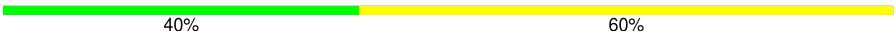
Chain pE:

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain rE:

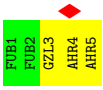


• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain tE: 

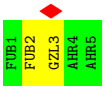
• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain yE:



• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain zE:



• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 0E:

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain AE:

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain LE:

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain NE:

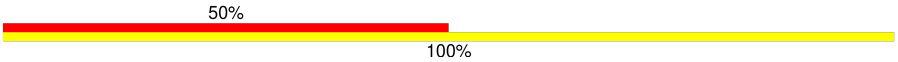
• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain aE:

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain qE:

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 1E: 

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CE:

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain EE:

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HE:

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TE:

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain UE:

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WE: 50% 50%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain gE: 75% 25%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain hE: 75% 25%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain jE: 75% 25%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain sE: 25% 75%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uE: 50% 50%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xE:

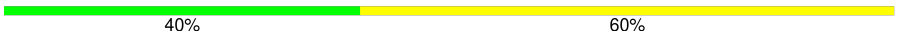
• Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain FE:

• Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

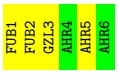
Chain kE:

• Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain vE: 

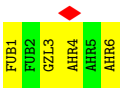
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain GE:

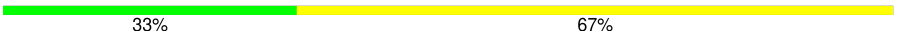


• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain QE:



• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain RE: 

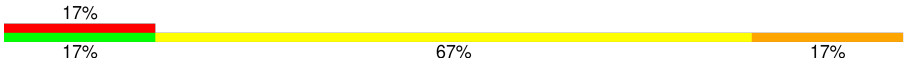
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

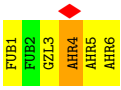
Chain VE:

• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain dE:

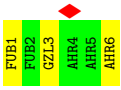
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain eE: 



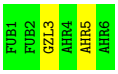
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain iE:



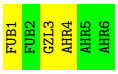
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain wE:

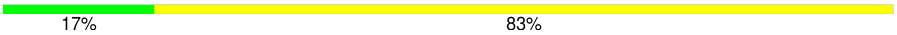


• Molecule 23: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

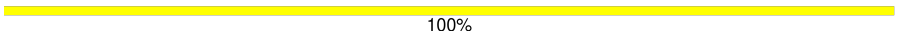
Chain XE:



• Molecule 24: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain YE: 

• Molecule 24: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain lE: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69065	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.527	Depositor
Minimum map value	-0.673	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	554.24, 554.24, 554.24	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FUB, BMA, NAG, MAN, AHR, CA, HYP, GZL, GLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.29	0/13724	0.54	2/18848 (0.0%)
1	B	0.29	0/13724	0.54	3/18848 (0.0%)
1	C	0.27	0/10873	0.51	0/14984
1	D	0.27	0/11422	0.53	2/15734 (0.0%)
1	E	0.27	0/10283	0.51	0/14106
1	F	0.31	2/10246 (0.0%)	0.56	4/14055 (0.0%)
2	G	0.25	0/139	0.58	0/174
2	H	0.21	0/69	0.43	0/89
2	I	0.23	0/71	0.45	0/87
All	All	0.28	2/70551 (0.0%)	0.53	11/96925 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	E	0	2
1	F	0	1
2	G	2	0
2	I	2	0
All	All	4	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	632	PRO	CB-CG	-10.50	0.97	1.50
1	F	632	PRO	CG-CD	-9.54	1.19	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	632	PRO	N-CD-CG	-16.73	78.11	103.20
1	F	632	PRO	CB-CG-CD	14.79	164.20	106.50
1	F	632	PRO	CA-CB-CG	-13.73	77.91	104.00
1	B	1846	PRO	CA-N-CD	-12.21	94.40	111.50
1	A	1839	PRO	CA-N-CD	-11.07	96.00	111.50
1	A	1842	LEU	CA-CB-CG	8.99	135.98	115.30
1	D	534	CYS	CA-CB-SG	7.89	128.20	114.00
1	B	1846	PRO	N-CD-CG	-6.07	94.10	103.20
1	D	915	PRO	CA-N-CD	-5.62	103.63	111.50
1	F	632	PRO	CA-N-CD	-5.58	103.69	111.50
1	B	1845	LYS	C-N-CD	5.27	139.46	128.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	23	HYP	CA
2	G	26	HYP	CA
2	I	23	HYP	CA
2	I	26	HYP	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1522	GLY	Peptide
1	A	1527	LYS	Peptide
1	B	1527	LYS	Peptide
1	E	1527	LYS	Peptide
1	E	1725	TYR	Peptide
1	F	1527	LYS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1848/1987 (93%)	1690 (92%)	150 (8%)	8 (0%)	30	66
1	B	1848/1987 (93%)	1691 (92%)	150 (8%)	7 (0%)	30	66
1	C	1461/1987 (74%)	1342 (92%)	115 (8%)	4 (0%)	37	70
1	D	1531/1987 (77%)	1411 (92%)	114 (7%)	6 (0%)	30	66
1	E	1390/1987 (70%)	1289 (93%)	97 (7%)	4 (0%)	37	70
1	F	1384/1987 (70%)	1273 (92%)	108 (8%)	3 (0%)	44	77
2	G	27/64 (42%)	17 (63%)	6 (22%)	4 (15%)	0	0
2	H	12/64 (19%)	11 (92%)	0	1 (8%)	0	3
2	I	14/64 (22%)	9 (64%)	3 (21%)	2 (14%)	0	1
All	All	9515/12114 (78%)	8733 (92%)	743 (8%)	39 (0%)	32	66

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	585	ALA
1	A	1523	PRO
1	B	1523	PRO
1	E	1523	PRO
1	F	1523	PRO
1	A	473	VAL
1	B	473	VAL
1	C	169	ASN
1	C	473	VAL
1	D	169	ASN
1	D	473	VAL
1	D	585	ALA
2	G	27	ALA
1	A	1909	ARG
1	B	602	TRP
1	C	602	TRP
1	D	1909	ARG
1	E	1909	ARG
1	F	602	TRP
1	A	169	ASN
1	A	602	TRP
1	A	914	ALA

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Mol	Chain	Res	Type
1	D	602	TRP
1	E	602	TRP
2	G	25	ALA
2	G	57	ALA
2	H	57	ALA
2	I	13	THR
2	I	25	ALA
1	B	914	ALA
1	C	914	ALA
1	D	914	ALA
2	G	13	THR
1	B	169	ASN
1	B	1398	SER
1	E	1398	SER
1	F	914	ALA
1	A	604	PRO
1	B	670	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1451/1514 (96%)	1314 (91%)	137 (9%)	7	28
1	B	1451/1514 (96%)	1331 (92%)	120 (8%)	9	34
1	C	1149/1514 (76%)	1064 (93%)	85 (7%)	11	38
1	D	1209/1514 (80%)	1099 (91%)	110 (9%)	7	30
1	E	1081/1514 (71%)	1005 (93%)	76 (7%)	12	41
1	F	1078/1514 (71%)	1009 (94%)	69 (6%)	14	44
2	G	5/5 (100%)	5 (100%)	0	100	100
2	H	2/5 (40%)	2 (100%)	0	100	100
2	I	3/5 (60%)	2 (67%)	1 (33%)	0	1
All	All	7429/9099 (82%)	6831 (92%)	598 (8%)	12	35

All (598) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	61	SER
1	A	62	ASP
1	A	77	THR
1	A	81	PHE
1	A	118	THR
1	A	161	LEU
1	A	180	SER
1	A	185	ASN
1	A	204	SER
1	A	225	ASP
1	A	235	THR
1	A	251	ARG
1	A	271	LEU
1	A	281	THR
1	A	287	THR
1	A	289	THR
1	A	291	THR
1	A	292	THR
1	A	314	ASP
1	A	332	SER
1	A	334	PHE
1	A	343	SER
1	A	347	SER
1	A	353	SER
1	A	361	LEU
1	A	382	ASN
1	A	393	THR
1	A	398	THR
1	A	399	THR
1	A	416	SER
1	A	430	SER
1	A	439	ASN
1	A	456	THR
1	A	491	THR
1	A	530	GLU
1	A	533	LYS
1	A	562	THR
1	A	568	SER
1	A	596	ILE
1	A	613	VAL
1	A	623	SER

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Mol	Chain	Res	Type
1	A	625	SER
1	A	626	VAL
1	A	631	VAL
1	A	664	ASP
1	A	696	THR
1	A	707	SER
1	A	708	THR
1	A	711	THR
1	A	755	SER
1	A	758	ASN
1	A	761	THR
1	A	763	VAL
1	A	792	MET
1	A	805	THR
1	A	816	VAL
1	A	820	SER
1	A	824	TYR
1	A	826	THR
1	A	832	TYR
1	A	860	THR
1	A	866	VAL
1	A	869	VAL
1	A	874	THR
1	A	923	ARG
1	A	924	VAL
1	A	944	THR
1	A	946	THR
1	A	967	VAL
1	A	979	THR
1	A	981	LEU
1	A	983	VAL
1	A	1000	VAL
1	A	1025	ASN
1	A	1052	CYS
1	A	1056	THR
1	A	1064	SER
1	A	1071	ASP
1	A	1076	THR
1	A	1078	THR
1	A	1084	VAL
1	A	1096	LEU
1	A	1108	VAL

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Mol	Chain	Res	Type
1	A	1110	CYS
1	A	1146	THR
1	A	1163	THR
1	A	1191	SER
1	A	1199	VAL
1	A	1208	TYR
1	A	1214	ARG
1	A	1222	THR
1	A	1223	MET
1	A	1237	SER
1	A	1245	THR
1	A	1337	GLU
1	A	1341	LEU
1	A	1377	SER
1	A	1387	THR
1	A	1398	SER
1	A	1459	MET
1	A	1460	SER
1	A	1479	CYS
1	A	1531	THR
1	A	1534	ASP
1	A	1537	PHE
1	A	1538	PHE
1	A	1543	SER
1	A	1548	THR
1	A	1556	ASP
1	A	1576	THR
1	A	1583	ASP
1	A	1584	THR
1	A	1621	LYS
1	A	1647	ASN
1	A	1648	THR
1	A	1658	LYS
1	A	1677	THR
1	A	1731	THR
1	A	1746	GLN
1	A	1748	THR
1	A	1770	ARG
1	A	1773	TYR
1	A	1788	PHE
1	A	1789	GLU
1	A	1799	TYR

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Mol	Chain	Res	Type
1	A	1800	ASP
1	A	1802	PHE
1	A	1808	VAL
1	A	1845	LYS
1	A	1854	SER
1	A	1874	SER
1	A	1884	SER
1	A	1891	ASN
1	A	1925	ARG
1	A	1934	SER
1	A	1938	ASN
1	B	50	ASP
1	B	51	LYS
1	B	72	SER
1	B	89	VAL
1	B	104	THR
1	B	134	SER
1	B	140	VAL
1	B	151	VAL
1	B	159	THR
1	B	160	LEU
1	B	161	LEU
1	B	169	ASN
1	B	176	LYS
1	B	222	VAL
1	B	252	THR
1	B	347	SER
1	B	353	SER
1	B	398	THR
1	B	418	VAL
1	B	429	SER
1	B	430	SER
1	B	433	THR
1	B	437	MET
1	B	457	SER
1	B	494	LEU
1	B	498	GLU
1	B	501	VAL
1	B	528	VAL
1	B	566	LEU
1	B	568	SER
1	B	573	ASP

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Mol	Chain	Res	Type
1	B	603	ASP
1	B	623	SER
1	B	625	SER
1	B	637	THR
1	B	708	THR
1	B	716	LEU
1	B	717	GLN
1	B	745	THR
1	B	755	SER
1	B	774	VAL
1	B	820	SER
1	B	824	TYR
1	B	826	THR
1	B	828	THR
1	B	849	THR
1	B	869	VAL
1	B	871	SER
1	B	923	ARG
1	B	924	VAL
1	B	927	THR
1	B	943	THR
1	B	956	VAL
1	B	962	THR
1	B	965	LEU
1	B	967	VAL
1	B	977	LEU
1	B	983	VAL
1	B	1000	VAL
1	B	1012	THR
1	B	1084	VAL
1	B	1087	ASP
1	B	1096	LEU
1	B	1100	THR
1	B	1108	VAL
1	B	1110	CYS
1	B	1145	ASP
1	B	1146	THR
1	B	1147	VAL
1	B	1166	THR
1	B	1192	ASN
1	B	1208	TYR
1	B	1237	SER

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Mol	Chain	Res	Type
1	B	1245	THR
1	B	1259	THR
1	B	1263	LYS
1	B	1270	THR
1	B	1306	SER
1	B	1318	THR
1	B	1340	SER
1	B	1367	LEU
1	B	1377	SER
1	B	1380	LEU
1	B	1387	THR
1	B	1393	GLU
1	B	1436	THR
1	B	1437	THR
1	B	1486	THR
1	B	1497	MET
1	B	1527	LYS
1	B	1534	ASP
1	B	1537	PHE
1	B	1538	PHE
1	B	1543	SER
1	B	1545	THR
1	B	1548	THR
1	B	1555	THR
1	B	1576	THR
1	B	1583	ASP
1	B	1588	VAL
1	B	1622	ARG
1	B	1627	CYS
1	B	1648	THR
1	B	1654	THR
1	B	1658	LYS
1	B	1683	CYS
1	B	1697	CYS
1	B	1764	SER
1	B	1788	PHE
1	B	1799	TYR
1	B	1802	PHE
1	B	1804	ASP
1	B	1831	ASP
1	B	1836	ARG
1	B	1840	CYS

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Mol	Chain	Res	Type
1	B	1853	GLN
1	B	1874	SER
1	B	1884	SER
1	B	1904	SER
1	B	1934	SER
1	C	46	THR
1	C	48	THR
1	C	67	THR
1	C	69	THR
1	C	72	SER
1	C	97	THR
1	C	117	VAL
1	C	159	THR
1	C	161	LEU
1	C	176	LYS
1	C	188	ASP
1	C	204	SER
1	C	235	THR
1	C	275	VAL
1	C	286	VAL
1	C	287	THR
1	C	292	THR
1	C	332	SER
1	C	395	ASP
1	C	429	SER
1	C	430	SER
1	C	433	THR
1	C	462	LEU
1	C	467	ILE
1	C	470	ARG
1	C	480	LEU
1	C	488	PHE
1	C	552	LEU
1	C	573	ASP
1	C	602	TRP
1	C	619	THR
1	C	622	LEU
1	C	623	SER
1	C	627	THR
1	C	642	ASN
1	C	667	THR
1	C	689	THR

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Mol	Chain	Res	Type
1	C	691	MET
1	C	699	THR
1	C	700	CYS
1	C	726	ASP
1	C	737	VAL
1	C	745	THR
1	C	756	TYR
1	C	760	VAL
1	C	761	THR
1	C	781	VAL
1	C	821	ILE
1	C	843	VAL
1	C	909	ASN
1	C	921	TYR
1	C	923	ARG
1	C	924	VAL
1	C	938	MET
1	C	943	THR
1	C	944	THR
1	C	950	THR
1	C	966	MET
1	C	967	VAL
1	C	979	THR
1	C	1011	THR
1	C	1017	TYR
1	C	1033	THR
1	C	1071	ASP
1	C	1076	THR
1	C	1078	THR
1	C	1123	SER
1	C	1128	VAL
1	C	1135	THR
1	C	1171	ARG
1	C	1172	VAL
1	C	1199	VAL
1	C	1208	TYR
1	C	1223	MET
1	C	1245	THR
1	C	1258	LEU
1	C	1269	THR
1	C	1289	LYS
1	C	1295	ASN

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Mol	Chain	Res	Type
1	C	1365	THR
1	C	1377	SER
1	C	1378	MET
1	C	1379	ASN
1	C	1384	SER
1	C	1397	TRP
1	D	46	THR
1	D	50	ASP
1	D	51	LYS
1	D	76	THR
1	D	85	TYR
1	D	105	PRO
1	D	110	VAL
1	D	116	THR
1	D	159	THR
1	D	160	LEU
1	D	161	LEU
1	D	179	VAL
1	D	181	SER
1	D	182	SER
1	D	185	ASN
1	D	204	SER
1	D	207	ILE
1	D	231	GLU
1	D	251	ARG
1	D	278	THR
1	D	280	VAL
1	D	281	THR
1	D	287	THR
1	D	289	THR
1	D	334	PHE
1	D	352	THR
1	D	379	THR
1	D	395	ASP
1	D	398	THR
1	D	399	THR
1	D	410	LYS
1	D	416	SER
1	D	429	SER
1	D	433	THR
1	D	437	MET
1	D	466	ARG

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Mol	Chain	Res	Type
1	D	470	ARG
1	D	479	LEU
1	D	487	THR
1	D	491	THR
1	D	501	VAL
1	D	524	THR
1	D	531	SER
1	D	540	ASP
1	D	573	ASP
1	D	587	SER
1	D	608	THR
1	D	619	THR
1	D	623	SER
1	D	639	TRP
1	D	662	PHE
1	D	667	THR
1	D	687	LYS
1	D	691	MET
1	D	696	THR
1	D	697	THR
1	D	729	THR
1	D	735	SER
1	D	745	THR
1	D	747	THR
1	D	750	SER
1	D	792	MET
1	D	794	ASP
1	D	807	ASP
1	D	820	SER
1	D	832	TYR
1	D	833	PHE
1	D	846	SER
1	D	888	ILE
1	D	909	ASN
1	D	921	TYR
1	D	922	TRP
1	D	923	ARG
1	D	934	VAL
1	D	938	MET
1	D	943	THR
1	D	962	THR
1	D	983	VAL

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Mol	Chain	Res	Type
1	D	1000	VAL
1	D	1028	THR
1	D	1037	ASP
1	D	1046	SER
1	D	1059	ASN
1	D	1096	LEU
1	D	1100	THR
1	D	1128	VAL
1	D	1133	SER
1	D	1145	ASP
1	D	1160	THR
1	D	1192	ASN
1	D	1208	TYR
1	D	1223	MET
1	D	1229	ILE
1	D	1242	ARG
1	D	1286	LYS
1	D	1299	THR
1	D	1337	GLU
1	D	1339	THR
1	D	1366	TYR
1	D	1370	ARG
1	D	1377	SER
1	D	1379	ASN
1	D	1398	SER
1	D	1399	LYS
1	D	1479	CYS
1	D	1490	MET
1	D	1492	ASP
1	D	1534	ASP
1	D	1539	MET
1	D	1925	ARG
1	E	568	SER
1	E	579	ARG
1	E	623	SER
1	E	635	THR
1	E	640	THR
1	E	701	SER
1	E	733	PHE
1	E	761	THR
1	E	770	VAL
1	E	774	VAL

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Mol	Chain	Res	Type
1	E	824	TYR
1	E	846	SER
1	E	847	HIS
1	E	848	ILE
1	E	907	PHE
1	E	908	PHE
1	E	913	THR
1	E	923	ARG
1	E	953	TYR
1	E	962	THR
1	E	999	MET
1	E	1000	VAL
1	E	1008	VAL
1	E	1012	THR
1	E	1078	THR
1	E	1127	PHE
1	E	1128	VAL
1	E	1146	THR
1	E	1208	TYR
1	E	1232	PRO
1	E	1237	SER
1	E	1259	THR
1	E	1271	TYR
1	E	1289	LYS
1	E	1318	THR
1	E	1334	THR
1	E	1387	THR
1	E	1413	TYR
1	E	1416	THR
1	E	1460	SER
1	E	1479	CYS
1	E	1507	ASP
1	E	1512	ARG
1	E	1515	THR
1	E	1534	ASP
1	E	1539	MET
1	E	1548	THR
1	E	1588	VAL
1	E	1648	THR
1	E	1677	THR
1	E	1678	THR
1	E	1721	THR

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Mol	Chain	Res	Type
1	E	1730	CYS
1	E	1737	THR
1	E	1738	VAL
1	E	1741	LYS
1	E	1744	SER
1	E	1773	TYR
1	E	1786	ASP
1	E	1788	PHE
1	E	1799	TYR
1	E	1805	ARG
1	E	1808	VAL
1	E	1818	ASP
1	E	1819	LEU
1	E	1829	THR
1	E	1832	LEU
1	E	1841	SER
1	E	1844	SER
1	E	1861	SER
1	E	1876	ASN
1	E	1884	SER
1	E	1891	ASN
1	E	1895	THR
1	E	1925	ARG
1	E	1938	ASN
1	F	524	THR
1	F	564	THR
1	F	566	LEU
1	F	619	THR
1	F	625	SER
1	F	646	SER
1	F	662	PHE
1	F	674	ASP
1	F	690	SER
1	F	699	THR
1	F	713	THR
1	F	743	PHE
1	F	761	THR
1	F	763	VAL
1	F	778	ASN
1	F	795	ASN
1	F	807	ASP
1	F	832	TYR

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Mol	Chain	Res	Type
1	F	833	PHE
1	F	867	THR
1	F	870	VAL
1	F	923	ARG
1	F	966	MET
1	F	993	HIS
1	F	1028	THR
1	F	1035	LEU
1	F	1056	THR
1	F	1084	VAL
1	F	1131	TYR
1	F	1191	SER
1	F	1208	TYR
1	F	1224	ASP
1	F	1233	SER
1	F	1251	THR
1	F	1274	VAL
1	F	1315	THR
1	F	1318	THR
1	F	1334	THR
1	F	1349	SER
1	F	1378	MET
1	F	1460	SER
1	F	1479	CYS
1	F	1512	ARG
1	F	1548	THR
1	F	1555	THR
1	F	1558	ASP
1	F	1583	ASP
1	F	1587	THR
1	F	1588	VAL
1	F	1627	CYS
1	F	1671	PHE
1	F	1677	THR
1	F	1678	THR
1	F	1681	THR
1	F	1742	THR
1	F	1761	SER
1	F	1766	ARG
1	F	1799	TYR
1	F	1808	VAL
1	F	1819	LEU

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Mol	Chain	Res	Type
1	F	1824	LEU
1	F	1839	PRO
1	F	1842	LEU
1	F	1861	SER
1	F	1871	ARG
1	F	1874	SER
1	F	1884	SER
1	F	1925	ARG
1	F	1926	SER
2	I	13	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1212	GLN
1	A	1406	GLN
1	A	1421	GLN
1	A	1487	ASN
1	A	1563	GLN
1	B	909	ASN
1	B	1212	GLN
1	B	1293	GLN
1	B	1536	ASN
1	B	1549	ASN
1	B	1672	GLN
1	B	1701	GLN
1	C	612	GLN
1	D	1212	GLN
1	E	1672	GLN
1	F	1536	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

358 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	C	1906	1	7,8,9	0.56	0	5,10,12	1.19	1 (20%)
1	HYP	A	1866	1	7,8,9	0.56	0	5,10,12	1.48	1 (20%)
1	HYP	F	1894	1	7,8,9	0.51	0	5,10,12	1.98	2 (40%)
1	HYP	E	1880	1	7,8,9	0.53	0	5,10,12	1.45	1 (20%)
2	HYP	G	9	2	7,8,9	0.55	0	5,10,12	1.80	2 (40%)
1	HYP	A	1878	1	7,8,9	0.52	0	5,10,12	1.75	2 (40%)
1	HYP	E	1914	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	E	1911	1	7,8,9	0.56	0	5,10,12	1.25	1 (20%)
1	HYP	D	1914	1	7,8,9	0.53	0	5,10,12	1.11	1 (20%)
1	HYP	C	1897	1	7,8,9	0.53	0	5,10,12	1.30	1 (20%)
2	HYP	G	33	2	7,8,9	0.51	0	5,10,12	1.65	1 (20%)
1	HYP	A	1894	1	7,8,9	0.55	0	5,10,12	1.93	2 (40%)
1	HYP	E	1898	1	7,8,9	0.57	0	5,10,12	1.22	1 (20%)
1	HYP	C	1903	1	7,8,9	0.54	0	5,10,12	1.84	3 (60%)
1	HYP	E	1912	1	7,8,9	0.57	0	5,10,12	1.29	1 (20%)
1	HYP	D	1932	1	7,8,9	0.56	0	5,10,12	1.87	3 (60%)
1	HYP	E	1865	1	7,8,9	0.55	0	5,10,12	1.66	1 (20%)
1	HYP	D	1918	1	7,8,9	0.55	0	5,10,12	1.86	2 (40%)
1	HYP	B	1873	1	7,8,9	0.49	0	5,10,12	1.37	1 (20%)
1	HYP	A	1870	1	7,8,9	0.50	0	5,10,12	1.60	2 (40%)
2	HYP	G	56	2	7,8,9	0.53	0	5,10,12	1.28	1 (20%)
2	HYP	G	46	2	7,8,9	0.57	0	5,10,12	1.57	1 (20%)
1	HYP	A	1887	1	7,8,9	0.55	0	5,10,12	1.27	1 (20%)
1	HYP	E	1893	1	7,8,9	0.58	0	5,10,12	1.26	1 (20%)
1	HYP	F	1898	1	7,8,9	0.58	0	5,10,12	1.19	1 (20%)
1	HYP	B	1917	1	7,8,9	0.60	0	5,10,12	1.68	1 (20%)
2	HYP	G	32	2	7,8,9	0.52	0	5,10,12	1.43	1 (20%)
1	HYP	A	1883	1	7,8,9	0.55	0	5,10,12	2.22	2 (40%)
1	HYP	A	1882	1	7,8,9	0.55	0	5,10,12	1.25	1 (20%)
1	HYP	E	1902	1	7,8,9	0.52	0	5,10,12	1.70	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	B	1894	1	7,8,9	0.55	0	5,10,12	2.01	2 (40%)
1	HYP	C	1899	1	7,8,9	0.59	0	5,10,12	1.32	1 (20%)
1	HYP	F	1917	1	7,8,9	0.54	0	5,10,12	1.41	1 (20%)
1	HYP	B	1907	1	7,8,9	0.56	0	5,10,12	1.68	1 (20%)
1	HYP	E	1916	1	7,8,9	0.59	0	5,10,12	1.34	1 (20%)
1	HYP	F	1914	1	7,8,9	0.54	0	5,10,12	1.48	1 (20%)
1	HYP	F	1899	1	7,8,9	0.61	0	5,10,12	1.33	1 (20%)
1	HYP	B	1908	1	7,8,9	0.56	0	5,10,12	2.17	3 (60%)
1	HYP	E	1888	1	7,8,9	0.50	0	5,10,12	1.86	2 (40%)
1	HYP	B	1875	1	7,8,9	0.56	0	5,10,12	1.20	1 (20%)
1	HYP	B	1888	1	7,8,9	0.54	0	5,10,12	1.72	2 (40%)
1	HYP	E	1929	1	7,8,9	0.59	0	5,10,12	1.27	1 (20%)
2	HYP	G	1	2	7,8,9	0.53	0	5,10,12	1.21	1 (20%)
1	HYP	E	1899	1	7,8,9	0.59	0	5,10,12	1.34	1 (20%)
1	HYP	F	1877	1	7,8,9	0.54	0	5,10,12	1.58	1 (20%)
1	HYP	E	1855	1	7,8,9	0.60	0	5,10,12	1.22	1 (20%)
1	HYP	C	1927	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	F	1929	1	7,8,9	0.57	0	5,10,12	1.22	1 (20%)
1	HYP	F	1865	1	7,8,9	0.57	0	5,10,12	1.68	2 (40%)
1	HYP	D	1921	1	7,8,9	0.59	0	5,10,12	1.25	1 (20%)
1	HYP	A	1903	1	7,8,9	0.58	0	5,10,12	1.81	2 (40%)
1	HYP	B	1929	1	7,8,9	0.68	0	5,10,12	1.40	1 (20%)
1	HYP	B	1887	1	7,8,9	0.58	0	5,10,12	1.30	1 (20%)
1	HYP	D	1923	1	7,8,9	0.53	0	5,10,12	1.86	3 (60%)
1	HYP	B	1910	1	7,8,9	0.54	0	5,10,12	1.18	1 (20%)
1	HYP	A	1910	1	7,8,9	0.55	0	5,10,12	1.19	1 (20%)
1	HYP	F	1905	1	7,8,9	0.59	0	5,10,12	1.30	1 (20%)
1	HYP	A	1918	1	7,8,9	0.57	0	5,10,12	1.62	1 (20%)
1	HYP	B	1866	1	7,8,9	0.51	0	5,10,12	1.32	1 (20%)
1	HYP	F	1893	1	7,8,9	0.57	0	5,10,12	1.34	1 (20%)
1	HYP	B	1928	1	7,8,9	0.56	0	5,10,12	1.54	1 (20%)
1	HYP	B	1897	1	7,8,9	0.57	0	5,10,12	1.17	1 (20%)
1	HYP	E	1877	1	7,8,9	0.54	0	5,10,12	1.80	2 (40%)
1	HYP	E	1892	1	7,8,9	0.52	0	5,10,12	1.32	1 (20%)
1	HYP	A	1890	1	7,8,9	0.59	0	5,10,12	1.25	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	E	1908	1	7,8,9	0.54	0	5,10,12	2.14	3 (60%)
2	HYP	I	2	2	7,8,9	0.48	0	5,10,12	1.48	1 (20%)
1	HYP	A	1916	1	7,8,9	0.58	0	5,10,12	1.47	1 (20%)
1	HYP	F	1890	1	7,8,9	0.57	0	5,10,12	1.18	1 (20%)
1	HYP	E	1862	1	7,8,9	0.54	0	5,10,12	1.49	1 (20%)
1	HYP	E	1858	1	7,8,9	0.54	0	5,10,12	1.70	1 (20%)
1	HYP	F	1916	1	7,8,9	0.54	0	5,10,12	1.28	1 (20%)
1	HYP	F	1928	1	7,8,9	0.56	0	5,10,12	1.28	1 (20%)
1	HYP	B	1877	1	7,8,9	0.51	0	5,10,12	1.68	1 (20%)
1	HYP	B	1892	1	7,8,9	0.51	0	5,10,12	1.27	1 (20%)
1	HYP	F	1855	1	7,8,9	0.62	0	5,10,12	1.46	1 (20%)
2	HYP	G	41	2	7,8,9	0.58	0	5,10,12	1.23	1 (20%)
1	HYP	C	1911	1	7,8,9	0.54	0	5,10,12	1.23	1 (20%)
1	HYP	D	1897	1	7,8,9	0.51	0	5,10,12	1.27	1 (20%)
1	HYP	F	1885	1	7,8,9	0.54	0	5,10,12	1.24	1 (20%)
2	HYP	G	5	2	7,8,9	0.47	0	5,10,12	1.20	1 (20%)
2	HYP	G	17	2	7,8,9	0.56	0	5,10,12	1.31	1 (20%)
1	HYP	B	1870	1	7,8,9	0.56	0	5,10,12	1.57	1 (20%)
1	HYP	C	1913	1	7,8,9	0.57	0	5,10,12	1.27	1 (20%)
1	HYP	B	1858	1	7,8,9	0.56	0	5,10,12	1.43	1 (20%)
1	HYP	A	1885	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	B	1901	1	7,8,9	0.57	0	5,10,12	1.20	1 (20%)
1	HYP	A	1911	1	7,8,9	0.56	0	5,10,12	1.24	1 (20%)
2	HYP	H	48	2	7,8,9	0.62	0	5,10,12	1.23	1 (20%)
1	HYP	A	1867	1	7,8,9	0.51	0	5,10,12	1.61	1 (20%)
1	HYP	C	1901	1	7,8,9	0.56	0	5,10,12	1.20	1 (20%)
1	HYP	D	1911	1	7,8,9	0.57	0	5,10,12	1.22	1 (20%)
1	HYP	A	1856	1	7,8,9	0.56	0	5,10,12	1.34	1 (20%)
1	HYP	C	1905	1	7,8,9	0.58	0	5,10,12	1.20	1 (20%)
1	HYP	E	1870	1	7,8,9	0.50	0	5,10,12	1.59	2 (40%)
1	HYP	A	1912	1	7,8,9	0.60	0	5,10,12	1.24	1 (20%)
1	HYP	F	1930	1	7,8,9	0.53	0	5,10,12	1.54	1 (20%)
1	HYP	A	1913	1	7,8,9	0.62	0	5,10,12	1.30	1 (20%)
2	HYP	G	8	2	7,8,9	0.59	0	5,10,12	1.62	1 (20%)
2	HYP	G	43	2	7,8,9	0.54	0	5,10,12	1.49	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HYP	I	7	2	7,8,9	0.52	0	5,10,12	1.67	1 (20%)
1	HYP	B	1890	1	7,8,9	0.59	0	5,10,12	1.21	1 (20%)
1	HYP	F	1872	1	7,8,9	0.56	0	5,10,12	1.25	1 (20%)
1	HYP	D	1908	1	7,8,9	0.54	0	5,10,12	1.74	2 (40%)
1	HYP	F	1915	1	7,8,9	0.52	0	5,10,12	1.24	1 (20%)
1	HYP	D	1907	1	7,8,9	0.50	0	5,10,12	1.61	1 (20%)
1	HYP	D	1905	1	7,8,9	0.55	0	5,10,12	1.22	1 (20%)
1	HYP	A	1917	1	7,8,9	0.55	0	5,10,12	1.62	1 (20%)
1	HYP	A	1915	1	7,8,9	0.57	0	5,10,12	1.27	1 (20%)
1	HYP	B	1864	1	7,8,9	0.53	0	5,10,12	1.49	1 (20%)
1	HYP	F	1863	1	7,8,9	0.54	0	5,10,12	1.41	1 (20%)
1	HYP	F	1862	1	7,8,9	0.50	0	5,10,12	1.37	1 (20%)
1	HYP	A	1880	1	7,8,9	0.53	0	5,10,12	1.41	1 (20%)
1	HYP	E	1864	1	7,8,9	0.58	0	5,10,12	1.58	1 (20%)
2	HYP	G	49	2	7,8,9	0.57	0	5,10,12	1.51	1 (20%)
1	HYP	A	1914	1	7,8,9	0.57	0	5,10,12	1.40	1 (20%)
1	HYP	D	1920	1	7,8,9	0.57	0	5,10,12	1.51	1 (20%)
1	HYP	C	1917	1	7,8,9	0.57	0	5,10,12	1.48	1 (20%)
1	HYP	A	1898	1	7,8,9	0.64	0	5,10,12	1.23	1 (20%)
1	HYP	B	1927	1	7,8,9	0.58	0	5,10,12	1.23	1 (20%)
2	HYP	G	29	2	7,8,9	0.53	0	5,10,12	1.24	1 (20%)
1	HYP	B	1857	1	7,8,9	0.57	0	5,10,12	1.63	2 (40%)
2	HYP	G	47	2	7,8,9	0.61	0	5,10,12	1.31	1 (20%)
2	HYP	G	45	2	7,8,9	0.59	0	5,10,12	1.29	1 (20%)
1	HYP	D	1910	1	7,8,9	0.50	0	5,10,12	1.17	1 (20%)
1	HYP	F	1870	1	7,8,9	0.52	0	5,10,12	1.60	1 (20%)
1	HYP	A	1929	1	7,8,9	0.62	0	5,10,12	1.27	1 (20%)
1	HYP	E	1863	1	7,8,9	0.54	0	5,10,12	1.44	1 (20%)
1	HYP	C	1912	1	7,8,9	0.56	0	5,10,12	1.21	1 (20%)
1	HYP	A	1928	1	7,8,9	0.56	0	5,10,12	1.16	1 (20%)
1	HYP	F	1868	1	7,8,9	0.58	0	5,10,12	2.08	3 (60%)
1	HYP	E	1932	1	7,8,9	0.54	0	5,10,12	1.48	1 (20%)
1	HYP	E	1910	1	7,8,9	0.52	0	5,10,12	1.22	1 (20%)
1	HYP	A	1921	1	7,8,9	0.66	0	5,10,12	1.42	1 (20%)
1	HYP	E	1918	1	7,8,9	0.54	0	5,10,12	1.73	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	A	1893	1	7,8,9	0.61	0	5,10,12	1.32	1 (20%)
1	HYP	B	1867	1	7,8,9	0.51	0	5,10,12	1.67	1 (20%)
1	HYP	C	1910	1	7,8,9	0.55	0	5,10,12	1.20	1 (20%)
1	HYP	D	1922	1	7,8,9	0.56	0	5,10,12	1.42	1 (20%)
2	HYP	I	4	2	7,8,9	0.54	0	5,10,12	1.29	1 (20%)
1	HYP	F	1902	1	7,8,9	0.57	0	5,10,12	1.72	2 (40%)
1	HYP	B	1856	1	7,8,9	0.50	0	5,10,12	1.28	1 (20%)
1	HYP	D	1931	1	7,8,9	0.54	0	5,10,12	1.41	1 (20%)
2	HYP	H	52	2	7,8,9	0.52	0	5,10,12	1.77	2 (40%)
1	HYP	F	1910	1	7,8,9	0.52	0	5,10,12	1.16	1 (20%)
2	HYP	G	50	2	7,8,9	0.58	0	5,10,12	1.21	1 (20%)
1	HYP	F	1882	1	7,8,9	0.53	0	5,10,12	1.20	1 (20%)
2	HYP	H	40	2	7,8,9	0.51	0	5,10,12	1.15	1 (20%)
2	HYP	I	23	2	7,8,9	0.42	0	5,10,12	1.45	1 (20%)
1	HYP	B	1905	1	7,8,9	0.59	0	5,10,12	1.23	1 (20%)
1	HYP	C	1931	1	7,8,9	0.56	0	5,10,12	1.40	1 (20%)
1	HYP	B	1898	1	7,8,9	0.64	0	5,10,12	1.29	1 (20%)
2	HYP	H	56	2	7,8,9	0.53	0	5,10,12	1.26	1 (20%)
1	HYP	E	1887	1	7,8,9	0.53	0	5,10,12	1.25	1 (20%)
1	HYP	A	1892	1	7,8,9	0.56	0	5,10,12	1.39	1 (20%)
1	HYP	A	1899	1	7,8,9	0.65	0	5,10,12	1.44	1 (20%)
1	HYP	C	1916	1	7,8,9	0.56	0	5,10,12	1.19	1 (20%)
1	HYP	F	1883	1	7,8,9	0.53	0	5,10,12	2.03	2 (40%)
1	HYP	F	1921	1	7,8,9	0.61	0	5,10,12	1.38	1 (20%)
2	HYP	G	11	2	7,8,9	0.51	0	5,10,12	1.98	2 (40%)
2	HYP	I	3	2	7,8,9	0.54	0	5,10,12	1.66	2 (40%)
1	HYP	B	1911	1	7,8,9	0.57	0	5,10,12	1.21	1 (20%)
1	HYP	A	1858	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
2	HYP	I	20	2	7,8,9	0.55	0	5,10,12	1.28	1 (20%)
2	HYP	G	26	2	7,8,9	0.55	0	5,10,12	1.19	1 (20%)
1	HYP	F	1912	1	7,8,9	0.57	0	5,10,12	1.17	1 (20%)
1	HYP	E	1882	1	7,8,9	0.53	0	5,10,12	1.26	1 (20%)
1	HYP	E	1873	1	7,8,9	0.47	0	5,10,12	1.34	1 (20%)
2	HYP	I	10	2	7,8,9	0.57	0	5,10,12	1.73	1 (20%)
1	HYP	B	1914	1	7,8,9	0.53	0	5,10,12	1.55	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	E	1906	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	B	1913	1	7,8,9	0.62	0	5,10,12	1.34	1 (20%)
1	HYP	B	1931	1	7,8,9	0.56	0	5,10,12	1.43	1 (20%)
1	HYP	E	1860	1	7,8,9	0.57	0	5,10,12	1.92	3 (60%)
1	HYP	E	1867	1	7,8,9	0.58	0	5,10,12	1.82	2 (40%)
1	HYP	E	1922	1	7,8,9	0.62	0	5,10,12	1.55	1 (20%)
2	HYP	G	48	2	7,8,9	0.59	0	5,10,12	1.23	1 (20%)
2	HYP	G	20	2	7,8,9	0.54	0	5,10,12	1.33	1 (20%)
1	HYP	C	1918	1	7,8,9	0.56	0	5,10,12	1.81	2 (40%)
1	HYP	E	1856	1	7,8,9	0.54	0	5,10,12	1.32	1 (20%)
1	HYP	F	1892	1	7,8,9	0.57	0	5,10,12	1.28	1 (20%)
1	HYP	F	1923	1	7,8,9	0.56	0	5,10,12	2.15	3 (60%)
2	HYP	G	52	2	7,8,9	0.55	0	5,10,12	1.68	2 (40%)
1	HYP	F	1888	1	7,8,9	0.50	0	5,10,12	1.90	2 (40%)
1	HYP	F	1932	1	7,8,9	0.50	0	5,10,12	1.75	2 (40%)
1	HYP	E	1921	1	7,8,9	0.60	0	5,10,12	1.35	1 (20%)
1	HYP	A	1877	1	7,8,9	0.50	0	5,10,12	1.34	1 (20%)
1	HYP	D	1917	1	7,8,9	0.57	0	5,10,12	1.53	1 (20%)
1	HYP	B	1915	1	7,8,9	0.57	0	5,10,12	1.29	1 (20%)
1	HYP	F	1918	1	7,8,9	0.53	0	5,10,12	2.04	2 (40%)
1	HYP	A	1865	1	7,8,9	0.56	0	5,10,12	1.68	1 (20%)
1	HYP	E	1920	1	7,8,9	0.56	0	5,10,12	1.47	1 (20%)
1	HYP	E	1923	1	7,8,9	0.53	0	5,10,12	2.15	2 (40%)
1	HYP	B	1860	1	7,8,9	0.51	0	5,10,12	1.75	3 (60%)
1	HYP	A	1862	1	7,8,9	0.54	0	5,10,12	1.45	1 (20%)
2	HYP	H	50	2	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	E	1915	1	7,8,9	0.52	0	5,10,12	1.17	1 (20%)
1	HYP	A	1931	1	7,8,9	0.58	0	5,10,12	1.43	1 (20%)
1	HYP	A	1868	1	7,8,9	0.56	0	5,10,12	1.98	3 (60%)
1	HYP	E	1930	1	7,8,9	0.59	0	5,10,12	1.24	1 (20%)
1	HYP	F	1927	1	7,8,9	0.53	0	5,10,12	1.18	1 (20%)
1	HYP	F	1887	1	7,8,9	0.54	0	5,10,12	1.19	1 (20%)
1	HYP	B	1921	1	7,8,9	0.61	0	5,10,12	1.25	1 (20%)
1	HYP	F	1857	1	7,8,9	0.56	0	5,10,12	1.61	1 (20%)
1	HYP	D	1916	1	7,8,9	0.57	0	5,10,12	1.40	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HYP	I	26	2	7,8,9	0.54	0	5,10,12	1.51	2 (40%)
2	HYP	I	17	2	7,8,9	0.56	0	5,10,12	1.24	1 (20%)
1	HYP	A	1857	1	7,8,9	0.57	0	5,10,12	1.34	1 (20%)
2	HYP	I	33	2	7,8,9	0.51	0	5,10,12	1.27	1 (20%)
1	HYP	A	1902	1	7,8,9	0.61	0	5,10,12	1.63	1 (20%)
1	HYP	F	1873	1	7,8,9	0.46	0	5,10,12	1.29	1 (20%)
1	HYP	A	1906	1	7,8,9	0.59	0	5,10,12	1.39	1 (20%)
2	HYP	G	2	2	7,8,9	0.55	0	5,10,12	1.66	2 (40%)
2	HYP	I	29	2	7,8,9	0.54	0	5,10,12	1.22	1 (20%)
1	HYP	B	1855	1	7,8,9	0.54	0	5,10,12	1.20	1 (20%)
1	HYP	B	1930	1	7,8,9	0.60	0	5,10,12	1.65	1 (20%)
2	HYP	I	1	2	7,8,9	0.50	0	5,10,12	1.27	1 (20%)
2	HYP	H	42	2	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	F	1906	1	7,8,9	0.55	0	5,10,12	1.33	1 (20%)
1	HYP	C	1898	1	7,8,9	0.56	0	5,10,12	1.22	1 (20%)
1	HYP	E	1907	1	7,8,9	0.54	0	5,10,12	1.67	2 (40%)
2	HYP	G	6	2	7,8,9	0.49	0	5,10,12	1.54	1 (20%)
1	HYP	C	1915	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
1	HYP	E	1901	1	7,8,9	0.55	0	5,10,12	1.44	1 (20%)
1	HYP	B	1920	1	7,8,9	0.57	0	5,10,12	1.39	1 (20%)
1	HYP	B	1885	1	7,8,9	0.58	0	5,10,12	1.19	1 (20%)
1	HYP	B	1899	1	7,8,9	0.64	0	5,10,12	1.47	1 (20%)
1	HYP	B	1918	1	7,8,9	0.61	0	5,10,12	1.62	1 (20%)
1	HYP	A	1872	1	7,8,9	0.53	0	5,10,12	1.33	1 (20%)
1	HYP	E	1927	1	7,8,9	0.55	0	5,10,12	1.22	1 (20%)
2	HYP	G	37	2	7,8,9	0.55	0	5,10,12	0.98	1 (20%)
1	HYP	E	1875	1	7,8,9	0.55	0	5,10,12	1.20	1 (20%)
1	HYP	C	1922	1	7,8,9	0.57	0	5,10,12	1.49	1 (20%)
1	HYP	C	1914	1	7,8,9	0.53	0	5,10,12	1.44	1 (20%)
1	HYP	B	1882	1	7,8,9	0.53	0	5,10,12	1.24	1 (20%)
1	HYP	A	1930	1	7,8,9	0.58	0	5,10,12	1.69	1 (20%)
1	HYP	E	1866	1	7,8,9	0.59	0	5,10,12	1.43	1 (20%)
1	HYP	B	1902	1	7,8,9	0.59	0	5,10,12	1.62	1 (20%)
1	HYP	F	1875	1	7,8,9	0.55	0	5,10,12	1.18	1 (20%)
1	HYP	E	1905	1	7,8,9	0.55	0	5,10,12	1.26	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HYP	G	51	2	7,8,9	0.57	0	5,10,12	1.62	1 (20%)
1	HYP	A	1908	1	7,8,9	0.52	0	5,10,12	2.25	3 (60%)
1	HYP	F	1878	1	7,8,9	0.57	0	5,10,12	1.57	2 (40%)
1	HYP	B	1893	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	C	1929	1	7,8,9	0.63	0	5,10,12	1.30	1 (20%)
1	HYP	C	1928	1	7,8,9	0.61	0	5,10,12	1.30	1 (20%)
1	HYP	D	1898	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	F	1866	1	7,8,9	0.57	0	5,10,12	1.37	1 (20%)
1	HYP	C	1921	1	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
2	HYP	H	37	2	7,8,9	0.56	0	5,10,12	1.16	1 (20%)
1	HYP	D	1912	1	7,8,9	0.56	0	5,10,12	1.33	1 (20%)
1	HYP	A	1888	1	7,8,9	0.54	0	5,10,12	1.55	1 (20%)
2	HYP	I	6	2	7,8,9	0.53	0	5,10,12	1.32	1 (20%)
1	HYP	D	1915	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
1	HYP	A	1932	1	7,8,9	0.54	0	5,10,12	1.82	3 (60%)
1	HYP	D	1929	1	7,8,9	0.59	0	5,10,12	1.24	1 (20%)
1	HYP	F	1897	1	7,8,9	0.55	0	5,10,12	1.30	1 (20%)
2	HYP	H	51	2	7,8,9	0.53	0	5,10,12	1.64	1 (20%)
1	HYP	D	1899	1	7,8,9	0.52	0	5,10,12	1.73	2 (40%)
1	HYP	E	1878	1	7,8,9	0.51	0	5,10,12	1.96	2 (40%)
1	HYP	A	1897	1	7,8,9	0.55	0	5,10,12	1.29	1 (20%)
1	HYP	A	1922	1	7,8,9	0.61	0	5,10,12	1.76	1 (20%)
1	HYP	A	1875	1	7,8,9	0.58	0	5,10,12	1.21	1 (20%)
1	HYP	E	1894	1	7,8,9	0.59	0	5,10,12	1.29	1 (20%)
1	HYP	B	1862	1	7,8,9	0.53	0	5,10,12	1.48	1 (20%)
2	HYP	I	8	2	7,8,9	0.55	0	5,10,12	1.52	1 (20%)
2	HYP	G	10	2	7,8,9	0.62	0	5,10,12	1.67	1 (20%)
1	HYP	F	1911	1	7,8,9	0.54	0	5,10,12	1.18	1 (20%)
2	HYP	G	7	2	7,8,9	0.63	0	5,10,12	1.41	1 (20%)
1	HYP	C	1932	1	7,8,9	0.55	0	5,10,12	1.89	2 (40%)
1	HYP	B	1868	1	7,8,9	0.52	0	5,10,12	2.03	3 (60%)
1	HYP	B	1916	1	7,8,9	0.58	0	5,10,12	1.47	1 (20%)
2	HYP	H	45	2	7,8,9	0.55	0	5,10,12	1.22	1 (20%)
1	HYP	D	1903	1	7,8,9	0.57	0	5,10,12	1.78	2 (40%)
2	HYP	G	3	2	7,8,9	0.56	0	5,10,12	1.64	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	E	1931	1	7,8,9	0.55	0	5,10,12	1.35	1 (20%)
2	HYP	I	34	2	7,8,9	0.52	0	5,10,12	1.63	1 (20%)
1	HYP	B	1912	1	7,8,9	0.59	0	5,10,12	1.28	1 (20%)
1	HYP	E	1928	1	7,8,9	0.54	0	5,10,12	1.25	1 (20%)
1	HYP	D	1928	1	7,8,9	0.57	0	5,10,12	1.16	1 (20%)
1	HYP	F	1931	1	7,8,9	0.54	0	5,10,12	1.39	1 (20%)
1	HYP	E	1857	1	7,8,9	0.54	0	5,10,12	1.59	1 (20%)
2	HYP	I	9	2	7,8,9	0.52	0	5,10,12	1.58	1 (20%)
1	HYP	A	1855	1	7,8,9	0.61	0	5,10,12	1.20	1 (20%)
1	HYP	E	1890	1	7,8,9	0.55	0	5,10,12	1.15	1 (20%)
1	HYP	A	1873	1	7,8,9	0.50	0	5,10,12	1.23	1 (20%)
1	HYP	C	1902	1	7,8,9	0.57	0	5,10,12	1.81	2 (40%)
2	HYP	H	49	2	7,8,9	0.59	0	5,10,12	1.49	1 (20%)
1	HYP	A	1860	1	7,8,9	0.53	0	5,10,12	1.82	3 (60%)
1	HYP	C	1923	1	7,8,9	0.57	0	5,10,12	1.99	3 (60%)
2	HYP	I	32	2	7,8,9	0.50	0	5,10,12	1.18	1 (20%)
2	HYP	H	46	2	7,8,9	0.51	0	5,10,12	1.63	1 (20%)
2	HYP	H	44	2	7,8,9	0.54	0	5,10,12	1.67	1 (20%)
1	HYP	B	1863	1	7,8,9	0.54	0	5,10,12	1.45	1 (20%)
1	HYP	B	1880	1	7,8,9	0.54	0	5,10,12	1.38	1 (20%)
2	HYP	G	14	2	7,8,9	0.57	0	5,10,12	1.37	1 (20%)
2	HYP	H	47	2	7,8,9	0.59	0	5,10,12	1.30	1 (20%)
1	HYP	B	1878	1	7,8,9	0.54	0	5,10,12	1.88	2 (40%)
1	HYP	F	1864	1	7,8,9	0.55	0	5,10,12	1.45	1 (20%)
1	HYP	B	1923	1	7,8,9	0.57	0	5,10,12	2.02	3 (60%)
1	HYP	A	1923	1	7,8,9	0.55	0	5,10,12	1.93	3 (60%)
2	HYP	G	55	2	7,8,9	0.53	0	5,10,12	1.21	1 (20%)
1	HYP	B	1922	1	7,8,9	0.60	0	5,10,12	1.64	1 (20%)
1	HYP	E	1903	1	7,8,9	0.54	0	5,10,12	1.92	3 (60%)
1	HYP	B	1932	1	7,8,9	0.54	0	5,10,12	1.57	1 (20%)
1	HYP	F	1922	1	7,8,9	0.60	0	5,10,12	1.60	1 (20%)
1	HYP	A	1863	1	7,8,9	0.49	0	5,10,12	1.38	1 (20%)
1	HYP	A	1927	1	7,8,9	0.55	0	5,10,12	1.43	1 (20%)
1	HYP	F	1880	1	7,8,9	0.53	0	5,10,12	1.44	1 (20%)
1	HYP	D	1927	1	7,8,9	0.55	0	5,10,12	1.23	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	E	1872	1	7,8,9	0.59	0	5,10,12	1.29	1 (20%)
2	HYP	G	44	2	7,8,9	0.56	0	5,10,12	1.55	1 (20%)
1	HYP	D	1913	1	7,8,9	0.56	0	5,10,12	1.26	1 (20%)
2	HYP	G	42	2	7,8,9	0.61	0	5,10,12	1.29	1 (20%)
1	HYP	D	1902	1	7,8,9	0.52	0	5,10,12	1.77	2 (40%)
1	HYP	C	1908	1	7,8,9	0.54	0	5,10,12	1.96	3 (60%)
1	HYP	F	1901	1	7,8,9	0.53	0	5,10,12	1.18	1 (20%)
1	HYP	F	1908	1	7,8,9	0.57	0	5,10,12	1.84	2 (40%)
2	HYP	I	11	2	7,8,9	0.50	0	5,10,12	1.84	2 (40%)
1	HYP	C	1920	1	7,8,9	0.56	0	5,10,12	1.49	1 (20%)
1	HYP	F	1860	1	7,8,9	0.59	0	5,10,12	1.59	2 (40%)
1	HYP	F	1867	1	7,8,9	0.54	0	5,10,12	1.67	1 (20%)
1	HYP	A	1907	1	7,8,9	0.53	0	5,10,12	1.91	2 (40%)
1	HYP	D	1906	1	7,8,9	0.54	0	5,10,12	1.37	1 (20%)
1	HYP	A	1901	1	7,8,9	0.58	0	5,10,12	1.19	1 (20%)
1	HYP	F	1856	1	7,8,9	0.56	0	5,10,12	1.37	1 (20%)
2	HYP	I	14	2	7,8,9	0.57	0	5,10,12	1.31	1 (20%)
1	HYP	D	1901	1	7,8,9	0.56	0	5,10,12	1.22	1 (20%)
1	HYP	F	1858	1	7,8,9	0.57	0	5,10,12	1.72	2 (40%)
1	HYP	C	1930	1	7,8,9	0.60	0	5,10,12	1.76	2 (40%)
1	HYP	E	1897	1	7,8,9	0.52	0	5,10,12	1.22	1 (20%)
2	HYP	H	55	2	7,8,9	0.52	0	5,10,12	1.22	1 (20%)
1	HYP	F	1903	1	7,8,9	0.57	0	5,10,12	1.74	2 (40%)
1	HYP	C	1907	1	7,8,9	0.55	0	5,10,12	1.77	2 (40%)
1	HYP	B	1883	1	7,8,9	0.54	0	5,10,12	2.07	2 (40%)
2	HYP	H	41	2	7,8,9	0.54	0	5,10,12	1.30	1 (20%)
1	HYP	E	1885	1	7,8,9	0.53	0	5,10,12	1.41	1 (20%)
1	HYP	A	1864	1	7,8,9	0.54	0	5,10,12	1.50	1 (20%)
2	HYP	G	4	2	7,8,9	0.59	0	5,10,12	1.40	1 (20%)
1	HYP	A	1905	1	7,8,9	0.60	0	5,10,12	1.24	1 (20%)
1	HYP	B	1872	1	7,8,9	0.49	0	5,10,12	1.35	1 (20%)
1	HYP	E	1913	1	7,8,9	0.56	0	5,10,12	1.22	1 (20%)
1	HYP	F	1907	1	7,8,9	0.55	0	5,10,12	1.78	3 (60%)
1	HYP	D	1930	1	7,8,9	0.63	0	5,10,12	1.30	1 (20%)
2	HYP	G	40	2	7,8,9	0.50	0	5,10,12	1.18	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	F	1920	1	7,8,9	0.56	0	5,10,12	1.58	2 (40%)
1	HYP	B	1906	1	7,8,9	0.59	0	5,10,12	1.20	1 (20%)
2	HYP	H	43	2	7,8,9	0.55	0	5,10,12	1.50	1 (20%)
1	HYP	B	1865	1	7,8,9	0.53	0	5,10,12	1.71	1 (20%)
1	HYP	F	1913	1	7,8,9	0.55	0	5,10,12	1.28	1 (20%)
2	HYP	G	23	2	7,8,9	0.44	0	5,10,12	1.51	1 (20%)
1	HYP	A	1920	1	7,8,9	0.55	0	5,10,12	1.58	1 (20%)
1	HYP	E	1917	1	7,8,9	0.56	0	5,10,12	1.40	1 (20%)
1	HYP	E	1883	1	7,8,9	0.55	0	5,10,12	2.08	2 (40%)
2	HYP	I	5	2	7,8,9	0.55	0	5,10,12	1.47	1 (20%)
2	HYP	G	34	2	7,8,9	0.51	0	5,10,12	1.70	2 (40%)
1	HYP	E	1868	1	7,8,9	0.57	0	5,10,12	1.83	2 (40%)
1	HYP	B	1903	1	7,8,9	0.57	0	5,10,12	1.97	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	C	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1880	1	-	0/0/11/13	0/1/1/1
2	HYP	G	9	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	G	33	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1870	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	G	56	2	-	0/0/11/13	0/1/1/1
2	HYP	G	46	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1917	1	-	0/0/11/13	0/1/1/1
2	HYP	G	32	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1929	1	-	0/0/11/13	0/1/1/1
2	HYP	G	1	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1897	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	I	2	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1855	1	-	0/0/11/13	0/1/1/1
2	HYP	G	41	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1885	1	-	0/0/11/13	0/1/1/1
2	HYP	G	5	2	-	0/0/11/13	0/1/1/1
2	HYP	G	17	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1911	1	-	0/0/11/13	0/1/1/1
2	HYP	H	48	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	G	8	2	-	0/0/11/13	0/1/1/1
2	HYP	G	43	2	-	0/0/11/13	0/1/1/1
2	HYP	I	7	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1908	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1864	1	-	0/0/11/13	0/1/1/1
2	HYP	G	49	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1927	1	-	0/0/11/13	0/1/1/1
2	HYP	G	29	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	G	47	2	-	0/0/11/13	0/1/1/1
2	HYP	G	45	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1922	1	-	0/0/11/13	0/1/1/1
2	HYP	I	4	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	H	52	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1910	1	-	0/0/11/13	0/1/1/1
2	HYP	G	50	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1882	1	-	0/0/11/13	0/1/1/1
2	HYP	H	40	2	-	0/0/11/13	0/1/1/1
2	HYP	I	23	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	B	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1898	1	-	0/0/11/13	0/1/1/1
2	HYP	H	56	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1921	1	-	0/0/11/13	0/1/1/1
2	HYP	G	11	2	-	0/0/11/13	0/1/1/1
2	HYP	I	3	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1858	1	-	0/0/11/13	0/1/1/1
2	HYP	G	26	2	1/1/2/4	0/0/11/13	0/1/1/1
2	HYP	I	20	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1873	1	-	0/0/11/13	0/1/1/1
2	HYP	I	10	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1922	1	-	0/0/11/13	0/1/1/1
2	HYP	G	48	2	-	0/0/11/13	0/1/1/1
2	HYP	G	20	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	G	52	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1917	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1862	1	-	0/0/11/13	0/1/1/1
2	HYP	H	50	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1857	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1916	1	-	0/0/11/13	0/1/1/1
2	HYP	I	26	2	1/1/2/4	0/0/11/13	0/1/1/1
2	HYP	I	17	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	I	33	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1906	1	-	0/0/11/13	0/1/1/1
2	HYP	G	2	2	-	0/0/11/13	0/1/1/1
2	HYP	I	29	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	I	1	2	-	0/0/11/13	0/1/1/1
2	HYP	H	42	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1907	1	-	0/0/11/13	0/1/1/1
2	HYP	G	6	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1927	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	G	37	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1905	1	-	0/0/11/13	0/1/1/1
2	HYP	G	51	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1921	1	-	0/0/11/13	0/1/1/1
2	HYP	H	37	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1888	1	-	0/0/11/13	0/1/1/1
2	HYP	I	6	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	H	51	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1862	1	-	0/0/11/13	0/1/1/1
2	HYP	I	8	2	-	0/0/11/13	0/1/1/1
2	HYP	G	10	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1911	1	-	0/0/11/13	0/1/1/1
2	HYP	G	7	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1916	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	H	45	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1903	1	-	0/0/11/13	0/1/1/1
2	HYP	G	3	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	I	34	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	I	9	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1902	1	-	0/0/11/13	0/1/1/1
2	HYP	H	49	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	I	32	2	-	0/0/11/13	0/1/1/1
2	HYP	H	46	2	-	0/0/11/13	0/1/1/1
2	HYP	H	44	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1880	1	-	0/0/11/13	0/1/1/1
2	HYP	G	14	2	-	0/0/11/13	0/1/1/1
2	HYP	H	47	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	G	55	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1872	1	-	0/0/11/13	0/1/1/1
2	HYP	G	44	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	G	42	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	D	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	I	11	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1856	1	-	0/0/11/13	0/1/1/1
2	HYP	I	14	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	H	55	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1883	1	-	0/0/11/13	0/1/1/1
2	HYP	H	41	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1864	1	-	0/0/11/13	0/1/1/1
2	HYP	G	4	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	G	40	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1906	1	-	0/0/11/13	0/1/1/1
2	HYP	H	43	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	G	23	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	A	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1883	1	-	0/0/11/13	0/1/1/1
2	HYP	I	5	2	-	0/0/11/13	0/1/1/1
2	HYP	G	34	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1903	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (454) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1883	HYP	CG-CB-CA	-3.64	99.55	103.75
1	A	1883	HYP	CG-CB-CA	-3.60	99.59	103.75
1	E	1923	HYP	CG-CB-CA	-3.50	99.71	103.75
1	F	1918	HYP	CG-CB-CA	-3.43	99.79	103.75
1	B	1883	HYP	CG-CB-CA	-3.39	99.84	103.75
1	F	1883	HYP	CG-CB-CA	-3.29	99.95	103.75
1	A	1908	HYP	CG-CB-CA	-3.24	100.00	103.75
2	G	11	HYP	CG-CB-CA	-3.17	100.09	103.75
1	F	1894	HYP	CG-CB-CA	-3.12	100.14	103.75
1	B	1894	HYP	CG-CB-CA	-3.08	100.19	103.75
1	F	1923	HYP	CG-CB-CA	-3.06	100.22	103.75
1	F	1888	HYP	CG-CB-CA	-3.05	100.22	103.75
1	B	1868	HYP	CG-CB-CA	-3.01	100.27	103.75
1	A	1907	HYP	CG-CB-CA	-3.01	100.27	103.75
1	E	1888	HYP	CG-CB-CA	-3.00	100.28	103.75
2	I	10	HYP	O-C-CA	-2.98	117.10	124.77
2	I	34	HYP	O-C-CA	-2.98	117.11	124.77
2	G	10	HYP	O-C-CA	-2.97	117.12	124.77
1	A	1908	HYP	O-C-CA	-2.92	117.25	124.77
2	I	11	HYP	CG-CB-CA	-2.92	100.37	103.75
1	B	1908	HYP	O-C-CA	-2.91	117.29	124.77
1	F	1868	HYP	CG-CB-CA	-2.88	100.42	103.75
1	B	1907	HYP	O-C-CA	-2.88	117.37	124.77
1	E	1867	HYP	O-C-CA	-2.86	117.42	124.77
1	E	1878	HYP	CG-CB-CA	-2.86	100.45	103.75
1	E	1908	HYP	CG-CB-CA	-2.83	100.48	103.75
1	F	1857	HYP	O-C-CA	-2.83	117.49	124.77
1	A	1922	HYP	O-C-CA	-2.83	117.50	124.77
2	G	4	HYP	O-C-CA	-2.82	117.52	124.77
1	E	1860	HYP	CG-CB-CA	-2.81	100.50	103.75
1	D	1906	HYP	O-C-CA	-2.81	117.55	124.77
1	A	1907	HYP	O-C-CA	-2.81	117.55	124.77
1	B	1931	HYP	O-C-CA	-2.80	117.57	124.77
1	E	1868	HYP	O-C-CA	-2.79	117.60	124.77
1	B	1917	HYP	O-C-CA	-2.79	117.60	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1865	HYP	O-C-CA	-2.78	117.62	124.77
1	B	1872	HYP	O-C-CA	-2.77	117.63	124.77
1	A	1865	HYP	O-C-CA	-2.77	117.64	124.77
1	B	1858	HYP	O-C-CA	-2.77	117.64	124.77
1	D	1918	HYP	O-C-CA	-2.77	117.64	124.77
1	A	1917	HYP	O-C-CA	-2.76	117.67	124.77
1	F	1893	HYP	O-C-CA	-2.75	117.69	124.77
1	B	1914	HYP	O-C-CA	-2.75	117.70	124.77
1	E	1858	HYP	O-C-CA	-2.75	117.70	124.77
1	F	1868	HYP	O-C-CA	-2.75	117.70	124.77
1	F	1880	HYP	O-C-CA	-2.75	117.70	124.77
1	B	1902	HYP	O-C-CA	-2.74	117.72	124.77
1	A	1902	HYP	O-C-CA	-2.74	117.73	124.77
1	B	1923	HYP	O-C-CA	-2.74	117.73	124.77
1	A	1931	HYP	O-C-CA	-2.73	117.74	124.77
2	I	5	HYP	O-C-CA	-2.73	117.74	124.77
1	E	1865	HYP	O-C-CA	-2.73	117.74	124.77
1	F	1864	HYP	O-C-CA	-2.73	117.75	124.77
1	B	1932	HYP	O-C-CA	-2.73	117.75	124.77
1	A	1868	HYP	O-C-CA	-2.73	117.75	124.77
2	H	44	HYP	O-C-CA	-2.73	117.76	124.77
1	E	1857	HYP	O-C-CA	-2.73	117.76	124.77
1	C	1932	HYP	O-C-CA	-2.72	117.77	124.77
1	C	1930	HYP	O-C-CA	-2.72	117.77	124.77
1	A	1923	HYP	O-C-CA	-2.72	117.77	124.77
1	E	1916	HYP	O-C-CA	-2.72	117.78	124.77
1	E	1908	HYP	O-C-CA	-2.72	117.78	124.77
1	F	1863	HYP	O-C-CA	-2.72	117.78	124.77
1	E	1864	HYP	O-C-CA	-2.72	117.78	124.77
2	G	3	HYP	O-C-CA	-2.71	117.80	124.77
1	F	1877	HYP	O-C-CA	-2.71	117.80	124.77
1	A	1916	HYP	O-C-CA	-2.71	117.81	124.77
1	C	1923	HYP	CG-CB-CA	-2.70	100.63	103.75
1	E	1903	HYP	CG-CB-CA	-2.70	100.63	103.75
2	G	11	HYP	O-C-CA	-2.70	117.83	124.77
2	G	42	HYP	O-C-CA	-2.70	117.83	124.77
1	A	1880	HYP	O-C-CA	-2.70	117.84	124.77
1	D	1908	HYP	O-C-CA	-2.70	117.84	124.77
1	A	1894	HYP	O-C-CA	-2.69	117.84	124.77
1	A	1893	HYP	O-C-CA	-2.69	117.84	124.77
1	B	1908	HYP	CG-CB-CA	-2.69	100.64	103.75
1	F	1931	HYP	O-C-CA	-2.69	117.86	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1902	HYP	O-C-CA	-2.69	117.86	124.77
1	B	1865	HYP	O-C-CA	-2.69	117.86	124.77
1	D	1931	HYP	O-C-CA	-2.68	117.87	124.77
1	C	1923	HYP	O-C-CA	-2.68	117.89	124.77
1	B	1922	HYP	O-C-CA	-2.68	117.89	124.77
2	G	43	HYP	O-C-CA	-2.67	117.89	124.77
2	H	43	HYP	O-C-CA	-2.67	117.90	124.77
1	D	1921	HYP	O-C-CA	-2.67	117.90	124.77
2	G	8	HYP	O-C-CA	-2.67	117.90	124.77
1	B	1878	HYP	O-C-CA	-2.67	117.91	124.77
1	E	1922	HYP	O-C-CA	-2.67	117.91	124.77
1	F	1858	HYP	O-C-CA	-2.67	117.91	124.77
1	B	1915	HYP	O-C-CA	-2.67	117.91	124.77
1	B	1887	HYP	O-C-CA	-2.67	117.91	124.77
1	A	1857	HYP	O-C-CA	-2.67	117.92	124.77
2	G	45	HYP	O-C-CA	-2.66	117.92	124.77
2	H	51	HYP	O-C-CA	-2.66	117.92	124.77
1	A	1894	HYP	CG-CB-CA	-2.66	100.68	103.75
1	C	1907	HYP	O-C-CA	-2.66	117.93	124.77
1	A	1918	HYP	O-C-CA	-2.66	117.94	124.77
2	I	3	HYP	O-C-CA	-2.66	117.94	124.77
2	I	8	HYP	O-C-CA	-2.66	117.94	124.77
1	B	1913	HYP	O-C-CA	-2.66	117.94	124.77
2	H	49	HYP	O-C-CA	-2.65	117.94	124.77
1	A	1899	HYP	O-C-CA	-2.65	117.95	124.77
1	A	1914	HYP	O-C-CA	-2.65	117.95	124.77
1	B	1863	HYP	O-C-CA	-2.65	117.95	124.77
1	E	1907	HYP	O-C-CA	-2.65	117.95	124.77
1	F	1902	HYP	O-C-CA	-2.65	117.95	124.77
1	B	1899	HYP	O-C-CA	-2.65	117.96	124.77
1	F	1855	HYP	O-C-CA	-2.65	117.96	124.77
2	I	4	HYP	O-C-CA	-2.65	117.96	124.77
2	G	51	HYP	O-C-CA	-2.65	117.96	124.77
1	A	1866	HYP	O-C-CA	-2.65	117.96	124.77
1	E	1918	HYP	O-C-CA	-2.65	117.96	124.77
1	E	1877	HYP	O-C-CA	-2.65	117.96	124.77
1	A	1927	HYP	O-C-CA	-2.65	117.97	124.77
1	C	1931	HYP	O-C-CA	-2.65	117.97	124.77
1	F	1906	HYP	O-C-CA	-2.64	117.97	124.77
1	B	1903	HYP	O-C-CA	-2.64	117.97	124.77
1	E	1863	HYP	O-C-CA	-2.64	117.97	124.77
1	F	1922	HYP	O-C-CA	-2.64	117.97	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1918	HYP	CG-CB-CA	-2.64	100.70	103.75
1	F	1914	HYP	O-C-CA	-2.64	117.97	124.77
1	F	1866	HYP	O-C-CA	-2.64	117.97	124.77
1	A	1903	HYP	O-C-CA	-2.64	117.98	124.77
1	A	1862	HYP	O-C-CA	-2.64	117.99	124.77
1	A	1864	HYP	O-C-CA	-2.64	117.99	124.77
1	C	1908	HYP	O-C-CA	-2.63	118.00	124.77
1	F	1873	HYP	O-C-CA	-2.63	118.00	124.77
1	D	1915	HYP	O-C-CA	-2.63	118.00	124.77
1	F	1899	HYP	O-C-CA	-2.63	118.00	124.77
1	D	1923	HYP	O-C-CA	-2.63	118.00	124.77
1	F	1862	HYP	O-C-CA	-2.63	118.00	124.77
1	B	1916	HYP	O-C-CA	-2.63	118.01	124.77
1	B	1921	HYP	O-C-CA	-2.63	118.02	124.77
1	D	1922	HYP	O-C-CA	-2.63	118.02	124.77
2	G	49	HYP	O-C-CA	-2.63	118.02	124.77
1	A	1930	HYP	O-C-CA	-2.62	118.02	124.77
1	E	1902	HYP	O-C-CA	-2.62	118.02	124.77
1	C	1899	HYP	O-C-CA	-2.62	118.02	124.77
1	A	1888	HYP	O-C-CA	-2.62	118.03	124.77
1	A	1872	HYP	O-C-CA	-2.62	118.03	124.77
1	E	1862	HYP	O-C-CA	-2.62	118.03	124.77
2	G	9	HYP	CG-CB-CA	-2.62	100.72	103.75
1	B	1930	HYP	O-C-CA	-2.62	118.04	124.77
1	F	1856	HYP	O-C-CA	-2.62	118.04	124.77
1	F	1872	HYP	O-C-CA	-2.62	118.04	124.77
1	F	1907	HYP	O-C-CA	-2.62	118.04	124.77
1	A	1921	HYP	O-C-CA	-2.62	118.04	124.77
1	F	1867	HYP	O-C-CA	-2.62	118.04	124.77
1	E	1880	HYP	O-C-CA	-2.61	118.05	124.77
2	G	46	HYP	O-C-CA	-2.61	118.05	124.77
2	H	46	HYP	O-C-CA	-2.61	118.05	124.77
2	H	41	HYP	O-C-CA	-2.61	118.06	124.77
1	B	1918	HYP	O-C-CA	-2.61	118.06	124.77
1	D	1898	HYP	O-C-CA	-2.61	118.07	124.77
2	H	42	HYP	O-C-CA	-2.60	118.07	124.77
1	A	1890	HYP	O-C-CA	-2.60	118.08	124.77
1	B	1857	HYP	O-C-CA	-2.60	118.08	124.77
2	G	2	HYP	O-C-CA	-2.60	118.08	124.77
1	B	1856	HYP	O-C-CA	-2.60	118.08	124.77
2	G	47	HYP	O-C-CA	-2.60	118.09	124.77
1	D	1907	HYP	O-C-CA	-2.60	118.09	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1930	HYP	O-C-CA	-2.60	118.09	124.77
1	E	1872	HYP	O-C-CA	-2.60	118.09	124.77
1	F	1915	HYP	O-C-CA	-2.60	118.09	124.77
1	E	1912	HYP	O-C-CA	-2.60	118.09	124.77
1	D	1913	HYP	O-C-CA	-2.59	118.10	124.77
1	C	1917	HYP	O-C-CA	-2.59	118.10	124.77
1	B	1928	HYP	O-C-CA	-2.59	118.10	124.77
1	C	1918	HYP	O-C-CA	-2.59	118.11	124.77
1	A	1887	HYP	O-C-CA	-2.59	118.11	124.77
1	C	1902	HYP	O-C-CA	-2.59	118.11	124.77
1	E	1914	HYP	O-C-CA	-2.59	118.11	124.77
1	D	1916	HYP	O-C-CA	-2.59	118.11	124.77
1	C	1914	HYP	O-C-CA	-2.59	118.11	124.77
1	E	1866	HYP	O-C-CA	-2.59	118.11	124.77
1	A	1877	HYP	O-C-CA	-2.59	118.11	124.77
1	B	1880	HYP	O-C-CA	-2.59	118.11	124.77
1	E	1918	HYP	CG-CB-CA	-2.59	100.76	103.75
1	B	1893	HYP	O-C-CA	-2.59	118.11	124.77
1	D	1899	HYP	O-C-CA	-2.59	118.11	124.77
2	I	20	HYP	O-C-CA	-2.59	118.12	124.77
1	E	1887	HYP	O-C-CA	-2.58	118.12	124.77
2	I	6	HYP	O-C-CA	-2.58	118.12	124.77
2	G	52	HYP	O-C-CA	-2.58	118.12	124.77
1	F	1913	HYP	O-C-CA	-2.58	118.13	124.77
1	F	1908	HYP	O-C-CA	-2.58	118.13	124.77
1	A	1915	HYP	O-C-CA	-2.58	118.13	124.77
1	B	1877	HYP	O-C-CA	-2.58	118.13	124.77
1	E	1885	HYP	O-C-CA	-2.58	118.14	124.77
1	F	1897	HYP	O-C-CA	-2.58	118.14	124.77
2	G	14	HYP	O-C-CA	-2.58	118.14	124.77
1	A	1868	HYP	CG-CB-CA	-2.58	100.77	103.75
2	G	7	HYP	O-C-CA	-2.58	118.14	124.77
1	E	1888	HYP	O-C-CA	-2.58	118.14	124.77
1	F	1928	HYP	O-C-CA	-2.58	118.15	124.77
1	A	1883	HYP	O-C-CA	-2.57	118.15	124.77
1	C	1921	HYP	O-C-CA	-2.57	118.15	124.77
1	F	1885	HYP	O-C-CA	-2.57	118.15	124.77
1	A	1898	HYP	O-C-CA	-2.57	118.15	124.77
1	D	1927	HYP	O-C-CA	-2.57	118.16	124.77
1	E	1856	HYP	O-C-CA	-2.57	118.16	124.77
1	D	1903	HYP	O-C-CA	-2.57	118.16	124.77
1	C	1915	HYP	O-C-CA	-2.57	118.16	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	56	HYP	O-C-CA	-2.57	118.17	124.77
1	A	1875	HYP	O-C-CA	-2.57	118.17	124.77
1	B	1927	HYP	O-C-CA	-2.57	118.17	124.77
1	B	1888	HYP	O-C-CA	-2.56	118.18	124.77
1	C	1929	HYP	O-C-CA	-2.56	118.18	124.77
1	F	1923	HYP	O-C-CA	-2.56	118.18	124.77
2	H	56	HYP	O-C-CA	-2.56	118.18	124.77
1	C	1903	HYP	O-C-CA	-2.56	118.19	124.77
1	E	1923	HYP	O-C-CA	-2.56	118.19	124.77
1	B	1878	HYP	CG-CB-CA	-2.56	100.79	103.75
1	E	1921	HYP	O-C-CA	-2.56	118.19	124.77
1	A	1855	HYP	O-C-CA	-2.56	118.19	124.77
1	B	1898	HYP	O-C-CA	-2.56	118.19	124.77
1	E	1882	HYP	O-C-CA	-2.56	118.19	124.77
1	C	1908	HYP	CG-CB-CA	-2.56	100.80	103.75
1	E	1928	HYP	O-C-CA	-2.55	118.20	124.77
1	F	1894	HYP	O-C-CA	-2.55	118.20	124.77
1	B	1882	HYP	O-C-CA	-2.55	118.20	124.77
2	G	33	HYP	O-C-CA	-2.55	118.20	124.77
2	G	44	HYP	O-C-CA	-2.55	118.20	124.77
1	C	1927	HYP	O-C-CA	-2.55	118.20	124.77
1	C	1897	HYP	O-C-CA	-2.55	118.20	124.77
1	E	1893	HYP	O-C-CA	-2.55	118.21	124.77
1	B	1867	HYP	O-C-CA	-2.55	118.21	124.77
1	C	1922	HYP	O-C-CA	-2.55	118.21	124.77
1	E	1873	HYP	O-C-CA	-2.55	118.21	124.77
1	E	1905	HYP	O-C-CA	-2.55	118.22	124.77
1	A	1892	HYP	O-C-CA	-2.55	118.22	124.77
1	C	1913	HYP	O-C-CA	-2.55	118.22	124.77
1	A	1885	HYP	O-C-CA	-2.55	118.22	124.77
1	B	1894	HYP	O-C-CA	-2.55	118.22	124.77
2	G	6	HYP	O-C-CA	-2.55	118.22	124.77
2	I	14	HYP	O-C-CA	-2.55	118.22	124.77
1	A	1929	HYP	O-C-CA	-2.55	118.22	124.77
1	A	1911	HYP	O-C-CA	-2.54	118.22	124.77
1	E	1911	HYP	O-C-CA	-2.54	118.23	124.77
1	A	1897	HYP	O-C-CA	-2.54	118.23	124.77
2	G	20	HYP	O-C-CA	-2.54	118.23	124.77
1	A	1863	HYP	O-C-CA	-2.54	118.23	124.77
1	E	1929	HYP	O-C-CA	-2.54	118.23	124.77
1	F	1888	HYP	O-C-CA	-2.54	118.23	124.77
1	F	1892	HYP	O-C-CA	-2.54	118.24	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1929	HYP	O-C-CA	-2.54	118.24	124.77
1	E	1931	HYP	O-C-CA	-2.54	118.24	124.77
1	F	1929	HYP	O-C-CA	-2.54	118.24	124.77
1	A	1906	HYP	O-C-CA	-2.54	118.24	124.77
2	I	17	HYP	O-C-CA	-2.54	118.25	124.77
1	F	1921	HYP	O-C-CA	-2.53	118.25	124.77
1	B	1862	HYP	O-C-CA	-2.53	118.26	124.77
1	F	1917	HYP	O-C-CA	-2.53	118.26	124.77
1	B	1923	HYP	CG-CB-CA	-2.53	100.83	103.75
2	G	48	HYP	O-C-CA	-2.53	118.26	124.77
1	D	1905	HYP	O-C-CA	-2.53	118.26	124.77
2	H	48	HYP	O-C-CA	-2.53	118.26	124.77
1	A	1882	HYP	O-C-CA	-2.53	118.27	124.77
1	B	1908	HYP	CB-CG-CD	-2.53	100.34	103.16
1	A	1913	HYP	O-C-CA	-2.53	118.27	124.77
2	I	1	HYP	O-C-CA	-2.53	118.27	124.77
1	B	1855	HYP	O-C-CA	-2.53	118.27	124.77
1	B	1883	HYP	O-C-CA	-2.53	118.28	124.77
1	E	1855	HYP	O-C-CA	-2.53	118.28	124.77
1	F	1930	HYP	O-C-CA	-2.52	118.28	124.77
1	E	1927	HYP	O-C-CA	-2.52	118.28	124.77
1	A	1912	HYP	O-C-CA	-2.52	118.29	124.77
1	C	1928	HYP	O-C-CA	-2.52	118.29	124.77
2	H	52	HYP	O-C-CA	-2.52	118.29	124.77
1	A	1856	HYP	O-C-CA	-2.52	118.30	124.77
1	E	1894	HYP	O-C-CA	-2.52	118.30	124.77
2	G	32	HYP	O-C-CA	-2.51	118.30	124.77
1	B	1903	HYP	CG-CB-CA	-2.51	100.85	103.75
1	B	1868	HYP	O-C-CA	-2.51	118.31	124.77
1	F	1916	HYP	O-C-CA	-2.51	118.31	124.77
2	I	11	HYP	O-C-CA	-2.51	118.31	124.77
1	C	1912	HYP	O-C-CA	-2.51	118.32	124.77
2	G	29	HYP	O-C-CA	-2.51	118.32	124.77
1	B	1905	HYP	O-C-CA	-2.51	118.32	124.77
1	B	1912	HYP	O-C-CA	-2.51	118.32	124.77
1	F	1918	HYP	O-C-CA	-2.51	118.32	124.77
2	G	41	HYP	O-C-CA	-2.51	118.32	124.77
1	B	1870	HYP	O-C-CA	-2.51	118.32	124.77
2	I	33	HYP	O-C-CA	-2.50	118.33	124.77
1	F	1903	HYP	O-C-CA	-2.50	118.33	124.77
1	E	1899	HYP	O-C-CA	-2.50	118.33	124.77
1	D	1911	HYP	O-C-CA	-2.50	118.34	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1932	HYP	O-C-CA	-2.50	118.34	124.77
1	E	1875	HYP	O-C-CA	-2.50	118.34	124.77
1	E	1908	HYP	CB-CG-CD	-2.50	100.37	103.16
1	B	1866	HYP	O-C-CA	-2.50	118.34	124.77
1	C	1932	HYP	CG-CB-CA	-2.50	100.86	103.75
2	G	26	HYP	O-C-CA	-2.50	118.35	124.77
1	E	1903	HYP	O-C-CA	-2.50	118.35	124.77
1	B	1890	HYP	O-C-CA	-2.49	118.36	124.77
2	H	50	HYP	O-C-CA	-2.49	118.36	124.77
1	A	1860	HYP	CG-CB-CA	-2.49	100.87	103.75
1	E	1898	HYP	O-C-CA	-2.49	118.37	124.77
1	E	1878	HYP	O-C-CA	-2.49	118.37	124.77
1	D	1912	HYP	O-C-CA	-2.49	118.37	124.77
1	F	1898	HYP	O-C-CA	-2.49	118.37	124.77
2	I	7	HYP	O-C-CA	-2.49	118.37	124.77
1	C	1906	HYP	O-C-CA	-2.49	118.38	124.77
2	G	17	HYP	O-C-CA	-2.49	118.38	124.77
2	I	29	HYP	O-C-CA	-2.48	118.38	124.77
1	B	1911	HYP	O-C-CA	-2.48	118.38	124.77
1	A	1905	HYP	O-C-CA	-2.48	118.39	124.77
1	A	1932	HYP	O-C-CA	-2.48	118.39	124.77
2	G	9	HYP	O-C-CA	-2.48	118.39	124.77
1	A	1867	HYP	O-C-CA	-2.48	118.39	124.77
1	C	1910	HYP	O-C-CA	-2.48	118.39	124.77
1	C	1905	HYP	O-C-CA	-2.48	118.39	124.77
2	H	47	HYP	O-C-CA	-2.48	118.39	124.77
1	B	1885	HYP	O-C-CA	-2.48	118.40	124.77
1	C	1911	HYP	O-C-CA	-2.48	118.40	124.77
1	A	1873	HYP	O-C-CA	-2.48	118.40	124.77
2	I	2	HYP	O-C-CA	-2.48	118.40	124.77
2	G	5	HYP	O-C-CA	-2.47	118.41	124.77
1	A	1858	HYP	O-C-CA	-2.47	118.42	124.77
1	B	1910	HYP	O-C-CA	-2.47	118.42	124.77
1	F	1932	HYP	O-C-CA	-2.47	118.42	124.77
1	F	1882	HYP	O-C-CA	-2.47	118.42	124.77
1	D	1917	HYP	O-C-CA	-2.47	118.42	124.77
2	G	50	HYP	O-C-CA	-2.46	118.43	124.77
1	D	1899	HYP	CG-CB-CA	-2.46	100.91	103.75
1	B	1901	HYP	O-C-CA	-2.46	118.44	124.77
1	B	1920	HYP	O-C-CA	-2.46	118.44	124.77
2	I	9	HYP	O-C-CA	-2.46	118.45	124.77
1	C	1898	HYP	O-C-CA	-2.46	118.45	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1883	HYP	O-C-CA	-2.46	118.45	124.77
1	D	1929	HYP	O-C-CA	-2.46	118.45	124.77
1	F	1905	HYP	O-C-CA	-2.45	118.46	124.77
1	E	1892	HYP	O-C-CA	-2.45	118.46	124.77
1	F	1911	HYP	O-C-CA	-2.45	118.46	124.77
1	A	1910	HYP	O-C-CA	-2.45	118.46	124.77
1	F	1875	HYP	O-C-CA	-2.45	118.47	124.77
1	F	1912	HYP	O-C-CA	-2.45	118.47	124.77
1	C	1920	HYP	O-C-CA	-2.45	118.48	124.77
2	H	55	HYP	O-C-CA	-2.44	118.48	124.77
1	E	1910	HYP	O-C-CA	-2.44	118.49	124.77
2	G	55	HYP	O-C-CA	-2.44	118.49	124.77
1	C	1916	HYP	O-C-CA	-2.44	118.49	124.77
1	E	1901	HYP	O-C-CA	-2.44	118.50	124.77
2	G	34	HYP	O-C-CA	-2.44	118.50	124.77
1	B	1875	HYP	O-C-CA	-2.44	118.50	124.77
2	G	40	HYP	O-C-CA	-2.44	118.50	124.77
1	D	1897	HYP	O-C-CA	-2.43	118.51	124.77
1	E	1917	HYP	O-C-CA	-2.43	118.51	124.77
2	I	32	HYP	O-C-CA	-2.43	118.52	124.77
1	B	1892	HYP	O-C-CA	-2.43	118.52	124.77
1	F	1878	HYP	O-C-CA	-2.43	118.52	124.77
1	A	1878	HYP	CG-CB-CA	-2.43	100.95	103.75
2	H	45	HYP	O-C-CA	-2.42	118.54	124.77
1	E	1907	HYP	CG-CB-CA	-2.42	100.96	103.75
1	B	1906	HYP	O-C-CA	-2.42	118.55	124.77
1	A	1901	HYP	O-C-CA	-2.41	118.56	124.77
1	F	1887	HYP	O-C-CA	-2.41	118.57	124.77
1	F	1890	HYP	O-C-CA	-2.41	118.57	124.77
1	E	1913	HYP	O-C-CA	-2.41	118.57	124.77
1	A	1928	HYP	O-C-CA	-2.41	118.57	124.77
1	D	1928	HYP	O-C-CA	-2.41	118.58	124.77
2	H	40	HYP	O-C-CA	-2.41	118.58	124.77
1	B	1864	HYP	O-C-CA	-2.41	118.58	124.77
1	B	1897	HYP	O-C-CA	-2.40	118.59	124.77
1	C	1903	HYP	CG-CB-CA	-2.40	100.98	103.75
1	E	1920	HYP	O-C-CA	-2.40	118.60	124.77
1	A	1920	HYP	O-C-CA	-2.40	118.61	124.77
1	F	1910	HYP	O-C-CA	-2.40	118.61	124.77
1	F	1927	HYP	O-C-CA	-2.39	118.61	124.77
1	F	1923	HYP	CB-CG-CD	-2.39	100.50	103.16
2	G	1	HYP	O-C-CA	-2.39	118.64	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1870	HYP	O-C-CA	-2.38	118.64	124.77
1	E	1932	HYP	O-C-CA	-2.38	118.64	124.77
1	A	1923	HYP	CG-CB-CA	-2.38	101.00	103.75
1	B	1873	HYP	O-C-CA	-2.37	118.66	124.77
1	E	1890	HYP	O-C-CA	-2.37	118.67	124.77
1	D	1920	HYP	O-C-CA	-2.37	118.68	124.77
1	B	1860	HYP	CG-CB-CA	-2.37	101.02	103.75
1	E	1915	HYP	O-C-CA	-2.36	118.69	124.77
2	I	26	HYP	O-C-CA	-2.36	118.70	124.77
2	H	37	HYP	O-C-CA	-2.36	118.70	124.77
1	E	1930	HYP	O-C-CA	-2.36	118.71	124.77
1	E	1897	HYP	O-C-CA	-2.36	118.71	124.77
1	E	1906	HYP	O-C-CA	-2.36	118.71	124.77
2	H	52	HYP	CG-CB-CA	-2.35	101.03	103.75
1	F	1908	HYP	CB-CG-CD	-2.35	100.54	103.16
2	G	34	HYP	CG-CB-CA	-2.35	101.03	103.75
1	D	1914	HYP	O-C-CA	-2.35	118.73	124.77
1	C	1901	HYP	O-C-CA	-2.35	118.74	124.77
1	E	1883	HYP	O-C-CA	-2.34	118.75	124.77
1	F	1860	HYP	O-C-CA	-2.33	118.77	124.77
1	D	1910	HYP	O-C-CA	-2.32	118.80	124.77
1	A	1860	HYP	O-C-CA	-2.32	118.81	124.77
1	D	1923	HYP	CG-CB-CA	-2.31	101.08	103.75
1	F	1920	HYP	O-C-CA	-2.31	118.82	124.77
1	B	1923	HYP	CB-CG-CD	-2.31	100.58	103.16
1	D	1932	HYP	CB-CG-CD	-2.30	100.59	103.16
1	A	1870	HYP	O-C-CA	-2.30	118.85	124.77
1	F	1901	HYP	O-C-CA	-2.30	118.86	124.77
1	E	1860	HYP	O-C-CA	-2.29	118.89	124.77
1	C	1918	HYP	CG-CB-CA	-2.28	101.11	103.75
2	G	23	HYP	O-C-CA	-2.28	118.90	124.77
1	C	1908	HYP	CB-CG-CD	-2.28	100.61	103.16
1	B	1903	HYP	CB-CG-CD	-2.28	100.62	103.16
1	A	1878	HYP	O-C-CA	-2.28	118.91	124.77
2	I	23	HYP	O-C-CA	-2.28	118.91	124.77
1	E	1870	HYP	O-C-CA	-2.28	118.91	124.77
1	B	1860	HYP	O-C-CA	-2.27	118.93	124.77
1	D	1901	HYP	O-C-CA	-2.25	118.97	124.77
1	E	1877	HYP	CG-CB-CA	-2.25	101.15	103.75
1	A	1932	HYP	CG-CB-CA	-2.25	101.15	103.75
1	D	1903	HYP	CB-CG-CD	-2.24	100.66	103.16
1	F	1932	HYP	CG-CB-CA	-2.24	101.16	103.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1902	HYP	CG-CB-CA	-2.22	101.19	103.75
1	F	1903	HYP	CB-CG-CD	-2.22	100.69	103.16
1	A	1903	HYP	CB-CG-CD	-2.21	100.70	103.16
1	D	1932	HYP	CG-CB-CA	-2.20	101.21	103.75
1	A	1908	HYP	CB-CG-CD	-2.19	100.72	103.16
1	A	1923	HYP	CB-CG-CD	-2.18	100.72	103.16
1	D	1908	HYP	CB-CG-CD	-2.18	100.72	103.16
1	C	1907	HYP	CG-CB-CA	-2.17	101.24	103.75
1	E	1870	HYP	CG-CB-CA	-2.17	101.24	103.75
2	I	26	HYP	CB-CG-CD	-2.16	100.75	103.16
1	A	1868	HYP	CB-CG-CD	-2.15	100.76	103.16
1	F	1907	HYP	CG-CB-CA	-2.14	101.27	103.75
1	E	1860	HYP	CB-CG-CD	-2.14	100.77	103.16
1	B	1888	HYP	CB-CG-CD	-2.14	100.78	103.16
1	C	1902	HYP	CB-CG-CD	-2.13	100.78	103.16
1	D	1923	HYP	CB-CG-CD	-2.12	100.79	103.16
1	F	1868	HYP	CB-CG-CD	-2.12	100.80	103.16
1	E	1868	HYP	CB-CG-CD	-2.12	100.80	103.16
2	G	37	HYP	O-C-CA	-2.12	119.33	124.77
1	A	1932	HYP	CB-CG-CD	-2.11	100.80	103.16
2	I	3	HYP	CB-CG-CD	-2.10	100.82	103.16
1	C	1923	HYP	CB-CG-CD	-2.10	100.82	103.16
1	A	1860	HYP	CB-CG-CD	-2.09	100.83	103.16
1	A	1870	HYP	CG-CB-CA	-2.09	101.34	103.75
1	F	1860	HYP	CB-CG-CD	-2.09	100.83	103.16
1	E	1903	HYP	CB-CG-CD	-2.08	100.84	103.16
1	B	1868	HYP	CB-CG-CD	-2.07	100.85	103.16
1	C	1903	HYP	CB-CG-CD	-2.06	100.86	103.16
1	F	1878	HYP	CB-CG-CD	-2.06	100.86	103.16
1	F	1920	HYP	CB-CG-CD	-2.04	100.88	103.16
1	E	1867	HYP	CB-CG-CD	-2.04	100.89	103.16
2	G	3	HYP	CB-CG-CD	-2.03	100.89	103.16
1	F	1907	HYP	CB-CG-CD	-2.03	100.89	103.16
1	B	1857	HYP	CB-CG-CD	-2.03	100.89	103.16
1	F	1858	HYP	CB-CG-CD	-2.03	100.90	103.16
2	G	2	HYP	CB-CG-CD	-2.02	100.90	103.16
1	B	1860	HYP	CB-CG-CD	-2.02	100.90	103.16
2	G	52	HYP	CB-CG-CD	-2.01	100.92	103.16
1	F	1902	HYP	CB-CG-CD	-2.01	100.92	103.16
1	F	1865	HYP	CB-CG-CD	-2.00	100.93	103.16
1	C	1930	HYP	CB-CG-CD	-2.00	100.93	103.16

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	23	HYP	CA
2	I	23	HYP	CA
2	G	26	HYP	CA
2	I	26	HYP	CA

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

1348 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	0	1	3	9,9,10	0.55	0	11,12,14	1.13	1 (9%)
3	FUB	0	2	3	9,9,10	0.52	0	11,12,14	0.88	0
3	FUB	0	3	3	9,9,10	0.55	0	11,12,14	0.93	0
3	FUB	0A	1	3	9,9,10	0.54	0	11,12,14	0.95	1 (9%)
3	FUB	0A	2	3	9,9,10	0.52	0	11,12,14	0.77	0
3	FUB	0A	3	3	9,9,10	0.53	0	11,12,14	0.88	0
6	FUB	0B	1	6	9,9,10	0.54	0	11,12,14	0.99	0
6	FUB	0B	2	6	9,9,10	0.55	0	11,12,14	1.20	2 (18%)
6	GZL	0B	3	6	11,11,12	6.84	6 (54%)	13,15,17	4.19	4 (30%)
6	FUB	0C	1	6	9,9,10	0.56	0	11,12,14	0.83	0
6	FUB	0C	2	6	9,9,10	0.54	0	11,12,14	1.11	1 (9%)
6	GZL	0C	3	6	11,11,12	6.56	7 (63%)	13,15,17	1.46	2 (15%)
13	FUB	0D	1	13	9,9,10	0.56	0	11,12,14	0.86	0
13	FUB	0D	2	13	9,9,10	0.54	0	11,12,14	1.03	0
13	GZL	0D	3	13	11,11,12	6.56	7 (63%)	13,15,17	1.43	2 (15%)
13	AHR	0D	4	13	9,9,10	0.54	0	11,12,14	0.88	0
18	FUB	0E	1	18	9,9,10	0.57	0	11,12,14	0.98	0
18	FUB	0E	2	18	9,9,10	0.54	0	11,12,14	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	GZL	0E	3	18	11,11,12	6.59	7 (63%)	13,15,17	1.33	1 (7%)
18	AHR	0E	4	18	9,9,10	0.56	0	11,12,14	0.95	0
18	AHR	0E	5	18	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
3	FUB	1	1	3	9,9,10	0.55	0	11,12,14	0.83	0
3	FUB	1	2	3	9,9,10	0.54	0	11,12,14	0.92	0
3	FUB	1	3	3	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
10	FUB	1A	1	10	9,9,10	0.50	0	11,12,14	1.05	1 (9%)
10	FUB	1A	2	10	9,9,10	0.52	0	11,12,14	0.76	0
10	FUB	1A	3	10	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
10	AHR	1A	4	10	9,9,10	0.55	0	11,12,14	0.84	1 (9%)
10	AHR	1A	5	10	9,9,10	0.55	0	11,12,14	0.87	1 (9%)
13	FUB	1B	1	13	9,9,10	0.53	0	11,12,14	0.84	0
13	FUB	1B	2	13	9,9,10	0.55	0	11,12,14	0.88	0
13	GZL	1B	3	13	11,11,12	6.63	7 (63%)	13,15,17	1.36	1 (7%)
13	AHR	1B	4	13	9,9,10	0.55	0	11,12,14	0.96	0
6	FUB	1C	1	6	9,9,10	0.53	0	11,12,14	0.71	0
6	FUB	1C	2	6	9,9,10	0.55	0	11,12,14	0.88	0
6	GZL	1C	3	6	11,11,12	6.58	7 (63%)	13,15,17	1.46	1 (7%)
15	FUB	1D	1	15	9,9,10	0.55	0	11,12,14	0.97	0
15	FUB	1D	2	15	9,9,10	0.56	0	11,12,14	0.95	0
15	GZL	1D	3	15	11,11,12	6.60	7 (63%)	13,15,17	1.29	1 (7%)
15	AHR	1D	4	15	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
15	AHR	1D	5	15	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
19	FUB	1E	1	19	9,9,10	0.53	0	11,12,14	1.06	1 (9%)
19	FUB	1E	2	19	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
19	GZL	1E	3	19	11,11,12	6.58	7 (63%)	13,15,17	1.47	1 (7%)
19	AHR	1E	4	19	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
3	FUB	2	1	3	9,9,10	0.53	0	11,12,14	0.95	0
3	FUB	2	2	3	9,9,10	0.51	0	11,12,14	0.74	0
3	FUB	2	3	3	9,9,10	0.54	0	11,12,14	0.97	0
13	FUB	2A	1	13	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
13	FUB	2A	2	13	9,9,10	0.45	0	11,12,14	1.30	2 (18%)
13	GZL	2A	3	13	11,11,12	6.71	6 (54%)	13,15,17	1.01	0
13	AHR	2A	4	13	9,9,10	0.56	0	11,12,14	1.06	1 (9%)
13	FUB	2B	1	13	9,9,10	0.54	0	11,12,14	1.01	0
13	FUB	2B	2	13	9,9,10	0.54	0	11,12,14	0.87	0
13	GZL	2B	3	13	11,11,12	6.57	7 (63%)	13,15,17	1.48	2 (15%)
13	AHR	2B	4	13	9,9,10	0.55	0	11,12,14	0.98	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FUB	2C	1	6	9,9,10	0.57	0	11,12,14	0.91	0
6	FUB	2C	2	6	9,9,10	0.56	0	11,12,14	1.05	1 (9%)
6	GZL	2C	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.42	1 (7%)
15	FUB	2D	1	15	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
15	FUB	2D	2	15	9,9,10	0.56	0	11,12,14	0.89	0
15	GZL	2D	3	15	11,11,12	6.60	7 (63%)	13,15,17	1.36	1 (7%)
15	AHR	2D	4	15	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
15	AHR	2D	5	15	9,9,10	0.56	0	11,12,14	0.96	0
10	FUB	3	1	10	9,9,10	0.53	0	11,12,14	1.05	1 (9%)
10	FUB	3	2	10	9,9,10	0.52	0	11,12,14	0.68	0
10	FUB	3	3	10	9,9,10	0.58	0	11,12,14	1.06	1 (9%)
10	AHR	3	4	10	9,9,10	0.54	0	11,12,14	0.92	0
10	AHR	3	5	10	9,9,10	0.55	0	11,12,14	0.80	1 (9%)
6	FUB	3A	1	6	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
6	FUB	3A	2	6	9,9,10	0.51	0	11,12,14	1.13	2 (18%)
6	GZL	3A	3	6	11,11,12	6.73	6 (54%)	13,15,17	4.98	4 (30%)
6	FUB	3B	1	6	9,9,10	0.53	0	11,12,14	0.94	0
6	FUB	3B	2	6	9,9,10	0.52	0	11,12,14	1.21	1 (9%)
6	GZL	3B	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.55	2 (15%)
13	FUB	3C	1	13	9,9,10	0.56	0	11,12,14	0.95	0
13	FUB	3C	2	13	9,9,10	0.53	0	11,12,14	1.13	1 (9%)
13	GZL	3C	3	13	11,11,12	6.54	7 (63%)	13,15,17	1.42	2 (15%)
13	AHR	3C	4	13	9,9,10	0.56	0	11,12,14	0.86	0
6	FUB	3D	1	6	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
6	FUB	3D	2	6	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
6	GZL	3D	3	6	11,11,12	6.58	7 (63%)	13,15,17	1.36	1 (7%)
13	FUB	4	1	13	9,9,10	0.51	0	11,12,14	0.85	0
13	FUB	4	2	13	9,9,10	0.49	0	11,12,14	1.29	1 (9%)
13	GZL	4	3	13	11,11,12	6.68	7 (63%)	13,15,17	3.35	6 (46%)
13	AHR	4	4	13	9,9,10	0.55	0	11,12,14	0.91	1 (9%)
13	FUB	4A	1	13	9,9,10	0.51	0	11,12,14	0.86	0
13	FUB	4A	2	13	9,9,10	0.54	0	11,12,14	0.82	0
13	GZL	4A	3	13	11,11,12	6.63	6 (54%)	13,15,17	1.41	1 (7%)
13	AHR	4A	4	13	9,9,10	0.52	0	11,12,14	1.07	1 (9%)
6	FUB	4B	1	6	9,9,10	0.55	0	11,12,14	0.87	1 (9%)
6	FUB	4B	2	6	9,9,10	0.56	0	11,12,14	0.83	0
6	GZL	4B	3	6	11,11,12	6.58	7 (63%)	13,15,17	1.63	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	FUB	4C	1	15	9,9,10	0.56	0	11,12,14	0.90	0
15	FUB	4C	2	15	9,9,10	0.55	0	11,12,14	0.96	0
15	GZL	4C	3	15	11,11,12	6.59	7 (63%)	13,15,17	1.34	1 (7%)
15	AHR	4C	4	15	9,9,10	0.54	0	11,12,14	1.03	0
15	AHR	4C	5	15	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
16	NAG	4D	1	1,16	14,14,15	0.34	0	17,19,21	0.53	0
16	NAG	4D	2	16	14,14,15	0.48	0	17,19,21	1.34	2 (11%)
6	FUB	5	1	6	9,9,10	0.52	0	11,12,14	0.97	1 (9%)
6	FUB	5	2	6	9,9,10	0.50	0	11,12,14	1.22	2 (18%)
6	GZL	5	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.55	1 (7%)
13	FUB	5A	1	13	9,9,10	0.53	0	11,12,14	0.88	0
13	FUB	5A	2	13	9,9,10	0.52	0	11,12,14	0.77	0
13	GZL	5A	3	13	11,11,12	6.57	7 (63%)	13,15,17	1.22	1 (7%)
13	AHR	5A	4	13	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
6	FUB	5B	1	6	9,9,10	0.52	0	11,12,14	0.79	0
6	FUB	5B	2	6	9,9,10	0.56	0	11,12,14	1.03	1 (9%)
6	GZL	5B	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.28	1 (7%)
15	FUB	5C	1	15	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
15	FUB	5C	2	15	9,9,10	0.56	0	11,12,14	0.95	0
15	GZL	5C	3	15	11,11,12	6.57	7 (63%)	13,15,17	1.49	1 (7%)
15	AHR	5C	4	15	9,9,10	0.55	0	11,12,14	0.97	1 (9%)
15	AHR	5C	5	15	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
17	NAG	5D	1	1,17	14,14,15	0.32	0	17,19,21	0.99	1 (5%)
17	NAG	5D	2	17	14,14,15	0.30	0	17,19,21	0.70	0
17	BMA	5D	3	17	11,11,12	0.25	0	15,15,17	1.22	3 (20%)
17	MAN	5D	4	17	11,11,12	0.40	0	15,15,17	2.06	3 (20%)
17	MAN	5D	5	17	11,11,12	0.26	0	15,15,17	0.52	0
17	MAN	5D	6	17	11,11,12	0.29	0	15,15,17	0.77	0
13	FUB	6	1	13	9,9,10	0.52	0	11,12,14	0.76	0
13	FUB	6	2	13	9,9,10	0.56	0	11,12,14	0.82	0
13	GZL	6	3	13	11,11,12	6.64	6 (54%)	13,15,17	1.37	1 (7%)
13	AHR	6	4	13	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
6	FUB	6A	1	6	9,9,10	0.53	0	11,12,14	0.86	0
6	FUB	6A	2	6	9,9,10	0.50	0	11,12,14	1.35	1 (9%)
6	GZL	6A	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.38	1 (7%)
13	FUB	6B	1	13	9,9,10	0.54	0	11,12,14	0.89	0
13	FUB	6B	2	13	9,9,10	0.52	0	11,12,14	1.15	2 (18%)
13	GZL	6B	3	13	11,11,12	6.57	7 (63%)	13,15,17	1.85	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	AHR	6B	4	13	9,9,10	0.52	0	11,12,14	0.92	0
6	FUB	6C	1	6	9,9,10	0.55	0	11,12,14	0.95	0
6	FUB	6C	2	6	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
6	GZL	6C	3	6	11,11,12	6.58	7 (63%)	13,15,17	1.39	1 (7%)
6	FUB	6D	1	6	9,9,10	0.56	0	11,12,14	1.03	0
6	FUB	6D	2	6	9,9,10	0.55	0	11,12,14	1.11	1 (9%)
6	GZL	6D	3	6	11,11,12	6.54	6 (54%)	13,15,17	1.75	2 (15%)
13	FUB	7	1	13	9,9,10	0.55	0	11,12,14	0.95	0
13	FUB	7	2	13	9,9,10	0.54	0	11,12,14	0.75	0
13	GZL	7	3	13	11,11,12	6.59	7 (63%)	13,15,17	1.32	1 (7%)
13	AHR	7	4	13	9,9,10	0.53	0	11,12,14	1.10	1 (9%)
6	FUB	7A	1	6	9,9,10	0.53	0	11,12,14	0.95	1 (9%)
6	FUB	7A	2	6	9,9,10	0.55	0	11,12,14	0.93	0
6	GZL	7A	3	6	11,11,12	6.57	6 (54%)	13,15,17	1.41	1 (7%)
15	FUB	7B	1	15	9,9,10	0.50	0	11,12,14	0.92	0
15	FUB	7B	2	15	9,9,10	0.53	0	11,12,14	0.85	0
15	GZL	7B	3	15	11,11,12	6.61	6 (54%)	13,15,17	1.39	1 (7%)
15	AHR	7B	4	15	9,9,10	0.57	0	11,12,14	1.17	1 (9%)
15	AHR	7B	5	15	9,9,10	0.56	0	11,12,14	0.89	0
17	NAG	7C	1	1,17	14,14,15	0.32	0	17,19,21	0.86	1 (5%)
17	NAG	7C	2	17	14,14,15	0.35	0	17,19,21	0.98	0
17	BMA	7C	3	17	11,11,12	0.20	0	15,15,17	1.11	1 (6%)
17	MAN	7C	4	17	11,11,12	0.31	0	15,15,17	1.08	1 (6%)
17	MAN	7C	5	17	11,11,12	0.23	0	15,15,17	0.63	0
17	MAN	7C	6	17	11,11,12	0.28	0	15,15,17	0.85	0
6	FUB	7D	1	6	9,9,10	0.55	0	11,12,14	0.96	0
6	FUB	7D	2	6	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
6	GZL	7D	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.52	2 (15%)
6	FUB	8	1	6	9,9,10	0.53	0	11,12,14	0.96	1 (9%)
6	FUB	8	2	6	9,9,10	0.53	0	11,12,14	0.80	0
6	GZL	8	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.35	1 (7%)
6	FUB	8A	1	6	9,9,10	0.51	0	11,12,14	0.99	1 (9%)
6	FUB	8A	2	6	9,9,10	0.58	0	11,12,14	1.04	1 (9%)
6	GZL	8A	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.45	1 (7%)
15	FUB	8B	1	15	9,9,10	0.56	0	11,12,14	0.92	0
15	FUB	8B	2	15	9,9,10	0.53	0	11,12,14	0.90	0
15	GZL	8B	3	15	11,11,12	6.60	7 (63%)	13,15,17	1.17	1 (7%)
15	AHR	8B	4	15	9,9,10	0.54	0	11,12,14	1.05	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	AHR	8B	5	15	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
3	FUB	8C	1	3	9,9,10	0.55	0	11,12,14	0.83	0
3	FUB	8C	2	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	8C	3	3	9,9,10	0.56	0	11,12,14	0.88	0
6	FUB	8D	1	6	9,9,10	0.54	0	11,12,14	0.83	0
6	FUB	8D	2	6	9,9,10	0.54	0	11,12,14	0.91	0
6	GZL	8D	3	6	11,11,12	6.60	6 (54%)	13,15,17	1.54	2 (15%)
6	FUB	9	1	6	9,9,10	0.52	0	11,12,14	0.87	1 (9%)
6	FUB	9	2	6	9,9,10	0.54	0	11,12,14	0.79	0
6	GZL	9	3	6	11,11,12	6.60	6 (54%)	13,15,17	1.29	1 (7%)
13	FUB	9A	1	13	9,9,10	0.53	0	11,12,14	0.89	0
13	FUB	9A	2	13	9,9,10	0.51	0	11,12,14	1.15	2 (18%)
13	GZL	9A	3	13	11,11,12	6.58	7 (63%)	13,15,17	1.94	4 (30%)
13	AHR	9A	4	13	9,9,10	0.53	0	11,12,14	0.96	0
6	FUB	9B	1	6	9,9,10	0.54	0	11,12,14	0.86	0
6	FUB	9B	2	6	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
6	GZL	9B	3	6	11,11,12	6.56	7 (63%)	13,15,17	1.58	2 (15%)
3	FUB	9C	1	3	9,9,10	0.55	0	11,12,14	0.99	0
3	FUB	9C	2	3	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
3	FUB	9C	3	3	9,9,10	0.54	0	11,12,14	0.82	1 (9%)
18	FUB	9D	1	18	9,9,10	0.57	0	11,12,14	2.51	5 (45%)
18	FUB	9D	2	18	9,9,10	0.54	0	11,12,14	0.87	0
18	GZL	9D	3	18	11,11,12	6.60	7 (63%)	13,15,17	1.29	1 (7%)
18	AHR	9D	4	18	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
18	AHR	9D	5	18	9,9,10	0.56	0	11,12,14	1.21	1 (9%)
6	FUB	AA	1	6	9,9,10	0.51	0	11,12,14	0.77	0
6	FUB	AA	2	6	9,9,10	0.58	0	11,12,14	1.07	1 (9%)
6	GZL	AA	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.22	1 (7%)
15	FUB	AB	1	15	9,9,10	0.52	0	11,12,14	0.97	1 (9%)
15	FUB	AB	2	15	9,9,10	0.55	0	11,12,14	0.88	0
15	GZL	AB	3	15	11,11,12	6.59	6 (54%)	13,15,17	1.26	1 (7%)
15	AHR	AB	4	15	9,9,10	0.60	0	11,12,14	1.18	1 (9%)
15	AHR	AB	5	15	9,9,10	0.55	0	11,12,14	1.10	1 (9%)
16	NAG	AC	1	1,16	14,14,15	0.55	0	17,19,21	0.97	1 (5%)
16	NAG	AC	2	16	14,14,15	0.41	0	17,19,21	1.30	2 (11%)
4	FUB	AD	1	4	9,9,10	0.54	0	11,12,14	0.91	1 (9%)
4	FUB	AD	2	4	9,9,10	0.52	0	11,12,14	0.80	0
4	FUB	AD	3	4	9,9,10	0.53	0	11,12,14	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	AHR	AD	4	4	9,9,10	0.53	0	11,12,14	1.07	1 (9%)
19	FUB	AE	1	19	9,9,10	0.55	0	11,12,14	1.18	1 (9%)
19	FUB	AE	2	19	9,9,10	0.54	0	11,12,14	0.85	0
19	GZL	AE	3	19	11,11,12	6.61	6 (54%)	13,15,17	1.40	1 (7%)
19	AHR	AE	4	19	9,9,10	0.54	0	11,12,14	0.85	0
13	FUB	BA	1	13	9,9,10	0.54	0	11,12,14	0.77	0
13	FUB	BA	2	13	9,9,10	0.52	0	11,12,14	1.33	3 (27%)
13	GZL	BA	3	13	11,11,12	6.53	7 (63%)	13,15,17	1.93	4 (30%)
13	AHR	BA	4	13	9,9,10	0.52	0	11,12,14	0.83	0
15	FUB	BB	1	15	9,9,10	0.52	0	11,12,14	0.96	1 (9%)
15	FUB	BB	2	15	9,9,10	0.54	0	11,12,14	0.70	0
15	GZL	BB	3	15	11,11,12	6.61	6 (54%)	13,15,17	1.13	1 (7%)
15	AHR	BB	4	15	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
15	AHR	BB	5	15	9,9,10	0.56	0	11,12,14	0.90	0
3	FUB	BC	1	3	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
3	FUB	BC	2	3	9,9,10	0.52	0	11,12,14	0.89	0
3	FUB	BC	3	3	9,9,10	0.54	0	11,12,14	0.86	0
5	FUB	BD	1	5	9,9,10	0.52	0	11,12,14	0.97	1 (9%)
5	FUB	BD	2	5	9,9,10	0.51	0	11,12,14	0.84	0
5	FUB	BD	3	5	9,9,10	0.55	0	11,12,14	0.89	0
5	AHR	BD	4	5	9,9,10	0.53	0	11,12,14	1.06	1 (9%)
5	AHR	BD	5	5	9,9,10	0.54	0	11,12,14	0.81	0
18	FUB	BE	1	18	9,9,10	0.58	0	11,12,14	0.92	0
18	FUB	BE	2	18	9,9,10	0.51	0	11,12,14	1.00	1 (9%)
18	GZL	BE	3	18	11,11,12	6.56	7 (63%)	13,15,17	1.50	2 (15%)
18	AHR	BE	4	18	9,9,10	0.54	0	11,12,14	0.82	0
18	AHR	BE	5	18	9,9,10	0.52	0	11,12,14	1.10	1 (9%)
15	FUB	CA	1	15	9,9,10	0.52	0	11,12,14	0.99	0
15	FUB	CA	2	15	9,9,10	0.51	0	11,12,14	0.82	0
15	GZL	CA	3	15	11,11,12	6.61	7 (63%)	13,15,17	1.17	1 (7%)
15	AHR	CA	4	15	9,9,10	0.56	0	11,12,14	1.22	2 (18%)
15	AHR	CA	5	15	9,9,10	0.56	0	11,12,14	1.04	0
6	FUB	CB	1	6	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
6	FUB	CB	2	6	9,9,10	0.53	0	11,12,14	0.84	0
6	GZL	CB	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.49	3 (23%)
3	FUB	CC	1	3	9,9,10	0.54	0	11,12,14	0.92	1 (9%)
3	FUB	CC	2	3	9,9,10	0.53	0	11,12,14	0.89	1 (9%)
3	FUB	CC	3	3	9,9,10	0.54	0	11,12,14	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FUB	CD	1	6	9,9,10	0.53	0	11,12,14	0.95	0
6	FUB	CD	2	6	9,9,10	0.48	0	11,12,14	1.08	2 (18%)
6	GZL	CD	3	6	11,11,12	6.96	6 (54%)	13,15,17	4.33	5 (38%)
20	FUB	CE	1	20	9,9,10	0.53	0	11,12,14	0.80	0
20	FUB	CE	2	20	9,9,10	0.50	0	11,12,14	0.80	0
20	GZL	CE	3	20	11,11,12	6.55	6 (54%)	13,15,17	1.48	1 (7%)
20	AHR	CE	4	20	9,9,10	0.56	0	11,12,14	0.86	0
15	FUB	DA	1	15	9,9,10	0.54	0	11,12,14	0.94	0
15	FUB	DA	2	15	9,9,10	0.53	0	11,12,14	0.81	0
15	GZL	DA	3	15	11,11,12	6.60	6 (54%)	13,15,17	1.30	1 (7%)
15	AHR	DA	4	15	9,9,10	0.53	0	11,12,14	1.08	1 (9%)
15	AHR	DA	5	15	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
17	NAG	DB	1	1,17	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
17	NAG	DB	2	17	14,14,15	0.32	0	17,19,21	1.06	1 (5%)
17	BMA	DB	3	17	11,11,12	0.22	0	15,15,17	1.13	1 (6%)
17	MAN	DB	4	17	11,11,12	0.31	0	15,15,17	1.06	2 (13%)
17	MAN	DB	5	17	11,11,12	0.23	0	15,15,17	0.62	0
17	MAN	DB	6	17	11,11,12	0.39	0	15,15,17	1.31	2 (13%)
4	FUB	DC	1	4	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
4	FUB	DC	2	4	9,9,10	0.54	0	11,12,14	0.82	0
4	FUB	DC	3	4	9,9,10	0.53	0	11,12,14	0.81	0
4	AHR	DC	4	4	9,9,10	0.54	0	11,12,14	0.97	1 (9%)
3	FUB	DD	1	3	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
3	FUB	DD	2	3	9,9,10	0.55	0	11,12,14	0.80	0
3	FUB	DD	3	3	9,9,10	0.54	0	11,12,14	0.95	0
18	FUB	DE	1	18	9,9,10	0.50	0	11,12,14	1.02	1 (9%)
18	FUB	DE	2	18	9,9,10	0.49	0	11,12,14	0.76	0
18	GZL	DE	3	18	11,11,12	6.56	7 (63%)	13,15,17	1.53	1 (7%)
18	AHR	DE	4	18	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
18	AHR	DE	5	18	9,9,10	0.56	0	11,12,14	0.90	0
6	FUB	EA	1	6	9,9,10	0.54	0	11,12,14	0.93	0
6	FUB	EA	2	6	9,9,10	0.52	0	11,12,14	0.88	0
6	GZL	EA	3	6	11,11,12	6.60	6 (54%)	13,15,17	1.37	1 (7%)
3	FUB	EB	1	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	FUB	EB	2	3	9,9,10	0.55	0	11,12,14	0.83	0
3	FUB	EB	3	3	9,9,10	0.55	0	11,12,14	0.97	0
5	FUB	EC	1	5	9,9,10	0.55	0	11,12,14	0.97	0
5	FUB	EC	2	5	9,9,10	0.56	0	11,12,14	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FUB	EC	3	5	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
5	AHR	EC	4	5	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
5	AHR	EC	5	5	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	ED	1	3	9,9,10	0.51	0	11,12,14	1.04	1 (9%)
3	FUB	ED	2	3	9,9,10	0.54	0	11,12,14	0.79	0
3	FUB	ED	3	3	9,9,10	0.55	0	11,12,14	0.81	0
20	FUB	EE	1	20	9,9,10	0.51	0	11,12,14	0.81	0
20	FUB	EE	2	20	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
20	GZL	EE	3	20	11,11,12	6.59	7 (63%)	13,15,17	1.43	1 (7%)
20	AHR	EE	4	20	9,9,10	0.57	0	11,12,14	0.83	0
16	NAG	FA	1	1,16	14,14,15	0.42	0	17,19,21	0.58	0
16	NAG	FA	2	16	14,14,15	0.40	0	17,19,21	1.40	2 (11%)
12	FUB	FB	1	12	9,9,10	0.56	0	11,12,14	0.99	0
12	FUB	FB	2	12	9,9,10	0.56	0	11,12,14	0.94	0
12	GZL	FB	3	12	11,11,12	6.53	7 (63%)	13,15,17	1.64	2 (15%)
12	AHR	FB	4	12	9,9,10	0.55	0	11,12,14	0.92	0
12	AHR	FB	5	12	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
6	FUB	FC	1	6	9,9,10	0.53	0	11,12,14	1.23	2 (18%)
6	FUB	FC	2	6	9,9,10	0.58	0	11,12,14	1.15	1 (9%)
6	GZL	FC	3	6	11,11,12	6.45	6 (54%)	13,15,17	2.37	3 (23%)
3	FUB	FD	1	3	9,9,10	0.52	0	11,12,14	1.04	1 (9%)
3	FUB	FD	2	3	9,9,10	0.52	0	11,12,14	0.73	0
3	FUB	FD	3	3	9,9,10	0.55	0	11,12,14	0.87	0
21	FUB	FE	1	21	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
21	FUB	FE	2	21	9,9,10	0.51	0	11,12,14	0.70	0
21	GZL	FE	3	21	11,11,12	6.61	6 (54%)	13,15,17	1.30	1 (7%)
21	AHR	FE	4	21	9,9,10	0.54	0	11,12,14	0.98	0
21	AHR	FE	5	21	9,9,10	0.59	0	11,12,14	0.95	1 (9%)
17	NAG	GA	1	1,17	14,14,15	0.34	0	17,19,21	0.80	1 (5%)
17	NAG	GA	2	17	14,14,15	0.33	0	17,19,21	0.92	0
17	BMA	GA	3	17	11,11,12	0.23	0	15,15,17	1.59	3 (20%)
17	MAN	GA	4	17	11,11,12	0.30	0	15,15,17	0.70	0
17	MAN	GA	5	17	11,11,12	0.24	0	15,15,17	0.55	0
17	MAN	GA	6	17	11,11,12	0.28	0	15,15,17	0.91	0
13	FUB	GB	1	13	9,9,10	0.55	0	11,12,14	0.87	0
13	FUB	GB	2	13	9,9,10	0.56	0	11,12,14	0.91	0
13	GZL	GB	3	13	11,11,12	6.60	7 (63%)	13,15,17	1.22	1 (7%)
13	AHR	GB	4	13	9,9,10	0.53	0	11,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	GC	1	3	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
3	FUB	GC	2	3	9,9,10	0.52	0	11,12,14	0.71	0
3	FUB	GC	3	3	9,9,10	0.55	0	11,12,14	0.85	0
6	FUB	GD	1	6	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
6	FUB	GD	2	6	9,9,10	0.53	0	11,12,14	0.82	0
6	GZL	GD	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.33	1 (7%)
22	FUB	GE	1	22	9,9,10	0.55	0	11,12,14	1.12	1 (9%)
22	FUB	GE	2	22	9,9,10	0.56	0	11,12,14	1.11	1 (9%)
22	GZL	GE	3	22	11,11,12	6.57	7 (63%)	13,15,17	1.34	1 (7%)
22	AHR	GE	4	22	9,9,10	0.53	0	11,12,14	0.78	0
22	AHR	GE	5	22	9,9,10	0.57	0	11,12,14	1.40	3 (27%)
22	AHR	GE	6	22	9,9,10	0.52	0	11,12,14	0.80	0
3	FUB	HA	1	3	9,9,10	0.52	0	11,12,14	0.85	0
3	FUB	HA	2	3	9,9,10	0.55	0	11,12,14	0.80	0
3	FUB	HA	3	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
14	FUB	HB	1	14	9,9,10	0.53	0	11,12,14	0.77	0
14	FUB	HB	2	14	9,9,10	0.54	0	11,12,14	0.86	0
14	GZL	HB	3	14	11,11,12	6.52	7 (63%)	13,15,17	1.71	3 (23%)
14	FUB	HB	4	14	9,9,10	0.56	0	11,12,14	1.04	1 (9%)
3	FUB	HC	1	3	9,9,10	0.52	0	11,12,14	1.12	1 (9%)
3	FUB	HC	2	3	9,9,10	0.53	0	11,12,14	0.75	0
3	FUB	HC	3	3	9,9,10	0.54	0	11,12,14	0.90	0
7	FUB	HD	1	7	9,9,10	0.56	0	11,12,14	1.10	1 (9%)
7	FUB	HD	2	7	9,9,10	0.54	0	11,12,14	0.84	0
7	FUB	HD	3	7	9,9,10	0.54	0	11,12,14	0.96	0
7	AHR	HD	4	7	9,9,10	0.53	0	11,12,14	0.94	1 (9%)
20	FUB	HE	1	20	9,9,10	0.56	0	11,12,14	1.14	0
20	FUB	HE	2	20	9,9,10	0.53	0	11,12,14	0.92	0
20	GZL	HE	3	20	11,11,12	6.58	7 (63%)	13,15,17	1.49	1 (7%)
20	AHR	HE	4	20	9,9,10	0.54	0	11,12,14	0.97	0
3	FUB	IA	1	3	9,9,10	0.52	0	11,12,14	0.74	0
3	FUB	IA	2	3	9,9,10	0.53	0	11,12,14	0.88	0
3	FUB	IA	3	3	9,9,10	0.53	0	11,12,14	0.78	0
12	FUB	IB	1	12	9,9,10	0.55	0	11,12,14	0.91	0
12	FUB	IB	2	12	9,9,10	0.54	0	11,12,14	0.93	1 (9%)
12	GZL	IB	3	12	11,11,12	6.58	7 (63%)	13,15,17	1.33	1 (7%)
12	AHR	IB	4	12	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
12	AHR	IB	5	12	9,9,10	0.54	0	11,12,14	1.05	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	IC	1	3	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
3	FUB	IC	2	3	9,9,10	0.49	0	11,12,14	0.80	0
3	FUB	IC	3	3	9,9,10	0.53	0	11,12,14	0.84	0
3	FUB	ID	1	3	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
3	FUB	ID	2	3	9,9,10	0.52	0	11,12,14	0.78	0
3	FUB	ID	3	3	9,9,10	0.56	0	11,12,14	0.85	0
18	FUB	IE	1	18	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
18	FUB	IE	2	18	9,9,10	0.50	0	11,12,14	0.84	0
18	GZL	IE	3	18	11,11,12	6.54	7 (63%)	13,15,17	1.55	1 (7%)
18	AHR	IE	4	18	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
18	AHR	IE	5	18	9,9,10	0.54	0	11,12,14	1.11	1 (9%)
3	FUB	J	1	3	9,9,10	0.53	0	11,12,14	0.76	0
3	FUB	J	2	3	9,9,10	0.53	0	11,12,14	0.94	0
3	FUB	J	3	3	9,9,10	0.57	0	11,12,14	0.92	0
4	FUB	JA	1	4	9,9,10	0.55	0	11,12,14	0.83	0
4	FUB	JA	2	4	9,9,10	0.55	0	11,12,14	1.00	0
4	FUB	JA	3	4	9,9,10	0.55	0	11,12,14	0.92	0
4	AHR	JA	4	4	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
4	FUB	JB	1	4	9,9,10	0.54	0	11,12,14	0.96	0
4	FUB	JB	2	4	9,9,10	0.56	0	11,12,14	0.98	0
4	FUB	JB	3	4	9,9,10	0.56	0	11,12,14	0.87	0
4	AHR	JB	4	4	9,9,10	0.54	0	11,12,14	0.68	0
6	FUB	JC	1	6	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
6	FUB	JC	2	6	9,9,10	0.53	0	11,12,14	0.82	0
6	GZL	JC	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.34	1 (7%)
8	FUB	JD	1	8	9,9,10	0.53	0	11,12,14	0.81	0
8	FUB	JD	2	8	9,9,10	0.54	0	11,12,14	0.77	0
8	FUB	JD	3	8	9,9,10	0.56	0	11,12,14	0.76	0
8	AHR	JD	4	8	9,9,10	0.55	0	11,12,14	1.09	1 (9%)
8	AHR	JD	5	8	9,9,10	0.55	0	11,12,14	0.94	0
18	FUB	JE	1	18	9,9,10	0.56	0	11,12,14	1.05	1 (9%)
18	FUB	JE	2	18	9,9,10	0.54	0	11,12,14	0.89	0
18	GZL	JE	3	18	11,11,12	6.56	7 (63%)	13,15,17	1.43	1 (7%)
18	AHR	JE	4	18	9,9,10	0.55	0	11,12,14	0.82	0
18	AHR	JE	5	18	9,9,10	0.54	0	11,12,14	0.98	0
3	FUB	K	1	3	9,9,10	0.54	0	11,12,14	0.64	0
3	FUB	K	2	3	9,9,10	0.52	0	11,12,14	0.78	0
3	FUB	K	3	3	9,9,10	0.53	0	11,12,14	0.76	0
5	FUB	KA	1	5	9,9,10	0.54	0	11,12,14	0.92	0
5	FUB	KA	2	5	9,9,10	0.56	0	11,12,14	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FUB	KA	3	5	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
5	AHR	KA	4	5	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
5	AHR	KA	5	5	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
14	FUB	KB	1	14	9,9,10	0.56	0	11,12,14	0.96	0
14	FUB	KB	2	14	9,9,10	0.56	0	11,12,14	0.97	0
14	GZL	KB	3	14	11,11,12	6.50	7 (63%)	13,15,17	1.80	2 (15%)
14	FUB	KB	4	14	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
7	FUB	KC	1	7	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
7	FUB	KC	2	7	9,9,10	0.53	0	11,12,14	0.75	0
7	FUB	KC	3	7	9,9,10	0.55	0	11,12,14	0.94	0
7	AHR	KC	4	7	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
3	FUB	KD	1	3	9,9,10	0.54	0	11,12,14	0.95	1 (9%)
3	FUB	KD	2	3	9,9,10	0.53	0	11,12,14	0.89	0
3	FUB	KD	3	3	9,9,10	0.54	0	11,12,14	0.95	0
18	FUB	KE	1	18	9,9,10	0.57	0	11,12,14	1.09	0
18	FUB	KE	2	18	9,9,10	0.54	0	11,12,14	0.92	0
18	GZL	KE	3	18	11,11,12	6.54	7 (63%)	13,15,17	1.39	1 (7%)
18	AHR	KE	4	18	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
18	AHR	KE	5	18	9,9,10	0.55	0	11,12,14	0.99	0
4	FUB	L	1	4	9,9,10	0.56	0	11,12,14	0.67	0
4	FUB	L	2	4	9,9,10	0.54	0	11,12,14	0.89	0
4	FUB	L	3	4	9,9,10	0.57	0	11,12,14	0.83	0
4	AHR	L	4	4	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
6	FUB	LA	1	6	9,9,10	0.56	0	11,12,14	0.96	0
6	FUB	LA	2	6	9,9,10	0.54	0	11,12,14	1.15	1 (9%)
6	GZL	LA	3	6	11,11,12	6.97	6 (54%)	13,15,17	4.26	5 (38%)
3	FUB	LB	1	3	9,9,10	0.55	0	11,12,14	0.89	0
3	FUB	LB	2	3	9,9,10	0.54	0	11,12,14	0.84	0
3	FUB	LB	3	3	9,9,10	0.54	0	11,12,14	0.94	0
3	FUB	LC	1	3	9,9,10	0.55	0	11,12,14	1.00	0
3	FUB	LC	2	3	9,9,10	0.52	0	11,12,14	0.77	0
3	FUB	LC	3	3	9,9,10	0.55	0	11,12,14	0.83	0
4	FUB	LD	1	4	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
4	FUB	LD	2	4	9,9,10	0.54	0	11,12,14	0.80	0
4	FUB	LD	3	4	9,9,10	0.55	0	11,12,14	0.80	0
4	AHR	LD	4	4	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
19	FUB	LE	1	19	9,9,10	0.55	0	11,12,14	1.08	0
19	FUB	LE	2	19	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
19	GZL	LE	3	19	11,11,12	6.60	7 (63%)	13,15,17	1.34	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	AHR	LE	4	19	9,9,10	0.53	0	11,12,14	0.93	0
5	FUB	M	1	5	9,9,10	0.53	0	11,12,14	0.89	0
5	FUB	M	2	5	9,9,10	0.55	0	11,12,14	1.19	2 (18%)
5	FUB	M	3	5	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
5	AHR	M	4	5	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
5	AHR	M	5	5	9,9,10	0.54	0	11,12,14	1.12	1 (9%)
3	FUB	MA	1	3	9,9,10	0.53	0	11,12,14	0.84	0
3	FUB	MA	2	3	9,9,10	0.53	0	11,12,14	0.82	0
3	FUB	MA	3	3	9,9,10	0.55	0	11,12,14	0.86	0
10	FUB	MB	1	10	9,9,10	0.55	0	11,12,14	0.97	0
10	FUB	MB	2	10	9,9,10	0.55	0	11,12,14	1.01	0
10	FUB	MB	3	10	9,9,10	0.55	0	11,12,14	0.83	0
10	AHR	MB	4	10	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
10	AHR	MB	5	10	9,9,10	0.54	0	11,12,14	1.13	1 (9%)
8	FUB	MC	1	8	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
8	FUB	MC	2	8	9,9,10	0.54	0	11,12,14	0.78	0
8	FUB	MC	3	8	9,9,10	0.54	0	11,12,14	0.82	0
8	AHR	MC	4	8	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
8	AHR	MC	5	8	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	FUB	MD	1	4	9,9,10	0.51	0	11,12,14	0.88	0
4	FUB	MD	2	4	9,9,10	0.52	0	11,12,14	0.83	0
4	FUB	MD	3	4	9,9,10	0.56	0	11,12,14	0.95	0
4	AHR	MD	4	4	9,9,10	0.54	0	11,12,14	0.81	0
6	FUB	ME	1	6	9,9,10	0.55	0	11,12,14	0.81	0
6	FUB	ME	2	6	9,9,10	0.55	0	11,12,14	0.81	0
6	GZL	ME	3	6	11,11,12	6.59	6 (54%)	13,15,17	1.40	1 (7%)
6	FUB	N	1	6	9,9,10	0.55	0	11,12,14	1.02	0
6	FUB	N	2	6	9,9,10	0.59	0	11,12,14	1.11	1 (9%)
6	GZL	N	3	6	11,11,12	6.50	7 (63%)	13,15,17	3.34	5 (38%)
3	FUB	NA	1	3	9,9,10	0.52	0	11,12,14	1.06	1 (9%)
3	FUB	NA	2	3	9,9,10	0.52	0	11,12,14	0.79	0
3	FUB	NA	3	3	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
4	FUB	NB	1	4	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	FUB	NB	2	4	9,9,10	0.56	0	11,12,14	0.93	0
4	FUB	NB	3	4	9,9,10	0.54	0	11,12,14	0.90	0
4	AHR	NB	4	4	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
3	FUB	NC	1	3	9,9,10	0.55	0	11,12,14	0.91	0
3	FUB	NC	2	3	9,9,10	0.54	0	11,12,14	0.84	0
3	FUB	NC	3	3	9,9,10	0.54	0	11,12,14	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	FUB	ND	1	9	9,9,10	0.59	0	11,12,14	1.02	0
9	FUB	ND	2	9	9,9,10	0.56	0	11,12,14	1.05	1 (9%)
19	FUB	NE	1	19	9,9,10	0.56	0	11,12,14	0.93	0
19	FUB	NE	2	19	9,9,10	0.54	0	11,12,14	0.76	0
19	GZL	NE	3	19	11,11,12	6.57	7 (63%)	13,15,17	1.40	1 (7%)
19	AHR	NE	4	19	9,9,10	0.55	0	11,12,14	0.92	0
3	FUB	O	1	3	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
3	FUB	O	2	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	O	3	3	9,9,10	0.56	0	11,12,14	0.95	0
3	FUB	OA	1	3	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
3	FUB	OA	2	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	OA	3	3	9,9,10	0.55	0	11,12,14	0.92	0
3	FUB	OB	1	3	9,9,10	0.56	0	11,12,14	0.97	0
3	FUB	OB	2	3	9,9,10	0.56	0	11,12,14	0.87	0
3	FUB	OB	3	3	9,9,10	0.56	0	11,12,14	0.95	0
4	FUB	OC	1	4	9,9,10	0.51	0	11,12,14	0.87	0
4	FUB	OC	2	4	9,9,10	0.56	0	11,12,14	0.71	0
4	FUB	OC	3	4	9,9,10	0.54	0	11,12,14	0.82	0
4	AHR	OC	4	4	9,9,10	0.53	0	11,12,14	1.08	1 (9%)
4	FUB	OD	1	4	9,9,10	0.51	0	11,12,14	1.02	0
4	FUB	OD	2	4	9,9,10	0.49	0	11,12,14	0.77	0
4	FUB	OD	3	4	9,9,10	0.55	0	11,12,14	0.85	0
4	AHR	OD	4	4	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
6	FUB	OE	1	6	9,9,10	0.60	0	11,12,14	0.85	0
6	FUB	OE	2	6	9,9,10	0.56	0	11,12,14	0.89	0
6	GZL	OE	3	6	11,11,12	6.59	6 (54%)	13,15,17	1.46	1 (7%)
3	FUB	P	1	3	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
3	FUB	P	2	3	9,9,10	0.54	0	11,12,14	0.86	0
3	FUB	P	3	3	9,9,10	0.56	0	11,12,14	0.92	0
6	FUB	PA	1	6	9,9,10	0.56	0	11,12,14	0.98	0
6	FUB	PA	2	6	9,9,10	0.54	0	11,12,14	0.88	0
6	GZL	PA	3	6	11,11,12	6.59	6 (54%)	13,15,17	1.42	1 (7%)
3	FUB	PB	1	3	9,9,10	0.54	0	11,12,14	0.91	0
3	FUB	PB	2	3	9,9,10	0.54	0	11,12,14	0.90	0
3	FUB	PB	3	3	9,9,10	0.53	0	11,12,14	0.86	0
4	FUB	PC	1	4	9,9,10	0.51	0	11,12,14	0.92	0
4	FUB	PC	2	4	9,9,10	0.52	0	11,12,14	0.81	0
4	FUB	PC	3	4	9,9,10	0.55	0	11,12,14	0.91	0
4	AHR	PC	4	4	9,9,10	0.61	0	11,12,14	1.18	1 (9%)
10	FUB	PD	1	10	9,9,10	0.52	0	11,12,14	1.01	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
10	FUB	PD	2	10	9,9,10	0.57	0	11,12,14	0.92	0
10	FUB	PD	3	10	9,9,10	0.56	0	11,12,14	0.87	0
10	AHR	PD	4	10	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
10	AHR	PD	5	10	9,9,10	0.55	0	11,12,14	0.98	0
18	FUB	PE	1	18	9,9,10	0.53	0	11,12,14	0.96	1 (9%)
18	FUB	PE	2	18	9,9,10	0.52	0	11,12,14	0.76	0
18	GZL	PE	3	18	11,11,12	6.60	6 (54%)	13,15,17	1.36	1 (7%)
18	AHR	PE	4	18	9,9,10	0.54	0	11,12,14	0.80	0
18	AHR	PE	5	18	9,9,10	0.54	0	11,12,14	0.98	0
3	FUB	Q	1	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	FUB	Q	2	3	9,9,10	0.52	0	11,12,14	0.80	0
3	FUB	Q	3	3	9,9,10	0.54	0	11,12,14	0.79	0
7	FUB	QA	1	7	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
7	FUB	QA	2	7	9,9,10	0.56	0	11,12,14	0.87	0
7	FUB	QA	3	7	9,9,10	0.57	0	11,12,14	1.01	1 (9%)
7	AHR	QA	4	7	9,9,10	0.53	0	11,12,14	0.88	0
3	FUB	QB	1	3	9,9,10	0.56	0	11,12,14	0.94	1 (9%)
3	FUB	QB	2	3	9,9,10	0.56	0	11,12,14	0.88	0
3	FUB	QB	3	3	9,9,10	0.52	0	11,12,14	0.80	0
9	FUB	QC	1	9	9,9,10	0.54	0	11,12,14	0.91	0
9	FUB	QC	2	9	9,9,10	0.54	0	11,12,14	0.91	0
3	FUB	QD	1	3	9,9,10	0.55	0	11,12,14	0.77	0
3	FUB	QD	2	3	9,9,10	0.56	0	11,12,14	0.95	0
3	FUB	QD	3	3	9,9,10	0.54	0	11,12,14	0.87	0
22	FUB	QE	1	22	9,9,10	0.54	0	11,12,14	0.79	1 (9%)
22	FUB	QE	2	22	9,9,10	0.54	0	11,12,14	0.93	0
22	GZL	QE	3	22	11,11,12	6.60	6 (54%)	13,15,17	1.37	1 (7%)
22	AHR	QE	4	22	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
22	AHR	QE	5	22	9,9,10	0.55	0	11,12,14	0.87	0
22	AHR	QE	6	22	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
6	FUB	R	1	6	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
6	FUB	R	2	6	9,9,10	0.54	0	11,12,14	0.89	0
6	GZL	R	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.39	1 (7%)
3	FUB	RA	1	3	9,9,10	0.53	0	11,12,14	1.06	1 (9%)
3	FUB	RA	2	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	RA	3	3	9,9,10	0.55	0	11,12,14	0.91	0
3	FUB	RB	1	3	9,9,10	0.53	0	11,12,14	1.04	0
3	FUB	RB	2	3	9,9,10	0.58	0	11,12,14	0.98	0
3	FUB	RB	3	3	9,9,10	0.55	0	11,12,14	1.03	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FUB	RC	1	4	9,9,10	0.53	0	11,12,14	0.93	0
4	FUB	RC	2	4	9,9,10	0.54	0	11,12,14	0.68	0
4	FUB	RC	3	4	9,9,10	0.57	0	11,12,14	0.93	0
4	AHR	RC	4	4	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
4	FUB	RD	1	4	9,9,10	0.52	0	11,12,14	0.81	0
4	FUB	RD	2	4	9,9,10	0.55	0	11,12,14	0.94	1 (9%)
4	FUB	RD	3	4	9,9,10	0.57	0	11,12,14	0.95	0
4	AHR	RD	4	4	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
22	FUB	RE	1	22	9,9,10	0.57	0	11,12,14	1.01	0
22	FUB	RE	2	22	9,9,10	0.54	0	11,12,14	0.87	0
22	GZL	RE	3	22	11,11,12	6.60	6 (54%)	13,15,17	1.35	1 (7%)
22	AHR	RE	4	22	9,9,10	0.54	0	11,12,14	0.95	0
22	AHR	RE	5	22	9,9,10	0.53	0	11,12,14	1.13	1 (9%)
22	AHR	RE	6	22	9,9,10	0.60	0	11,12,14	1.16	1 (9%)
7	FUB	S	1	7	9,9,10	0.54	0	11,12,14	1.09	1 (9%)
7	FUB	S	2	7	9,9,10	0.53	0	11,12,14	0.81	0
7	FUB	S	3	7	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
7	AHR	S	4	7	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
8	FUB	SA	1	8	9,9,10	0.55	0	11,12,14	0.94	0
8	FUB	SA	2	8	9,9,10	0.54	0	11,12,14	0.84	0
8	FUB	SA	3	8	9,9,10	0.53	0	11,12,14	0.92	0
8	AHR	SA	4	8	9,9,10	0.57	0	11,12,14	0.99	0
8	AHR	SA	5	8	9,9,10	0.56	0	11,12,14	0.85	0
3	FUB	SB	1	3	9,9,10	0.56	0	11,12,14	1.08	1 (9%)
3	FUB	SB	2	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	FUB	SB	3	3	9,9,10	0.55	0	11,12,14	0.99	0
10	FUB	SC	1	10	9,9,10	0.54	0	11,12,14	0.90	0
10	FUB	SC	2	10	9,9,10	0.55	0	11,12,14	0.82	0
10	FUB	SC	3	10	9,9,10	0.58	0	11,12,14	0.90	0
10	AHR	SC	4	10	9,9,10	0.54	0	11,12,14	0.87	0
10	AHR	SC	5	10	9,9,10	0.56	0	11,12,14	1.02	1 (9%)
4	FUB	SD	1	4	9,9,10	0.55	0	11,12,14	0.97	0
4	FUB	SD	2	4	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
4	FUB	SD	3	4	9,9,10	0.55	0	11,12,14	0.88	0
4	AHR	SD	4	4	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
18	FUB	SE	1	18	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
18	FUB	SE	2	18	9,9,10	0.51	0	11,12,14	0.82	0
18	GZL	SE	3	18	11,11,12	6.61	6 (54%)	13,15,17	1.36	1 (7%)
18	AHR	SE	4	18	9,9,10	0.54	0	11,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	AHR	SE	5	18	9,9,10	0.54	0	11,12,14	0.96	0
3	FUB	T	1	3	9,9,10	0.51	0	11,12,14	1.08	1 (9%)
3	FUB	T	2	3	9,9,10	0.53	0	11,12,14	0.81	0
3	FUB	T	3	3	9,9,10	0.56	0	11,12,14	0.93	0
3	FUB	TA	1	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	FUB	TA	2	3	9,9,10	0.51	0	11,12,14	0.98	1 (9%)
3	FUB	TA	3	3	9,9,10	0.54	0	11,12,14	0.81	0
3	FUB	TB	1	3	9,9,10	0.53	0	11,12,14	0.75	0
3	FUB	TB	2	3	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
3	FUB	TB	3	3	9,9,10	0.54	0	11,12,14	0.85	0
3	FUB	TC	1	3	9,9,10	0.56	0	11,12,14	1.07	1 (9%)
3	FUB	TC	2	3	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
3	FUB	TC	3	3	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
3	FUB	TD	1	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	TD	2	3	9,9,10	0.57	0	11,12,14	0.91	0
3	FUB	TD	3	3	9,9,10	0.54	0	11,12,14	0.89	0
20	FUB	TE	1	20	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
20	FUB	TE	2	20	9,9,10	0.54	0	11,12,14	0.80	0
20	GZL	TE	3	20	11,11,12	6.60	7 (63%)	13,15,17	1.55	1 (7%)
20	AHR	TE	4	20	9,9,10	0.53	0	11,12,14	0.80	0
8	FUB	U	1	8	9,9,10	0.53	0	11,12,14	1.01	0
8	FUB	U	2	8	9,9,10	0.54	0	11,12,14	0.96	1 (9%)
8	FUB	U	3	8	9,9,10	0.56	0	11,12,14	0.88	0
8	AHR	U	4	8	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
8	AHR	U	5	8	9,9,10	0.57	0	11,12,14	0.92	0
4	FUB	UA	1	4	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
4	FUB	UA	2	4	9,9,10	0.54	0	11,12,14	0.84	0
4	FUB	UA	3	4	9,9,10	0.54	0	11,12,14	0.88	0
4	AHR	UA	4	4	9,9,10	0.55	0	11,12,14	0.89	0
3	FUB	UB	1	3	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
3	FUB	UB	2	3	9,9,10	0.54	0	11,12,14	0.75	0
3	FUB	UB	3	3	9,9,10	0.55	0	11,12,14	0.94	0
4	FUB	UC	1	4	9,9,10	0.50	0	11,12,14	0.88	0
4	FUB	UC	2	4	9,9,10	0.53	0	11,12,14	0.91	0
4	FUB	UC	3	4	9,9,10	0.54	0	11,12,14	0.93	0
4	AHR	UC	4	4	9,9,10	0.56	0	11,12,14	0.93	0
7	FUB	UD	1	7	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
7	FUB	UD	2	7	9,9,10	0.53	0	11,12,14	0.71	0
7	FUB	UD	3	7	9,9,10	0.55	0	11,12,14	0.84	0
7	AHR	UD	4	7	9,9,10	0.55	0	11,12,14	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	FUB	UE	1	20	9,9,10	0.52	0	11,12,14	0.87	0
20	FUB	UE	2	20	9,9,10	0.48	0	11,12,14	0.99	0
20	GZL	UE	3	20	11,11,12	6.61	6 (54%)	13,15,17	1.29	1 (7%)
20	AHR	UE	4	20	9,9,10	0.56	0	11,12,14	0.81	0
3	FUB	V	1	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	V	2	3	9,9,10	0.54	0	11,12,14	0.88	0
3	FUB	V	3	3	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
4	FUB	VA	1	4	9,9,10	0.53	0	11,12,14	0.92	0
4	FUB	VA	2	4	9,9,10	0.54	0	11,12,14	0.89	0
4	FUB	VA	3	4	9,9,10	0.53	0	11,12,14	0.83	0
4	AHR	VA	4	4	9,9,10	0.58	0	11,12,14	0.77	0
10	FUB	VB	1	10	9,9,10	0.52	0	11,12,14	0.91	0
10	FUB	VB	2	10	9,9,10	0.53	0	11,12,14	0.80	0
10	FUB	VB	3	10	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
10	AHR	VB	4	10	9,9,10	0.56	0	11,12,14	0.80	0
10	AHR	VB	5	10	9,9,10	0.56	0	11,12,14	0.95	1 (9%)
4	FUB	VC	1	4	9,9,10	0.53	0	11,12,14	0.85	0
4	FUB	VC	2	4	9,9,10	0.56	0	11,12,14	0.91	0
4	FUB	VC	3	4	9,9,10	0.56	0	11,12,14	0.85	0
4	AHR	VC	4	4	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
4	FUB	VD	1	4	9,9,10	0.55	0	11,12,14	0.92	0
4	FUB	VD	2	4	9,9,10	0.55	0	11,12,14	0.97	1 (9%)
4	FUB	VD	3	4	9,9,10	0.55	0	11,12,14	0.87	0
4	AHR	VD	4	4	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
22	FUB	VE	1	22	9,9,10	0.53	0	11,12,14	1.24	1 (9%)
22	FUB	VE	2	22	9,9,10	0.52	0	11,12,14	0.92	0
22	GZL	VE	3	22	11,11,12	6.59	6 (54%)	13,15,17	1.38	1 (7%)
22	AHR	VE	4	22	9,9,10	0.54	0	11,12,14	1.11	1 (9%)
22	AHR	VE	5	22	9,9,10	0.55	0	11,12,14	0.87	1 (9%)
22	AHR	VE	6	22	9,9,10	0.56	0	11,12,14	0.92	0
4	FUB	W	1	4	9,9,10	0.55	0	11,12,14	0.84	0
4	FUB	W	2	4	9,9,10	0.55	0	11,12,14	0.78	0
4	FUB	W	3	4	9,9,10	0.55	0	11,12,14	0.84	0
4	AHR	W	4	4	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
9	FUB	WA	1	9	9,9,10	0.54	0	11,12,14	0.84	0
9	FUB	WA	2	9	9,9,10	0.55	0	11,12,14	0.92	0
13	FUB	WB	1	13	9,9,10	0.51	0	11,12,14	0.93	0
13	FUB	WB	2	13	9,9,10	0.52	0	11,12,14	1.03	1 (9%)
13	GZL	WB	3	13	11,11,12	6.66	7 (63%)	13,15,17	1.24	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	AHR	WB	4	13	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
3	FUB	WC	1	3	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
3	FUB	WC	2	3	9,9,10	0.55	0	11,12,14	0.89	0
3	FUB	WC	3	3	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
7	FUB	WD	1	7	9,9,10	0.58	0	11,12,14	0.92	0
7	FUB	WD	2	7	9,9,10	0.56	0	11,12,14	1.06	0
7	FUB	WD	3	7	9,9,10	0.55	0	11,12,14	0.93	0
7	AHR	WD	4	7	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
20	FUB	WE	1	20	9,9,10	0.52	0	11,12,14	0.90	0
20	FUB	WE	2	20	9,9,10	0.54	0	11,12,14	0.81	0
20	GZL	WE	3	20	11,11,12	6.59	7 (63%)	13,15,17	1.32	1 (7%)
20	AHR	WE	4	20	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
4	FUB	X	1	4	9,9,10	0.51	0	11,12,14	0.92	0
4	FUB	X	2	4	9,9,10	0.52	0	11,12,14	0.79	0
4	FUB	X	3	4	9,9,10	0.55	0	11,12,14	0.84	0
4	AHR	X	4	4	9,9,10	0.56	0	11,12,14	0.96	0
3	FUB	XA	1	3	9,9,10	0.54	0	11,12,14	1.00	0
3	FUB	XA	2	3	9,9,10	0.52	0	11,12,14	0.63	0
3	FUB	XA	3	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
6	FUB	XB	1	6	9,9,10	0.55	0	11,12,14	1.00	0
6	FUB	XB	2	6	9,9,10	0.56	0	11,12,14	1.03	1 (9%)
6	GZL	XB	3	6	11,11,12	6.86	6 (54%)	13,15,17	4.11	4 (30%)
7	FUB	XC	1	7	9,9,10	0.56	0	11,12,14	1.03	0
7	FUB	XC	2	7	9,9,10	0.52	0	11,12,14	0.94	1 (9%)
7	FUB	XC	3	7	9,9,10	0.57	0	11,12,14	0.87	0
7	AHR	XC	4	7	9,9,10	0.55	0	11,12,14	0.81	0
11	FUB	XD	1	11	9,9,10	0.63	0	11,12,14	1.21	1 (9%)
11	AHR	XD	2	11	9,9,10	0.55	0	11,12,14	0.98	0
11	AHR	XD	3	11	9,9,10	0.53	0	11,12,14	1.05	1 (9%)
23	FUB	XE	1	23	9,9,10	0.56	0	11,12,14	1.14	1 (9%)
23	FUB	XE	2	23	9,9,10	0.53	0	11,12,14	0.74	0
23	GZL	XE	3	23	11,11,12	6.58	6 (54%)	13,15,17	1.38	1 (7%)
23	AHR	XE	4	23	9,9,10	0.56	0	11,12,14	0.85	1 (9%)
23	AHR	XE	5	23	9,9,10	0.55	0	11,12,14	0.91	0
23	AHR	XE	6	23	9,9,10	0.53	0	11,12,14	0.96	0
9	FUB	Y	1	9	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
9	FUB	Y	2	9	9,9,10	0.55	0	11,12,14	0.99	0
10	FUB	YA	1	10	9,9,10	0.54	0	11,12,14	0.80	0
10	FUB	YA	2	10	9,9,10	0.55	0	11,12,14	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	FUB	YA	3	10	9,9,10	0.55	0	11,12,14	0.81	0
10	AHR	YA	4	10	9,9,10	0.55	0	11,12,14	0.97	0
10	AHR	YA	5	10	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
13	FUB	YB	1	13	9,9,10	0.51	0	11,12,14	0.76	0
13	FUB	YB	2	13	9,9,10	0.55	0	11,12,14	0.76	0
13	GZL	YB	3	13	11,11,12	6.63	6 (54%)	13,15,17	1.16	1 (7%)
13	AHR	YB	4	13	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
4	FUB	YC	1	4	9,9,10	0.55	0	11,12,14	0.87	0
4	FUB	YC	2	4	9,9,10	0.53	0	11,12,14	0.94	1 (9%)
4	FUB	YC	3	4	9,9,10	0.54	0	11,12,14	0.81	0
4	AHR	YC	4	4	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
9	FUB	YD	1	9	9,9,10	0.52	0	11,12,14	0.63	0
9	FUB	YD	2	9	9,9,10	0.53	0	11,12,14	0.79	0
24	FUB	YE	1	24	9,9,10	0.52	0	11,12,14	1.35	1 (9%)
24	FUB	YE	2	24	9,9,10	0.53	0	11,12,14	0.79	0
24	GZL	YE	3	24	11,11,12	6.59	7 (63%)	13,15,17	1.35	1 (7%)
24	AHR	YE	4	24	9,9,10	0.56	0	11,12,14	1.06	2 (18%)
24	AHR	YE	5	24	9,9,10	0.55	0	11,12,14	1.12	1 (9%)
24	AHR	YE	6	24	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
4	FUB	Z	1	4	9,9,10	0.53	0	11,12,14	1.09	1 (9%)
4	FUB	Z	2	4	9,9,10	0.54	0	11,12,14	0.91	0
4	FUB	Z	3	4	9,9,10	0.53	0	11,12,14	0.81	0
4	AHR	Z	4	4	9,9,10	0.55	0	11,12,14	1.10	1 (9%)
3	FUB	ZA	1	3	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
3	FUB	ZA	2	3	9,9,10	0.54	0	11,12,14	0.88	0
3	FUB	ZA	3	3	9,9,10	0.54	0	11,12,14	0.91	0
13	FUB	ZB	1	13	9,9,10	0.56	0	11,12,14	0.97	0
13	FUB	ZB	2	13	9,9,10	0.54	0	11,12,14	0.90	0
13	GZL	ZB	3	13	11,11,12	6.59	7 (63%)	13,15,17	1.43	2 (15%)
13	AHR	ZB	4	13	9,9,10	0.54	0	11,12,14	0.92	0
7	FUB	ZC	1	7	9,9,10	0.53	0	11,12,14	0.82	0
7	FUB	ZC	2	7	9,9,10	0.54	0	11,12,14	0.90	0
7	FUB	ZC	3	7	9,9,10	0.52	0	11,12,14	1.09	1 (9%)
7	AHR	ZC	4	7	9,9,10	0.55	0	11,12,14	0.99	0
4	FUB	ZD	1	4	9,9,10	0.54	0	11,12,14	0.96	1 (9%)
4	FUB	ZD	2	4	9,9,10	0.55	0	11,12,14	0.84	0
4	FUB	ZD	3	4	9,9,10	0.56	0	11,12,14	0.91	0
4	AHR	ZD	4	4	9,9,10	0.55	0	11,12,14	0.97	0
6	FUB	ZE	1	6	9,9,10	0.54	0	11,12,14	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FUB	ZE	2	6	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
6	GZL	ZE	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.40	1 (7%)
10	FUB	a	1	10	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
10	FUB	a	2	10	9,9,10	0.54	0	11,12,14	0.95	0
10	FUB	a	3	10	9,9,10	0.55	0	11,12,14	0.83	0
10	AHR	a	4	10	9,9,10	0.53	0	11,12,14	1.12	1 (9%)
10	AHR	a	5	10	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
4	FUB	aA	1	4	9,9,10	0.53	0	11,12,14	0.78	0
4	FUB	aA	2	4	9,9,10	0.56	0	11,12,14	0.90	0
4	FUB	aA	3	4	9,9,10	0.54	0	11,12,14	0.95	0
4	AHR	aA	4	4	9,9,10	0.54	0	11,12,14	0.96	0
6	FUB	aB	1	6	9,9,10	0.54	0	11,12,14	0.88	0
6	FUB	aB	2	6	9,9,10	0.51	0	11,12,14	1.18	2 (18%)
6	GZL	aB	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.34	1 (7%)
11	FUB	aC	1	11	9,9,10	0.61	0	11,12,14	1.10	0
11	AHR	aC	2	11	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
11	AHR	aC	3	11	9,9,10	0.56	0	11,12,14	0.98	0
3	FUB	aD	1	3	9,9,10	0.55	0	11,12,14	0.91	0
3	FUB	aD	2	3	9,9,10	0.55	0	11,12,14	0.93	0
3	FUB	aD	3	3	9,9,10	0.55	0	11,12,14	0.87	0
19	FUB	aE	1	19	9,9,10	0.56	0	11,12,14	0.87	0
19	FUB	aE	2	19	9,9,10	0.54	0	11,12,14	0.96	0
19	GZL	aE	3	19	11,11,12	6.55	7 (63%)	13,15,17	1.49	2 (15%)
19	AHR	aE	4	19	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
3	FUB	b	1	3	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
3	FUB	b	2	3	9,9,10	0.54	0	11,12,14	0.93	0
3	FUB	b	3	3	9,9,10	0.56	0	11,12,14	0.89	0
4	FUB	bA	1	4	9,9,10	0.52	0	11,12,14	0.87	0
4	FUB	bA	2	4	9,9,10	0.55	0	11,12,14	0.86	0
4	FUB	bA	3	4	9,9,10	0.54	0	11,12,14	0.95	0
4	AHR	bA	4	4	9,9,10	0.55	0	11,12,14	0.88	0
6	FUB	bB	1	6	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
6	FUB	bB	2	6	9,9,10	0.57	0	11,12,14	0.94	0
6	GZL	bB	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.35	1 (7%)
9	FUB	bC	1	9	9,9,10	0.54	0	11,12,14	0.72	0
9	FUB	bC	2	9	9,9,10	0.52	0	11,12,14	0.83	0
3	FUB	bD	1	3	9,9,10	0.49	0	11,12,14	0.85	0
3	FUB	bD	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	bD	3	3	9,9,10	0.55	0	11,12,14	0.82	0
6	FUB	bE	1	6	9,9,10	0.59	0	11,12,14	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FUB	bE	2	6	9,9,10	0.53	0	11,12,14	0.83	0
6	GZL	bE	3	6	11,11,12	6.62	7 (63%)	13,15,17	1.46	1 (7%)
4	FUB	c	1	4	9,9,10	0.54	0	11,12,14	0.79	0
4	FUB	c	2	4	9,9,10	0.55	0	11,12,14	0.88	0
4	FUB	c	3	4	9,9,10	0.52	0	11,12,14	0.90	0
4	AHR	c	4	4	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
3	FUB	cA	1	3	9,9,10	0.53	0	11,12,14	0.84	0
3	FUB	cA	2	3	9,9,10	0.56	0	11,12,14	0.96	1 (9%)
3	FUB	cA	3	3	9,9,10	0.56	0	11,12,14	1.03	1 (9%)
6	FUB	cB	1	6	9,9,10	0.54	0	11,12,14	0.95	1 (9%)
6	FUB	cB	2	6	9,9,10	0.56	0	11,12,14	1.06	1 (9%)
6	GZL	cB	3	6	11,11,12	6.60	6 (54%)	13,15,17	1.52	2 (15%)
4	FUB	cC	1	4	9,9,10	0.54	0	11,12,14	1.15	1 (9%)
4	FUB	cC	2	4	9,9,10	0.54	0	11,12,14	0.84	0
4	FUB	cC	3	4	9,9,10	0.54	0	11,12,14	0.93	0
4	AHR	cC	4	4	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
12	FUB	cD	1	12	9,9,10	0.54	0	11,12,14	0.80	0
12	FUB	cD	2	12	9,9,10	0.56	0	11,12,14	0.94	0
12	GZL	cD	3	12	11,11,12	6.58	7 (63%)	13,15,17	1.29	1 (7%)
12	AHR	cD	4	12	9,9,10	0.55	0	11,12,14	0.96	0
12	AHR	cD	5	12	9,9,10	0.57	0	11,12,14	0.98	1 (9%)
18	FUB	cE	1	18	9,9,10	0.52	0	11,12,14	0.97	1 (9%)
18	FUB	cE	2	18	9,9,10	0.56	0	11,12,14	0.88	0
18	GZL	cE	3	18	11,11,12	6.59	7 (63%)	13,15,17	1.50	1 (7%)
18	AHR	cE	4	18	9,9,10	0.55	0	11,12,14	0.93	0
18	AHR	cE	5	18	9,9,10	0.55	0	11,12,14	0.85	0
4	FUB	d	1	4	9,9,10	0.53	0	11,12,14	0.94	1 (9%)
4	FUB	d	2	4	9,9,10	0.54	0	11,12,14	0.89	0
4	FUB	d	3	4	9,9,10	0.55	0	11,12,14	0.98	0
4	AHR	d	4	4	9,9,10	0.54	0	11,12,14	1.09	1 (9%)
7	FUB	dA	1	7	9,9,10	0.53	0	11,12,14	1.06	1 (9%)
7	FUB	dA	2	7	9,9,10	0.52	0	11,12,14	1.03	1 (9%)
7	FUB	dA	3	7	9,9,10	0.53	0	11,12,14	0.86	0
7	AHR	dA	4	7	9,9,10	0.55	0	11,12,14	0.81	0
13	FUB	dB	1	13	9,9,10	0.55	0	11,12,14	0.77	0
13	FUB	dB	2	13	9,9,10	0.53	0	11,12,14	1.09	1 (9%)
13	GZL	dB	3	13	11,11,12	6.61	7 (63%)	13,15,17	1.89	4 (30%)
13	AHR	dB	4	13	9,9,10	0.54	0	11,12,14	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	dC	1	3	9,9,10	0.53	0	11,12,14	0.85	0
3	FUB	dC	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	dC	3	3	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
13	FUB	dD	1	13	9,9,10	0.57	0	11,12,14	0.87	0
13	FUB	dD	2	13	9,9,10	0.53	0	11,12,14	0.84	0
13	GZL	dD	3	13	11,11,12	6.58	7 (63%)	13,15,17	1.22	1 (7%)
13	AHR	dD	4	13	9,9,10	0.53	0	11,12,14	0.91	0
22	FUB	dE	1	22	9,9,10	0.54	0	11,12,14	0.88	1 (9%)
22	FUB	dE	2	22	9,9,10	0.55	0	11,12,14	0.97	1 (9%)
22	GZL	dE	3	22	11,11,12	6.58	7 (63%)	13,15,17	1.45	1 (7%)
22	AHR	dE	4	22	9,9,10	0.53	0	11,12,14	1.10	1 (9%)
22	AHR	dE	5	22	9,9,10	0.55	0	11,12,14	1.05	0
22	AHR	dE	6	22	9,9,10	0.53	0	11,12,14	1.05	1 (9%)
3	FUB	e	1	3	9,9,10	0.56	0	11,12,14	0.83	0
3	FUB	e	2	3	9,9,10	0.56	0	11,12,14	0.91	0
3	FUB	e	3	3	9,9,10	0.55	0	11,12,14	1.06	1 (9%)
4	FUB	eA	1	4	9,9,10	0.55	0	11,12,14	0.96	0
4	FUB	eA	2	4	9,9,10	0.54	0	11,12,14	0.82	0
4	FUB	eA	3	4	9,9,10	0.56	0	11,12,14	0.99	0
4	AHR	eA	4	4	9,9,10	0.56	0	11,12,14	0.93	0
15	FUB	eB	1	15	9,9,10	0.52	0	11,12,14	0.96	1 (9%)
15	FUB	eB	2	15	9,9,10	0.54	0	11,12,14	0.89	0
15	GZL	eB	3	15	11,11,12	6.61	6 (54%)	13,15,17	1.38	1 (7%)
15	AHR	eB	4	15	9,9,10	0.58	0	11,12,14	1.18	1 (9%)
15	AHR	eB	5	15	9,9,10	0.56	0	11,12,14	0.95	0
3	FUB	eC	1	3	9,9,10	0.53	0	11,12,14	0.72	0
3	FUB	eC	2	3	9,9,10	0.55	0	11,12,14	0.88	0
3	FUB	eC	3	3	9,9,10	0.56	0	11,12,14	0.89	0
14	FUB	eD	1	14	9,9,10	0.54	0	11,12,14	0.89	0
14	FUB	eD	2	14	9,9,10	0.55	0	11,12,14	0.83	0
14	GZL	eD	3	14	11,11,12	6.56	7 (63%)	13,15,17	1.73	2 (15%)
14	FUB	eD	4	14	9,9,10	0.57	0	11,12,14	0.99	0
22	FUB	eE	1	22	9,9,10	0.58	0	11,12,14	1.15	1 (9%)
22	FUB	eE	2	22	9,9,10	0.55	0	11,12,14	0.88	0
22	GZL	eE	3	22	11,11,12	6.60	6 (54%)	13,15,17	1.47	1 (7%)
22	AHR	eE	4	22	9,9,10	0.54	0	11,12,14	0.96	1 (9%)
22	AHR	eE	5	22	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
22	AHR	eE	6	22	9,9,10	0.56	0	11,12,14	1.12	1 (9%)
7	FUB	f	1	7	9,9,10	0.53	0	11,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	FUB	f	2	7	9,9,10	0.52	0	11,12,14	1.01	1 (9%)
7	FUB	f	3	7	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
7	AHR	f	4	7	9,9,10	0.51	0	11,12,14	0.82	0
7	FUB	fA	1	7	9,9,10	0.55	0	11,12,14	0.96	0
7	FUB	fA	2	7	9,9,10	0.55	0	11,12,14	0.90	0
7	FUB	fA	3	7	9,9,10	0.56	0	11,12,14	0.94	0
7	AHR	fA	4	7	9,9,10	0.54	0	11,12,14	0.96	0
15	FUB	fB	1	15	9,9,10	0.54	0	11,12,14	0.97	0
15	FUB	fB	2	15	9,9,10	0.55	0	11,12,14	0.86	0
15	GZL	fB	3	15	11,11,12	6.60	6 (54%)	13,15,17	1.26	1 (7%)
15	AHR	fB	4	15	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
15	AHR	fB	5	15	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
12	FUB	fC	1	12	9,9,10	0.56	0	11,12,14	0.92	0
12	FUB	fC	2	12	9,9,10	0.54	0	11,12,14	0.85	0
12	GZL	fC	3	12	11,11,12	6.60	6 (54%)	13,15,17	1.26	1 (7%)
12	AHR	fC	4	12	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
12	AHR	fC	5	12	9,9,10	0.56	0	11,12,14	1.00	0
12	FUB	fD	1	12	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
12	FUB	fD	2	12	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
12	GZL	fD	3	12	11,11,12	6.56	7 (63%)	13,15,17	1.14	1 (7%)
12	AHR	fD	4	12	9,9,10	0.53	0	11,12,14	0.91	0
12	AHR	fD	5	12	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
18	FUB	fE	1	18	9,9,10	0.51	0	11,12,14	1.04	1 (9%)
18	FUB	fE	2	18	9,9,10	0.52	0	11,12,14	0.87	0
18	GZL	fE	3	18	11,11,12	6.58	6 (54%)	13,15,17	1.28	1 (7%)
18	AHR	fE	4	18	9,9,10	0.54	0	11,12,14	1.00	0
18	AHR	fE	5	18	9,9,10	0.55	0	11,12,14	0.85	0
4	FUB	g	1	4	9,9,10	0.53	0	11,12,14	0.99	0
4	FUB	g	2	4	9,9,10	0.56	0	11,12,14	0.88	0
4	FUB	g	3	4	9,9,10	0.54	0	11,12,14	0.90	0
4	AHR	g	4	4	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
11	FUB	gA	1	11	9,9,10	0.63	0	11,12,14	1.38	1 (9%)
11	AHR	gA	2	11	9,9,10	0.55	0	11,12,14	0.93	0
11	AHR	gA	3	11	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
6	FUB	gB	1	6	9,9,10	0.55	0	11,12,14	0.83	0
6	FUB	gB	2	6	9,9,10	0.53	0	11,12,14	0.88	0
6	GZL	gB	3	6	11,11,12	6.57	7 (63%)	13,15,17	1.50	2 (15%)
13	FUB	gC	1	13	9,9,10	0.56	0	11,12,14	0.85	0
13	FUB	gC	2	13	9,9,10	0.56	0	11,12,14	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	GZL	gC	3	13	11,11,12	6.61	7 (63%)	13,15,17	1.25	1 (7%)
13	AHR	gC	4	13	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
4	FUB	gD	1	4	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
4	FUB	gD	2	4	9,9,10	0.54	0	11,12,14	0.97	0
4	FUB	gD	3	4	9,9,10	0.54	0	11,12,14	0.78	0
4	AHR	gD	4	4	9,9,10	0.54	0	11,12,14	0.72	0
20	FUB	gE	1	20	9,9,10	0.53	0	11,12,14	0.87	0
20	FUB	gE	2	20	9,9,10	0.56	0	11,12,14	1.00	0
20	GZL	gE	3	20	11,11,12	6.60	7 (63%)	13,15,17	1.26	1 (7%)
20	AHR	gE	4	20	9,9,10	0.55	0	11,12,14	0.84	0
7	FUB	h	1	7	9,9,10	0.54	0	11,12,14	0.96	0
7	FUB	h	2	7	9,9,10	0.57	0	11,12,14	0.94	0
7	FUB	h	3	7	9,9,10	0.55	0	11,12,14	0.97	0
7	AHR	h	4	7	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
9	FUB	hA	1	9	9,9,10	0.52	0	11,12,14	0.87	1 (9%)
9	FUB	hA	2	9	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	hB	1	3	9,9,10	0.55	0	11,12,14	0.81	0
3	FUB	hB	2	3	9,9,10	0.55	0	11,12,14	0.85	0
3	FUB	hB	3	3	9,9,10	0.56	0	11,12,14	0.92	0
14	FUB	hC	1	14	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
14	FUB	hC	2	14	9,9,10	0.54	0	11,12,14	0.86	0
14	GZL	hC	3	14	11,11,12	6.58	7 (63%)	13,15,17	1.62	2 (15%)
14	FUB	hC	4	14	9,9,10	0.57	0	11,12,14	0.85	0
14	FUB	hD	1	14	9,9,10	0.54	0	11,12,14	0.95	0
14	FUB	hD	2	14	9,9,10	0.55	0	11,12,14	1.02	0
14	GZL	hD	3	14	11,11,12	6.48	7 (63%)	13,15,17	1.57	2 (15%)
14	FUB	hD	4	14	9,9,10	0.54	0	11,12,14	0.91	0
20	FUB	hE	1	20	9,9,10	0.54	0	11,12,14	0.95	0
20	FUB	hE	2	20	9,9,10	0.54	0	11,12,14	0.83	0
20	GZL	hE	3	20	11,11,12	6.58	7 (63%)	13,15,17	1.38	1 (7%)
20	AHR	hE	4	20	9,9,10	0.54	0	11,12,14	0.87	0
11	FUB	i	1	11	9,9,10	0.62	0	11,12,14	1.29	1 (9%)
11	AHR	i	2	11	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
11	AHR	i	3	11	9,9,10	0.52	0	11,12,14	1.04	1 (9%)
4	FUB	iA	1	4	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
4	FUB	iA	2	4	9,9,10	0.54	0	11,12,14	0.94	0
4	FUB	iA	3	4	9,9,10	0.54	0	11,12,14	0.85	0
4	AHR	iA	4	4	9,9,10	0.54	0	11,12,14	1.13	1 (9%)
12	FUB	iB	1	12	9,9,10	0.57	0	11,12,14	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FUB	iB	2	12	9,9,10	0.56	0	11,12,14	0.98	0
12	GZL	iB	3	12	11,11,12	6.57	7 (63%)	13,15,17	1.50	2 (15%)
12	AHR	iB	4	12	9,9,10	0.55	0	11,12,14	0.99	0
12	AHR	iB	5	12	9,9,10	0.57	0	11,12,14	0.95	0
12	FUB	iC	1	12	9,9,10	0.54	0	11,12,14	1.07	1 (9%)
12	FUB	iC	2	12	9,9,10	0.55	0	11,12,14	0.95	1 (9%)
12	GZL	iC	3	12	11,11,12	6.54	7 (63%)	13,15,17	1.33	1 (7%)
12	AHR	iC	4	12	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
12	AHR	iC	5	12	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
3	FUB	iD	1	3	9,9,10	0.54	0	11,12,14	0.96	0
3	FUB	iD	2	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	iD	3	3	9,9,10	0.54	0	11,12,14	0.91	0
22	FUB	iE	1	22	9,9,10	0.52	0	11,12,14	1.10	1 (9%)
22	FUB	iE	2	22	9,9,10	0.53	0	11,12,14	0.86	0
22	GZL	iE	3	22	11,11,12	6.61	6 (54%)	13,15,17	1.28	1 (7%)
22	AHR	iE	4	22	9,9,10	0.57	0	11,12,14	0.98	0
22	AHR	iE	5	22	9,9,10	0.54	0	11,12,14	0.60	0
22	AHR	iE	6	22	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
9	FUB	j	1	9	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
9	FUB	j	2	9	9,9,10	0.54	0	11,12,14	0.77	0
3	FUB	jA	1	3	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
3	FUB	jA	2	3	9,9,10	0.56	0	11,12,14	0.88	0
3	FUB	jA	3	3	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
13	FUB	jB	1	13	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
13	FUB	jB	2	13	9,9,10	0.54	0	11,12,14	0.88	0
13	GZL	jB	3	13	11,11,12	6.61	7 (63%)	13,15,17	1.33	1 (7%)
13	AHR	jB	4	13	9,9,10	0.56	0	11,12,14	0.96	0
4	FUB	jC	1	4	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
4	FUB	jC	2	4	9,9,10	0.55	0	11,12,14	0.94	0
4	FUB	jC	3	4	9,9,10	0.54	0	11,12,14	0.96	0
4	AHR	jC	4	4	9,9,10	0.54	0	11,12,14	0.85	0
10	FUB	jD	1	10	9,9,10	0.52	0	11,12,14	1.11	1 (9%)
10	FUB	jD	2	10	9,9,10	0.56	0	11,12,14	0.95	0
10	FUB	jD	3	10	9,9,10	0.55	0	11,12,14	0.91	0
10	AHR	jD	4	10	9,9,10	0.56	0	11,12,14	0.95	0
10	AHR	jD	5	10	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
20	FUB	jE	1	20	9,9,10	0.56	0	11,12,14	0.99	0
20	FUB	jE	2	20	9,9,10	0.54	0	11,12,14	0.90	0
20	GZL	jE	3	20	11,11,12	6.58	6 (54%)	13,15,17	1.51	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
20	AHR	jE	4	20	9,9,10	0.55	0	11,12,14	0.88	0
4	FUB	k	1	4	9,9,10	0.56	0	11,12,14	0.83	0
4	FUB	k	2	4	9,9,10	0.56	0	11,12,14	0.94	0
4	FUB	k	3	4	9,9,10	0.53	0	11,12,14	0.90	0
4	AHR	k	4	4	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	kA	1	3	9,9,10	0.51	0	11,12,14	0.76	0
3	FUB	kA	2	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	kA	3	3	9,9,10	0.55	0	11,12,14	0.86	0
14	FUB	kB	1	14	9,9,10	0.56	0	11,12,14	0.89	0
14	FUB	kB	2	14	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
14	GZL	kB	3	14	11,11,12	6.51	7 (63%)	13,15,17	1.61	3 (23%)
14	FUB	kB	4	14	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
14	FUB	kC	1	14	9,9,10	0.55	0	11,12,14	0.95	0
14	FUB	kC	2	14	9,9,10	0.56	0	11,12,14	0.95	0
14	GZL	kC	3	14	11,11,12	6.52	7 (63%)	13,15,17	1.89	2 (15%)
14	FUB	kC	4	14	9,9,10	0.58	0	11,12,14	0.87	0
4	FUB	kD	1	4	9,9,10	0.57	0	11,12,14	0.94	0
4	FUB	kD	2	4	9,9,10	0.55	0	11,12,14	0.85	0
4	FUB	kD	3	4	9,9,10	0.53	0	11,12,14	0.89	0
4	AHR	kD	4	4	9,9,10	0.54	0	11,12,14	0.92	0
21	FUB	kE	1	21	9,9,10	0.54	0	11,12,14	1.09	1 (9%)
21	FUB	kE	2	21	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
21	GZL	kE	3	21	11,11,12	6.60	6 (54%)	13,15,17	1.23	1 (7%)
21	AHR	kE	4	21	9,9,10	0.56	0	11,12,14	0.96	0
21	AHR	kE	5	21	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
3	FUB	l	1	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	l	2	3	9,9,10	0.51	0	11,12,14	0.82	0
3	FUB	l	3	3	9,9,10	0.54	0	11,12,14	0.87	0
12	FUB	lA	1	12	9,9,10	0.52	0	11,12,14	0.90	0
12	FUB	lA	2	12	9,9,10	0.56	0	11,12,14	0.92	0
12	GZL	lA	3	12	11,11,12	6.59	7 (63%)	13,15,17	1.22	1 (7%)
12	AHR	lA	4	12	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
12	AHR	lA	5	12	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
12	FUB	lB	1	12	9,9,10	0.52	0	11,12,14	1.10	1 (9%)
12	FUB	lB	2	12	9,9,10	0.55	0	11,12,14	0.93	0
12	GZL	lB	3	12	11,11,12	6.57	7 (63%)	13,15,17	1.25	1 (7%)
12	AHR	lB	4	12	9,9,10	0.54	0	11,12,14	0.98	0
12	AHR	lB	5	12	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	lC	1	3	9,9,10	0.54	0	11,12,14	0.81	0
3	FUB	lC	2	3	9,9,10	0.54	0	11,12,14	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	FUB	lC	3	3	9,9,10	0.56	0	11,12,14	0.97	0
3	FUB	lD	1	3	9,9,10	0.56	0	11,12,14	0.87	0
3	FUB	lD	2	3	9,9,10	0.54	0	11,12,14	0.92	0
3	FUB	lD	3	3	9,9,10	0.56	0	11,12,14	0.85	0
24	FUB	lE	1	24	9,9,10	0.52	0	11,12,14	1.22	1 (9%)
24	FUB	lE	2	24	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
24	GZL	lE	3	24	11,11,12	6.57	7 (63%)	13,15,17	1.43	1 (7%)
24	AHR	lE	4	24	9,9,10	0.57	0	11,12,14	1.11	2 (18%)
24	AHR	lE	5	24	9,9,10	0.53	0	11,12,14	1.05	1 (9%)
24	AHR	lE	6	24	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
3	FUB	m	1	3	9,9,10	0.51	0	11,12,14	0.86	0
3	FUB	m	2	3	9,9,10	0.54	0	11,12,14	0.80	0
3	FUB	m	3	3	9,9,10	0.55	0	11,12,14	0.86	0
13	FUB	mA	1	13	9,9,10	0.54	0	11,12,14	0.83	0
13	FUB	mA	2	13	9,9,10	0.57	0	11,12,14	0.88	0
13	GZL	mA	3	13	11,11,12	6.61	6 (54%)	13,15,17	1.26	1 (7%)
13	AHR	mA	4	13	9,9,10	0.52	0	11,12,14	1.03	1 (9%)
4	FUB	mB	1	4	9,9,10	0.53	0	11,12,14	0.96	1 (9%)
4	FUB	mB	2	4	9,9,10	0.53	0	11,12,14	0.92	0
4	FUB	mB	3	4	9,9,10	0.55	0	11,12,14	1.00	0
4	AHR	mB	4	4	9,9,10	0.55	0	11,12,14	0.87	1 (9%)
10	FUB	mC	1	10	9,9,10	0.55	0	11,12,14	1.09	1 (9%)
10	FUB	mC	2	10	9,9,10	0.56	0	11,12,14	0.97	0
10	FUB	mC	3	10	9,9,10	0.55	0	11,12,14	0.82	0
10	AHR	mC	4	10	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
10	AHR	mC	5	10	9,9,10	0.54	0	11,12,14	1.13	1 (9%)
3	FUB	mD	1	3	9,9,10	0.54	0	11,12,14	0.71	0
3	FUB	mD	2	3	9,9,10	0.55	0	11,12,14	0.96	0
3	FUB	mD	3	3	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
6	FUB	mE	1	6	9,9,10	0.56	0	11,12,14	0.96	0
6	FUB	mE	2	6	9,9,10	0.55	0	11,12,14	0.95	0
6	GZL	mE	3	6	11,11,12	6.58	6 (54%)	13,15,17	1.64	2 (15%)
12	FUB	n	1	12	9,9,10	0.53	0	11,12,14	0.84	0
12	FUB	n	2	12	9,9,10	0.55	0	11,12,14	0.82	0
12	GZL	n	3	12	11,11,12	6.58	7 (63%)	13,15,17	1.28	1 (7%)
12	AHR	n	4	12	9,9,10	0.53	0	11,12,14	1.09	1 (9%)
12	AHR	n	5	12	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
14	FUB	nA	1	14	9,9,10	0.50	0	11,12,14	0.88	0
14	FUB	nA	2	14	9,9,10	0.56	0	11,12,14	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	GZL	nA	3	14	11,11,12	6.58	6 (54%)	13,15,17	1.92	4 (30%)
14	FUB	nA	4	14	9,9,10	0.56	0	11,12,14	1.05	0
14	FUB	nB	1	14	9,9,10	0.55	0	11,12,14	0.89	0
14	FUB	nB	2	14	9,9,10	0.55	0	11,12,14	0.99	0
14	GZL	nB	3	14	11,11,12	6.53	7 (63%)	13,15,17	1.61	3 (23%)
14	FUB	nB	4	14	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
4	FUB	nC	1	4	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
4	FUB	nC	2	4	9,9,10	0.54	0	11,12,14	0.96	0
4	FUB	nC	3	4	9,9,10	0.55	0	11,12,14	0.94	0
4	AHR	nC	4	4	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
3	FUB	nD	1	3	9,9,10	0.57	0	11,12,14	0.98	0
3	FUB	nD	2	3	9,9,10	0.56	0	11,12,14	0.93	0
3	FUB	nD	3	3	9,9,10	0.52	0	11,12,14	0.65	0
6	FUB	nE	1	6	9,9,10	0.55	0	11,12,14	1.08	1 (9%)
6	FUB	nE	2	6	9,9,10	0.55	0	11,12,14	0.95	0
6	GZL	nE	3	6	11,11,12	6.55	7 (63%)	13,15,17	1.49	1 (7%)
13	FUB	o	1	13	9,9,10	0.55	0	11,12,14	0.78	0
13	FUB	o	2	13	9,9,10	0.56	0	11,12,14	0.85	0
13	GZL	o	3	13	11,11,12	6.62	7 (63%)	13,15,17	1.26	1 (7%)
13	AHR	o	4	13	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
12	FUB	oA	1	12	9,9,10	0.52	0	11,12,14	1.06	1 (9%)
12	FUB	oA	2	12	9,9,10	0.54	0	11,12,14	0.91	0
12	GZL	oA	3	12	11,11,12	6.60	6 (54%)	13,15,17	1.27	1 (7%)
12	AHR	oA	4	12	9,9,10	0.57	0	11,12,14	0.91	0
12	AHR	oA	5	12	9,9,10	0.57	0	11,12,14	1.02	0
3	FUB	oB	1	3	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
3	FUB	oB	2	3	9,9,10	0.54	0	11,12,14	0.82	0
3	FUB	oB	3	3	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
3	FUB	oC	1	3	9,9,10	0.57	0	11,12,14	0.91	0
3	FUB	oC	2	3	9,9,10	0.54	0	11,12,14	0.90	0
3	FUB	oC	3	3	9,9,10	0.57	0	11,12,14	0.88	0
3	FUB	oD	1	3	9,9,10	0.56	0	11,12,14	0.96	0
3	FUB	oD	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	oD	3	3	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
6	FUB	oE	1	6	9,9,10	0.55	0	11,12,14	0.78	0
6	FUB	oE	2	6	9,9,10	0.54	0	11,12,14	0.96	1 (9%)
6	GZL	oE	3	6	11,11,12	6.55	7 (63%)	13,15,17	1.65	2 (15%)
14	FUB	p	1	14	9,9,10	0.52	0	11,12,14	0.85	0
14	FUB	p	2	14	9,9,10	0.55	0	11,12,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	GZL	p	3	14	11,11,12	6.56	6 (54%)	13,15,17	1.72	4 (30%)
14	FUB	p	4	14	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
4	FUB	pA	1	4	9,9,10	0.54	0	11,12,14	0.74	0
4	FUB	pA	2	4	9,9,10	0.54	0	11,12,14	0.83	0
4	FUB	pA	3	4	9,9,10	0.55	0	11,12,14	0.80	0
4	AHR	pA	4	4	9,9,10	0.53	0	11,12,14	0.83	0
10	FUB	pB	1	10	9,9,10	0.56	0	11,12,14	1.05	0
10	FUB	pB	2	10	9,9,10	0.55	0	11,12,14	1.02	0
10	FUB	pB	3	10	9,9,10	0.55	0	11,12,14	0.83	0
10	AHR	pB	4	10	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
10	AHR	pB	5	10	9,9,10	0.55	0	11,12,14	1.11	1 (9%)
3	FUB	pC	1	3	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
3	FUB	pC	2	3	9,9,10	0.55	0	11,12,14	1.01	0
3	FUB	pC	3	3	9,9,10	0.55	0	11,12,14	0.88	0
3	FUB	pD	1	3	9,9,10	0.56	0	11,12,14	1.07	0
3	FUB	pD	2	3	9,9,10	0.53	0	11,12,14	0.95	0
3	FUB	pD	3	3	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
18	FUB	pE	1	18	9,9,10	0.53	0	11,12,14	2.22	5 (45%)
18	FUB	pE	2	18	9,9,10	0.55	0	11,12,14	0.95	0
18	GZL	pE	3	18	11,11,12	6.57	7 (63%)	13,15,17	1.42	1 (7%)
18	AHR	pE	4	18	9,9,10	0.56	0	11,12,14	1.01	0
18	AHR	pE	5	18	9,9,10	0.58	0	11,12,14	1.15	1 (9%)
12	FUB	q	1	12	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
12	FUB	q	2	12	9,9,10	0.54	0	11,12,14	0.91	0
12	GZL	q	3	12	11,11,12	6.58	7 (63%)	13,15,17	1.30	1 (7%)
12	AHR	q	4	12	9,9,10	0.55	0	11,12,14	0.95	1 (9%)
12	AHR	q	5	12	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
14	FUB	qA	1	14	9,9,10	0.57	0	11,12,14	0.78	0
14	FUB	qA	2	14	9,9,10	0.56	0	11,12,14	0.89	0
14	GZL	qA	3	14	11,11,12	6.59	6 (54%)	13,15,17	1.72	2 (15%)
14	FUB	qA	4	14	9,9,10	0.56	0	11,12,14	0.99	0
4	FUB	qB	1	4	9,9,10	0.56	0	11,12,14	1.02	1 (9%)
4	FUB	qB	2	4	9,9,10	0.55	0	11,12,14	0.97	1 (9%)
4	FUB	qB	3	4	9,9,10	0.55	0	11,12,14	0.96	0
4	AHR	qB	4	4	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
3	FUB	qC	1	3	9,9,10	0.54	0	11,12,14	0.95	0
3	FUB	qC	2	3	9,9,10	0.54	0	11,12,14	0.81	0
3	FUB	qC	3	3	9,9,10	0.52	0	11,12,14	0.63	0
3	FUB	qD	1	3	9,9,10	0.56	0	11,12,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	qD	2	3	9,9,10	0.55	0	11,12,14	0.91	0
3	FUB	qD	3	3	9,9,10	0.53	0	11,12,14	0.91	0
19	FUB	qE	1	19	9,9,10	0.55	0	11,12,14	1.16	1 (9%)
19	FUB	qE	2	19	9,9,10	0.56	0	11,12,14	0.86	0
19	GZL	qE	3	19	11,11,12	6.59	6 (54%)	13,15,17	1.49	2 (15%)
19	AHR	qE	4	19	9,9,10	0.56	0	11,12,14	0.83	0
4	FUB	r	1	4	9,9,10	0.53	0	11,12,14	0.77	0
4	FUB	r	2	4	9,9,10	0.54	0	11,12,14	0.85	0
4	FUB	r	3	4	9,9,10	0.55	0	11,12,14	0.88	0
4	AHR	r	4	4	9,9,10	0.55	0	11,12,14	0.76	0
3	FUB	rA	1	3	9,9,10	0.52	0	11,12,14	0.80	0
3	FUB	rA	2	3	9,9,10	0.53	0	11,12,14	0.78	0
3	FUB	rA	3	3	9,9,10	0.56	0	11,12,14	0.90	0
3	FUB	rB	1	3	9,9,10	0.54	0	11,12,14	0.93	1 (9%)
3	FUB	rB	2	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	rB	3	3	9,9,10	0.54	0	11,12,14	0.96	0
3	FUB	rC	1	3	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
3	FUB	rC	2	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	rC	3	3	9,9,10	0.56	0	11,12,14	0.96	0
3	FUB	rD	1	3	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
3	FUB	rD	2	3	9,9,10	0.56	0	11,12,14	0.88	0
3	FUB	rD	3	3	9,9,10	0.54	0	11,12,14	0.95	0
18	FUB	rE	1	18	9,9,10	0.58	0	11,12,14	1.02	0
18	FUB	rE	2	18	9,9,10	0.54	0	11,12,14	1.06	1 (9%)
18	GZL	rE	3	18	11,11,12	6.61	7 (63%)	13,15,17	1.35	1 (7%)
18	AHR	rE	4	18	9,9,10	0.53	0	11,12,14	0.78	0
18	AHR	rE	5	18	9,9,10	0.55	0	11,12,14	1.10	1 (9%)
14	FUB	s	1	14	9,9,10	0.52	0	11,12,14	0.86	0
14	FUB	s	2	14	9,9,10	0.56	0	11,12,14	0.92	0
14	GZL	s	3	14	11,11,12	6.56	7 (63%)	13,15,17	1.95	3 (23%)
14	FUB	s	4	14	9,9,10	0.57	0	11,12,14	0.88	0
10	FUB	sA	1	10	9,9,10	0.55	0	11,12,14	0.98	0
10	FUB	sA	2	10	9,9,10	0.54	0	11,12,14	0.84	0
10	FUB	sA	3	10	9,9,10	0.53	0	11,12,14	0.79	0
10	AHR	sA	4	10	9,9,10	0.55	0	11,12,14	1.07	1 (9%)
10	AHR	sA	5	10	9,9,10	0.54	0	11,12,14	1.12	1 (9%)
3	FUB	sB	1	3	9,9,10	0.58	0	11,12,14	0.92	0
3	FUB	sB	2	3	9,9,10	0.55	0	11,12,14	1.01	0
3	FUB	sB	3	3	9,9,10	0.55	0	11,12,14	0.82	0
3	FUB	sC	1	3	9,9,10	0.52	0	11,12,14	1.04	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	sC	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	sC	3	3	9,9,10	0.55	0	11,12,14	0.99	0
10	FUB	sD	1	10	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
10	FUB	sD	2	10	9,9,10	0.55	0	11,12,14	0.82	0
10	FUB	sD	3	10	9,9,10	0.55	0	11,12,14	0.98	0
10	AHR	sD	4	10	9,9,10	0.55	0	11,12,14	0.89	0
10	AHR	sD	5	10	9,9,10	0.55	0	11,12,14	0.73	0
20	FUB	sE	1	20	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
20	FUB	sE	2	20	9,9,10	0.55	0	11,12,14	0.99	0
20	GZL	sE	3	20	11,11,12	6.59	6 (54%)	13,15,17	1.45	1 (7%)
20	AHR	sE	4	20	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
3	FUB	t	1	3	9,9,10	0.54	0	11,12,14	0.94	0
3	FUB	t	2	3	9,9,10	0.54	0	11,12,14	0.77	0
3	FUB	t	3	3	9,9,10	0.55	0	11,12,14	0.95	0
4	FUB	tA	1	4	9,9,10	0.52	0	11,12,14	1.05	1 (9%)
4	FUB	tA	2	4	9,9,10	0.55	0	11,12,14	0.80	0
4	FUB	tA	3	4	9,9,10	0.54	0	11,12,14	0.78	0
4	AHR	tA	4	4	9,9,10	0.54	0	11,12,14	1.10	1 (9%)
3	FUB	tB	1	3	9,9,10	0.56	0	11,12,14	0.82	0
3	FUB	tB	2	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	tB	3	3	9,9,10	0.53	0	11,12,14	0.73	0
3	FUB	tC	1	3	9,9,10	0.56	0	11,12,14	0.98	0
3	FUB	tC	2	3	9,9,10	0.56	0	11,12,14	0.91	0
3	FUB	tC	3	3	9,9,10	0.56	0	11,12,14	1.04	1 (9%)
13	FUB	tD	1	13	9,9,10	0.55	0	11,12,14	1.02	0
13	FUB	tD	2	13	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
13	GZL	tD	3	13	11,11,12	6.65	6 (54%)	13,15,17	1.12	2 (15%)
13	AHR	tD	4	13	9,9,10	0.56	0	11,12,14	1.14	1 (9%)
18	FUB	tE	1	18	9,9,10	0.51	0	11,12,14	0.88	1 (9%)
18	FUB	tE	2	18	9,9,10	0.51	0	11,12,14	0.71	0
18	GZL	tE	3	18	11,11,12	6.57	7 (63%)	13,15,17	1.46	1 (7%)
18	AHR	tE	4	18	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
18	AHR	tE	5	18	9,9,10	0.56	0	11,12,14	0.94	0
10	FUB	u	1	10	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
10	FUB	u	2	10	9,9,10	0.55	0	11,12,14	0.86	0
10	FUB	u	3	10	9,9,10	0.53	0	11,12,14	0.91	0
10	AHR	u	4	10	9,9,10	0.56	0	11,12,14	0.96	0
10	AHR	u	5	10	9,9,10	0.54	0	11,12,14	1.14	1 (9%)
3	FUB	uA	1	3	9,9,10	0.53	0	11,12,14	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	uA	2	3	9,9,10	0.55	0	11,12,14	0.82	0
3	FUB	uA	3	3	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
3	FUB	uB	1	3	9,9,10	0.54	0	11,12,14	0.95	0
3	FUB	uB	2	3	9,9,10	0.55	0	11,12,14	0.86	0
3	FUB	uB	3	3	9,9,10	0.55	0	11,12,14	0.88	0
3	FUB	uC	1	3	9,9,10	0.52	0	11,12,14	0.89	0
3	FUB	uC	2	3	9,9,10	0.54	0	11,12,14	0.94	0
3	FUB	uC	3	3	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
6	FUB	uD	1	6	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
6	FUB	uD	2	6	9,9,10	0.57	0	11,12,14	1.00	0
6	GZL	uD	3	6	11,11,12	6.87	6 (54%)	13,15,17	4.15	4 (30%)
20	FUB	uE	1	20	9,9,10	0.52	0	11,12,14	0.87	1 (9%)
20	FUB	uE	2	20	9,9,10	0.50	0	11,12,14	0.88	0
20	GZL	uE	3	20	11,11,12	6.57	7 (63%)	13,15,17	1.39	1 (7%)
20	AHR	uE	4	20	9,9,10	0.56	0	11,12,14	0.85	0
4	FUB	v	1	4	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
4	FUB	v	2	4	9,9,10	0.54	0	11,12,14	0.87	0
4	FUB	v	3	4	9,9,10	0.54	0	11,12,14	0.88	0
4	AHR	v	4	4	9,9,10	0.55	0	11,12,14	0.98	0
3	FUB	vA	1	3	9,9,10	0.55	0	11,12,14	0.81	0
3	FUB	vA	2	3	9,9,10	0.55	0	11,12,14	0.87	0
3	FUB	vA	3	3	9,9,10	0.55	0	11,12,14	1.05	1 (9%)
3	FUB	vB	1	3	9,9,10	0.52	0	11,12,14	1.12	1 (9%)
3	FUB	vB	2	3	9,9,10	0.56	0	11,12,14	0.85	0
3	FUB	vB	3	3	9,9,10	0.56	0	11,12,14	0.90	0
10	FUB	vC	1	10	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
10	FUB	vC	2	10	9,9,10	0.54	0	11,12,14	0.79	0
10	FUB	vC	3	10	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
10	AHR	vC	4	10	9,9,10	0.58	0	11,12,14	0.87	0
10	AHR	vC	5	10	9,9,10	0.54	0	11,12,14	0.84	1 (9%)
13	FUB	vD	1	13	9,9,10	0.53	0	11,12,14	0.93	0
13	FUB	vD	2	13	9,9,10	0.56	0	11,12,14	0.93	0
13	GZL	vD	3	13	11,11,12	6.56	7 (63%)	13,15,17	1.38	1 (7%)
13	AHR	vD	4	13	9,9,10	0.54	0	11,12,14	1.08	1 (9%)
21	FUB	vE	1	21	9,9,10	0.51	0	11,12,14	0.93	1 (9%)
21	FUB	vE	2	21	9,9,10	0.54	0	11,12,14	0.79	0
21	GZL	vE	3	21	11,11,12	6.60	6 (54%)	13,15,17	1.37	1 (7%)
21	AHR	vE	4	21	9,9,10	0.55	0	11,12,14	0.98	0
21	AHR	vE	5	21	9,9,10	0.54	0	11,12,14	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	w	1	3	9,9,10	0.55	0	11,12,14	0.85	0
3	FUB	w	2	3	9,9,10	0.56	0	11,12,14	0.91	0
3	FUB	w	3	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	FUB	wA	1	3	9,9,10	0.55	0	11,12,14	0.74	0
3	FUB	wA	2	3	9,9,10	0.55	0	11,12,14	0.83	0
3	FUB	wA	3	3	9,9,10	0.55	0	11,12,14	0.85	1 (9%)
3	FUB	wB	1	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	wB	2	3	9,9,10	0.54	0	11,12,14	0.84	0
3	FUB	wB	3	3	9,9,10	0.56	0	11,12,14	0.84	0
13	FUB	wC	1	13	9,9,10	0.53	0	11,12,14	0.94	0
13	FUB	wC	2	13	9,9,10	0.51	0	11,12,14	1.05	1 (9%)
13	GZL	wC	3	13	11,11,12	6.69	7 (63%)	13,15,17	1.25	3 (23%)
13	AHR	wC	4	13	9,9,10	0.57	0	11,12,14	1.16	1 (9%)
13	FUB	wD	1	13	9,9,10	0.53	0	11,12,14	0.96	1 (9%)
13	FUB	wD	2	13	9,9,10	0.55	0	11,12,14	0.80	0
13	GZL	wD	3	13	11,11,12	6.58	7 (63%)	13,15,17	1.43	2 (15%)
13	AHR	wD	4	13	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
22	FUB	wE	1	22	9,9,10	0.56	0	11,12,14	1.01	0
22	FUB	wE	2	22	9,9,10	0.56	0	11,12,14	0.93	0
22	GZL	wE	3	22	11,11,12	6.61	7 (63%)	13,15,17	1.33	1 (7%)
22	AHR	wE	4	22	9,9,10	0.53	0	11,12,14	0.93	0
22	AHR	wE	5	22	9,9,10	0.56	0	11,12,14	1.44	3 (27%)
22	AHR	wE	6	22	9,9,10	0.53	0	11,12,14	0.79	0
3	FUB	x	1	3	9,9,10	0.55	0	11,12,14	0.80	0
3	FUB	x	2	3	9,9,10	0.56	0	11,12,14	0.96	0
3	FUB	x	3	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	FUB	xA	1	3	9,9,10	0.57	0	11,12,14	0.90	0
3	FUB	xA	2	3	9,9,10	0.56	0	11,12,14	0.88	0
3	FUB	xA	3	3	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	xB	1	3	9,9,10	0.52	0	11,12,14	1.04	1 (9%)
3	FUB	xB	2	3	9,9,10	0.53	0	11,12,14	0.80	0
3	FUB	xB	3	3	9,9,10	0.54	0	11,12,14	0.97	0
6	FUB	xC	1	6	9,9,10	0.52	0	11,12,14	1.05	1 (9%)
6	FUB	xC	2	6	9,9,10	0.56	0	11,12,14	1.02	0
6	GZL	xC	3	6	11,11,12	6.86	6 (54%)	13,15,17	4.12	4 (30%)
6	FUB	xD	1	6	9,9,10	0.55	0	11,12,14	0.82	0
6	FUB	xD	2	6	9,9,10	0.55	0	11,12,14	1.15	2 (18%)
6	GZL	xD	3	6	11,11,12	6.52	7 (63%)	13,15,17	1.63	2 (15%)
20	FUB	xE	1	20	9,9,10	0.55	0	11,12,14	1.11	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	FUB	xE	2	20	9,9,10	0.54	0	11,12,14	0.70	0
20	GZL	xE	3	20	11,11,12	6.55	7 (63%)	13,15,17	1.44	1 (7%)
20	AHR	xE	4	20	9,9,10	0.53	0	11,12,14	0.96	0
3	FUB	y	1	3	9,9,10	0.54	0	11,12,14	0.99	0
3	FUB	y	2	3	9,9,10	0.55	0	11,12,14	0.90	0
3	FUB	y	3	3	9,9,10	0.53	0	11,12,14	0.83	0
3	FUB	yA	1	3	9,9,10	0.55	0	11,12,14	1.10	1 (9%)
3	FUB	yA	2	3	9,9,10	0.52	0	11,12,14	0.78	0
3	FUB	yA	3	3	9,9,10	0.55	0	11,12,14	0.84	0
10	FUB	yB	1	10	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
10	FUB	yB	2	10	9,9,10	0.55	0	11,12,14	0.74	0
10	FUB	yB	3	10	9,9,10	0.56	0	11,12,14	1.08	0
10	AHR	yB	4	10	9,9,10	0.55	0	11,12,14	0.91	0
10	AHR	yB	5	10	9,9,10	0.55	0	11,12,14	0.73	0
13	FUB	yC	1	13	9,9,10	0.54	0	11,12,14	0.90	0
13	FUB	yC	2	13	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
13	GZL	yC	3	13	11,11,12	6.56	7 (63%)	13,15,17	1.41	1 (7%)
13	AHR	yC	4	13	9,9,10	0.56	0	11,12,14	0.95	0
6	FUB	yD	1	6	9,9,10	0.52	0	11,12,14	0.89	1 (9%)
6	FUB	yD	2	6	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
6	GZL	yD	3	6	11,11,12	6.60	7 (63%)	13,15,17	1.38	1 (7%)
18	FUB	yE	1	18	9,9,10	0.53	0	11,12,14	0.90	0
18	FUB	yE	2	18	9,9,10	0.50	0	11,12,14	0.86	0
18	GZL	yE	3	18	11,11,12	6.50	7 (63%)	13,15,17	1.62	2 (15%)
18	AHR	yE	4	18	9,9,10	0.55	0	11,12,14	1.09	1 (9%)
18	AHR	yE	5	18	9,9,10	0.53	0	11,12,14	1.08	1 (9%)
3	FUB	z	1	3	9,9,10	0.53	0	11,12,14	0.95	1 (9%)
3	FUB	z	2	3	9,9,10	0.54	0	11,12,14	0.88	0
3	FUB	z	3	3	9,9,10	0.54	0	11,12,14	0.83	0
3	FUB	zA	1	3	9,9,10	0.50	0	11,12,14	0.85	0
3	FUB	zA	2	3	9,9,10	0.56	0	11,12,14	0.85	0
3	FUB	zA	3	3	9,9,10	0.54	0	11,12,14	0.85	0
13	FUB	zB	1	13	9,9,10	0.52	0	11,12,14	1.00	0
13	FUB	zB	2	13	9,9,10	0.51	0	11,12,14	1.03	1 (9%)
13	GZL	zB	3	13	11,11,12	6.62	7 (63%)	13,15,17	1.17	1 (7%)
13	AHR	zB	4	13	9,9,10	0.56	0	11,12,14	1.08	1 (9%)
13	FUB	zC	1	13	9,9,10	0.54	0	11,12,14	0.91	0
13	FUB	zC	2	13	9,9,10	0.53	0	11,12,14	0.94	1 (9%)
13	GZL	zC	3	13	11,11,12	6.57	7 (63%)	13,15,17	1.41	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	AHR	zC	4	13	9,9,10	0.54	0	11,12,14	0.97	0
6	FUB	zD	1	6	9,9,10	0.55	0	11,12,14	1.00	0
6	FUB	zD	2	6	9,9,10	0.55	0	11,12,14	0.96	1 (9%)
6	GZL	zD	3	6	11,11,12	6.59	7 (63%)	13,15,17	1.37	1 (7%)
18	FUB	zE	1	18	9,9,10	0.57	0	11,12,14	1.00	0
18	FUB	zE	2	18	9,9,10	0.56	0	11,12,14	1.05	1 (9%)
18	GZL	zE	3	18	11,11,12	6.53	7 (63%)	13,15,17	1.57	2 (15%)
18	AHR	zE	4	18	9,9,10	0.56	0	11,12,14	0.80	0
18	AHR	zE	5	18	9,9,10	0.55	0	11,12,14	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	0	1	3	-	0/2/15/18	0/1/1/1
3	FUB	0	2	3	-	0/2/15/18	0/1/1/1
3	FUB	0	3	3	-	0/2/15/18	0/1/1/1
3	FUB	0A	1	3	-	0/2/15/18	0/1/1/1
3	FUB	0A	2	3	-	0/2/15/18	0/1/1/1
3	FUB	0A	3	3	-	0/2/15/18	0/1/1/1
6	FUB	0B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	0B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	0B	3	6	2/2/4/5	5/6/19/22	0/1/1/1
6	FUB	0C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	0C	2	6	-	0/2/15/18	0/1/1/1
6	GZL	0C	3	6	-	2/6/19/22	0/1/1/1
13	FUB	0D	1	13	-	0/2/15/18	0/1/1/1
13	FUB	0D	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	0D	3	13	-	6/6/19/22	0/1/1/1
13	AHR	0D	4	13	-	0/2/15/18	0/1/1/1
18	FUB	0E	1	18	-	0/2/15/18	0/1/1/1
18	FUB	0E	2	18	-	0/2/15/18	0/1/1/1
18	GZL	0E	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	0E	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	0E	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	1	1	3	-	0/2/15/18	0/1/1/1
3	FUB	1	2	3	-	0/2/15/18	0/1/1/1
3	FUB	1	3	3	-	0/2/15/18	0/1/1/1
10	FUB	1A	1	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FUB	1A	2	10	-	0/2/15/18	0/1/1/1
10	FUB	1A	3	10	-	0/2/15/18	0/1/1/1
10	AHR	1A	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	1A	5	10	-	0/2/15/18	0/1/1/1
13	FUB	1B	1	13	-	0/2/15/18	0/1/1/1
13	FUB	1B	2	13	-	0/2/15/18	0/1/1/1
13	GZL	1B	3	13	1/1/4/5	2/6/19/22	0/1/1/1
13	AHR	1B	4	13	-	0/2/15/18	0/1/1/1
6	FUB	1C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	1C	2	6	-	0/2/15/18	0/1/1/1
6	GZL	1C	3	6	1/1/4/5	0/6/19/22	0/1/1/1
15	FUB	1D	1	15	-	0/2/15/18	0/1/1/1
15	FUB	1D	2	15	-	0/2/15/18	0/1/1/1
15	GZL	1D	3	15	1/1/4/5	4/6/19/22	0/1/1/1
15	AHR	1D	4	15	-	0/2/15/18	0/1/1/1
15	AHR	1D	5	15	1/1/3/4	0/2/15/18	0/1/1/1
19	FUB	1E	1	19	-	0/2/15/18	0/1/1/1
19	FUB	1E	2	19	-	0/2/15/18	0/1/1/1
19	GZL	1E	3	19	1/1/4/5	4/6/19/22	0/1/1/1
19	AHR	1E	4	19	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	2	1	3	-	0/2/15/18	0/1/1/1
3	FUB	2	2	3	-	0/2/15/18	0/1/1/1
3	FUB	2	3	3	-	0/2/15/18	0/1/1/1
13	FUB	2A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	2A	2	13	-	0/2/15/18	0/1/1/1
13	GZL	2A	3	13	3/3/4/5	2/6/19/22	0/1/1/1
13	AHR	2A	4	13	-	0/2/15/18	0/1/1/1
13	FUB	2B	1	13	-	0/2/15/18	0/1/1/1
13	FUB	2B	2	13	-	0/2/15/18	0/1/1/1
13	GZL	2B	3	13	1/1/4/5	0/6/19/22	0/1/1/1
13	AHR	2B	4	13	-	0/2/15/18	0/1/1/1
6	FUB	2C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	2C	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	2C	3	6	1/1/4/5	4/6/19/22	0/1/1/1
15	FUB	2D	1	15	-	0/2/15/18	0/1/1/1
15	FUB	2D	2	15	-	0/2/15/18	0/1/1/1
15	GZL	2D	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	2D	4	15	-	0/2/15/18	0/1/1/1
15	AHR	2D	5	15	-	0/2/15/18	0/1/1/1
10	FUB	3	1	10	-	0/2/15/18	0/1/1/1
10	FUB	3	2	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FUB	3	3	10	-	0/2/15/18	0/1/1/1
10	AHR	3	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	3	5	10	-	0/2/15/18	0/1/1/1
6	FUB	3A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	3A	2	6	-	0/2/15/18	0/1/1/1
6	GZL	3A	3	6	2/2/4/5	4/6/19/22	0/1/1/1
6	FUB	3B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	3B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	3B	3	6	-	2/6/19/22	0/1/1/1
13	FUB	3C	1	13	-	0/2/15/18	0/1/1/1
13	FUB	3C	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	3C	3	13	-	4/6/19/22	0/1/1/1
13	AHR	3C	4	13	-	0/2/15/18	0/1/1/1
6	FUB	3D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	3D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	3D	3	6	1/1/4/5	0/6/19/22	0/1/1/1
13	FUB	4	1	13	-	0/2/15/18	0/1/1/1
13	FUB	4	2	13	-	0/2/15/18	0/1/1/1
13	GZL	4	3	13	2/2/4/5	5/6/19/22	0/1/1/1
13	AHR	4	4	13	-	0/2/15/18	0/1/1/1
13	FUB	4A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	4A	2	13	-	0/2/15/18	0/1/1/1
13	GZL	4A	3	13	1/1/4/5	0/6/19/22	0/1/1/1
13	AHR	4A	4	13	-	0/2/15/18	0/1/1/1
6	FUB	4B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	4B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	4B	3	6	1/1/4/5	4/6/19/22	0/1/1/1
15	FUB	4C	1	15	-	0/2/15/18	0/1/1/1
15	FUB	4C	2	15	-	0/2/15/18	0/1/1/1
15	GZL	4C	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	4C	4	15	-	0/2/15/18	0/1/1/1
15	AHR	4C	5	15	1/1/3/4	0/2/15/18	0/1/1/1
16	NAG	4D	1	1,16	-	3/6/23/26	0/1/1/1
16	NAG	4D	2	16	-	0/6/23/26	0/1/1/1
6	FUB	5	1	6	-	0/2/15/18	0/1/1/1
6	FUB	5	2	6	-	0/2/15/18	0/1/1/1
6	GZL	5	3	6	3/3/4/5	2/6/19/22	0/1/1/1
13	FUB	5A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	5A	2	13	-	0/2/15/18	0/1/1/1
13	GZL	5A	3	13	1/1/4/5	2/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	AHR	5A	4	13	-	0/2/15/18	0/1/1/1
6	FUB	5B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	5B	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	5B	3	6	1/1/4/5	6/6/19/22	0/1/1/1
15	FUB	5C	1	15	-	0/2/15/18	0/1/1/1
15	FUB	5C	2	15	-	0/2/15/18	0/1/1/1
15	GZL	5C	3	15	1/1/4/5	0/6/19/22	0/1/1/1
15	AHR	5C	4	15	-	0/2/15/18	0/1/1/1
15	AHR	5C	5	15	-	0/2/15/18	0/1/1/1
17	NAG	5D	1	1,17	-	1/6/23/26	0/1/1/1
17	NAG	5D	2	17	-	2/6/23/26	0/1/1/1
17	BMA	5D	3	17	-	2/2/19/22	0/1/1/1
17	MAN	5D	4	17	1/1/4/5	2/2/19/22	0/1/1/1
17	MAN	5D	5	17	-	0/2/19/22	0/1/1/1
17	MAN	5D	6	17	1/1/4/5	2/2/19/22	0/1/1/1
13	FUB	6	1	13	-	0/2/15/18	0/1/1/1
13	FUB	6	2	13	-	0/2/15/18	0/1/1/1
13	GZL	6	3	13	1/1/4/5	3/6/19/22	0/1/1/1
13	AHR	6	4	13	-	0/2/15/18	0/1/1/1
6	FUB	6A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	6A	2	6	-	0/2/15/18	0/1/1/1
6	GZL	6A	3	6	-	2/6/19/22	0/1/1/1
13	FUB	6B	1	13	-	0/2/15/18	0/1/1/1
13	FUB	6B	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	6B	3	13	-	4/6/19/22	0/1/1/1
13	AHR	6B	4	13	-	0/2/15/18	0/1/1/1
6	FUB	6C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	6C	2	6	-	0/2/15/18	0/1/1/1
6	GZL	6C	3	6	1/1/4/5	2/6/19/22	0/1/1/1
6	FUB	6D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	6D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	6D	3	6	1/1/4/5	4/6/19/22	0/1/1/1
13	FUB	7	1	13	-	0/2/15/18	0/1/1/1
13	FUB	7	2	13	-	0/2/15/18	0/1/1/1
13	GZL	7	3	13	1/1/4/5	0/6/19/22	0/1/1/1
13	AHR	7	4	13	-	0/2/15/18	0/1/1/1
6	FUB	7A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	7A	2	6	-	0/2/15/18	0/1/1/1
6	GZL	7A	3	6	1/1/4/5	2/6/19/22	0/1/1/1
15	FUB	7B	1	15	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FUB	7B	2	15	-	0/2/15/18	0/1/1/1
15	GZL	7B	3	15	1/1/4/5	6/6/19/22	0/1/1/1
15	AHR	7B	4	15	-	0/2/15/18	0/1/1/1
15	AHR	7B	5	15	1/1/3/4	0/2/15/18	0/1/1/1
17	NAG	7C	1	1,17	-	1/6/23/26	0/1/1/1
17	NAG	7C	2	17	-	0/6/23/26	0/1/1/1
17	BMA	7C	3	17	-	2/2/19/22	0/1/1/1
17	MAN	7C	4	17	1/1/4/5	2/2/19/22	0/1/1/1
17	MAN	7C	5	17	-	2/2/19/22	0/1/1/1
17	MAN	7C	6	17	1/1/4/5	1/2/19/22	0/1/1/1
6	FUB	7D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	7D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	7D	3	6	1/1/4/5	6/6/19/22	0/1/1/1
6	FUB	8	1	6	-	0/2/15/18	0/1/1/1
6	FUB	8	2	6	-	0/2/15/18	0/1/1/1
6	GZL	8	3	6	1/1/4/5	0/6/19/22	0/1/1/1
6	FUB	8A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	8A	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	8A	3	6	1/1/4/5	4/6/19/22	0/1/1/1
15	FUB	8B	1	15	-	0/2/15/18	0/1/1/1
15	FUB	8B	2	15	-	0/2/15/18	0/1/1/1
15	GZL	8B	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	8B	4	15	-	0/2/15/18	0/1/1/1
15	AHR	8B	5	15	-	0/2/15/18	0/1/1/1
3	FUB	8C	1	3	-	0/2/15/18	0/1/1/1
3	FUB	8C	2	3	-	0/2/15/18	0/1/1/1
3	FUB	8C	3	3	-	0/2/15/18	0/1/1/1
6	FUB	8D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	8D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	8D	3	6	1/1/4/5	2/6/19/22	0/1/1/1
6	FUB	9	1	6	-	0/2/15/18	0/1/1/1
6	FUB	9	2	6	-	0/2/15/18	0/1/1/1
6	GZL	9	3	6	1/1/4/5	2/6/19/22	0/1/1/1
13	FUB	9A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	9A	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	9A	3	13	-	4/6/19/22	0/1/1/1
13	AHR	9A	4	13	-	0/2/15/18	0/1/1/1
6	FUB	9B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	9B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	9B	3	6	1/1/4/5	2/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	9C	1	3	-	0/2/15/18	0/1/1/1
3	FUB	9C	2	3	-	0/2/15/18	0/1/1/1
3	FUB	9C	3	3	-	0/2/15/18	0/1/1/1
18	FUB	9D	1	18	-	0/2/15/18	0/1/1/1
18	FUB	9D	2	18	-	0/2/15/18	0/1/1/1
18	GZL	9D	3	18	1/1/4/5	3/6/19/22	0/1/1/1
18	AHR	9D	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	9D	5	18	-	0/2/15/18	0/1/1/1
6	FUB	AA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	AA	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	AA	3	6	1/1/4/5	6/6/19/22	0/1/1/1
15	FUB	AB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	AB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	AB	3	15	1/1/4/5	4/6/19/22	0/1/1/1
15	AHR	AB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	AB	5	15	1/1/3/4	0/2/15/18	0/1/1/1
16	NAG	AC	1	1,16	-	3/6/23/26	0/1/1/1
16	NAG	AC	2	16	-	2/6/23/26	0/1/1/1
4	FUB	AD	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	AD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	AD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	AD	4	4	-	0/2/15/18	0/1/1/1
19	FUB	AE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	AE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	AE	3	19	1/1/4/5	6/6/19/22	0/1/1/1
19	AHR	AE	4	19	-	0/2/15/18	0/1/1/1
13	FUB	BA	1	13	-	0/2/15/18	0/1/1/1
13	FUB	BA	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	BA	3	13	-	4/6/19/22	0/1/1/1
13	AHR	BA	4	13	-	0/2/15/18	0/1/1/1
15	FUB	BB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	BB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	BB	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	BB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	BB	5	15	-	0/2/15/18	0/1/1/1
3	FUB	BC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	BC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	BC	3	3	-	0/2/15/18	0/1/1/1
5	FUB	BD	1	5	-	0/2/15/18	0/1/1/1
5	FUB	BD	2	5	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUB	BD	3	5	-	0/2/15/18	0/1/1/1
5	AHR	BD	4	5	-	0/2/15/18	0/1/1/1
5	AHR	BD	5	5	1/1/3/4	0/2/15/18	0/1/1/1
18	FUB	BE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	BE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	BE	3	18	1/1/4/5	5/6/19/22	0/1/1/1
18	AHR	BE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	BE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
15	FUB	CA	1	15	-	0/2/15/18	0/1/1/1
15	FUB	CA	2	15	-	0/2/15/18	0/1/1/1
15	GZL	CA	3	15	1/1/4/5	4/6/19/22	0/1/1/1
15	AHR	CA	4	15	-	0/2/15/18	0/1/1/1
15	AHR	CA	5	15	1/1/3/4	0/2/15/18	0/1/1/1
6	FUB	CB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	CB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	CB	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	CC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	CC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	CC	3	3	-	0/2/15/18	0/1/1/1
6	FUB	CD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	CD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	CD	3	6	3/3/4/5	1/6/19/22	0/1/1/1
20	FUB	CE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	CE	2	20	-	1/2/15/18	0/1/1/1
20	GZL	CE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	CE	4	20	-	0/2/15/18	0/1/1/1
15	FUB	DA	1	15	-	0/2/15/18	0/1/1/1
15	FUB	DA	2	15	-	0/2/15/18	0/1/1/1
15	GZL	DA	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	DA	4	15	-	0/2/15/18	0/1/1/1
15	AHR	DA	5	15	-	0/2/15/18	0/1/1/1
17	NAG	DB	1	1,17	-	2/6/23/26	0/1/1/1
17	NAG	DB	2	17	-	2/6/23/26	0/1/1/1
17	BMA	DB	3	17	-	2/2/19/22	0/1/1/1
17	MAN	DB	4	17	1/1/4/5	2/2/19/22	0/1/1/1
17	MAN	DB	5	17	-	2/2/19/22	0/1/1/1
17	MAN	DB	6	17	1/1/4/5	1/2/19/22	0/1/1/1
4	FUB	DC	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	DC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	DC	3	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	DC	4	4	-	0/2/15/18	0/1/1/1
3	FUB	DD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	DD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	DD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	DE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	DE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	DE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	DE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	DE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
6	FUB	EA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	EA	2	6	-	0/2/15/18	0/1/1/1
6	GZL	EA	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	EB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	EB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	EB	3	3	-	0/2/15/18	0/1/1/1
5	FUB	EC	1	5	-	0/2/15/18	0/1/1/1
5	FUB	EC	2	5	-	0/2/15/18	0/1/1/1
5	FUB	EC	3	5	-	0/2/15/18	0/1/1/1
5	AHR	EC	4	5	-	0/2/15/18	0/1/1/1
5	AHR	EC	5	5	-	0/2/15/18	0/1/1/1
3	FUB	ED	1	3	-	0/2/15/18	0/1/1/1
3	FUB	ED	2	3	-	0/2/15/18	0/1/1/1
3	FUB	ED	3	3	-	0/2/15/18	0/1/1/1
20	FUB	EE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	EE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	EE	3	20	1/1/4/5	0/6/19/22	0/1/1/1
20	AHR	EE	4	20	-	0/2/15/18	0/1/1/1
16	NAG	FA	1	1,16	-	3/6/23/26	0/1/1/1
16	NAG	FA	2	16	-	2/6/23/26	0/1/1/1
12	FUB	FB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	FB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	FB	3	12	2/2/4/5	3/6/19/22	0/1/1/1
12	AHR	FB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	FB	5	12	-	0/2/15/18	0/1/1/1
6	FUB	FC	1	6	-	0/2/15/18	0/1/1/1
6	FUB	FC	2	6	-	0/2/15/18	0/1/1/1
6	GZL	FC	3	6	1/1/4/5	4/6/19/22	0/1/1/1
3	FUB	FD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	FD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	FD	3	3	-	0/2/15/18	0/1/1/1
21	FUB	FE	1	21	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	FUB	FE	2	21	-	0/2/15/18	0/1/1/1
21	GZL	FE	3	21	1/1/4/5	2/6/19/22	0/1/1/1
21	AHR	FE	4	21	1/1/3/4	0/2/15/18	0/1/1/1
21	AHR	FE	5	21	1/1/3/4	0/2/15/18	0/1/1/1
17	NAG	GA	1	1,17	-	1/6/23/26	0/1/1/1
17	NAG	GA	2	17	-	2/6/23/26	0/1/1/1
17	BMA	GA	3	17	-	2/2/19/22	0/1/1/1
17	MAN	GA	4	17	1/1/4/5	1/2/19/22	0/1/1/1
17	MAN	GA	5	17	-	1/2/19/22	0/1/1/1
17	MAN	GA	6	17	1/1/4/5	1/2/19/22	0/1/1/1
13	FUB	GB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	GB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	GB	3	13	2/2/4/5	3/6/19/22	0/1/1/1
13	AHR	GB	4	13	-	0/2/15/18	0/1/1/1
3	FUB	GC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	GC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	GC	3	3	-	0/2/15/18	0/1/1/1
6	FUB	GD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	GD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	GD	3	6	1/1/4/5	4/6/19/22	0/1/1/1
22	FUB	GE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	GE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	GE	3	22	1/1/4/5	6/6/19/22	0/1/1/1
22	AHR	GE	4	22	-	0/2/15/18	0/1/1/1
22	AHR	GE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	GE	6	22	-	0/2/15/18	0/1/1/1
3	FUB	HA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	HA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	HA	3	3	-	0/2/15/18	0/1/1/1
14	FUB	HB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	HB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	HB	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	HB	4	14	-	0/2/15/18	0/1/1/1
3	FUB	HC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	HC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	HC	3	3	-	0/2/15/18	0/1/1/1
7	FUB	HD	1	7	-	0/2/15/18	0/1/1/1
7	FUB	HD	2	7	-	0/2/15/18	0/1/1/1
7	FUB	HD	3	7	-	0/2/15/18	0/1/1/1
7	AHR	HD	4	7	-	0/2/15/18	0/1/1/1
20	FUB	HE	1	20	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	FUB	HE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	HE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	HE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	IA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	IA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	IA	3	3	-	0/2/15/18	0/1/1/1
12	FUB	IB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	IB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	IB	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	IB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	IB	5	12	-	0/2/15/18	0/1/1/1
3	FUB	IC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	IC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	IC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	ID	1	3	-	0/2/15/18	0/1/1/1
3	FUB	ID	2	3	-	0/2/15/18	0/1/1/1
3	FUB	ID	3	3	-	0/2/15/18	0/1/1/1
18	FUB	IE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	IE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	IE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	IE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	IE	5	18	-	0/2/15/18	0/1/1/1
3	FUB	J	1	3	-	0/2/15/18	0/1/1/1
3	FUB	J	2	3	-	0/2/15/18	0/1/1/1
3	FUB	J	3	3	-	0/2/15/18	0/1/1/1
4	FUB	JA	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	JA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	JA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	JA	4	4	-	0/2/15/18	0/1/1/1
4	FUB	JB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	JB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	JB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	JB	4	4	-	0/2/15/18	0/1/1/1
6	FUB	JC	1	6	-	0/2/15/18	0/1/1/1
6	FUB	JC	2	6	-	0/2/15/18	0/1/1/1
6	GZL	JC	3	6	1/1/4/5	0/6/19/22	0/1/1/1
8	FUB	JD	1	8	-	0/2/15/18	0/1/1/1
8	FUB	JD	2	8	-	0/2/15/18	0/1/1/1
8	FUB	JD	3	8	-	0/2/15/18	0/1/1/1
8	AHR	JD	4	8	-	0/2/15/18	0/1/1/1
8	AHR	JD	5	8	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	FUB	JE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	JE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	JE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	JE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	JE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	K	1	3	-	0/2/15/18	0/1/1/1
3	FUB	K	2	3	-	0/2/15/18	0/1/1/1
3	FUB	K	3	3	-	0/2/15/18	0/1/1/1
5	FUB	KA	1	5	-	0/2/15/18	0/1/1/1
5	FUB	KA	2	5	-	0/2/15/18	0/1/1/1
5	FUB	KA	3	5	-	0/2/15/18	0/1/1/1
5	AHR	KA	4	5	-	0/2/15/18	0/1/1/1
5	AHR	KA	5	5	-	0/2/15/18	0/1/1/1
14	FUB	KB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	KB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	KB	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	KB	4	14	-	0/2/15/18	0/1/1/1
7	FUB	KC	1	7	-	0/2/15/18	0/1/1/1
7	FUB	KC	2	7	-	0/2/15/18	0/1/1/1
7	FUB	KC	3	7	-	0/2/15/18	0/1/1/1
7	AHR	KC	4	7	-	0/2/15/18	0/1/1/1
3	FUB	KD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	KD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	KD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	KE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	KE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	KE	3	18	1/1/4/5	4/6/19/22	0/1/1/1
18	AHR	KE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	KE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	L	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	L	2	4	-	0/2/15/18	0/1/1/1
4	FUB	L	3	4	-	0/2/15/18	0/1/1/1
4	AHR	L	4	4	-	0/2/15/18	0/1/1/1
6	FUB	LA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	LA	2	6	-	0/2/15/18	0/1/1/1
6	GZL	LA	3	6	2/2/4/5	2/6/19/22	0/1/1/1
3	FUB	LB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	LB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	LB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	LC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	LC	2	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	LC	3	3	-	0/2/15/18	0/1/1/1
4	FUB	LD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	LD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	LD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	LD	4	4	-	0/2/15/18	0/1/1/1
19	FUB	LE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	LE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	LE	3	19	1/1/4/5	2/6/19/22	0/1/1/1
19	AHR	LE	4	19	1/1/3/4	0/2/15/18	0/1/1/1
5	FUB	M	1	5	-	0/2/15/18	0/1/1/1
5	FUB	M	2	5	-	0/2/15/18	0/1/1/1
5	FUB	M	3	5	-	0/2/15/18	0/1/1/1
5	AHR	M	4	5	-	0/2/15/18	0/1/1/1
5	AHR	M	5	5	-	0/2/15/18	0/1/1/1
3	FUB	MA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	MA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	MA	3	3	-	0/2/15/18	0/1/1/1
10	FUB	MB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	MB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	MB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	MB	4	10	-	0/2/15/18	0/1/1/1
10	AHR	MB	5	10	-	0/2/15/18	0/1/1/1
8	FUB	MC	1	8	-	0/2/15/18	0/1/1/1
8	FUB	MC	2	8	-	0/2/15/18	0/1/1/1
8	FUB	MC	3	8	-	0/2/15/18	0/1/1/1
8	AHR	MC	4	8	-	0/2/15/18	0/1/1/1
8	AHR	MC	5	8	-	0/2/15/18	0/1/1/1
4	FUB	MD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	MD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	MD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	MD	4	4	-	0/2/15/18	0/1/1/1
6	FUB	ME	1	6	-	0/2/15/18	0/1/1/1
6	FUB	ME	2	6	-	0/2/15/18	0/1/1/1
6	GZL	ME	3	6	1/1/4/5	4/6/19/22	0/1/1/1
6	FUB	N	1	6	-	0/2/15/18	0/1/1/1
6	FUB	N	2	6	-	0/2/15/18	0/1/1/1
6	GZL	N	3	6	2/2/4/5	2/6/19/22	0/1/1/1
3	FUB	NA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	NA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	NA	3	3	-	0/2/15/18	0/1/1/1
4	FUB	NB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	NB	2	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	NB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	NB	4	4	-	0/2/15/18	0/1/1/1
3	FUB	NC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	NC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	NC	3	3	-	0/2/15/18	0/1/1/1
9	FUB	ND	1	9	-	0/2/15/18	0/1/1/1
9	FUB	ND	2	9	-	0/2/15/18	0/1/1/1
19	FUB	NE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	NE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	NE	3	19	1/1/4/5	2/6/19/22	0/1/1/1
19	AHR	NE	4	19	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	O	1	3	-	0/2/15/18	0/1/1/1
3	FUB	O	2	3	-	0/2/15/18	0/1/1/1
3	FUB	O	3	3	-	0/2/15/18	0/1/1/1
3	FUB	OA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	OA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	OA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	OB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	OB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	OB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	OC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	OC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	OC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	OC	4	4	-	0/2/15/18	0/1/1/1
4	FUB	OD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	OD	2	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	OD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	OD	4	4	-	0/2/15/18	0/1/1/1
6	FUB	OE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	OE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	OE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
3	FUB	P	1	3	-	0/2/15/18	0/1/1/1
3	FUB	P	2	3	-	0/2/15/18	0/1/1/1
3	FUB	P	3	3	-	0/2/15/18	0/1/1/1
6	FUB	PA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	PA	2	6	-	0/2/15/18	0/1/1/1
6	GZL	PA	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	PB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	PB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	PB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	PC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	PC	2	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	PC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	PC	4	4	1/1/3/4	0/2/15/18	0/1/1/1
10	FUB	PD	1	10	-	0/2/15/18	0/1/1/1
10	FUB	PD	2	10	-	0/2/15/18	0/1/1/1
10	FUB	PD	3	10	-	0/2/15/18	0/1/1/1
10	AHR	PD	4	10	-	0/2/15/18	0/1/1/1
10	AHR	PD	5	10	-	0/2/15/18	0/1/1/1
18	FUB	PE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	PE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	PE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	PE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	PE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	Q	1	3	-	0/2/15/18	0/1/1/1
3	FUB	Q	2	3	-	0/2/15/18	0/1/1/1
3	FUB	Q	3	3	-	0/2/15/18	0/1/1/1
7	FUB	QA	1	7	-	0/2/15/18	0/1/1/1
7	FUB	QA	2	7	-	0/2/15/18	0/1/1/1
7	FUB	QA	3	7	-	0/2/15/18	0/1/1/1
7	AHR	QA	4	7	-	0/2/15/18	0/1/1/1
3	FUB	QB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	QB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	QB	3	3	-	0/2/15/18	0/1/1/1
9	FUB	QC	1	9	-	0/2/15/18	0/1/1/1
9	FUB	QC	2	9	-	0/2/15/18	0/1/1/1
3	FUB	QD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	QD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	QD	3	3	-	0/2/15/18	0/1/1/1
22	FUB	QE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	QE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	QE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	QE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	QE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	QE	6	22	1/1/3/4	0/2/15/18	0/1/1/1
6	FUB	R	1	6	-	0/2/15/18	0/1/1/1
6	FUB	R	2	6	-	0/2/15/18	0/1/1/1
6	GZL	R	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	RA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	RA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	RA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	RB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	RB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	RB	3	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	RC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	RC	2	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	RC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	RC	4	4	-	0/2/15/18	0/1/1/1
4	FUB	RD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	RD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	RD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	RD	4	4	-	0/2/15/18	0/1/1/1
22	FUB	RE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	RE	2	22	-	1/2/15/18	0/1/1/1
22	GZL	RE	3	22	1/1/4/5	3/6/19/22	0/1/1/1
22	AHR	RE	4	22	2/2/3/4	0/2/15/18	0/1/1/1
22	AHR	RE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	RE	6	22	-	0/2/15/18	0/1/1/1
7	FUB	S	1	7	-	0/2/15/18	0/1/1/1
7	FUB	S	2	7	-	0/2/15/18	0/1/1/1
7	FUB	S	3	7	-	0/2/15/18	0/1/1/1
7	AHR	S	4	7	-	0/2/15/18	0/1/1/1
8	FUB	SA	1	8	-	0/2/15/18	0/1/1/1
8	FUB	SA	2	8	-	0/2/15/18	0/1/1/1
8	FUB	SA	3	8	-	0/2/15/18	0/1/1/1
8	AHR	SA	4	8	-	0/2/15/18	0/1/1/1
8	AHR	SA	5	8	-	0/2/15/18	0/1/1/1
3	FUB	SB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	SB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	SB	3	3	-	0/2/15/18	0/1/1/1
10	FUB	SC	1	10	-	0/2/15/18	0/1/1/1
10	FUB	SC	2	10	-	0/2/15/18	0/1/1/1
10	FUB	SC	3	10	-	0/2/15/18	0/1/1/1
10	AHR	SC	4	10	-	0/2/15/18	0/1/1/1
10	AHR	SC	5	10	-	0/2/15/18	0/1/1/1
4	FUB	SD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	SD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	SD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	SD	4	4	-	0/2/15/18	0/1/1/1
18	FUB	SE	1	18	1/1/3/4	0/2/15/18	0/1/1/1
18	FUB	SE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	SE	3	18	1/1/4/5	3/6/19/22	0/1/1/1
18	AHR	SE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	SE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	T	1	3	-	0/2/15/18	0/1/1/1
3	FUB	T	2	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	T	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TD	3	3	-	0/2/15/18	0/1/1/1
20	FUB	TE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	TE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	TE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	TE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
8	FUB	U	1	8	-	0/2/15/18	0/1/1/1
8	FUB	U	2	8	-	0/2/15/18	0/1/1/1
8	FUB	U	3	8	-	0/2/15/18	0/1/1/1
8	AHR	U	4	8	-	0/2/15/18	0/1/1/1
8	AHR	U	5	8	-	0/2/15/18	0/1/1/1
4	FUB	UA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	UA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	UA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	UA	4	4	-	0/2/15/18	0/1/1/1
3	FUB	UB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	UB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	UB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	UC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	UC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	UC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	UC	4	4	-	0/2/15/18	0/1/1/1
7	FUB	UD	1	7	-	0/2/15/18	0/1/1/1
7	FUB	UD	2	7	-	0/2/15/18	0/1/1/1
7	FUB	UD	3	7	-	0/2/15/18	0/1/1/1
7	AHR	UD	4	7	-	0/2/15/18	0/1/1/1
20	FUB	UE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	UE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	UE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	UE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	V	1	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	V	2	3	-	0/2/15/18	0/1/1/1
3	FUB	V	3	3	-	0/2/15/18	0/1/1/1
4	FUB	VA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	VA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	VA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	VA	4	4	2/2/3/4	0/2/15/18	0/1/1/1
10	FUB	VB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	VB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	VB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	VB	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	VB	5	10	-	0/2/15/18	0/1/1/1
4	FUB	VC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	VC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	VC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	VC	4	4	-	0/2/15/18	0/1/1/1
4	FUB	VD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	VD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	VD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	VD	4	4	-	0/2/15/18	0/1/1/1
22	FUB	VE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	VE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	VE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	VE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	VE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	VE	6	22	-	0/2/15/18	0/1/1/1
4	FUB	W	1	4	-	0/2/15/18	0/1/1/1
4	FUB	W	2	4	-	0/2/15/18	0/1/1/1
4	FUB	W	3	4	-	0/2/15/18	0/1/1/1
4	AHR	W	4	4	-	0/2/15/18	0/1/1/1
9	FUB	WA	1	9	-	0/2/15/18	0/1/1/1
9	FUB	WA	2	9	-	0/2/15/18	0/1/1/1
13	FUB	WB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	WB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	WB	3	13	3/3/4/5	1/6/19/22	0/1/1/1
13	AHR	WB	4	13	-	0/2/15/18	0/1/1/1
3	FUB	WC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	WC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	WC	3	3	-	0/2/15/18	0/1/1/1
7	FUB	WD	1	7	-	0/2/15/18	0/1/1/1
7	FUB	WD	2	7	-	0/2/15/18	0/1/1/1
7	FUB	WD	3	7	-	0/2/15/18	0/1/1/1
7	AHR	WD	4	7	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	FUB	WE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	WE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	WE	3	20	1/1/4/5	2/6/19/22	0/1/1/1
20	AHR	WE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	X	1	4	-	0/2/15/18	0/1/1/1
4	FUB	X	2	4	-	0/2/15/18	0/1/1/1
4	FUB	X	3	4	-	0/2/15/18	0/1/1/1
4	AHR	X	4	4	-	0/2/15/18	0/1/1/1
3	FUB	XA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	XA	2	3	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	XA	3	3	-	0/2/15/18	0/1/1/1
6	FUB	XB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	XB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	XB	3	6	2/2/4/5	5/6/19/22	0/1/1/1
7	FUB	XC	1	7	-	0/2/15/18	0/1/1/1
7	FUB	XC	2	7	-	0/2/15/18	0/1/1/1
7	FUB	XC	3	7	-	0/2/15/18	0/1/1/1
7	AHR	XC	4	7	-	0/2/15/18	0/1/1/1
11	FUB	XD	1	11	-	0/2/15/18	0/1/1/1
11	AHR	XD	2	11	-	0/2/15/18	0/1/1/1
11	AHR	XD	3	11	-	0/2/15/18	0/1/1/1
23	FUB	XE	1	23	-	0/2/15/18	0/1/1/1
23	FUB	XE	2	23	-	1/2/15/18	0/1/1/1
23	GZL	XE	3	23	1/1/4/5	2/6/19/22	0/1/1/1
23	AHR	XE	4	23	1/1/3/4	0/2/15/18	0/1/1/1
23	AHR	XE	5	23	1/1/3/4	0/2/15/18	0/1/1/1
23	AHR	XE	6	23	-	0/2/15/18	0/1/1/1
9	FUB	Y	1	9	-	0/2/15/18	0/1/1/1
9	FUB	Y	2	9	-	0/2/15/18	0/1/1/1
10	FUB	YA	1	10	-	0/2/15/18	0/1/1/1
10	FUB	YA	2	10	-	0/2/15/18	0/1/1/1
10	FUB	YA	3	10	-	0/2/15/18	0/1/1/1
10	AHR	YA	4	10	-	0/2/15/18	0/1/1/1
10	AHR	YA	5	10	-	0/2/15/18	0/1/1/1
13	FUB	YB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	YB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	YB	3	13	1/1/4/5	4/6/19/22	0/1/1/1
13	AHR	YB	4	13	-	0/2/15/18	0/1/1/1
4	FUB	YC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	YC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	YC	3	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	YC	4	4	-	0/2/15/18	0/1/1/1
9	FUB	YD	1	9	-	0/2/15/18	0/1/1/1
9	FUB	YD	2	9	-	0/2/15/18	0/1/1/1
24	FUB	YE	1	24	-	0/2/15/18	0/1/1/1
24	FUB	YE	2	24	-	0/2/15/18	0/1/1/1
24	GZL	YE	3	24	1/1/4/5	4/6/19/22	0/1/1/1
24	AHR	YE	4	24	1/1/3/4	0/2/15/18	0/1/1/1
24	AHR	YE	5	24	-	0/2/15/18	0/1/1/1
24	AHR	YE	6	24	-	0/2/15/18	0/1/1/1
4	FUB	Z	1	4	-	0/2/15/18	0/1/1/1
4	FUB	Z	2	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	Z	3	4	-	0/2/15/18	0/1/1/1
4	AHR	Z	4	4	-	0/2/15/18	0/1/1/1
3	FUB	ZA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	ZA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	ZA	3	3	-	0/2/15/18	0/1/1/1
13	FUB	ZB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	ZB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	ZB	3	13	1/1/4/5	2/6/19/22	0/1/1/1
13	AHR	ZB	4	13	-	0/2/15/18	0/1/1/1
7	FUB	ZC	1	7	-	0/2/15/18	0/1/1/1
7	FUB	ZC	2	7	-	0/2/15/18	0/1/1/1
7	FUB	ZC	3	7	-	0/2/15/18	0/1/1/1
7	AHR	ZC	4	7	-	0/2/15/18	0/1/1/1
4	FUB	ZD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	ZD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	ZD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	ZD	4	4	-	0/2/15/18	0/1/1/1
6	FUB	ZE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	ZE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	ZE	3	6	1/1/4/5	2/6/19/22	0/1/1/1
10	FUB	a	1	10	-	0/2/15/18	0/1/1/1
10	FUB	a	2	10	-	0/2/15/18	0/1/1/1
10	FUB	a	3	10	-	0/2/15/18	0/1/1/1
10	AHR	a	4	10	-	0/2/15/18	0/1/1/1
10	AHR	a	5	10	-	0/2/15/18	0/1/1/1
4	FUB	aA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	aA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	aA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	aA	4	4	-	0/2/15/18	0/1/1/1
6	FUB	aB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	aB	2	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GZL	aB	3	6	-	2/6/19/22	0/1/1/1
11	FUB	aC	1	11	-	0/2/15/18	0/1/1/1
11	AHR	aC	2	11	-	0/2/15/18	0/1/1/1
11	AHR	aC	3	11	-	0/2/15/18	0/1/1/1
3	FUB	aD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	aD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	aD	3	3	-	0/2/15/18	0/1/1/1
19	FUB	aE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	aE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	aE	3	19	1/1/4/5	2/6/19/22	0/1/1/1
19	AHR	aE	4	19	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	b	1	3	-	0/2/15/18	0/1/1/1
3	FUB	b	2	3	-	0/2/15/18	0/1/1/1
3	FUB	b	3	3	-	0/2/15/18	0/1/1/1
4	FUB	bA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	bA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	bA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	bA	4	4	-	0/2/15/18	0/1/1/1
6	FUB	bB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	bB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	bB	3	6	1/1/4/5	4/6/19/22	0/1/1/1
9	FUB	bC	1	9	-	0/2/15/18	0/1/1/1
9	FUB	bC	2	9	-	0/2/15/18	0/1/1/1
3	FUB	bD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	bD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	bD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	bE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	bE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	bE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
4	FUB	c	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c	2	4	-	0/2/15/18	0/1/1/1
4	FUB	c	3	4	-	0/2/15/18	0/1/1/1
4	AHR	c	4	4	-	0/2/15/18	0/1/1/1
3	FUB	cA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	cA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	cA	3	3	-	0/2/15/18	0/1/1/1
6	FUB	cB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	cB	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	cB	3	6	1/1/4/5	4/6/19/22	0/1/1/1
4	FUB	cC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	cC	2	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	cC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	cC	4	4	-	0/2/15/18	0/1/1/1
12	FUB	cD	1	12	-	0/2/15/18	0/1/1/1
12	FUB	cD	2	12	-	0/2/15/18	0/1/1/1
12	GZL	cD	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	cD	4	12	-	0/2/15/18	0/1/1/1
12	AHR	cD	5	12	-	0/2/15/18	0/1/1/1
18	FUB	cE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	cE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	cE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	cE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	cE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	d	1	4	-	0/2/15/18	0/1/1/1
4	FUB	d	2	4	-	0/2/15/18	0/1/1/1
4	FUB	d	3	4	-	0/2/15/18	0/1/1/1
4	AHR	d	4	4	-	0/2/15/18	0/1/1/1
7	FUB	dA	1	7	-	0/2/15/18	0/1/1/1
7	FUB	dA	2	7	-	0/2/15/18	0/1/1/1
7	FUB	dA	3	7	-	0/2/15/18	0/1/1/1
7	AHR	dA	4	7	-	0/2/15/18	0/1/1/1
13	FUB	dB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	dB	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	dB	3	13	-	4/6/19/22	0/1/1/1
13	AHR	dB	4	13	-	0/2/15/18	0/1/1/1
3	FUB	dC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	dC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	dC	3	3	-	0/2/15/18	0/1/1/1
13	FUB	dD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	dD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	dD	3	13	2/2/4/5	3/6/19/22	0/1/1/1
13	AHR	dD	4	13	-	0/2/15/18	0/1/1/1
22	FUB	dE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	dE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	dE	3	22	1/1/4/5	4/6/19/22	0/1/1/1
22	AHR	dE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	dE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	dE	6	22	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	e	1	3	-	0/2/15/18	0/1/1/1
3	FUB	e	2	3	-	0/2/15/18	0/1/1/1
3	FUB	e	3	3	-	0/2/15/18	0/1/1/1
4	FUB	eA	1	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	eA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	eA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	eA	4	4	-	0/2/15/18	0/1/1/1
15	FUB	eB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	eB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	eB	3	15	1/1/4/5	6/6/19/22	0/1/1/1
15	AHR	eB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	eB	5	15	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	eC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	eC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	eC	3	3	-	0/2/15/18	0/1/1/1
14	FUB	eD	1	14	-	0/2/15/18	0/1/1/1
14	FUB	eD	2	14	-	0/2/15/18	0/1/1/1
14	GZL	eD	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	eD	4	14	-	0/2/15/18	0/1/1/1
22	FUB	eE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	eE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	eE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	eE	4	22	2/2/3/4	0/2/15/18	0/1/1/1
22	AHR	eE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	eE	6	22	-	0/2/15/18	0/1/1/1
7	FUB	f	1	7	-	0/2/15/18	0/1/1/1
7	FUB	f	2	7	-	0/2/15/18	0/1/1/1
7	FUB	f	3	7	-	0/2/15/18	0/1/1/1
7	AHR	f	4	7	-	0/2/15/18	0/1/1/1
7	FUB	fA	1	7	-	0/2/15/18	0/1/1/1
7	FUB	fA	2	7	-	0/2/15/18	0/1/1/1
7	FUB	fA	3	7	-	0/2/15/18	0/1/1/1
7	AHR	fA	4	7	-	0/2/15/18	0/1/1/1
15	FUB	fB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	fB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	fB	3	15	1/1/4/5	0/6/19/22	0/1/1/1
15	AHR	fB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	fB	5	15	-	0/2/15/18	0/1/1/1
12	FUB	fC	1	12	-	0/2/15/18	0/1/1/1
12	FUB	fC	2	12	-	0/2/15/18	0/1/1/1
12	GZL	fC	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	fC	4	12	-	0/2/15/18	0/1/1/1
12	AHR	fC	5	12	-	0/2/15/18	0/1/1/1
12	FUB	fD	1	12	-	0/2/15/18	0/1/1/1
12	FUB	fD	2	12	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	GZL	fD	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	fD	4	12	-	0/2/15/18	0/1/1/1
12	AHR	fD	5	12	-	0/2/15/18	0/1/1/1
18	FUB	fE	1	18	1/1/3/4	0/2/15/18	0/1/1/1
18	FUB	fE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	fE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	fE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	fE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	g	1	4	-	0/2/15/18	0/1/1/1
4	FUB	g	2	4	-	0/2/15/18	0/1/1/1
4	FUB	g	3	4	-	0/2/15/18	0/1/1/1
4	AHR	g	4	4	-	0/2/15/18	0/1/1/1
11	FUB	gA	1	11	-	1/2/15/18	0/1/1/1
11	AHR	gA	2	11	-	0/2/15/18	0/1/1/1
11	AHR	gA	3	11	-	0/2/15/18	0/1/1/1
6	FUB	gB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	gB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	gB	3	6	1/1/4/5	6/6/19/22	0/1/1/1
13	FUB	gC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	gC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	gC	3	13	2/2/4/5	2/6/19/22	0/1/1/1
13	AHR	gC	4	13	-	0/2/15/18	0/1/1/1
4	FUB	gD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	gD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	gD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	gD	4	4	-	0/2/15/18	0/1/1/1
20	FUB	gE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	gE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	gE	3	20	1/1/4/5	2/6/19/22	0/1/1/1
20	AHR	gE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
7	FUB	h	1	7	-	0/2/15/18	0/1/1/1
7	FUB	h	2	7	-	0/2/15/18	0/1/1/1
7	FUB	h	3	7	-	0/2/15/18	0/1/1/1
7	AHR	h	4	7	-	0/2/15/18	0/1/1/1
9	FUB	hA	1	9	-	0/2/15/18	0/1/1/1
9	FUB	hA	2	9	-	0/2/15/18	0/1/1/1
3	FUB	hB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	hB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	hB	3	3	-	0/2/15/18	0/1/1/1
14	FUB	hC	1	14	-	0/2/15/18	0/1/1/1
14	FUB	hC	2	14	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	GZL	hC	3	14	2/2/4/5	3/6/19/22	0/1/1/1
14	FUB	hC	4	14	-	0/2/15/18	0/1/1/1
14	FUB	hD	1	14	-	0/2/15/18	0/1/1/1
14	FUB	hD	2	14	-	0/2/15/18	0/1/1/1
14	GZL	hD	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	hD	4	14	-	0/2/15/18	0/1/1/1
20	FUB	hE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	hE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	hE	3	20	1/1/4/5	3/6/19/22	0/1/1/1
20	AHR	hE	4	20	-	0/2/15/18	0/1/1/1
11	FUB	i	1	11	-	0/2/15/18	0/1/1/1
11	AHR	i	2	11	-	0/2/15/18	0/1/1/1
11	AHR	i	3	11	-	0/2/15/18	0/1/1/1
4	FUB	iA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	iA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	iA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	iA	4	4	-	0/2/15/18	0/1/1/1
12	FUB	iB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	iB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	iB	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	iB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	iB	5	12	-	0/2/15/18	0/1/1/1
12	FUB	iC	1	12	-	0/2/15/18	0/1/1/1
12	FUB	iC	2	12	-	0/2/15/18	0/1/1/1
12	GZL	iC	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	iC	4	12	-	0/2/15/18	0/1/1/1
12	AHR	iC	5	12	-	0/2/15/18	0/1/1/1
3	FUB	iD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	iD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	iD	3	3	-	0/2/15/18	0/1/1/1
22	FUB	iE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	iE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	iE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	iE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	iE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	iE	6	22	-	0/2/15/18	0/1/1/1
9	FUB	j	1	9	-	0/2/15/18	0/1/1/1
9	FUB	j	2	9	-	0/2/15/18	0/1/1/1
3	FUB	jA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	jA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	jA	3	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FUB	jB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	jB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	jB	3	13	2/2/4/5	3/6/19/22	0/1/1/1
13	AHR	jB	4	13	-	0/2/15/18	0/1/1/1
4	FUB	jC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	jC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	jC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	jC	4	4	-	0/2/15/18	0/1/1/1
10	FUB	jD	1	10	-	0/2/15/18	0/1/1/1
10	FUB	jD	2	10	-	0/2/15/18	0/1/1/1
10	FUB	jD	3	10	-	0/2/15/18	0/1/1/1
10	AHR	jD	4	10	-	0/2/15/18	0/1/1/1
10	AHR	jD	5	10	-	0/2/15/18	0/1/1/1
20	FUB	jE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	jE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	jE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	jE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	k	1	4	-	0/2/15/18	0/1/1/1
4	FUB	k	2	4	-	0/2/15/18	0/1/1/1
4	FUB	k	3	4	-	0/2/15/18	0/1/1/1
4	AHR	k	4	4	-	0/2/15/18	0/1/1/1
3	FUB	kA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	kA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	kA	3	3	-	0/2/15/18	0/1/1/1
14	FUB	kB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	kB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	kB	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	kB	4	14	-	0/2/15/18	0/1/1/1
14	FUB	kC	1	14	-	0/2/15/18	0/1/1/1
14	FUB	kC	2	14	-	0/2/15/18	0/1/1/1
14	GZL	kC	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	kC	4	14	-	0/2/15/18	0/1/1/1
4	FUB	kD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	kD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	kD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	kD	4	4	-	0/2/15/18	0/1/1/1
21	FUB	kE	1	21	-	0/2/15/18	0/1/1/1
21	FUB	kE	2	21	-	0/2/15/18	0/1/1/1
21	GZL	kE	3	21	1/1/4/5	0/6/19/22	0/1/1/1
21	AHR	kE	4	21	1/1/3/4	0/2/15/18	0/1/1/1
21	AHR	kE	5	21	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	l	1	3	-	0/2/15/18	0/1/1/1
3	FUB	l	2	3	-	0/2/15/18	0/1/1/1
3	FUB	l	3	3	-	0/2/15/18	0/1/1/1
12	FUB	lA	1	12	-	0/2/15/18	0/1/1/1
12	FUB	lA	2	12	-	0/2/15/18	0/1/1/1
12	GZL	lA	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	lA	4	12	-	0/2/15/18	0/1/1/1
12	AHR	lA	5	12	-	0/2/15/18	0/1/1/1
12	FUB	lB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	lB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	lB	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	lB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	lB	5	12	-	0/2/15/18	0/1/1/1
3	FUB	lC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	lC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	lC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	lD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	lD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	lD	3	3	-	0/2/15/18	0/1/1/1
24	FUB	lE	1	24	-	0/2/15/18	0/1/1/1
24	FUB	lE	2	24	-	0/2/15/18	0/1/1/1
24	GZL	lE	3	24	1/1/4/5	5/6/19/22	0/1/1/1
24	AHR	lE	4	24	1/1/3/4	0/2/15/18	0/1/1/1
24	AHR	lE	5	24	-	0/2/15/18	0/1/1/1
24	AHR	lE	6	24	-	0/2/15/18	0/1/1/1
3	FUB	m	1	3	-	0/2/15/18	0/1/1/1
3	FUB	m	2	3	-	0/2/15/18	0/1/1/1
3	FUB	m	3	3	-	0/2/15/18	0/1/1/1
13	FUB	mA	1	13	-	0/2/15/18	0/1/1/1
13	FUB	mA	2	13	-	0/2/15/18	0/1/1/1
13	GZL	mA	3	13	2/2/4/5	4/6/19/22	0/1/1/1
13	AHR	mA	4	13	-	0/2/15/18	0/1/1/1
4	FUB	mB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	mB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	mB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	mB	4	4	-	0/2/15/18	0/1/1/1
10	FUB	mC	1	10	-	0/2/15/18	0/1/1/1
10	FUB	mC	2	10	-	0/2/15/18	0/1/1/1
10	FUB	mC	3	10	-	0/2/15/18	0/1/1/1
10	AHR	mC	4	10	-	0/2/15/18	0/1/1/1
10	AHR	mC	5	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	mD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	mD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	mD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	mE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	mE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	mE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
12	FUB	n	1	12	-	0/2/15/18	0/1/1/1
12	FUB	n	2	12	-	0/2/15/18	0/1/1/1
12	GZL	n	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	n	4	12	-	0/2/15/18	0/1/1/1
12	AHR	n	5	12	-	0/2/15/18	0/1/1/1
14	FUB	nA	1	14	-	0/2/15/18	0/1/1/1
14	FUB	nA	2	14	-	0/2/15/18	0/1/1/1
14	GZL	nA	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	nA	4	14	-	0/2/15/18	0/1/1/1
14	FUB	nB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	nB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	nB	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	nB	4	14	-	0/2/15/18	0/1/1/1
4	FUB	nC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	nC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	nC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	nC	4	4	-	0/2/15/18	0/1/1/1
3	FUB	nD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	nD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	nD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	nE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	nE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	nE	3	6	1/1/4/5	6/6/19/22	0/1/1/1
13	FUB	o	1	13	-	0/2/15/18	0/1/1/1
13	FUB	o	2	13	-	0/2/15/18	0/1/1/1
13	GZL	o	3	13	2/2/4/5	2/6/19/22	0/1/1/1
13	AHR	o	4	13	-	0/2/15/18	0/1/1/1
12	FUB	oA	1	12	-	0/2/15/18	0/1/1/1
12	FUB	oA	2	12	-	0/2/15/18	0/1/1/1
12	GZL	oA	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	oA	4	12	-	0/2/15/18	0/1/1/1
12	AHR	oA	5	12	-	0/2/15/18	0/1/1/1
3	FUB	oB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	oB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	oB	3	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	oC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	oC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	oC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	oD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	oD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	oD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	oE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	oE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	oE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
14	FUB	p	1	14	-	0/2/15/18	0/1/1/1
14	FUB	p	2	14	-	0/2/15/18	0/1/1/1
14	GZL	p	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	p	4	14	-	0/2/15/18	0/1/1/1
4	FUB	pA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	pA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	pA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	pA	4	4	-	0/2/15/18	0/1/1/1
10	FUB	pB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	pB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	pB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	pB	4	10	-	0/2/15/18	0/1/1/1
10	AHR	pB	5	10	-	0/2/15/18	0/1/1/1
3	FUB	pC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	pC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	pC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	pE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	pE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	pE	3	18	1/1/4/5	4/6/19/22	0/1/1/1
18	AHR	pE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	pE	5	18	-	0/2/15/18	0/1/1/1
12	FUB	q	1	12	-	0/2/15/18	0/1/1/1
12	FUB	q	2	12	-	0/2/15/18	0/1/1/1
12	GZL	q	3	12	2/2/4/5	1/6/19/22	0/1/1/1
12	AHR	q	4	12	-	0/2/15/18	0/1/1/1
12	AHR	q	5	12	1/1/3/4	0/2/15/18	0/1/1/1
14	FUB	qA	1	14	-	0/2/15/18	0/1/1/1
14	FUB	qA	2	14	-	0/2/15/18	0/1/1/1
14	GZL	qA	3	14	2/2/4/5	4/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FUB	qA	4	14	-	0/2/15/18	0/1/1/1
4	FUB	qB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	qB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	qB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	qB	4	4	-	0/2/15/18	0/1/1/1
3	FUB	qC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	qC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	qC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	qD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	qD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	qD	3	3	-	0/2/15/18	0/1/1/1
19	FUB	qE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	qE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	qE	3	19	1/1/4/5	4/6/19/22	0/1/1/1
19	AHR	qE	4	19	-	0/2/15/18	0/1/1/1
4	FUB	r	1	4	-	0/2/15/18	0/1/1/1
4	FUB	r	2	4	-	0/2/15/18	0/1/1/1
4	FUB	r	3	4	-	0/2/15/18	0/1/1/1
4	AHR	r	4	4	-	0/2/15/18	0/1/1/1
3	FUB	rA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	rB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	rC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	rD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	rE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	rE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	rE	3	18	1/1/4/5	3/6/19/22	0/1/1/1
18	AHR	rE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	rE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
14	FUB	s	1	14	-	0/2/15/18	0/1/1/1
14	FUB	s	2	14	-	0/2/15/18	0/1/1/1
14	GZL	s	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	s	4	14	-	0/2/15/18	0/1/1/1
10	FUB	sA	1	10	-	0/2/15/18	0/1/1/1
10	FUB	sA	2	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FUB	sA	3	10	-	0/2/15/18	0/1/1/1
10	AHR	sA	4	10	-	0/2/15/18	0/1/1/1
10	AHR	sA	5	10	-	0/2/15/18	0/1/1/1
3	FUB	sB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	sB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	sB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	sC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	sC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	sC	3	3	-	0/2/15/18	0/1/1/1
10	FUB	sD	1	10	-	0/2/15/18	0/1/1/1
10	FUB	sD	2	10	-	0/2/15/18	0/1/1/1
10	FUB	sD	3	10	-	0/2/15/18	0/1/1/1
10	AHR	sD	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	sD	5	10	-	0/2/15/18	0/1/1/1
20	FUB	sE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	sE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	sE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	sE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	t	1	3	-	0/2/15/18	0/1/1/1
3	FUB	t	2	3	-	0/2/15/18	0/1/1/1
3	FUB	t	3	3	-	0/2/15/18	0/1/1/1
4	FUB	tA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	tA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	tA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	tA	4	4	-	0/2/15/18	0/1/1/1
3	FUB	tB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	tB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	tB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	tC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	tC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	tC	3	3	-	0/2/15/18	0/1/1/1
13	FUB	tD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	tD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	tD	3	13	3/3/4/5	0/6/19/22	0/1/1/1
13	AHR	tD	4	13	-	0/2/15/18	0/1/1/1
18	FUB	tE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	tE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	tE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	tE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	tE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
10	FUB	u	1	10	-	0/2/15/18	0/1/1/1
10	FUB	u	2	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FUB	u	3	10	-	0/2/15/18	0/1/1/1
10	AHR	u	4	10	-	0/2/15/18	0/1/1/1
10	AHR	u	5	10	-	0/2/15/18	0/1/1/1
3	FUB	uA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	uA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	uA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	uB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	uB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	uB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	uC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	uC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	uC	3	3	-	0/2/15/18	0/1/1/1
6	FUB	uD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	uD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	uD	3	6	2/2/4/5	6/6/19/22	0/1/1/1
20	FUB	uE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	uE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	uE	3	20	1/1/4/5	5/6/19/22	0/1/1/1
20	AHR	uE	4	20	-	0/2/15/18	0/1/1/1
4	FUB	v	1	4	-	0/2/15/18	0/1/1/1
4	FUB	v	2	4	-	0/2/15/18	0/1/1/1
4	FUB	v	3	4	-	0/2/15/18	0/1/1/1
4	AHR	v	4	4	-	0/2/15/18	0/1/1/1
3	FUB	vA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	vA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	vA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	vB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	vB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	vB	3	3	-	0/2/15/18	0/1/1/1
10	FUB	vC	1	10	-	0/2/15/18	0/1/1/1
10	FUB	vC	2	10	-	0/2/15/18	0/1/1/1
10	FUB	vC	3	10	-	0/2/15/18	0/1/1/1
10	AHR	vC	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	vC	5	10	-	0/2/15/18	0/1/1/1
13	FUB	vD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	vD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	vD	3	13	1/1/4/5	4/6/19/22	0/1/1/1
13	AHR	vD	4	13	-	0/2/15/18	0/1/1/1
21	FUB	vE	1	21	-	0/2/15/18	0/1/1/1
21	FUB	vE	2	21	-	0/2/15/18	0/1/1/1
21	GZL	vE	3	21	1/1/4/5	4/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	AHR	vE	4	21	1/1/3/4	0/2/15/18	0/1/1/1
21	AHR	vE	5	21	2/2/3/4	0/2/15/18	0/1/1/1
3	FUB	w	1	3	-	0/2/15/18	0/1/1/1
3	FUB	w	2	3	-	0/2/15/18	0/1/1/1
3	FUB	w	3	3	-	0/2/15/18	0/1/1/1
3	FUB	wA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	wA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	wA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	wB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	wB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	wB	3	3	-	0/2/15/18	0/1/1/1
13	FUB	wC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	wC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	wC	3	13	3/3/4/5	1/6/19/22	0/1/1/1
13	AHR	wC	4	13	-	0/2/15/18	0/1/1/1
13	FUB	wD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	wD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	wD	3	13	1/1/4/5	6/6/19/22	0/1/1/1
13	AHR	wD	4	13	-	0/2/15/18	0/1/1/1
22	FUB	wE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	wE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	wE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	wE	4	22	-	0/2/15/18	0/1/1/1
22	AHR	wE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	wE	6	22	-	0/2/15/18	0/1/1/1
3	FUB	x	1	3	-	0/2/15/18	0/1/1/1
3	FUB	x	2	3	-	0/2/15/18	0/1/1/1
3	FUB	x	3	3	-	0/2/15/18	0/1/1/1
3	FUB	xA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	xA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	xA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	xB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	xB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	xB	3	3	-	0/2/15/18	0/1/1/1
6	FUB	xC	1	6	-	0/2/15/18	0/1/1/1
6	FUB	xC	2	6	-	0/2/15/18	0/1/1/1
6	GZL	xC	3	6	2/2/4/5	5/6/19/22	0/1/1/1
6	FUB	xD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	xD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	xD	3	6	-	6/6/19/22	0/1/1/1
20	FUB	xE	1	20	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	FUB	xE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	xE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	xE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	y	1	3	-	0/2/15/18	0/1/1/1
3	FUB	y	2	3	-	0/2/15/18	0/1/1/1
3	FUB	y	3	3	-	0/2/15/18	0/1/1/1
3	FUB	yA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	yA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	yA	3	3	-	0/2/15/18	0/1/1/1
10	FUB	yB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	yB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	yB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	yB	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	yB	5	10	-	0/2/15/18	0/1/1/1
13	FUB	yC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	yC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	yC	3	13	1/1/4/5	2/6/19/22	0/1/1/1
13	AHR	yC	4	13	-	0/2/15/18	0/1/1/1
6	FUB	yD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	yD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	yD	3	6	1/1/4/5	2/6/19/22	0/1/1/1
18	FUB	yE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	yE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	yE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	yE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	yE	5	18	-	0/2/15/18	0/1/1/1
3	FUB	z	1	3	-	0/2/15/18	0/1/1/1
3	FUB	z	2	3	-	0/2/15/18	0/1/1/1
3	FUB	z	3	3	-	0/2/15/18	0/1/1/1
3	FUB	zA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	zA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	zA	3	3	-	0/2/15/18	0/1/1/1
13	FUB	zB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	zB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	zB	3	13	3/3/4/5	2/6/19/22	0/1/1/1
13	AHR	zB	4	13	-	0/2/15/18	0/1/1/1
13	FUB	zC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	zC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	zC	3	13	1/1/4/5	6/6/19/22	0/1/1/1
13	AHR	zC	4	13	-	0/2/15/18	0/1/1/1
6	FUB	zD	1	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUB	zD	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	zD	3	6	1/1/4/5	2/6/19/22	0/1/1/1
18	FUB	zE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	zE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	zE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	zE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	zE	5	18	1/1/3/4	0/2/15/18	0/1/1/1

