



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2025 – 04:34 PM JST

PDB ID : 9JJ8 / pdb\_00009jj8  
EMDB ID : EMD-61519  
Title : Structural insights into the PSI-FCPI supercomplex from the coccolithophore  
Emiliana huxleyi  
Authors : Shen, L.L.; Li, Z.H.; Wang, W.D.  
Deposited on : 2024-09-13  
Resolution : 2.79 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

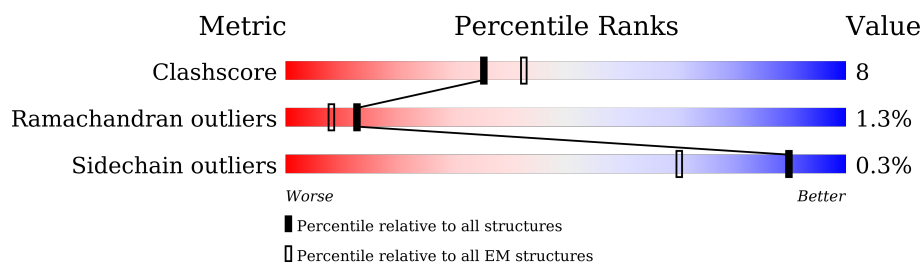
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.79 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)
Clashscore	210492	15764
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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	a	752	84% 15% .
2	b	734	88% 12%
3	c	81	85% 12% ..
4	d	142	87% 10% ..
5	e	131	46% . 52%
6	f	184	79% 8% 12%
7	i	36	78% 14% 8%
8	j	40	78% 22%
9	l	145	86% 13% .

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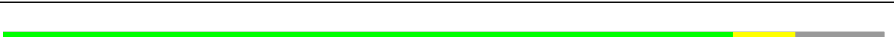


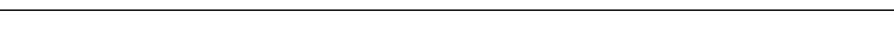
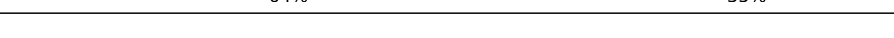
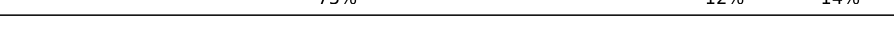



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Mol	Chain	Length	Quality of chain
10	m	30	
11	k	145	
12	o	123	
13	A	201	
14	B	177	
15	C	233	
16	D	231	
17	E	217	
18	F	239	
19	G	204	
20	H	210	
21	J	251	
22	K	198	
23	L	244	
24	M	224	
24	P	224	
24	W	224	
25	O	219	
26	Q	257	
27	5	219	
27	R	219	
27	V	219	
27	X	219	
28	4	255	
28	7	255	

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Mol	Chain	Length	Quality of chain
28	S	255	
28	x	255	
28	y	255	
28	z	255	
29	T	211	
30	U	198	
31	0	254	
32	1	253	
33	3	268	
34	6	250	
34	8	250	
35	9	245	
36	I	209	
37	h	133	
38	2	260	
38	Y	260	
38	Z	260	

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
39	CLA	0	310	X	-	-	-
39	CLA	0	312	X	-	-	-
39	CLA	0	313	X	-	-	-
39	CLA	0	315	X	-	-	-
39	CLA	0	318	X	-	-	-
39	CLA	0	320	X	-	-	-
39	CLA	0	322	X	-	-	-
39	CLA	0	323	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	1	308	X	-	-	-
39	CLA	1	309	X	-	-	-
39	CLA	1	310	X	-	-	-
39	CLA	1	311	X	-	-	-
39	CLA	1	313	X	-	-	-
39	CLA	1	316	X	-	-	-
39	CLA	1	317	X	-	-	-
39	CLA	1	319	X	-	-	-
39	CLA	1	320	X	-	-	-
39	CLA	2	307	X	-	-	-
39	CLA	2	308	X	-	-	-
39	CLA	2	309	X	-	-	-
39	CLA	2	310	X	-	-	-
39	CLA	2	312	X	-	-	-
39	CLA	2	315	X	-	-	-
39	CLA	2	316	X	-	-	-
39	CLA	2	318	X	-	-	-
39	CLA	3	311	X	-	-	-
39	CLA	3	312	X	-	-	-
39	CLA	3	313	X	-	-	-
39	CLA	3	314	X	-	-	-
39	CLA	3	316	X	-	-	-
39	CLA	3	319	X	-	-	-
39	CLA	3	320	X	-	-	-
39	CLA	3	322	X	-	-	-
39	CLA	3	323	X	-	-	-
39	CLA	4	311	X	-	-	-
39	CLA	4	313	X	-	-	-
39	CLA	4	314	X	-	-	-
39	CLA	4	316	X	-	-	-
39	CLA	4	319	X	-	-	-
39	CLA	4	322	X	-	-	-
39	CLA	4	323	X	-	-	-
39	CLA	5	306	X	-	-	-
39	CLA	5	307	X	-	-	-
39	CLA	5	308	X	-	-	-
39	CLA	5	310	X	-	-	-
39	CLA	5	315	X	-	-	-
39	CLA	5	316	X	-	-	-
39	CLA	6	310	X	-	-	-
39	CLA	6	311	X	-	-	-
39	CLA	6	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	6	313	X	-	-	-
39	CLA	6	315	X	-	-	-
39	CLA	6	318	X	-	-	-
39	CLA	6	321	X	-	-	-
39	CLA	6	322	X	-	-	-
39	CLA	7	313	X	-	-	-
39	CLA	7	314	X	-	-	-
39	CLA	7	315	X	-	-	-
39	CLA	7	316	X	-	-	-
39	CLA	7	318	X	-	-	-
39	CLA	7	321	X	-	-	-
39	CLA	7	324	X	-	-	-
39	CLA	8	310	X	-	-	-
39	CLA	8	311	X	-	-	-
39	CLA	8	312	X	-	-	-
39	CLA	8	313	X	-	-	-
39	CLA	8	315	X	-	-	-
39	CLA	8	318	X	-	-	-
39	CLA	8	321	X	-	-	-
39	CLA	9	307	X	-	-	-
39	CLA	9	308	X	-	-	-
39	CLA	9	309	X	-	-	-
39	CLA	9	310	X	-	-	-
39	CLA	9	312	X	-	-	-
39	CLA	9	315	X	-	-	-
39	CLA	9	319	X	-	-	-
39	CLA	9	320	X	-	-	-
39	CLA	A	305	X	-	-	-
39	CLA	A	306	X	-	-	-
39	CLA	A	307	X	-	-	-
39	CLA	A	308	X	-	-	-
39	CLA	A	309	X	-	-	-
39	CLA	A	311	X	-	-	-
39	CLA	A	312	X	-	-	-
39	CLA	A	314	X	-	-	-
39	CLA	A	315	X	-	-	-
39	CLA	B	203	X	-	-	-
39	CLA	B	204	X	-	-	-
39	CLA	B	205	X	-	-	-
39	CLA	B	206	X	-	-	-
39	CLA	B	207	X	-	-	-
39	CLA	B	209	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	C	304	X	-	-	-
39	CLA	C	305	X	-	-	-
39	CLA	C	306	X	-	-	-
39	CLA	C	307	X	-	-	-
39	CLA	C	308	X	-	-	-
39	CLA	C	309	X	-	-	-
39	CLA	C	310	X	-	-	-
39	CLA	C	311	X	-	-	-
39	CLA	D	309	X	-	-	-
39	CLA	D	310	X	-	-	-
39	CLA	D	311	X	-	-	-
39	CLA	D	312	X	-	-	-
39	CLA	D	313	X	-	-	-
39	CLA	D	314	X	-	-	-
39	CLA	D	315	X	-	-	-
39	CLA	D	316	X	-	-	-
39	CLA	D	317	X	-	-	-
39	CLA	D	318	X	-	-	-
39	CLA	D	319	X	-	-	-
39	CLA	E	306	X	-	-	-
39	CLA	E	307	X	-	-	-
39	CLA	E	308	X	-	-	-
39	CLA	E	309	X	-	-	-
39	CLA	E	310	X	-	-	-
39	CLA	E	312	X	-	-	-
39	CLA	E	313	X	-	-	-
39	CLA	E	314	X	-	-	-
39	CLA	E	315	X	-	-	-
39	CLA	E	316	X	-	-	-
39	CLA	E	317	X	-	-	-
39	CLA	E	318	X	-	-	-
39	CLA	E	319	X	-	-	-
39	CLA	F	306	X	-	-	-
39	CLA	F	308	X	-	-	-
39	CLA	F	309	X	-	-	-
39	CLA	F	310	X	-	-	-
39	CLA	F	312	X	-	-	-
39	CLA	F	313	X	-	-	-
39	CLA	F	314	X	-	-	-
39	CLA	F	315	X	-	-	-
39	CLA	F	316	X	-	-	-
39	CLA	F	321	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	G	309	X	-	-	-
39	CLA	G	310	X	-	-	-
39	CLA	G	312	X	-	-	-
39	CLA	G	314	X	-	-	-
39	CLA	G	318	X	-	-	-
39	CLA	H	306	X	-	-	-
39	CLA	H	307	X	-	-	-
39	CLA	H	308	X	-	-	-
39	CLA	H	309	X	-	-	-
39	CLA	H	310	X	-	-	-
39	CLA	H	312	X	-	-	-
39	CLA	H	313	X	-	-	-
39	CLA	H	315	X	-	-	-
39	CLA	H	316	X	-	-	-
39	CLA	I	301	X	-	-	-
39	CLA	I	308	X	-	-	-
39	CLA	I	309	X	-	-	-
39	CLA	I	310	X	-	-	-
39	CLA	I	311	X	-	-	-
39	CLA	I	313	X	-	-	-
39	CLA	I	314	X	-	-	-
39	CLA	I	315	X	-	-	-
39	CLA	I	316	X	-	-	-
39	CLA	J	307	X	-	-	-
39	CLA	J	308	X	-	-	-
39	CLA	J	309	X	-	-	-
39	CLA	J	310	X	-	-	-
39	CLA	J	311	X	-	-	-
39	CLA	J	312	X	-	-	-
39	CLA	J	313	X	-	-	-
39	CLA	J	314	X	-	-	-
39	CLA	J	316	X	-	-	-
39	CLA	J	317	X	-	-	-
39	CLA	J	318	X	-	-	-
39	CLA	K	306	X	-	-	-
39	CLA	K	307	X	-	-	-
39	CLA	K	308	X	-	-	-
39	CLA	K	309	X	-	-	-
39	CLA	K	311	X	-	-	-
39	CLA	K	312	X	-	-	-
39	CLA	K	314	X	-	-	-
39	CLA	L	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	L	309	X	-	-	-
39	CLA	L	310	X	-	-	-
39	CLA	L	311	X	-	-	-
39	CLA	L	313	X	-	-	-
39	CLA	L	316	X	-	-	-
39	CLA	L	319	X	-	-	-
39	CLA	L	320	X	-	-	-
39	CLA	M	308	X	-	-	-
39	CLA	M	309	X	-	-	-
39	CLA	M	310	X	-	-	-
39	CLA	M	312	X	-	-	-
39	CLA	M	315	X	-	-	-
39	CLA	M	317	X	-	-	-
39	CLA	M	318	X	-	-	-
39	CLA	M	321	X	-	-	-
39	CLA	O	308	X	-	-	-
39	CLA	O	309	X	-	-	-
39	CLA	O	310	X	-	-	-
39	CLA	O	311	X	-	-	-
39	CLA	O	312	X	-	-	-
39	CLA	O	313	X	-	-	-
39	CLA	O	314	X	-	-	-
39	CLA	O	316	X	-	-	-
39	CLA	O	318	X	-	-	-
39	CLA	P	307	X	-	-	-
39	CLA	P	308	X	-	-	-
39	CLA	P	309	X	-	-	-
39	CLA	P	311	X	-	-	-
39	CLA	P	314	X	-	-	-
39	CLA	P	316	X	-	-	-
39	CLA	Q	309	X	-	-	-
39	CLA	Q	310	X	-	-	-
39	CLA	Q	311	X	-	-	-
39	CLA	Q	312	X	-	-	-
39	CLA	Q	314	X	-	-	-
39	CLA	Q	317	X	-	-	-
39	CLA	Q	320	X	-	-	-
39	CLA	Q	321	X	-	-	-
39	CLA	R	307	X	-	-	-
39	CLA	R	308	X	-	-	-
39	CLA	R	309	X	-	-	-
39	CLA	R	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	R	315	X	-	-	-
39	CLA	R	316	X	-	-	-
39	CLA	S	308	X	-	-	-
39	CLA	S	310	X	-	-	-
39	CLA	S	311	X	-	-	-
39	CLA	S	313	X	-	-	-
39	CLA	S	316	X	-	-	-
39	CLA	S	319	X	-	-	-
39	CLA	S	320	X	-	-	-
39	CLA	T	308	X	-	-	-
39	CLA	T	309	X	-	-	-
39	CLA	T	310	X	-	-	-
39	CLA	T	311	X	-	-	-
39	CLA	T	313	X	-	-	-
39	CLA	T	318	X	-	-	-
39	CLA	T	319	X	-	-	-
39	CLA	T	320	X	-	-	-
39	CLA	U	201	X	-	-	-
39	CLA	U	207	X	-	-	-
39	CLA	U	208	X	-	-	-
39	CLA	U	209	X	-	-	-
39	CLA	U	210	X	-	-	-
39	CLA	U	211	X	-	-	-
39	CLA	U	212	X	-	-	-
39	CLA	U	213	X	-	-	-
39	CLA	U	214	X	-	-	-
39	CLA	U	215	X	-	-	-
39	CLA	V	309	X	-	-	-
39	CLA	V	310	X	-	-	-
39	CLA	V	311	X	-	-	-
39	CLA	V	313	X	-	-	-
39	CLA	V	316	X	-	-	-
39	CLA	V	319	X	-	-	-
39	CLA	W	309	X	-	-	-
39	CLA	W	310	X	-	-	-
39	CLA	W	311	X	-	-	-
39	CLA	W	313	X	-	-	-
39	CLA	W	316	X	-	-	-
39	CLA	W	318	X	-	-	-
39	CLA	W	319	X	-	-	-
39	CLA	X	307	X	-	-	-
39	CLA	X	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	X	309	X	-	-	-
39	CLA	X	311	X	-	-	-
39	CLA	X	316	X	-	-	-
39	CLA	X	317	X	-	-	-
39	CLA	Y	302	X	-	-	-
39	CLA	Y	303	X	-	-	-
39	CLA	Y	304	X	-	-	-
39	CLA	Y	305	X	-	-	-
39	CLA	Y	307	X	-	-	-
39	CLA	Y	310	X	-	-	-
39	CLA	Y	311	X	-	-	-
39	CLA	Y	313	X	-	-	-
39	CLA	Y	314	X	-	-	-
39	CLA	Z	304	X	-	-	-
39	CLA	Z	305	X	-	-	-
39	CLA	Z	306	X	-	-	-
39	CLA	Z	307	X	-	-	-
39	CLA	Z	309	X	-	-	-
39	CLA	Z	312	X	-	-	-
39	CLA	Z	313	X	-	-	-
39	CLA	Z	315	X	-	-	-
39	CLA	a	801	X	-	-	-
39	CLA	a	802	X	-	-	-
39	CLA	a	803	X	-	-	-
39	CLA	a	804	X	-	-	-
39	CLA	a	805	X	-	-	-
39	CLA	a	806	X	-	-	-
39	CLA	a	807	X	-	-	-
39	CLA	a	808	X	-	-	-
39	CLA	a	809	X	-	-	-
39	CLA	a	810	X	-	-	-
39	CLA	a	811	X	-	-	-
39	CLA	a	812	X	-	-	-
39	CLA	a	813	X	-	-	-
39	CLA	a	814	X	-	-	-
39	CLA	a	815	X	-	-	-
39	CLA	a	816	X	-	-	-
39	CLA	a	817	X	-	-	-
39	CLA	a	818	X	-	-	-
39	CLA	a	819	X	-	-	-
39	CLA	a	820	X	-	-	-
39	CLA	a	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	a	822	X	-	-	-
39	CLA	a	823	X	-	-	-
39	CLA	a	824	X	-	-	-
39	CLA	a	825	X	-	-	-
39	CLA	a	826	X	-	-	-
39	CLA	a	827	X	-	-	-
39	CLA	a	828	X	-	-	-
39	CLA	a	829	X	-	-	-
39	CLA	a	830	X	-	-	-
39	CLA	a	831	X	-	-	-
39	CLA	a	832	X	-	-	-
39	CLA	a	833	X	-	-	-
39	CLA	a	834	X	-	-	-
39	CLA	a	835	X	-	-	-
39	CLA	a	837	X	-	-	-
39	CLA	a	838	X	-	-	-
39	CLA	a	847	X	-	-	-
39	CLA	b	801	X	-	-	-
39	CLA	b	802	X	-	-	-
39	CLA	b	803	X	-	-	-
39	CLA	b	805	X	-	-	-
39	CLA	b	806	X	-	-	-
39	CLA	b	807	X	-	-	-
39	CLA	b	808	X	-	-	-
39	CLA	b	809	X	-	-	-
39	CLA	b	810	X	-	-	-
39	CLA	b	811	X	-	-	-
39	CLA	b	812	X	-	-	-
39	CLA	b	813	X	-	-	-
39	CLA	b	814	X	-	-	-
39	CLA	b	815	X	-	-	-
39	CLA	b	816	X	-	-	-
39	CLA	b	817	X	-	-	-
39	CLA	b	818	X	-	-	-
39	CLA	b	819	X	-	-	-
39	CLA	b	820	X	-	-	-
39	CLA	b	821	X	-	-	-
39	CLA	b	822	X	-	-	-
39	CLA	b	823	X	-	-	-
39	CLA	b	824	X	-	-	-
39	CLA	b	825	X	-	-	-
39	CLA	b	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	b	827	X	-	-	-
39	CLA	b	828	X	-	-	-
39	CLA	b	829	X	-	-	-
39	CLA	b	830	X	-	-	-
39	CLA	b	831	X	-	-	-
39	CLA	b	832	X	-	-	-
39	CLA	b	833	X	-	-	-
39	CLA	b	834	X	-	-	-
39	CLA	b	835	X	-	-	-
39	CLA	b	836	X	-	-	-
39	CLA	b	837	X	-	-	-
39	CLA	b	838	X	-	-	-
39	CLA	b	839	X	-	-	-
39	CLA	b	840	X	-	-	-
39	CLA	b	841	X	-	-	-
39	CLA	b	842	X	-	-	-
39	CLA	b	851	X	-	-	-
39	CLA	f	802	X	-	-	-
39	CLA	f	803	X	-	-	-
39	CLA	h	201	X	-	-	-
39	CLA	i	101	X	-	-	-
39	CLA	i	103	X	-	-	-
39	CLA	j	101	X	-	-	-
39	CLA	k	201	X	-	-	-
39	CLA	k	202	X	-	-	-
39	CLA	k	203	X	-	-	-
39	CLA	l	201	X	-	-	-
39	CLA	l	204	X	-	-	-
39	CLA	l	205	X	-	-	-
39	CLA	o	201	X	-	-	-
39	CLA	o	202	X	-	-	-
39	CLA	o	203	X	-	-	-
39	CLA	o	205	X	-	-	-
39	CLA	o	206	X	-	-	-
39	CLA	x	306	X	-	-	-
39	CLA	x	307	X	-	-	-
39	CLA	x	308	X	-	-	-
39	CLA	x	309	X	-	-	-
39	CLA	x	311	X	-	-	-
39	CLA	x	314	X	-	-	-
39	CLA	x	317	X	-	-	-
39	CLA	x	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CLA	y	307	X	-	-	-
39	CLA	y	308	X	-	-	-
39	CLA	y	309	X	-	-	-
39	CLA	y	310	X	-	-	-
39	CLA	y	312	X	-	-	-
39	CLA	y	315	X	-	-	-
39	CLA	y	318	X	-	-	-
39	CLA	y	319	X	-	-	-
39	CLA	z	306	X	-	-	-
39	CLA	z	307	X	-	-	-
39	CLA	z	308	X	-	-	-
39	CLA	z	309	X	-	-	-
39	CLA	z	311	X	-	-	-
39	CLA	z	314	X	-	-	-
39	CLA	z	317	X	-	-	-
39	CLA	z	318	X	-	-	-
46	LMG	4	326	-	-	X	-
48	A86	Q	304	-	-	X	-
49	KC2	5	313	-	-	X	-
51	A1ECV	0	321	X	-	-	-
51	A1ECV	1	318	X	-	-	-
51	A1ECV	2	311	X	-	-	-
51	A1ECV	4	315	X	-	-	-
51	A1ECV	4	321	X	-	-	-
51	A1ECV	5	309	X	-	-	-
51	A1ECV	5	312	X	-	-	-
51	A1ECV	6	320	X	-	-	-
51	A1ECV	7	317	X	-	-	-
51	A1ECV	7	323	X	-	-	-
51	A1ECV	9	314	X	-	-	-
51	A1ECV	9	317	X	-	-	-
51	A1ECV	E	311	X	-	-	-
51	A1ECV	G	316	X	-	-	-
51	A1ECV	L	318	X	-	-	-
51	A1ECV	M	316	X	-	-	-
51	A1ECV	O	315	X	-	-	-
51	A1ECV	P	315	X	-	-	-
51	A1ECV	Q	316	X	-	-	-
51	A1ECV	Q	319	X	-	-	-
51	A1ECV	R	310	X	-	-	-
51	A1ECV	R	313	X	-	-	-
51	A1ECV	S	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
51	A1ECV	S	318	X	-	-	-
51	A1ECV	T	317	X	-	-	-
51	A1ECV	V	317	X	-	-	-
51	A1ECV	W	317	X	-	-	-
51	A1ECV	X	310	X	-	-	-
51	A1ECV	X	313	X	-	-	-
51	A1ECV	Y	306	X	-	-	-
51	A1ECV	Y	312	X	-	-	-
51	A1ECV	Z	308	X	-	-	-
51	A1ECV	Z	314	X	-	-	-
51	A1ECV	x	310	X	-	-	-
51	A1ECV	x	316	X	-	-	-
51	A1ECV	y	311	X	-	-	-
51	A1ECV	y	317	X	-	-	-
51	A1ECV	z	310	X	-	-	-
51	A1ECV	z	316	X	-	-	-

## 2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 114135 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	741	Total	C	N	O	S	0	0
			5835	3817	993	995	30		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	733	Total	C	N	O	S	0	0
			5818	3828	982	987	21		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	80	Total	C	N	O	S	0	0
			598	365	105	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	140	Total	C	N	O	S	0	0
			1103	710	184	206	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	63	Total	C	N	O	S	0	0
			491	314	86	90	1		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	161	Total	C	N	O	S	0	0
			1232	797	207	224	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	33	Total	C	N	O	S	0	0
			254	176	34	43	1		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			318	211	47	57	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	143	Total	C	N	O	S	0	0
			1084	716	172	195	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	30	Total	C	N	O	S	0	0
			224	149	35	38	2		

- Molecule 11 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	73	Total	C	N	O	S	0	0
			533	347	87	93	6		

- Molecule 12 is a protein called Linker-protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	o	48	Total	C	N	O	S	0	0
			360	231	61	66	2		

- Molecule 13 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	183	Total	C	N	O	S	0	0
			1419	916	229	264	10		

- Molecule 14 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	172	Total	C	N	O	S	0	0
			1255	805	212	231	7		

- Molecule 15 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	176	Total	C	N	O	S	0	0
			1329	857	221	242	9		

- Molecule 16 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	189	Total	C	N	O	S	0	0
			1424	921	226	271	6		

- Molecule 17 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	187	Total	C	N	O	S	0	0
			1384	896	222	258	8		

- Molecule 18 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	188	Total	C	N	O	S	0	0
			1411	907	244	251	9		

- Molecule 19 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	171	Total	C	N	O	S	0	0
			1340	875	226	232	7		

- Molecule 20 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	168	Total	C	N	O	S	0	0
			1263	810	206	235	12		

- Molecule 21 is a protein called Light harvesting protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	171	Total	C	N	O	S	0	0
			1270	810	223	230	7		

- Molecule 22 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	168	Total	C	N	O	S	0	0
			1251	806	206	231	8		

- Molecule 23 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	210	Total	C	N	O	S	0	0
			1626	1064	273	281	8		

- Molecule 24 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
24	P	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
24	W	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		

- Molecule 25 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	155	Total	C	N	O	S	0	0
			1133	717	200	209	7		

- Molecule 26 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	215	Total	C	N	O	S	0	0
			1666	1094	273	294	5		

- Molecule 27 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	188	Total	C	N	O	S	0	0
			1353	872	227	248	6		
27	X	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		
27	5	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		

- Molecule 28 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	4	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	7	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	x	228	Total	C	N	O		0	0
			1113	657	228	228			
28	y	228	Total	C	N	O		0	0
			1113	657	228	228			
28	z	228	Total	C	N	O		0	0
			1113	657	228	228			

- Molecule 29 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	197	Total	C	N	O	S	0	0
			1482	973	246	257	6		

- Molecule 30 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	158	Total	C	N	O	S	0	0
			1240	801	207	226	6		

- Molecule 31 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	0	218	Total	C	N	O	S	0	0
			1706	1114	278	309	5		

- Molecule 32 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	201	Total	C	N	O	S	0	0
			1255	794	223	237	1		

- Molecule 33 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	3	236	Total	C	N	O	S	0	0
			1775	1155	294	318	8		

- Molecule 34 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	224	Total	C	N	O	S	0	0
			1415	892	255	261	7		
34	6	224	Total	C	N	O	S	0	0
			1326	825	249	250	2		

- Molecule 35 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	209	Total	C	N	O	S	0	0
			1490	970	246	267	7		

- Molecule 36 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	I	156	Total	C	N	O	S	0	0
			1203	780	201	213	9		

- Molecule 37 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	87	Total	C	N	O	S	0	0
			650	425	104	120	1		

- Molecule 38 is a protein called Light harvesting protein.

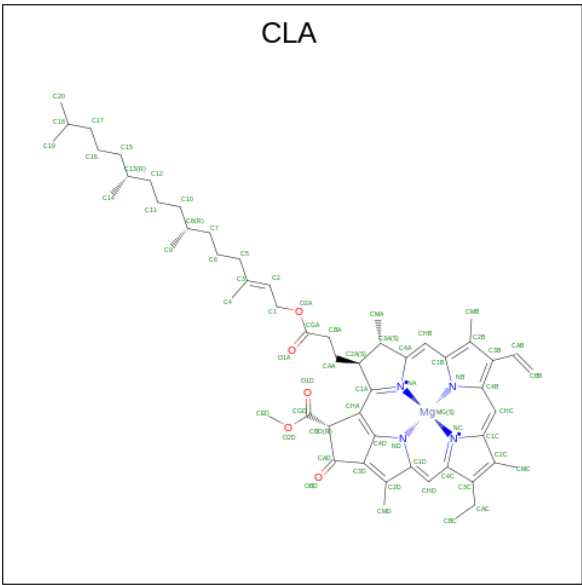
Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	225	Total	C	N	O		0	0
			1099	649	225	225			
38	Z	225	Total	C	N	O		0	0
			1099	649	225	225			

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Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	224	Total	C	N	O	S	0	0
			1383	858	256	263	6		

- Molecule 39 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
39	b	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
39	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
39	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	l	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	l	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	k	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	o	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	o	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	o	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	o	1	Total 58	C 48	Mg 1	N 4	O 5	0
39	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
39	C	1	Total 43	C 35	Mg 1	N 4	O 3	0
39	C	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	D	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	E	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	E	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
39	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	H	1	Total 48	C 38	Mg 1	N 4	O 5	0
39	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	H	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	H	1	Total 57	C 47	Mg 1	N 4	O 5	0
39	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	J	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	J	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	K	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	K	1	Total 59	C 49	Mg 1	N 4	O 5	0
39	K	1	Total 62	C 52	Mg 1	N 4	O 5	0
39	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	L	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	L	1	Total 54	C 44	Mg 1	N 4	O 5	0
39	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	L	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	M	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	M	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	M	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	O	1	Total 38	C 32	Mg 1	N 4	O 1	0
39	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	O	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	P	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	Q	1	Total 54	C 44	Mg 1	N 4	O 5	0
39	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	Q	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	Q	1	Total 53	C 43	Mg 1	N 4	O 5	0
39	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	R	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	R	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	S	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	T	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	V	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	W	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	W	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	X	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	0	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	0	1	Total 53	C 43	Mg 1	N 4	O 5	0
39	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	0	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	0	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
39	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	0	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	0	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	3	1	Total 53	C 43	Mg 1	N 4	O 5	0
39	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	4	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	5	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	7	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
39	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	7	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
39	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	I	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	I	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	I	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	I	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	I	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	y	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	y	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	y	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
39	y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	z	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0

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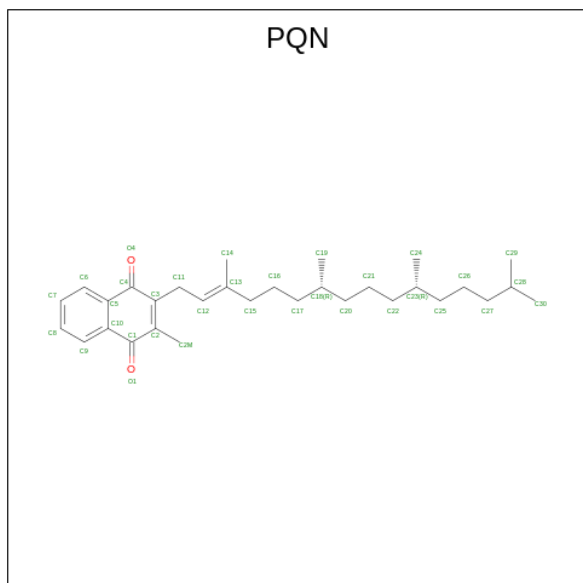
Mol	Chain	Residues	Atoms					AltConf
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
39	6	1	Total 52	C 44	Mg 1	N 4	O 3	0
39	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	6	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
39	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

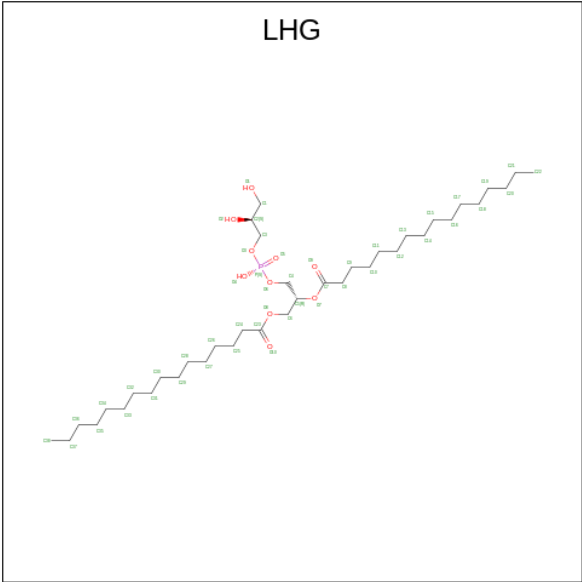
- Molecule 40 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
40	a	1	Total	C	O	0
			33	31	2	
40	b	1	Total	C	O	0
			33	31	2	

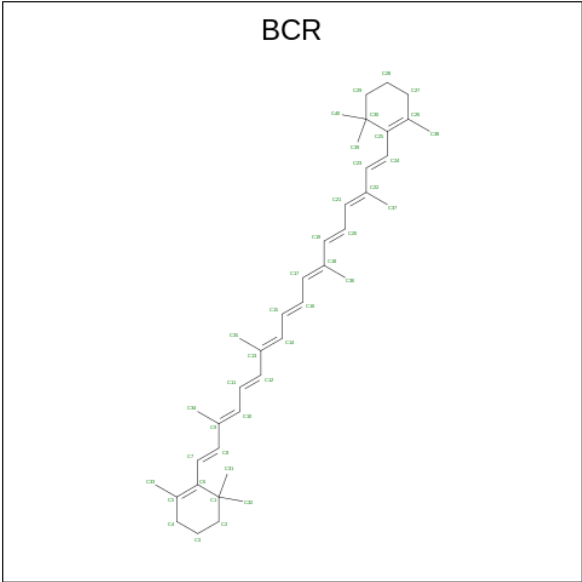
- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf
41	a	1	Total	C	O	P	0
			49	38	10	1	
41	a	1	Total	C	O	P	0
			27	16	10	1	
41	j	1	Total	C	O	P	0
			30	19	10	1	
41	D	1	Total	C	O	P	0
			35	24	10	1	
41	D	1	Total	C	O	P	0
			35	24	10	1	
41	H	1	Total	C	O	P	0
			35	24	10	1	
41	X	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 42 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



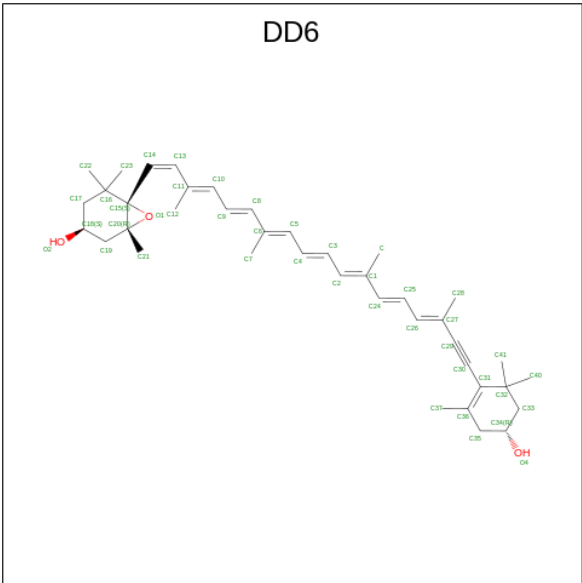
Mol	Chain	Residues	Atoms	AltConf
42	a	1	Total C 40 40	0
42	a	1	Total C 40 40	0
42	a	1	Total C 40 40	0
42	a	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	f	1	Total C 40 40	0
42	f	1	Total C 40 40	0
42	i	1	Total C 40 40	0
42	j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
42	l	1	Total C 40 40	0
42	l	1	Total C 40 40	0
42	l	1	Total C 40 40	0
42	m	1	Total C 40 40	0
42	k	1	Total C 40 40	0
42	h	1	Total C 40 40	0

- Molecule 43 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
43	a	1	Total C O 43 40 3	0
43	j	1	Total C O 43 40 3	0
43	o	1	Total C O 43 40 3	0
43	A	1	Total C O 43 40 3	0

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Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total 43	C 40	O 3	0
43	A	1	Total 43	C 40	O 3	0
43	A	1	Total 43	C 40	O 3	0
43	B	1	Total 43	C 40	O 3	0
43	C	1	Total 43	C 40	O 3	0
43	D	1	Total 43	C 40	O 3	0
43	D	1	Total 43	C 40	O 3	0
43	D	1	Total 43	C 40	O 3	0
43	E	1	Total 43	C 40	O 3	0
43	E	1	Total 43	C 40	O 3	0
43	E	1	Total 43	C 40	O 3	0
43	F	1	Total 43	C 40	O 3	0
43	F	1	Total 43	C 40	O 3	0
43	G	1	Total 43	C 40	O 3	0
43	G	1	Total 43	C 40	O 3	0
43	H	1	Total 43	C 40	O 3	0
43	H	1	Total 43	C 40	O 3	0
43	J	1	Total 43	C 40	O 3	0
43	J	1	Total 43	C 40	O 3	0
43	J	1	Total 43	C 40	O 3	0
43	K	1	Total 43	C 40	O 3	0

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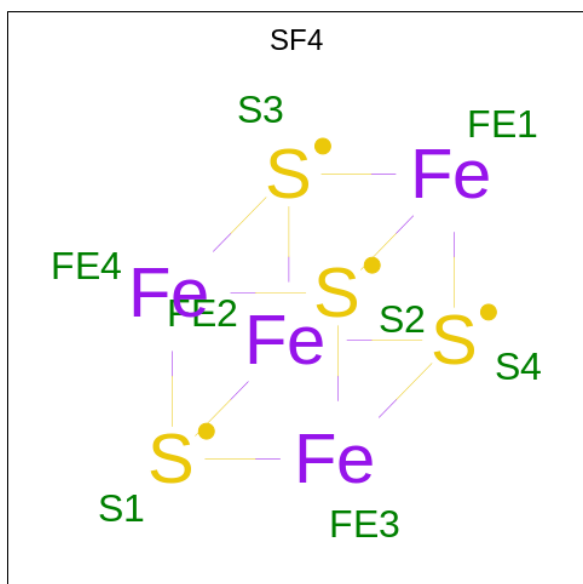
Mol	Chain	Residues	Atoms			AltConf
43	M	1	Total 43	C 40	O 3	0
43	O	1	Total 43	C 40	O 3	0
43	O	1	Total 43	C 40	O 3	0
43	O	1	Total 43	C 40	O 3	0
43	P	1	Total 43	C 40	O 3	0
43	Q	1	Total 43	C 40	O 3	0
43	Q	1	Total 43	C 40	O 3	0
43	R	1	Total 43	C 40	O 3	0
43	S	1	Total 43	C 40	O 3	0
43	T	1	Total 43	C 40	O 3	0
43	U	1	Total 43	C 40	O 3	0
43	V	1	Total 43	C 40	O 3	0
43	W	1	Total 43	C 40	O 3	0
43	X	1	Total 43	C 40	O 3	0
43	1	1	Total 43	C 40	O 3	0
43	3	1	Total 43	C 40	O 3	0
43	3	1	Total 43	C 40	O 3	0
43	4	1	Total 43	C 40	O 3	0
43	4	1	Total 43	C 40	O 3	0
43	5	1	Total 43	C 40	O 3	0
43	7	1	Total 43	C 40	O 3	0

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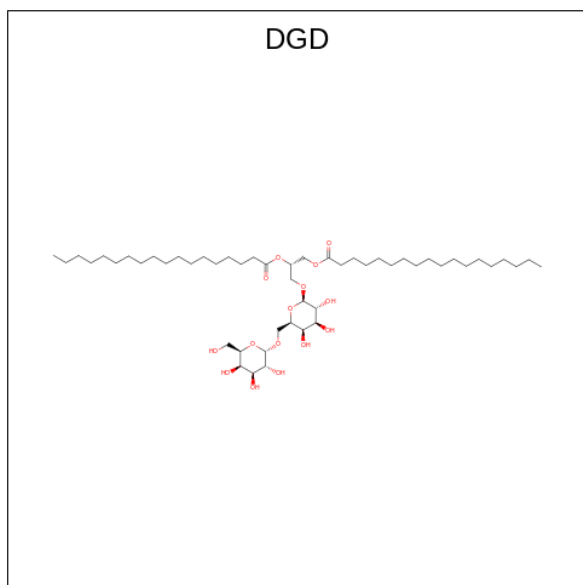
Mol	Chain	Residues	Atoms			AltConf
43	7	1	Total	C	O	0
			43	40	3	
43	I	1	Total	C	O	0
			43	40	3	
43	I	1	Total	C	O	0
			43	40	3	
43	I	1	Total	C	O	0
			43	40	3	
43	x	1	Total	C	O	0
			43	40	3	
43	x	1	Total	C	O	0
			43	40	3	
43	y	1	Total	C	O	0
			43	40	3	
43	y	1	Total	C	O	0
			43	40	3	
43	z	1	Total	C	O	0
			43	40	3	
43	z	1	Total	C	O	0
			43	40	3	
43	Z	1	Total	C	O	0
			43	40	3	
43	2	1	Total	C	O	0
			43	40	3	

- Molecule 44 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



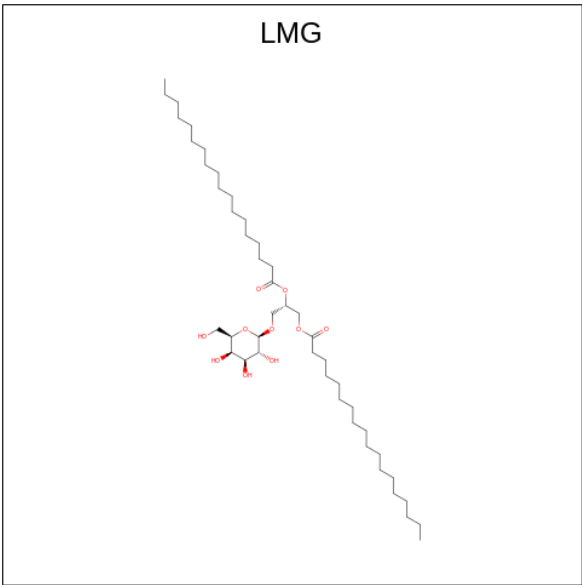
Mol	Chain	Residues	Atoms			AltConf
44	b	1	Total	Fe	S	0
			8	4	4	
44	c	1	Total	Fe	S	0
			8	4	4	
44	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
45	b	1	Total	C	O	0
			60	45	15	
45	C	1	Total	C	O	0
			40	25	15	

- Molecule 46 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
46	I	1	Total	C	O	0
			39	29	10	
46	A	1	Total	C	O	0
			29	19	10	
46	D	1	Total	C	O	0
			37	27	10	
46	F	1	Total	C	O	0
			39	29	10	
46	F	1	Total	C	O	0
			34	24	10	
46	M	1	Total	C	O	0
			39	29	10	
46	M	1	Total	C	O	0
			33	23	10	
46	P	1	Total	C	O	0
			39	29	10	
46	Q	1	Total	C	O	0
			28	18	10	
46	S	1	Total	C	O	0
			32	22	10	
46	S	1	Total	C	O	0
			46	36	10	
46	W	1	Total	C	O	0
			39	29	10	
46	W	1	Total	C	O	0
			33	23	10	
46	0	1	Total	C	O	0
			27	17	10	

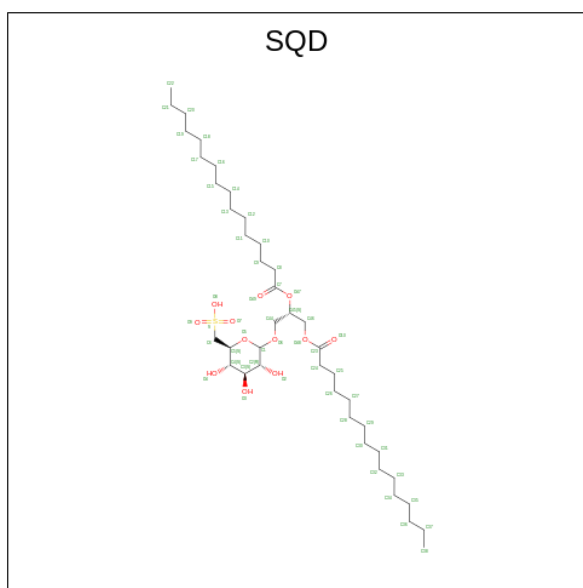
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Mol	Chain	Residues	Atoms			AltConf
46	4	1	Total	C	O	0
			32	22	10	
46	4	1	Total	C	O	0
			46	36	10	
46	7	1	Total	C	O	0
			46	36	10	
46	7	1	Total	C	O	0
			32	22	10	
46	9	1	Total	C	O	0
			36	26	10	
46	I	1	Total	C	O	0
			42	32	10	

- Molecule 47 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



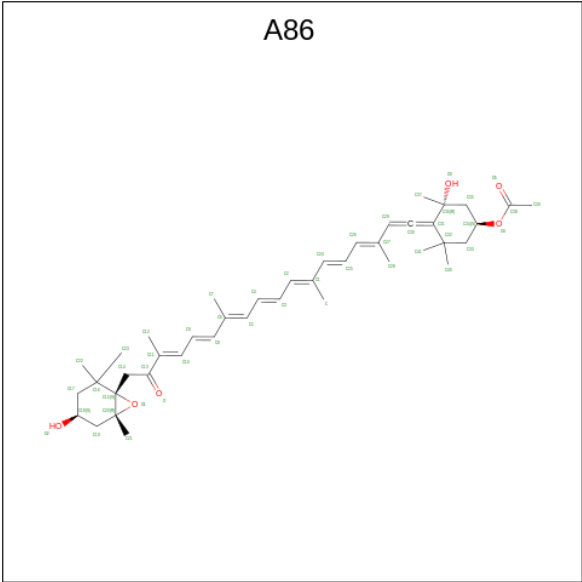
Mol	Chain	Residues	Atoms				AltConf
47	k	1	Total	C	O	S	0
			38	25	12	1	
47	D	1	Total	C	O	S	0
			38	25	12	1	
47	D	1	Total	C	O	S	0
			37	24	12	1	
47	D	1	Total	C	O	S	0
			39	26	12	1	

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Mol	Chain	Residues	Atoms				AltConf
47	E	1	Total	C	O	S	0
			35	22	12	1	
47	F	1	Total	C	O	S	0
			42	29	12	1	
47	F	1	Total	C	O	S	0
			37	24	12	1	
47	H	1	Total	C	O	S	0
			38	25	12	1	
47	M	1	Total	C	O	S	0
			39	26	12	1	
47	P	1	Total	C	O	S	0
			38	25	12	1	
47	S	1	Total	C	O	S	0
			39	26	12	1	
47	T	1	Total	C	O	S	0
			36	23	12	1	
47	W	1	Total	C	O	S	0
			28	15	12	1	
47	4	1	Total	C	O	S	0
			39	26	12	1	
47	7	1	Total	C	O	S	0
			39	26	12	1	
47	9	1	Total	C	O	S	0
			36	23	12	1	

- Molecule 48 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C<sub>42</sub>H<sub>58</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
48	k	1	Total	C	O	0
			48	42	6	
48	B	1	Total	C	O	0
			48	42	6	
48	C	1	Total	C	O	0
			48	42	6	
48	D	1	Total	C	O	0
			48	42	6	
48	E	1	Total	C	O	0
			48	42	6	
48	F	1	Total	C	O	0
			48	42	6	
48	F	1	Total	C	O	0
			48	42	6	
48	G	1	Total	C	O	0
			48	42	6	
48	G	1	Total	C	O	0
			48	42	6	
48	H	1	Total	C	O	0
			48	42	6	
48	J	1	Total	C	O	0
			48	42	6	
48	J	1	Total	C	O	0
			48	42	6	
48	K	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
48	L	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	
48	M	1	Total	C	O	0
			48	42	6	
48	M	1	Total	C	O	0
			48	42	6	
48	M	1	Total	C	O	0
			48	42	6	
48	O	1	Total	C	O	0
			48	42	6	
48	O	1	Total	C	O	0
			48	42	6	
48	O	1	Total	C	O	0
			48	42	6	
48	P	1	Total	C	O	0
			48	42	6	
48	P	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	R	1	Total	C	O	0
			48	42	6	
48	R	1	Total	C	O	0
			48	42	6	
48	R	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
48	S	1	Total	C	O	0
			48	42	6	
48	S	1	Total	C	O	0
			48	42	6	
48	S	1	Total	C	O	0
			48	42	6	
48	T	1	Total	C	O	0
			48	42	6	
48	T	1	Total	C	O	0
			48	42	6	
48	T	1	Total	C	O	0
			48	42	6	
48	U	1	Total	C	O	0
			48	42	6	
48	U	1	Total	C	O	0
			48	42	6	
48	V	1	Total	C	O	0
			48	42	6	
48	V	1	Total	C	O	0
			48	42	6	
48	W	1	Total	C	O	0
			48	42	6	
48	W	1	Total	C	O	0
			48	42	6	
48	W	1	Total	C	O	0
			48	42	6	
48	X	1	Total	C	O	0
			48	42	6	
48	X	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	1	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
48	1	1	Total	C	O	0
			48	42	6	
48	1	1	Total	C	O	0
			48	42	6	
48	1	1	Total	C	O	0
			48	42	6	
48	3	1	Total	C	O	0
			48	42	6	
48	3	1	Total	C	O	0
			48	42	6	
48	3	1	Total	C	O	0
			48	42	6	
48	3	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	5	1	Total	C	O	0
			48	42	6	
48	7	1	Total	C	O	0
			48	42	6	
48	7	1	Total	C	O	0
			48	42	6	
48	7	1	Total	C	O	0
			48	42	6	
48	7	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	

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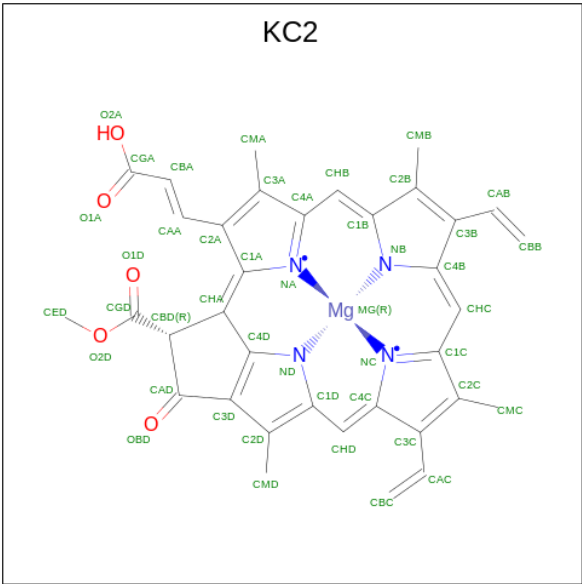
Mol	Chain	Residues	Atoms			AltConf
48	8	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	
48	9	1	Total	C	O	0
			48	42	6	
48	9	1	Total	C	O	0
			48	42	6	
48	9	1	Total	C	O	0
			48	42	6	
48	9	1	Total	C	O	0
			48	42	6	
48	I	1	Total	C	O	0
			48	42	6	
48	x	1	Total	C	O	0
			48	42	6	
48	y	1	Total	C	O	0
			48	42	6	
48	y	1	Total	C	O	0
			48	42	6	
48	z	1	Total	C	O	0
			48	42	6	
48	Y	1	Total	C	O	0
			48	42	6	
48	Z	1	Total	C	O	0
			48	42	6	
48	Z	1	Total	C	O	0
			48	42	6	
48	2	1	Total	C	O	0
			48	42	6	
48	2	1	Total	C	O	0
			48	42	6	
48	2	1	Total	C	O	0
			48	42	6	
48	6	1	Total	C	O	0
			48	42	6	
48	6	1	Total	C	O	0
			48	42	6	
48	6	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
48	6	1	Total	C	O	0
			48	42	6	
48	6	1	Total	C	O	0
			48	42	6	

- Molecule 49 is Chlorophyll c2 (CCD ID: KC2) (formula: C<sub>35</sub>H<sub>28</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
49	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	F	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
49	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	M	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	O	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	P	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	P	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
49	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Q	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
49	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	W	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	X	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	0	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
49	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	5	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	I	1	Total 44	C 35	Mg 1	N 4	O 4	0

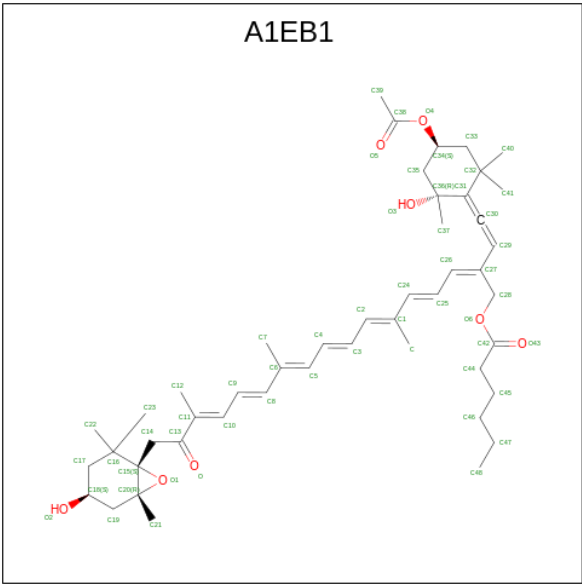
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Mol	Chain	Residues	Atoms					AltConf
49	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	z	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	z	1	Total 44	C 34	Mg 1	N 4	O 5	0
49	z	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
49	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	6	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 50 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-2-[2-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]ethenyl]-6,11,15-trimethyl-16-oxidanylidene-17-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]heptadec

a-2,4,6,8,10,12,14-heptaenyl] hexanoate (CCD ID: A1EB1) (formula: C<sub>48</sub>H<sub>68</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			56	48	8	
50	D	1	Total	C	O	0
			56	48	8	
50	E	1	Total	C	O	0
			56	48	8	
50	F	1	Total	C	O	0
			56	48	8	
50	G	1	Total	C	O	0
			56	48	8	
50	G	1	Total	C	O	0
			56	48	8	
50	G	1	Total	C	O	0
			56	48	8	
50	G	1	Total	C	O	0
			56	48	8	
50	H	1	Total	C	O	0
			56	48	8	
50	H	1	Total	C	O	0
			56	48	8	
50	J	1	Total	C	O	0
			56	48	8	
50	K	1	Total	C	O	0
			56	48	8	

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Mol	Chain	Residues	Atoms			AltConf
50	K	1	Total	C	O	0
			56	48	8	
50	K	1	Total	C	O	0
			56	48	8	
50	L	1	Total	C	O	0
			56	48	8	
50	O	1	Total	C	O	0
			56	48	8	
50	Q	1	Total	C	O	0
			56	48	8	
50	Q	1	Total	C	O	0
			56	48	8	
50	R	1	Total	C	O	0
			56	48	8	
50	S	1	Total	C	O	0
			56	48	8	
50	S	1	Total	C	O	0
			56	48	8	
50	T	1	Total	C	O	0
			56	48	8	
50	T	1	Total	C	O	0
			56	48	8	
50	U	1	Total	C	O	0
			56	48	8	
50	U	1	Total	C	O	0
			56	48	8	
50	V	1	Total	C	O	0
			56	48	8	
50	V	1	Total	C	O	0
			56	48	8	
50	V	1	Total	C	O	0
			56	48	8	
50	V	1	Total	C	O	0
			56	48	8	
50	0	1	Total	C	O	0
			56	48	8	
50	0	1	Total	C	O	0
			56	48	8	
50	0	1	Total	C	O	0
			56	48	8	
50	0	1	Total	C	O	0
			56	48	8	

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Mol	Chain	Residues	Atoms			AltConf
50	1	1	Total	C	O	0
			56	48	8	
50	1	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	4	1	Total	C	O	0
			56	48	8	
50	4	1	Total	C	O	0
			56	48	8	
50	4	1	Total	C	O	0
			56	48	8	
50	4	1	Total	C	O	0
			56	48	8	
50	5	1	Total	C	O	0
			56	48	8	
50	7	1	Total	C	O	0
			56	48	8	
50	7	1	Total	C	O	0
			56	48	8	
50	7	1	Total	C	O	0
			56	48	8	
50	7	1	Total	C	O	0
			56	48	8	
50	8	1	Total	C	O	0
			56	48	8	
50	8	1	Total	C	O	0
			56	48	8	
50	8	1	Total	C	O	0
			56	48	8	
50	8	1	Total	C	O	0
			56	48	8	
50	9	1	Total	C	O	0
			56	48	8	

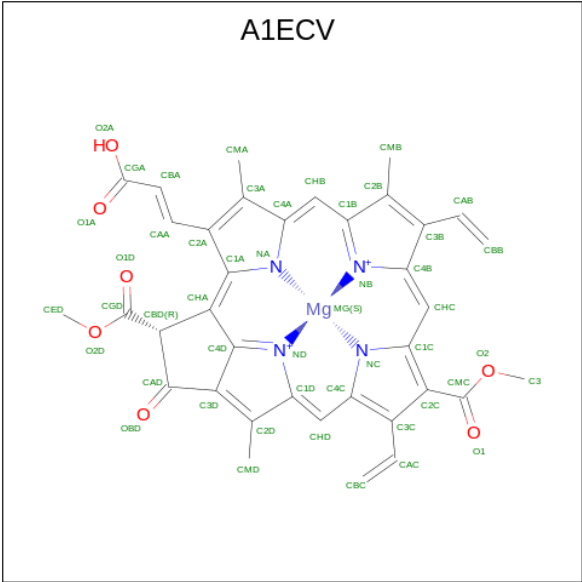
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Mol	Chain	Residues	Atoms			AltConf
50	h	1	Total	C	O	0
			56	48	8	
50	x	1	Total	C	O	0
			56	48	8	
50	x	1	Total	C	O	0
			56	48	8	
50	y	1	Total	C	O	0
			56	48	8	
50	y	1	Total	C	O	0
			56	48	8	
50	z	1	Total	C	O	0
			48	42	6	
50	z	1	Total	C	O	0
			56	48	8	
50	2	1	Total	C	O	0
			56	48	8	
50	2	1	Total	C	O	0
			56	48	8	
50	6	1	Total	C	O	0
			56	48	8	
50	6	1	Total	C	O	0
			53	45	8	
50	6	1	Total	C	O	0
			48	42	6	
50	6	1	Total	C	O	0
			56	48	8	

- Molecule 51 is Chlorophyll C3 (CCD ID: A1ECV) (formula:  $C_{36}H_{28}MgN_4O_7$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
51	E	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	G	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	L	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	M	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	O	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	P	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Q	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Q	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	R	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	R	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	S	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	S	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	T	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	V	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

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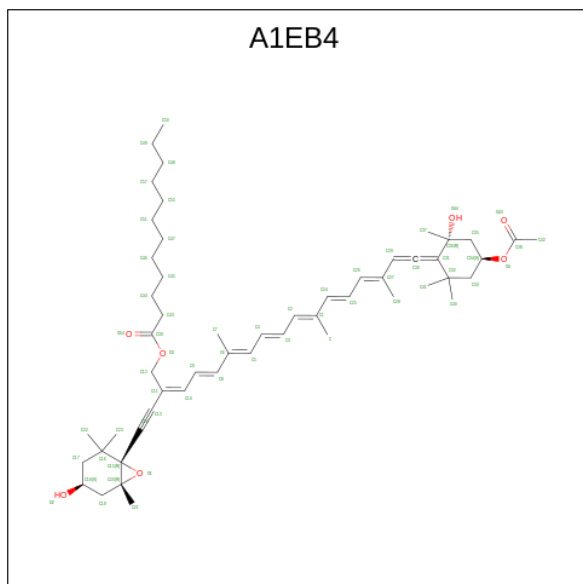
Mol	Chain	Residues	Atoms					AltConf
51	W	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	X	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	X	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	0	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	1	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	4	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	4	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	5	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	5	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	7	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	7	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	9	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	9	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	x	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	x	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	y	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	y	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	z	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	z	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	Y	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	Y	1	Total 48	C 36	Mg 1	N 4	O 7	0

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Mol	Chain	Residues	Atoms					AltConf
51	Z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	2	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	6	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

- Molecule 52 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyl oxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[2-[(1 {R},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethynyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] dodecanoate (CCD ID: A1EB4) (formula: C<sub>54</sub>H<sub>78</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
52	M	1	Total	C	O		0
			58	51	7		
52	M	1	Total	C	O		0
			57	50	7		
52	P	1	Total	C	O		0
			56	49	7		
52	P	1	Total	C	O		0
			54	47	7		
52	P	1	Total	C	O		0
			57	50	7		

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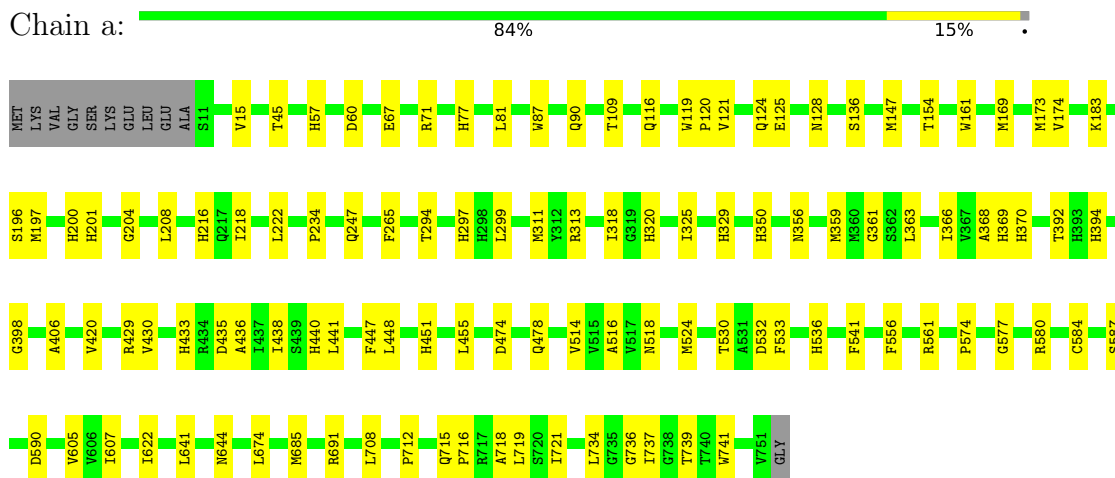
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Mol	Chain	Residues	Atoms			AltConf
52	R	1	Total	C	O	0
			57	50	7	
52	T	1	Total	C	O	0
			55	48	7	
52	W	1	Total	C	O	0
			56	49	7	
52	W	1	Total	C	O	0
			57	50	7	
52	X	1	Total	C	O	0
			57	50	7	
52	5	1	Total	C	O	0
			57	50	7	

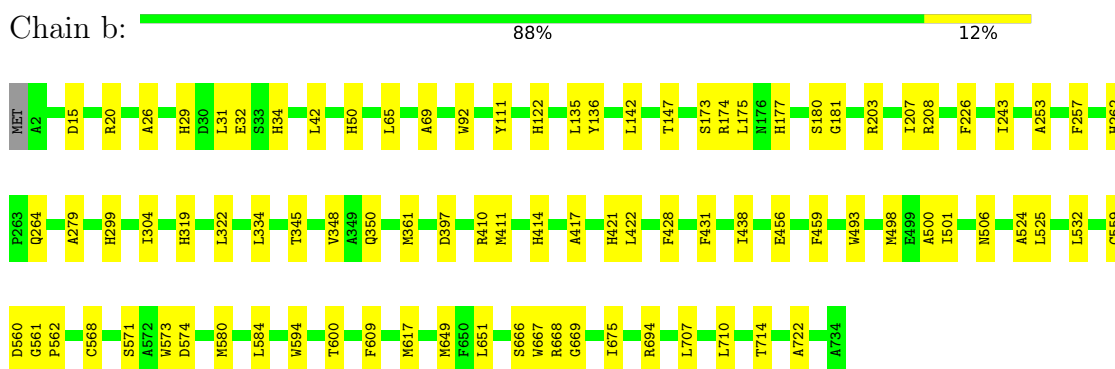
### 3 Residue-property plots [i](#)

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. 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. 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.

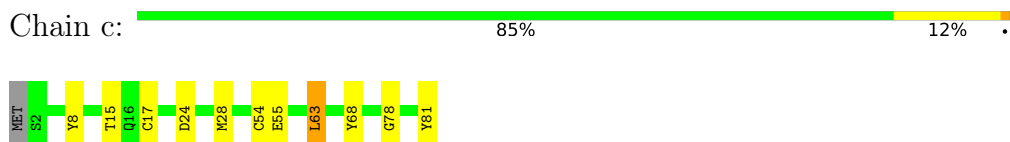
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

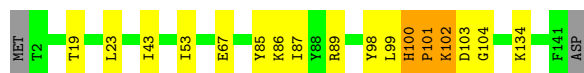


- Molecule 3: Photosystem I iron-sulfur center



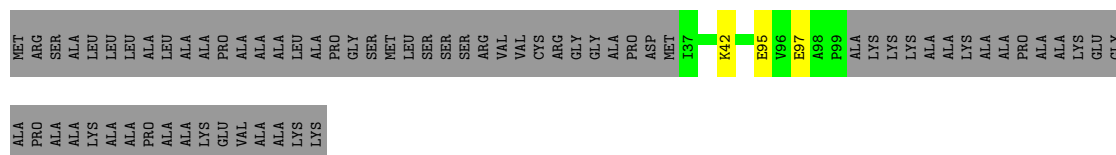
- Molecule 4: Photosystem I reaction center subunit II

Chain d:  87% 10% ..




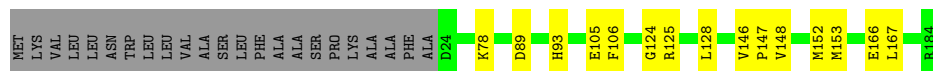
• Molecule 5: Photosystem I reaction center subunit IV

Chain e:  46% 52%




• Molecule 6: Photosystem I reaction center subunit III

Chain f:  79% 8% 12%




• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:  78% 14% 8%




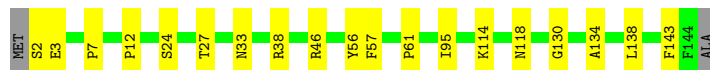
• Molecule 8: Photosystem I reaction center subunit IX

Chain j:  78% 22%




• Molecule 9: Photosystem I reaction center subunit XI

Chain l:  86% 13%



• Molecule 10: Photosystem I reaction center subunit XII

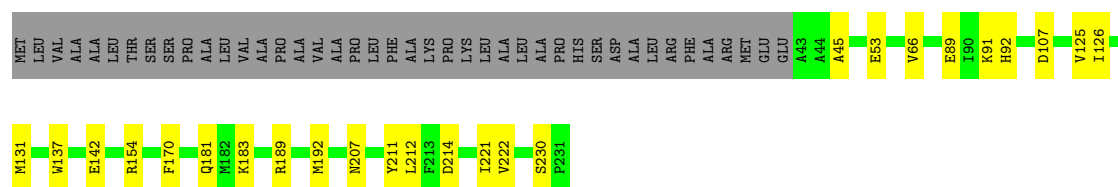
Chain m:  80% 20%





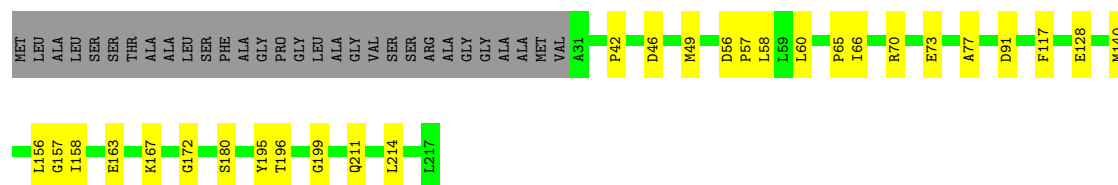


Chain D:  71% 11% 18%



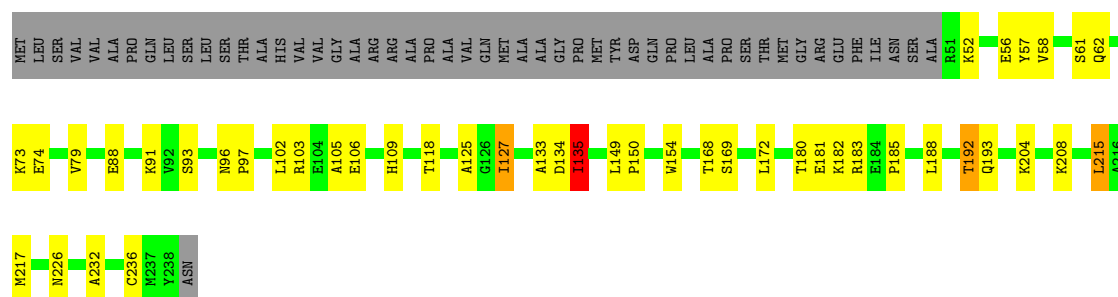
- Molecule 17: Light harvesting protein

Chain E:  73% 13% 14%



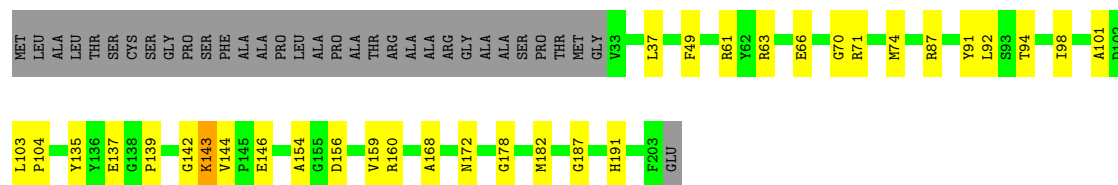
- Molecule 18: Light harvesting protein

Chain F:  59% 18% 21%



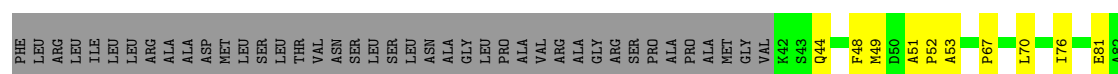
- Molecule 19: Light harvesting protein

Chain G:  68% 16% 16%

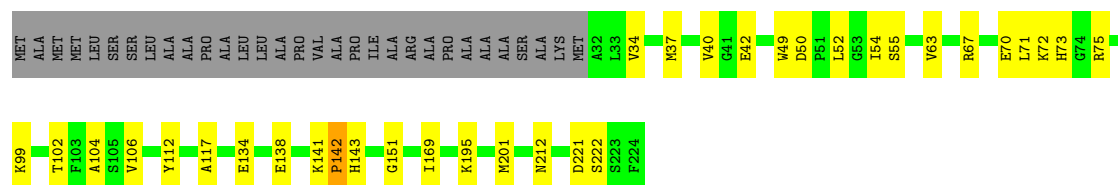


- Molecule 20: Light harvesting protein

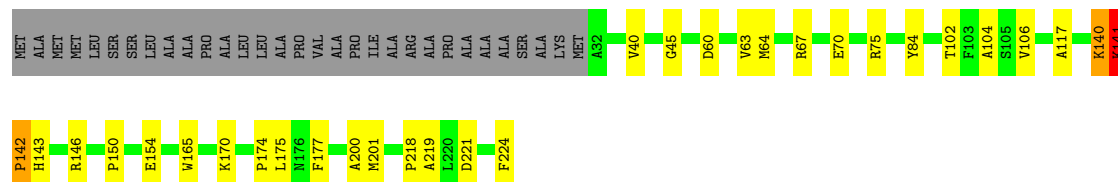
Chain H:  66% 14% 20%



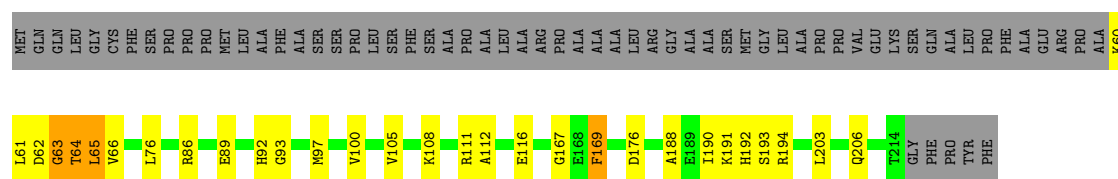




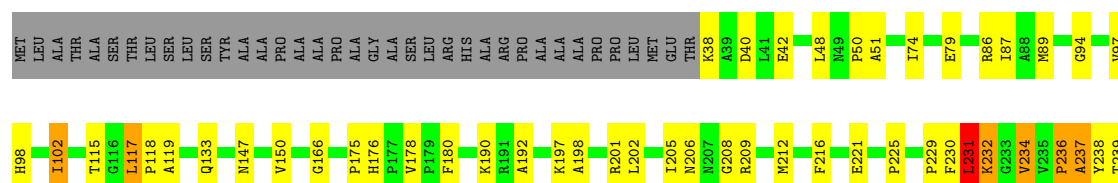
• Molecule 24: Light harvesting protein



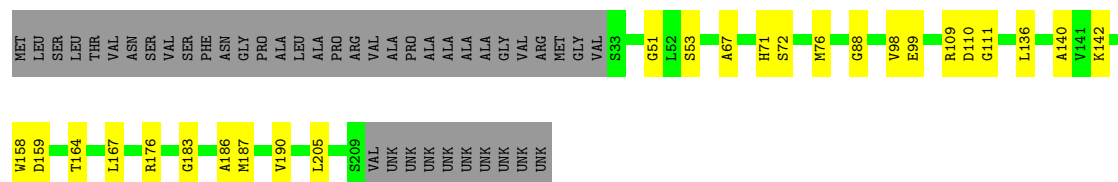
• Molecule 25: Light harvesting protein



• Molecule 26: Light harvesting protein

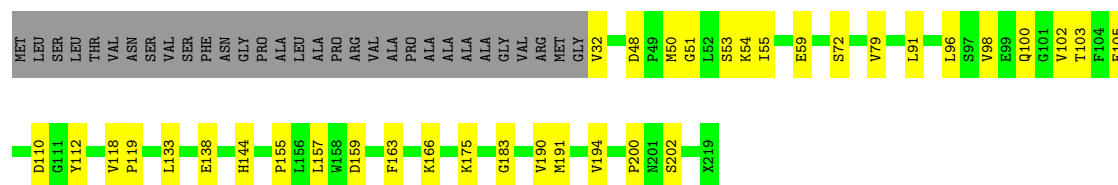


• Molecule 27: Light harvesting protein



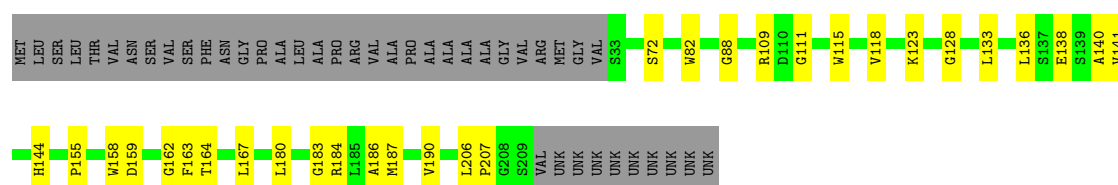
- Molecule 27: Light harvesting protein

Chain V:  69% 16% 14%



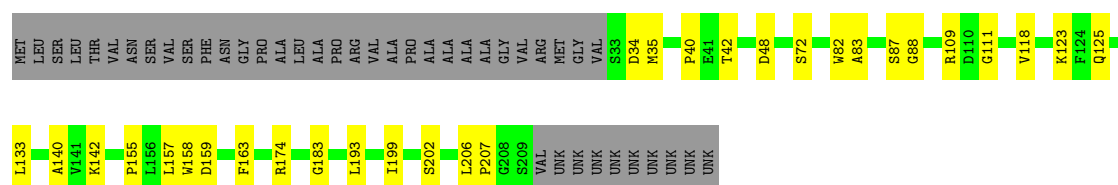
- Molecule 27: Light harvesting protein

Chain X:  67% 14% 19%



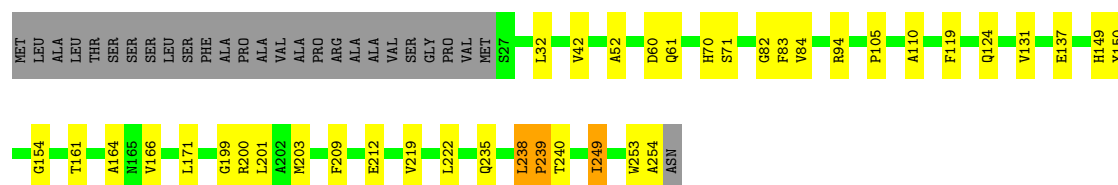
- Molecule 27: Light harvesting protein

Chain 5:  67% 14% 19%




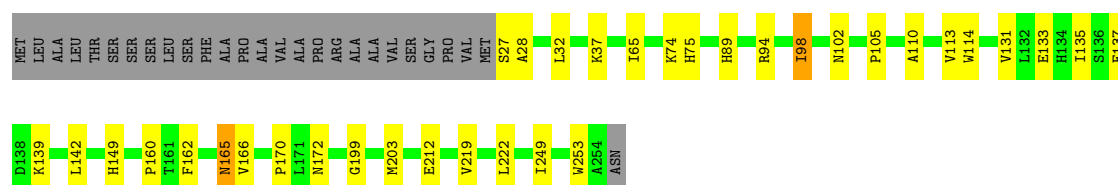
- Molecule 28: Light harvesting protein

Chain S:  74% 14% 11%




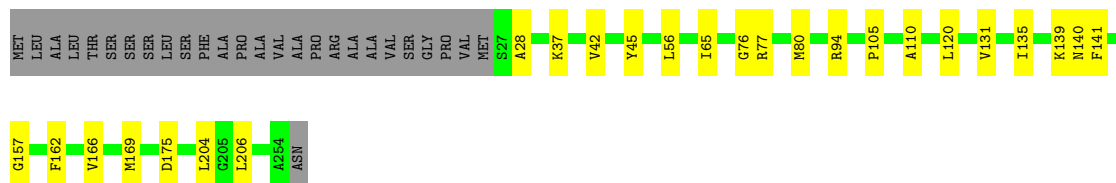
- Molecule 28: Light harvesting protein

Chain 4:  76% 13% 11%




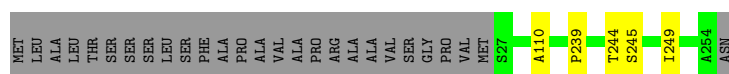
- Molecule 28: Light harvesting protein

Chain 7:  80% 10% 11%




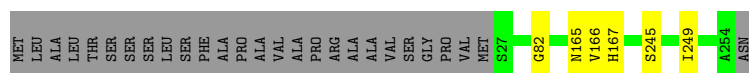
- Molecule 28: Light harvesting protein

Chain x:  87% 11%




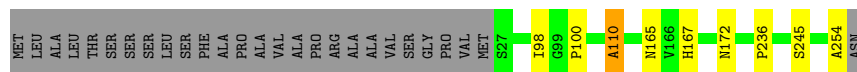
- Molecule 28: Light harvesting protein

Chain y:  87% 11%




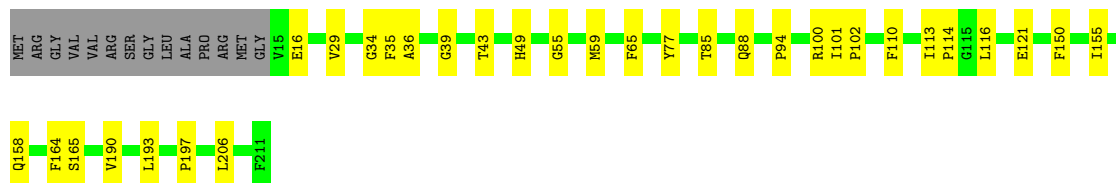
- Molecule 28: Light harvesting protein

Chain z:  86% 11%



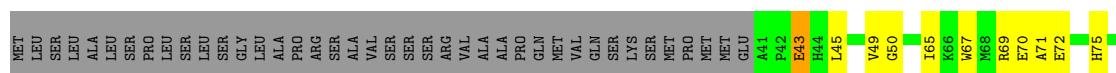
- Molecule 29: Light harvesting protein

Chain T:  78% 15% 7%



- Molecule 30: Light harvesting protein

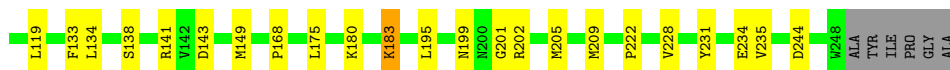
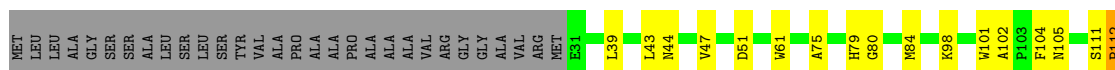
Chain U:  63% 16% 20%





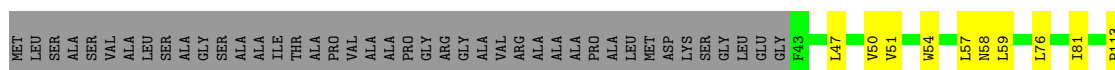
- Molecule 31: Light harvesting protein

Chain 0: 70% 15% 14%



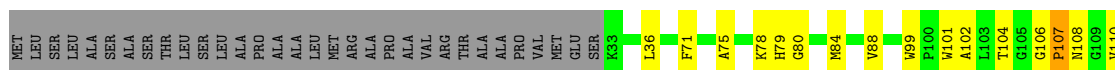
- Molecule 32: Light harvesting protein

Chain 1: 67% 12% 21%



- Molecule 33: Light harvesting protein

Chain 3: 74% 14% 12%



- Molecule 34: Light harvesting protein

Chain 8: 82% 7% 10%




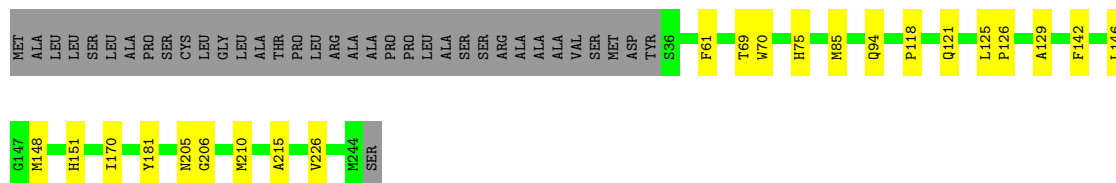
- Molecule 34: Light harvesting protein

Chain 6: 84% 6% 10%



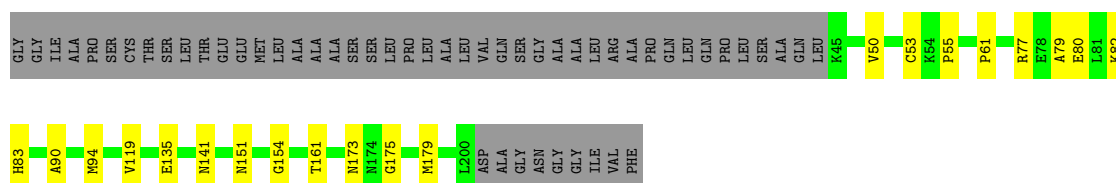
- Molecule 35: Light harvesting protein

Chain 9:  76% 9% 15%



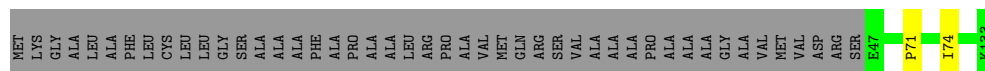
- Molecule 36: Light harvesting protein

Chain I:  65% 10% 25%




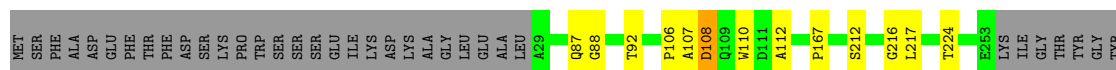
- Molecule 37: PsaR

Chain h:  64% 0% 35%




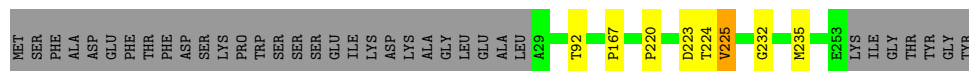
- Molecule 38: Light harvesting protein

Chain Y:  82% 5% 13%



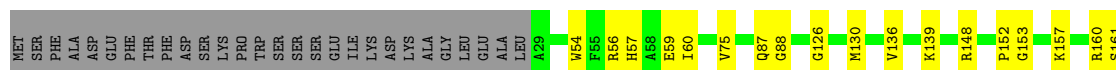
- Molecule 38: Light harvesting protein

Chain Z:  83% 0% 13%



- Molecule 38: Light harvesting protein

Chain 2:  75% 12% 14%



F166	P167	W175	A195	E196	V197	N198	N199	G200	R201	F208	I211	P220	T224	V225	L252	GLU	LYS	ILE	GLY	THR	TYR	GLY	TYR
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1ECV, DGD, A86, SQD, KC2, BCR, A1EB1, DD6, CLA, LMG, LHG, A1EB4, SF4, PQN

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	0.18	0/6028	0.40	0/8207
2	b	0.22	0/6028	0.46	1/8222 (0.0%)
3	c	0.16	0/608	0.54	0/824
4	d	0.18	0/1128	0.47	0/1525
5	e	0.24	0/503	0.45	0/683
6	f	0.18	0/1263	0.45	0/1714
7	i	0.30	0/261	0.56	0/357
8	j	0.14	0/325	0.33	0/438
9	l	0.19	0/1113	0.41	0/1513
10	m	0.21	0/226	0.62	0/306
11	k	0.19	0/545	0.43	0/737
12	o	0.21	0/371	0.59	0/503
13	A	0.18	0/1458	0.43	0/1979
14	B	0.20	0/1285	0.49	0/1750
15	C	0.21	0/1357	0.48	0/1836
16	D	0.19	0/1462	0.47	0/1988
17	E	0.22	0/1417	0.51	0/1933
18	F	0.28	0/1449	0.64	3/1967 (0.2%)
19	G	0.22	0/1386	0.55	2/1885 (0.1%)
20	H	0.25	0/1296	0.54	0/1757
21	J	0.23	0/1294	0.54	0/1749
22	K	0.24	0/1281	0.56	1/1744 (0.1%)
23	L	0.20	0/1684	0.49	0/2298
24	M	0.21	0/1491	0.42	0/2020
24	P	0.18	0/1491	0.42	0/2020
24	W	0.21	0/1491	0.45	0/2020
25	O	0.25	0/1152	0.60	0/1555
26	Q	0.26	0/1719	0.60	0/2340
27	5	0.24	0/1346	0.60	0/1830
27	R	0.22	0/1346	0.57	0/1830
27	V	0.23	0/1339	0.57	0/1820
27	X	0.23	0/1346	0.54	0/1830

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
28	4	0.21	0/1801	0.51	2/2451 (0.1%)
28	7	0.20	0/1801	0.48	0/2451
28	S	0.21	0/1801	0.49	0/2451
28	x	0.17	0/1112	0.43	0/1539
28	y	0.16	0/1112	0.38	0/1539
28	z	0.15	0/1112	0.41	0/1539
29	T	0.24	0/1534	0.55	1/2091 (0.0%)
30	U	0.21	0/1274	0.48	0/1726
31	0	0.24	0/1764	0.59	2/2410 (0.1%)
32	1	0.26	0/1284	0.56	0/1770
33	3	0.21	0/1828	0.54	3/2483 (0.1%)
34	6	0.16	0/1317	0.42	0/1813
34	8	0.20	0/1413	0.48	0/1941
35	9	0.25	0/1537	0.57	0/2106
36	I	0.23	0/1233	0.50	0/1666
37	h	0.17	0/669	0.37	0/915
38	2	0.23	0/1401	0.64	0/1911
38	Y	0.19	0/1098	0.59	1/1520 (0.1%)
38	Z	0.18	0/1098	0.58	0/1520
All	All	0.21	0/72678	0.50	16/99022 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	668	ARG	N-CA-C	10.45	123.65	111.11
22	K	36	VAL	N-CA-C	-6.07	107.94	113.71
28	4	165	ASN	CA-C-N	5.99	132.74	121.97
28	4	165	ASN	C-N-CA	5.99	132.74	121.97
33	3	231	SER	CA-C-N	5.66	132.60	122.13

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5835	0	5733	90	0
2	b	5818	0	5640	71	0
3	c	598	0	581	7	0
4	d	1103	0	1113	20	0
5	e	491	0	480	1	0
6	f	1232	0	1231	13	0
7	i	254	0	262	5	0
8	j	318	0	333	7	0
9	l	1084	0	1090	15	0
10	m	224	0	243	7	0
11	k	533	0	547	11	0
12	o	360	0	363	6	0
13	A	1419	0	1408	20	0
14	B	1255	0	1223	28	0
15	C	1329	0	1352	16	0
16	D	1424	0	1361	20	0
17	E	1384	0	1399	22	0
18	F	1411	0	1407	41	0
19	G	1340	0	1303	17	0
20	H	1263	0	1232	23	0
21	J	1270	0	1295	33	0
22	K	1251	0	1249	16	0
23	L	1626	0	1560	19	0
24	M	1455	0	1468	40	0
24	P	1455	0	1468	26	0
24	W	1455	0	1468	29	0
25	O	1133	0	1141	28	0
26	Q	1666	0	1649	69	0
27	5	1311	0	1326	19	0
27	R	1311	0	1326	18	0
27	V	1353	0	1332	22	0
27	X	1311	0	1326	20	0
28	4	1744	0	1703	23	0
28	7	1744	0	1703	19	0
28	S	1744	0	1703	34	0
28	x	1113	0	529	2	0
28	y	1113	0	529	3	0
28	z	1113	0	529	4	0
29	T	1482	0	1457	22	0
30	U	1240	0	1212	22	0
31	0	1706	0	1662	24	0
32	1	1255	0	932	19	0
33	3	1775	0	1765	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	6	1326	0	910	8	0
34	8	1415	0	1126	9	0
35	9	1490	0	1326	17	0
36	I	1203	0	1215	15	0
37	h	650	0	636	1	0
38	2	1383	0	1078	18	0
38	Y	1099	0	529	4	0
38	Z	1099	0	529	2	0
39	0	457	0	379	18	0
39	1	384	0	279	6	0
39	2	385	0	275	5	0
39	3	477	0	425	12	0
39	4	460	0	454	14	0
39	5	339	0	320	7	0
39	6	345	0	258	3	0
39	7	410	0	353	19	0
39	8	353	0	266	7	0
39	9	347	0	258	10	0
39	A	531	0	527	12	0
39	B	287	0	228	7	0
39	C	470	0	474	13	0
39	D	685	0	725	25	0
39	E	728	0	683	20	0
39	F	551	0	512	13	0
39	G	280	0	257	3	0
39	H	479	0	430	13	0
39	I	520	0	512	12	0
39	J	576	0	506	15	0
39	K	418	0	427	13	0
39	L	420	0	364	7	0
39	M	444	0	424	11	0
39	O	423	0	332	8	0
39	P	352	0	358	8	0
39	Q	437	0	399	13	0
39	R	339	0	320	7	0
39	S	456	0	452	18	0
39	T	406	0	330	15	0
39	U	498	0	410	8	0
39	V	357	0	357	22	0
39	W	398	0	391	13	0
39	X	339	0	320	11	0
39	Y	374	0	265	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Z	374	0	265	3	0
39	a	2327	0	2356	90	0
39	b	2553	0	2635	106	0
39	f	120	0	121	2	0
39	h	55	0	49	0	0
39	i	130	0	144	10	0
39	j	65	0	72	5	0
39	k	162	0	141	3	0
39	l	229	0	222	13	0
39	o	258	0	219	6	0
39	x	337	0	240	5	0
39	y	339	0	244	2	0
39	z	335	0	240	2	0
40	a	33	0	46	4	0
40	b	33	0	46	3	0
41	D	70	0	80	3	0
41	H	35	0	40	3	0
41	X	41	0	55	2	0
41	a	76	0	98	3	0
41	j	30	0	30	1	0
42	a	160	0	224	16	0
42	b	240	0	336	23	0
42	f	80	0	112	6	0
42	h	40	0	56	4	0
42	i	40	0	56	6	0
42	j	40	0	56	1	0
42	k	40	0	56	2	0
42	l	120	0	168	10	0
42	m	40	0	56	5	0
43	1	43	0	0	2	0
43	2	43	0	0	1	0
43	3	86	0	0	3	0
43	4	86	0	0	1	0
43	5	43	0	0	1	0
43	7	86	0	0	5	0
43	A	172	0	0	1	0
43	B	43	0	0	0	0
43	C	43	0	0	0	0
43	D	129	0	0	1	0
43	E	129	0	0	1	0
43	F	86	0	0	7	0
43	G	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	H	86	0	0	1	0
43	I	129	0	0	1	0
43	J	129	0	0	1	0
43	K	43	0	0	0	0
43	M	43	0	0	2	0
43	O	129	0	0	2	0
43	P	43	0	0	2	0
43	Q	86	0	0	5	0
43	R	43	0	0	0	0
43	S	43	0	0	1	0
43	T	43	0	0	0	0
43	U	43	0	0	1	0
43	V	43	0	0	0	0
43	W	43	0	0	0	0
43	X	43	0	0	0	0
43	Z	43	0	0	0	0
43	a	43	0	0	0	0
43	j	43	0	0	0	0
43	o	43	0	0	0	0
43	x	86	0	0	0	0
43	y	86	0	0	0	0
43	z	86	0	0	1	0
44	b	8	0	0	0	0
44	c	16	0	0	0	0
45	C	40	0	38	0	0
45	b	60	0	81	3	0
46	0	27	0	23	4	0
46	4	78	0	93	35	0
46	7	78	0	93	22	0
46	9	36	0	42	0	0
46	A	29	0	28	1	0
46	D	37	0	44	1	0
46	F	73	0	84	21	0
46	I	42	0	54	1	0
46	M	72	0	82	10	0
46	P	39	0	46	5	0
46	Q	28	0	25	2	0
46	S	78	0	93	23	0
46	W	72	0	82	14	0
46	l	39	0	47	4	0
47	4	39	0	42	1	0
47	7	39	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	9	36	0	36	1	0
47	D	114	0	119	6	0
47	E	35	0	34	0	0
47	F	79	0	86	1	0
47	H	38	0	40	3	0
47	M	39	0	42	3	0
47	P	38	0	40	1	0
47	S	39	0	42	4	0
47	T	36	0	35	1	0
47	W	28	0	20	1	0
47	k	38	0	40	2	0
48	0	240	0	0	1	0
48	1	192	0	0	1	0
48	2	144	0	0	1	0
48	3	192	0	0	0	0
48	4	240	0	0	0	0
48	5	48	0	0	2	0
48	6	240	0	0	0	0
48	7	192	0	0	1	0
48	8	288	0	0	0	0
48	9	240	0	0	1	0
48	B	48	0	0	0	0
48	C	48	0	0	0	0
48	D	48	0	0	1	0
48	E	48	0	0	1	0
48	F	96	0	0	9	0
48	G	96	0	0	0	0
48	H	48	0	0	0	0
48	I	48	0	0	1	0
48	J	96	0	0	0	0
48	K	48	0	0	0	0
48	L	288	0	0	4	0
48	M	144	0	0	0	0
48	O	144	0	0	0	0
48	P	96	0	0	0	0
48	Q	240	0	0	31	0
48	R	144	0	0	2	0
48	S	144	0	0	0	0
48	T	144	0	0	0	0
48	U	96	0	0	1	0
48	V	96	0	0	0	0
48	W	144	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	X	96	0	0	0	0
48	Y	48	0	0	0	0
48	Z	96	0	0	1	0
48	k	48	0	0	0	0
48	x	48	0	0	0	0
48	y	96	0	0	0	0
48	z	48	0	0	0	0
49	0	179	0	0	2	0
49	1	135	0	0	0	0
49	2	134	0	0	1	0
49	3	180	0	0	1	0
49	4	180	0	0	1	0
49	5	179	0	0	27	0
49	6	180	0	0	1	0
49	7	135	0	0	1	0
49	8	225	0	0	1	0
49	9	180	0	0	0	0
49	A	90	0	0	0	0
49	B	45	0	0	0	0
49	C	90	0	0	0	0
49	F	89	0	0	8	0
49	G	180	0	0	0	0
49	H	90	0	0	0	0
49	I	89	0	0	0	0
49	J	45	0	0	0	0
49	K	90	0	0	0	0
49	L	225	0	0	1	0
49	M	179	0	0	1	0
49	O	44	0	0	1	0
49	P	224	0	0	3	0
49	Q	134	0	0	1	0
49	R	179	0	0	16	0
49	S	135	0	0	0	0
49	T	180	0	0	2	0
49	V	270	0	0	1	0
49	W	179	0	0	3	0
49	X	224	0	0	20	0
49	Y	90	0	0	1	0
49	Z	90	0	0	0	0
49	x	135	0	0	1	0
49	y	135	0	0	0	0
49	z	134	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	0	224	0	0	4	0
50	1	112	0	0	0	0
50	2	112	0	0	1	0
50	3	280	0	0	0	0
50	4	224	0	0	1	0
50	5	56	0	0	0	0
50	6	213	0	0	0	0
50	7	224	0	0	1	0
50	8	224	0	0	0	0
50	9	56	0	0	1	0
50	C	56	0	0	0	0
50	D	56	0	0	0	0
50	E	56	0	0	0	0
50	F	56	0	0	4	0
50	G	224	0	0	0	0
50	H	112	0	0	1	0
50	J	56	0	0	0	0
50	K	168	0	0	0	0
50	L	56	0	0	0	0
50	O	56	0	0	0	0
50	Q	112	0	0	0	0
50	R	56	0	0	0	0
50	S	112	0	0	1	0
50	T	112	0	0	0	0
50	U	112	0	0	0	0
50	V	224	0	0	0	0
50	h	56	0	0	0	0
50	x	112	0	0	2	0
50	y	112	0	0	0	0
50	z	104	0	0	1	0
51	0	48	0	0	2	0
51	1	48	0	0	1	0
51	2	48	0	0	1	0
51	4	96	0	0	0	0
51	5	96	0	0	0	0
51	6	48	0	0	0	0
51	7	96	0	0	6	0
51	9	96	0	0	2	0
51	E	48	0	0	0	0
51	G	48	0	0	0	0
51	L	48	0	0	0	0
51	M	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	O	48	0	0	0	0
51	P	48	0	0	0	0
51	Q	96	0	0	0	0
51	R	96	0	0	0	0
51	S	96	0	0	0	0
51	T	48	0	0	1	0
51	V	48	0	0	0	0
51	W	48	0	0	0	0
51	X	96	0	0	0	0
51	Y	96	0	0	1	0
51	Z	96	0	0	0	0
51	x	96	0	0	1	0
51	y	96	0	0	1	0
51	z	96	0	0	1	0
52	5	57	0	0	1	0
52	M	115	0	0	0	0
52	P	167	0	0	5	0
52	R	57	0	0	1	0
52	T	55	0	0	0	0
52	W	113	0	0	5	0
52	X	57	0	0	0	0
All	All	114135	0	89288	1556	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1556 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:4:326:LMG:H311	49:5:313:KC2:C3A	1.15	1.56
49:X:314:KC2:C3A	46:7:301:LMG:H311	1.26	1.55
46:4:326:LMG:C31	49:5:313:KC2:C3A	2.03	1.35
46:4:326:LMG:C32	49:5:313:KC2:C4A	2.09	1.30
46:4:326:LMG:C31	49:5:313:KC2:C4A	2.12	1.27

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	739/752 (98%)	706 (96%)	33 (4%)	0	100	100
2	b	731/734 (100%)	698 (96%)	32 (4%)	1 (0%)	48	77
3	c	78/81 (96%)	74 (95%)	3 (4%)	1 (1%)	10	32
4	d	138/142 (97%)	125 (91%)	12 (9%)	1 (1%)	19	48
5	e	61/131 (47%)	58 (95%)	2 (3%)	1 (2%)	8	27
6	f	159/184 (86%)	154 (97%)	5 (3%)	0	100	100
7	i	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	l	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
10	m	28/30 (93%)	27 (96%)	0	1 (4%)	3	10
11	k	71/145 (49%)	69 (97%)	1 (1%)	1 (1%)	9	30
12	o	46/123 (37%)	36 (78%)	9 (20%)	1 (2%)	5	20
13	A	181/201 (90%)	167 (92%)	13 (7%)	1 (1%)	22	51
14	B	170/177 (96%)	153 (90%)	15 (9%)	2 (1%)	11	34
15	C	174/233 (75%)	164 (94%)	9 (5%)	1 (1%)	22	51
16	D	187/231 (81%)	172 (92%)	14 (8%)	1 (0%)	25	56
17	E	185/217 (85%)	169 (91%)	16 (9%)	0	100	100
18	F	186/239 (78%)	157 (84%)	23 (12%)	6 (3%)	3	12
19	G	169/204 (83%)	148 (88%)	16 (10%)	5 (3%)	3	13
20	H	166/210 (79%)	147 (89%)	18 (11%)	1 (1%)	22	51
21	J	169/251 (67%)	150 (89%)	18 (11%)	1 (1%)	22	51
22	K	166/198 (84%)	149 (90%)	12 (7%)	5 (3%)	3	13
23	L	208/244 (85%)	182 (88%)	24 (12%)	2 (1%)	13	39
24	M	191/224 (85%)	170 (89%)	18 (9%)	3 (2%)	8	27
24	P	191/224 (85%)	175 (92%)	14 (7%)	2 (1%)	13	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	W	191/224 (85%)	176 (92%)	12 (6%)	3 (2%)	8	27
25	O	153/219 (70%)	135 (88%)	13 (8%)	5 (3%)	3	11
26	Q	213/257 (83%)	178 (84%)	24 (11%)	11 (5%)	1	5
27	5	175/219 (80%)	153 (87%)	22 (13%)	0	100	100
27	R	175/219 (80%)	151 (86%)	24 (14%)	0	100	100
27	V	178/219 (81%)	147 (83%)	24 (14%)	7 (4%)	2	9
27	X	175/219 (80%)	157 (90%)	18 (10%)	0	100	100
28	4	226/255 (89%)	202 (89%)	21 (9%)	3 (1%)	10	32
28	7	226/255 (89%)	201 (89%)	24 (11%)	1 (0%)	30	61
28	S	226/255 (89%)	204 (90%)	18 (8%)	4 (2%)	7	24
28	x	226/255 (89%)	203 (90%)	20 (9%)	3 (1%)	10	32
28	y	226/255 (89%)	211 (93%)	13 (6%)	2 (1%)	14	42
28	z	226/255 (89%)	203 (90%)	19 (8%)	4 (2%)	7	24
29	T	195/211 (92%)	169 (87%)	23 (12%)	3 (2%)	8	29
30	U	156/198 (79%)	138 (88%)	16 (10%)	2 (1%)	10	32
31	0	216/254 (85%)	186 (86%)	25 (12%)	5 (2%)	5	19
32	1	199/253 (79%)	163 (82%)	29 (15%)	7 (4%)	3	10
33	3	234/268 (87%)	204 (87%)	26 (11%)	4 (2%)	7	26
34	6	217/250 (87%)	182 (84%)	31 (14%)	4 (2%)	7	24
34	8	217/250 (87%)	186 (86%)	25 (12%)	6 (3%)	4	14
35	9	207/245 (84%)	173 (84%)	32 (16%)	2 (1%)	13	39
36	I	154/209 (74%)	142 (92%)	12 (8%)	0	100	100
37	h	85/133 (64%)	83 (98%)	2 (2%)	0	100	100
38	2	222/260 (85%)	186 (84%)	31 (14%)	5 (2%)	5	19
38	Y	223/260 (86%)	186 (83%)	31 (14%)	6 (3%)	4	15
38	Z	223/260 (86%)	191 (86%)	26 (12%)	6 (3%)	4	15
All	All	9768/11553 (84%)	8765 (90%)	873 (9%)	130 (1%)	13	32

5 of 130 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	101	PRO
13	A	200	SER

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Mol	Chain	Res	Type
15	C	171	ASN
18	F	135	ILE
18	F	181	GLU

### 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	608/616 (99%)	608 (100%)	0	100	100
2	b	591/592 (100%)	591 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	d	120/122 (98%)	118 (98%)	2 (2%)	56	84
5	e	51/91 (56%)	51 (100%)	0	100	100
6	f	126/144 (88%)	126 (100%)	0	100	100
7	i	29/32 (91%)	29 (100%)	0	100	100
8	j	36/36 (100%)	36 (100%)	0	100	100
9	l	114/115 (99%)	114 (100%)	0	100	100
10	m	23/23 (100%)	23 (100%)	0	100	100
11	k	56/107 (52%)	56 (100%)	0	100	100
12	o	40/85 (47%)	40 (100%)	0	100	100
13	A	155/170 (91%)	155 (100%)	0	100	100
14	B	120/131 (92%)	119 (99%)	1 (1%)	79	93
15	C	140/181 (77%)	140 (100%)	0	100	100
16	D	140/171 (82%)	140 (100%)	0	100	100
17	E	146/163 (90%)	146 (100%)	0	100	100
18	F	140/180 (78%)	138 (99%)	2 (1%)	62	87
19	G	132/153 (86%)	132 (100%)	0	100	100
20	H	131/163 (80%)	131 (100%)	0	100	100
21	J	128/194 (66%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	K	127/149 (85%)	126 (99%)	1 (1%)	79	93
23	L	161/183 (88%)	160 (99%)	1 (1%)	84	95
24	M	146/165 (88%)	145 (99%)	1 (1%)	81	94
24	P	146/165 (88%)	146 (100%)	0	100	100
24	W	146/165 (88%)	144 (99%)	2 (1%)	62	87
25	O	112/160 (70%)	111 (99%)	1 (1%)	75	92
26	Q	171/199 (86%)	167 (98%)	4 (2%)	45	78
27	5	134/157 (85%)	134 (100%)	0	100	100
27	R	134/157 (85%)	134 (100%)	0	100	100
27	V	132/157 (84%)	132 (100%)	0	100	100
27	X	134/157 (85%)	134 (100%)	0	100	100
28	4	179/199 (90%)	179 (100%)	0	100	100
28	7	179/199 (90%)	179 (100%)	0	100	100
28	S	179/199 (90%)	177 (99%)	2 (1%)	70	90
29	T	150/161 (93%)	150 (100%)	0	100	100
30	U	128/162 (79%)	128 (100%)	0	100	100
31	0	177/198 (89%)	177 (100%)	0	100	100
32	1	74/194 (38%)	74 (100%)	0	100	100
33	3	181/204 (89%)	181 (100%)	0	100	100
34	6	58/183 (32%)	58 (100%)	0	100	100
34	8	91/183 (50%)	89 (98%)	2 (2%)	47	79
35	9	126/188 (67%)	126 (100%)	0	100	100
36	I	126/163 (77%)	126 (100%)	0	100	100
37	h	67/94 (71%)	67 (100%)	0	100	100
38	2	82/204 (40%)	82 (100%)	0	100	100
All	All	6434/7883 (82%)	6415 (100%)	19 (0%)	90	97

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	S	240	THR
34	8	160	ASP
34	8	161	THR

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Mol	Chain	Res	Type
24	W	141	LYS
25	O	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
33	3	54	ASN
34	6	195	ASN
33	3	210	ASN
28	7	140	ASN
13	A	82	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