All (1076) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CD	3	GZL	C2-C3	-18.93	1.22	1.53
6	LA	3	GZL	C2-C3	-18.87	1.22	1.53
6	uD	3	GZL	C2-C3	-18.70	1.22	1.53
6	xC	3	GZL	C2-C3	-18.69	1.22	1.53
6	XB	3	GZL	C2-C3	-18.66	1.22	1.53
13	4	3	GZL	C2-C3	-18.56	1.22	1.53
6	0B	3	GZL	C2-C3	-18.56	1.22	1.53
6	3A	3	GZL	C2-C3	-18.44	1.22	1.53
13	6	3	GZL	C2-C3	-18.27	1.23	1.53
13	wC	3	GZL	C2-C3	-18.22	1.23	1.53
13	YB	3	GZL	C2-C3	-18.20	1.23	1.53
13	4A	3	GZL	C2-C3	-18.20	1.23	1.53
6	5	3	GZL	C2-C3	-18.18	1.23	1.53
13	WB	3	GZL	C2-C3	-18.18	1.23	1.53
18	rE	3	GZL	C2-C3	-18.13	1.23	1.53
21	FE	3	GZL	C2-C3	-18.13	1.23	1.53
13	mA	3	GZL	C2-C3	-18.12	1.23	1.53
6	bE	3	GZL	C2-C3	-18.12	1.23	1.53
13	dB	3	GZL	C2-C3	-18.12	1.23	1.53
13	1B	3	GZL	C2-C3	-18.11	1.23	1.53
12	oA	3	GZL	C2-C3	-18.10	1.23	1.53
15	BB	3	GZL	C2-C3	-18.10	1.23	1.53
18	9D	3	GZL	C2-C3	-18.10	1.23	1.53
15	DA	3	GZL	C2-C3	-18.10	1.23	1.53
22	wE	3	GZL	C2-C3	-18.09	1.23	1.53
15	eB	3	GZL	C2-C3	-18.09	1.23	1.53
18	SE	3	GZL	C2-C3	-18.08	1.23	1.53
20	UE	3	GZL	C2-C3	-18.08	1.23	1.53
22	iE	3	GZL	C2-C3	-18.08	1.23	1.53
13	o	3	GZL	C2-C3	-18.08	1.23	1.53
18	PE	3	GZL	C2-C3	-18.08	1.23	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	OE	3	GZL	C2-C3	-18.07	1.23	1.53
15	fB	3	GZL	C2-C3	-18.07	1.23	1.53
6	9	3	GZL	C2-C3	-18.07	1.23	1.53
6	5B	3	GZL	C2-C3	-18.06	1.23	1.53
15	CA	3	GZL	C2-C3	-18.06	1.23	1.53
6	yD	3	GZL	C2-C3	-18.05	1.23	1.53
13	gC	3	GZL	C2-C3	-18.05	1.23	1.53
22	RE	3	GZL	C2-C3	-18.04	1.23	1.53
6	FC	3	GZL	C2-C3	-18.04	1.23	1.53
13	zB	3	GZL	C2-C3	-18.04	1.23	1.53
22	QE	3	GZL	C2-C3	-18.04	1.23	1.53
6	7D	3	GZL	C2-C3	-18.04	1.23	1.53
20	HE	3	GZL	C2-C3	-18.03	1.23	1.53
12	fC	3	GZL	C2-C3	-18.03	1.23	1.53
13	tD	3	GZL	C2-C3	-18.03	1.23	1.53
6	ME	3	GZL	C2-C3	-18.03	1.23	1.53
22	eE	3	GZL	C2-C3	-18.03	1.23	1.53
6	cB	3	GZL	C2-C3	-18.03	1.23	1.53
6	AA	3	GZL	C2-C3	-18.03	1.23	1.53
15	8B	3	GZL	C2-C3	-18.03	1.23	1.53
18	fE	3	GZL	C2-C3	-18.02	1.23	1.53
15	7B	3	GZL	C2-C3	-18.02	1.23	1.53
15	2D	3	GZL	C2-C3	-18.02	1.23	1.53
20	sE	3	GZL	C2-C3	-18.02	1.23	1.53
21	kE	3	GZL	C2-C3	-18.01	1.23	1.53
15	1D	3	GZL	C2-C3	-18.01	1.23	1.53
22	VE	3	GZL	C2-C3	-18.01	1.23	1.53
6	6A	3	GZL	C2-C3	-18.00	1.23	1.53
6	8A	3	GZL	C2-C3	-18.00	1.23	1.53
15	4C	3	GZL	C2-C3	-18.00	1.23	1.53
18	cE	3	GZL	C2-C3	-17.99	1.23	1.53
13	9A	3	GZL	C2-C3	-17.99	1.23	1.53
13	7	3	GZL	C2-C3	-17.99	1.23	1.53
12	q	3	GZL	C2-C3	-17.98	1.23	1.53
15	AB	3	GZL	C2-C3	-17.98	1.23	1.53
18	0E	3	GZL	C2-C3	-17.98	1.23	1.53
23	XE	3	GZL	C2-C3	-17.98	1.23	1.53
24	YE	3	GZL	C2-C3	-17.98	1.23	1.53
20	WE	3	GZL	C2-C3	-17.98	1.23	1.53
19	AE	3	GZL	C2-C3	-17.98	1.23	1.53
6	JC	3	GZL	C2-C3	-17.98	1.23	1.53
13	GB	3	GZL	C2-C3	-17.98	1.23	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	LE	3	GZL	C2-C3	-17.98	1.23	1.53
20	TE	3	GZL	C2-C3	-17.97	1.23	1.53
6	R	3	GZL	C2-C3	-17.97	1.23	1.53
20	EE	3	GZL	C2-C3	-17.97	1.23	1.53
22	GE	3	GZL	C2-C3	-17.97	1.23	1.53
20	gE	3	GZL	C2-C3	-17.97	1.23	1.53
14	qA	3	GZL	C2-C3	-17.97	1.23	1.53
6	8D	3	GZL	C2-C3	-17.96	1.23	1.53
12	lA	3	GZL	C2-C3	-17.96	1.23	1.53
21	vE	3	GZL	C2-C3	-17.96	1.23	1.53
19	NE	3	GZL	C2-C3	-17.96	1.23	1.53
13	2A	3	GZL	C2-C3	-17.95	1.23	1.53
22	dE	3	GZL	C2-C3	-17.95	1.23	1.53
6	8	3	GZL	C2-C3	-17.95	1.23	1.53
6	1C	3	GZL	C2-C3	-17.95	1.23	1.53
6	EA	3	GZL	C2-C3	-17.95	1.23	1.53
19	1E	3	GZL	C2-C3	-17.94	1.23	1.53
13	ZB	3	GZL	C2-C3	-17.94	1.23	1.53
6	zD	3	GZL	C2-C3	-17.94	1.23	1.53
20	uE	3	GZL	C2-C3	-17.94	1.23	1.53
13	jB	3	GZL	C2-C3	-17.94	1.23	1.53
6	bB	3	GZL	C2-C3	-17.94	1.23	1.53
6	mE	3	GZL	C2-C3	-17.94	1.23	1.53
12	cD	3	GZL	C2-C3	-17.94	1.23	1.53
18	tE	3	GZL	C2-C3	-17.94	1.23	1.53
18	DE	3	GZL	C2-C3	-17.93	1.23	1.53
20	CE	3	GZL	C2-C3	-17.93	1.23	1.53
6	aB	3	GZL	C2-C3	-17.93	1.23	1.53
6	7A	3	GZL	C2-C3	-17.92	1.23	1.53
12	n	3	GZL	C2-C3	-17.91	1.23	1.53
13	6B	3	GZL	C2-C3	-17.91	1.23	1.53
6	PA	3	GZL	C2-C3	-17.91	1.23	1.53
13	dD	3	GZL	C2-C3	-17.91	1.23	1.53
19	qE	3	GZL	C2-C3	-17.90	1.23	1.53
20	xE	3	GZL	C2-C3	-17.90	1.23	1.53
6	GD	3	GZL	C2-C3	-17.90	1.23	1.53
18	pE	3	GZL	C2-C3	-17.90	1.23	1.53
12	lB	3	GZL	C2-C3	-17.90	1.23	1.53
6	6C	3	GZL	C2-C3	-17.90	1.23	1.53
6	CB	3	GZL	C2-C3	-17.89	1.23	1.53
13	5A	3	GZL	C2-C3	-17.89	1.23	1.53
20	hE	3	GZL	C2-C3	-17.89	1.23	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	jE	3	GZL	C2-C3	-17.89	1.23	1.53
14	nA	3	GZL	C2-C3	-17.89	1.23	1.53
12	IB	3	GZL	C2-C3	-17.88	1.23	1.53
13	vD	3	GZL	C2-C3	-17.88	1.23	1.53
15	5C	3	GZL	C2-C3	-17.87	1.23	1.53
13	wD	3	GZL	C2-C3	-17.87	1.23	1.53
6	3D	3	GZL	C2-C3	-17.86	1.23	1.53
6	4B	3	GZL	C2-C3	-17.86	1.23	1.53
12	fD	3	GZL	C2-C3	-17.85	1.23	1.53
13	2B	3	GZL	C2-C3	-17.85	1.23	1.53
24	lE	3	GZL	C2-C3	-17.85	1.23	1.53
18	JE	3	GZL	C2-C3	-17.85	1.23	1.53
18	BE	3	GZL	C2-C3	-17.84	1.23	1.53
13	0D	3	GZL	C2-C3	-17.83	1.23	1.53
6	2C	3	GZL	C2-C3	-17.83	1.23	1.53
18	IE	3	GZL	C2-C3	-17.83	1.23	1.53
6	gB	3	GZL	C2-C3	-17.82	1.23	1.53
13	BA	3	GZL	C2-C3	-17.82	1.23	1.53
13	zC	3	GZL	C2-C3	-17.81	1.23	1.53
14	s	3	GZL	C2-C3	-17.81	1.23	1.53
6	nE	3	GZL	C2-C3	-17.79	1.23	1.53
18	KE	3	GZL	C2-C3	-17.78	1.23	1.53
14	p	3	GZL	C2-C3	-17.78	1.23	1.53
19	aE	3	GZL	C2-C3	-17.77	1.24	1.53
13	3C	3	GZL	C2-C3	-17.77	1.24	1.53
13	yC	3	GZL	C2-C3	-17.77	1.24	1.53
12	iB	3	GZL	C2-C3	-17.76	1.24	1.53
6	ZE	3	GZL	C2-C3	-17.76	1.24	1.53
14	hC	3	GZL	C2-C3	-17.76	1.24	1.53
6	6D	3	GZL	C2-C3	-17.76	1.24	1.53
12	iC	3	GZL	C2-C3	-17.76	1.24	1.53
6	oE	3	GZL	C2-C3	-17.75	1.24	1.53
14	eD	3	GZL	C2-C3	-17.75	1.24	1.53
6	9B	3	GZL	C2-C3	-17.73	1.24	1.53
6	0C	3	GZL	C2-C3	-17.72	1.24	1.53
6	3B	3	GZL	C2-C3	-17.69	1.24	1.53
14	nB	3	GZL	C2-C3	-17.67	1.24	1.53
14	kC	3	GZL	C2-C3	-17.66	1.24	1.53
18	zE	3	GZL	C2-C3	-17.64	1.24	1.53
14	HB	3	GZL	C2-C3	-17.61	1.24	1.53
18	yE	3	GZL	C2-C3	-17.61	1.24	1.53
12	FB	3	GZL	C2-C3	-17.57	1.24	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	kB	3	GZL	C2-C3	-17.56	1.24	1.53
14	KB	3	GZL	C2-C3	-17.54	1.24	1.53
6	xD	3	GZL	C2-C3	-17.51	1.24	1.53
14	hD	3	GZL	C2-C3	-17.49	1.24	1.53
6	N	3	GZL	C2-C3	-17.25	1.24	1.53
6	CD	3	GZL	O4-C4	-8.15	1.26	1.43
6	LA	3	GZL	O4-C4	-8.02	1.26	1.43
6	3A	3	GZL	O4-C4	-7.99	1.26	1.43
6	0B	3	GZL	O4-C4	-7.94	1.26	1.43
6	XB	3	GZL	O4-C4	-7.91	1.26	1.43
6	uD	3	GZL	O4-C4	-7.89	1.26	1.43
6	xC	3	GZL	O4-C4	-7.84	1.26	1.43
6	N	3	GZL	O4-C4	-7.57	1.27	1.43
13	2A	3	GZL	O4-C4	-7.57	1.27	1.43
14	hC	3	GZL	O4-C4	-7.49	1.27	1.43
18	BE	3	GZL	O4-C4	-7.48	1.27	1.43
6	3B	3	GZL	O4-C4	-7.47	1.27	1.43
14	nA	3	GZL	O4-C4	-7.47	1.27	1.43
14	p	3	GZL	O4-C4	-7.46	1.27	1.43
6	oE	3	GZL	O4-C4	-7.45	1.27	1.43
6	8D	3	GZL	O4-C4	-7.45	1.27	1.43
22	QE	3	GZL	O4-C4	-7.44	1.27	1.43
14	eD	3	GZL	O4-C4	-7.44	1.27	1.43
6	EA	3	GZL	O4-C4	-7.43	1.27	1.43
14	s	3	GZL	O4-C4	-7.42	1.27	1.43
6	8A	3	GZL	O4-C4	-7.42	1.27	1.43
6	9B	3	GZL	O4-C4	-7.42	1.27	1.43
13	tD	3	GZL	O4-C4	-7.42	1.27	1.43
15	7B	3	GZL	O4-C4	-7.41	1.27	1.43
6	CB	3	GZL	O4-C4	-7.41	1.27	1.43
14	qA	3	GZL	O4-C4	-7.41	1.27	1.43
6	PA	3	GZL	O4-C4	-7.40	1.27	1.43
6	xD	3	GZL	O4-C4	-7.40	1.27	1.43
22	RE	3	GZL	O4-C4	-7.40	1.27	1.43
14	kB	3	GZL	O4-C4	-7.39	1.27	1.43
6	4B	3	GZL	O4-C4	-7.39	1.27	1.43
20	TE	3	GZL	O4-C4	-7.39	1.27	1.43
24	lE	3	GZL	O4-C4	-7.39	1.27	1.43
6	gB	3	GZL	O4-C4	-7.39	1.27	1.43
14	KB	3	GZL	O4-C4	-7.39	1.27	1.43
21	vE	3	GZL	O4-C4	-7.39	1.27	1.43
12	FB	3	GZL	O4-C4	-7.38	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	HB	3	GZL	O4-C4	-7.37	1.27	1.43
6	GD	3	GZL	O4-C4	-7.37	1.27	1.43
13	4	3	GZL	O4-C4	-7.37	1.27	1.43
22	eE	3	GZL	O4-C4	-7.37	1.27	1.43
15	AB	3	GZL	O4-C4	-7.37	1.27	1.43
14	hD	3	GZL	O4-C4	-7.37	1.27	1.43
20	UE	3	GZL	O4-C4	-7.37	1.27	1.43
14	nB	3	GZL	O4-C4	-7.37	1.27	1.43
22	dE	3	GZL	O4-C4	-7.36	1.27	1.43
14	kC	3	GZL	O4-C4	-7.36	1.27	1.43
18	SE	3	GZL	O4-C4	-7.36	1.27	1.43
6	ZE	3	GZL	O4-C4	-7.36	1.27	1.43
12	iB	3	GZL	O4-C4	-7.35	1.27	1.43
13	2B	3	GZL	O4-C4	-7.35	1.27	1.43
6	mE	3	GZL	O4-C4	-7.35	1.27	1.43
19	qE	3	GZL	O4-C4	-7.35	1.27	1.43
6	cB	3	GZL	O4-C4	-7.35	1.27	1.43
20	gE	3	GZL	O4-C4	-7.35	1.27	1.43
23	XE	3	GZL	O4-C4	-7.35	1.27	1.43
15	CA	3	GZL	O4-C4	-7.34	1.27	1.43
21	kE	3	GZL	O4-C4	-7.34	1.27	1.43
19	AE	3	GZL	O4-C4	-7.34	1.27	1.43
6	0C	3	GZL	O4-C4	-7.34	1.27	1.43
20	WE	3	GZL	O4-C4	-7.33	1.27	1.43
6	9	3	GZL	O4-C4	-7.33	1.27	1.43
20	hE	3	GZL	O4-C4	-7.33	1.27	1.43
13	BA	3	GZL	O4-C4	-7.32	1.27	1.43
15	eB	3	GZL	O4-C4	-7.32	1.27	1.43
20	jE	3	GZL	O4-C4	-7.32	1.27	1.43
6	JC	3	GZL	O4-C4	-7.32	1.27	1.43
12	n	3	GZL	O4-C4	-7.32	1.27	1.43
13	o	3	GZL	O4-C4	-7.32	1.27	1.43
13	6	3	GZL	O4-C4	-7.32	1.27	1.43
6	3D	3	GZL	O4-C4	-7.32	1.27	1.43
20	EE	3	GZL	O4-C4	-7.32	1.27	1.43
6	7A	3	GZL	O4-C4	-7.31	1.27	1.43
18	PE	3	GZL	O4-C4	-7.31	1.27	1.43
21	FE	3	GZL	O4-C4	-7.31	1.27	1.43
6	8	3	GZL	O4-C4	-7.31	1.27	1.43
6	R	3	GZL	O4-C4	-7.31	1.27	1.43
18	IE	3	GZL	O4-C4	-7.30	1.27	1.43
6	bE	3	GZL	O4-C4	-7.30	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	yE	3	GZL	O4-C4	-7.30	1.27	1.43
6	AA	3	GZL	O4-C4	-7.30	1.27	1.43
12	iC	3	GZL	O4-C4	-7.30	1.27	1.43
13	4A	3	GZL	O4-C4	-7.29	1.27	1.43
6	6D	3	GZL	O4-C4	-7.29	1.27	1.43
13	wD	3	GZL	O4-C4	-7.29	1.27	1.43
18	zE	3	GZL	O4-C4	-7.29	1.27	1.43
13	jB	3	GZL	O4-C4	-7.29	1.28	1.43
15	DA	3	GZL	O4-C4	-7.29	1.28	1.43
13	mA	3	GZL	O4-C4	-7.28	1.28	1.43
13	5A	3	GZL	O4-C4	-7.28	1.28	1.43
24	YE	3	GZL	O4-C4	-7.28	1.28	1.43
6	ME	3	GZL	O4-C4	-7.28	1.28	1.43
15	BB	3	GZL	O4-C4	-7.27	1.28	1.43
22	VE	3	GZL	O4-C4	-7.27	1.28	1.43
13	wC	3	GZL	O4-C4	-7.27	1.28	1.43
13	yC	3	GZL	O4-C4	-7.27	1.28	1.43
20	CE	3	GZL	O4-C4	-7.26	1.28	1.43
6	bB	3	GZL	O4-C4	-7.26	1.28	1.43
15	8B	3	GZL	O4-C4	-7.26	1.28	1.43
12	oA	3	GZL	O4-C4	-7.26	1.28	1.43
13	ZB	3	GZL	O4-C4	-7.26	1.28	1.43
20	uE	3	GZL	O4-C4	-7.26	1.28	1.43
19	LE	3	GZL	O4-C4	-7.25	1.28	1.43
12	fC	3	GZL	O4-C4	-7.25	1.28	1.43
18	pE	3	GZL	O4-C4	-7.24	1.28	1.43
13	zC	3	GZL	O4-C4	-7.24	1.28	1.43
6	2C	3	GZL	O4-C4	-7.24	1.28	1.43
6	5B	3	GZL	O4-C4	-7.24	1.28	1.43
6	OE	3	GZL	O4-C4	-7.24	1.28	1.43
20	sE	3	GZL	O4-C4	-7.23	1.28	1.43
22	wE	3	GZL	O4-C4	-7.23	1.28	1.43
19	NE	3	GZL	O4-C4	-7.23	1.28	1.43
13	dD	3	GZL	O4-C4	-7.23	1.28	1.43
12	q	3	GZL	O4-C4	-7.23	1.28	1.43
12	lA	3	GZL	O4-C4	-7.23	1.28	1.43
18	rE	3	GZL	O4-C4	-7.22	1.28	1.43
20	HE	3	GZL	O4-C4	-7.22	1.28	1.43
15	fB	3	GZL	O4-C4	-7.22	1.28	1.43
13	1B	3	GZL	O4-C4	-7.22	1.28	1.43
6	6C	3	GZL	O4-C4	-7.22	1.28	1.43
18	JE	3	GZL	O4-C4	-7.21	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	5C	3	GZL	O4-C4	-7.21	1.28	1.43
13	zB	3	GZL	O4-C4	-7.21	1.28	1.43
19	1E	3	GZL	O4-C4	-7.20	1.28	1.43
13	7	3	GZL	O4-C4	-7.20	1.28	1.43
13	gC	3	GZL	O4-C4	-7.20	1.28	1.43
20	xE	3	GZL	O4-C4	-7.20	1.28	1.43
6	nE	3	GZL	O4-C4	-7.19	1.28	1.43
18	DE	3	GZL	O4-C4	-7.19	1.28	1.43
22	GE	3	GZL	O4-C4	-7.19	1.28	1.43
22	iE	3	GZL	O4-C4	-7.19	1.28	1.43
6	zD	3	GZL	O4-C4	-7.19	1.28	1.43
12	IB	3	GZL	O4-C4	-7.19	1.28	1.43
18	KE	3	GZL	O4-C4	-7.19	1.28	1.43
19	aE	3	GZL	O4-C4	-7.19	1.28	1.43
18	cE	3	GZL	O4-C4	-7.19	1.28	1.43
18	tE	3	GZL	O4-C4	-7.18	1.28	1.43
18	0E	3	GZL	O4-C4	-7.18	1.28	1.43
18	9D	3	GZL	O4-C4	-7.17	1.28	1.43
6	1C	3	GZL	O4-C4	-7.17	1.28	1.43
12	fD	3	GZL	O4-C4	-7.16	1.28	1.43
15	4C	3	GZL	O4-C4	-7.16	1.28	1.43
12	cD	3	GZL	O4-C4	-7.16	1.28	1.43
13	YB	3	GZL	O4-C4	-7.16	1.28	1.43
6	aB	3	GZL	O4-C4	-7.16	1.28	1.43
13	WB	3	GZL	O4-C4	-7.16	1.28	1.43
15	1D	3	GZL	O4-C4	-7.15	1.28	1.43
6	6A	3	GZL	O4-C4	-7.15	1.28	1.43
18	fE	3	GZL	O4-C4	-7.15	1.28	1.43
13	9A	3	GZL	C3-C4	7.15	1.68	1.53
13	GB	3	GZL	O4-C4	-7.14	1.28	1.43
15	2D	3	GZL	O4-C4	-7.12	1.28	1.43
6	yD	3	GZL	O4-C4	-7.12	1.28	1.43
13	6B	3	GZL	O4-C4	-7.12	1.28	1.43
13	9A	3	GZL	O4-C4	-7.12	1.28	1.43
13	0D	3	GZL	O4-C4	-7.12	1.28	1.43
6	5	3	GZL	O4-C4	-7.11	1.28	1.43
13	3C	3	GZL	O4-C4	-7.11	1.28	1.43
13	dB	3	GZL	O4-C4	-7.10	1.28	1.43
6	7D	3	GZL	O4-C4	-7.10	1.28	1.43
13	vD	3	GZL	O4-C4	-7.09	1.28	1.43
12	lB	3	GZL	O4-C4	-7.09	1.28	1.43
13	dB	3	GZL	C3-C4	7.08	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BA	3	GZL	C3-C4	7.08	1.68	1.53
13	6B	3	GZL	C3-C4	7.04	1.68	1.53
13	2A	3	GZL	C3-C4	6.92	1.68	1.53
13	3C	3	GZL	C3-C4	6.89	1.68	1.53
13	0D	3	GZL	C3-C4	6.86	1.68	1.53
6	nE	3	GZL	C3-C4	6.82	1.67	1.53
18	0E	3	GZL	C3-C4	6.79	1.67	1.53
13	wC	3	GZL	C3-C4	6.78	1.67	1.53
18	zE	3	GZL	C3-C4	6.78	1.67	1.53
14	hD	3	GZL	C3-C4	6.77	1.67	1.53
18	KE	3	GZL	C3-C4	6.74	1.67	1.53
15	2D	3	GZL	C3-C4	6.74	1.67	1.53
18	JE	3	GZL	C3-C4	6.73	1.67	1.53
6	FC	3	GZL	O4-C4	-6.72	1.29	1.43
13	vD	3	GZL	C3-C4	6.71	1.67	1.53
12	cD	3	GZL	C3-C4	6.70	1.67	1.53
6	1C	3	GZL	C3-C4	6.69	1.67	1.53
6	7D	3	GZL	C3-C4	6.69	1.67	1.53
13	7	3	GZL	C3-C4	6.68	1.67	1.53
18	9D	3	GZL	C3-C4	6.68	1.67	1.53
19	1E	3	GZL	C3-C4	6.68	1.67	1.53
13	ZB	3	GZL	C3-C4	6.68	1.67	1.53
13	5A	3	GZL	C3-C4	6.67	1.67	1.53
19	aE	3	GZL	C3-C4	6.67	1.67	1.53
18	yE	3	GZL	C3-C4	6.67	1.67	1.53
20	sE	3	GZL	C3-C4	6.67	1.67	1.53
18	tE	3	GZL	C3-C4	6.67	1.67	1.53
13	zB	3	GZL	C3-C4	6.65	1.67	1.53
14	kB	3	GZL	C3-C4	6.65	1.67	1.53
20	xE	3	GZL	C3-C4	6.65	1.67	1.53
13	WB	3	GZL	C3-C4	6.64	1.67	1.53
12	FB	3	GZL	C3-C4	6.64	1.67	1.53
6	aB	3	GZL	C3-C4	6.64	1.67	1.53
18	rE	3	GZL	C3-C4	6.63	1.67	1.53
18	IE	3	GZL	C3-C4	6.62	1.67	1.53
13	tD	3	GZL	C3-C4	6.62	1.67	1.53
13	zC	3	GZL	C3-C4	6.62	1.67	1.53
12	lB	3	GZL	C3-C4	6.61	1.67	1.53
13	yC	3	GZL	C3-C4	6.61	1.67	1.53
15	8B	3	GZL	C3-C4	6.61	1.67	1.53
6	2C	3	GZL	C3-C4	6.61	1.67	1.53
15	5C	3	GZL	C3-C4	6.60	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	NE	3	GZL	C3-C4	6.60	1.67	1.53
6	xD	3	GZL	C3-C4	6.60	1.67	1.53
12	fD	3	GZL	C3-C4	6.59	1.67	1.53
13	wD	3	GZL	C3-C4	6.59	1.67	1.53
14	HB	3	GZL	C3-C4	6.59	1.67	1.53
6	zD	3	GZL	C3-C4	6.58	1.67	1.53
6	yD	3	GZL	C3-C4	6.58	1.67	1.53
14	hC	3	GZL	C3-C4	6.57	1.67	1.53
20	HE	3	GZL	C3-C4	6.57	1.67	1.53
18	cE	3	GZL	C3-C4	6.57	1.67	1.53
13	GB	3	GZL	C3-C4	6.56	1.67	1.53
12	IB	3	GZL	C3-C4	6.56	1.67	1.53
15	4C	3	GZL	C3-C4	6.56	1.67	1.53
14	KB	3	GZL	C3-C4	6.55	1.67	1.53
14	eD	3	GZL	C3-C4	6.55	1.67	1.53
22	GE	3	GZL	C3-C4	6.55	1.67	1.53
20	CE	3	GZL	C3-C4	6.55	1.67	1.53
12	lA	3	GZL	C3-C4	6.54	1.67	1.53
18	pE	3	GZL	C3-C4	6.54	1.67	1.53
15	eB	3	GZL	C3-C4	6.54	1.67	1.53
6	OE	3	GZL	C3-C4	6.53	1.67	1.53
6	9B	3	GZL	C3-C4	6.52	1.67	1.53
13	dD	3	GZL	C3-C4	6.52	1.67	1.53
6	6D	3	GZL	C3-C4	6.52	1.67	1.53
18	DE	3	GZL	C3-C4	6.51	1.67	1.53
6	6C	3	GZL	C3-C4	6.51	1.67	1.53
6	3D	3	GZL	C3-C4	6.51	1.67	1.53
14	kC	3	GZL	C3-C4	6.51	1.67	1.53
6	R	3	GZL	C3-C4	6.51	1.67	1.53
6	6A	3	GZL	C3-C4	6.51	1.67	1.53
12	iB	3	GZL	C3-C4	6.51	1.67	1.53
6	5B	3	GZL	C3-C4	6.50	1.67	1.53
15	CA	3	GZL	C3-C4	6.50	1.67	1.53
12	iC	3	GZL	C3-C4	6.50	1.67	1.53
14	s	3	GZL	C3-C4	6.49	1.67	1.53
19	qE	3	GZL	C3-C4	6.49	1.67	1.53
20	uE	3	GZL	C3-C4	6.49	1.67	1.53
14	p	3	GZL	C3-C4	6.49	1.67	1.53
15	BB	3	GZL	C3-C4	6.48	1.67	1.53
14	nB	3	GZL	C3-C4	6.48	1.67	1.53
22	wE	3	GZL	C3-C4	6.48	1.67	1.53
6	bB	3	GZL	C3-C4	6.48	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	GD	3	GZL	C3-C4	6.48	1.67	1.53
6	0C	3	GZL	C3-C4	6.48	1.67	1.53
15	fB	3	GZL	C3-C4	6.48	1.67	1.53
18	fE	3	GZL	C3-C4	6.48	1.67	1.53
22	eE	3	GZL	C3-C4	6.48	1.67	1.53
14	nA	3	GZL	C3-C4	6.48	1.67	1.53
12	fC	3	GZL	C3-C4	6.48	1.67	1.53
22	iE	3	GZL	C3-C4	6.47	1.67	1.53
6	4B	3	GZL	C3-C4	6.47	1.67	1.53
13	jB	3	GZL	C3-C4	6.47	1.67	1.53
6	JC	3	GZL	C3-C4	6.46	1.67	1.53
20	jE	3	GZL	C3-C4	6.46	1.67	1.53
6	ZE	3	GZL	C3-C4	6.46	1.67	1.53
6	3B	3	GZL	C3-C4	6.45	1.67	1.53
13	gC	3	GZL	C3-C4	6.45	1.67	1.53
6	bE	3	GZL	C3-C4	6.45	1.67	1.53
20	hE	3	GZL	C3-C4	6.45	1.67	1.53
20	EE	3	GZL	C3-C4	6.45	1.67	1.53
19	LE	3	GZL	C3-C4	6.44	1.67	1.53
19	AE	3	GZL	C3-C4	6.44	1.67	1.53
6	ME	3	GZL	C3-C4	6.44	1.67	1.53
6	gB	3	GZL	C3-C4	6.44	1.67	1.53
12	n	3	GZL	C3-C4	6.44	1.67	1.53
6	AA	3	GZL	C3-C4	6.44	1.67	1.53
13	o	3	GZL	C3-C4	6.43	1.67	1.53
15	1D	3	GZL	C3-C4	6.43	1.67	1.53
24	lE	3	GZL	C3-C4	6.43	1.67	1.53
13	2B	3	GZL	C3-C4	6.42	1.67	1.53
12	q	3	GZL	C3-C4	6.42	1.67	1.53
13	YB	3	GZL	C3-C4	6.42	1.67	1.53
22	dE	3	GZL	C3-C4	6.42	1.67	1.53
24	YE	3	GZL	C3-C4	6.41	1.67	1.53
6	8	3	GZL	C3-C4	6.41	1.67	1.53
6	cB	3	GZL	C3-C4	6.40	1.67	1.53
20	WE	3	GZL	C3-C4	6.40	1.67	1.53
13	4A	3	GZL	C3-C4	6.39	1.67	1.53
21	FE	3	GZL	C3-C4	6.39	1.67	1.53
6	8D	3	GZL	C3-C4	6.39	1.67	1.53
22	QE	3	GZL	C3-C4	6.39	1.67	1.53
21	kE	3	GZL	C3-C4	6.39	1.67	1.53
6	oE	3	GZL	C3-C4	6.38	1.66	1.53
12	oA	3	GZL	C3-C4	6.38	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	AB	3	GZL	C3-C4	6.38	1.66	1.53
15	DA	3	GZL	C3-C4	6.38	1.66	1.53
20	gE	3	GZL	C3-C4	6.37	1.66	1.53
18	PE	3	GZL	C3-C4	6.37	1.66	1.53
6	mE	3	GZL	C3-C4	6.36	1.66	1.53
6	PA	3	GZL	C3-C4	6.36	1.66	1.53
22	RE	3	GZL	C3-C4	6.36	1.66	1.53
6	8A	3	GZL	C3-C4	6.36	1.66	1.53
22	VE	3	GZL	C3-C4	6.36	1.66	1.53
21	vE	3	GZL	C3-C4	6.36	1.66	1.53
6	9	3	GZL	C3-C4	6.36	1.66	1.53
6	EA	3	GZL	C3-C4	6.36	1.66	1.53
18	BE	3	GZL	C3-C4	6.35	1.66	1.53
13	mA	3	GZL	C3-C4	6.35	1.66	1.53
15	7B	3	GZL	C3-C4	6.35	1.66	1.53
6	CB	3	GZL	C3-C4	6.35	1.66	1.53
13	1B	3	GZL	C3-C4	6.35	1.66	1.53
14	qA	3	GZL	C3-C4	6.34	1.66	1.53
18	SE	3	GZL	C3-C4	6.34	1.66	1.53
20	TE	3	GZL	C3-C4	6.31	1.66	1.53
23	XE	3	GZL	C3-C4	6.31	1.66	1.53
13	6	3	GZL	C3-C4	6.31	1.66	1.53
20	UE	3	GZL	C3-C4	6.28	1.66	1.53
6	7A	3	GZL	C3-C4	6.28	1.66	1.53
6	N	3	GZL	C3-C4	6.23	1.66	1.53
6	0B	3	GZL	C1-C2	6.21	1.62	1.51
6	5	3	GZL	C3-C4	6.18	1.66	1.53
6	LA	3	GZL	C1-C2	6.16	1.62	1.51
6	XB	3	GZL	C1-C2	6.16	1.62	1.51
6	xC	3	GZL	C1-C2	6.13	1.62	1.51
6	uD	3	GZL	C1-C2	6.08	1.62	1.51
13	4	3	GZL	C3-C4	5.99	1.66	1.53
6	CD	3	GZL	C1-C2	5.98	1.62	1.51
6	FC	3	GZL	C3-C4	5.95	1.66	1.53
6	N	3	GZL	C1-C2	5.92	1.62	1.51
6	LA	3	GZL	C3-C4	5.89	1.65	1.53
6	CD	3	GZL	C3-C4	5.74	1.65	1.53
6	3A	3	GZL	C1-C2	5.50	1.61	1.51
13	2A	3	GZL	C1-C2	5.47	1.61	1.51
6	uD	3	GZL	C3-C4	5.40	1.64	1.53
6	XB	3	GZL	C3-C4	5.37	1.64	1.53
6	0B	3	GZL	C3-C4	5.36	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	xC	3	GZL	C3-C4	5.31	1.64	1.53
6	3A	3	GZL	C3-C4	5.30	1.64	1.53
13	tD	3	GZL	C1-C2	4.97	1.60	1.51
6	5	3	GZL	C1-C2	4.93	1.60	1.51
6	3B	3	GZL	C1-C2	4.91	1.60	1.51
13	WB	3	GZL	C1-C2	4.89	1.60	1.51
6	0C	3	GZL	C1-C2	4.88	1.60	1.51
13	wC	3	GZL	C1-C2	4.87	1.60	1.51
6	CB	3	GZL	C1-C2	4.84	1.60	1.51
14	kB	3	GZL	C1-C2	4.84	1.60	1.51
14	nB	3	GZL	C1-C2	4.83	1.60	1.51
12	iB	3	GZL	C1-C2	4.83	1.60	1.51
13	jB	3	GZL	C1-C2	4.80	1.60	1.51
6	ZE	3	GZL	C1-C2	4.80	1.60	1.51
14	p	3	GZL	C1-C2	4.80	1.60	1.51
14	hC	3	GZL	C1-C2	4.79	1.60	1.51
13	zB	3	GZL	C1-C2	4.79	1.60	1.51
6	xD	3	GZL	C1-C2	4.78	1.60	1.51
6	9B	3	GZL	C1-C2	4.77	1.60	1.51
12	FB	3	GZL	C1-C2	4.76	1.60	1.51
6	gB	3	GZL	C1-C2	4.76	1.60	1.51
14	HB	3	GZL	C1-C2	4.76	1.60	1.51
14	kC	3	GZL	C1-C2	4.76	1.60	1.51
14	eD	3	GZL	C1-C2	4.75	1.60	1.51
14	KB	3	GZL	C1-C2	4.74	1.60	1.51
6	EA	3	GZL	C1-C2	4.74	1.60	1.51
19	qE	3	GZL	C1-C2	4.74	1.60	1.51
6	3D	3	GZL	C1-C2	4.74	1.60	1.51
12	n	3	GZL	C1-C2	4.73	1.60	1.51
13	4	3	GZL	C1-C2	4.73	1.60	1.51
6	PA	3	GZL	C1-C2	4.73	1.60	1.51
19	LE	3	GZL	C1-C2	4.72	1.60	1.51
13	2B	3	GZL	C1-C2	4.72	1.60	1.51
14	nA	3	GZL	C1-C2	4.72	1.60	1.51
21	vE	3	GZL	C1-C2	4.72	1.60	1.51
6	7A	3	GZL	C1-C2	4.71	1.60	1.51
19	AE	3	GZL	C1-C2	4.71	1.60	1.51
6	4B	3	GZL	C1-C2	4.71	1.60	1.51
6	6C	3	GZL	C1-C2	4.70	1.59	1.51
20	gE	3	GZL	C1-C2	4.70	1.59	1.51
14	qA	3	GZL	C1-C2	4.69	1.59	1.51
20	TE	3	GZL	C1-C2	4.68	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1B	3	GZL	C1-C2	4.67	1.59	1.51
6	oE	3	GZL	C1-C2	4.67	1.59	1.51
6	bB	3	GZL	C1-C2	4.65	1.59	1.51
20	jE	3	GZL	C1-C2	4.65	1.59	1.51
12	IB	3	GZL	C1-C2	4.65	1.59	1.51
13	yC	3	GZL	C1-C2	4.65	1.59	1.51
13	wD	3	GZL	C1-C2	4.65	1.59	1.51
6	2C	3	GZL	C1-C2	4.64	1.59	1.51
13	GB	3	GZL	C1-C2	4.64	1.59	1.51
14	s	3	GZL	C1-C2	4.63	1.59	1.51
12	fC	3	GZL	C1-C2	4.63	1.59	1.51
13	zC	3	GZL	C1-C2	4.63	1.59	1.51
21	kE	3	GZL	C1-C2	4.63	1.59	1.51
15	1D	3	GZL	C1-C2	4.62	1.59	1.51
18	BE	3	GZL	C1-C2	4.62	1.59	1.51
20	hE	3	GZL	C1-C2	4.62	1.59	1.51
24	lE	3	GZL	C1-C2	4.61	1.59	1.51
6	6D	3	GZL	C1-C2	4.61	1.59	1.51
6	bE	3	GZL	C1-C2	4.61	1.59	1.51
6	8D	3	GZL	C1-C2	4.60	1.59	1.51
18	cE	3	GZL	C1-C2	4.60	1.59	1.51
13	dD	3	GZL	C1-C2	4.59	1.59	1.51
19	aE	3	GZL	C1-C2	4.59	1.59	1.51
13	o	3	GZL	C1-C2	4.59	1.59	1.51
6	cB	3	GZL	C1-C2	4.59	1.59	1.51
6	8	3	GZL	C1-C2	4.59	1.59	1.51
12	lA	3	GZL	C1-C2	4.58	1.59	1.51
24	YE	3	GZL	C1-C2	4.58	1.59	1.51
15	7B	3	GZL	C1-C2	4.58	1.59	1.51
6	uD	3	GZL	O4-C1	4.58	1.53	1.43
6	mE	3	GZL	C1-C2	4.57	1.59	1.51
15	AB	3	GZL	C1-C2	4.57	1.59	1.51
13	gC	3	GZL	C1-C2	4.57	1.59	1.51
6	R	3	GZL	C1-C2	4.56	1.59	1.51
13	4A	3	GZL	C1-C2	4.56	1.59	1.51
6	xC	3	GZL	O4-C1	4.55	1.53	1.43
20	UE	3	GZL	C1-C2	4.55	1.59	1.51
22	VE	3	GZL	C1-C2	4.55	1.59	1.51
12	iC	3	GZL	C1-C2	4.54	1.59	1.51
20	WE	3	GZL	C1-C2	4.54	1.59	1.51
15	5C	3	GZL	C1-C2	4.54	1.59	1.51
20	EE	3	GZL	C1-C2	4.54	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	CA	3	GZL	C1-C2	4.54	1.59	1.51
22	dE	3	GZL	C1-C2	4.53	1.59	1.51
6	zD	3	GZL	C1-C2	4.53	1.59	1.51
18	SE	3	GZL	C1-C2	4.53	1.59	1.51
6	8A	3	GZL	C1-C2	4.52	1.59	1.51
13	ZB	3	GZL	C1-C2	4.52	1.59	1.51
12	cD	3	GZL	C1-C2	4.52	1.59	1.51
23	XE	3	GZL	C1-C2	4.52	1.59	1.51
18	zE	3	GZL	C1-C2	4.51	1.59	1.51
6	XB	3	GZL	O4-C1	4.51	1.53	1.43
18	PE	3	GZL	C1-C2	4.51	1.59	1.51
6	GD	3	GZL	C1-C2	4.51	1.59	1.51
22	iE	3	GZL	C1-C2	4.51	1.59	1.51
12	lB	3	GZL	C1-C2	4.50	1.59	1.51
22	RE	3	GZL	C1-C2	4.50	1.59	1.51
6	ME	3	GZL	C1-C2	4.49	1.59	1.51
6	9	3	GZL	C1-C2	4.49	1.59	1.51
18	yE	3	GZL	C1-C2	4.49	1.59	1.51
14	hD	3	GZL	C1-C2	4.49	1.59	1.51
6	aB	3	GZL	C1-C2	4.49	1.59	1.51
6	yD	3	GZL	C1-C2	4.48	1.59	1.51
18	fE	3	GZL	C1-C2	4.48	1.59	1.51
19	1E	3	GZL	C1-C2	4.48	1.59	1.51
21	FE	3	GZL	C1-C2	4.48	1.59	1.51
13	mA	3	GZL	C1-C2	4.48	1.59	1.51
6	AA	3	GZL	C1-C2	4.48	1.59	1.51
22	eE	3	GZL	C1-C2	4.48	1.59	1.51
6	LA	3	GZL	O4-C1	4.48	1.53	1.43
18	pE	3	GZL	C1-C2	4.47	1.59	1.51
12	q	3	GZL	C1-C2	4.47	1.59	1.51
12	oA	3	GZL	C1-C2	4.47	1.59	1.51
13	YB	3	GZL	C1-C2	4.46	1.59	1.51
6	JC	3	GZL	C1-C2	4.46	1.59	1.51
6	0B	3	GZL	O4-C1	4.46	1.53	1.43
13	vD	3	GZL	C1-C2	4.46	1.59	1.51
18	DE	3	GZL	C1-C2	4.45	1.59	1.51
15	DA	3	GZL	C1-C2	4.44	1.59	1.51
20	uE	3	GZL	C1-C2	4.44	1.59	1.51
15	4C	3	GZL	C1-C2	4.44	1.59	1.51
15	eB	3	GZL	C1-C2	4.43	1.59	1.51
12	fD	3	GZL	C1-C2	4.43	1.59	1.51
6	6A	3	GZL	C1-C2	4.43	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QE	3	GZL	C1-C2	4.43	1.59	1.51
15	BB	3	GZL	C1-C2	4.42	1.59	1.51
15	fB	3	GZL	C1-C2	4.42	1.59	1.51
15	2D	3	GZL	C1-C2	4.42	1.59	1.51
18	JE	3	GZL	C1-C2	4.41	1.59	1.51
18	tE	3	GZL	C1-C2	4.41	1.59	1.51
22	wE	3	GZL	C1-C2	4.41	1.59	1.51
20	sE	3	GZL	C1-C2	4.40	1.59	1.51
6	5B	3	GZL	C1-C2	4.40	1.59	1.51
6	OE	3	GZL	C1-C2	4.40	1.59	1.51
6	1C	3	GZL	C1-C2	4.39	1.59	1.51
13	0D	3	GZL	C1-C2	4.39	1.59	1.51
18	KE	3	GZL	C1-C2	4.38	1.59	1.51
6	nE	3	GZL	C1-C2	4.38	1.59	1.51
13	7	3	GZL	C1-C2	4.38	1.59	1.51
13	5A	3	GZL	C1-C2	4.36	1.59	1.51
13	6	3	GZL	C1-C2	4.35	1.59	1.51
13	3C	3	GZL	C1-C2	4.35	1.59	1.51
19	NE	3	GZL	C1-C2	4.35	1.59	1.51
15	8B	3	GZL	C1-C2	4.34	1.59	1.51
18	IE	3	GZL	C1-C2	4.32	1.59	1.51
6	CD	3	GZL	O4-C1	4.32	1.53	1.43
13	YB	3	GZL	O4-C1	4.30	1.53	1.43
15	1D	3	GZL	O4-C1	4.30	1.53	1.43
13	1B	3	GZL	O4-C1	4.29	1.53	1.43
22	GE	3	GZL	C1-C2	4.28	1.59	1.51
18	0E	3	GZL	C1-C2	4.27	1.59	1.51
20	HE	3	GZL	C1-C2	4.27	1.59	1.51
20	CE	3	GZL	C1-C2	4.27	1.59	1.51
18	rE	3	GZL	C1-C2	4.27	1.59	1.51
13	wC	3	GZL	O4-C1	4.26	1.53	1.43
20	xE	3	GZL	C1-C2	4.25	1.59	1.51
13	WB	3	GZL	O4-C1	4.25	1.53	1.43
19	LE	3	GZL	O4-C1	4.23	1.53	1.43
13	jB	3	GZL	O4-C1	4.23	1.53	1.43
13	zB	3	GZL	O4-C1	4.23	1.52	1.43
6	7D	3	GZL	C1-C2	4.22	1.59	1.51
13	tD	3	GZL	O4-C1	4.21	1.52	1.43
13	o	3	GZL	O4-C1	4.21	1.52	1.43
13	2A	3	GZL	O4-C1	4.21	1.52	1.43
15	4C	3	GZL	O4-C1	4.20	1.52	1.43
13	gC	3	GZL	O4-C1	4.20	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	gE	3	GZL	O4-C1	4.19	1.52	1.43
18	9D	3	GZL	C1-C2	4.19	1.59	1.51
6	N	3	GZL	O4-C1	4.19	1.52	1.43
6	5	3	GZL	O4-C1	4.19	1.52	1.43
22	VE	3	GZL	O4-C1	4.19	1.52	1.43
12	IB	3	GZL	O4-C1	4.18	1.52	1.43
13	GB	3	GZL	O4-C1	4.18	1.52	1.43
15	fB	3	GZL	O4-C1	4.18	1.52	1.43
22	iE	3	GZL	O4-C1	4.18	1.52	1.43
6	6A	3	GZL	O4-C1	4.18	1.52	1.43
13	mA	3	GZL	O4-C1	4.18	1.52	1.43
23	XE	3	GZL	O4-C1	4.17	1.52	1.43
12	q	3	GZL	O4-C1	4.17	1.52	1.43
13	6B	3	GZL	C1-C2	4.17	1.59	1.51
12	lB	3	GZL	O4-C1	4.16	1.52	1.43
13	dD	3	GZL	O4-C1	4.16	1.52	1.43
21	kE	3	GZL	O4-C1	4.16	1.52	1.43
12	fC	3	GZL	O4-C1	4.15	1.52	1.43
6	3B	3	GZL	O4-C1	4.15	1.52	1.43
14	qA	3	GZL	O4-C1	4.15	1.52	1.43
20	TE	3	GZL	O4-C1	4.15	1.52	1.43
6	zD	3	GZL	O4-C1	4.15	1.52	1.43
24	YE	3	GZL	O4-C1	4.15	1.52	1.43
12	oA	3	GZL	O4-C1	4.15	1.52	1.43
6	ZE	3	GZL	O4-C1	4.15	1.52	1.43
18	fE	3	GZL	O4-C1	4.14	1.52	1.43
6	7A	3	GZL	O4-C1	4.14	1.52	1.43
6	oE	3	GZL	O4-C1	4.14	1.52	1.43
13	6	3	GZL	O4-C1	4.14	1.52	1.43
22	wE	3	GZL	O4-C1	4.14	1.52	1.43
21	vE	3	GZL	O4-C1	4.14	1.52	1.43
13	yC	3	GZL	O4-C1	4.13	1.52	1.43
15	7B	3	GZL	O4-C1	4.13	1.52	1.43
18	pE	3	GZL	O4-C1	4.13	1.52	1.43
6	ME	3	GZL	O4-C1	4.12	1.52	1.43
6	mE	3	GZL	O4-C1	4.12	1.52	1.43
6	FC	3	GZL	O4-C1	4.12	1.52	1.43
19	AE	3	GZL	O4-C1	4.12	1.52	1.43
15	DA	3	GZL	O4-C1	4.11	1.52	1.43
15	AB	3	GZL	O4-C1	4.11	1.52	1.43
24	lE	3	GZL	O4-C1	4.11	1.52	1.43
12	lA	3	GZL	O4-C1	4.11	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	0C	3	GZL	O4-C1	4.11	1.52	1.43
12	fD	3	GZL	O4-C1	4.11	1.52	1.43
18	SE	3	GZL	O4-C1	4.10	1.52	1.43
6	bB	3	GZL	O4-C1	4.10	1.52	1.43
6	3D	3	GZL	O4-C1	4.10	1.52	1.43
12	iB	3	GZL	O4-C1	4.10	1.52	1.43
20	UE	3	GZL	O4-C1	4.10	1.52	1.43
6	AA	3	GZL	O4-C1	4.10	1.52	1.43
6	PA	3	GZL	O4-C1	4.10	1.52	1.43
6	6C	3	GZL	O4-C1	4.09	1.52	1.43
6	yD	3	GZL	O4-C1	4.09	1.52	1.43
13	2B	3	GZL	O4-C1	4.09	1.52	1.43
14	nA	3	GZL	O4-C1	4.09	1.52	1.43
14	s	3	GZL	O4-C1	4.09	1.52	1.43
20	WE	3	GZL	O4-C1	4.09	1.52	1.43
6	CB	3	GZL	O4-C1	4.09	1.52	1.43
18	PE	3	GZL	O4-C1	4.09	1.52	1.43
12	iC	3	GZL	O4-C1	4.09	1.52	1.43
20	jE	3	GZL	O4-C1	4.09	1.52	1.43
18	cE	3	GZL	O4-C1	4.09	1.52	1.43
6	FC	3	GZL	C1-C2	4.09	1.58	1.51
15	2D	3	GZL	O4-C1	4.09	1.52	1.43
13	4A	3	GZL	O4-C1	4.08	1.52	1.43
15	BB	3	GZL	O4-C1	4.08	1.52	1.43
12	n	3	GZL	O4-C1	4.08	1.52	1.43
6	8	3	GZL	O4-C1	4.08	1.52	1.43
6	xD	3	GZL	O4-C1	4.08	1.52	1.43
14	p	3	GZL	O4-C1	4.08	1.52	1.43
6	3A	3	GZL	O4-C1	4.07	1.52	1.43
6	EA	3	GZL	O4-C1	4.07	1.52	1.43
6	9	3	GZL	O4-C1	4.07	1.52	1.43
6	6D	3	GZL	O4-C1	4.07	1.52	1.43
22	RE	3	GZL	O4-C1	4.07	1.52	1.43
15	8B	3	GZL	O4-C1	4.07	1.52	1.43
6	aB	3	GZL	O4-C1	4.07	1.52	1.43
14	eD	3	GZL	O4-C1	4.06	1.52	1.43
6	5B	3	GZL	O4-C1	4.06	1.52	1.43
6	bE	3	GZL	O4-C1	4.06	1.52	1.43
19	qE	3	GZL	O4-C1	4.06	1.52	1.43
22	GE	3	GZL	O4-C1	4.06	1.52	1.43
6	8D	3	GZL	O4-C1	4.05	1.52	1.43
20	hE	3	GZL	O4-C1	4.05	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2C	3	GZL	O4-C1	4.05	1.52	1.43
22	dE	3	GZL	O4-C1	4.05	1.52	1.43
15	CA	3	GZL	O4-C1	4.05	1.52	1.43
13	wD	3	GZL	O4-C1	4.05	1.52	1.43
20	EE	3	GZL	O4-C1	4.05	1.52	1.43
6	cB	3	GZL	O4-C1	4.05	1.52	1.43
12	cD	3	GZL	O4-C1	4.04	1.52	1.43
13	zC	3	GZL	O4-C1	4.04	1.52	1.43
15	5C	3	GZL	O4-C1	4.04	1.52	1.43
13	vD	3	GZL	O4-C1	4.04	1.52	1.43
6	8A	3	GZL	O4-C1	4.04	1.52	1.43
22	eE	3	GZL	O4-C1	4.03	1.52	1.43
19	1E	3	GZL	O4-C1	4.03	1.52	1.43
6	gB	3	GZL	O4-C1	4.03	1.52	1.43
21	FE	3	GZL	O4-C1	4.03	1.52	1.43
18	9D	3	GZL	O4-C1	4.02	1.52	1.43
22	QE	3	GZL	O4-C1	4.02	1.52	1.43
13	7	3	GZL	O4-C1	4.02	1.52	1.43
20	uE	3	GZL	O4-C1	4.02	1.52	1.43
14	nB	3	GZL	O4-C1	4.02	1.52	1.43
13	dB	3	GZL	C1-C2	4.02	1.58	1.51
14	kC	3	GZL	O4-C1	4.01	1.52	1.43
6	1C	3	GZL	O4-C1	4.01	1.52	1.43
6	JC	3	GZL	O4-C1	4.01	1.52	1.43
6	R	3	GZL	O4-C1	4.01	1.52	1.43
14	KB	3	GZL	O4-C1	4.00	1.52	1.43
18	0E	3	GZL	O4-C1	4.00	1.52	1.43
13	ZB	3	GZL	O4-C1	4.00	1.52	1.43
20	xE	3	GZL	O4-C1	3.99	1.52	1.43
19	NE	3	GZL	O4-C1	3.99	1.52	1.43
12	FB	3	GZL	O4-C1	3.99	1.52	1.43
6	4B	3	GZL	O4-C1	3.99	1.52	1.43
6	7D	3	GZL	O4-C1	3.98	1.52	1.43
18	DE	3	GZL	O4-C1	3.98	1.52	1.43
15	eB	3	GZL	O4-C1	3.98	1.52	1.43
18	rE	3	GZL	O4-C1	3.98	1.52	1.43
13	0D	3	GZL	O4-C1	3.96	1.52	1.43
14	hC	3	GZL	O4-C1	3.96	1.52	1.43
19	aE	3	GZL	O4-C1	3.95	1.52	1.43
18	JE	3	GZL	O4-C1	3.94	1.52	1.43
6	GD	3	GZL	O4-C1	3.94	1.52	1.43
14	HB	3	GZL	O4-C1	3.94	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	HE	3	GZL	O4-C1	3.93	1.52	1.43
18	tE	3	GZL	O4-C1	3.93	1.52	1.43
6	9B	3	GZL	O4-C1	3.93	1.52	1.43
18	KE	3	GZL	O4-C1	3.92	1.52	1.43
13	5A	3	GZL	O4-C1	3.92	1.52	1.43
6	nE	3	GZL	O4-C1	3.91	1.52	1.43
13	3C	3	GZL	O4-C1	3.91	1.52	1.43
14	hC	3	GZL	O2-C2	3.91	1.51	1.43
19	aE	3	GZL	O2-C2	3.91	1.51	1.43
12	FB	3	GZL	O2-C2	3.91	1.51	1.43
20	sE	3	GZL	O4-C1	3.90	1.52	1.43
18	BE	3	GZL	O4-C1	3.90	1.52	1.43
6	OE	3	GZL	O4-C1	3.90	1.52	1.43
6	0C	3	GZL	O2-C2	3.90	1.51	1.43
18	yE	3	GZL	O4-C1	3.90	1.52	1.43
13	4	3	GZL	O2-C2	3.90	1.51	1.43
14	nB	3	GZL	O2-C2	3.90	1.51	1.43
14	kB	3	GZL	O4-C1	3.89	1.52	1.43
12	iB	3	GZL	O2-C2	3.89	1.51	1.43
13	yC	3	GZL	O2-C2	3.89	1.51	1.43
18	zE	3	GZL	O2-C2	3.89	1.51	1.43
13	9A	3	GZL	C1-C2	3.89	1.58	1.51
18	zE	3	GZL	O4-C1	3.89	1.52	1.43
13	zC	3	GZL	O2-C2	3.88	1.51	1.43
6	zD	3	GZL	O2-C2	3.88	1.51	1.43
15	5C	3	GZL	O2-C2	3.88	1.51	1.43
12	IB	3	GZL	O2-C2	3.88	1.51	1.43
12	lB	3	GZL	O2-C2	3.88	1.51	1.43
13	zB	3	GZL	O2-C2	3.87	1.51	1.43
19	qE	3	GZL	O2-C2	3.87	1.51	1.43
15	4C	3	GZL	O2-C2	3.87	1.51	1.43
6	xD	3	GZL	O2-C2	3.86	1.51	1.43
13	dD	3	GZL	O2-C2	3.86	1.51	1.43
20	jE	3	GZL	O2-C2	3.86	1.51	1.43
6	nE	3	GZL	O2-C2	3.86	1.51	1.43
6	8D	3	GZL	O2-C2	3.86	1.51	1.43
18	0E	3	GZL	O2-C2	3.86	1.51	1.43
13	vD	3	GZL	O2-C2	3.86	1.51	1.43
15	2D	3	GZL	O2-C2	3.86	1.51	1.43
6	2C	3	GZL	O2-C2	3.86	1.51	1.43
14	HB	3	GZL	O2-C2	3.86	1.51	1.43
14	kB	3	GZL	O2-C2	3.86	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	ZE	3	GZL	O2-C2	3.86	1.51	1.43
6	9B	3	GZL	O2-C2	3.86	1.51	1.43
6	6C	3	GZL	O2-C2	3.86	1.51	1.43
6	3D	3	GZL	O2-C2	3.86	1.51	1.43
18	JE	3	GZL	O2-C2	3.86	1.51	1.43
18	cE	3	GZL	O2-C2	3.86	1.51	1.43
14	KB	3	GZL	O2-C2	3.85	1.51	1.43
13	1B	3	GZL	O2-C2	3.85	1.51	1.43
13	wD	3	GZL	O2-C2	3.85	1.51	1.43
13	6B	3	GZL	O4-C1	3.85	1.52	1.43
15	1D	3	GZL	O2-C2	3.85	1.51	1.43
20	CE	3	GZL	O4-C1	3.85	1.52	1.43
6	1C	3	GZL	O2-C2	3.85	1.51	1.43
13	gC	3	GZL	O2-C2	3.85	1.51	1.43
19	AE	3	GZL	O2-C2	3.85	1.51	1.43
20	hE	3	GZL	O2-C2	3.85	1.51	1.43
6	oE	3	GZL	O2-C2	3.84	1.51	1.43
14	hD	3	GZL	O2-C2	3.84	1.51	1.43
13	jB	3	GZL	O2-C2	3.84	1.51	1.43
6	3B	3	GZL	O2-C2	3.84	1.51	1.43
14	eD	3	GZL	O2-C2	3.84	1.51	1.43
12	fD	3	GZL	O2-C2	3.84	1.51	1.43
24	lE	3	GZL	O2-C2	3.84	1.51	1.43
13	WB	3	GZL	O2-C2	3.84	1.51	1.43
13	dB	3	GZL	O4-C1	3.84	1.52	1.43
14	s	3	GZL	O2-C2	3.84	1.51	1.43
13	YB	3	GZL	O2-C2	3.84	1.51	1.43
18	pE	3	GZL	O2-C2	3.84	1.51	1.43
12	iC	3	GZL	O2-C2	3.83	1.51	1.43
6	6D	3	GZL	O2-C2	3.83	1.51	1.43
13	GB	3	GZL	O2-C2	3.83	1.51	1.43
22	iE	3	GZL	O2-C2	3.83	1.51	1.43
20	HE	3	GZL	O2-C2	3.83	1.51	1.43
6	bB	3	GZL	O2-C2	3.83	1.51	1.43
20	TE	3	GZL	O2-C2	3.83	1.51	1.43
22	QE	3	GZL	O2-C2	3.83	1.51	1.43
6	4B	3	GZL	O2-C2	3.82	1.51	1.43
20	gE	3	GZL	O2-C2	3.82	1.51	1.43
20	uE	3	GZL	O2-C2	3.82	1.51	1.43
6	R	3	GZL	O2-C2	3.82	1.51	1.43
14	kC	3	GZL	O2-C2	3.82	1.51	1.43
13	3C	3	GZL	O2-C2	3.82	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	yE	3	GZL	O2-C2	3.82	1.51	1.43
6	7D	3	GZL	O2-C2	3.82	1.51	1.43
6	gB	3	GZL	O2-C2	3.82	1.51	1.43
19	NE	3	GZL	O2-C2	3.82	1.51	1.43
13	tD	3	GZL	O2-C2	3.82	1.51	1.43
13	wC	3	GZL	O2-C2	3.81	1.51	1.43
18	tE	3	GZL	O2-C2	3.81	1.51	1.43
6	ME	3	GZL	O2-C2	3.81	1.51	1.43
22	VE	3	GZL	O2-C2	3.81	1.51	1.43
22	eE	3	GZL	O2-C2	3.81	1.51	1.43
6	PA	3	GZL	O2-C2	3.81	1.51	1.43
15	7B	3	GZL	O2-C2	3.81	1.51	1.43
18	PE	3	GZL	O2-C2	3.81	1.51	1.43
18	KE	3	GZL	O2-C2	3.81	1.51	1.43
13	0D	3	GZL	O2-C2	3.81	1.51	1.43
18	BE	3	GZL	O2-C2	3.81	1.51	1.43
6	8	3	GZL	O2-C2	3.81	1.51	1.43
13	2A	3	GZL	O2-C2	3.81	1.51	1.43
6	yD	3	GZL	O2-C2	3.81	1.51	1.43
13	o	3	GZL	O2-C2	3.80	1.51	1.43
13	ZB	3	GZL	O2-C2	3.80	1.51	1.43
6	cB	3	GZL	O2-C2	3.80	1.51	1.43
6	GD	3	GZL	O2-C2	3.80	1.51	1.43
6	mE	3	GZL	O2-C2	3.80	1.51	1.43
14	qA	3	GZL	O2-C2	3.80	1.51	1.43
18	rE	3	GZL	O2-C2	3.80	1.51	1.43
15	fB	3	GZL	O2-C2	3.80	1.51	1.43
23	XE	3	GZL	O2-C2	3.80	1.51	1.43
22	GE	3	GZL	O2-C2	3.80	1.51	1.43
6	aB	3	GZL	O2-C2	3.80	1.51	1.43
12	lA	3	GZL	O2-C2	3.80	1.51	1.43
6	JC	3	GZL	O2-C2	3.80	1.51	1.43
20	xE	3	GZL	O2-C2	3.80	1.51	1.43
22	wE	3	GZL	O2-C2	3.80	1.51	1.43
18	9D	3	GZL	O2-C2	3.80	1.51	1.43
14	p	3	GZL	O2-C2	3.79	1.51	1.43
13	BA	3	GZL	C1-C2	3.79	1.58	1.51
18	IE	3	GZL	O4-C1	3.79	1.52	1.43
6	EA	3	GZL	O2-C2	3.79	1.51	1.43
13	5A	3	GZL	O2-C2	3.79	1.51	1.43
6	7A	3	GZL	O2-C2	3.79	1.51	1.43
13	7	3	GZL	O2-C2	3.79	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2B	3	GZL	O2-C2	3.79	1.51	1.43
21	kE	3	GZL	O2-C2	3.79	1.51	1.43
18	IE	3	GZL	O2-C2	3.79	1.51	1.43
13	mA	3	GZL	O2-C2	3.79	1.51	1.43
19	1E	3	GZL	O2-C2	3.79	1.51	1.43
12	fC	3	GZL	O2-C2	3.79	1.51	1.43
12	cD	3	GZL	O2-C2	3.79	1.51	1.43
22	RE	3	GZL	O2-C2	3.79	1.51	1.43
6	LA	3	GZL	O2-C2	3.78	1.51	1.43
6	OE	3	GZL	O2-C2	3.78	1.51	1.43
18	DE	3	GZL	O2-C2	3.78	1.51	1.43
18	fE	3	GZL	O2-C2	3.78	1.51	1.43
20	sE	3	GZL	O2-C2	3.78	1.51	1.43
6	6A	3	GZL	O2-C2	3.78	1.51	1.43
20	EE	3	GZL	O2-C2	3.78	1.51	1.43
24	YE	3	GZL	O2-C2	3.77	1.51	1.43
20	CE	3	GZL	O2-C2	3.77	1.51	1.43
6	bE	3	GZL	O2-C2	3.77	1.51	1.43
13	6	3	GZL	O2-C2	3.77	1.51	1.43
20	WE	3	GZL	O2-C2	3.77	1.51	1.43
12	q	3	GZL	O2-C2	3.77	1.51	1.43
18	SE	3	GZL	O2-C2	3.77	1.51	1.43
22	dE	3	GZL	O2-C2	3.77	1.51	1.43
6	8A	3	GZL	O2-C2	3.77	1.51	1.43
6	CB	3	GZL	O2-C2	3.76	1.51	1.43
20	UE	3	GZL	O2-C2	3.76	1.51	1.43
15	8B	3	GZL	O2-C2	3.76	1.51	1.43
14	hD	3	GZL	O4-C1	3.76	1.51	1.43
15	BB	3	GZL	O2-C2	3.76	1.51	1.43
21	vE	3	GZL	O2-C2	3.75	1.51	1.43
15	eB	3	GZL	O2-C2	3.75	1.51	1.43
12	n	3	GZL	O2-C2	3.74	1.51	1.43
13	9A	3	GZL	O4-C1	3.74	1.51	1.43
6	CD	3	GZL	O2-C2	3.74	1.51	1.43
13	4A	3	GZL	O2-C2	3.74	1.51	1.43
6	5B	3	GZL	O2-C2	3.74	1.51	1.43
13	6B	3	GZL	O2-C2	3.74	1.51	1.43
15	AB	3	GZL	O2-C2	3.74	1.51	1.43
21	FE	3	GZL	O2-C2	3.73	1.51	1.43
6	uD	3	GZL	O2-C2	3.73	1.51	1.43
15	DA	3	GZL	O2-C2	3.73	1.51	1.43
6	AA	3	GZL	O2-C2	3.73	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	3	GZL	O2-C2	3.72	1.51	1.43
12	oA	3	GZL	O2-C2	3.72	1.51	1.43
14	nA	3	GZL	O2-C2	3.72	1.51	1.43
13	dB	3	GZL	O2-C2	3.72	1.51	1.43
15	CA	3	GZL	O2-C2	3.70	1.51	1.43
6	XB	3	GZL	O2-C2	3.69	1.51	1.43
13	9A	3	GZL	O2-C2	3.69	1.51	1.43
19	LE	3	GZL	O2-C2	3.69	1.51	1.43
13	BA	3	GZL	O2-C2	3.67	1.51	1.43
6	N	3	GZL	O2-C2	3.67	1.51	1.43
6	FC	3	GZL	O2-C2	3.65	1.51	1.43
6	xC	3	GZL	O2-C2	3.64	1.51	1.43
6	0B	3	GZL	O2-C2	3.60	1.50	1.43
13	BA	3	GZL	O4-C1	3.57	1.51	1.43
6	3A	3	GZL	O2-C2	3.46	1.50	1.43
13	4	3	GZL	O4-C1	3.28	1.50	1.43
6	5	3	GZL	O2-C2	3.26	1.50	1.43
12	fD	3	GZL	O3-C3	2.20	1.48	1.43
13	6B	3	GZL	O3-C3	2.15	1.48	1.43
12	FB	3	GZL	O3-C3	2.15	1.48	1.43
13	3C	3	GZL	O3-C3	2.14	1.48	1.43
13	0D	3	GZL	O3-C3	2.13	1.48	1.43
13	4	3	GZL	O3-C3	2.13	1.48	1.43
13	zC	3	GZL	O3-C3	2.13	1.48	1.43
13	5A	3	GZL	O3-C3	2.12	1.48	1.43
13	yC	3	GZL	O3-C3	2.11	1.48	1.43
12	lB	3	GZL	O3-C3	2.11	1.48	1.43
12	iC	3	GZL	O3-C3	2.11	1.48	1.43
13	ZB	3	GZL	O3-C3	2.09	1.48	1.43
13	dD	3	GZL	O3-C3	2.09	1.48	1.43
6	xD	3	GZL	O3-C3	2.09	1.48	1.43
20	EE	3	GZL	O3-C3	2.09	1.48	1.43
14	eD	3	GZL	O3-C3	2.09	1.48	1.43
13	9A	3	GZL	O3-C3	2.09	1.48	1.43
12	n	3	GZL	O3-C3	2.08	1.48	1.43
13	GB	3	GZL	O3-C3	2.08	1.48	1.43
13	BA	3	GZL	O3-C3	2.08	1.48	1.43
18	KE	3	GZL	O3-C3	2.07	1.48	1.43
13	o	3	GZL	O3-C3	2.07	1.48	1.43
13	jB	3	GZL	O3-C3	2.07	1.48	1.43
13	wD	3	GZL	O3-C3	2.07	1.48	1.43
14	kB	3	GZL	O3-C3	2.07	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	zE	3	GZL	O3-C3	2.07	1.48	1.43
6	GD	3	GZL	O3-C3	2.07	1.48	1.43
6	6C	3	GZL	O3-C3	2.07	1.48	1.43
6	2C	3	GZL	O3-C3	2.06	1.48	1.43
15	5C	3	GZL	O3-C3	2.06	1.48	1.43
14	KB	3	GZL	O3-C3	2.06	1.48	1.43
13	2B	3	GZL	O3-C3	2.06	1.48	1.43
15	1D	3	GZL	O3-C3	2.06	1.48	1.43
6	zD	3	GZL	O3-C3	2.06	1.48	1.43
12	lA	3	GZL	O3-C3	2.06	1.48	1.43
12	IB	3	GZL	O3-C3	2.06	1.48	1.43
6	nE	3	GZL	O3-C3	2.06	1.48	1.43
6	N	3	GZL	O3-C3	2.06	1.48	1.43
6	0C	3	GZL	O3-C3	2.06	1.48	1.43
13	1B	3	GZL	O3-C3	2.05	1.48	1.43
12	q	3	GZL	O3-C3	2.05	1.48	1.43
14	HB	3	GZL	O3-C3	2.05	1.48	1.43
6	ZE	3	GZL	O3-C3	2.05	1.48	1.43
19	aE	3	GZL	O3-C3	2.05	1.48	1.43
6	3B	3	GZL	O3-C3	2.05	1.48	1.43
19	NE	3	GZL	O3-C3	2.05	1.48	1.43
6	3D	3	GZL	O3-C3	2.04	1.48	1.43
12	cD	3	GZL	O3-C3	2.04	1.48	1.43
6	bB	3	GZL	O3-C3	2.04	1.48	1.43
12	iB	3	GZL	O3-C3	2.04	1.48	1.43
13	zB	3	GZL	O3-C3	2.04	1.48	1.43
6	4B	3	GZL	O3-C3	2.04	1.48	1.43
14	hD	3	GZL	O3-C3	2.04	1.48	1.43
15	8B	3	GZL	O3-C3	2.04	1.48	1.43
22	dE	3	GZL	O3-C3	2.04	1.48	1.43
13	7	3	GZL	O3-C3	2.04	1.48	1.43
18	0E	3	GZL	O3-C3	2.04	1.48	1.43
6	gB	3	GZL	O3-C3	2.03	1.48	1.43
15	4C	3	GZL	O3-C3	2.03	1.48	1.43
22	GE	3	GZL	O3-C3	2.03	1.48	1.43
18	pE	3	GZL	O3-C3	2.03	1.48	1.43
20	gE	3	GZL	O3-C3	2.03	1.48	1.43
20	xE	3	GZL	O3-C3	2.03	1.48	1.43
20	WE	3	GZL	O3-C3	2.03	1.48	1.43
14	s	3	GZL	O3-C3	2.03	1.48	1.43
18	BE	3	GZL	O3-C3	2.03	1.48	1.43
20	HE	3	GZL	O3-C3	2.02	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	TE	3	GZL	O3-C3	2.02	1.48	1.43
19	1E	3	GZL	O3-C3	2.02	1.48	1.43
6	yD	3	GZL	O3-C3	2.02	1.48	1.43
13	dB	3	GZL	O3-C3	2.02	1.48	1.43
15	CA	3	GZL	O3-C3	2.02	1.48	1.43
18	DE	3	GZL	O3-C3	2.02	1.48	1.43
20	uE	3	GZL	O3-C3	2.02	1.48	1.43
6	1C	3	GZL	O3-C3	2.02	1.48	1.43
18	9D	3	GZL	O3-C3	2.02	1.48	1.43
18	rE	3	GZL	O3-C3	2.02	1.48	1.43
18	yE	3	GZL	O3-C3	2.02	1.48	1.43
6	9B	3	GZL	O3-C3	2.02	1.48	1.43
13	vD	3	GZL	O3-C3	2.02	1.48	1.43
19	LE	3	GZL	O3-C3	2.02	1.48	1.43
18	JE	3	GZL	O3-C3	2.02	1.47	1.43
13	wC	3	GZL	O3-C3	2.02	1.47	1.43
14	nB	3	GZL	O3-C3	2.01	1.47	1.43
18	IE	3	GZL	O3-C3	2.01	1.47	1.43
20	hE	3	GZL	O3-C3	2.01	1.47	1.43
6	oE	3	GZL	O3-C3	2.01	1.47	1.43
13	gC	3	GZL	O3-C3	2.01	1.47	1.43
6	5B	3	GZL	O3-C3	2.01	1.47	1.43
13	WB	3	GZL	O3-C3	2.01	1.47	1.43
18	tE	3	GZL	O3-C3	2.01	1.47	1.43
6	R	3	GZL	O3-C3	2.01	1.47	1.43
14	hC	3	GZL	O3-C3	2.01	1.47	1.43
18	cE	3	GZL	O3-C3	2.01	1.47	1.43
24	YE	3	GZL	O3-C3	2.01	1.47	1.43
15	2D	3	GZL	O3-C3	2.01	1.47	1.43
24	lE	3	GZL	O3-C3	2.01	1.47	1.43
6	CB	3	GZL	O3-C3	2.00	1.47	1.43
6	AA	3	GZL	O3-C3	2.00	1.47	1.43
6	8A	3	GZL	O3-C3	2.00	1.47	1.43
6	aB	3	GZL	O3-C3	2.00	1.47	1.43
22	wE	3	GZL	O3-C3	2.00	1.47	1.43
6	bE	3	GZL	O3-C3	2.00	1.47	1.43
14	kC	3	GZL	O3-C3	2.00	1.47	1.43

All (723) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	3A	3	GZL	C1-O4-C4	-12.94	82.02	107.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	CD	3	GZL	C1-O4-C4	-9.95	87.98	107.84
6	0B	3	GZL	C1-O4-C4	-9.64	88.59	107.84
6	LA	3	GZL	C1-O4-C4	-9.57	88.73	107.84
6	uD	3	GZL	C1-O4-C4	-9.30	89.28	107.84
6	N	3	GZL	C5-C4-C3	-9.30	102.60	115.95
13	4	3	GZL	O5-C5-C4	-9.28	87.02	109.18
6	XB	3	GZL	C1-O4-C4	-9.17	89.53	107.84
6	xC	3	GZL	C1-O4-C4	-9.11	89.65	107.84
6	3A	3	GZL	O5-C5-C4	-9.09	87.47	109.18
6	0B	3	GZL	O5-C5-C4	-8.12	89.78	109.18
6	uD	3	GZL	O5-C5-C4	-8.06	89.92	109.18
6	xC	3	GZL	O5-C5-C4	-7.99	90.10	109.18
6	XB	3	GZL	O5-C5-C4	-7.95	90.19	109.18
6	CD	3	GZL	O5-C5-C4	-7.80	90.56	109.18
6	LA	3	GZL	O4-C4-C5	7.68	125.67	109.08
6	3A	3	GZL	O4-C4-C5	7.59	125.49	109.08
6	CD	3	GZL	O4-C4-C5	7.56	125.43	109.08
6	LA	3	GZL	O5-C5-C4	-7.47	91.35	109.18
6	uD	3	GZL	O4-C4-C5	7.30	124.86	109.08
6	xC	3	GZL	O4-C4-C5	7.24	124.73	109.08
6	0B	3	GZL	O4-C4-C5	7.20	124.64	109.08
6	XB	3	GZL	O4-C4-C5	7.13	124.49	109.08
6	FC	3	GZL	C5-C4-C3	-6.95	105.97	115.95
6	N	3	GZL	O2-C2-C3	5.64	122.53	111.43
14	s	3	GZL	C5-C4-C3	-5.63	107.86	115.95
18	9D	1	FUB	O2-C2-C3	5.49	122.23	111.43
14	kC	3	GZL	C5-C4-C3	-5.38	108.23	115.95
17	5D	4	MAN	C1-C2-C3	4.95	116.85	109.64
14	nA	3	GZL	C5-C4-C3	-4.91	108.90	115.95
6	6D	3	GZL	C5-C4-C3	-4.90	108.91	115.95
14	qA	3	GZL	C5-C4-C3	-4.85	108.98	115.95
17	5D	4	MAN	C1-O5-C5	4.81	118.63	112.19
18	pE	1	FUB	O2-C2-C3	4.76	120.80	111.43
14	eD	3	GZL	C5-C4-C3	-4.73	109.16	115.95
6	4B	3	GZL	C5-C4-C3	-4.62	109.31	115.95
14	KB	3	GZL	C5-C4-C3	-4.61	109.33	115.95
6	mE	3	GZL	C5-C4-C3	-4.59	109.36	115.95
18	DE	3	GZL	C5-C4-C3	-4.58	109.37	115.95
22	eE	3	GZL	C5-C4-C3	-4.54	109.43	115.95
6	OE	3	GZL	C5-C4-C3	-4.48	109.51	115.95
18	cE	3	GZL	C5-C4-C3	-4.46	109.55	115.95
15	5C	3	GZL	C5-C4-C3	-4.45	109.55	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	CE	3	GZL	C5-C4-C3	-4.45	109.57	115.95
18	yE	3	GZL	C5-C4-C3	-4.44	109.57	115.95
14	hC	3	GZL	C5-C4-C3	-4.43	109.59	115.95
6	cB	3	GZL	C5-C4-C3	-4.43	109.59	115.95
6	nE	3	GZL	C5-C4-C3	-4.42	109.60	115.95
20	jE	3	GZL	C5-C4-C3	-4.42	109.61	115.95
19	aE	3	GZL	C5-C4-C3	-4.41	109.62	115.95
18	IE	3	GZL	C5-C4-C3	-4.41	109.62	115.95
20	HE	3	GZL	C5-C4-C3	-4.40	109.63	115.95
19	1E	3	GZL	C5-C4-C3	-4.39	109.64	115.95
6	oE	3	GZL	C5-C4-C3	-4.39	109.65	115.95
22	dE	3	GZL	C5-C4-C3	-4.37	109.67	115.95
20	TE	3	GZL	C5-C4-C3	-4.36	109.68	115.95
6	8A	3	GZL	C5-C4-C3	-4.35	109.70	115.95
6	bE	3	GZL	C5-C4-C3	-4.35	109.71	115.95
18	pE	3	GZL	C5-C4-C3	-4.34	109.72	115.95
18	zE	3	GZL	C5-C4-C3	-4.33	109.73	115.95
20	uE	3	GZL	C5-C4-C3	-4.29	109.78	115.95
20	xE	3	GZL	C5-C4-C3	-4.29	109.79	115.95
6	R	3	GZL	C5-C4-C3	-4.29	109.80	115.95
13	9A	3	GZL	C1-C2-C3	-4.28	94.78	101.63
6	8D	3	GZL	C5-C4-C3	-4.27	109.81	115.95
13	4A	3	GZL	C5-C4-C3	-4.27	109.81	115.95
6	ME	3	GZL	C5-C4-C3	-4.27	109.81	115.95
20	sE	3	GZL	C5-C4-C3	-4.26	109.83	115.95
6	1C	3	GZL	C5-C4-C3	-4.26	109.83	115.95
13	yC	3	GZL	C5-C4-C3	-4.26	109.84	115.95
20	EE	3	GZL	C5-C4-C3	-4.25	109.84	115.95
22	VE	3	GZL	C5-C4-C3	-4.25	109.85	115.95
6	yD	3	GZL	C5-C4-C3	-4.23	109.88	115.95
15	4C	3	GZL	C5-C4-C3	-4.20	109.92	115.95
13	vD	3	GZL	C5-C4-C3	-4.19	109.93	115.95
19	NE	3	GZL	C5-C4-C3	-4.18	109.95	115.95
14	HB	3	GZL	C5-C4-C3	-4.17	109.96	115.95
6	2C	3	GZL	C5-C4-C3	-4.17	109.97	115.95
13	wD	3	GZL	C5-C4-C3	-4.16	109.98	115.95
12	FB	3	GZL	C5-C4-C3	-4.15	109.99	115.95
6	zD	3	GZL	C5-C4-C3	-4.14	110.00	115.95
18	tE	3	GZL	C5-C4-C3	-4.12	110.04	115.95
18	9D	1	FUB	C1-C2-C3	-4.11	95.05	101.63
6	6C	3	GZL	C5-C4-C3	-4.10	110.06	115.95
6	bB	3	GZL	C5-C4-C3	-4.09	110.07	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	qE	3	GZL	C5-C4-C3	-4.09	110.08	115.95
18	JE	3	GZL	C5-C4-C3	-4.09	110.08	115.95
24	lE	3	GZL	C5-C4-C3	-4.09	110.08	115.95
18	SE	3	GZL	C5-C4-C3	-4.08	110.09	115.95
22	QE	3	GZL	C5-C4-C3	-4.07	110.10	115.95
15	eB	3	GZL	C5-C4-C3	-4.07	110.10	115.95
13	1B	3	GZL	C5-C4-C3	-4.07	110.11	115.95
13	2B	3	GZL	C5-C4-C3	-4.06	110.11	115.95
15	2D	3	GZL	C5-C4-C3	-4.06	110.11	115.95
6	6A	3	GZL	C5-C4-C3	-4.06	110.12	115.95
12	iB	3	GZL	C5-C4-C3	-4.06	110.12	115.95
6	JC	3	GZL	C5-C4-C3	-4.06	110.13	115.95
20	hE	3	GZL	C5-C4-C3	-4.05	110.14	115.95
6	7D	3	GZL	C5-C4-C3	-4.04	110.14	115.95
22	iE	3	GZL	C5-C4-C3	-4.04	110.15	115.95
18	rE	3	GZL	C5-C4-C3	-4.03	110.16	115.95
13	6	3	GZL	C5-C4-C3	-4.02	110.18	115.95
18	PE	3	GZL	C5-C4-C3	-4.02	110.18	115.95
22	GE	3	GZL	C5-C4-C3	-4.01	110.19	115.95
12	IB	3	GZL	C5-C4-C3	-4.01	110.19	115.95
18	BE	3	GZL	C5-C4-C3	-4.01	110.19	115.95
6	9B	3	GZL	C5-C4-C3	-4.00	110.20	115.95
6	xD	3	GZL	C5-C4-C3	-4.00	110.20	115.95
23	XE	3	GZL	C5-C4-C3	-4.00	110.20	115.95
6	PA	3	GZL	C5-C4-C3	-4.00	110.21	115.95
24	YE	3	GZL	C5-C4-C3	-4.00	110.21	115.95
6	8	3	GZL	C5-C4-C3	-3.99	110.22	115.95
19	AE	3	GZL	C5-C4-C3	-3.99	110.22	115.95
6	7A	3	GZL	C5-C4-C3	-3.98	110.23	115.95
6	GD	3	GZL	C5-C4-C3	-3.97	110.25	115.95
13	4	3	GZL	C5-C4-C3	3.97	121.66	115.95
6	aB	3	GZL	C5-C4-C3	-3.97	110.25	115.95
15	DA	3	GZL	C5-C4-C3	-3.97	110.25	115.95
22	wE	3	GZL	C5-C4-C3	-3.97	110.26	115.95
14	kB	3	GZL	C5-C4-C3	-3.96	110.26	115.95
12	iC	3	GZL	C5-C4-C3	-3.95	110.28	115.95
6	5	3	GZL	C5-C4-C3	-3.94	110.29	115.95
15	7B	3	GZL	C5-C4-C3	-3.94	110.29	115.95
20	WE	3	GZL	C5-C4-C3	-3.93	110.30	115.95
6	3B	3	GZL	C5-C4-C3	-3.92	110.33	115.95
18	KE	3	GZL	C5-C4-C3	-3.91	110.33	115.95
13	zC	3	GZL	C5-C4-C3	-3.90	110.35	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	p	3	GZL	C5-C4-C3	-3.90	110.35	115.95
6	5B	3	GZL	C5-C4-C3	-3.90	110.36	115.95
6	0C	3	GZL	C5-C4-C3	-3.89	110.37	115.95
6	9	3	GZL	C5-C4-C3	-3.87	110.39	115.95
13	ZB	3	GZL	C5-C4-C3	-3.87	110.39	115.95
18	fE	3	GZL	C5-C4-C3	-3.87	110.39	115.95
6	gB	3	GZL	C5-C4-C3	-3.87	110.40	115.95
13	BA	3	GZL	C1-C2-C3	-3.86	95.45	101.63
12	lB	3	GZL	C5-C4-C3	-3.85	110.42	115.95
21	FE	3	GZL	C5-C4-C3	-3.85	110.42	115.95
13	3C	3	GZL	C5-C4-C3	-3.85	110.43	115.95
19	LE	3	GZL	C5-C4-C3	-3.84	110.43	115.95
6	6A	2	FUB	O2-C2-C3	3.84	118.98	111.43
12	q	3	GZL	C5-C4-C3	-3.83	110.44	115.95
18	0E	3	GZL	C5-C4-C3	-3.83	110.45	115.95
15	1D	3	GZL	C5-C4-C3	-3.83	110.45	115.95
15	fB	3	GZL	C5-C4-C3	-3.83	110.45	115.95
16	FA	2	NAG	O5-C1-C2	3.82	117.20	111.29
12	cD	3	GZL	C5-C4-C3	-3.81	110.48	115.95
13	mA	3	GZL	C5-C4-C3	-3.80	110.49	115.95
14	nB	3	GZL	C5-C4-C3	-3.80	110.49	115.95
22	RE	3	GZL	C5-C4-C3	-3.80	110.49	115.95
6	ZE	3	GZL	C5-C4-C3	-3.79	110.51	115.95
13	GB	3	GZL	C5-C4-C3	-3.79	110.51	115.95
6	3D	3	GZL	C5-C4-C3	-3.76	110.55	115.95
21	vE	3	GZL	C5-C4-C3	-3.76	110.55	115.95
13	dB	3	GZL	C1-C2-C3	-3.74	95.64	101.63
13	0D	3	GZL	C5-C4-C3	-3.74	110.58	115.95
14	hD	3	GZL	C5-C4-C3	-3.73	110.59	115.95
13	gC	3	GZL	C5-C4-C3	-3.73	110.60	115.95
18	9D	3	GZL	C5-C4-C3	-3.72	110.60	115.95
18	pE	1	FUB	C1-C2-C3	-3.70	95.70	101.63
20	UE	3	GZL	C5-C4-C3	-3.70	110.64	115.95
12	fC	3	GZL	C5-C4-C3	-3.69	110.66	115.95
6	AA	3	GZL	C5-C4-C3	-3.68	110.66	115.95
12	oA	3	GZL	C5-C4-C3	-3.68	110.66	115.95
6	EA	3	GZL	C5-C4-C3	-3.68	110.67	115.95
6	CB	3	GZL	C5-C4-C3	-3.64	110.72	115.95
13	dD	3	GZL	C5-C4-C3	-3.64	110.73	115.95
16	4D	2	NAG	C1-O5-C5	3.64	117.06	112.19
16	AC	2	NAG	O5-C1-C2	3.63	116.90	111.29
6	XB	3	GZL	C1-C2-C3	-3.62	95.84	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	CD	3	GZL	C5-C4-C3	-3.61	110.77	115.95
13	6B	3	GZL	C5-C4-C3	-3.61	110.77	115.95
20	gE	3	GZL	C5-C4-C3	-3.59	110.80	115.95
6	LA	3	GZL	C5-C4-C3	-3.59	110.80	115.95
13	4	3	GZL	O3-C3-C2	-3.59	103.47	111.97
13	o	3	GZL	C5-C4-C3	-3.57	110.83	115.95
6	xC	3	GZL	C1-C2-C3	-3.56	95.93	101.63
13	WB	3	GZL	C5-C4-C3	-3.56	110.84	115.95
13	jB	3	GZL	C5-C4-C3	-3.55	110.85	115.95
13	7	3	GZL	C5-C4-C3	-3.55	110.85	115.95
17	GA	3	BMA	C1-O5-C5	3.49	116.87	112.19
21	kE	3	GZL	C5-C4-C3	-3.46	110.99	115.95
13	zB	3	GZL	C5-C4-C3	-3.45	110.99	115.95
12	fD	3	GZL	C5-C4-C3	-3.44	111.02	115.95
16	FA	2	NAG	C1-O5-C5	3.42	116.77	112.19
6	uD	3	GZL	C1-C2-C3	-3.40	96.19	101.63
13	6B	3	GZL	C1-C2-C3	-3.39	96.21	101.63
6	xD	3	GZL	C1-C2-C3	3.38	107.04	101.63
13	dB	3	GZL	C5-C4-C3	-3.36	111.12	115.95
17	5D	1	NAG	C1-O5-C5	3.35	116.68	112.19
6	LA	3	GZL	O5-C5-C6	3.30	116.53	109.03
15	8B	3	GZL	C5-C4-C3	-3.28	111.23	115.95
13	BA	3	GZL	C1-O4-C4	-3.23	101.39	107.84
6	FC	3	GZL	O4-C1-C2	-3.21	100.23	105.76
12	FB	3	GZL	C1-C2-C3	3.21	106.75	101.63
6	6D	3	GZL	C1-C2-C3	3.20	106.75	101.63
12	n	3	GZL	C5-C4-C3	-3.20	111.36	115.95
13	9A	3	GZL	C1-O4-C4	-3.19	101.47	107.84
6	0B	3	GZL	C1-C2-C3	-3.19	96.53	101.63
14	KB	3	GZL	C1-C2-C3	3.15	106.67	101.63
13	2A	2	FUB	O2-C2-C3	3.15	117.62	111.43
6	FC	2	FUB	O2-C2-C1	3.15	120.68	110.89
17	DB	6	MAN	C3-C4-C5	3.14	115.92	110.23
14	HB	3	GZL	C1-C2-C3	3.13	106.63	101.63
17	7C	1	NAG	C1-O5-C5	3.10	116.34	112.19
17	7C	4	MAN	C1-O5-C5	3.09	116.32	112.19
16	4D	2	NAG	O5-C1-C2	3.08	116.05	111.29
13	BA	3	GZL	C5-C4-C3	-3.08	111.53	115.95
19	qE	1	FUB	C1-C2-C3	3.07	106.53	101.63
17	5D	4	MAN	O5-C1-C2	3.07	118.10	110.79
14	p	3	GZL	O5-C5-C6	3.06	115.99	109.03
15	AB	3	GZL	C5-C4-C3	-3.06	111.56	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	lE	1	FUB	C1-C2-C3	3.01	106.45	101.63
15	BB	3	GZL	C5-C4-C3	-3.01	111.62	115.95
24	YE	1	FUB	C1-C2-C3	3.01	106.44	101.63
13	YB	3	GZL	C5-C4-C3	-2.98	111.67	115.95
6	3B	3	GZL	C1-C2-C3	2.98	106.39	101.63
6	3B	2	FUB	O2-C2-C3	2.94	117.22	111.43
15	CA	3	GZL	C5-C4-C3	-2.93	111.75	115.95
13	dB	3	GZL	O4-C1-C2	-2.92	100.72	105.76
6	LA	2	FUB	C1-C2-C3	2.91	106.28	101.63
13	BA	3	GZL	O4-C1-C2	-2.91	100.75	105.76
12	lA	3	GZL	C5-C4-C3	-2.91	111.77	115.95
6	N	3	GZL	O5-C5-C6	2.91	115.64	109.03
6	CD	3	GZL	O5-C5-C6	2.90	115.61	109.03
13	4	3	GZL	O4-C1-C2	-2.89	100.78	105.76
21	FE	1	FUB	C1-C2-C3	2.88	106.24	101.63
6	cB	2	FUB	C1-C2-C3	2.87	106.22	101.63
13	6B	3	GZL	O4-C1-C2	-2.86	100.83	105.76
6	5B	2	FUB	C1-C2-C3	2.86	106.19	101.63
4	DC	1	FUB	C1-C2-C3	2.85	106.19	101.63
20	TE	1	FUB	C1-C2-C3	2.85	106.18	101.63
18	cE	1	FUB	C1-C2-C3	2.84	106.16	101.63
13	5A	3	GZL	C5-C4-C3	-2.83	111.89	115.95
7	KC	1	FUB	C1-C2-C3	2.82	106.13	101.63
13	9A	3	GZL	O4-C1-C2	-2.82	100.91	105.76
3	NA	1	FUB	C1-C2-C3	2.82	106.13	101.63
6	2C	2	FUB	C1-C2-C3	2.82	106.13	101.63
4	d	4	AHR	C1-C2-C3	2.81	106.12	101.63
7	QA	1	FUB	C1-C2-C3	2.80	106.10	101.63
13	9A	3	GZL	C5-C4-C3	-2.80	111.93	115.95
18	yE	3	GZL	C1-C2-C3	2.80	106.10	101.63
6	FC	1	FUB	O2-C2-C3	2.79	116.93	111.43
18	9D	5	AHR	C1-C2-C3	2.79	106.09	101.63
12	oA	1	FUB	C1-C2-C3	2.79	106.09	101.63
7	S	1	FUB	C1-C2-C3	2.78	106.08	101.63
13	4	2	FUB	O2-C2-C3	2.78	116.90	111.43
18	DE	1	FUB	C1-C2-C3	2.78	106.07	101.63
6	5	2	FUB	O2-C2-C3	2.77	116.89	111.43
16	AC	1	NAG	C4-C3-C2	2.77	115.08	111.02
19	AE	1	FUB	C1-C2-C3	2.77	106.05	101.63
14	kB	3	GZL	C1-C2-C3	2.77	106.05	101.63
7	HD	1	FUB	C1-C2-C3	2.76	106.05	101.63
13	dB	3	GZL	C1-O4-C4	-2.76	102.33	107.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	mC	5	AHR	C1-C2-C3	2.76	106.03	101.63
12	lB	1	FUB	C1-C2-C3	2.75	106.03	101.63
6	9B	3	GZL	C1-C2-C3	2.75	106.03	101.63
10	3	1	FUB	C1-C2-C3	2.75	106.02	101.63
15	DA	4	AHR	C1-C2-C3	2.73	105.99	101.63
14	nA	3	GZL	O5-C5-C6	2.72	115.20	109.03
11	i	1	FUB	O2-C2-C3	2.72	116.77	111.43
4	PC	4	AHR	O2-C2-C1	2.71	119.34	110.89
12	n	4	AHR	C1-C2-C3	2.71	105.97	101.63
10	MB	5	AHR	C1-C2-C3	2.71	105.97	101.63
4	OC	4	AHR	C1-C2-C3	2.71	105.97	101.63
17	GA	3	BMA	C2-C3-C4	-2.71	106.09	110.86
6	AA	2	FUB	C1-C2-C3	2.70	105.95	101.63
13	4	3	GZL	C1-C2-C3	2.70	105.94	101.63
7	UD	1	FUB	C1-C2-C3	2.68	105.91	101.63
4	RD	4	AHR	C1-C2-C3	2.68	105.91	101.63
3	vB	1	FUB	C1-C2-C3	2.67	105.90	101.63
6	4B	3	GZL	C1-C2-C3	2.67	105.90	101.63
10	VB	3	FUB	O3-C3-C2	2.67	118.29	111.97
22	VE	1	FUB	O2-C2-C3	2.67	116.68	111.43
13	6B	3	GZL	C1-O4-C4	-2.66	102.52	107.84
10	1A	1	FUB	C1-C2-C3	2.66	105.88	101.63
6	zD	2	FUB	C1-C2-C3	2.65	105.87	101.63
10	a	4	AHR	C1-C2-C3	2.65	105.87	101.63
22	dE	4	AHR	C1-C2-C3	2.65	105.87	101.63
6	8A	2	FUB	C1-C2-C3	2.65	105.86	101.63
6	7D	3	GZL	O4-C1-C2	-2.64	101.20	105.76
3	rD	1	FUB	C1-C2-C3	2.64	105.85	101.63
8	MC	4	AHR	C1-C2-C3	2.63	105.84	101.63
6	oE	3	GZL	C1-C2-C3	2.63	105.84	101.63
6	bB	1	FUB	C1-C2-C3	2.62	105.83	101.63
18	pE	5	AHR	C1-C2-C3	2.62	105.83	101.63
14	eD	3	GZL	C1-C2-C3	2.62	105.82	101.63
12	lA	4	AHR	C1-C2-C3	2.62	105.82	101.63
16	AC	2	NAG	C1-O5-C5	2.62	115.70	112.19
4	tA	4	AHR	C1-C2-C3	2.62	105.82	101.63
6	nE	1	FUB	C1-C2-C3	2.62	105.82	101.63
22	GE	5	AHR	O2-C2-C1	2.62	119.04	110.89
18	PE	1	FUB	C1-C2-C3	2.62	105.81	101.63
5	M	5	AHR	C1-C2-C3	2.62	105.81	101.63
13	wC	3	GZL	C5-C4-C3	-2.61	112.20	115.95
4	Z	4	AHR	C1-C2-C3	2.61	105.80	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	iA	4	AHR	C1-C2-C3	2.61	105.80	101.63
6	0C	2	FUB	O2-C2-C3	2.61	116.56	111.43
7	dA	2	FUB	C1-C2-C3	2.61	105.80	101.63
3	ZA	1	FUB	C1-C2-C3	2.61	105.80	101.63
18	rE	2	FUB	C1-C2-C3	2.60	105.79	101.63
11	gA	1	FUB	O2-C2-C3	2.60	116.55	111.43
6	0B	2	FUB	O2-C2-C3	2.60	116.55	111.43
9	j	1	FUB	C1-C2-C3	2.60	105.79	101.63
13	BA	2	FUB	C1-C2-C3	2.60	105.78	101.63
14	hC	3	GZL	C1-C2-C3	2.60	105.78	101.63
18	IE	5	AHR	C1-C2-C3	2.58	105.76	101.63
17	GA	1	NAG	C1-O5-C5	2.58	115.64	112.19
13	4A	4	AHR	C1-C2-C3	2.58	105.75	101.63
6	GD	1	FUB	C1-C2-C3	2.57	105.74	101.63
10	pB	5	AHR	C1-C2-C3	2.57	105.74	101.63
10	u	5	AHR	C1-C2-C3	2.57	105.73	101.63
22	wE	5	AHR	O2-C2-C3	2.57	116.48	111.43
3	sC	1	FUB	C1-C2-C3	2.56	105.73	101.63
13	vD	4	AHR	C1-C2-C3	2.56	105.73	101.63
22	wE	5	AHR	O2-C2-C1	2.56	118.86	110.89
10	PD	1	FUB	C1-C2-C3	2.55	105.71	101.63
10	sA	5	AHR	C1-C2-C3	2.55	105.71	101.63
19	1E	1	FUB	C1-C2-C3	2.55	105.70	101.63
3	b	1	FUB	C1-C2-C3	2.55	105.70	101.63
18	rE	5	AHR	C1-C2-C3	2.55	105.70	101.63
6	6D	2	FUB	C1-C2-C3	2.54	105.69	101.63
18	9D	1	FUB	O3-C3-C4	2.54	118.38	111.08
13	7	4	AHR	C1-C2-C3	2.54	105.69	101.63
22	VE	4	AHR	C1-C2-C3	2.54	105.69	101.63
17	7C	3	BMA	C2-C3-C4	-2.54	106.40	110.86
18	yE	5	AHR	C1-C2-C3	2.54	105.68	101.63
17	GA	3	BMA	C3-C4-C5	-2.53	105.64	110.23
6	gB	3	GZL	C1-C2-C3	2.53	105.67	101.63
4	gD	1	FUB	C1-C2-C3	2.53	105.67	101.63
4	iA	1	FUB	C1-C2-C3	2.53	105.67	101.63
5	BD	4	AHR	C1-C2-C3	2.52	105.66	101.63
24	lE	2	FUB	C1-C2-C3	2.52	105.66	101.63
18	BE	5	AHR	C1-C2-C3	2.52	105.65	101.63
10	sD	1	FUB	C1-C2-C3	2.51	105.65	101.63
12	lA	5	AHR	C1-C2-C3	2.51	105.65	101.63
18	zE	3	GZL	C1-C2-C3	2.51	105.65	101.63
15	AB	5	AHR	C1-C2-C3	2.51	105.64	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	1	FUB	O2-C2-C3	2.51	116.37	111.43
22	iE	6	AHR	C1-C2-C3	2.51	105.64	101.63
17	DB	3	BMA	C2-C3-C4	-2.51	106.45	110.86
4	AD	1	FUB	C1-C2-C3	2.51	105.64	101.63
20	WE	4	AHR	C1-C2-C3	2.51	105.64	101.63
22	dE	1	FUB	C1-C2-C3	2.51	105.64	101.63
12	iC	1	FUB	C1-C2-C3	2.51	105.63	101.63
7	f	2	FUB	C1-C2-C3	2.50	105.63	101.63
6	N	2	FUB	O2-C2-C1	2.50	118.67	110.89
18	IE	4	AHR	C1-C2-C3	2.50	105.63	101.63
10	PD	4	AHR	C1-C2-C3	2.49	105.61	101.63
18	BE	2	FUB	C1-C2-C3	2.49	105.61	101.63
13	4	3	GZL	C1-O4-C4	-2.49	102.87	107.84
17	5D	3	BMA	C2-C3-C4	-2.49	106.49	110.86
6	yD	2	FUB	C1-C2-C3	2.48	105.59	101.63
18	yE	4	AHR	C1-C2-C3	2.47	105.58	101.63
13	YB	4	AHR	C1-C2-C3	2.47	105.58	101.63
4	AD	4	AHR	C1-C2-C3	2.47	105.58	101.63
4	tA	1	FUB	C1-C2-C3	2.47	105.57	101.63
18	9D	1	FUB	O3-C3-C2	2.46	117.81	111.97
22	eE	1	FUB	O2-C2-C3	2.46	116.27	111.43
12	fC	4	AHR	C1-C2-C3	2.46	105.56	101.63
11	XD	3	AHR	C1-C2-C3	2.46	105.56	101.63
22	iE	1	FUB	O2-C2-C3	2.46	116.26	111.43
3	e	3	FUB	C1-C2-C3	2.45	105.55	101.63
10	a	1	FUB	C1-C2-C3	2.45	105.55	101.63
24	lE	6	AHR	C1-C2-C3	2.45	105.55	101.63
10	sA	4	AHR	C1-C2-C3	2.45	105.54	101.63
3	SB	2	FUB	C1-C2-C3	2.45	105.54	101.63
22	QE	4	AHR	C1-C2-C3	2.44	105.54	101.63
3	T	1	FUB	C1-C2-C3	2.44	105.53	101.63
19	LE	2	FUB	C1-C2-C3	2.44	105.53	101.63
6	FC	3	GZL	O2-C2-C1	2.44	118.49	110.89
7	ZC	3	FUB	C1-C2-C3	2.44	105.53	101.63
6	N	3	GZL	O6-C6-C5	-2.44	106.03	111.16
10	VB	5	AHR	C1-C2-C3	2.44	105.53	101.63
20	sE	1	FUB	C1-C2-C3	2.43	105.52	101.63
3	uA	3	FUB	C1-C2-C3	2.43	105.52	101.63
3	vA	3	FUB	C1-C2-C3	2.43	105.52	101.63
13	3C	2	FUB	C1-C2-C3	2.43	105.52	101.63
15	CA	4	AHR	O2-C2-C1	2.42	118.42	110.89
13	gC	4	AHR	C1-C2-C3	2.42	105.49	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	wC	4	AHR	C1-C2-C3	2.42	105.49	101.63
18	pE	1	FUB	O3-C3-C2	2.42	117.69	111.97
6	mE	3	GZL	C1-C2-C3	2.42	105.49	101.63
3	SB	1	FUB	C1-C2-C3	2.41	105.49	101.63
17	DB	6	MAN	O5-C1-C2	-2.41	105.03	110.79
3	TC	3	FUB	C1-C2-C3	2.41	105.48	101.63
17	DB	4	MAN	C1-C2-C3	2.41	113.15	109.64
3	dC	3	FUB	C1-C2-C3	2.41	105.48	101.63
22	GE	5	AHR	O2-C2-C3	2.41	116.17	111.43
15	5C	1	FUB	C1-C2-C3	2.40	105.47	101.63
3	TA	2	FUB	C1-C2-C3	2.40	105.47	101.63
6	aB	2	FUB	O2-C2-C3	2.40	116.16	111.43
6	0C	3	GZL	C1-C2-C3	2.40	105.47	101.63
21	kE	5	AHR	C1-C2-C3	2.39	105.46	101.63
6	9B	2	FUB	C1-C2-C3	2.38	105.44	101.63
3	xB	1	FUB	C1-C2-C3	2.38	105.44	101.63
12	IB	5	AHR	C1-C2-C3	2.38	105.44	101.63
10	mC	1	FUB	C1-C2-C3	2.38	105.44	101.63
24	YE	5	AHR	C1-C2-C3	2.38	105.43	101.63
10	1A	3	FUB	O3-C3-C2	2.38	117.60	111.97
10	vC	1	FUB	C1-C2-C3	2.38	105.43	101.63
22	QE	6	AHR	C1-C2-C3	2.38	105.43	101.63
4	YC	4	AHR	C1-C2-C3	2.37	105.42	101.63
4	OD	4	AHR	C1-C2-C3	2.37	105.42	101.63
14	s	3	GZL	C1-C2-C3	2.37	105.42	101.63
22	dE	6	AHR	C1-C2-C3	2.37	105.42	101.63
22	RE	5	AHR	C1-C2-C3	2.37	105.42	101.63
22	wE	5	AHR	C1-C2-C3	2.37	105.41	101.63
14	nA	3	GZL	C1-O4-C4	-2.37	103.11	107.84
13	6B	2	FUB	O3-C3-C2	2.36	117.57	111.97
6	3D	2	FUB	C1-C2-C3	2.36	105.41	101.63
15	AB	4	AHR	O2-C2-C1	2.36	118.24	110.89
3	WC	1	FUB	O2-C2-C3	2.36	116.07	111.43
14	kC	3	GZL	C1-C2-C3	2.36	105.40	101.63
4	jC	1	FUB	C1-C2-C3	2.36	105.40	101.63
19	1E	4	AHR	C1-C2-C3	2.35	105.39	101.63
3	RA	1	FUB	C1-C2-C3	2.35	105.38	101.63
12	iB	3	GZL	C1-C2-C3	2.35	105.38	101.63
13	zC	3	GZL	C1-C2-C3	2.35	105.38	101.63
10	yB	1	FUB	C1-C2-C3	2.35	105.38	101.63
13	tD	4	AHR	C1-C2-C3	2.35	105.38	101.63
13	4	4	AHR	C1-C2-C3	2.34	105.37	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	4	AHR	C1-C2-C3	2.34	105.37	101.63
4	g	4	AHR	C1-C2-C3	2.34	105.37	101.63
3	HC	1	FUB	C1-C2-C3	2.34	105.37	101.63
12	fD	1	FUB	C1-C2-C3	2.34	105.37	101.63
13	zB	4	AHR	C1-C2-C3	2.34	105.36	101.63
6	CD	2	FUB	O2-C2-C3	2.33	116.02	111.43
10	YA	5	AHR	C1-C2-C3	2.33	105.36	101.63
24	lE	5	AHR	C1-C2-C3	2.33	105.36	101.63
20	xE	1	FUB	C1-C2-C3	2.33	105.36	101.63
15	1D	5	AHR	C1-C2-C3	2.33	105.35	101.63
13	WB	4	AHR	C1-C2-C3	2.32	105.34	101.63
11	i	3	AHR	C1-C2-C3	2.32	105.34	101.63
22	GE	1	FUB	O2-C2-C3	2.32	116.00	111.43
6	8A	1	FUB	C1-C2-C3	2.32	105.34	101.63
3	TC	1	FUB	C1-C2-C3	2.32	105.34	101.63
18	9D	4	AHR	C1-C2-C3	2.32	105.34	101.63
22	RE	6	AHR	C1-C2-C3	2.32	105.34	101.63
22	GE	2	FUB	O2-C2-C3	2.32	115.99	111.43
15	5C	5	AHR	C1-C2-C3	2.32	105.34	101.63
22	eE	6	AHR	C1-C2-C3	2.32	105.33	101.63
23	XE	1	FUB	C1-C2-C3	2.31	105.33	101.63
3	V	3	FUB	C1-C2-C3	2.31	105.32	101.63
5	KA	3	FUB	C1-C2-C3	2.31	105.32	101.63
6	7A	1	FUB	C1-C2-C3	2.31	105.32	101.63
13	2A	1	FUB	C1-C2-C3	2.31	105.32	101.63
4	L	4	AHR	C1-C2-C3	2.31	105.32	101.63
3	9C	2	FUB	C1-C2-C3	2.31	105.32	101.63
10	1A	5	AHR	C1-C2-C3	2.31	105.31	101.63
13	BA	2	FUB	O3-C3-C2	2.30	117.43	111.97
8	JD	4	AHR	C1-C2-C3	2.30	105.31	101.63
15	8B	5	AHR	C1-C2-C3	2.30	105.31	101.63
4	VD	4	AHR	C1-C2-C3	2.30	105.31	101.63
4	v	1	FUB	C1-C2-C3	2.30	105.31	101.63
13	ZB	3	GZL	C1-C2-C3	2.30	105.31	101.63
14	hD	3	GZL	O4-C1-C2	-2.30	101.80	105.76
3	O	1	FUB	C1-C2-C3	2.30	105.31	101.63
6	xC	1	FUB	C1-C2-C3	2.30	105.30	101.63
14	nB	3	GZL	C1-C2-C3	2.30	105.30	101.63
3	tC	3	FUB	C1-C2-C3	2.30	105.30	101.63
3	oB	1	FUB	C1-C2-C3	2.29	105.30	101.63
18	BE	3	GZL	C1-C2-C3	2.29	105.29	101.63
5	M	2	FUB	C1-C2-C3	2.29	105.29	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	i	2	AHR	C1-C2-C3	2.29	105.29	101.63
3	DD	1	FUB	C1-C2-C3	2.29	105.29	101.63
3	P	1	FUB	C1-C2-C3	2.29	105.28	101.63
6	3A	2	FUB	O2-C2-C3	2.28	115.92	111.43
3	XA	3	FUB	C1-C2-C3	2.28	105.28	101.63
3	OA	1	FUB	C1-C2-C3	2.28	105.27	101.63
4	SD	4	AHR	C1-C2-C3	2.28	105.27	101.63
4	JA	4	AHR	C1-C2-C3	2.28	105.27	101.63
3	jA	3	FUB	C1-C2-C3	2.28	105.27	101.63
6	N	3	GZL	C6-C5-C4	2.28	116.58	112.05
12	iC	4	AHR	C1-C2-C3	2.27	105.26	101.63
17	DB	1	NAG	C1-O5-C5	2.27	115.23	112.19
22	GE	5	AHR	C1-C2-C3	2.27	105.25	101.63
10	3	3	FUB	O3-C3-C2	2.27	117.34	111.97
24	lE	4	AHR	C1-C2-C3	2.27	105.25	101.63
3	TB	2	FUB	C1-C2-C3	2.26	105.25	101.63
13	o	4	AHR	C1-C2-C3	2.26	105.24	101.63
13	jB	1	FUB	C1-C2-C3	2.26	105.24	101.63
3	0	1	FUB	C1-C2-C3	2.26	105.24	101.63
8	U	4	AHR	C1-C2-C3	2.26	105.24	101.63
12	fD	2	FUB	C1-C2-C3	2.26	105.24	101.63
4	qB	4	AHR	C1-C2-C3	2.26	105.24	101.63
5	KA	4	AHR	C1-C2-C3	2.26	105.23	101.63
12	IB	4	AHR	C1-C2-C3	2.26	105.23	101.63
8	MC	5	AHR	C1-C2-C3	2.25	105.23	101.63
14	nB	4	FUB	C1-C2-C3	2.25	105.23	101.63
18	KE	4	AHR	C1-C2-C3	2.25	105.22	101.63
4	mB	1	FUB	C1-C2-C3	2.25	105.22	101.63
18	tE	1	FUB	C1-C2-C3	2.25	105.22	101.63
13	2A	2	FUB	O3-C3-C2	2.25	117.30	111.97
3	cA	3	FUB	C1-C2-C3	2.25	105.22	101.63
4	W	4	AHR	C1-C2-C3	2.25	105.22	101.63
6	3A	3	GZL	O2-C2-C3	-2.25	107.00	111.43
13	mA	4	AHR	C1-C2-C3	2.24	105.22	101.63
12	iC	5	AHR	C1-C2-C3	2.24	105.22	101.63
15	fB	5	AHR	C1-C2-C3	2.24	105.22	101.63
6	FC	1	FUB	O2-C2-C1	2.24	117.87	110.89
13	2A	4	AHR	C1-C2-C3	2.24	105.21	101.63
3	z	1	FUB	C1-C2-C3	2.24	105.21	101.63
4	LD	1	FUB	O2-C2-C3	2.23	115.83	111.43
13	WB	2	FUB	O2-C2-C3	2.23	115.83	111.43
6	8D	3	GZL	C1-C2-C3	2.23	105.20	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	DB	4	MAN	C1-O5-C5	2.23	115.18	112.19
6	R	1	FUB	C1-C2-C3	2.23	105.20	101.63
14	qA	3	GZL	O5-C5-C4	2.23	114.51	109.18
6	7D	2	FUB	C1-C2-C3	2.23	105.20	101.63
6	oE	2	FUB	C1-C2-C3	2.23	105.20	101.63
6	3D	1	FUB	C1-C2-C3	2.23	105.20	101.63
14	kB	3	GZL	O5-C5-C4	2.23	114.50	109.18
3	UB	1	FUB	C1-C2-C3	2.23	105.19	101.63
12	n	5	AHR	C1-C2-C3	2.23	105.19	101.63
22	VE	5	AHR	C1-C2-C3	2.22	105.18	101.63
7	WD	4	AHR	C1-C2-C3	2.22	105.18	101.63
14	p	3	GZL	C1-O4-C4	-2.22	103.40	107.84
13	zB	2	FUB	O2-C2-C3	2.22	115.80	111.43
19	qE	3	GZL	C1-C2-C3	2.22	105.18	101.63
14	p	3	GZL	C1-C2-C3	2.22	105.18	101.63
4	LD	4	AHR	C1-C2-C3	2.22	105.17	101.63
13	0D	3	GZL	O4-C1-C2	-2.22	101.94	105.76
21	kE	2	FUB	C1-C2-C3	2.22	105.17	101.63
4	qB	1	FUB	C1-C2-C3	2.21	105.17	101.63
17	5D	3	BMA	C1-O5-C5	2.21	115.15	112.19
4	cC	4	AHR	C1-C2-C3	2.21	105.17	101.63
3	IC	1	FUB	C1-C2-C3	2.21	105.16	101.63
14	nA	3	GZL	C1-C2-C3	2.21	105.16	101.63
18	SE	1	FUB	C1-C2-C3	2.21	105.16	101.63
24	YE	4	AHR	C1-C2-C3	2.21	105.16	101.63
9	ND	2	FUB	C1-C2-C3	2.21	105.16	101.63
14	nB	3	GZL	C1-O4-C4	-2.21	103.44	107.84
3	FD	1	FUB	C1-C2-C3	2.20	105.15	101.63
10	jD	1	FUB	C1-C2-C3	2.20	105.15	101.63
13	wD	4	AHR	C1-C2-C3	2.20	105.15	101.63
13	9A	2	FUB	O3-C3-C2	2.20	117.19	111.97
5	M	3	FUB	C1-C2-C3	2.20	105.15	101.63
10	a	5	AHR	C1-C2-C3	2.20	105.15	101.63
20	sE	4	AHR	C1-C2-C3	2.20	105.15	101.63
14	kB	2	FUB	C1-C2-C3	2.20	105.14	101.63
4	cC	1	FUB	C1-C2-C3	2.20	105.14	101.63
6	6C	2	FUB	C1-C2-C3	2.20	105.14	101.63
13	wC	2	FUB	O2-C2-C3	2.20	115.75	111.43
6	yD	1	FUB	C1-C2-C3	2.19	105.14	101.63
5	EC	4	AHR	C1-C2-C3	2.19	105.13	101.63
4	SD	2	FUB	C1-C2-C3	2.19	105.13	101.63
15	BB	4	AHR	C1-C2-C3	2.19	105.13	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	BA	2	FUB	O2-C2-C3	2.19	115.74	111.43
12	fD	5	AHR	C1-C2-C3	2.19	105.13	101.63
6	cB	1	FUB	C1-C2-C3	2.19	105.13	101.63
14	hC	1	FUB	C1-C2-C3	2.19	105.13	101.63
14	HB	4	FUB	C1-C2-C3	2.19	105.13	101.63
19	aE	3	GZL	C1-C2-C3	2.19	105.13	101.63
15	fB	4	AHR	C1-C2-C3	2.19	105.12	101.63
4	YC	2	FUB	C1-C2-C3	2.19	105.12	101.63
13	tD	3	GZL	C5-C4-C3	-2.18	112.81	115.95
15	2D	4	AHR	C1-C2-C3	2.18	105.12	101.63
17	DB	2	NAG	C4-C3-C2	-2.18	107.82	111.02
4	NB	1	FUB	C1-C2-C3	2.18	105.11	101.63
22	eE	5	AHR	C1-C2-C3	2.18	105.11	101.63
13	2B	3	GZL	C1-C2-C3	2.18	105.11	101.63
10	pB	4	AHR	C1-C2-C3	2.18	105.11	101.63
18	0E	5	AHR	C1-C2-C3	2.18	105.11	101.63
15	AB	1	FUB	C1-C2-C3	2.18	105.11	101.63
13	5A	4	AHR	C1-C2-C3	2.17	105.11	101.63
3	RB	3	FUB	C1-C2-C3	2.17	105.10	101.63
6	9	1	FUB	C1-C2-C3	2.17	105.10	101.63
9	hA	1	FUB	C1-C2-C3	2.17	105.10	101.63
18	JE	1	FUB	C1-C2-C3	2.17	105.10	101.63
21	vE	1	FUB	C1-C2-C3	2.17	105.10	101.63
4	qB	2	FUB	C1-C2-C3	2.17	105.09	101.63
4	nC	1	FUB	C1-C2-C3	2.16	105.08	101.63
5	M	4	AHR	C1-C2-C3	2.16	105.08	101.63
13	6B	2	FUB	O2-C2-C3	2.16	115.68	111.43
13	wD	3	GZL	C1-C2-C3	2.16	105.08	101.63
4	UA	1	FUB	O2-C2-C3	2.16	115.67	111.43
19	aE	4	AHR	C1-C2-C3	2.16	105.08	101.63
8	MC	1	FUB	C1-C2-C3	2.15	105.07	101.63
18	9D	1	FUB	O2-C2-C1	2.15	117.59	110.89
10	vC	3	FUB	O3-C3-C2	2.15	117.07	111.97
15	8B	4	AHR	C1-C2-C3	2.15	105.07	101.63
10	MB	4	AHR	C1-C2-C3	2.15	105.07	101.63
12	FB	5	AHR	C1-C2-C3	2.15	105.06	101.63
3	ED	1	FUB	C1-C2-C3	2.15	105.06	101.63
15	eB	4	AHR	O2-C2-C1	2.15	117.56	110.89
7	S	3	FUB	C1-C2-C3	2.14	105.06	101.63
5	BD	1	FUB	C1-C2-C3	2.14	105.05	101.63
3	rC	1	FUB	C1-C2-C3	2.14	105.05	101.63
7	QA	3	FUB	C1-C2-C3	2.14	105.05	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	CB	3	GZL	C1-O4-C4	-2.14	103.57	107.84
6	3A	1	FUB	C1-C2-C3	2.14	105.05	101.63
15	4C	5	AHR	C1-C2-C3	2.14	105.05	101.63
3	wA	3	FUB	O4-C4-C3	2.14	106.61	104.63
3	BC	1	FUB	C1-C2-C3	2.14	105.04	101.63
3	oD	3	FUB	C1-C2-C3	2.14	105.04	101.63
13	tD	2	FUB	O2-C2-C3	2.13	115.63	111.43
7	dA	1	FUB	C1-C2-C3	2.13	105.03	101.63
20	jE	3	GZL	C1-C2-C3	2.13	105.03	101.63
3	mD	3	FUB	C1-C2-C3	2.13	105.03	101.63
18	DE	4	AHR	C1-C2-C3	2.12	105.02	101.63
6	CB	1	FUB	C1-C2-C3	2.12	105.02	101.63
3	TC	2	FUB	C1-C2-C3	2.12	105.02	101.63
4	VD	2	FUB	C1-C2-C3	2.12	105.02	101.63
12	q	1	FUB	C1-C2-C3	2.12	105.02	101.63
6	4B	1	FUB	C1-C2-C3	2.12	105.02	101.63
15	2D	1	FUB	C1-C2-C3	2.12	105.01	101.63
3	pD	3	FUB	C1-C2-C3	2.12	105.01	101.63
14	kB	4	FUB	C1-C2-C3	2.11	105.01	101.63
7	KC	4	AHR	C1-C2-C3	2.11	105.01	101.63
3	QB	1	FUB	C1-C2-C3	2.11	105.00	101.63
6	aB	2	FUB	C1-C2-C3	2.11	105.00	101.63
15	DA	5	AHR	C1-C2-C3	2.11	105.00	101.63
20	uE	1	FUB	C1-C2-C3	2.11	105.00	101.63
4	VC	4	AHR	C1-C2-C3	2.11	105.00	101.63
3	0A	1	FUB	C1-C2-C3	2.11	105.00	101.63
3	pC	1	FUB	C1-C2-C3	2.10	104.99	101.63
14	s	3	GZL	O5-C5-C4	2.10	114.20	109.18
11	gA	3	AHR	C1-C2-C3	2.10	104.99	101.63
10	vC	5	AHR	C1-C2-C3	2.10	104.98	101.63
3	yA	1	FUB	C1-C2-C3	2.09	104.97	101.63
15	7B	4	AHR	O2-C2-C1	2.09	117.40	110.89
3	KD	1	FUB	C1-C2-C3	2.09	104.97	101.63
6	XB	2	FUB	O2-C2-C3	2.09	115.54	111.43
15	CA	4	AHR	C1-C2-C3	2.09	104.97	101.63
15	1D	4	AHR	C1-C2-C3	2.09	104.97	101.63
5	KA	5	AHR	C1-C2-C3	2.09	104.96	101.63
9	Y	1	FUB	O2-C2-C3	2.09	115.53	111.43
3	oB	3	FUB	C1-C2-C3	2.08	104.96	101.63
18	IE	1	FUB	O2-C2-C3	2.08	115.53	111.43
6	xD	2	FUB	O2-C2-C3	2.08	115.53	111.43
11	aC	2	AHR	C1-C2-C3	2.08	104.95	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	TA	1	FUB	C1-C2-C3	2.07	104.94	101.63
14	HB	3	GZL	O5-C5-C4	2.07	114.13	109.18
18	pE	1	FUB	O3-C3-C4	2.07	117.03	111.08
23	XE	4	AHR	O4-C4-C3	2.07	106.55	104.63
15	eB	1	FUB	C1-C2-C3	2.07	104.94	101.63
22	QE	1	FUB	C1-C2-C3	2.07	104.94	101.63
13	3C	3	GZL	O4-C1-C2	-2.07	102.19	105.76
3	w	3	FUB	C1-C2-C3	2.07	104.93	101.63
4	mB	4	AHR	C1-C2-C3	2.07	104.93	101.63
3	Q	1	FUB	C1-C2-C3	2.06	104.93	101.63
3	NA	3	FUB	C1-C2-C3	2.06	104.93	101.63
3	ID	1	FUB	C1-C2-C3	2.06	104.93	101.63
3	rB	1	FUB	C1-C2-C3	2.06	104.92	101.63
4	RC	4	AHR	C1-C2-C3	2.06	104.92	101.63
10	SC	5	AHR	C1-C2-C3	2.06	104.92	101.63
14	KB	4	FUB	C1-C2-C3	2.06	104.92	101.63
10	mC	4	AHR	C1-C2-C3	2.06	104.92	101.63
3	EB	1	FUB	C1-C2-C3	2.06	104.92	101.63
3	uC	3	FUB	C1-C2-C3	2.06	104.92	101.63
5	EC	3	FUB	C1-C2-C3	2.06	104.92	101.63
13	zC	2	FUB	C1-C2-C3	2.05	104.91	101.63
22	eE	4	AHR	C1-C2-C3	2.05	104.91	101.63
14	p	4	FUB	C1-C2-C3	2.05	104.91	101.63
10	jD	5	AHR	C1-C2-C3	2.05	104.91	101.63
7	XC	2	FUB	C1-C2-C3	-2.05	98.35	101.63
13	dB	2	FUB	O3-C3-C2	2.05	116.83	111.97
12	q	4	AHR	C1-C2-C3	2.05	104.90	101.63
6	uD	1	FUB	C1-C2-C3	2.05	104.90	101.63
22	dE	2	FUB	C1-C2-C3	2.05	104.90	101.63
18	fE	1	FUB	C1-C2-C3	2.05	104.90	101.63
6	CB	3	GZL	C1-C2-C3	2.05	104.90	101.63
13	9A	2	FUB	O2-C2-C3	2.04	115.45	111.43
6	5	1	FUB	C1-C2-C3	2.04	104.89	101.63
20	EE	2	FUB	O4-C4-C3	2.04	106.52	104.63
21	kE	1	FUB	O4-C4-C3	2.04	106.51	104.63
11	XD	1	FUB	O2-C2-C3	2.03	115.43	111.43
6	ZE	2	FUB	C1-C2-C3	2.03	104.88	101.63
12	cD	5	AHR	C1-C2-C3	2.03	104.88	101.63
8	U	2	FUB	C1-C2-C3	2.03	104.88	101.63
7	S	4	AHR	C1-C2-C3	2.03	104.88	101.63
3	cA	2	FUB	C1-C2-C3	2.03	104.88	101.63
6	cB	3	GZL	C1-C2-C3	2.03	104.88	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	2	FUB	O2-C2-C1	2.03	117.20	110.89
3	9C	3	FUB	C1-C2-C3	2.03	104.87	101.63
15	5C	4	AHR	C1-C2-C3	2.03	104.87	101.63
19	1E	2	FUB	C1-C2-C3	2.03	104.87	101.63
21	FE	5	AHR	C1-C2-C3	2.03	104.87	101.63
10	3	5	AHR	C1-C2-C3	2.03	104.87	101.63
3	x	3	FUB	C1-C2-C3	2.03	104.87	101.63
18	tE	4	AHR	C1-C2-C3	2.03	104.87	101.63
6	3A	2	FUB	O3-C3-C2	2.02	116.77	111.97
3	1	3	FUB	C1-C2-C3	2.02	104.86	101.63
15	BB	1	FUB	C1-C2-C3	2.02	104.86	101.63
24	YE	4	AHR	O2-C2-C1	2.02	117.18	110.89
18	pE	1	FUB	O2-C2-C1	2.02	117.18	110.89
13	2B	4	AHR	C1-C2-C3	2.02	104.86	101.63
6	5	2	FUB	O3-C3-C2	2.02	116.75	111.97
17	5D	3	BMA	C1-C2-C3	-2.02	106.70	109.64
4	NB	4	AHR	C1-C2-C3	2.02	104.86	101.63
4	d	1	FUB	C1-C2-C3	2.02	104.85	101.63
4	RD	2	FUB	C1-C2-C3	2.02	104.85	101.63
4	nC	4	AHR	C1-C2-C3	2.02	104.85	101.63
12	IB	2	FUB	C1-C2-C3	2.02	104.85	101.63
6	CD	2	FUB	O3-C3-C2	2.02	116.75	111.97
13	wC	3	GZL	O4-C1-C2	-2.01	102.29	105.76
6	0B	2	FUB	O3-C3-C2	2.01	116.74	111.97
13	wC	3	GZL	C1-C2-C3	-2.01	98.41	101.63
6	8	1	FUB	C1-C2-C3	2.01	104.85	101.63
12	q	5	AHR	C1-C2-C3	2.01	104.85	101.63
24	YE	6	AHR	C1-C2-C3	2.01	104.85	101.63
4	c	4	AHR	C1-C2-C3	2.01	104.84	101.63
13	yC	2	FUB	C1-C2-C3	2.01	104.84	101.63
6	JC	1	FUB	C1-C2-C3	2.01	104.84	101.63
24	lE	4	AHR	O2-C2-C1	2.01	117.14	110.89
3	WC	3	FUB	C1-C2-C3	2.01	104.84	101.63
4	ZD	1	FUB	C1-C2-C3	2.01	104.84	101.63
3	CC	1	FUB	C1-C2-C3	2.01	104.84	101.63
13	tD	3	GZL	C6-C5-C4	-2.01	108.06	112.05
7	HD	4	AHR	C1-C2-C3	2.01	104.84	101.63
18	zE	2	FUB	C1-C2-C3	2.01	104.84	101.63
4	DC	4	AHR	C1-C2-C3	2.01	104.83	101.63
7	h	4	AHR	C1-C2-C3	2.01	104.83	101.63
3	GC	1	FUB	C1-C2-C3	2.00	104.83	101.63
10	u	1	FUB	C1-C2-C3	2.00	104.83	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	iC	2	FUB	C1-C2-C3	2.00	104.83	101.63
6	xD	2	FUB	C1-C2-C3	2.00	104.83	101.63
13	wD	1	FUB	C1-C2-C3	2.00	104.83	101.63
3	jA	1	FUB	C1-C2-C3	2.00	104.83	101.63
3	CC	2	FUB	C1-C2-C3	2.00	104.83	101.63
7	f	3	FUB	C1-C2-C3	2.00	104.83	101.63
3	HA	3	FUB	C1-C2-C3	2.00	104.83	101.63
10	1A	4	AHR	O2-C2-C1	2.00	117.11	110.89

All (302) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	XA	2	FUB	C1
4	L	1	FUB	C4
4	Z	2	FUB	C1
4	JA	1	FUB	C4
4	VA	4	AHR	C2
4	VA	4	AHR	C1
4	DC	1	FUB	C4
4	PC	4	AHR	C1
4	RC	2	FUB	C1
4	AD	1	FUB	C4
4	OD	2	FUB	C1
5	BD	5	AHR	C1
6	N	3	GZL	C5
6	N	3	GZL	C1
6	R	3	GZL	C1
6	5	3	GZL	C4
6	5	3	GZL	C5
6	5	3	GZL	C1
6	8	3	GZL	C1
6	9	3	GZL	C1
6	AA	2	FUB	C4
6	AA	3	GZL	C1
6	EA	3	GZL	C1
6	LA	3	GZL	C5
6	LA	3	GZL	C1
6	PA	3	GZL	C1
6	3A	3	GZL	C5
6	3A	3	GZL	C1
6	7A	3	GZL	C1
6	8A	2	FUB	C4

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Mol	Chain	Res	Type	Atom
6	8A	3	GZL	C1
6	CB	3	GZL	C1
6	XB	3	GZL	C5
6	XB	3	GZL	C1
6	bB	3	GZL	C1
6	cB	2	FUB	C4
6	cB	3	GZL	C1
6	gB	3	GZL	C1
6	0B	3	GZL	C5
6	0B	3	GZL	C1
6	4B	3	GZL	C1
6	5B	2	FUB	C4
6	5B	3	GZL	C1
6	9B	3	GZL	C1
6	FC	3	GZL	C1
6	JC	3	GZL	C1
6	xC	3	GZL	C5
6	xC	3	GZL	C1
6	1C	3	GZL	C1
6	2C	2	FUB	C4
6	2C	3	GZL	C1
6	6C	3	GZL	C1
6	CD	3	GZL	C3
6	CD	3	GZL	C5
6	CD	3	GZL	C1
6	GD	3	GZL	C1
6	uD	3	GZL	C5
6	uD	3	GZL	C1
6	yD	3	GZL	C1
6	zD	2	FUB	C4
6	zD	3	GZL	C1
6	3D	3	GZL	C1
6	6D	3	GZL	C1
6	7D	3	GZL	C1
6	8D	3	GZL	C1
6	ME	3	GZL	C1
6	OE	3	GZL	C1
6	ZE	3	GZL	C1
6	bE	3	GZL	C1
6	mE	3	GZL	C1
6	nE	3	GZL	C1
6	oE	3	GZL	C1

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Mol	Chain	Res	Type	Atom
10	3	4	AHR	C1
10	1A	4	AHR	C1
10	VB	4	AHR	C1
10	yB	4	AHR	C1
10	vC	4	AHR	C1
10	sD	4	AHR	C1
12	n	3	GZL	C5
12	n	3	GZL	C1
12	q	3	GZL	C5
12	q	3	GZL	C1
12	q	5	AHR	C4
12	lA	3	GZL	C5
12	lA	3	GZL	C1
12	oA	3	GZL	C5
12	oA	3	GZL	C1
12	FB	3	GZL	C5
12	FB	3	GZL	C1
12	IB	3	GZL	C5
12	IB	3	GZL	C1
12	iB	3	GZL	C5
12	iB	3	GZL	C1
12	lB	3	GZL	C5
12	lB	3	GZL	C1
12	fC	3	GZL	C5
12	fC	3	GZL	C1
12	iC	3	GZL	C5
12	iC	3	GZL	C1
12	cD	3	GZL	C5
12	cD	3	GZL	C1
12	fD	3	GZL	C5
12	fD	3	GZL	C1
13	o	3	GZL	C5
13	o	3	GZL	C1
13	4	3	GZL	C5
13	4	3	GZL	C1
13	6	3	GZL	C1
13	7	3	GZL	C1
13	BA	2	FUB	C2
13	mA	3	GZL	C5
13	mA	3	GZL	C1
13	2A	3	GZL	C4
13	2A	3	GZL	C5

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Mol	Chain	Res	Type	Atom
13	2A	3	GZL	C1
13	4A	3	GZL	C1
13	5A	3	GZL	C1
13	9A	2	FUB	C2
13	GB	3	GZL	C5
13	GB	3	GZL	C1
13	WB	3	GZL	C4
13	WB	3	GZL	C5
13	WB	3	GZL	C1
13	YB	3	GZL	C1
13	ZB	3	GZL	C1
13	dB	2	FUB	C2
13	jB	3	GZL	C5
13	jB	3	GZL	C1
13	zB	3	GZL	C4
13	zB	3	GZL	C5
13	zB	3	GZL	C1
13	1B	3	GZL	C1
13	2B	3	GZL	C1
13	6B	2	FUB	C2
13	gC	3	GZL	C5
13	gC	3	GZL	C1
13	wC	3	GZL	C4
13	wC	3	GZL	C5
13	wC	3	GZL	C1
13	yC	3	GZL	C1
13	zC	3	GZL	C1
13	3C	2	FUB	C2
13	dD	3	GZL	C5
13	dD	3	GZL	C1
13	tD	3	GZL	C4
13	tD	3	GZL	C5
13	tD	3	GZL	C1
13	vD	3	GZL	C1
13	wD	3	GZL	C1
13	0D	2	FUB	C2
14	p	3	GZL	C5
14	p	3	GZL	C1
14	s	3	GZL	C5
14	s	3	GZL	C1
14	nA	3	GZL	C5
14	nA	3	GZL	C1

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Mol	Chain	Res	Type	Atom
14	qA	3	GZL	C5
14	qA	3	GZL	C1
14	HB	3	GZL	C5
14	HB	3	GZL	C1
14	KB	3	GZL	C5
14	KB	3	GZL	C1
14	kB	3	GZL	C5
14	kB	3	GZL	C1
14	nB	3	GZL	C5
14	nB	3	GZL	C1
14	hC	3	GZL	C5
14	hC	3	GZL	C1
14	kC	3	GZL	C5
14	kC	3	GZL	C1
14	eD	3	GZL	C5
14	eD	3	GZL	C1
14	hD	3	GZL	C5
14	hD	3	GZL	C1
15	CA	3	GZL	C1
15	CA	5	AHR	C1
15	DA	3	GZL	C1
15	AB	3	GZL	C1
15	AB	5	AHR	C1
15	BB	3	GZL	C1
15	eB	3	GZL	C1
15	eB	5	AHR	C1
15	fB	3	GZL	C1
15	7B	3	GZL	C1
15	7B	5	AHR	C1
15	8B	3	GZL	C1
15	4C	3	GZL	C1
15	4C	5	AHR	C1
15	5C	3	GZL	C1
15	1D	3	GZL	C1
15	1D	5	AHR	C1
15	2D	3	GZL	C1
17	GA	4	MAN	C1
17	GA	6	MAN	C1
17	DB	4	MAN	C1
17	DB	6	MAN	C1
17	7C	4	MAN	C1
17	7C	6	MAN	C1

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Mol	Chain	Res	Type	Atom
17	5D	4	MAN	C1
17	5D	6	MAN	C1
18	9D	3	GZL	C1
18	9D	4	AHR	C1
18	BE	3	GZL	C1
18	BE	4	AHR	C1
18	BE	5	AHR	C1
18	DE	3	GZL	C1
18	DE	5	AHR	C1
18	IE	3	GZL	C1
18	IE	4	AHR	C1
18	JE	3	GZL	C1
18	JE	5	AHR	C1
18	KE	3	GZL	C1
18	KE	4	AHR	C1
18	KE	5	AHR	C1
18	PE	3	GZL	C1
18	PE	4	AHR	C1
18	PE	5	AHR	C1
18	SE	1	FUB	C4
18	SE	3	GZL	C1
18	SE	4	AHR	C1
18	SE	5	AHR	C1
18	cE	3	GZL	C1
18	cE	4	AHR	C1
18	cE	5	AHR	C1
18	fE	1	FUB	C4
18	fE	3	GZL	C1
18	fE	4	AHR	C1
18	fE	5	AHR	C1
18	pE	3	GZL	C1
18	pE	4	AHR	C1
18	rE	3	GZL	C1
18	rE	4	AHR	C1
18	rE	5	AHR	C1
18	tE	3	GZL	C1
18	tE	5	AHR	C1
18	yE	3	GZL	C1
18	yE	4	AHR	C1
18	zE	3	GZL	C1
18	zE	5	AHR	C1
18	0E	3	GZL	C1

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Mol	Chain	Res	Type	Atom
18	0E	4	AHR	C1
18	0E	5	AHR	C1
19	AE	3	GZL	C1
19	LE	3	GZL	C1
19	LE	4	AHR	C1
19	NE	3	GZL	C1
19	NE	4	AHR	C1
19	aE	3	GZL	C1
19	aE	4	AHR	C1
19	qE	3	GZL	C1
19	1E	3	GZL	C1
19	1E	4	AHR	C1
20	CE	3	GZL	C1
20	EE	3	GZL	C1
20	HE	3	GZL	C1
20	TE	3	GZL	C1
20	TE	4	AHR	C1
20	UE	3	GZL	C1
20	WE	3	GZL	C1
20	WE	4	AHR	C1
20	gE	3	GZL	C1
20	gE	4	AHR	C1
20	hE	3	GZL	C1
20	jE	3	GZL	C1
20	jE	4	AHR	C1
20	sE	3	GZL	C1
20	uE	3	GZL	C1
20	xE	3	GZL	C1
21	FE	3	GZL	C1
21	FE	4	AHR	C1
21	FE	5	AHR	C3
21	kE	3	GZL	C1
21	kE	4	AHR	C1
21	vE	3	GZL	C1
21	vE	4	AHR	C1
21	vE	5	AHR	C3
21	vE	5	AHR	C2
22	GE	3	GZL	C1
22	QE	3	GZL	C1
22	QE	4	AHR	C1
22	QE	6	AHR	C1
22	RE	3	GZL	C1

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Mol	Chain	Res	Type	Atom
22	RE	4	AHR	C2
22	RE	4	AHR	C1
22	VE	3	GZL	C1
22	VE	4	AHR	C1
22	dE	3	GZL	C1
22	dE	4	AHR	C1
22	dE	6	AHR	C1
22	eE	3	GZL	C1
22	eE	4	AHR	C2
22	eE	4	AHR	C1
22	iE	3	GZL	C1
22	iE	4	AHR	C1
22	wE	3	GZL	C1
23	XE	3	GZL	C1
23	XE	4	AHR	C1
23	XE	5	AHR	C1
24	YE	3	GZL	C1
24	YE	4	AHR	C1
24	lE	3	GZL	C1
24	lE	4	AHR	C1

All (607) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	3	GZL	C4-C5-C6-O6
6	N	3	GZL	O5-C5-C6-O6
6	5	3	GZL	O5-C5-C6-O6
6	AA	3	GZL	C3-C4-C5-C6
6	AA	3	GZL	O4-C4-C5-C6
6	AA	3	GZL	C3-C4-C5-O5
6	AA	3	GZL	O4-C4-C5-O5
6	EA	3	GZL	O5-C5-C6-O6
6	LA	3	GZL	C4-C5-C6-O6
6	LA	3	GZL	O5-C5-C6-O6
6	PA	3	GZL	O5-C5-C6-O6
6	3A	3	GZL	O4-C4-C5-C6
6	3A	3	GZL	C3-C4-C5-O5
6	3A	3	GZL	O4-C4-C5-O5
6	7A	3	GZL	C4-C5-C6-O6
6	7A	3	GZL	O5-C5-C6-O6
6	8A	3	GZL	O4-C4-C5-C6
6	XB	3	GZL	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	XB	3	GZL	O4-C4-C5-C6
6	XB	3	GZL	C3-C4-C5-O5
6	XB	3	GZL	O4-C4-C5-O5
6	bB	3	GZL	C3-C4-C5-C6
6	bB	3	GZL	O4-C4-C5-C6
6	bB	3	GZL	C3-C4-C5-O5
6	bB	3	GZL	O4-C4-C5-O5
6	gB	3	GZL	C4-C5-C6-O6
6	gB	3	GZL	C3-C4-C5-C6
6	gB	3	GZL	O4-C4-C5-C6
6	gB	3	GZL	C3-C4-C5-O5
6	gB	3	GZL	O4-C4-C5-O5
6	0B	3	GZL	C3-C4-C5-C6
6	0B	3	GZL	O4-C4-C5-C6
6	0B	3	GZL	C3-C4-C5-O5
6	0B	3	GZL	O4-C4-C5-O5
6	4B	3	GZL	O4-C4-C5-C6
6	5B	3	GZL	O4-C4-C5-O5
6	FC	3	GZL	O4-C4-C5-C6
6	xC	3	GZL	C3-C4-C5-C6
6	xC	3	GZL	O4-C4-C5-C6
6	xC	3	GZL	C3-C4-C5-O5
6	xC	3	GZL	O4-C4-C5-O5
6	0C	3	GZL	O5-C5-C6-O6
6	2C	3	GZL	O4-C4-C5-C6
6	2C	3	GZL	O4-C4-C5-O5
6	6C	3	GZL	O5-C5-C6-O6
6	GD	3	GZL	O4-C4-C5-C6
6	uD	3	GZL	C4-C5-C6-O6
6	uD	3	GZL	C3-C4-C5-C6
6	uD	3	GZL	O4-C4-C5-C6
6	uD	3	GZL	C3-C4-C5-O5
6	uD	3	GZL	O4-C4-C5-O5
6	xD	3	GZL	O5-C5-C6-O6
6	xD	3	GZL	C3-C4-C5-C6
6	xD	3	GZL	O4-C4-C5-C6
6	xD	3	GZL	C3-C4-C5-O5
6	xD	3	GZL	O4-C4-C5-O5
6	yD	3	GZL	O5-C5-C6-O6
6	6D	3	GZL	O4-C4-C5-O5
6	7D	3	GZL	C3-C4-C5-C6
6	7D	3	GZL	O4-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	7D	3	GZL	C3-C4-C5-O5
6	7D	3	GZL	O4-C4-C5-O5
6	8D	3	GZL	O4-C4-C5-C6
6	ME	3	GZL	O4-C4-C5-C6
6	OE	3	GZL	C3-C4-C5-C6
6	OE	3	GZL	O4-C4-C5-C6
6	OE	3	GZL	C3-C4-C5-O5
6	ZE	3	GZL	C4-C5-C6-O6
6	ZE	3	GZL	O5-C5-C6-O6
6	bE	3	GZL	C4-C5-C6-O6
6	bE	3	GZL	O4-C4-C5-C6
6	mE	3	GZL	C3-C4-C5-C6
6	mE	3	GZL	O4-C4-C5-C6
6	mE	3	GZL	C3-C4-C5-O5
6	mE	3	GZL	O4-C4-C5-O5
6	nE	3	GZL	C3-C4-C5-C6
6	nE	3	GZL	O4-C4-C5-C6
6	nE	3	GZL	C3-C4-C5-O5
6	nE	3	GZL	O4-C4-C5-O5
6	oE	3	GZL	C3-C4-C5-C6
6	oE	3	GZL	O4-C4-C5-C6
6	oE	3	GZL	C3-C4-C5-O5
12	n	3	GZL	O5-C5-C6-O6
12	lA	3	GZL	O5-C5-C6-O6
12	FB	3	GZL	C4-C5-C6-O6
12	IB	3	GZL	C3-C4-C5-O5
12	IB	3	GZL	O4-C4-C5-O5
12	iB	3	GZL	C4-C5-C6-O6
12	iB	3	GZL	O4-C4-C5-C6
12	iB	3	GZL	O4-C4-C5-O5
12	lB	3	GZL	O4-C4-C5-C6
12	lB	3	GZL	O4-C4-C5-O5
12	fC	3	GZL	O4-C4-C5-C6
12	fC	3	GZL	O4-C4-C5-O5
12	iC	3	GZL	O4-C4-C5-C6
12	iC	3	GZL	O4-C4-C5-O5
12	cD	3	GZL	C4-C5-C6-O6
12	fD	3	GZL	C4-C5-C6-O6
13	o	3	GZL	C4-C5-C6-O6
13	4	3	GZL	C3-C4-C5-O5
13	BA	3	GZL	O4-C4-C5-O5
13	mA	3	GZL	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
13	2A	3	GZL	O5-C5-C6-O6
13	5A	3	GZL	O5-C5-C6-O6
13	GB	3	GZL	O5-C5-C6-O6
13	YB	3	GZL	C3-C4-C5-C6
13	YB	3	GZL	O4-C4-C5-C6
13	YB	3	GZL	C3-C4-C5-O5
13	YB	3	GZL	O4-C4-C5-O5
13	ZB	3	GZL	O5-C5-C6-O6
13	dB	3	GZL	O4-C4-C5-C6
13	dB	3	GZL	C3-C4-C5-O5
13	dB	3	GZL	O4-C4-C5-O5
13	jB	3	GZL	O5-C5-C6-O6
13	6B	3	GZL	C3-C4-C5-O5
13	6B	3	GZL	O4-C4-C5-O5
13	gC	3	GZL	O5-C5-C6-O6
13	zC	3	GZL	C3-C4-C5-C6
13	zC	3	GZL	O4-C4-C5-C6
13	zC	3	GZL	C3-C4-C5-O5
13	3C	3	GZL	O4-C4-C5-O5
13	dD	3	GZL	O5-C5-C6-O6
13	vD	3	GZL	C3-C4-C5-C6
13	vD	3	GZL	O4-C4-C5-C6
13	vD	3	GZL	C3-C4-C5-O5
13	vD	3	GZL	O4-C4-C5-O5
13	wD	3	GZL	C3-C4-C5-C6
13	wD	3	GZL	O4-C4-C5-C6
13	wD	3	GZL	C3-C4-C5-O5
13	wD	3	GZL	O4-C4-C5-O5
13	0D	3	GZL	O4-C4-C5-O5
14	p	3	GZL	O4-C4-C5-C6
14	p	3	GZL	O4-C4-C5-O5
14	s	3	GZL	O4-C4-C5-C6
14	s	3	GZL	O4-C4-C5-O5
14	nA	3	GZL	C4-C5-C6-O6
14	nA	3	GZL	O5-C5-C6-O6
14	nA	3	GZL	O4-C4-C5-C6
14	nA	3	GZL	O4-C4-C5-O5
14	qA	3	GZL	O4-C4-C5-C6
14	qA	3	GZL	O4-C4-C5-O5
14	HB	3	GZL	O4-C4-C5-C6
14	HB	3	GZL	O4-C4-C5-O5
14	KB	3	GZL	O4-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
14	KB	3	GZL	C3-C4-C5-O5
14	KB	3	GZL	O4-C4-C5-O5
14	kB	3	GZL	O4-C4-C5-C6
14	kB	3	GZL	O4-C4-C5-O5
14	nB	3	GZL	O4-C4-C5-C6
14	nB	3	GZL	O4-C4-C5-O5
14	hC	3	GZL	C3-C4-C5-C6
14	hC	3	GZL	C3-C4-C5-O5
14	kC	3	GZL	O5-C5-C6-O6
14	kC	3	GZL	O4-C4-C5-C6
14	kC	3	GZL	O4-C4-C5-O5
14	eD	3	GZL	O4-C4-C5-C6
14	eD	3	GZL	O4-C4-C5-O5
14	hD	3	GZL	O4-C4-C5-C6
14	hD	3	GZL	O4-C4-C5-O5
15	CA	3	GZL	C4-C5-C6-O6
15	CA	3	GZL	O5-C5-C6-O6
15	CA	3	GZL	O4-C4-C5-C6
15	AB	3	GZL	C4-C5-C6-O6
15	AB	3	GZL	O5-C5-C6-O6
15	AB	3	GZL	O4-C4-C5-C6
15	eB	3	GZL	C3-C4-C5-C6
15	eB	3	GZL	O4-C4-C5-C6
15	eB	3	GZL	C3-C4-C5-O5
15	7B	3	GZL	C4-C5-C6-O6
15	7B	3	GZL	C3-C4-C5-C6
15	7B	3	GZL	O4-C4-C5-C6
15	7B	3	GZL	C3-C4-C5-O5
15	1D	3	GZL	C3-C4-C5-C6
15	1D	3	GZL	O4-C4-C5-C6
15	1D	3	GZL	C3-C4-C5-O5
15	1D	3	GZL	O4-C4-C5-O5
16	AC	1	NAG	C3-C2-N2-C7
16	AC	1	NAG	C8-C7-N2-C2
16	AC	1	NAG	O7-C7-N2-C2
16	4D	1	NAG	C8-C7-N2-C2
16	4D	1	NAG	O7-C7-N2-C2
18	BE	3	GZL	C3-C4-C5-C6
18	BE	3	GZL	O4-C4-C5-C6
18	BE	3	GZL	C3-C4-C5-O5
18	BE	3	GZL	O4-C4-C5-O5
18	DE	3	GZL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
18	IE	3	GZL	C3-C4-C5-C6
18	IE	3	GZL	O4-C4-C5-C6
18	IE	3	GZL	C3-C4-C5-O5
18	IE	3	GZL	O4-C4-C5-O5
18	JE	3	GZL	O5-C5-C6-O6
18	KE	3	GZL	O4-C4-C5-C6
18	KE	3	GZL	C3-C4-C5-O5
18	KE	3	GZL	O4-C4-C5-O5
18	PE	3	GZL	C4-C5-C6-O6
18	PE	3	GZL	O5-C5-C6-O6
18	SE	3	GZL	C4-C5-C6-O6
18	SE	3	GZL	O5-C5-C6-O6
18	cE	3	GZL	C4-C5-C6-O6
18	cE	3	GZL	O5-C5-C6-O6
18	fE	3	GZL	C3-C4-C5-C6
18	fE	3	GZL	O4-C4-C5-C6
18	fE	3	GZL	C3-C4-C5-O5
18	fE	3	GZL	O4-C4-C5-O5
18	pE	3	GZL	C4-C5-C6-O6
18	tE	3	GZL	C4-C5-C6-O6
18	tE	3	GZL	O5-C5-C6-O6
18	yE	3	GZL	O5-C5-C6-O6
18	yE	3	GZL	C3-C4-C5-O5
18	zE	3	GZL	C3-C4-C5-C6
18	zE	3	GZL	O4-C4-C5-C6
18	zE	3	GZL	C3-C4-C5-O5
18	zE	3	GZL	O4-C4-C5-O5
18	0E	3	GZL	O4-C4-C5-C6
18	0E	3	GZL	C3-C4-C5-O5
18	0E	3	GZL	O4-C4-C5-O5
19	AE	3	GZL	C4-C5-C6-O6
19	AE	3	GZL	C3-C4-C5-C6
19	AE	3	GZL	O4-C4-C5-C6
19	AE	3	GZL	C3-C4-C5-O5
19	AE	3	GZL	O4-C4-C5-O5
19	qE	3	GZL	C3-C4-C5-C6
19	qE	3	GZL	O4-C4-C5-C6
19	qE	3	GZL	C3-C4-C5-O5
19	qE	3	GZL	O4-C4-C5-O5
19	1E	3	GZL	C3-C4-C5-C6
19	1E	3	GZL	O4-C4-C5-C6
19	1E	3	GZL	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
19	1E	3	GZL	O4-C4-C5-O5
20	CE	3	GZL	C3-C4-C5-C6
20	CE	3	GZL	O4-C4-C5-C6
20	CE	3	GZL	C3-C4-C5-O5
20	CE	3	GZL	O4-C4-C5-O5
20	HE	3	GZL	C3-C4-C5-C6
20	HE	3	GZL	O4-C4-C5-C6
20	HE	3	GZL	C3-C4-C5-O5
20	HE	3	GZL	O4-C4-C5-O5
20	TE	3	GZL	O5-C5-C6-O6
20	UE	3	GZL	C4-C5-C6-O6
20	UE	3	GZL	O4-C4-C5-C6
20	gE	3	GZL	O5-C5-C6-O6
20	hE	3	GZL	O4-C4-C5-C6
20	jE	3	GZL	O5-C5-C6-O6
20	sE	3	GZL	C3-C4-C5-C6
20	sE	3	GZL	O4-C4-C5-C6
20	sE	3	GZL	C3-C4-C5-O5
20	sE	3	GZL	O4-C4-C5-O5
20	uE	3	GZL	C3-C4-C5-C6
20	uE	3	GZL	O4-C4-C5-C6
20	uE	3	GZL	C3-C4-C5-O5
20	xE	3	GZL	C3-C4-C5-C6
20	xE	3	GZL	O4-C4-C5-C6
20	xE	3	GZL	C3-C4-C5-O5
20	xE	3	GZL	O4-C4-C5-O5
21	FE	3	GZL	O4-C4-C5-C6
21	vE	3	GZL	C4-C5-C6-O6
22	GE	3	GZL	C4-C5-C6-O6
22	GE	3	GZL	O5-C5-C6-O6
22	GE	3	GZL	O4-C4-C5-C6
22	GE	3	GZL	O4-C4-C5-O5
22	QE	3	GZL	C4-C5-C6-O6
22	RE	3	GZL	O5-C5-C6-O6
22	dE	3	GZL	O4-C4-C5-C6
22	eE	3	GZL	C4-C5-C6-O6
22	eE	3	GZL	O5-C5-C6-O6
22	iE	3	GZL	C4-C5-C6-O6
22	iE	3	GZL	O5-C5-C6-O6
22	wE	3	GZL	O5-C5-C6-O6
23	XE	3	GZL	C4-C5-C6-O6
23	XE	3	GZL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
24	YE	3	GZL	C3-C4-C5-C6
24	YE	3	GZL	C3-C4-C5-O5
24	YE	3	GZL	O4-C4-C5-O5
24	lE	3	GZL	C3-C4-C5-O5
24	lE	3	GZL	O4-C4-C5-O5
17	DB	2	NAG	C8-C7-N2-C2
17	DB	2	NAG	O7-C7-N2-C2
20	HE	2	FUB	O4-C4-C5-O5
6	gB	3	GZL	O5-C5-C6-O6
6	GD	3	GZL	O5-C5-C6-O6
6	uD	3	GZL	O5-C5-C6-O6
6	bE	3	GZL	O5-C5-C6-O6
12	FB	3	GZL	O5-C5-C6-O6
12	iB	3	GZL	O5-C5-C6-O6
12	lB	3	GZL	O5-C5-C6-O6
12	cD	3	GZL	O5-C5-C6-O6
12	fD	3	GZL	O5-C5-C6-O6
13	o	3	GZL	O5-C5-C6-O6
13	zC	3	GZL	O5-C5-C6-O6
14	kB	3	GZL	O5-C5-C6-O6
15	DA	3	GZL	O5-C5-C6-O6
15	8B	3	GZL	O5-C5-C6-O6
18	fE	3	GZL	O5-C5-C6-O6
18	pE	3	GZL	O5-C5-C6-O6
18	zE	3	GZL	O5-C5-C6-O6
19	AE	3	GZL	O5-C5-C6-O6
19	LE	3	GZL	O5-C5-C6-O6
19	aE	3	GZL	O5-C5-C6-O6
20	HE	3	GZL	O5-C5-C6-O6
20	UE	3	GZL	O5-C5-C6-O6
20	xE	3	GZL	O5-C5-C6-O6
21	vE	3	GZL	O5-C5-C6-O6
22	QE	3	GZL	O5-C5-C6-O6
17	DB	4	MAN	O5-C5-C6-O6
17	5D	4	MAN	O5-C5-C6-O6
6	5	3	GZL	C4-C5-C6-O6
6	EA	3	GZL	C4-C5-C6-O6
6	PA	3	GZL	C4-C5-C6-O6
6	6A	3	GZL	C4-C5-C6-O6
6	CB	3	GZL	C4-C5-C6-O6
6	XB	3	GZL	C4-C5-C6-O6
6	aB	3	GZL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	cB	3	GZL	C4-C5-C6-O6
6	0C	3	GZL	C4-C5-C6-O6
6	6C	3	GZL	C4-C5-C6-O6
6	GD	3	GZL	C4-C5-C6-O6
6	xD	3	GZL	C4-C5-C6-O6
6	yD	3	GZL	C4-C5-C6-O6
6	7D	3	GZL	C4-C5-C6-O6
6	ME	3	GZL	C4-C5-C6-O6
6	nE	3	GZL	C4-C5-C6-O6
12	n	3	GZL	C4-C5-C6-O6
12	lA	3	GZL	C4-C5-C6-O6
13	mA	3	GZL	C4-C5-C6-O6
13	2A	3	GZL	C4-C5-C6-O6
13	5A	3	GZL	C4-C5-C6-O6
13	GB	3	GZL	C4-C5-C6-O6
13	ZB	3	GZL	C4-C5-C6-O6
13	jB	3	GZL	C4-C5-C6-O6
13	gC	3	GZL	C4-C5-C6-O6
13	yC	3	GZL	C4-C5-C6-O6
13	zC	3	GZL	C4-C5-C6-O6
13	dD	3	GZL	C4-C5-C6-O6
13	wD	3	GZL	C4-C5-C6-O6
13	0D	3	GZL	C4-C5-C6-O6
14	p	3	GZL	C4-C5-C6-O6
14	kC	3	GZL	C4-C5-C6-O6
14	eD	3	GZL	C4-C5-C6-O6
15	DA	3	GZL	C4-C5-C6-O6
15	8B	3	GZL	C4-C5-C6-O6
18	DE	3	GZL	C4-C5-C6-O6
18	JE	3	GZL	C4-C5-C6-O6
18	fE	3	GZL	C4-C5-C6-O6
18	yE	3	GZL	C4-C5-C6-O6
19	LE	3	GZL	C4-C5-C6-O6
19	NE	3	GZL	C4-C5-C6-O6
19	aE	3	GZL	C4-C5-C6-O6
20	TE	3	GZL	C4-C5-C6-O6
20	gE	3	GZL	C4-C5-C6-O6
20	jE	3	GZL	C4-C5-C6-O6
20	xE	3	GZL	C4-C5-C6-O6
22	RE	3	GZL	C4-C5-C6-O6
22	wE	3	GZL	C4-C5-C6-O6
20	xE	2	FUB	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
17	DB	4	MAN	C4-C5-C6-O6
17	5D	4	MAN	C4-C5-C6-O6
17	DB	1	NAG	O5-C5-C6-O6
20	HE	2	FUB	C3-C4-C5-O5
17	7C	4	MAN	O5-C5-C6-O6
17	7C	4	MAN	C4-C5-C6-O6
16	FA	1	NAG	C8-C7-N2-C2
19	NE	3	GZL	O5-C5-C6-O6
20	hE	2	FUB	C3-C4-C5-O5
6	8A	3	GZL	C4-C5-C6-O6
12	lB	3	GZL	C4-C5-C6-O6
12	iC	3	GZL	C4-C5-C6-O6
18	zE	3	GZL	C4-C5-C6-O6
20	HE	3	GZL	C4-C5-C6-O6
17	7C	5	MAN	O5-C5-C6-O6
16	AC	2	NAG	C8-C7-N2-C2
17	5D	2	NAG	C8-C7-N2-C2
17	DB	1	NAG	C4-C5-C6-O6
6	6A	3	GZL	O5-C5-C6-O6
6	CB	3	GZL	O5-C5-C6-O6
6	0B	3	GZL	O5-C5-C6-O6
6	ME	3	GZL	O5-C5-C6-O6
6	nE	3	GZL	O5-C5-C6-O6
13	mA	3	GZL	O5-C5-C6-O6
13	yC	3	GZL	O5-C5-C6-O6
13	wD	3	GZL	O5-C5-C6-O6
15	7B	3	GZL	O5-C5-C6-O6
16	FA	1	NAG	O7-C7-N2-C2
16	AC	2	NAG	O7-C7-N2-C2
17	GA	2	NAG	C8-C7-N2-C2
17	5D	2	NAG	O7-C7-N2-C2
20	hE	2	FUB	O4-C4-C5-O5
17	5D	6	MAN	O5-C5-C6-O6
6	5B	3	GZL	C4-C5-C6-O6
20	sE	3	GZL	C4-C5-C6-O6
20	xE	2	FUB	C3-C4-C5-O5
6	cB	3	GZL	O5-C5-C6-O6
12	iC	3	GZL	O5-C5-C6-O6
13	0D	3	GZL	O5-C5-C6-O6
14	HB	3	GZL	O5-C5-C6-O6
17	7C	3	BMA	C4-C5-C6-O6
6	R	3	GZL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	AA	3	GZL	C4-C5-C6-O6
6	xC	3	GZL	C4-C5-C6-O6
13	1B	3	GZL	C4-C5-C6-O6
14	kB	3	GZL	C4-C5-C6-O6
18	rE	3	GZL	C4-C5-C6-O6
17	7C	5	MAN	C4-C5-C6-O6
6	8A	3	GZL	O5-C5-C6-O6
6	9B	3	GZL	O5-C5-C6-O6
17	7C	3	BMA	O5-C5-C6-O6
17	GA	2	NAG	O7-C7-N2-C2
17	DB	6	MAN	O5-C5-C6-O6
12	IB	3	GZL	C4-C5-C6-O6
6	3A	3	GZL	O5-C5-C6-O6
12	oA	3	GZL	O5-C5-C6-O6
12	fC	3	GZL	O5-C5-C6-O6
18	rE	3	GZL	O5-C5-C6-O6
6	5B	3	GZL	C3-C4-C5-O5
6	FC	3	GZL	C3-C4-C5-O5
6	2C	3	GZL	C3-C4-C5-O5
6	6D	3	GZL	C3-C4-C5-O5
12	iB	3	GZL	C3-C4-C5-O5
12	lB	3	GZL	C3-C4-C5-O5
12	fC	3	GZL	C3-C4-C5-O5
12	iC	3	GZL	C3-C4-C5-O5
13	BA	3	GZL	C3-C4-C5-O5
13	3C	3	GZL	C3-C4-C5-O5
13	0D	3	GZL	C3-C4-C5-O5
14	p	3	GZL	C3-C4-C5-O5
14	s	3	GZL	C3-C4-C5-O5
14	nA	3	GZL	C3-C4-C5-O5
14	qA	3	GZL	C3-C4-C5-O5
14	HB	3	GZL	C3-C4-C5-O5
14	kB	3	GZL	C3-C4-C5-O5
14	nB	3	GZL	C3-C4-C5-O5
14	kC	3	GZL	C3-C4-C5-O5
14	eD	3	GZL	C3-C4-C5-O5
14	hD	3	GZL	C3-C4-C5-O5
20	TE	3	GZL	C3-C4-C5-O5
22	GE	3	GZL	C3-C4-C5-O5
6	8A	3	GZL	O4-C4-C5-O5
6	4B	3	GZL	O4-C4-C5-O5
6	FC	3	GZL	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
6	GD	3	GZL	O4-C4-C5-O5
6	8D	3	GZL	O4-C4-C5-O5
6	OE	3	GZL	O4-C4-C5-O5
6	bE	3	GZL	O4-C4-C5-O5
6	oE	3	GZL	O4-C4-C5-O5
13	9A	3	GZL	O4-C4-C5-O5
13	WB	3	GZL	O4-C4-C5-O5
13	zB	3	GZL	O4-C4-C5-O5
13	wC	3	GZL	O4-C4-C5-O5
13	zC	3	GZL	O4-C4-C5-O5
14	hC	3	GZL	O4-C4-C5-O5
15	CA	3	GZL	O4-C4-C5-O5
15	AB	3	GZL	O4-C4-C5-O5
15	eB	3	GZL	O4-C4-C5-O5
15	7B	3	GZL	O4-C4-C5-O5
15	4C	3	GZL	O4-C4-C5-O5
18	SE	3	GZL	O4-C4-C5-O5
18	pE	3	GZL	O4-C4-C5-O5
18	rE	3	GZL	O4-C4-C5-O5
18	yE	3	GZL	O4-C4-C5-O5
20	UE	3	GZL	O4-C4-C5-O5
20	WE	3	GZL	O4-C4-C5-O5
20	hE	3	GZL	O4-C4-C5-O5
20	jE	3	GZL	O4-C4-C5-O5
20	uE	3	GZL	O4-C4-C5-O5
21	FE	3	GZL	O4-C4-C5-O5
21	vE	3	GZL	O4-C4-C5-O5
22	dE	3	GZL	O4-C4-C5-O5
20	CE	3	GZL	C4-C5-C6-O6
6	aB	3	GZL	O5-C5-C6-O6
6	5B	3	GZL	O5-C5-C6-O6
6	7D	3	GZL	O5-C5-C6-O6
12	IB	3	GZL	O5-C5-C6-O6
14	p	3	GZL	O5-C5-C6-O6
14	eD	3	GZL	O5-C5-C6-O6
15	2D	3	GZL	O5-C5-C6-O6
17	DB	5	MAN	O5-C5-C6-O6
20	TE	2	FUB	O4-C4-C5-O5
20	TE	2	FUB	C3-C4-C5-O5
18	IE	3	GZL	O5-C5-C6-O6
20	sE	3	GZL	O5-C5-C6-O6
17	7C	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
17	7C	1	NAG	O5-C5-C6-O6
6	2C	3	GZL	C3-C4-C5-C6
6	6D	3	GZL	C3-C4-C5-C6
12	iB	3	GZL	C3-C4-C5-C6
13	4	3	GZL	C3-C4-C5-C6
13	BA	3	GZL	C3-C4-C5-C6
13	dB	3	GZL	C3-C4-C5-C6
13	jB	3	GZL	C3-C4-C5-C6
13	6B	3	GZL	C3-C4-C5-C6
14	p	3	GZL	C3-C4-C5-C6
14	s	3	GZL	C3-C4-C5-C6
14	nA	3	GZL	C3-C4-C5-C6
14	HB	3	GZL	C3-C4-C5-C6
14	KB	3	GZL	C3-C4-C5-C6
14	nB	3	GZL	C3-C4-C5-C6
14	kC	3	GZL	C3-C4-C5-C6
14	eD	3	GZL	C3-C4-C5-C6
14	hD	3	GZL	C3-C4-C5-C6
18	KE	3	GZL	C3-C4-C5-C6
18	0E	3	GZL	C3-C4-C5-C6
22	GE	3	GZL	C3-C4-C5-C6
22	dE	3	GZL	C3-C4-C5-C6
24	lE	3	GZL	C3-C4-C5-C6
17	GA	4	MAN	O5-C5-C6-O6
15	eB	3	GZL	C4-C5-C6-O6
15	2D	3	GZL	C4-C5-C6-O6
17	GA	1	NAG	O5-C5-C6-O6
17	GA	6	MAN	O5-C5-C6-O6
6	6D	3	GZL	O4-C4-C5-C6
13	4	3	GZL	O4-C4-C5-C6
13	BA	3	GZL	O4-C4-C5-C6
13	6B	3	GZL	O4-C4-C5-C6
18	yE	3	GZL	O4-C4-C5-C6
20	jE	3	GZL	O4-C4-C5-C6
24	YE	3	GZL	O4-C4-C5-C6
24	lE	3	GZL	O4-C4-C5-C6
17	5D	1	NAG	O5-C5-C6-O6
12	oA	3	GZL	C4-C5-C6-O6
12	fC	3	GZL	C4-C5-C6-O6
17	DB	3	BMA	C4-C5-C6-O6
16	FA	1	NAG	C3-C2-N2-C7
13	6	3	GZL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	1B	3	GZL	O5-C5-C6-O6
6	zD	3	GZL	C4-C5-C6-O6
18	9D	3	GZL	C4-C5-C6-O6
6	R	3	GZL	O5-C5-C6-O6
6	9B	3	GZL	C4-C5-C6-O6
13	4	3	GZL	C4-C5-C6-O6
13	9A	3	GZL	C4-C5-C6-O6
14	HB	3	GZL	C4-C5-C6-O6
6	4B	3	GZL	C3-C4-C5-O5
13	9A	3	GZL	C3-C4-C5-O5
22	VE	3	GZL	C3-C4-C5-O5
22	dE	3	GZL	C3-C4-C5-O5
6	ME	3	GZL	O4-C4-C5-O5
22	VE	3	GZL	O4-C4-C5-O5
14	nB	3	GZL	C4-C5-C6-O6
6	AA	3	GZL	O5-C5-C6-O6
6	3B	3	GZL	O5-C5-C6-O6
13	zB	3	GZL	O5-C5-C6-O6
15	eB	3	GZL	O5-C5-C6-O6
18	0E	3	GZL	O5-C5-C6-O6
20	CE	3	GZL	O5-C5-C6-O6
16	FA	2	NAG	C8-C7-N2-C2
17	GA	5	MAN	O5-C5-C6-O6
6	4B	3	GZL	C3-C4-C5-C6
6	FC	3	GZL	C3-C4-C5-C6
12	lB	3	GZL	C3-C4-C5-C6
12	fC	3	GZL	C3-C4-C5-C6
12	iC	3	GZL	C3-C4-C5-C6
14	qA	3	GZL	C3-C4-C5-C6
14	kB	3	GZL	C3-C4-C5-C6
15	4C	3	GZL	O4-C4-C5-C6
6	CD	3	GZL	C4-C5-C6-O6
13	6	3	GZL	C4-C5-C6-O6
6	cB	3	GZL	C3-C4-C5-O5
13	6	3	GZL	C3-C4-C5-O5
17	5D	3	BMA	C4-C5-C6-O6
12	FB	3	GZL	O4-C4-C5-O5
13	4	3	GZL	O4-C4-C5-O5
20	TE	3	GZL	O4-C4-C5-O5
18	9D	3	GZL	O5-C5-C6-O6
17	5D	6	MAN	C4-C5-C6-O6
16	FA	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
17	GA	3	BMA	C4-C5-C6-O6
17	DB	3	BMA	O5-C5-C6-O6
6	3B	3	GZL	C4-C5-C6-O6
18	0E	3	GZL	C4-C5-C6-O6
6	9	3	GZL	O5-C5-C6-O6
20	CE	2	FUB	O4-C4-C5-O5
11	gA	1	FUB	O4-C4-C5-O5
6	zD	3	GZL	O5-C5-C6-O6
22	RE	2	FUB	O4-C4-C5-O5
12	IB	3	GZL	C3-C4-C5-C6
13	dD	3	GZL	C3-C4-C5-C6
13	0D	3	GZL	C3-C4-C5-C6
18	yE	3	GZL	C3-C4-C5-C6
6	cB	3	GZL	O4-C4-C5-O5
12	IB	3	GZL	O4-C4-C5-C6
13	0D	3	GZL	O4-C4-C5-C6
18	IE	3	GZL	C4-C5-C6-O6
24	lE	3	GZL	C4-C5-C6-O6
23	XE	2	FUB	O4-C4-C5-O5
16	4D	1	NAG	C3-C2-N2-C7
18	9D	3	GZL	O4-C4-C5-O5
13	9A	3	GZL	O5-C5-C6-O6
15	BB	3	GZL	O5-C5-C6-O6
6	5B	3	GZL	C3-C4-C5-C6
13	GB	3	GZL	C3-C4-C5-C6
13	3C	3	GZL	C3-C4-C5-C6
20	hE	3	GZL	C3-C4-C5-C6
17	GA	3	BMA	O5-C5-C6-O6
6	5B	3	GZL	O4-C4-C5-C6
13	mA	3	GZL	O4-C4-C5-C6
13	3C	3	GZL	O4-C4-C5-C6
18	pE	3	GZL	O4-C4-C5-C6
20	WE	3	GZL	O4-C4-C5-C6
21	vE	3	GZL	O4-C4-C5-C6
14	nB	3	GZL	O5-C5-C6-O6
17	DB	5	MAN	C4-C5-C6-O6
18	BE	3	GZL	C4-C5-C6-O6
15	BB	3	GZL	C4-C5-C6-O6
20	uE	3	GZL	C4-C5-C6-O6
22	RE	3	GZL	C3-C4-C5-O5
12	q	3	GZL	O5-C5-C6-O6
6	9	3	GZL	C4-C5-C6-O6

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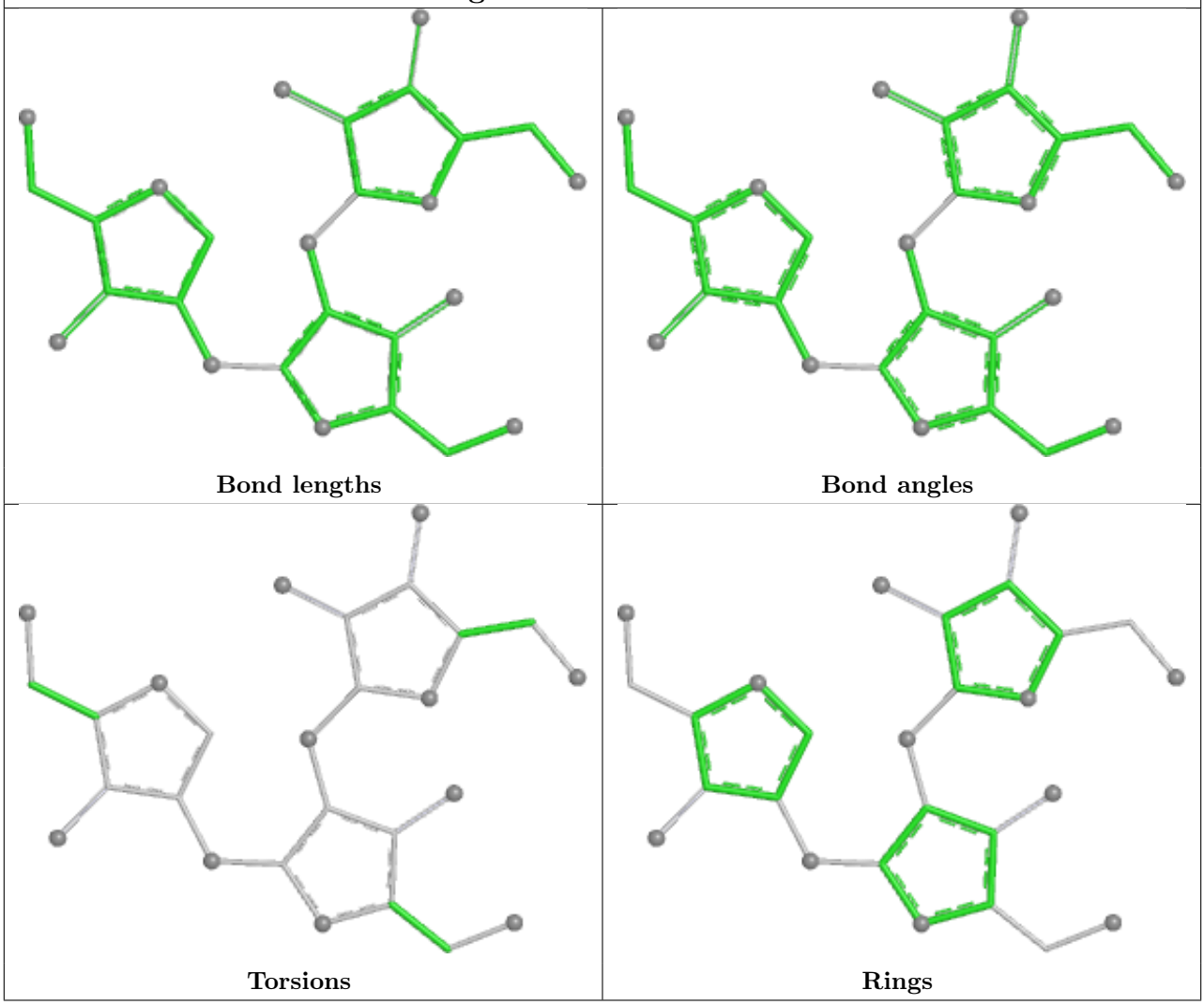
Mol	Chain	Res	Type	Atoms
17	5D	3	BMA	O5-C5-C6-O6

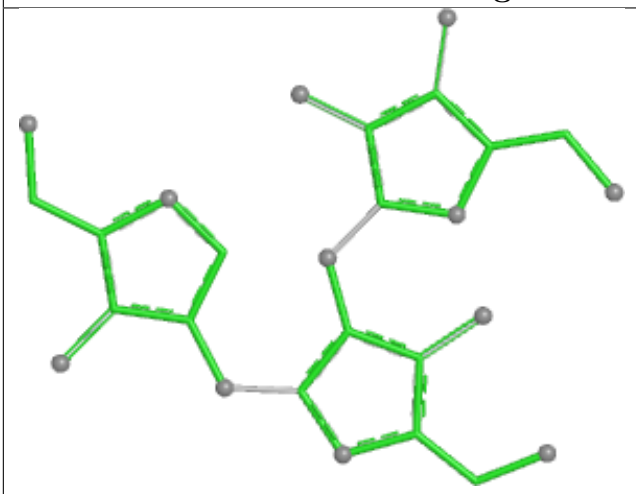
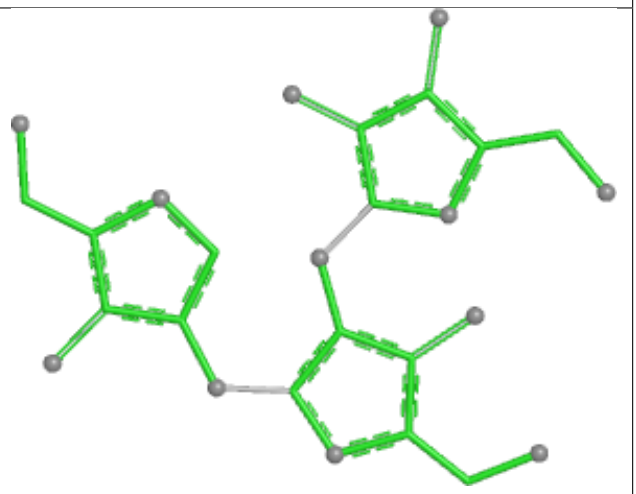
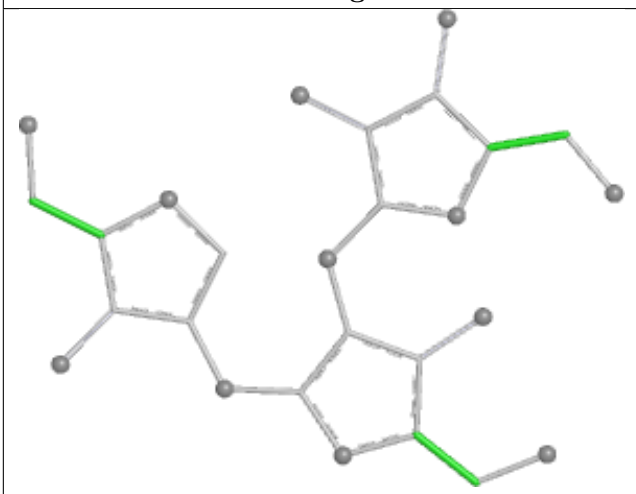
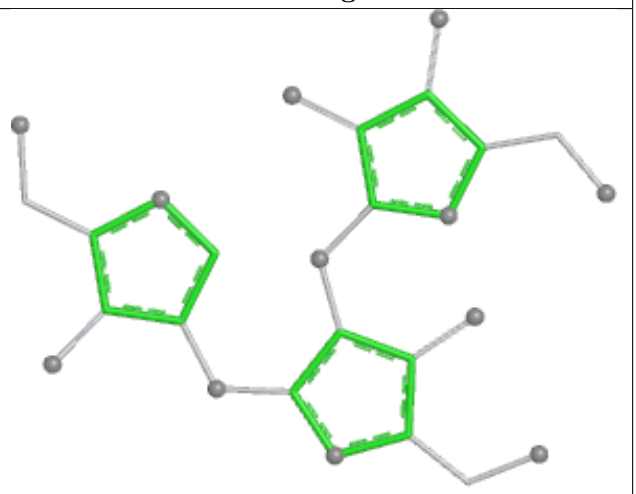
There are no ring outliers.

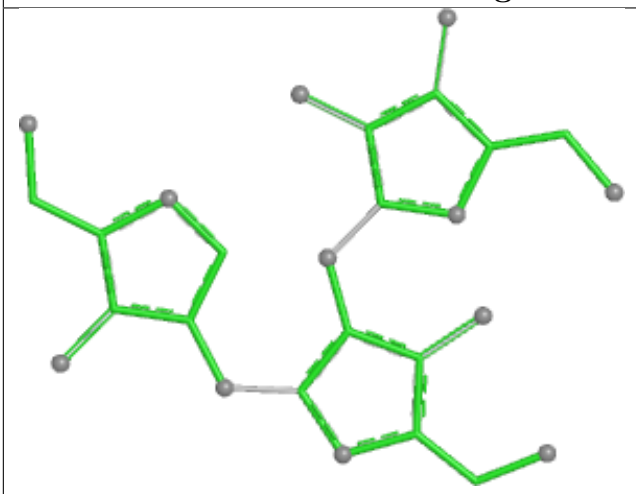
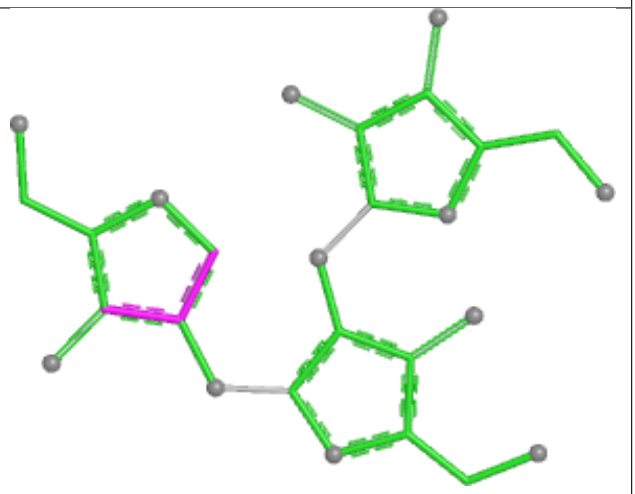
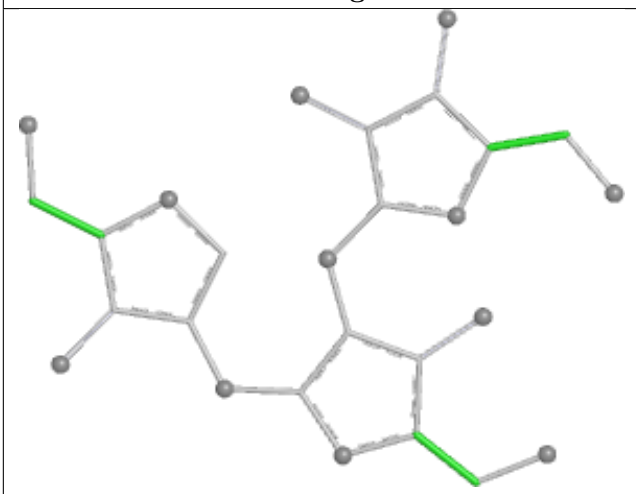
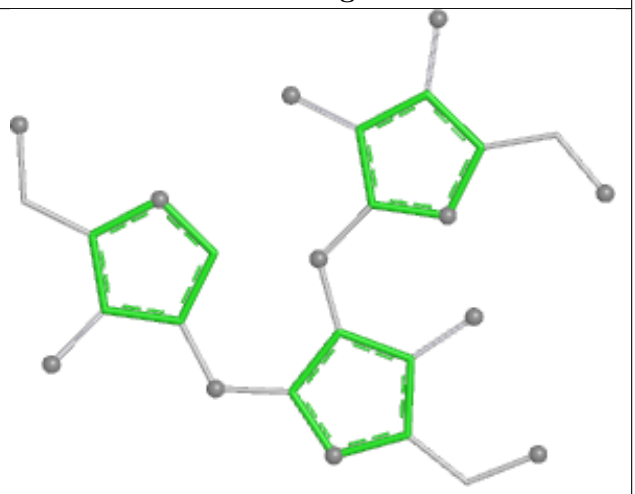
No monomer is involved in short contacts.

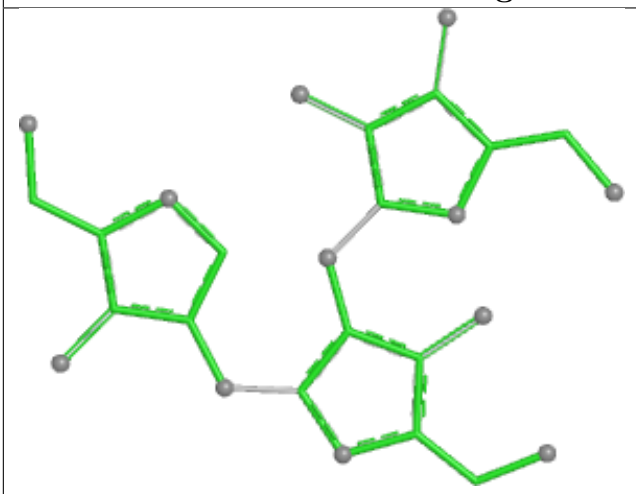
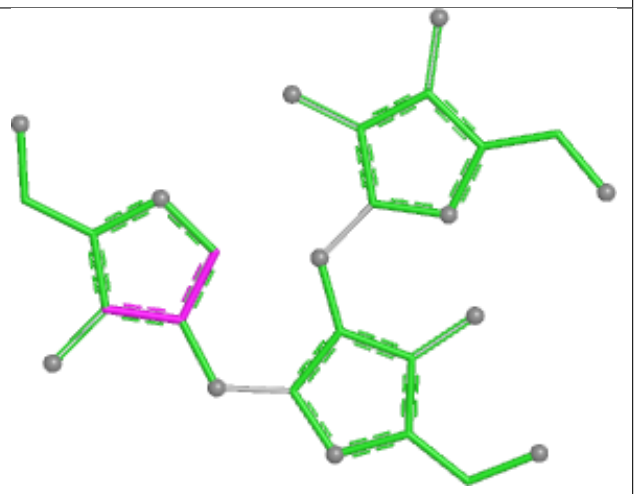
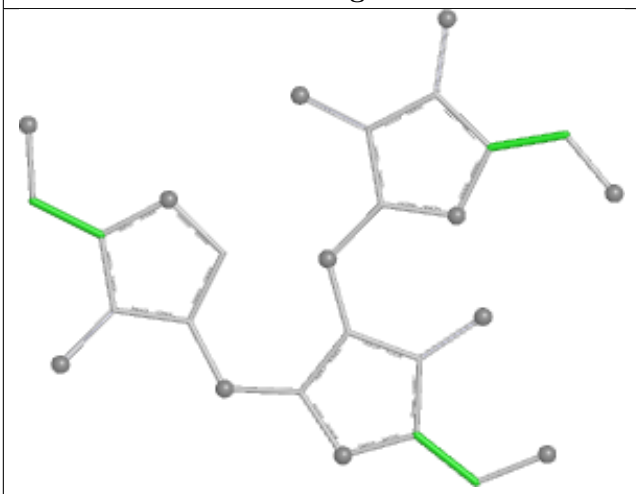
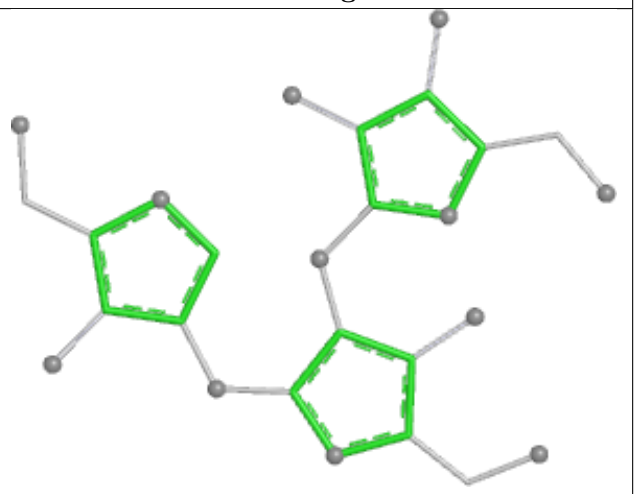
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

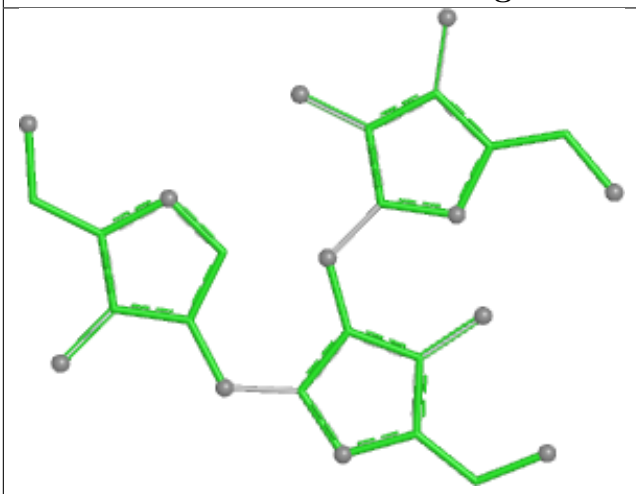
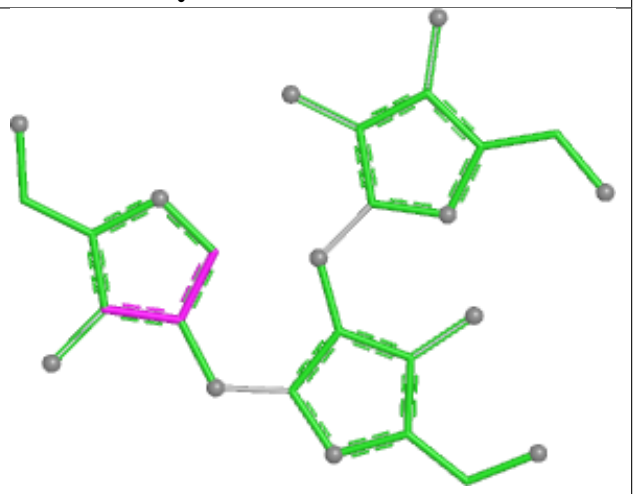
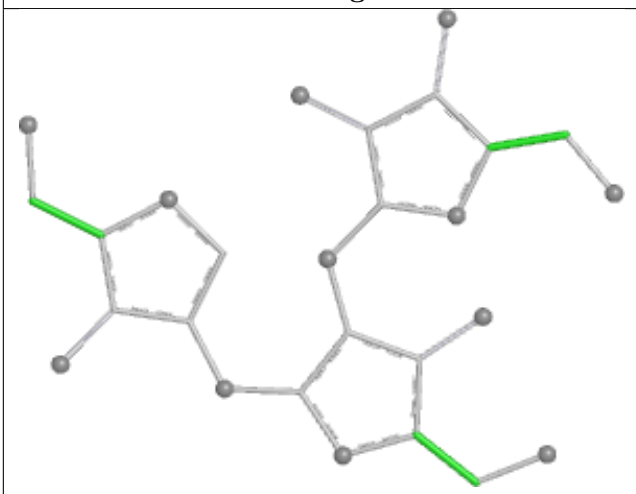
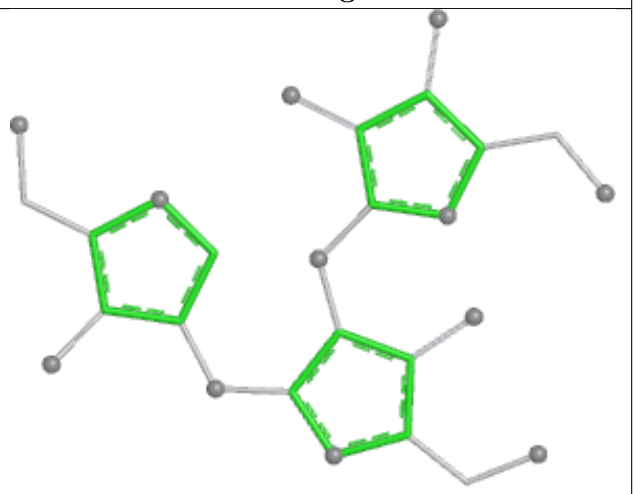
Oligosaccharide Chain J



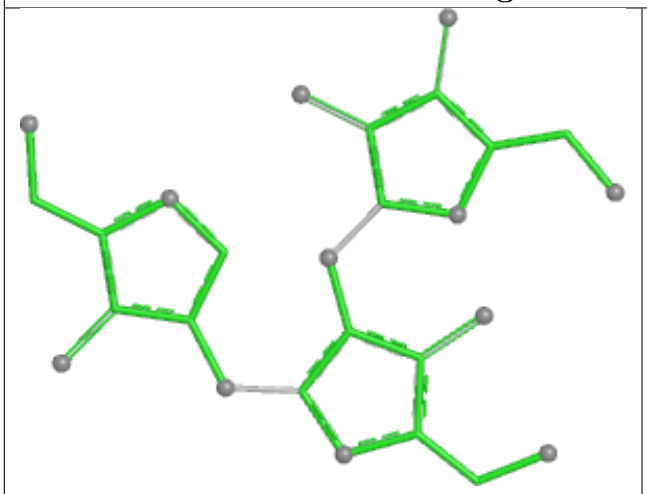
Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

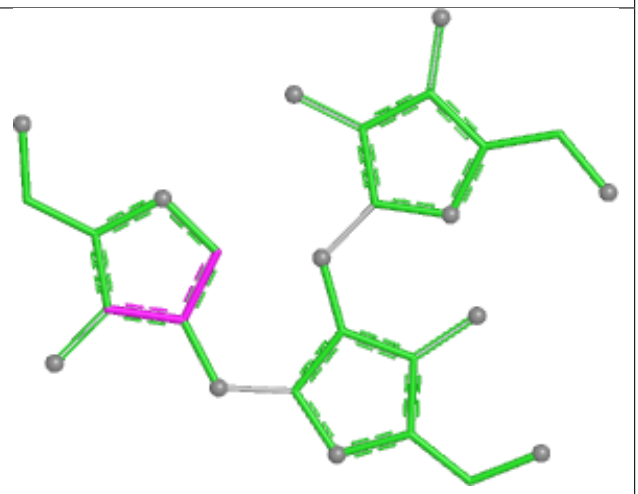
Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

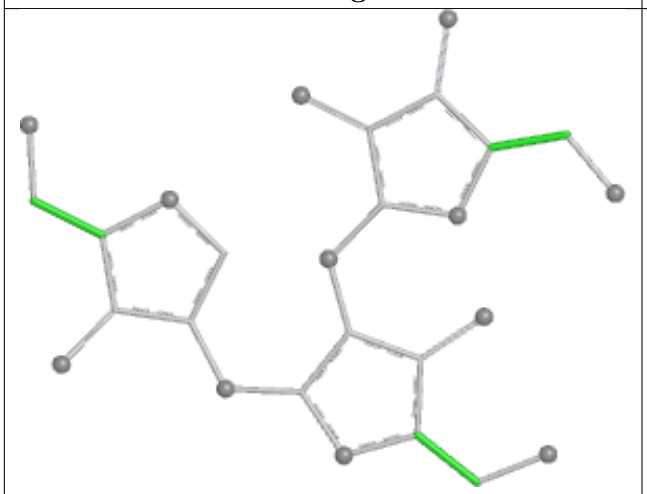
Oligosaccharide Chain T



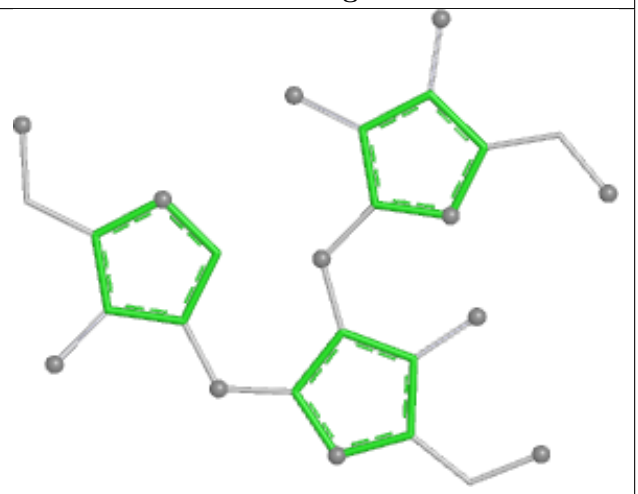
Bond lengths



Bond angles

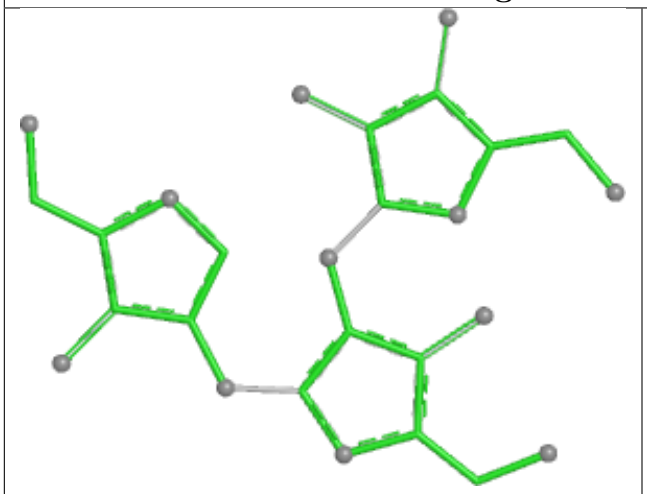


Torsions



Rings

Oligosaccharide Chain V



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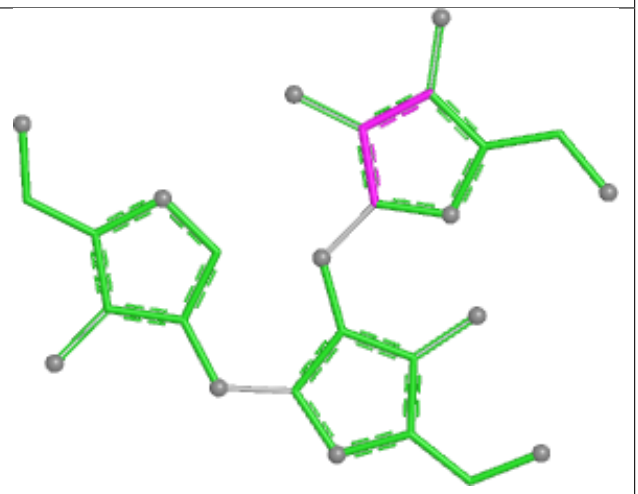

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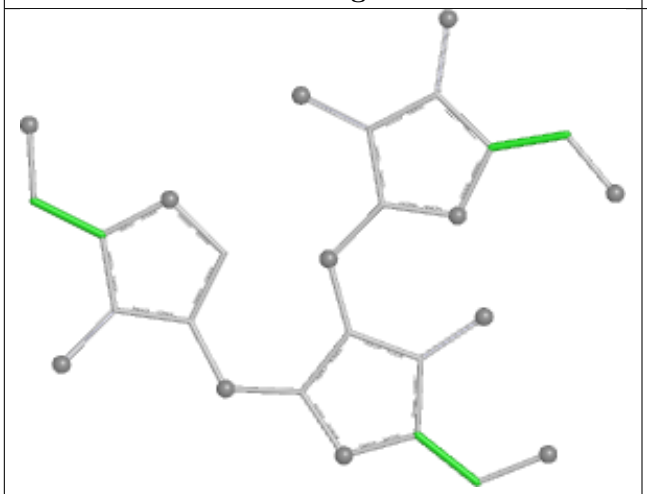

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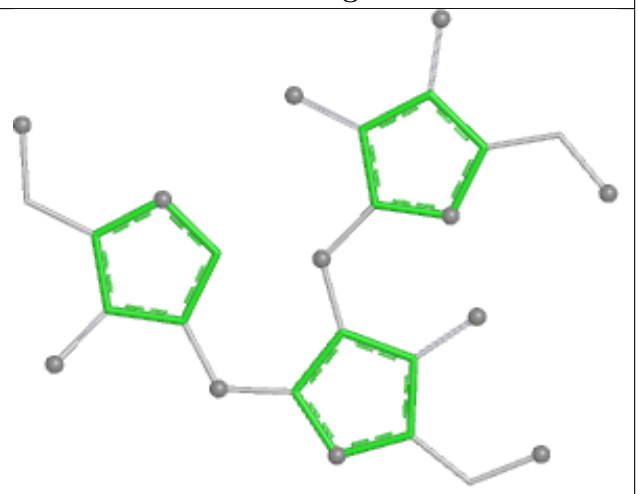
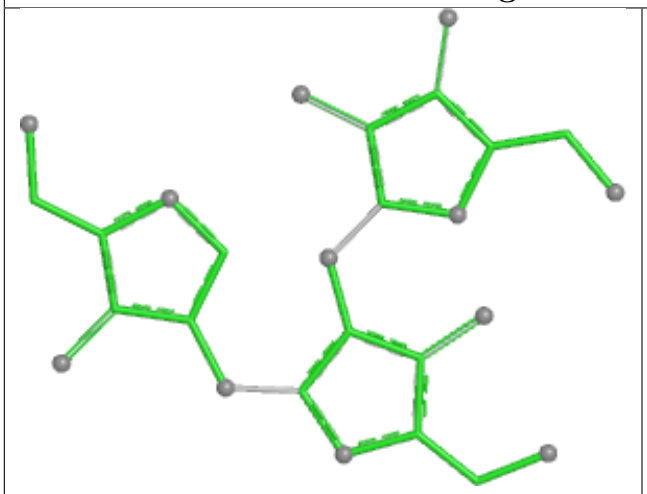


Rings

Oligosaccharide Chain b



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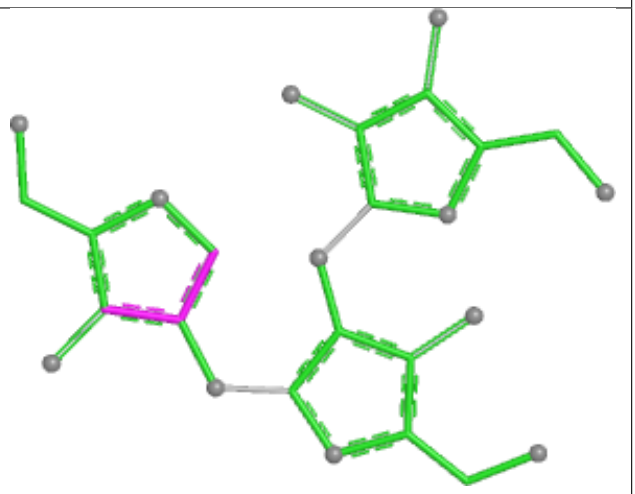

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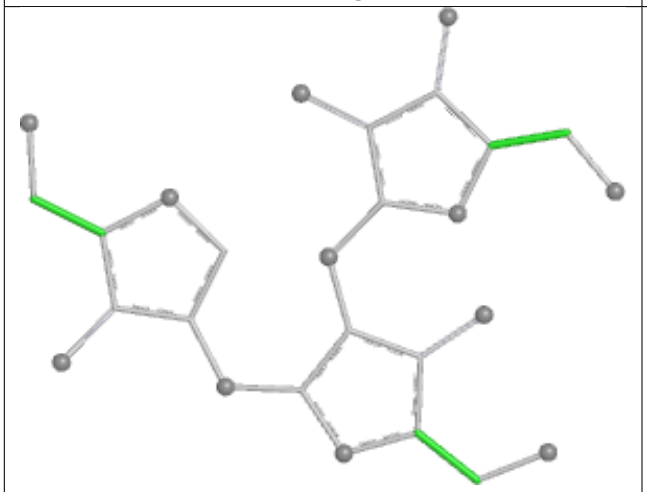

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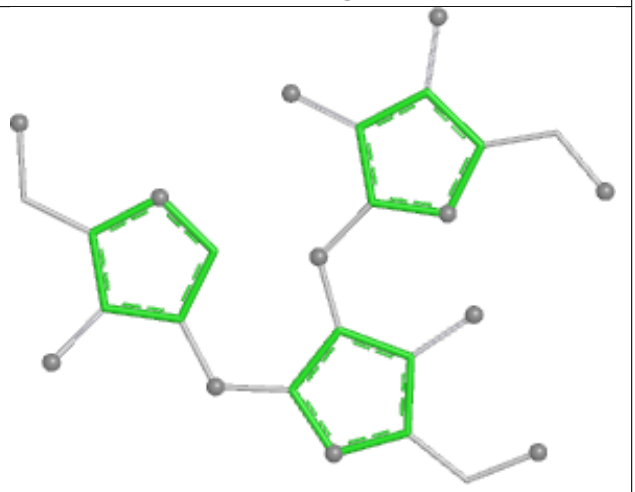
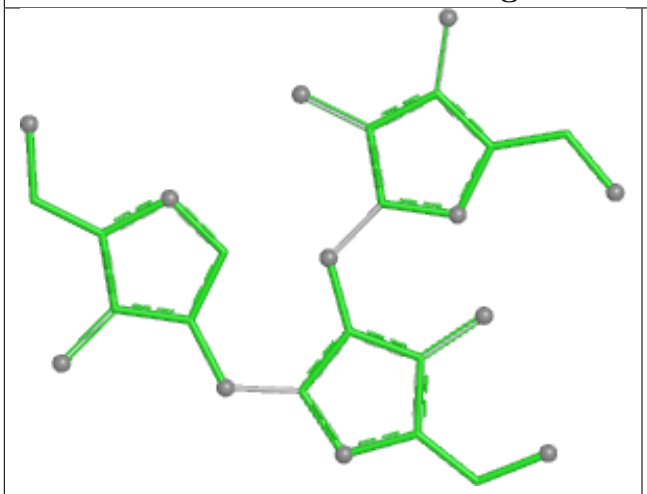
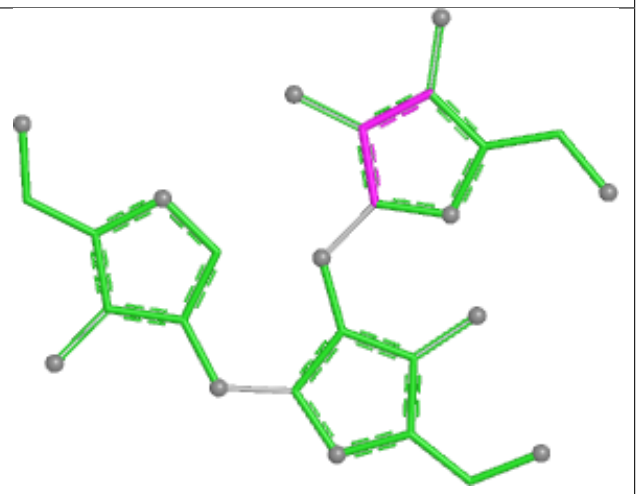


Rings

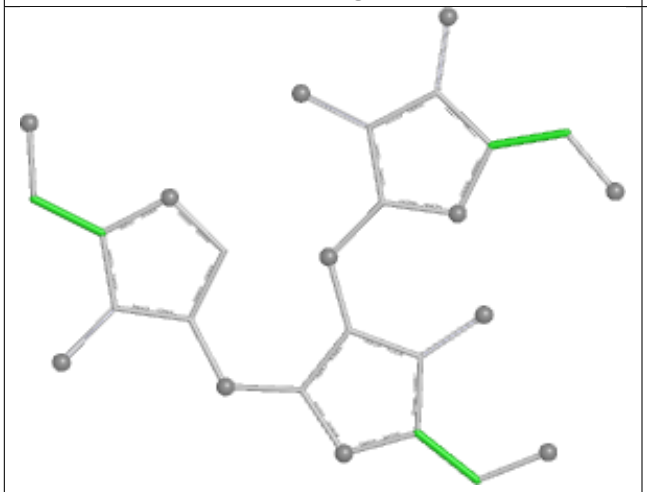
Oligosaccharide Chain e



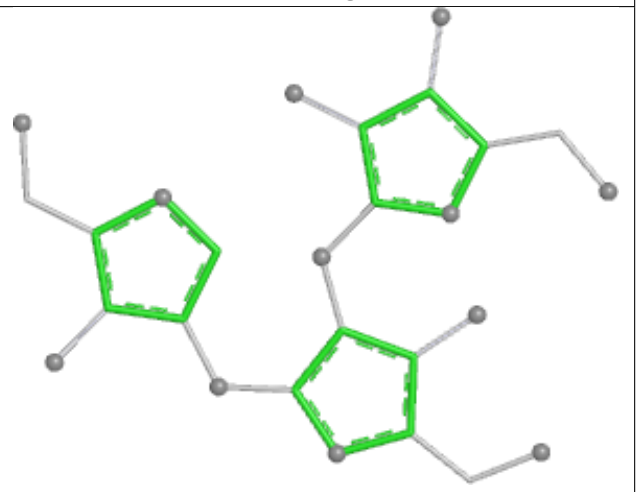
Bond lengths



Bond angles

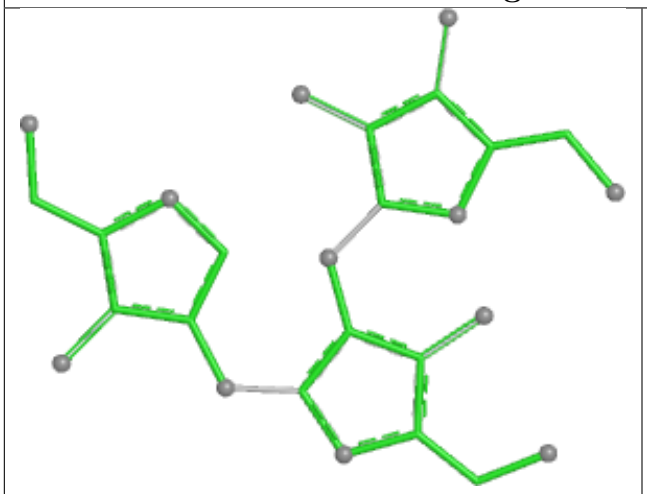


Torsions

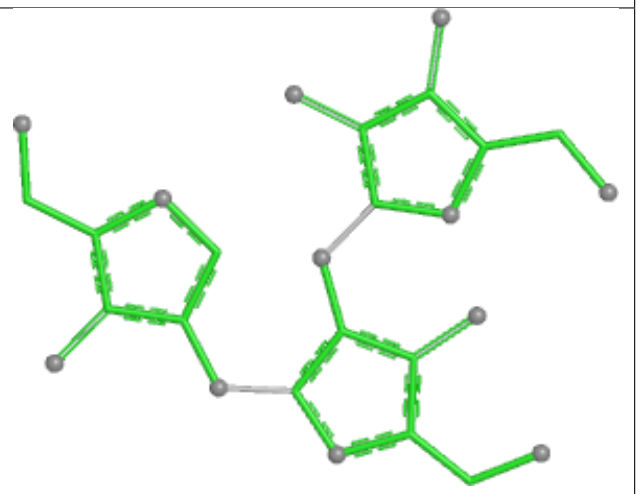


Rings

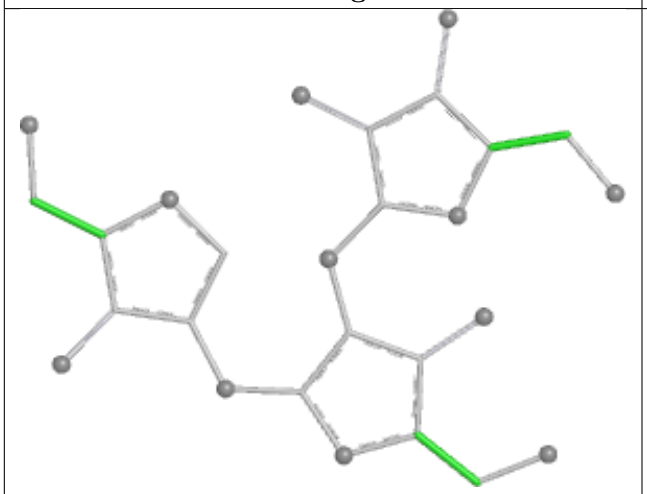
Oligosaccharide Chain l



Bond lengths



Bond angles



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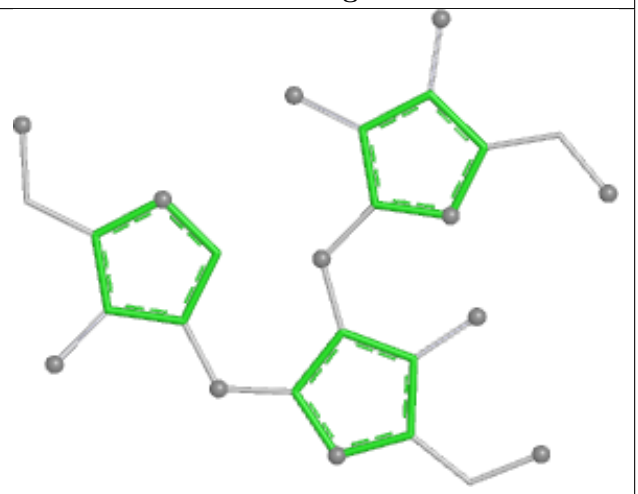
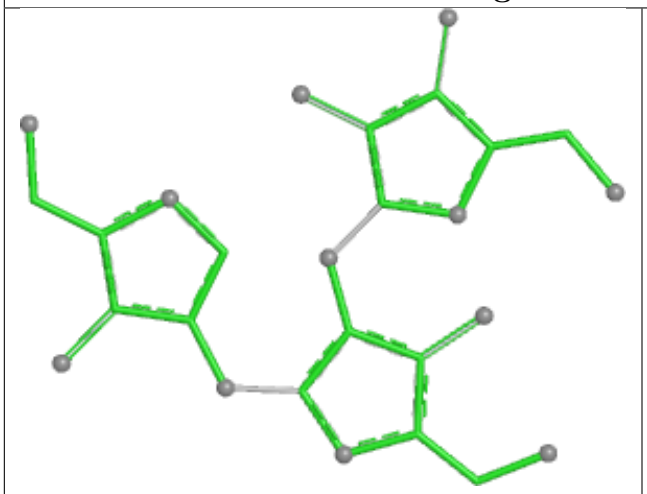


Rings

Oligosaccharide Chain m



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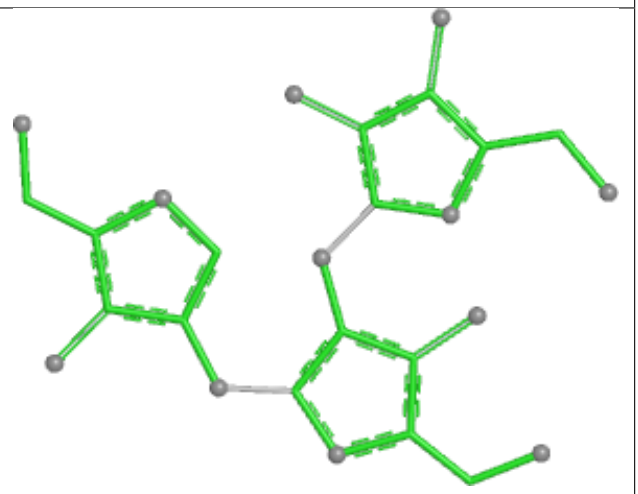
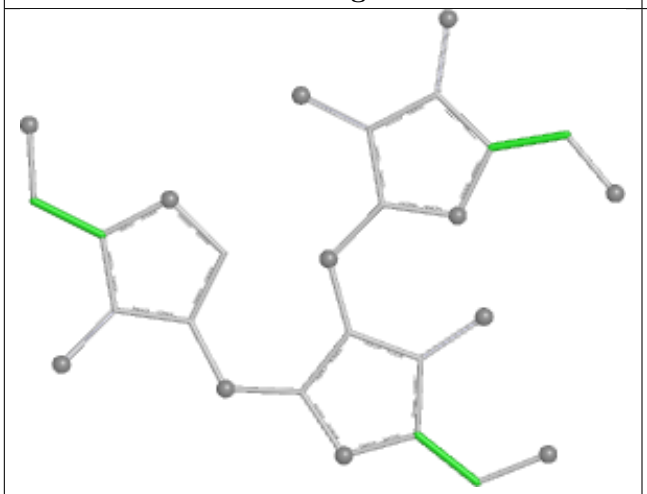


Bond angles



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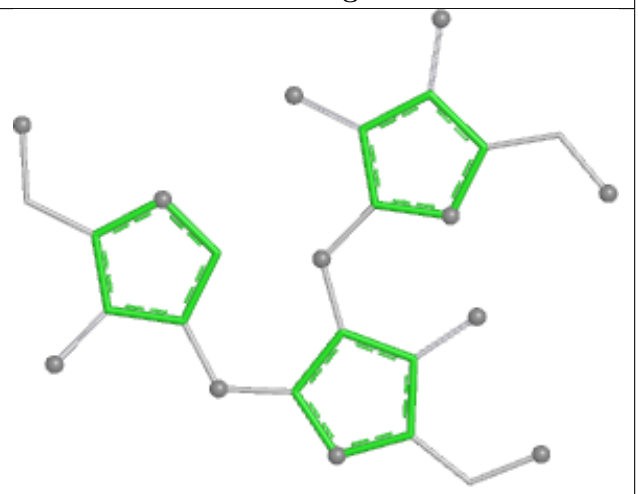
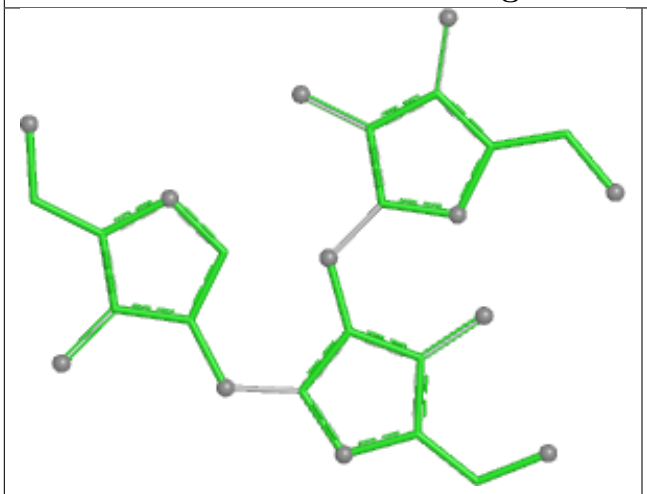


Rings

Oligosaccharide Chain t



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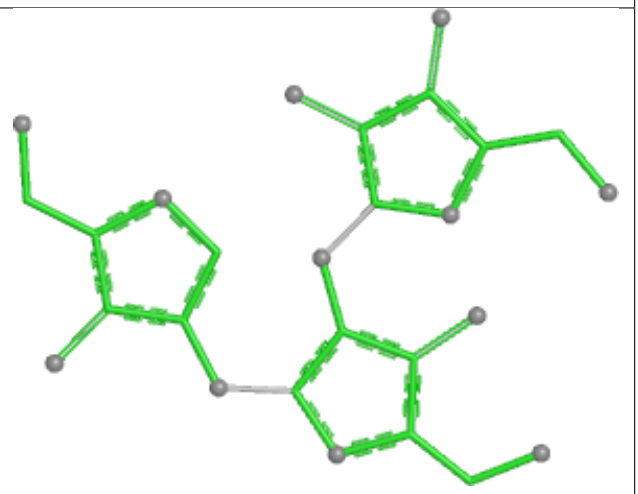
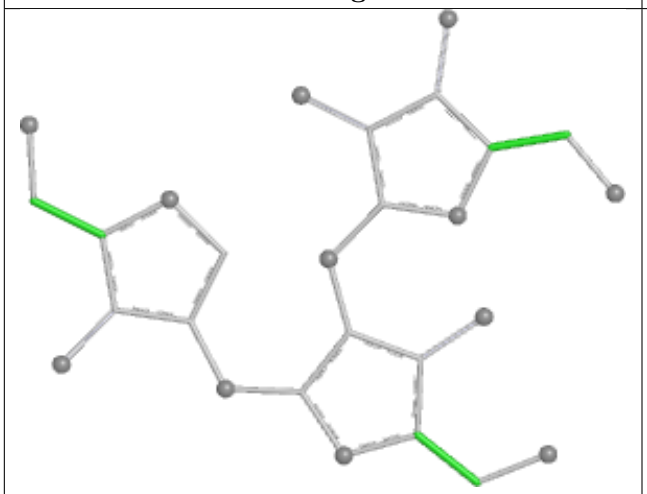


Bond angles



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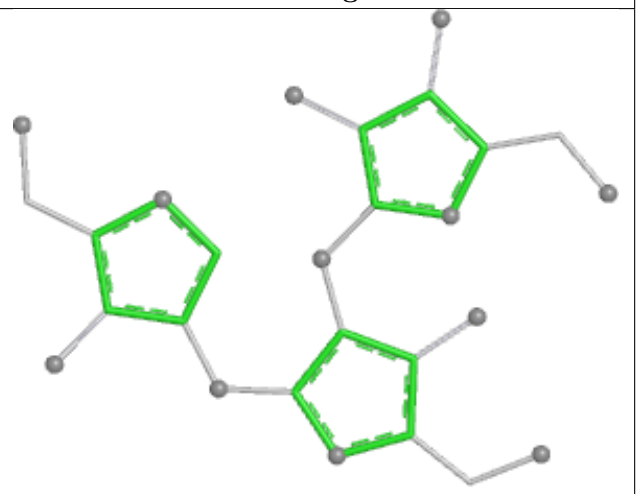
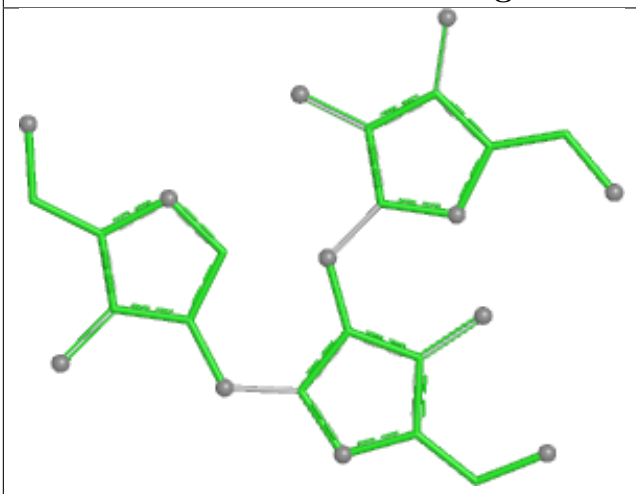
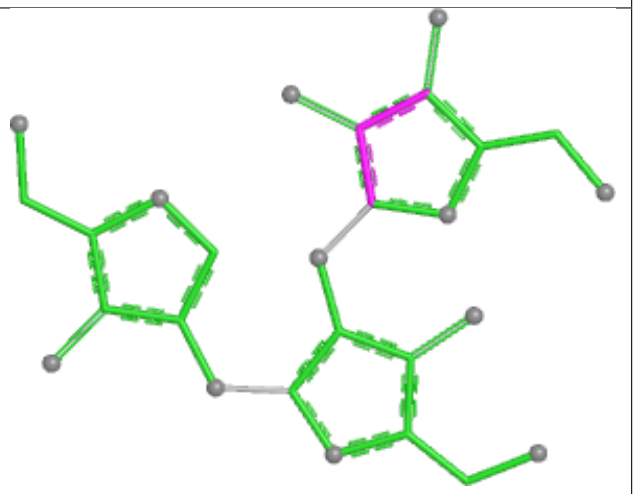
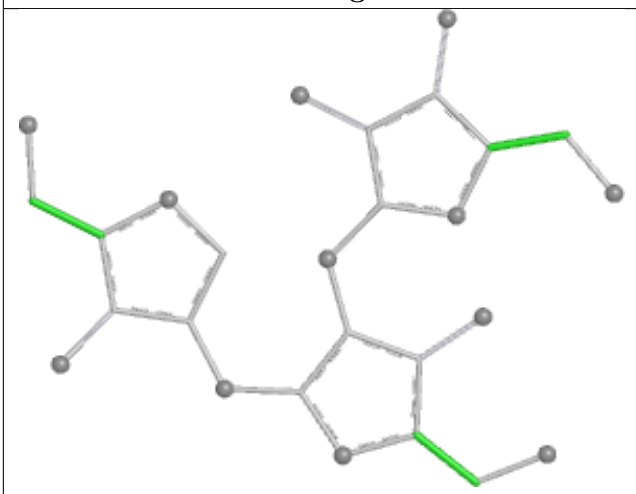
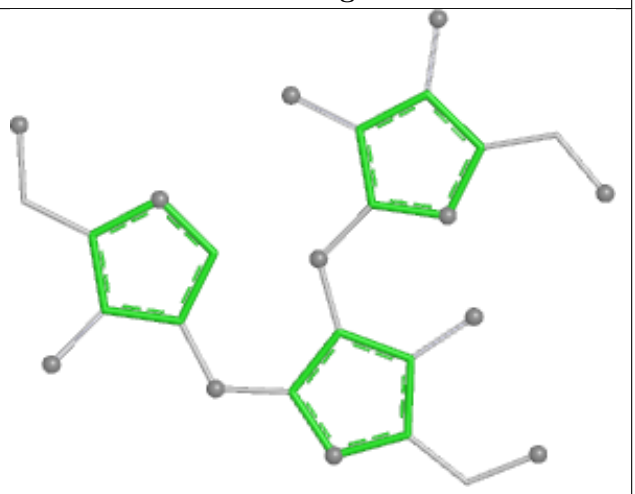
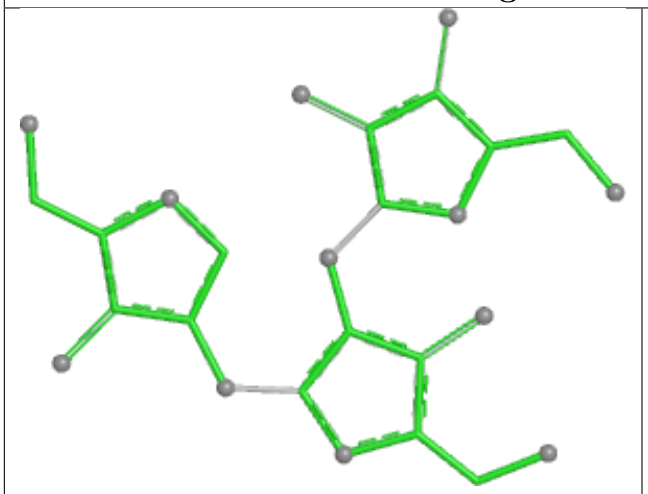


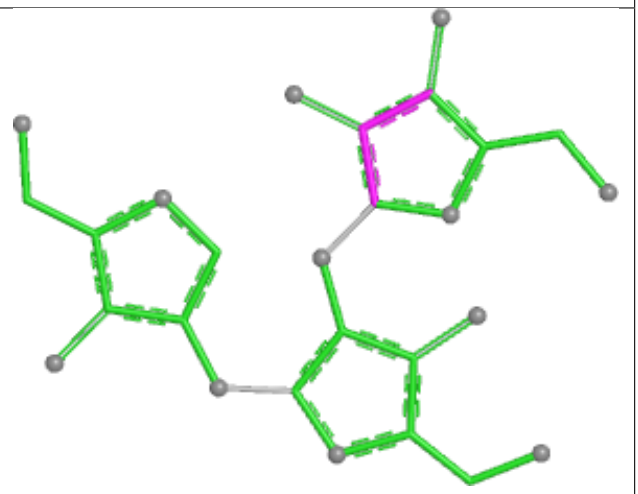
Rings

Oligosaccharide Chain w	
 Bond lengths	 Bond angles
 Torsions	 Rings

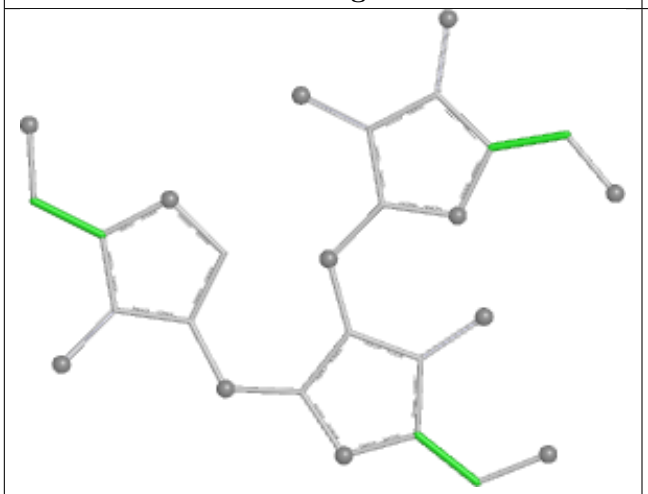
Oligosaccharide Chain x



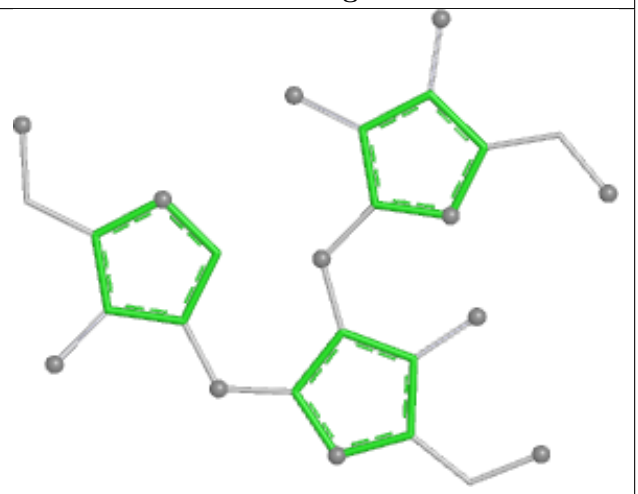
Bond lengths



Bond angles

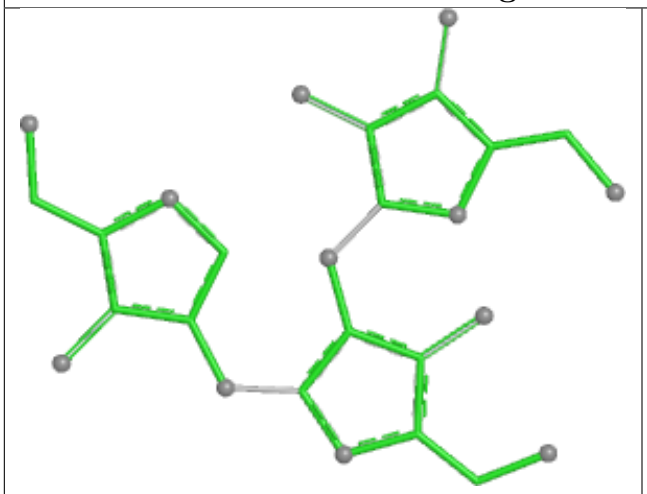


Torsions



Rings

Oligosaccharide Chain y



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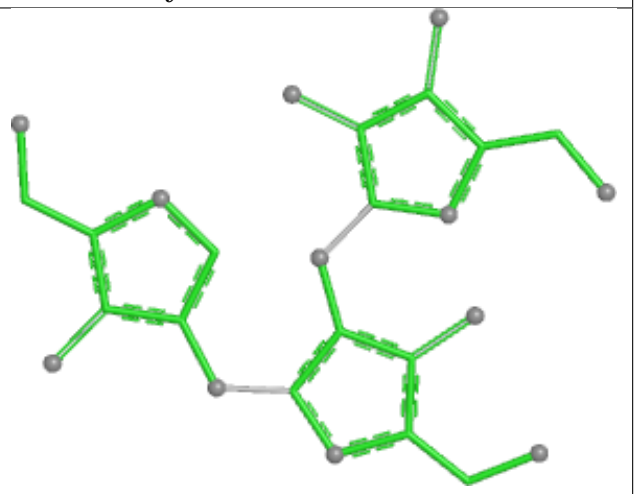
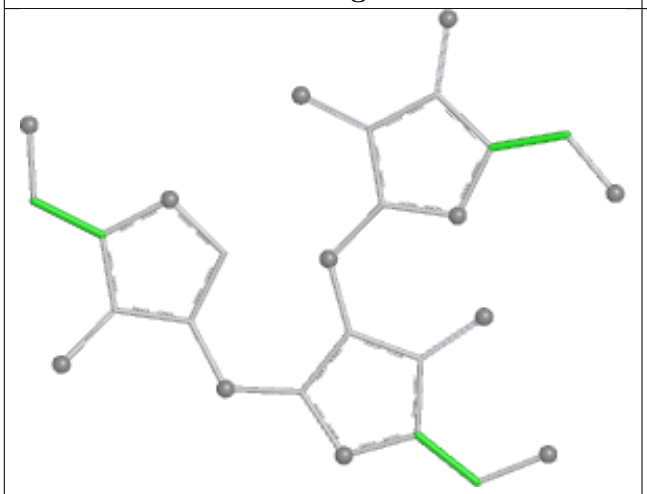
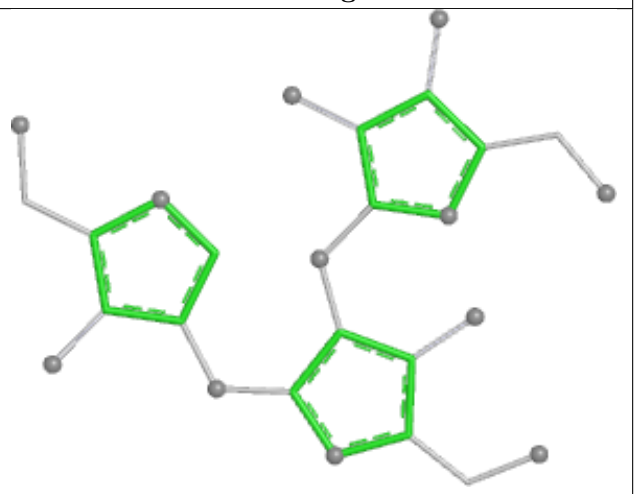


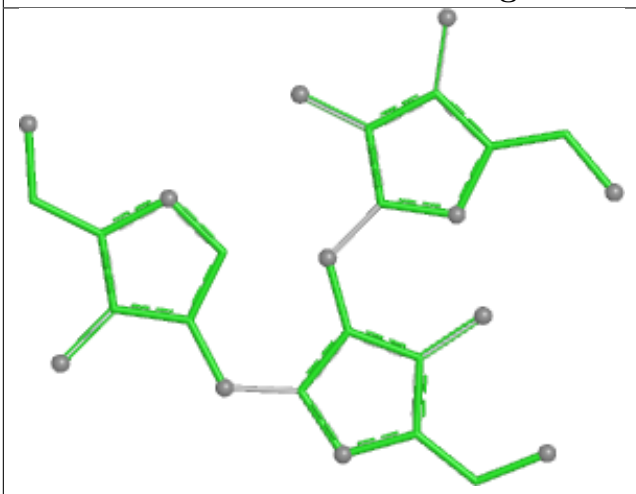
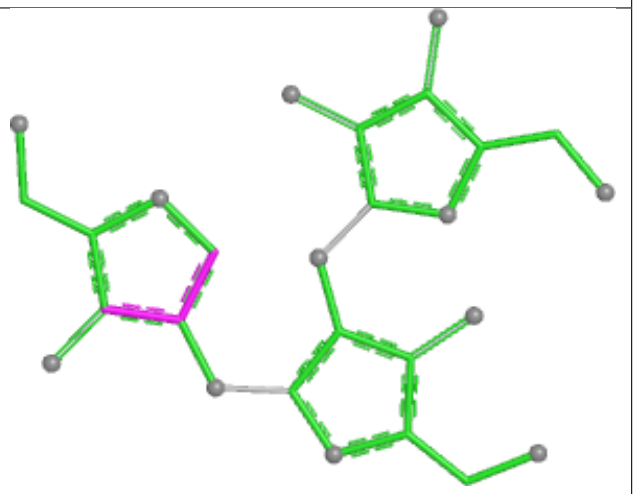
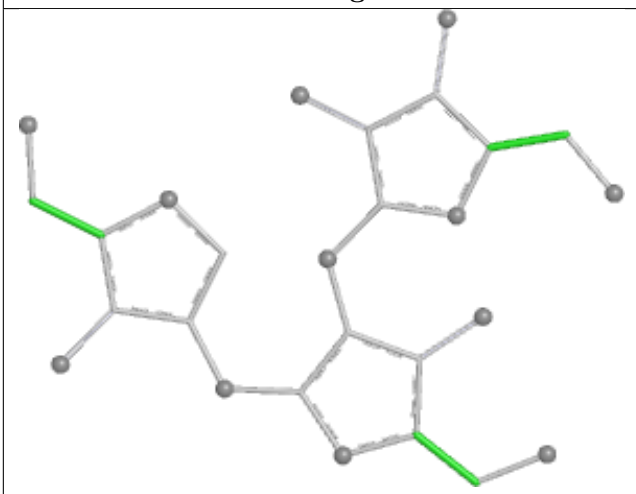
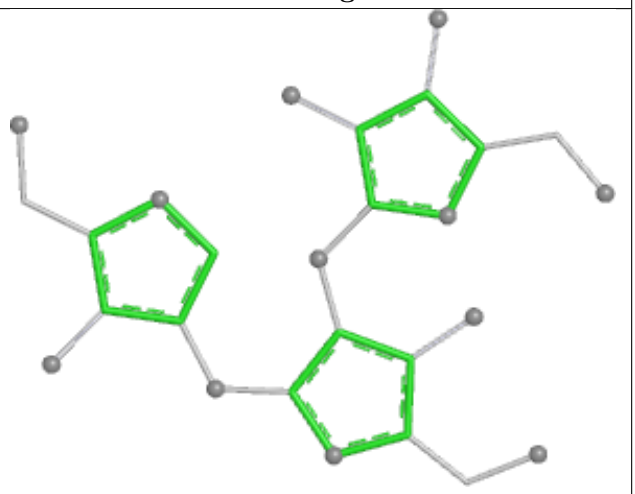
Bond angles



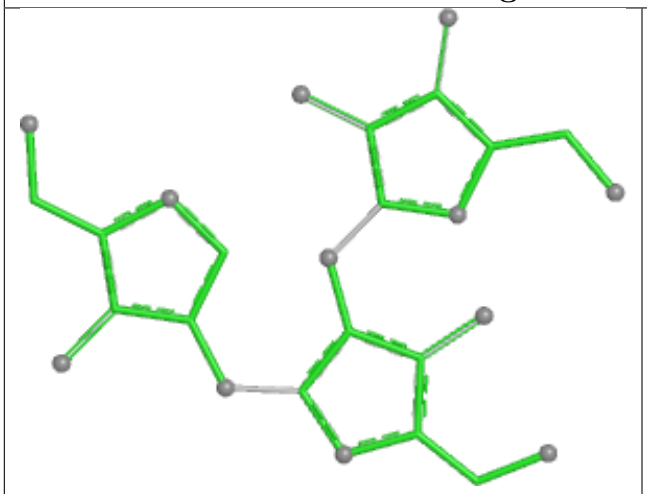
Torsions



Rings

Oligosaccharide Chain z	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 0



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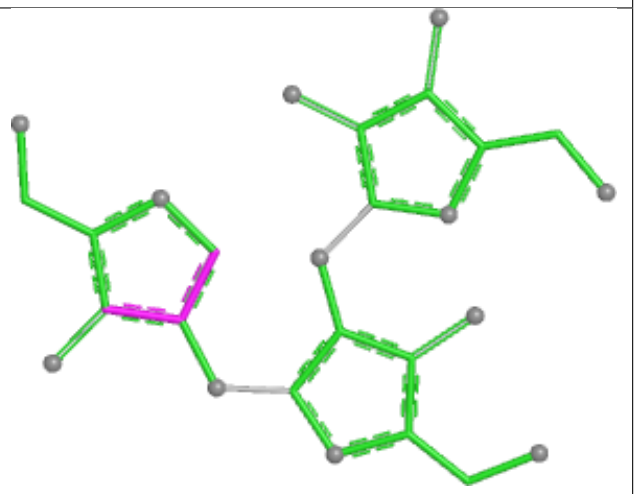

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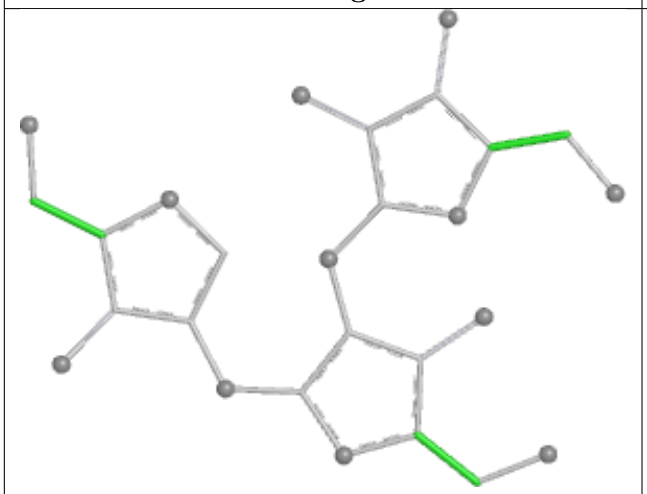

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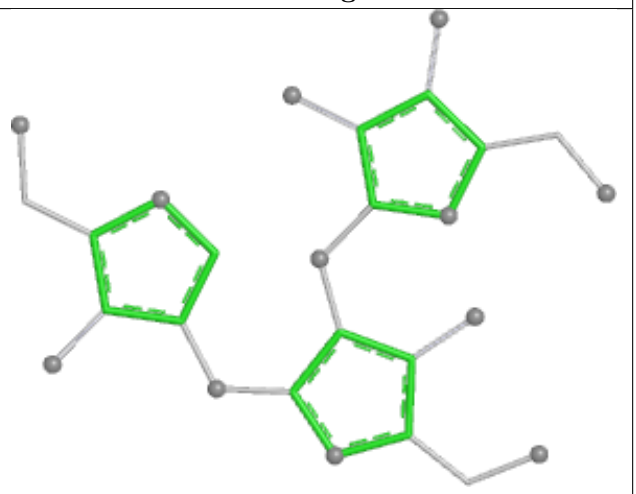
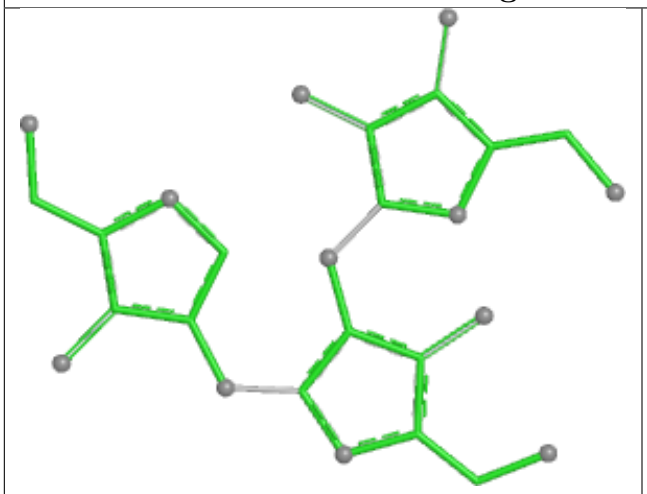


Rings

Oligosaccharide Chain 1



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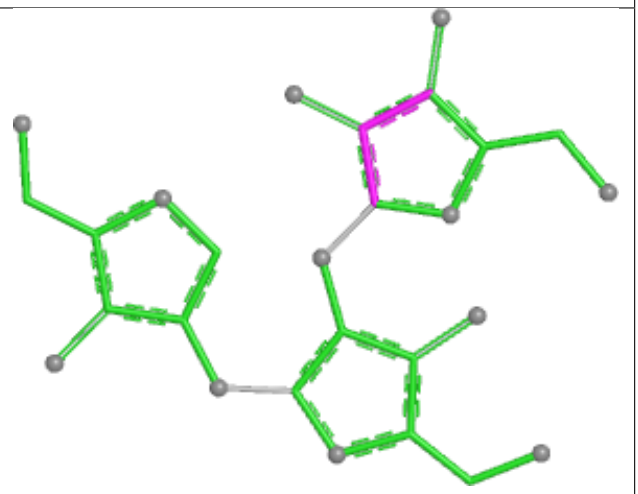
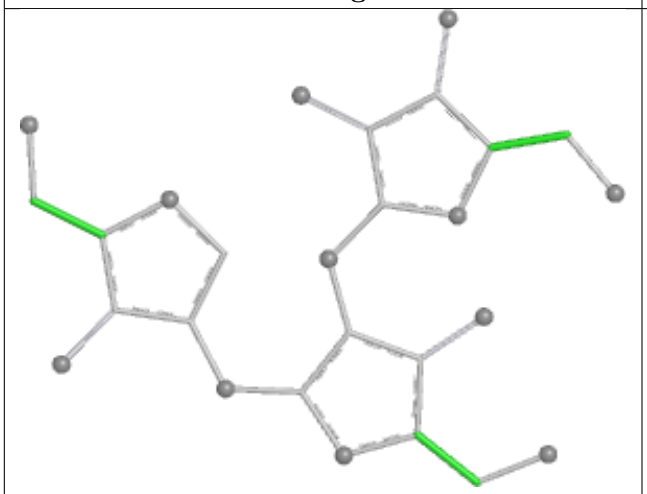


Bond angles



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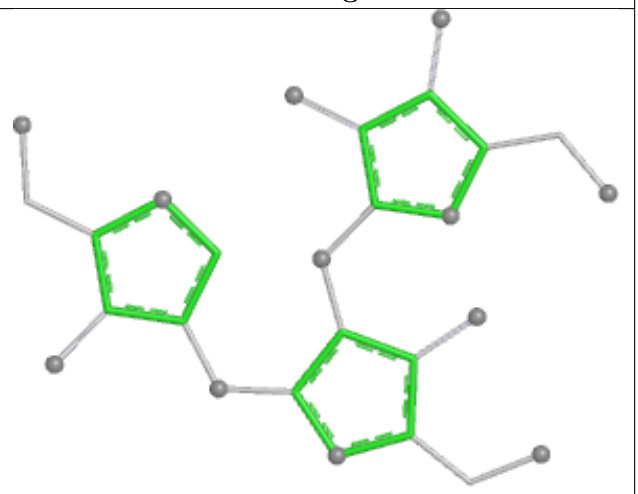
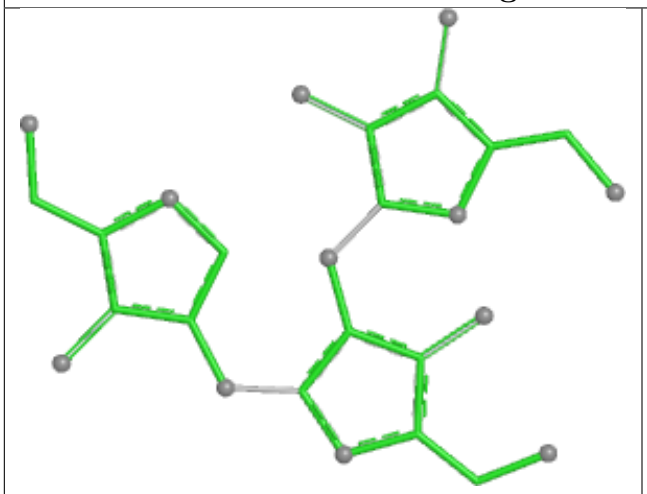


Rings

Oligosaccharide Chain 2



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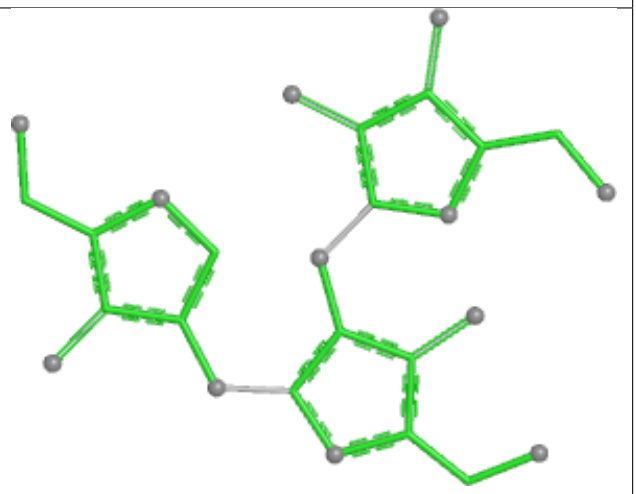
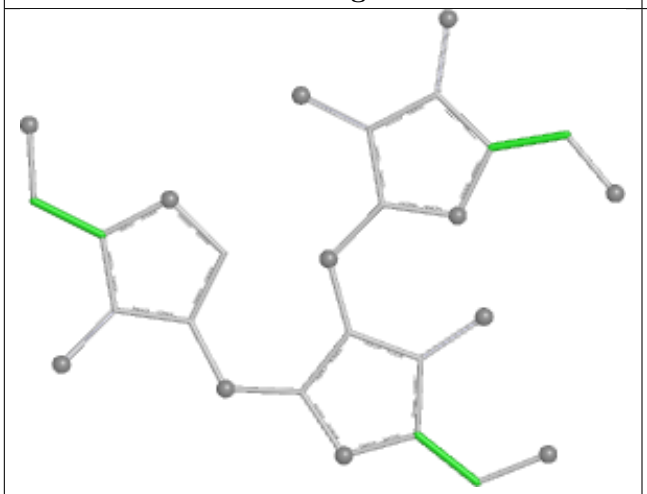
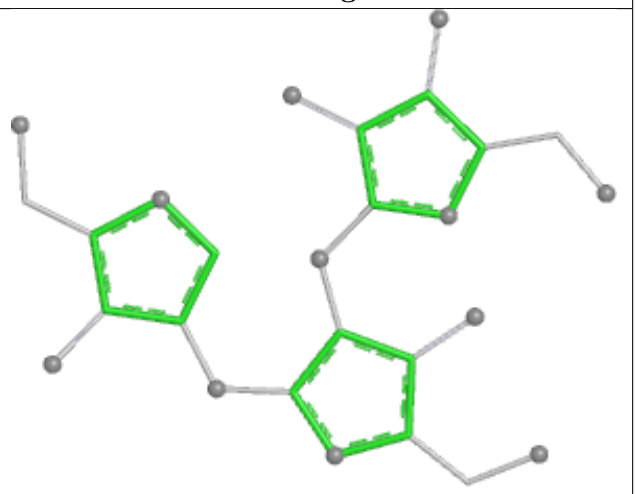


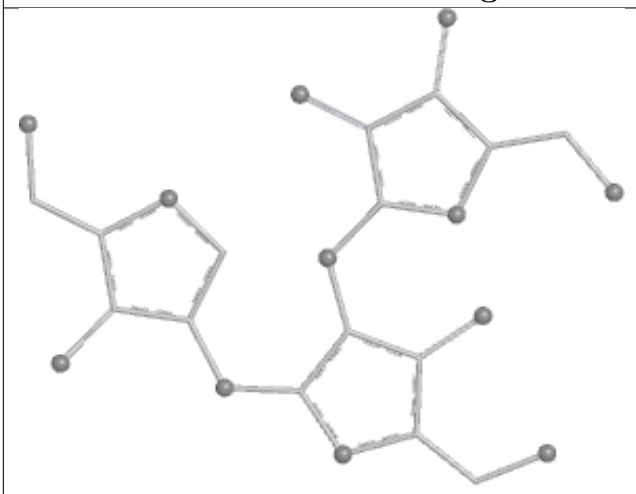
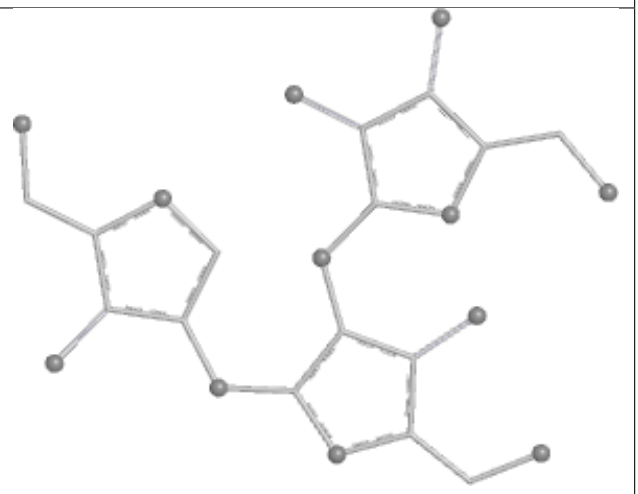
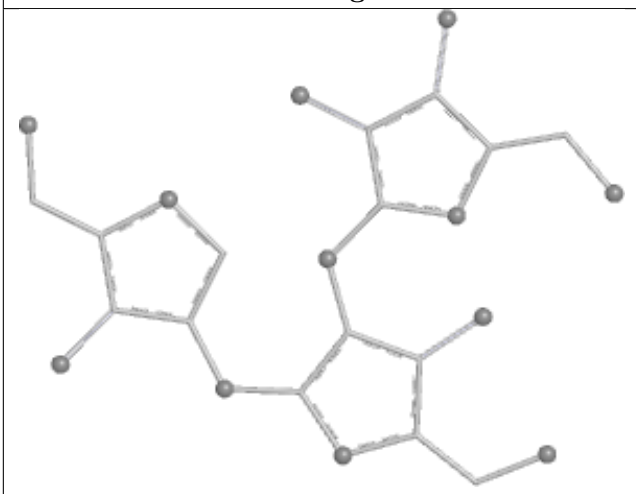
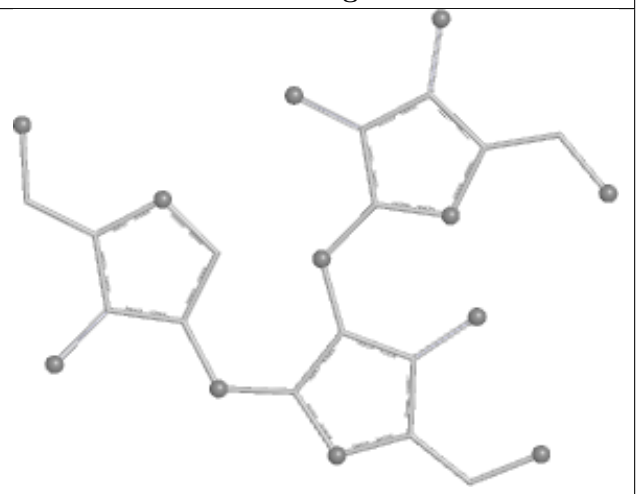
Bond angles

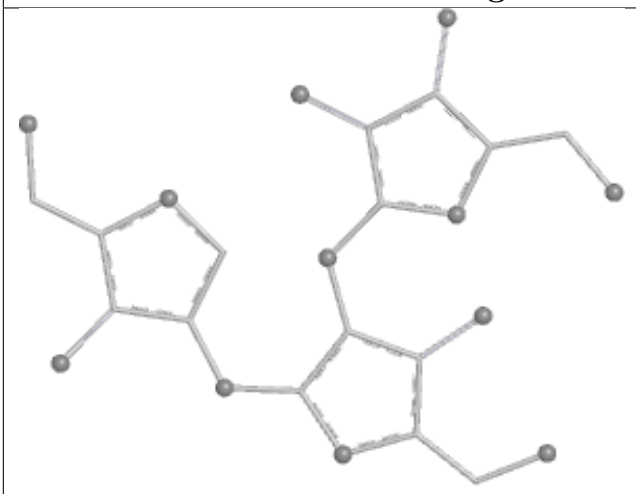
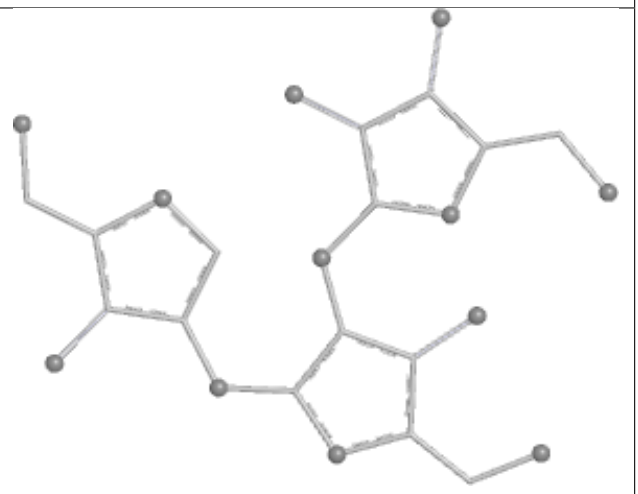
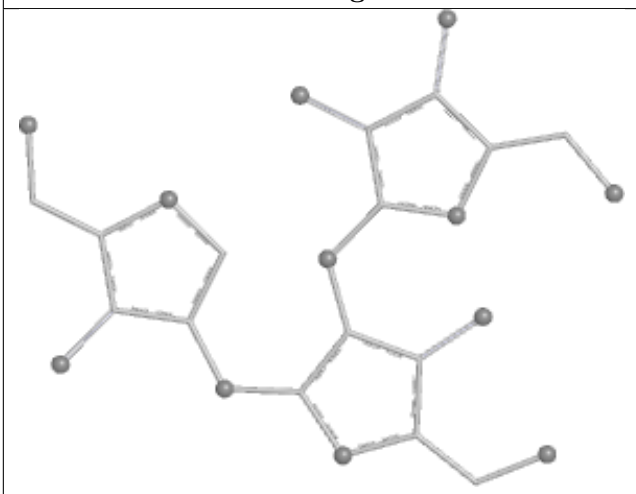
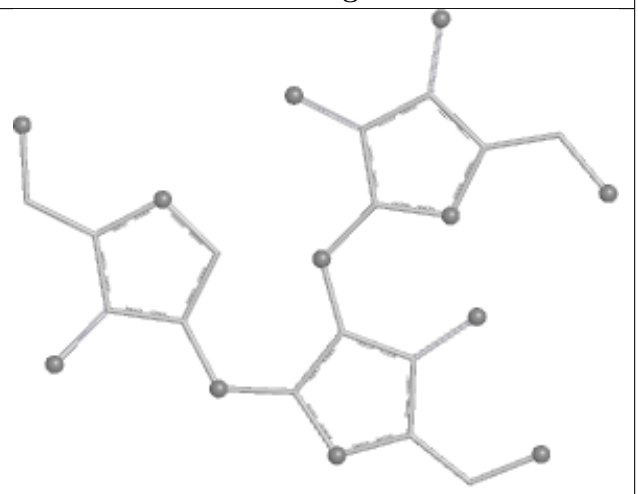


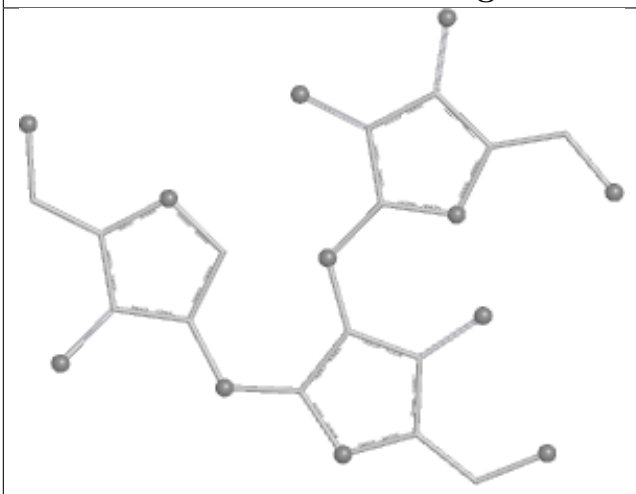
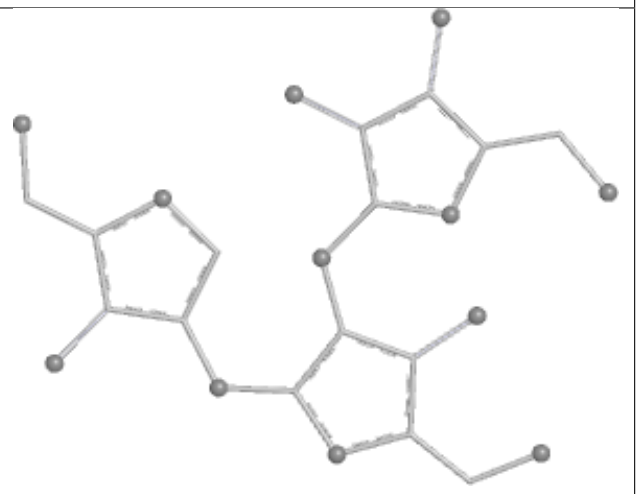
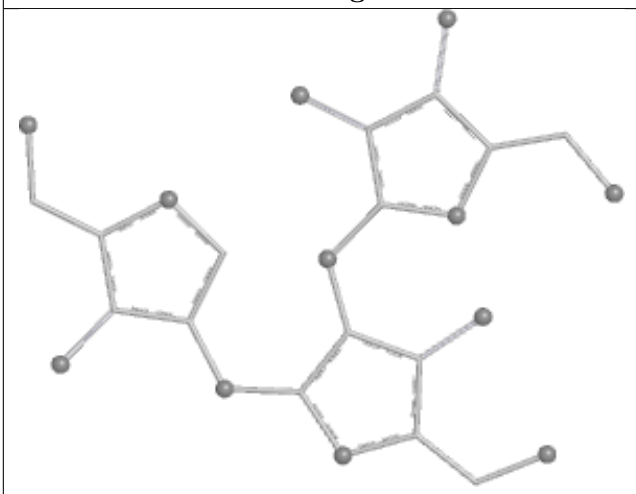
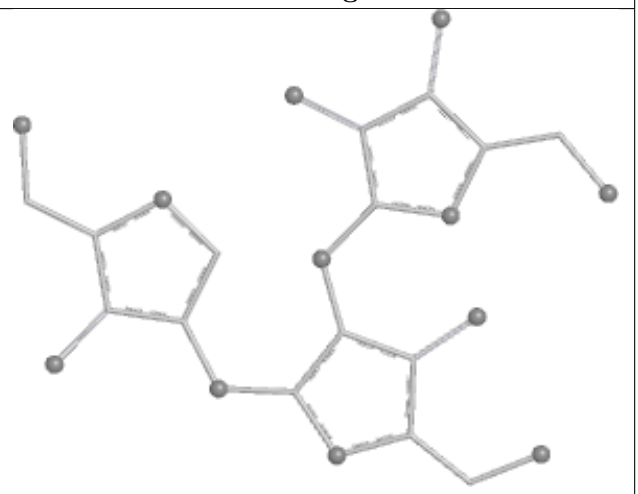
Torsions

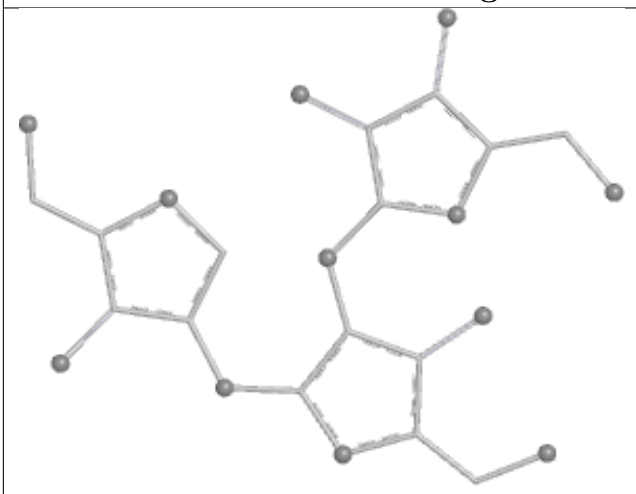
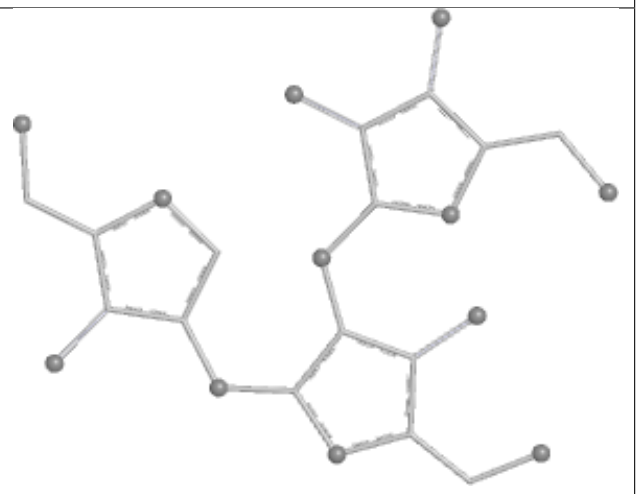
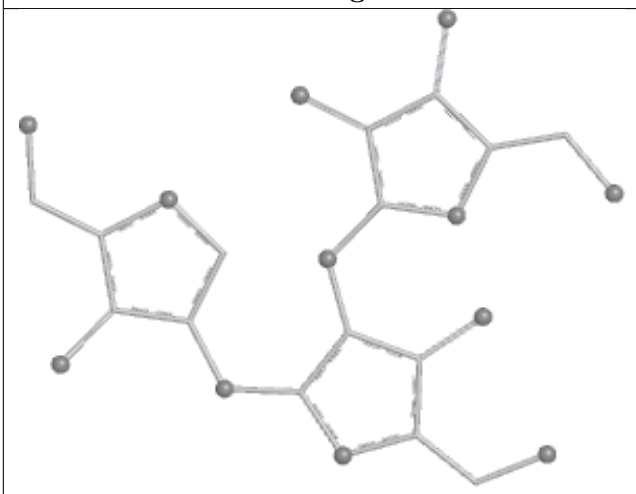
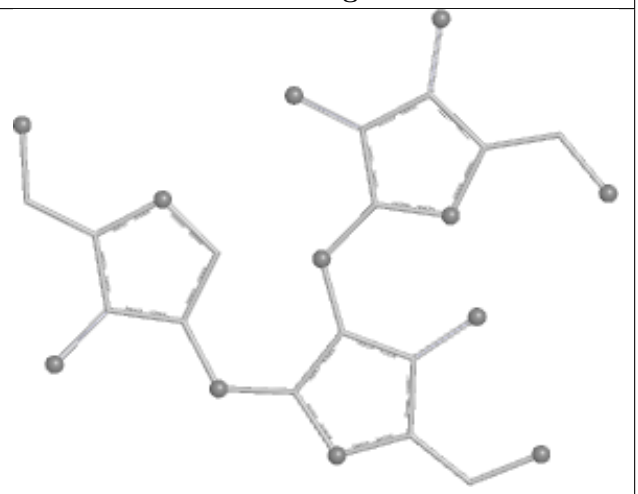


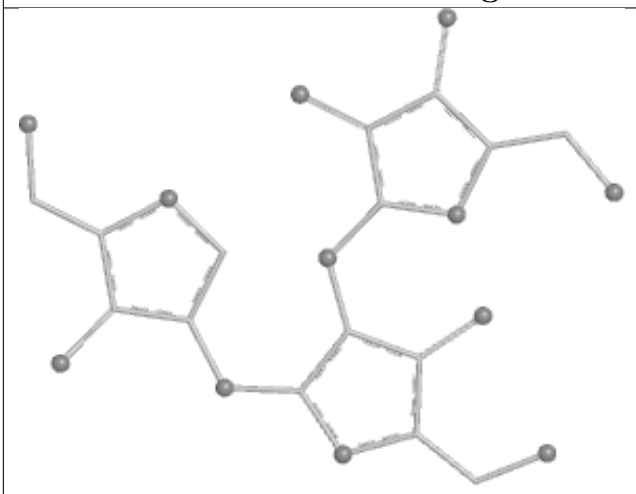
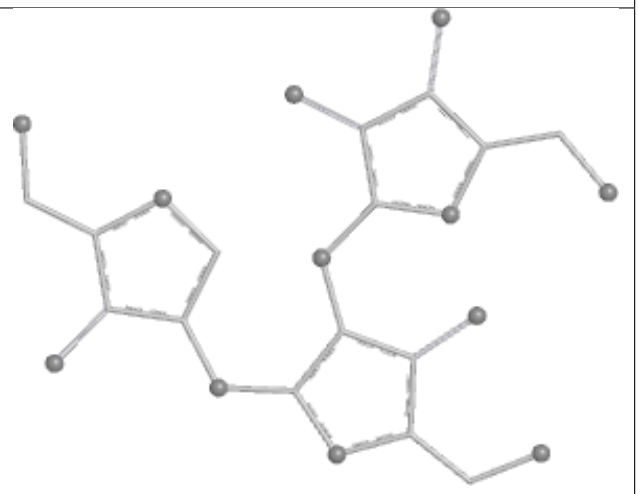
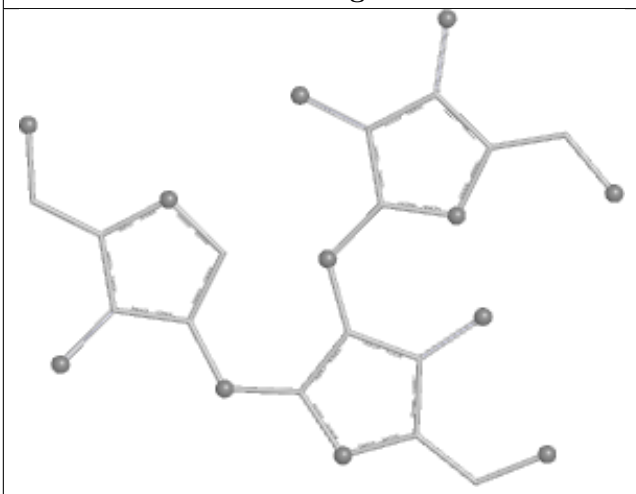
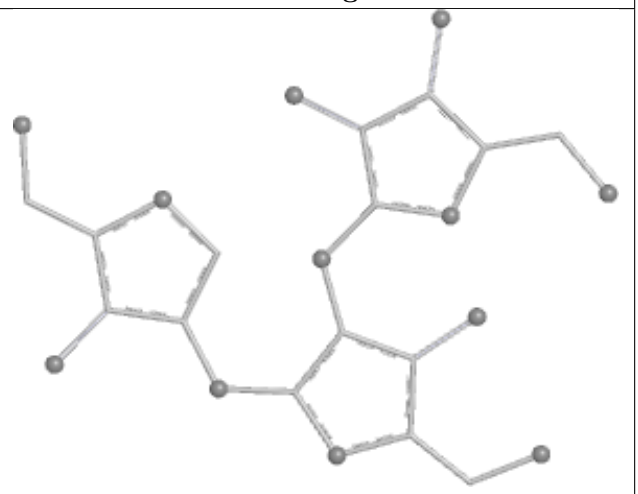
Rings

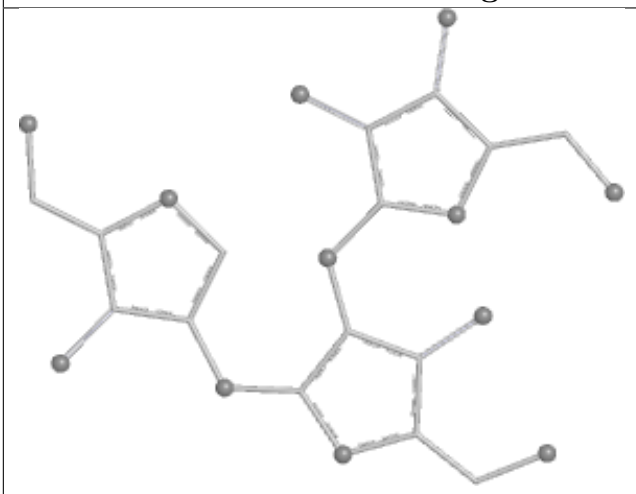
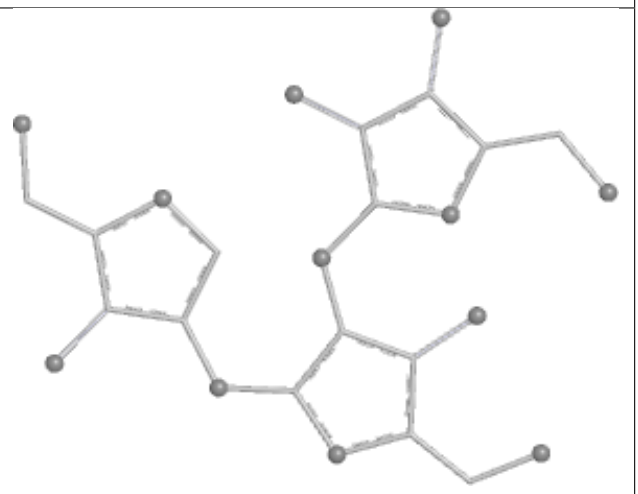
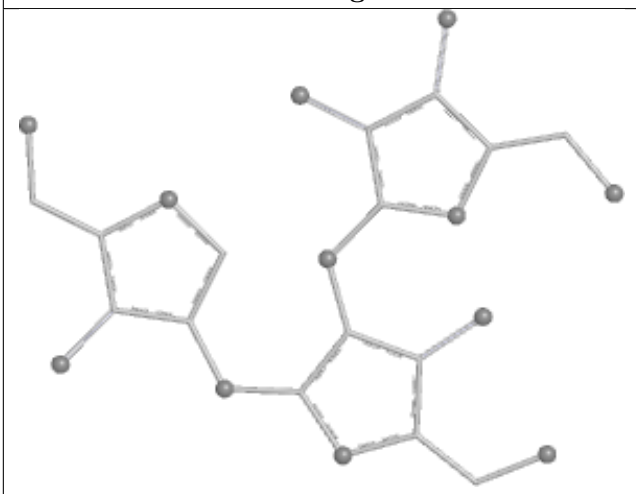
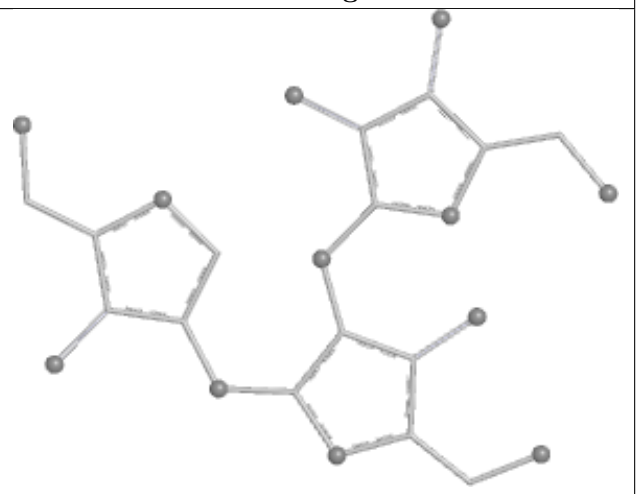
Oligosaccharide Chain HA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

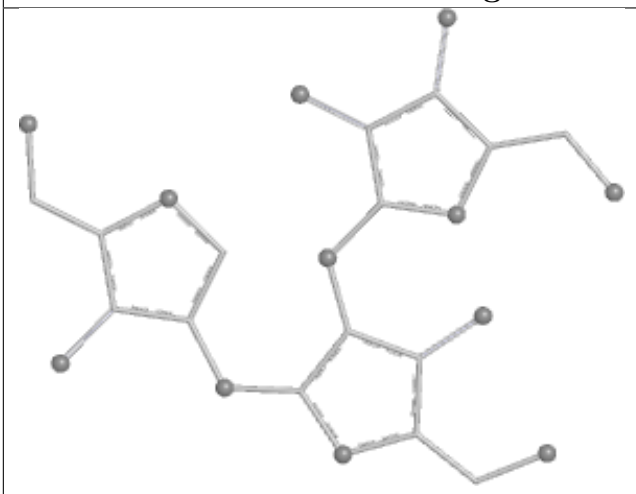
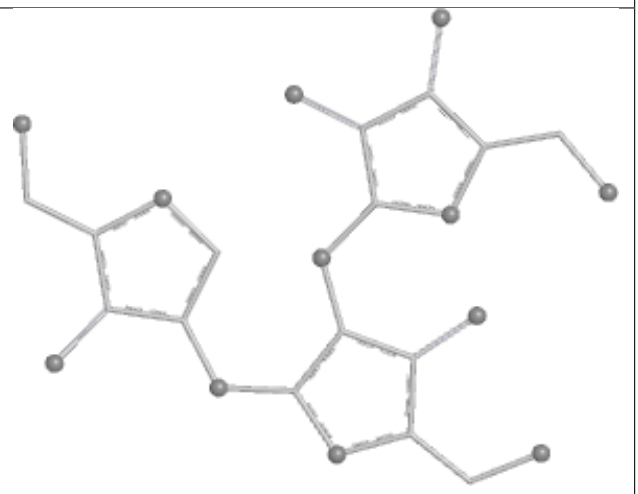
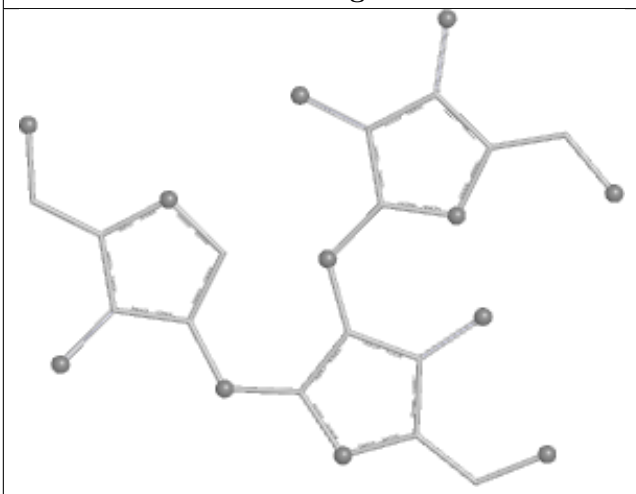
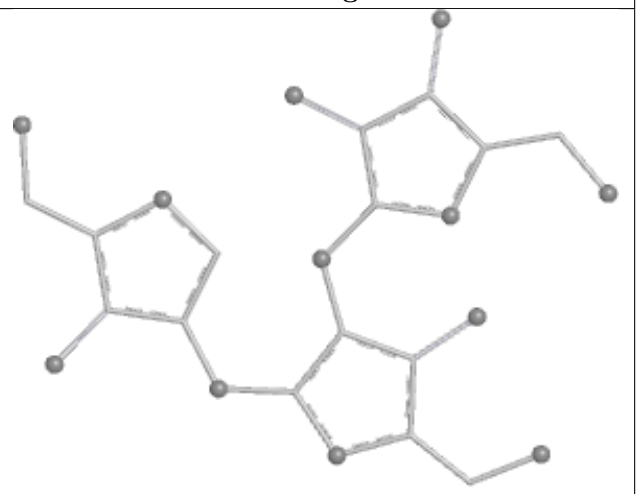
Oligosaccharide Chain IA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

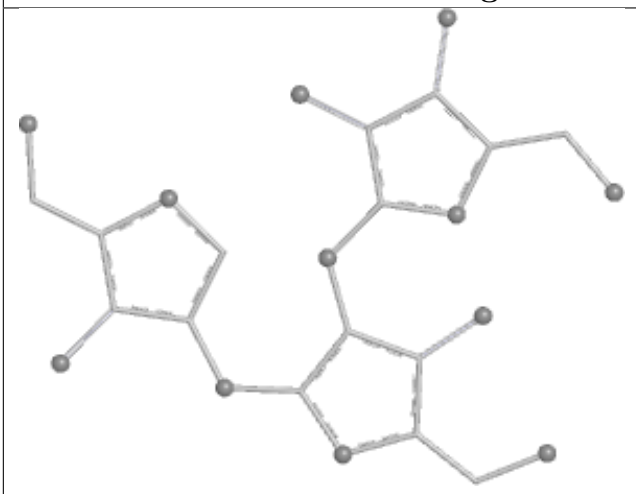
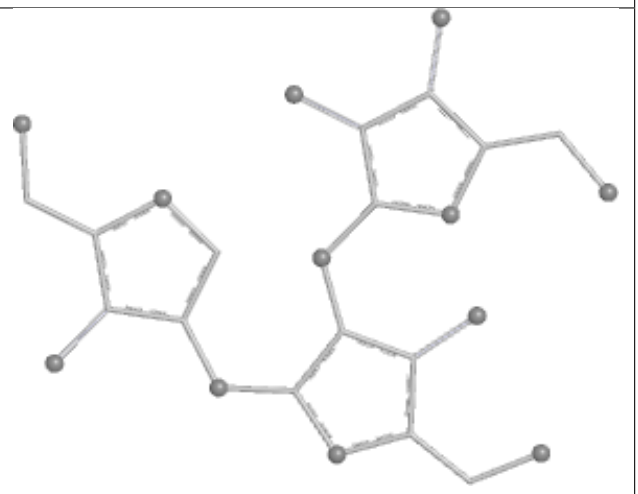
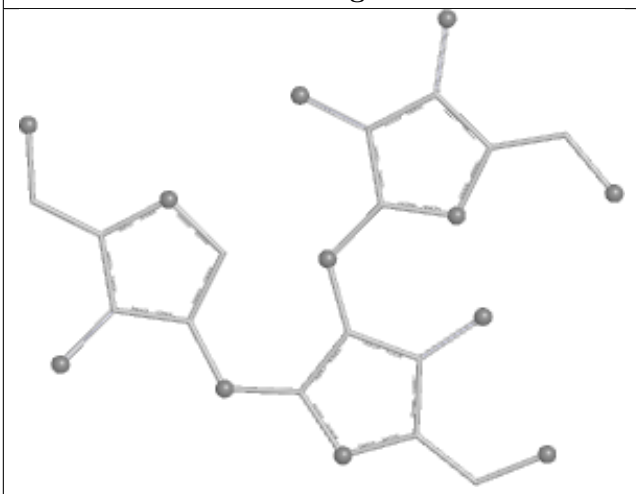
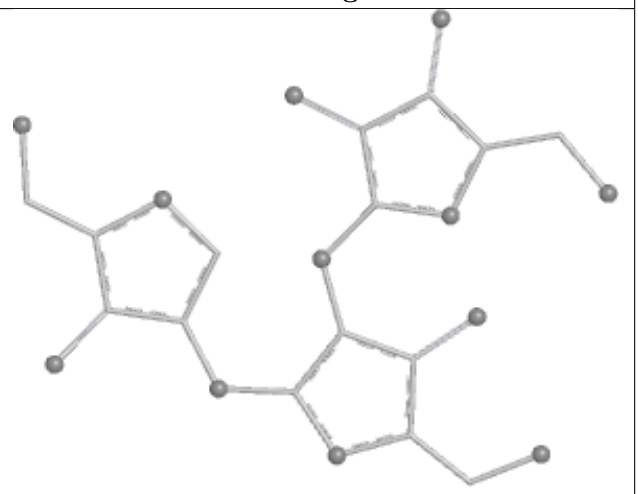
Oligosaccharide Chain MA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

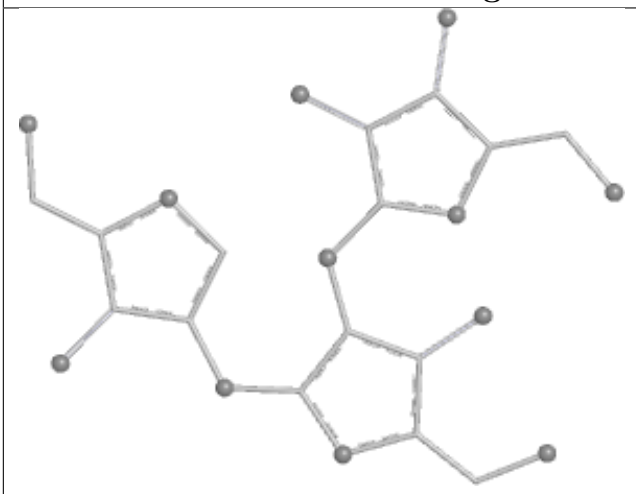
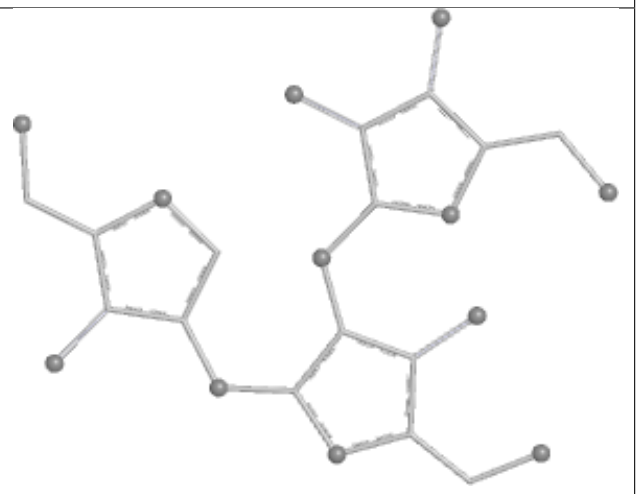
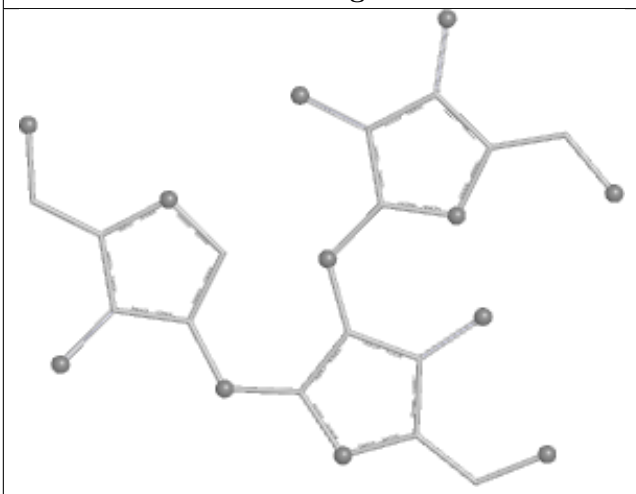
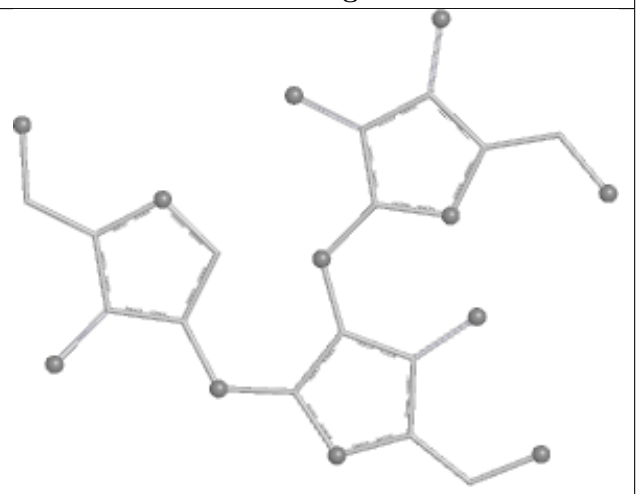
Oligosaccharide Chain NA	
 Bond lengths	 Bond angles
 Torsions	 Rings

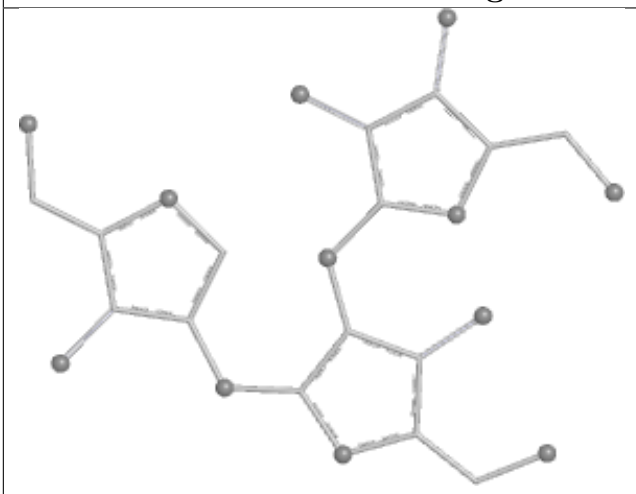
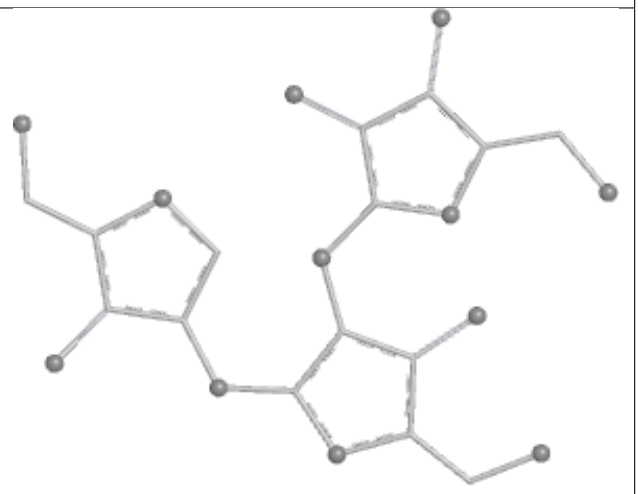
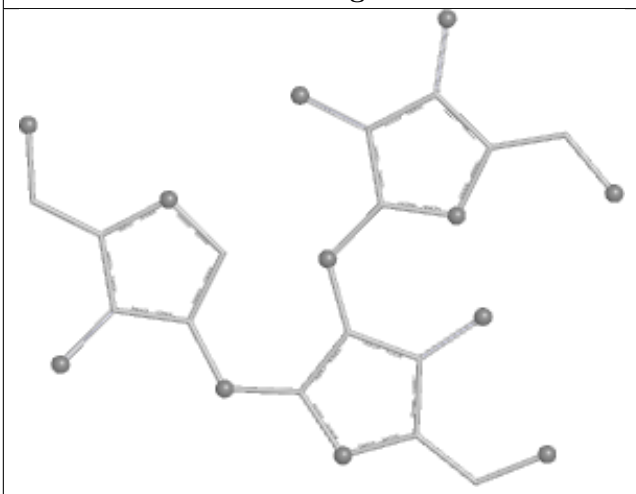
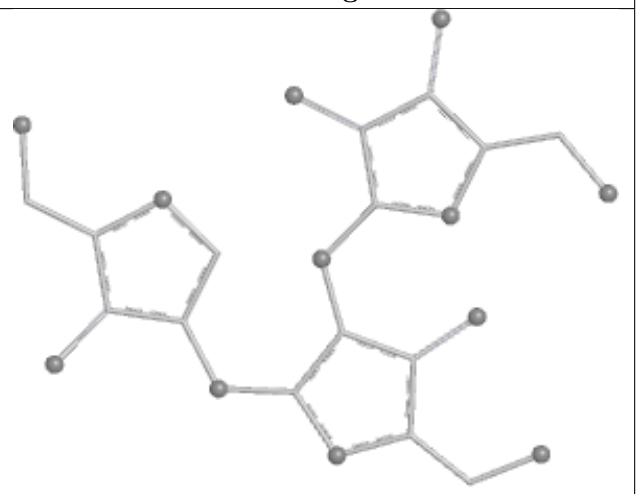
Oligosaccharide Chain OA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain RA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain TA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain XA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain ZA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain cA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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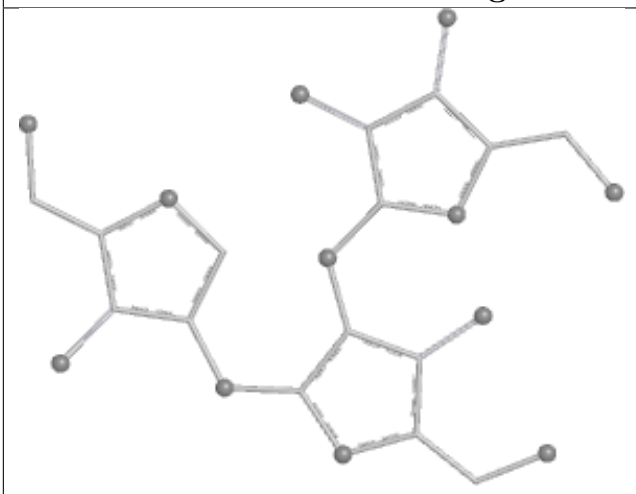
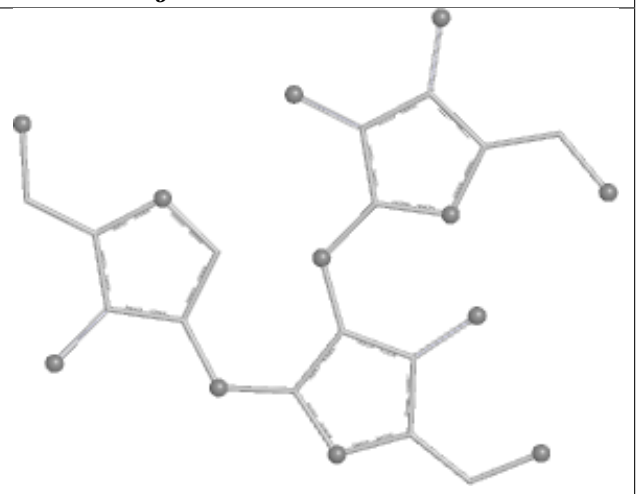
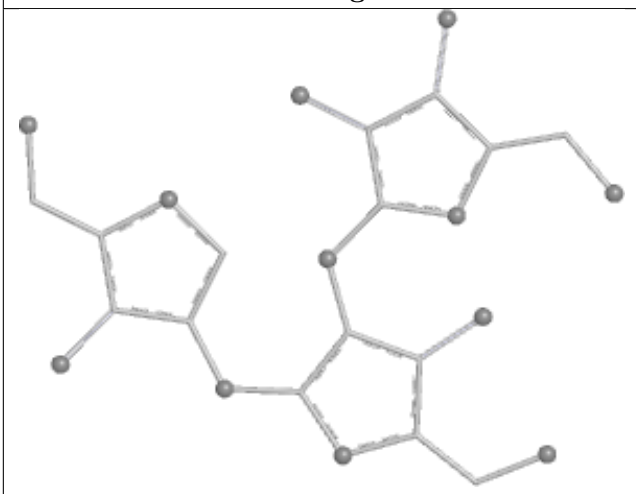
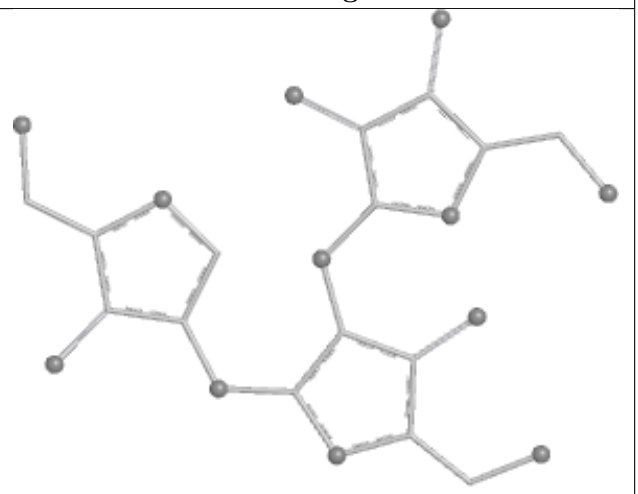
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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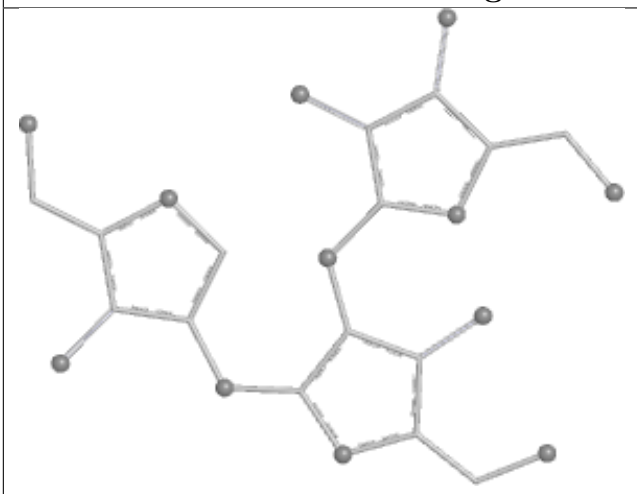
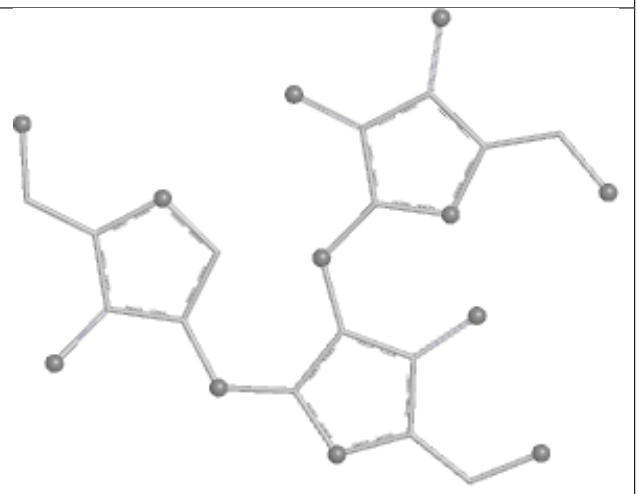
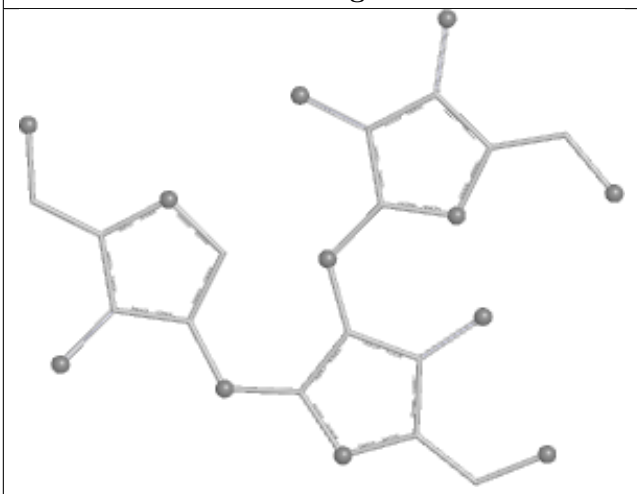
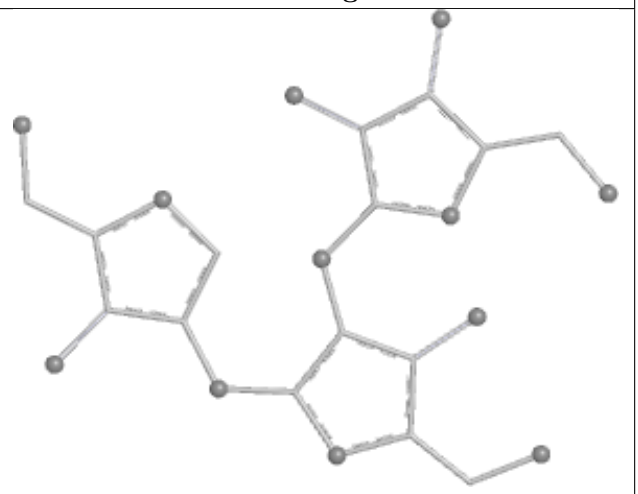
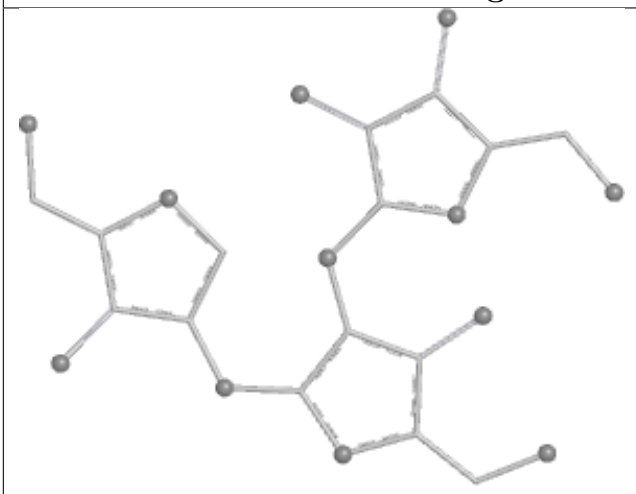
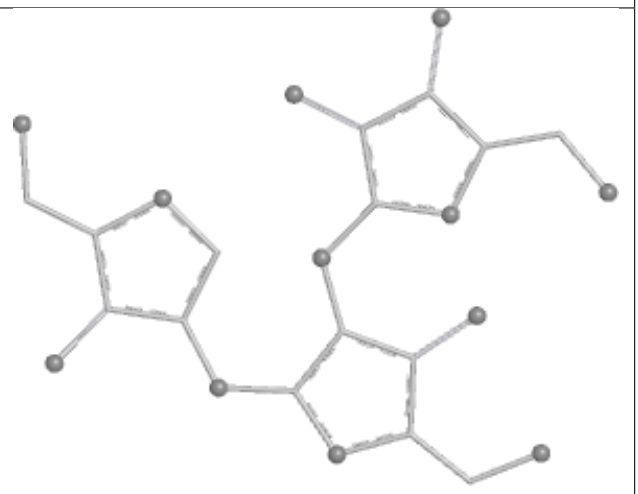
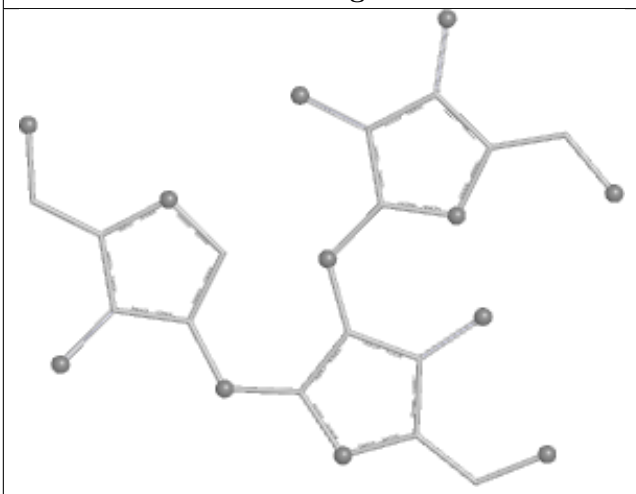
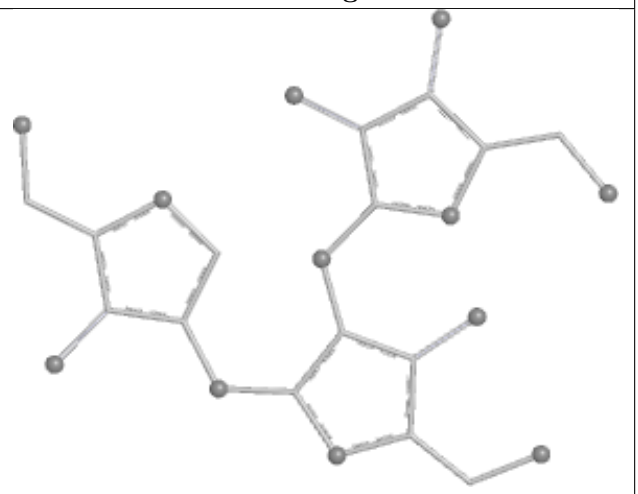
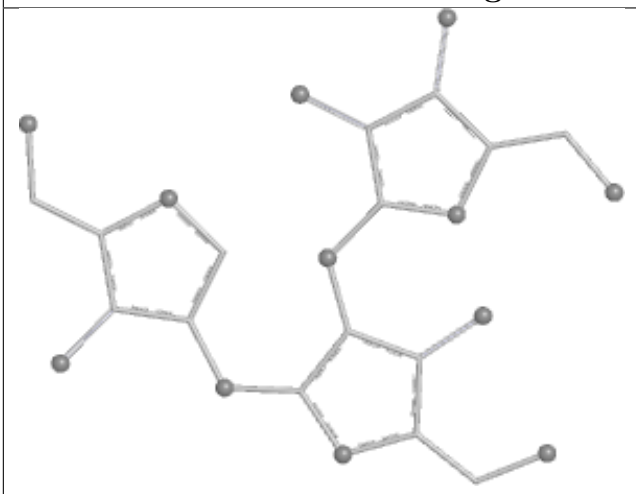
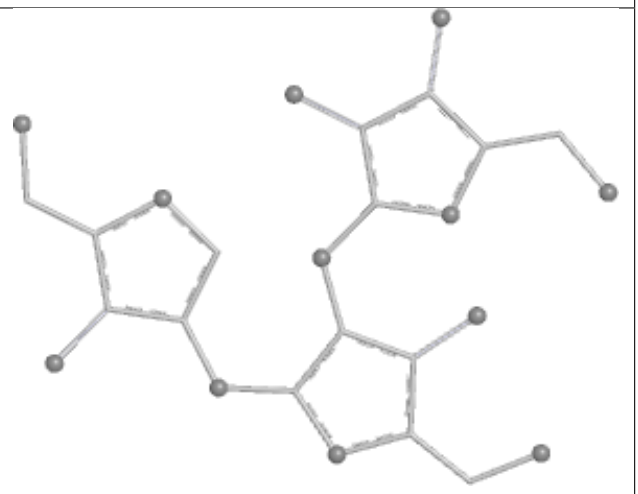
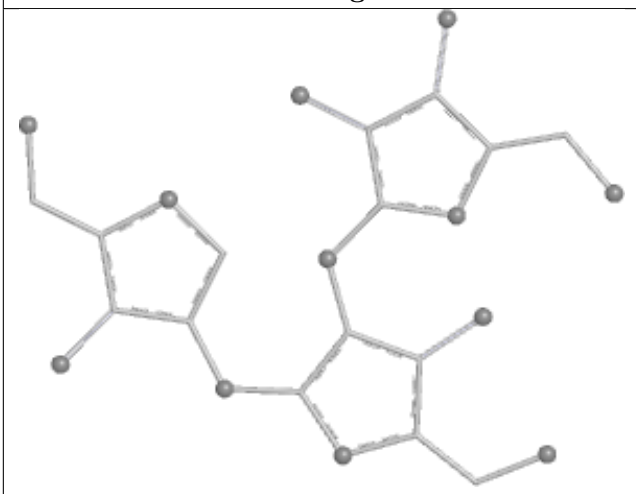
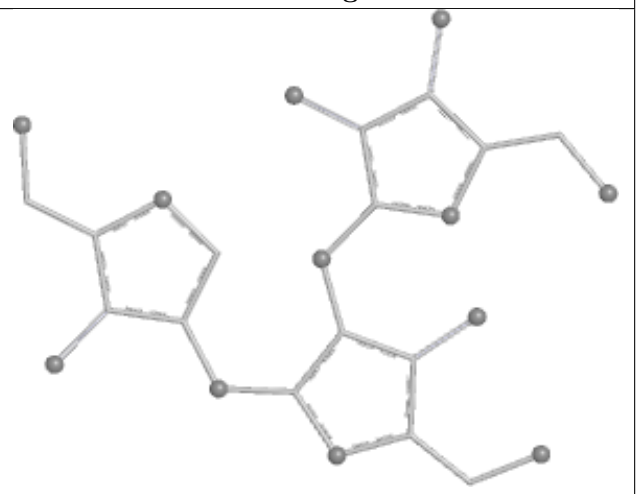
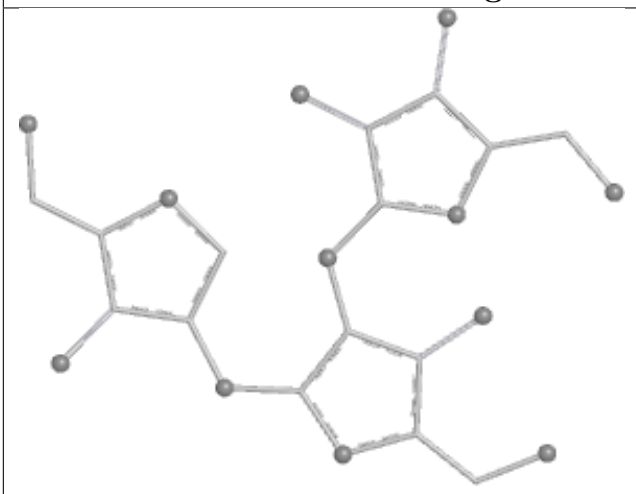
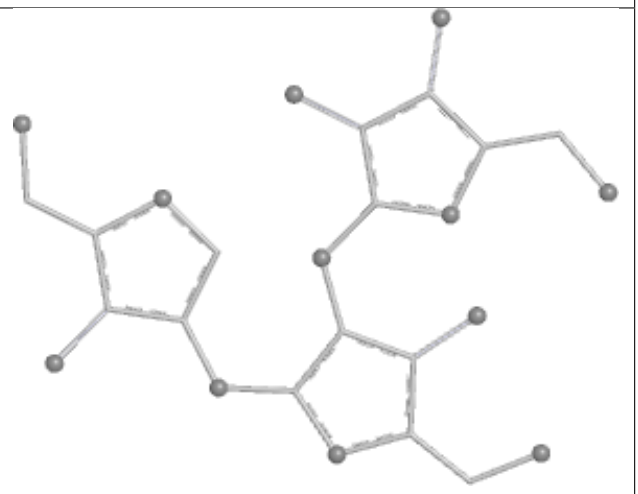
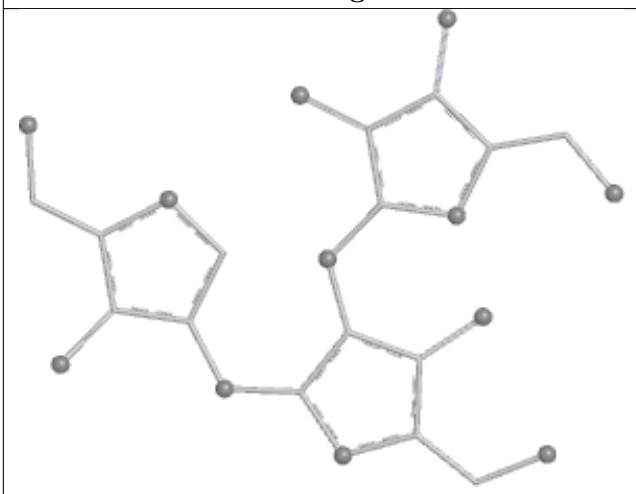
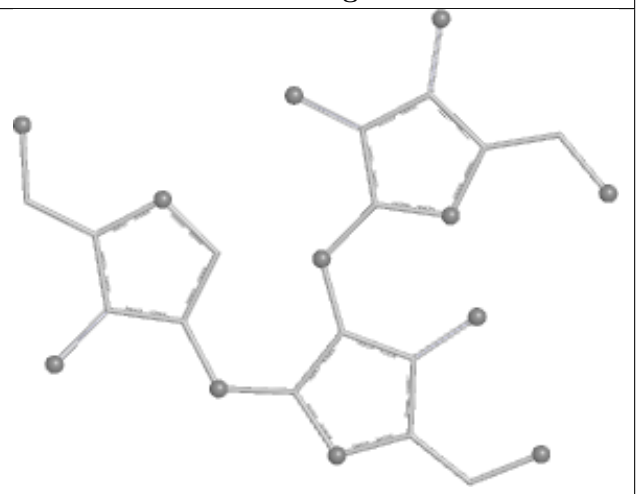
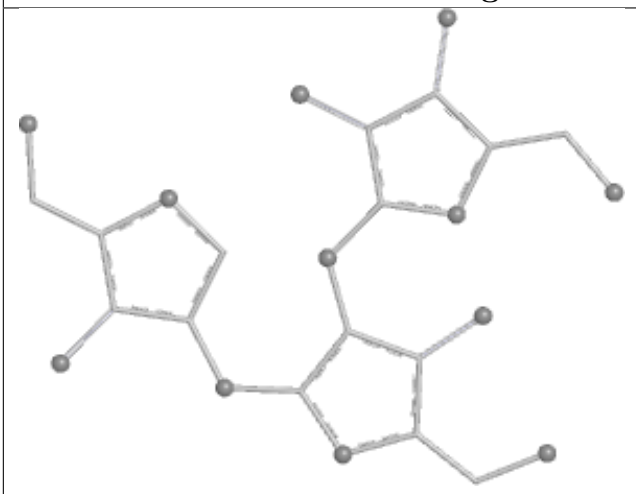
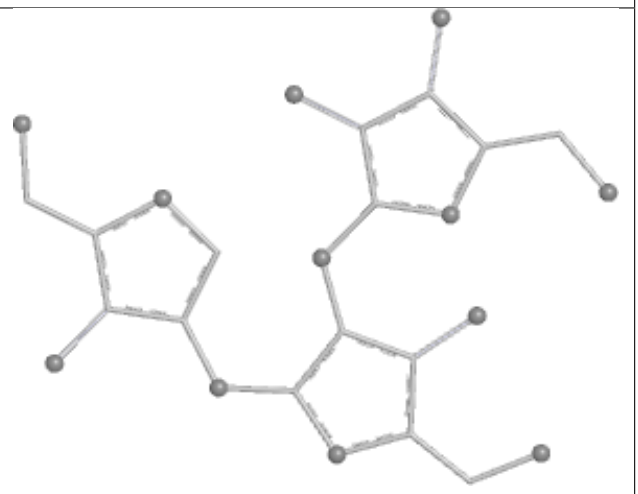
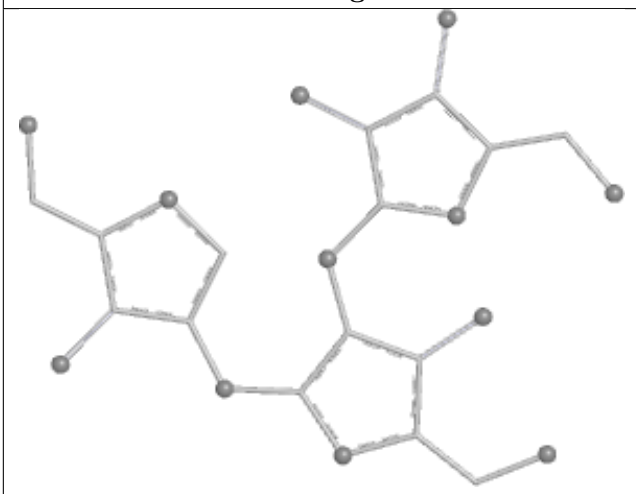
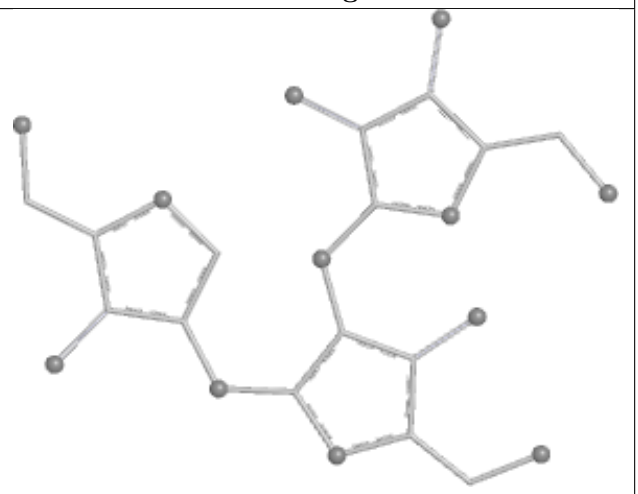
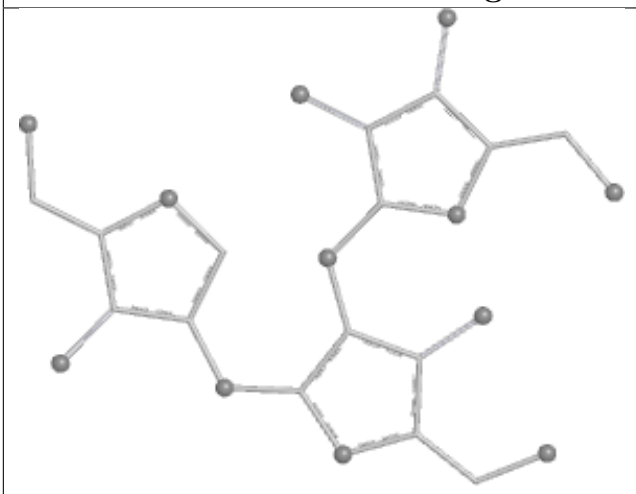
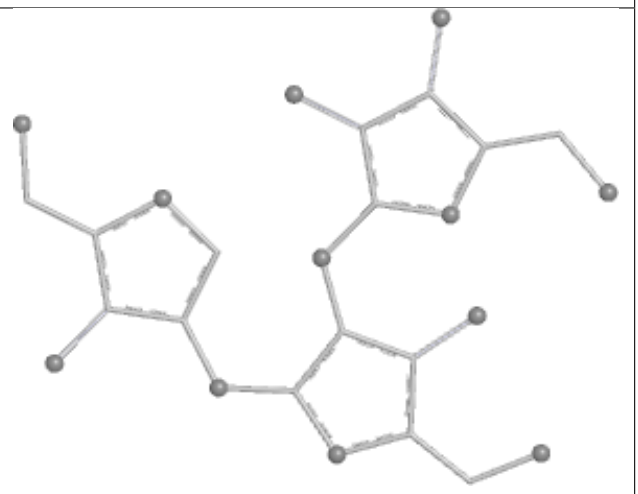
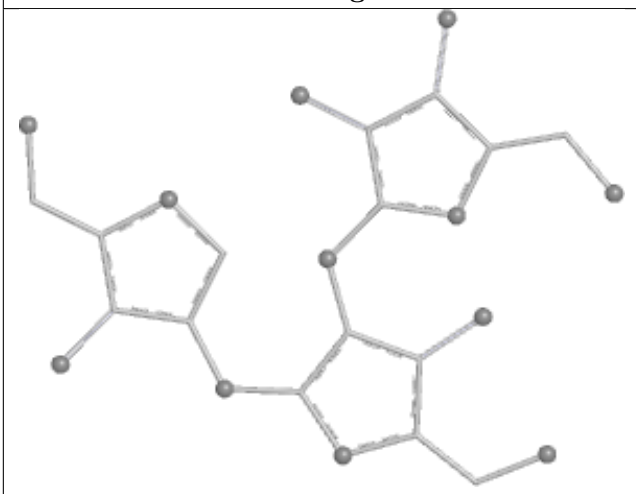
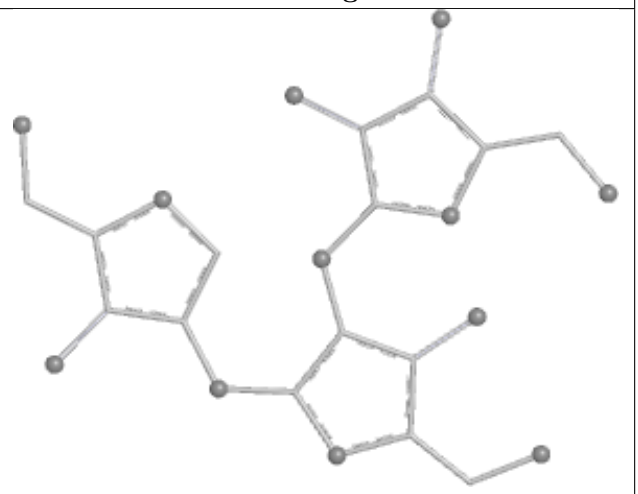
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

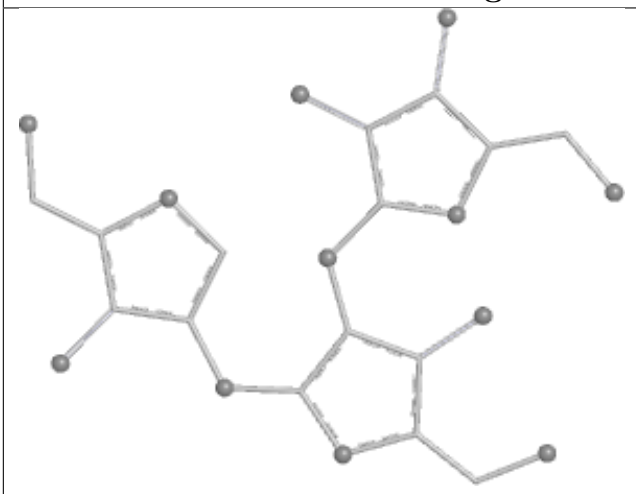
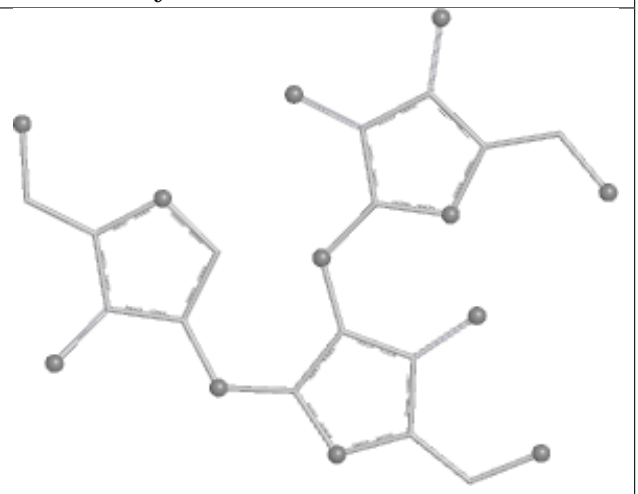
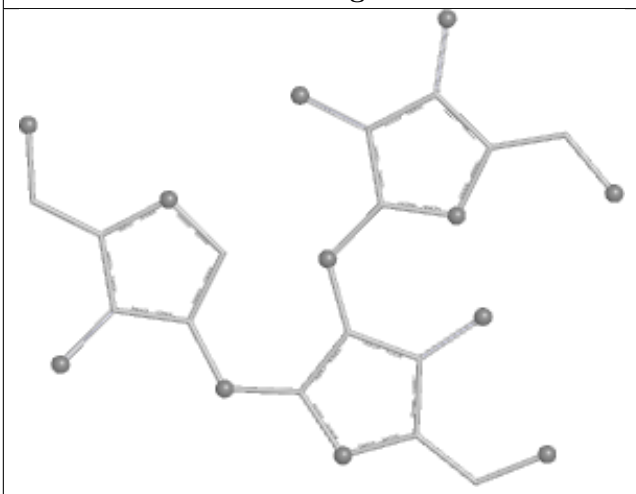
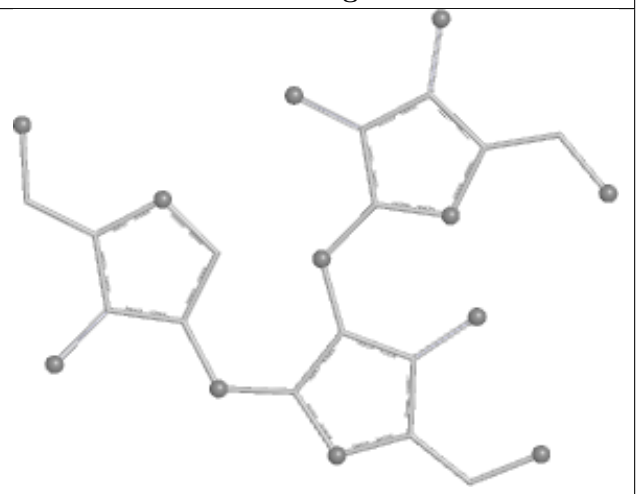
Oligosaccharide Chain rA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain uA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain vA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain wA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain xA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain yA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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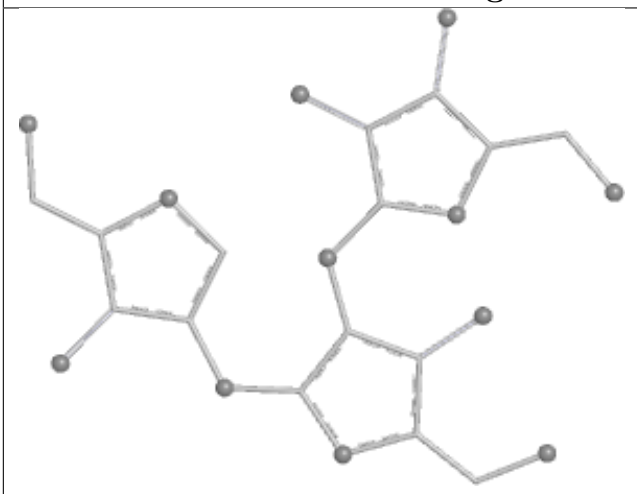
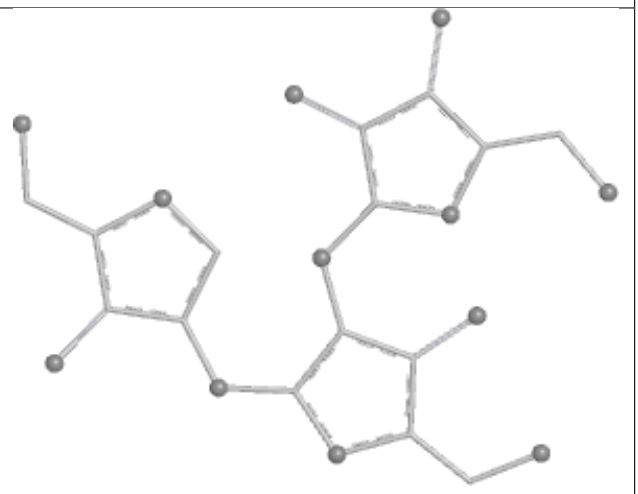
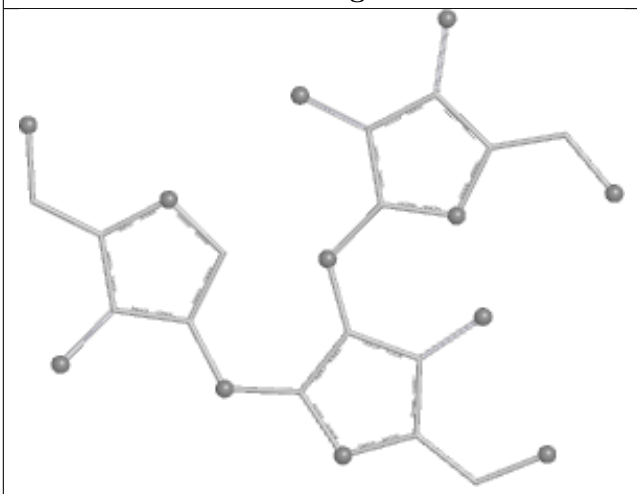
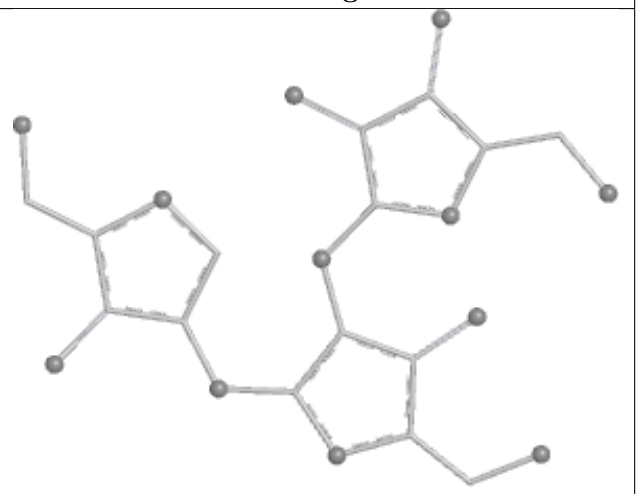
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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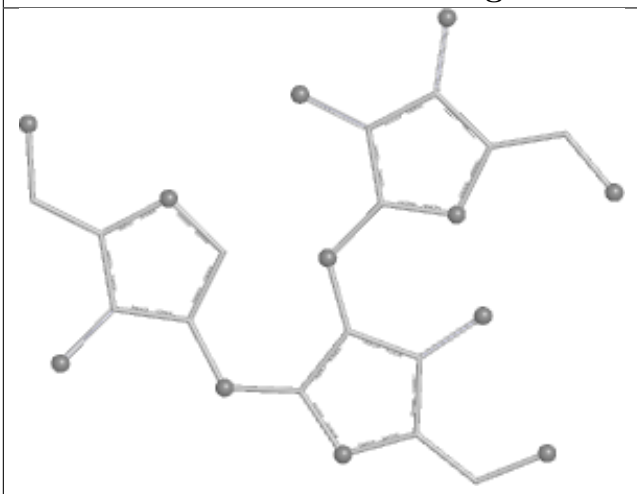
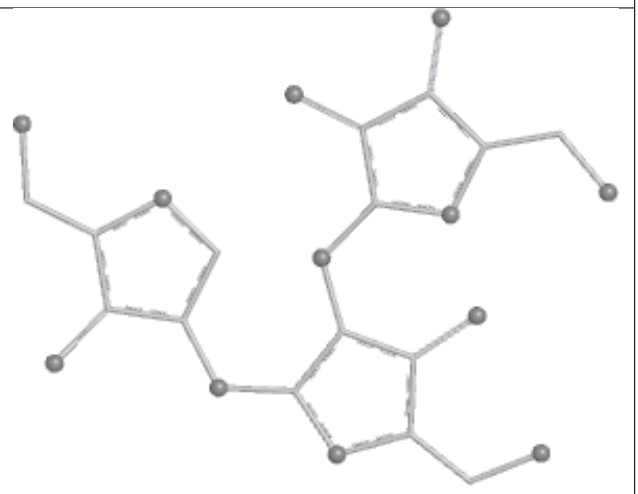
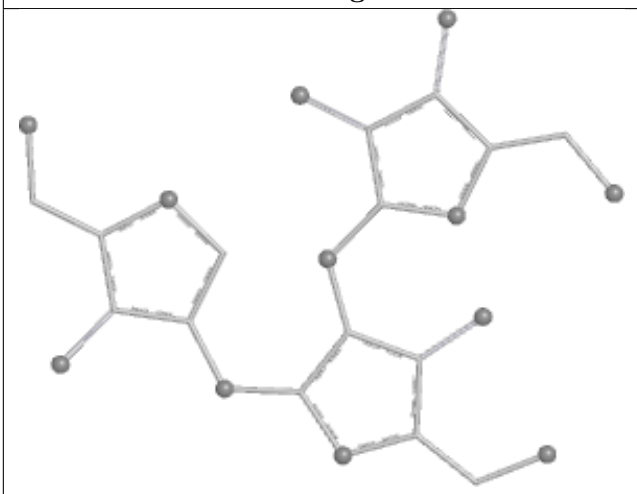
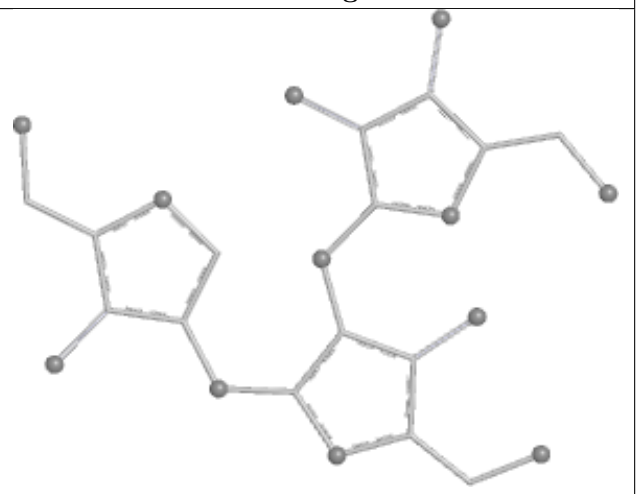
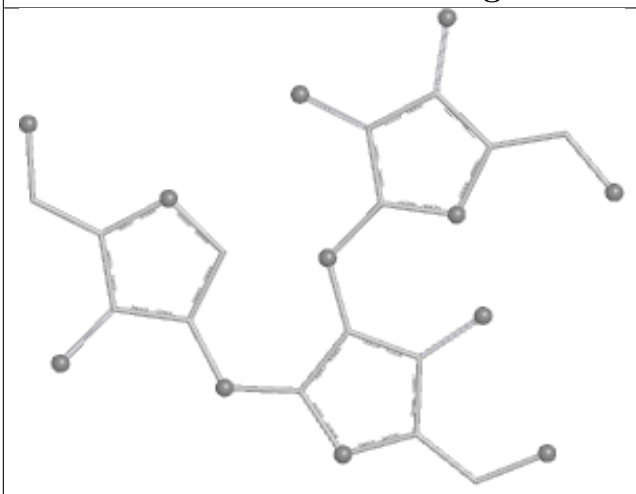
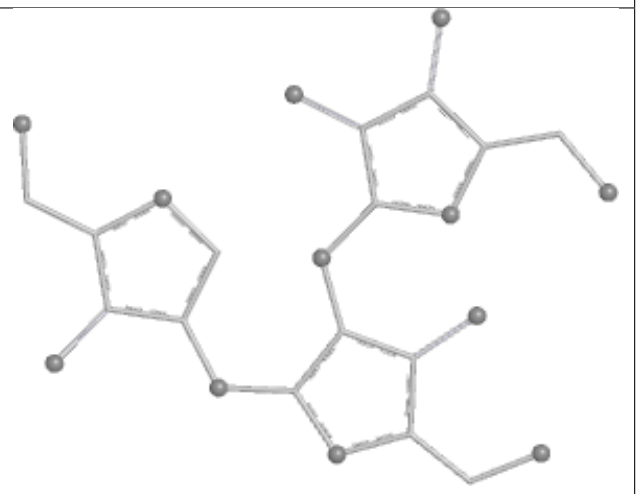
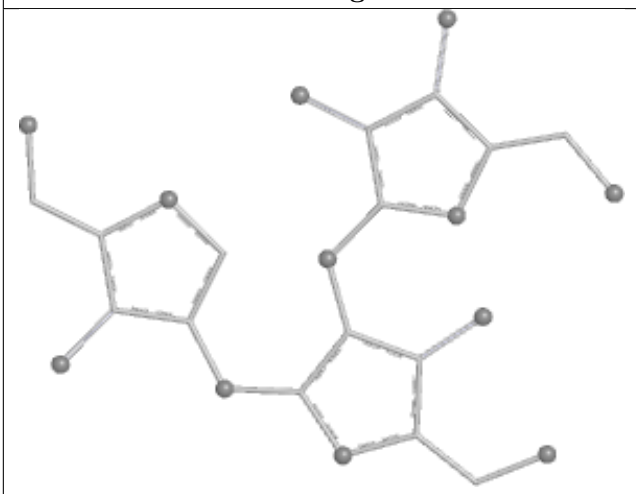
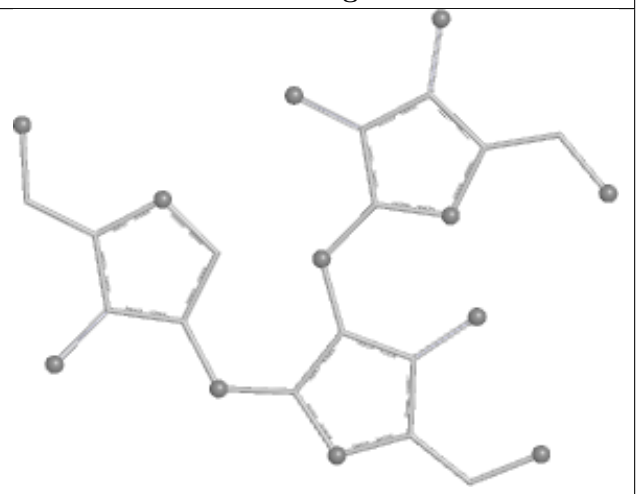
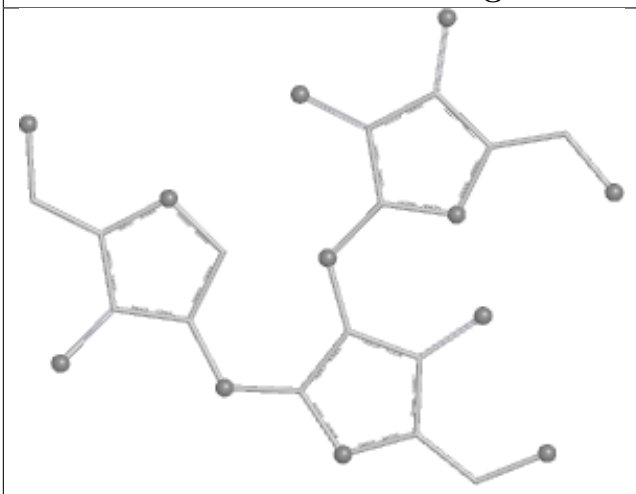
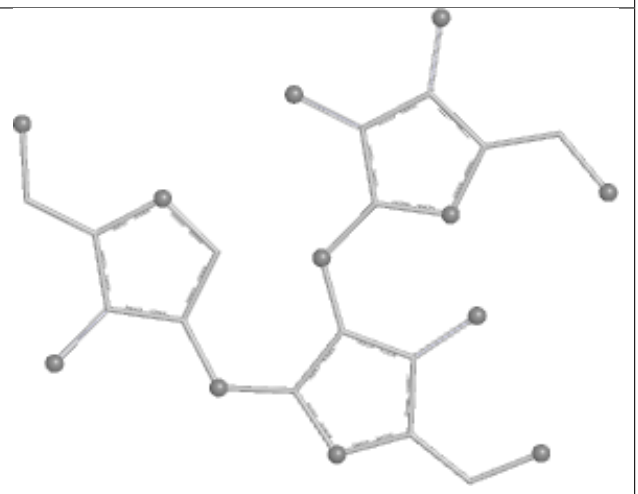
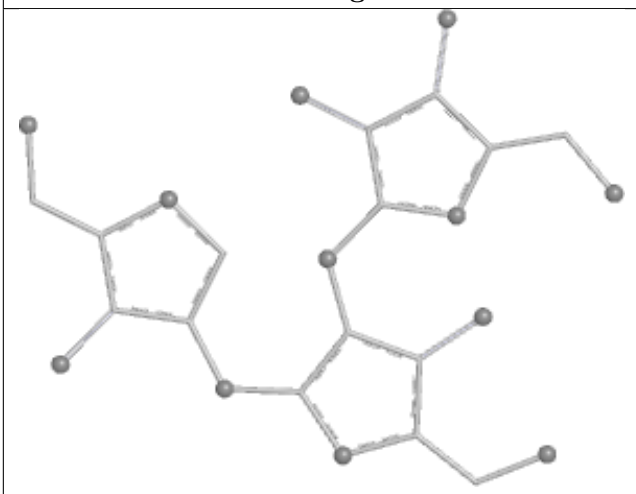
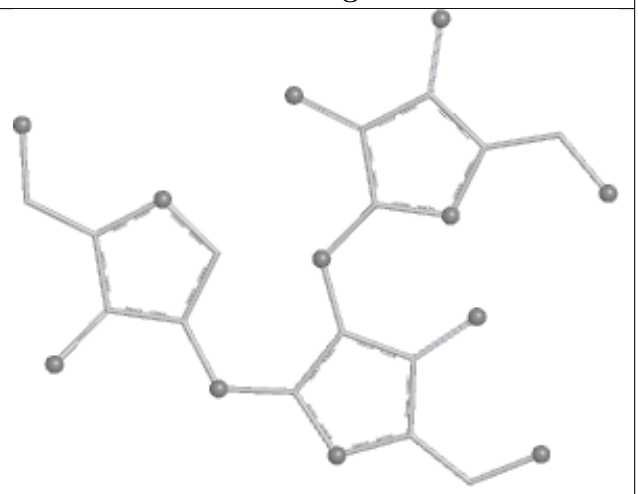
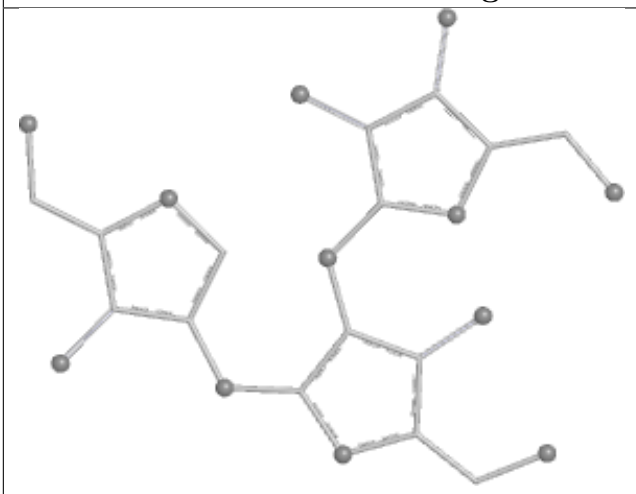
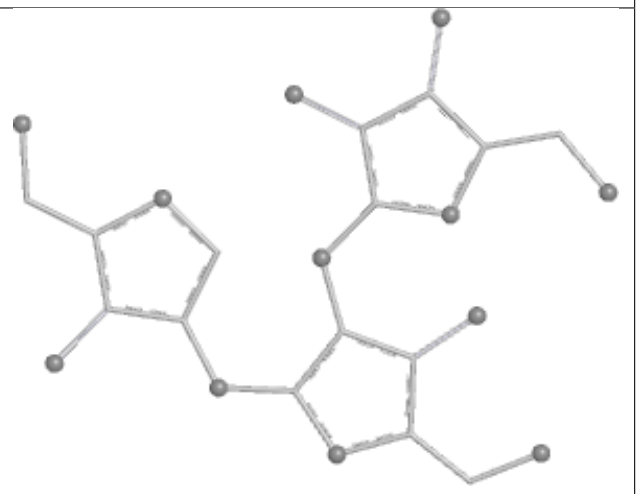
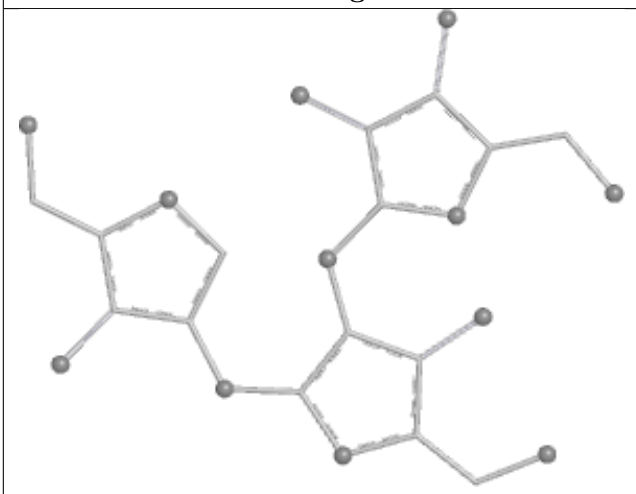
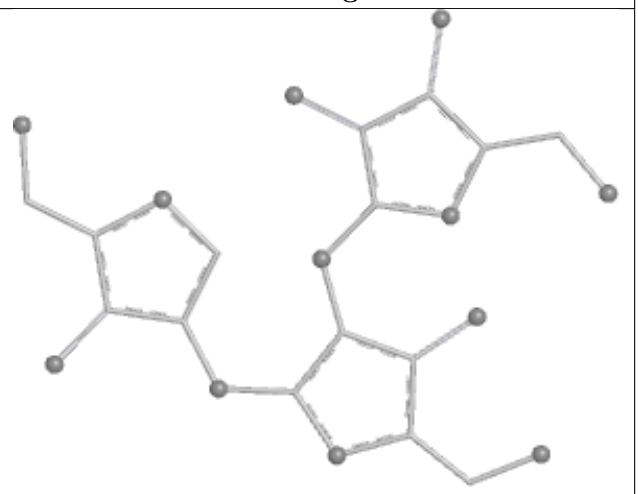
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain EB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain LB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain OB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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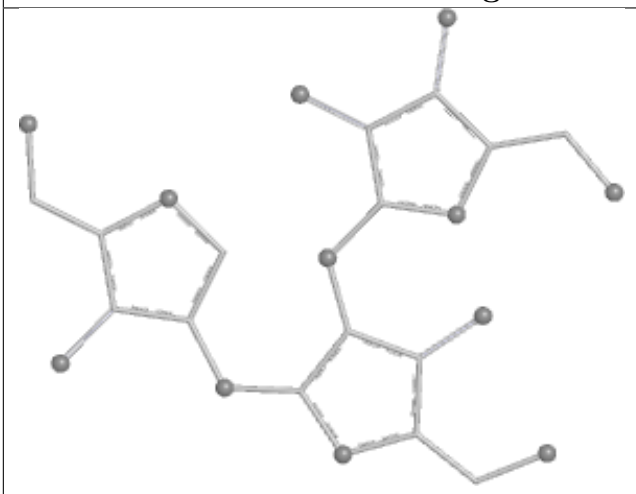
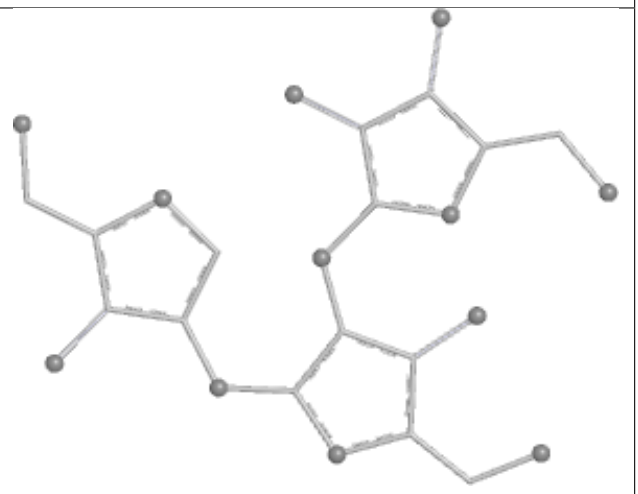
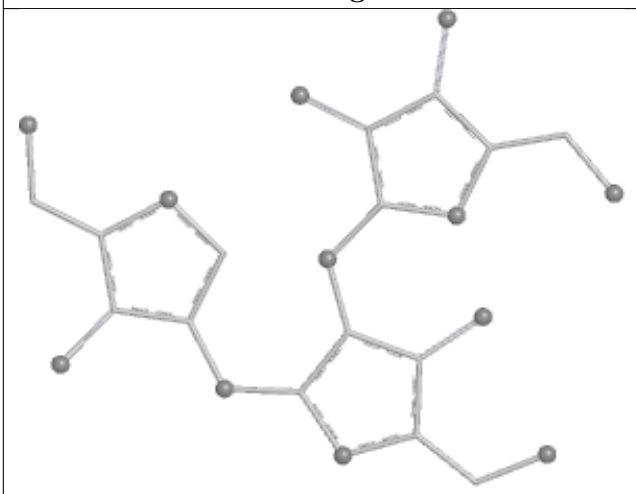
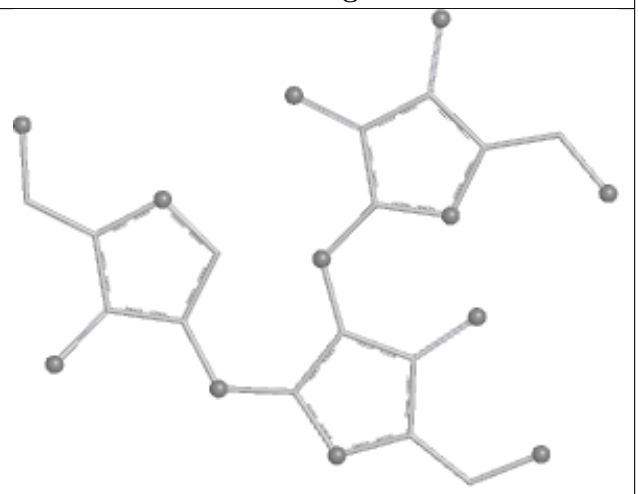
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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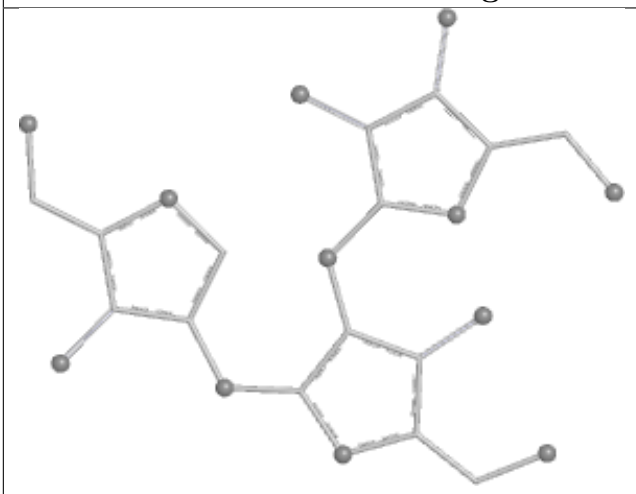
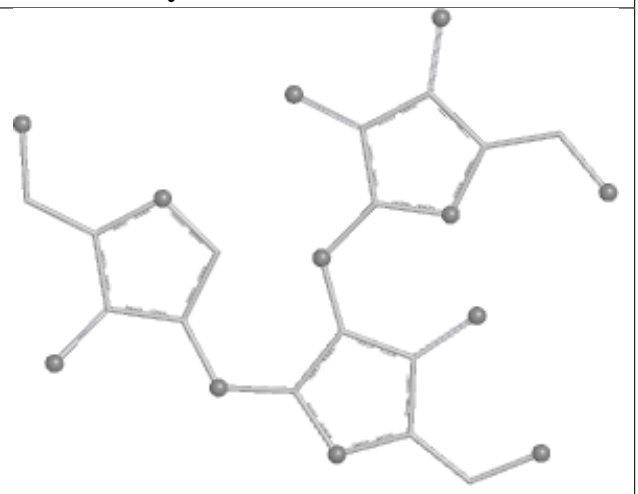
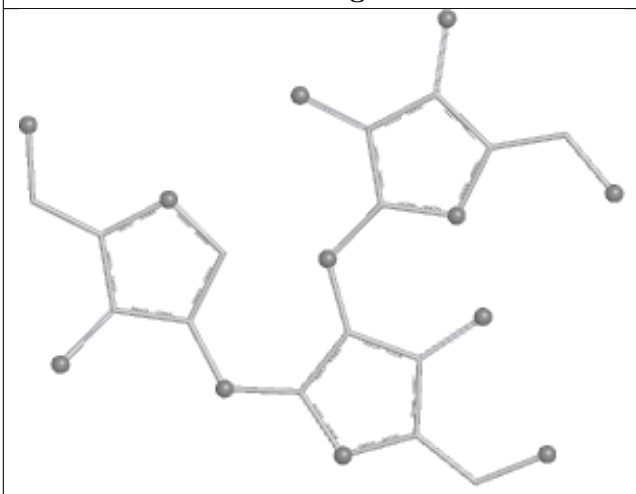
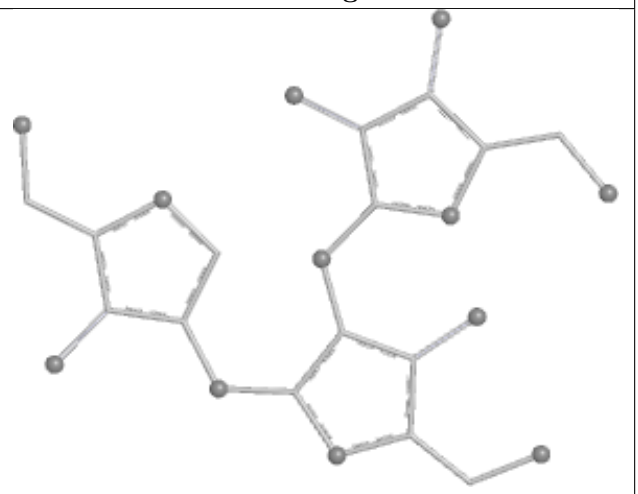
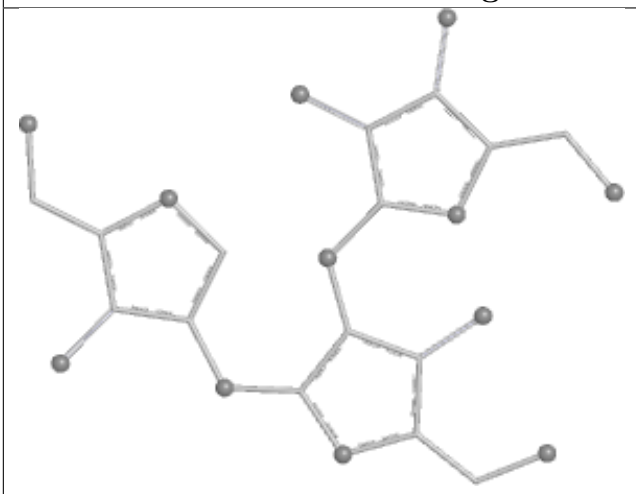
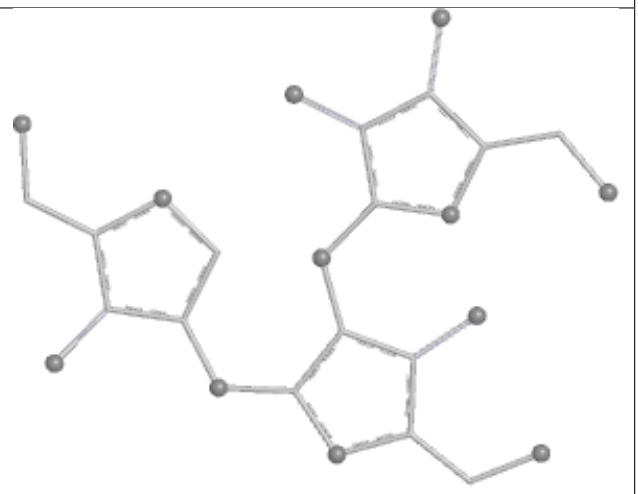
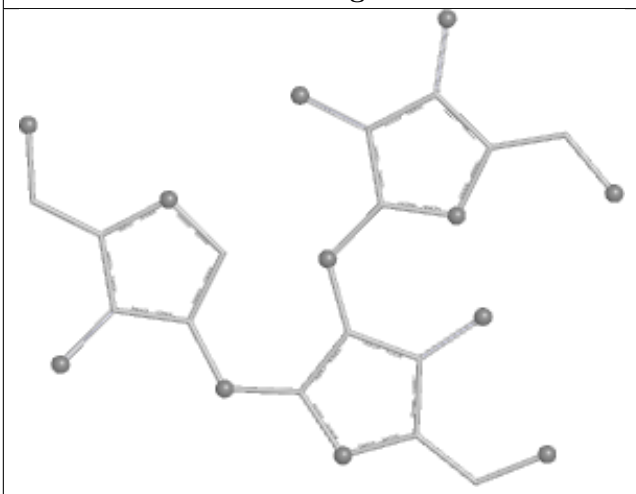
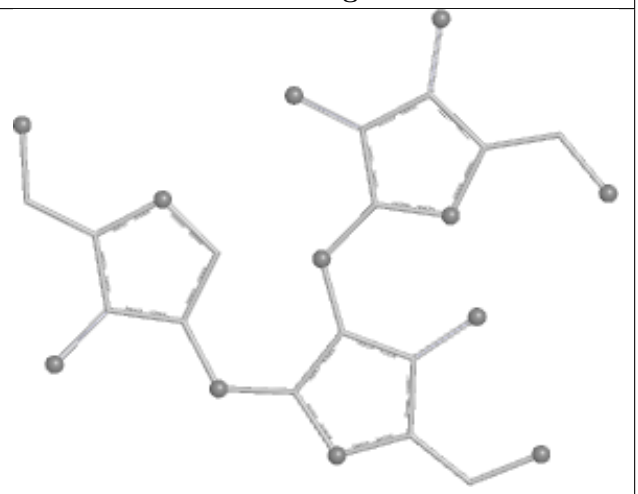
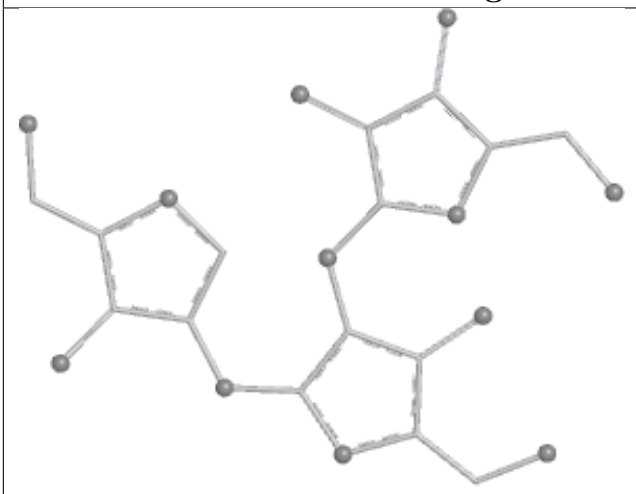
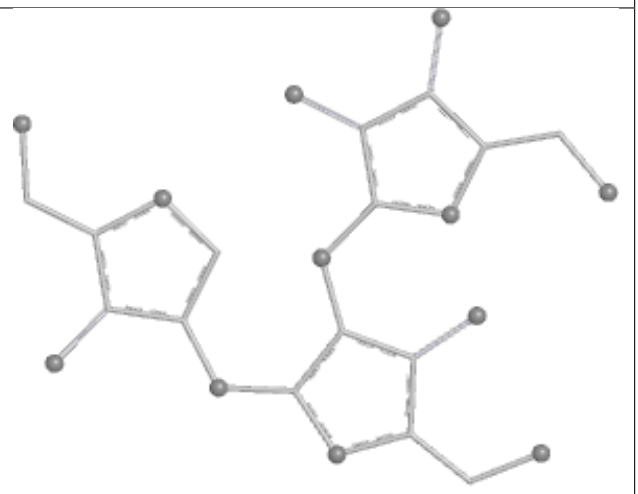
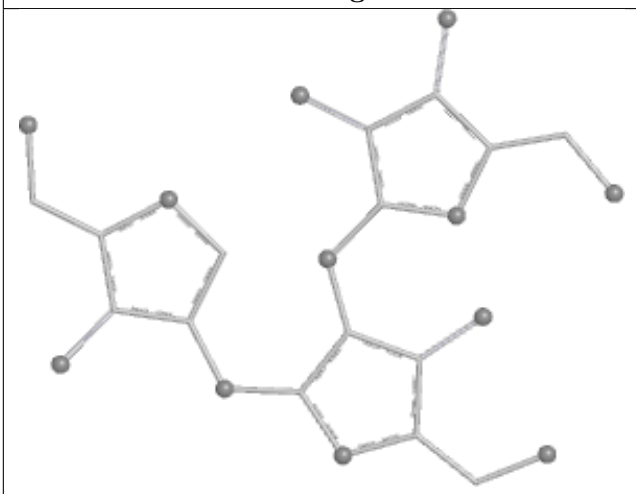
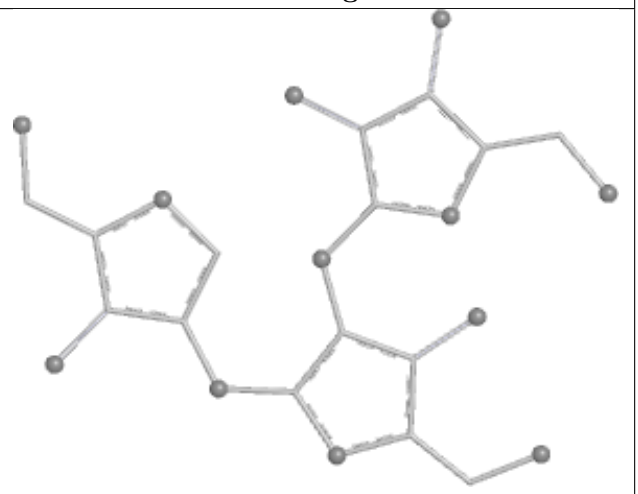
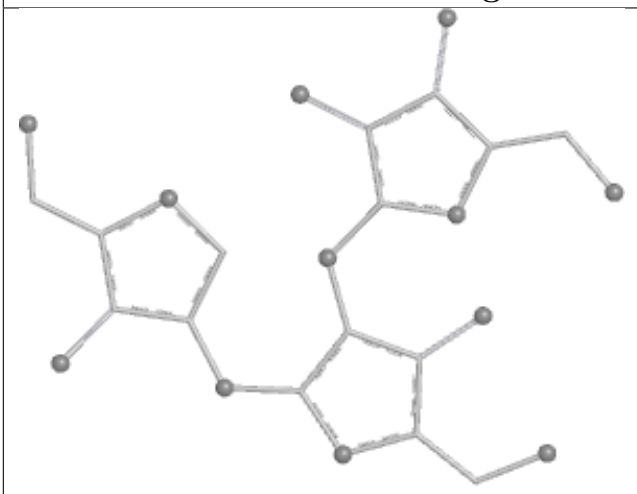
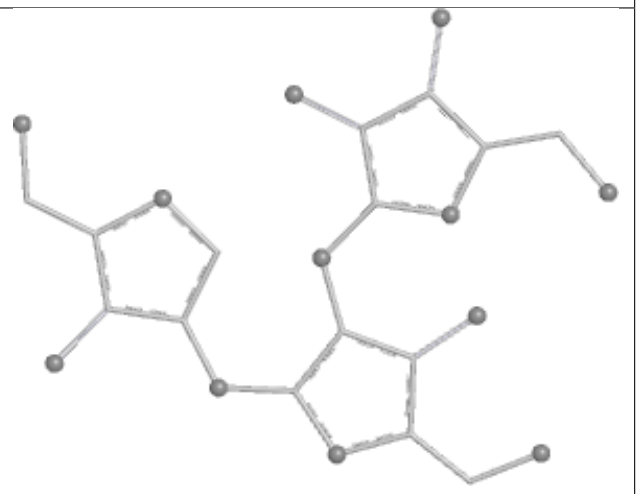
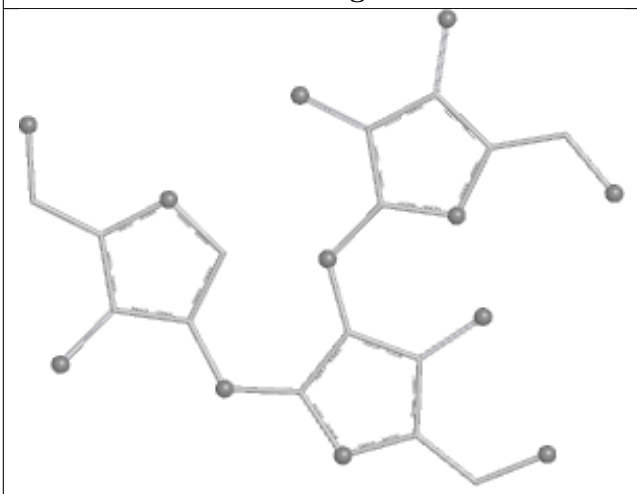
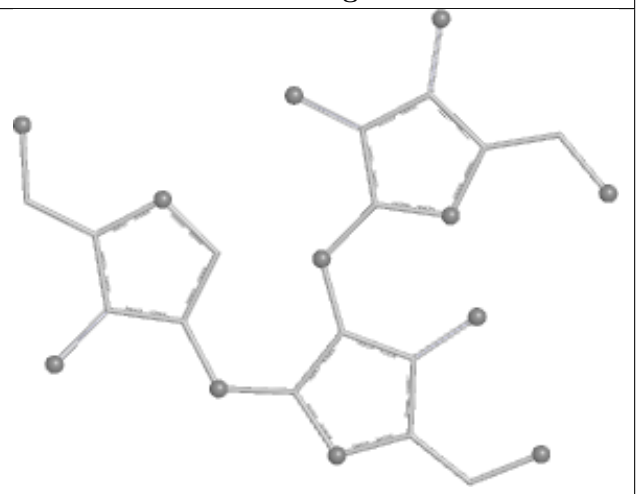
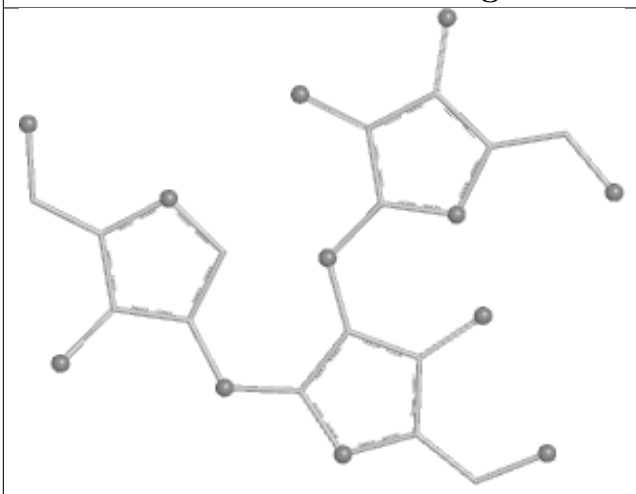
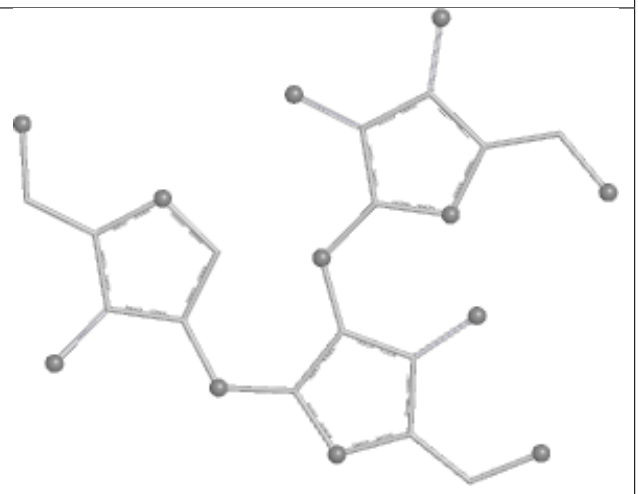
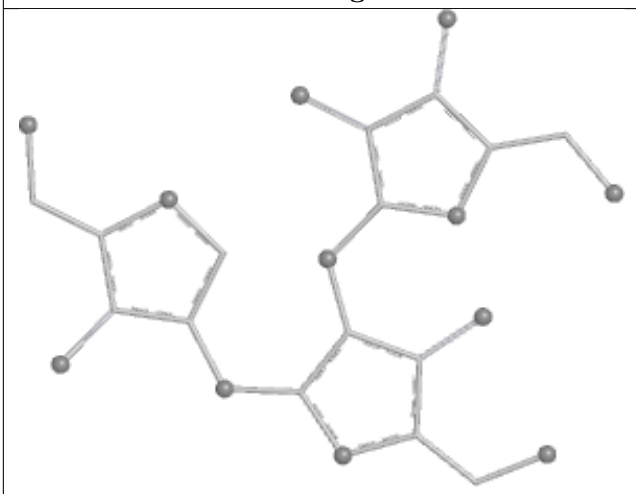
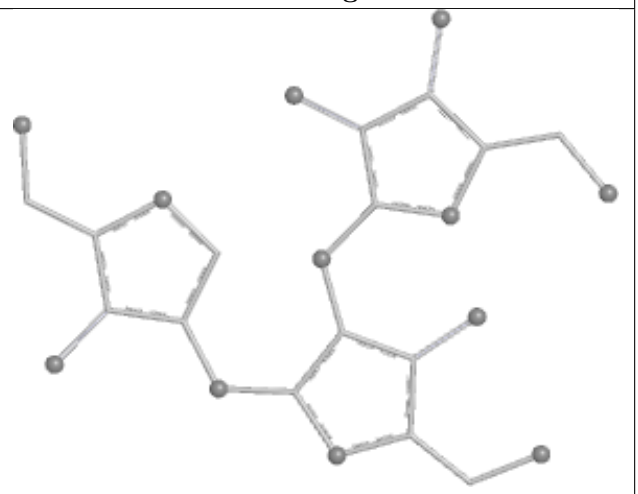
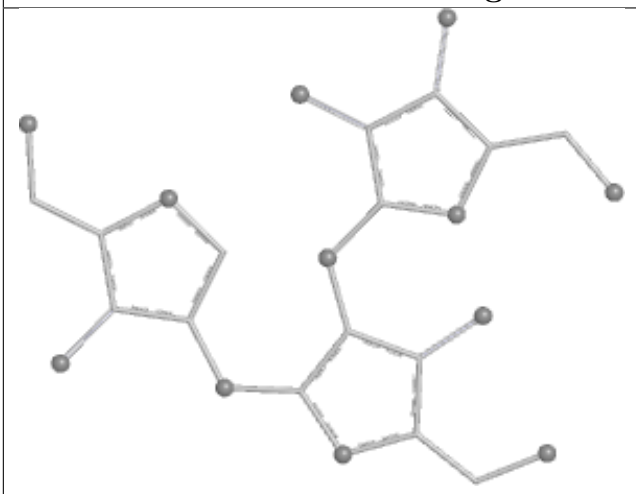
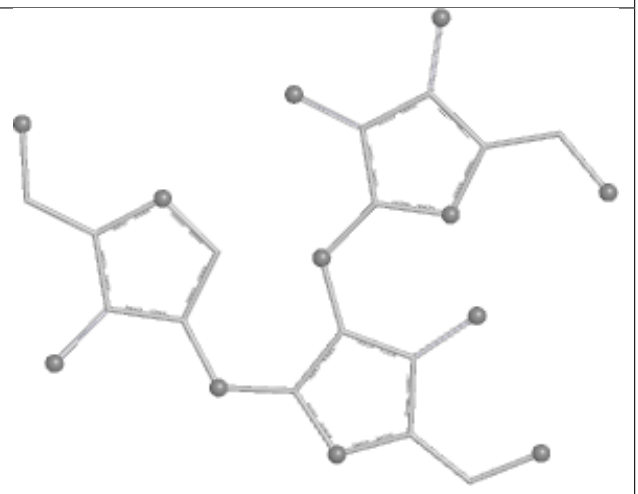
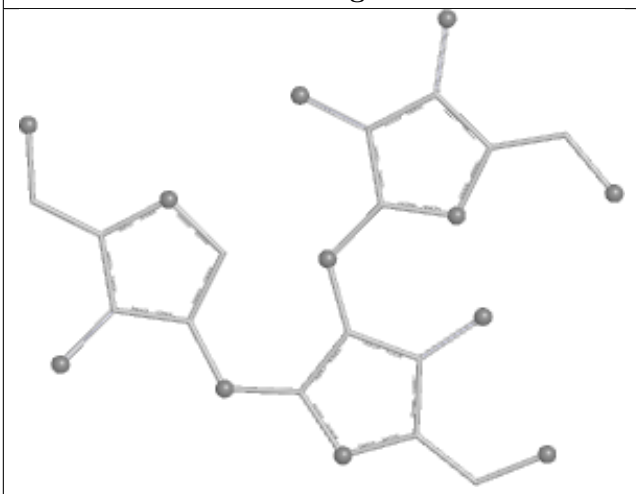
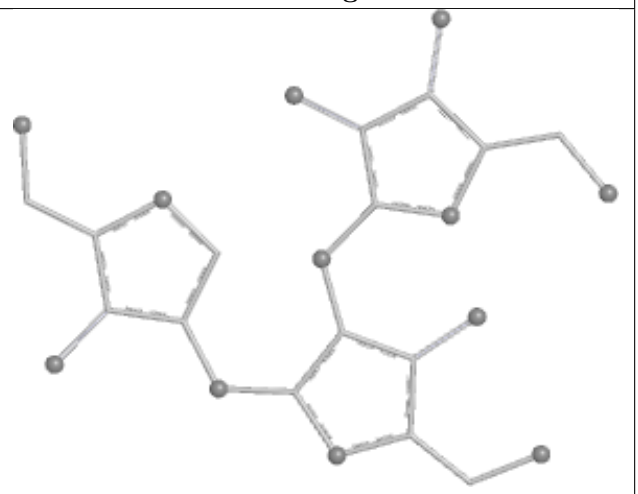
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

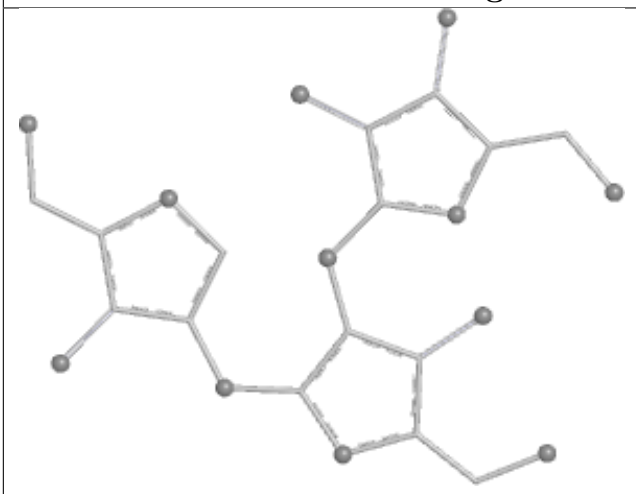
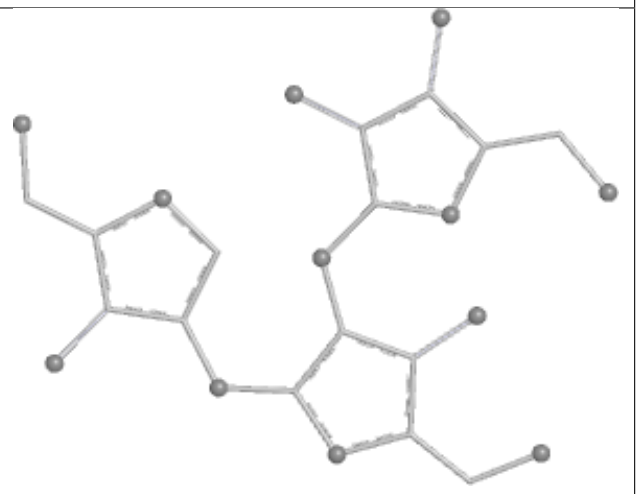
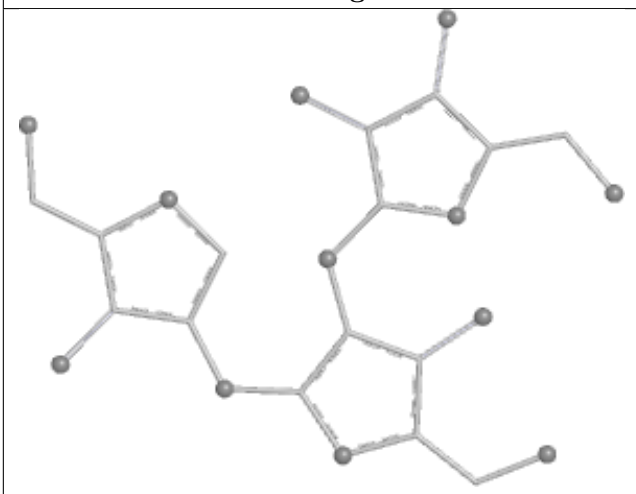
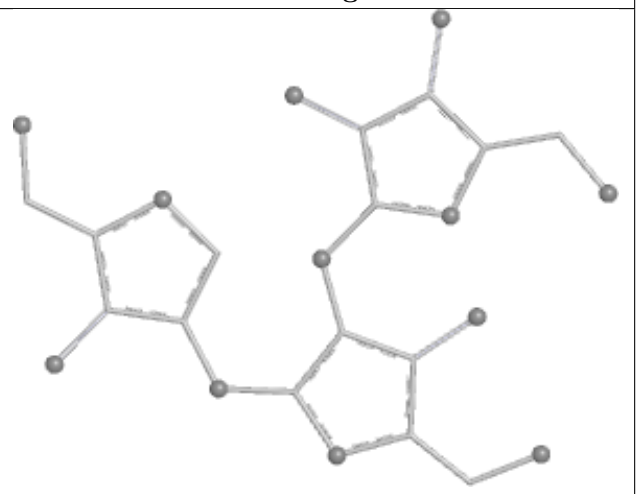
Oligosaccharide Chain RB	
 Bond lengths	 Bond angles
 Torsions	 Rings

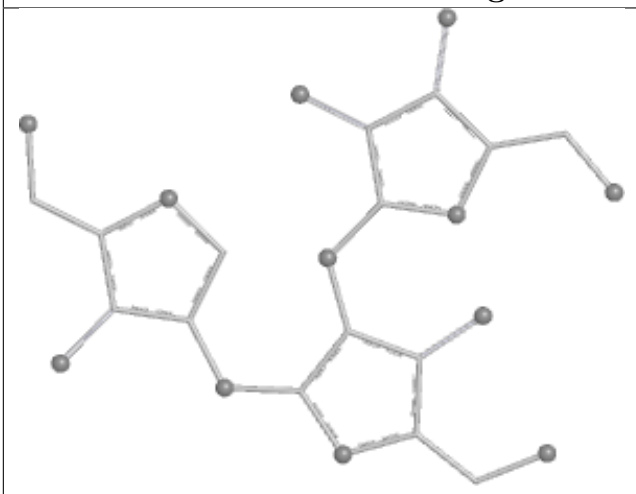
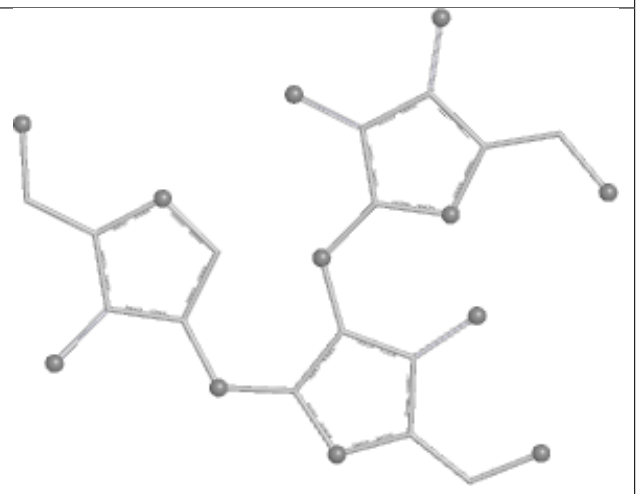
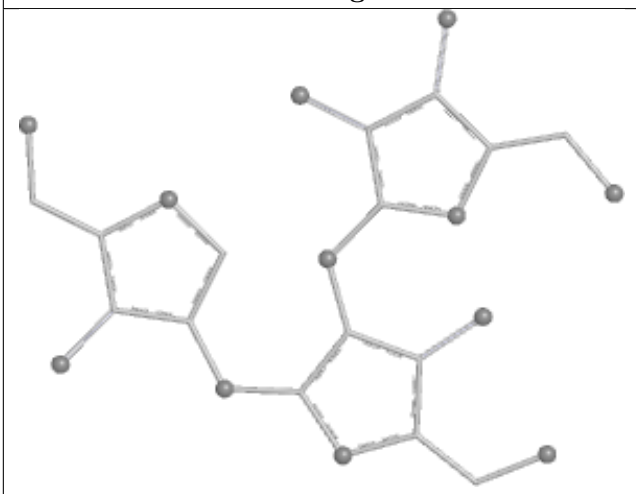
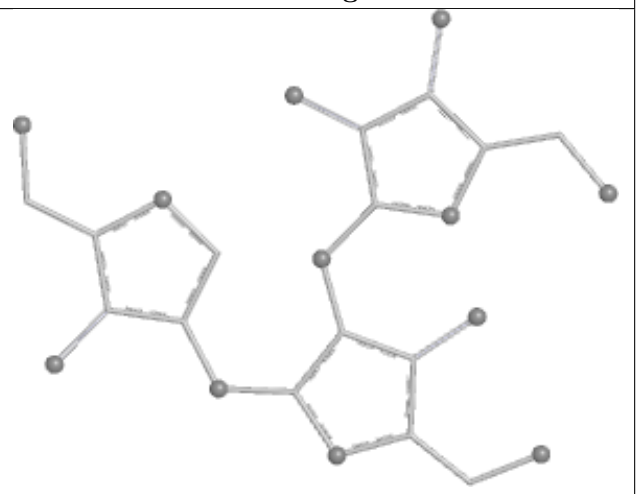
Oligosaccharide Chain SB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

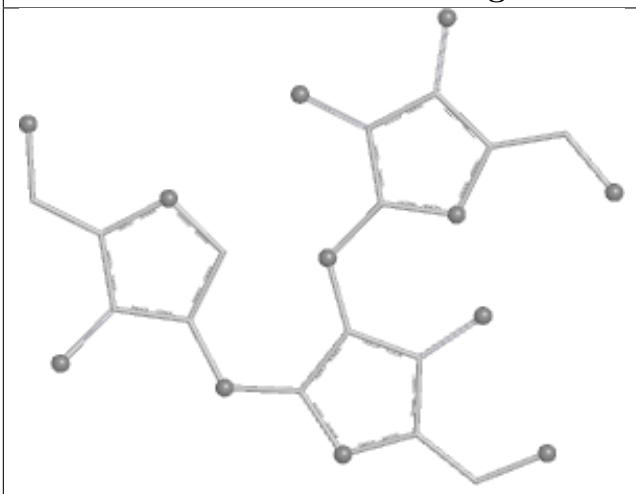
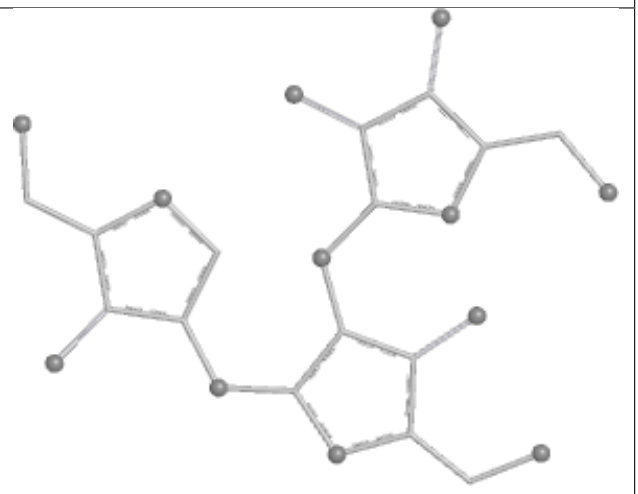
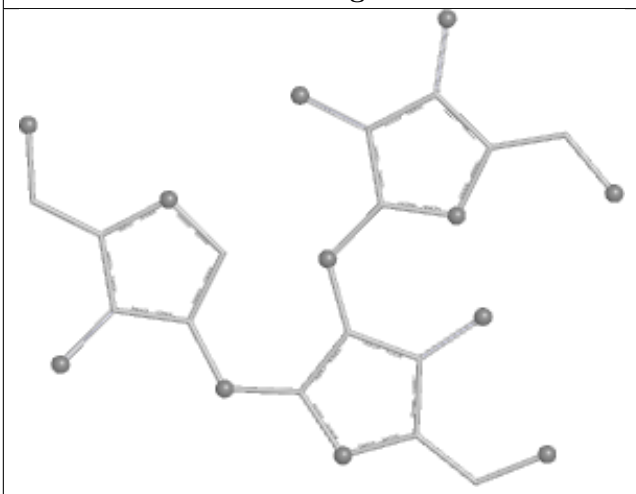
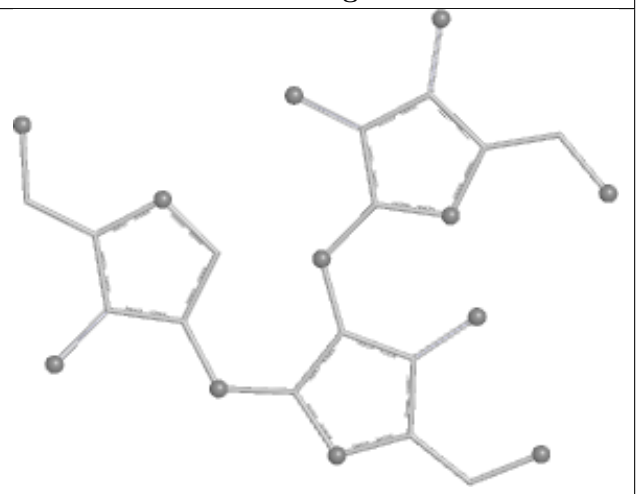
Oligosaccharide Chain TB	
 Bond lengths	 Bond angles
 Torsions	 Rings

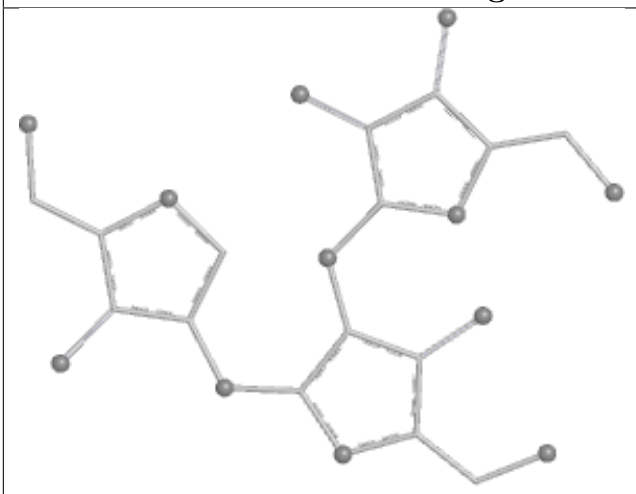
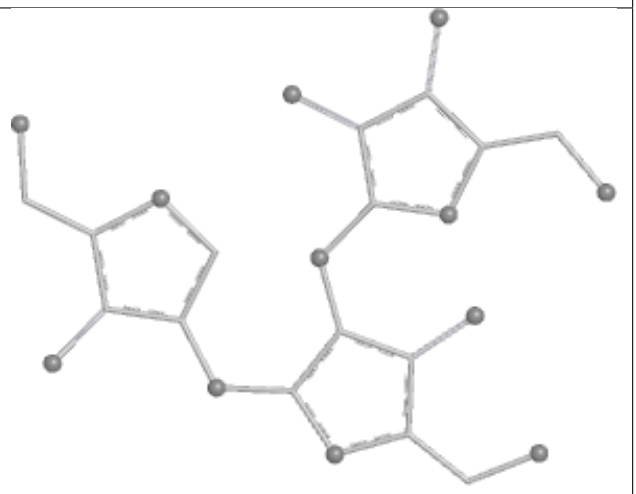
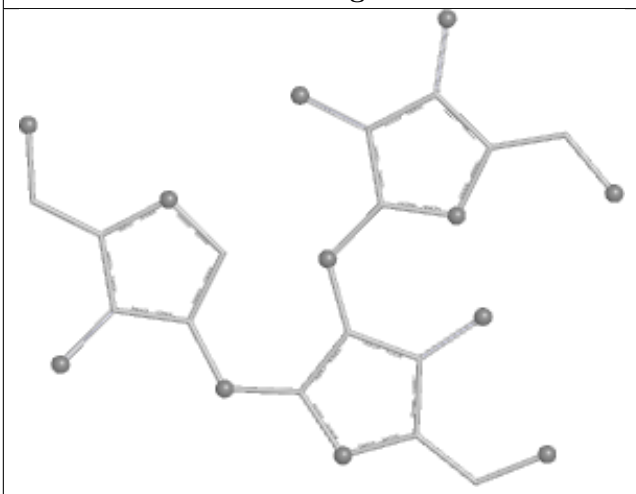
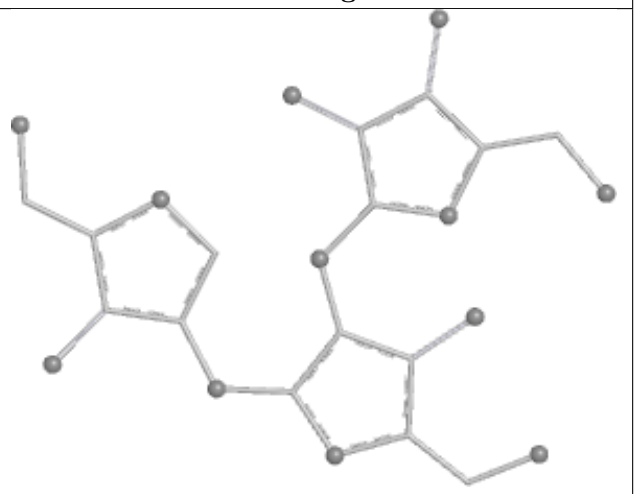
Oligosaccharide Chain UB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

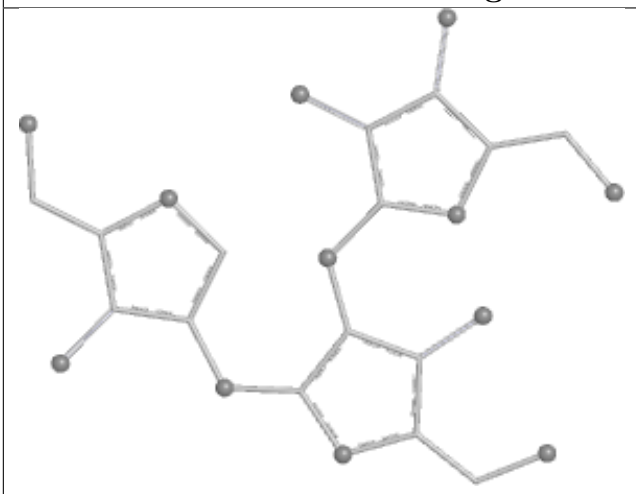
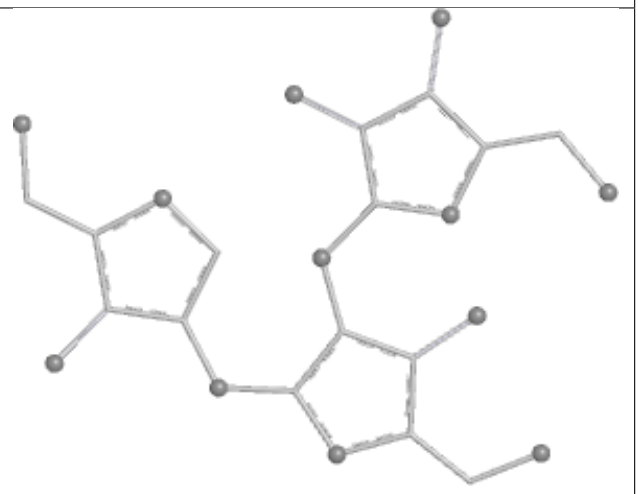
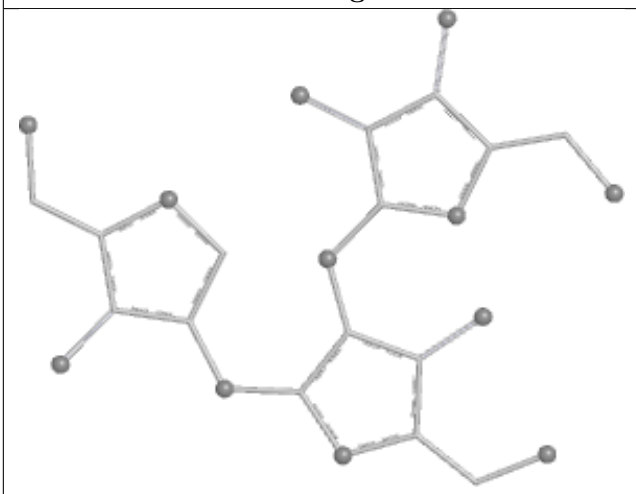
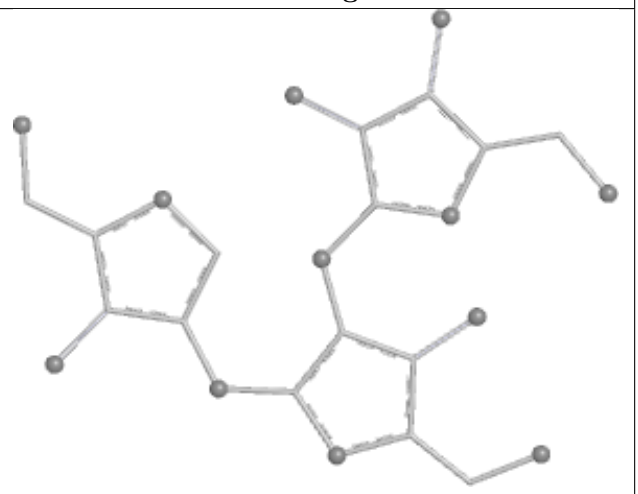
Oligosaccharide Chain hB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

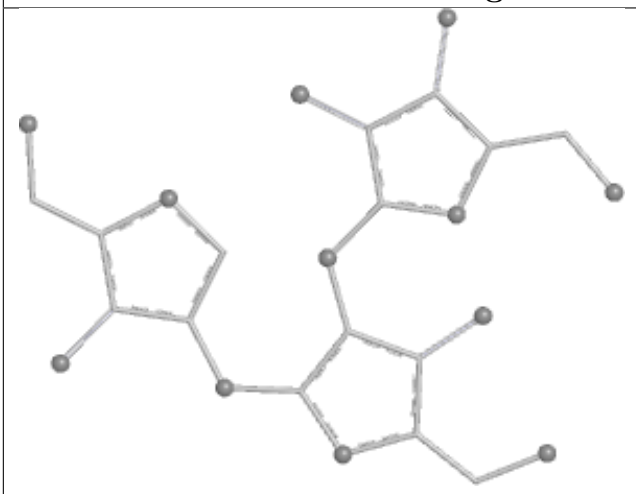
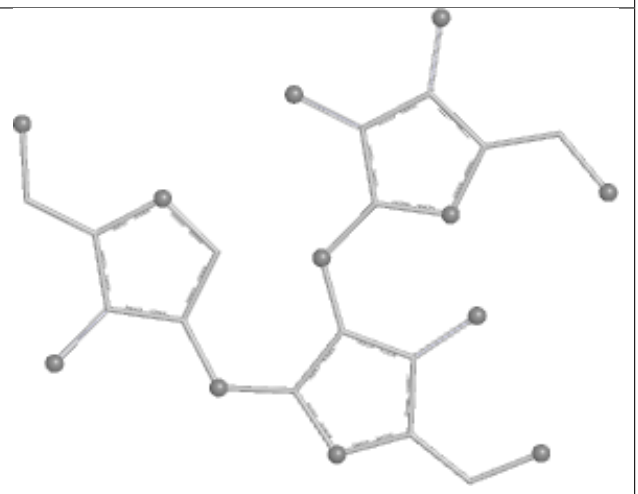
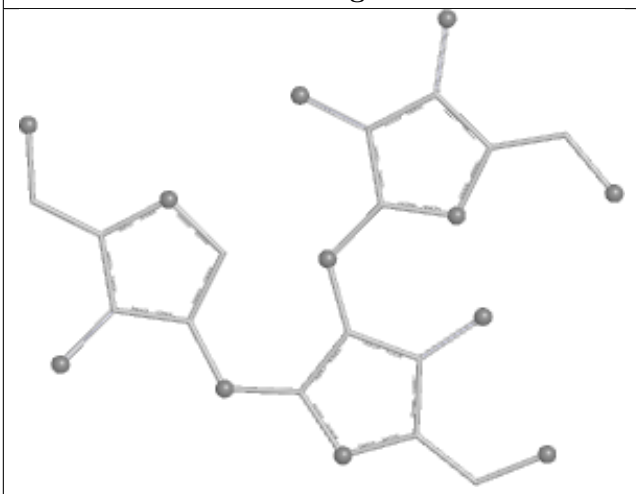
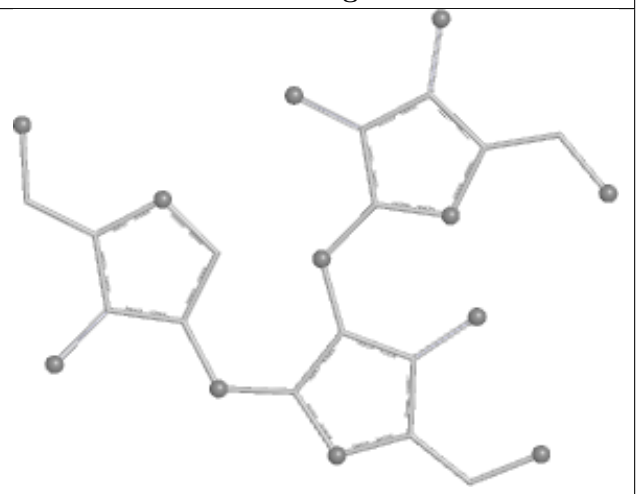
Oligosaccharide Chain oB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

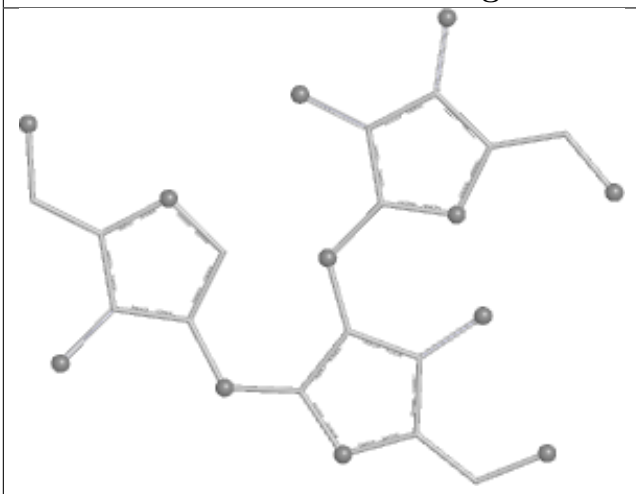
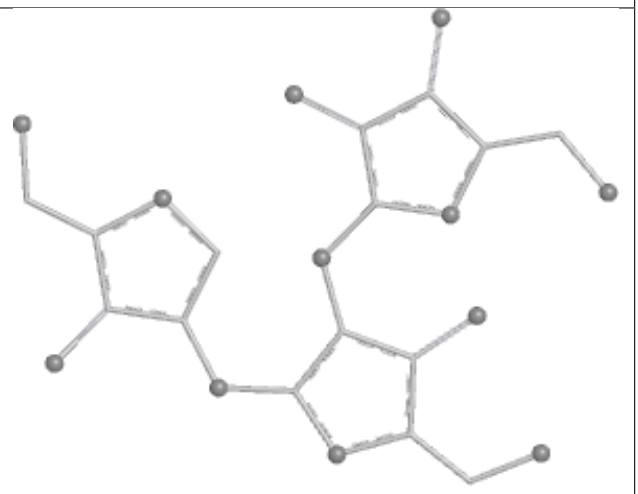
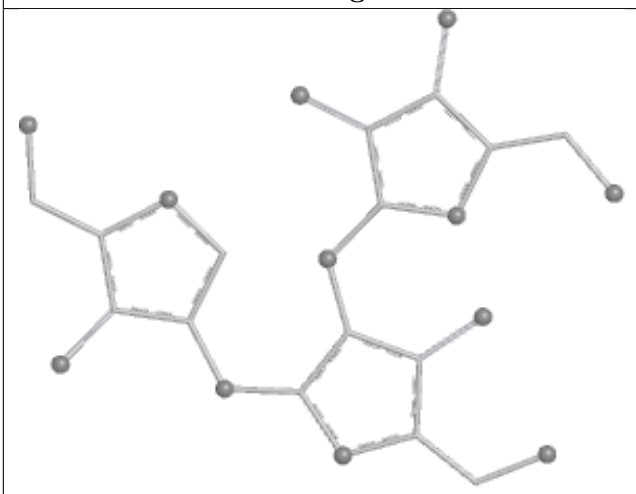
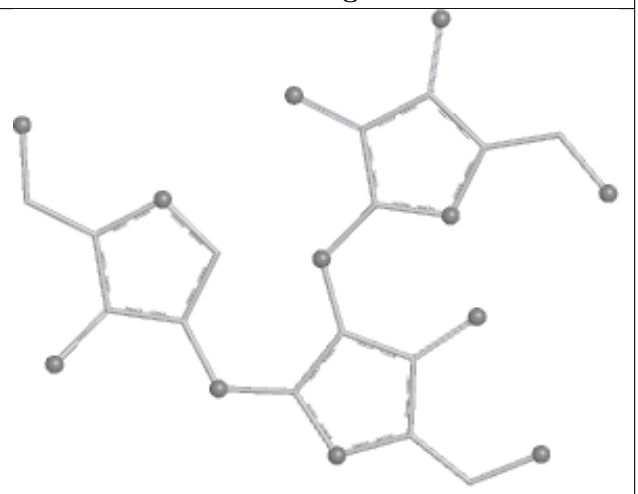
Oligosaccharide Chain rB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

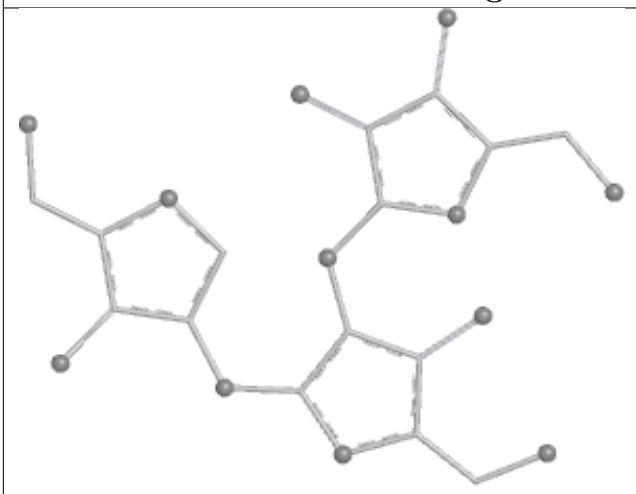
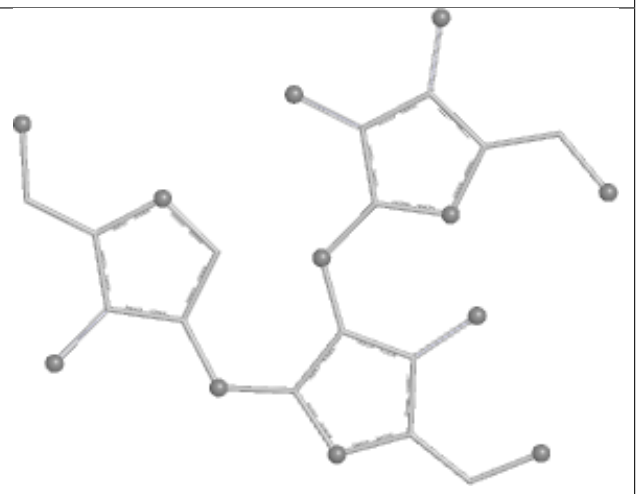
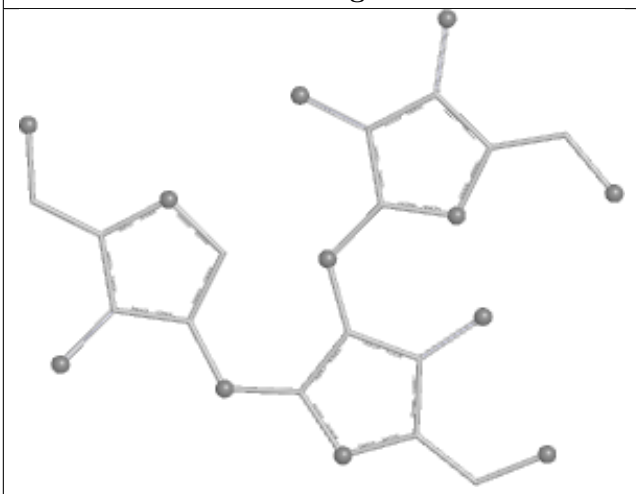
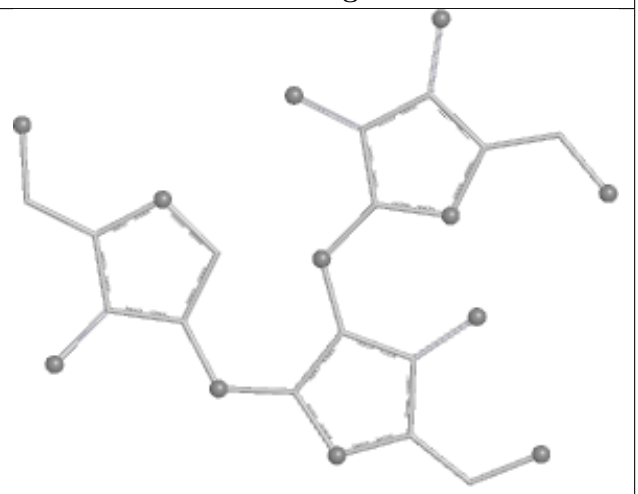
Oligosaccharide Chain sB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

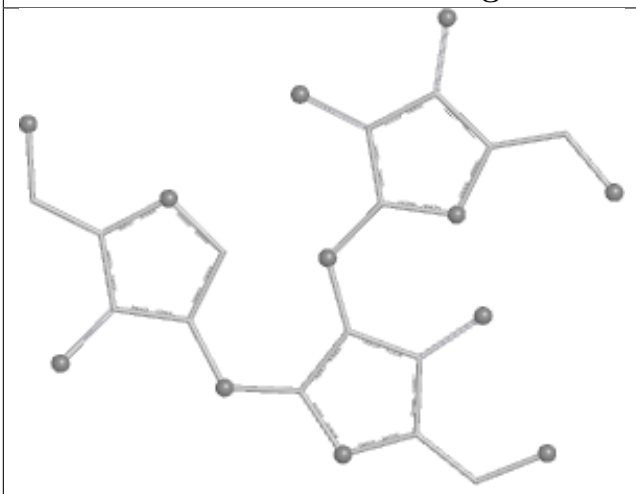
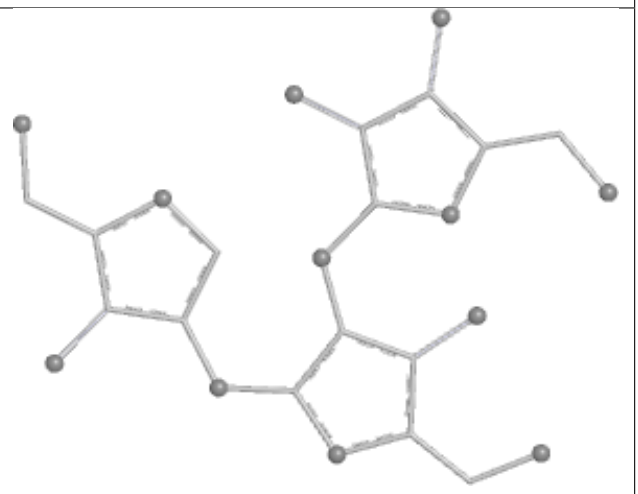
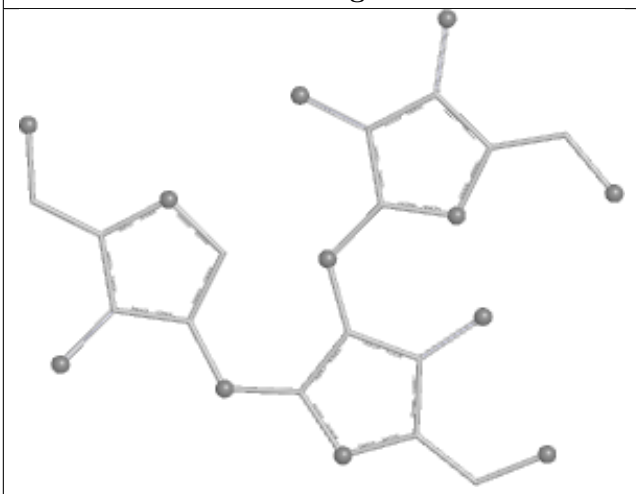
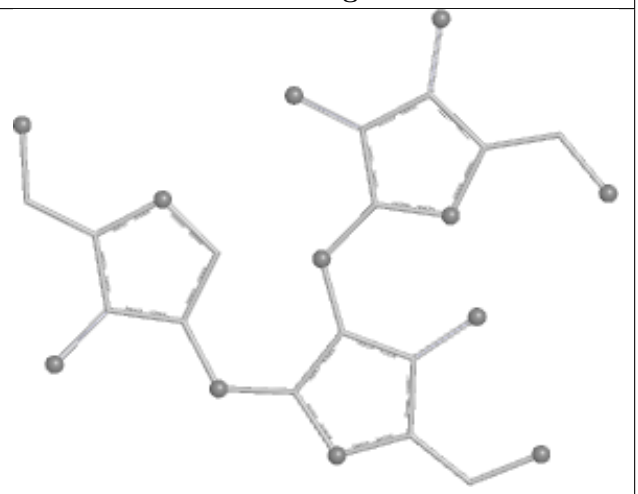
Oligosaccharide Chain tB	
 Bond lengths	 Bond angles
 Torsions	 Rings

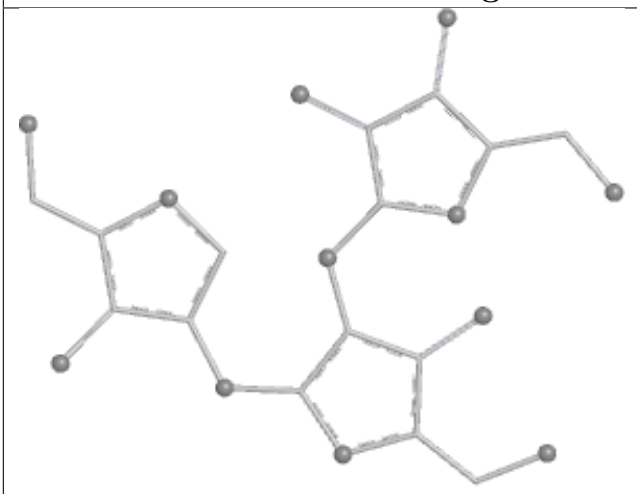
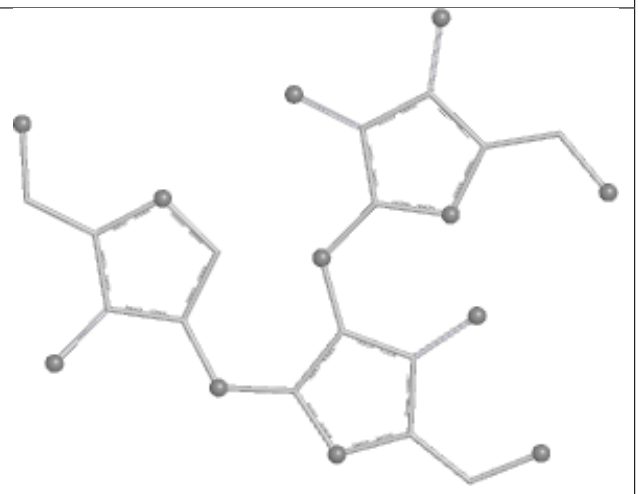
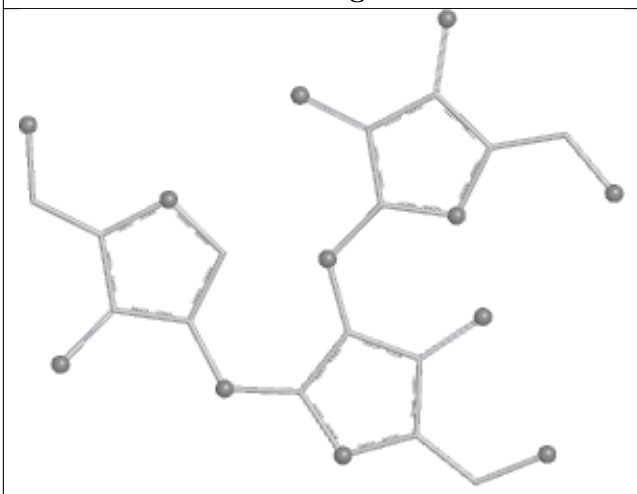
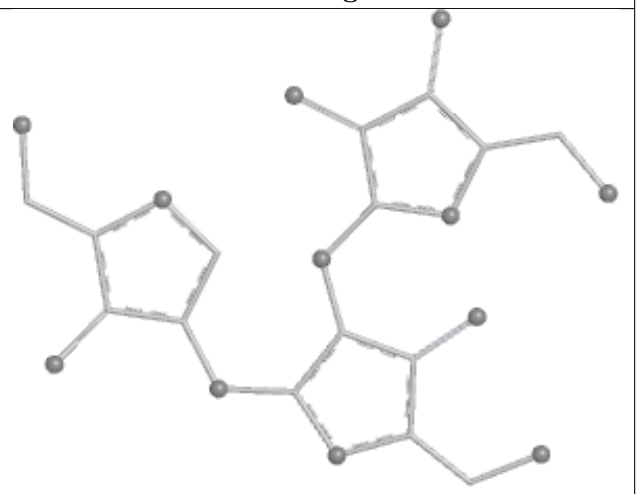
Oligosaccharide Chain uB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

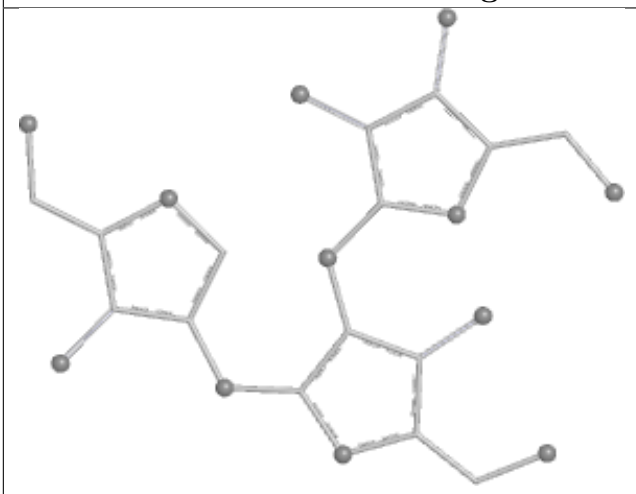
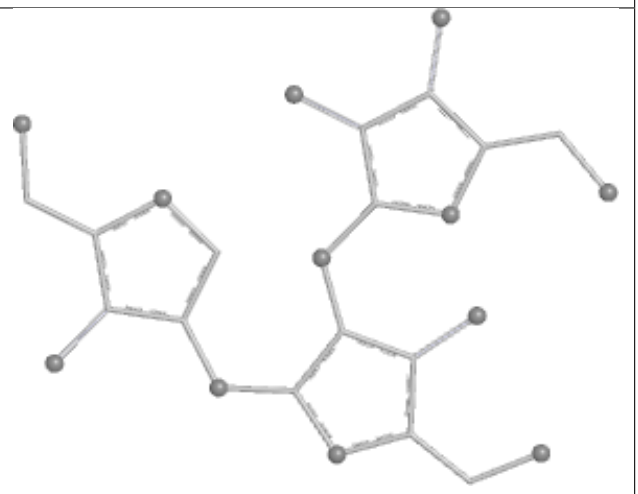
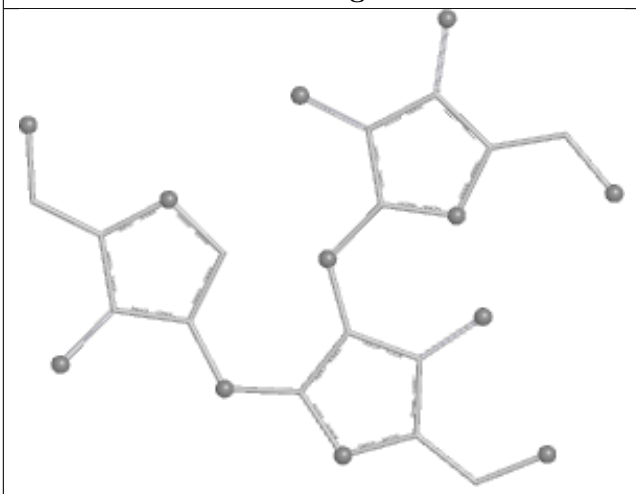
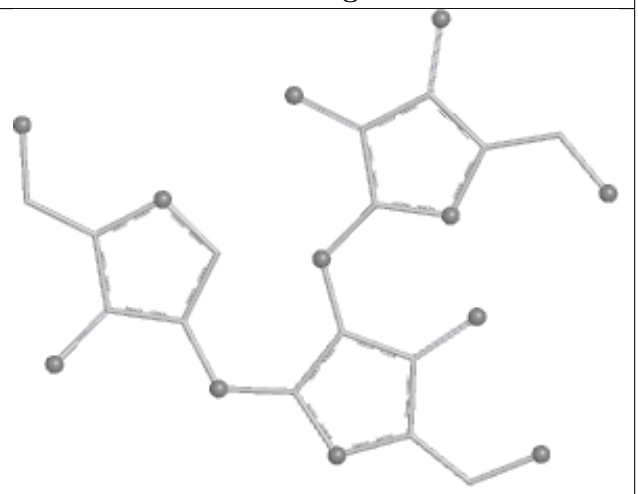
Oligosaccharide Chain vB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

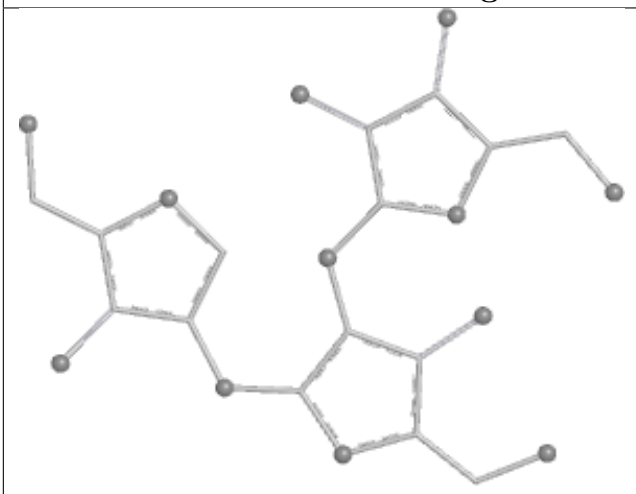
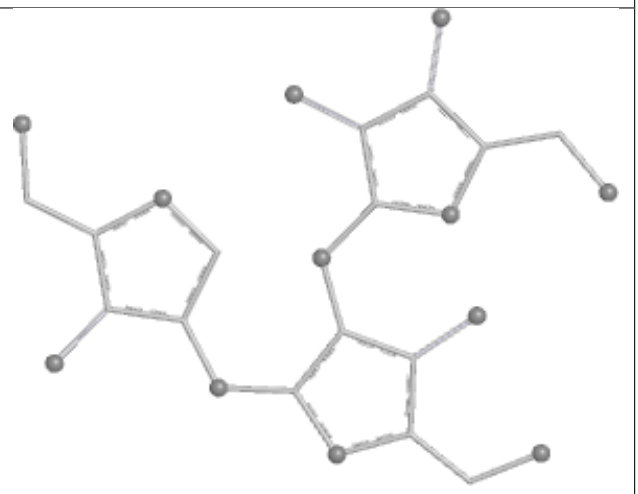
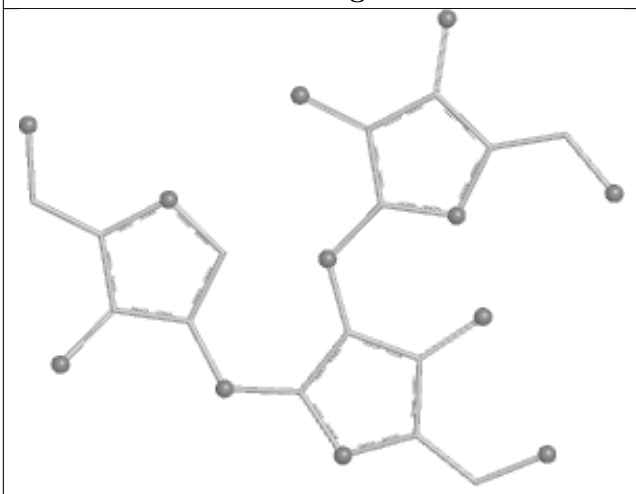
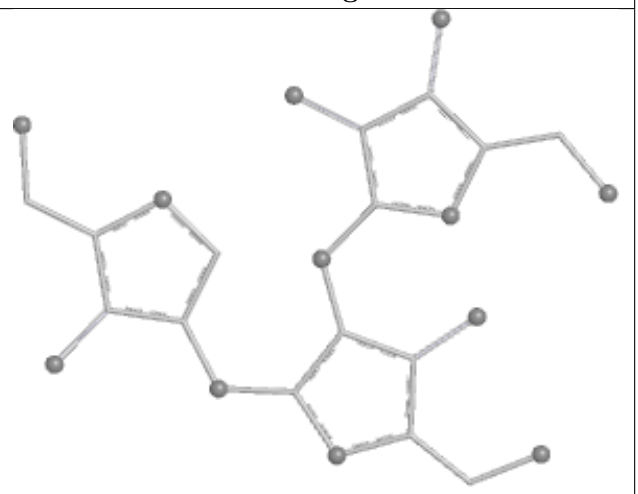
Oligosaccharide Chain wB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

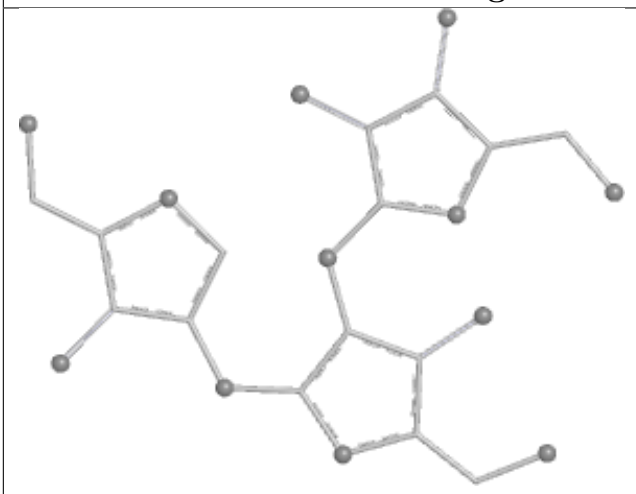
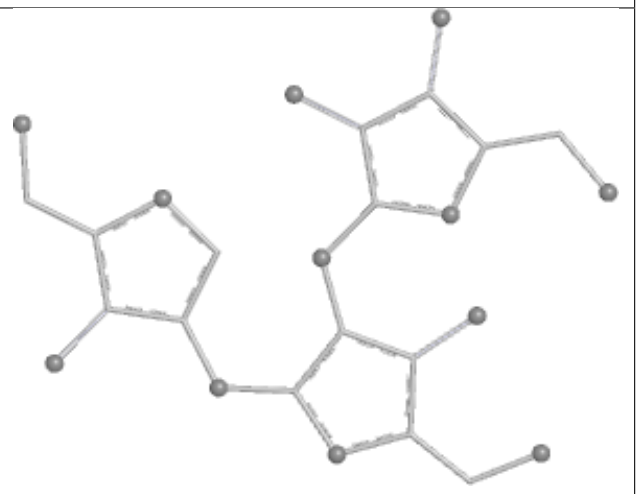
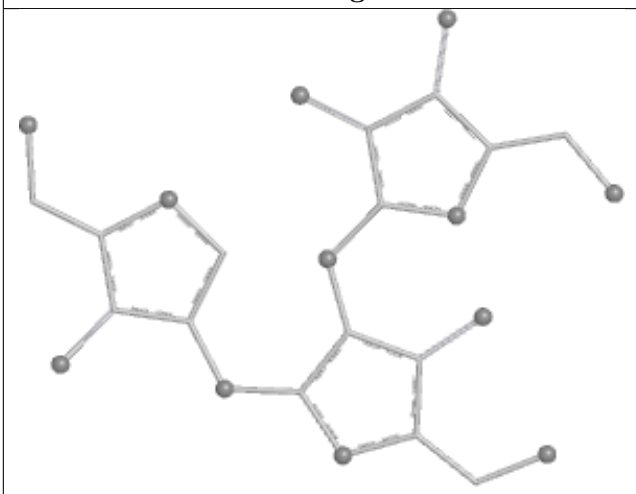
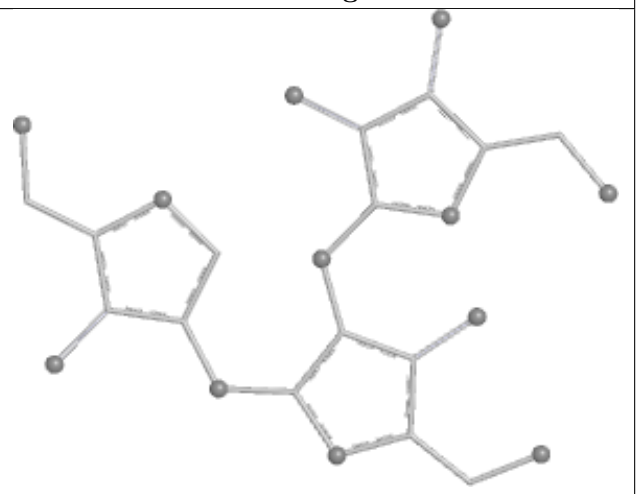
Oligosaccharide Chain xB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

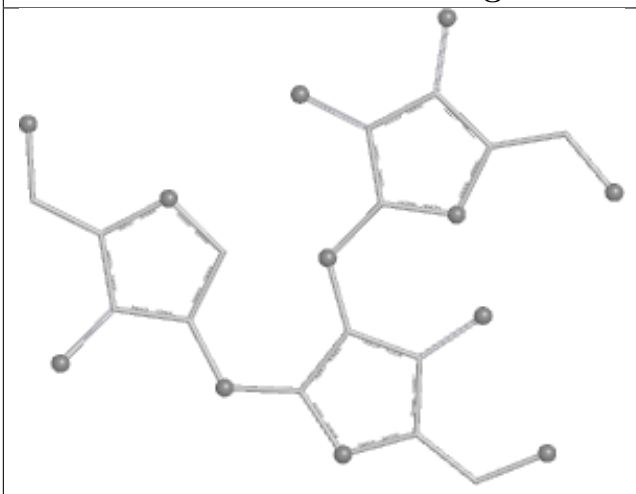
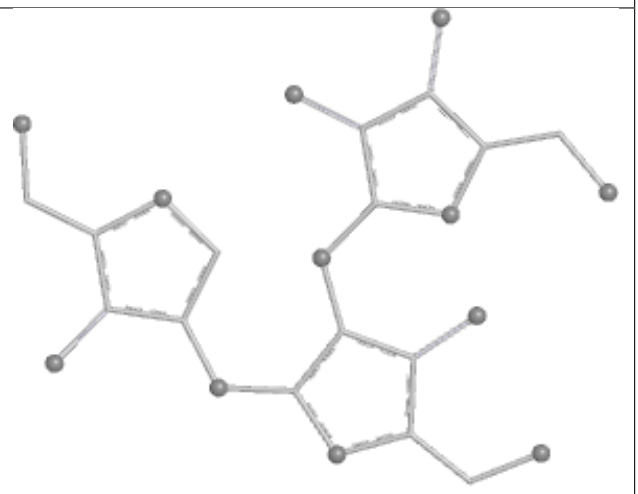
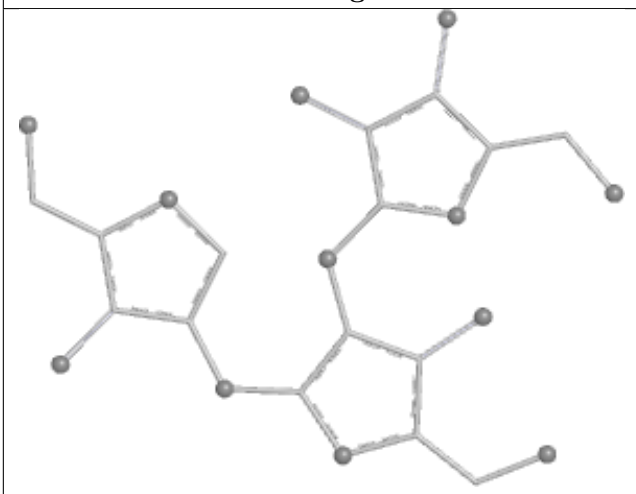
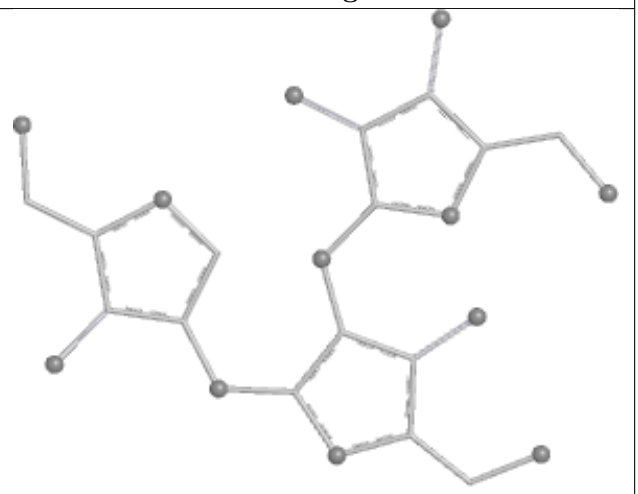
Oligosaccharide Chain BC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain CC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain GC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain HC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain IC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain LC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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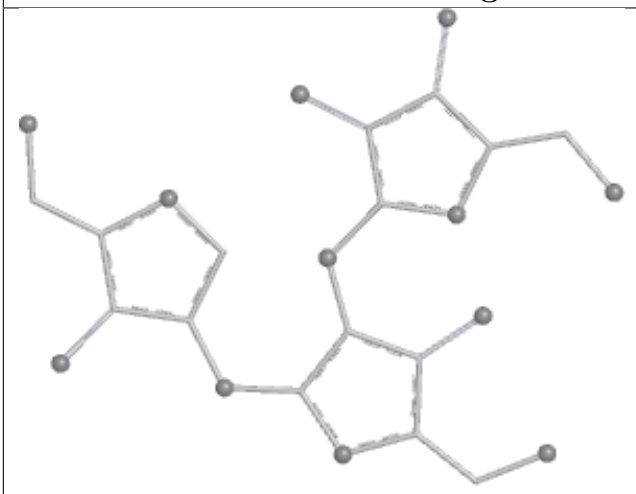
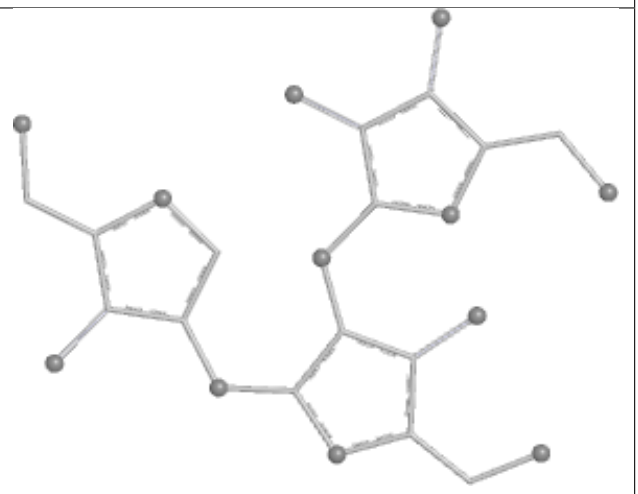
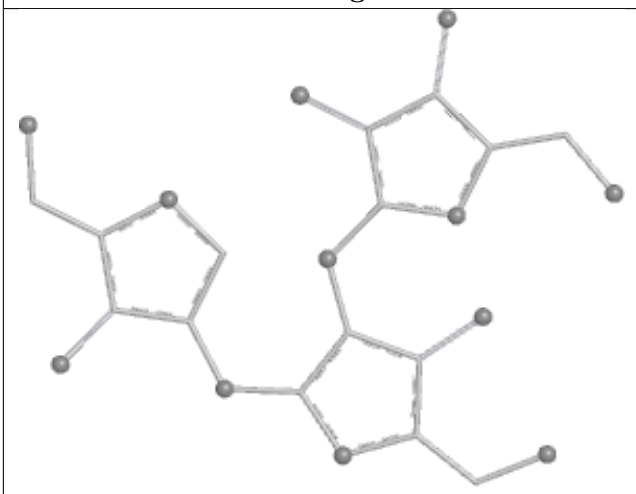
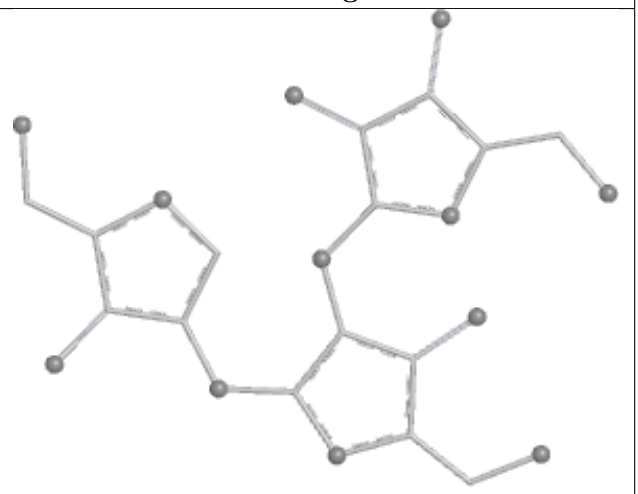
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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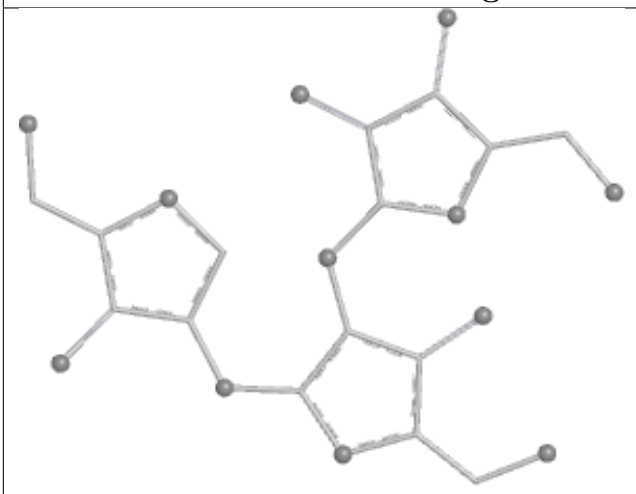
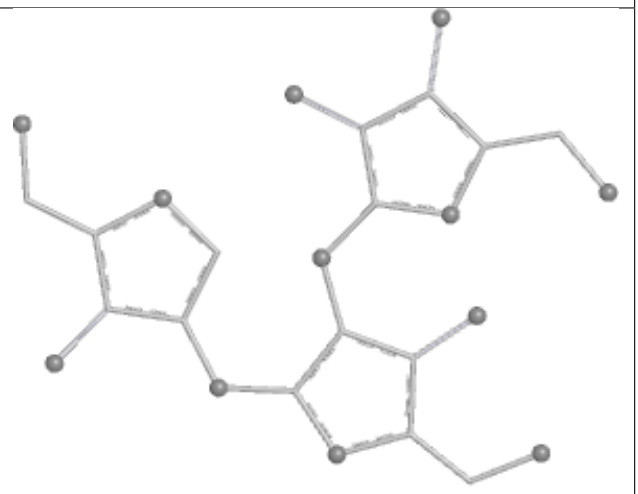
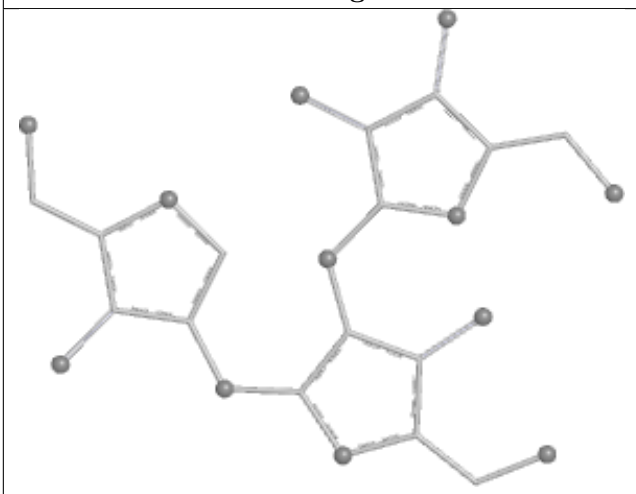
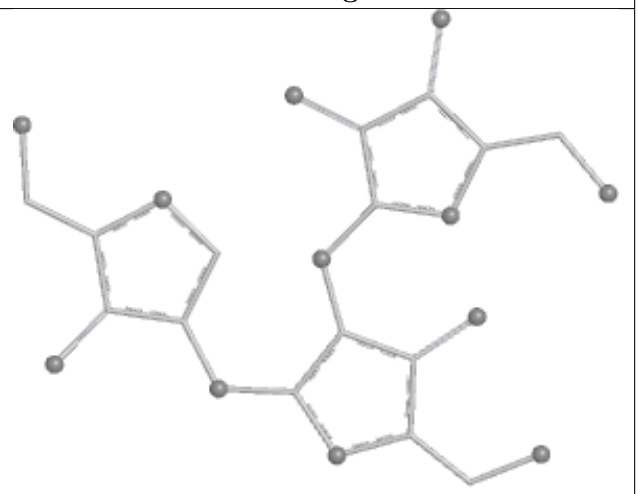
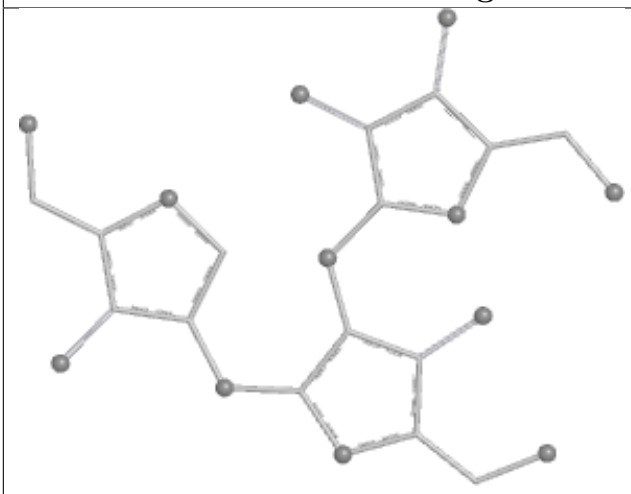
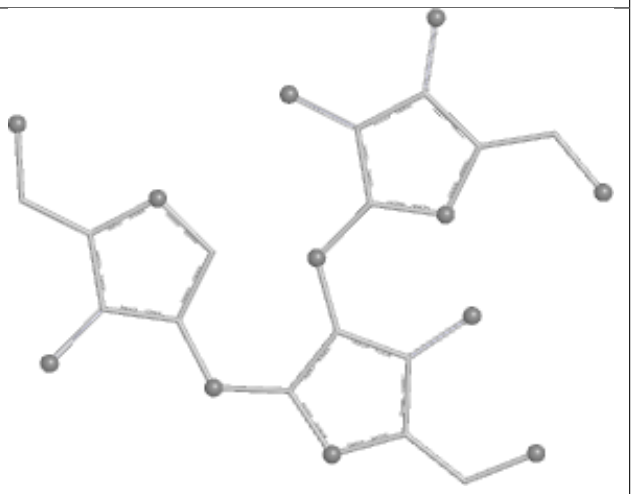
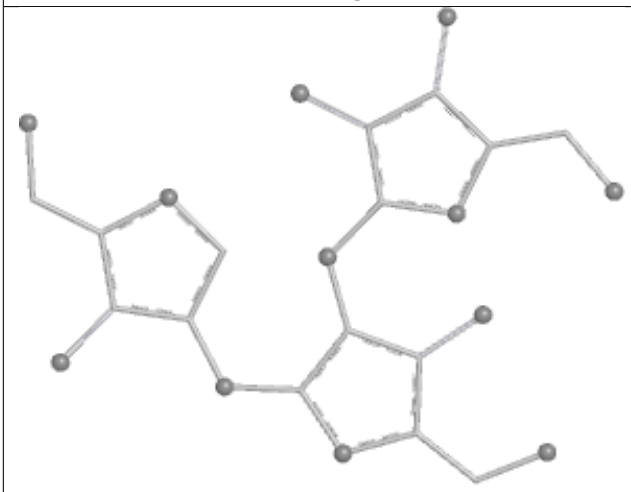
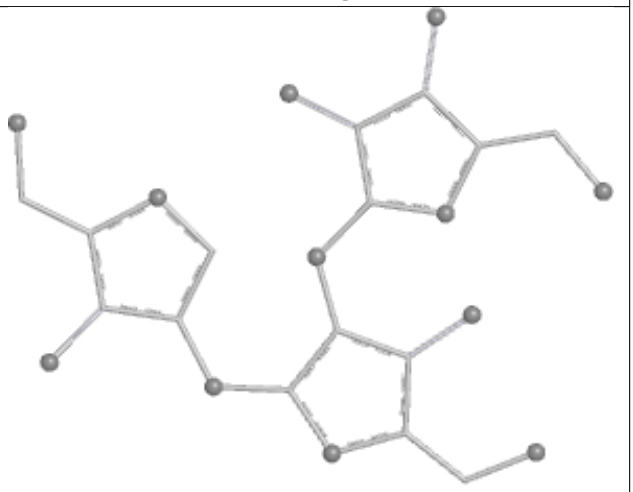
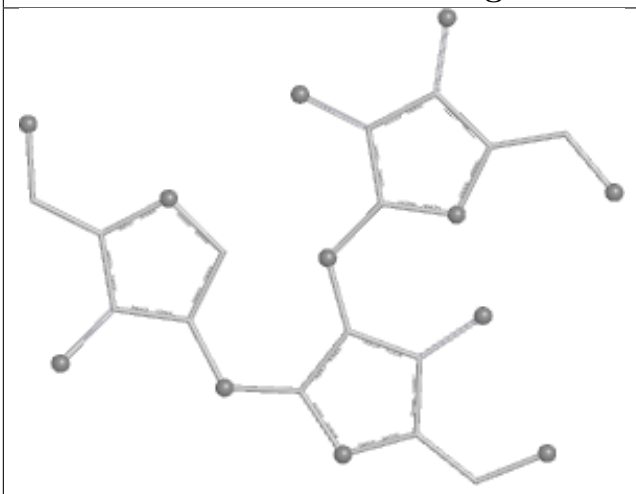
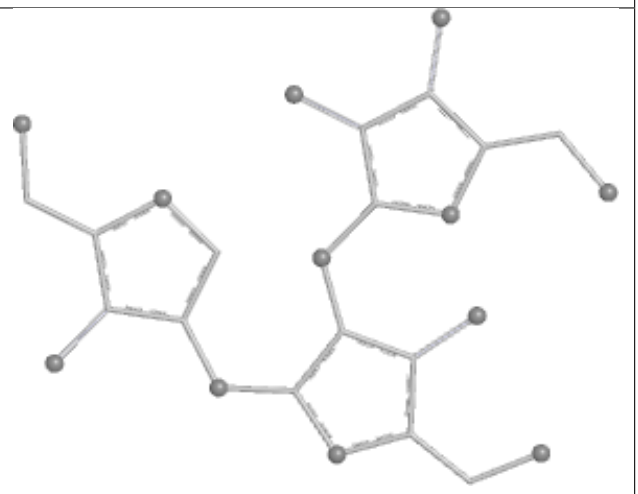
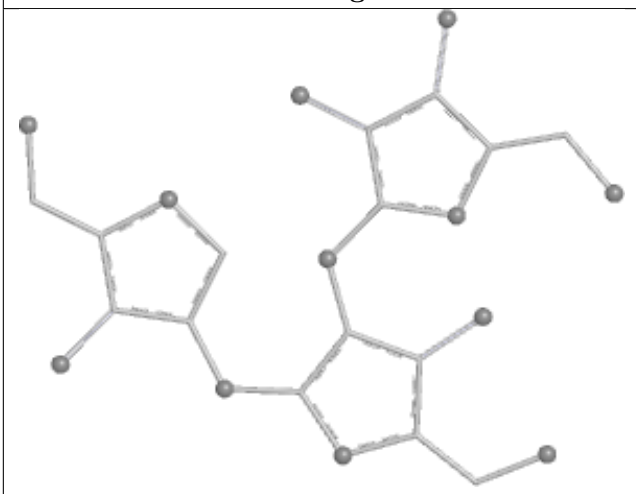
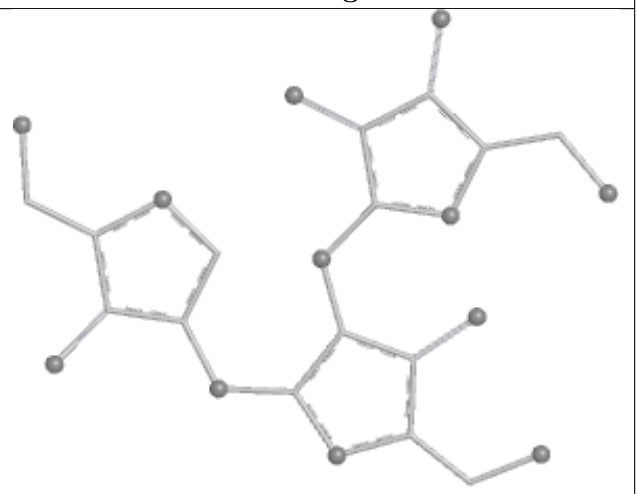
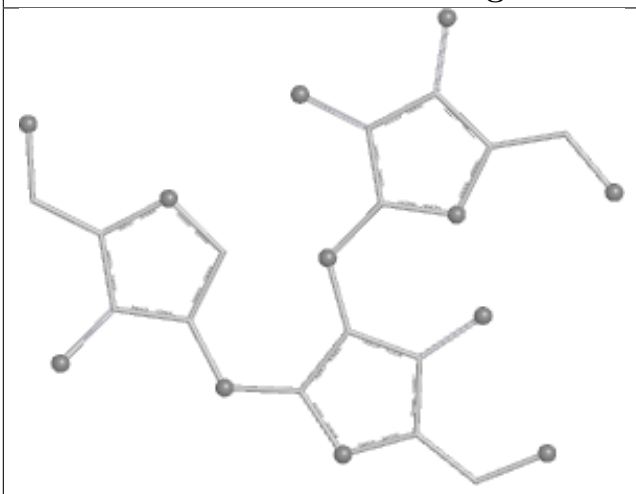
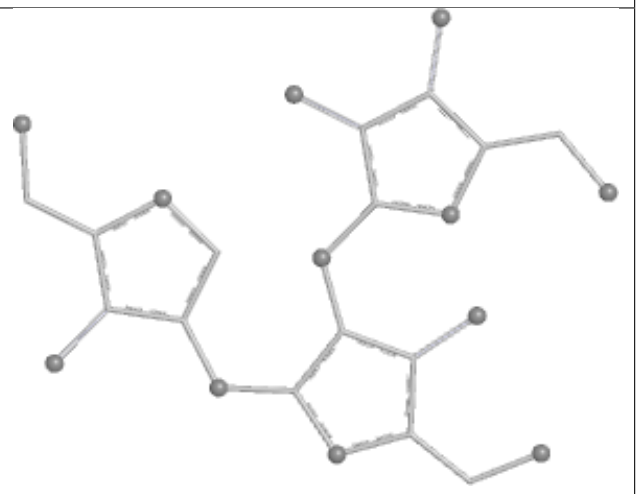
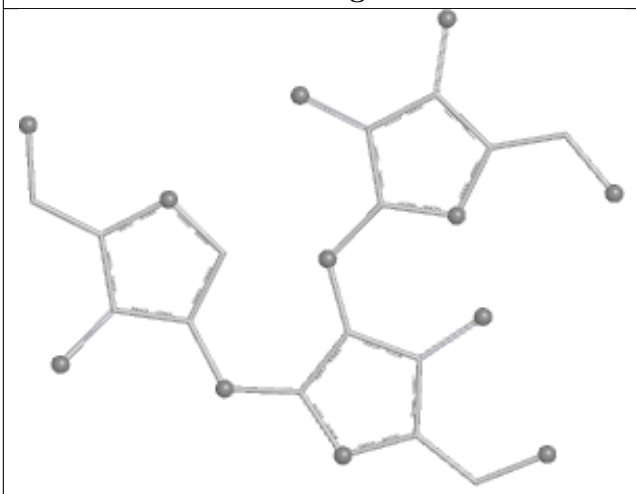
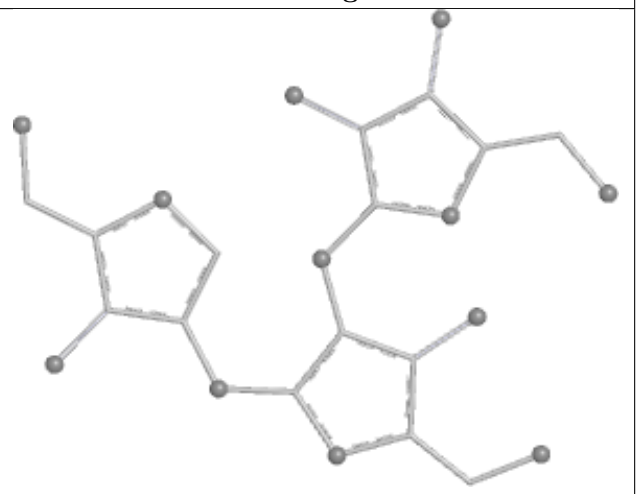
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain WC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain dC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain eC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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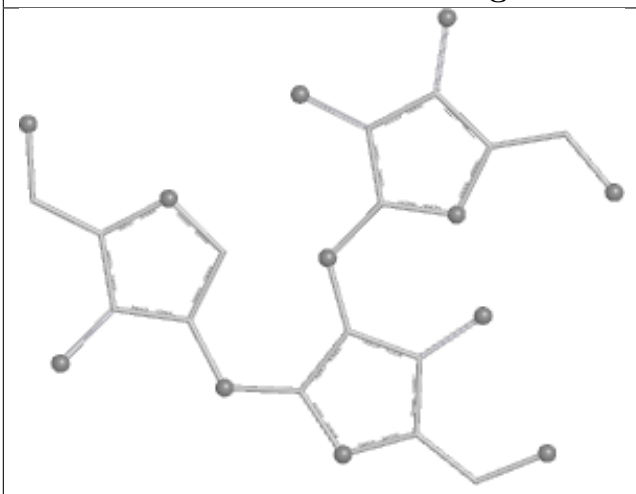
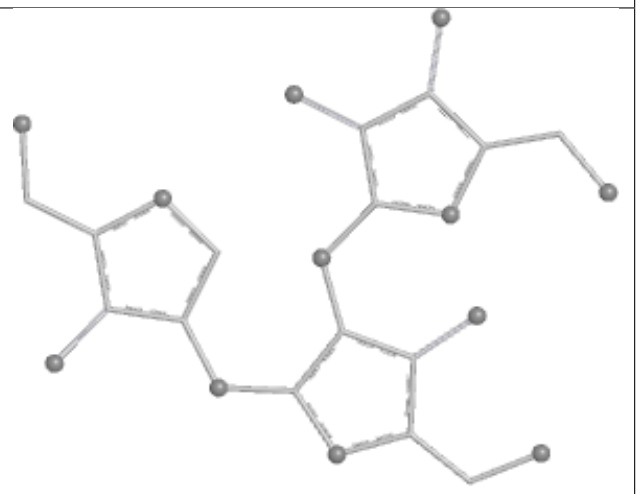
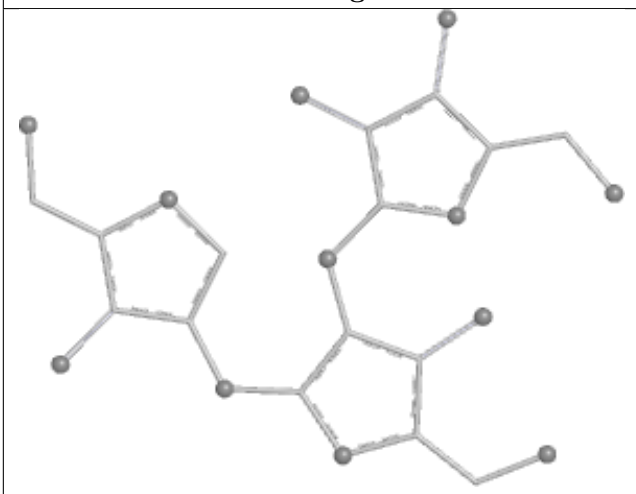
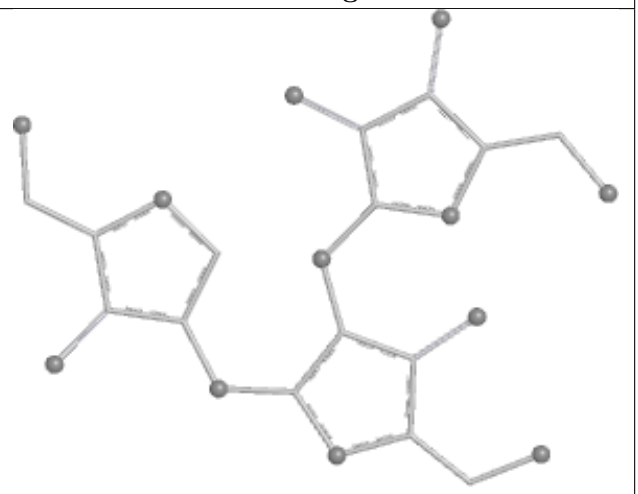
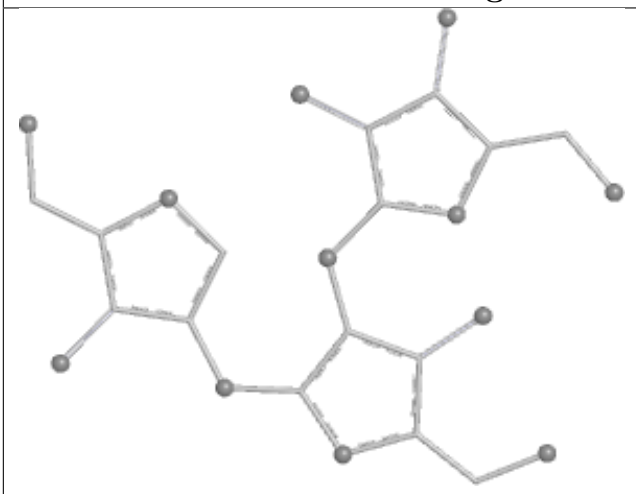
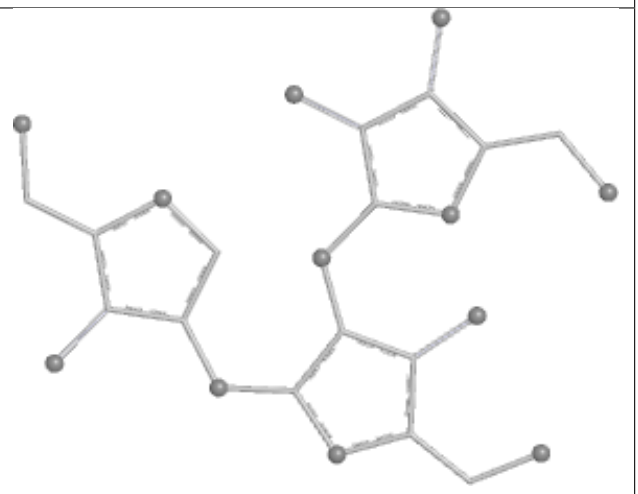
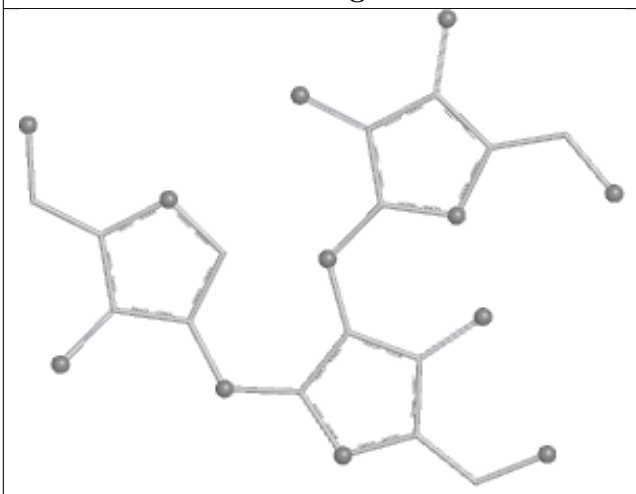
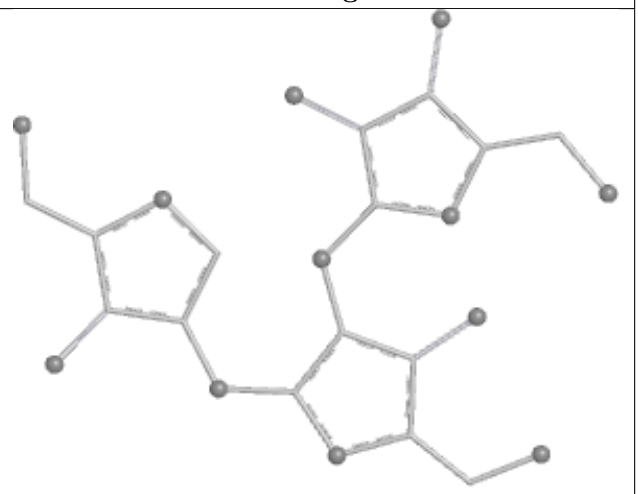
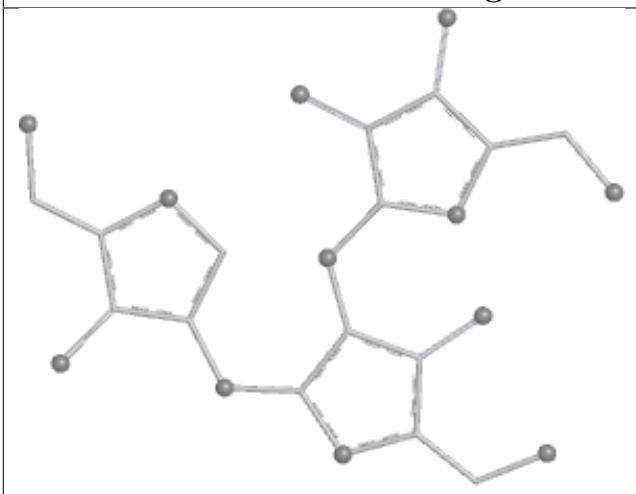
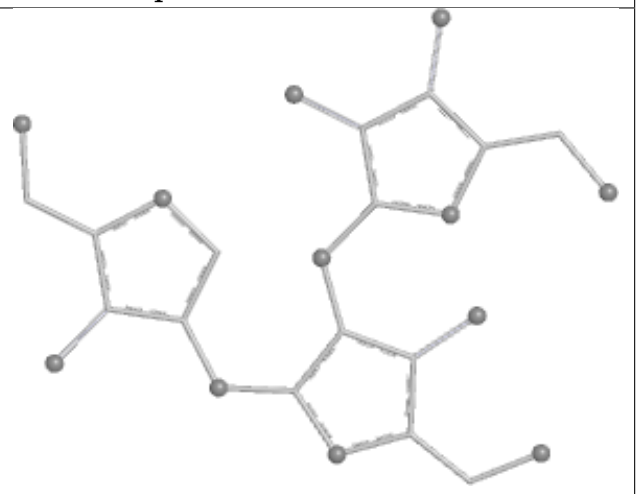
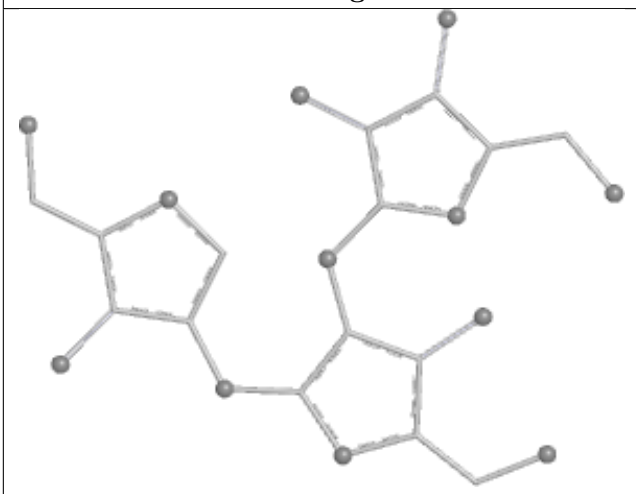
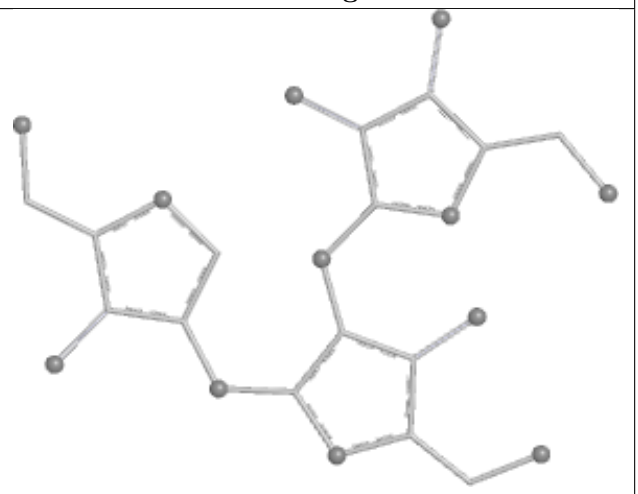
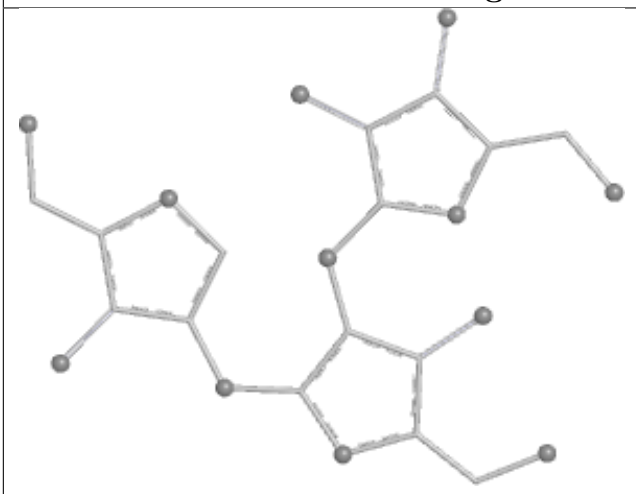
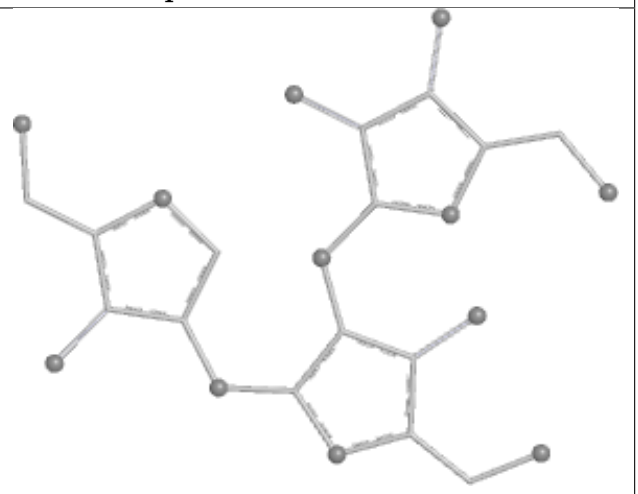
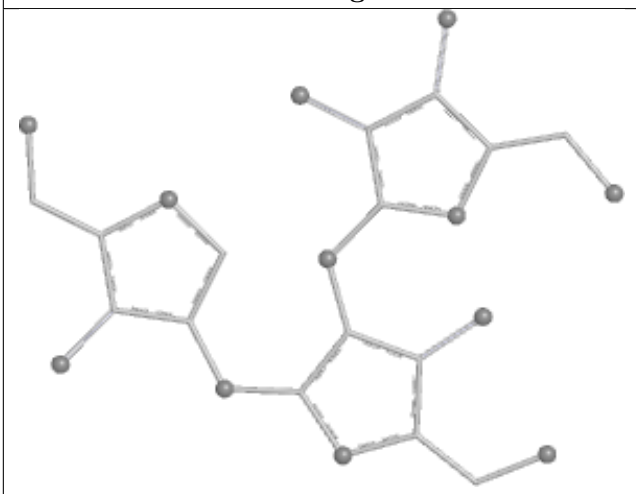
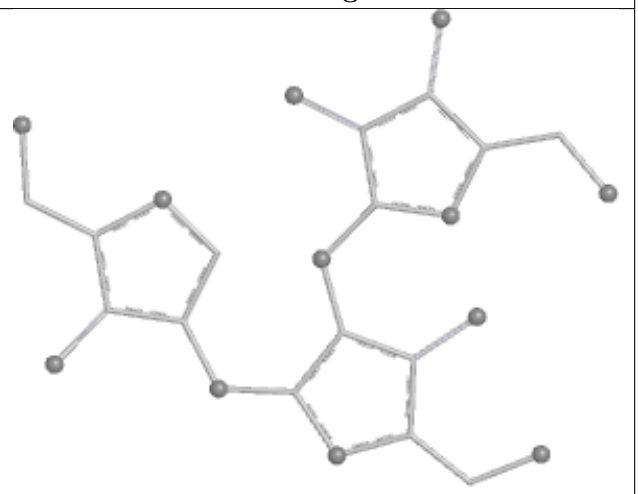
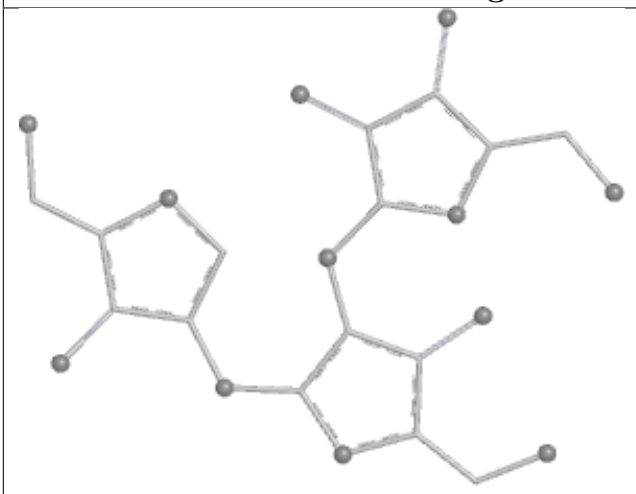
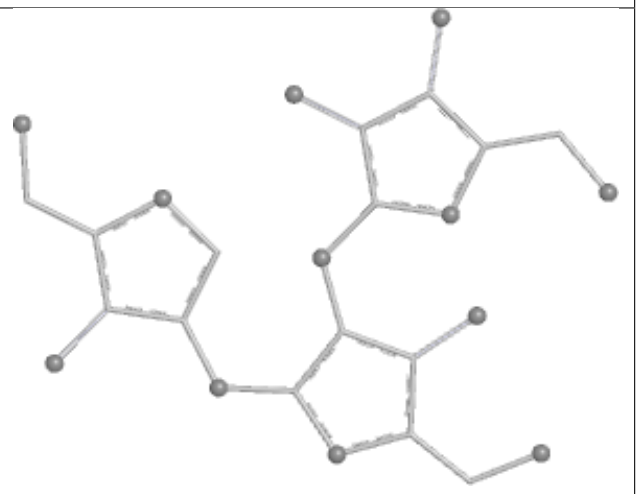
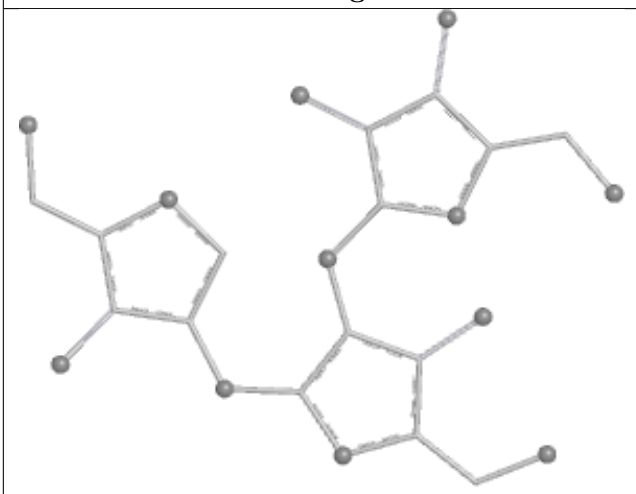
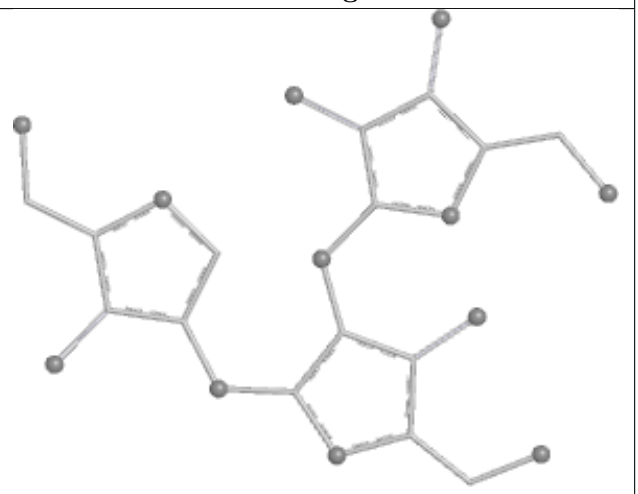
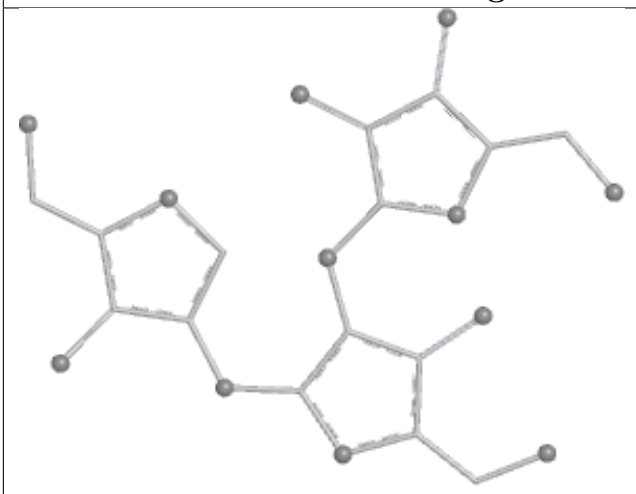
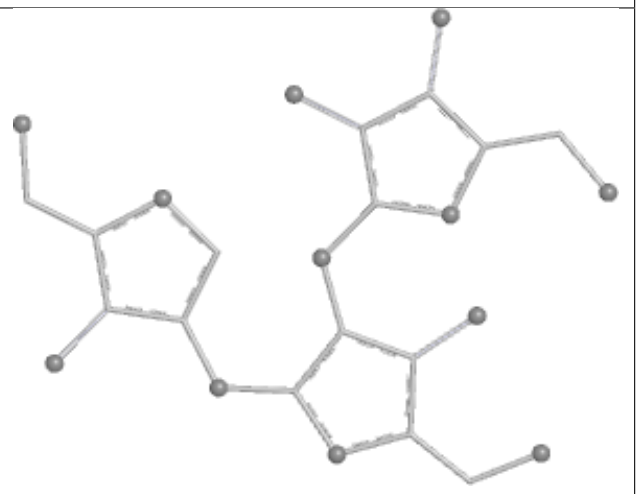
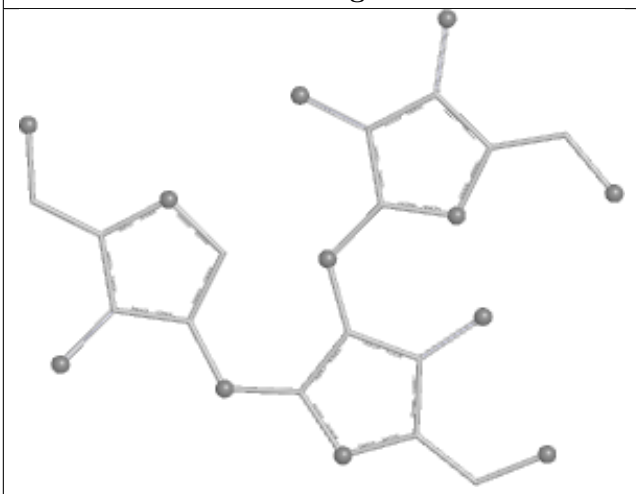
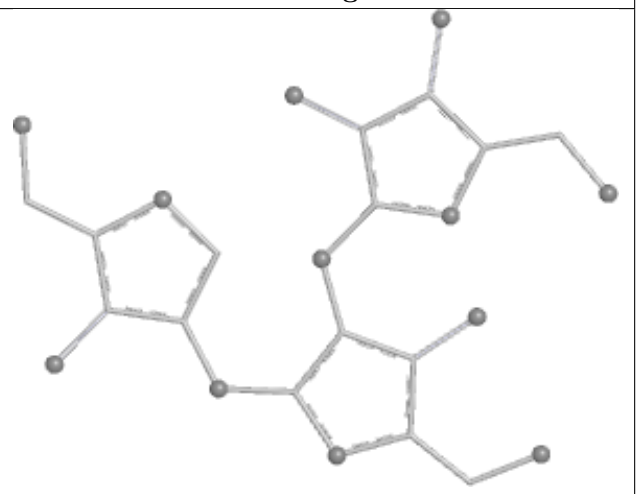
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

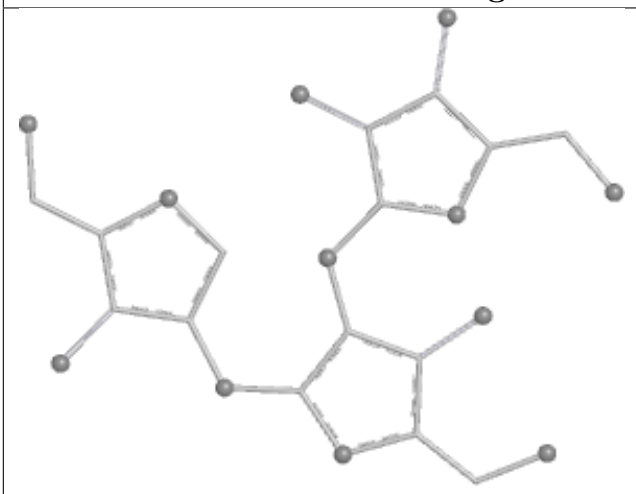
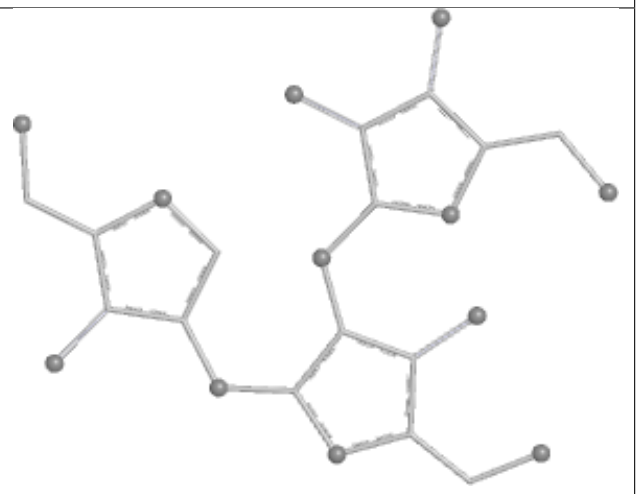
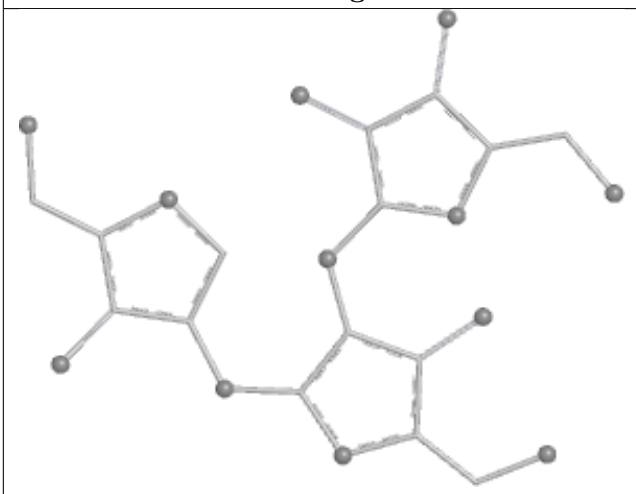
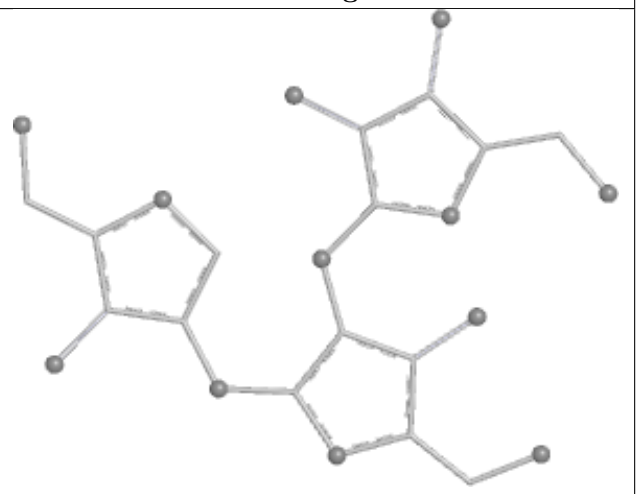
Oligosaccharide Chain oC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain pC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain qC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain rC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain sC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain tC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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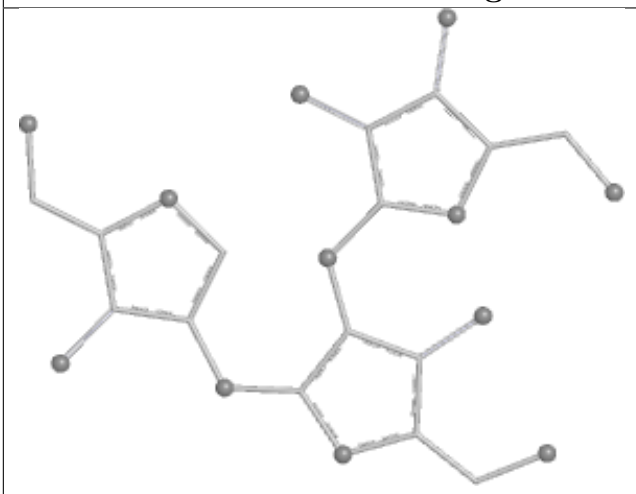
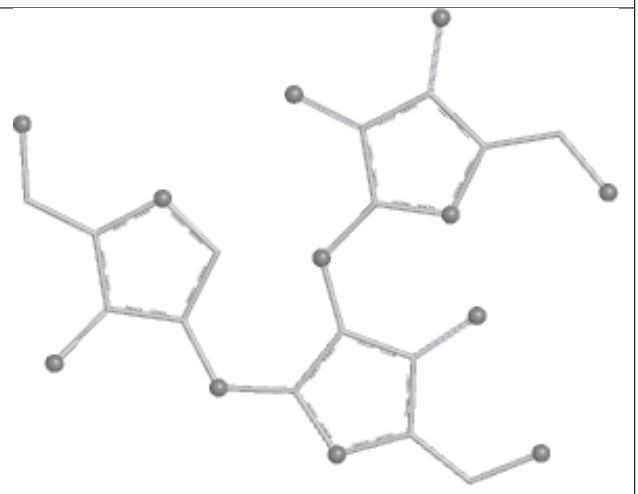
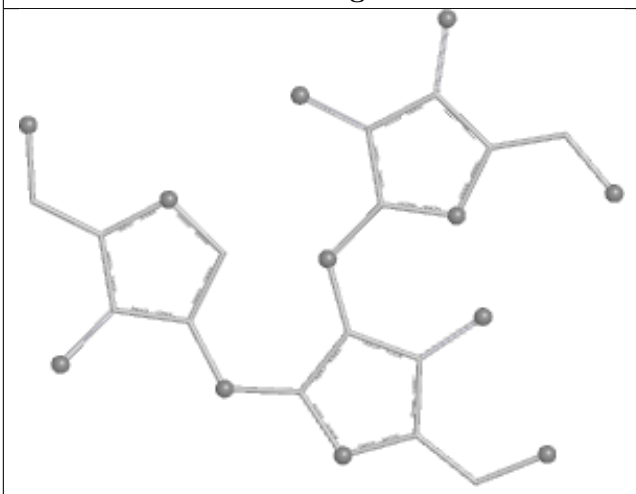
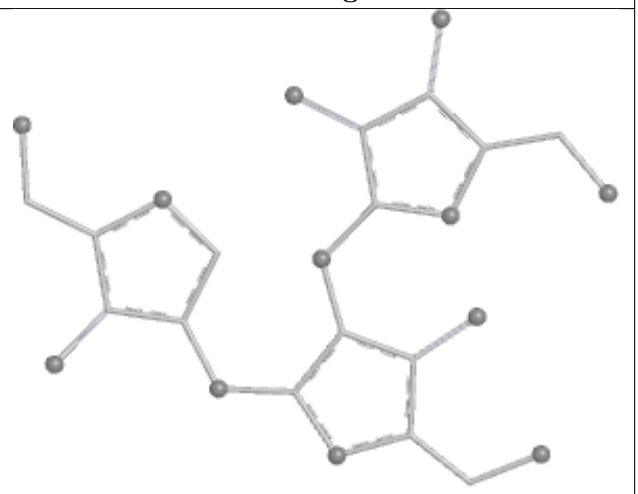
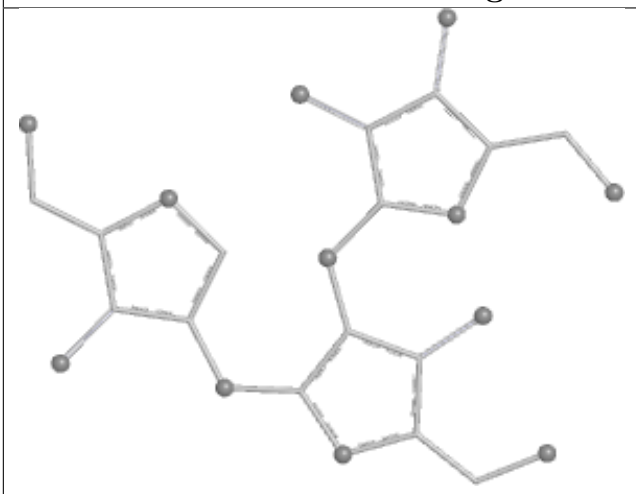
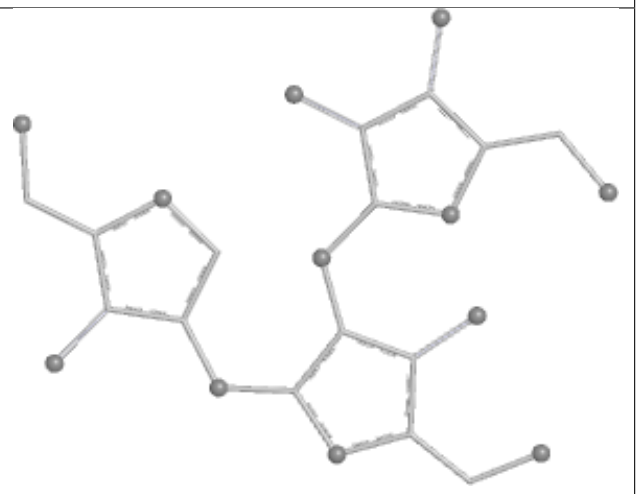
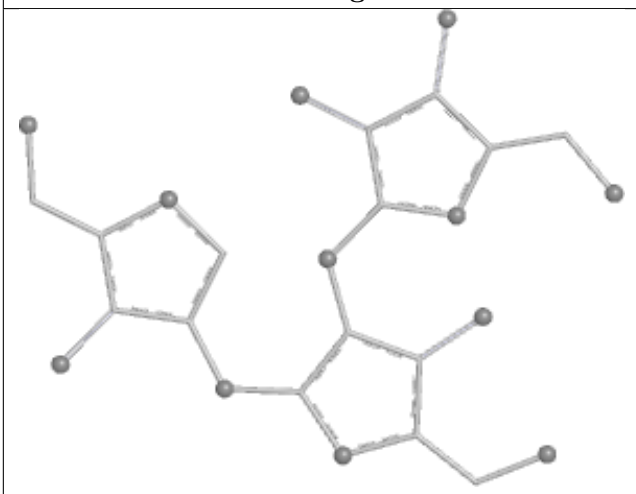
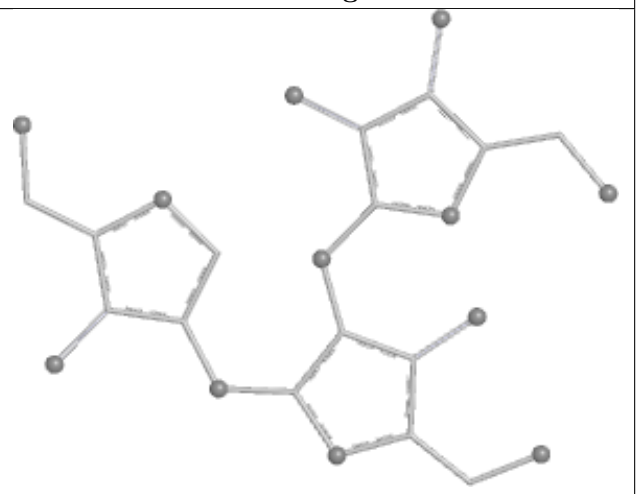
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 8C	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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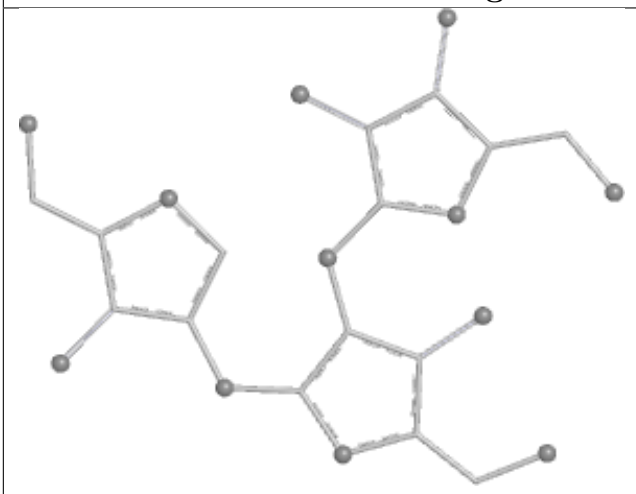
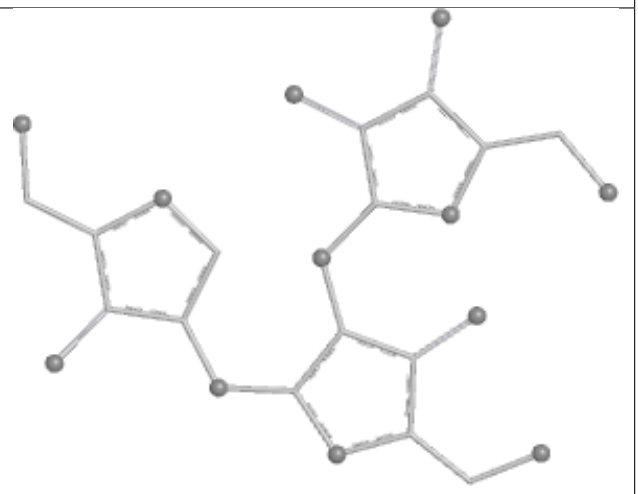
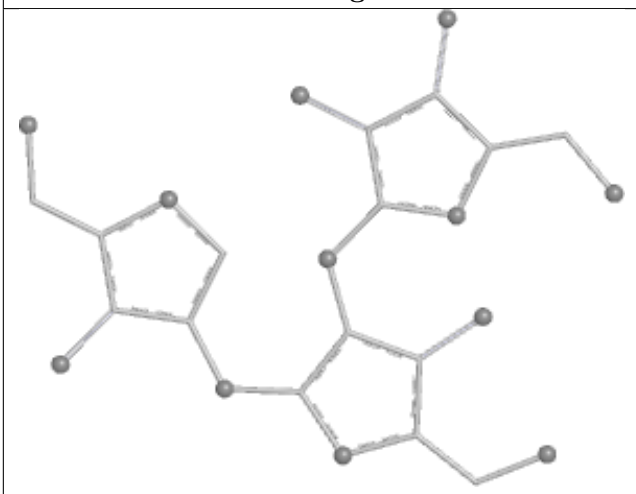
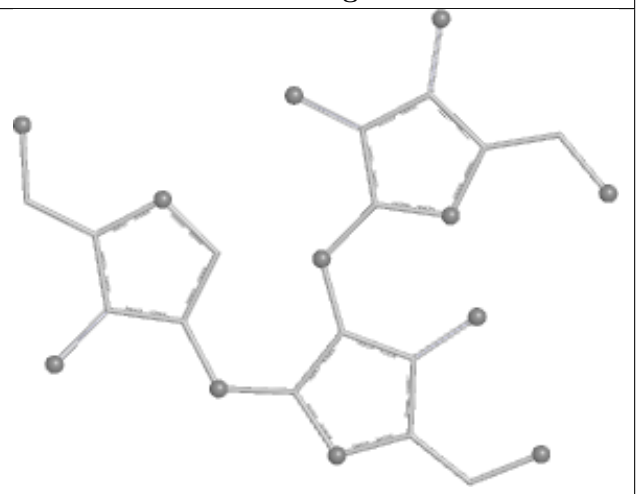
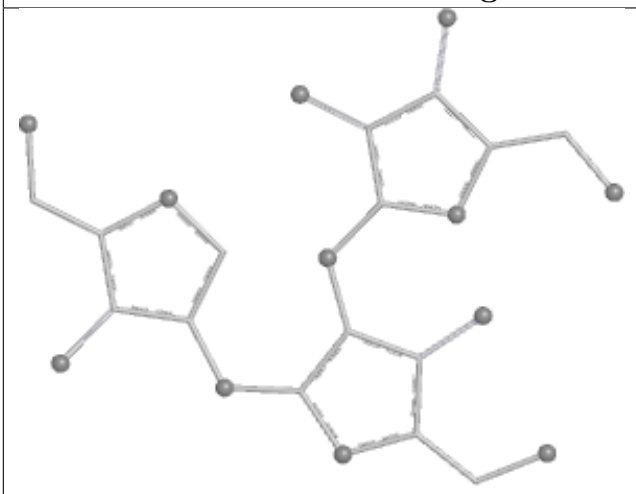
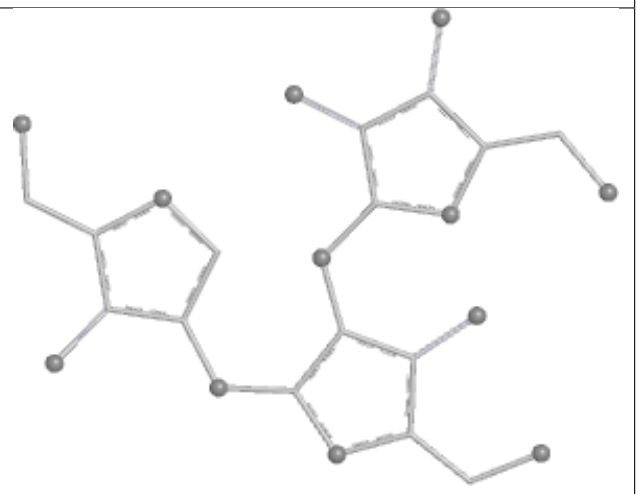
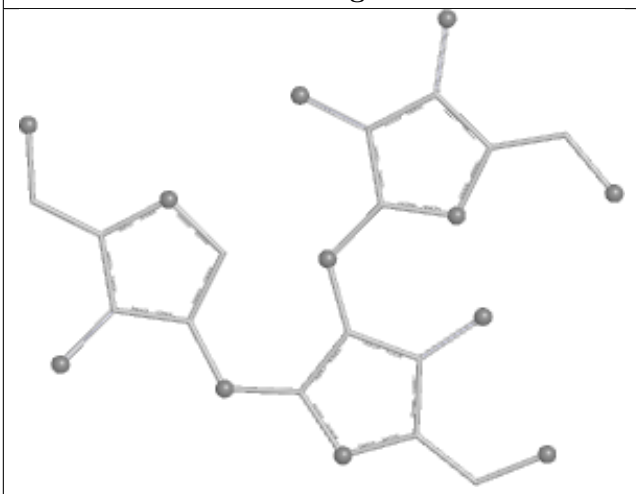
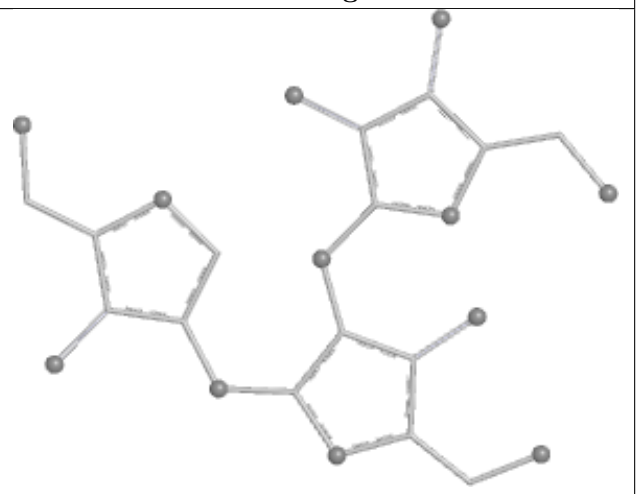
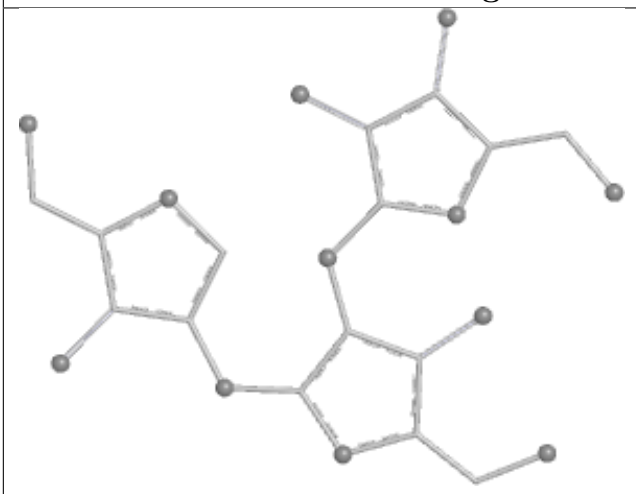
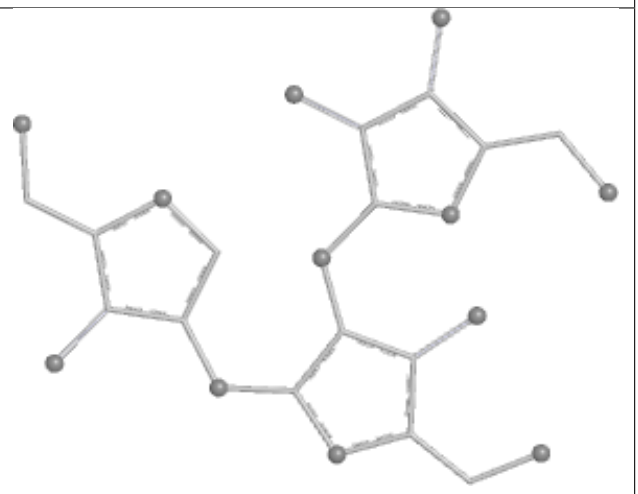
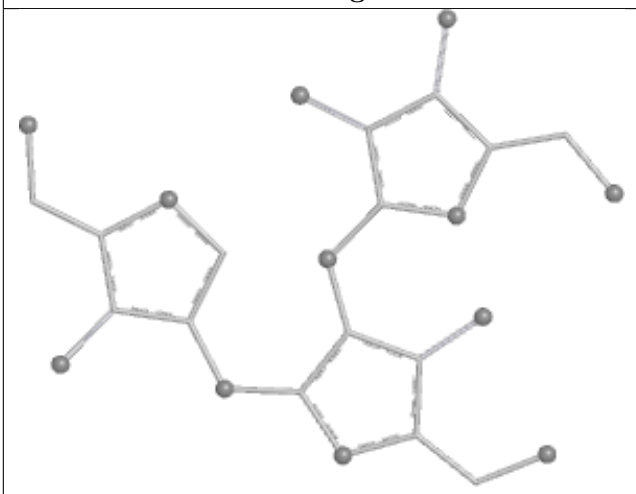
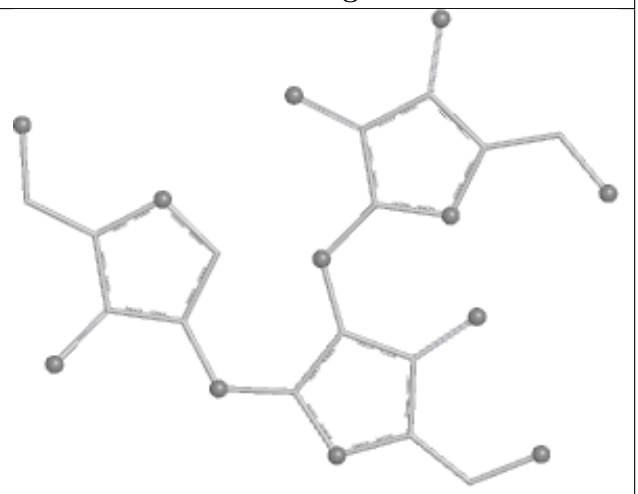
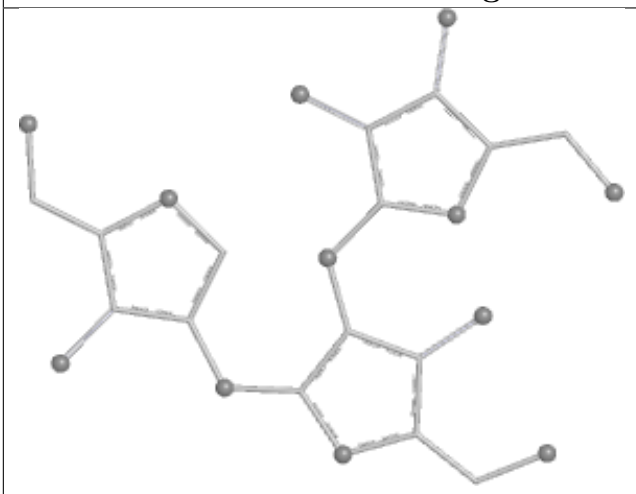
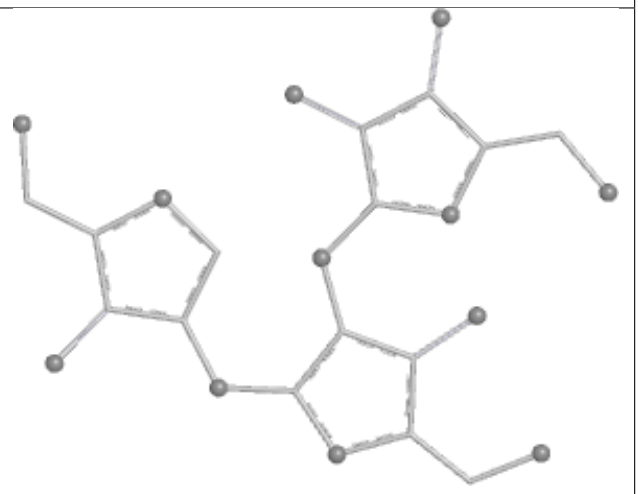
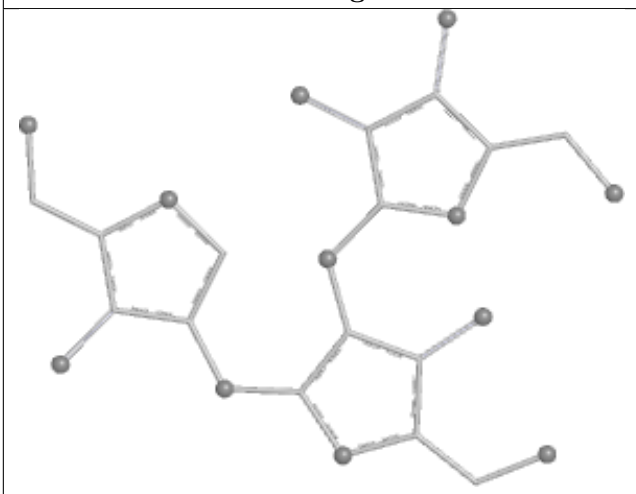
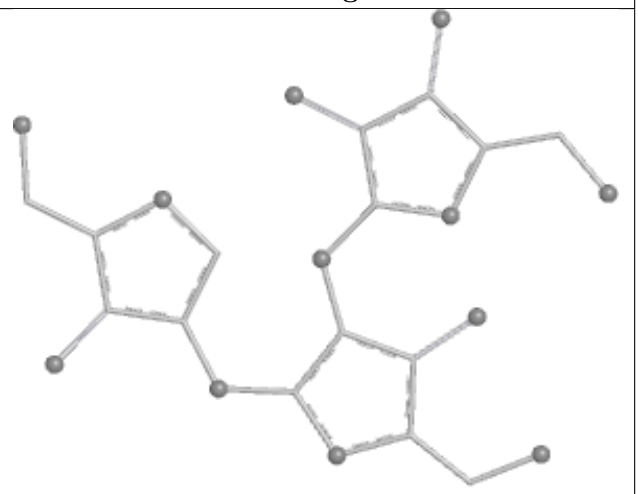
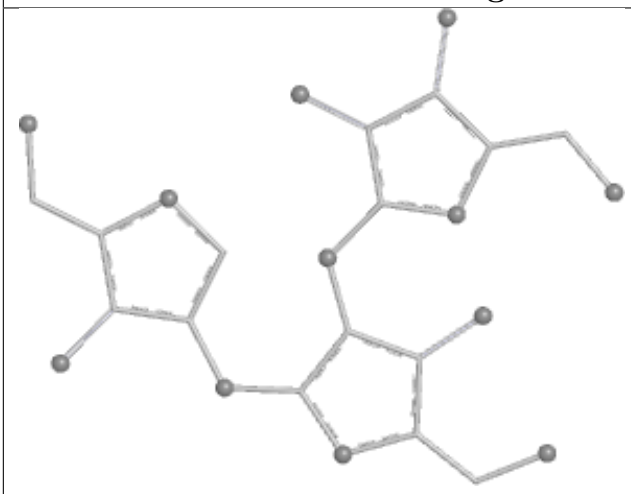
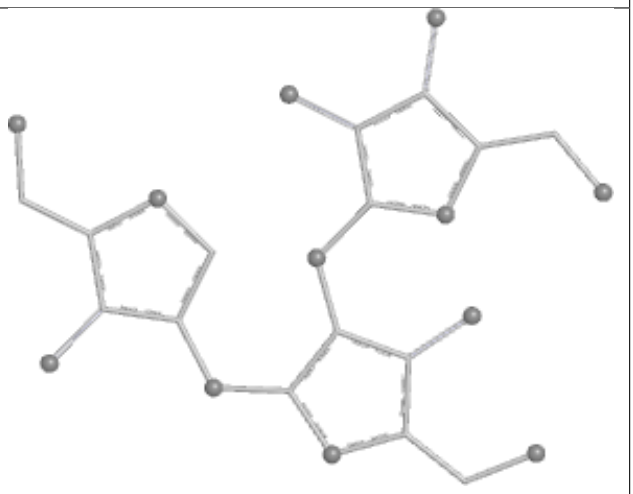
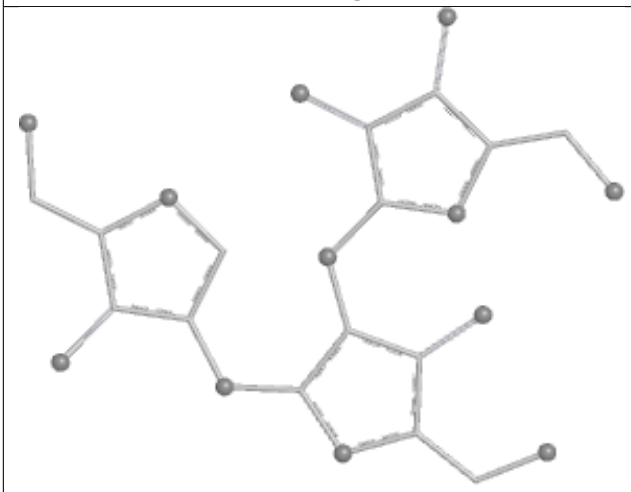
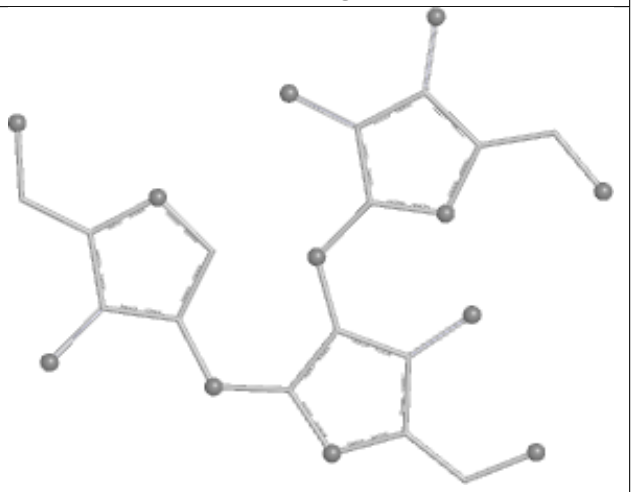
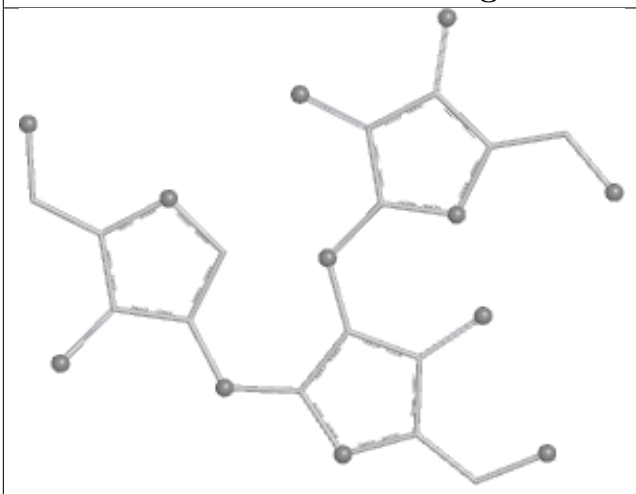
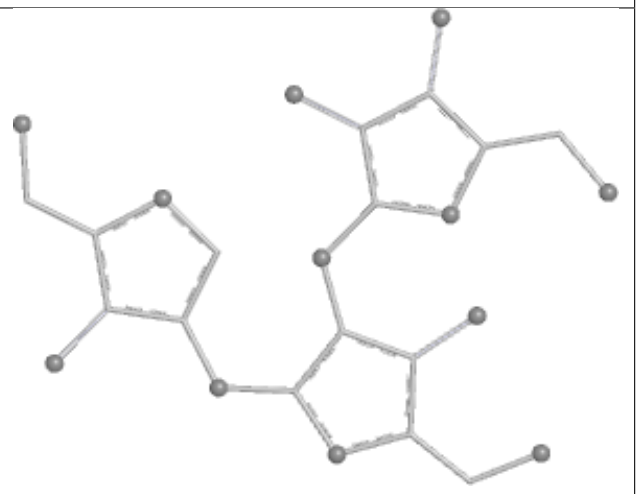
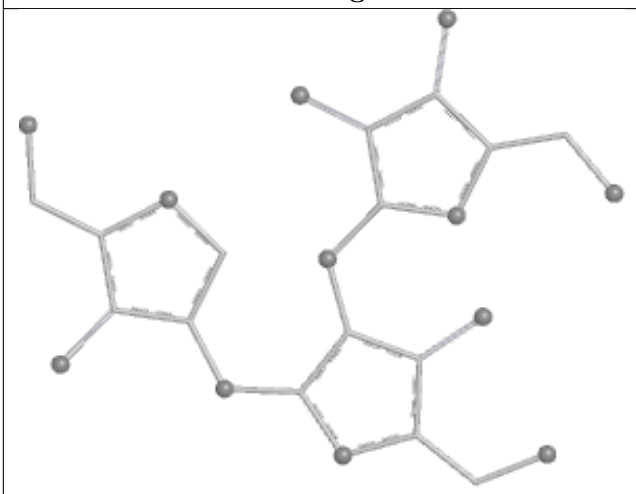
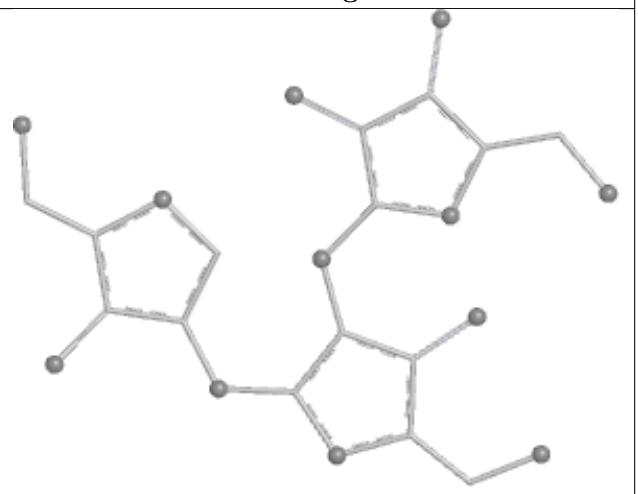
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

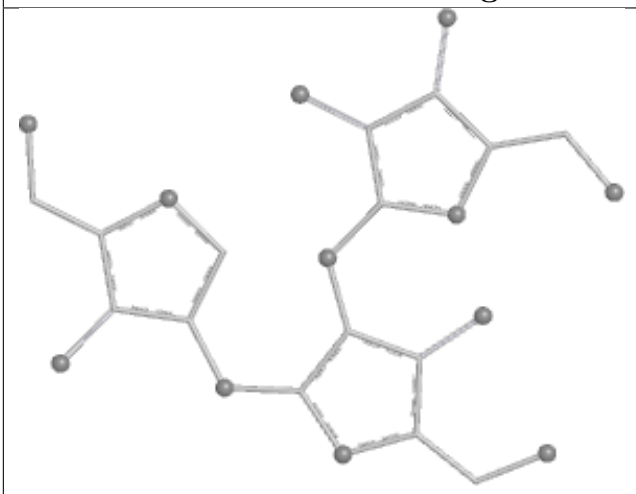
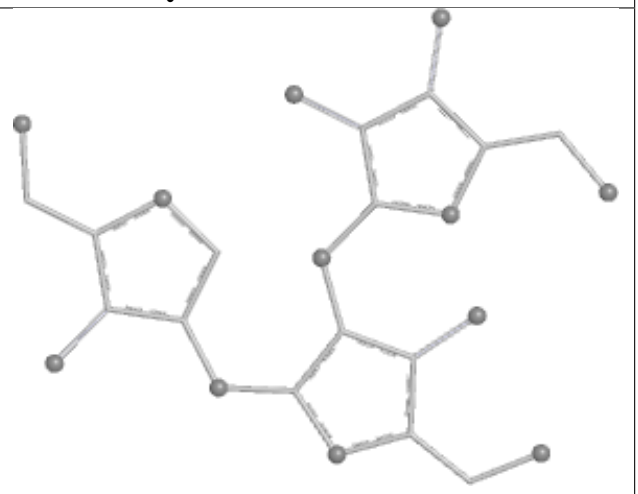
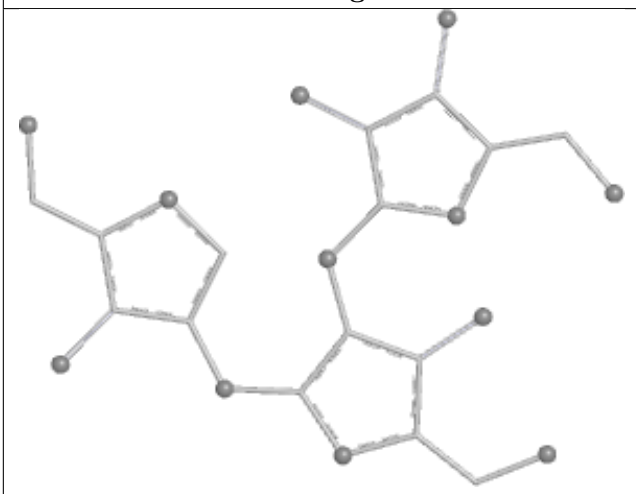
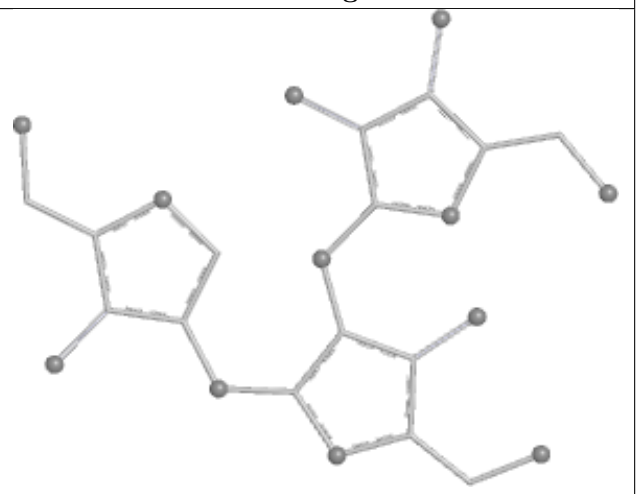
Oligosaccharide Chain DD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

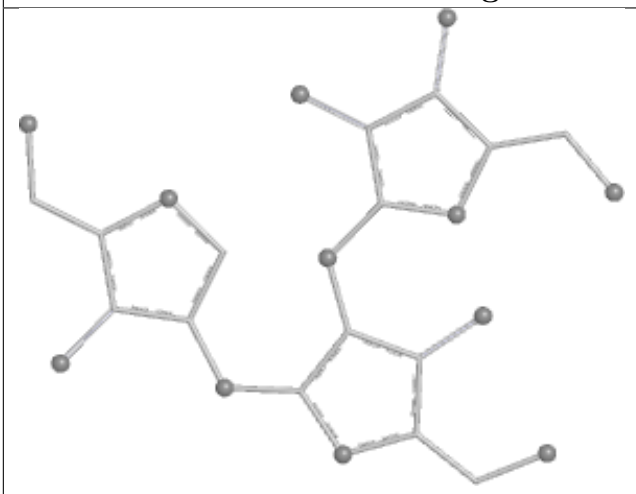
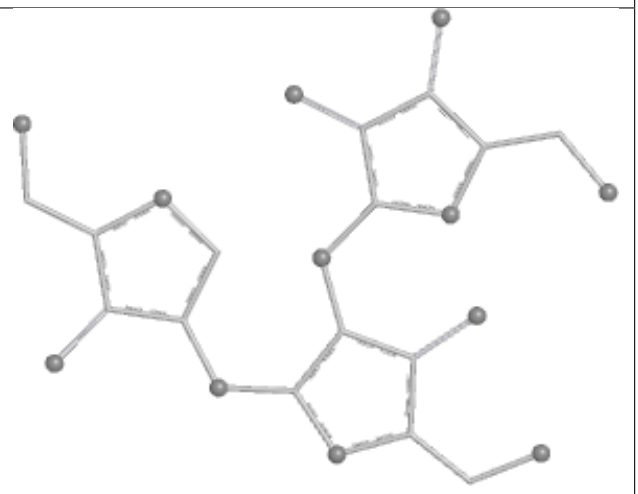
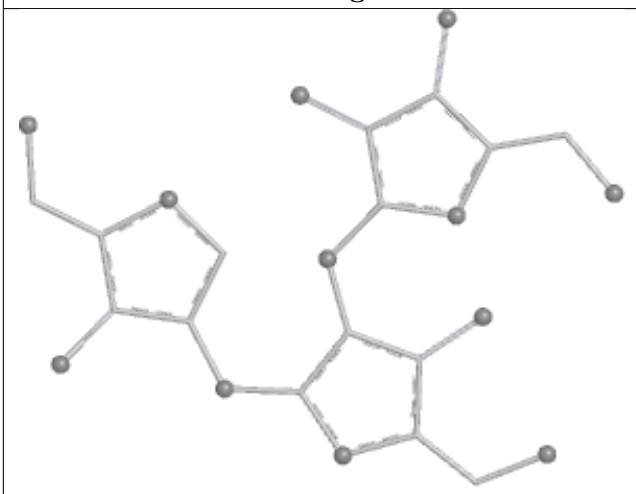
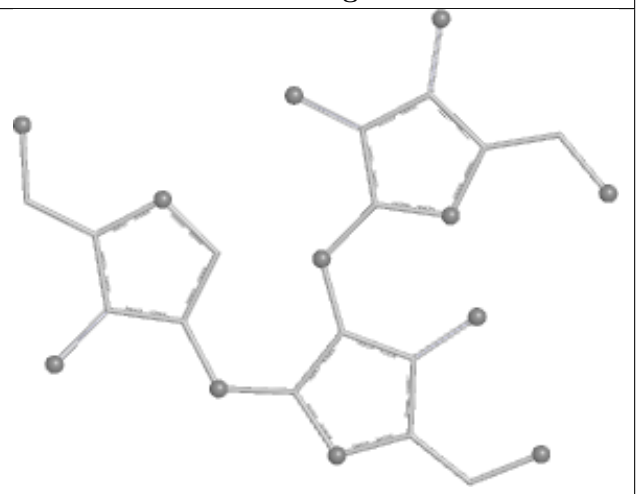
Oligosaccharide Chain ED	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

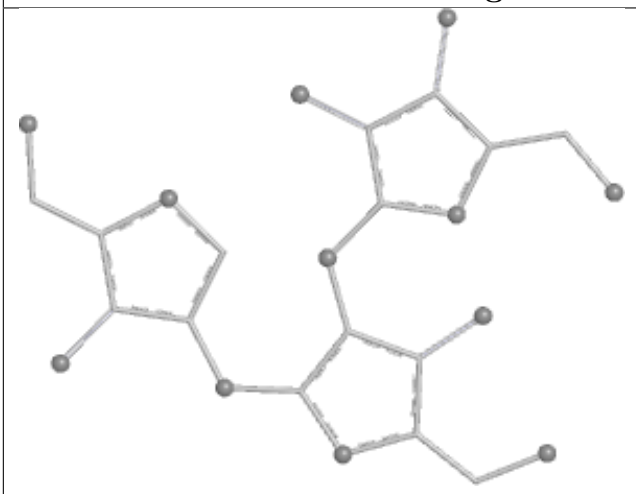
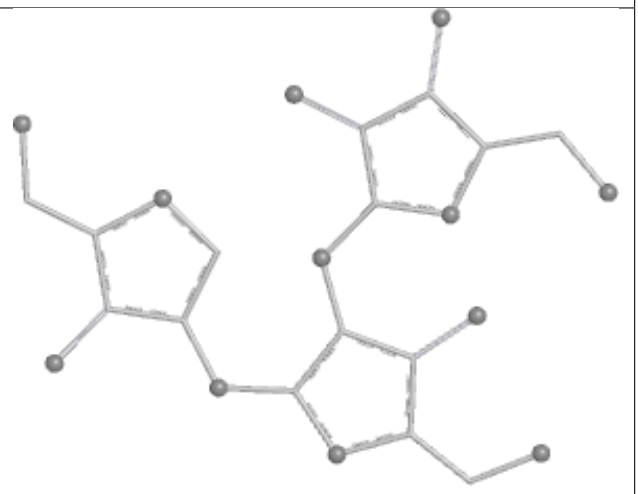
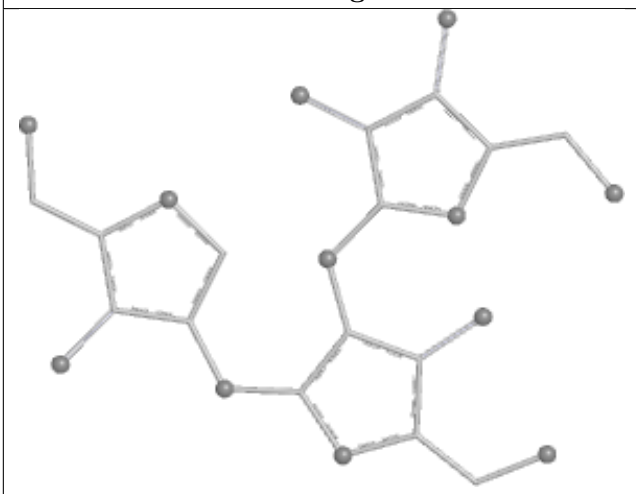
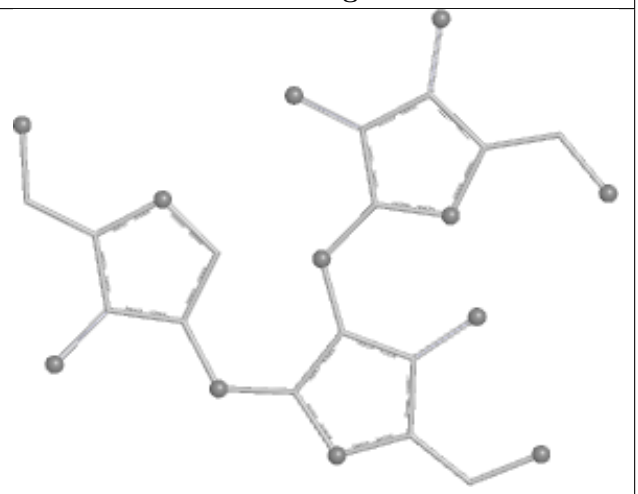
Oligosaccharide Chain FD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

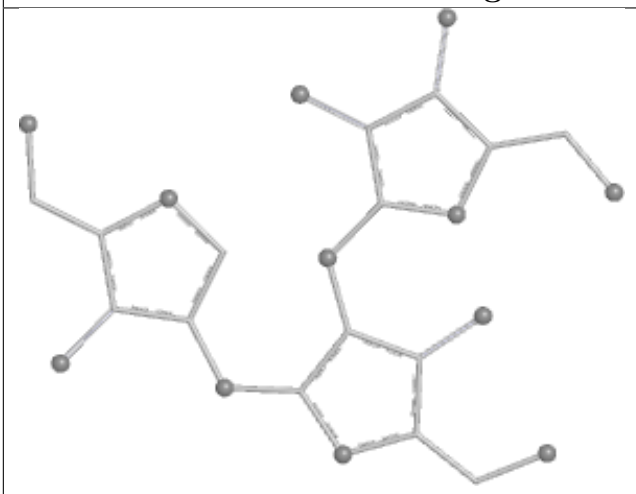
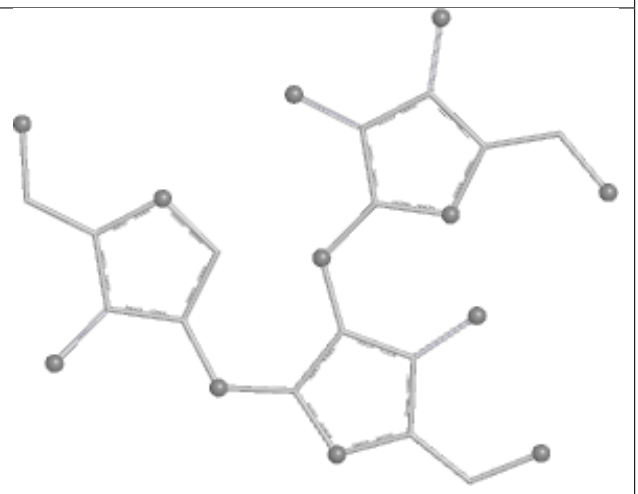
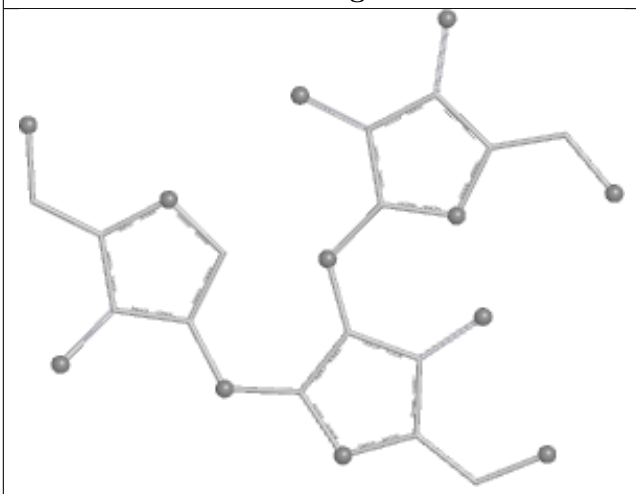
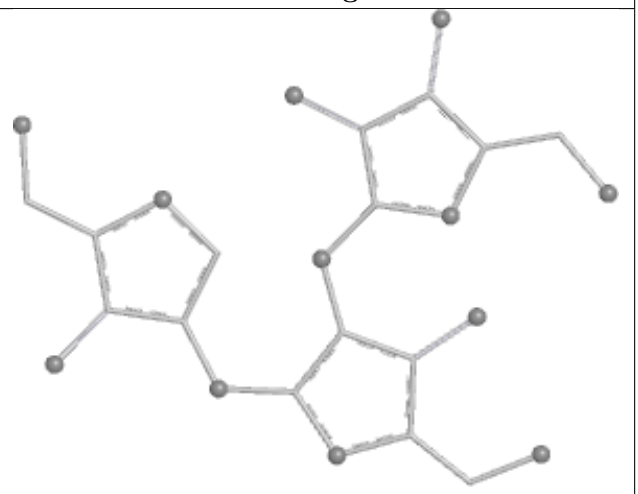
Oligosaccharide Chain ID	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

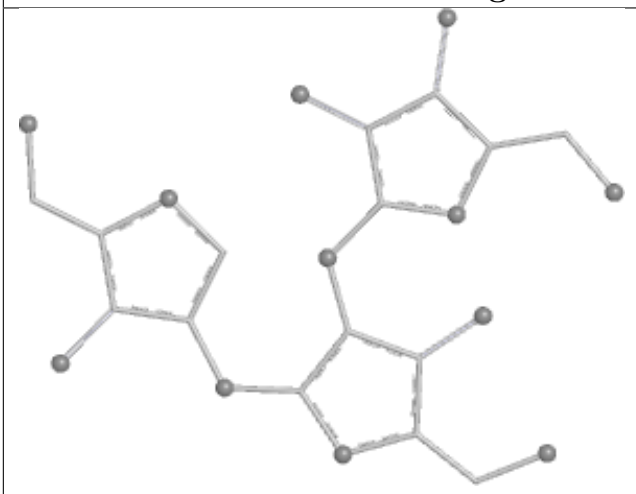
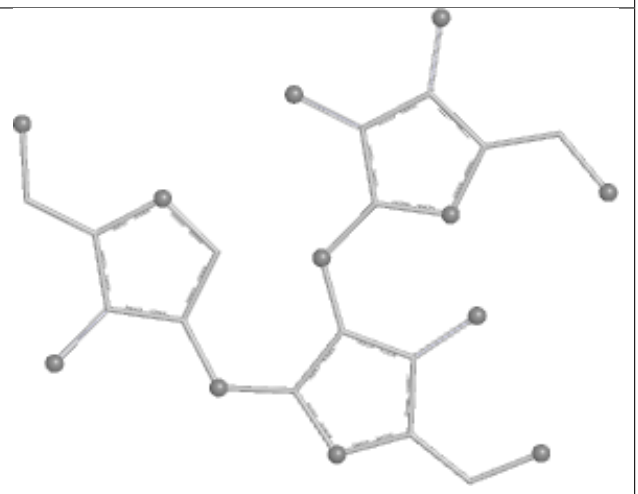
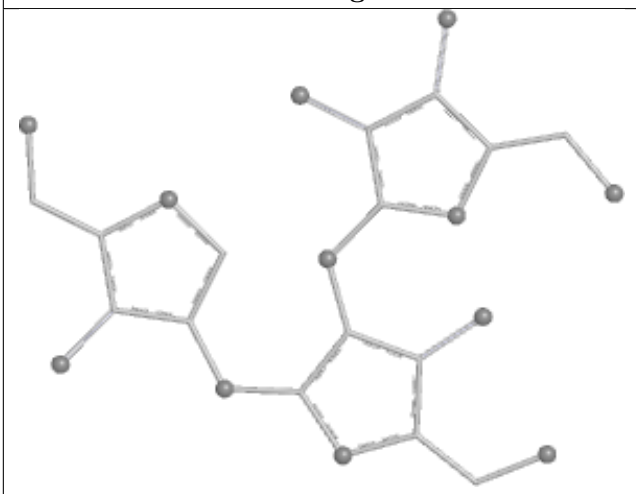
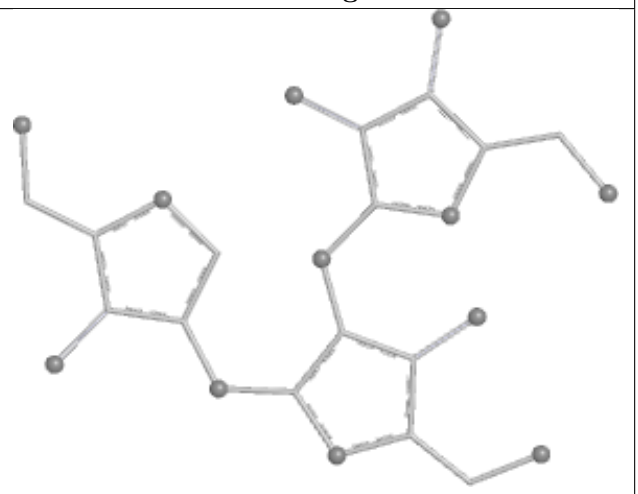
Oligosaccharide Chain KD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain QD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain TD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain aD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain bD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain iD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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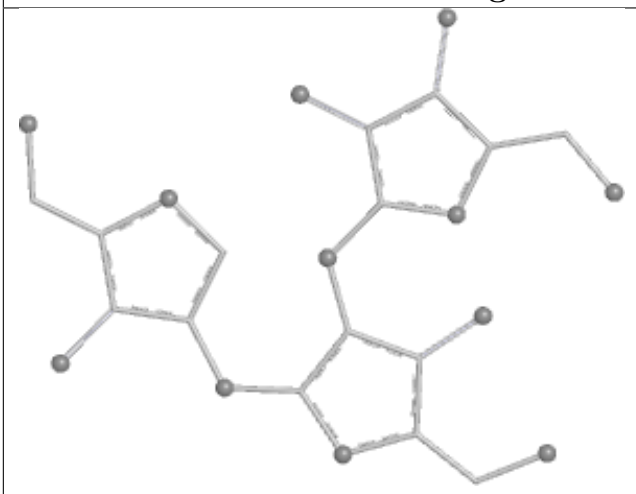
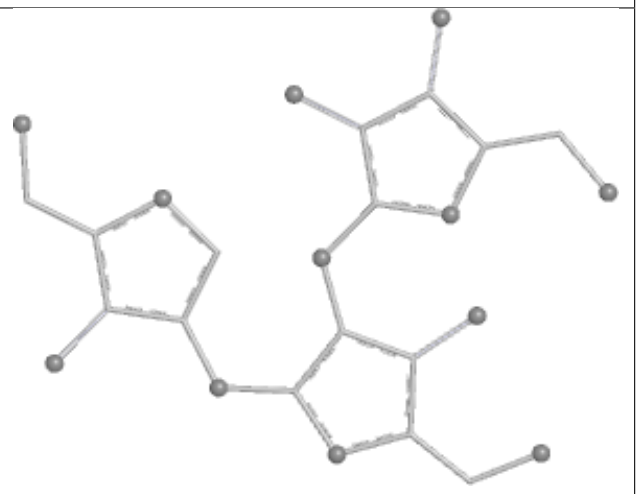
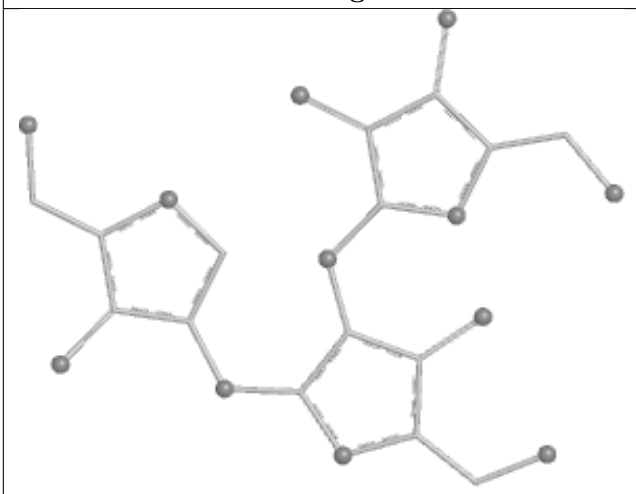
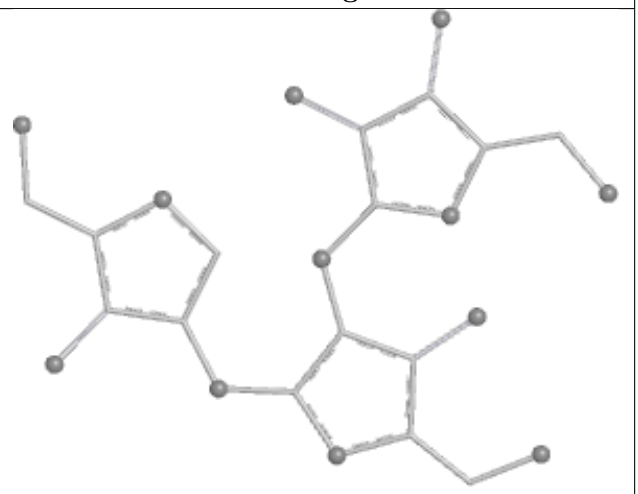
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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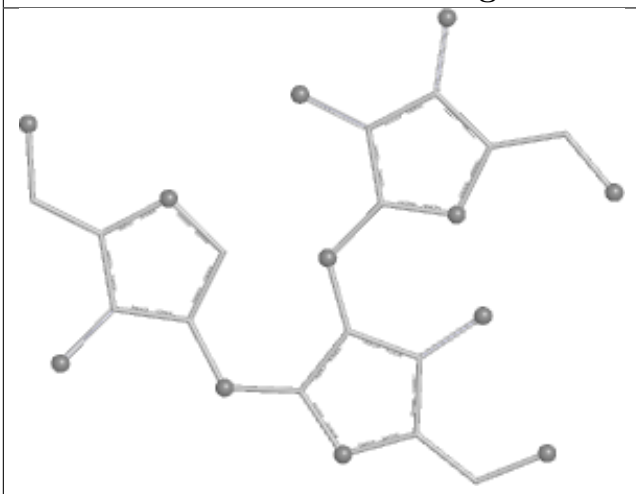
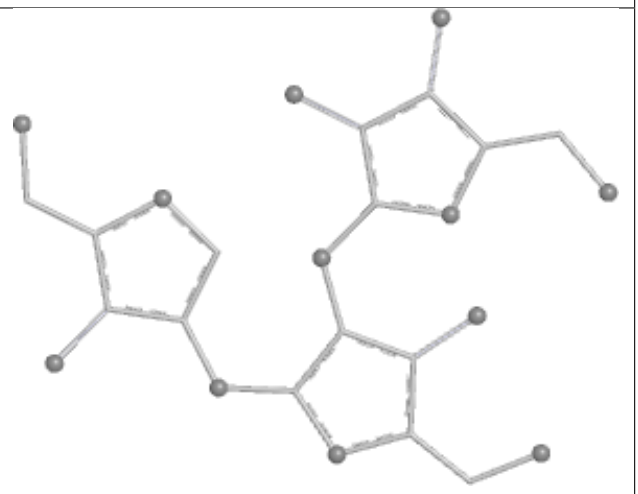
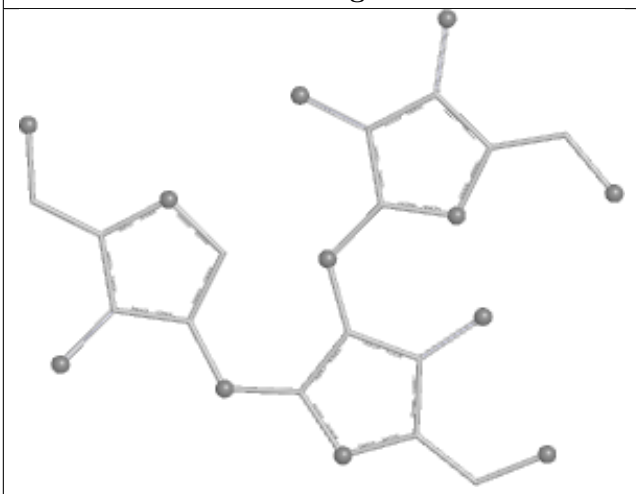
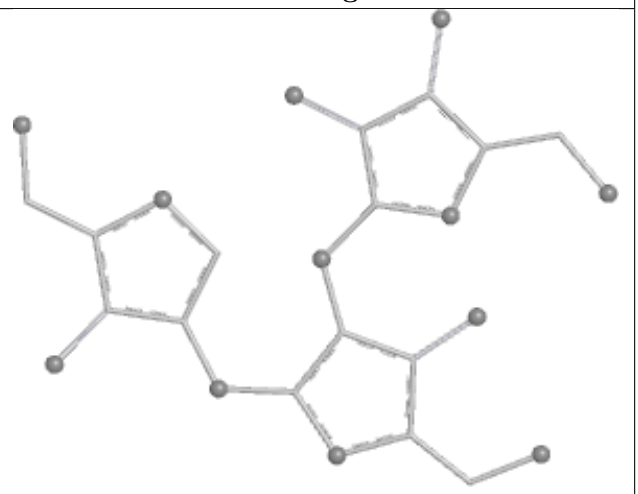
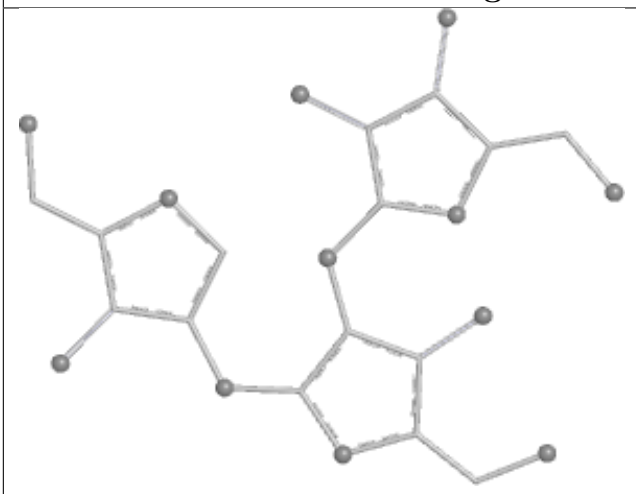
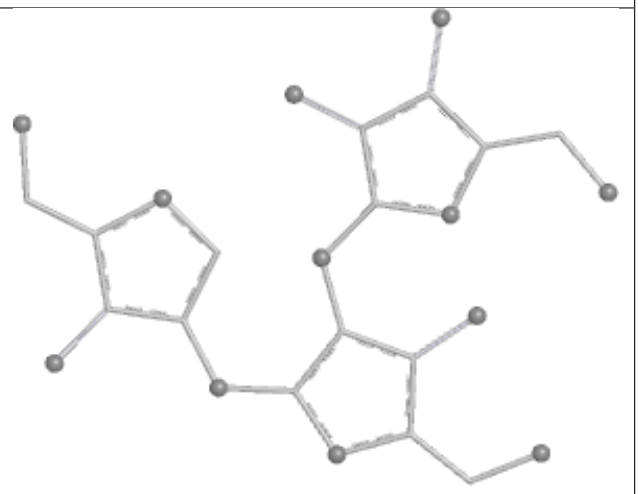
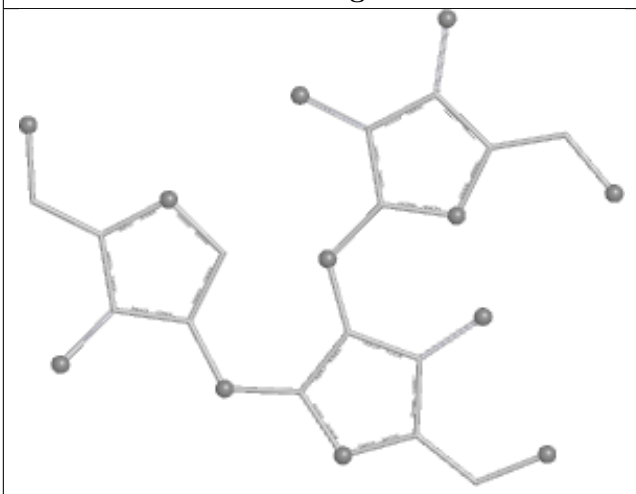
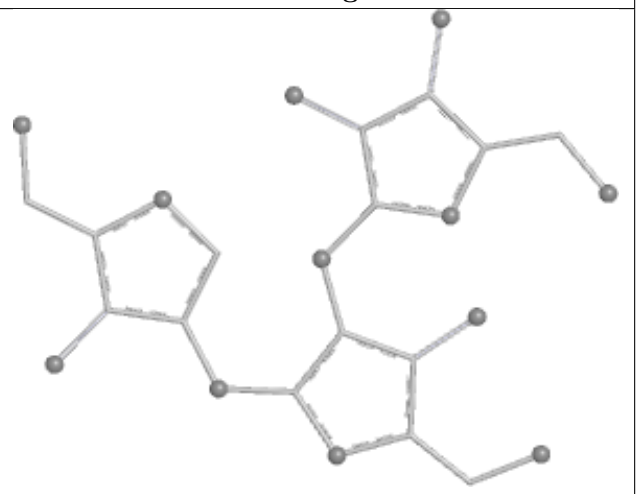
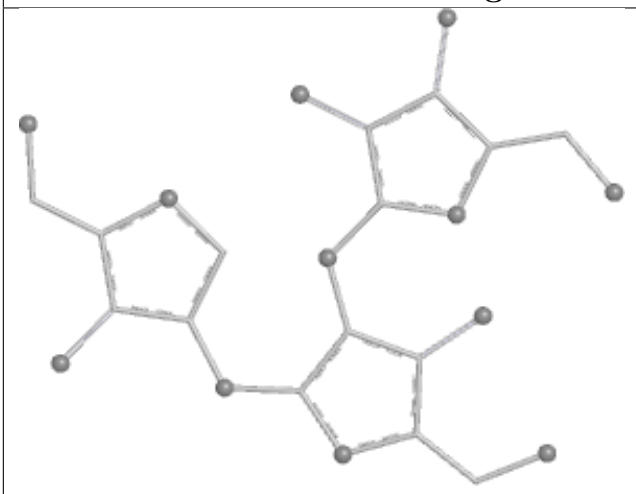
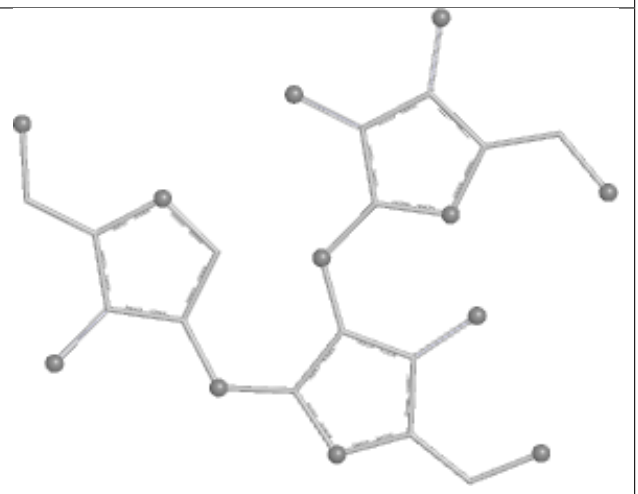
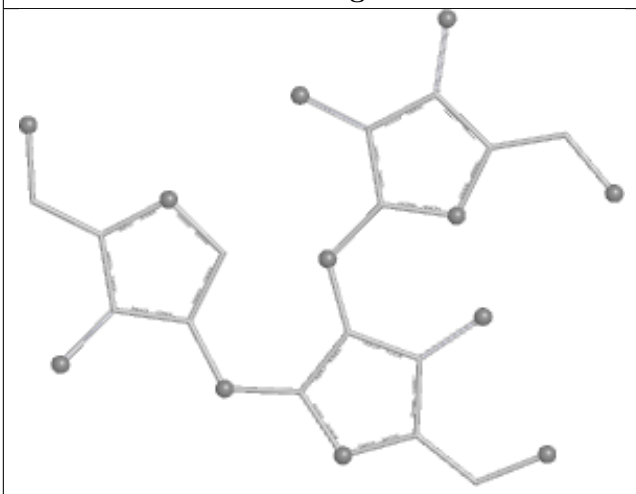
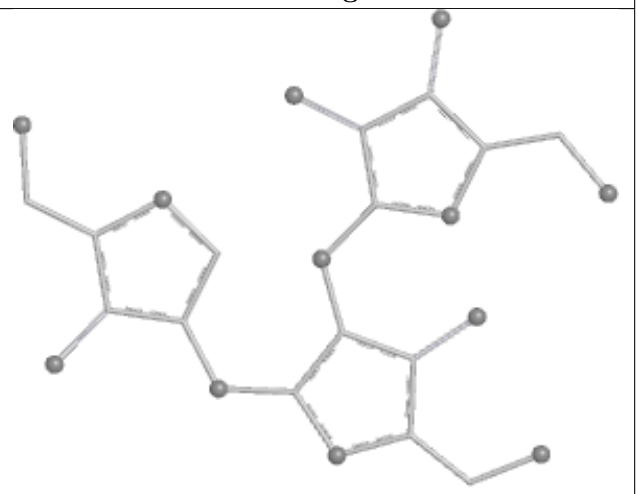
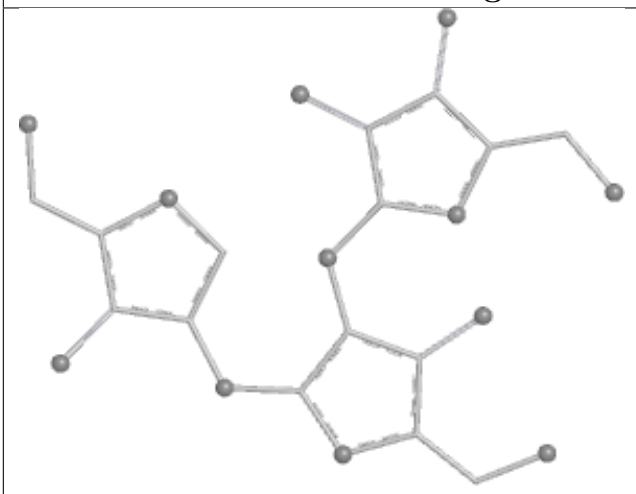
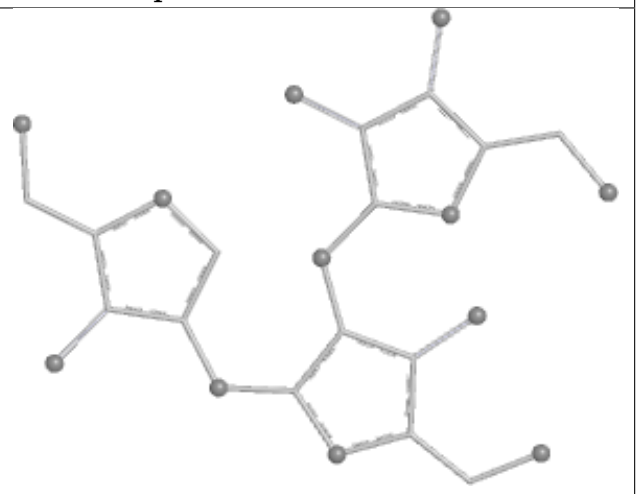
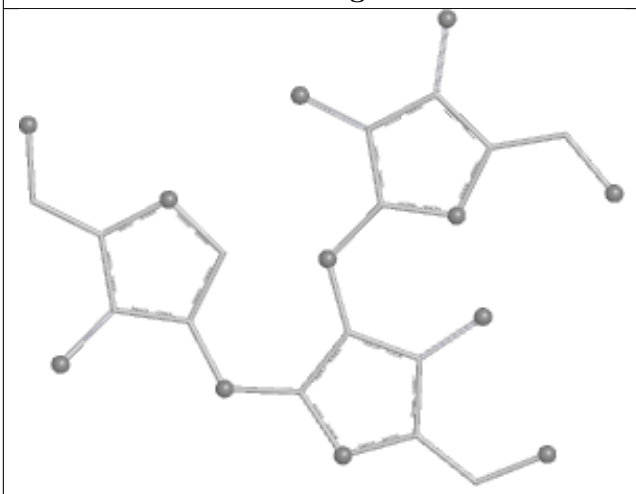
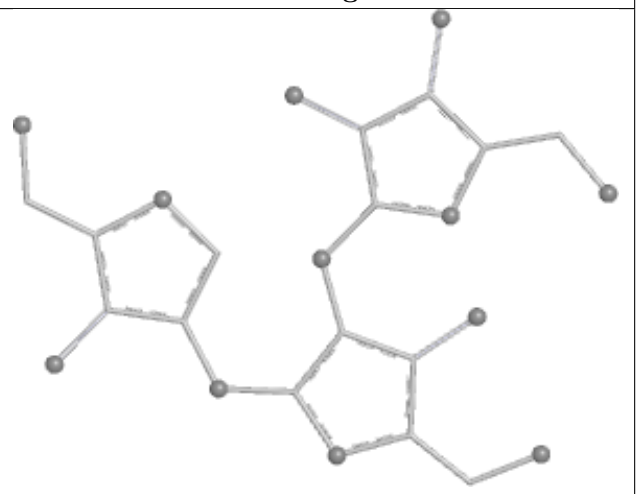
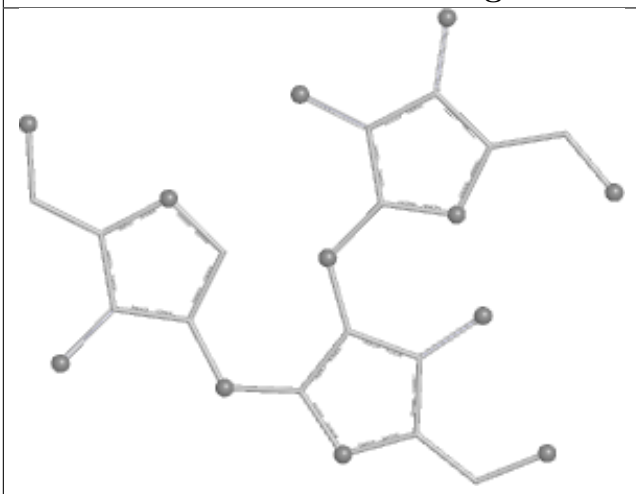
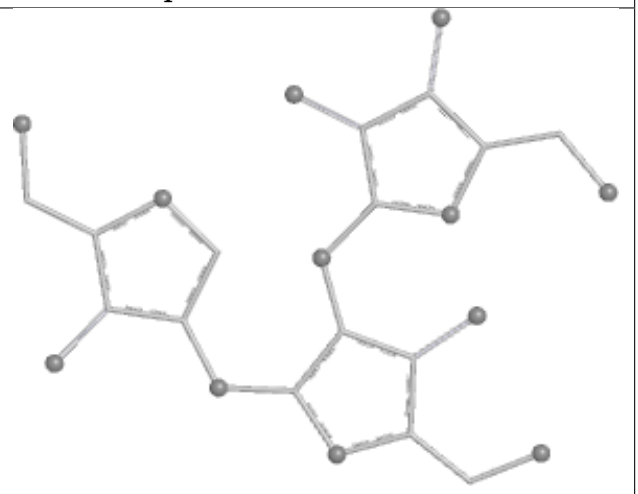
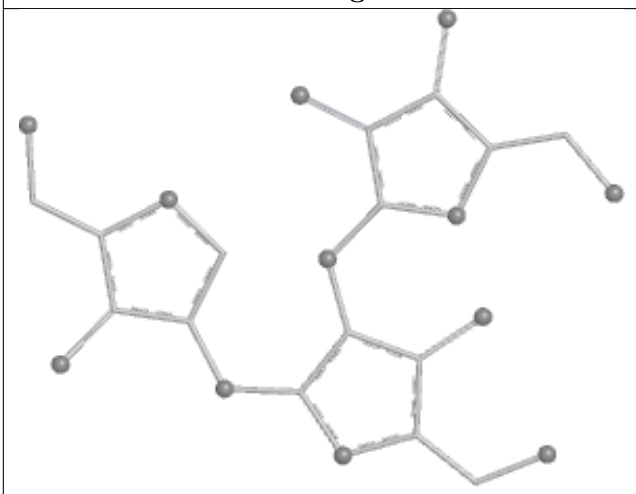
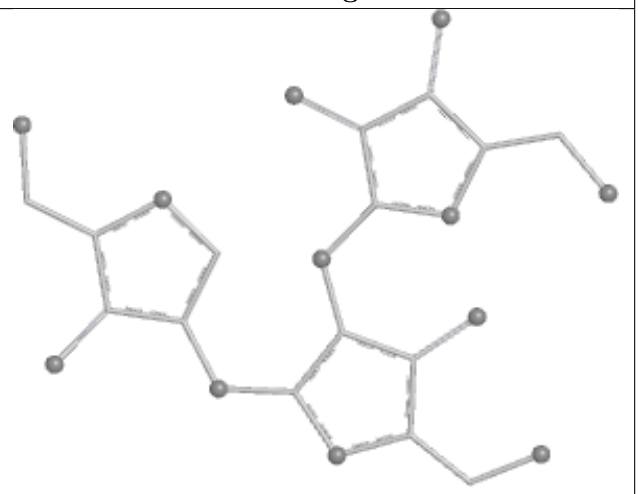
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain nD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain oD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain pD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain qD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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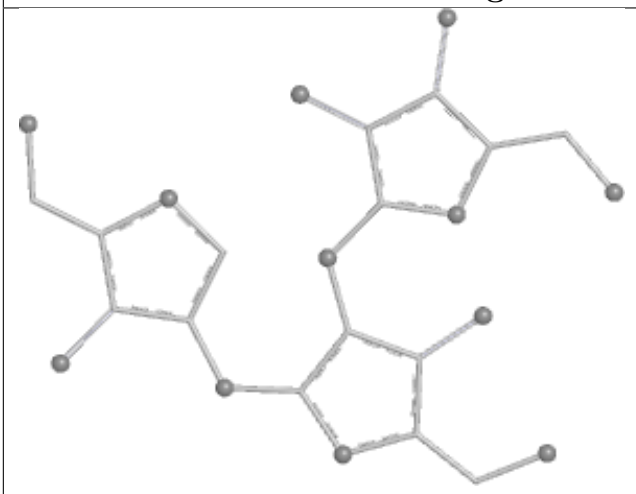
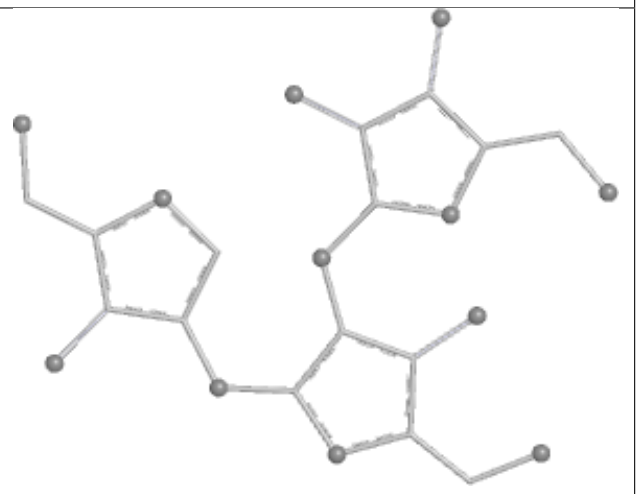
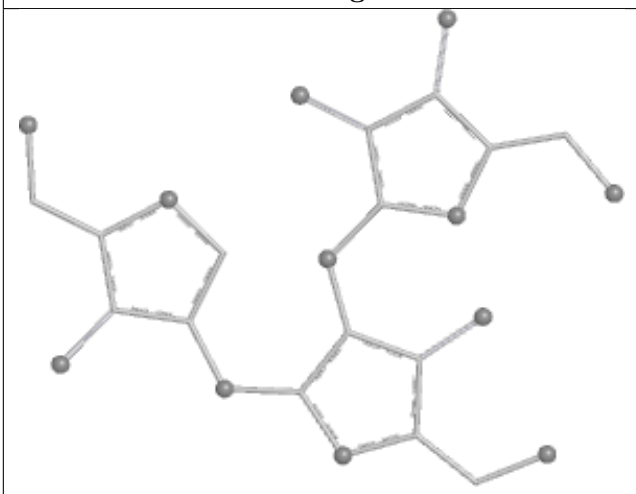
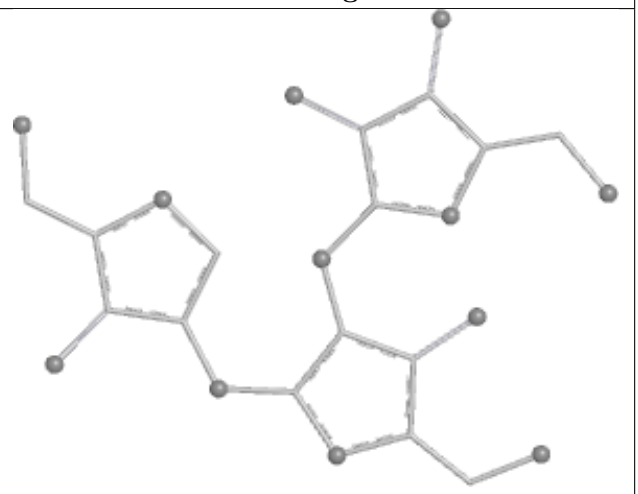
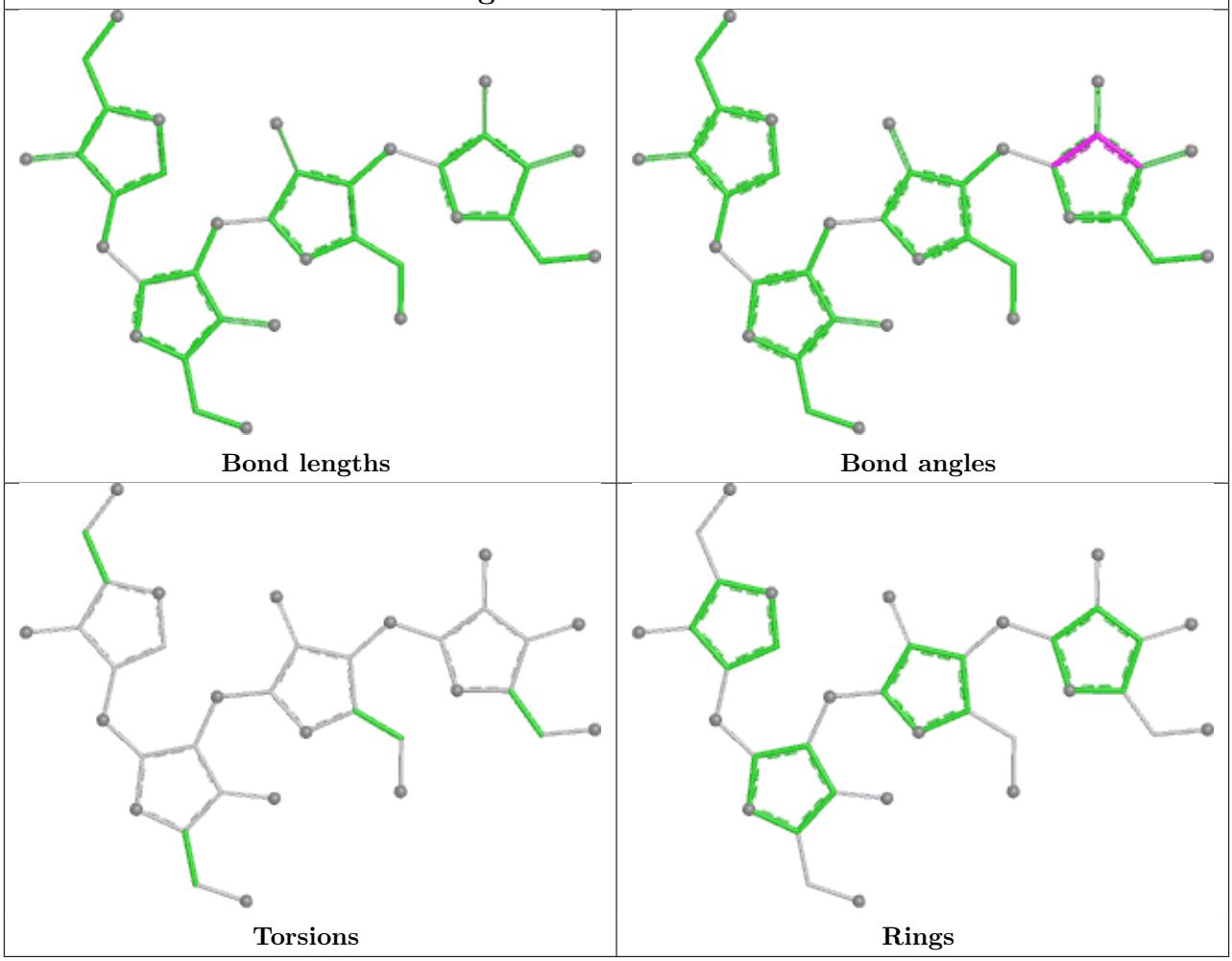
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain L