869 ligands 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	$\# Z  > 2$
39	CLA	X	308	-	60,68,73	1.57	5 (8%)	70,107,113	1.45	7 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	8	313	-	41,49,73	1.83	5 (12%)	47,84,113	1.69	8 (17%)
39	CLA	2	307	-	41,49,73	1.86	6 (14%)	47,84,113	1.75	7 (14%)
41	LHG	D	302	-	34,34,48	0.70	0	37,40,54	1.27	3 (8%)
48	A86	T	306	-	44,50,50	1.19	2 (4%)	51,76,76	2.35	15 (29%)
49	KC2	M	307	-	48,53,53	1.84	10 (20%)	54,89,89	2.13	15 (27%)
42	BCR	l	207	-	41,41,41	0.69	0	56,56,56	1.81	11 (19%)
49	KC2	Y	309	-	48,53,53	1.85	9 (18%)	54,89,89	2.05	13 (24%)
39	CLA	b	824	-	60,68,73	1.53	7 (11%)	70,107,113	1.45	6 (8%)
39	CLA	a	828	1	50,58,73	1.69	6 (12%)	58,95,113	1.54	7 (12%)
39	CLA	3	316	-	50,58,73	1.70	6 (12%)	58,95,113	1.55	8 (13%)
39	CLA	b	836	-	45,53,73	1.80	5 (11%)	52,89,113	1.72	7 (13%)
39	CLA	F	306	-	46,54,73	1.75	6 (13%)	53,90,113	1.59	7 (13%)
49	KC2	V	315	-	48,53,53	1.86	11 (22%)	54,89,89	2.10	13 (24%)
39	CLA	A	306	-	61,69,73	1.54	6 (9%)	71,108,113	1.51	6 (8%)
39	CLA	o	206	-	58,66,73	1.57	5 (8%)	67,104,113	1.48	7 (10%)
48	A86	8	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.24	19 (37%)
49	KC2	8	319	34	48,53,53	1.86	10 (20%)	54,89,89	2.06	13 (24%)
43	DD6	o	204	-	39,45,45	1.99	2 (5%)	52,67,67	1.88	12 (23%)
39	CLA	7	313	-	61,69,73	1.56	5 (8%)	71,108,113	1.43	9 (12%)
46	LMG	A	316	-	29,29,55	1.00	0	37,37,63	1.23	4 (10%)
39	CLA	a	812	-	45,53,73	1.78	5 (11%)	52,89,113	1.63	9 (17%)
39	CLA	E	306	17	49,57,73	1.71	6 (12%)	55,93,113	1.55	7 (12%)
49	KC2	P	320	-	48,53,53	1.85	10 (20%)	54,89,89	2.11	15 (27%)
39	CLA	7	318	28	46,54,73	1.72	7 (15%)	53,90,113	1.53	5 (9%)
50	A1EB1	1	301	-	51,58,58	1.22	3 (5%)	60,85,85	1.92	17 (28%)
50	A1EB1	3	302	-	51,58,58	1.30	4 (7%)	60,85,85	2.09	18 (30%)
39	CLA	a	806	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
39	CLA	l	203	-	49,57,73	1.74	5 (10%)	55,93,113	1.55	8 (14%)
48	A86	M	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.16	19 (37%)
49	KC2	R	306	-	48,53,53	1.84	10 (20%)	54,89,89	1.96	11 (20%)
48	A86	0	304	-	44,50,50	1.20	2 (4%)	51,76,76	1.94	15 (29%)
49	KC2	x	313	-	48,53,53	1.85	9 (18%)	54,89,89	2.08	13 (24%)
39	CLA	a	827	-	65,73,73	1.52	7 (10%)	76,113,113	1.53	8 (10%)
39	CLA	E	319	17	49,57,73	1.72	5 (10%)	55,93,113	1.53	7 (12%)
39	CLA	F	316	-	51,59,73	1.69	6 (11%)	59,96,113	1.51	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	A86	2	302	-	44,50,50	1.17	3 (6%)	51,76,76	2.32	18 (35%)
48	A86	O	306	-	44,50,50	1.18	3 (6%)	51,76,76	2.57	20 (39%)
50	A1EB1	K	304	-	51,58,58	1.26	4 (7%)	60,85,85	1.95	18 (30%)
39	CLA	V	313	27	65,73,73	1.45	8 (12%)	76,113,113	1.36	6 (7%)
46	LMG	F	317	49	39,39,55	1.05	2 (5%)	47,47,63	1.23	6 (12%)
50	A1EB1	x	301	-	51,58,58	1.26	4 (7%)	60,85,85	1.97	14 (23%)
39	CLA	b	818	-	55,63,73	1.60	6 (10%)	64,101,113	1.54	7 (10%)
39	CLA	2	309	-	46,54,73	1.75	6 (13%)	53,90,113	1.58	6 (11%)
39	CLA	7	316	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	6 (7%)
39	CLA	E	312	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
39	CLA	b	805	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
47	SQD	7	302	-	38,39,54	1.13	5 (13%)	47,50,65	1.69	11 (23%)
48	A86	F	301	-	44,50,50	1.19	3 (6%)	51,76,76	2.23	15 (29%)
48	A86	V	301	-	44,50,50	1.19	3 (6%)	51,76,76	2.45	17 (33%)
49	KC2	W	308	-	48,53,53	1.83	10 (20%)	54,89,89	2.13	13 (24%)
49	KC2	5	305	27	48,53,53	1.82	9 (18%)	54,89,89	2.10	12 (22%)
39	CLA	O	316	-	41,49,73	1.85	5 (12%)	47,84,113	1.74	7 (14%)
51	A1ECV	x	310	-	51,56,56	2.69	20 (39%)	53,93,93	4.24	28 (52%)
49	KC2	4	324	-	48,53,53	1.83	10 (20%)	54,89,89	2.17	14 (25%)
48	A86	8	309	-	44,50,50	1.17	3 (6%)	51,76,76	2.32	19 (37%)
50	A1EB1	2	304	-	51,58,58	1.26	4 (7%)	60,85,85	2.16	20 (33%)
39	CLA	H	315	-	41,49,73	1.86	6 (14%)	47,84,113	1.64	7 (14%)
51	A1ECV	Y	312	-	51,56,56	2.64	17 (33%)	53,93,93	4.17	27 (50%)
39	CLA	T	308	-	46,54,73	1.73	8 (17%)	53,90,113	1.56	7 (13%)
39	CLA	z	309	-	41,49,73	1.83	6 (14%)	47,84,113	1.73	7 (14%)
39	CLA	D	315	-	65,73,73	1.49	5 (7%)	76,113,113	1.35	7 (9%)
39	CLA	I	308	-	61,69,73	1.50	5 (8%)	71,108,113	1.45	7 (9%)
43	DD6	O	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	13 (25%)
39	CLA	J	318	-	46,54,73	1.75	6 (13%)	53,90,113	1.65	6 (11%)
49	KC2	8	317	-	48,53,53	1.87	9 (18%)	54,89,89	2.08	14 (25%)
42	BCR	b	846	-	41,41,41	0.74	0	56,56,56	2.13	16 (28%)
48	A86	4	328	-	44,50,50	1.14	2 (4%)	51,76,76	2.28	15 (29%)
49	KC2	V	318	-	48,53,53	1.86	9 (18%)	54,89,89	2.08	13 (24%)
39	CLA	6	312	-	51,59,73	1.66	6 (11%)	58,95,113	1.52	7 (12%)
48	A86	Y	301	-	44,50,50	1.16	3 (6%)	51,76,76	2.05	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	A1EB1	D	308	-	51,58,58	1.28	3 (5%)	60,85,85	2.34	20 (33%)
39	CLA	z	306	-	41,49,73	1.87	5 (12%)	47,84,113	1.66	7 (14%)
50	A1EB1	y	301	-	51,58,58	1.23	4 (7%)	60,85,85	2.16	23 (38%)
39	CLA	E	309	-	53,61,73	1.65	5 (9%)	61,98,113	1.50	7 (11%)
39	CLA	y	309	-	46,54,73	1.80	6 (13%)	53,90,113	1.58	6 (11%)
39	CLA	D	310	47	61,69,73	1.57	6 (9%)	71,108,113	1.44	7 (9%)
48	A86	0	308	51	44,50,50	1.27	3 (6%)	51,76,76	2.18	19 (37%)
39	CLA	F	321	-	65,73,73	1.50	5 (7%)	76,113,113	1.42	10 (13%)
39	CLA	Q	311	-	46,54,73	1.74	7 (15%)	53,90,113	1.69	7 (13%)
39	CLA	0	310	-	61,69,73	1.57	6 (9%)	71,108,113	1.43	8 (11%)
39	CLA	I	310	-	54,62,73	1.61	6 (11%)	62,99,113	1.52	7 (11%)
48	A86	Q	308	-	44,50,50	1.15	2 (4%)	51,76,76	2.25	15 (29%)
49	KC2	2	317	-	48,53,53	1.88	11 (22%)	54,89,89	2.20	15 (27%)
39	CLA	5	307	-	60,68,73	1.57	5 (8%)	70,107,113	1.40	7 (10%)
49	KC2	K	310	-	48,53,53	1.86	10 (20%)	54,89,89	2.15	14 (25%)
46	LMG	7	326	-	32,32,55	0.93	1 (3%)	40,40,63	1.23	3 (7%)
51	A1ECV	R	310	-	51,56,56	2.61	18 (35%)	53,93,93	4.25	28 (52%)
42	BCR	h	202	-	41,41,41	0.74	0	56,56,56	1.87	17 (30%)
39	CLA	4	319	-	41,49,73	1.85	5 (12%)	47,84,113	1.72	7 (14%)
42	BCR	m	101	-	41,41,41	1.16	4 (9%)	56,56,56	1.34	7 (12%)
45	DGD	b	849	-	61,61,67	0.93	2 (3%)	75,75,81	1.37	8 (10%)
39	CLA	b	837	-	60,68,73	1.52	7 (11%)	70,107,113	1.55	7 (10%)
49	KC2	Z	310	-	48,53,53	1.86	10 (20%)	54,89,89	2.11	14 (25%)
39	CLA	Q	314	-	54,62,73	1.62	6 (11%)	62,99,113	1.51	7 (11%)
39	CLA	a	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	6 (7%)
48	A86	H	302	-	44,50,50	1.15	3 (6%)	51,76,76	2.29	17 (33%)
48	A86	X	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.10	18 (35%)
48	A86	W	307	-	44,50,50	1.23	4 (9%)	51,76,76	1.94	13 (25%)
50	A1EB1	0	305	-	51,58,58	1.27	3 (5%)	60,85,85	2.03	17 (28%)
39	CLA	R	309	-	65,73,73	1.48	5 (7%)	76,113,113	1.43	9 (11%)
39	CLA	8	315	-	43,51,73	1.80	6 (13%)	49,86,113	1.59	6 (12%)
39	CLA	a	833	1	45,53,73	1.80	5 (11%)	52,89,113	1.64	7 (13%)
49	KC2	0	314	46,31	47,52,53	1.82	9 (19%)	51,87,89	2.18	13 (25%)
39	CLA	3	314	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	7 (9%)
39	CLA	Y	313	-	41,49,73	1.88	5 (12%)	47,84,113	1.70	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	A86	C	303	-	44,50,50	1.21	2 (4%)	51,76,76	1.92	14 (27%)
48	A86	x	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.26	17 (33%)
49	KC2	G	311	19	48,53,53	1.85	10 (20%)	54,89,89	2.09	13 (24%)
49	KC2	z	313	-	41,50,53	1.78	7 (17%)	44,80,89	2.01	9 (20%)
46	LMG	P	317	49	39,39,55	1.08	2 (5%)	47,47,63	1.23	4 (8%)
47	SQD	D	304	-	37,38,54	1.14	5 (13%)	46,49,65	1.74	10 (21%)
49	KC2	M	314	-	48,53,53	1.85	9 (18%)	54,89,89	2.04	15 (27%)
49	KC2	L	312	-	48,53,53	1.86	10 (20%)	54,89,89	1.86	11 (20%)
39	CLA	V	311	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	6 (7%)
39	CLA	9	307	-	41,49,73	1.87	5 (12%)	47,84,113	1.63	7 (14%)
49	KC2	2	313	-	47,52,53	1.88	10 (21%)	54,88,89	2.11	15 (27%)
39	CLA	T	311	-	56,64,73	1.60	5 (8%)	65,102,113	1.48	7 (10%)
49	KC2	y	314	-	48,53,53	1.86	9 (18%)	54,89,89	1.95	11 (20%)
39	CLA	b	807	-	65,73,73	1.45	7 (10%)	76,113,113	1.58	8 (10%)
49	KC2	P	306	24	48,53,53	1.88	12 (25%)	54,89,89	2.12	13 (24%)
39	CLA	B	206	-	42,50,73	1.81	6 (14%)	48,85,113	1.63	8 (16%)
39	CLA	E	308	-	65,73,73	1.46	5 (7%)	76,113,113	1.41	8 (10%)
39	CLA	G	314	19	58,66,73	1.56	6 (10%)	67,104,113	1.55	8 (11%)
50	A1EB1	V	306	-	51,58,58	1.25	3 (5%)	60,85,85	1.97	19 (31%)
46	LMG	M	320	-	33,33,55	0.94	0	41,41,63	1.19	4 (9%)
52	A1EB4	5	304	-	52,59,63	2.56	4 (7%)	61,85,89	1.93	19 (31%)
49	KC2	6	317	-	48,53,53	1.86	9 (18%)	54,89,89	2.09	14 (25%)
51	A1ECV	4	315	-	51,56,56	2.65	19 (37%)	53,93,93	4.25	29 (54%)
39	CLA	A	305	13	49,57,73	1.72	6 (12%)	55,93,113	1.53	6 (10%)
48	A86	7	307	-	44,50,50	1.24	3 (6%)	51,76,76	2.22	17 (33%)
39	CLA	1	317	-	41,49,73	1.86	5 (12%)	47,84,113	1.68	7 (14%)
39	CLA	Q	312	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	6 (7%)
43	DD6	x	303	-	39,45,45	2.06	3 (7%)	52,67,67	1.96	16 (30%)
39	CLA	V	310	-	60,68,73	1.55	6 (10%)	70,107,113	1.55	11 (15%)
49	KC2	J	315	-	48,53,53	1.87	9 (18%)	54,89,89	2.05	16 (29%)
48	A86	G	301	-	44,50,50	1.18	2 (4%)	51,76,76	2.46	19 (37%)
39	CLA	L	309	-	53,62,73	1.62	6 (11%)	61,100,113	1.58	6 (9%)
43	DD6	z	305	-	39,45,45	2.02	2 (5%)	52,67,67	1.89	16 (30%)
48	A86	B	201	-	44,50,50	1.19	3 (6%)	51,76,76	2.49	19 (37%)
49	KC2	9	313	-	48,53,53	1.86	11 (22%)	54,89,89	2.05	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	KC2	P	312	-	48,53,53	1.90	10 (20%)	54,89,89	2.13	13 (24%)
39	CLA	9	320	-	41,49,73	1.86	5 (12%)	47,84,113	1.72	9 (19%)
48	A86	1	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.18	17 (33%)
50	A1EB1	4	302	-	51,58,58	1.24	4 (7%)	60,85,85	2.12	20 (33%)
39	CLA	b	821	-	65,73,73	1.52	6 (9%)	76,113,113	1.37	8 (10%)
39	CLA	S	309	-	65,73,73	1.52	6 (9%)	76,113,113	1.48	9 (11%)
39	CLA	3	312	-	65,73,73	1.50	6 (9%)	76,113,113	1.47	10 (13%)
39	CLA	D	319	16	65,73,73	1.48	5 (7%)	76,113,113	1.42	7 (9%)
39	CLA	C	307	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	7 (9%)
50	A1EB1	H	301	-	51,58,58	1.27	3 (5%)	60,85,85	2.10	17 (28%)
39	CLA	4	314	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
39	CLA	L	319	-	51,59,73	1.69	5 (9%)	59,96,113	1.53	6 (10%)
41	LHG	j	104	-	29,29,48	0.74	1 (3%)	32,35,54	1.23	3 (9%)
39	CLA	0	322	-	51,59,73	1.71	7 (13%)	59,96,113	1.54	7 (11%)
43	DD6	5	303	-	39,45,45	1.90	3 (7%)	52,67,67	1.73	12 (23%)
47	SQD	4	327	-	38,39,54	1.14	5 (13%)	47,50,65	1.69	11 (23%)
51	A1ECV	6	320	-	51,56,56	2.67	17 (33%)	53,93,93	4.10	28 (52%)
43	DD6	A	301	-	39,45,45	1.98	3 (7%)	52,67,67	1.88	12 (23%)
39	CLA	a	816	-	65,73,73	1.50	5 (7%)	76,113,113	1.47	9 (11%)
39	CLA	M	318	24	46,54,73	1.76	5 (10%)	53,90,113	1.63	6 (11%)
39	CLA	Y	305	-	41,49,73	1.85	5 (12%)	47,84,113	1.72	7 (14%)
39	CLA	1	313	32	41,49,73	1.85	6 (14%)	47,84,113	1.63	7 (14%)
48	A86	R	317	-	44,50,50	1.17	2 (4%)	51,76,76	2.06	12 (23%)
39	CLA	a	803	-	65,73,73	1.48	7 (10%)	76,113,113	1.40	7 (9%)
39	CLA	0	323	-	46,54,73	1.75	6 (13%)	53,90,113	1.64	7 (13%)
43	DD6	J	304	-	39,45,45	2.23	5 (12%)	52,67,67	2.35	14 (26%)
44	SF4	b	804	-	0,12,12	-	-	-	-	-
39	CLA	C	305	-	61,69,73	1.56	5 (8%)	71,108,113	1.39	7 (9%)
49	KC2	B	208	-	48,53,53	1.84	10 (20%)	54,89,89	2.18	15 (27%)
39	CLA	A	311	-	65,73,73	1.49	6 (9%)	76,113,113	1.33	7 (9%)
49	KC2	X	314	46	47,52,53	1.83	9 (19%)	51,87,89	2.14	13 (25%)
42	BCR	b	848	-	41,41,41	0.75	0	56,56,56	1.78	14 (25%)
39	CLA	l	204	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	9 (11%)
50	A1EB1	4	304	-	51,58,58	1.28	3 (5%)	60,85,85	2.17	21 (35%)
48	A86	3	306	-	44,50,50	1.14	3 (6%)	51,76,76	2.24	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
51	A1ECV	9	314	-	51,56,56	2.66	19 (37%)	53,93,93	4.14	27 (50%)
39	CLA	i	103	-	65,73,73	1.49	6 (9%)	76,113,113	1.49	9 (11%)
47	SQD	D	320	39	36,37,54	1.16	5 (13%)	45,48,65	1.86	10 (22%)
39	CLA	a	815	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
49	KC2	3	315	-	48,53,53	1.87	10 (20%)	54,89,89	2.03	11 (20%)
39	CLA	8	321	-	42,50,73	1.86	5 (11%)	48,85,113	1.61	6 (12%)
51	A1ECV	2	311	-	51,56,56	2.68	19 (37%)	53,93,93	4.25	27 (50%)
39	CLA	D	317	-	65,73,73	1.48	7 (10%)	76,113,113	1.47	8 (10%)
39	CLA	a	831	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	7 (9%)
51	A1ECV	9	317	-	51,56,56	2.59	19 (37%)	53,93,93	4.05	28 (52%)
39	CLA	Z	316	-	41,49,73	1.86	5 (12%)	47,84,113	1.76	8 (17%)
42	BCR	l	202	-	41,41,41	0.76	0	56,56,56	1.93	13 (23%)
39	CLA	6	313	-	42,50,73	1.82	5 (11%)	48,85,113	1.63	6 (12%)
51	A1ECV	M	316	-	51,56,56	2.62	17 (33%)	53,93,93	4.03	29 (54%)
42	BCR	f	801	-	41,41,41	0.68	0	56,56,56	1.92	14 (25%)
48	A86	9	305	-	44,50,50	1.19	3 (6%)	51,76,76	1.91	17 (33%)
39	CLA	M	312	-	65,73,73	1.50	7 (10%)	76,113,113	1.39	6 (7%)
39	CLA	E	316	-	52,60,73	1.66	6 (11%)	60,97,113	1.54	8 (13%)
49	KC2	7	320	-	48,53,53	1.86	9 (18%)	54,89,89	2.01	13 (24%)
39	CLA	9	312	35	42,50,73	1.81	6 (14%)	48,85,113	1.66	8 (16%)
50	A1EB1	3	303	-	51,58,58	1.28	4 (7%)	60,85,85	2.05	18 (30%)
50	A1EB1	8	306	-	51,58,58	1.28	3 (5%)	60,85,85	2.08	19 (31%)
39	CLA	X	317	-	52,60,73	1.68	6 (11%)	60,97,113	1.58	7 (11%)
48	A86	E	304	-	44,50,50	1.26	3 (6%)	51,76,76	2.41	19 (37%)
39	CLA	O	313	-	50,58,73	1.67	6 (12%)	58,95,113	1.59	7 (12%)
39	CLA	9	309	-	41,49,73	1.83	6 (14%)	47,84,113	1.77	7 (14%)
51	A1ECV	S	318	-	51,56,56	2.69	18 (35%)	53,93,93	4.01	28 (52%)
39	CLA	E	310	-	65,73,73	1.48	6 (9%)	76,113,113	1.43	9 (11%)
39	CLA	8	318	-	41,49,73	1.87	5 (12%)	47,84,113	1.67	8 (17%)
49	KC2	3	317	-	48,53,53	1.86	9 (18%)	54,89,89	2.11	15 (27%)
50	A1EB1	z	302	-	51,58,58	1.28	3 (5%)	60,85,85	2.12	20 (33%)
39	CLA	V	319	-	52,60,73	1.68	6 (11%)	60,97,113	1.48	7 (11%)
39	CLA	O	308	-	37,46,73	1.94	6 (16%)	44,80,113	2.22	13 (29%)
39	CLA	a	825	-	62,70,73	1.51	6 (9%)	72,109,113	1.51	8 (11%)
43	DD6	E	305	-	39,45,45	1.99	3 (7%)	52,67,67	1.92	14 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	KC2	V	314	-	48,53,53	1.86	9 (18%)	54,89,89	2.09	15 (27%)
39	CLA	h	201	-	55,63,73	1.61	6 (10%)	64,101,113	1.49	8 (12%)
52	A1EB4	X	305	-	52,59,63	2.59	4 (7%)	61,85,89	1.90	19 (31%)
43	DD6	U	204	-	39,45,45	2.04	4 (10%)	52,67,67	1.72	12 (23%)
39	CLA	z	318	-	41,49,73	1.82	5 (12%)	47,84,113	1.80	7 (14%)
50	A1EB1	G	308	-	51,58,58	1.22	3 (5%)	60,85,85	2.28	16 (26%)
48	A86	M	306	-	44,50,50	1.24	3 (6%)	51,76,76	2.08	17 (33%)
48	A86	9	306	-	44,50,50	1.18	2 (4%)	51,76,76	2.38	15 (29%)
39	CLA	G	310	-	65,73,73	1.50	7 (10%)	76,113,113	1.42	8 (10%)
39	CLA	a	818	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	7 (9%)
39	CLA	b	825	-	65,73,73	1.50	6 (9%)	76,113,113	1.46	10 (13%)
39	CLA	C	310	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	7 (9%)
39	CLA	K	312	-	65,73,73	1.46	6 (9%)	76,113,113	1.46	7 (9%)
39	CLA	2	312	-	41,49,73	1.83	6 (14%)	47,84,113	1.69	8 (17%)
50	A1EB1	T	302	-	51,58,58	1.27	3 (5%)	60,85,85	2.04	12 (20%)
48	A86	Z	303	-	44,50,50	1.16	3 (6%)	51,76,76	2.27	18 (35%)
50	A1EB1	H	304	-	51,58,58	1.22	3 (5%)	60,85,85	1.63	11 (18%)
39	CLA	y	319	-	41,49,73	1.86	5 (12%)	47,84,113	1.81	7 (14%)
47	SQD	W	301	-	27,28,54	1.22	4 (14%)	36,39,65	1.79	9 (25%)
48	A86	L	306	-	44,50,50	1.16	3 (6%)	51,76,76	2.15	15 (29%)
52	A1EB4	M	322	-	52,59,63	2.81	6 (11%)	61,85,89	2.80	22 (36%)
48	A86	L	302	-	44,50,50	1.13	3 (6%)	51,76,76	2.99	22 (43%)
49	KC2	y	313	-	48,53,53	1.85	10 (20%)	54,89,89	2.08	13 (24%)
48	A86	I	304	-	44,50,50	1.13	3 (6%)	51,76,76	2.14	14 (27%)
49	KC2	S	314	-	48,53,53	1.86	9 (18%)	54,89,89	2.04	13 (24%)
39	CLA	6	310	-	42,50,73	1.85	5 (11%)	48,85,113	1.59	7 (14%)
39	CLA	Z	307	-	41,49,73	1.83	6 (14%)	47,84,113	1.73	7 (14%)
46	LMG	Q	322	49	28,28,55	1.26	2 (7%)	36,36,63	1.44	6 (16%)
39	CLA	a	811	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
48	A86	P	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.25	18 (35%)
49	KC2	5	314	-	48,53,53	1.85	10 (20%)	54,89,89	2.10	14 (25%)
49	KC2	z	312	-	48,53,53	1.85	10 (20%)	54,89,89	1.96	11 (20%)
47	SQD	F	318	-	41,42,54	1.07	5 (12%)	50,53,65	1.70	10 (20%)
39	CLA	a	814	-	61,69,73	1.54	7 (11%)	71,108,113	1.46	8 (11%)
39	CLA	a	834	-	51,59,73	1.64	6 (11%)	59,96,113	1.61	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	E	315	-	46,54,73	1.78	6 (13%)	53,90,113	1.55	6 (11%)
39	CLA	y	307	-	41,49,73	1.86	6 (14%)	47,84,113	1.69	7 (14%)
39	CLA	x	306	-	45,53,73	1.80	5 (11%)	52,89,113	1.60	6 (11%)
39	CLA	8	311	-	55,63,73	1.58	5 (9%)	64,101,113	1.58	8 (12%)
49	KC2	T	316	-	48,53,53	1.86	9 (18%)	54,89,89	2.10	13 (24%)
39	CLA	a	809	-	62,70,73	1.51	6 (9%)	72,109,113	1.44	7 (9%)
39	CLA	S	320	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	8 (10%)
49	KC2	Q	318	26	48,53,53	1.84	10 (20%)	54,89,89	2.12	13 (24%)
39	CLA	W	313	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	8 (10%)
39	CLA	P	309	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
50	A1EB1	G	307	-	51,58,58	1.29	4 (7%)	60,85,85	1.87	17 (28%)
49	KC2	L	317	-	48,53,53	1.85	10 (20%)	54,89,89	2.12	14 (25%)
43	DD6	F	305	-	39,45,45	2.14	3 (7%)	52,67,67	2.66	17 (32%)
39	CLA	R	308	-	60,68,73	1.54	5 (8%)	70,107,113	1.41	6 (8%)
39	CLA	U	212	-	46,54,73	1.78	5 (10%)	53,90,113	1.56	6 (11%)
39	CLA	W	309	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	6 (7%)
39	CLA	Y	311	-	41,49,73	1.87	5 (12%)	47,84,113	1.73	8 (17%)
48	A86	P	302	-	44,50,50	1.23	2 (4%)	51,76,76	2.31	17 (33%)
39	CLA	k	201	-	52,60,73	1.66	7 (13%)	60,97,113	1.53	7 (11%)
51	A1ECV	X	310	-	51,56,56	2.65	18 (35%)	53,93,93	4.20	27 (50%)
48	A86	4	305	-	44,50,50	1.16	2 (4%)	51,76,76	1.94	11 (21%)
52	A1EB4	W	321	-	52,59,63	2.65	5 (9%)	61,85,89	2.25	20 (32%)
39	CLA	I	314	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	8 (10%)
39	CLA	x	308	-	41,49,73	1.81	6 (14%)	47,84,113	1.83	7 (14%)
39	CLA	2	318	-	41,49,73	1.87	5 (12%)	47,84,113	1.70	7 (14%)
49	KC2	3	318	-	48,53,53	1.88	10 (20%)	54,89,89	2.07	15 (27%)
39	CLA	a	820	-	51,59,73	1.70	6 (11%)	59,96,113	1.46	7 (11%)
50	A1EB1	J	302	-	51,58,58	1.26	4 (7%)	60,85,85	2.25	23 (38%)
39	CLA	O	318	-	46,54,73	1.75	5 (10%)	53,90,113	1.69	7 (13%)
48	A86	1	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.29	18 (35%)
48	A86	Q	301	-	44,50,50	1.22	3 (6%)	51,76,76	2.35	19 (37%)
50	A1EB1	E	301	-	51,58,58	1.31	4 (7%)	60,85,85	1.91	19 (31%)
43	DD6	D	303	-	39,45,45	2.10	2 (5%)	52,67,67	2.77	15 (28%)
49	KC2	Y	308	-	48,53,53	1.86	9 (18%)	54,89,89	1.93	11 (20%)
49	KC2	1	315	-	48,53,53	1.86	10 (20%)	54,89,89	2.08	11 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	a	832	-	50,58,73	1.71	6 (12%)	58,95,113	1.53	7 (12%)
49	KC2	x	315	-	48,53,53	1.84	9 (18%)	54,89,89	1.96	12 (22%)
50	A1EB1	x	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.07	19 (31%)
39	CLA	M	315	-	41,49,73	1.82	5 (12%)	47,84,113	1.77	9 (19%)
50	A1EB1	R	303	-	51,58,58	1.31	5 (9%)	60,85,85	2.18	19 (31%)
48	A86	5	301	-	44,50,50	1.21	2 (4%)	51,76,76	2.19	16 (31%)
51	A1ECV	4	321	-	51,56,56	2.66	18 (35%)	53,93,93	4.02	29 (54%)
39	CLA	1	309	-	42,50,73	1.84	6 (14%)	48,85,113	1.62	6 (12%)
42	BCR	i	102	-	41,41,41	0.72	0	56,56,56	2.26	19 (33%)
51	A1ECV	7	323	-	51,56,56	2.63	19 (37%)	53,93,93	4.18	26 (49%)
39	CLA	K	307	-	65,73,73	1.50	6 (9%)	76,113,113	1.40	6 (7%)
39	CLA	5	308	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	7 (9%)
48	A86	2	305	-	44,50,50	1.12	2 (4%)	51,76,76	2.43	15 (29%)
39	CLA	J	316	-	46,54,73	1.75	6 (13%)	53,90,113	1.64	6 (11%)
39	CLA	1	316	-	41,49,73	1.86	5 (12%)	47,84,113	1.68	7 (14%)
39	CLA	a	819	-	49,57,73	1.70	5 (10%)	55,93,113	1.59	9 (16%)
46	LMG	M	319	49	39,39,55	1.08	2 (5%)	47,47,63	1.56	8 (17%)
50	A1EB1	Q	323	-	51,58,58	1.24	3 (5%)	60,85,85	2.08	15 (25%)
48	A86	8	323	-	44,50,50	1.19	3 (6%)	51,76,76	2.21	16 (31%)
39	CLA	F	310	-	54,62,73	1.63	5 (9%)	62,99,113	1.53	7 (11%)
51	A1ECV	z	316	-	51,56,56	2.66	19 (37%)	53,93,93	4.26	28 (52%)
39	CLA	b	817	-	59,67,73	1.56	5 (8%)	68,105,113	1.48	8 (11%)
39	CLA	I	309	-	65,73,73	1.50	6 (9%)	76,113,113	1.39	6 (7%)
39	CLA	6	311	-	39,48,73	1.88	6 (15%)	44,83,113	1.73	9 (20%)
39	CLA	O	311	-	42,50,73	1.89	6 (14%)	48,85,113	1.59	7 (14%)
49	KC2	4	317	-	48,53,53	1.86	9 (18%)	54,89,89	2.05	13 (24%)
43	DD6	Q	306	-	39,45,45	2.01	3 (7%)	52,67,67	1.83	14 (26%)
51	A1ECV	z	310	-	51,56,56	2.66	19 (37%)	53,93,93	4.25	26 (49%)
48	A86	y	306	-	44,50,50	1.16	2 (4%)	51,76,76	2.50	18 (35%)
39	CLA	9	319	-	45,53,73	1.80	5 (11%)	52,89,113	1.60	7 (13%)
39	CLA	Y	302	-	41,49,73	1.85	5 (12%)	47,84,113	1.72	7 (14%)
39	CLA	b	808	-	45,53,73	1.77	6 (13%)	52,89,113	1.69	7 (13%)
39	CLA	a	813	1	50,58,73	1.67	6 (12%)	58,95,113	1.67	8 (13%)
39	CLA	1	319	-	51,59,73	1.69	6 (11%)	59,96,113	1.54	7 (11%)
39	CLA	Z	313	-	41,49,73	1.85	6 (14%)	47,84,113	2.08	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	A	314	-	65,73,73	1.48	5 (7%)	76,113,113	1.46	9 (11%)
39	CLA	K	311	-	65,73,73	1.45	5 (7%)	76,113,113	1.43	6 (7%)
39	CLA	b	826	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	7 (9%)
49	KC2	9	318	-	48,53,53	1.85	9 (18%)	54,89,89	1.93	11 (20%)
49	KC2	F	311	46	47,52,53	1.80	9 (19%)	51,87,89	2.24	15 (29%)
49	KC2	1	312	-	48,53,53	1.85	11 (22%)	54,89,89	1.92	12 (22%)
43	DD6	y	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.84	14 (26%)
39	CLA	i	101	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	7 (9%)
48	A86	4	306	-	44,50,50	1.18	2 (4%)	51,76,76	1.99	15 (29%)
48	A86	4	310	-	44,50,50	1.18	2 (4%)	51,76,76	2.34	17 (33%)
51	A1ECV	5	312	27	51,56,56	2.66	18 (35%)	53,93,93	4.08	28 (52%)
42	BCR	a	845	-	41,41,41	0.75	0	56,56,56	2.14	15 (26%)
51	A1ECV	T	317	-	51,56,56	2.64	19 (37%)	53,93,93	3.94	28 (52%)
39	CLA	x	309	-	41,49,73	1.85	6 (14%)	47,84,113	1.73	7 (14%)
39	CLA	y	312	-	42,50,73	1.83	5 (11%)	48,85,113	1.61	6 (12%)
48	A86	L	305	-	44,50,50	1.22	3 (6%)	51,76,76	2.17	16 (31%)
43	DD6	J	305	-	39,45,45	2.05	3 (7%)	52,67,67	2.29	17 (32%)
49	KC2	x	312	-	48,53,53	1.85	10 (20%)	54,89,89	2.04	13 (24%)
43	DD6	H	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	10 (19%)
39	CLA	M	309	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	8 (10%)
39	CLA	1	308	-	41,49,73	1.87	5 (12%)	47,84,113	1.70	7 (14%)
39	CLA	M	308	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
39	CLA	8	312	-	45,53,73	1.80	5 (11%)	52,89,113	1.64	6 (11%)
39	CLA	b	842	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
50	A1EB1	G	304	-	51,58,58	1.31	4 (7%)	60,85,85	2.04	20 (33%)
39	CLA	A	307	-	60,68,73	1.57	6 (10%)	70,107,113	1.43	7 (10%)
43	DD6	D	307	-	39,45,45	1.97	3 (7%)	52,67,67	1.79	10 (19%)
48	A86	4	309	-	44,50,50	1.21	3 (6%)	51,76,76	2.13	17 (33%)
39	CLA	L	316	-	41,49,73	1.84	5 (12%)	47,84,113	1.75	8 (17%)
50	A1EB1	U	205	-	51,58,58	1.23	4 (7%)	60,85,85	1.99	19 (31%)
39	CLA	T	309	-	56,64,73	1.63	6 (10%)	65,102,113	1.50	8 (12%)
39	CLA	b	838	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	10 (13%)
49	KC2	A	310	13	48,53,53	1.85	9 (18%)	54,89,89	1.94	9 (16%)
39	CLA	2	308	-	46,54,73	1.78	6 (13%)	53,90,113	1.59	7 (13%)
39	CLA	2	316	-	41,49,73	1.86	6 (14%)	47,84,113	1.69	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	A1EB1	0	303	-	51,58,58	1.26	3 (5%)	60,85,85	2.23	17 (28%)
49	KC2	6	319	-	48,53,53	1.87	10 (20%)	54,89,89	1.94	10 (18%)
43	DD6	j	102	-	39,45,45	1.96	2 (5%)	52,67,67	1.85	12 (23%)
49	KC2	y	316	-	48,53,53	1.83	10 (20%)	54,89,89	2.09	14 (25%)
39	CLA	C	309	-	46,54,73	1.78	5 (10%)	53,90,113	1.54	6 (11%)
39	CLA	M	321	24	46,54,73	1.76	5 (10%)	53,90,113	1.58	7 (13%)
46	LMG	9	321	-	36,36,55	0.91	0	44,44,63	1.20	3 (6%)
51	A1ECV	E	311	-	51,56,56	2.68	21 (41%)	53,93,93	4.09	24 (45%)
49	KC2	T	315	29	48,53,53	1.86	10 (20%)	54,89,89	2.04	15 (27%)
39	CLA	7	314	-	56,64,73	1.60	5 (8%)	65,102,113	1.60	11 (16%)
39	CLA	a	804	-	65,73,73	1.46	6 (9%)	76,113,113	1.36	7 (9%)
43	DD6	K	303	-	39,45,45	1.95	3 (7%)	52,67,67	1.73	11 (21%)
50	A1EB1	O	301	-	51,58,58	1.24	4 (7%)	60,85,85	1.95	18 (30%)
50	A1EB1	4	303	-	51,58,58	1.27	3 (5%)	60,85,85	1.84	14 (23%)
49	KC2	A	313	-	48,53,53	1.87	10 (20%)	54,89,89	2.07	15 (27%)
50	A1EB1	9	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.05	19 (31%)
50	A1EB1	L	303	-	51,58,58	1.29	3 (5%)	60,85,85	2.24	19 (31%)
48	A86	6	302	-	44,50,50	1.16	3 (6%)	51,76,76	2.16	15 (29%)
48	A86	R	302	-	44,50,50	1.15	2 (4%)	51,76,76	2.19	13 (25%)
39	CLA	z	308	-	46,54,73	1.77	5 (10%)	53,90,113	1.56	6 (11%)
39	CLA	0	313	-	55,63,73	1.62	6 (10%)	64,101,113	1.51	8 (12%)
43	DD6	W	305	-	39,45,45	1.91	3 (7%)	52,67,67	1.78	12 (23%)
48	A86	0	306	-	44,50,50	1.14	3 (6%)	51,76,76	2.25	17 (33%)
39	CLA	b	834	-	58,66,73	1.60	7 (12%)	67,104,113	1.46	8 (11%)
39	CLA	a	805	-	65,73,73	1.44	6 (9%)	76,113,113	1.49	8 (10%)
39	CLA	x	311	-	45,53,73	1.80	5 (11%)	52,89,113	1.61	6 (11%)
39	CLA	K	309	-	62,70,73	1.50	5 (8%)	72,109,113	1.42	7 (9%)
49	KC2	0	319	-	48,53,53	1.90	10 (20%)	54,89,89	1.88	11 (20%)
39	CLA	J	313	-	46,54,73	1.78	6 (13%)	53,90,113	1.56	6 (11%)
49	KC2	X	306	27	48,53,53	1.87	10 (20%)	54,89,89	1.92	12 (22%)
39	CLA	a	802	-	55,63,73	1.60	6 (10%)	64,101,113	1.54	8 (12%)
39	CLA	L	313	-	50,58,73	1.67	6 (12%)	58,95,113	1.54	6 (10%)
49	KC2	V	312	-	48,53,53	1.86	10 (20%)	54,89,89	2.13	14 (25%)
49	KC2	8	316	-	48,53,53	1.85	10 (20%)	54,89,89	2.22	13 (24%)
39	CLA	b	816	-	60,68,73	1.56	6 (10%)	70,107,113	1.43	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	3	323	-	46,54,73	1.76	6 (13%)	53,90,113	1.64	6 (11%)
49	KC2	V	320	-	48,53,53	1.82	10 (20%)	54,89,89	2.18	14 (25%)
49	KC2	Q	313	46	47,52,53	1.91	9 (19%)	51,87,89	2.18	14 (27%)
39	CLA	J	311	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	7 (9%)
48	A86	X	302	-	44,50,50	1.17	2 (4%)	51,76,76	2.19	17 (33%)
39	CLA	T	310	29	52,60,73	1.65	7 (13%)	60,97,113	1.54	7 (11%)
43	DD6	3	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	13 (25%)
39	CLA	W	316	24	41,49,73	1.81	6 (14%)	47,84,113	1.79	9 (19%)
48	A86	7	308	-	44,50,50	1.19	2 (4%)	51,76,76	2.06	16 (31%)
44	SF4	c	101	-	0,12,12	-	-	-	-	-
39	CLA	a	823	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	11 (14%)
39	CLA	U	201	-	46,54,73	1.70	8 (17%)	53,90,113	1.60	8 (15%)
48	A86	8	307	-	44,50,50	1.23	3 (6%)	51,76,76	2.45	23 (45%)
39	CLA	b	830	-	65,73,73	1.50	6 (9%)	76,113,113	1.55	7 (9%)
39	CLA	P	316	-	51,59,73	1.69	5 (9%)	59,96,113	1.54	7 (11%)
39	CLA	H	309	20	52,60,73	1.66	6 (11%)	60,97,113	1.53	7 (11%)
51	A1ECV	y	311	-	51,56,56	2.66	19 (37%)	53,93,93	4.23	28 (52%)
39	CLA	x	318	-	41,49,73	1.88	5 (12%)	47,84,113	1.76	8 (17%)
48	A86	U	206	-	44,50,50	1.20	3 (6%)	51,76,76	2.39	19 (37%)
39	CLA	a	836	-	65,73,73	1.48	5 (7%)	76,113,113	1.43	6 (7%)
39	CLA	a	821	-	55,63,73	1.61	6 (10%)	64,101,113	1.49	7 (10%)
48	A86	L	301	-	44,50,50	1.16	3 (6%)	51,76,76	2.05	14 (27%)
51	A1ECV	S	312	-	51,56,56	2.66	20 (39%)	53,93,93	4.24	28 (52%)
39	CLA	Q	310	-	65,73,73	1.51	6 (9%)	76,113,113	1.40	9 (11%)
39	CLA	b	832	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	6 (7%)
39	CLA	L	308	-	61,69,73	1.56	5 (8%)	71,108,113	1.45	8 (11%)
39	CLA	k	203	-	55,63,73	1.63	5 (9%)	64,101,113	1.47	7 (10%)
39	CLA	o	203	12	55,63,73	1.61	6 (10%)	64,101,113	1.51	7 (10%)
39	CLA	2	315	-	41,49,73	1.86	7 (17%)	47,84,113	1.67	7 (14%)
49	KC2	0	317	31	48,53,53	1.86	10 (20%)	54,89,89	2.09	15 (27%)
39	CLA	1	320	-	41,49,73	1.87	5 (12%)	47,84,113	1.71	9 (19%)
48	A86	O	307	-	44,50,50	1.17	2 (4%)	51,76,76	2.35	19 (37%)
43	DD6	T	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.87	13 (25%)
39	CLA	b	811	-	65,73,73	1.47	7 (10%)	76,113,113	1.49	9 (11%)
39	CLA	y	315	-	41,49,73	1.83	6 (14%)	47,84,113	1.72	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
42	BCR	f	804	-	41,41,41	0.68	0	56,56,56	1.98	14 (25%)
39	CLA	b	851	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	7 (9%)
39	CLA	1	310	-	45,53,73	1.80	5 (11%)	52,89,113	1.61	6 (11%)
39	CLA	5	310	27	50,58,73	1.69	5 (10%)	58,95,113	1.58	8 (13%)
44	SF4	c	102	-	0,12,12	-	-	-	-	-
48	A86	U	202	-	44,50,50	1.17	3 (6%)	51,76,76	2.30	20 (39%)
48	A86	y	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.00	16 (31%)
39	CLA	O	314	-	55,63,73	1.66	7 (12%)	64,101,113	1.42	7 (10%)
43	DD6	4	307	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	15 (28%)
50	A1EB1	h	203	-	51,58,58	1.27	4 (7%)	60,85,85	2.00	19 (31%)
46	LMG	0	324	49	27,27,55	1.31	2 (7%)	35,35,63	1.47	4 (11%)
49	KC2	L	321	-	48,53,53	1.85	11 (22%)	54,89,89	1.98	12 (22%)
47	SQD	E	320	-	34,35,54	1.17	5 (14%)	43,46,65	1.98	11 (25%)
46	LMG	4	325	-	32,32,55	0.90	0	40,40,63	1.25	4 (10%)
48	A86	8	305	-	44,50,50	1.20	3 (6%)	51,76,76	2.63	22 (43%)
39	CLA	A	312	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	8 (10%)
50	A1EB1	7	305	-	51,58,58	1.29	4 (7%)	60,85,85	2.22	18 (30%)
41	LHG	D	301	-	34,34,48	0.72	0	37,40,54	1.25	3 (8%)
48	A86	9	304	-	44,50,50	1.16	3 (6%)	51,76,76	2.06	16 (31%)
39	CLA	B	205	-	42,50,73	1.83	5 (11%)	48,85,113	1.67	7 (14%)
48	A86	F	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.12	15 (29%)
51	A1ECV	x	316	-	51,56,56	2.68	17 (33%)	53,93,93	4.16	28 (52%)
39	CLA	2	319	-	46,54,73	1.77	6 (13%)	53,90,113	1.81	10 (18%)
43	DD6	x	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.89	16 (30%)
39	CLA	X	311	27	50,58,73	1.70	5 (10%)	58,95,113	1.55	9 (15%)
43	DD6	O	304	-	39,45,45	2.10	4 (10%)	52,67,67	1.91	15 (28%)
50	A1EB1	U	203	-	51,58,58	1.25	3 (5%)	60,85,85	2.17	19 (31%)
51	A1ECV	Q	319	-	51,56,56	2.62	19 (37%)	53,93,93	4.14	28 (52%)
39	CLA	S	319	-	52,60,73	1.67	6 (11%)	60,97,113	1.66	10 (16%)
50	A1EB1	K	302	-	51,58,58	1.29	4 (7%)	60,85,85	2.12	21 (35%)
39	CLA	7	315	-	50,58,73	1.70	6 (12%)	58,95,113	1.53	8 (13%)
39	CLA	7	324	-	41,49,73	1.85	5 (12%)	47,84,113	1.81	8 (17%)
48	A86	7	311	-	44,50,50	1.19	3 (6%)	51,76,76	2.16	16 (31%)
43	DD6	Z	302	-	39,45,45	2.09	4 (10%)	52,67,67	3.79	20 (38%)
39	CLA	b	835	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	LMG	I	302	-	42,42,55	0.89	1 (2%)	50,50,63	1.22	4 (8%)
39	CLA	W	318	-	51,59,73	1.69	5 (9%)	59,96,113	1.54	6 (10%)
50	A1EB1	1	305	-	51,58,58	1.25	4 (7%)	60,85,85	2.08	16 (26%)
39	CLA	b	831	-	50,58,73	1.68	6 (12%)	58,95,113	1.54	9 (15%)
39	CLA	b	815	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	9 (11%)
43	DD6	I	305	-	39,45,45	1.98	3 (7%)	52,67,67	1.86	13 (25%)
47	SQD	9	322	-	35,36,54	1.16	5 (14%)	44,47,65	1.65	9 (20%)
42	BCR	b	844	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
48	A86	S	304	-	44,50,50	1.13	2 (4%)	51,76,76	1.98	11 (21%)
39	CLA	b	820	-	60,68,73	1.56	6 (10%)	70,107,113	1.42	7 (10%)
48	A86	2	301	-	44,50,50	1.18	3 (6%)	51,76,76	2.31	17 (33%)
48	A86	k	206	-	44,50,50	1.18	3 (6%)	51,76,76	2.00	13 (25%)
39	CLA	R	307	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	7 (9%)
48	A86	8	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.04	15 (29%)
39	CLA	M	310	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
39	CLA	E	307	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	7 (9%)
39	CLA	Z	315	-	41,49,73	1.86	5 (12%)	47,84,113	1.69	7 (14%)
51	A1ECV	O	315	-	51,56,56	2.66	17 (33%)	53,93,93	4.03	28 (52%)
47	SQD	H	318	-	37,38,54	1.13	5 (13%)	46,49,65	1.64	8 (17%)
39	CLA	R	311	27	50,58,73	1.69	7 (14%)	58,95,113	1.54	7 (12%)
43	DD6	D	306	-	39,45,45	2.66	4 (10%)	52,67,67	2.39	12 (23%)
39	CLA	a	810	-	54,62,73	1.64	6 (11%)	62,99,113	1.48	8 (12%)
39	CLA	7	325	-	50,58,73	1.72	5 (10%)	58,95,113	1.54	9 (15%)
39	CLA	y	308	-	45,53,73	1.78	6 (13%)	52,89,113	1.69	8 (15%)
39	CLA	W	311	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	7 (9%)
39	CLA	Y	310	-	41,49,73	1.86	5 (12%)	47,84,113	1.70	7 (14%)
39	CLA	z	311	-	41,49,73	1.86	5 (12%)	47,84,113	1.64	7 (14%)
39	CLA	b	827	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	6 (7%)
43	DD6	1	304	-	39,45,45	2.22	3 (7%)	52,67,67	3.19	18 (34%)
39	CLA	1	311	-	41,49,73	1.88	6 (14%)	47,84,113	1.63	7 (14%)
39	CLA	o	201	-	51,59,73	1.67	5 (9%)	59,96,113	1.55	7 (11%)
43	DD6	3	304	-	39,45,45	2.05	3 (7%)	52,67,67	3.25	19 (36%)
42	BCR	l	206	-	41,41,41	0.69	0	56,56,56	1.76	13 (23%)
39	CLA	U	213	-	41,49,73	1.86	6 (14%)	47,84,113	1.72	7 (14%)
43	DD6	G	303	-	39,45,45	1.93	3 (7%)	52,67,67	1.82	11 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	L	310	23	65,73,73	1.49	5 (7%)	76,113,113	1.41	6 (7%)
39	CLA	U	214	-	46,54,73	1.77	6 (13%)	53,90,113	1.56	6 (11%)
50	A1EB1	7	304	-	51,58,58	1.23	4 (7%)	60,85,85	2.03	19 (31%)
39	CLA	W	319	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	6 (11%)
39	CLA	b	801	-	65,73,73	1.41	10 (15%)	76,113,113	1.42	9 (11%)
39	CLA	6	322	-	46,54,73	1.78	5 (10%)	53,90,113	1.59	6 (11%)
40	PQN	b	843	-	34,34,34	1.53	2 (5%)	42,45,45	1.26	4 (9%)
50	A1EB1	V	307	-	51,58,58	1.26	4 (7%)	60,85,85	2.09	21 (35%)
48	A86	W	304	-	44,50,50	1.21	3 (6%)	51,76,76	2.29	18 (35%)
39	CLA	6	315	-	41,49,73	1.81	6 (14%)	47,84,113	1.80	7 (14%)
50	A1EB1	3	310	-	51,58,58	1.27	4 (7%)	60,85,85	2.05	17 (28%)
50	A1EB1	F	304	-	51,58,58	1.30	4 (7%)	60,85,85	2.12	18 (30%)
39	CLA	O	309	-	45,53,73	1.78	7 (15%)	52,89,113	1.60	6 (11%)
39	CLA	B	207	-	55,63,73	1.64	5 (9%)	64,101,113	1.53	8 (12%)
39	CLA	b	823	-	46,54,73	1.78	5 (10%)	53,90,113	1.60	7 (13%)
48	A86	S	307	-	44,50,50	1.19	2 (4%)	51,76,76	2.32	18 (35%)
49	KC2	9	316	35	48,53,53	1.83	10 (20%)	54,89,89	2.03	13 (24%)
39	CLA	T	319	29	46,54,73	1.78	5 (10%)	53,90,113	1.63	7 (13%)
41	LHG	a	840	-	48,48,48	0.62	1 (2%)	51,54,54	1.28	7 (13%)
50	A1EB1	2	306	-	51,58,58	1.24	3 (5%)	60,85,85	2.09	20 (33%)
39	CLA	F	314	18	55,63,73	1.62	5 (9%)	64,101,113	1.62	11 (17%)
39	CLA	J	314	-	65,73,73	1.50	5 (7%)	76,113,113	1.33	7 (9%)
49	KC2	K	313	22	48,53,53	1.87	10 (20%)	54,89,89	2.11	14 (25%)
51	A1ECV	Y	306	-	51,56,56	2.68	18 (35%)	53,93,93	4.22	27 (50%)
49	KC2	2	314	-	48,53,53	1.86	10 (20%)	54,89,89	2.11	14 (25%)
39	CLA	6	321	-	41,49,73	1.85	5 (12%)	47,84,113	1.67	7 (14%)
41	LHG	a	841	39	26,26,48	0.85	1 (3%)	29,32,54	1.33	3 (10%)
39	CLA	B	203	-	46,54,73	1.75	5 (10%)	53,90,113	1.60	7 (13%)
50	A1EB1	6	308	-	51,58,58	1.29	4 (7%)	60,85,85	2.25	19 (31%)
50	A1EB1	K	305	-	51,58,58	1.25	3 (5%)	60,85,85	2.22	18 (30%)
47	SQD	P	301	-	37,38,54	1.11	5 (13%)	46,49,65	1.73	12 (26%)
43	DD6	C	301	-	39,45,45	2.32	4 (10%)	52,67,67	2.51	14 (26%)
39	CLA	b	829	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
39	CLA	x	314	-	41,49,73	1.85	5 (12%)	47,84,113	1.71	7 (14%)
50	A1EB1	y	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.21	20 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
42	BCR	b	845	-	41,41,41	0.72	0	56,56,56	1.96	17 (30%)
39	CLA	a	822	-	65,73,73	1.47	5 (7%)	76,113,113	1.49	8 (10%)
39	CLA	j	101	-	65,73,73	1.44	6 (9%)	76,113,113	1.49	8 (10%)
51	A1ECV	P	315	-	51,56,56	2.64	17 (33%)	53,93,93	4.12	27 (50%)
39	CLA	f	802	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	8 (10%)
39	CLA	Z	309	-	41,49,73	1.85	5 (12%)	47,84,113	1.63	6 (12%)
39	CLA	I	316	36	41,49,73	1.84	5 (12%)	47,84,113	1.69	8 (17%)
42	BCR	k	204	-	41,41,41	0.71	0	56,56,56	1.90	15 (26%)
48	A86	9	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.01	14 (27%)
49	KC2	X	318	-	48,53,53	1.85	9 (18%)	54,89,89	2.10	13 (24%)
39	CLA	b	822	2	50,58,73	1.70	6 (12%)	58,95,113	1.53	7 (12%)
39	CLA	D	313	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	7 (9%)
39	CLA	H	306	-	48,56,73	1.73	7 (14%)	55,92,113	1.57	7 (12%)
43	DD6	M	304	-	39,45,45	1.92	3 (7%)	52,67,67	1.71	12 (23%)
39	CLA	P	311	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	7 (9%)
43	DD6	2	303	-	39,45,45	2.09	4 (10%)	52,67,67	3.79	20 (38%)
43	DD6	A	302	-	39,45,45	1.97	3 (7%)	52,67,67	1.84	11 (21%)
48	A86	3	307	-	44,50,50	1.22	3 (6%)	51,76,76	2.40	20 (39%)
39	CLA	G	309	-	56,64,73	1.59	6 (10%)	65,102,113	1.49	7 (10%)
50	A1EB1	z	301	-	44,50,58	1.15	2 (4%)	51,76,85	1.70	12 (23%)
43	DD6	E	303	-	39,45,45	1.93	3 (7%)	52,67,67	1.84	11 (21%)
47	SQD	D	321	-	38,39,54	1.10	5 (13%)	47,50,65	1.70	11 (23%)
39	CLA	J	317	-	42,50,73	1.87	6 (14%)	48,85,113	1.64	6 (12%)
39	CLA	4	312	-	65,73,73	1.50	6 (9%)	76,113,113	1.47	10 (13%)
39	CLA	b	819	-	59,67,73	1.58	5 (8%)	68,105,113	1.45	6 (8%)
39	CLA	4	311	-	61,69,73	1.56	6 (9%)	71,108,113	1.47	9 (12%)
39	CLA	6	318	-	41,49,73	1.85	6 (14%)	47,84,113	1.70	7 (14%)
41	LHG	H	317	-	34,34,48	0.71	0	37,40,54	1.19	3 (8%)
39	CLA	b	803	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
39	CLA	b	839	-	47,55,73	1.77	6 (12%)	54,91,113	1.52	8 (14%)
48	A86	J	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.28	18 (35%)
49	KC2	G	317	-	48,53,53	1.83	10 (20%)	54,89,89	2.19	15 (27%)
39	CLA	z	314	-	41,49,73	1.86	5 (12%)	47,84,113	1.69	7 (14%)
39	CLA	5	306	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
39	CLA	4	313	-	46,54,73	1.77	5 (10%)	53,90,113	1.55	6 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	D	309	16	49,57,73	1.72	5 (10%)	55,93,113	1.65	8 (14%)
39	CLA	I	301	41	52,60,73	1.68	5 (9%)	60,97,113	1.49	8 (13%)
49	KC2	X	312	-	48,53,53	1.86	9 (18%)	54,89,89	2.16	15 (27%)
48	A86	7	312	-	44,50,50	1.21	2 (4%)	51,76,76	2.29	18 (35%)
39	CLA	G	312	-	52,60,73	1.67	5 (9%)	60,97,113	1.60	8 (13%)
39	CLA	U	207	-	60,68,73	1.55	6 (10%)	70,107,113	1.45	7 (10%)
39	CLA	a	835	-	65,73,73	1.48	5 (7%)	76,113,113	1.43	8 (10%)
48	A86	T	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.22	19 (37%)
39	CLA	a	829	-	56,64,73	1.60	5 (8%)	65,102,113	1.55	6 (9%)
49	KC2	F	307	-	48,53,53	1.86	10 (20%)	54,89,89	2.10	14 (25%)
39	CLA	O	312	-	46,54,73	1.76	6 (13%)	53,90,113	1.59	6 (11%)
39	CLA	M	317	-	51,59,73	1.69	6 (11%)	59,96,113	1.53	6 (10%)
39	CLA	J	307	21	49,57,73	1.72	6 (12%)	55,93,113	1.58	7 (12%)
39	CLA	Q	317	-	46,54,73	1.80	5 (10%)	53,90,113	1.54	7 (13%)
39	CLA	8	310	-	45,53,73	1.82	5 (11%)	52,89,113	1.66	9 (17%)
47	SQD	M	301	-	38,39,54	1.11	5 (13%)	47,50,65	1.69	13 (27%)
42	BCR	b	847	-	41,41,41	0.71	0	56,56,56	2.01	16 (28%)
49	KC2	P	310	46	47,52,53	1.82	9 (19%)	51,87,89	2.17	14 (27%)
39	CLA	a	817	1	45,53,73	1.80	6 (13%)	52,89,113	1.62	6 (11%)
49	KC2	W	315	-	48,53,53	1.85	9 (18%)	54,89,89	1.99	11 (20%)
48	A86	L	304	-	44,50,50	1.21	3 (6%)	51,76,76	2.32	18 (35%)
49	KC2	L	315	-	48,53,53	1.86	10 (20%)	54,89,89	2.12	12 (22%)
50	A1EB1	6	306	-	44,50,58	1.15	2 (4%)	51,76,85	1.86	11 (21%)
39	CLA	H	307	-	45,53,73	1.80	5 (11%)	52,89,113	1.61	6 (11%)
39	CLA	x	307	-	41,49,73	1.86	6 (14%)	47,84,113	1.68	9 (19%)
48	A86	O	302	-	44,50,50	1.22	3 (6%)	51,76,76	2.36	20 (39%)
50	A1EB1	3	324	-	51,58,58	1.29	3 (5%)	60,85,85	2.03	18 (30%)
43	DD6	P	304	-	39,45,45	2.10	3 (7%)	52,67,67	2.77	14 (26%)
49	KC2	8	314	-	48,53,53	1.84	9 (18%)	54,89,89	2.03	13 (24%)
52	A1EB4	P	305	-	51,58,63	2.60	4 (7%)	60,84,89	2.09	19 (31%)
39	CLA	0	311	-	55,63,73	1.66	6 (10%)	64,101,113	1.57	10 (15%)
52	A1EB4	M	305	-	53,60,63	2.51	4 (7%)	62,86,89	2.08	16 (25%)
39	CLA	l	201	-	65,73,73	1.50	5 (7%)	76,113,113	1.33	8 (10%)
47	SQD	k	205	-	37,38,54	1.13	5 (13%)	46,49,65	1.66	9 (19%)
39	CLA	b	810	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	y	310	-	41,49,73	1.86	6 (14%)	47,84,113	1.66	7 (14%)
39	CLA	5	316	-	52,60,73	1.68	6 (11%)	60,97,113	1.52	7 (11%)
49	KC2	G	315	-	48,53,53	1.88	9 (18%)	54,89,89	2.13	16 (29%)
39	CLA	o	205	-	52,60,73	1.67	6 (11%)	60,97,113	1.51	7 (11%)
43	DD6	R	304	-	39,45,45	1.95	4 (10%)	52,67,67	1.84	15 (28%)
48	A86	L	307	-	44,50,50	1.18	3 (6%)	51,76,76	2.52	20 (39%)
39	CLA	U	209	-	52,60,73	1.65	6 (11%)	60,97,113	1.58	8 (13%)
39	CLA	F	313	-	57,65,73	1.58	6 (10%)	66,103,113	1.45	8 (12%)
49	KC2	S	317	-	48,53,53	1.84	10 (20%)	54,89,89	2.10	13 (24%)
39	CLA	K	314	-	41,49,73	1.85	5 (12%)	47,84,113	1.68	9 (19%)
50	A1EB1	4	301	-	51,58,58	1.25	3 (5%)	60,85,85	1.93	18 (30%)
46	LMG	4	326	49	46,46,55	0.96	2 (4%)	54,54,63	1.28	6 (11%)
39	CLA	Z	312	-	41,49,73	1.85	5 (12%)	47,84,113	1.68	7 (14%)
39	CLA	C	306	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
39	CLA	D	318	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	7 (9%)
39	CLA	L	311	23	52,60,73	1.67	6 (11%)	60,97,113	1.48	8 (13%)
39	CLA	4	323	-	65,73,73	1.52	6 (9%)	76,113,113	1.36	6 (7%)
46	LMG	l	208	49	39,39,55	1.06	2 (5%)	47,47,63	1.23	5 (10%)
48	A86	9	301	-	44,50,50	1.20	3 (6%)	51,76,76	2.14	15 (29%)
49	KC2	I	312	46	47,52,53	1.79	9 (19%)	51,87,89	2.24	15 (29%)
50	A1EB1	T	307	-	51,58,58	1.24	4 (7%)	60,85,85	1.95	19 (31%)
39	CLA	0	318	-	41,49,73	1.88	5 (12%)	47,84,113	1.66	7 (14%)
43	DD6	y	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.93	15 (28%)
49	KC2	M	311	46	47,52,53	1.82	9 (19%)	51,87,89	2.15	13 (25%)
39	CLA	Y	314	-	41,49,73	1.86	5 (12%)	47,84,113	1.76	8 (17%)
51	A1ECV	V	317	-	51,56,56	2.63	18 (35%)	53,93,93	3.97	28 (52%)
39	CLA	9	315	-	41,49,73	1.88	5 (12%)	47,84,113	1.72	7 (14%)
51	A1ECV	X	313	-	51,56,56	2.65	20 (39%)	53,93,93	4.04	28 (52%)
39	CLA	D	316	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
42	BCR	b	850	-	41,41,41	0.68	0	56,56,56	1.86	12 (21%)
39	CLA	E	314	-	56,64,73	1.62	7 (12%)	65,102,113	1.45	6 (9%)
43	DD6	7	310	-	39,45,45	2.06	3 (7%)	52,67,67	2.49	14 (26%)
49	KC2	5	311	-	48,53,53	1.86	10 (20%)	54,89,89	2.19	16 (29%)
49	KC2	9	311	-	48,53,53	1.86	10 (20%)	54,89,89	2.01	11 (20%)
39	CLA	f	803	-	55,63,73	1.63	6 (10%)	64,101,113	1.43	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	A1EB1	7	303	-	51,58,58	1.33	3 (5%)	60,85,85	2.01	20 (33%)
50	A1EB1	5	302	-	51,58,58	1.26	3 (5%)	60,85,85	2.12	16 (26%)
43	DD6	4	308	-	39,45,45	2.06	3 (7%)	52,67,67	2.04	14 (26%)
51	A1ECV	y	317	-	51,56,56	2.69	17 (33%)	53,93,93	4.16	28 (52%)
39	CLA	U	208	-	46,54,73	1.78	7 (15%)	53,90,113	1.49	6 (11%)
39	CLA	X	316	-	47,55,73	1.73	6 (12%)	54,91,113	1.60	8 (14%)
46	LMG	D	322	-	37,37,55	0.91	0	45,45,63	1.21	5 (11%)
49	KC2	5	313	46	47,52,53	1.83	9 (19%)	51,87,89	2.14	13 (25%)
51	A1ECV	1	318	-	51,56,56	2.65	19 (37%)	53,93,93	4.26	28 (52%)
50	A1EB1	0	307	-	51,58,58	1.25	3 (5%)	60,85,85	2.24	17 (28%)
39	CLA	b	814	-	55,63,73	1.63	6 (10%)	64,101,113	1.48	7 (10%)
43	DD6	z	304	-	39,45,45	2.05	4 (10%)	52,67,67	1.88	14 (26%)
48	A86	G	305	-	44,50,50	1.19	2 (4%)	51,76,76	2.29	16 (31%)
51	A1ECV	Z	308	-	51,56,56	2.68	19 (37%)	53,93,93	4.24	27 (50%)
39	CLA	0	312	31	53,61,73	1.63	8 (15%)	61,98,113	1.53	8 (13%)
48	A86	1	307	-	44,50,50	1.24	3 (6%)	51,76,76	2.20	18 (35%)
39	CLA	b	809	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	8 (10%)
49	KC2	7	319	-	48,53,53	1.85	10 (20%)	54,89,89	2.12	13 (24%)
51	A1ECV	L	318	-	51,56,56	2.64	15 (29%)	53,93,93	4.03	28 (52%)
39	CLA	J	312	-	46,54,73	1.78	6 (13%)	53,90,113	1.60	6 (11%)
48	A86	z	303	-	44,50,50	1.14	2 (4%)	51,76,76	1.90	11 (21%)
43	DD6	E	302	-	39,45,45	1.98	3 (7%)	52,67,67	1.77	8 (15%)
39	CLA	Q	320	-	47,55,73	1.72	6 (12%)	54,91,113	1.56	6 (11%)
39	CLA	k	202	-	55,63,73	1.62	6 (10%)	64,101,113	1.44	8 (12%)
50	A1EB1	6	304	-	48,55,58	1.32	3 (6%)	57,82,85	2.32	19 (33%)
50	A1EB1	8	301	-	51,58,58	1.26	4 (7%)	60,85,85	1.95	16 (26%)
50	A1EB1	V	302	-	51,58,58	1.27	4 (7%)	60,85,85	2.00	20 (33%)
48	A86	Q	302	-	44,50,50	1.21	3 (6%)	51,76,76	2.27	18 (35%)
39	CLA	H	312	20	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
39	CLA	P	314	-	41,49,73	1.85	7 (17%)	47,84,113	1.75	8 (17%)
42	BCR	a	843	-	41,41,41	0.73	0	56,56,56	1.94	17 (30%)
39	CLA	Y	304	-	46,54,73	1.76	5 (10%)	53,90,113	1.61	6 (11%)
51	A1ECV	R	313	-	51,56,56	2.66	19 (37%)	53,93,93	3.99	29 (54%)
49	KC2	Q	315	-	48,53,53	1.84	10 (20%)	54,89,89	2.05	14 (25%)
52	A1EB4	P	318	-	49,56,63	2.77	5 (10%)	58,82,89	2.27	18 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	3	320	-	45,53,73	1.79	5 (11%)	52,89,113	1.66	8 (15%)
43	DD6	G	306	-	39,45,45	2.02	3 (7%)	52,67,67	2.07	12 (23%)
39	CLA	R	315	-	47,55,73	1.74	6 (12%)	54,91,113	1.61	10 (18%)
48	A86	6	305	-	44,50,50	1.17	2 (4%)	51,76,76	2.19	16 (31%)
43	DD6	I	306	-	39,45,45	1.95	3 (7%)	52,67,67	1.76	11 (21%)
43	DD6	B	202	-	39,45,45	2.03	3 (7%)	52,67,67	1.99	12 (23%)
39	CLA	C	308	-	60,68,73	1.55	6 (10%)	70,107,113	1.45	8 (11%)
46	LMG	7	301	49	46,46,55	0.95	2 (4%)	54,54,63	1.28	6 (11%)
43	DD6	Q	303	-	39,45,45	2.12	3 (7%)	52,67,67	2.59	17 (32%)
49	KC2	R	318	-	48,53,53	1.87	10 (20%)	54,89,89	2.07	13 (24%)
39	CLA	B	204	-	46,54,73	1.77	6 (13%)	53,90,113	1.60	6 (11%)
48	A86	K	301	-	44,50,50	1.23	3 (6%)	51,76,76	2.15	18 (35%)
49	KC2	z	315	-	48,53,53	1.85	10 (20%)	54,89,89	2.15	14 (25%)
39	CLA	K	308	22	59,67,73	1.57	6 (10%)	68,105,113	1.39	6 (8%)
46	LMG	F	320	49	34,34,55	1.14	2 (5%)	42,42,63	1.20	6 (14%)
39	CLA	I	315	-	52,60,73	1.64	5 (9%)	60,97,113	1.63	8 (13%)
39	CLA	R	316	-	52,60,73	1.69	6 (11%)	60,97,113	1.56	7 (11%)
39	CLA	4	316	-	65,73,73	1.47	7 (10%)	76,113,113	1.44	7 (9%)
39	CLA	Y	307	-	41,49,73	1.87	5 (12%)	47,84,113	1.59	7 (14%)
39	CLA	H	308	-	60,68,73	1.56	5 (8%)	70,107,113	1.43	8 (11%)
48	A86	Q	304	-	44,50,50	1.19	3 (6%)	51,76,76	2.14	17 (33%)
39	CLA	b	828	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
49	KC2	0	316	-	48,53,53	1.85	10 (20%)	54,89,89	2.08	15 (27%)
49	KC2	O	317	46	47,52,53	1.83	10 (21%)	51,87,89	1.90	10 (19%)
51	A1ECV	0	321	48	51,56,56	2.59	18 (35%)	53,93,93	3.84	30 (56%)
49	KC2	S	315	28	48,53,53	1.90	10 (20%)	54,89,89	2.10	15 (27%)
39	CLA	z	317	-	42,50,73	1.85	5 (11%)	48,85,113	1.63	6 (12%)
39	CLA	D	312	16	55,63,73	1.60	6 (10%)	64,101,113	1.52	8 (12%)
39	CLA	a	801	-	65,73,73	1.48	9 (13%)	76,113,113	1.46	9 (11%)
50	A1EB1	S	302	-	51,58,58	1.30	3 (5%)	60,85,85	1.97	17 (28%)
52	A1EB4	R	305	-	52,59,63	2.56	4 (7%)	61,85,89	1.92	21 (34%)
39	CLA	a	847	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
48	A86	W	303	-	44,50,50	1.19	2 (4%)	51,76,76	2.16	19 (37%)
49	KC2	I	303	-	48,53,53	1.84	10 (20%)	54,89,89	2.29	17 (31%)
49	KC2	8	320	-	48,53,53	1.83	9 (18%)	54,89,89	2.07	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	5	315	-	47,55,73	1.72	6 (12%)	54,91,113	1.56	8 (14%)
39	CLA	S	308	-	61,69,73	1.54	6 (9%)	71,108,113	1.41	8 (11%)
47	SQD	F	319	-	36,37,54	1.14	5 (13%)	45,48,65	1.72	10 (22%)
47	SQD	S	301	-	38,39,54	1.14	5 (13%)	47,50,65	1.67	10 (21%)
48	A86	S	305	-	44,50,50	1.17	2 (4%)	51,76,76	2.02	14 (27%)
39	CLA	J	310	-	55,63,73	1.63	5 (9%)	64,101,113	1.51	6 (9%)
51	A1ECV	7	317	-	51,56,56	2.65	20 (39%)	53,93,93	4.25	29 (54%)
50	A1EB1	Q	307	-	51,58,58	1.31	5 (9%)	60,85,85	2.01	15 (25%)
50	A1EB1	8	304	-	51,58,58	1.25	3 (5%)	60,85,85	2.21	17 (28%)
39	CLA	H	313	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	8 (10%)
39	CLA	3	313	-	53,61,73	1.66	6 (11%)	61,98,113	1.47	6 (9%)
51	A1ECV	W	317	-	51,56,56	2.62	17 (33%)	53,93,93	4.04	27 (50%)
50	A1EB1	S	303	-	51,58,58	1.25	3 (5%)	60,85,85	2.14	21 (35%)
50	A1EB1	6	301	-	51,58,58	1.28	3 (5%)	60,85,85	2.00	16 (26%)
51	A1ECV	Q	316	26	51,56,56	2.66	20 (39%)	53,93,93	4.16	27 (50%)
39	CLA	S	316	-	41,49,73	1.86	5 (12%)	47,84,113	1.68	8 (17%)
43	DD6	V	303	-	39,45,45	1.97	3 (7%)	52,67,67	1.75	10 (19%)
49	KC2	P	313	24	48,53,53	1.89	10 (20%)	54,89,89	2.07	15 (27%)
39	CLA	2	310	-	42,50,73	1.81	5 (11%)	48,85,113	1.71	7 (14%)
49	KC2	R	312	-	48,53,53	1.86	10 (20%)	54,89,89	2.14	16 (29%)
39	CLA	b	812	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
49	KC2	W	312	46,24	47,52,53	1.82	9 (19%)	51,87,89	2.17	14 (27%)
46	LMG	S	322	49	46,46,55	0.95	2 (4%)	54,54,63	1.32	5 (9%)
39	CLA	Z	306	-	46,54,73	1.76	5 (10%)	53,90,113	1.60	7 (13%)
48	A86	M	302	-	44,50,50	1.18	2 (4%)	51,76,76	2.19	17 (33%)
39	CLA	b	806	-	65,73,73	1.46	6 (9%)	76,113,113	1.32	9 (11%)
49	KC2	H	314	-	48,53,53	1.86	10 (20%)	54,89,89	2.11	15 (27%)
39	CLA	b	840	-	65,73,73	1.49	7 (10%)	76,113,113	1.41	7 (9%)
49	KC2	G	313	-	48,53,53	1.86	10 (20%)	54,89,89	2.17	16 (29%)
49	KC2	C	313	-	48,53,53	1.84	9 (18%)	54,89,89	2.09	14 (25%)
49	KC2	6	316	-	48,53,53	1.85	9 (18%)	54,89,89	2.08	15 (27%)
50	A1EB1	V	305	-	51,58,58	1.29	4 (7%)	60,85,85	2.09	17 (28%)
39	CLA	4	322	-	52,60,73	1.69	6 (11%)	60,97,113	1.57	7 (11%)
49	KC2	4	318	28	48,53,53	1.88	10 (20%)	54,89,89	2.10	13 (24%)
39	CLA	E	318	17	46,54,73	1.75	6 (13%)	53,90,113	1.57	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	C	311	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	6 (7%)
52	A1EB4	T	304	-	50,57,63	2.65	5 (10%)	59,83,89	2.20	19 (32%)
49	KC2	C	312	-	48,53,53	1.86	10 (20%)	54,89,89	2.13	14 (25%)
39	CLA	b	813	-	54,62,73	1.66	7 (12%)	67,100,113	1.52	8 (11%)
39	CLA	b	841	2	65,73,73	1.52	5 (7%)	76,113,113	1.39	7 (9%)
39	CLA	L	320	-	46,54,73	1.77	5 (10%)	53,90,113	1.71	9 (16%)
39	CLA	P	307	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
39	CLA	T	313	-	51,59,73	1.74	6 (11%)	59,96,113	1.39	8 (13%)
39	CLA	9	310	-	41,49,73	1.80	6 (14%)	47,84,113	1.80	8 (17%)
46	LMG	W	320	-	33,33,55	0.94	1 (3%)	41,41,63	1.21	4 (9%)
39	CLA	a	824	-	65,73,73	1.51	7 (10%)	76,113,113	1.41	7 (9%)
39	CLA	o	202	-	42,50,73	1.83	5 (11%)	48,85,113	1.65	7 (14%)
50	A1EB1	G	302	-	51,58,58	1.30	4 (7%)	60,85,85	2.07	19 (31%)
39	CLA	F	309	-	52,60,73	1.66	5 (9%)	60,97,113	1.53	6 (10%)
48	A86	Z	301	-	44,50,50	1.17	3 (6%)	51,76,76	2.18	19 (37%)
48	A86	6	307	-	44,50,50	1.15	3 (6%)	51,76,76	2.11	17 (33%)
43	DD6	F	303	-	39,45,45	1.93	2 (5%)	52,67,67	1.79	10 (19%)
50	A1EB1	C	302	-	51,58,58	1.24	3 (5%)	60,85,85	1.81	16 (26%)
39	CLA	B	209	-	56,64,73	1.64	6 (10%)	65,102,113	1.43	7 (10%)
39	CLA	0	315	31	50,58,73	1.63	6 (12%)	58,95,113	1.61	9 (15%)
49	KC2	3	321	-	48,53,53	1.82	9 (18%)	54,89,89	2.07	15 (27%)
39	CLA	G	318	-	49,57,73	1.71	7 (14%)	55,93,113	1.51	8 (14%)
39	CLA	W	310	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	6 (7%)
42	BCR	j	103	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
48	A86	6	303	-	44,50,50	1.15	3 (6%)	51,76,76	2.21	15 (29%)
39	CLA	D	311	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	7 (9%)
47	SQD	T	321	-	35,36,54	1.15	5 (14%)	44,47,65	1.80	10 (22%)
39	CLA	F	312	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	7 (9%)
39	CLA	V	316	-	50,58,73	1.70	5 (10%)	58,95,113	1.61	8 (13%)
52	A1EB4	P	319	-	52,59,63	2.81	6 (11%)	61,85,89	2.79	21 (34%)
39	CLA	Y	303	-	41,49,73	1.86	5 (12%)	47,84,113	1.68	8 (17%)
48	A86	3	308	-	44,50,50	1.25	3 (6%)	51,76,76	2.33	18 (35%)
51	A1ECV	Z	314	-	51,56,56	2.65	17 (33%)	53,93,93	4.20	27 (50%)
39	CLA	K	306	-	61,69,73	1.58	6 (9%)	71,108,113	1.45	9 (12%)
49	KC2	T	314	-	48,53,53	1.86	10 (20%)	54,89,89	2.15	16 (29%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	E	317	-	52,60,73	1.64	5 (9%)	60,97,113	1.58	7 (11%)
39	CLA	S	310	-	42,50,73	1.83	5 (11%)	48,85,113	1.79	8 (16%)
43	DD6	A	303	-	39,45,45	2.03	3 (7%)	52,67,67	2.88	20 (38%)
39	CLA	9	308	-	55,63,73	1.59	6 (10%)	64,101,113	1.67	12 (18%)
39	CLA	D	314	-	65,73,73	1.52	6 (9%)	76,113,113	1.33	9 (11%)
50	A1EB1	0	302	-	51,58,58	1.22	3 (5%)	60,85,85	2.11	19 (31%)
39	CLA	U	210	-	60,68,73	1.57	6 (10%)	70,107,113	1.40	8 (11%)
39	CLA	U	211	-	60,68,73	1.55	5 (8%)	70,107,113	1.47	9 (12%)
46	LMG	W	302	49	39,39,55	1.08	2 (5%)	47,47,63	1.23	4 (8%)
41	LHG	X	301	-	40,40,48	0.67	1 (2%)	43,46,54	1.30	6 (13%)
39	CLA	b	802	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	6 (7%)
48	A86	D	305	-	44,50,50	1.21	3 (6%)	51,76,76	2.71	21 (41%)
51	A1ECV	5	309	27	51,56,56	2.64	18 (35%)	53,93,93	4.20	28 (52%)
39	CLA	0	320	-	45,53,73	1.81	5 (11%)	52,89,113	1.57	7 (13%)
42	BCR	a	842	-	41,41,41	0.67	0	56,56,56	1.82	14 (25%)
48	A86	R	301	-	44,50,50	1.22	3 (6%)	51,76,76	2.06	16 (31%)
43	DD6	S	306	-	39,45,45	2.01	2 (5%)	52,67,67	1.92	16 (30%)
39	CLA	I	311	-	65,73,73	1.47	6 (9%)	76,113,113	1.47	7 (9%)
50	A1EB1	8	308	-	51,58,58	1.26	4 (7%)	60,85,85	1.97	18 (30%)
48	A86	V	304	-	44,50,50	1.18	3 (6%)	51,76,76	2.02	17 (33%)
39	CLA	T	320	-	52,60,73	1.68	5 (9%)	60,97,113	1.48	7 (11%)
49	KC2	T	312	-	48,53,53	1.89	10 (20%)	54,89,89	2.15	14 (25%)
39	CLA	3	319	-	41,49,73	1.85	5 (12%)	47,84,113	1.75	8 (17%)
43	DD6	J	306	-	39,45,45	1.99	3 (7%)	52,67,67	2.16	12 (23%)
46	LMG	S	321	-	32,32,55	0.92	0	40,40,63	1.21	5 (12%)
49	KC2	1	314	-	48,53,53	1.86	10 (20%)	54,89,89	2.05	13 (24%)
39	CLA	b	833	-	65,73,73	1.51	5 (7%)	76,113,113	1.39	7 (9%)
43	DD6	X	304	-	39,45,45	1.92	3 (7%)	52,67,67	1.87	16 (30%)
39	CLA	F	308	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
39	CLA	J	308	-	50,58,73	1.70	5 (10%)	58,95,113	1.52	8 (13%)
49	KC2	Z	311	-	48,53,53	1.85	9 (18%)	54,89,89	2.10	13 (24%)
39	CLA	z	307	-	42,50,73	1.80	5 (11%)	48,85,113	1.73	6 (12%)
39	CLA	a	830	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	6 (7%)
39	CLA	E	313	-	65,73,73	1.45	5 (7%)	76,113,113	1.46	8 (10%)
48	A86	0	301	-	44,50,50	1.26	3 (6%)	51,76,76	2.19	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	7	321	-	41,49,73	1.86	5 (12%)	47,84,113	1.76	8 (17%)
39	CLA	A	309	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
39	CLA	T	318	-	47,55,73	1.75	6 (12%)	54,91,113	1.61	7 (12%)
48	A86	J	301	-	44,50,50	1.17	3 (6%)	51,76,76	2.13	18 (35%)
39	CLA	H	316	-	46,54,73	1.76	6 (13%)	53,90,113	1.63	6 (11%)
49	KC2	V	308	27	48,53,53	1.84	10 (20%)	54,89,89	2.12	14 (25%)
39	CLA	X	307	-	65,73,73	1.49	5 (7%)	76,113,113	1.36	8 (10%)
39	CLA	a	838	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	7 (9%)
39	CLA	H	310	-	57,65,73	1.56	6 (10%)	66,103,113	1.50	6 (9%)
39	CLA	X	309	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	7 (9%)
43	DD6	O	305	-	39,45,45	1.99	2 (5%)	52,67,67	1.62	12 (23%)
39	CLA	a	808	-	56,64,73	1.60	5 (8%)	65,102,113	1.52	6 (9%)
48	A86	0	309	-	44,50,50	1.20	2 (4%)	51,76,76	2.35	18 (35%)
48	A86	6	309	-	44,50,50	1.18	2 (4%)	51,76,76	2.22	17 (33%)
39	CLA	l	205	-	50,58,73	1.67	6 (12%)	58,95,113	1.58	9 (15%)
39	CLA	y	318	-	42,50,73	1.84	5 (11%)	48,85,113	1.62	6 (12%)
50	A1EB1	7	306	-	51,58,58	1.26	3 (5%)	60,85,85	2.11	22 (36%)
39	CLA	3	311	-	61,69,73	1.55	5 (8%)	71,108,113	1.38	7 (9%)
43	DD6	H	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.93	10 (19%)
43	DD6	I	307	-	39,45,45	2.01	3 (7%)	52,67,67	1.90	10 (19%)
49	KC2	R	314	46	47,52,53	1.83	9 (19%)	51,87,89	2.14	13 (25%)
49	KC2	6	314	-	48,53,53	1.84	10 (20%)	54,89,89	2.11	15 (27%)
39	CLA	x	317	-	41,49,73	1.86	5 (12%)	47,84,113	1.69	8 (17%)
39	CLA	P	308	24	65,73,73	1.46	6 (9%)	76,113,113	1.42	7 (9%)
49	KC2	4	320	-	48,53,53	1.85	10 (20%)	54,89,89	2.10	13 (24%)
49	KC2	W	314	-	48,53,53	1.87	9 (18%)	54,89,89	2.13	15 (27%)
49	KC2	X	315	-	48,53,53	1.85	10 (20%)	54,89,89	2.08	13 (24%)
39	CLA	8	322	-	41,49,73	1.87	5 (12%)	47,84,113	1.78	10 (21%)
43	DD6	A	304	-	39,45,45	2.00	2 (5%)	52,67,67	1.75	13 (25%)
43	DD6	a	846	-	39,45,45	2.00	3 (7%)	52,67,67	1.84	12 (23%)
39	CLA	Z	304	-	41,49,73	1.84	6 (14%)	47,84,113	1.72	7 (14%)
39	CLA	C	304	-	43,51,73	1.82	5 (11%)	49,86,113	1.58	6 (12%)
39	CLA	Z	305	-	41,49,73	1.86	5 (12%)	47,84,113	1.69	8 (17%)
49	KC2	7	322	-	48,53,53	1.85	10 (20%)	54,89,89	2.03	13 (24%)
39	CLA	a	837	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	7 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CLA	U	215	-	41,49,73	1.88	5 (12%)	47,84,113	1.70	7 (14%)
49	KC2	H	311	-	48,53,53	1.85	10 (20%)	54,89,89	2.04	12 (22%)
39	CLA	3	322	-	51,59,73	1.68	6 (11%)	59,96,113	1.57	8 (13%)
49	KC2	M	313	-	48,53,53	1.89	9 (18%)	54,89,89	2.15	14 (25%)
48	A86	Q	305	-	44,50,50	1.14	3 (6%)	51,76,76	2.03	14 (27%)
39	CLA	S	311	-	65,73,73	1.49	6 (9%)	76,113,113	1.33	6 (7%)
48	A86	T	301	-	44,50,50	1.29	3 (6%)	51,76,76	2.33	17 (33%)
39	CLA	a	807	1	65,73,73	1.51	6 (9%)	76,113,113	1.37	7 (9%)
51	A1ECV	G	316	-	51,56,56	2.63	17 (33%)	53,93,93	4.17	29 (54%)
52	A1EB4	W	306	-	51,58,63	2.60	4 (7%)	60,84,89	2.09	19 (31%)
45	DGD	C	314	-	41,41,67	1.10	2 (4%)	55,55,81	1.38	6 (10%)
48	A86	1	306	-	44,50,50	1.18	2 (4%)	51,76,76	2.05	13 (25%)
39	CLA	Q	309	-	61,69,73	1.52	6 (9%)	71,108,113	1.41	6 (8%)
42	BCR	a	844	-	41,41,41	0.72	0	56,56,56	1.91	17 (30%)
39	CLA	A	308	-	51,59,73	1.69	6 (11%)	59,96,113	1.45	6 (10%)
39	CLA	O	310	-	60,68,73	1.58	6 (10%)	70,107,113	1.50	10 (14%)
39	CLA	J	309	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	7 (9%)
50	A1EB1	3	309	-	51,58,58	1.28	4 (7%)	60,85,85	1.97	15 (25%)
39	CLA	F	315	18	41,49,73	1.83	5 (12%)	47,84,113	1.82	8 (17%)
40	PQN	a	839	-	34,34,34	1.60	2 (5%)	42,45,45	1.10	2 (4%)
39	CLA	A	315	-	50,58,73	1.71	5 (10%)	58,95,113	1.55	8 (13%)
39	CLA	S	313	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
39	CLA	I	313	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	7 (9%)
43	DD6	7	309	-	39,45,45	1.99	3 (7%)	52,67,67	1.87	15 (28%)
48	A86	3	305	-	44,50,50	1.19	2 (4%)	51,76,76	1.79	10 (19%)
49	KC2	L	314	-	48,53,53	1.85	9 (18%)	54,89,89	2.12	15 (27%)
39	CLA	V	309	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	8 (10%)
39	CLA	Q	321	-	53,61,73	1.71	6 (11%)	61,98,113	1.43	9 (14%)

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
39	CLA	X	308	-	1/1/14/20	16/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	8	313	-	1/1/10/20	3/8/86/115	-
39	CLA	2	307	-	1/1/10/20	2/8/86/115	-
41	LHG	D	302	-	-	21/39/39/53	-
48	A86	T	306	-	-	6/34/90/90	0/3/3/3
49	KC2	M	307	-	-	7/15/71/71	-
42	BCR	l	207	-	-	2/29/63/63	0/2/2/2
49	KC2	Y	309	-	-	8/15/71/71	-
39	CLA	b	824	-	1/1/14/20	10/31/109/115	-
39	CLA	a	828	1	1/1/12/20	4/19/97/115	-
39	CLA	3	316	-	1/1/12/20	5/19/97/115	-
39	CLA	b	836	-	1/1/11/20	3/13/91/115	-
39	CLA	F	306	-	1/1/11/20	4/15/93/115	-
49	KC2	V	315	-	-	9/15/71/71	-
39	CLA	A	306	-	1/1/14/20	11/33/111/115	-
39	CLA	o	206	-	1/1/13/20	12/29/107/115	-
48	A86	8	302	-	-	8/34/90/90	0/3/3/3
49	KC2	8	319	34	-	12/15/71/71	-
43	DD6	o	204	-	-	2/26/80/80	0/3/3/3
39	CLA	7	313	-	1/1/14/20	19/33/111/115	-
46	LMG	A	316	-	-	13/24/44/70	0/1/1/1
39	CLA	a	812	-	1/1/11/20	3/13/91/115	-
39	CLA	E	306	17	1/1/11/20	4/18/96/115	-
49	KC2	P	320	-	-	9/15/71/71	-
39	CLA	7	318	28	1/1/11/20	3/15/93/115	-
50	A1EB1	1	301	-	-	11/42/100/100	0/3/3/3
50	A1EB1	3	302	-	-	15/42/100/100	0/3/3/3
39	CLA	a	806	-	1/1/15/20	17/37/115/115	-
39	CLA	l	203	-	-	6/18/96/115	-
48	A86	M	303	-	-	0/34/90/90	0/3/3/3
49	KC2	R	306	-	-	8/15/71/71	-
48	A86	0	304	-	-	12/34/90/90	0/3/3/3
49	KC2	x	313	-	-	6/15/71/71	-
39	CLA	a	827	-	1/1/15/20	6/37/115/115	-
39	CLA	E	319	17	1/1/11/20	11/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	F	316	-	1/1/12/20	8/21/99/115	-
48	A86	2	302	-	-	5/34/90/90	0/3/3/3
48	A86	O	306	-	-	6/34/90/90	0/3/3/3
50	A1EB1	K	304	-	-	8/42/100/100	0/3/3/3
39	CLA	V	313	27	1/1/15/20	8/37/115/115	-
46	LMG	F	317	49	-	20/34/54/70	0/1/1/1
50	A1EB1	x	301	-	-	14/42/100/100	0/3/3/3
39	CLA	b	818	-	1/1/13/20	11/25/103/115	-
39	CLA	2	309	-	1/1/11/20	6/15/93/115	-
39	CLA	7	316	-	1/1/15/20	10/37/115/115	-
39	CLA	E	312	-	1/1/15/20	21/37/115/115	-
39	CLA	b	805	-	1/1/15/20	9/37/115/115	-
51	A1ECV	x	310	-	3/3/17/24	5/19/117/117	-
47	SQD	7	302	-	-	15/34/54/69	0/1/1/1
48	A86	F	301	-	-	4/34/90/90	0/3/3/3
48	A86	V	301	-	-	2/34/90/90	0/3/3/3
49	KC2	W	308	-	-	6/15/71/71	-
39	CLA	O	316	-	1/1/10/20	4/8/86/115	-
49	KC2	5	305	27	-	7/15/71/71	-
49	KC2	4	324	-	-	8/15/71/71	-
48	A86	8	309	-	-	4/34/90/90	0/3/3/3
50	A1EB1	2	304	-	-	16/42/100/100	0/3/3/3
39	CLA	H	315	-	1/1/10/20	4/8/86/115	-
51	A1ECV	Y	312	-	3/3/17/24	7/19/117/117	-
39	CLA	T	308	-	1/1/11/20	8/15/93/115	-
39	CLA	z	309	-	1/1/10/20	5/8/86/115	-
39	CLA	D	315	-	1/1/15/20	7/37/115/115	-
39	CLA	I	308	-	1/1/14/20	10/33/111/115	-
43	DD6	O	303	-	-	3/26/80/80	0/3/3/3
39	CLA	J	318	-	1/1/11/20	7/15/93/115	-
49	KC2	8	317	-	-	8/15/71/71	-
42	BCR	b	846	-	-	3/29/63/63	0/2/2/2
48	A86	4	328	-	-	15/34/90/90	0/3/3/3
49	KC2	V	318	-	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	6	312	-	1/1/12/20	6/18/96/115	-
48	A86	Y	301	-	-	5/34/90/90	0/3/3/3
50	A1EB1	D	308	-	-	8/42/100/100	0/3/3/3
39	CLA	z	306	-	1/1/10/20	2/8/86/115	-
50	A1EB1	y	301	-	-	11/42/100/100	0/3/3/3
39	CLA	E	309	-	1/1/12/20	6/23/101/115	-
39	CLA	y	309	-	1/1/11/20	4/15/93/115	-
39	CLA	D	310	47	1/1/14/20	17/33/111/115	-
48	A86	0	308	51	-	2/34/90/90	0/3/3/3
39	CLA	F	321	-	1/1/15/20	17/37/115/115	-
39	CLA	Q	311	-	1/1/11/20	5/15/93/115	-
39	CLA	0	310	-	1/1/14/20	23/33/111/115	-
39	CLA	I	310	-	1/1/12/20	9/24/102/115	-
48	A86	Q	308	-	-	8/34/90/90	0/3/3/3
49	KC2	2	317	-	-	7/15/71/71	-
39	CLA	5	307	-	1/1/14/20	3/31/109/115	-
49	KC2	K	310	-	-	7/15/71/71	-
46	LMG	7	326	-	-	6/27/47/70	0/1/1/1
51	A1ECV	R	310	-	3/3/17/24	11/19/117/117	-
42	BCR	h	202	-	-	6/29/63/63	0/2/2/2
39	CLA	4	319	-	1/1/10/20	2/8/86/115	-
42	BCR	m	101	-	-	9/29/63/63	0/2/2/2
45	DGD	b	849	-	-	27/49/89/95	0/2/2/2
39	CLA	b	837	-	1/1/14/20	10/31/109/115	-
49	KC2	Z	310	-	-	9/15/71/71	-
39	CLA	Q	314	-	1/1/12/20	6/24/102/115	-
39	CLA	a	826	-	1/1/15/20	18/37/115/115	-
48	A86	H	302	-	-	6/34/90/90	0/3/3/3
48	A86	X	303	-	-	8/34/90/90	0/3/3/3
48	A86	W	307	-	-	2/34/90/90	0/3/3/3
50	A1EB1	0	305	-	-	16/42/100/100	0/3/3/3
39	CLA	R	309	-	1/1/15/20	13/37/115/115	-
39	CLA	8	315	-	1/1/10/20	1/11/89/115	-
39	CLA	a	833	1	1/1/11/20	9/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	0	314	46,31	-	8/14/70/71	-
39	CLA	3	314	-	1/1/15/20	17/37/115/115	-
39	CLA	Y	313	-	1/1/10/20	3/8/86/115	-
48	A86	C	303	-	-	6/34/90/90	0/3/3/3
48	A86	x	305	-	-	8/34/90/90	0/3/3/3
49	KC2	G	311	19	-	9/15/71/71	-
49	KC2	z	313	-	-	6/16/59/71	-
46	LMG	P	317	49	-	18/34/54/70	0/1/1/1
47	SQD	D	304	-	-	8/33/53/69	0/1/1/1
49	KC2	M	314	-	-	7/15/71/71	-
49	KC2	L	312	-	-	8/15/71/71	-
39	CLA	V	311	-	1/1/15/20	15/37/115/115	-
39	CLA	9	307	-	1/1/10/20	2/8/86/115	-
49	KC2	2	313	-	-	6/13/69/71	-
39	CLA	T	311	-	1/1/13/20	5/27/105/115	-
49	KC2	y	314	-	-	7/15/71/71	-
39	CLA	b	807	-	1/1/15/20	14/37/115/115	-
49	KC2	P	306	24	-	7/15/71/71	-
39	CLA	B	206	-	1/1/10/20	4/10/88/115	-
39	CLA	E	308	-	1/1/15/20	11/37/115/115	-
39	CLA	G	314	19	1/1/13/20	6/29/107/115	-
50	A1EB1	V	306	-	-	7/42/100/100	0/3/3/3
46	LMG	M	320	-	-	10/28/48/70	0/1/1/1
52	A1EB4	5	304	-	-	5/38/99/103	0/3/3/3
49	KC2	6	317	-	-	9/15/71/71	-
51	A1ECV	4	315	-	3/3/17/24	9/19/117/117	-
39	CLA	A	305	13	1/1/11/20	4/18/96/115	-
48	A86	7	307	-	-	3/34/90/90	0/3/3/3
39	CLA	1	317	-	1/1/10/20	4/8/86/115	-
39	CLA	Q	312	-	1/1/15/20	9/37/115/115	-
43	DD6	x	303	-	-	1/26/80/80	0/3/3/3
39	CLA	V	310	-	1/1/14/20	9/31/109/115	-
49	KC2	J	315	-	-	10/15/71/71	-
48	A86	G	301	-	-	11/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	L	309	-	1/1/13/20	11/23/101/115	-
43	DD6	z	305	-	-	1/26/80/80	0/3/3/3
48	A86	B	201	-	-	5/34/90/90	0/3/3/3
49	KC2	9	313	-	-	6/15/71/71	-
49	KC2	P	312	-	-	7/15/71/71	-
39	CLA	9	320	-	1/1/10/20	2/8/86/115	-
48	A86	1	303	-	-	2/34/90/90	0/3/3/3
50	A1EB1	4	302	-	-	11/42/100/100	0/3/3/3
39	CLA	b	821	-	1/1/15/20	9/37/115/115	-
39	CLA	S	309	-	-	19/37/115/115	-
39	CLA	3	312	-	1/1/15/20	20/37/115/115	-
39	CLA	D	319	16	1/1/15/20	20/37/115/115	-
39	CLA	C	307	-	1/1/15/20	12/37/115/115	-
50	A1EB1	H	301	-	-	12/42/100/100	0/3/3/3
39	CLA	4	314	-	1/1/15/20	10/37/115/115	-
39	CLA	L	319	-	1/1/12/20	6/21/99/115	-
41	LHG	j	104	-	-	22/34/34/53	-
39	CLA	0	322	-	1/1/12/20	12/21/99/115	-
43	DD6	5	303	-	-	1/26/80/80	0/3/3/3
47	SQD	4	327	-	-	17/34/54/69	0/1/1/1
51	A1ECV	6	320	-	3/3/17/24	12/19/117/117	-
43	DD6	A	301	-	-	0/26/80/80	0/3/3/3
39	CLA	a	816	-	1/1/15/20	15/37/115/115	-
39	CLA	M	318	24	1/1/11/20	5/15/93/115	-
39	CLA	Y	305	-	1/1/10/20	2/8/86/115	-
39	CLA	1	313	32	1/1/10/20	3/8/86/115	-
48	A86	R	317	-	-	3/34/90/90	0/3/3/3
39	CLA	a	803	-	1/1/15/20	15/37/115/115	-
39	CLA	0	323	-	1/1/11/20	9/15/93/115	-
43	DD6	J	304	-	-	3/26/80/80	0/3/3/3
44	SF4	b	804	-	-	-	0/6/5/5
39	CLA	C	305	-	1/1/14/20	15/33/111/115	-
49	KC2	B	208	-	-	9/15/71/71	-
39	CLA	A	311	-	1/1/15/20	11/37/115/115	-
49	KC2	X	314	46	-	7/14/70/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	BCR	b	848	-	-	1/29/63/63	0/2/2/2
39	CLA	l	204	-	1/1/15/20	9/37/115/115	-
50	A1EB1	4	304	-	-	9/42/100/100	0/3/3/3
51	A1ECV	9	314	-	3/3/17/24	9/19/117/117	-
48	A86	3	306	-	-	8/34/90/90	0/3/3/3
39	CLA	i	103	-	1/1/15/20	17/37/115/115	-
47	SQD	D	320	39	-	11/32/52/69	0/1/1/1
39	CLA	a	815	-	1/1/15/20	14/37/115/115	-
49	KC2	3	315	-	-	8/15/71/71	-
39	CLA	8	321	-	1/1/10/20	2/10/88/115	-
51	A1ECV	2	311	-	3/3/17/24	8/19/117/117	-
39	CLA	D	317	-	1/1/15/20	16/37/115/115	-
39	CLA	a	831	-	1/1/15/20	10/37/115/115	-
51	A1ECV	9	317	-	3/3/17/24	7/19/117/117	-
39	CLA	Z	316	-	-	6/8/86/115	-
42	BCR	l	202	-	-	4/29/63/63	0/2/2/2
39	CLA	6	313	-	1/1/10/20	3/10/88/115	-
51	A1ECV	M	316	-	3/3/17/24	8/19/117/117	-
42	BCR	f	801	-	-	4/29/63/63	0/2/2/2
48	A86	9	305	-	-	6/34/90/90	0/3/3/3
39	CLA	M	312	-	1/1/15/20	12/37/115/115	-
39	CLA	E	316	-	1/1/12/20	6/22/100/115	-
49	KC2	7	320	-	-	7/15/71/71	-
39	CLA	9	312	35	1/1/10/20	3/10/88/115	-
50	A1EB1	3	303	-	-	8/42/100/100	0/3/3/3
50	A1EB1	8	306	-	-	13/42/100/100	0/3/3/3
39	CLA	X	317	-	1/1/12/20	8/22/100/115	-
48	A86	E	304	-	-	2/34/90/90	0/3/3/3
39	CLA	O	313	-	1/1/12/20	2/19/97/115	-
39	CLA	9	309	-	1/1/10/20	3/8/86/115	-
51	A1ECV	S	318	-	3/3/17/24	5/19/117/117	-
39	CLA	E	310	-	1/1/15/20	8/37/115/115	-
39	CLA	8	318	-	1/1/10/20	3/8/86/115	-
49	KC2	3	317	-	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	A1EB1	z	302	-	-	13/42/100/100	0/3/3/3
39	CLA	V	319	-	1/1/12/20	4/22/100/115	-
39	CLA	O	308	-	1/1/9/20	2/2/80/115	-
39	CLA	a	825	-	1/1/14/20	11/34/112/115	-
43	DD6	E	305	-	-	3/26/80/80	0/3/3/3
49	KC2	V	314	-	-	9/15/71/71	-
39	CLA	h	201	-	1/1/13/20	8/25/103/115	-
52	A1EB4	X	305	-	-	10/38/99/103	0/3/3/3
43	DD6	U	204	-	-	1/26/80/80	0/3/3/3
39	CLA	z	318	-	1/1/10/20	6/8/86/115	-
50	A1EB1	G	308	-	-	10/42/100/100	0/3/3/3
48	A86	M	306	-	-	2/34/90/90	0/3/3/3
48	A86	9	306	-	-	6/34/90/90	0/3/3/3
39	CLA	G	310	-	1/1/15/20	10/37/115/115	-
39	CLA	a	818	-	1/1/15/20	9/37/115/115	-
39	CLA	b	825	-	1/1/15/20	12/37/115/115	-
39	CLA	C	310	-	1/1/15/20	16/37/115/115	-
39	CLA	K	312	-	1/1/15/20	17/37/115/115	-
39	CLA	2	312	-	1/1/10/20	5/8/86/115	-
50	A1EB1	T	302	-	-	14/42/100/100	0/3/3/3
48	A86	Z	303	-	-	8/34/90/90	0/3/3/3
50	A1EB1	H	304	-	-	14/42/100/100	0/3/3/3
39	CLA	y	319	-	1/1/10/20	5/8/86/115	-
47	SQD	W	301	-	-	8/22/42/69	0/1/1/1
48	A86	L	306	-	-	12/34/90/90	0/3/3/3
52	A1EB4	M	322	-	-	6/38/99/103	0/3/3/3
48	A86	L	302	-	-	13/34/90/90	0/3/3/3
49	KC2	y	313	-	-	8/15/71/71	-
48	A86	I	304	-	-	11/34/90/90	0/3/3/3
49	KC2	S	314	-	-	6/15/71/71	-
39	CLA	6	310	-	1/1/10/20	4/10/88/115	-
39	CLA	Z	307	-	1/1/10/20	0/8/86/115	-
46	LMG	Q	322	49	-	13/23/43/70	0/1/1/1
39	CLA	a	811	-	1/1/15/20	17/37/115/115	-
48	A86	P	303	-	-	0/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	5	314	-	-	8/15/71/71	-
49	KC2	z	312	-	-	7/15/71/71	-
47	SQD	F	318	-	-	17/37/57/69	0/1/1/1
39	CLA	a	814	-	1/1/14/20	13/33/111/115	-
39	CLA	a	834	-	1/1/12/20	6/21/99/115	-
39	CLA	E	315	-	1/1/11/20	10/15/93/115	-
39	CLA	y	307	-	1/1/10/20	2/8/86/115	-
39	CLA	x	306	-	1/1/11/20	5/13/91/115	-
39	CLA	8	311	-	1/1/13/20	11/25/103/115	-
49	KC2	T	316	-	-	7/15/71/71	-
39	CLA	a	809	-	1/1/14/20	12/34/112/115	-
39	CLA	S	320	-	1/1/15/20	13/37/115/115	-
49	KC2	Q	318	26	-	6/15/71/71	-
39	CLA	W	313	-	1/1/15/20	8/37/115/115	-
39	CLA	P	309	-	1/1/15/20	14/37/115/115	-
50	A1EB1	G	307	-	-	17/42/100/100	0/3/3/3
49	KC2	L	317	-	-	11/15/71/71	-
43	DD6	F	305	-	-	1/26/80/80	0/3/3/3
39	CLA	R	308	-	1/1/14/20	9/31/109/115	-
39	CLA	U	212	-	1/1/11/20	5/15/93/115	-
39	CLA	W	309	-	1/1/15/20	10/37/115/115	-
39	CLA	Y	311	-	1/1/10/20	4/8/86/115	-
48	A86	P	302	-	-	12/34/90/90	0/3/3/3
39	CLA	k	201	-	1/1/12/20	5/22/100/115	-
51	A1ECV	X	310	-	3/3/17/24	10/19/117/117	-
48	A86	4	305	-	-	6/34/90/90	0/3/3/3
52	A1EB4	W	321	-	-	8/38/99/103	0/3/3/3
39	CLA	I	314	-	1/1/15/20	13/37/115/115	-
39	CLA	x	308	-	1/1/10/20	2/8/86/115	-
39	CLA	2	318	-	1/1/10/20	3/8/86/115	-
49	KC2	3	318	-	-	6/15/71/71	-
39	CLA	a	820	-	1/1/12/20	9/21/99/115	-
50	A1EB1	J	302	-	-	9/42/100/100	0/3/3/3
39	CLA	O	318	-	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	1	302	-	-	5/34/90/90	0/3/3/3
48	A86	Q	301	-	-	5/34/90/90	0/3/3/3
50	A1EB1	E	301	-	-	9/42/100/100	0/3/3/3
43	DD6	D	303	-	-	0/26/80/80	0/3/3/3
49	KC2	Y	308	-	-	9/15/71/71	-
49	KC2	1	315	-	-	11/15/71/71	-
39	CLA	a	832	-	1/1/12/20	5/19/97/115	-
49	KC2	x	315	-	-	10/15/71/71	-
50	A1EB1	x	302	-	-	15/42/100/100	0/3/3/3
39	CLA	M	315	-	1/1/10/20	4/8/86/115	-
50	A1EB1	R	303	-	-	10/42/100/100	0/3/3/3
51	A1ECV	4	321	-	3/3/17/24	10/19/117/117	-
48	A86	5	301	-	-	3/34/90/90	0/3/3/3
39	CLA	1	309	-	1/1/10/20	4/10/88/115	-
51	A1ECV	7	323	-	2/2/17/24	8/19/117/117	-
42	BCR	i	102	-	-	4/29/63/63	0/2/2/2
39	CLA	K	307	-	1/1/15/20	14/37/115/115	-
39	CLA	5	308	-	1/1/15/20	12/37/115/115	-
48	A86	2	305	-	-	12/34/90/90	0/3/3/3
39	CLA	J	316	-	1/1/11/20	5/15/93/115	-
39	CLA	1	316	-	1/1/10/20	3/8/86/115	-
39	CLA	a	819	-	1/1/11/20	9/18/96/115	-
46	LMG	M	319	49	-	13/34/54/70	0/1/1/1
50	A1EB1	Q	323	-	-	9/42/100/100	0/3/3/3
48	A86	8	323	-	-	4/34/90/90	0/3/3/3
39	CLA	F	310	-	1/1/12/20	7/24/102/115	-
51	A1ECV	z	316	-	3/3/17/24	6/19/117/117	-
39	CLA	b	817	-	1/1/13/20	7/30/108/115	-
39	CLA	I	309	-	1/1/15/20	10/37/115/115	-
39	CLA	6	311	-	1/1/10/20	1/6/84/115	-
39	CLA	O	311	-	1/1/10/20	2/10/88/115	-
49	KC2	4	317	-	-	5/15/71/71	-
43	DD6	Q	306	-	-	1/26/80/80	0/3/3/3
51	A1ECV	z	310	-	3/3/17/24	11/19/117/117	-
48	A86	y	306	-	-	6/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	9	319	-	1/1/11/20	6/13/91/115	-
39	CLA	Y	302	-	1/1/10/20	2/8/86/115	-
39	CLA	b	808	-	1/1/11/20	7/13/91/115	-
39	CLA	a	813	1	1/1/12/20	4/19/97/115	-
39	CLA	1	319	-	1/1/12/20	10/21/99/115	-
39	CLA	Z	313	-	1/1/10/20	4/8/86/115	-
39	CLA	A	314	-	1/1/15/20	17/37/115/115	-
39	CLA	K	311	-	1/1/15/20	14/37/115/115	-
39	CLA	b	826	-	1/1/15/20	7/37/115/115	-
49	KC2	9	318	-	-	10/15/71/71	-
49	KC2	F	311	46	-	7/14/70/71	-
49	KC2	1	312	-	-	7/15/71/71	-
43	DD6	y	303	-	-	1/26/80/80	0/3/3/3
39	CLA	i	101	-	1/1/15/20	8/37/115/115	-
48	A86	4	306	-	-	8/34/90/90	0/3/3/3
51	A1ECV	5	312	27	3/3/17/24	11/19/117/117	-
48	A86	4	310	-	-	5/34/90/90	0/3/3/3
42	BCR	a	845	-	-	4/29/63/63	0/2/2/2
51	A1ECV	T	317	-	3/3/17/24	6/19/117/117	-
39	CLA	x	309	-	1/1/10/20	3/8/86/115	-
39	CLA	y	312	-	1/1/10/20	3/10/88/115	-
48	A86	L	305	-	-	2/34/90/90	0/3/3/3
43	DD6	J	305	-	-	3/26/80/80	0/3/3/3
49	KC2	x	312	-	-	8/15/71/71	-
43	DD6	H	303	-	-	1/26/80/80	0/3/3/3
39	CLA	M	309	-	1/1/15/20	15/37/115/115	-
39	CLA	1	308	-	1/1/10/20	4/8/86/115	-
39	CLA	M	308	-	1/1/15/20	12/37/115/115	-
39	CLA	8	312	-	1/1/11/20	6/13/91/115	-
39	CLA	b	842	-	1/1/15/20	12/37/115/115	-
50	A1EB1	G	304	-	-	8/42/100/100	0/3/3/3
39	CLA	A	307	-	1/1/14/20	8/31/109/115	-
43	DD6	D	307	-	-	2/26/80/80	0/3/3/3
48	A86	4	309	-	-	1/34/90/90	0/3/3/3
39	CLA	L	316	-	1/1/10/20	6/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	A1EB1	U	205	-	-	11/42/100/100	0/3/3/3
39	CLA	T	309	-	1/1/13/20	11/27/105/115	-
39	CLA	b	838	-	1/1/15/20	13/37/115/115	-
49	KC2	A	310	13	-	7/15/71/71	-
39	CLA	2	308	-	1/1/11/20	9/15/93/115	-
39	CLA	2	316	-	1/1/10/20	4/8/86/115	-
50	A1EB1	0	303	-	-	10/42/100/100	0/3/3/3
49	KC2	6	319	-	-	11/15/71/71	-
43	DD6	j	102	-	-	6/26/80/80	0/3/3/3
49	KC2	y	316	-	-	7/15/71/71	-
39	CLA	C	309	-	1/1/11/20	11/15/93/115	-
39	CLA	M	321	24	1/1/11/20	3/15/93/115	-
46	LMG	9	321	-	-	16/31/51/70	0/1/1/1
51	A1ECV	E	311	-	3/3/17/24	6/19/117/117	-
49	KC2	T	315	29	-	7/15/71/71	-
39	CLA	7	314	-	1/1/13/20	11/27/105/115	-
39	CLA	a	804	-	1/1/15/20	16/37/115/115	-
43	DD6	K	303	-	-	0/26/80/80	0/3/3/3
50	A1EB1	O	301	-	-	16/42/100/100	0/3/3/3
50	A1EB1	4	303	-	-	12/42/100/100	0/3/3/3
49	KC2	A	313	-	-	11/15/71/71	-
50	A1EB1	9	302	-	-	18/42/100/100	0/3/3/3
50	A1EB1	L	303	-	-	15/42/100/100	0/3/3/3
48	A86	6	302	-	-	7/34/90/90	0/3/3/3
48	A86	R	302	-	-	11/34/90/90	0/3/3/3
39	CLA	z	308	-	1/1/11/20	2/15/93/115	-
39	CLA	0	313	-	1/1/13/20	10/25/103/115	-
43	DD6	W	305	-	-	1/26/80/80	0/3/3/3
48	A86	0	306	-	-	2/34/90/90	0/3/3/3
39	CLA	b	834	-	1/1/13/20	5/29/107/115	-
39	CLA	a	805	-	1/1/15/20	11/37/115/115	-
39	CLA	x	311	-	1/1/11/20	0/13/91/115	-
39	CLA	K	309	-	1/1/14/20	9/34/112/115	-
49	KC2	0	319	-	-	10/15/71/71	-
39	CLA	J	313	-	1/1/11/20	7/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	X	306	27	-	10/15/71/71	-
39	CLA	a	802	-	1/1/13/20	7/25/103/115	-
39	CLA	L	313	-	1/1/12/20	1/19/97/115	-
49	KC2	V	312	-	-	6/15/71/71	-
49	KC2	8	316	-	-	11/15/71/71	-
39	CLA	b	816	-	1/1/14/20	9/31/109/115	-
39	CLA	3	323	-	1/1/11/20	9/15/93/115	-
49	KC2	V	320	-	-	8/15/71/71	-
49	KC2	Q	313	46	-	9/14/70/71	-
39	CLA	J	311	-	1/1/15/20	12/37/115/115	-
48	A86	X	302	-	-	7/34/90/90	0/3/3/3
39	CLA	T	310	29	1/1/12/20	6/22/100/115	-
43	DD6	3	301	-	-	2/26/80/80	0/3/3/3
39	CLA	W	316	24	1/1/10/20	3/8/86/115	-
48	A86	7	308	-	-	8/34/90/90	0/3/3/3
44	SF4	c	101	-	-	-	0/6/5/5
39	CLA	a	823	-	1/1/15/20	9/37/115/115	-
39	CLA	U	201	-	1/1/11/20	9/15/93/115	-
48	A86	8	307	-	-	12/34/90/90	0/3/3/3
39	CLA	b	830	-	1/1/15/20	13/37/115/115	-
39	CLA	P	316	-	1/1/12/20	5/21/99/115	-
39	CLA	H	309	20	1/1/12/20	3/22/100/115	-
51	A1ECV	y	311	-	3/3/17/24	10/19/117/117	-
39	CLA	x	318	-	1/1/10/20	6/8/86/115	-
48	A86	U	206	-	-	3/34/90/90	0/3/3/3
39	CLA	a	836	-	-	9/37/115/115	-
39	CLA	a	821	-	1/1/13/20	11/25/103/115	-
48	A86	L	301	-	-	7/34/90/90	0/3/3/3
51	A1ECV	S	312	-	3/3/17/24	9/19/117/117	-
39	CLA	Q	310	-	1/1/15/20	20/37/115/115	-
39	CLA	b	832	-	1/1/15/20	15/37/115/115	-
39	CLA	L	308	-	1/1/14/20	13/33/111/115	-
39	CLA	k	203	-	1/1/13/20	7/25/103/115	-
39	CLA	o	203	12	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	2	315	-	1/1/10/20	3/8/86/115	-
49	KC2	0	317	31	-	3/15/71/71	-
39	CLA	1	320	-	1/1/10/20	4/8/86/115	-
48	A86	O	307	-	-	9/34/90/90	0/3/3/3
43	DD6	T	303	-	-	1/26/80/80	0/3/3/3
39	CLA	b	811	-	1/1/15/20	8/37/115/115	-
39	CLA	y	315	-	1/1/10/20	6/8/86/115	-
42	BCR	f	804	-	-	2/29/63/63	0/2/2/2
39	CLA	b	851	-	1/1/15/20	11/37/115/115	-
39	CLA	1	310	-	1/1/11/20	4/13/91/115	-
39	CLA	5	310	27	1/1/12/20	4/19/97/115	-
48	A86	U	202	-	-	4/34/90/90	0/3/3/3
48	A86	y	305	-	-	0/34/90/90	0/3/3/3
50	A1EB1	h	203	-	-	10/42/100/100	0/3/3/3
39	CLA	O	314	-	1/1/13/20	5/25/103/115	-
43	DD6	4	307	-	-	1/26/80/80	0/3/3/3
44	SF4	c	102	-	-	-	0/6/5/5
46	LMG	0	324	49	-	13/21/41/70	0/1/1/1
49	KC2	L	321	-	-	7/15/71/71	-
47	SQD	E	320	-	-	12/30/50/69	0/1/1/1
46	LMG	4	325	-	-	16/27/47/70	0/1/1/1
48	A86	8	305	-	-	12/34/90/90	0/3/3/3
39	CLA	A	312	-	1/1/15/20	13/37/115/115	-
50	A1EB1	7	305	-	-	16/42/100/100	0/3/3/3
41	LHG	D	301	-	-	8/39/39/53	-
48	A86	9	304	-	-	9/34/90/90	0/3/3/3
39	CLA	B	205	-	1/1/10/20	3/10/88/115	-
51	A1ECV	x	316	-	3/3/17/24	7/19/117/117	-
48	A86	F	302	-	-	2/34/90/90	0/3/3/3
39	CLA	2	319	-	-	11/15/93/115	-
43	DD6	x	304	-	-	0/26/80/80	0/3/3/3
39	CLA	X	311	27	1/1/12/20	3/19/97/115	-
43	DD6	O	304	-	-	1/26/80/80	0/3/3/3
50	A1EB1	U	203	-	-	9/42/100/100	0/3/3/3
51	A1ECV	Q	319	-	3/3/17/24	11/19/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	S	319	-	1/1/12/20	8/22/100/115	-
50	A1EB1	K	302	-	-	6/42/100/100	0/3/3/3
39	CLA	7	315	-	1/1/12/20	4/19/97/115	-
39	CLA	7	324	-	1/1/10/20	3/8/86/115	-
48	A86	7	311	-	-	3/34/90/90	0/3/3/3
43	DD6	Z	302	-	-	2/26/80/80	0/3/3/3
39	CLA	b	835	-	1/1/15/20	14/37/115/115	-
46	LMG	I	302	-	-	23/37/57/70	0/1/1/1
39	CLA	W	318	-	1/1/12/20	5/21/99/115	-
50	A1EB1	1	305	-	-	10/42/100/100	0/3/3/3
39	CLA	b	831	-	1/1/12/20	5/19/97/115	-
39	CLA	b	815	-	1/1/15/20	14/37/115/115	-
43	DD6	I	305	-	-	1/26/80/80	0/3/3/3
47	SQD	9	322	-	-	10/31/51/69	0/1/1/1
42	BCR	b	844	-	-	6/29/63/63	0/2/2/2
48	A86	S	304	-	-	8/34/90/90	0/3/3/3
39	CLA	b	820	-	1/1/14/20	14/31/109/115	-
48	A86	2	301	-	-	3/34/90/90	0/3/3/3
48	A86	k	206	-	-	5/34/90/90	0/3/3/3
39	CLA	R	307	-	1/1/15/20	12/37/115/115	-
48	A86	8	303	-	-	6/34/90/90	0/3/3/3
39	CLA	M	310	-	1/1/15/20	14/37/115/115	-
39	CLA	E	307	-	1/1/15/20	20/37/115/115	-
39	CLA	Z	315	-	1/1/10/20	2/8/86/115	-
51	A1ECV	O	315	-	3/3/17/24	7/19/117/117	-
47	SQD	H	318	-	-	9/33/53/69	0/1/1/1
39	CLA	R	311	27	1/1/12/20	3/19/97/115	-
43	DD6	D	306	-	-	0/26/80/80	0/3/3/3
39	CLA	a	810	-	1/1/12/20	6/24/102/115	-
39	CLA	7	325	-	-	7/19/97/115	-
39	CLA	y	308	-	1/1/11/20	9/13/91/115	-
39	CLA	W	311	-	1/1/15/20	15/37/115/115	-
39	CLA	Y	310	-	1/1/10/20	2/8/86/115	-
39	CLA	z	311	-	1/1/10/20	3/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	b	827	-	1/1/15/20	8/37/115/115	-
43	DD6	1	304	-	-	4/26/80/80	0/3/3/3
39	CLA	1	311	-	1/1/10/20	5/8/86/115	-
39	CLA	o	201	-	1/1/12/20	5/21/99/115	-
43	DD6	3	304	-	-	3/26/80/80	0/3/3/3
42	BCR	1	206	-	-	6/29/63/63	0/2/2/2
39	CLA	U	213	-	1/1/10/20	4/8/86/115	-
43	DD6	G	303	-	-	1/26/80/80	0/3/3/3
39	CLA	L	310	23	1/1/15/20	14/37/115/115	-
39	CLA	U	214	-	1/1/11/20	2/15/93/115	-
50	A1EB1	7	304	-	-	14/42/100/100	0/3/3/3
39	CLA	W	319	-	1/1/11/20	6/15/93/115	-
39	CLA	b	801	-	1/1/15/20	10/37/115/115	-
39	CLA	6	322	-	1/1/11/20	9/15/93/115	-
40	PQN	b	843	-	-	3/23/43/43	0/2/2/2
50	A1EB1	V	307	-	-	12/42/100/100	0/3/3/3
48	A86	W	304	-	-	0/34/90/90	0/3/3/3
39	CLA	6	315	-	1/1/10/20	1/8/86/115	-
50	A1EB1	3	310	-	-	11/42/100/100	0/3/3/3
50	A1EB1	F	304	-	-	11/42/100/100	0/3/3/3
39	CLA	O	309	-	1/1/11/20	4/13/91/115	-
39	CLA	B	207	-	1/1/13/20	12/25/103/115	-
39	CLA	b	823	-	1/1/11/20	7/15/93/115	-
48	A86	S	307	-	-	6/34/90/90	0/3/3/3
49	KC2	9	316	35	-	9/15/71/71	-
39	CLA	T	319	29	1/1/11/20	8/15/93/115	-
51	A1ECV	Y	306	-	3/3/17/24	8/19/117/117	-
41	LHG	a	840	-	-	26/53/53/53	-
39	CLA	F	314	18	1/1/13/20	10/25/103/115	-
39	CLA	J	314	-	1/1/15/20	18/37/115/115	-
49	KC2	K	313	22	-	9/15/71/71	-
50	A1EB1	2	306	-	-	16/42/100/100	0/3/3/3
49	KC2	2	314	-	-	10/15/71/71	-
39	CLA	6	321	-	1/1/10/20	3/8/86/115	-
41	LHG	a	841	39	-	13/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	B	203	-	1/1/11/20	5/15/93/115	-
50	A1EB1	6	308	-	-	15/42/100/100	0/3/3/3
50	A1EB1	K	305	-	-	7/42/100/100	0/3/3/3
47	SQD	P	301	-	-	12/33/53/69	0/1/1/1
43	DD6	C	301	-	-	3/26/80/80	0/3/3/3
39	CLA	b	829	-	1/1/15/20	8/37/115/115	-
39	CLA	x	314	-	1/1/10/20	5/8/86/115	-
50	A1EB1	y	302	-	-	10/42/100/100	0/3/3/3
42	BCR	b	845	-	-	1/29/63/63	0/2/2/2
39	CLA	a	822	-	1/1/15/20	9/37/115/115	-
39	CLA	j	101	-	1/1/15/20	19/37/115/115	-
51	A1ECV	P	315	-	3/3/17/24	12/19/117/117	-
39	CLA	f	802	-	1/1/15/20	9/37/115/115	-
39	CLA	Z	309	-	1/1/10/20	0/8/86/115	-
39	CLA	I	316	36	1/1/10/20	2/8/86/115	-
42	BCR	k	204	-	-	2/29/63/63	0/2/2/2
48	A86	9	303	-	-	7/34/90/90	0/3/3/3
49	KC2	X	318	-	-	7/15/71/71	-
39	CLA	b	822	2	1/1/12/20	2/19/97/115	-
39	CLA	D	313	-	1/1/15/20	12/37/115/115	-
39	CLA	H	306	-	1/1/11/20	8/17/95/115	-
43	DD6	M	304	-	-	0/26/80/80	0/3/3/3
39	CLA	P	311	-	1/1/15/20	9/37/115/115	-
43	DD6	2	303	-	-	2/26/80/80	0/3/3/3
43	DD6	A	302	-	-	0/26/80/80	0/3/3/3
48	A86	3	307	-	-	6/34/90/90	0/3/3/3
39	CLA	G	309	-	1/1/13/20	13/27/105/115	-
50	A1EB1	z	301	-	-	12/34/90/100	0/3/3/3
43	DD6	E	303	-	-	1/26/80/80	0/3/3/3
47	SQD	D	321	-	-	16/34/54/69	0/1/1/1
39	CLA	J	317	-	1/1/10/20	2/10/88/115	-
39	CLA	4	312	-	-	18/37/115/115	-
39	CLA	b	819	-	1/1/13/20	9/30/108/115	-
39	CLA	4	311	-	1/1/14/20	17/33/111/115	-
39	CLA	6	318	-	1/1/10/20	6/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	H	317	-	-	18/39/39/53	-
39	CLA	b	803	-	1/1/15/20	14/37/115/115	-
39	CLA	b	839	-	1/1/11/20	2/16/94/115	-
48	A86	J	303	-	-	6/34/90/90	0/3/3/3
49	KC2	G	317	-	-	7/15/71/71	-
39	CLA	z	314	-	1/1/10/20	3/8/86/115	-
39	CLA	5	306	-	1/1/15/20	11/37/115/115	-
39	CLA	4	313	-	1/1/11/20	1/15/93/115	-
39	CLA	D	309	16	1/1/11/20	6/18/96/115	-
39	CLA	I	301	41	1/1/12/20	5/22/100/115	-
49	KC2	X	312	-	-	7/15/71/71	-
48	A86	7	312	-	-	4/34/90/90	0/3/3/3
39	CLA	G	312	-	1/1/12/20	10/22/100/115	-
39	CLA	U	207	-	1/1/14/20	15/31/109/115	-
39	CLA	a	835	-	1/1/15/20	11/37/115/115	-
48	A86	T	305	-	-	6/34/90/90	0/3/3/3
39	CLA	a	829	-	1/1/13/20	7/27/105/115	-
49	KC2	F	307	-	-	9/15/71/71	-
39	CLA	O	312	-	1/1/11/20	5/15/93/115	-
39	CLA	M	317	-	1/1/12/20	4/21/99/115	-
39	CLA	J	307	21	1/1/11/20	8/18/96/115	-
39	CLA	Q	317	-	1/1/11/20	5/15/93/115	-
39	CLA	8	310	-	1/1/11/20	6/13/91/115	-
47	SQD	M	301	-	-	15/34/54/69	0/1/1/1
42	BCR	b	847	-	-	4/29/63/63	0/2/2/2
49	KC2	P	310	46	-	8/14/70/71	-
39	CLA	a	817	1	1/1/11/20	4/13/91/115	-
49	KC2	W	315	-	-	8/15/71/71	-
48	A86	L	304	-	-	12/34/90/90	0/3/3/3
49	KC2	L	315	-	-	9/15/71/71	-
50	A1EB1	6	306	-	-	5/34/90/100	0/3/3/3
39	CLA	H	307	-	1/1/11/20	2/13/91/115	-
39	CLA	x	307	-	1/1/10/20	4/8/86/115	-
48	A86	O	302	-	-	2/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	A1EB1	3	324	-	-	20/42/100/100	0/3/3/3
43	DD6	P	304	-	-	2/26/80/80	0/3/3/3
49	KC2	8	314	-	-	10/15/71/71	-
52	A1EB4	P	305	-	-	10/37/98/103	0/3/3/3
39	CLA	0	311	-	-	11/25/103/115	-
52	A1EB4	M	305	-	-	9/39/100/103	0/3/3/3
39	CLA	l	201	-	1/1/15/20	14/37/115/115	-
47	SQD	k	205	-	-	13/33/53/69	0/1/1/1
39	CLA	b	810	-	1/1/15/20	13/37/115/115	-
39	CLA	y	310	-	1/1/10/20	5/8/86/115	-
39	CLA	5	316	-	1/1/12/20	8/22/100/115	-
49	KC2	G	315	-	-	11/15/71/71	-
39	CLA	o	205	-	1/1/12/20	10/22/100/115	-
43	DD6	R	304	-	-	0/26/80/80	0/3/3/3
48	A86	L	307	-	-	3/34/90/90	0/3/3/3
39	CLA	U	209	-	1/1/12/20	8/22/100/115	-
39	CLA	F	313	-	1/1/13/20	10/28/106/115	-
49	KC2	S	317	-	-	7/15/71/71	-
39	CLA	K	314	-	1/1/10/20	4/8/86/115	-
50	A1EB1	4	301	-	-	12/42/100/100	0/3/3/3
46	LMG	4	326	49	-	23/41/61/70	0/1/1/1
39	CLA	Z	312	-	1/1/10/20	2/8/86/115	-
39	CLA	C	306	-	1/1/15/20	8/37/115/115	-
39	CLA	D	318	-	1/1/15/20	14/37/115/115	-
39	CLA	L	311	23	1/1/12/20	8/22/100/115	-
39	CLA	4	323	-	1/1/15/20	11/37/115/115	-
46	LMG	l	208	49	-	15/34/54/70	0/1/1/1
48	A86	9	301	-	-	9/34/90/90	0/3/3/3
49	KC2	I	312	46	-	7/14/70/71	-
50	A1EB1	T	307	-	-	6/42/100/100	0/3/3/3
39	CLA	0	318	-	1/1/10/20	1/8/86/115	-
43	DD6	y	304	-	-	0/26/80/80	0/3/3/3
49	KC2	M	311	46	-	7/14/70/71	-
39	CLA	Y	314	-	1/1/10/20	6/8/86/115	-
51	A1ECV	V	317	-	3/3/17/24	11/19/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	9	315	-	1/1/10/20	1/8/86/115	-
51	A1ECV	X	313	-	3/3/17/24	7/19/117/117	-
39	CLA	D	316	-	1/1/15/20	14/37/115/115	-
42	BCR	b	850	-	-	6/29/63/63	0/2/2/2
39	CLA	E	314	-	1/1/13/20	10/27/105/115	-
43	DD6	7	310	-	-	4/26/80/80	0/3/3/3
49	KC2	5	311	-	-	6/15/71/71	-
49	KC2	9	311	-	-	7/15/71/71	-
39	CLA	f	803	-	1/1/13/20	9/25/103/115	-
50	A1EB1	7	303	-	-	17/42/100/100	0/3/3/3
50	A1EB1	5	302	-	-	9/42/100/100	0/3/3/3
51	A1ECV	y	317	-	3/3/17/24	8/19/117/117	-
43	DD6	4	308	-	-	1/26/80/80	0/3/3/3
39	CLA	U	208	-	1/1/11/20	3/15/93/115	-
39	CLA	X	316	-	1/1/11/20	7/16/94/115	-
46	LMG	D	322	-	-	14/32/52/70	0/1/1/1
51	A1ECV	1	318	-	3/3/17/24	6/19/117/117	-
49	KC2	5	313	46	-	7/14/70/71	-
50	A1EB1	0	307	-	-	11/42/100/100	0/3/3/3
39	CLA	b	814	-	1/1/13/20	5/25/103/115	-
43	DD6	z	304	-	-	6/26/80/80	0/3/3/3
48	A86	G	305	-	-	7/34/90/90	0/3/3/3
51	A1ECV	Z	308	-	3/3/17/24	10/19/117/117	-
39	CLA	0	312	31	1/1/12/20	8/23/101/115	-
48	A86	1	307	-	-	0/34/90/90	0/3/3/3
39	CLA	b	809	-	1/1/15/20	16/37/115/115	-
51	A1ECV	L	318	-	3/3/17/24	12/19/117/117	-
49	KC2	7	319	-	-	7/15/71/71	-
39	CLA	J	312	-	1/1/11/20	5/15/93/115	-
48	A86	z	303	-	-	9/34/90/90	0/3/3/3
43	DD6	E	302	-	-	0/26/80/80	0/3/3/3
39	CLA	Q	320	-	1/1/11/20	6/16/94/115	-
39	CLA	k	202	-	1/1/13/20	11/25/103/115	-
50	A1EB1	6	304	-	-	11/39/97/100	0/3/3/3
50	A1EB1	8	301	-	-	13/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	A1EB1	V	302	-	-	12/42/100/100	0/3/3/3
48	A86	Q	302	-	-	7/34/90/90	0/3/3/3
39	CLA	H	312	20	1/1/15/20	17/37/115/115	-
39	CLA	P	314	-	1/1/10/20	4/8/86/115	-
42	BCR	a	843	-	-	0/29/63/63	0/2/2/2
39	CLA	Y	304	-	1/1/11/20	7/15/93/115	-
51	A1ECV	R	313	-	3/3/17/24	9/19/117/117	-
49	KC2	Q	315	-	-	8/15/71/71	-
52	A1EB4	P	318	-	-	9/35/96/103	0/3/3/3
39	CLA	3	320	-	1/1/11/20	3/13/91/115	-
43	DD6	G	306	-	-	4/26/80/80	0/3/3/3
39	CLA	R	315	-	1/1/11/20	5/16/94/115	-
48	A86	6	305	-	-	11/34/90/90	0/3/3/3
43	DD6	I	306	-	-	2/26/80/80	0/3/3/3
43	DD6	B	202	-	-	3/26/80/80	0/3/3/3
39	CLA	C	308	-	1/1/14/20	14/31/109/115	-
46	LMG	7	301	49	-	23/41/61/70	0/1/1/1
43	DD6	Q	303	-	-	4/26/80/80	0/3/3/3
49	KC2	R	318	-	-	7/15/71/71	-
39	CLA	B	204	-	1/1/11/20	2/15/93/115	-
48	A86	K	301	-	-	6/34/90/90	0/3/3/3
49	KC2	z	315	-	-	10/15/71/71	-
39	CLA	K	308	22	1/1/13/20	11/30/108/115	-
46	LMG	F	320	49	-	14/29/49/70	0/1/1/1
39	CLA	I	315	-	1/1/12/20	6/22/100/115	-
39	CLA	R	316	-	1/1/12/20	8/22/100/115	-
39	CLA	4	316	-	1/1/15/20	13/37/115/115	-
39	CLA	Y	307	-	1/1/10/20	3/8/86/115	-
39	CLA	H	308	-	1/1/14/20	7/31/109/115	-
48	A86	Q	304	-	-	2/34/90/90	0/3/3/3
39	CLA	b	828	-	1/1/15/20	14/37/115/115	-
49	KC2	0	316	-	-	4/15/71/71	-
49	KC2	O	317	46	-	7/14/70/71	-
51	A1ECV	0	321	48	2/2/17/24	8/19/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	S	315	28	-	7/15/71/71	-
39	CLA	z	317	-	1/1/10/20	5/10/88/115	-
39	CLA	D	312	16	1/1/13/20	9/25/103/115	-
39	CLA	a	801	-	1/1/15/20	14/37/115/115	-
50	A1EB1	S	302	-	-	11/42/100/100	0/3/3/3
52	A1EB4	R	305	-	-	10/38/99/103	0/3/3/3
39	CLA	a	847	-	1/1/15/20	18/37/115/115	-
48	A86	W	303	-	-	4/34/90/90	0/3/3/3
49	KC2	I	303	-	-	7/15/71/71	-
49	KC2	8	320	-	-	8/15/71/71	-
39	CLA	5	315	-	1/1/11/20	3/16/94/115	-
39	CLA	S	308	-	1/1/14/20	16/33/111/115	-
47	SQD	F	319	-	-	13/32/52/69	0/1/1/1
47	SQD	S	301	-	-	13/34/54/69	0/1/1/1
48	A86	S	305	-	-	6/34/90/90	0/3/3/3
39	CLA	J	310	-	1/1/13/20	8/25/103/115	-
51	A1ECV	7	317	-	3/3/17/24	7/19/117/117	-
50	A1EB1	Q	307	-	-	8/42/100/100	0/3/3/3
50	A1EB1	8	304	-	-	10/42/100/100	0/3/3/3
39	CLA	H	313	-	1/1/15/20	7/37/115/115	-
39	CLA	3	313	-	1/1/12/20	3/23/101/115	-
51	A1ECV	W	317	-	3/3/17/24	8/19/117/117	-
50	A1EB1	S	303	-	-	14/42/100/100	0/3/3/3
51	A1ECV	Q	316	26	3/3/17/24	7/19/117/117	-
50	A1EB1	6	301	-	-	12/42/100/100	0/3/3/3
39	CLA	S	316	-	1/1/10/20	4/8/86/115	-
43	DD6	V	303	-	-	0/26/80/80	0/3/3/3
49	KC2	P	313	24	-	10/15/71/71	-
39	CLA	2	310	-	1/1/10/20	6/10/88/115	-
49	KC2	R	312	-	-	8/15/71/71	-
39	CLA	b	812	-	1/1/15/20	10/37/115/115	-
49	KC2	W	312	46,24	-	8/14/70/71	-
46	LMG	S	322	49	-	28/41/61/70	0/1/1/1
39	CLA	Z	306	-	1/1/11/20	7/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	M	302	-	-	8/34/90/90	0/3/3/3
39	CLA	b	806	-	1/1/15/20	13/37/115/115	-
49	KC2	H	314	-	-	11/15/71/71	-
39	CLA	b	840	-	1/1/15/20	9/37/115/115	-
49	KC2	G	313	-	-	6/15/71/71	-
49	KC2	C	313	-	-	11/15/71/71	-
49	KC2	6	316	-	-	10/15/71/71	-
50	A1EB1	V	305	-	-	12/42/100/100	0/3/3/3
39	CLA	4	322	-	1/1/12/20	5/22/100/115	-
49	KC2	4	318	28	-	9/15/71/71	-
39	CLA	E	318	17	1/1/11/20	9/15/93/115	-
39	CLA	C	311	-	1/1/15/20	15/37/115/115	-
52	A1EB4	T	304	-	-	9/36/97/103	0/3/3/3
49	KC2	C	312	-	-	10/15/71/71	-
39	CLA	b	813	-	1/1/13/20	3/25/101/115	-
39	CLA	b	841	2	1/1/15/20	12/37/115/115	-
39	CLA	L	320	-	1/1/11/20	8/15/93/115	-
39	CLA	P	307	-	1/1/15/20	10/37/115/115	-
39	CLA	T	313	-	1/1/12/20	6/21/99/115	-
39	CLA	9	310	-	1/1/10/20	3/8/86/115	-
46	LMG	W	320	-	-	15/28/48/70	0/1/1/1
39	CLA	a	824	-	1/1/15/20	5/37/115/115	-
39	CLA	o	202	-	1/1/10/20	3/10/88/115	-
50	A1EB1	G	302	-	-	8/42/100/100	0/3/3/3
39	CLA	F	309	-	1/1/12/20	4/22/100/115	-
48	A86	Z	301	-	-	11/34/90/90	0/3/3/3
48	A86	6	307	-	-	10/34/90/90	0/3/3/3
43	DD6	F	303	-	-	0/26/80/80	0/3/3/3
50	A1EB1	C	302	-	-	10/42/100/100	0/3/3/3
39	CLA	B	209	-	1/1/13/20	10/27/105/115	-
39	CLA	0	315	31	1/1/12/20	5/19/97/115	-
49	KC2	3	321	-	-	10/15/71/71	-
39	CLA	G	318	-	1/1/11/20	11/18/96/115	-
39	CLA	W	310	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	BCR	j	103	-	-	4/29/63/63	0/2/2/2
48	A86	6	303	-	-	2/34/90/90	0/3/3/3
39	CLA	D	311	-	1/1/15/20	21/37/115/115	-
47	SQD	T	321	-	-	13/31/51/69	0/1/1/1
39	CLA	F	312	-	1/1/15/20	6/37/115/115	-
39	CLA	V	316	-	1/1/12/20	6/19/97/115	-
52	A1EB4	P	319	-	-	6/38/99/103	0/3/3/3
39	CLA	Y	303	-	1/1/10/20	2/8/86/115	-
51	A1ECV	Z	314	-	3/3/17/24	7/19/117/117	-
48	A86	3	308	-	-	6/34/90/90	0/3/3/3
39	CLA	K	306	-	1/1/14/20	11/33/111/115	-
49	KC2	T	314	-	-	7/15/71/71	-
39	CLA	E	317	-	1/1/12/20	8/22/100/115	-
39	CLA	S	310	-	1/1/10/20	4/10/88/115	-
43	DD6	A	303	-	-	5/26/80/80	0/3/3/3
39	CLA	9	308	-	1/1/13/20	17/25/103/115	-
39	CLA	D	314	-	1/1/15/20	9/37/115/115	-
50	A1EB1	0	302	-	-	13/42/100/100	0/3/3/3
39	CLA	U	210	-	1/1/14/20	7/31/109/115	-
39	CLA	U	211	-	1/1/14/20	7/31/109/115	-
46	LMG	W	302	49	-	18/34/54/70	0/1/1/1
41	LHG	X	301	-	-	25/45/45/53	-
39	CLA	b	802	-	1/1/15/20	6/37/115/115	-
51	A1ECV	5	309	27	3/3/17/24	11/19/117/117	-
48	A86	D	305	-	-	8/34/90/90	0/3/3/3
39	CLA	0	320	-	1/1/11/20	6/13/91/115	-
42	BCR	a	842	-	-	4/29/63/63	0/2/2/2
48	A86	R	301	-	-	2/34/90/90	0/3/3/3
43	DD6	S	306	-	-	4/26/80/80	0/3/3/3
39	CLA	I	311	-	1/1/15/20	15/37/115/115	-
50	A1EB1	8	308	-	-	11/42/100/100	0/3/3/3
48	A86	V	304	-	-	3/34/90/90	0/3/3/3
39	CLA	T	320	-	1/1/12/20	8/22/100/115	-
49	KC2	T	312	-	-	10/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	3	319	-	1/1/10/20	4/8/86/115	-
43	DD6	J	306	-	-	3/26/80/80	0/3/3/3
46	LMG	S	321	-	-	11/27/47/70	0/1/1/1
49	KC2	1	314	-	-	11/15/71/71	-
39	CLA	b	833	-	1/1/15/20	13/37/115/115	-
43	DD6	X	304	-	-	0/26/80/80	0/3/3/3
39	CLA	F	308	-	1/1/15/20	14/37/115/115	-
39	CLA	J	308	-	1/1/12/20	4/19/97/115	-
49	KC2	Z	311	-	-	10/15/71/71	-
39	CLA	z	307	-	1/1/10/20	3/10/88/115	-
39	CLA	a	830	-	1/1/15/20	18/37/115/115	-
39	CLA	E	313	-	1/1/15/20	13/37/115/115	-
48	A86	0	301	-	-	4/34/90/90	0/3/3/3
39	CLA	7	321	-	1/1/10/20	4/8/86/115	-
39	CLA	A	309	-	1/1/15/20	13/37/115/115	-
39	CLA	T	318	-	1/1/11/20	7/16/94/115	-
48	A86	J	301	-	-	2/34/90/90	0/3/3/3
39	CLA	H	316	-	1/1/11/20	8/15/93/115	-
49	KC2	V	308	27	-	8/15/71/71	-
39	CLA	X	307	-	1/1/15/20	8/37/115/115	-
39	CLA	a	838	-	1/1/15/20	10/37/115/115	-
39	CLA	H	310	-	1/1/13/20	7/28/106/115	-
39	CLA	X	309	-	1/1/15/20	14/37/115/115	-
43	DD6	O	305	-	-	5/26/80/80	0/3/3/3
39	CLA	a	808	-	1/1/13/20	10/27/105/115	-
48	A86	0	309	-	-	7/34/90/90	0/3/3/3
48	A86	6	309	-	-	13/34/90/90	0/3/3/3
39	CLA	l	205	-	1/1/12/20	2/19/97/115	-
39	CLA	y	318	-	1/1/10/20	5/10/88/115	-
50	A1EB1	7	306	-	-	10/42/100/100	0/3/3/3
39	CLA	3	311	-	1/1/14/20	14/33/111/115	-
43	DD6	H	305	-	-	2/26/80/80	0/3/3/3
43	DD6	I	307	-	-	1/26/80/80	0/3/3/3
49	KC2	R	314	46	-	7/14/70/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	6	314	-	-	8/15/71/71	-
39	CLA	x	317	-	1/1/10/20	3/8/86/115	-
39	CLA	P	308	24	1/1/15/20	22/37/115/115	-
49	KC2	4	320	-	-	10/15/71/71	-
49	KC2	W	314	-	-	7/15/71/71	-
49	KC2	X	315	-	-	8/15/71/71	-
39	CLA	8	322	-	-	2/8/86/115	-
43	DD6	A	304	-	-	3/26/80/80	0/3/3/3
43	DD6	a	846	-	-	5/26/80/80	0/3/3/3
39	CLA	Z	304	-	1/1/10/20	3/8/86/115	-
39	CLA	C	304	-	1/1/10/20	3/11/89/115	-
39	CLA	Z	305	-	1/1/10/20	2/8/86/115	-
49	KC2	7	322	-	-	12/15/71/71	-
39	CLA	a	837	-	1/1/15/20	3/37/115/115	-
39	CLA	U	215	-	1/1/10/20	5/8/86/115	-
49	KC2	H	311	-	-	9/15/71/71	-
39	CLA	3	322	-	1/1/12/20	10/21/99/115	-
49	KC2	M	313	-	-	6/15/71/71	-
48	A86	Q	305	-	-	16/34/90/90	0/3/3/3
39	CLA	S	311	-	1/1/15/20	11/37/115/115	-
48	A86	T	301	-	-	2/34/90/90	0/3/3/3
39	CLA	a	807	1	1/1/15/20	11/37/115/115	-
51	A1ECV	G	316	-	3/3/17/24	11/19/117/117	-
52	A1EB4	W	306	-	-	10/37/98/103	0/3/3/3
45	DGD	C	314	-	-	15/29/69/95	0/2/2/2
48	A86	1	306	-	-	9/34/90/90	0/3/3/3
39	CLA	Q	309	-	1/1/14/20	7/33/111/115	-
42	BCR	a	844	-	-	0/29/63/63	0/2/2/2
39	CLA	A	308	-	1/1/12/20	7/21/99/115	-
39	CLA	O	310	-	1/1/14/20	13/31/109/115	-
39	CLA	J	309	-	1/1/15/20	17/37/115/115	-
50	A1EB1	3	309	-	-	9/42/100/100	0/3/3/3
39	CLA	F	315	18	1/1/10/20	2/8/86/115	-
40	PQN	a	839	-	-	7/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	A	315	-	1/1/12/20	6/19/97/115	-
39	CLA	S	313	-	1/1/15/20	7/37/115/115	-
39	CLA	I	313	-	1/1/15/20	17/37/115/115	-
43	DD6	7	309	-	-	2/26/80/80	0/3/3/3
48	A86	3	305	-	-	12/34/90/90	0/3/3/3
49	KC2	L	314	-	-	7/15/71/71	-
39	CLA	V	309	-	1/1/15/20	9/37/115/115	-
39	CLA	Q	321	-	1/1/12/20	6/23/101/115	-

The worst 5 of 5002 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	M	322	A1EB4	C13-C11	-17.07	1.25	1.43
52	P	319	A1EB4	C13-C11	-17.07	1.25	1.43
52	P	318	A1EB4	C13-C11	-16.98	1.25	1.43
52	W	321	A1EB4	C13-C11	-16.67	1.25	1.43
52	T	304	A1EB4	C13-C11	-16.45	1.25	1.43

The worst 5 of 10101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2	303	DD6	O1-C20-C21	17.30	135.78	115.06
43	Z	302	DD6	O1-C20-C21	17.29	135.77	115.06
43	F	305	DD6	O1-C20-C21	13.19	130.87	115.06
51	R	310	A1ECV	C3A-C4A-NA	12.90	119.61	110.10
51	Q	316	A1ECV	C3A-C4A-NA	12.89	119.60	110.10

5 of 517 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
39	a	801	CLA	ND
39	a	802	CLA	ND
39	a	803	CLA	ND
39	a	804	CLA	ND
39	a	805	CLA	ND

5 of 6960 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	a	801	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	a	802	CLA	C1A-C2A-CAA-CBA
39	a	803	CLA	CHA-CBD-CGD-O1D
39	a	803	CLA	CHA-CBD-CGD-O2D
39	a	803	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

444 monomers are involved in 929 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	X	308	CLA	4	0
39	8	313	CLA	1	0
41	D	302	LHG	3	0
42	l	207	BCR	4	0
39	b	824	CLA	4	0
49	V	315	KC2	1	0
39	A	306	CLA	3	0
39	o	206	CLA	2	0
39	7	313	CLA	2	0
46	A	316	LMG	1	0
39	a	812	CLA	1	0
39	7	318	CLA	3	0
39	a	806	CLA	1	0
39	l	203	CLA	2	0
48	0	304	A86	1	0
39	a	827	CLA	2	0
39	F	316	CLA	2	0
39	V	313	CLA	5	0
46	F	317	LMG	14	0
39	b	818	CLA	3	0
39	2	309	CLA	1	0
39	7	316	CLA	4	0
39	E	312	CLA	3	0
39	b	805	CLA	3	0
47	7	302	SQD	1	0
48	F	301	A86	1	0
49	5	305	KC2	1	0
39	O	316	CLA	1	0
51	x	310	A1ECV	1	0
49	4	324	KC2	1	0
50	2	304	A1EB1	1	0
39	T	308	CLA	9	0
39	D	315	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	I	308	CLA	3	0
39	J	318	CLA	2	0
42	b	846	BCR	4	0
39	z	306	CLA	1	0
39	D	310	CLA	2	0
39	F	321	CLA	1	0
39	Q	311	CLA	3	0
39	0	310	CLA	2	0
46	7	326	LMG	2	0
42	h	202	BCR	4	0
42	m	101	BCR	5	0
45	b	849	DGD	3	0
39	b	837	CLA	1	0
39	Q	314	CLA	2	0
39	a	826	CLA	3	0
48	W	307	A86	1	0
39	R	309	CLA	1	0
49	0	314	KC2	2	0
39	3	314	CLA	3	0
39	Y	313	CLA	1	0
46	P	317	LMG	5	0
47	D	304	SQD	2	0
39	V	311	CLA	1	0
39	9	307	CLA	1	0
49	2	313	KC2	1	0
39	T	311	CLA	1	0
39	b	807	CLA	3	0
39	B	206	CLA	1	0
39	E	308	CLA	1	0
52	5	304	A1EB4	1	0
39	A	305	CLA	1	0
39	Q	312	CLA	1	0
39	V	310	CLA	5	0
43	z	305	DD6	1	0
49	P	312	KC2	2	0
39	b	821	CLA	2	0
39	S	309	CLA	2	0
39	3	312	CLA	4	0
39	D	319	CLA	3	0
39	C	307	CLA	2	0
39	4	314	CLA	4	0
41	j	104	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	5	303	DD6	1	0
47	4	327	SQD	1	0
39	a	816	CLA	7	0
39	Y	305	CLA	1	0
39	1	313	CLA	2	0
39	a	803	CLA	3	0
39	0	323	CLA	2	0
39	C	305	CLA	1	0
39	A	311	CLA	2	0
49	X	314	KC2	19	0
42	b	848	BCR	5	0
39	l	204	CLA	1	0
50	4	304	A1EB1	1	0
39	i	103	CLA	6	0
47	D	320	SQD	2	0
39	a	815	CLA	4	0
39	8	321	CLA	1	0
51	2	311	A1ECV	1	0
39	D	317	CLA	5	0
39	a	831	CLA	4	0
51	9	317	A1ECV	2	0
39	Z	316	CLA	1	0
42	l	202	BCR	5	0
39	6	313	CLA	1	0
42	f	801	BCR	3	0
39	M	312	CLA	4	0
39	E	316	CLA	1	0
39	9	312	CLA	4	0
39	X	317	CLA	3	0
48	E	304	A86	1	0
39	O	313	CLA	1	0
39	E	310	CLA	4	0
49	3	317	KC2	1	0
50	z	302	A1EB1	1	0
39	V	319	CLA	1	0
39	O	308	CLA	1	0
39	a	825	CLA	7	0
43	U	204	DD6	1	0
39	G	310	CLA	1	0
39	a	818	CLA	3	0
39	b	825	CLA	2	0
39	C	310	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	K	312	CLA	2	0
48	Z	303	A86	1	0
50	H	304	A1EB1	1	0
47	W	301	SQD	1	0
48	I	304	A86	1	0
39	6	310	CLA	1	0
46	Q	322	LMG	2	0
39	a	811	CLA	5	0
39	a	814	CLA	2	0
39	E	315	CLA	2	0
39	y	307	CLA	1	0
39	x	306	CLA	1	0
39	8	311	CLA	2	0
39	a	809	CLA	3	0
39	S	320	CLA	3	0
39	W	313	CLA	2	0
39	P	309	CLA	1	0
43	F	305	DD6	1	0
39	R	308	CLA	1	0
39	W	309	CLA	2	0
39	k	201	CLA	2	0
52	W	321	A1EB4	1	0
39	x	308	CLA	1	0
39	2	318	CLA	1	0
39	a	820	CLA	2	0
48	Q	301	A86	1	0
49	Y	308	KC2	1	0
39	a	832	CLA	1	0
50	x	302	A1EB1	2	0
48	5	301	A86	2	0
39	1	309	CLA	1	0
42	i	102	BCR	6	0
51	7	323	A1ECV	4	0
39	K	307	CLA	1	0
39	5	308	CLA	2	0
48	2	305	A86	1	0
46	M	319	LMG	10	0
39	F	310	CLA	1	0
51	z	316	A1ECV	1	0
39	b	817	CLA	3	0
39	I	309	CLA	2	0
39	9	319	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	b	808	CLA	1	0
39	a	813	CLA	3	0
39	Z	313	CLA	1	0
39	A	314	CLA	3	0
39	K	311	CLA	1	0
39	b	826	CLA	7	0
49	F	311	KC2	7	0
39	i	101	CLA	4	0
42	a	845	BCR	5	0
51	T	317	A1ECV	1	0
43	J	305	DD6	1	0
49	x	312	KC2	1	0
43	H	303	DD6	1	0
39	M	309	CLA	2	0
39	1	308	CLA	2	0
39	M	308	CLA	1	0
39	b	842	CLA	2	0
39	b	838	CLA	4	0
39	2	308	CLA	1	0
39	2	316	CLA	1	0
50	0	303	A1EB1	2	0
49	T	315	KC2	2	0
39	7	314	CLA	5	0
39	a	804	CLA	2	0
50	9	302	A1EB1	1	0
48	R	302	A86	2	0
39	0	313	CLA	2	0
39	b	834	CLA	2	0
39	x	311	CLA	1	0
39	K	309	CLA	1	0
39	J	313	CLA	1	0
39	a	802	CLA	2	0
39	L	313	CLA	1	0
49	8	316	KC2	1	0
39	J	311	CLA	4	0
39	a	823	CLA	3	0
39	U	201	CLA	1	0
39	b	830	CLA	3	0
39	P	316	CLA	1	0
39	H	309	CLA	2	0
51	y	311	A1ECV	1	0
48	U	206	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	a	836	CLA	6	0
39	a	821	CLA	2	0
39	Q	310	CLA	3	0
39	b	832	CLA	5	0
39	L	308	CLA	3	0
39	k	203	CLA	1	0
39	b	811	CLA	2	0
42	f	804	BCR	3	0
39	b	851	CLA	4	0
39	1	310	CLA	1	0
46	0	324	LMG	4	0
46	4	325	LMG	2	0
39	A	312	CLA	1	0
48	F	302	A86	8	0
39	X	311	CLA	1	0
43	O	304	DD6	1	0
39	S	319	CLA	2	0
39	7	324	CLA	4	0
39	b	835	CLA	1	0
46	I	302	LMG	1	0
39	W	318	CLA	1	0
39	b	831	CLA	2	0
39	b	815	CLA	4	0
47	9	322	SQD	1	0
42	b	844	BCR	2	0
39	b	820	CLA	3	0
39	R	307	CLA	2	0
39	M	310	CLA	3	0
47	H	318	SQD	3	0
39	R	311	CLA	1	0
43	D	306	DD6	1	0
39	7	325	CLA	1	0
39	W	311	CLA	2	0
39	z	311	CLA	1	0
39	b	827	CLA	7	0
43	1	304	DD6	2	0
39	o	201	CLA	2	0
43	3	304	DD6	3	0
42	l	206	BCR	1	0
39	L	310	CLA	2	0
39	b	801	CLA	7	0
40	b	843	PQN	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	W	304	A86	5	0
50	F	304	A1EB1	4	0
39	O	309	CLA	1	0
39	B	207	CLA	2	0
39	b	823	CLA	1	0
39	T	319	CLA	1	0
41	a	840	LHG	3	0
39	F	314	CLA	3	0
39	J	314	CLA	3	0
51	Y	306	A1ECV	1	0
39	6	321	CLA	1	0
47	P	301	SQD	1	0
39	b	829	CLA	2	0
42	b	845	BCR	3	0
39	a	822	CLA	5	0
39	j	101	CLA	5	0
39	f	802	CLA	1	0
39	Z	309	CLA	1	0
42	k	204	BCR	2	0
48	9	303	A86	1	0
39	b	822	CLA	2	0
39	D	313	CLA	1	0
39	H	306	CLA	3	0
43	M	304	DD6	2	0
43	2	303	DD6	1	0
43	A	302	DD6	1	0
39	G	309	CLA	1	0
43	E	303	DD6	1	0
47	D	321	SQD	2	0
39	4	312	CLA	2	0
39	b	819	CLA	1	0
41	H	317	LHG	3	0
39	b	803	CLA	2	0
39	b	839	CLA	3	0
39	5	306	CLA	2	0
39	D	309	CLA	1	0
39	I	301	CLA	3	0
49	X	312	KC2	1	0
48	7	312	A86	1	0
39	U	207	CLA	3	0
39	a	835	CLA	3	0
39	a	829	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	F	307	KC2	1	0
39	M	317	CLA	2	0
39	J	307	CLA	1	0
39	8	310	CLA	3	0
47	M	301	SQD	3	0
42	b	847	BCR	4	0
49	P	310	KC2	1	0
39	a	817	CLA	2	0
49	W	315	KC2	1	0
48	L	304	A86	4	0
49	L	315	KC2	1	0
39	x	307	CLA	2	0
43	P	304	DD6	2	0
39	0	311	CLA	3	0
39	l	201	CLA	3	0
47	k	205	SQD	2	0
39	b	810	CLA	3	0
39	y	310	CLA	1	0
39	5	316	CLA	2	0
39	o	205	CLA	2	0
39	U	209	CLA	1	0
39	F	313	CLA	3	0
39	K	314	CLA	1	0
46	4	326	LMG	33	0
39	C	306	CLA	2	0
39	D	318	CLA	5	0
39	L	311	CLA	2	0
39	4	323	CLA	7	0
46	l	208	LMG	4	0
39	D	316	CLA	2	0
42	b	850	BCR	5	0
39	E	314	CLA	5	0
43	7	310	DD6	5	0
39	f	803	CLA	1	0
43	4	308	DD6	1	0
39	U	208	CLA	2	0
46	D	322	LMG	1	0
49	5	313	KC2	26	0
51	1	318	A1ECV	1	0
50	0	307	A1EB1	2	0
39	b	814	CLA	2	0
39	0	312	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	1	307	A86	1	0
39	b	809	CLA	5	0
49	7	319	KC2	1	0
39	Q	320	CLA	1	0
48	Q	302	A86	2	0
39	H	312	CLA	2	0
42	a	843	BCR	4	0
49	Q	315	KC2	1	0
52	P	318	A1EB4	3	0
39	3	320	CLA	1	0
43	I	306	DD6	1	0
39	C	308	CLA	3	0
46	7	301	LMG	20	0
43	Q	303	DD6	5	0
39	B	204	CLA	1	0
39	K	308	CLA	1	0
46	F	320	LMG	7	0
39	I	315	CLA	1	0
39	R	316	CLA	2	0
39	4	316	CLA	1	0
39	H	308	CLA	2	0
48	Q	304	A86	28	0
39	b	828	CLA	6	0
49	O	317	KC2	1	0
51	0	321	A1ECV	2	0
39	D	312	CLA	2	0
39	a	801	CLA	6	0
52	R	305	A1EB4	1	0
39	a	847	CLA	2	0
39	5	315	CLA	2	0
39	S	308	CLA	2	0
47	F	319	SQD	1	0
47	S	301	SQD	4	0
39	J	310	CLA	1	0
51	7	317	A1ECV	2	0
39	H	313	CLA	2	0
39	3	313	CLA	1	0
50	S	303	A1EB1	1	0
39	2	310	CLA	1	0
49	R	312	KC2	1	0
39	b	812	CLA	3	0
46	S	322	LMG	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	Z	306	CLA	1	0
39	b	806	CLA	1	0
39	b	840	CLA	4	0
49	6	316	KC2	1	0
39	E	318	CLA	1	0
39	C	311	CLA	1	0
39	b	813	CLA	2	0
39	b	841	CLA	4	0
39	P	307	CLA	3	0
39	T	313	CLA	2	0
39	a	824	CLA	5	0
39	F	309	CLA	1	0
43	F	303	DD6	6	0
39	B	209	CLA	4	0
39	0	315	CLA	2	0
39	G	318	CLA	1	0
39	W	310	CLA	7	0
42	j	103	BCR	1	0
39	D	311	CLA	2	0
47	T	321	SQD	1	0
39	F	312	CLA	1	0
39	V	316	CLA	10	0
52	P	319	A1EB4	2	0
39	K	306	CLA	6	0
39	E	317	CLA	3	0
39	9	308	CLA	3	0
39	D	314	CLA	2	0
46	W	302	LMG	14	0
41	X	301	LHG	2	0
39	b	802	CLA	1	0
48	D	305	A86	1	0
42	a	842	BCR	5	0
43	S	306	DD6	1	0
39	I	311	CLA	1	0
39	T	320	CLA	2	0
46	S	321	LMG	3	0
39	b	833	CLA	3	0
39	F	308	CLA	3	0
39	a	830	CLA	4	0
39	E	313	CLA	2	0
39	7	321	CLA	1	0
39	A	309	CLA	1	0

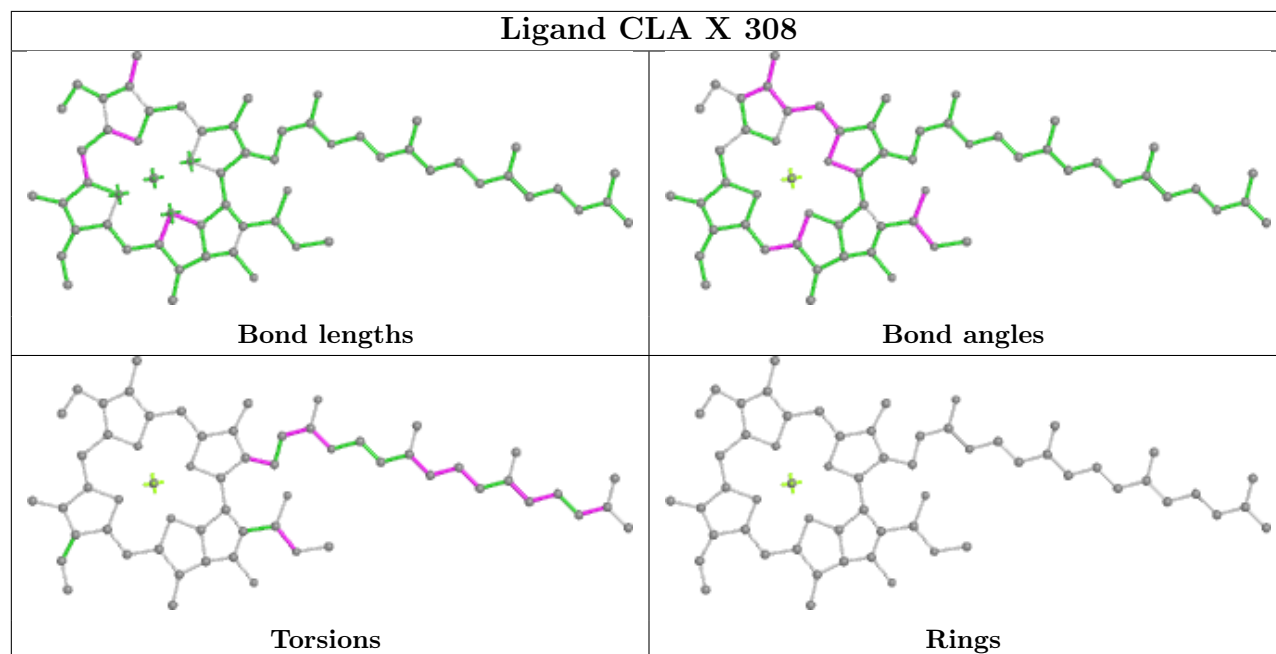
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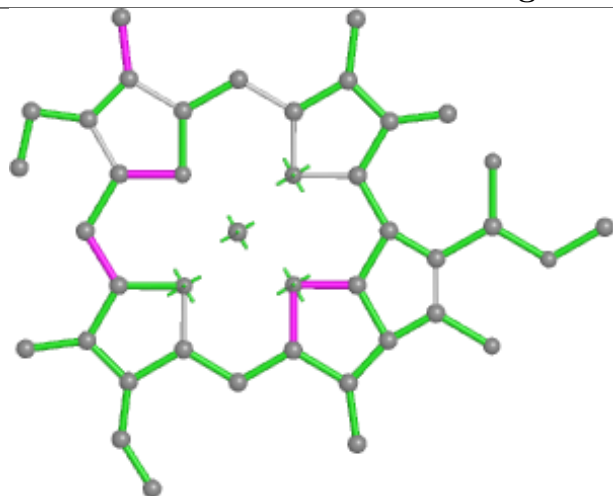
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	T	318	CLA	1	0
39	H	316	CLA	1	0
39	X	307	CLA	2	0
39	a	838	CLA	3	0
39	H	310	CLA	3	0
39	X	309	CLA	2	0
43	O	305	DD6	1	0
39	a	808	CLA	1	0
39	l	205	CLA	7	0
50	7	306	A1EB1	1	0
39	3	311	CLA	2	0
49	R	314	KC2	15	0
39	x	317	CLA	1	0
39	P	308	CLA	5	0
49	W	314	KC2	2	0
39	C	304	CLA	1	0
39	a	837	CLA	1	0
39	U	215	CLA	1	0
39	3	322	CLA	2	0
49	M	313	KC2	1	0
39	S	311	CLA	5	0
39	a	807	CLA	3	0
52	W	306	A1EB4	4	0
39	Q	309	CLA	2	0
42	a	844	BCR	3	0
39	O	310	CLA	4	0
39	J	309	CLA	3	0
40	a	839	PQN	4	0
39	A	315	CLA	2	0
39	S	313	CLA	4	0
39	I	313	CLA	2	0
39	V	309	CLA	2	0
39	Q	321	CLA	3	0

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 than 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

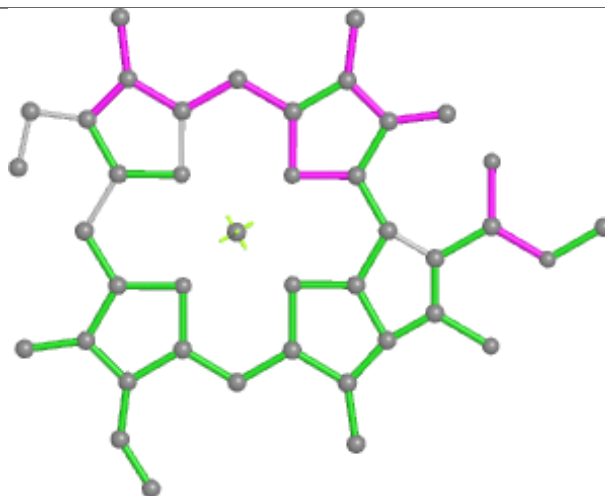
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



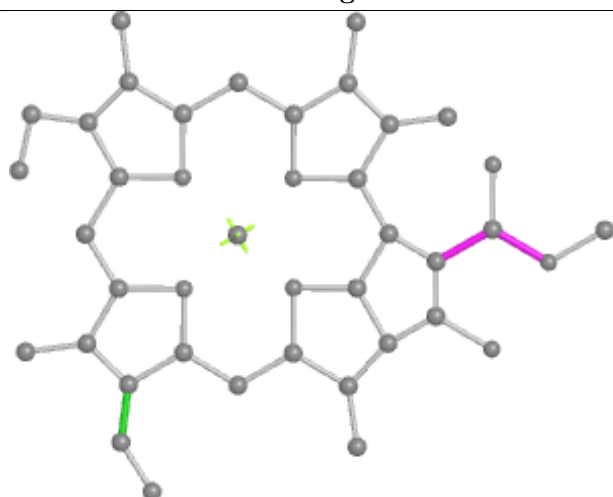
## Ligand CLA 8 313



Bond lengths



Bond angles



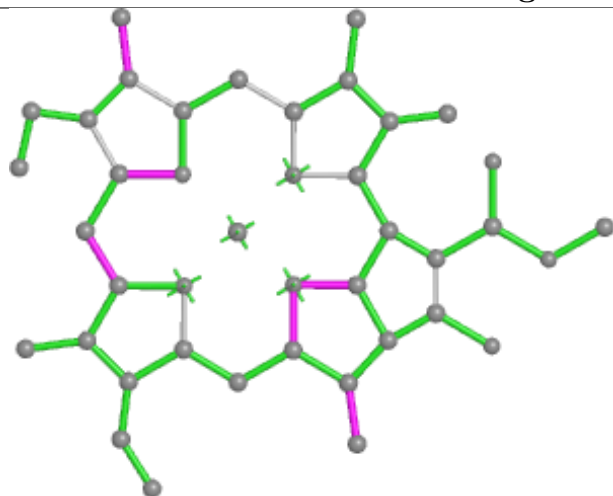
Torsions



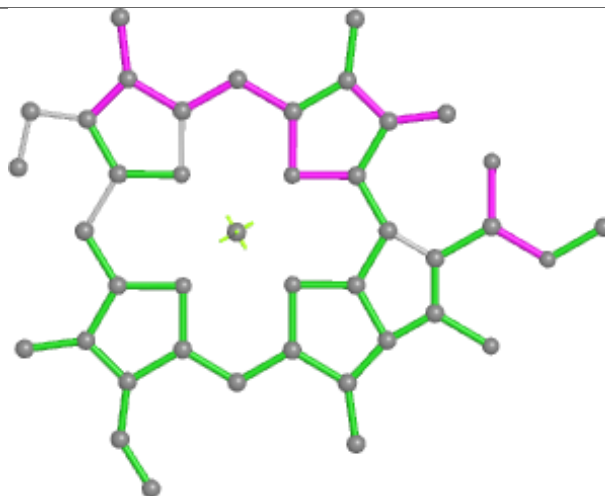
Rings



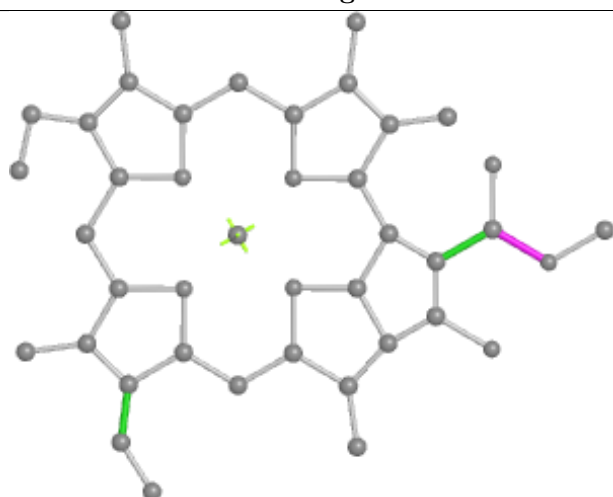
## Ligand CLA 2 307



Bond lengths



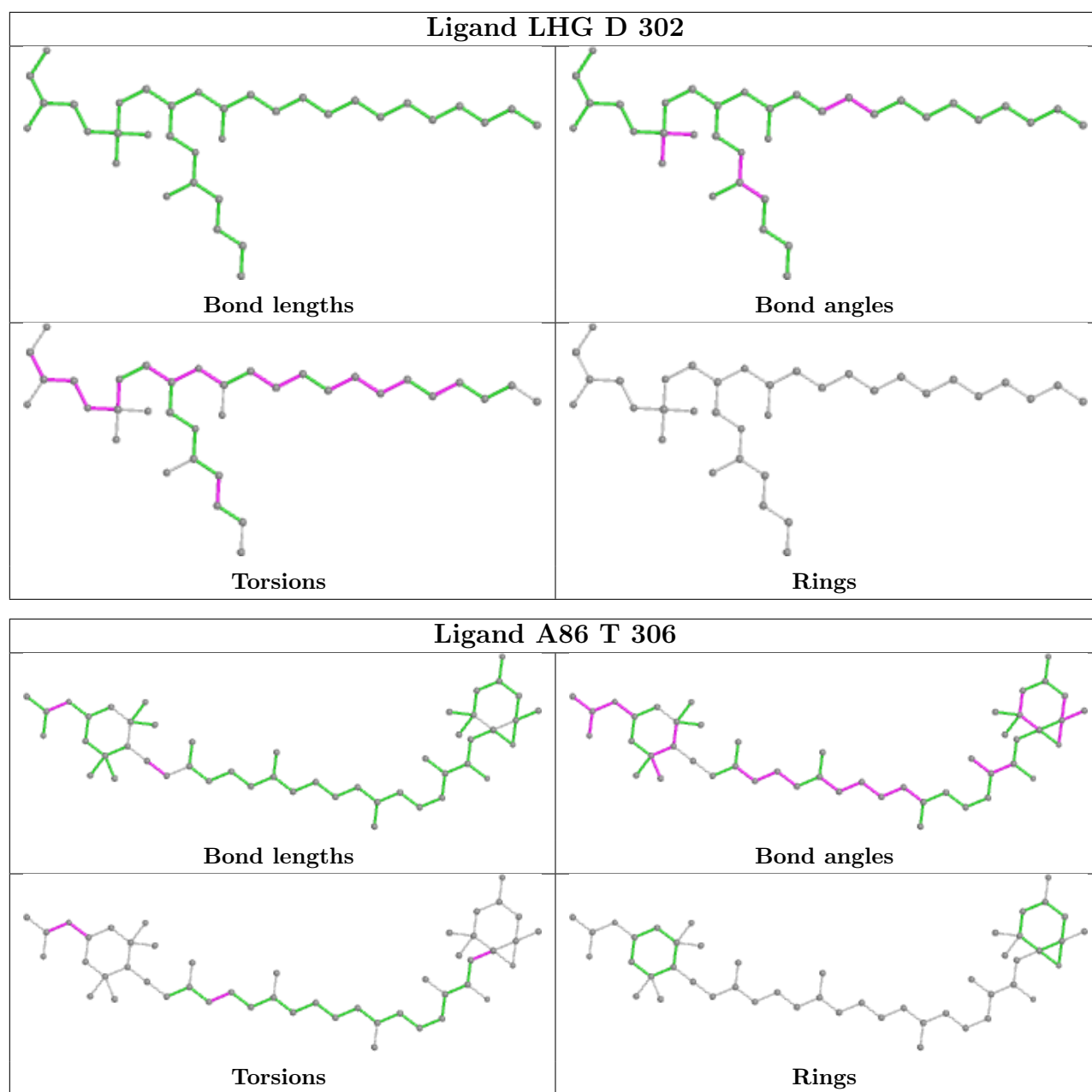
Bond angles

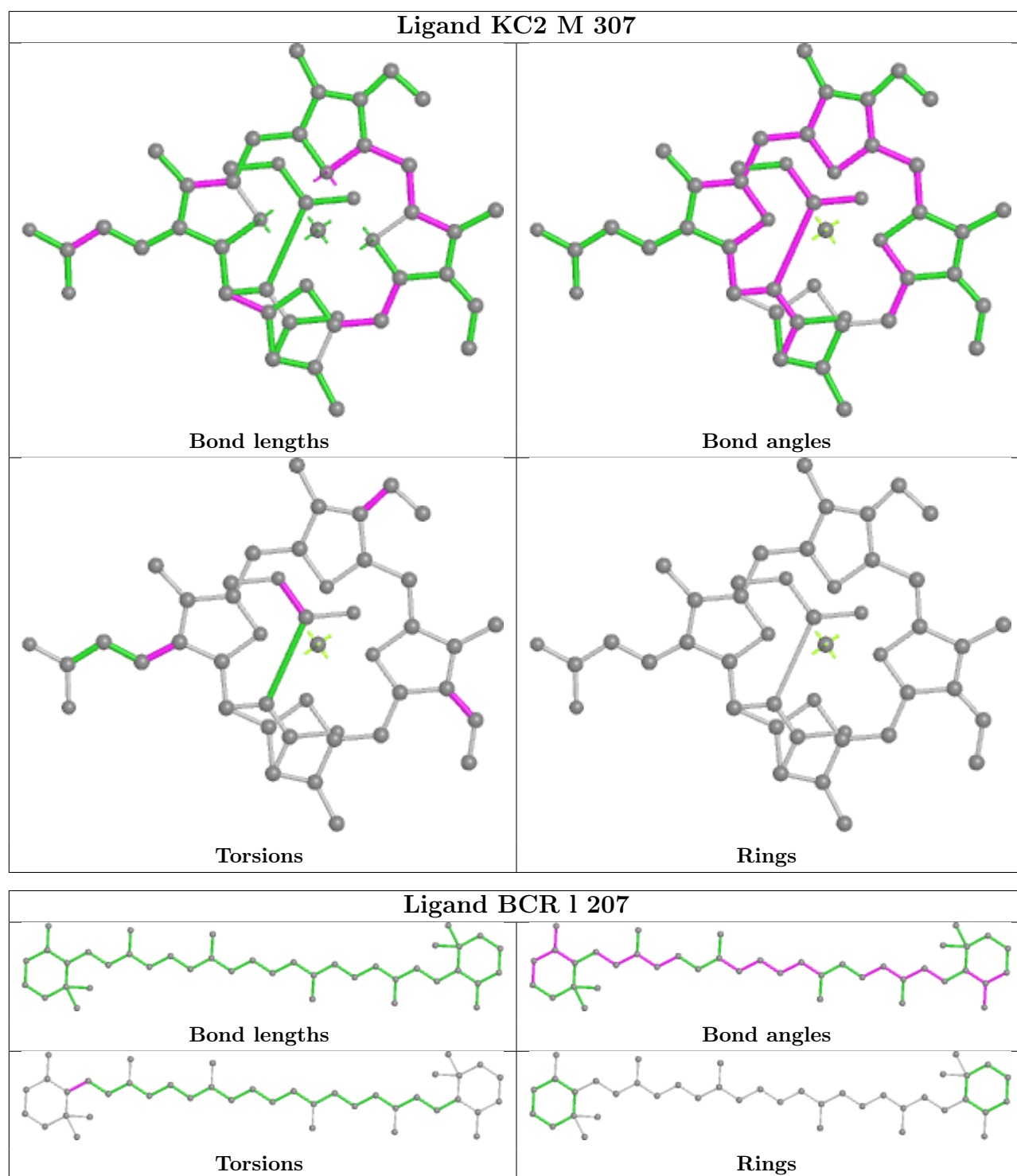


Torsions

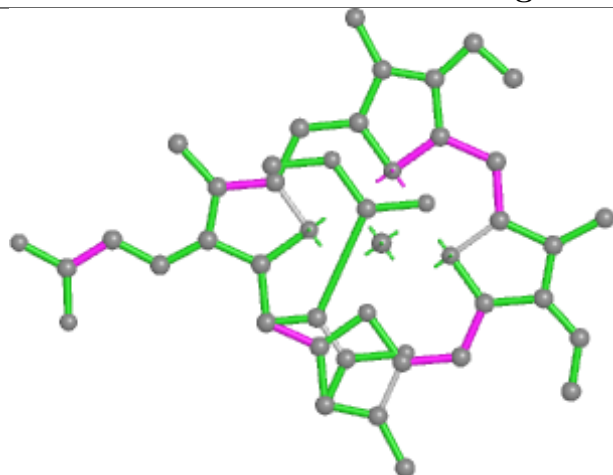


Rings

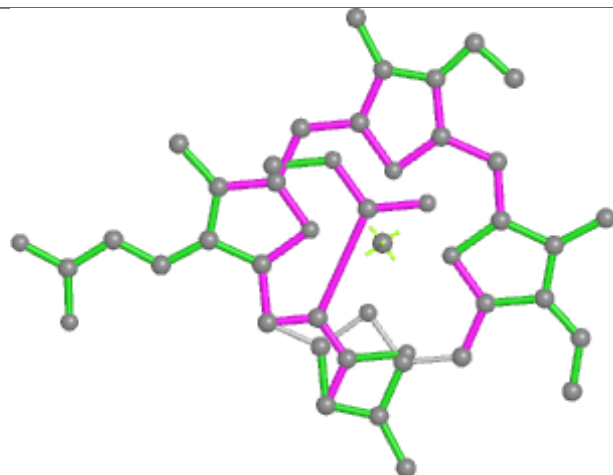




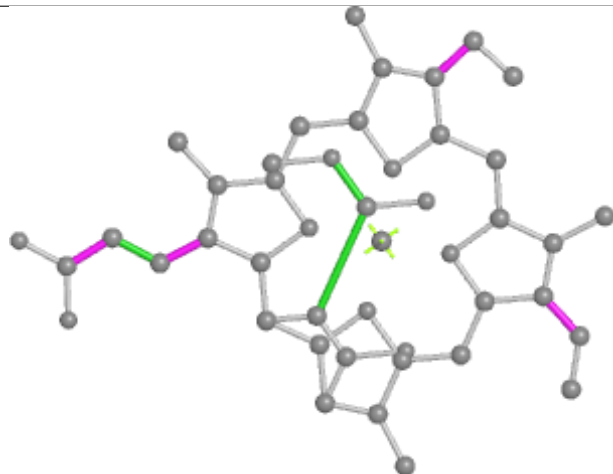
## Ligand KC2 Y 309



Bond lengths



Bond angles

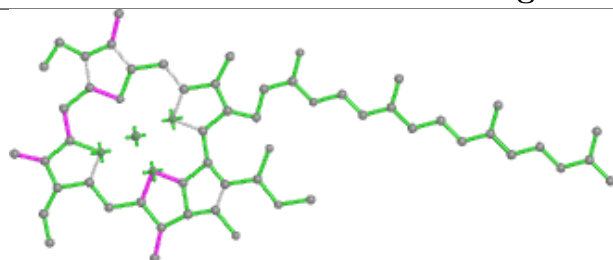


Torsions

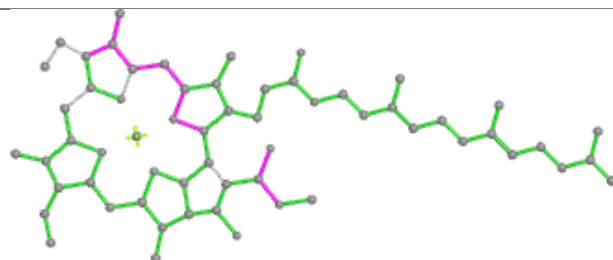


Rings

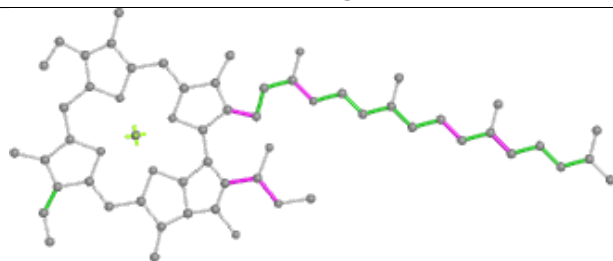
## Ligand CLA b 824



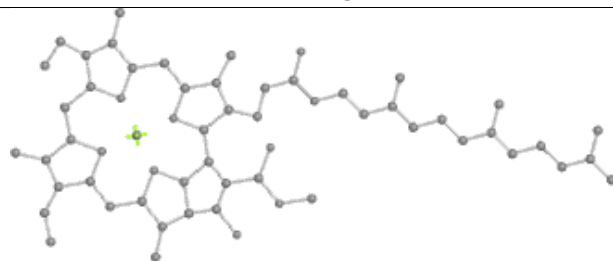
Bond lengths



Bond angles

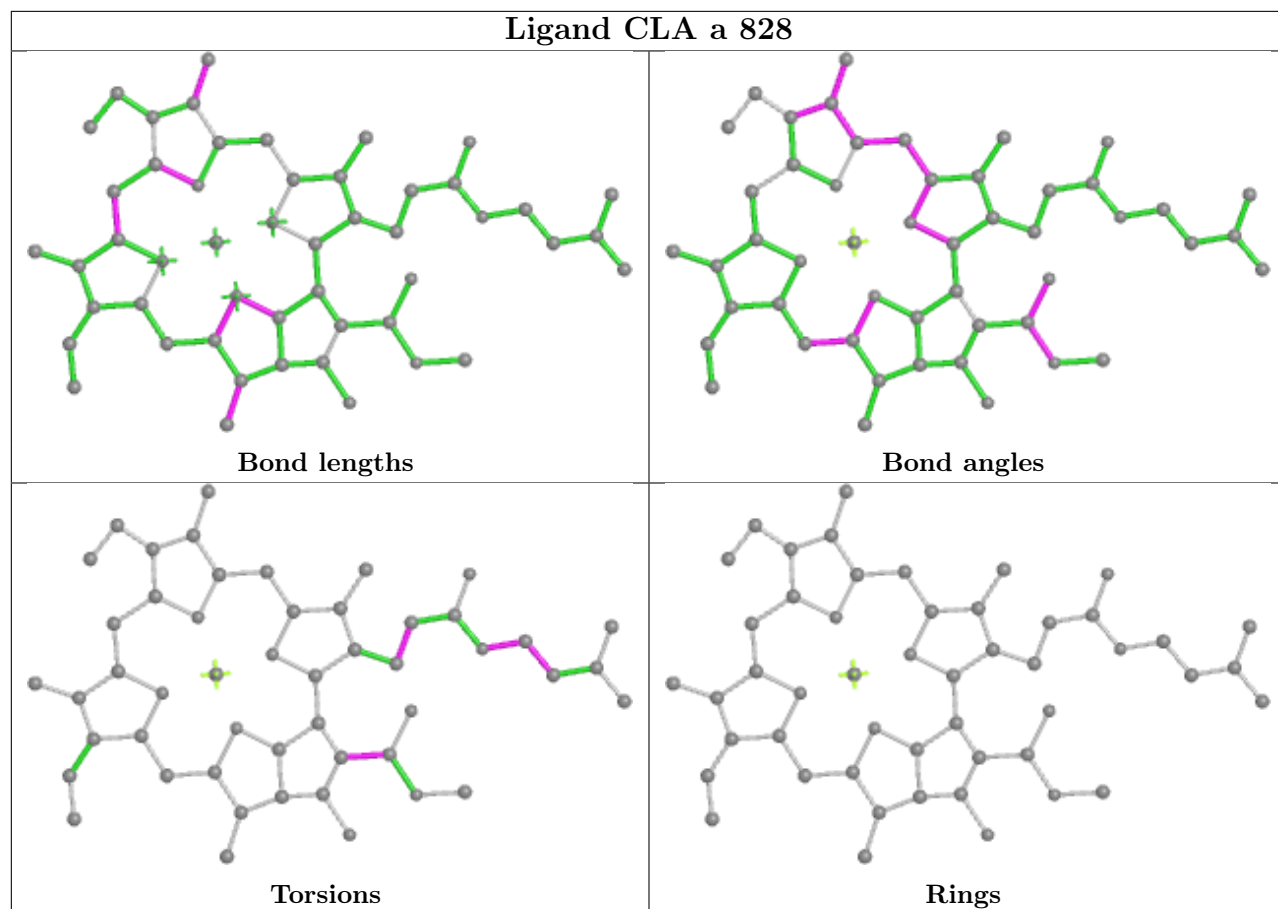


Torsions

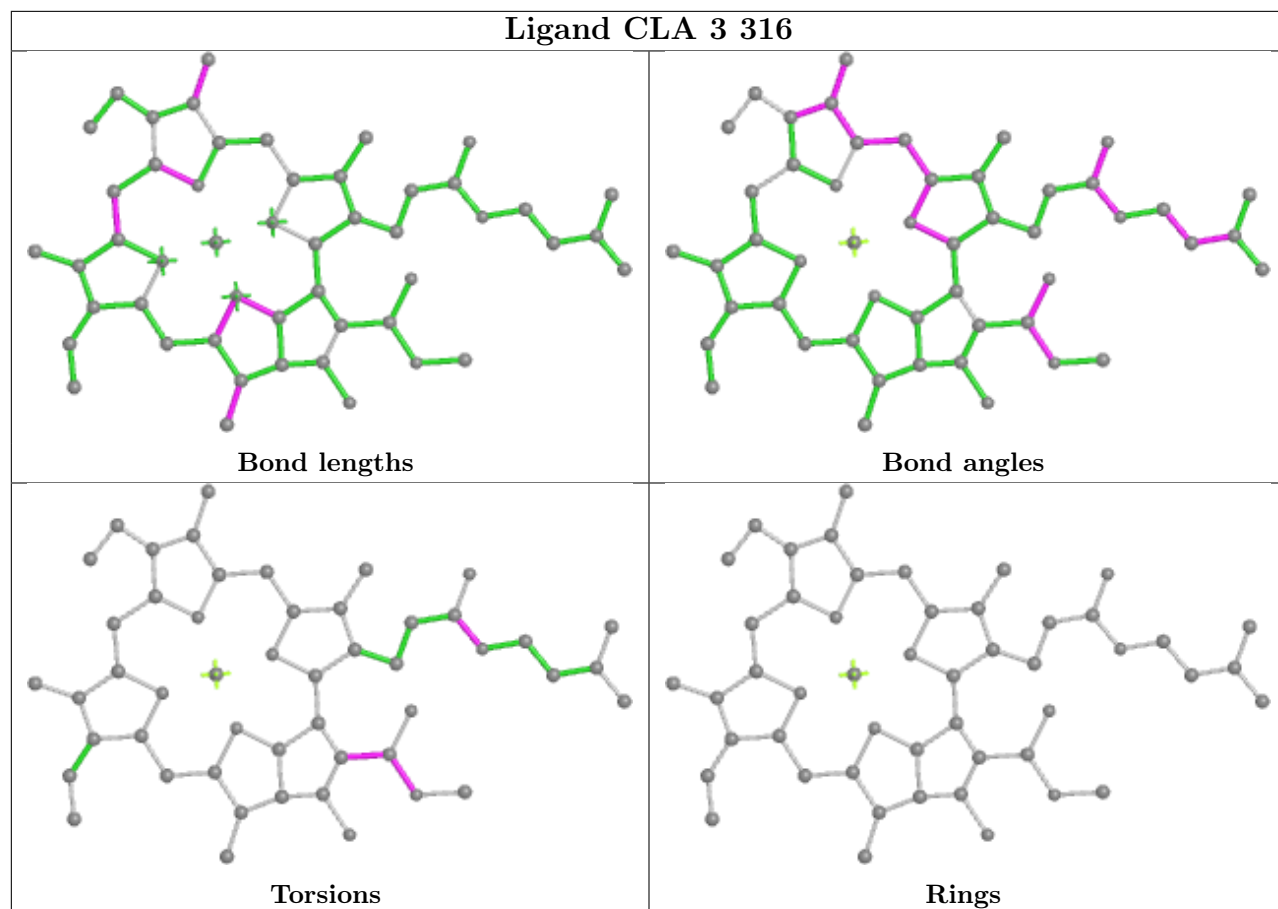


Rings

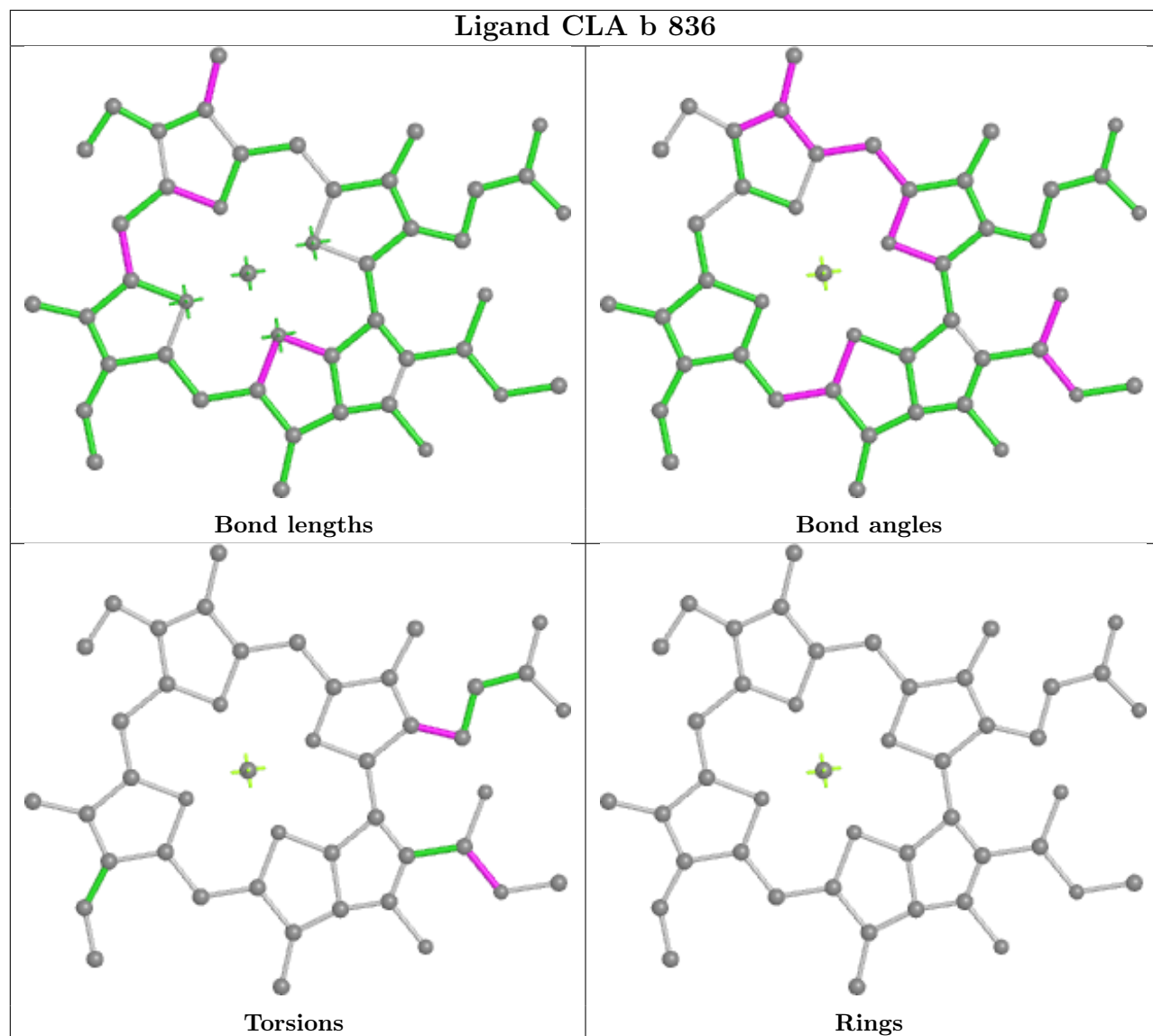
## Ligand CLA a 828



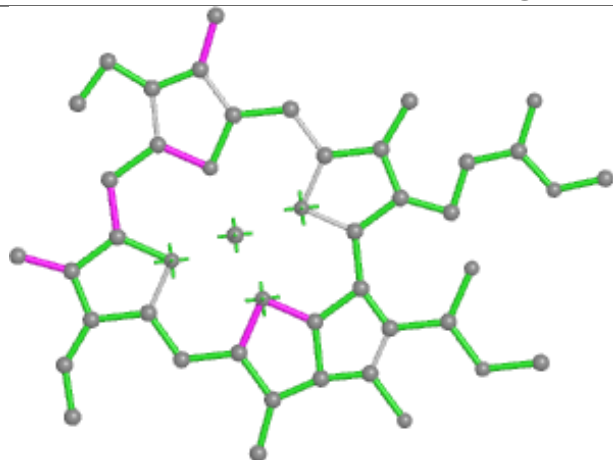
## Ligand CLA 3 316



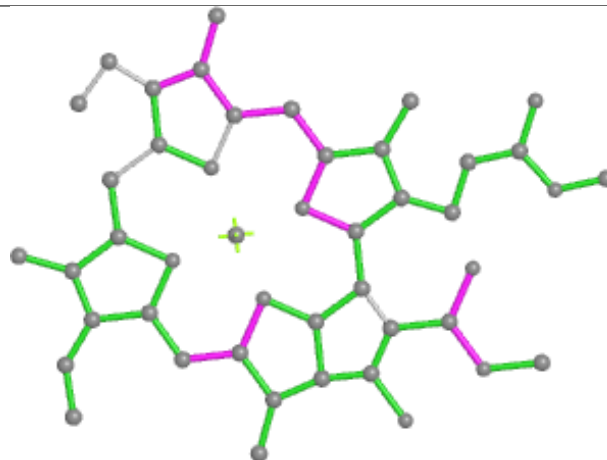
## Ligand CLA b 836



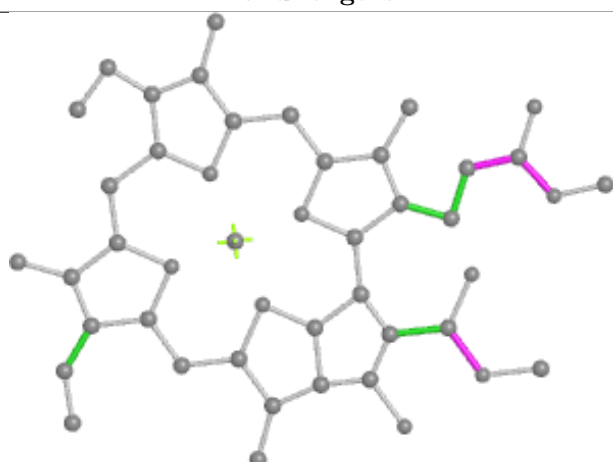
## Ligand CLA F 306



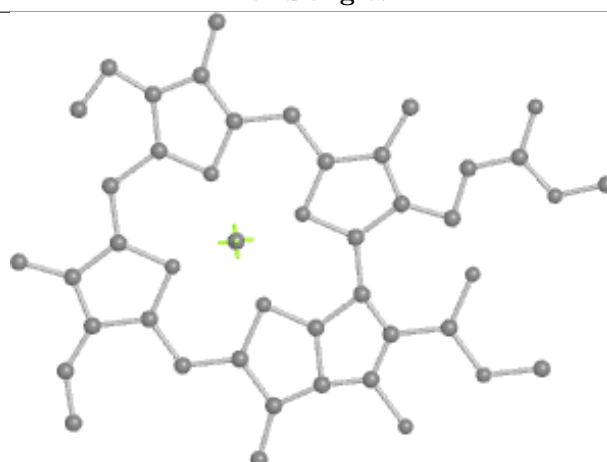
Bond lengths



Bond angles



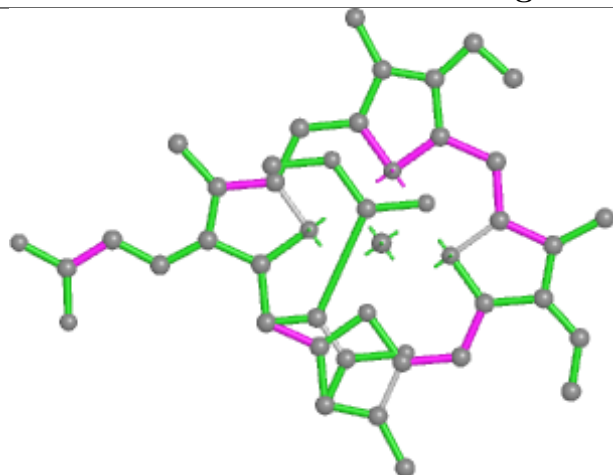
Torsions



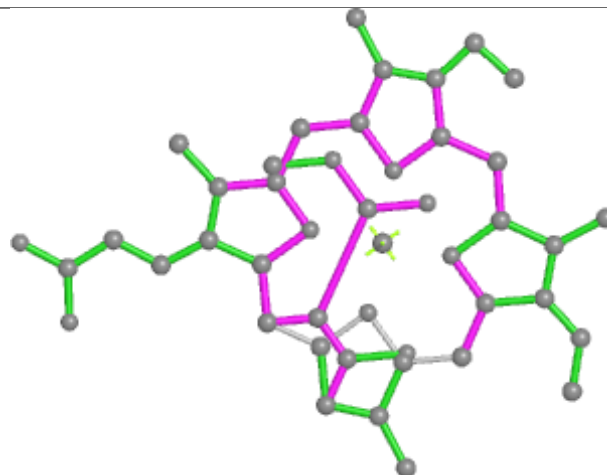
Rings



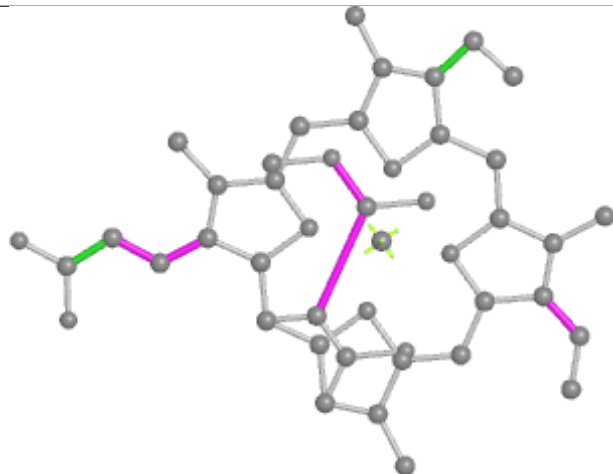
## Ligand KC2 V 315



Bond lengths



Bond angles

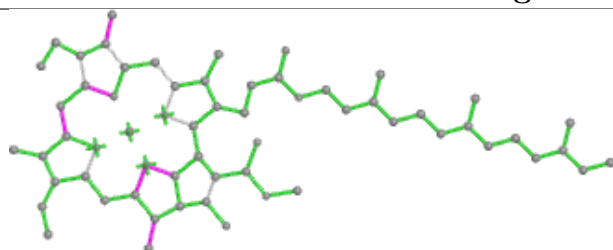


Torsions

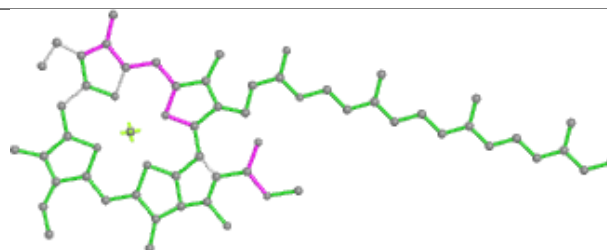


Rings

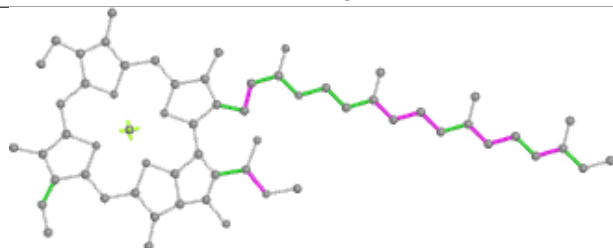
## Ligand CLA A 306



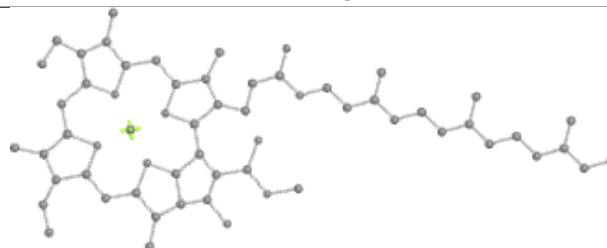
Bond lengths



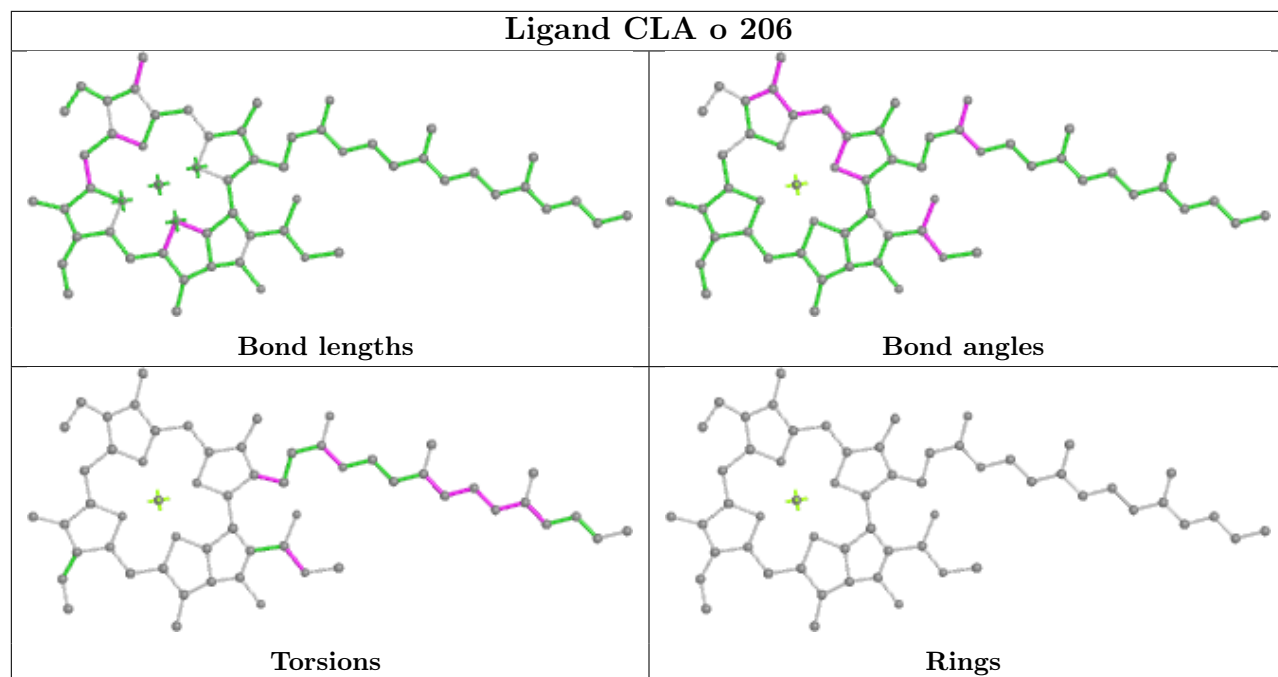
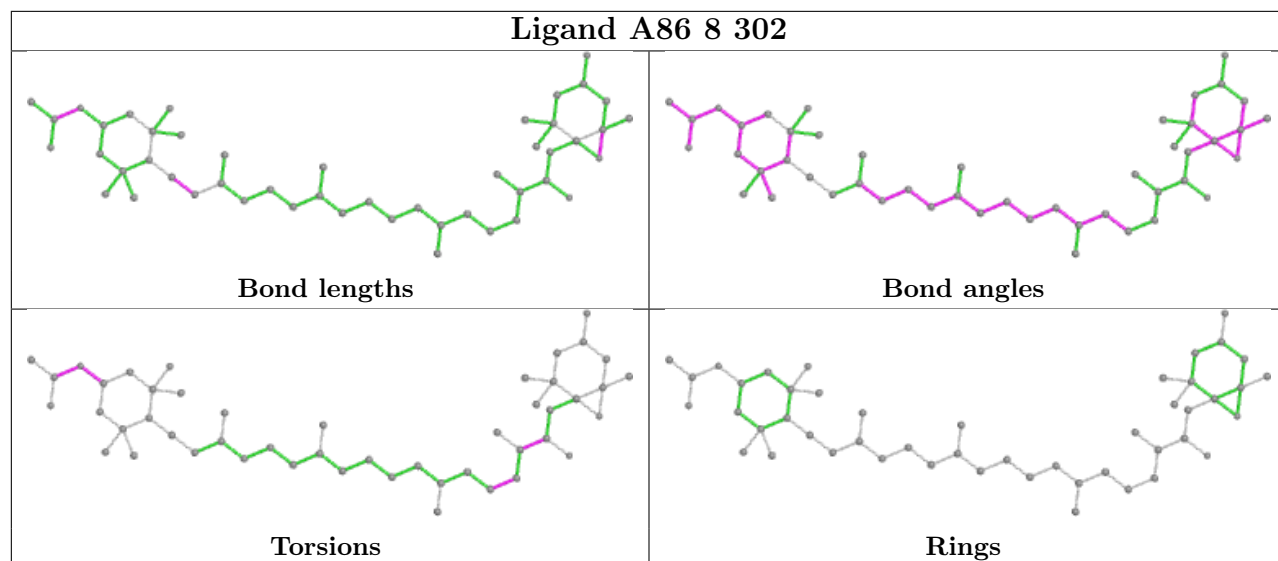
Bond angles



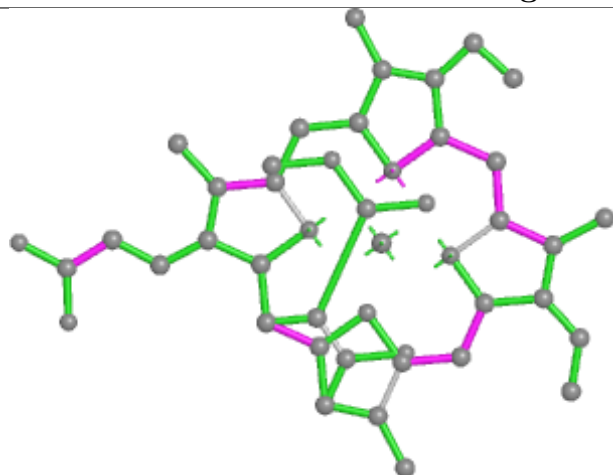
Torsions



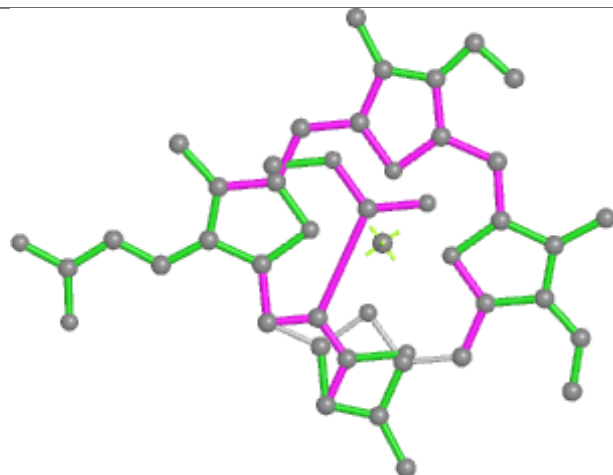
Rings

**Ligand CLA o 206****Ligand A86 8 302**

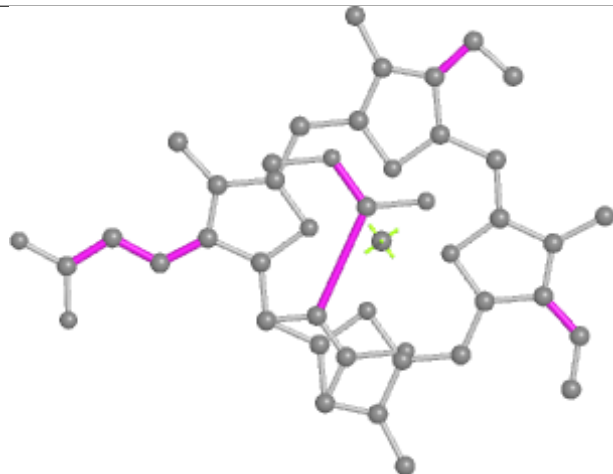
## Ligand KC2 8 319



Bond lengths



Bond angles

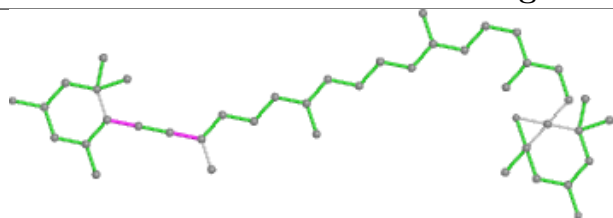


Torsions

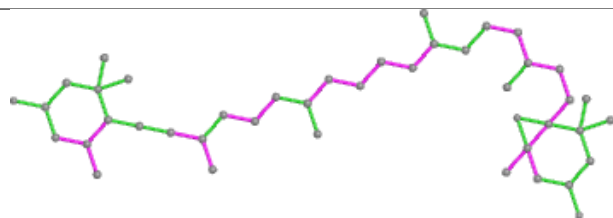


Rings

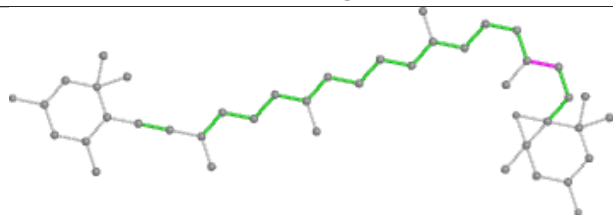
## Ligand DD6 o 204



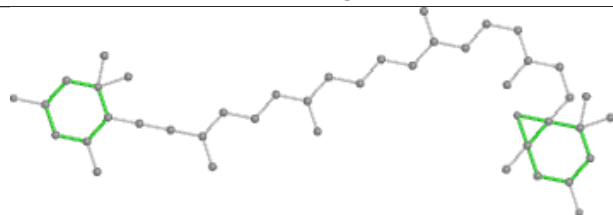
Bond lengths



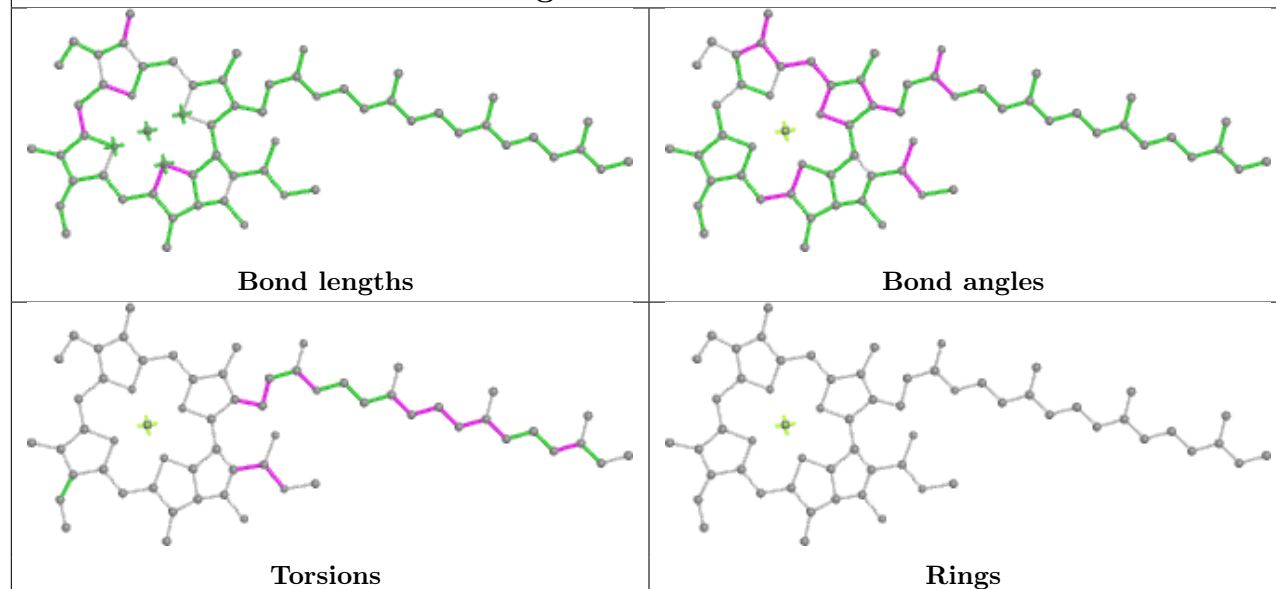
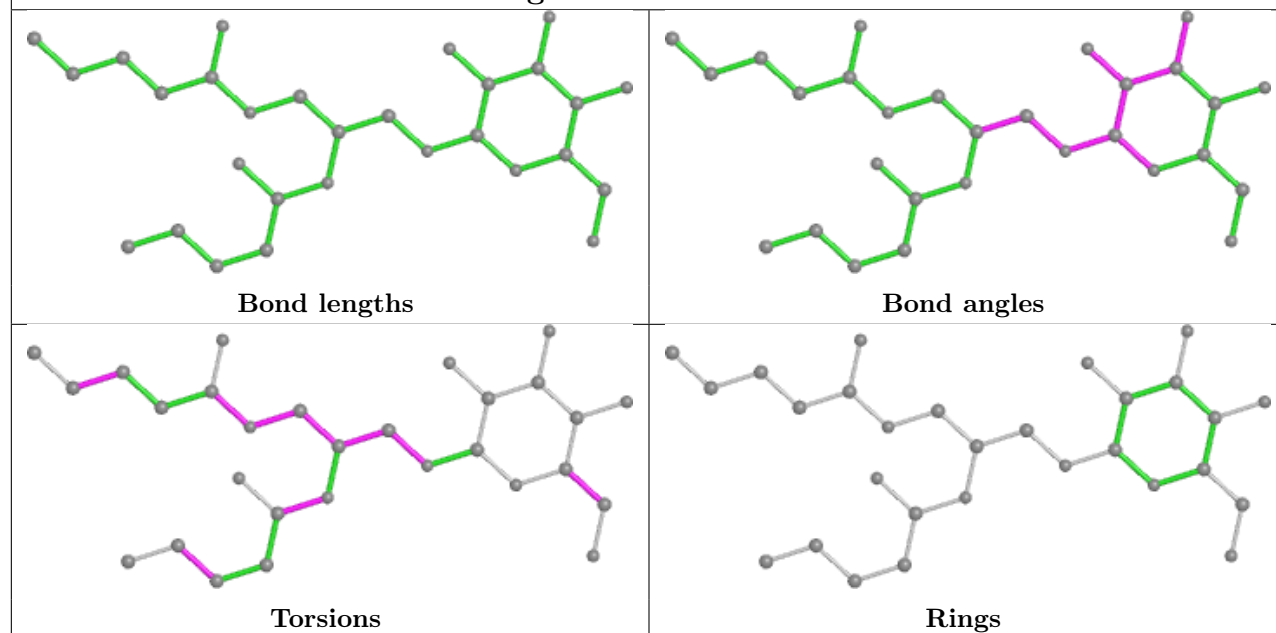
Bond angles



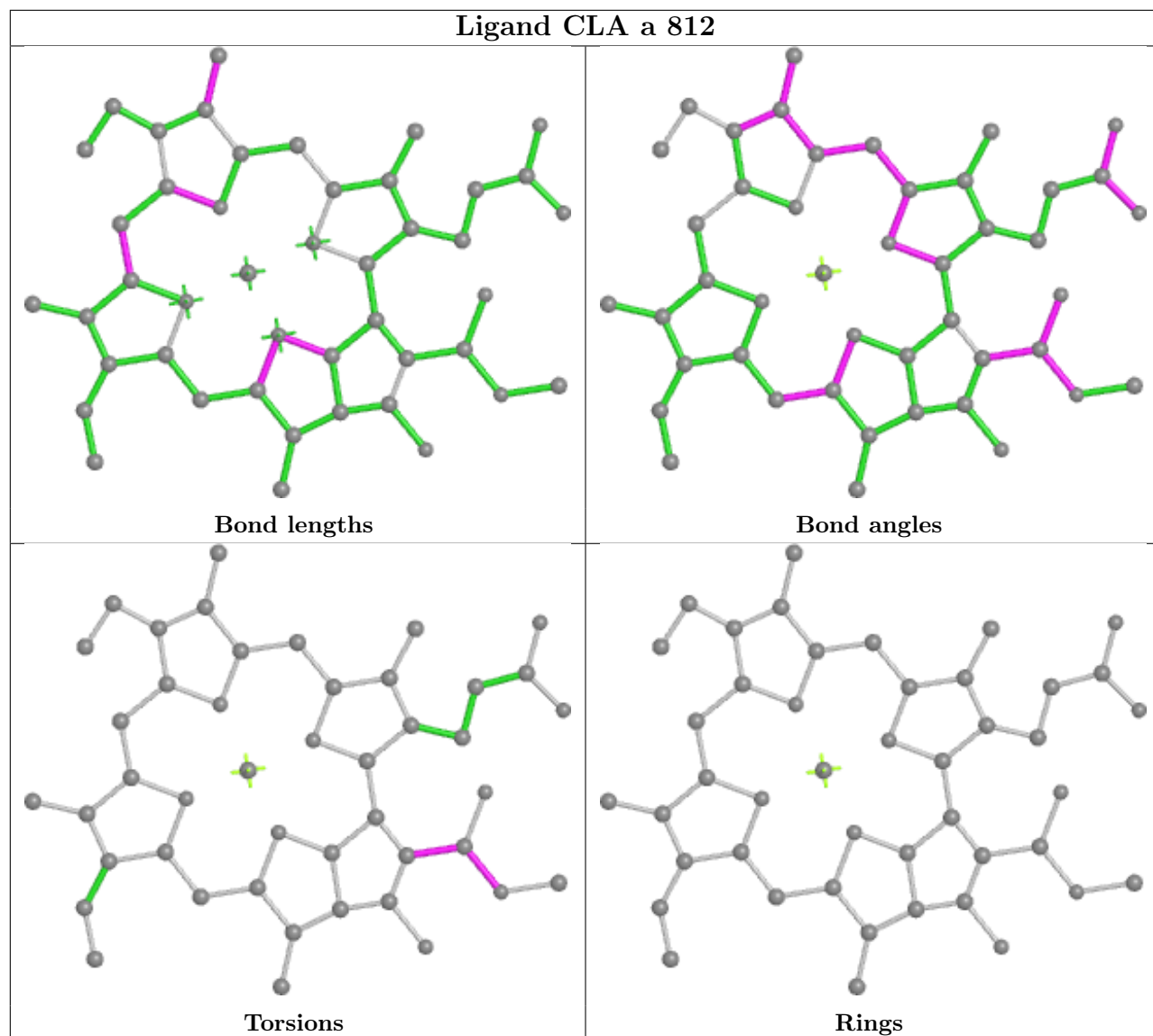
Torsions



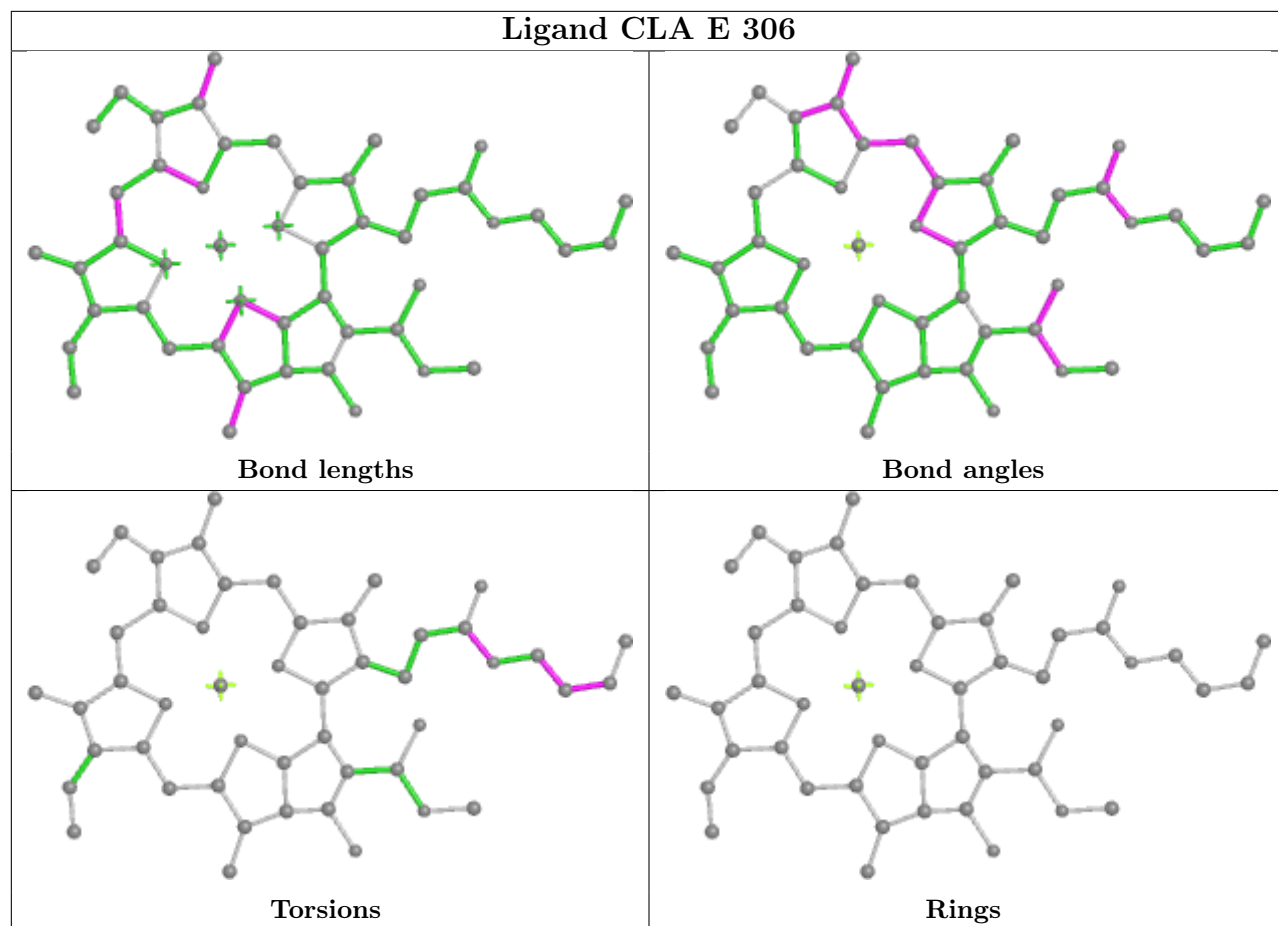
Rings

**Ligand CLA 7 313****Ligand LMG A 316**

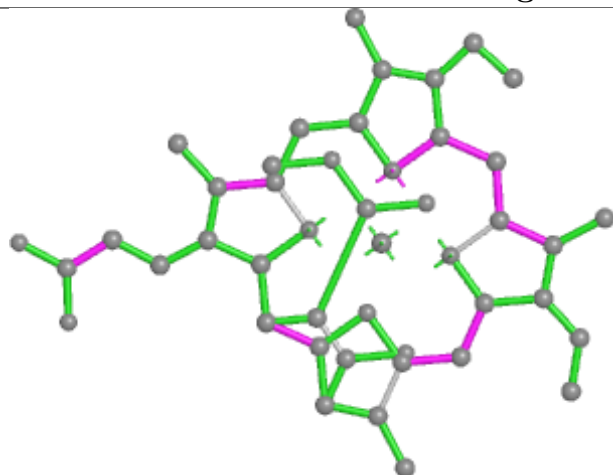
## Ligand CLA a 812



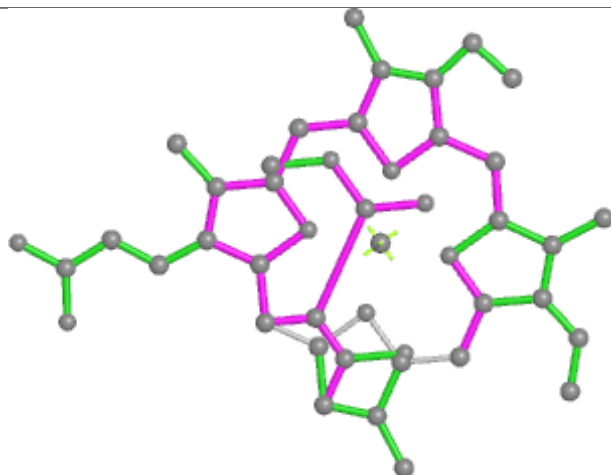
## Ligand CLA E 306



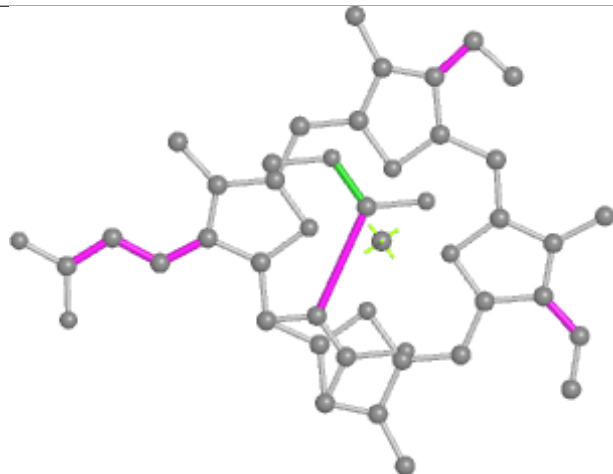
## Ligand KC2 P 320



Bond lengths



Bond angles

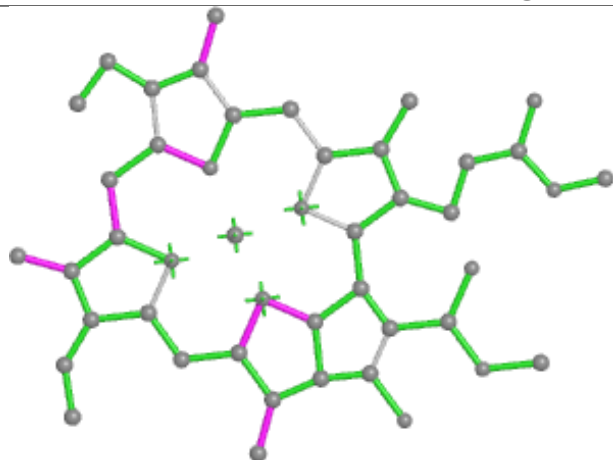


Torsions

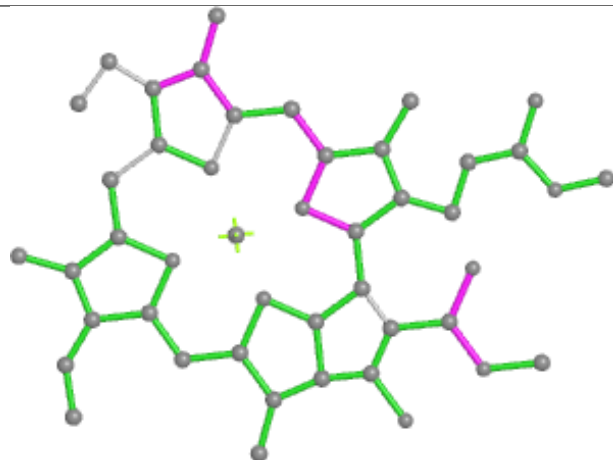


Rings

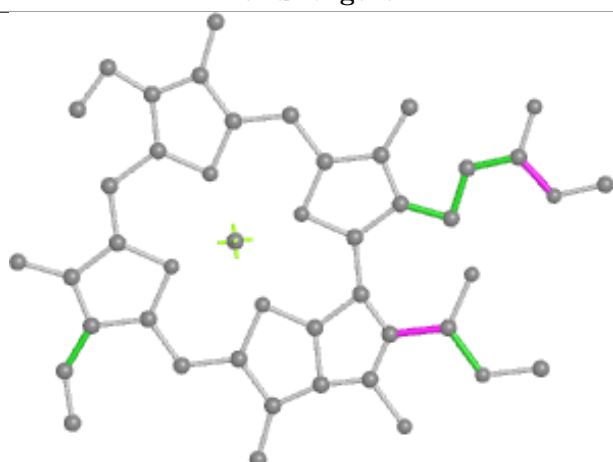
## Ligand CLA 7 318



Bond lengths



Bond angles

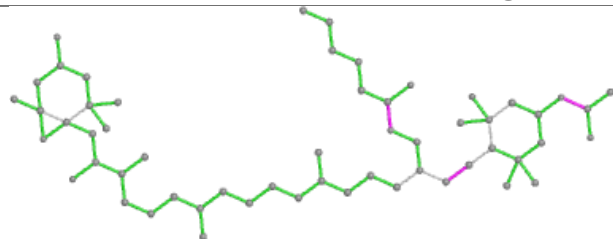


Torsions

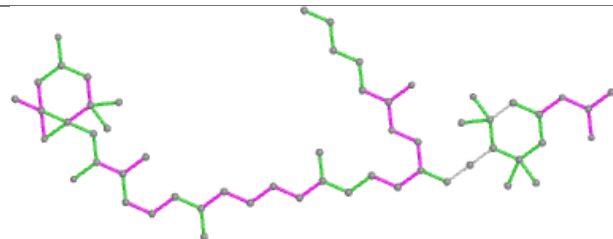


Rings

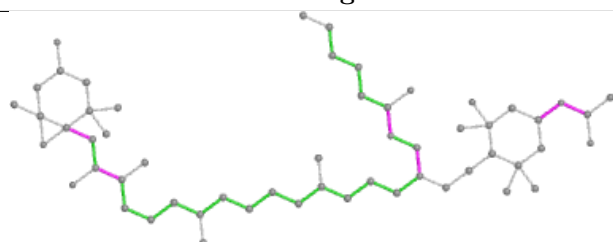
## Ligand A1EB1 1 301



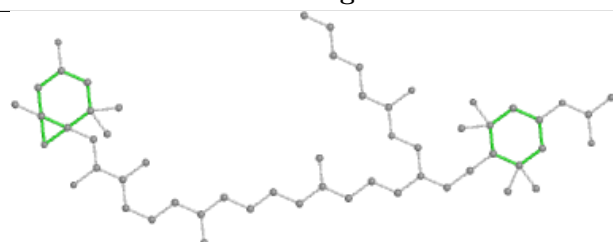
Bond lengths



Bond angles

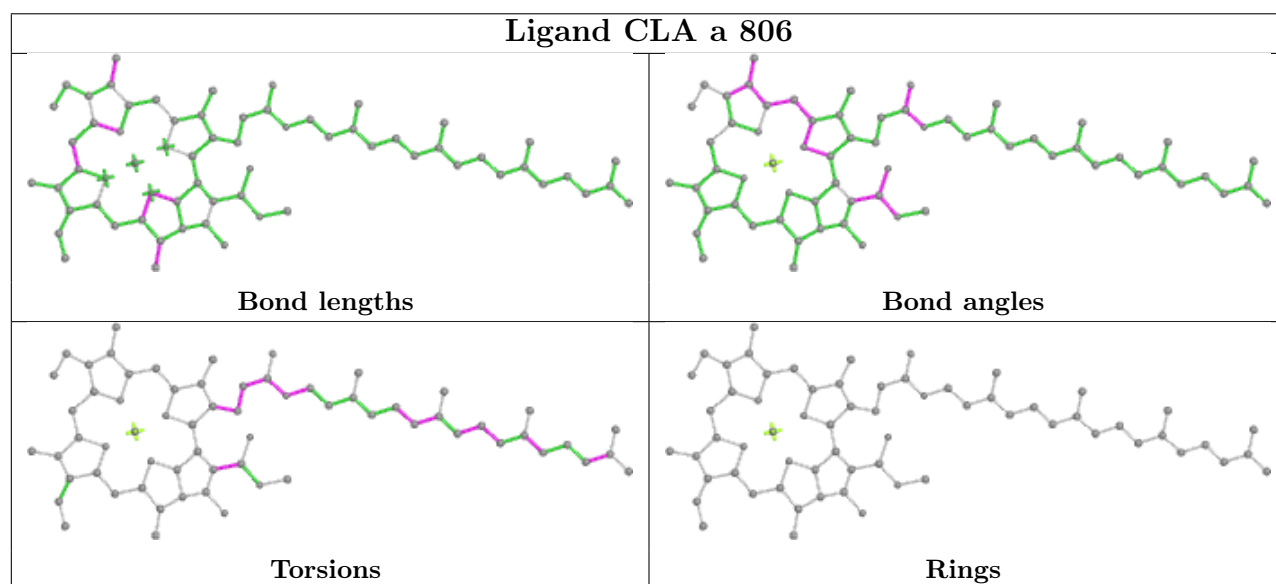
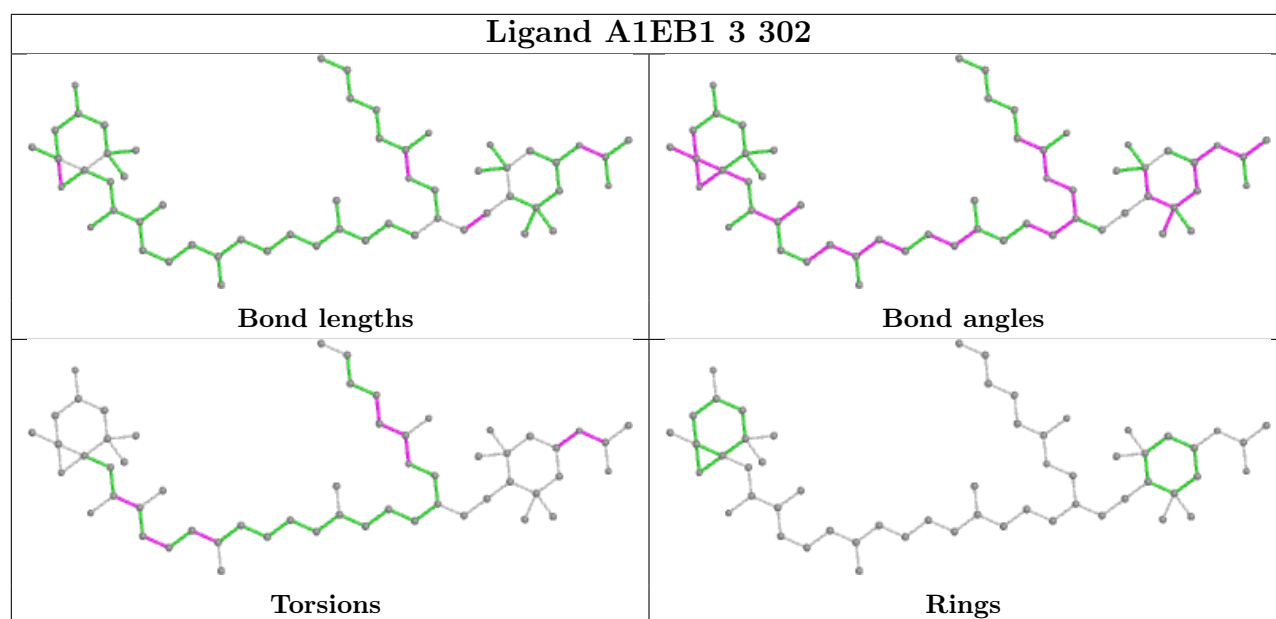


Torsions

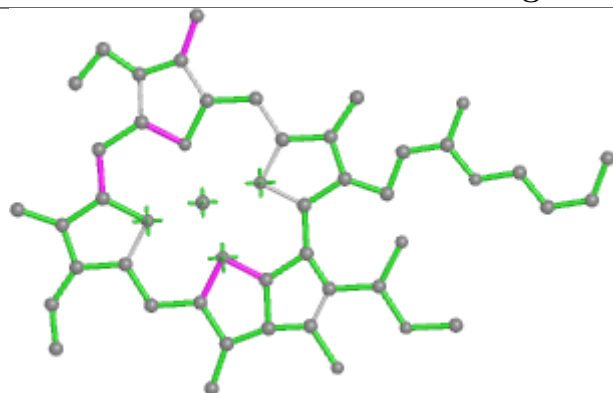


Rings

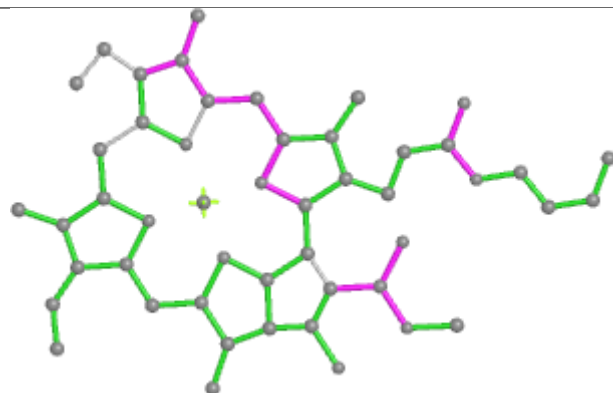




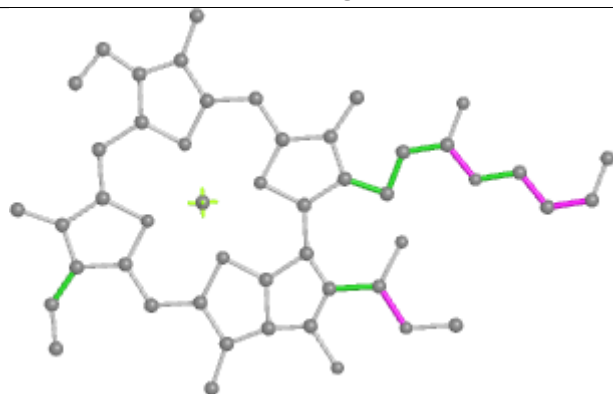
## Ligand CLA 1 203



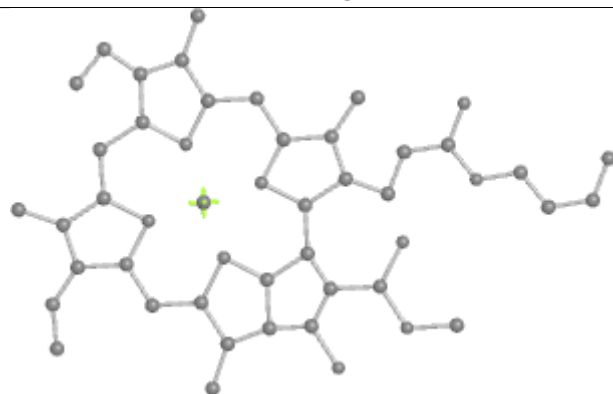
Bond lengths



Bond angles

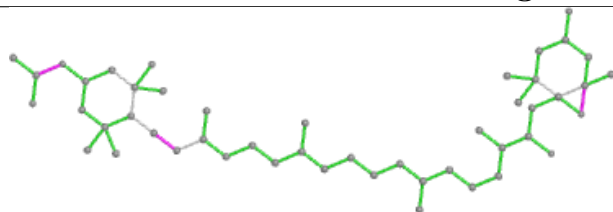


Torsions

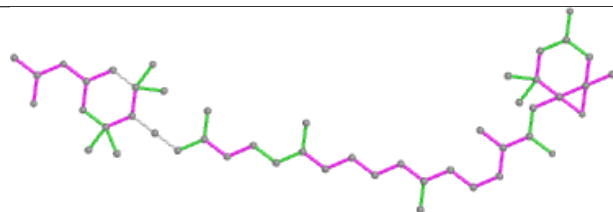


Rings

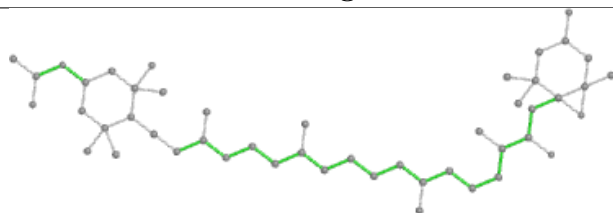
## Ligand A86 M 303



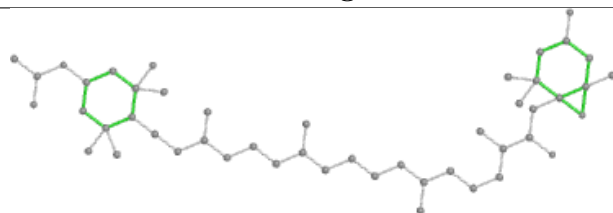
Bond lengths



Bond angles

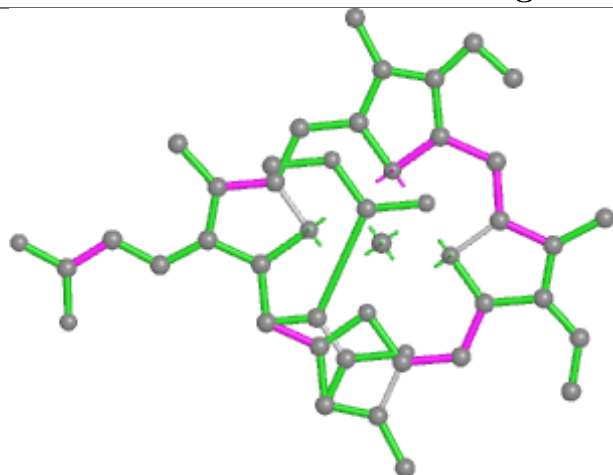


Torsions

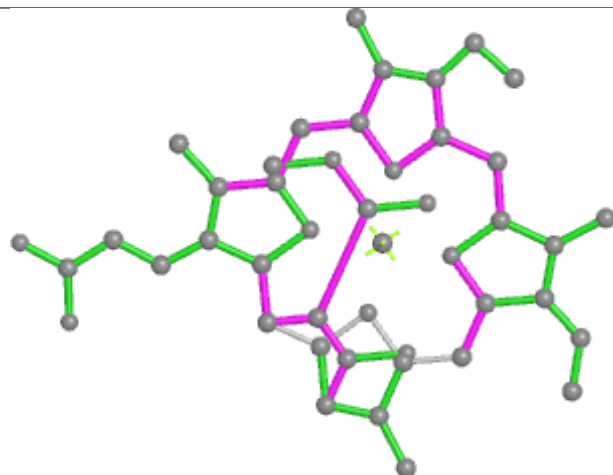


Rings

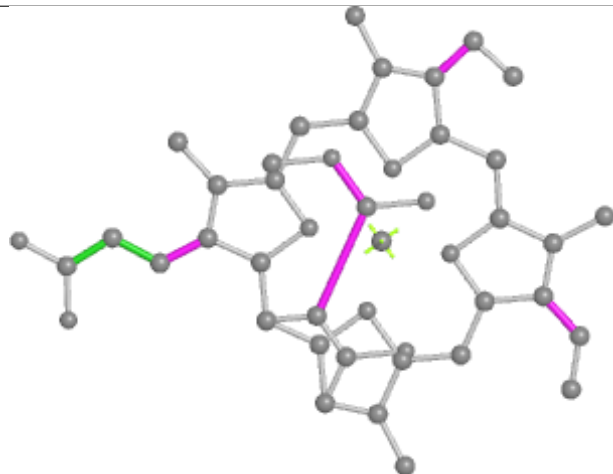
## Ligand KC2 R 306



Bond lengths



Bond angles

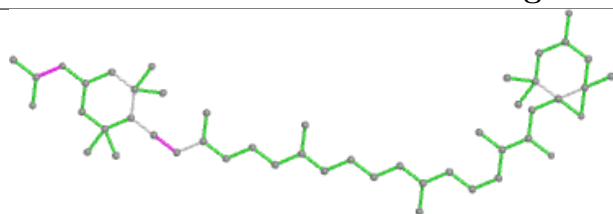


Torsions

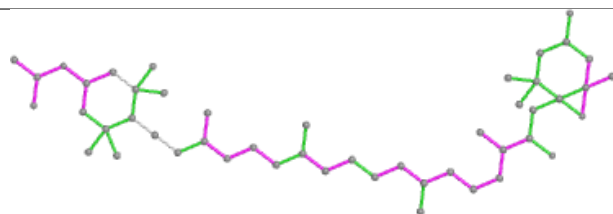


Rings

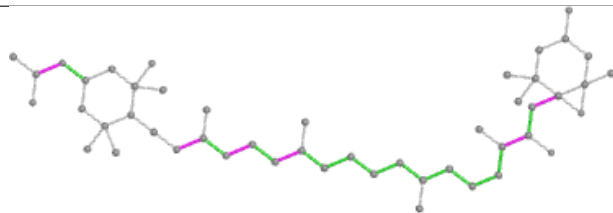
## Ligand A86 0 304



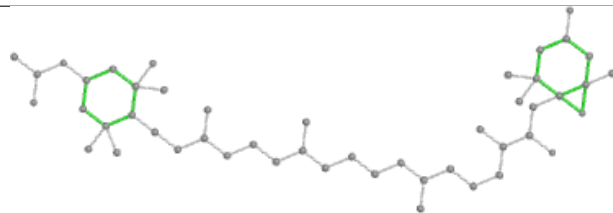
Bond lengths



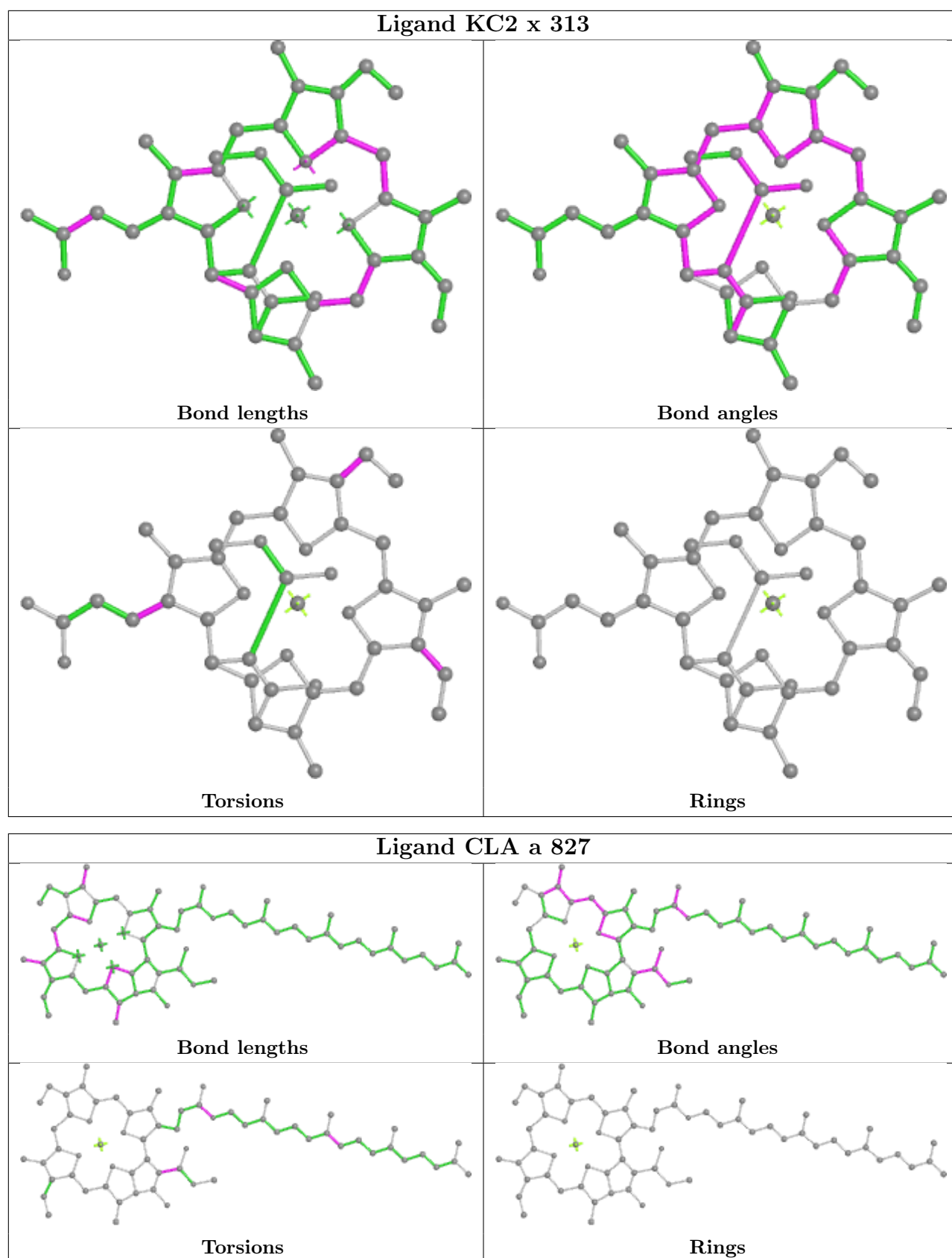
Bond angles



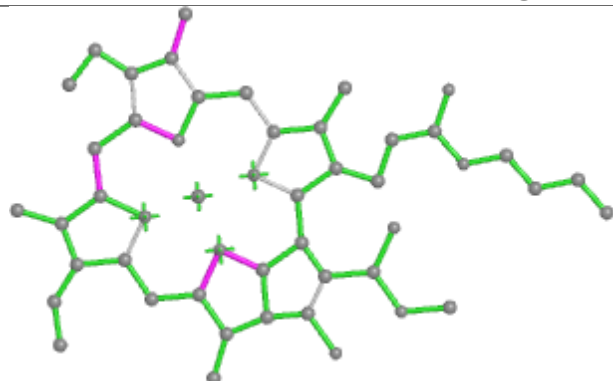
Torsions



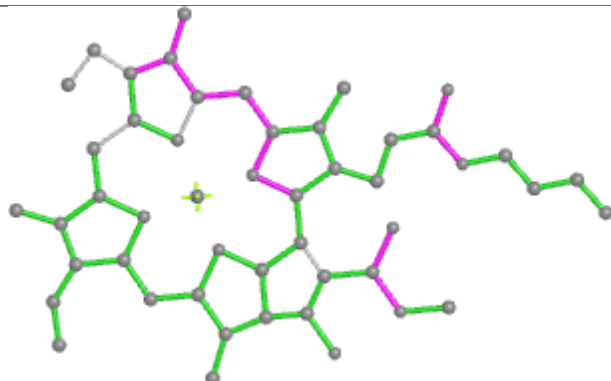
Rings



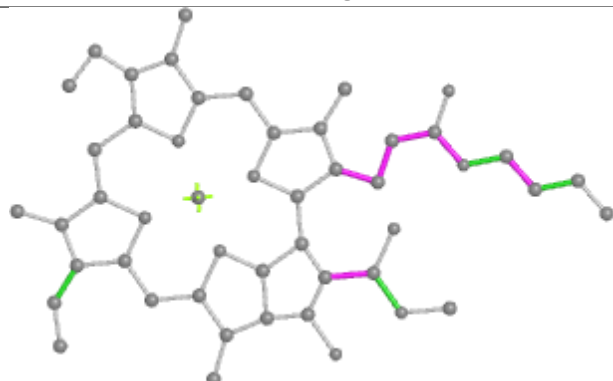
## Ligand CLA E 319



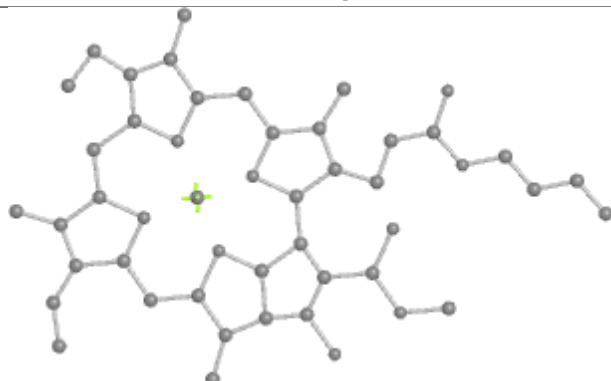
Bond lengths



Bond angles

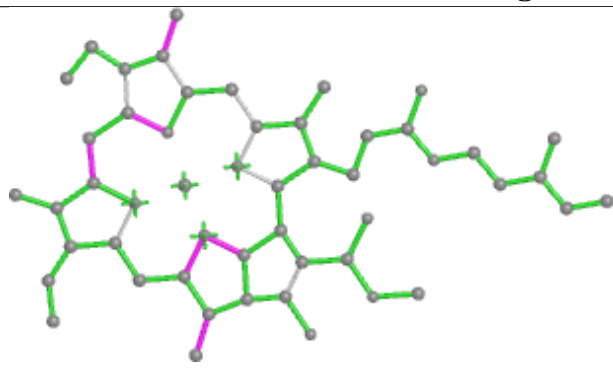


Torsions

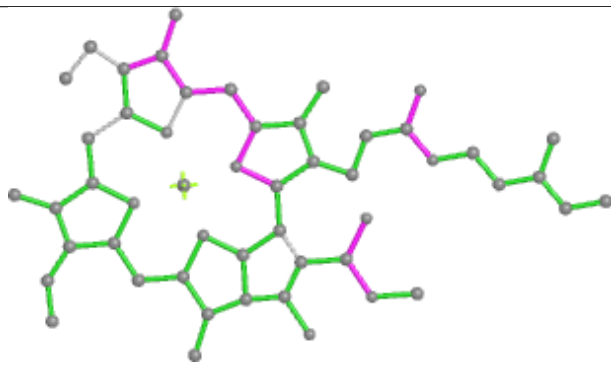


Rings

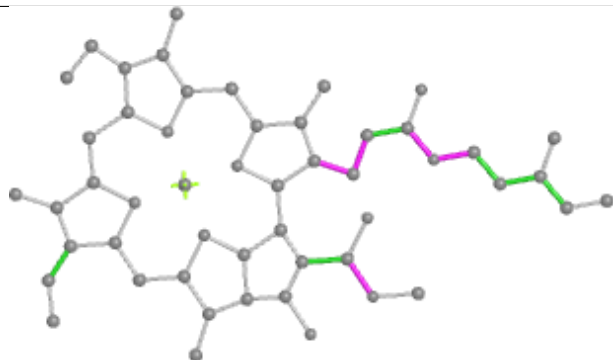
## Ligand CLA F 316



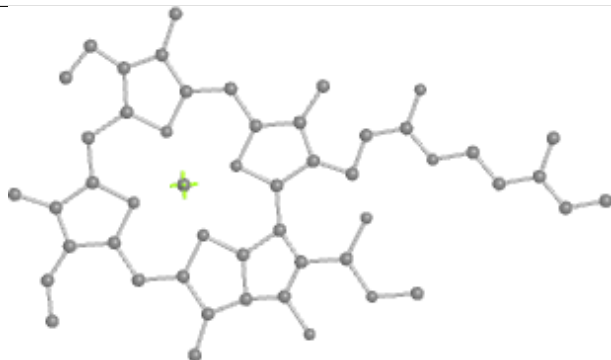
Bond lengths



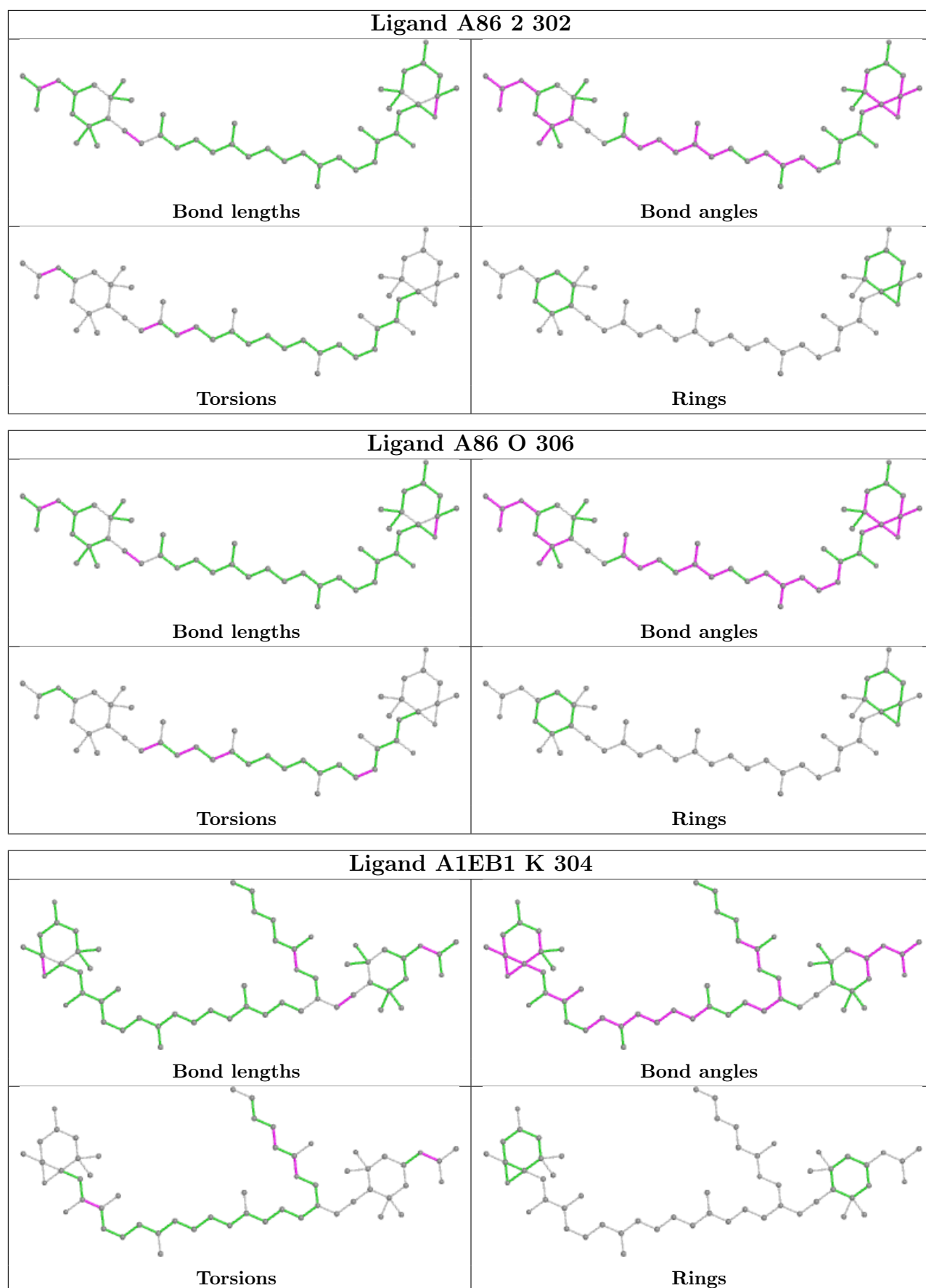
Bond angles

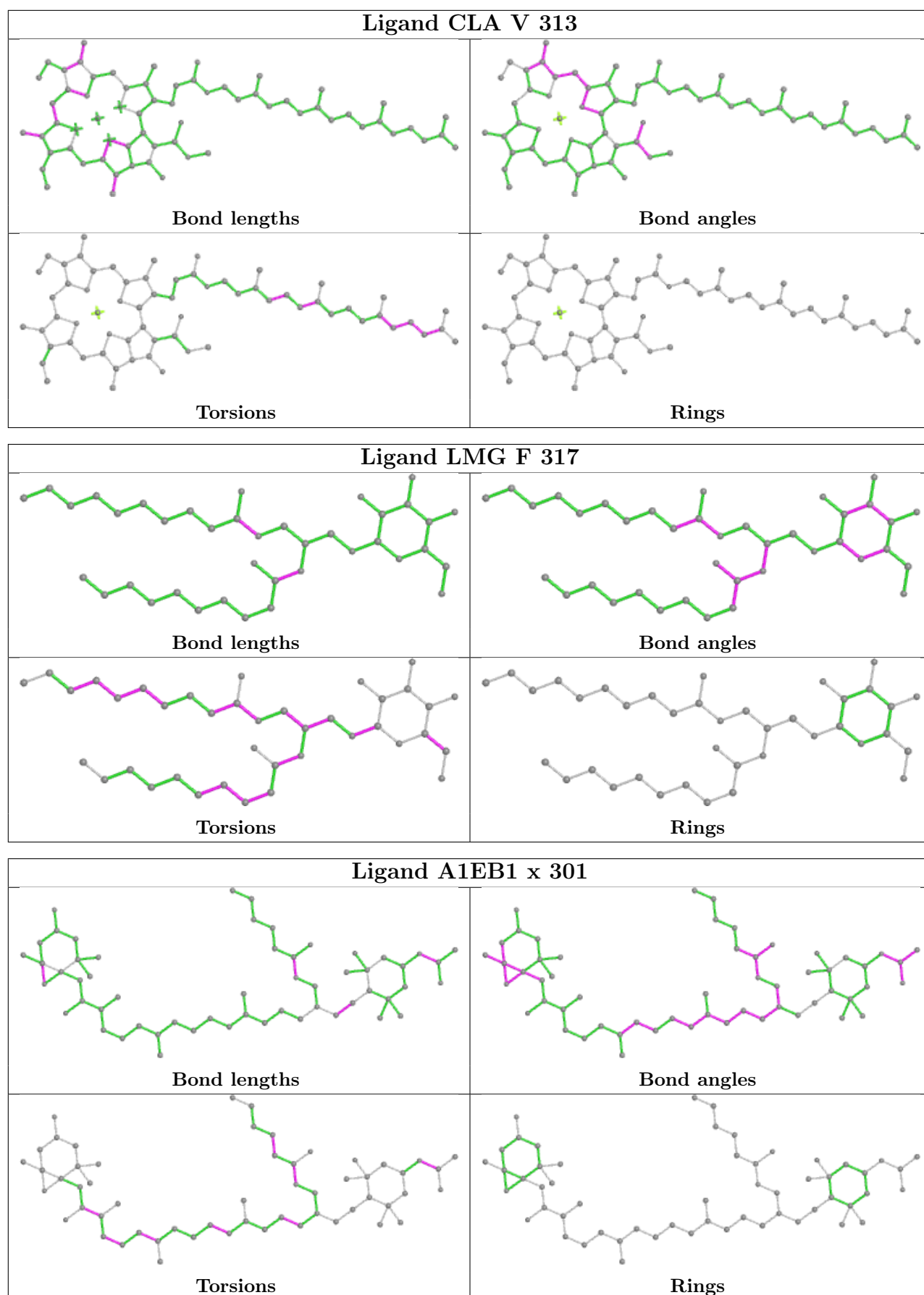


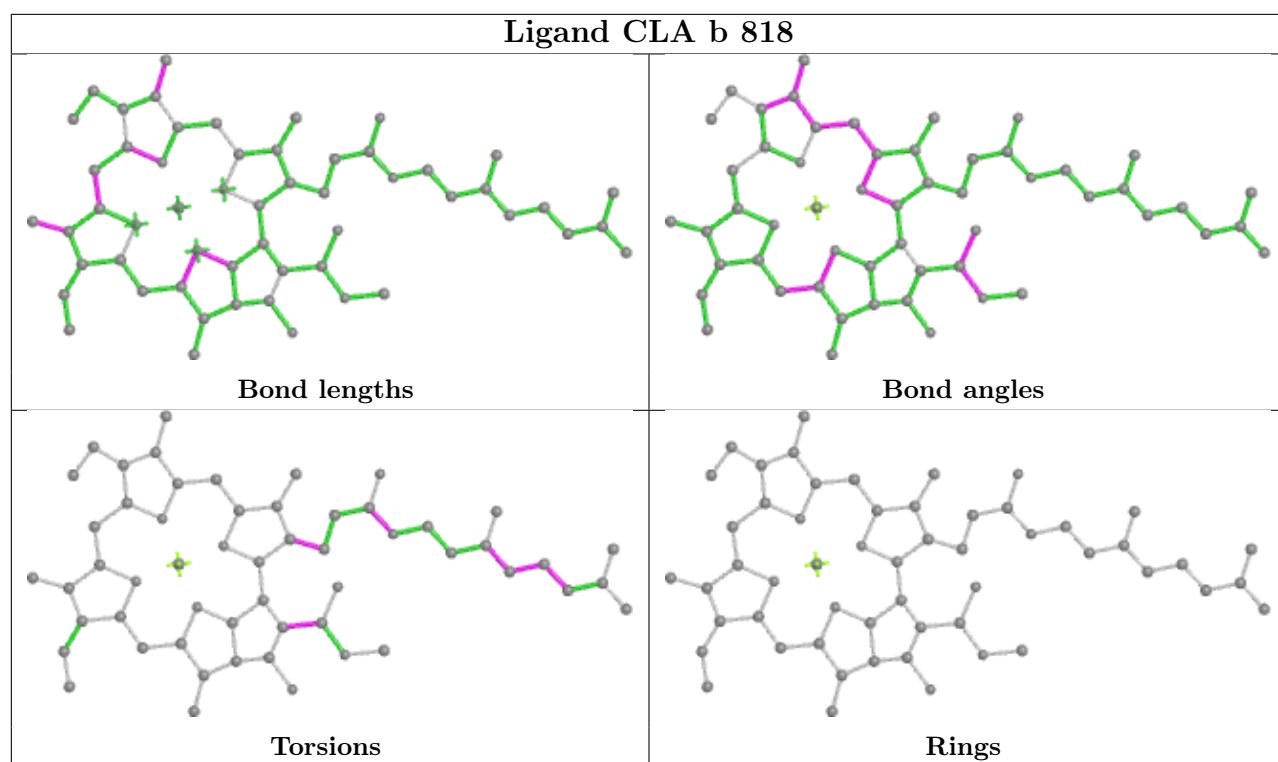
Torsions



Rings

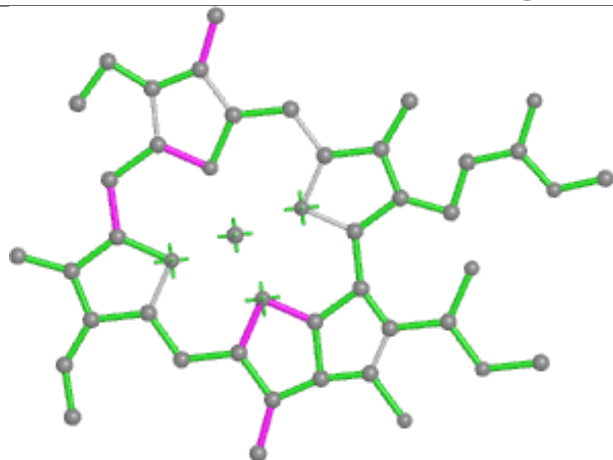




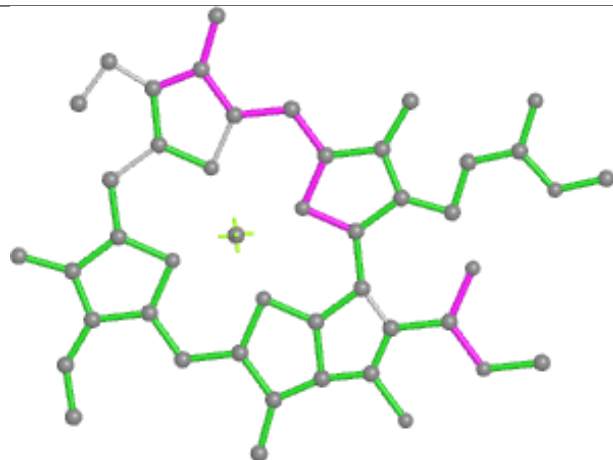




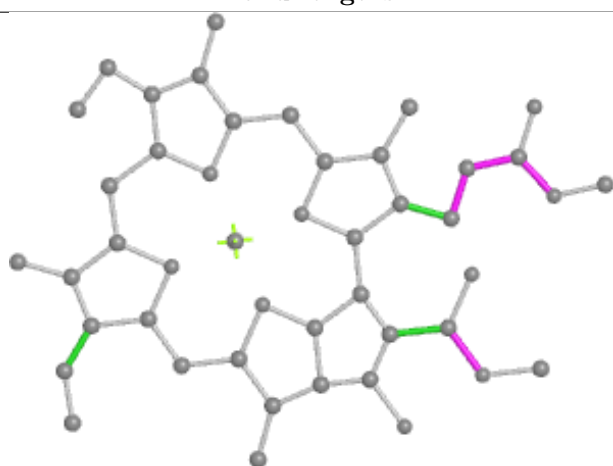
## Ligand CLA 2 309



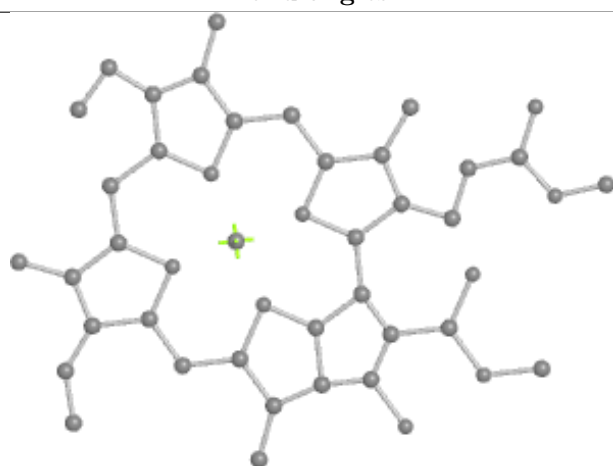
Bond lengths



Bond angles

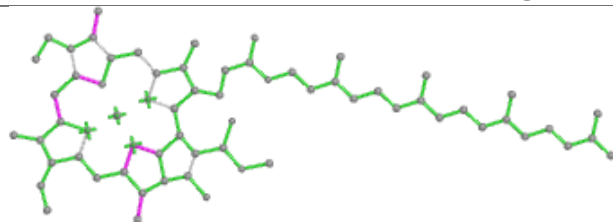


Torsions

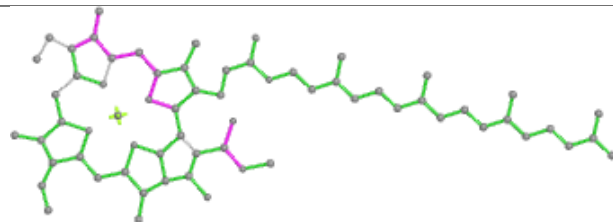


Rings

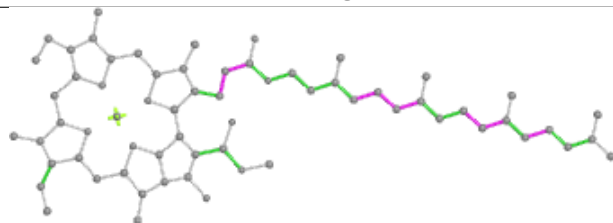
## Ligand CLA 7 316



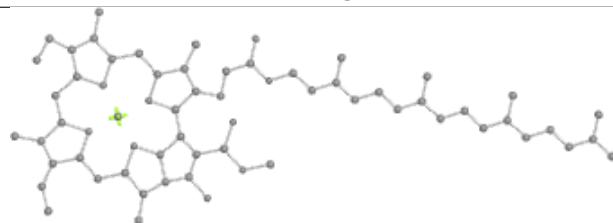
Bond lengths



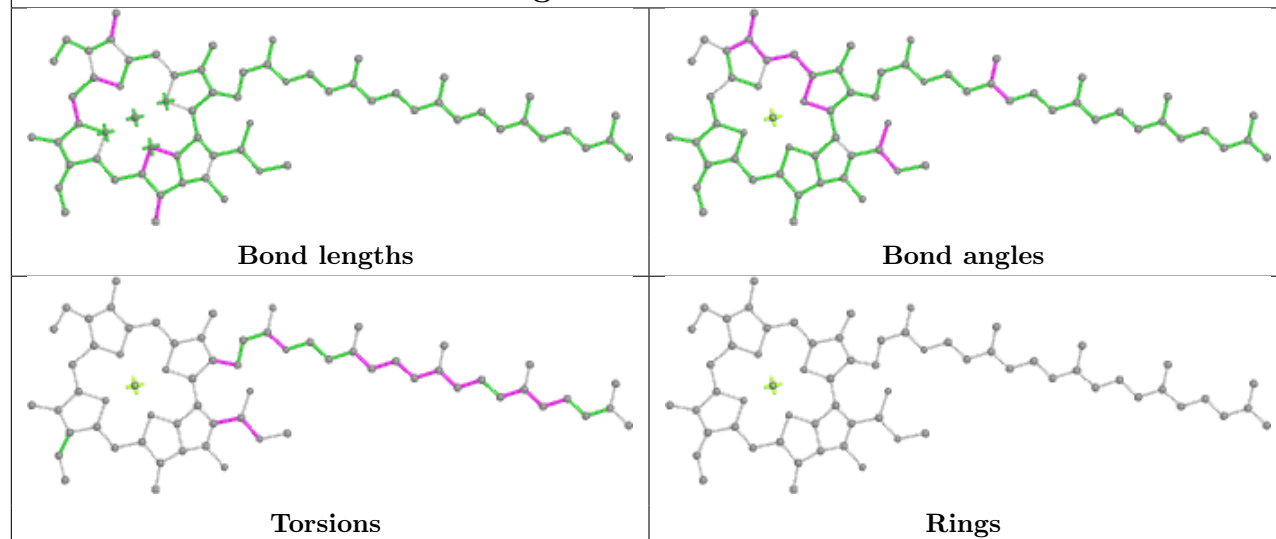
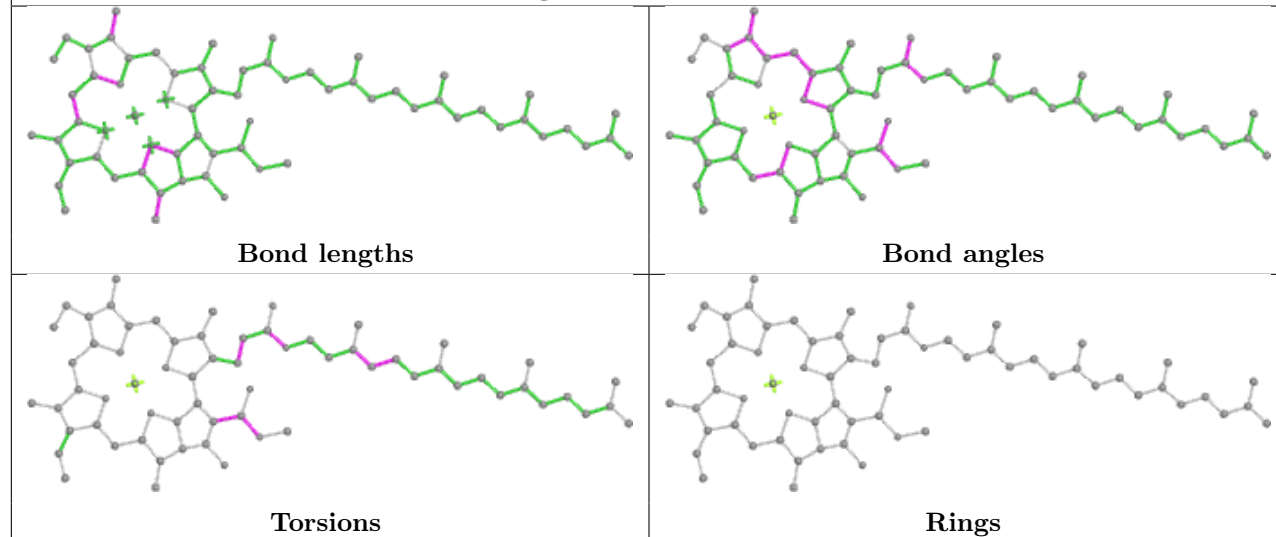
Bond angles



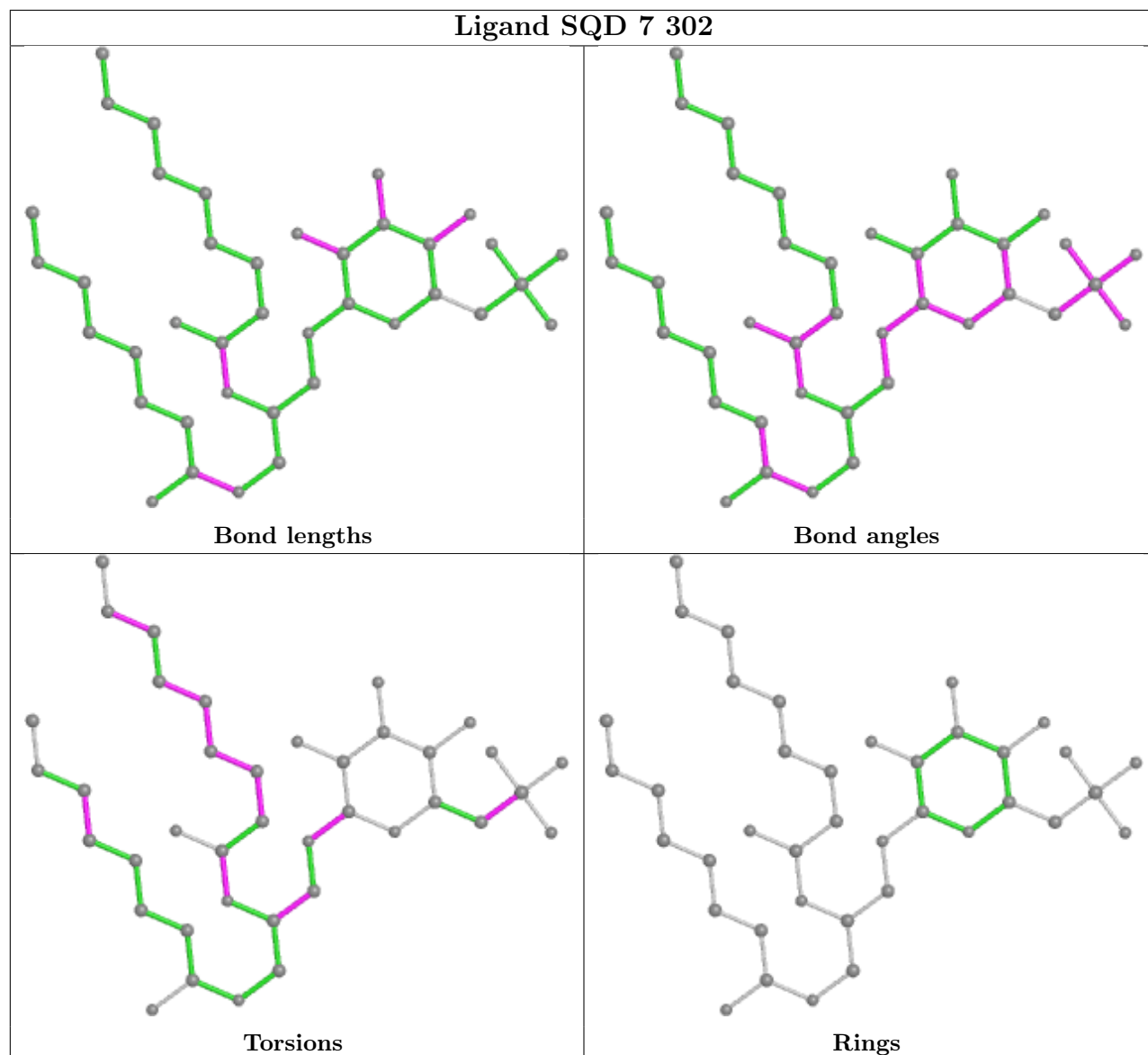
Torsions



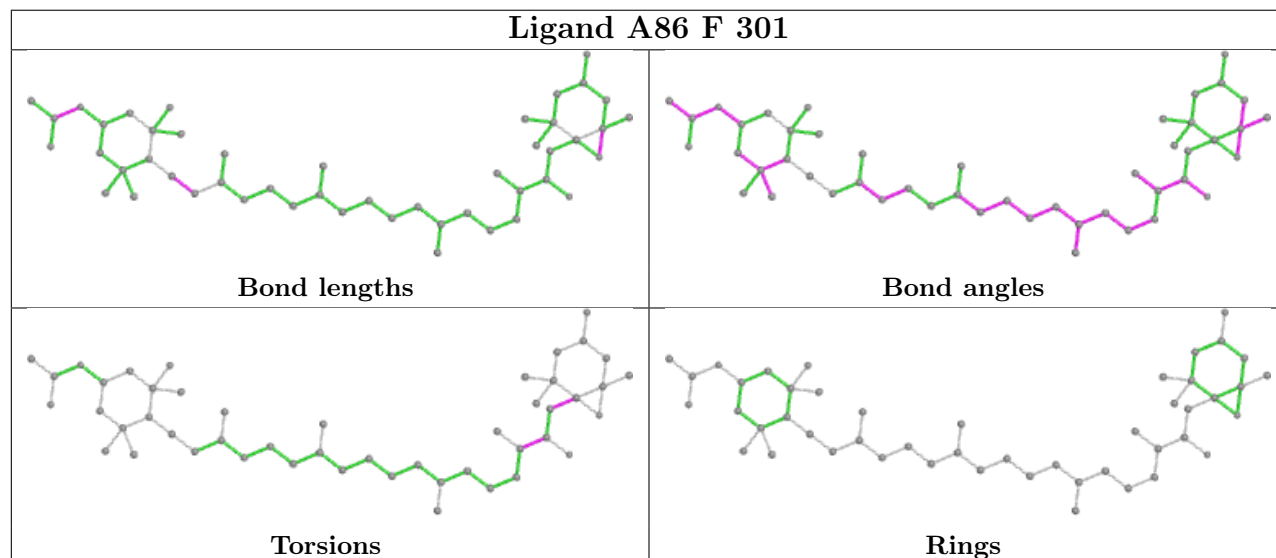
Rings

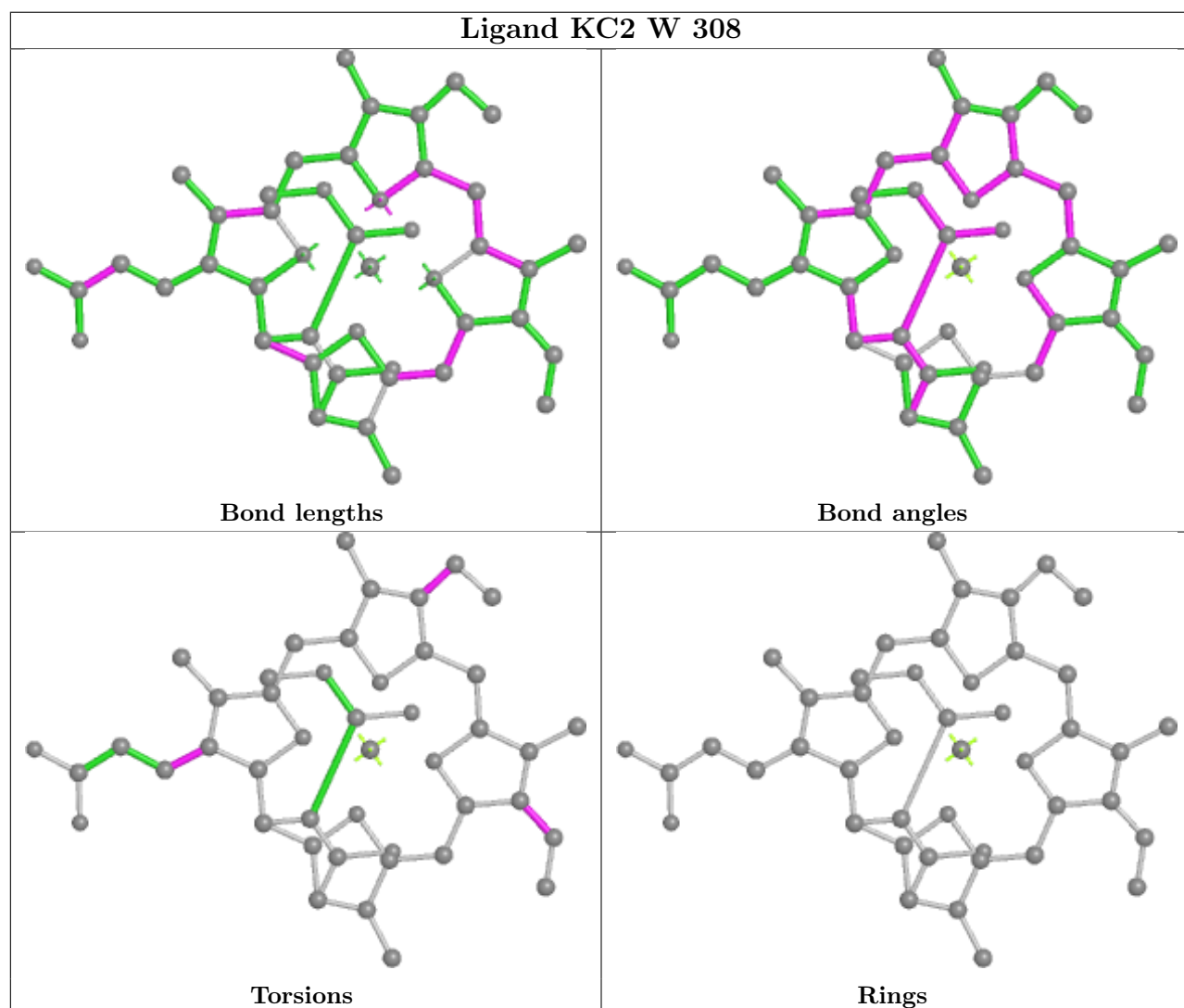
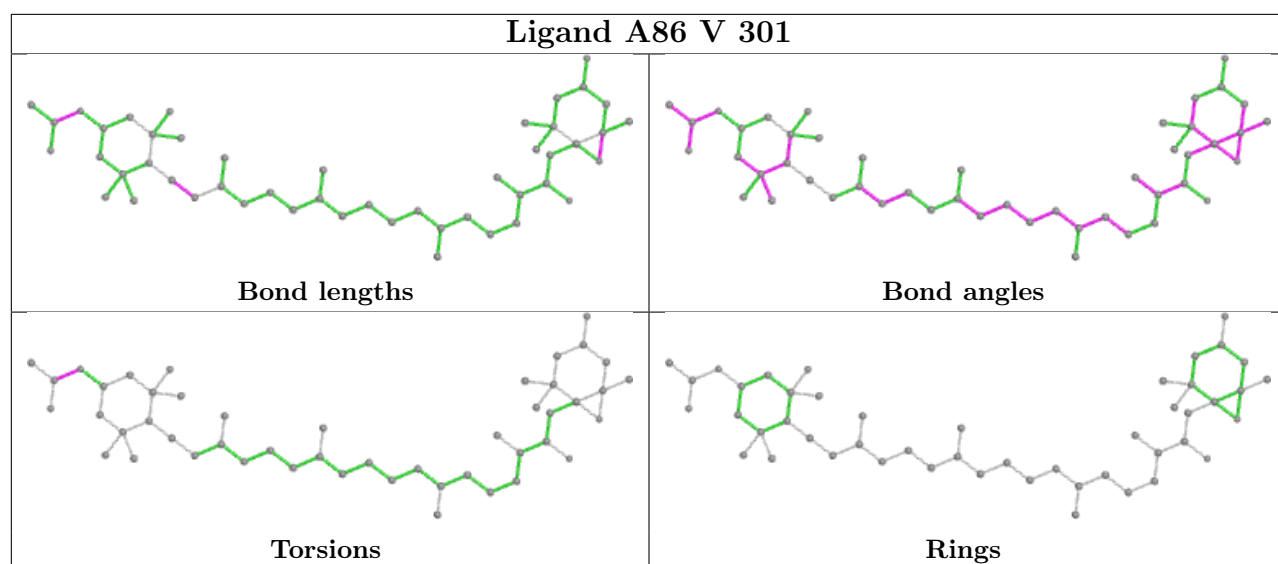
**Ligand CLA E 312****Ligand CLA b 805**

## Ligand SQD 7 302

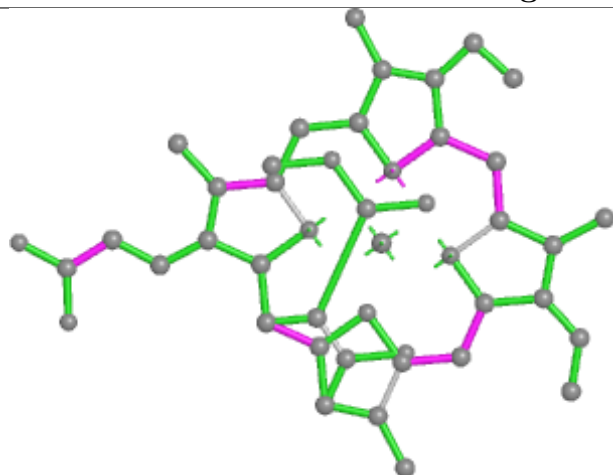


## Ligand A86 F 301

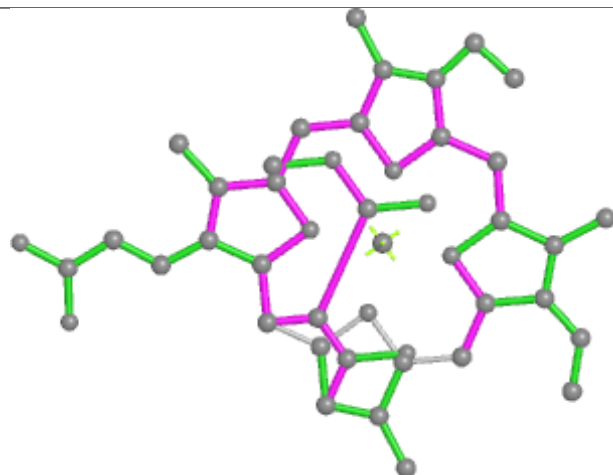




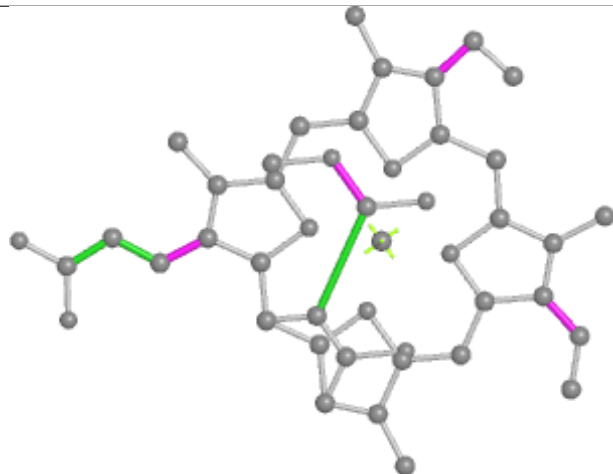
## Ligand KC2 5 305



Bond lengths



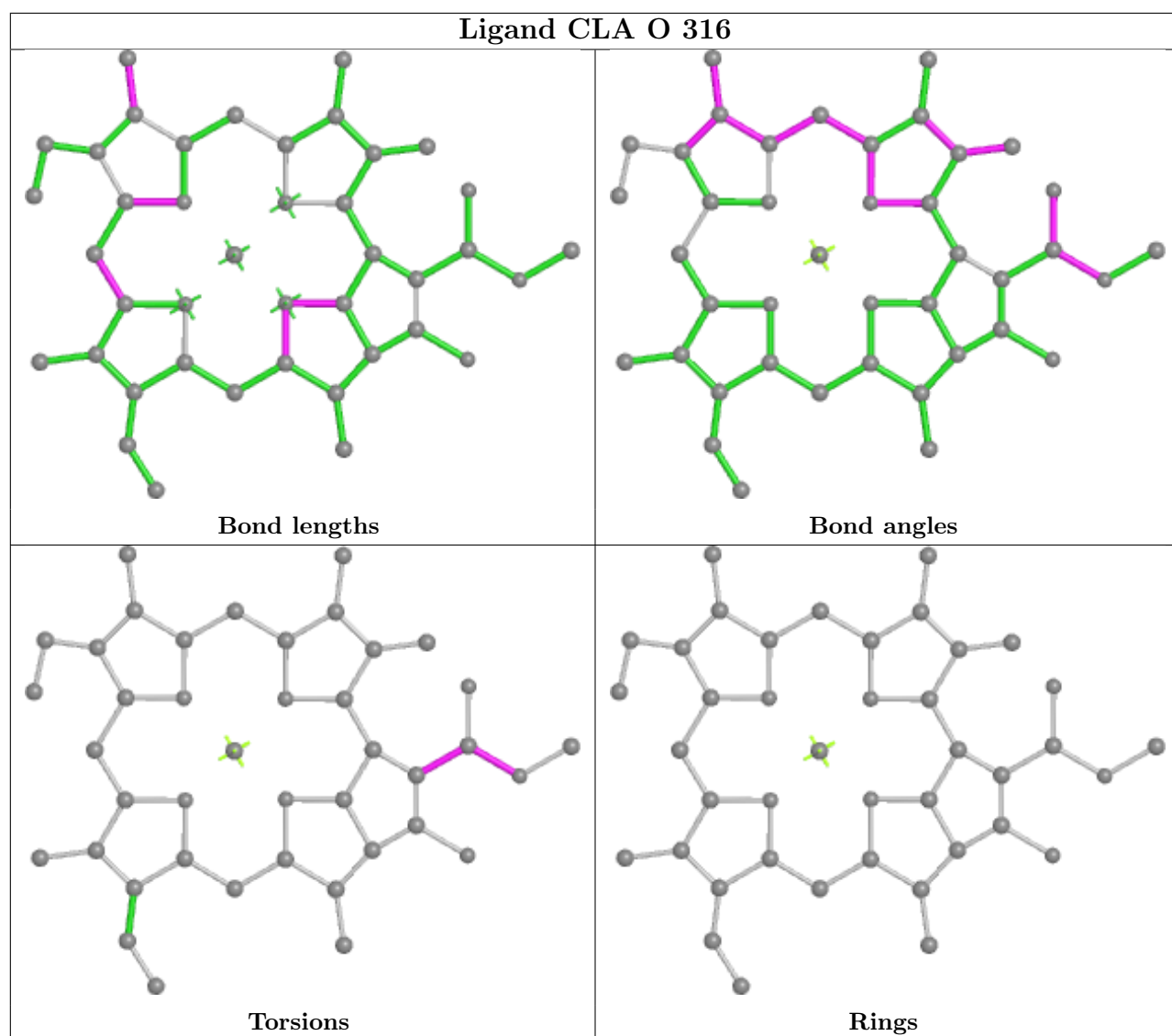
Bond angles

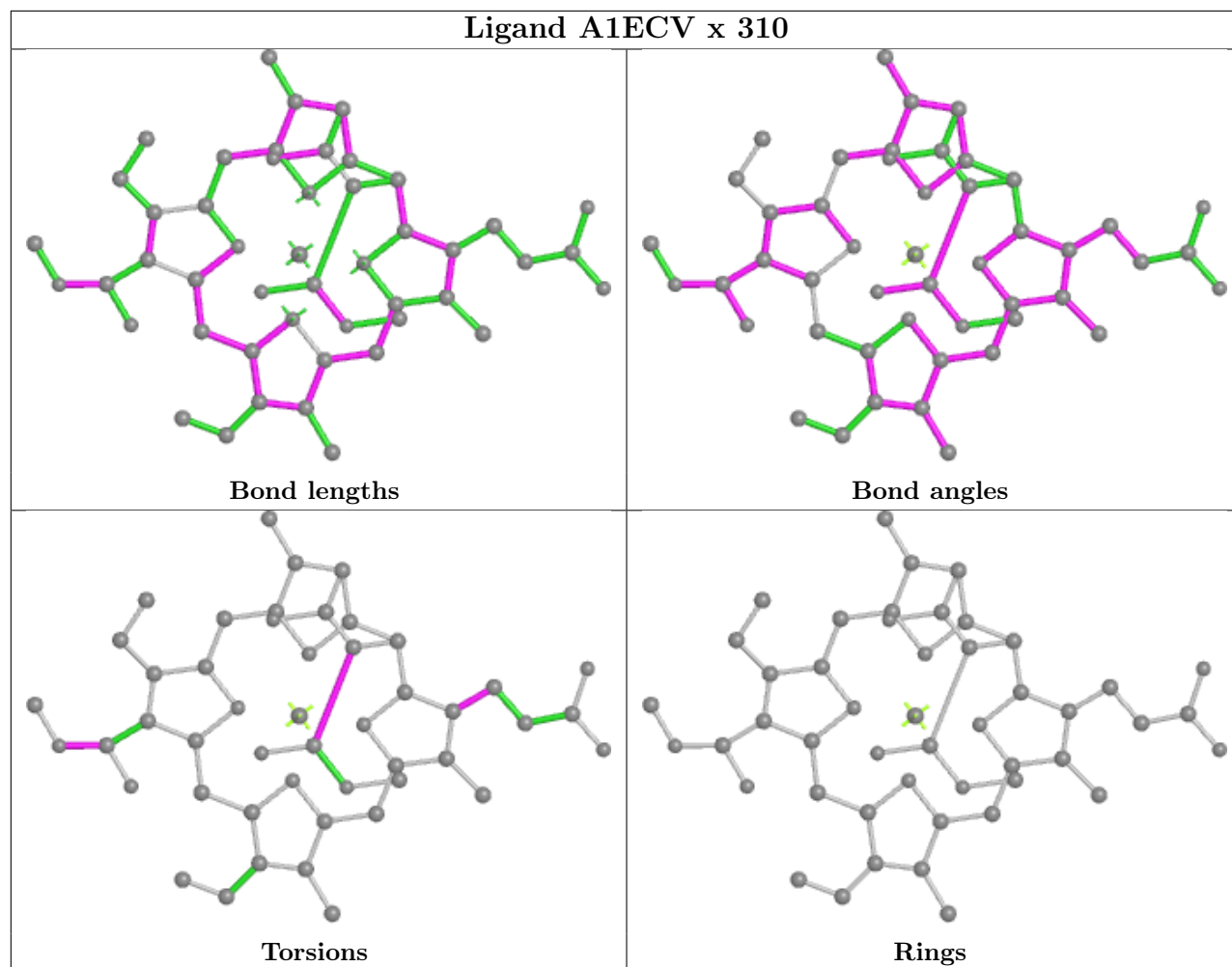


Torsions

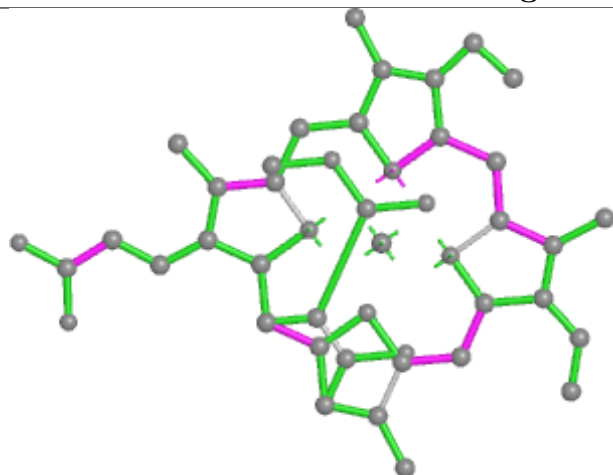


Rings

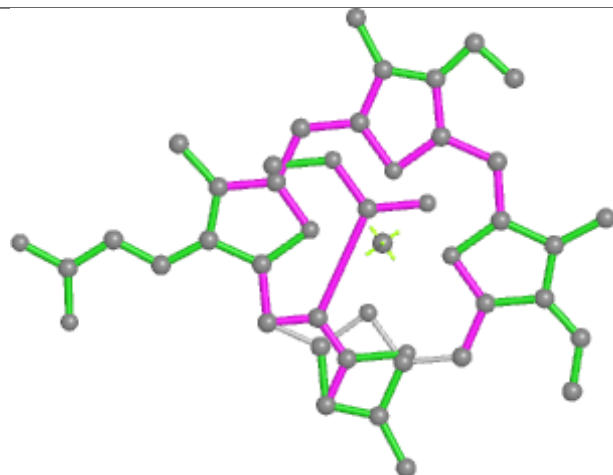




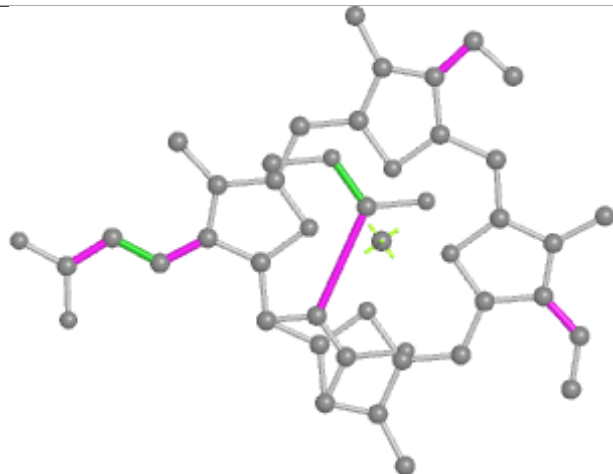
## Ligand KC2 4 324



Bond lengths



Bond angles

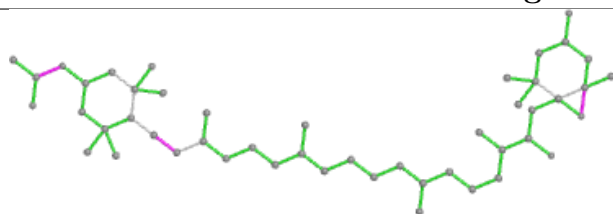


Torsions

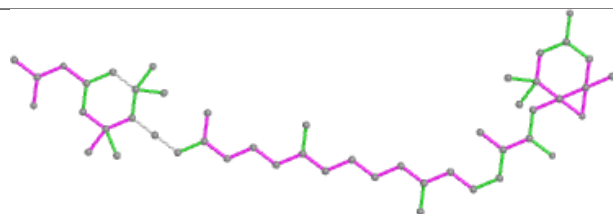


Rings

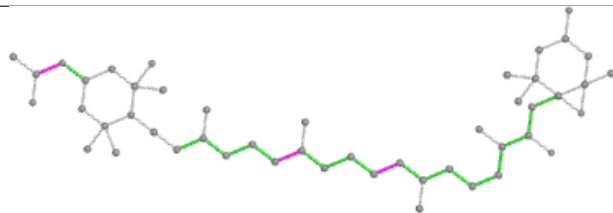
## Ligand A86 8 309



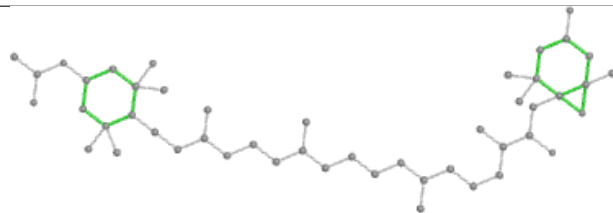
Bond lengths



Bond angles



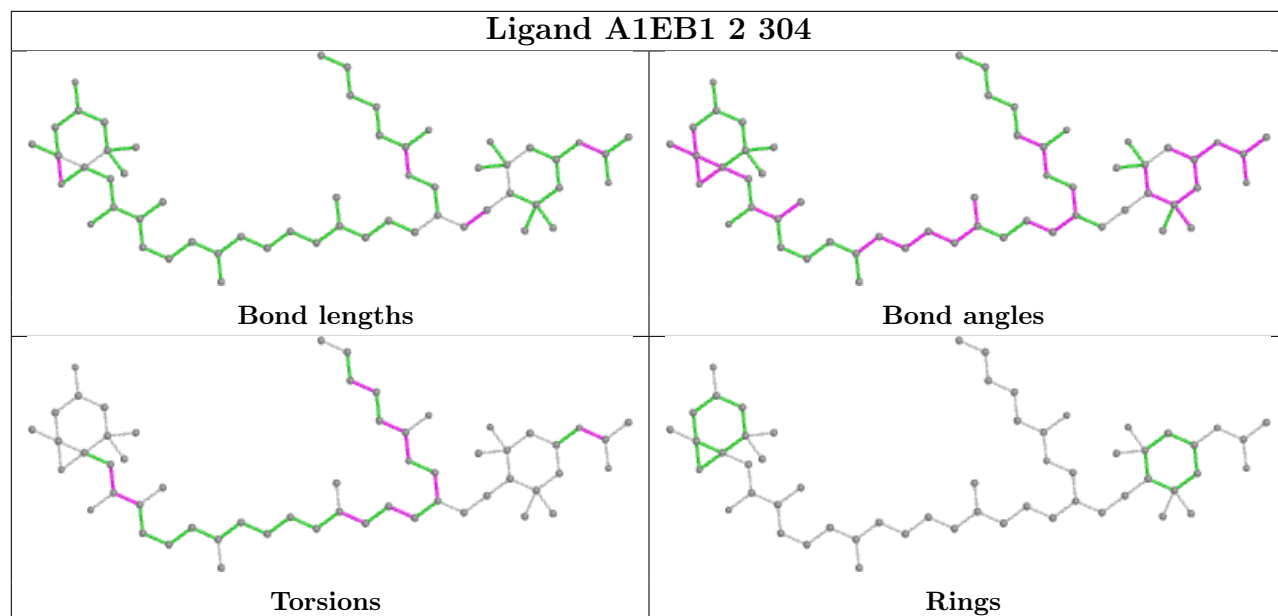
Torsions



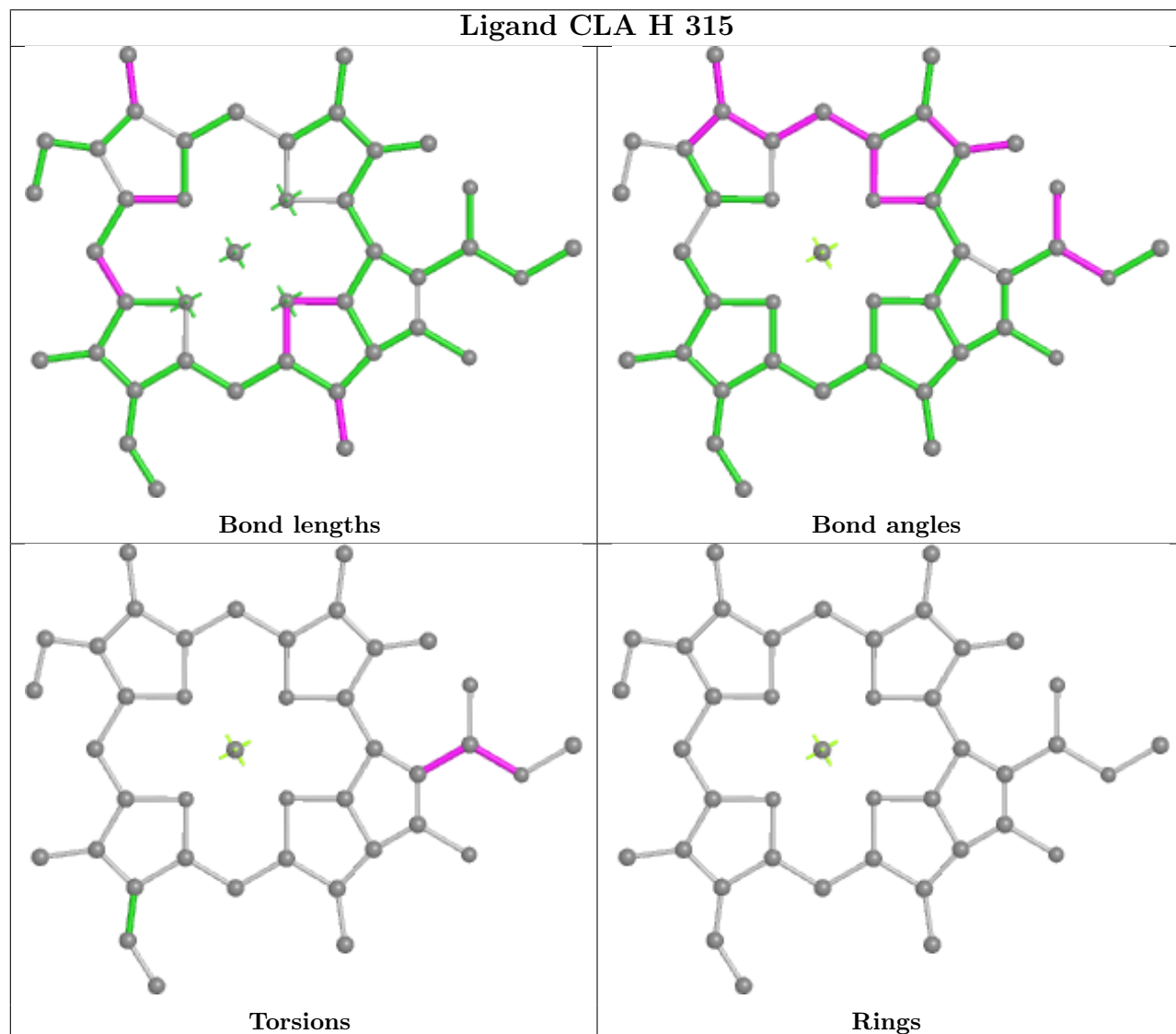
Rings



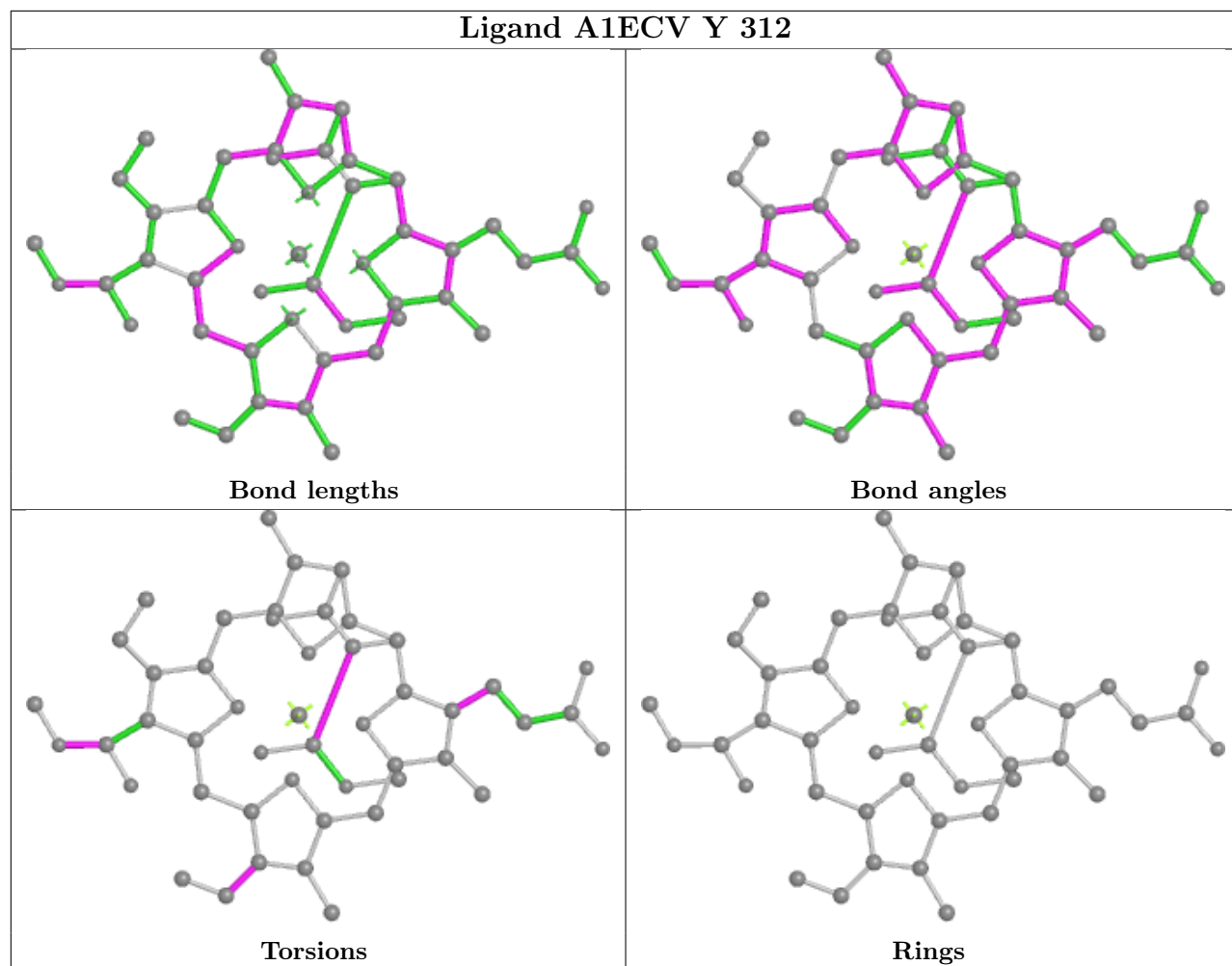
## Ligand A1EB1 2 304



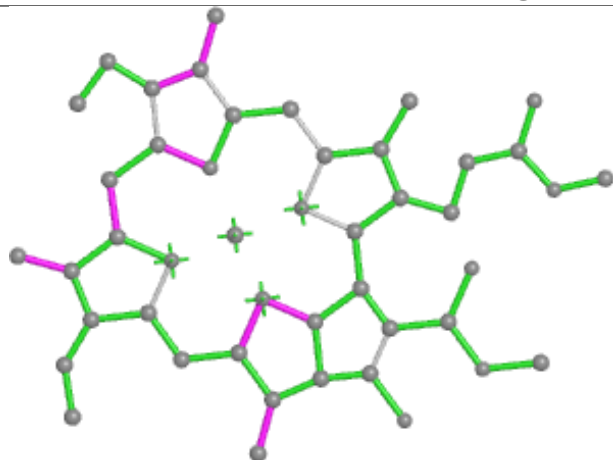
## Ligand CLA H 315



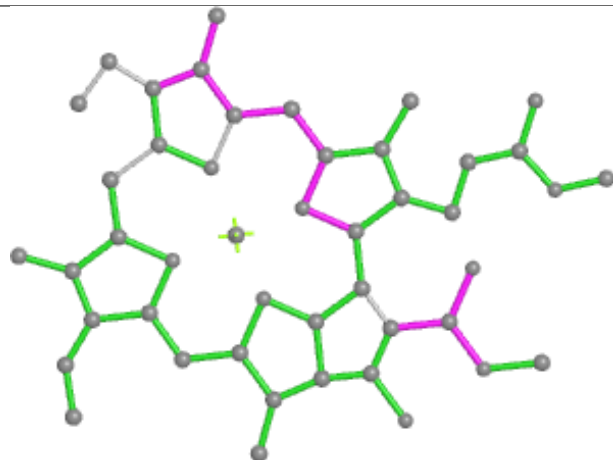
## Ligand A1ECV Y 312



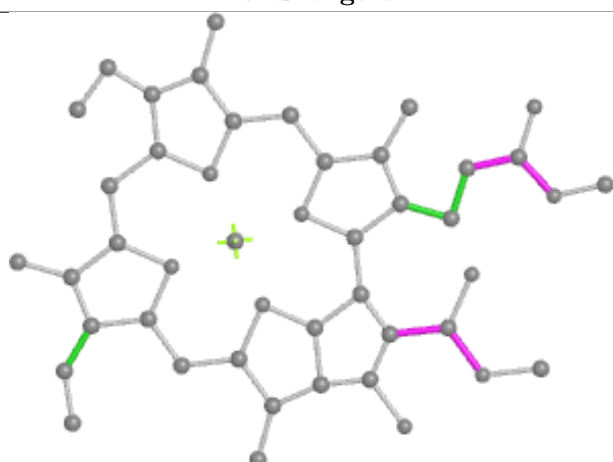
## Ligand CLA T 308



Bond lengths



Bond angles

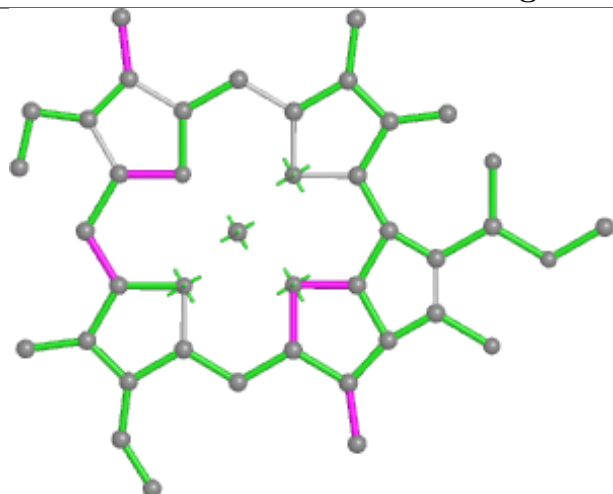


Torsions

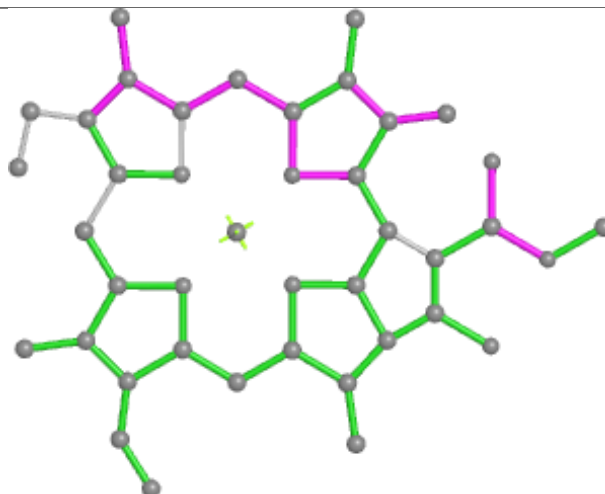


Rings

## Ligand CLA z 309



Bond lengths



Bond angles

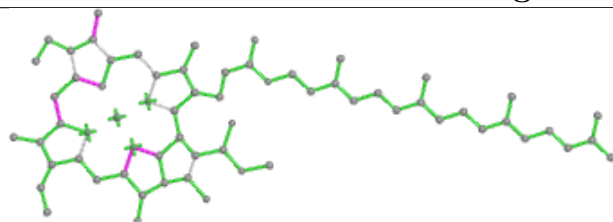


Torsions

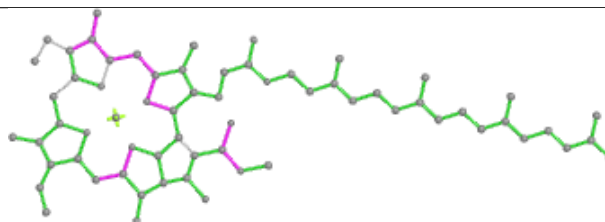


Rings

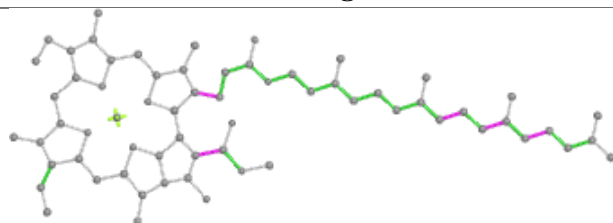
## Ligand CLA D 315



Bond lengths



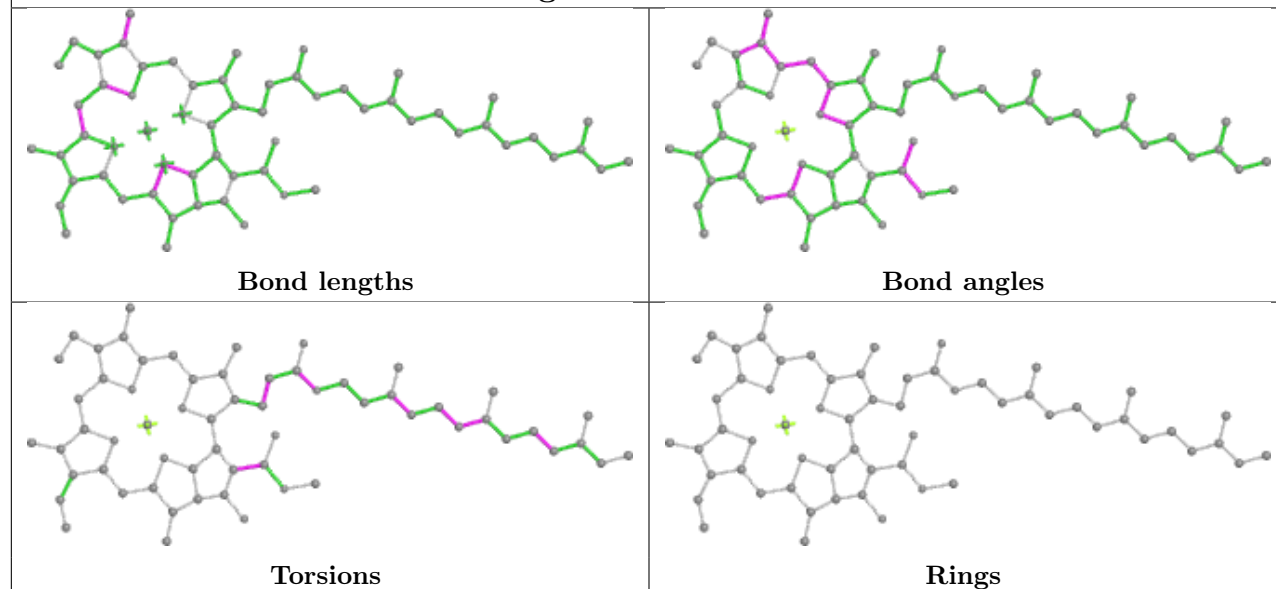
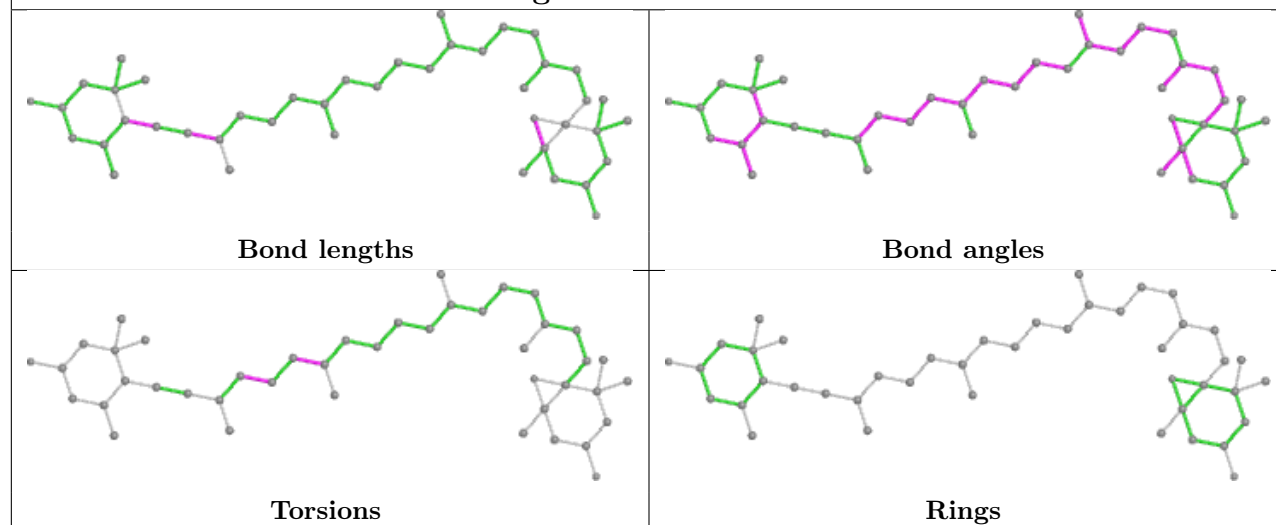
Bond angles