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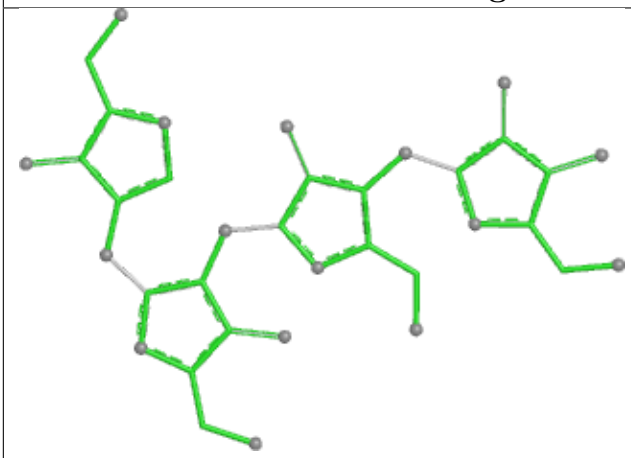
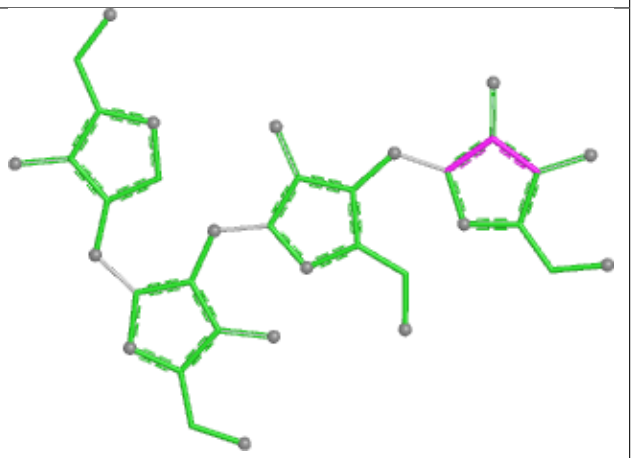
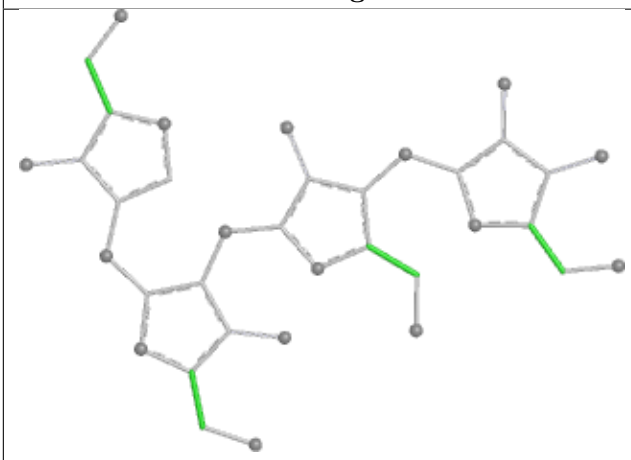
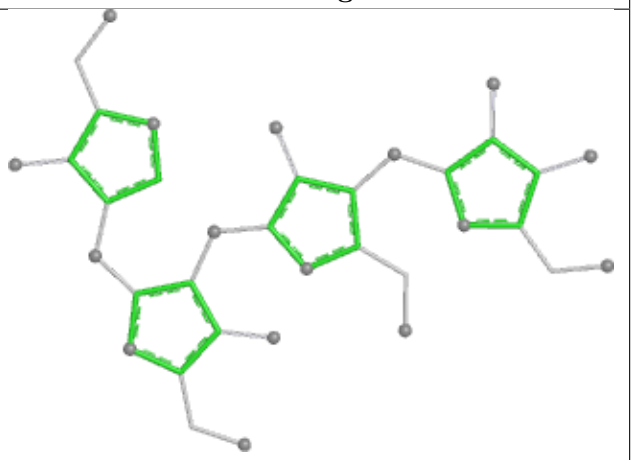
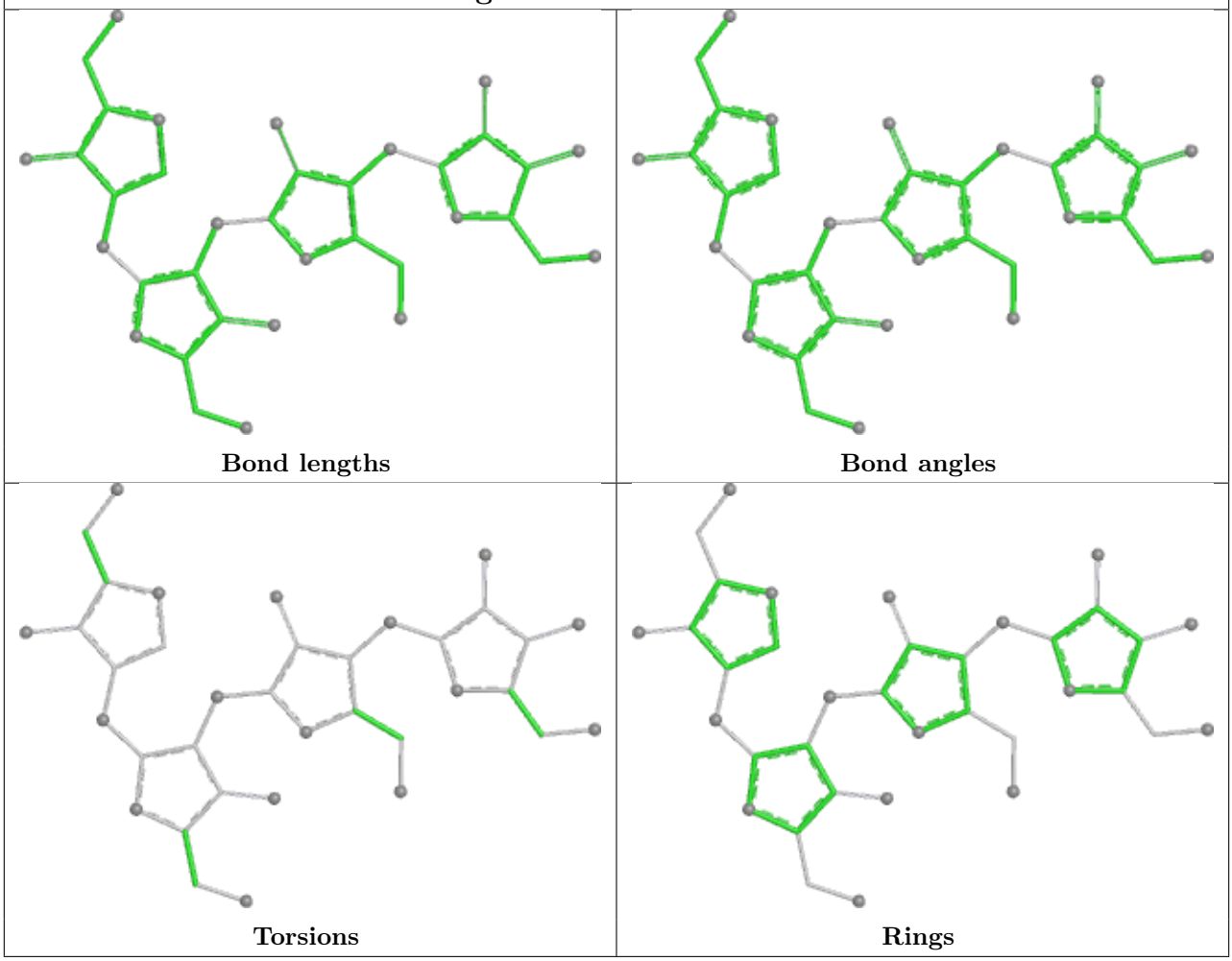
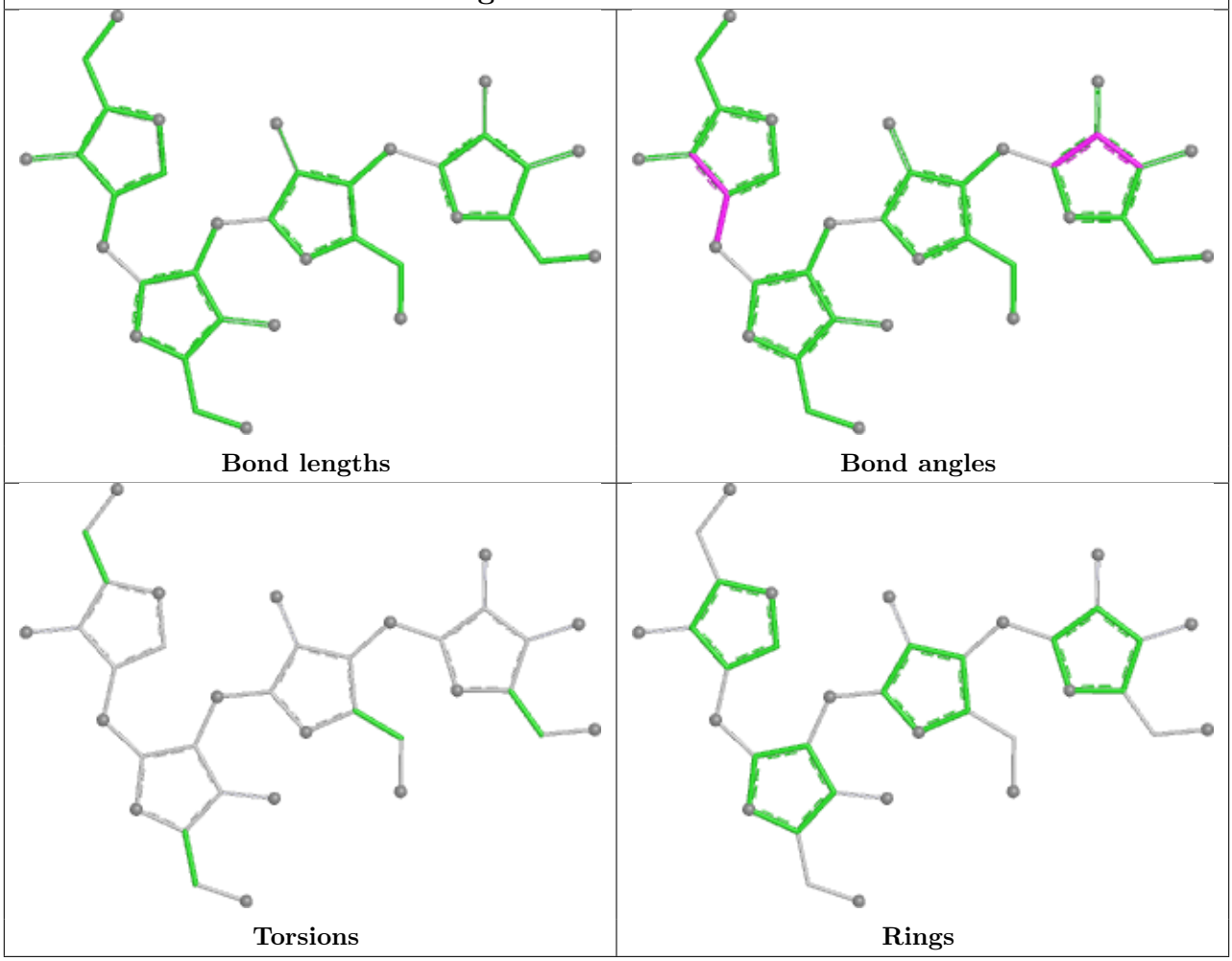
 Bond lengths	 Bond angles
 Torsions	 Rings

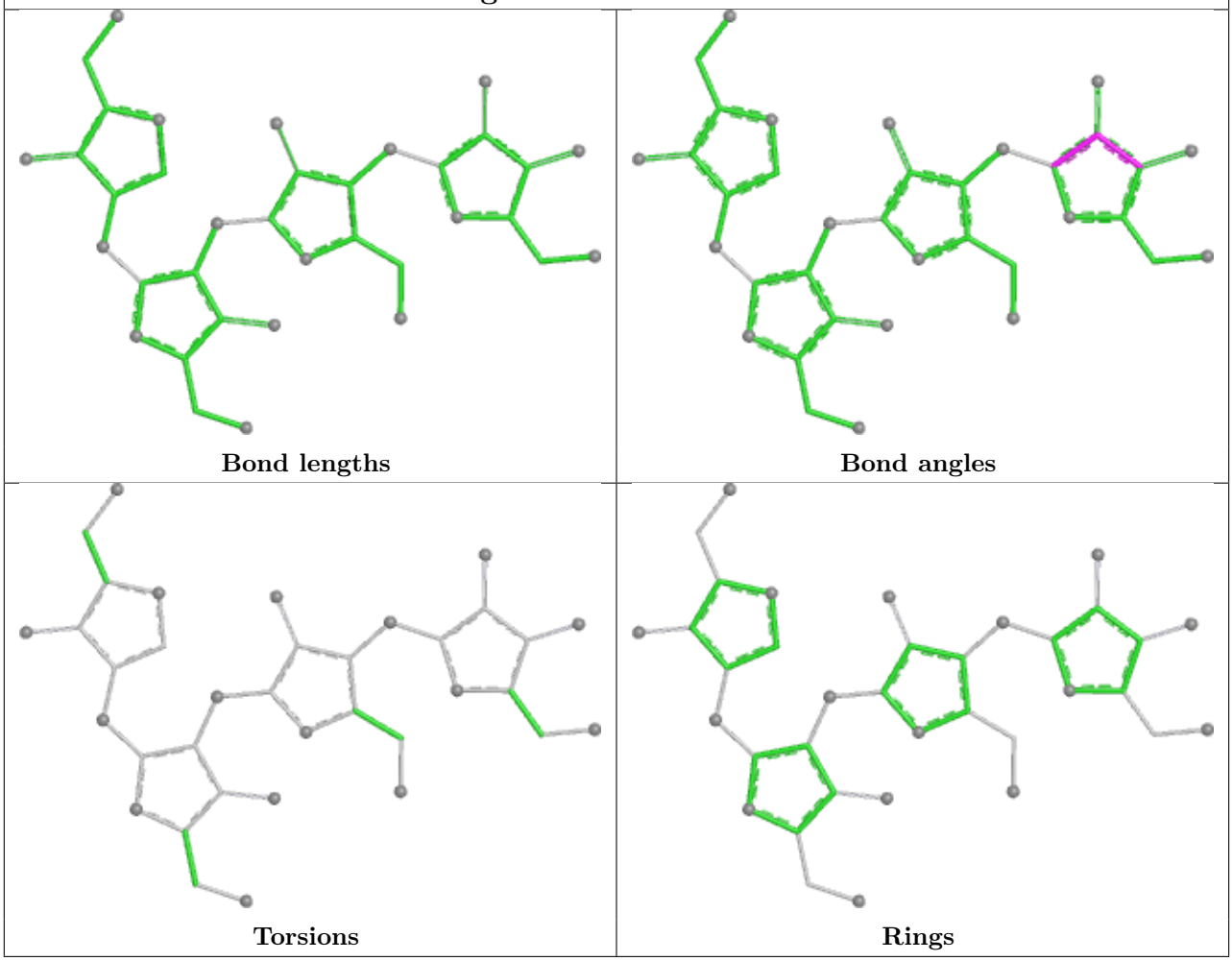
Oligosaccharide Chain X



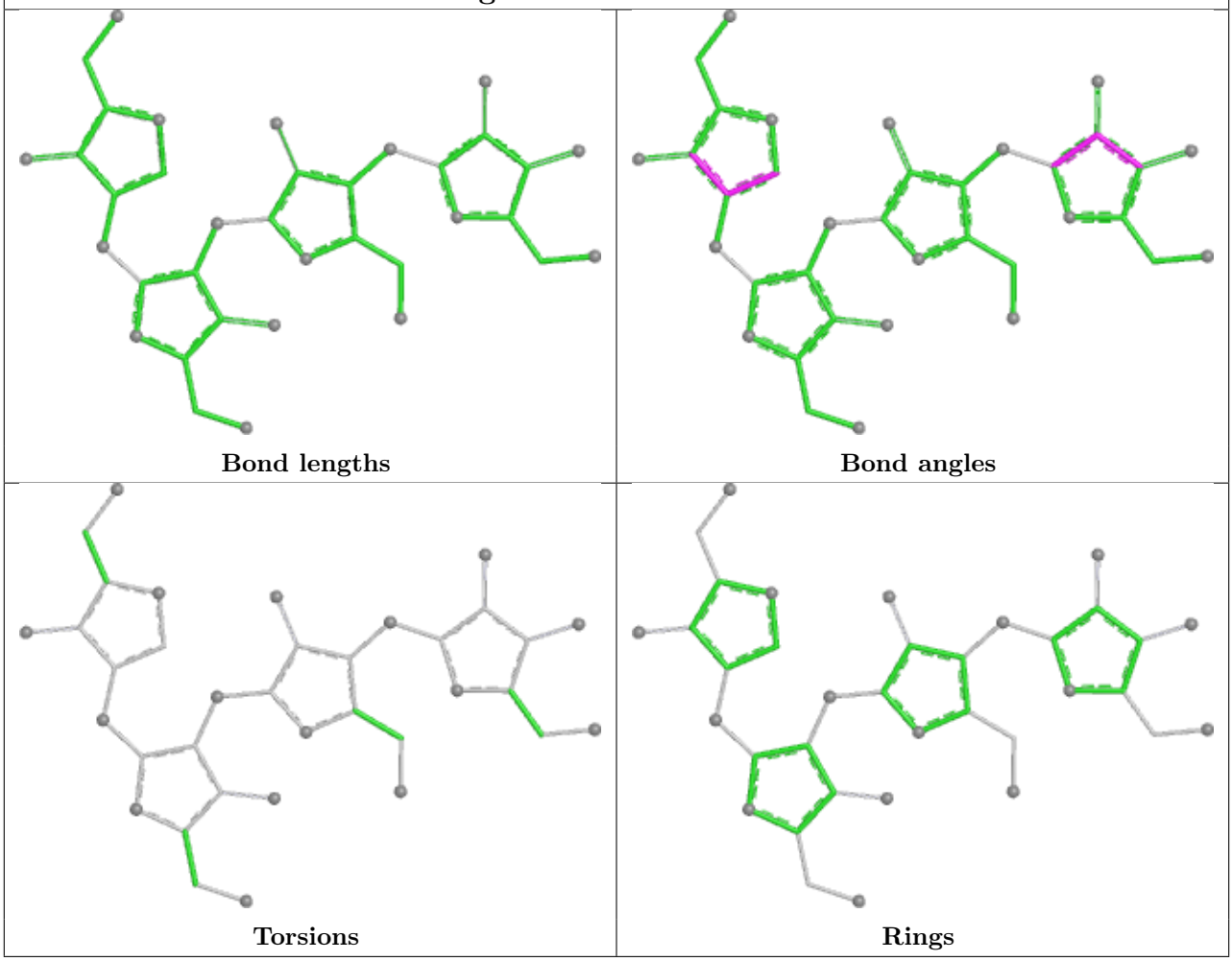
Oligosaccharide Chain Z



Oligosaccharide Chain c



Oligosaccharide Chain d



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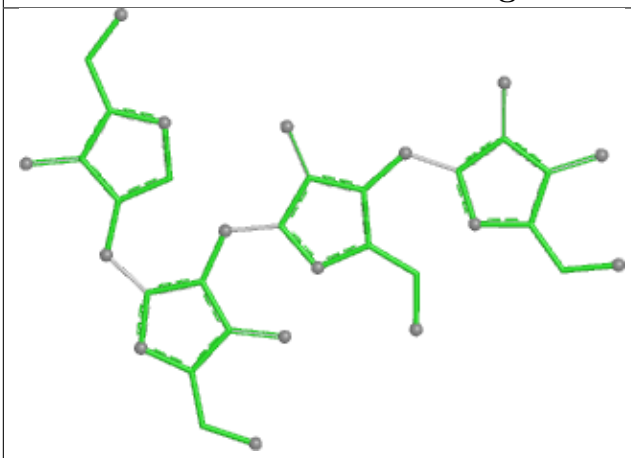
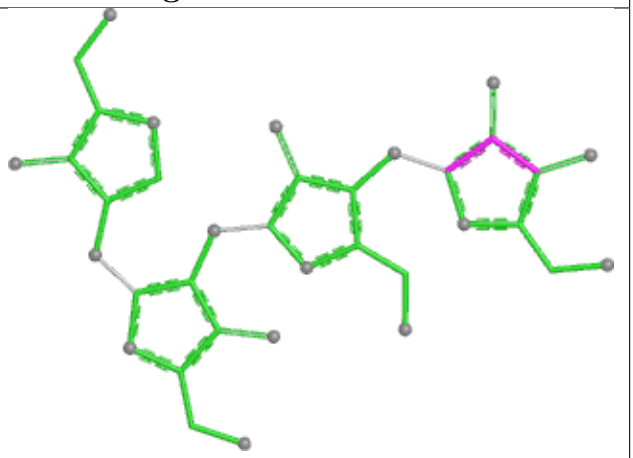
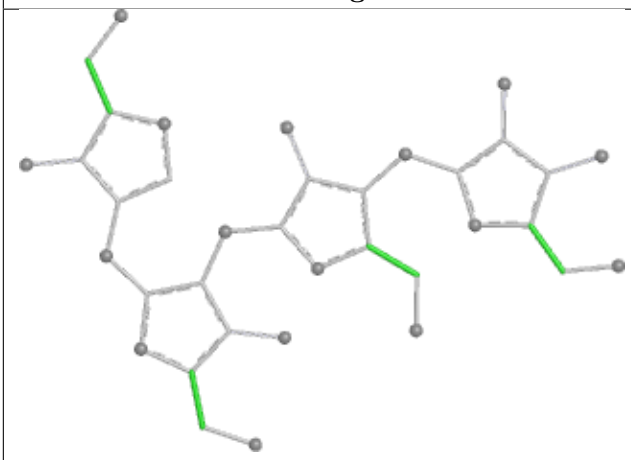
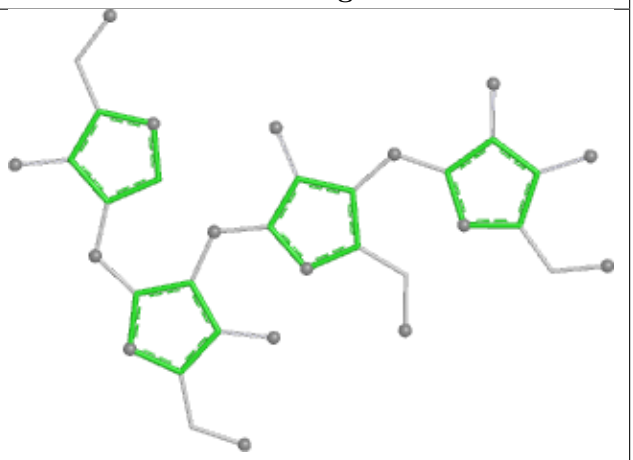
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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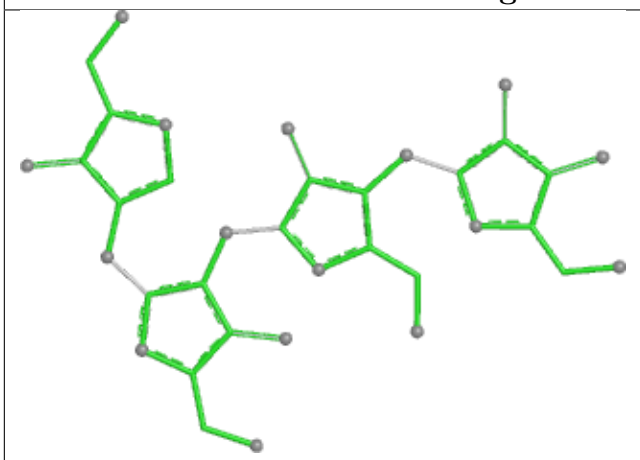
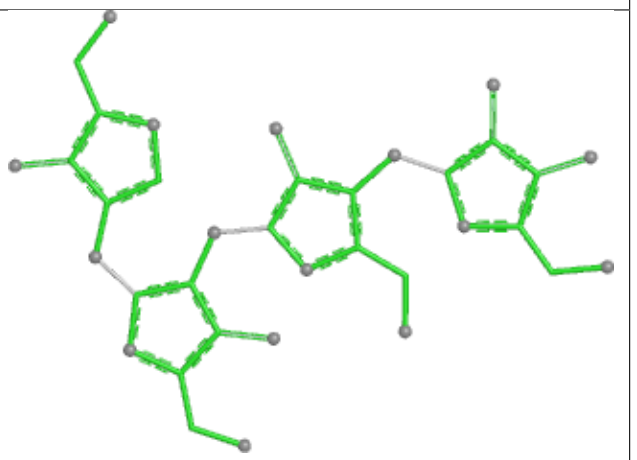
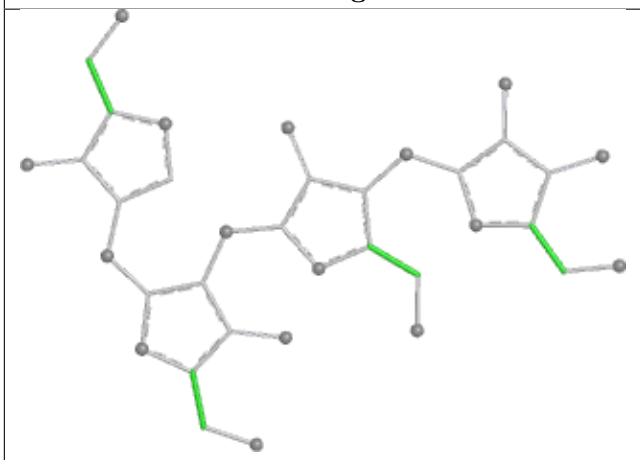
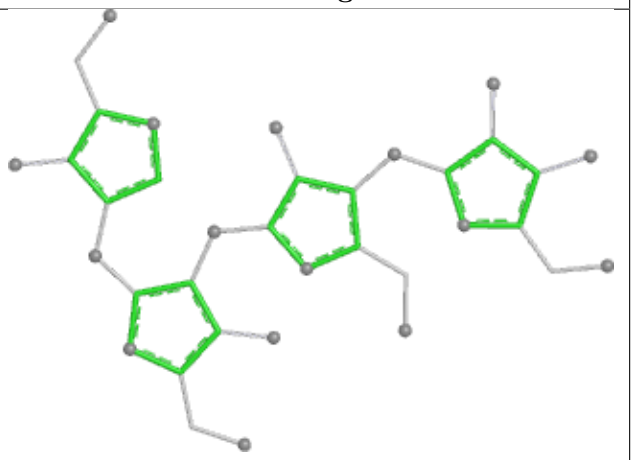
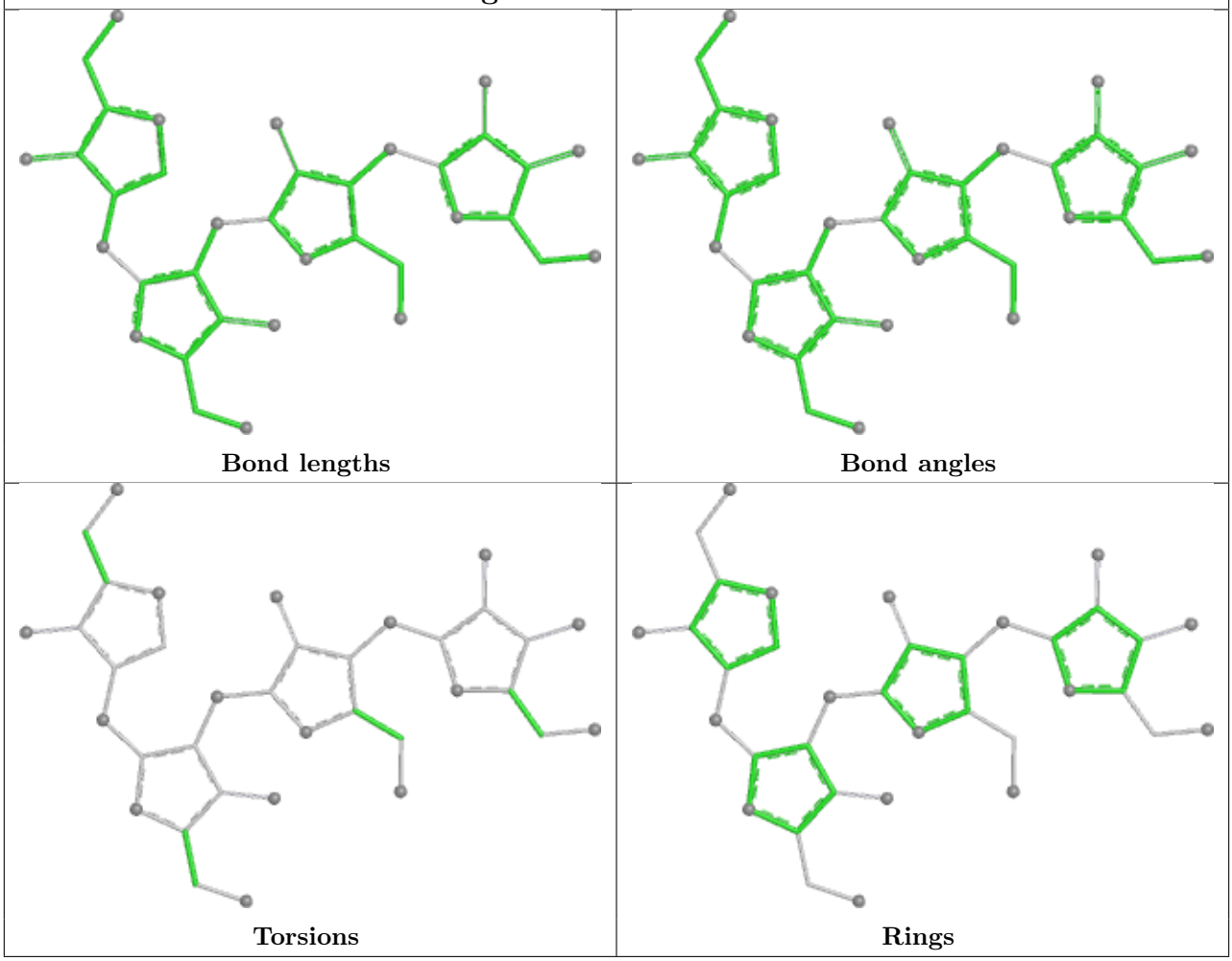
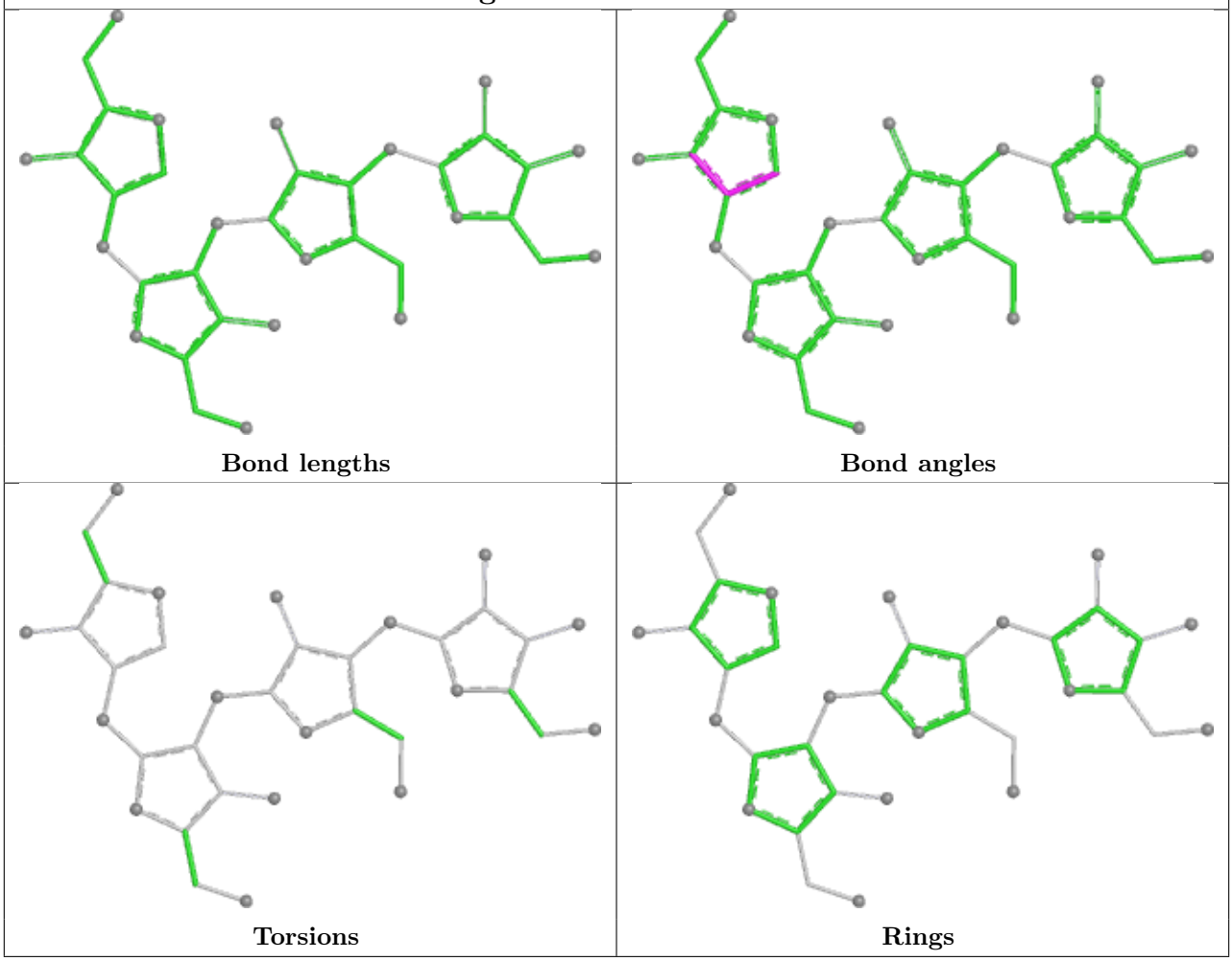
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain r



Oligosaccharide Chain v



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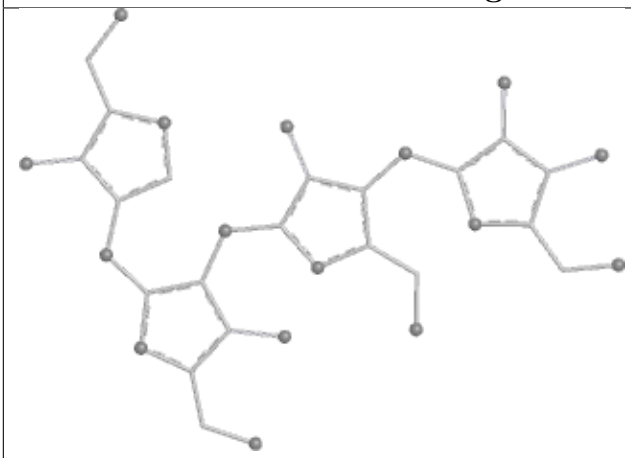
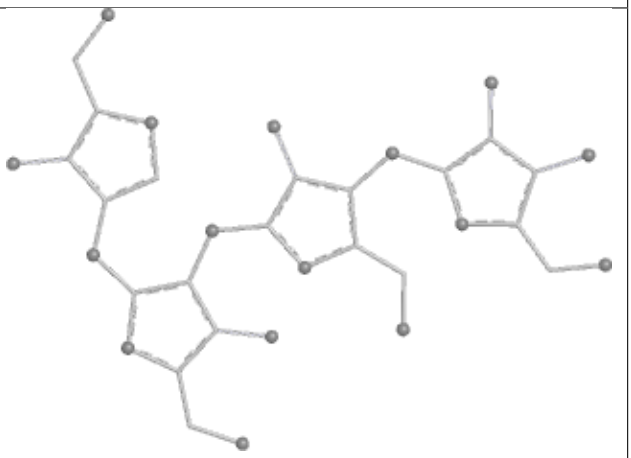
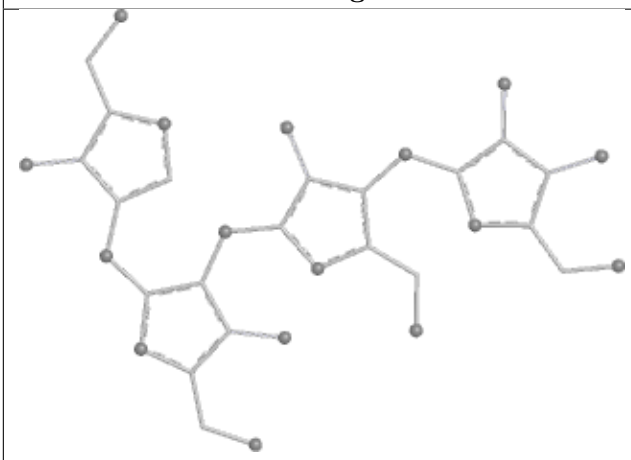
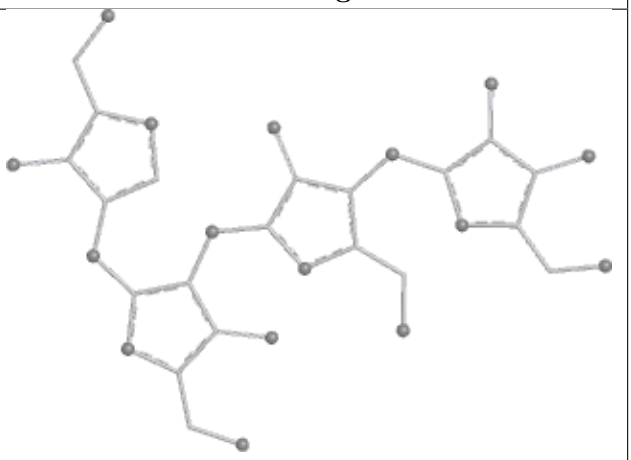
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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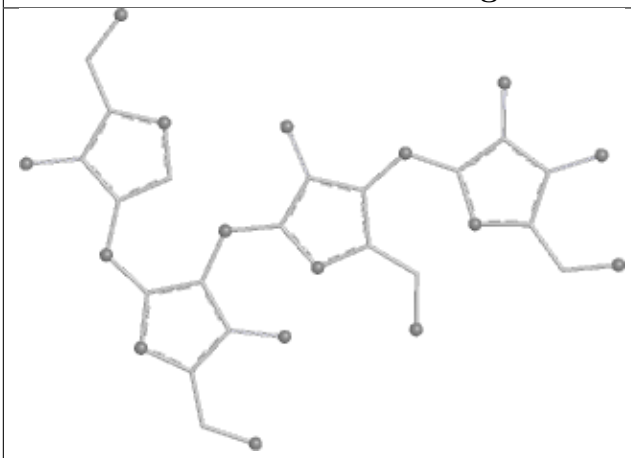
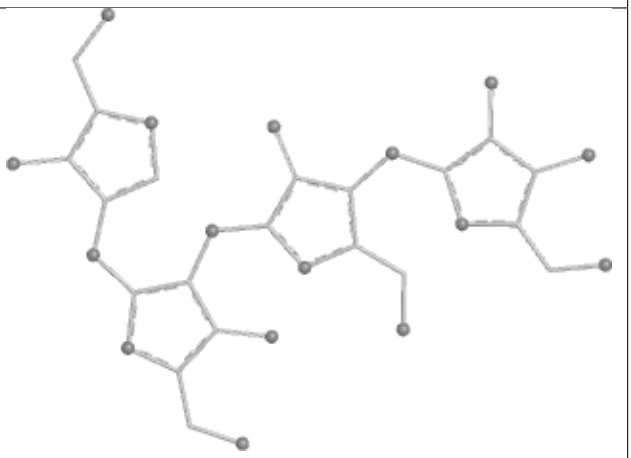
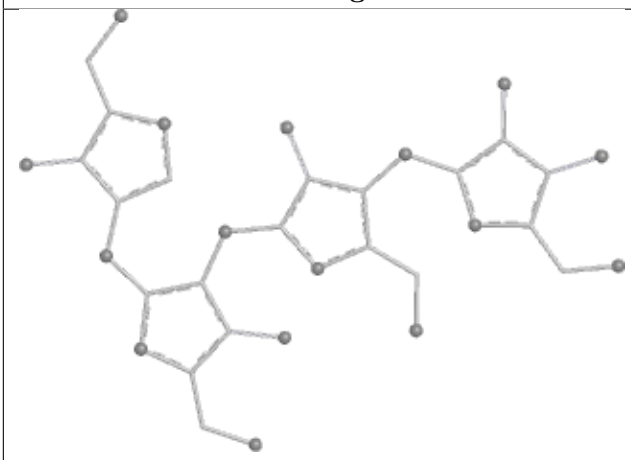
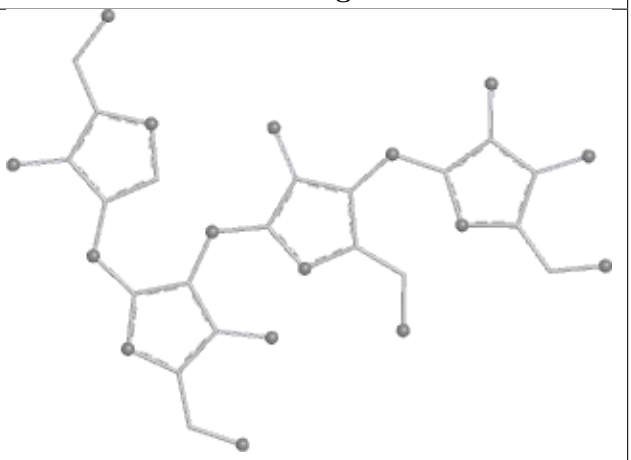
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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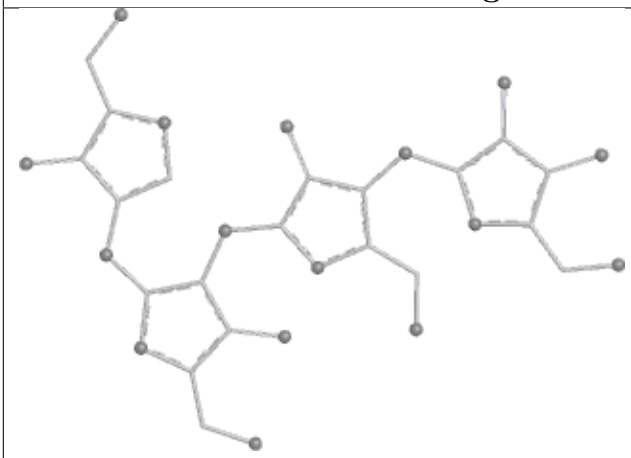
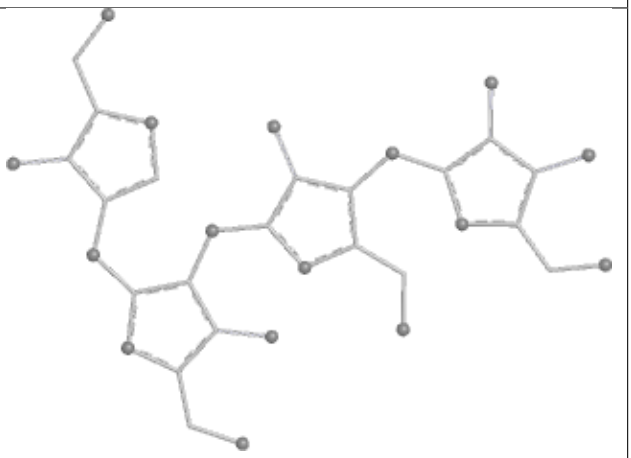
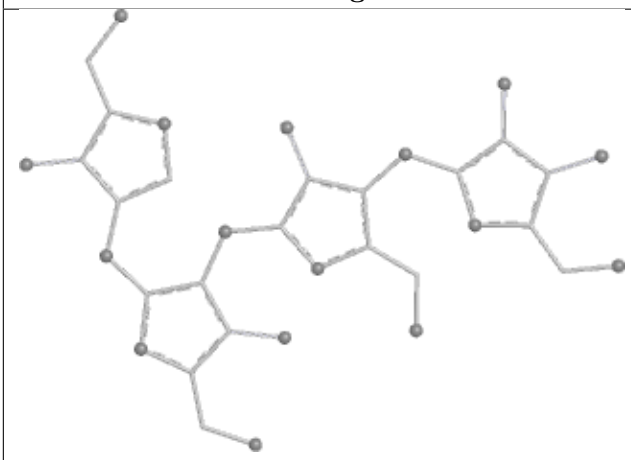
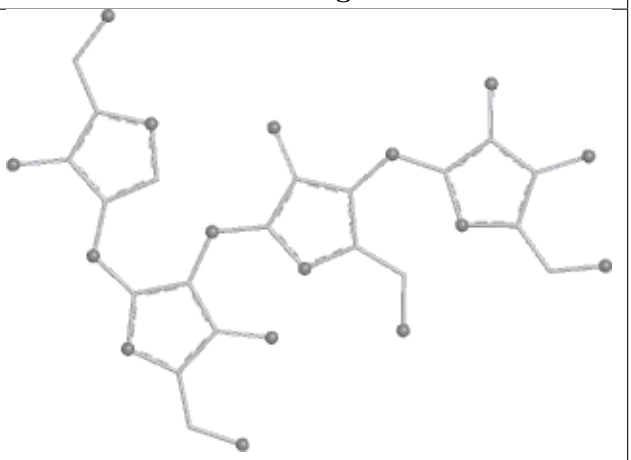
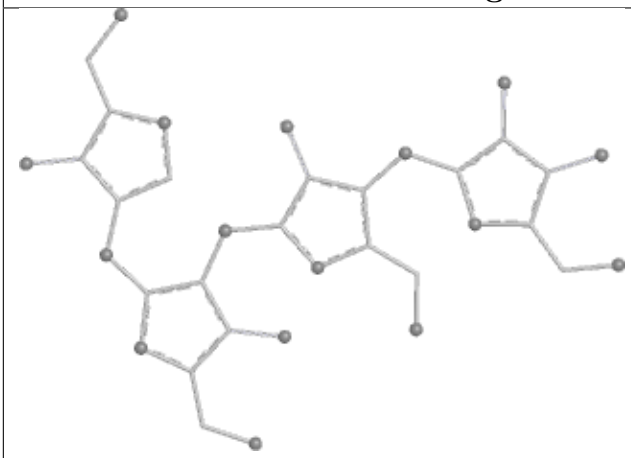
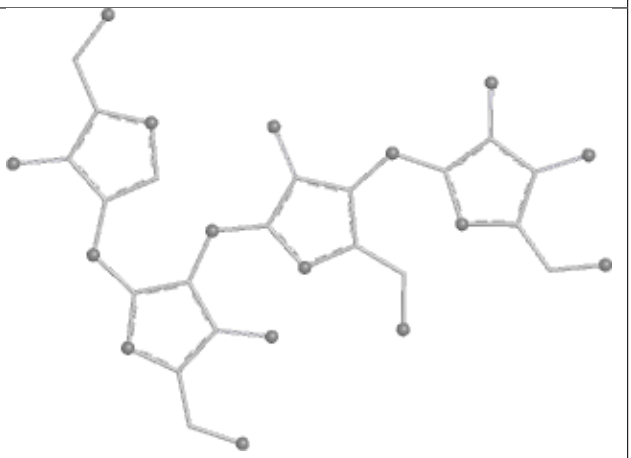
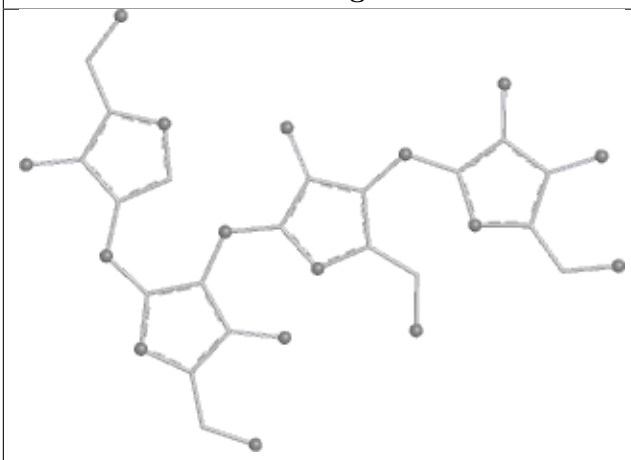
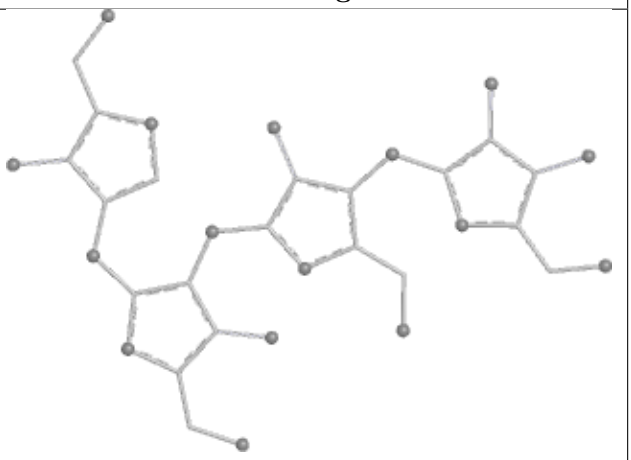
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain aA	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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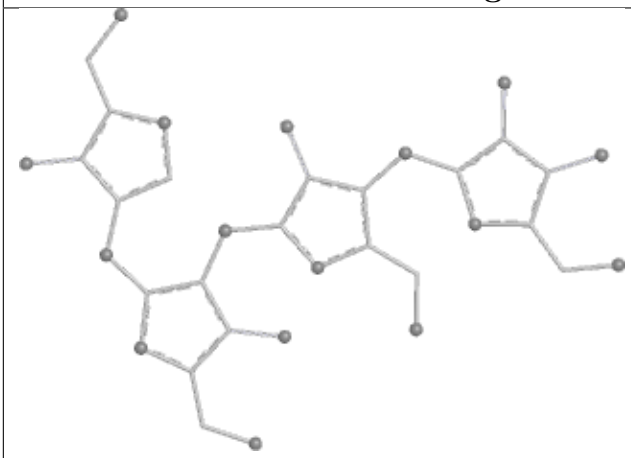
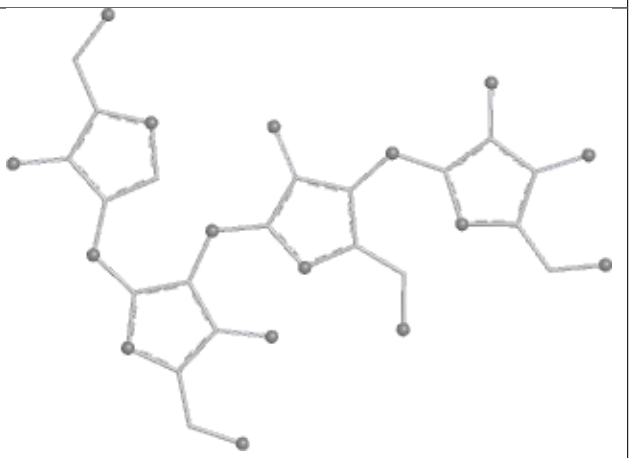
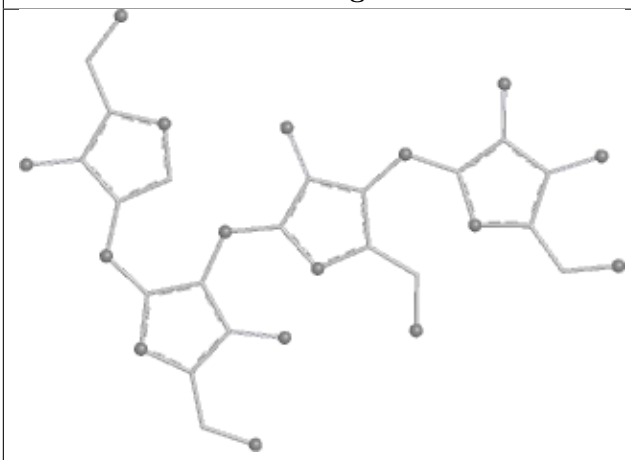
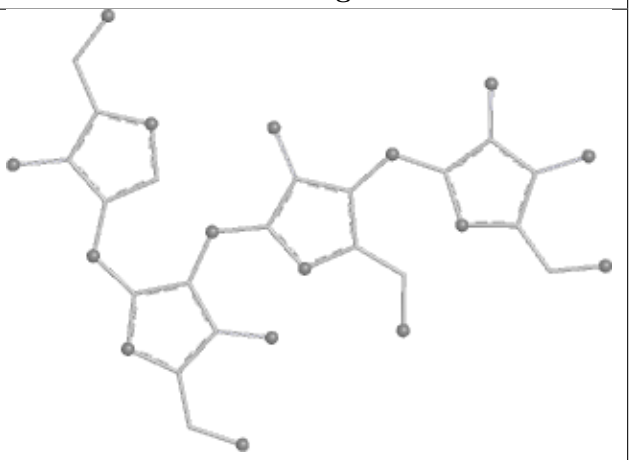
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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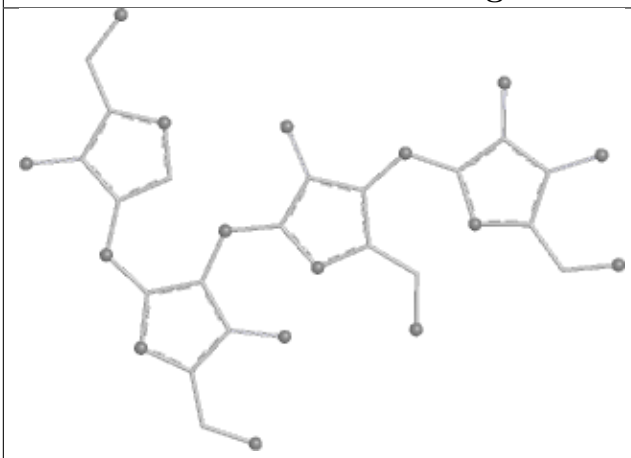
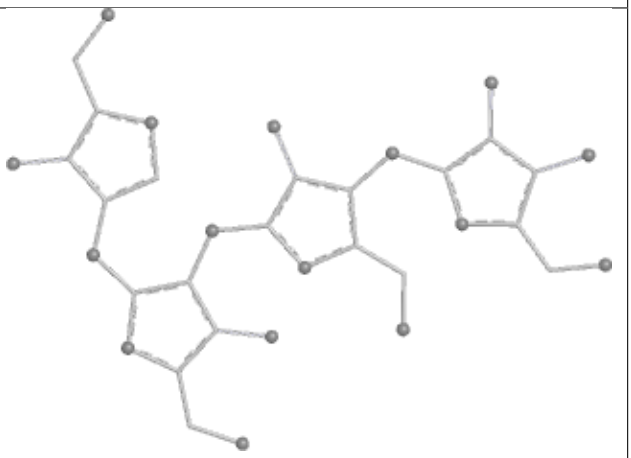
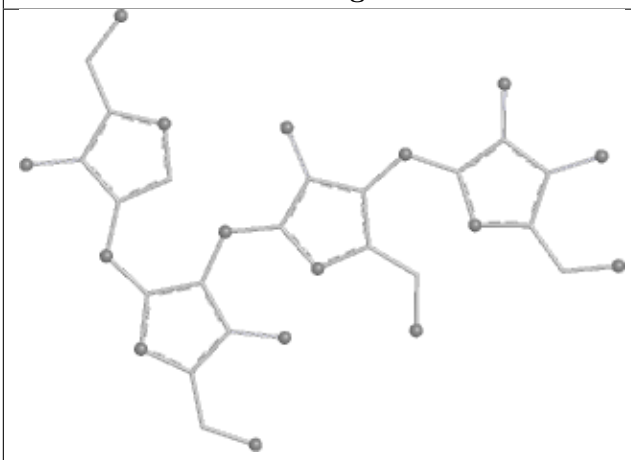
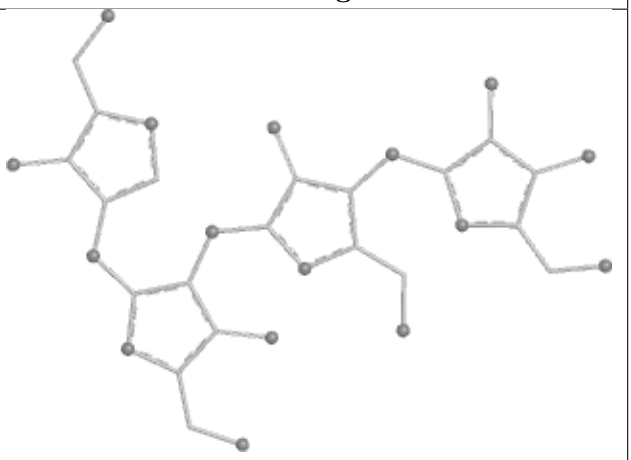
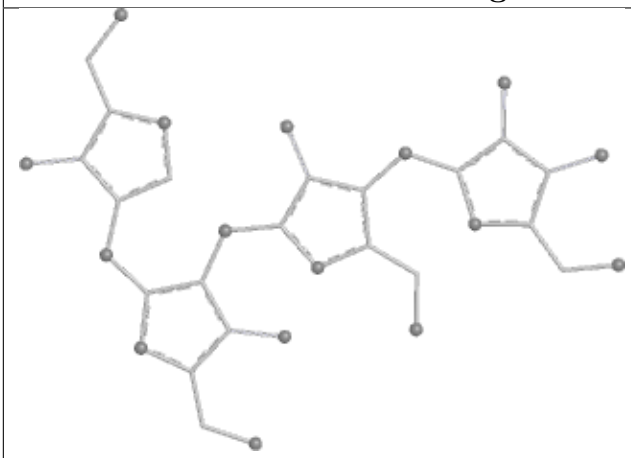
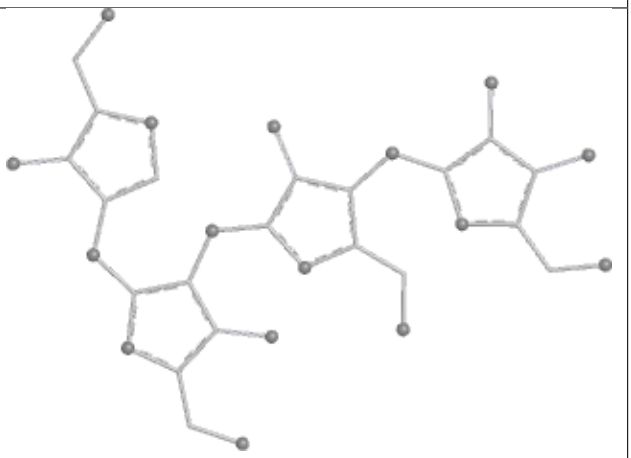
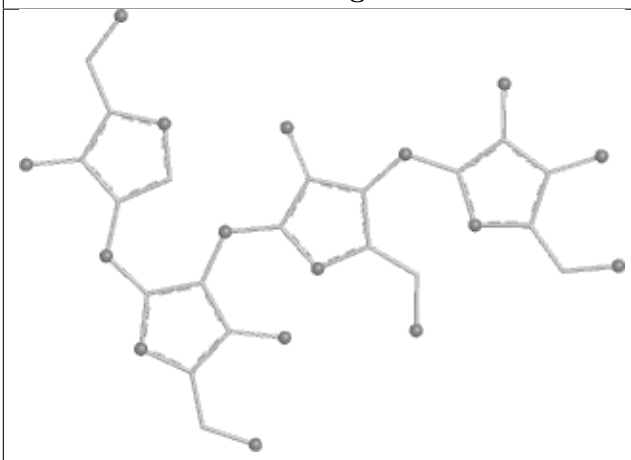
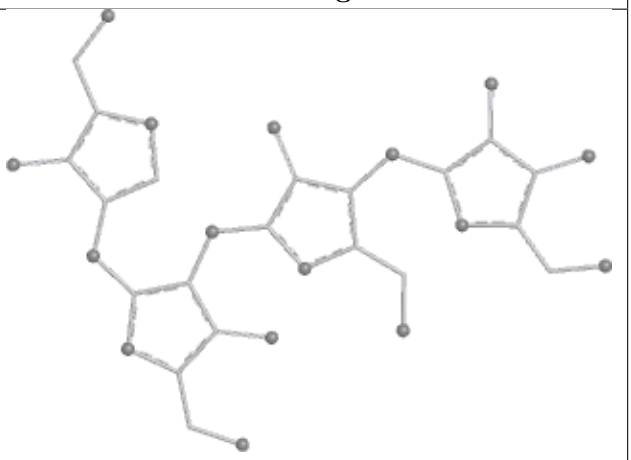
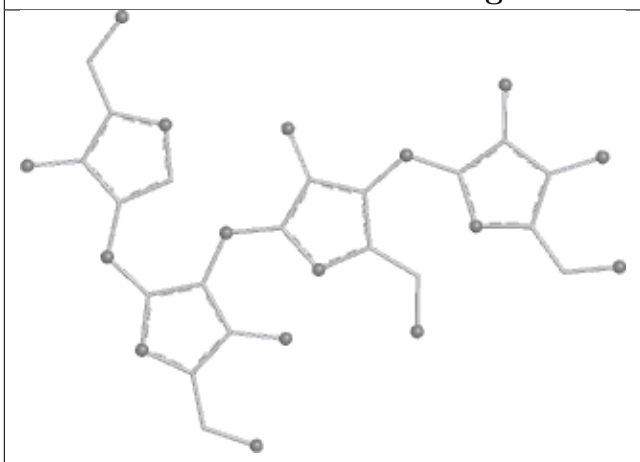
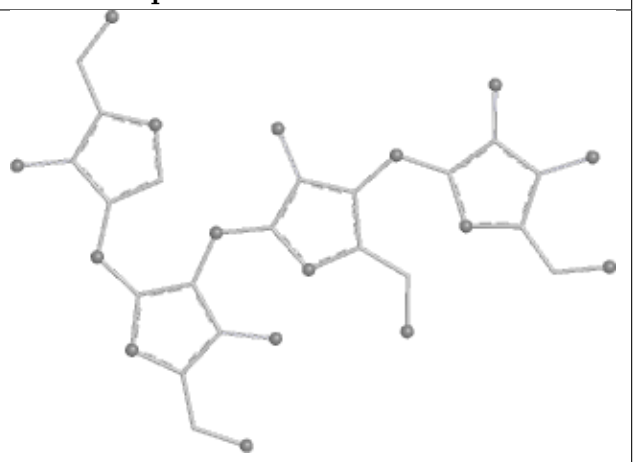
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain iA	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain pA	
	
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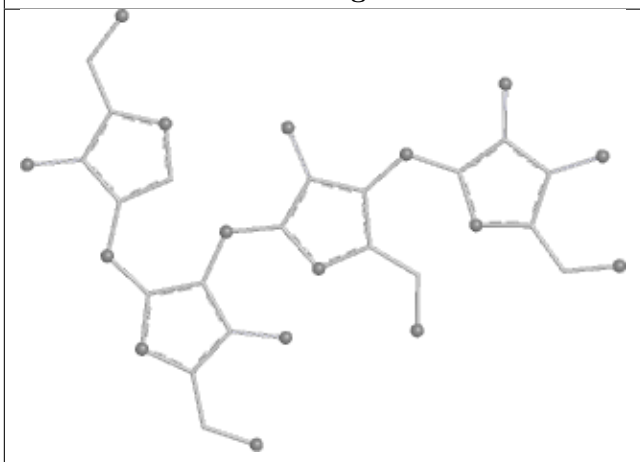	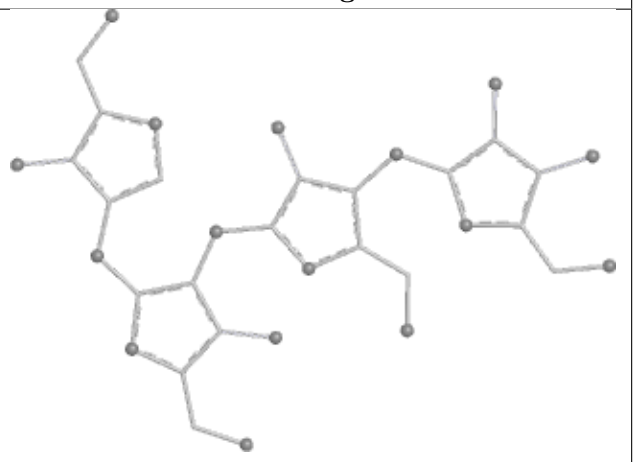
Torsions	**Rings**

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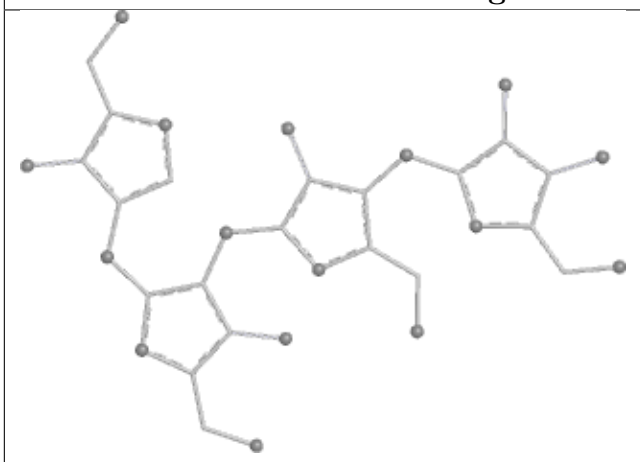	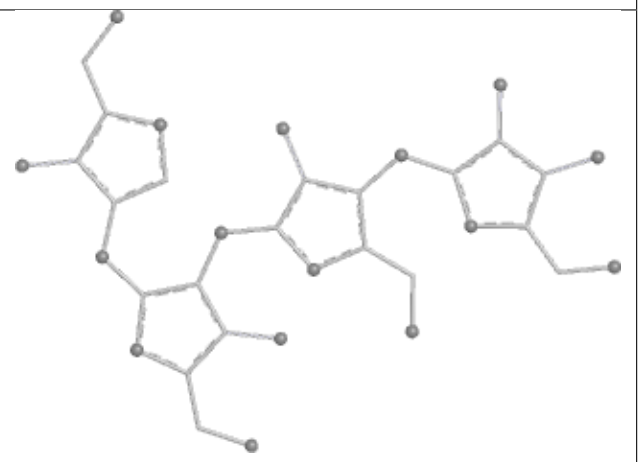
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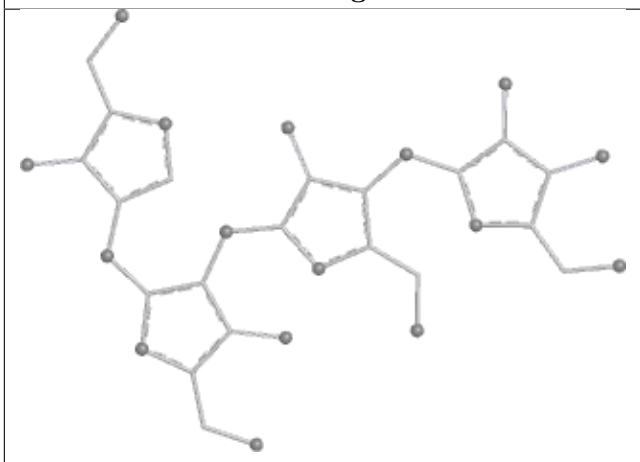	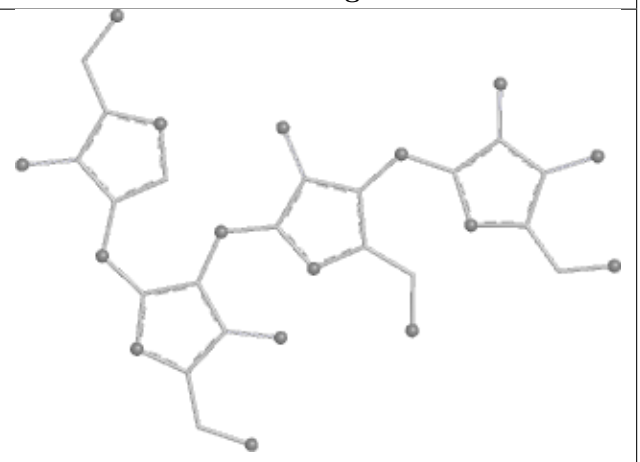
Torsions	**Rings**

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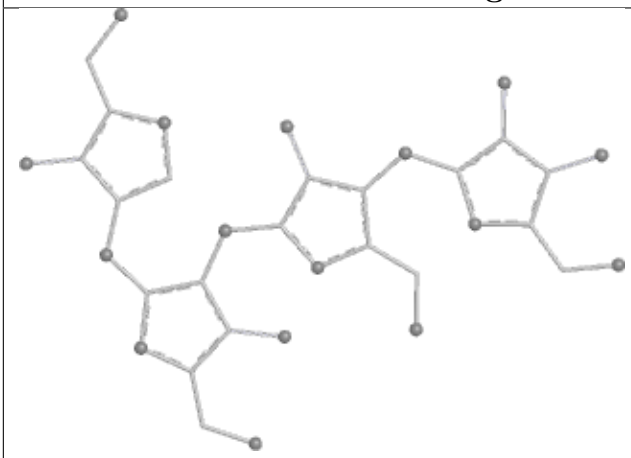
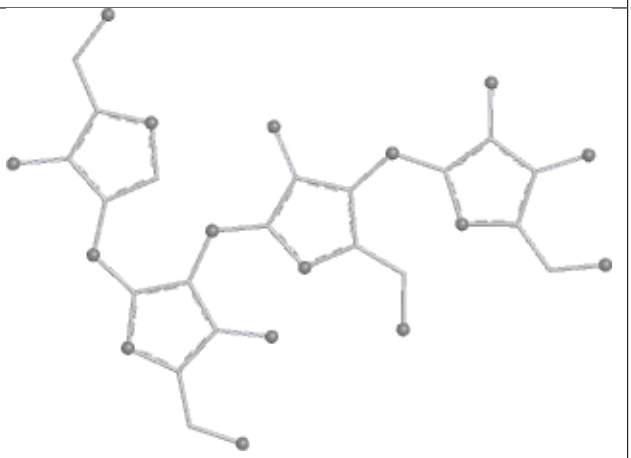
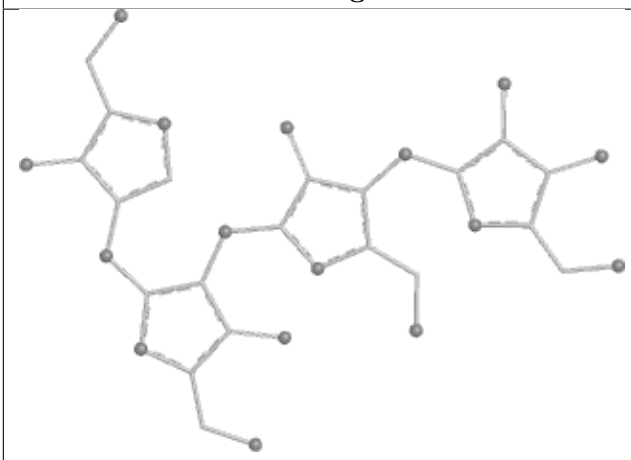
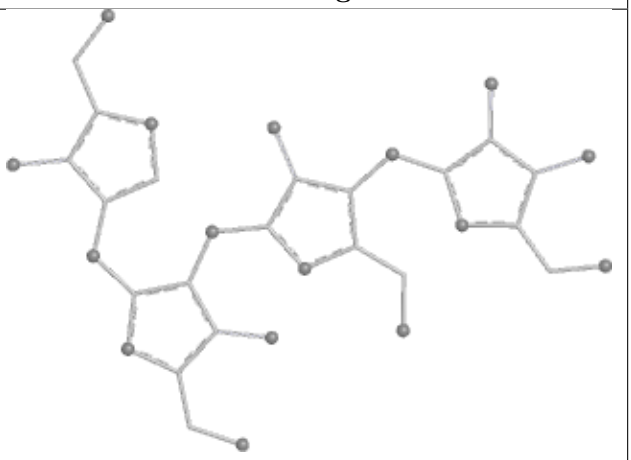
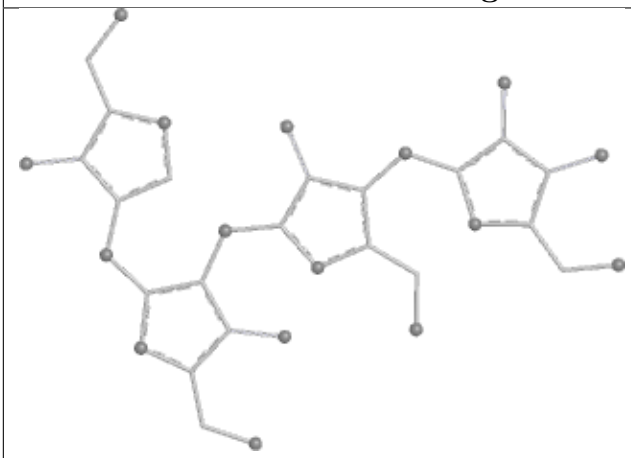
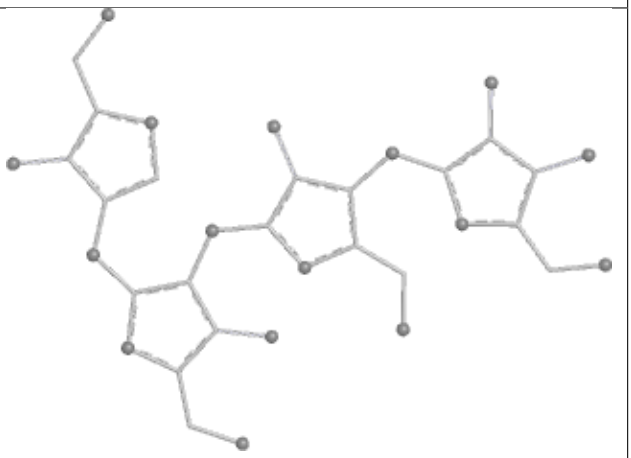
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain NB	
	
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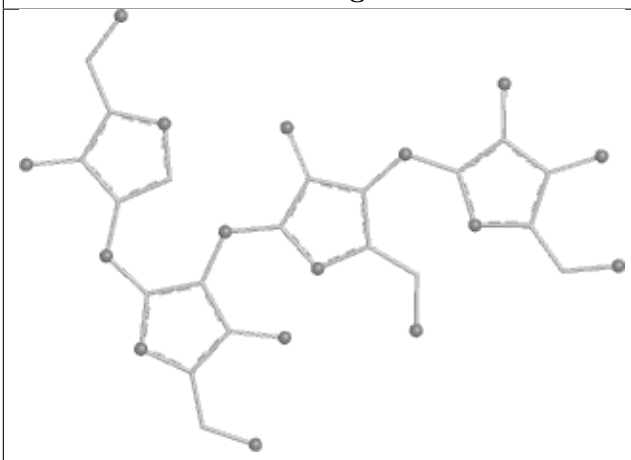	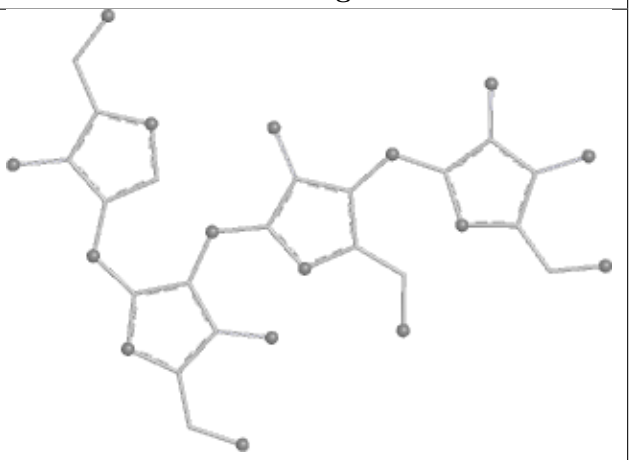
Torsions	**Rings**

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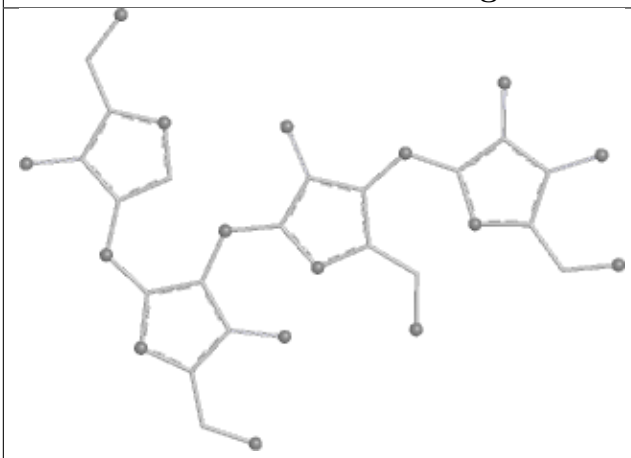	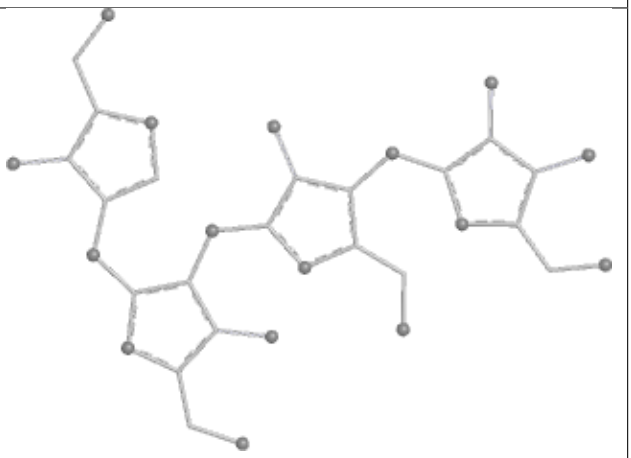
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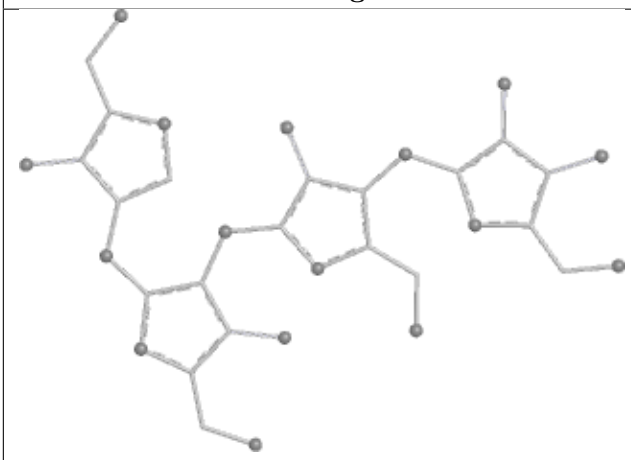	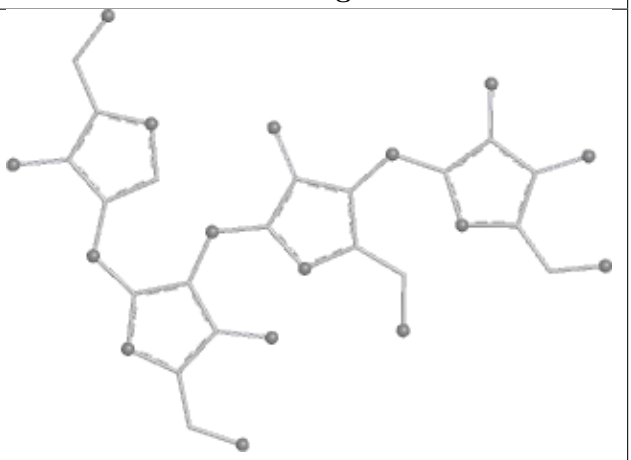
Torsions	**Rings**

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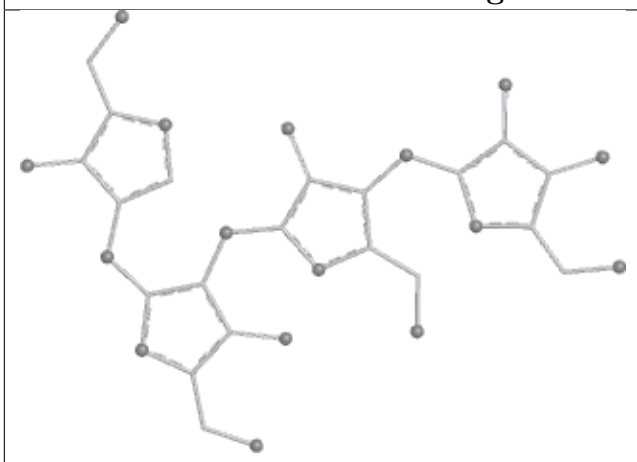
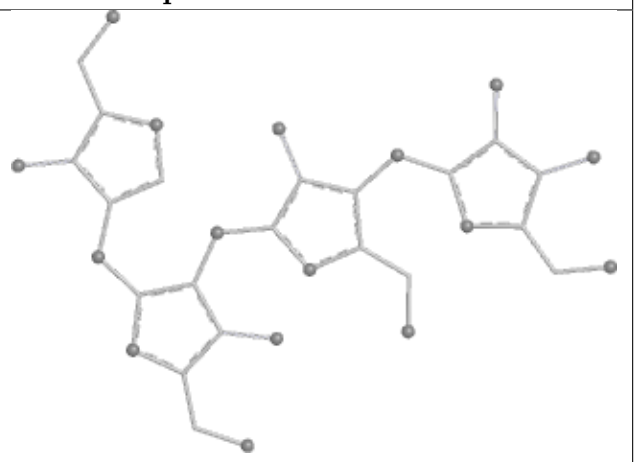
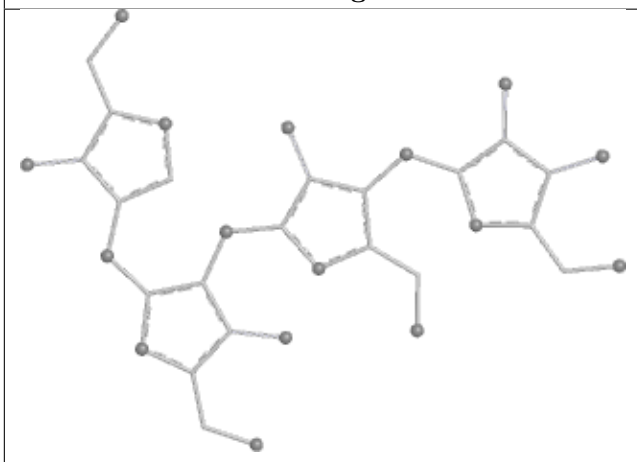
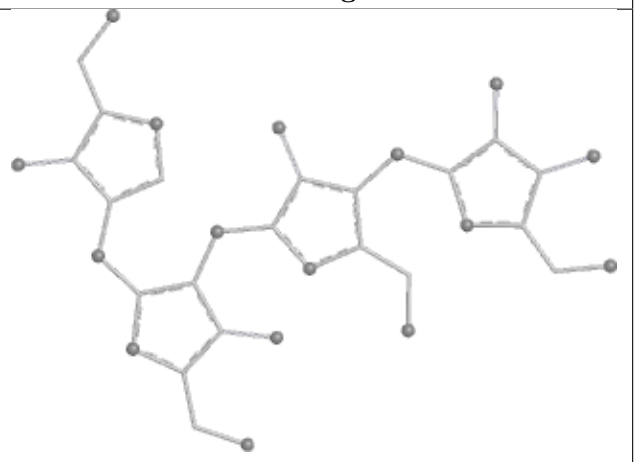
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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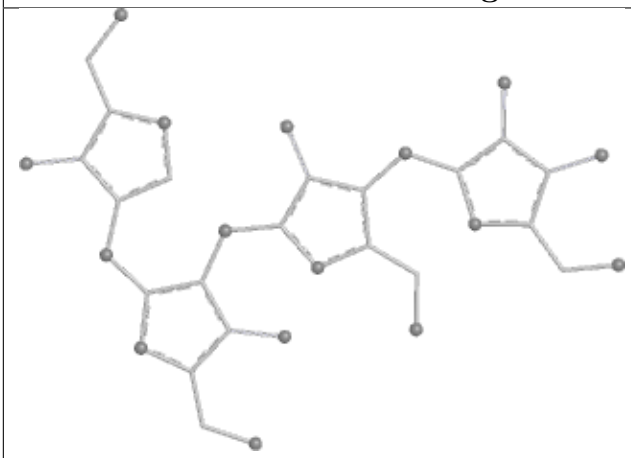
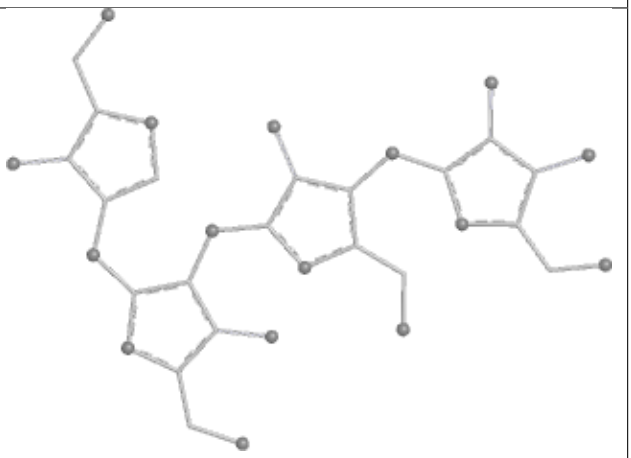
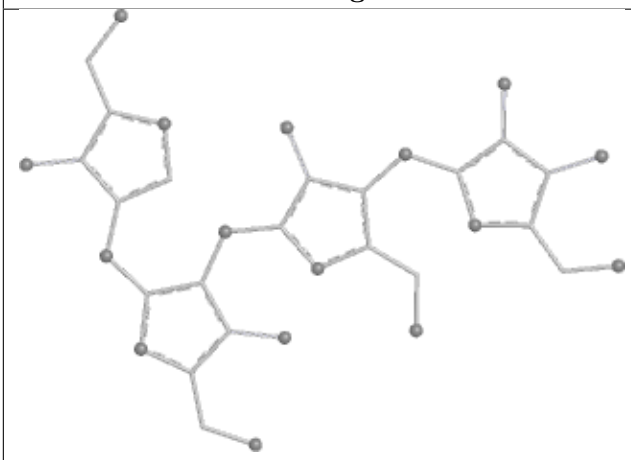
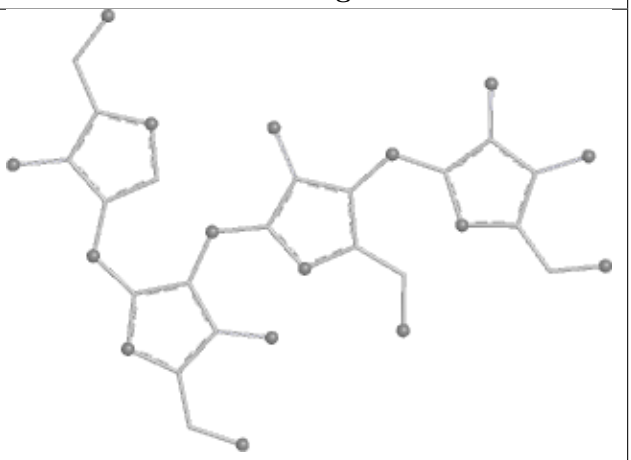
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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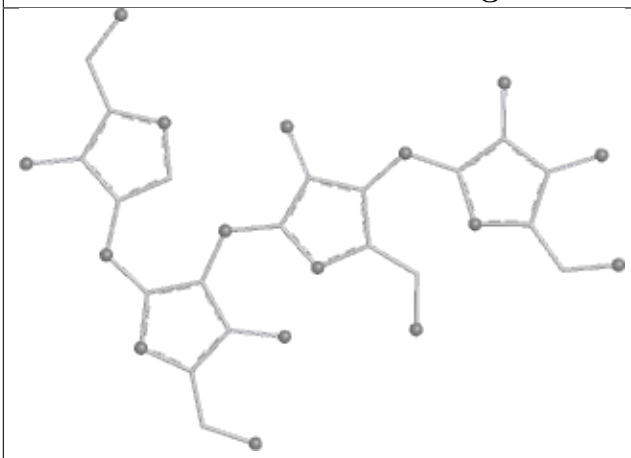	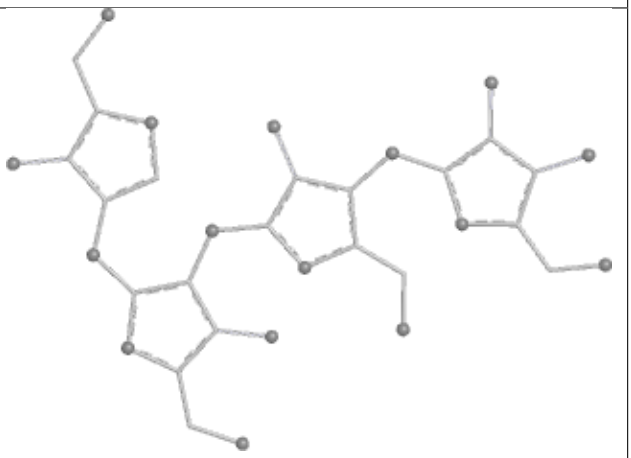
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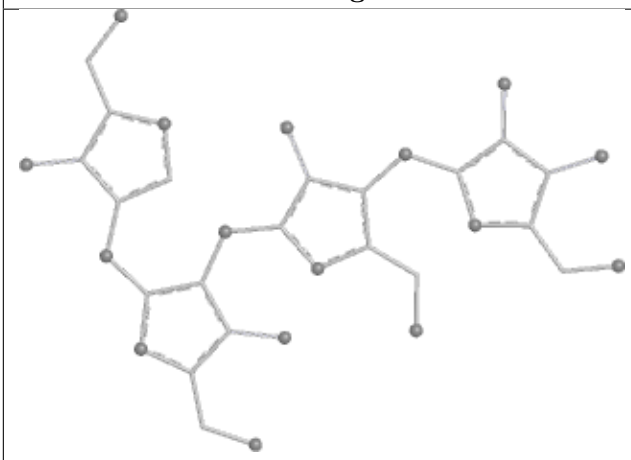	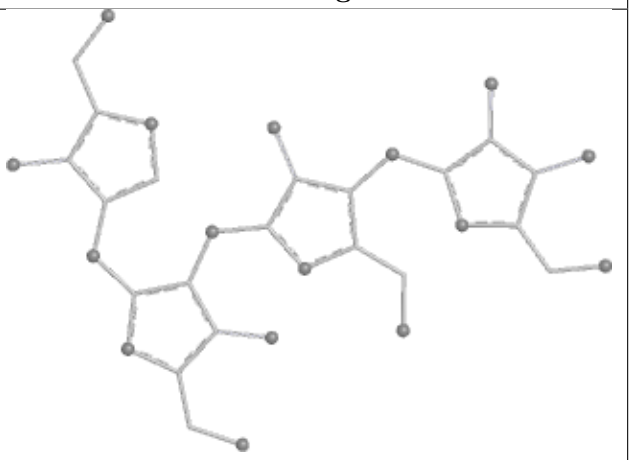
Torsions	**Rings**

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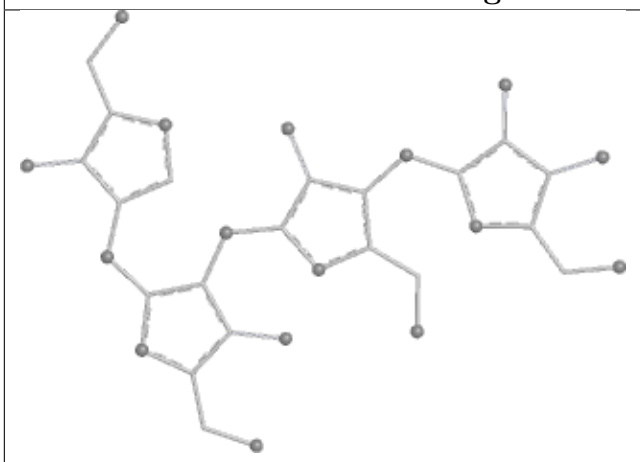
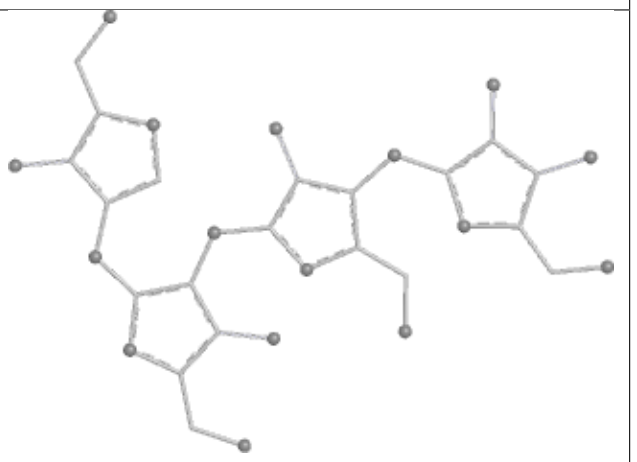
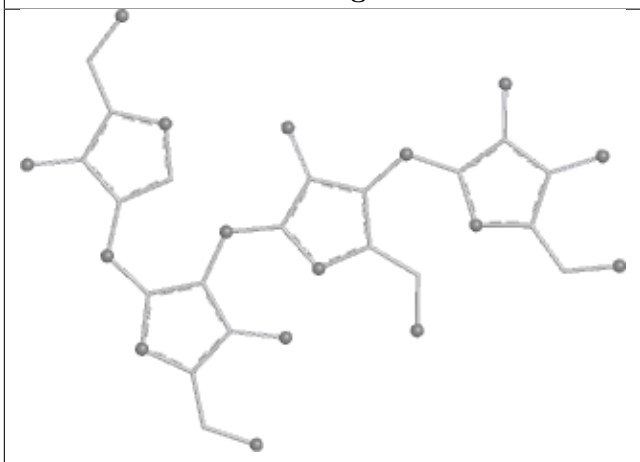
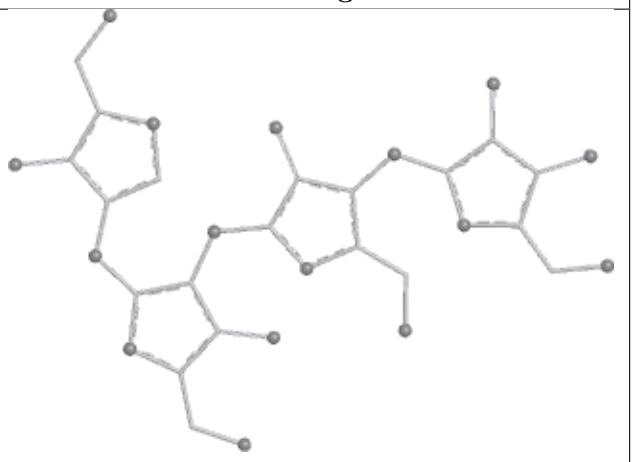
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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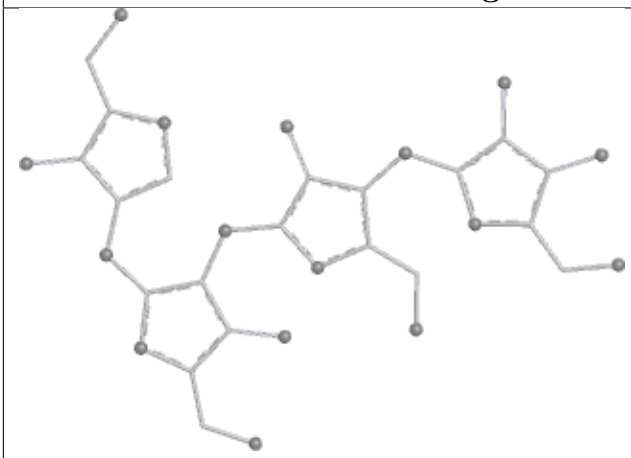	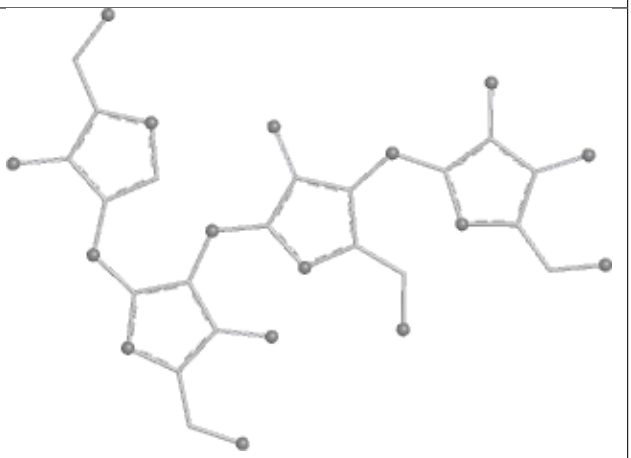
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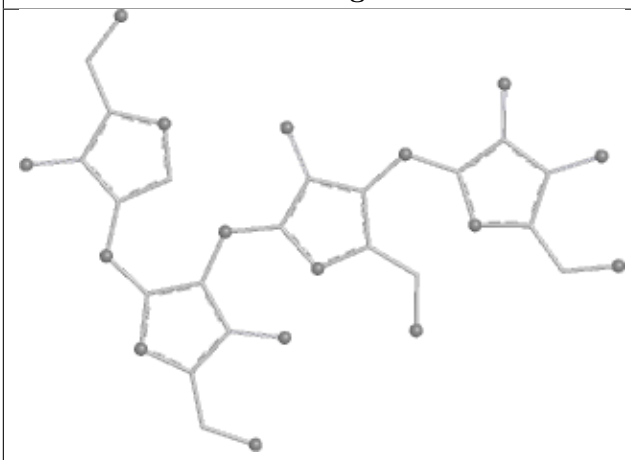	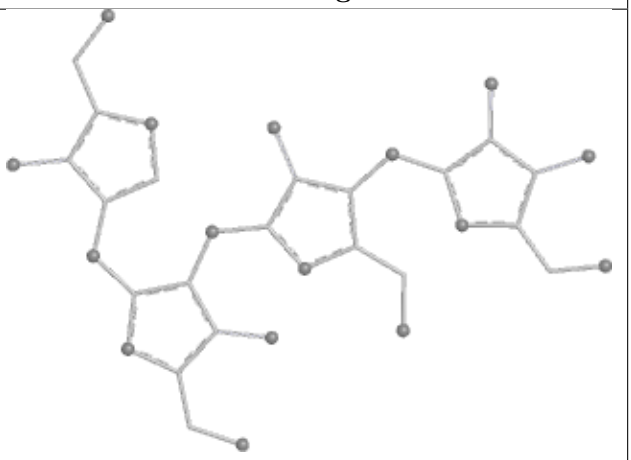
Torsions	**Rings**

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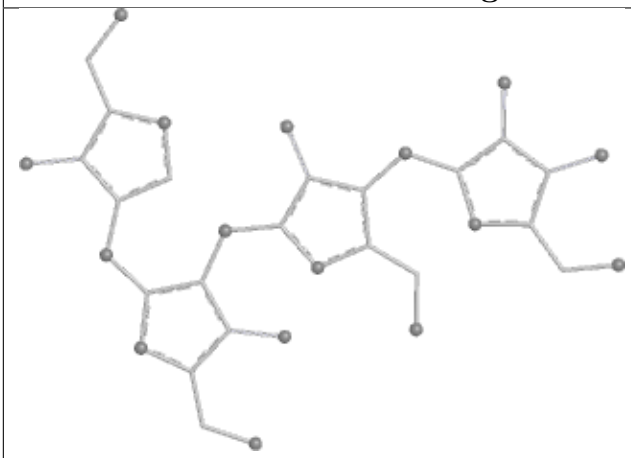	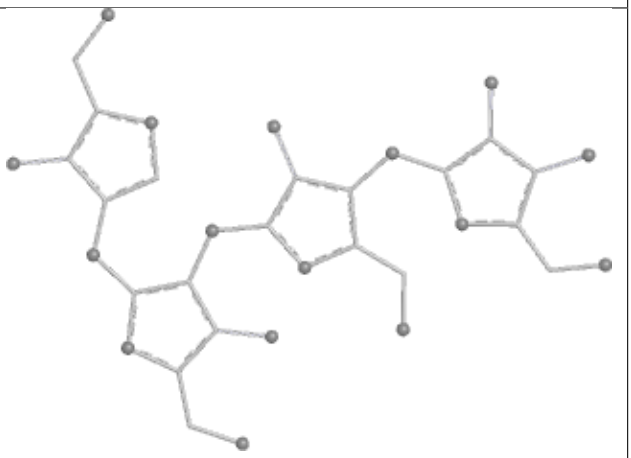
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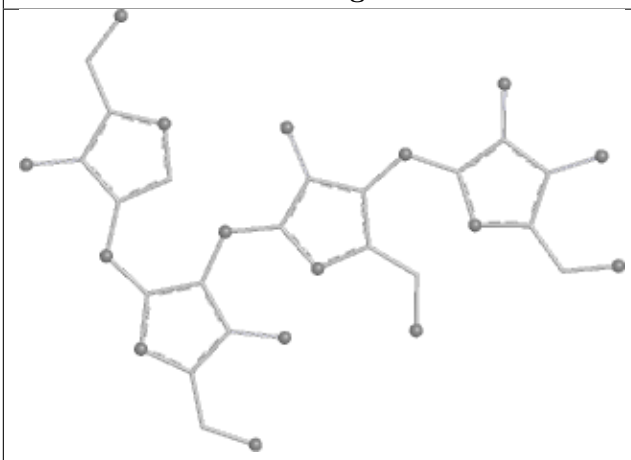	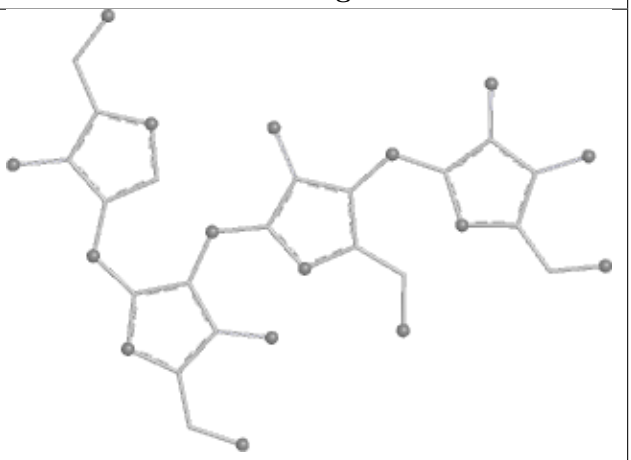
Torsions	**Rings**

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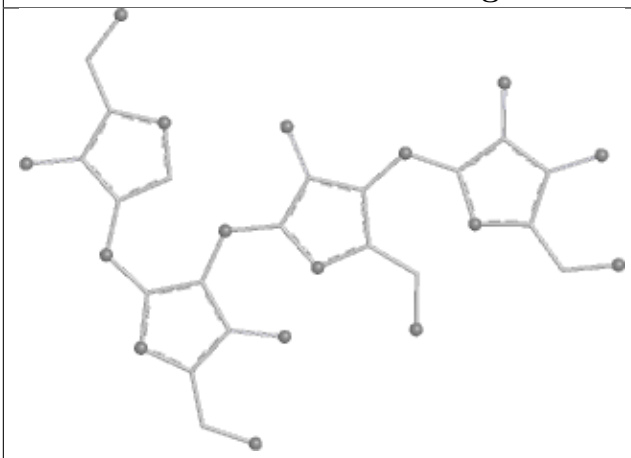	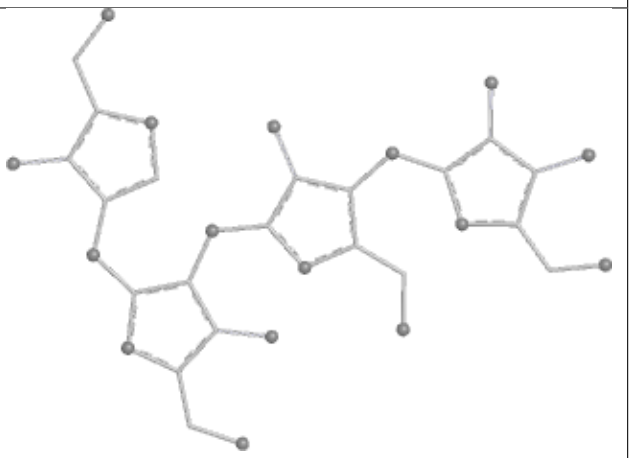
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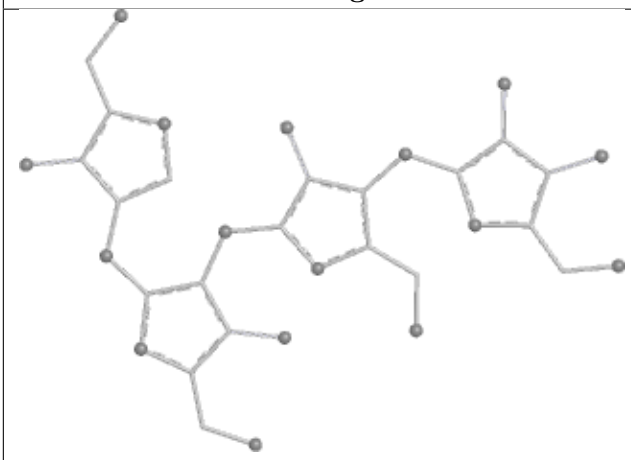	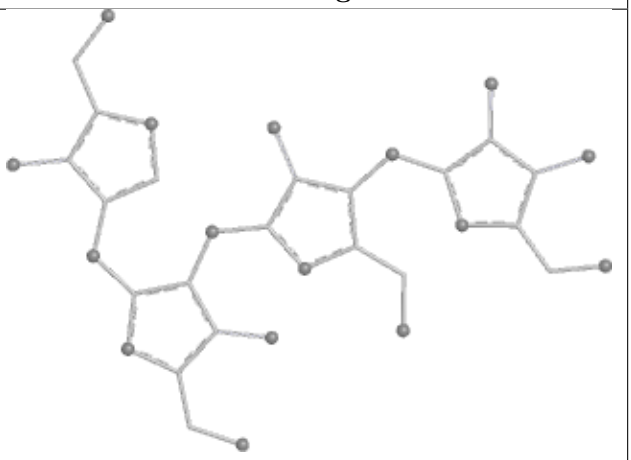
Torsions	**Rings**

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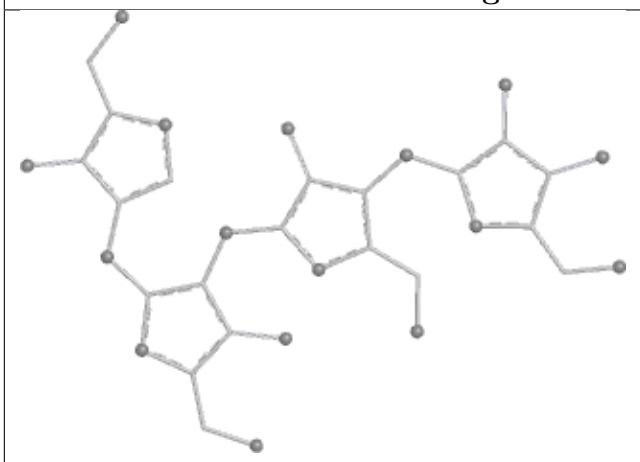	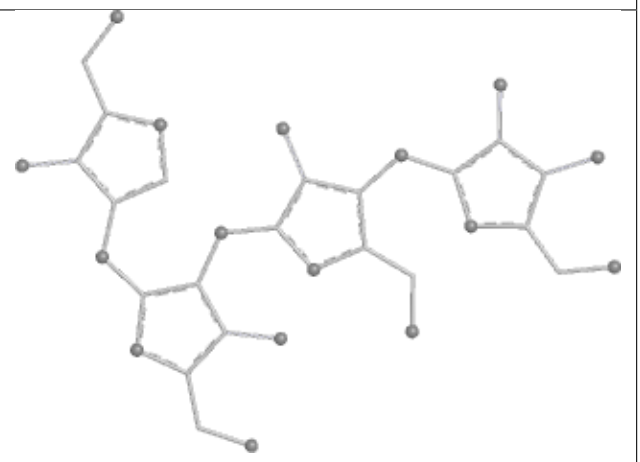
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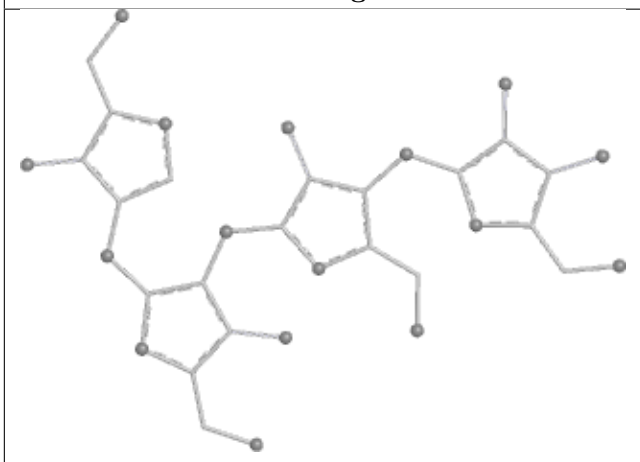	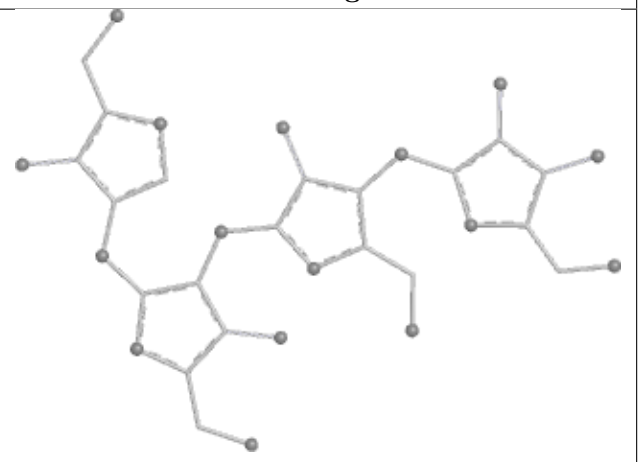
Torsions	**Rings**

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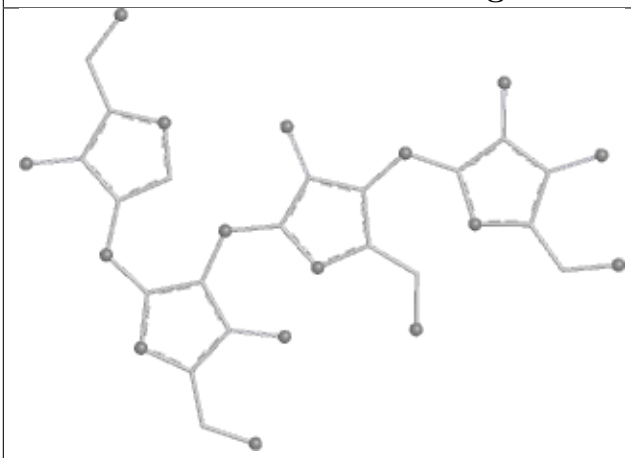	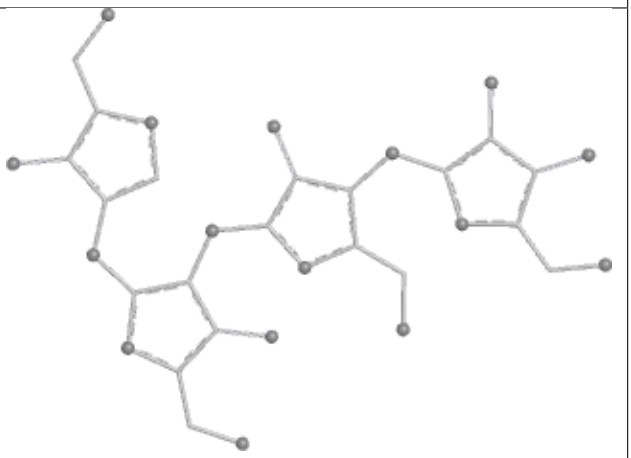
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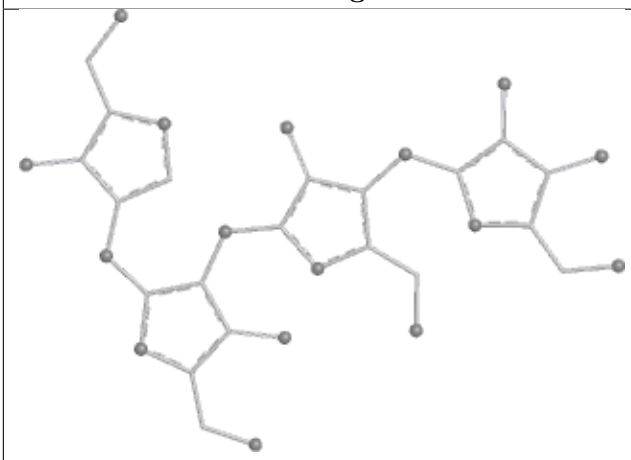	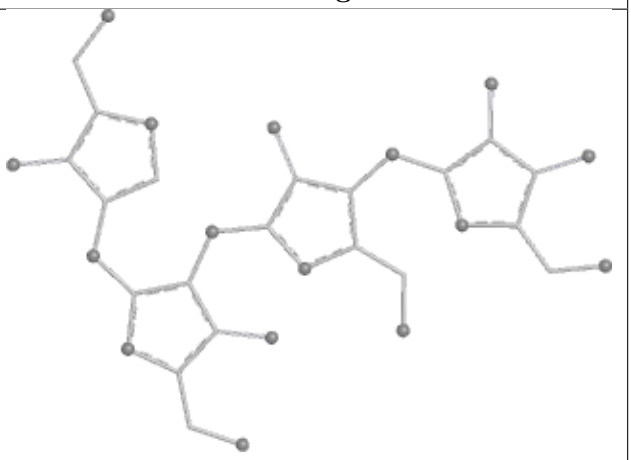
Torsions	**Rings**

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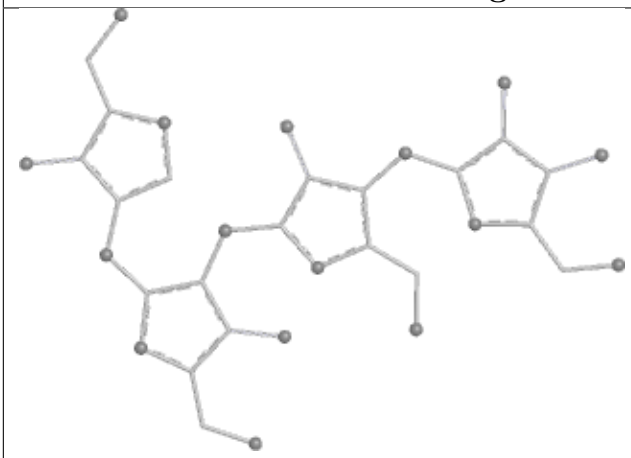	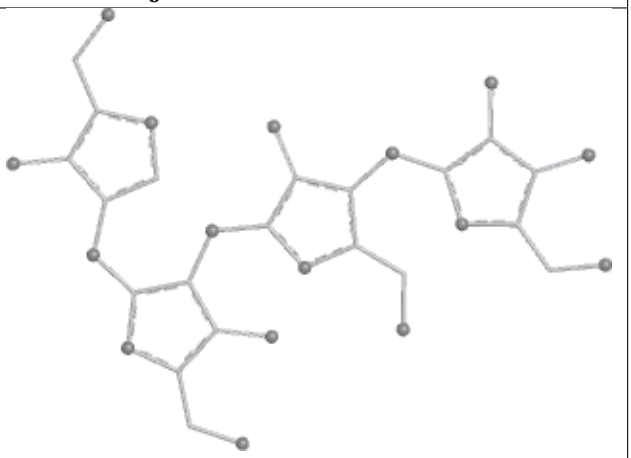
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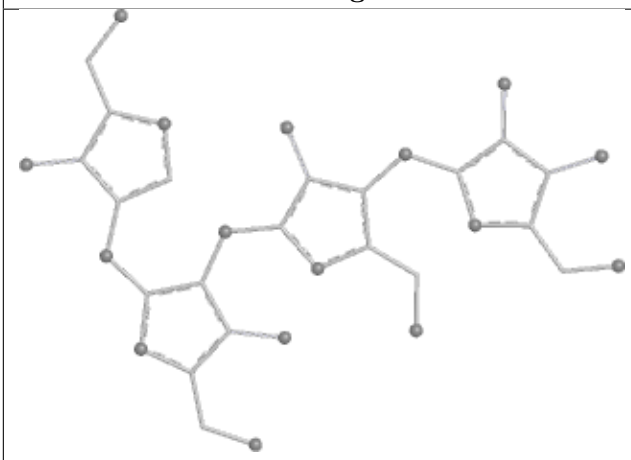	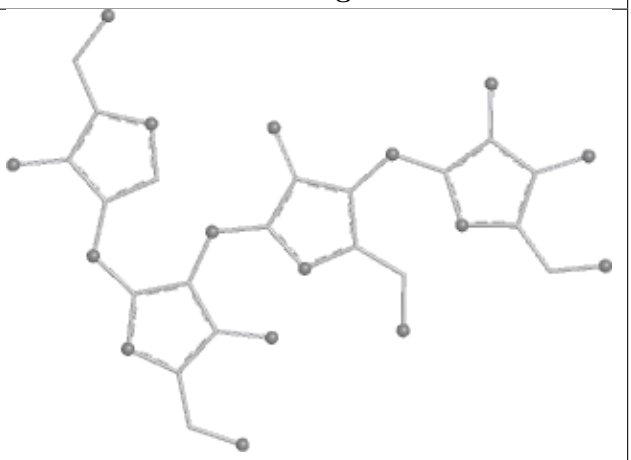
Torsions	**Rings**

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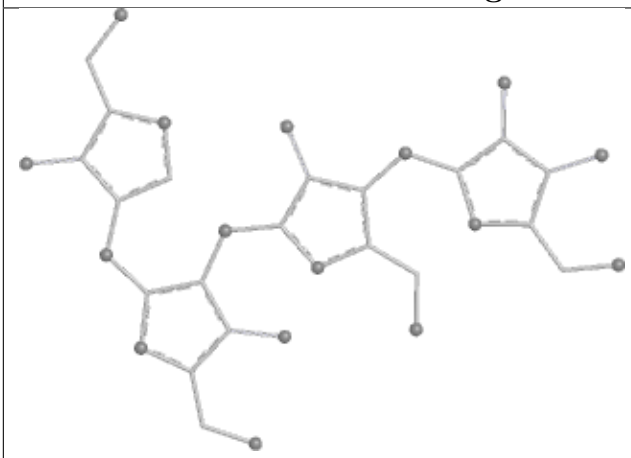	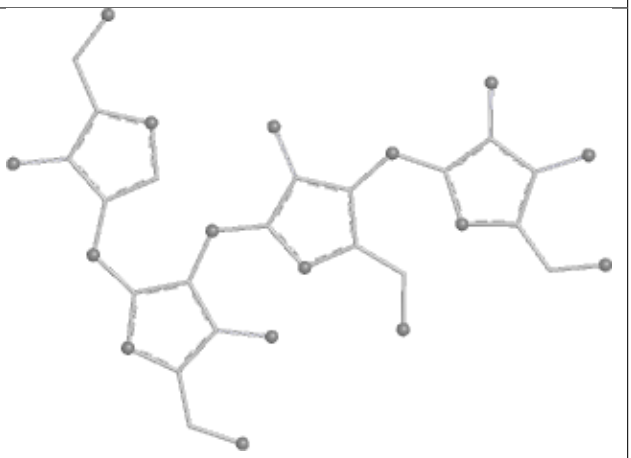
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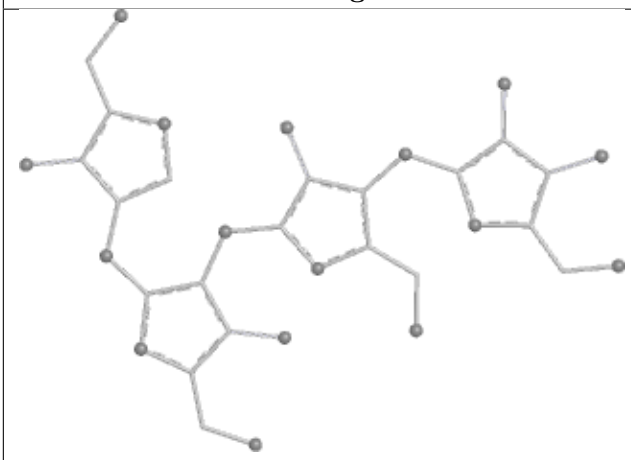	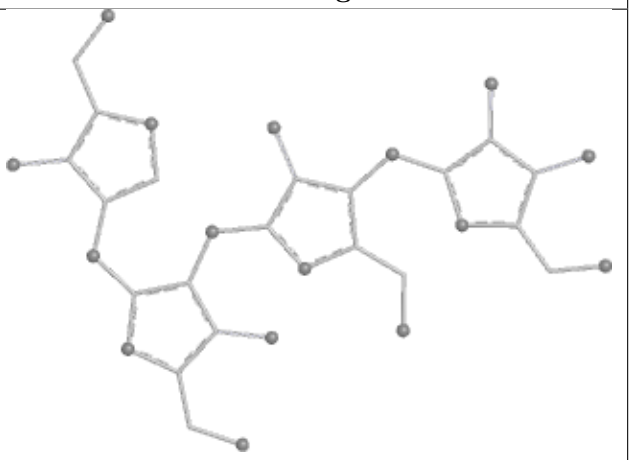
Torsions	**Rings**

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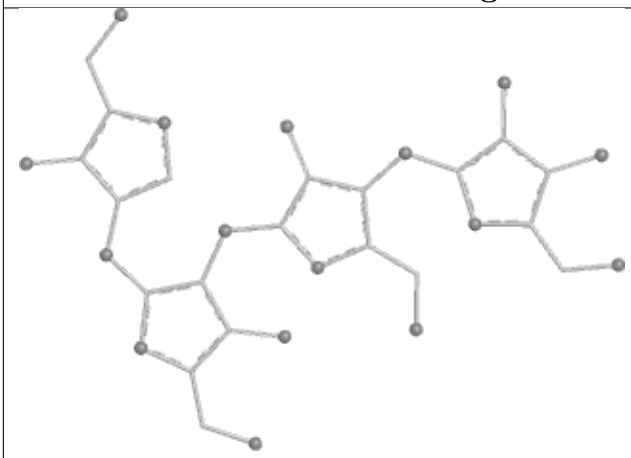	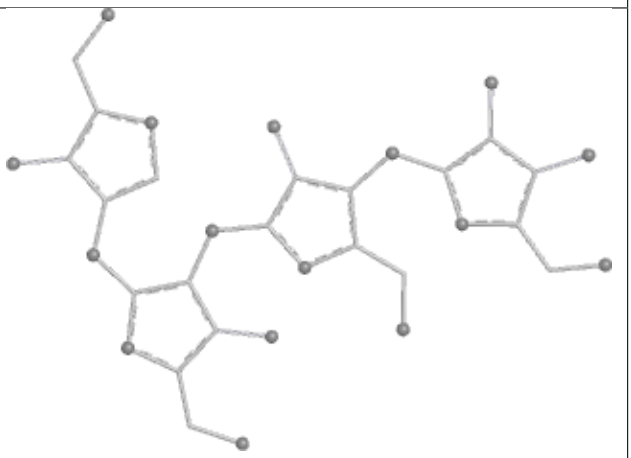
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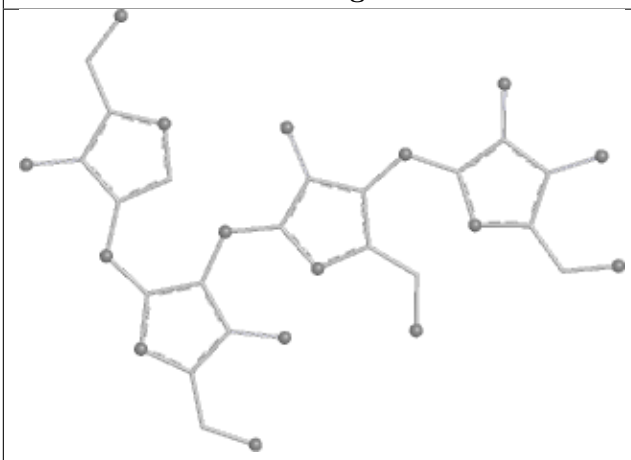	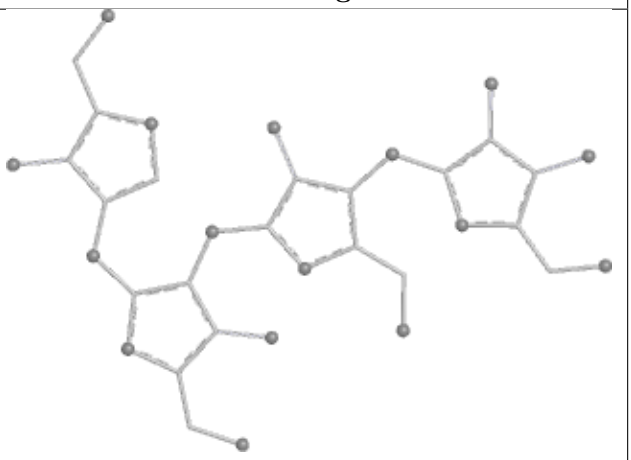
Torsions	**Rings**

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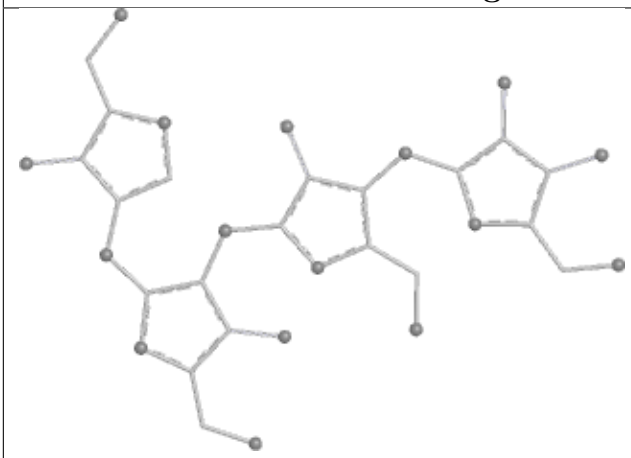	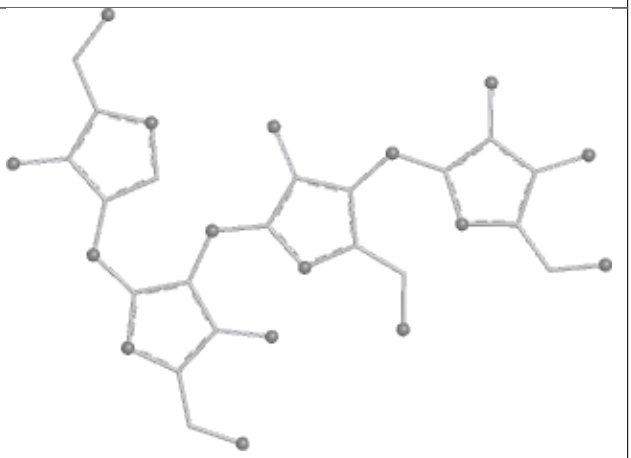
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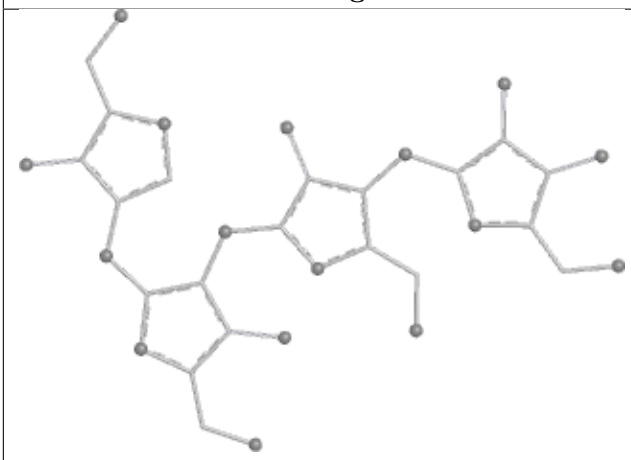	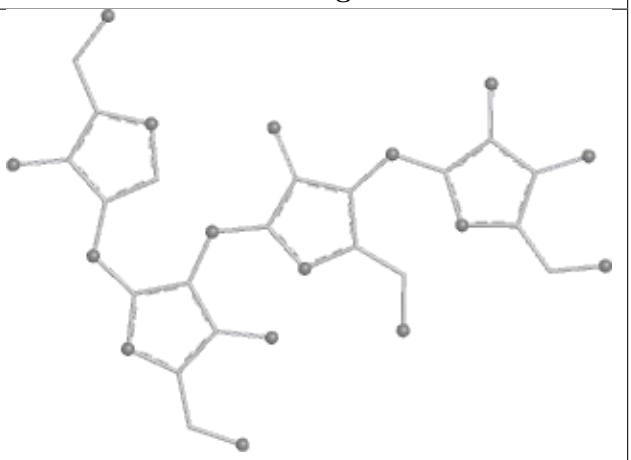
Torsions	**Rings**

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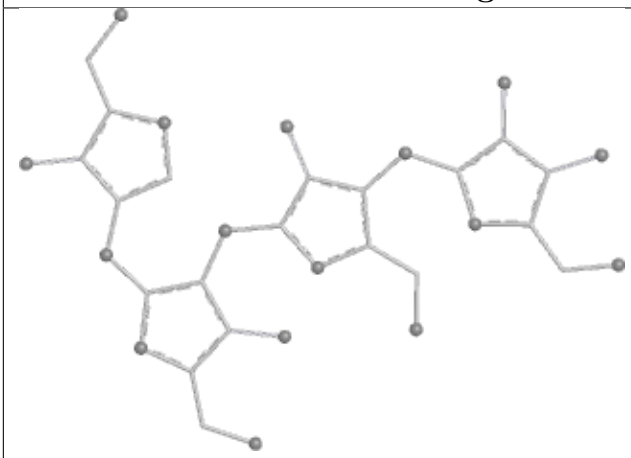
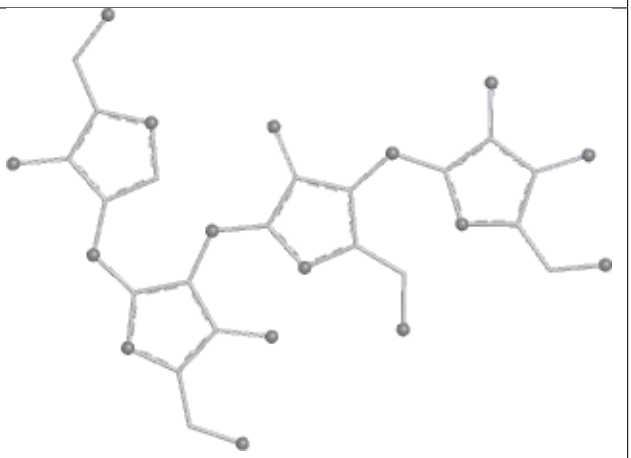
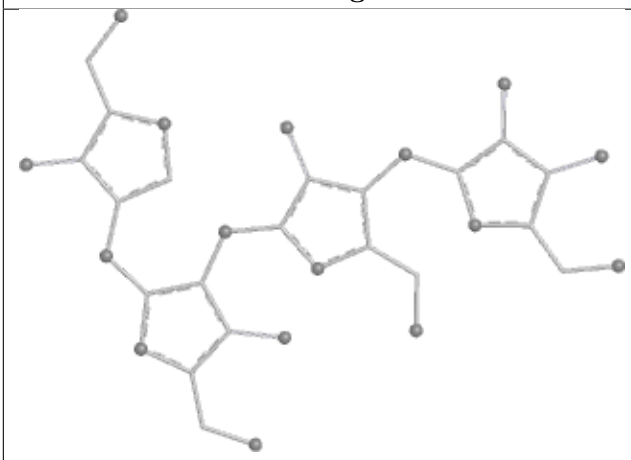
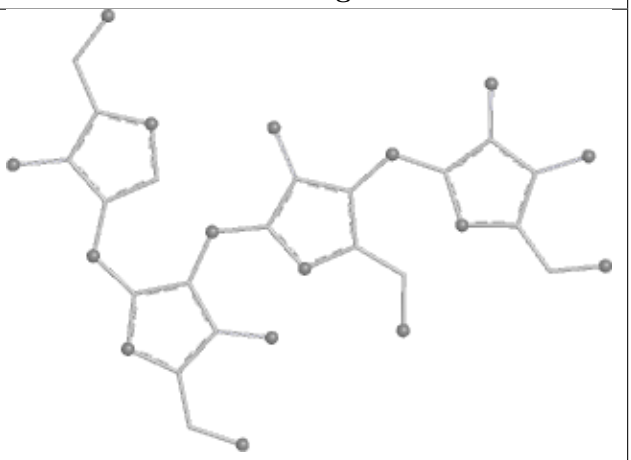
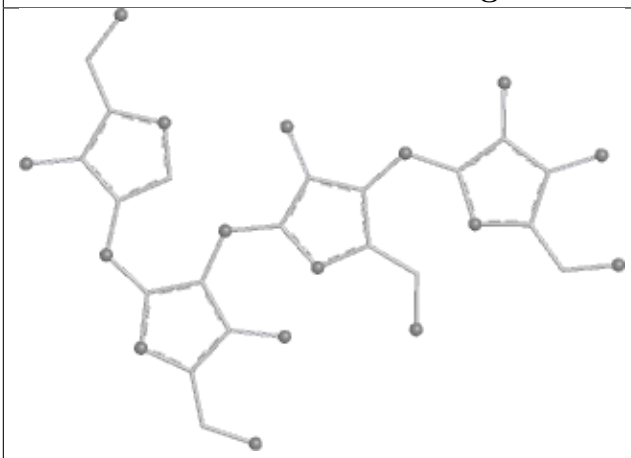
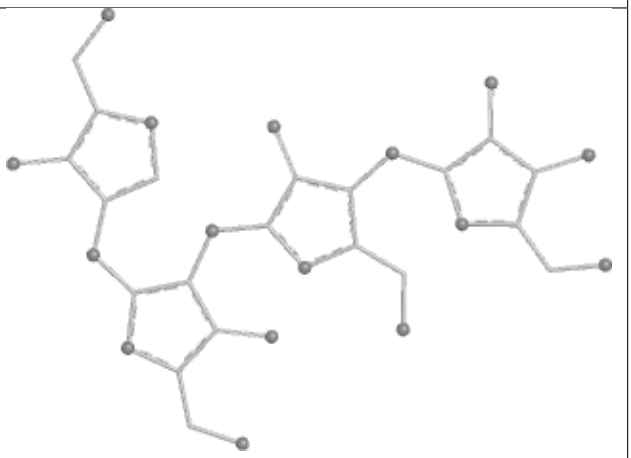
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain OD	
	
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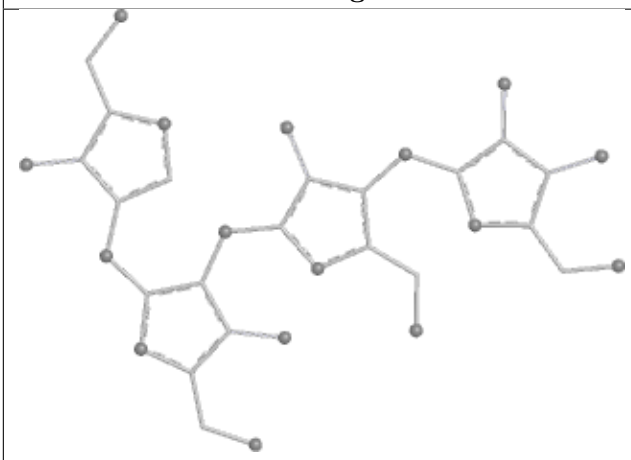	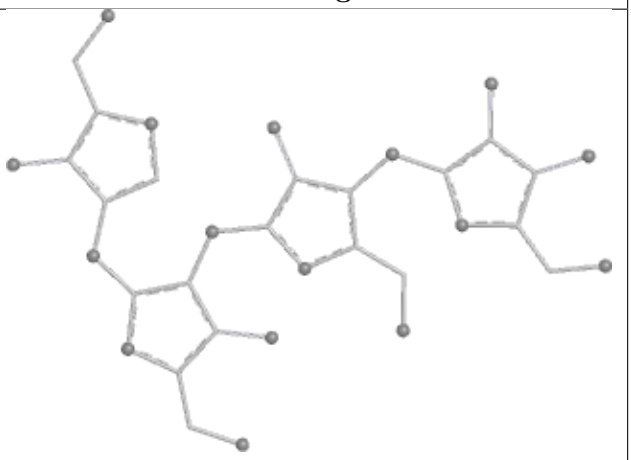
Torsions	**Rings**

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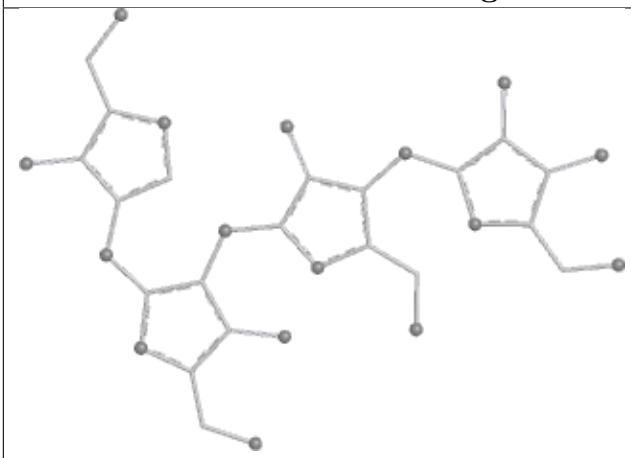
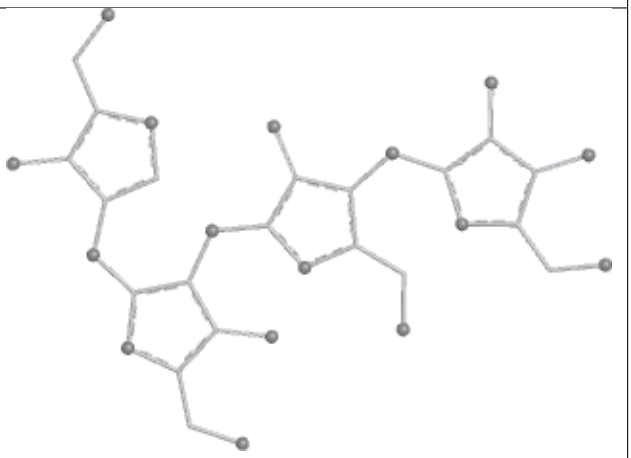
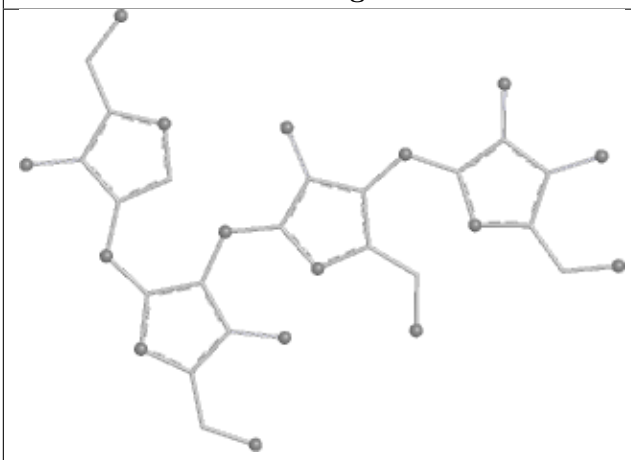
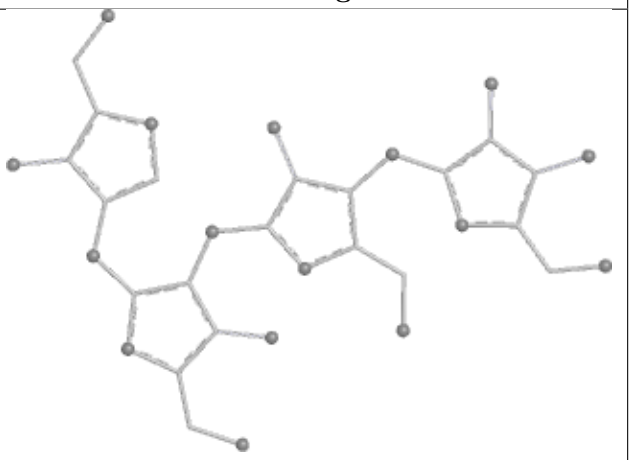
 Bond lengths	 Bond angles
 Torsions	 Rings

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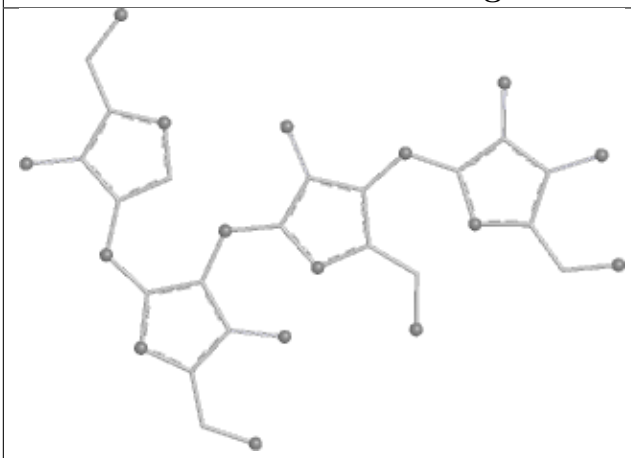
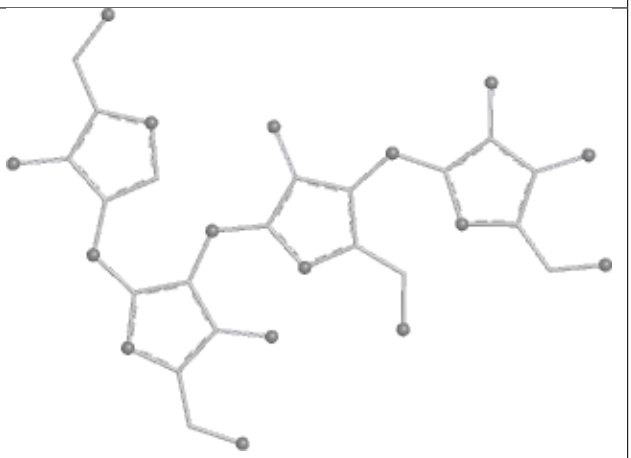
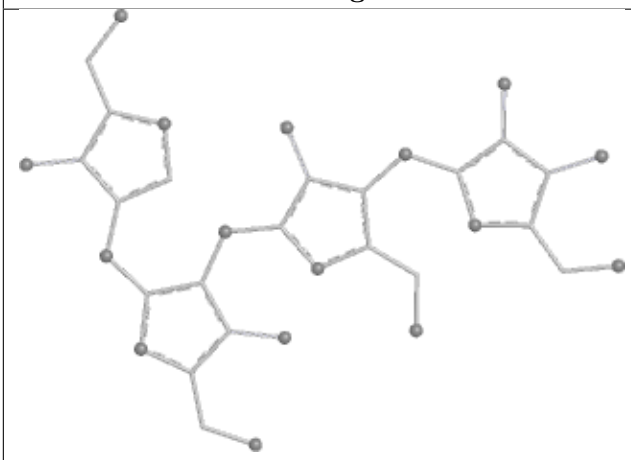
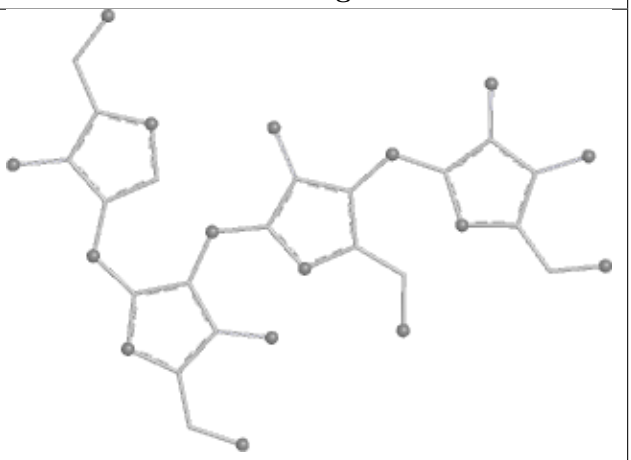
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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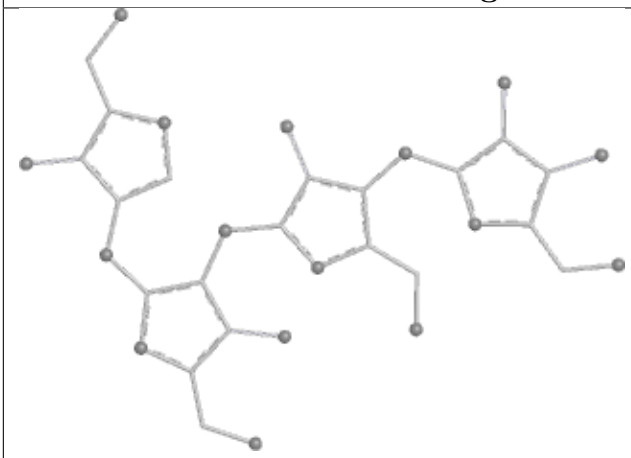
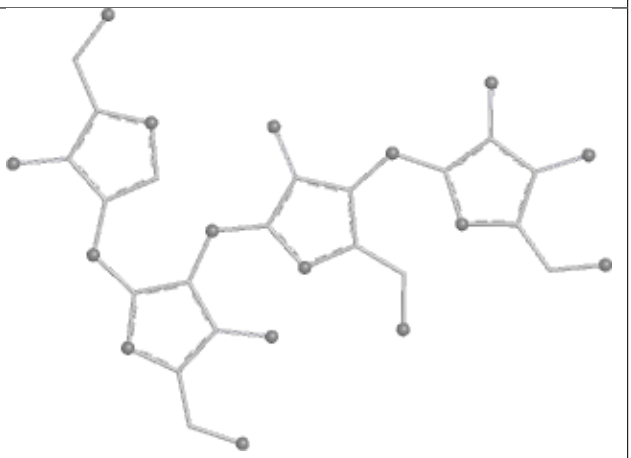
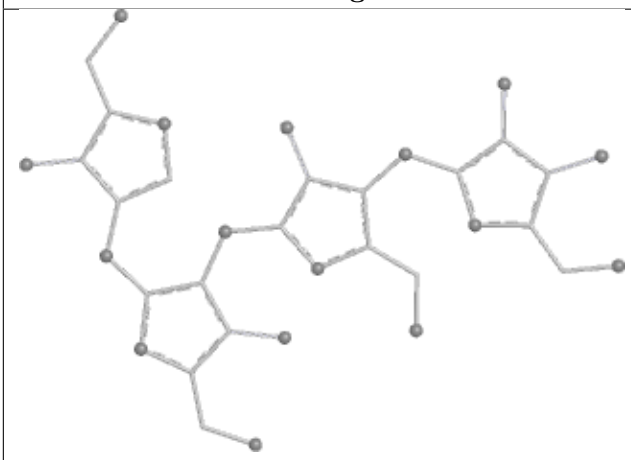
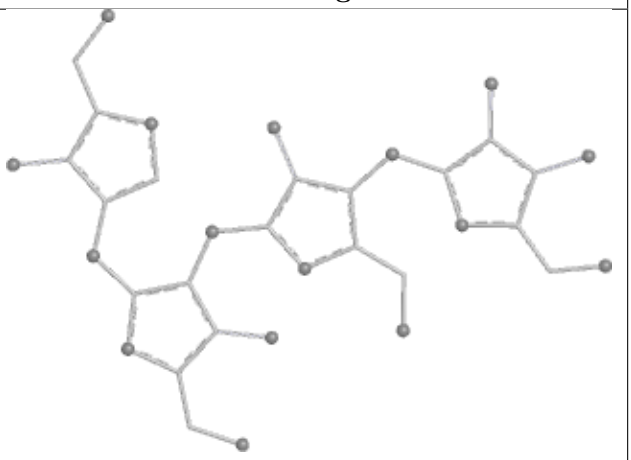
 Bond lengths	 Bond angles
 Torsions	 Rings

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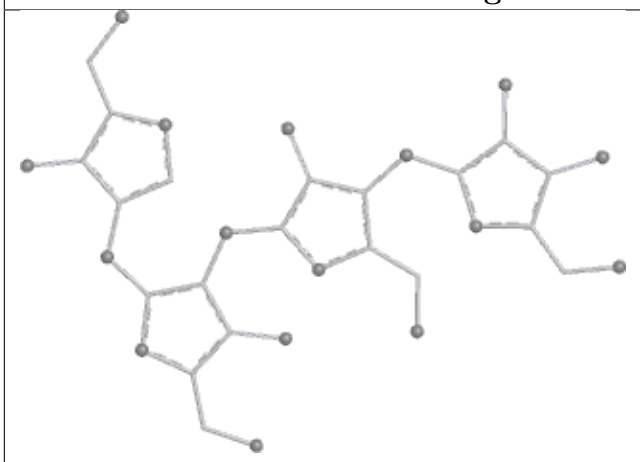
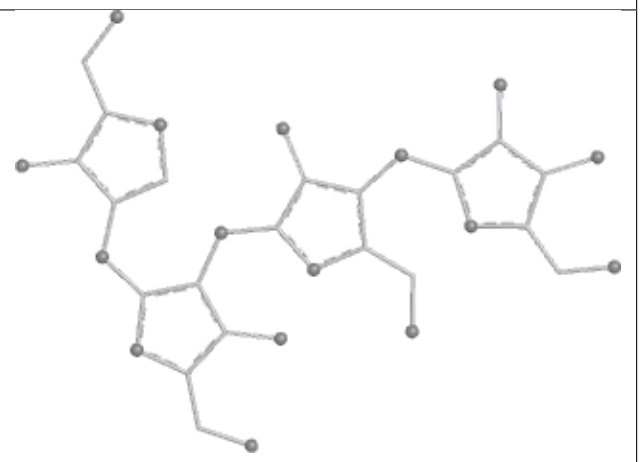
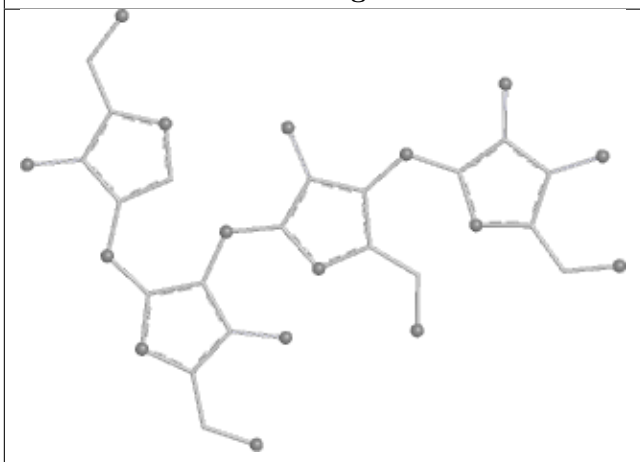
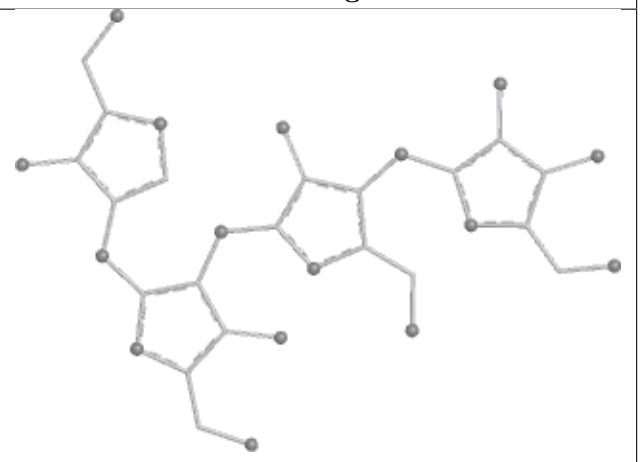
 Bond lengths	 Bond angles
 Torsions	 Rings

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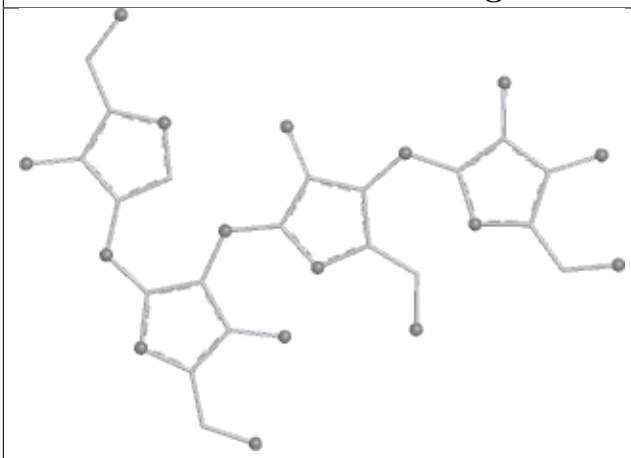
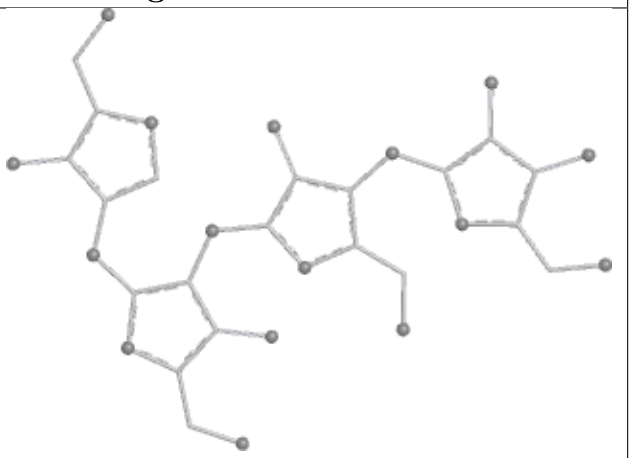
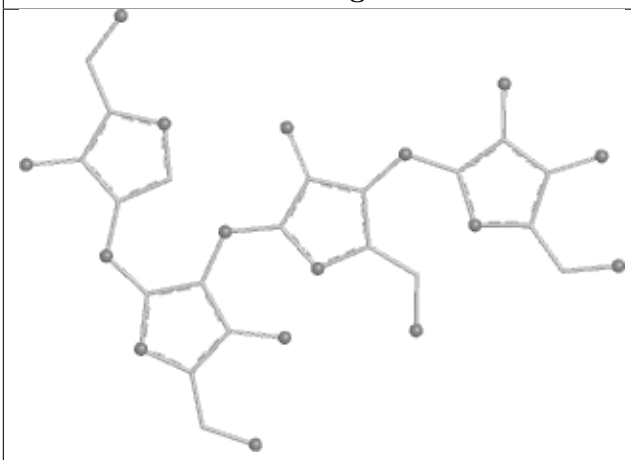
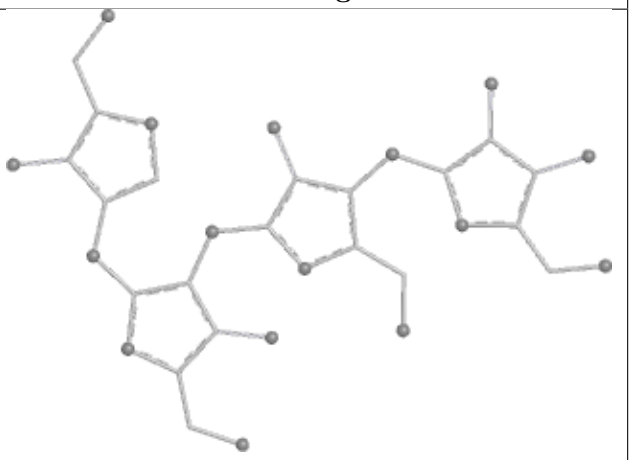
 Bond lengths	 Bond angles
 Torsions	 Rings

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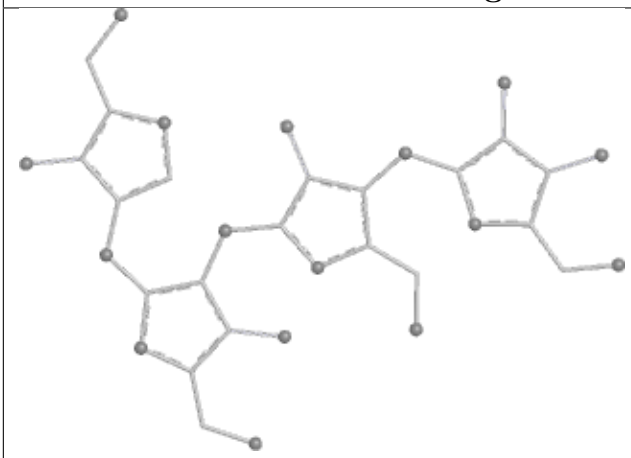
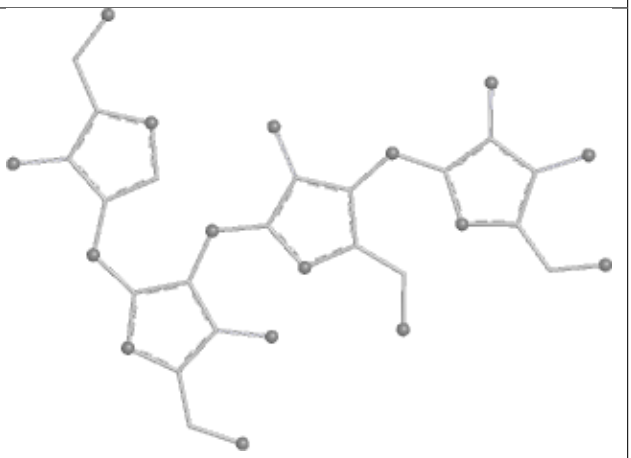
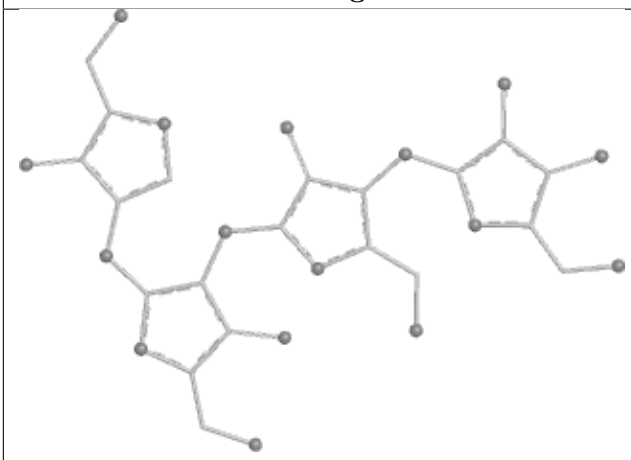
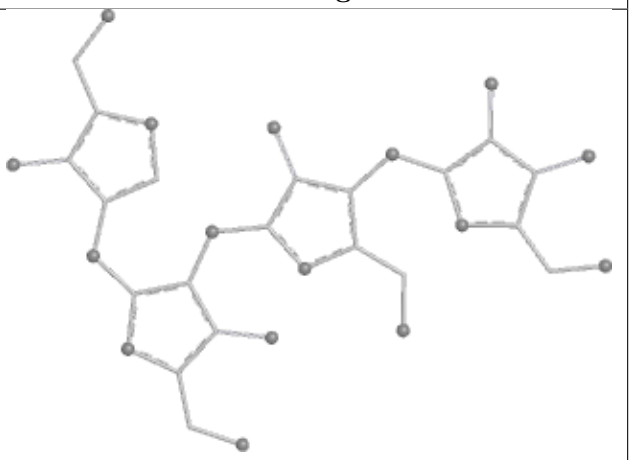
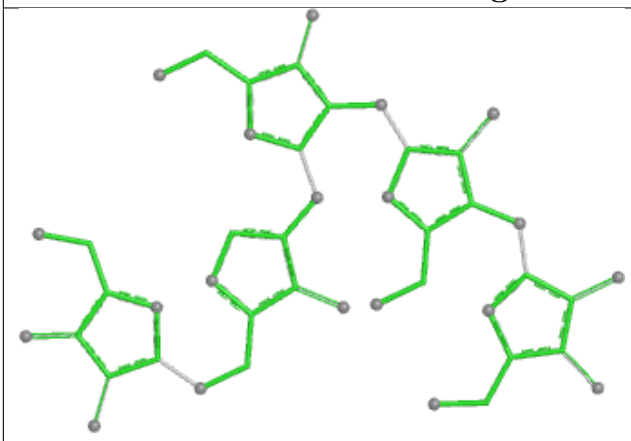
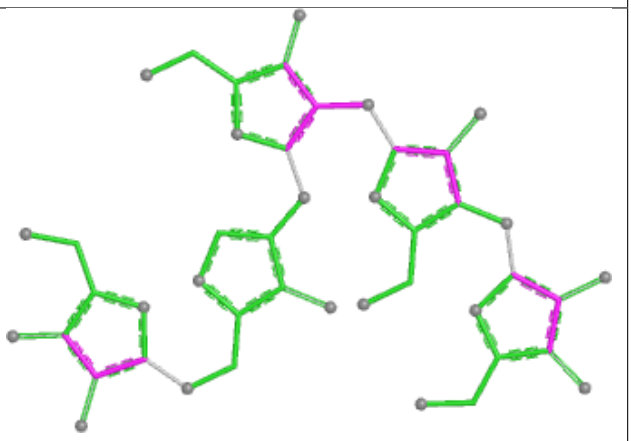
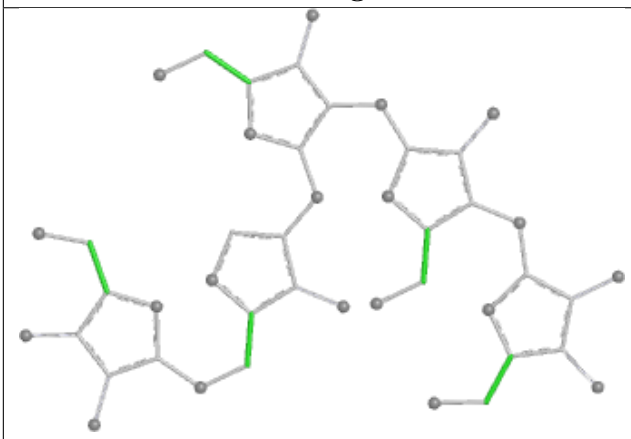
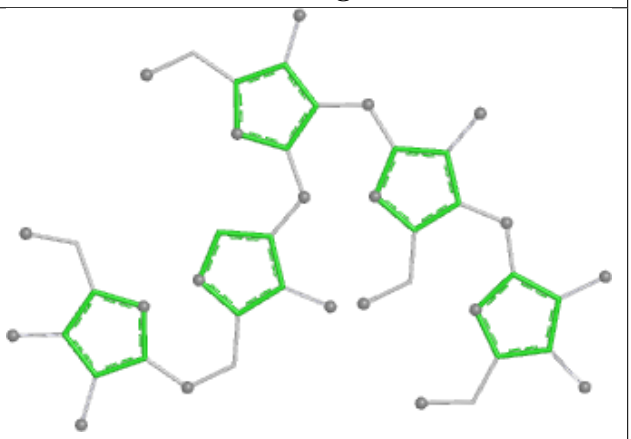
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

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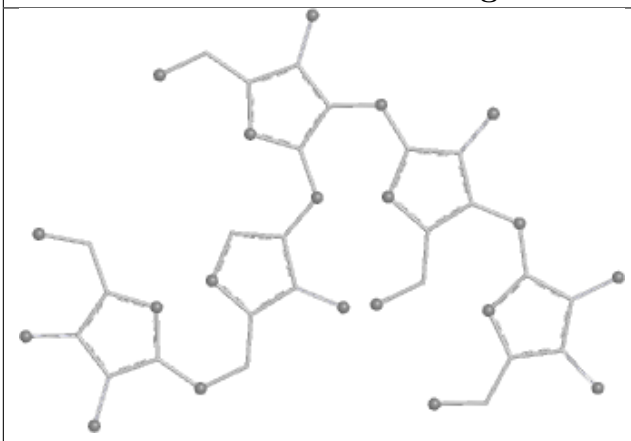
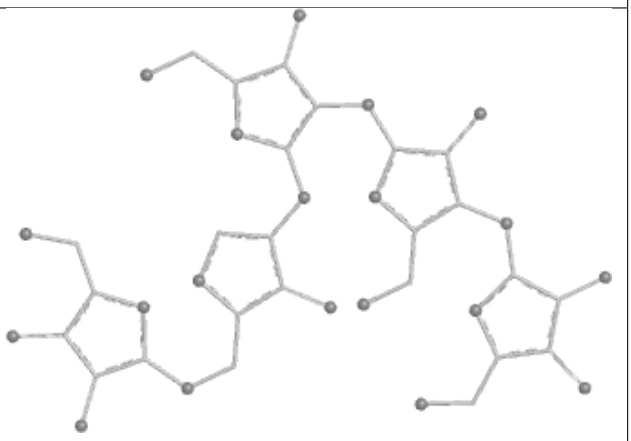
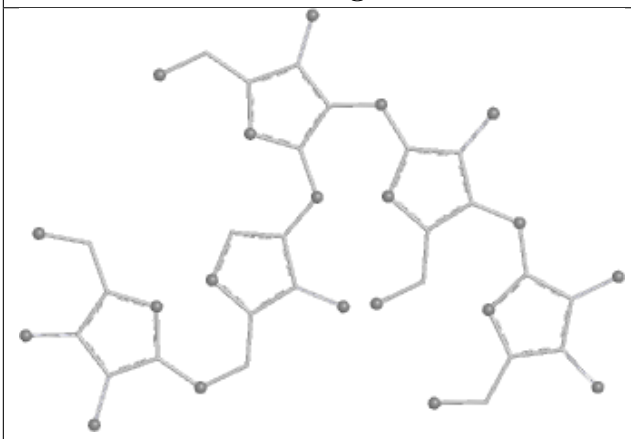
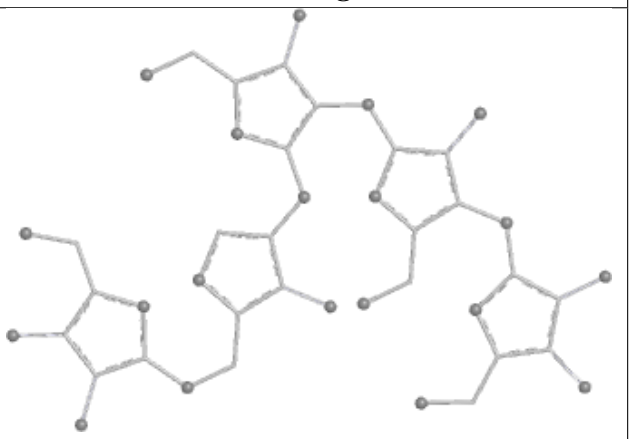
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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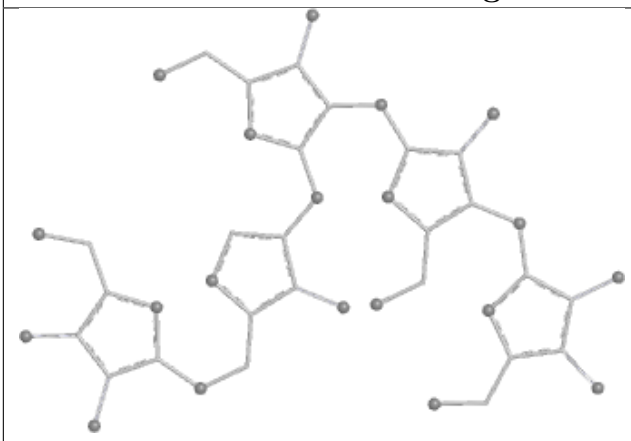
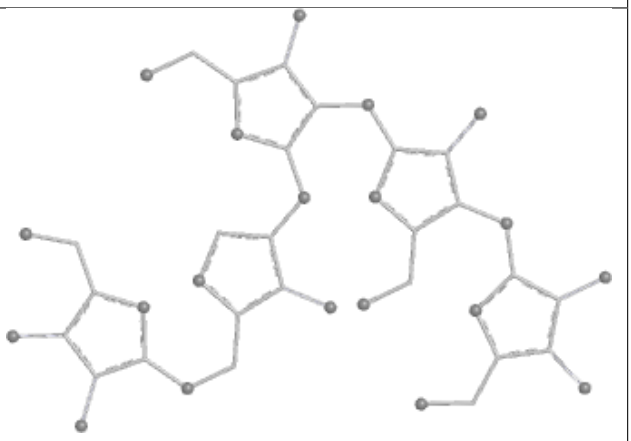
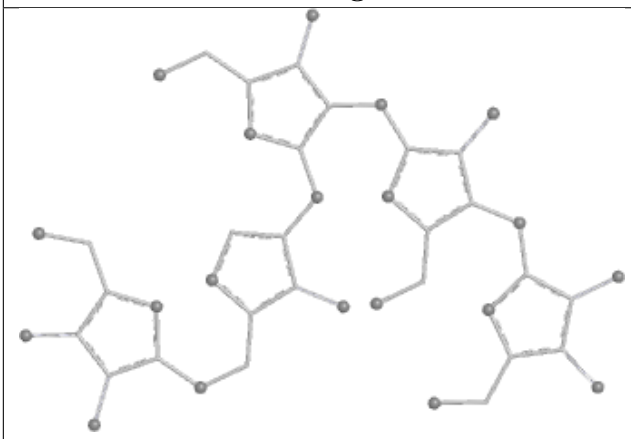
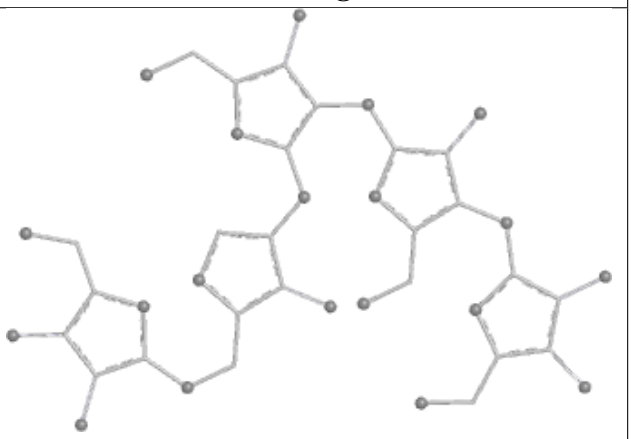
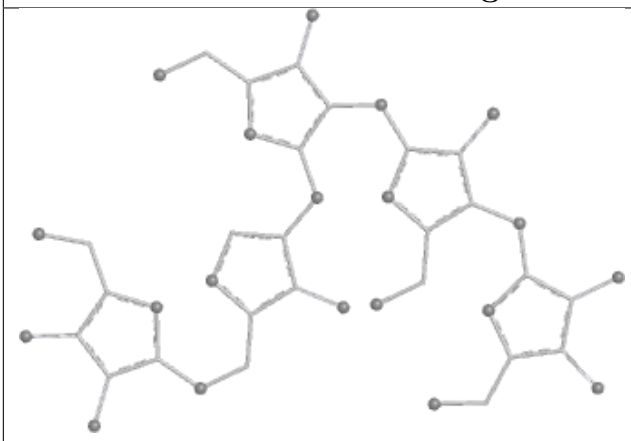
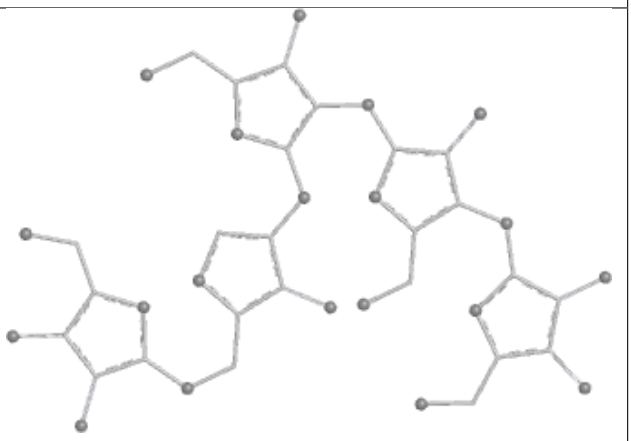
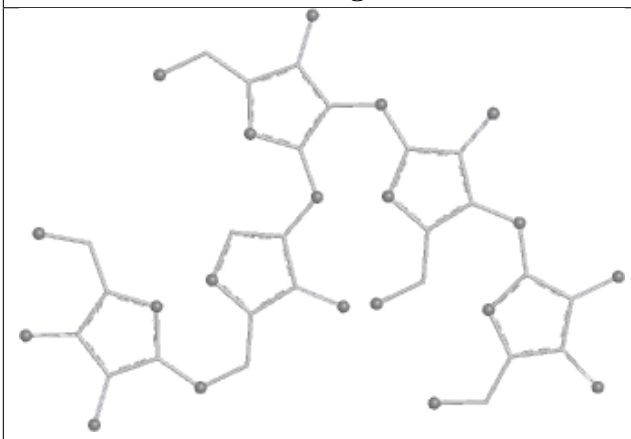
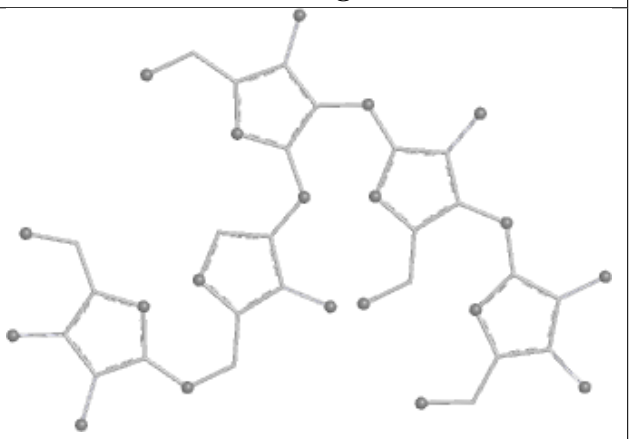
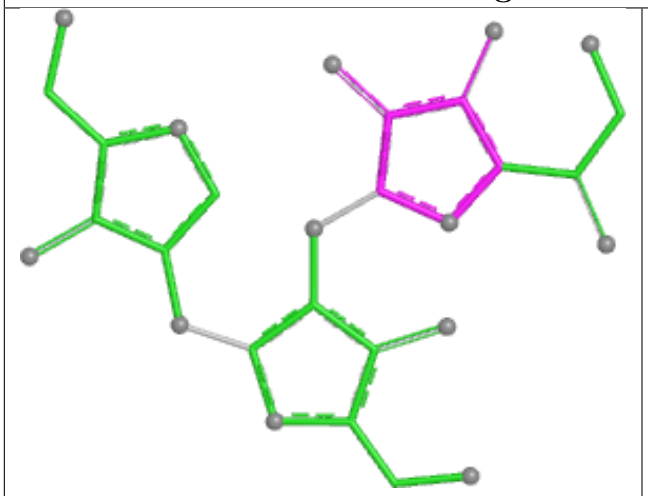
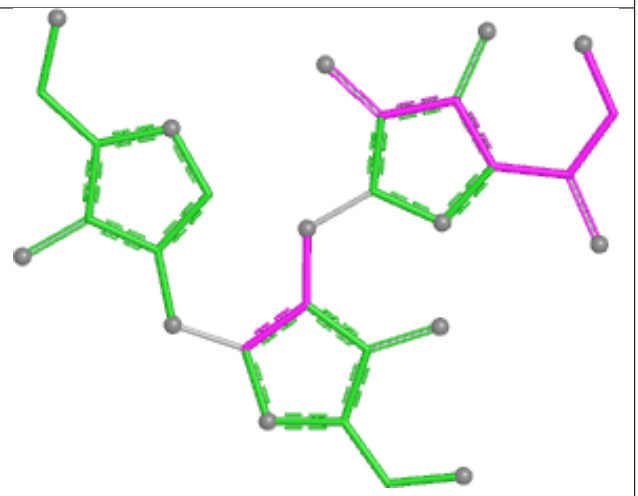
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain BD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

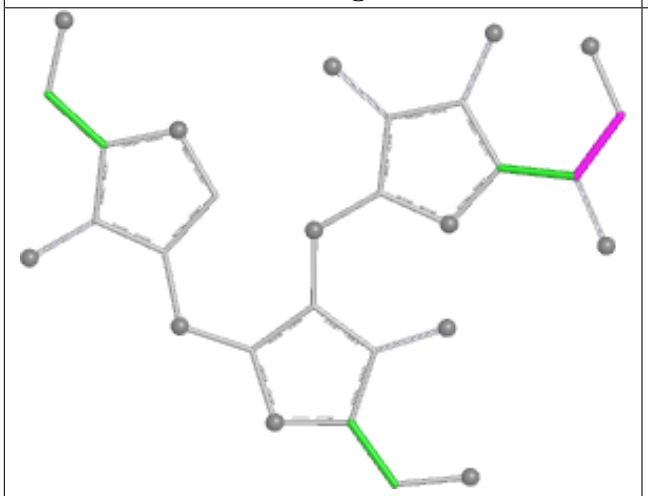
Oligosaccharide Chain N



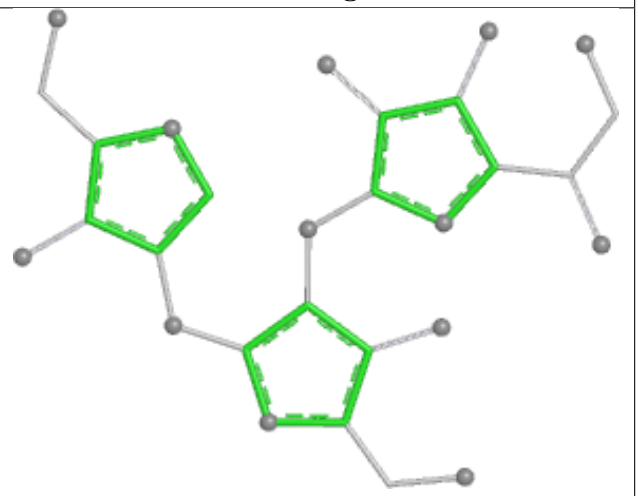
Bond lengths



Bond angles

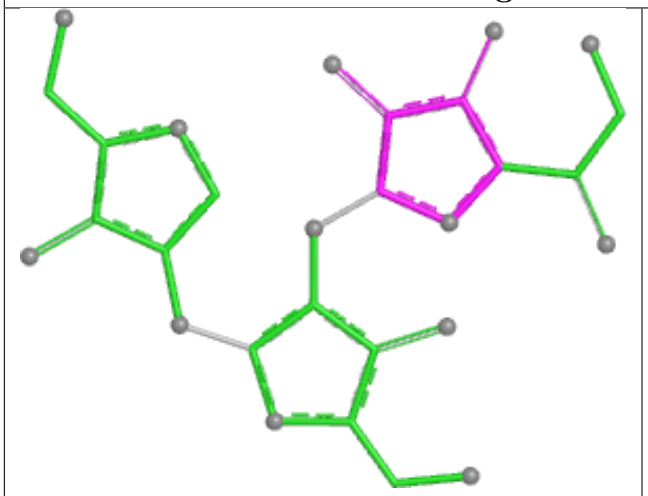


Torsions



Rings

Oligosaccharide Chain R



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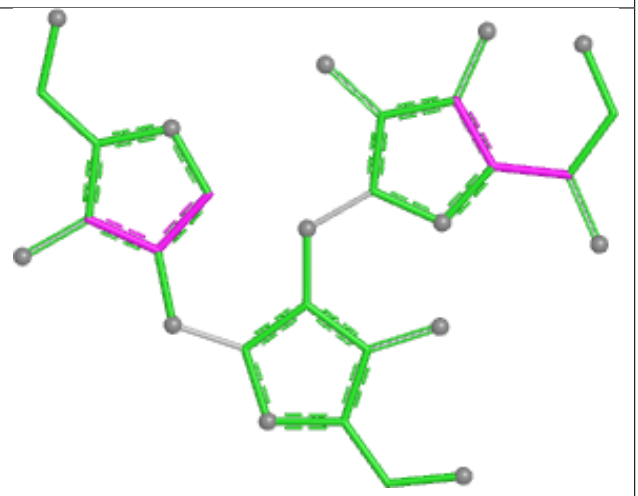
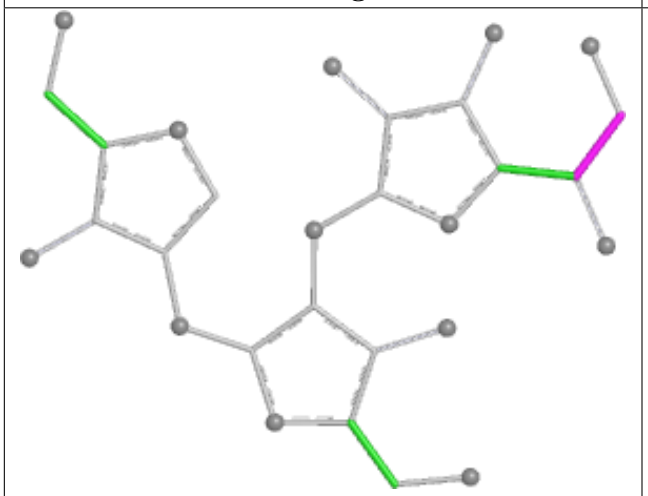


Bond angles



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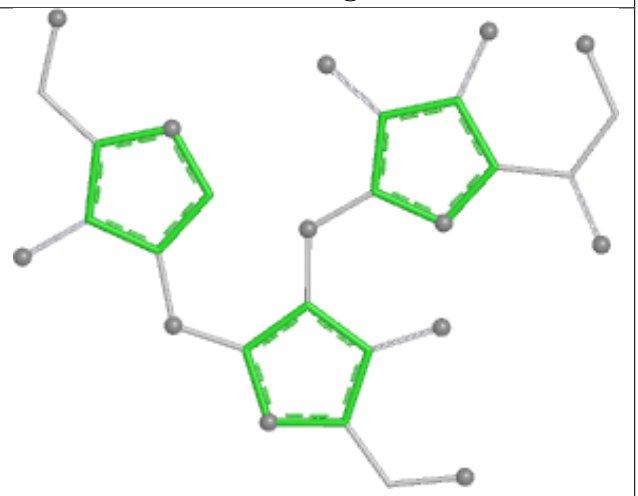
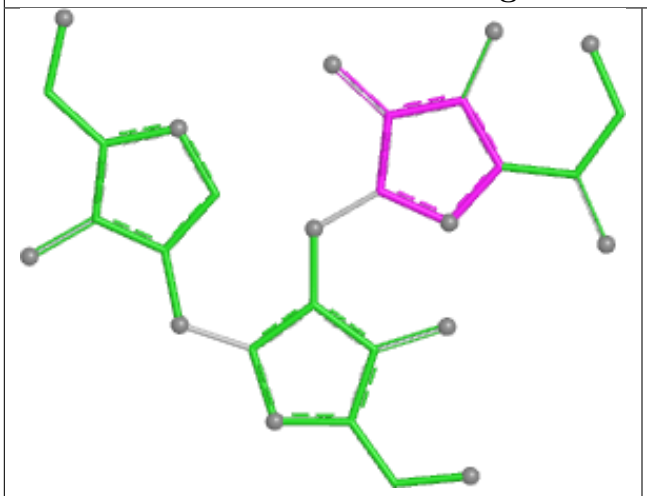


Rings

Oligosaccharide Chain 5



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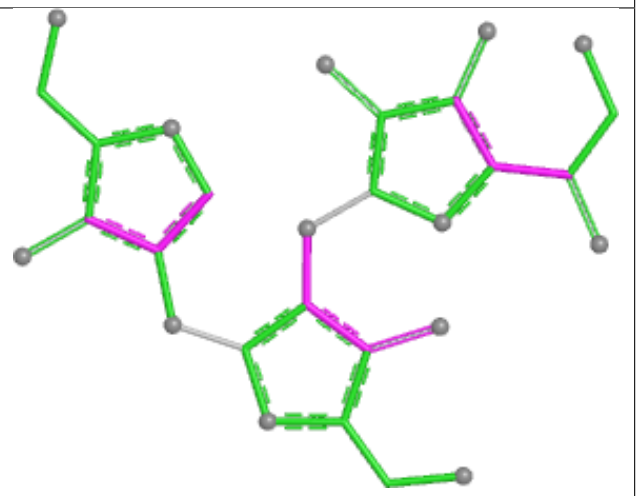

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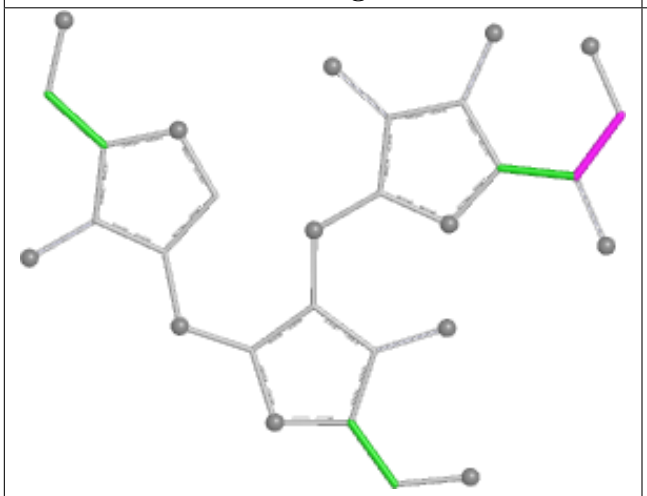

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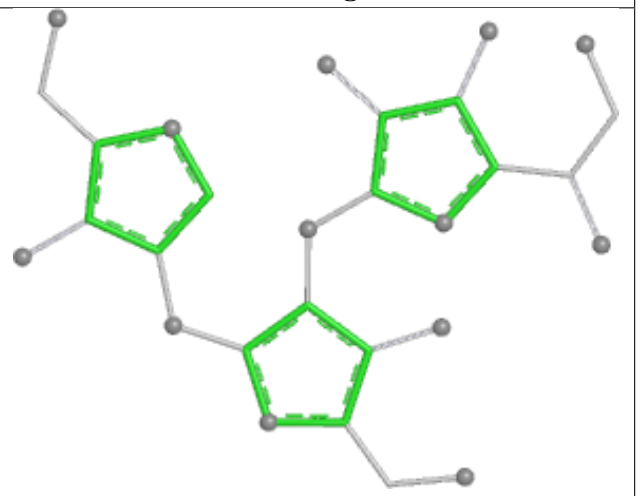
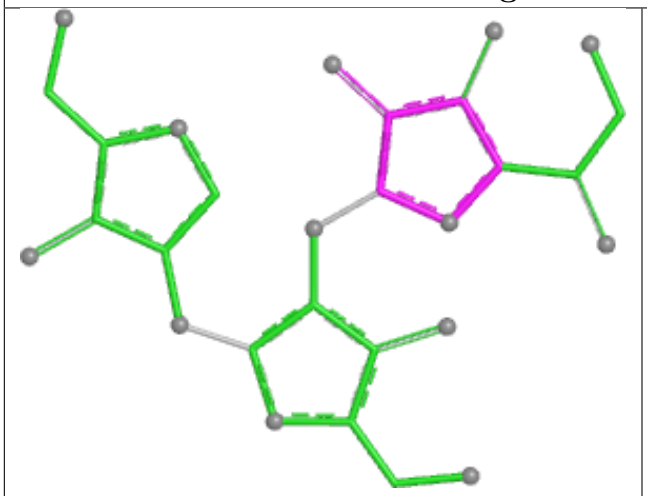
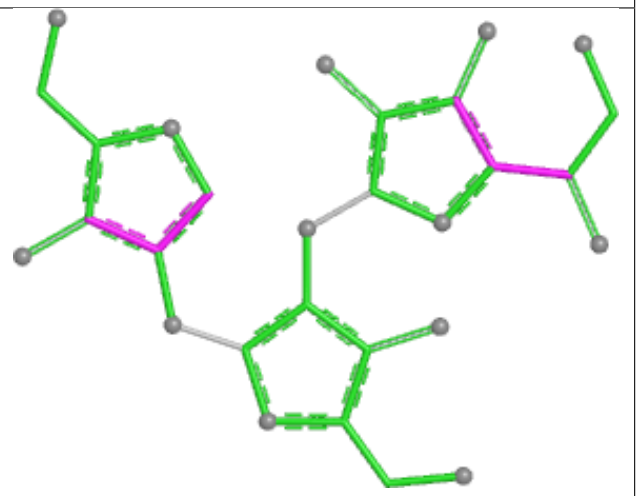


Rings

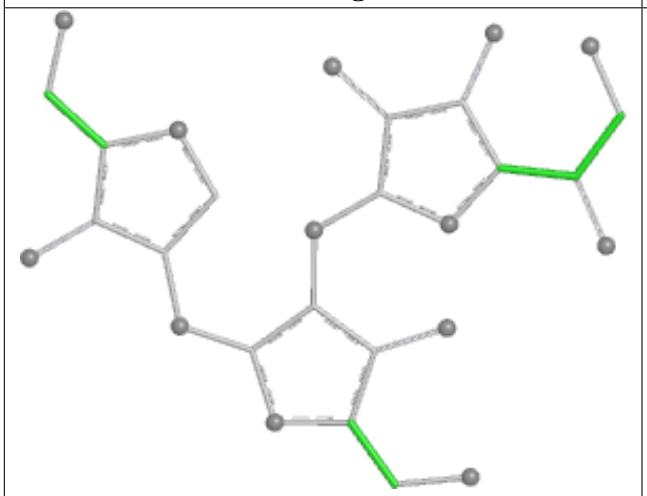
Oligosaccharide Chain 8



Bond lengths



Bond angles



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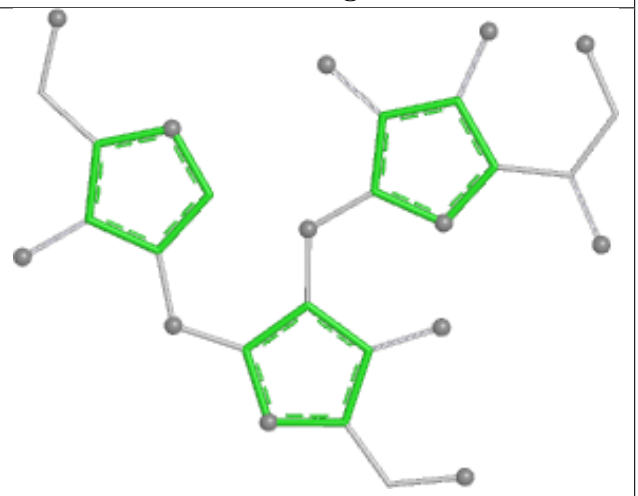
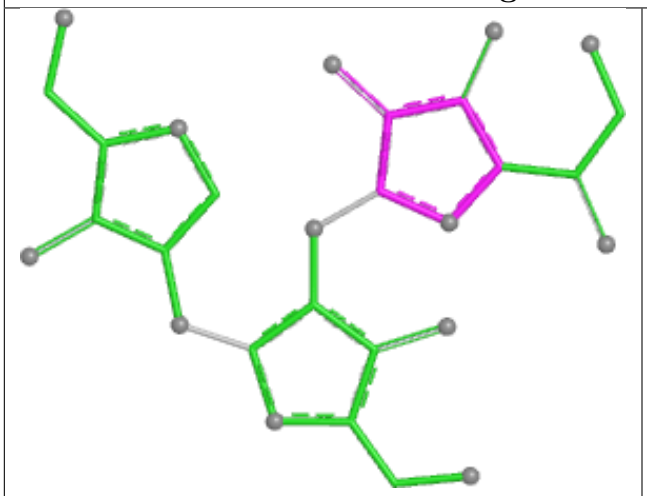


Rings

Oligosaccharide Chain 9



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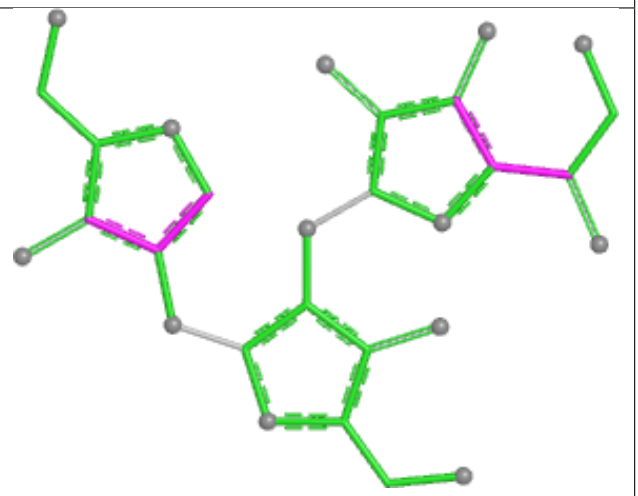
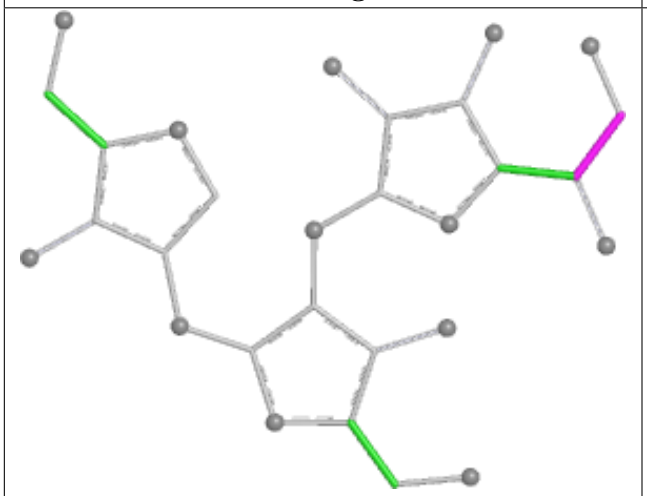


Bond angles



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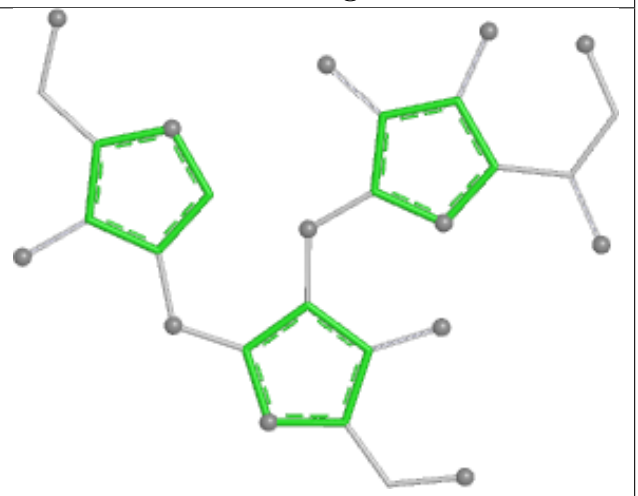
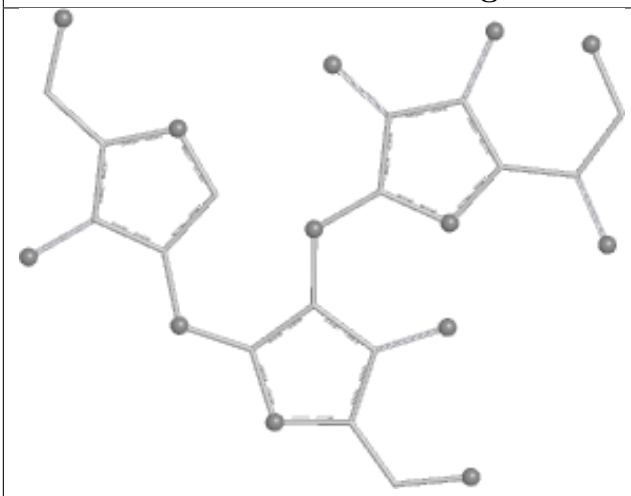
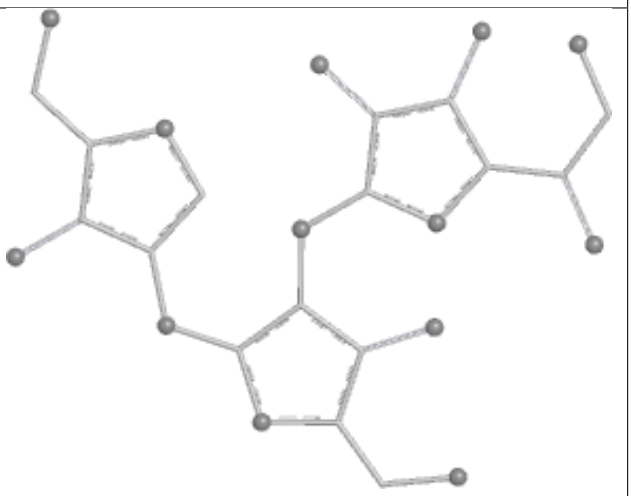
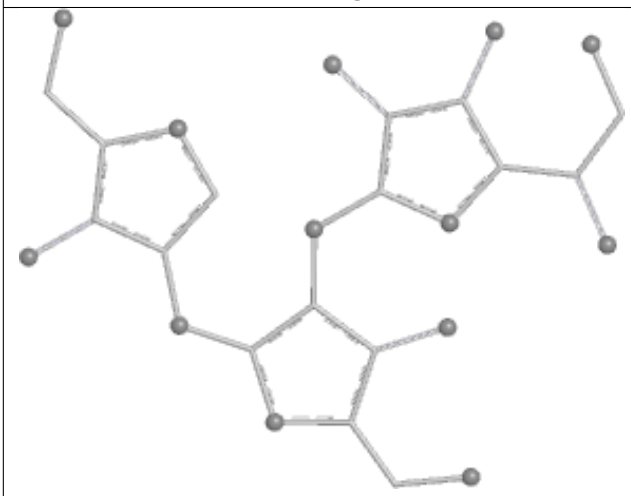
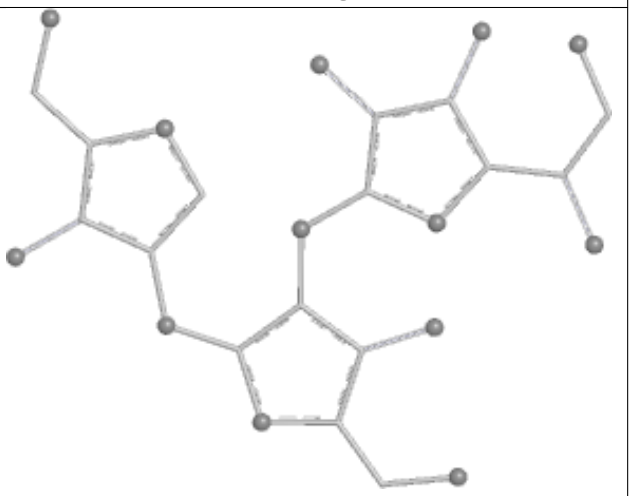


Rings

Oligosaccharide Chain AA	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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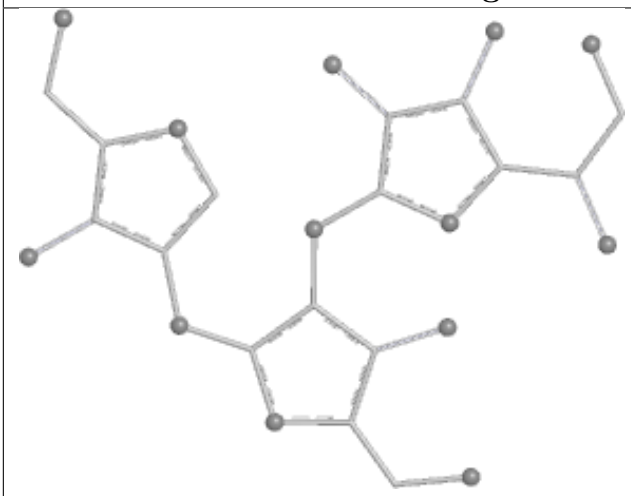
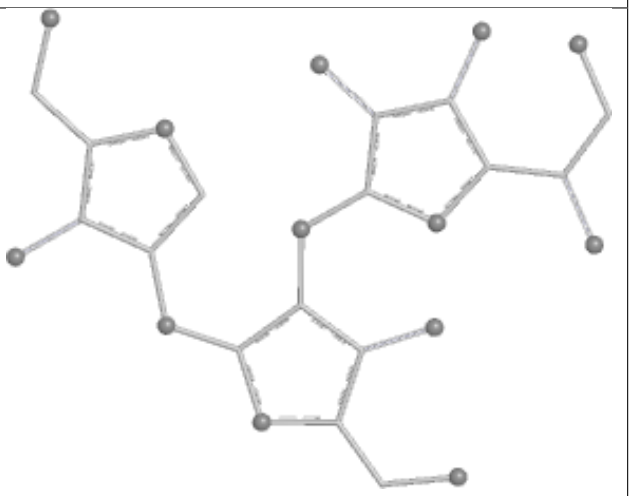
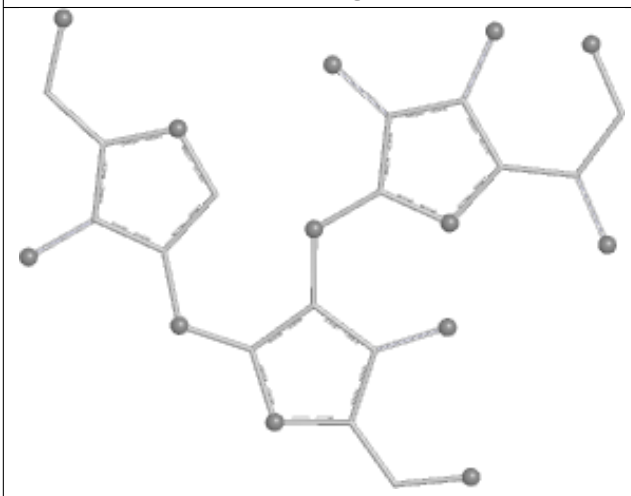
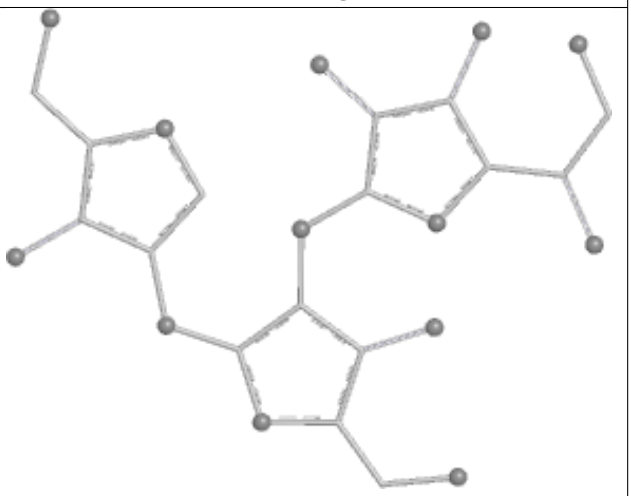
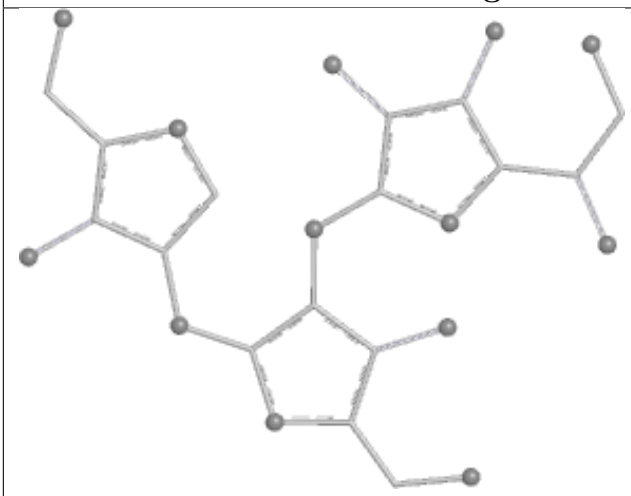
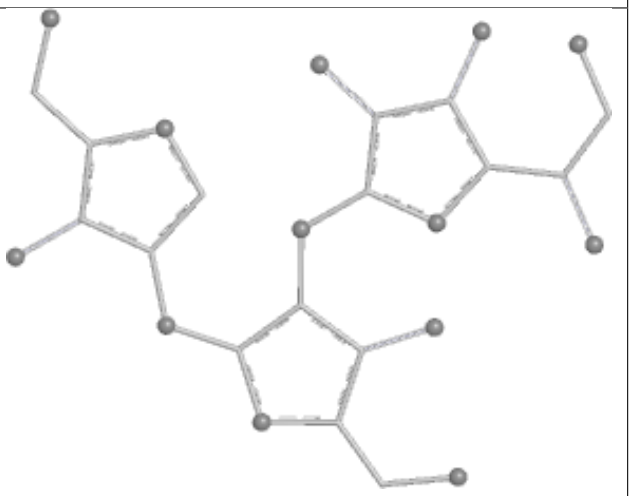
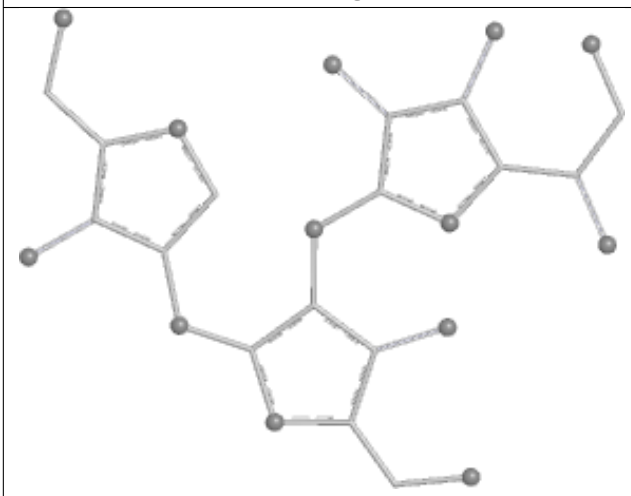
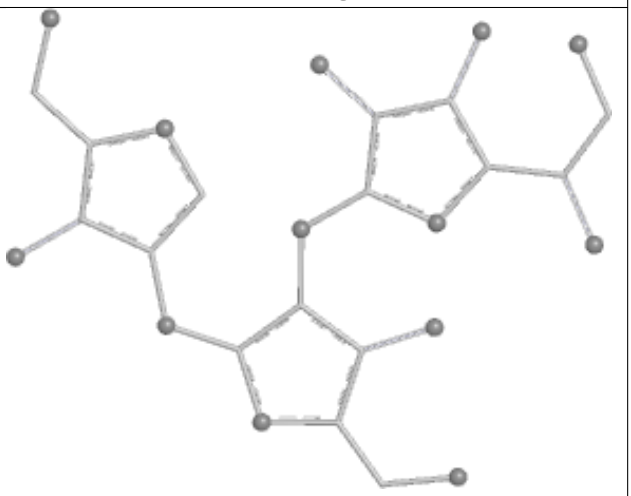
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain LA	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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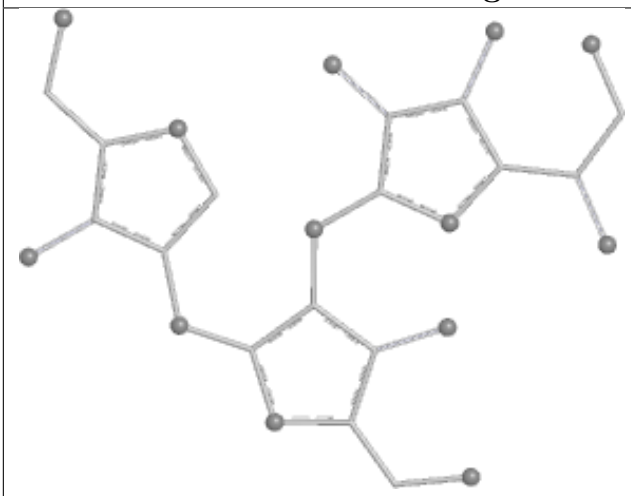
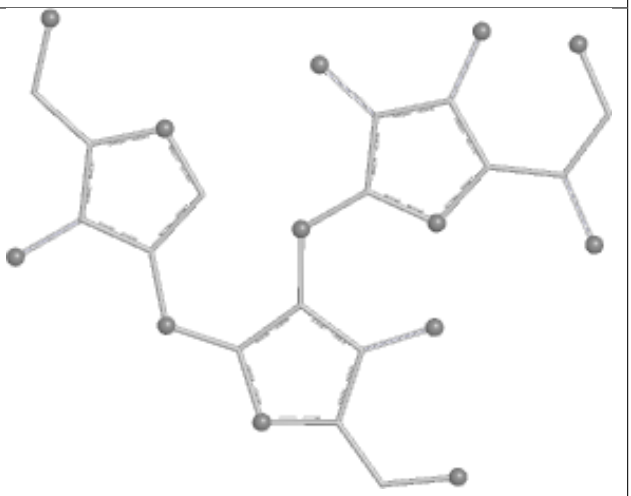
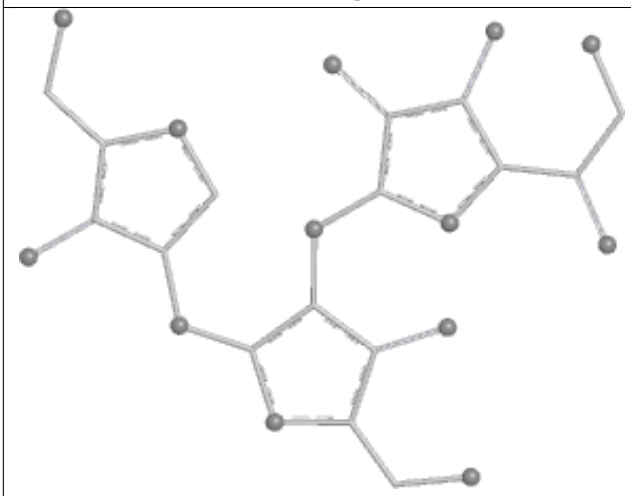
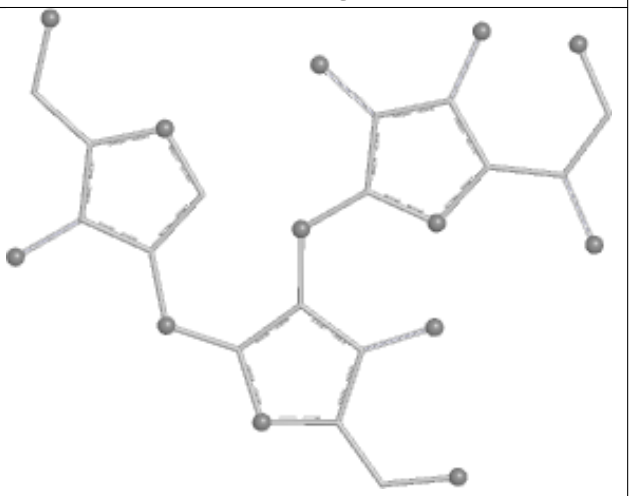
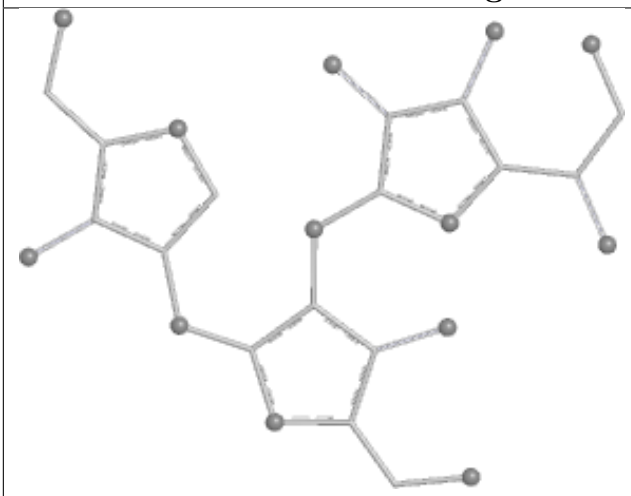
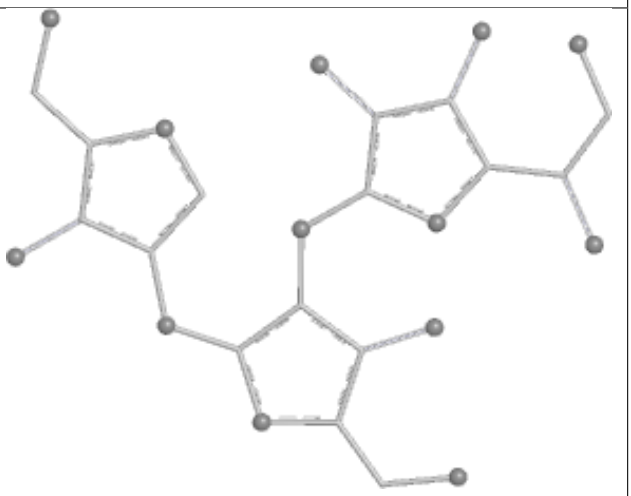
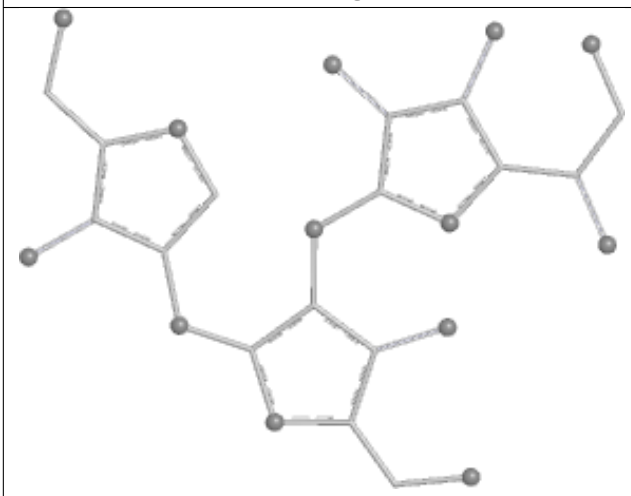
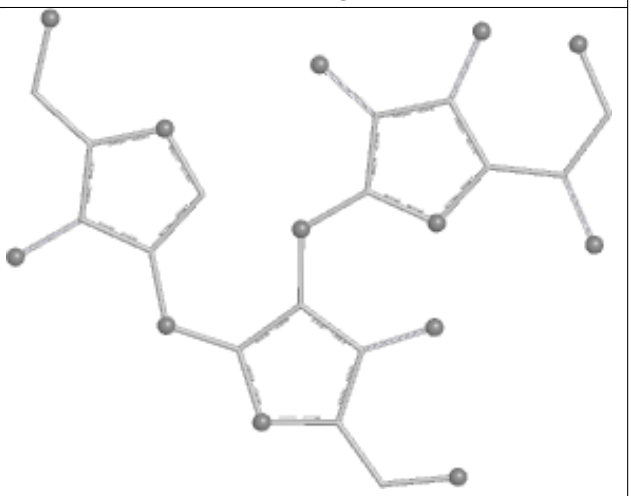
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain 3A	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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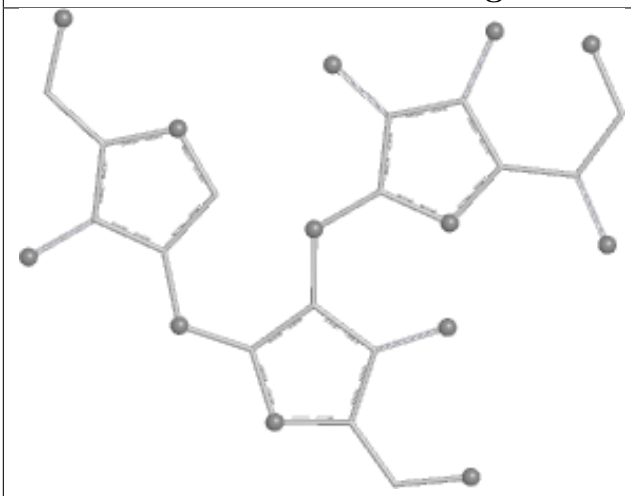	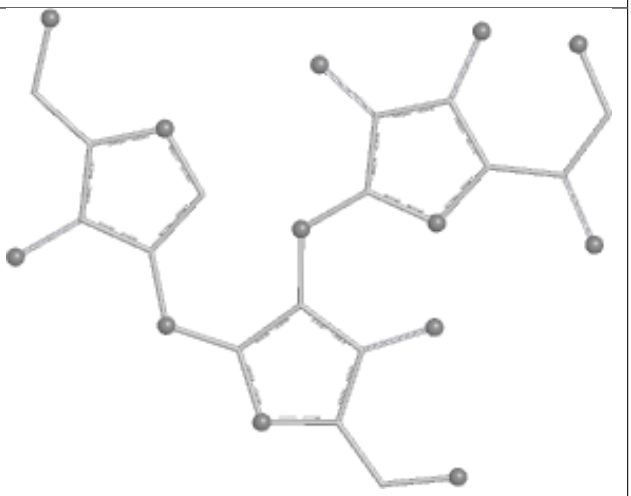
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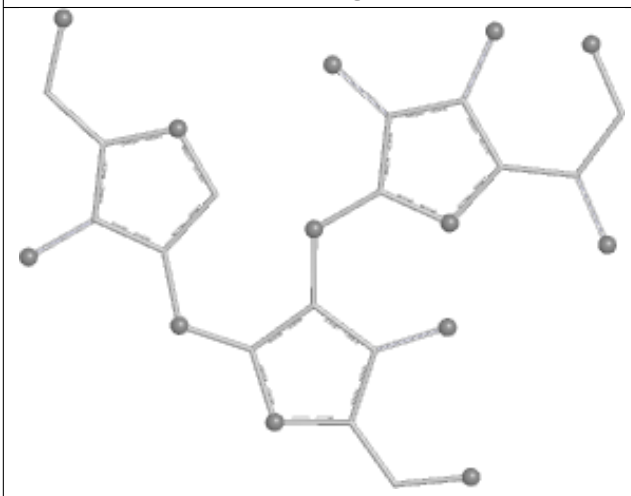	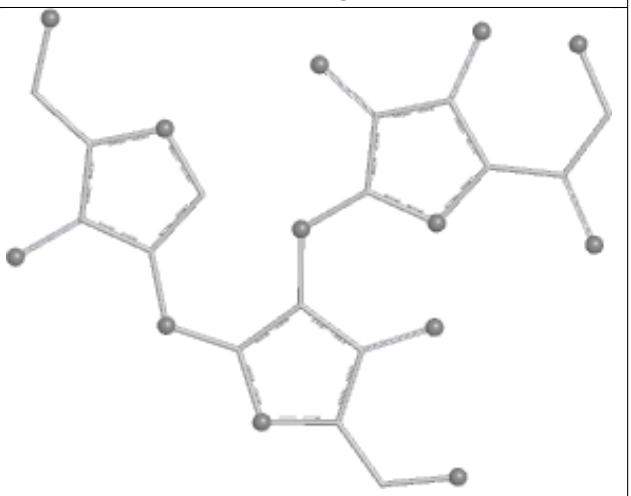
Torsions	**Rings**

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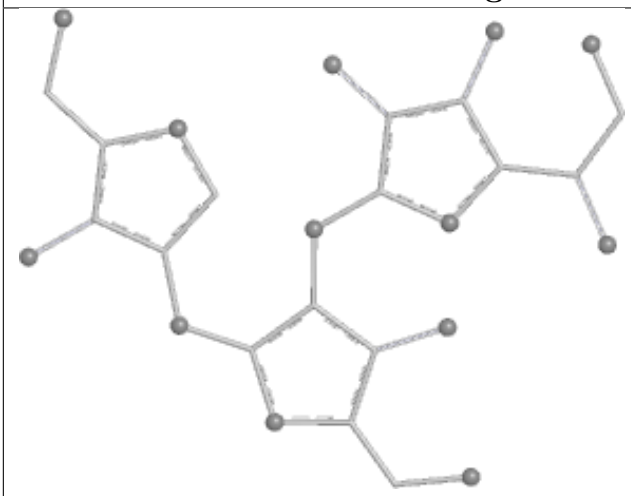	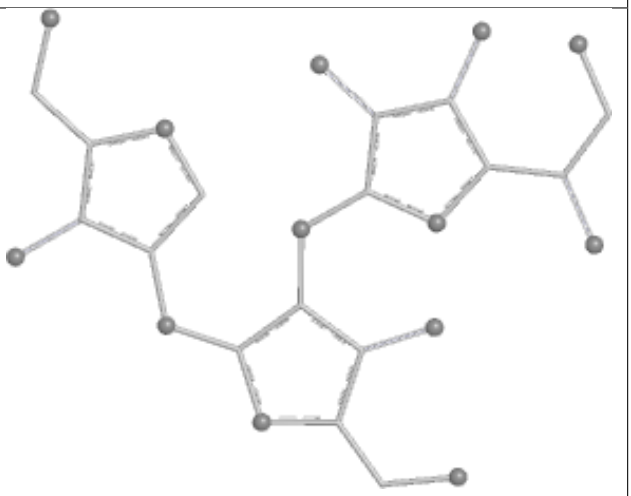
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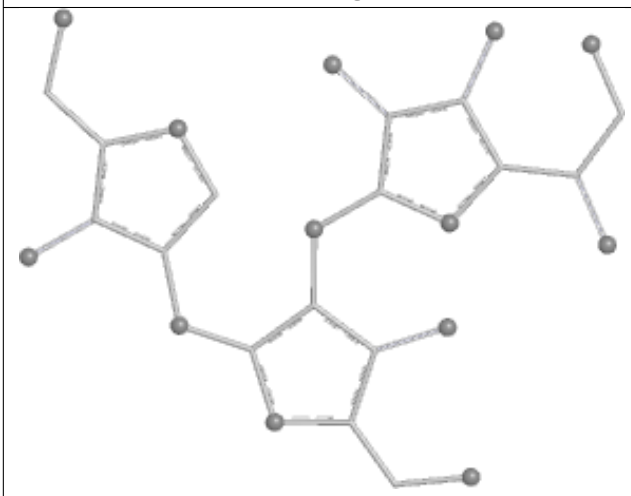	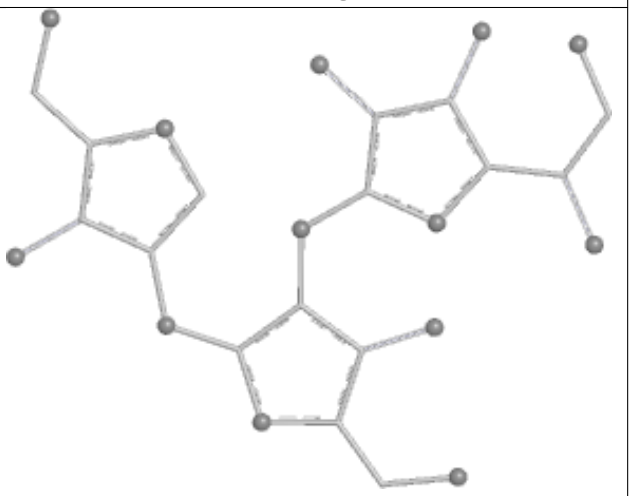
Torsions	**Rings**

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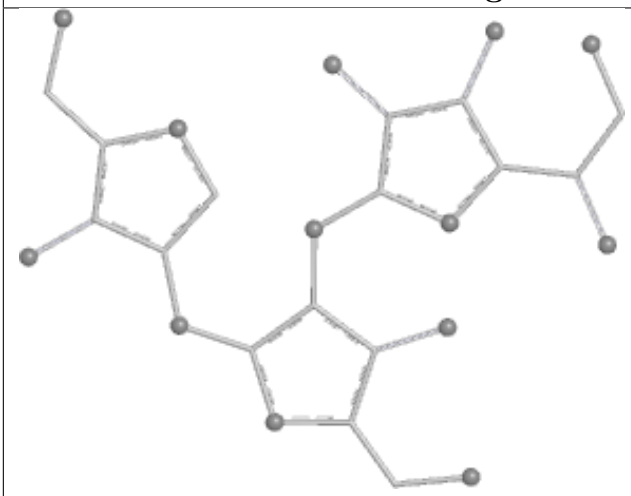
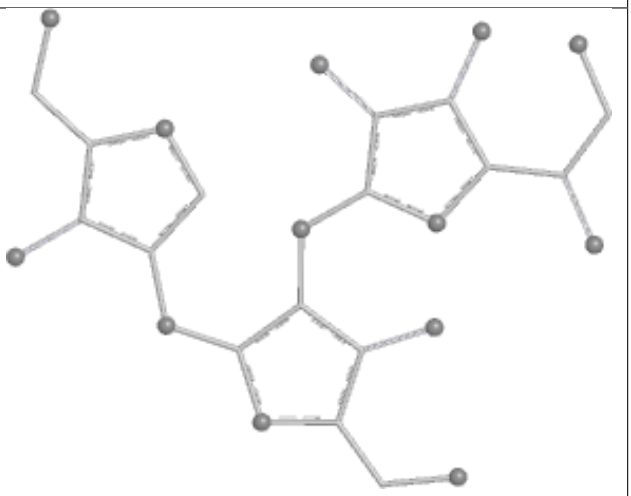
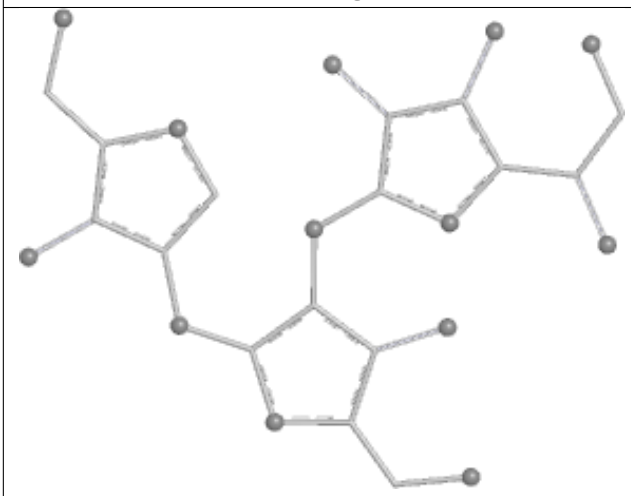
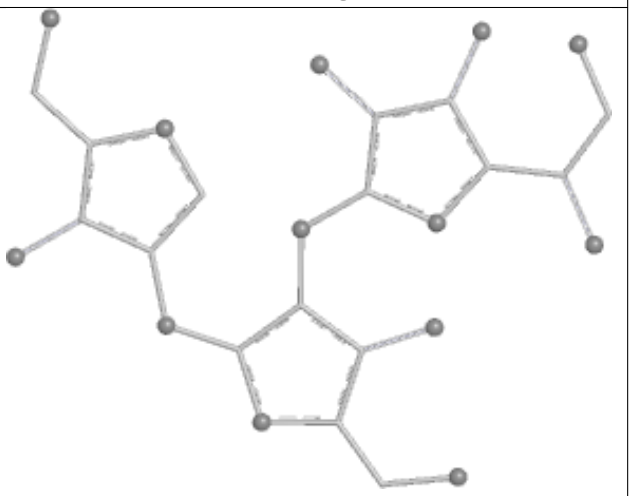
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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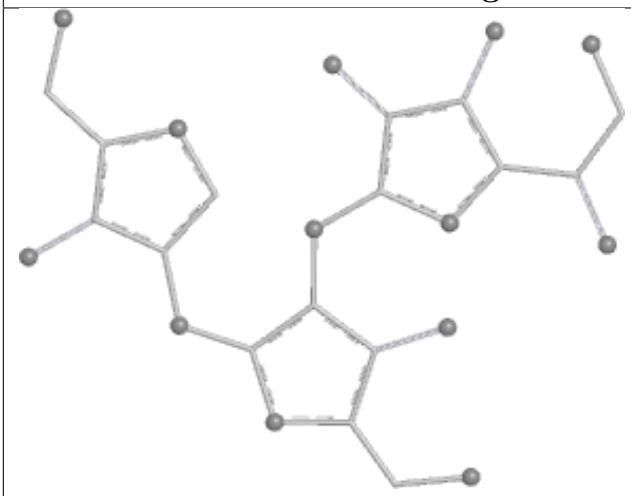
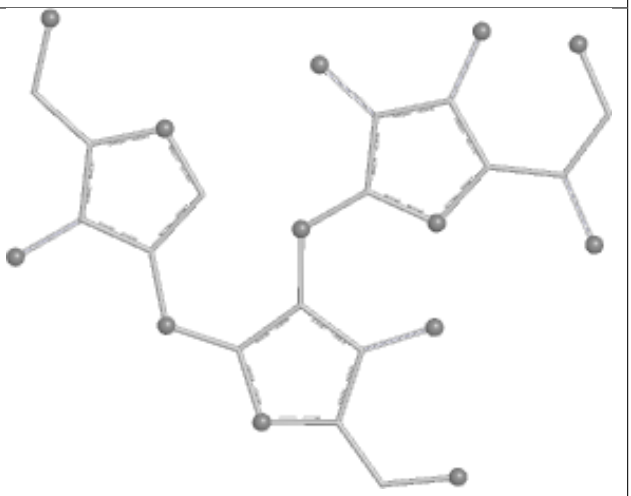
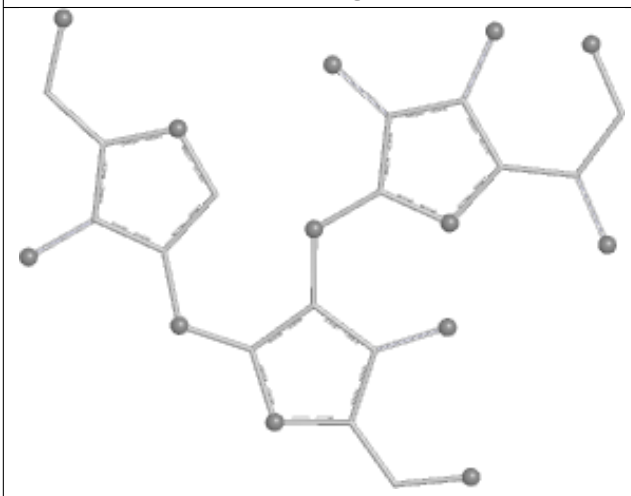
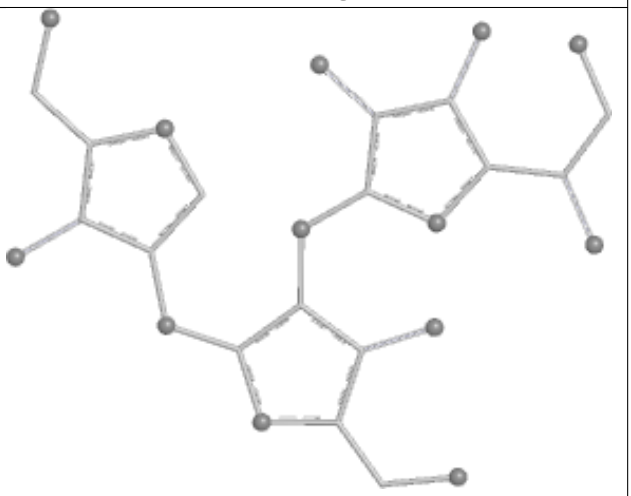
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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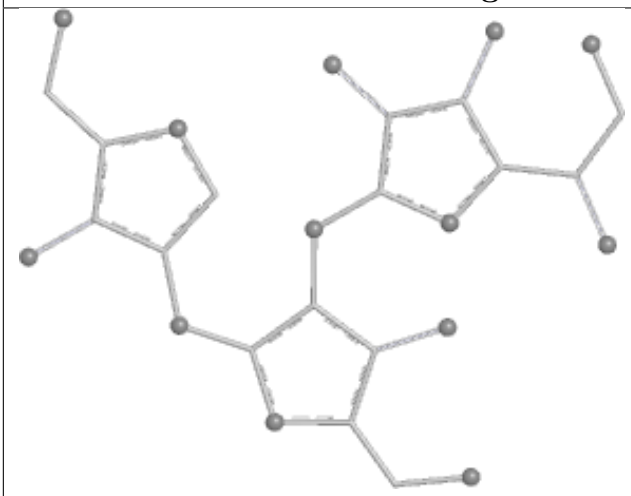
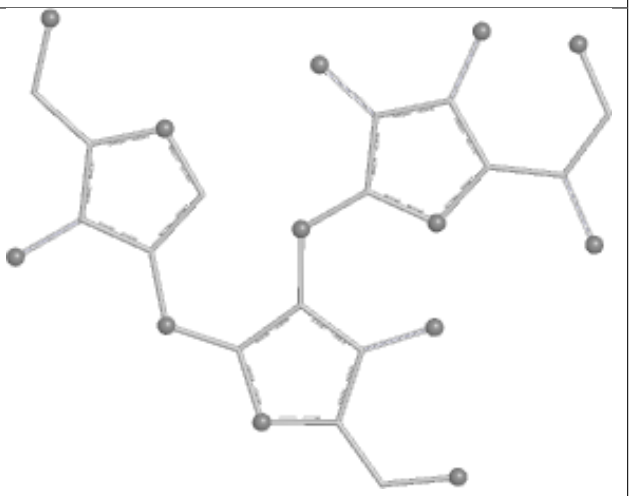
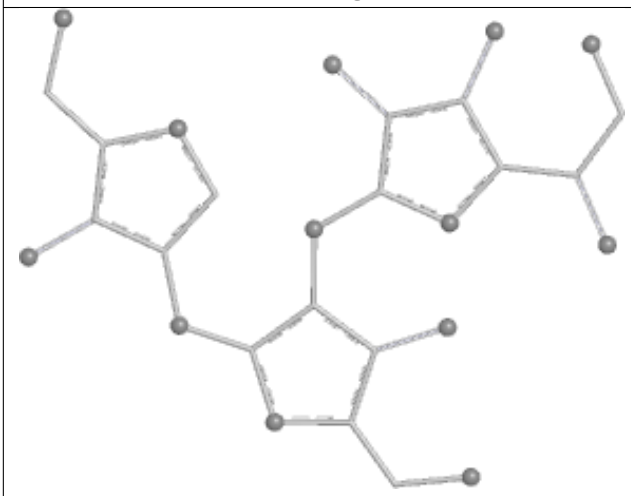
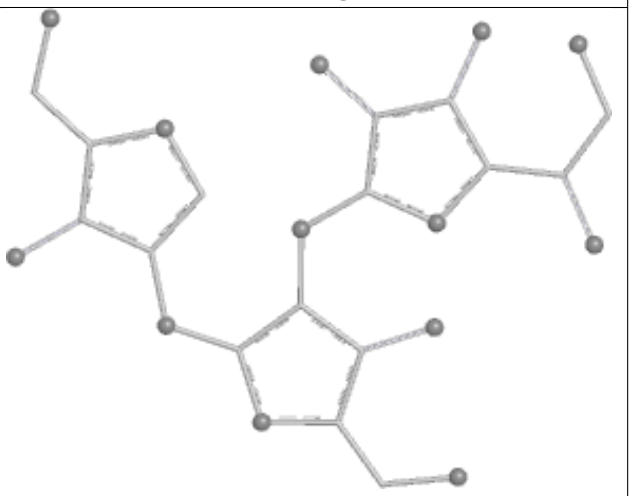
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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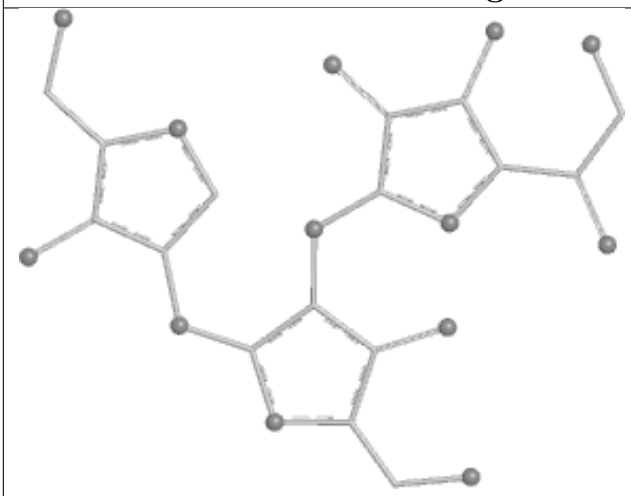	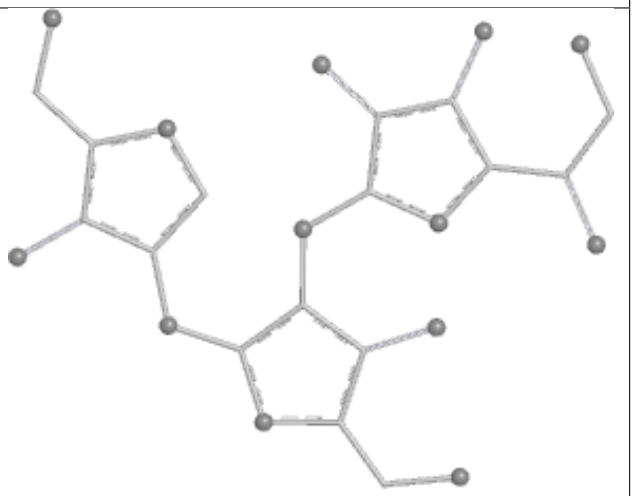
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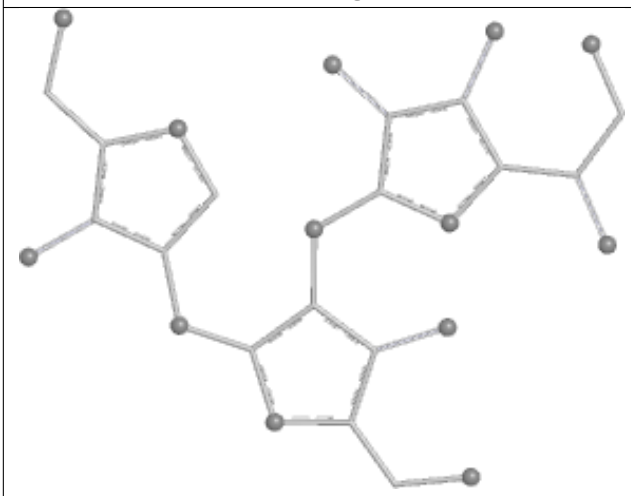	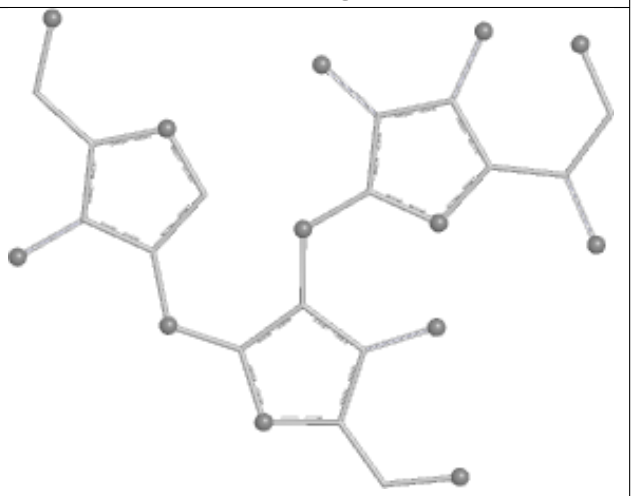
Torsions	**Rings**

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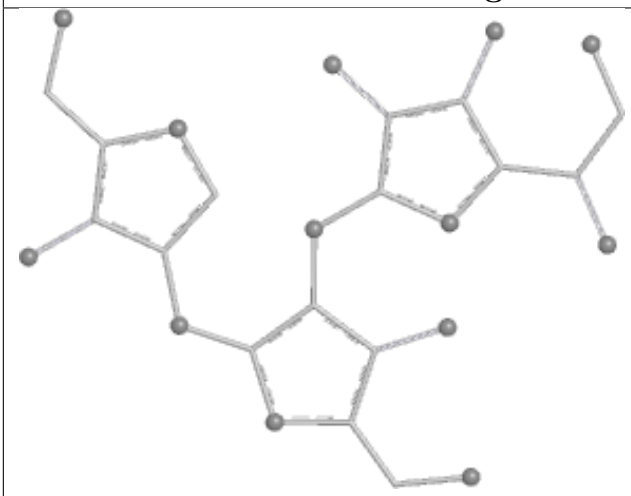	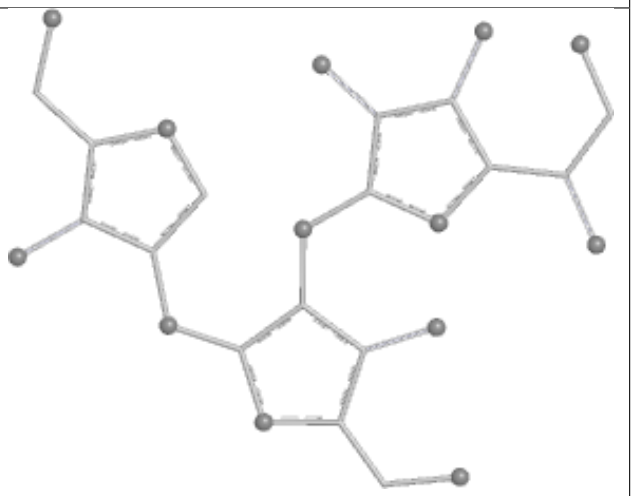
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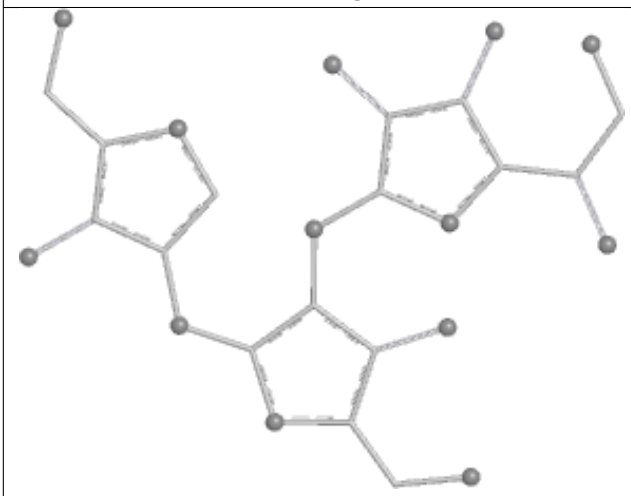	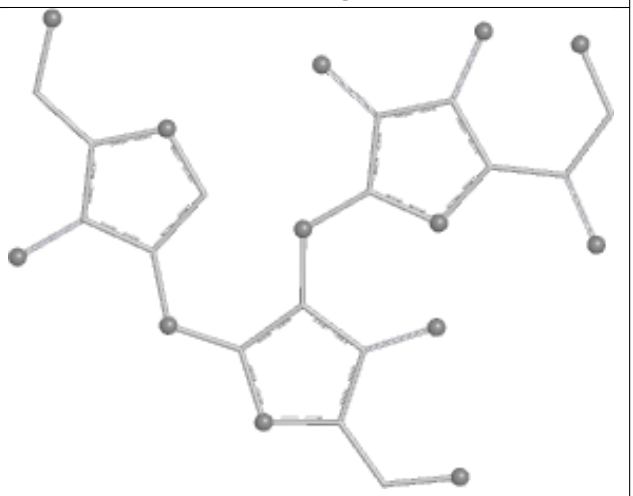
Torsions	**Rings**

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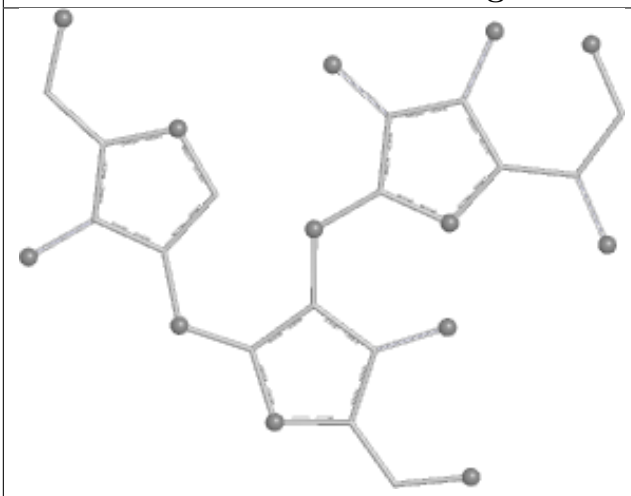	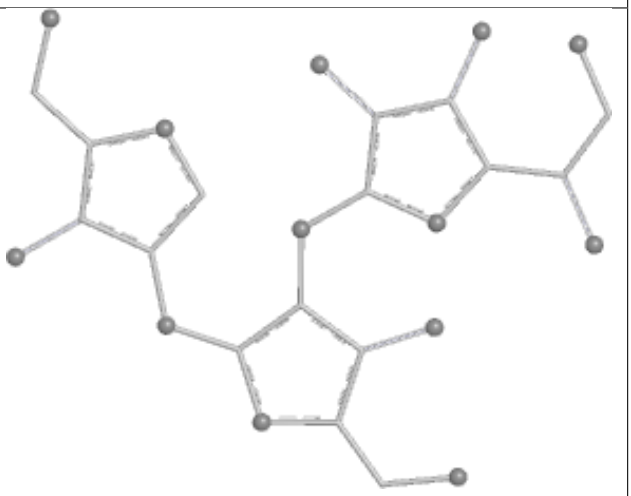
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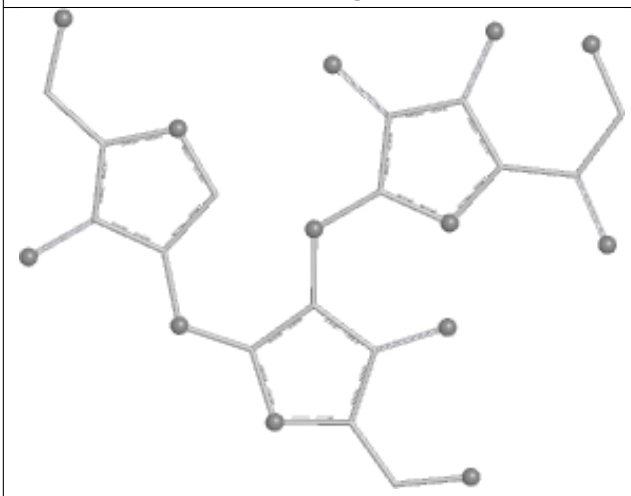	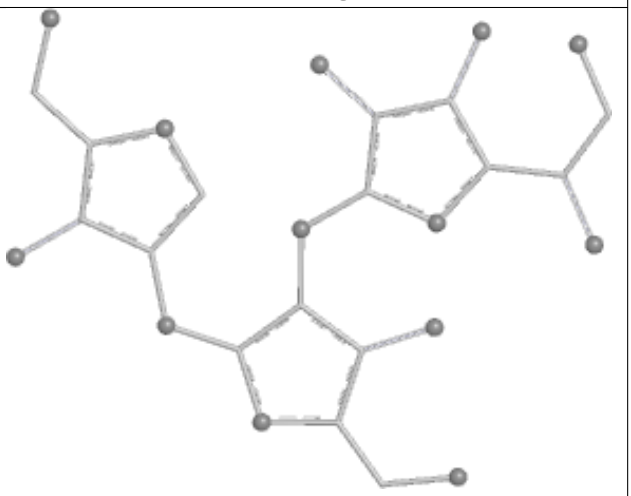
Torsions	**Rings**

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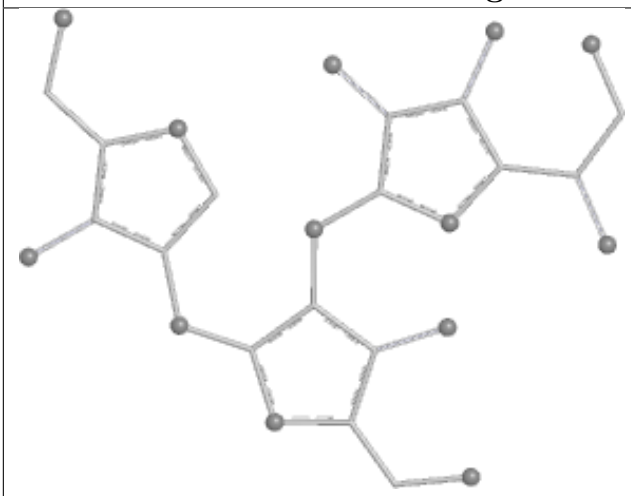	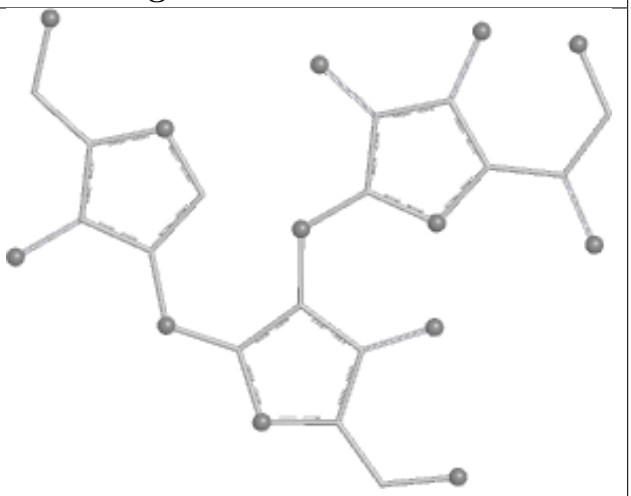
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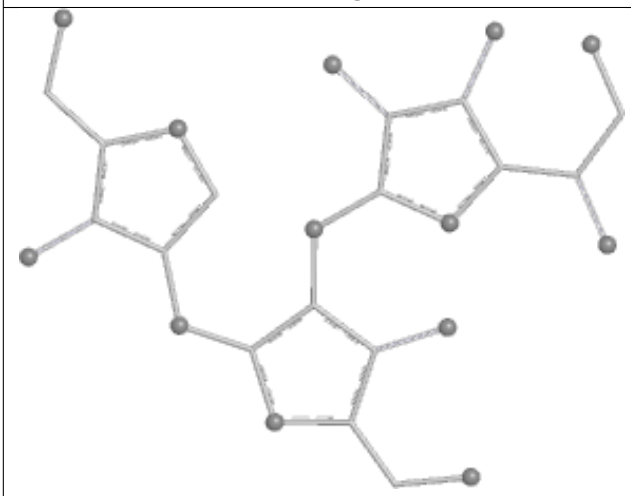	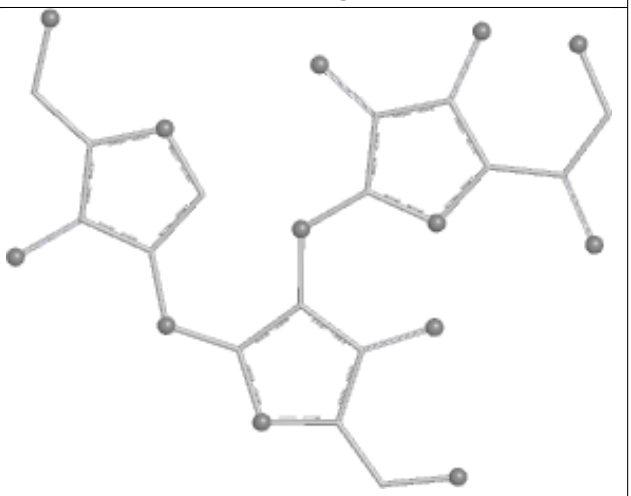
Torsions	**Rings**

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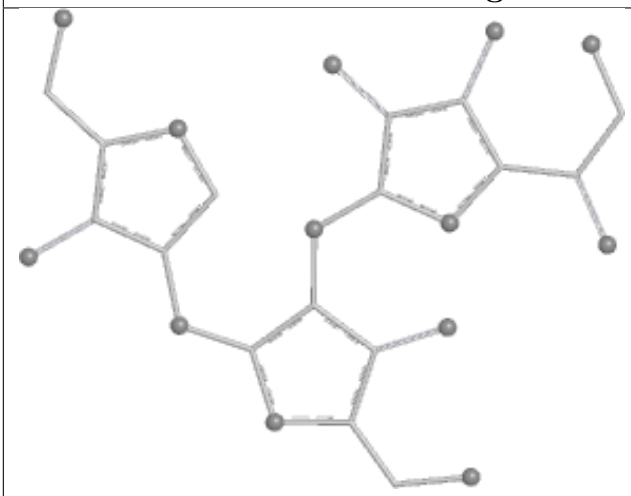
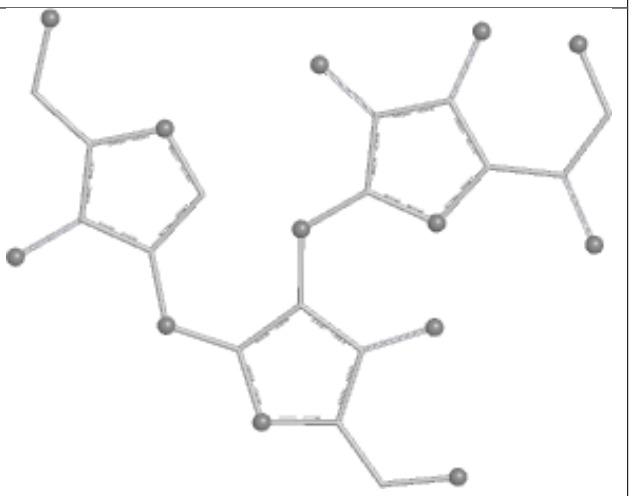
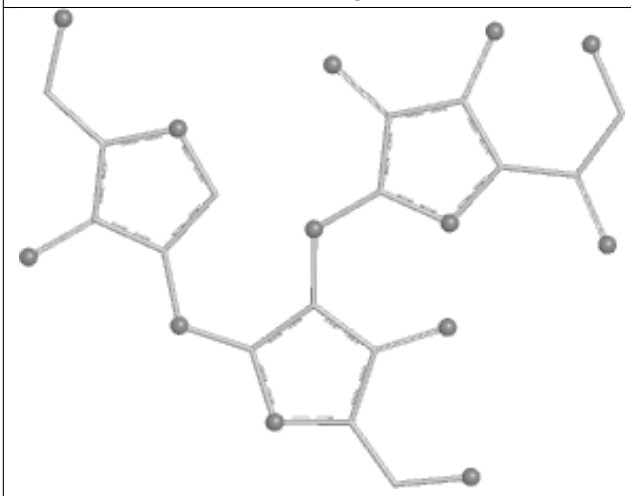
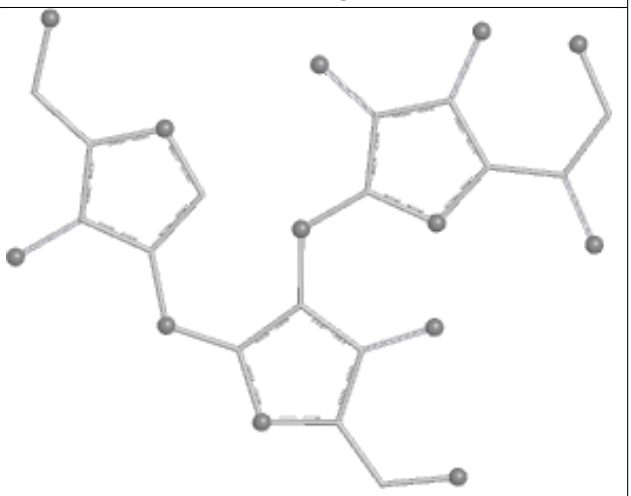
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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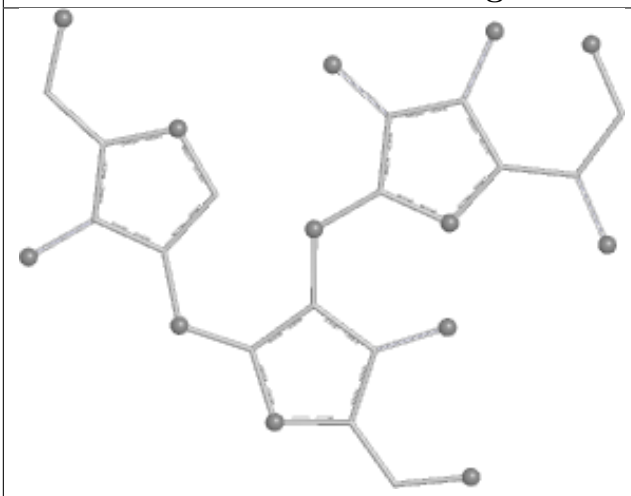
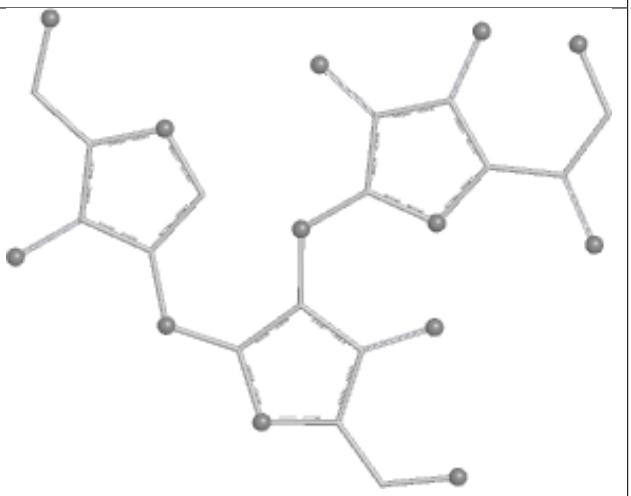
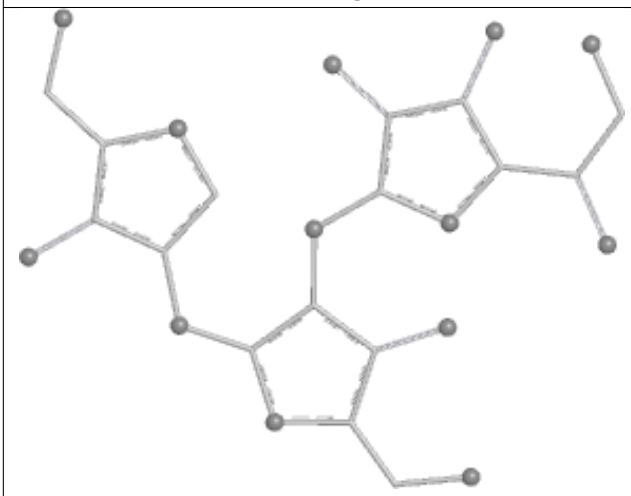
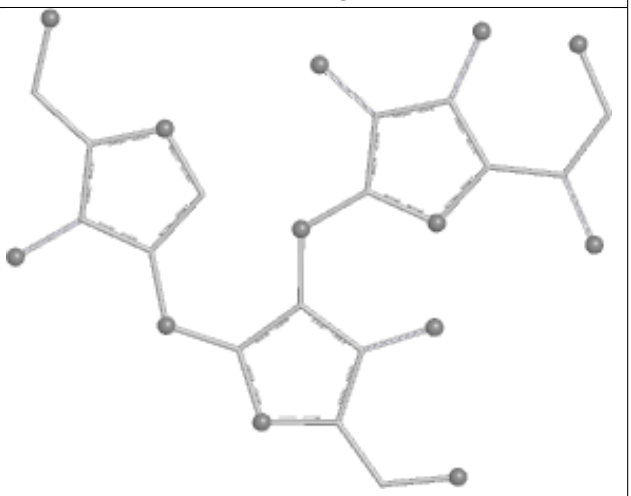
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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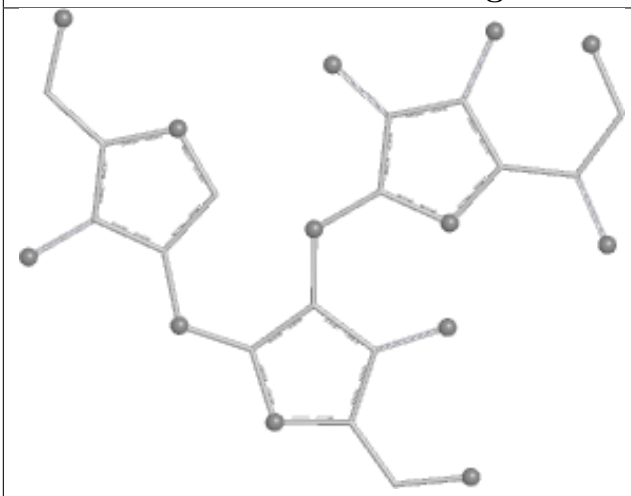
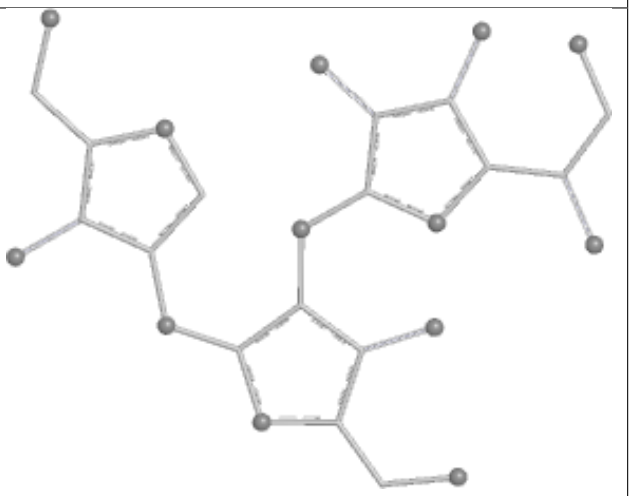
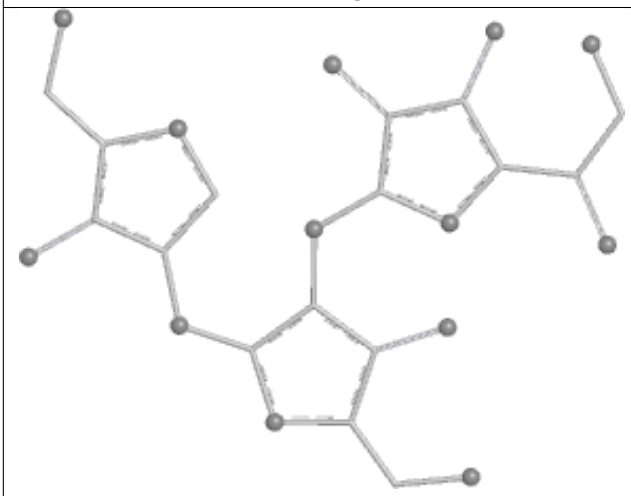
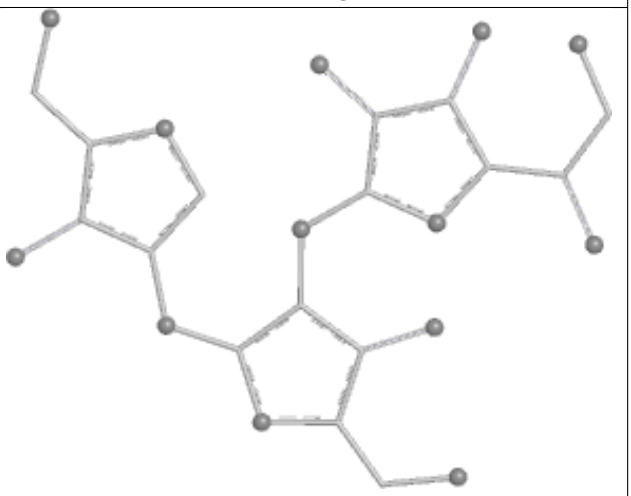
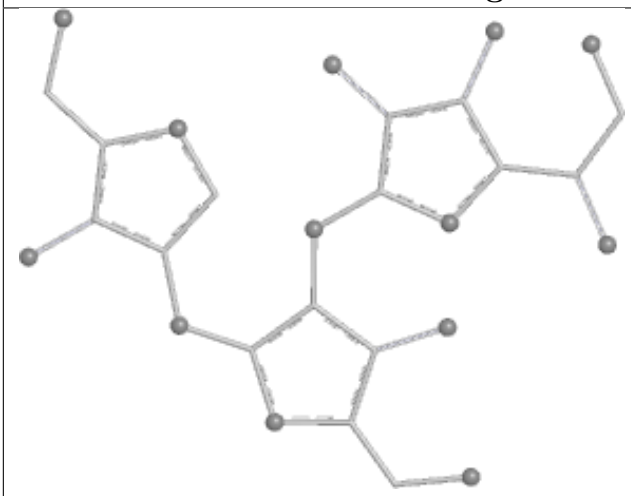
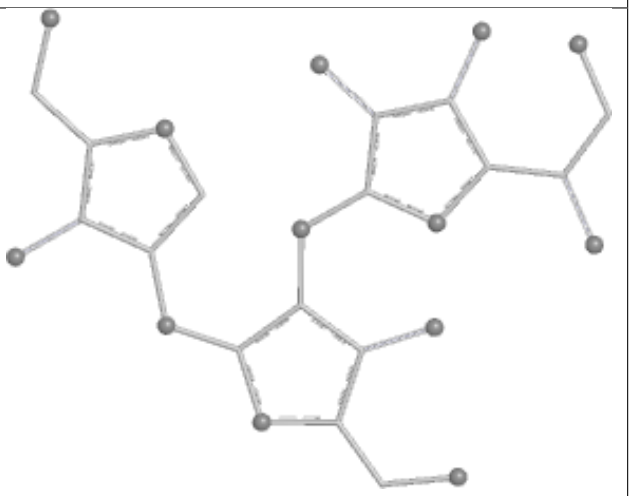
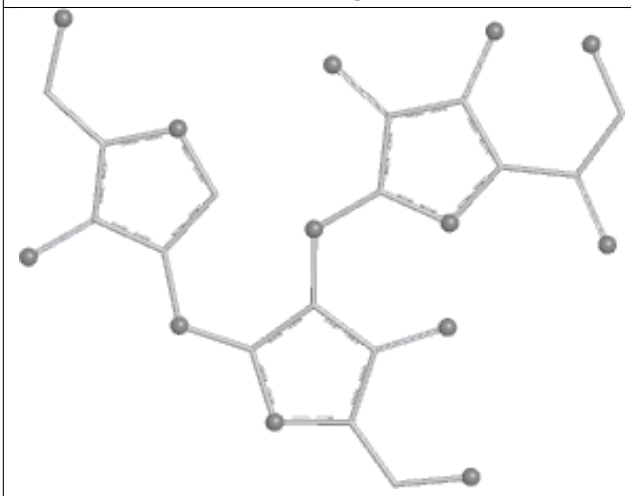
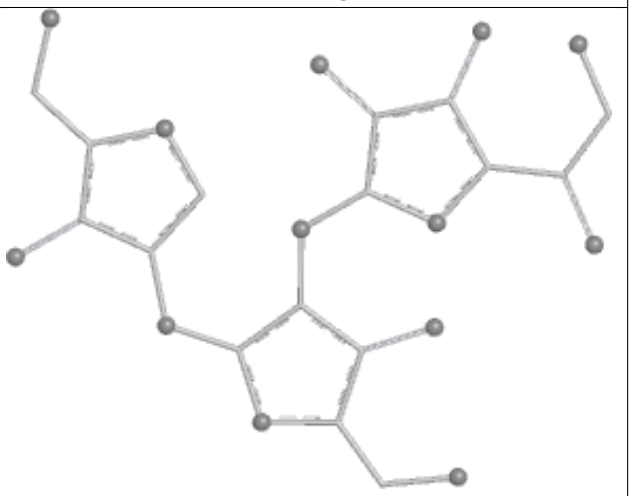
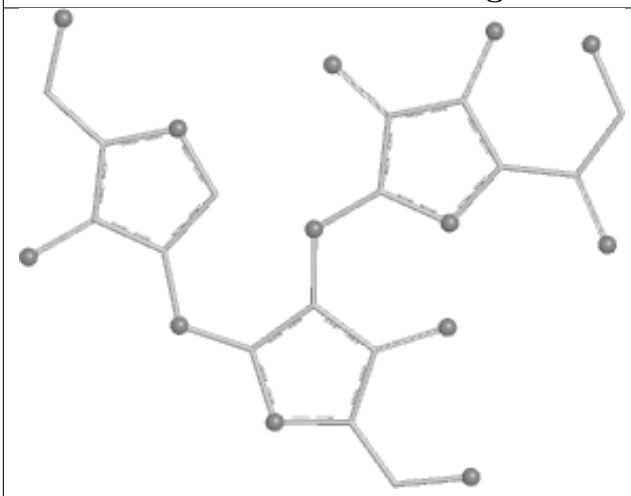
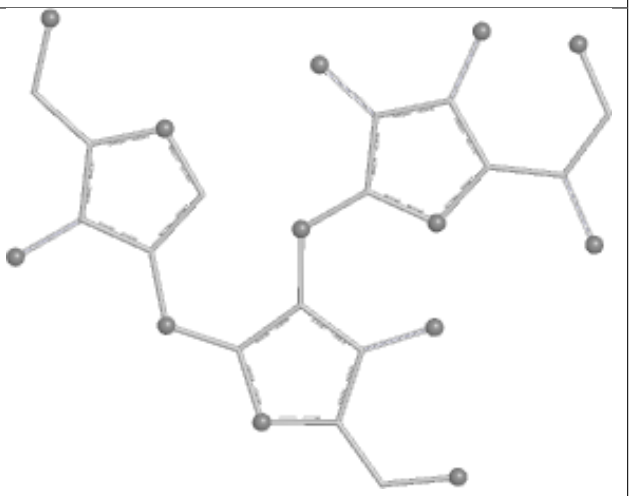
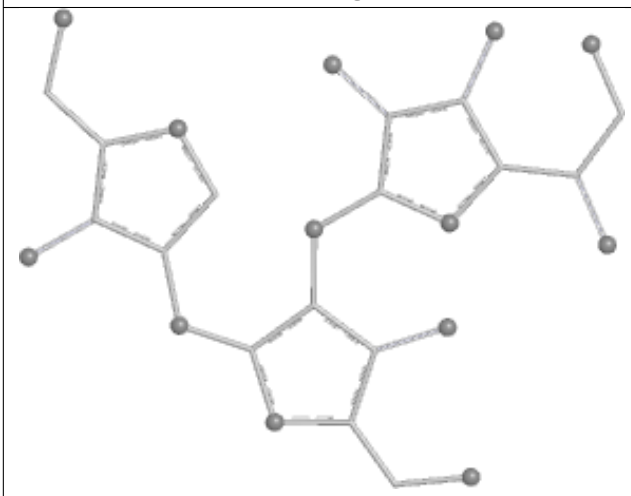
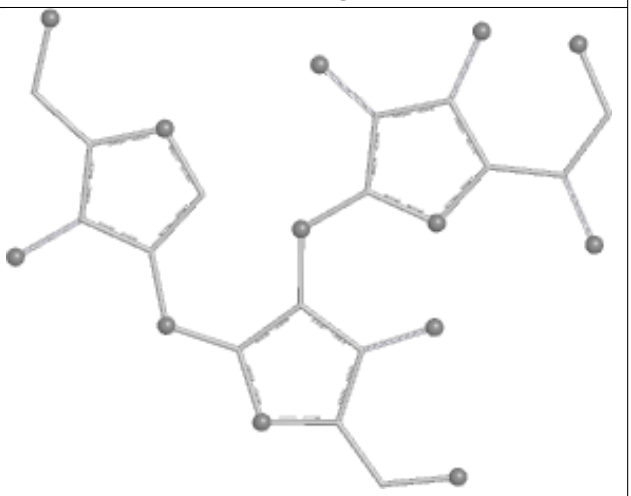
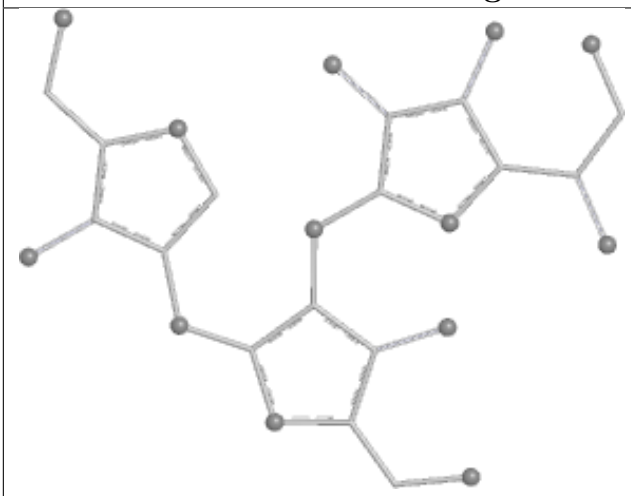
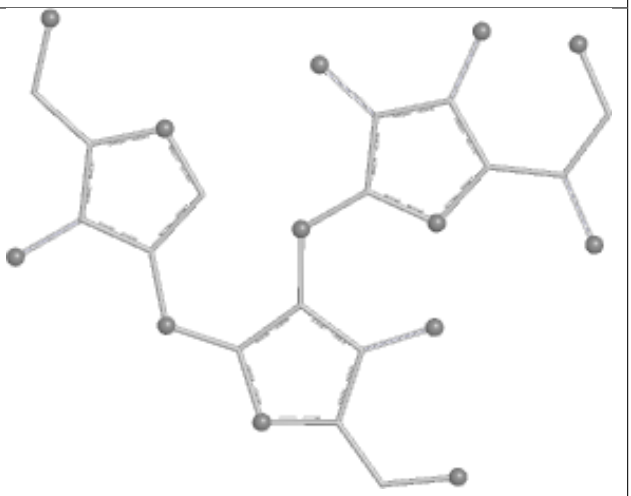
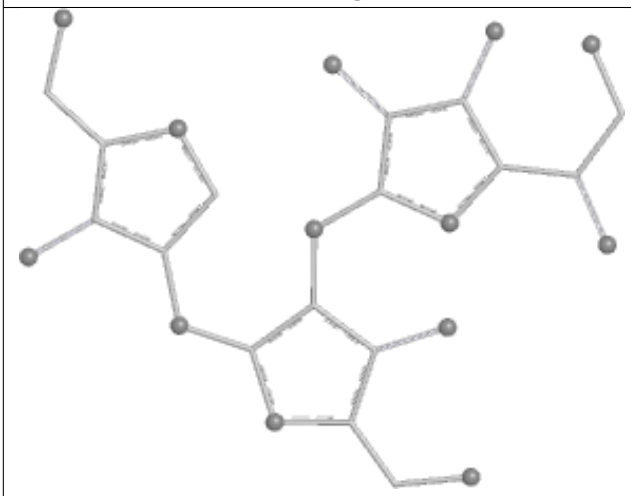
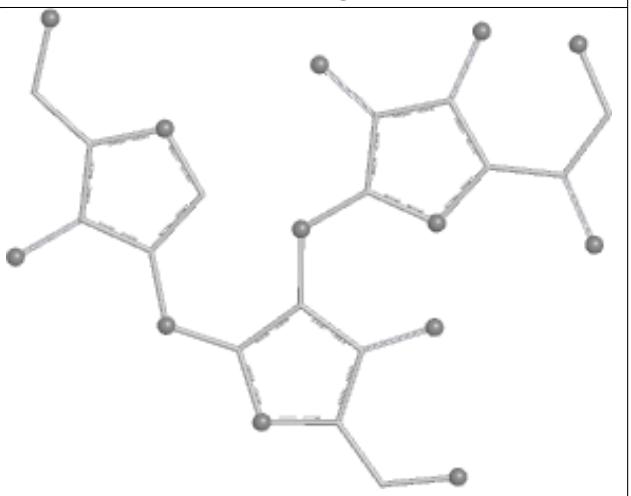
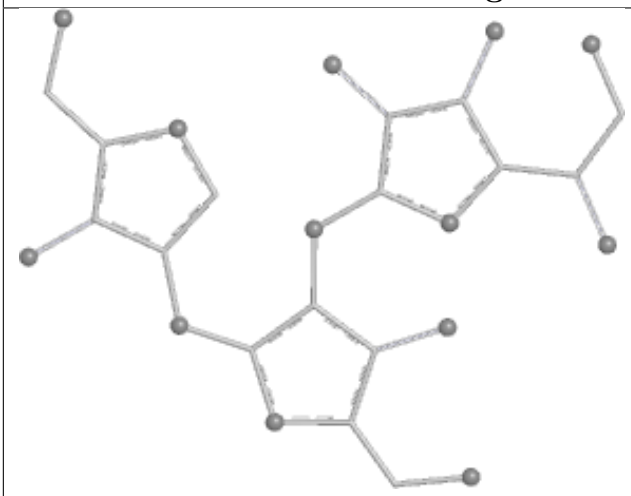
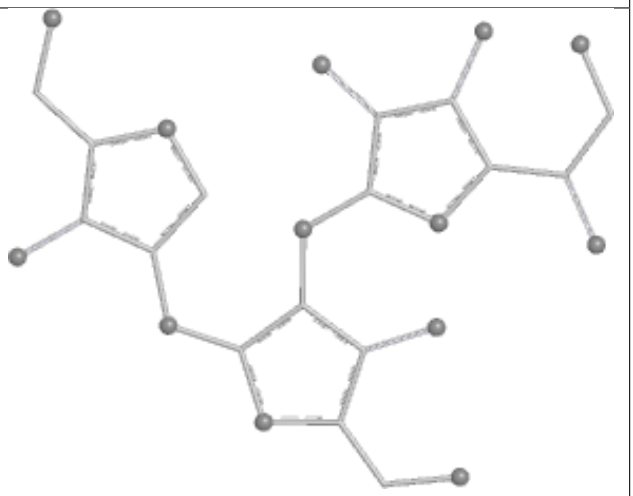
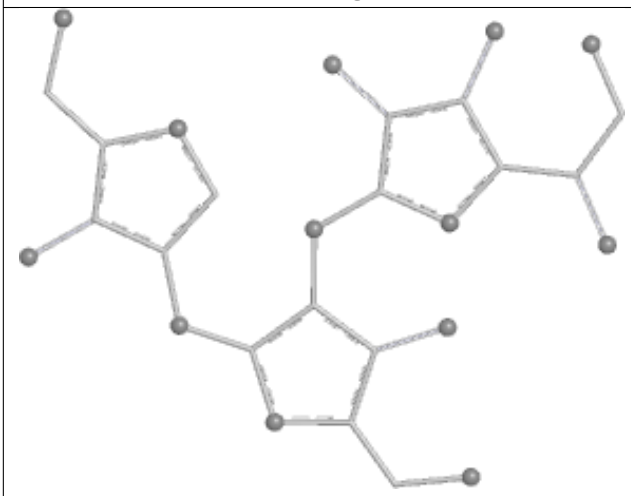
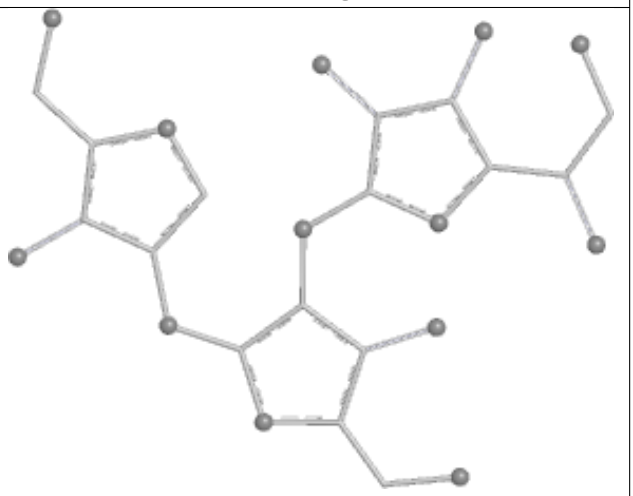
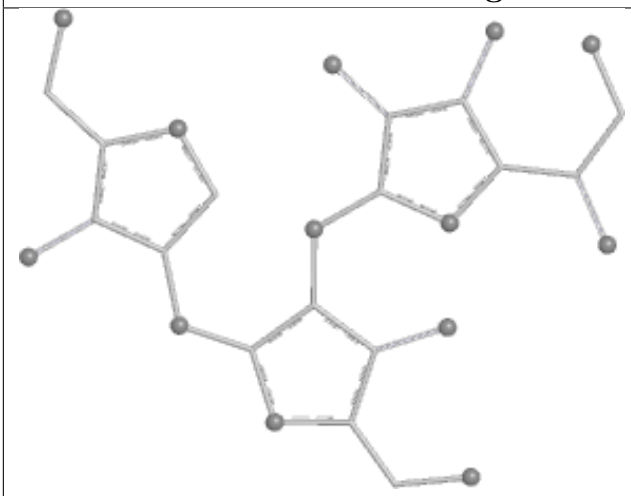
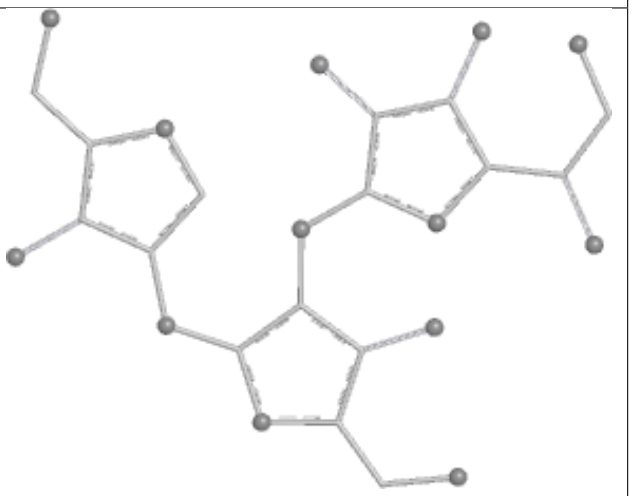
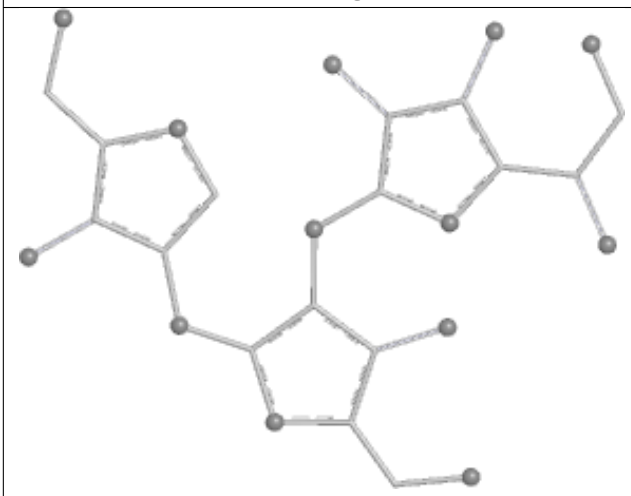
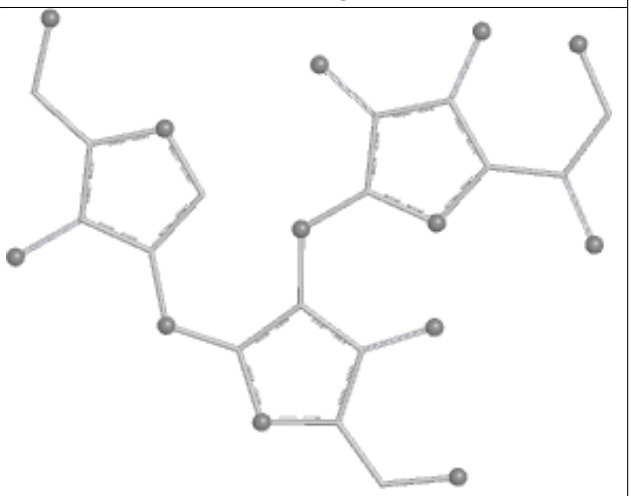
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