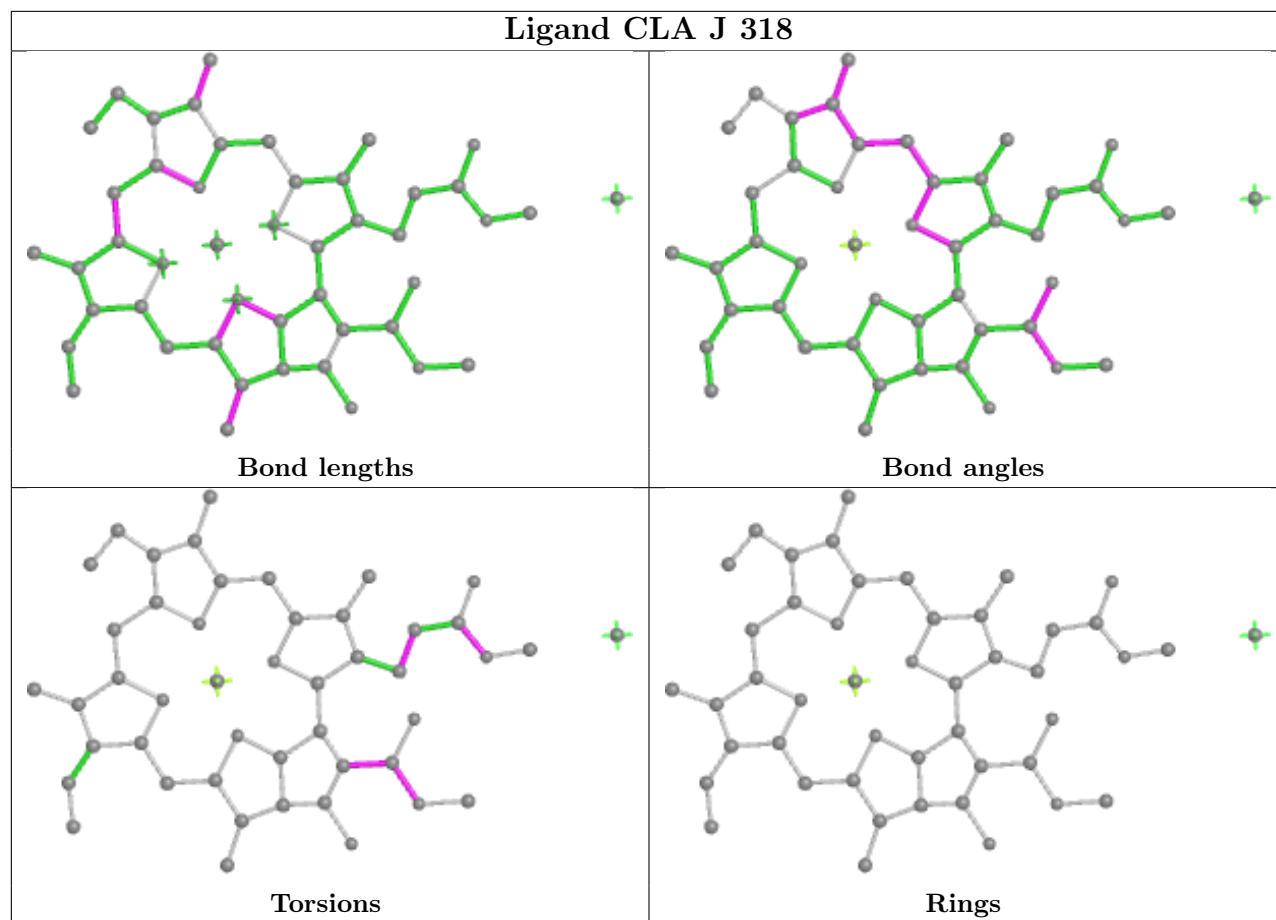
Torsions



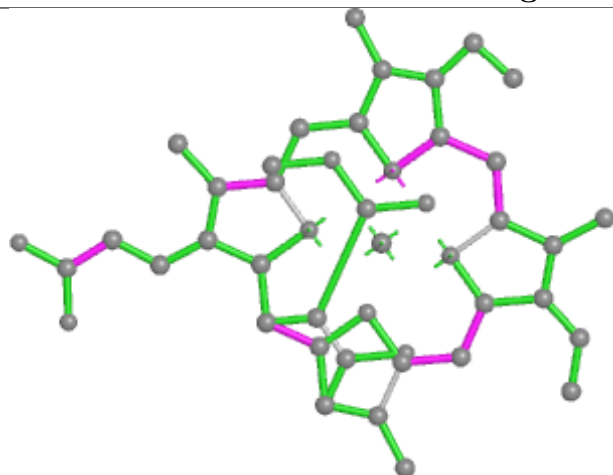
Rings

**Ligand CLA I 308****Ligand DD6 O 303**

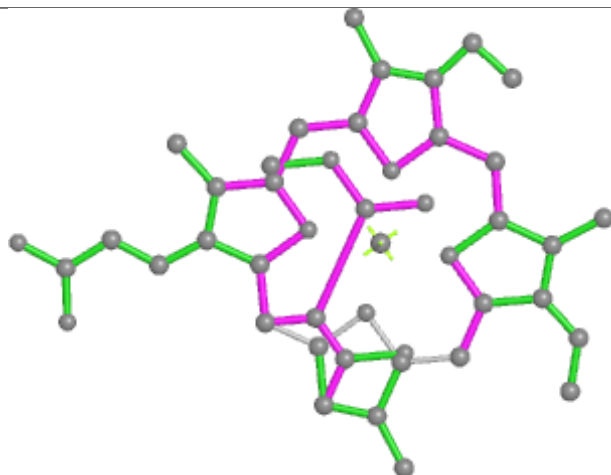
## Ligand CLA J 318



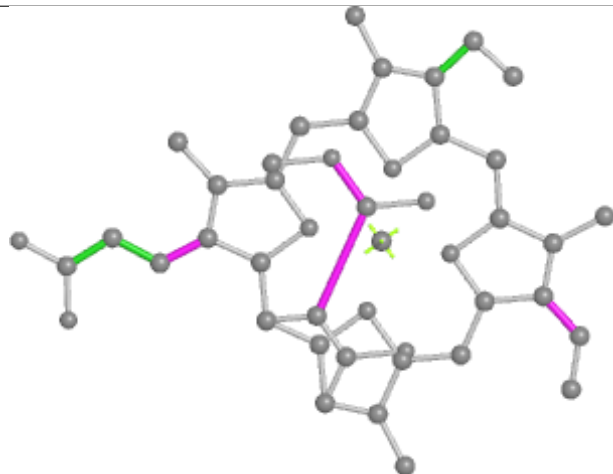
## Ligand KC2 8 317



Bond lengths



Bond angles

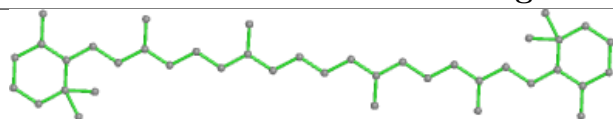


Torsions

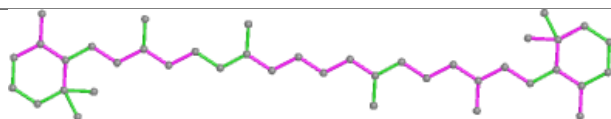


Rings

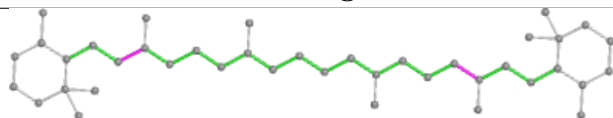
## Ligand BCR b 846



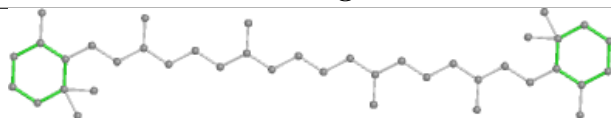
Bond lengths



Bond angles

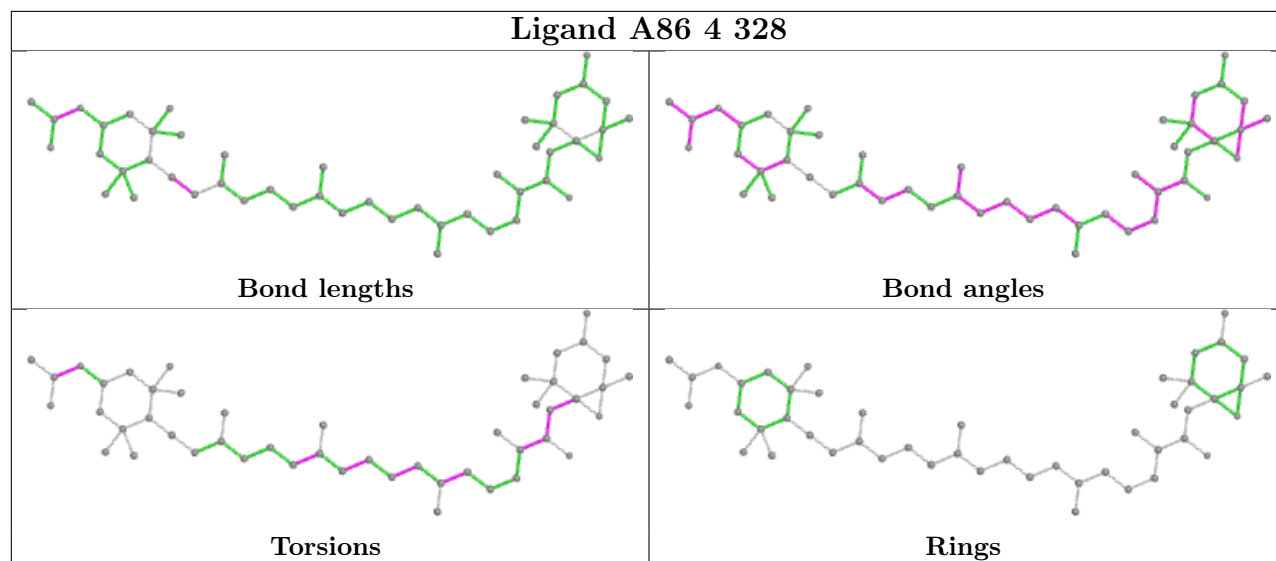


Torsions

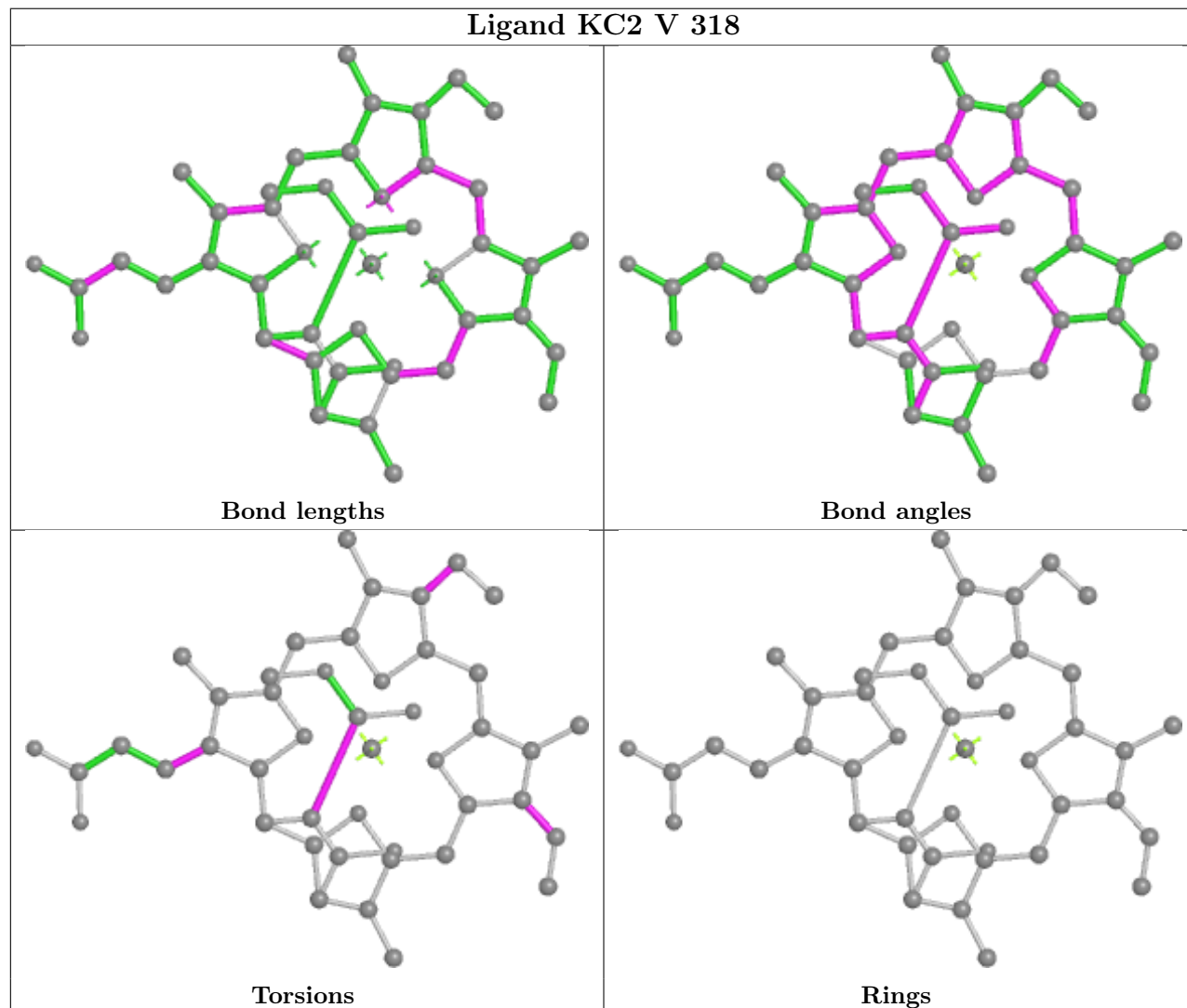


Rings

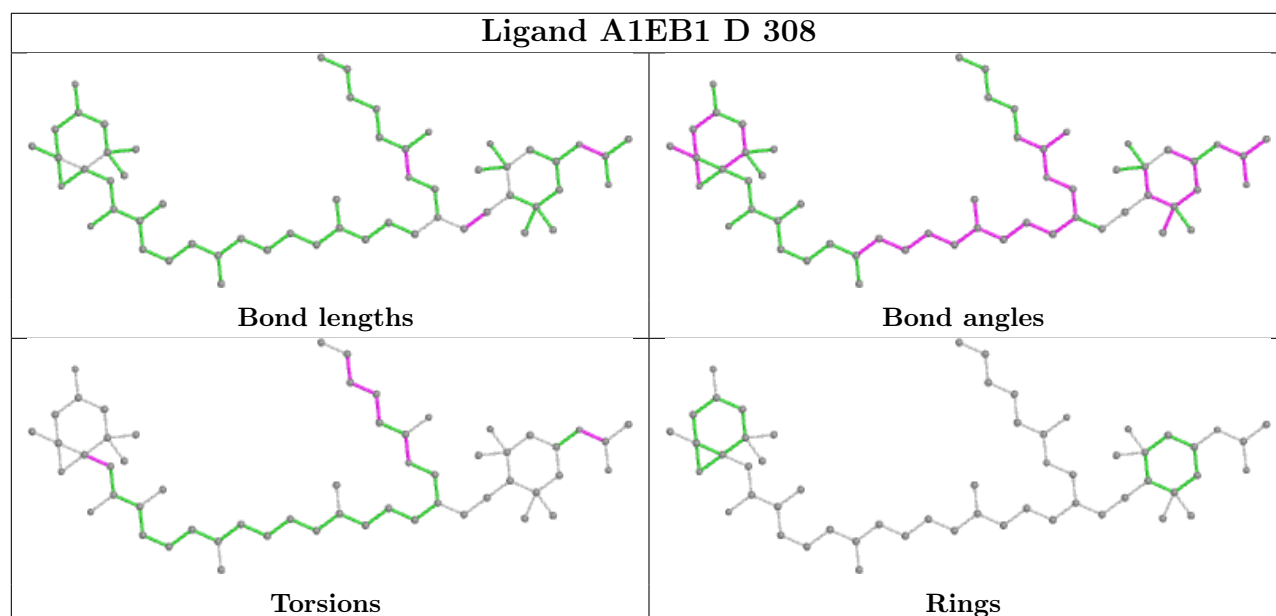
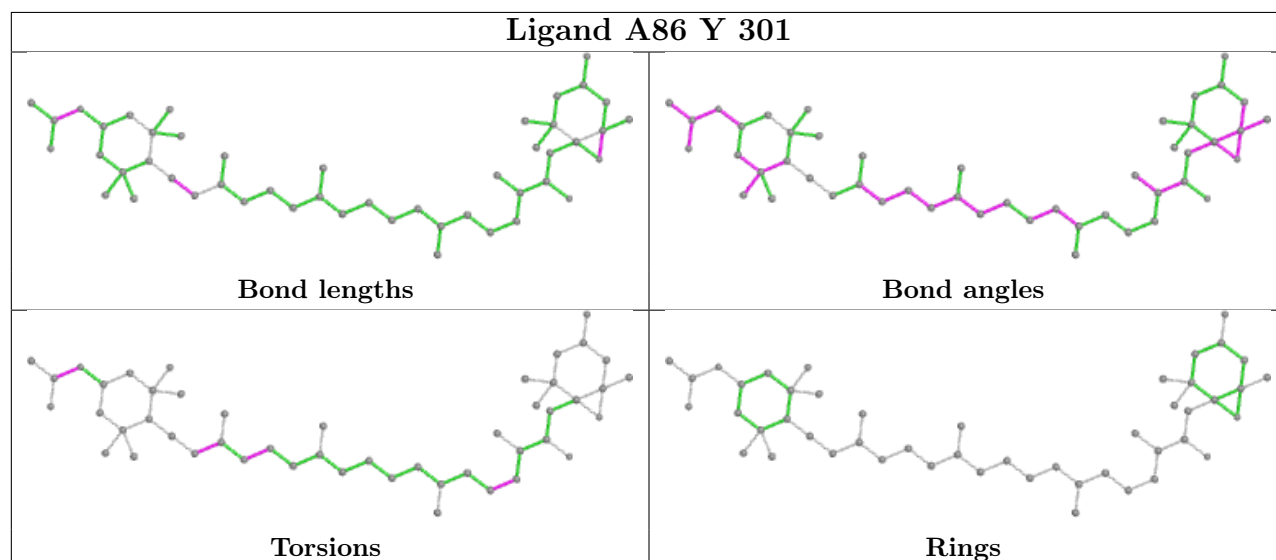
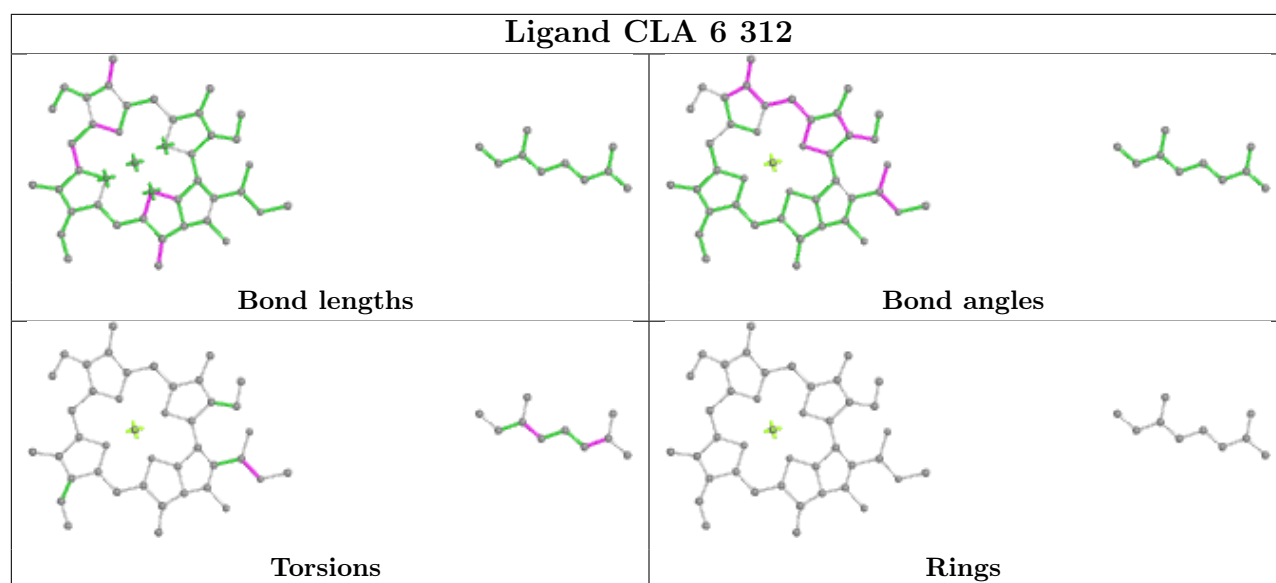
## Ligand A86 4 328



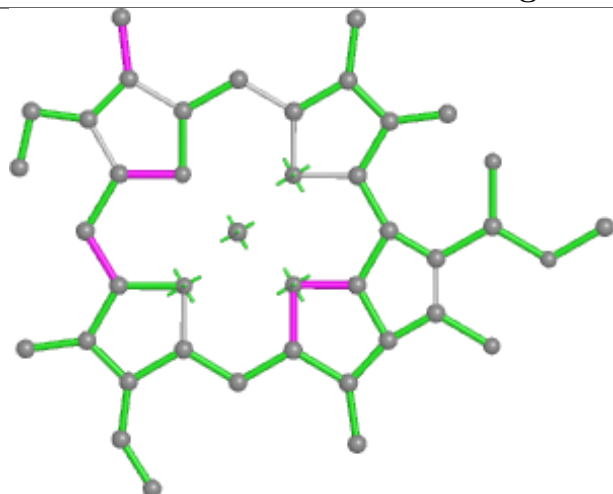
## Ligand KC2 V 318



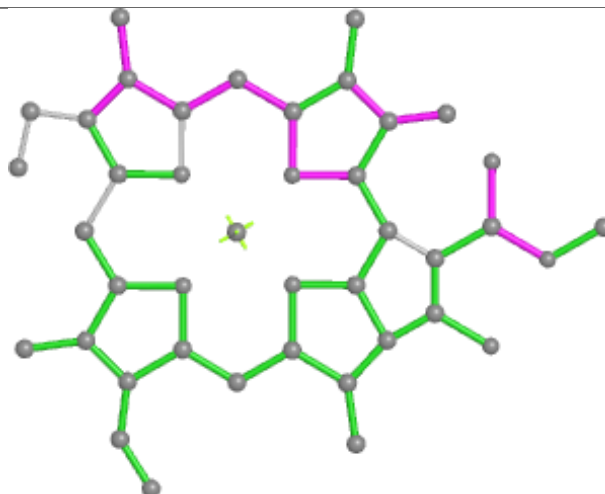




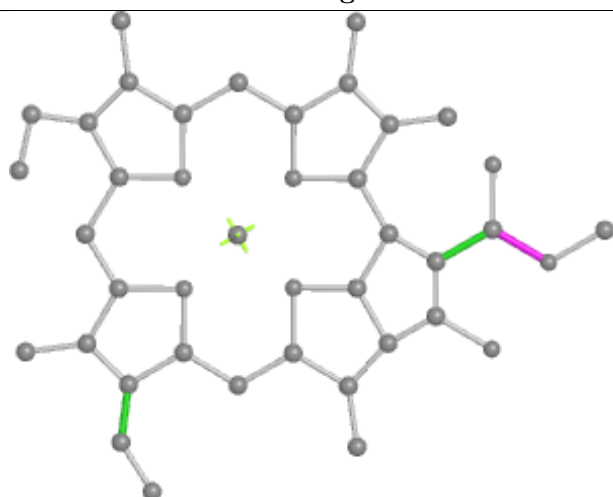
## Ligand CLA z 306



Bond lengths



Bond angles

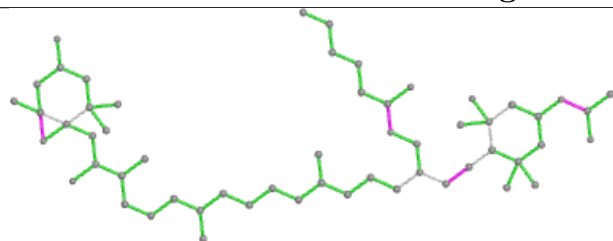


Torsions

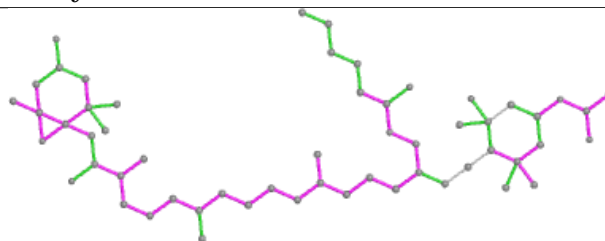


Rings

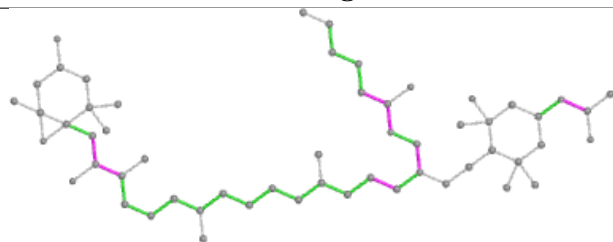
## Ligand A1EB1 y 301



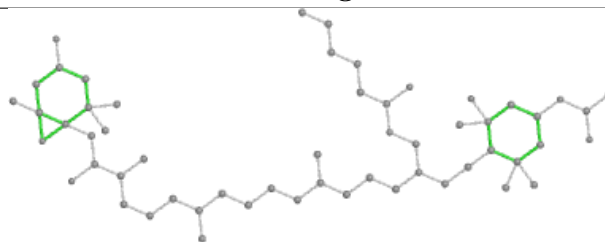
Bond lengths



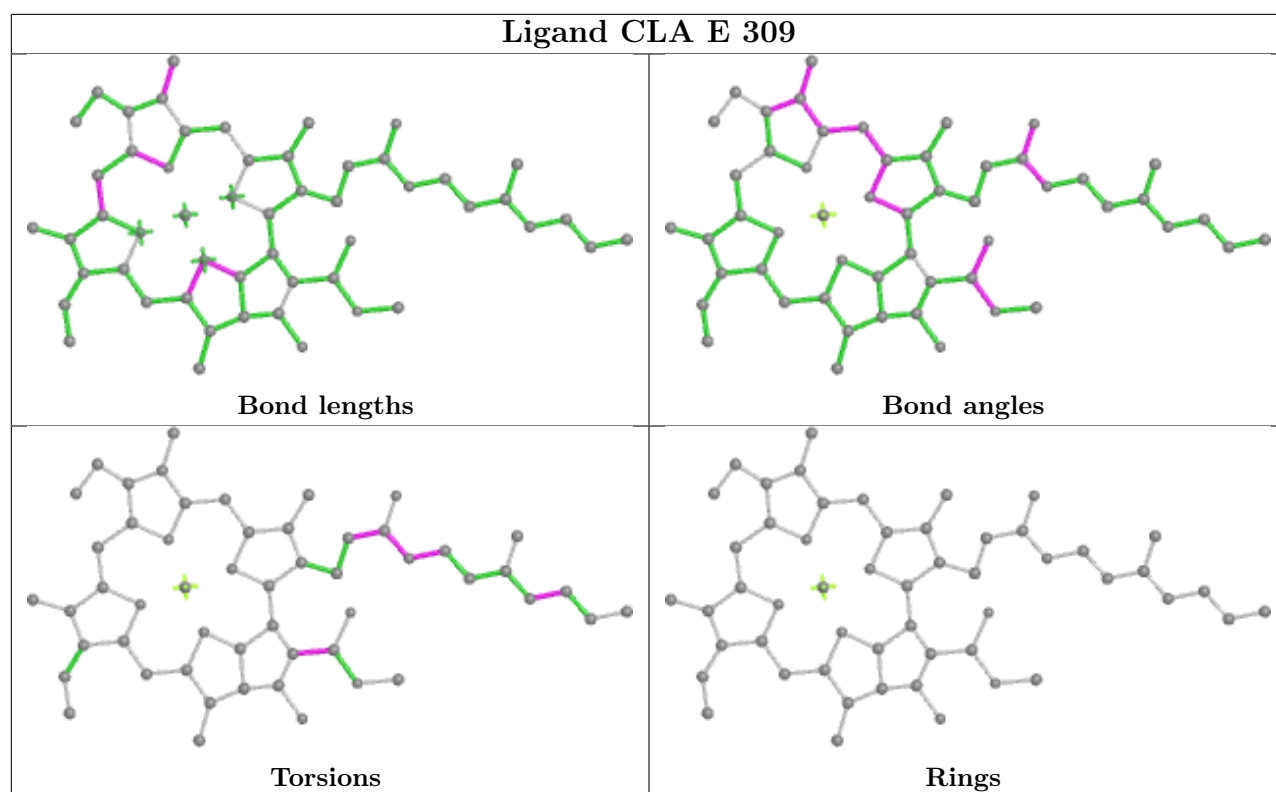
Bond angles



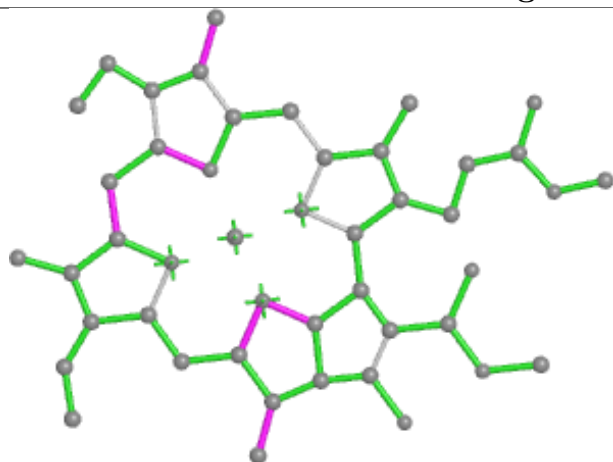
Torsions



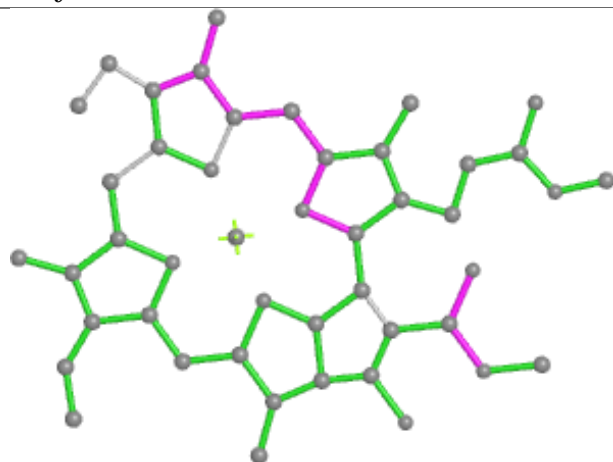
Rings



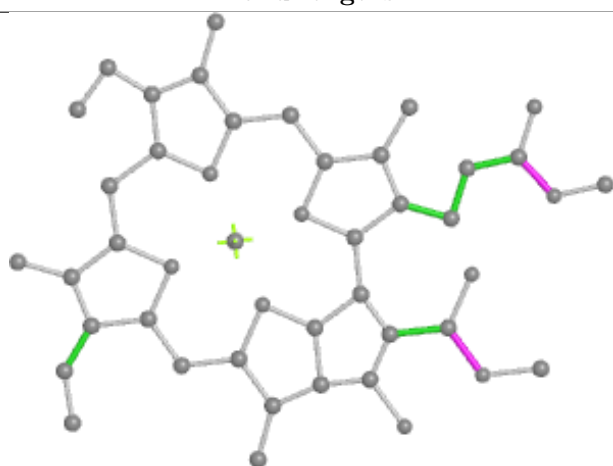
## Ligand CLA y 309



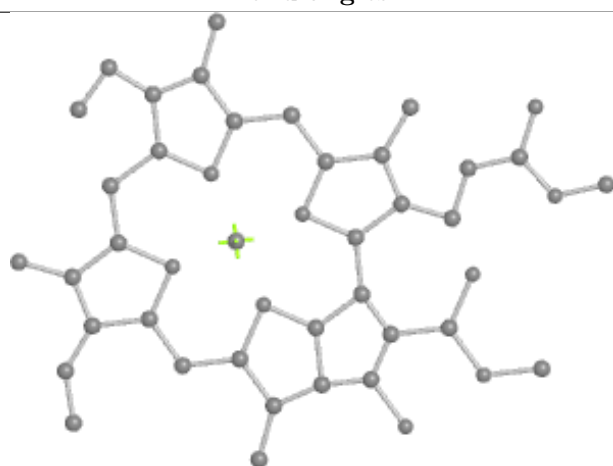
Bond lengths



Bond angles

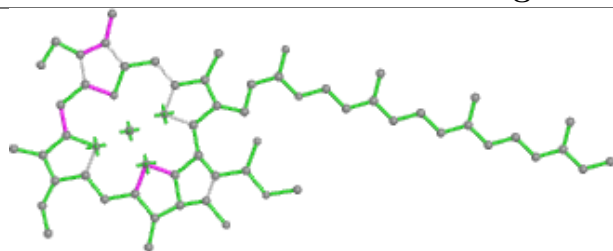


Torsions

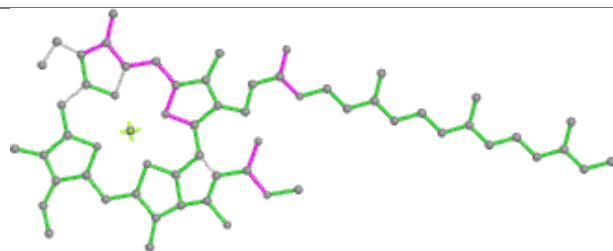


Rings

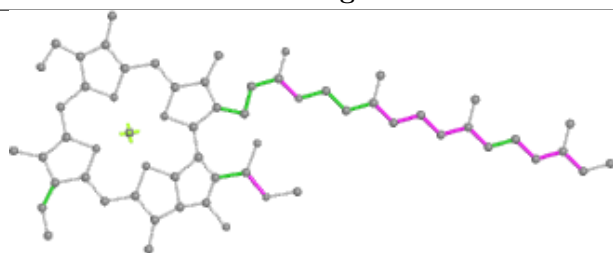
## Ligand CLA D 310



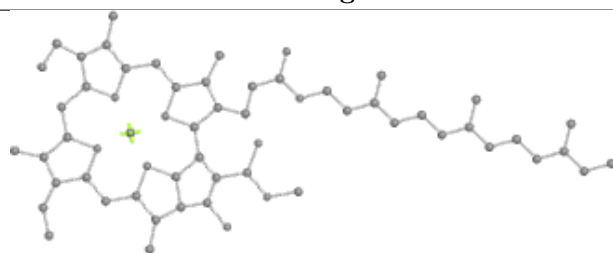
Bond lengths



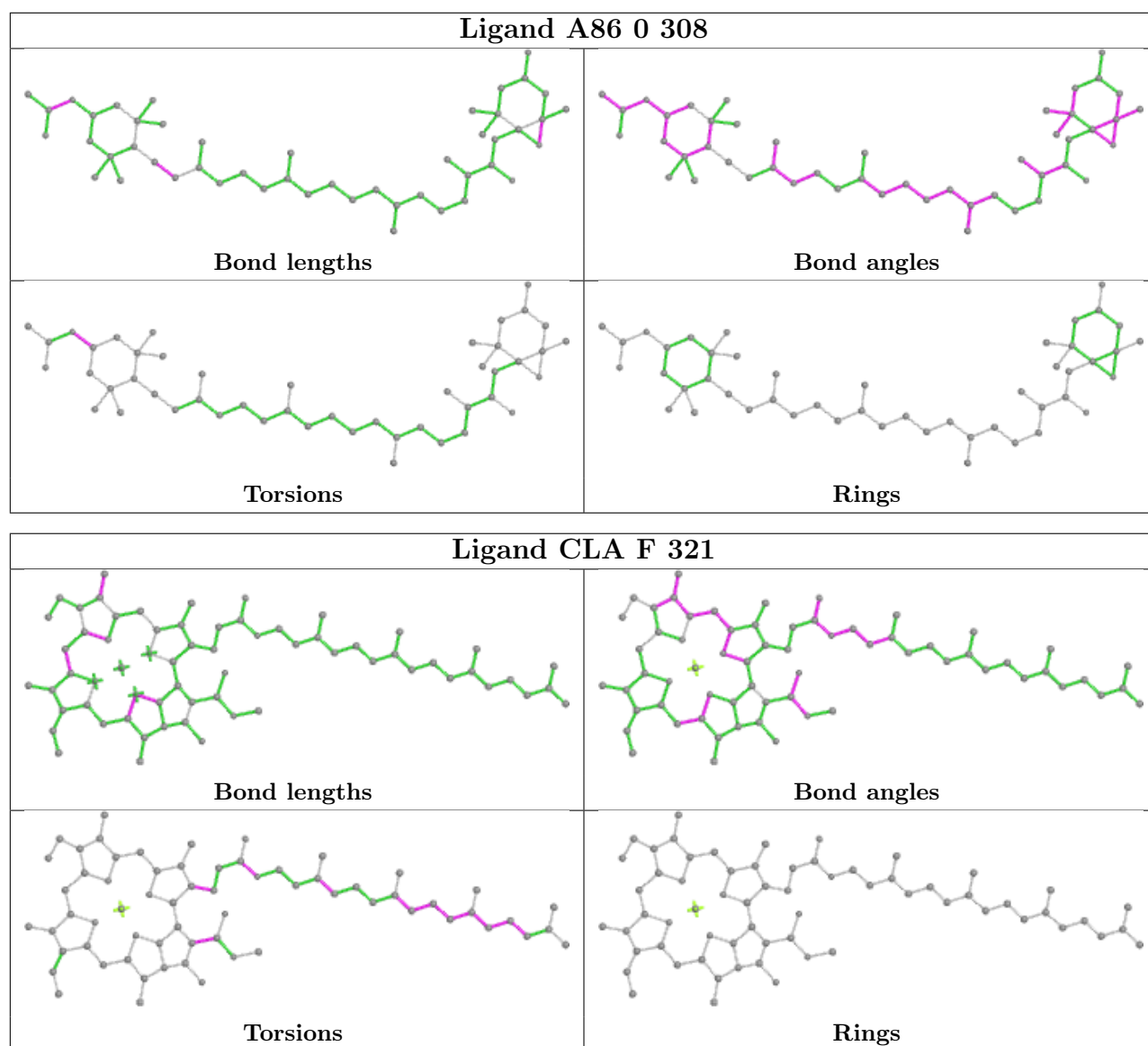
Bond angles



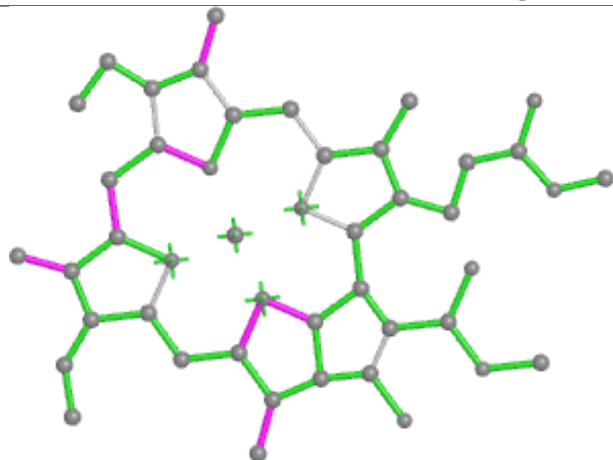
Torsions



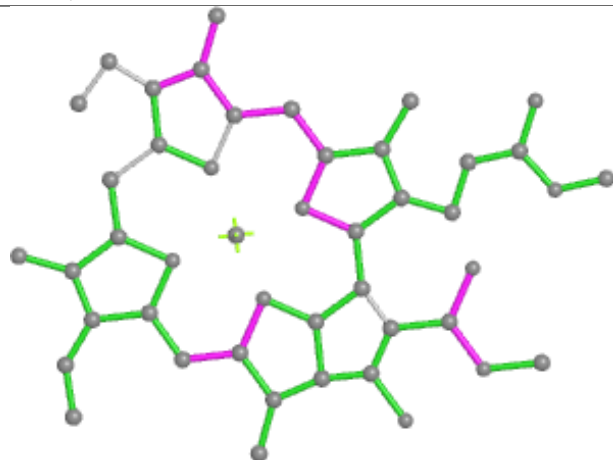
Rings



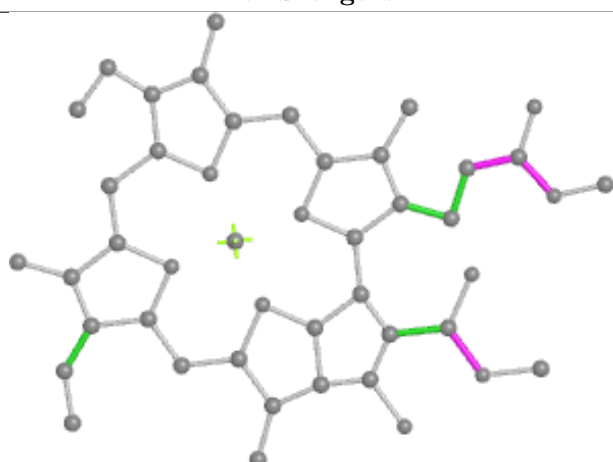
## Ligand CLA Q 311



Bond lengths



Bond angles

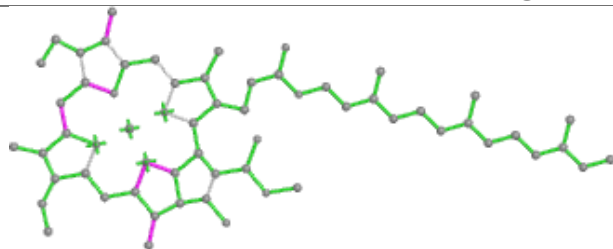


Torsions

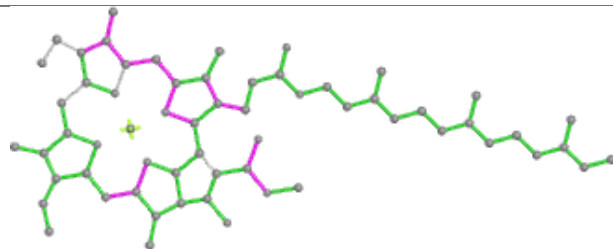


Rings

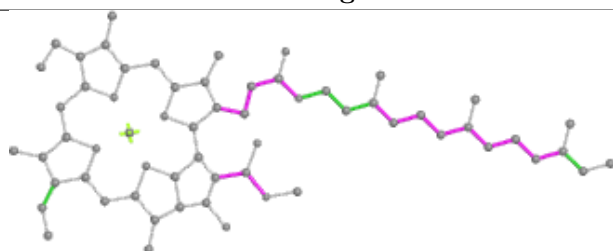
## Ligand CLA O 310



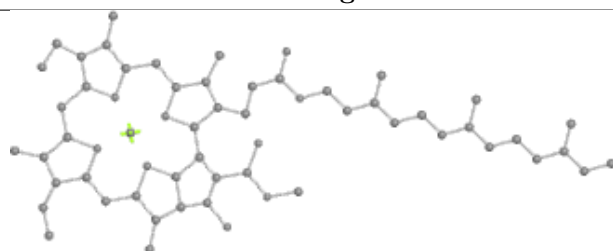
Bond lengths



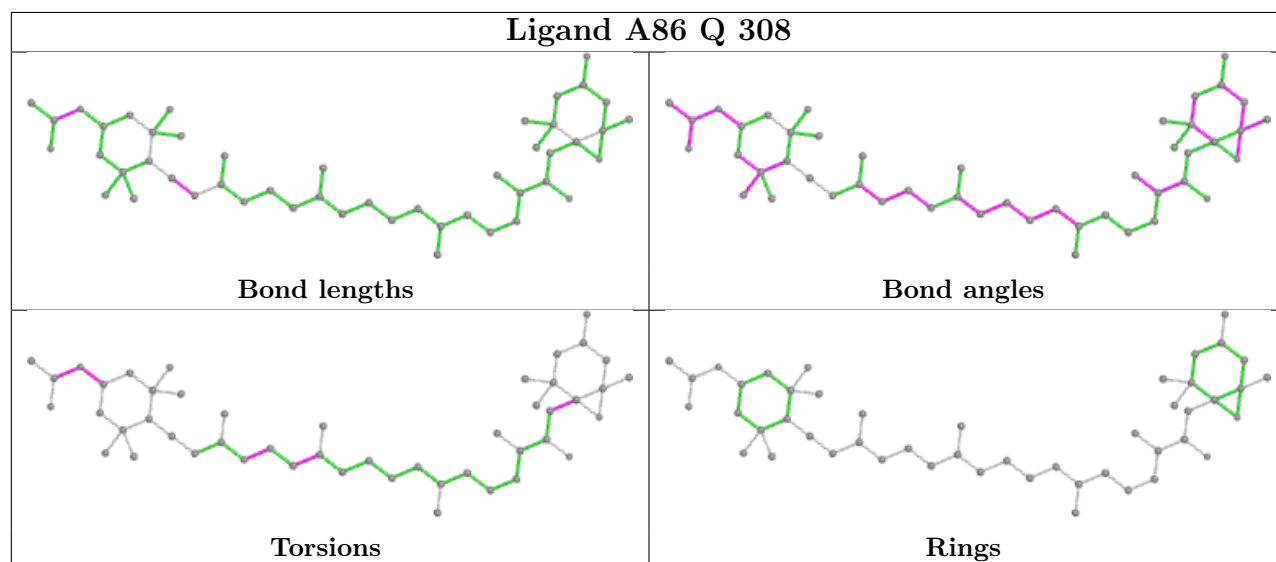
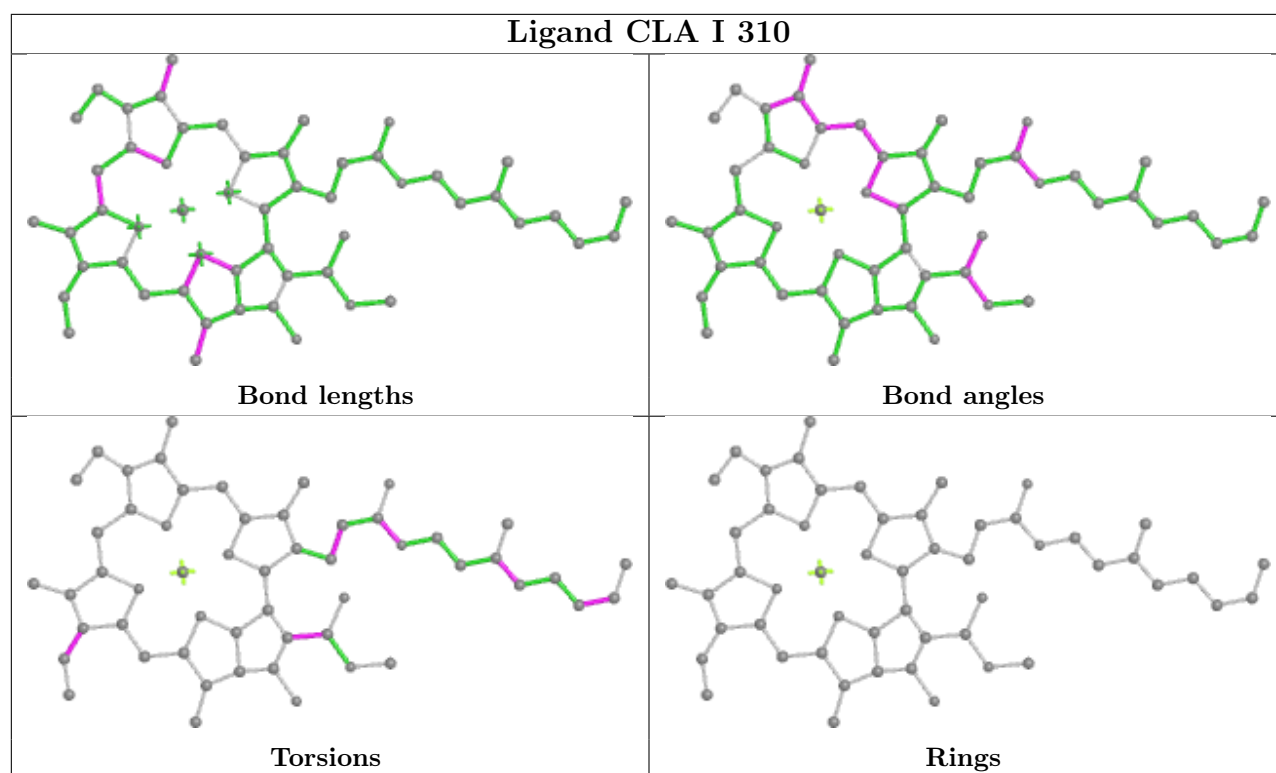
Bond angles



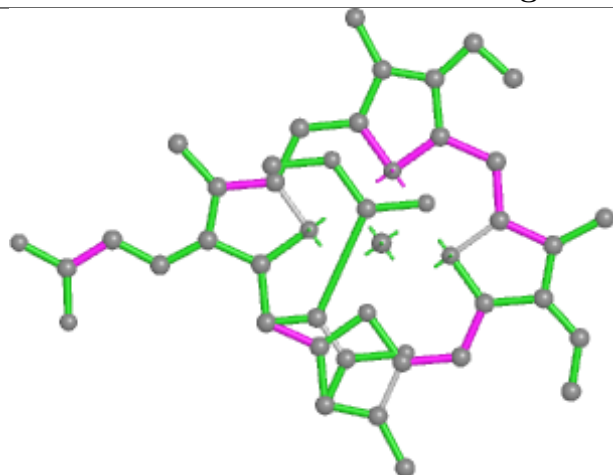
Torsions



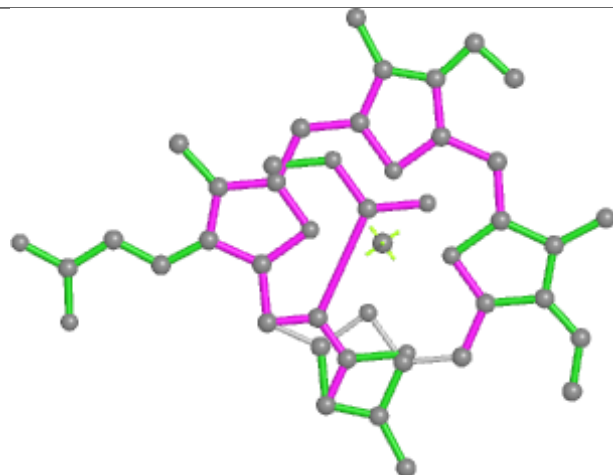
Rings



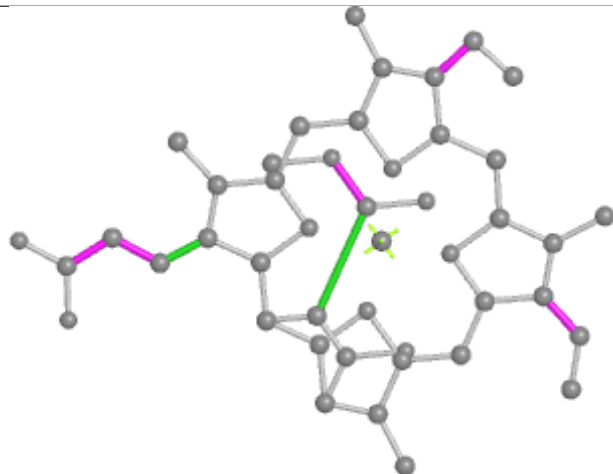
## Ligand KC2 2 317



Bond lengths



Bond angles

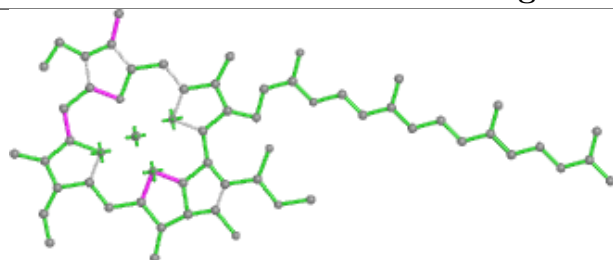


Torsions

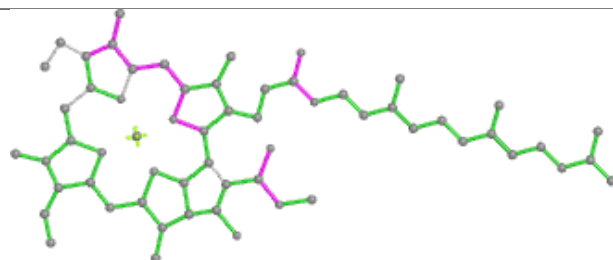


Rings

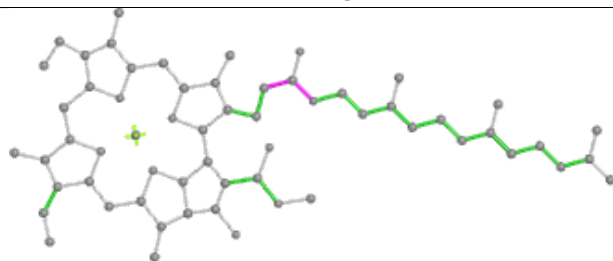
## Ligand CLA 5 307



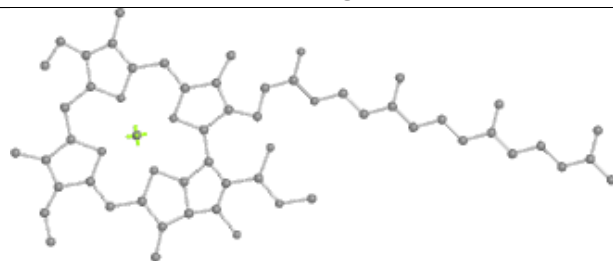
Bond lengths



Bond angles



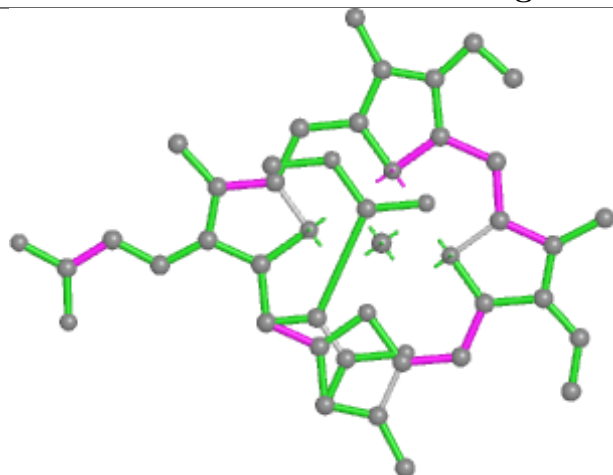
Torsions



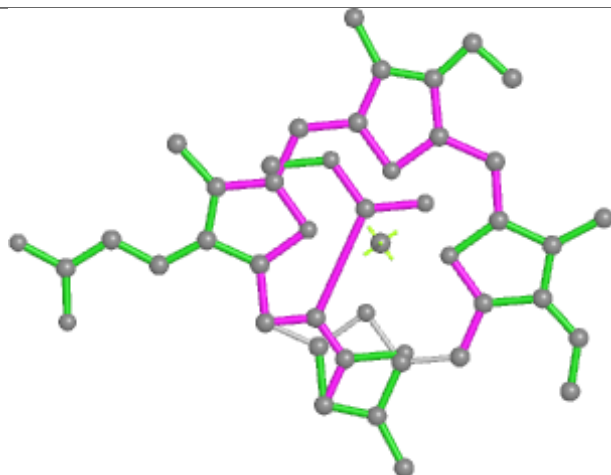
Rings



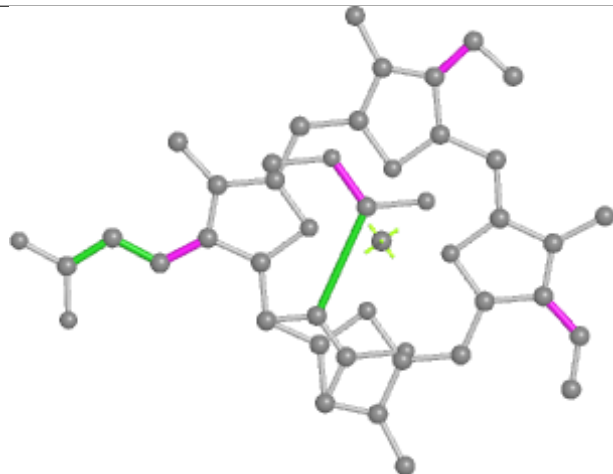
## Ligand KC2 K 310



Bond lengths



Bond angles

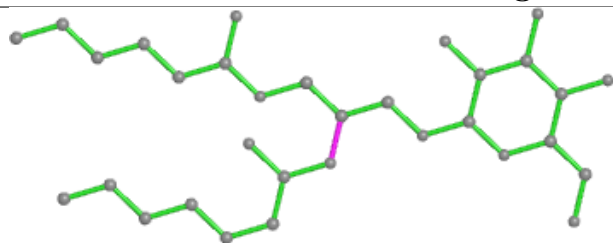


Torsions

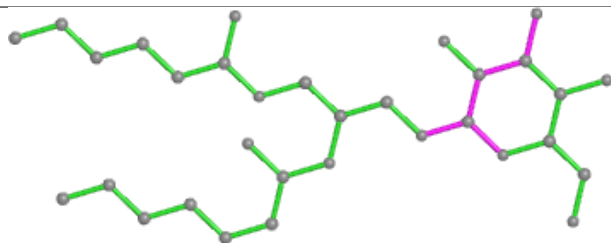


Rings

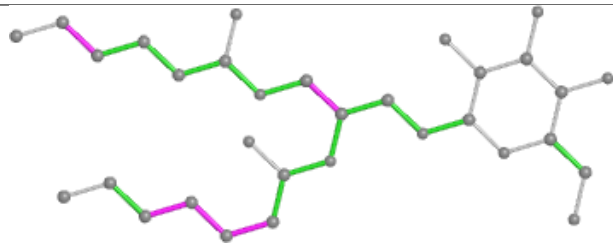
## Ligand LMG 7 326



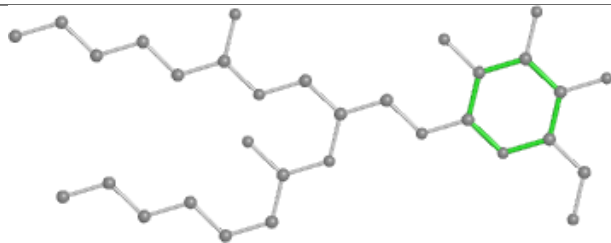
Bond lengths



Bond angles

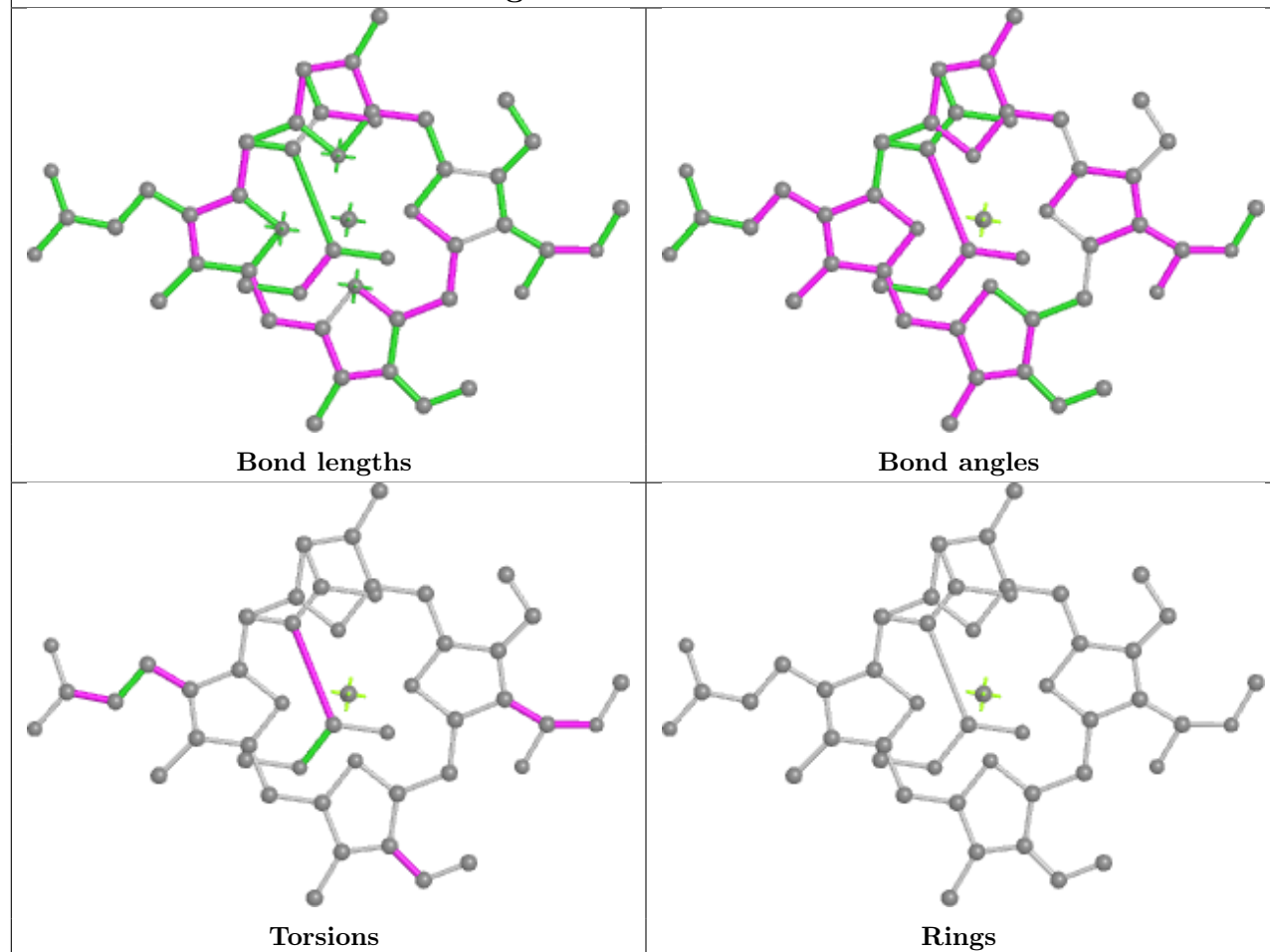


Torsions

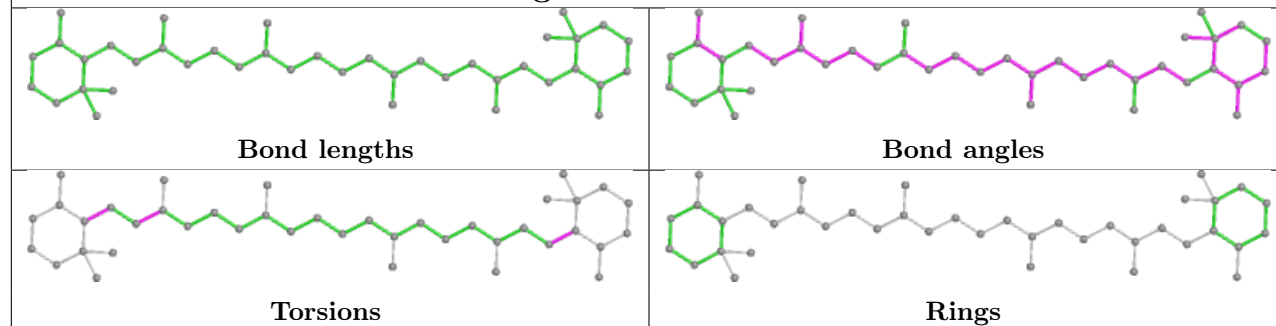


Rings

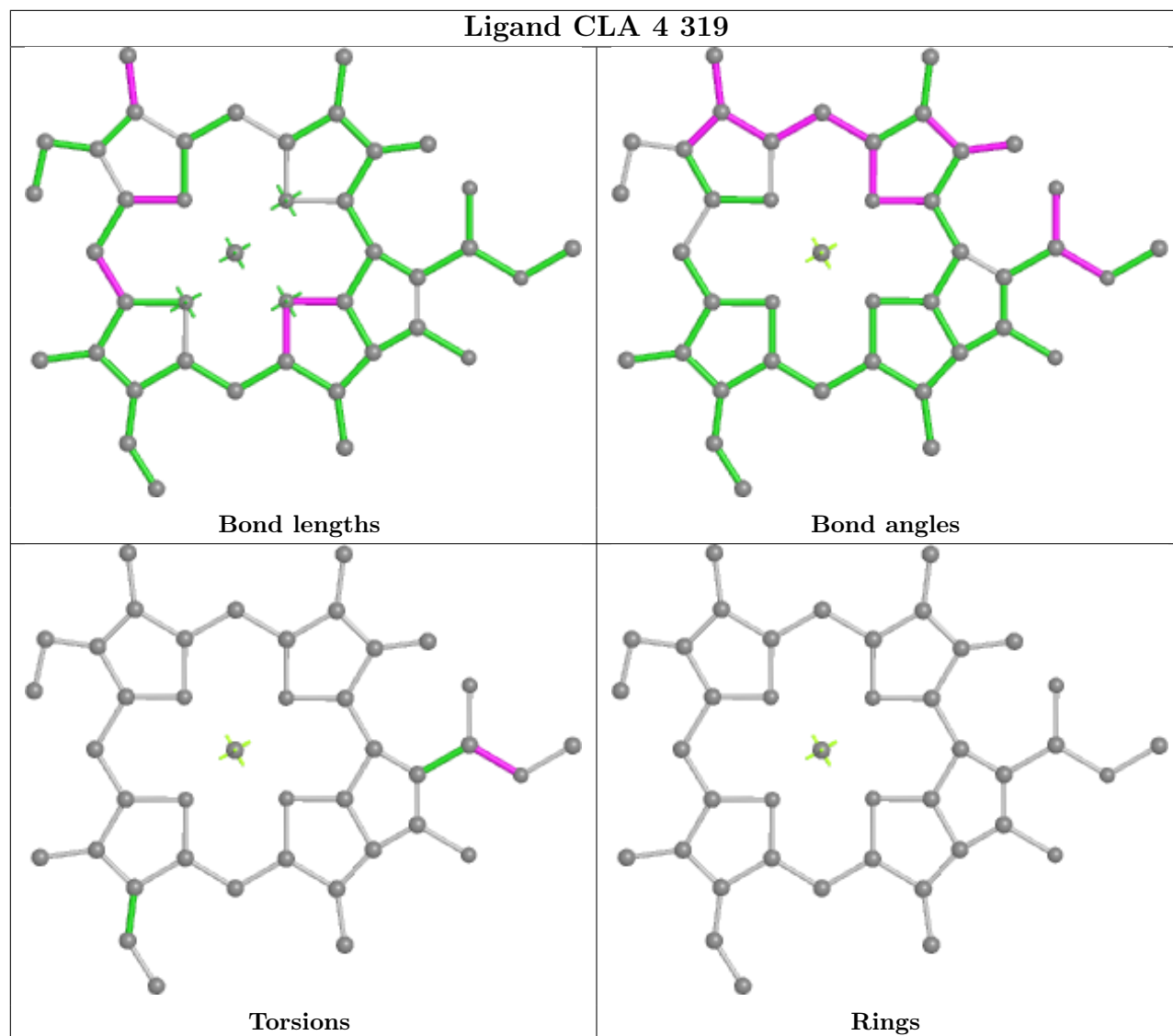
## Ligand A1ECV R 310



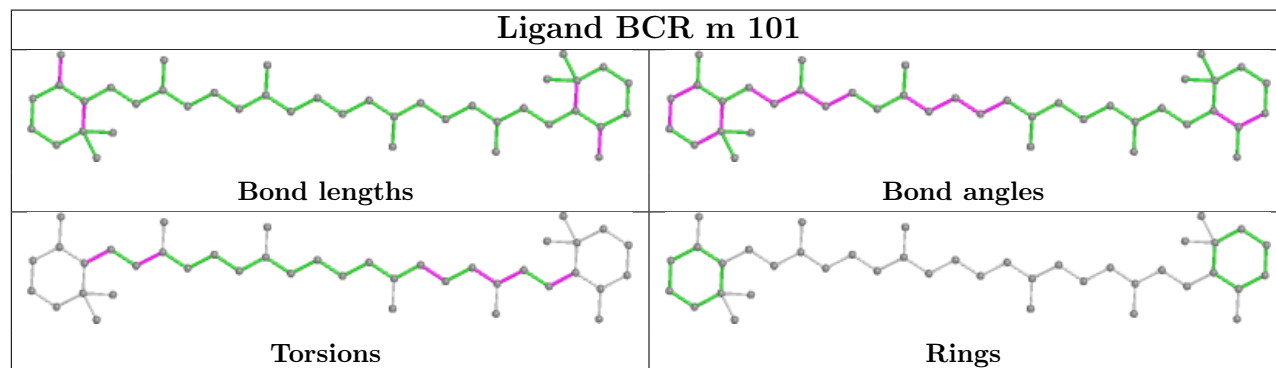
## Ligand BCR h 202

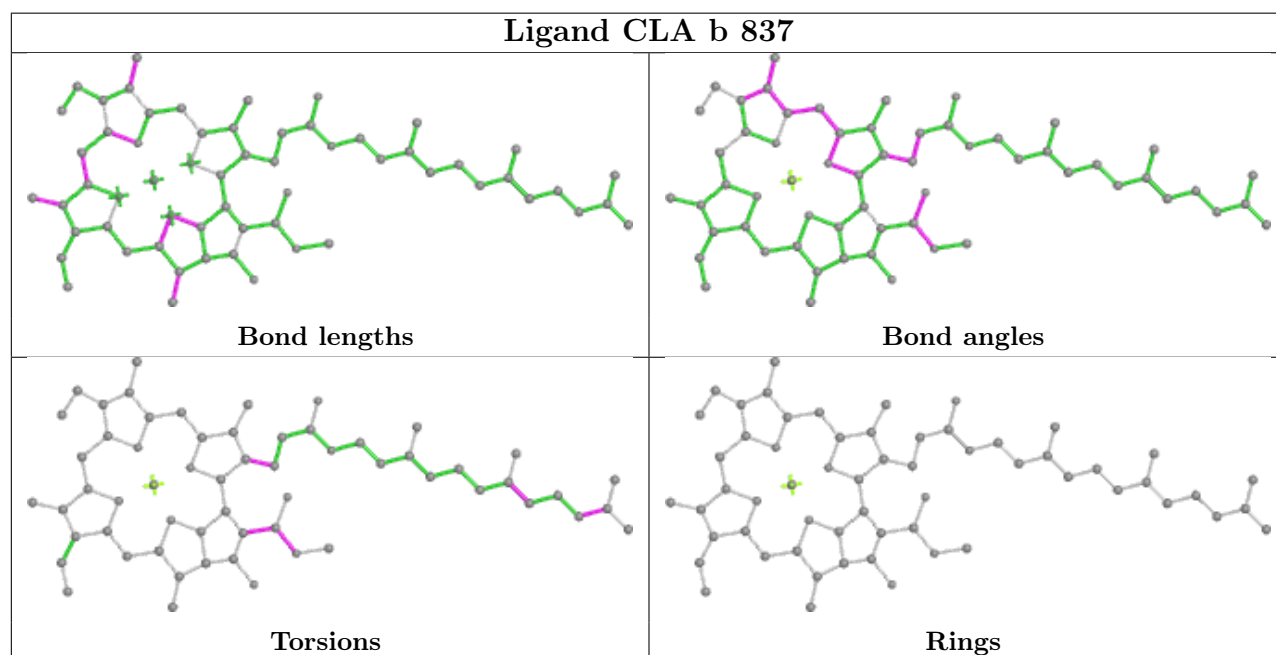
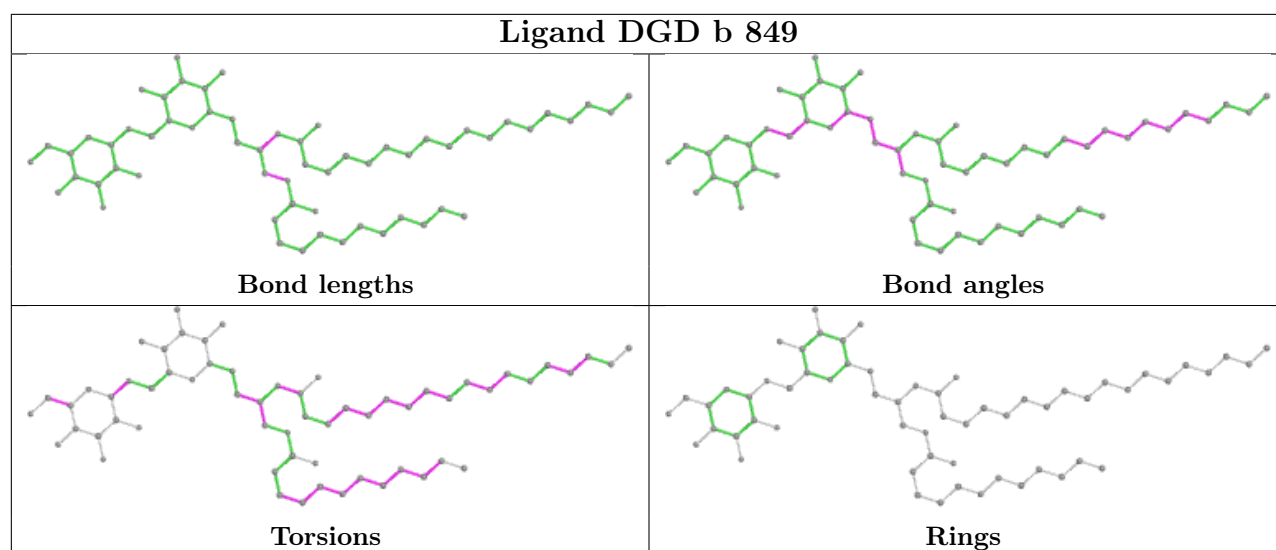


## Ligand CLA 4 319

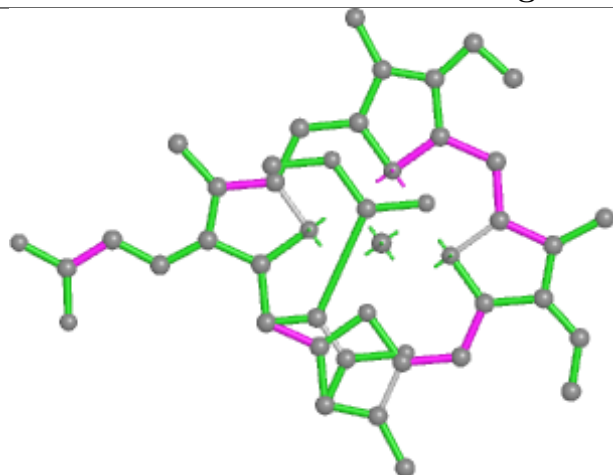


## Ligand BCR m 101

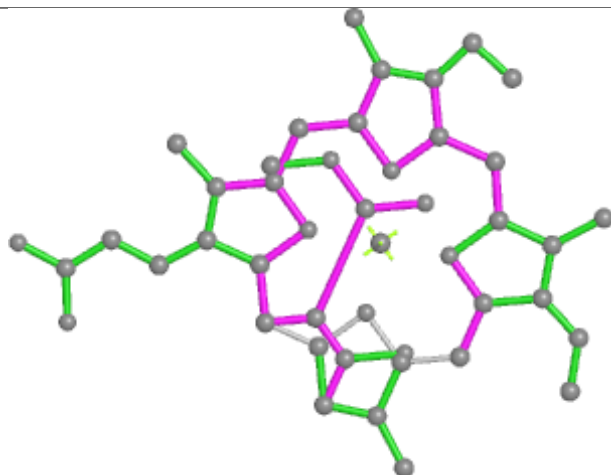




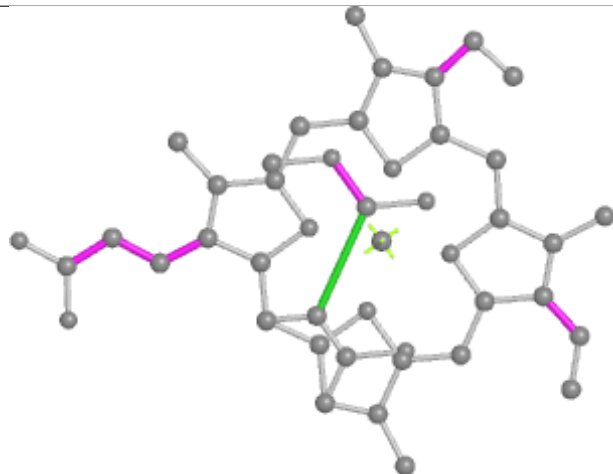
## Ligand KC2 Z 310



Bond lengths



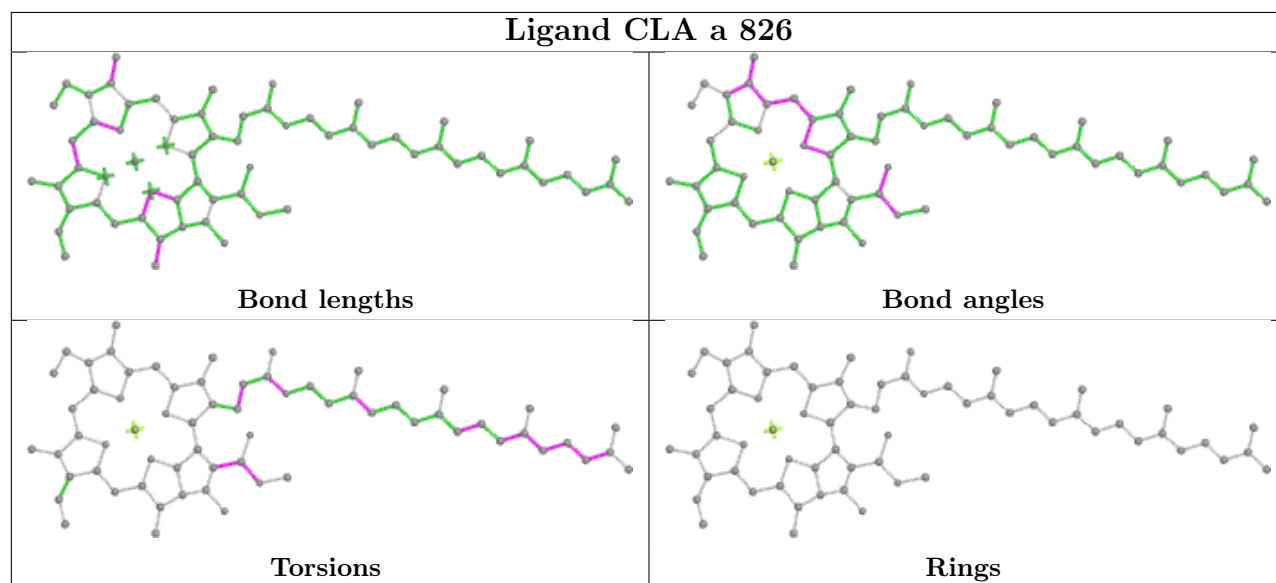
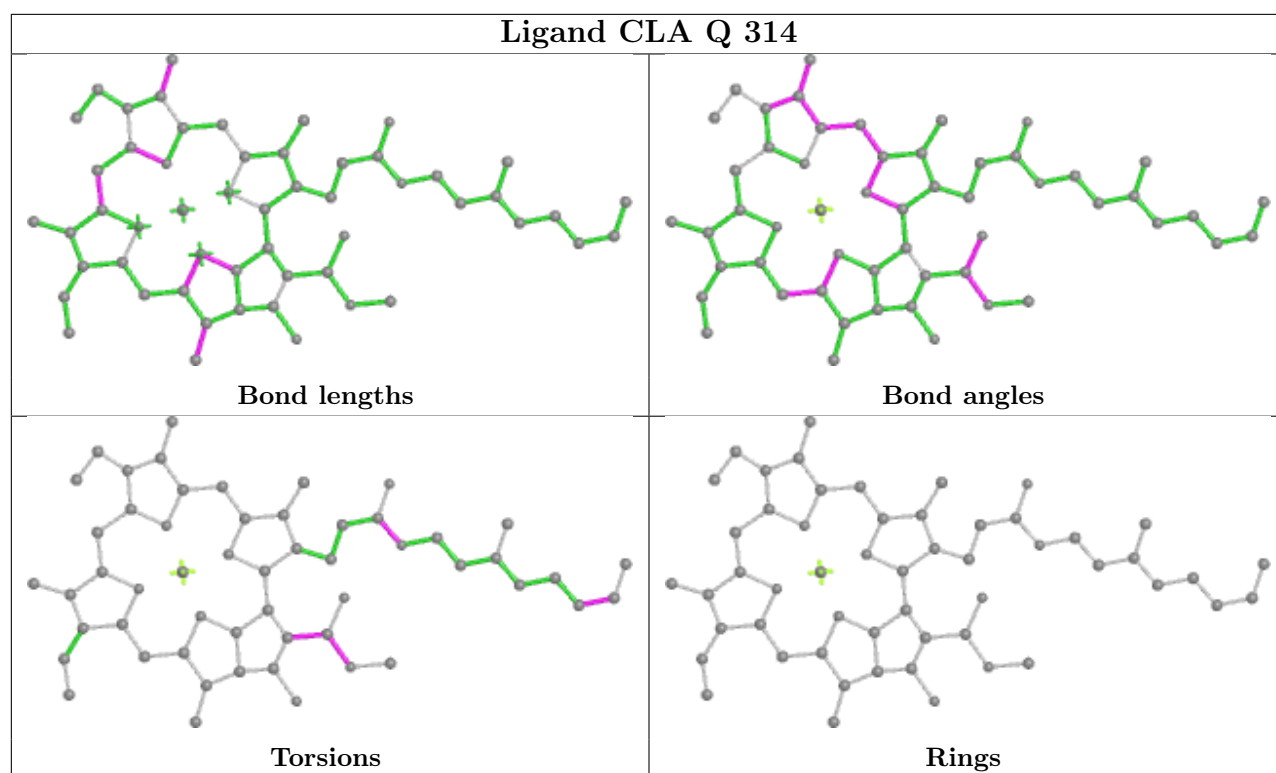
Bond angles

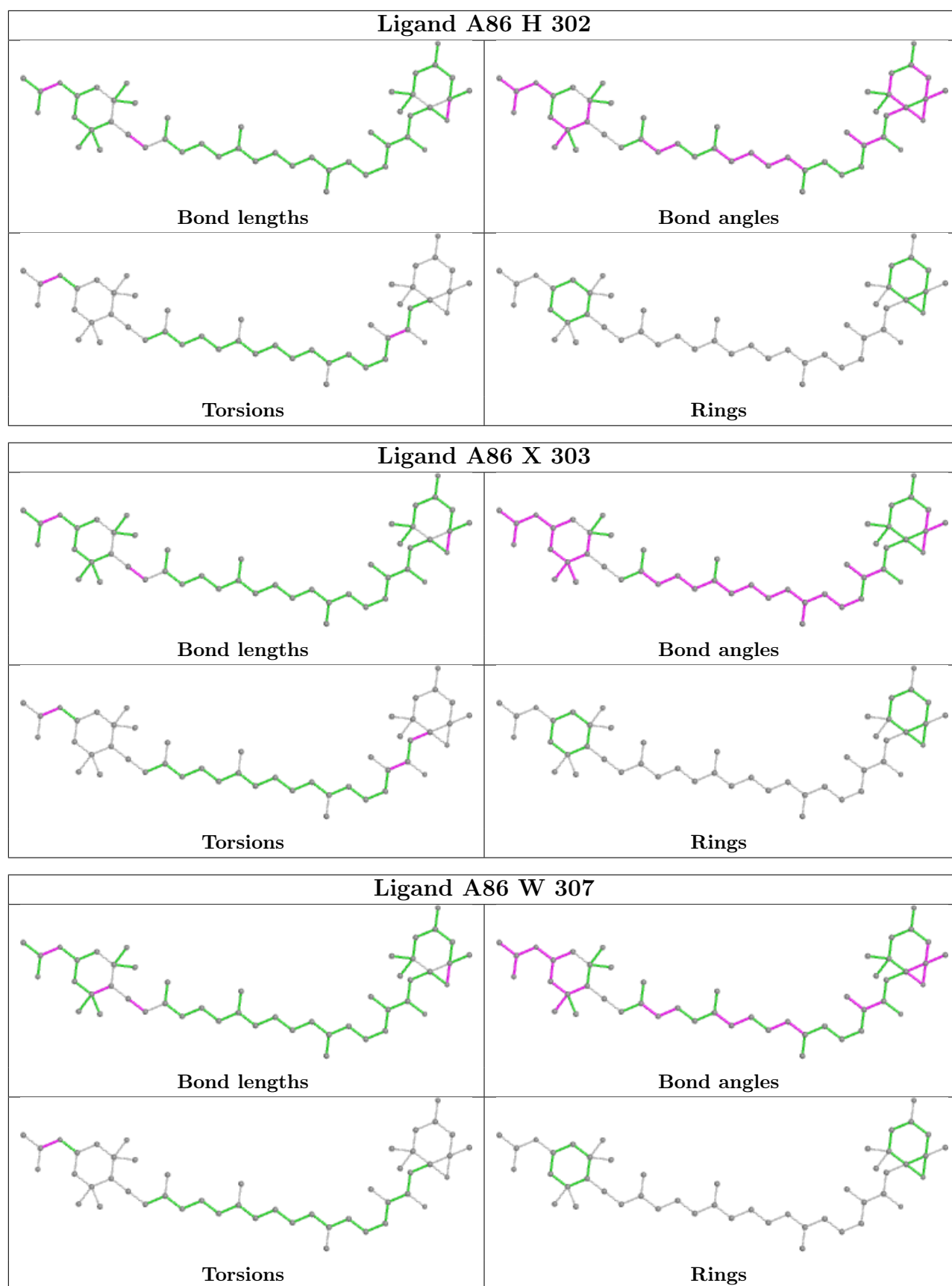


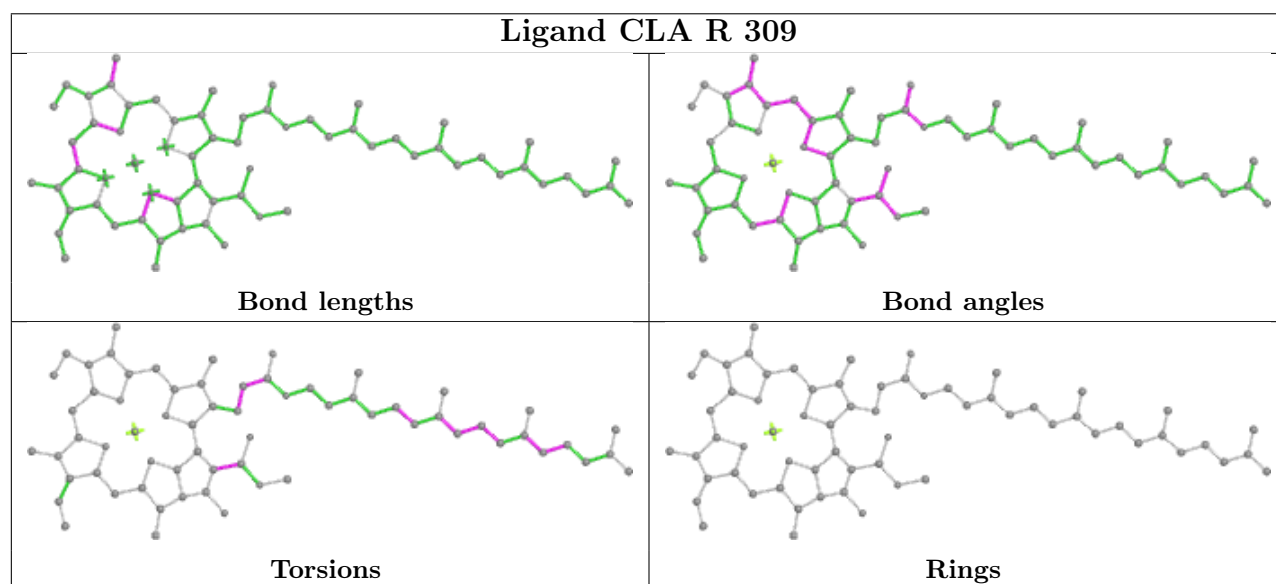
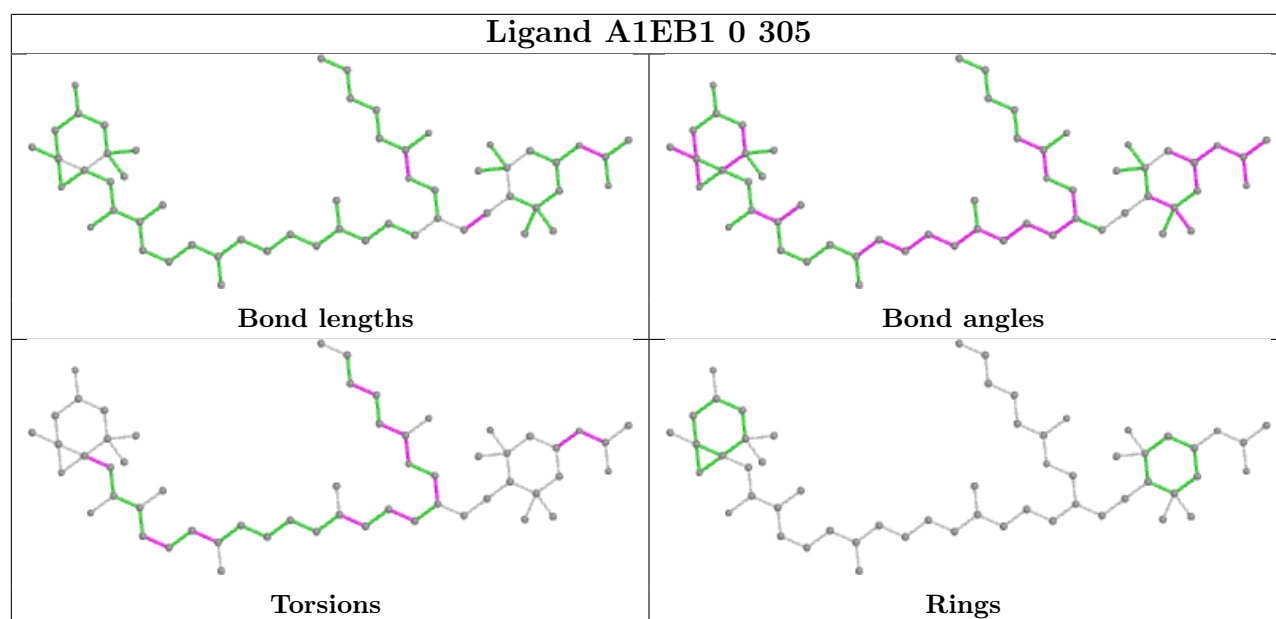
Torsions



Rings

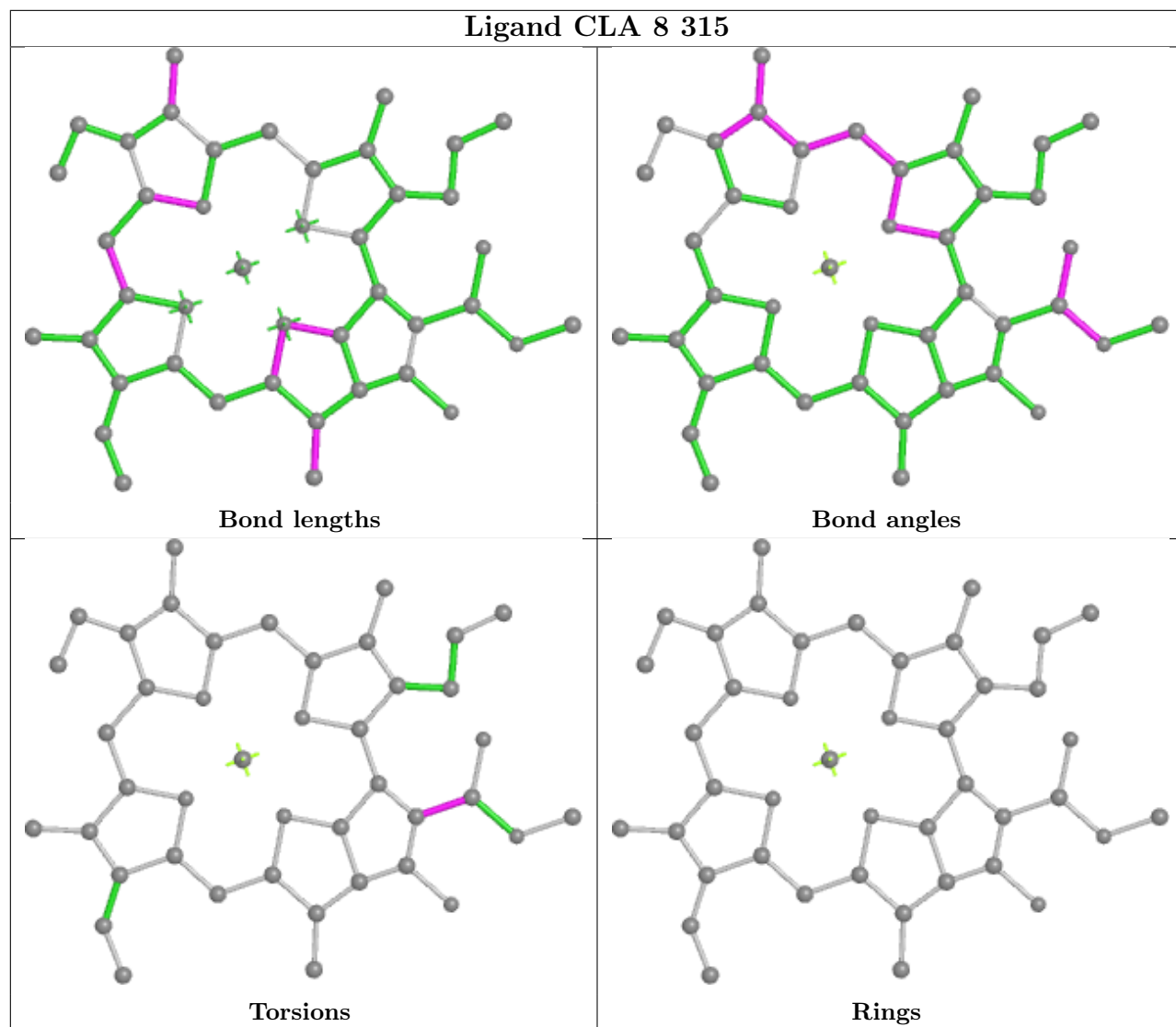




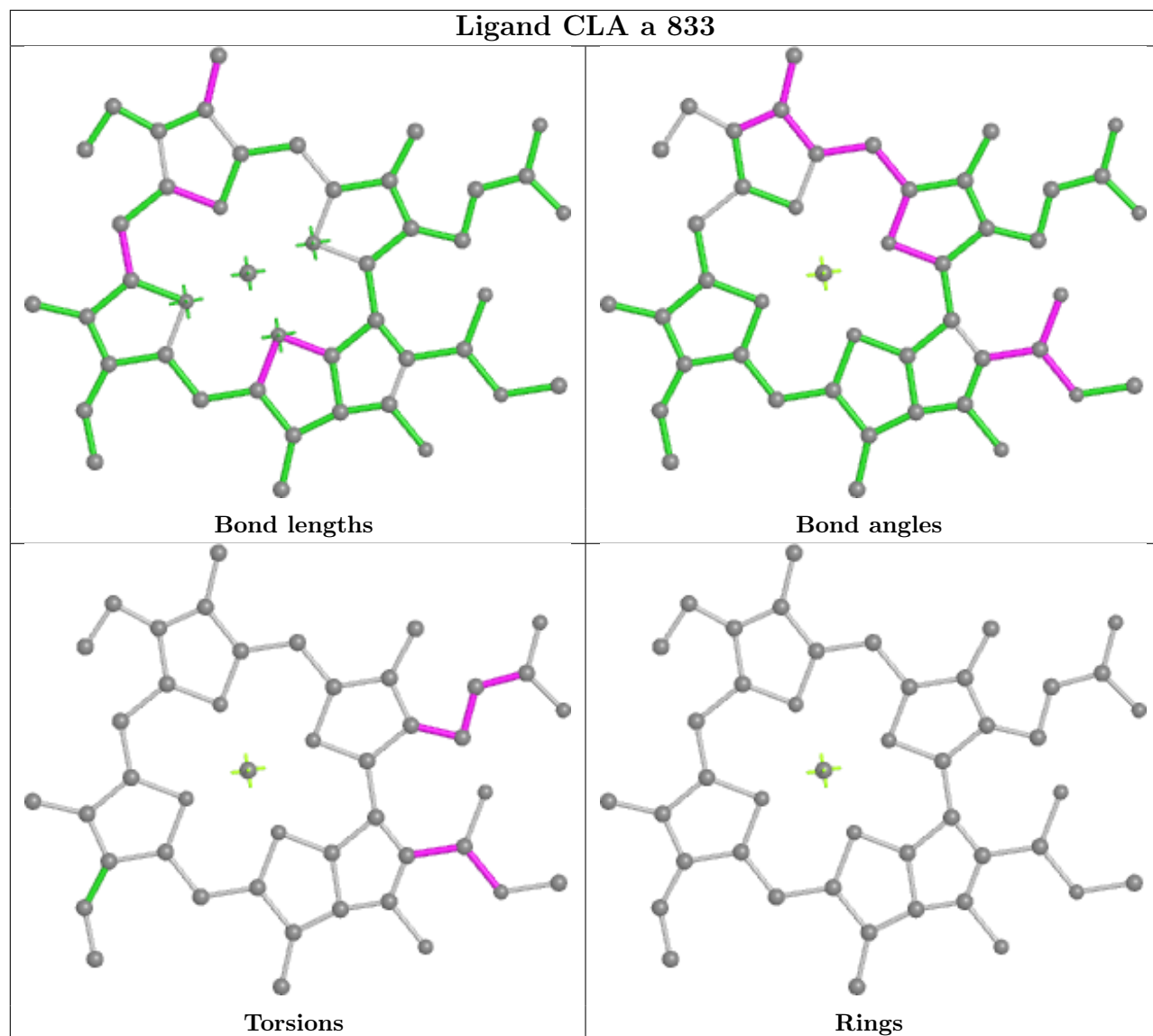




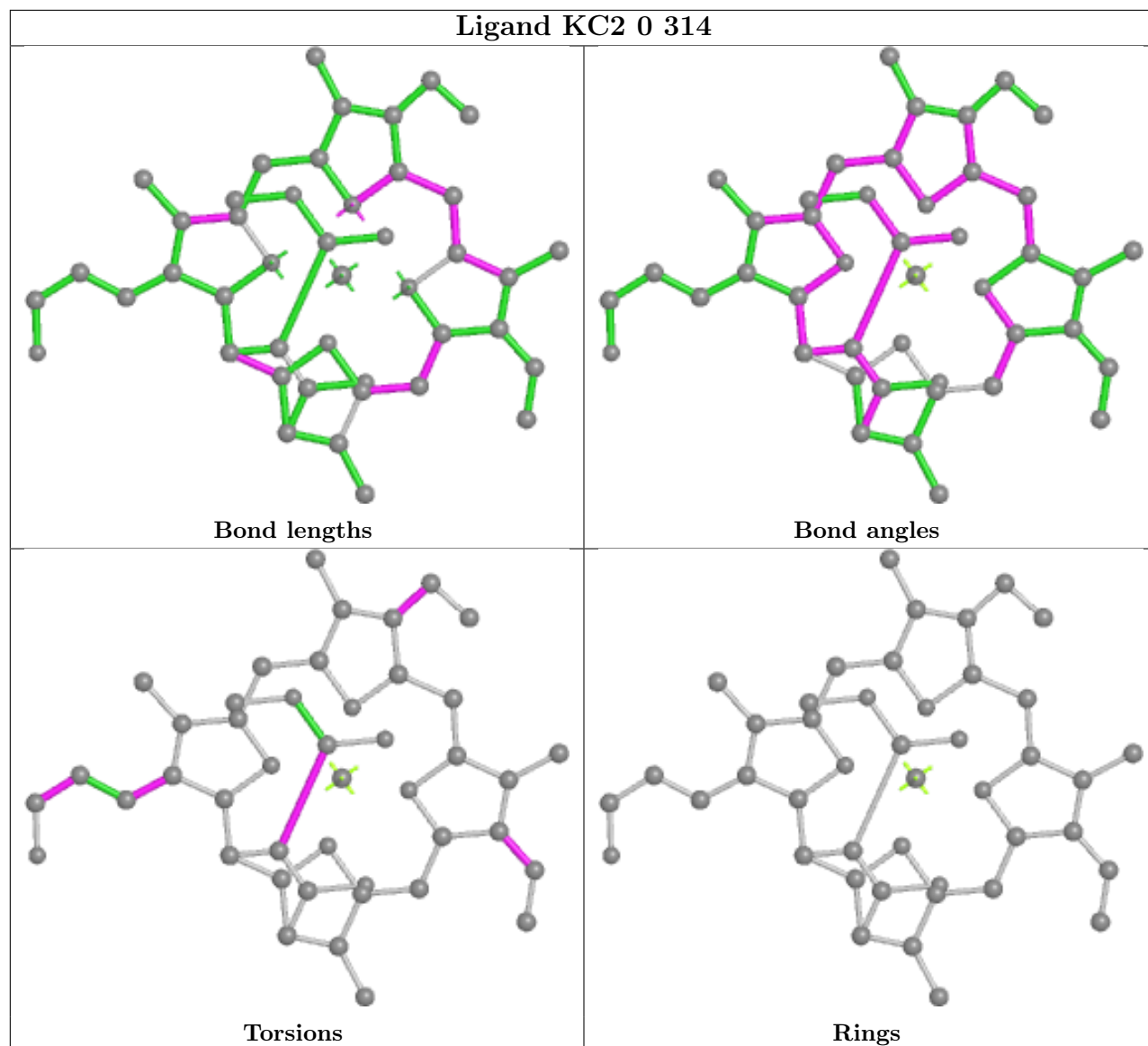
## Ligand CLA 8 315



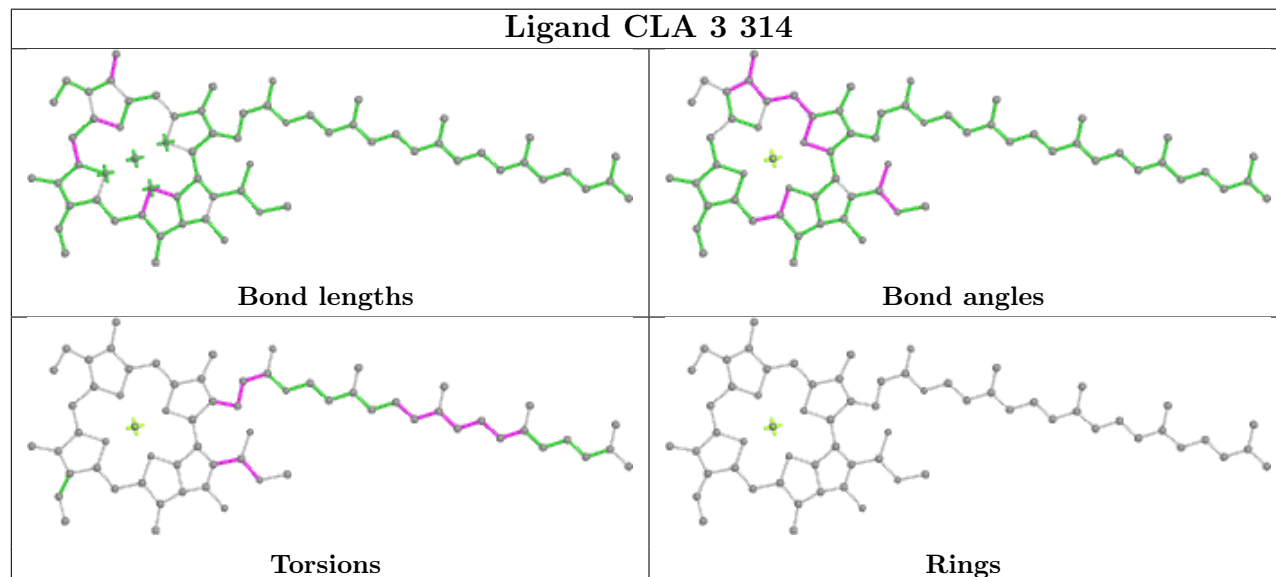
## Ligand CLA a 833



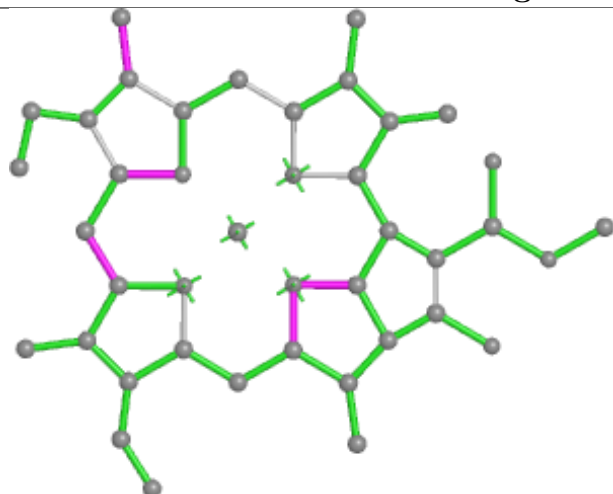
## Ligand KC2 0 314



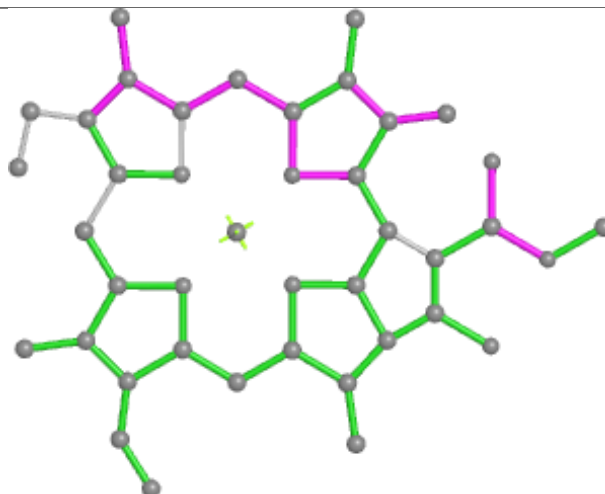
## Ligand CLA 3 314



## Ligand CLA Y 313



Bond lengths



Bond angles

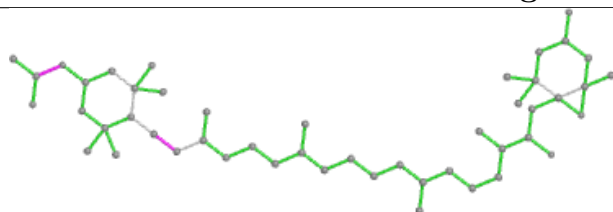


Torsions

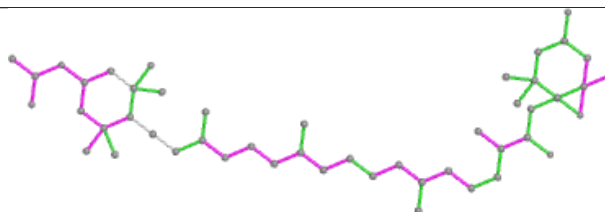


Rings

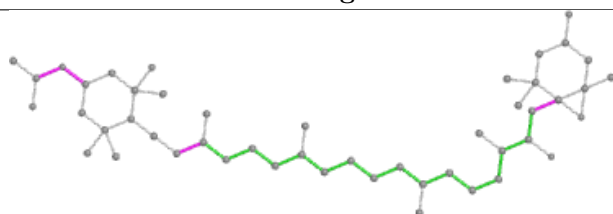
## Ligand A86 C 303



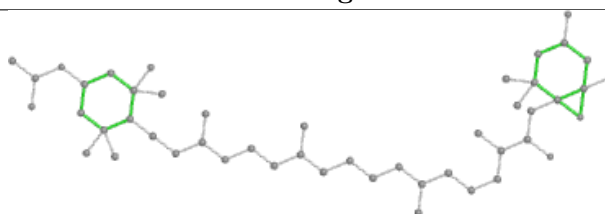
Bond lengths



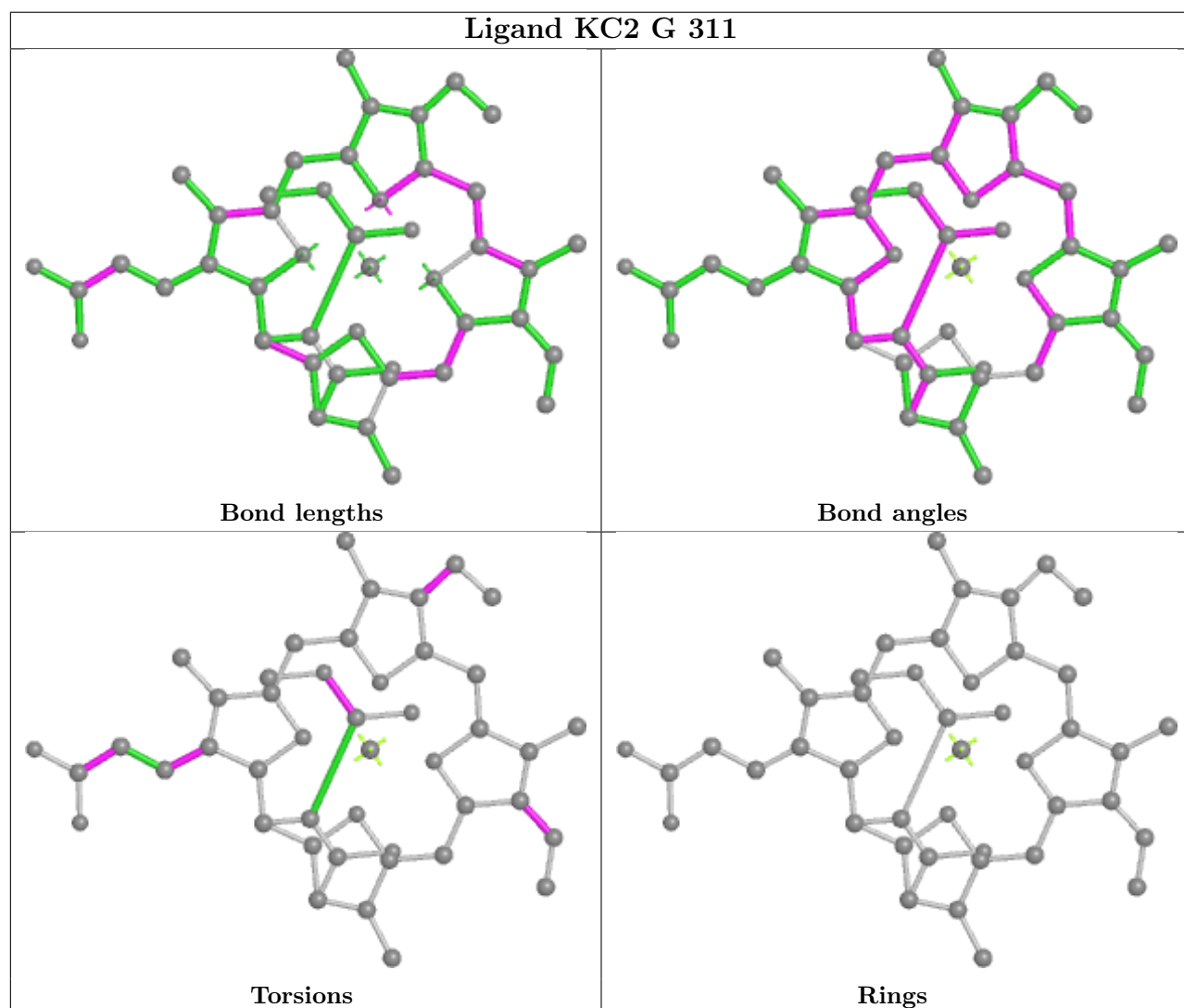
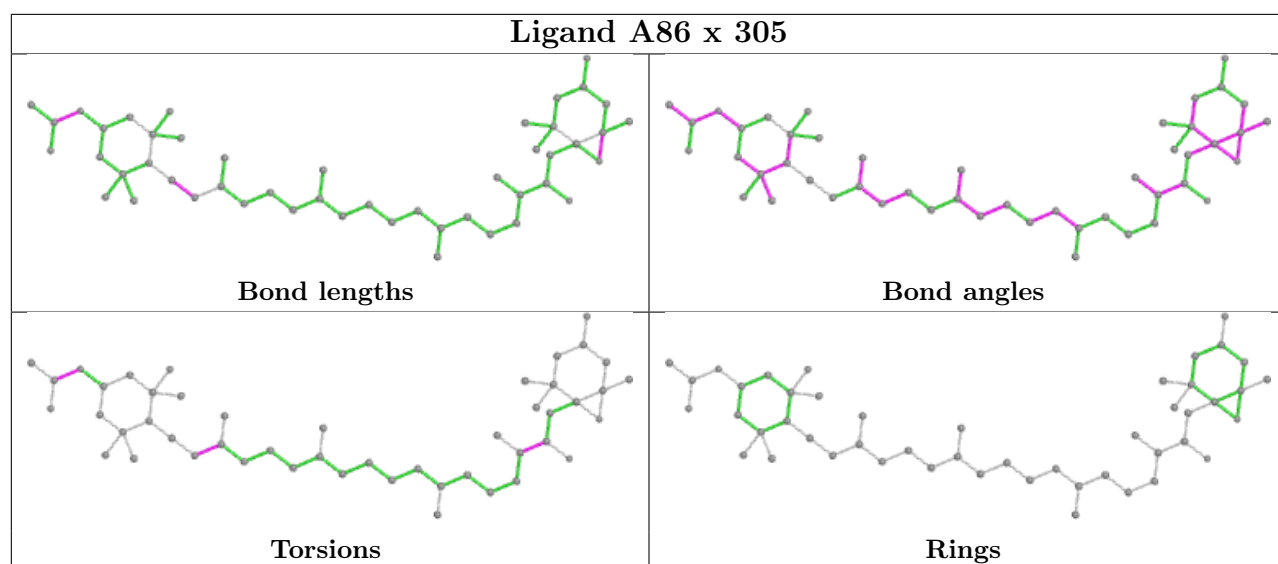
Bond angles



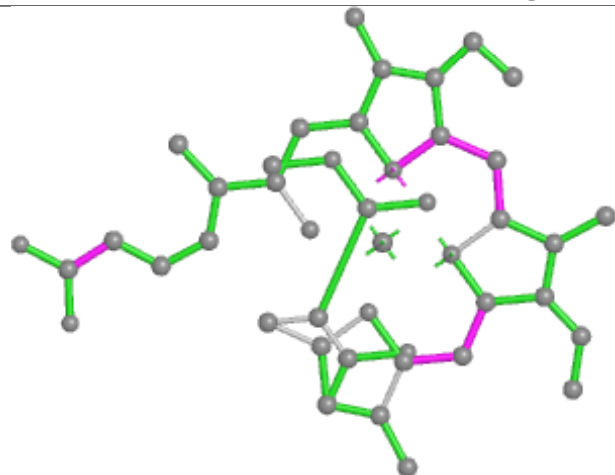
Torsions



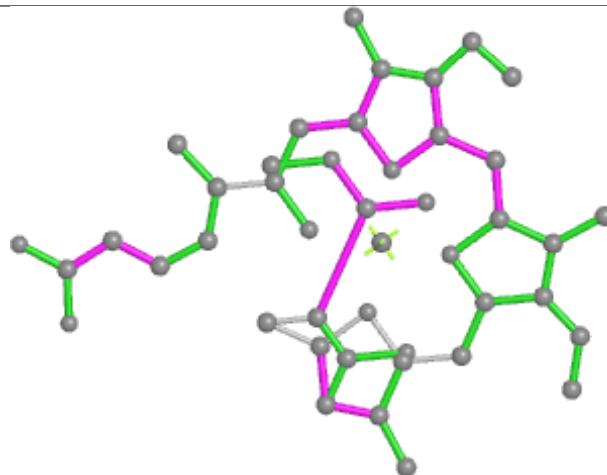
Rings



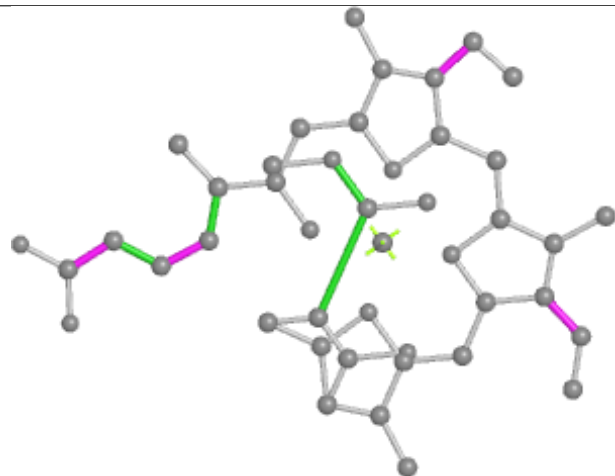
## Ligand KC2 z 313



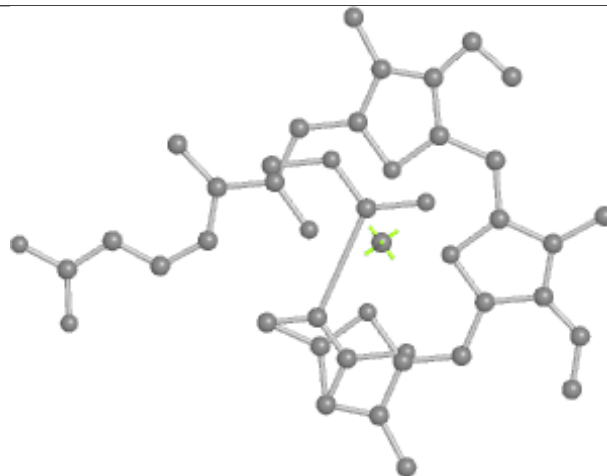
Bond lengths



Bond angles

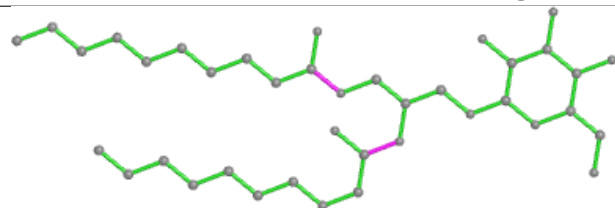


Torsions

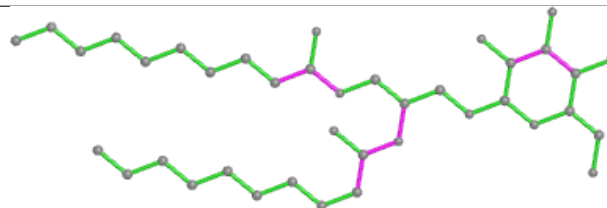


Rings

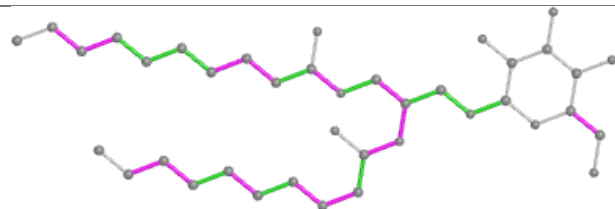
## Ligand LMG P 317



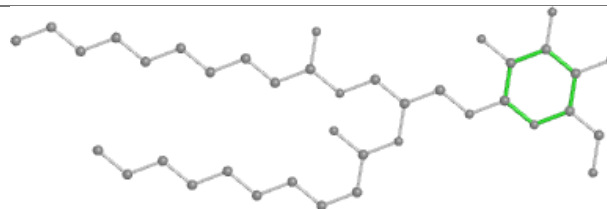
Bond lengths



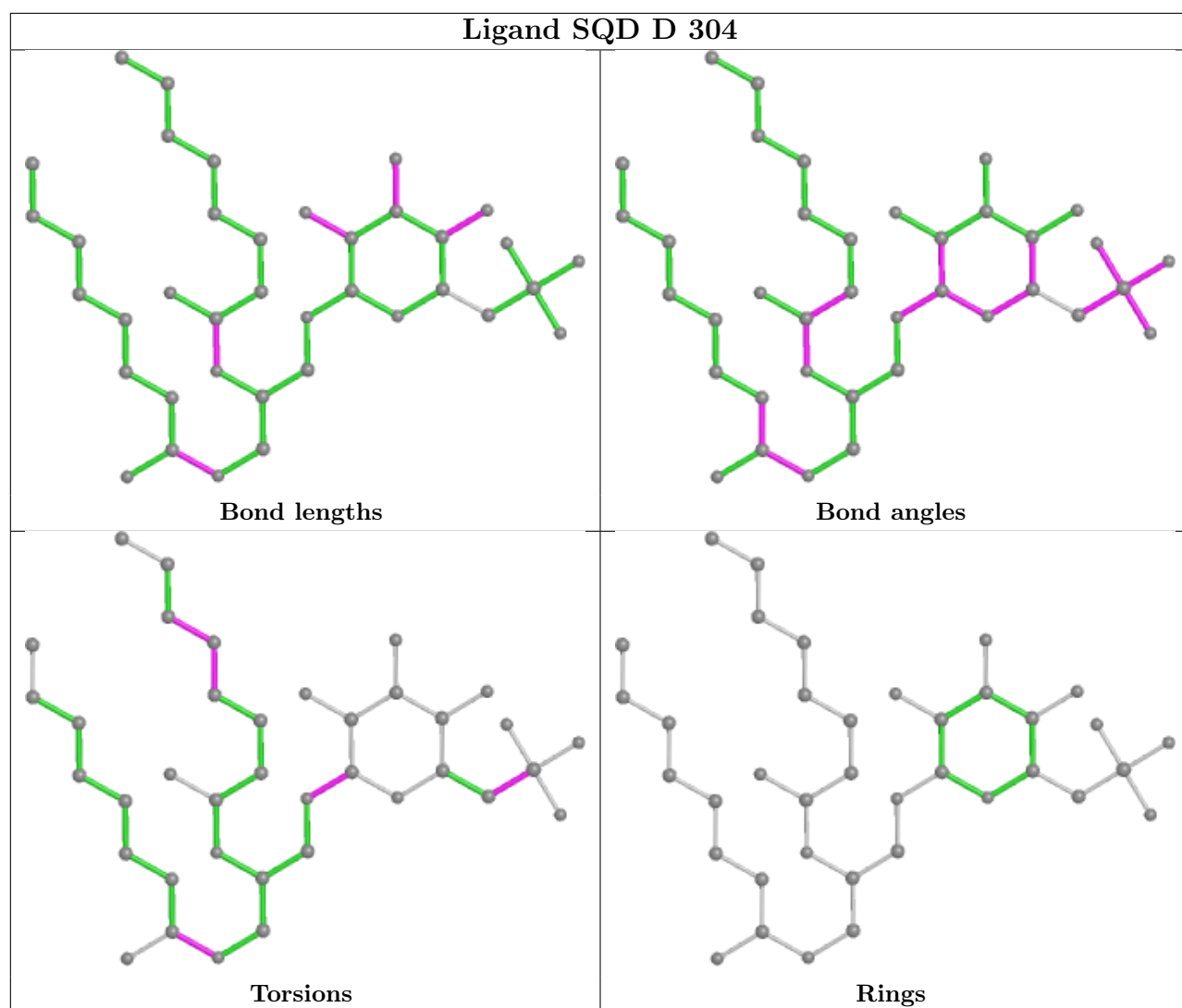
Bond angles

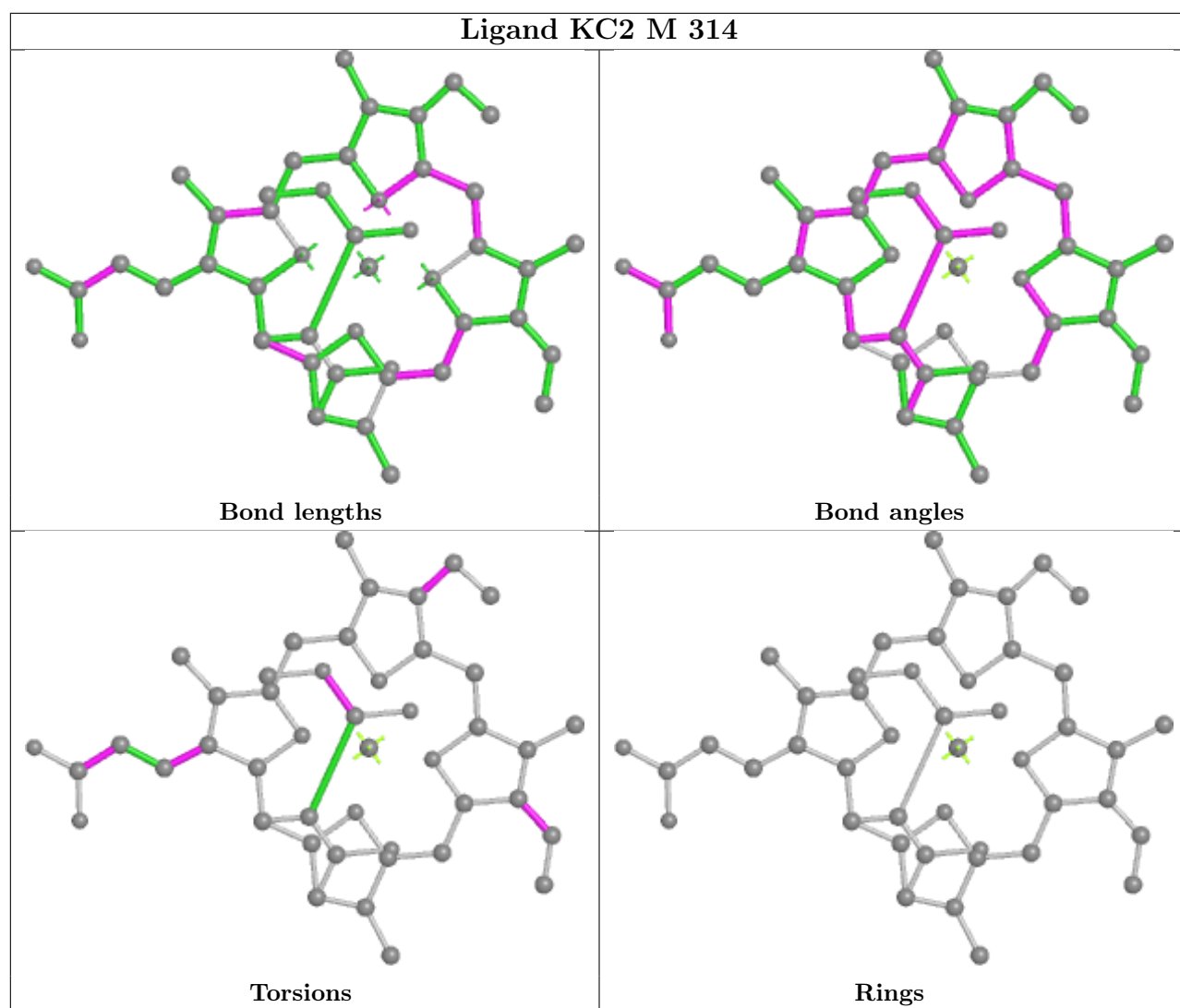


Torsions



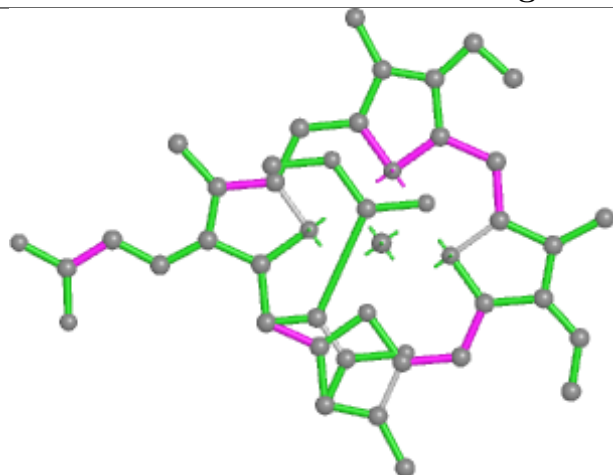
Rings



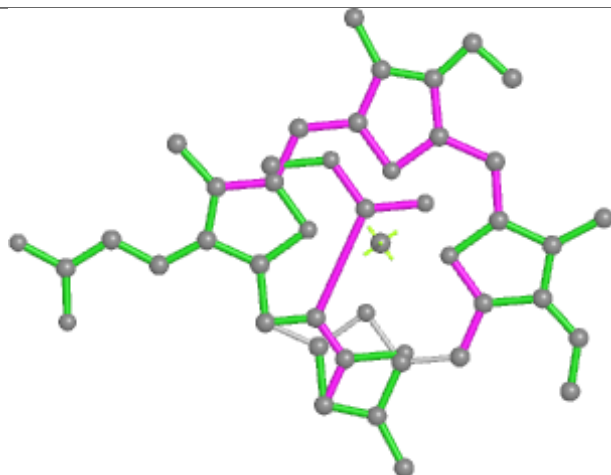




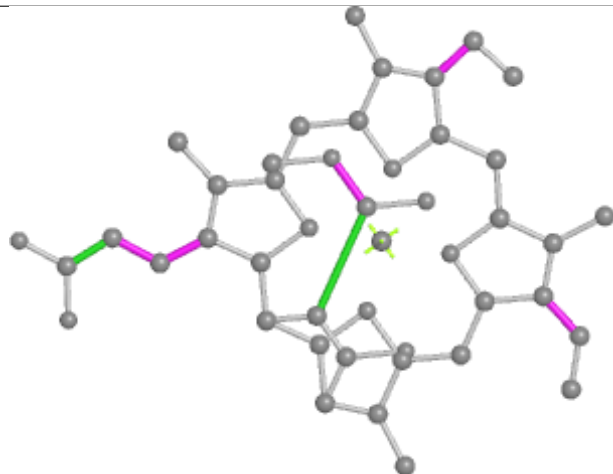
## Ligand KC2 L 312



Bond lengths



Bond angles

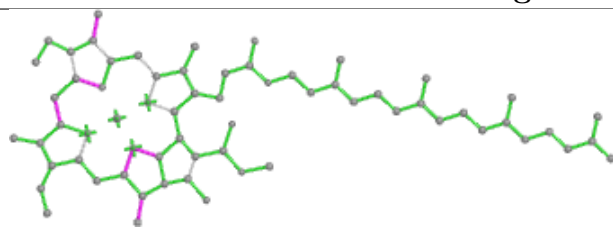


Torsions

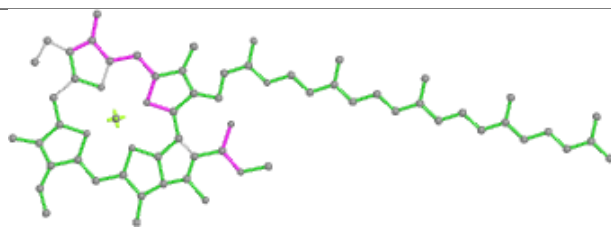


Rings

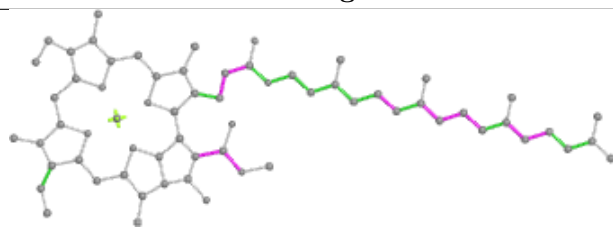
## Ligand CLA V 311



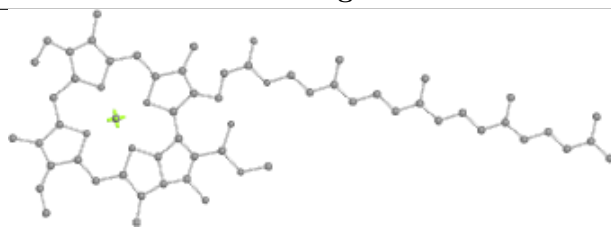
Bond lengths



Bond angles

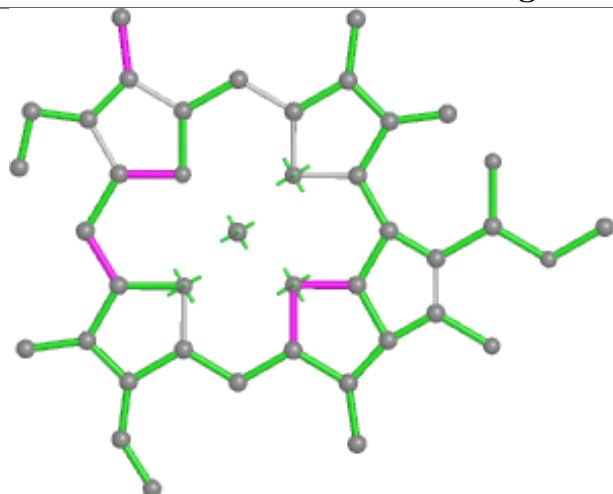


Torsions

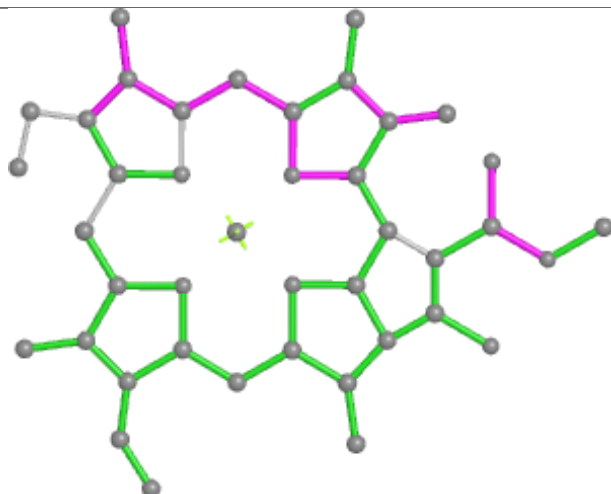


Rings

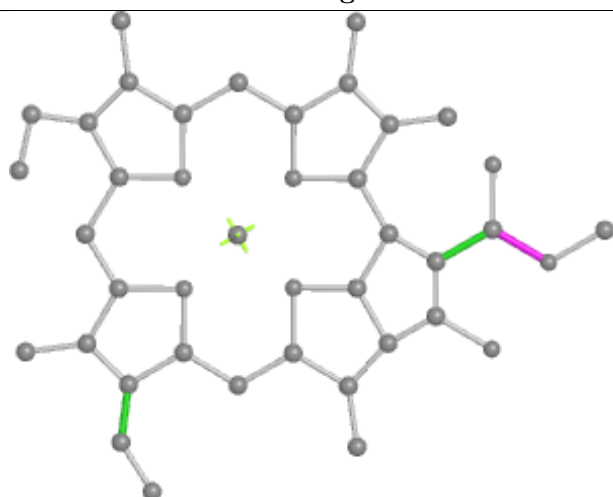
## Ligand CLA 9 307



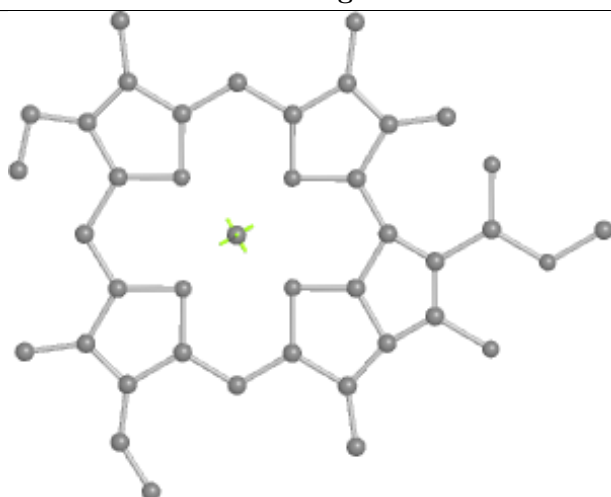
Bond lengths



Bond angles

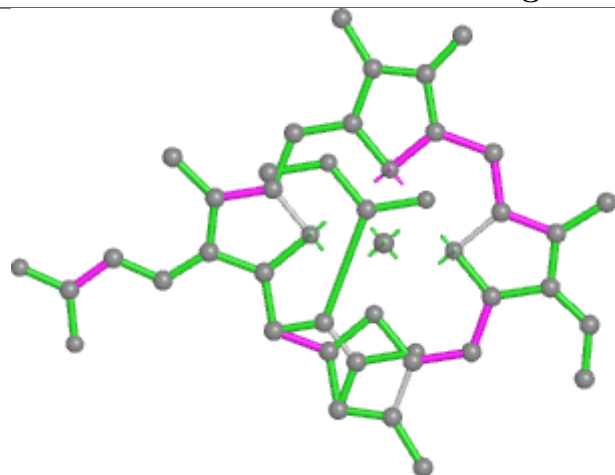


Torsions

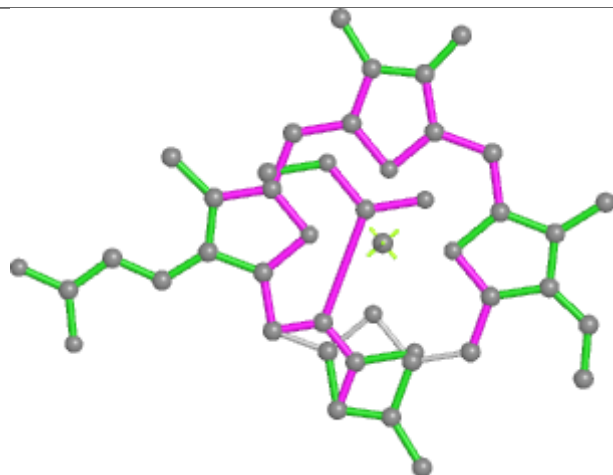


Rings

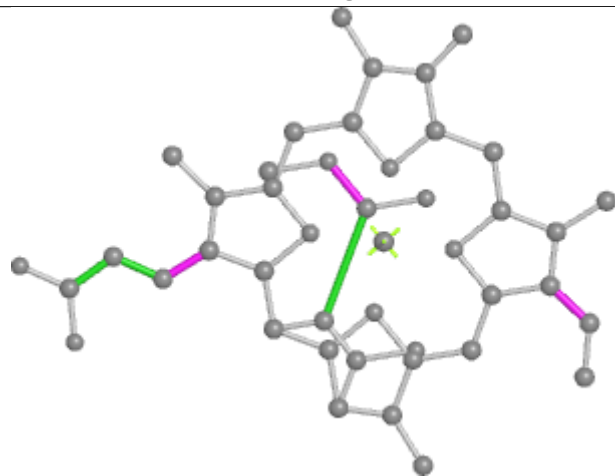
## Ligand KC2 2 313



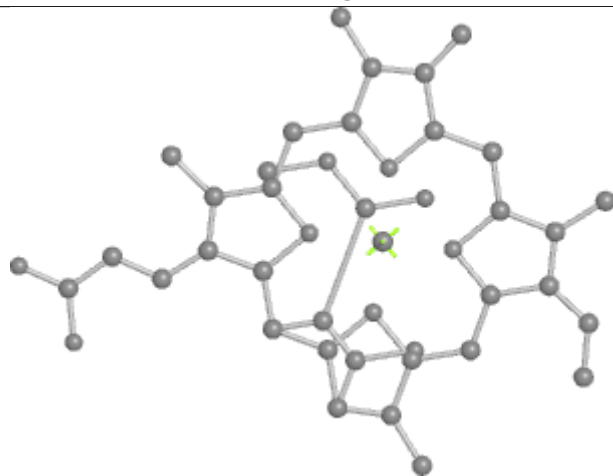
Bond lengths



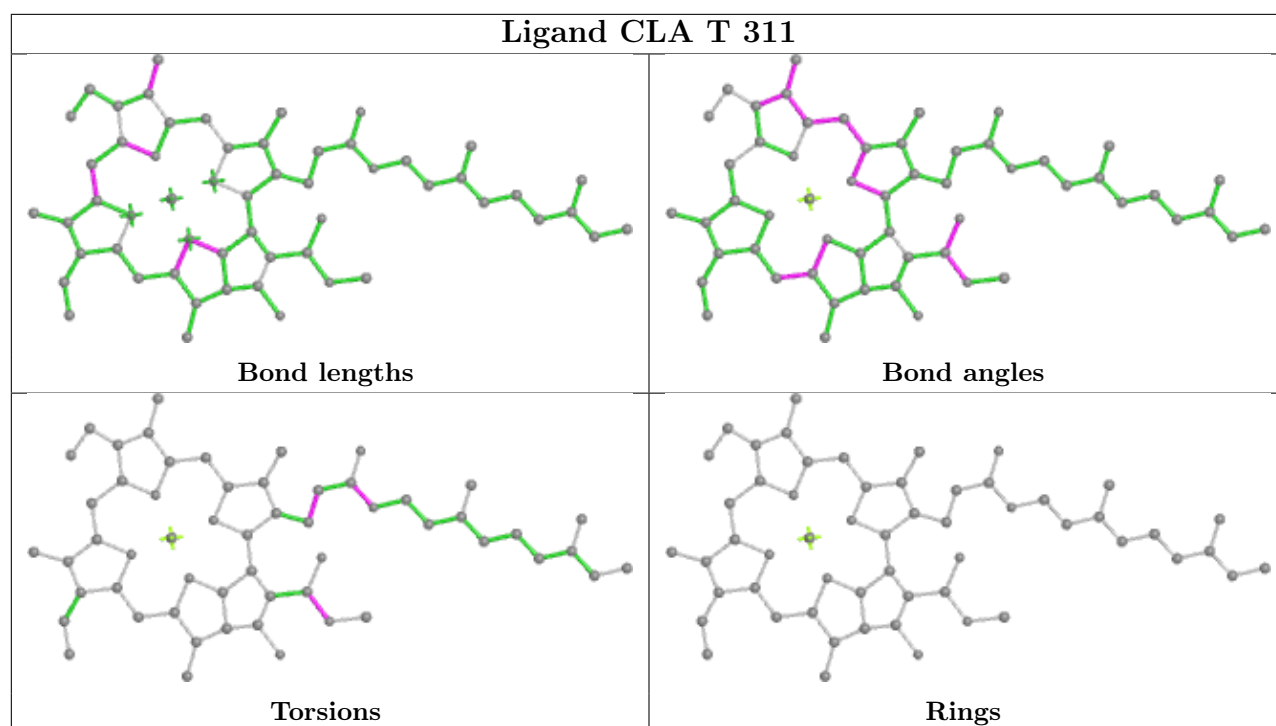
Bond angles



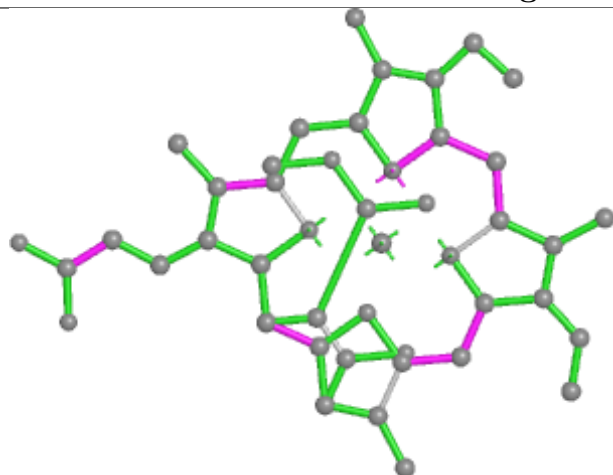
Torsions



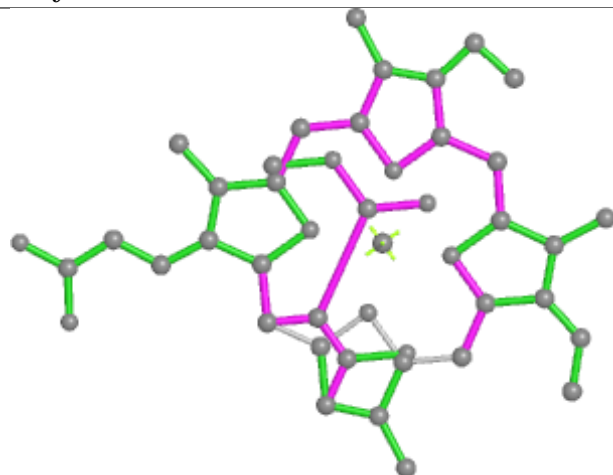
Rings



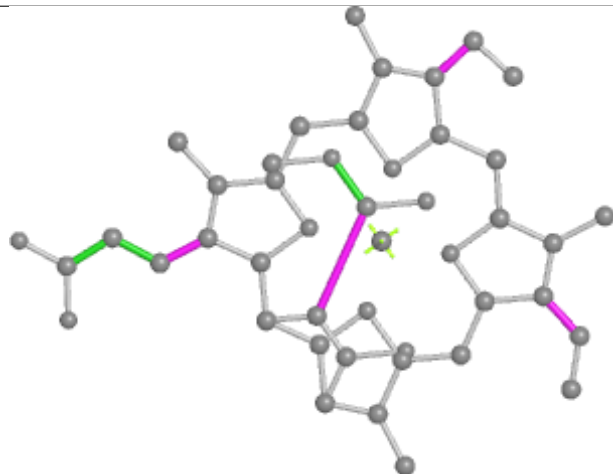
## Ligand KC2 y 314



Bond lengths



Bond angles

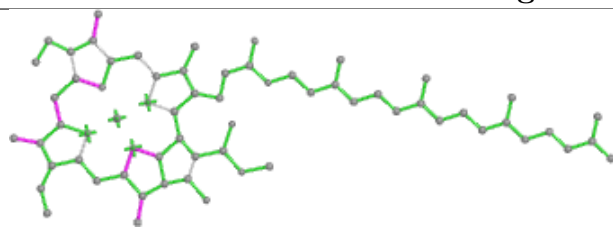


Torsions

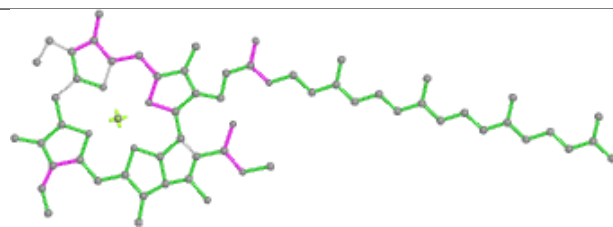


Rings

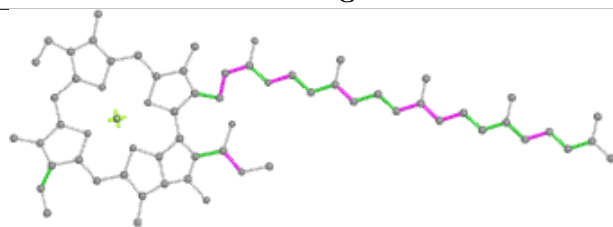
## Ligand CLA b 807



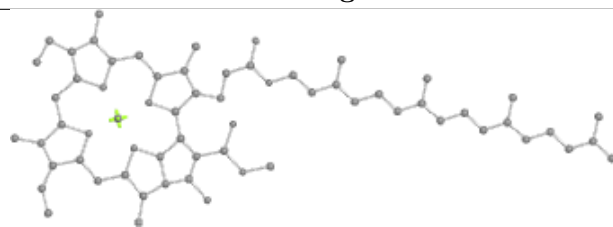
Bond lengths



Bond angles

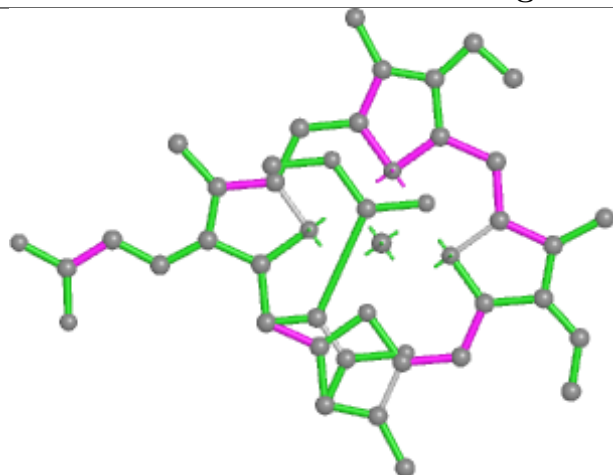


Torsions

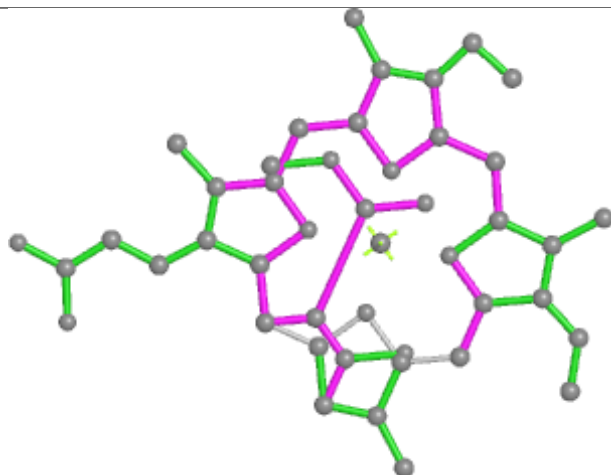


Rings

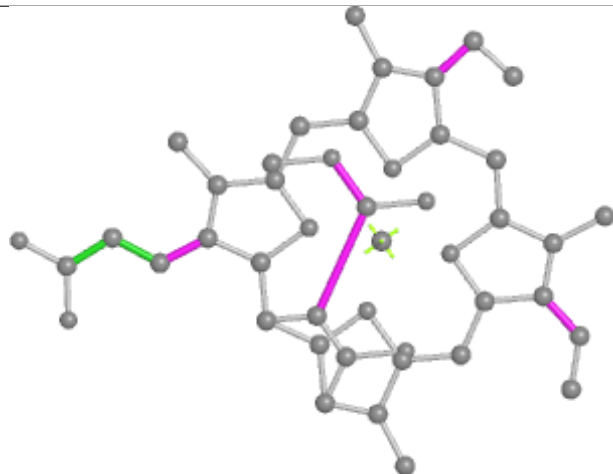
## Ligand KC2 P 306



Bond lengths



Bond angles

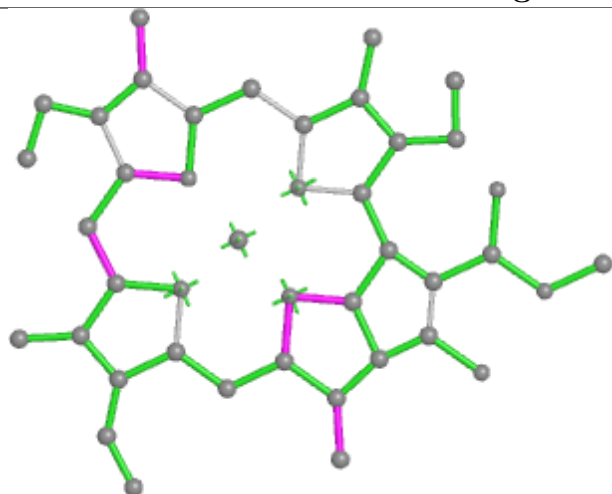


Torsions

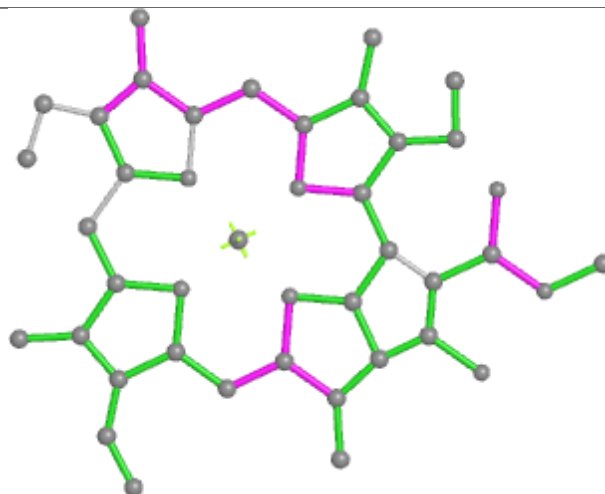


Rings

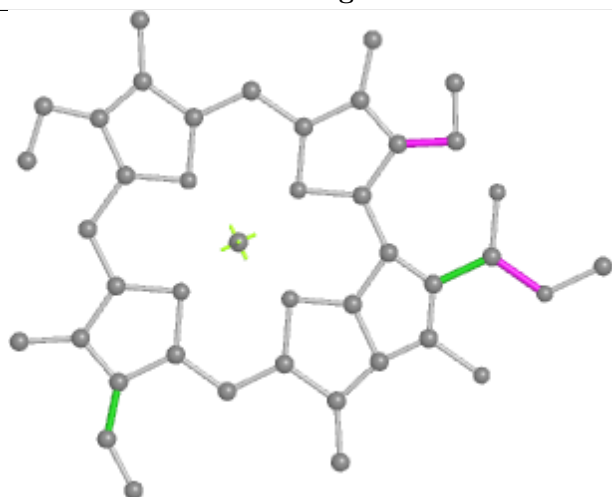
## Ligand CLA B 206



Bond lengths



Bond angles

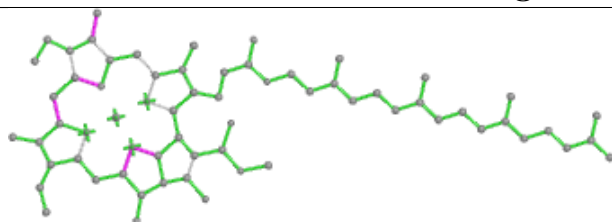


Torsions

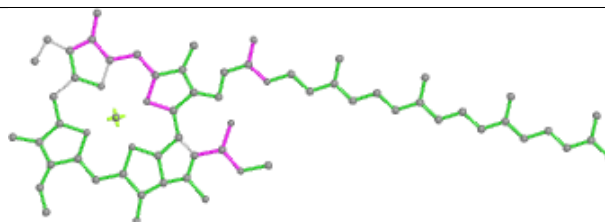


Rings

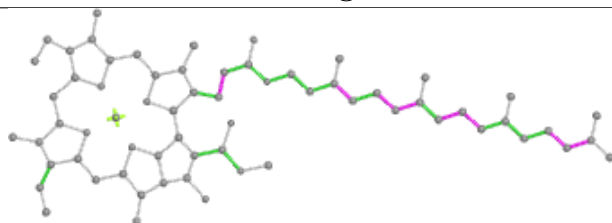
## Ligand CLA E 308



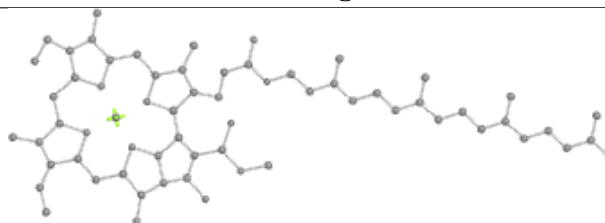
Bond lengths



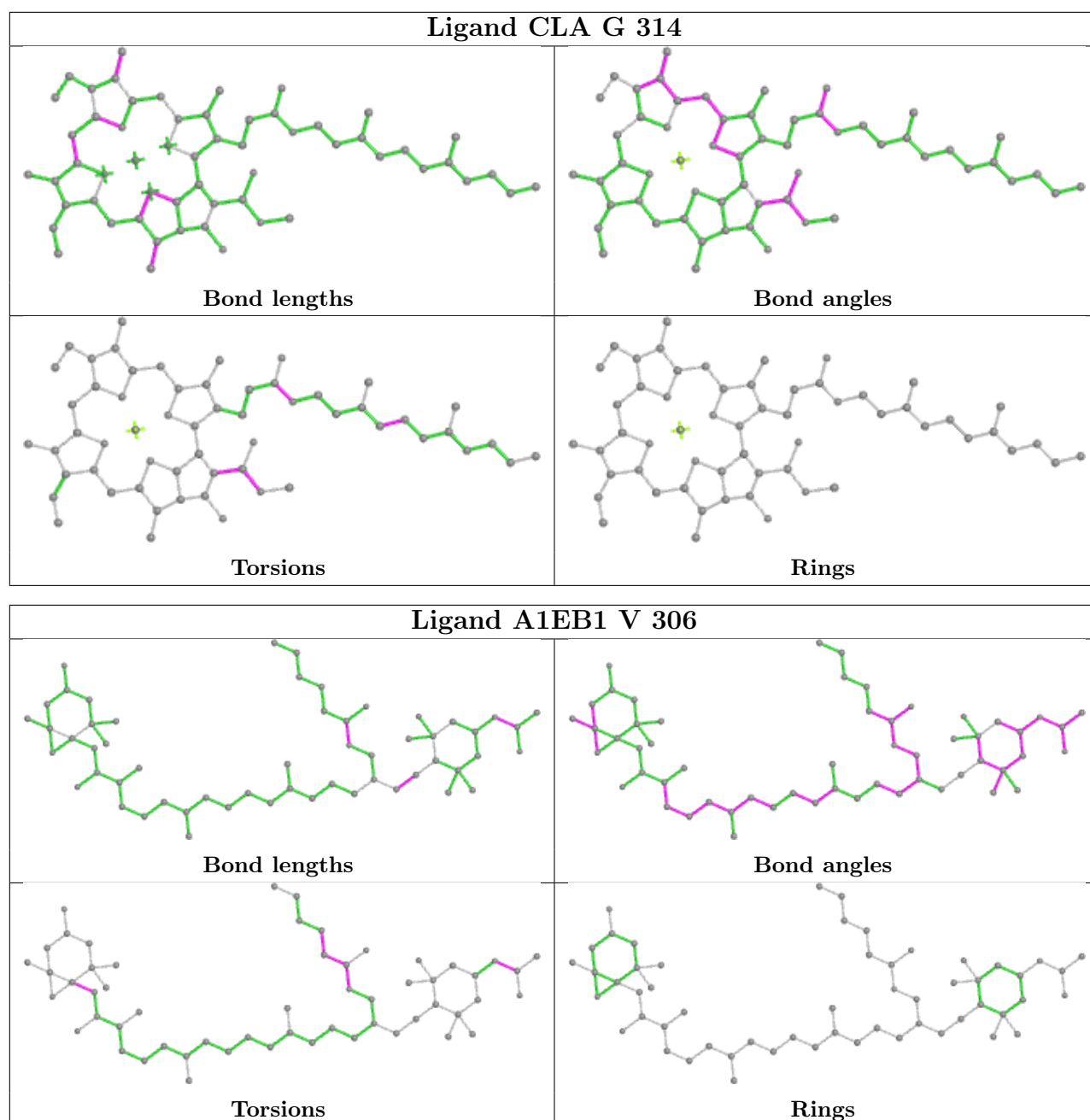
Bond angles



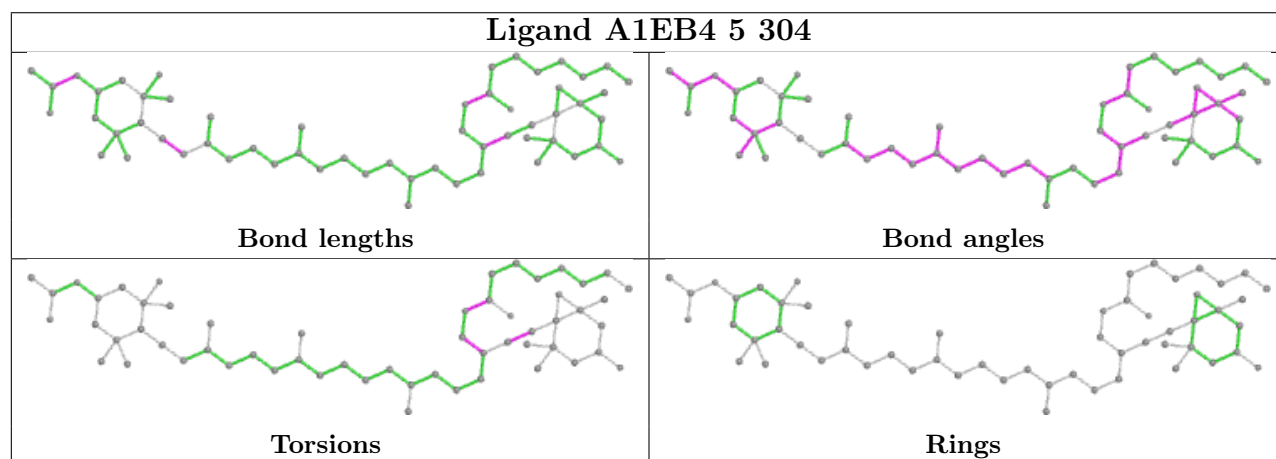
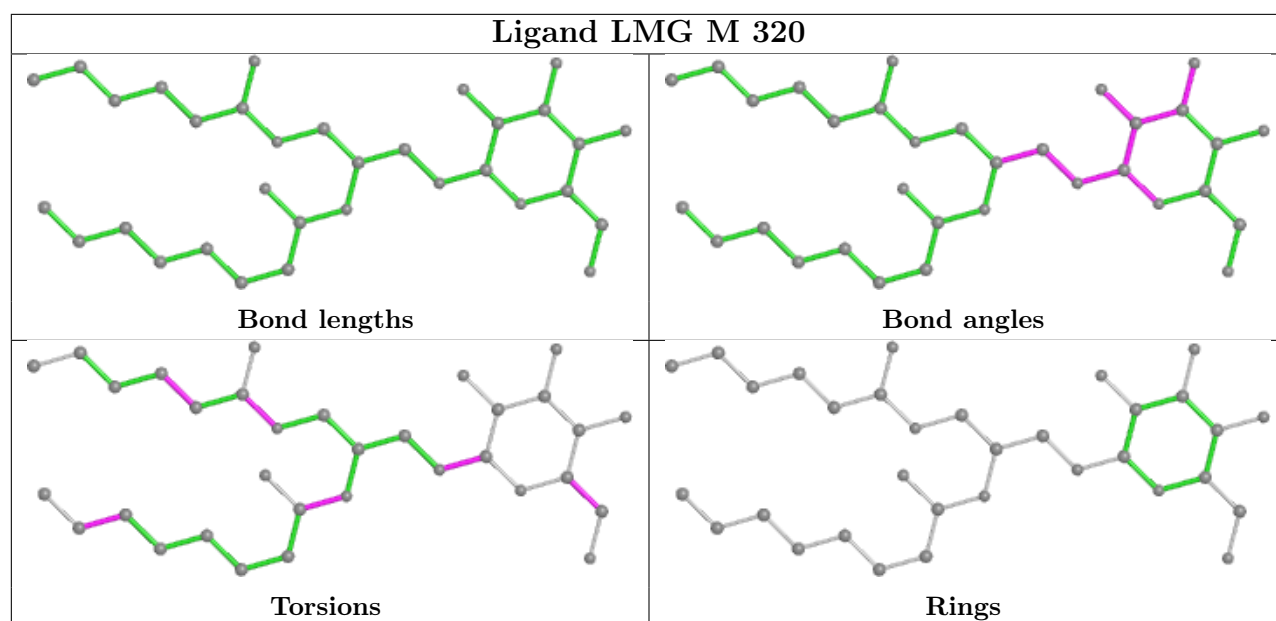
Torsions



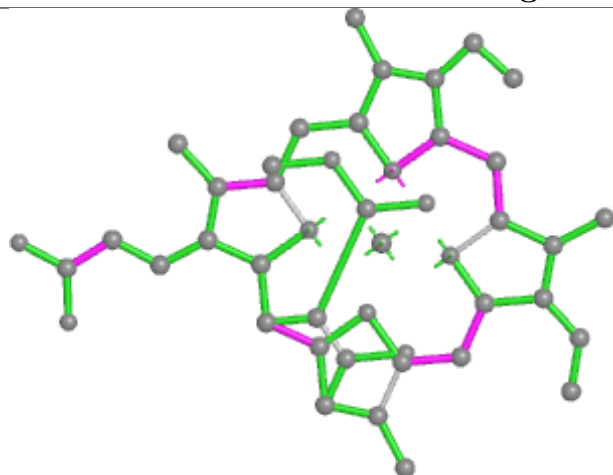
Rings



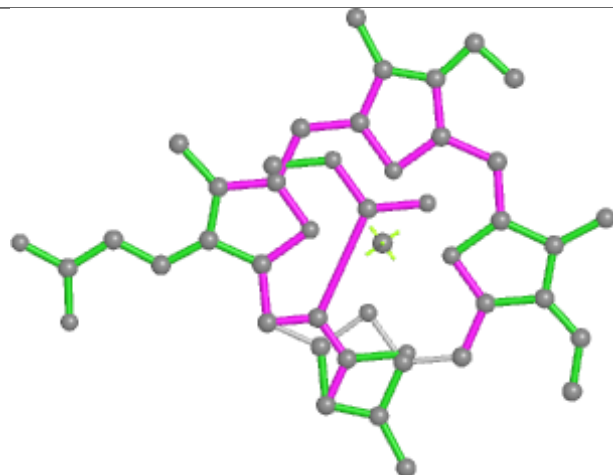




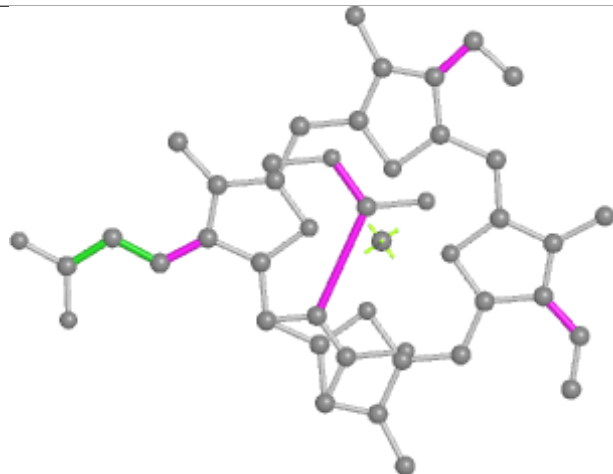
## Ligand KC2 6 317



Bond lengths



Bond angles

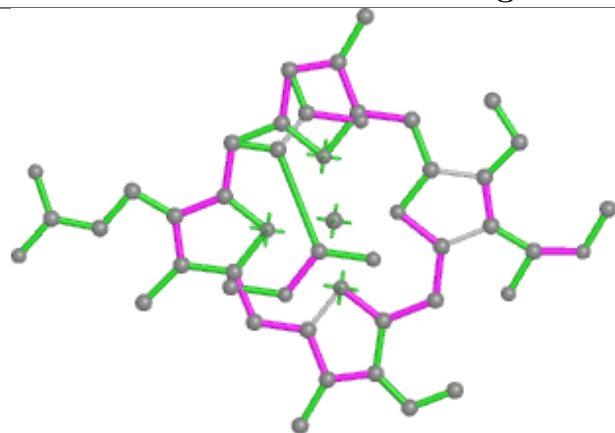


Torsions

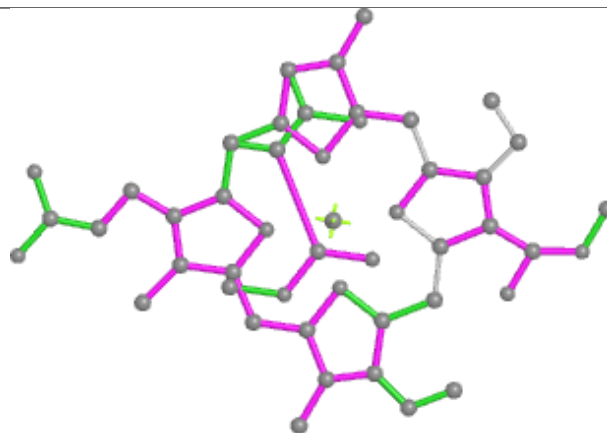


Rings

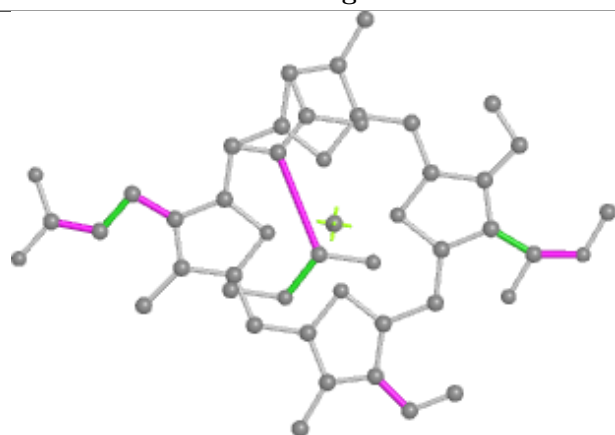
## Ligand A1ECV 4 315



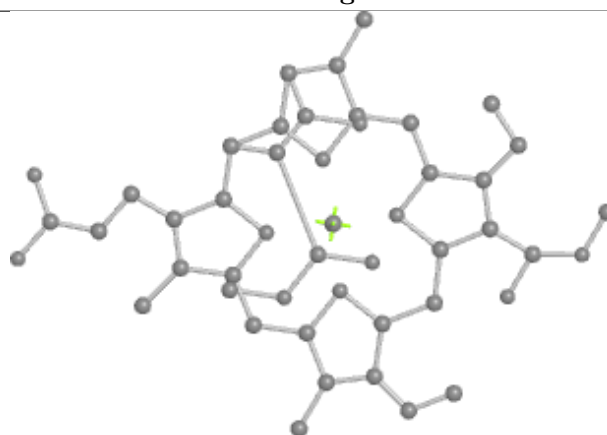
Bond lengths



Bond angles

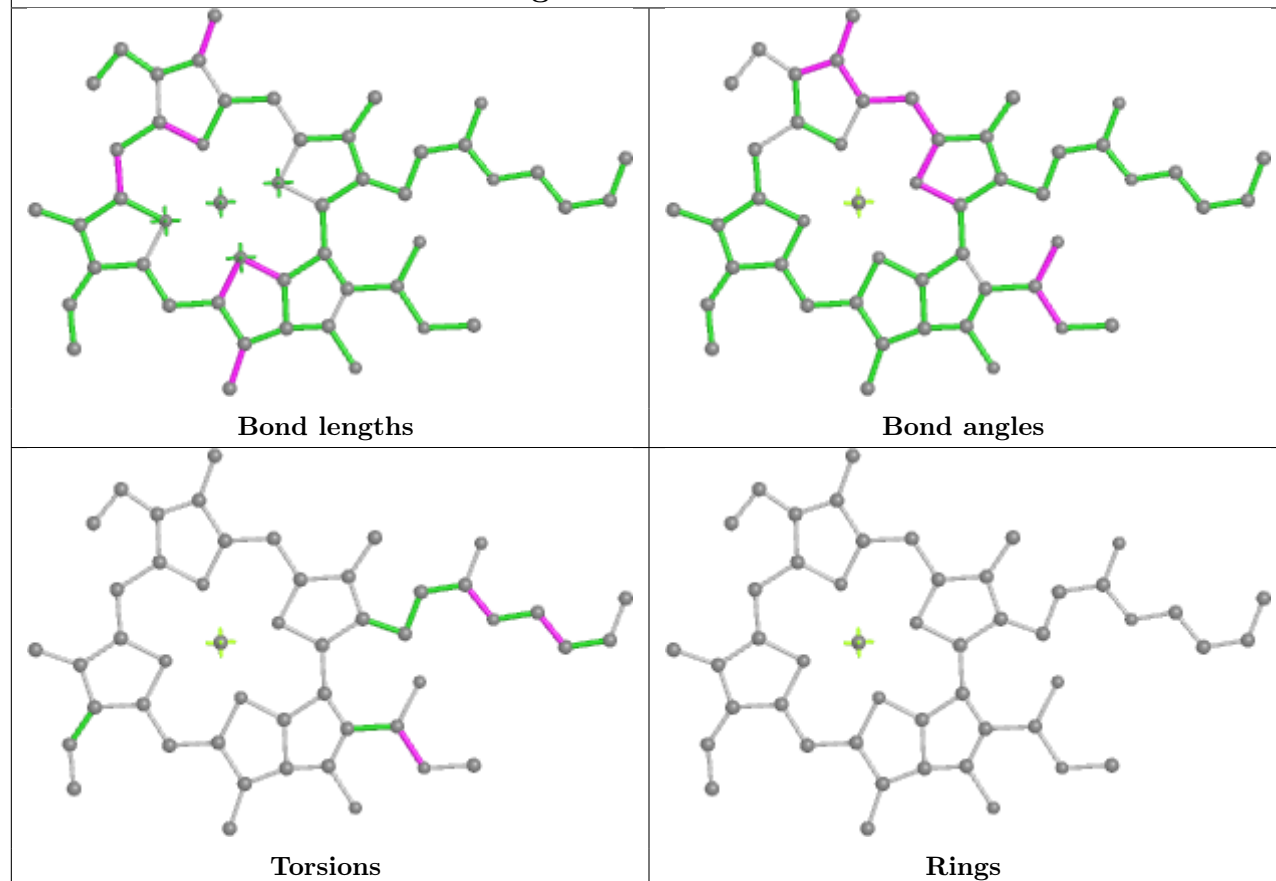


Torsions

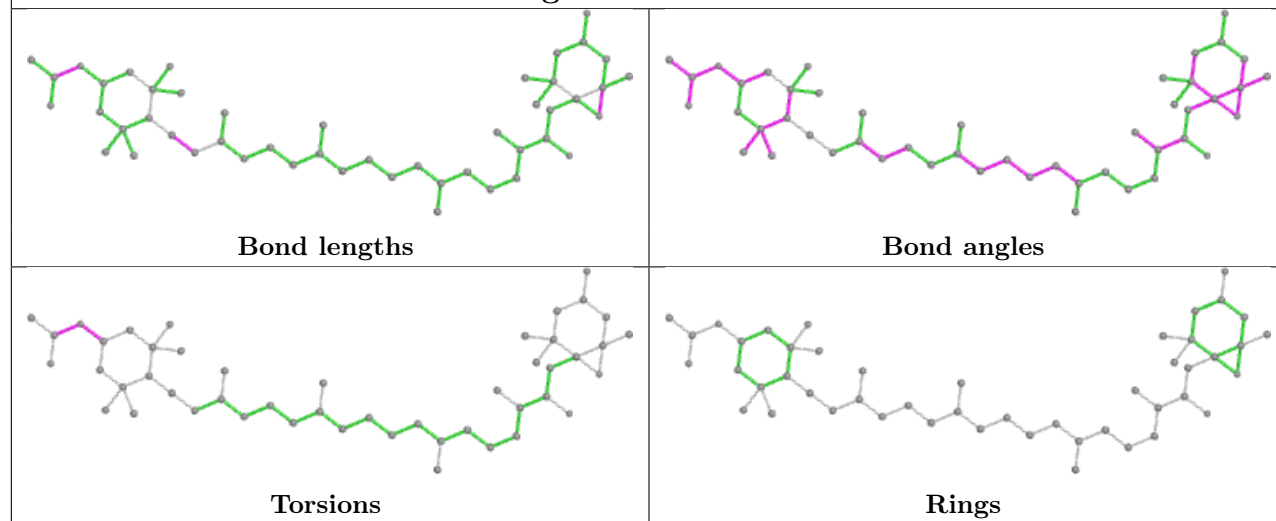


Rings

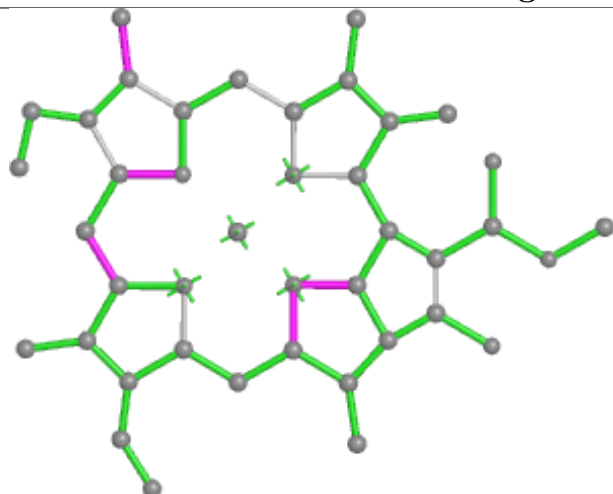
## Ligand CLA A 305



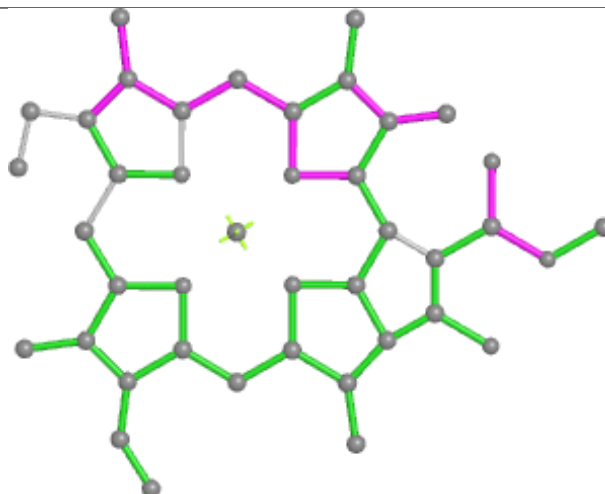
## Ligand A86 7 307



## Ligand CLA 1 317



Bond lengths



Bond angles

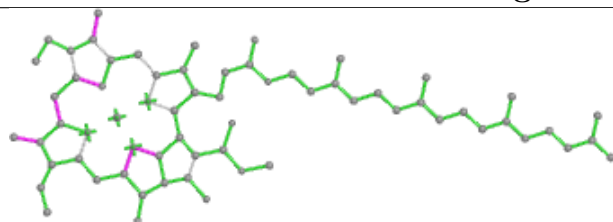


Torsions

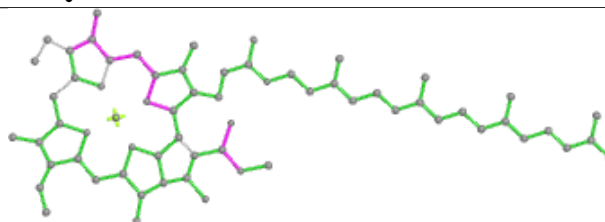


Rings

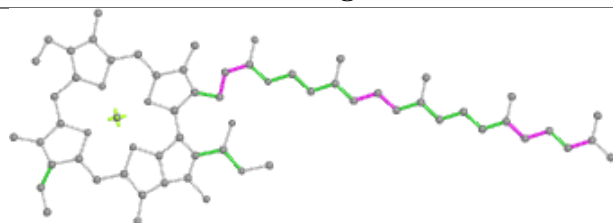
## Ligand CLA Q 312



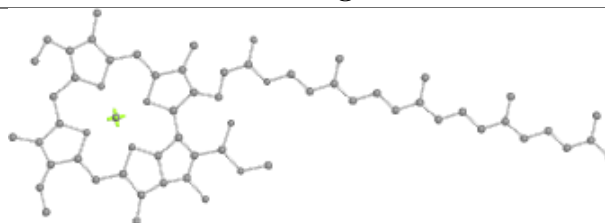
Bond lengths



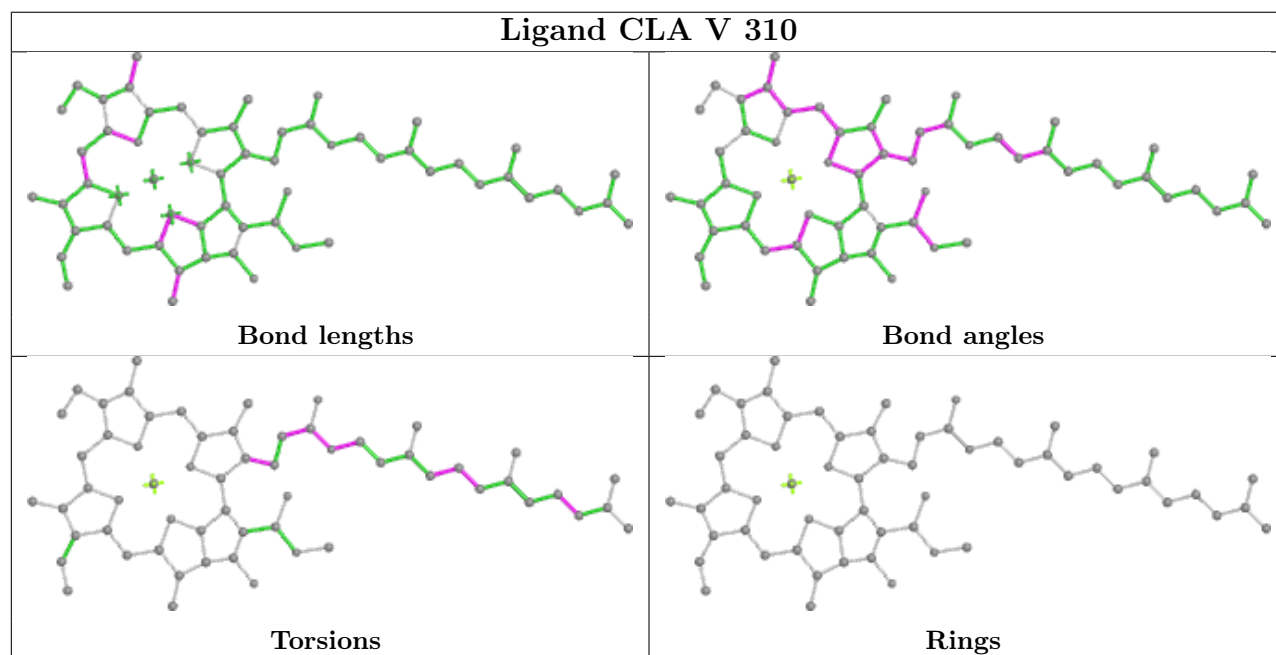
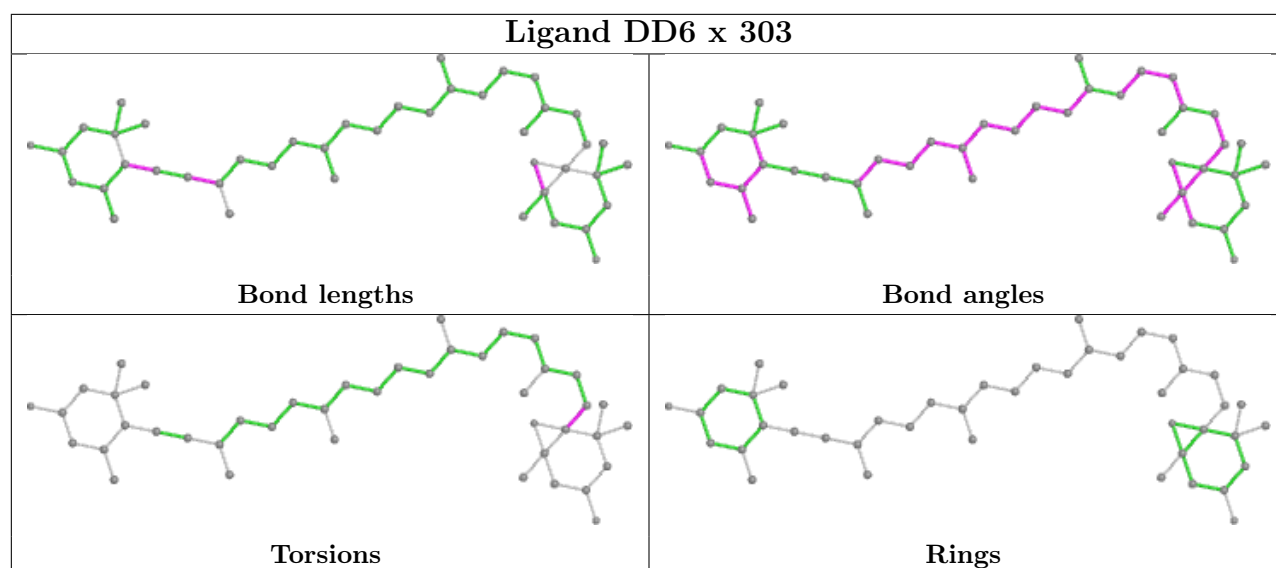
Bond angles



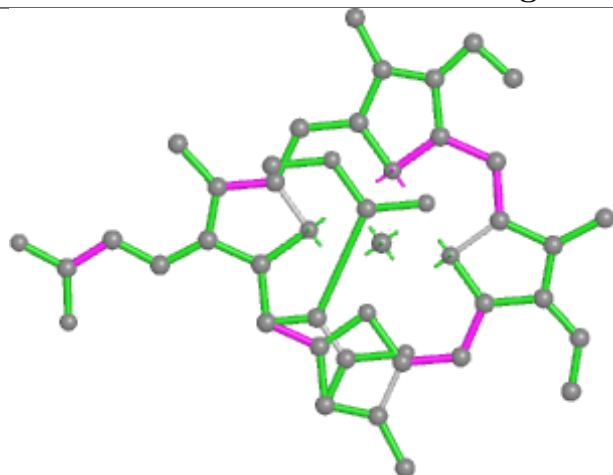
Torsions



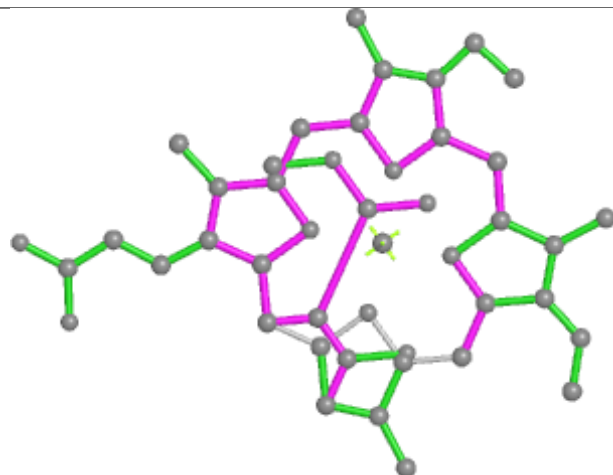
Rings



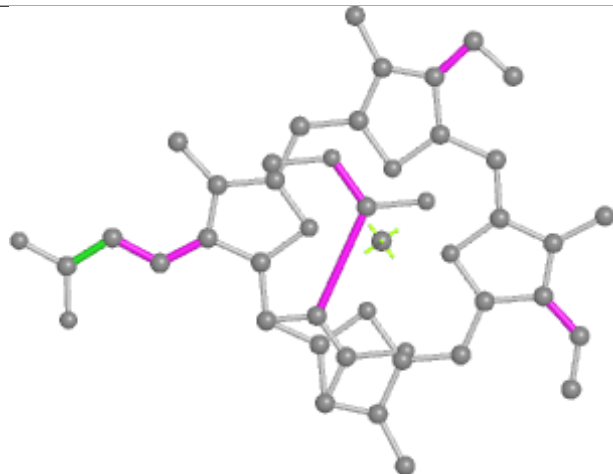
## Ligand KC2 J 315



Bond lengths



Bond angles

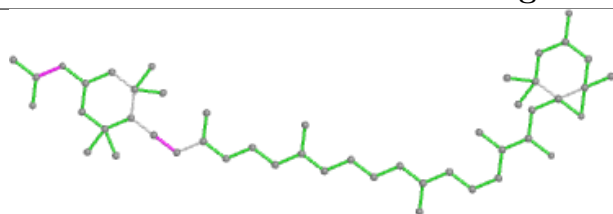


Torsions

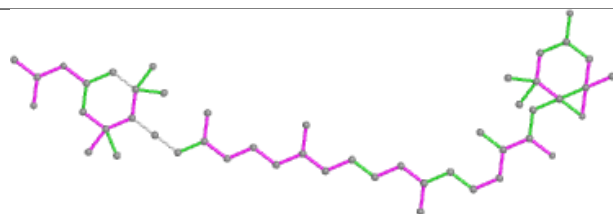


Rings

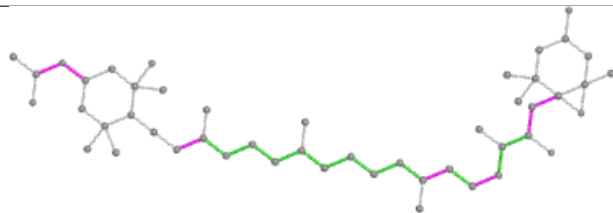
## Ligand A86 G 301



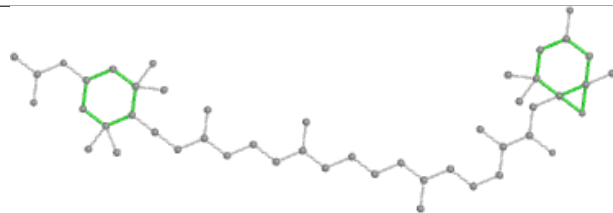
Bond lengths



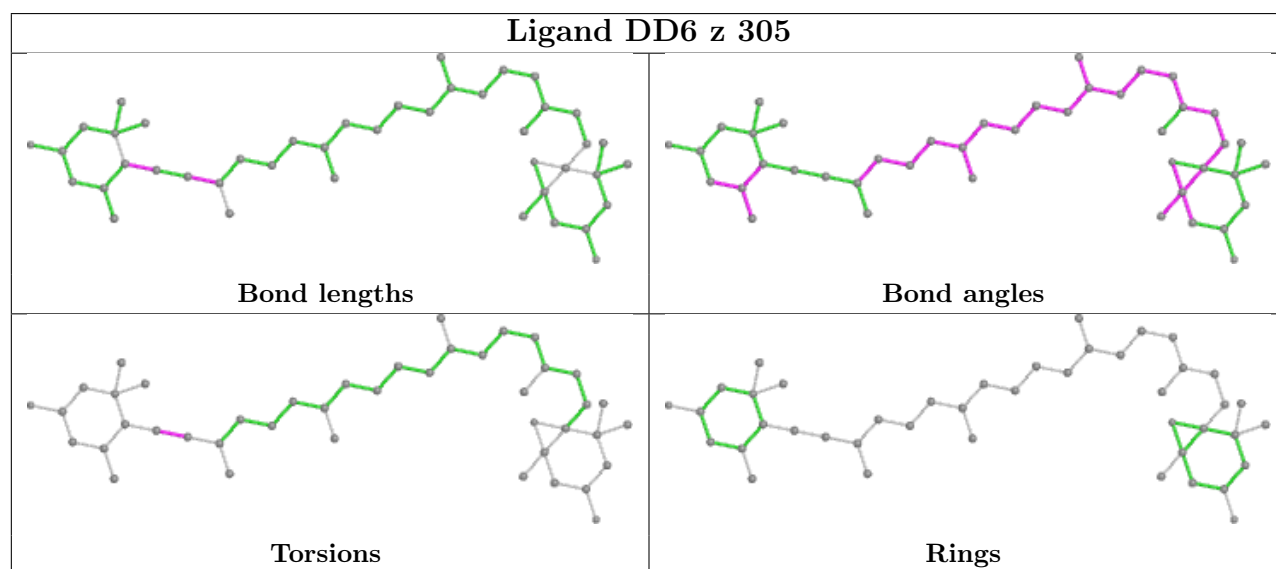
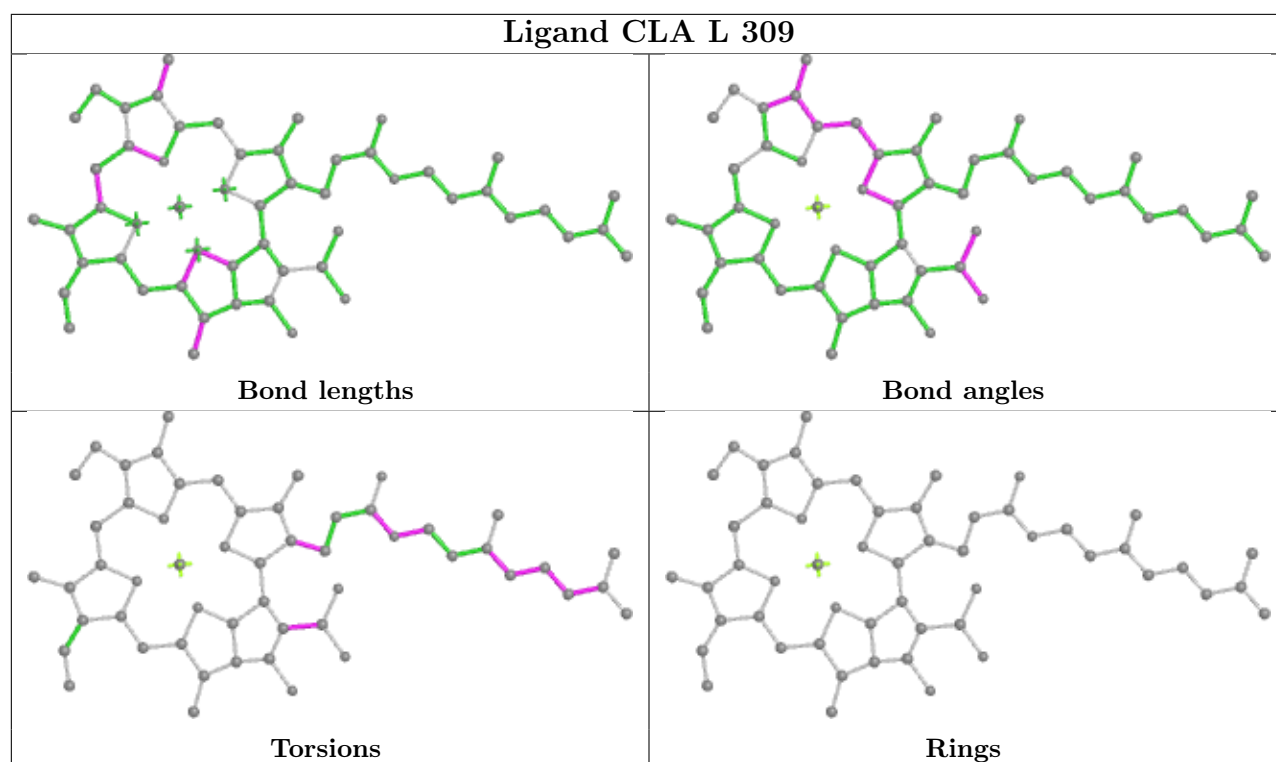
Bond angles



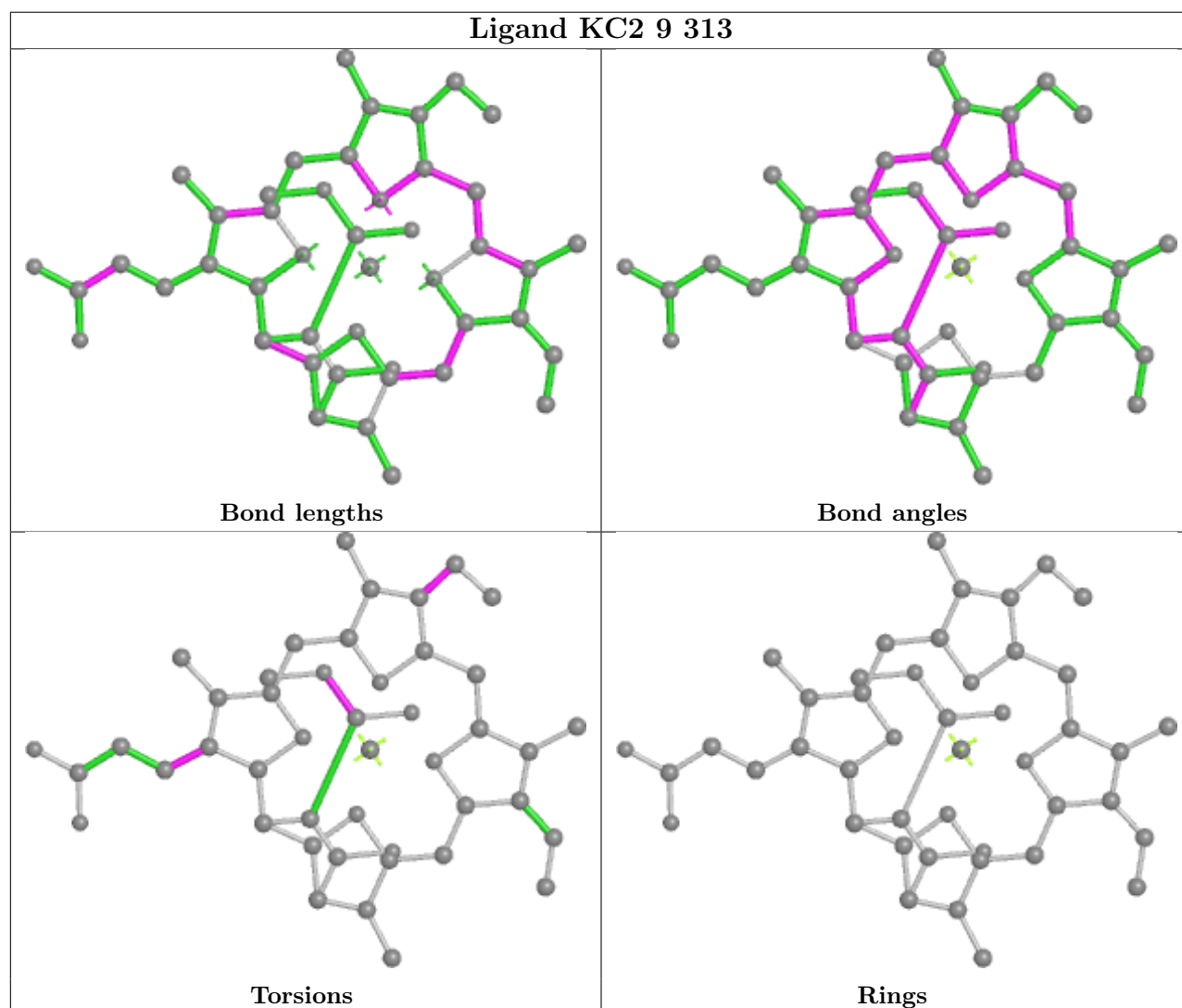
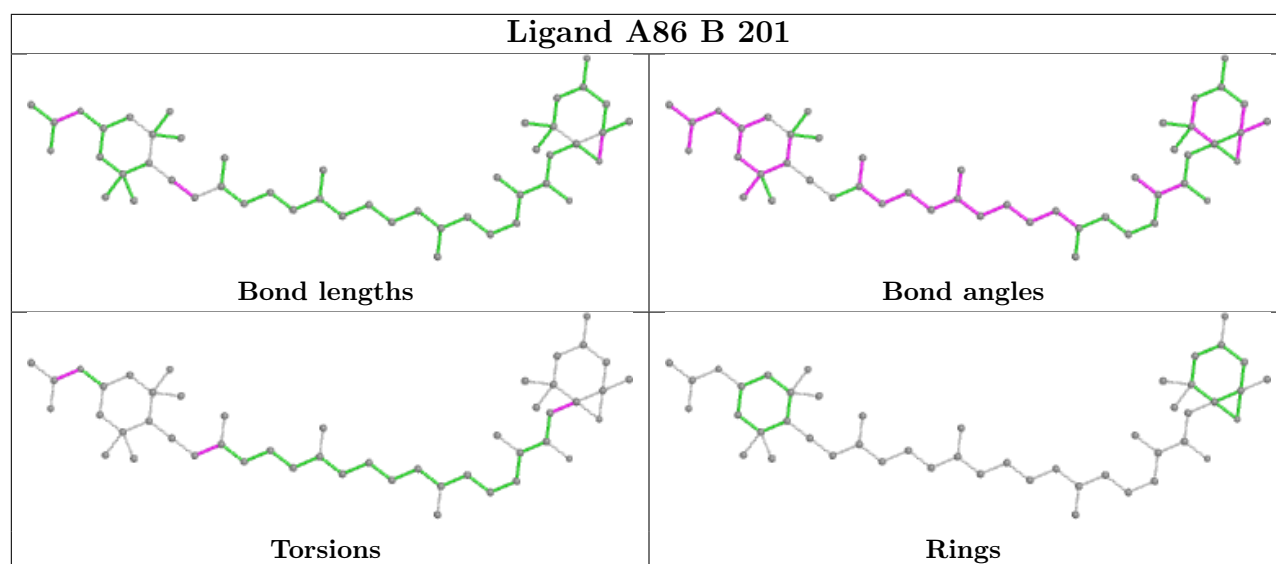
Torsions



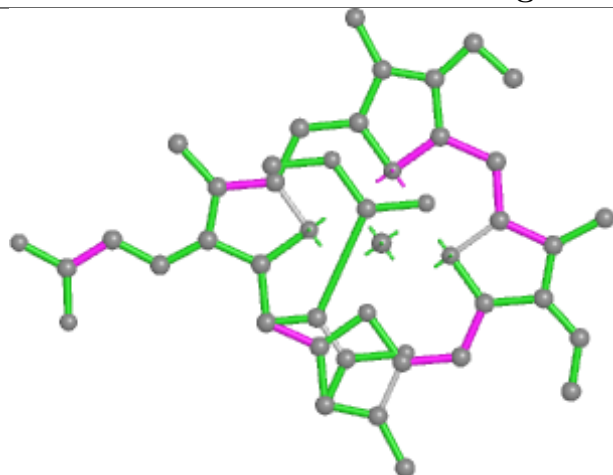
Rings



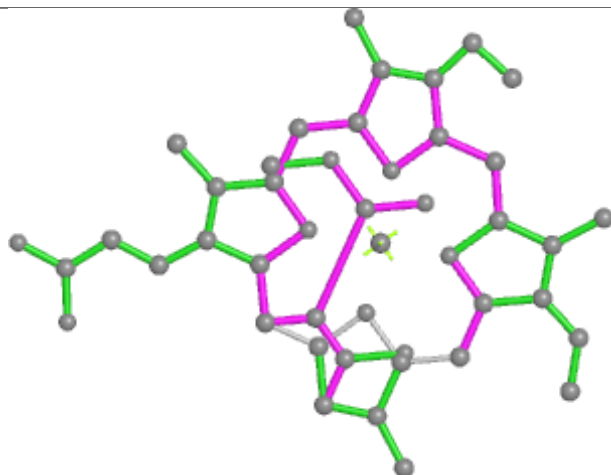




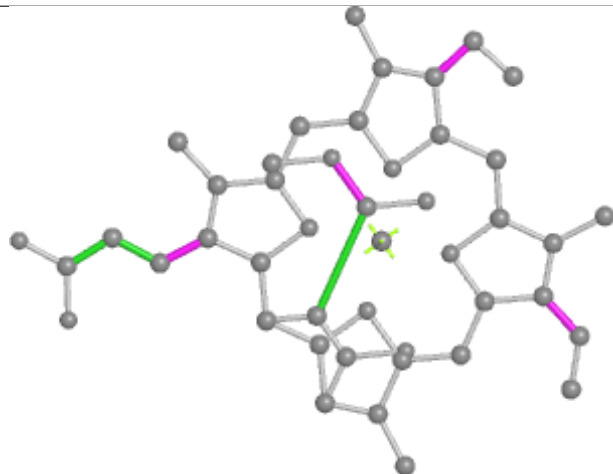
## Ligand KC2 P 312



Bond lengths



Bond angles

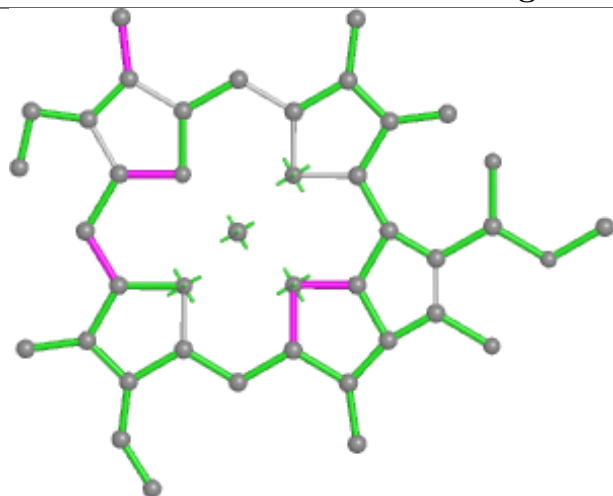


Torsions

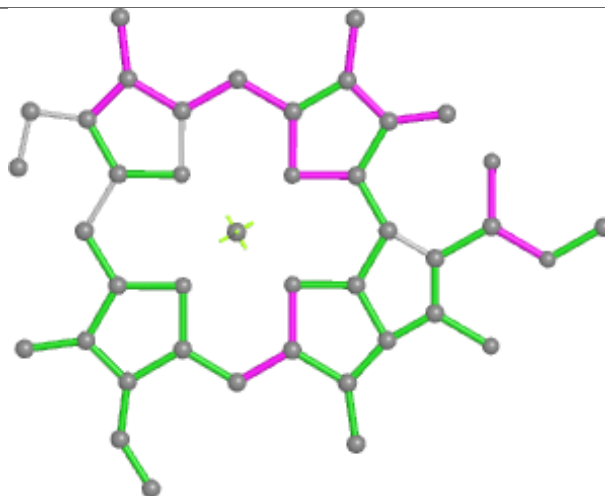


Rings

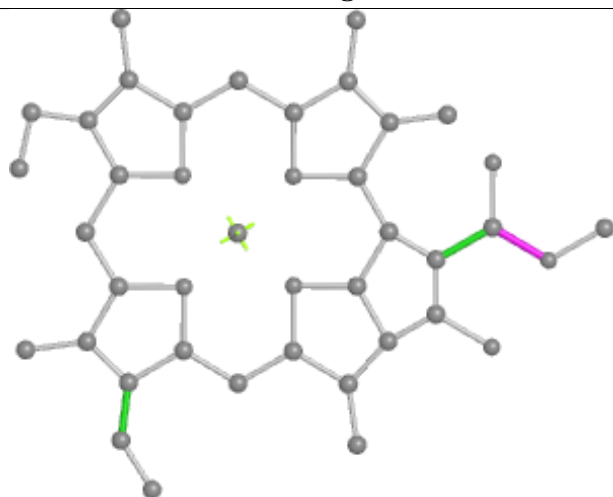
## Ligand CLA 9 320



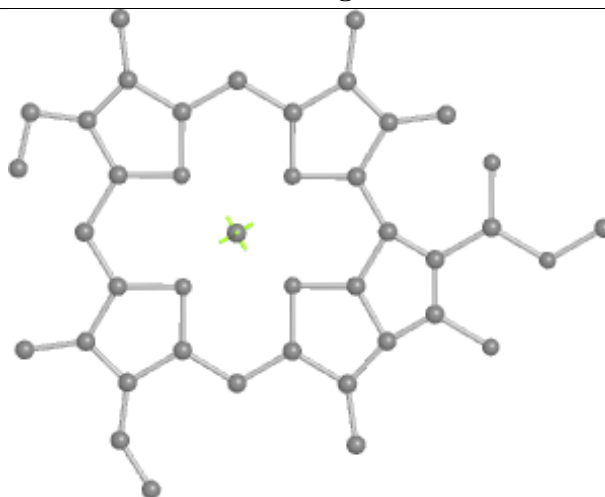
Bond lengths



Bond angles

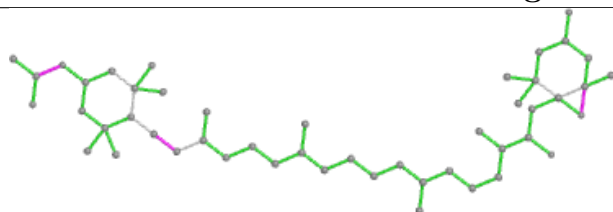


Torsions

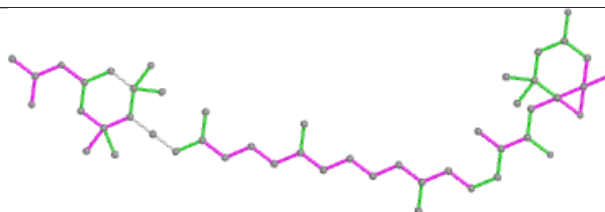


Rings

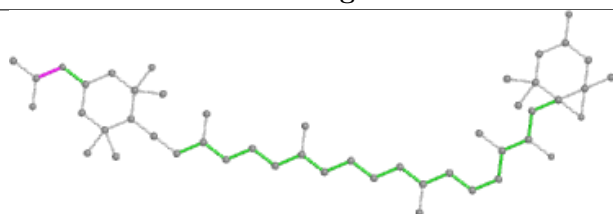
## Ligand A86 1 303



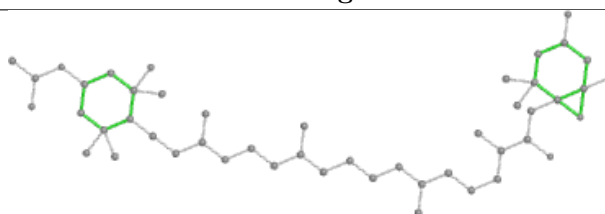
Bond lengths



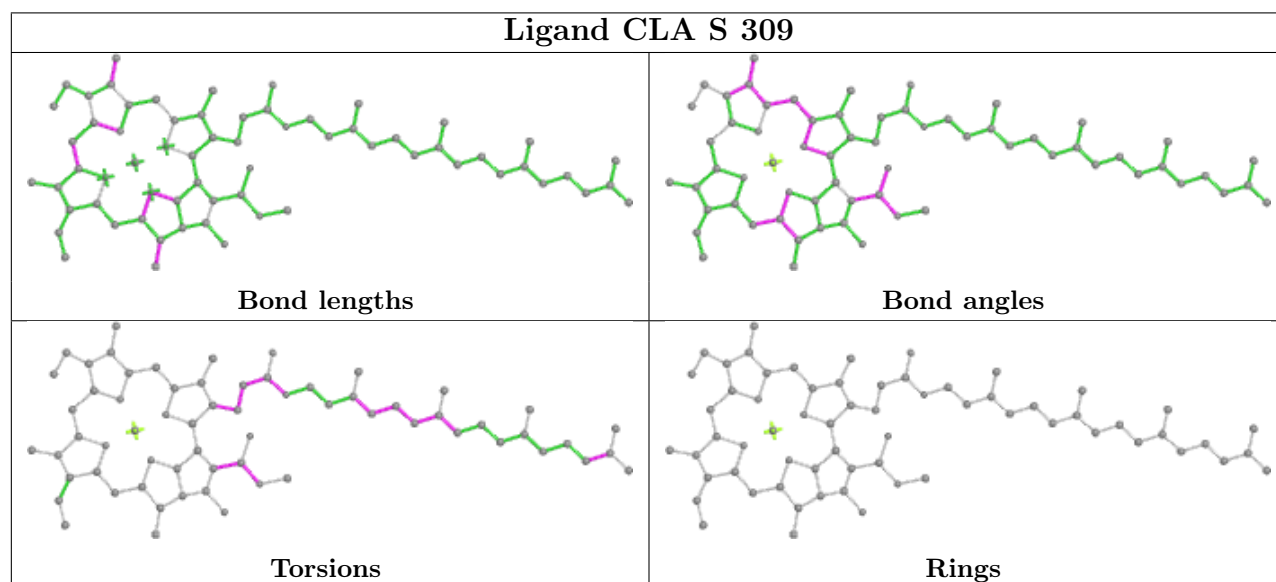
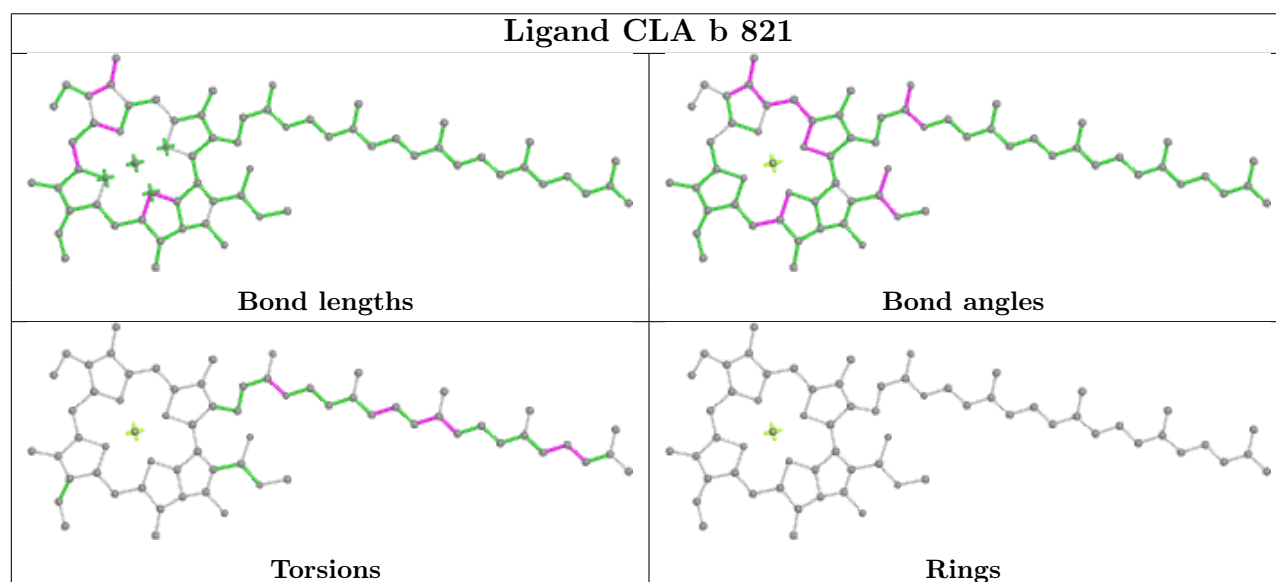
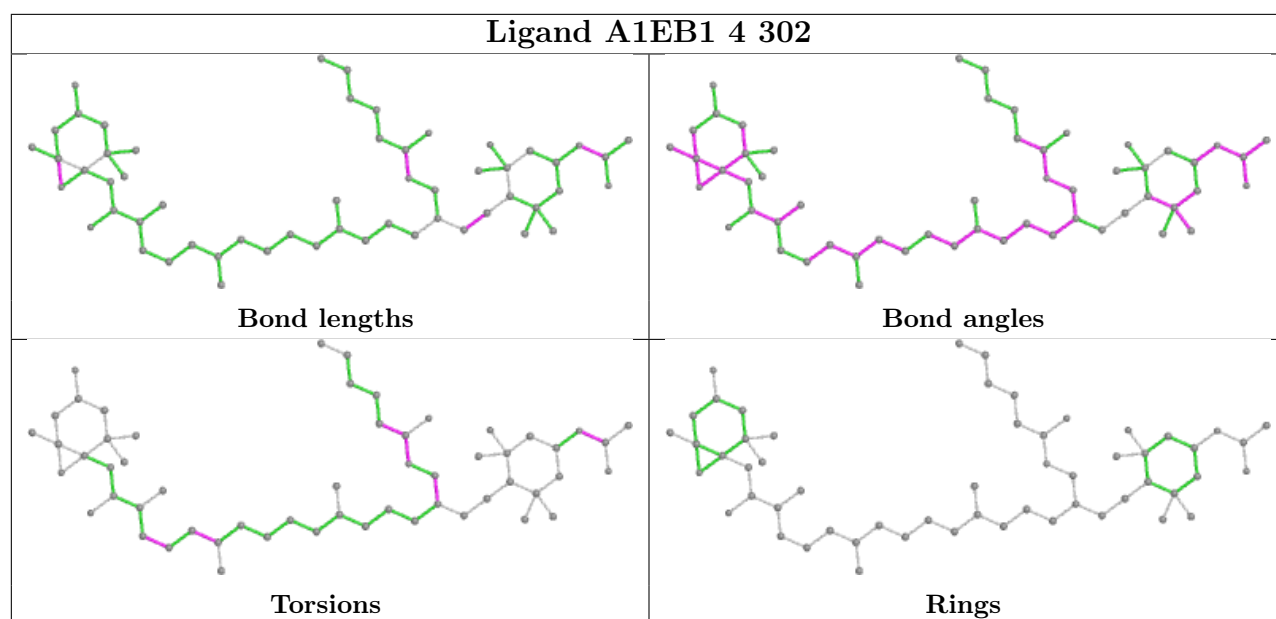
Bond angles



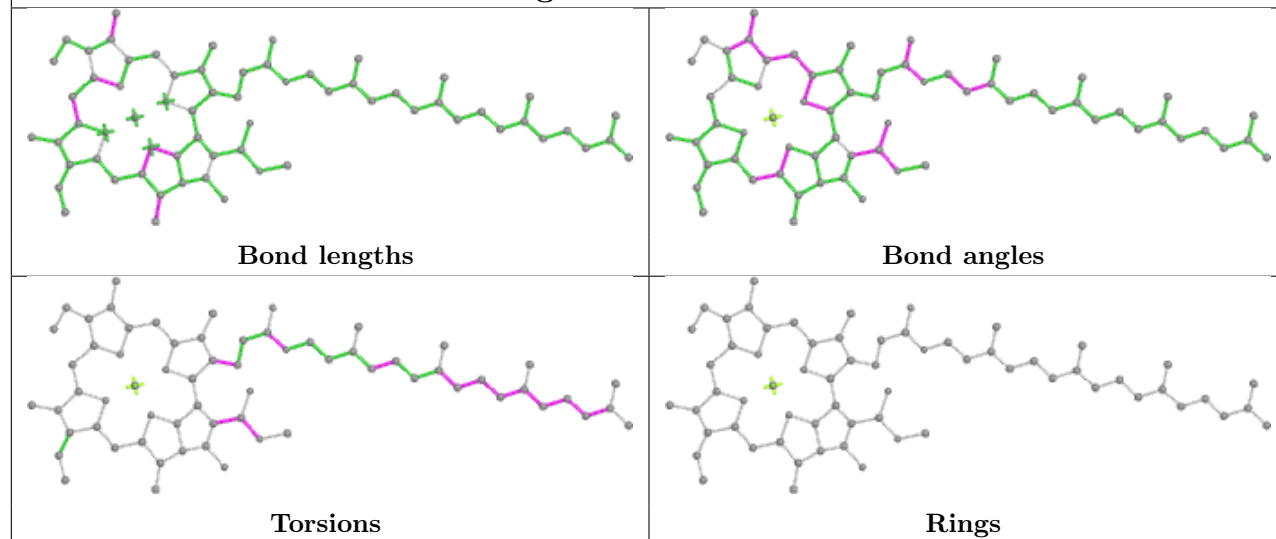
Torsions



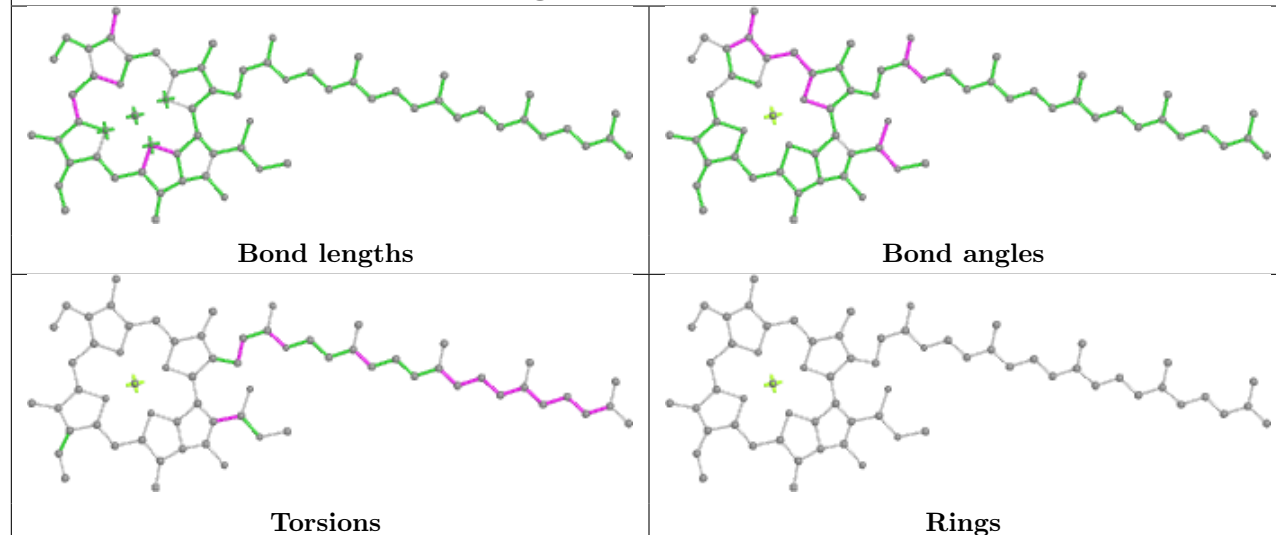
Rings



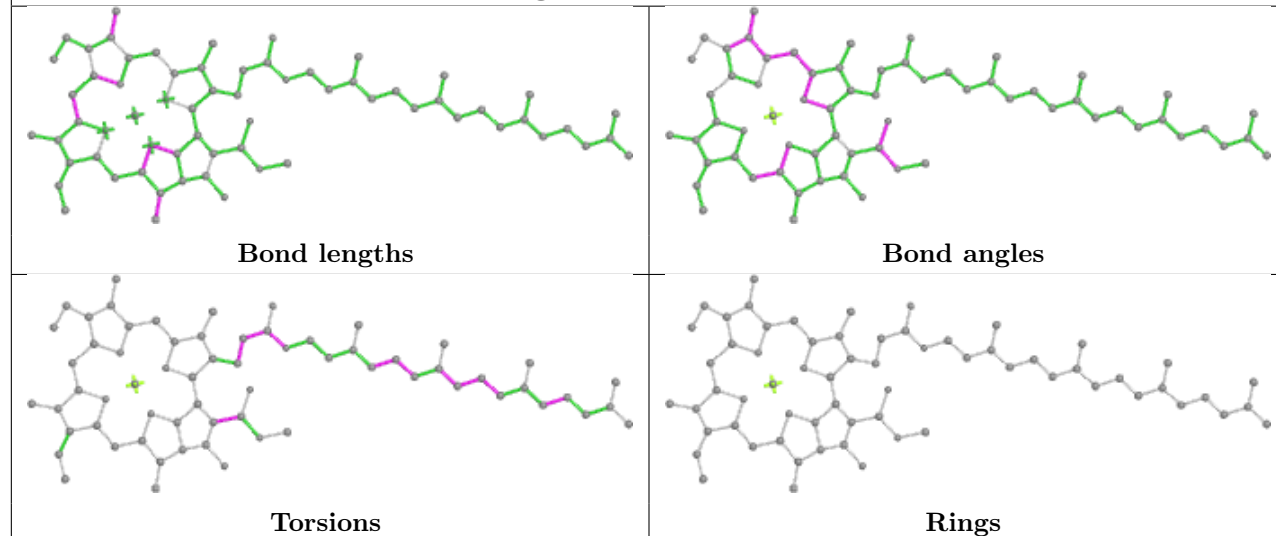
## Ligand CLA 3 312

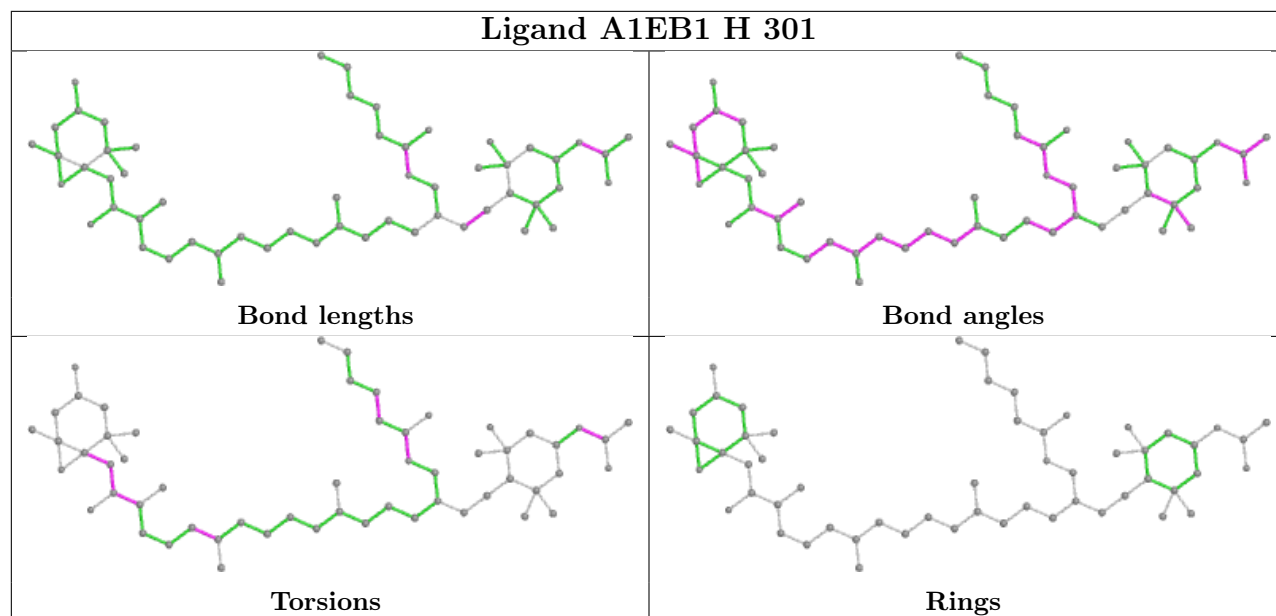
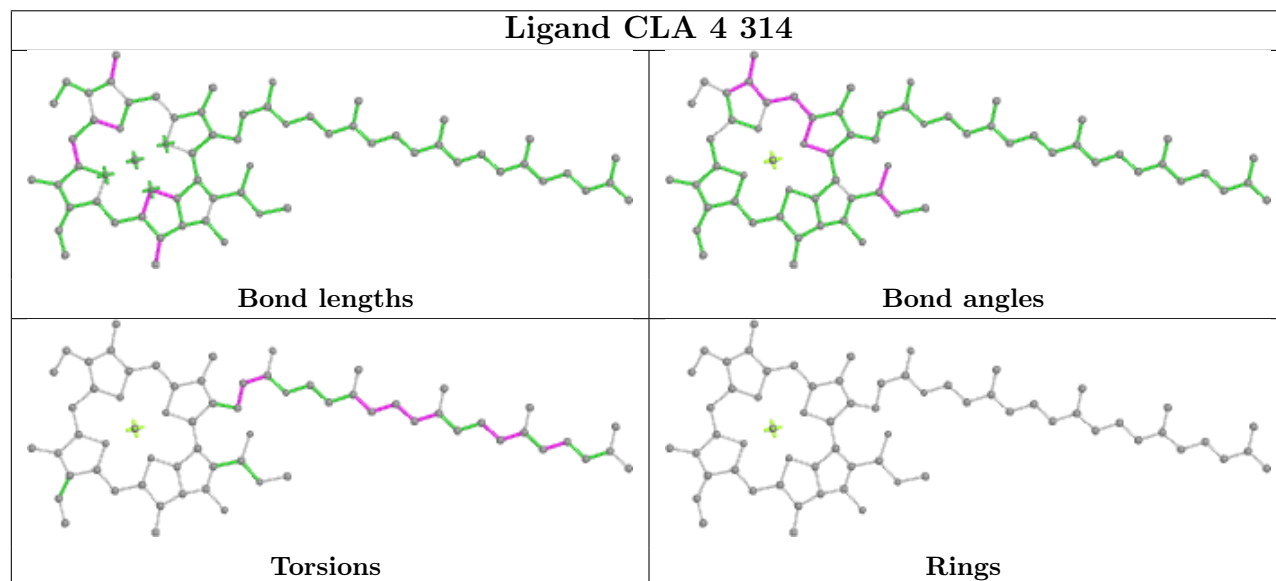


## Ligand CLA D 319

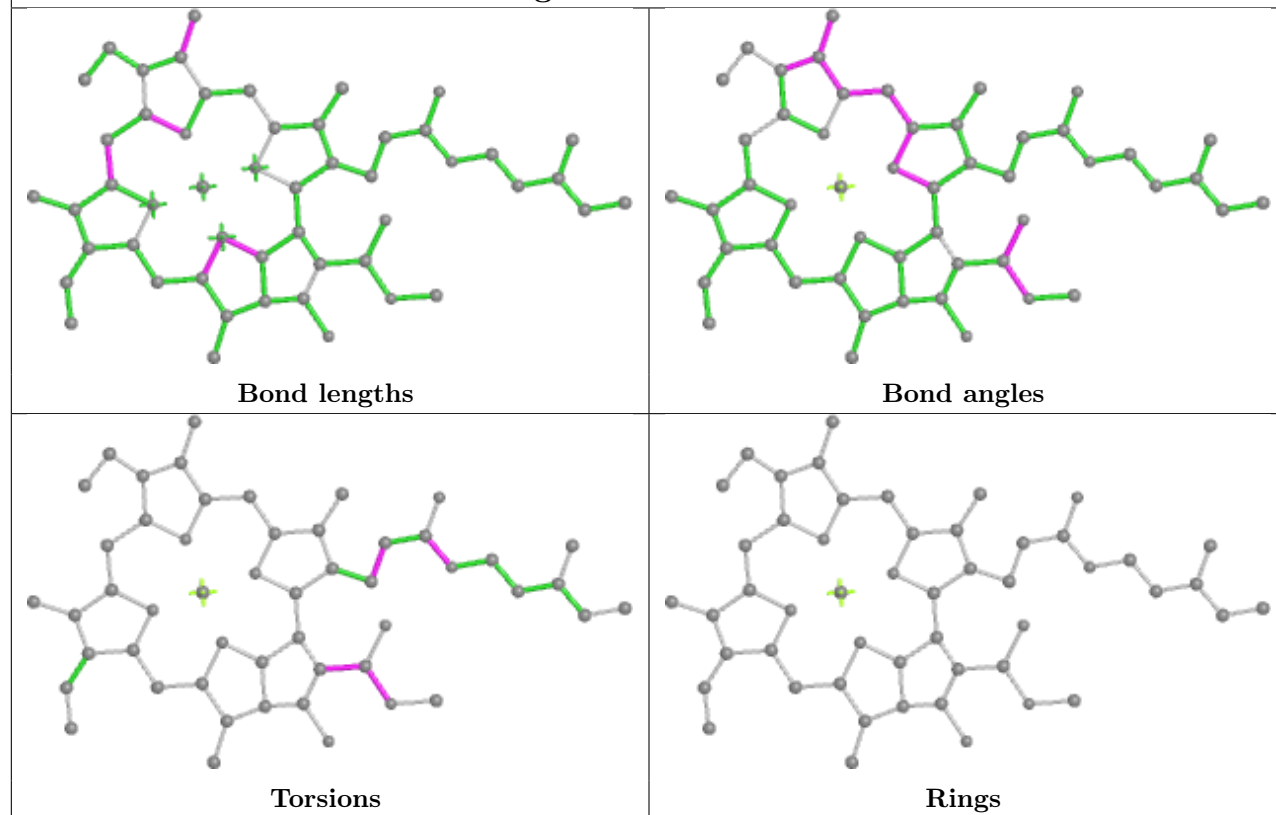


## Ligand CLA C 307

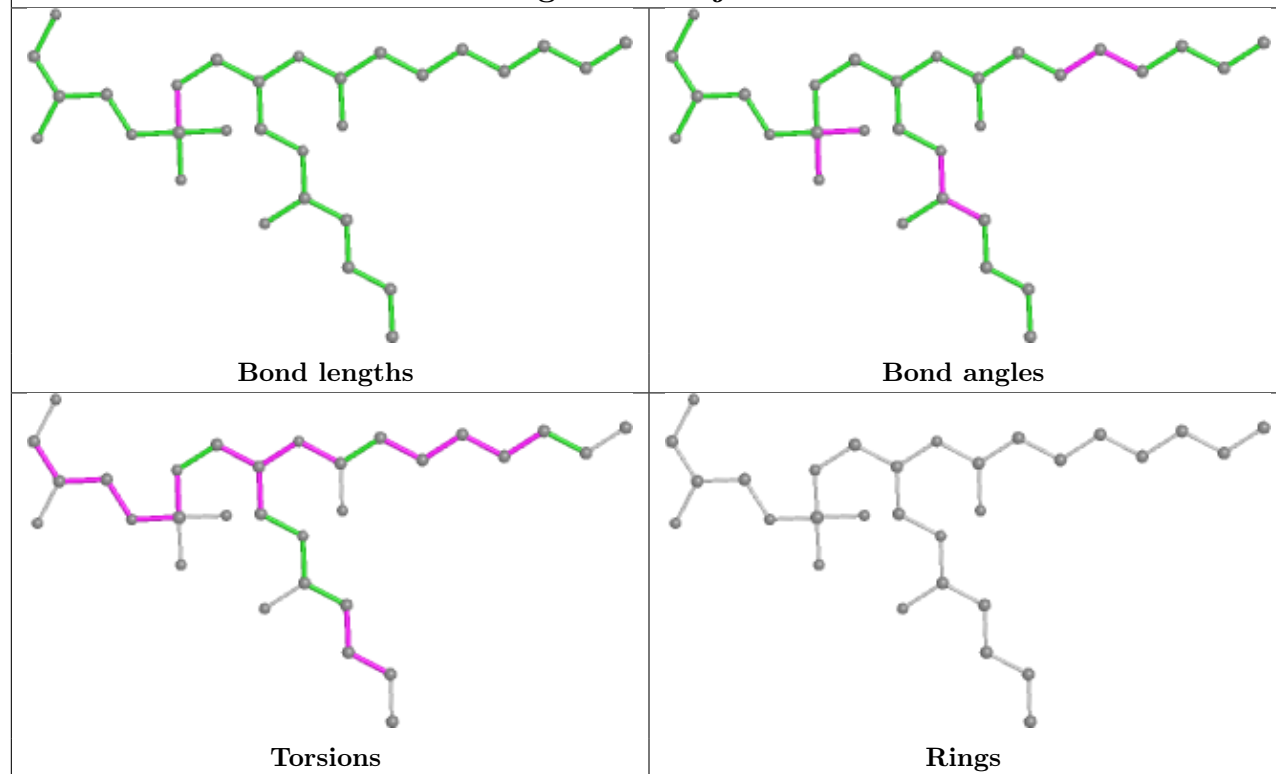


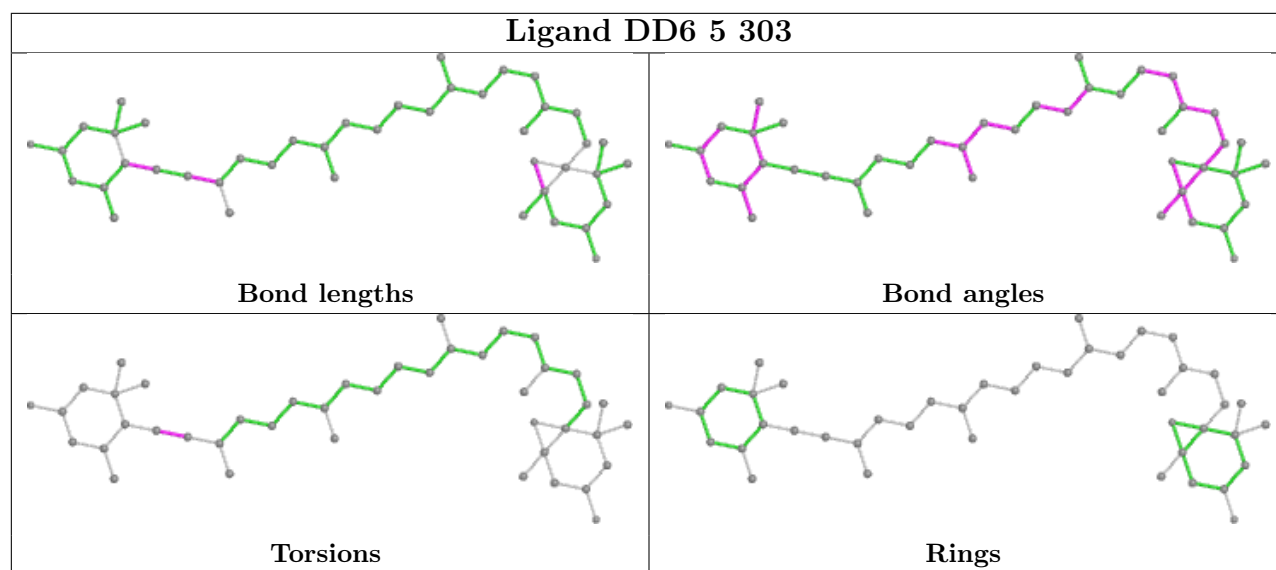
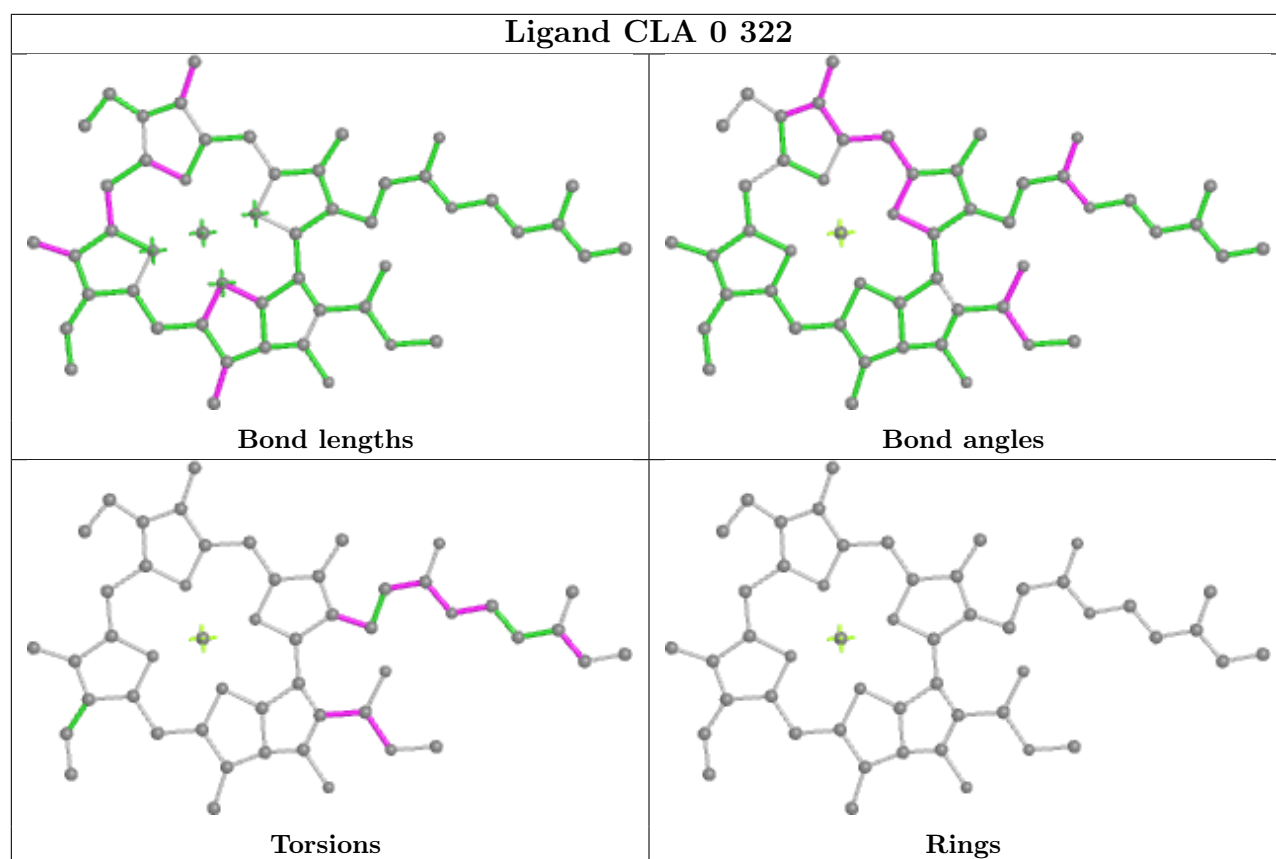
**Ligand A1EB1 H 301****Ligand CLA 4 314**

## Ligand CLA L 319



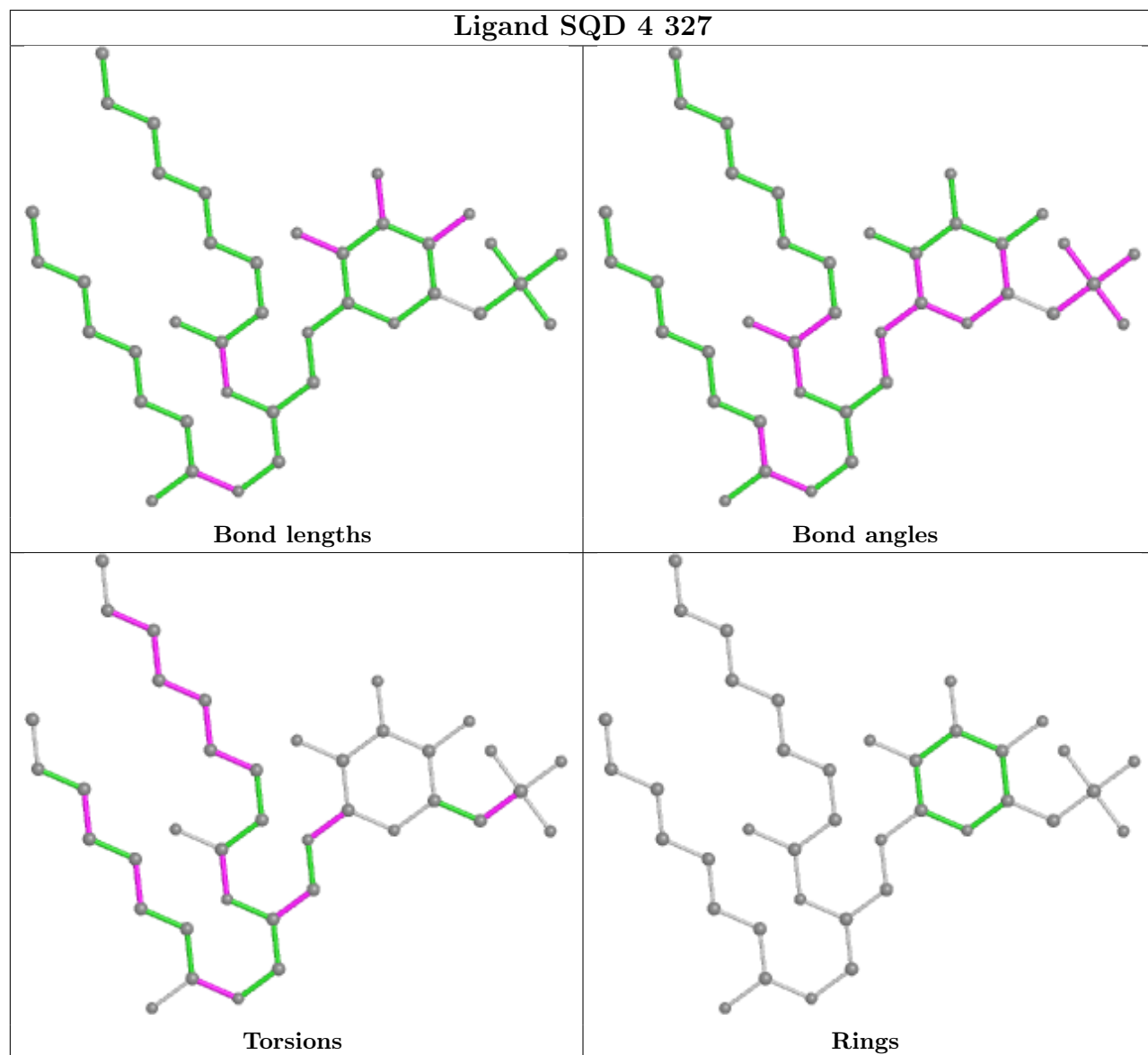
## Ligand LHG j 104



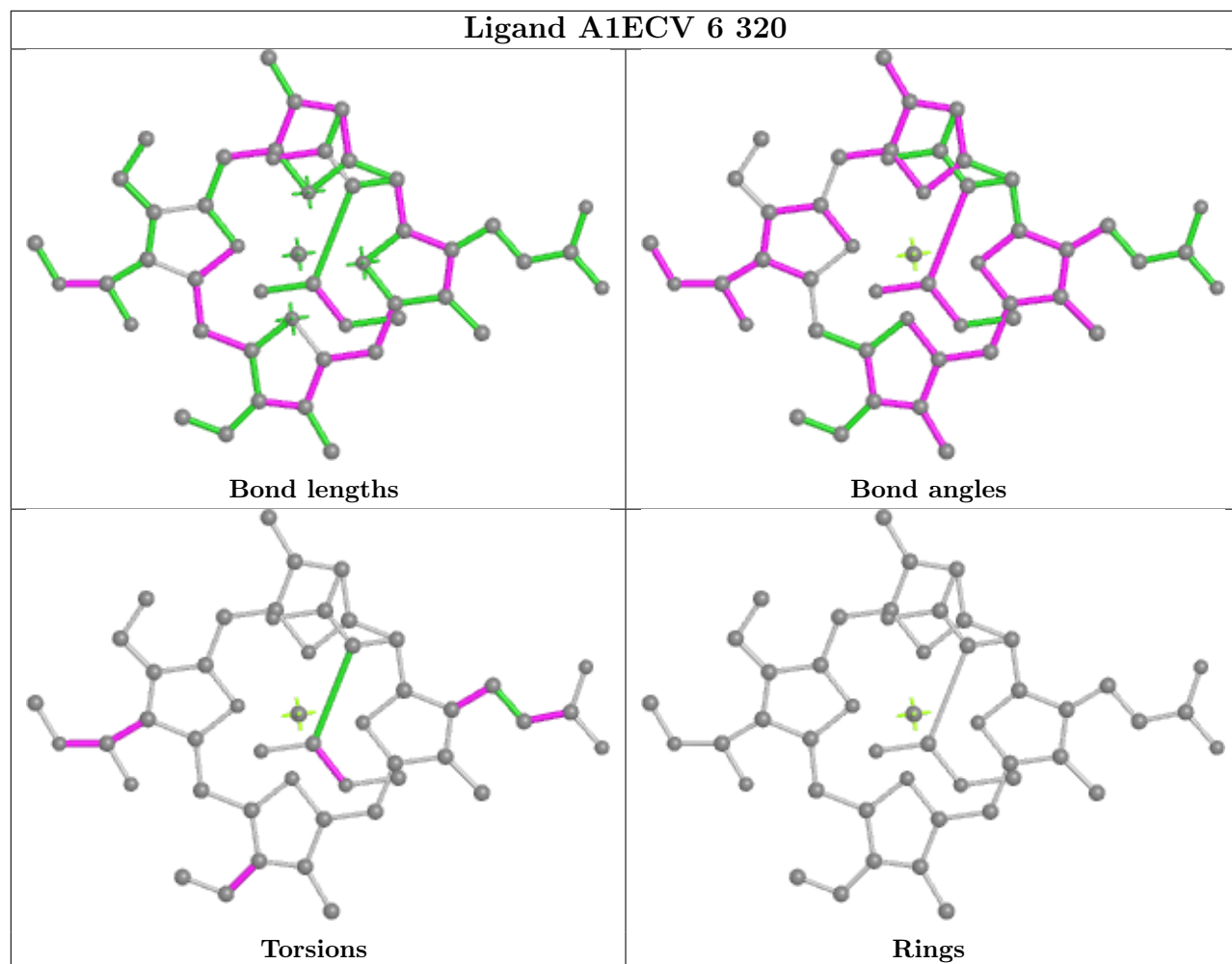




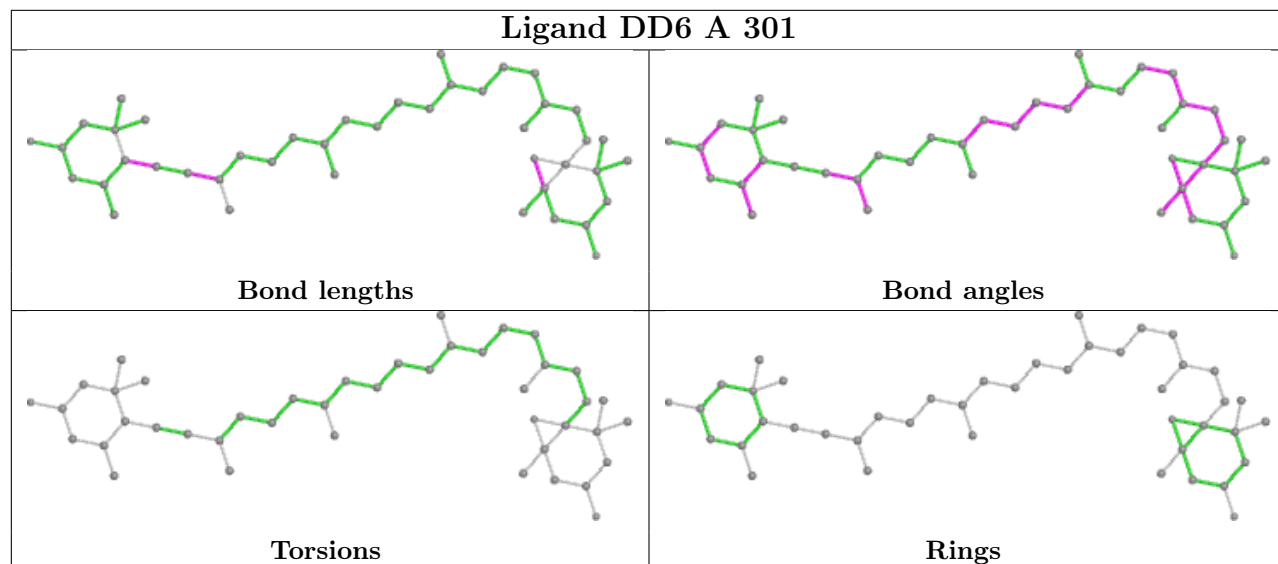
## Ligand SQD 4 327



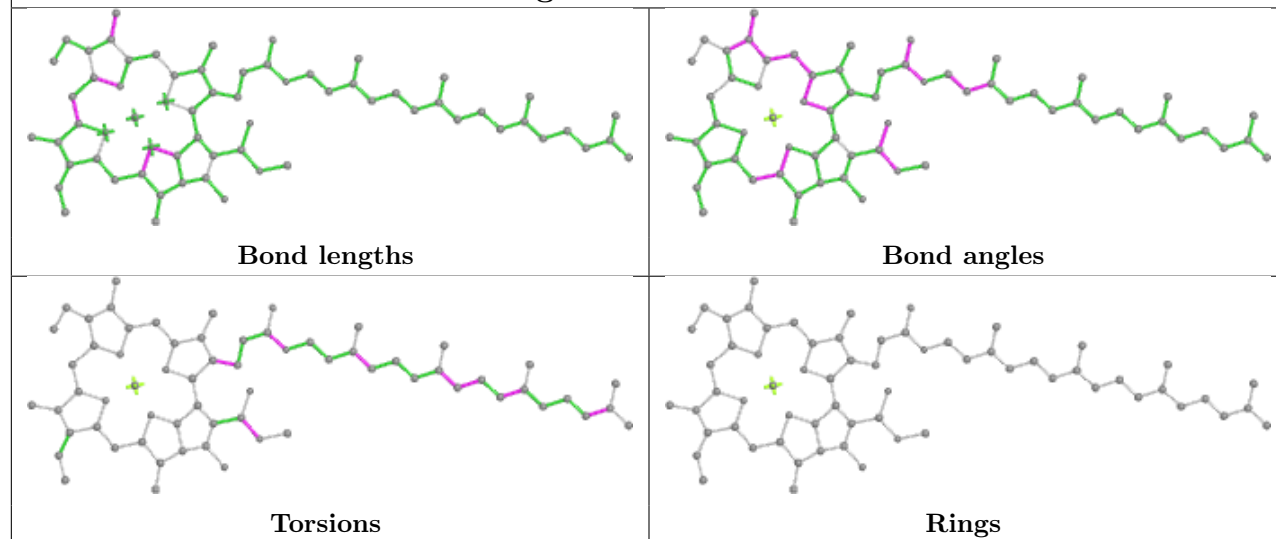
## Ligand A1ECV 6 320



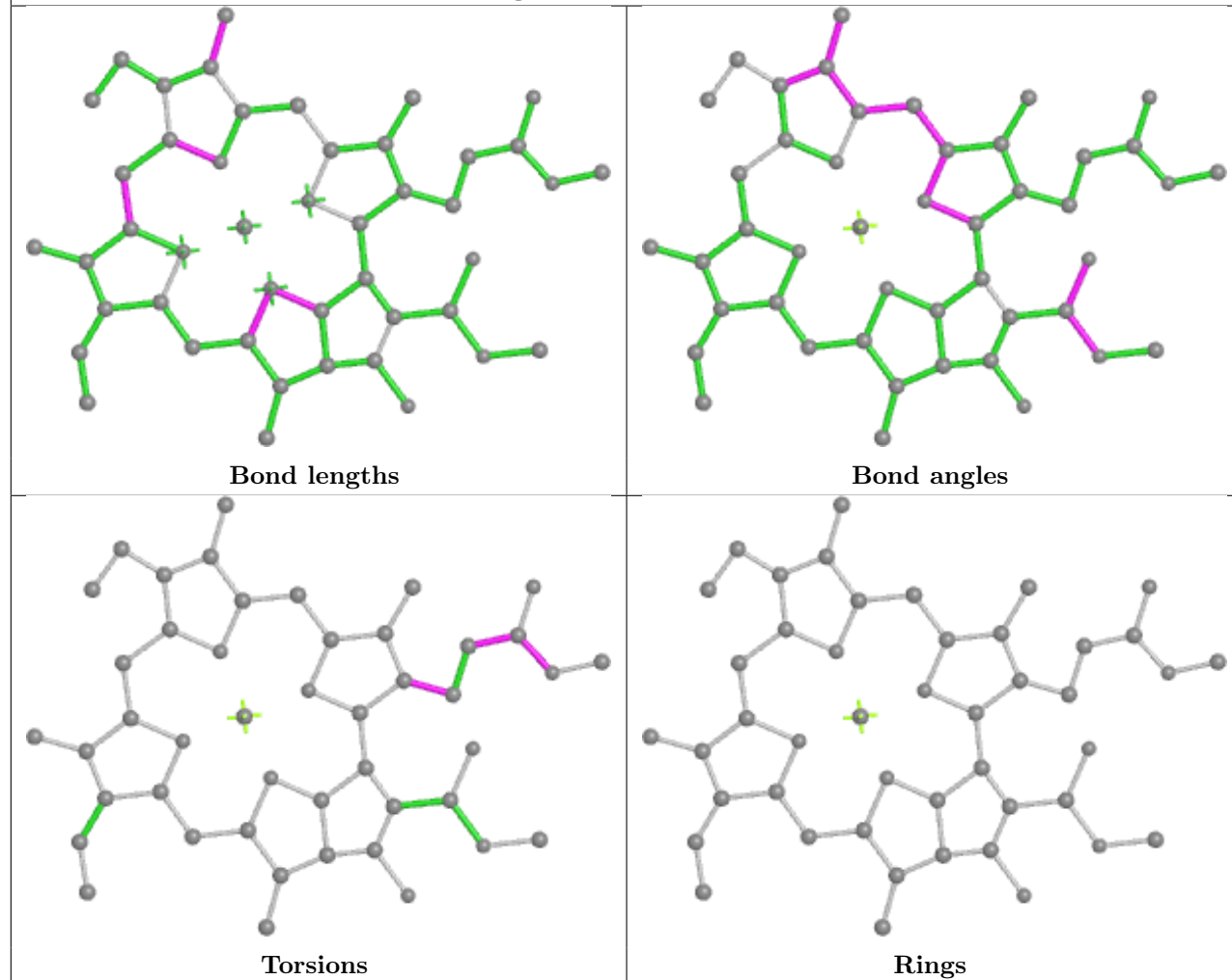
## Ligand DD6 A 301



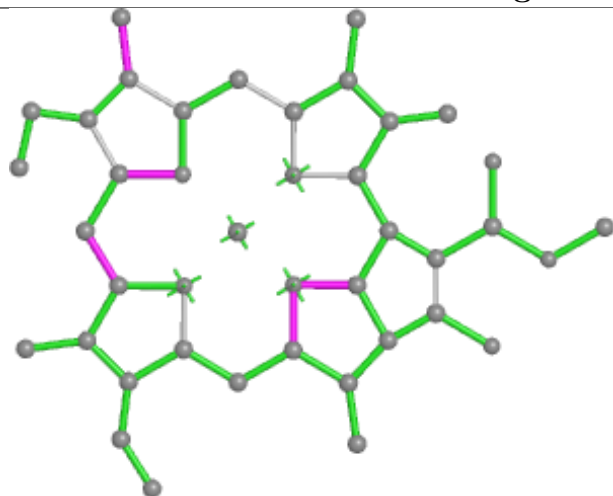
## Ligand CLA a 816



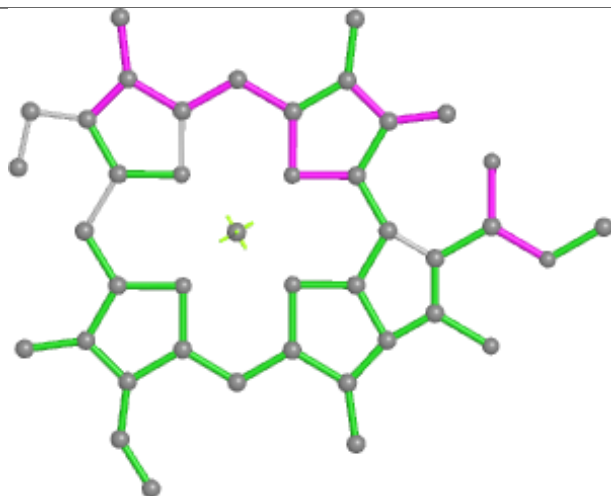
## Ligand CLA M 318



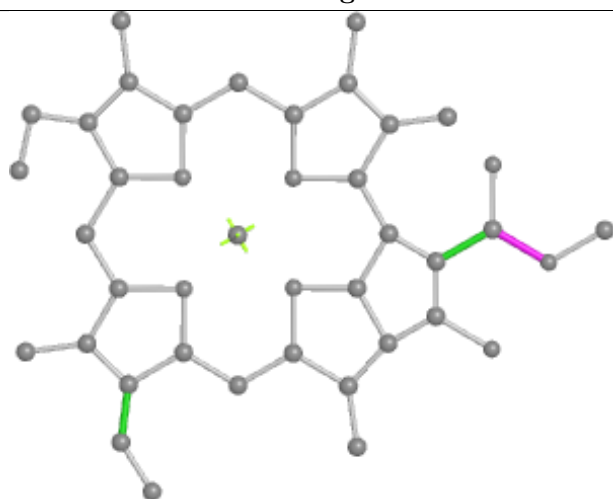
## Ligand CLA Y 305



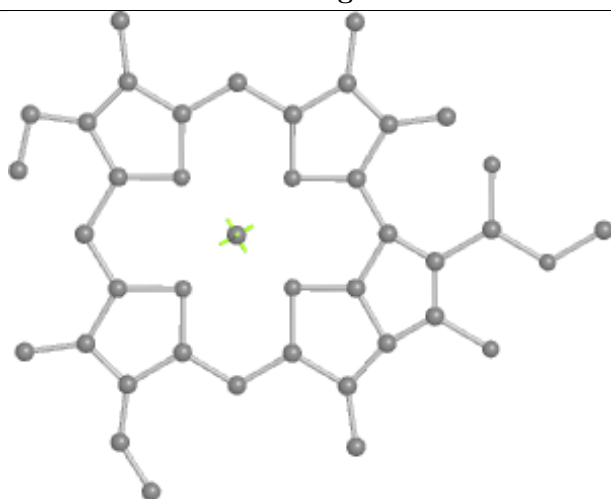
Bond lengths



Bond angles

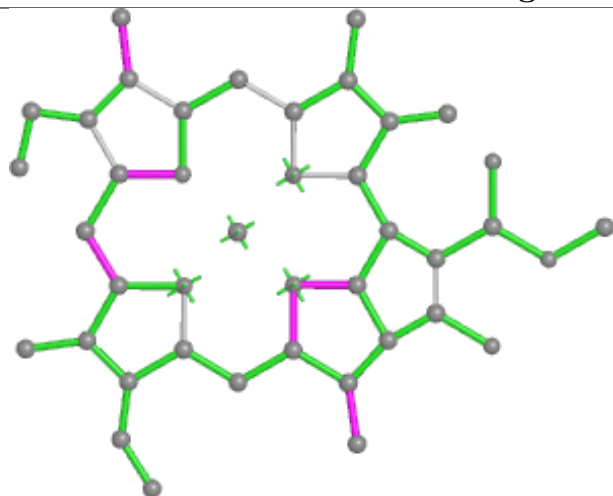


Torsions

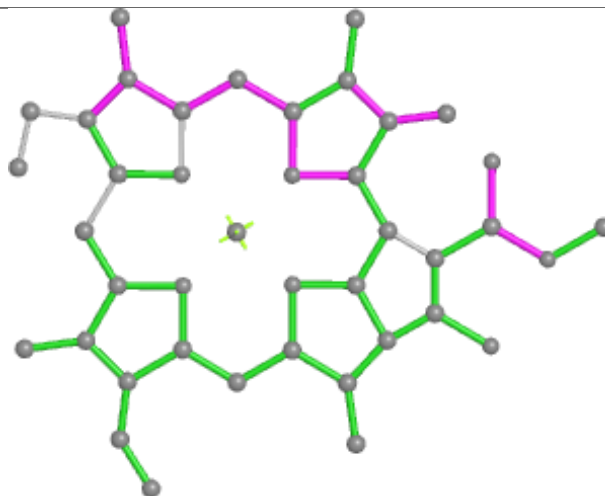


Rings

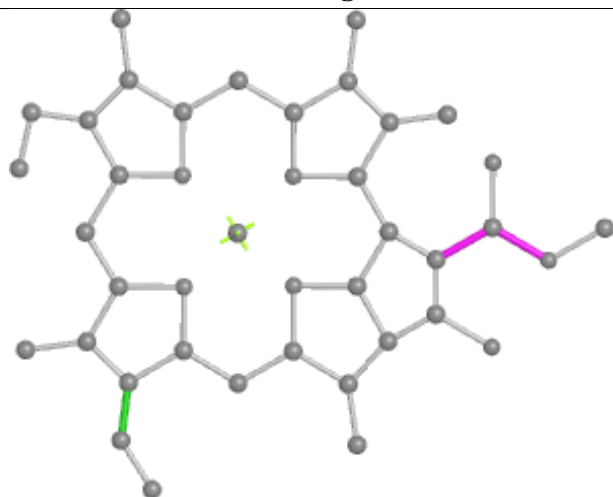
## Ligand CLA 1 313



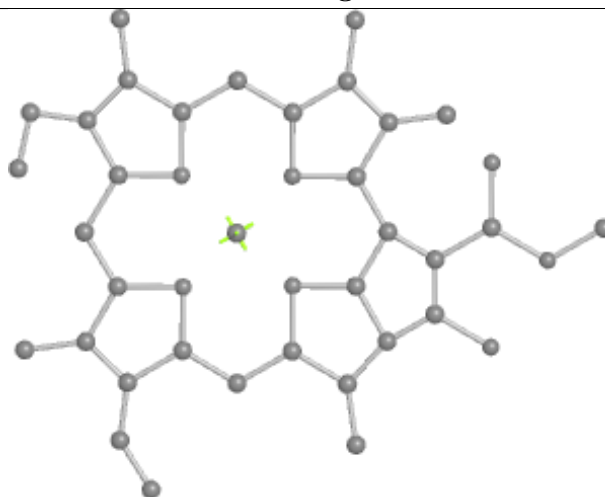
Bond lengths



Bond angles

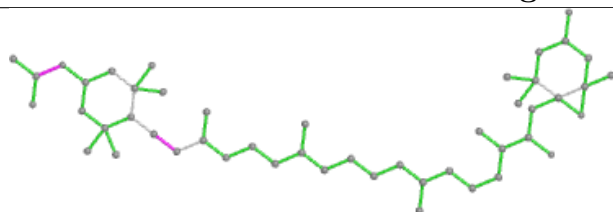


Torsions

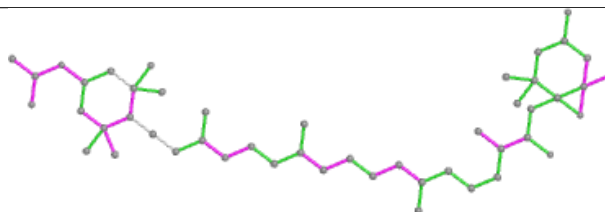


Rings

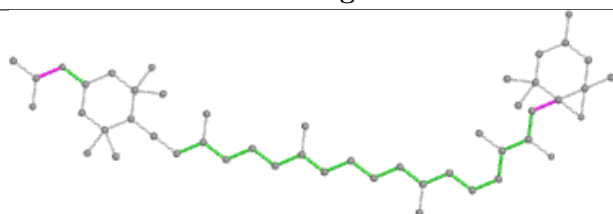
## Ligand A86 R 317



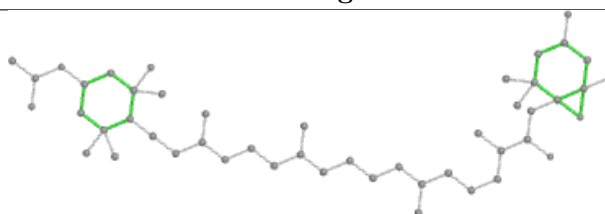
Bond lengths



Bond angles

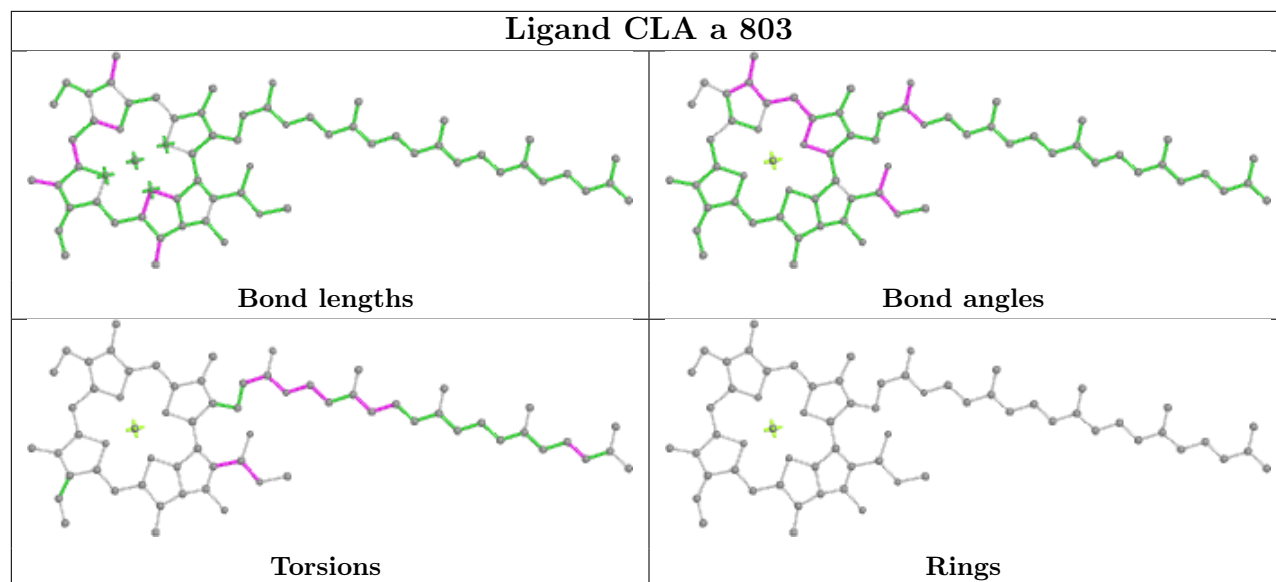


Torsions

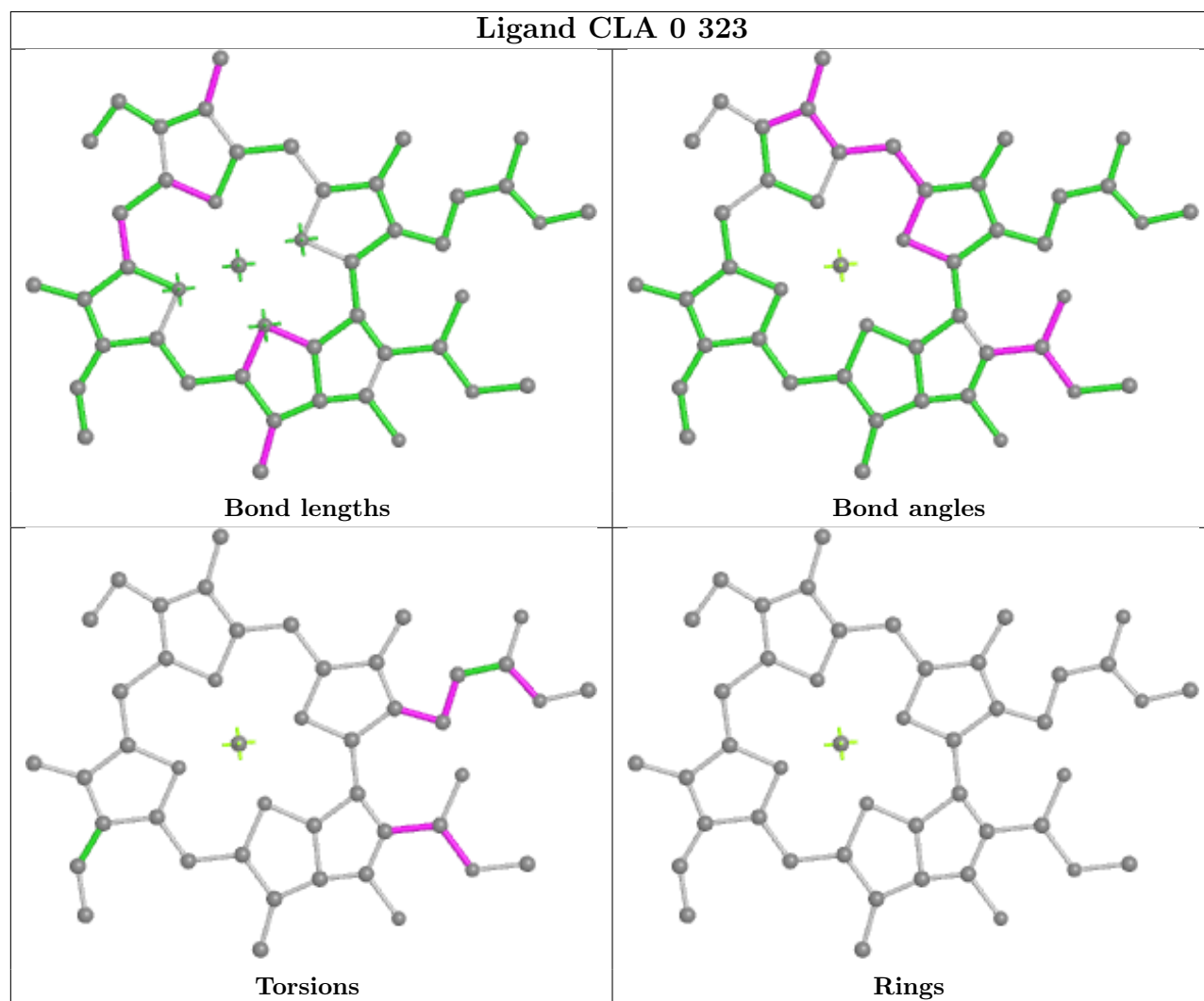


Rings

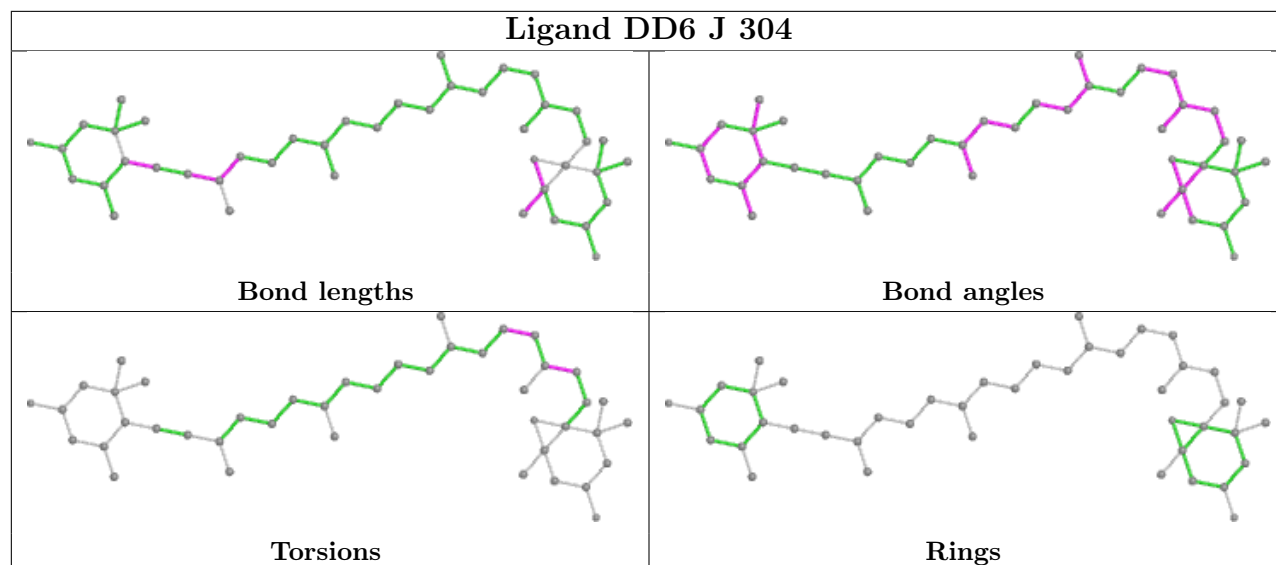
## Ligand CLA a 803



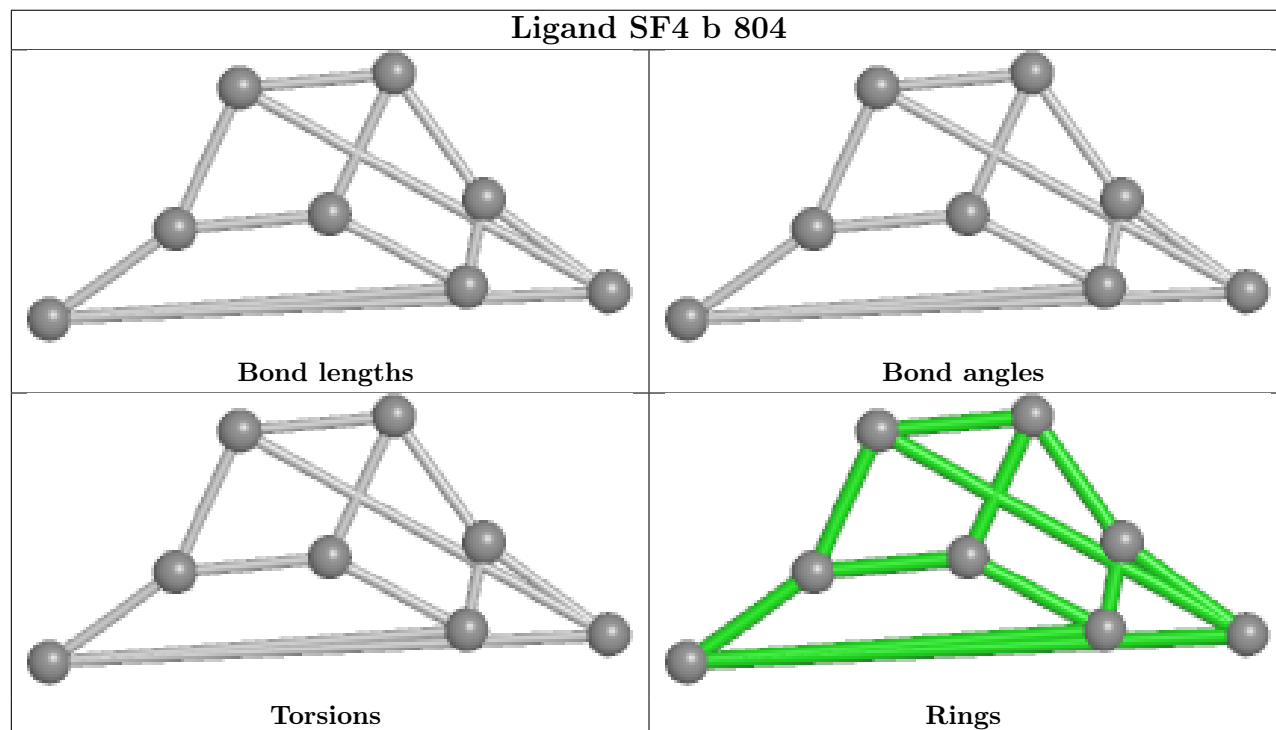
## Ligand CLA 0 323

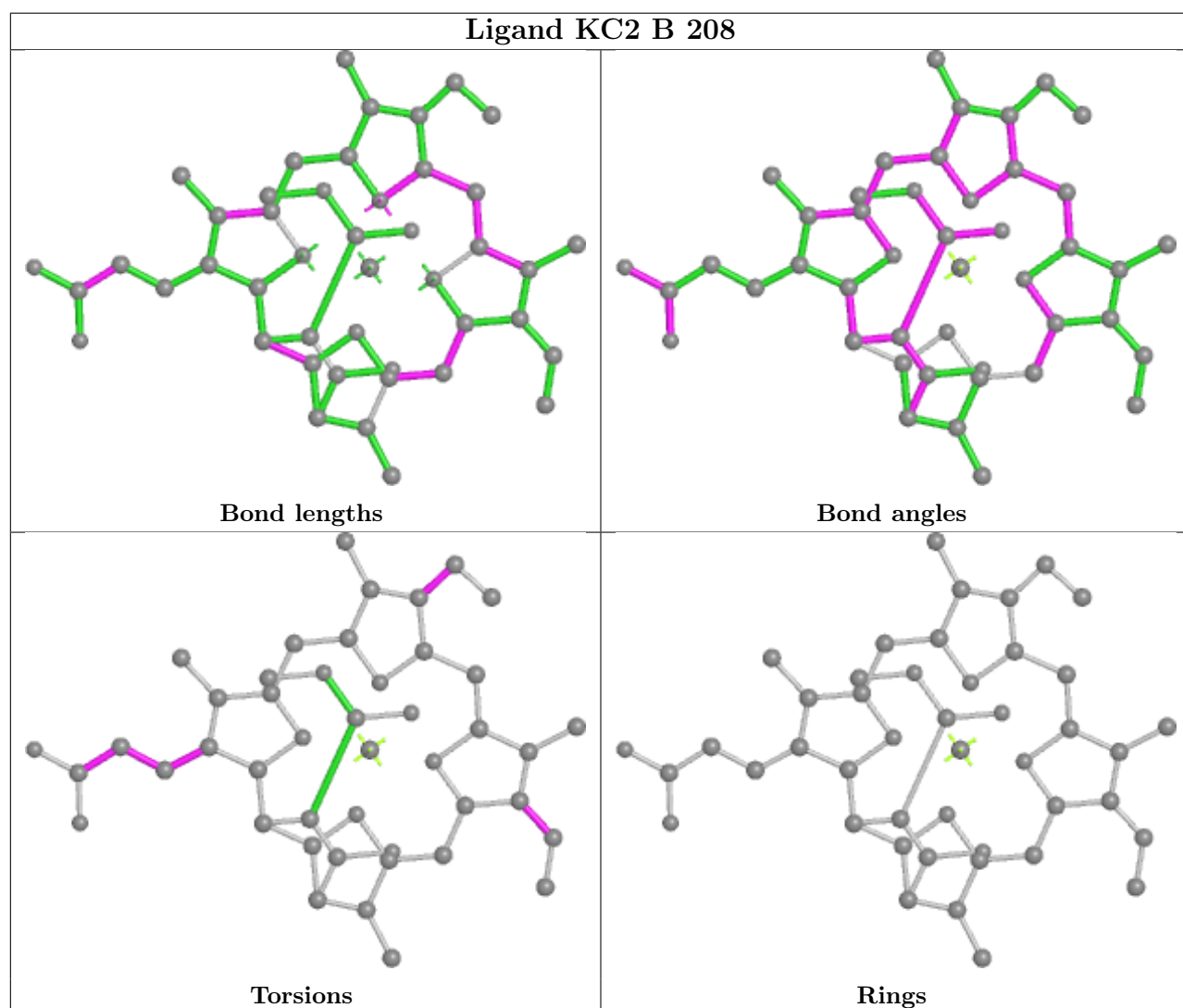
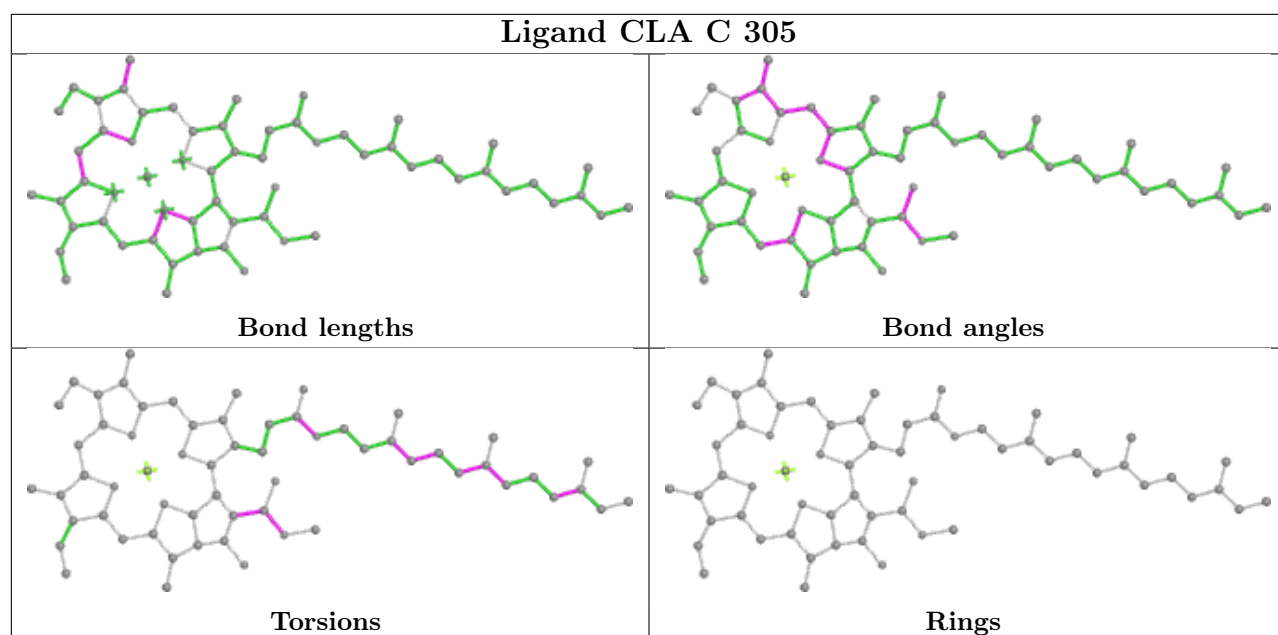