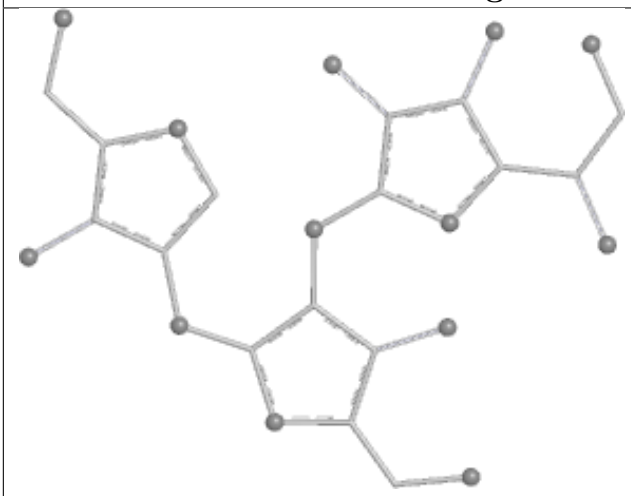
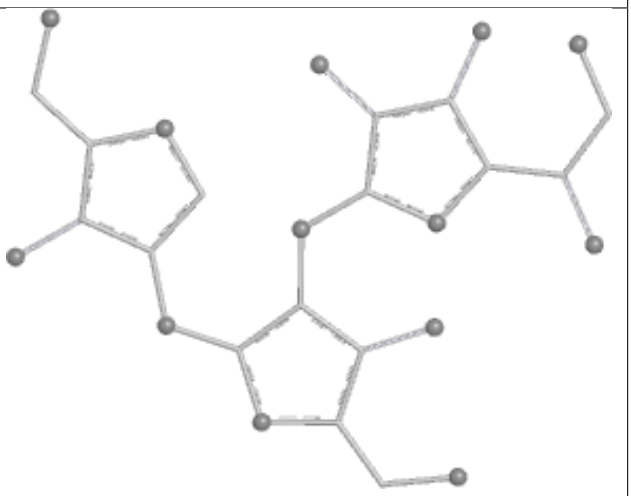
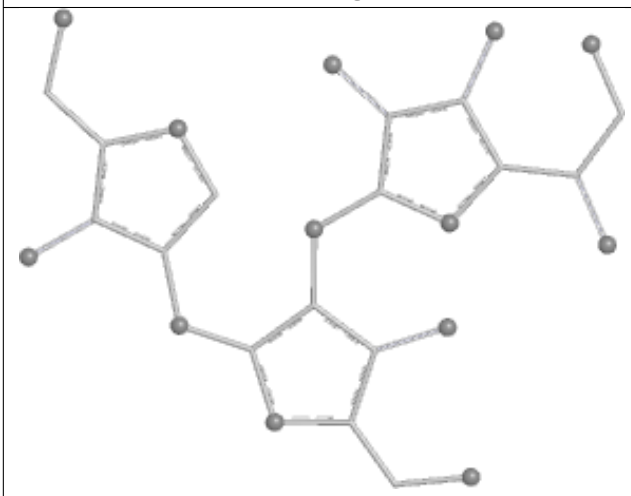
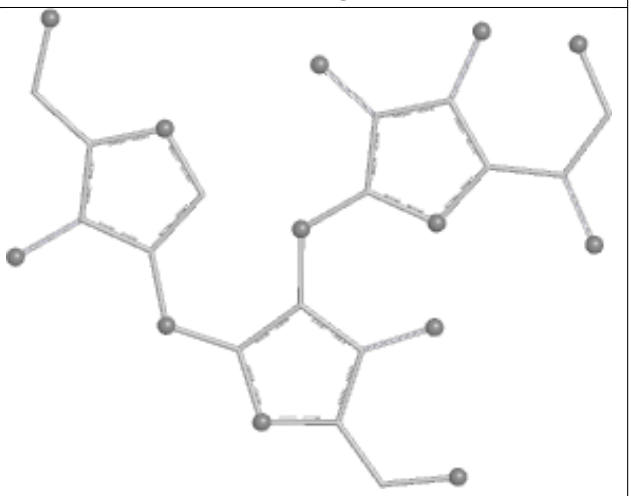
Oligosaccharide Chain 5B	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

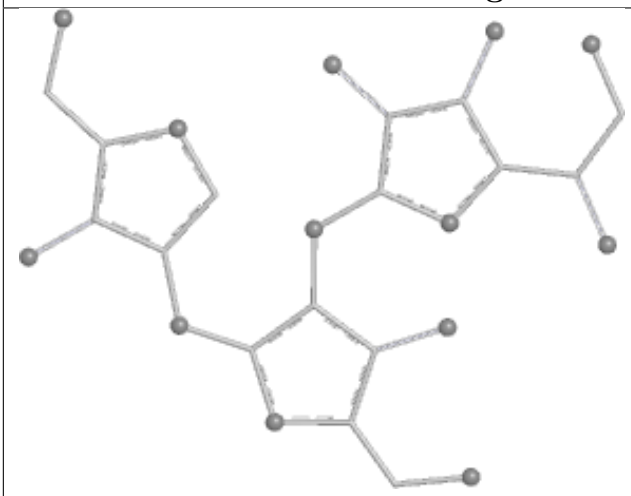
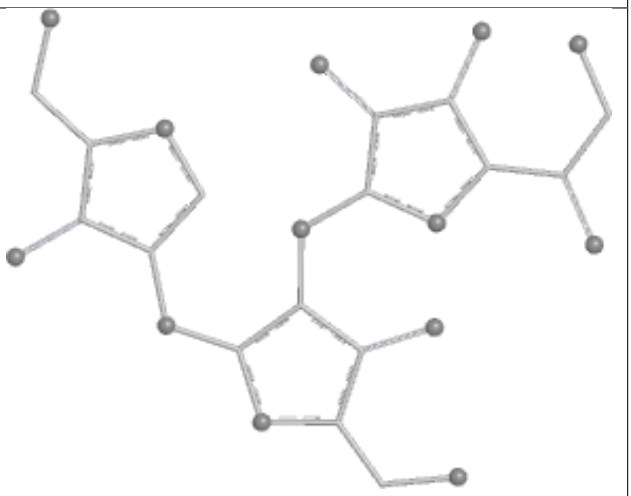
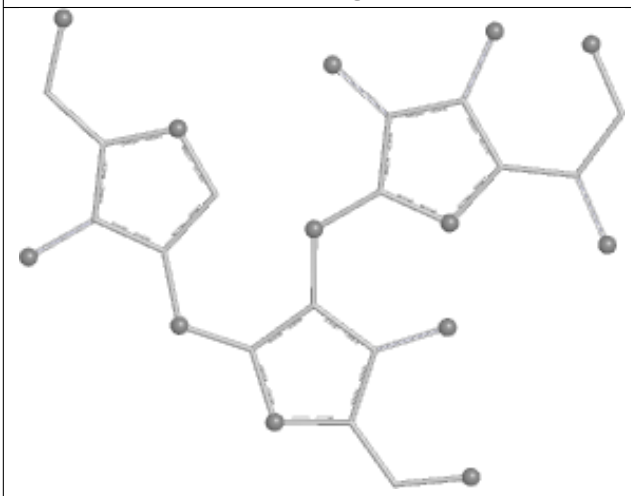
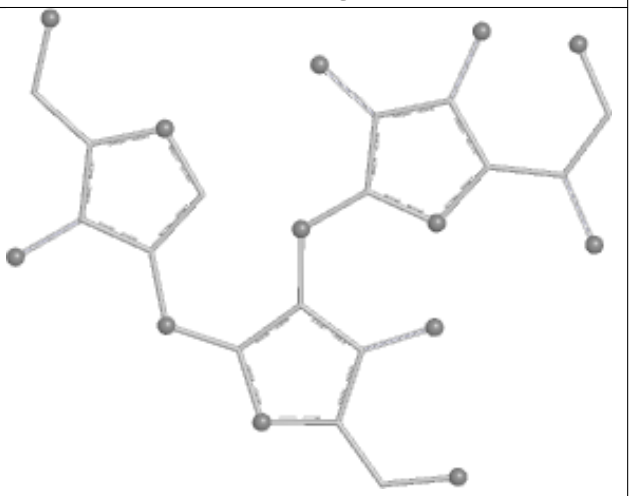
Oligosaccharide Chain 9B	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain FC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain JC	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain xC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 0C	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain 1C	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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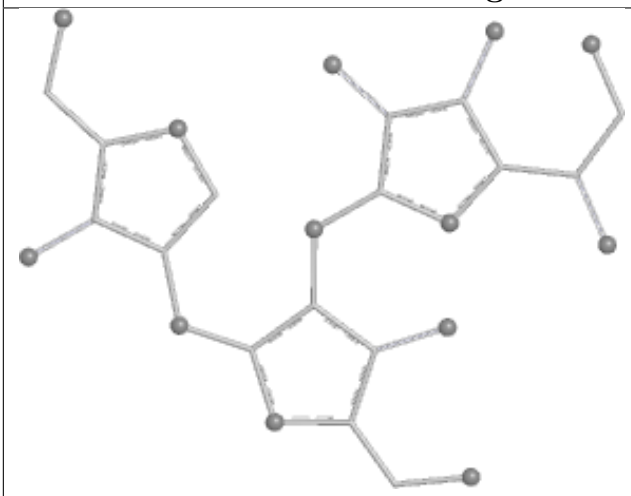
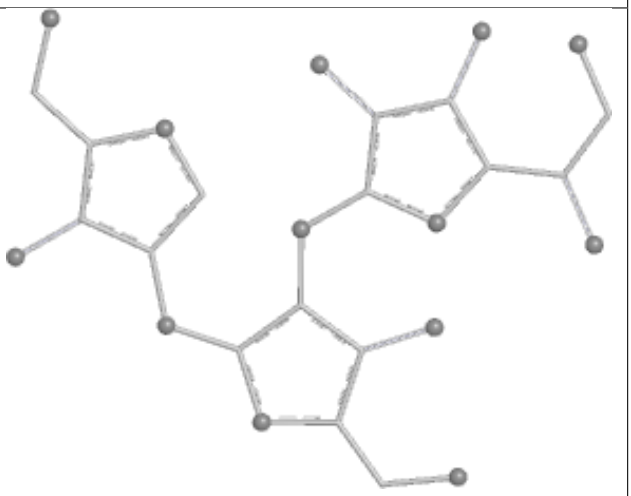
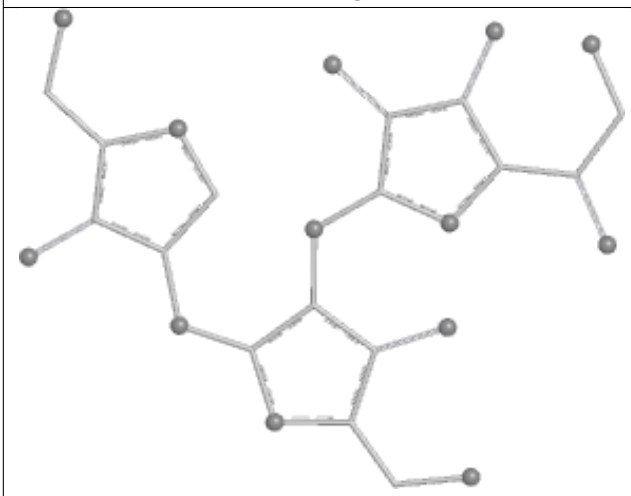
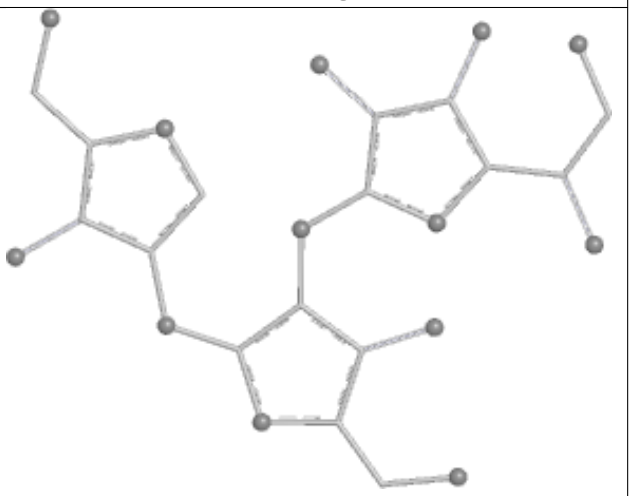
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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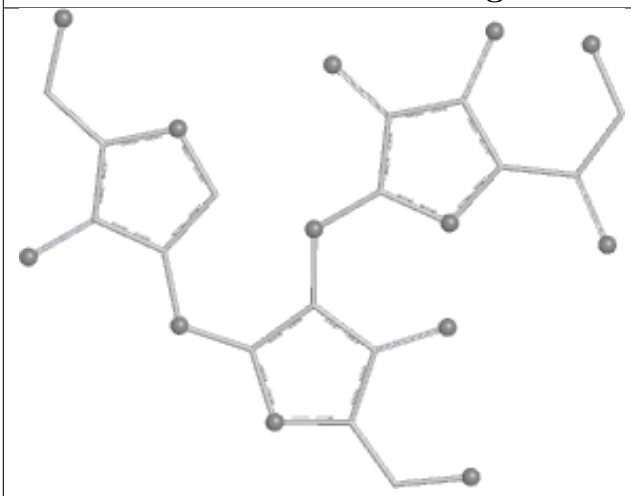
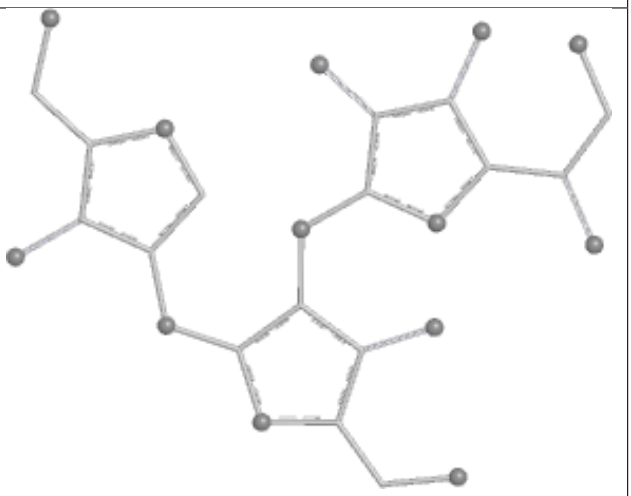
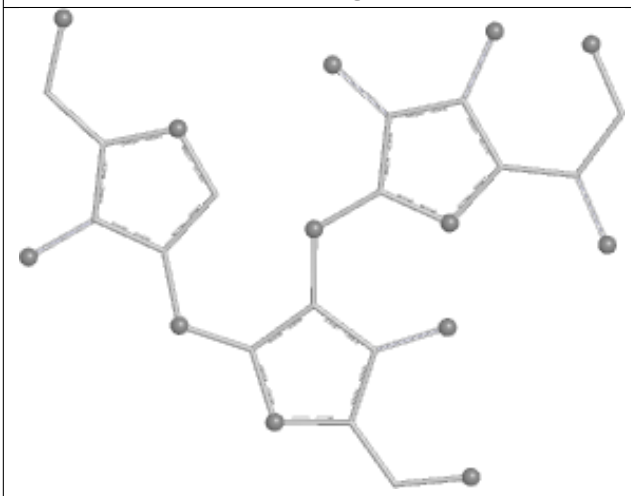
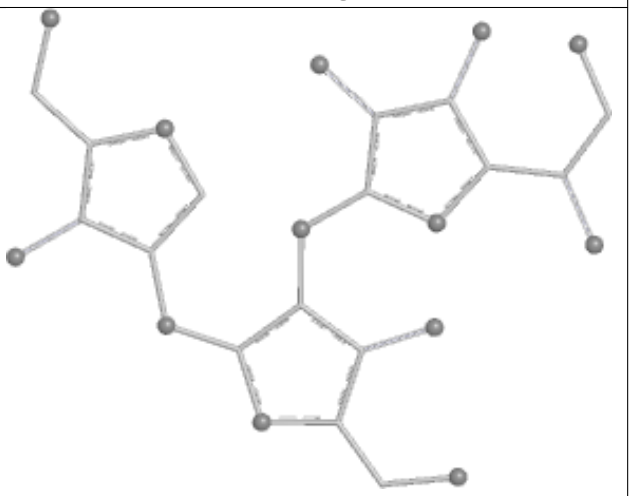
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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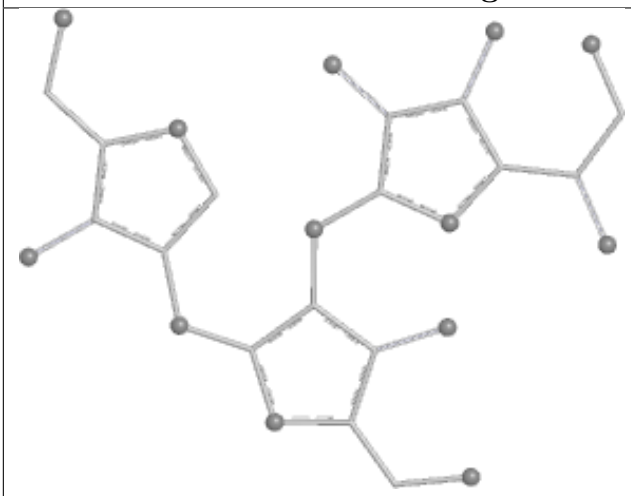
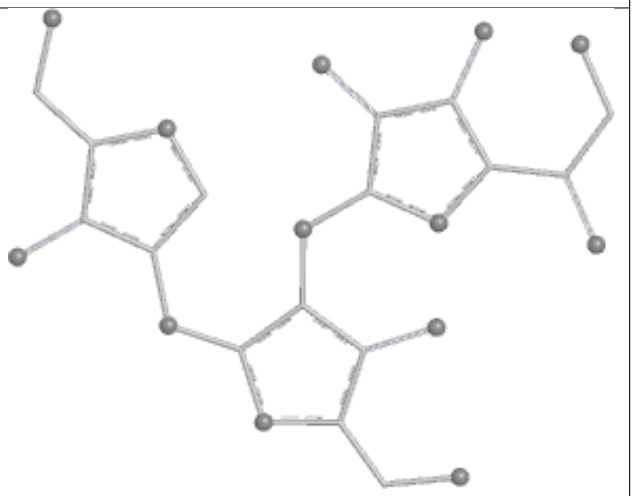
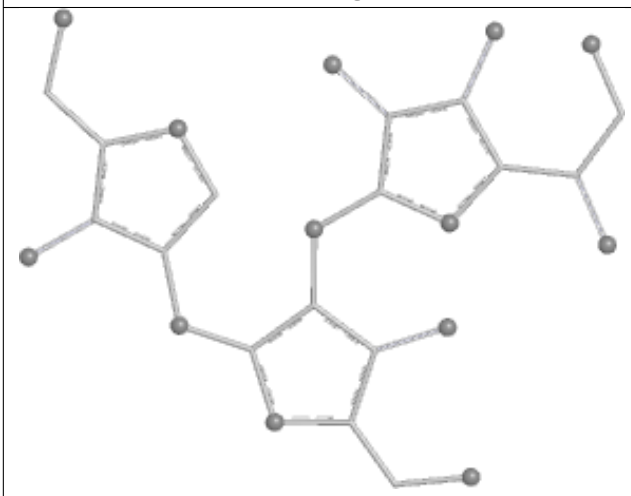
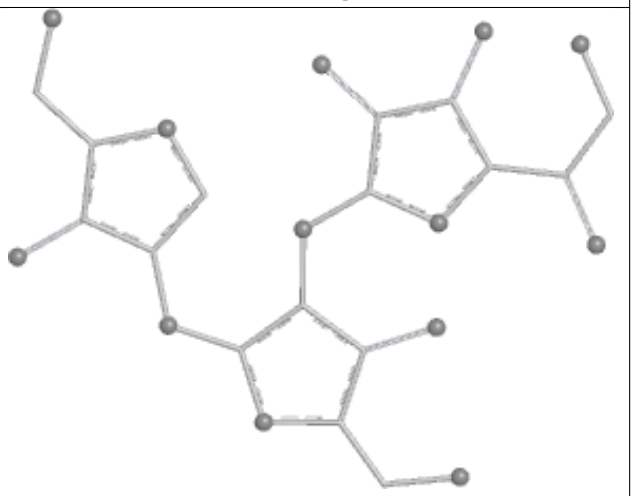
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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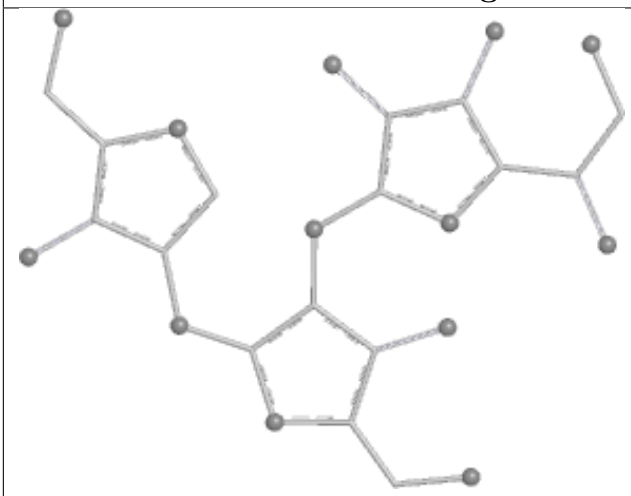
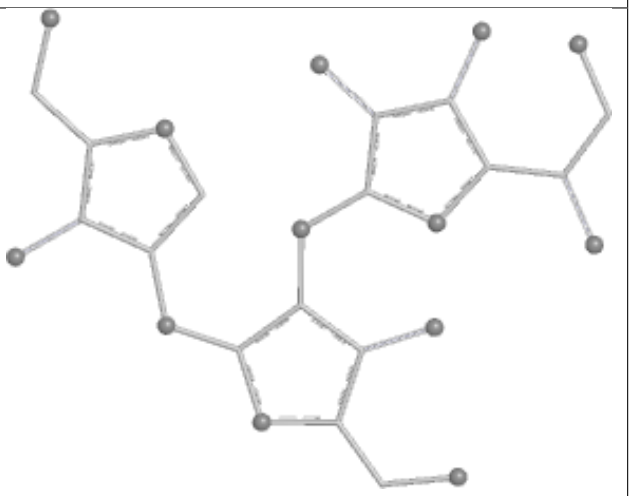
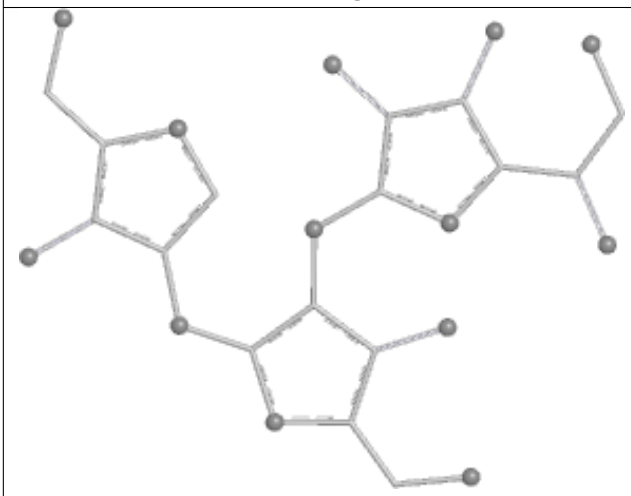
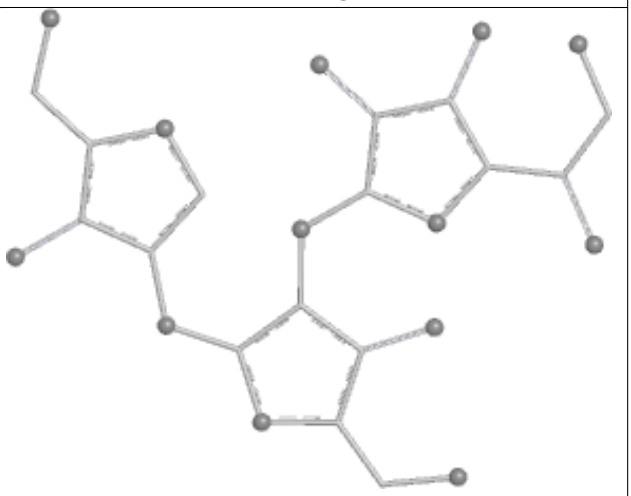
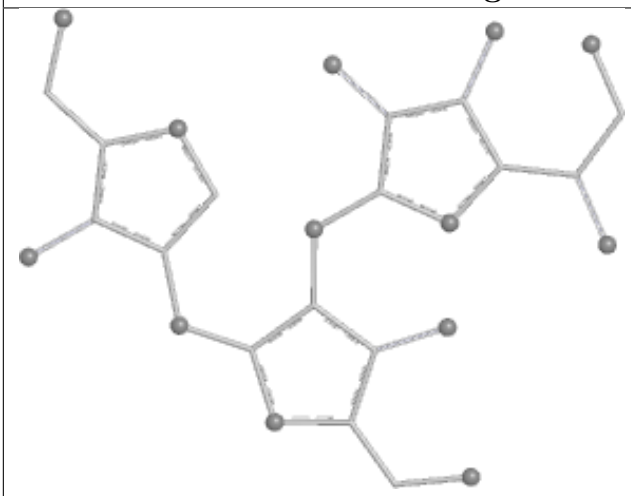
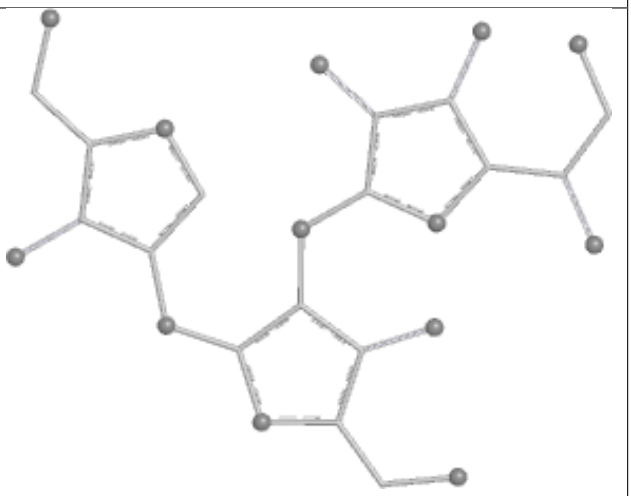
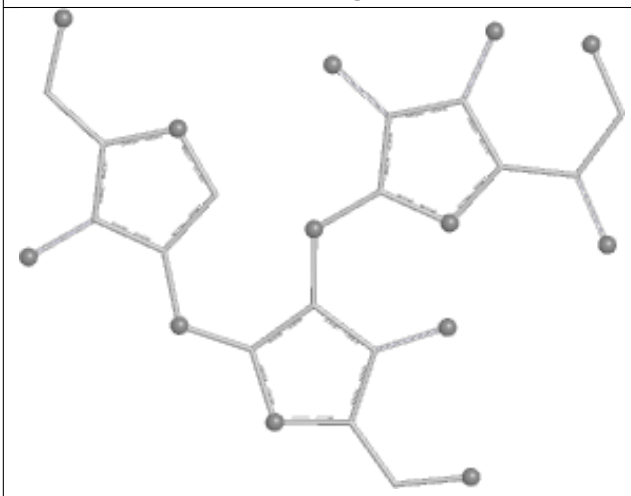
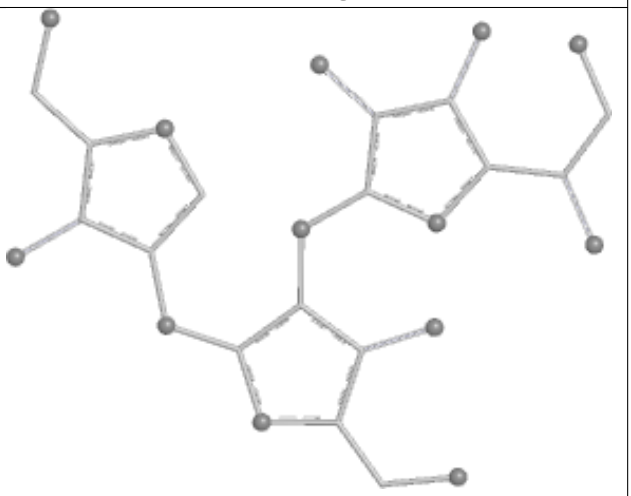
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain uD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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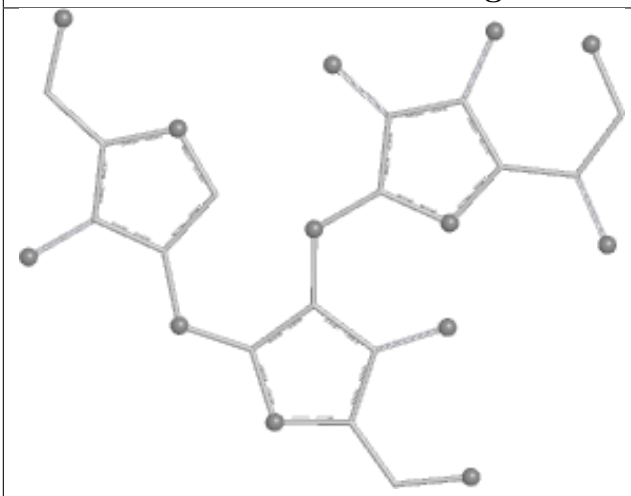
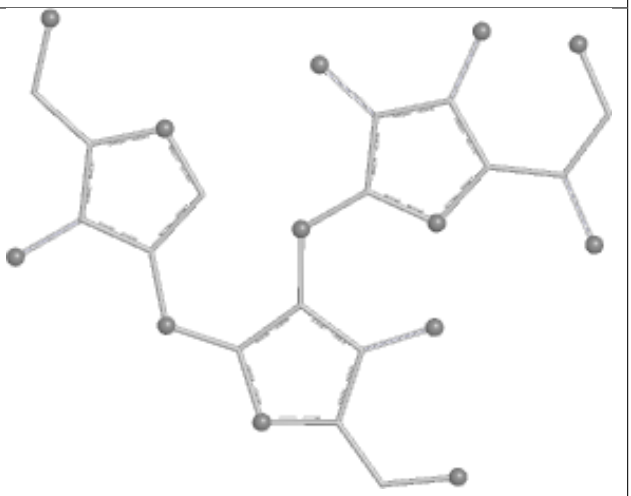
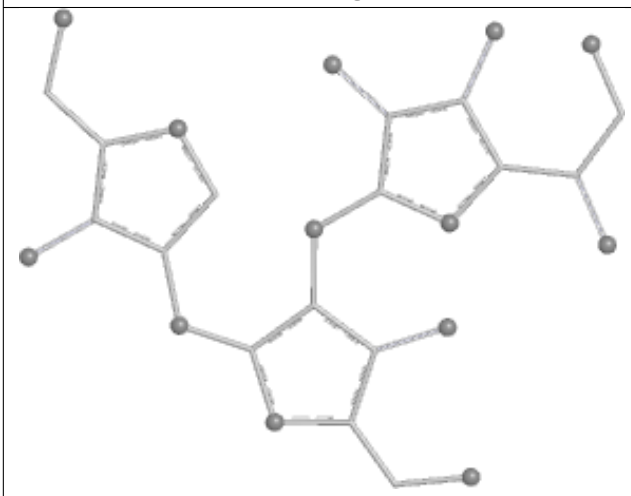
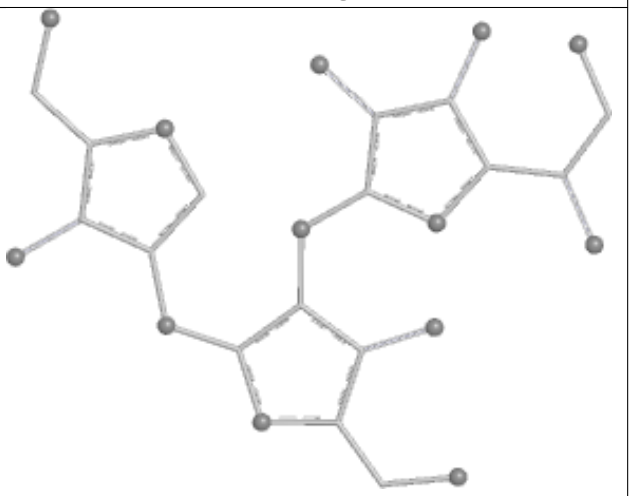
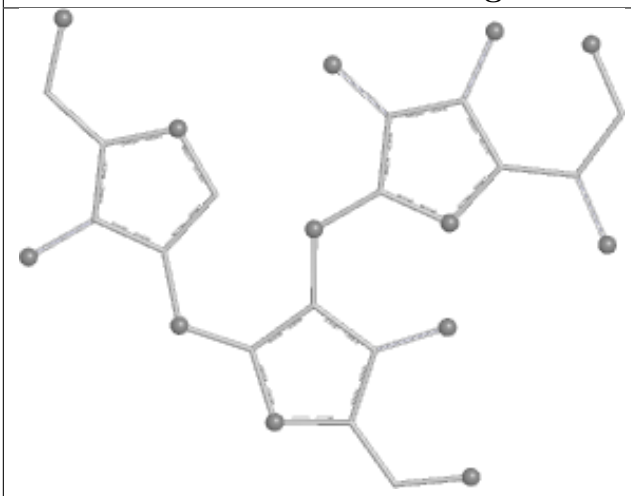
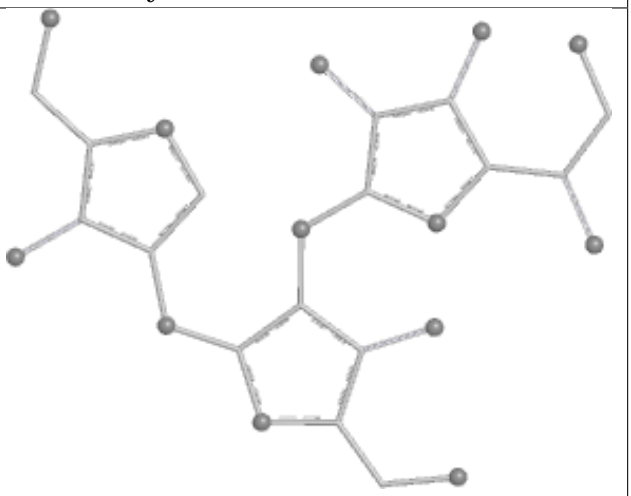
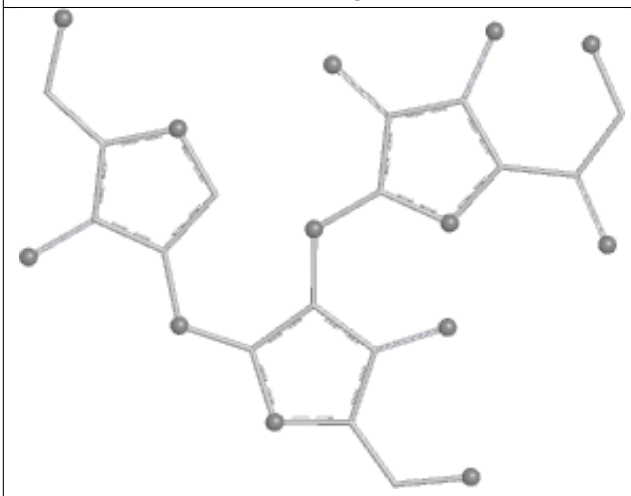
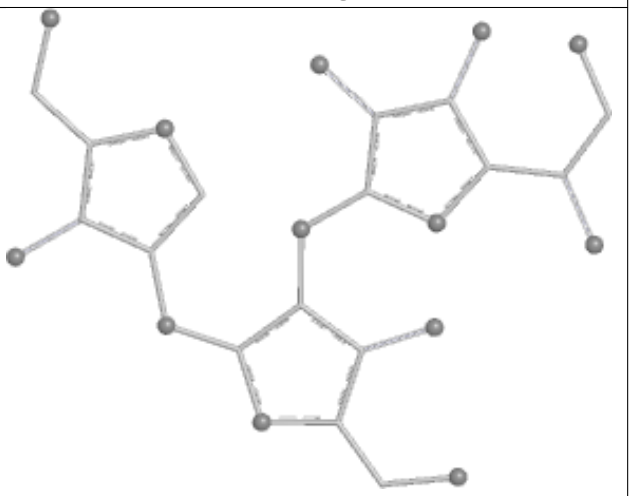
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain yD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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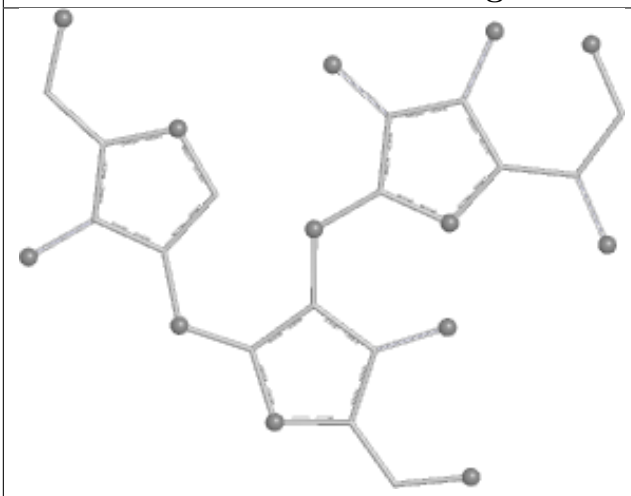
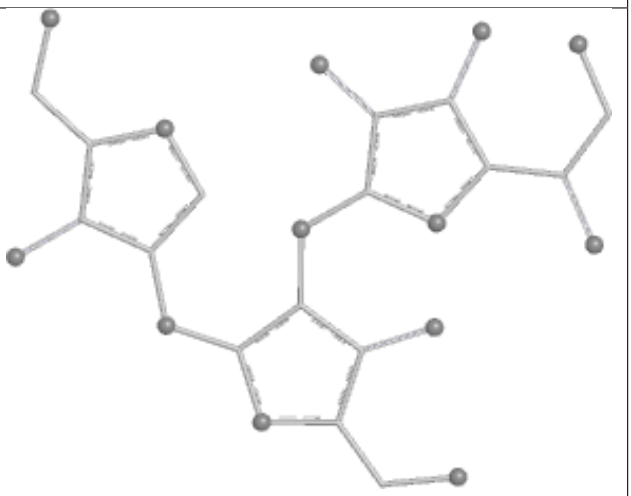
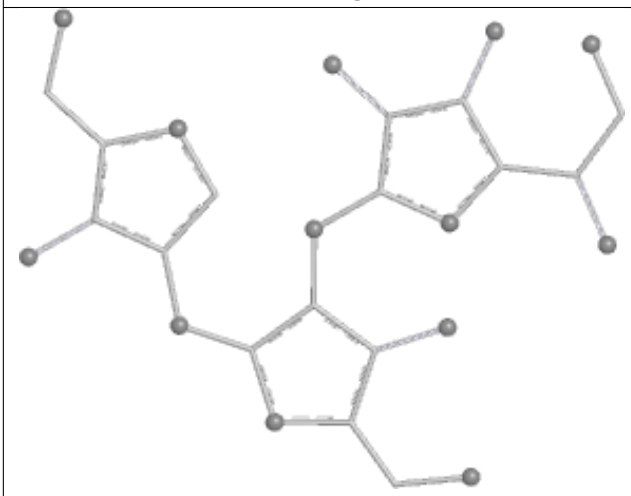
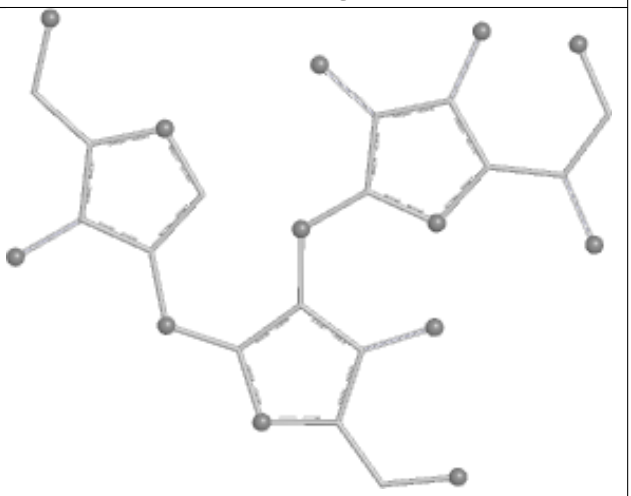
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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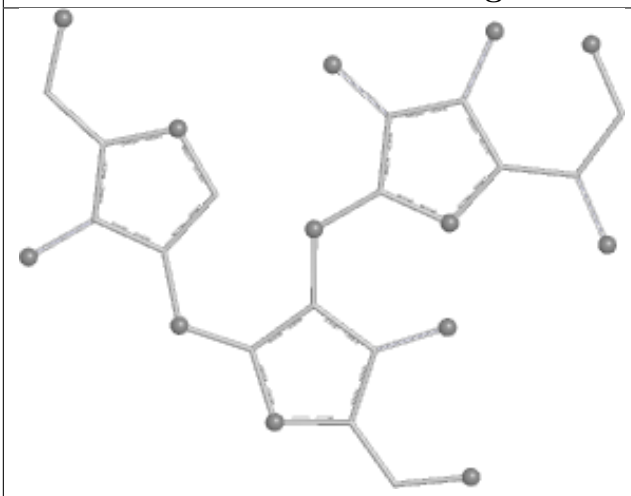
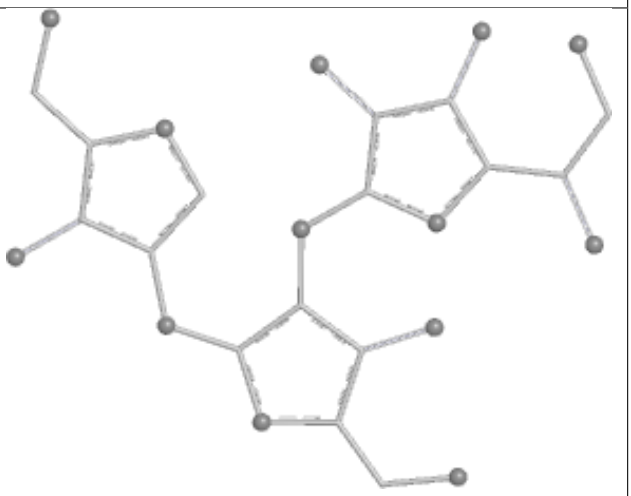
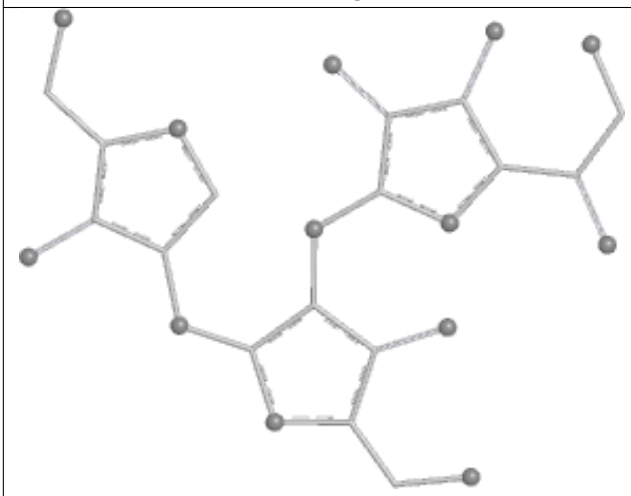
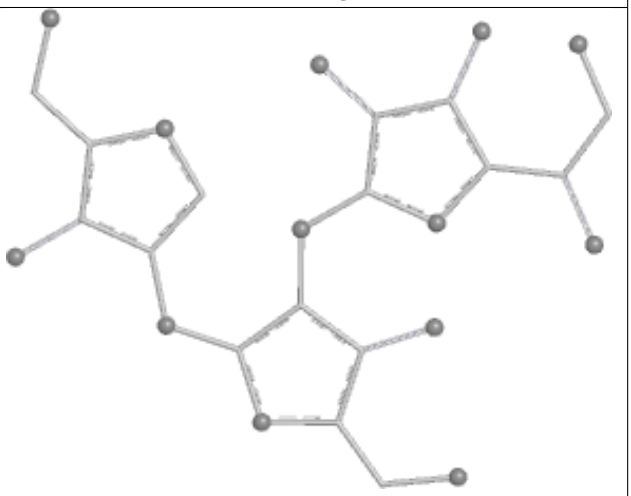
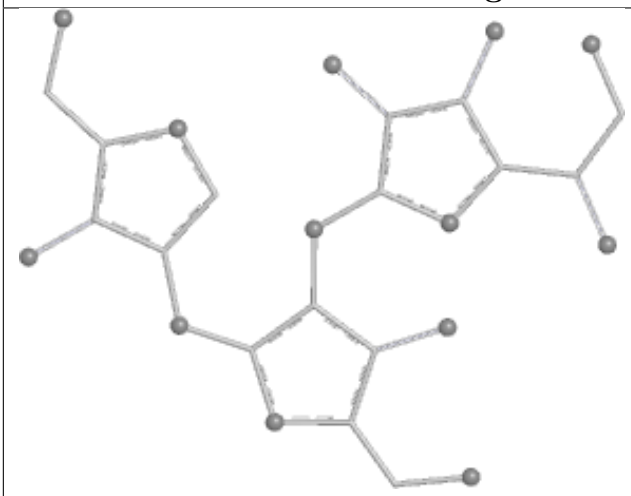
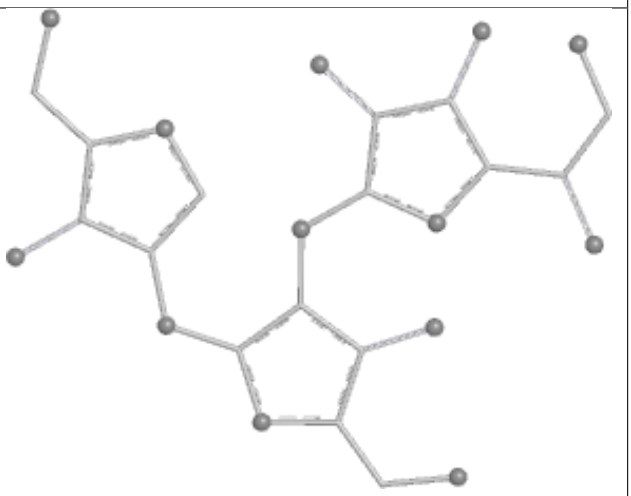
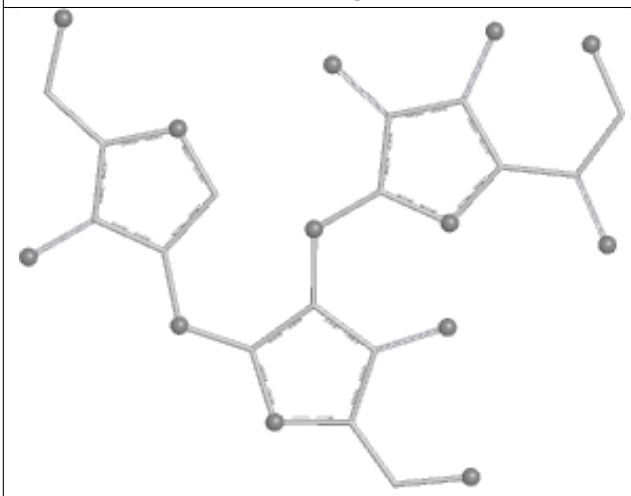
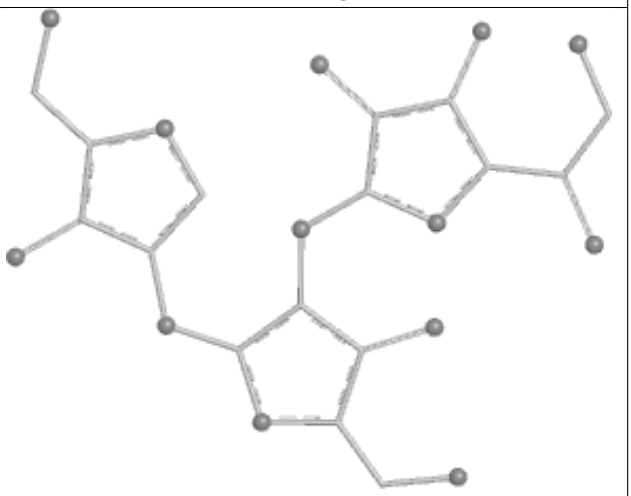
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 6D	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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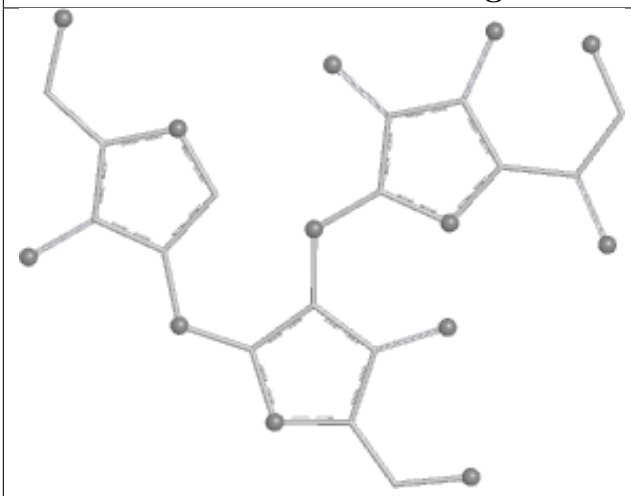	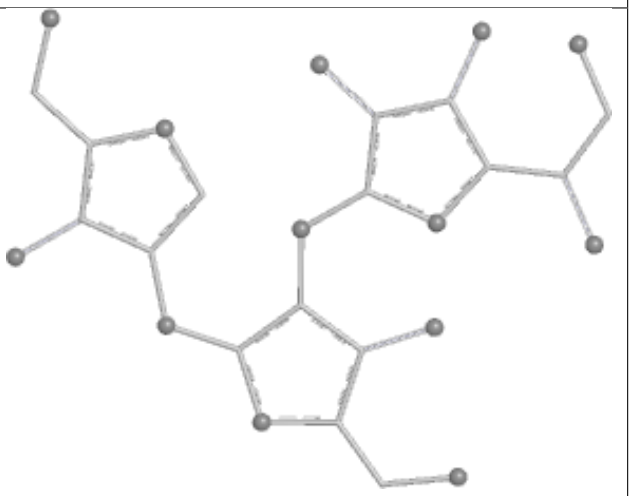
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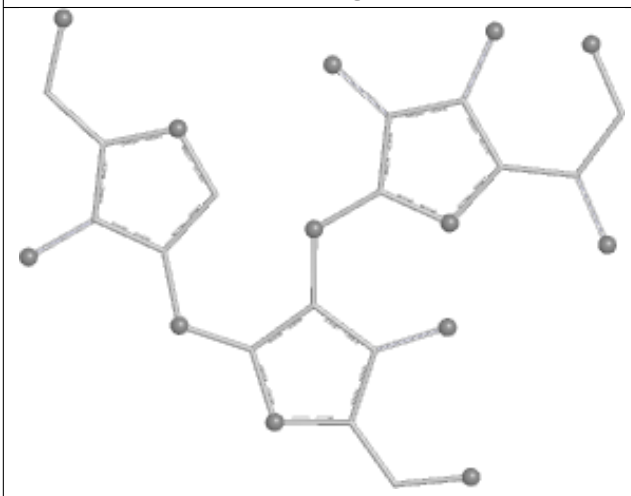	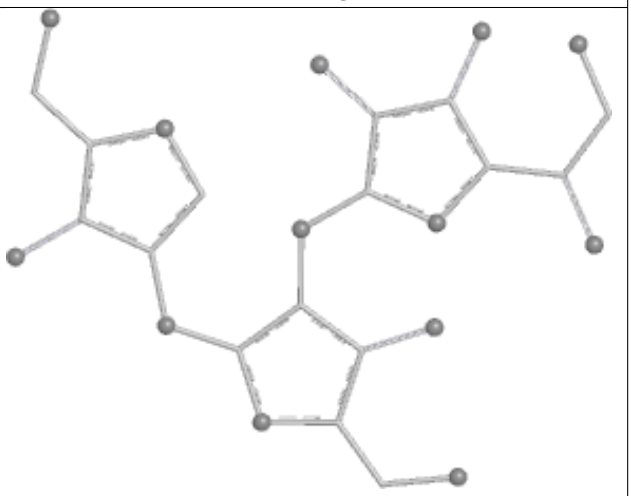
Torsions	**Rings**

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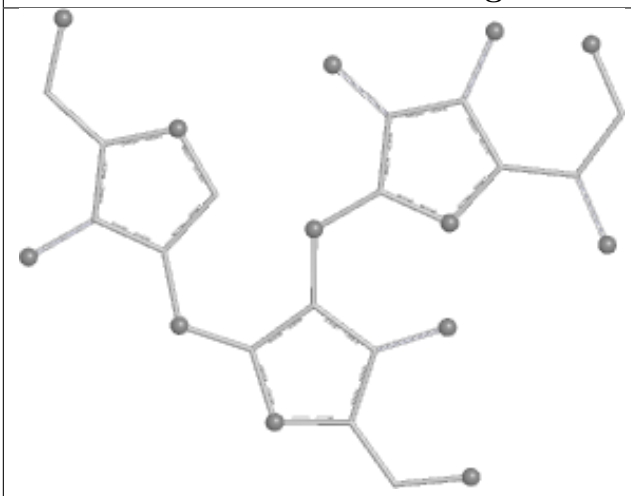
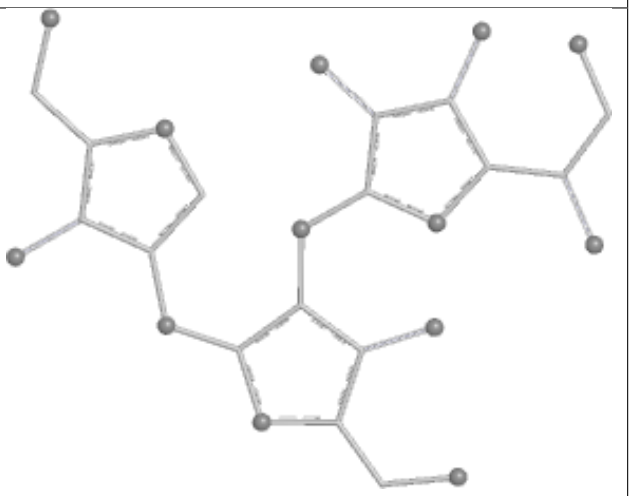
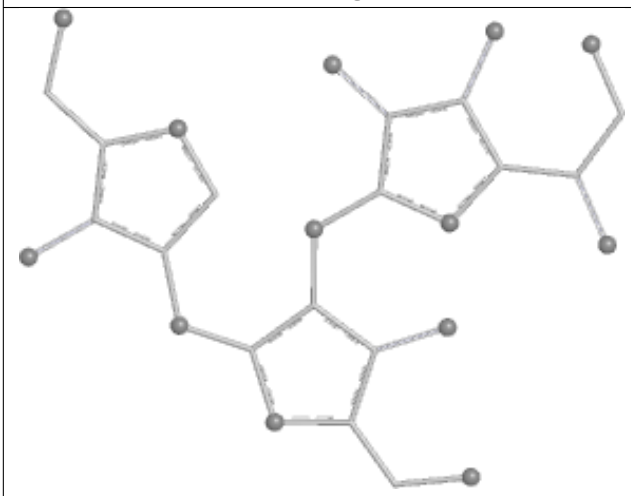
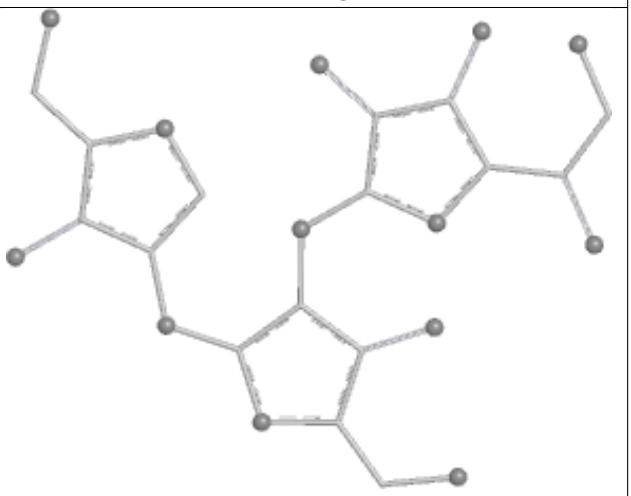
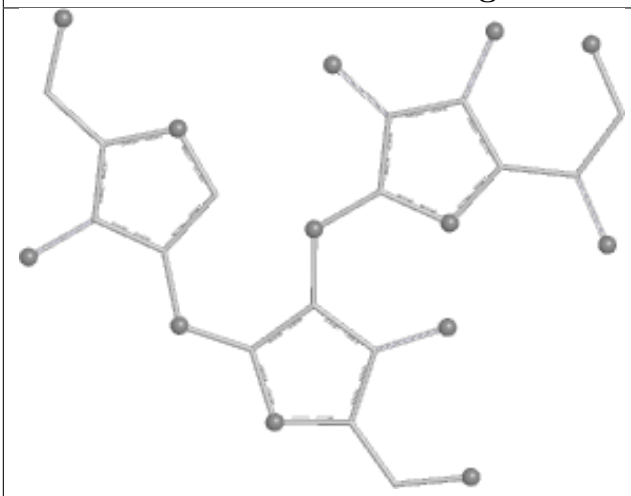
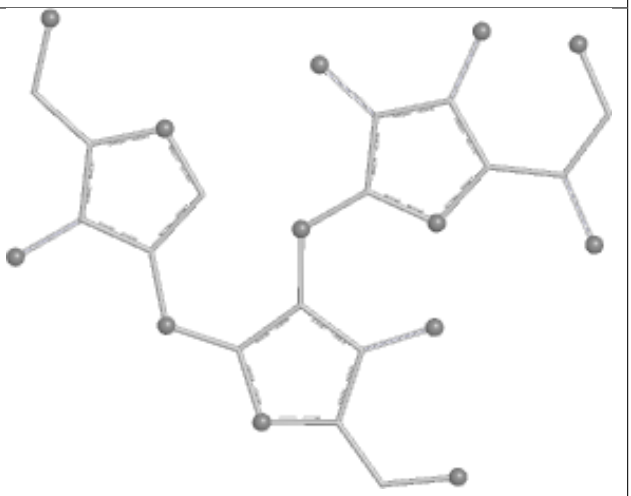
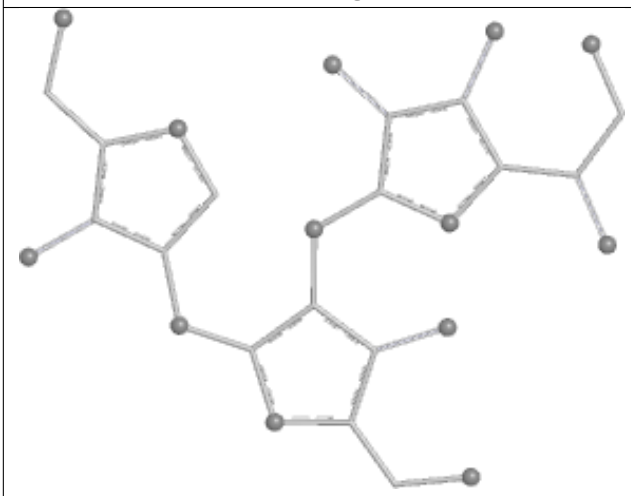
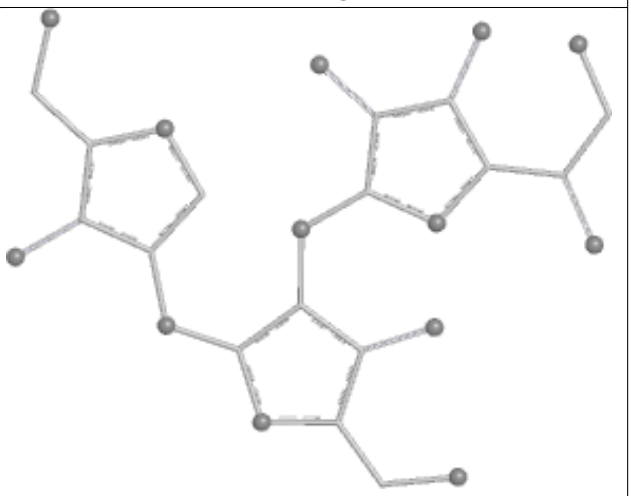
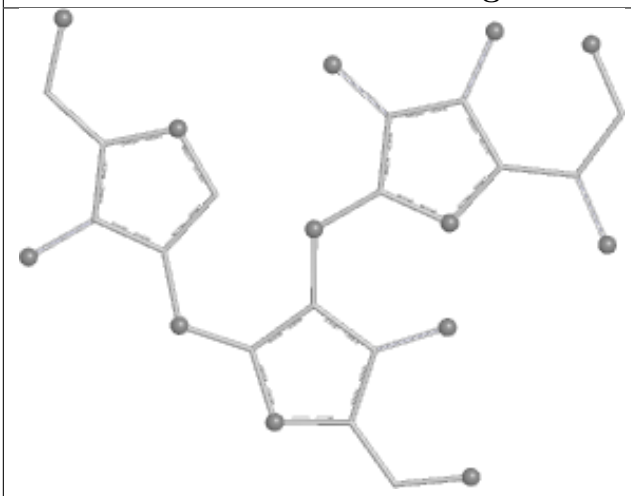
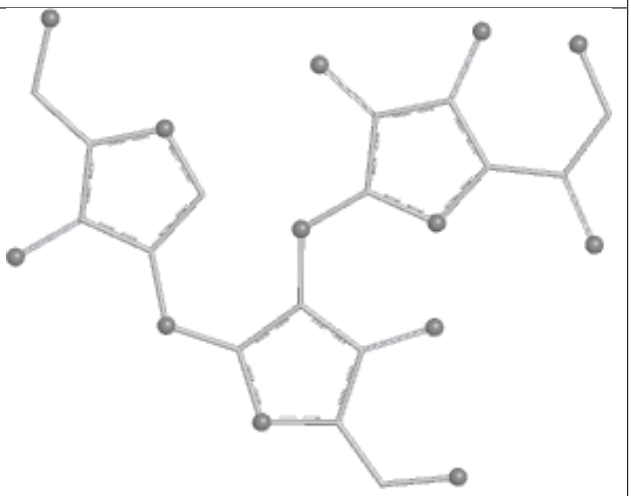
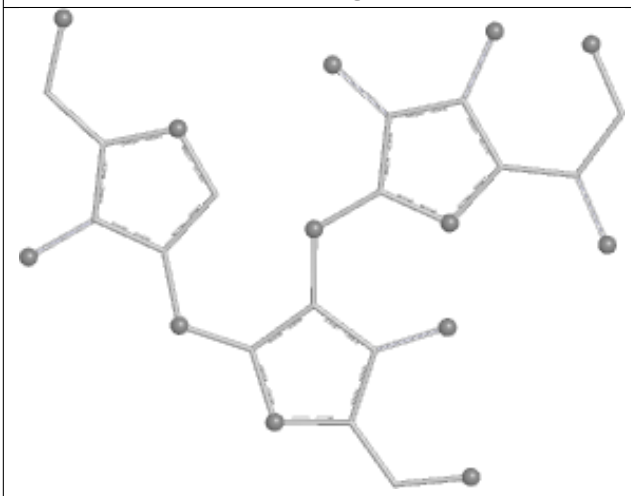
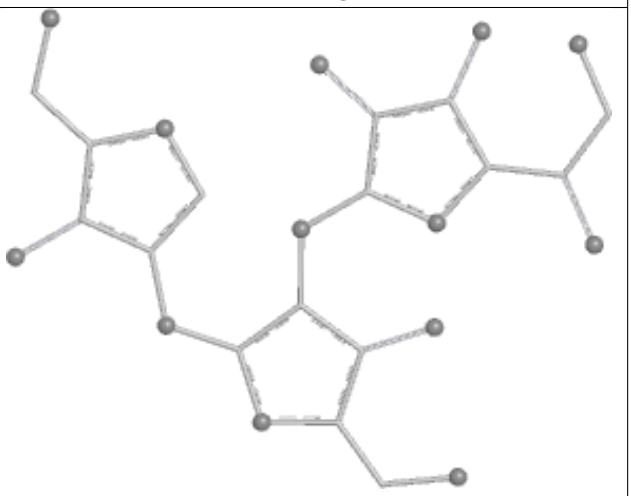
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain ME	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain OE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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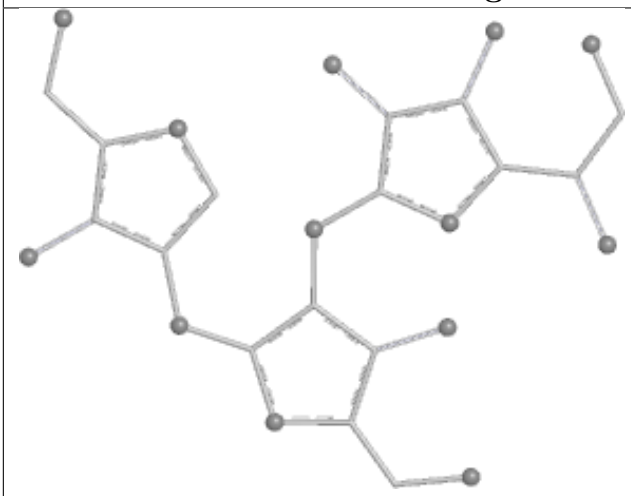
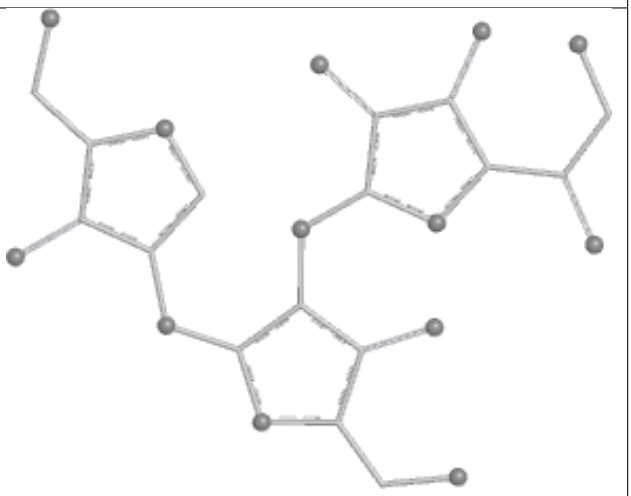
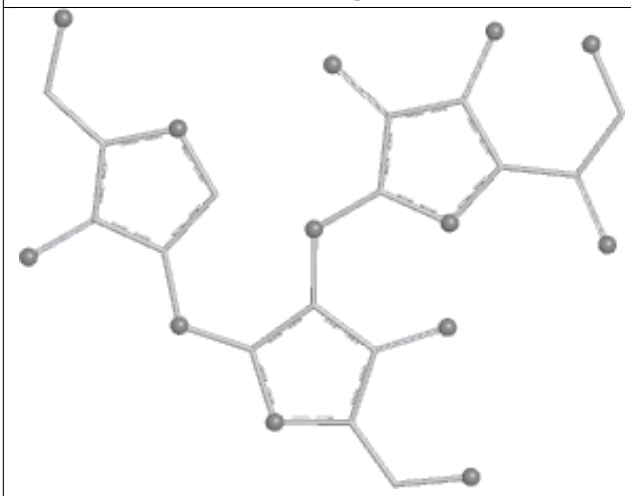
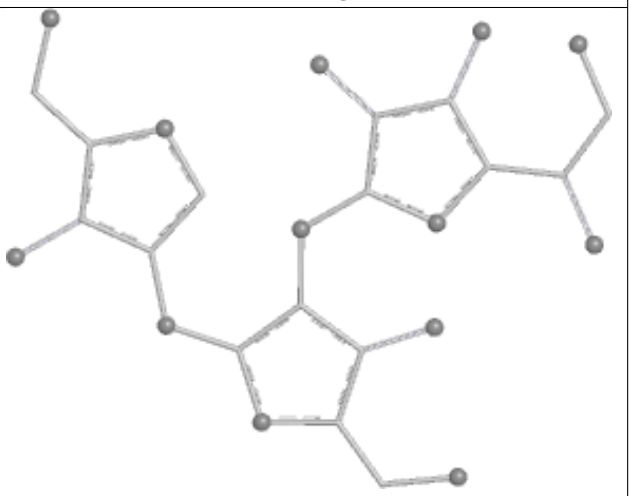
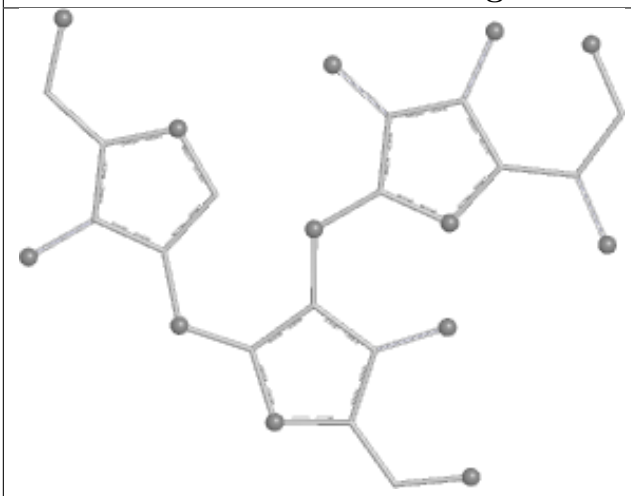
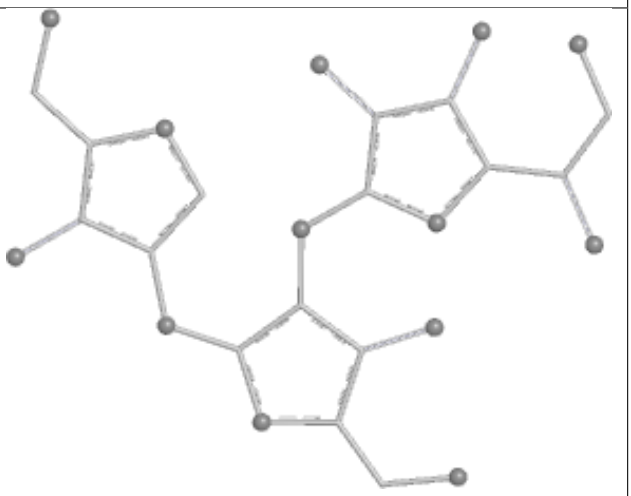
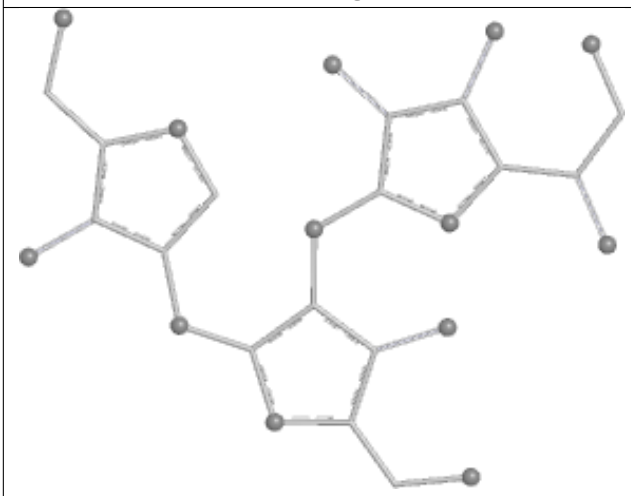
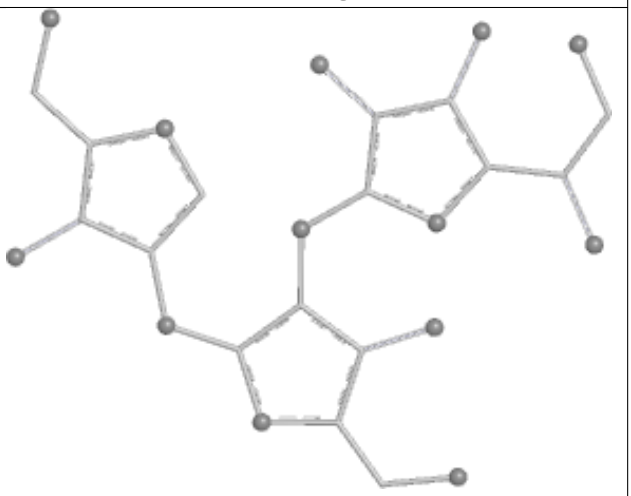
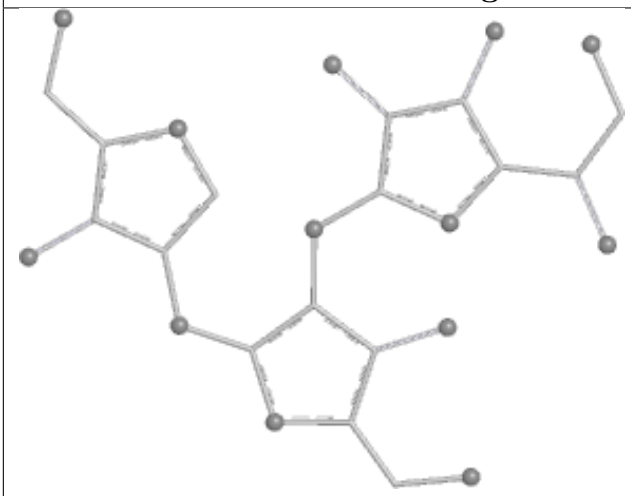
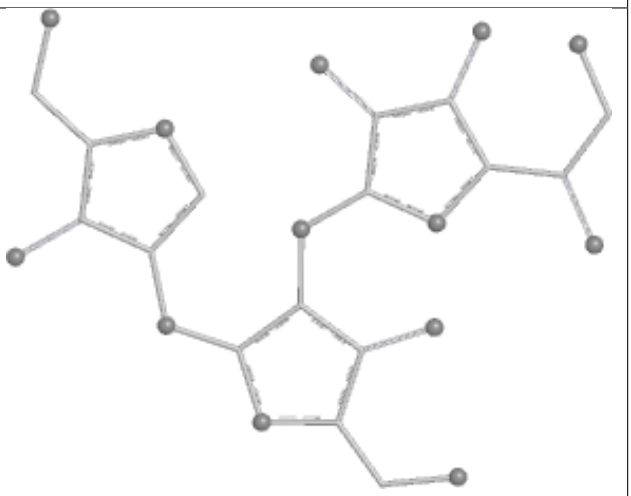
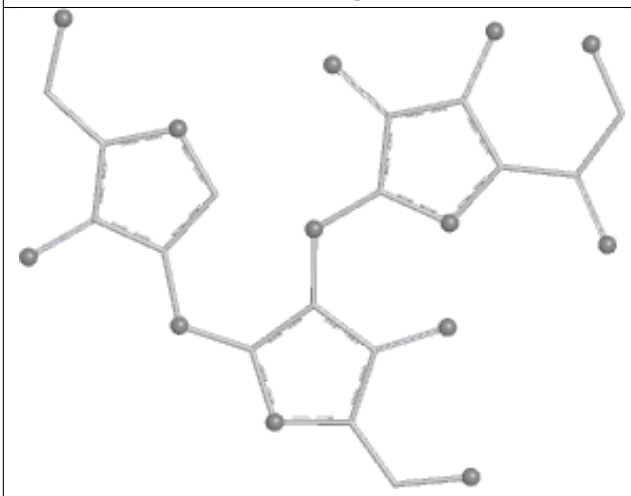
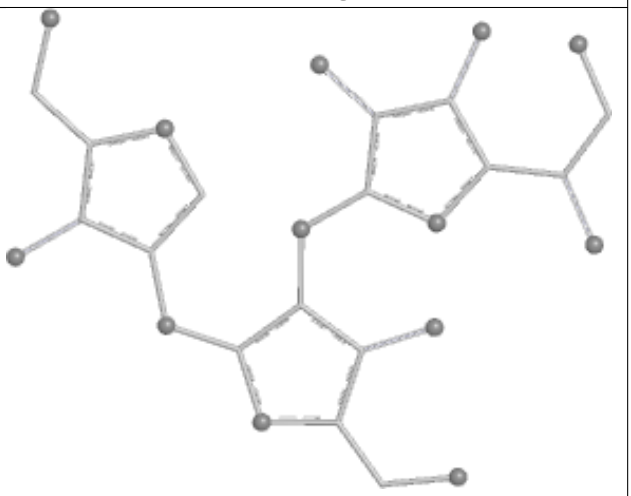
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain bE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain mE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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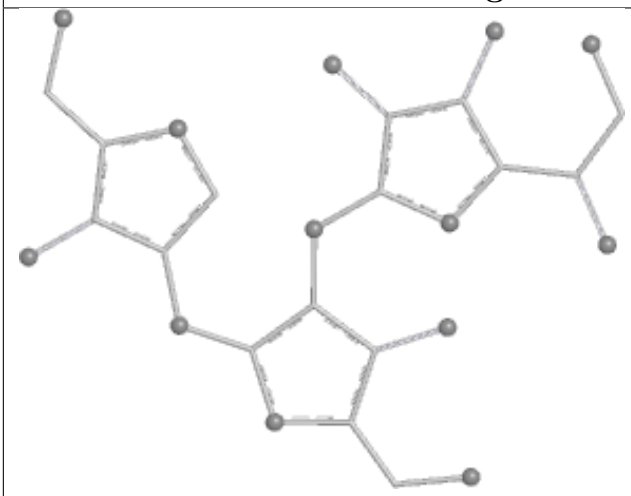
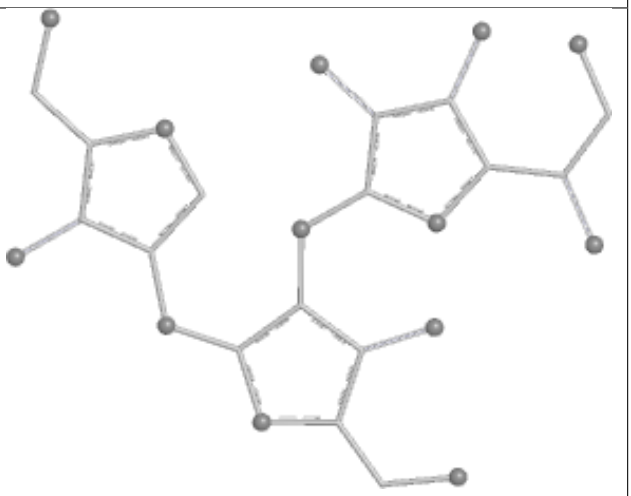
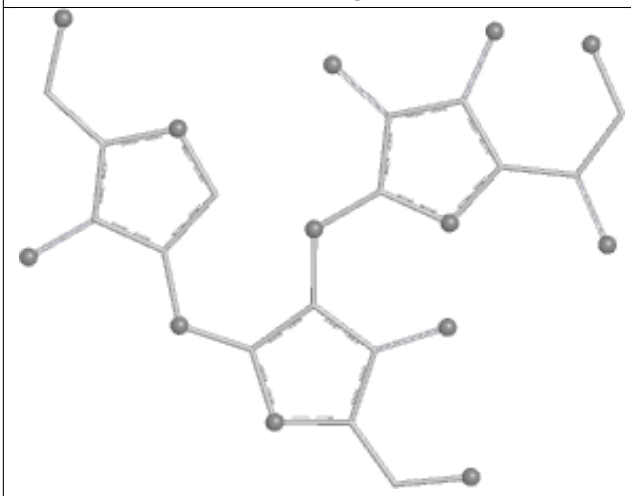
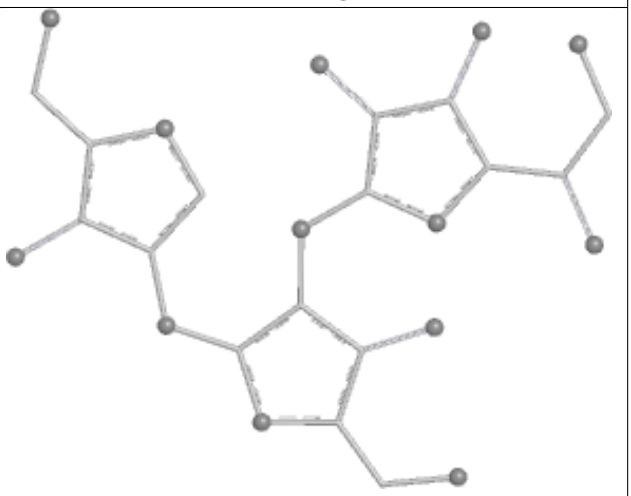
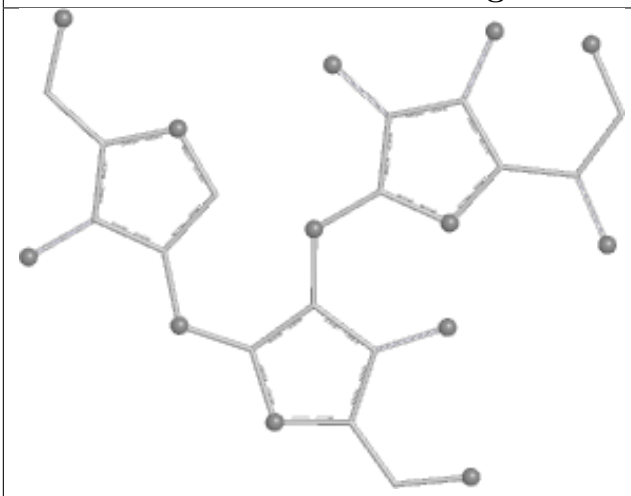
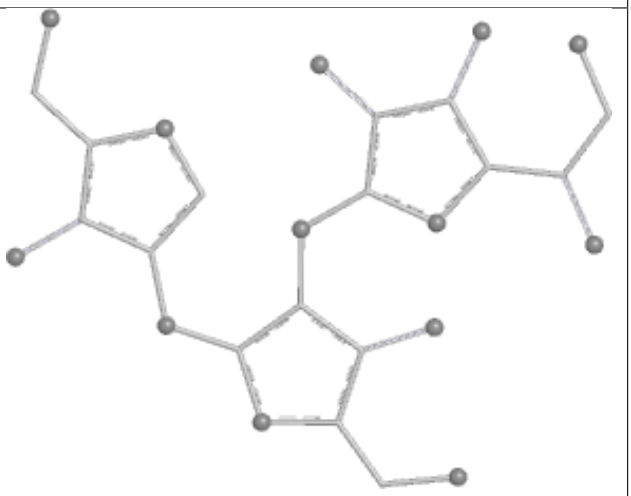
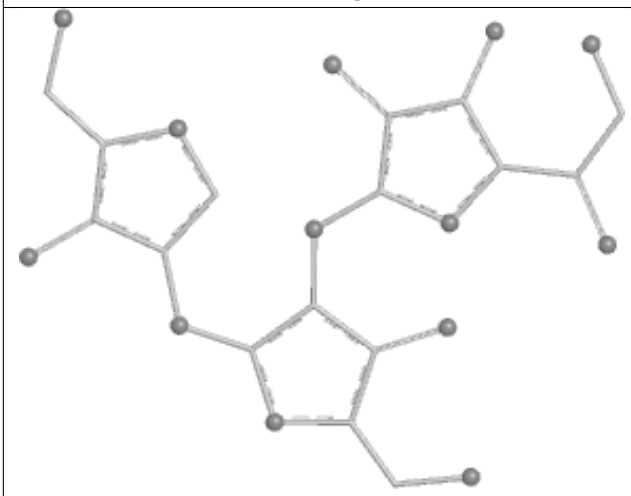
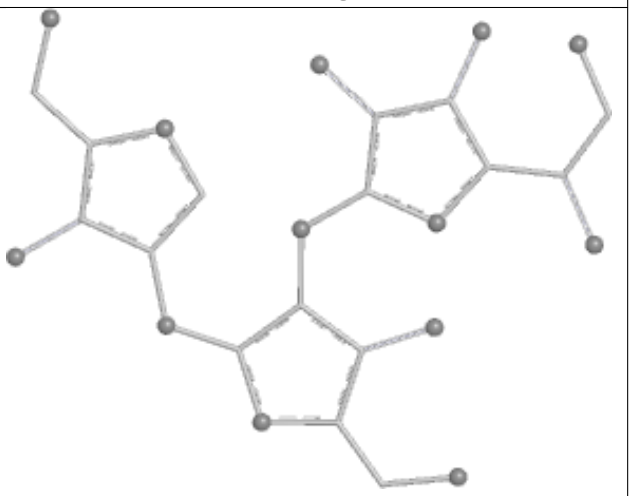
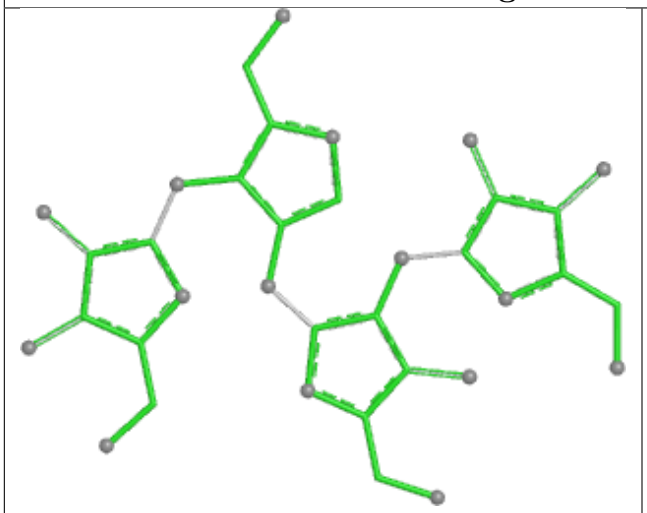
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain oE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain S



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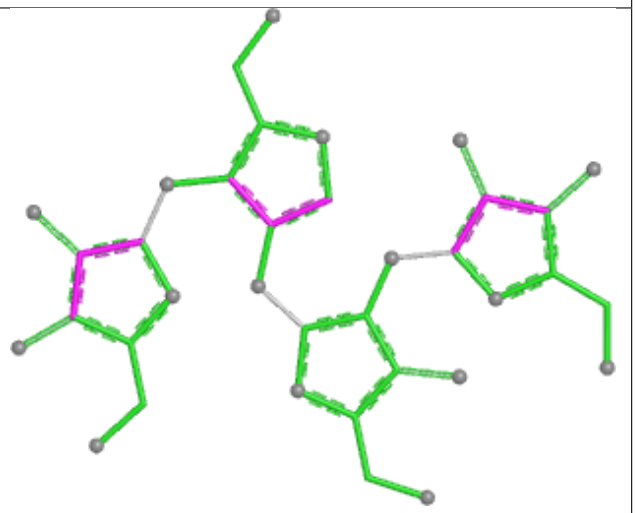

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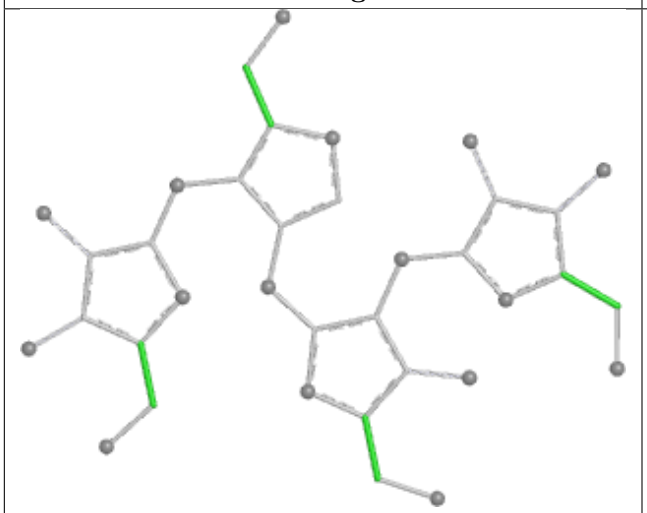

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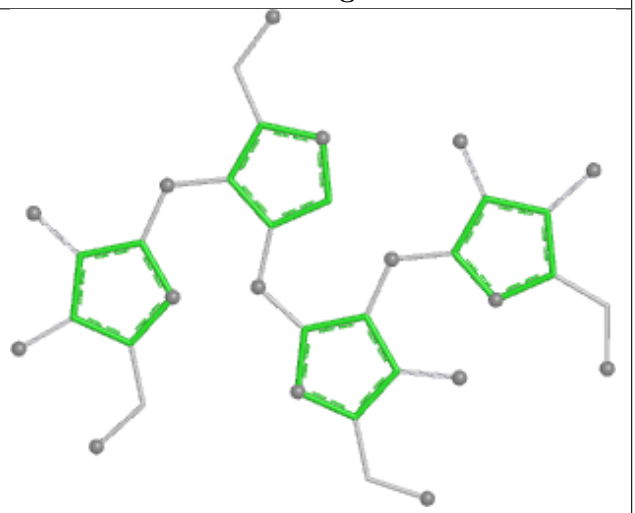
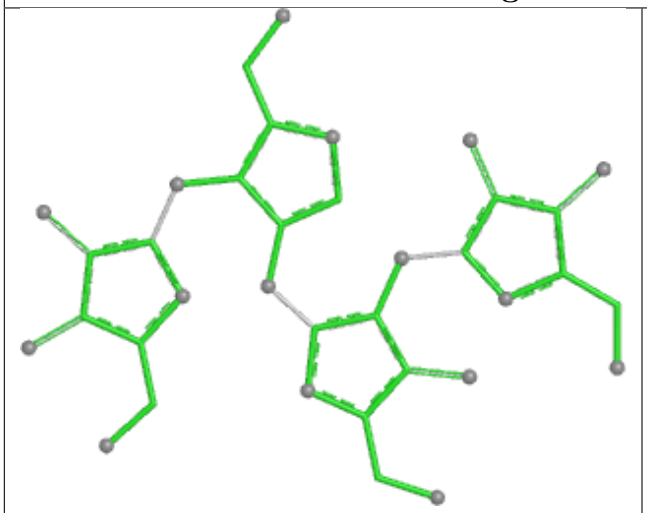


Rings

Oligosaccharide Chain f



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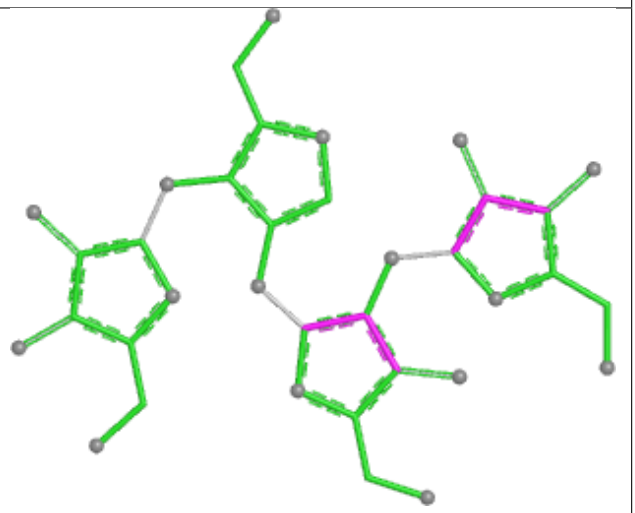

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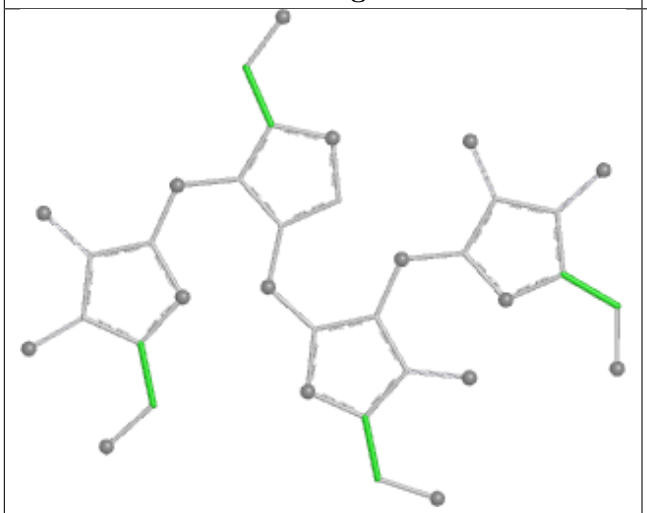

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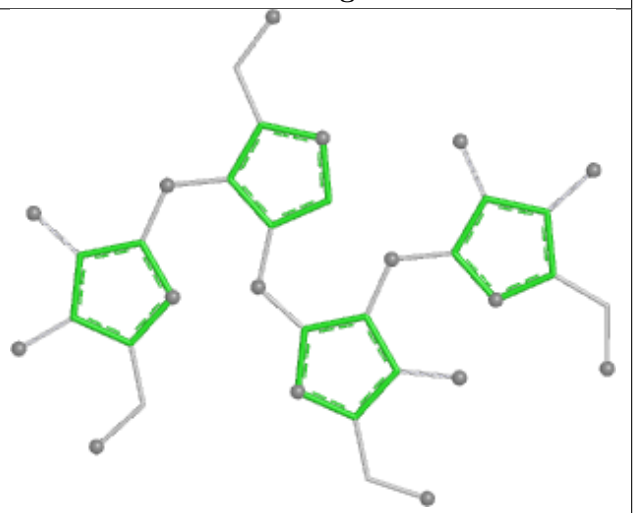
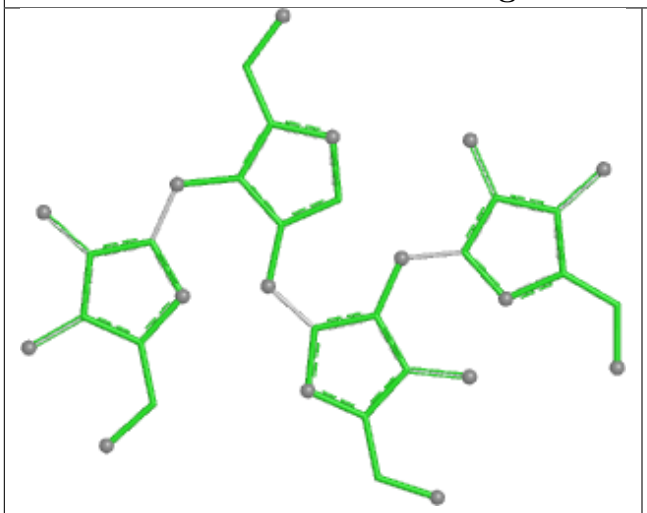


Rings

Oligosaccharide Chain h



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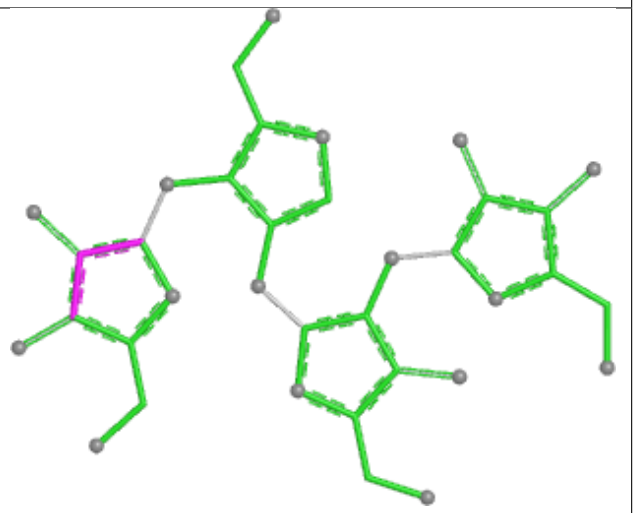

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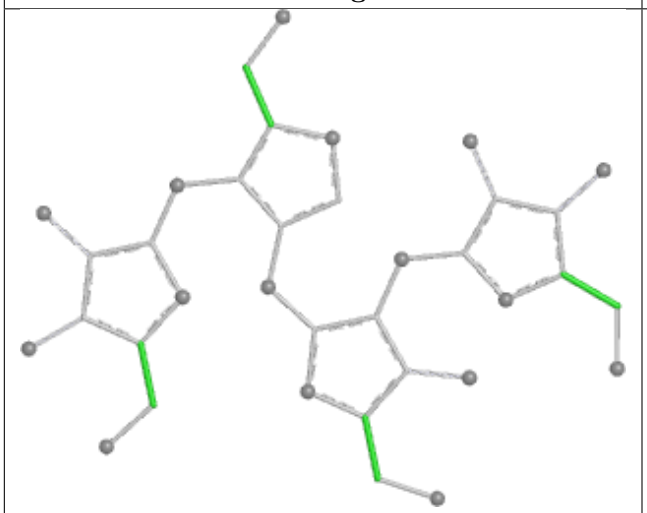

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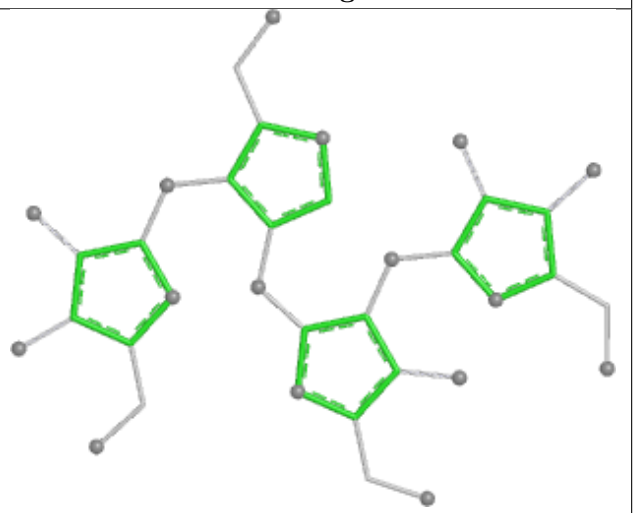
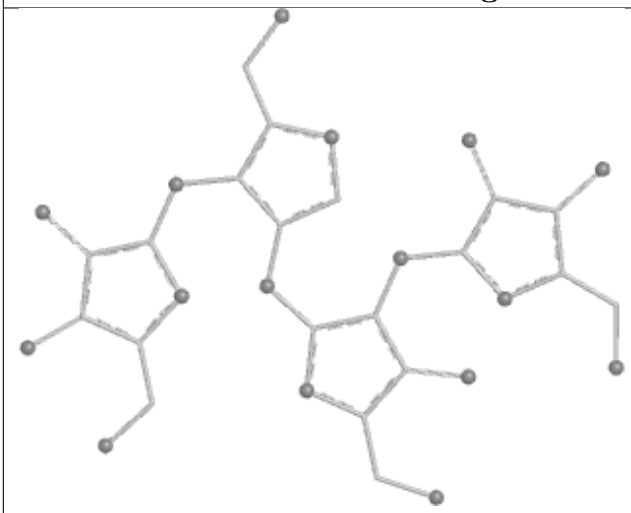
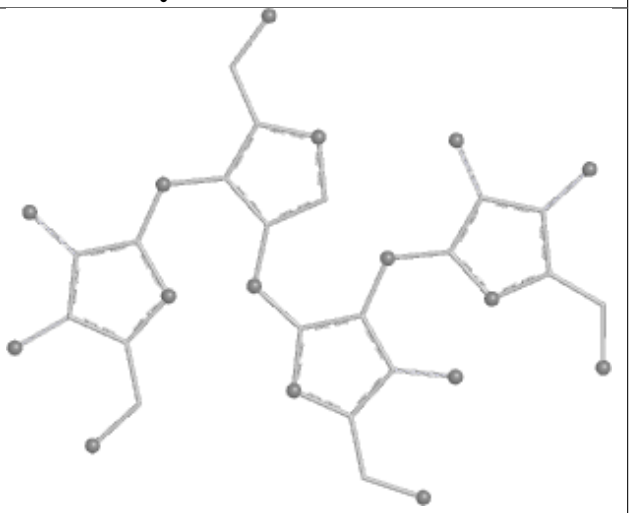
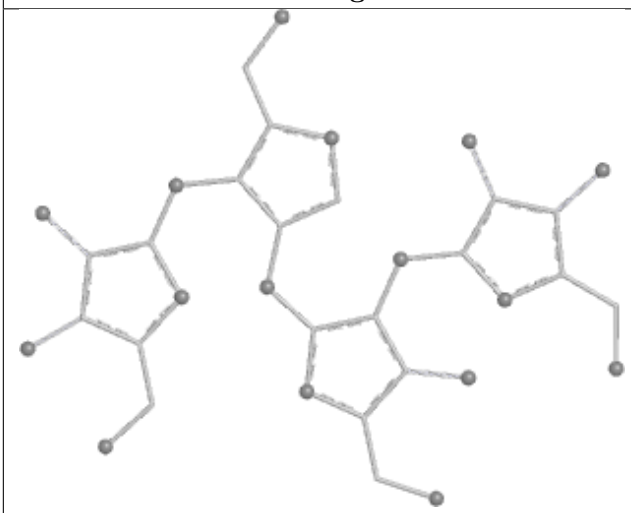
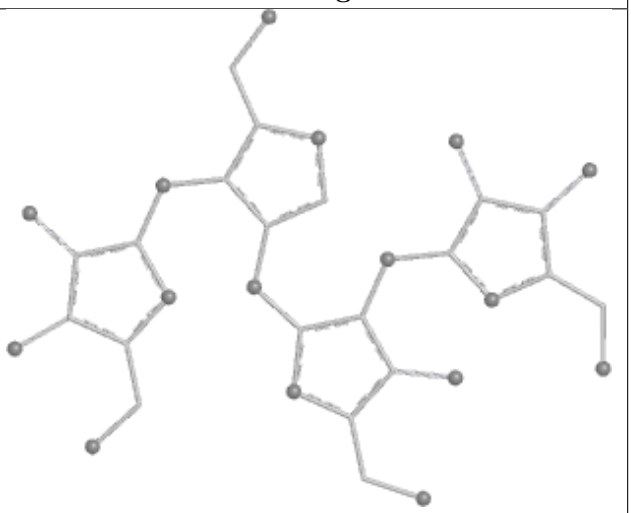
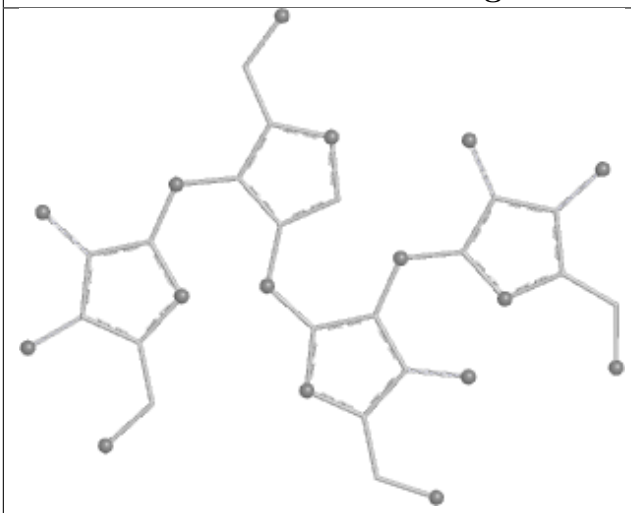
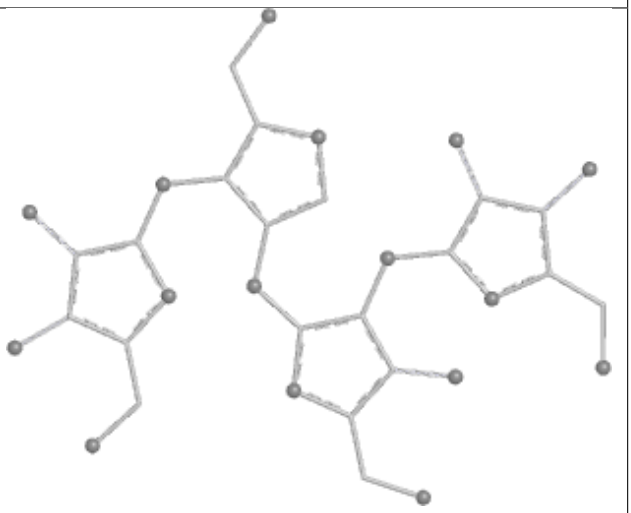
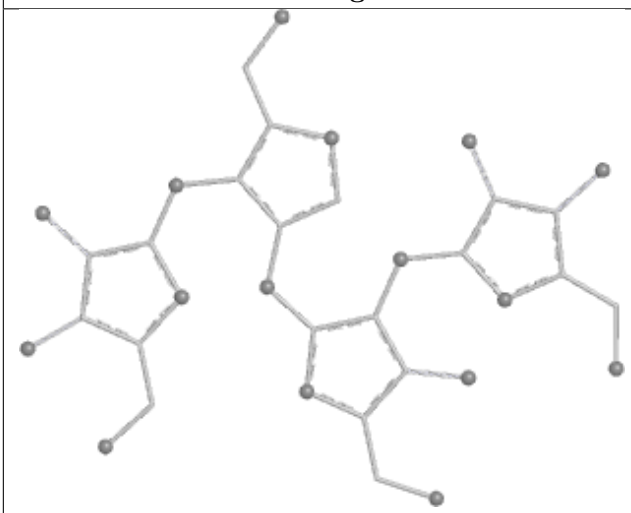
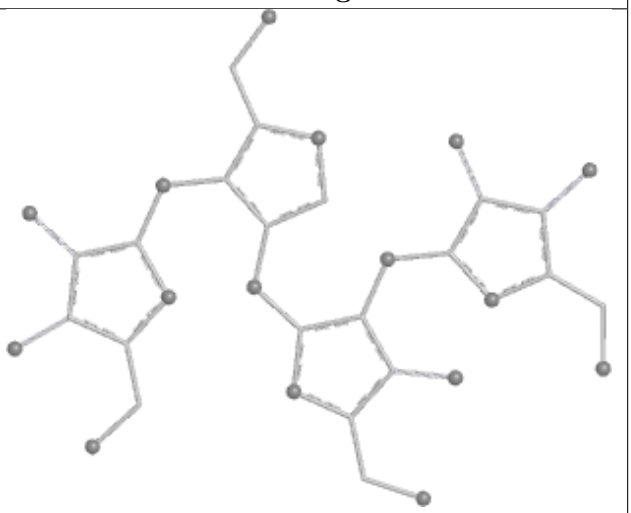


Rings

Oligosaccharide Chain QA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain dA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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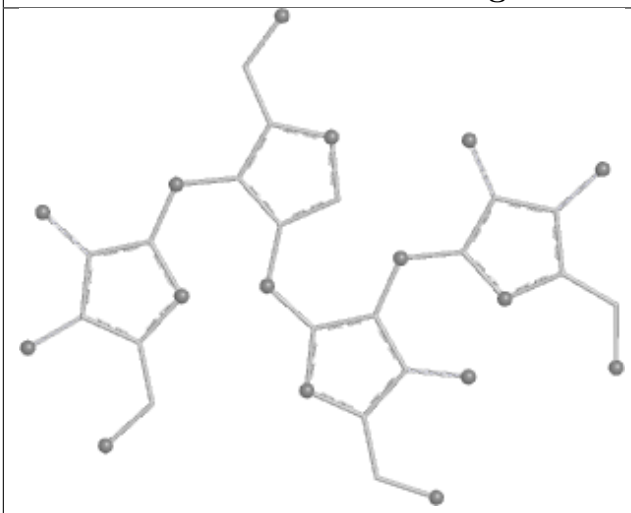
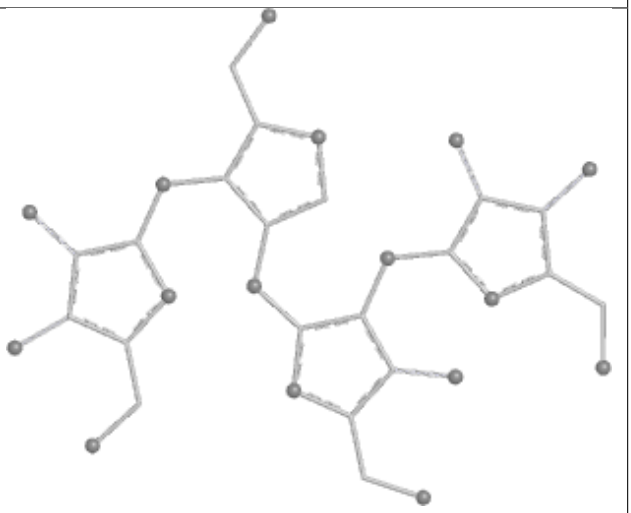
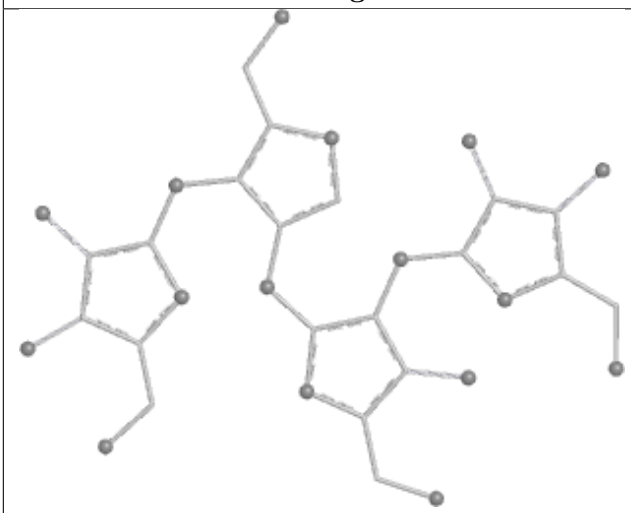
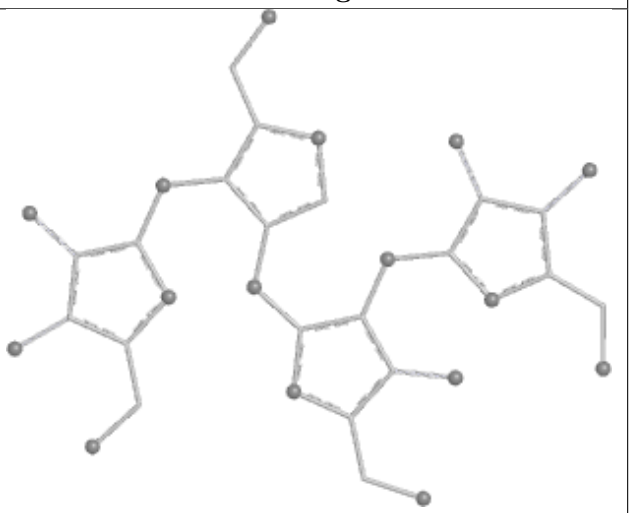
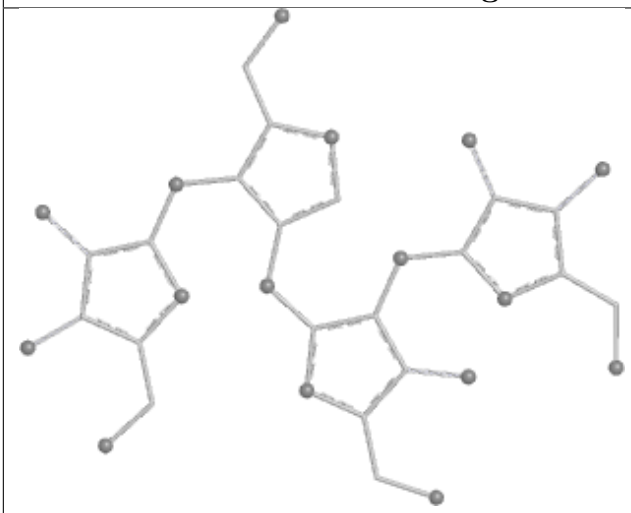
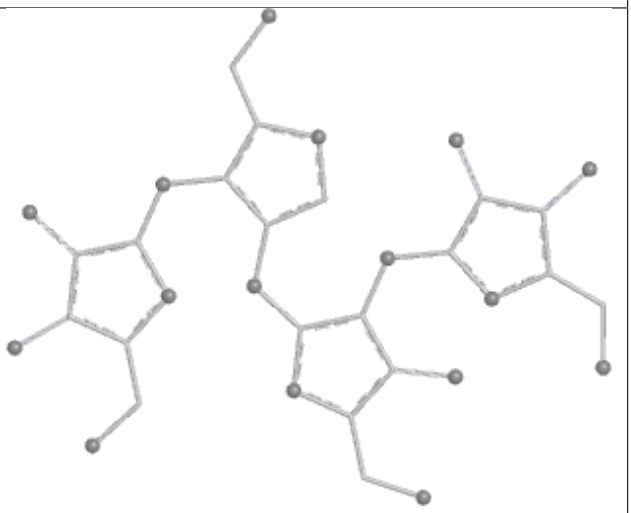
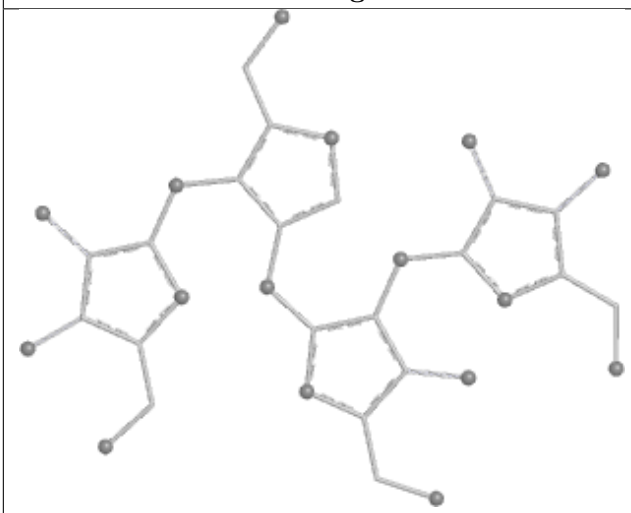
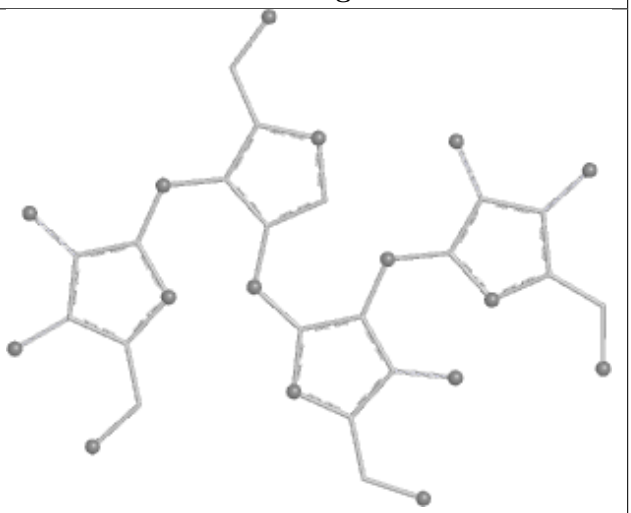
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain KC	
 Bond lengths	 Bond angles
 Torsions	 Rings

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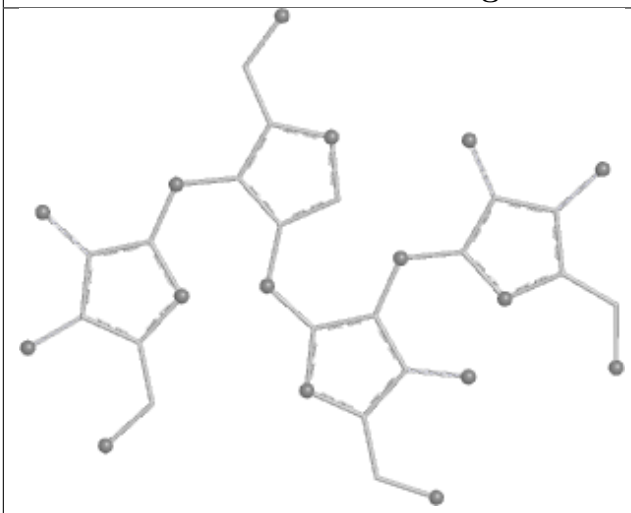
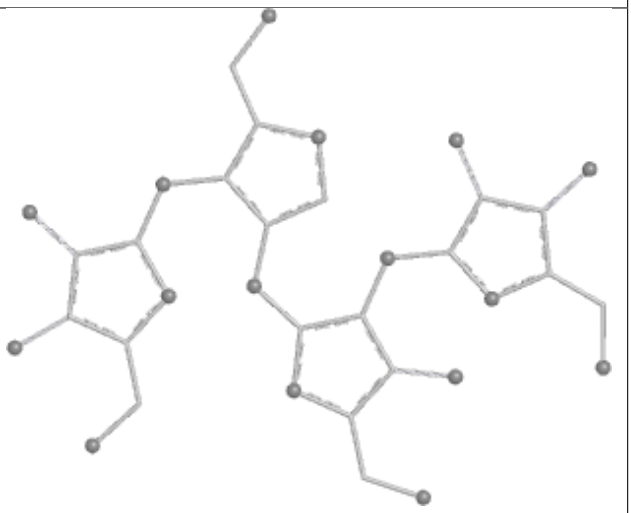
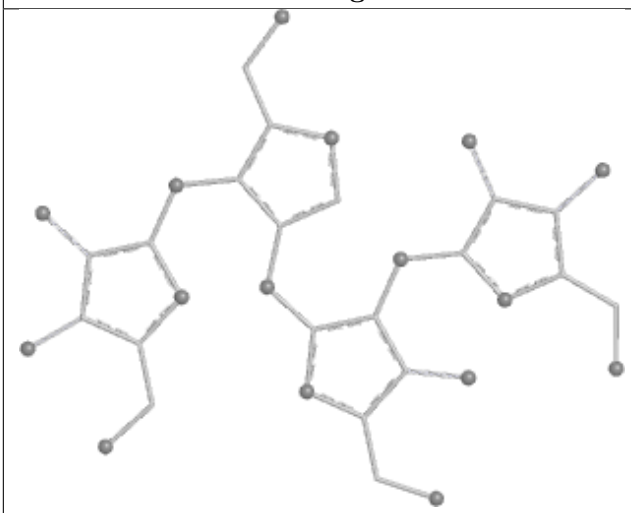
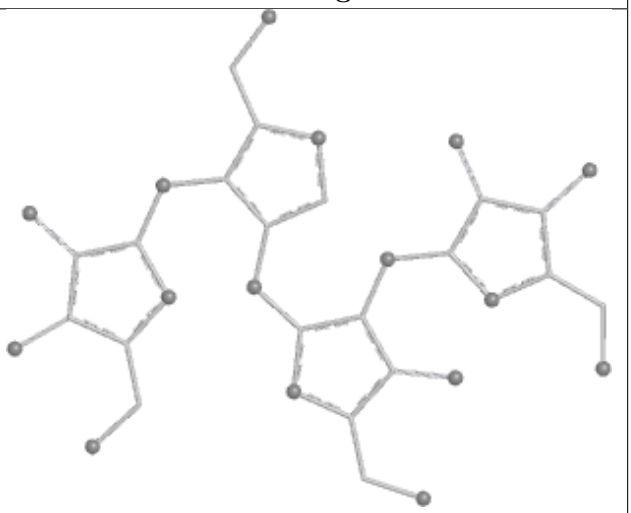
 Bond lengths	 Bond angles
 Torsions	 Rings

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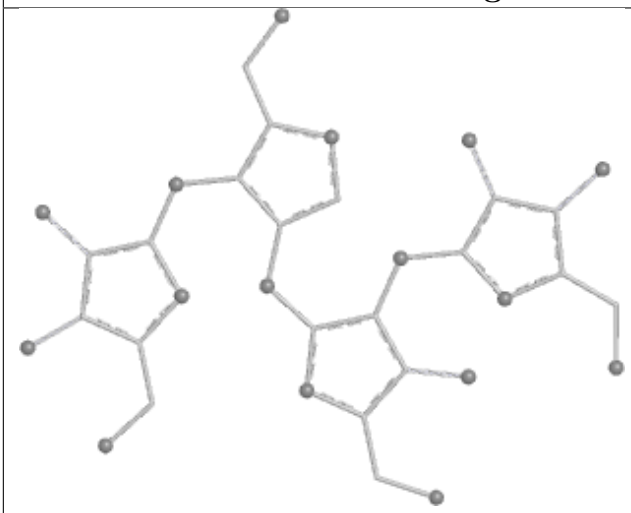
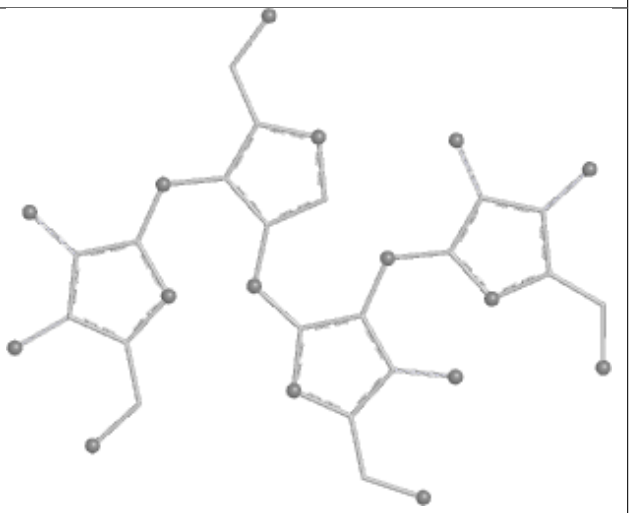
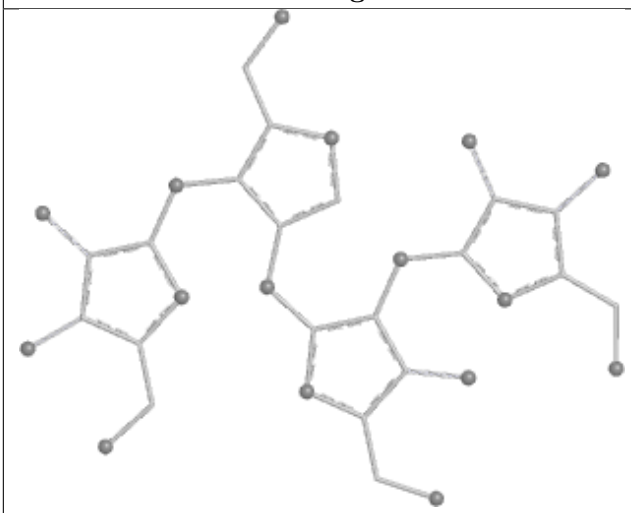
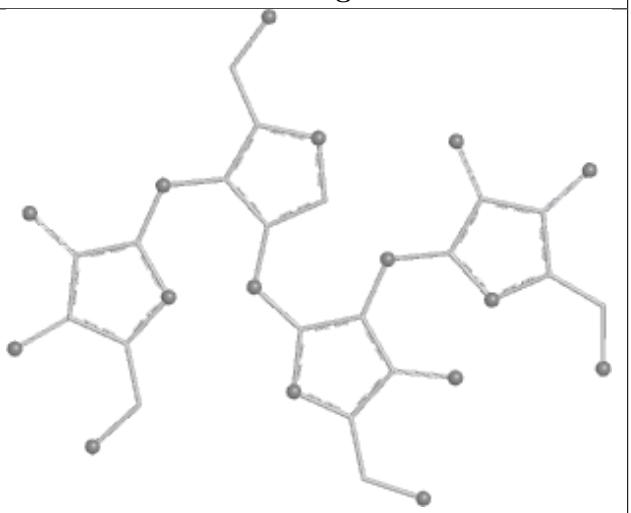
 Bond lengths	 Bond angles
 Torsions	 Rings

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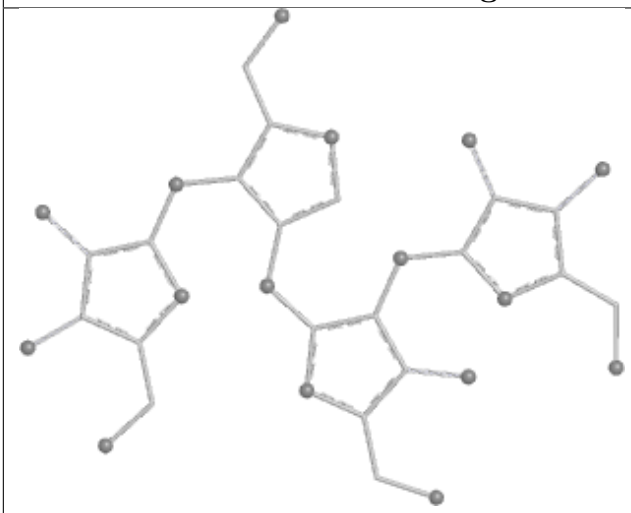
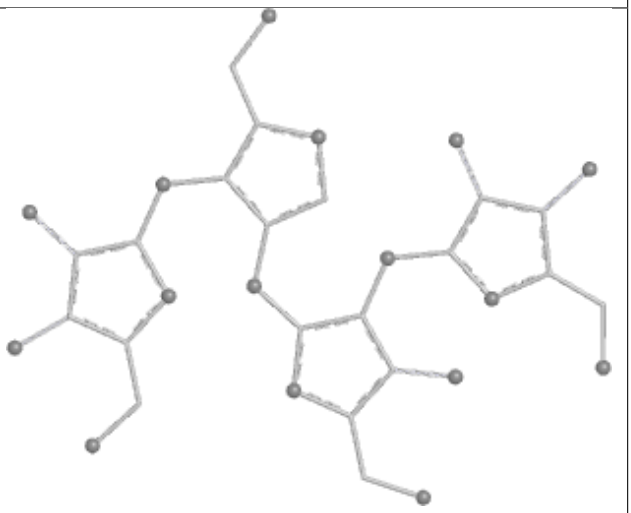
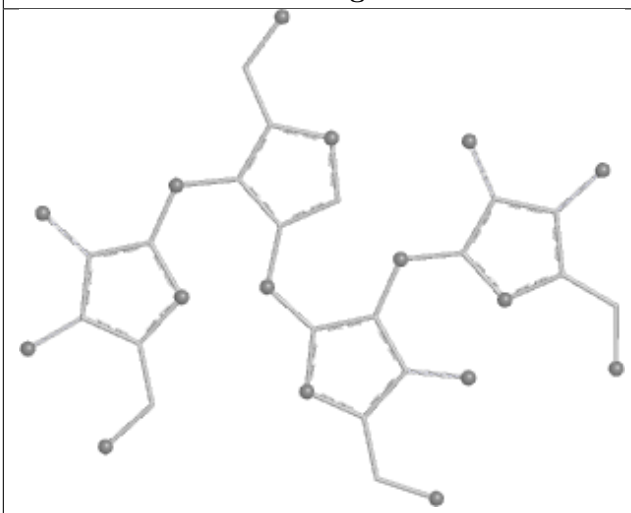
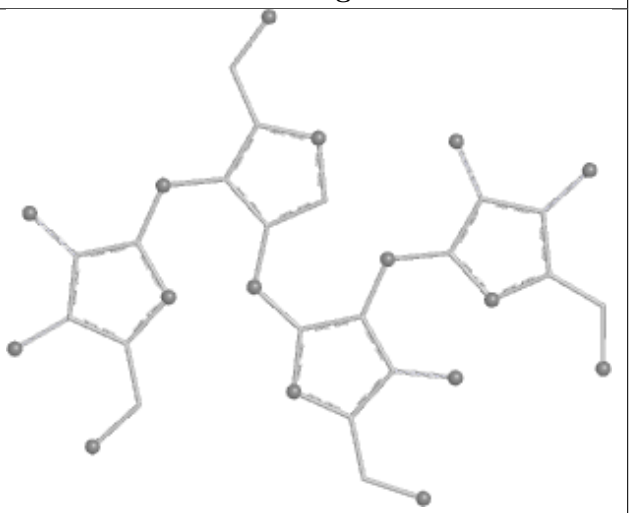
 Bond lengths	 Bond angles
 Torsions	 Rings

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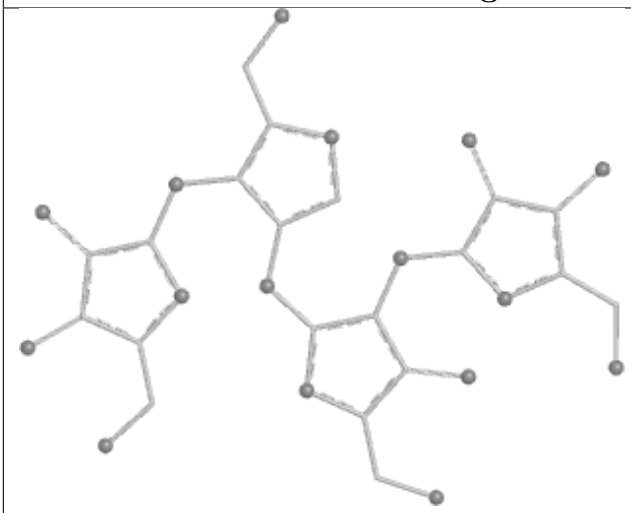
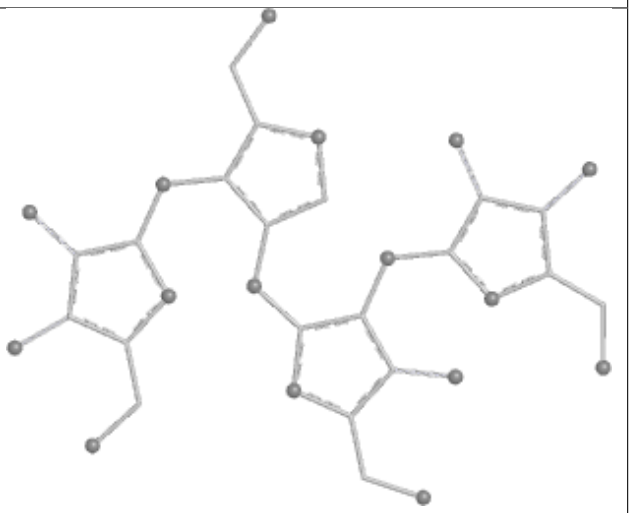
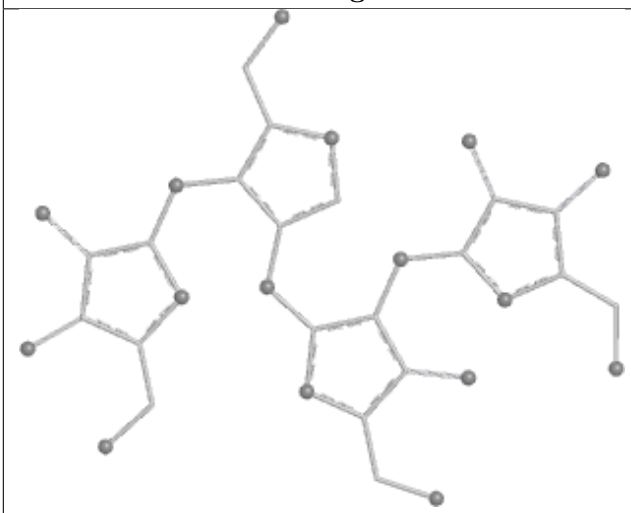
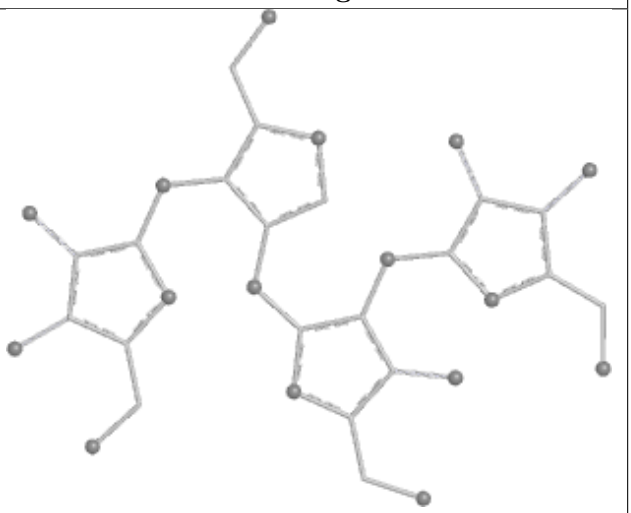
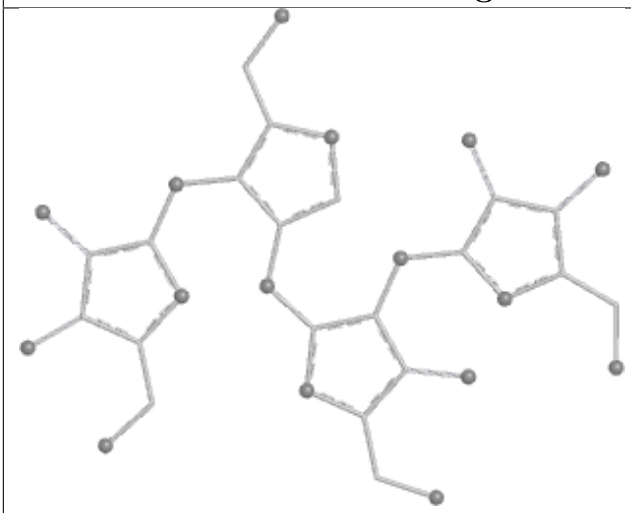
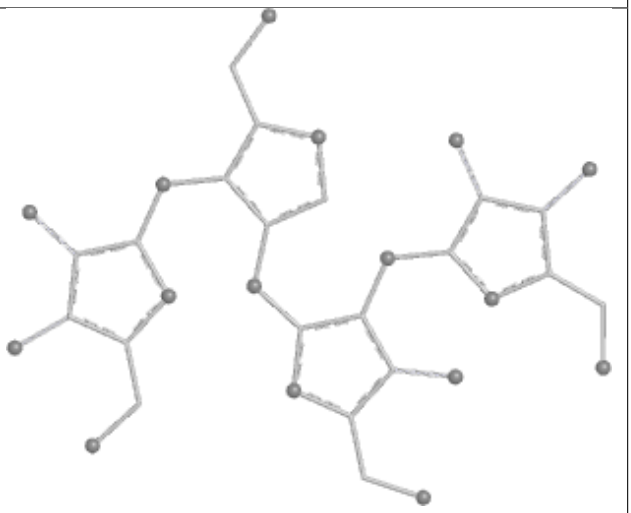
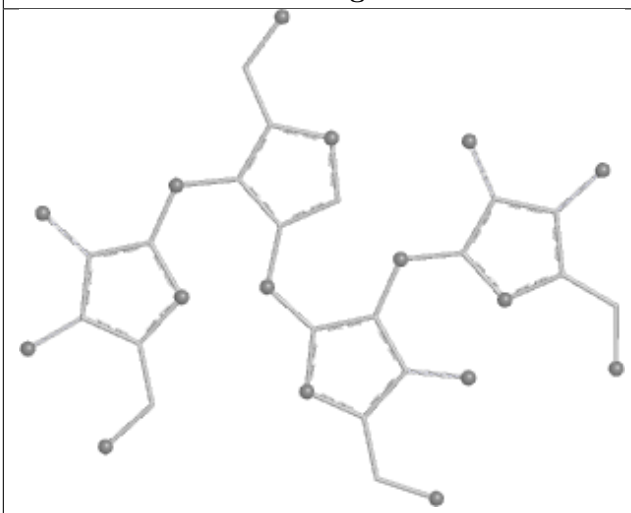
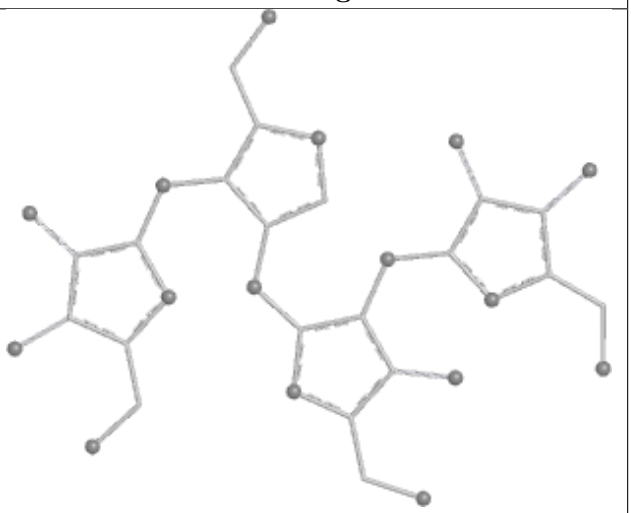
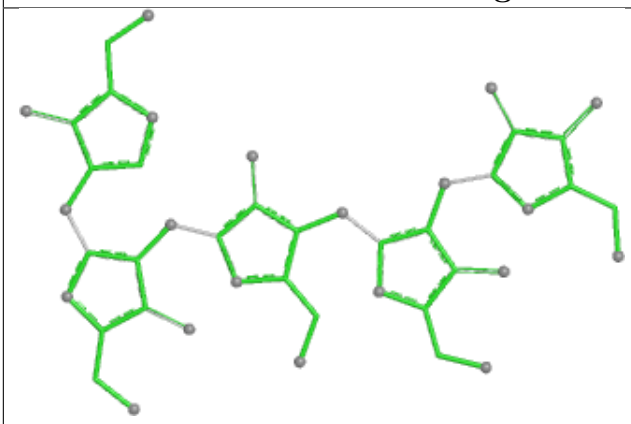
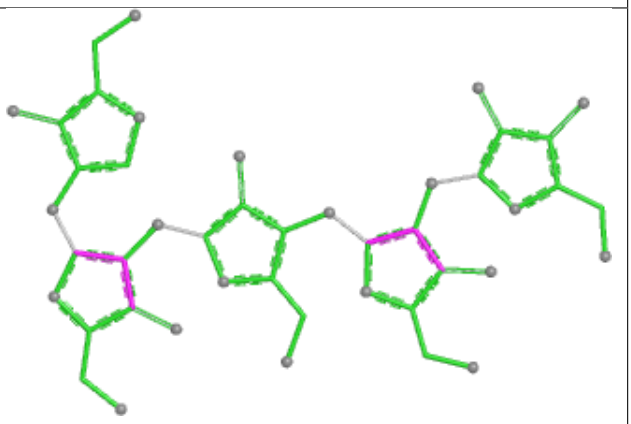
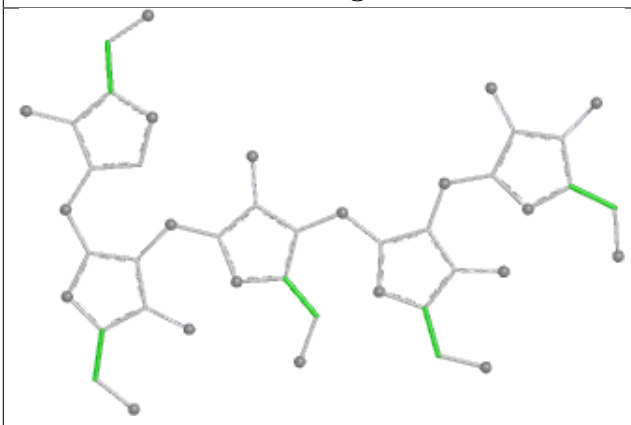
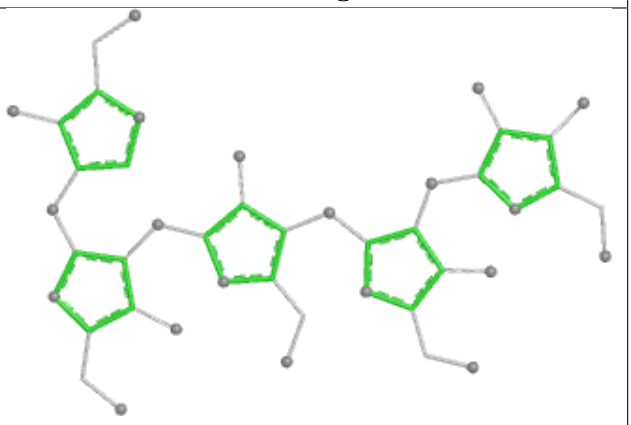
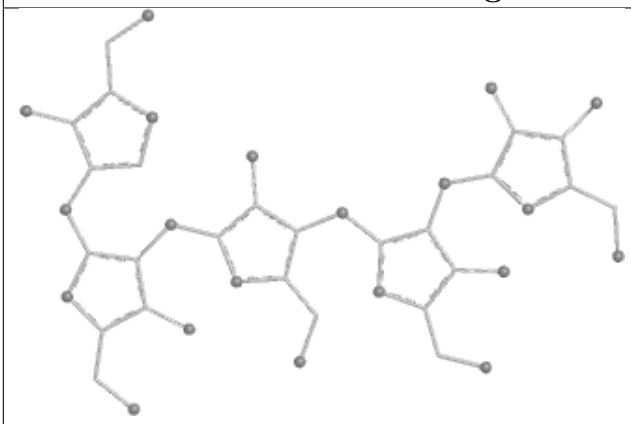
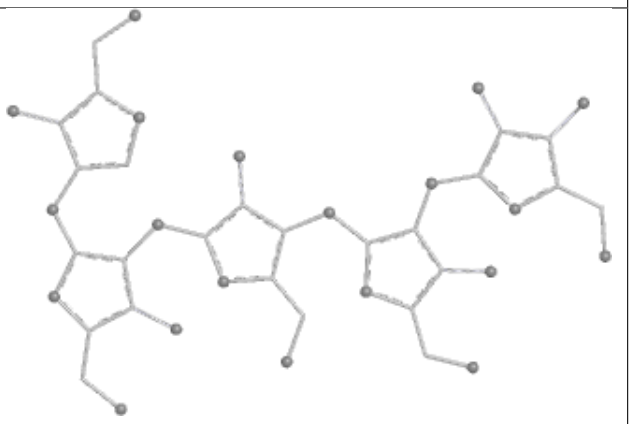
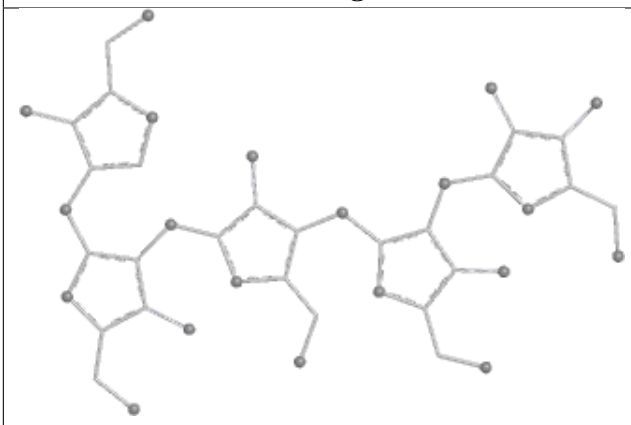
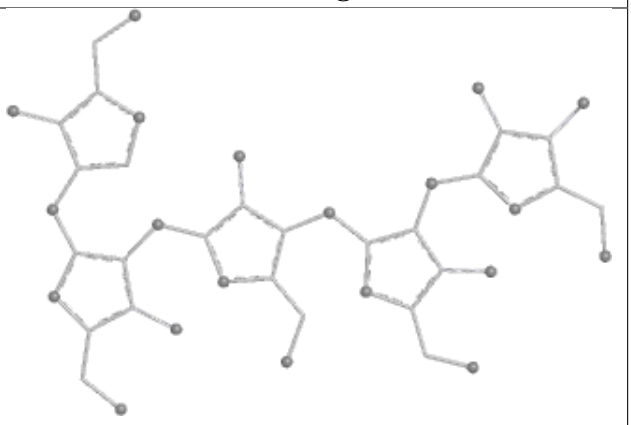
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain WD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain U	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain SA	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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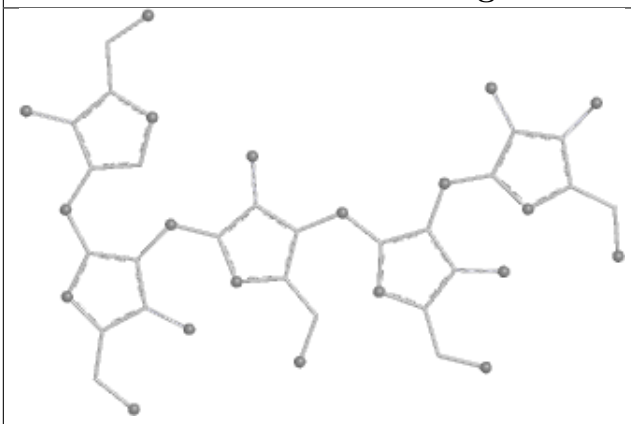
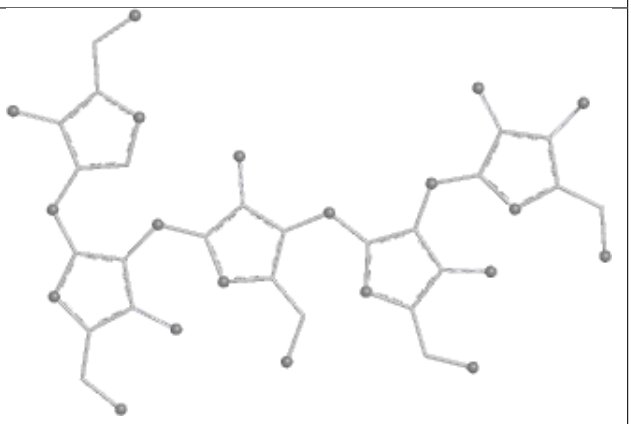
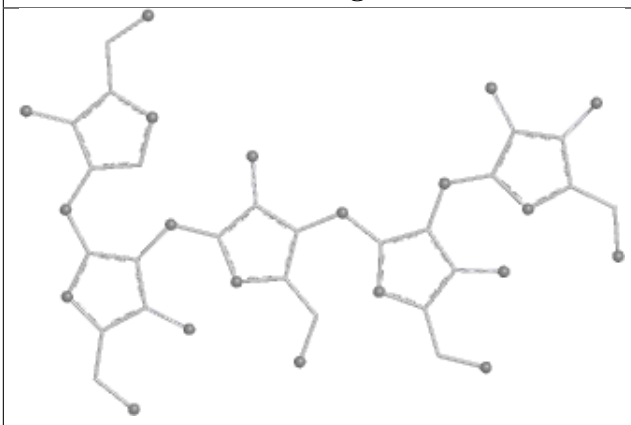
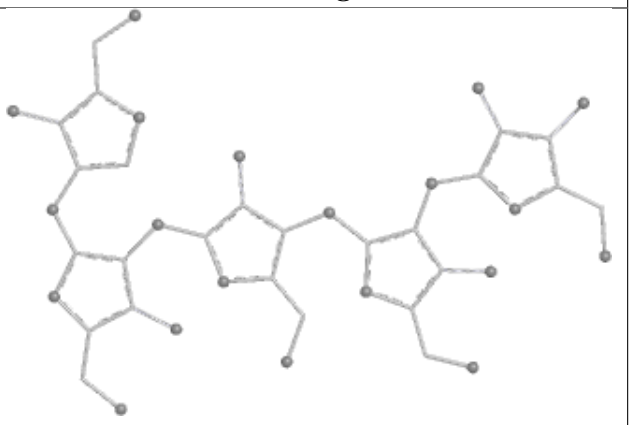
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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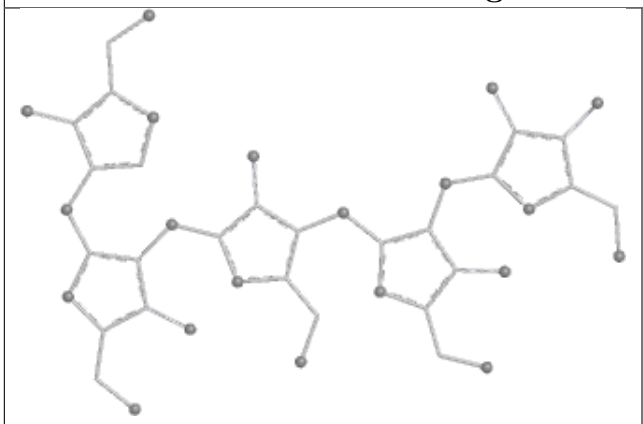
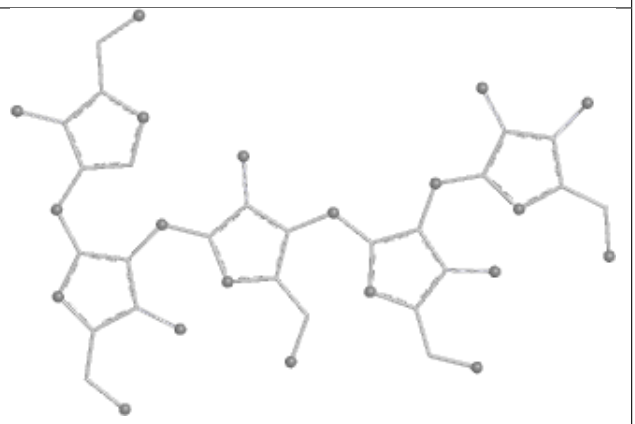
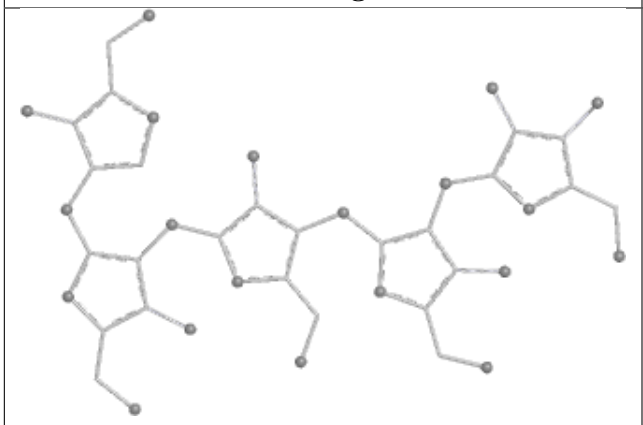


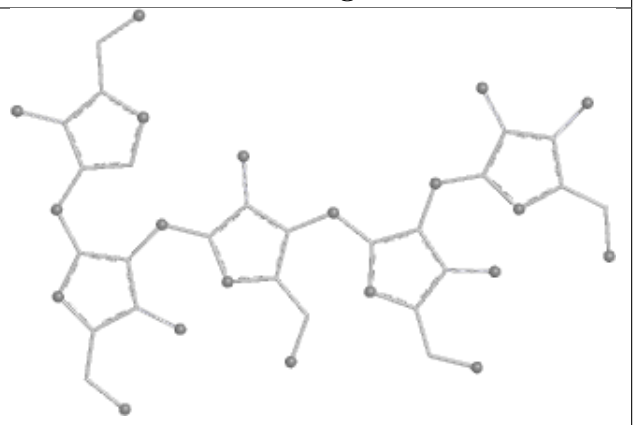
Bond lengths



Bond angles

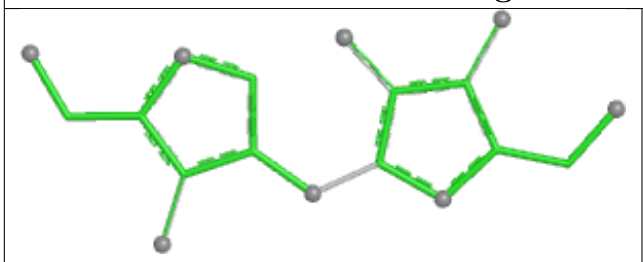


Torsions



Rings

Oligosaccharide Chain Y



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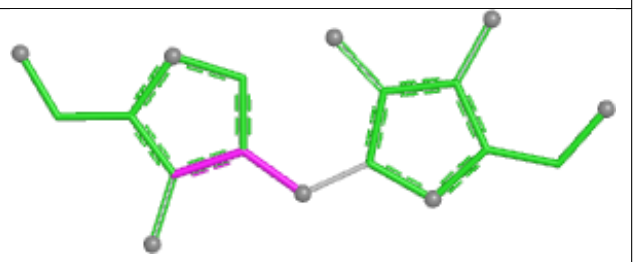

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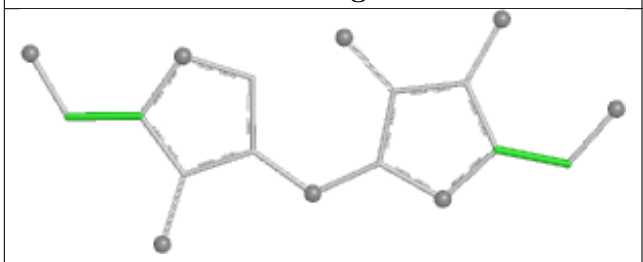
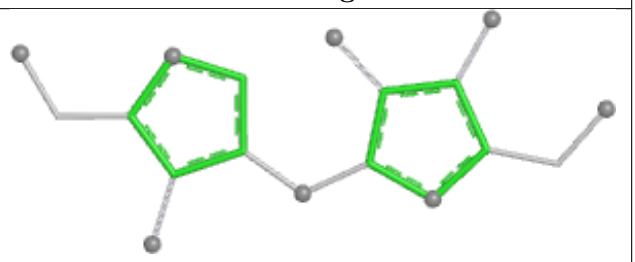
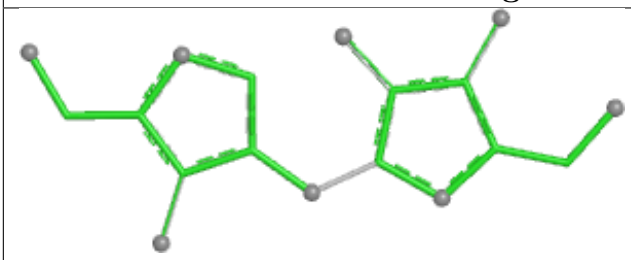
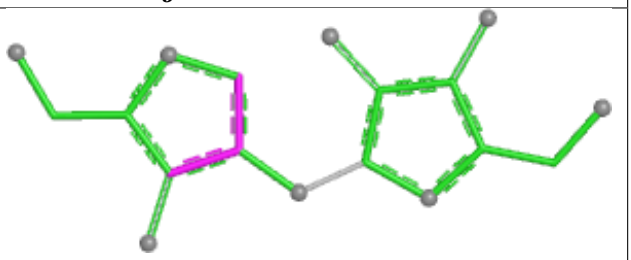
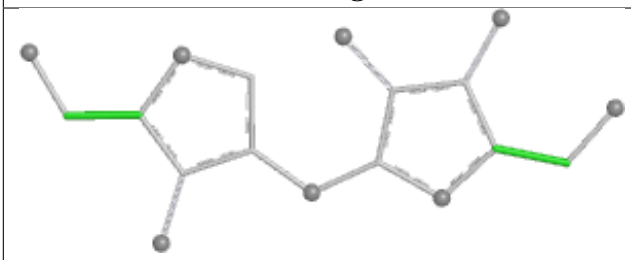
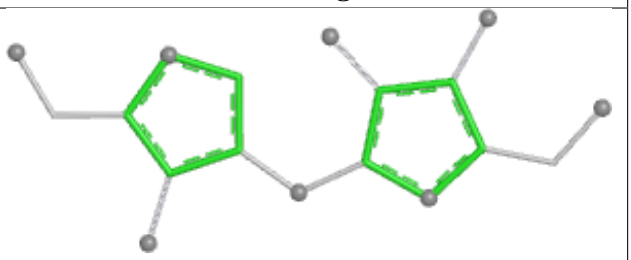


Torsions



Rings

Oligosaccharide Chain j	
 Bond lengths	 Bond angles
 Torsions	 Rings

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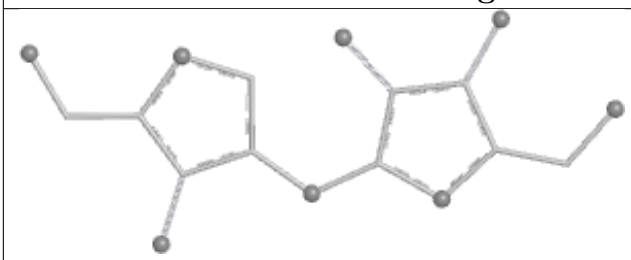
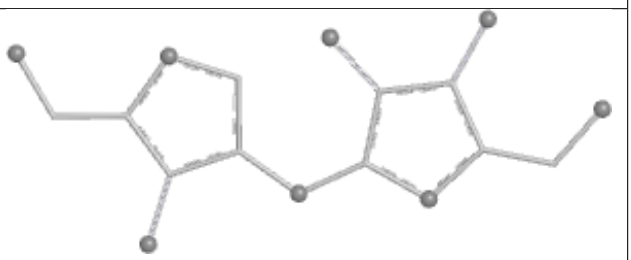
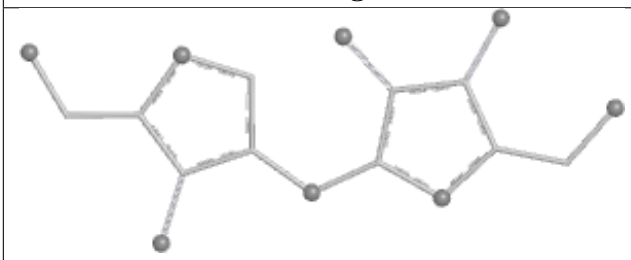
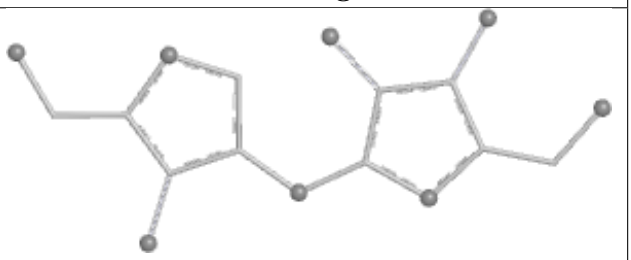
 Bond lengths	 Bond angles
 Torsions	 Rings

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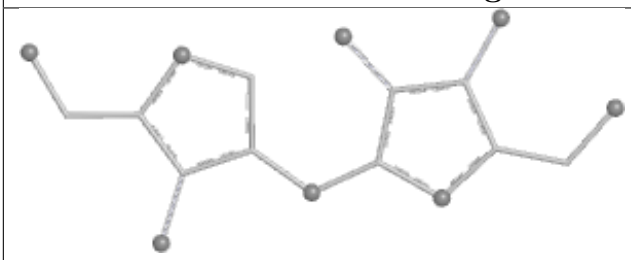
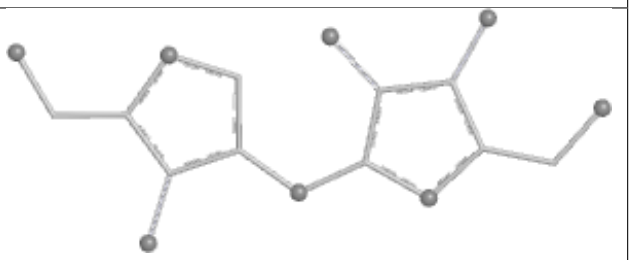
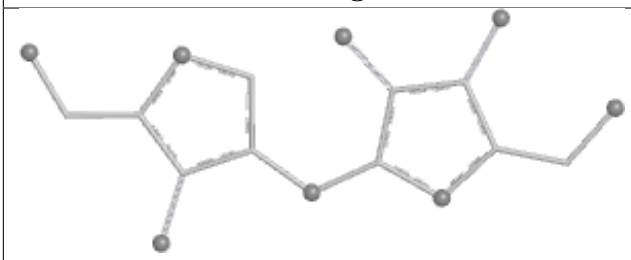
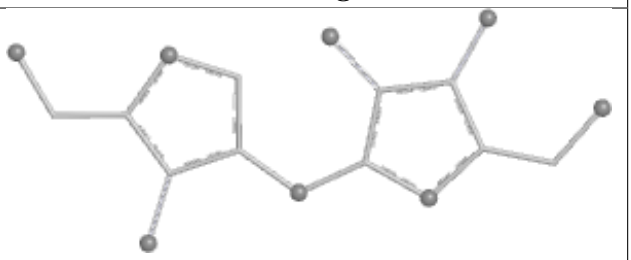
 Bond lengths	 Bond angles
 Torsions	 Rings

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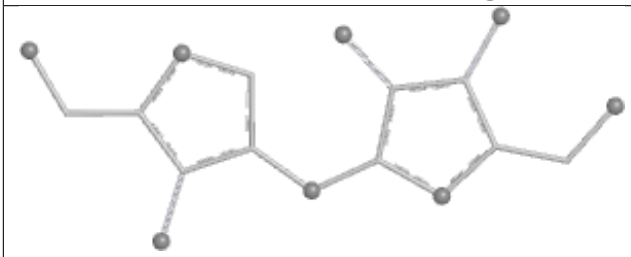
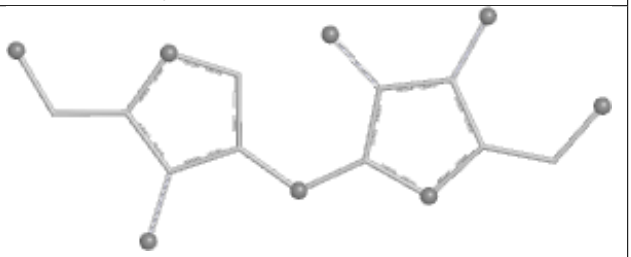
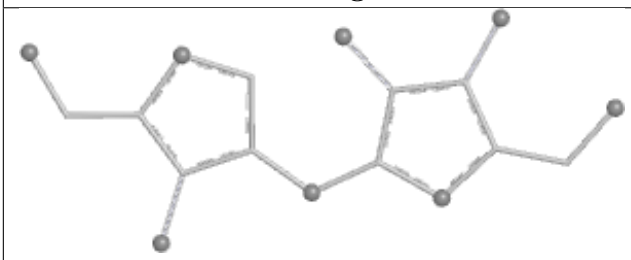
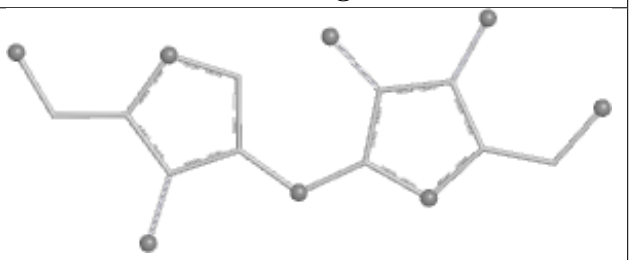
 Bond lengths	 Bond angles
 Torsions	 Rings

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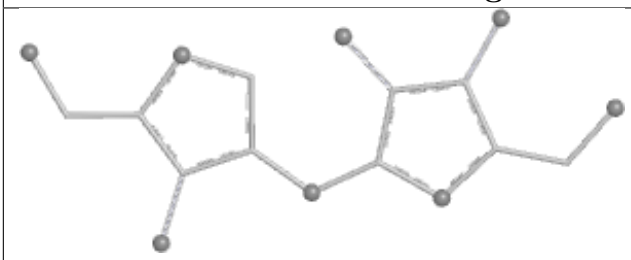
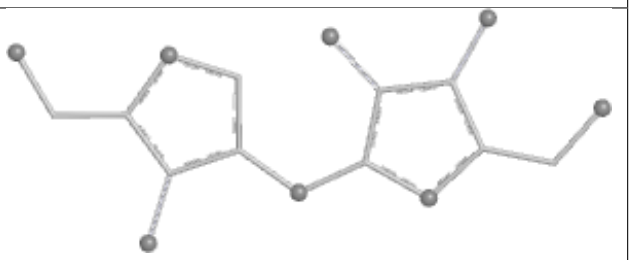
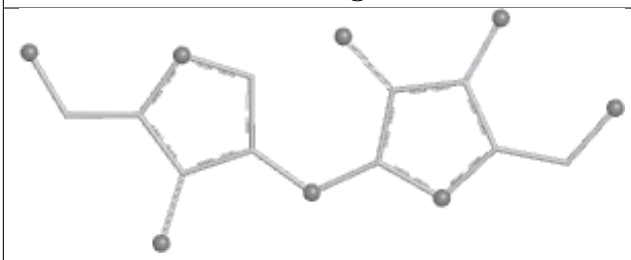
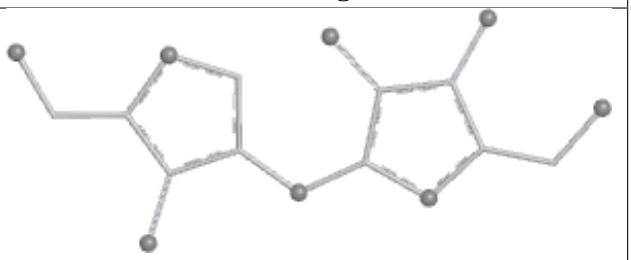
 Bond lengths	 Bond angles
 Torsions	 Rings

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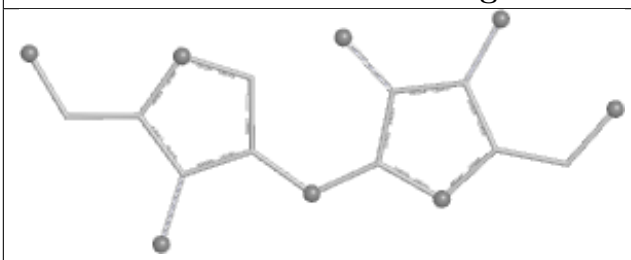
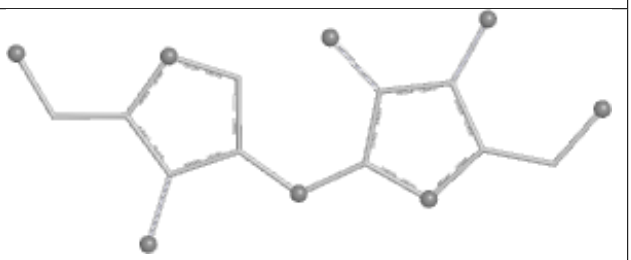
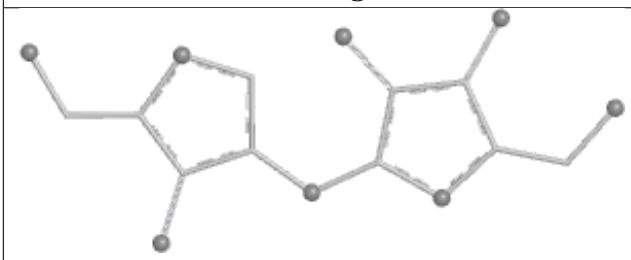
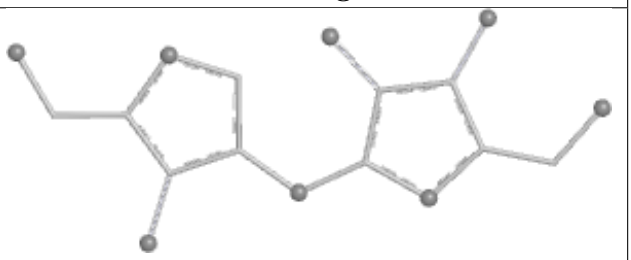
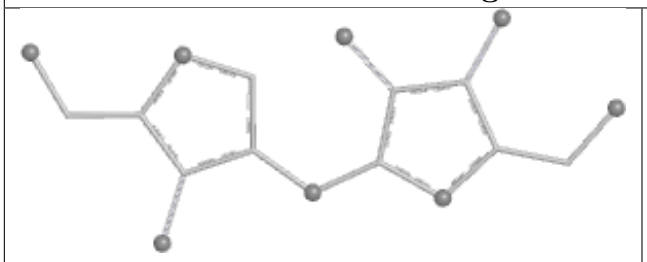
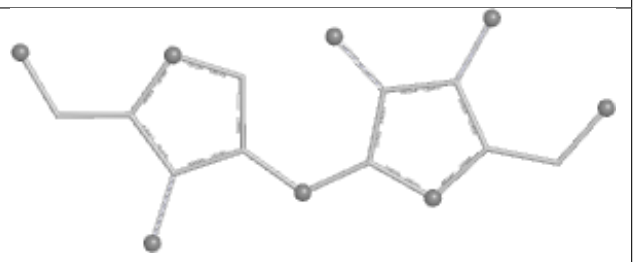
 Bond lengths	 Bond angles
 Torsions	 Rings

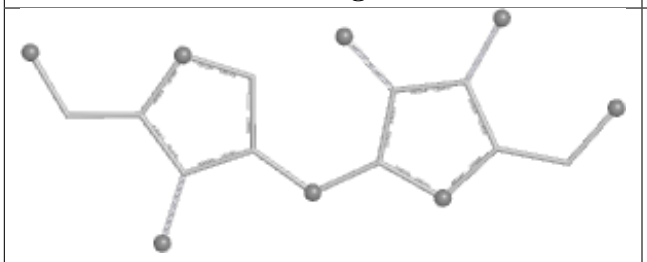
Oligosaccharide Chain YD



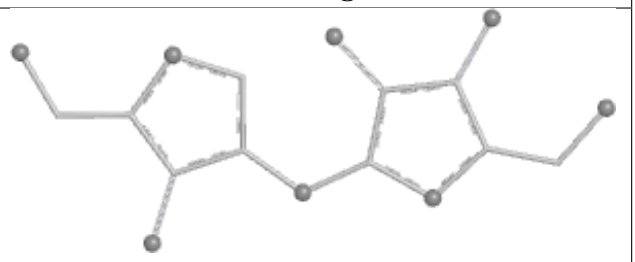
Bond lengths



Bond angles

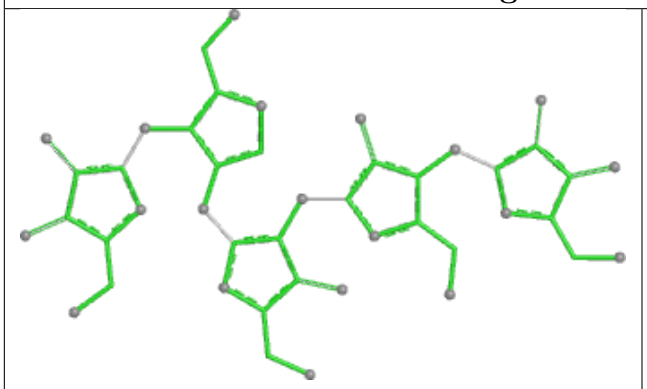


Torsions



Rings

Oligosaccharide Chain a



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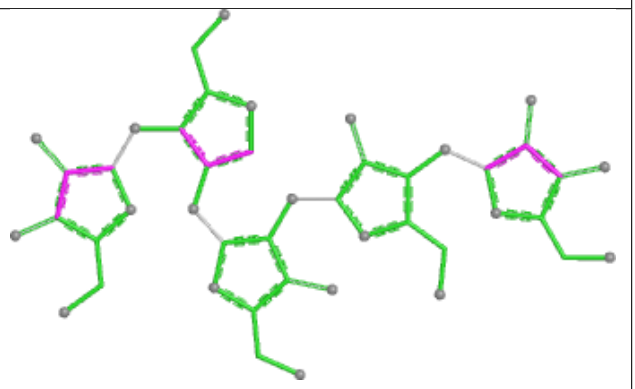
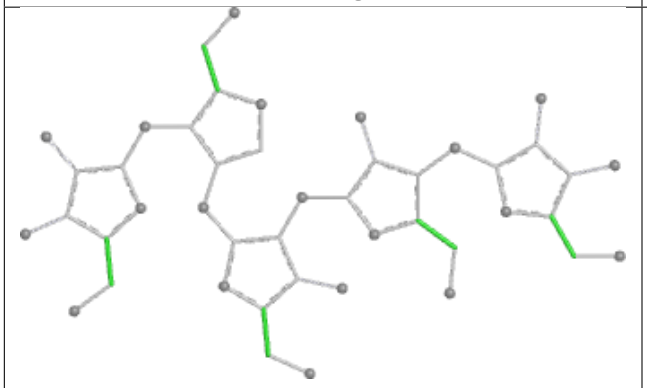


Bond angles



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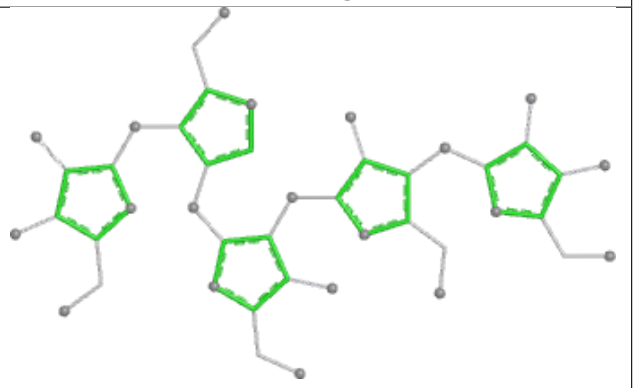
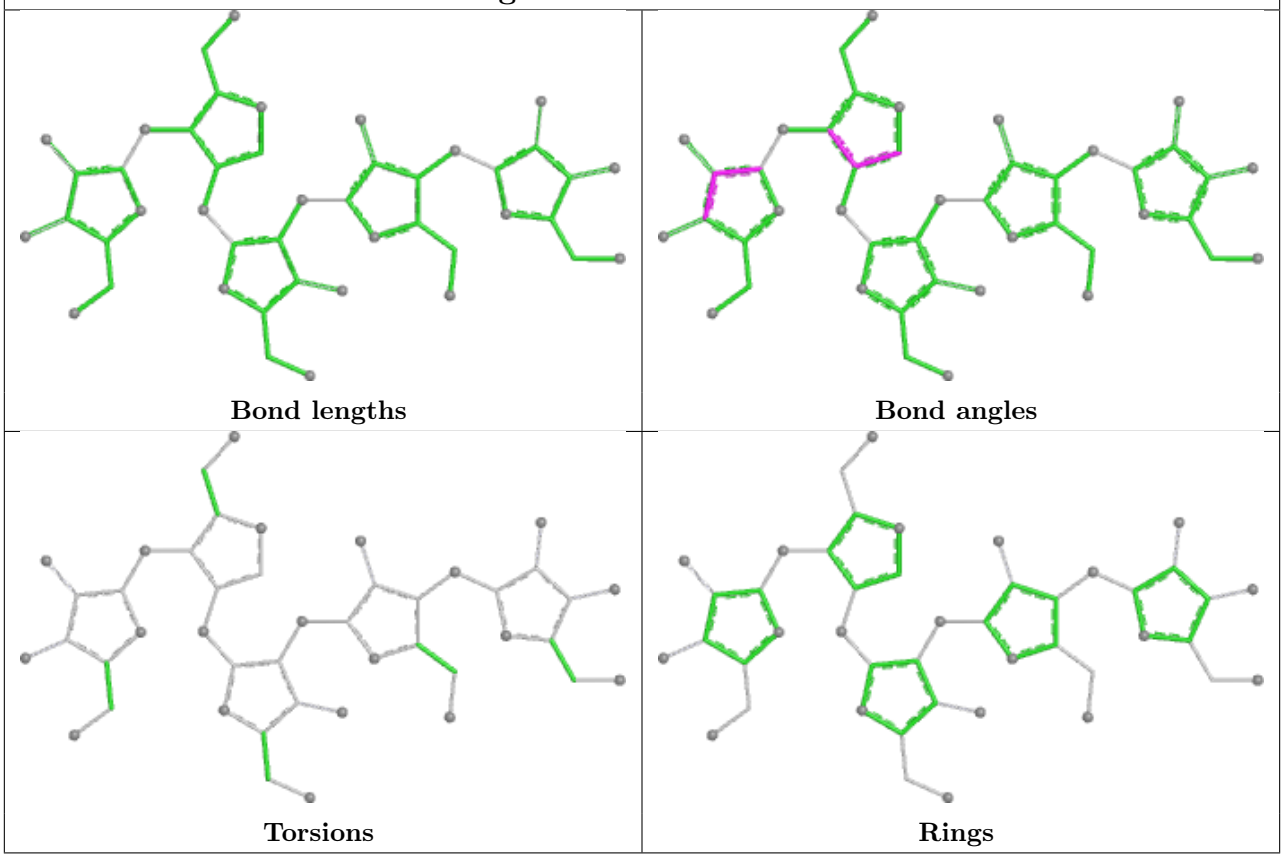
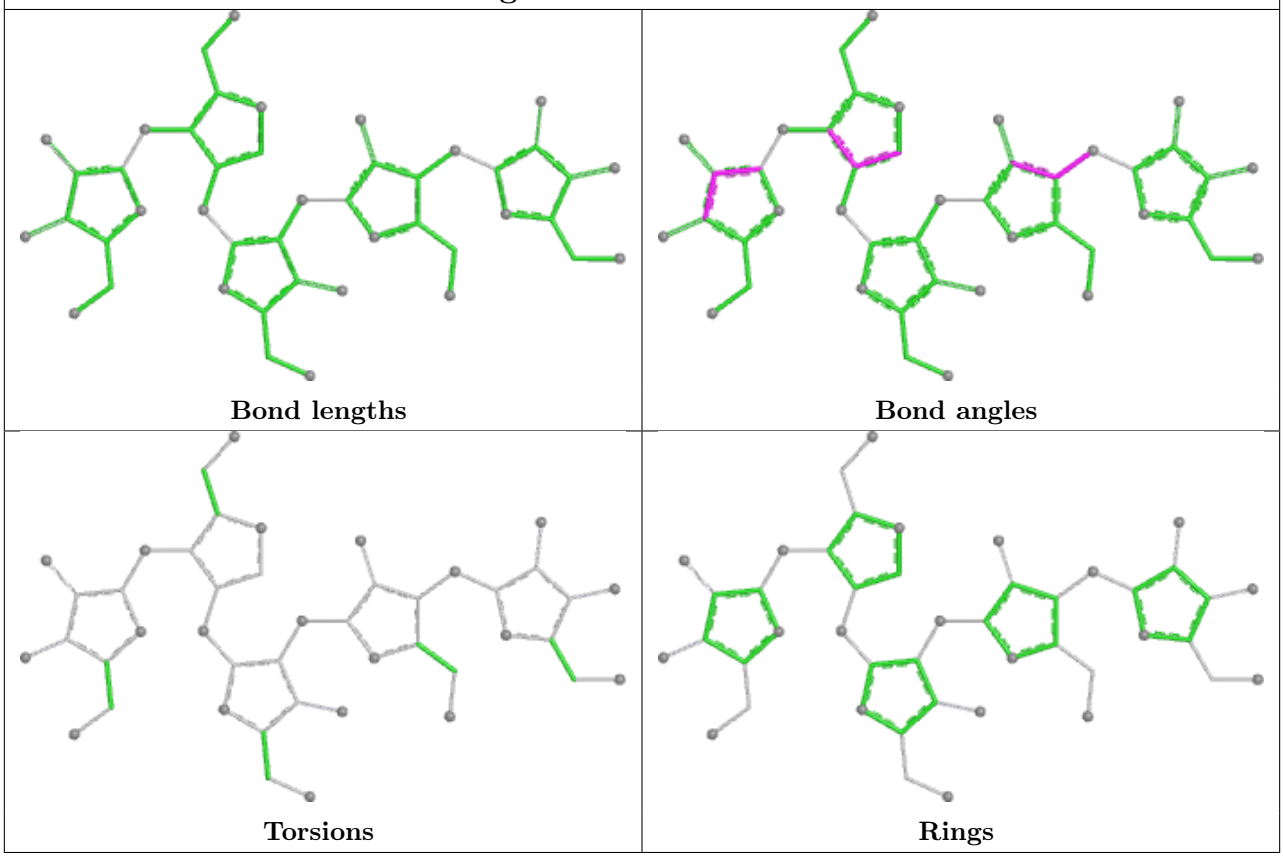


Rings

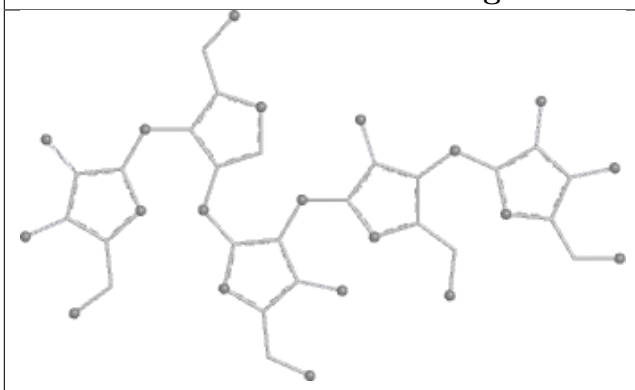
Oligosaccharide Chain u



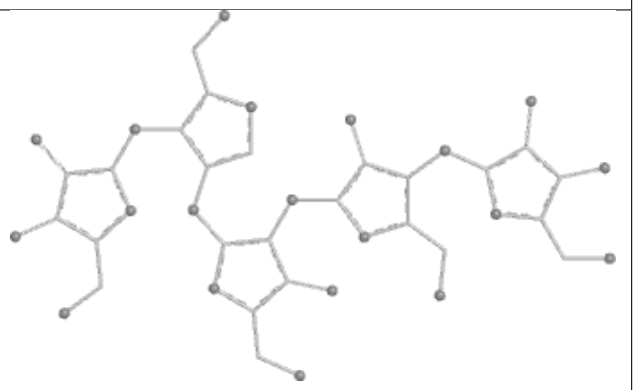
Oligosaccharide Chain 3



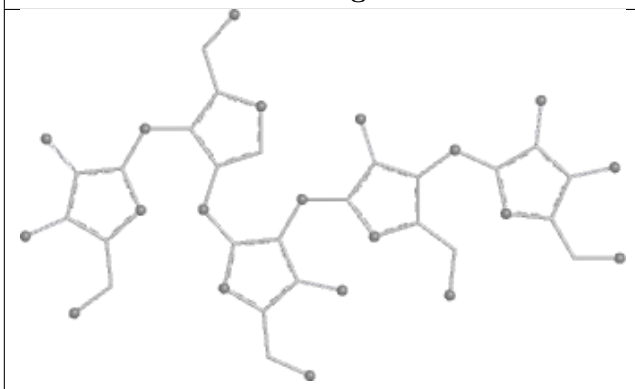
Oligosaccharide Chain YA



Bond lengths



Bond angles



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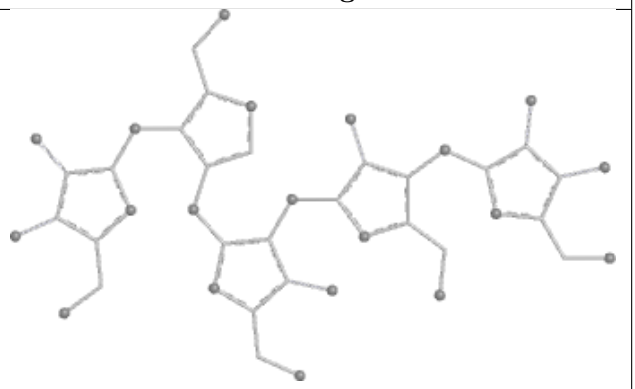
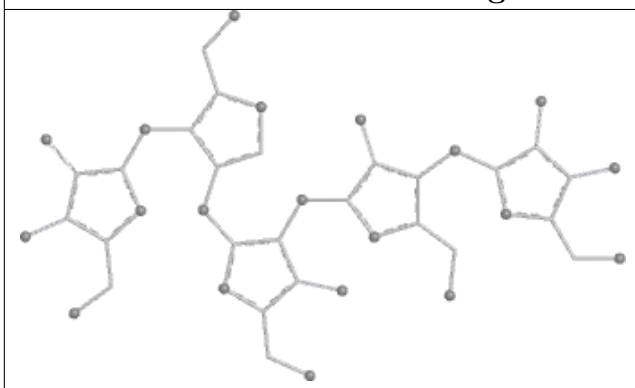
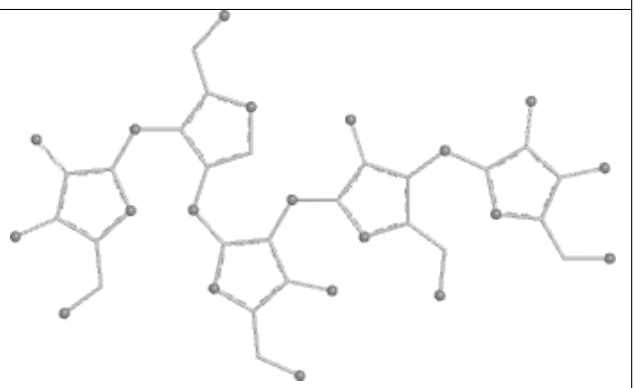


Rings

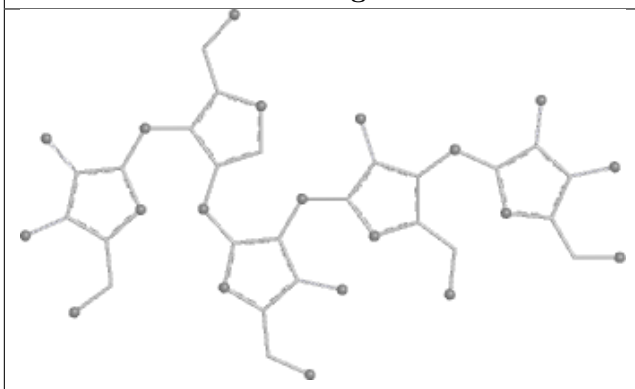
Oligosaccharide Chain sA



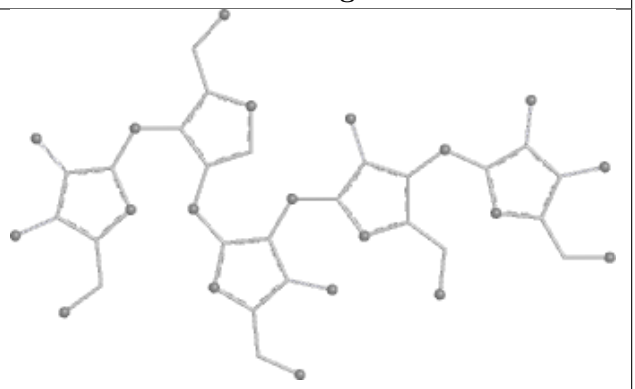
Bond lengths



Bond angles

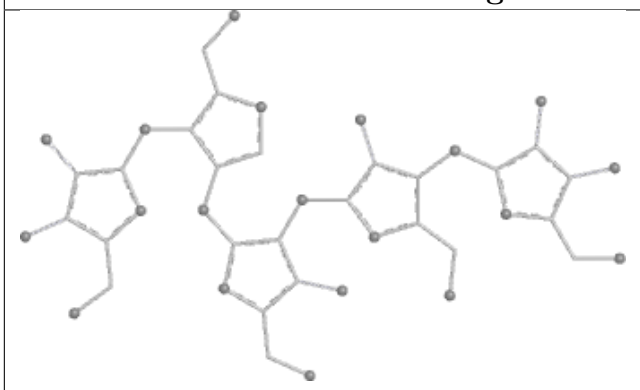


Torsions



Rings

Oligosaccharide Chain 1A



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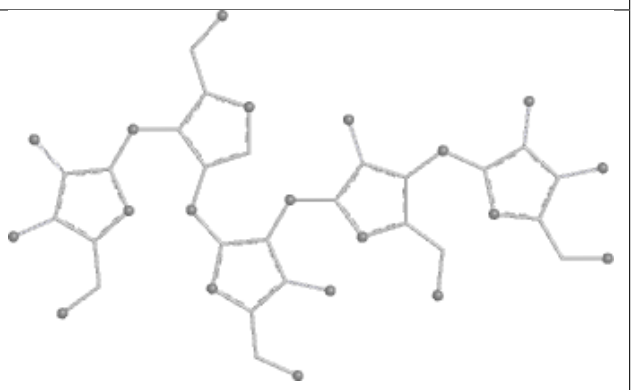

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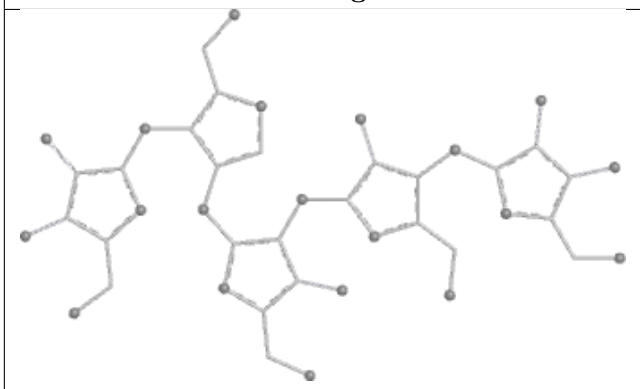

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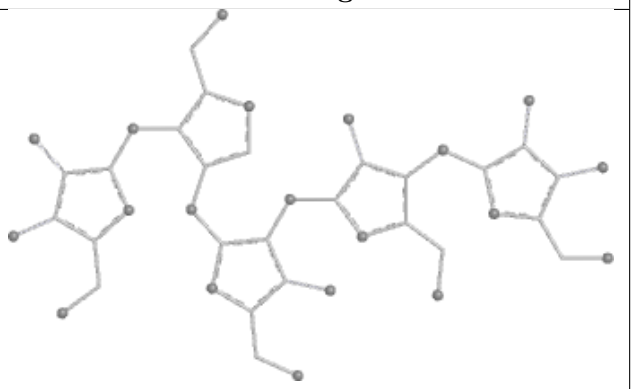
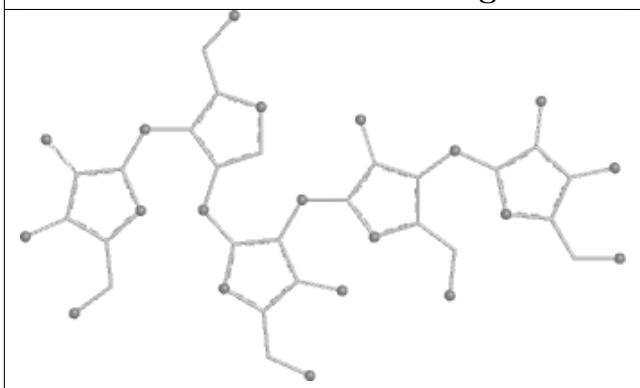


Rings

Oligosaccharide Chain MB



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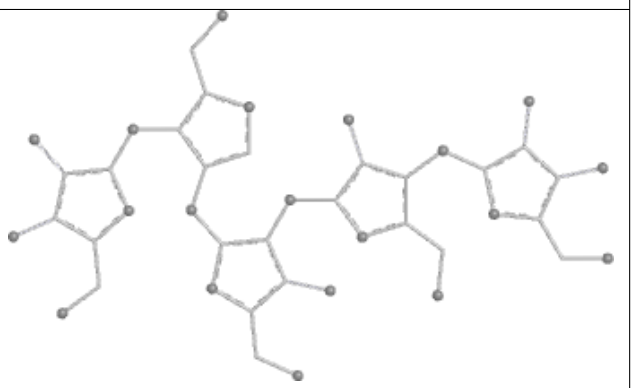

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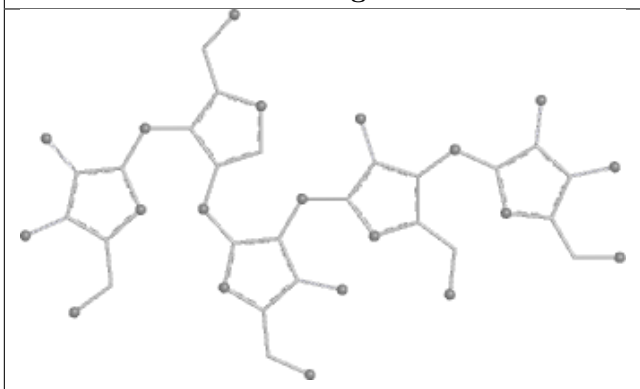

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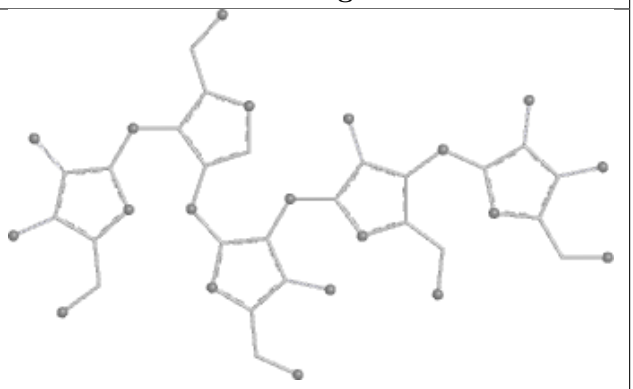
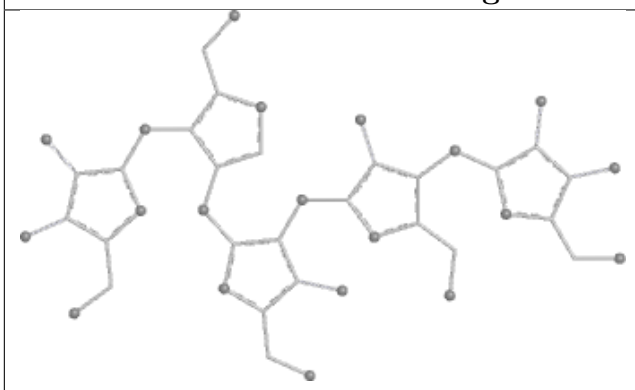


Rings

Oligosaccharide Chain VB



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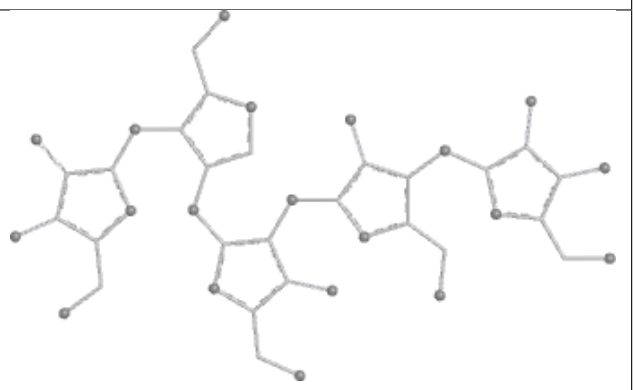

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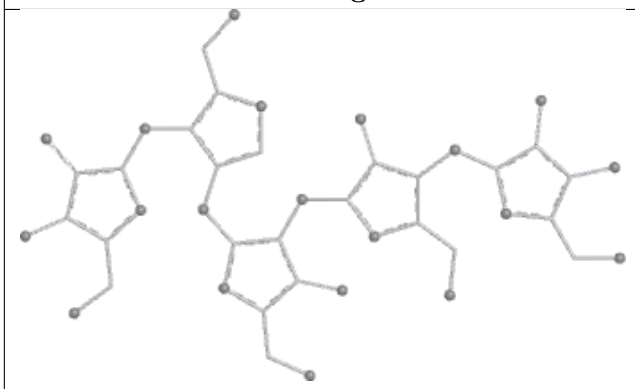

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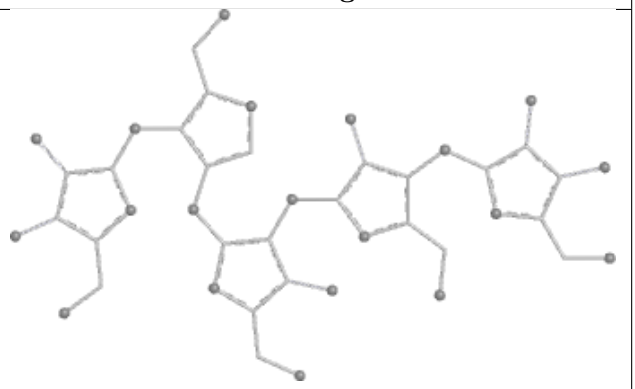
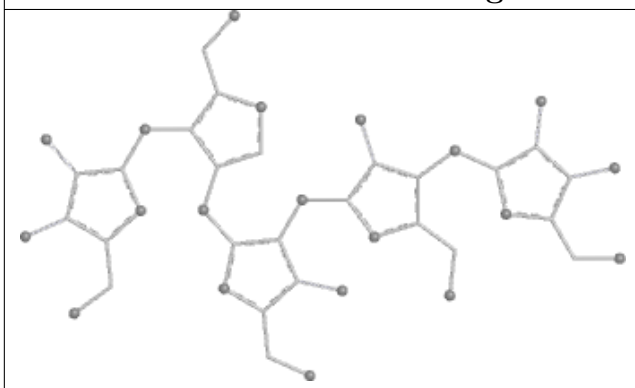


Rings

Oligosaccharide Chain pB



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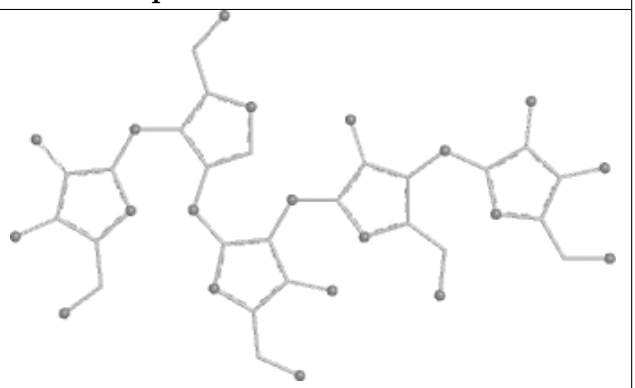

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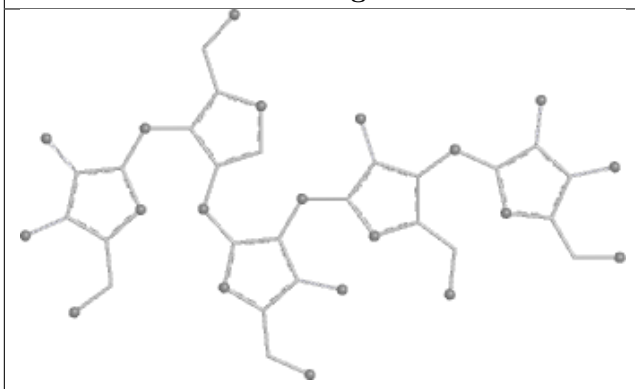

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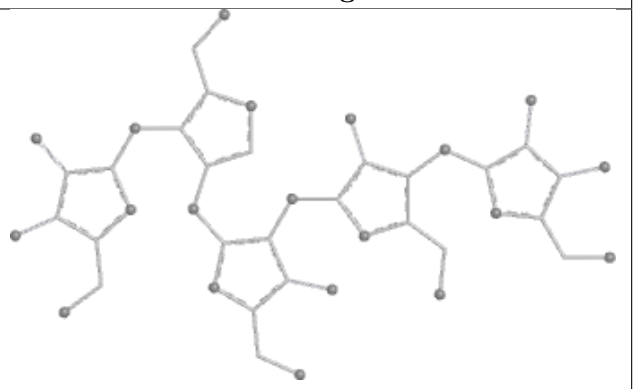
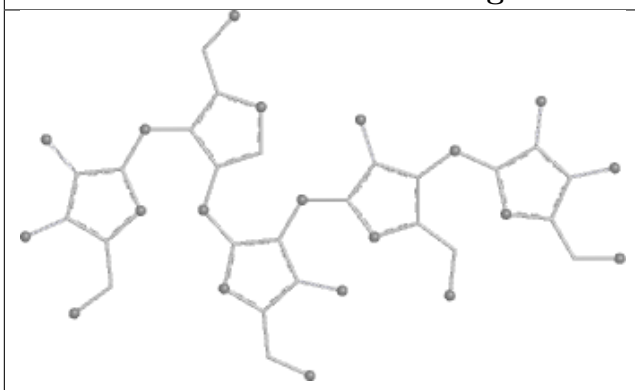


Rings

Oligosaccharide Chain yB



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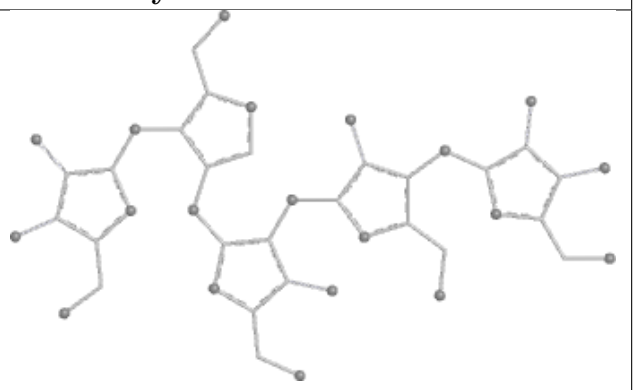

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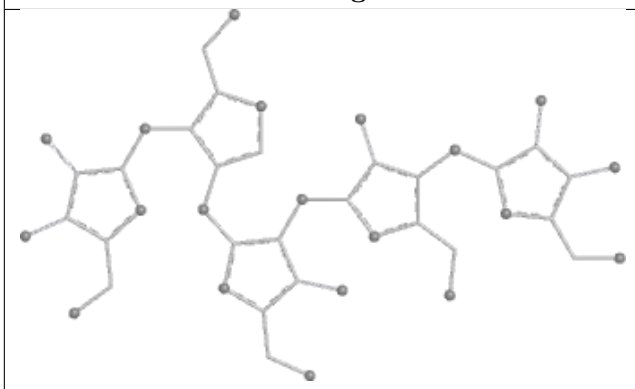

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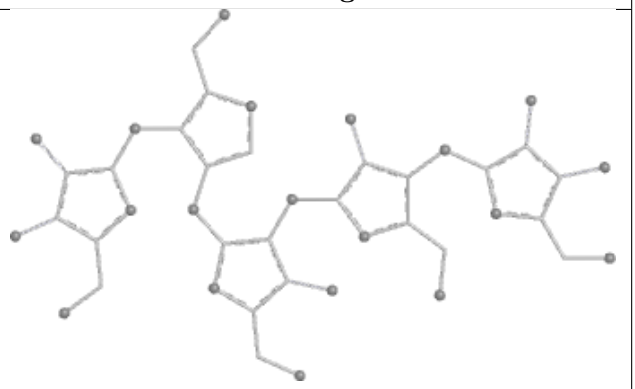
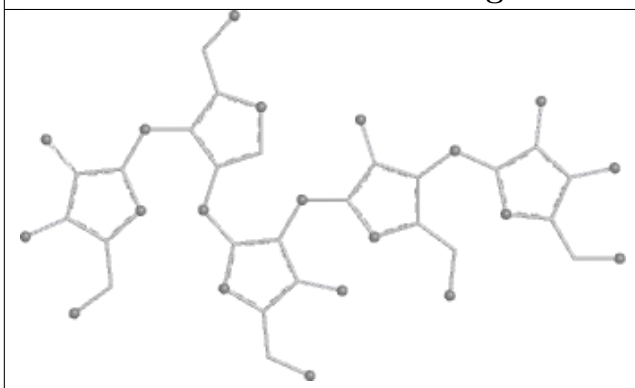


Rings

Oligosaccharide Chain SC



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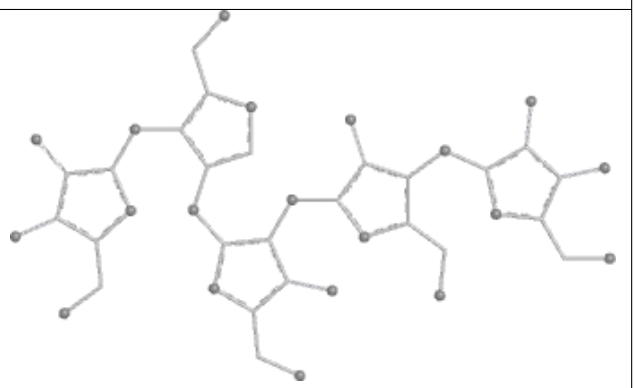
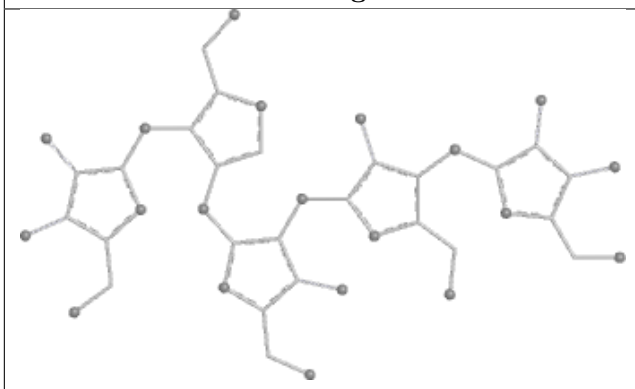


Bond angles



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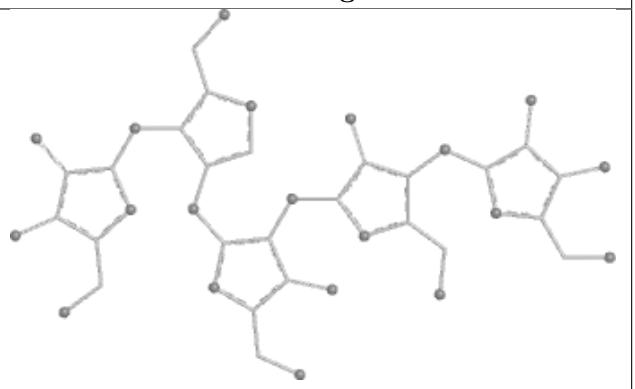
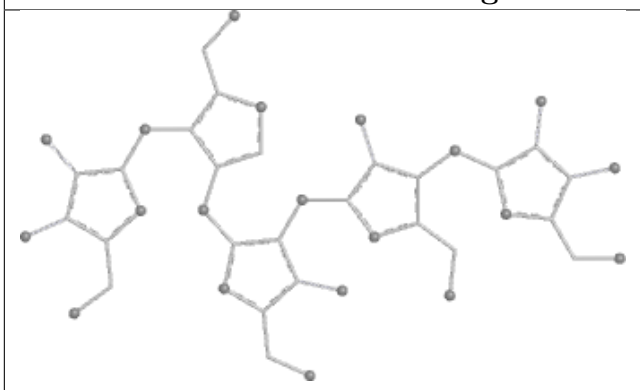
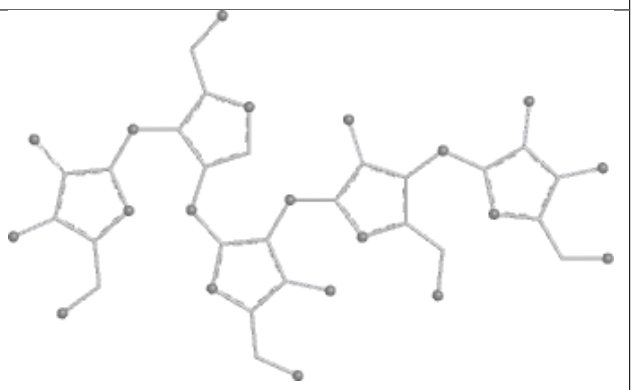
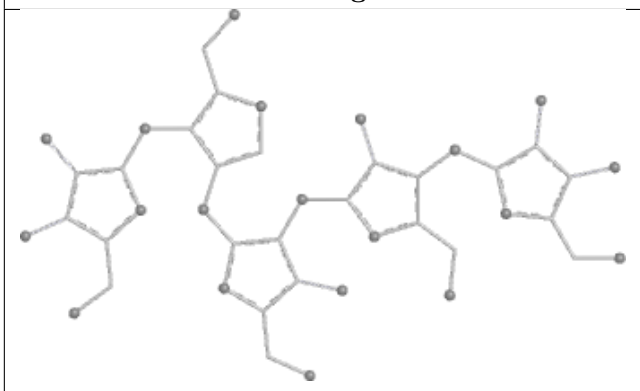
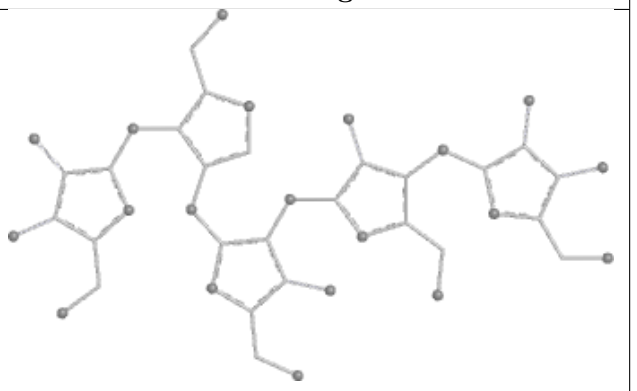
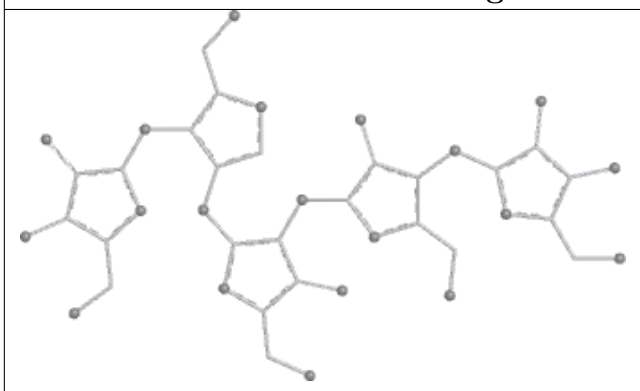
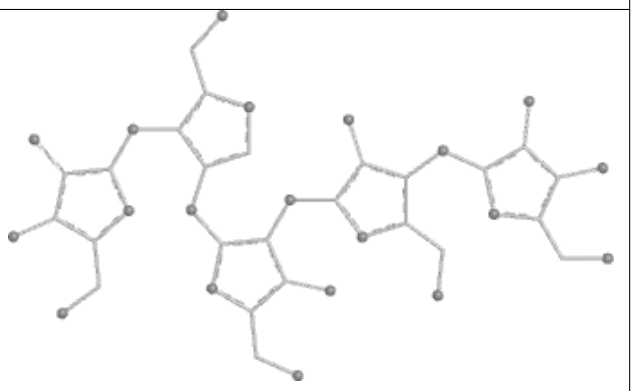
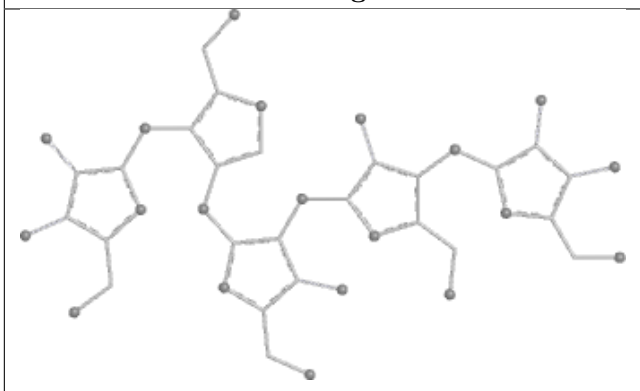
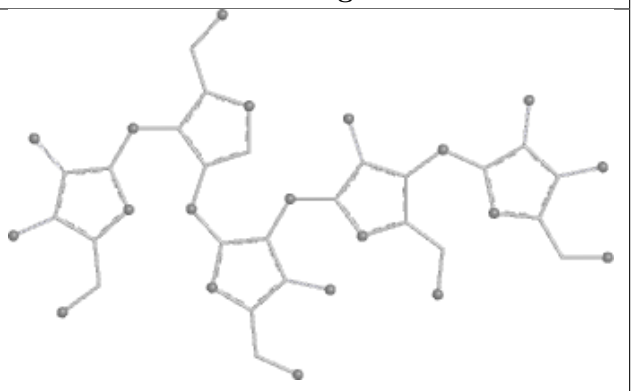
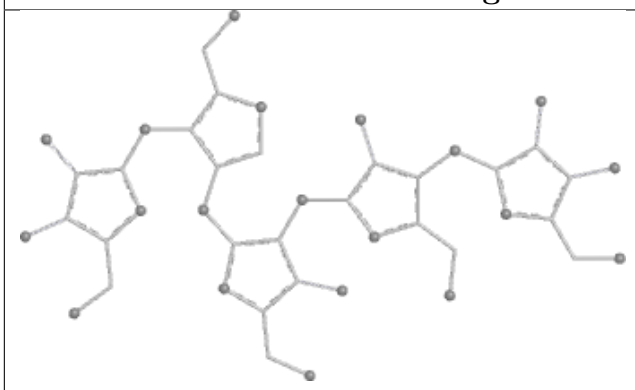


Rings

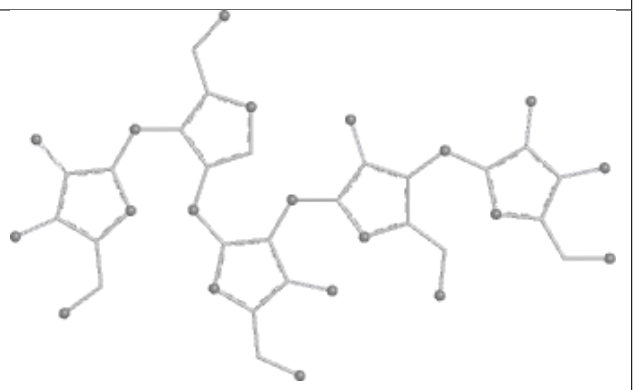
Oligosaccharide Chain mC	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain vC	
 Bond lengths	 Bond angles
 Torsions	 Rings

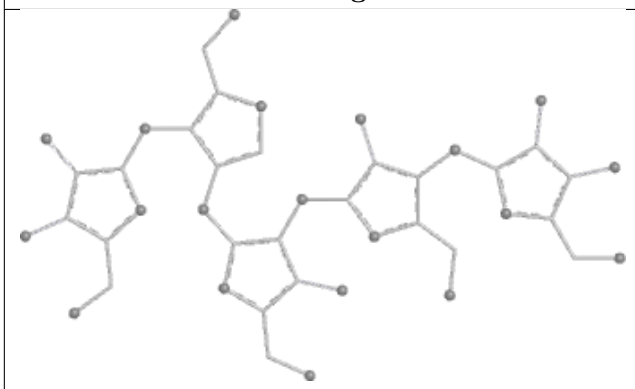
Oligosaccharide Chain PD



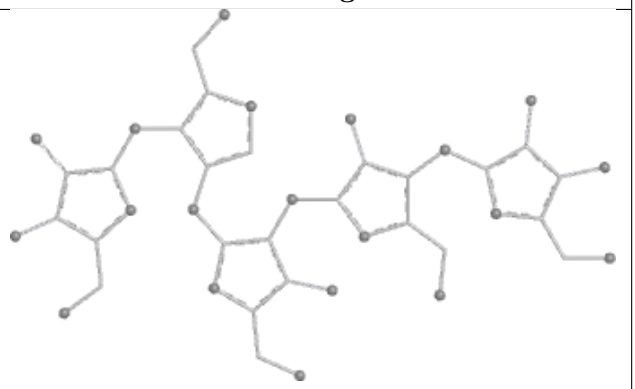
Bond lengths



Bond angles

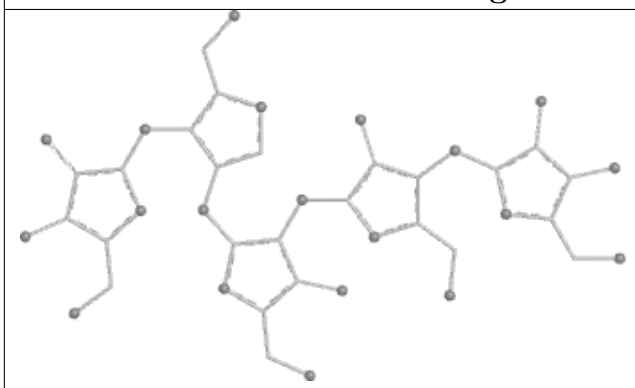


Torsions



Rings

Oligosaccharide Chain jD



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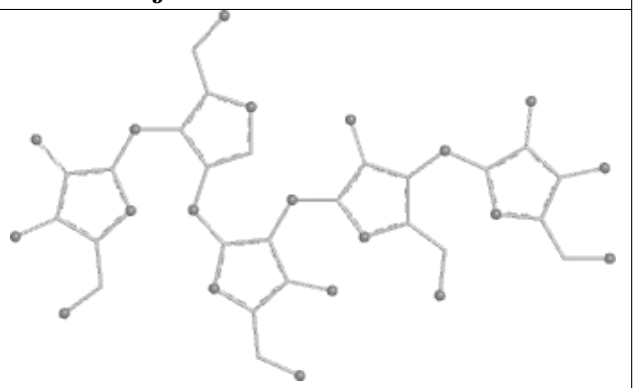
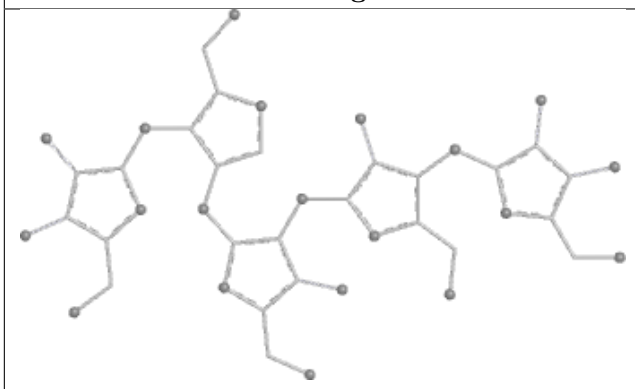
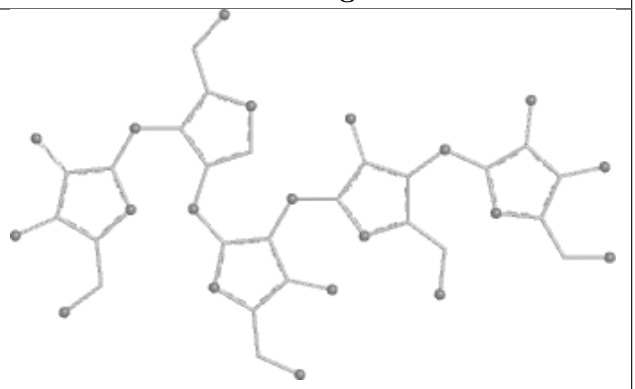


Bond angles

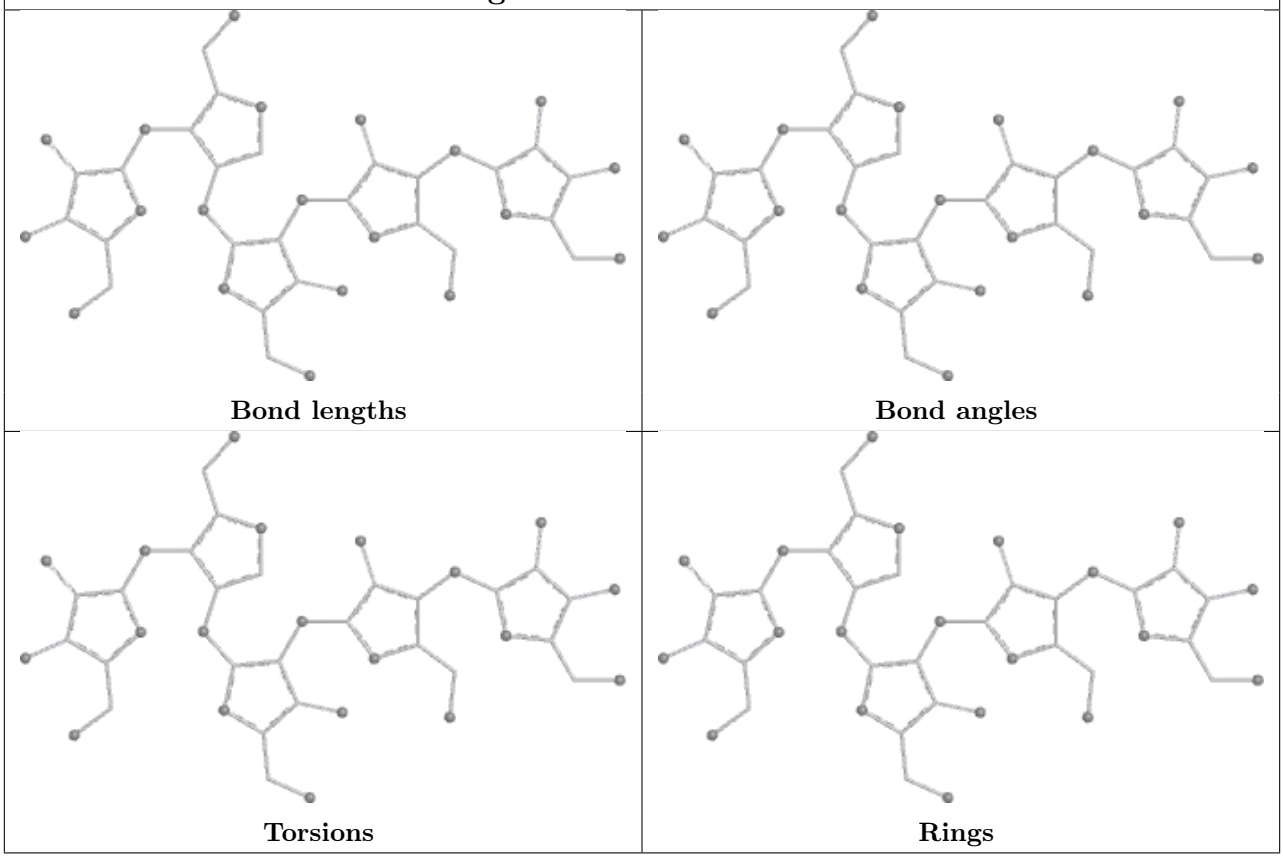


Torsions

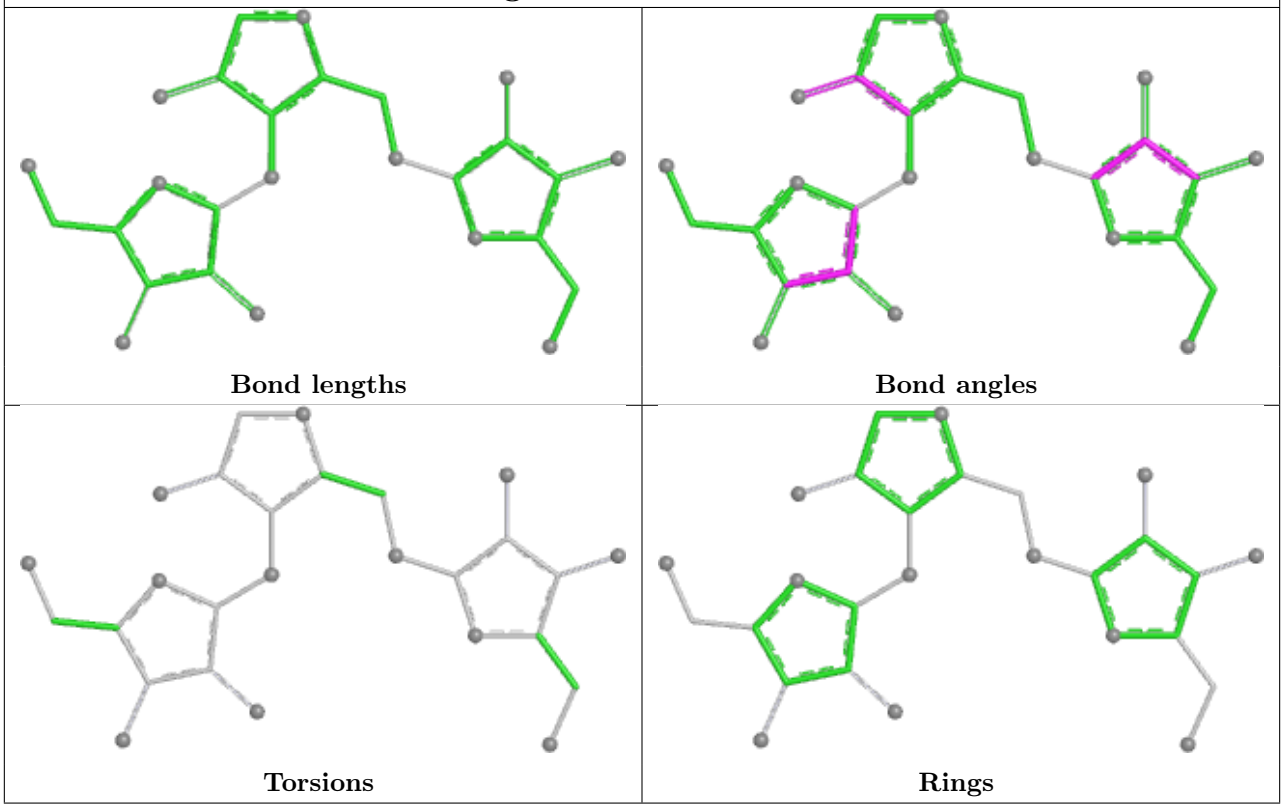


Rings

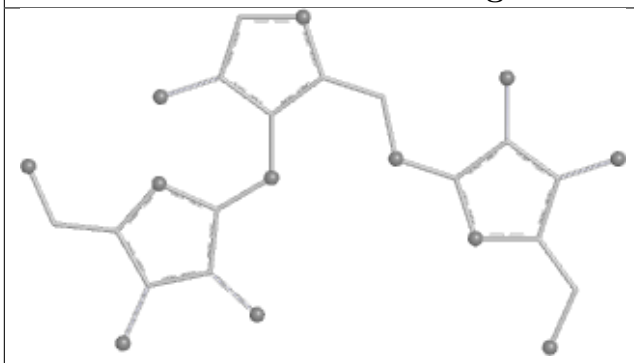
Oligosaccharide Chain sD



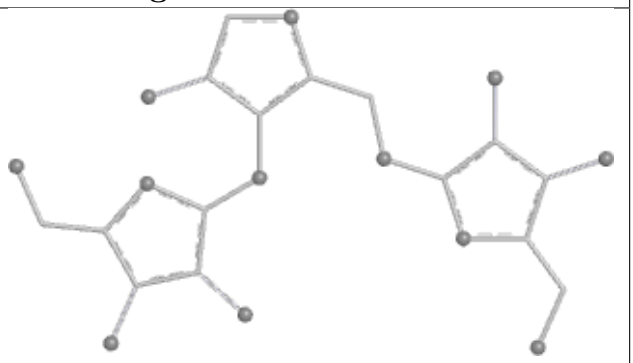
Oligosaccharide Chain i



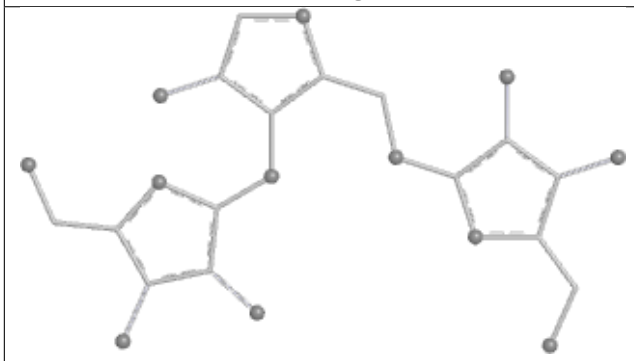
Oligosaccharide Chain gA



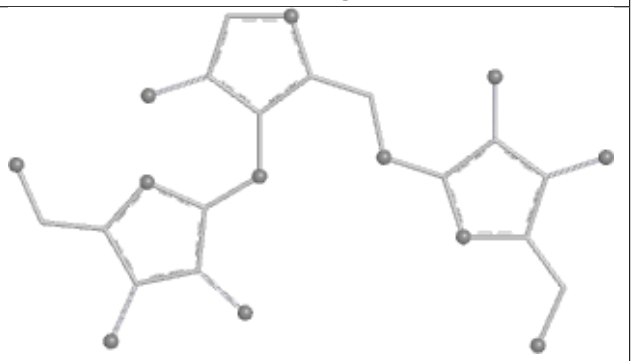
Bond lengths



Bond angles

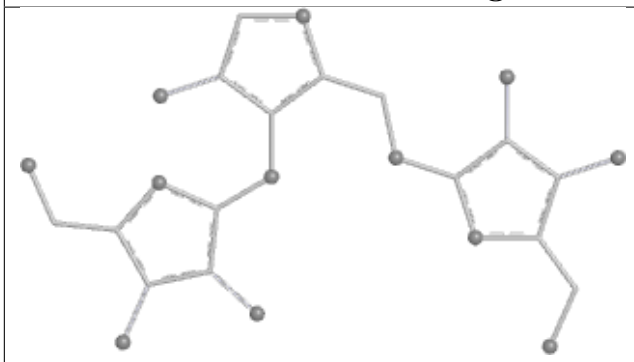


Torsions

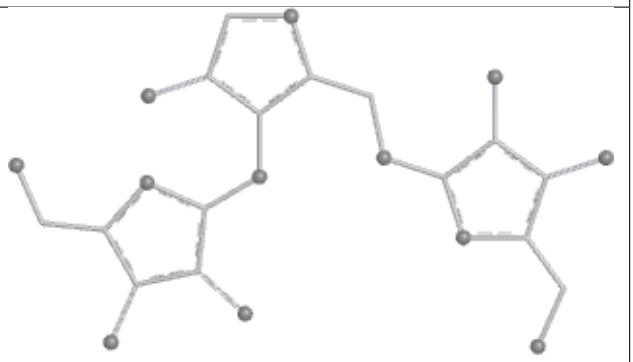


Rings

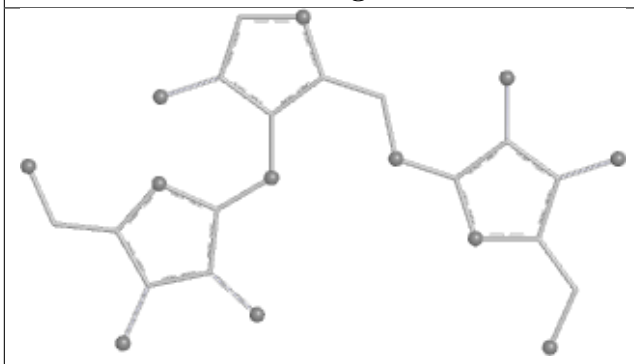
Oligosaccharide Chain aC



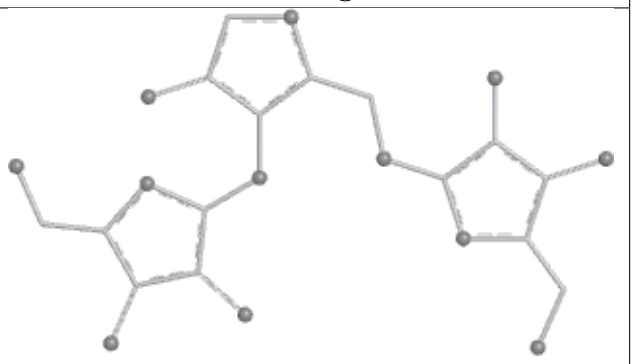
Bond lengths



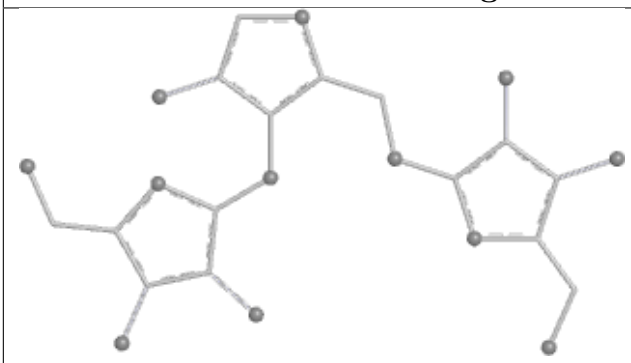
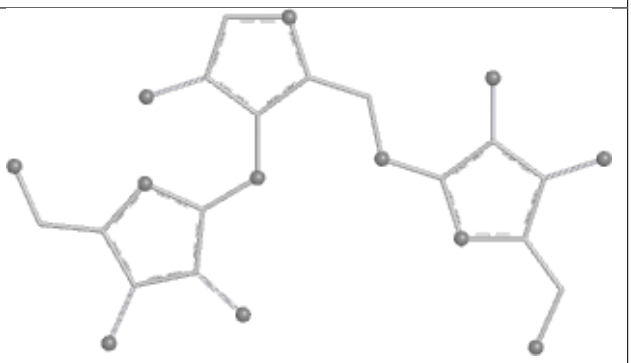
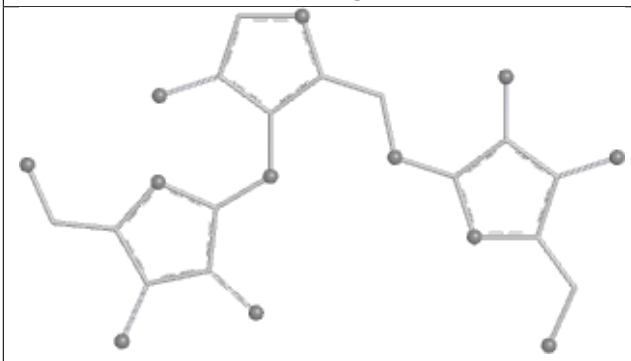
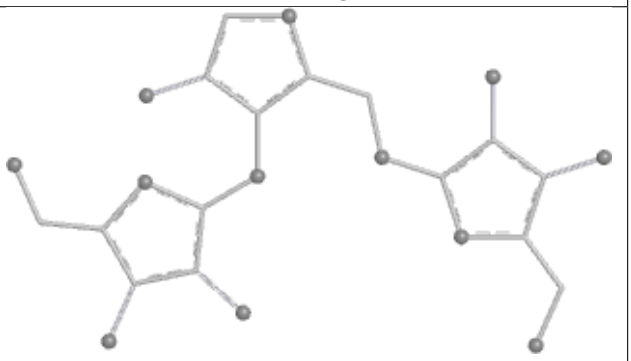
Bond angles

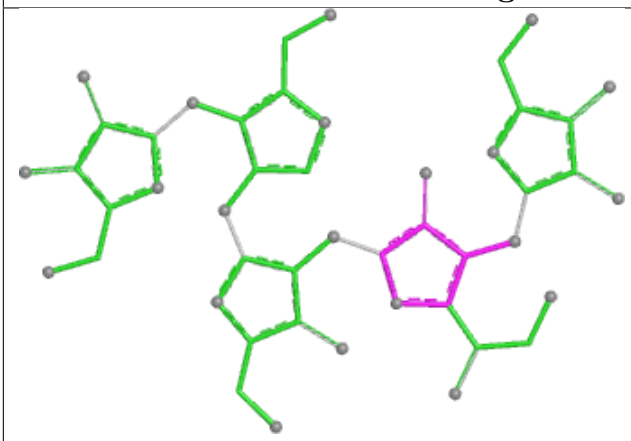
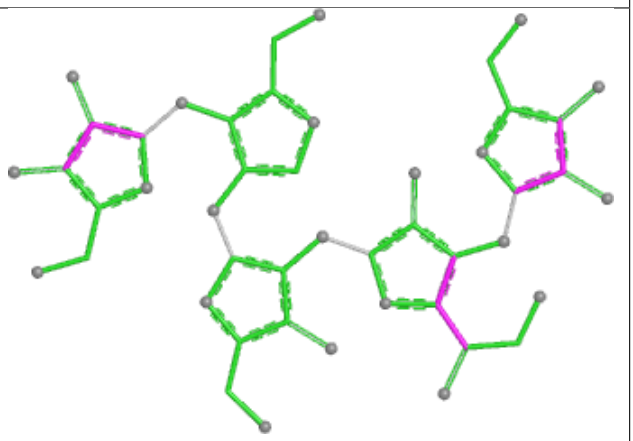


Torsions



Rings

Oligosaccharide Chain XD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain n	
	
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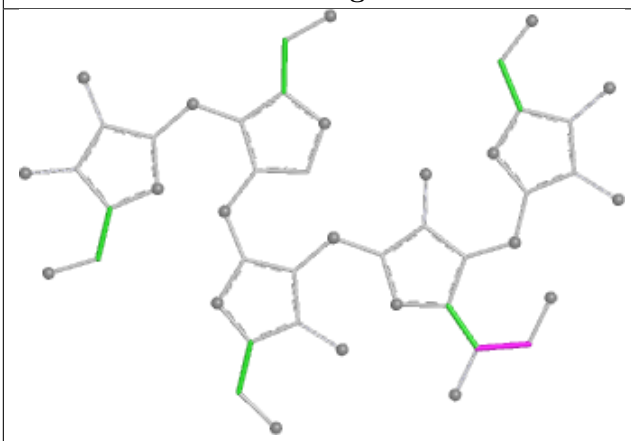	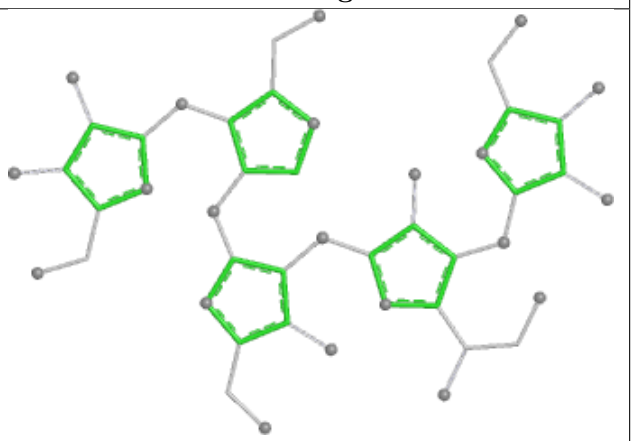
Torsions	**Rings**

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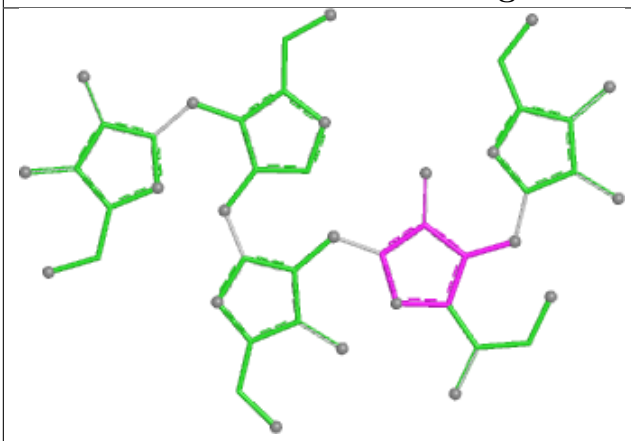	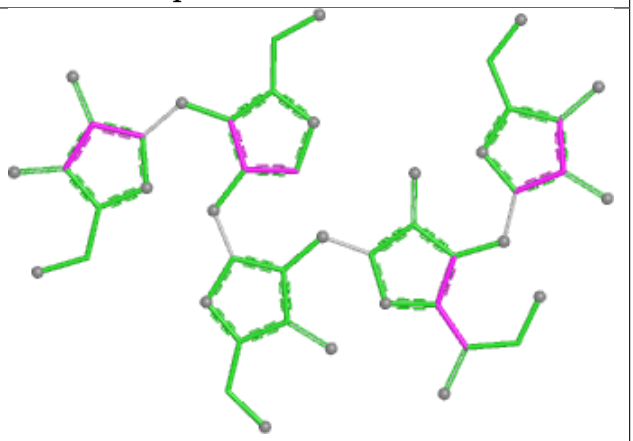
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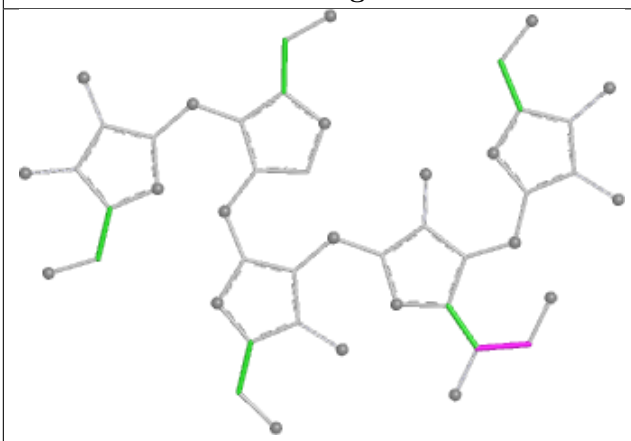	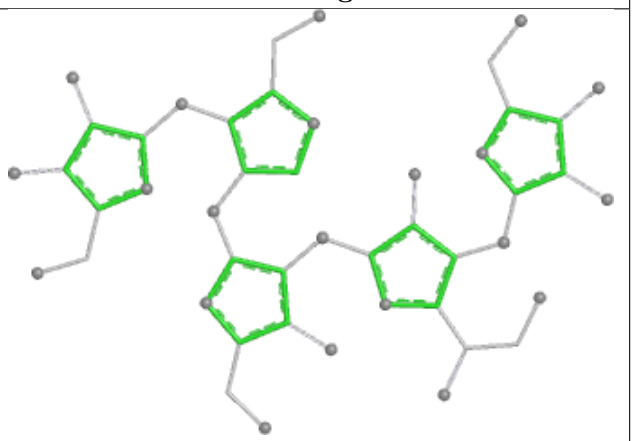
Torsions	**Rings**

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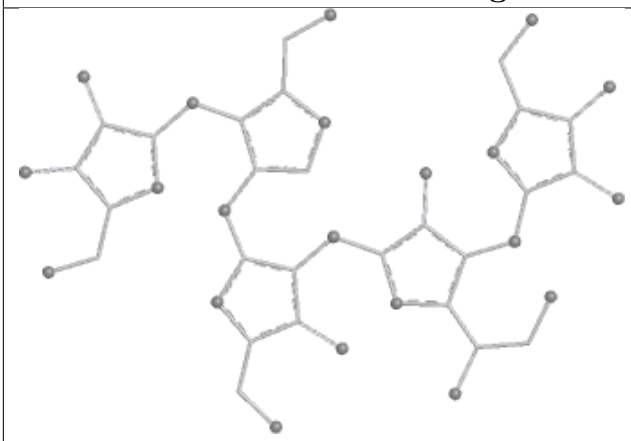
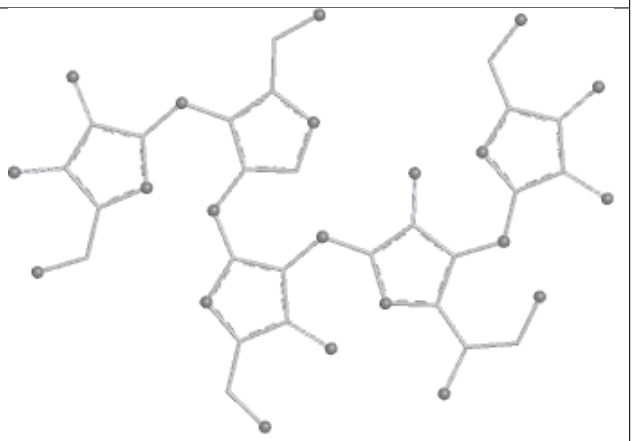
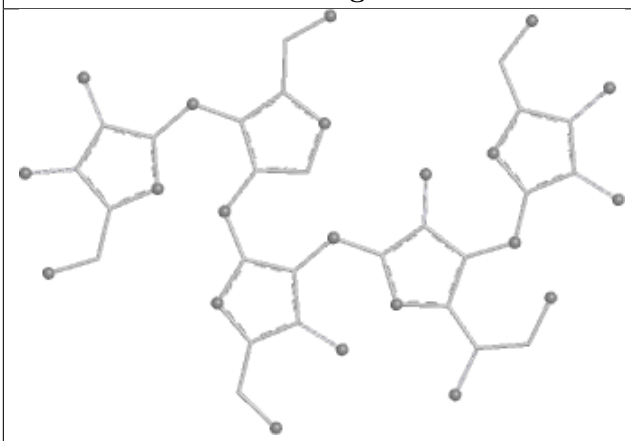
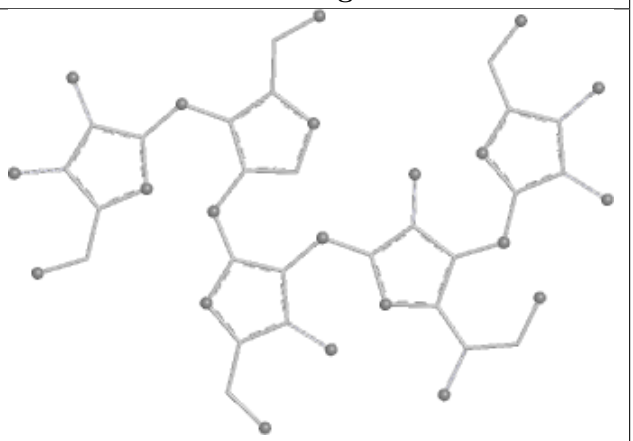
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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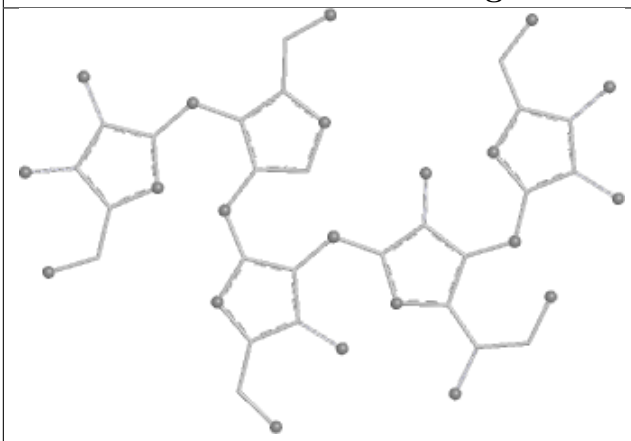
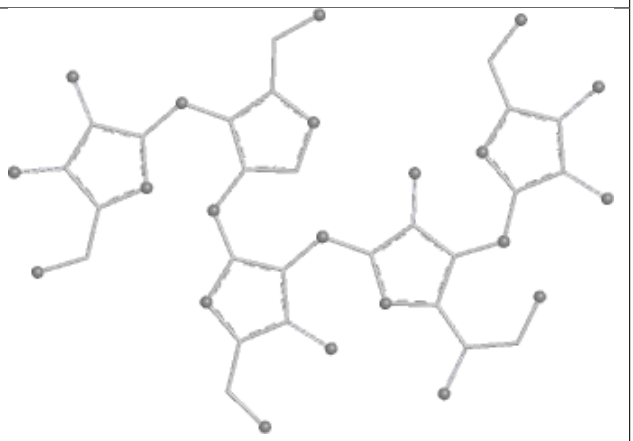
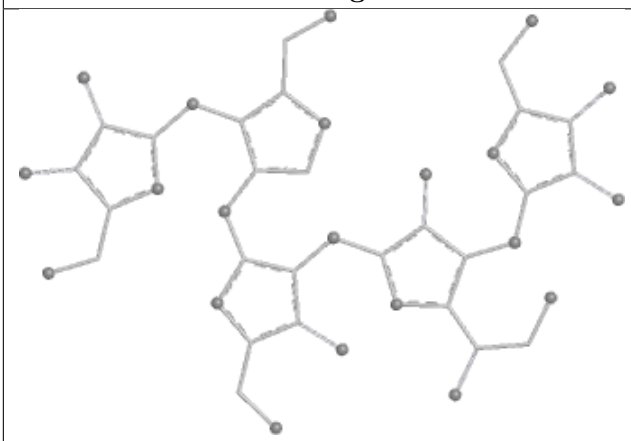
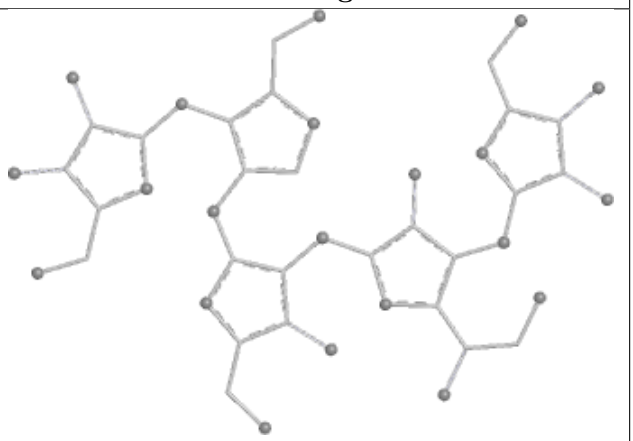
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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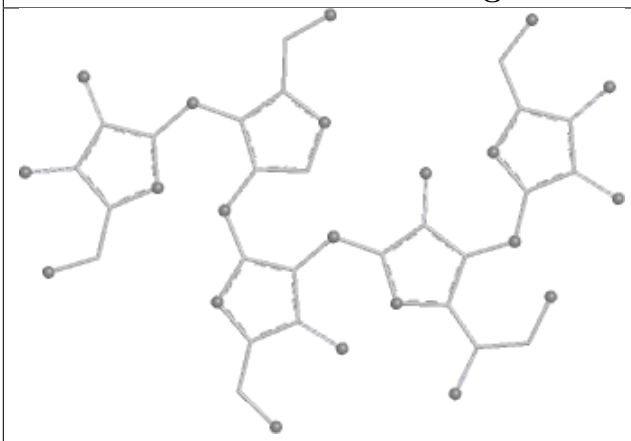	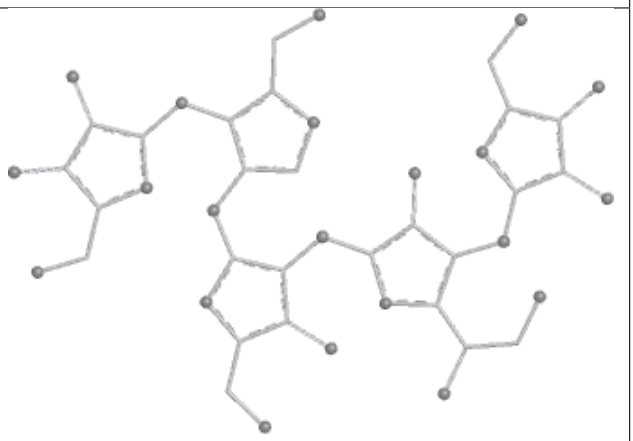
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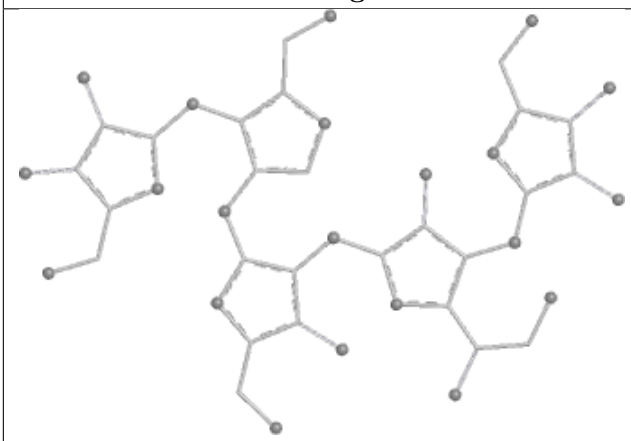	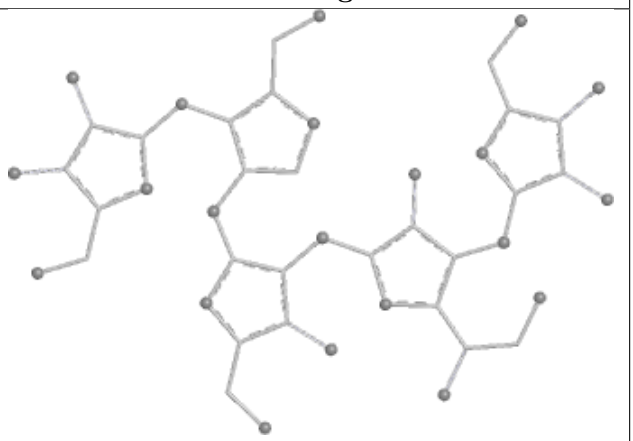
Torsions	**Rings**

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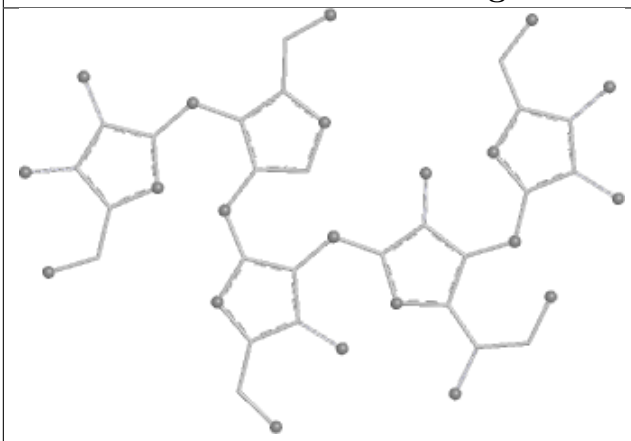	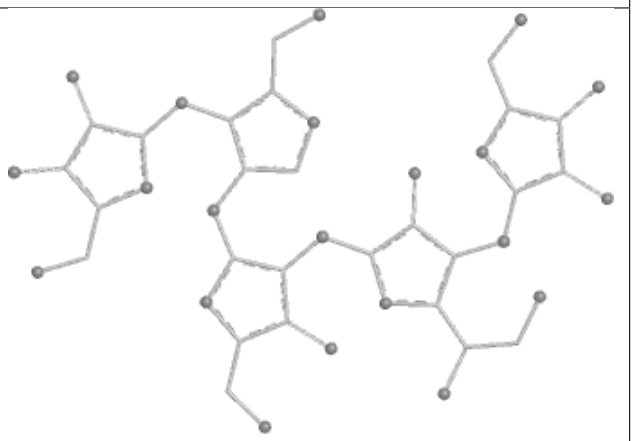
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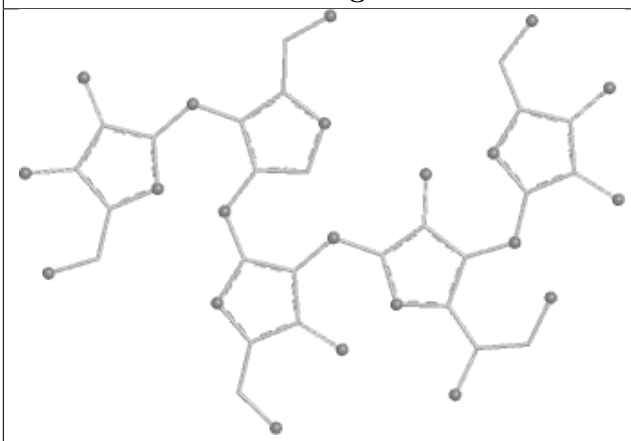	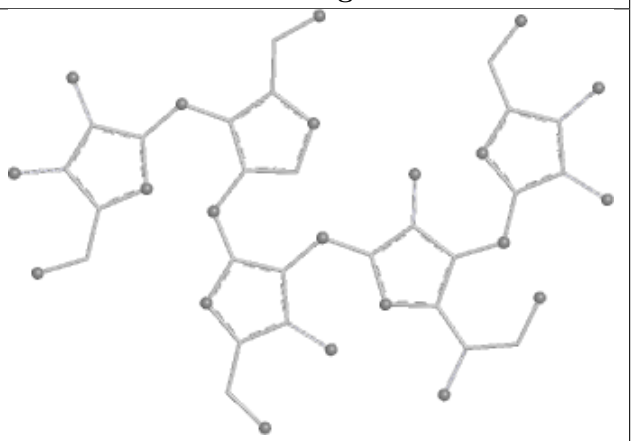
Torsions	**Rings**

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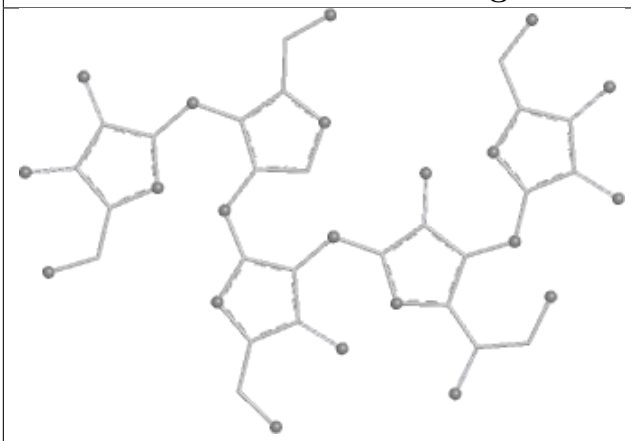	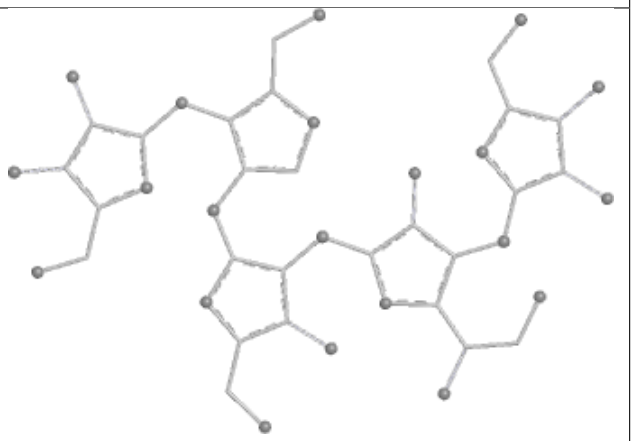
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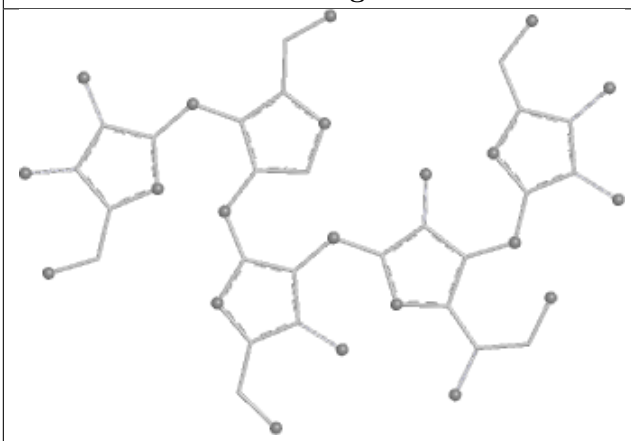	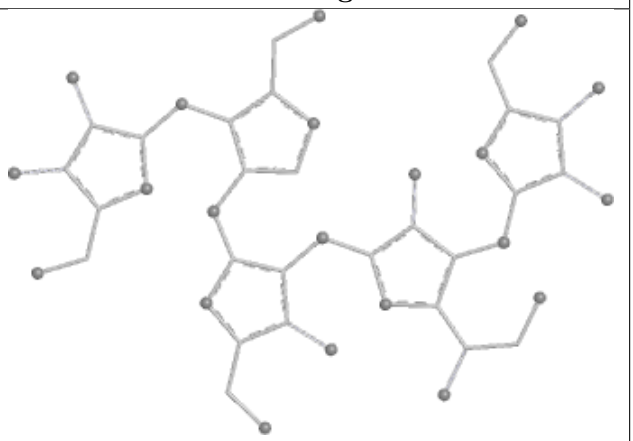
Torsions	**Rings**

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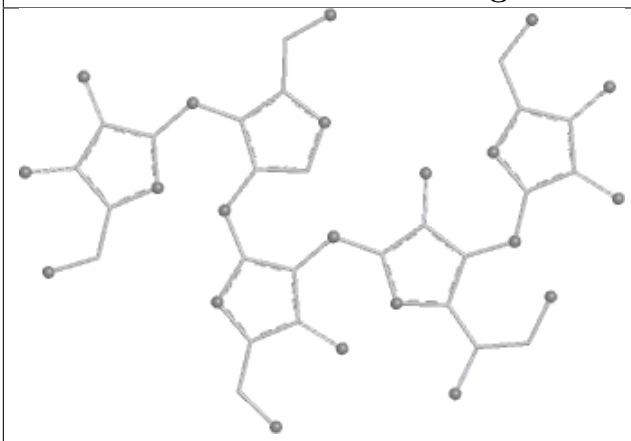	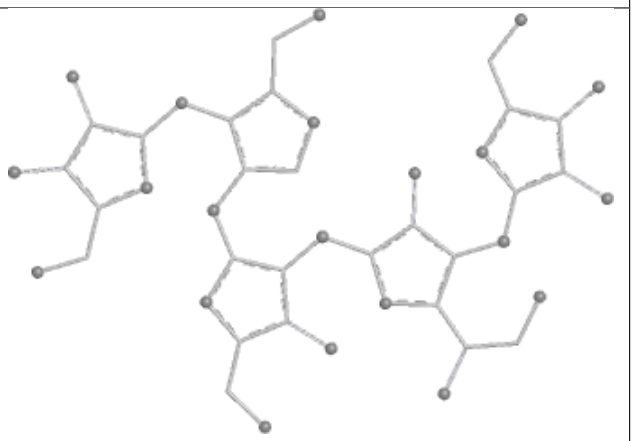
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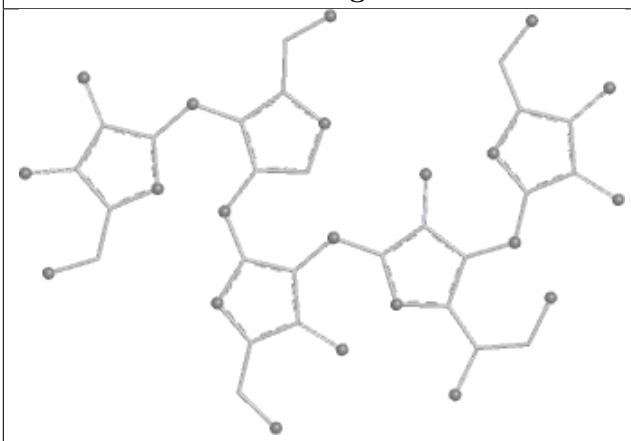	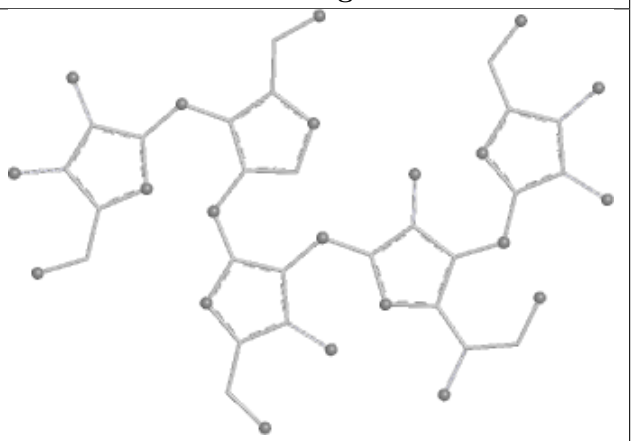
Torsions	**Rings**

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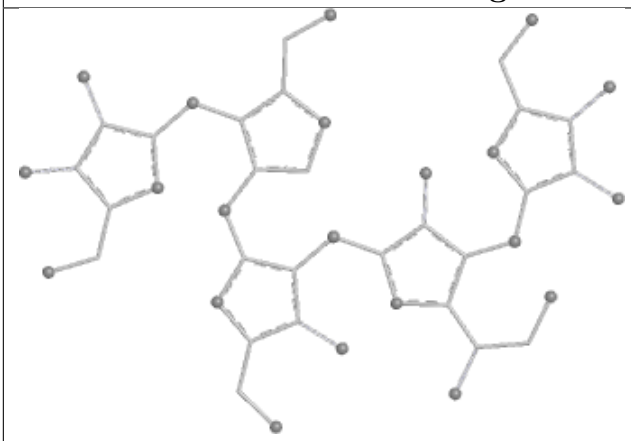
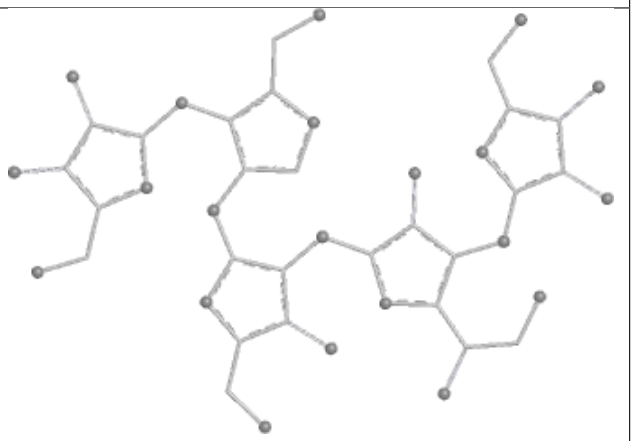
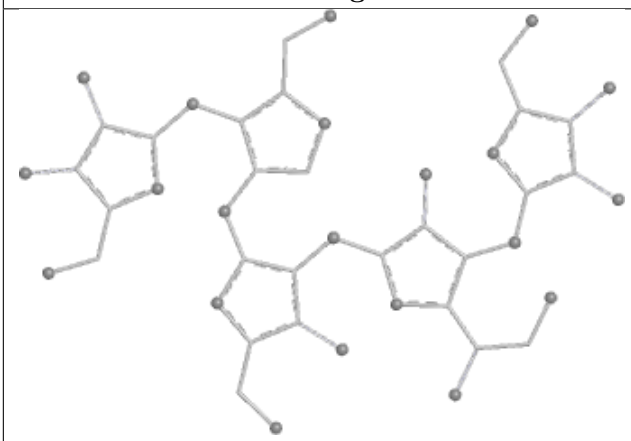
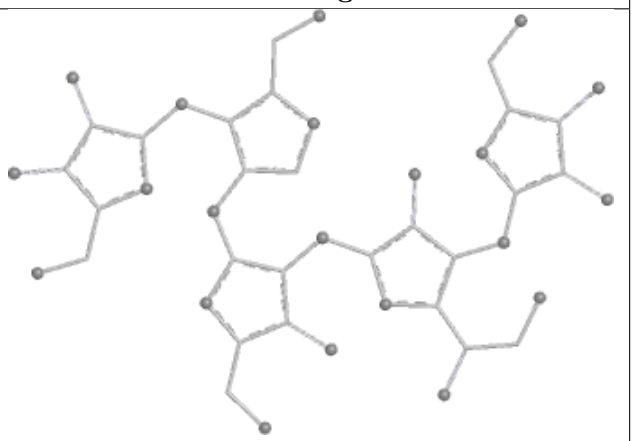
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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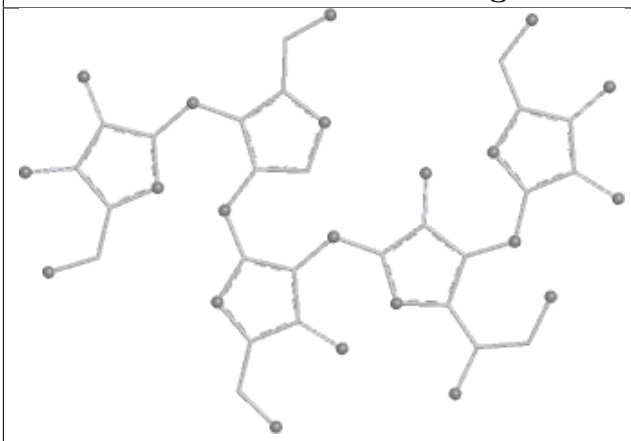	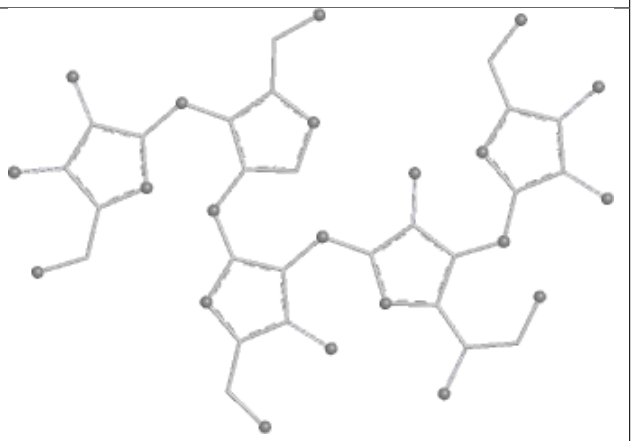
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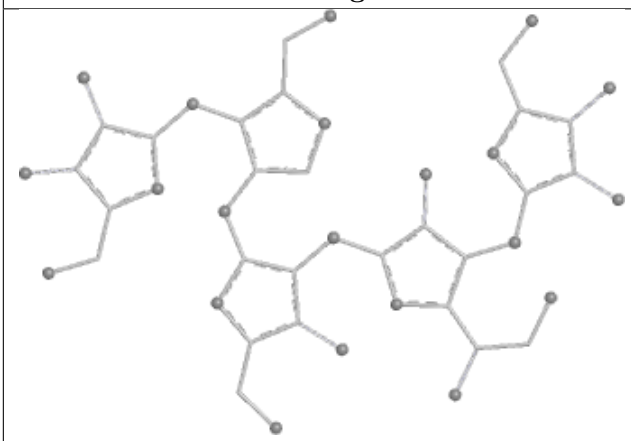	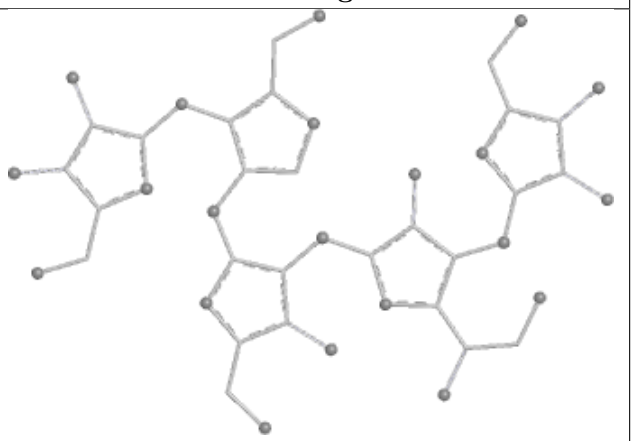
Torsions	**Rings**