## Ligand DD6 J 304



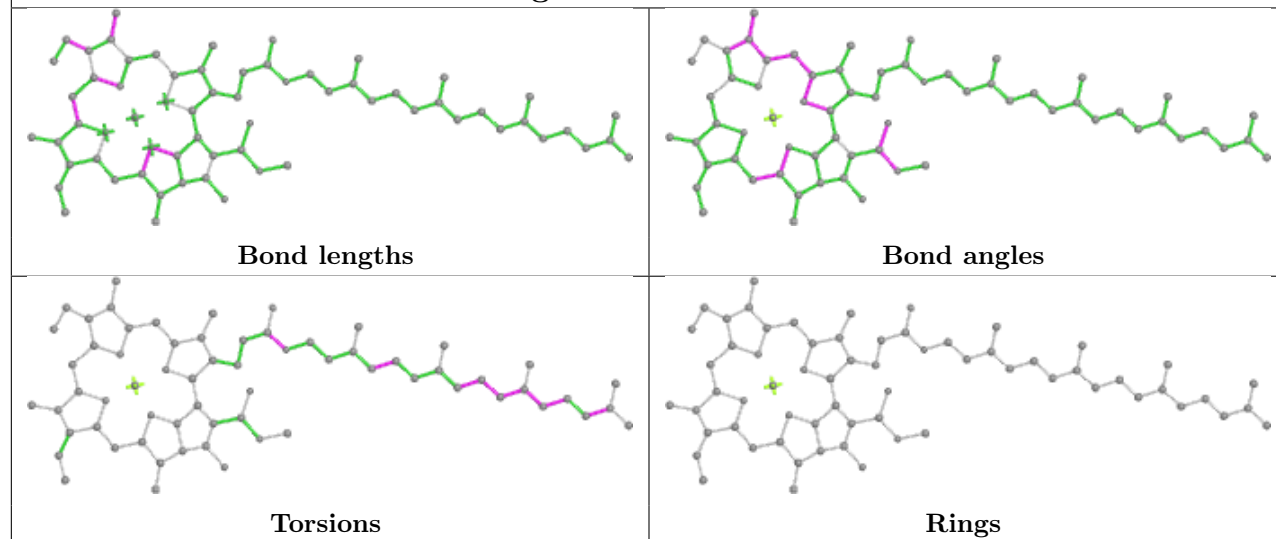
## Ligand SF4 b 804



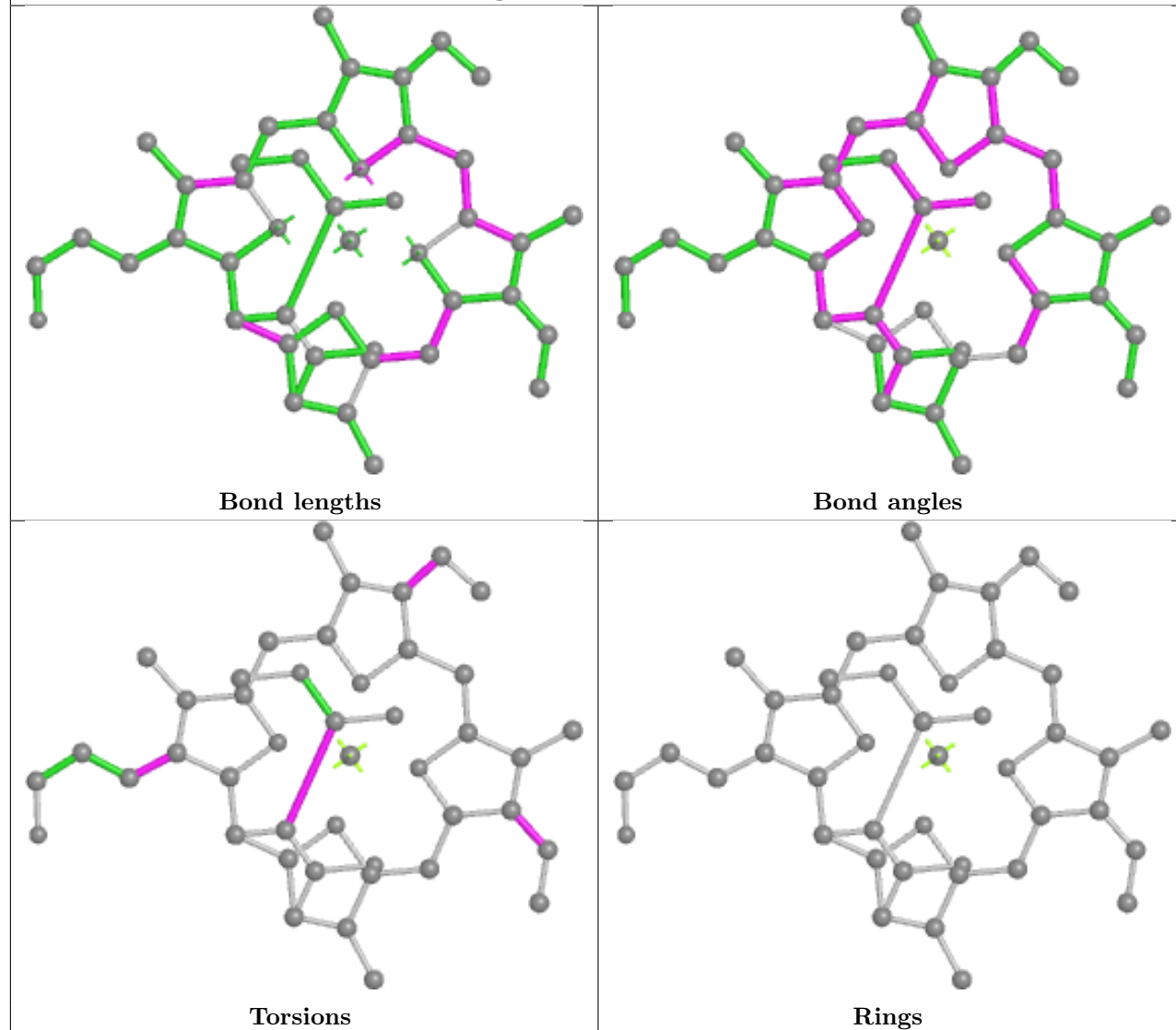


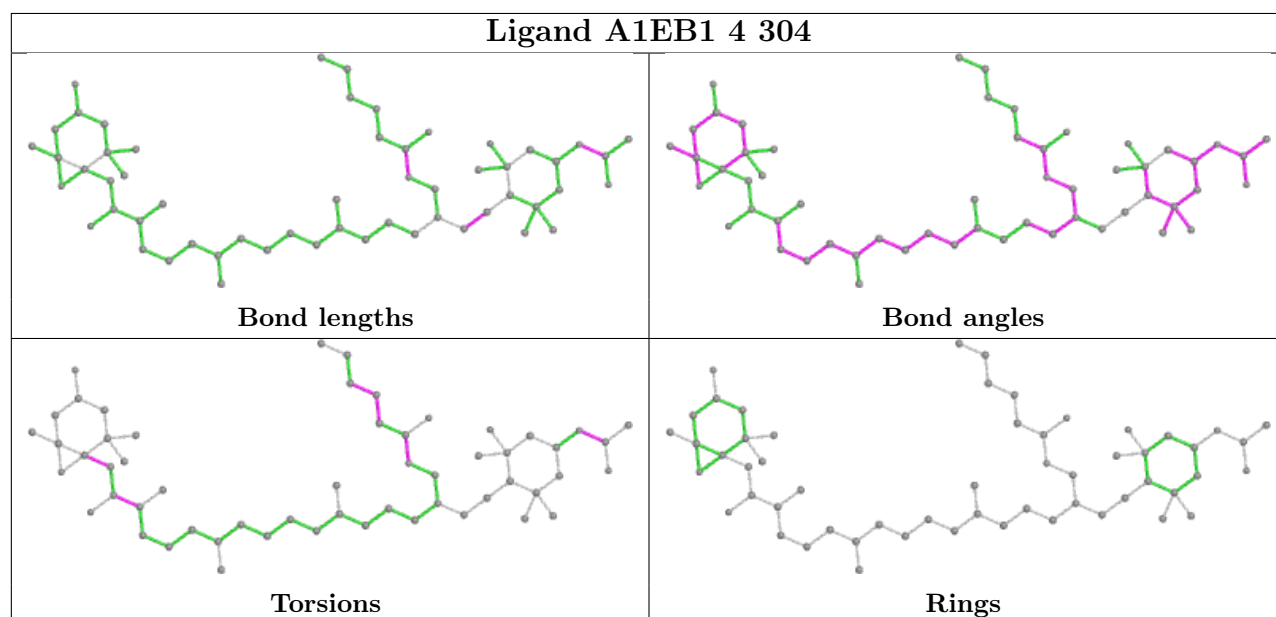
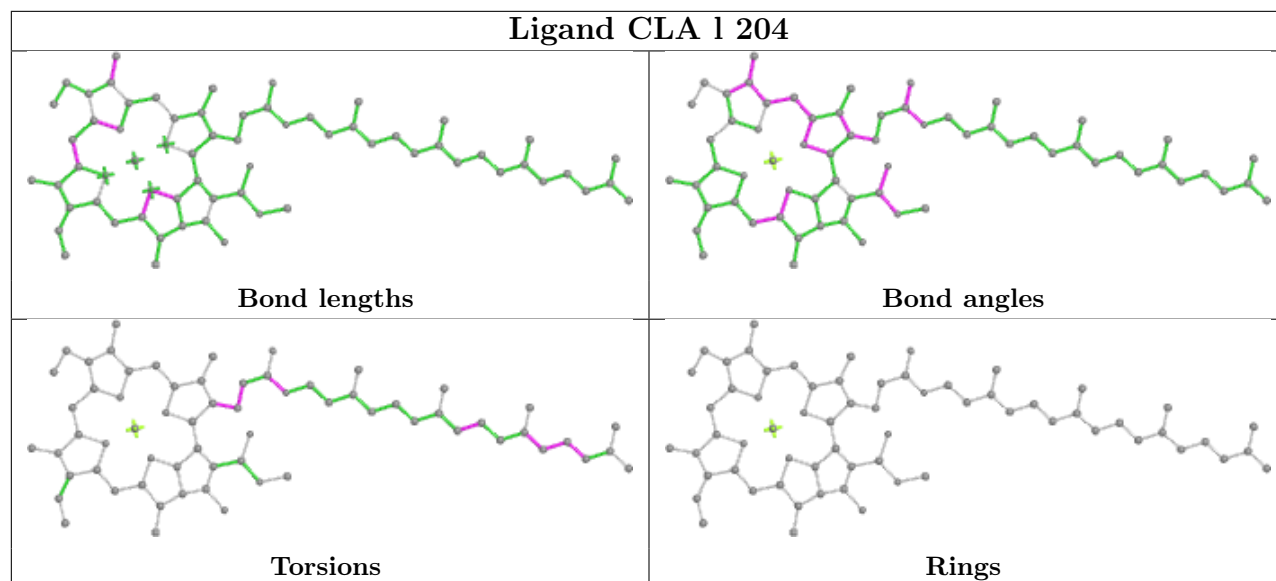
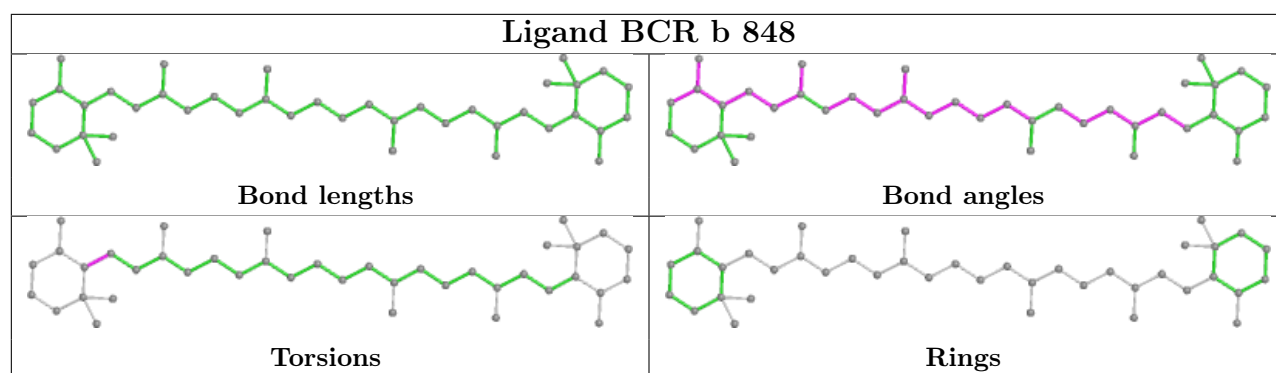


## Ligand CLA A 311

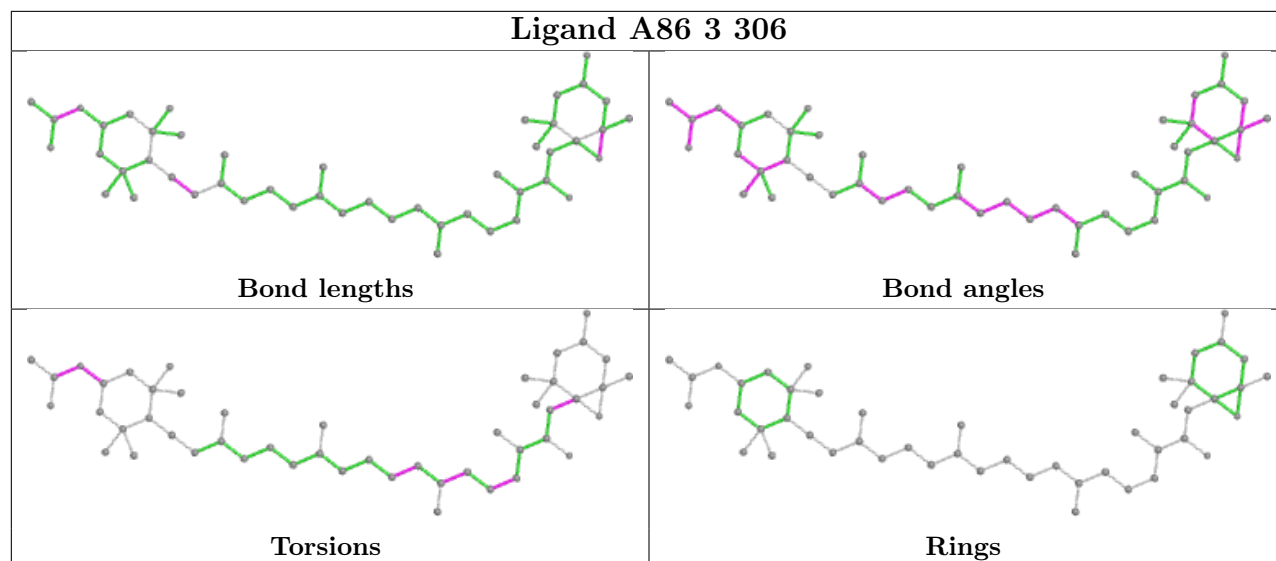


## Ligand KC2 X 314

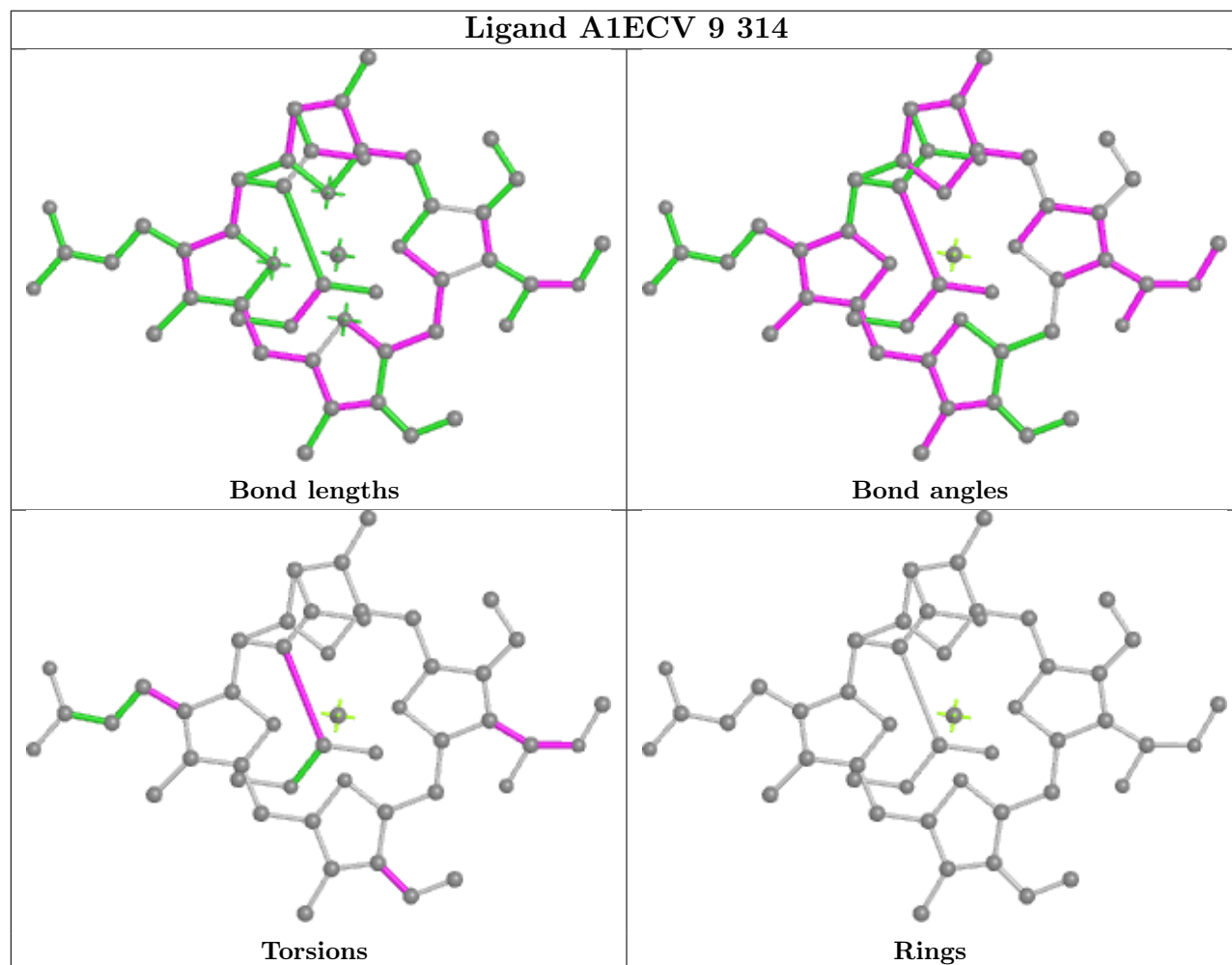




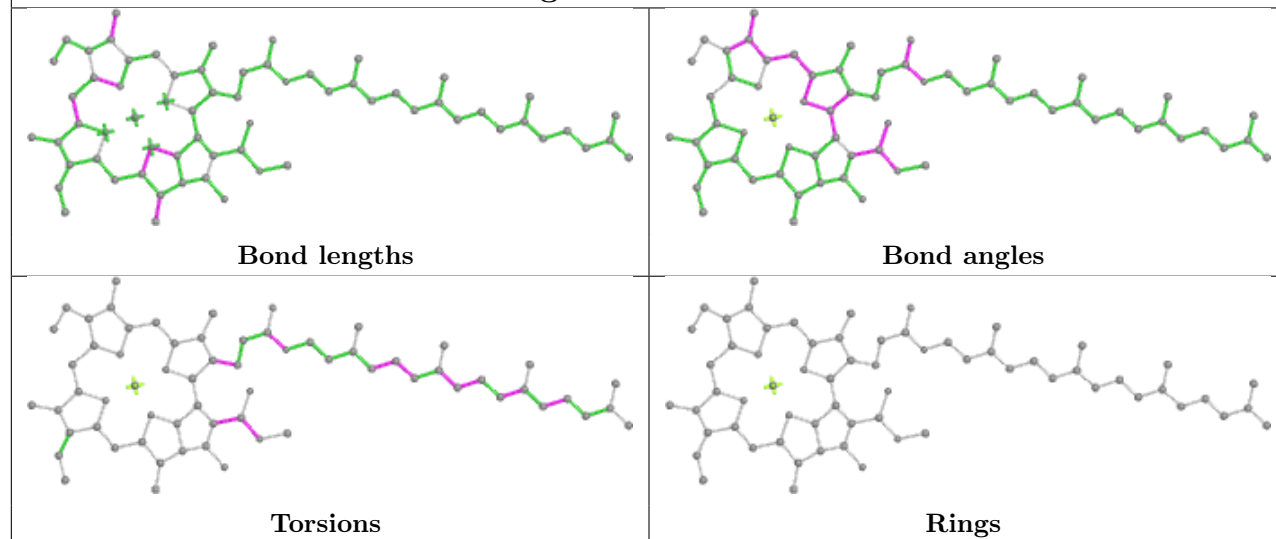
## Ligand A86 3 306



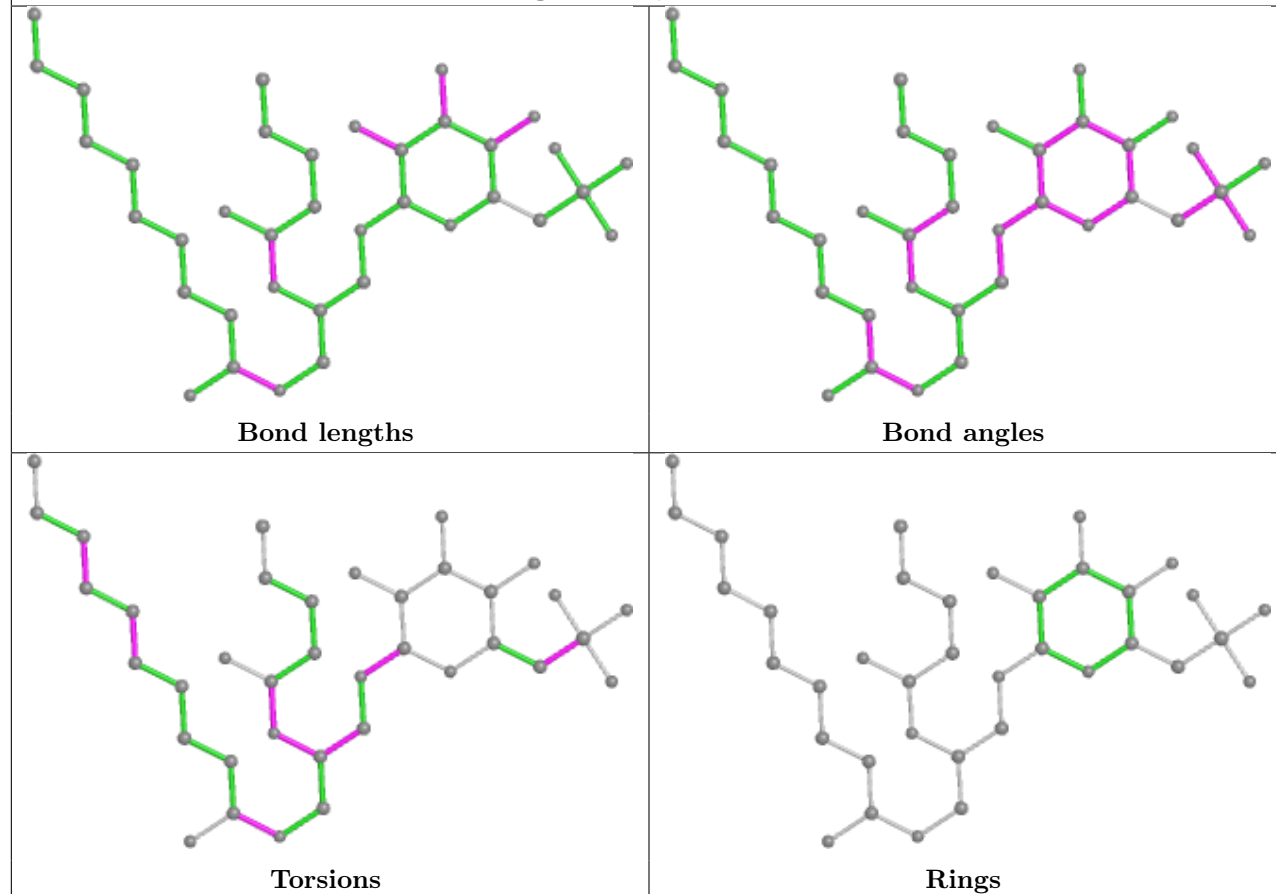
## Ligand A1ECV 9 314



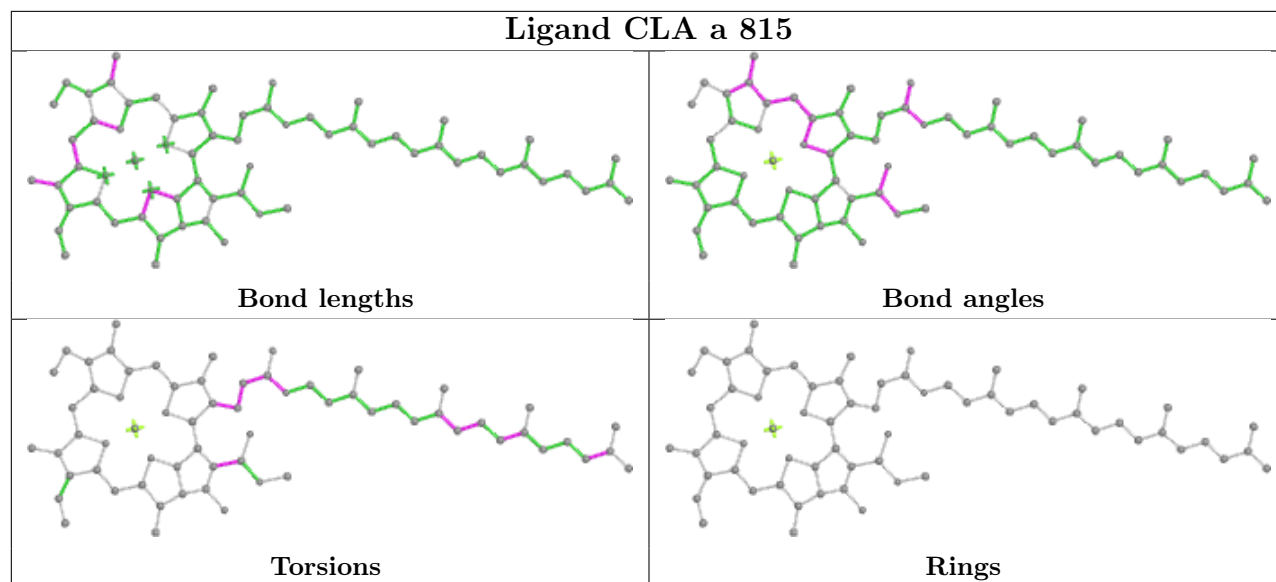
## Ligand CLA i 103



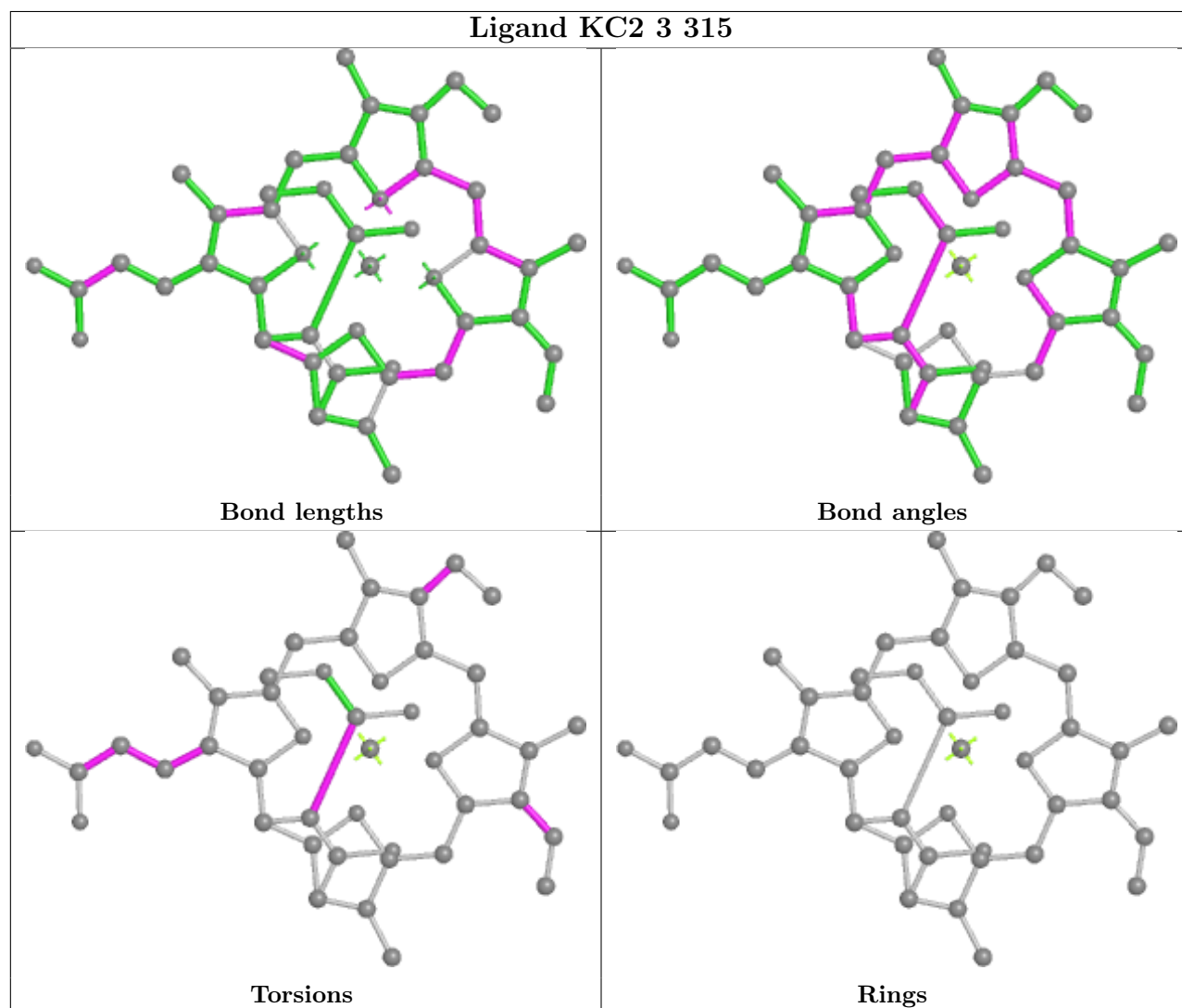
## Ligand SQD D 320



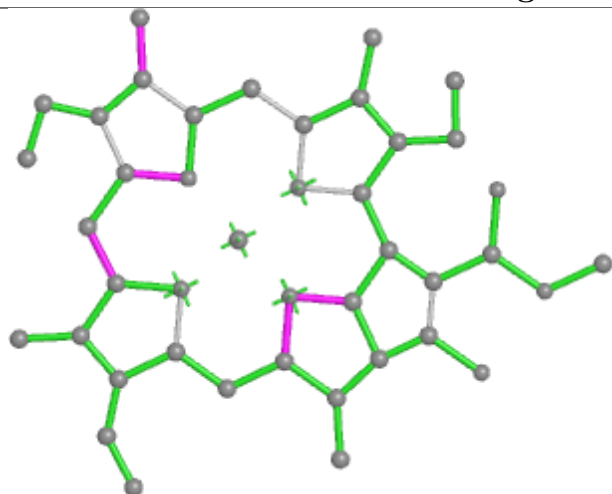
## Ligand CLA a 815



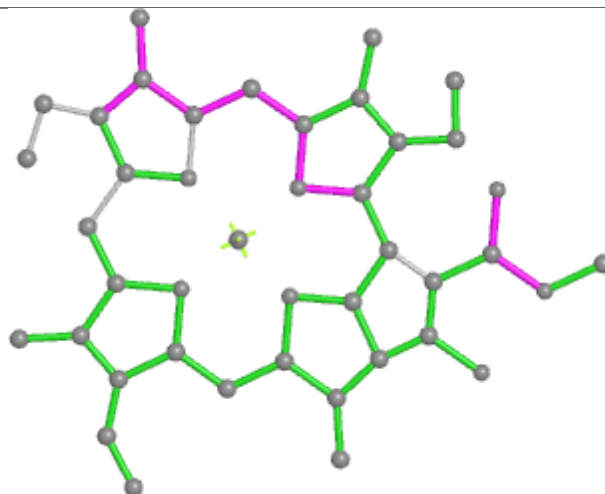
## Ligand KC2 3 315



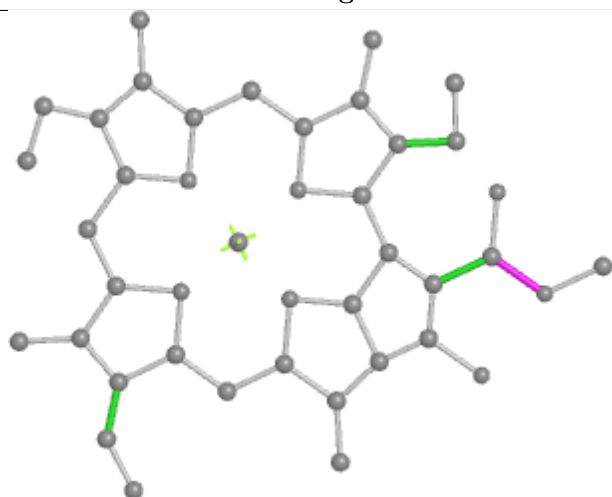
## Ligand CLA 8 321



Bond lengths



Bond angles

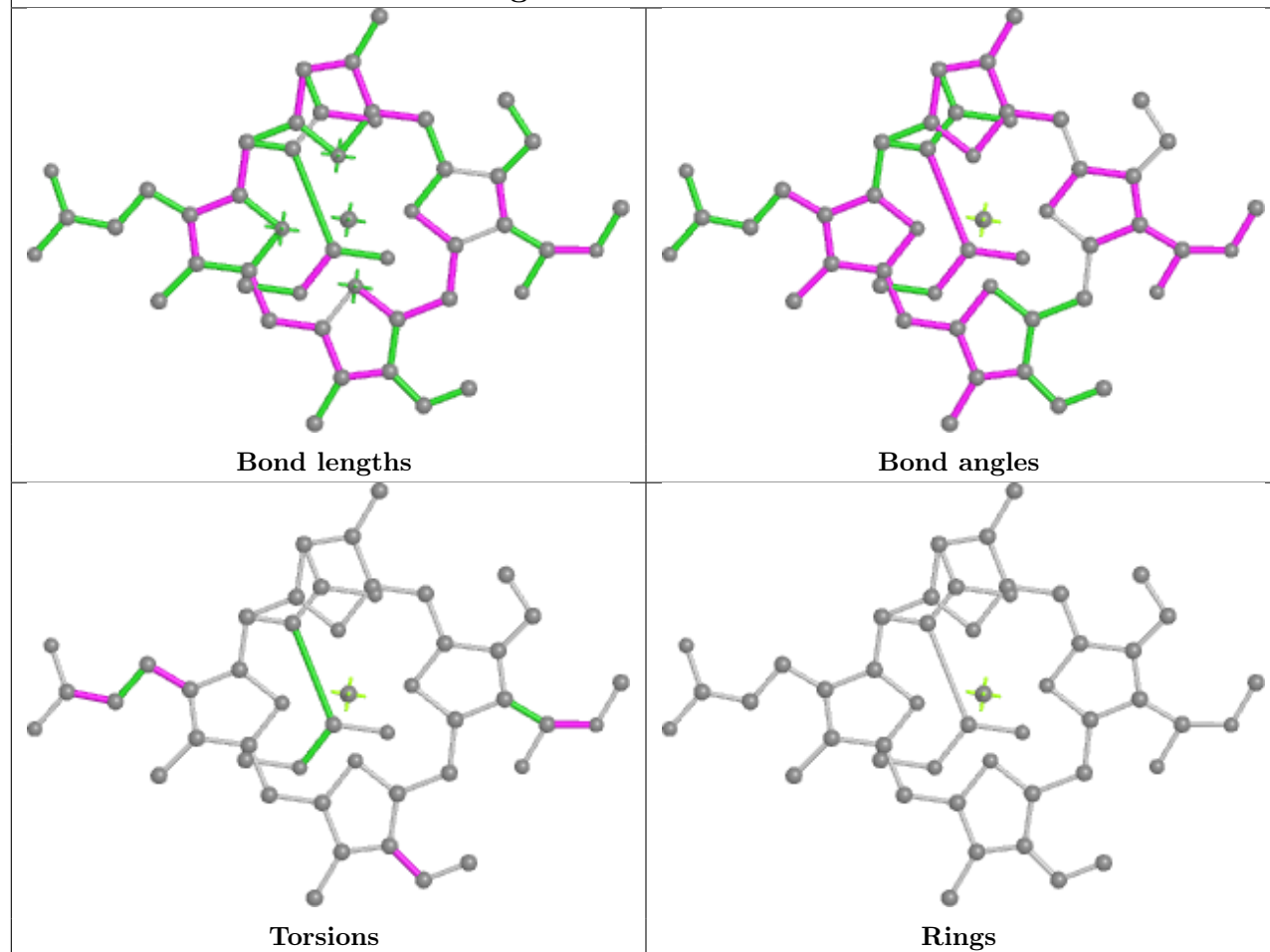


Torsions

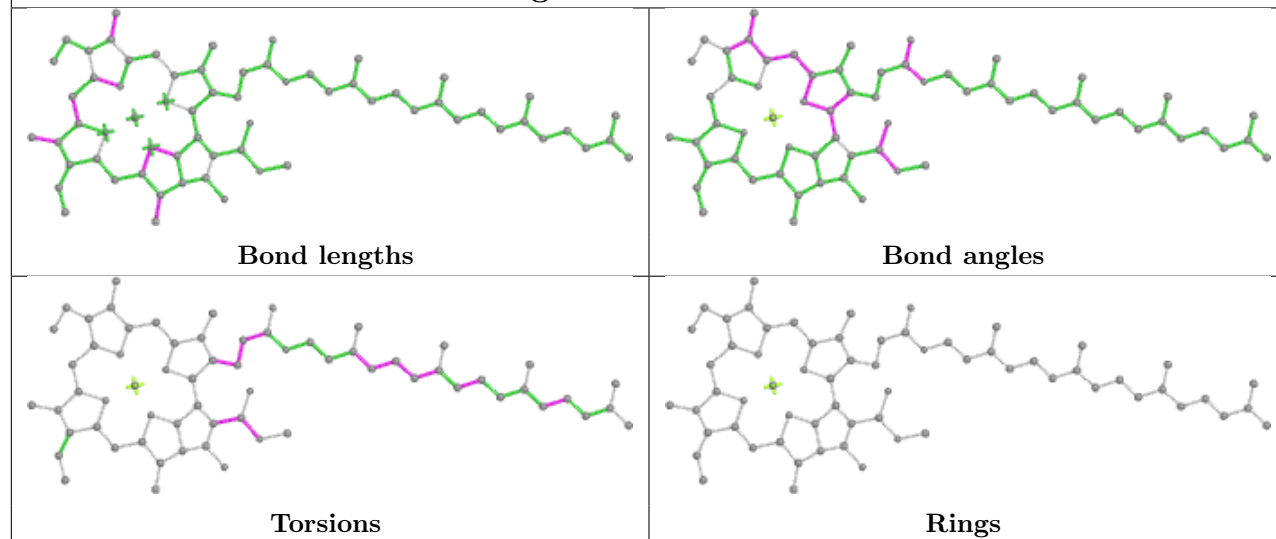


Rings

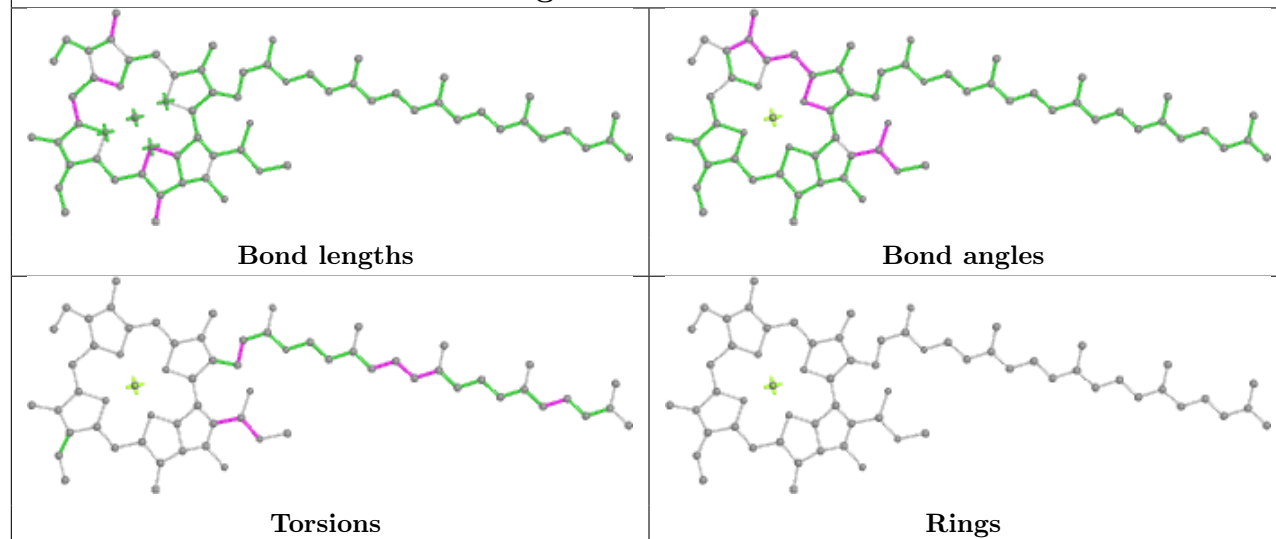
## Ligand A1ECV 2 311



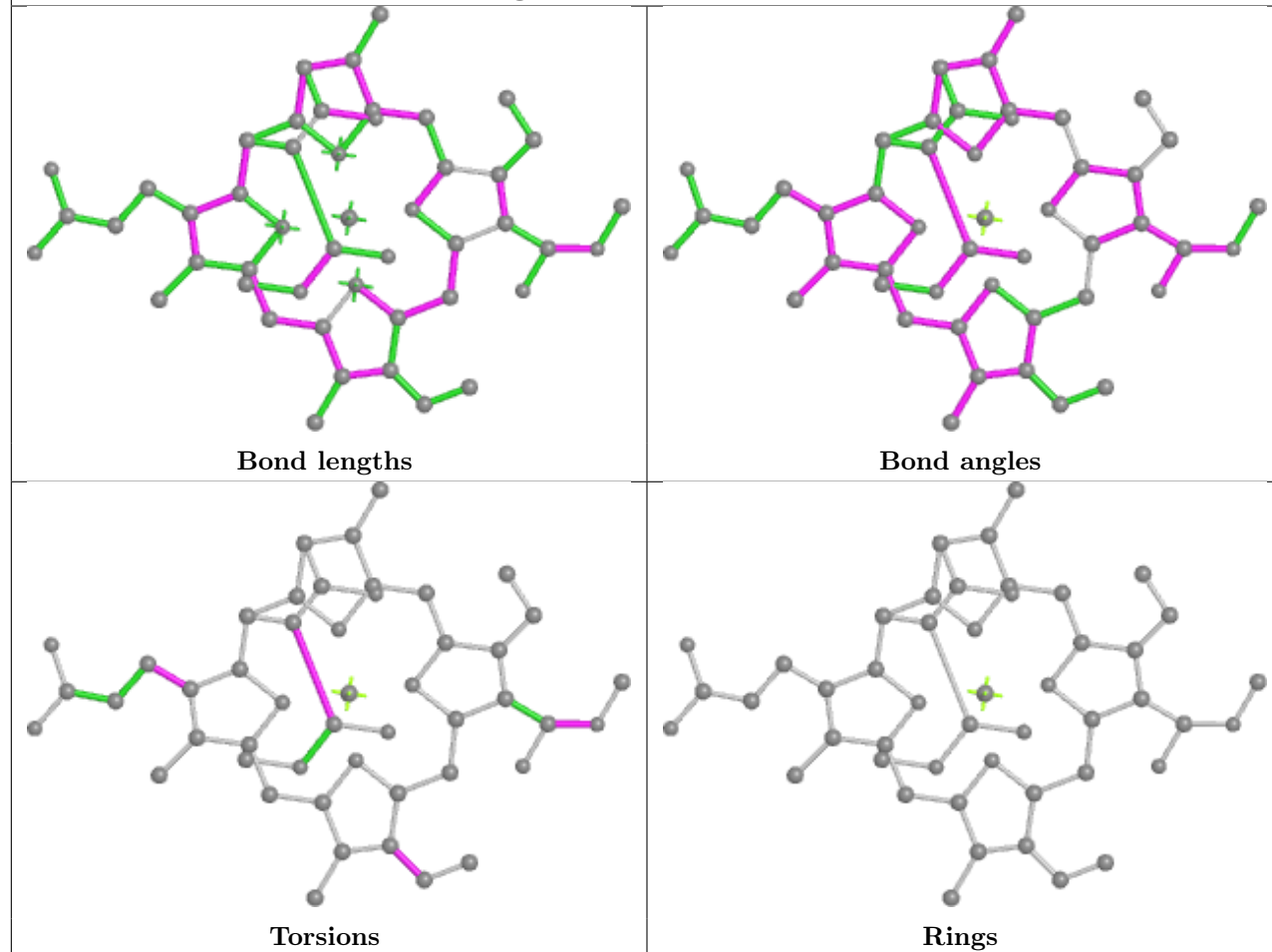
## Ligand CLA D 317



## Ligand CLA a 831

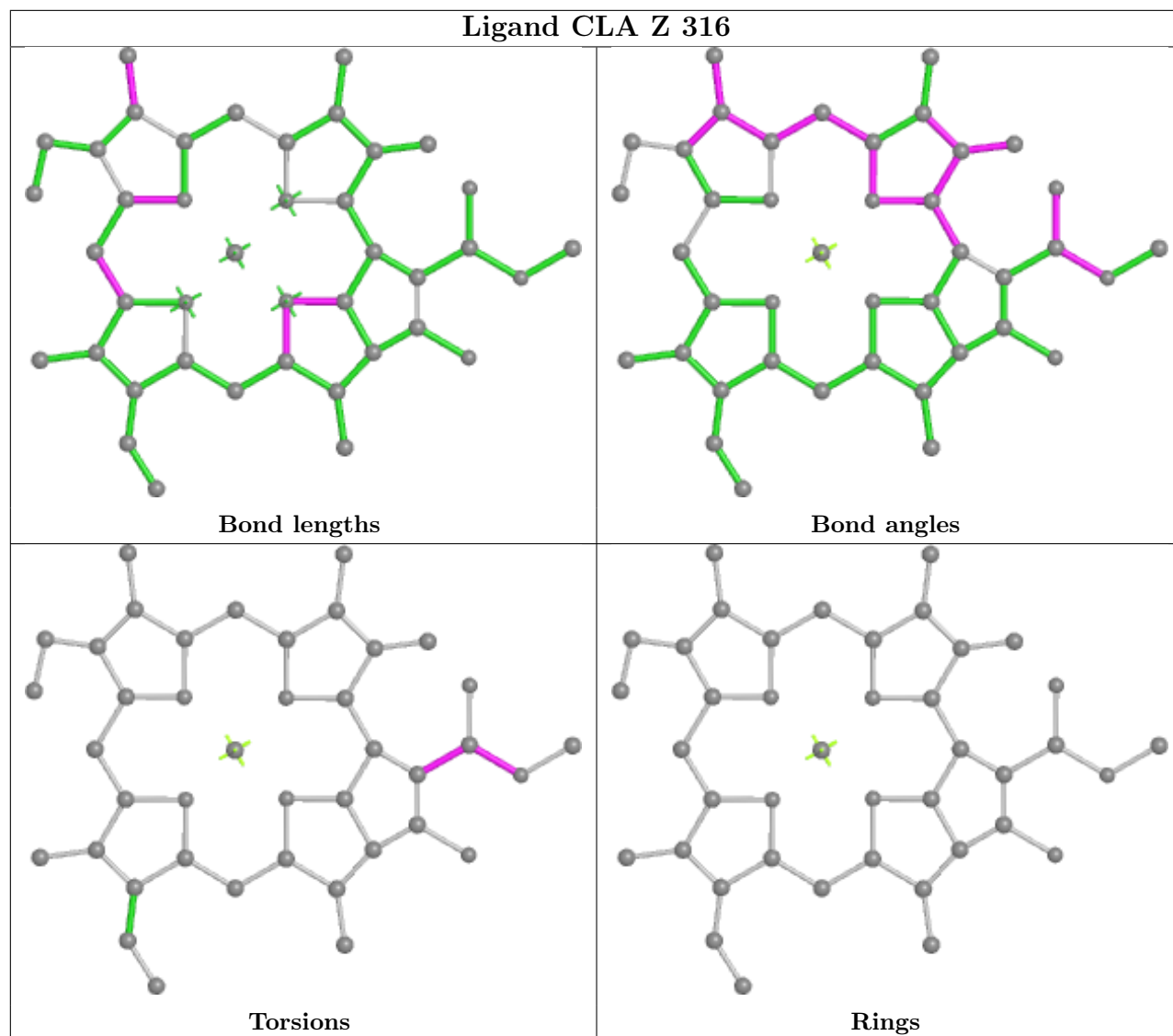


## Ligand A1ECV 9 317

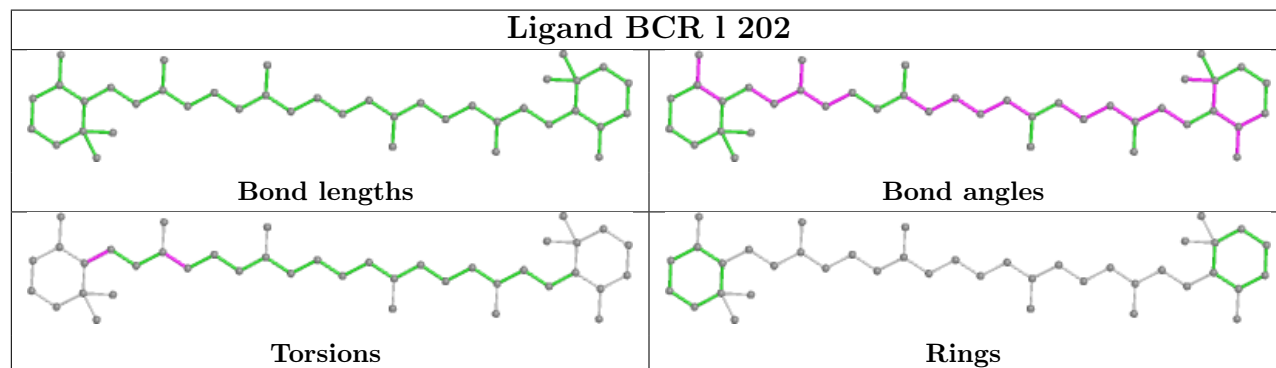




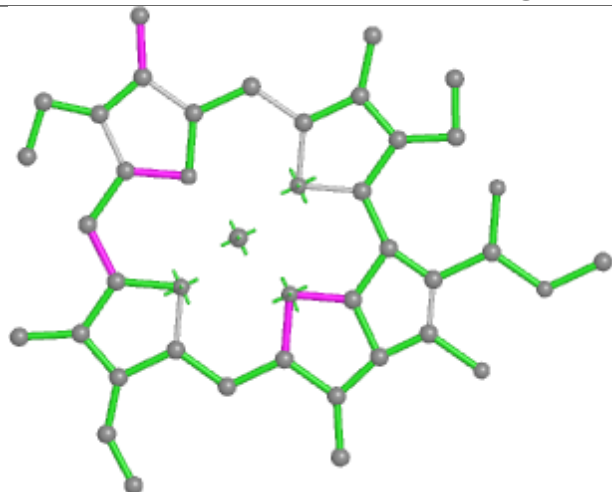
## Ligand CLA Z 316



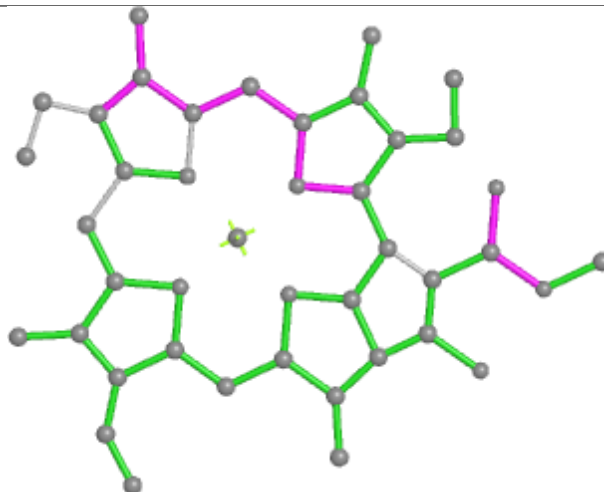
## Ligand BCR 1 202



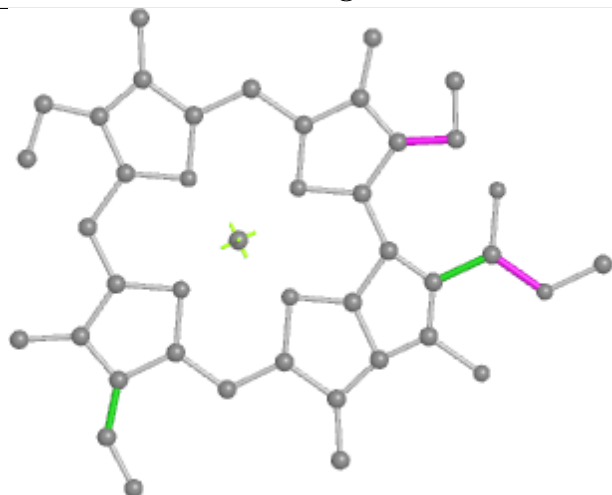
## Ligand CLA 6 313



Bond lengths



Bond angles

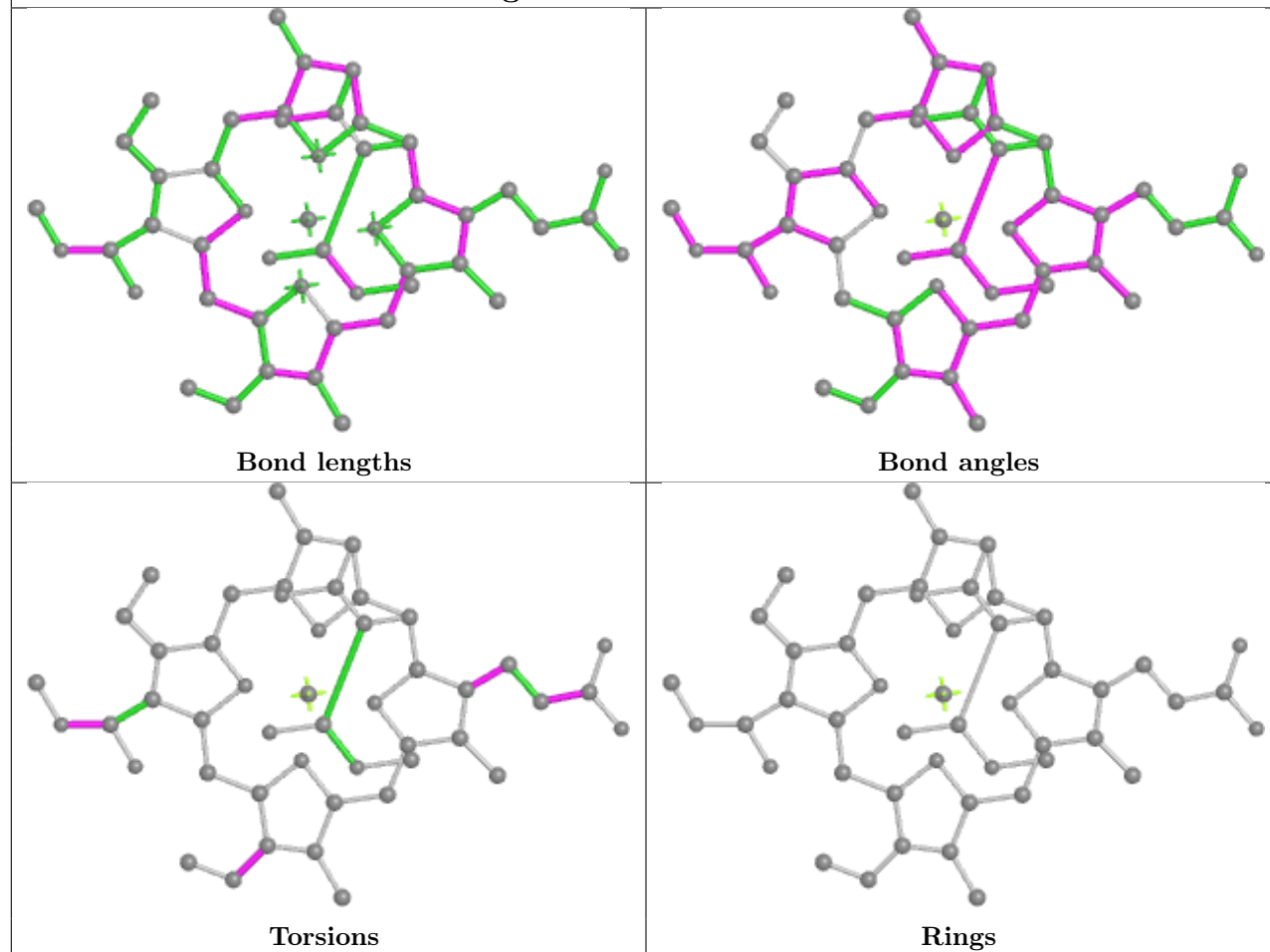


Torsions

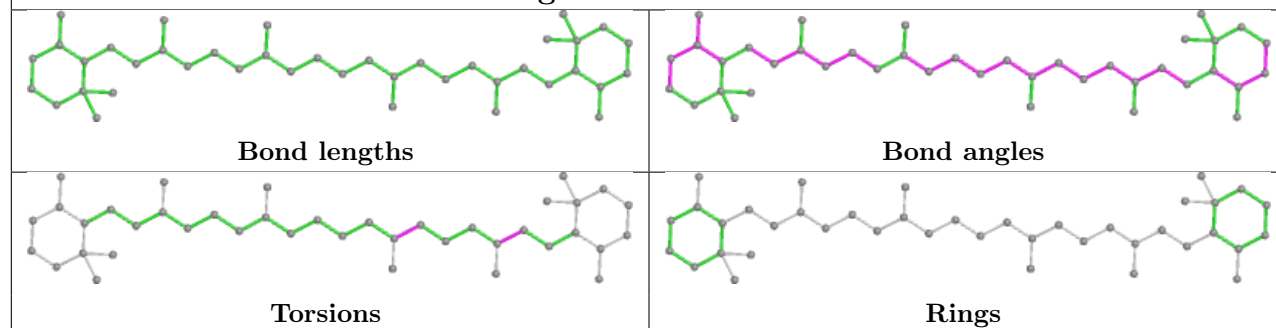


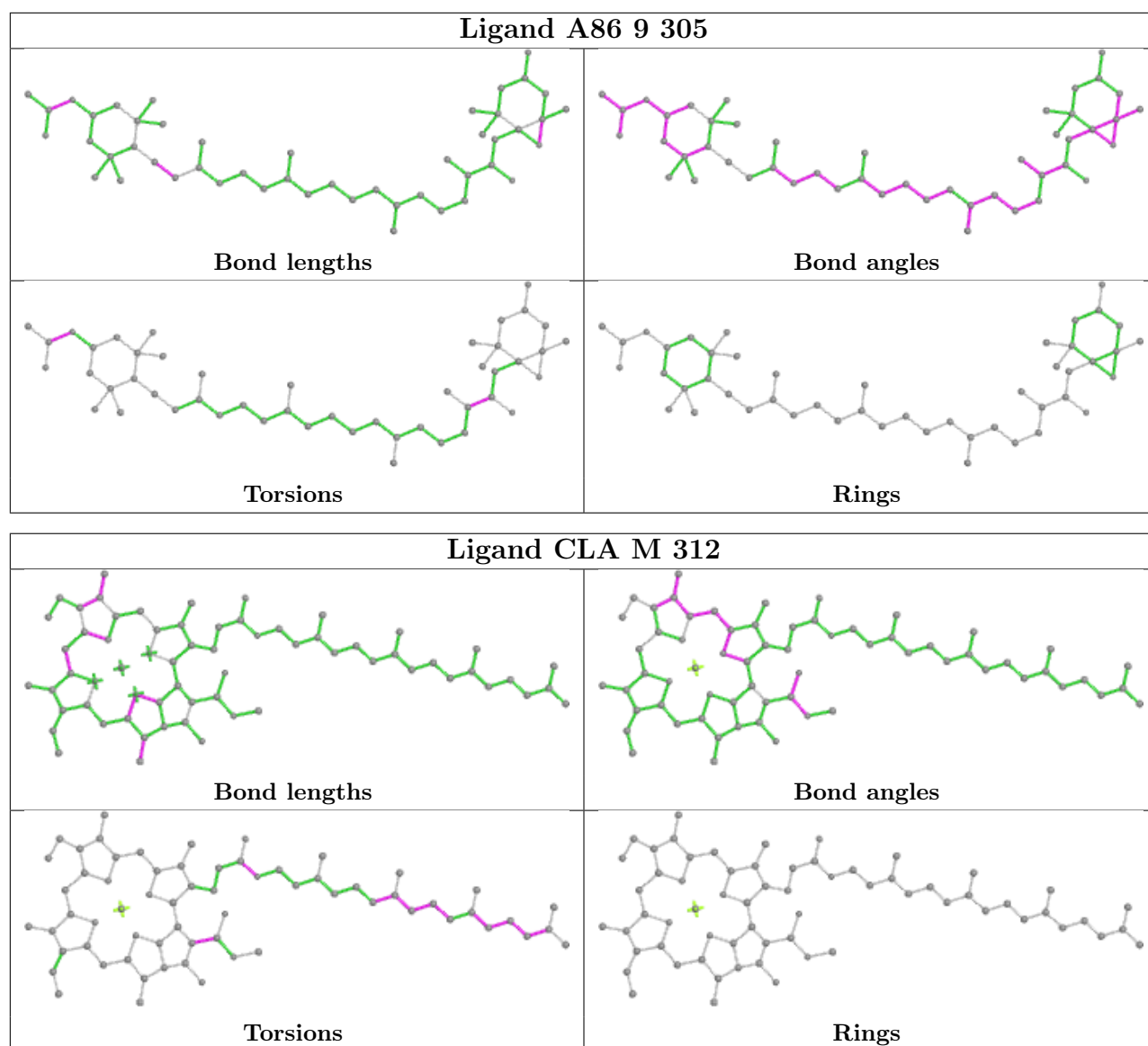
Rings

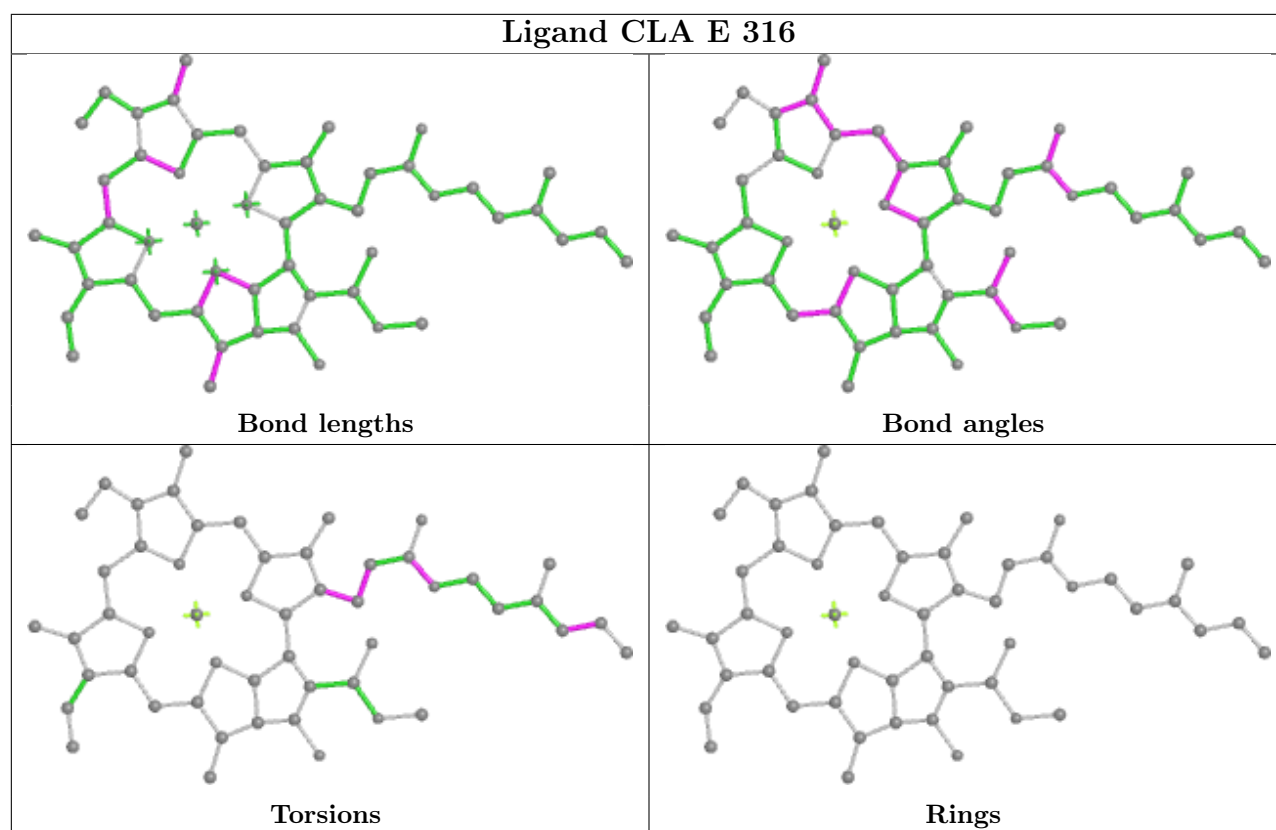
## Ligand A1ECV M 316



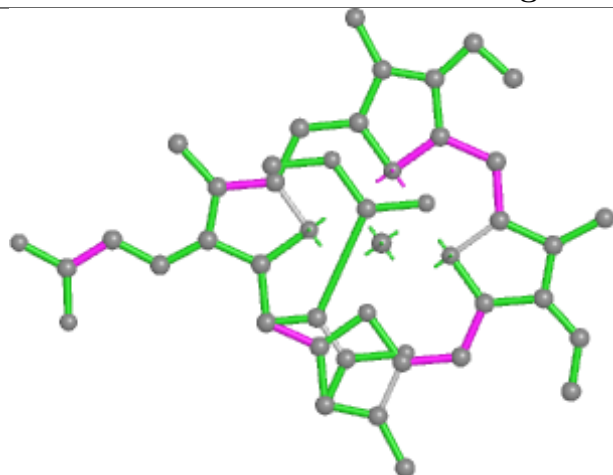
## Ligand BCR f 801



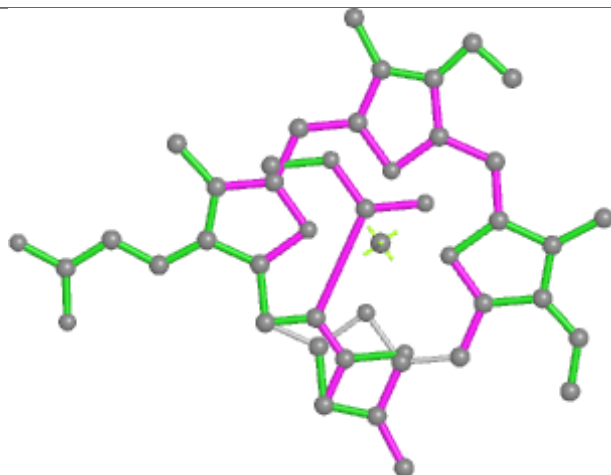




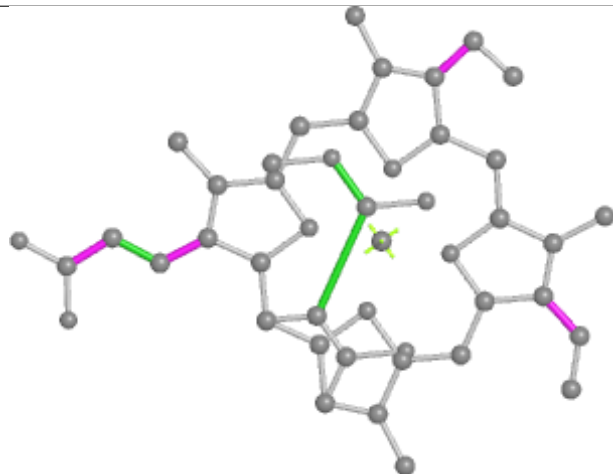
## Ligand KC2 7 320



Bond lengths



Bond angles

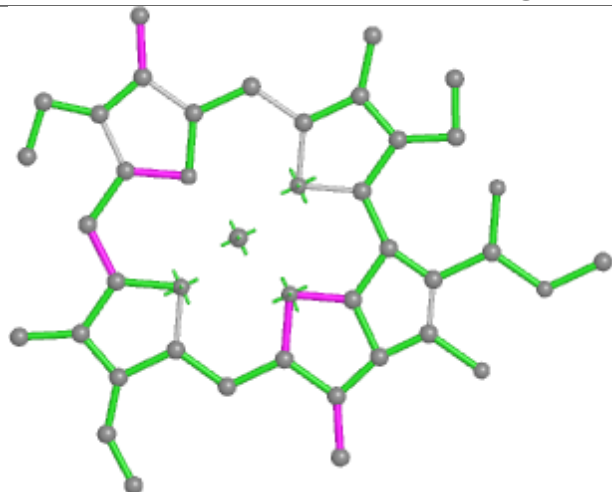


Torsions

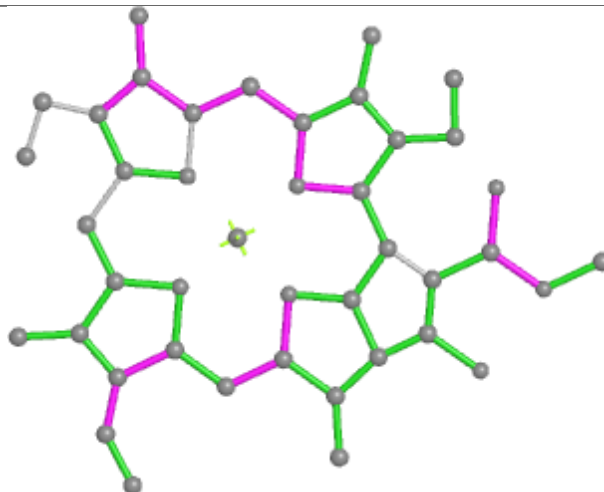


Rings

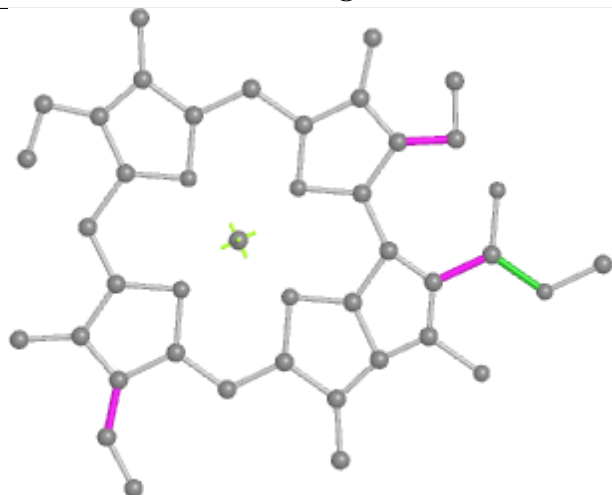
## Ligand CLA 9 312



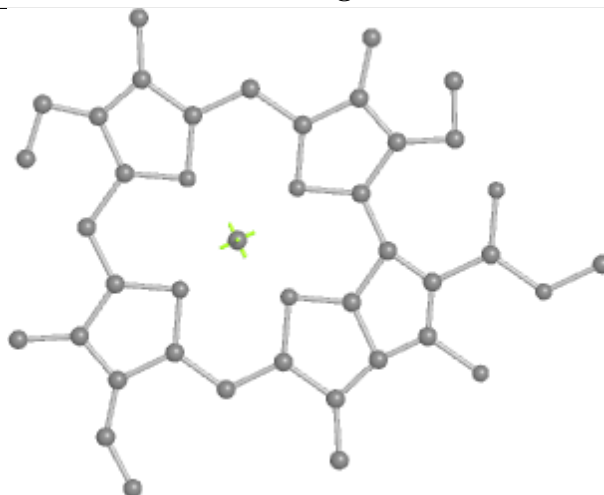
Bond lengths



Bond angles

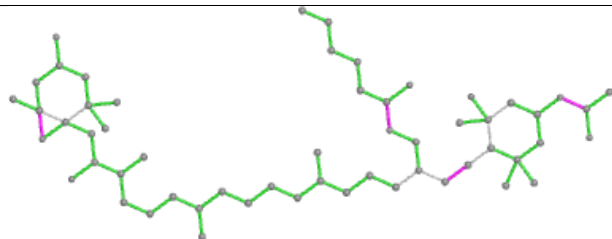


Torsions

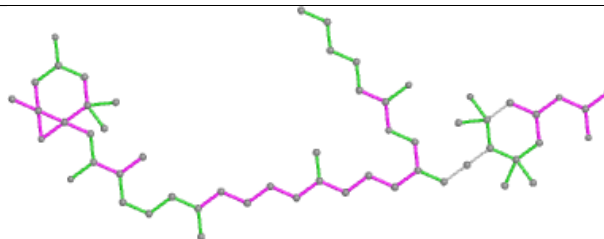


Rings

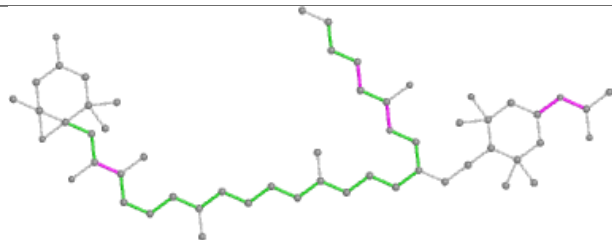
## Ligand A1EB1 3 303



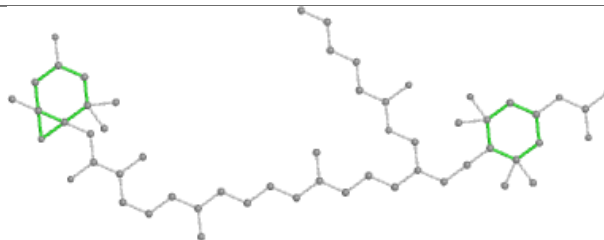
Bond lengths



Bond angles

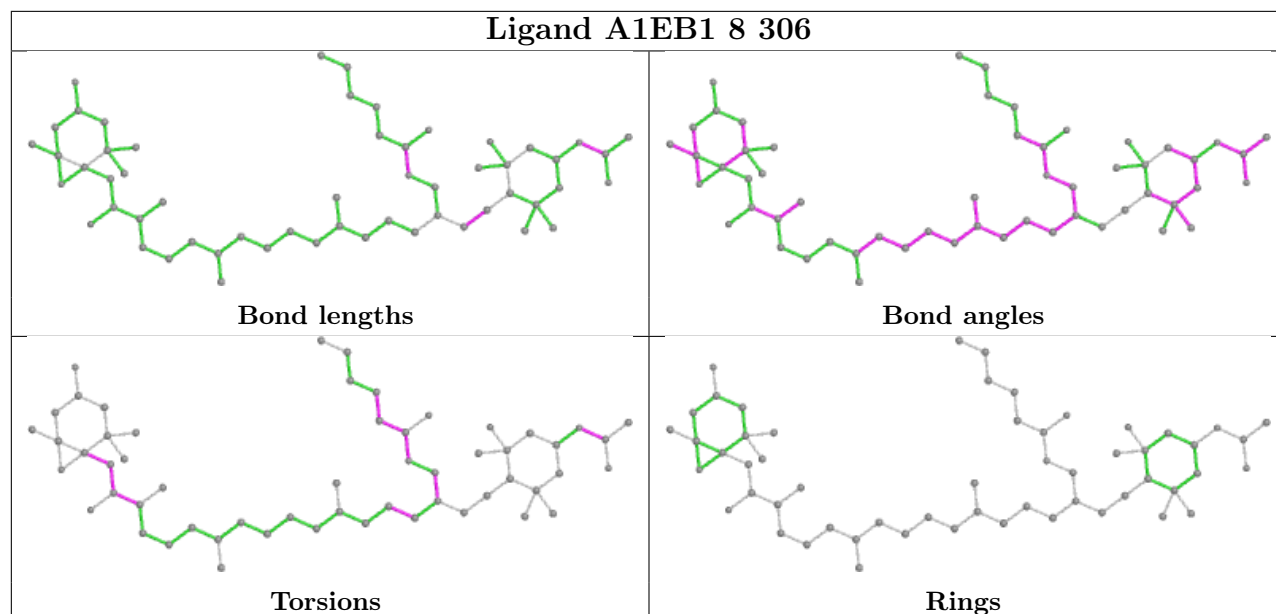


Torsions

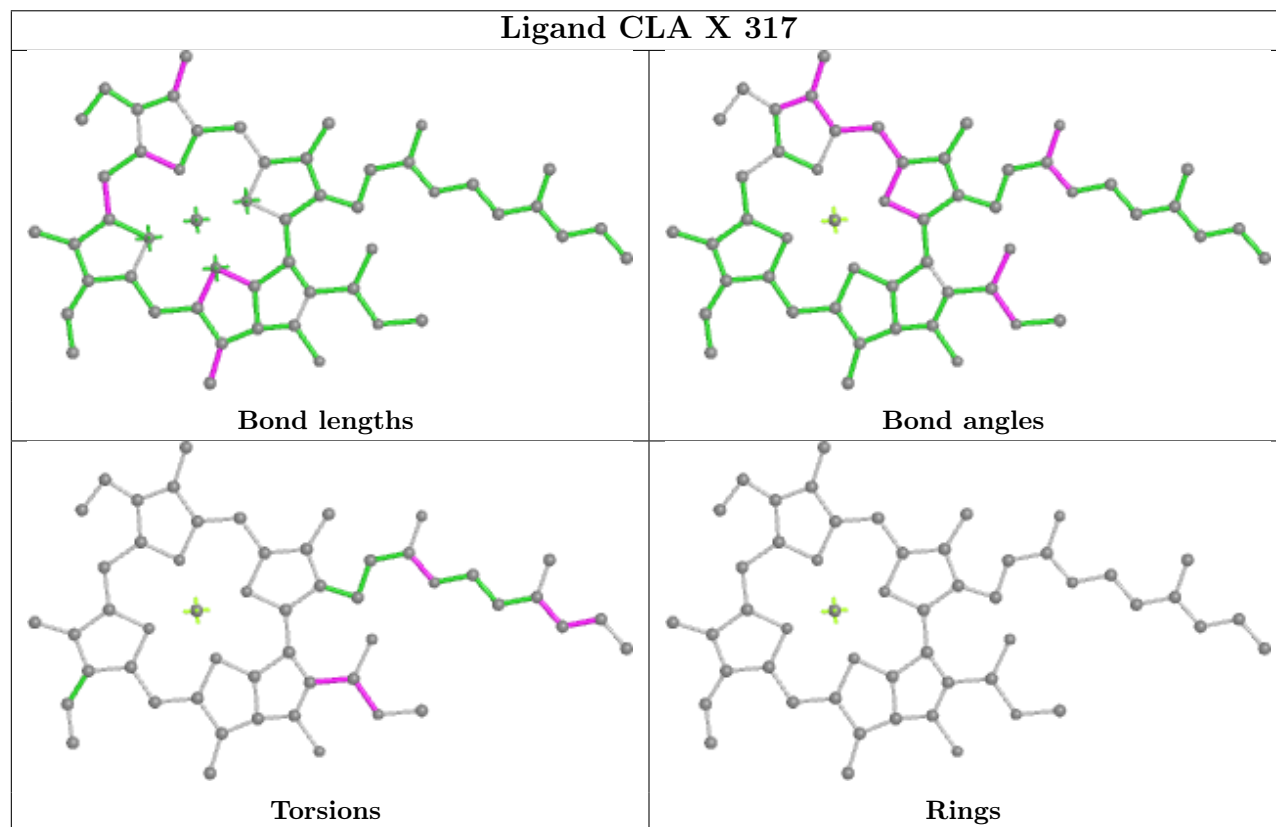


Rings

## Ligand A1EB1 8 306

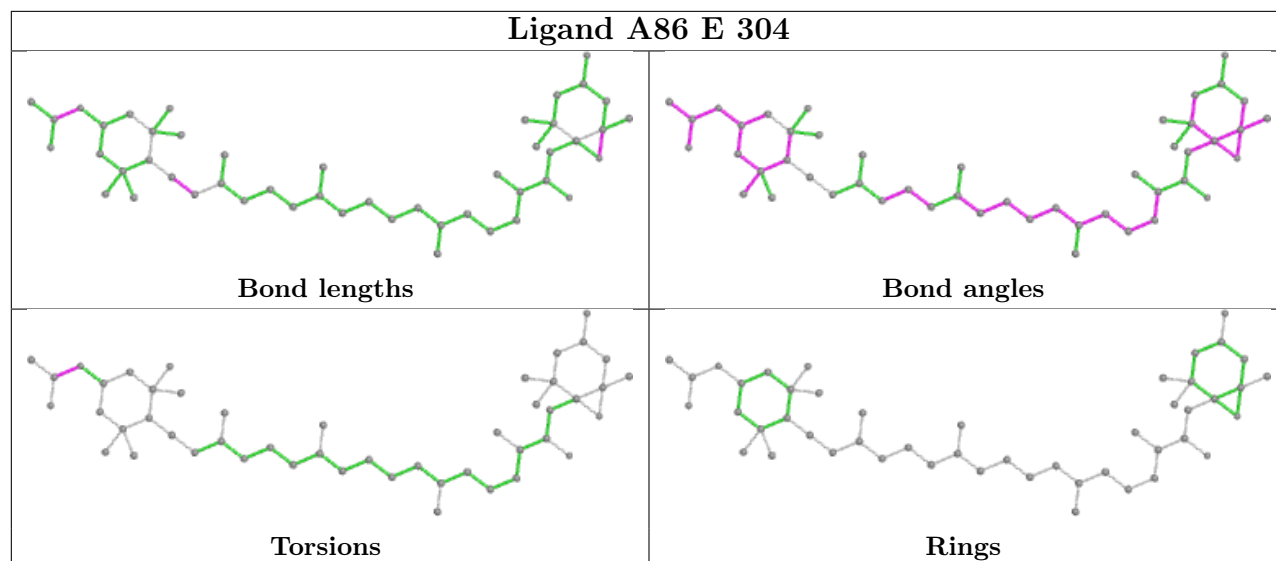


## Ligand CLA X 317

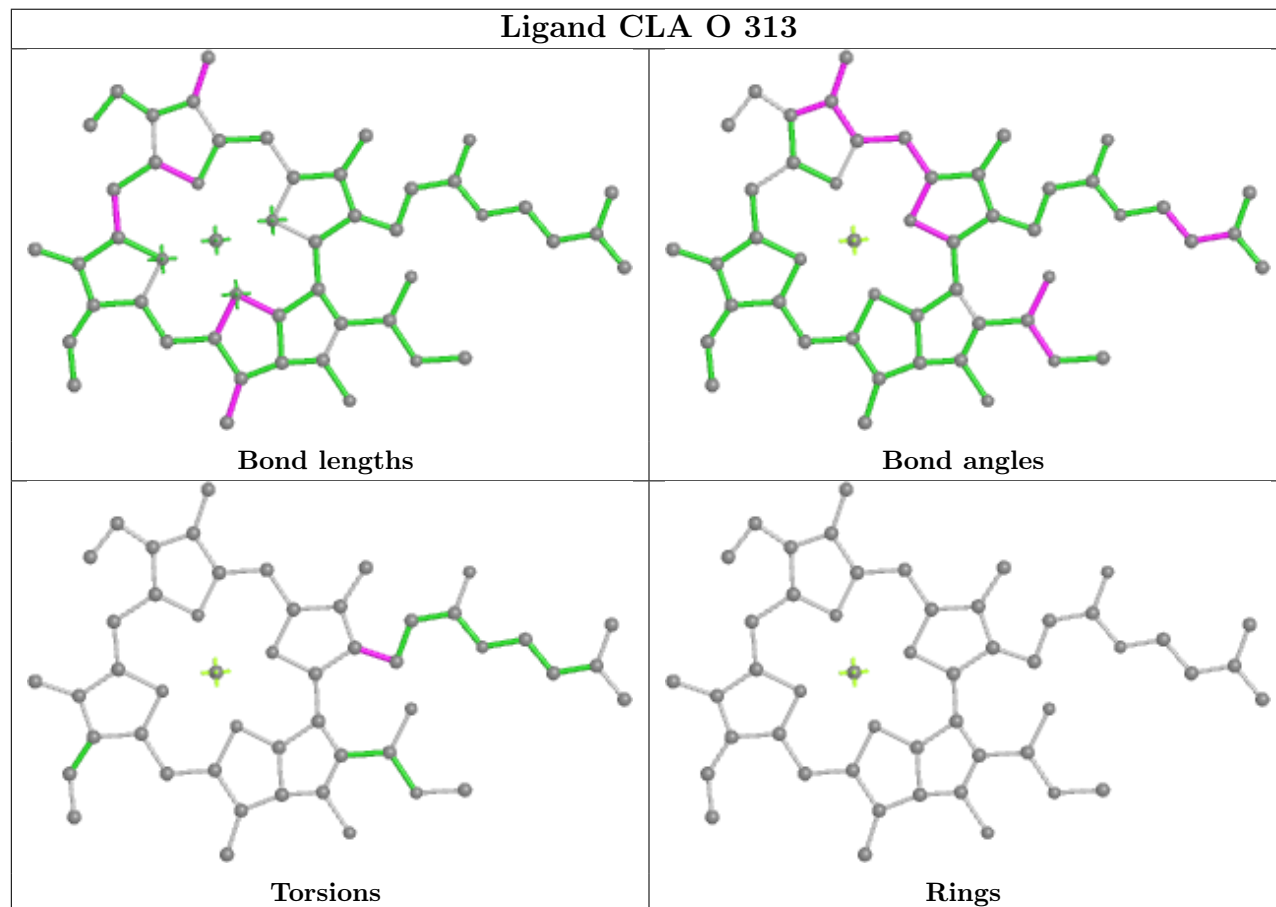




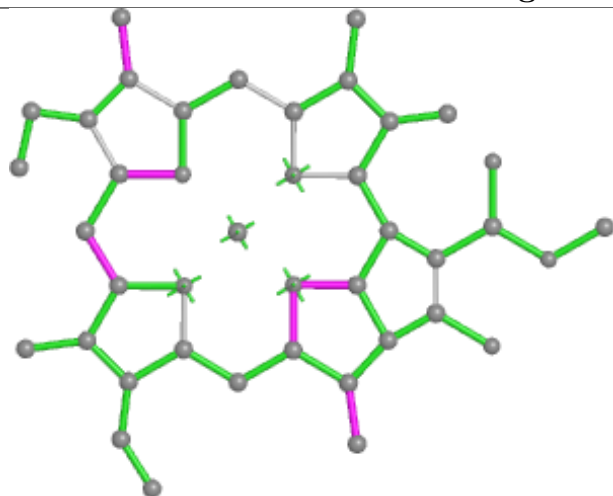
## Ligand A86 E 304



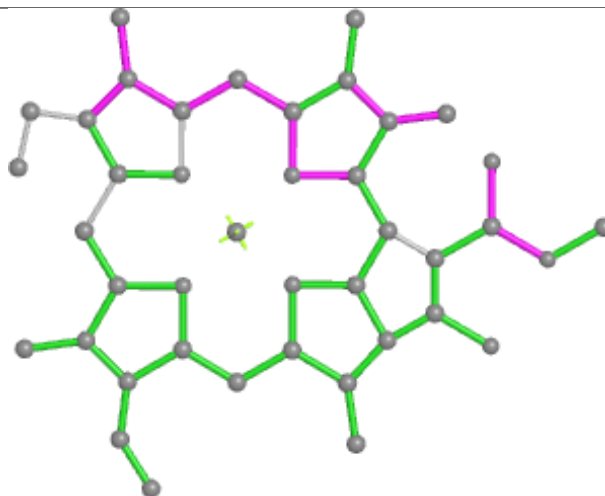
## Ligand CLA O 313



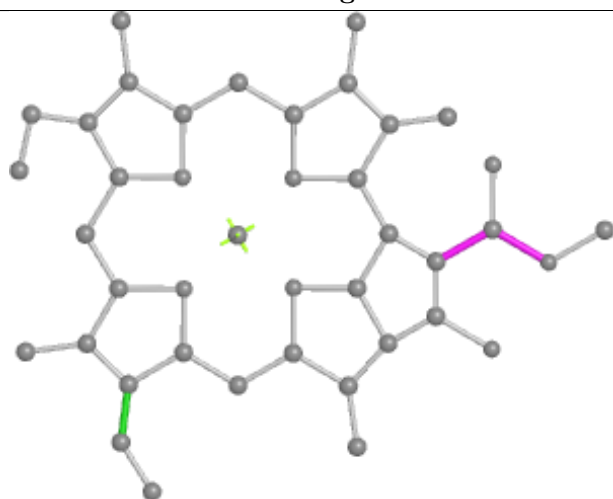
## Ligand CLA 9 309



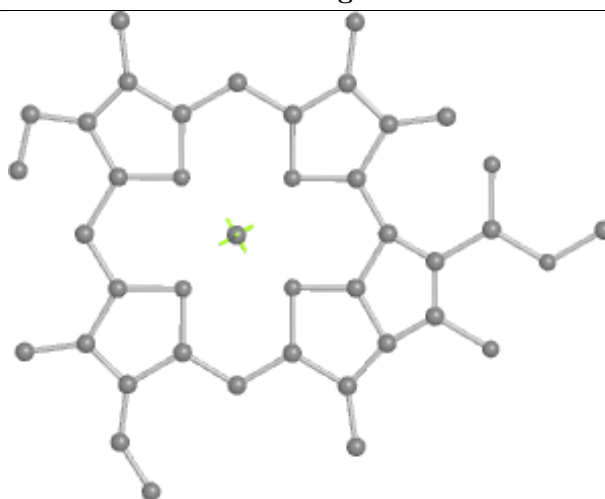
Bond lengths



Bond angles

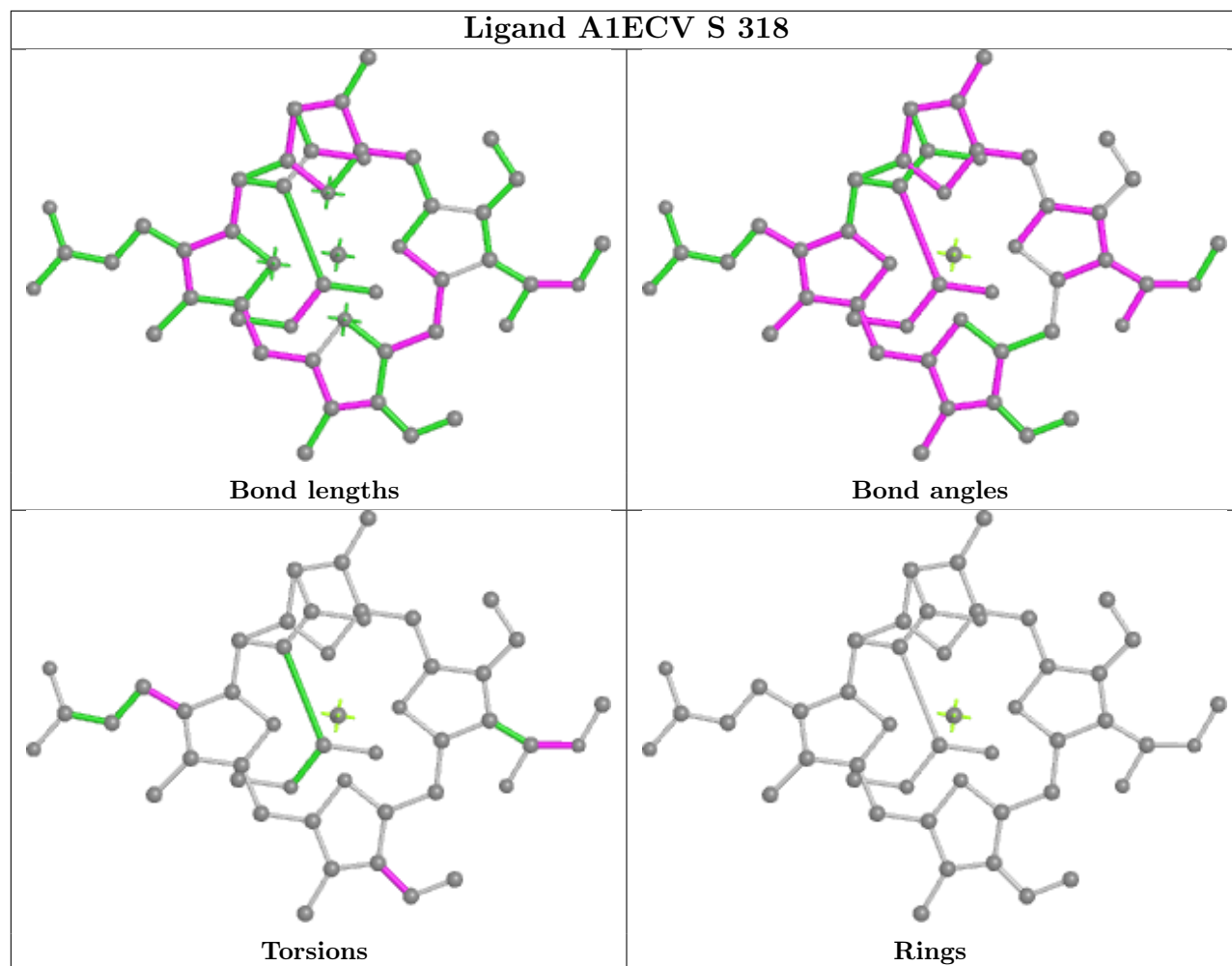


Torsions

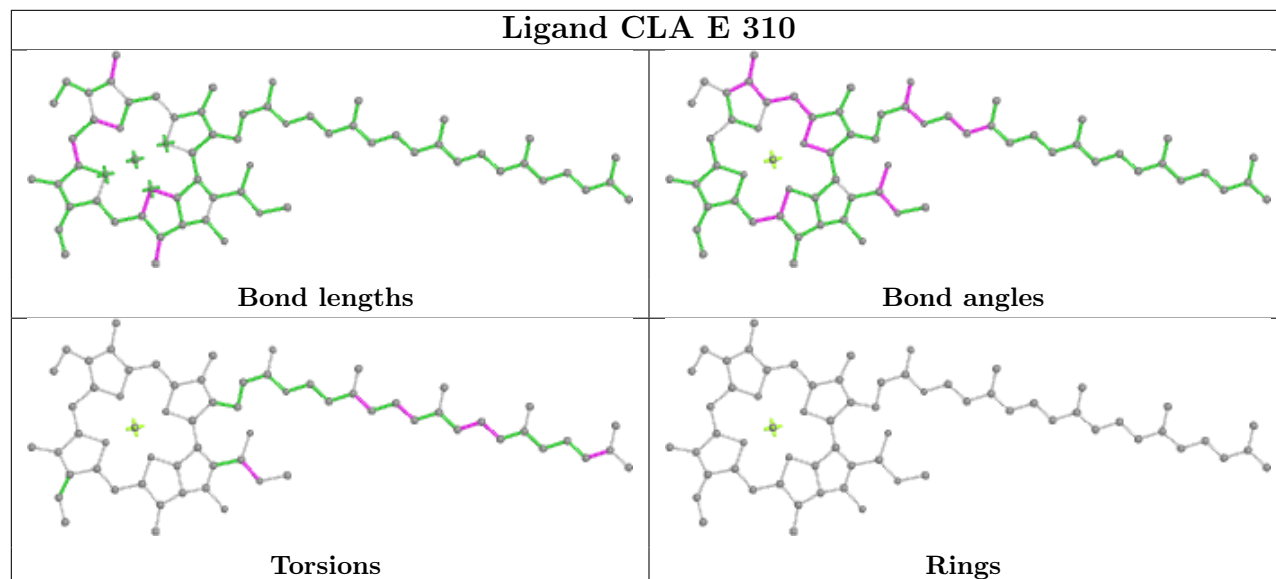


Rings

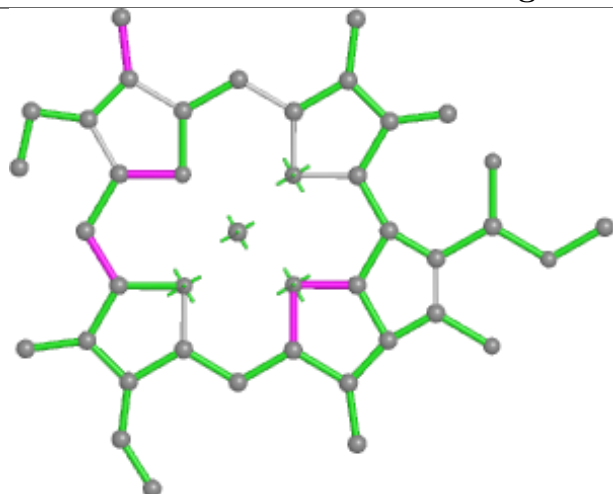
## Ligand A1ECV S 318



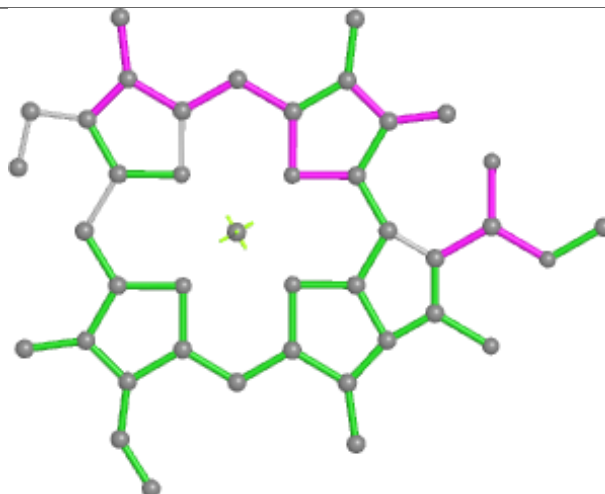
## Ligand CLA E 310



## Ligand CLA 8 318



Bond lengths



Bond angles

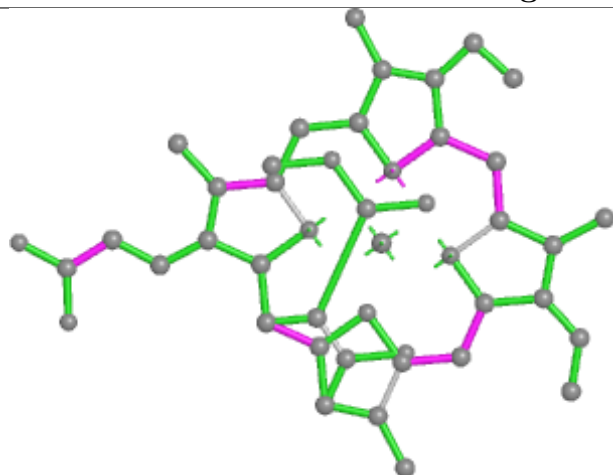


Torsions

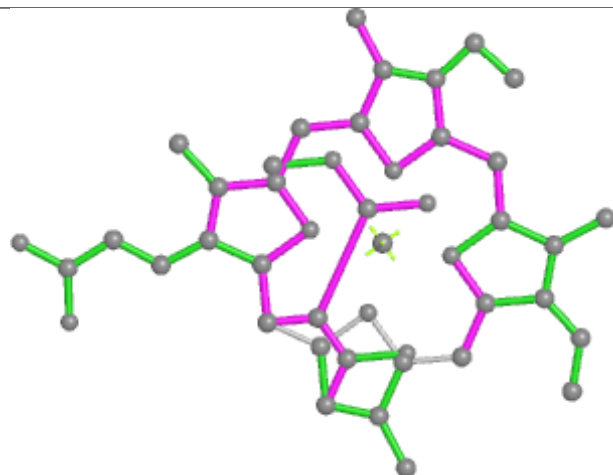


Rings

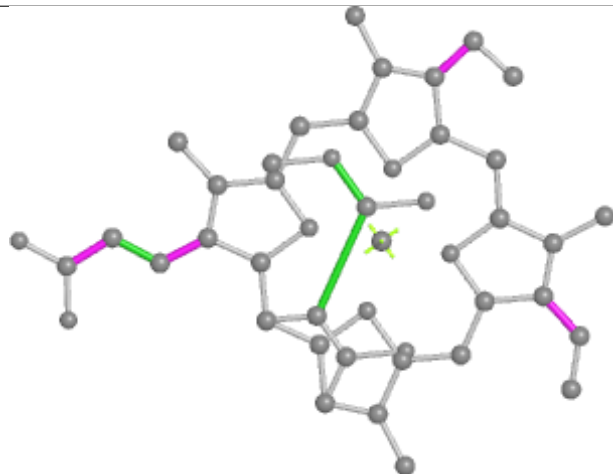
## Ligand KC2 3 317



Bond lengths



Bond angles

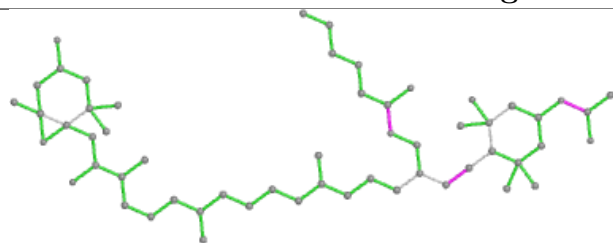


Torsions

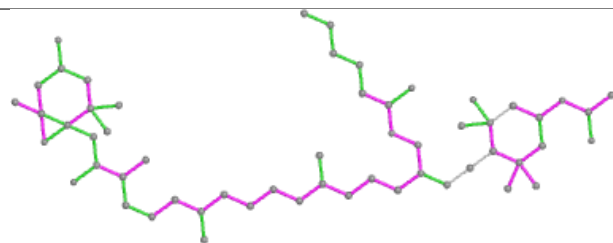


Rings

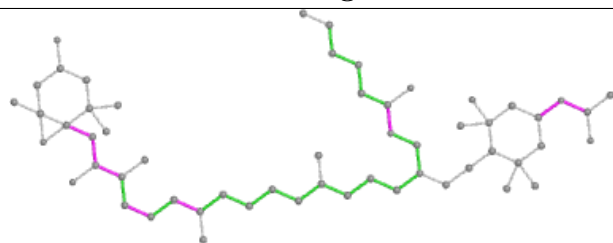
## Ligand A1EB1 z 302



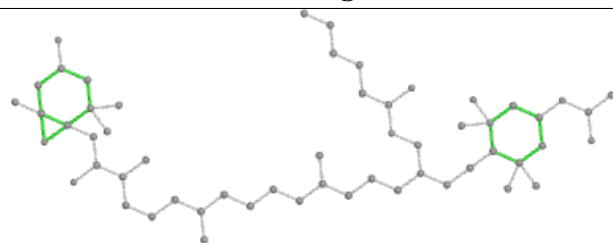
Bond lengths



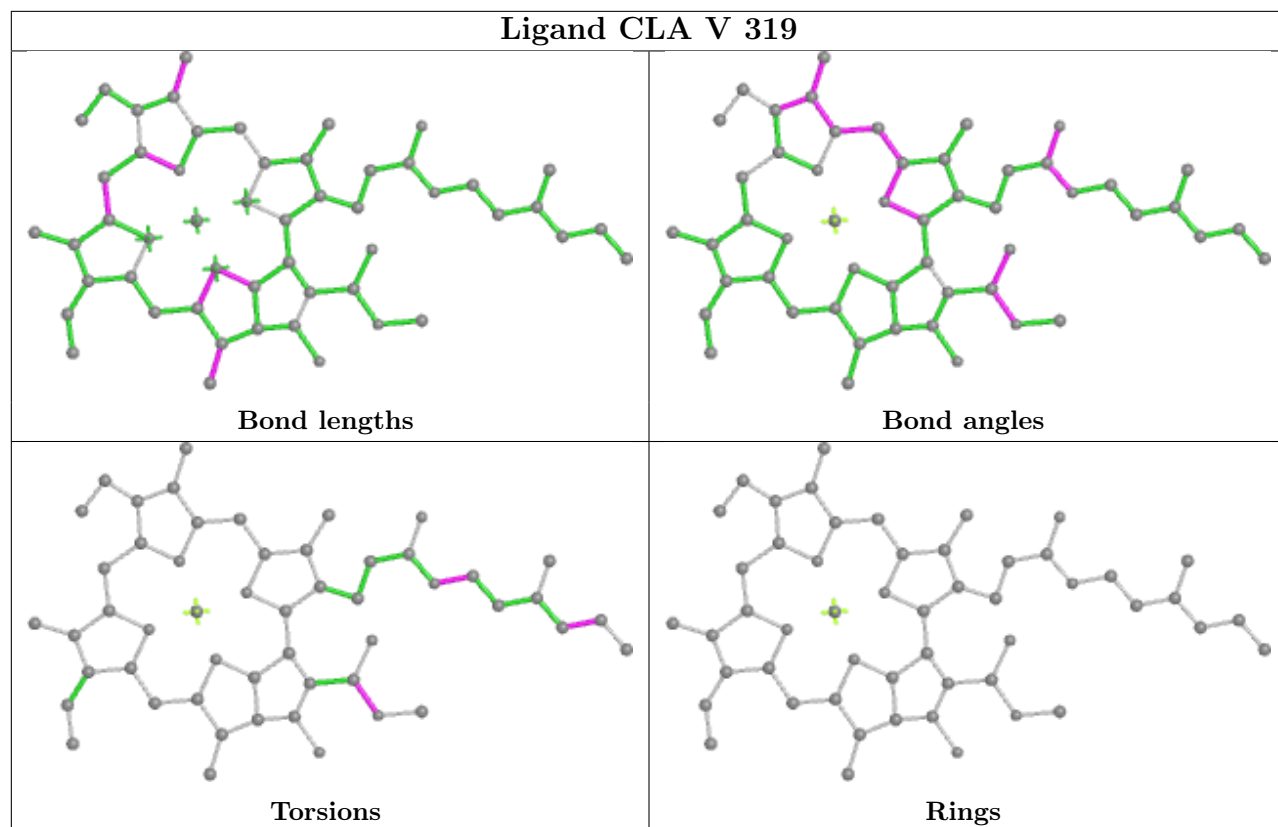
Bond angles



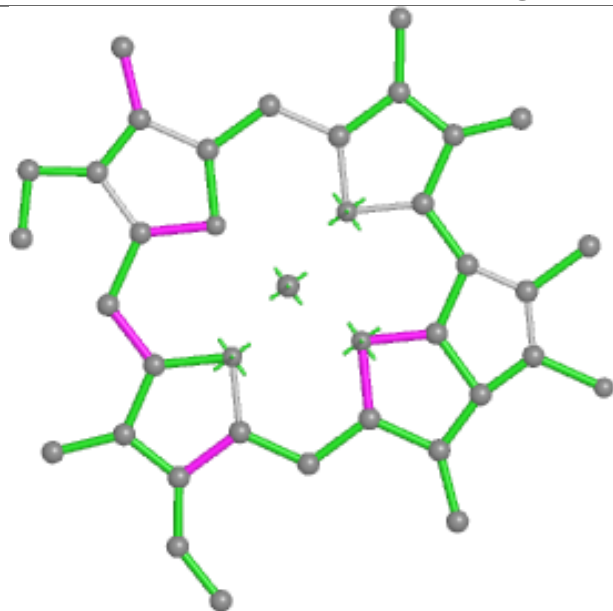
Torsions



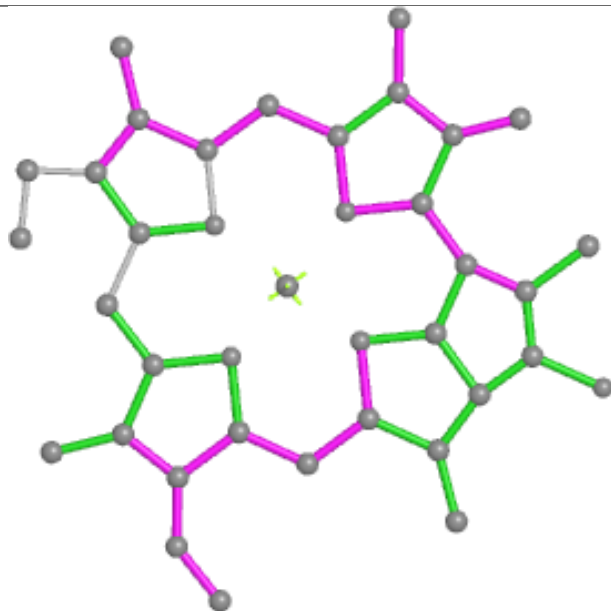
Rings



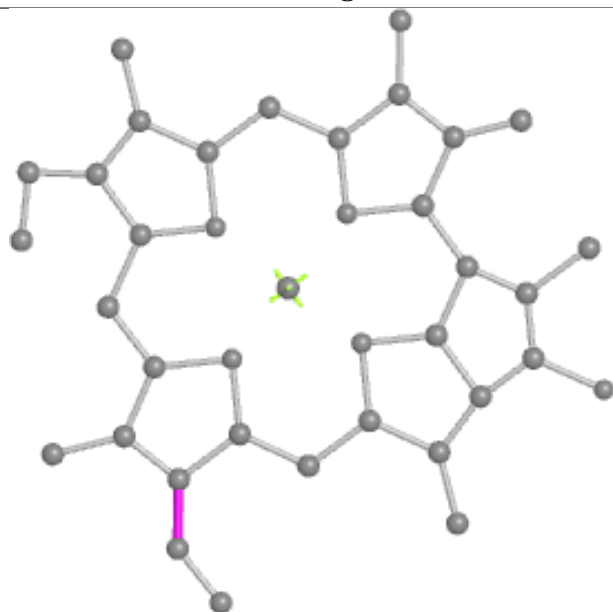
## Ligand CLA O 308



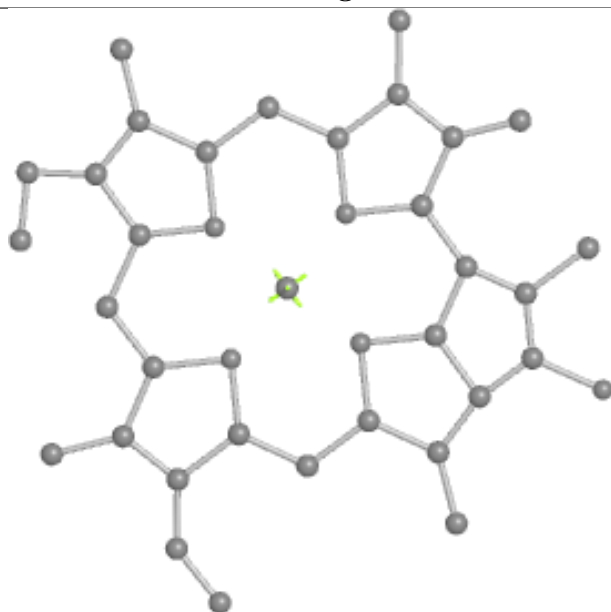
Bond lengths



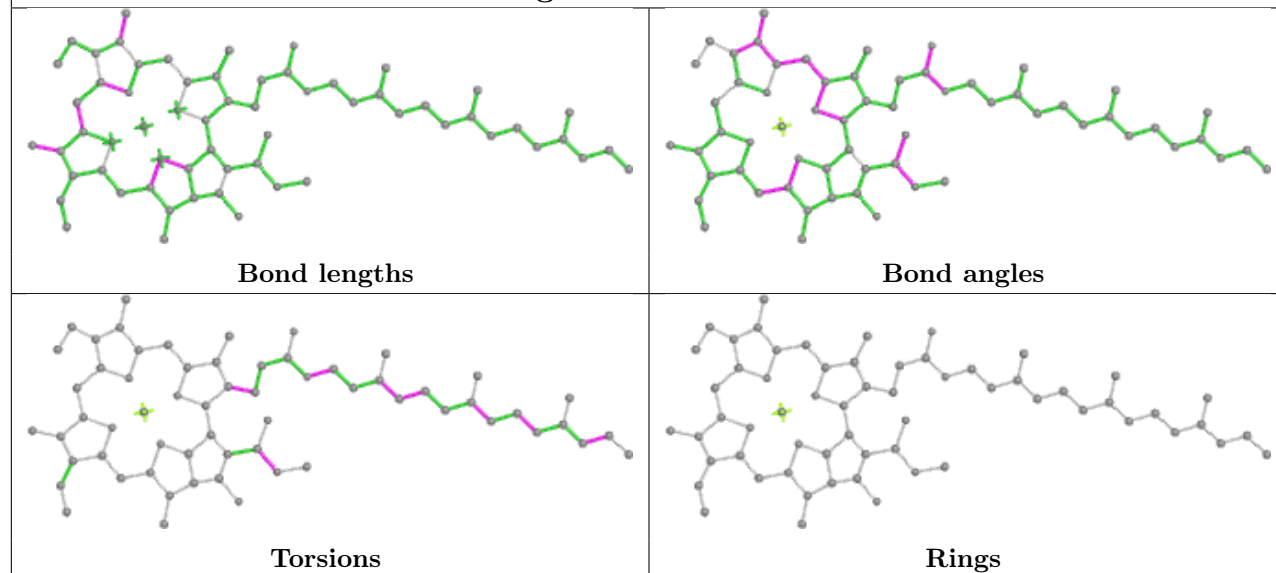
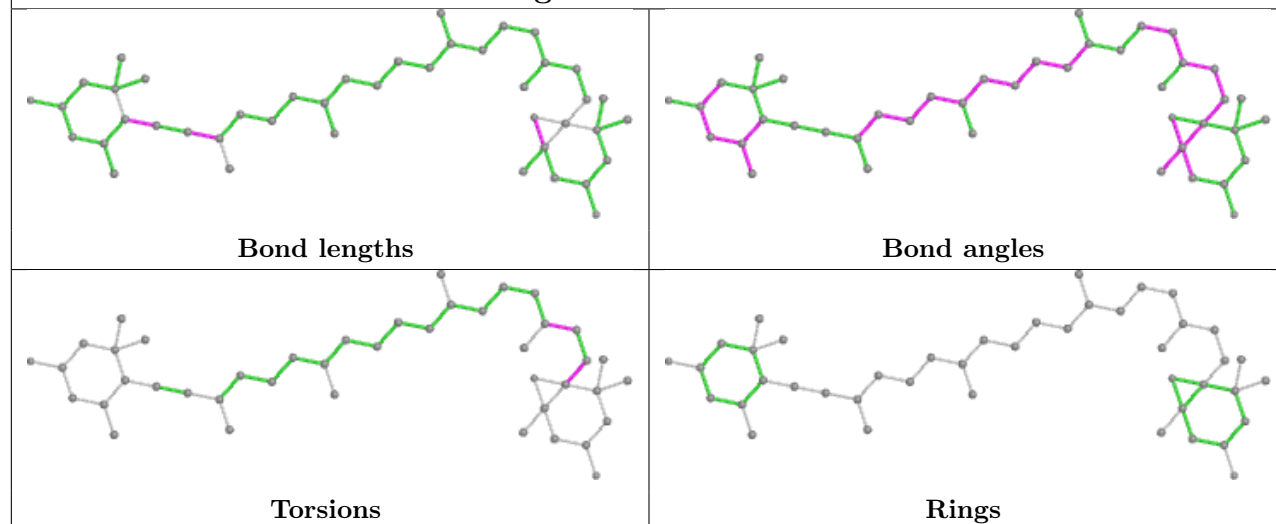
Bond angles



Torsions

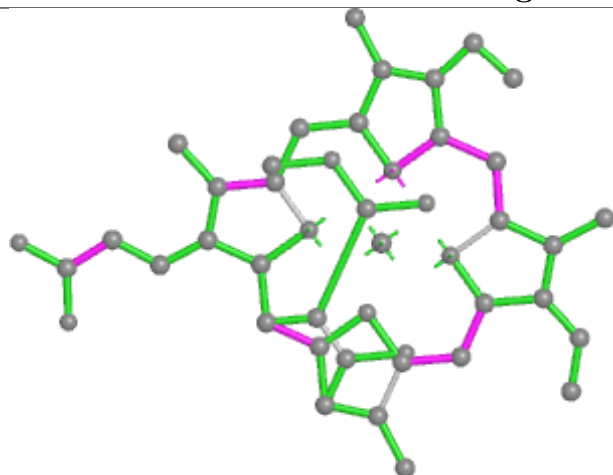


Rings

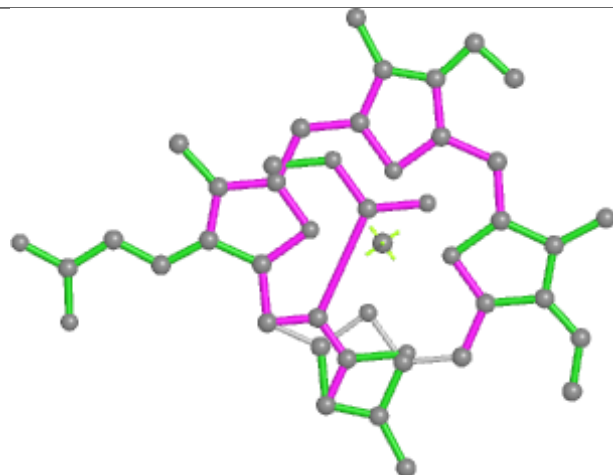
**Ligand CLA a 825****Ligand DD6 E 305**



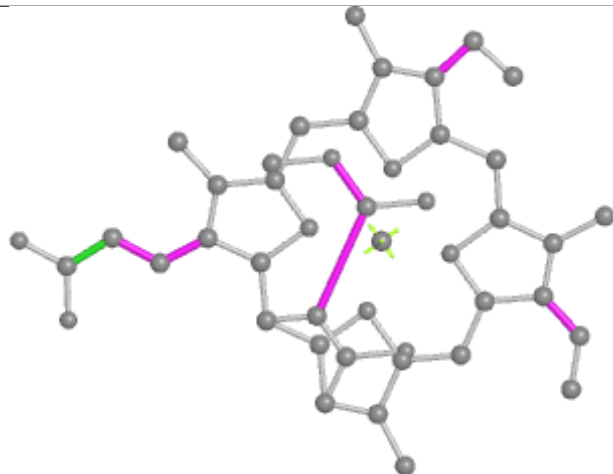
## Ligand KC2 V 314



Bond lengths



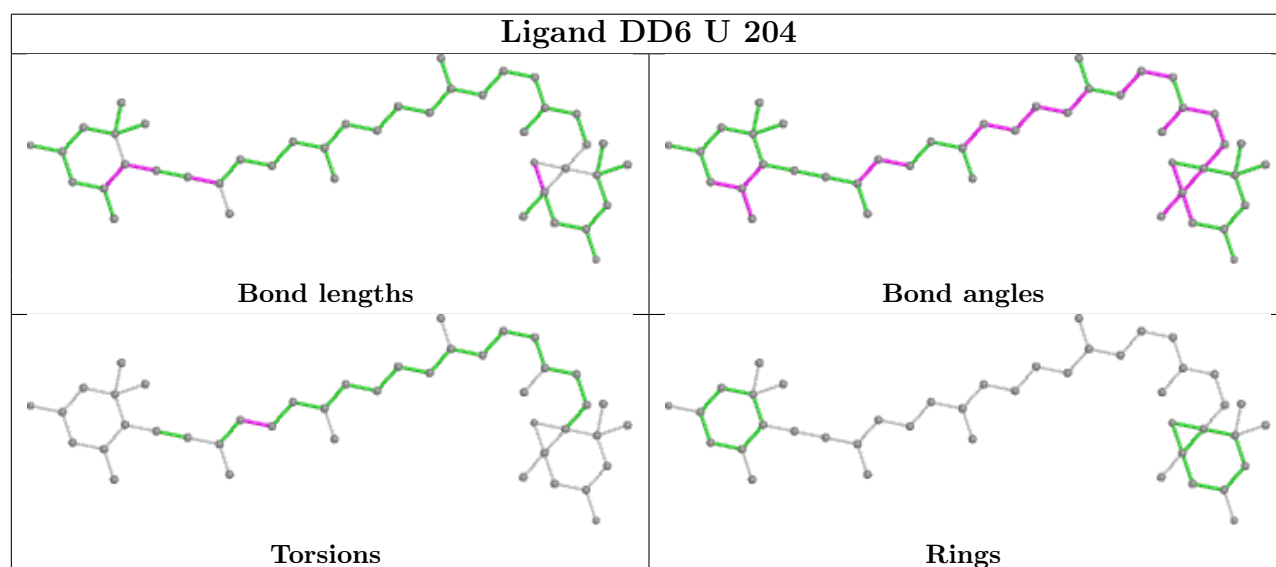
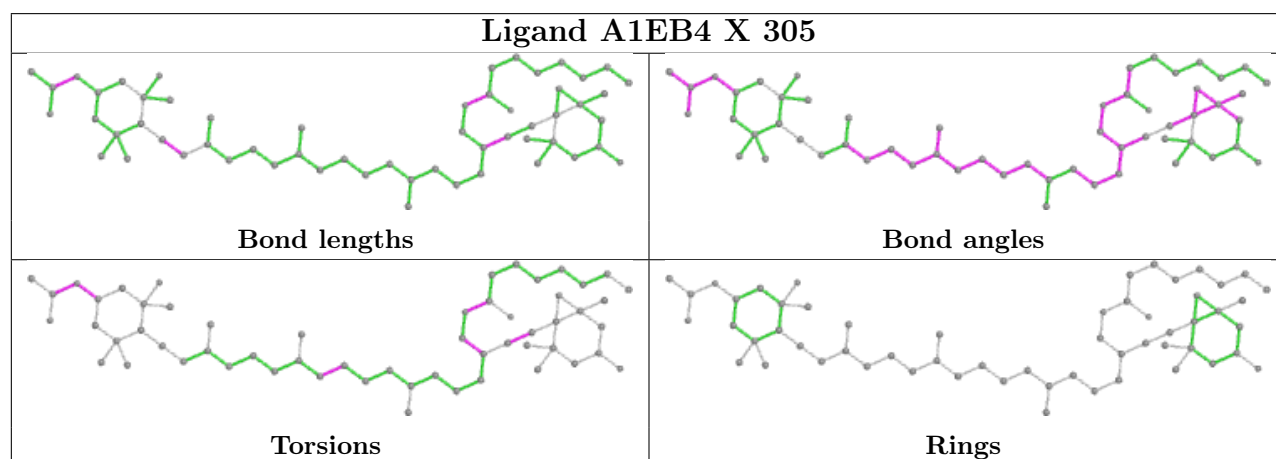
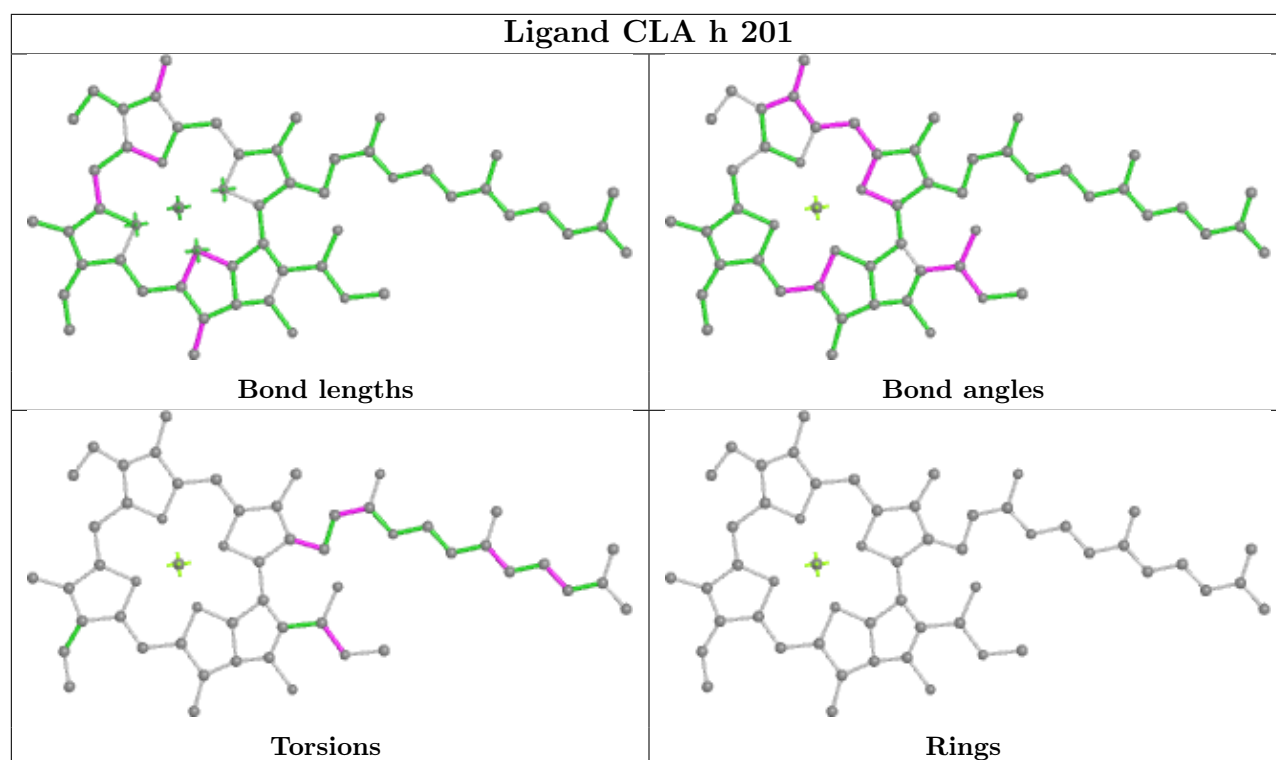
Bond angles



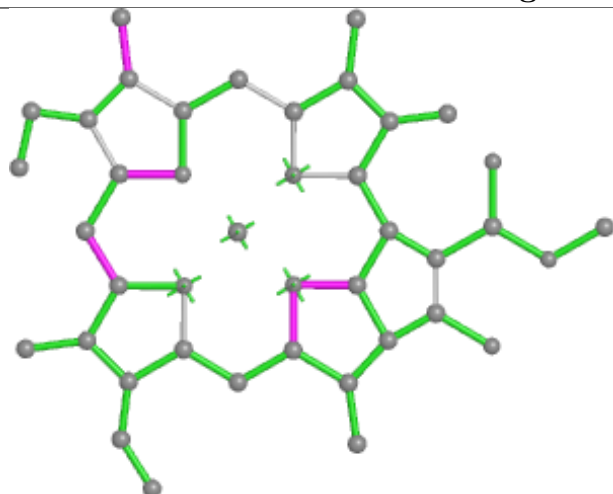
Torsions



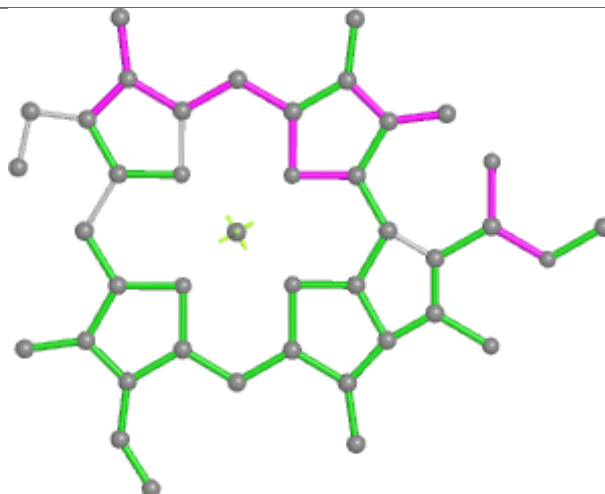
Rings



## Ligand CLA z 318



Bond lengths



Bond angles

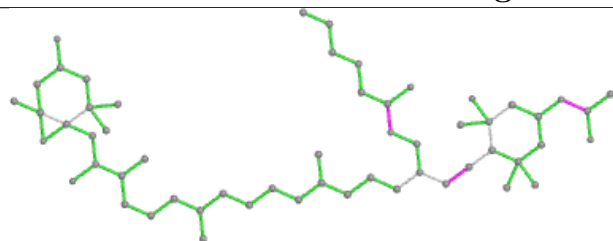


Torsions

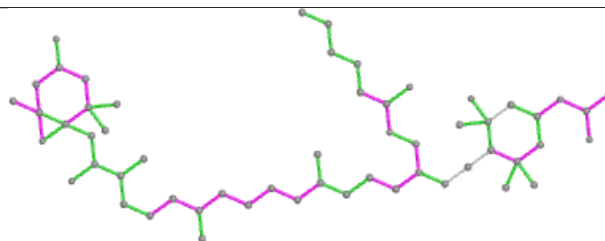


Rings

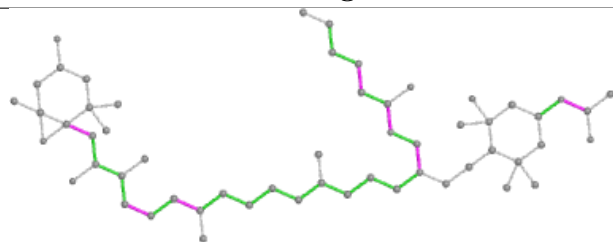
## Ligand A1EB1 G 308



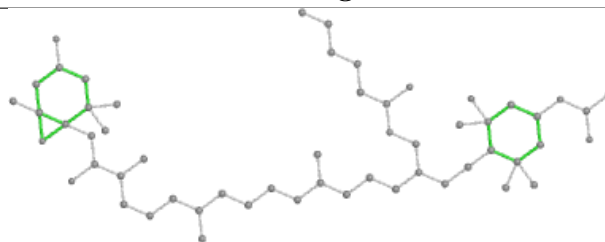
Bond lengths



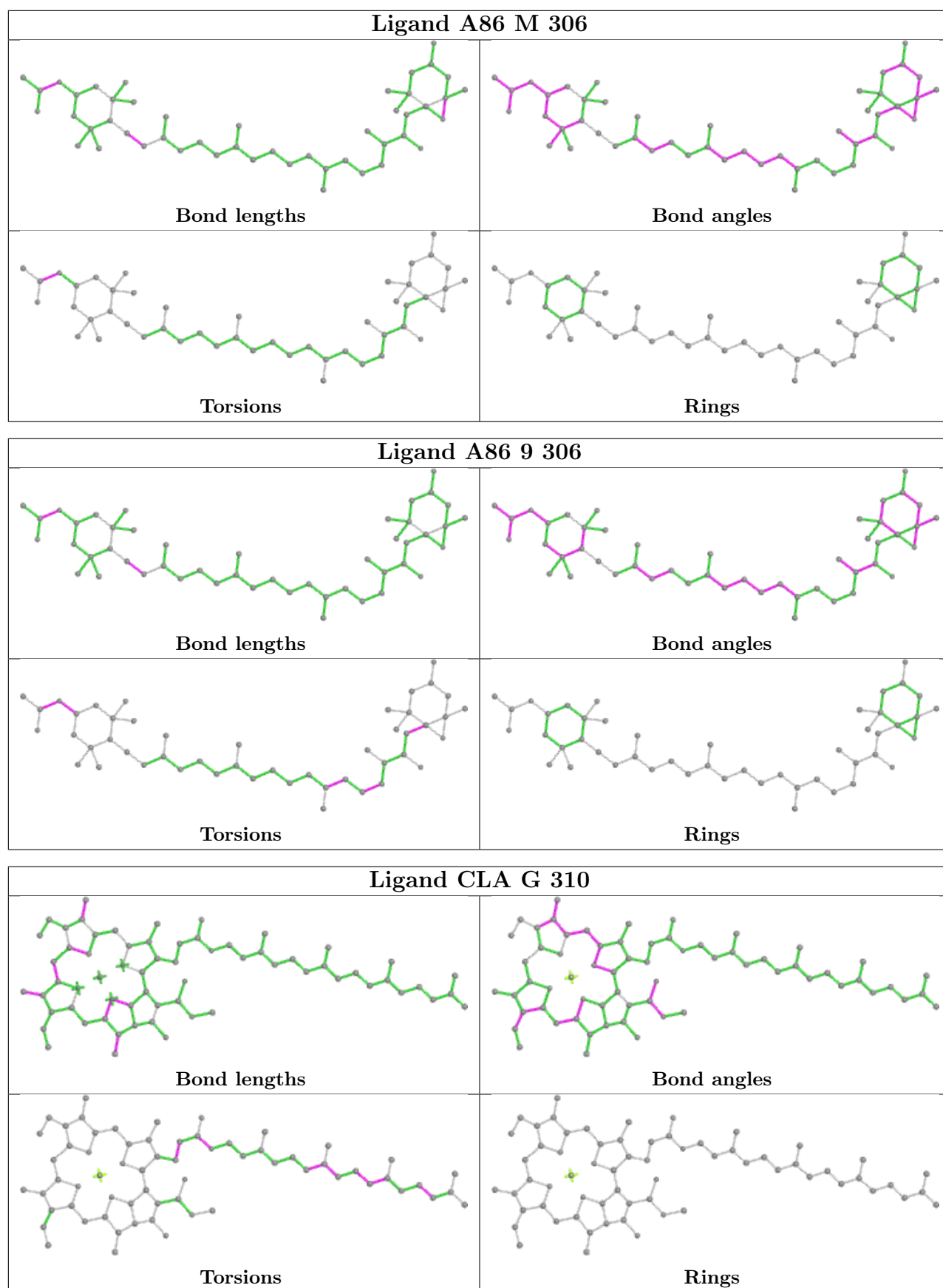
Bond angles

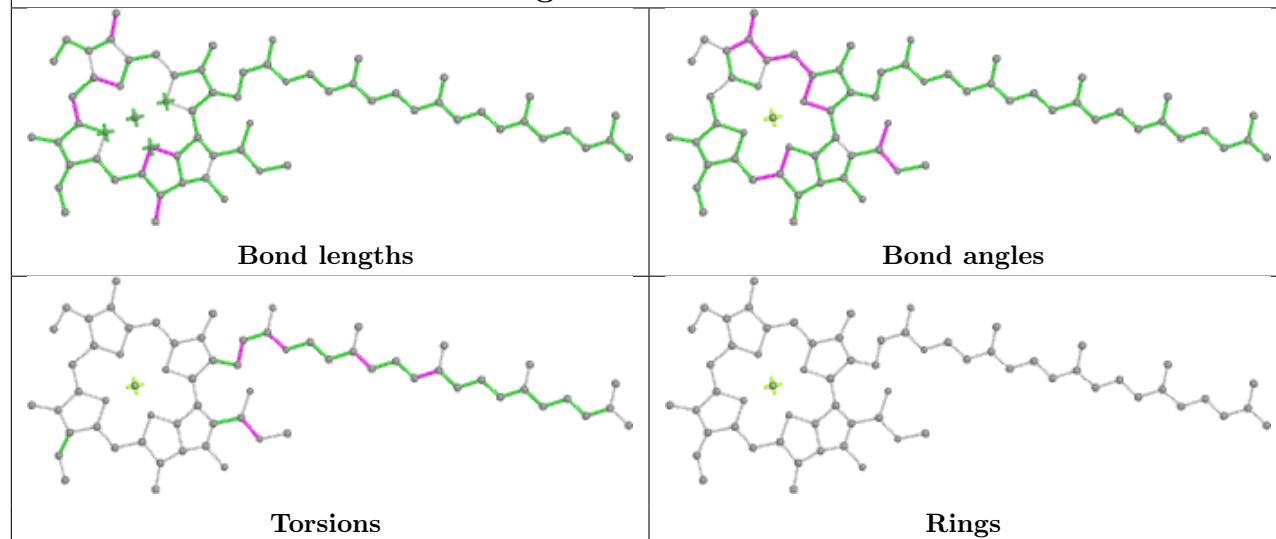
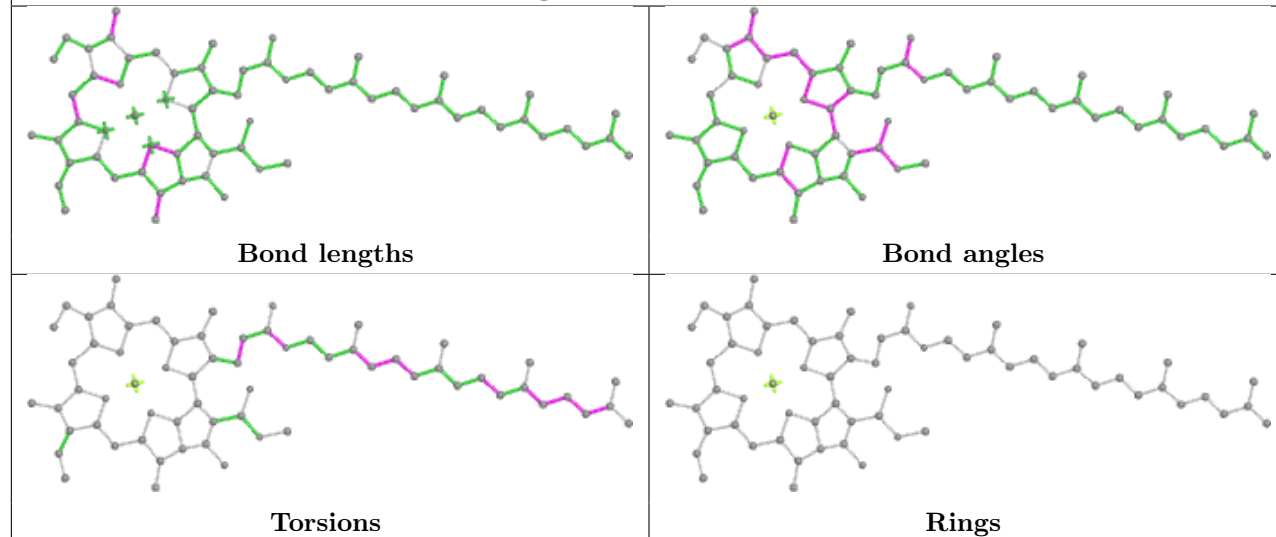
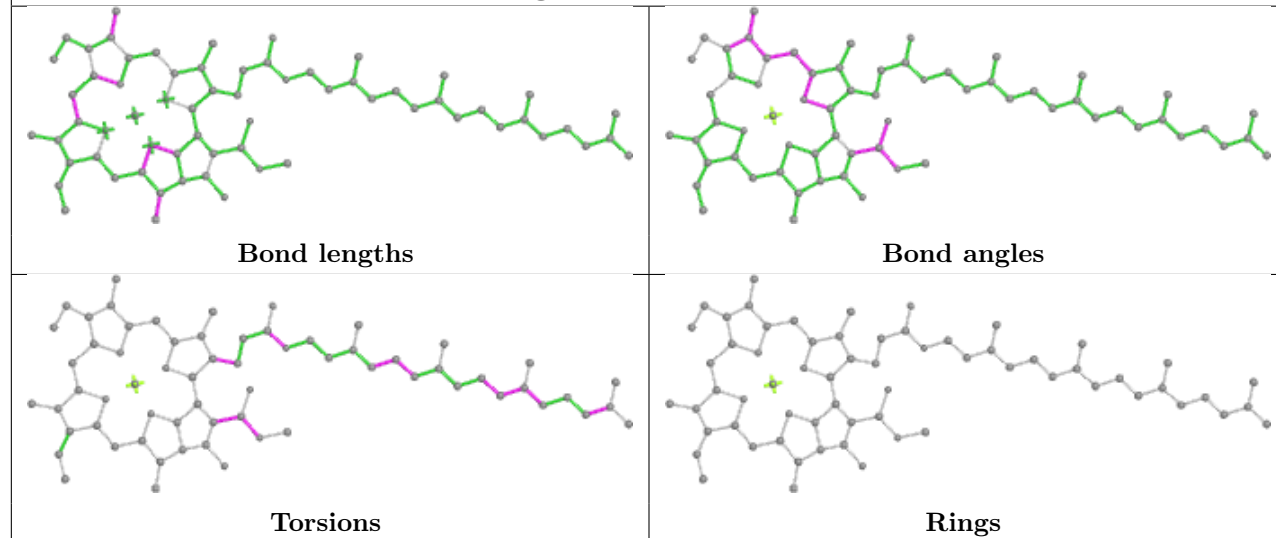


Torsions

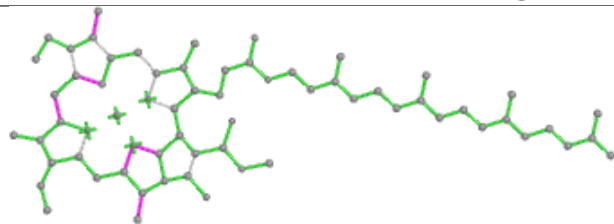


Rings

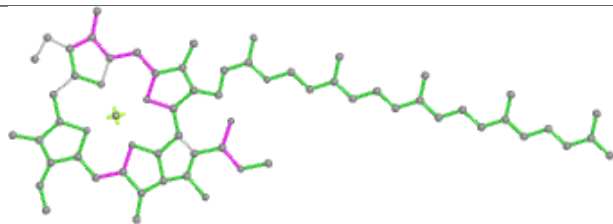


**Ligand CLA a 818****Ligand CLA b 825****Ligand CLA C 310**

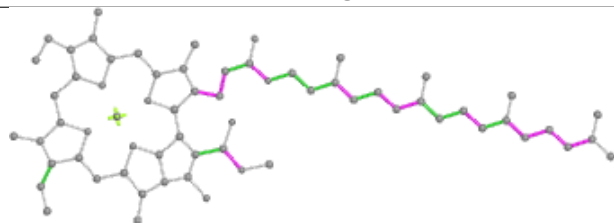
## Ligand CLA K 312



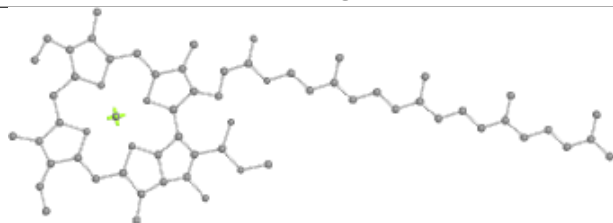
Bond lengths



Bond angles

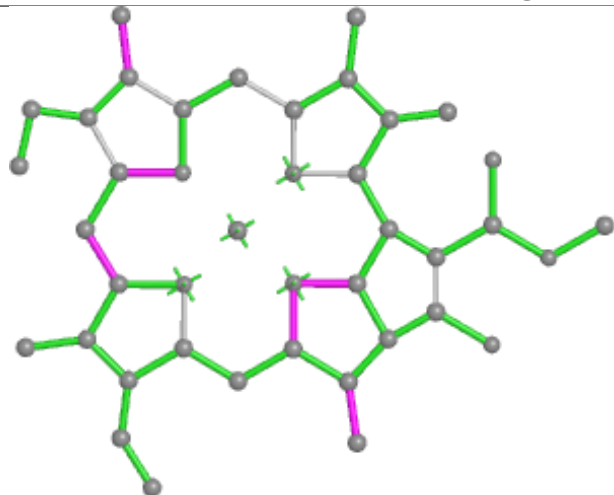


Torsions

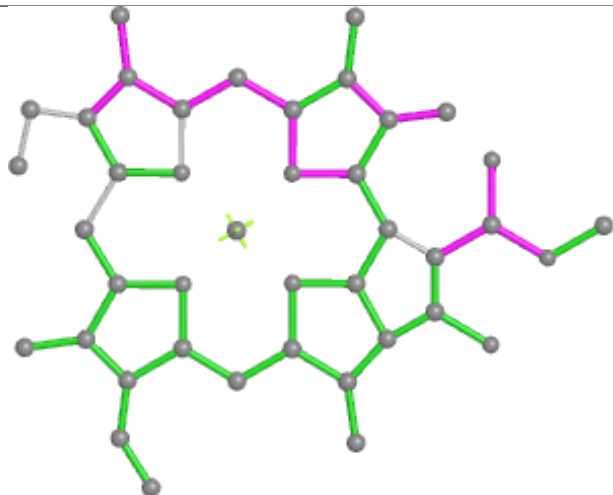


Rings

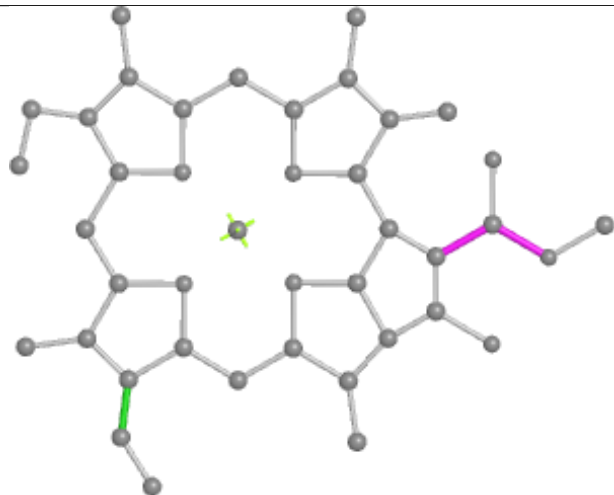
## Ligand CLA 2 312



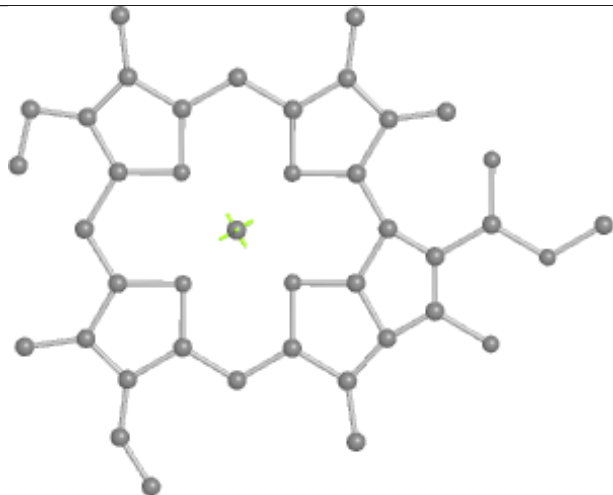
Bond lengths



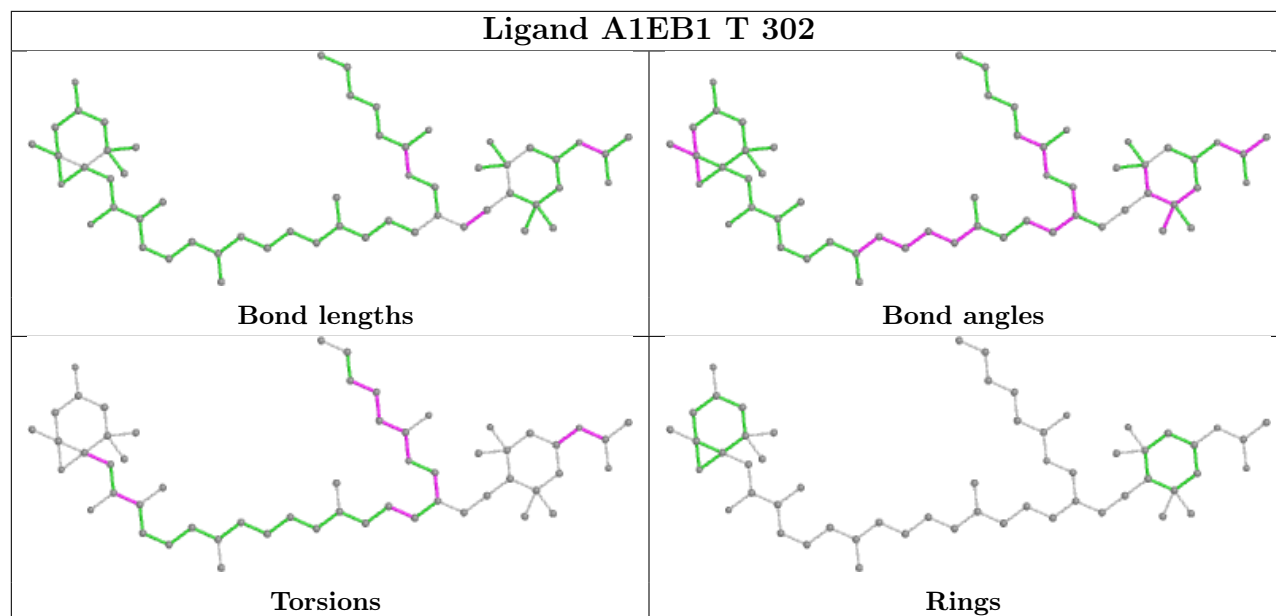
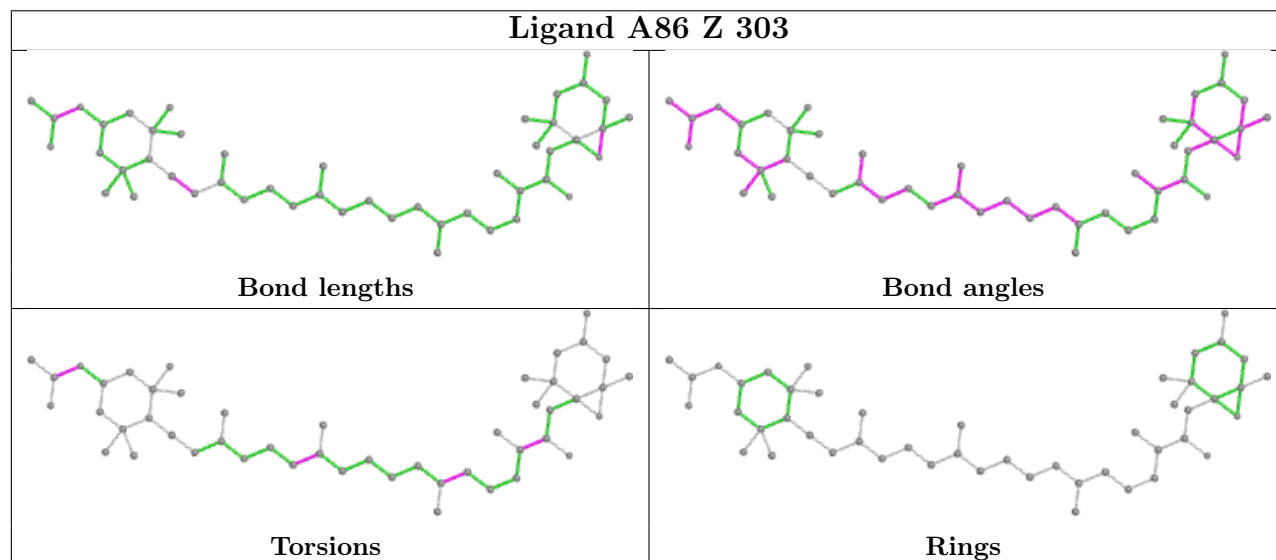
Bond angles



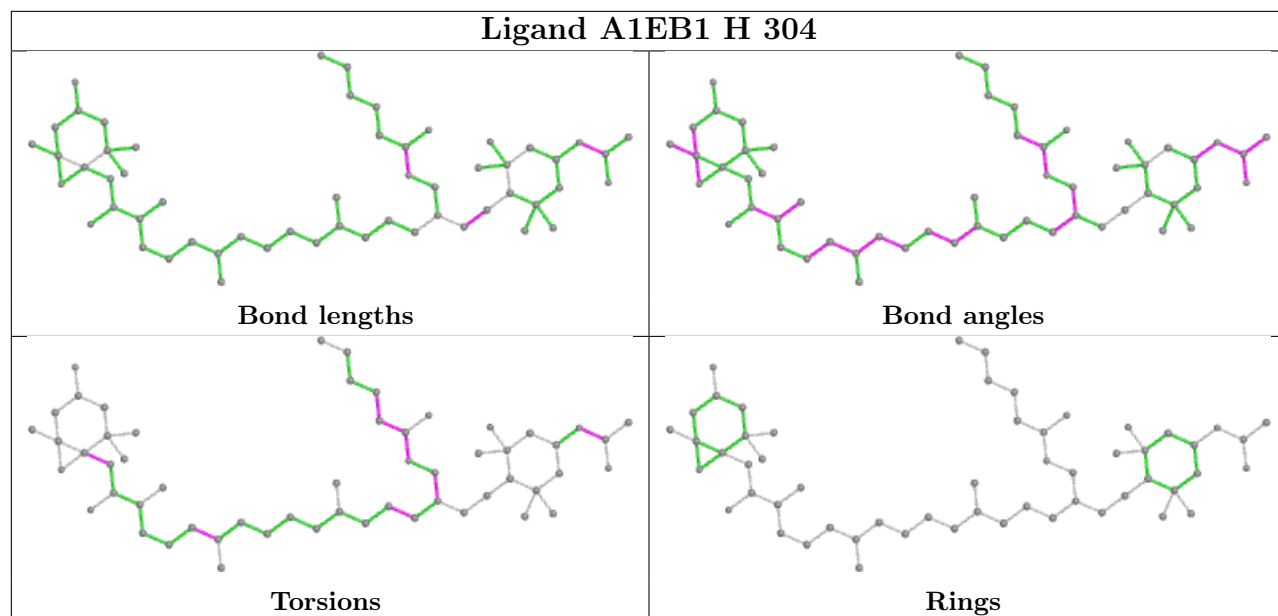
Torsions



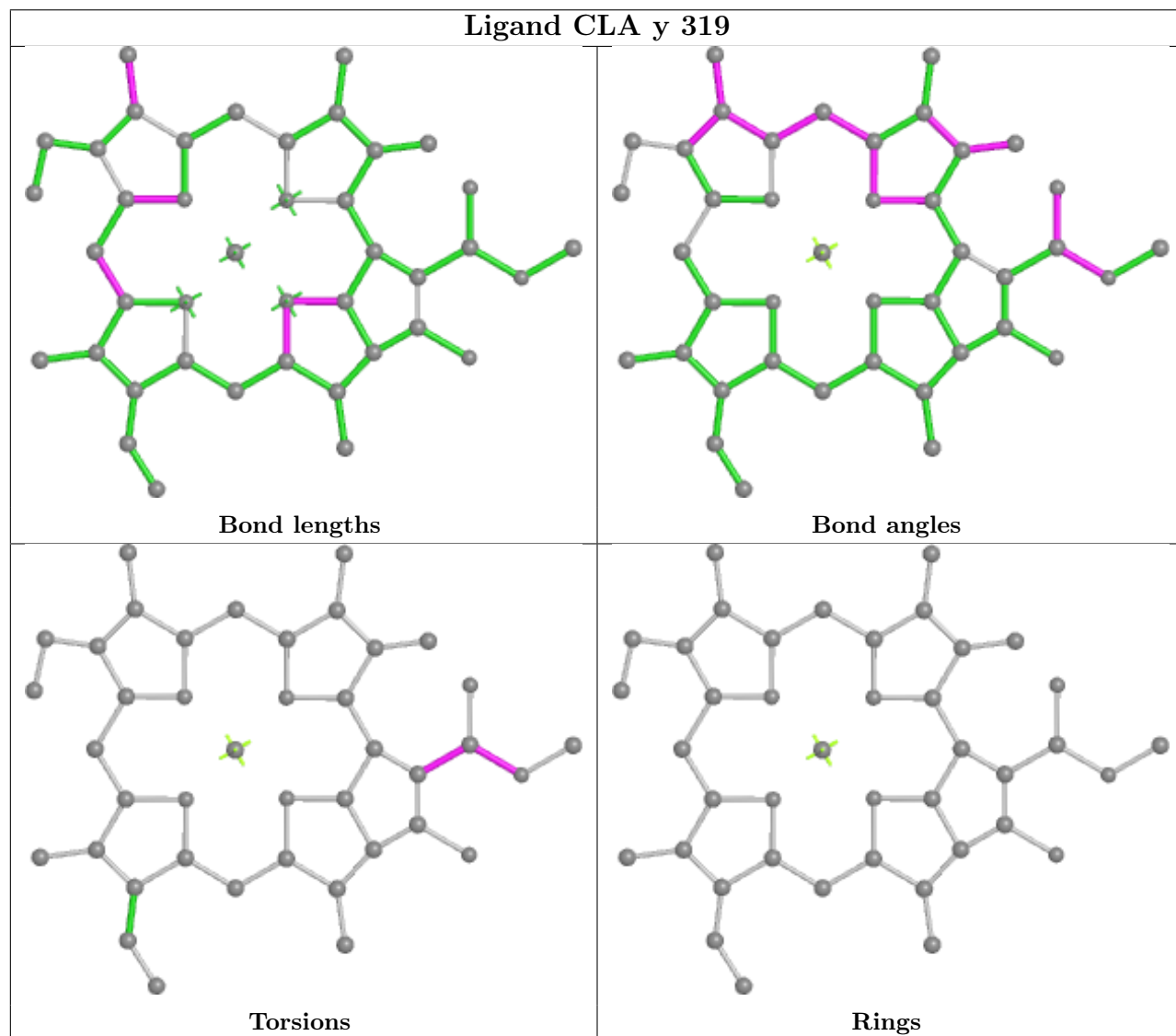
Rings

**Ligand A1EB1 T 302****Ligand A86 Z 303**

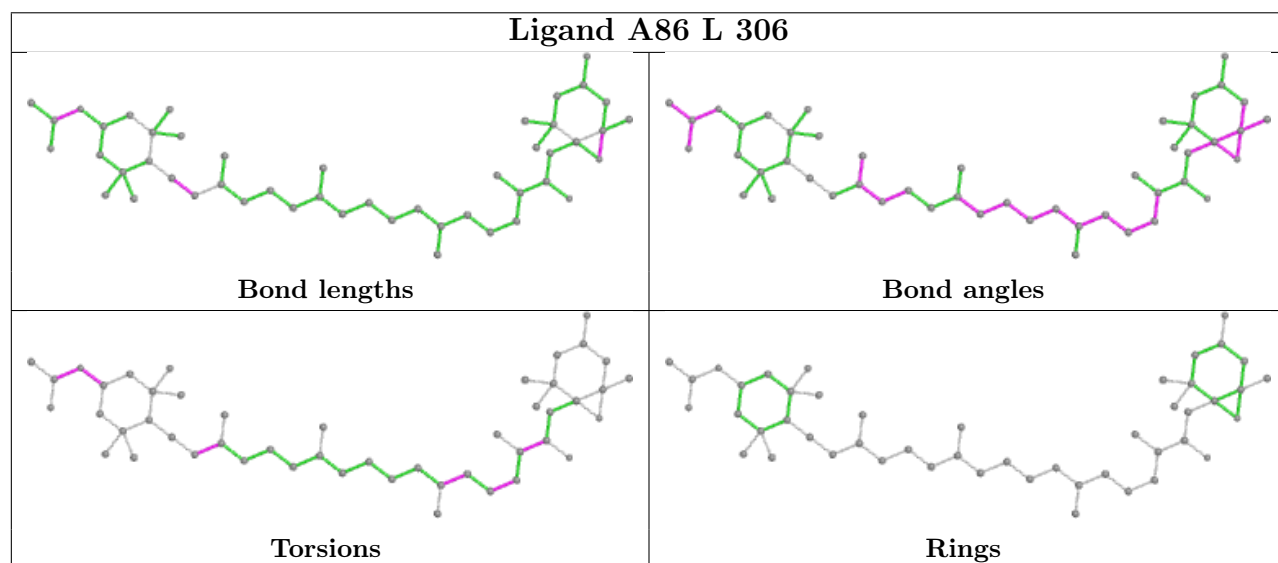
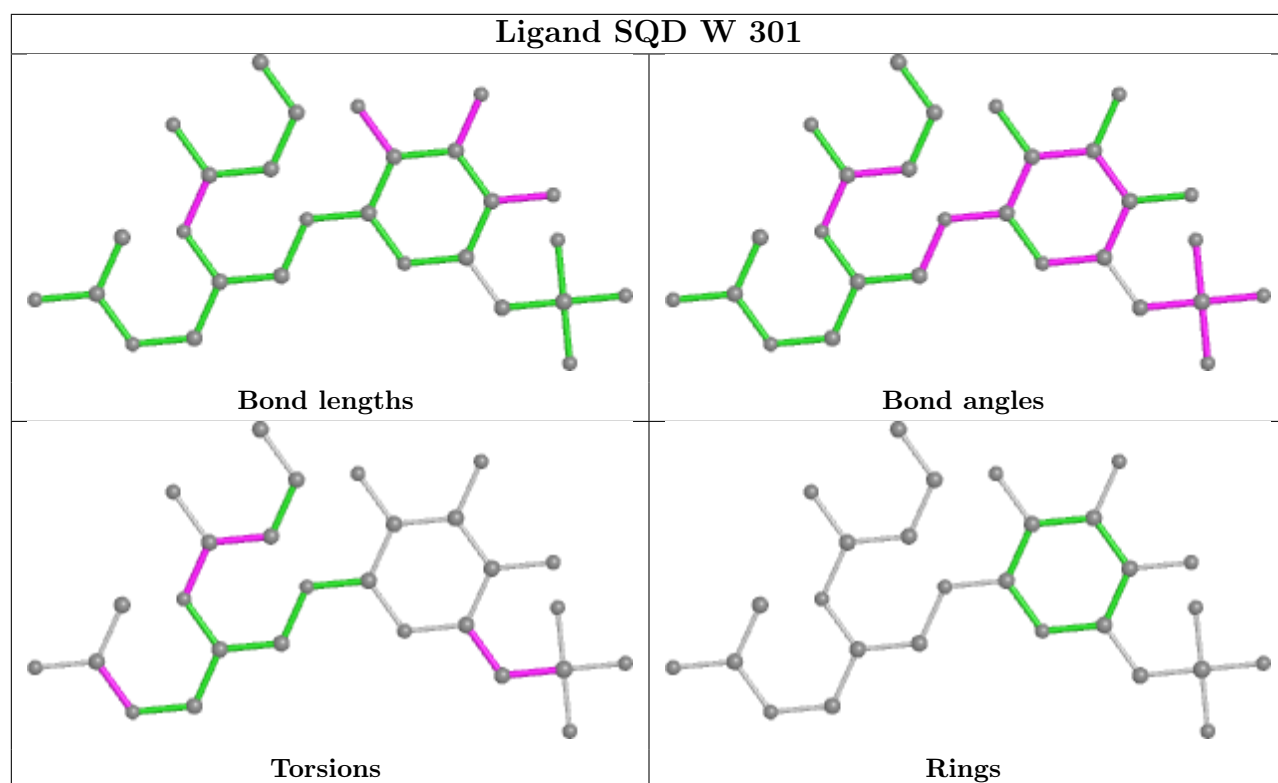
## Ligand A1EB1 H 304

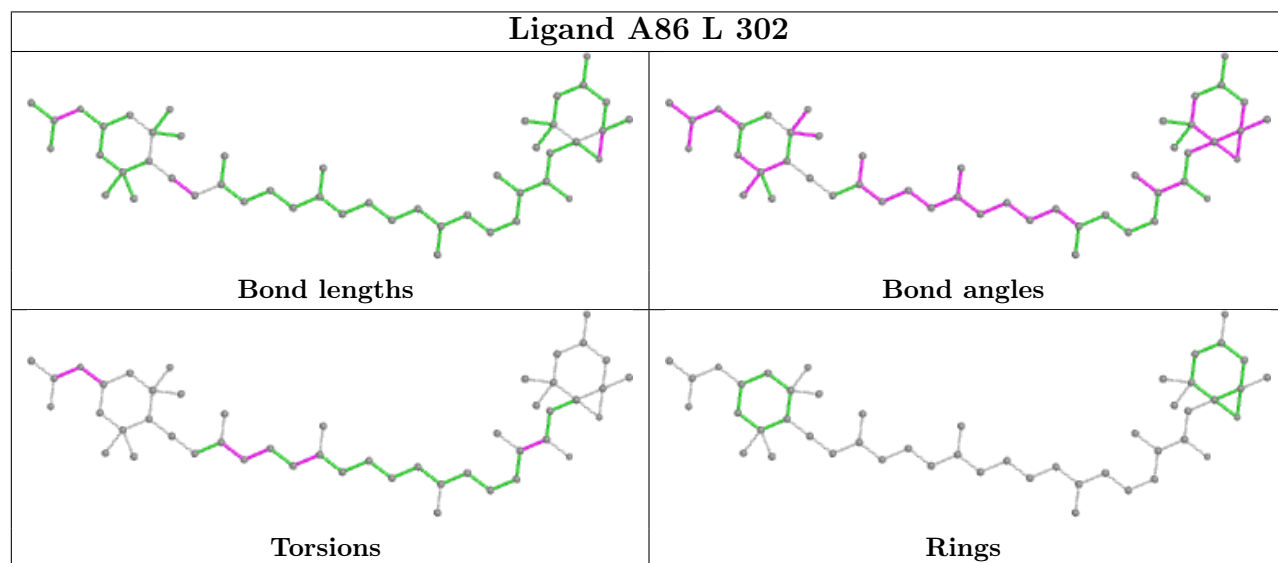
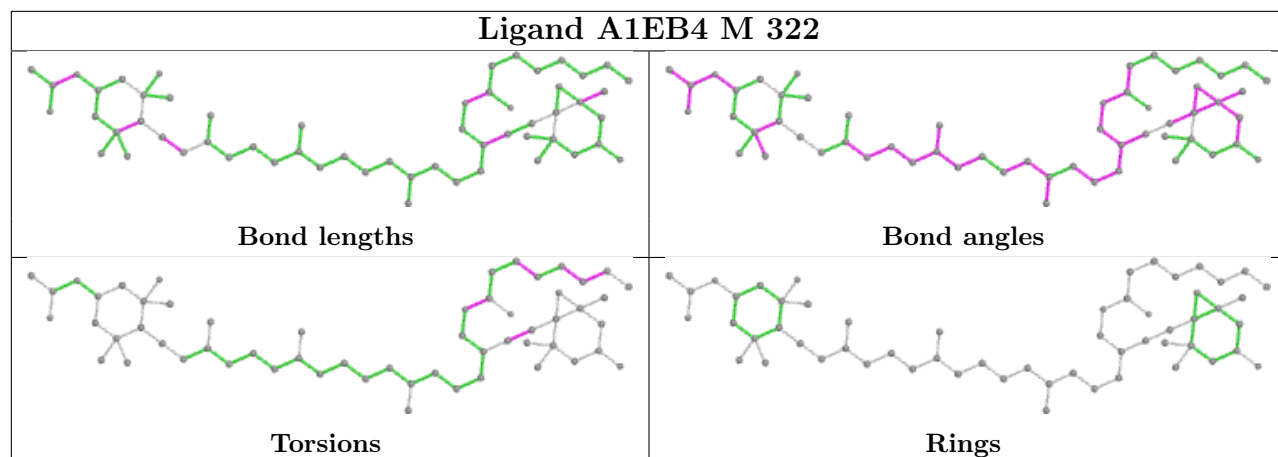


## Ligand CLA y 319

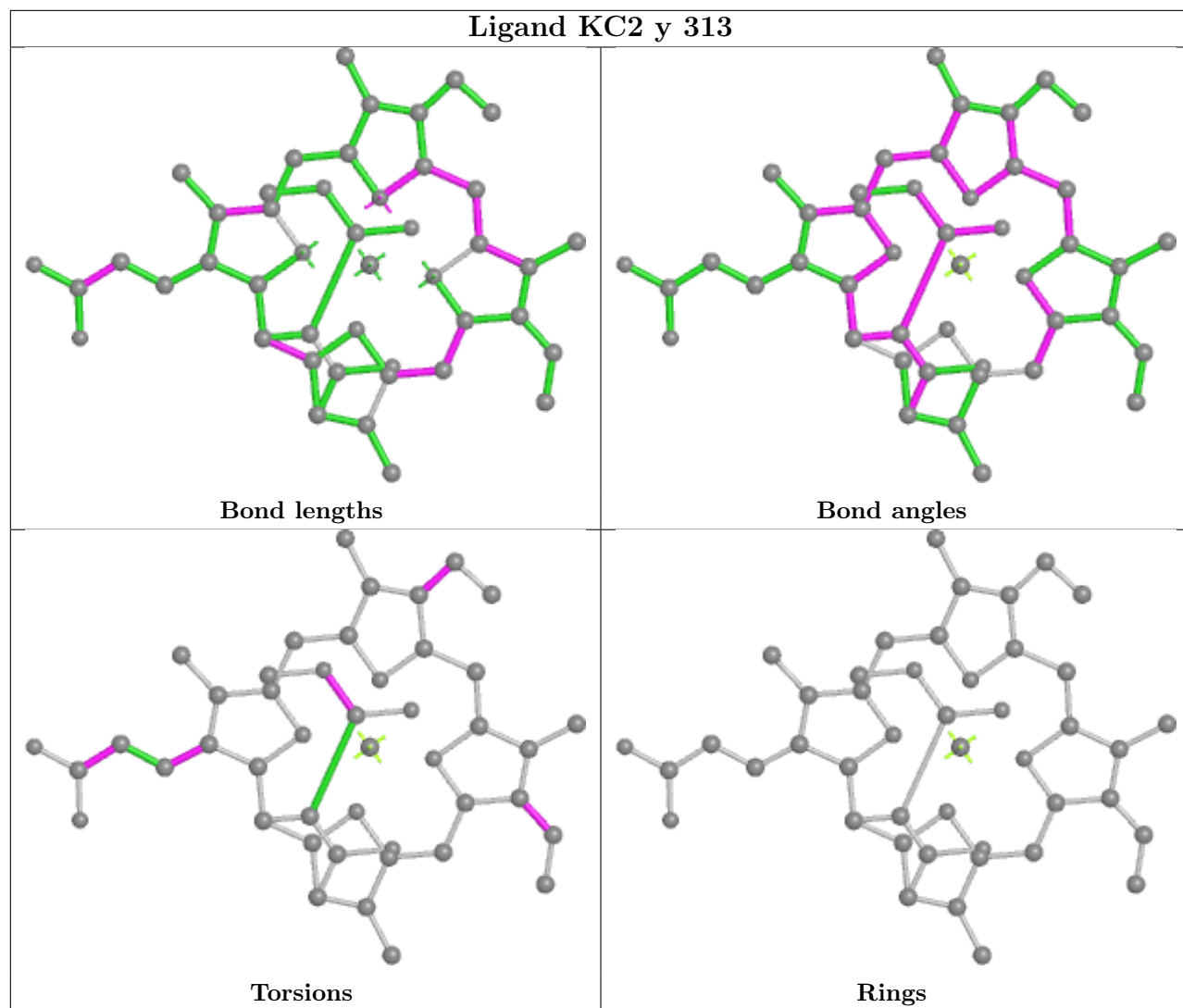




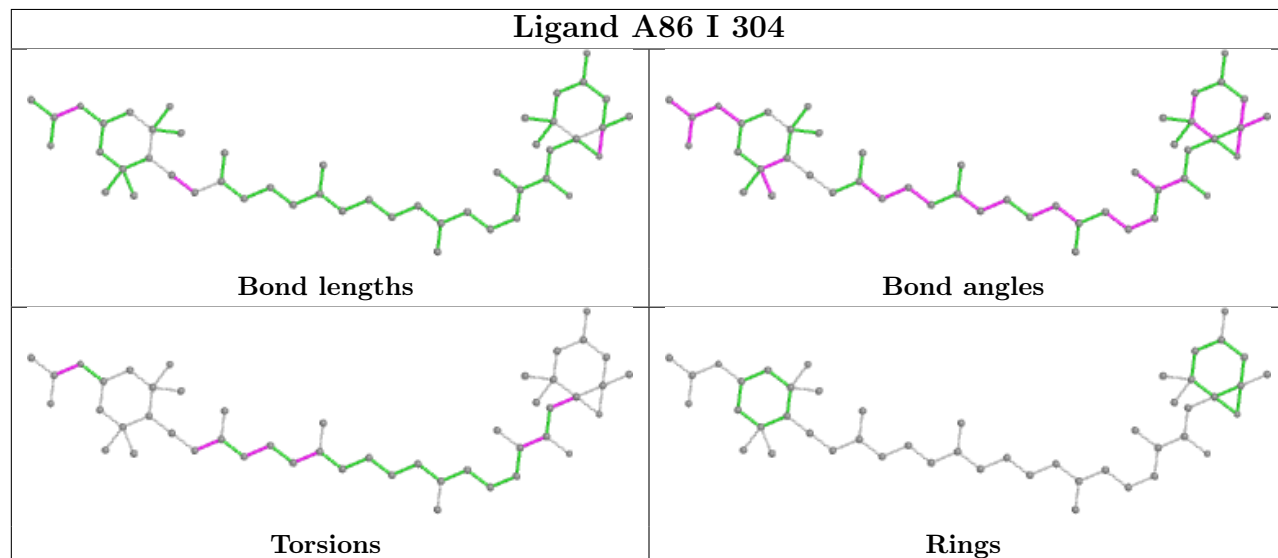




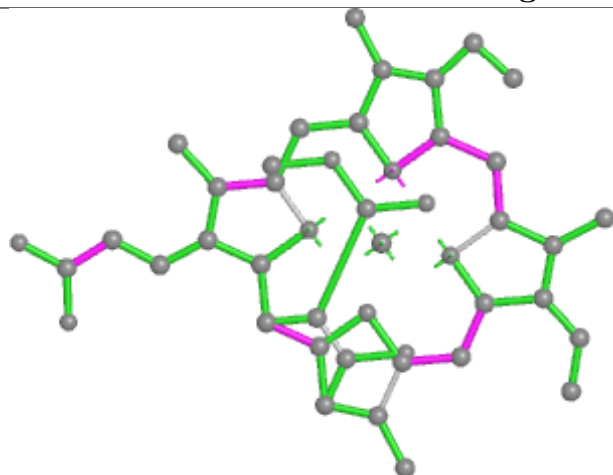
## Ligand KC2 y 313



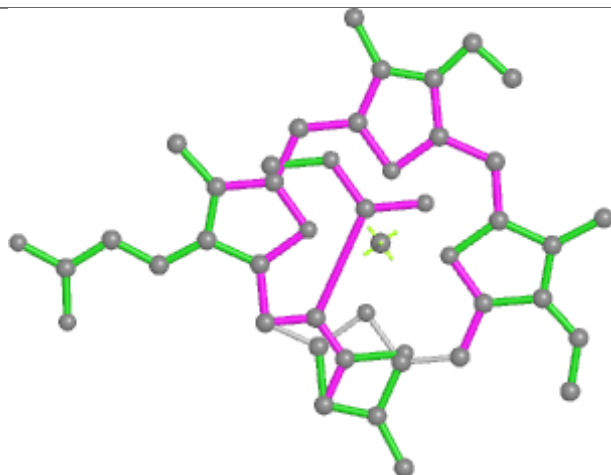
## Ligand A86 I 304



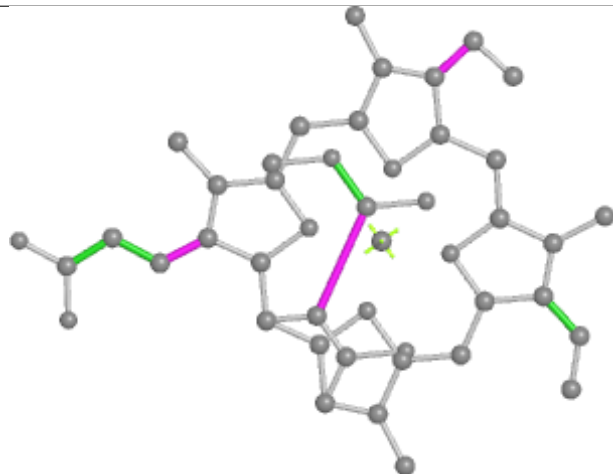
## Ligand KC2 S 314



Bond lengths



Bond angles

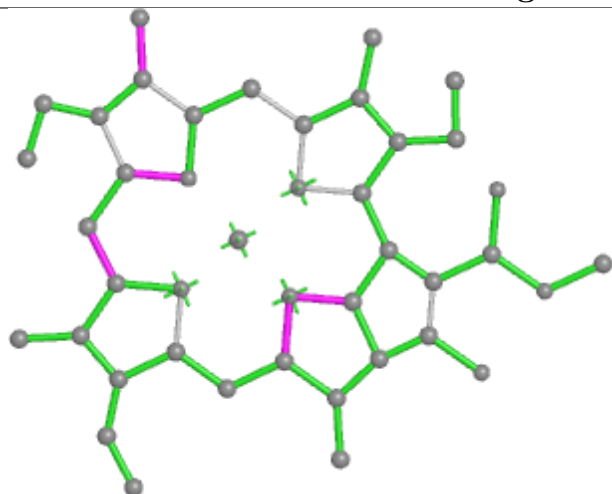


Torsions

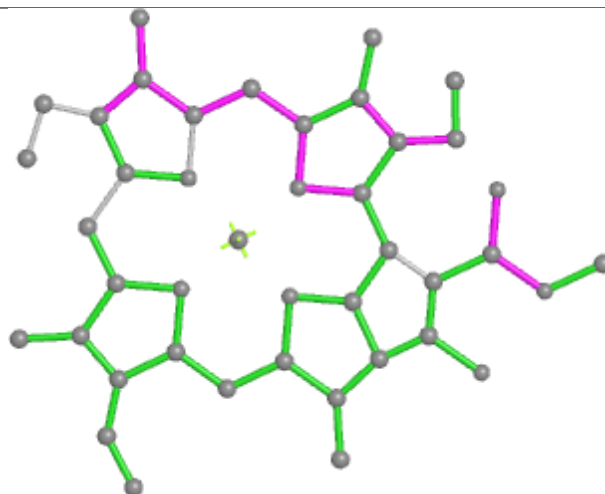


Rings

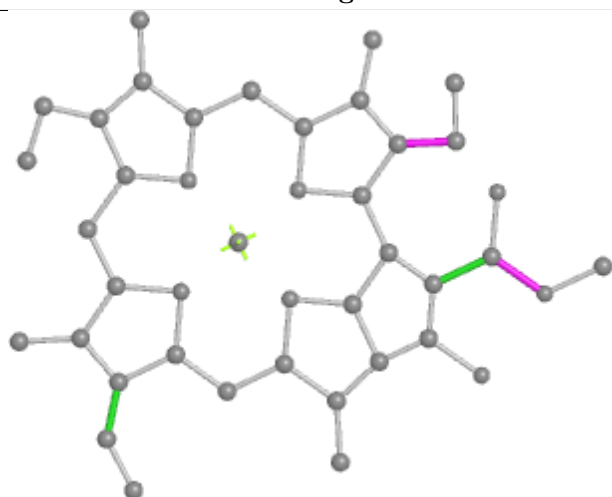
## Ligand CLA 6 310



Bond lengths



Bond angles

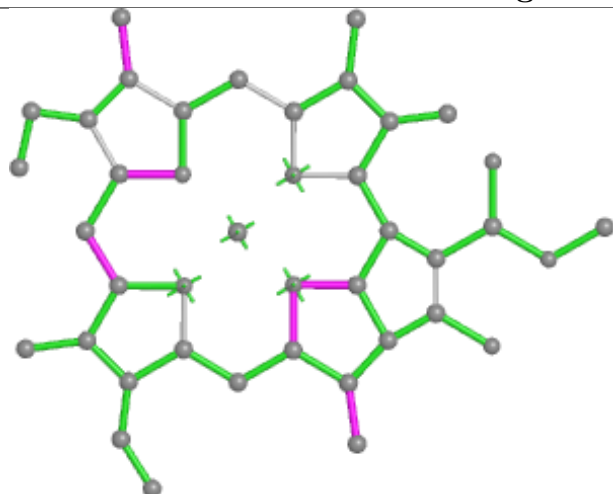


Torsions

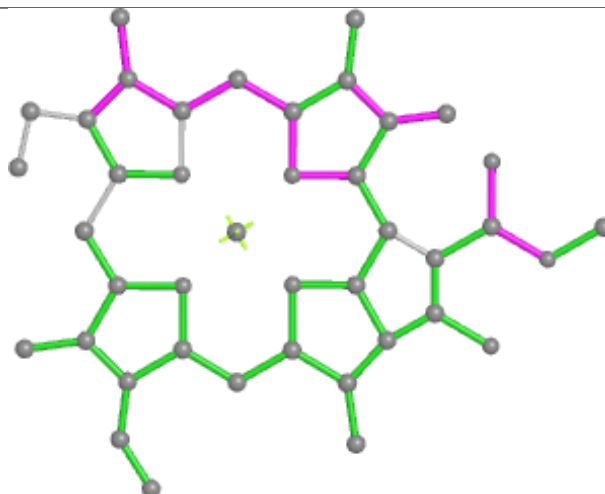


Rings

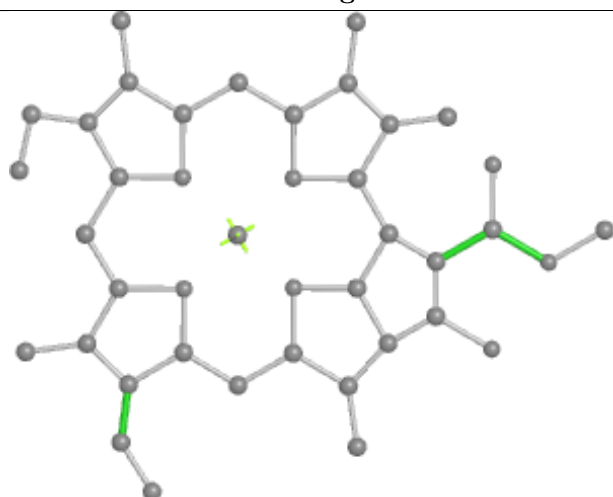
## Ligand CLA Z 307



Bond lengths



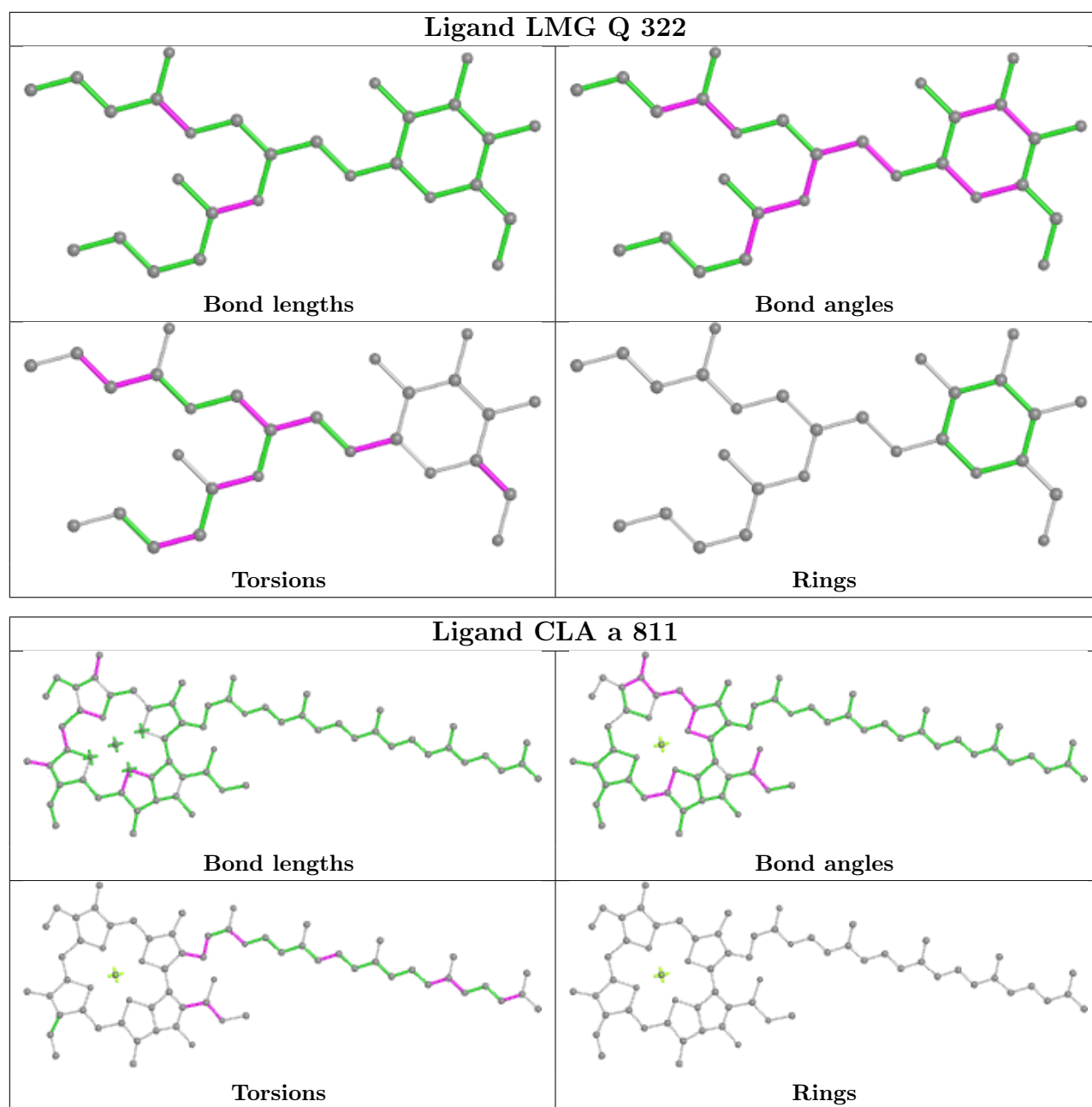
Bond angles



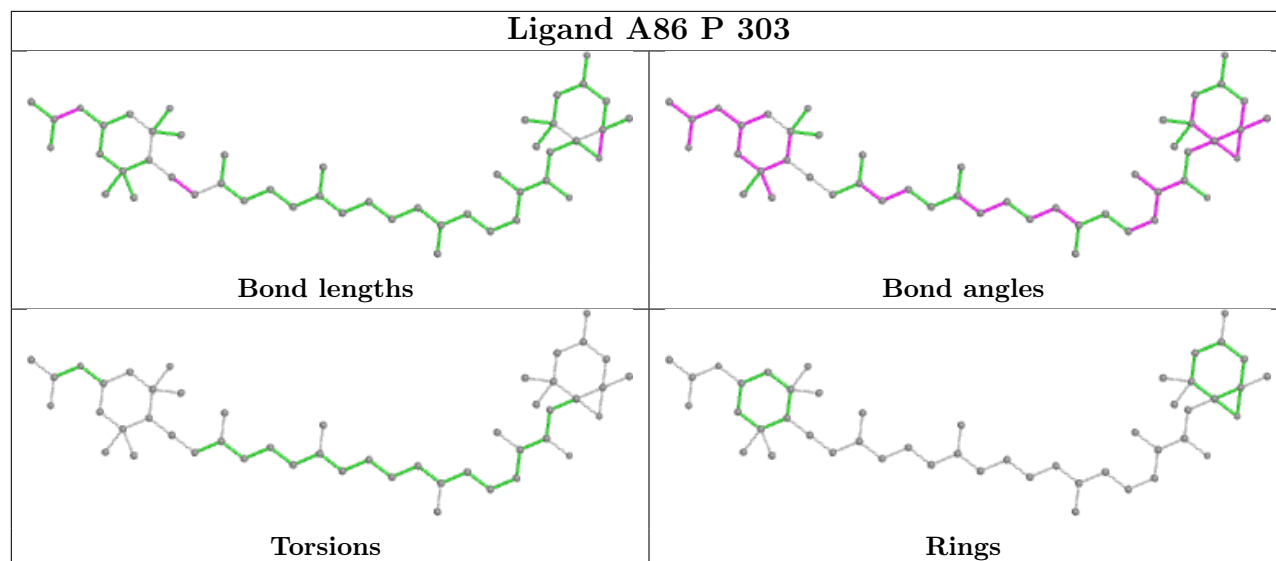
Torsions



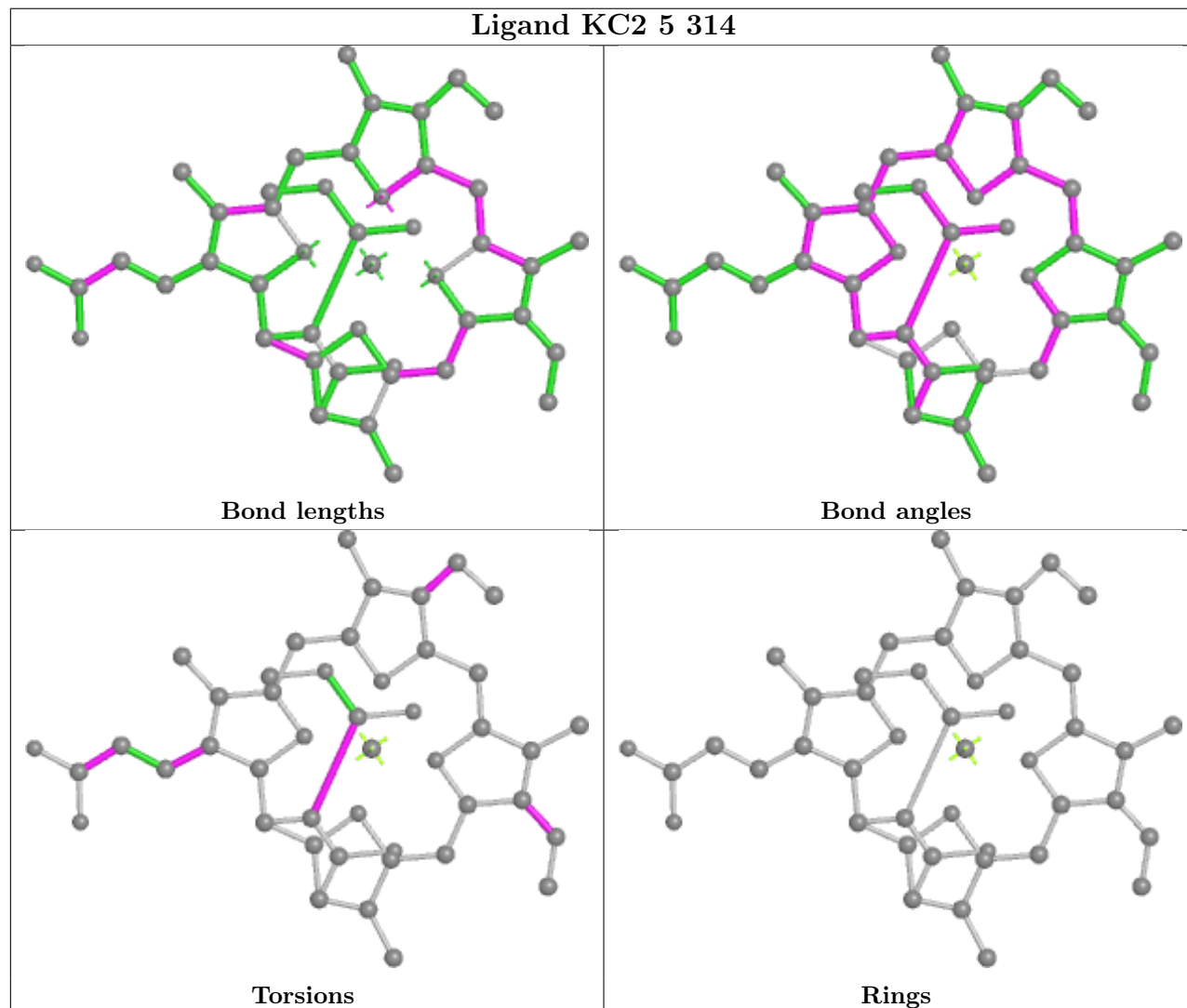
Rings



## Ligand A86 P 303

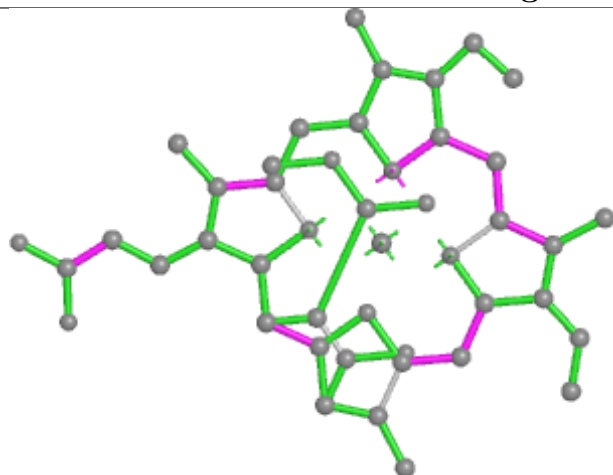


## Ligand KC2 5 314

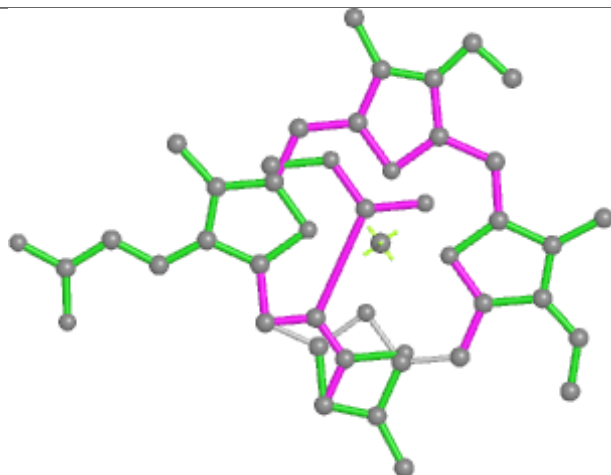




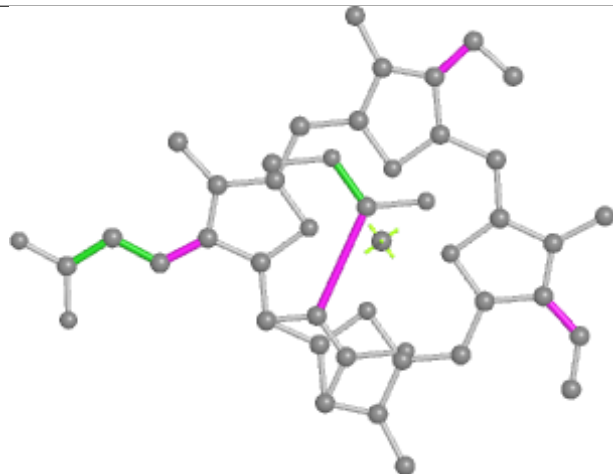
## Ligand KC2 z 312



Bond lengths



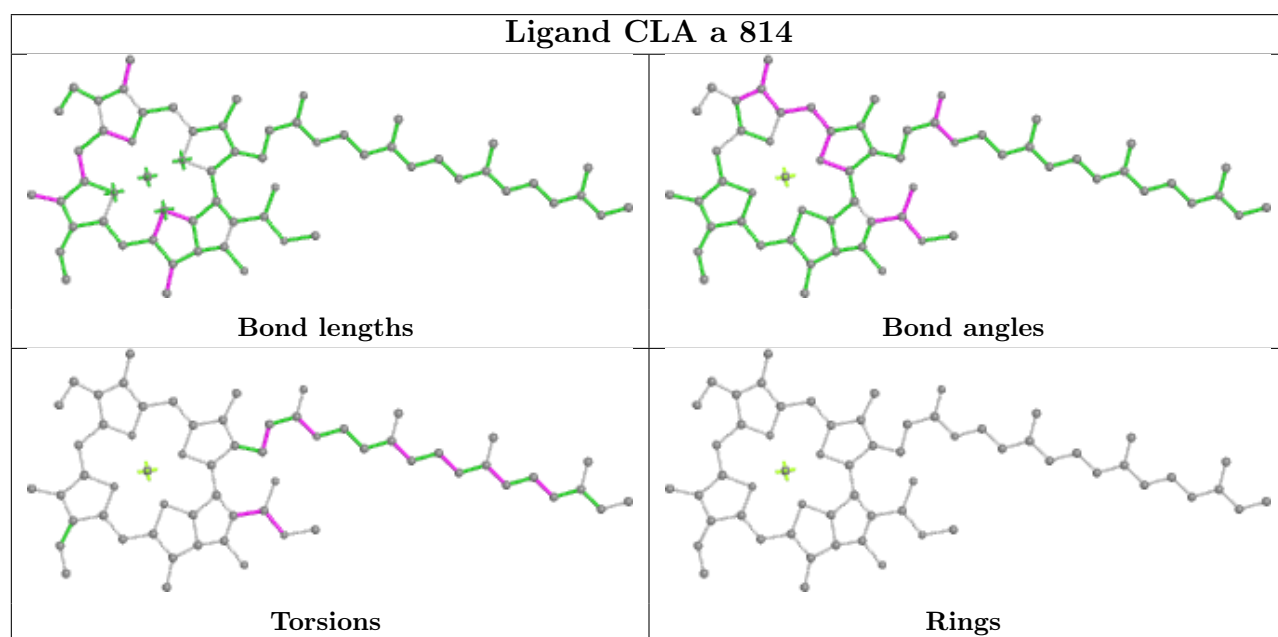
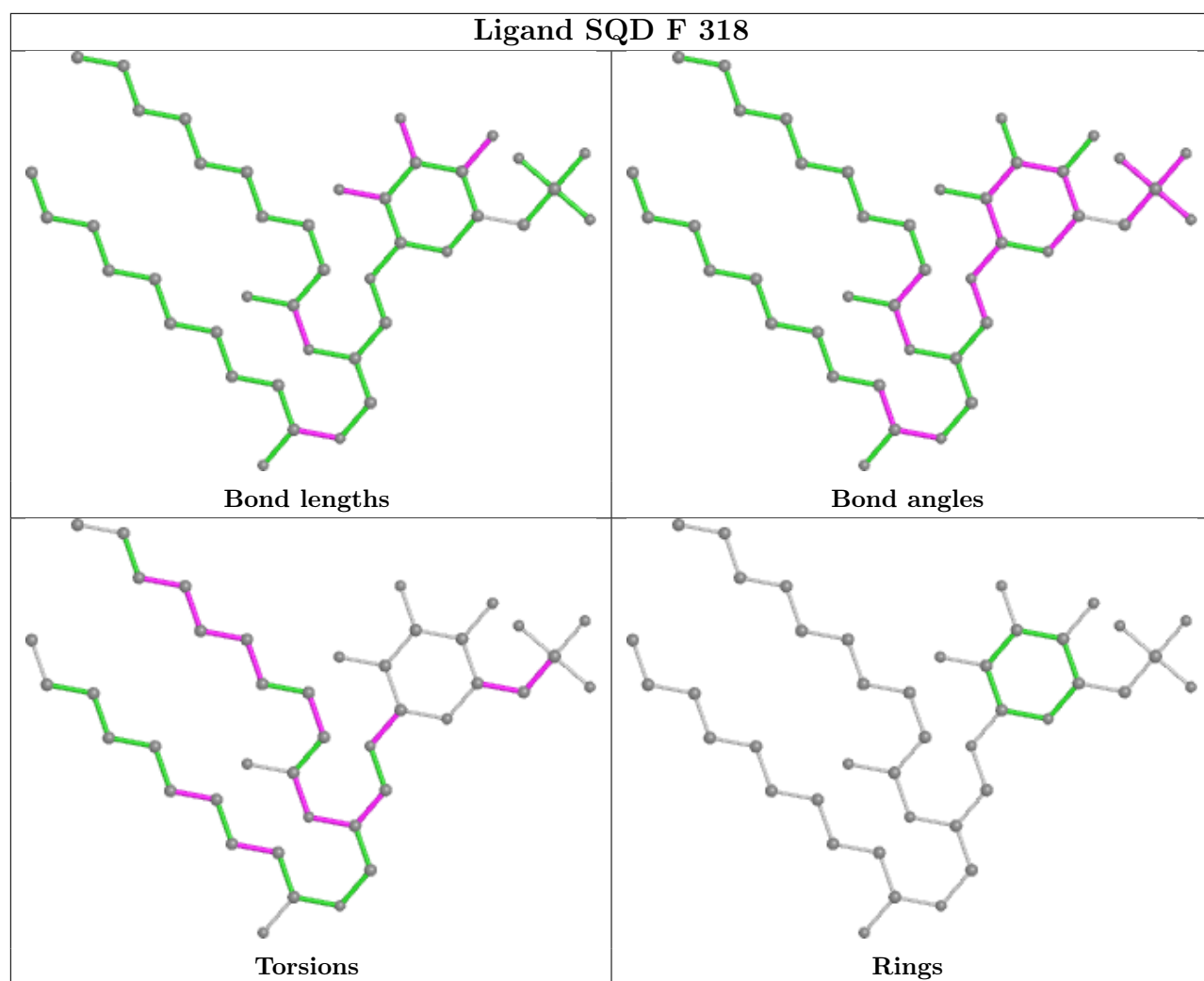
Bond angles

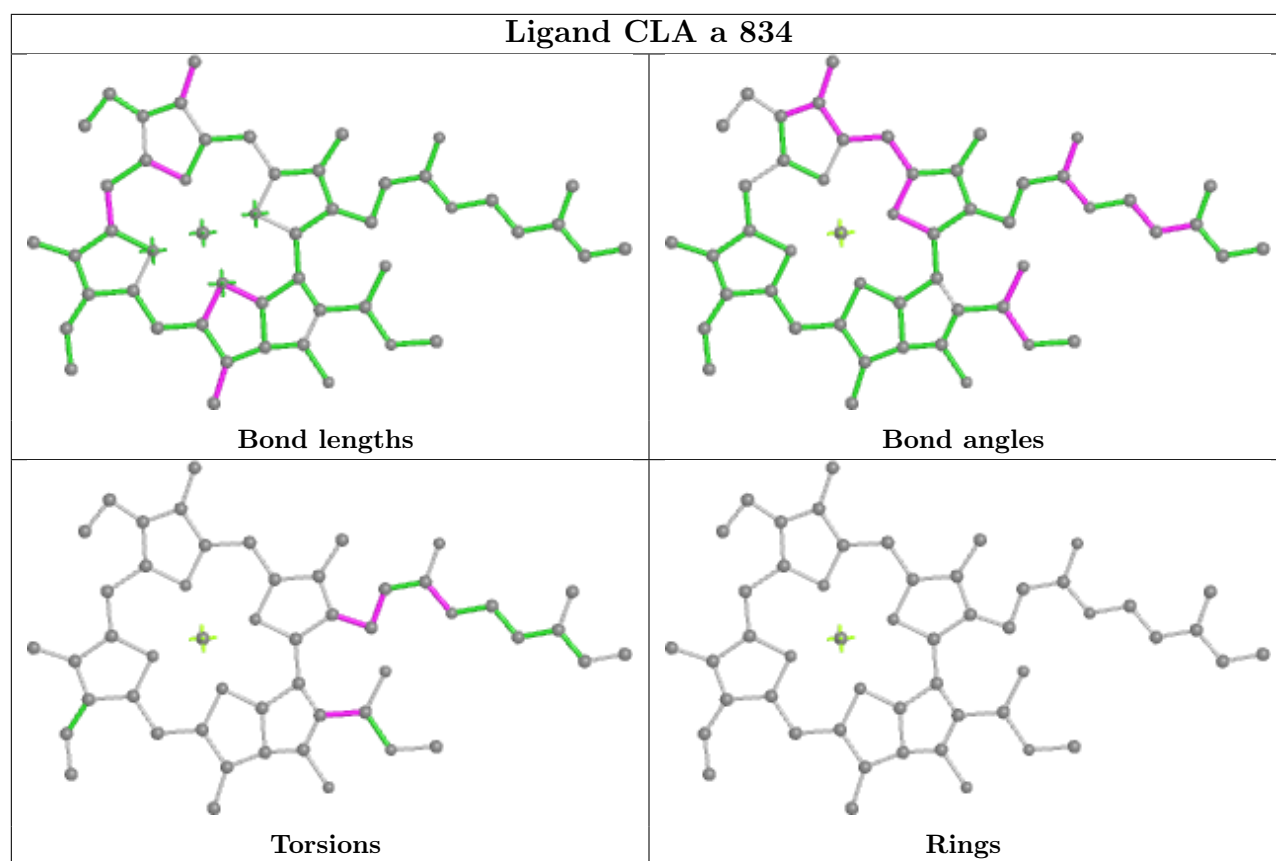


Torsions

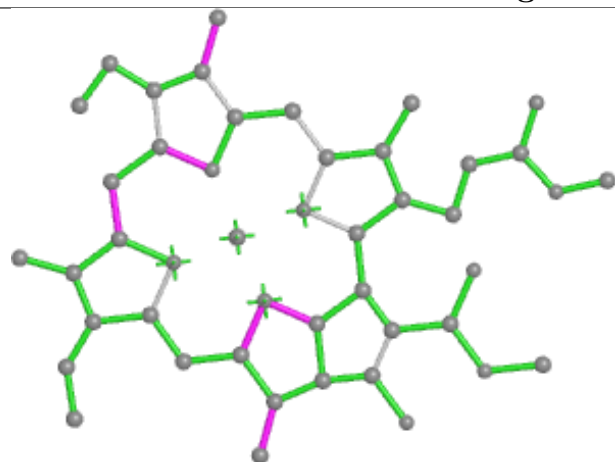


Rings

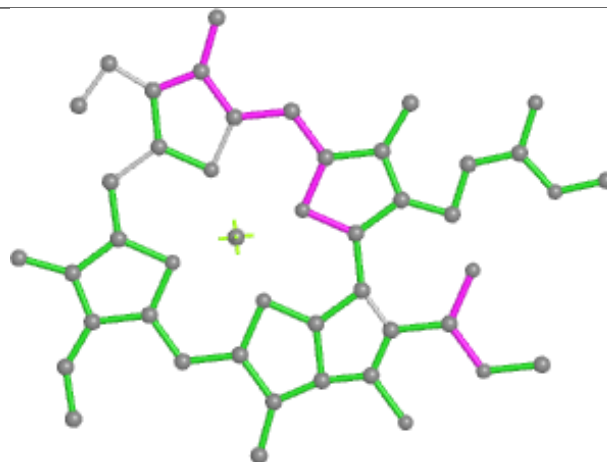




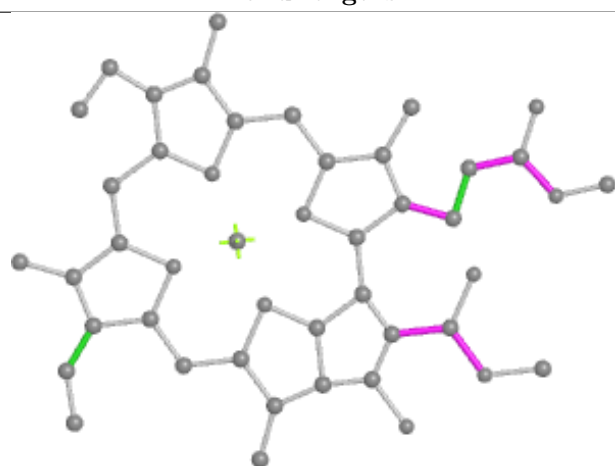
## Ligand CLA E 315



Bond lengths



Bond angles

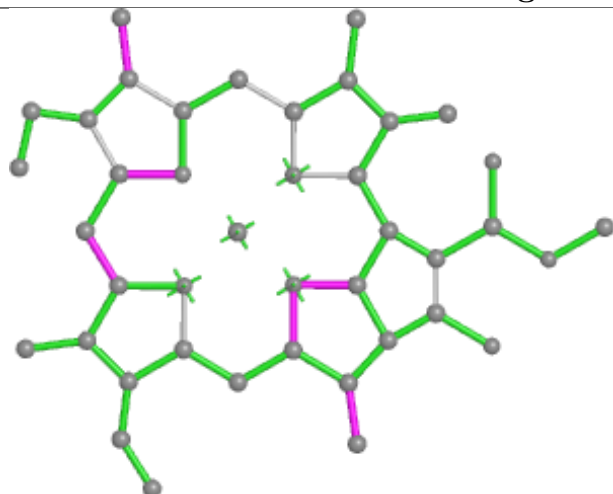


Torsions

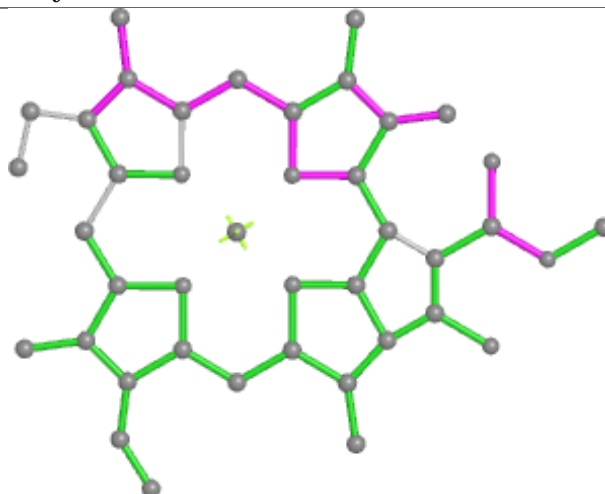


Rings

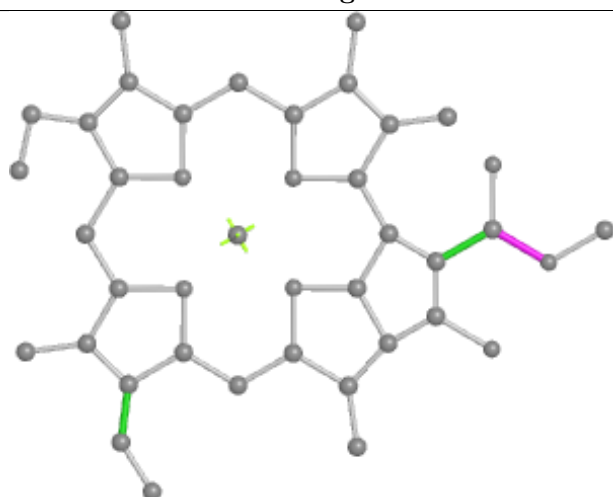
## Ligand CLA y 307



Bond lengths



Bond angles

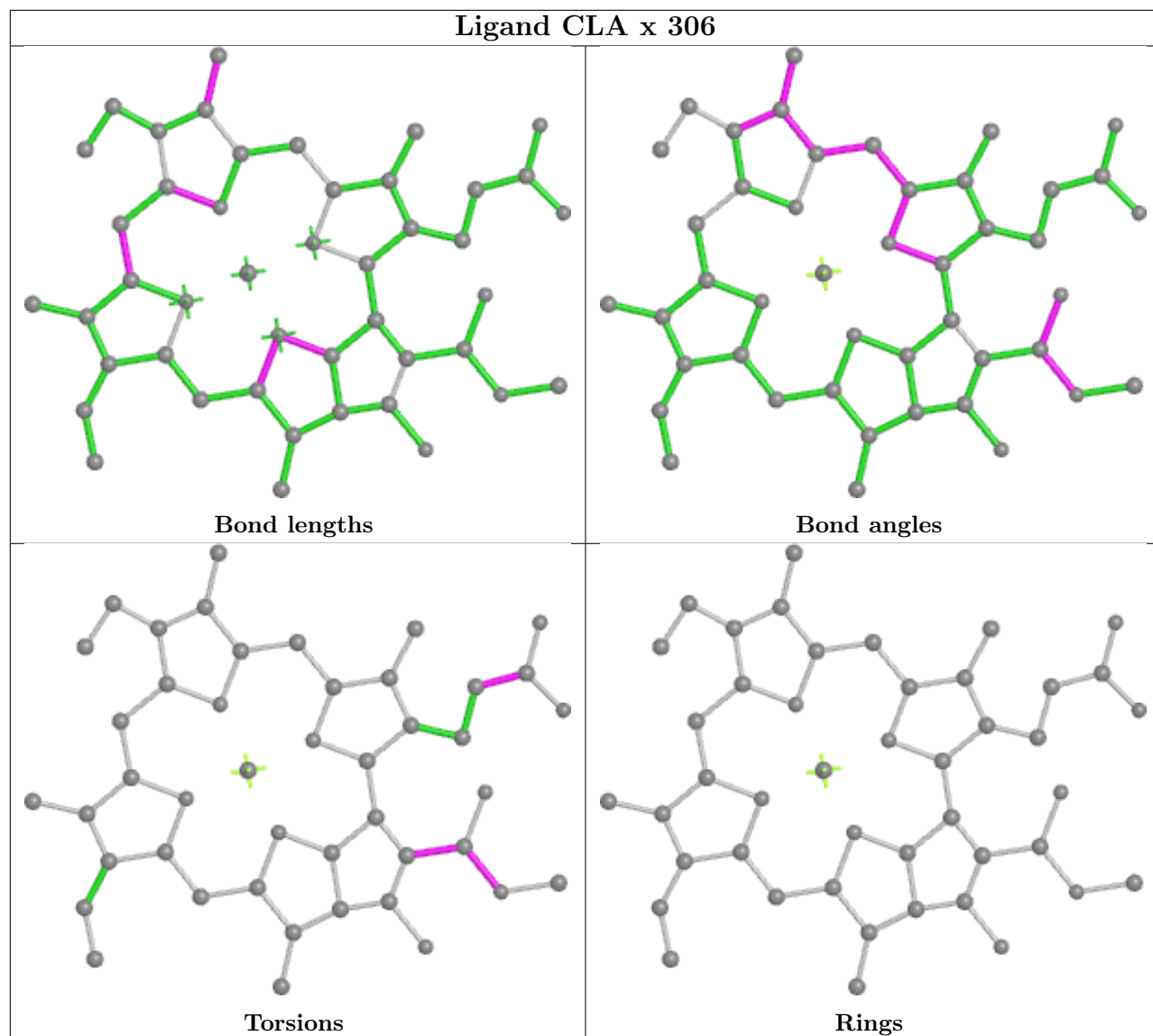


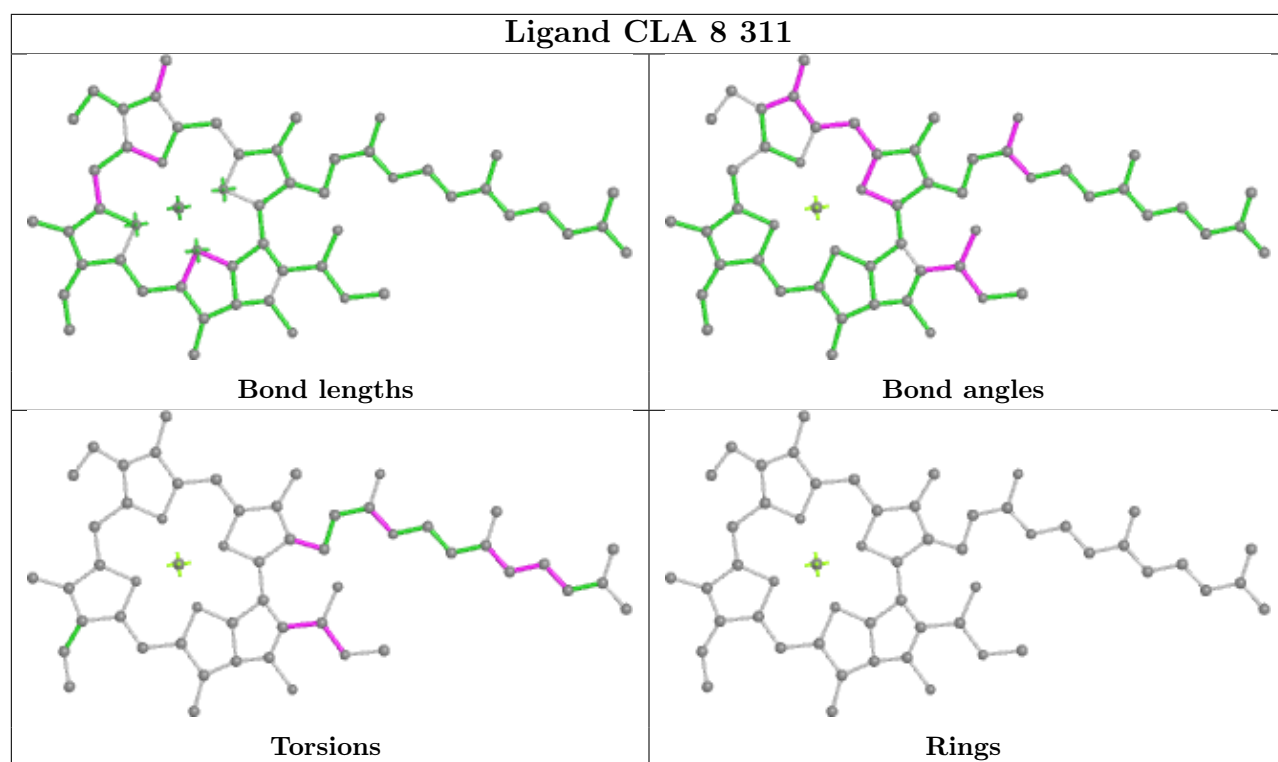
Torsions



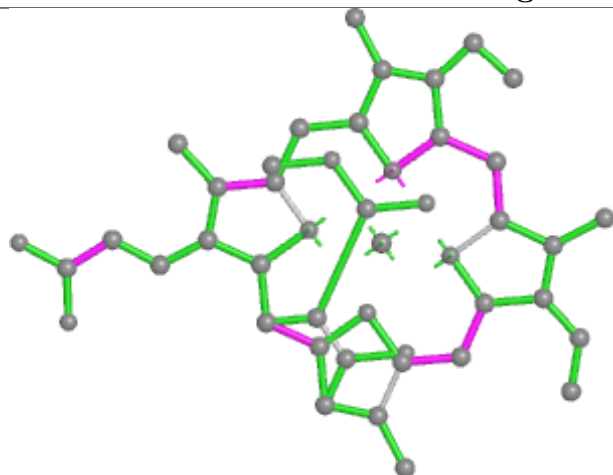
Rings

## Ligand CLA x 306

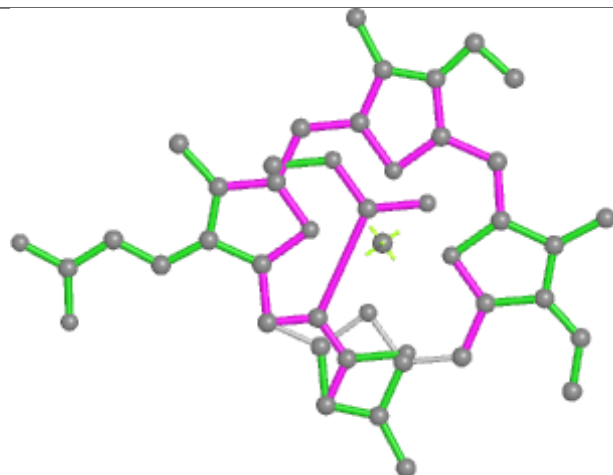




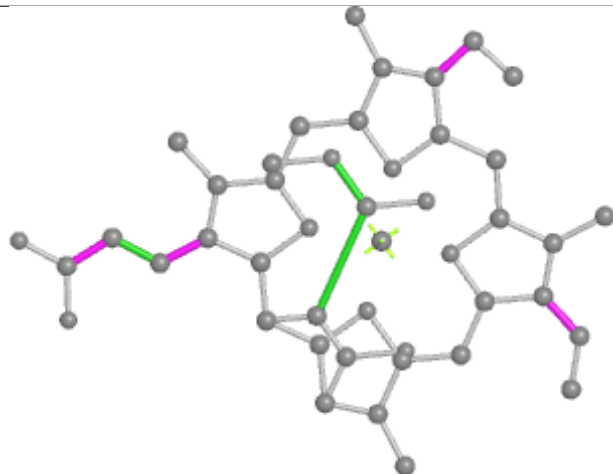
## Ligand KC2 T 316



Bond lengths



Bond angles

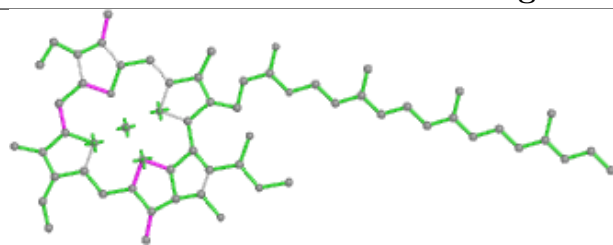


Torsions

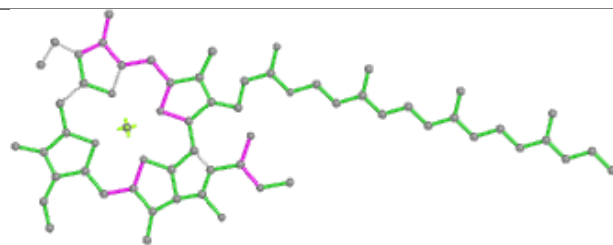


Rings

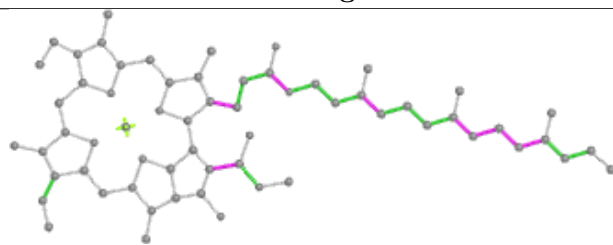
## Ligand CLA a 809



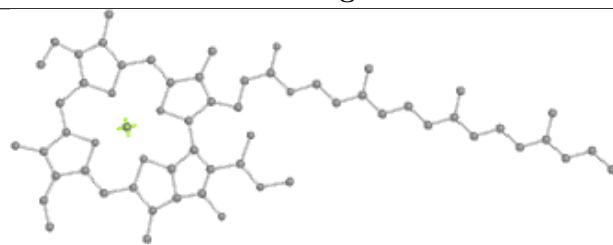
Bond lengths



Bond angles



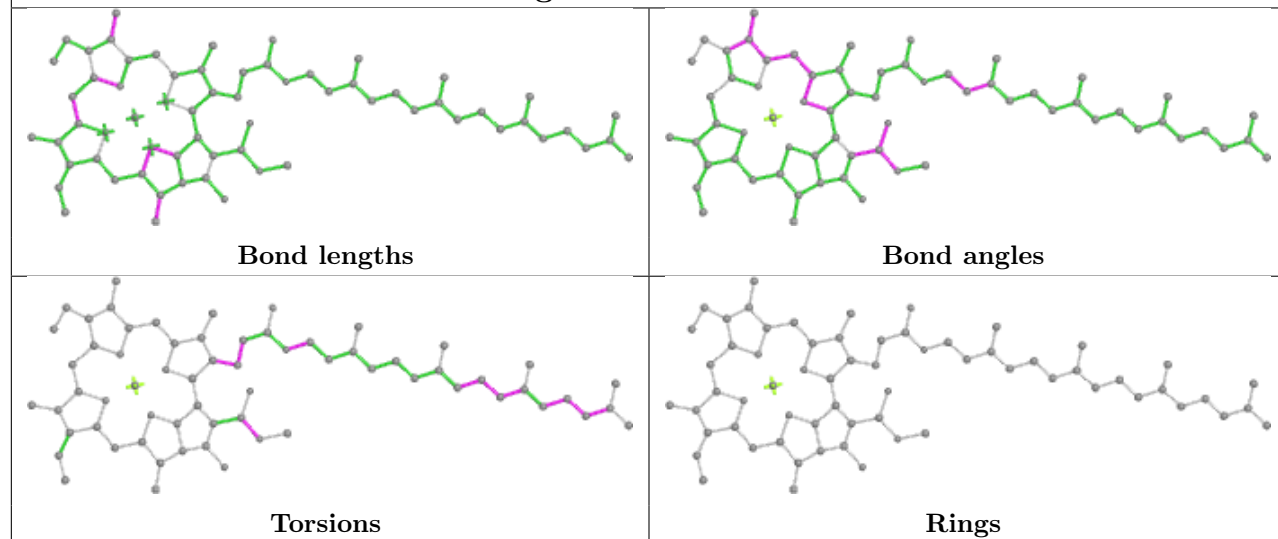
Torsions



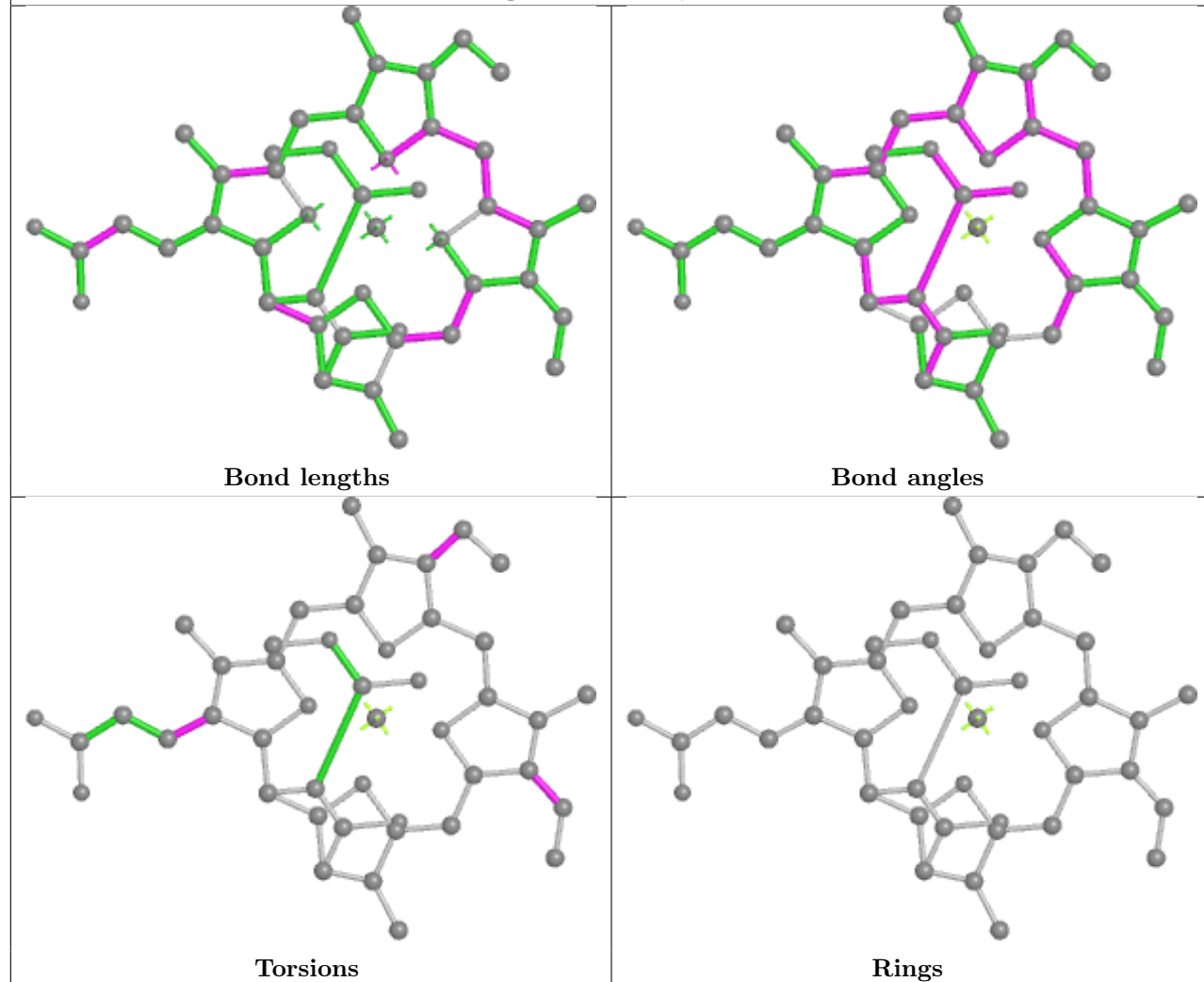
Rings

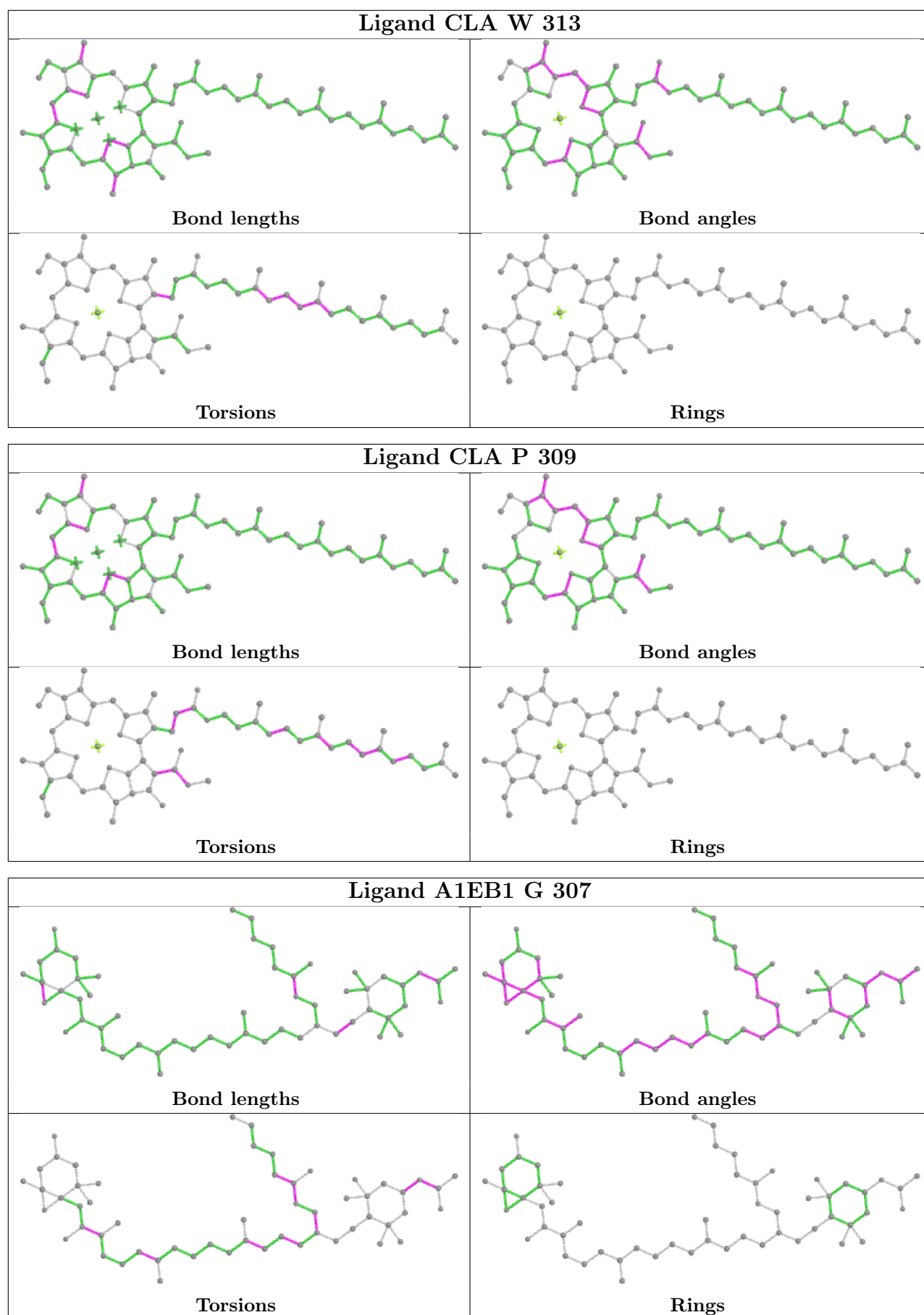


## Ligand CLA S 320

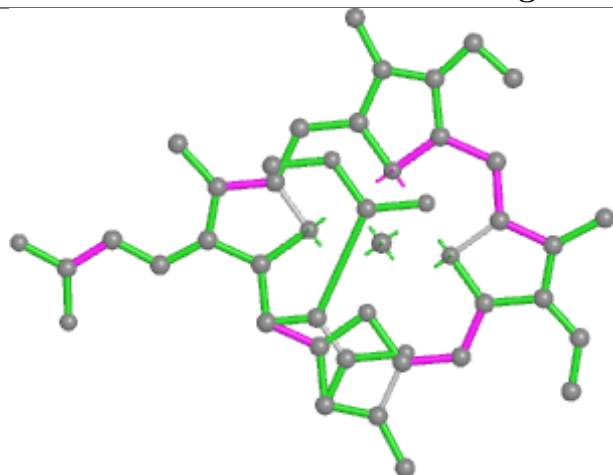


## Ligand KC2 Q 318

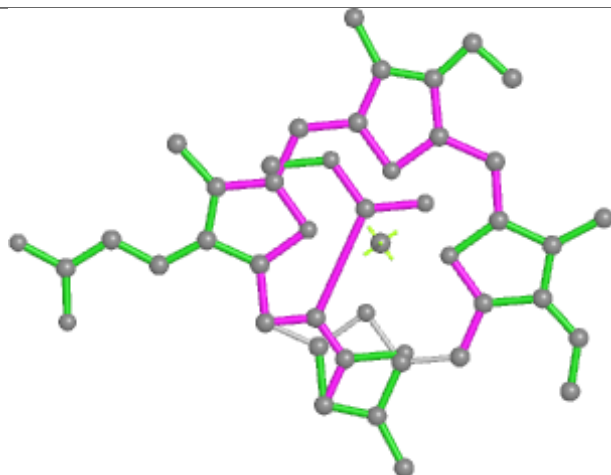




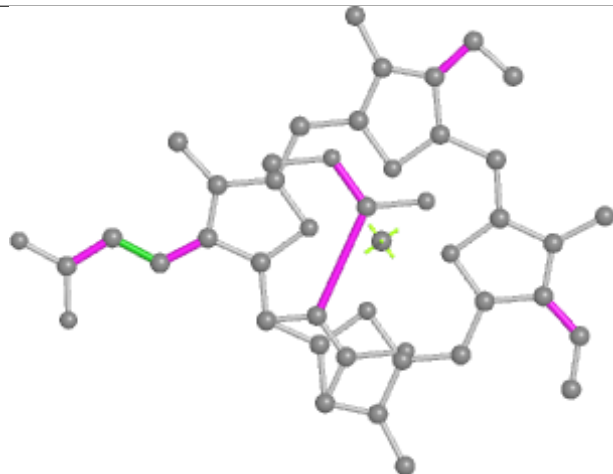
## Ligand KC2 L 317



Bond lengths



Bond angles

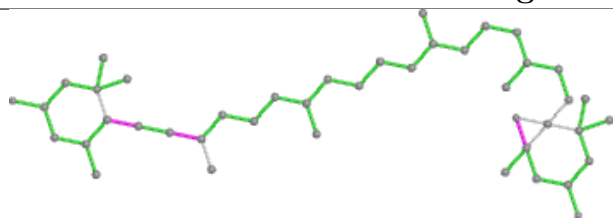


Torsions

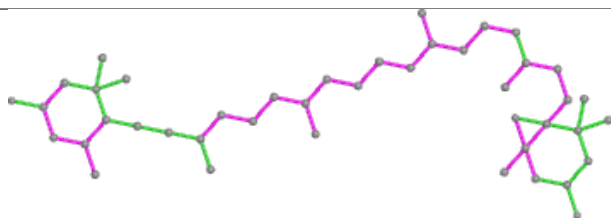


Rings

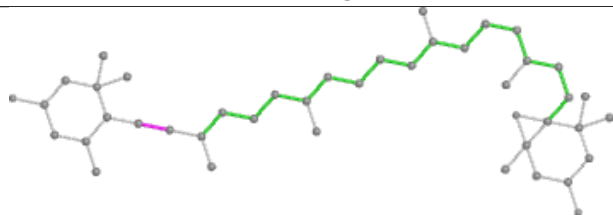
## Ligand DD6 F 305



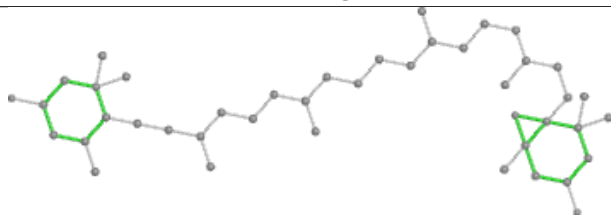
Bond lengths



Bond angles

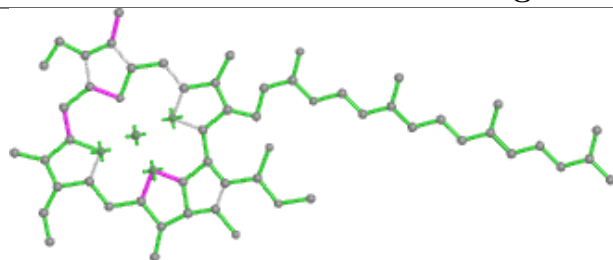


Torsions

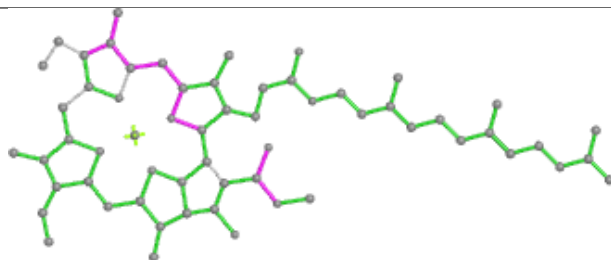


Rings

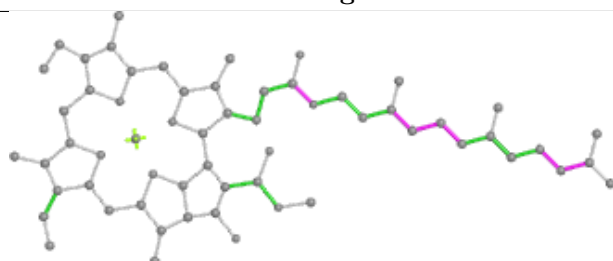
## Ligand CLA R 308



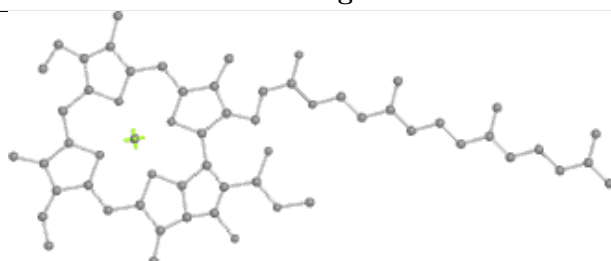
Bond lengths



Bond angles

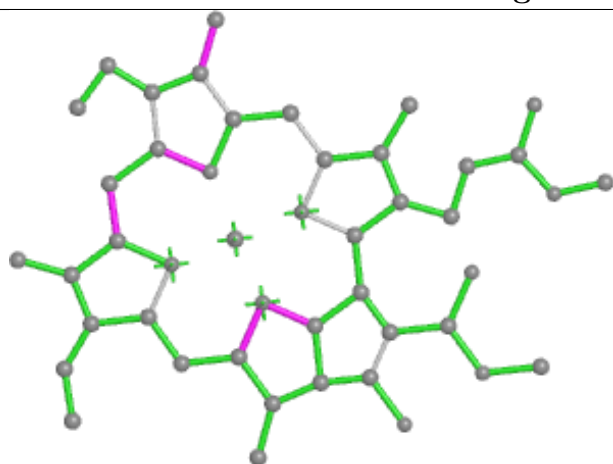


Torsions

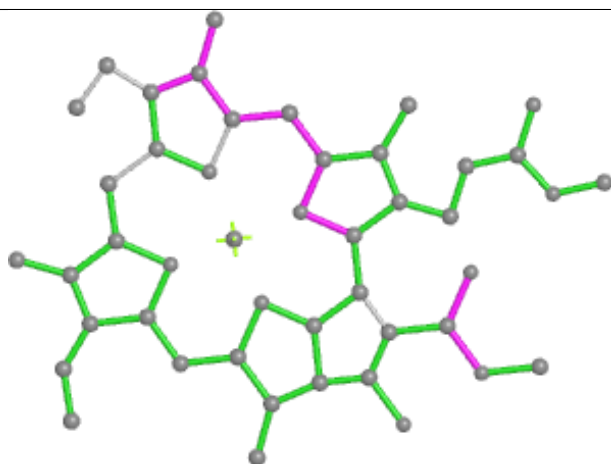


Rings

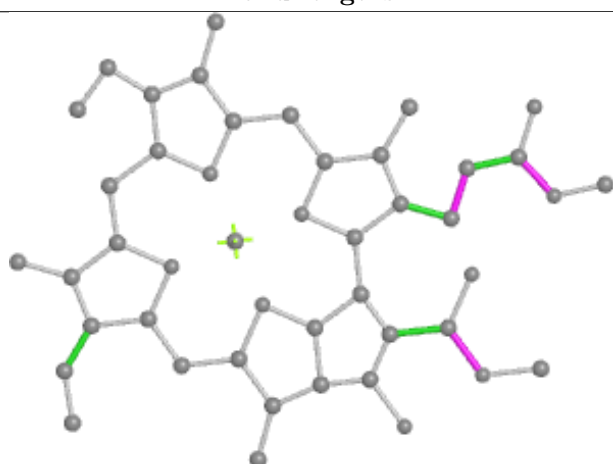
## Ligand CLA U 212



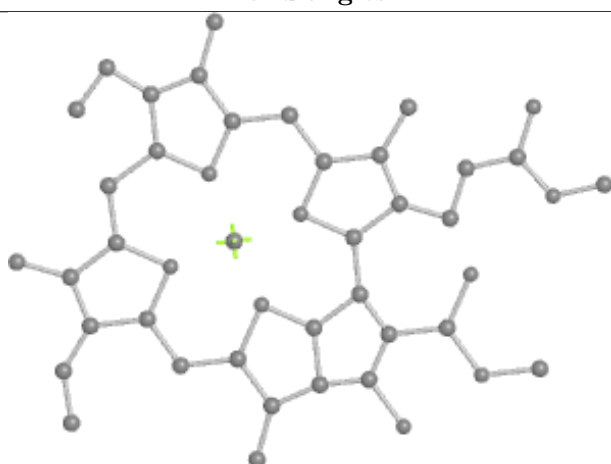
Bond lengths



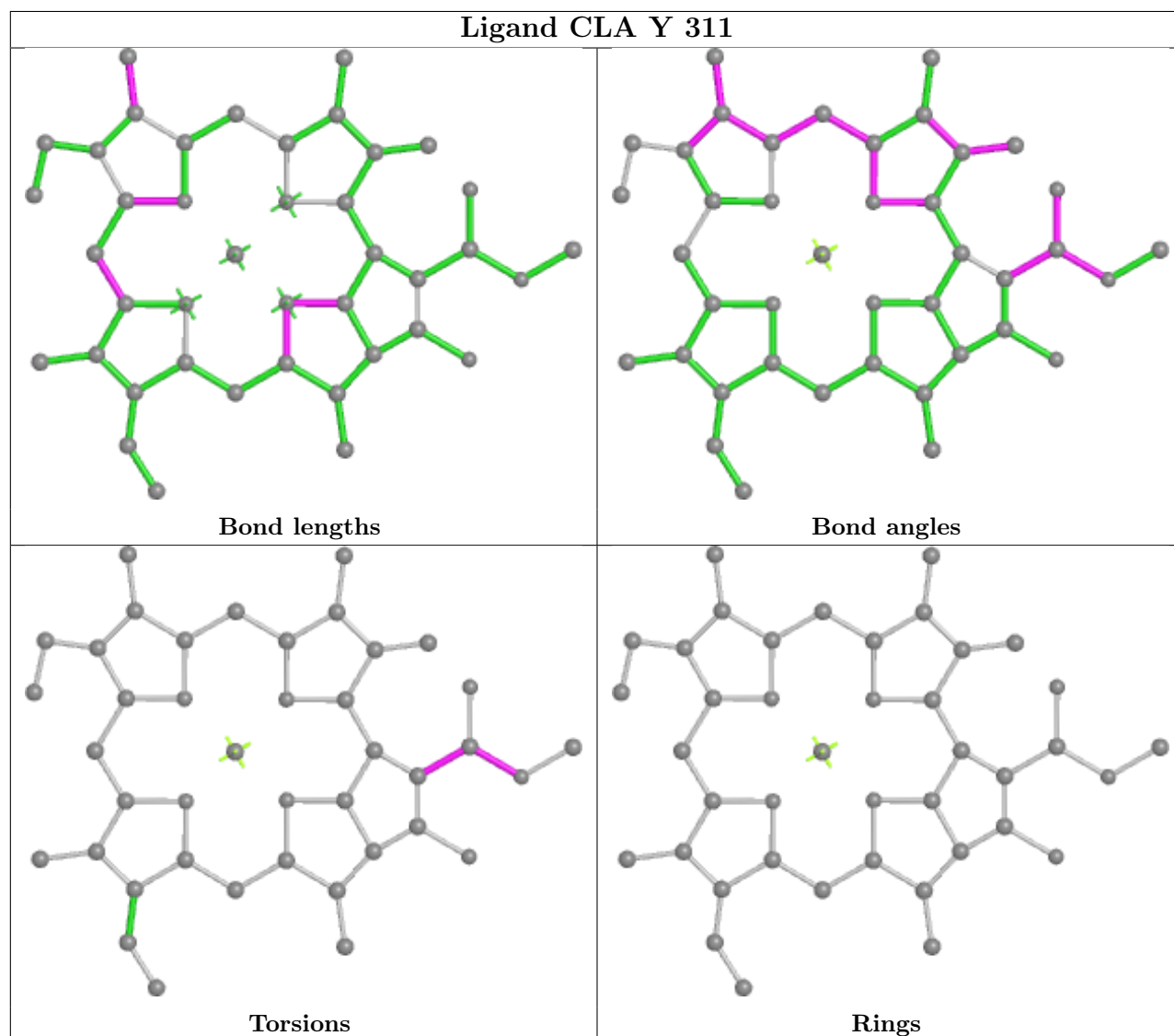
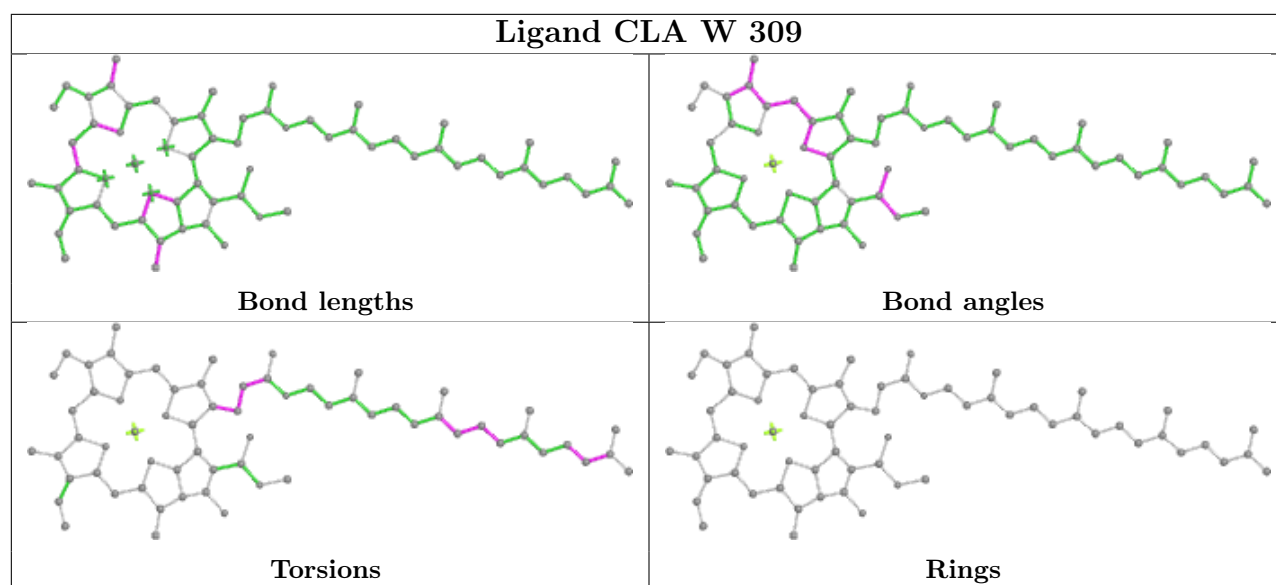
Bond angles

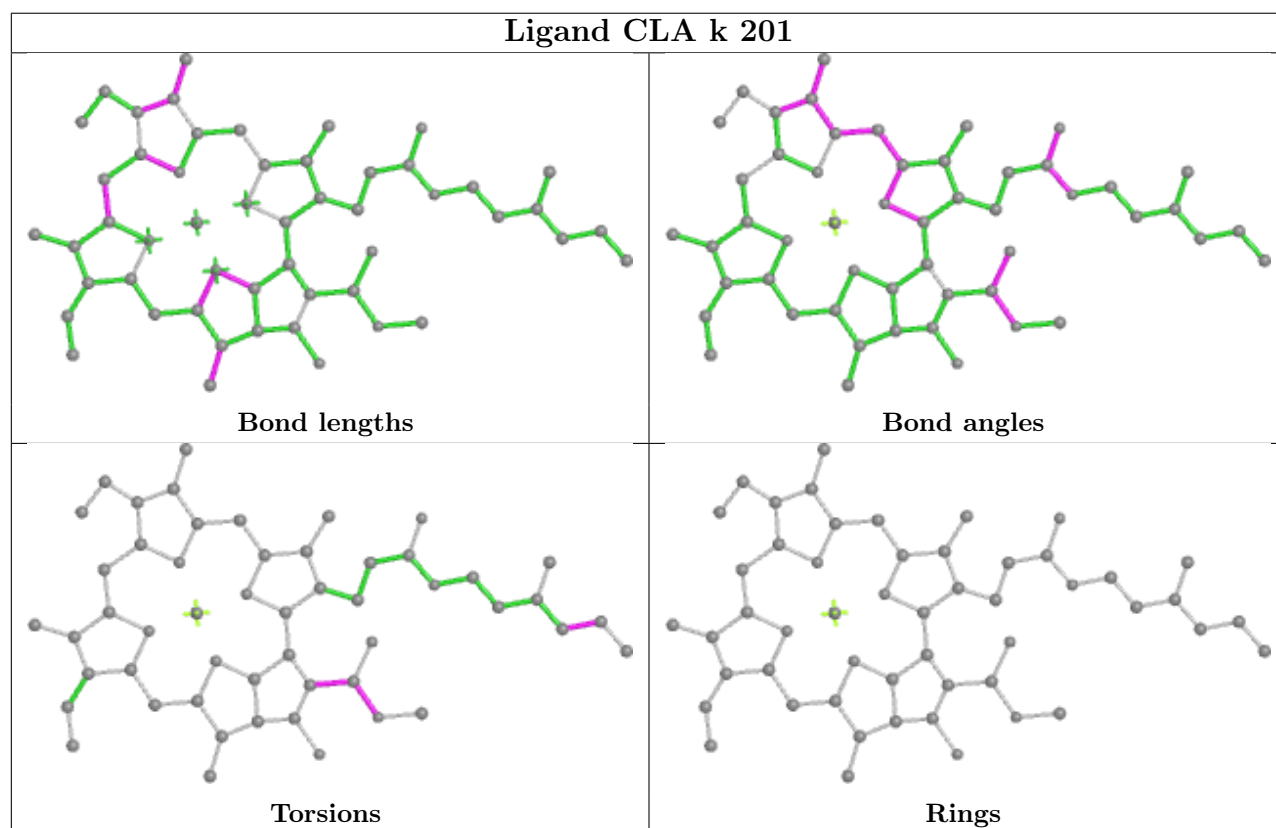
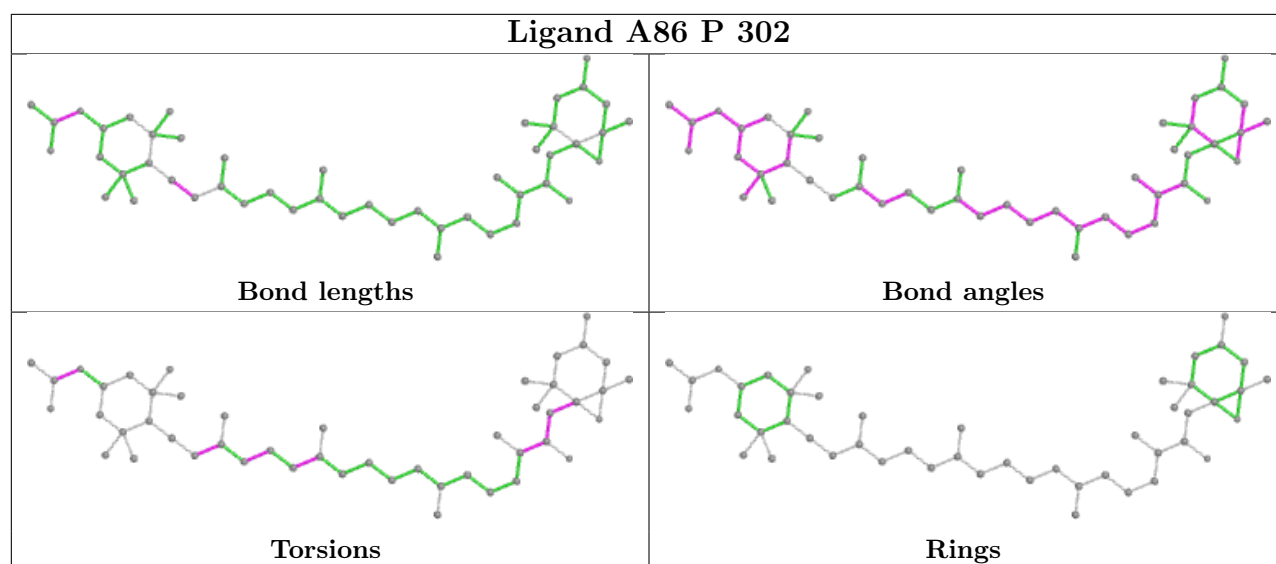


Torsions

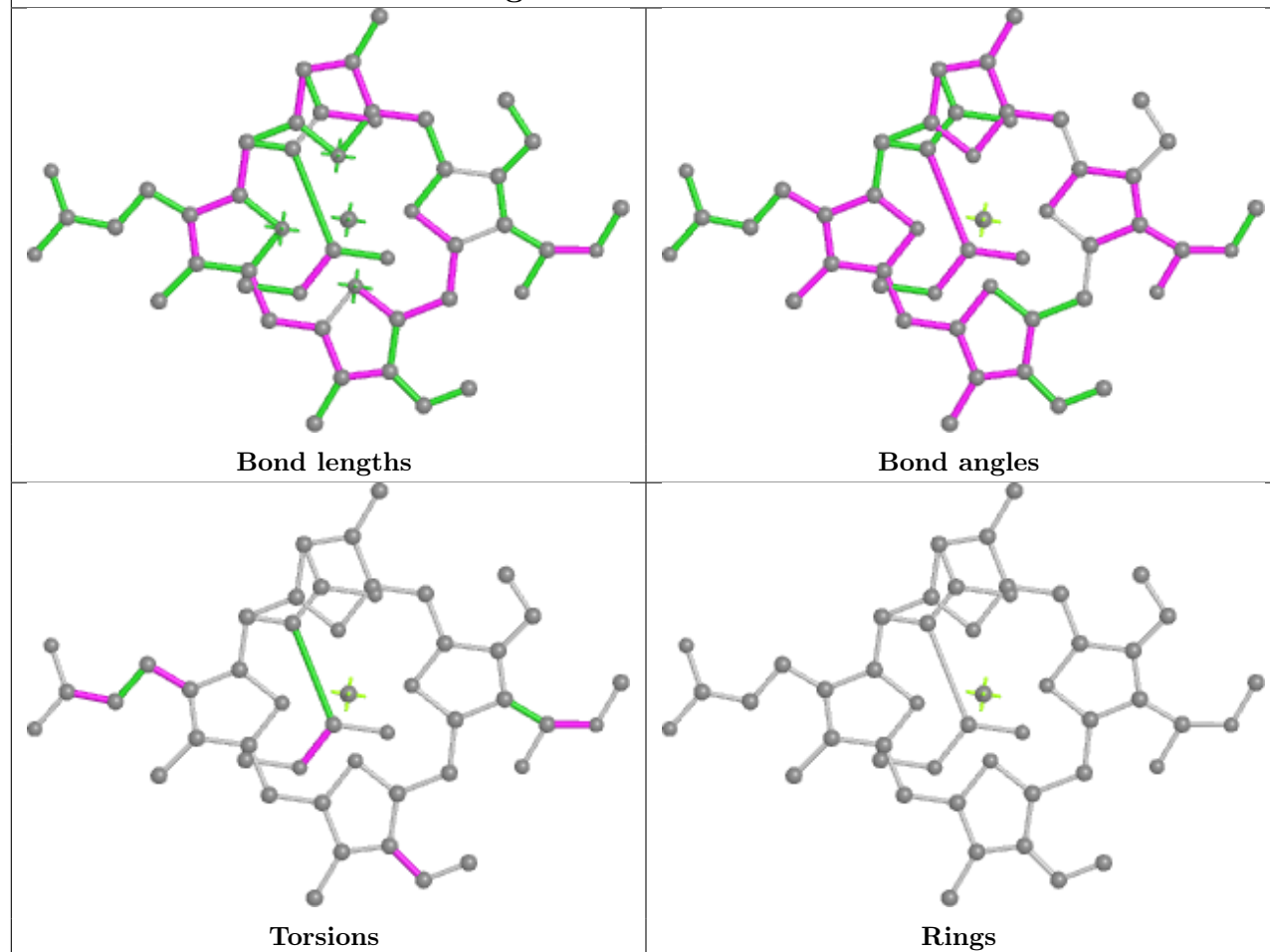


Rings

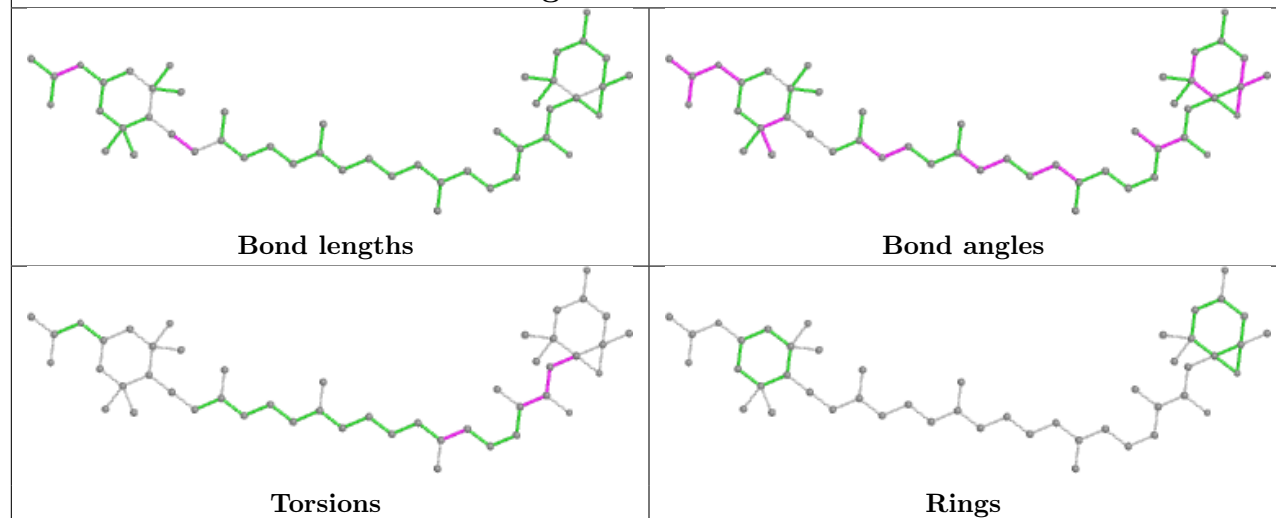


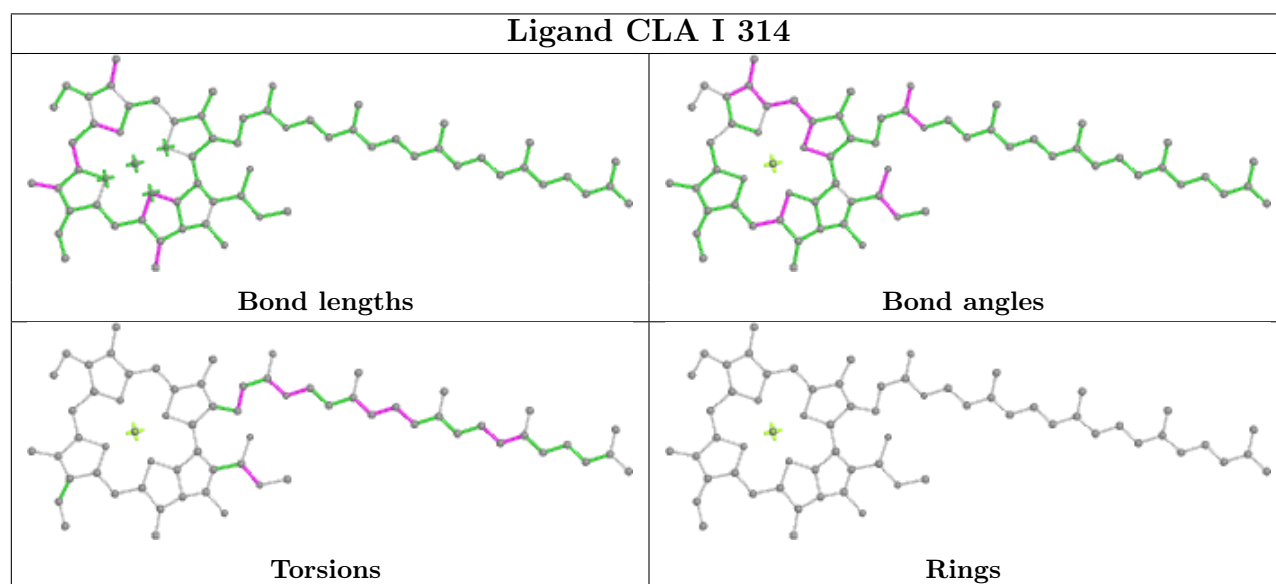
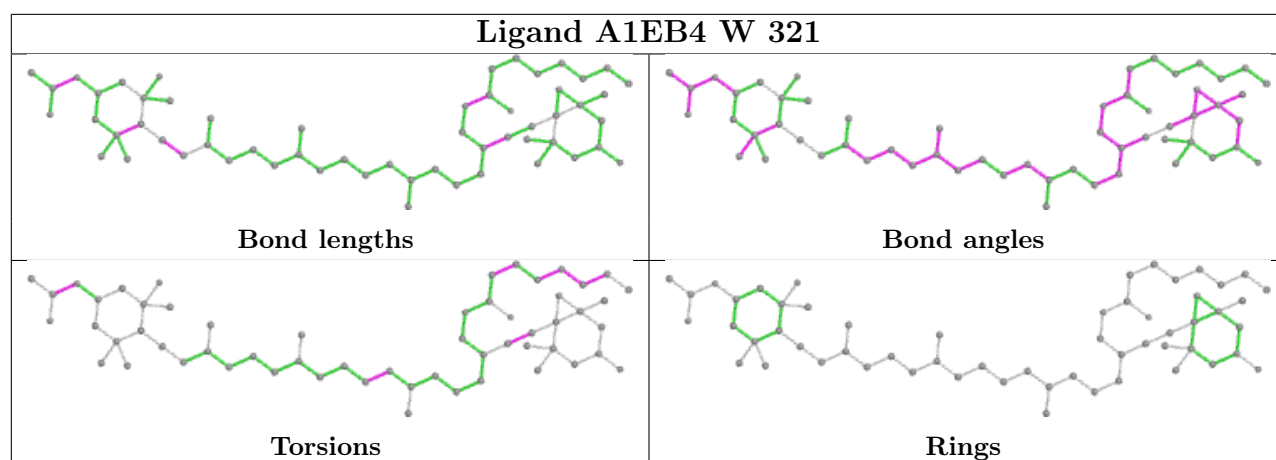


## Ligand A1ECV X 310



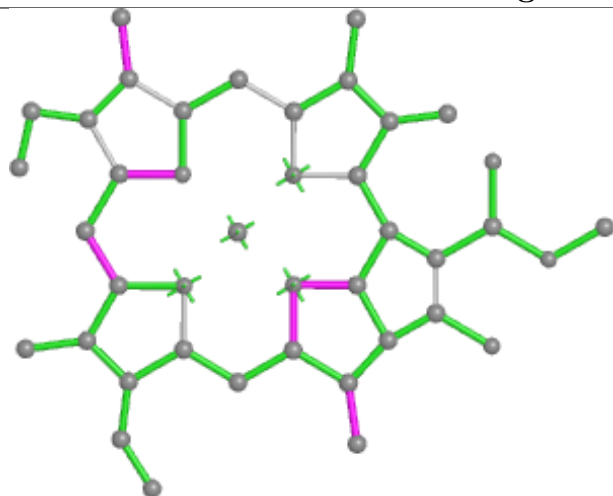
## Ligand A86 4 305



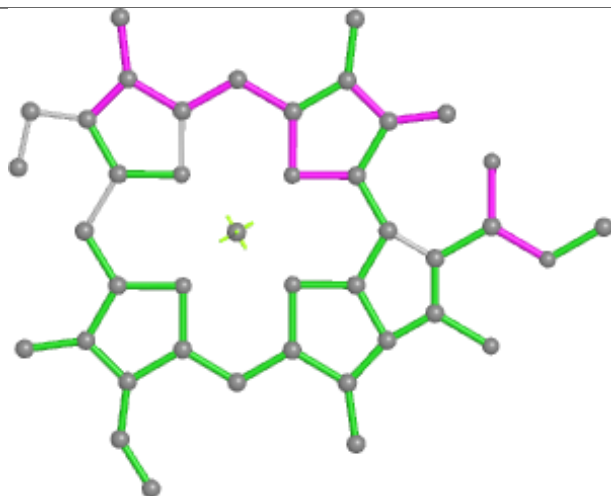




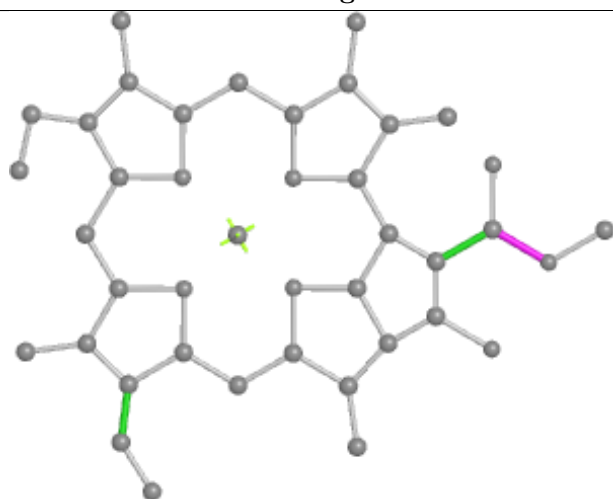
## Ligand CLA x 308



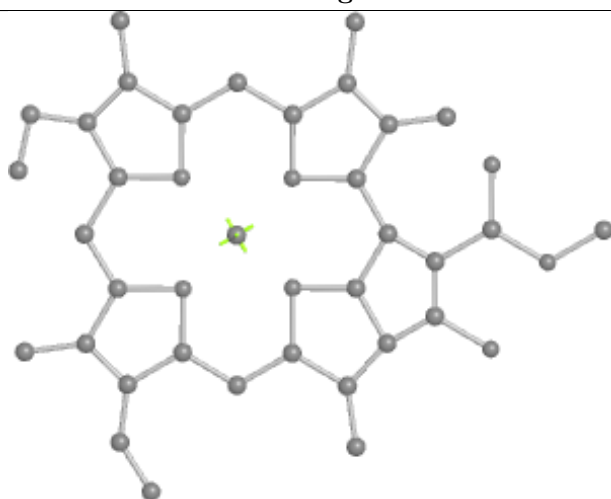
Bond lengths



Bond angles

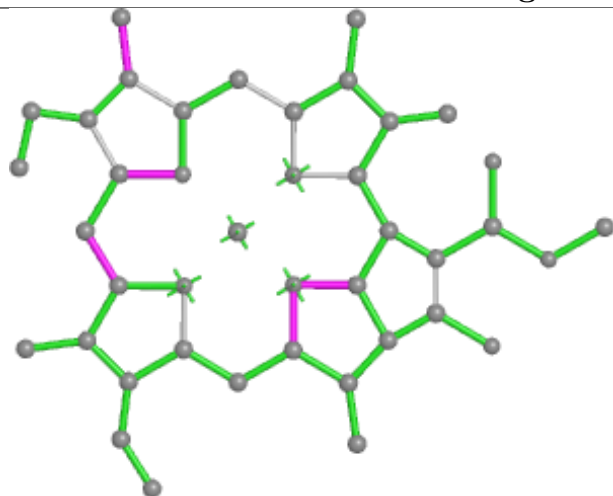


Torsions

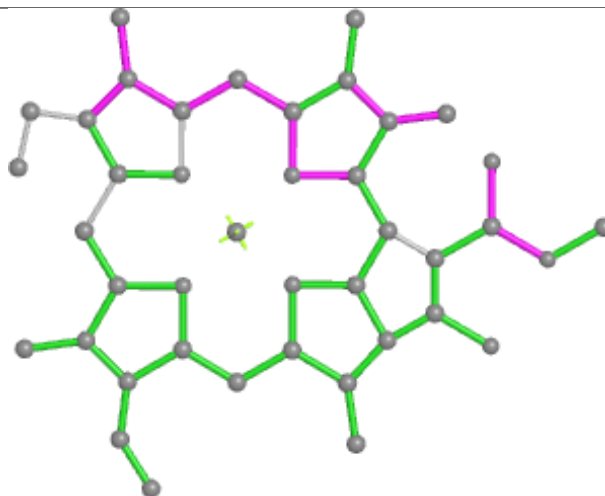


Rings

## Ligand CLA 2 318



Bond lengths



Bond angles

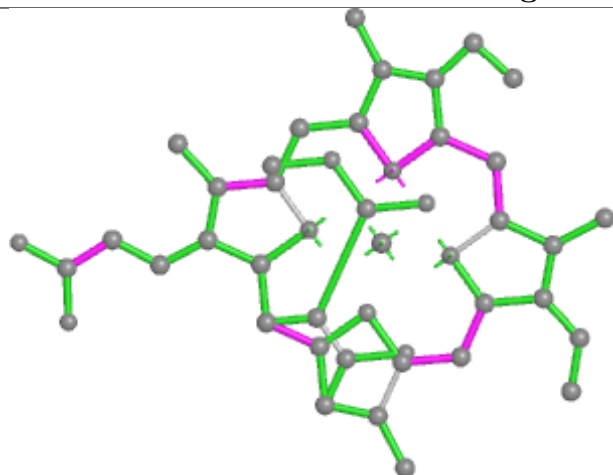


Torsions

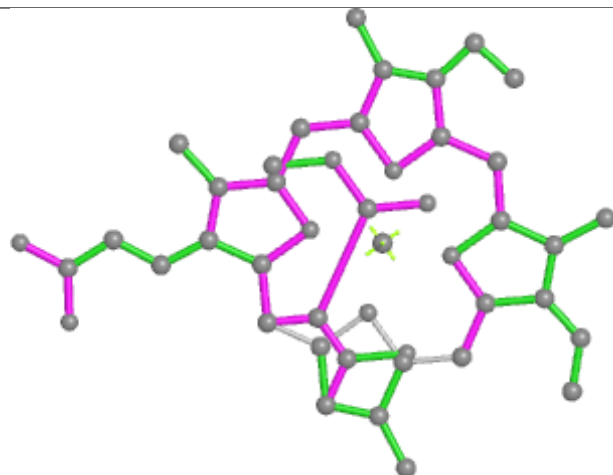


Rings

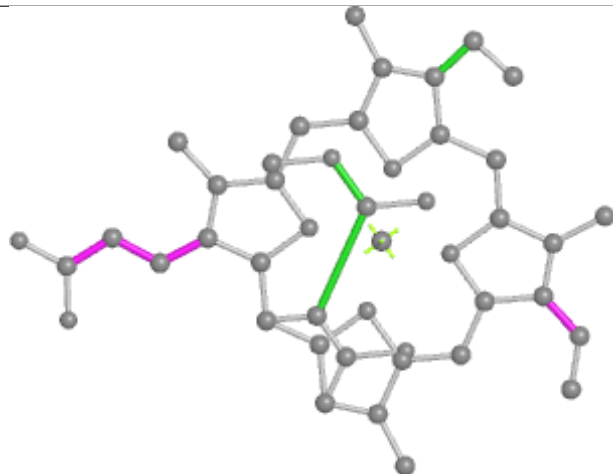
## Ligand KC2 3 318



Bond lengths



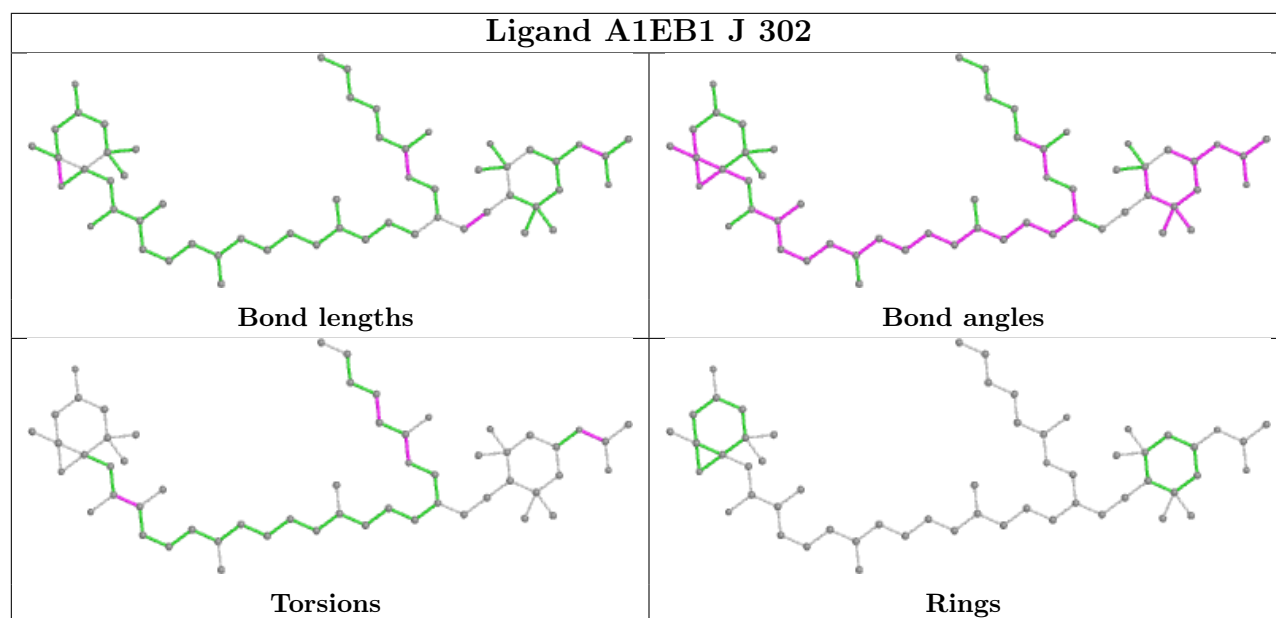
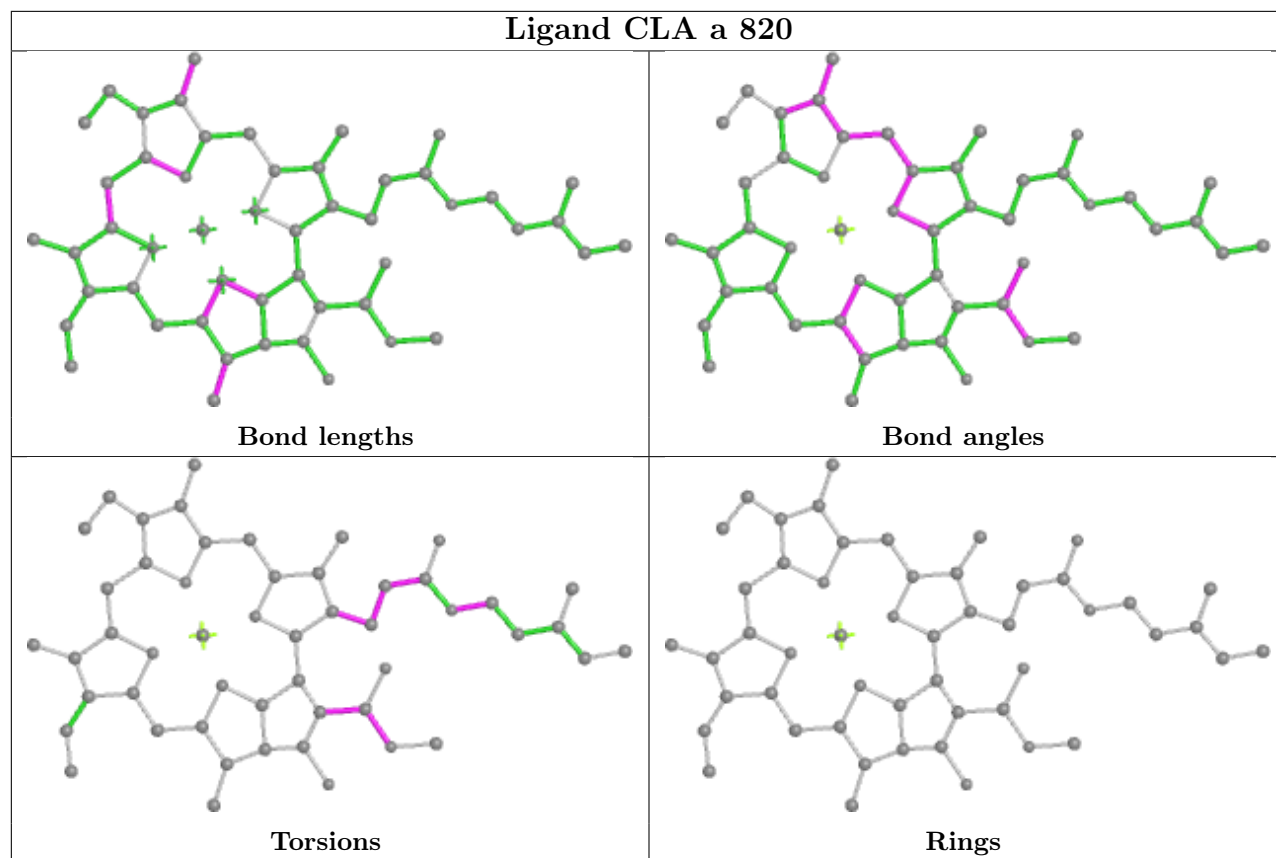
Bond angles