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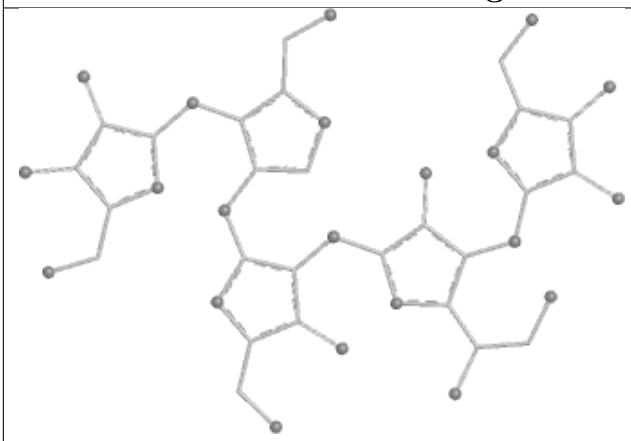	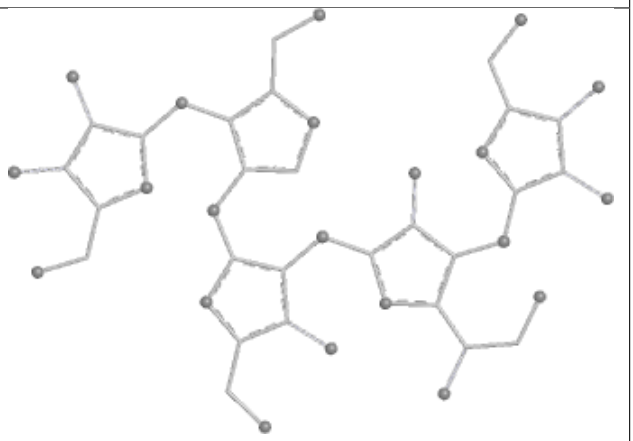
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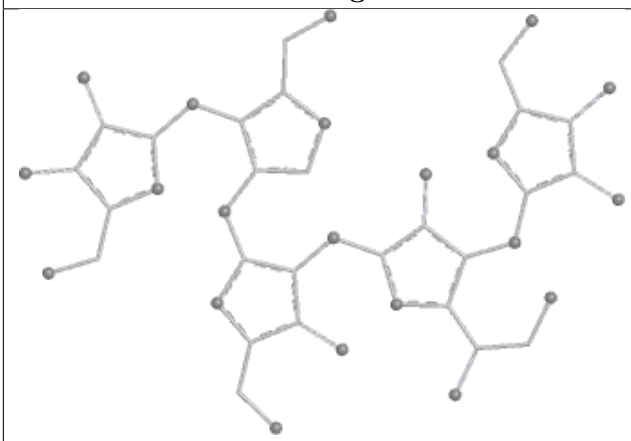	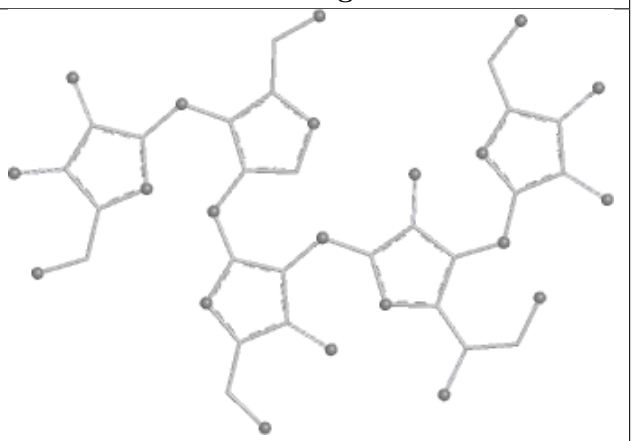
Torsions	**Rings**

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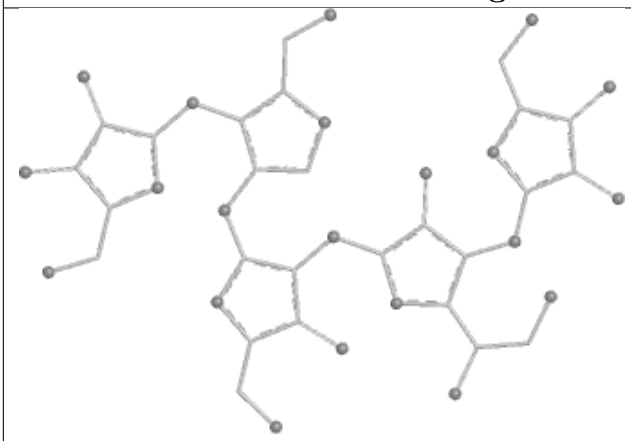	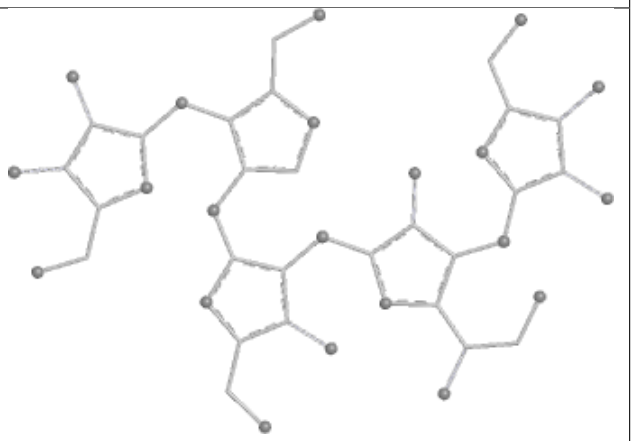
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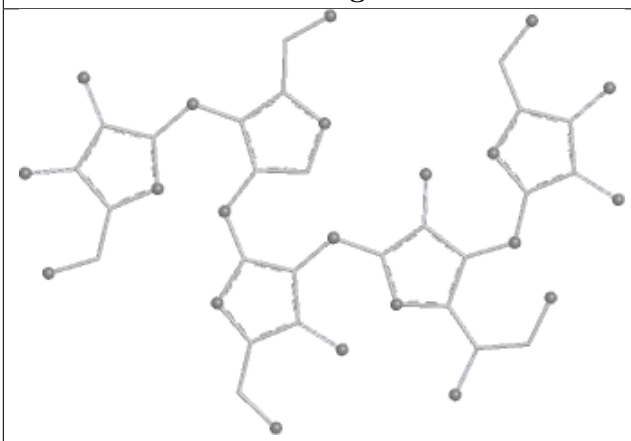	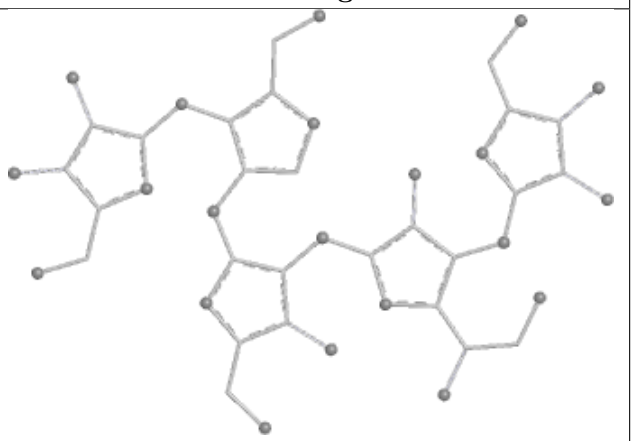
Torsions	**Rings**

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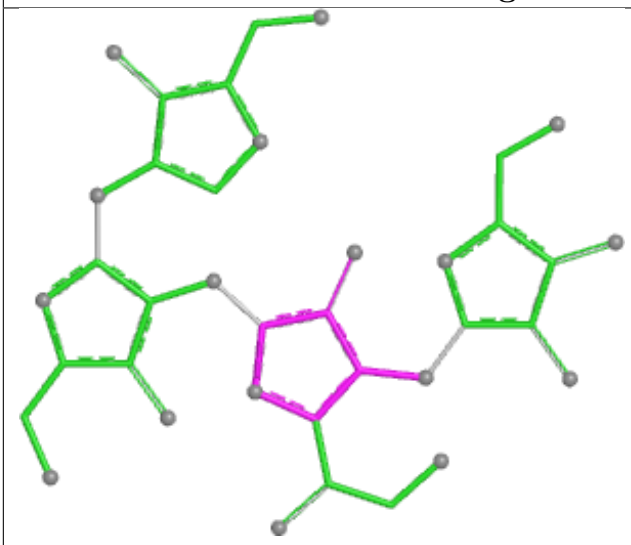
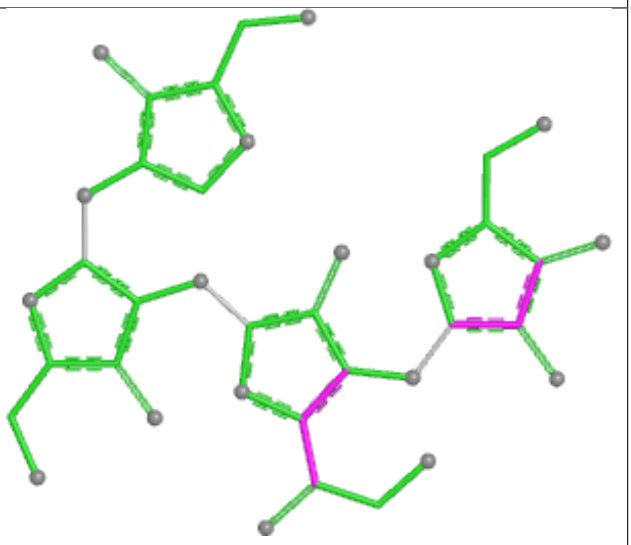
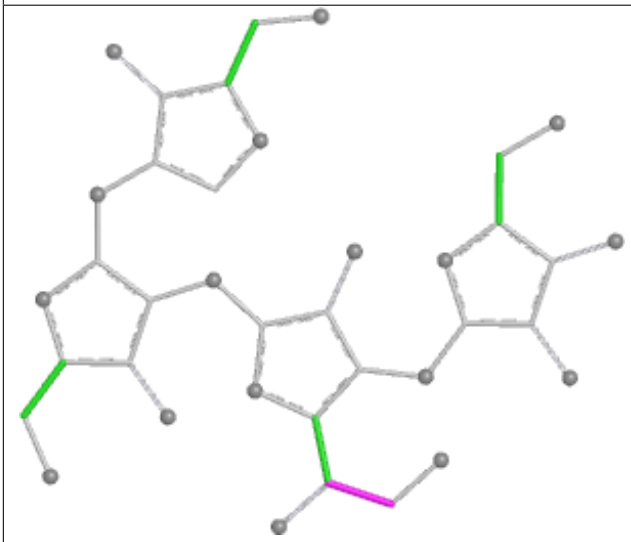
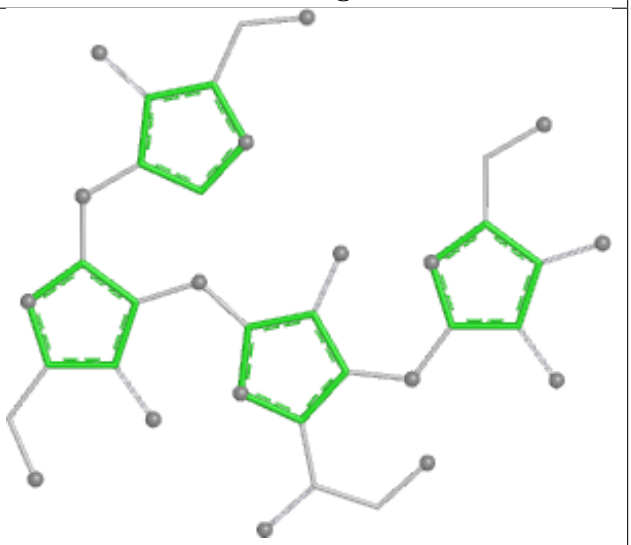
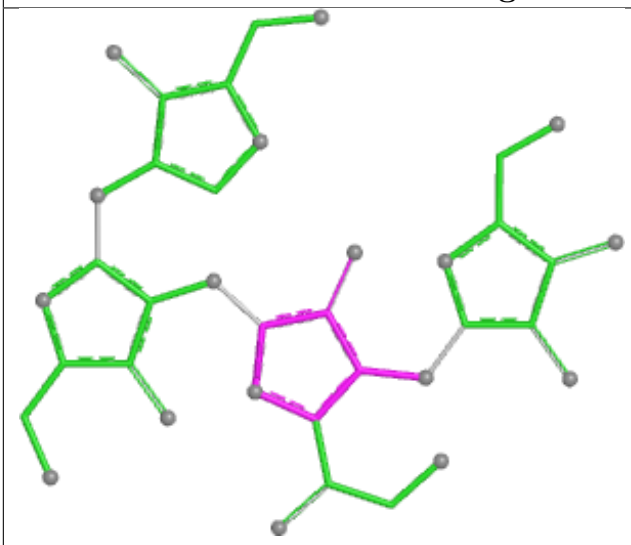
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 4



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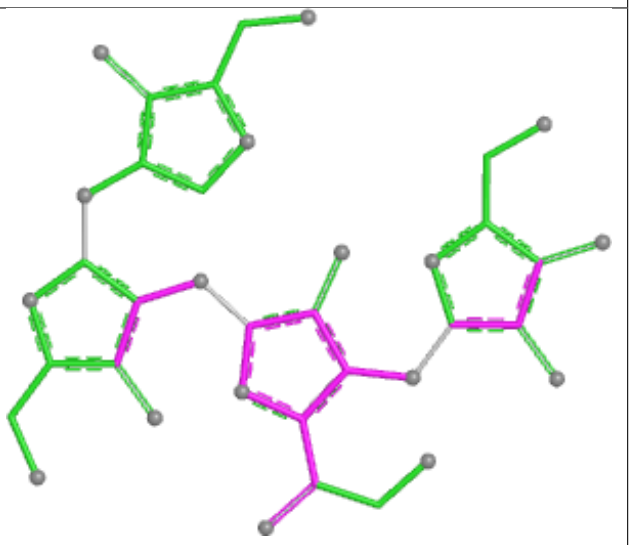

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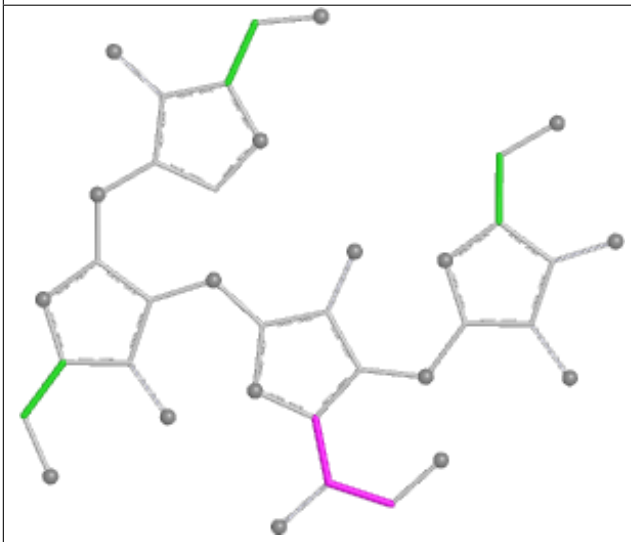

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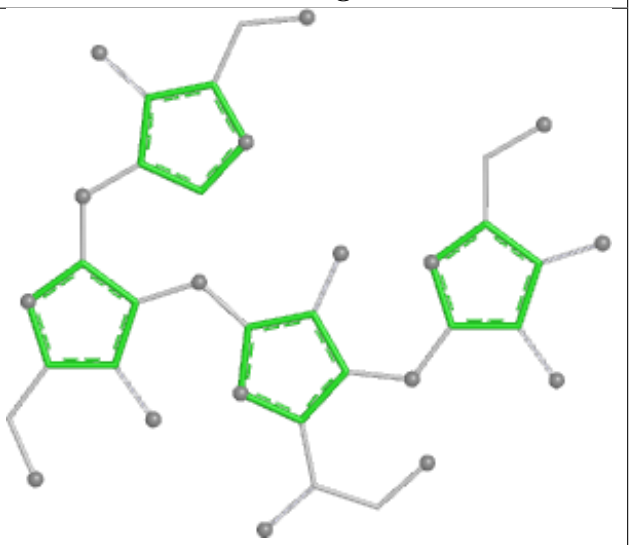

Rings

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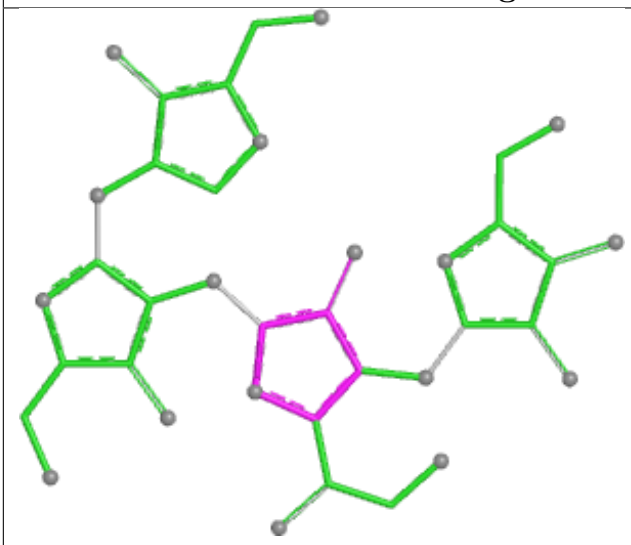
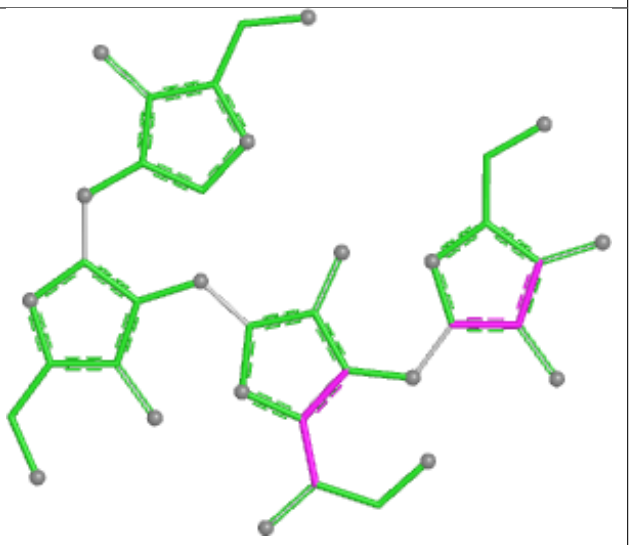
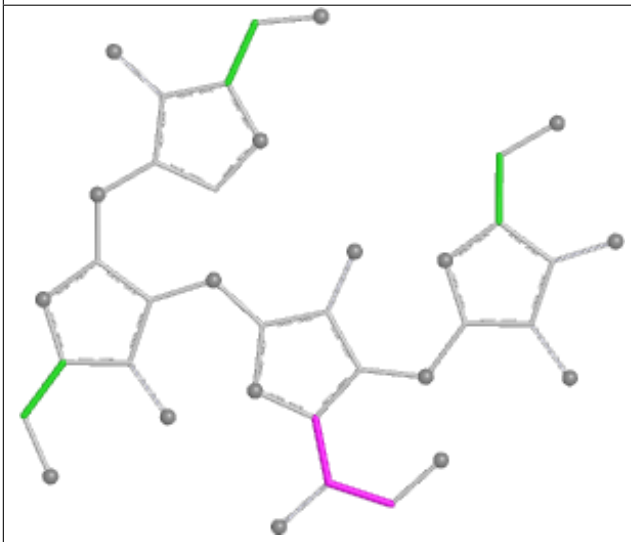
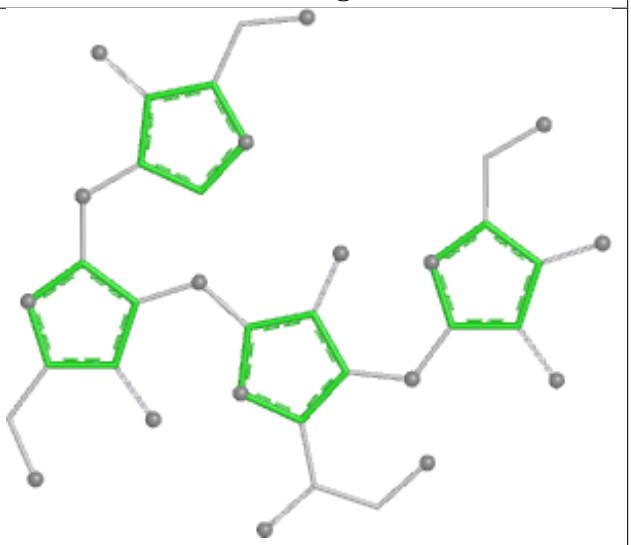
 Bond lengths	 Bond angles
 Torsions	 Rings

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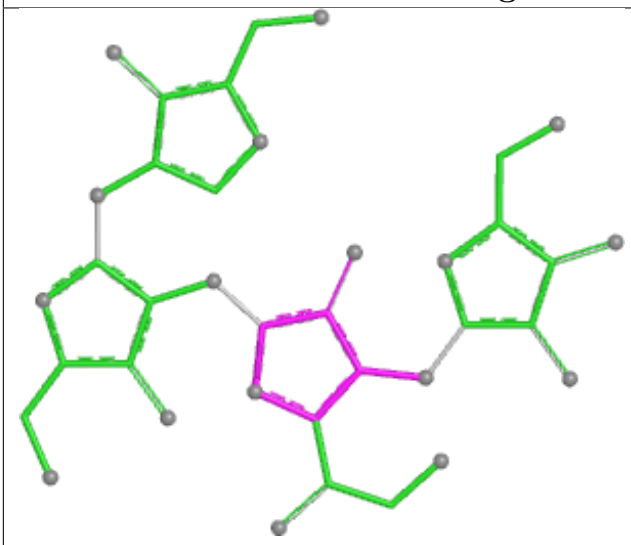
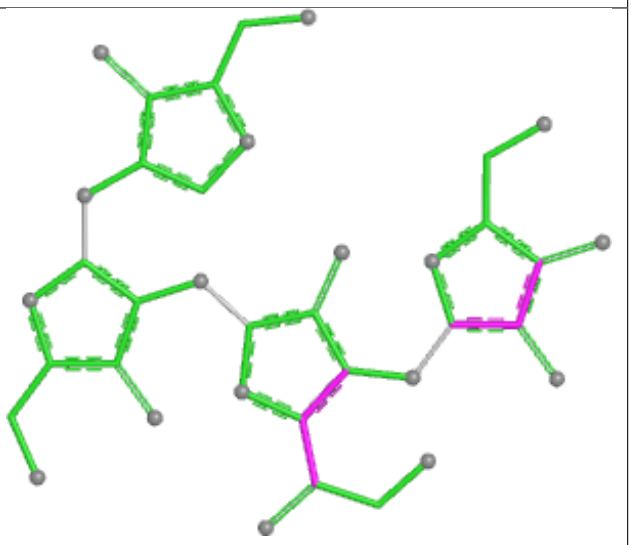
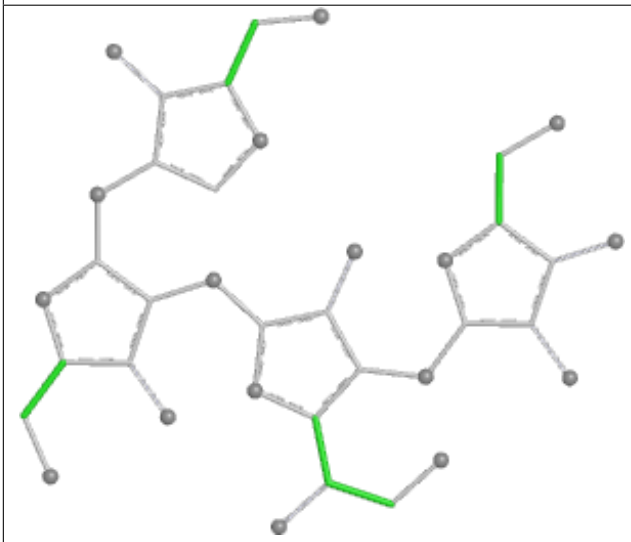
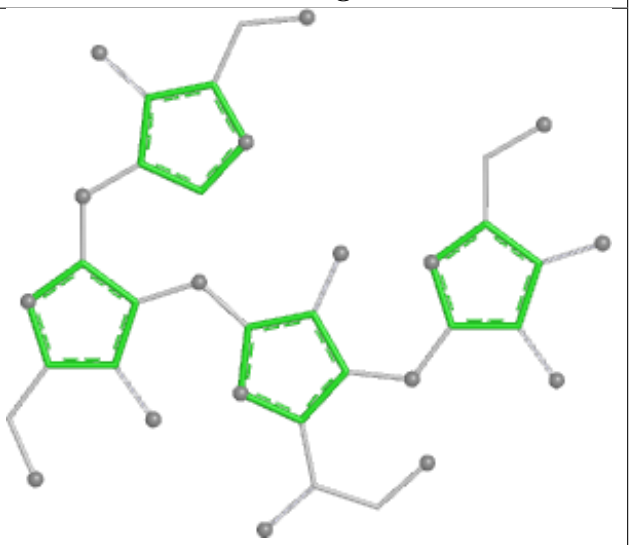
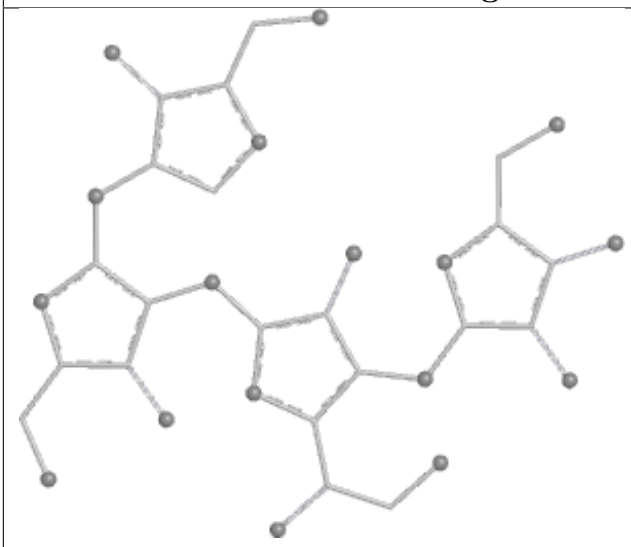
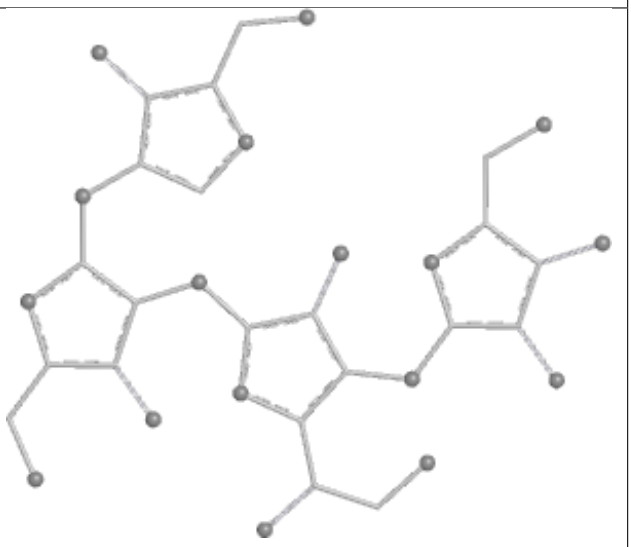
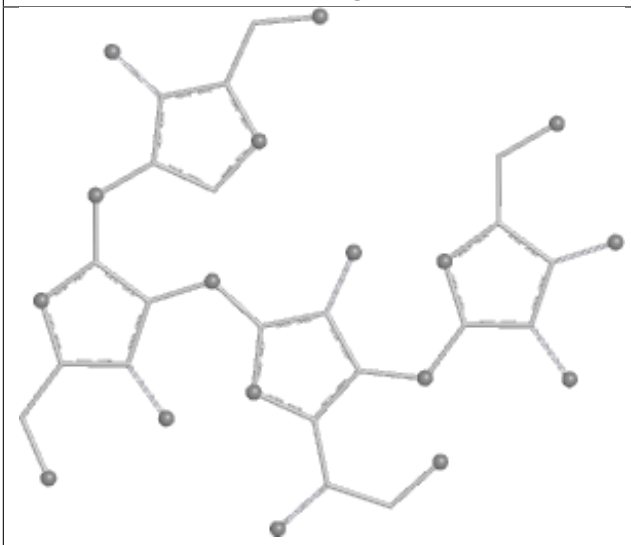
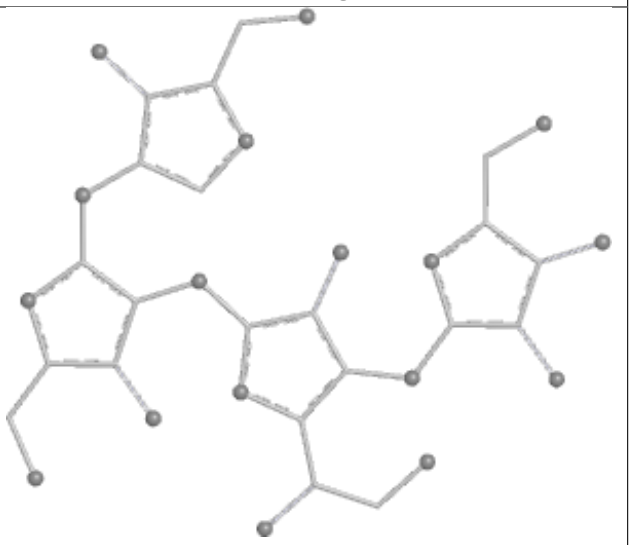
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain BA	
 Bond lengths	 Bond angles
 Torsions	 Rings

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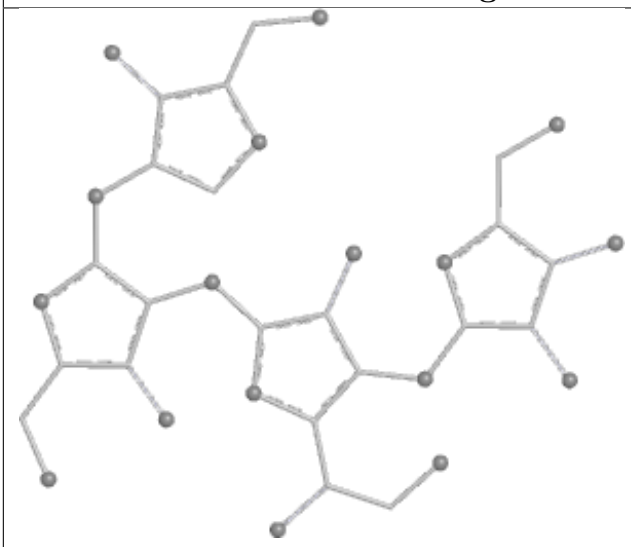
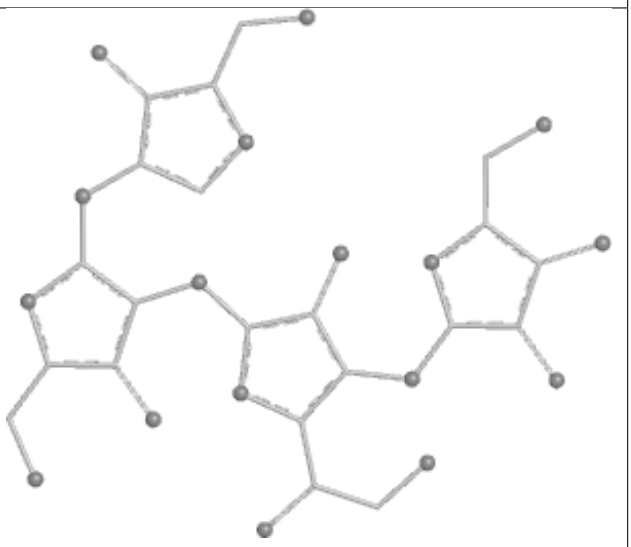
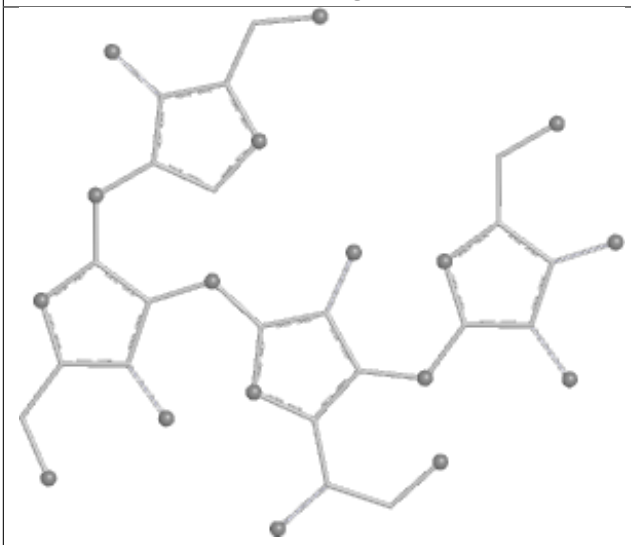
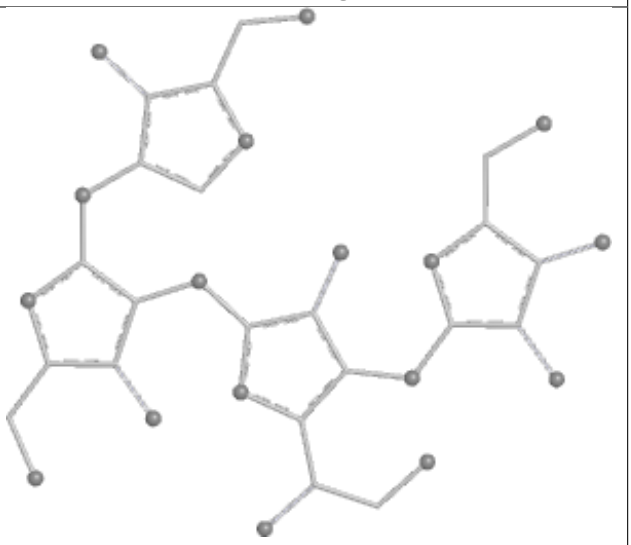
 Bond lengths	 Bond angles
 Torsions	 Rings

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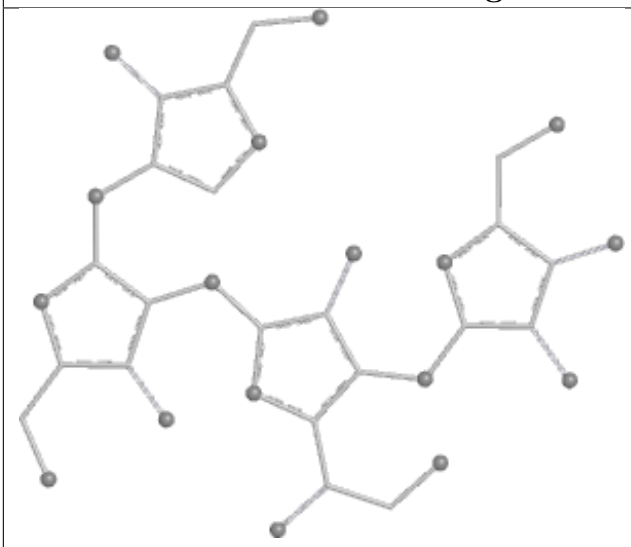
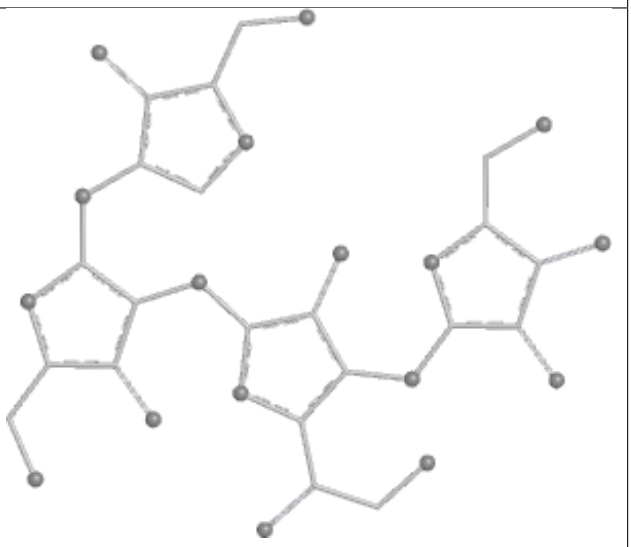
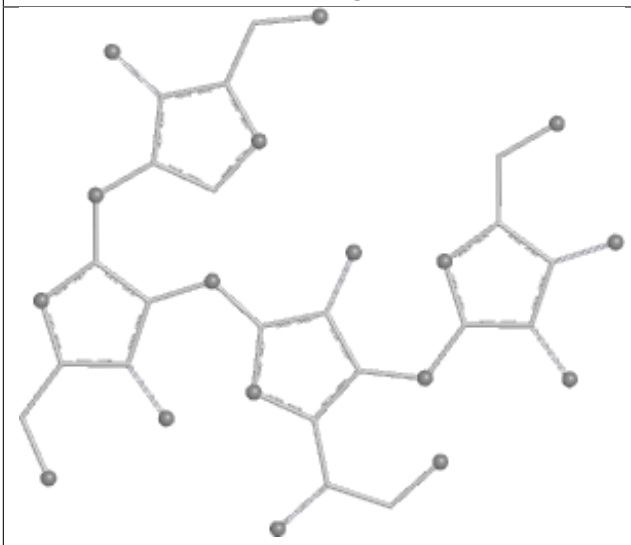
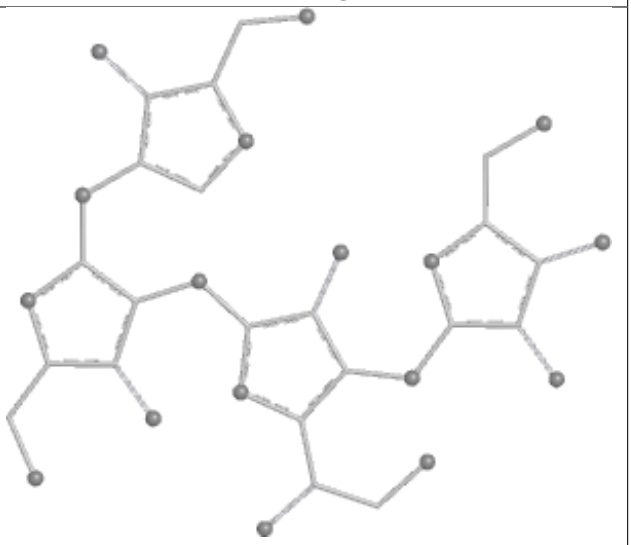
 Bond lengths	 Bond angles
 Torsions	 Rings

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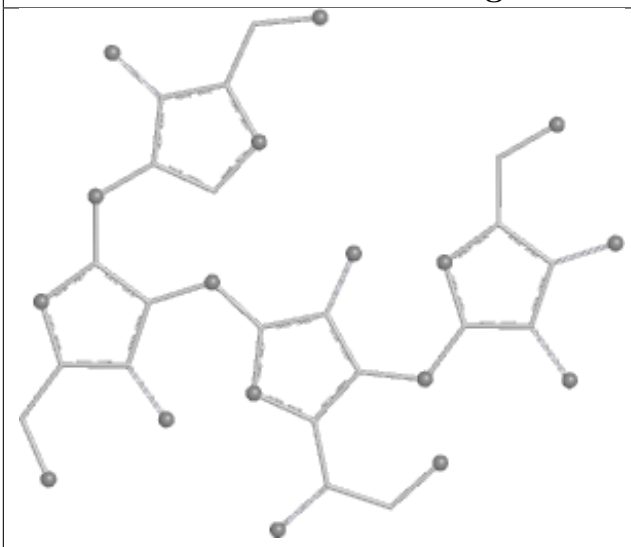
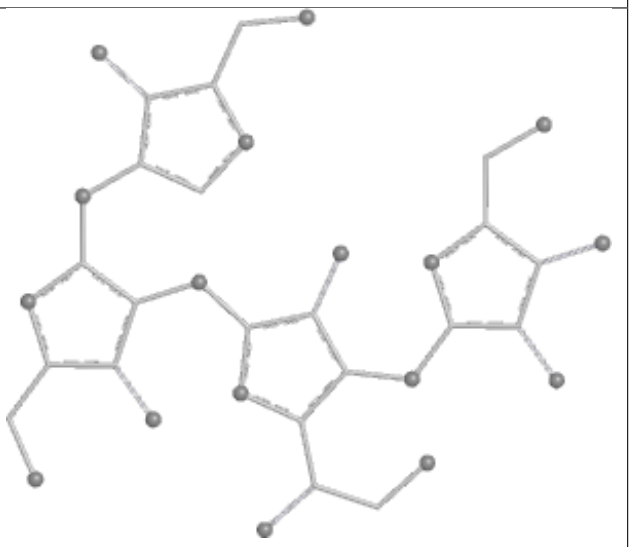
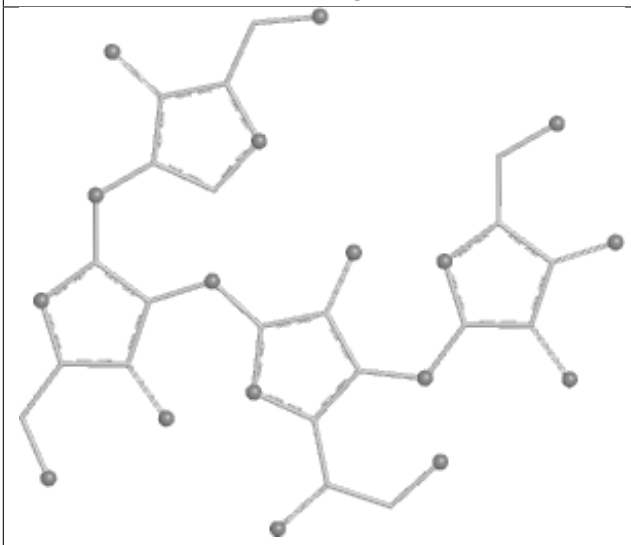
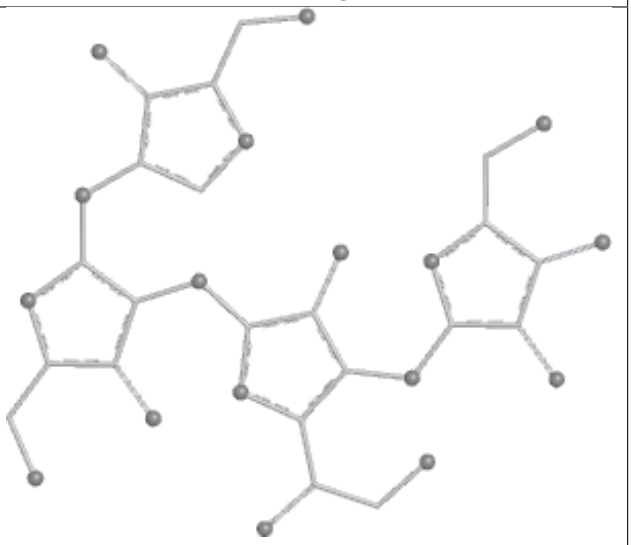
 Bond lengths	 Bond angles
 Torsions	 Rings

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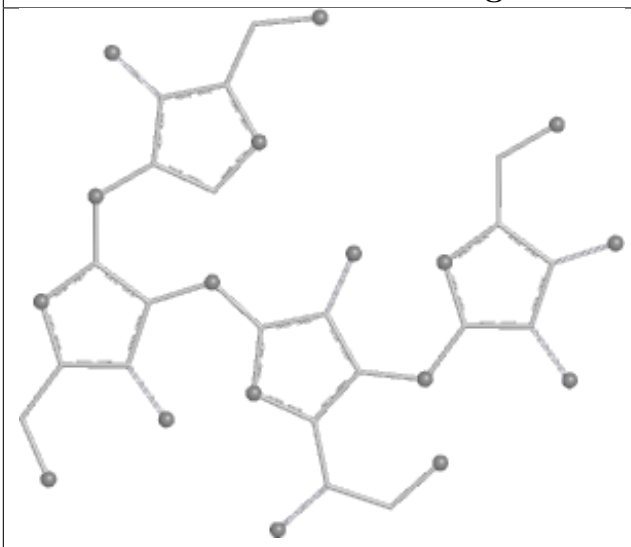
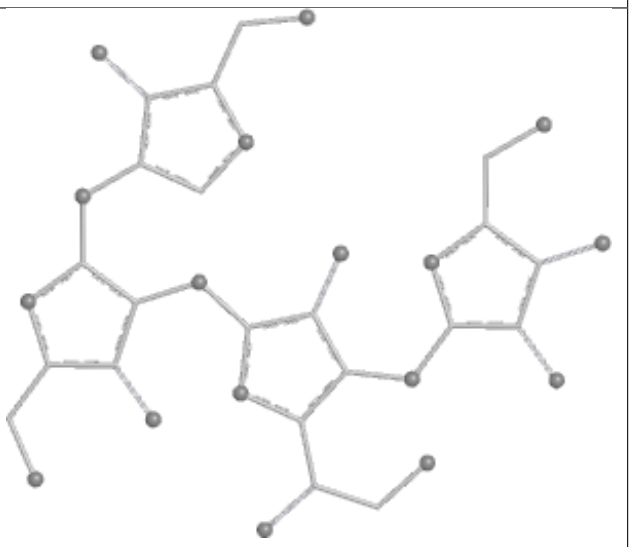
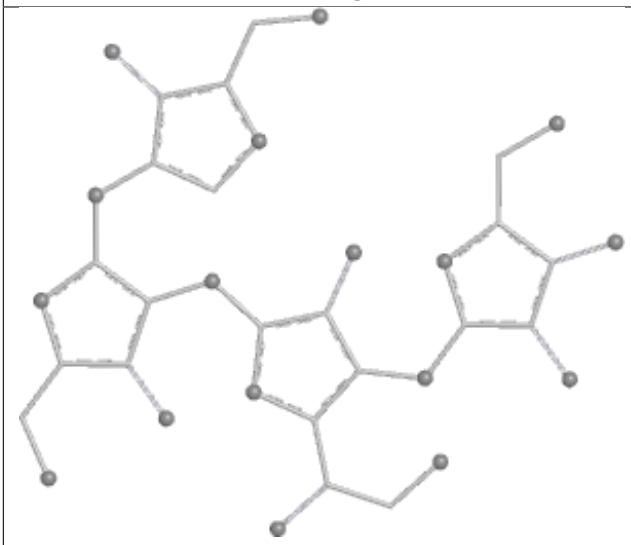
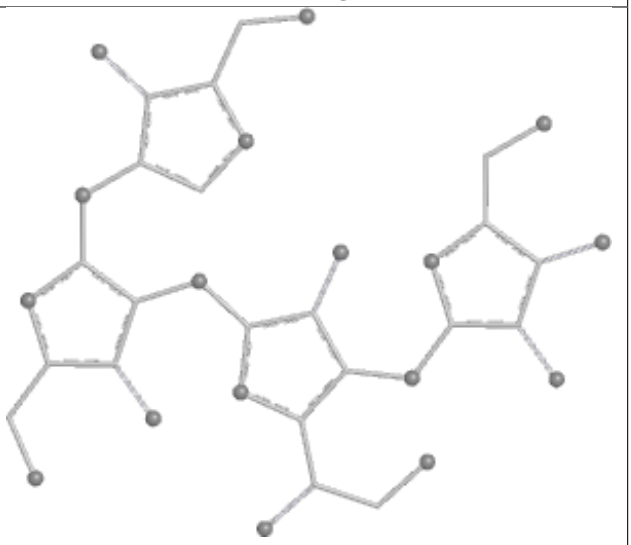
 Bond lengths	 Bond angles
 Torsions	 Rings

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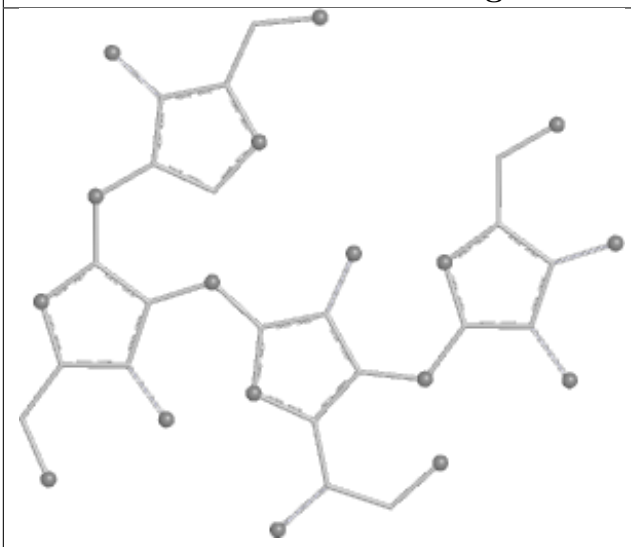
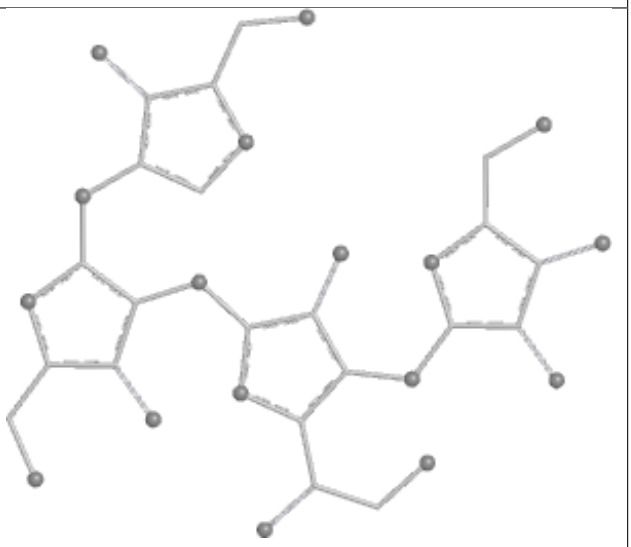
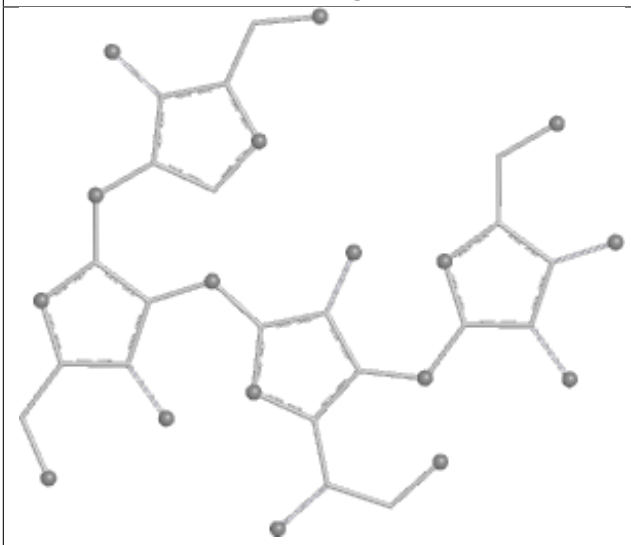
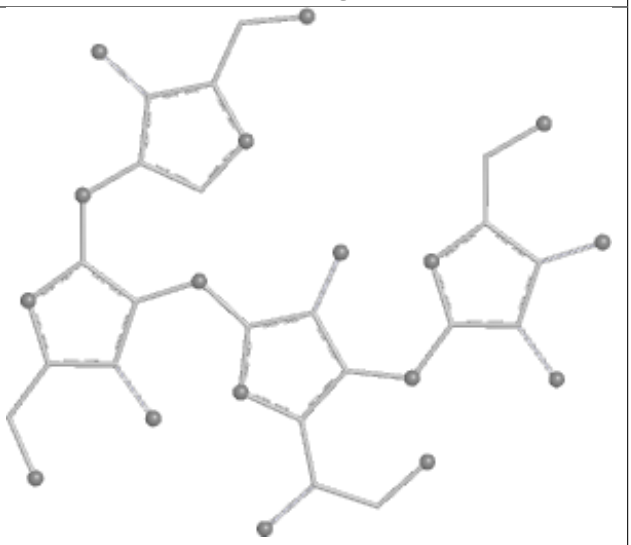
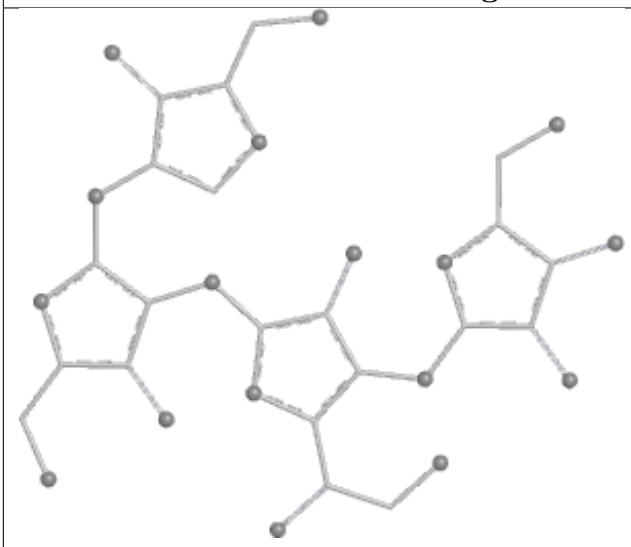
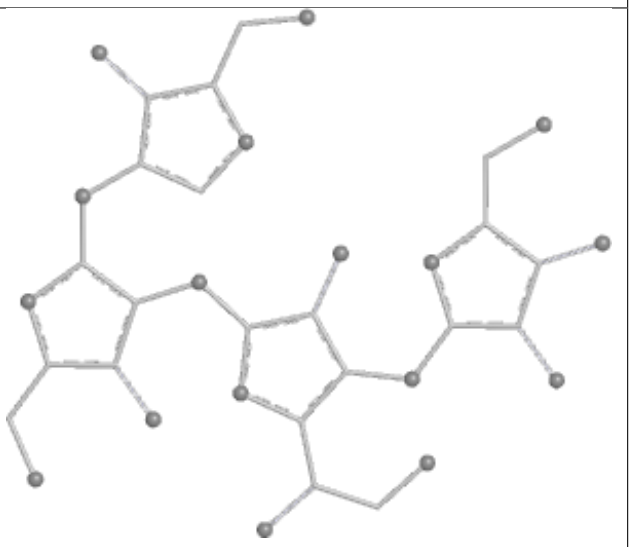
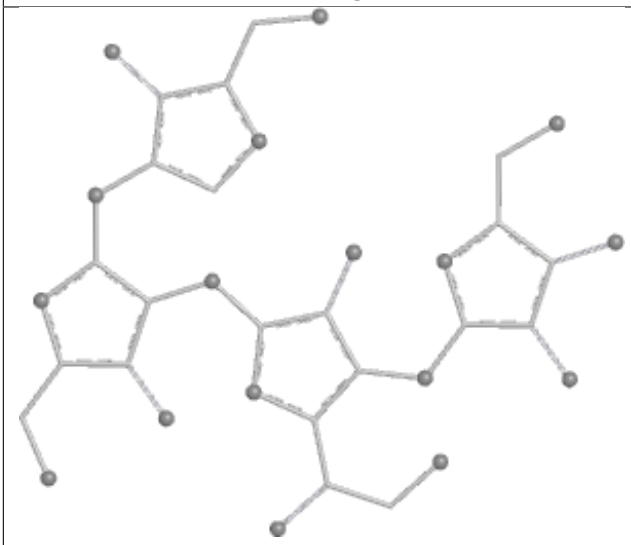
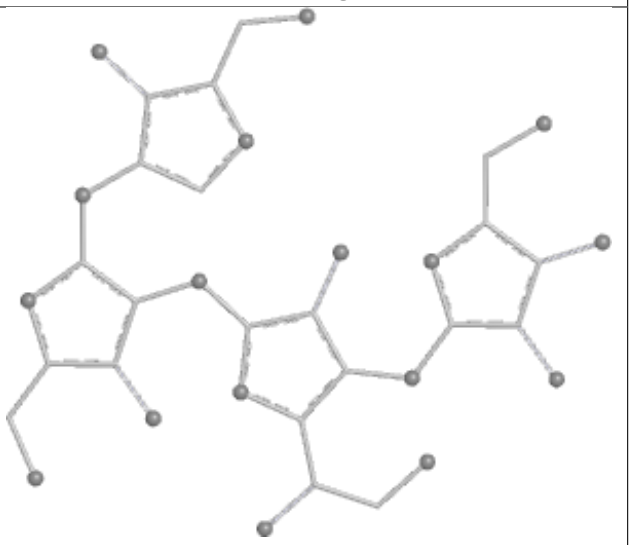
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain GB	
 Bond lengths	 Bond angles
 Torsions	 Rings

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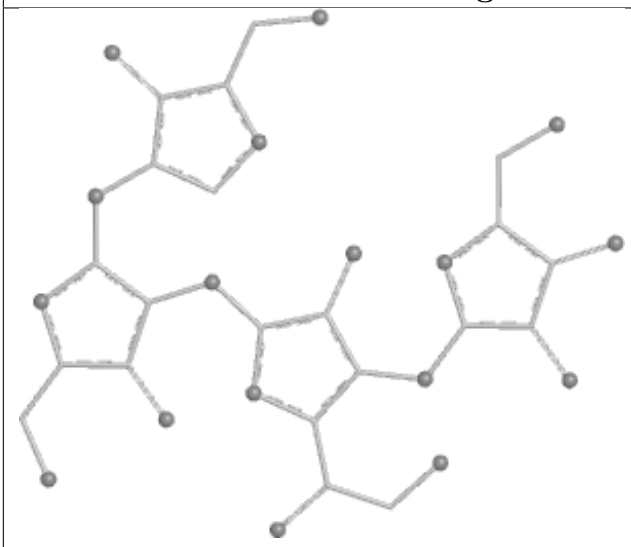
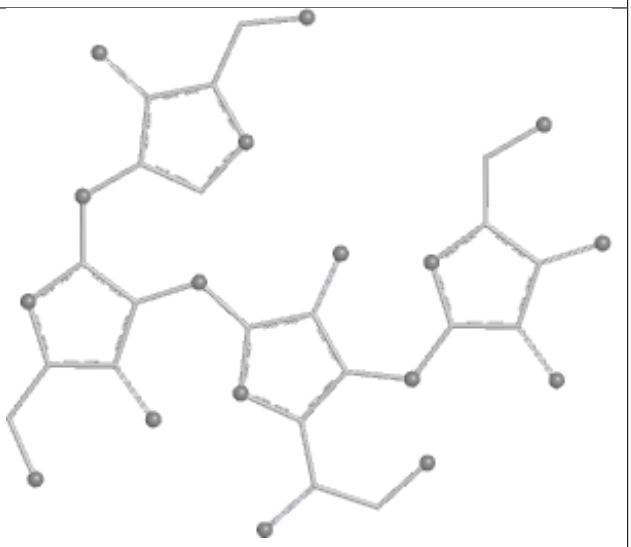
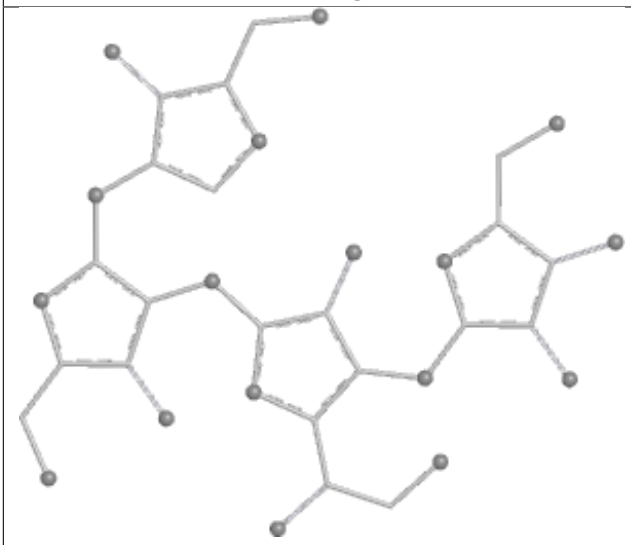
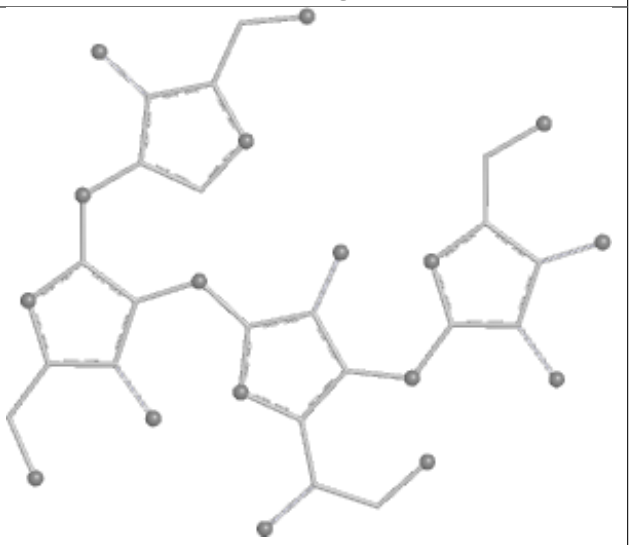
 Bond lengths	 Bond angles
 Torsions	 Rings

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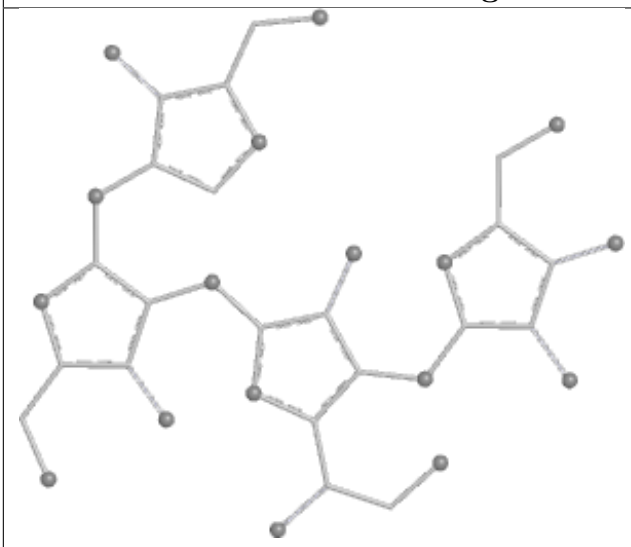
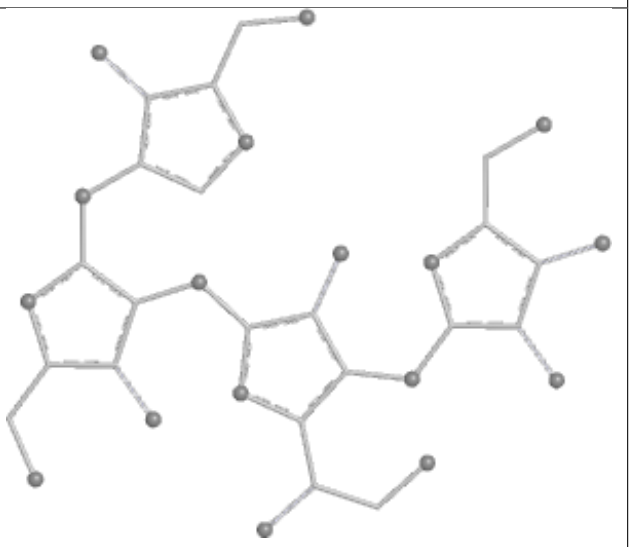
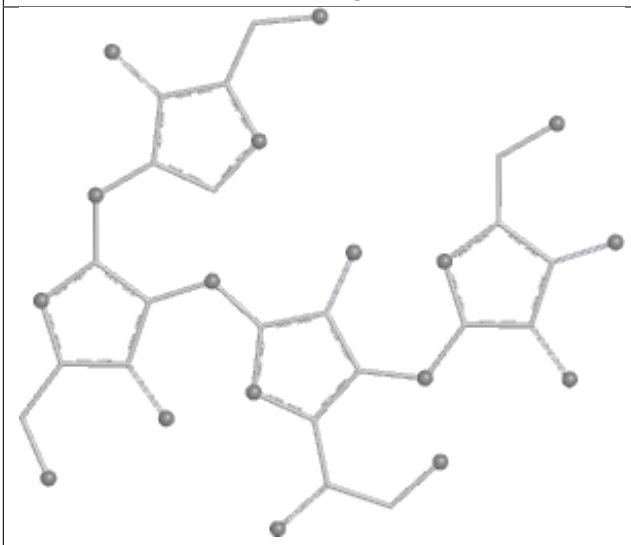
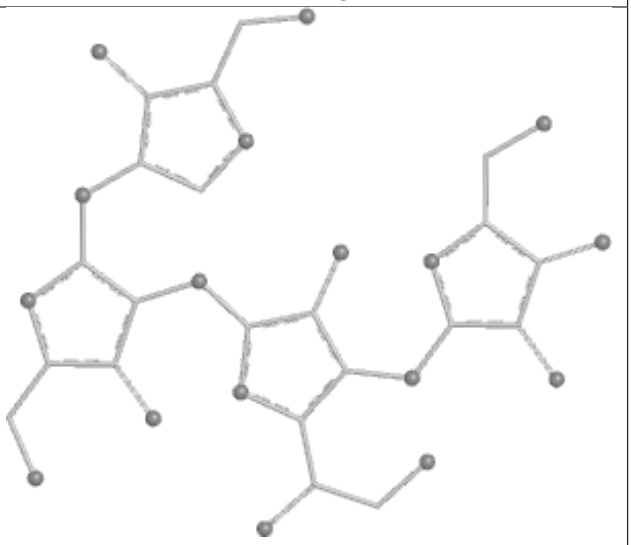
 Bond lengths	 Bond angles
 Torsions	 Rings

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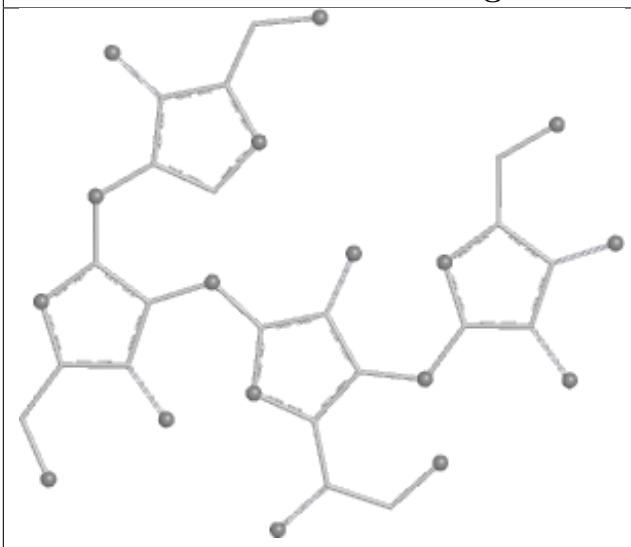
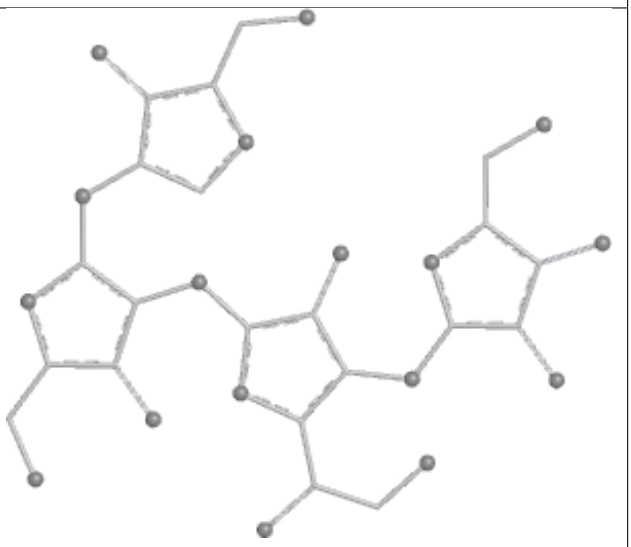
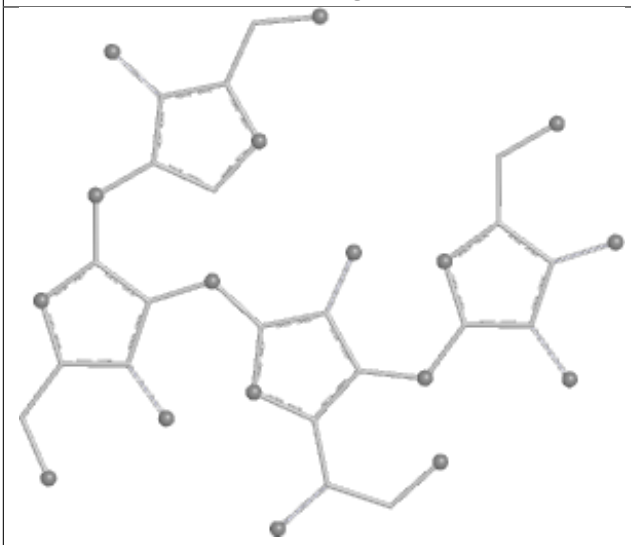
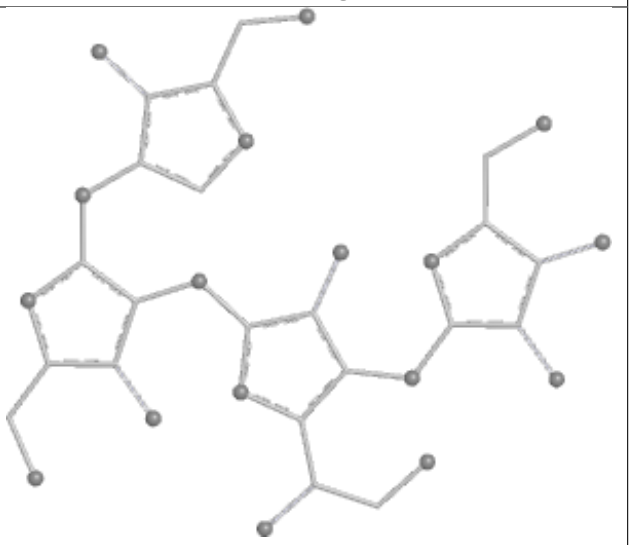
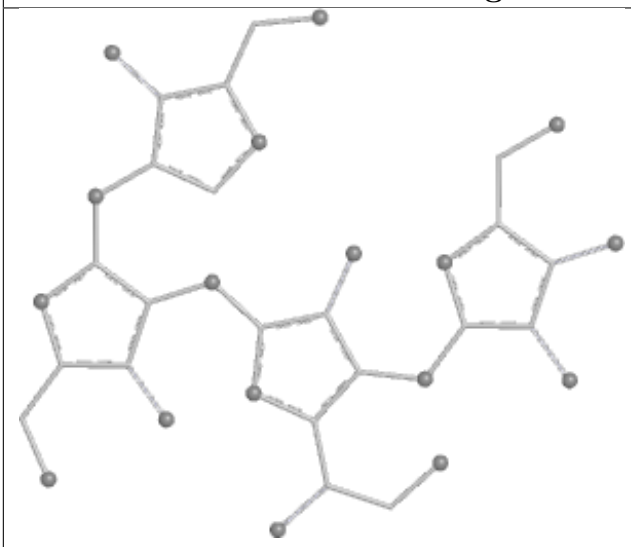
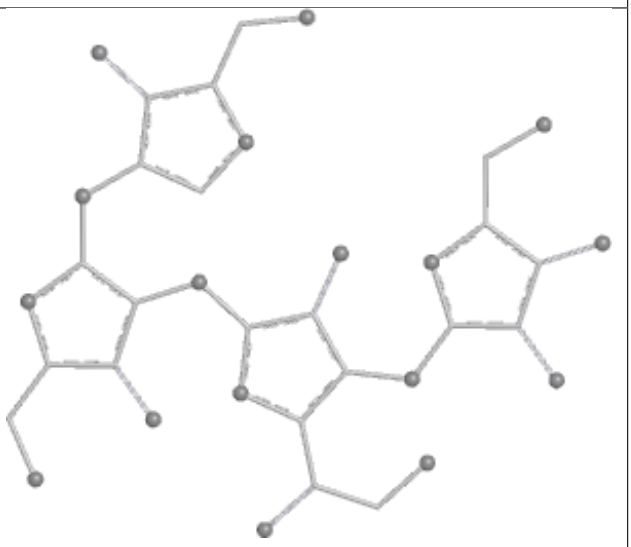
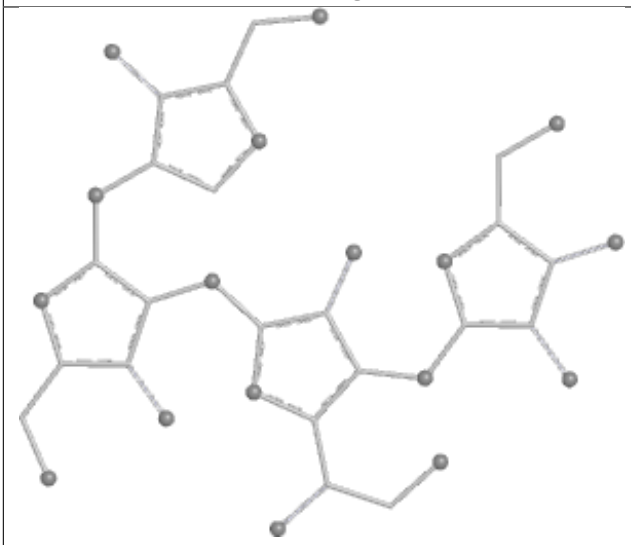
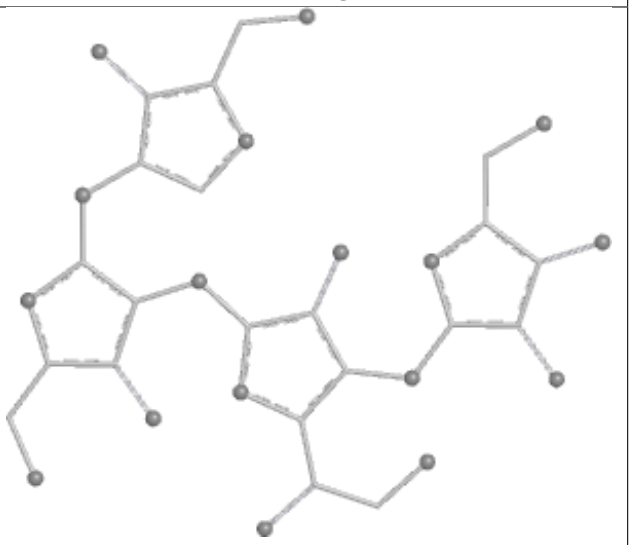
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain dB	
 Bond lengths	 Bond angles
 Torsions	 Rings

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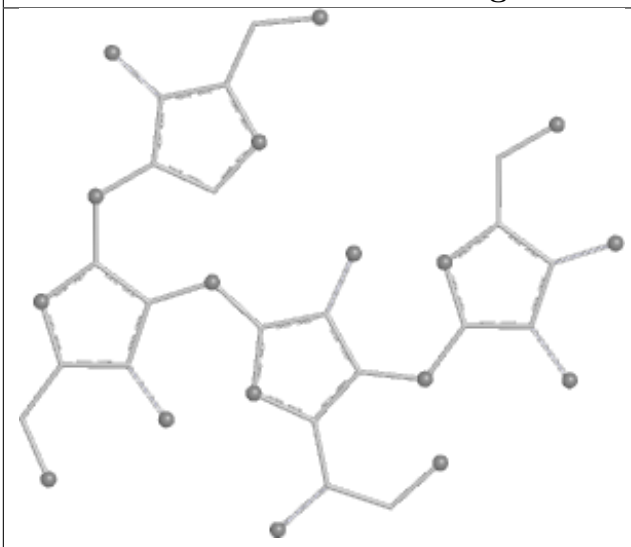
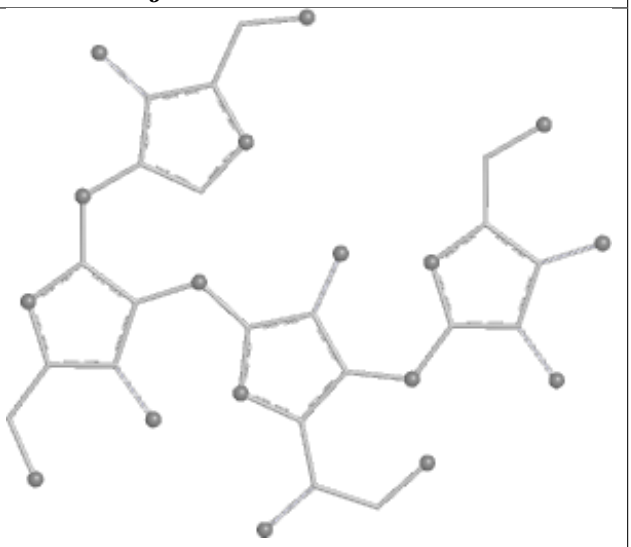
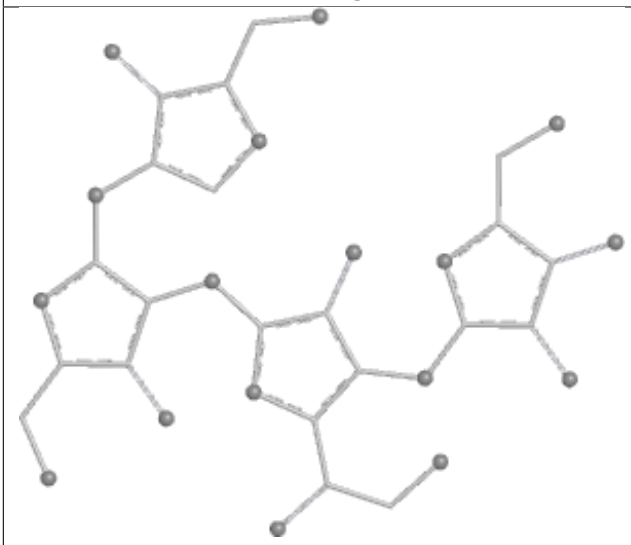
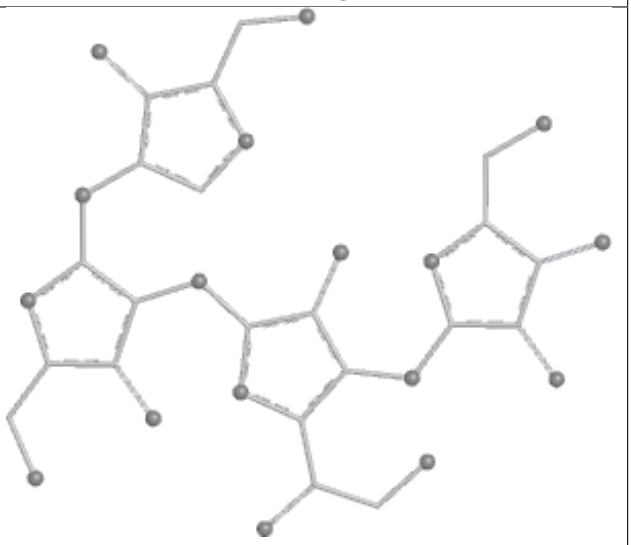
 Bond lengths	 Bond angles
 Torsions	 Rings

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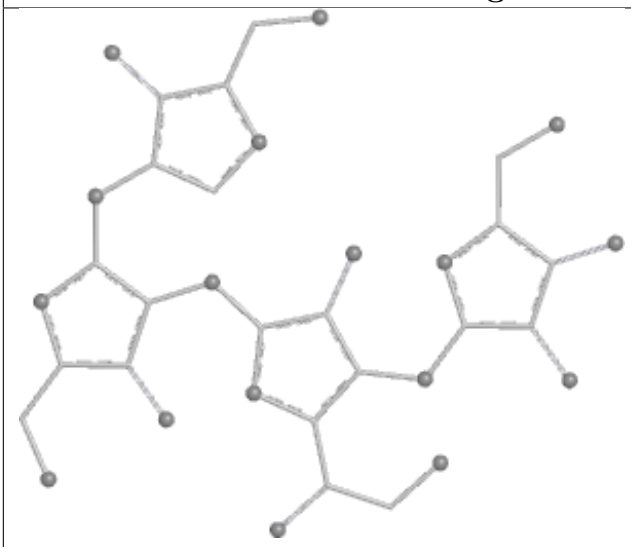
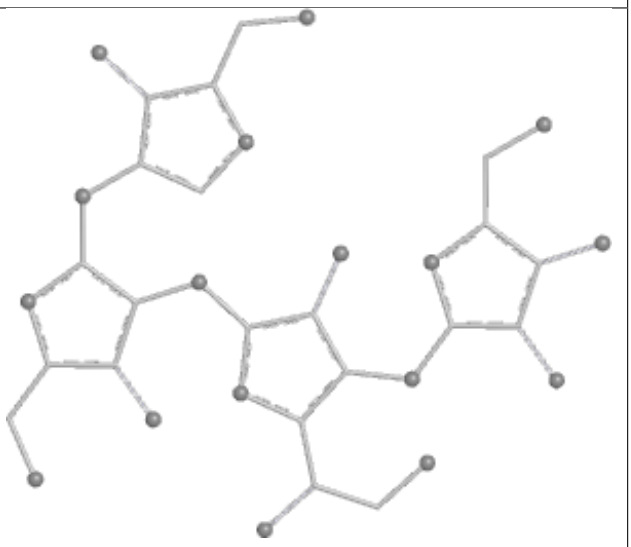
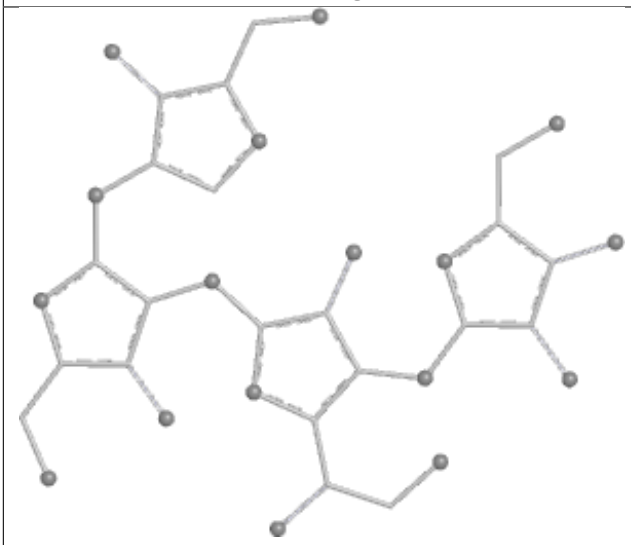
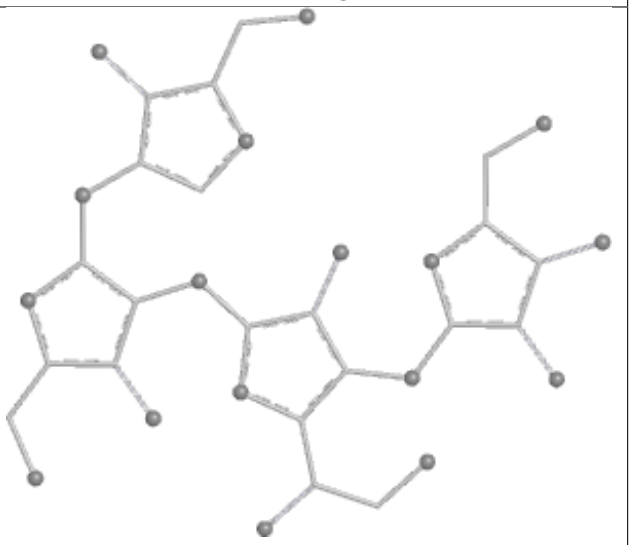
 Bond lengths	 Bond angles
 Torsions	 Rings

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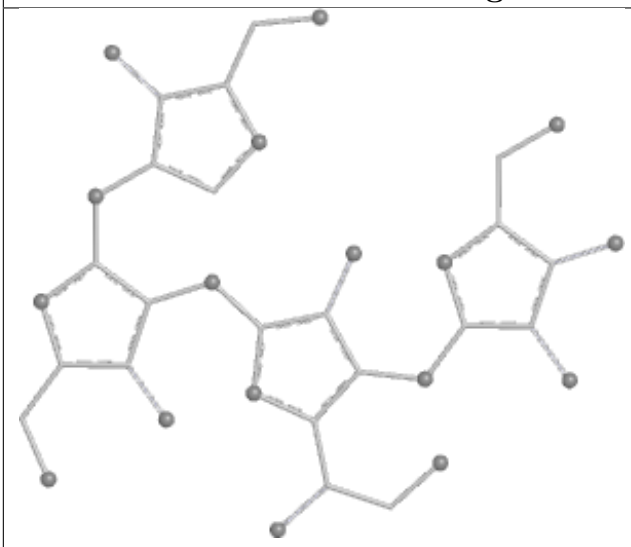
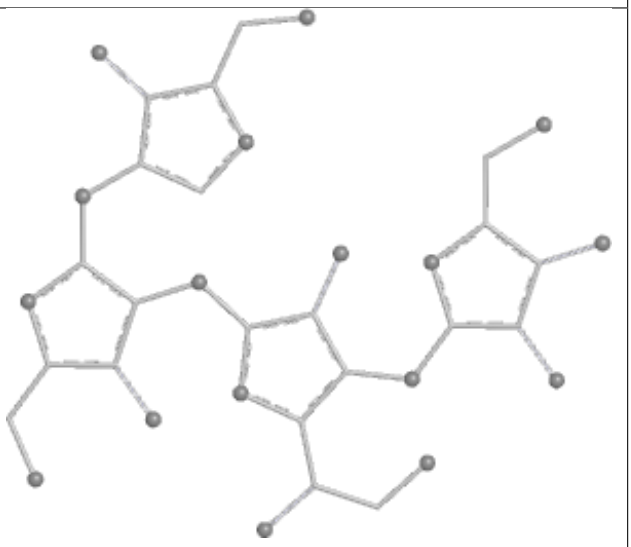
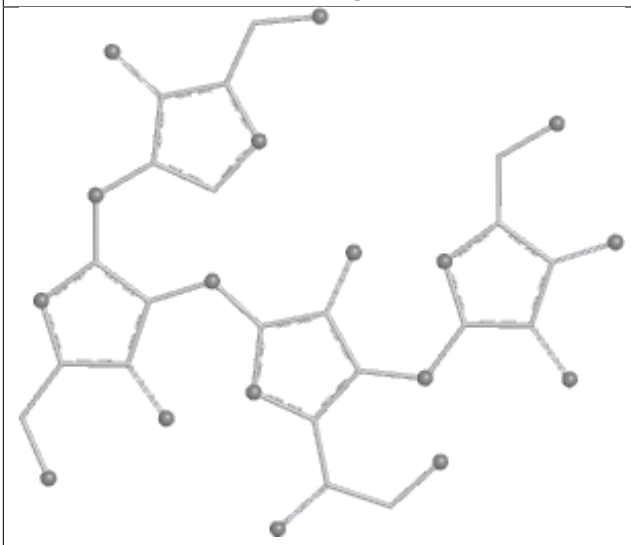
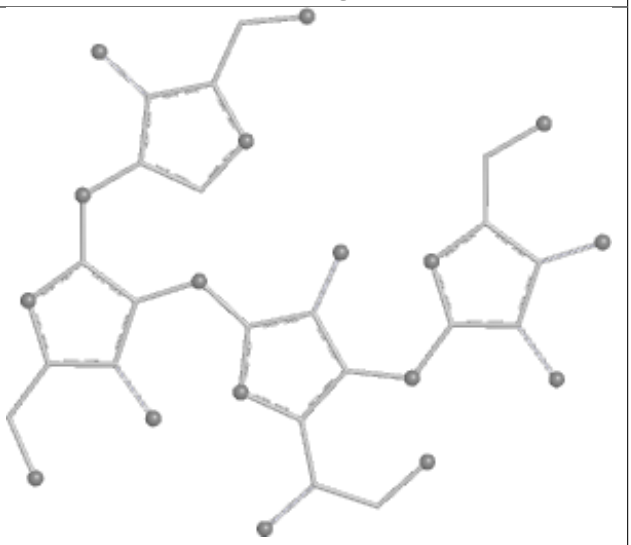
 Bond lengths	 Bond angles
 Torsions	 Rings

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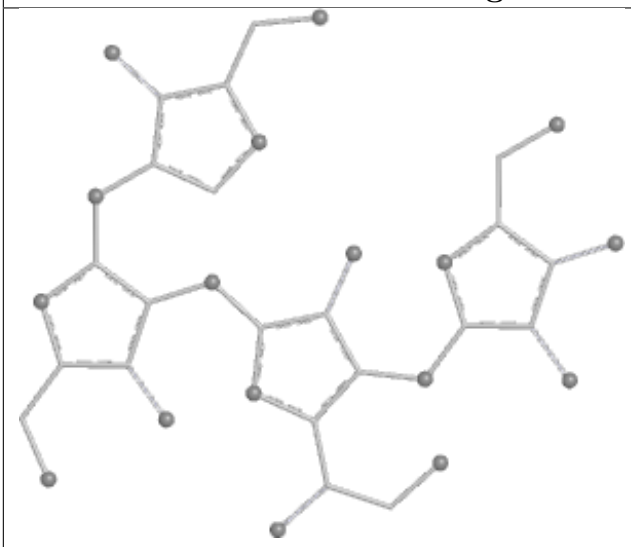
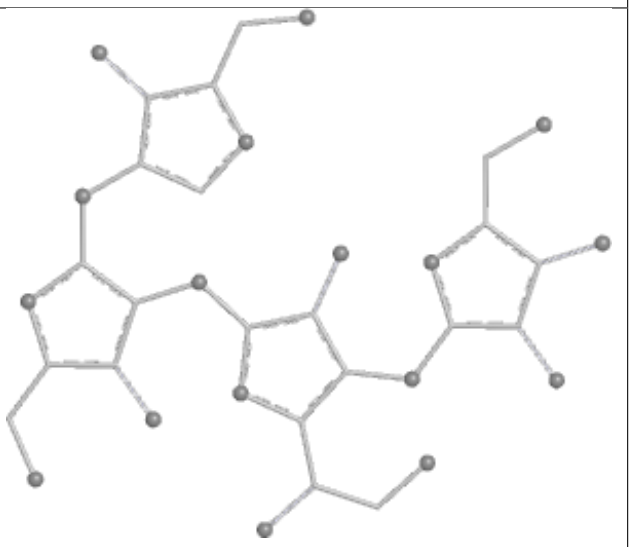
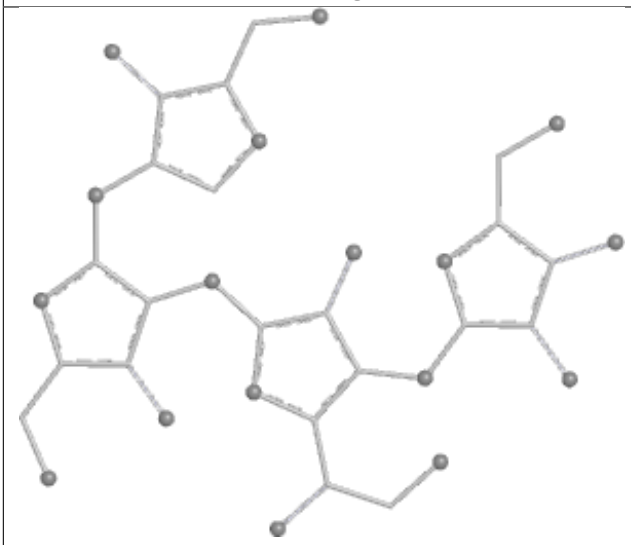
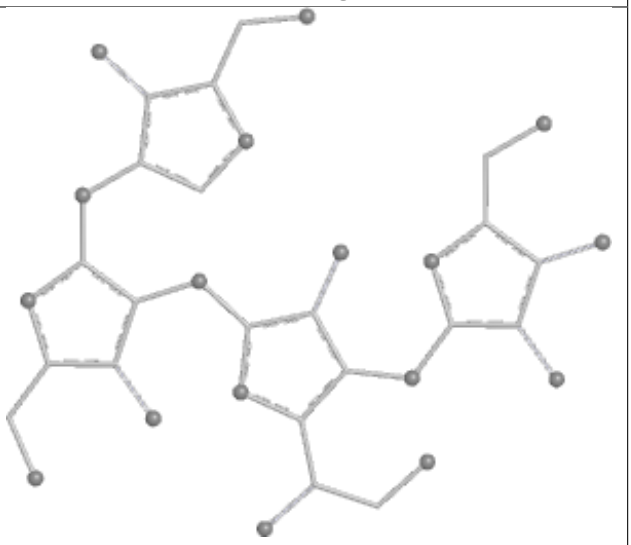
 Bond lengths	 Bond angles
 Torsions	 Rings

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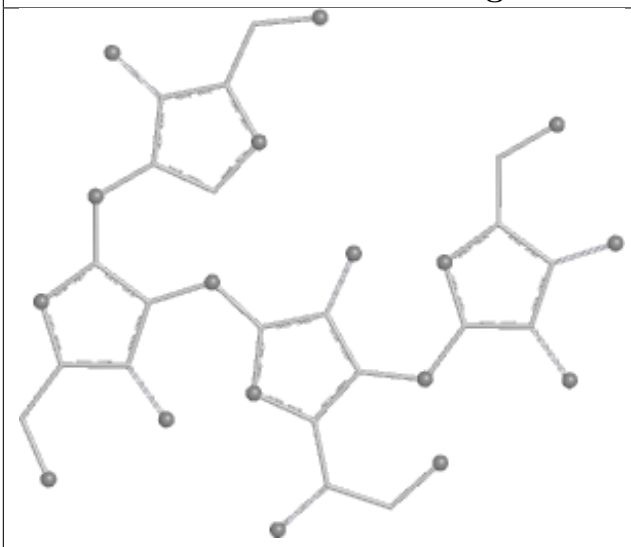
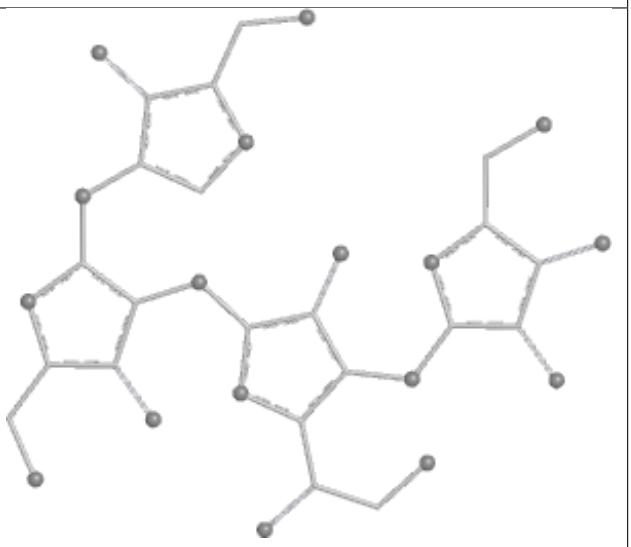
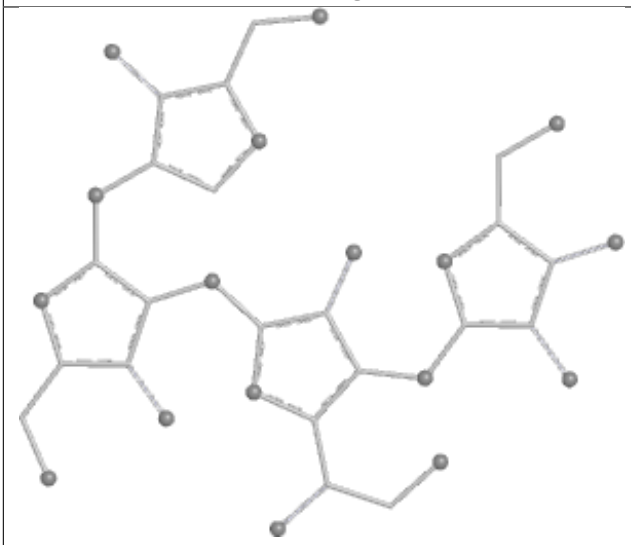
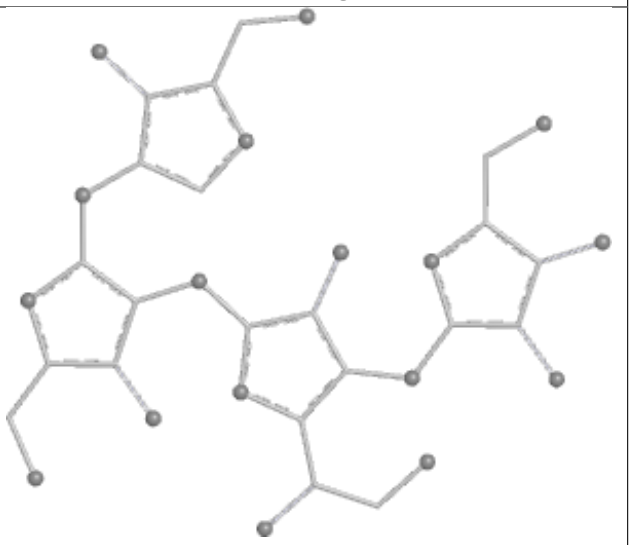
 Bond lengths	 Bond angles
 Torsions	 Rings

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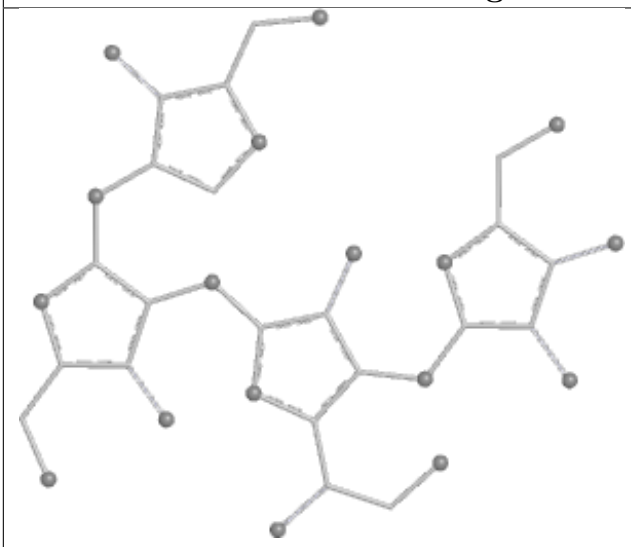
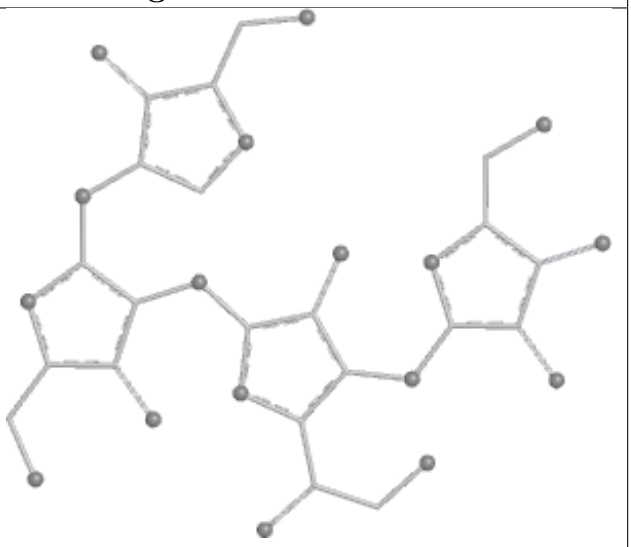
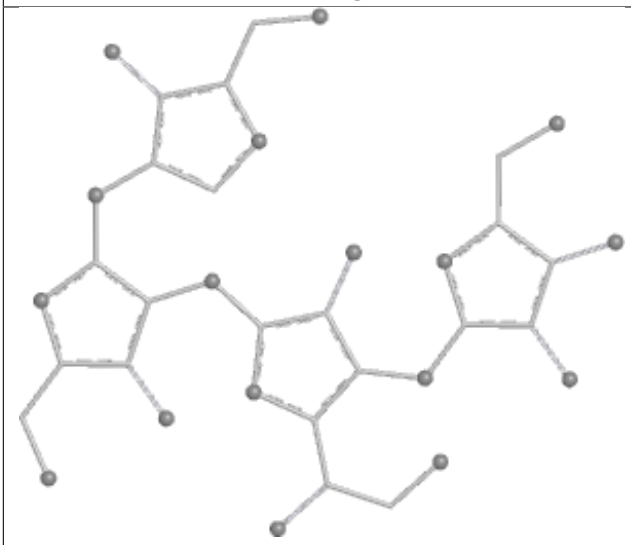
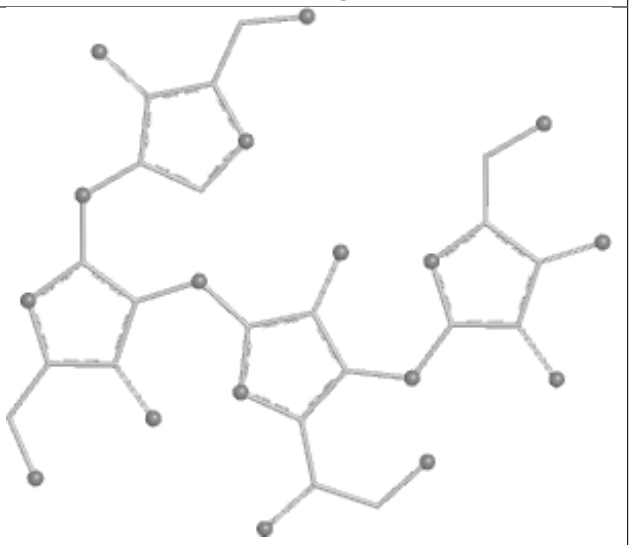
 Bond lengths	 Bond angles
 Torsions	 Rings

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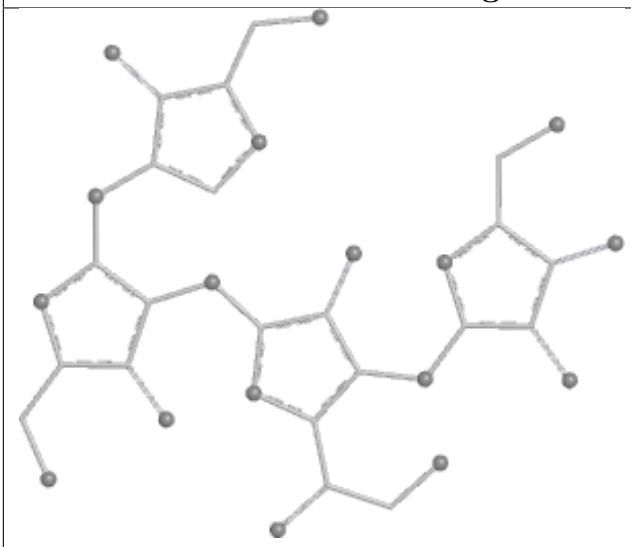
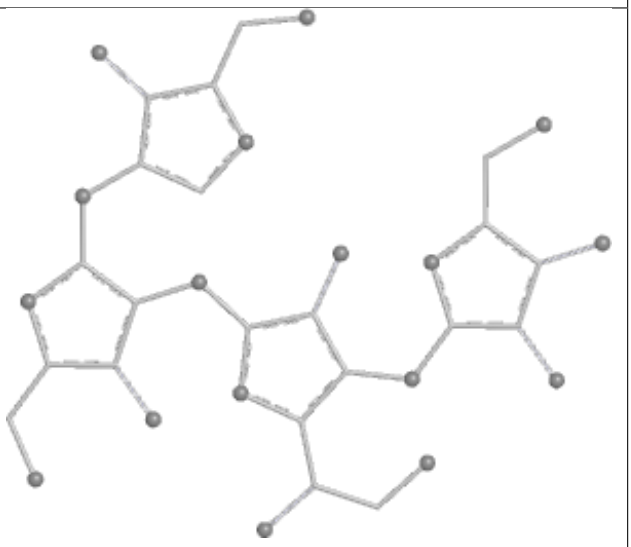
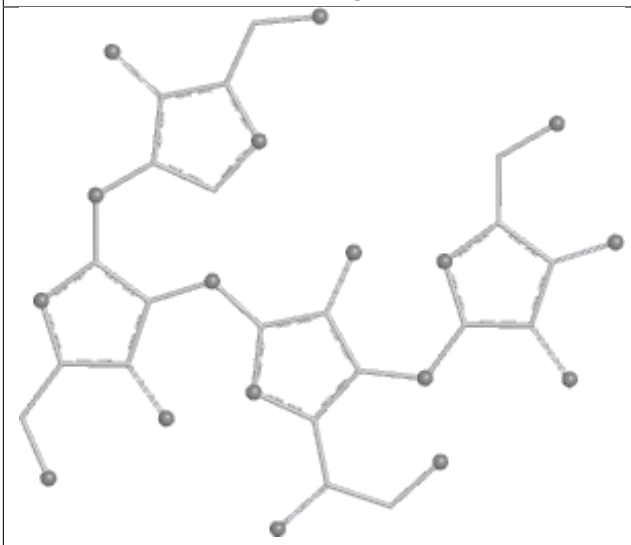
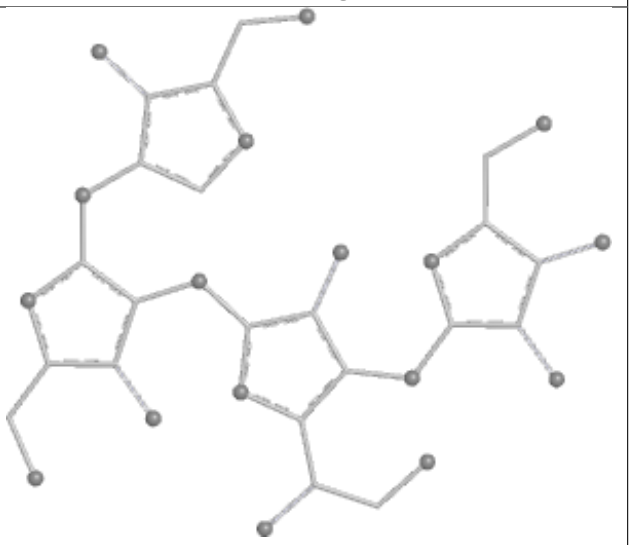
 Bond lengths	 Bond angles
 Torsions	 Rings

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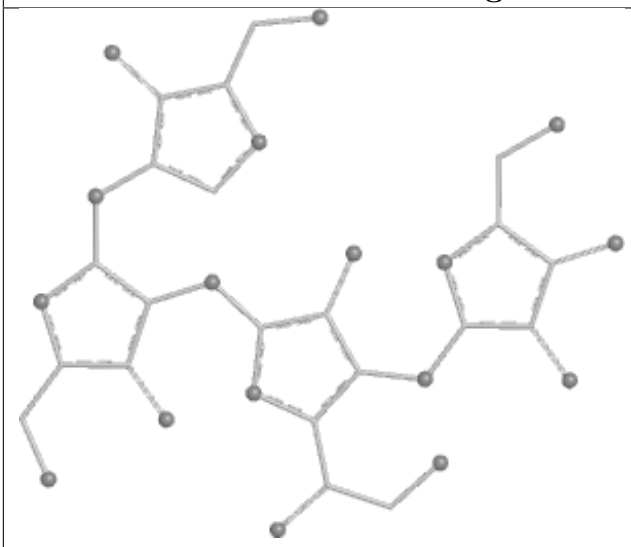	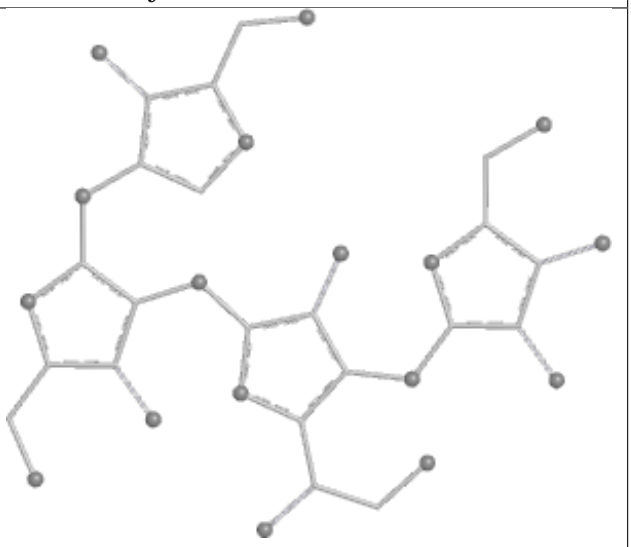
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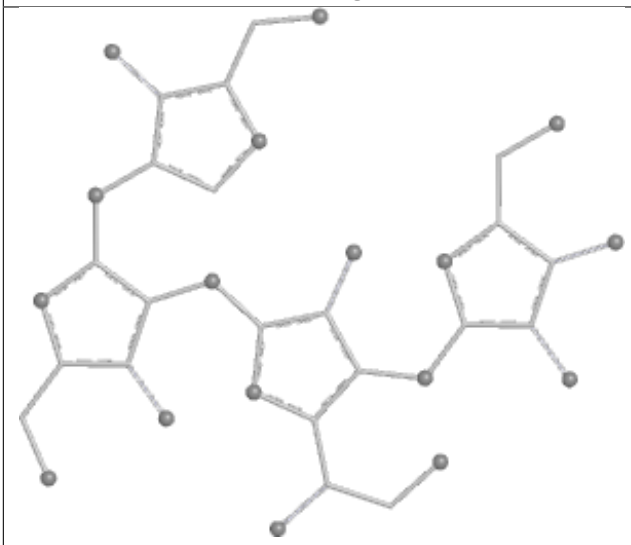	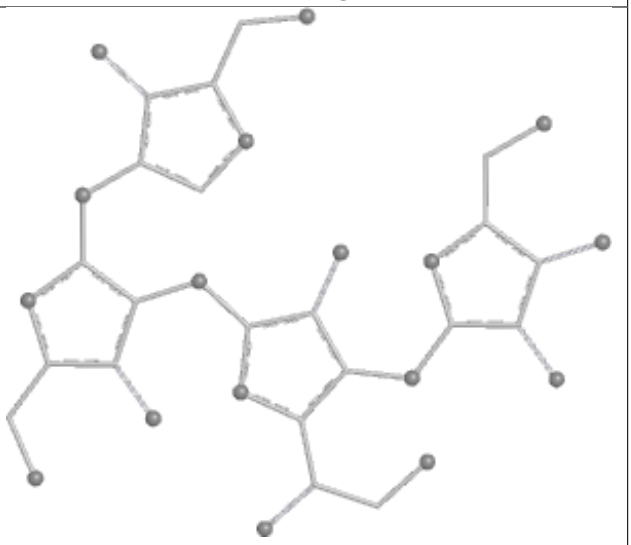
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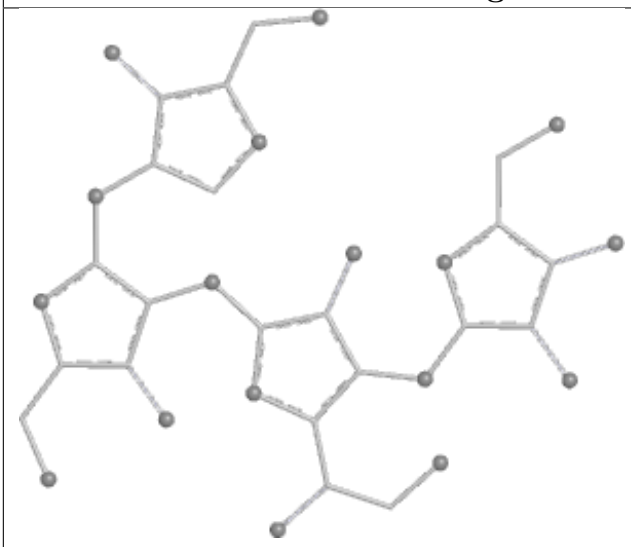	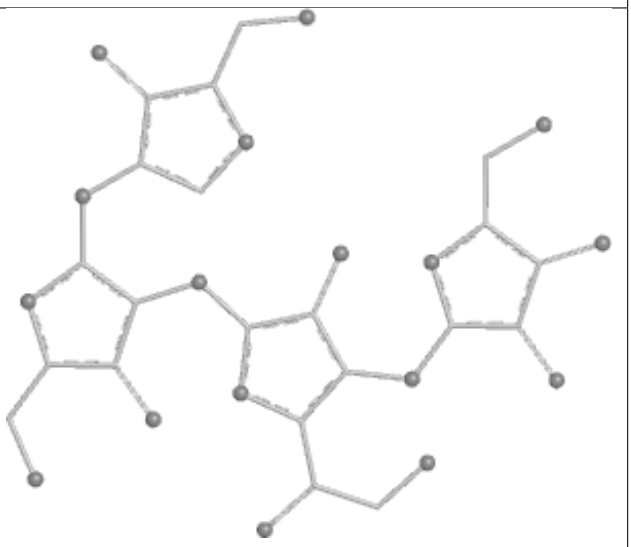
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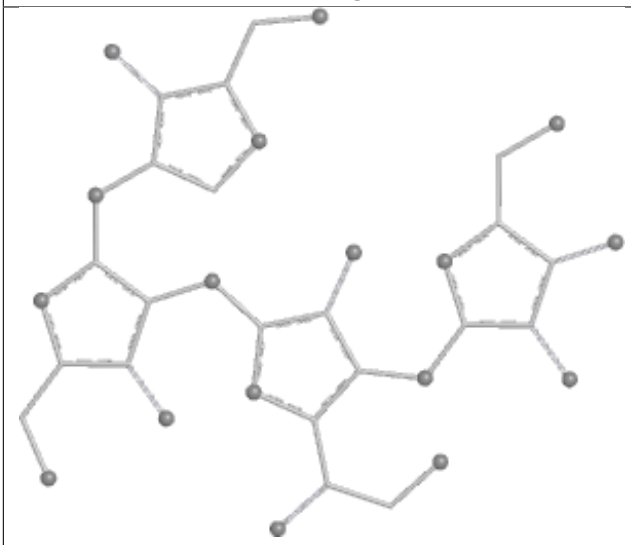	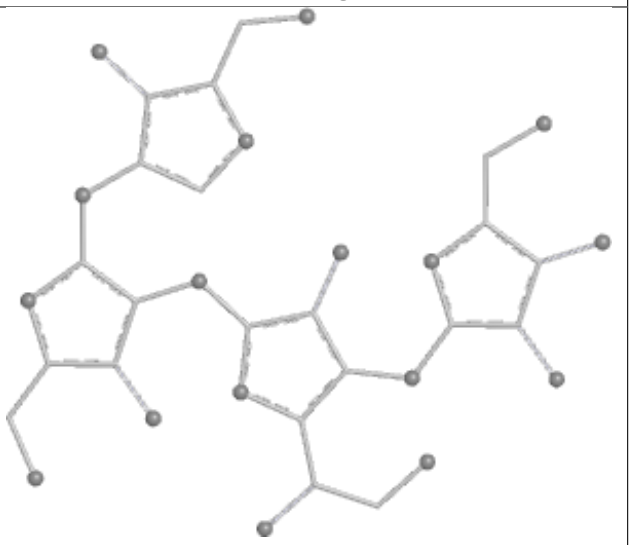
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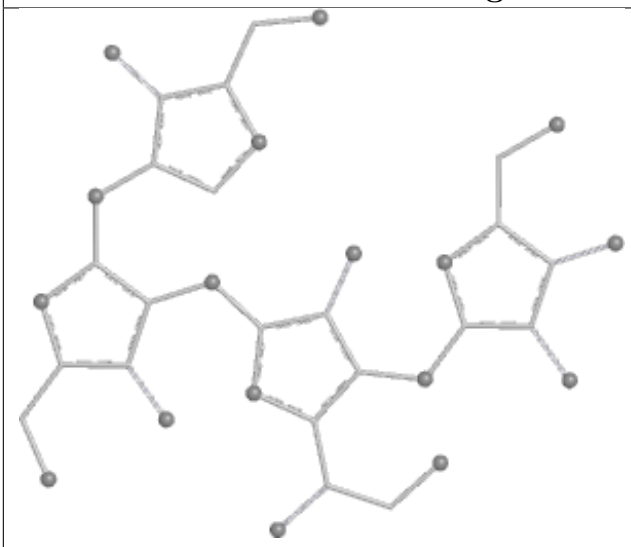
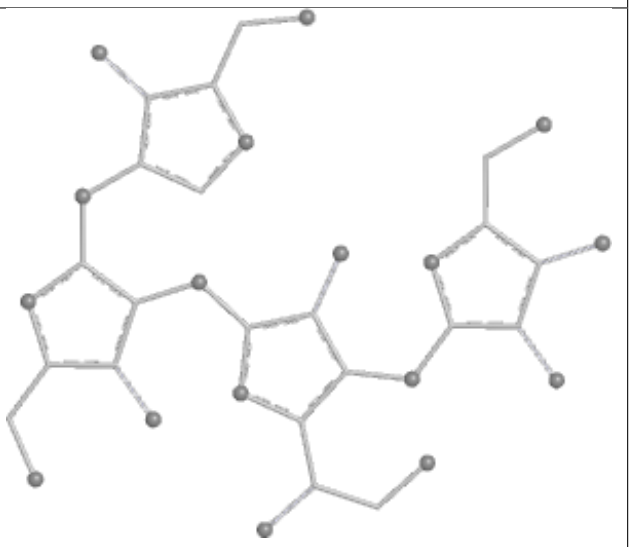
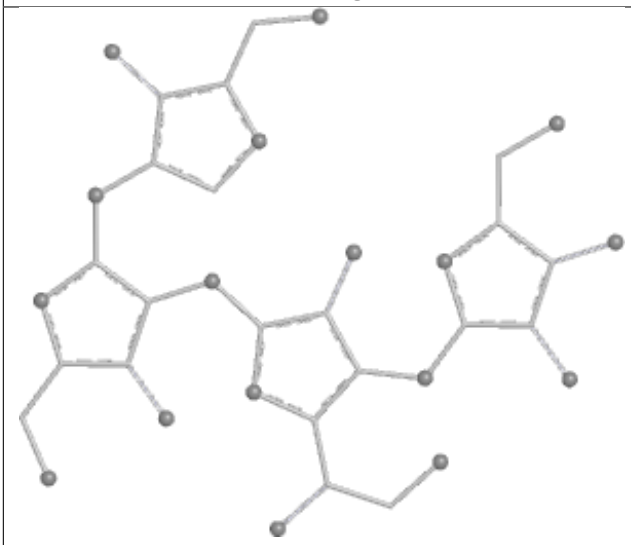
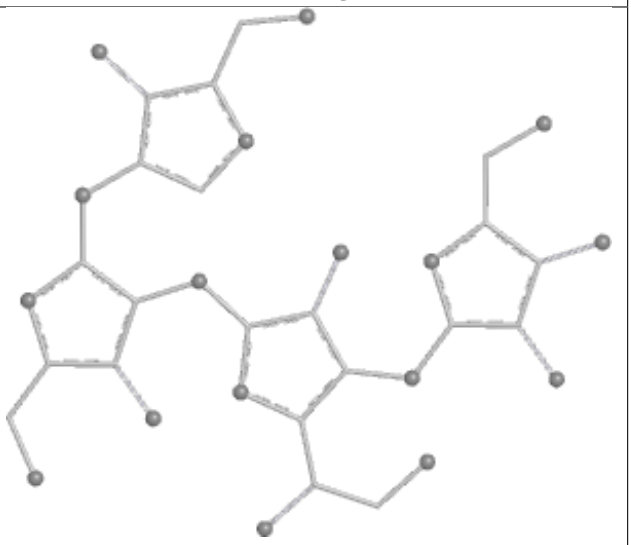
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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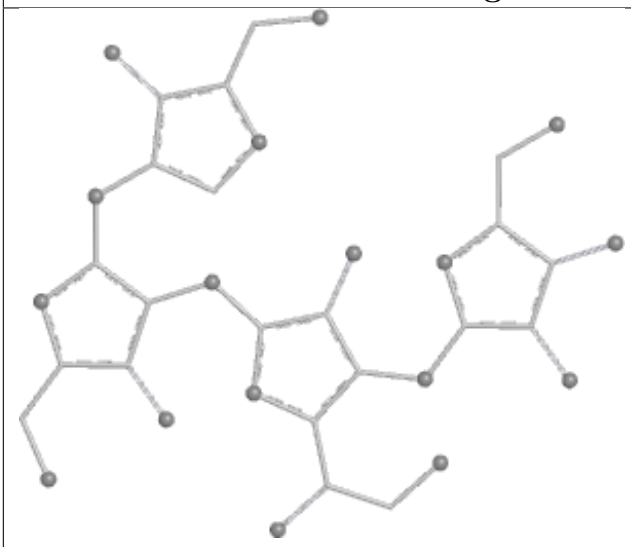
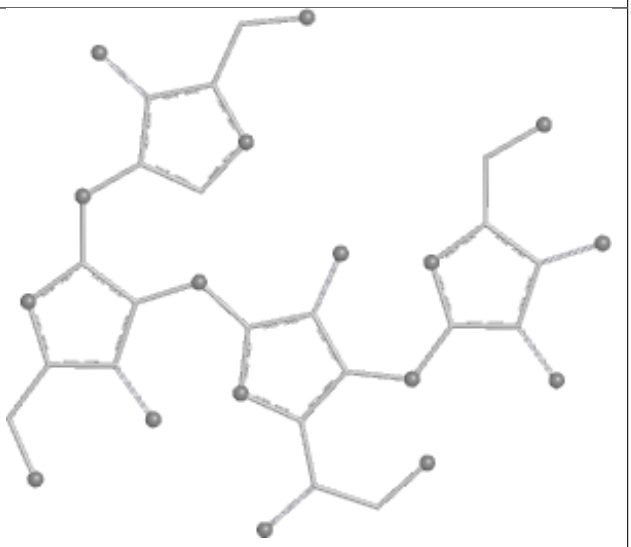
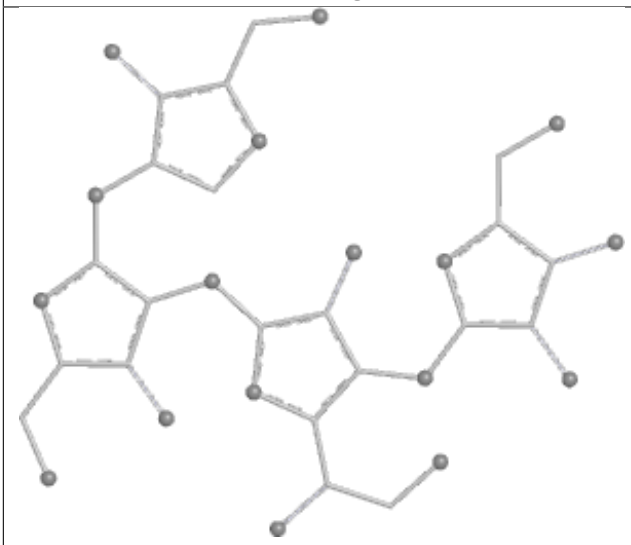
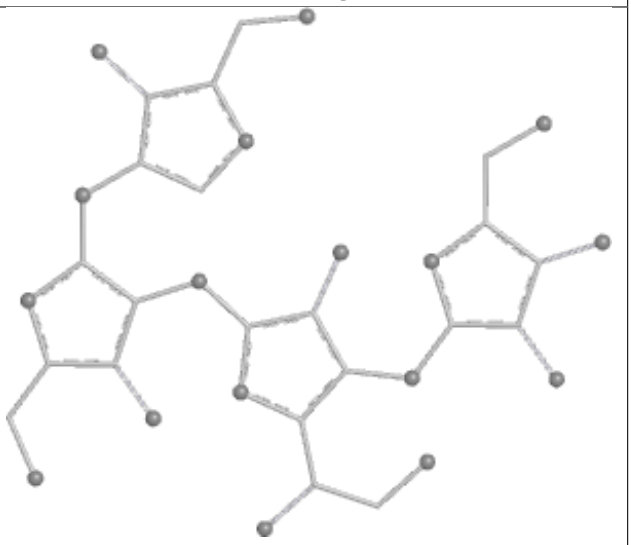
 Bond lengths	 Bond angles
 Torsions	 Rings

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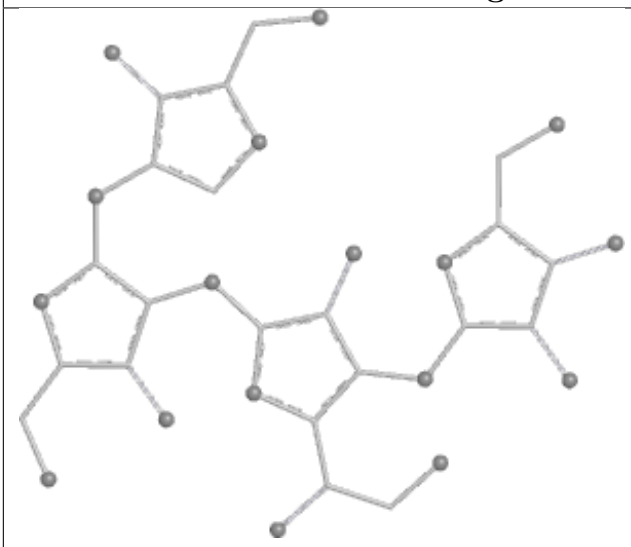
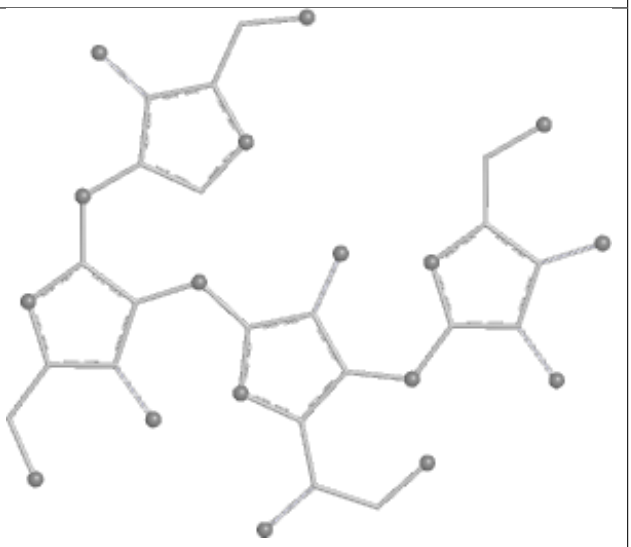
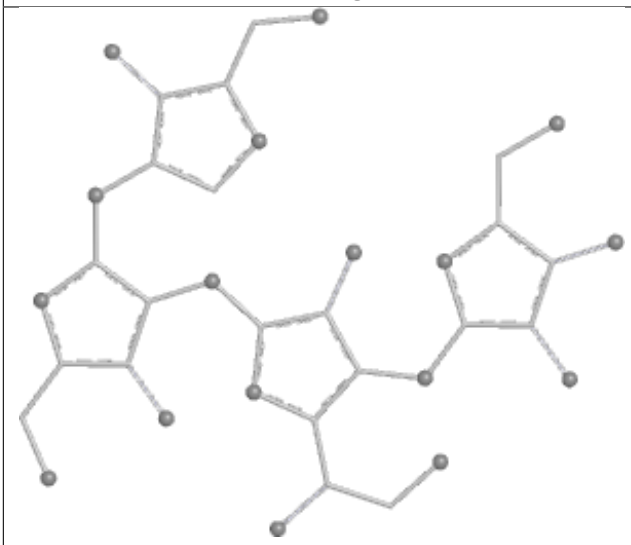
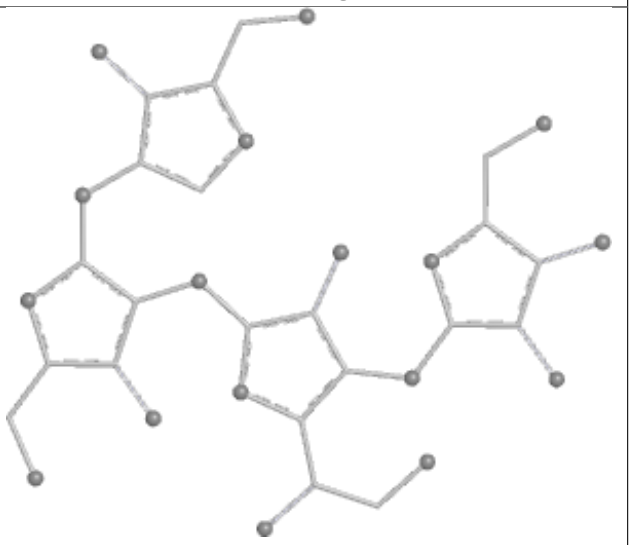
 Bond lengths	 Bond angles
 Torsions	 Rings

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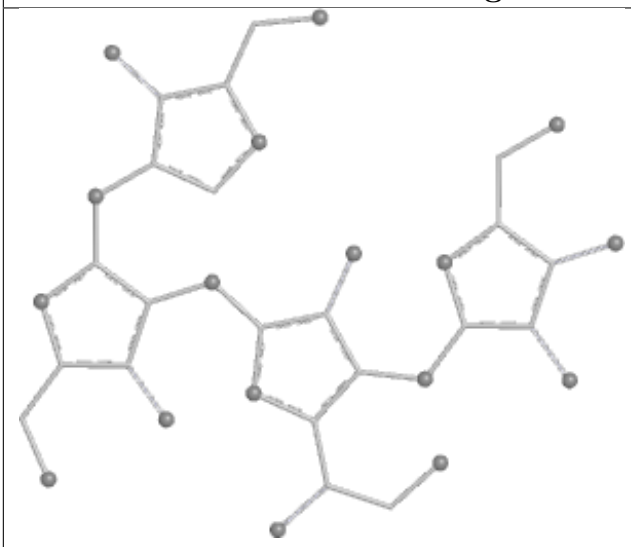
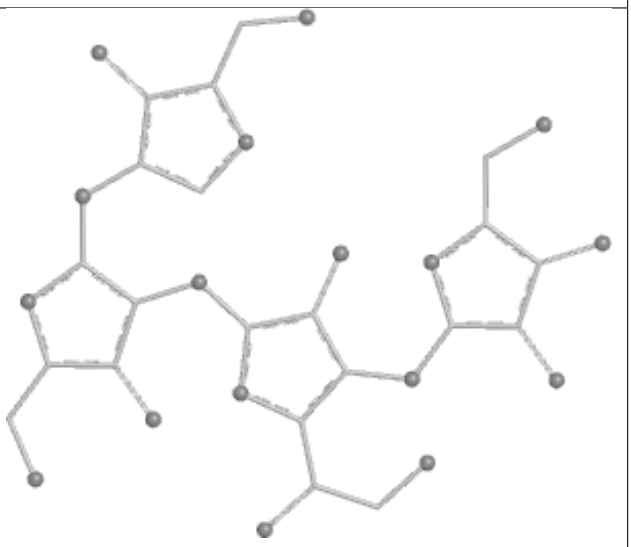
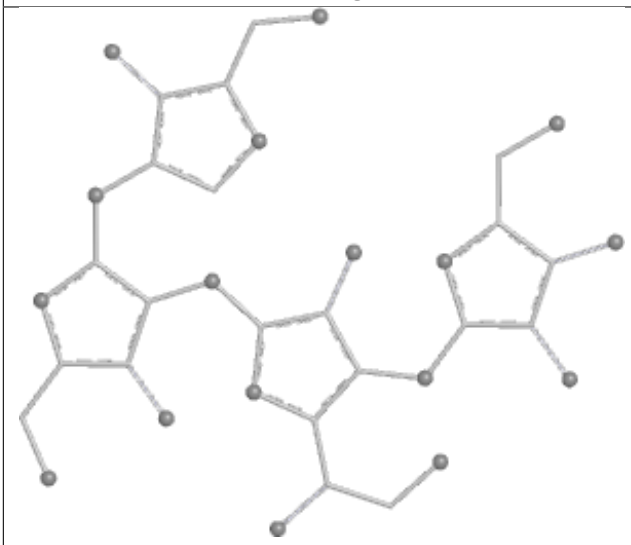
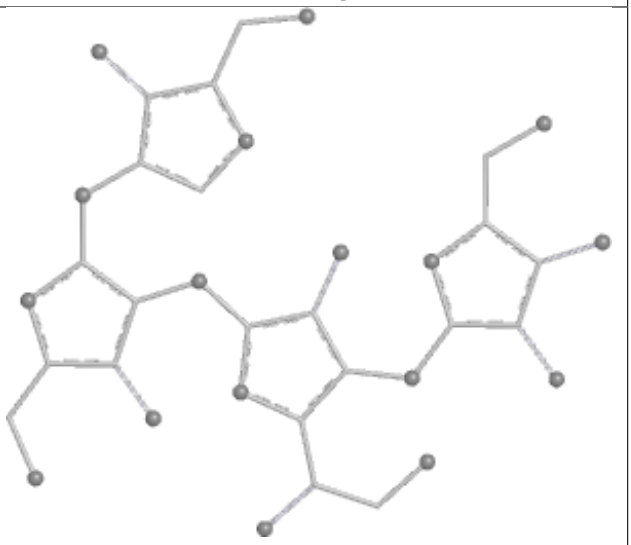
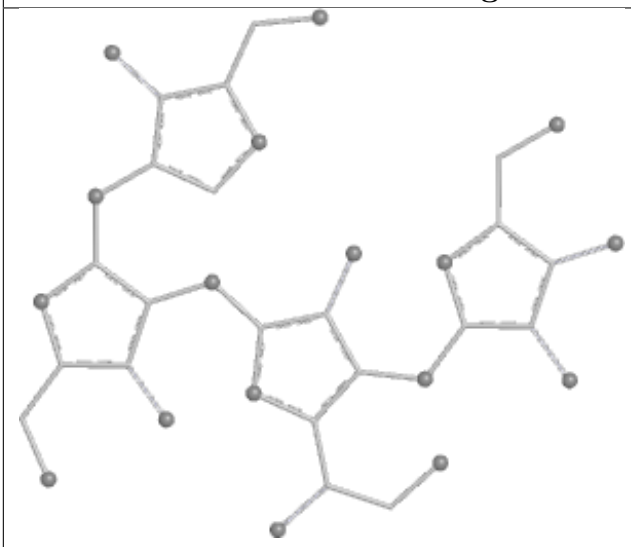
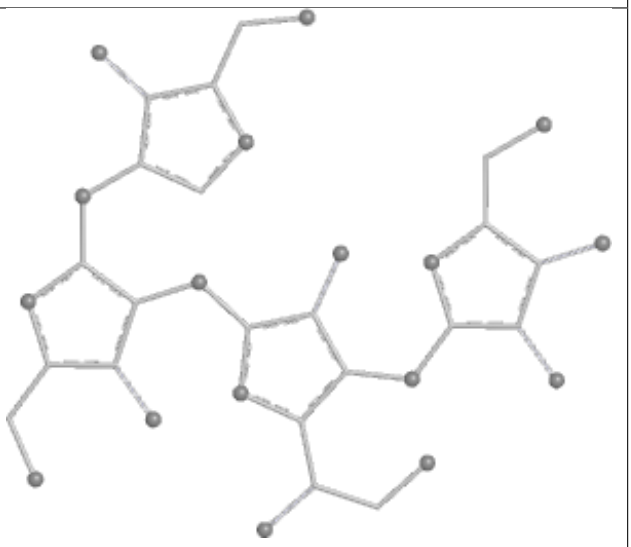
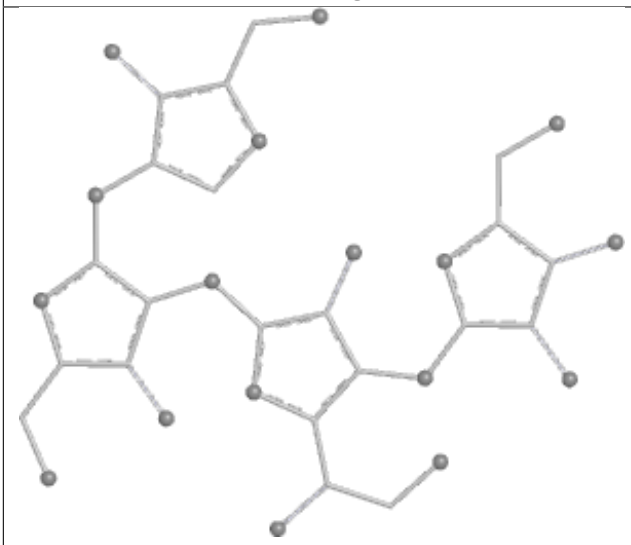
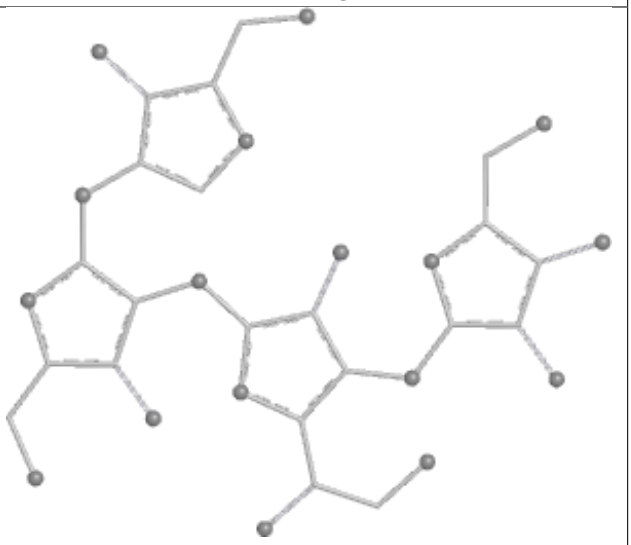
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain wD	
 Bond lengths	 Bond angles
 Torsions	 Rings

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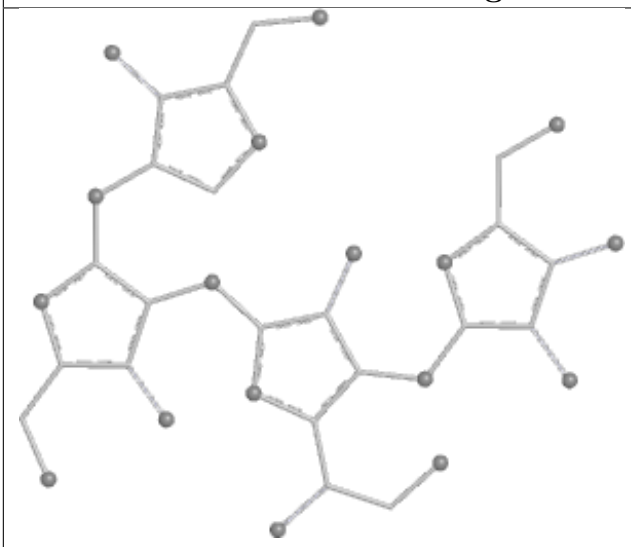
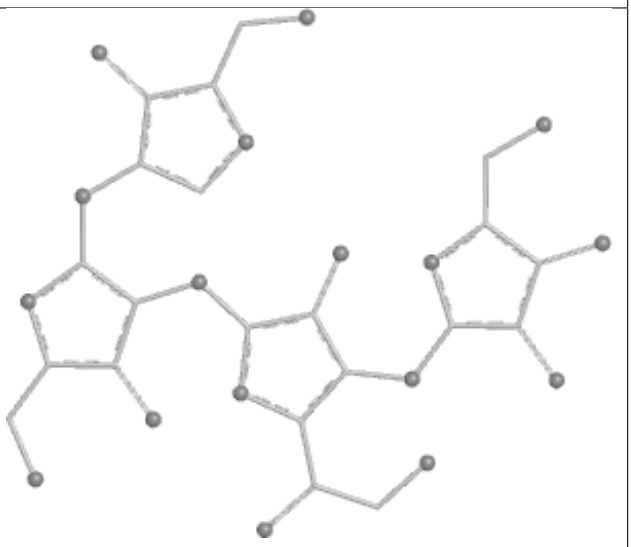
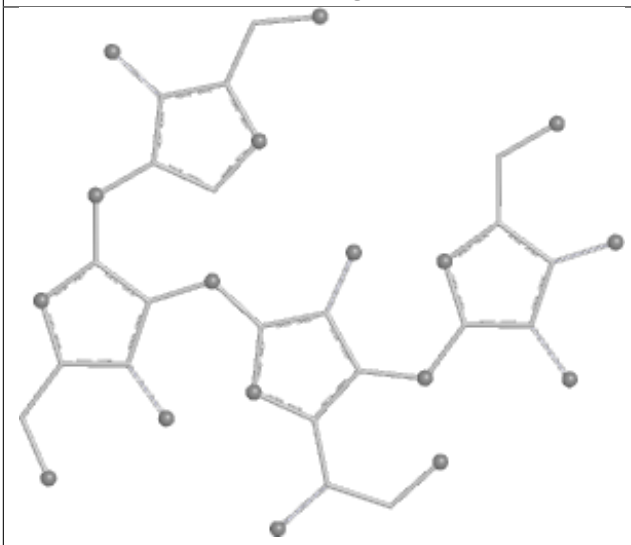
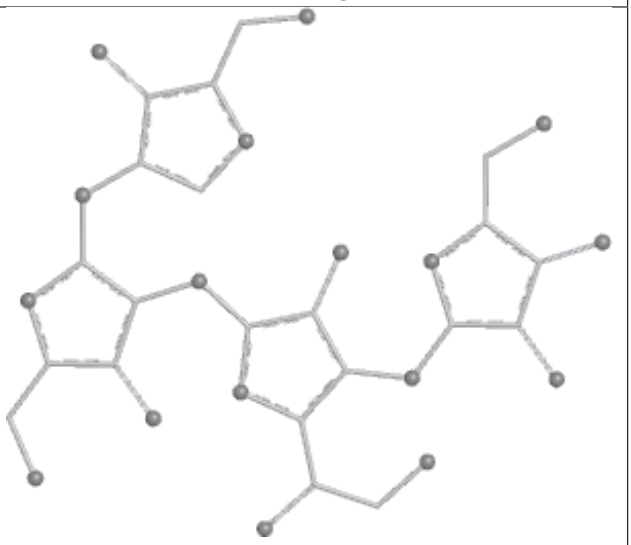
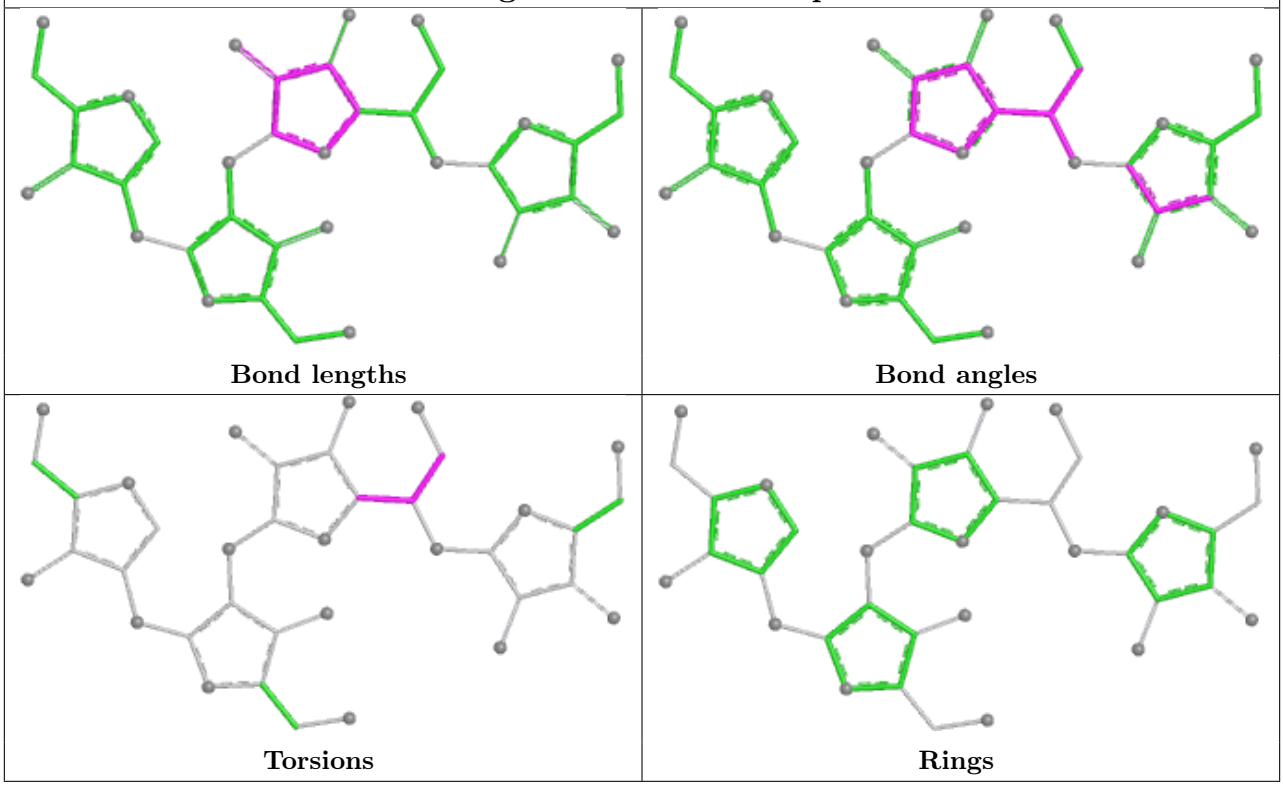
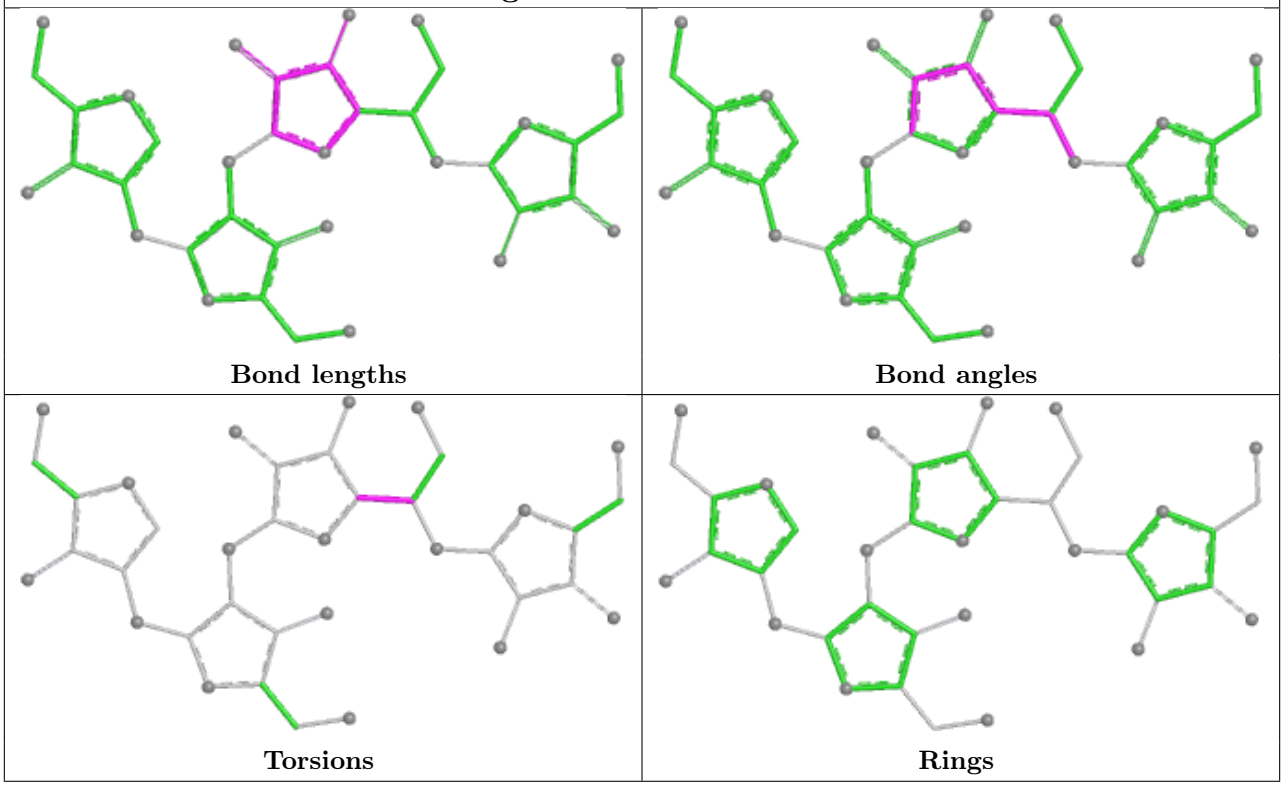
 Bond lengths	 Bond angles
 Torsions	 Rings

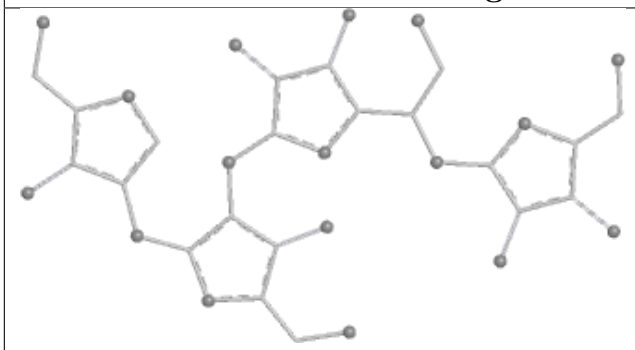
Oligosaccharide Chain p



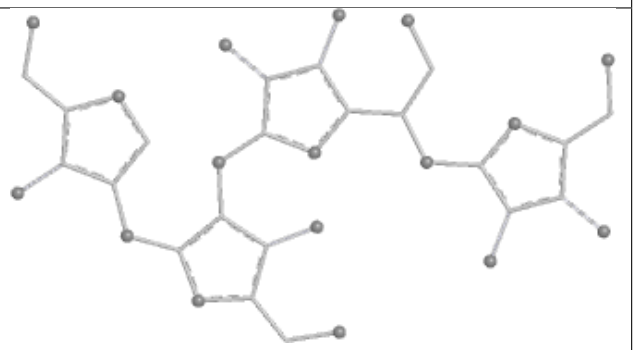
Oligosaccharide Chain s



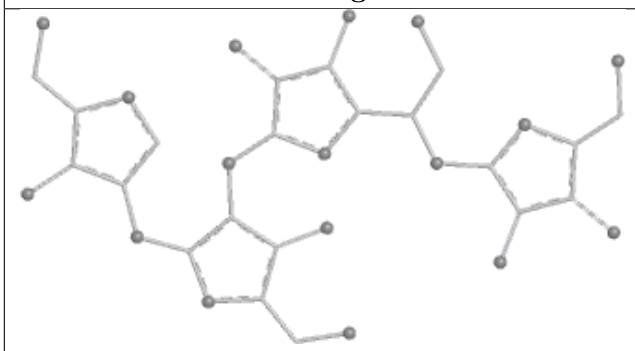
Oligosaccharide Chain nA



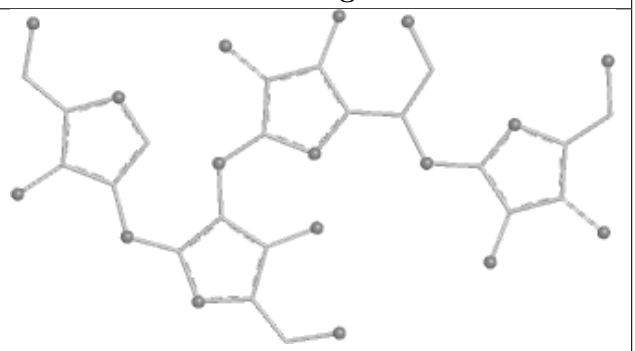
Bond lengths



Bond angles

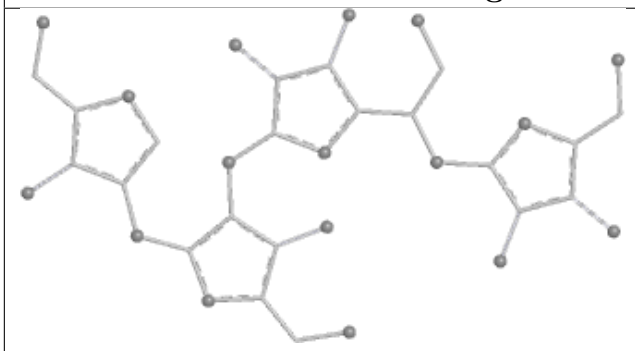


Torsions



Rings

Oligosaccharide Chain qA



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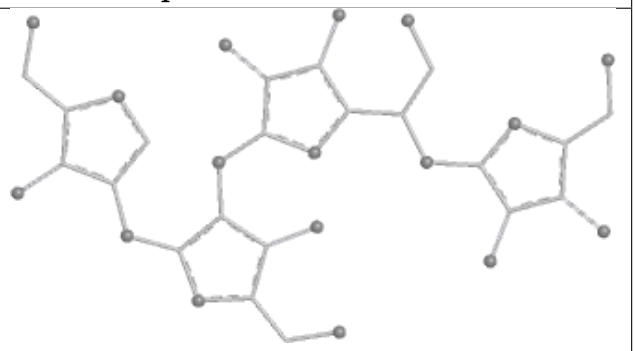

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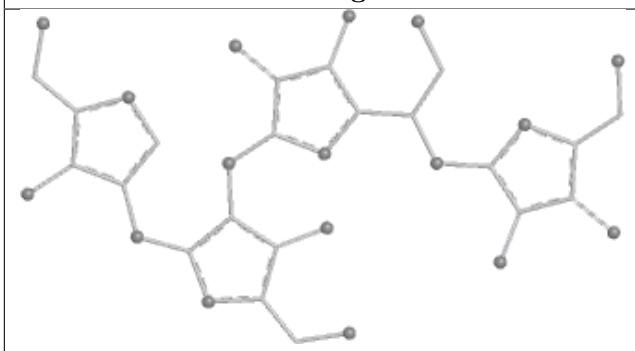

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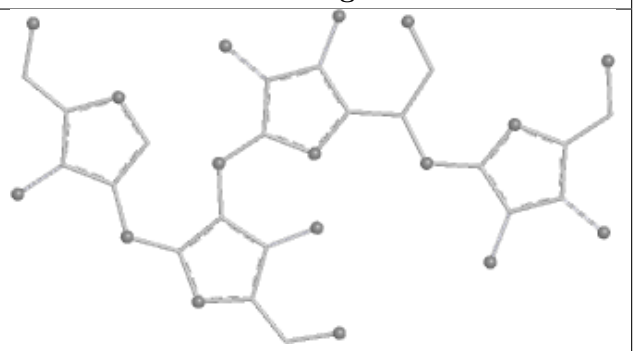
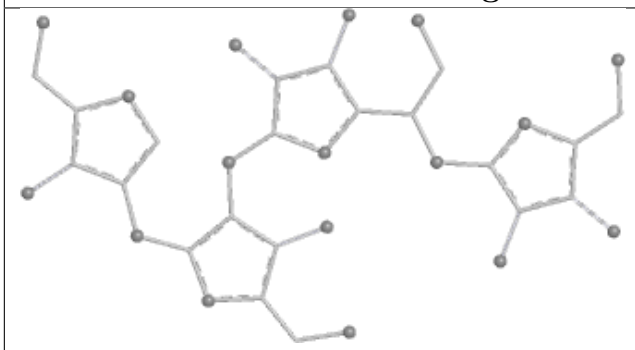


Rings

Oligosaccharide Chain HB



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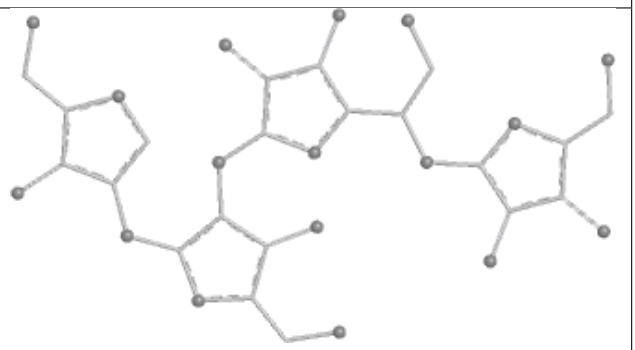

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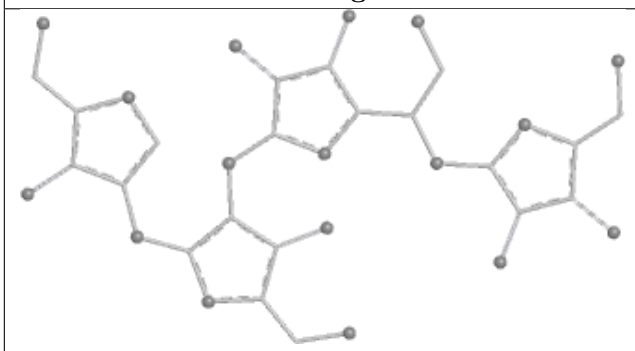

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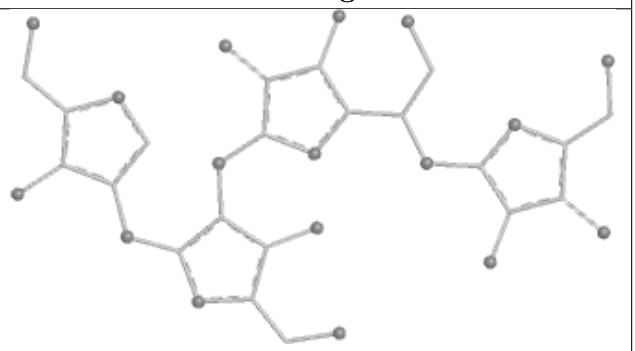
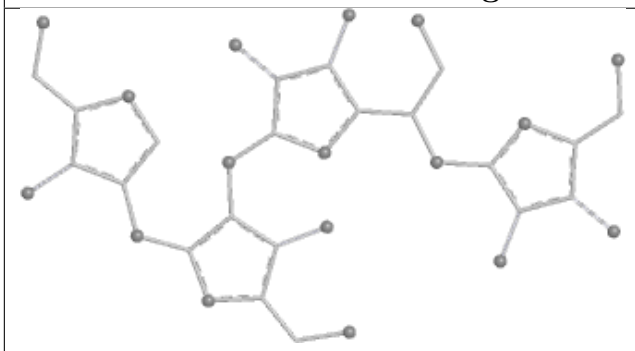


Rings

Oligosaccharide Chain KB



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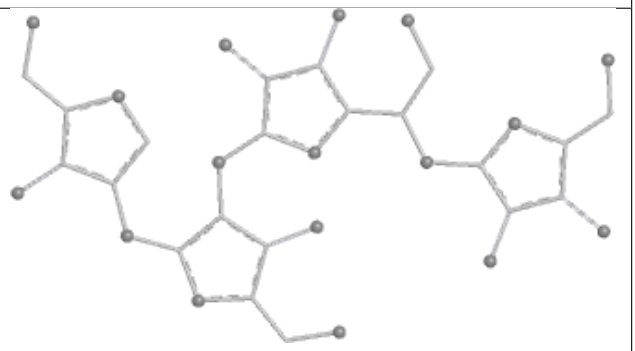

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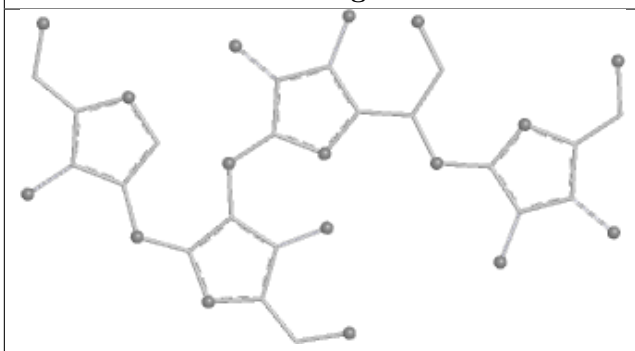

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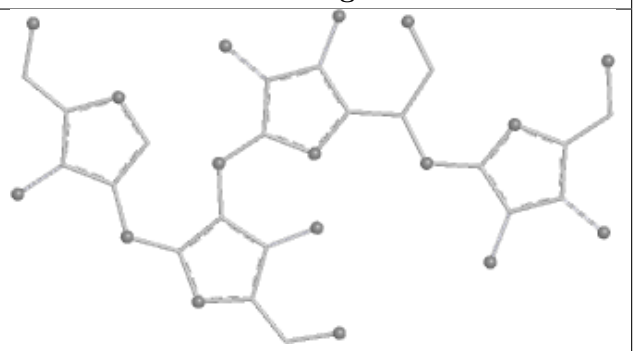
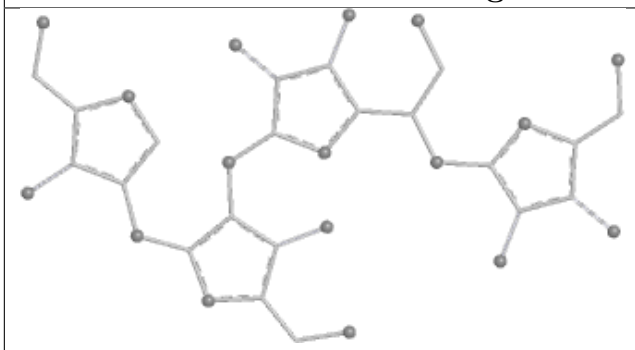


Rings

Oligosaccharide Chain kB



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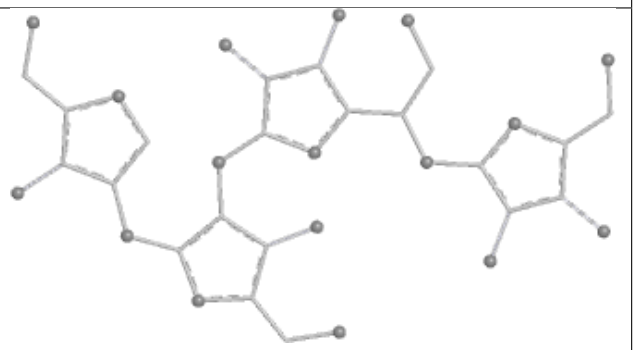

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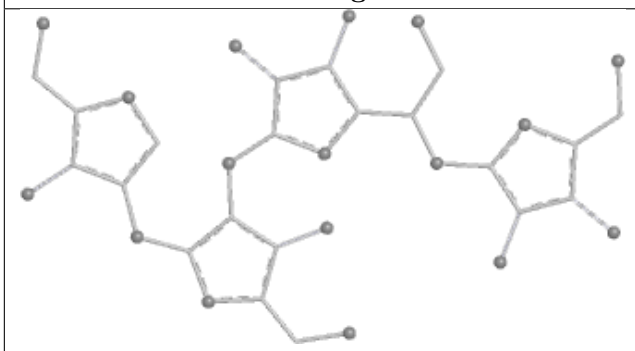

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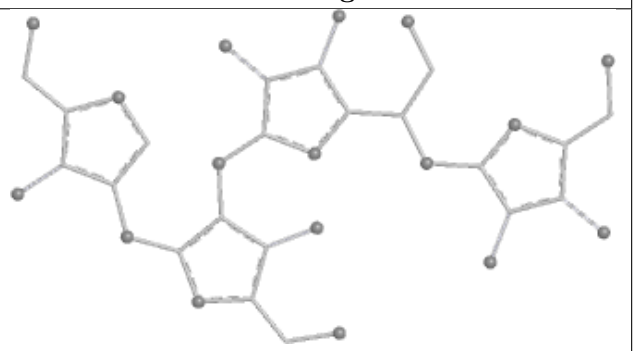
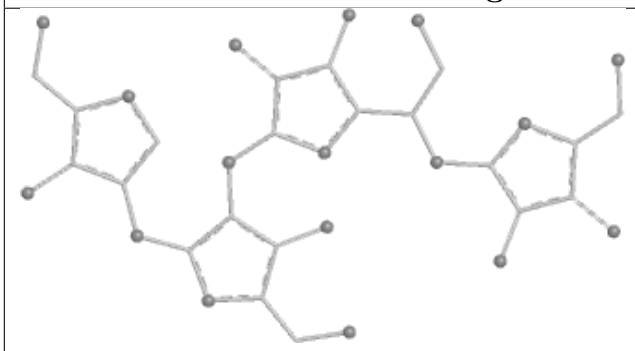


Rings

Oligosaccharide Chain nB



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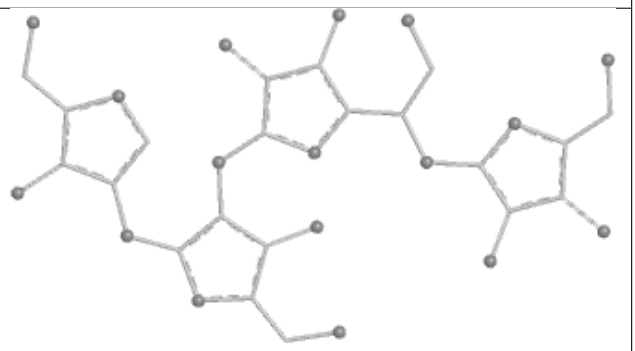

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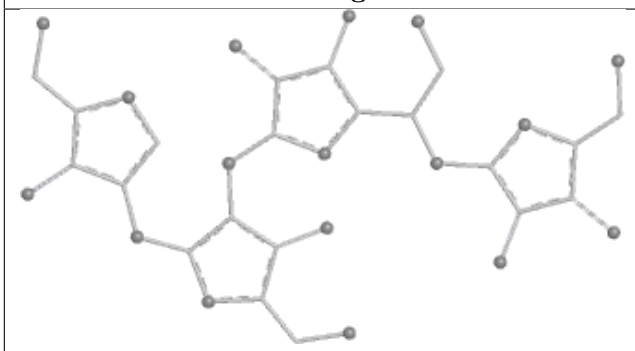

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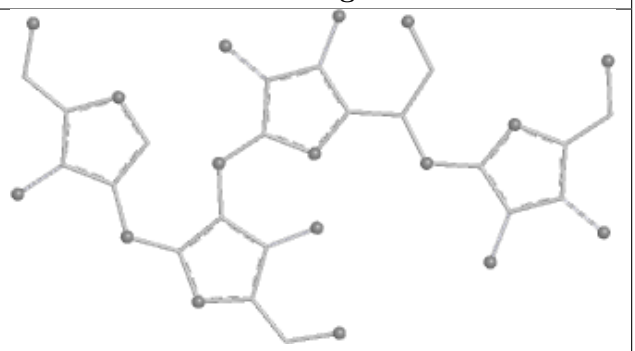
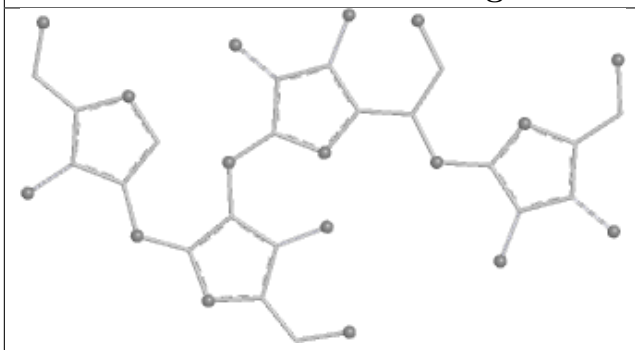


Rings

Oligosaccharide Chain hC



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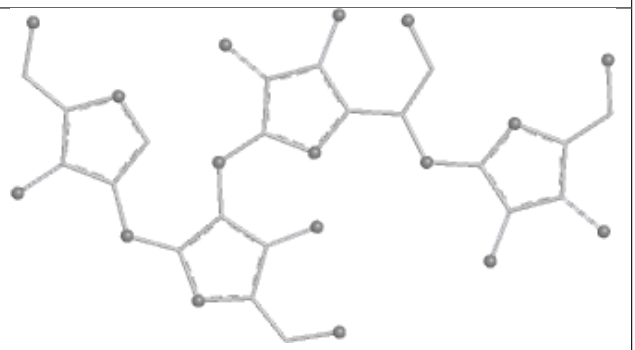

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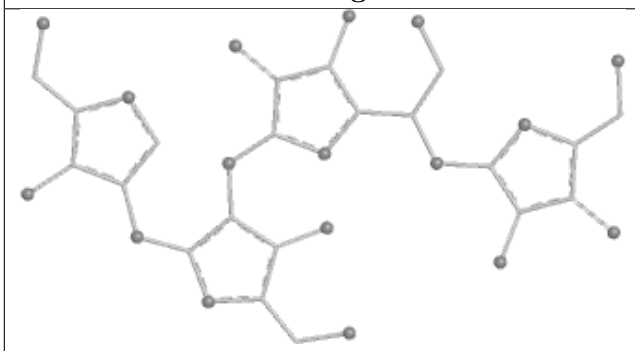

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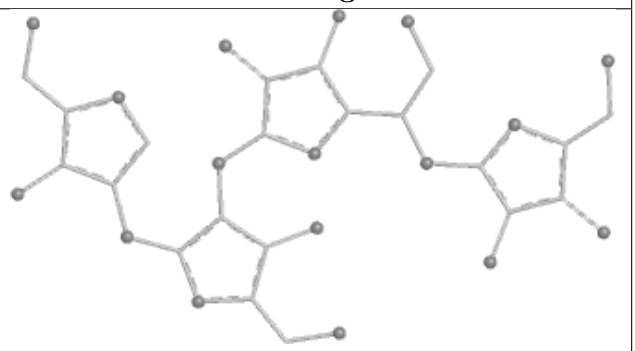
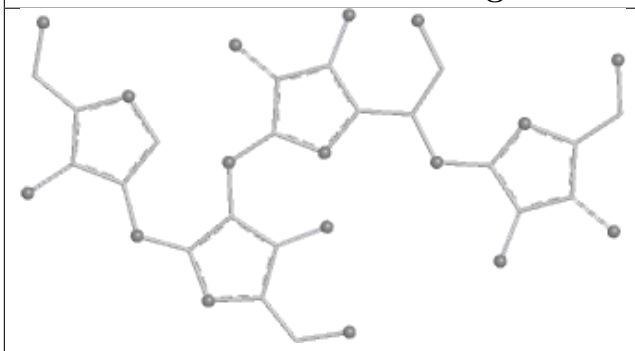


Rings

Oligosaccharide Chain kC



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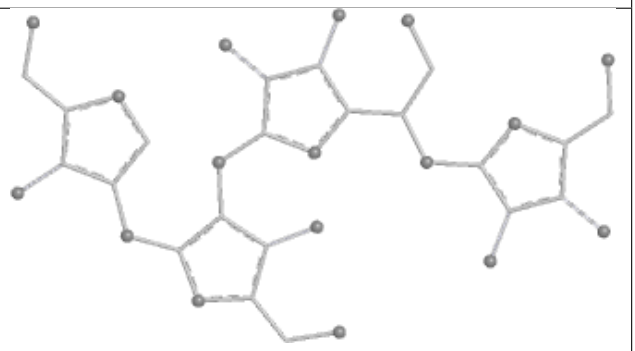

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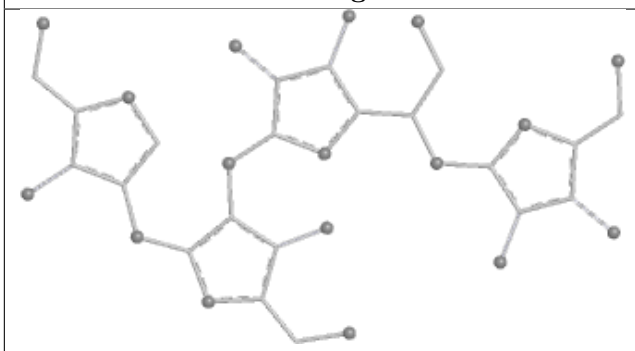

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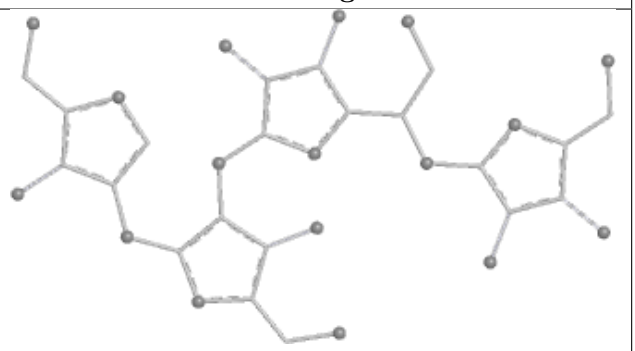
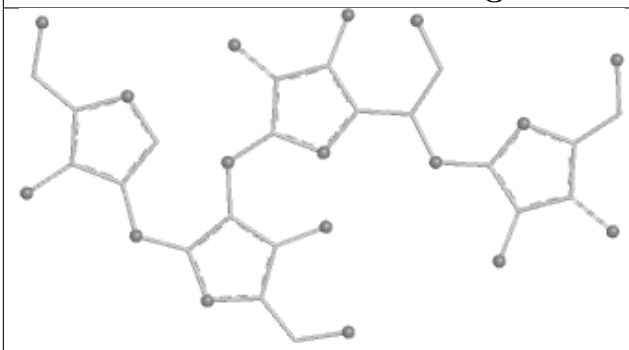
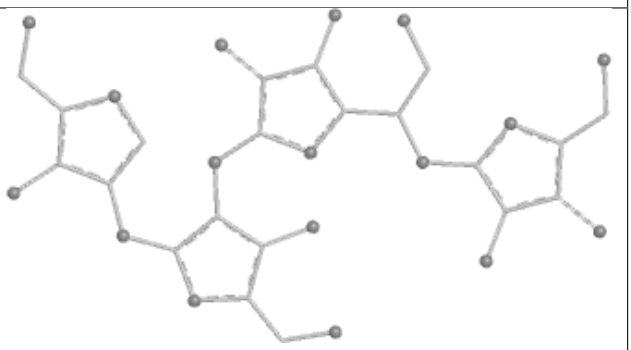
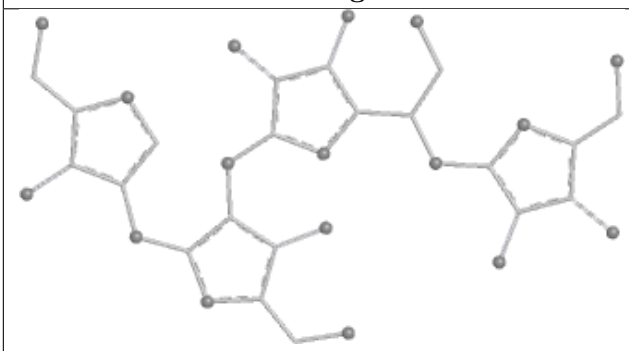
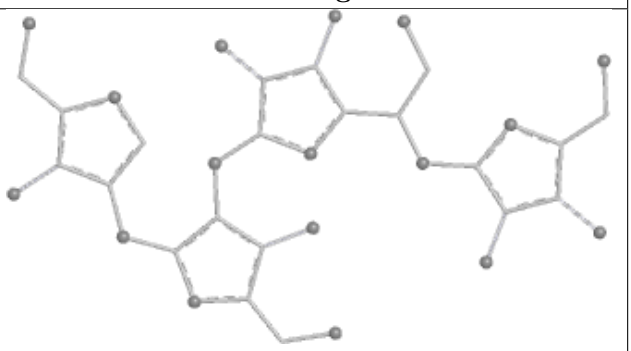
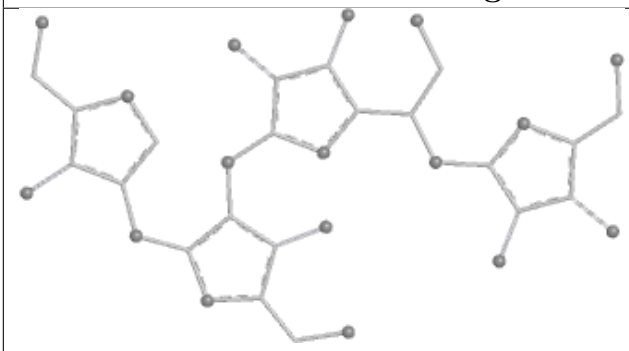
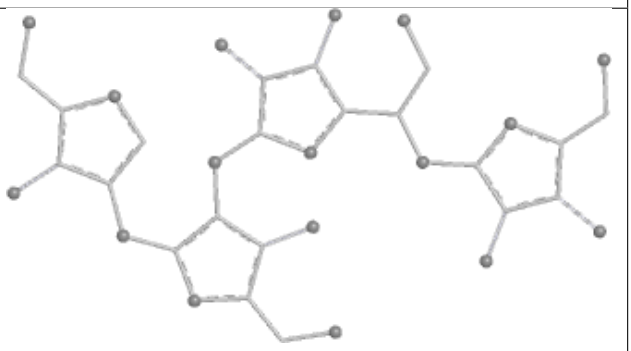
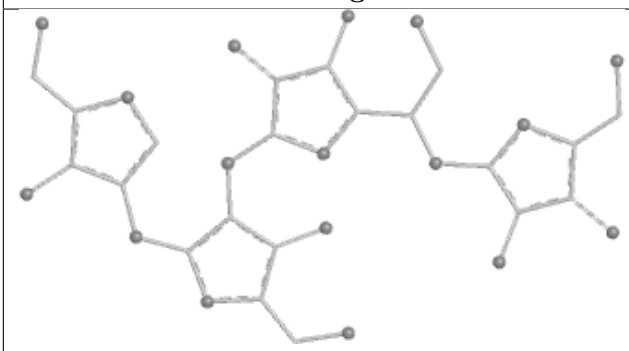
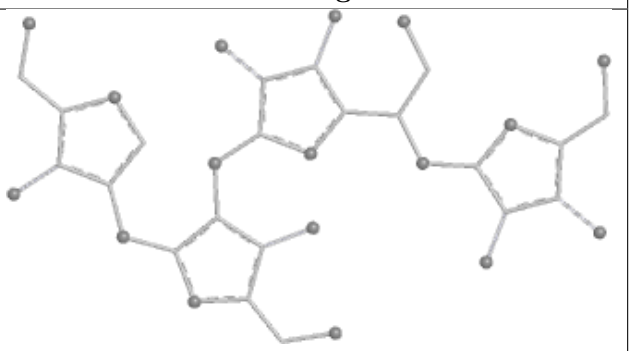
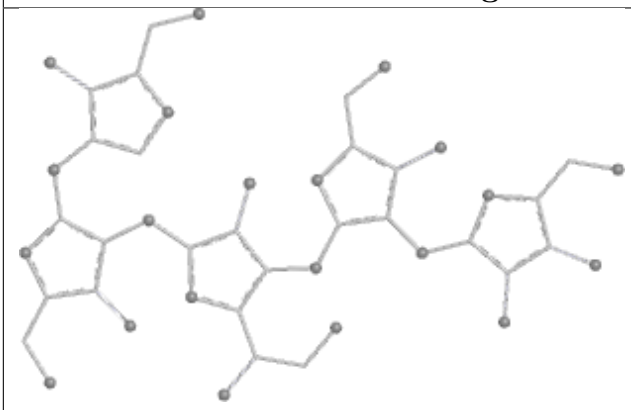
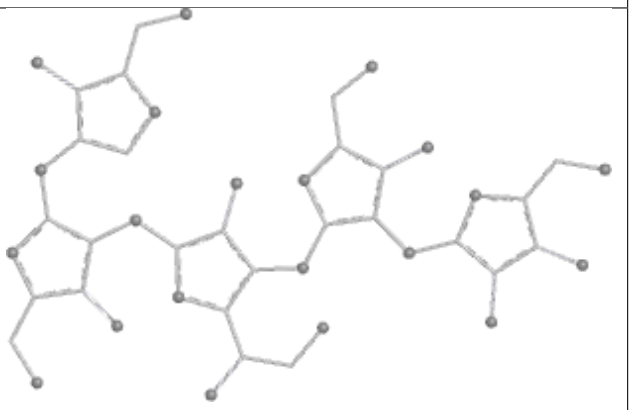
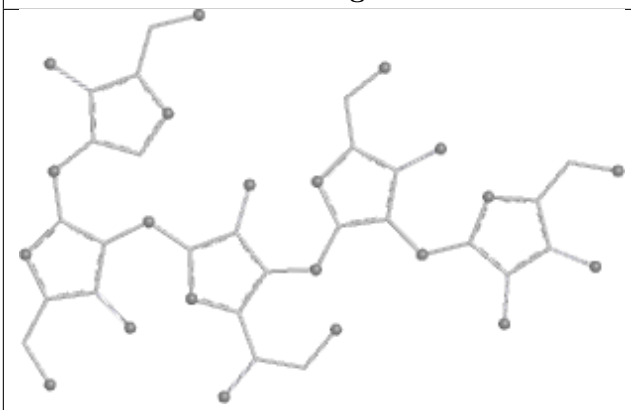
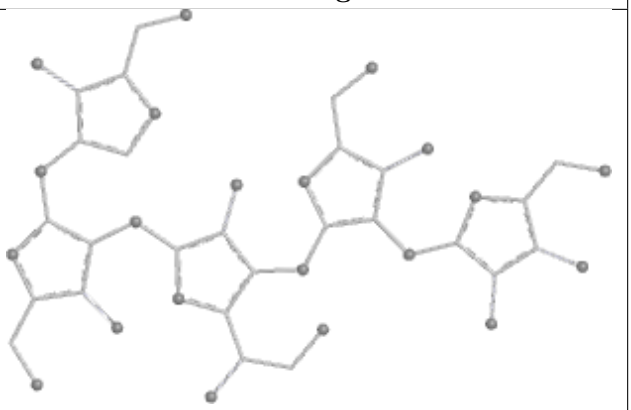


Rings

Oligosaccharide Chain eD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain hD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain CA	
 Bond lengths	 Bond angles
 Torsions	 Rings

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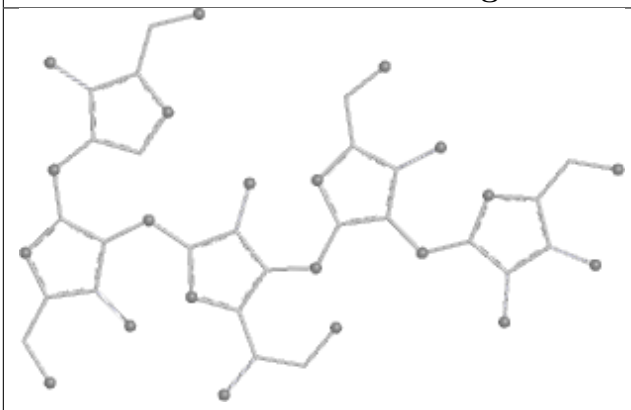
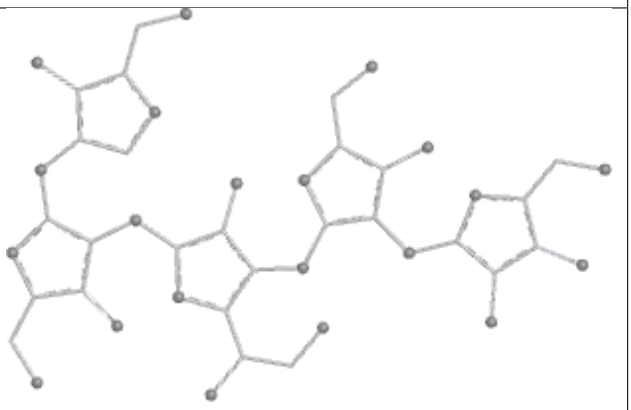
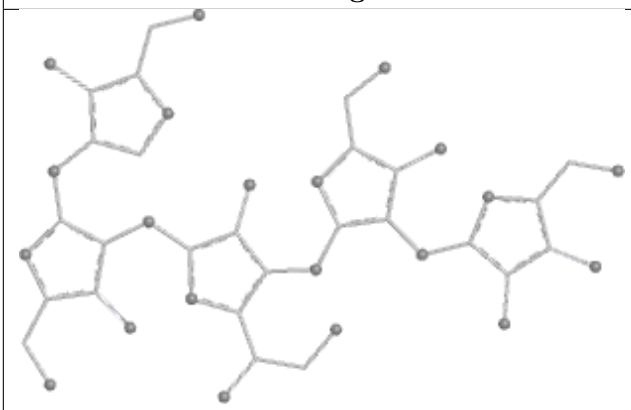
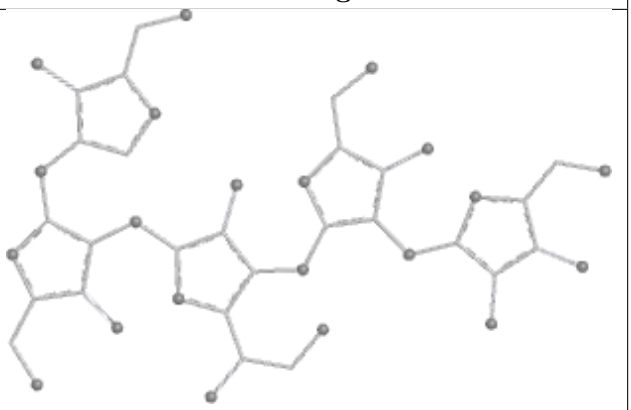
 Bond lengths	 Bond angles
 Torsions	 Rings

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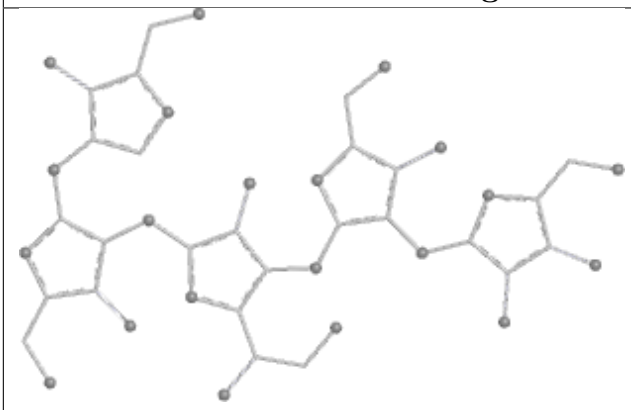
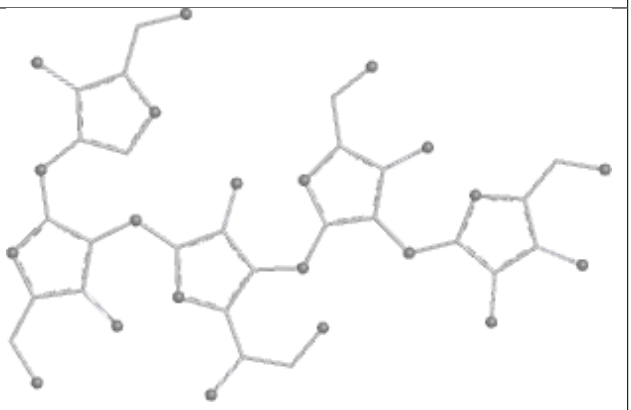
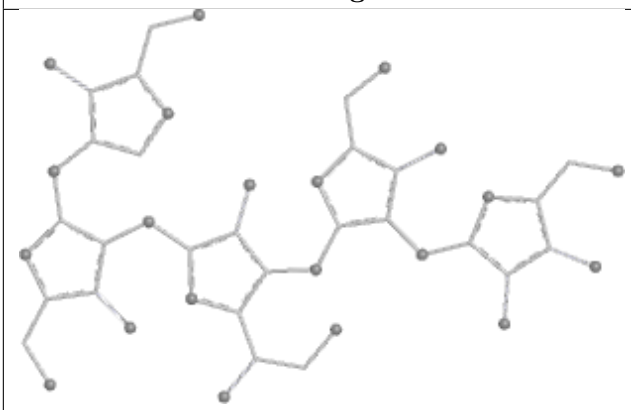
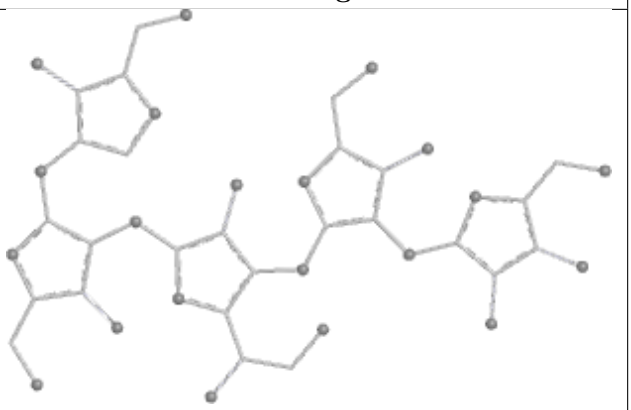
 Bond lengths	 Bond angles
 Torsions	 Rings

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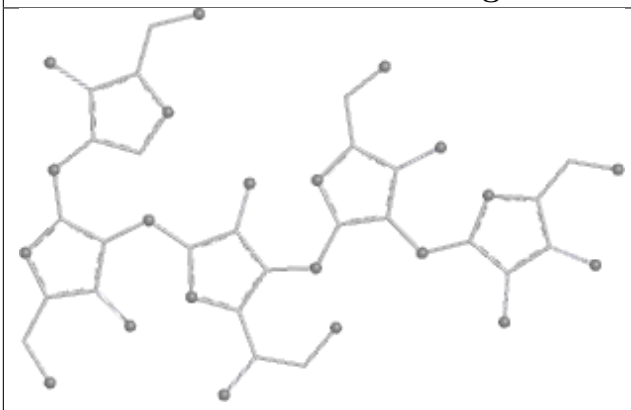
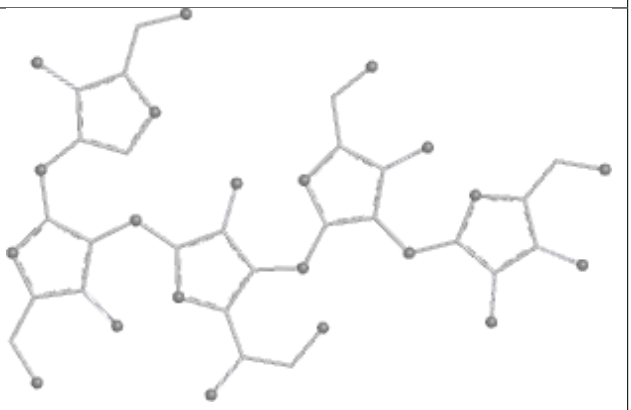
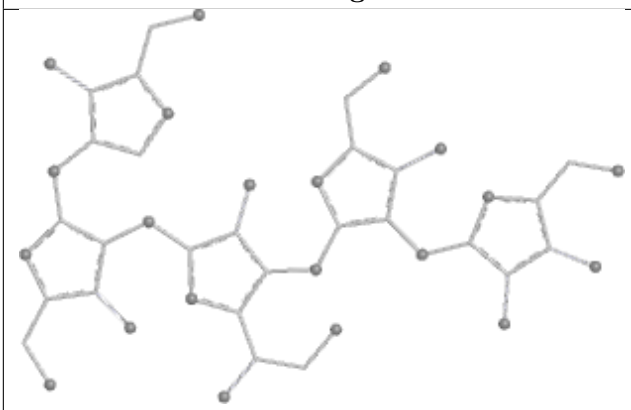
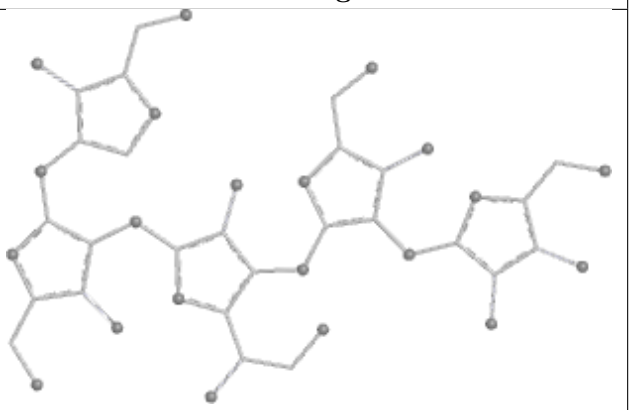
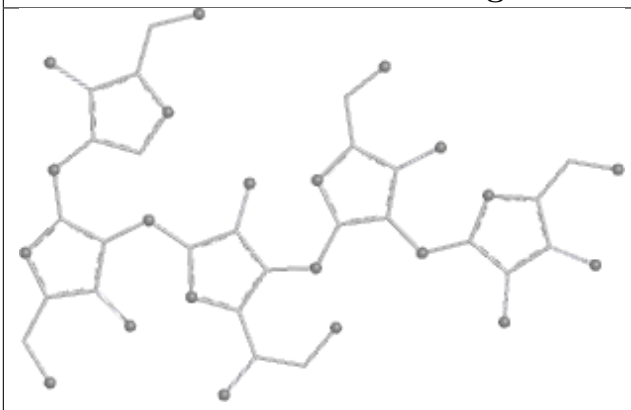
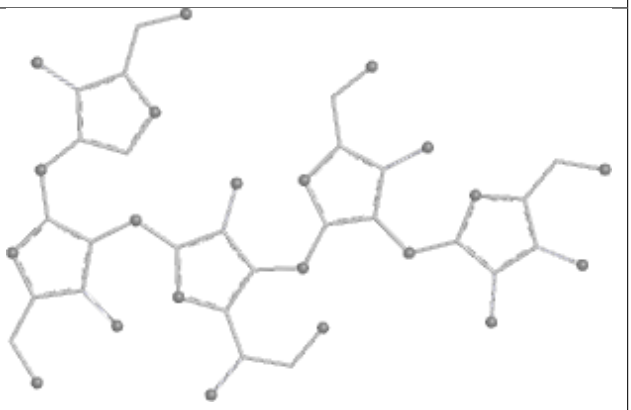
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain eB	
	
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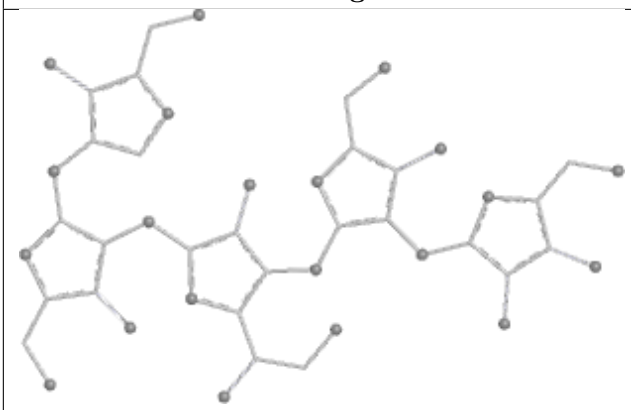
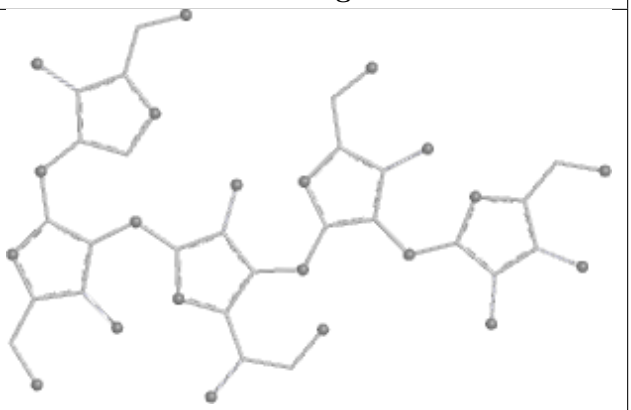
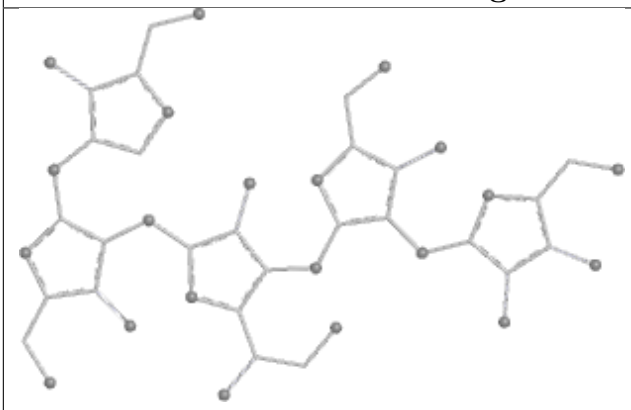
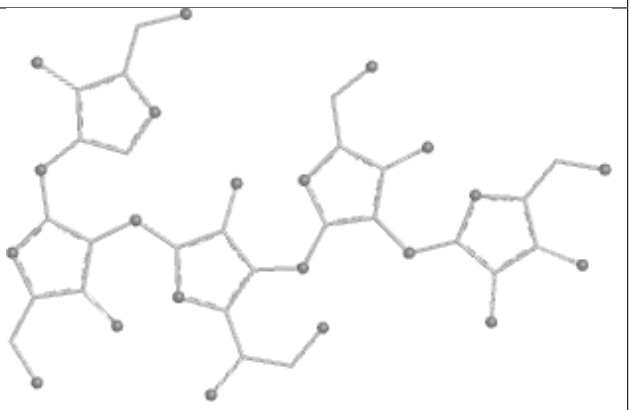
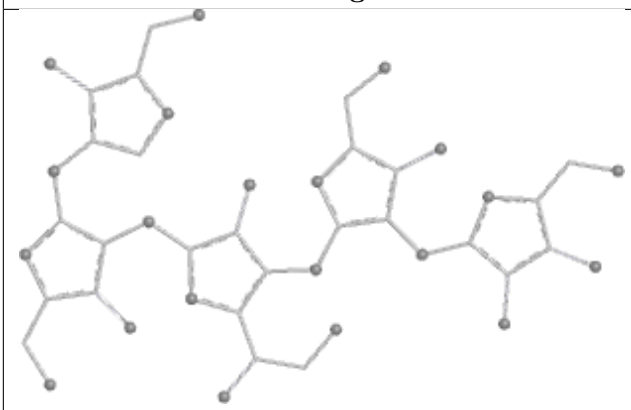
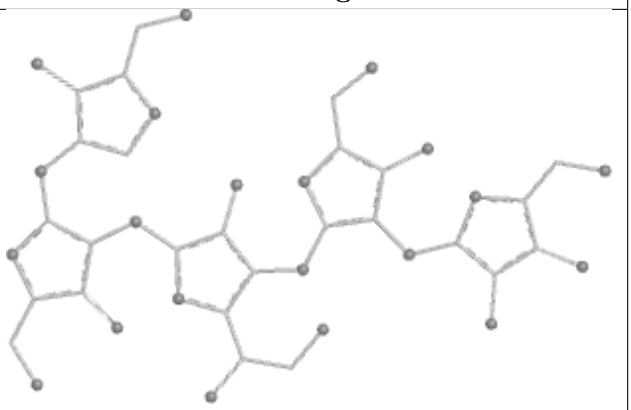
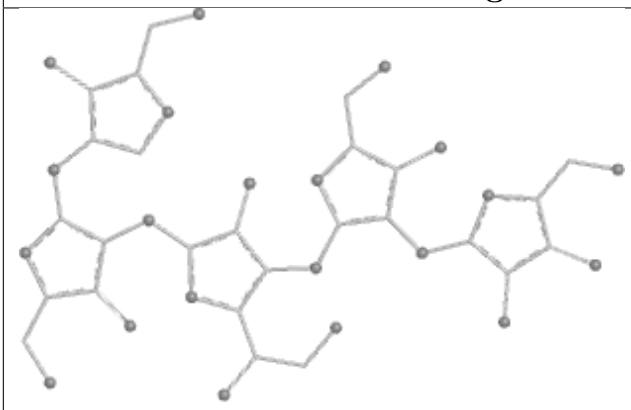
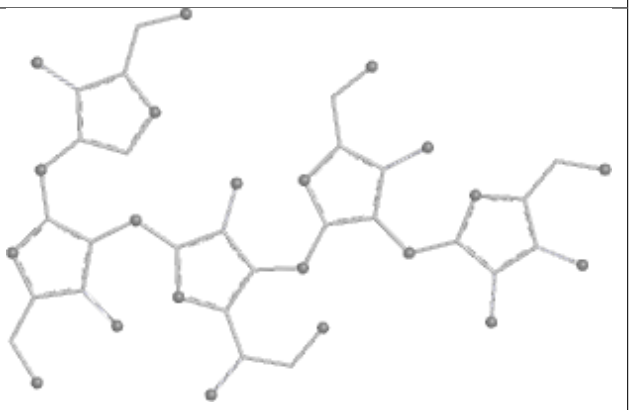
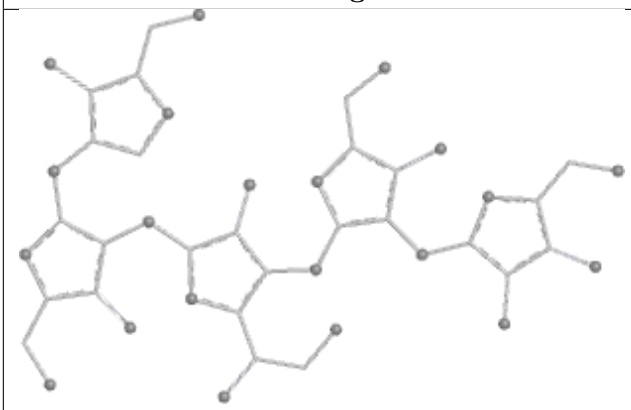
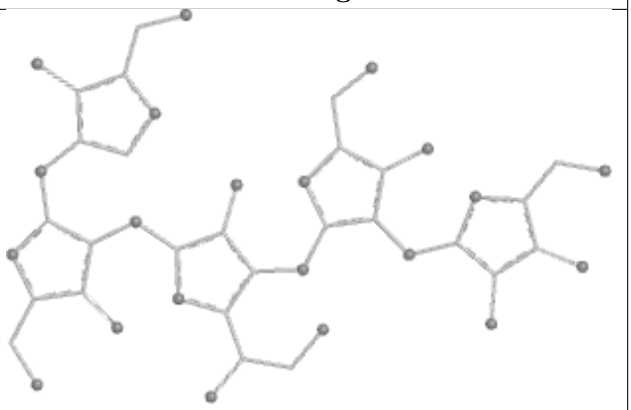
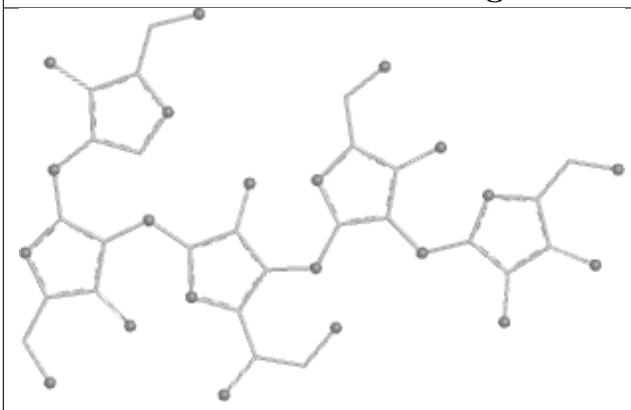
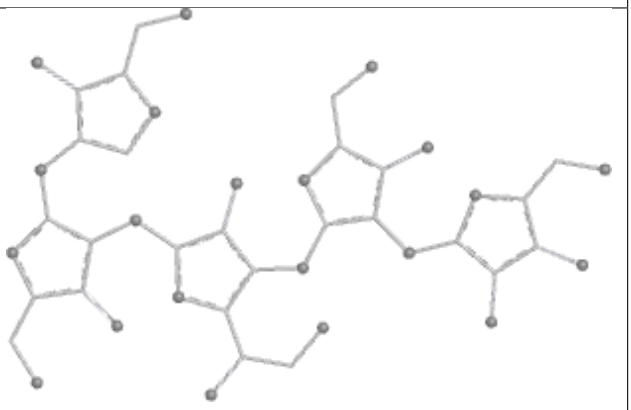
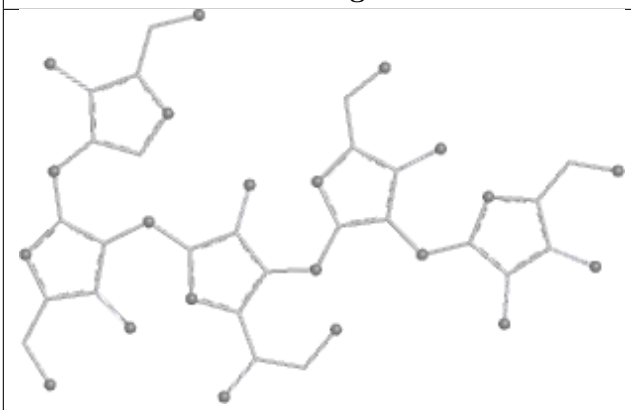
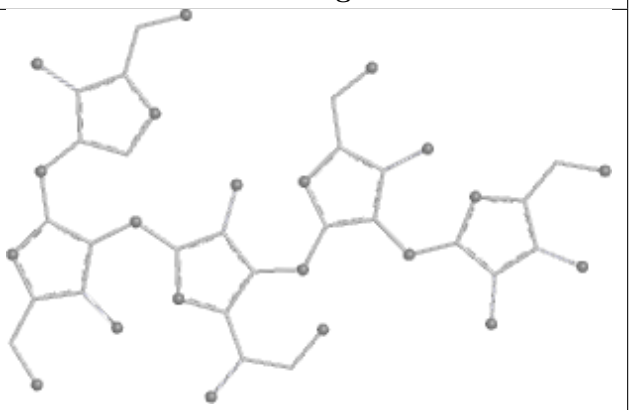
	
Torsions	**Rings**

Oligosaccharide Chain fB	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 7B	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 8B	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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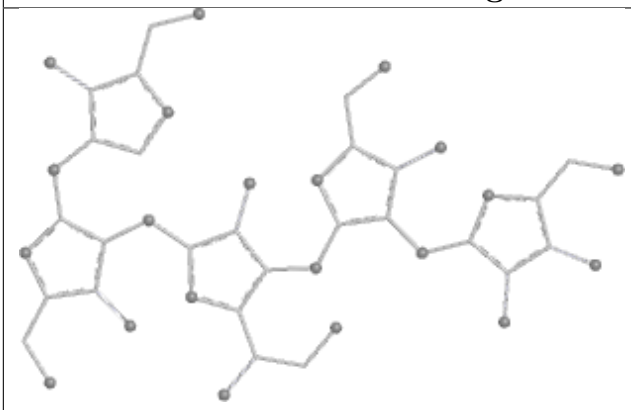
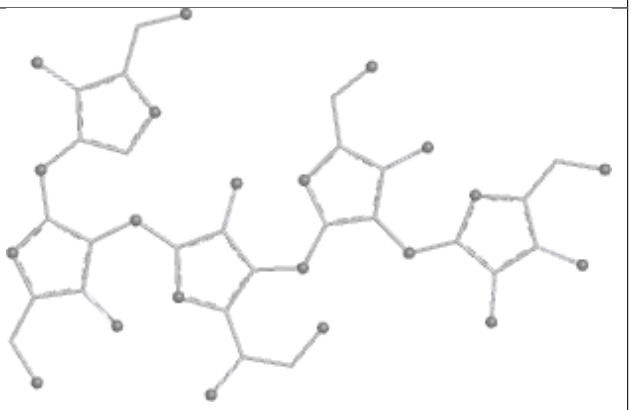
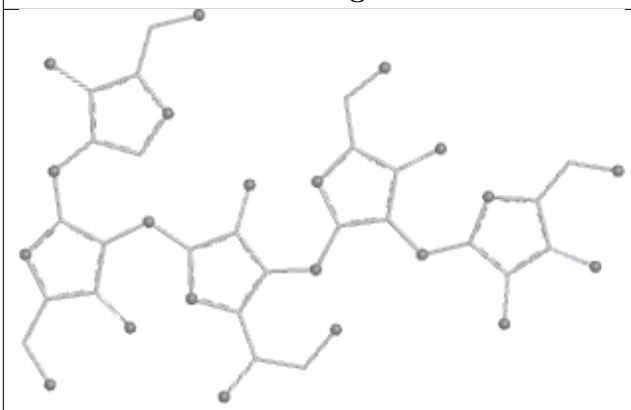
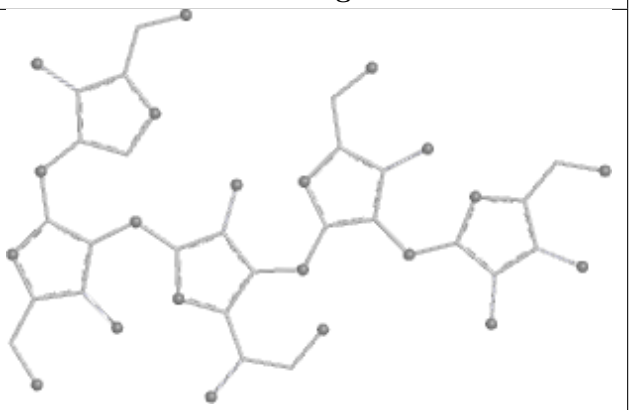
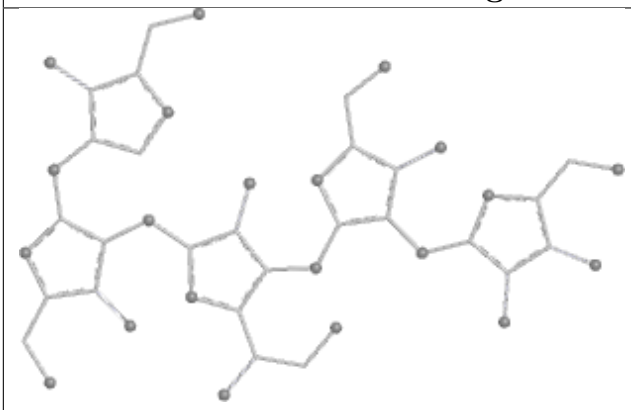
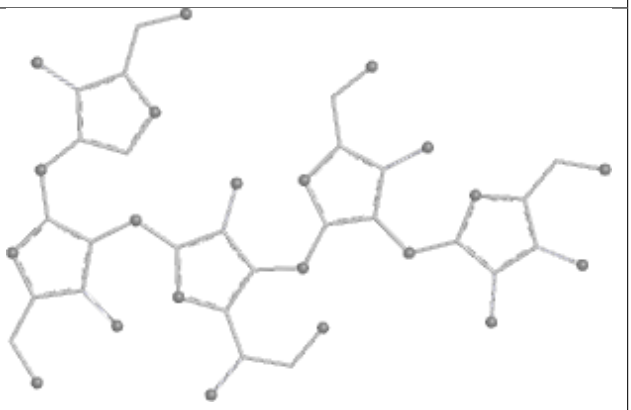
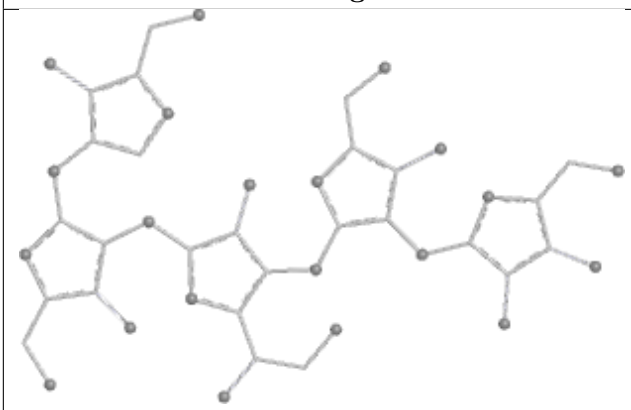
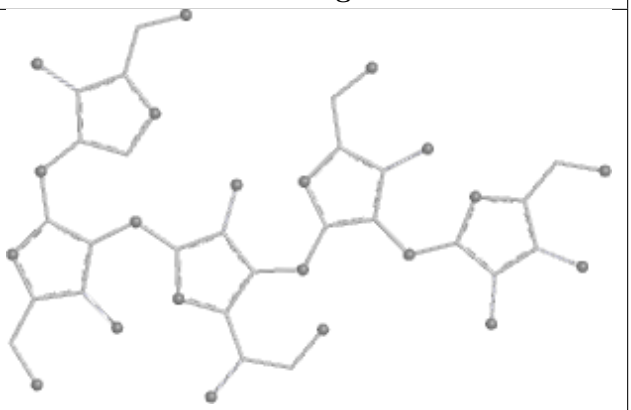
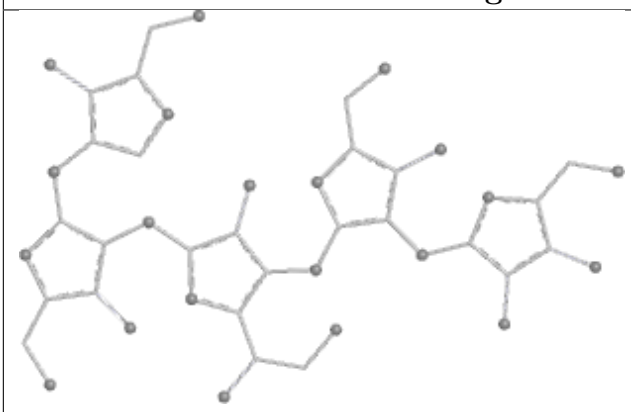
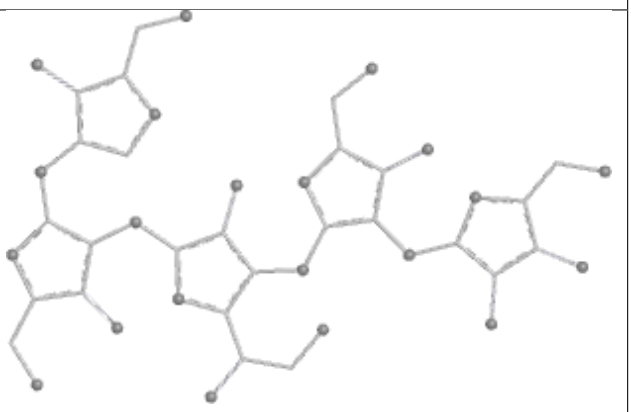
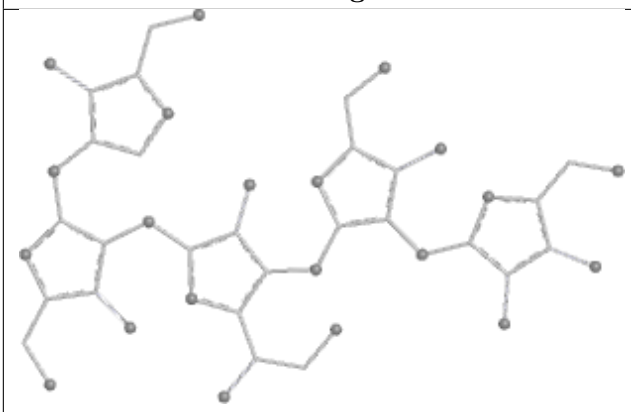
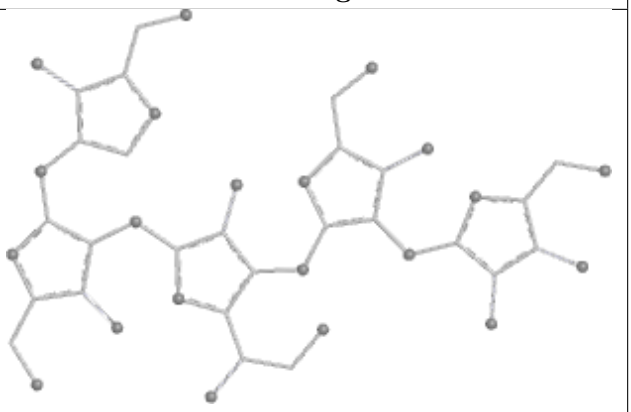
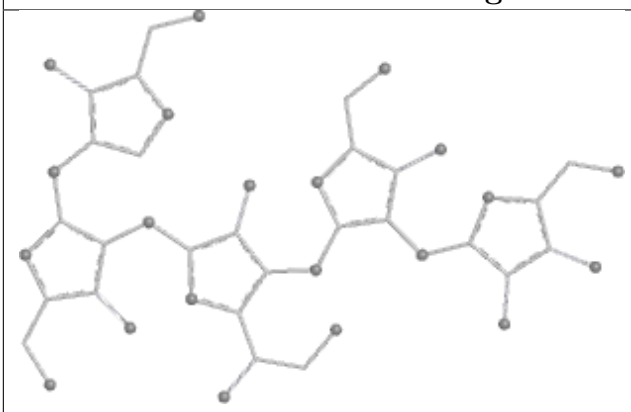
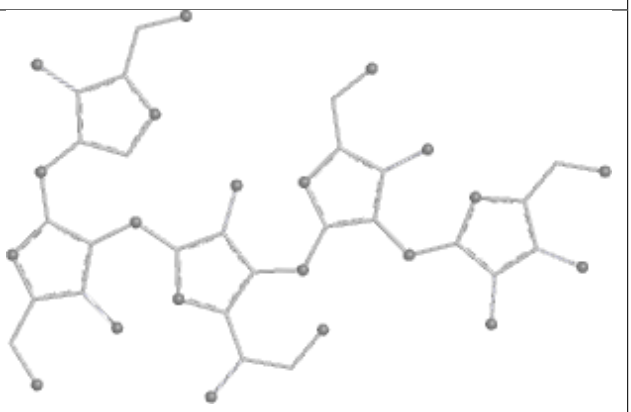
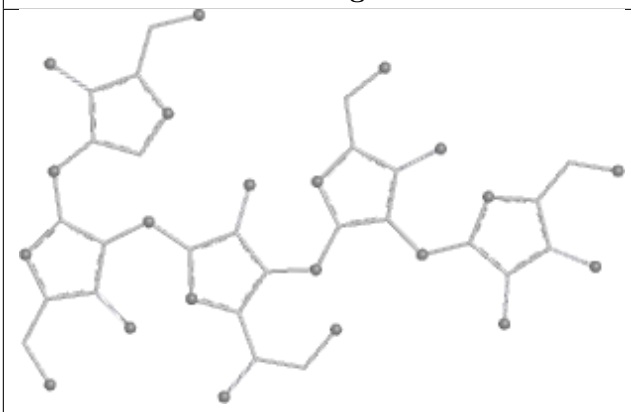
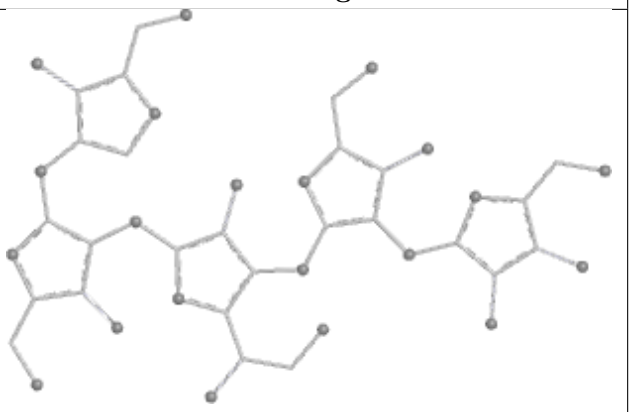
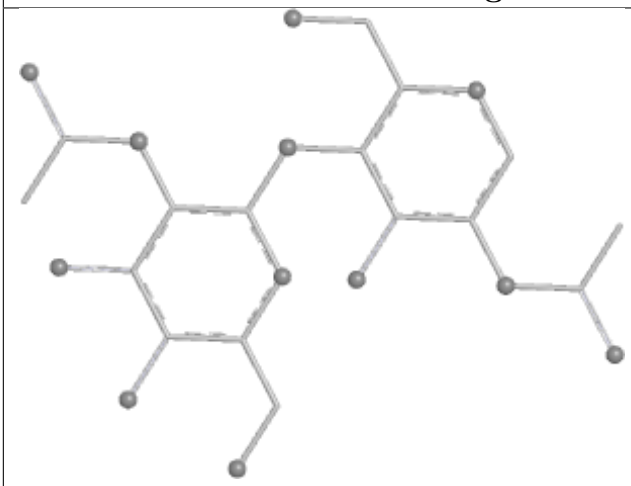
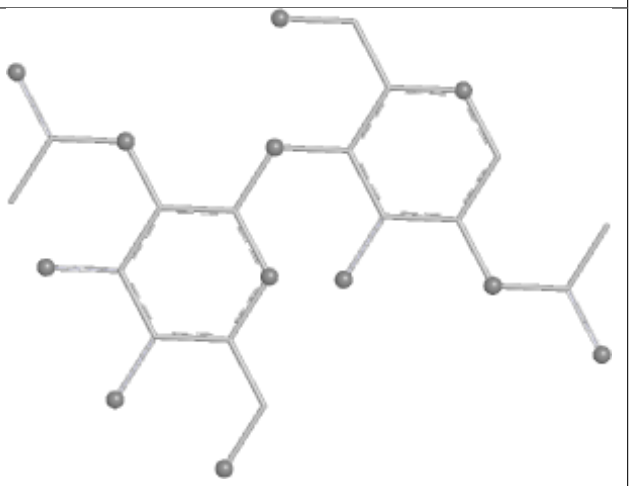
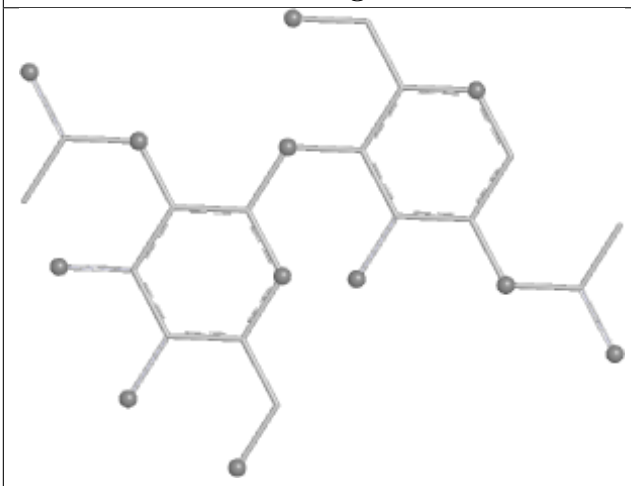
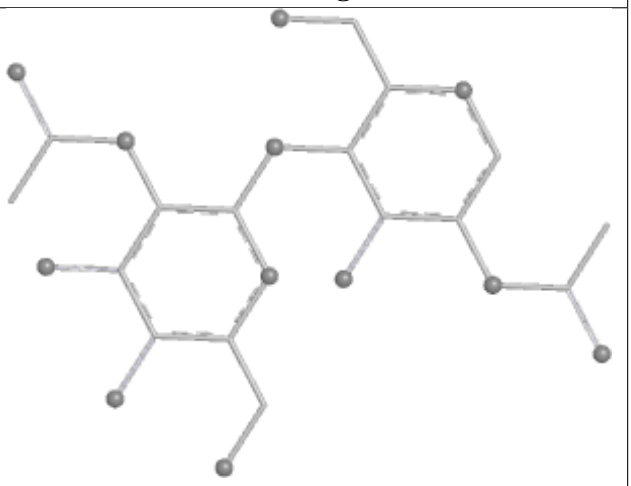
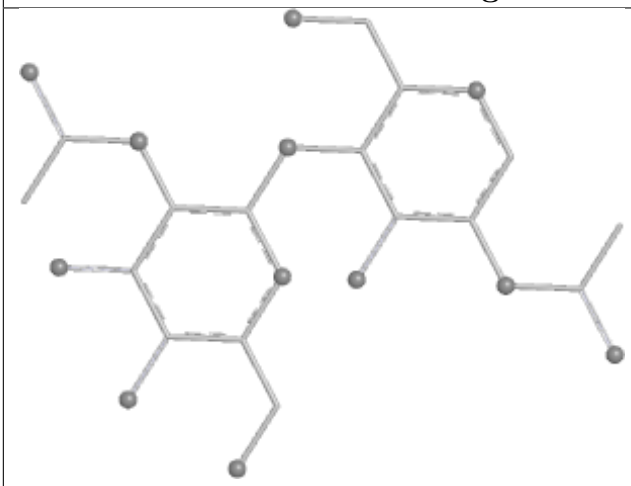
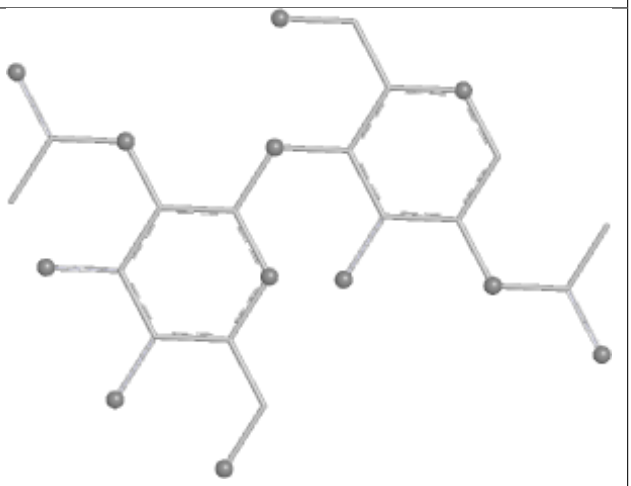
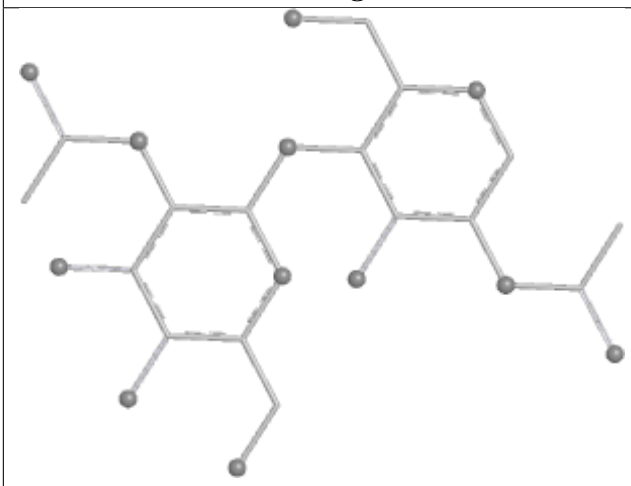
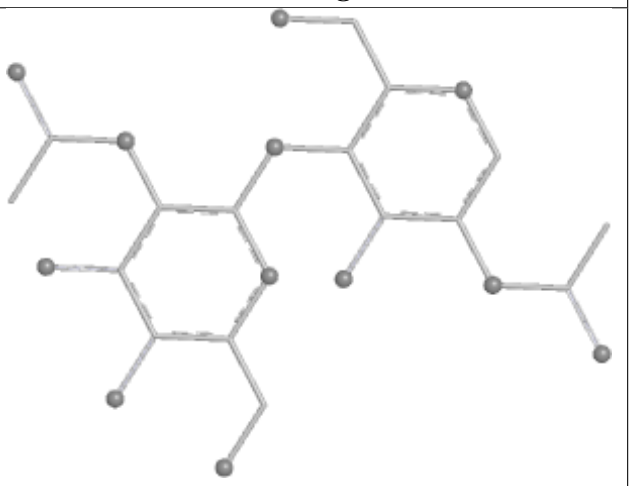
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

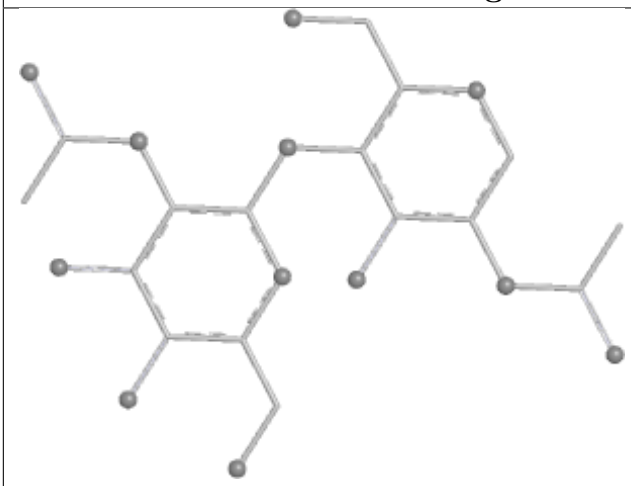
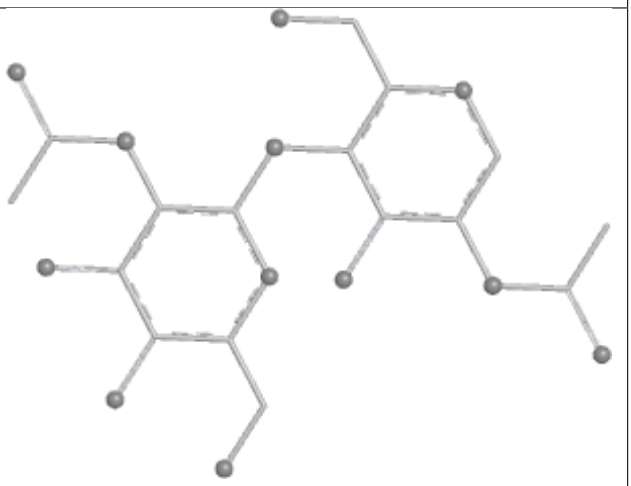
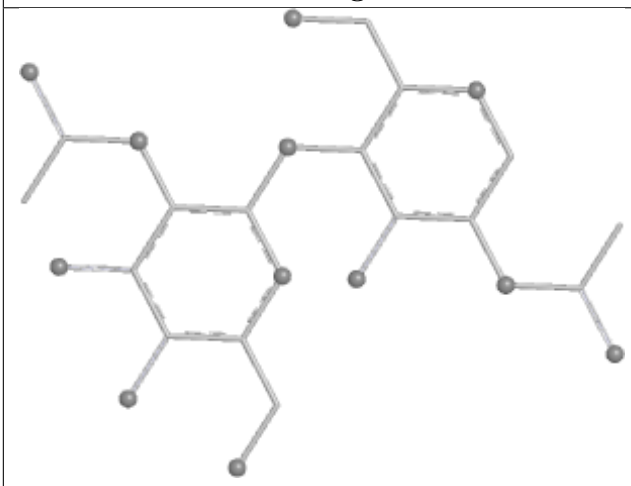
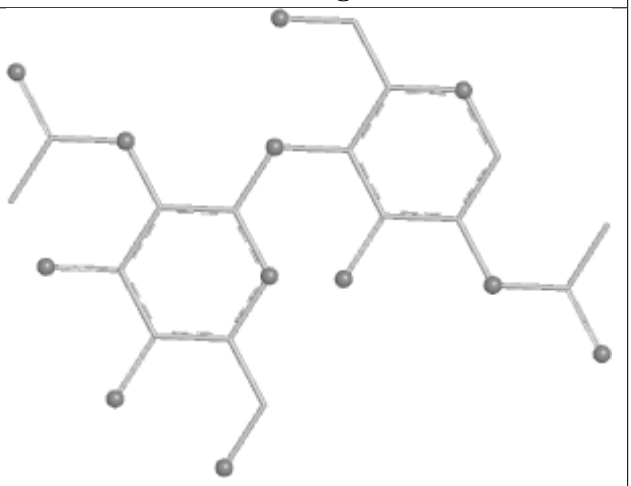
Oligosaccharide Chain 5C	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

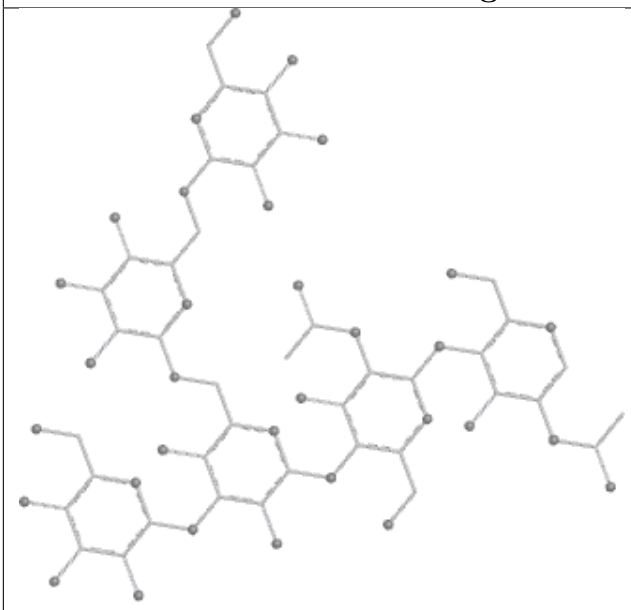
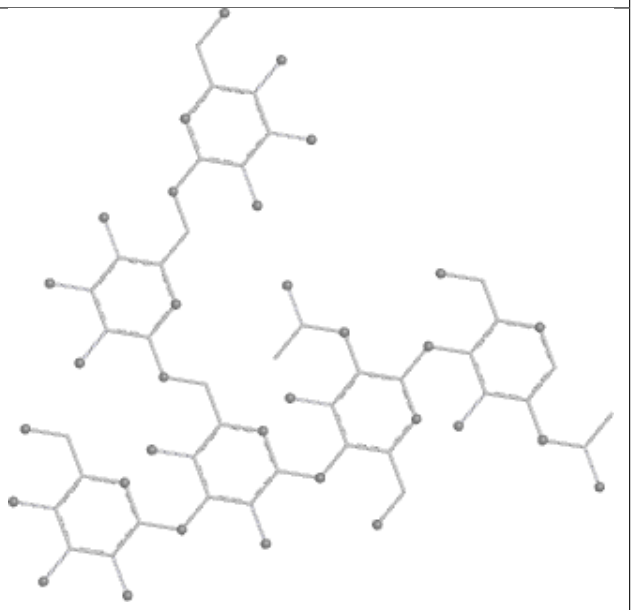
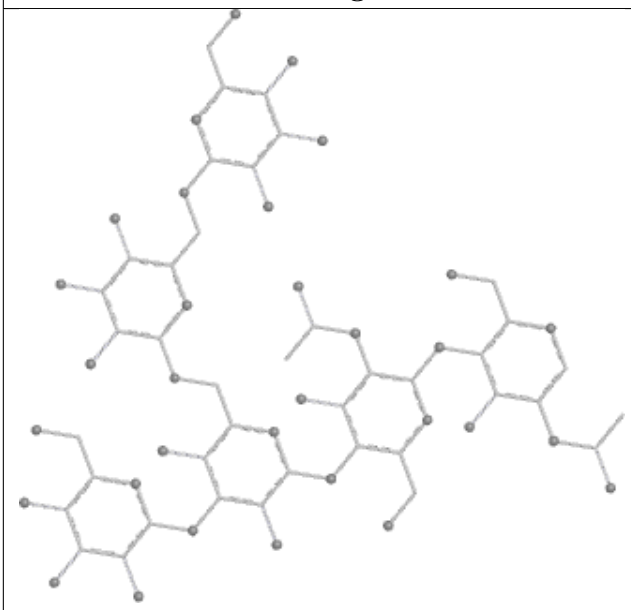
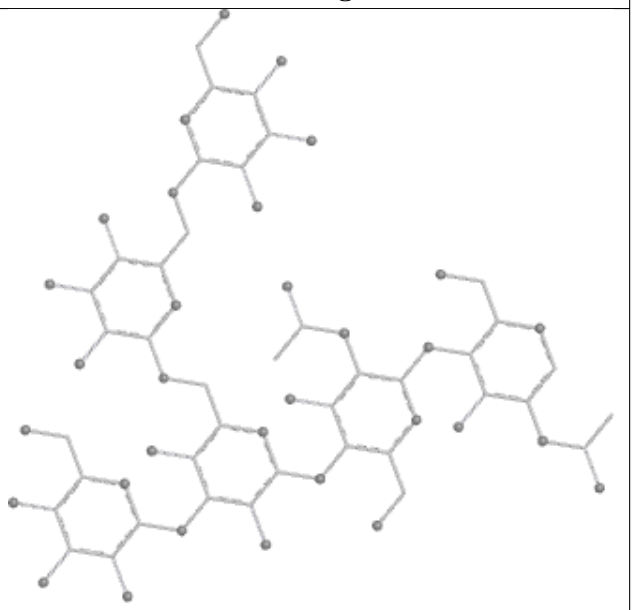
Oligosaccharide Chain 1D	
 Bond lengths	 Bond angles
 Torsions	 Rings

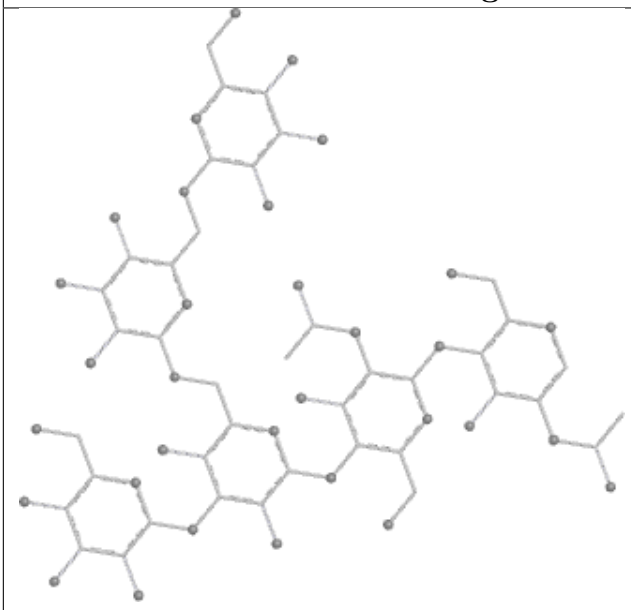
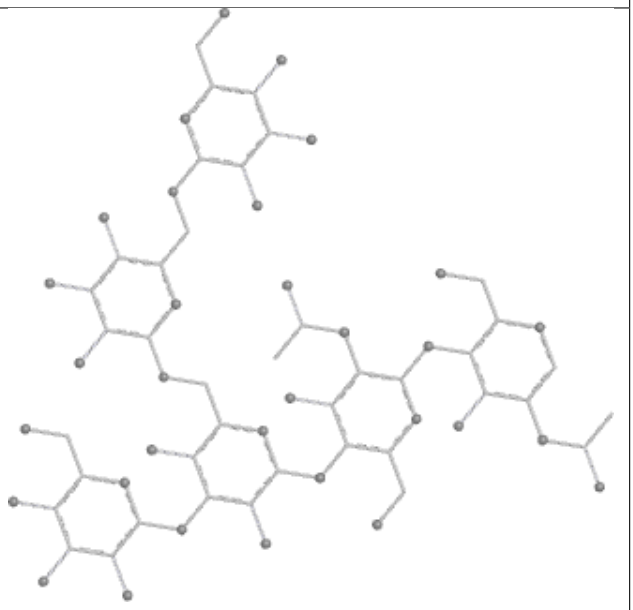
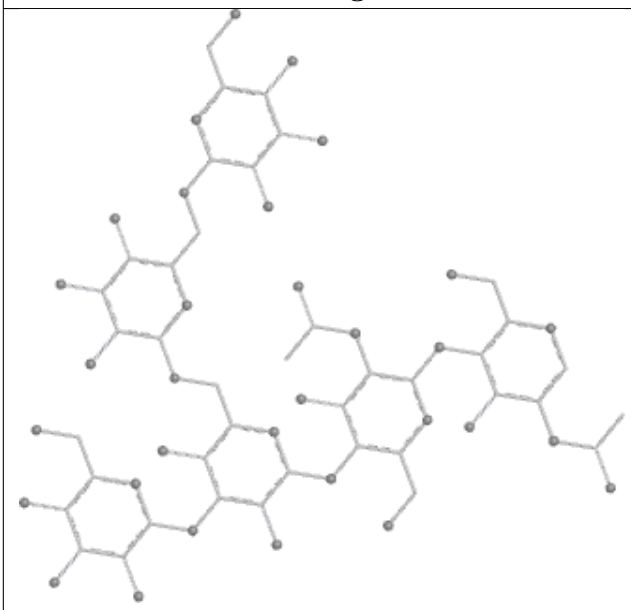
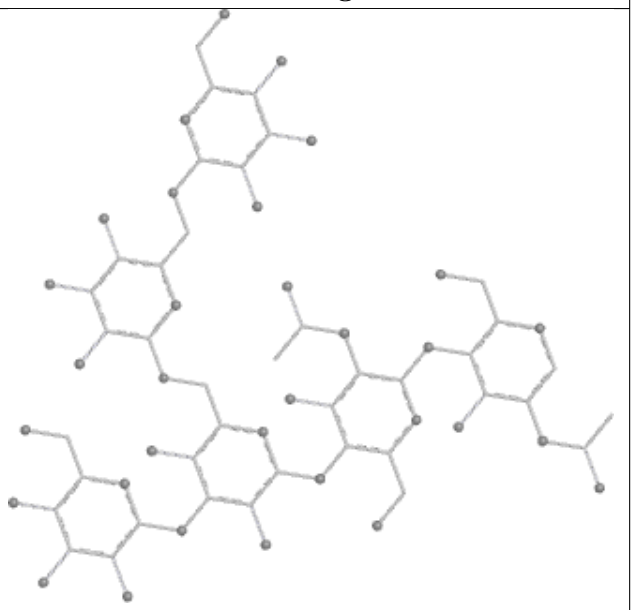
Oligosaccharide Chain 2D	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

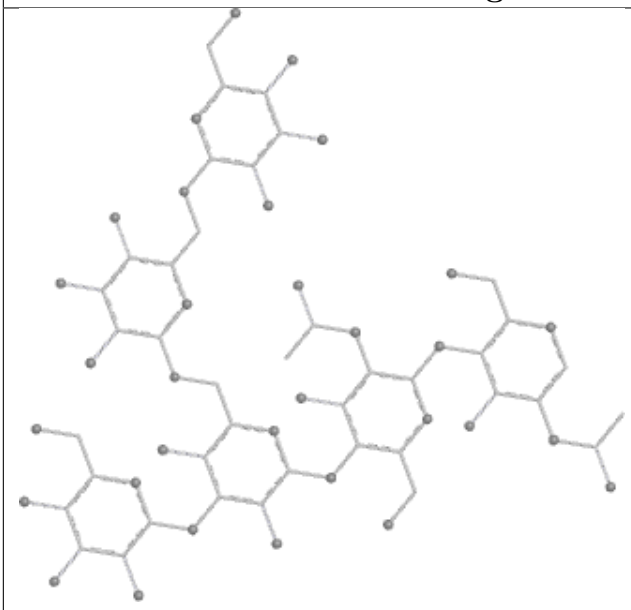
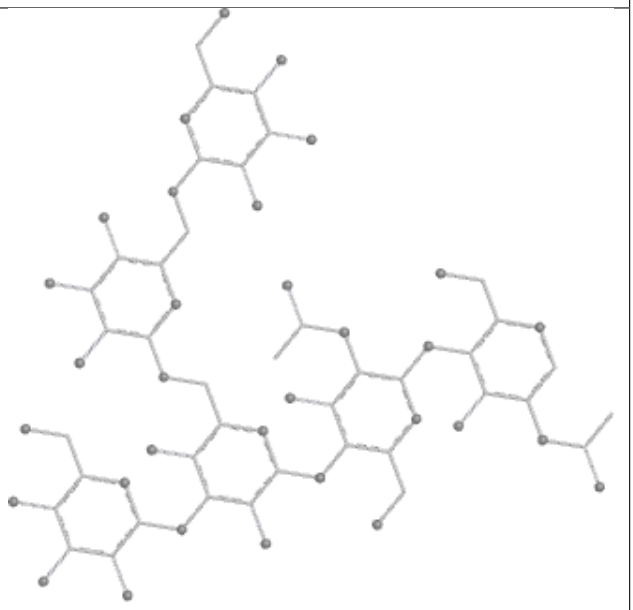
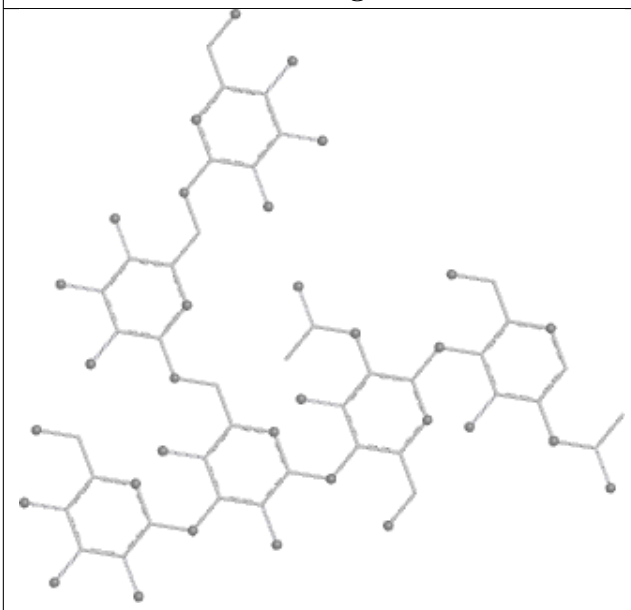
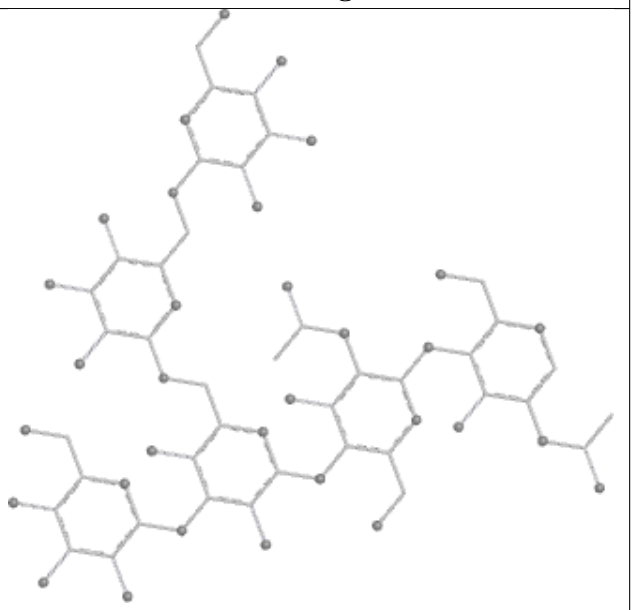
Oligosaccharide Chain FA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

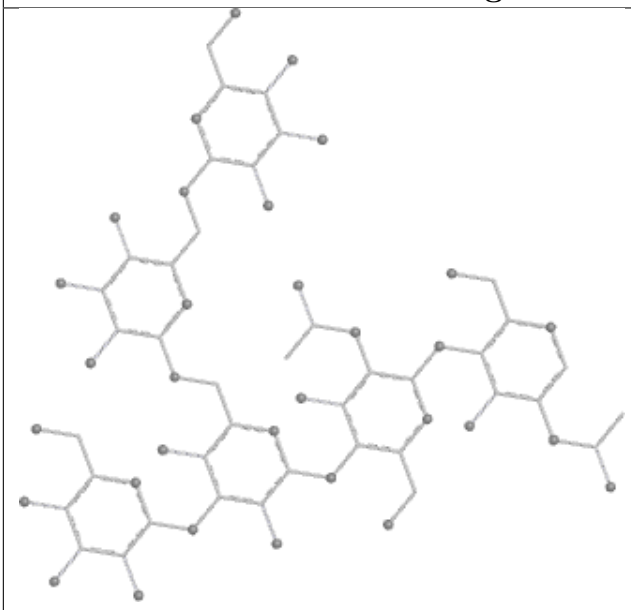
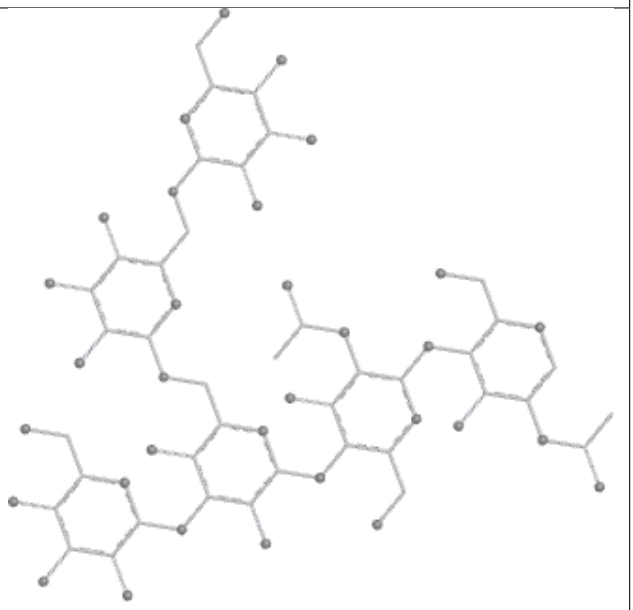
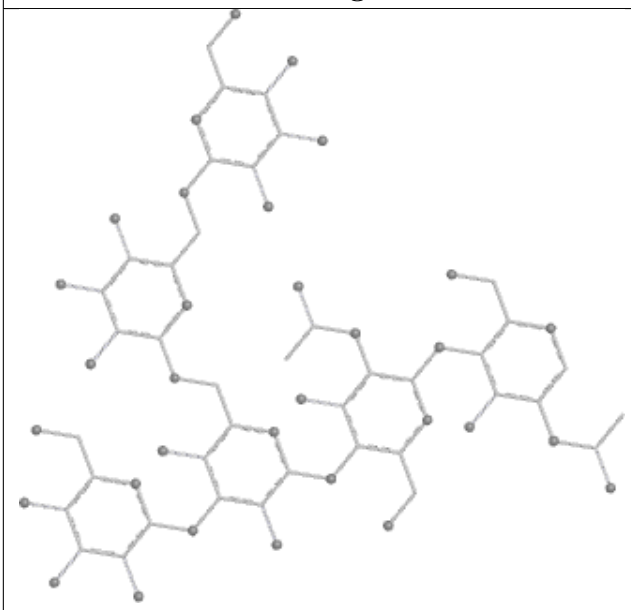
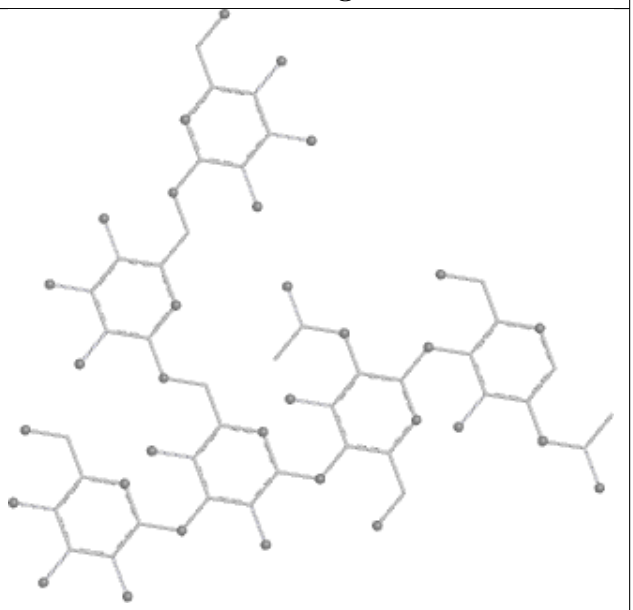
Oligosaccharide Chain AC	
 Bond lengths	 Bond angles
 Torsions	 Rings

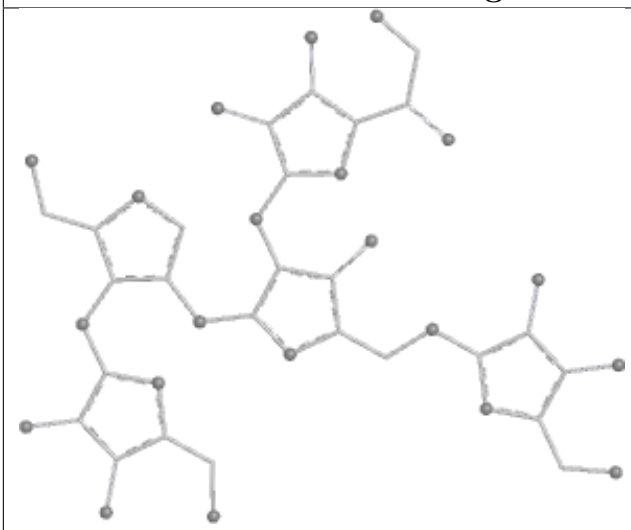
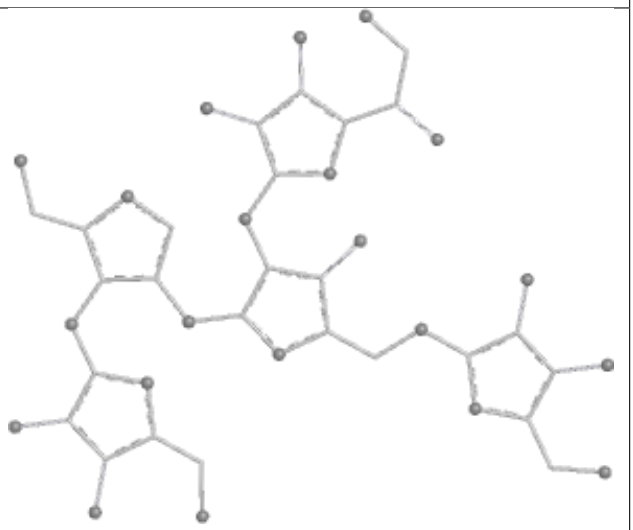
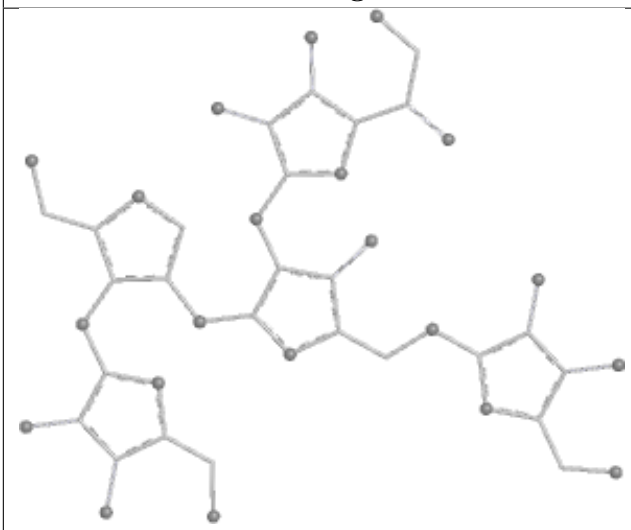
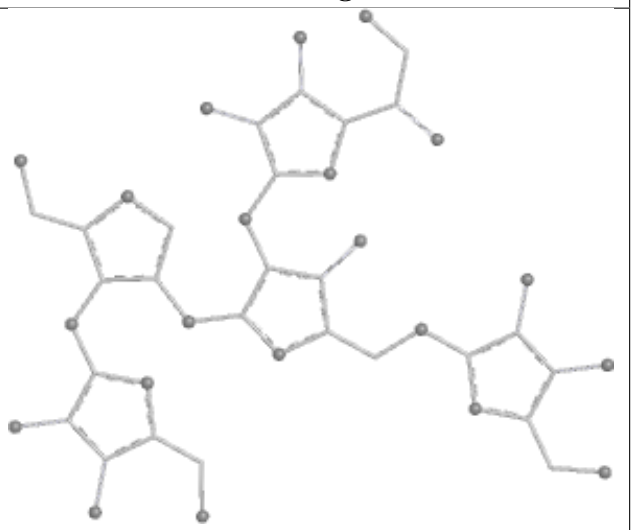
Oligosaccharide Chain 4D	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain GA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain DB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 7C	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 5D	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 9D	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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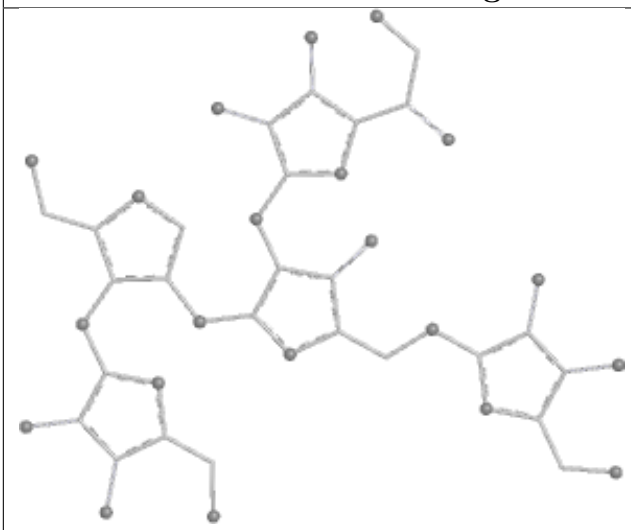
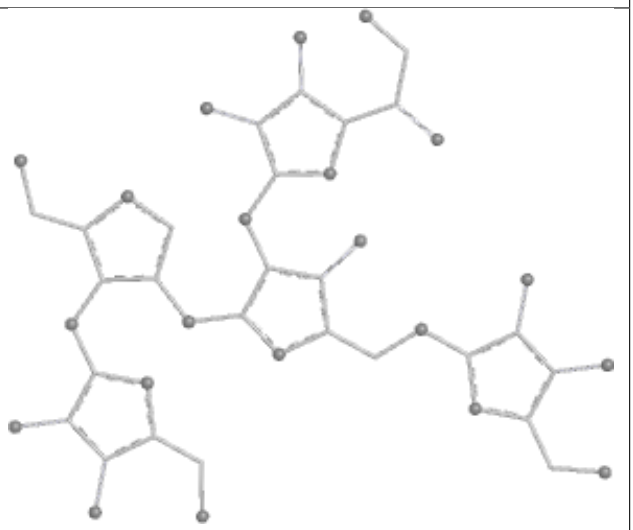
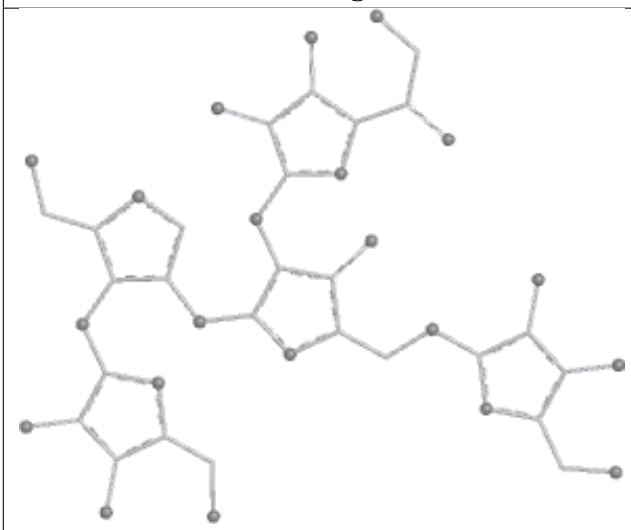
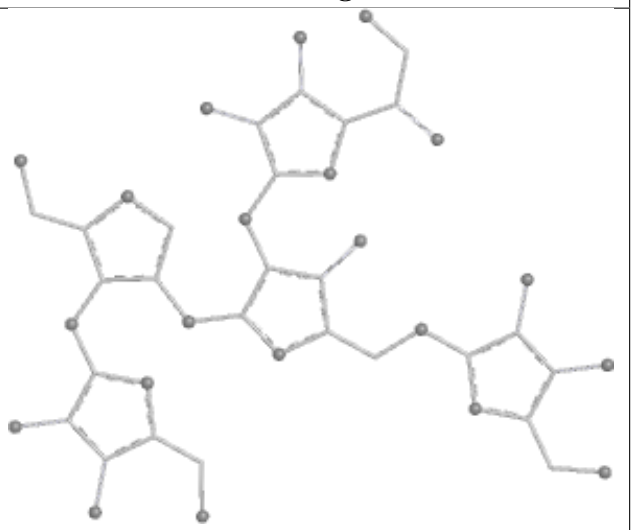
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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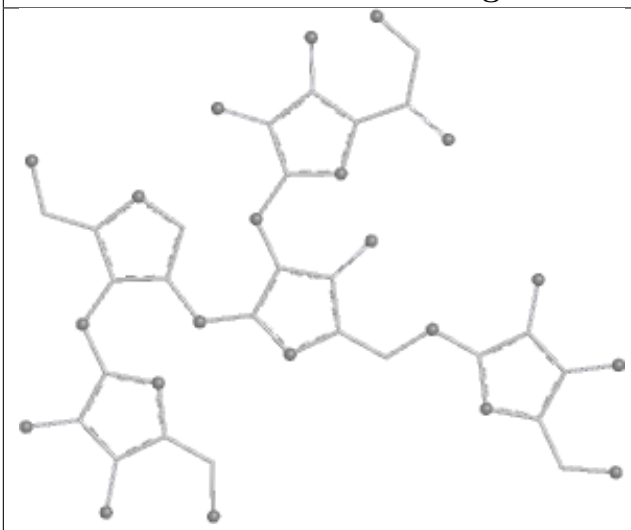
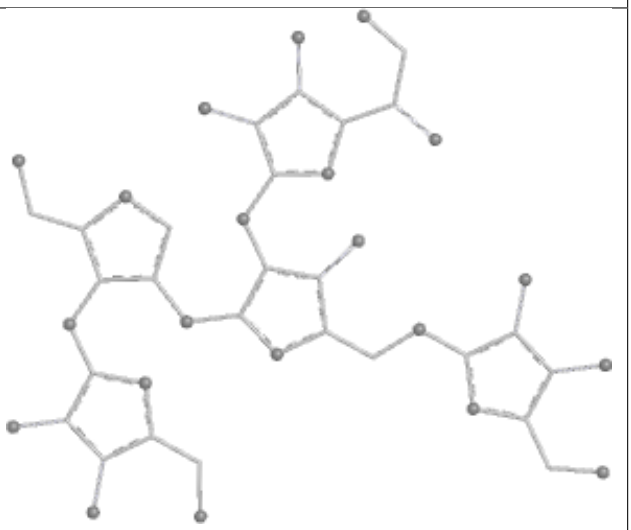
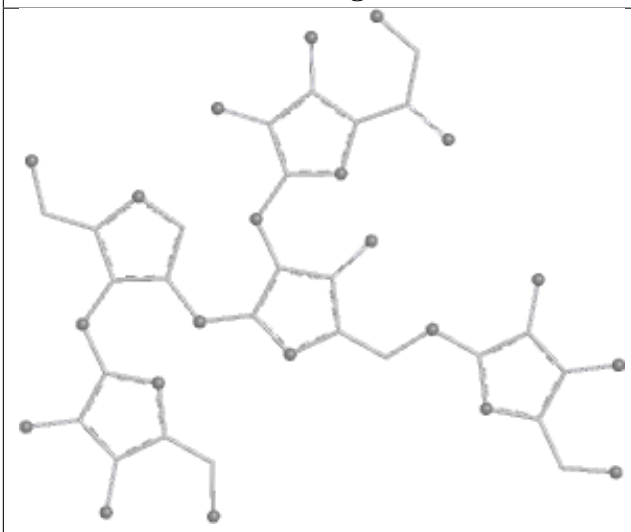
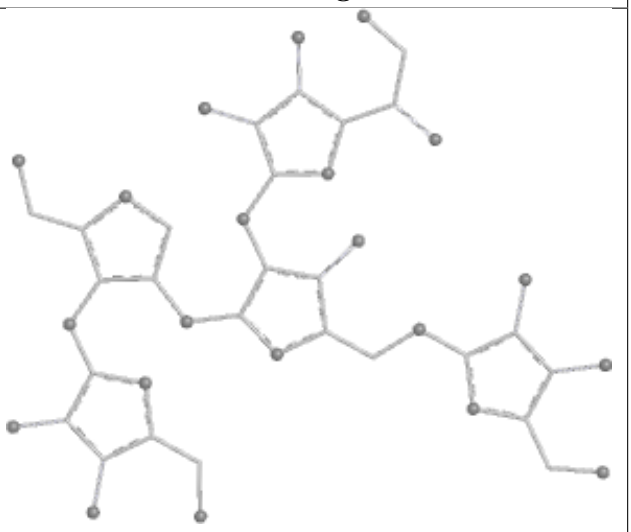
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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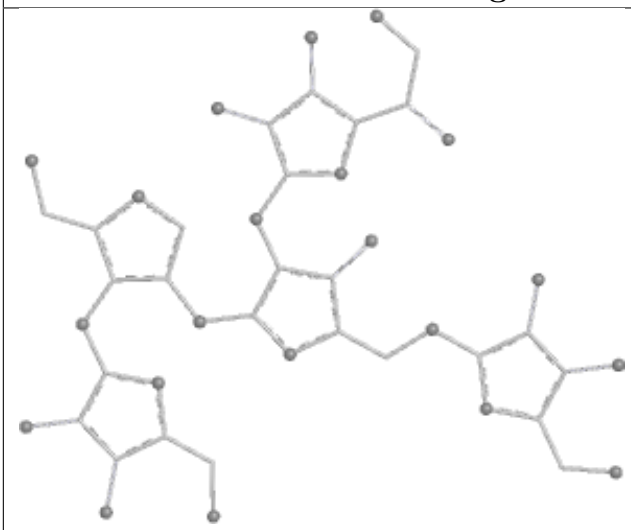
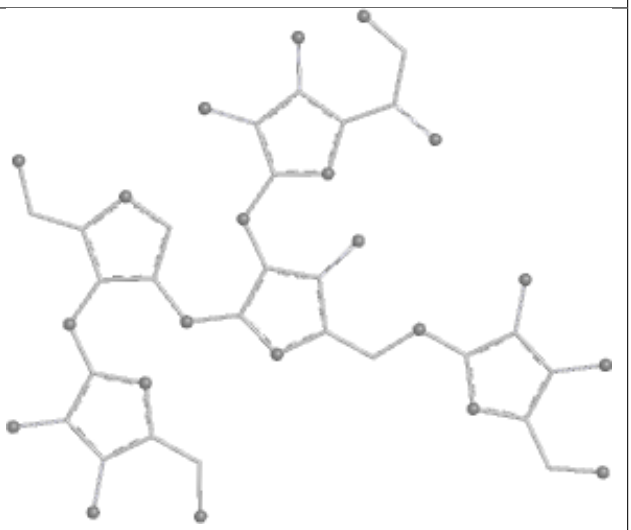
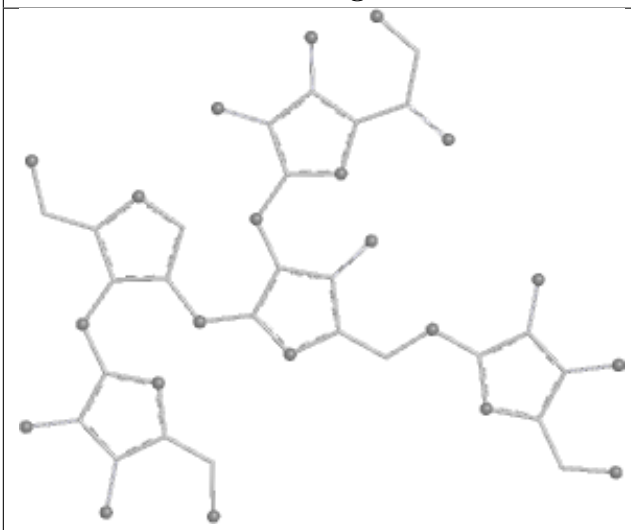
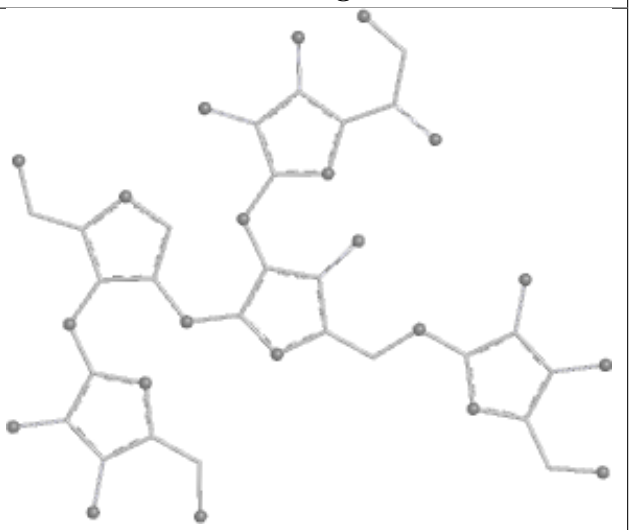
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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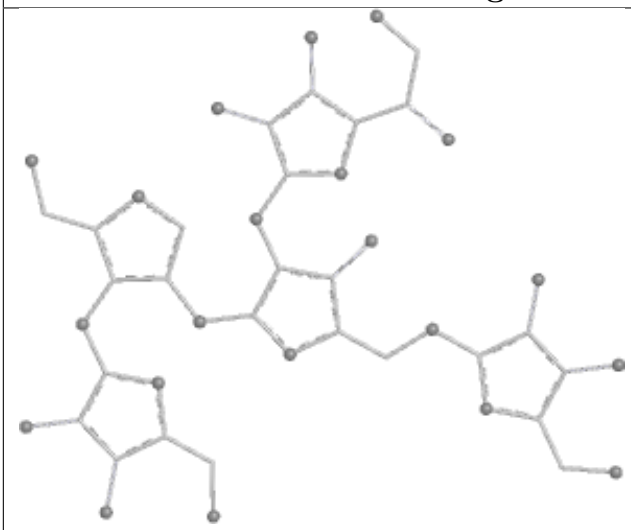
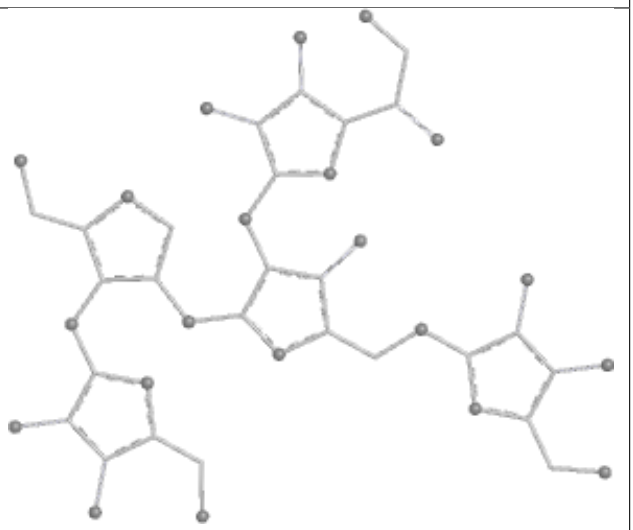
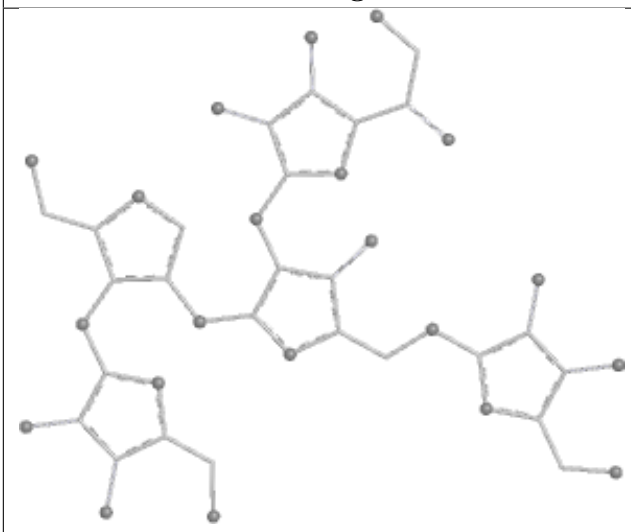
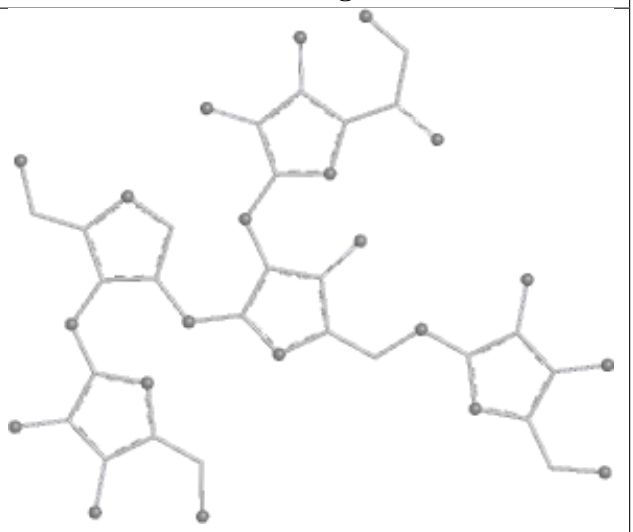
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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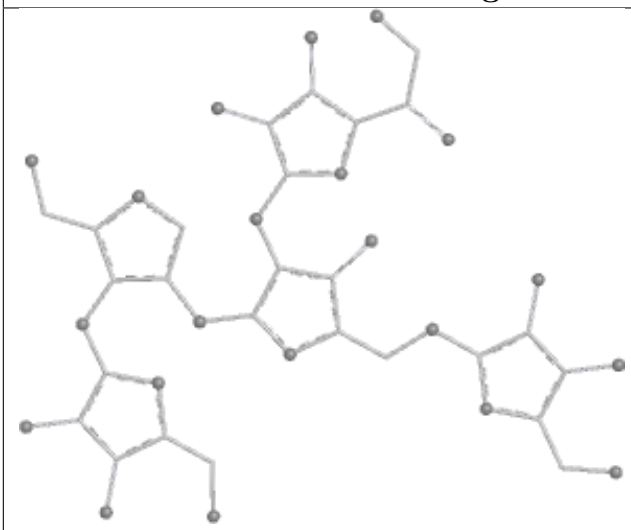
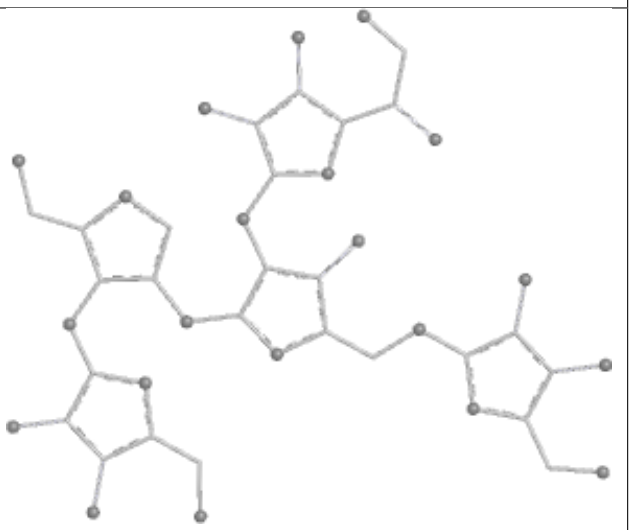
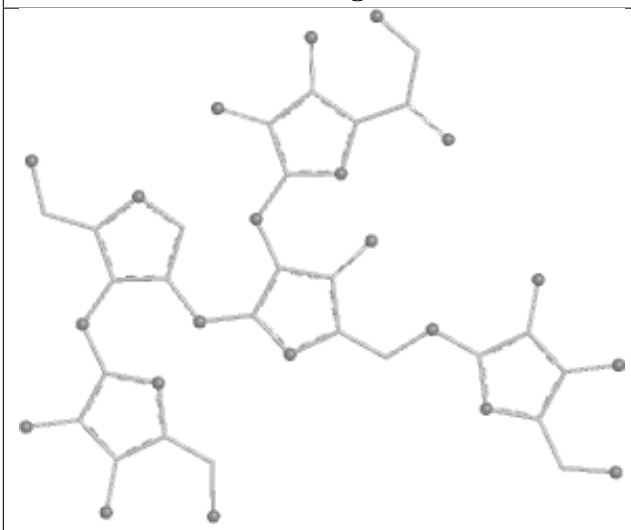
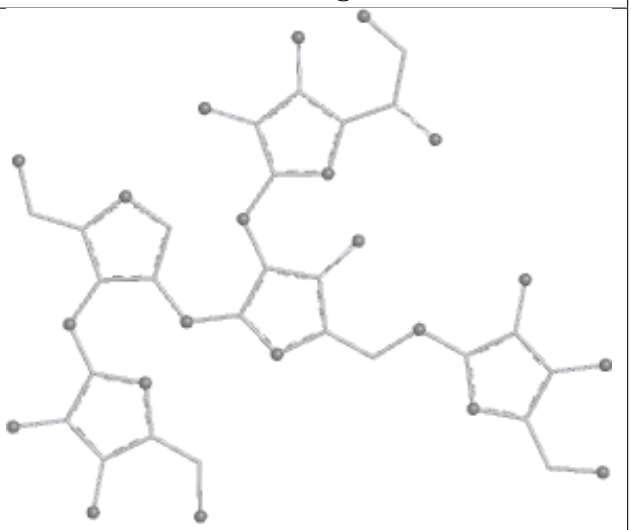
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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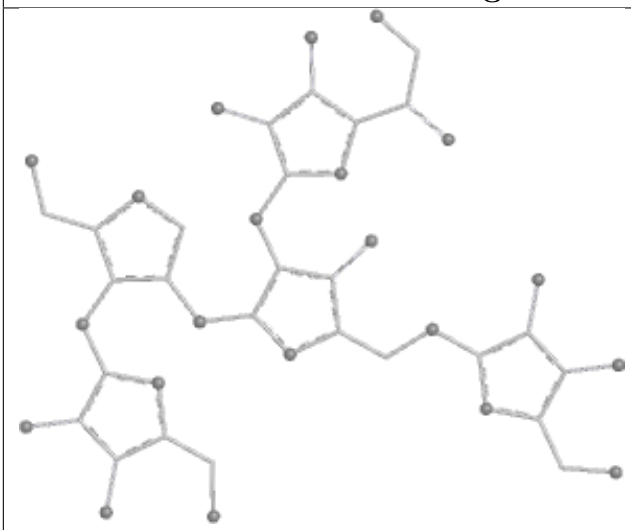
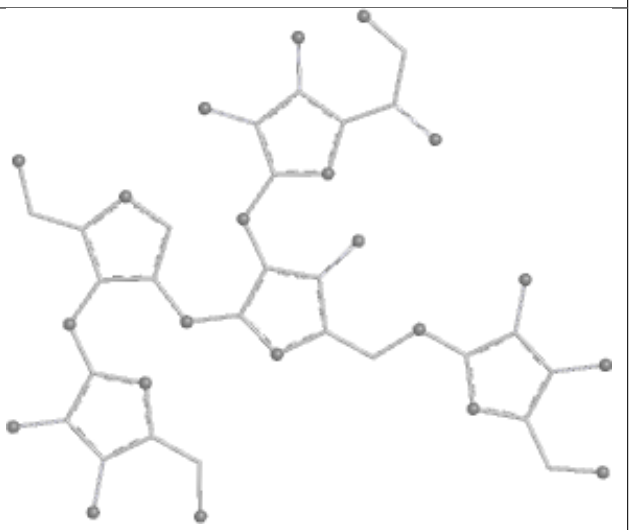
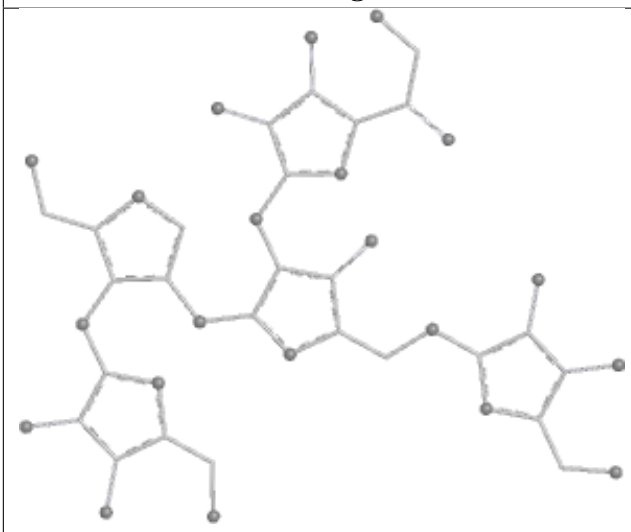
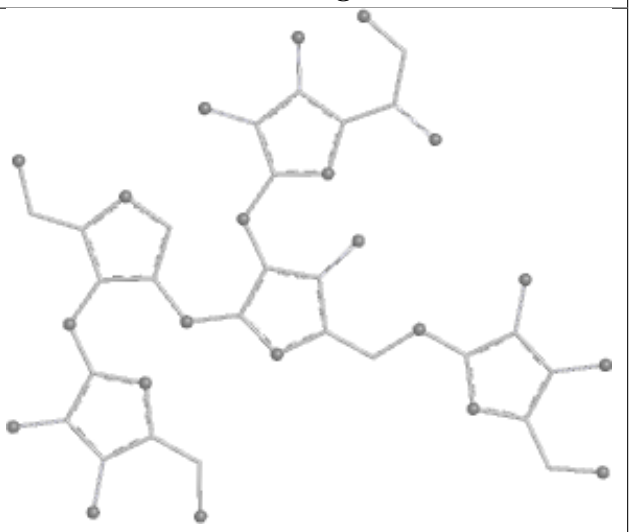
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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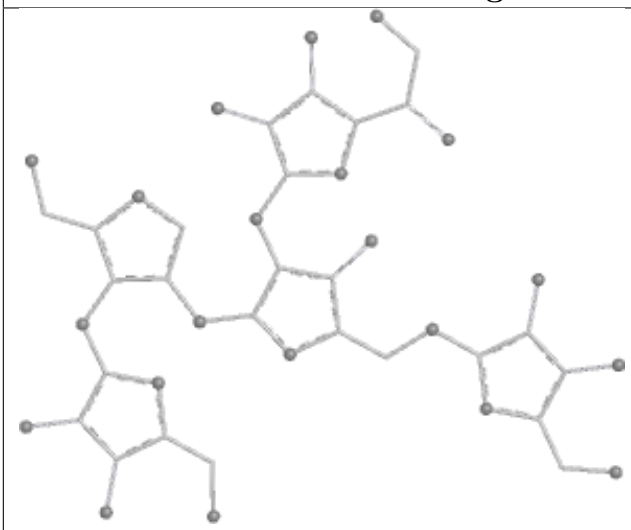
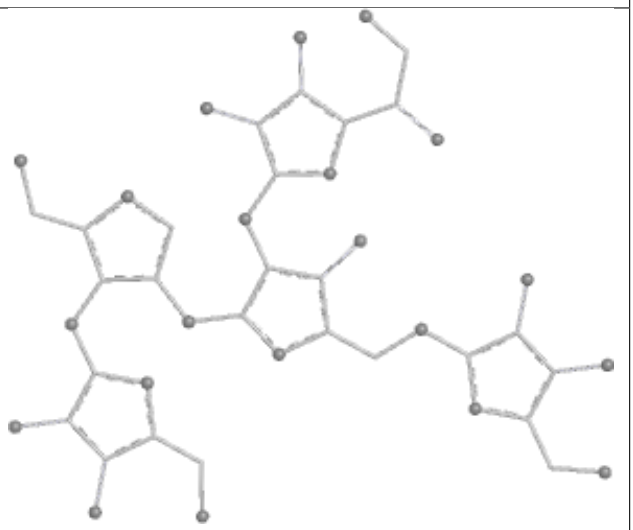
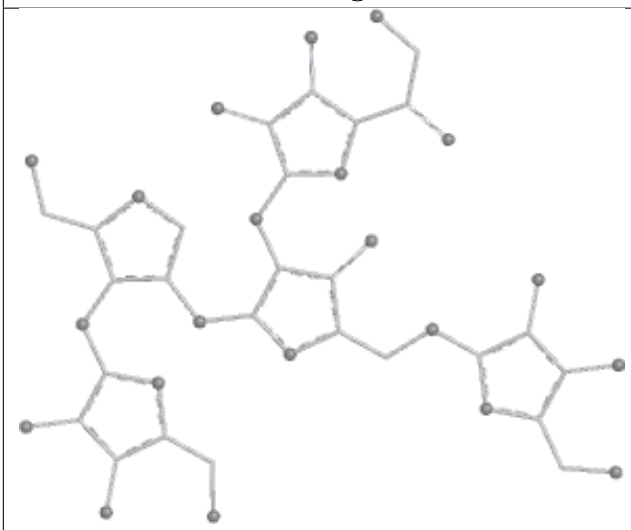
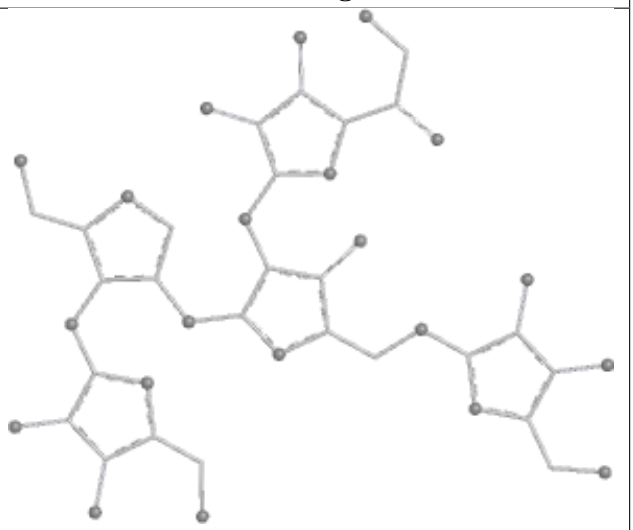
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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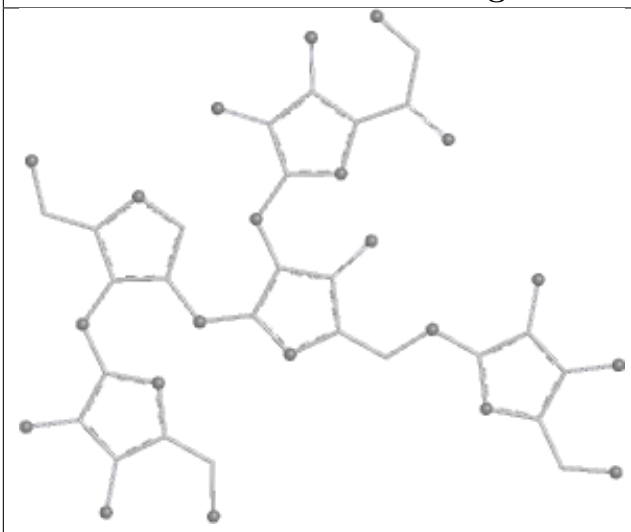	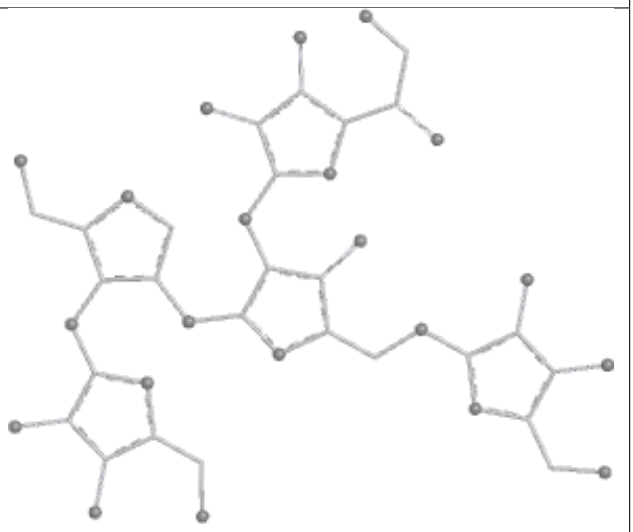
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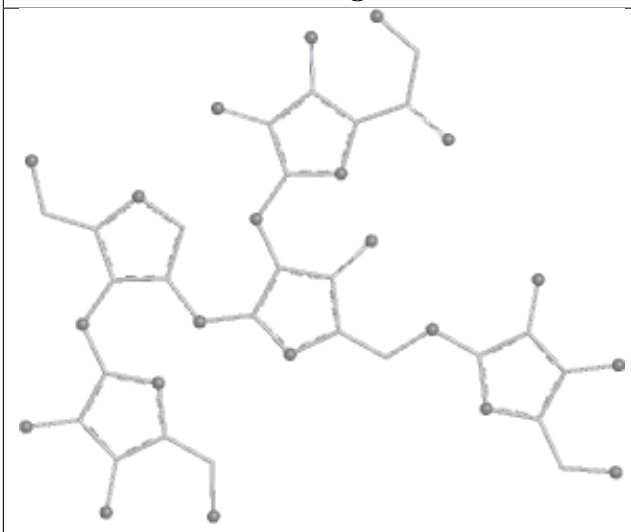	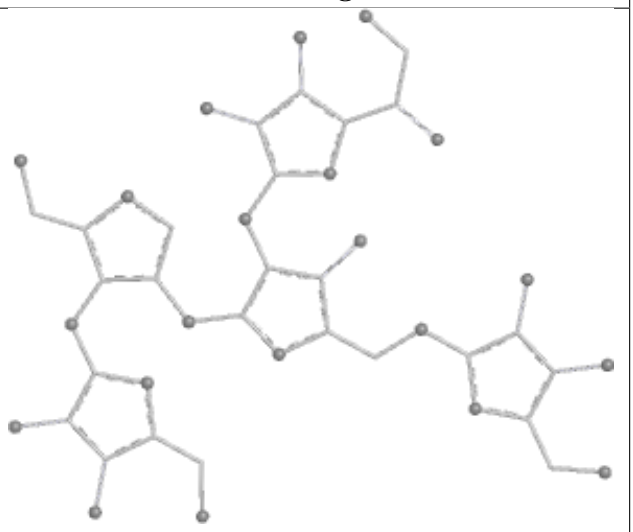
Torsions	**Rings**

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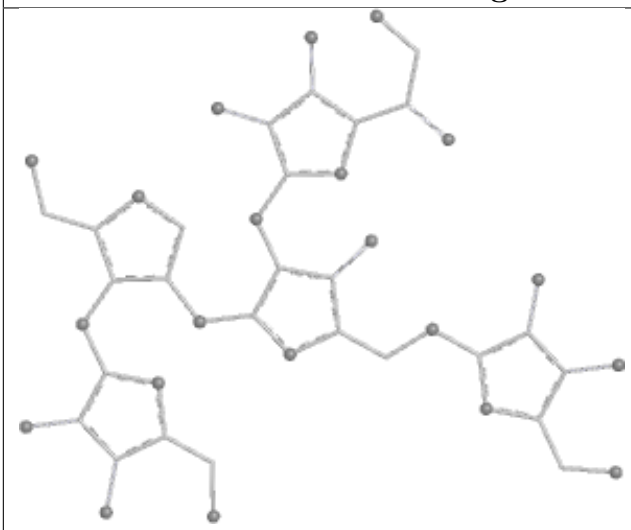
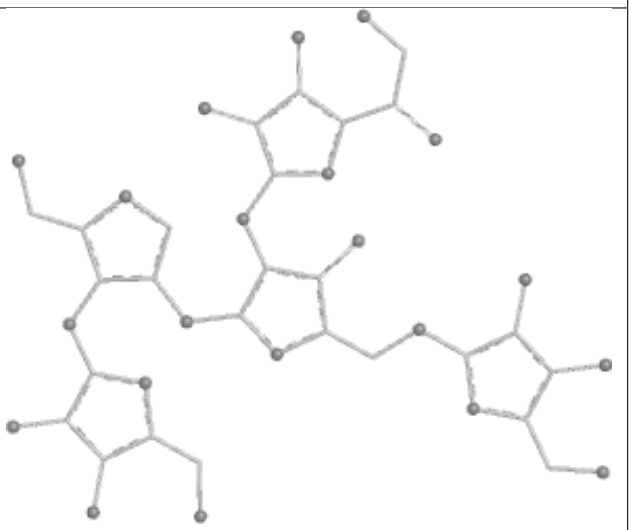
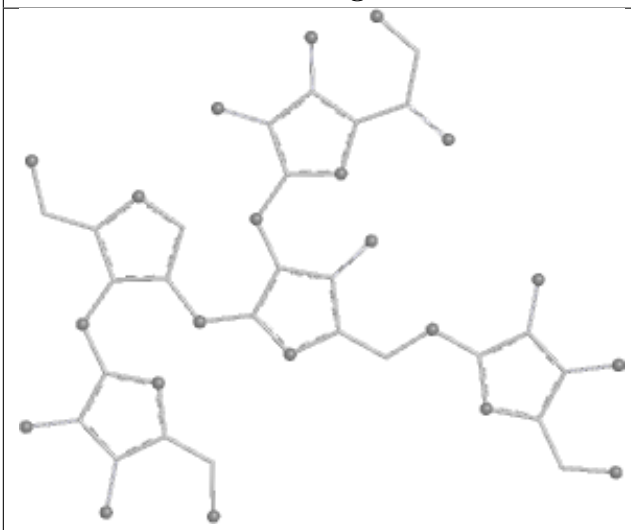
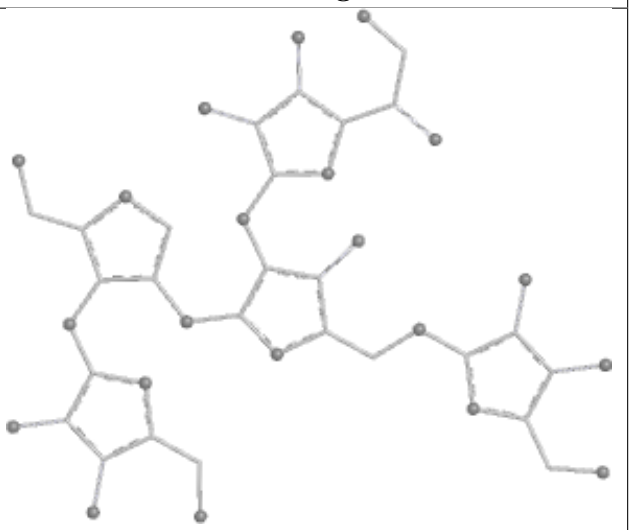
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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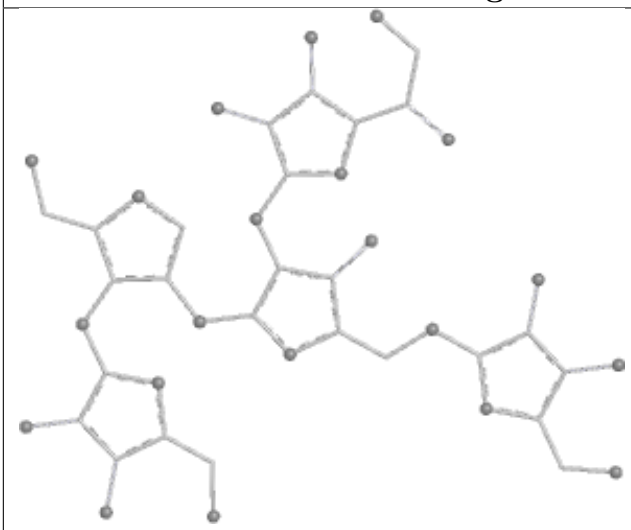	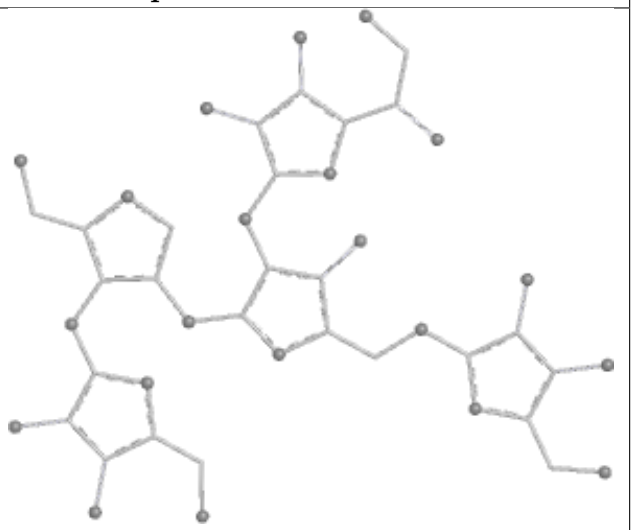
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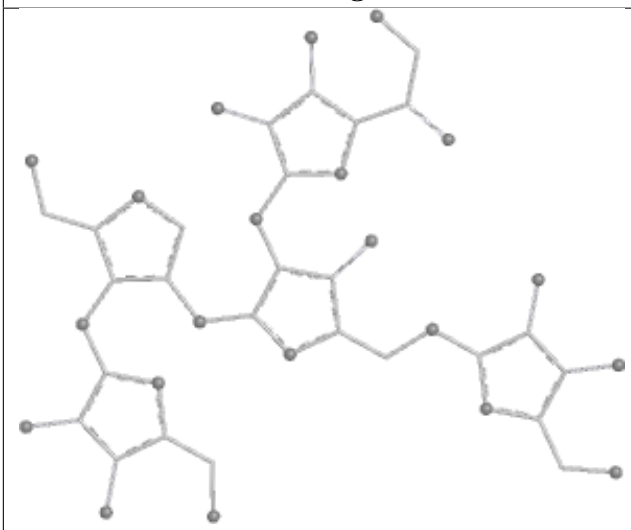	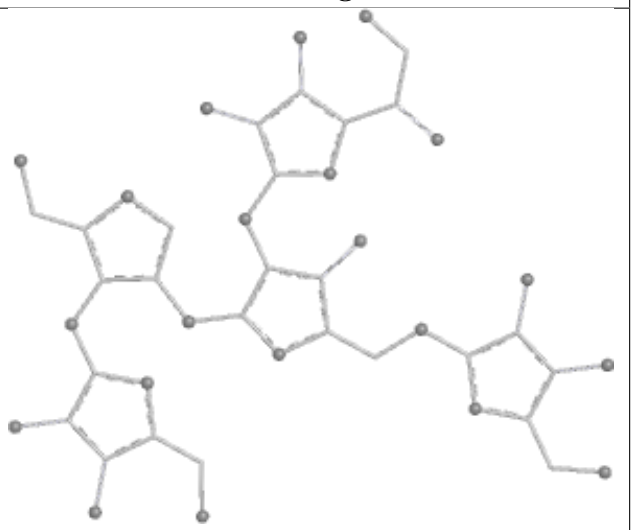
Torsions	**Rings**

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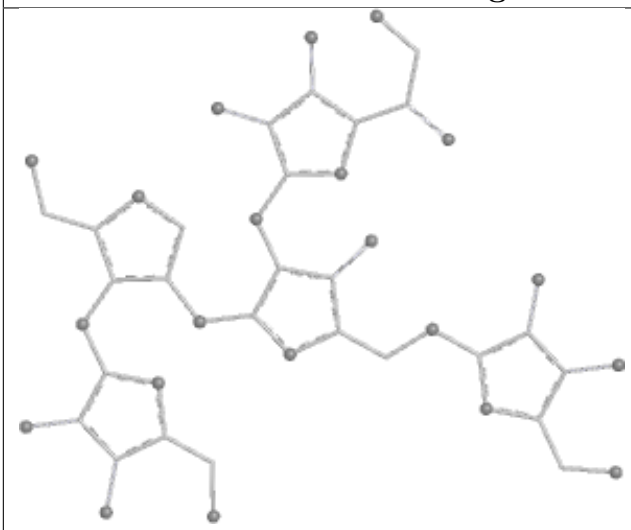	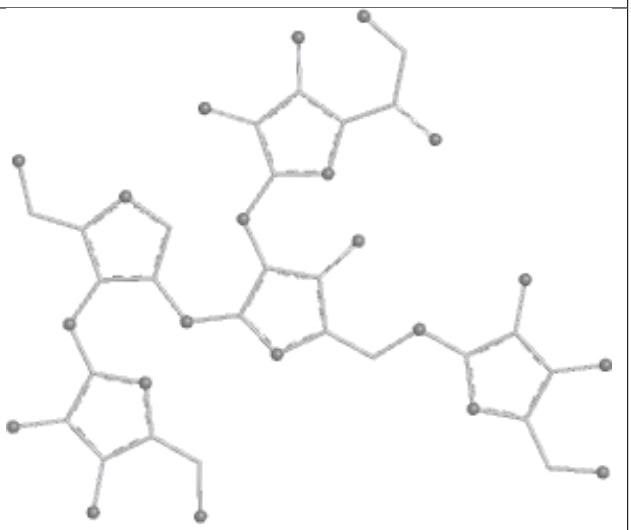
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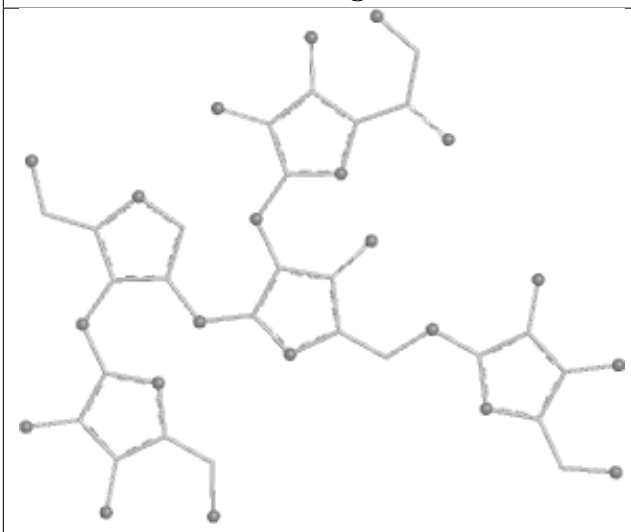	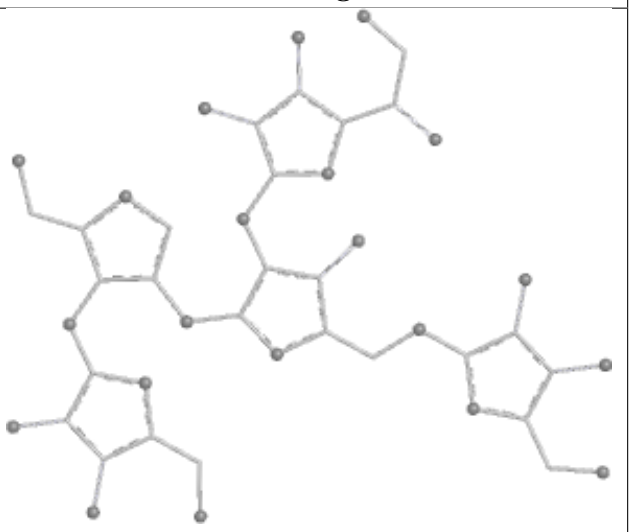
Torsions	**Rings**

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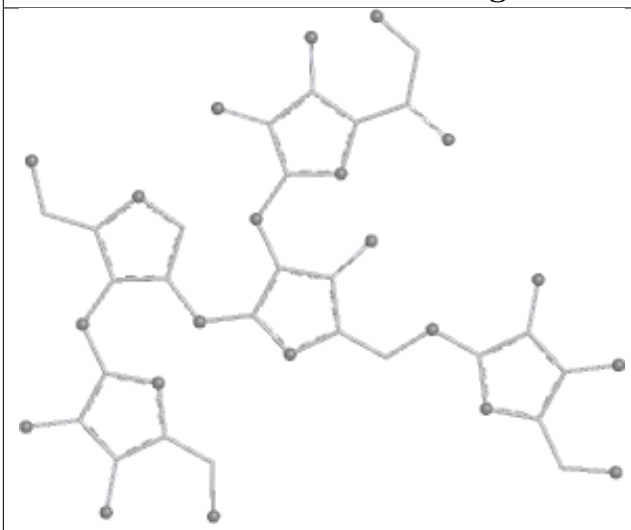	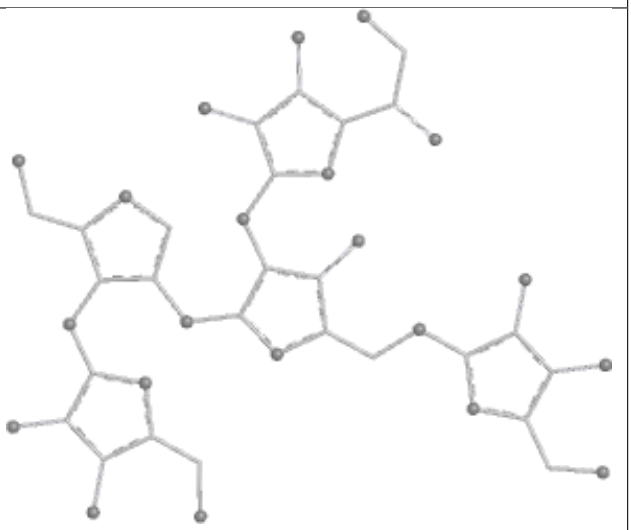
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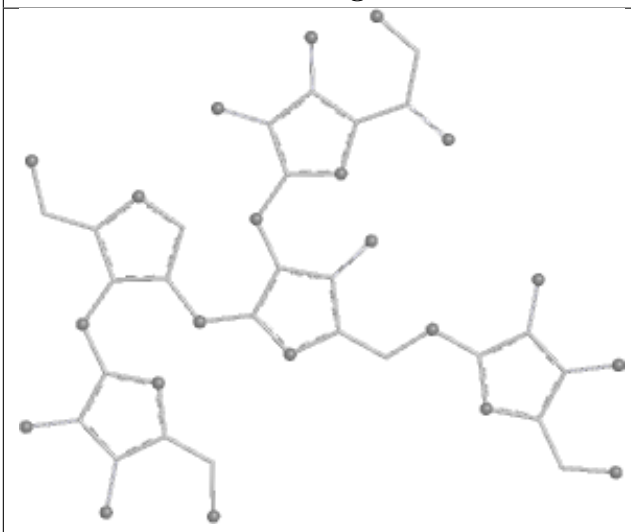	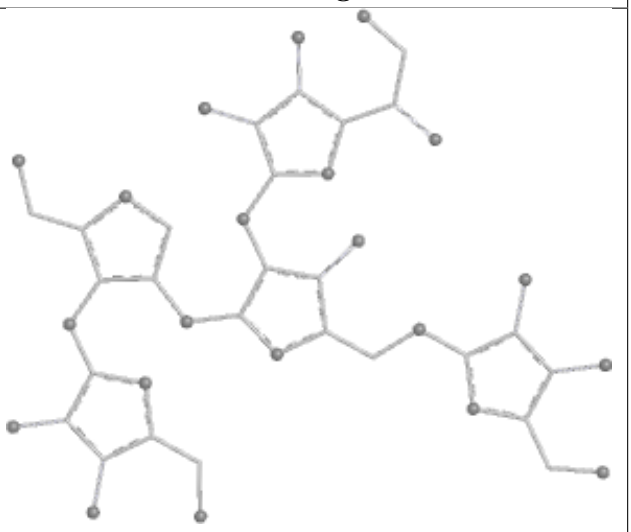
Torsions	**Rings**

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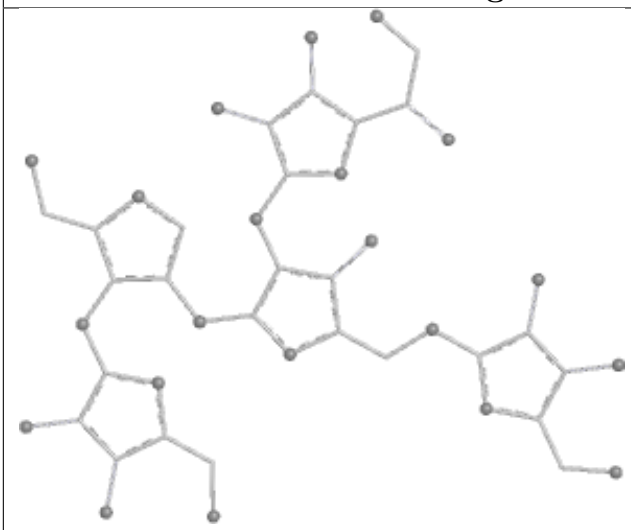	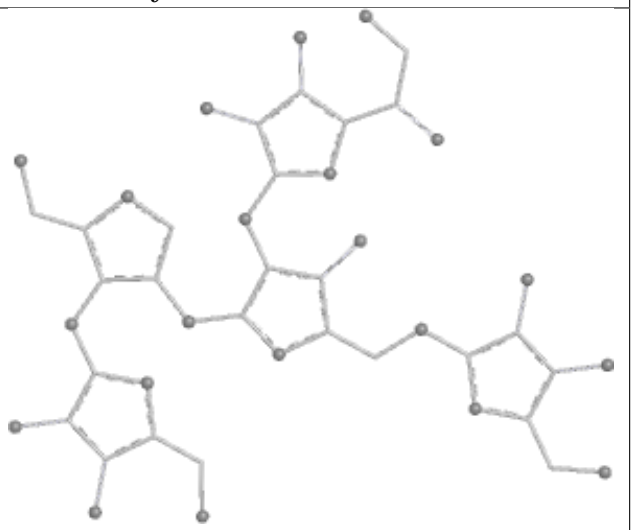
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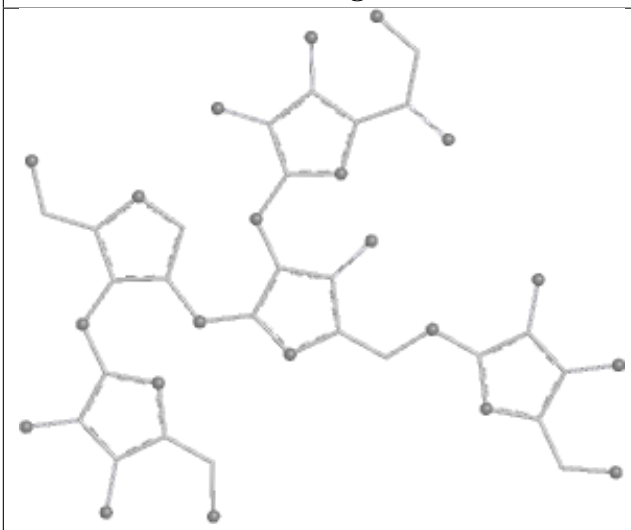	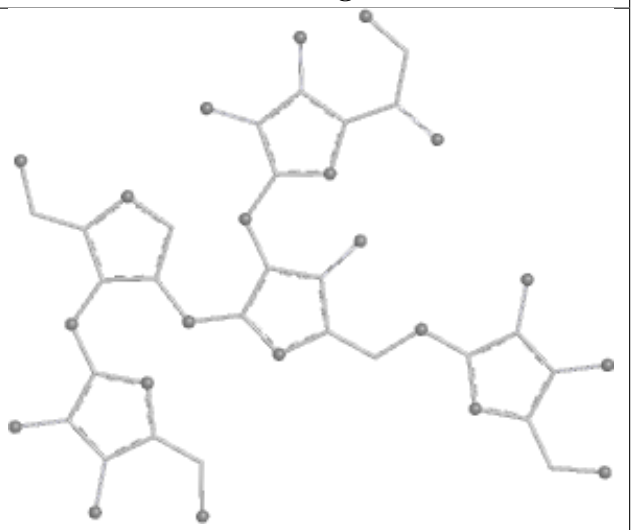
Torsions	**Rings**

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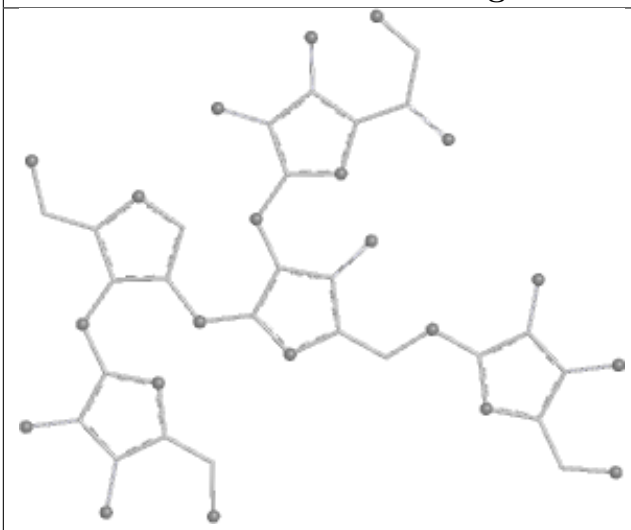	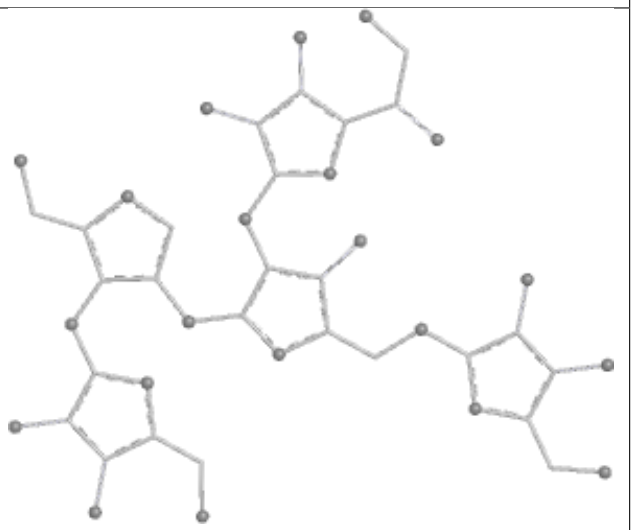
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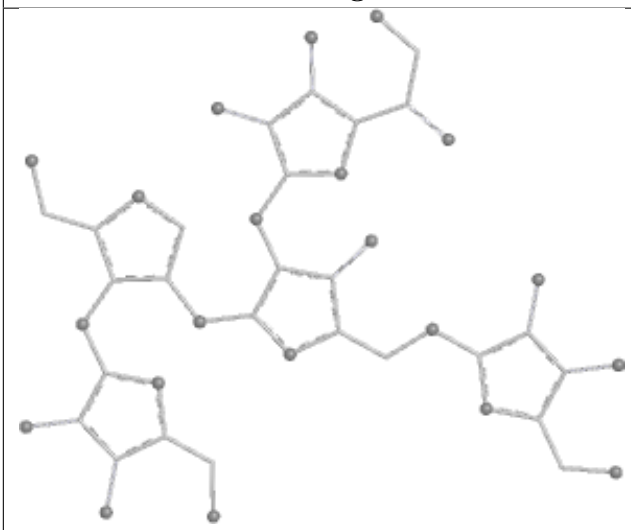	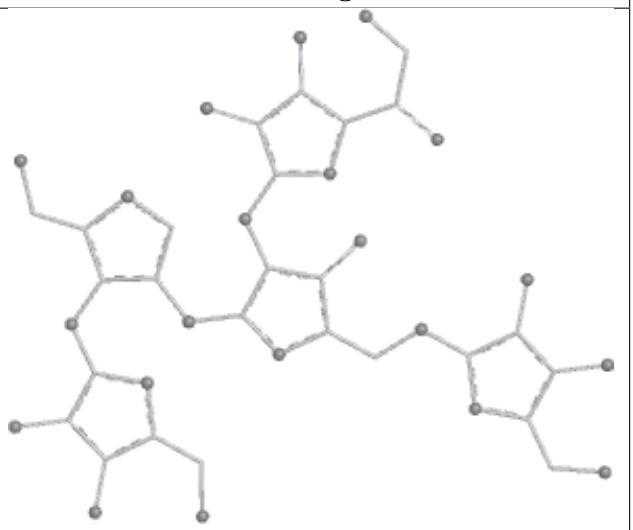
Torsions	**Rings**

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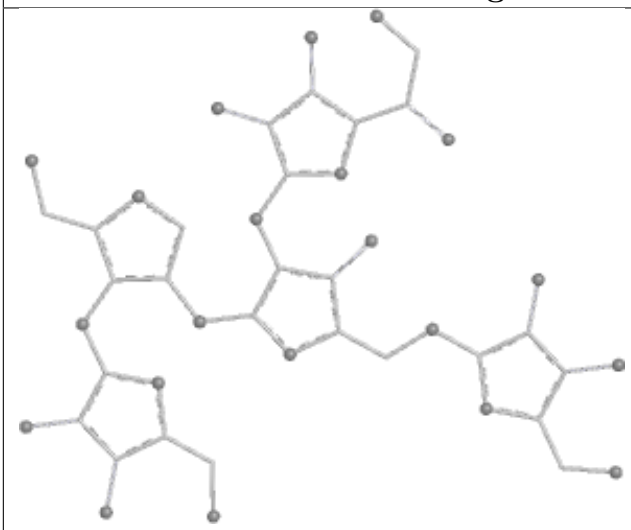	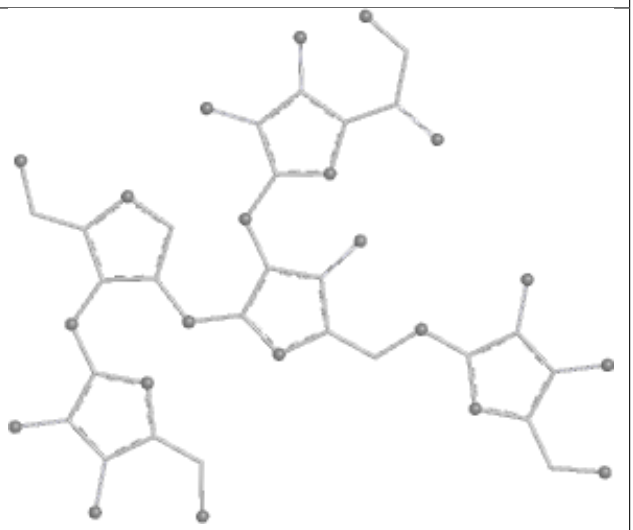
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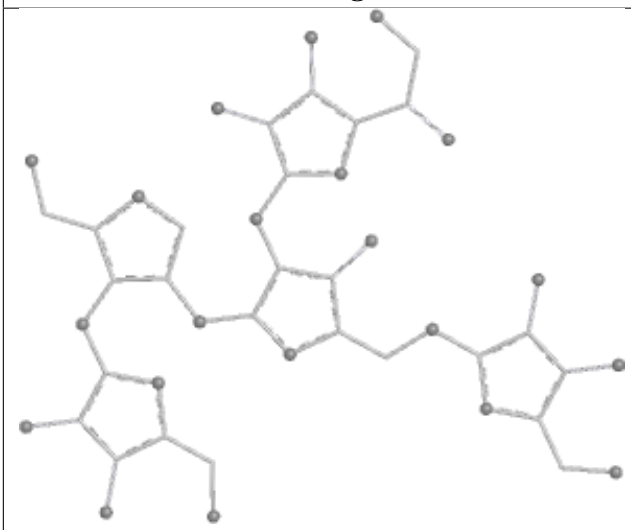	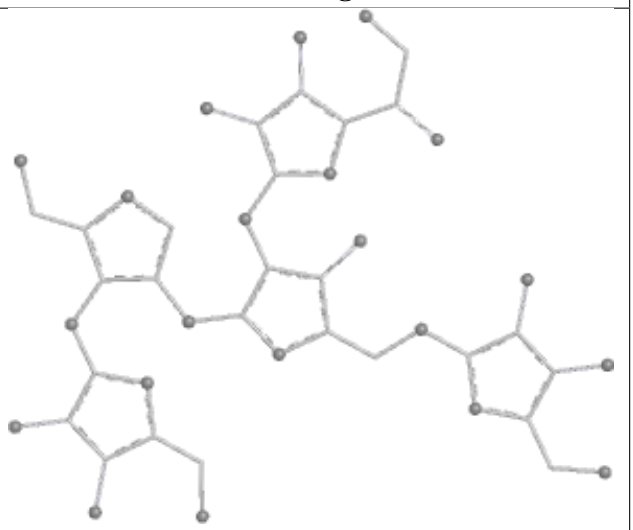
Torsions	**Rings**

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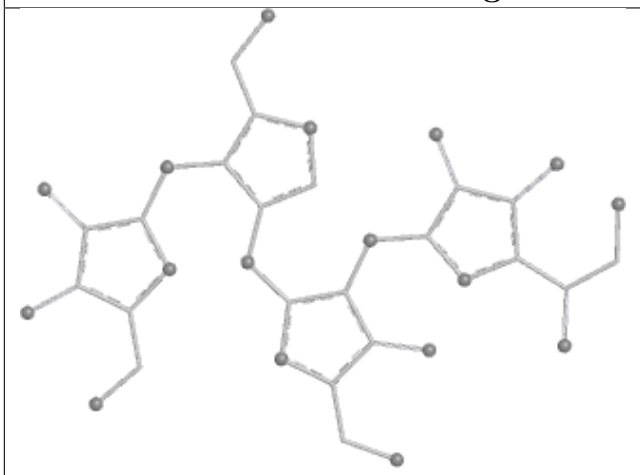
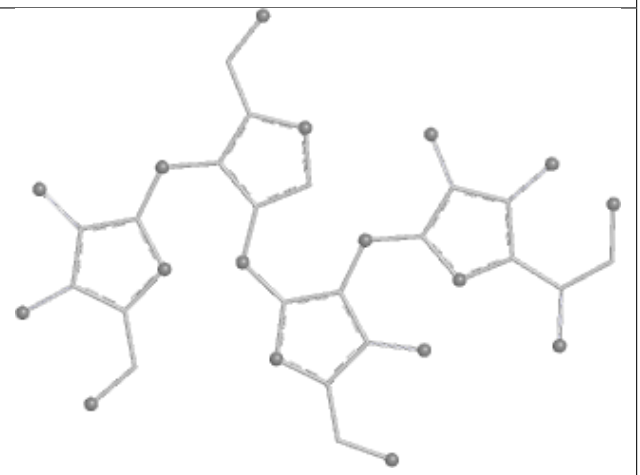
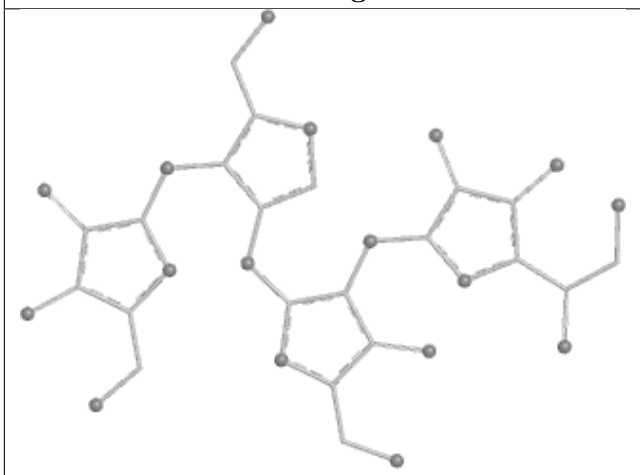
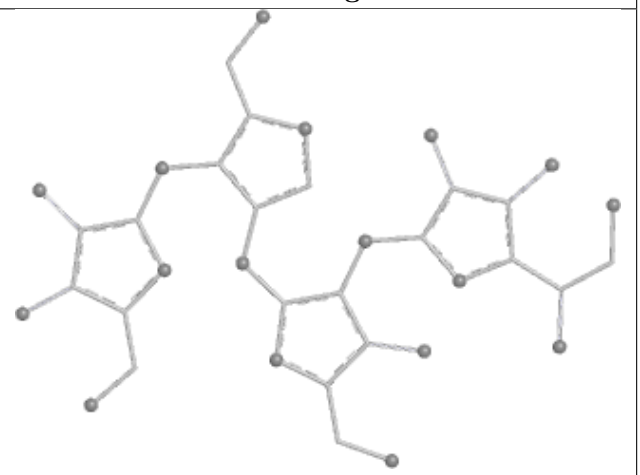
 Bond lengths	 Bond angles
 Torsions	 Rings

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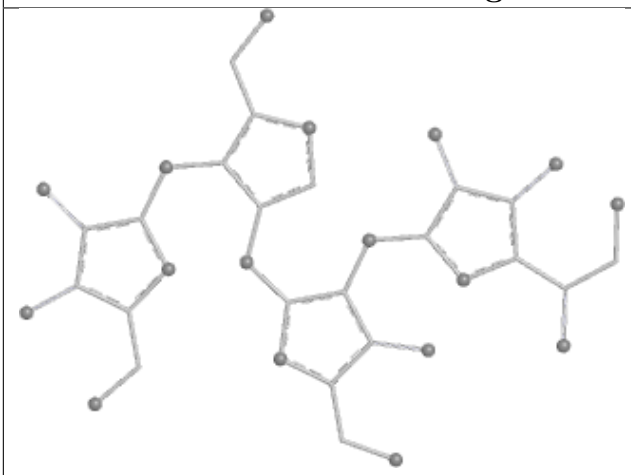
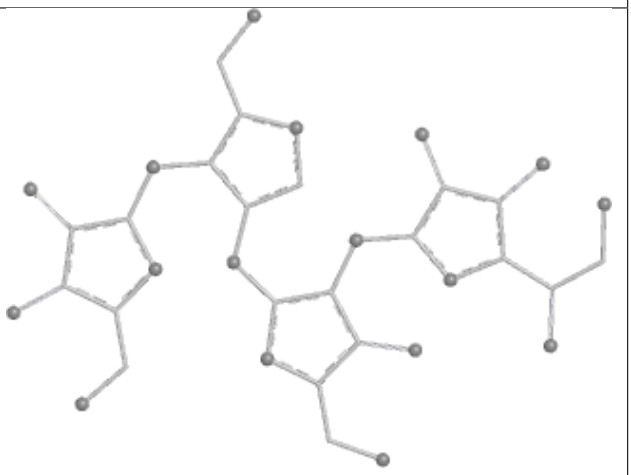
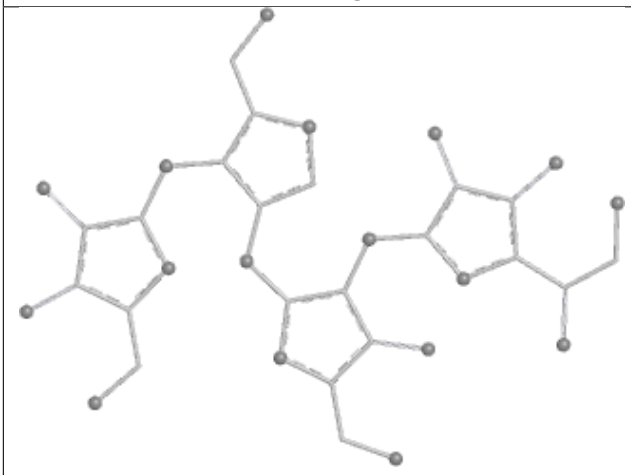
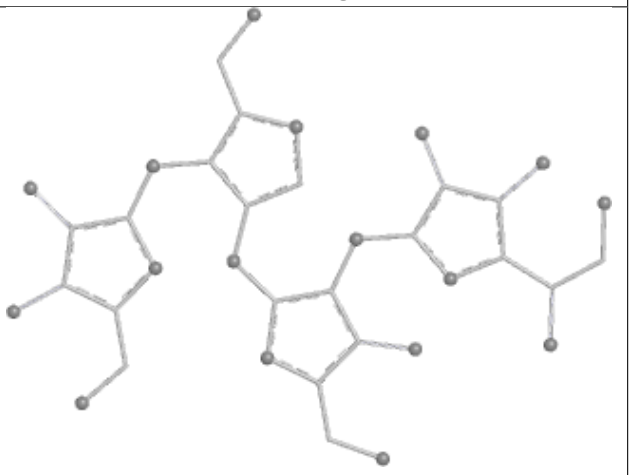
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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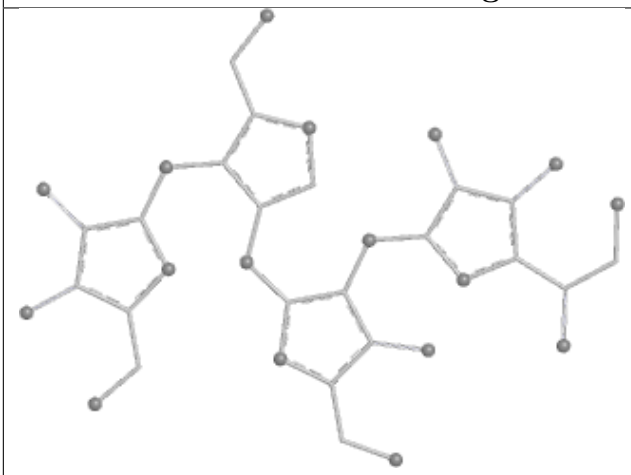
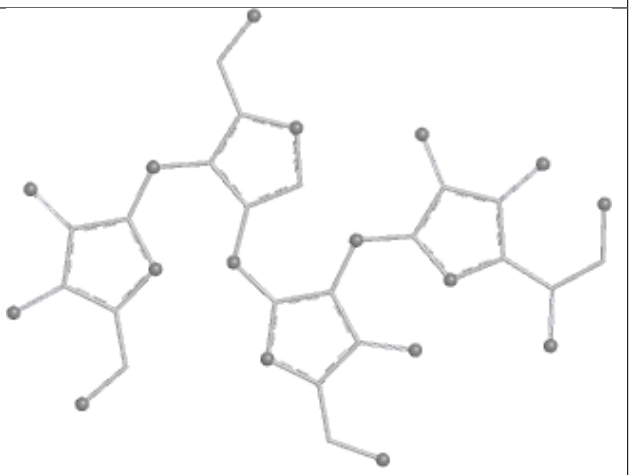
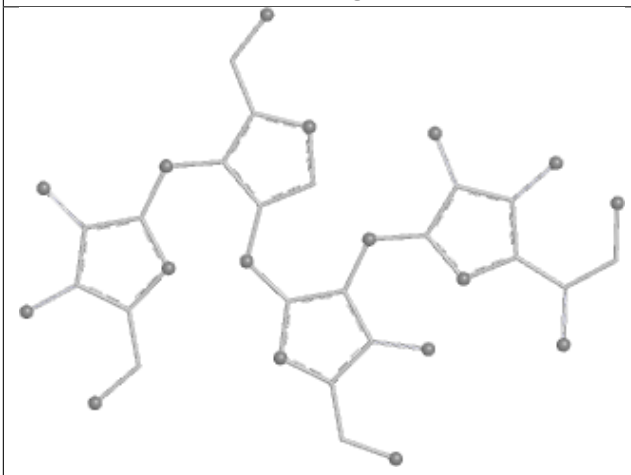
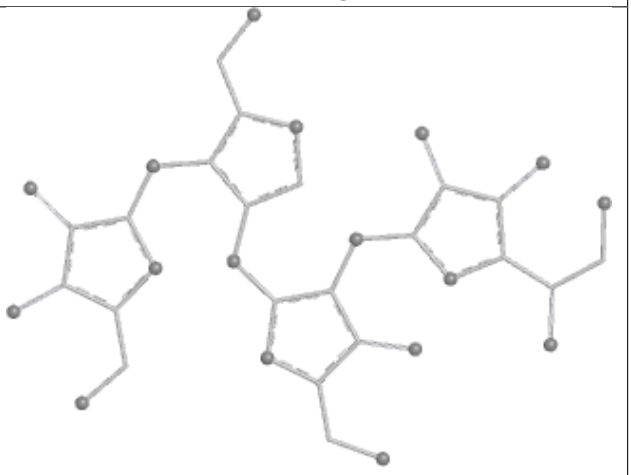
 Bond lengths	 Bond angles
 Torsions	 Rings

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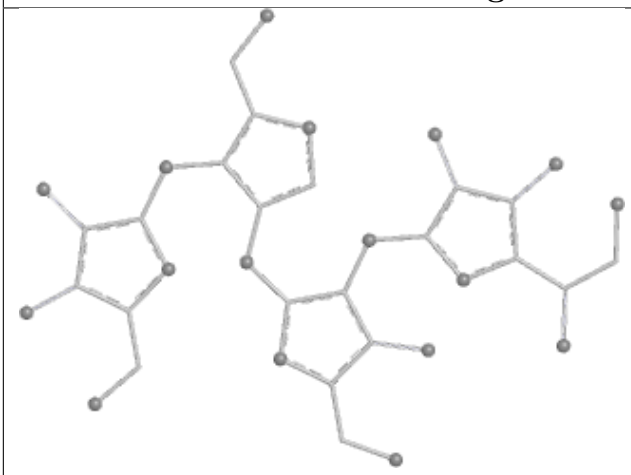
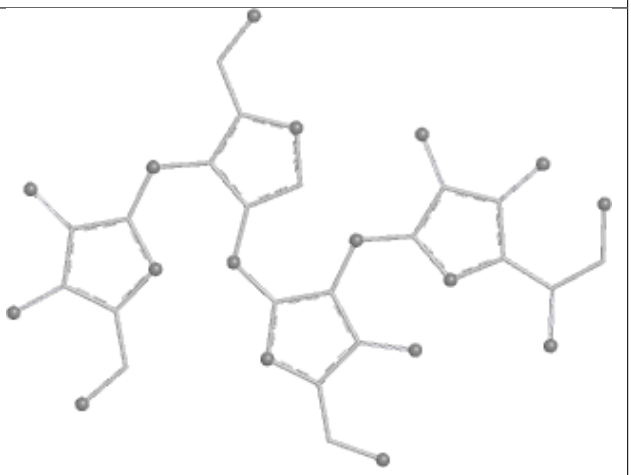
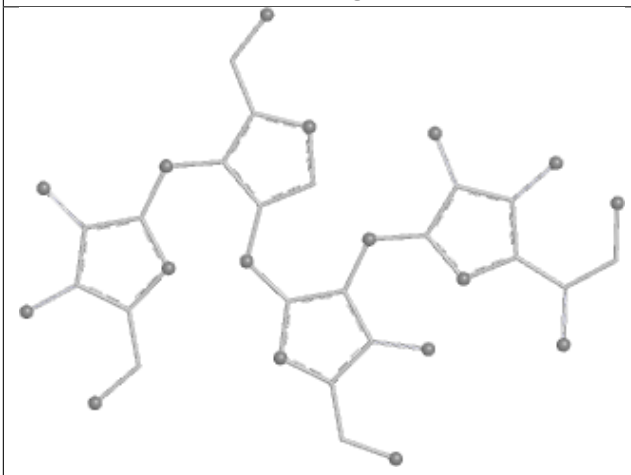
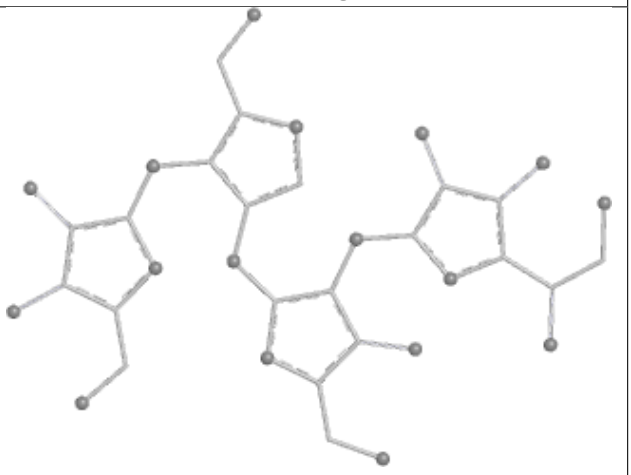
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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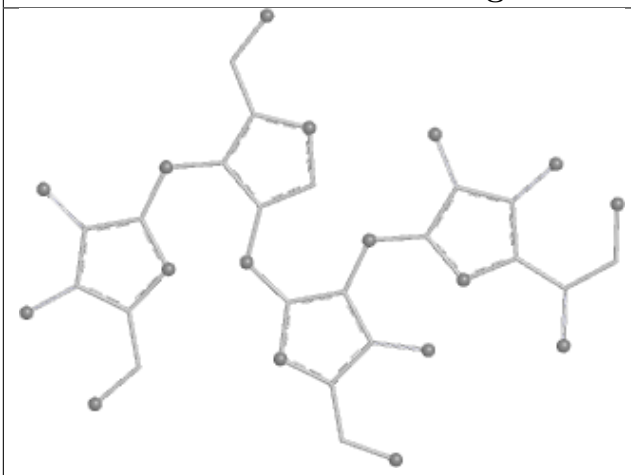
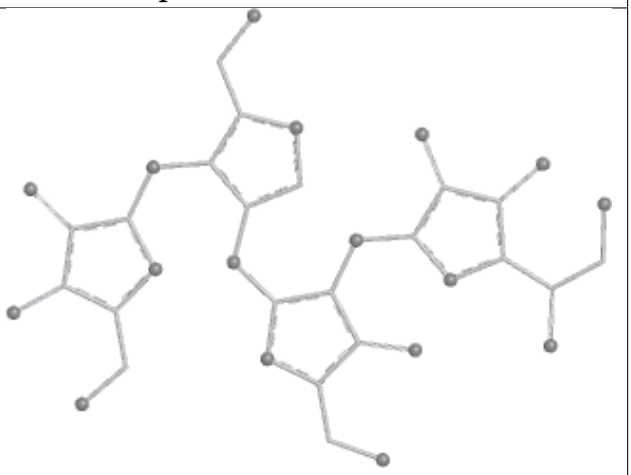
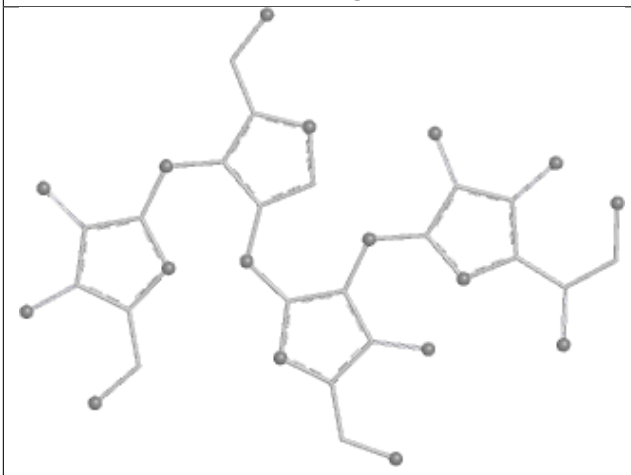
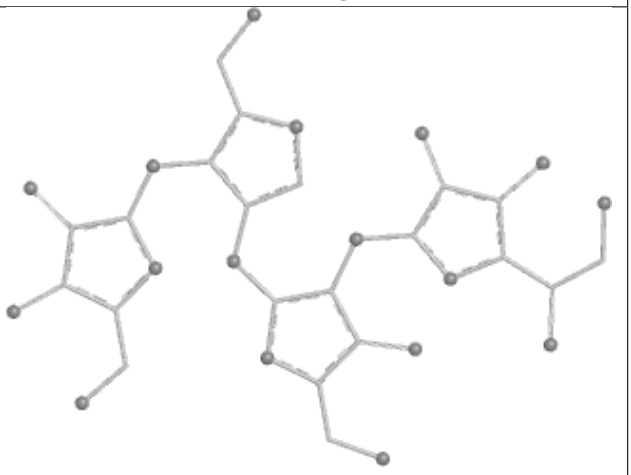
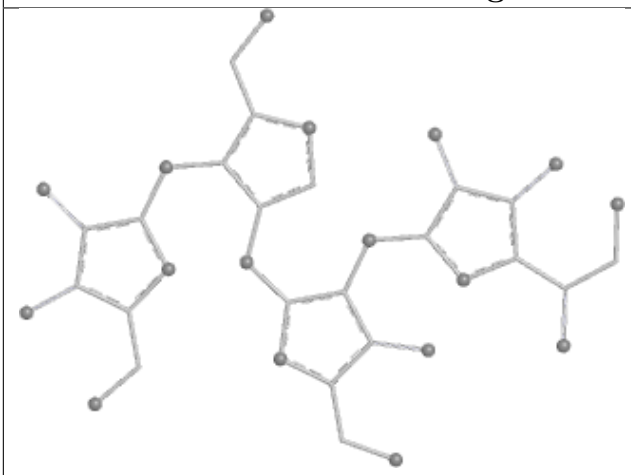
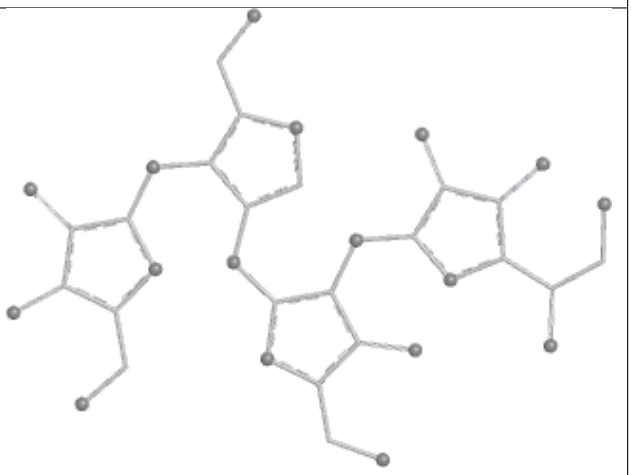
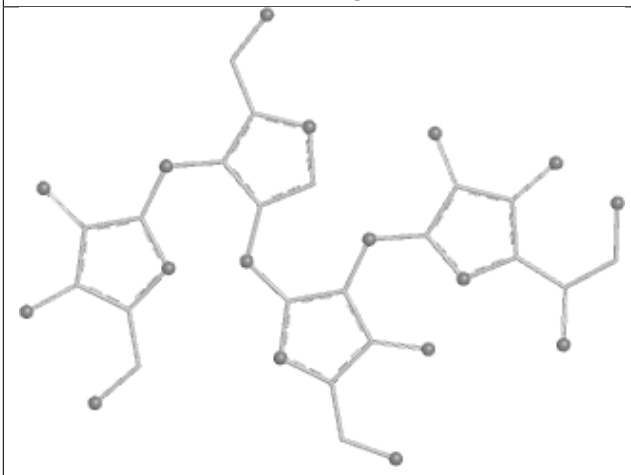
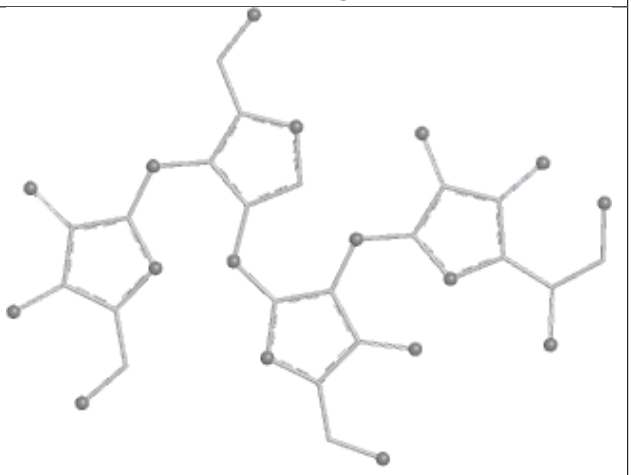
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 1E	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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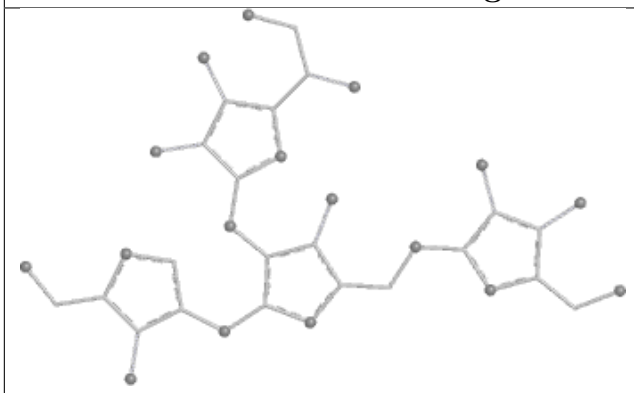
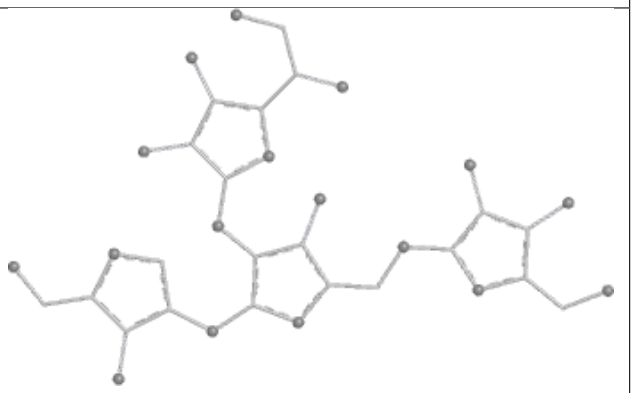
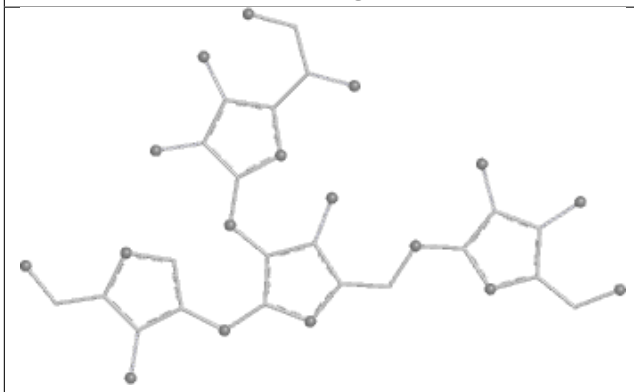
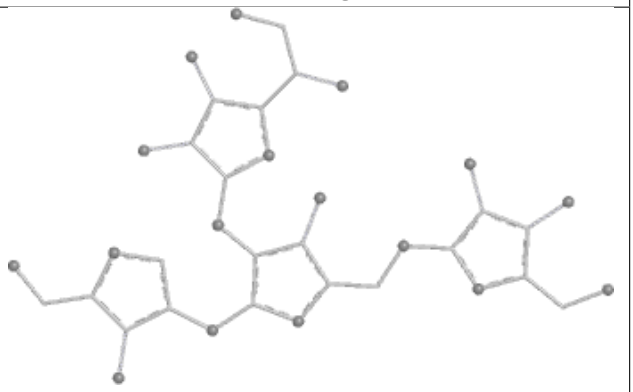
 Bond lengths	 Bond angles
 Torsions	 Rings

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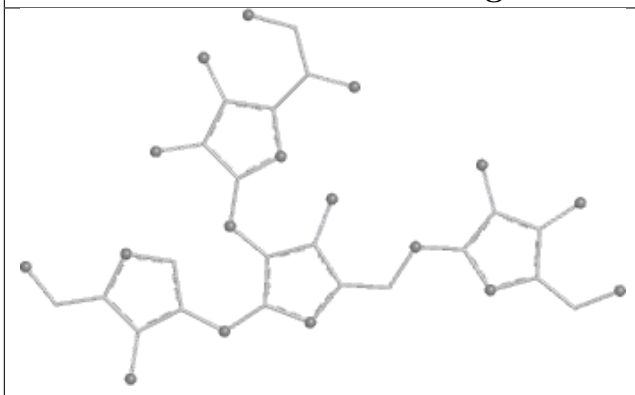
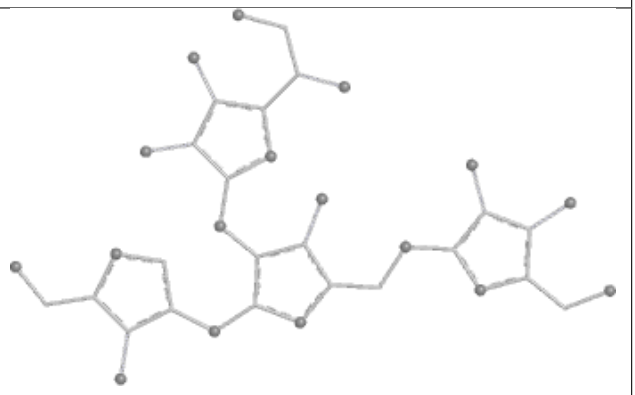
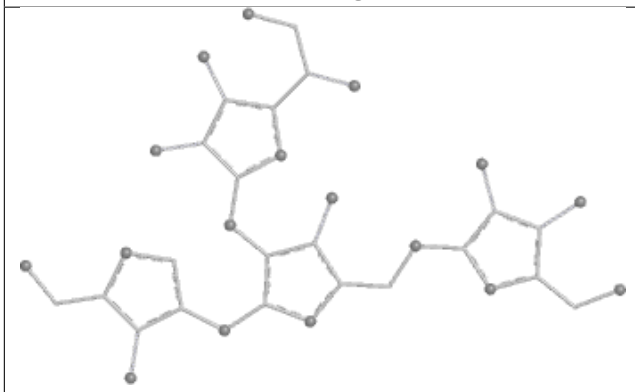
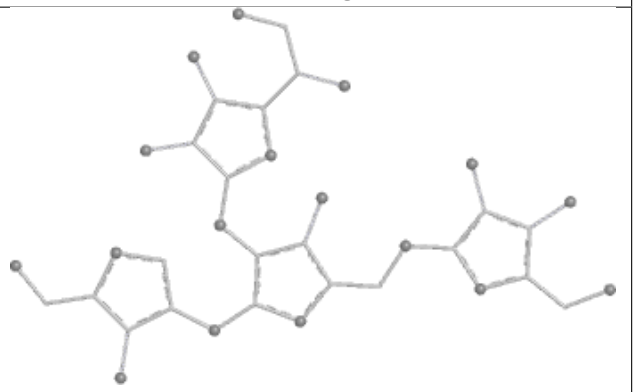
 Bond lengths	 Bond angles
 Torsions	 Rings

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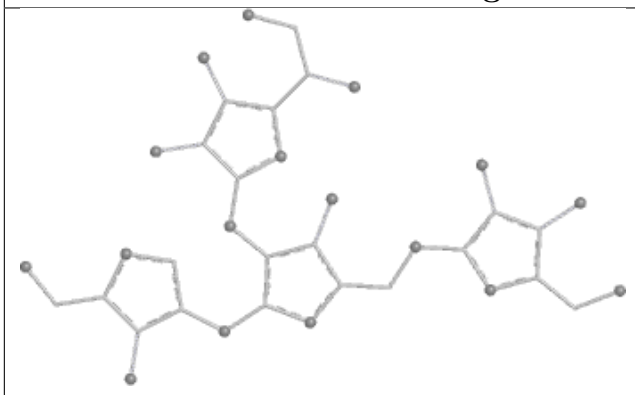
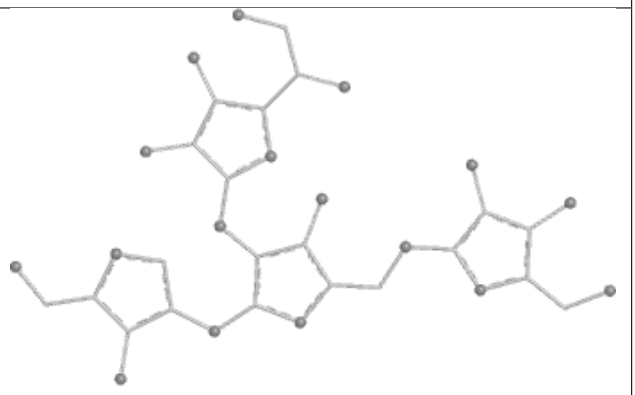
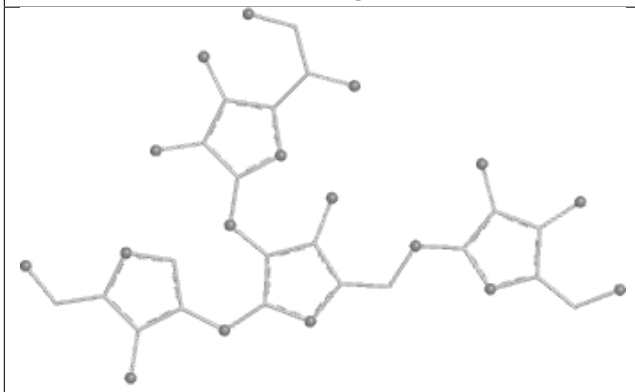
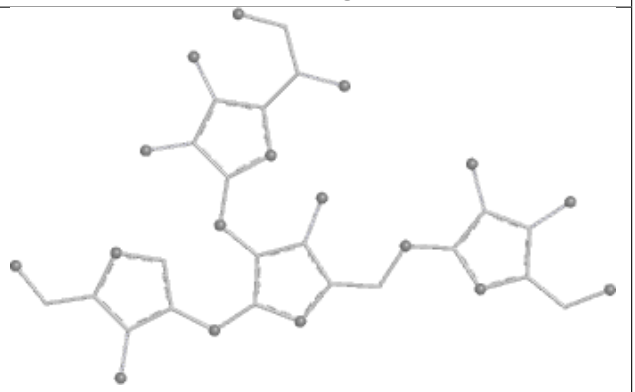
 Bond lengths	 Bond angles
 Torsions	 Rings

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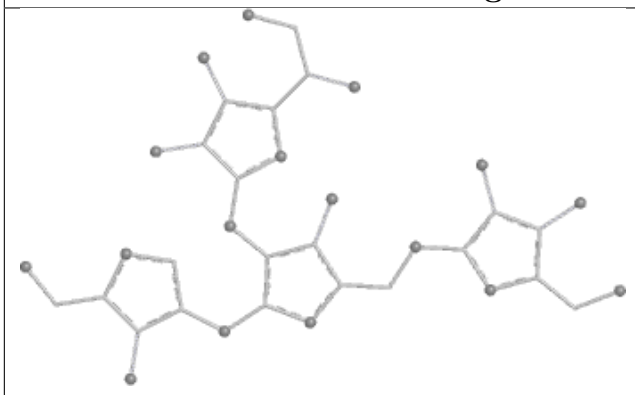
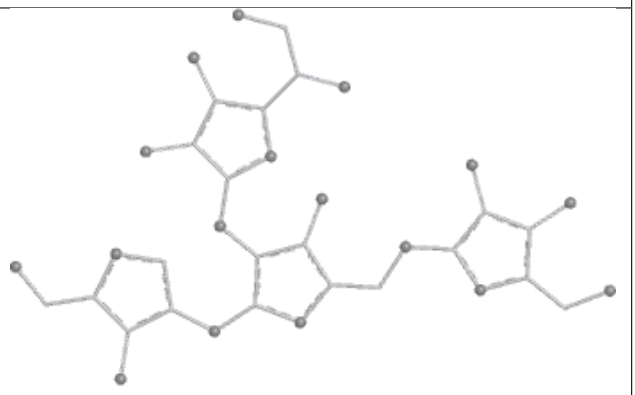
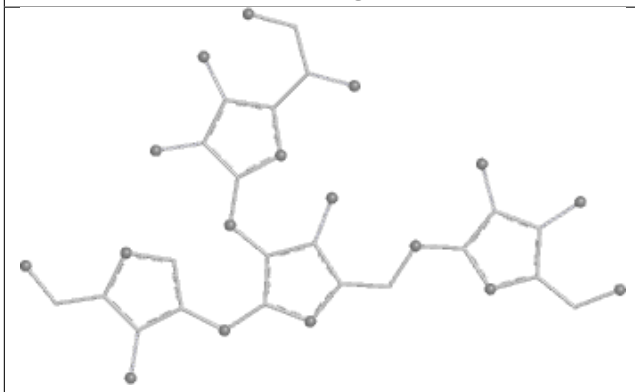
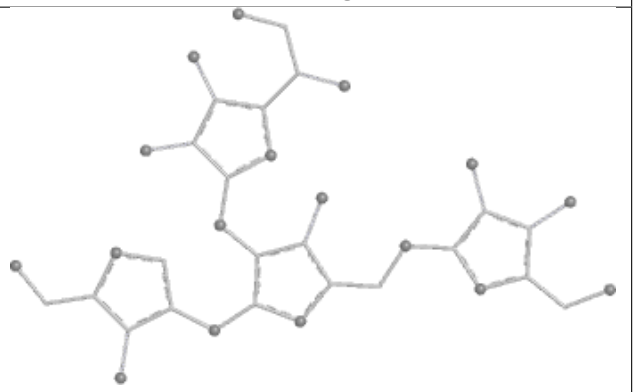
 Bond lengths	 Bond angles
 Torsions	 Rings

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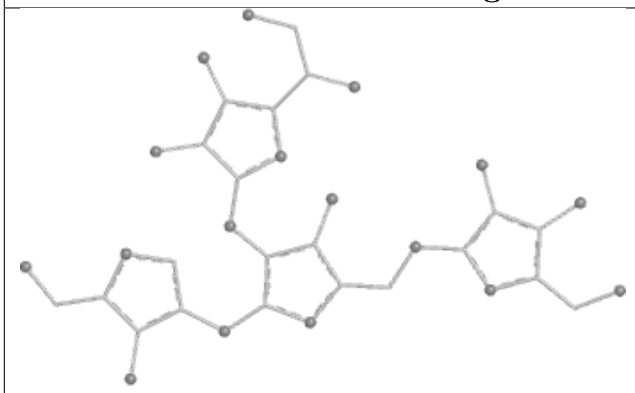
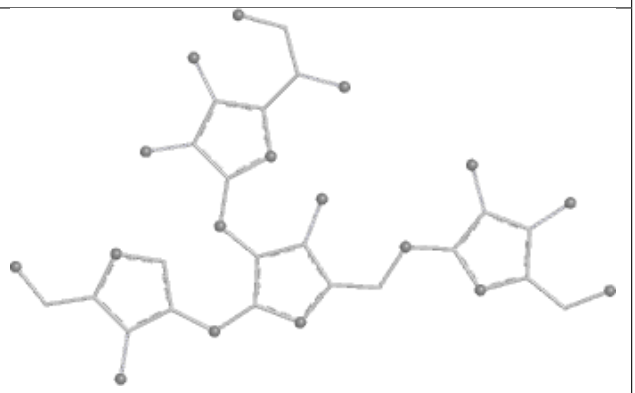
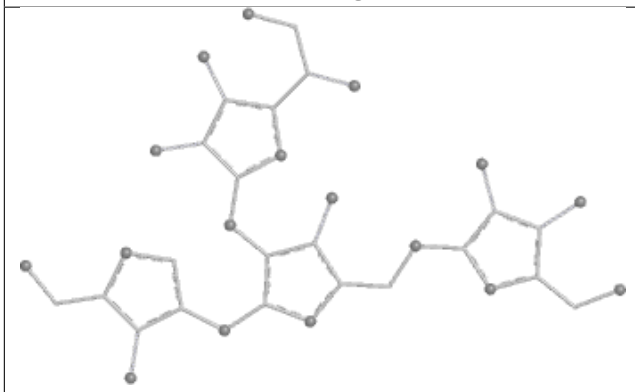
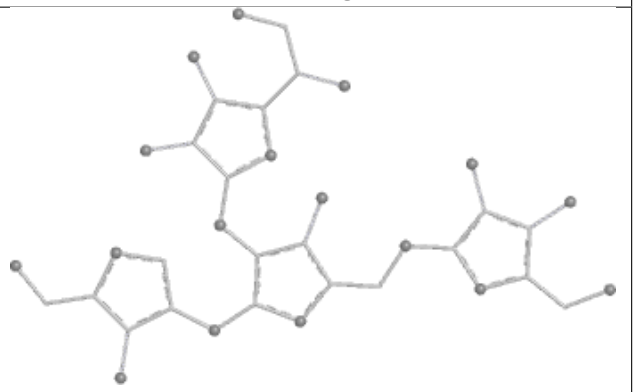
 Bond lengths	 Bond angles
 Torsions	 Rings

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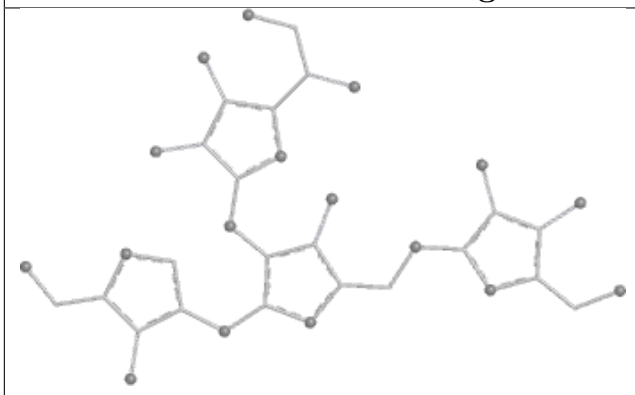
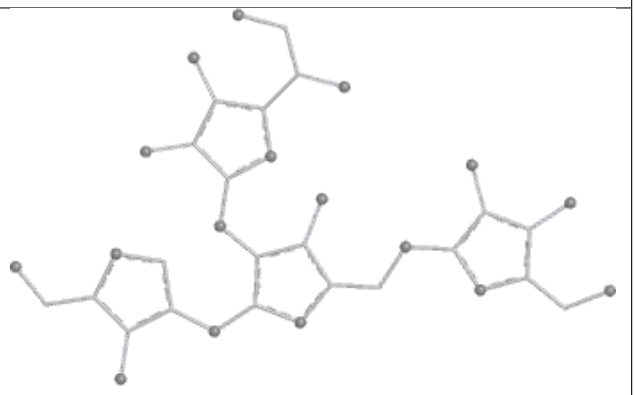
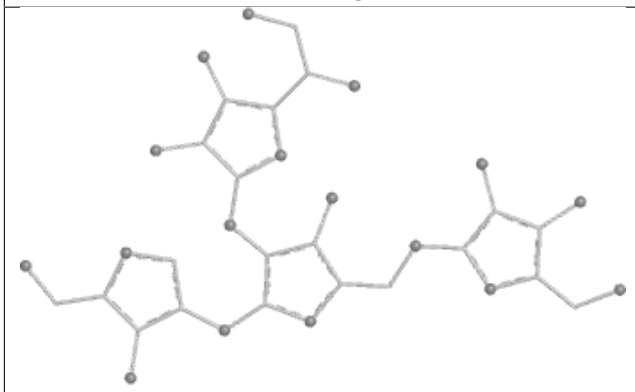
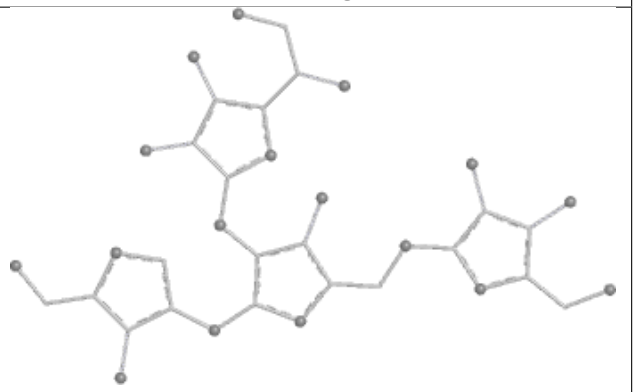
 Bond lengths	 Bond angles
 Torsions	 Rings

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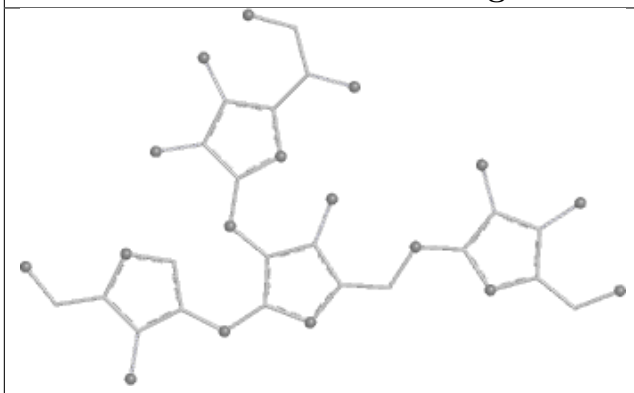
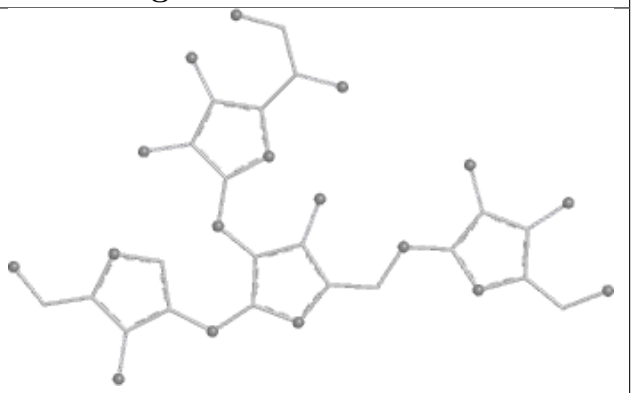
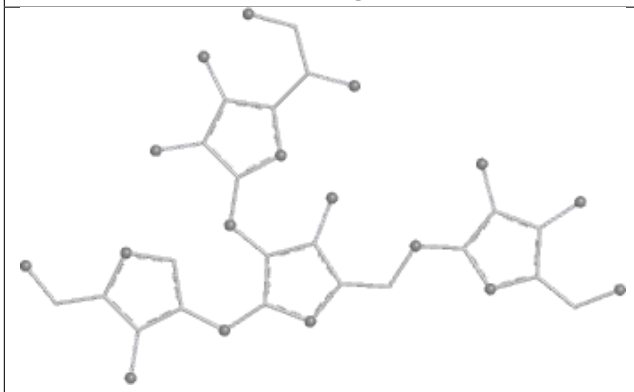
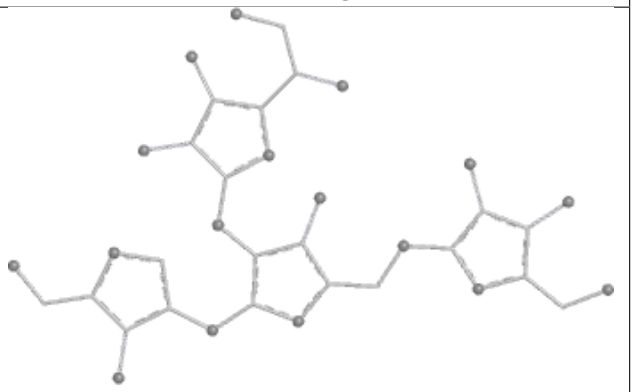
 Bond lengths	 Bond angles
 Torsions	 Rings

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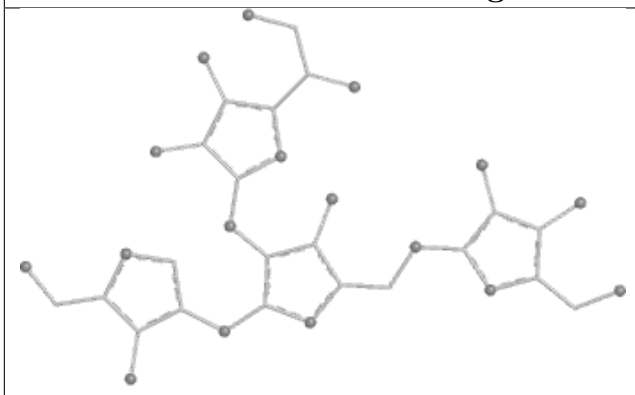
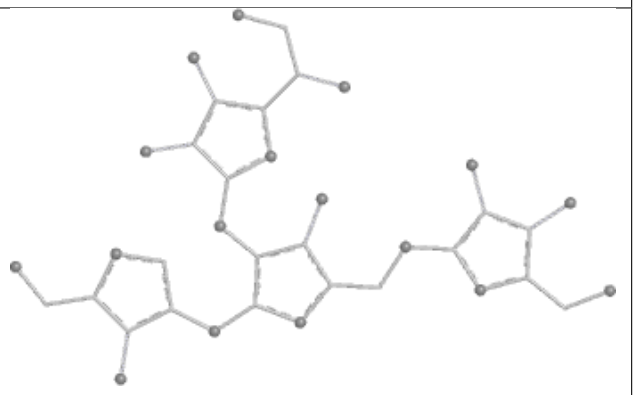
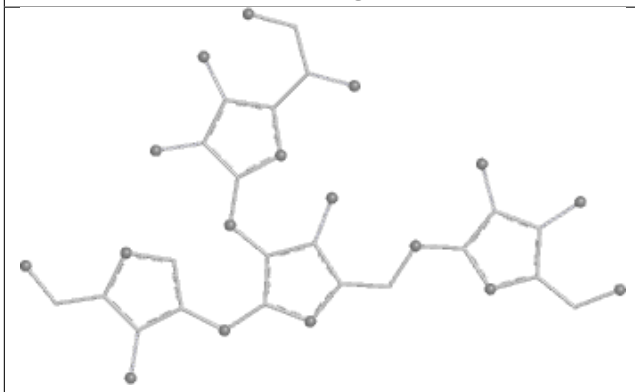
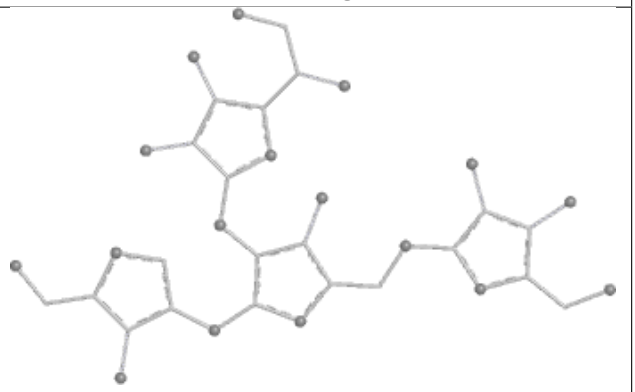
 Bond lengths	 Bond angles
 Torsions	 Rings

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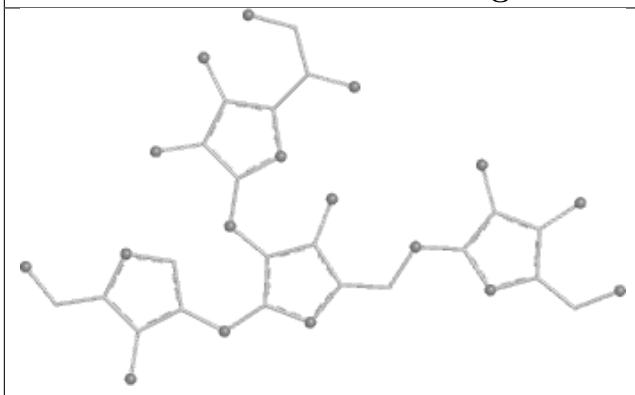
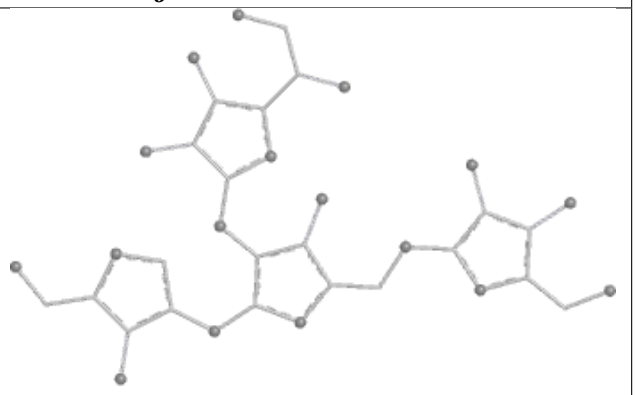
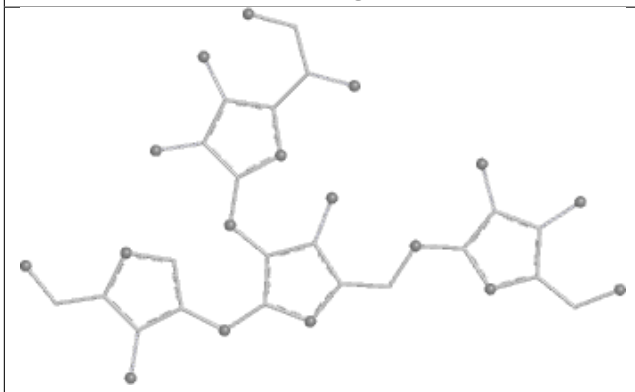
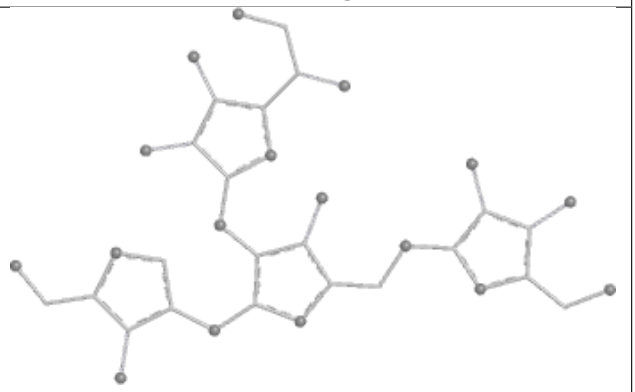
 Bond lengths	 Bond angles
 Torsions	 Rings

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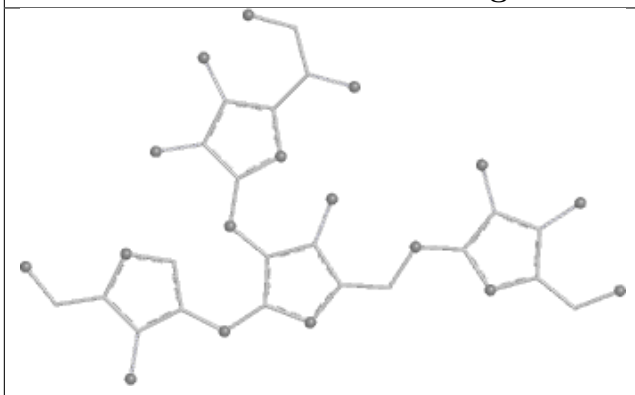
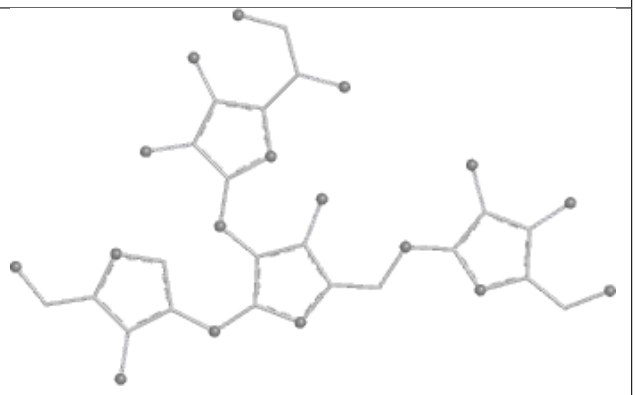
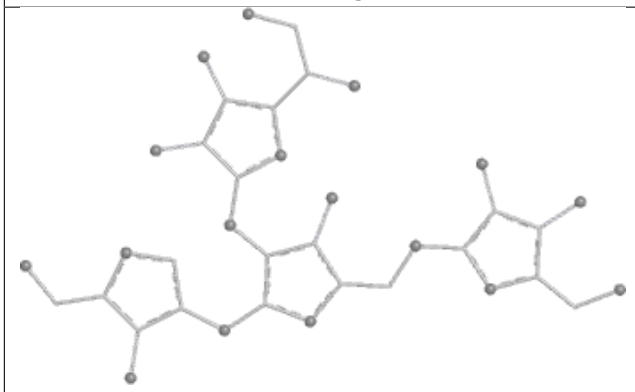
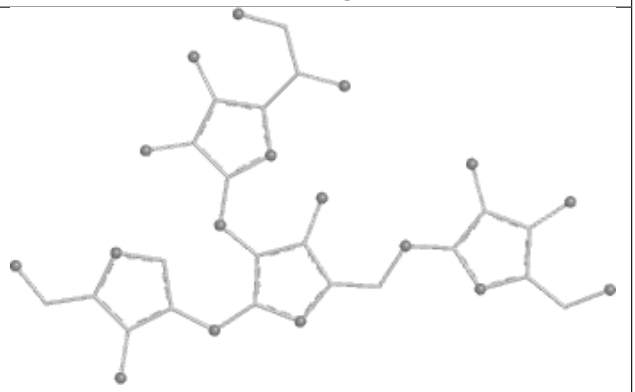
 Bond lengths	 Bond angles
 Torsions	 Rings

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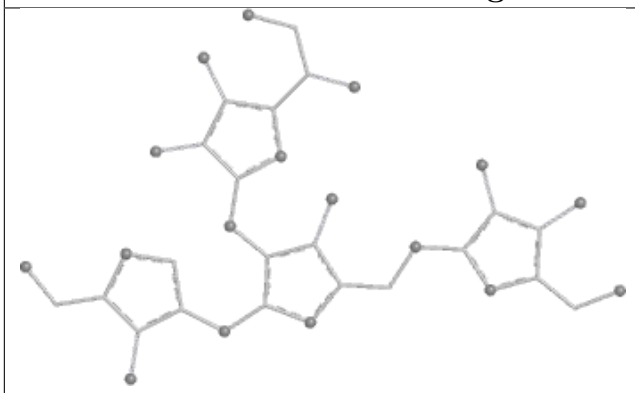
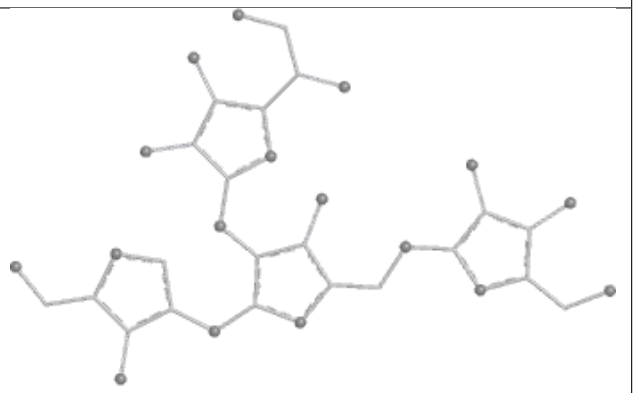
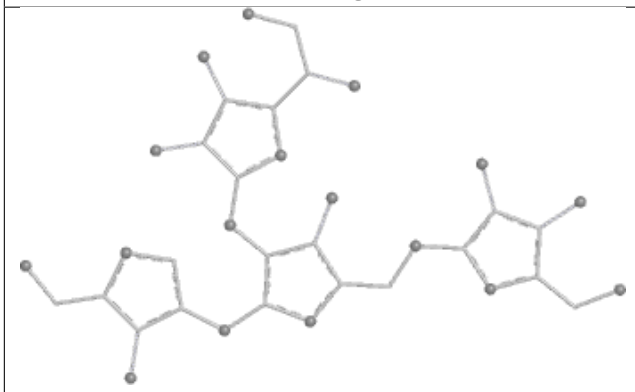
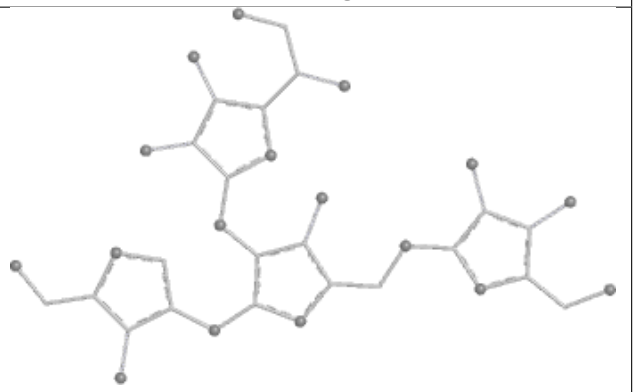
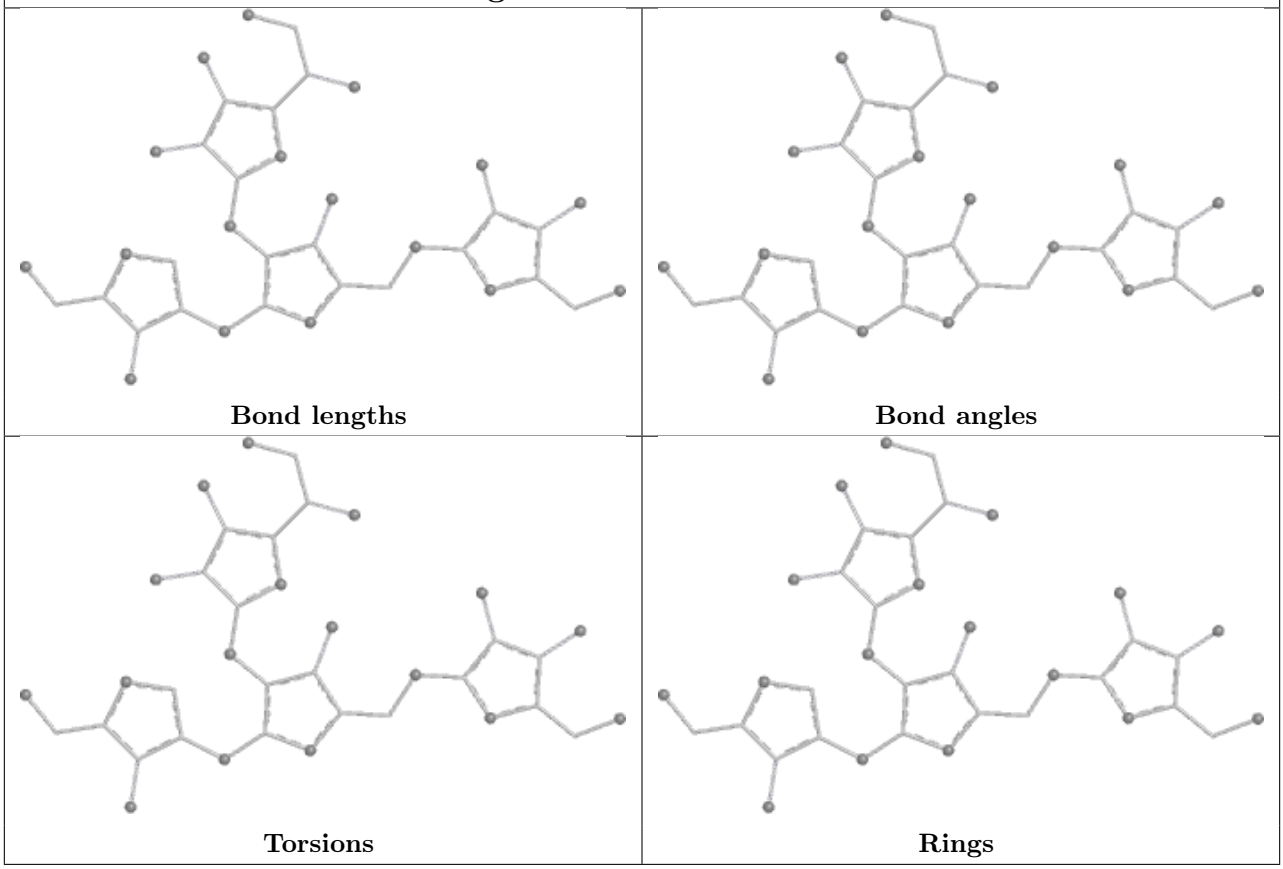
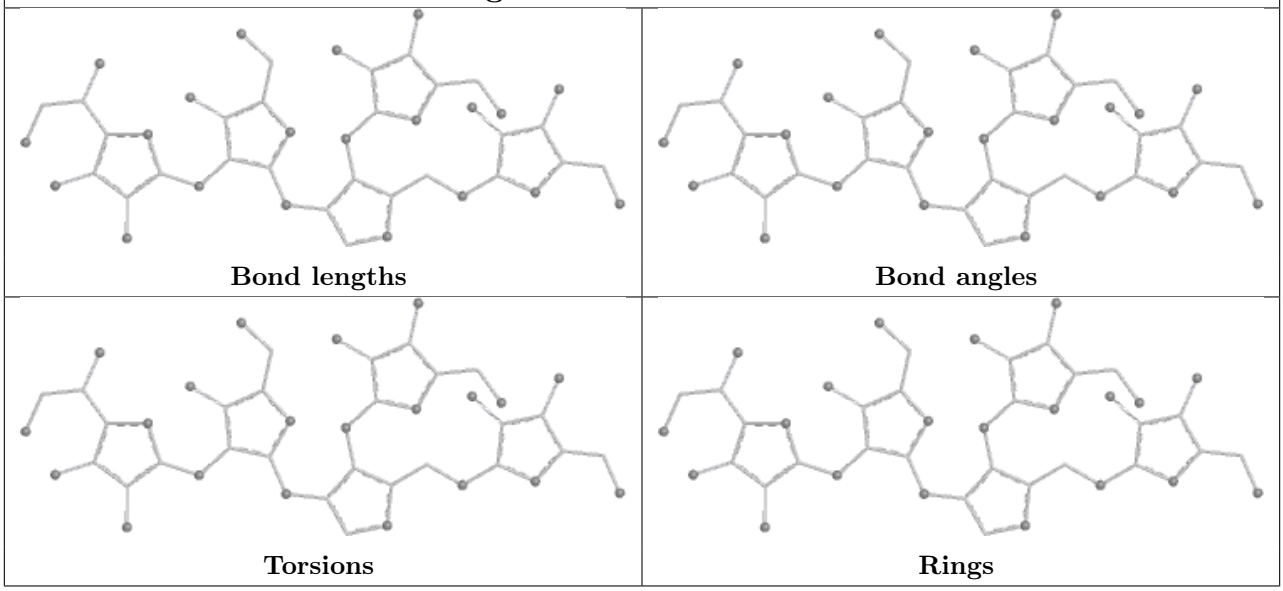
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain xE



Oligosaccharide Chain FE



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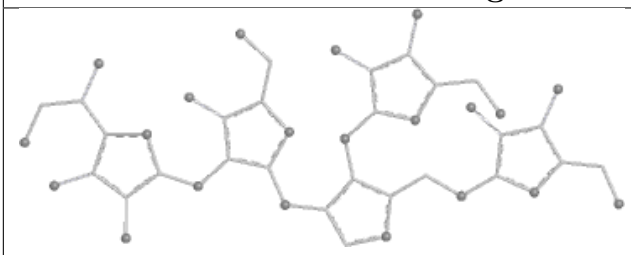
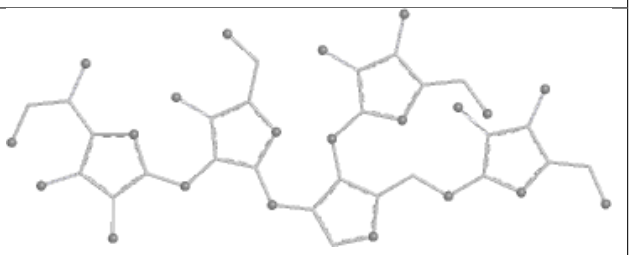
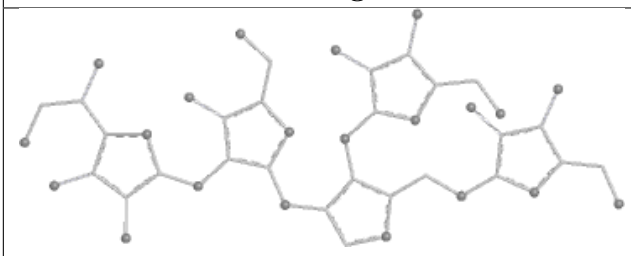
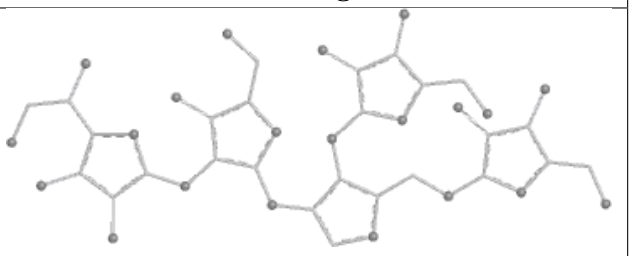
 Bond lengths	 Bond angles
 Torsions	 Rings

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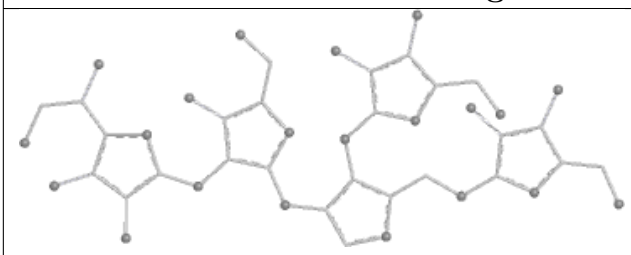
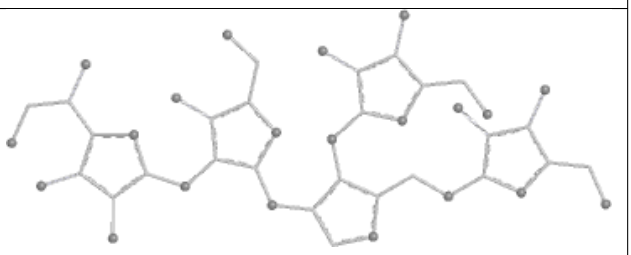
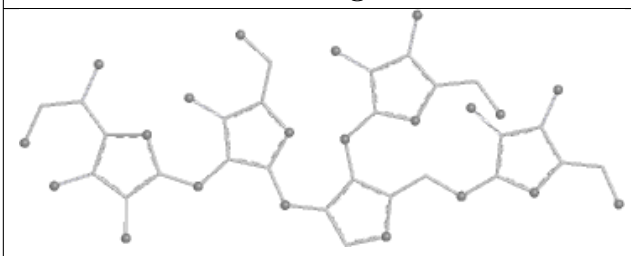
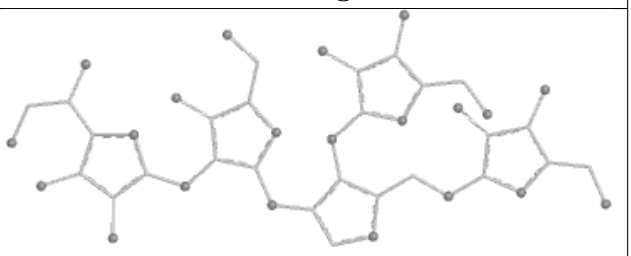
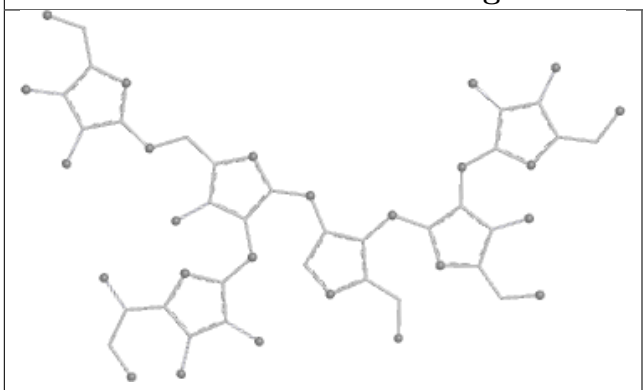
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain GE



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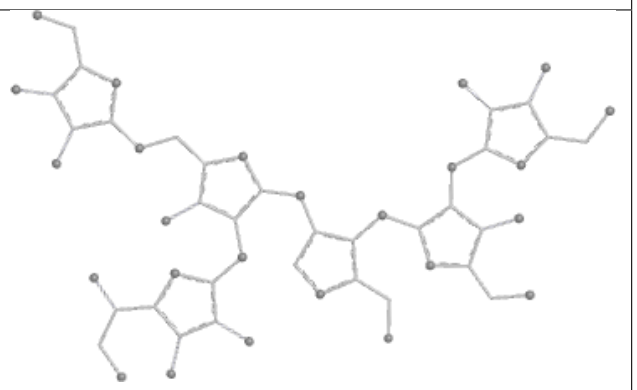

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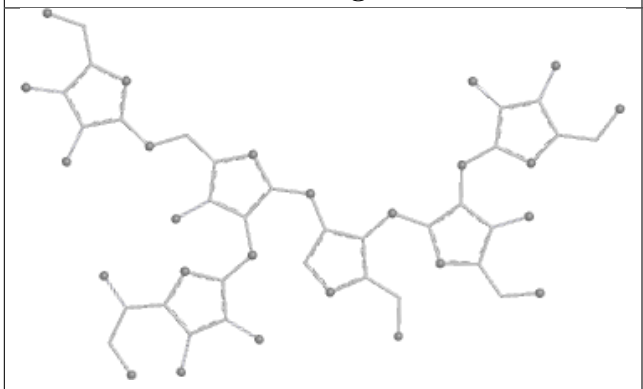

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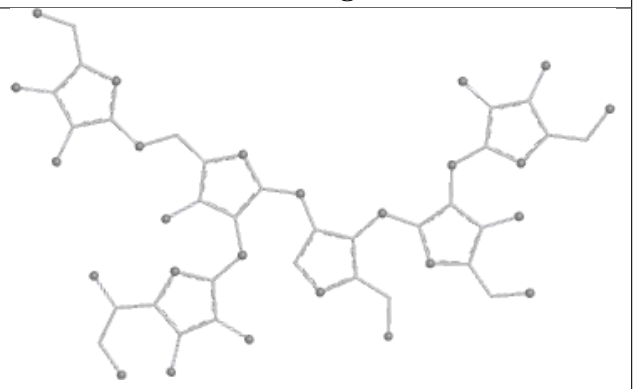
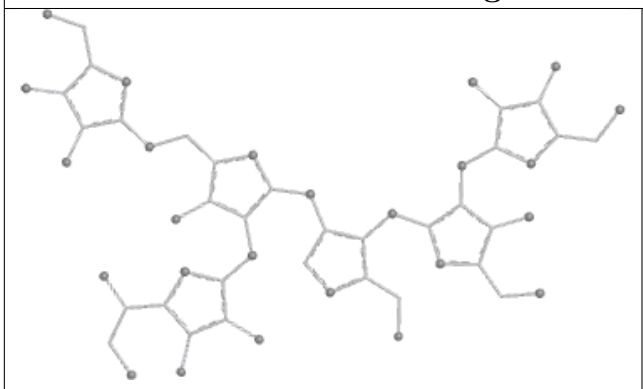


Rings

Oligosaccharide Chain QE



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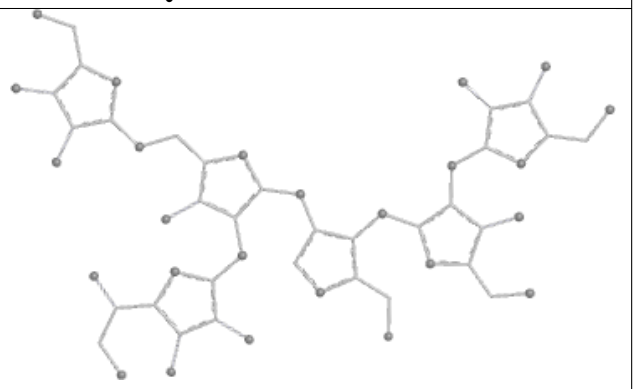

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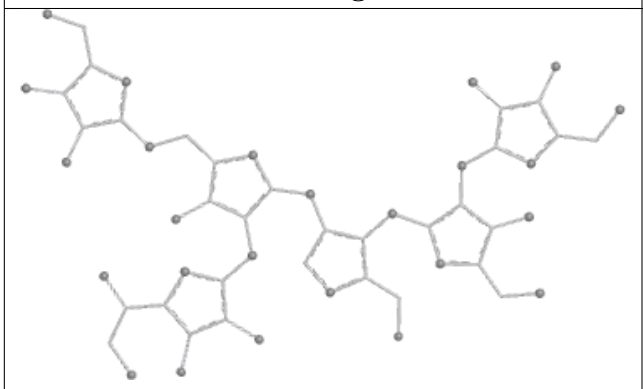

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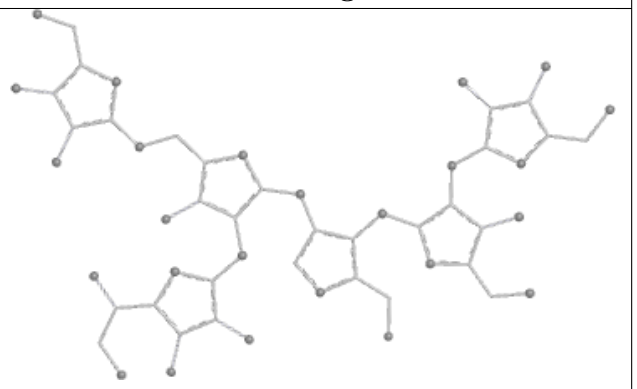
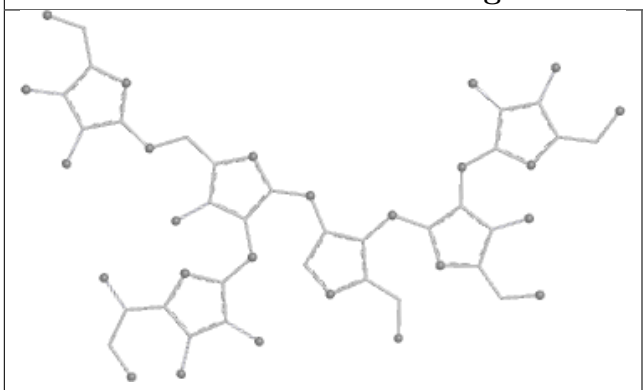


Rings

Oligosaccharide Chain RE



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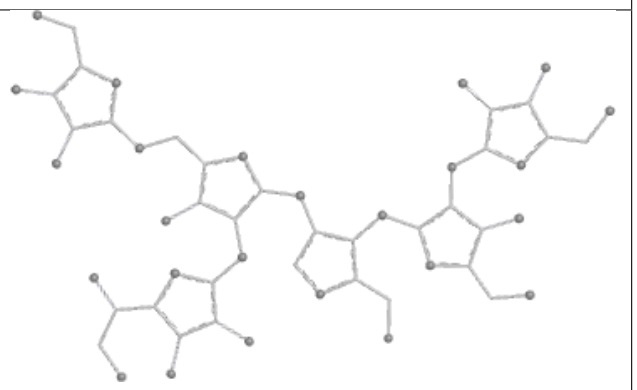

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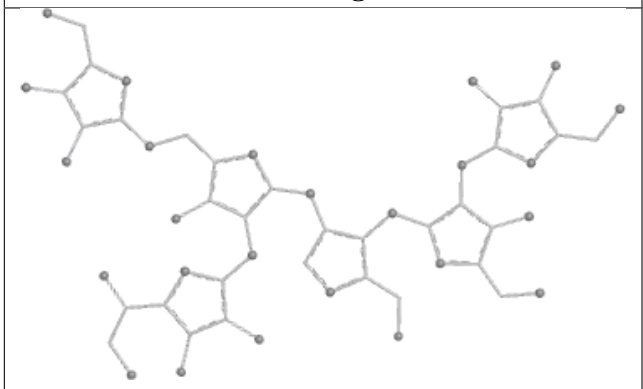

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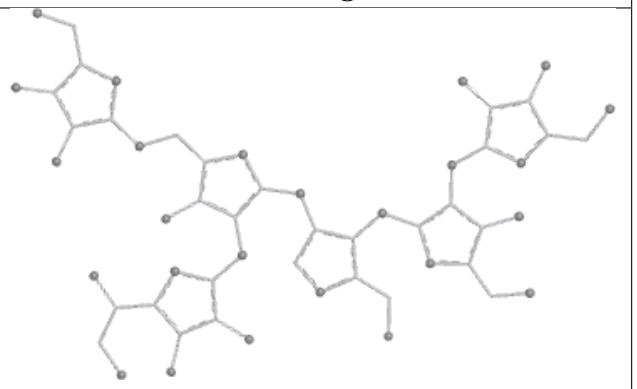
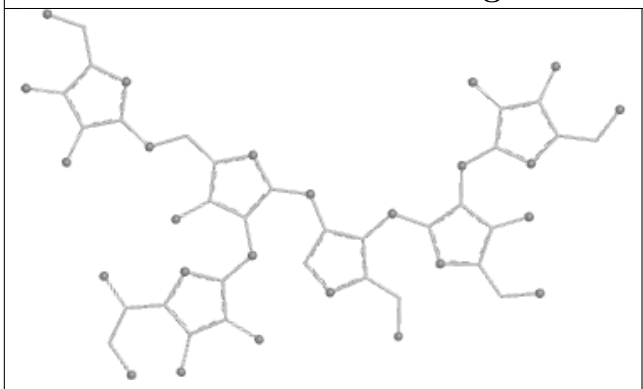


Rings

Oligosaccharide Chain VE



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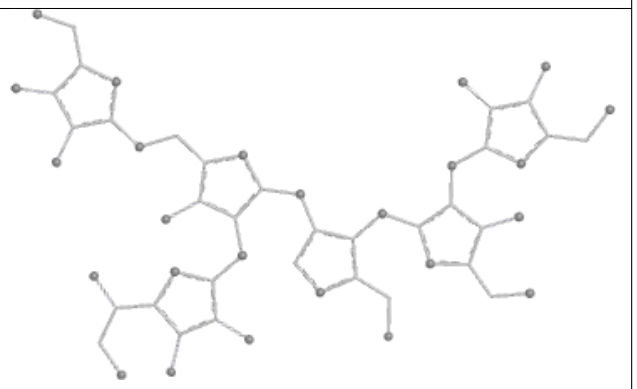

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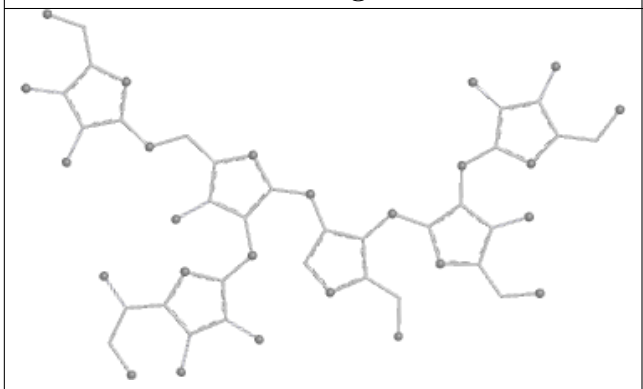

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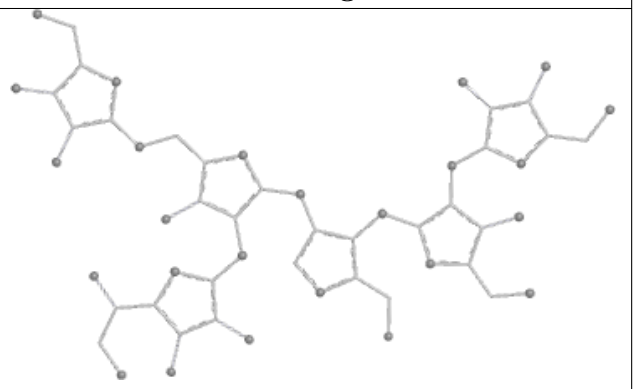
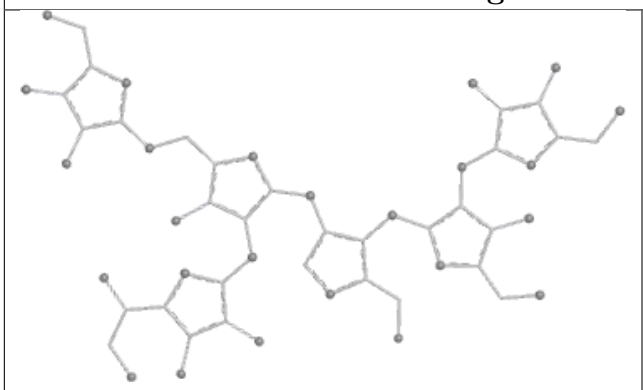


Rings

Oligosaccharide Chain dE



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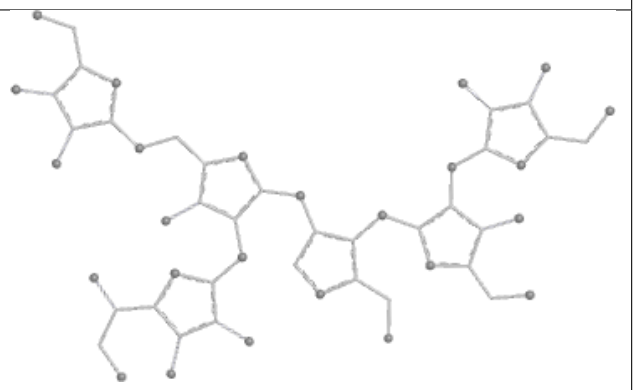
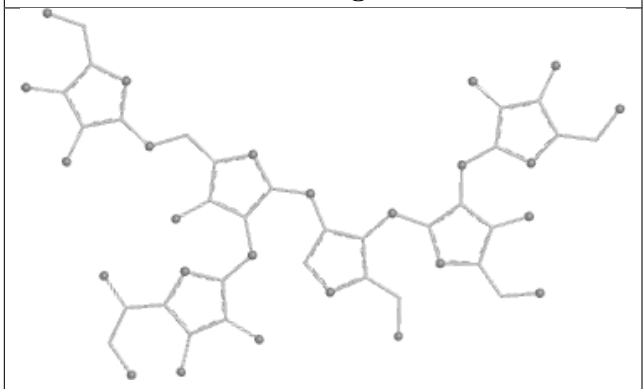


Bond angles



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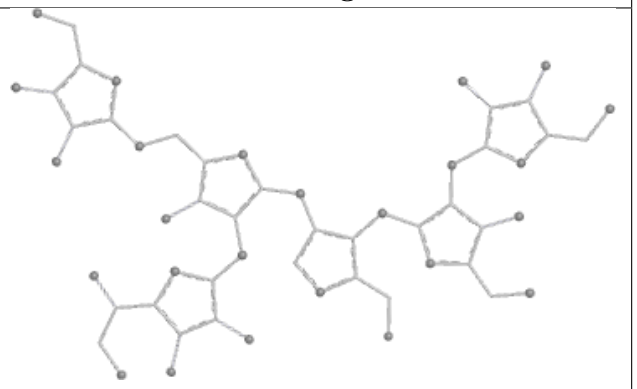
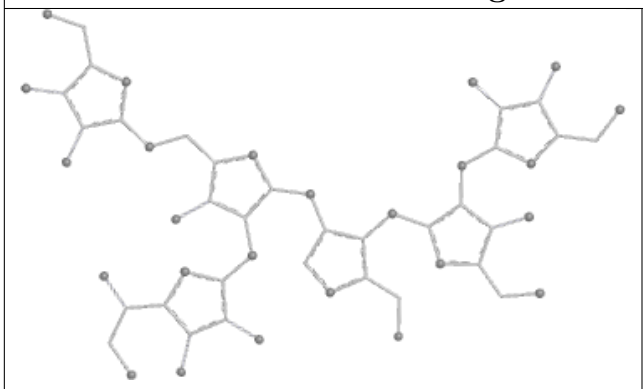


Rings

Oligosaccharide Chain eE



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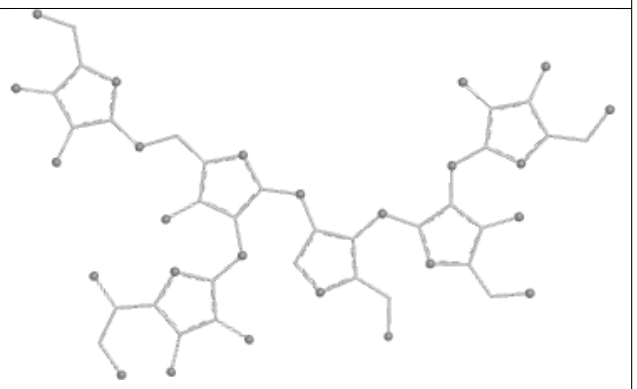

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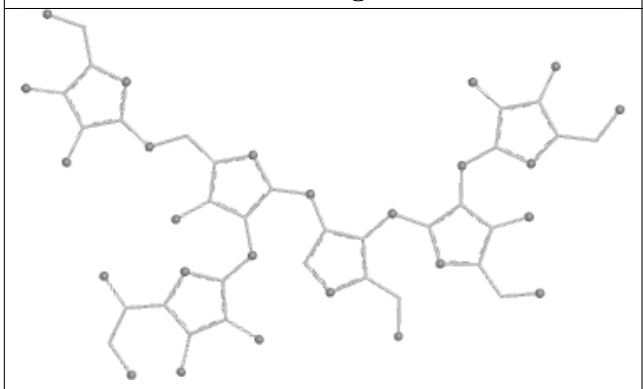

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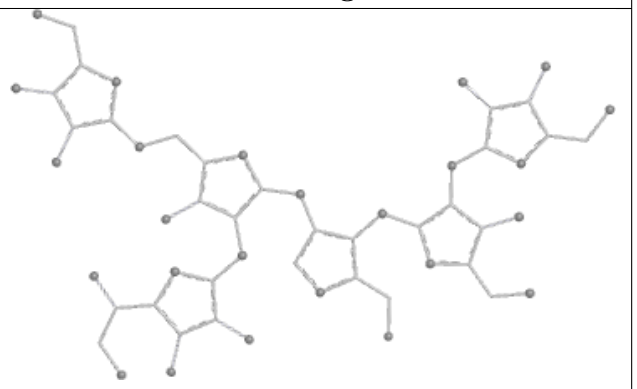

Rings

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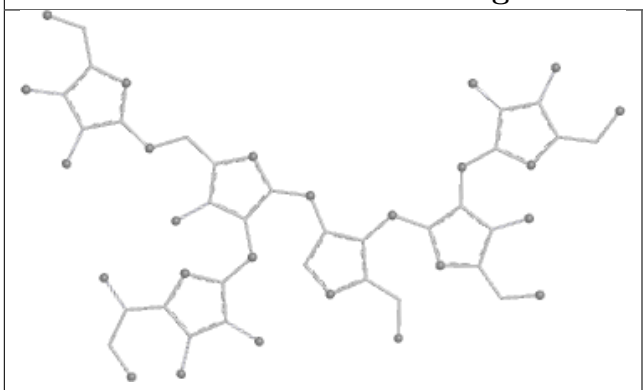

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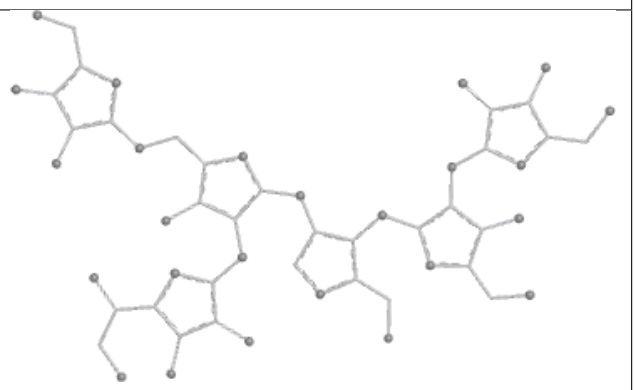

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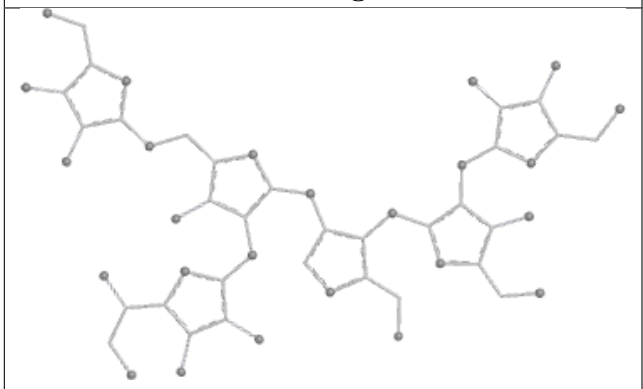

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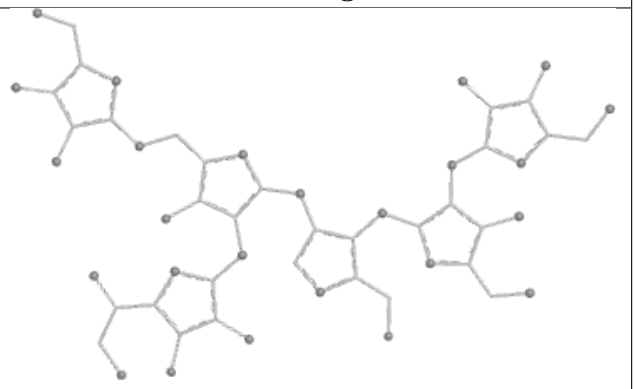
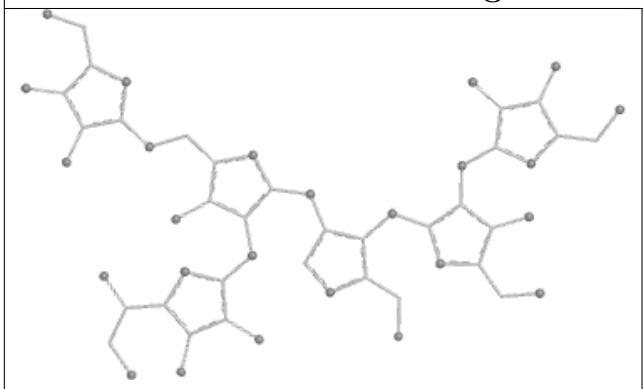


Rings

Oligosaccharide Chain wE



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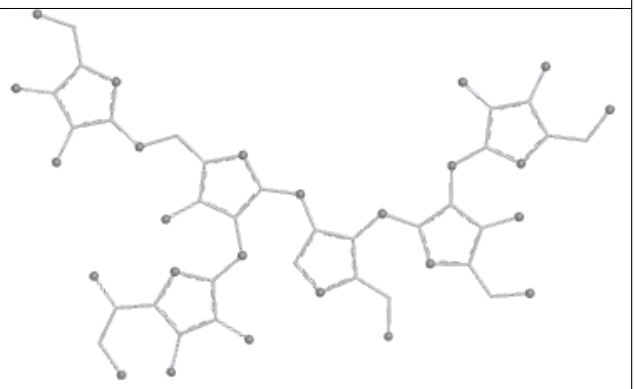
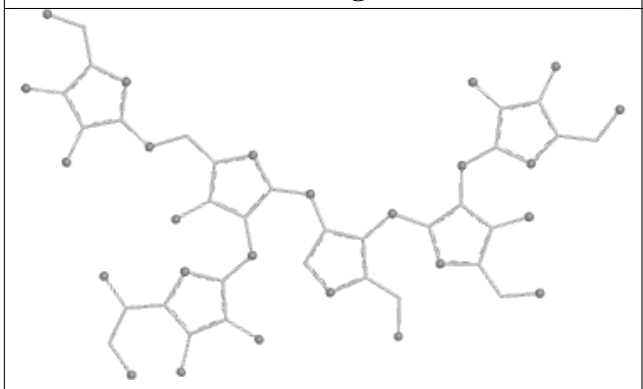


Bond angles



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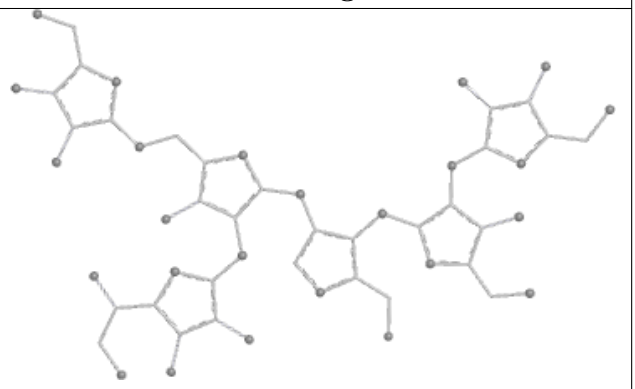
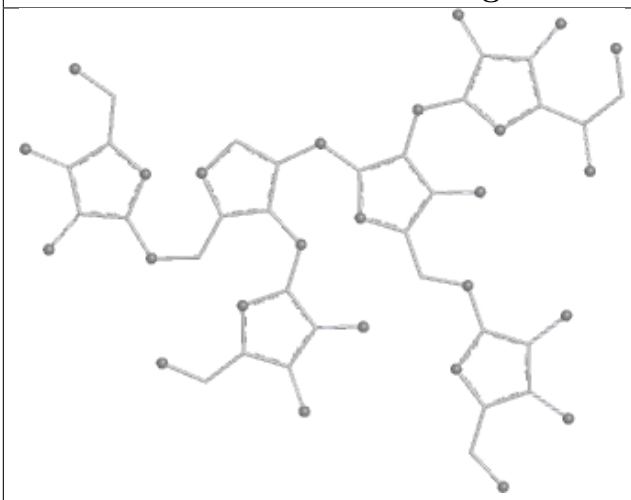
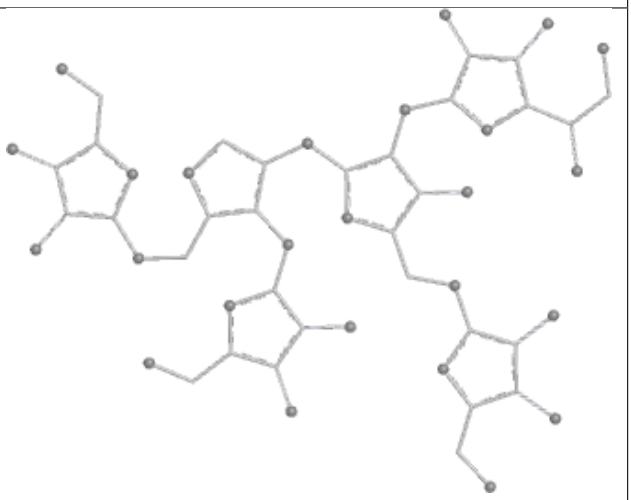
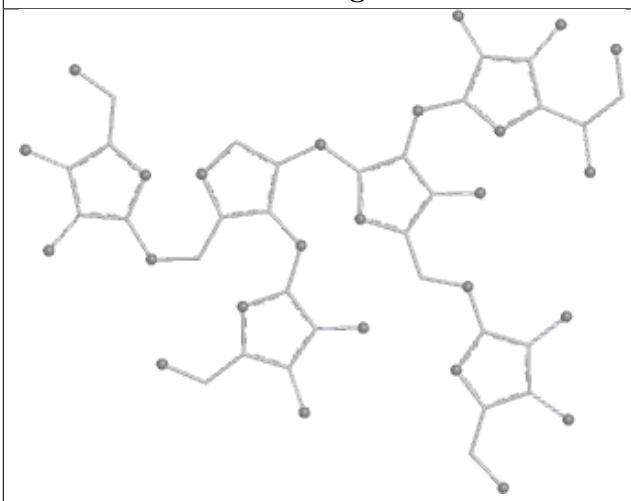
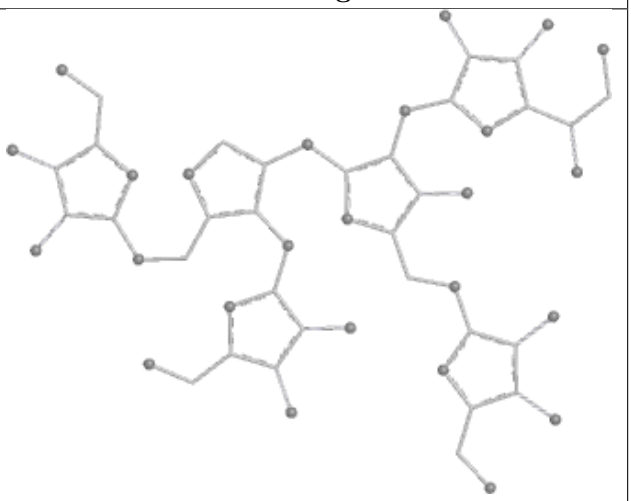


Rings

Oligosaccharide Chain XE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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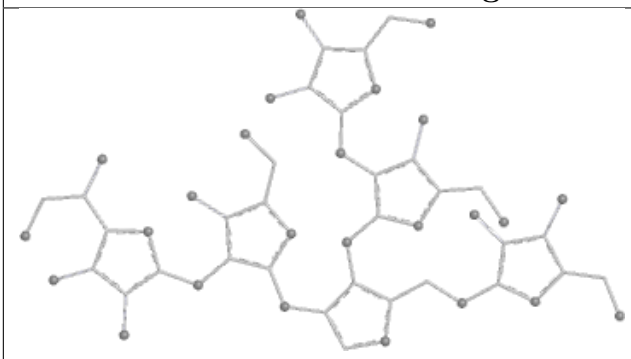
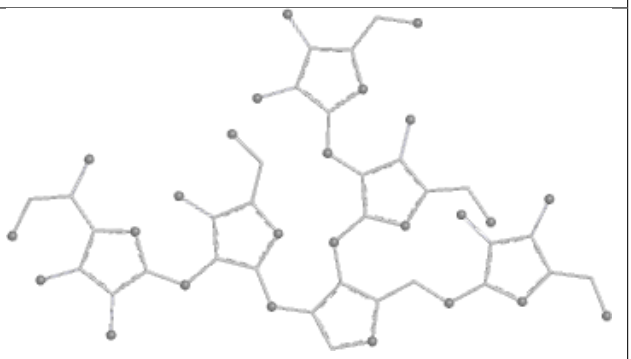
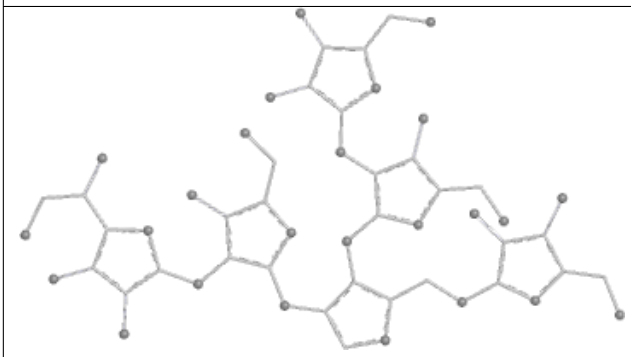
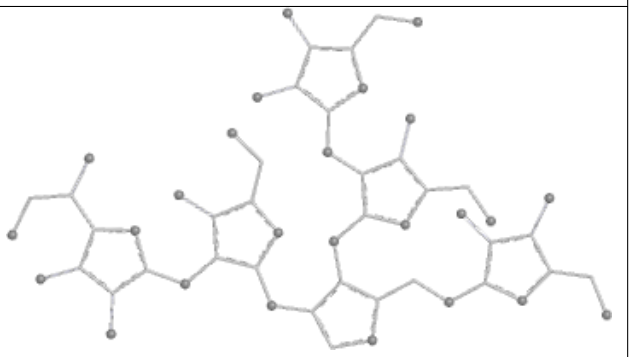
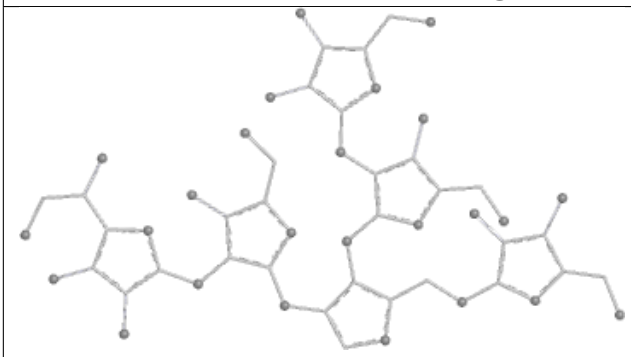
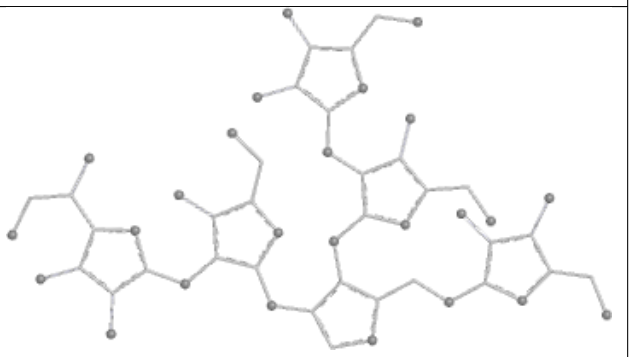
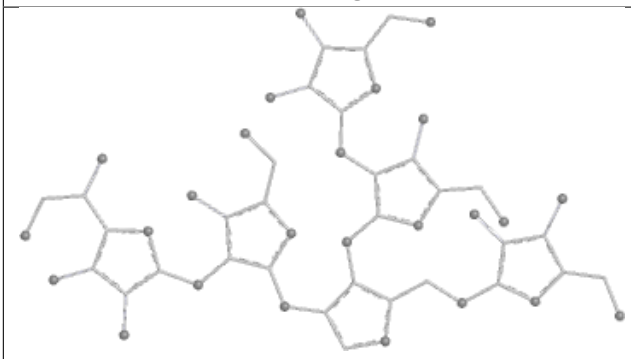
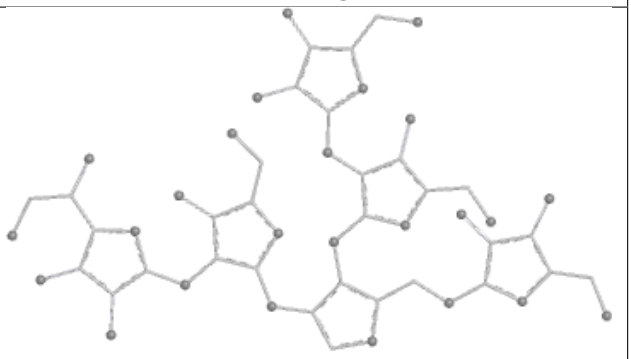
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain lE	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry (i)

Of 95 ligands modelled in this entry, 6 are monoatomic - leaving 89 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	GLA	B	2015	1	11,11,12	1.71	3 (27%)	15,15,17	0.81	0
28	NAG	A	2017	1	14,14,15	0.32	0	17,19,21	0.64	0
26	AHR	F	2005	-	9,9,10	0.64	0	11,12,14	1.54	3 (27%)
27	GLA	C	2007	1	11,11,12	1.74	3 (27%)	15,15,17	0.82	0
26	AHR	F	2019	-	9,9,10	0.54	0	11,12,14	0.64	0
27	GLA	F	2014	1	11,11,12	1.73	3 (27%)	15,15,17	0.81	0
27	GLA	F	2017	1	11,11,12	1.69	3 (27%)	15,15,17	1.02	1 (6%)
26	AHR	A	2002	-	9,9,10	0.83	1 (11%)	11,12,14	1.36	2 (18%)
27	GLA	A	2011	1	11,11,12	1.74	3 (27%)	15,15,17	0.90	1 (6%)
27	GLA	B	2013	1	11,11,12	1.68	3 (27%)	15,15,17	0.90	0
27	GLA	A	2010	1	11,11,12	1.68	3 (27%)	15,15,17	0.87	1 (6%)
27	GLA	F	2018	1	11,11,12	1.72	3 (27%)	15,15,17	0.61	0
27	GLA	A	2007	1	11,11,12	1.71	3 (27%)	15,15,17	0.62	0
27	GLA	A	2016	1	11,11,12	1.71	3 (27%)	15,15,17	0.95	1 (6%)
27	GLA	E	2004	1	11,11,12	1.83	3 (27%)	15,15,17	1.73	4 (26%)
26	AHR	A	2019	-	9,9,10	0.54	0	11,12,14	0.81	0
27	GLA	E	2010	1	11,11,12	1.64	2 (18%)	15,15,17	1.26	1 (6%)
27	GLA	D	2006	1	11,11,12	1.65	3 (27%)	15,15,17	0.95	1 (6%)
28	NAG	C	2009	1	14,14,15	0.37	0	17,19,21	0.73	0
27	GLA	B	2010	1	11,11,12	1.72	3 (27%)	15,15,17	0.77	0
27	GLA	C	2006	1	11,11,12	1.65	3 (27%)	15,15,17	0.78	0
27	GLA	D	2005	1	11,11,12	1.73	3 (27%)	15,15,17	0.87	0
26	AHR	B	2002	-	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
26	AHR	A	2018	-	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
28	NAG	D	2010	1	14,14,15	0.31	0	17,19,21	0.71	0
26	AHR	F	2004	-	9,9,10	0.64	0	11,12,14	1.56	3 (27%)
27	GLA	F	2016	1	11,11,12	1.65	2 (18%)	15,15,17	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	GLA	A	2004	1	11,11,12	1.83	3 (27%)	15,15,17	1.63	4 (26%)
27	GLA	B	2012	1	11,11,12	1.75	3 (27%)	15,15,17	0.70	0
27	GLA	E	2014	1	11,11,12	1.69	3 (27%)	15,15,17	0.91	0
27	GLA	D	2008	1	11,11,12	1.72	3 (27%)	15,15,17	0.71	0
27	GLA	F	2012	1	11,11,12	1.69	3 (27%)	15,15,17	0.84	0
27	GLA	C	2008	1	11,11,12	1.74	3 (27%)	15,15,17	0.94	0
26	AHR	B	2020	-	9,9,10	0.88	0	11,12,14	0.92	1 (9%)
26	AHR	D	2003	-	9,9,10	0.82	0	11,12,14	1.70	3 (27%)
27	GLA	B	2008	1	11,11,12	1.70	3 (27%)	15,15,17	0.76	0
27	GLA	F	2013	1	11,11,12	1.71	3 (27%)	15,15,17	0.90	0
28	NAG	B	2019	1	14,14,15	0.36	0	17,19,21	0.97	1 (5%)
27	GLA	E	2009	1	11,11,12	1.68	3 (27%)	15,15,17	1.04	1 (6%)
27	GLA	D	2009	1	11,11,12	1.76	3 (27%)	15,15,17	0.78	0
27	GLA	F	2011	1	11,11,12	1.72	3 (27%)	15,15,17	0.82	0
27	GLA	F	2008	1	11,11,12	1.70	3 (27%)	15,15,17	0.96	1 (6%)
27	GLA	A	2006	1	11,11,12	1.75	3 (27%)	15,15,17	0.95	1 (6%)
27	GLA	D	2007	1	11,11,12	1.67	3 (27%)	15,15,17	0.87	0
26	AHR	D	2004	-	9,9,10	0.65	0	11,12,14	1.55	3 (27%)
27	GLA	B	2009	-	11,11,12	1.72	3 (27%)	15,15,17	1.45	1 (6%)
27	GLA	F	2009	1	11,11,12	1.63	2 (18%)	15,15,17	0.86	1 (6%)
27	GLA	C	2004	1	11,11,12	1.72	3 (27%)	15,15,17	0.74	0
28	NAG	B	2018	1	14,14,15	0.35	0	17,19,21	0.80	0
26	AHR	B	2004	-	9,9,10	0.77	0	11,12,14	1.78	4 (36%)
27	GLA	B	2006	1	11,11,12	1.72	3 (27%)	15,15,17	0.71	0
27	GLA	E	2015	1	11,11,12	1.65	2 (18%)	15,15,17	1.17	1 (6%)
27	GLA	F	2006	1	11,11,12	1.77	3 (27%)	15,15,17	1.81	4 (26%)
27	GLA	A	2012	1	11,11,12	1.70	3 (27%)	15,15,17	0.84	0
27	GLA	B	2014	1	11,11,12	1.62	2 (18%)	15,15,17	0.83	1 (6%)
27	GLA	F	2015	1	11,11,12	1.72	3 (27%)	15,15,17	0.66	0
27	GLA	B	2017	1	11,11,12	1.61	2 (18%)	15,15,17	1.33	1 (6%)
27	GLA	E	2005	1	11,11,12	1.71	3 (27%)	15,15,17	0.90	0
27	GLA	B	2016	1	11,11,12	1.79	3 (27%)	15,15,17	0.78	0
27	GLA	A	2009	1	11,11,12	1.67	3 (27%)	15,15,17	1.03	1 (6%)
27	GLA	C	2005	1	11,11,12	1.64	3 (27%)	15,15,17	0.87	1 (6%)
27	GLA	B	2007	1	11,11,12	1.75	3 (27%)	15,15,17	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	GLA	F	2010	-	11,11,12	1.74	3 (27%)	15,15,17	0.84	0
27	GLA	E	2011	1	11,11,12	1.69	3 (27%)	15,15,17	0.87	0
28	NAG	C	2010	1	14,14,15	0.32	0	17,19,21	0.91	1 (5%)
26	AHR	E	2003	-	9,9,10	0.64	0	11,12,14	1.54	3 (27%)
26	AHR	C	2001	-	9,9,10	0.53	0	11,12,14	1.61	1 (9%)
27	GLA	F	2007	1	11,11,12	1.64	3 (27%)	15,15,17	1.04	0
26	AHR	B	2003	-	9,9,10	0.90	0	11,12,14	1.88	4 (36%)
26	AHR	C	2003	-	9,9,10	0.79	0	11,12,14	1.72	4 (36%)
26	AHR	F	2003	-	9,9,10	0.55	0	11,12,14	1.59	1 (9%)
27	GLA	A	2015	1	11,11,12	1.75	3 (27%)	15,15,17	0.78	0
26	AHR	A	2003	-	9,9,10	0.75	1 (11%)	11,12,14	1.63	3 (27%)
26	AHR	D	2001	-	9,9,10	0.65	0	11,12,14	1.49	2 (18%)
27	GLA	B	2011	1	11,11,12	1.67	3 (27%)	15,15,17	0.98	1 (6%)
27	GLA	E	2006	1	11,11,12	1.73	3 (27%)	15,15,17	0.75	0
28	NAG	E	2017	1	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
27	GLA	A	2005	1	11,11,12	1.66	3 (27%)	15,15,17	0.84	0
27	GLA	A	2013	1	11,11,12	1.72	3 (27%)	15,15,17	0.64	0
27	GLA	E	2016	1	11,11,12	1.79	3 (27%)	15,15,17	0.82	0
26	AHR	E	2002	-	9,9,10	0.78	1 (11%)	11,12,14	1.78	3 (27%)
27	GLA	E	2012	1	11,11,12	1.60	1 (9%)	15,15,17	1.17	1 (6%)
27	GLA	E	2013	1	11,11,12	1.76	3 (27%)	15,15,17	0.74	0
27	GLA	B	2005	1	11,11,12	1.82	3 (27%)	15,15,17	1.54	3 (20%)
27	GLA	A	2008	-	11,11,12	1.72	2 (18%)	15,15,17	1.33	1 (6%)
27	GLA	A	2014	1	11,11,12	1.73	3 (27%)	15,15,17	0.86	0
27	GLA	E	2007	1	11,11,12	1.76	3 (27%)	15,15,17	1.35	3 (20%)
26	AHR	F	2001	-	9,9,10	0.65	0	11,12,14	1.53	3 (27%)
27	GLA	E	2008	-	11,11,12	1.70	3 (27%)	15,15,17	0.99	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GLA	B	2015	1	-	2/2/19/22	0/1/1/1
28	NAG	A	2017	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	AHR	F	2005	-	-	2/2/15/18	0/1/1/1
27	GLA	C	2007	1	-	2/2/19/22	0/1/1/1
26	AHR	F	2019	-	-	0/2/15/18	0/1/1/1
27	GLA	F	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2017	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2002	-	-	2/2/15/18	0/1/1/1
27	GLA	A	2011	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2013	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2010	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2018	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2007	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	A	2016	1	-	1/2/19/22	0/1/1/1
27	GLA	E	2004	1	-	1/2/19/22	0/1/1/1
26	AHR	A	2019	-	-	0/2/15/18	0/1/1/1
27	GLA	E	2010	1	-	1/2/19/22	0/1/1/1
27	GLA	D	2006	1	-	0/2/19/22	0/1/1/1
28	NAG	C	2009	1	-	4/6/23/26	0/1/1/1
27	GLA	B	2010	1	-	2/2/19/22	0/1/1/1
27	GLA	C	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	D	2005	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2018	-	-	0/2/15/18	0/1/1/1
26	AHR	B	2002	-	-	0/2/15/18	0/1/1/1
28	NAG	D	2010	1	-	0/6/23/26	0/1/1/1
26	AHR	F	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2016	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2004	1	-	0/2/19/22	0/1/1/1
27	GLA	B	2012	1	-	1/2/19/22	0/1/1/1
27	GLA	E	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	D	2008	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2012	1	-	2/2/19/22	0/1/1/1
27	GLA	C	2008	1	-	2/2/19/22	0/1/1/1
26	AHR	B	2020	-	-	1/2/15/18	0/1/1/1
26	AHR	D	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2008	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	F	2013	1	-	0/2/19/22	0/1/1/1
28	NAG	B	2019	1	-	2/6/23/26	0/1/1/1
27	GLA	E	2009	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GLA	D	2009	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2011	1	-	1/2/19/22	0/1/1/1
27	GLA	F	2008	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2006	1	-	1/2/19/22	0/1/1/1
27	GLA	D	2007	1	-	2/2/19/22	0/1/1/1
26	AHR	D	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2009	-	-	2/2/19/22	0/1/1/1
27	GLA	F	2009	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	C	2004	1	-	2/2/19/22	0/1/1/1
28	NAG	B	2018	1	-	4/6/23/26	0/1/1/1
26	AHR	B	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	B	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2015	1	-	0/2/19/22	0/1/1/1
27	GLA	F	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2012	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2014	1	1/1/4/5	0/2/19/22	0/1/1/1
27	GLA	F	2015	1	-	0/2/19/22	0/1/1/1
27	GLA	B	2017	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2005	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2016	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2009	1	-	1/2/19/22	0/1/1/1
27	GLA	C	2005	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2007	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2010	-	-	2/2/19/22	0/1/1/1
27	GLA	E	2011	1	-	2/2/19/22	0/1/1/1
28	NAG	C	2010	1	-	4/6/23/26	0/1/1/1
26	AHR	E	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	C	2001	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2007	1	-	2/2/19/22	0/1/1/1
26	AHR	B	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	C	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	F	2003	-	-	1/2/15/18	0/1/1/1
27	GLA	A	2015	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	D	2001	-	-	1/2/15/18	0/1/1/1
27	GLA	B	2011	1	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GLA	E	2006	1	-	2/2/19/22	0/1/1/1
28	NAG	E	2017	1	-	4/6/23/26	0/1/1/1
27	GLA	A	2005	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2013	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2016	1	-	2/2/19/22	0/1/1/1
26	AHR	E	2002	-	-	2/2/15/18	0/1/1/1
27	GLA	E	2012	1	-	1/2/19/22	0/1/1/1
27	GLA	E	2013	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2005	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2008	-	-	2/2/19/22	0/1/1/1
27	GLA	A	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2007	1	1/1/4/5	2/2/19/22	0/1/1/1
26	AHR	F	2001	-	-	2/2/15/18	0/1/1/1
27	GLA	E	2008	-	-	2/2/19/22	0/1/1/1

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	2004	GLA	O5-C1	4.66	1.51	1.43
27	B	2005	GLA	O5-C1	4.63	1.51	1.43
27	B	2009	GLA	O5-C1	4.55	1.51	1.43
27	E	2004	GLA	O5-C1	4.51	1.51	1.43
27	A	2008	GLA	O5-C1	4.51	1.51	1.43
27	B	2010	GLA	O5-C1	4.47	1.51	1.43
27	E	2016	GLA	O5-C1	4.46	1.51	1.43
27	F	2013	GLA	O5-C1	4.45	1.51	1.43
27	E	2013	GLA	O5-C1	4.45	1.51	1.43
27	B	2016	GLA	O5-C1	4.44	1.51	1.43
27	D	2005	GLA	O5-C1	4.44	1.51	1.43
27	D	2009	GLA	O5-C1	4.44	1.51	1.43
27	B	2012	GLA	O5-C1	4.43	1.51	1.43
27	E	2008	GLA	O5-C1	4.41	1.51	1.43
27	C	2007	GLA	O5-C1	4.40	1.51	1.43
27	F	2011	GLA	O5-C1	4.40	1.51	1.43
27	F	2014	GLA	O5-C1	4.40	1.51	1.43
27	A	2014	GLA	O5-C1	4.39	1.51	1.43
27	F	2010	GLA	O5-C1	4.38	1.51	1.43
27	F	2015	GLA	O5-C1	4.38	1.51	1.43
27	A	2015	GLA	O5-C1	4.38	1.51	1.43
27	F	2018	GLA	O5-C1	4.38	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	2006	GLA	O5-C1	4.37	1.51	1.43
27	F	2006	GLA	O5-C1	4.37	1.51	1.43
27	C	2008	GLA	O5-C1	4.37	1.51	1.43
27	F	2017	GLA	O5-C1	4.37	1.51	1.43
27	C	2004	GLA	O5-C1	4.35	1.51	1.43
27	A	2011	GLA	O5-C1	4.33	1.51	1.43
27	A	2013	GLA	O5-C1	4.33	1.51	1.43
27	A	2012	GLA	O5-C1	4.32	1.51	1.43
27	B	2015	GLA	O5-C1	4.32	1.50	1.43
27	A	2016	GLA	O5-C1	4.32	1.50	1.43
27	B	2013	GLA	O5-C1	4.32	1.50	1.43
27	E	2007	GLA	O5-C1	4.31	1.50	1.43
27	B	2008	GLA	O5-C1	4.31	1.50	1.43
27	E	2014	GLA	O5-C1	4.31	1.50	1.43
27	E	2009	GLA	O5-C1	4.30	1.50	1.43
27	F	2016	GLA	O5-C1	4.30	1.50	1.43
27	B	2007	GLA	O5-C1	4.30	1.50	1.43
27	A	2009	GLA	O5-C1	4.29	1.50	1.43
27	A	2006	GLA	O5-C1	4.29	1.50	1.43
27	E	2015	GLA	O5-C1	4.28	1.50	1.43
27	B	2006	GLA	O5-C1	4.28	1.50	1.43
27	E	2012	GLA	O5-C1	4.26	1.50	1.43
27	A	2007	GLA	O5-C1	4.26	1.50	1.43
27	D	2006	GLA	O5-C1	4.25	1.50	1.43
27	C	2005	GLA	O5-C1	4.25	1.50	1.43
27	A	2005	GLA	O5-C1	4.24	1.50	1.43
27	D	2007	GLA	O5-C1	4.23	1.50	1.43
27	E	2010	GLA	O5-C1	4.22	1.50	1.43
27	E	2005	GLA	O5-C1	4.21	1.50	1.43
27	C	2006	GLA	O5-C1	4.21	1.50	1.43
27	D	2008	GLA	O5-C1	4.21	1.50	1.43
27	F	2008	GLA	O5-C1	4.19	1.50	1.43
27	E	2011	GLA	O5-C1	4.17	1.50	1.43
27	F	2012	GLA	O5-C1	4.17	1.50	1.43
27	B	2017	GLA	O5-C1	4.15	1.50	1.43
27	F	2007	GLA	O5-C1	4.10	1.50	1.43
27	B	2014	GLA	O5-C1	4.09	1.50	1.43
27	F	2009	GLA	O5-C1	4.08	1.50	1.43
27	A	2010	GLA	O5-C1	4.03	1.50	1.43
27	B	2011	GLA	O5-C1	3.96	1.50	1.43
27	E	2004	GLA	C2-C3	-2.94	1.48	1.52
27	F	2006	GLA	C2-C3	-2.85	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	2016	GLA	C2-C3	-2.84	1.48	1.52
27	A	2006	GLA	C2-C3	-2.83	1.48	1.52
27	B	2007	GLA	C2-C3	-2.77	1.48	1.52
27	A	2010	GLA	C2-C3	-2.75	1.48	1.52
27	A	2015	GLA	C2-C3	-2.74	1.48	1.52
27	E	2016	GLA	C2-C3	-2.74	1.48	1.52
27	E	2005	GLA	C2-C3	-2.71	1.48	1.52
27	B	2011	GLA	C2-C3	-2.70	1.48	1.52
27	A	2014	GLA	C2-C3	-2.69	1.48	1.52
27	D	2008	GLA	C2-C3	-2.68	1.48	1.52
27	F	2008	GLA	C2-C3	-2.67	1.48	1.52
27	A	2011	GLA	C2-C3	-2.66	1.48	1.52
27	E	2007	GLA	C2-C3	-2.66	1.48	1.52
27	A	2007	GLA	C2-C3	-2.66	1.48	1.52
27	F	2010	GLA	C2-C3	-2.65	1.48	1.52
27	F	2012	GLA	C2-C3	-2.65	1.48	1.52
27	E	2013	GLA	C2-C3	-2.64	1.48	1.52
27	B	2015	GLA	C2-C3	-2.64	1.48	1.52
27	C	2007	GLA	C2-C3	-2.64	1.48	1.52
27	D	2009	GLA	C2-C3	-2.64	1.48	1.52
27	C	2008	GLA	C2-C3	-2.63	1.48	1.52
27	A	2004	GLA	C2-C3	-2.63	1.48	1.52
27	B	2005	GLA	C2-C3	-2.62	1.48	1.52
27	A	2013	GLA	C2-C3	-2.61	1.48	1.52
27	E	2006	GLA	C2-C3	-2.60	1.48	1.52
27	B	2006	GLA	C2-C3	-2.59	1.48	1.52
27	B	2012	GLA	C2-C3	-2.59	1.48	1.52
27	B	2008	GLA	C2-C3	-2.59	1.48	1.52
27	E	2011	GLA	C2-C3	-2.58	1.48	1.52
27	A	2016	GLA	C2-C3	-2.53	1.48	1.52
27	F	2014	GLA	C2-C3	-2.52	1.48	1.52
27	A	2012	GLA	C2-C3	-2.51	1.48	1.52
27	F	2007	GLA	C2-C3	-2.50	1.48	1.52
27	B	2014	GLA	C2-C3	-2.49	1.48	1.52
27	F	2018	GLA	C2-C3	-2.49	1.48	1.52
27	D	2007	GLA	C2-C3	-2.49	1.48	1.52
27	F	2015	GLA	C2-C3	-2.49	1.48	1.52
27	E	2014	GLA	C2-C3	-2.47	1.48	1.52
27	F	2011	GLA	C2-C3	-2.46	1.48	1.52
27	C	2004	GLA	C2-C3	-2.45	1.48	1.52
27	F	2009	GLA	C2-C3	-2.45	1.48	1.52
27	D	2005	GLA	C2-C3	-2.44	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	2007	GLA	O5-C5	2.43	1.48	1.43
27	B	2010	GLA	C2-C3	-2.42	1.48	1.52
27	C	2006	GLA	C2-C3	-2.41	1.48	1.52
27	F	2013	GLA	C2-C3	-2.40	1.48	1.52
27	A	2008	GLA	C2-C3	-2.39	1.48	1.52
27	A	2005	GLA	C2-C3	-2.38	1.48	1.52
27	B	2013	GLA	C2-C3	-2.34	1.48	1.52
27	A	2009	GLA	C2-C3	-2.33	1.48	1.52
27	B	2005	GLA	O5-C5	2.32	1.48	1.43
27	A	2004	GLA	O5-C5	2.32	1.47	1.43
27	F	2017	GLA	C2-C3	-2.32	1.48	1.52
27	E	2016	GLA	O5-C5	2.30	1.47	1.43
26	A	2002	AHR	C1-C2	2.29	1.55	1.51
27	B	2017	GLA	C2-C3	-2.27	1.49	1.52
27	B	2016	GLA	O5-C5	2.27	1.47	1.43
27	D	2008	GLA	O5-C5	2.27	1.47	1.43
27	E	2004	GLA	O5-C5	2.26	1.47	1.43
27	E	2008	GLA	C2-C3	-2.26	1.49	1.52
27	E	2010	GLA	C2-C3	-2.25	1.49	1.52
27	B	2006	GLA	O5-C5	2.24	1.47	1.43
27	F	2016	GLA	C2-C3	-2.24	1.49	1.52
27	B	2011	GLA	O5-C5	2.24	1.47	1.43
27	E	2009	GLA	C2-C3	-2.23	1.49	1.52
27	C	2005	GLA	C2-C3	-2.22	1.49	1.52
27	D	2006	GLA	C2-C3	-2.22	1.49	1.52
27	C	2004	GLA	O5-C5	2.22	1.47	1.43
27	A	2011	GLA	O5-C5	2.21	1.47	1.43
27	F	2015	GLA	O5-C5	2.21	1.47	1.43
27	D	2009	GLA	O5-C5	2.20	1.47	1.43
27	E	2015	GLA	C2-C3	-2.20	1.49	1.52
27	C	2008	GLA	O5-C5	2.20	1.47	1.43
27	D	2005	GLA	O5-C5	2.20	1.47	1.43
27	F	2006	GLA	O5-C5	2.19	1.47	1.43
27	E	2005	GLA	O5-C5	2.19	1.47	1.43
27	E	2009	GLA	O5-C5	2.18	1.47	1.43
27	B	2009	GLA	C2-C3	-2.18	1.49	1.52
27	F	2011	GLA	O5-C5	2.18	1.47	1.43
27	B	2012	GLA	O5-C5	2.17	1.47	1.43
27	E	2013	GLA	O5-C5	2.17	1.47	1.43
27	E	2008	GLA	O5-C5	2.17	1.47	1.43
27	F	2018	GLA	O5-C5	2.17	1.47	1.43
27	B	2010	GLA	O5-C5	2.16	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	2007	GLA	O5-C5	2.16	1.47	1.43
27	E	2011	GLA	O5-C5	2.16	1.47	1.43
27	A	2015	GLA	O5-C5	2.15	1.47	1.43
27	A	2010	GLA	O5-C5	2.15	1.47	1.43
27	F	2010	GLA	O5-C5	2.14	1.47	1.43
27	A	2006	GLA	O5-C5	2.14	1.47	1.43
27	F	2012	GLA	O5-C5	2.14	1.47	1.43
27	F	2014	GLA	O5-C5	2.13	1.47	1.43
27	A	2012	GLA	O5-C5	2.12	1.47	1.43
27	B	2007	GLA	O5-C5	2.12	1.47	1.43
27	E	2006	GLA	O5-C5	2.12	1.47	1.43
27	A	2009	GLA	O5-C5	2.12	1.47	1.43
27	A	2013	GLA	O5-C5	2.12	1.47	1.43
27	F	2017	GLA	O5-C5	2.11	1.47	1.43
27	F	2008	GLA	O5-C5	2.11	1.47	1.43
27	F	2007	GLA	O5-C5	2.10	1.47	1.43
27	A	2007	GLA	O5-C5	2.09	1.47	1.43
27	A	2016	GLA	O5-C5	2.08	1.47	1.43
27	B	2008	GLA	O5-C5	2.07	1.47	1.43
27	E	2014	GLA	O5-C5	2.07	1.47	1.43
27	D	2007	GLA	O5-C5	2.07	1.47	1.43
27	B	2015	GLA	O5-C5	2.07	1.47	1.43
27	F	2013	GLA	O5-C5	2.07	1.47	1.43
27	A	2005	GLA	O5-C5	2.06	1.47	1.43
27	B	2013	GLA	O5-C5	2.06	1.47	1.43
26	A	2003	AHR	C1-C2	2.05	1.55	1.51
27	C	2006	GLA	O5-C5	2.04	1.47	1.43
27	D	2006	GLA	O5-C5	2.03	1.47	1.43
26	E	2002	AHR	C1-C2	2.03	1.55	1.51
27	A	2014	GLA	O5-C5	2.02	1.47	1.43
27	B	2009	GLA	O5-C5	2.02	1.47	1.43
27	C	2005	GLA	O5-C5	2.01	1.47	1.43

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	F	2003	AHR	O4-C1-C2	-4.29	98.37	105.76
26	C	2001	AHR	O4-C1-C2	-4.23	98.47	105.76
27	B	2009	GLA	C1-C2-C3	4.20	115.76	109.64
27	A	2008	GLA	C1-C2-C3	3.74	115.10	109.64
26	F	2004	AHR	O4-C1-C2	-3.72	99.36	105.76
26	F	2005	AHR	O4-C1-C2	-3.64	99.50	105.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	2004	GLA	C1-O5-C5	3.63	117.06	112.19
27	F	2006	GLA	O5-C1-C2	3.59	119.35	110.79
26	D	2004	AHR	O4-C1-C2	-3.59	99.58	105.76
26	E	2003	AHR	O4-C1-C2	-3.56	99.62	105.76
26	F	2001	AHR	O4-C1-C2	-3.54	99.65	105.76
27	B	2017	GLA	C1-C2-C3	3.41	114.60	109.64
26	A	2003	AHR	C1-C2-C3	3.40	107.07	101.63
27	F	2006	GLA	C1-O5-C5	3.40	116.74	112.19
27	E	2004	GLA	C1-O5-C5	3.38	116.71	112.19
27	E	2010	GLA	C1-C2-C3	3.29	114.44	109.64
26	E	2002	AHR	O4-C4-C5	-3.27	103.42	109.36
26	D	2001	AHR	O4-C1-C2	-3.26	100.15	105.76
27	E	2012	GLA	C1-C2-C3	3.25	114.37	109.64
27	E	2015	GLA	C1-C2-C3	3.15	114.24	109.64
26	E	2002	AHR	C1-C2-C3	3.15	106.67	101.63
26	B	2003	AHR	O4-C1-C2	-3.14	100.35	105.76
28	B	2019	NAG	C1-O5-C5	3.13	116.38	112.19
27	B	2005	GLA	C1-O5-C5	3.05	116.28	112.19
27	E	2004	GLA	O5-C1-C2	3.04	118.04	110.79
26	B	2003	AHR	C1-O4-C4	-3.03	101.37	108.06
27	B	2005	GLA	O5-C1-C2	3.00	117.95	110.79
27	E	2004	GLA	C1-C2-C3	2.97	113.97	109.64
27	B	2005	GLA	C1-C2-C3	2.93	113.91	109.64
27	F	2006	GLA	C1-C2-C3	2.89	113.86	109.64
27	A	2004	GLA	O5-C1-C2	2.89	117.67	110.79
27	A	2004	GLA	C1-C2-C3	2.85	113.80	109.64
26	C	2003	AHR	O4-C4-C5	-2.83	104.22	109.36
26	D	2003	AHR	O4-C1-C2	-2.78	100.97	105.76
26	A	2002	AHR	C1-C2-C3	2.76	106.04	101.63
26	C	2003	AHR	C1-C2-C3	2.74	106.01	101.63
26	B	2004	AHR	O4-C1-C2	-2.68	101.15	105.76
26	B	2003	AHR	O5-C5-C4	-2.67	102.26	111.33
26	D	2003	AHR	O5-C5-C4	-2.66	102.28	111.33
26	C	2003	AHR	O5-C5-C4	-2.66	102.29	111.33
26	E	2002	AHR	O5-C5-C4	-2.63	102.38	111.33
28	C	2010	NAG	C1-O5-C5	2.62	115.69	112.19
27	E	2007	GLA	C3-C4-C5	2.59	114.92	110.23
27	F	2017	GLA	C1-C2-C3	2.59	113.41	109.64
26	D	2001	AHR	O2-C2-C1	2.57	118.88	110.89
26	D	2003	AHR	O4-C4-C5	-2.54	104.74	109.36
26	B	2004	AHR	C1-O4-C4	-2.50	102.54	108.06
26	B	2002	AHR	C1-C2-C3	2.48	105.59	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	2004	AHR	C5-C4-C3	2.47	120.92	115.10
26	A	2018	AHR	C1-C2-C3	2.42	105.50	101.63
27	E	2004	GLA	C6-C5-C4	-2.40	107.12	113.02
26	A	2003	AHR	O4-C4-C5	-2.39	105.02	109.36
26	B	2003	AHR	C5-C4-C3	2.37	120.70	115.10
26	B	2020	AHR	C1-C2-C3	2.35	105.38	101.63
27	E	2007	GLA	C1-O5-C5	2.33	115.30	112.19
27	F	2006	GLA	C6-C5-C4	-2.30	107.37	113.02
26	D	2004	AHR	O2-C2-C1	2.30	118.04	110.89
27	A	2010	GLA	C6-C5-C4	-2.29	107.41	113.02
26	B	2004	AHR	O5-C5-C4	-2.25	103.69	111.33
26	F	2005	AHR	O2-C2-C3	2.25	115.85	111.43
26	E	2003	AHR	O2-C2-C3	2.24	115.84	111.43
27	A	2006	GLA	C6-C5-C4	-2.24	107.52	113.02
27	F	2008	GLA	C6-C5-C4	-2.24	107.53	113.02
26	E	2003	AHR	O2-C2-C1	2.23	117.83	110.89
27	E	2009	GLA	C1-C2-C3	2.23	112.89	109.64
26	F	2005	AHR	O2-C2-C1	2.22	117.81	110.89
27	D	2006	GLA	C1-C2-C3	2.22	112.88	109.64
26	F	2001	AHR	O2-C2-C3	2.22	115.80	111.43
26	D	2004	AHR	O2-C2-C3	2.21	115.78	111.43
27	A	2009	GLA	C1-C2-C3	2.21	112.86	109.64
26	F	2001	AHR	O2-C2-C1	2.21	117.75	110.89
27	E	2008	GLA	C1-C2-C3	2.20	112.85	109.64
26	A	2002	AHR	O4-C4-C3	-2.20	102.60	104.63
27	F	2009	GLA	C3-C4-C5	2.20	114.21	110.23
27	A	2004	GLA	C6-C5-C4	-2.19	107.64	113.02
28	E	2017	NAG	C1-O5-C5	2.18	115.10	112.19
27	A	2016	GLA	C1-C2-C3	2.16	112.78	109.64
26	A	2003	AHR	O5-C5-C4	-2.15	104.02	111.33
26	F	2004	AHR	O2-C2-C1	2.15	117.57	110.89
27	B	2011	GLA	C3-C4-C5	2.14	114.12	110.23
26	F	2004	AHR	O2-C2-C3	2.13	115.63	111.43
27	C	2005	GLA	C1-C2-C3	2.10	112.70	109.64
27	E	2007	GLA	C1-C2-C3	2.09	112.68	109.64
27	A	2011	GLA	C6-C5-C4	-2.05	107.98	113.02
27	B	2014	GLA	C1-O5-C5	-2.05	109.44	112.19
26	C	2003	AHR	O4-C1-C2	-2.03	102.27	105.76

All (5) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
27	A	2007	GLA	C1
27	B	2008	GLA	C1
27	B	2014	GLA	C1
27	E	2007	GLA	C1
27	F	2009	GLA	C1

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	B	2018	NAG	C3-C2-N2-C7
28	B	2018	NAG	C8-C7-N2-C2
28	B	2018	NAG	O7-C7-N2-C2
28	C	2009	NAG	C3-C2-N2-C7
28	C	2009	NAG	C8-C7-N2-C2
28	C	2009	NAG	O7-C7-N2-C2
28	E	2017	NAG	C8-C7-N2-C2
28	E	2017	NAG	O7-C7-N2-C2
26	A	2002	AHR	C3-C4-C5-O5
26	A	2003	AHR	C3-C4-C5-O5
27	F	2010	GLA	O5-C5-C6-O6
27	C	2004	GLA	O5-C5-C6-O6
26	A	2002	AHR	O4-C4-C5-O5
26	A	2003	AHR	O4-C4-C5-O5
26	E	2002	AHR	O4-C4-C5-O5
27	C	2007	GLA	O5-C5-C6-O6
26	C	2003	AHR	C3-C4-C5-O5
26	E	2002	AHR	C3-C4-C5-O5
27	F	2009	GLA	C4-C5-C6-O6
27	C	2005	GLA	O5-C5-C6-O6
27	A	2007	GLA	C4-C5-C6-O6
26	D	2003	AHR	C3-C4-C5-O5
27	A	2008	GLA	O5-C5-C6-O6
27	E	2008	GLA	O5-C5-C6-O6
27	E	2014	GLA	O5-C5-C6-O6
27	F	2014	GLA	O5-C5-C6-O6
27	C	2005	GLA	C4-C5-C6-O6
27	F	2018	GLA	C4-C5-C6-O6
27	A	2011	GLA	O5-C5-C6-O6
27	B	2009	GLA	O5-C5-C6-O6
27	B	2016	GLA	O5-C5-C6-O6
27	C	2004	GLA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
27	F	2010	GLA	C4-C5-C6-O6
27	F	2014	GLA	C4-C5-C6-O6
27	E	2007	GLA	O5-C5-C6-O6
27	F	2018	GLA	O5-C5-C6-O6
26	C	2003	AHR	O4-C4-C5-O5
27	D	2009	GLA	O5-C5-C6-O6
27	A	2008	GLA	C4-C5-C6-O6
27	B	2008	GLA	C4-C5-C6-O6
27	A	2010	GLA	O5-C5-C6-O6
27	E	2005	GLA	O5-C5-C6-O6
27	F	2007	GLA	O5-C5-C6-O6
27	E	2016	GLA	C4-C5-C6-O6
27	B	2007	GLA	O5-C5-C6-O6
27	E	2016	GLA	O5-C5-C6-O6
27	C	2008	GLA	O5-C5-C6-O6
27	D	2007	GLA	O5-C5-C6-O6
27	C	2007	GLA	C4-C5-C6-O6
27	A	2007	GLA	O5-C5-C6-O6
27	F	2009	GLA	O5-C5-C6-O6
28	E	2017	NAG	C4-C5-C6-O6
27	A	2012	GLA	C4-C5-C6-O6
28	C	2010	NAG	O5-C5-C6-O6
27	E	2014	GLA	C4-C5-C6-O6
26	D	2003	AHR	O4-C4-C5-O5
26	D	2004	AHR	O4-C4-C5-O5
26	E	2003	AHR	O4-C4-C5-O5
26	F	2001	AHR	O4-C4-C5-O5
27	A	2011	GLA	C4-C5-C6-O6
27	A	2015	GLA	C4-C5-C6-O6
27	D	2009	GLA	C4-C5-C6-O6
27	E	2011	GLA	C4-C5-C6-O6
27	B	2008	GLA	O5-C5-C6-O6
27	B	2015	GLA	O5-C5-C6-O6
28	A	2017	NAG	O5-C5-C6-O6
28	B	2019	NAG	O5-C5-C6-O6
27	B	2016	GLA	C4-C5-C6-O6
27	C	2008	GLA	C4-C5-C6-O6
28	C	2010	NAG	C4-C5-C6-O6
27	D	2005	GLA	O5-C5-C6-O6
27	F	2012	GLA	O5-C5-C6-O6
27	E	2006	GLA	C4-C5-C6-O6
28	A	2017	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
28	B	2019	NAG	C4-C5-C6-O6
26	C	2001	AHR	O4-C4-C5-O5
26	F	2005	AHR	O4-C4-C5-O5
27	A	2012	GLA	O5-C5-C6-O6
27	B	2010	GLA	O5-C5-C6-O6
27	B	2009	GLA	C4-C5-C6-O6
26	D	2004	AHR	C3-C4-C5-O5
27	E	2005	GLA	C4-C5-C6-O6
26	F	2004	AHR	O4-C4-C5-O5
27	E	2007	GLA	C4-C5-C6-O6
27	F	2007	GLA	C4-C5-C6-O6
27	A	2015	GLA	O5-C5-C6-O6
26	E	2003	AHR	C3-C4-C5-O5
26	F	2001	AHR	C3-C4-C5-O5
26	F	2005	AHR	C3-C4-C5-O5
27	E	2008	GLA	C4-C5-C6-O6
27	E	2011	GLA	O5-C5-C6-O6
26	B	2003	AHR	C3-C4-C5-O5
27	E	2013	GLA	O5-C5-C6-O6
27	D	2007	GLA	C4-C5-C6-O6
26	B	2003	AHR	O4-C4-C5-O5
27	B	2011	GLA	O5-C5-C6-O6
27	B	2017	GLA	C4-C5-C6-O6
27	E	2006	GLA	O5-C5-C6-O6
28	E	2017	NAG	O5-C5-C6-O6
27	B	2015	GLA	C4-C5-C6-O6
27	E	2010	GLA	O5-C5-C6-O6
27	D	2008	GLA	C4-C5-C6-O6
27	A	2009	GLA	O5-C5-C6-O6
26	B	2020	AHR	O4-C4-C5-O5
27	A	2014	GLA	O5-C5-C6-O6
27	B	2007	GLA	C4-C5-C6-O6
27	A	2016	GLA	O5-C5-C6-O6
26	B	2004	AHR	C3-C4-C5-O5
27	A	2010	GLA	C4-C5-C6-O6
26	B	2004	AHR	O4-C4-C5-O5
27	B	2017	GLA	O5-C5-C6-O6
27	A	2006	GLA	O5-C5-C6-O6
27	F	2016	GLA	C4-C5-C6-O6
27	F	2017	GLA	C4-C5-C6-O6
28	C	2009	NAG	O5-C5-C6-O6
27	D	2005	GLA	C4-C5-C6-O6

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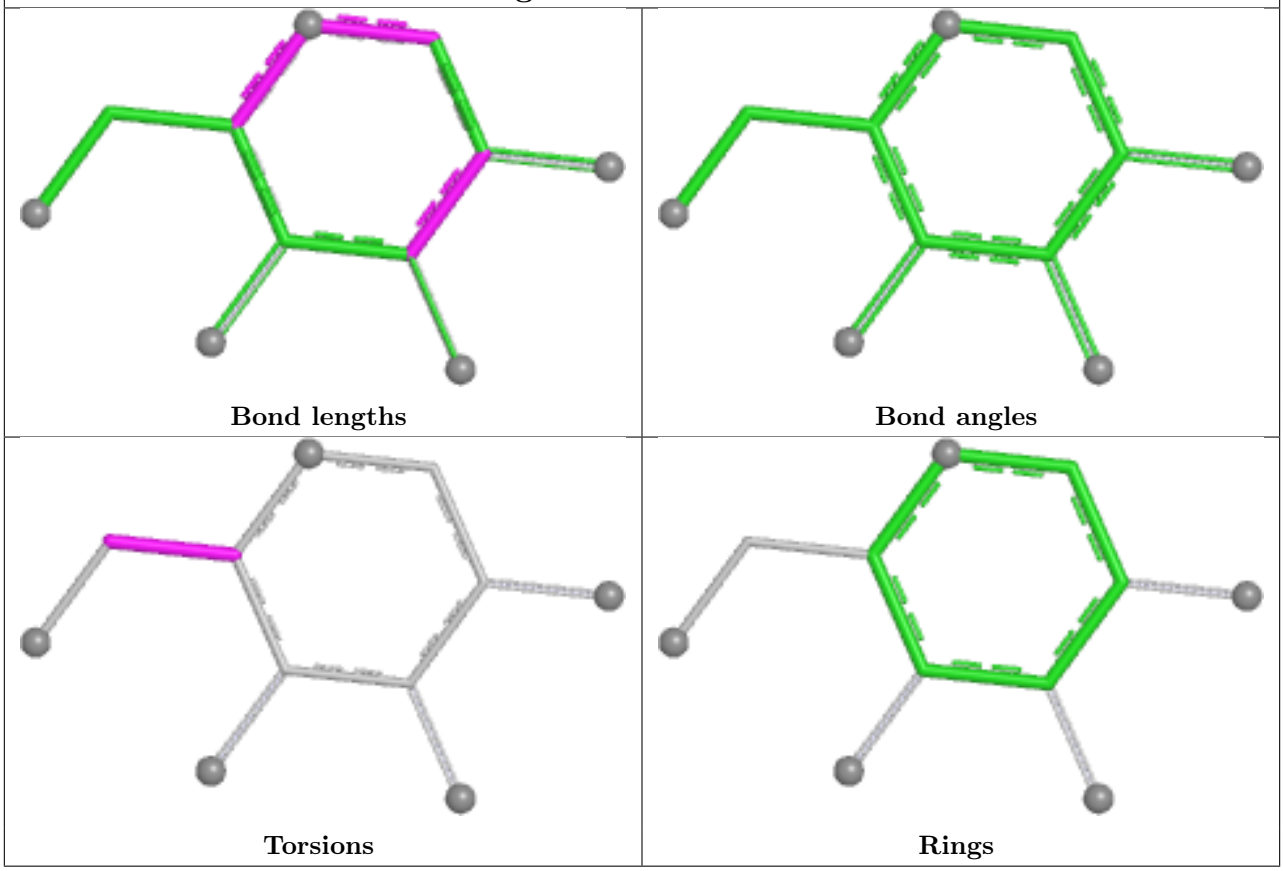
Mol	Chain	Res	Type	Atoms
27	F	2008	GLA	O5-C5-C6-O6
27	B	2013	GLA	O5-C5-C6-O6
26	C	2001	AHR	C3-C4-C5-O5
26	F	2004	AHR	C3-C4-C5-O5
27	B	2010	GLA	C4-C5-C6-O6
27	F	2012	GLA	C4-C5-C6-O6
27	D	2008	GLA	O5-C5-C6-O6
27	F	2016	GLA	O5-C5-C6-O6
27	F	2011	GLA	O5-C5-C6-O6
27	F	2017	GLA	O5-C5-C6-O6
27	E	2013	GLA	C4-C5-C6-O6
27	E	2012	GLA	C4-C5-C6-O6
28	B	2018	NAG	O5-C5-C6-O6
26	D	2001	AHR	O4-C4-C5-O5
27	B	2012	GLA	C4-C5-C6-O6
26	F	2003	AHR	O4-C4-C5-O5
28	C	2010	NAG	C8-C7-N2-C2
27	A	2014	GLA	C4-C5-C6-O6
28	C	2010	NAG	O7-C7-N2-C2
27	E	2004	GLA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GLA B 2015



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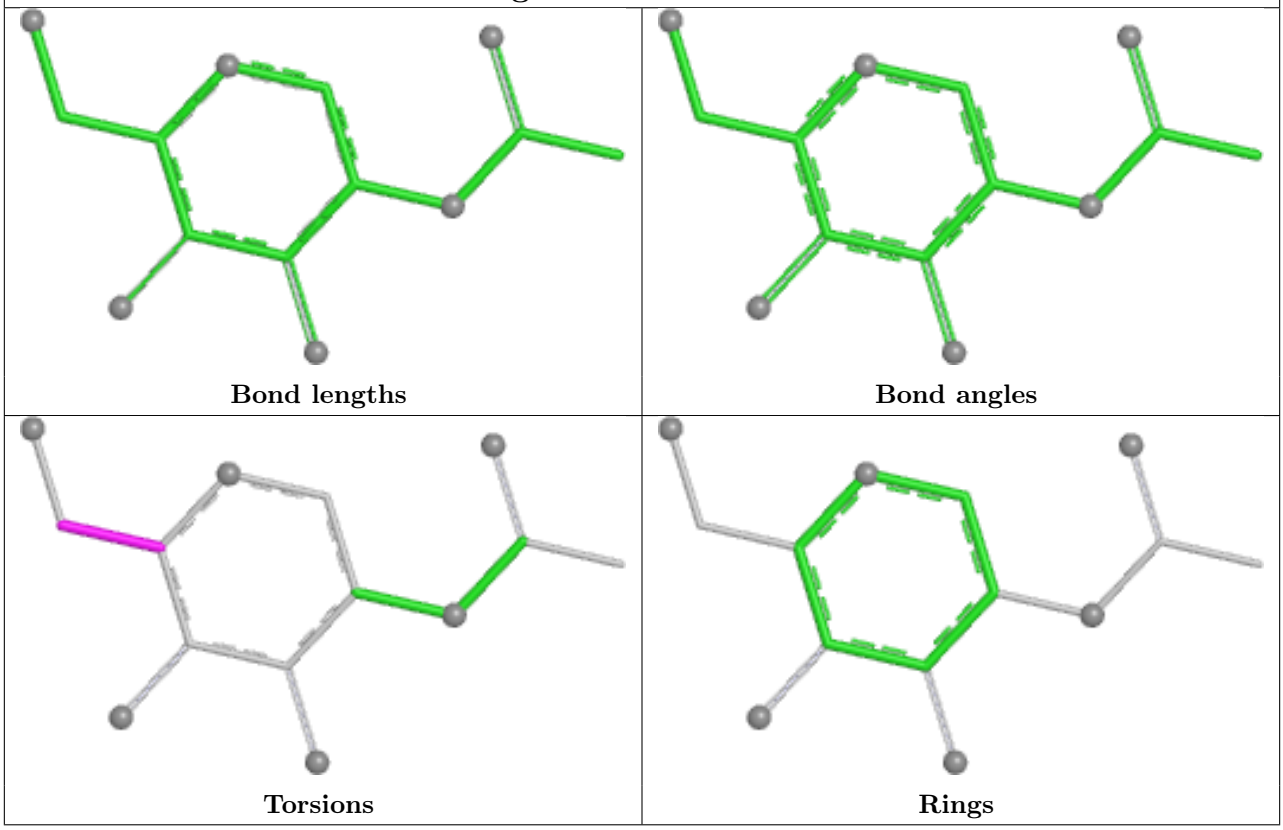

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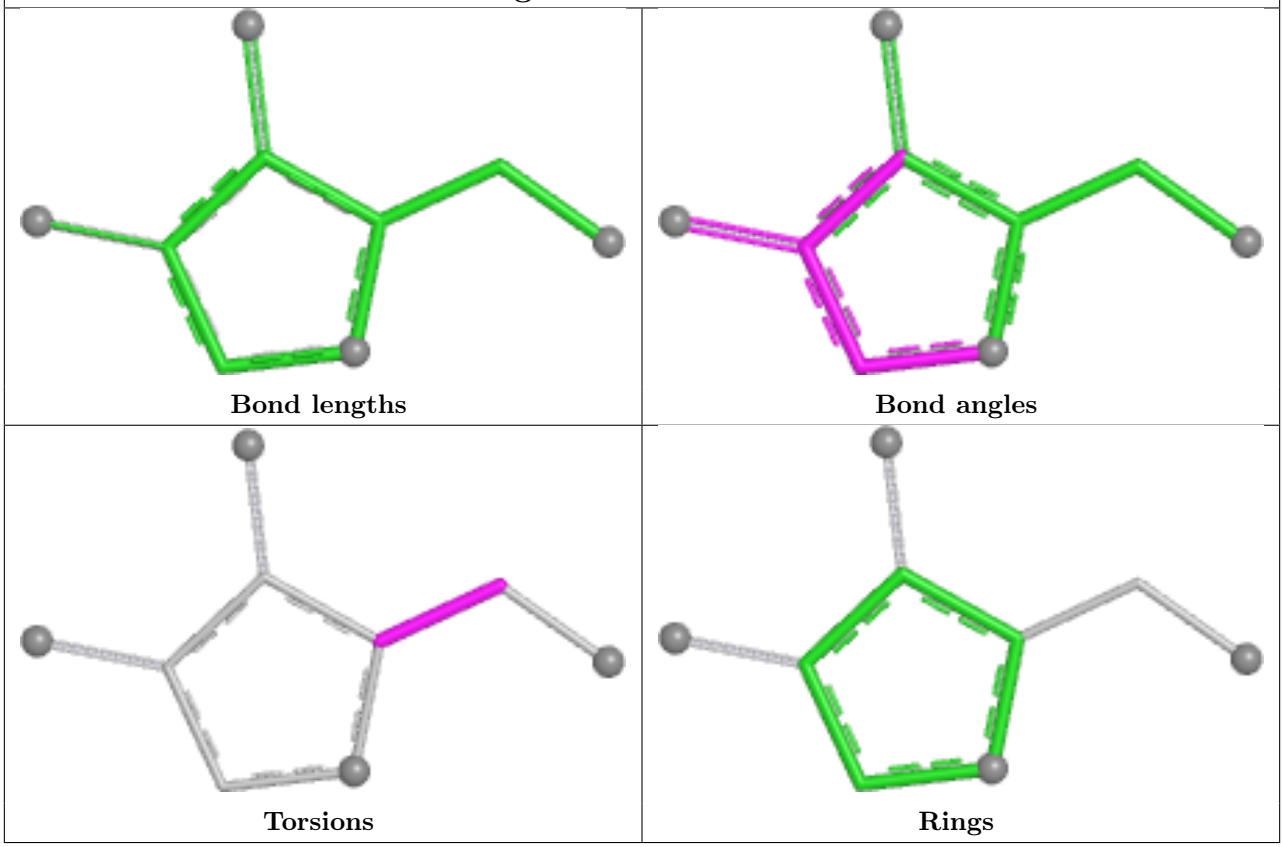

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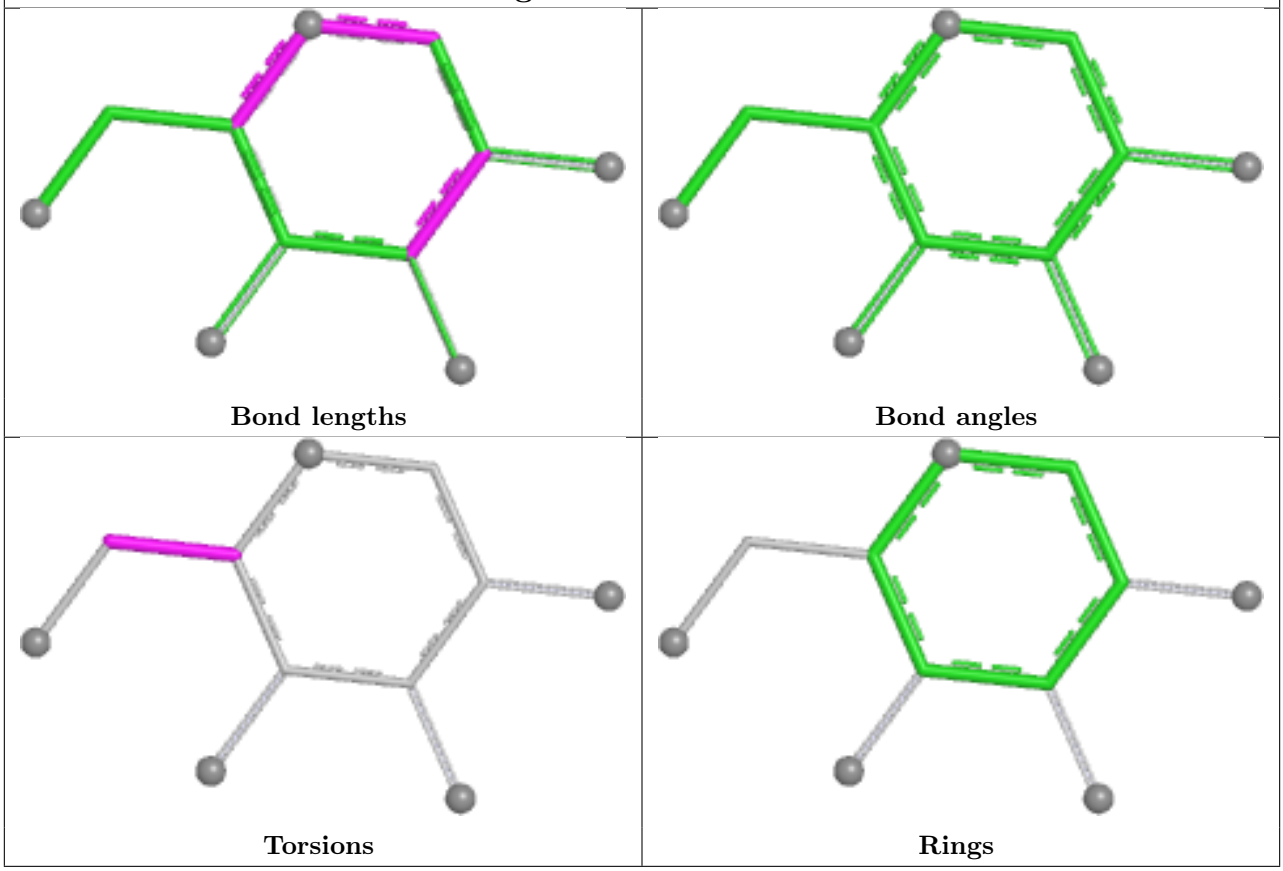

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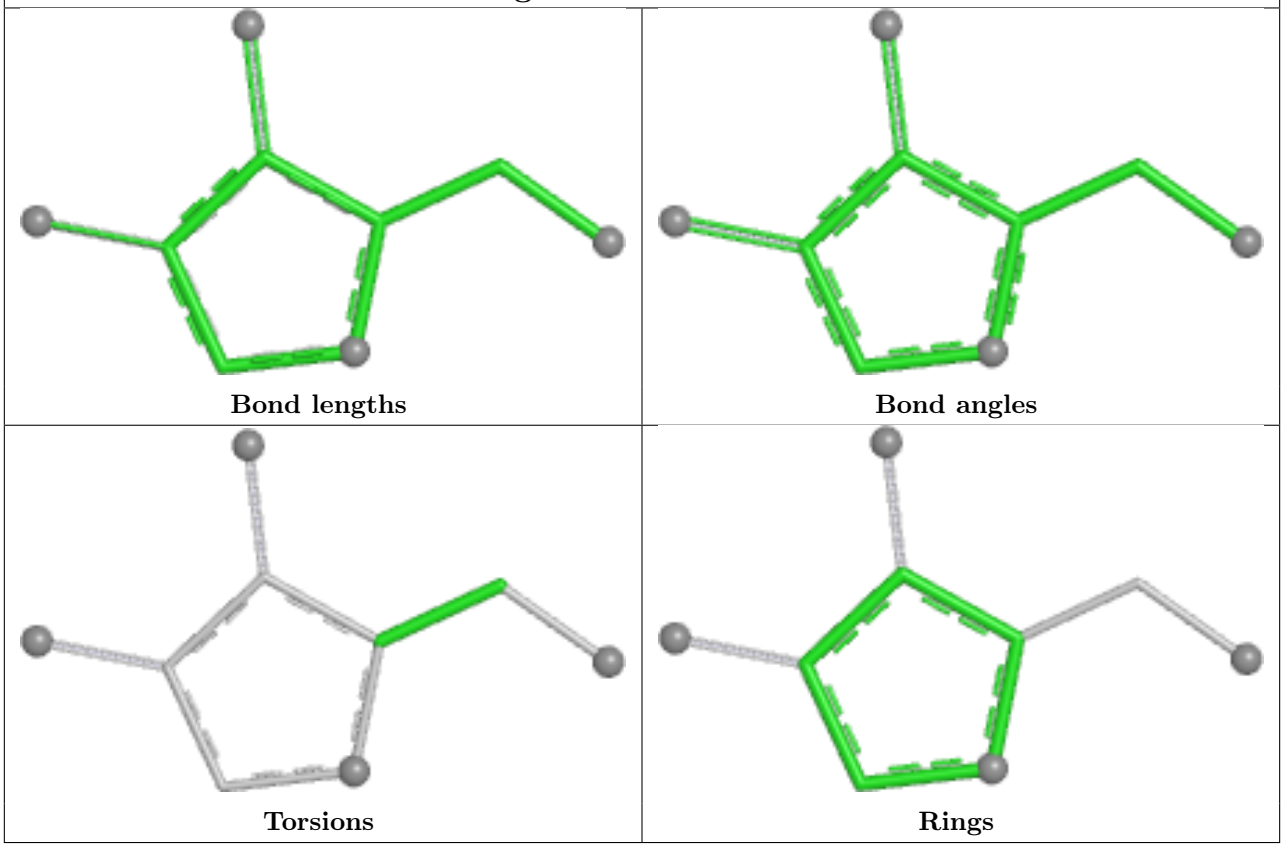

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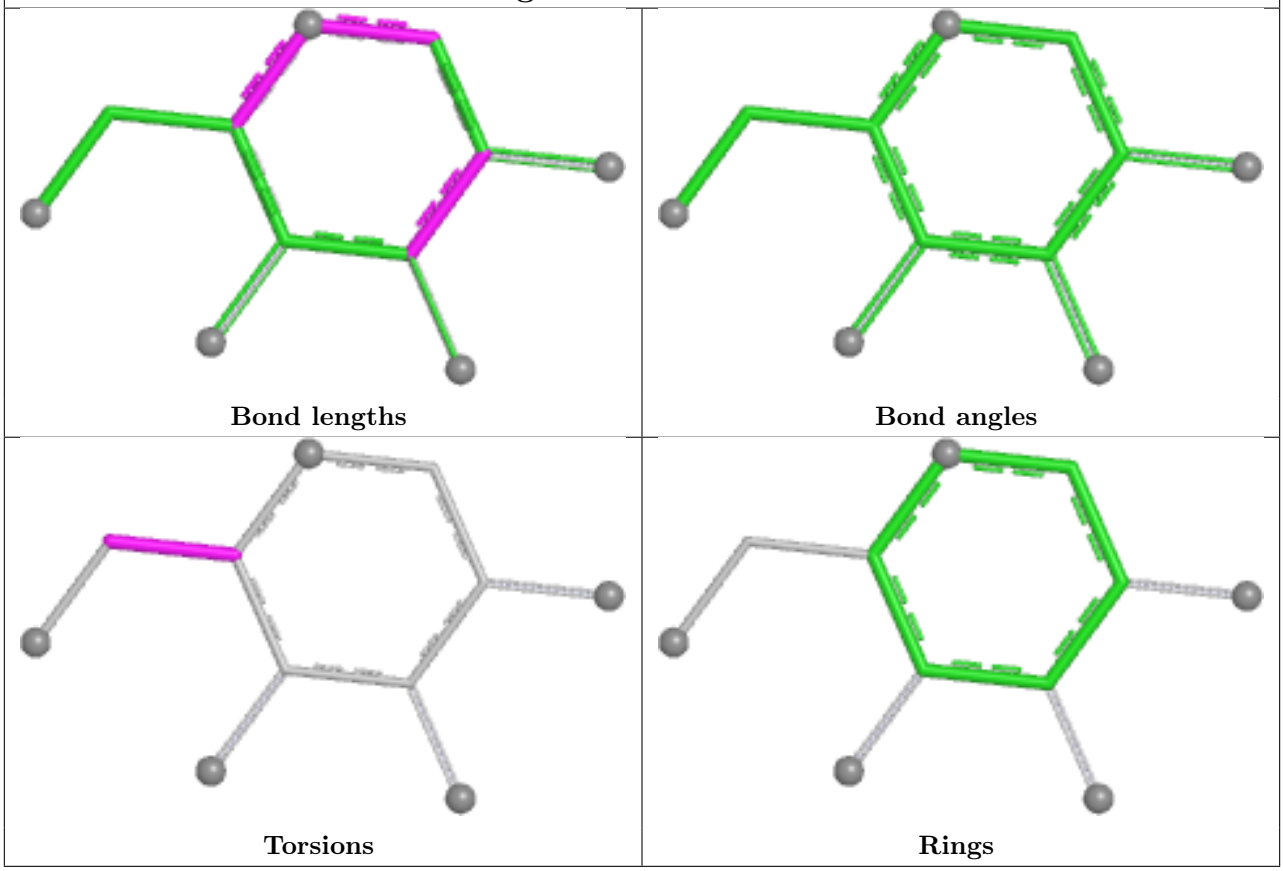

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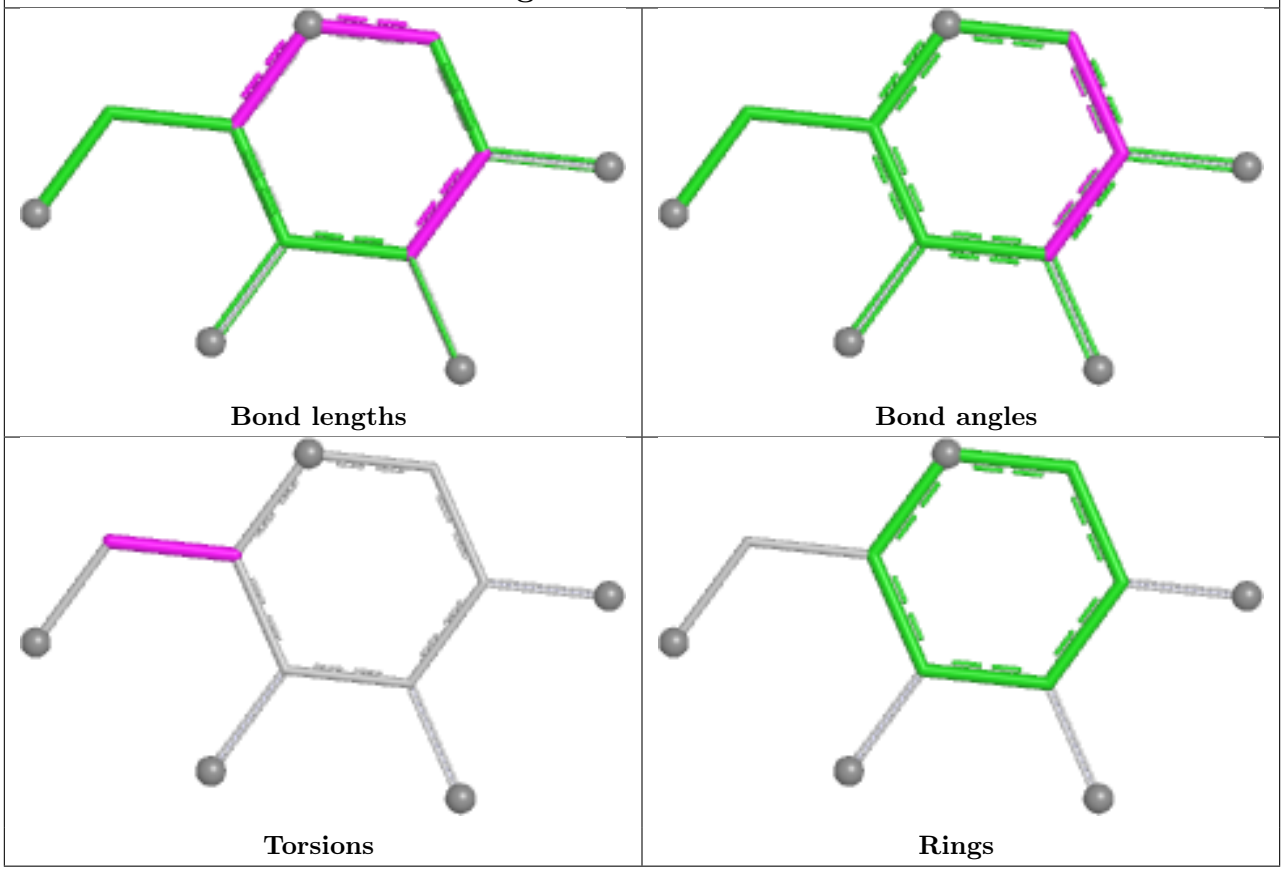
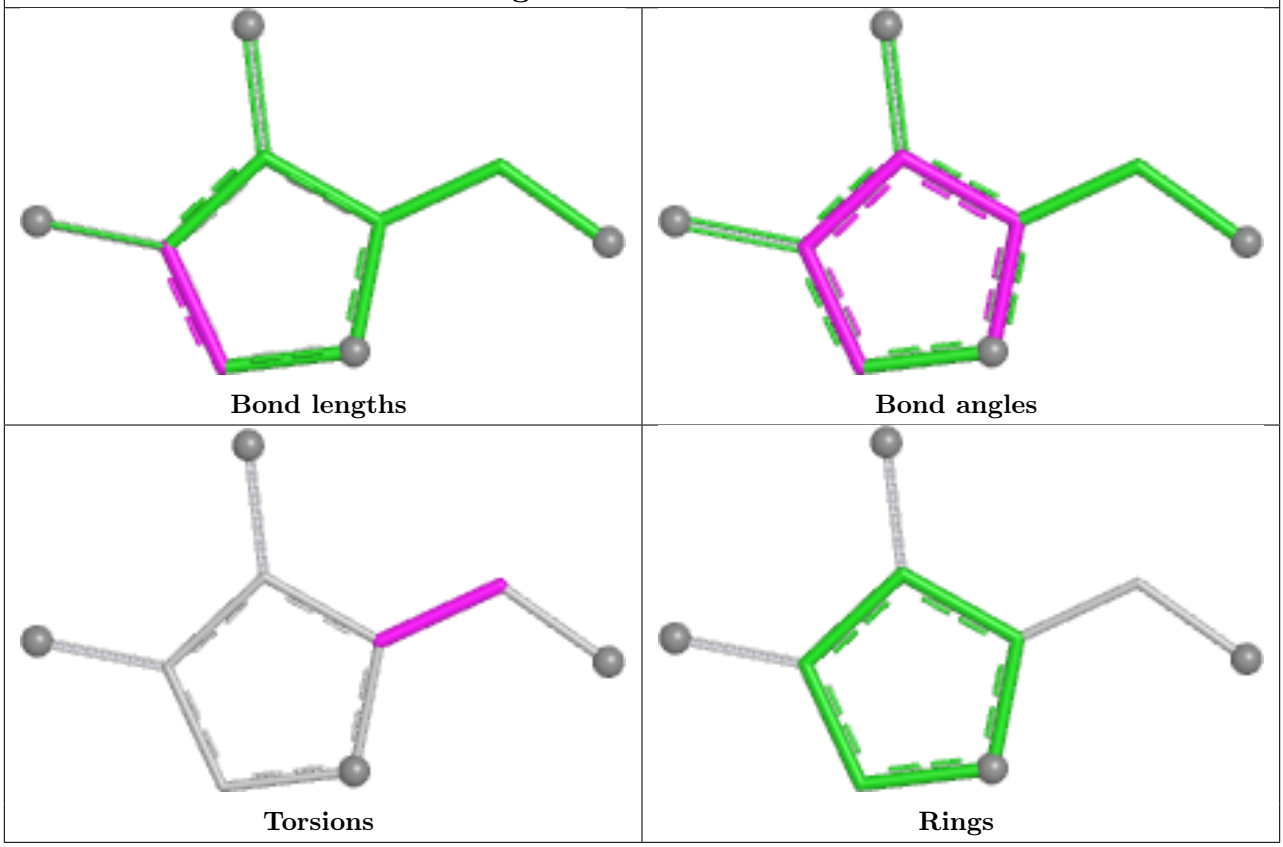


Ligand AHR A 2002



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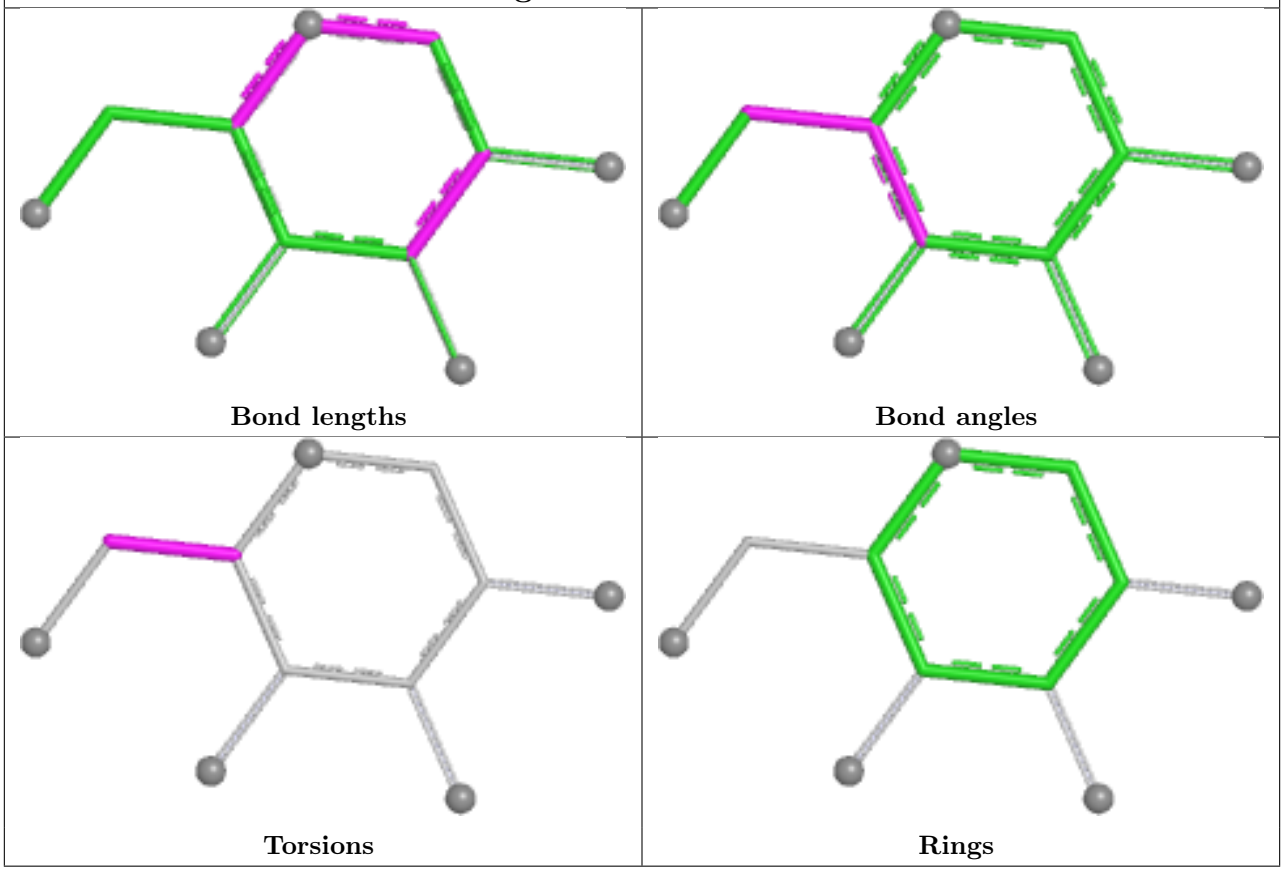

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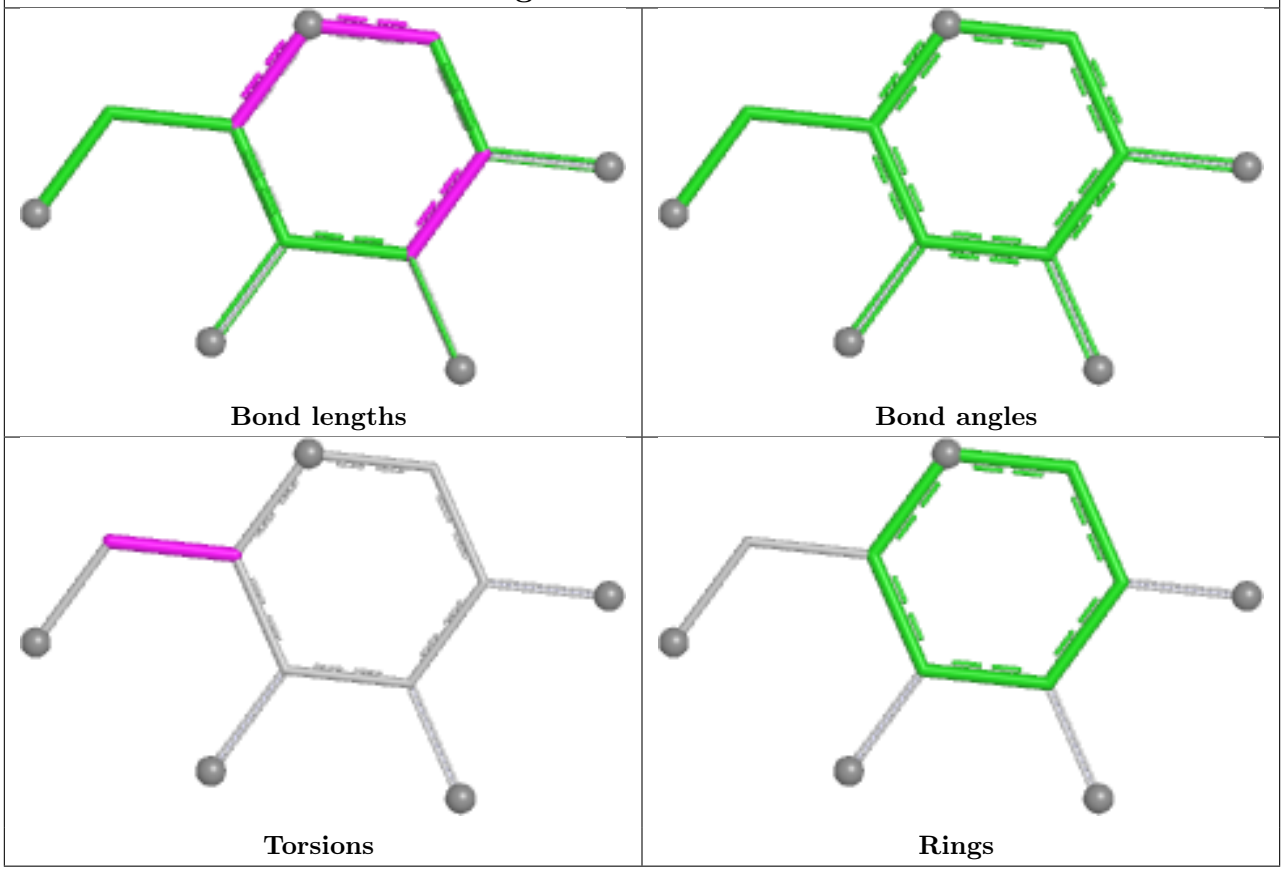

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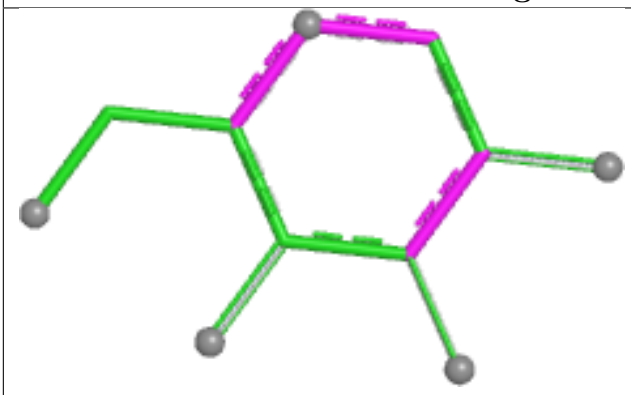	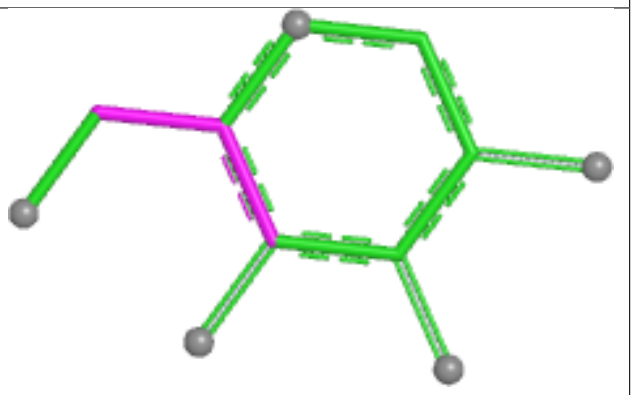
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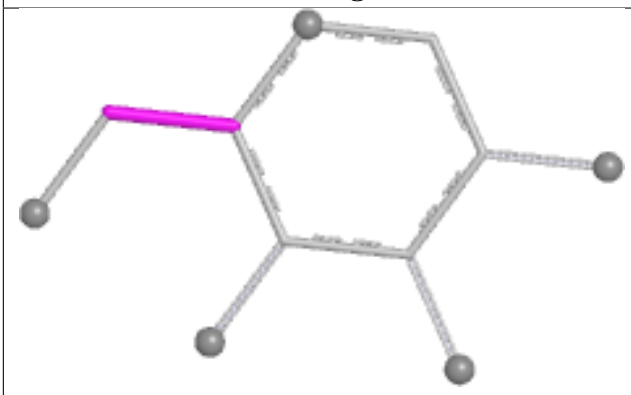
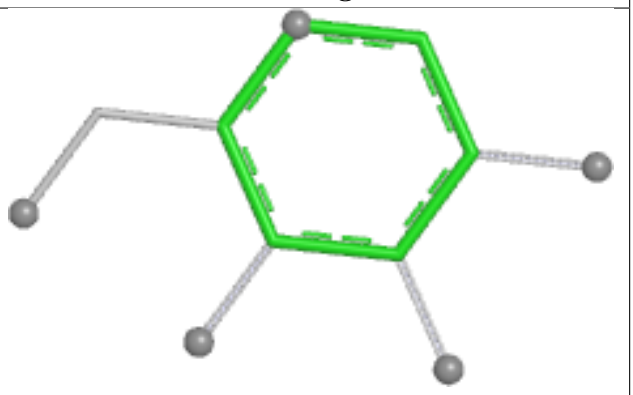
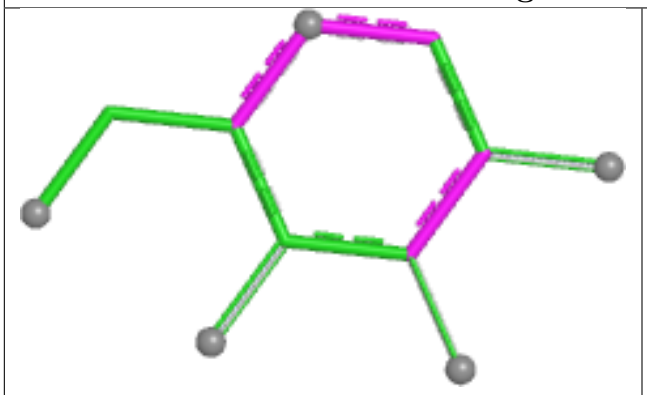
	
Torsions	**Rings**

Ligand GLA F 2018



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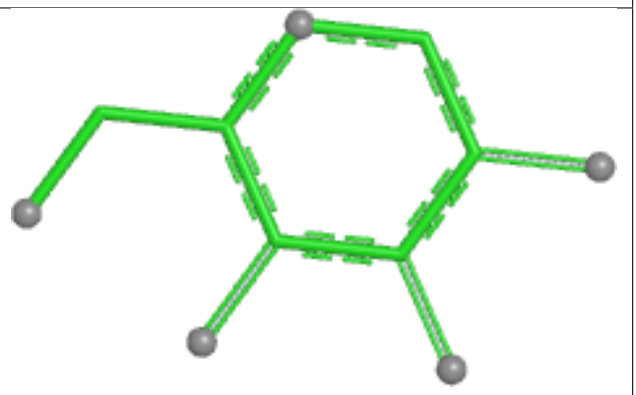

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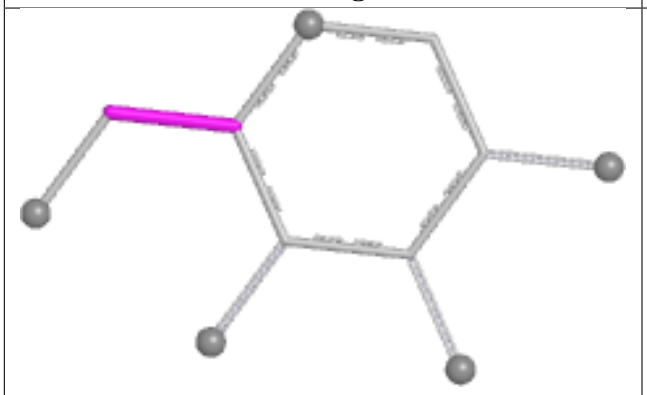
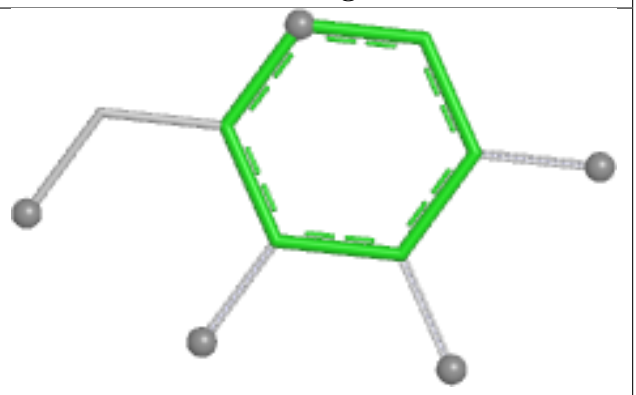


Torsions



Rings

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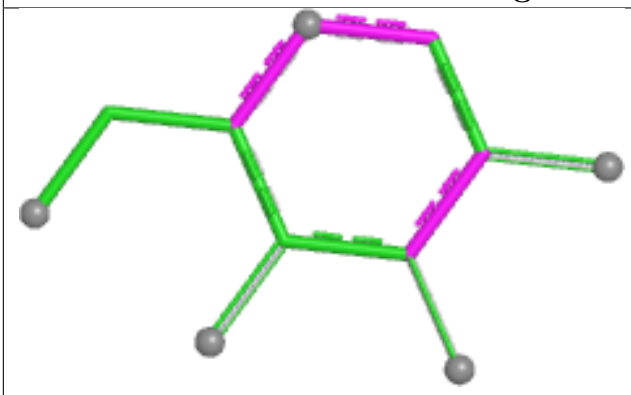
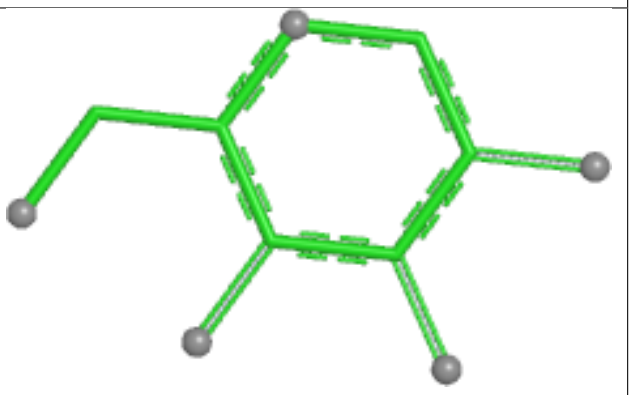
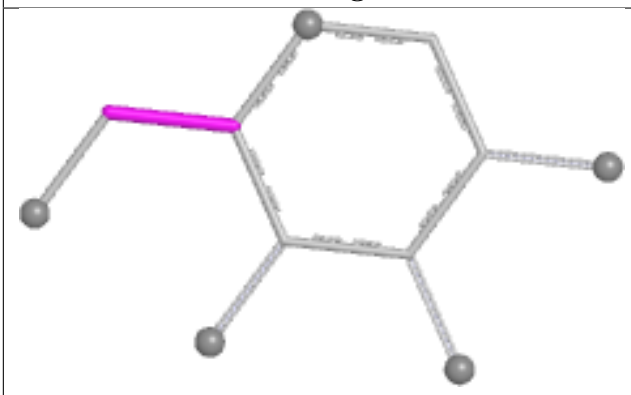
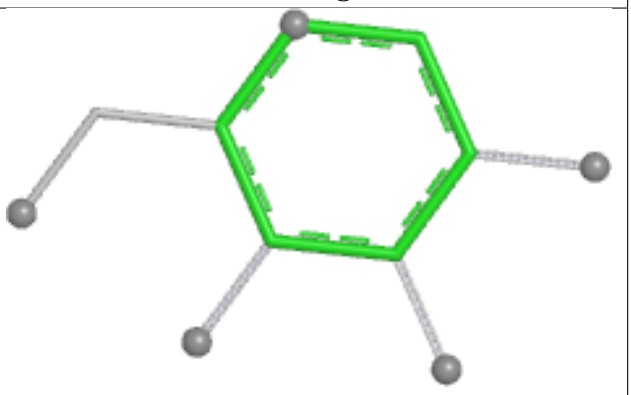
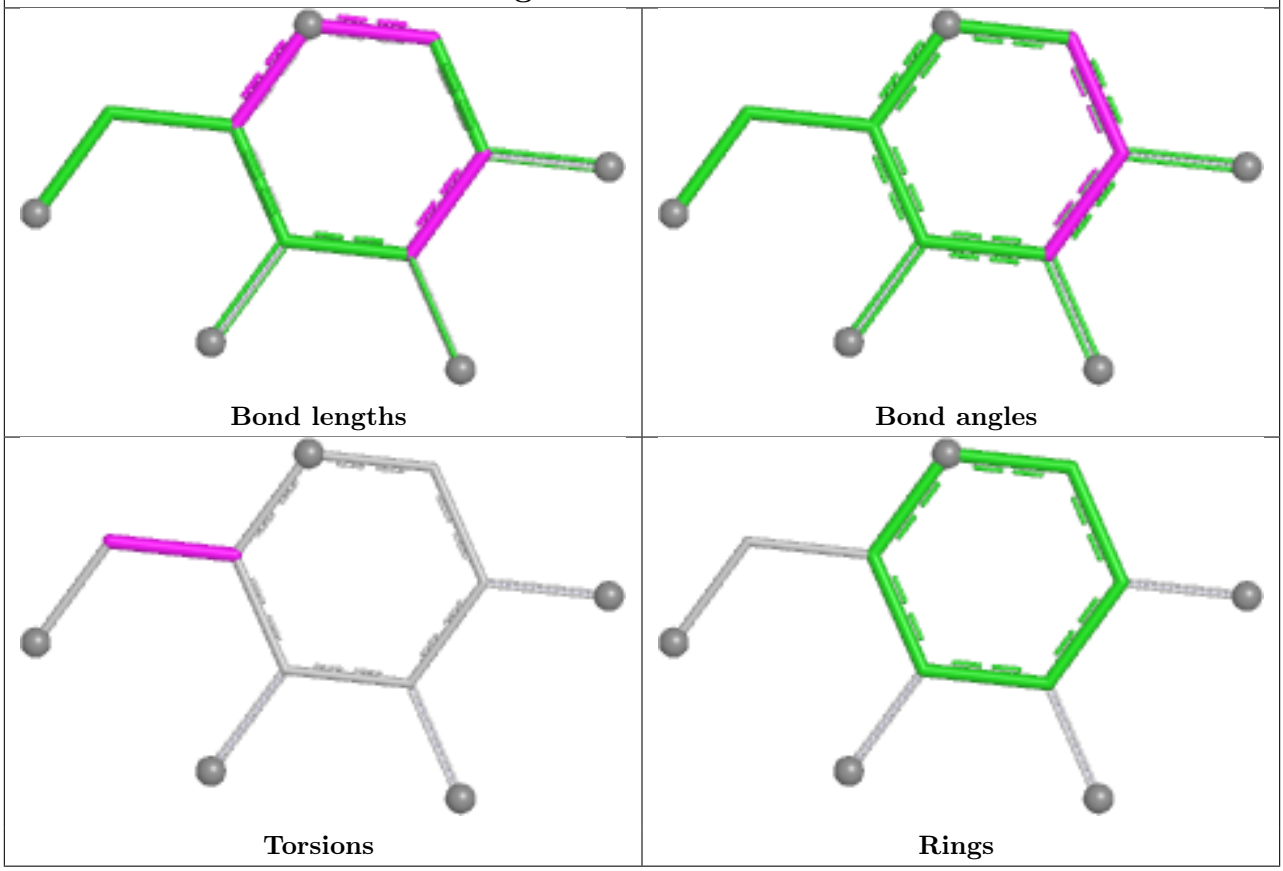
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA A 2016



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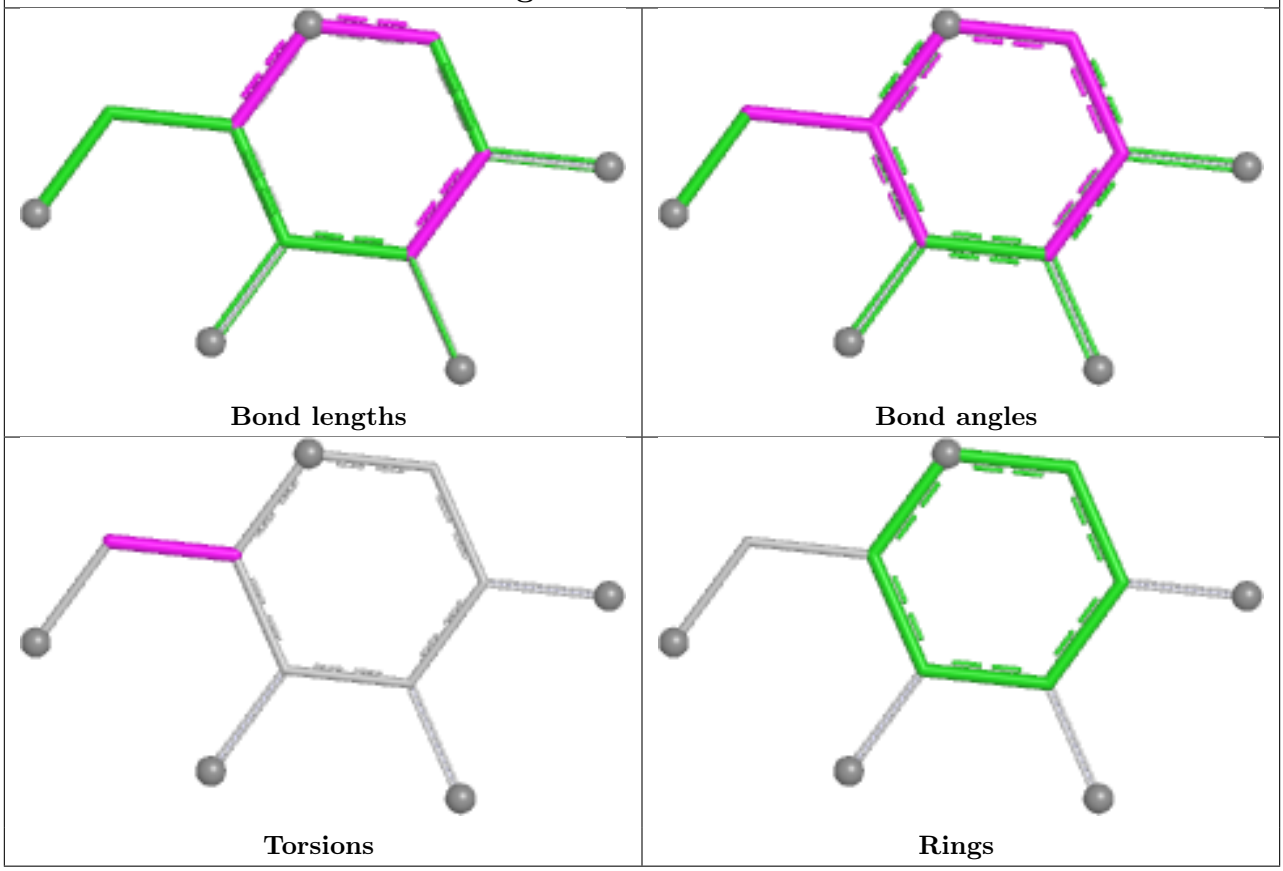

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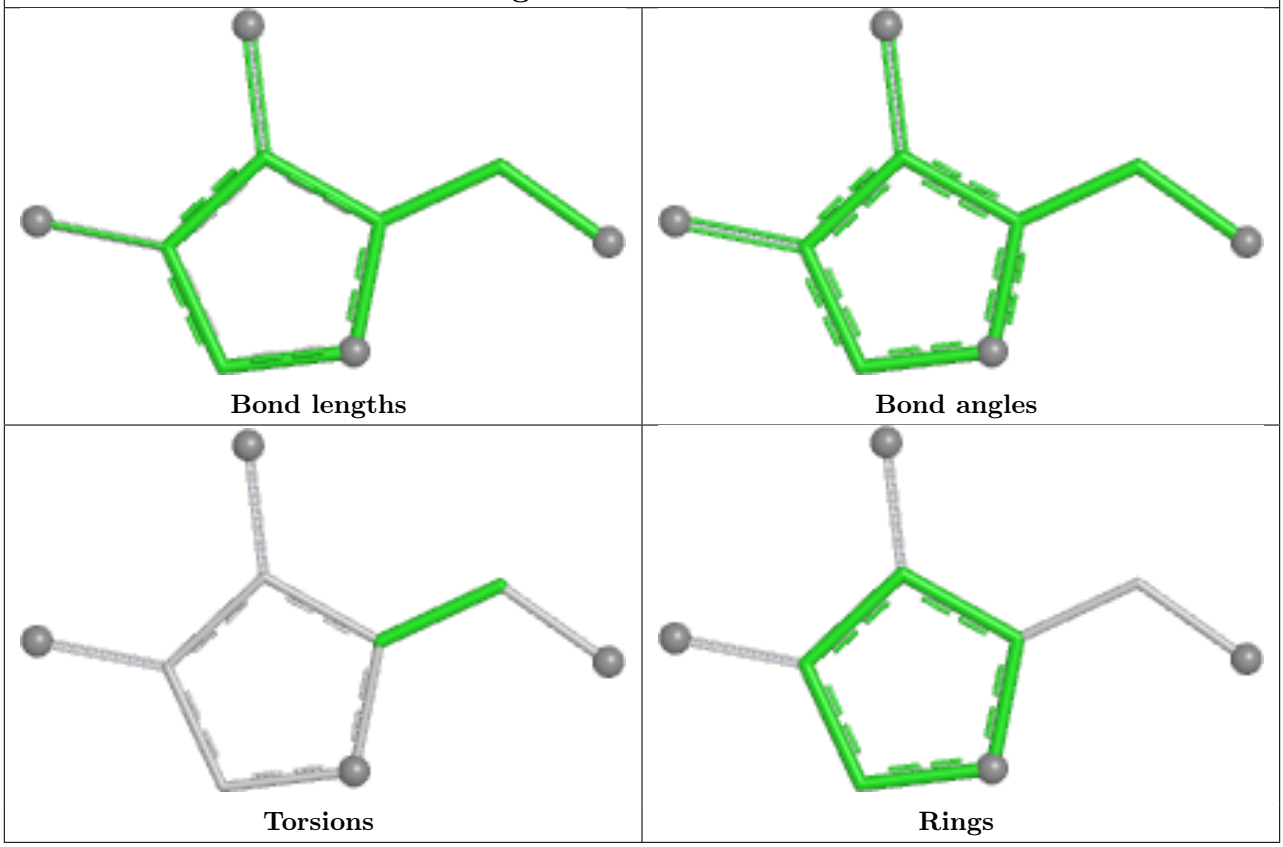

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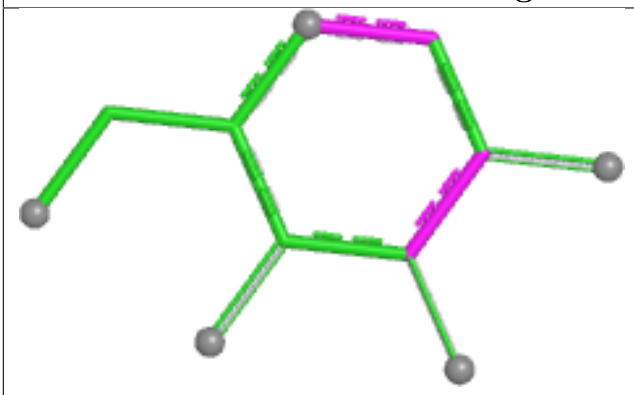	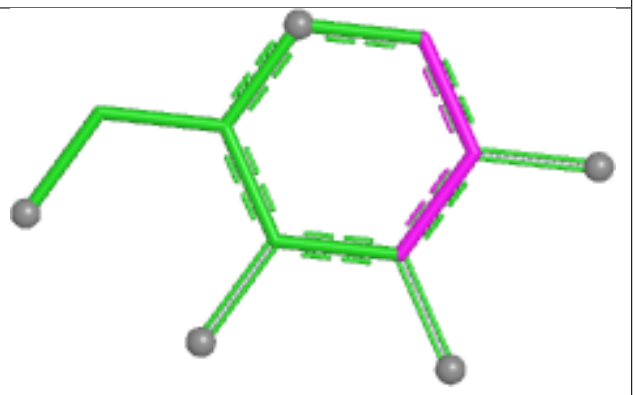
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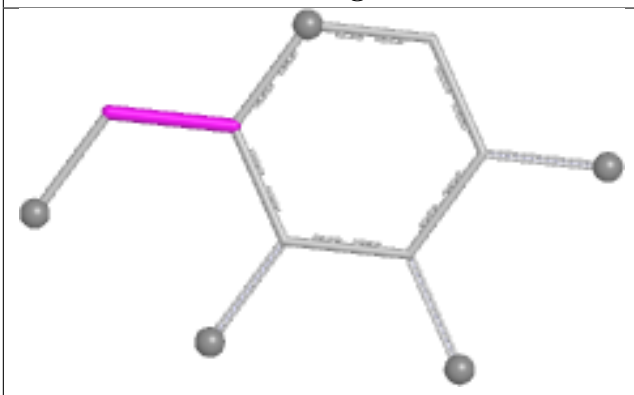	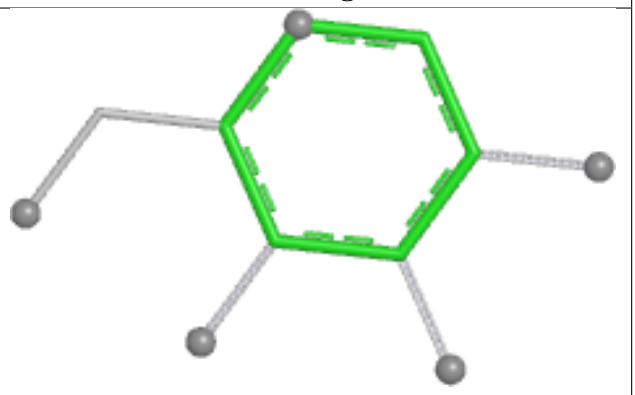
Torsions	**Rings**

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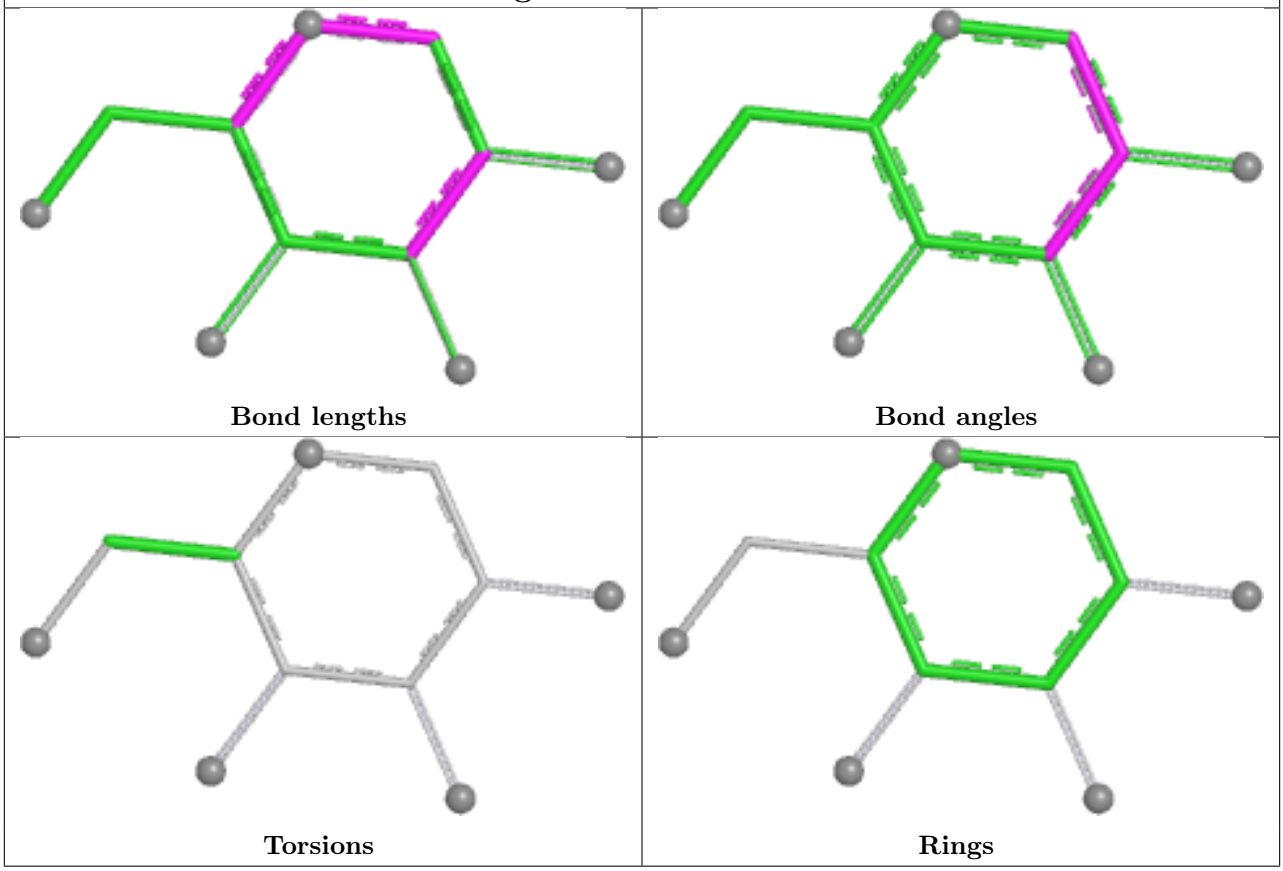
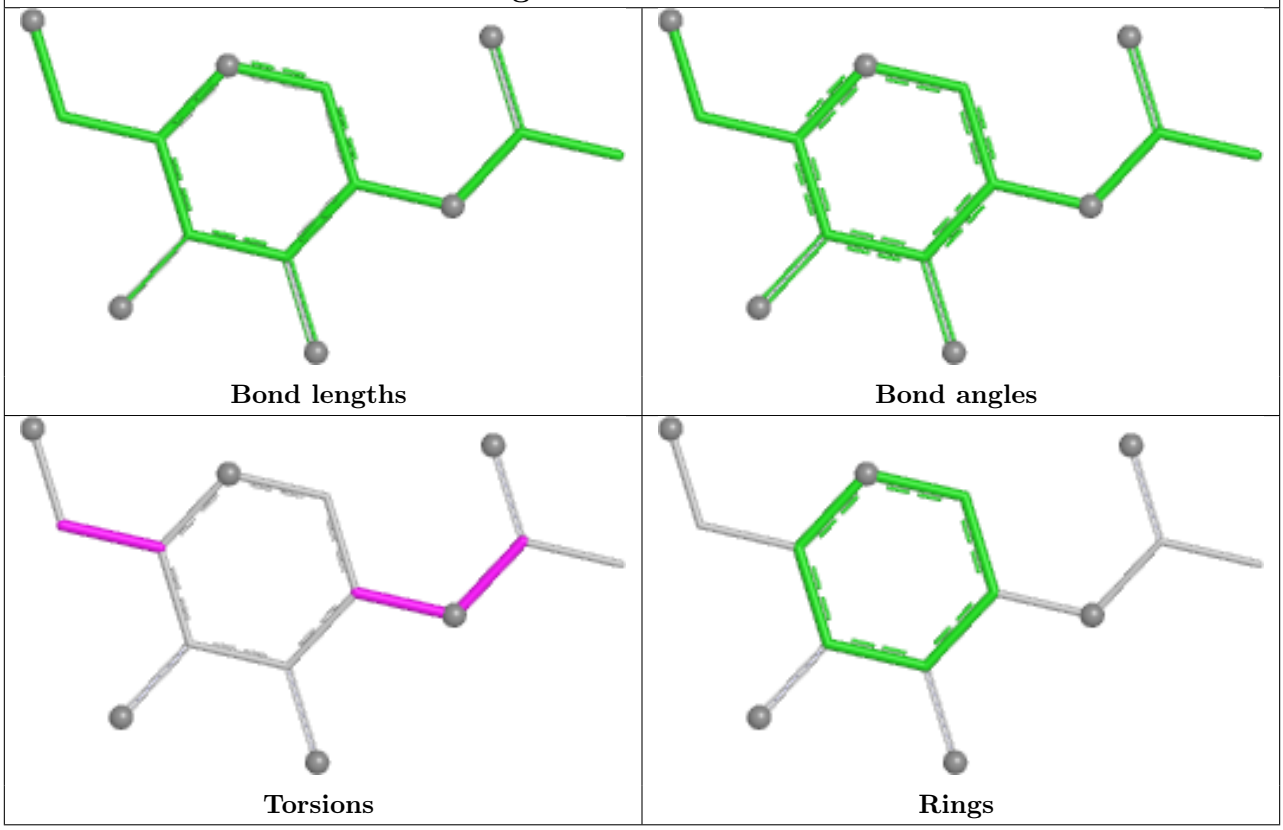


Ligand NAG C 2009



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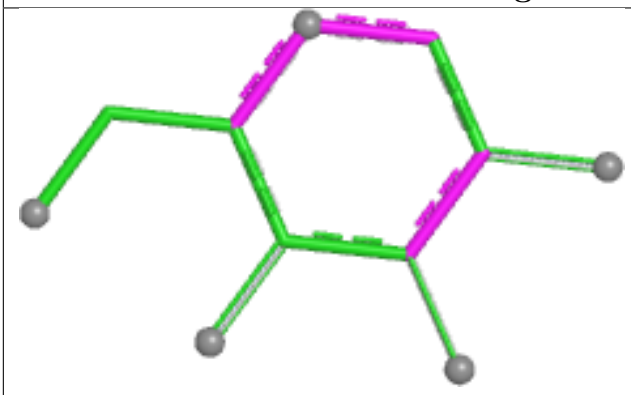
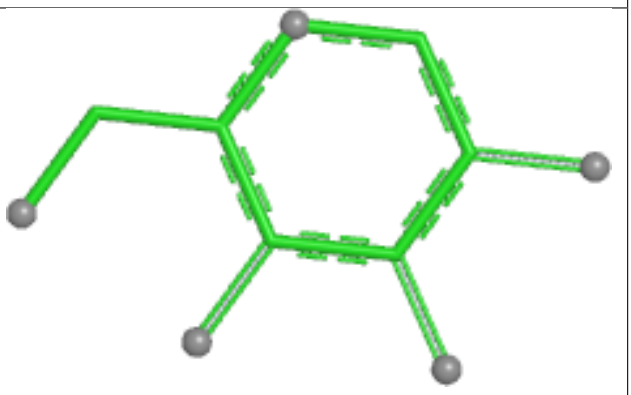
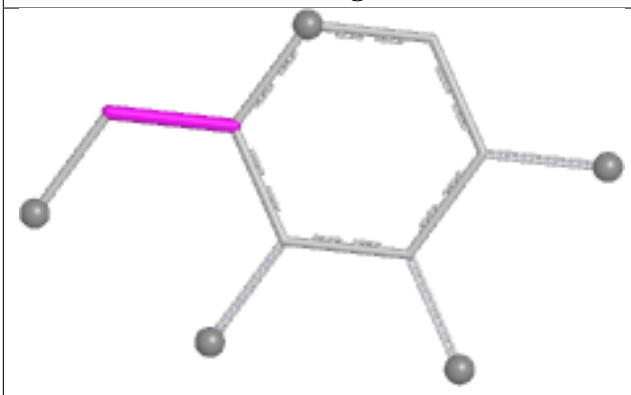
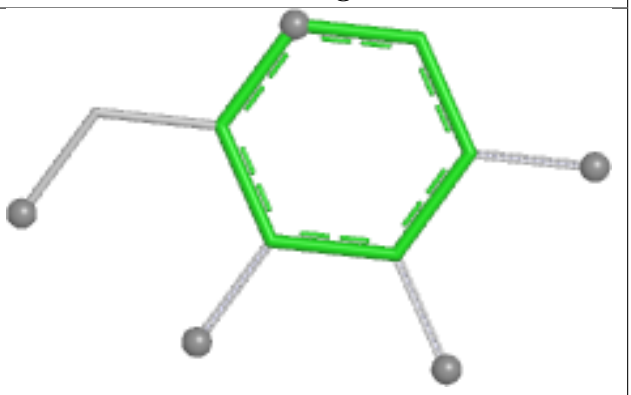
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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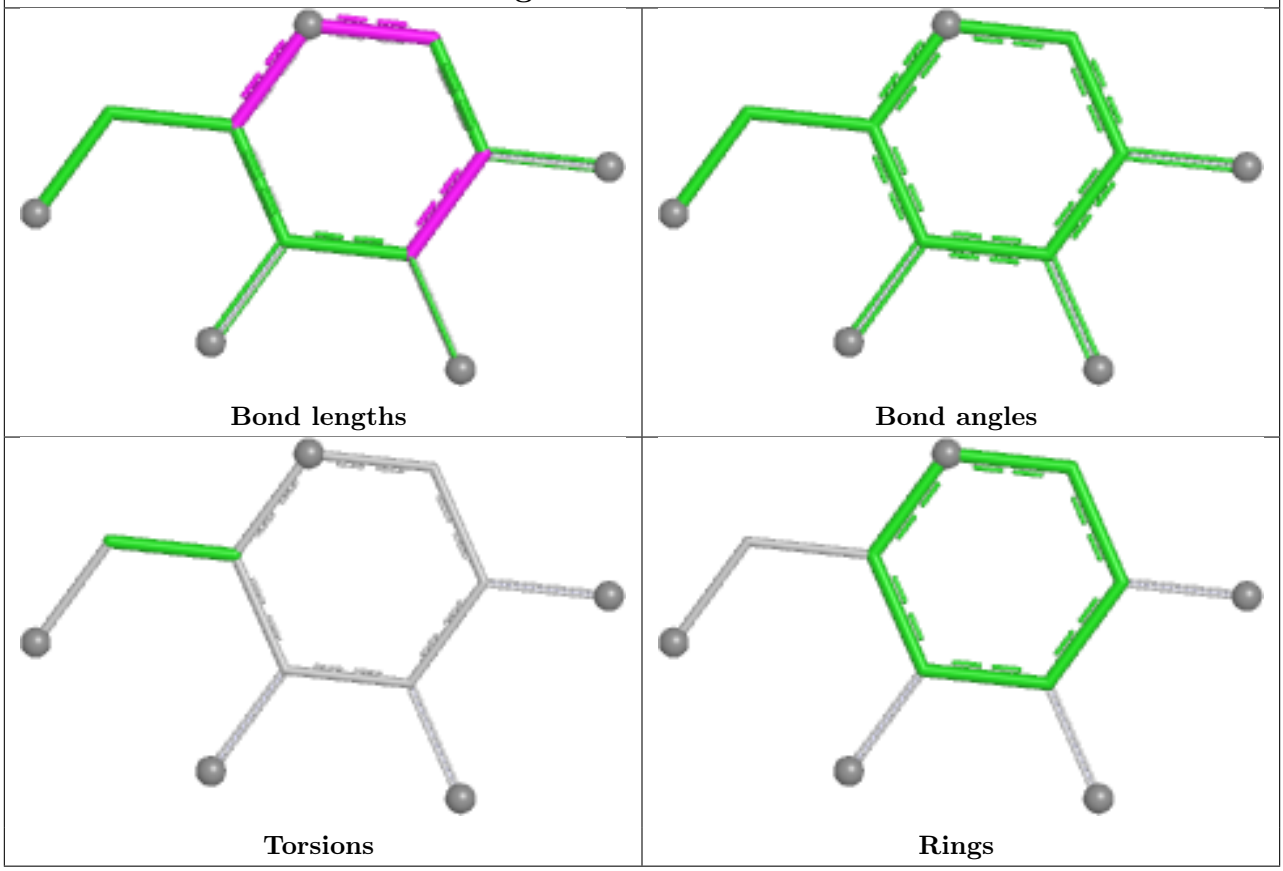
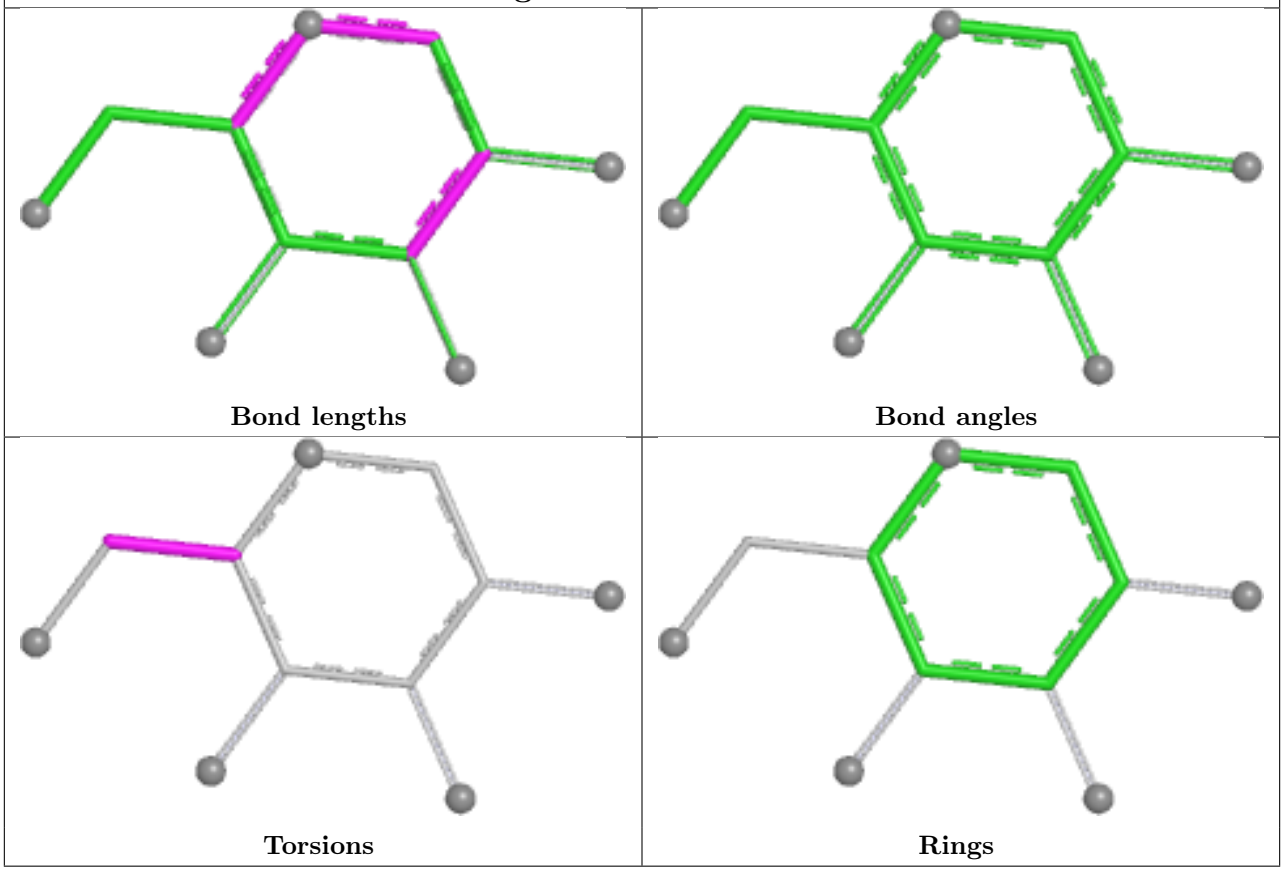
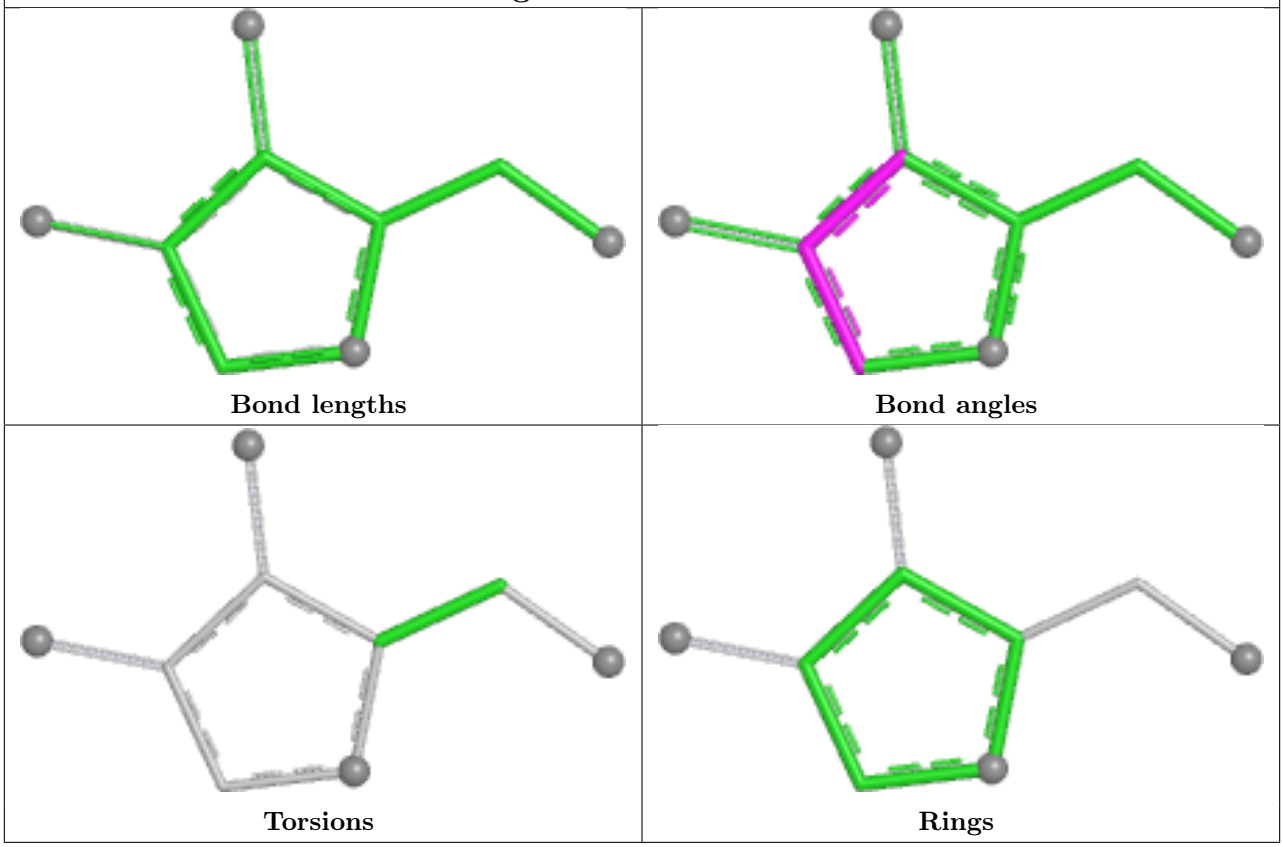


Ligand GLA D 2005



Ligand AHR B 2002



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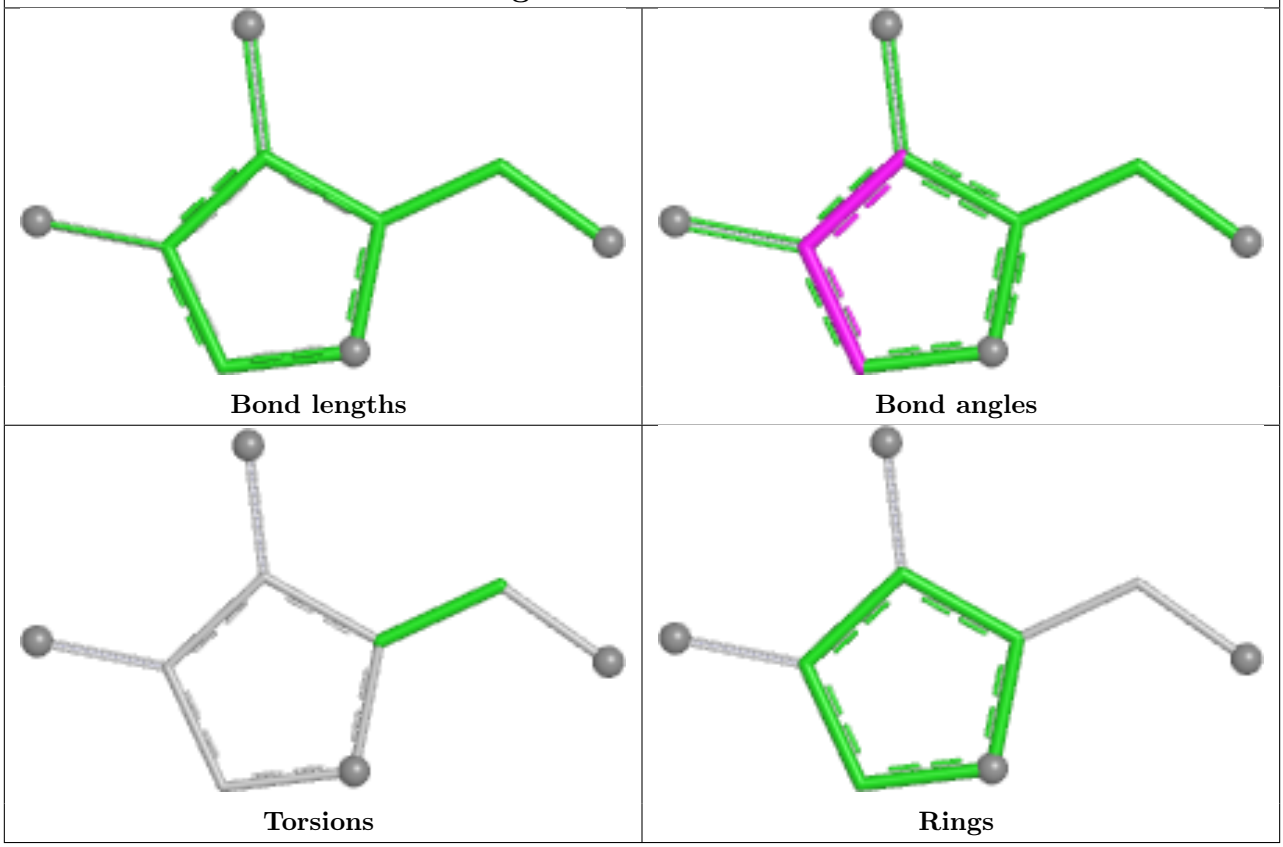

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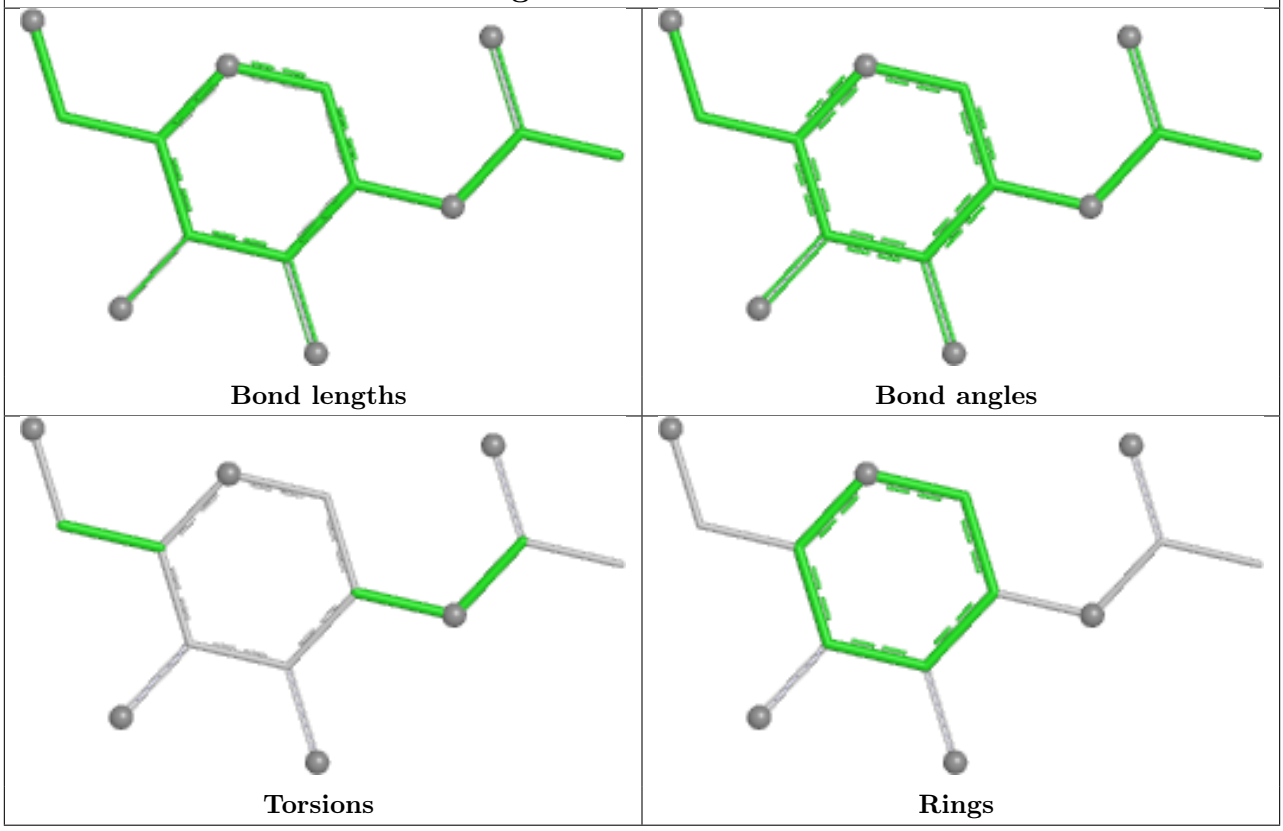

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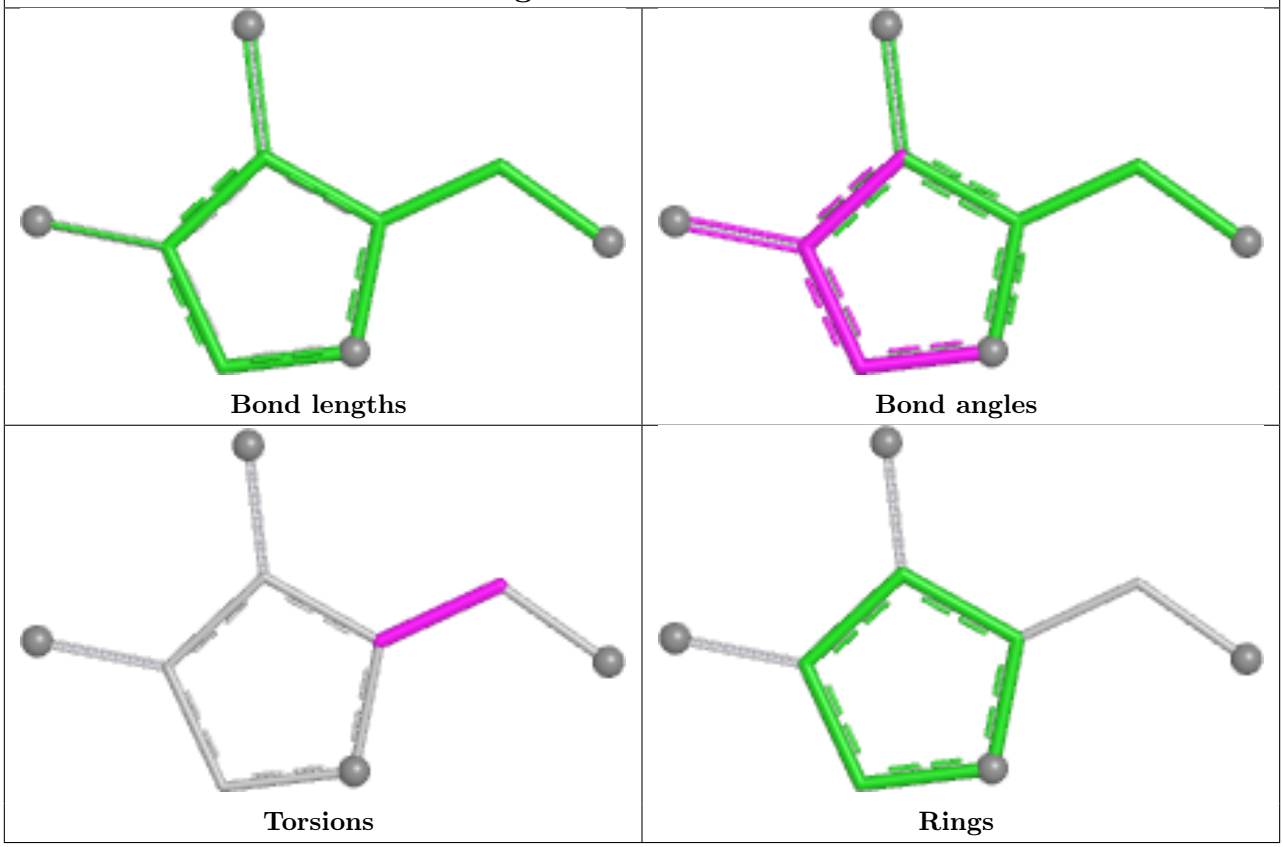
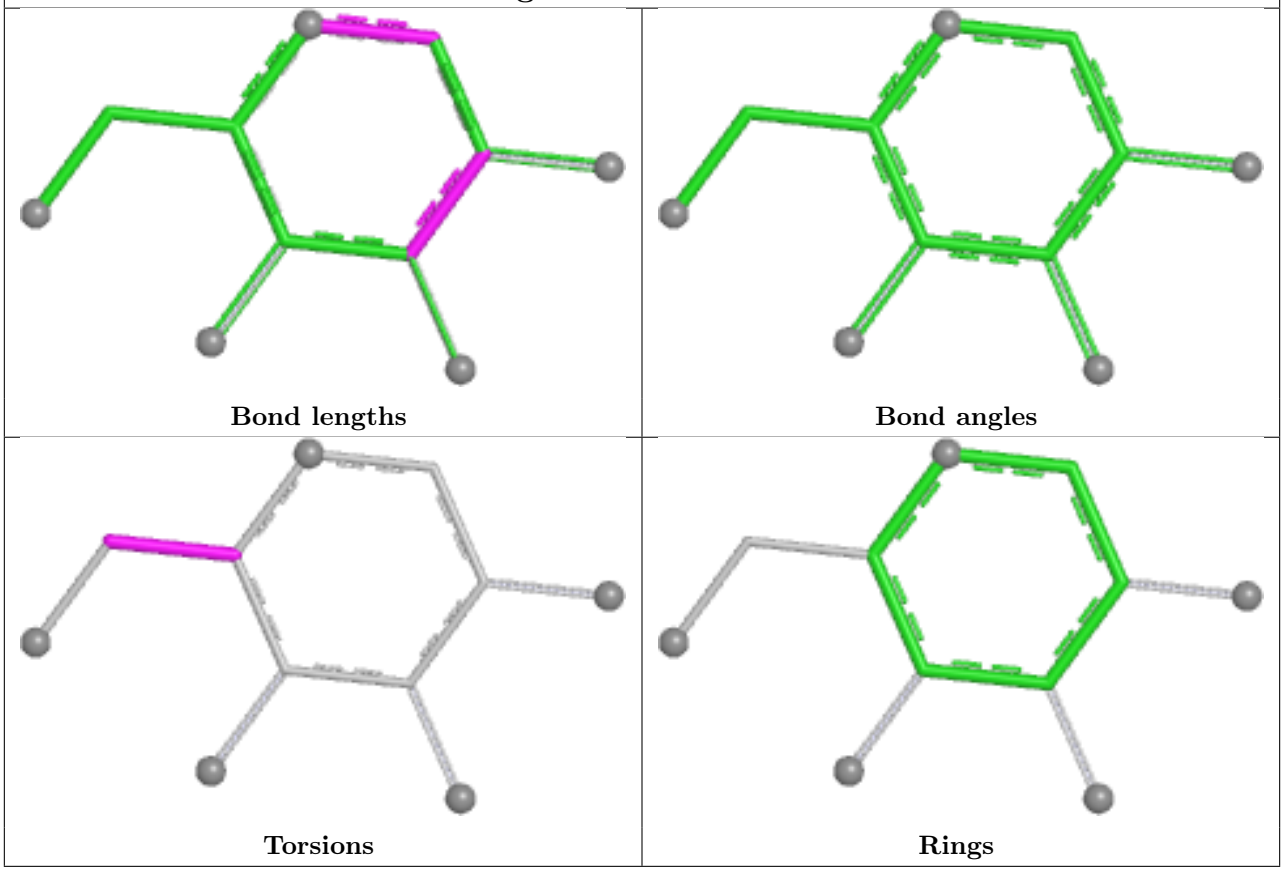


Ligand GLA F 2016



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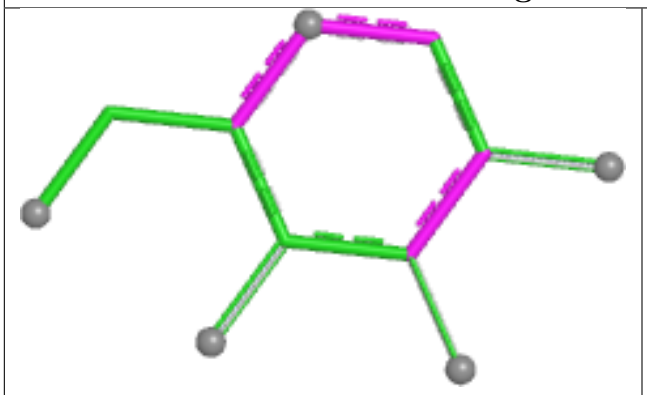
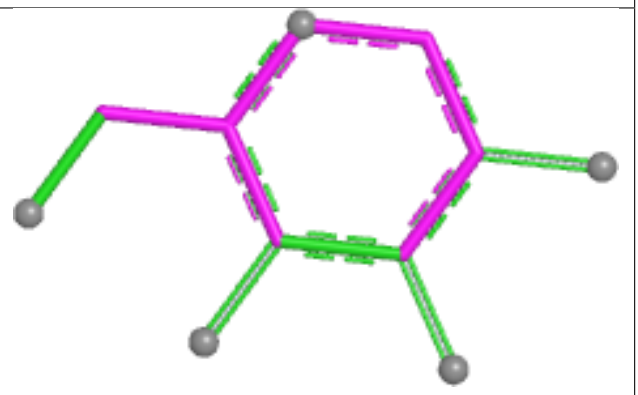
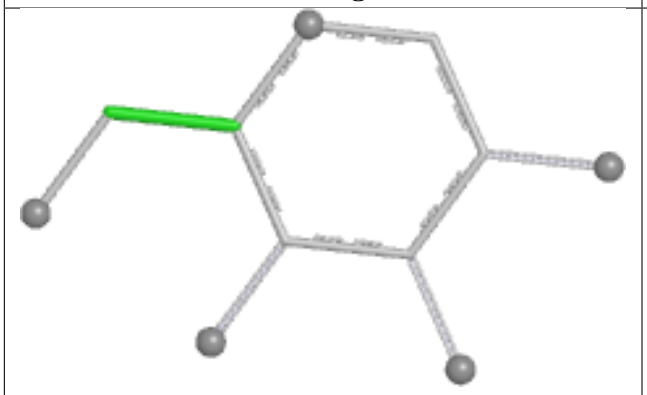


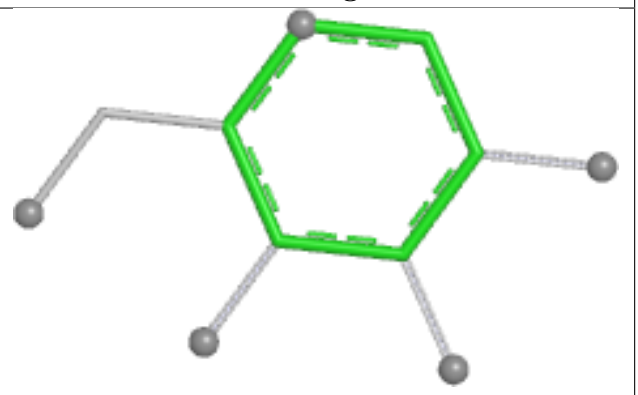
Bond lengths



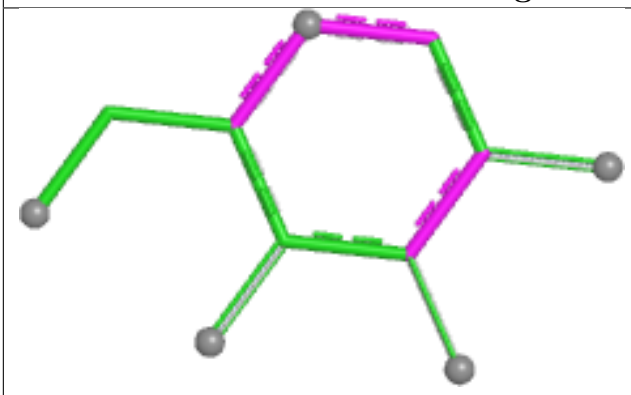
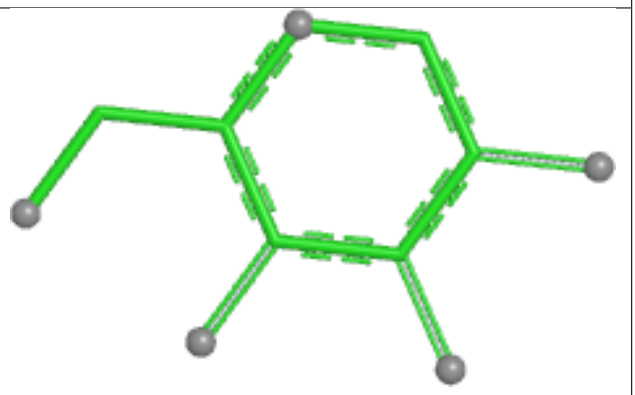
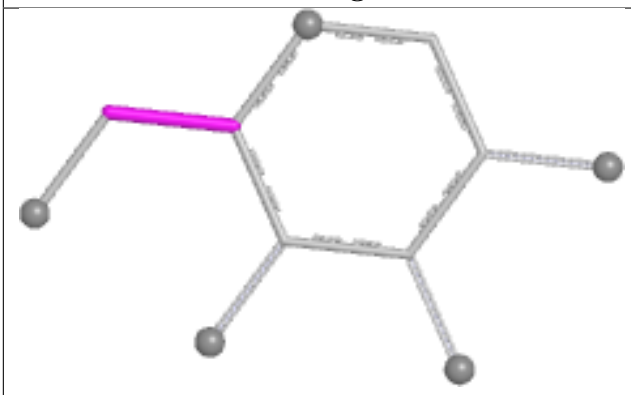
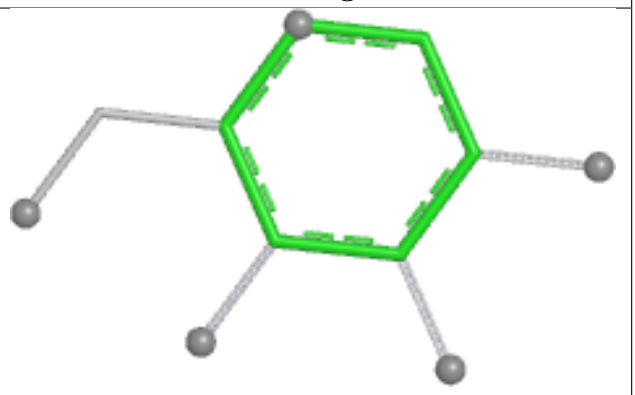
Bond angles



Torsions



Rings

Ligand GLA B 2012	
 Bond lengths	 Bond angles
 Torsions	 Rings

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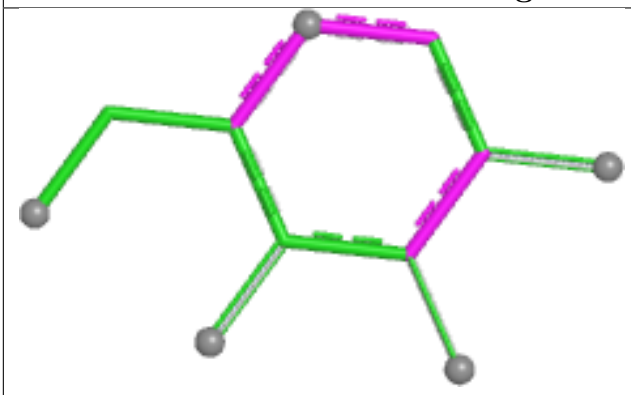	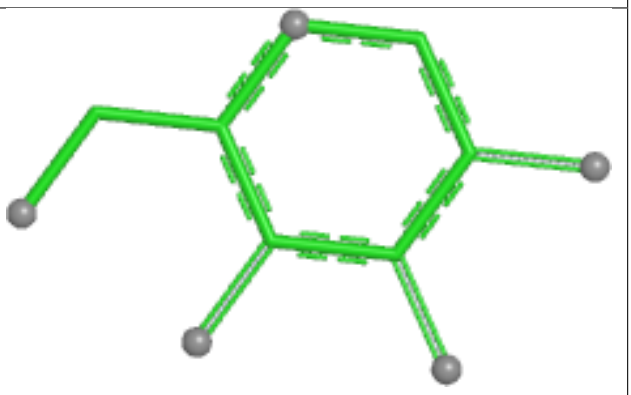
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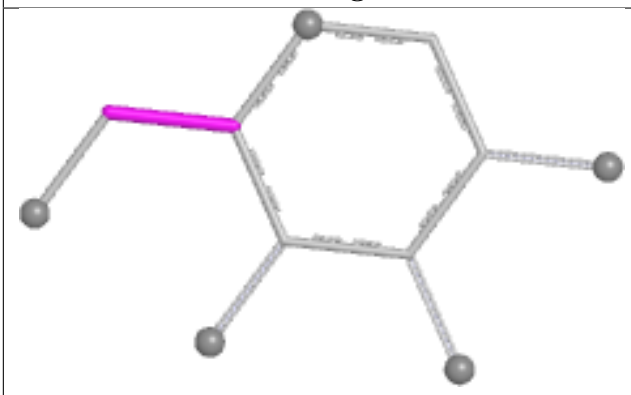
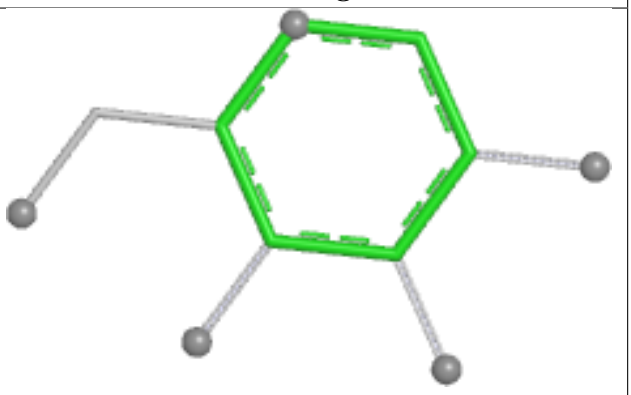
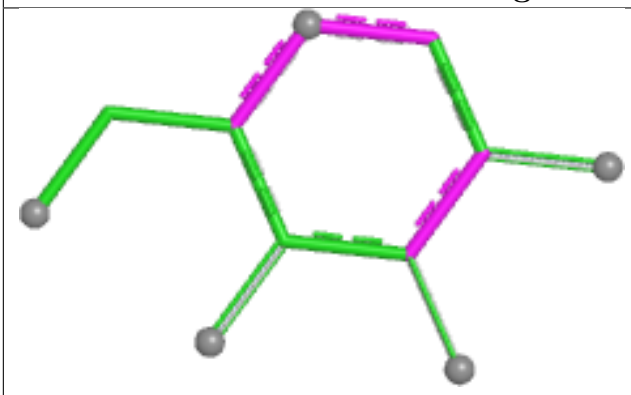
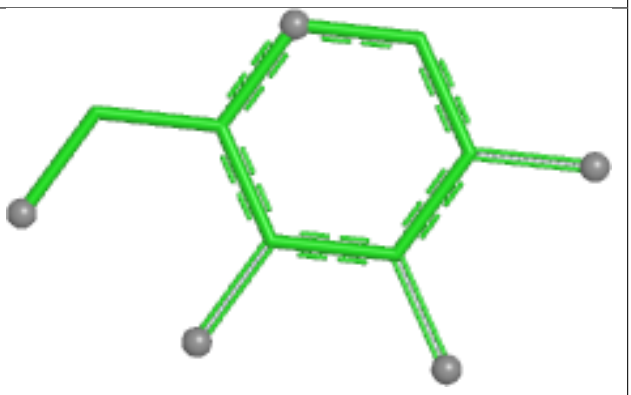
	
Torsions	**Rings**

Ligand GLA D 2008	
	
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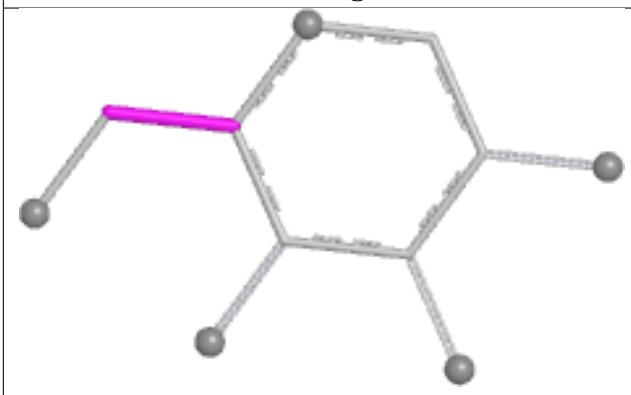
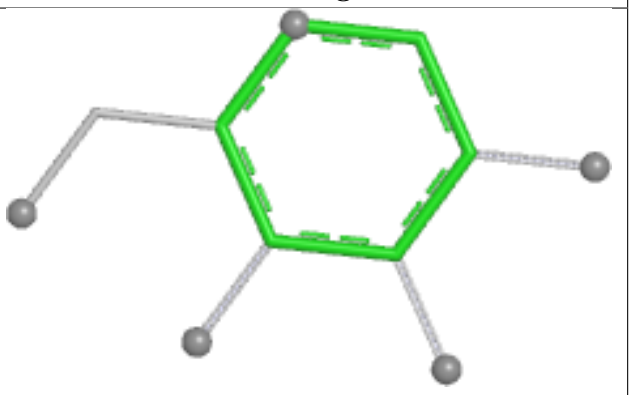
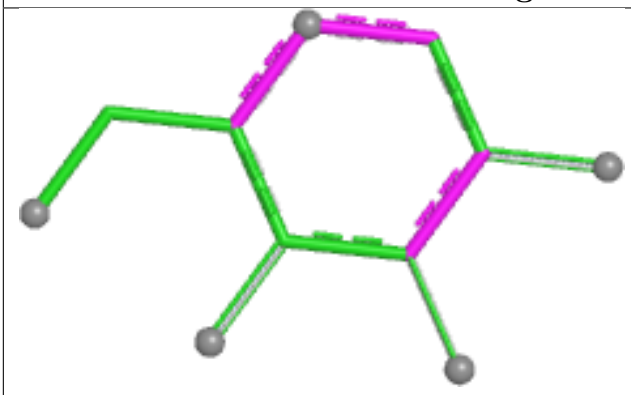
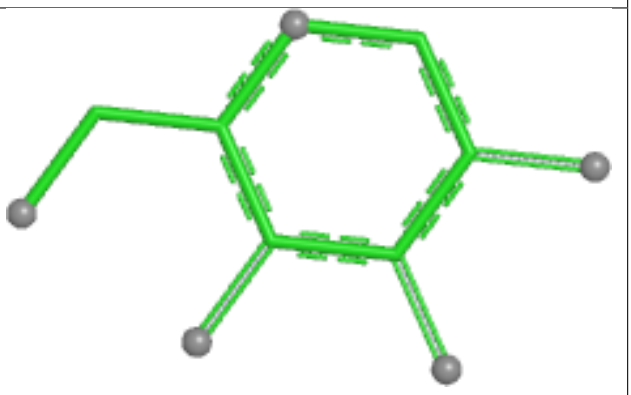
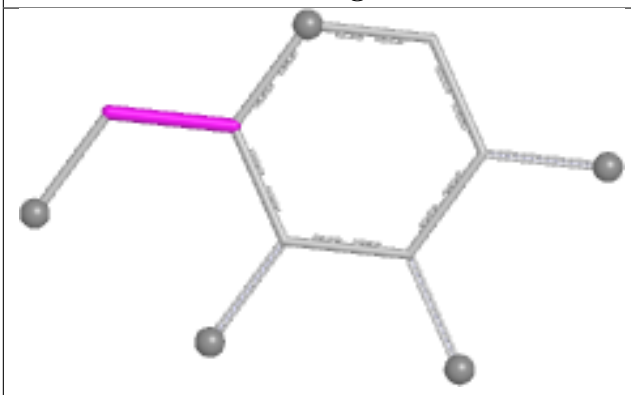
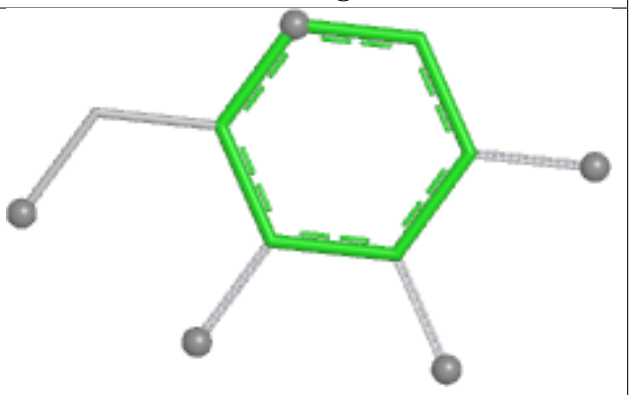
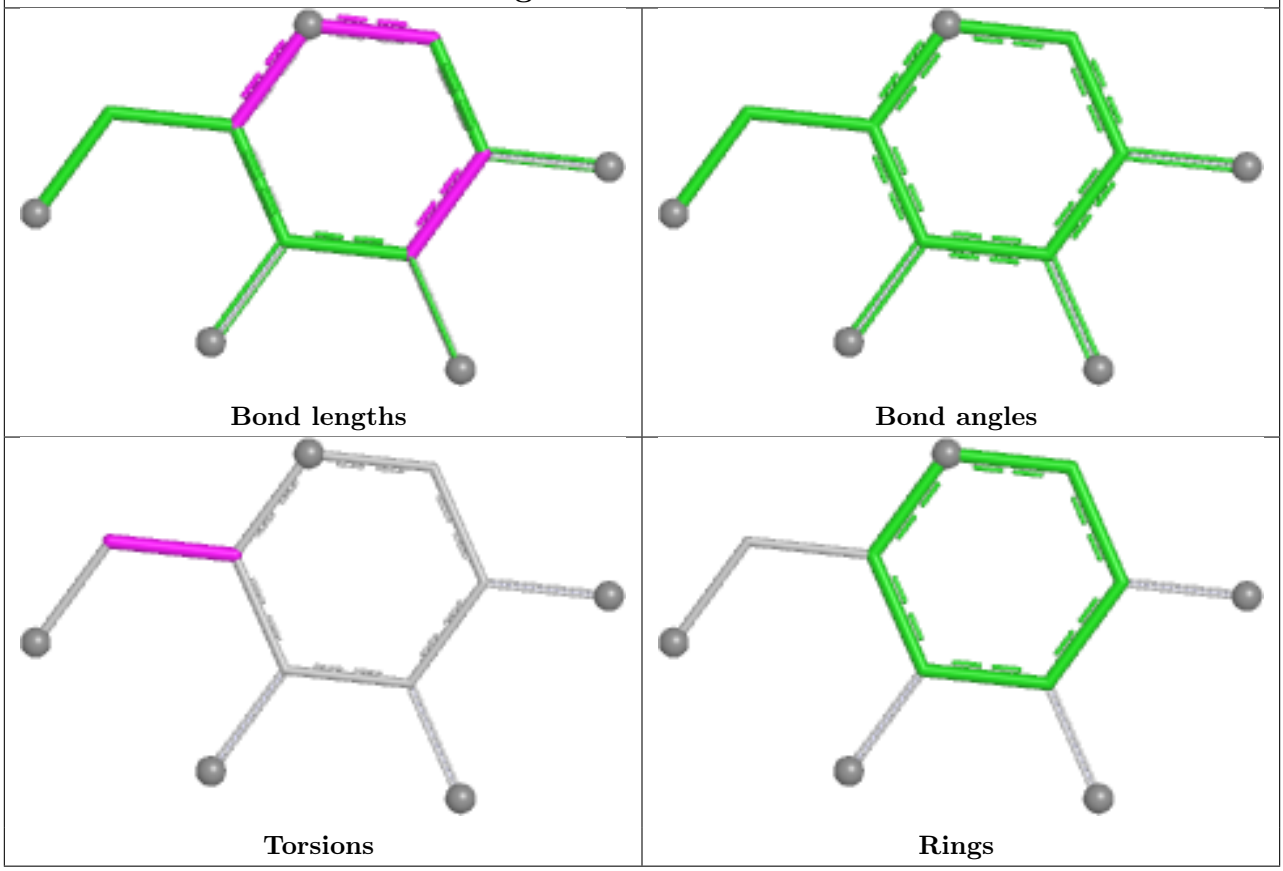
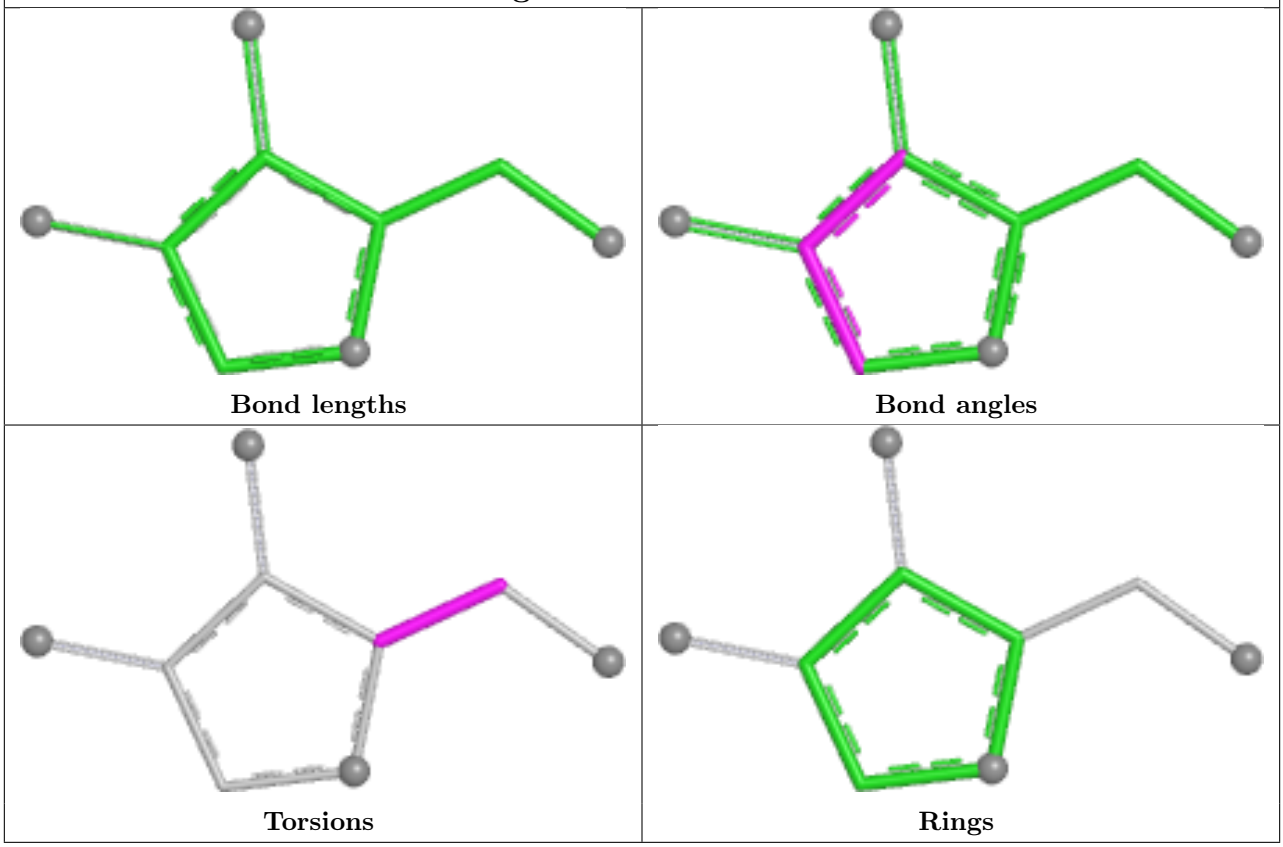
	
Torsions	**Rings**

Ligand GLA F 2012	
 Bond lengths	 Bond angles
 Torsions	 Rings

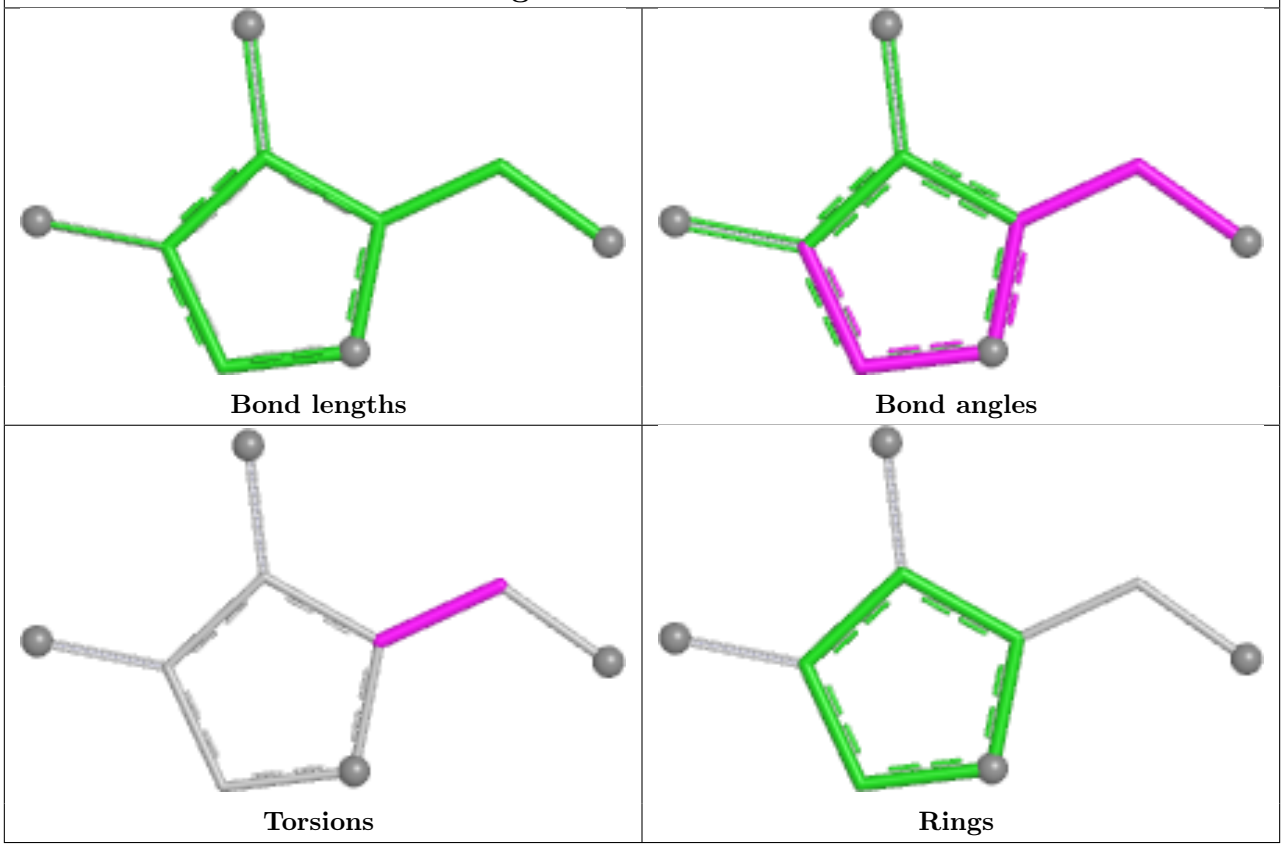
Ligand GLA C 2008



Ligand AHR B 2020



Ligand AHR D 2003



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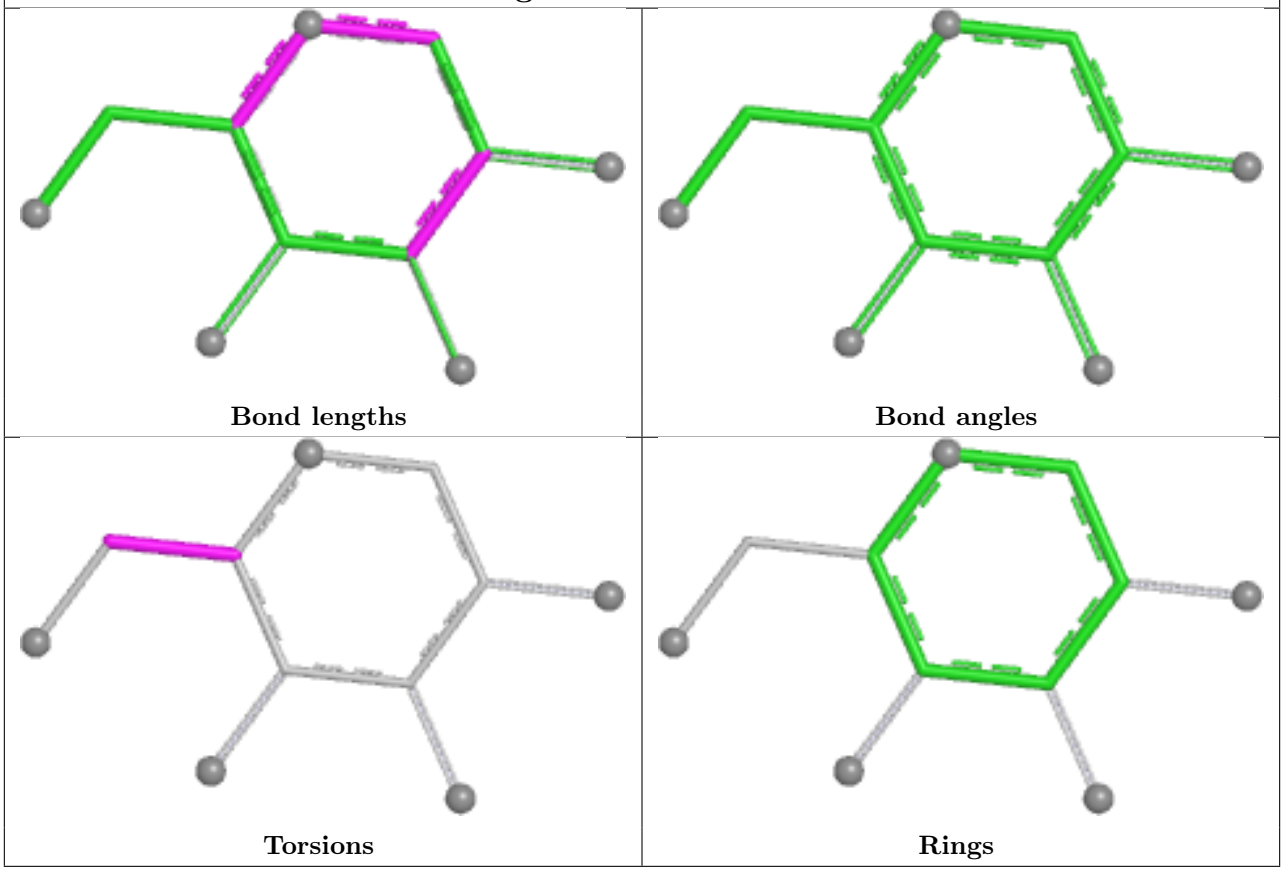

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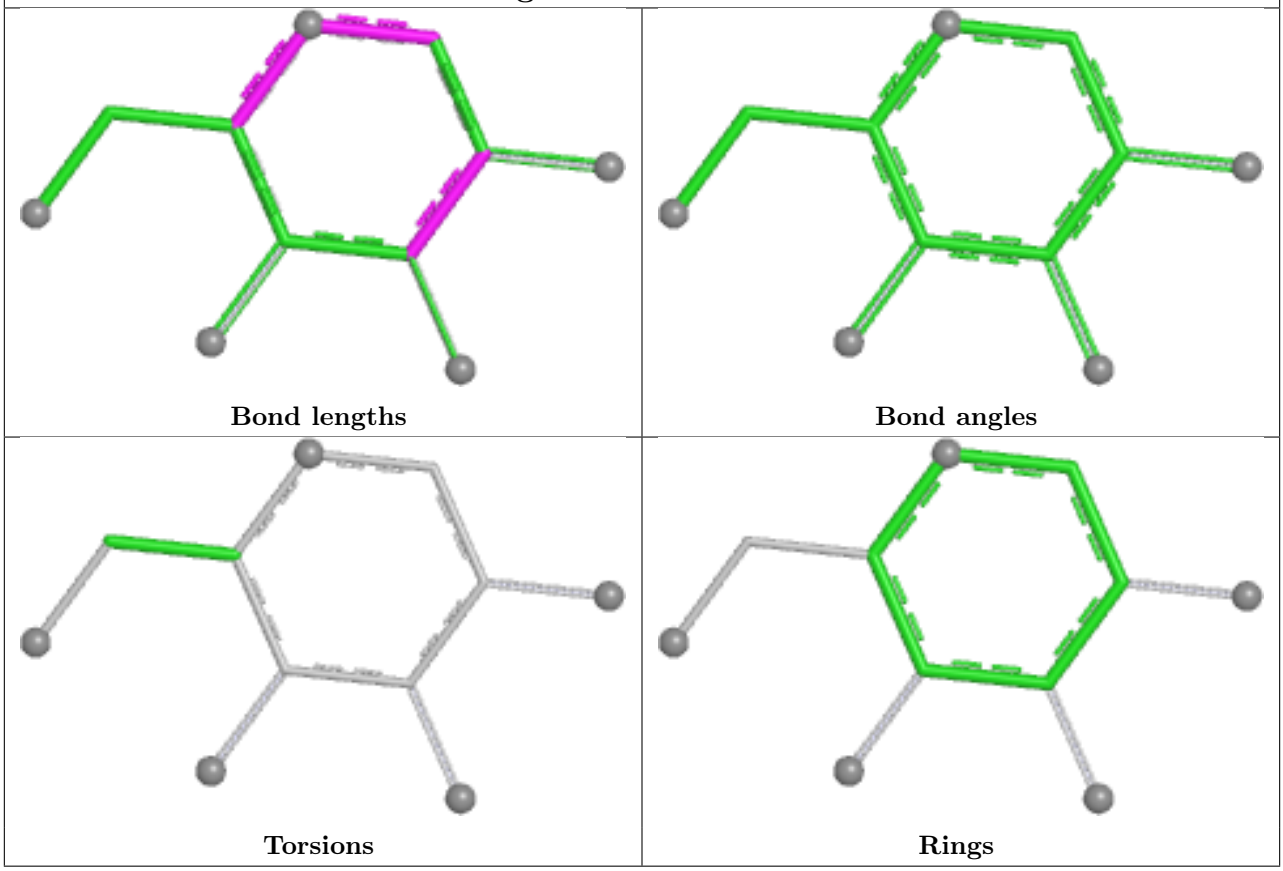

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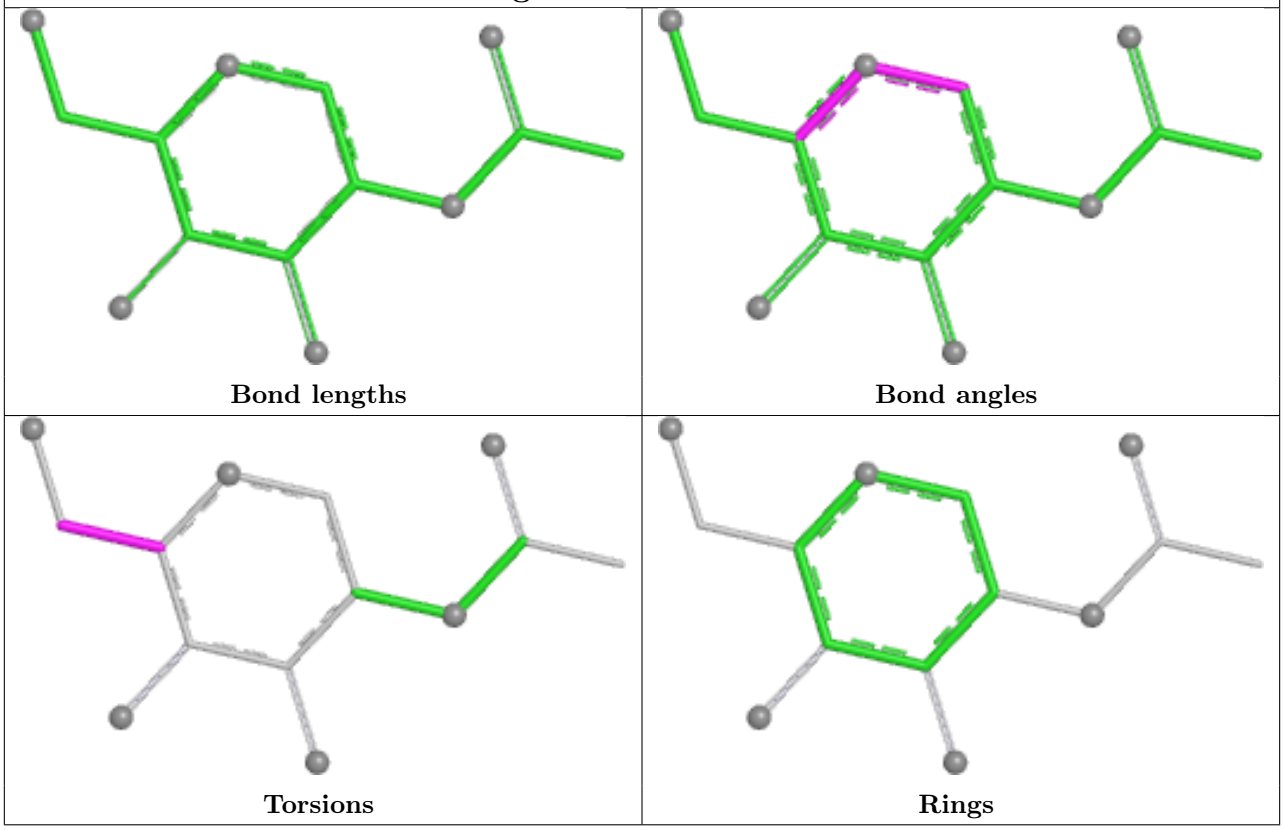
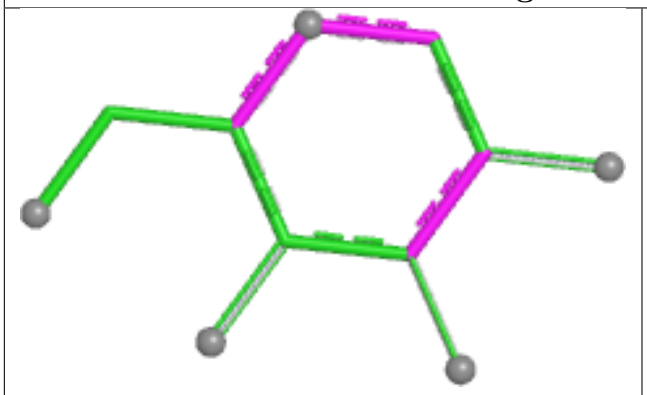
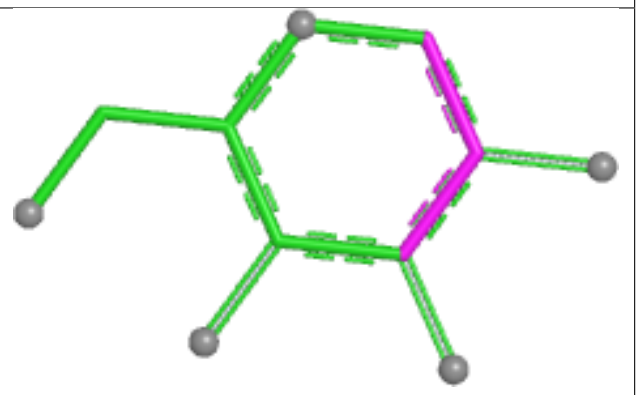


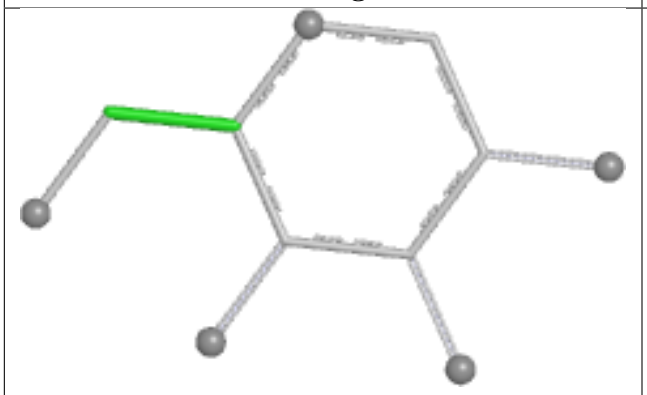
Ligand GLA E 2009



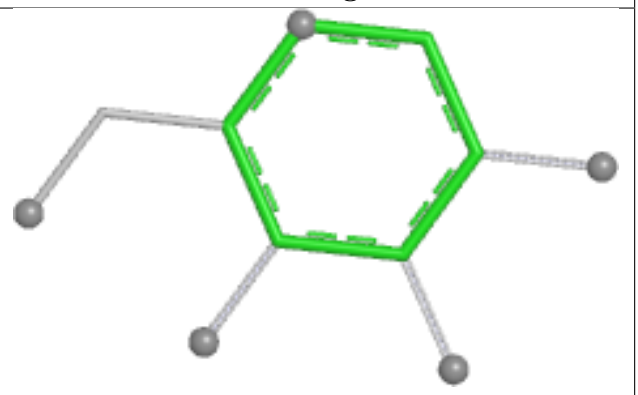
Bond lengths



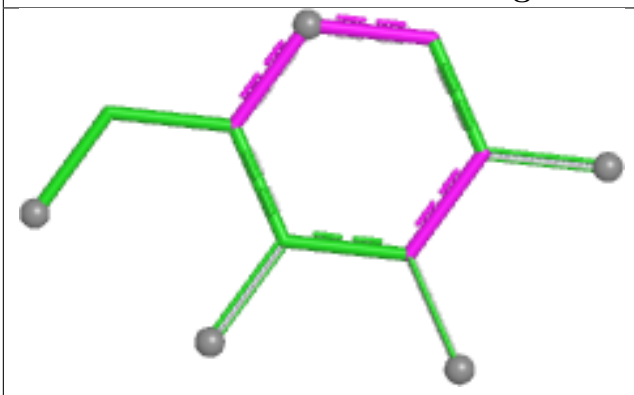
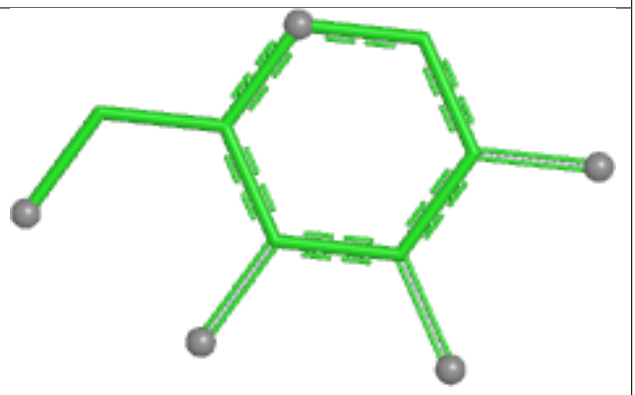
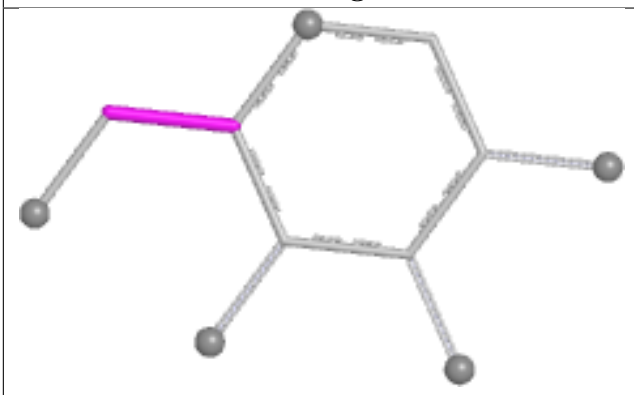
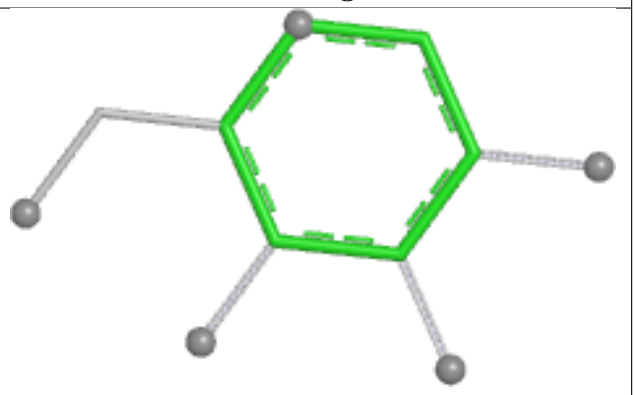
Bond angles



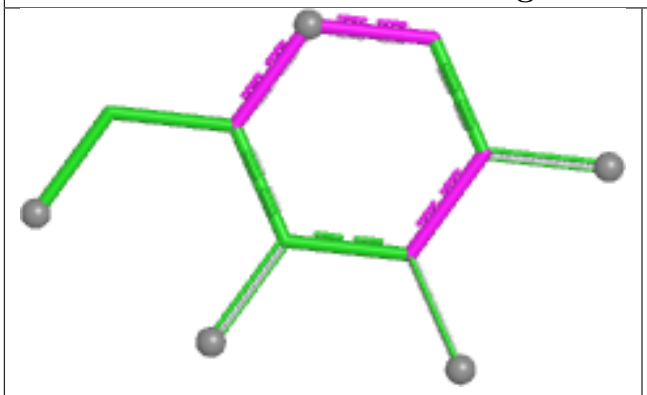
Torsions



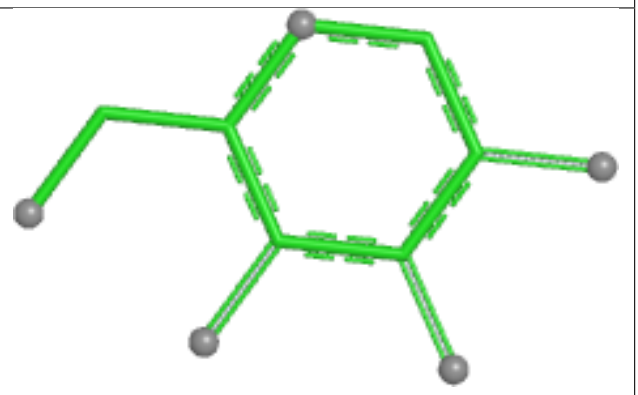
Rings

Ligand GLA D 2009	
 Bond lengths	 Bond angles
 Torsions	 Rings

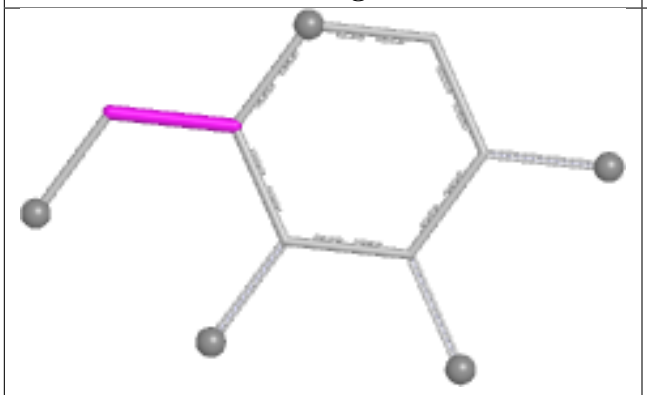
Ligand GLA F 2011



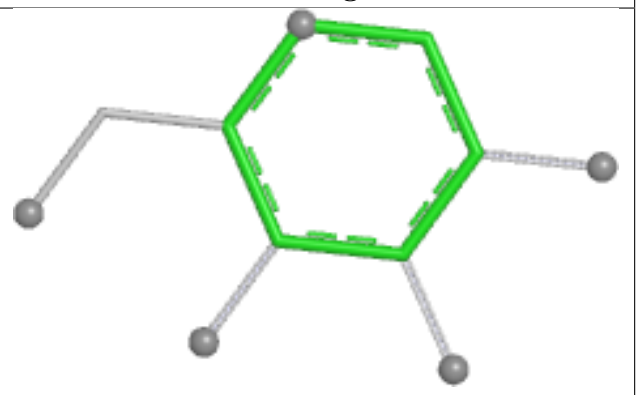
Bond lengths



Bond angles

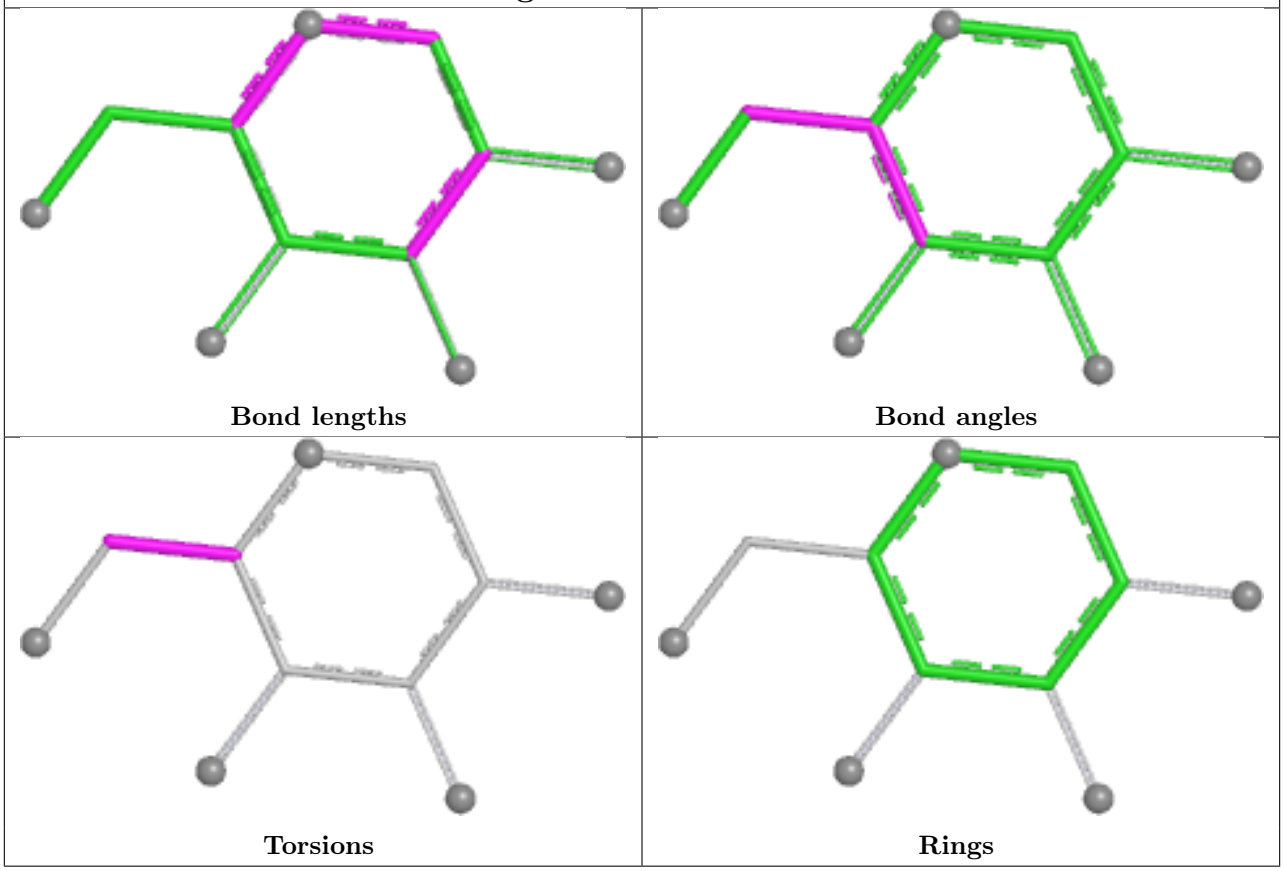


Torsions

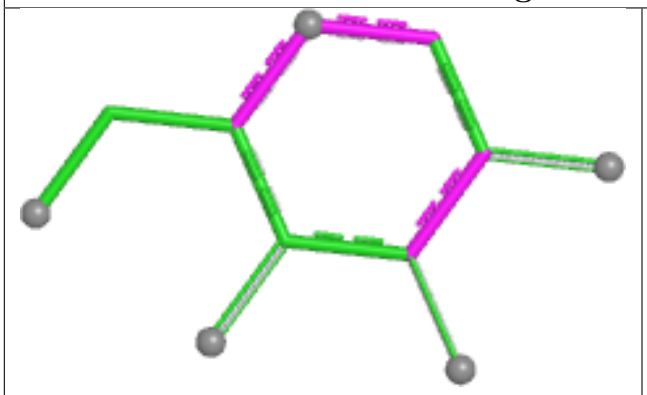


Rings

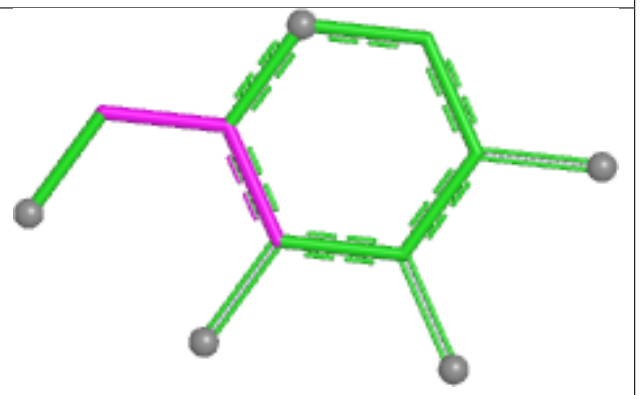
Ligand GLA F 2008



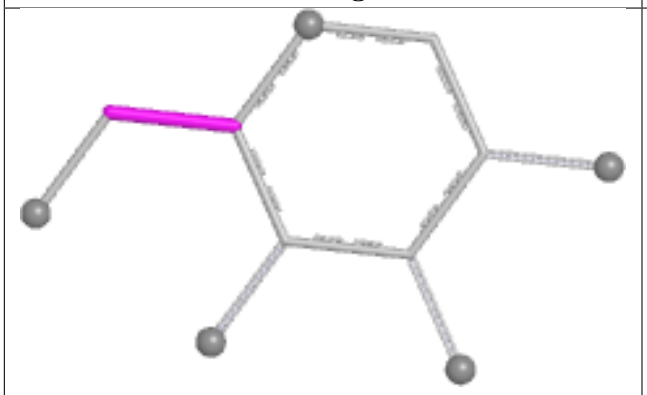
Ligand GLA A 2006



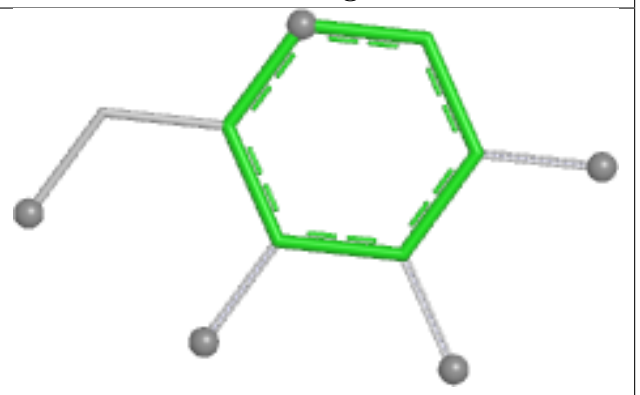
Bond lengths



Bond angles

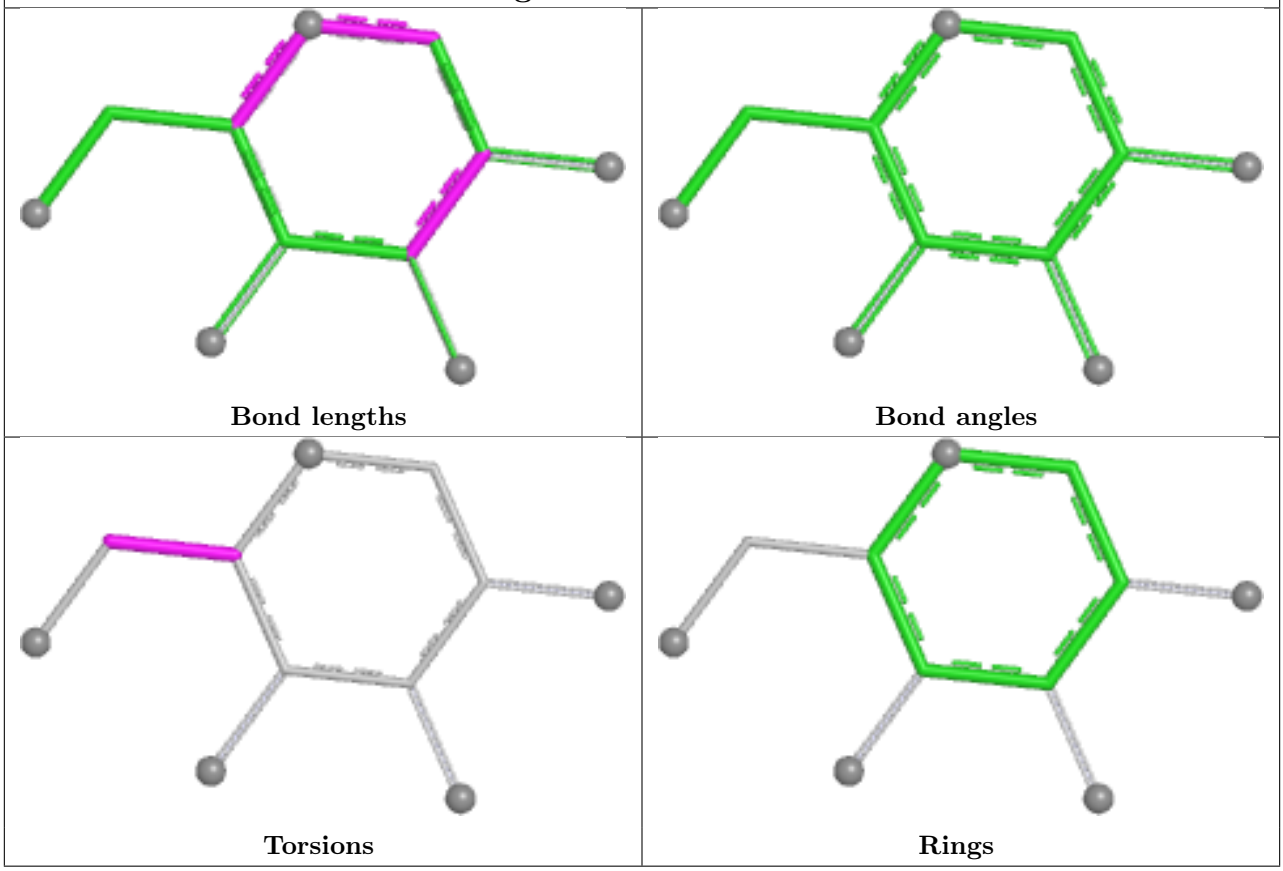


Torsions

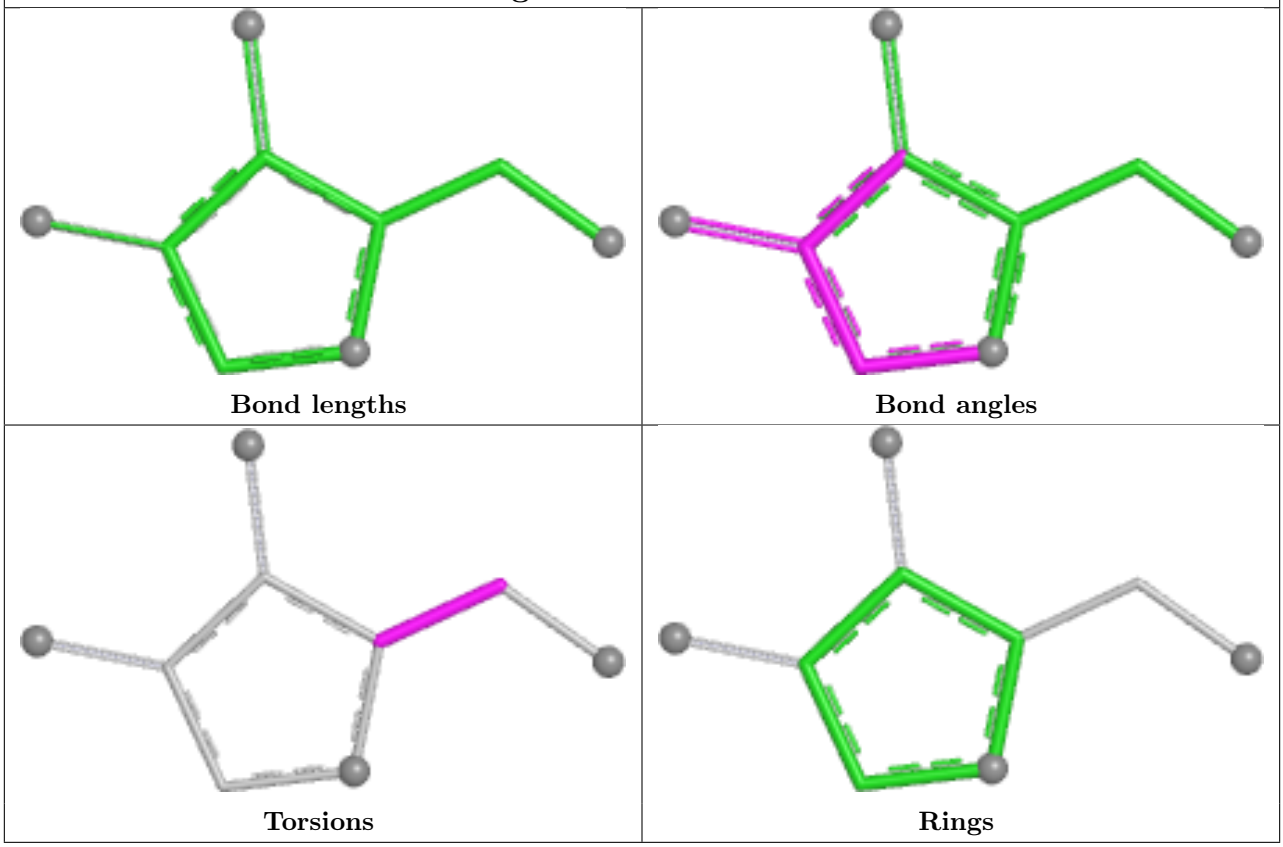


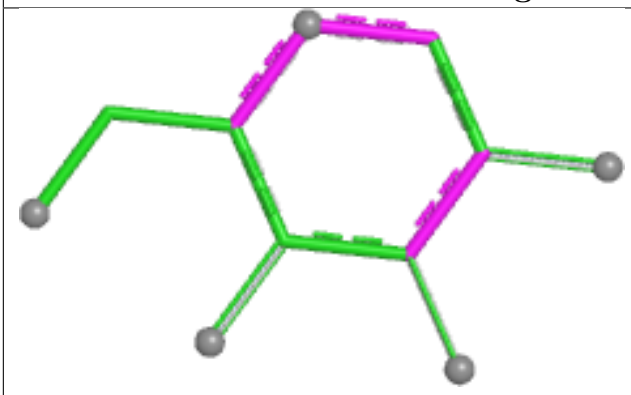
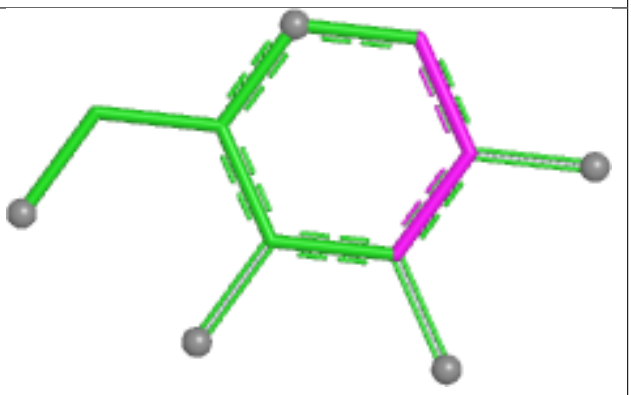
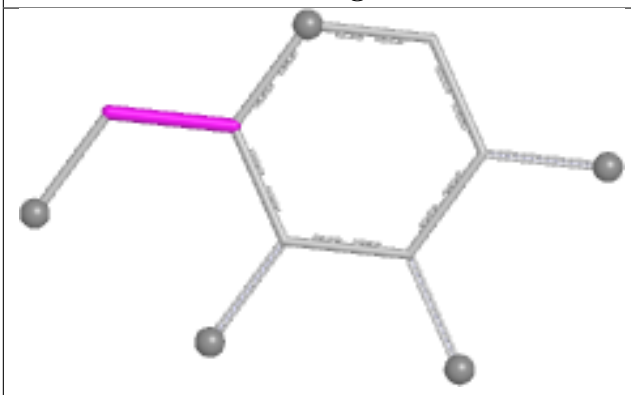
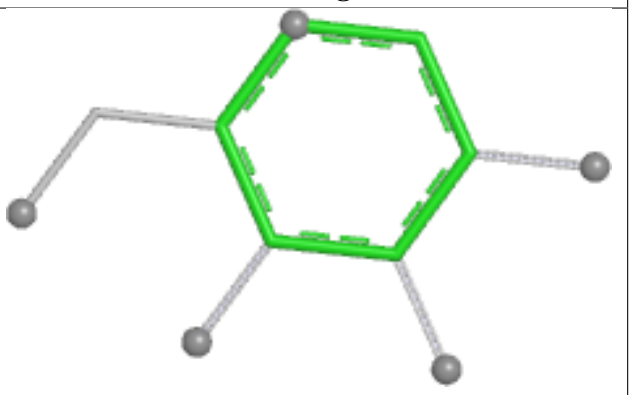
Rings

Ligand GLA D 2007

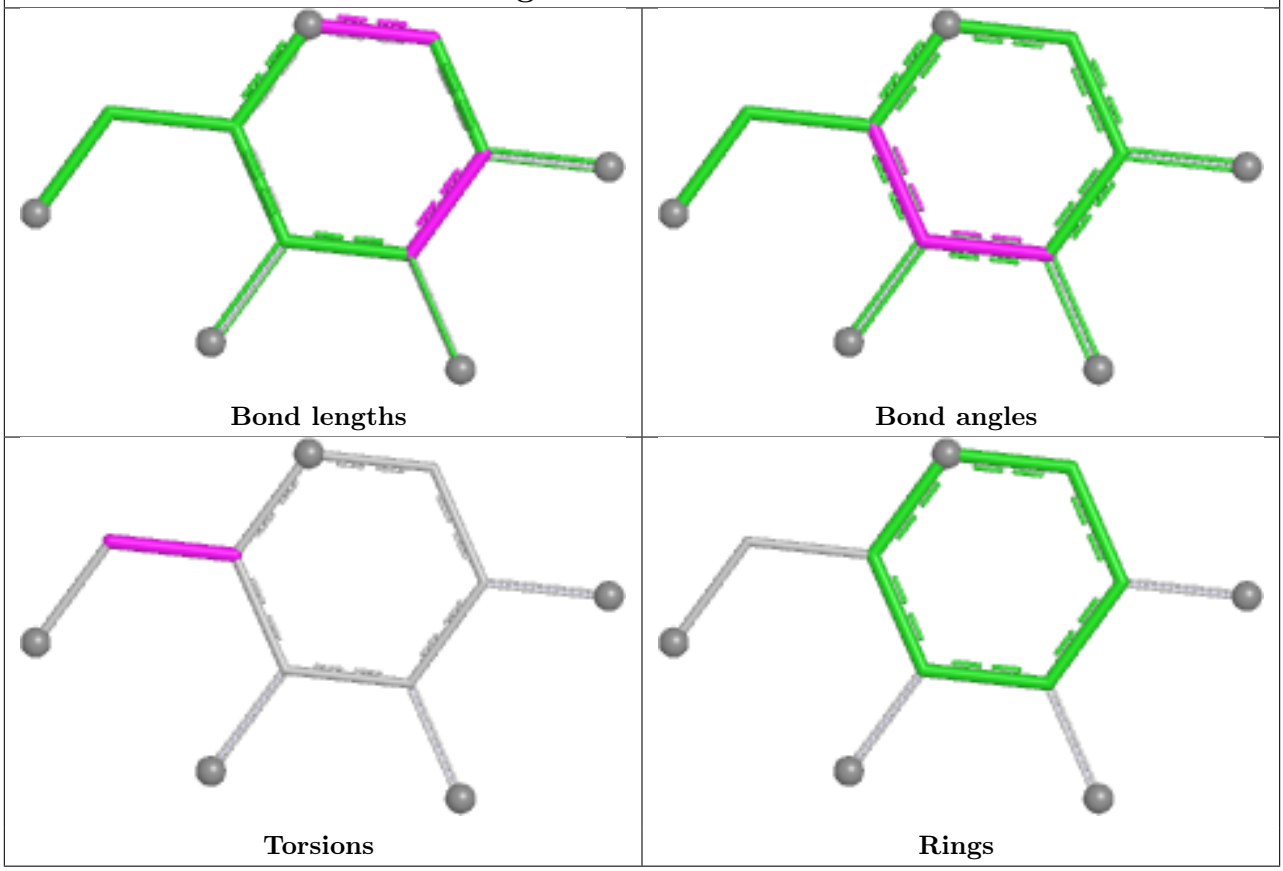


Ligand AHR D 2004

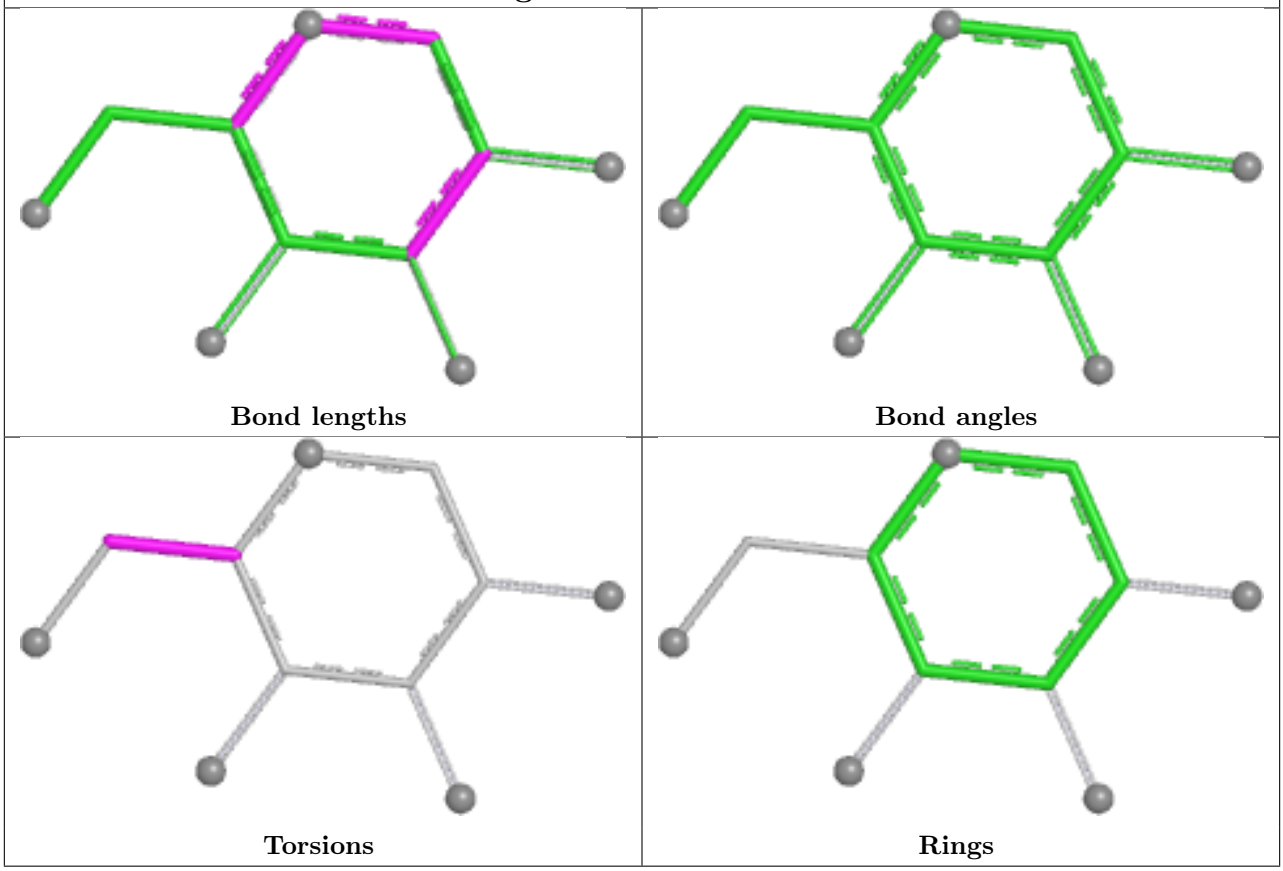


Ligand GLA B 2009	
 Bond lengths	 Bond angles
 Torsions	 Rings

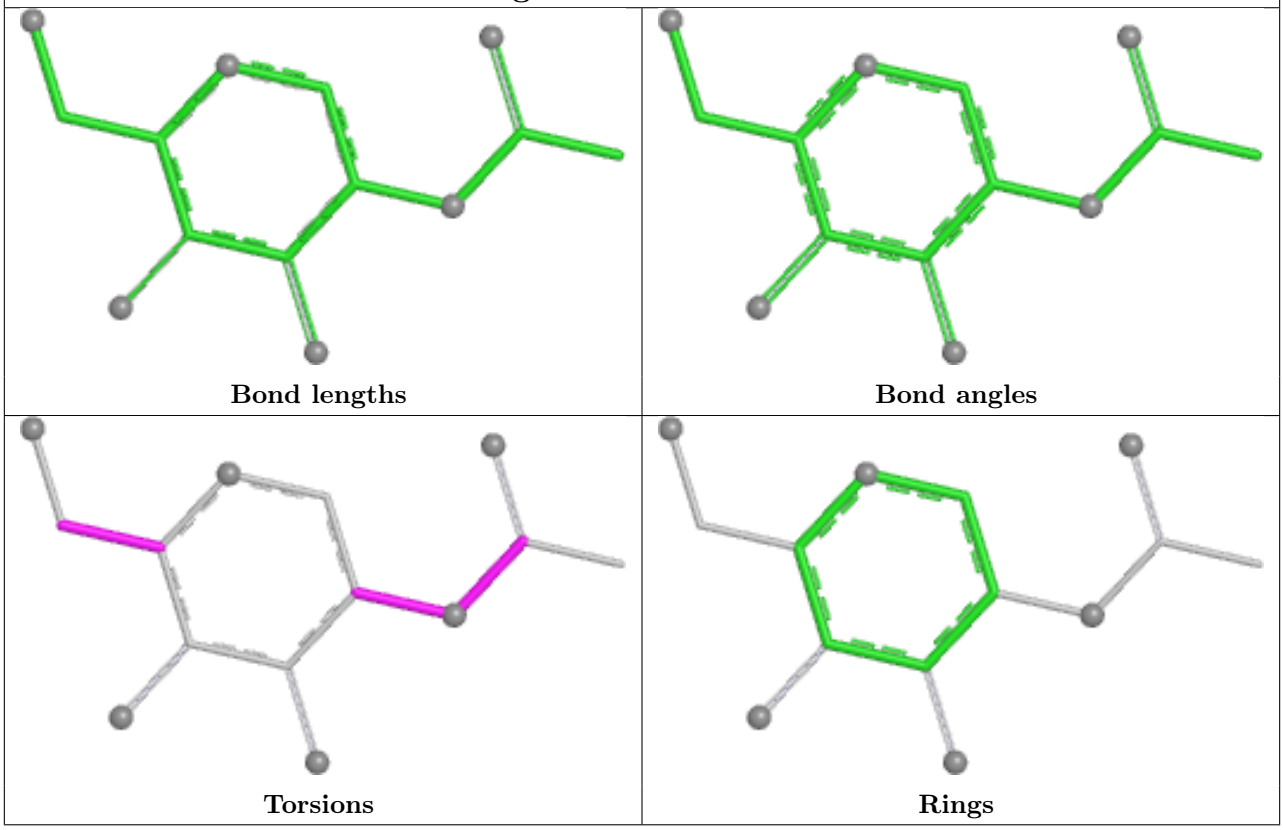
Ligand GLA F 2009



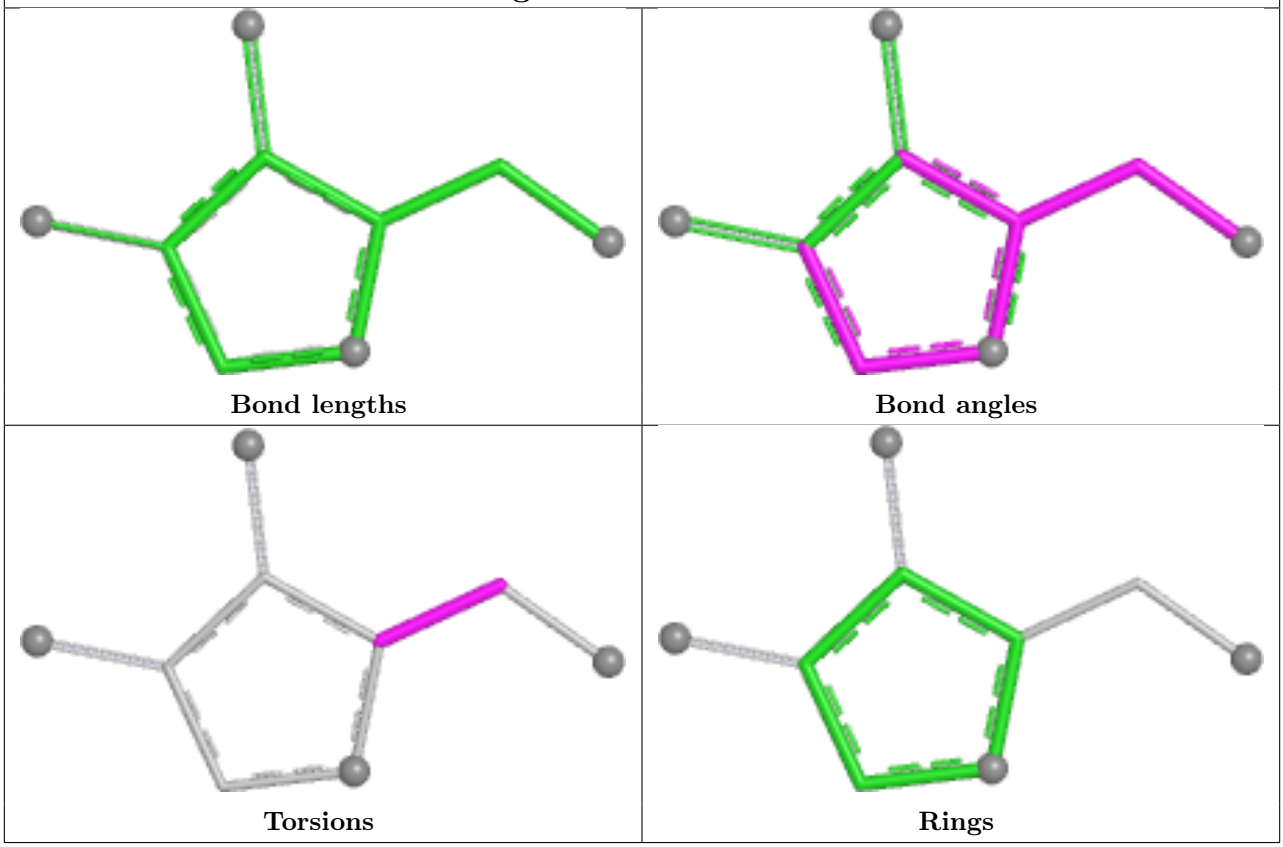
Ligand GLA C 2004



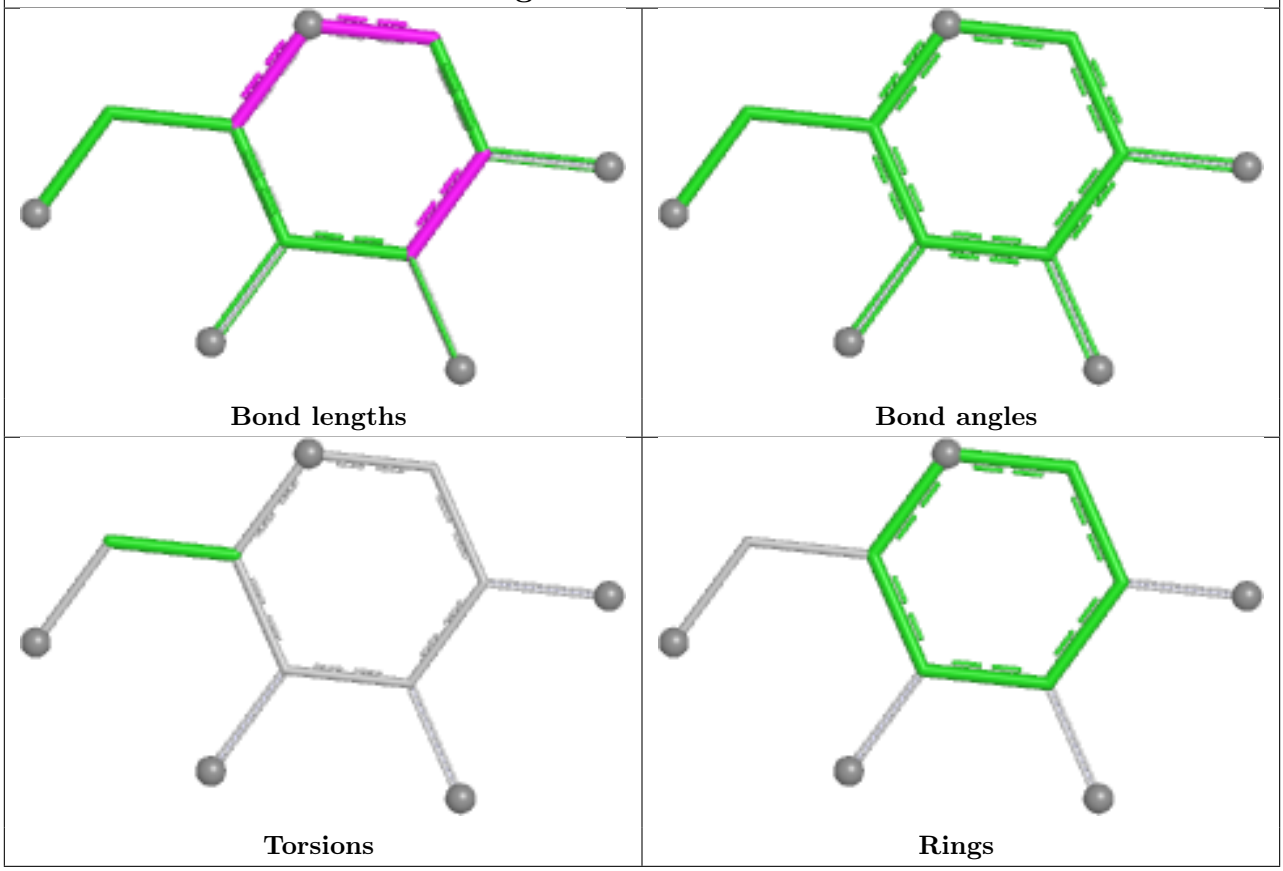
Ligand NAG B 2018

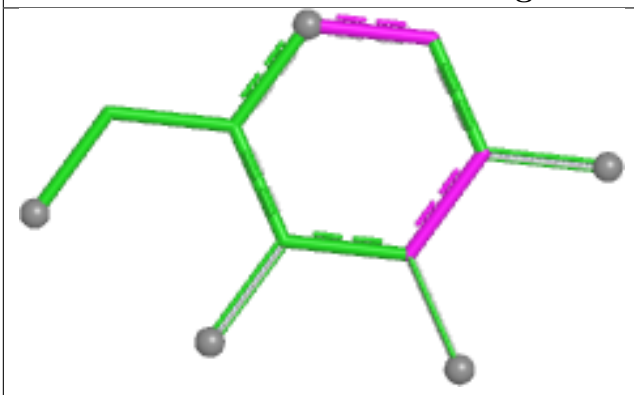
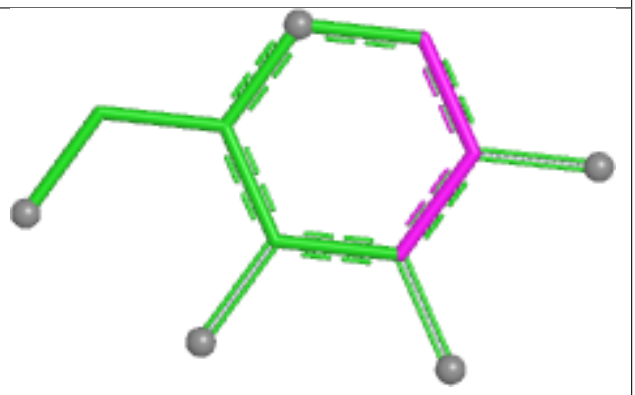
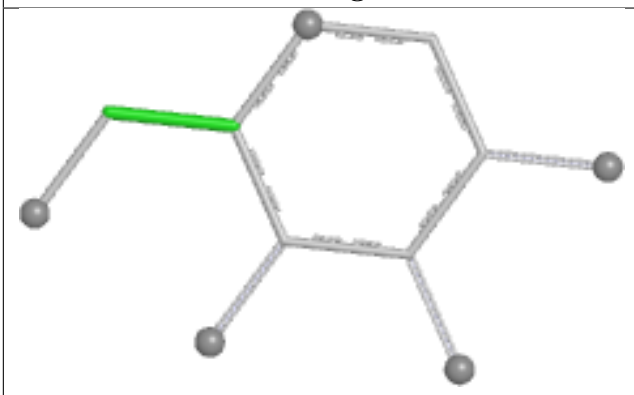
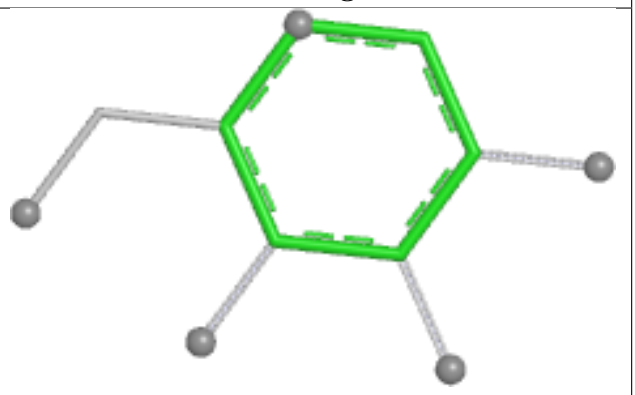


Ligand AHR B 2004

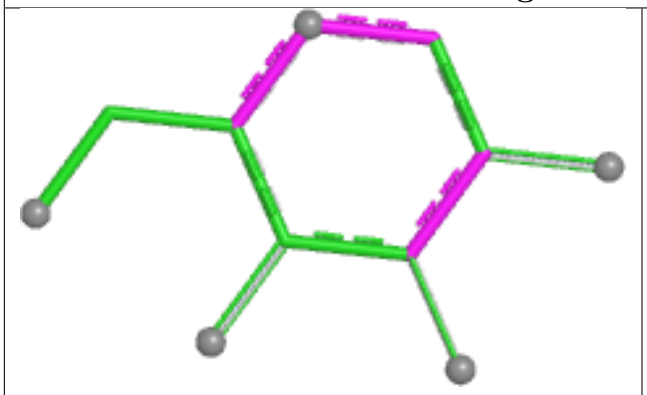


Ligand GLA B 2006

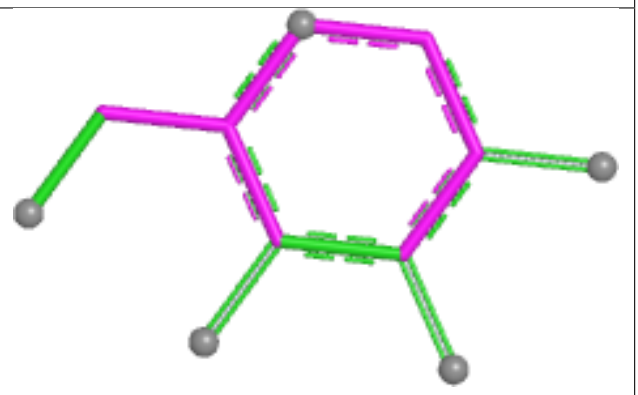


Ligand GLA E 2015	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

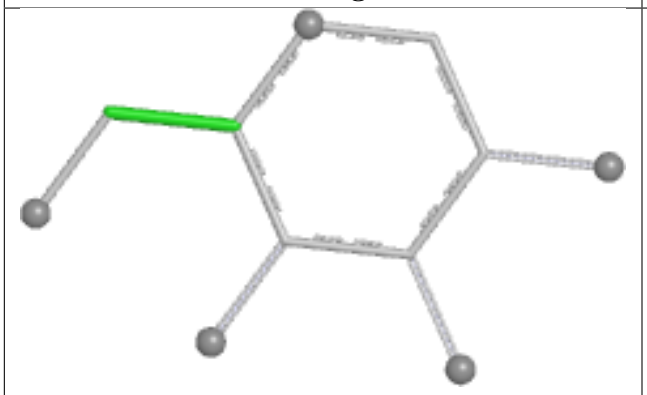
Ligand GLA F 2006



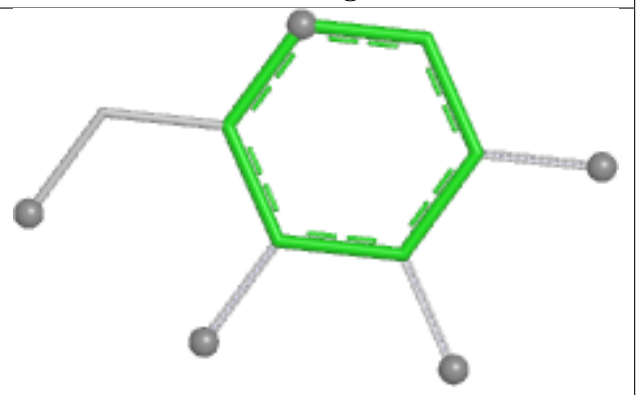
Bond lengths



Bond angles

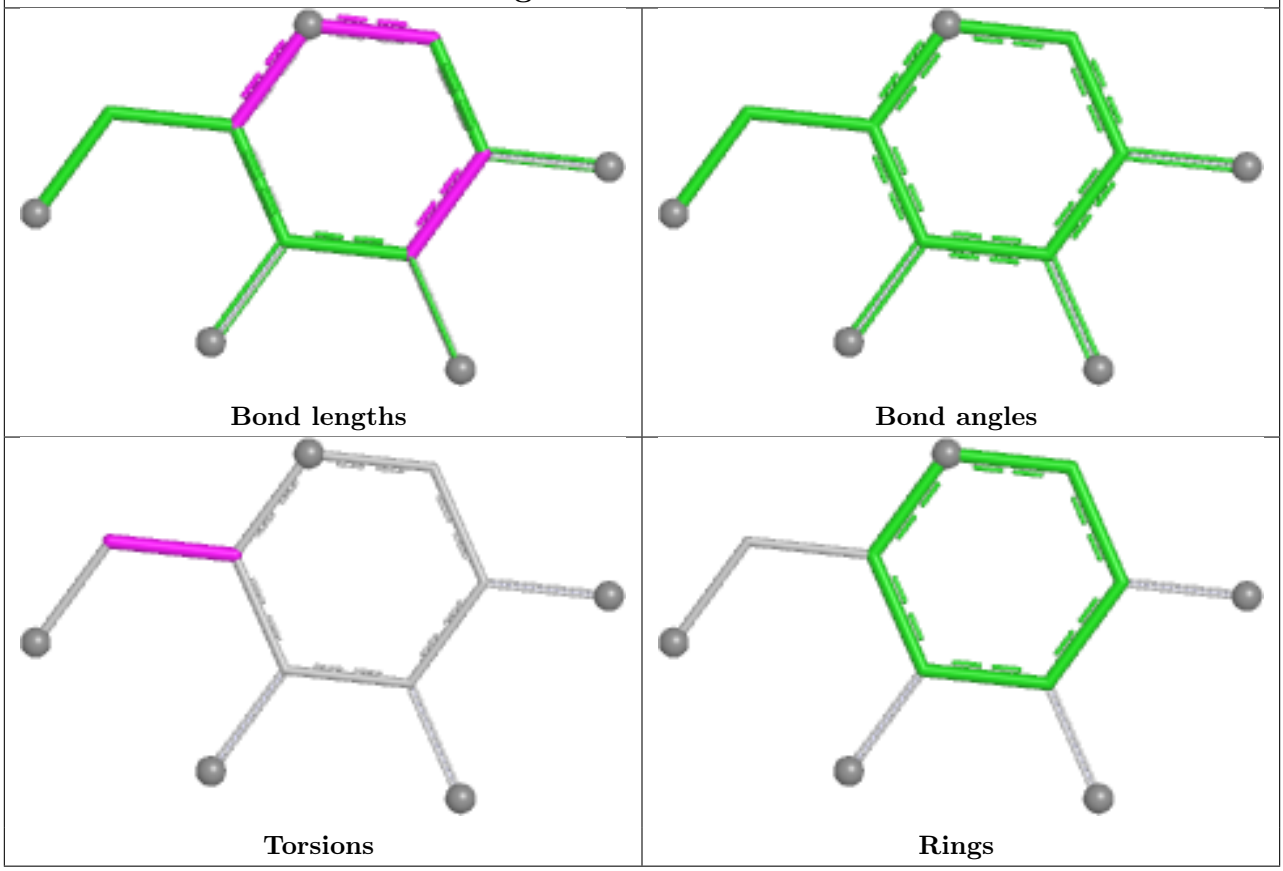


Torsions



Rings

Ligand GLA A 2012



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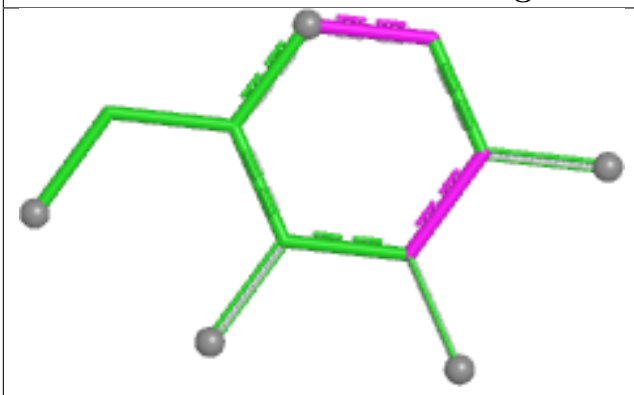
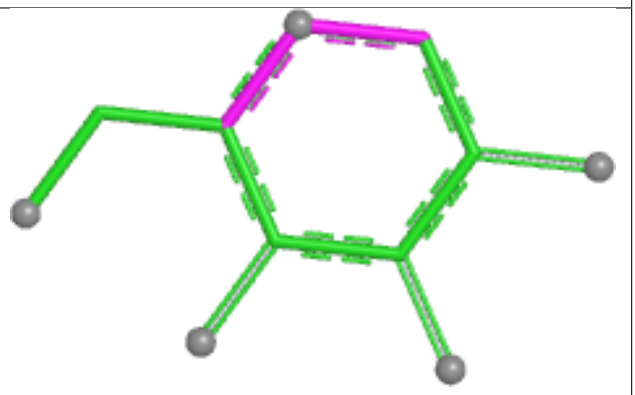
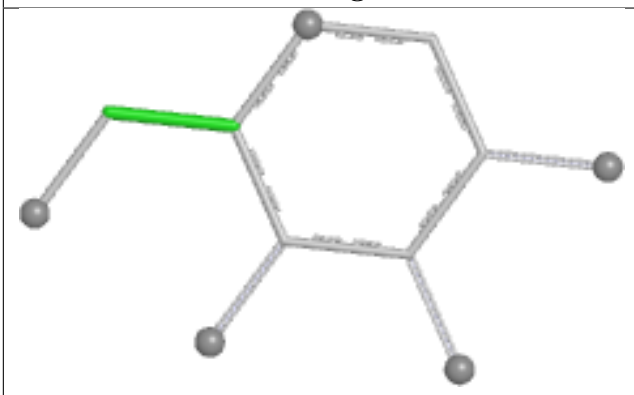
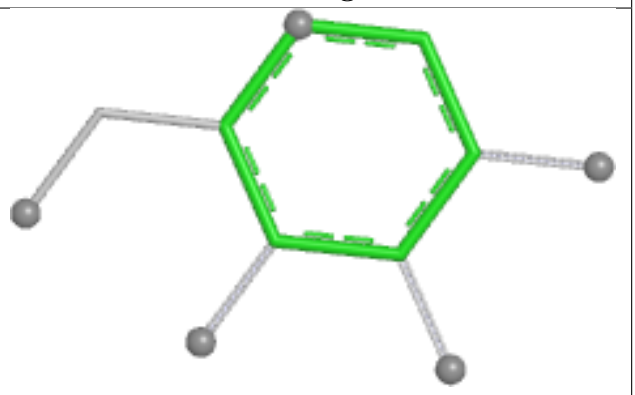
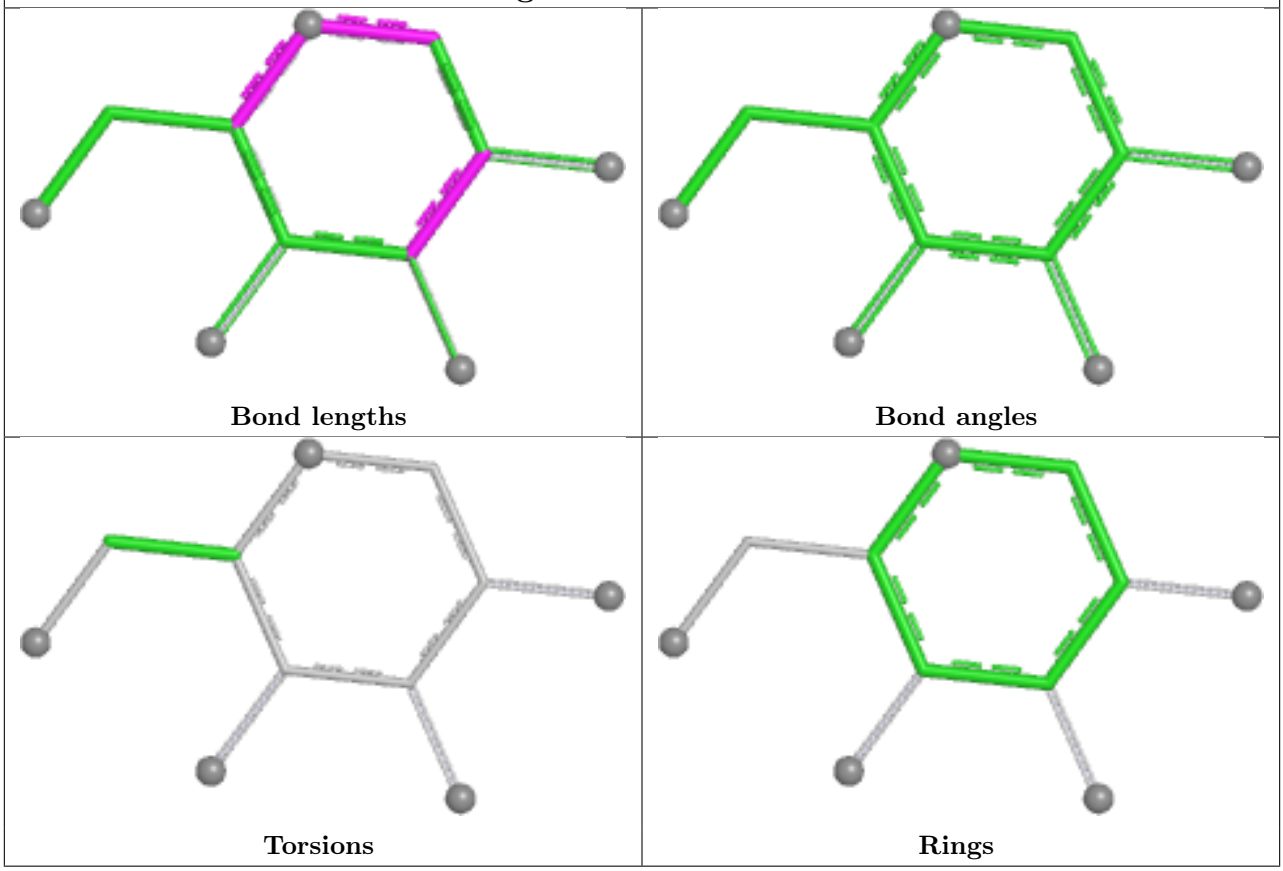
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA F 2015



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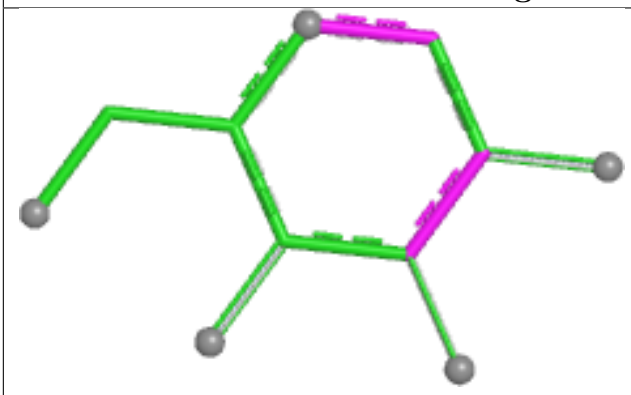
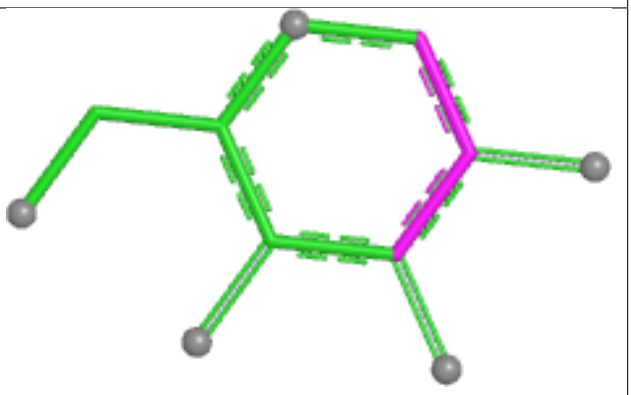
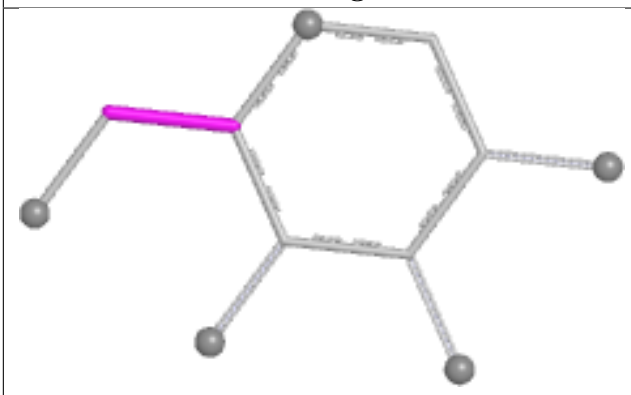
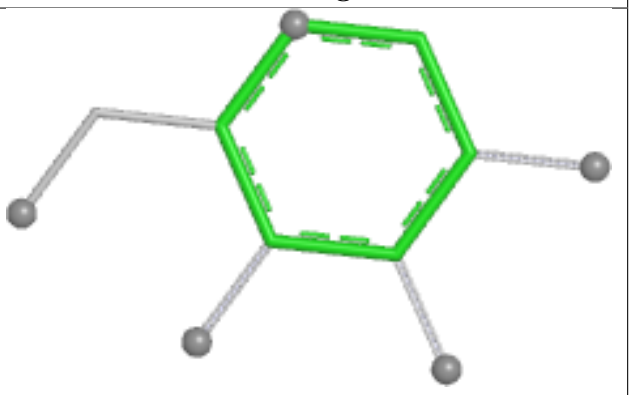
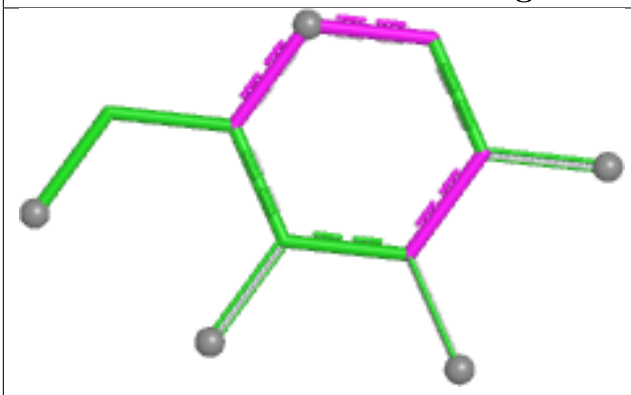
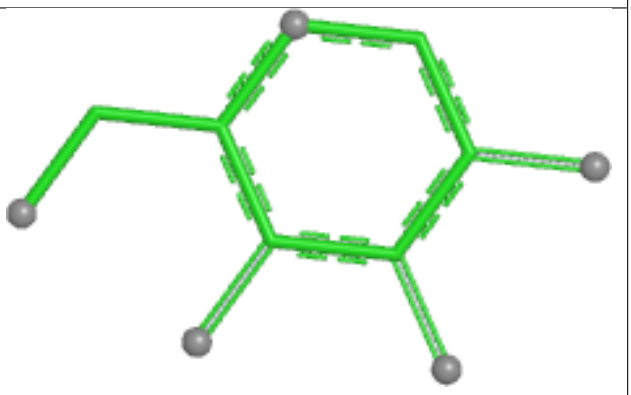
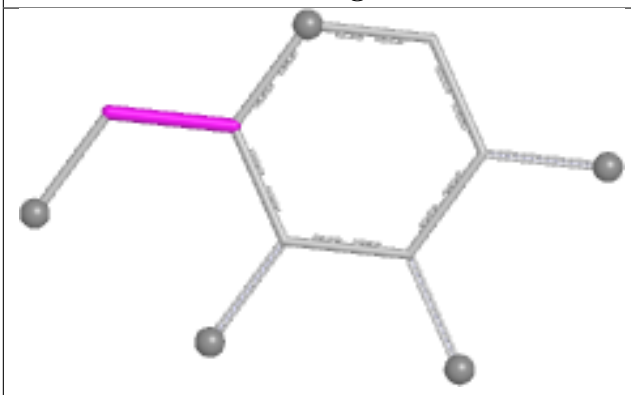
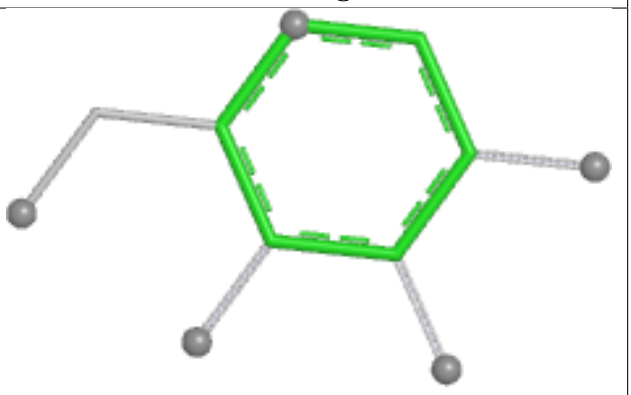
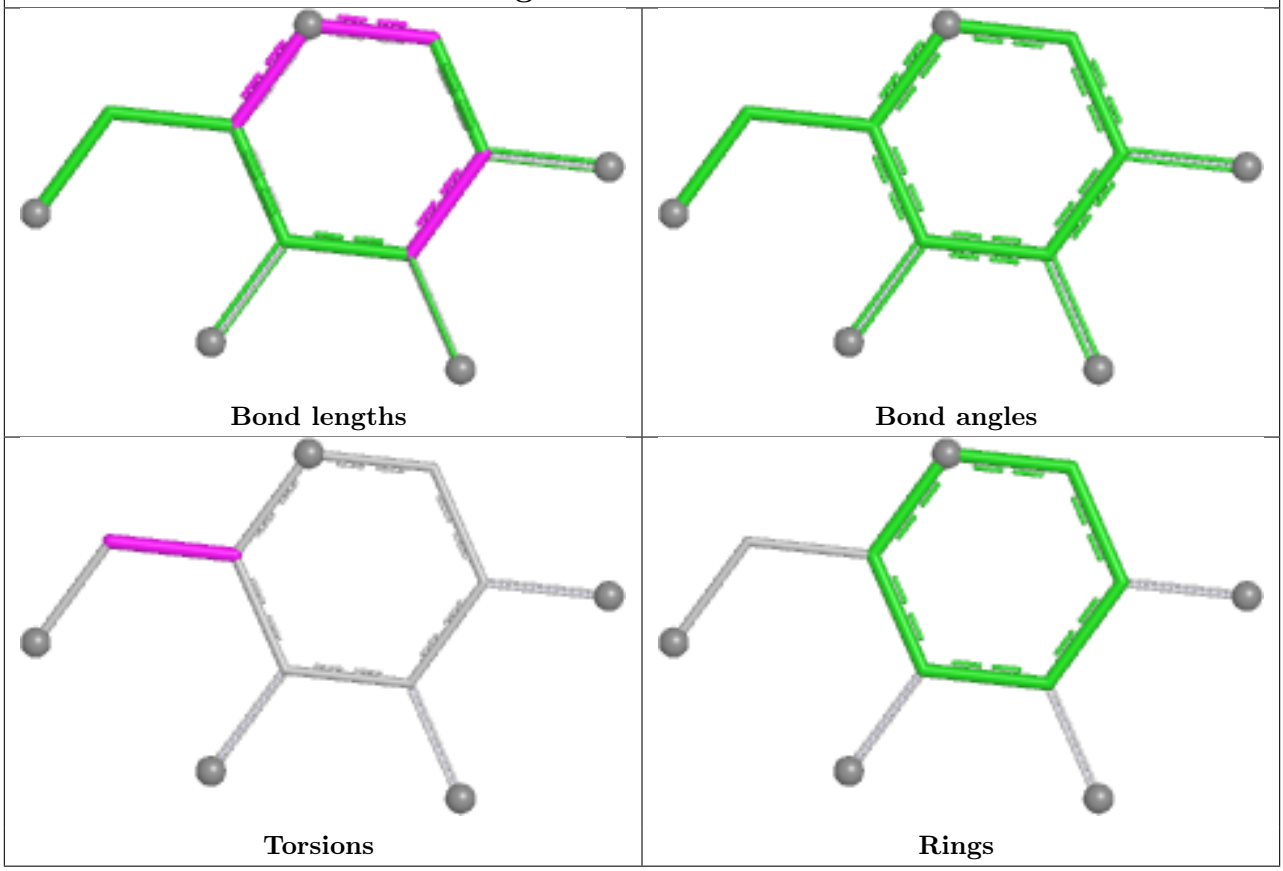
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand GLA E 2005	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA B 2016



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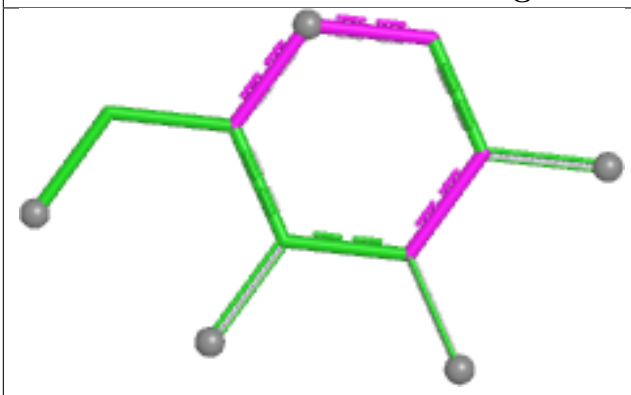	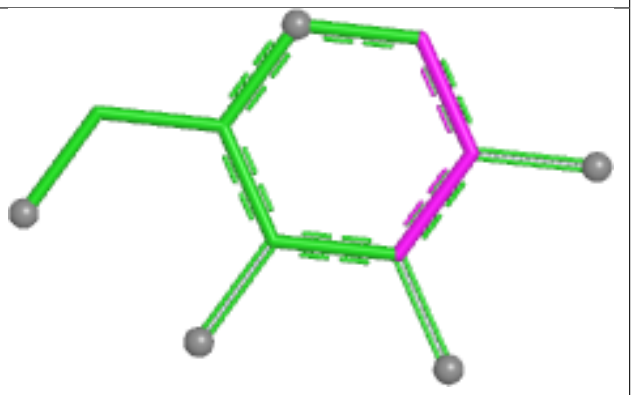
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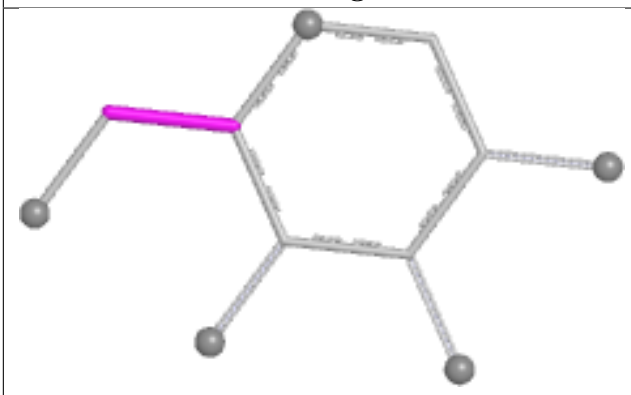	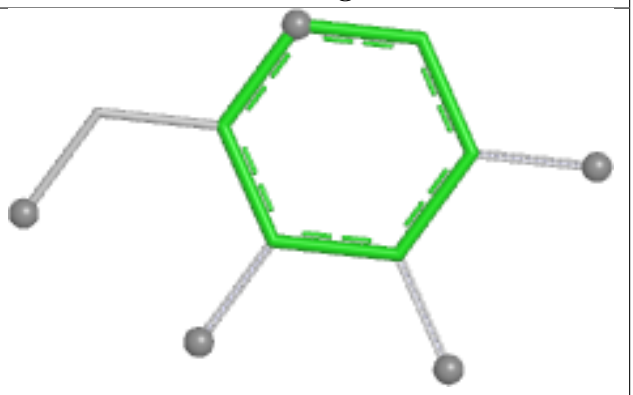
Torsions	**Rings**

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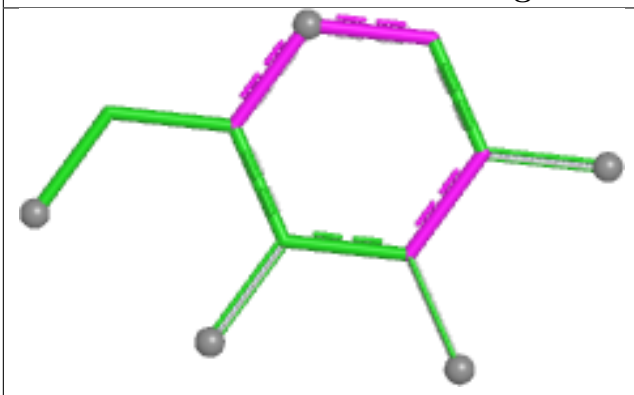	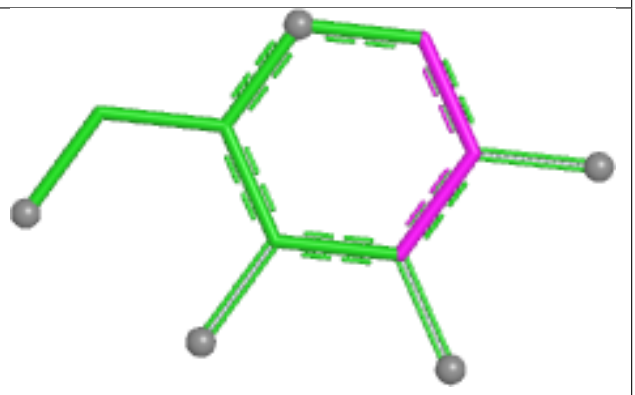
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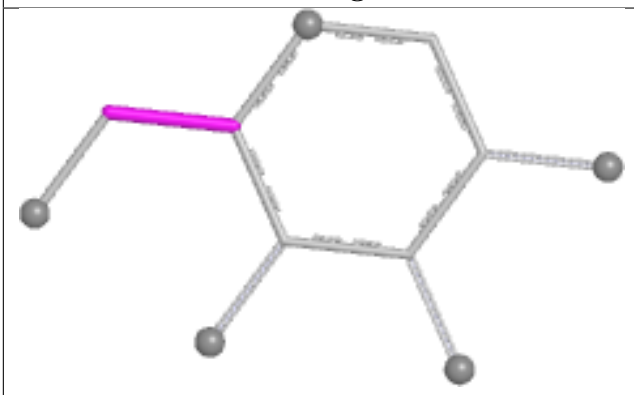	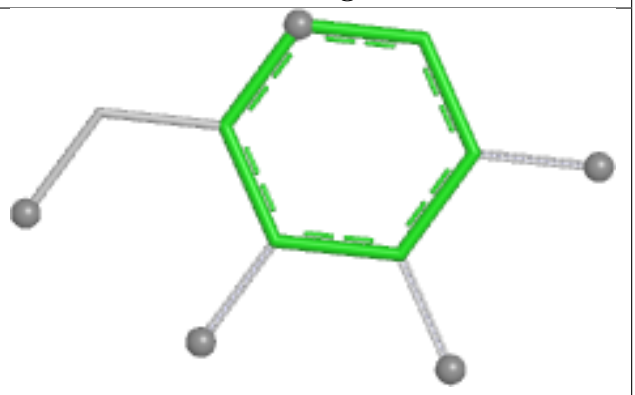
Torsions	**Rings**

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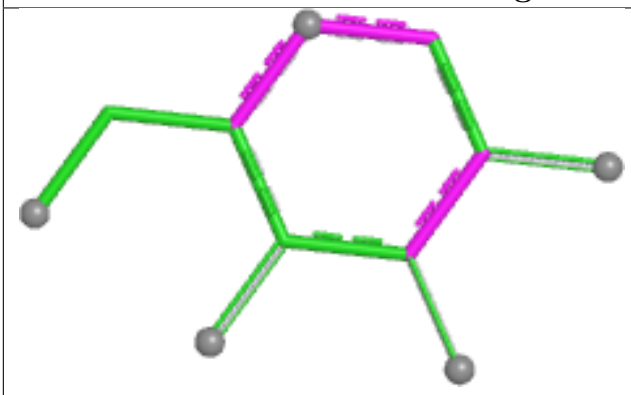
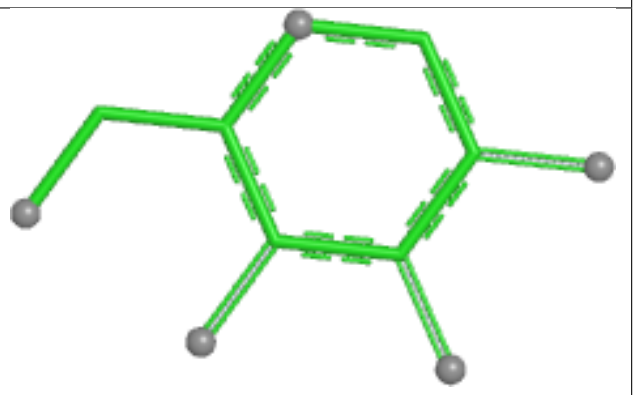
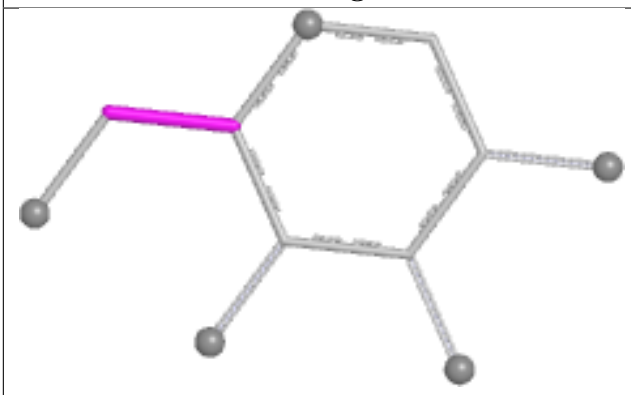
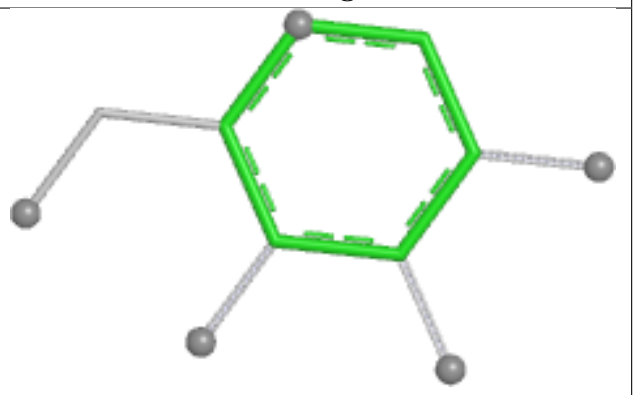
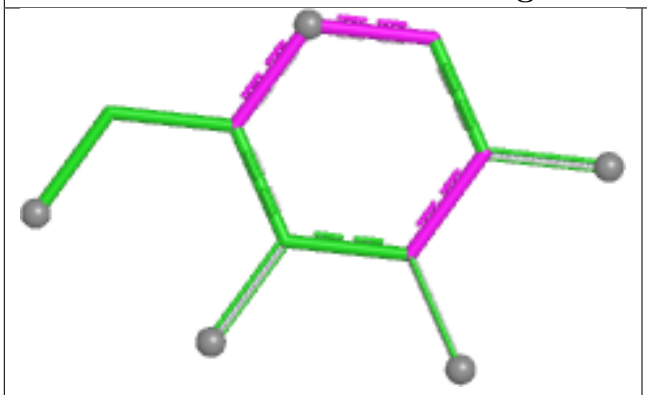
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA F 2010



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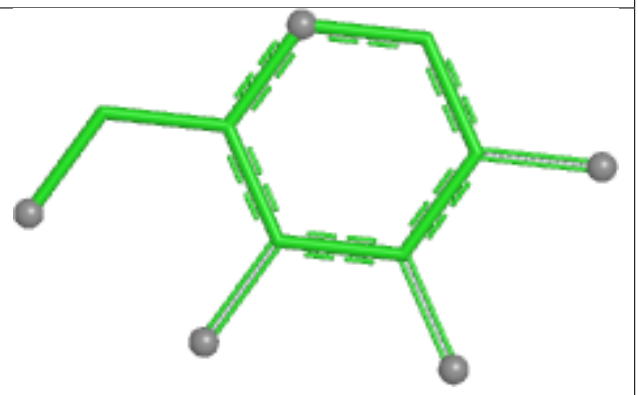

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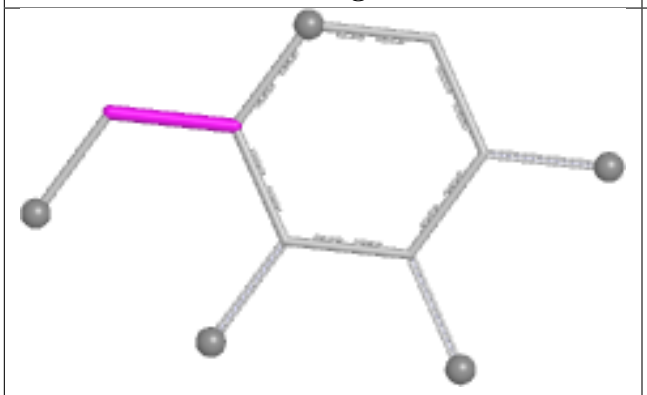
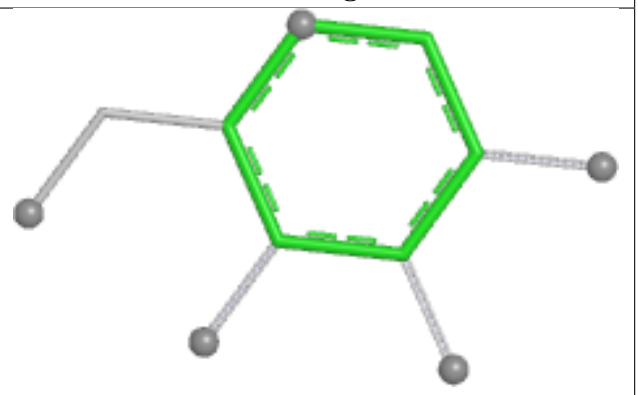
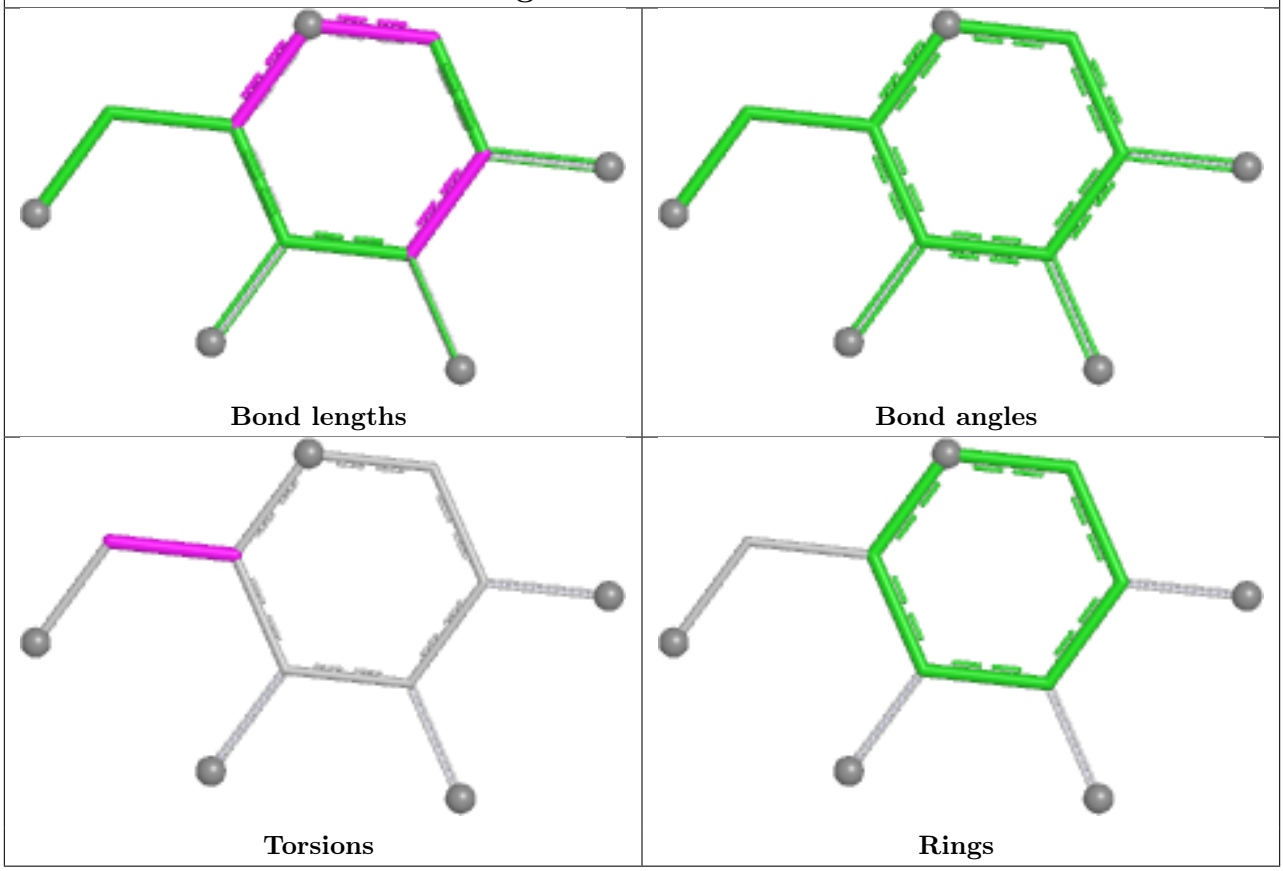


Torsions

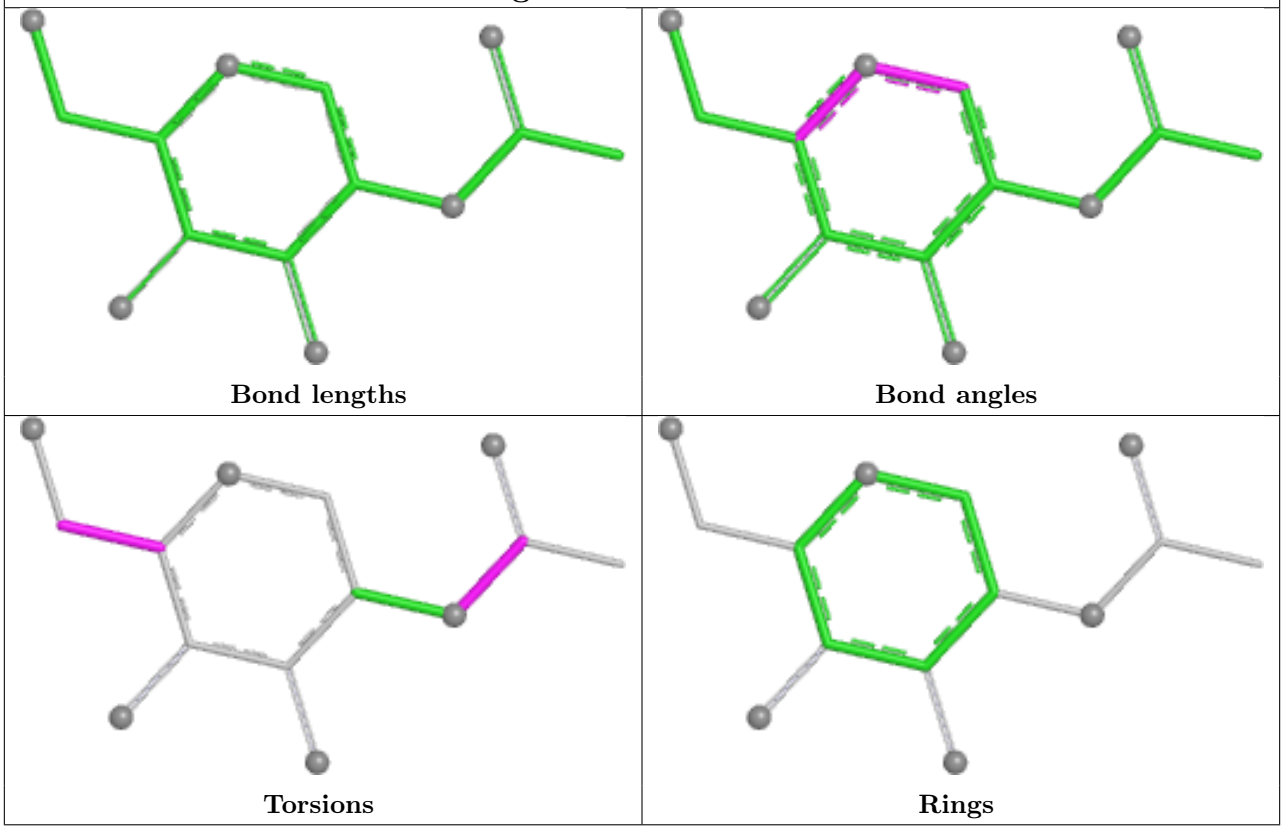


Rings

Ligand GLA E 2011



Ligand NAG C 2010



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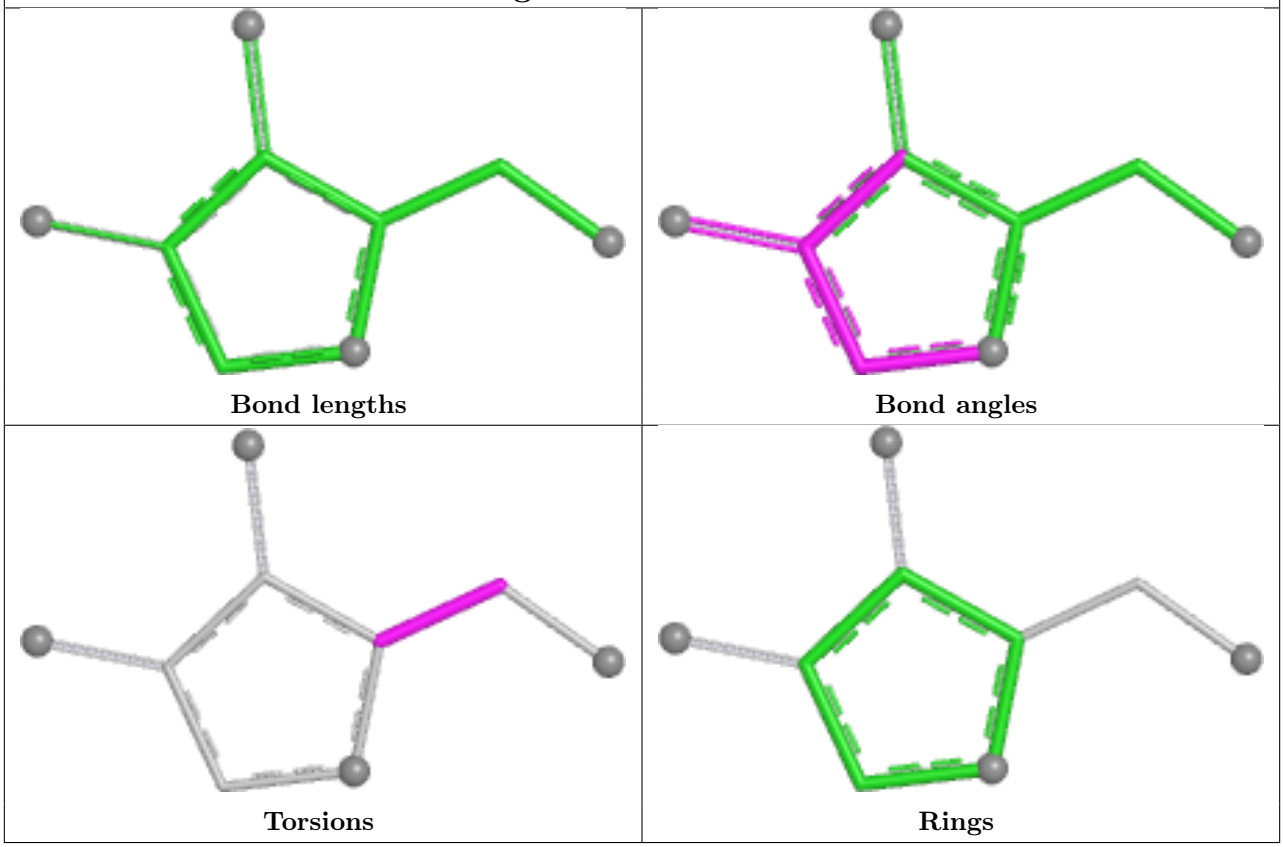
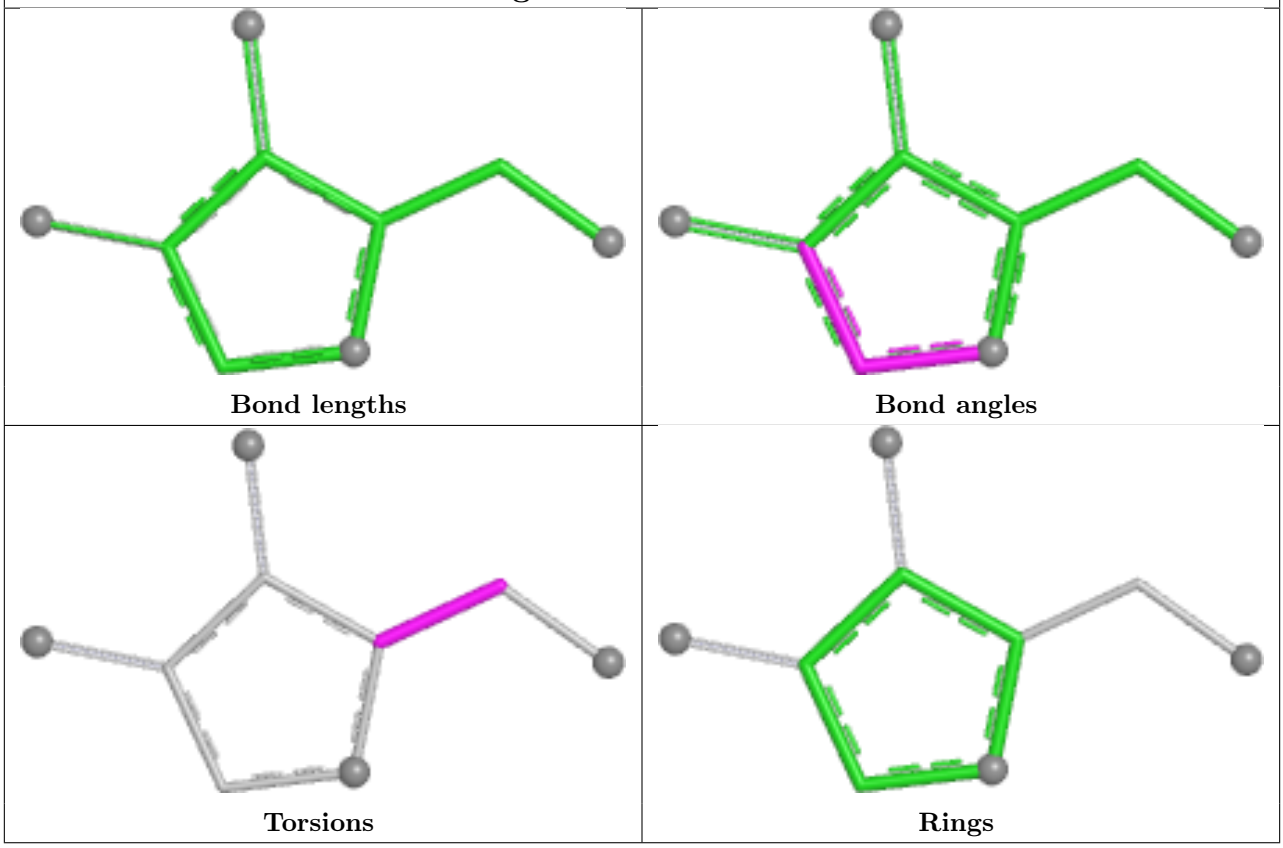
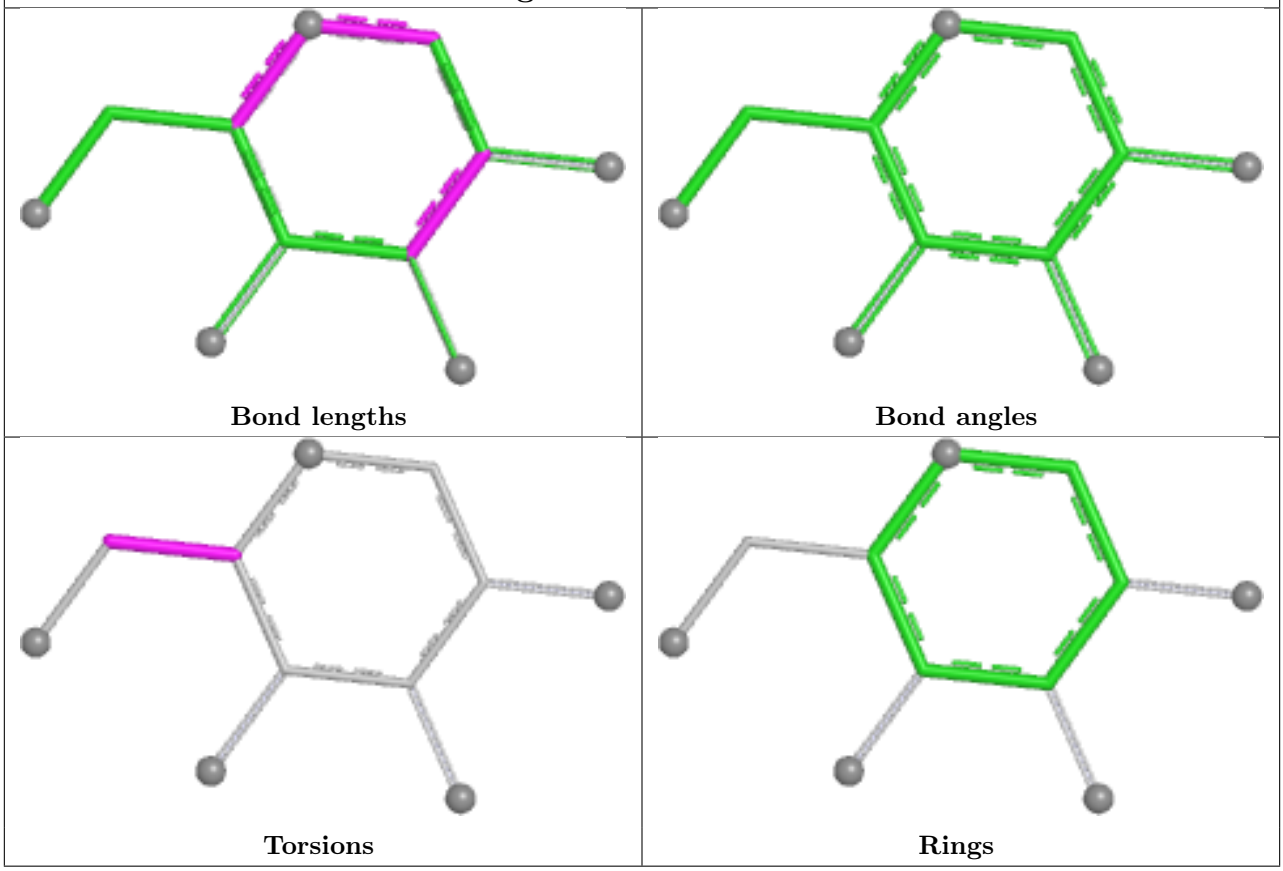


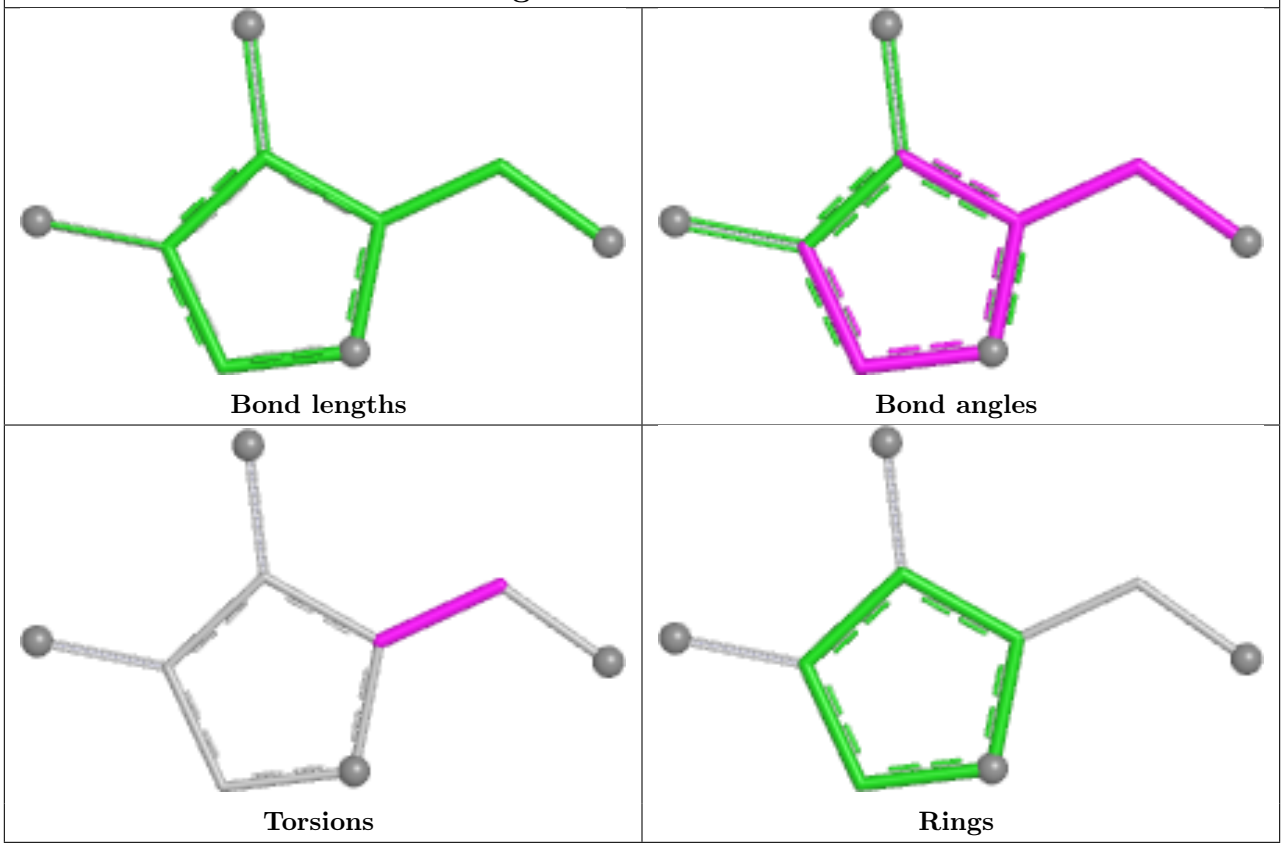
Ligand AHR C 2001



Ligand GLA F 2007



Ligand AHR B 2003



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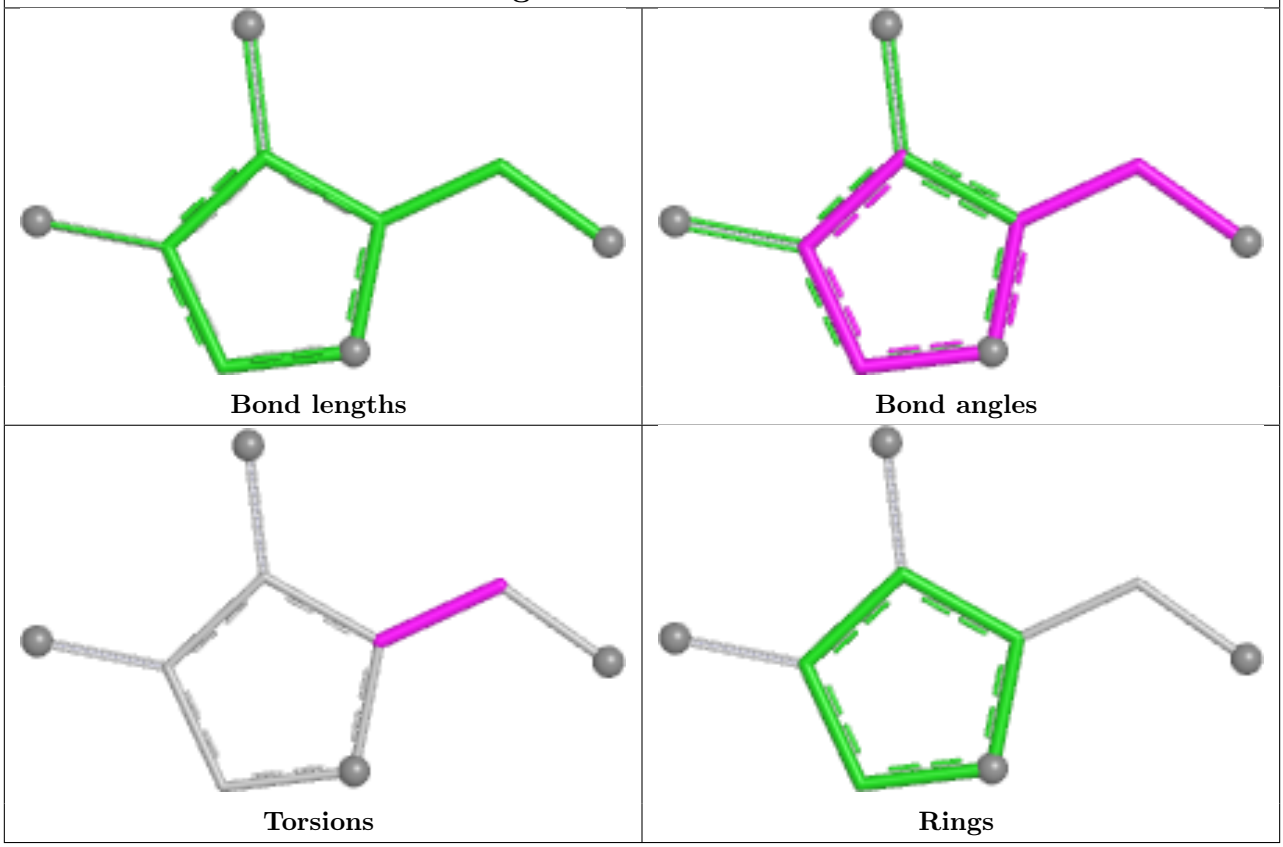

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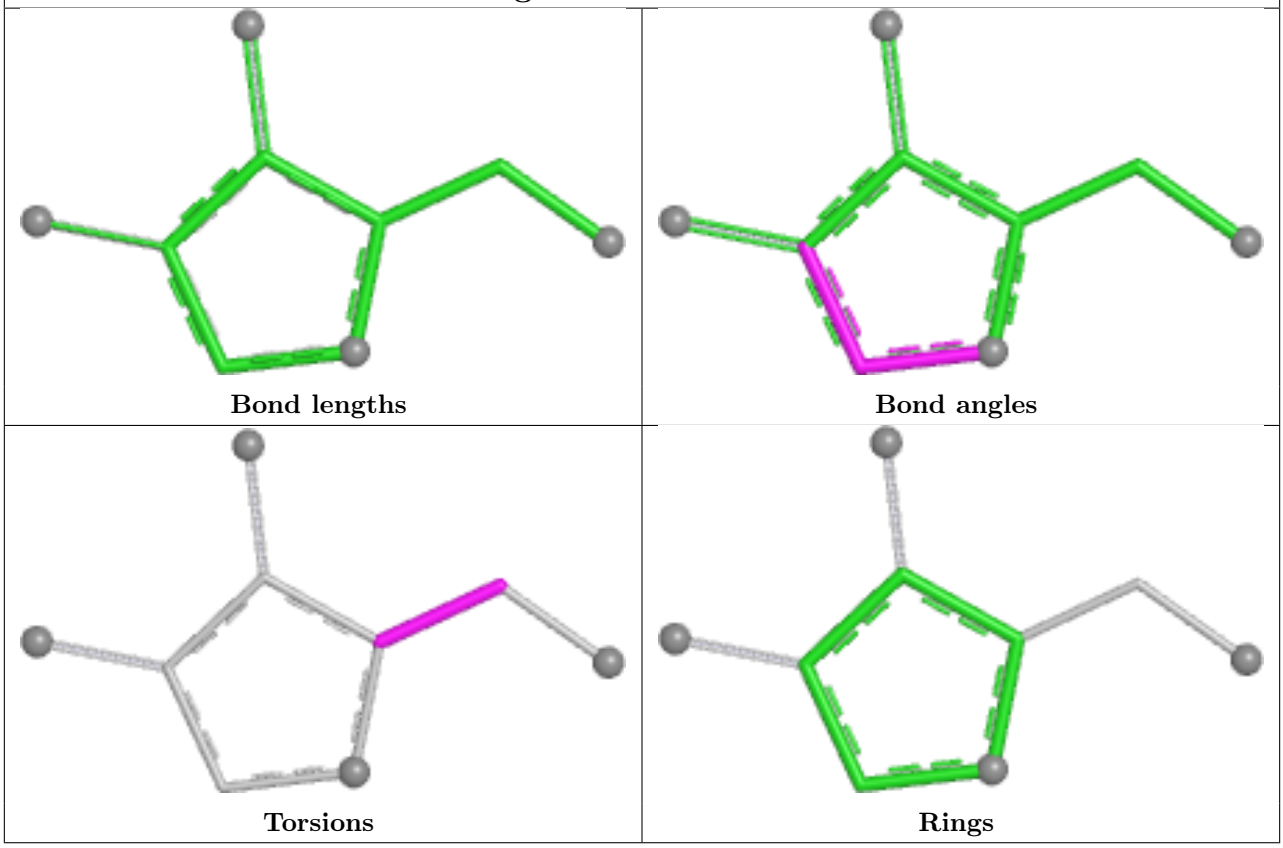

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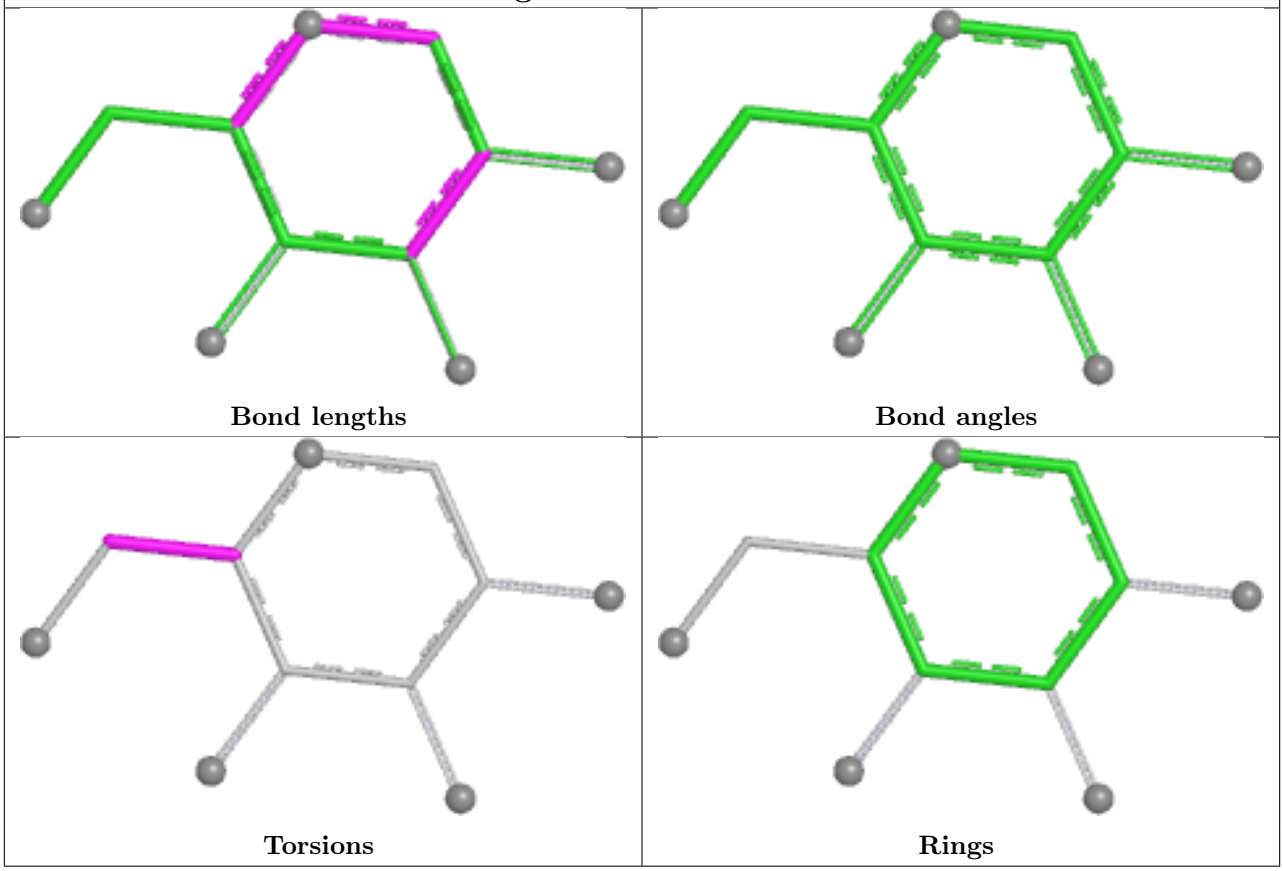

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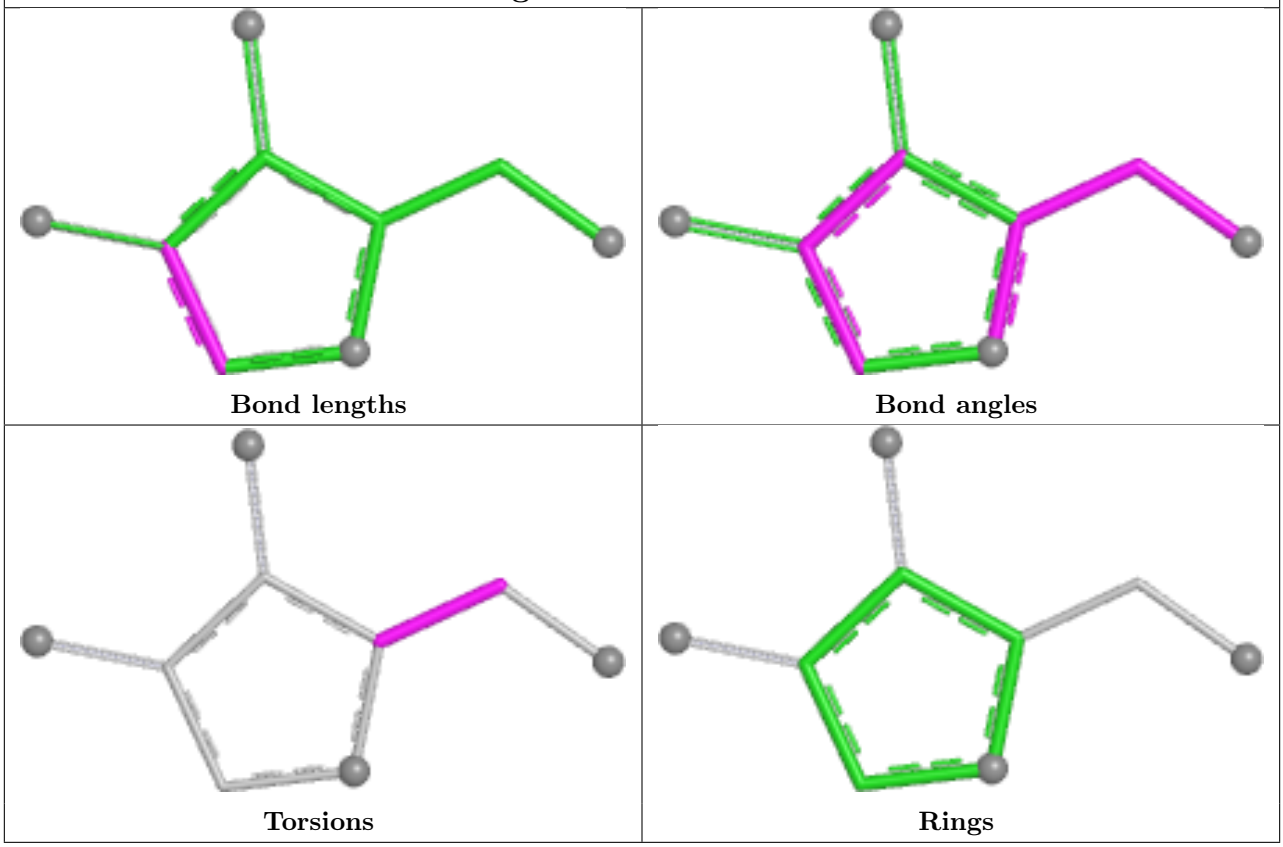

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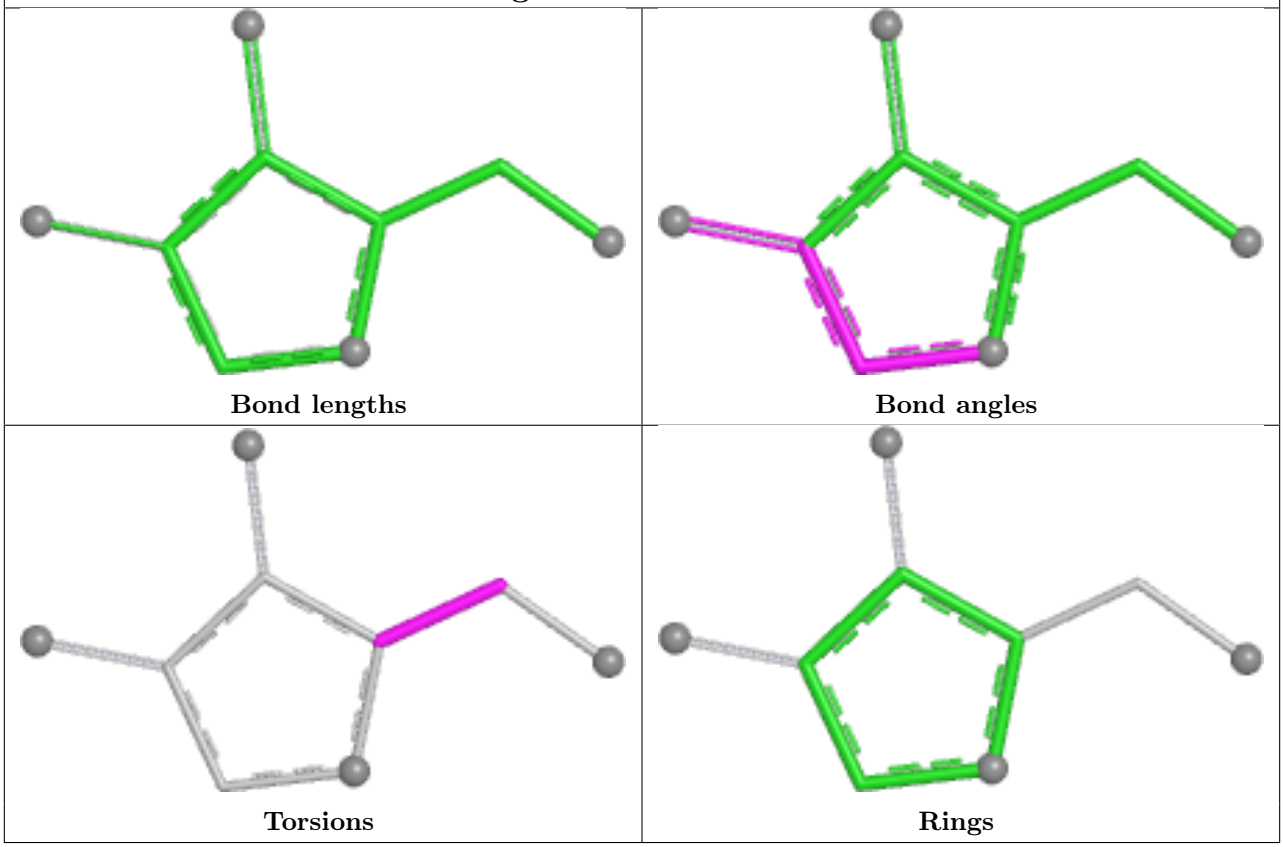
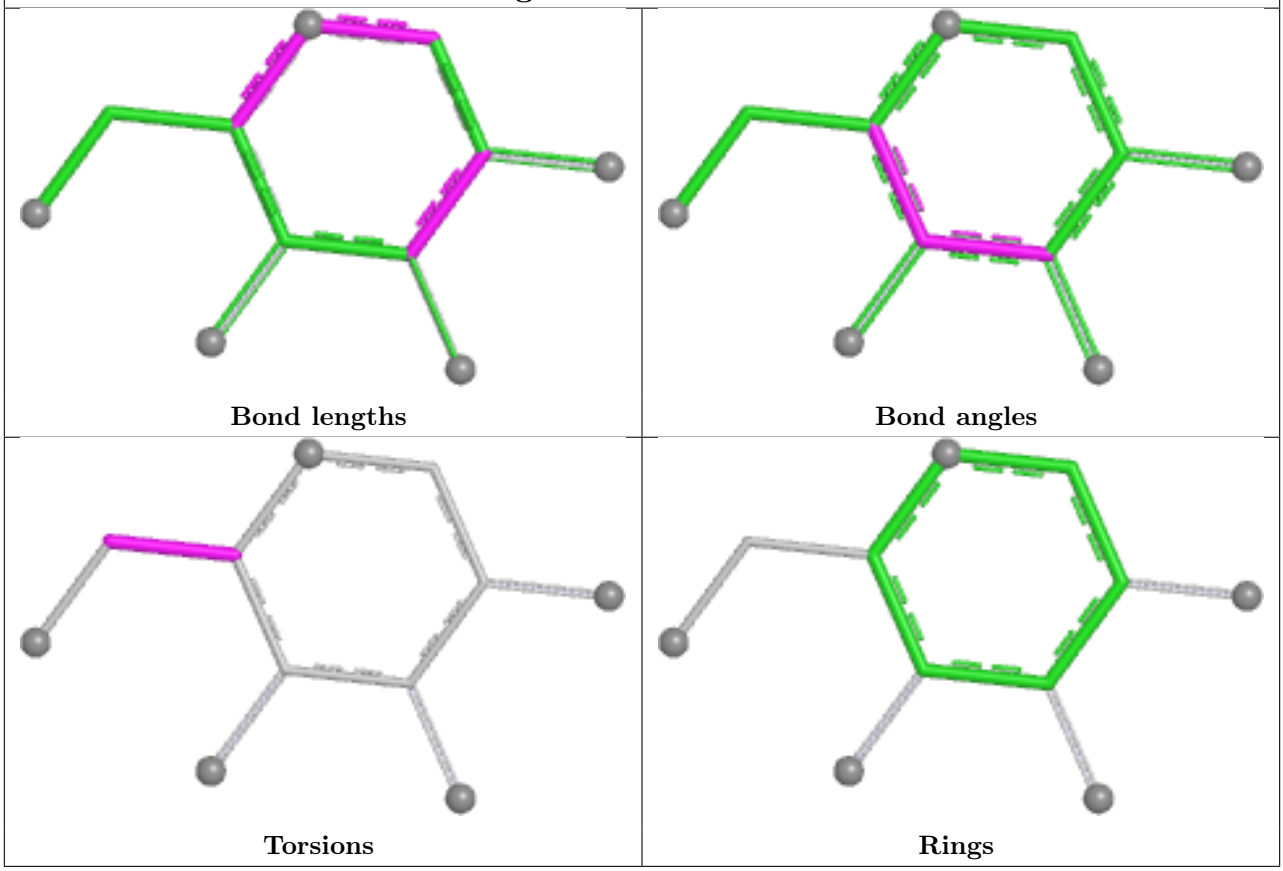
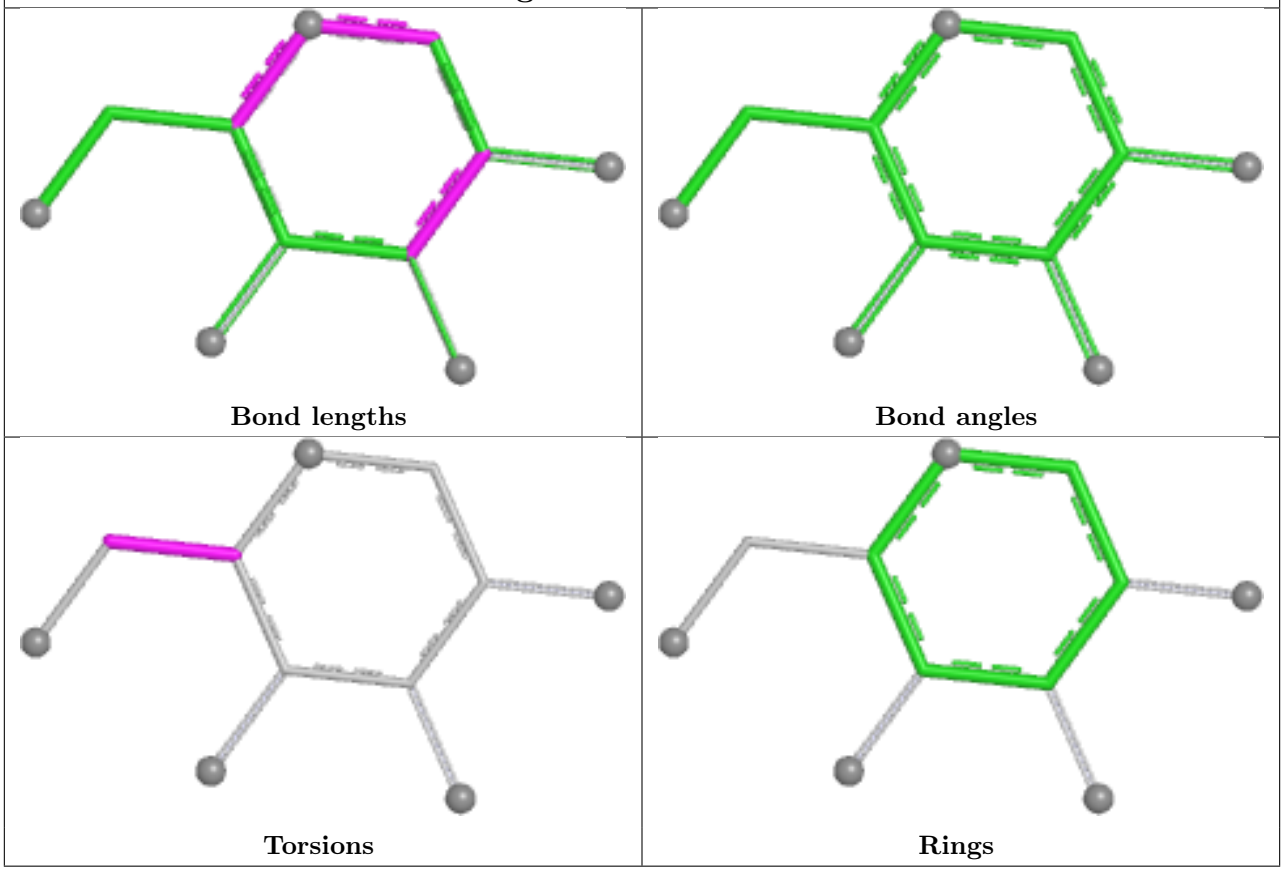


Ligand GLA B 2011



Ligand GLA E 2006



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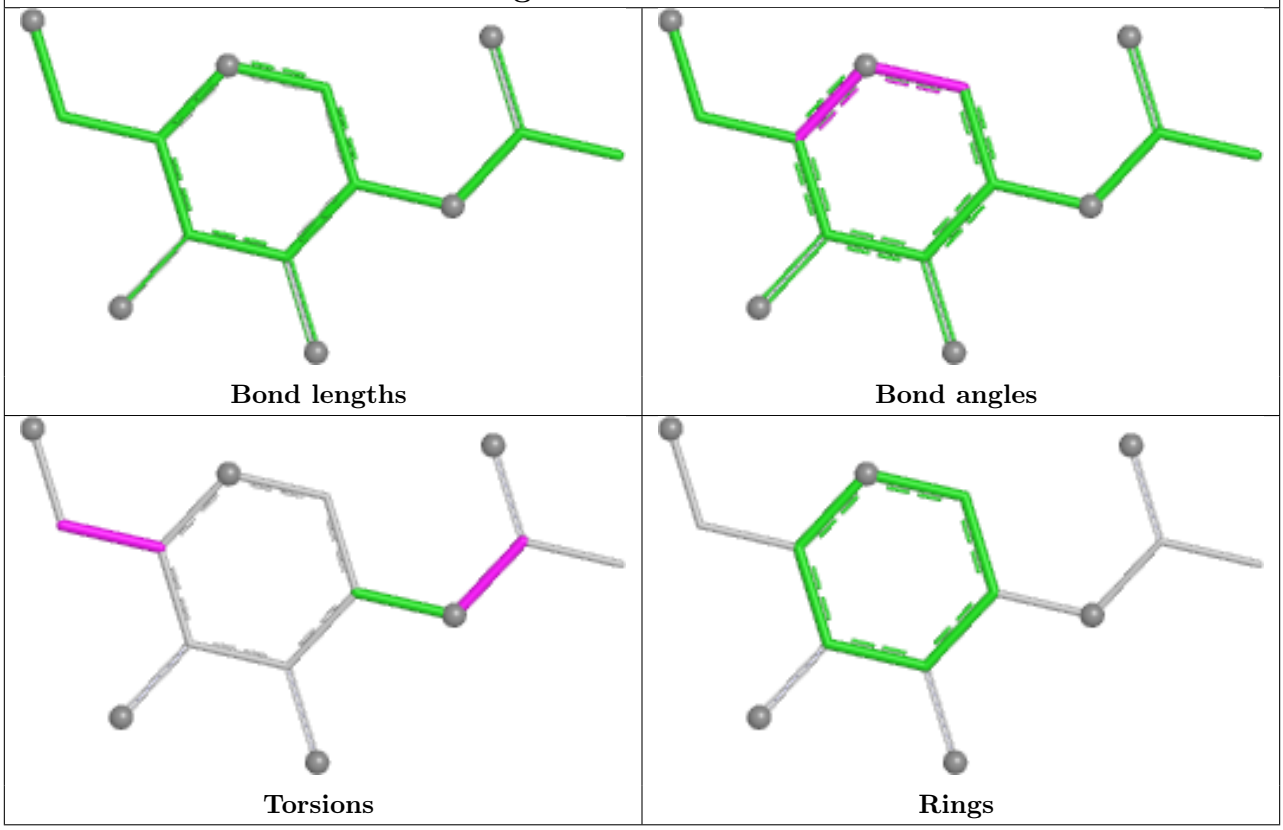
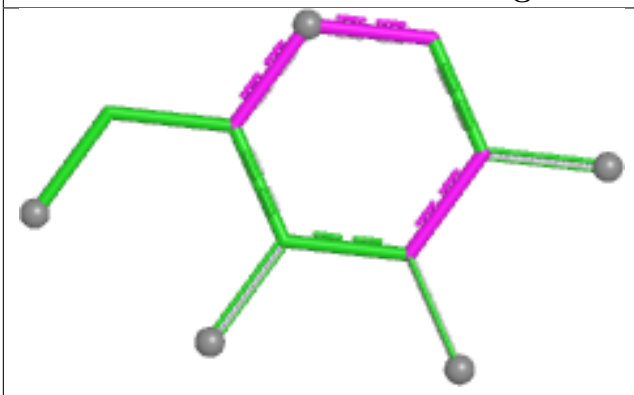
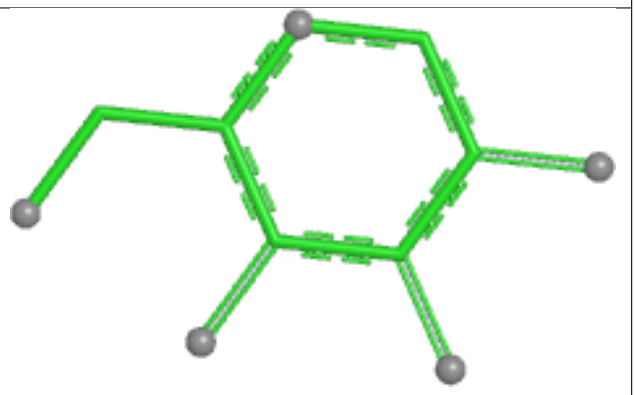
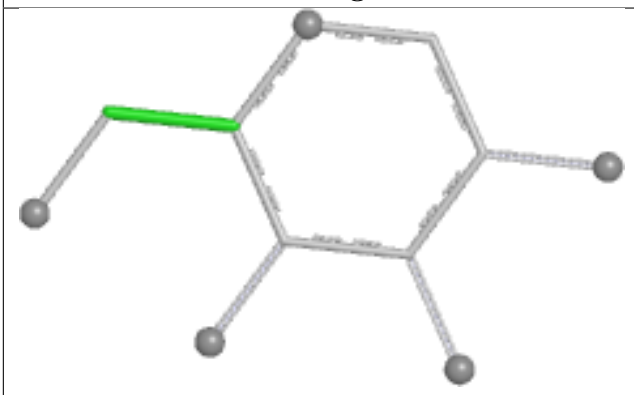
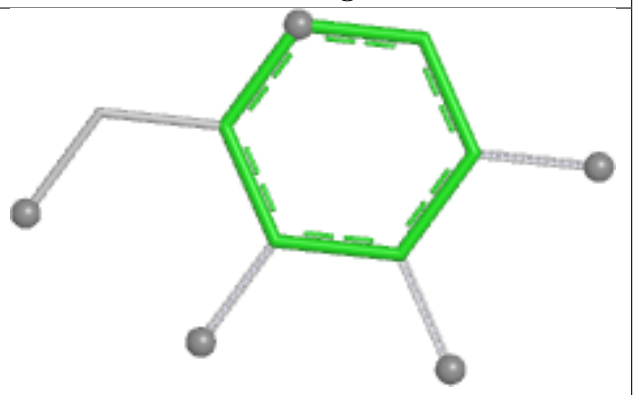
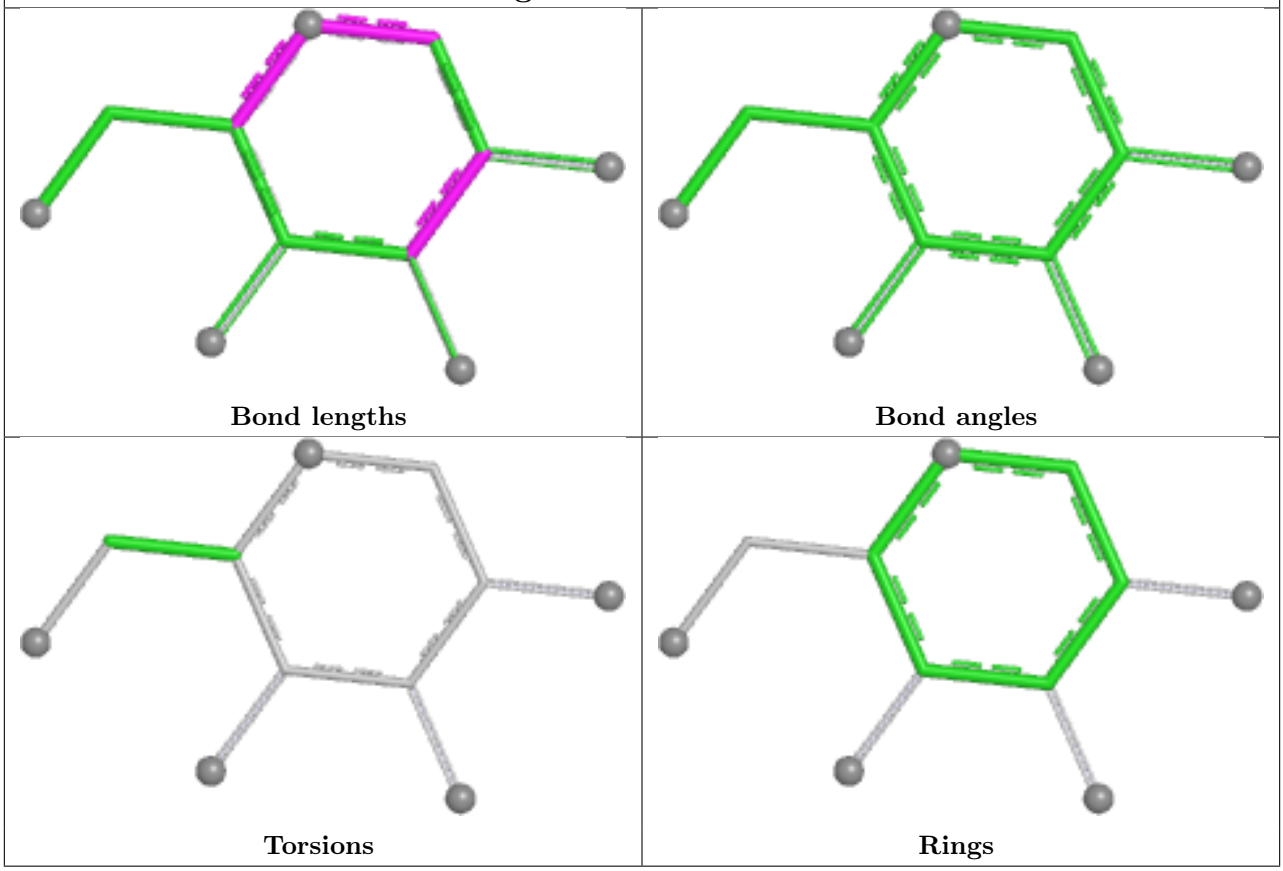
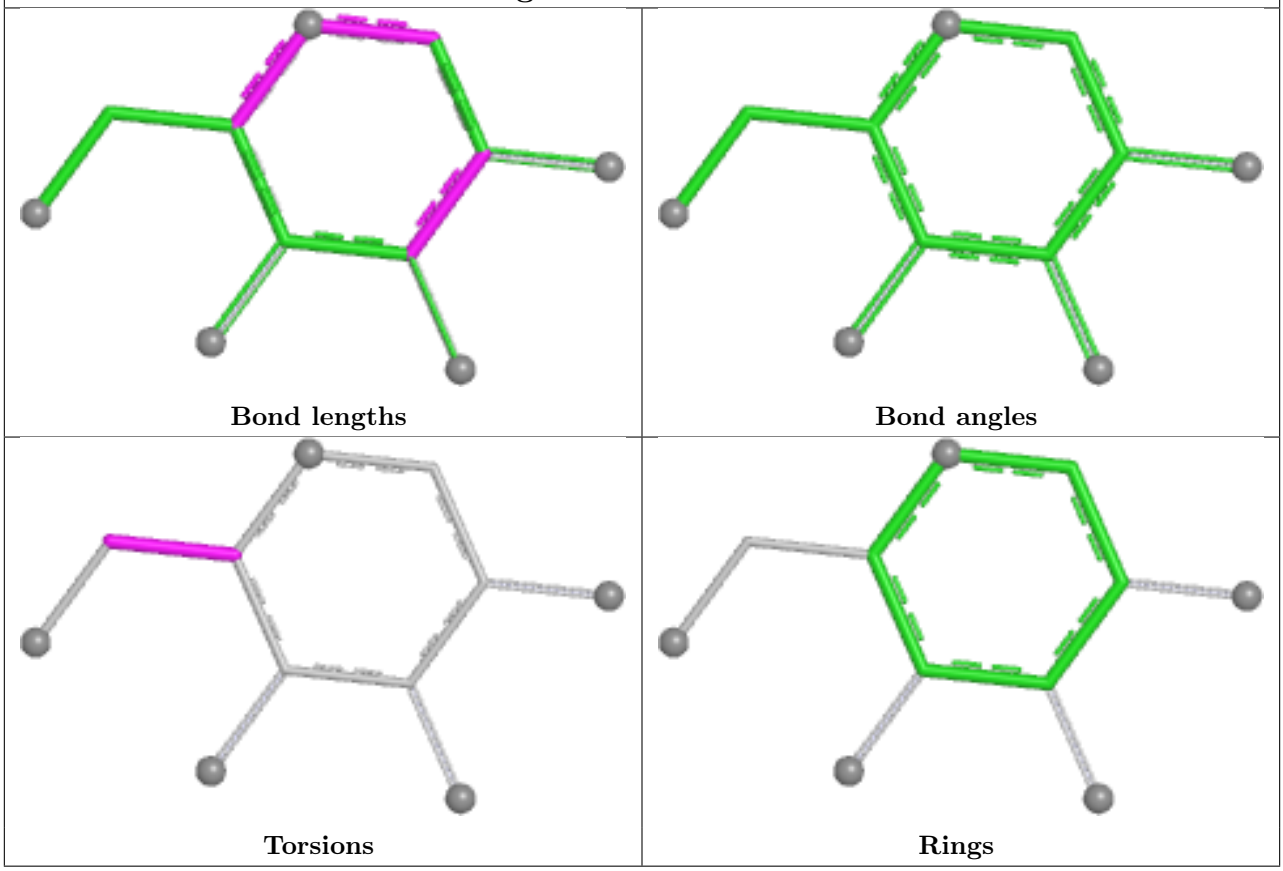


Ligand GLA A 2005	
 Bond lengths	 Bond angles
 Torsions	 Rings

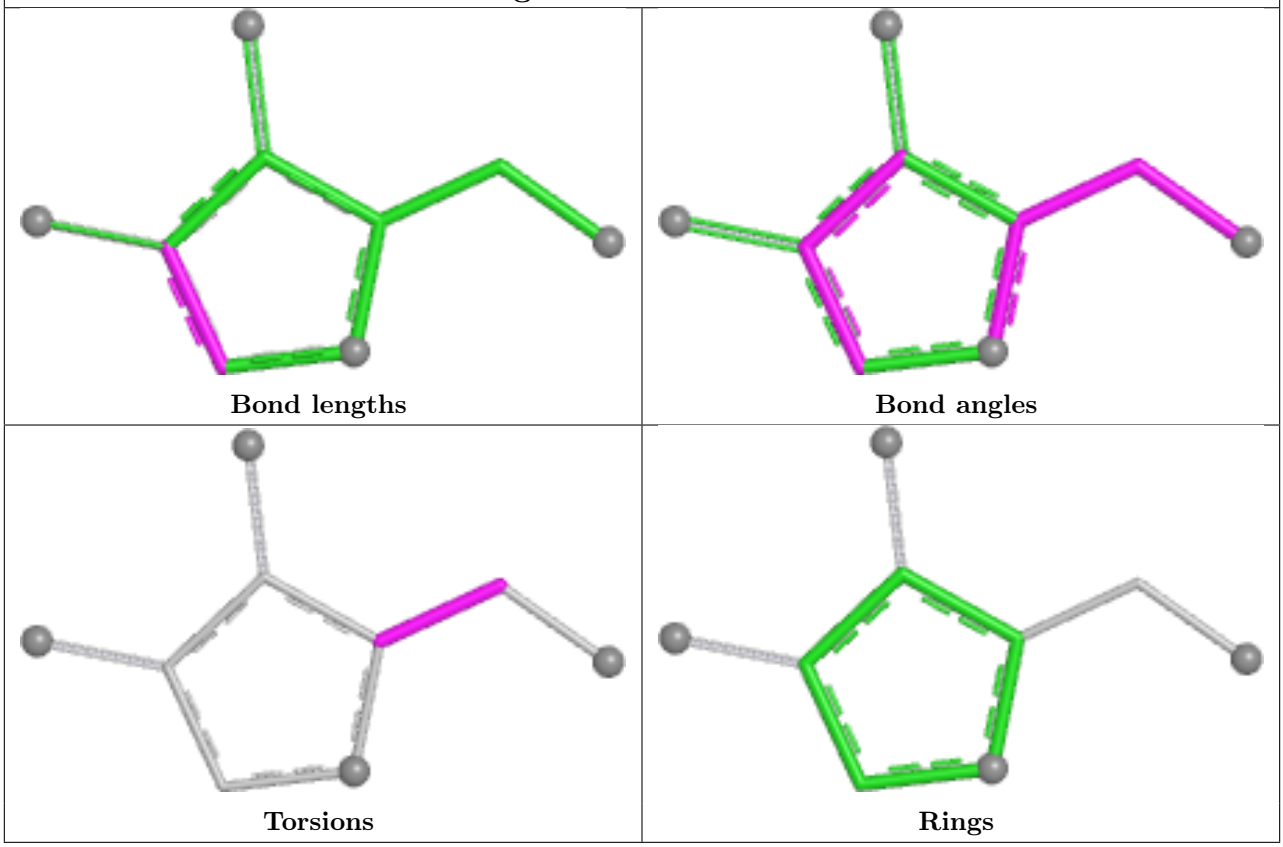
Ligand GLA A 2013

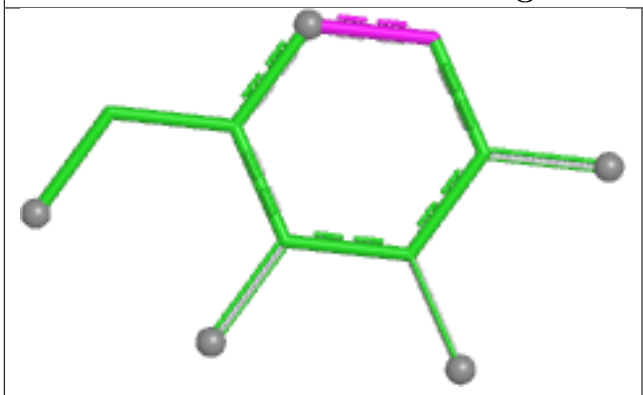
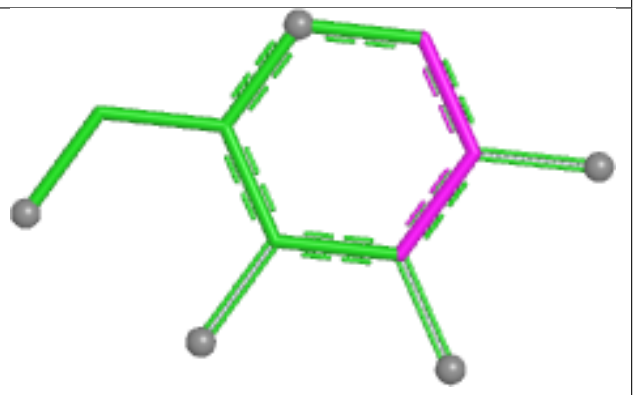
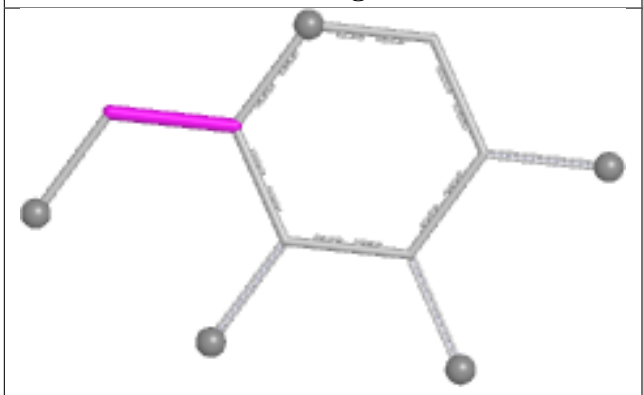
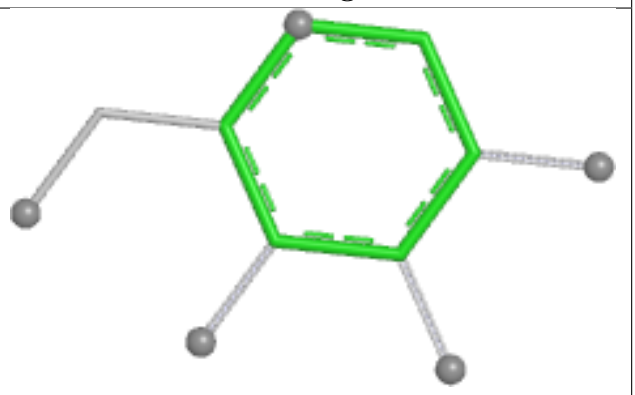


Ligand GLA E 2016

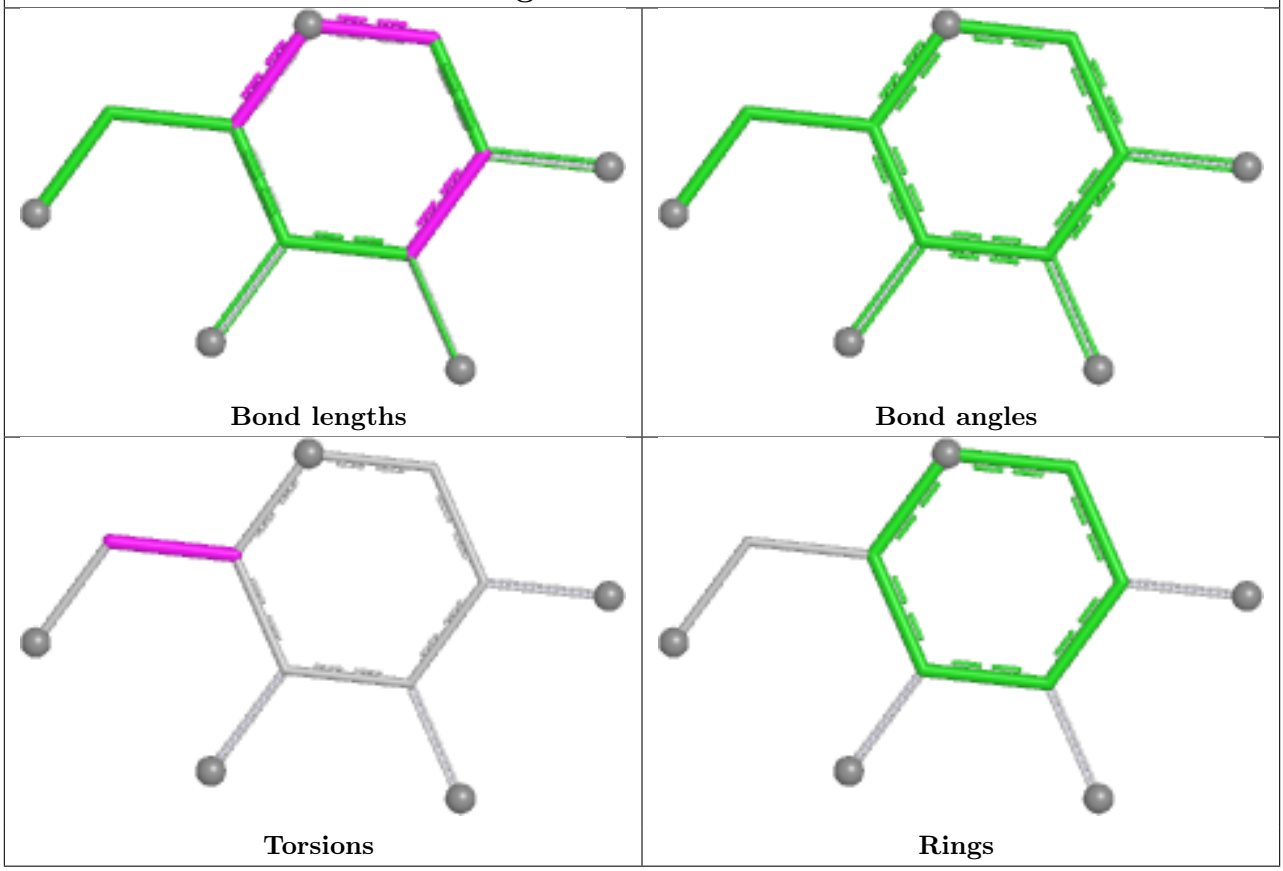


Ligand AHR E 2002

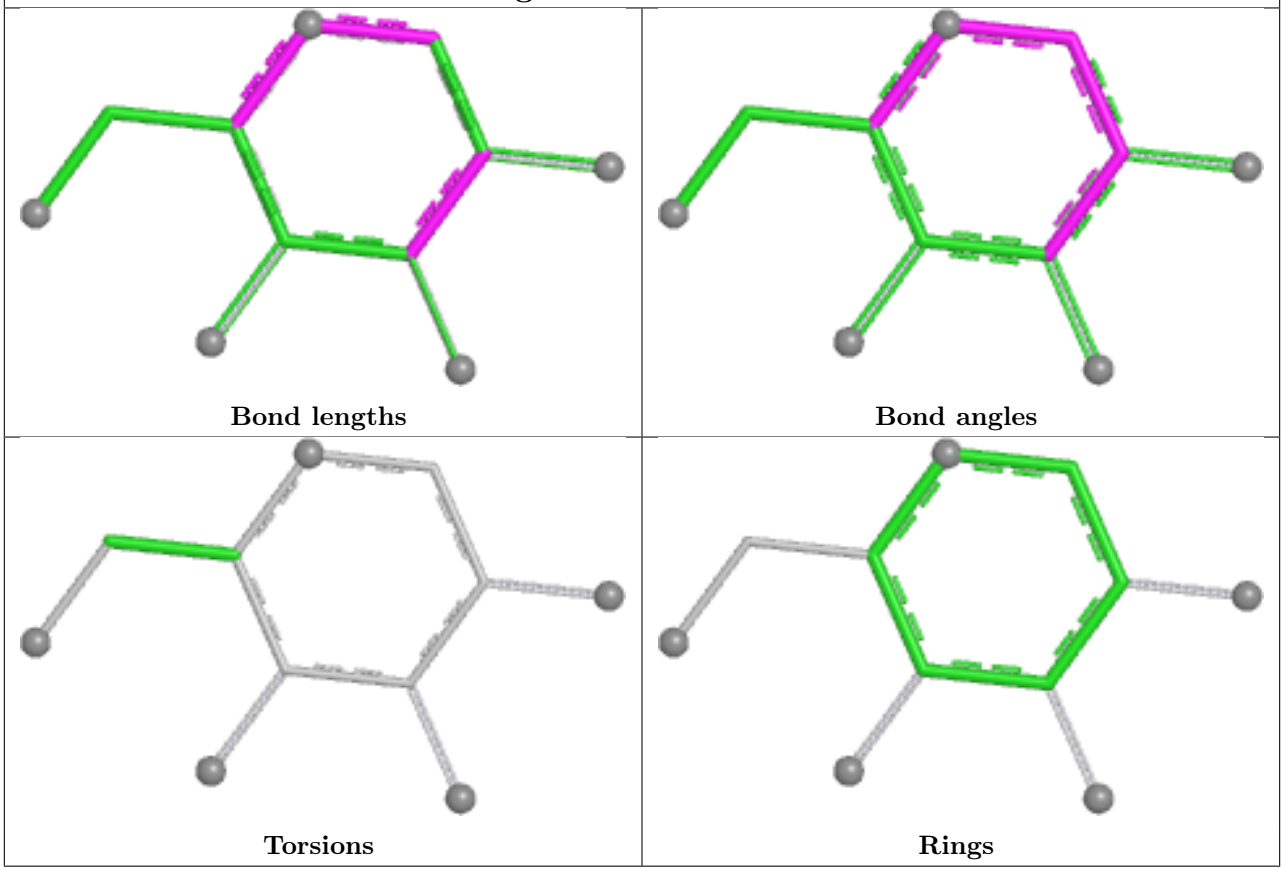


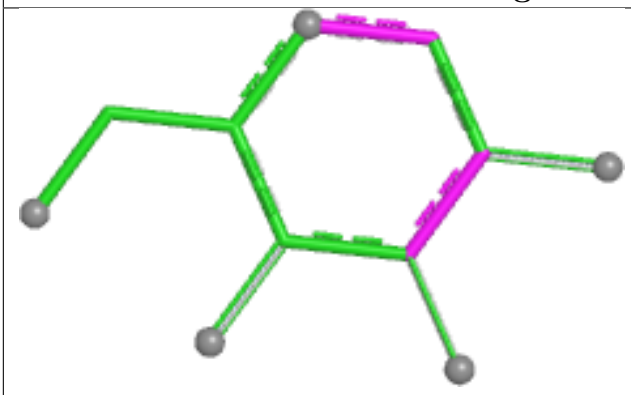
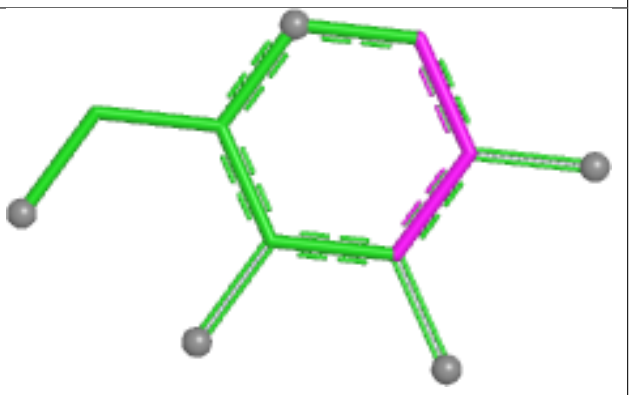
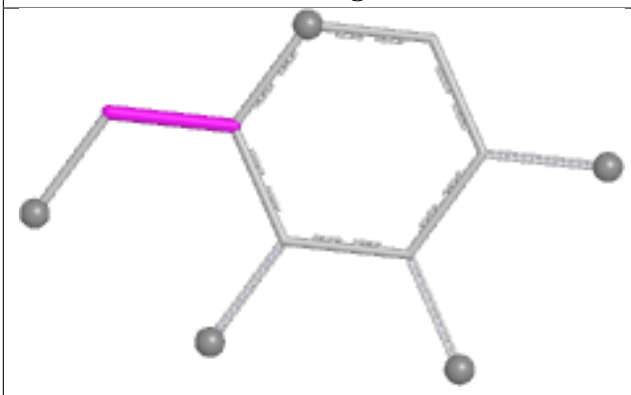
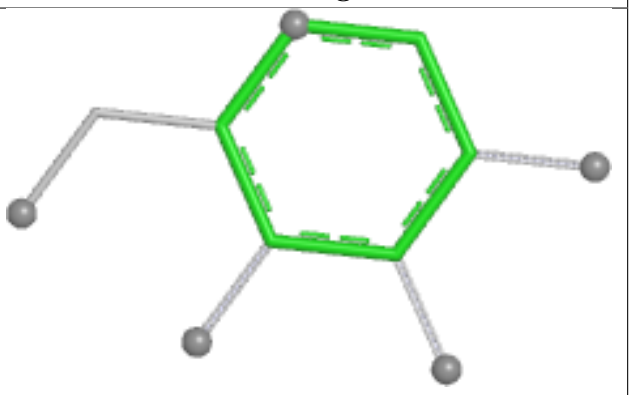
Ligand GLA E 2012	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

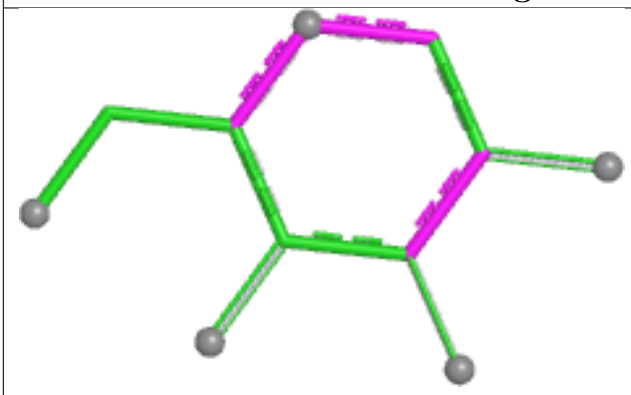
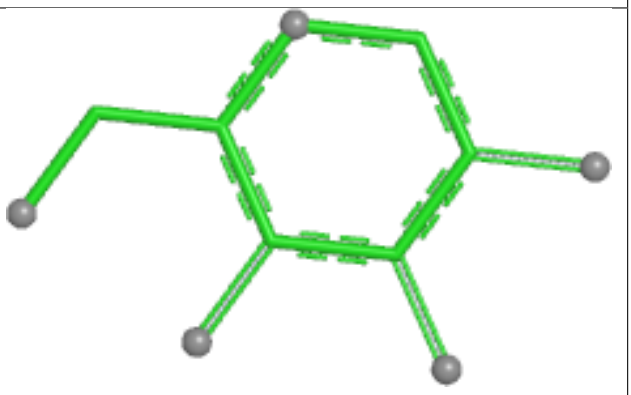
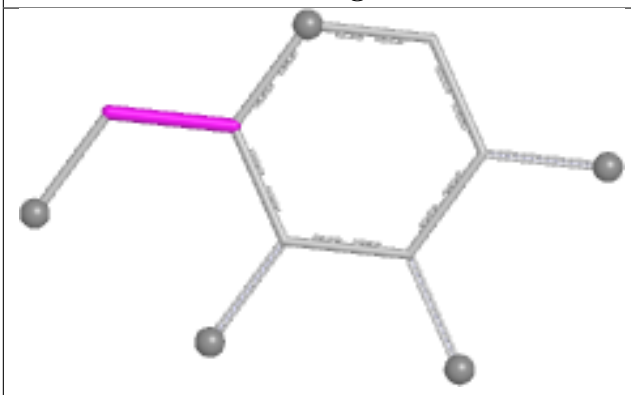
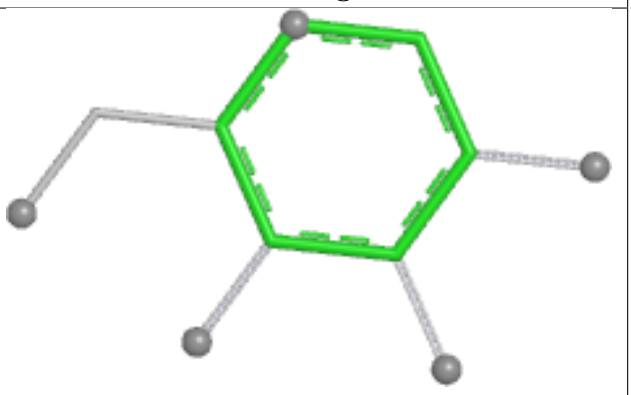
Ligand GLA E 2013



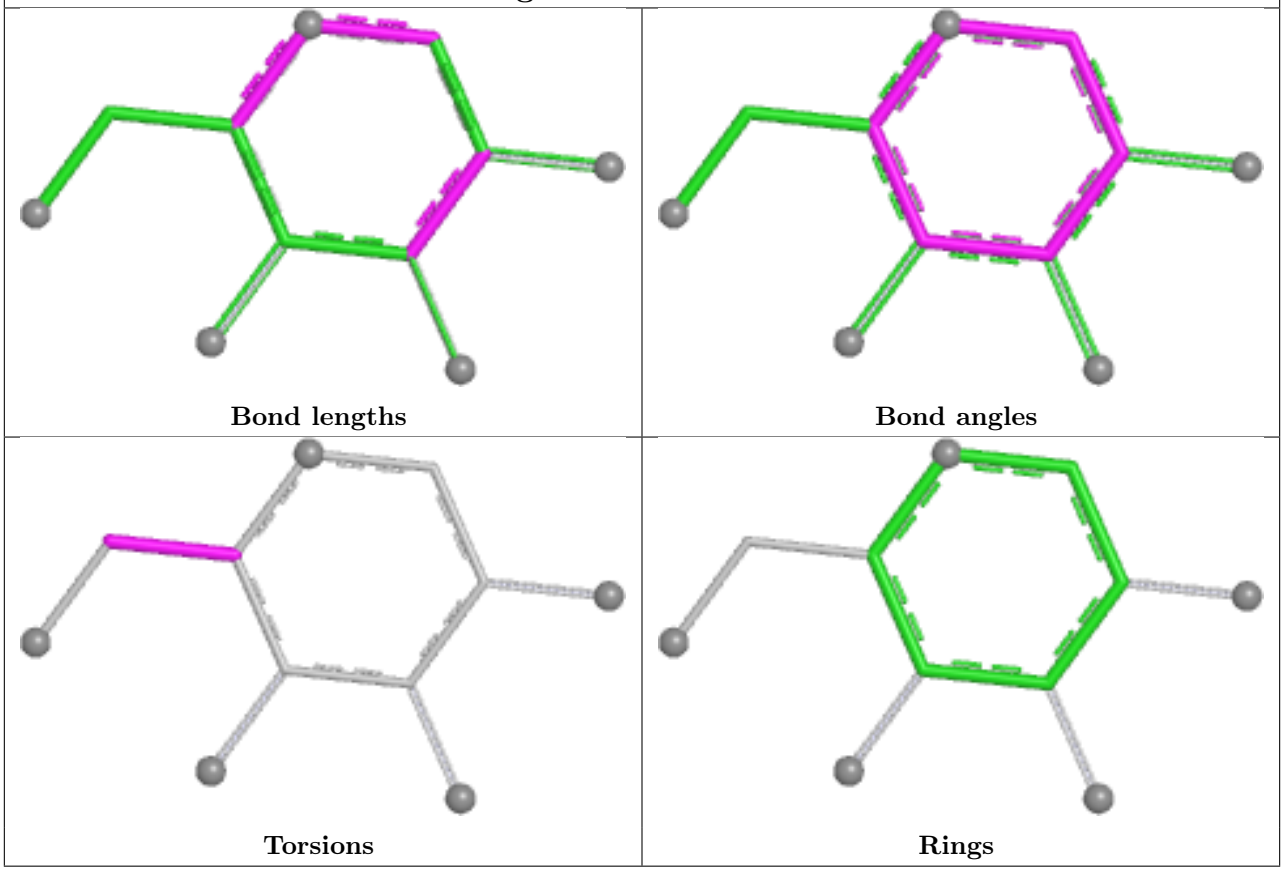
Ligand GLA B 2005



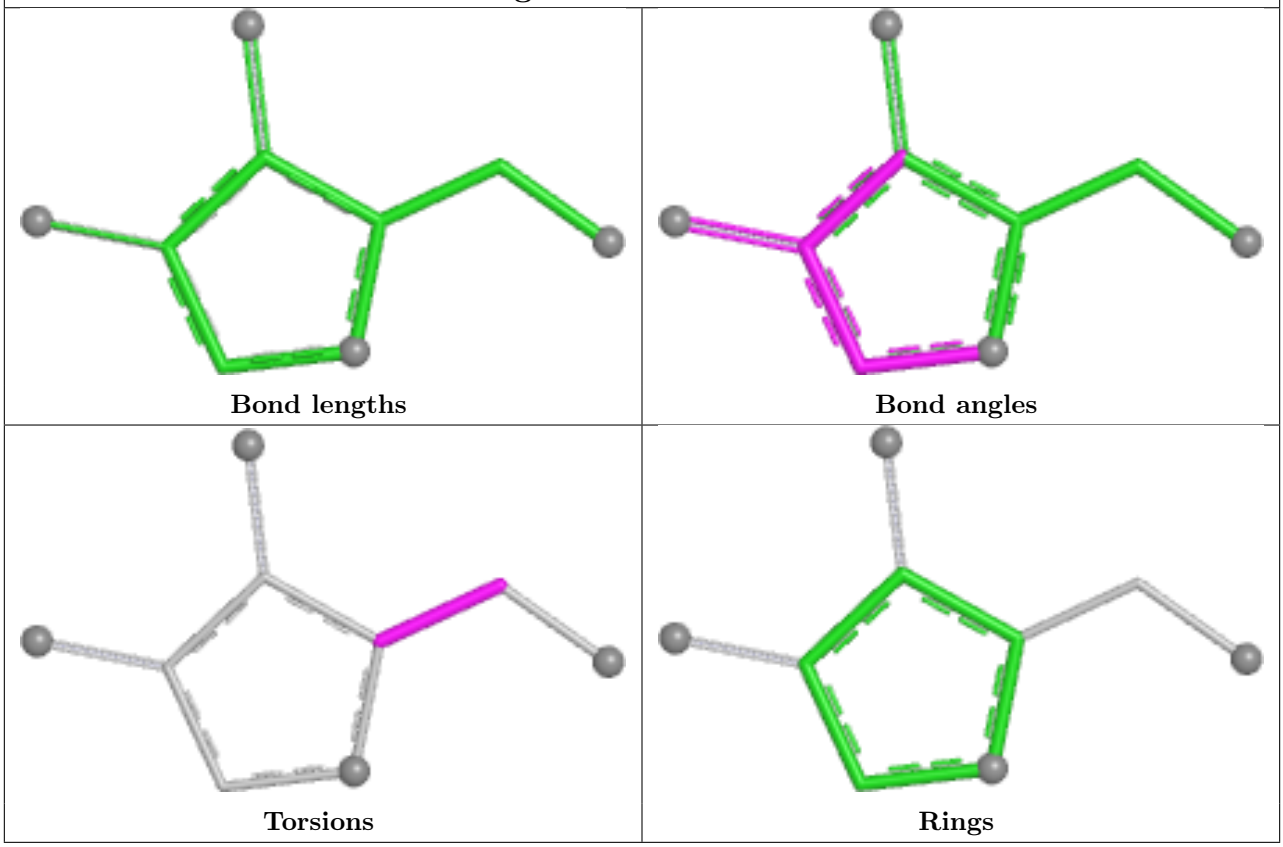
Ligand GLA A 2008	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

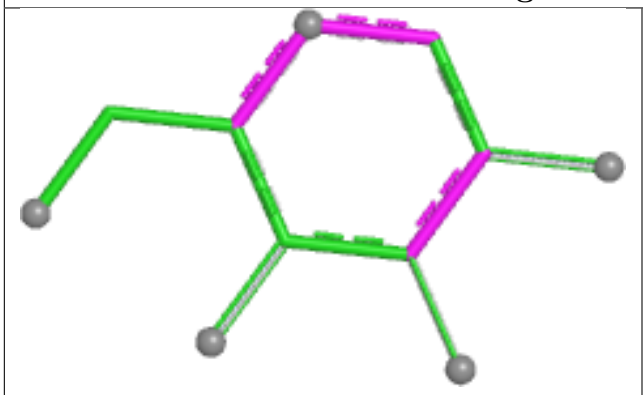
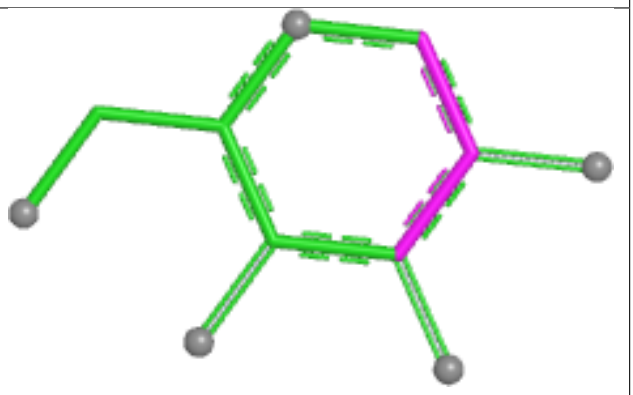
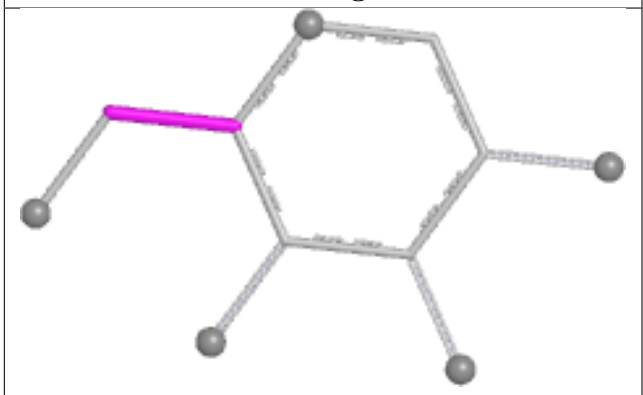
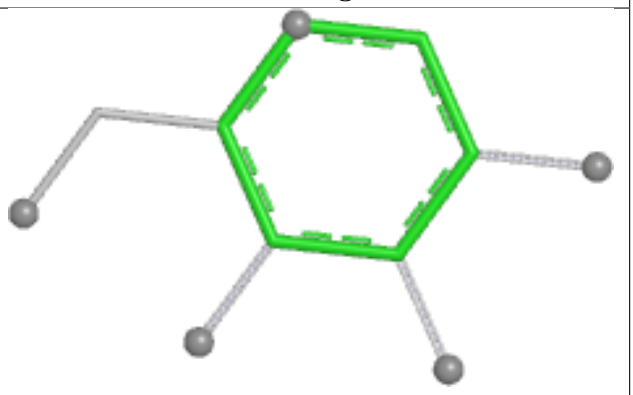
Ligand GLA A 2014	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand GLA E 2007



Ligand AHR F 2001



Ligand GLA E 2008	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

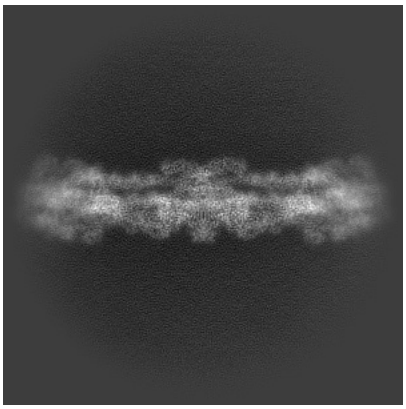
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37389. These allow visual inspection of the internal detail of the map and identification of artifacts.

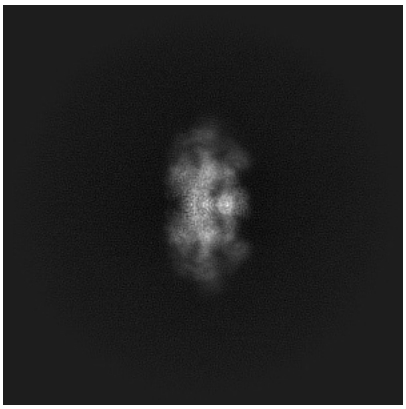
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

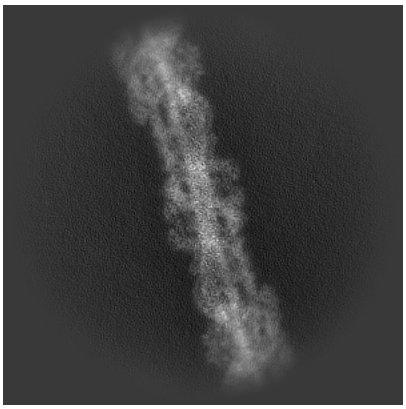
6.1.1 Primary map



X

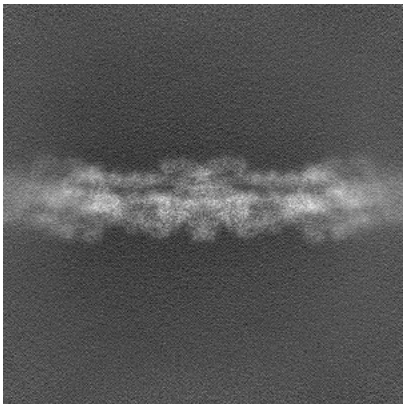


Y

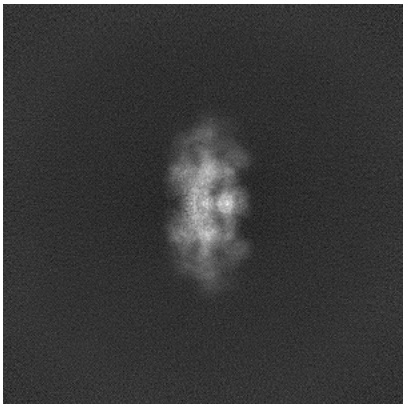


Z

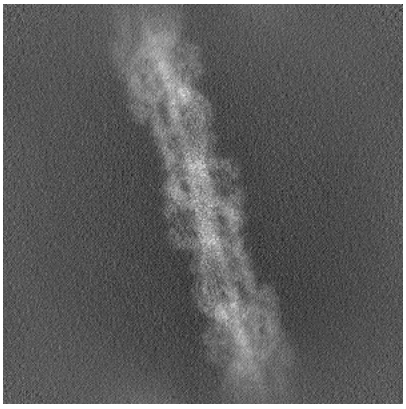
6.1.2 Raw map



X



Y

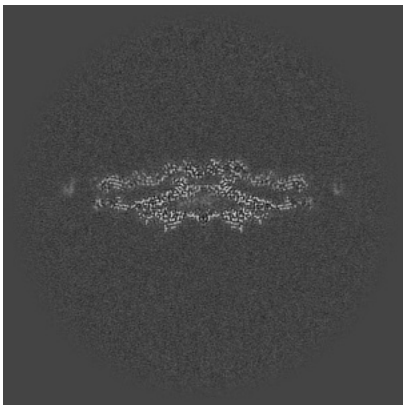


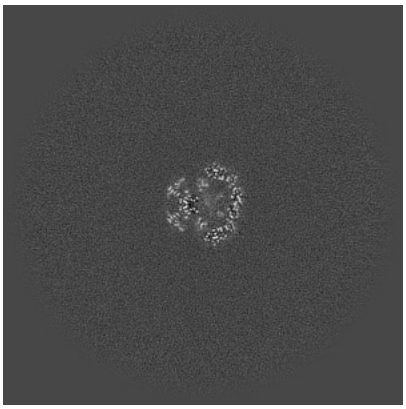
Z

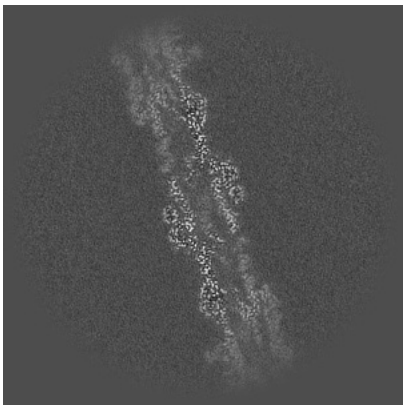
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

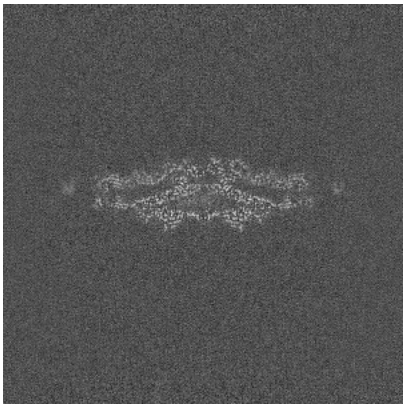
6.2.1 Primary map

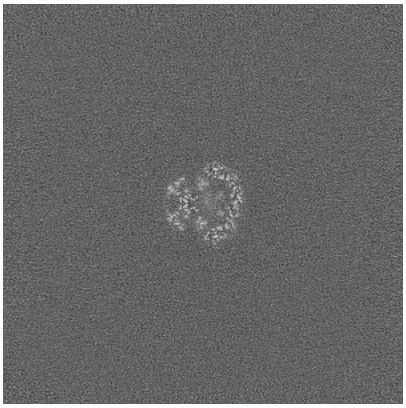

X Index: 256

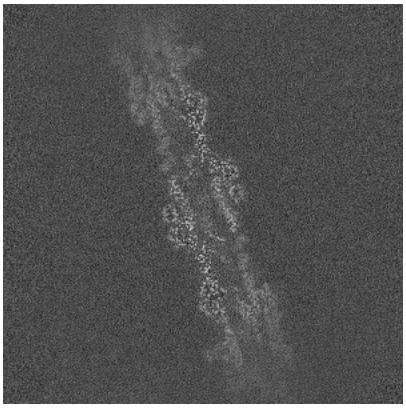

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

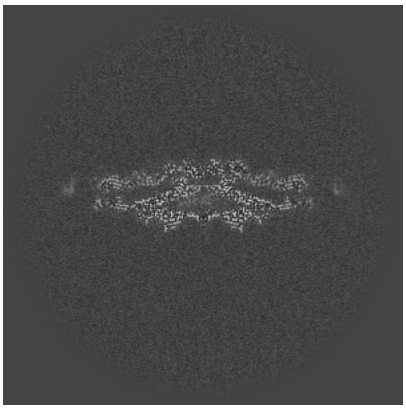

Y Index: 256


Z Index: 256

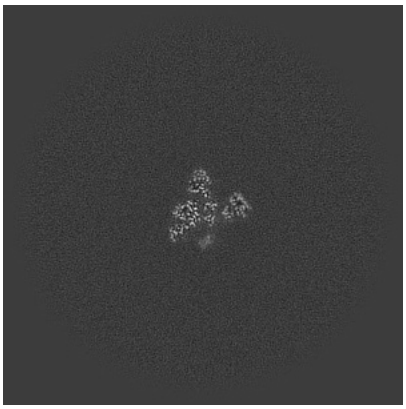
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

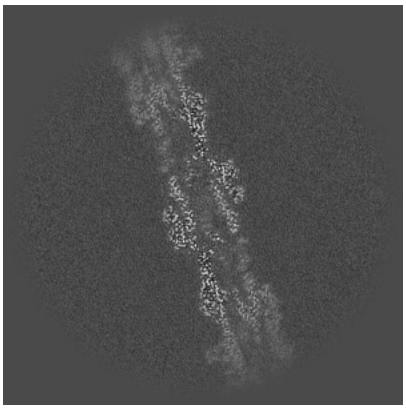
6.3.1 Primary map



X Index: 256

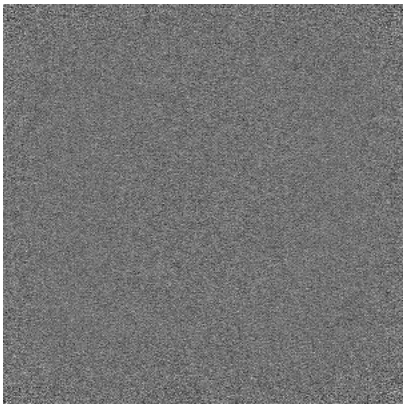


Y Index: 302

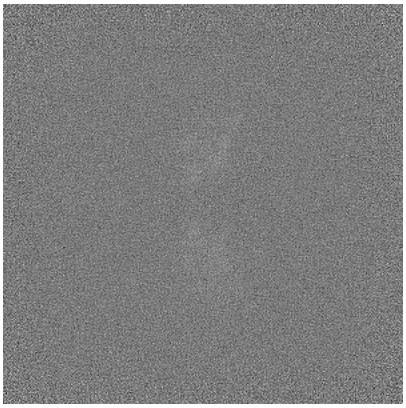


Z Index: 255

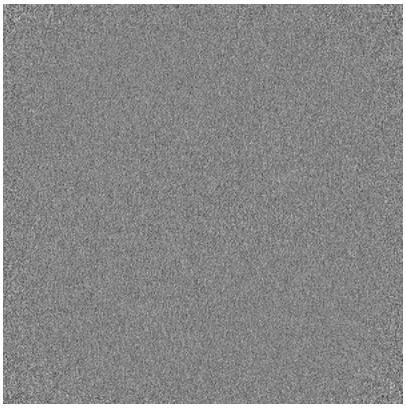
6.3.2 Raw map



X Index: 0



Y Index: 0

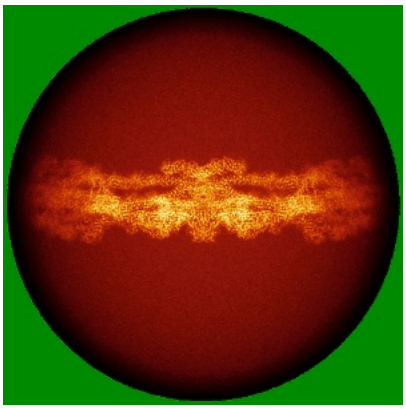


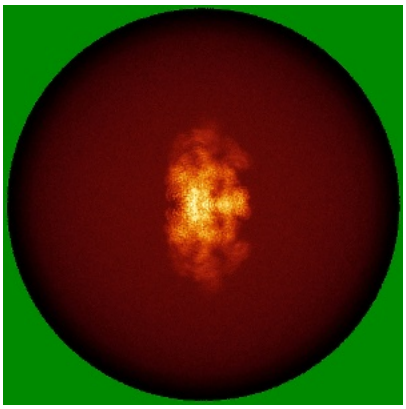
Z Index: 0

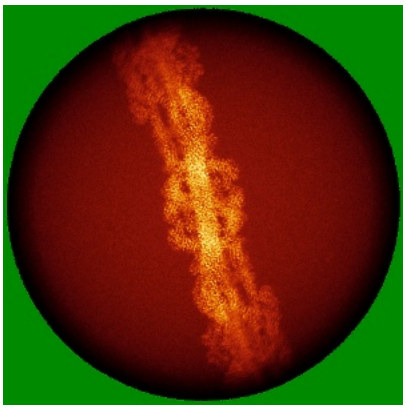
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

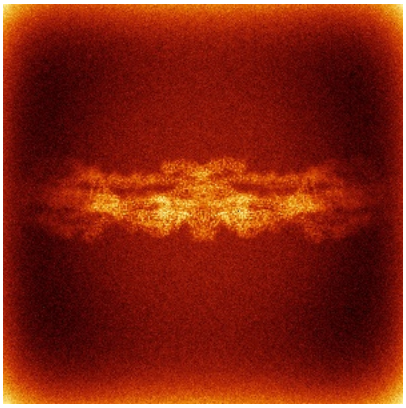
6.4.1 Primary map

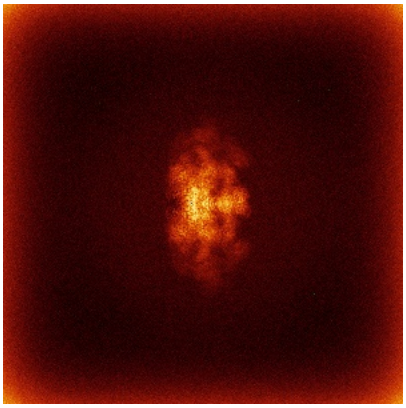

X

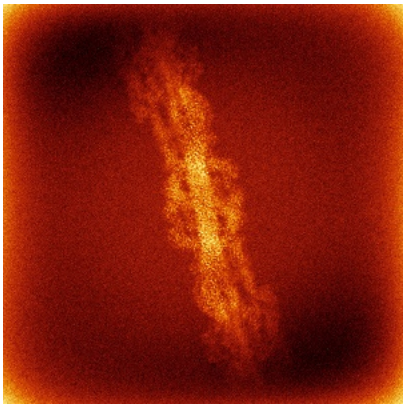

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

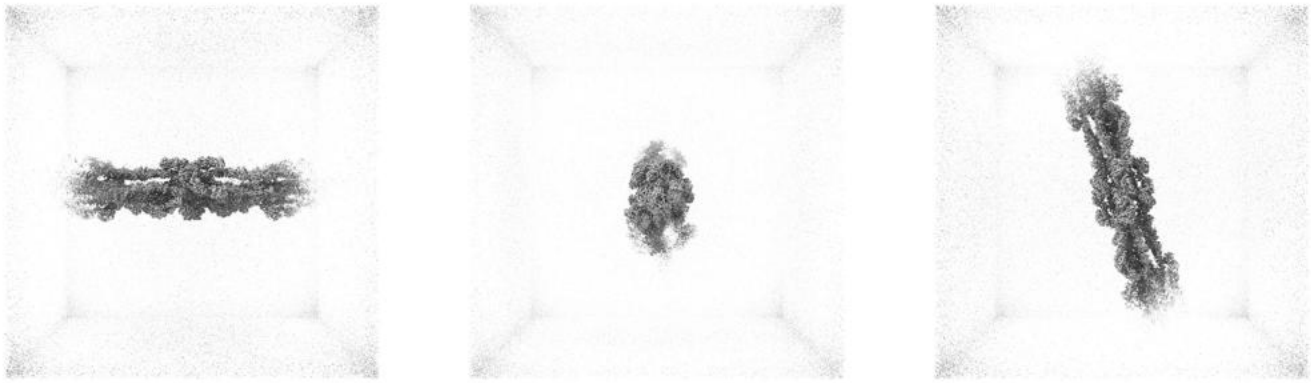
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

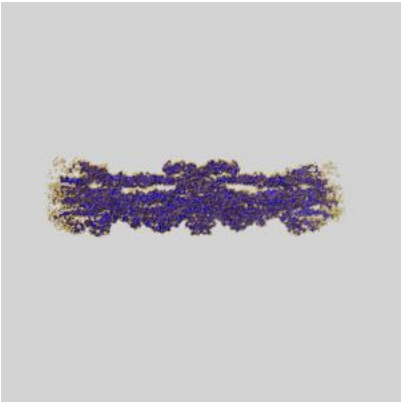
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

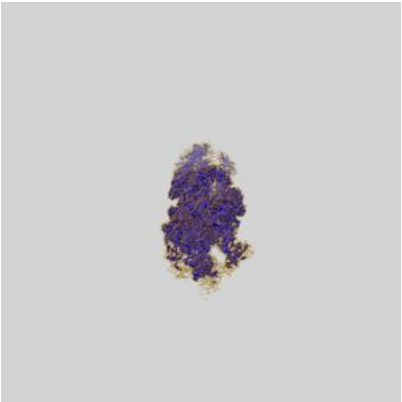
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

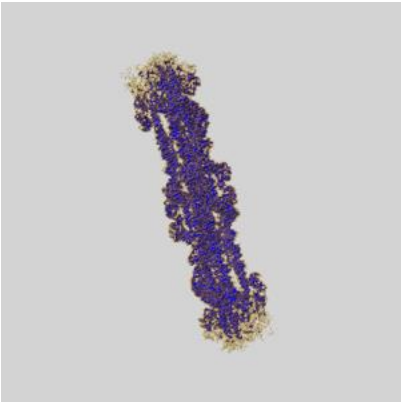
6.6.1 emd_37389_msk_1.map (i)



X



Y

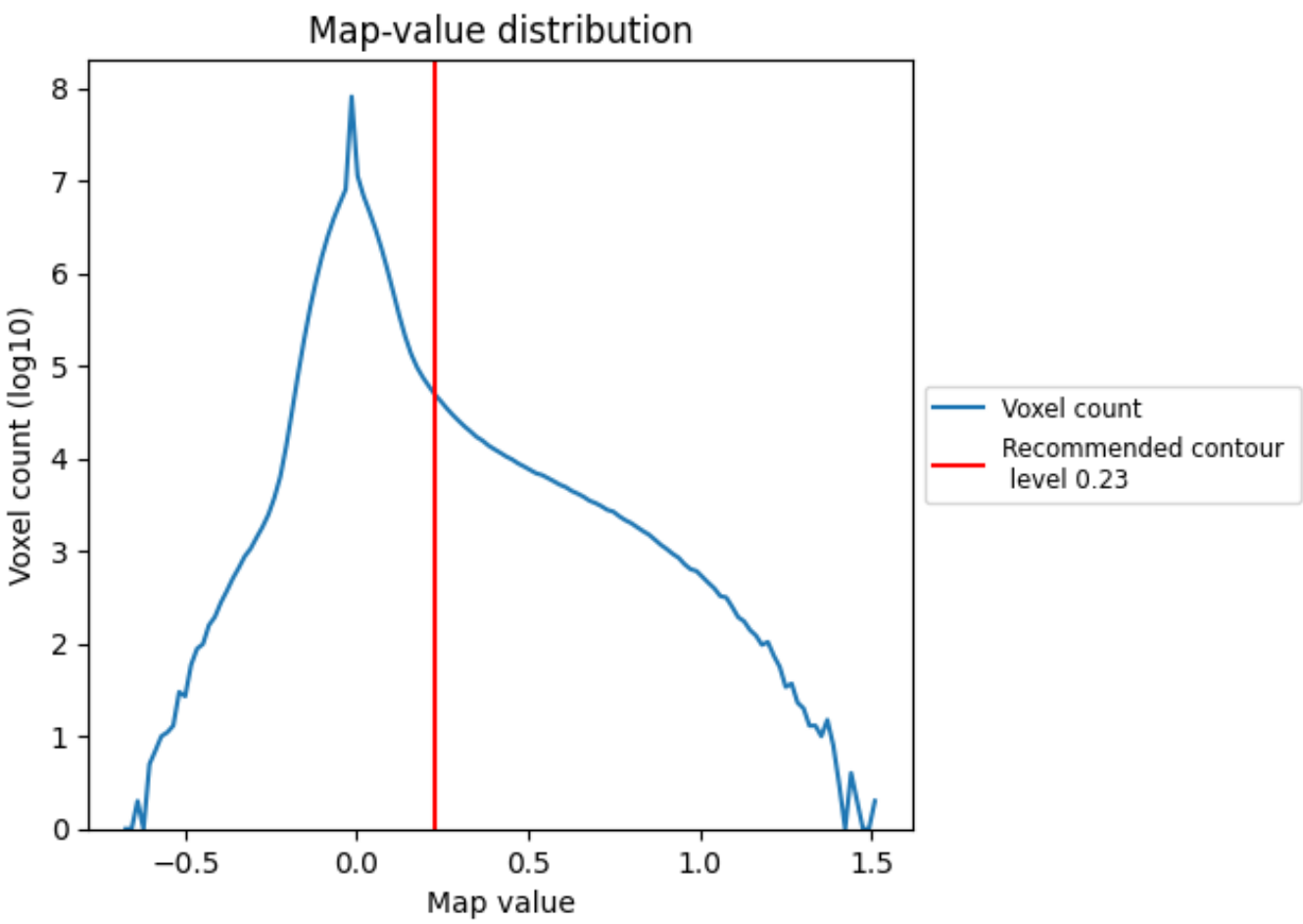


Z

7 Map analysis (i)

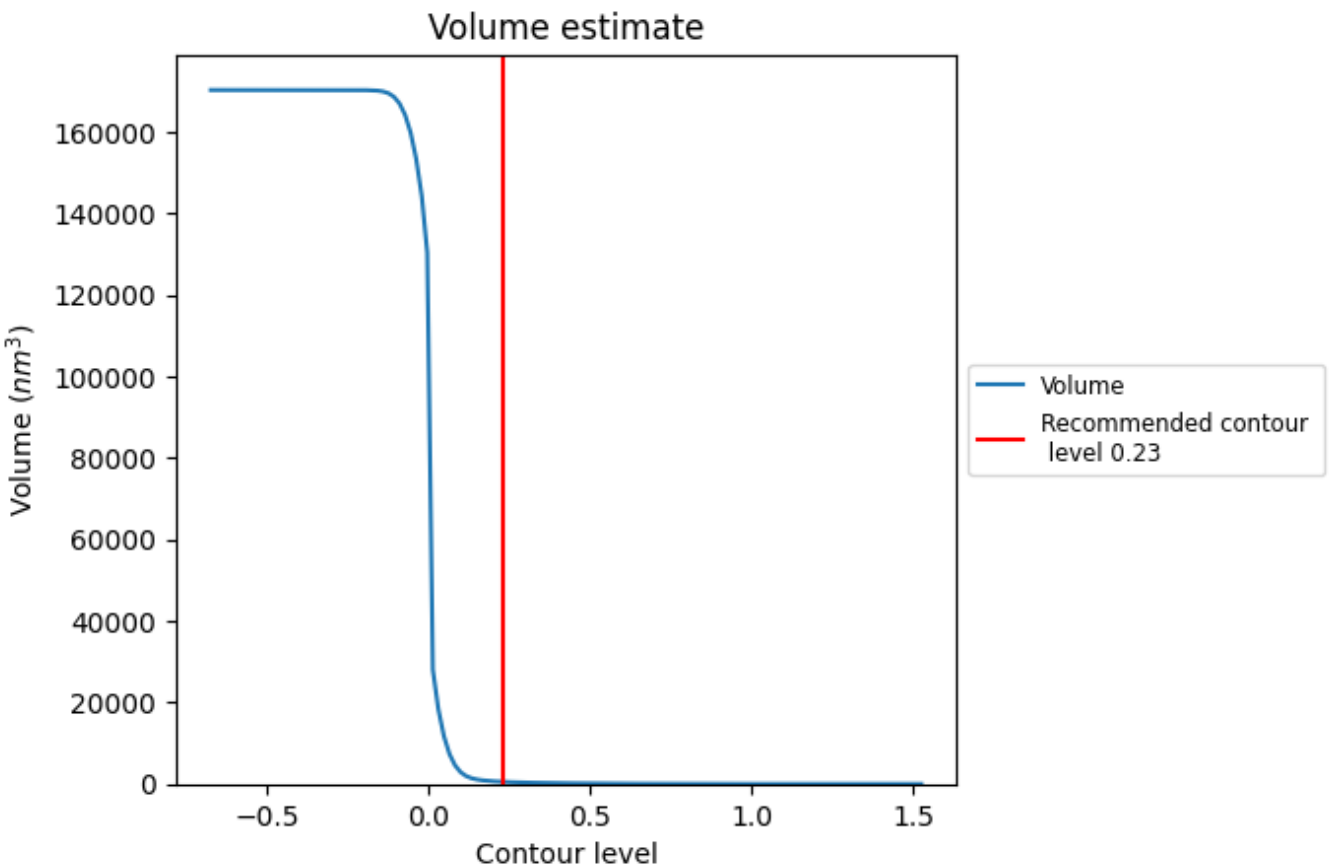
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

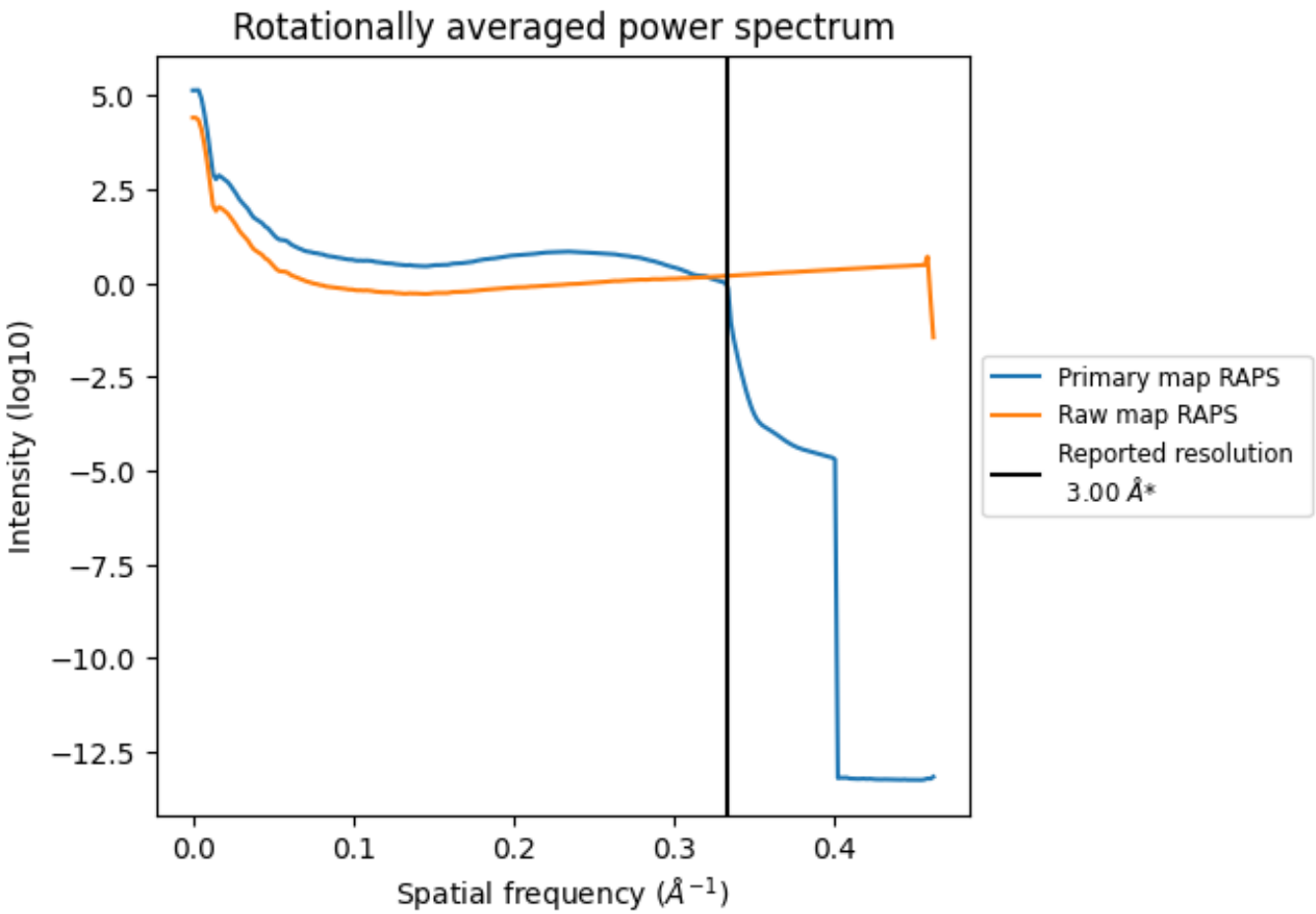
7.2 Volume estimate (i)



The volume at the recommended contour level is 527 nm^3; this corresponds to an approximate mass of 476 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

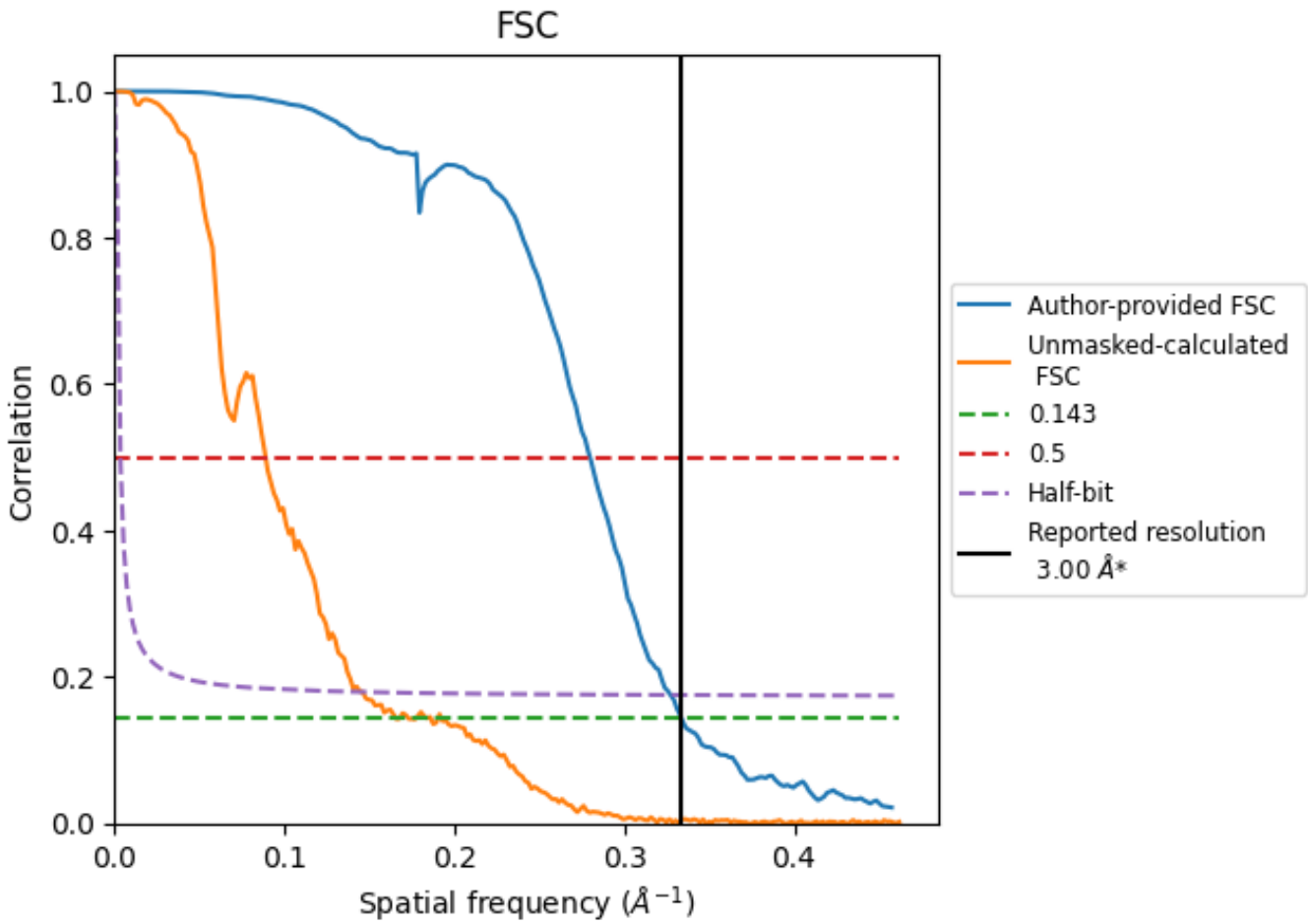


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

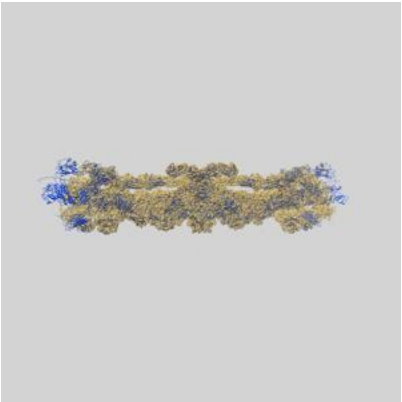
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.57	3.06
Unmasked-calculated*	6.04	11.24	6.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.04 differs from the reported value 3.0 by more than 10 %

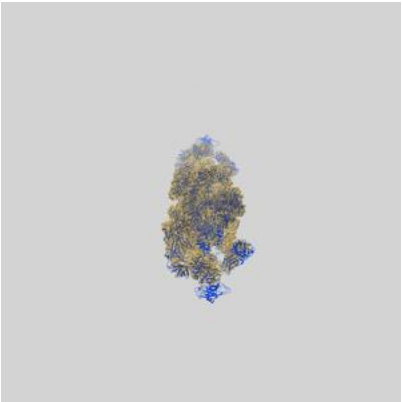
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37389 and PDB model 8WA2. Per-residue inclusion information can be found in section 3 on page 53.

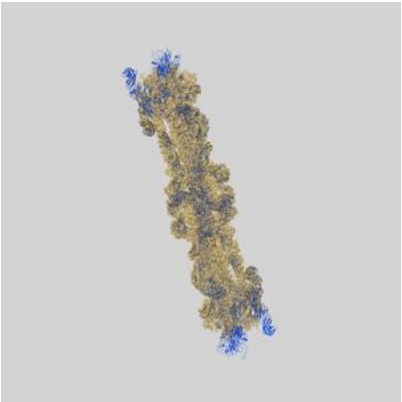
9.1 Map-model overlay (i)



X



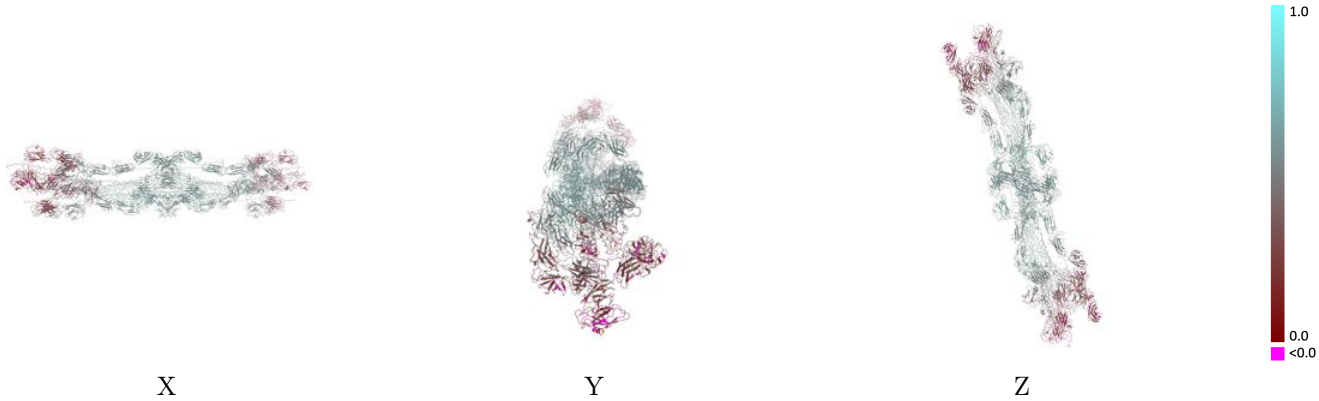
Y



Z

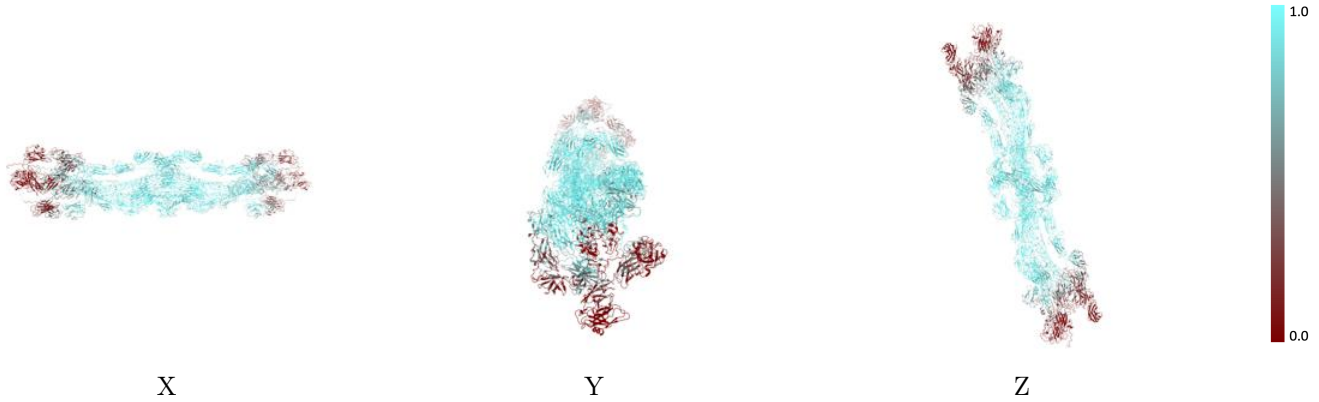
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



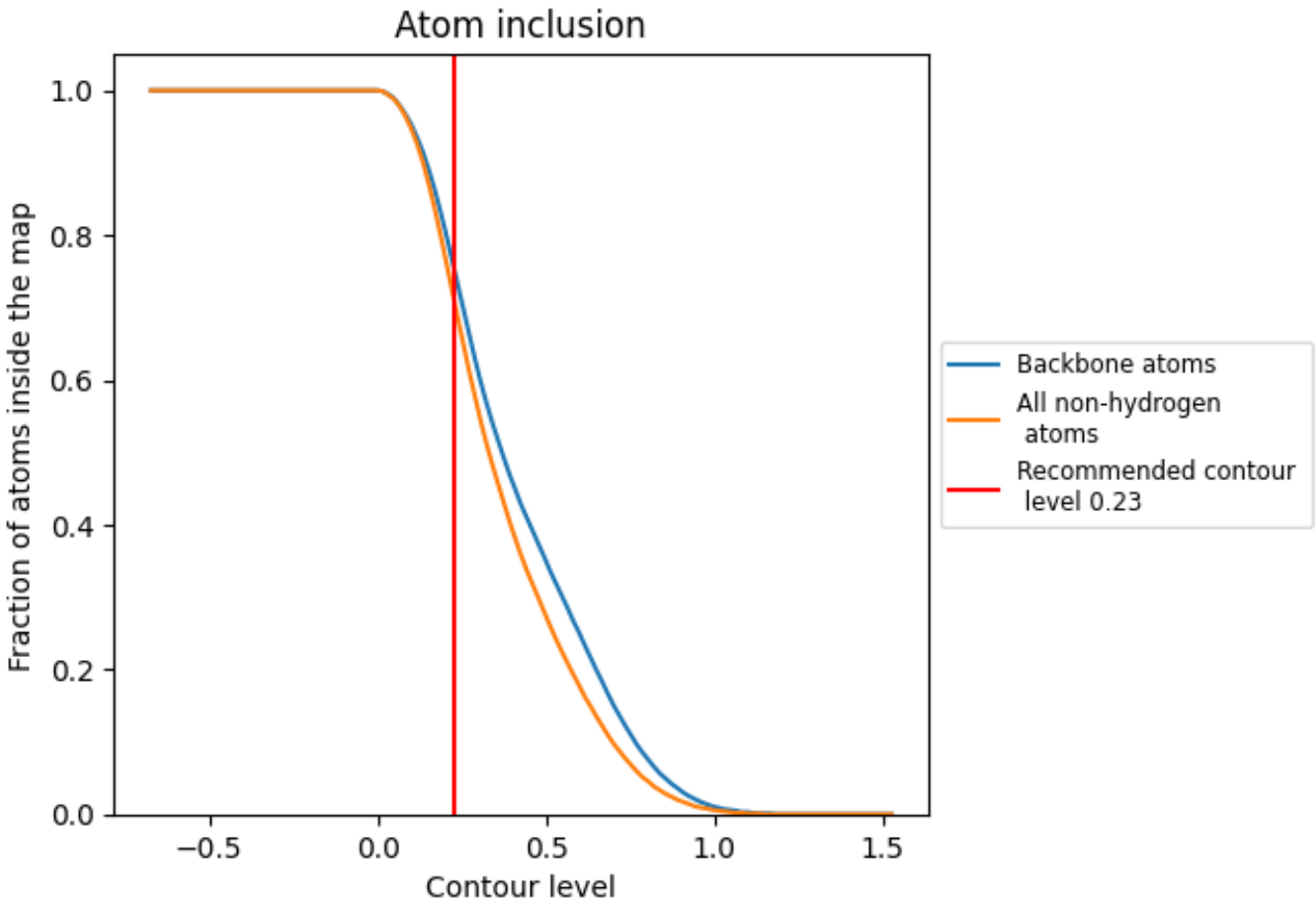
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.23).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.4570
0	0.7780	0.5390
0A	0.9630	0.5780
0B	0.5170	0.3330
0C	0.1030	0.2620
0D	0.0000	0.1240
0E	0.7020	0.3580
1	0.8520	0.5260
1A	0.8440	0.5240
1B	0.8680	0.5140
1C	0.0000	0.2620
1D	0.0000	0.2680
1E	0.3680	0.3570
2	0.9260	0.5380
2A	0.7110	0.4020
2B	0.6840	0.4460
2C	0.0000	0.0900
2D	0.0000	0.0530
3	0.9110	0.4940
3A	0.6900	0.3980
3B	0.7240	0.4480
3C	0.0000	0.2000
3D	0.0000	0.1280
4	0.8160	0.4770
4A	0.9470	0.5720
4B	0.8280	0.5020
4C	0.0000	0.1630
4D	0.5360	0.4130
5	0.7240	0.4800
5A	0.8420	0.5660
5B	0.8620	0.5280
5C	0.0000	0.1930
5D	0.9170	0.5420
6	0.9470	0.5720
6A	0.9310	0.5780

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Chain	Atom inclusion	Q-score
6B	0.8160	0.5310
6C	0.0000	0.1720
6D	0.6550	0.4610
7	0.8680	0.5540
7A	0.8620	0.5180
7B	0.9360	0.5350
7C	0.8750	0.5120
7D	0.7590	0.4250
8	0.8970	0.5490
8A	1.0000	0.6020
8B	0.7870	0.5060
8C	0.9260	0.5860
8D	0.7590	0.5330
9	0.8970	0.5620
9A	0.8680	0.5550
9B	0.9310	0.5480
9C	0.7780	0.5220
9D	0.7450	0.4270
A	0.9040	0.5460
AA	0.8970	0.5580
AB	0.9790	0.5770
AC	0.1070	0.1330
AD	0.9170	0.5680
AE	0.9470	0.5010
B	0.9040	0.5440
BA	0.8950	0.5540
BB	0.8940	0.5440
BC	0.9630	0.5780
BD	0.9330	0.5860
BE	0.7450	0.4390
C	0.6800	0.4450
CA	0.9790	0.5780
CB	0.9310	0.5860
CC	0.7780	0.4690
CD	0.7930	0.4910
CE	0.8420	0.5000
D	0.6430	0.4310
DA	0.8720	0.5340
DB	0.8470	0.5200
DC	0.8890	0.5450
DD	0.9260	0.5220
DE	0.8080	0.5160

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Chain	Atom inclusion	Q-score
E	0.4780	0.3750
EA	0.9310	0.5840
EB	0.0000	0.1940
EC	0.9560	0.5550
ED	0.8890	0.5400
EE	0.9210	0.5520
F	0.4870	0.3680
FA	0.7860	0.4320
FB	0.0000	0.2820
FC	0.7930	0.4170
FD	0.9260	0.5590
FE	0.9570	0.5680
G	0.8520	0.4770
GA	0.9030	0.5140
GB	0.0530	0.1760
GC	1.0000	0.5770
GD	0.8970	0.5680
GE	0.8390	0.5100
H	0.8010	0.4250
HA	0.7410	0.4240
HB	0.1050	0.3060
HC	0.9260	0.5570
HD	0.8610	0.5370
HE	0.8420	0.4860
I	0.7730	0.4450
IA	0.7410	0.4510
IB	0.2340	0.3620
IC	0.9260	0.5610
ID	0.9260	0.5270
IE	0.8940	0.5000
J	0.7780	0.3940
JA	0.7780	0.3850
JB	0.2500	0.3280
JC	0.8970	0.5550
JD	0.8440	0.4440
JE	0.8720	0.5120
K	0.7410	0.4130
KA	0.8440	0.4740
KB	0.1840	0.3940
KC	0.8890	0.5240
KD	0.8890	0.5280
KE	0.8080	0.4650

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Chain	Atom inclusion	Q-score
L	0.7780	0.4480
LA	0.6900	0.3950
LB	0.4810	0.3960
LC	0.8890	0.5170
LD	0.8890	0.5310
LE	0.5790	0.4390
M	0.8220	0.4470
MA	0.8520	0.4740
MB	0.2440	0.3120
MC	0.8440	0.5570
MD	0.8610	0.4970
ME	0.8970	0.5040
N	0.6210	0.2840
NA	0.8520	0.4270
NB	0.3330	0.3090
NC	0.8150	0.4630
ND	0.7220	0.4700
NE	0.7890	0.4830
O	0.7780	0.4630
OA	0.8520	0.5060
OB	0.1850	0.1930
OC	0.8060	0.4770
OD	0.6940	0.3100
OE	0.9310	0.5220
P	0.7780	0.4600
PA	0.8280	0.5150
PB	0.5180	0.4800
PC	0.8060	0.4790
PD	0.8670	0.4610
PE	0.8510	0.4710
Q	0.8520	0.4620
QA	0.7780	0.4610
QB	0.4810	0.2860
QC	0.8330	0.5180
QD	0.8890	0.5130
QE	0.7500	0.4370
R	0.9310	0.5370
RA	0.8150	0.4940
RB	0.4440	0.2560
RC	0.8060	0.3840
RD	0.7780	0.3870
RE	0.9110	0.5200

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Chain	Atom inclusion	Q-score
S	0.7780	0.4730
SA	0.7110	0.4530
SB	0.7410	0.4440
SC	0.8440	0.4550
SD	0.8060	0.3980
SE	0.9150	0.5260
T	0.8150	0.4580
TA	0.7410	0.4780
TB	0.6300	0.3990
TC	0.8150	0.4830
TD	0.8150	0.4730
TE	0.8420	0.4880
U	0.8000	0.4630
UA	0.8890	0.4630
UB	0.7040	0.4000
UC	0.7780	0.3260
UD	0.8610	0.3960
UE	0.8160	0.5000
V	0.7780	0.4470
VA	0.9170	0.4570
VB	0.6440	0.4450
VC	0.8890	0.4570
VD	0.8060	0.4110
VE	0.8750	0.5190
W	0.8330	0.4910
WA	0.7780	0.4080
WB	0.5530	0.3180
WC	0.7780	0.4970
WD	0.7780	0.4540
WE	0.7890	0.5130
X	0.8610	0.4700
XA	0.7780	0.3600
XB	0.4480	0.2390
XC	0.8610	0.4050
XD	0.8150	0.3350
XE	0.8040	0.5410
Y	0.8330	0.4590
YA	0.8000	0.3910
YB	0.7630	0.4680
YC	0.8890	0.4860
YD	0.7780	0.2770
YE	0.8930	0.5300

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Chain	Atom inclusion	Q-score
Z	0.8610	0.4340
ZA	0.7410	0.4490
ZB	0.7630	0.4570
ZC	0.6670	0.4550
ZD	0.6390	0.4140
ZE	0.7930	0.3920
a	0.8440	0.4410
aA	0.8330	0.4450
aB	0.7930	0.4980
aC	0.8520	0.4480
aD	0.5180	0.3540
aE	0.6050	0.3810
b	0.7780	0.4510
bA	0.8330	0.4410
bB	0.8280	0.5180
bC	0.5000	0.2290
bD	0.7780	0.4130
bE	0.7590	0.4020
c	0.8060	0.4370
cA	0.7780	0.4530
cB	0.8970	0.5360
cC	0.5280	0.3360
cD	0.6810	0.4300
cE	0.7660	0.3640
d	0.7780	0.4580
dA	0.8610	0.3890
dB	0.8420	0.4970
dC	0.6300	0.3600
dD	0.6580	0.4100
dE	0.7140	0.4370
e	0.8150	0.4870
eA	0.9170	0.4630
eB	0.9150	0.5530
eC	0.6300	0.4180
eD	0.7630	0.3990
eE	0.7860	0.4490
f	0.9440	0.5040
fA	0.6940	0.4290
fB	0.7870	0.5330
fC	0.5750	0.3830
fD	0.7230	0.4490
fE	0.8720	0.4850

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Chain	Atom inclusion	Q-score
g	0.8330	0.4840
gA	0.8150	0.4250
gB	0.8280	0.5060
gC	0.6580	0.4490
gD	0.6390	0.4450
gE	0.8160	0.4100
h	0.7500	0.4980
hA	0.8330	0.4740
hB	0.0000	0.1560
hC	0.7890	0.4280
hD	0.6320	0.3890
hE	0.8420	0.5460
i	0.8520	0.4700
iA	0.7780	0.4720
iB	0.0000	0.2310
iC	0.6170	0.4160
iD	0.6670	0.4500
iE	0.7680	0.4430
j	0.8890	0.4050
jA	0.8150	0.4760
jB	0.0260	0.2520
jC	0.7220	0.4740
jD	0.6670	0.3890
jE	0.6580	0.4430
k	0.6670	0.4760
kA	0.7780	0.4850
kB	0.0790	0.3290
kC	0.6050	0.4680
kD	0.5000	0.3100
kE	0.7870	0.5230
l	0.8520	0.5100
lA	0.7450	0.5000
lB	0.1280	0.2920
lC	0.7410	0.4410
lD	0.4070	0.3160
lE	0.7140	0.4250
m	0.8150	0.5080
mA	0.7630	0.4890
mB	0.1940	0.3010
mC	0.4890	0.3020
mD	0.4440	0.3290
mE	0.6900	0.3890

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Chain	Atom inclusion	Q-score
n	0.8080	0.5140
nA	0.8950	0.5250
nB	0.1840	0.3300
nC	0.5280	0.3920
nD	0.5560	0.3220
nE	0.6550	0.3630
o	0.7630	0.5030
oA	0.8510	0.5520
oB	0.3330	0.3180
oC	0.5180	0.3730
oD	0.4440	0.2630
oE	0.7590	0.4430
p	0.8680	0.5220
pA	0.8330	0.5440
pB	0.2220	0.2920
pC	0.6300	0.4570
pD	0.3330	0.2780
pE	0.7230	0.4180
q	0.8720	0.5400
qA	0.7890	0.5110
qB	0.3330	0.3340
qC	0.6300	0.4800
qD	0.4440	0.3680
qE	0.9470	0.4750
r	0.8890	0.5240
rA	0.8520	0.5530
rB	0.2220	0.3440
rC	0.2220	0.2050
rD	0.4440	0.3570
rE	0.6170	0.3780
s	0.8680	0.5100
sA	0.8220	0.5170
sB	0.5180	0.4020
sC	0.2960	0.1860
sD	0.3560	0.2430
sE	0.7630	0.4880
t	0.8890	0.5320
tA	0.8060	0.5160
tB	0.4810	0.3170
tC	0.5180	0.3590
tD	0.2630	0.1910
tE	0.8300	0.4560

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Chain	Atom inclusion	Q-score
u	0.8000	0.4770
uA	0.8150	0.5290
uB	0.5180	0.3210
uC	0.2960	0.4020
uD	0.1380	0.3240
uE	0.8420	0.4630
v	0.8060	0.5020
vA	0.8150	0.5300
vB	0.4810	0.3010
vC	0.4220	0.3310
vD	0.3160	0.3560
vE	0.8300	0.5180
w	0.7780	0.4950
wA	0.8520	0.5070
wB	0.7040	0.4330
wC	0.3420	0.1360
wD	0.3420	0.3580
wE	0.8210	0.4240
x	0.7040	0.4250
xA	0.8520	0.5250
xB	0.8520	0.5470
xC	0.1380	0.2600
xD	0.1030	0.2690
xE	0.7630	0.4430
y	0.8520	0.5030
yA	0.8520	0.5570
yB	0.7110	0.4230
yC	0.3420	0.2610
yD	0.0000	0.2070
yE	0.7660	0.4270
z	0.7780	0.4980
zA	0.8890	0.5340
zB	0.6320	0.3580
zC	0.1050	0.2530
zD	0.0000	0.1780
zE	0.6810	0.4300