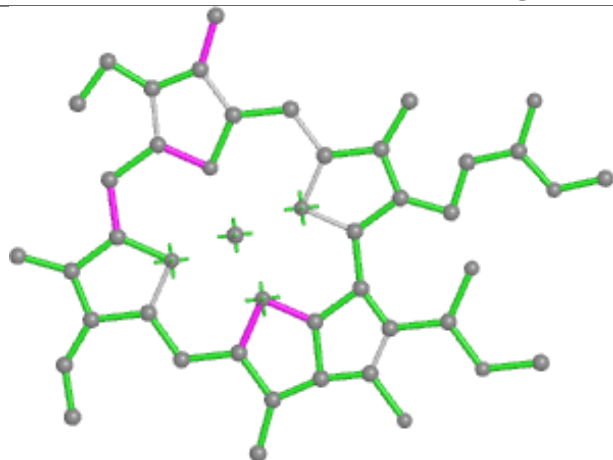
Torsions



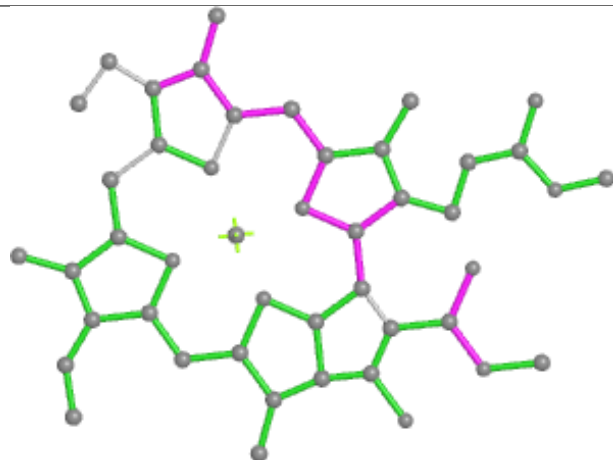
Rings



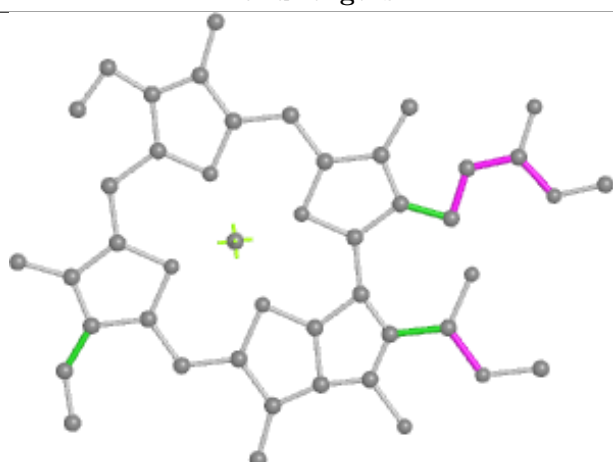
## Ligand CLA O 318



Bond lengths



Bond angles

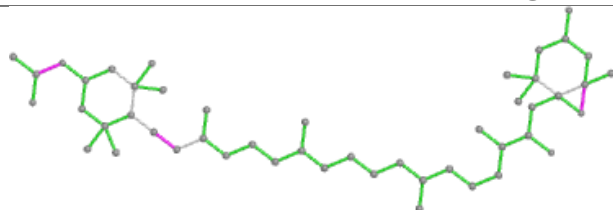


Torsions

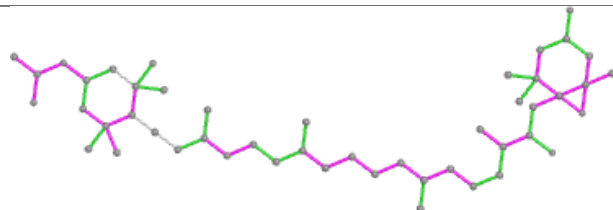


Rings

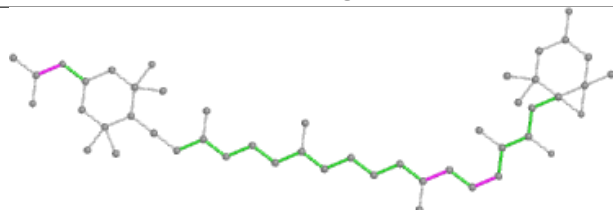
## Ligand A86 1 302



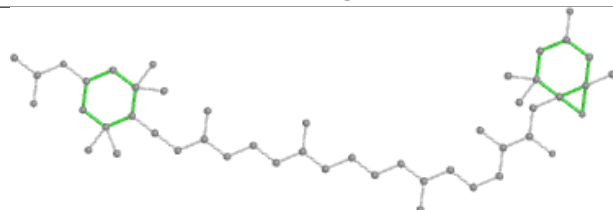
Bond lengths



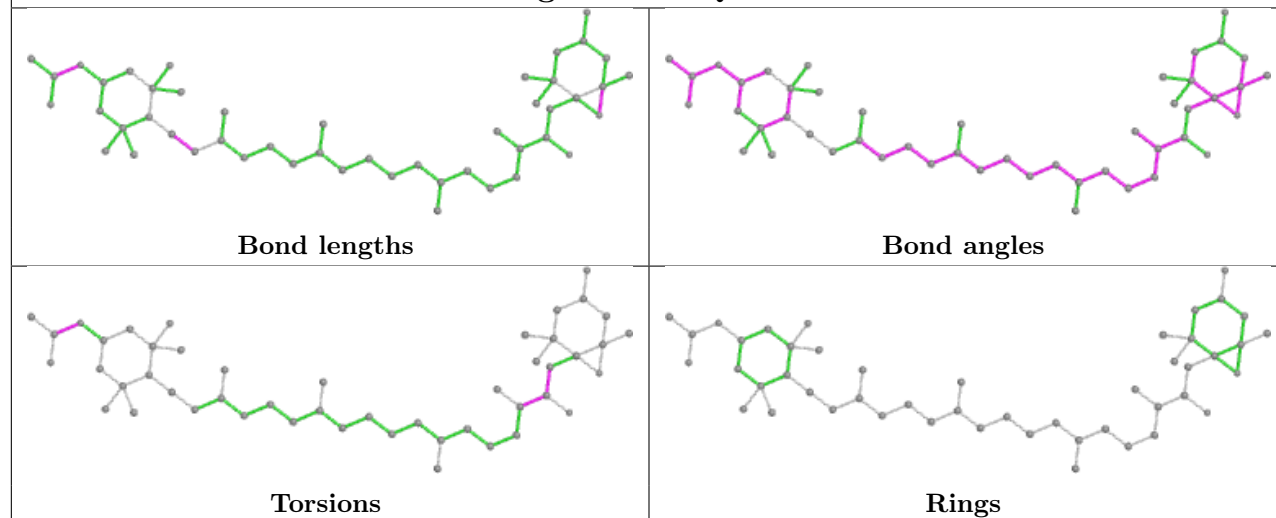
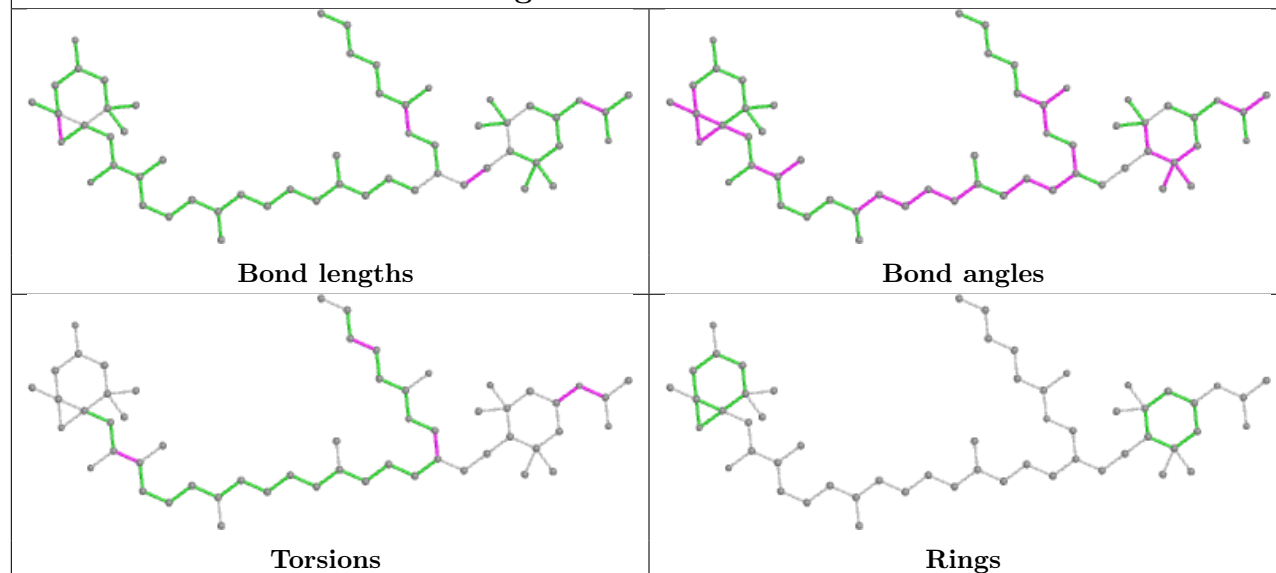
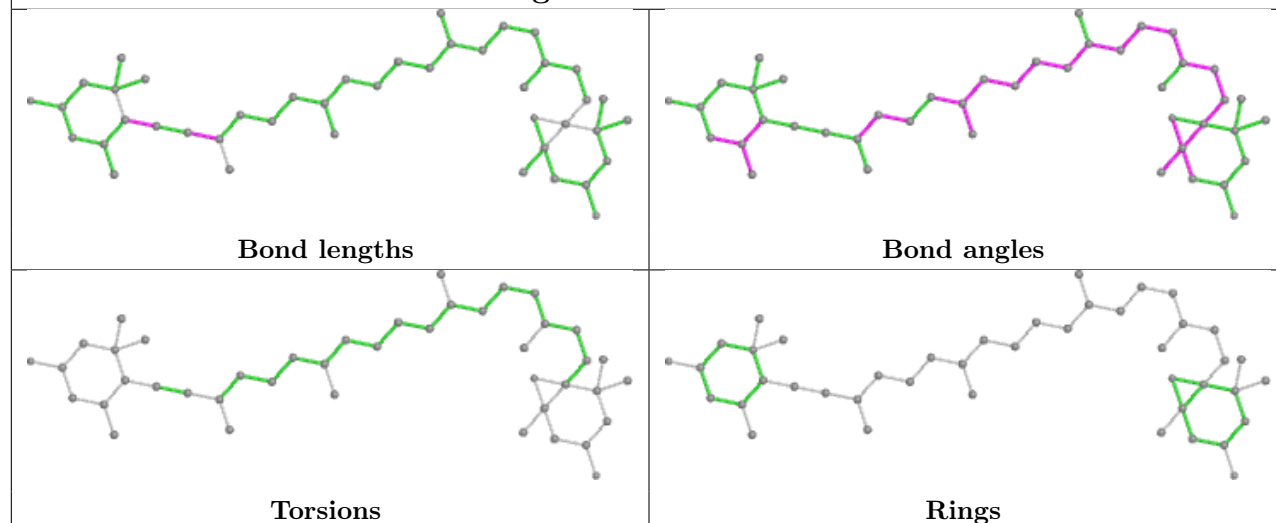
Bond angles



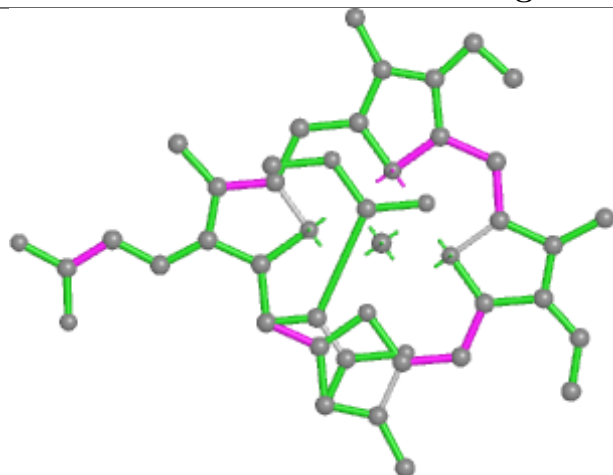
Torsions



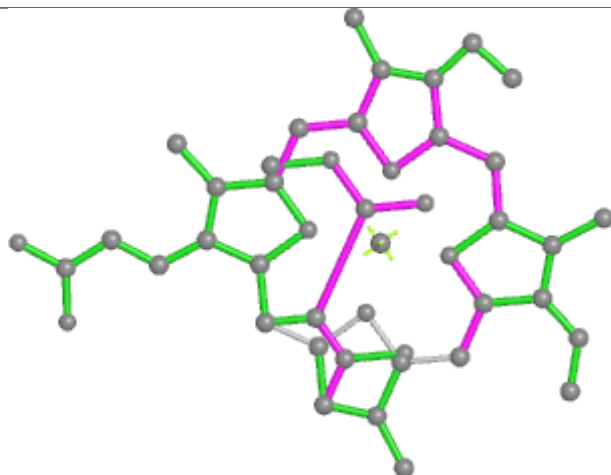
Rings

**Ligand A86 Q 301****Ligand A1EB1 E 301****Ligand DD6 D 303**

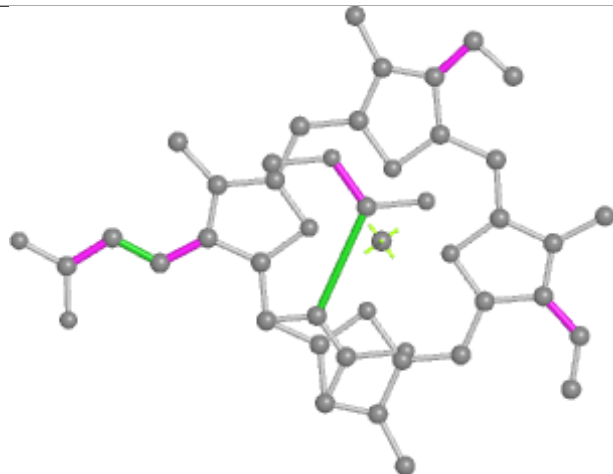
## Ligand KC2 Y 308



Bond lengths



Bond angles

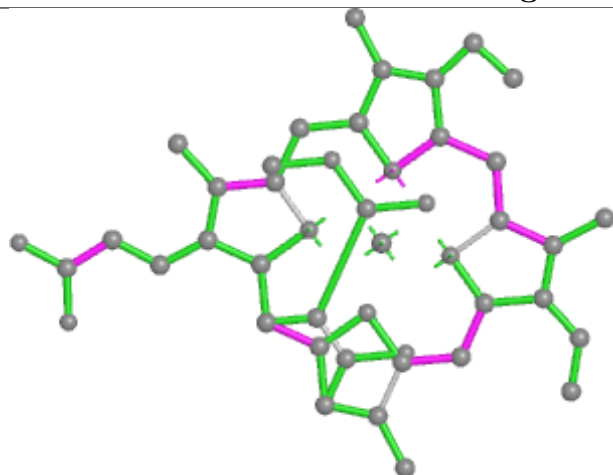


Torsions

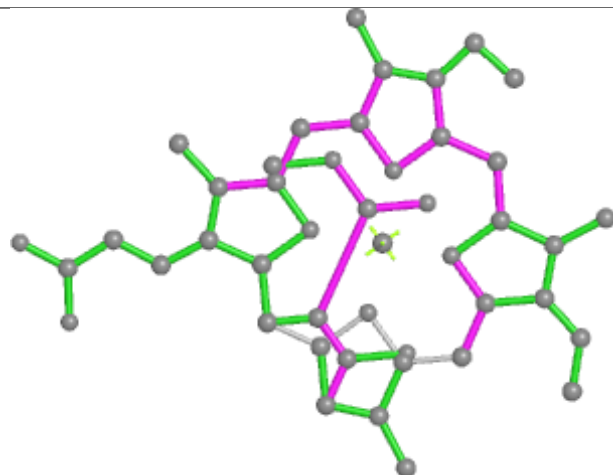


Rings

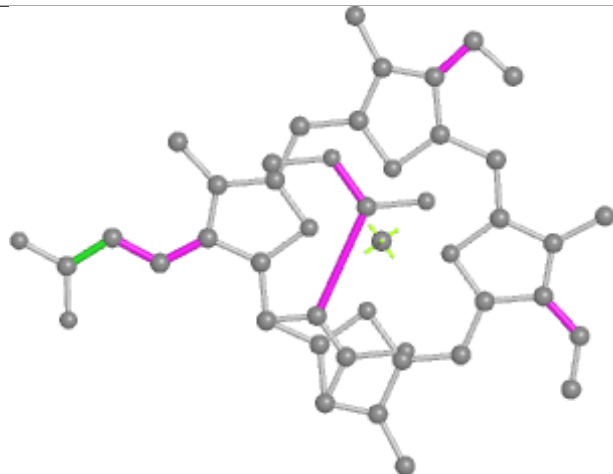
## Ligand KC2 1 315



Bond lengths



Bond angles



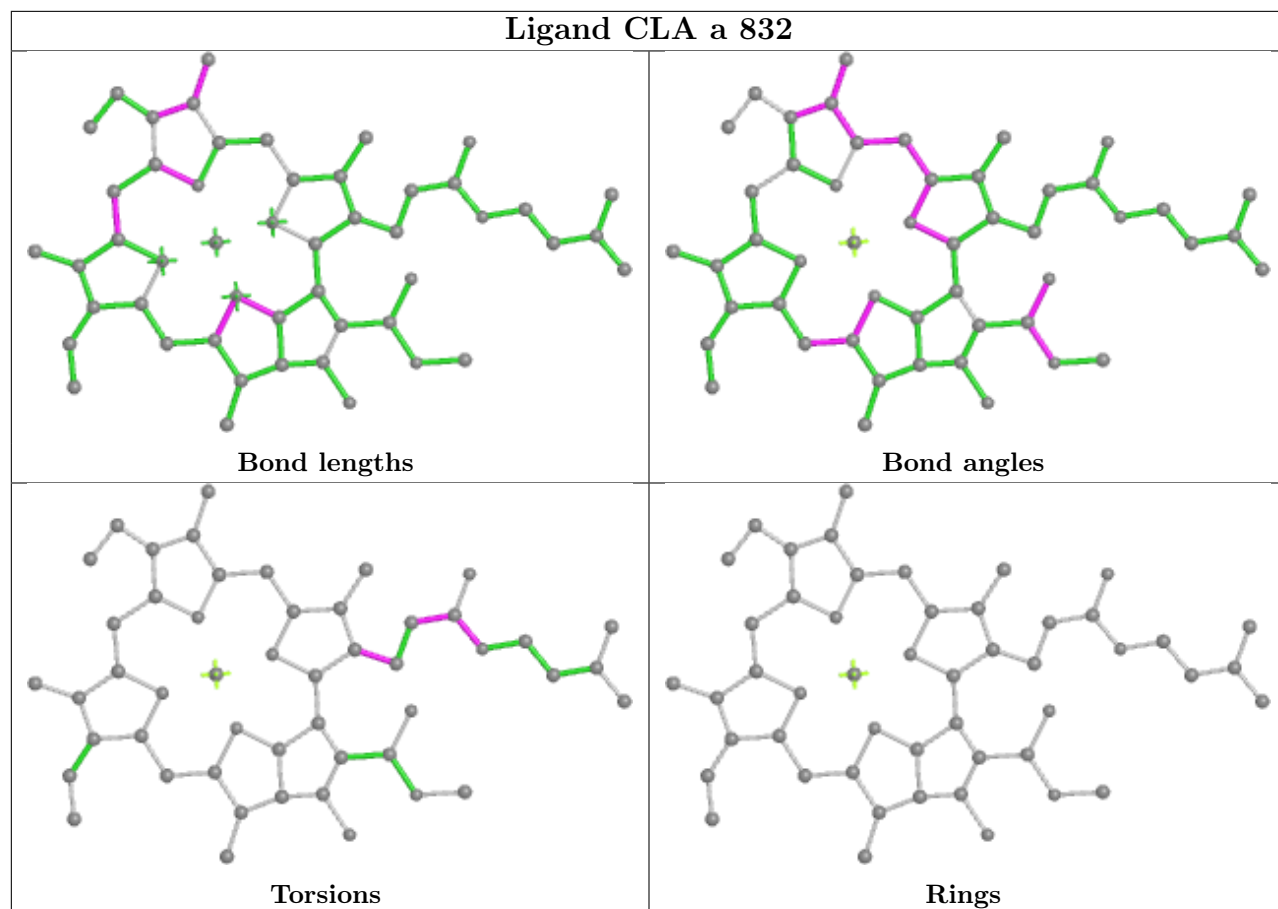
Torsions



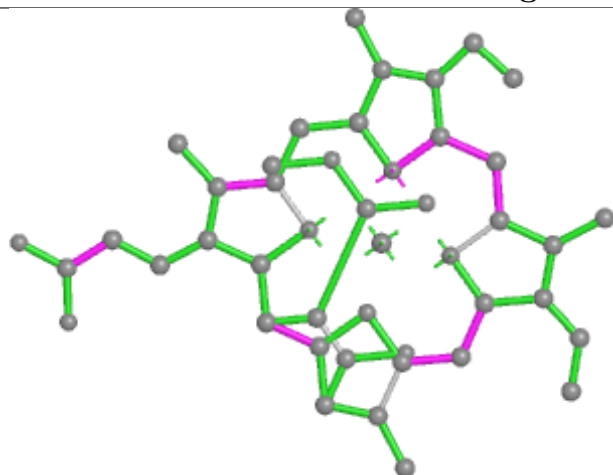
Rings



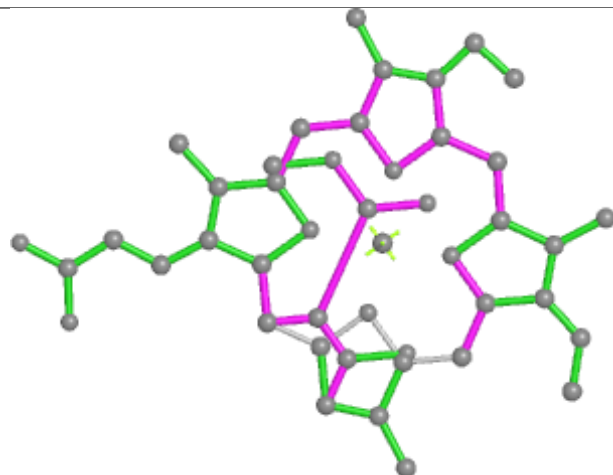
## Ligand CLA a 832



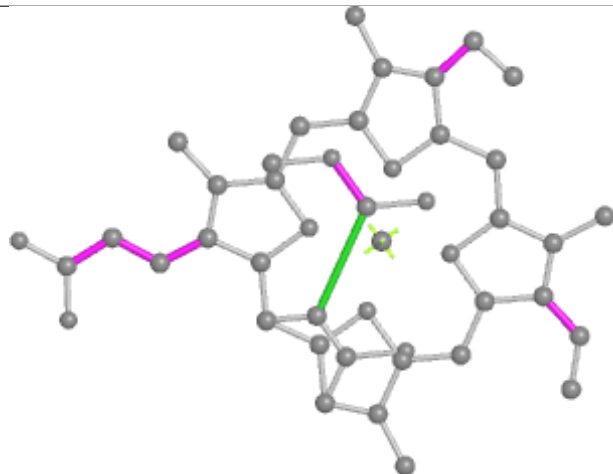
## Ligand KC2 x 315



Bond lengths



Bond angles

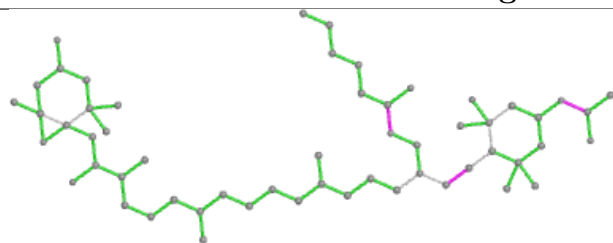


Torsions

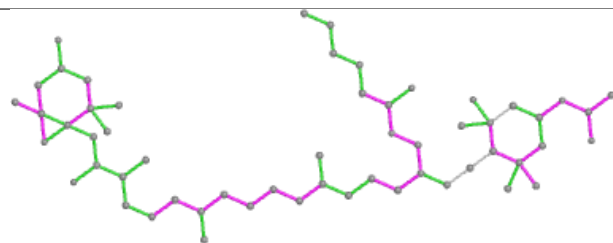


Rings

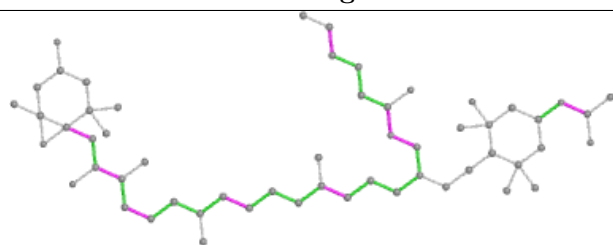
## Ligand A1EB1 x 302



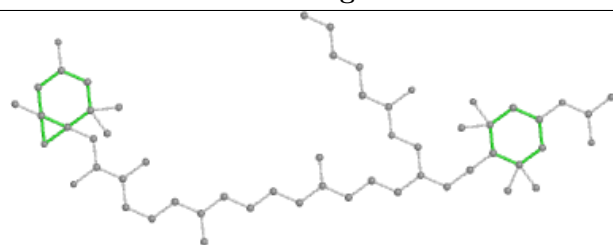
Bond lengths



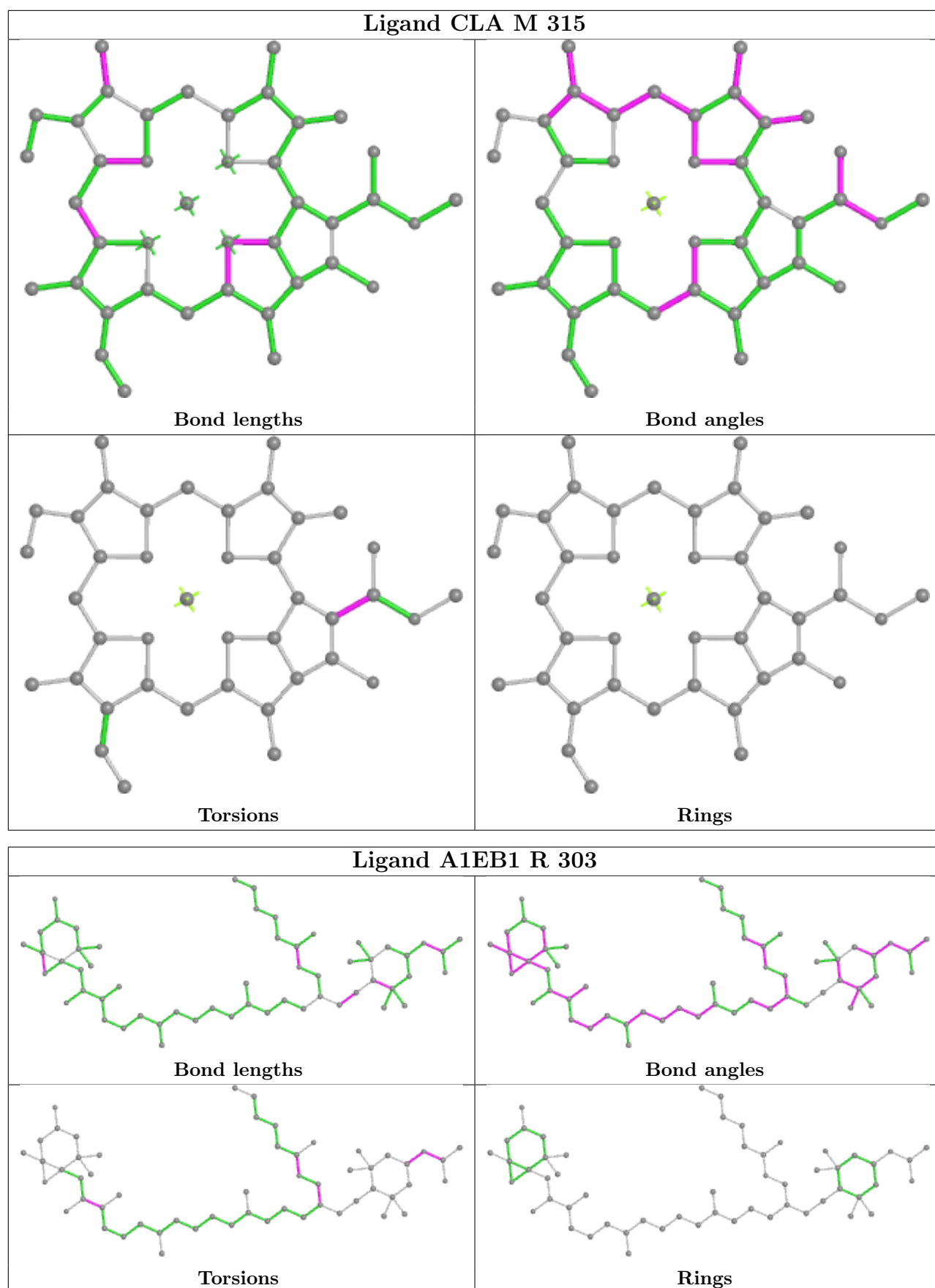
Bond angles



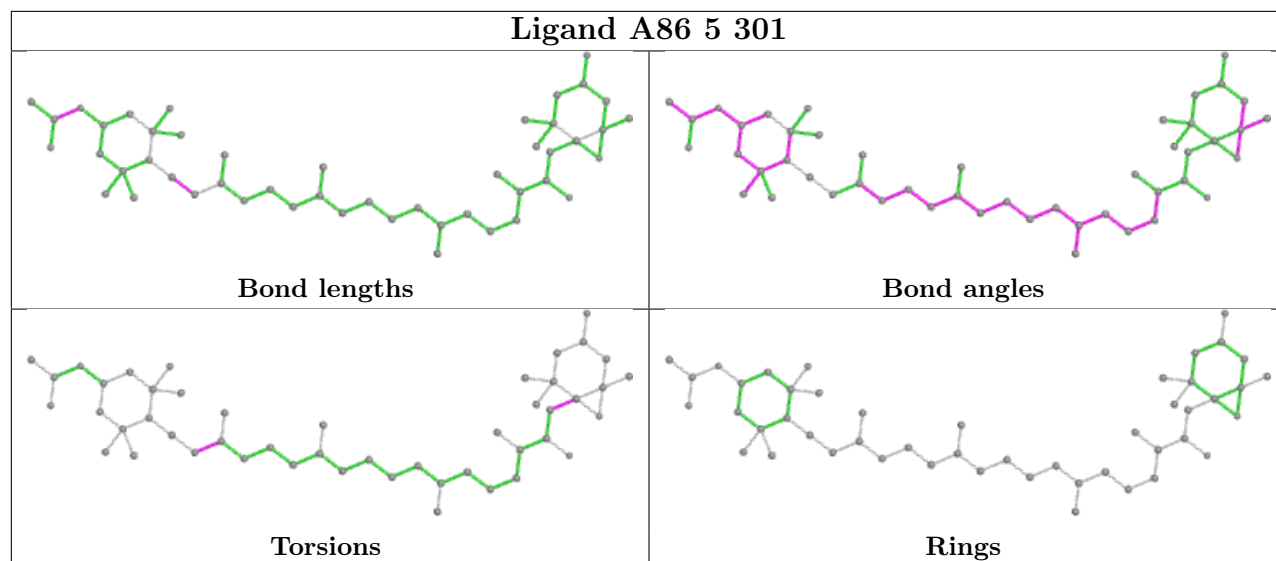
Torsions



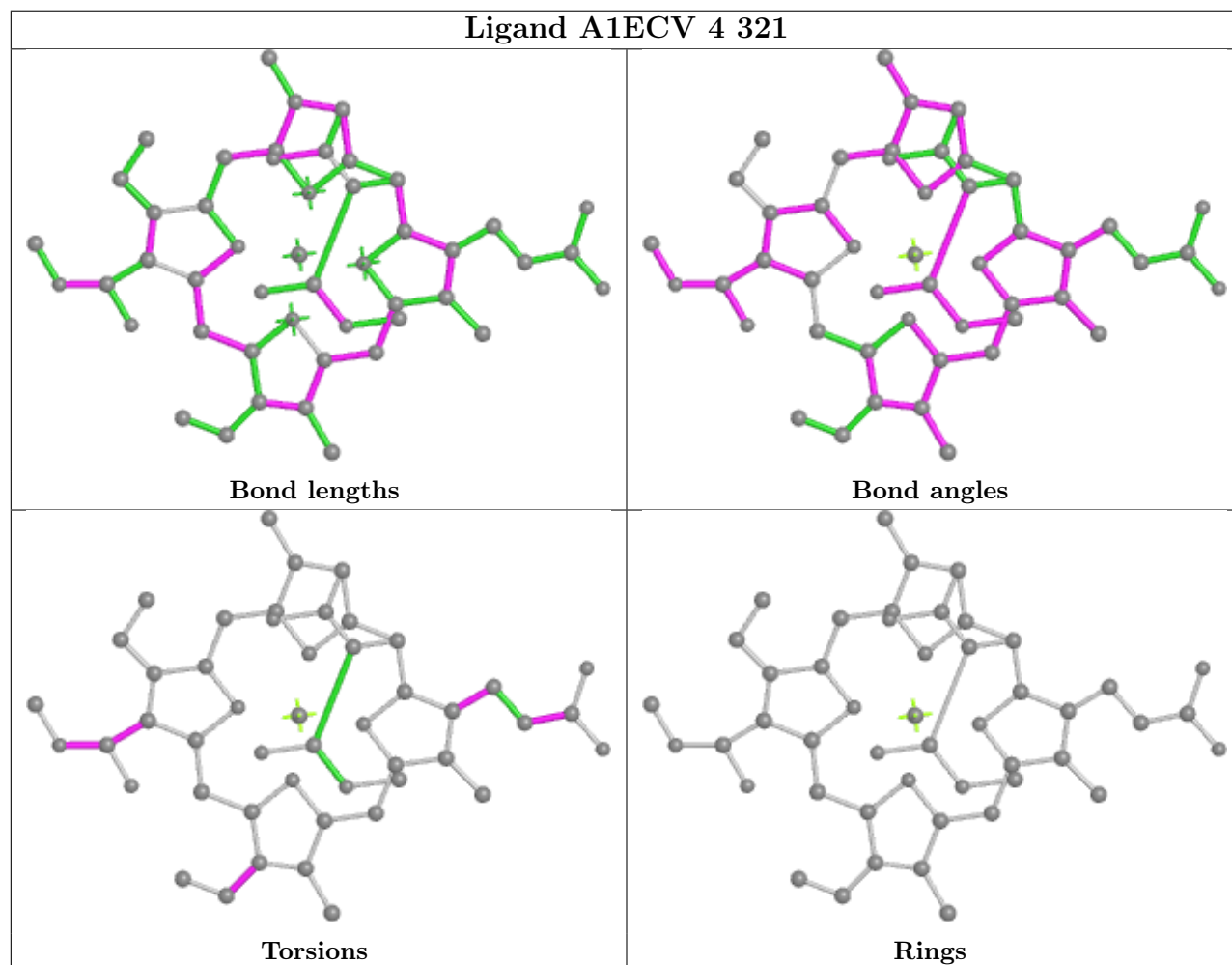
Rings



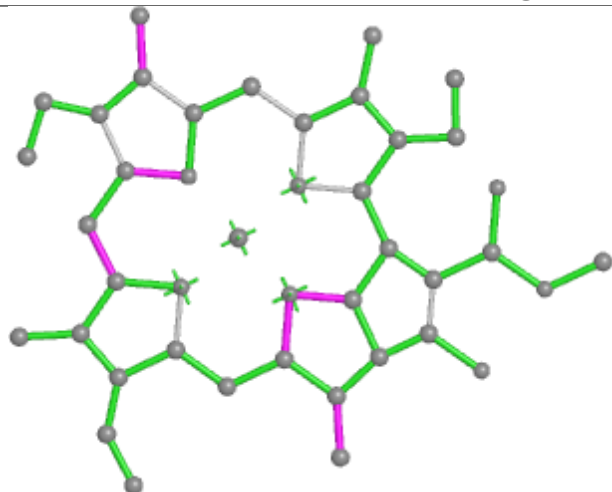
## Ligand A86 5 301



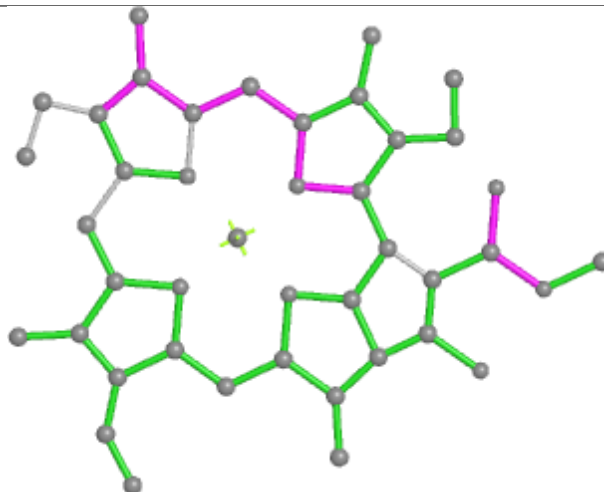
## Ligand A1ECV 4 321



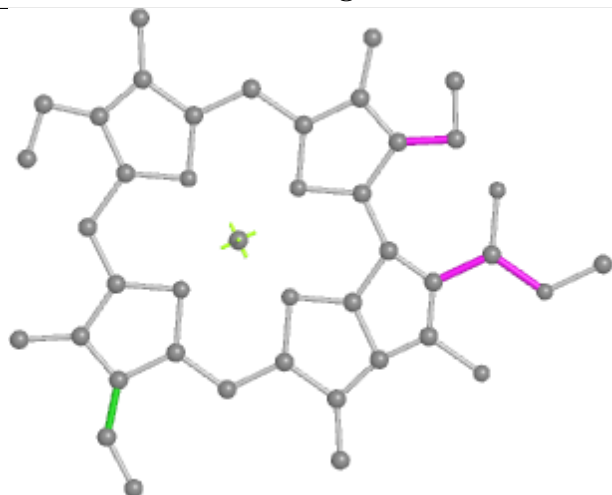
## Ligand CLA 1 309



Bond lengths



Bond angles

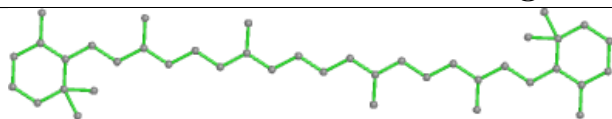


Torsions

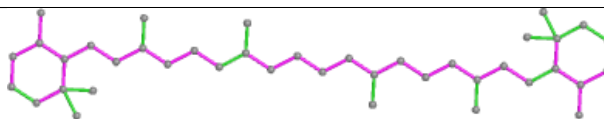


Rings

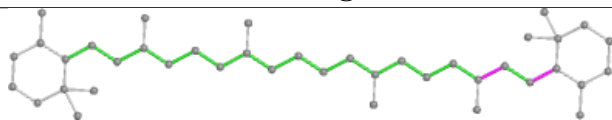
## Ligand BCR i 102



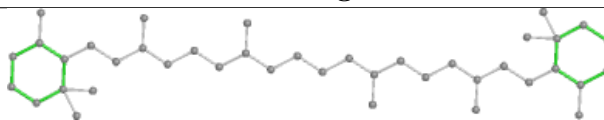
Bond lengths



Bond angles

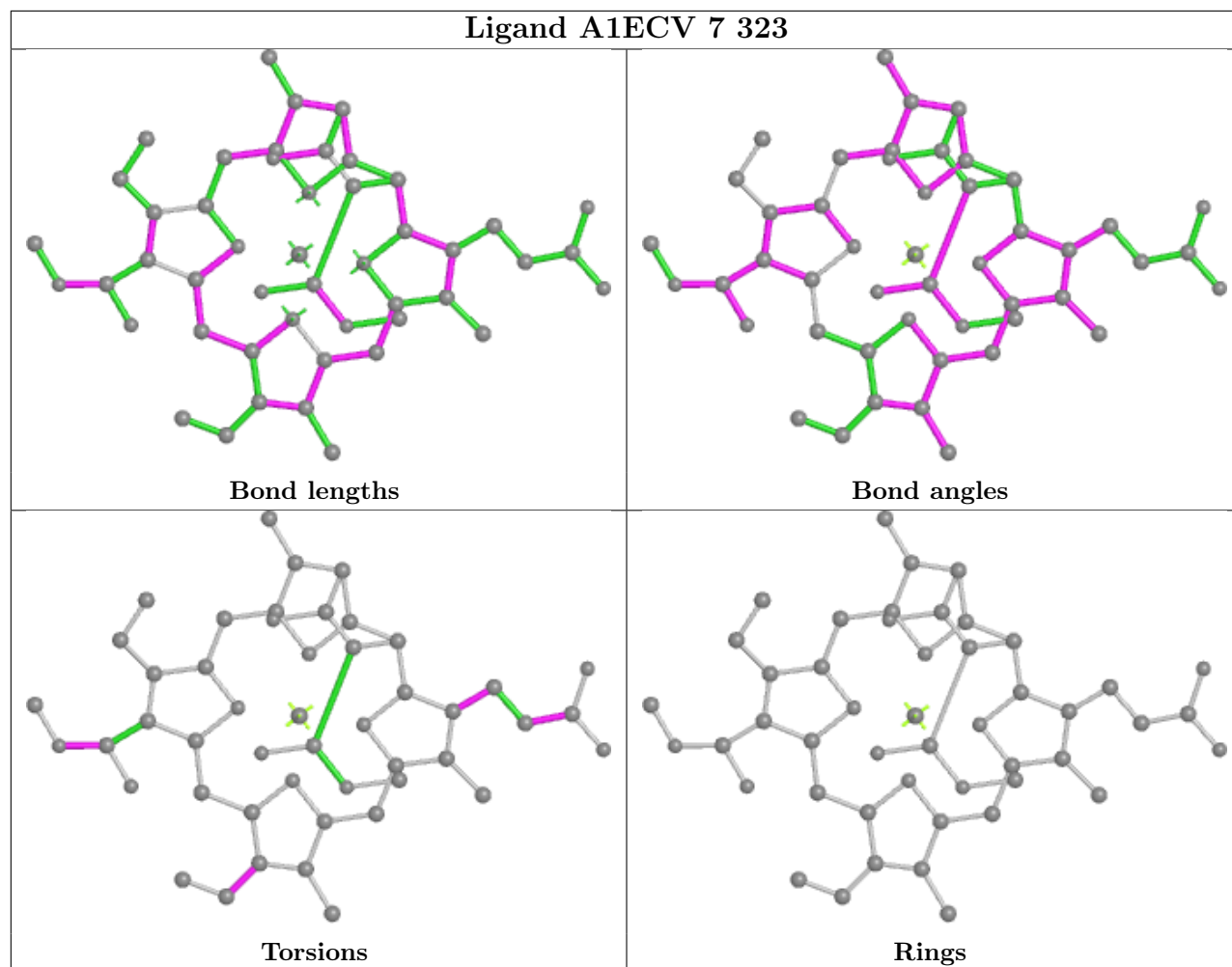


Torsions

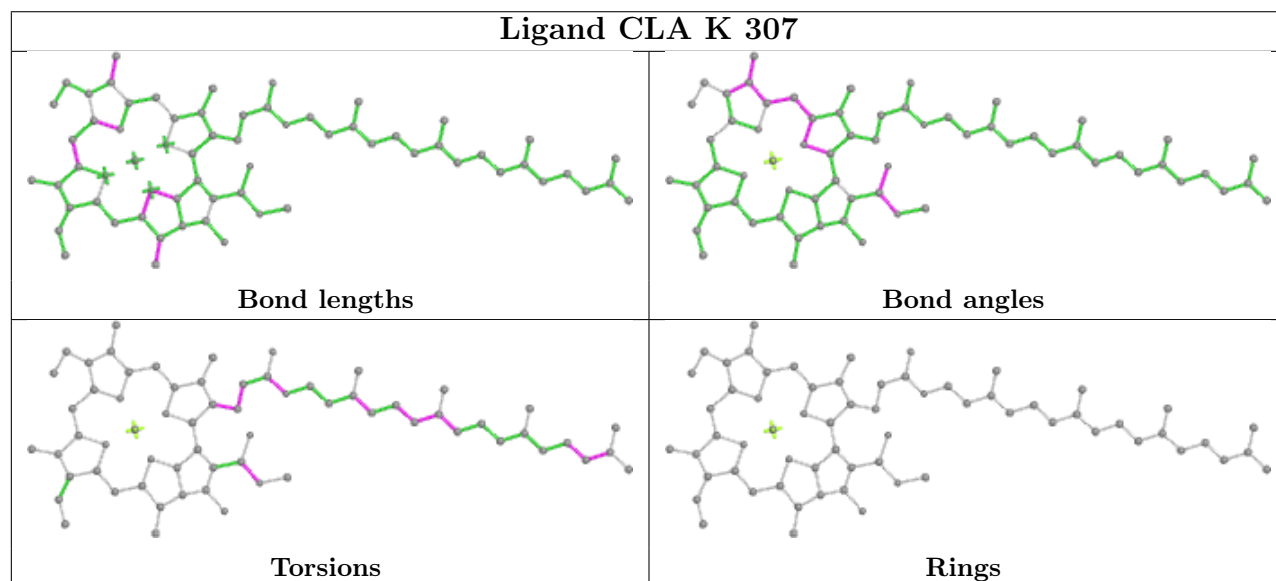


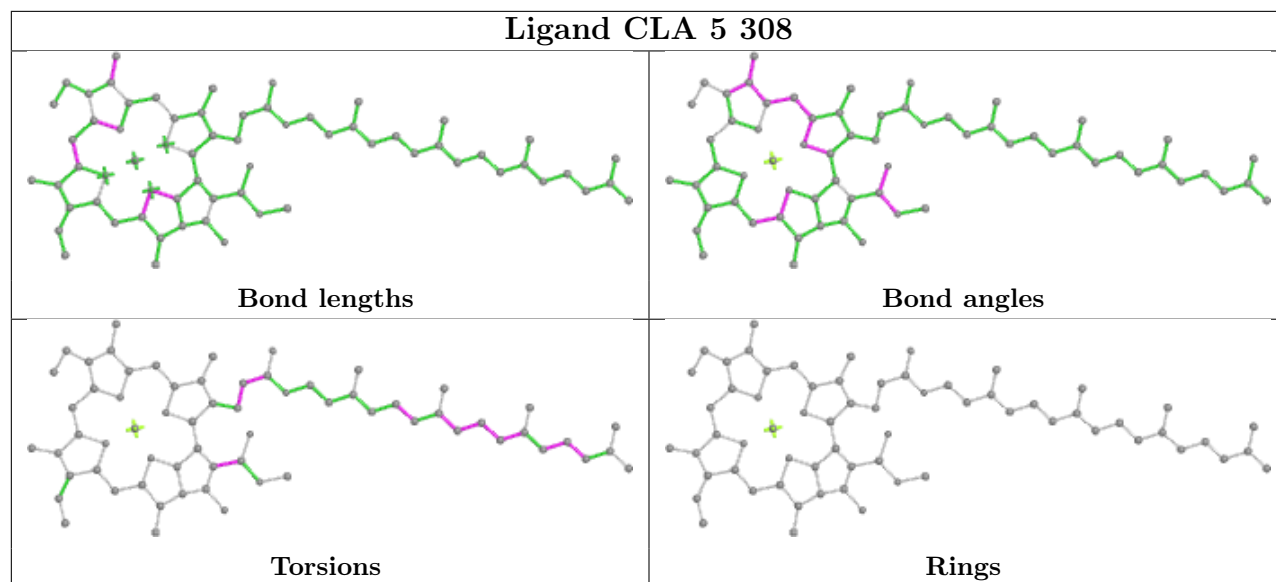
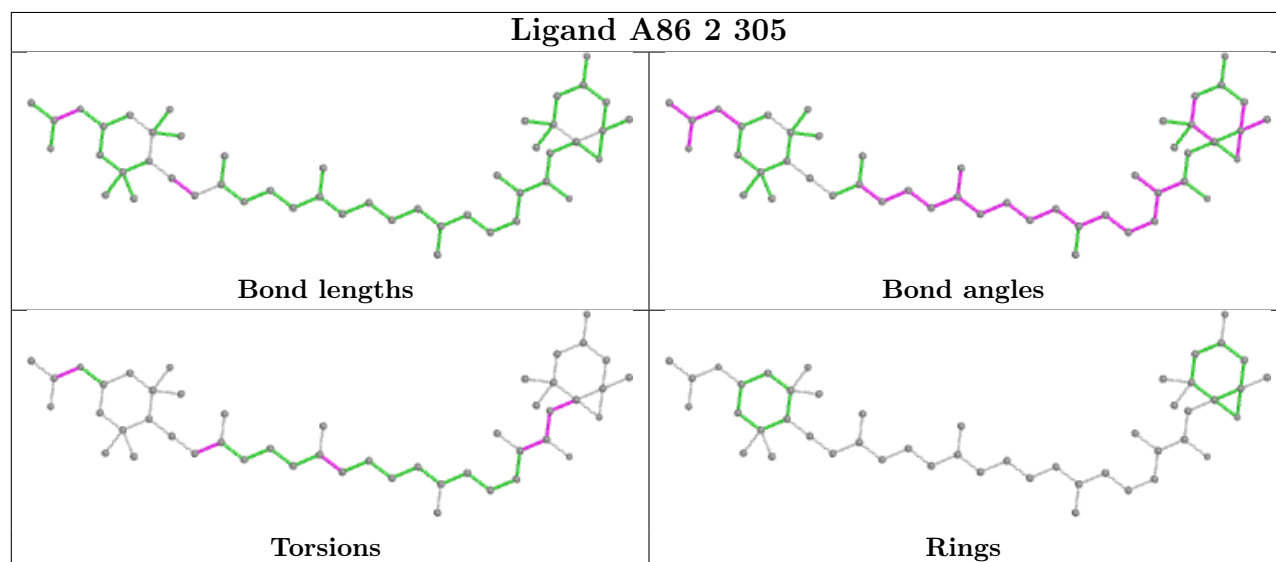
Rings

## Ligand A1ECV 7 323

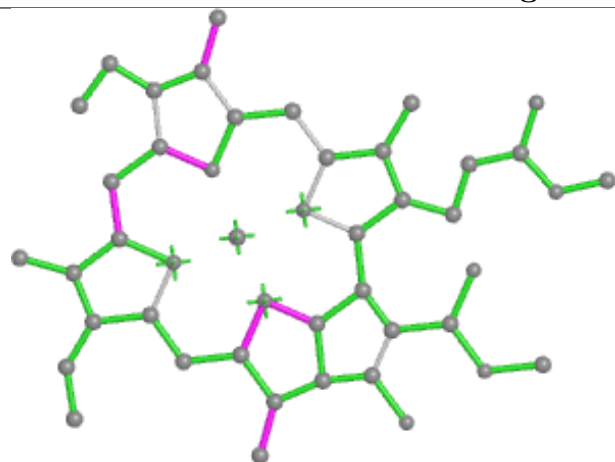


## Ligand CLA K 307

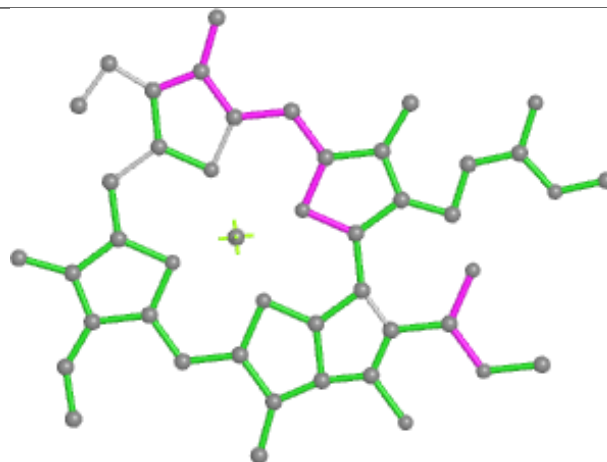


**Ligand CLA 5 308****Ligand A86 2 305**

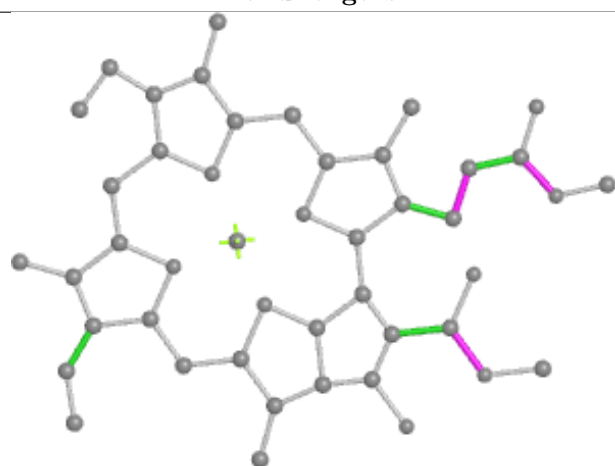
## Ligand CLA J 316



Bond lengths



Bond angles



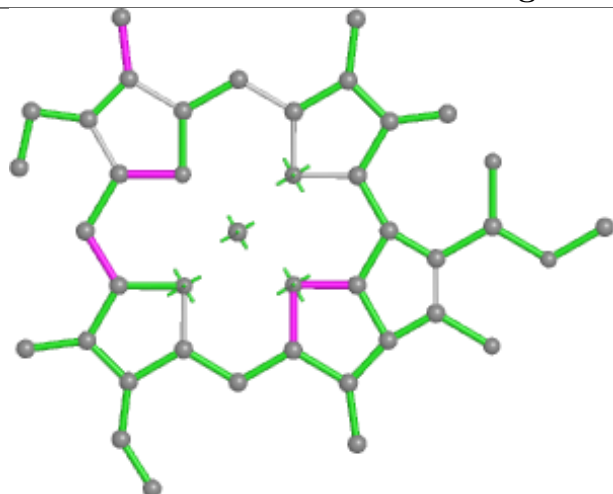
Torsions



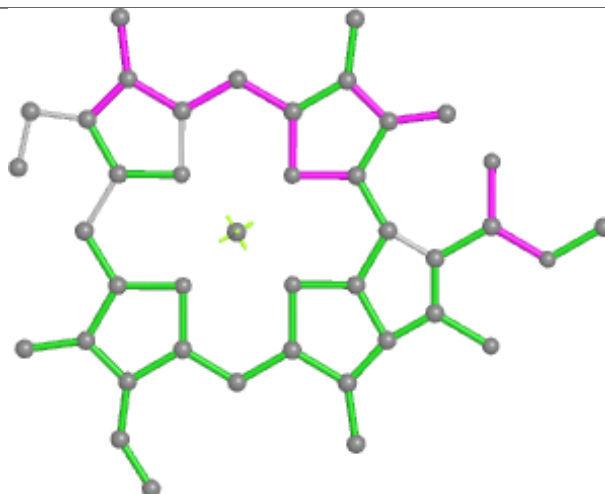
Rings



## Ligand CLA 1 316



Bond lengths



Bond angles

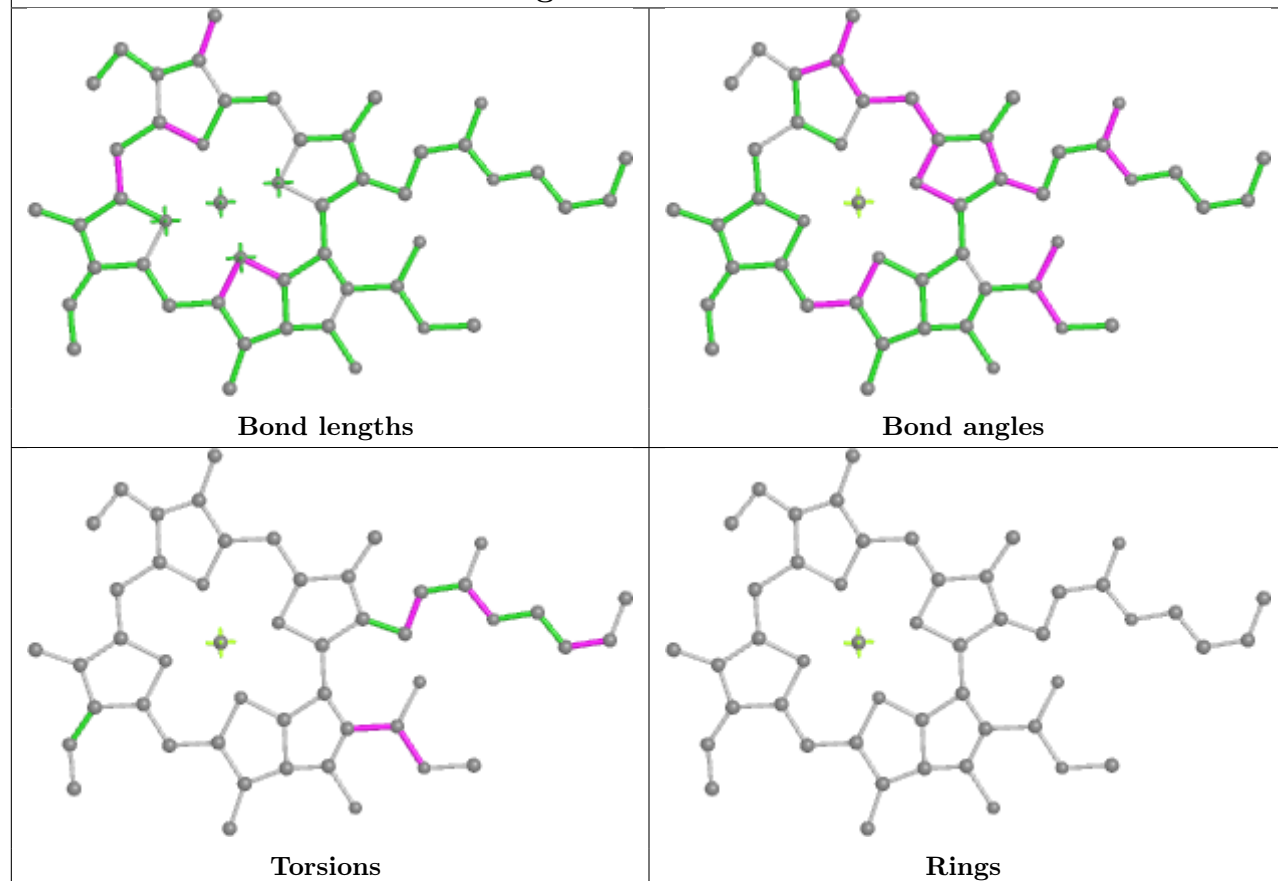


Torsions

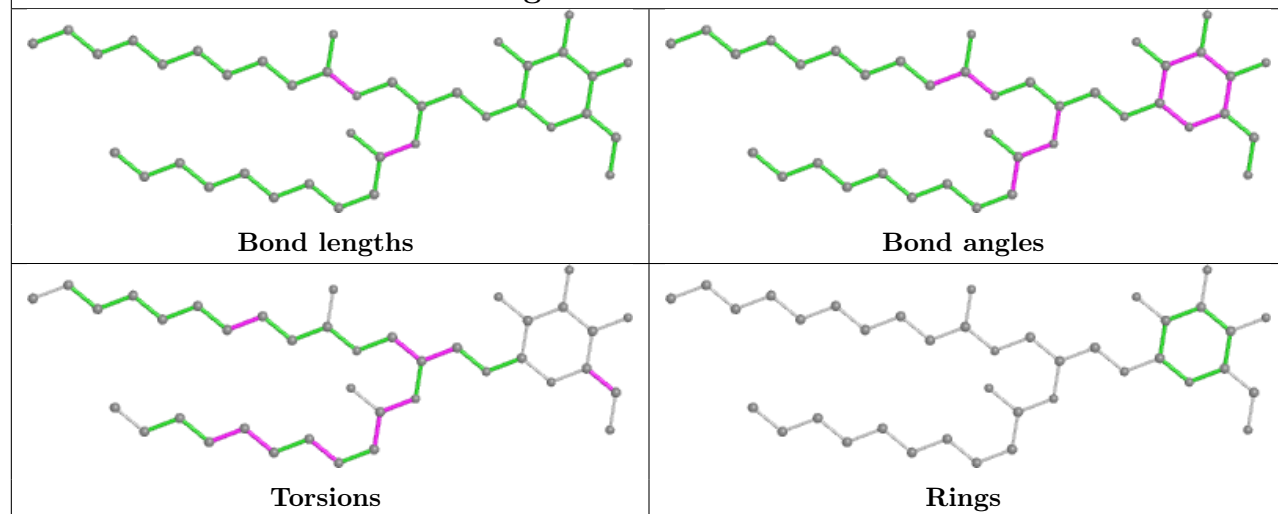


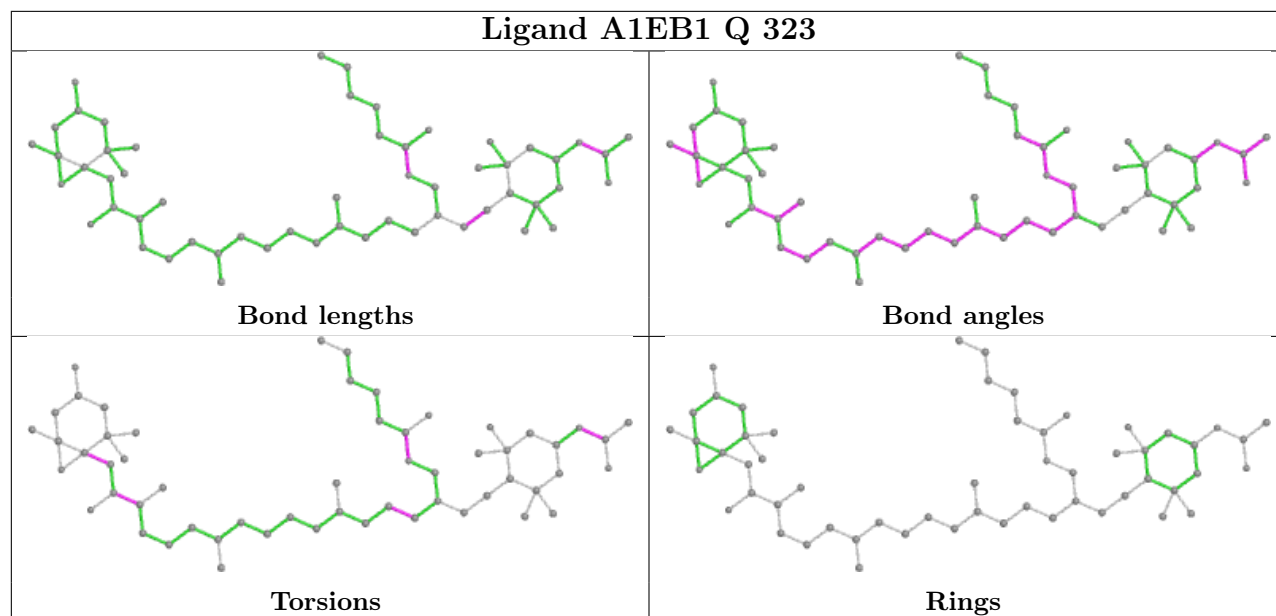
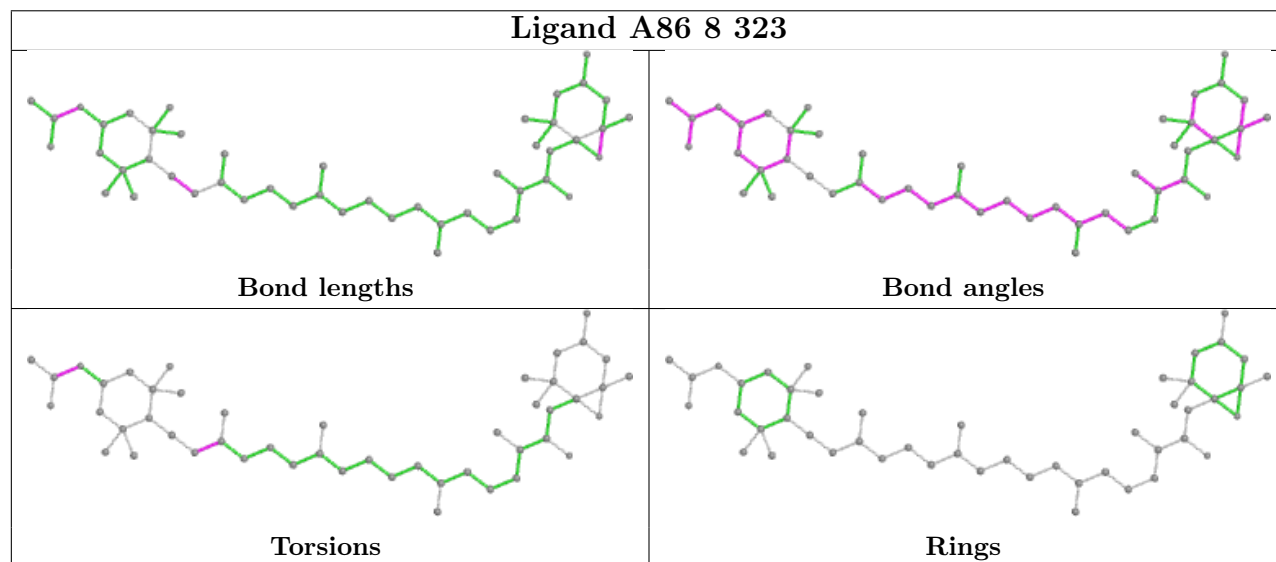
Rings

## Ligand CLA a 819

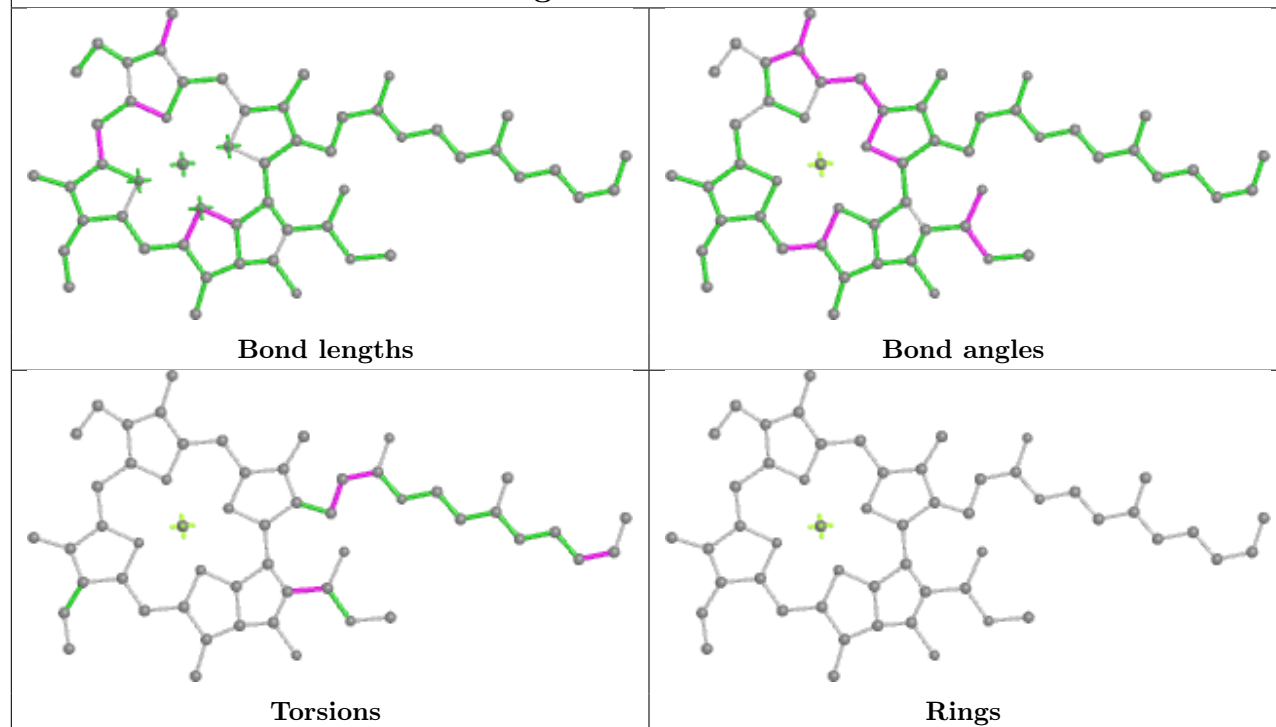


## Ligand LMG M 319

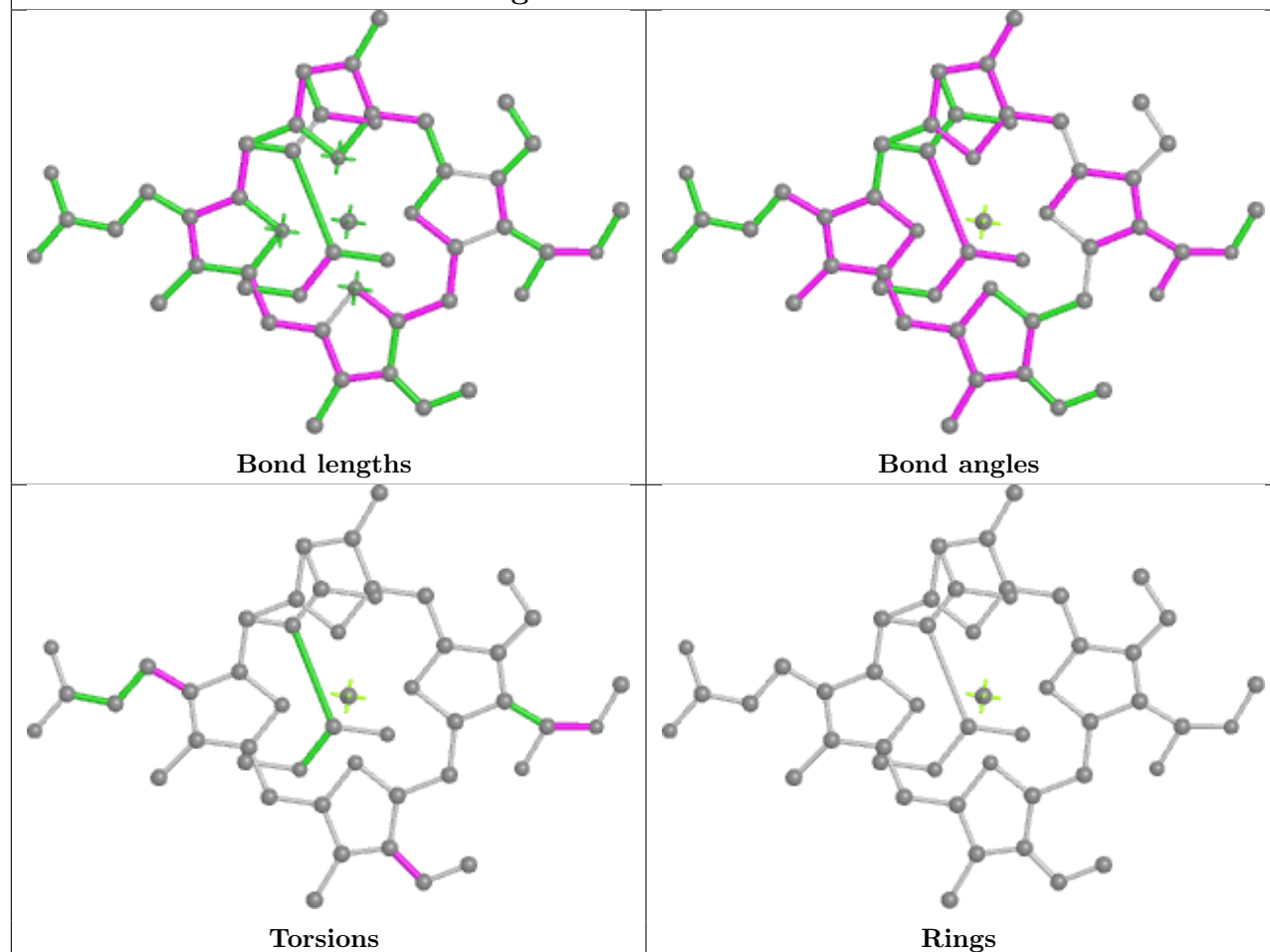


**Ligand A1EB1 Q 323****Ligand A86 8 323**

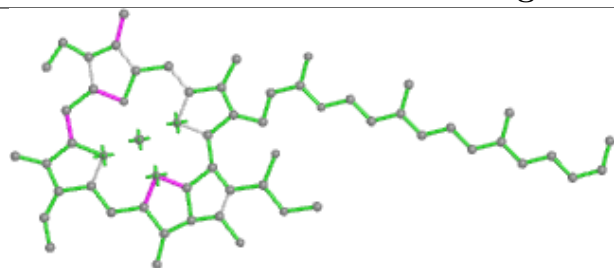
## Ligand CLA F 310



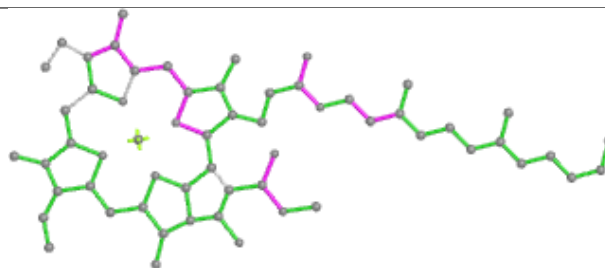
## Ligand A1ECV z 316



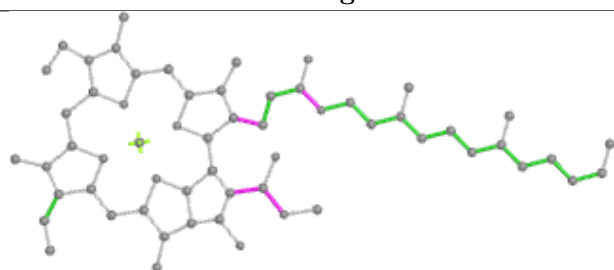
## Ligand CLA b 817



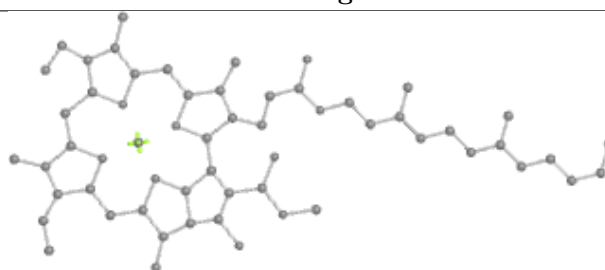
Bond lengths



Bond angles

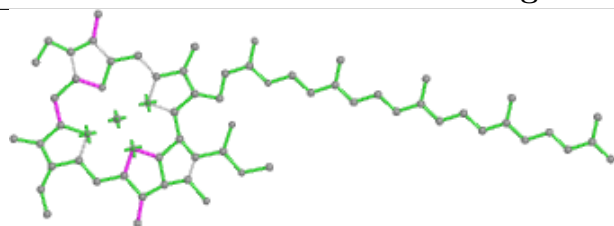


Torsions

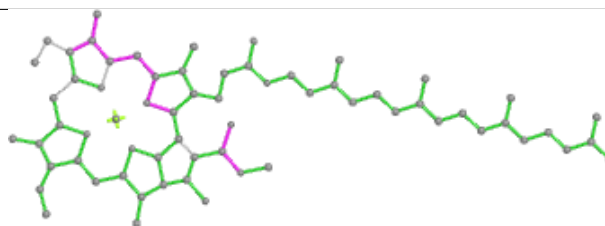


Rings

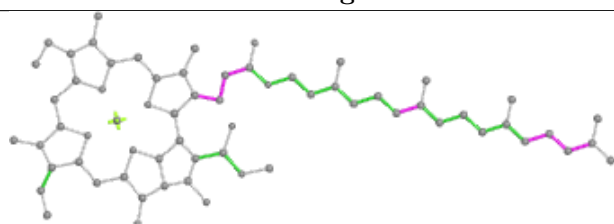
## Ligand CLA I 309



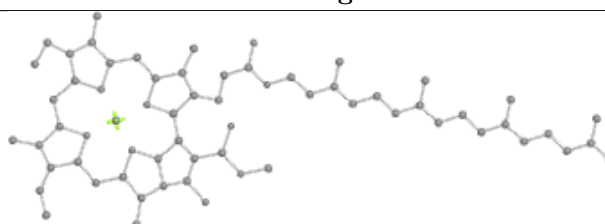
Bond lengths



Bond angles

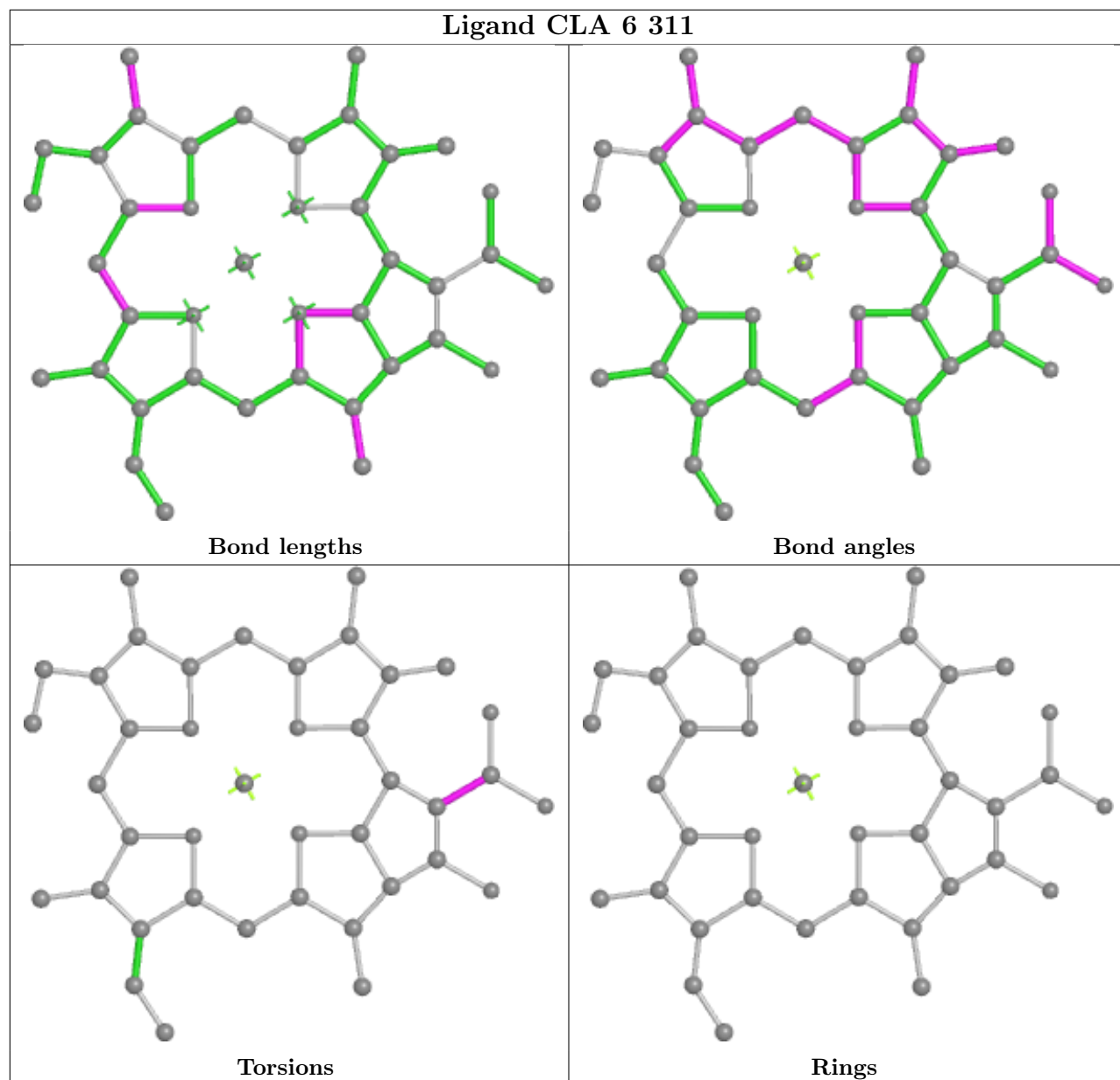


Torsions

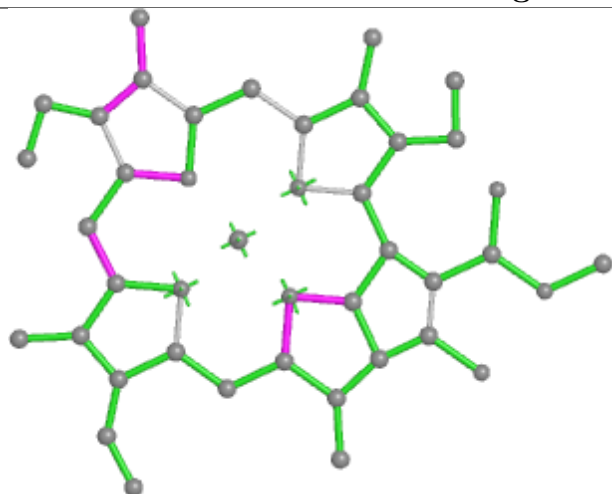


Rings

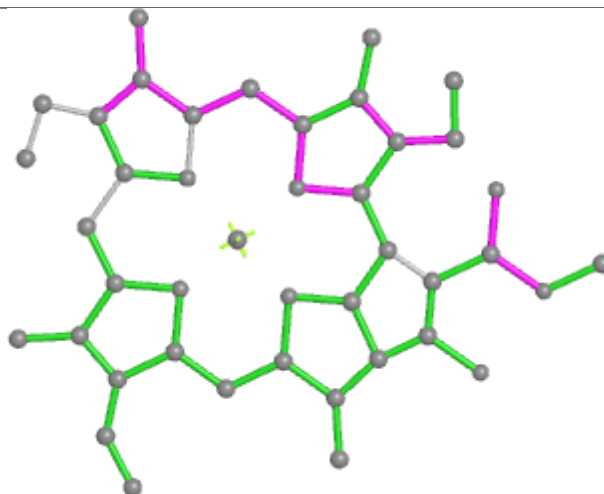
## Ligand CLA 6 311



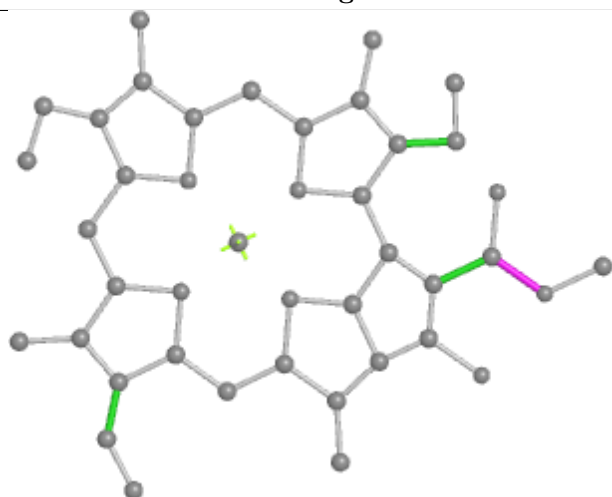
## Ligand CLA O 311



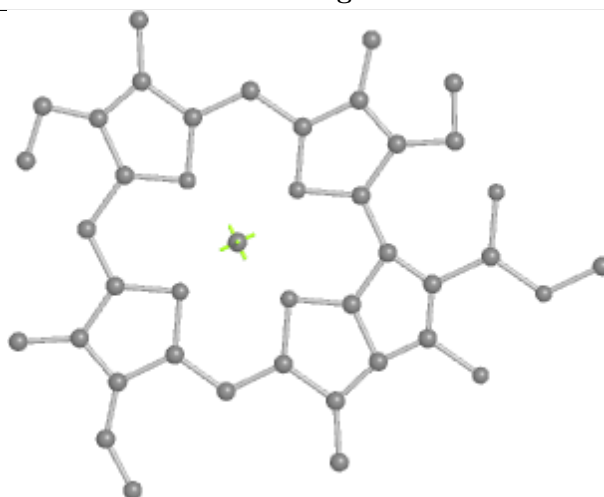
Bond lengths



Bond angles

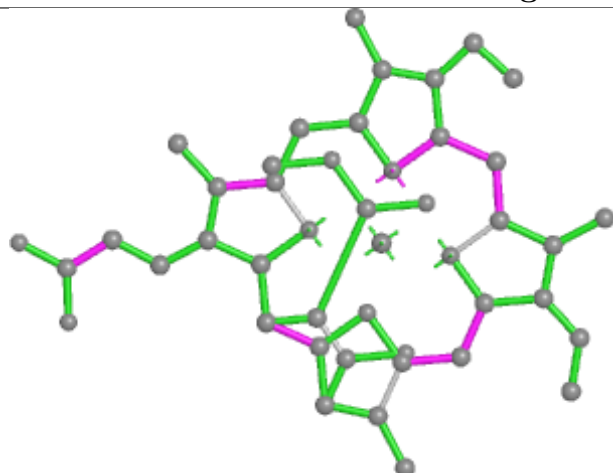


Torsions

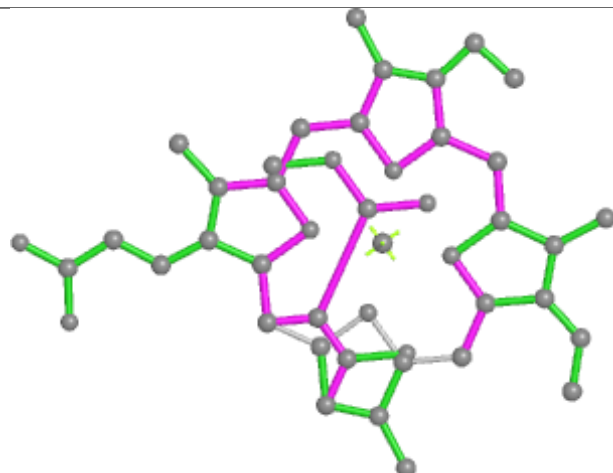


Rings

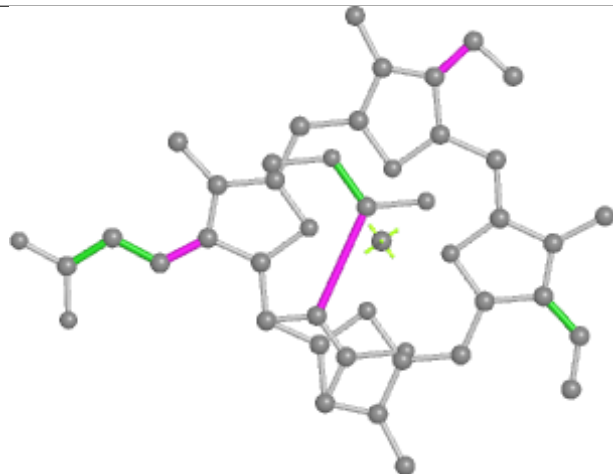
## Ligand KC2 4 317



Bond lengths



Bond angles

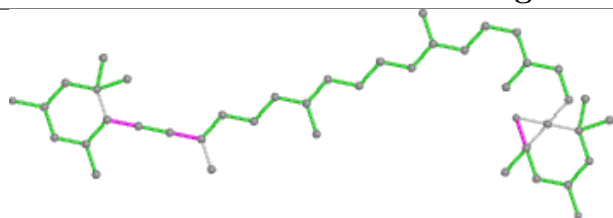


Torsions

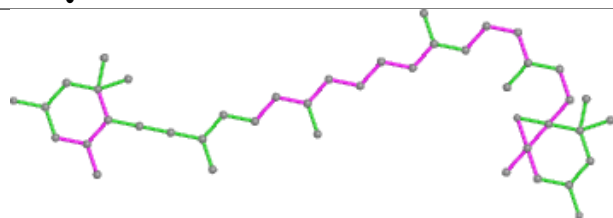


Rings

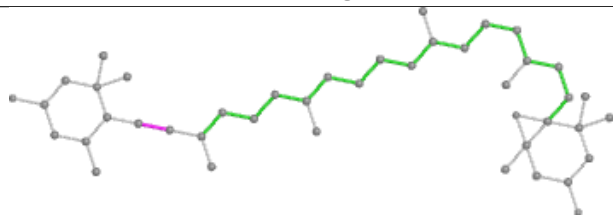
## Ligand DD6 Q 306



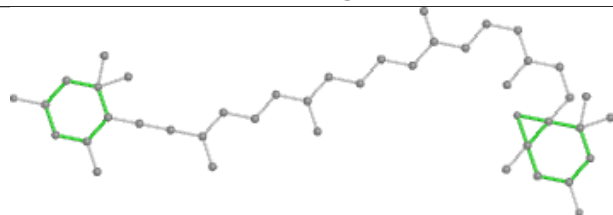
Bond lengths



Bond angles



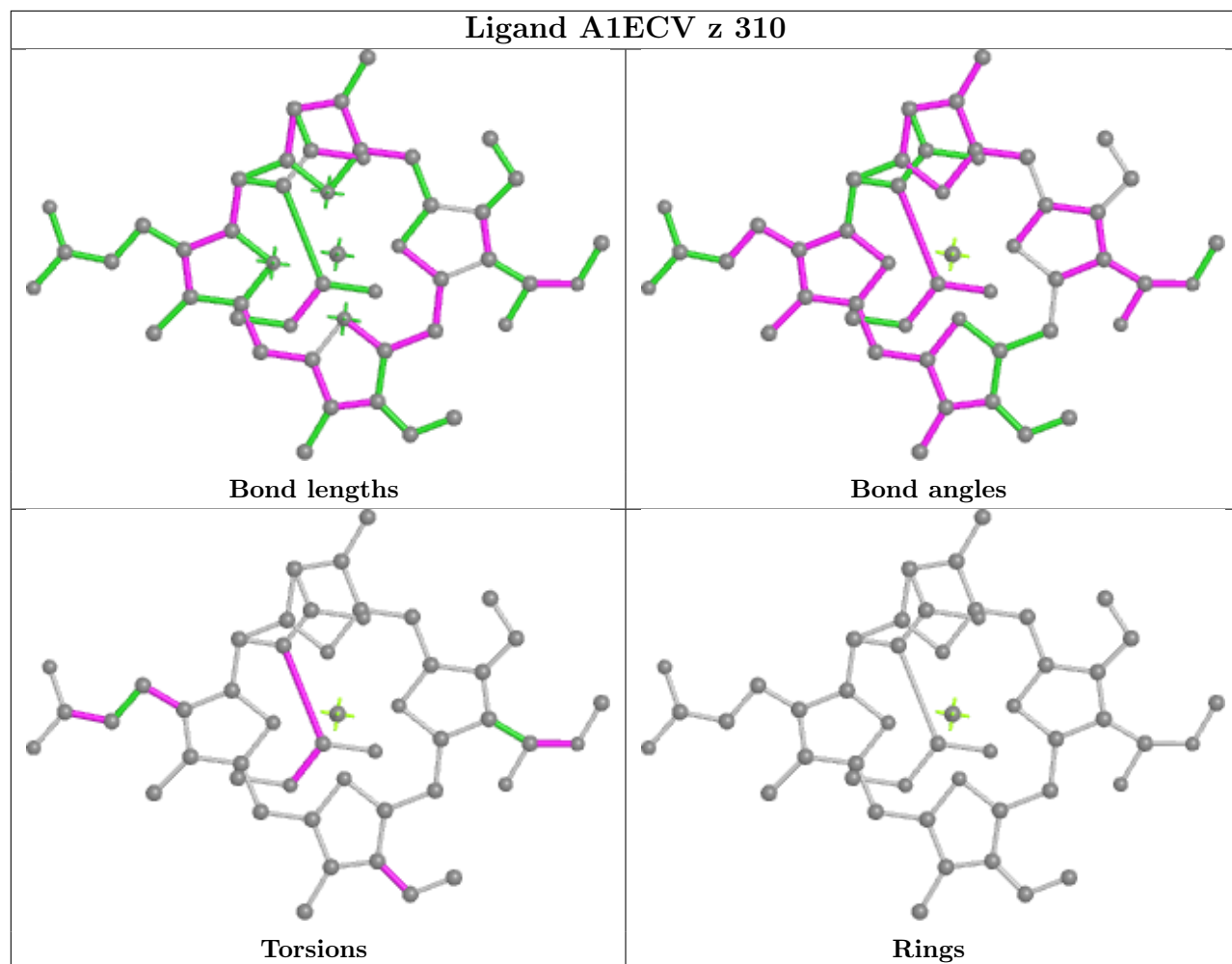
Torsions



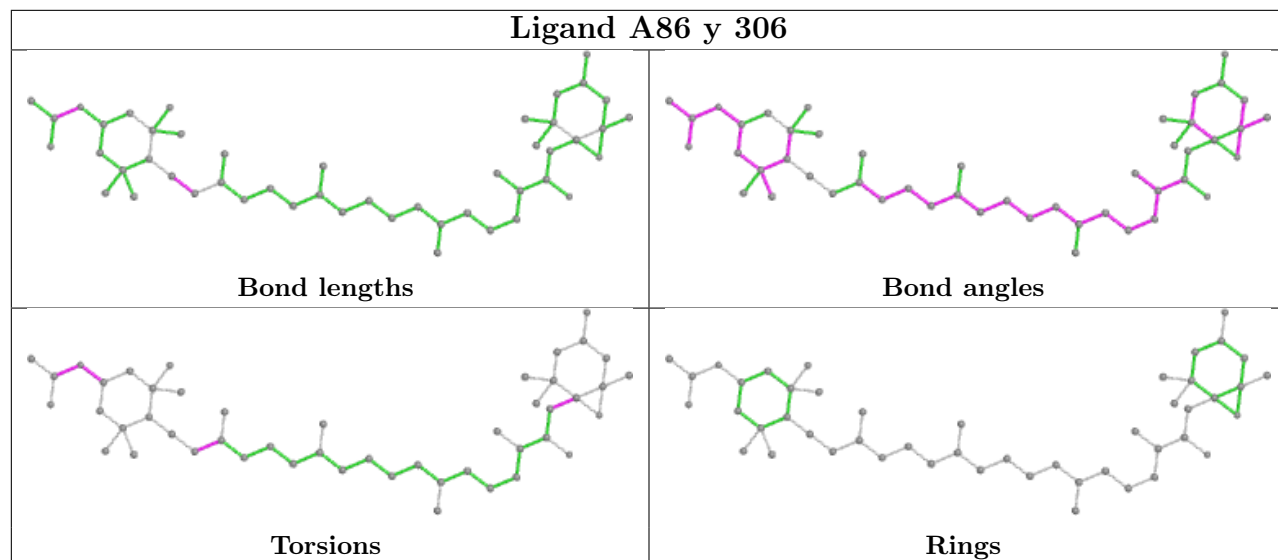
Rings



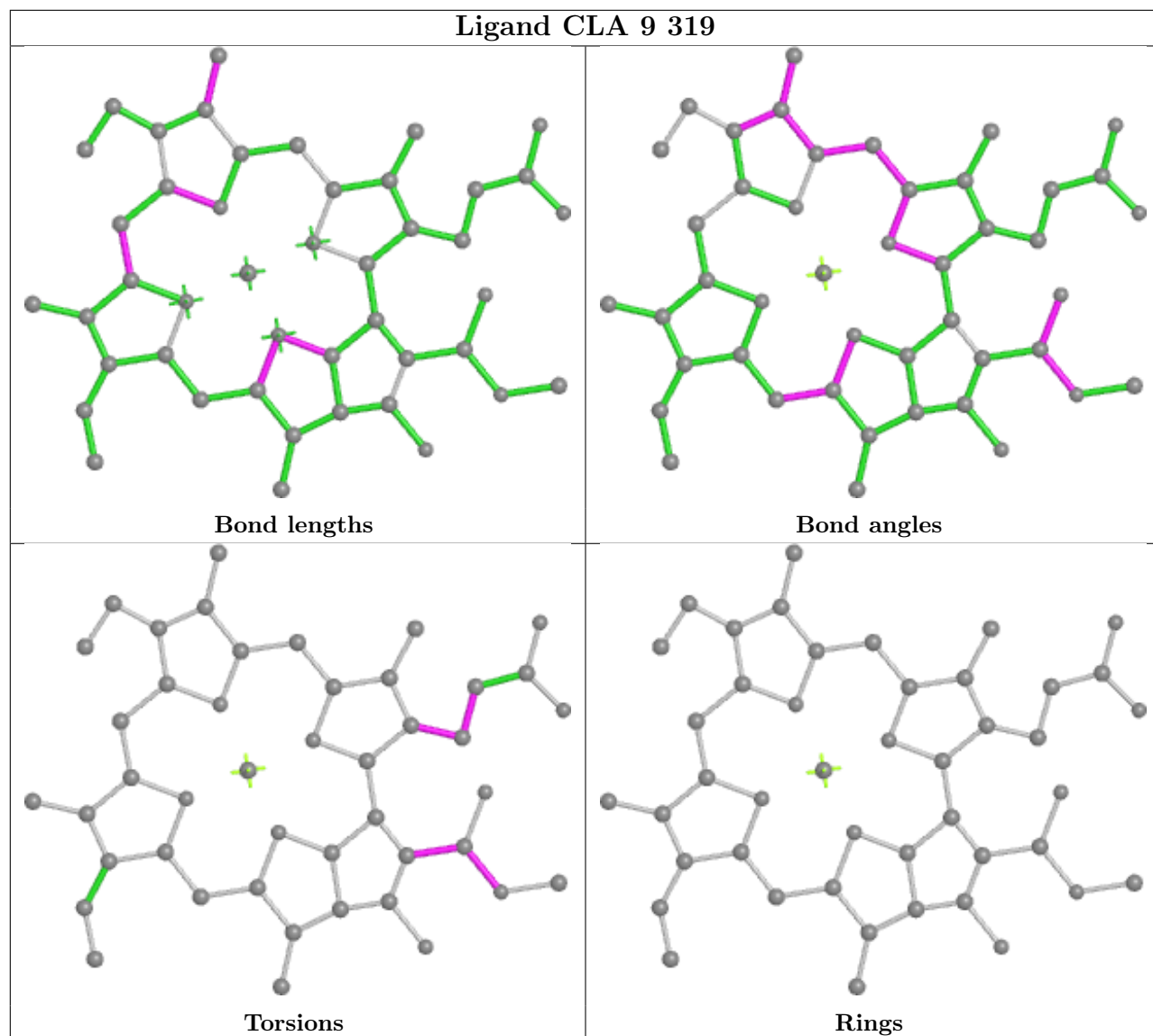
## Ligand A1ECV z 310



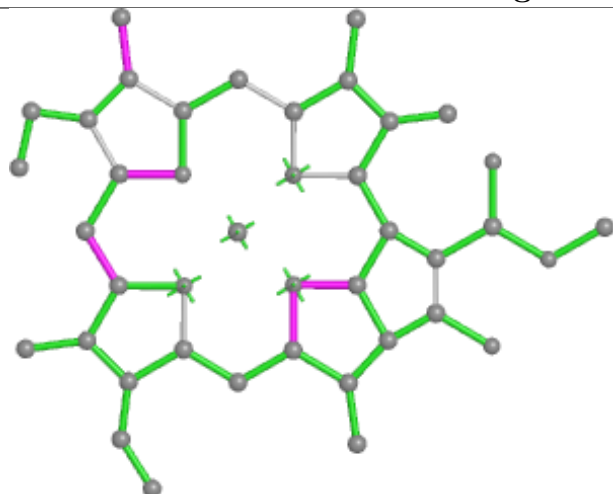
## Ligand A86 y 306



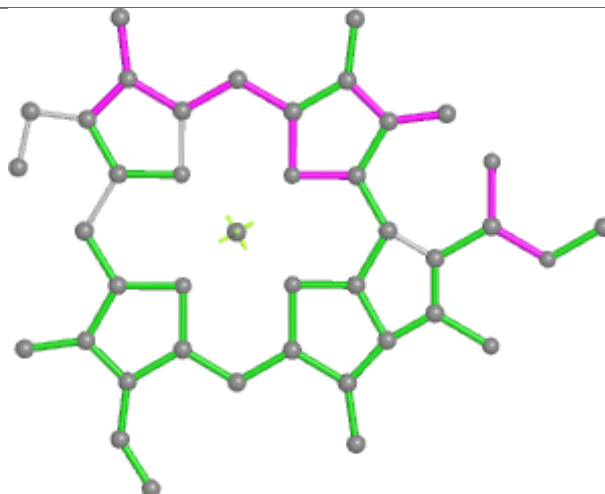
## Ligand CLA 9 319



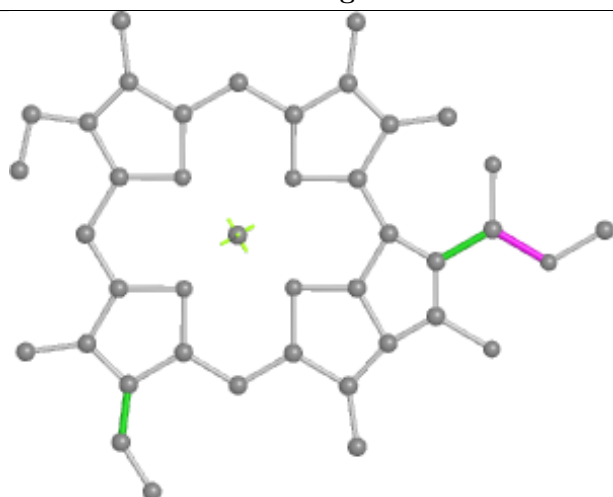
## Ligand CLA Y 302



Bond lengths



Bond angles

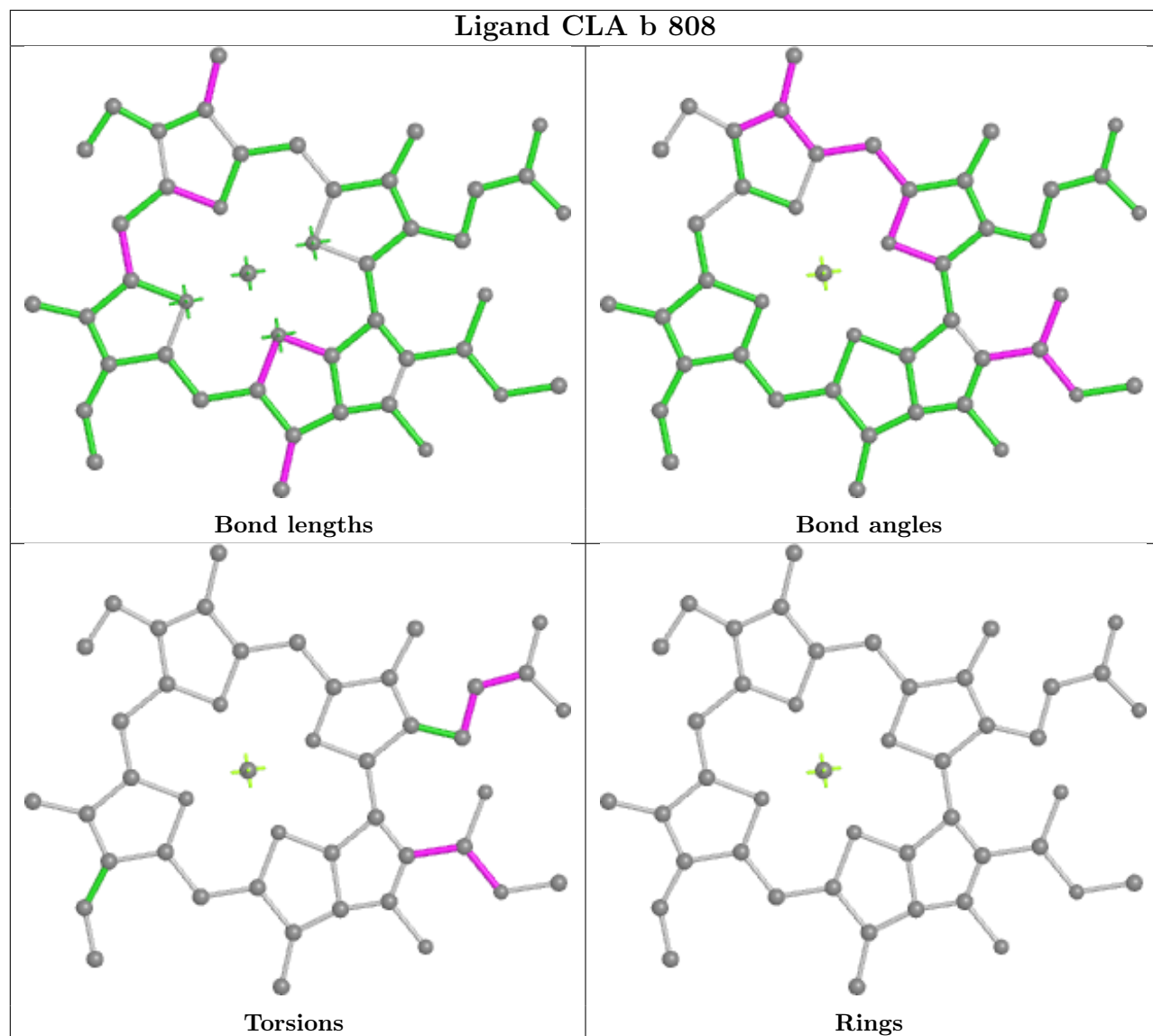


Torsions

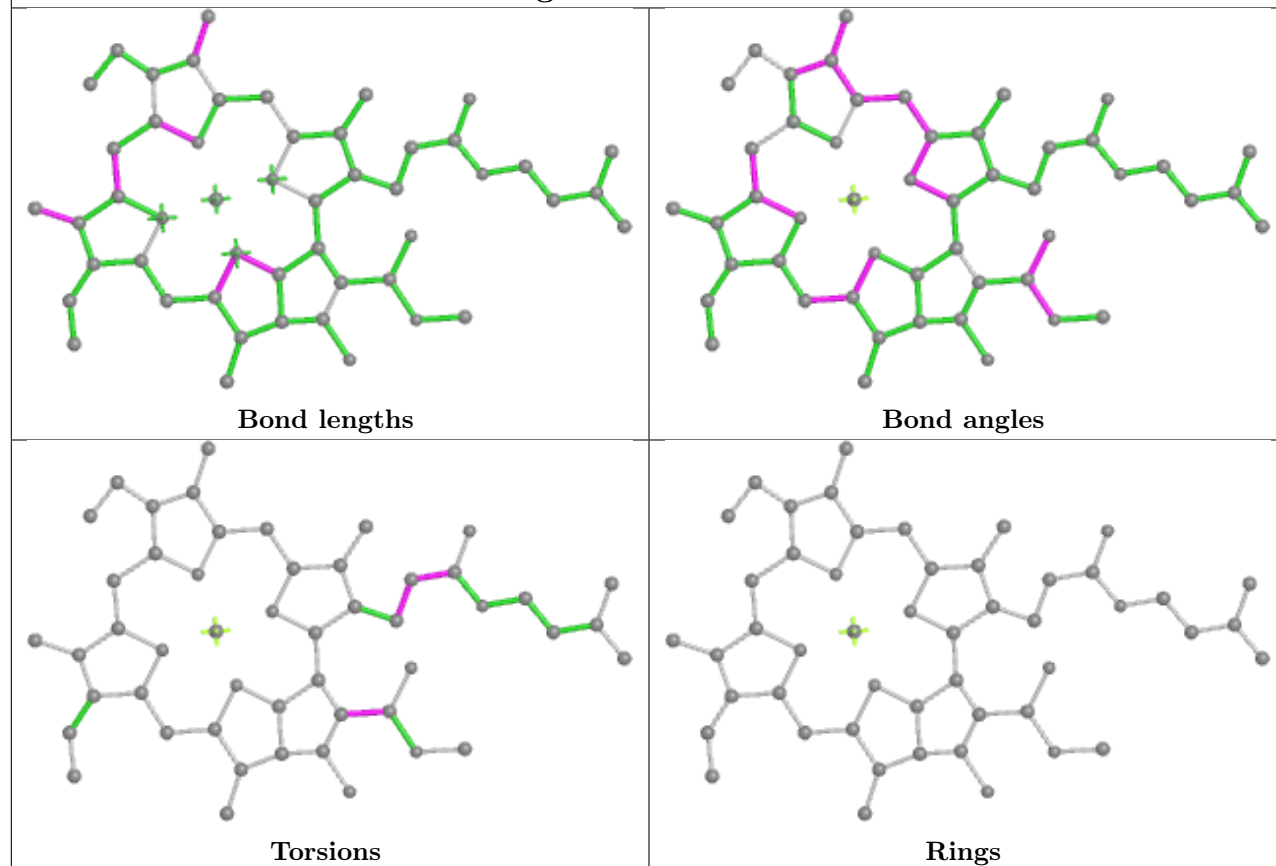


Rings

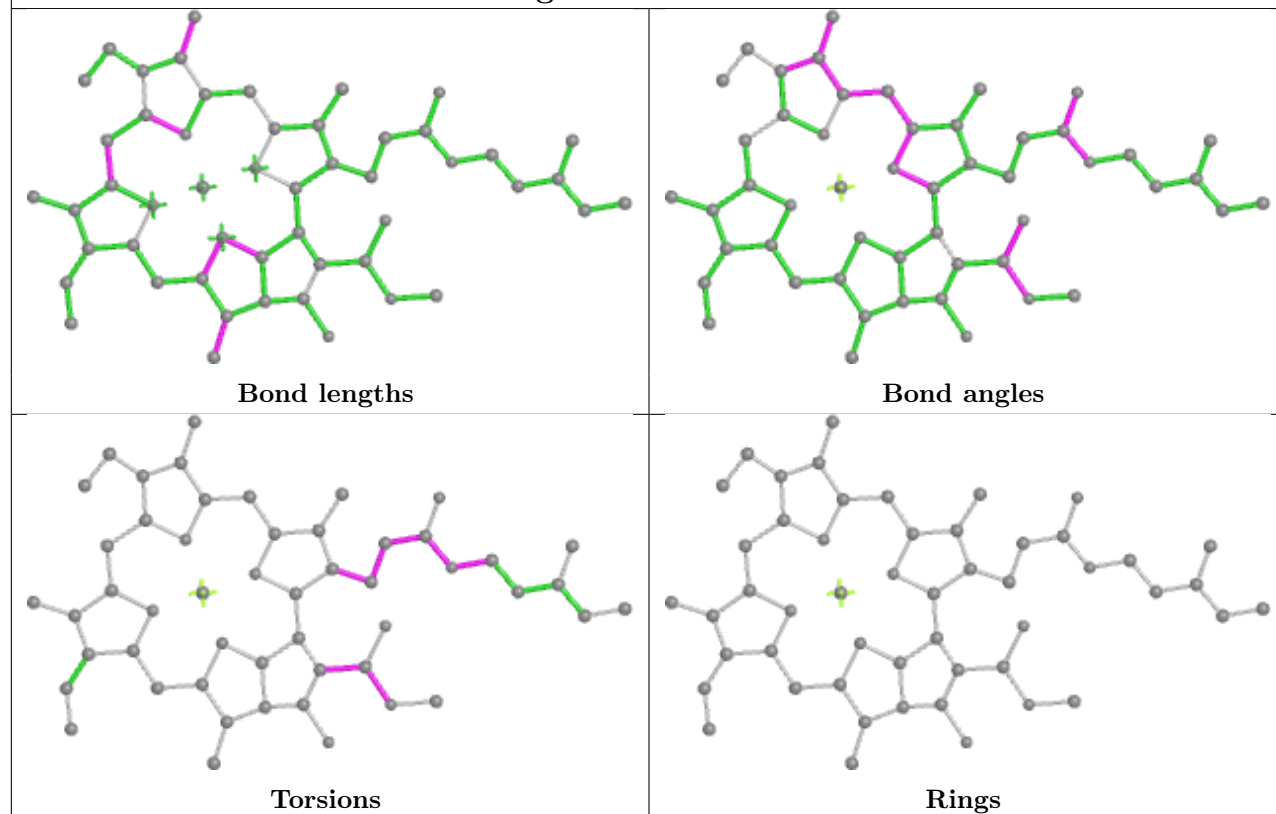
## Ligand CLA b 808



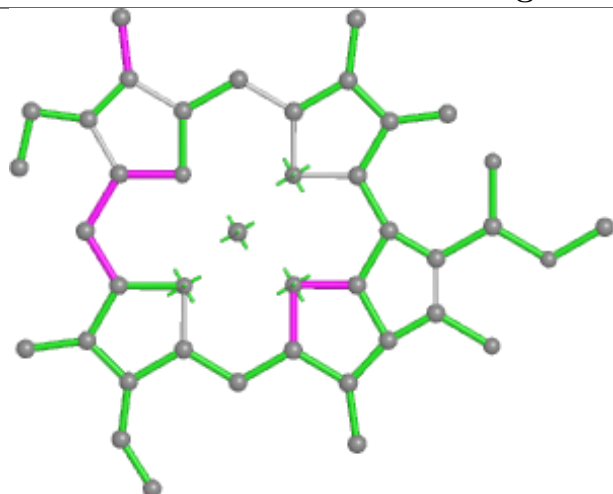
## Ligand CLA a 813



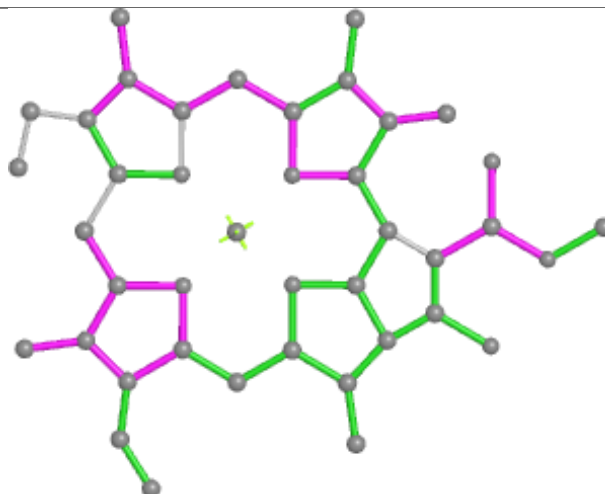
## Ligand CLA 1 319



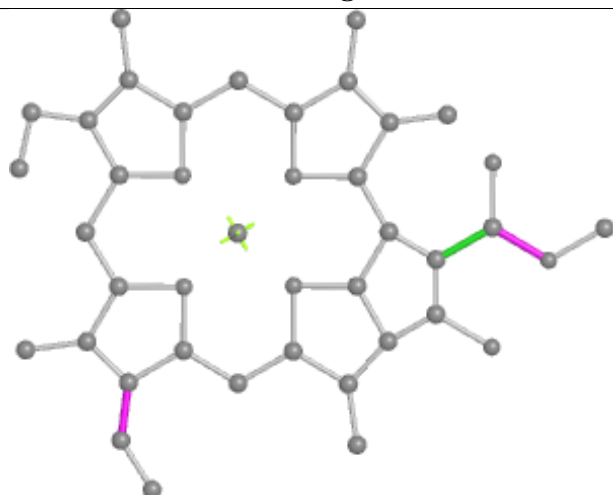
## Ligand CLA Z 313



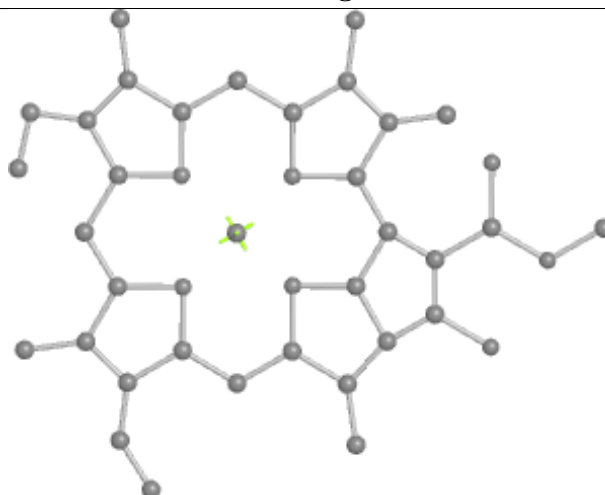
Bond lengths



Bond angles

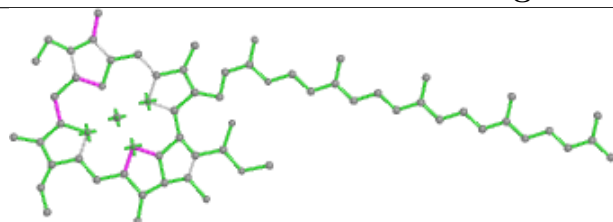


Torsions

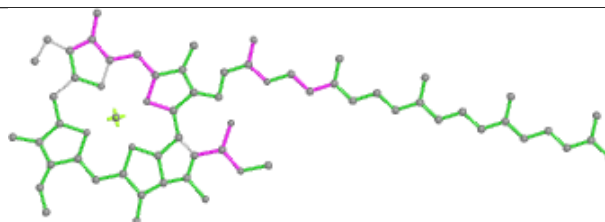


Rings

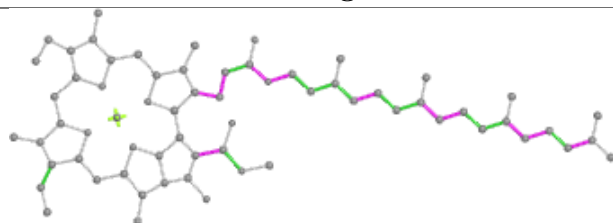
## Ligand CLA A 314



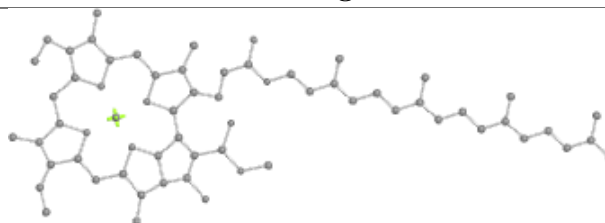
Bond lengths



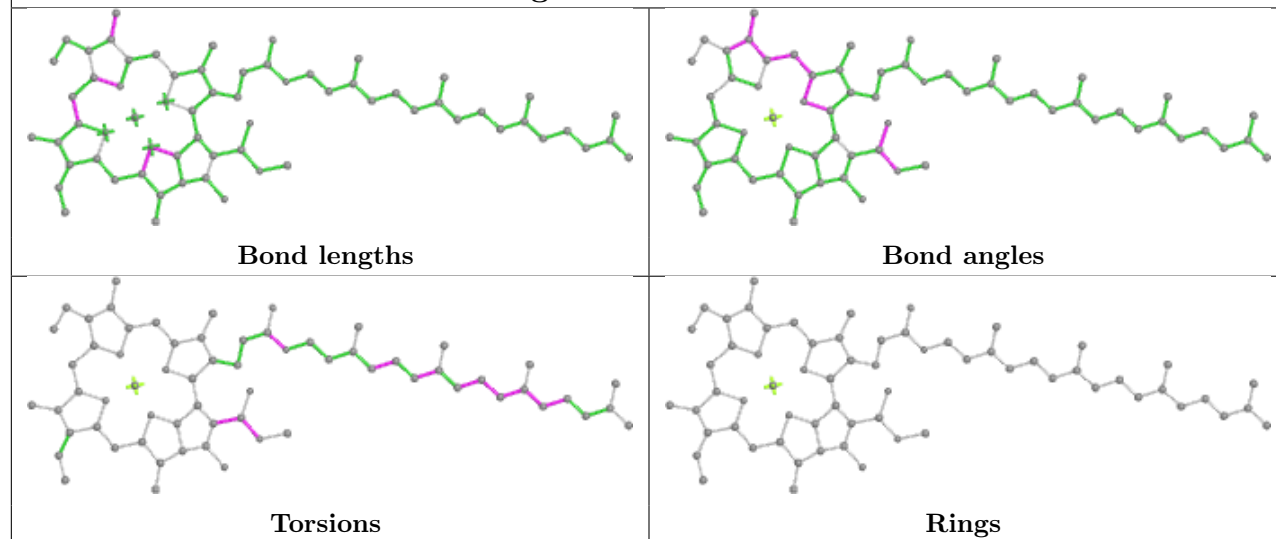
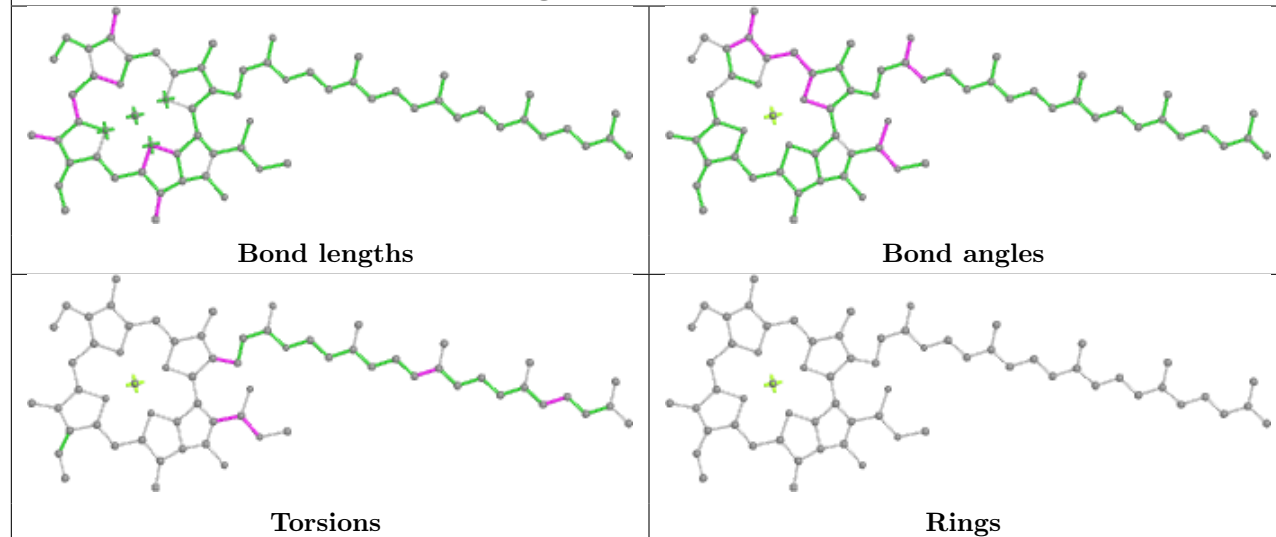
Bond angles



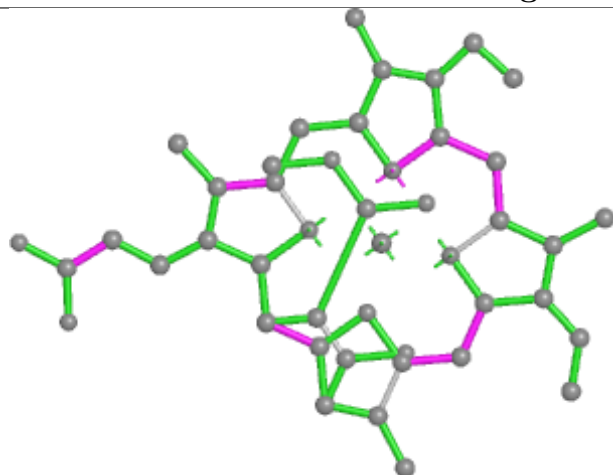
Torsions



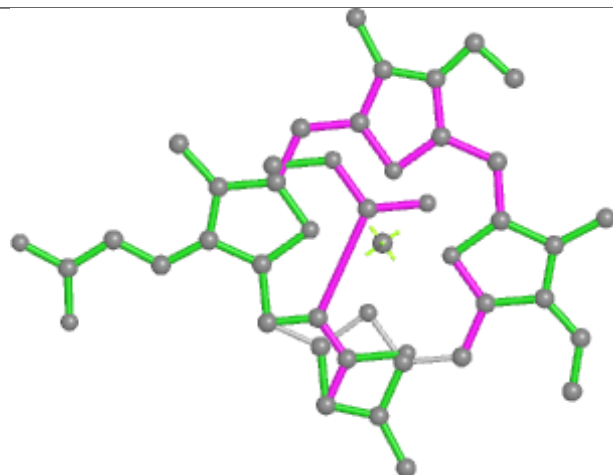
Rings

**Ligand CLA K 311****Ligand CLA b 826**

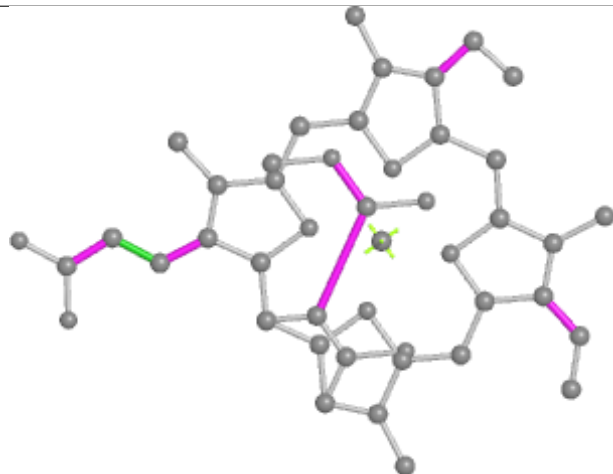
## Ligand KC2 9 318



Bond lengths



Bond angles



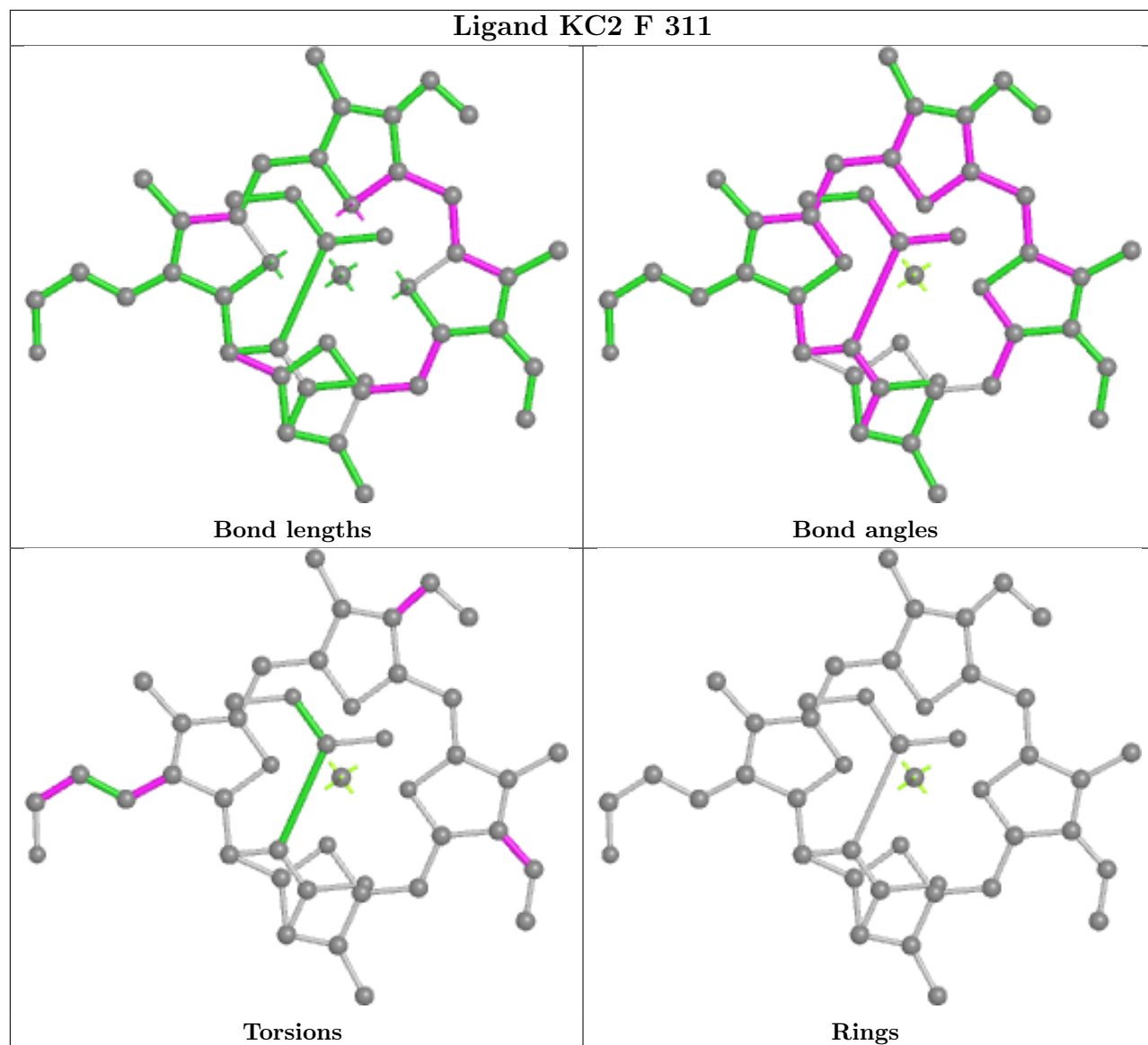
Torsions



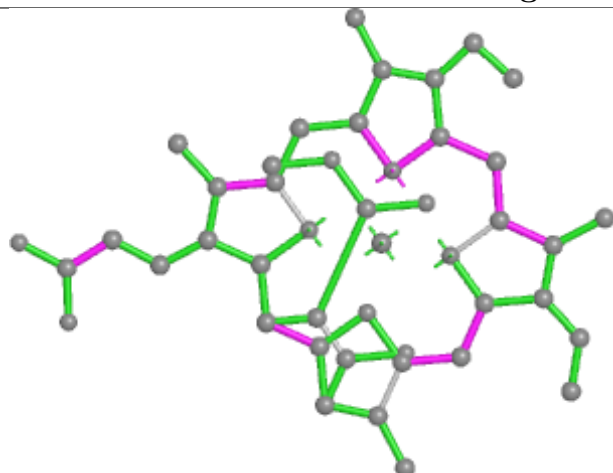
Rings



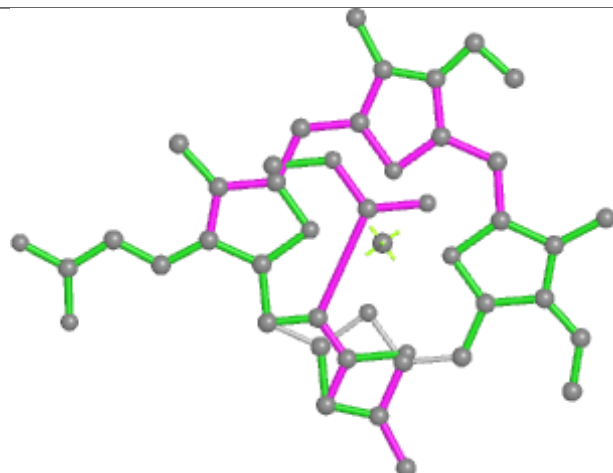
## Ligand KC2 F 311



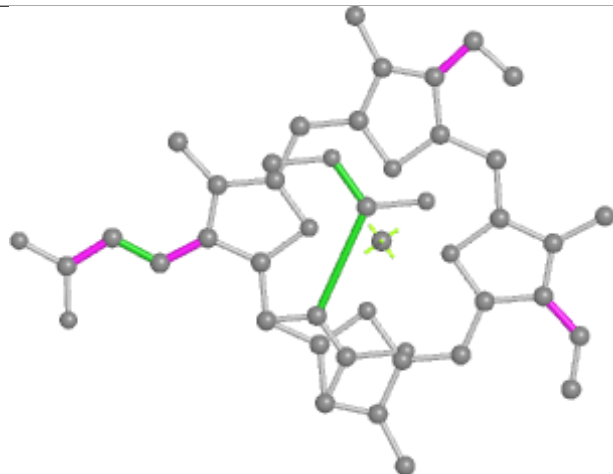
## Ligand KC2 1 312



Bond lengths



Bond angles

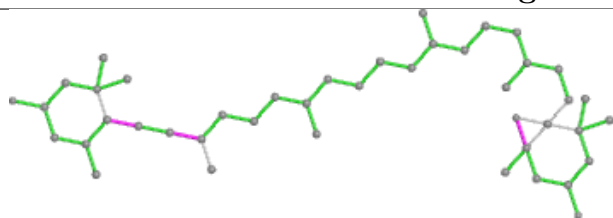


Torsions

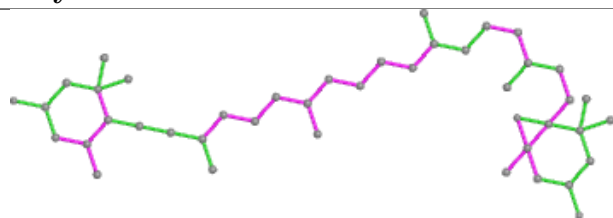


Rings

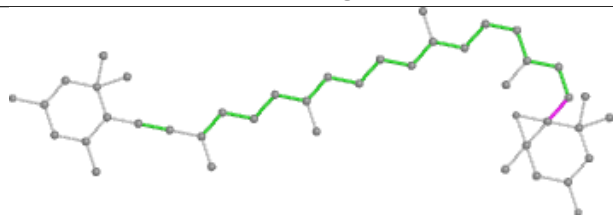
## Ligand DD6 y 303



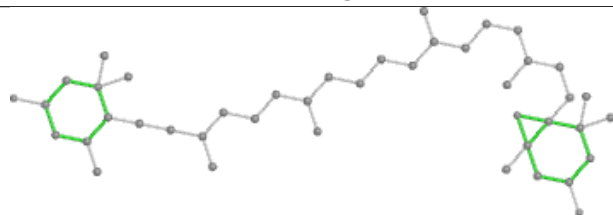
Bond lengths



Bond angles

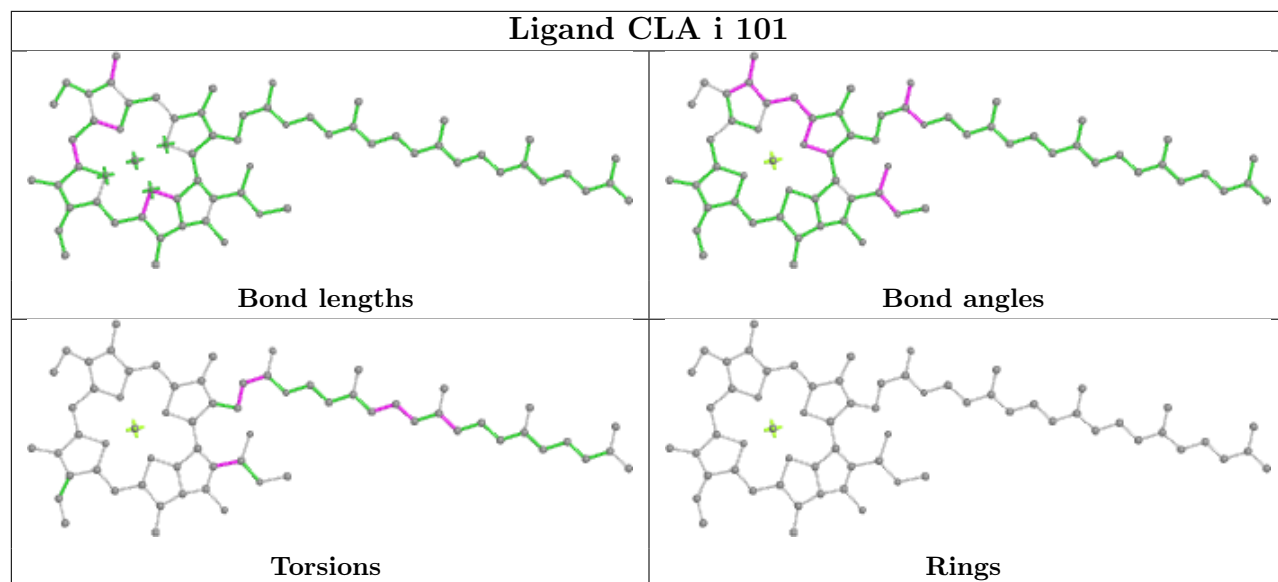


Torsions

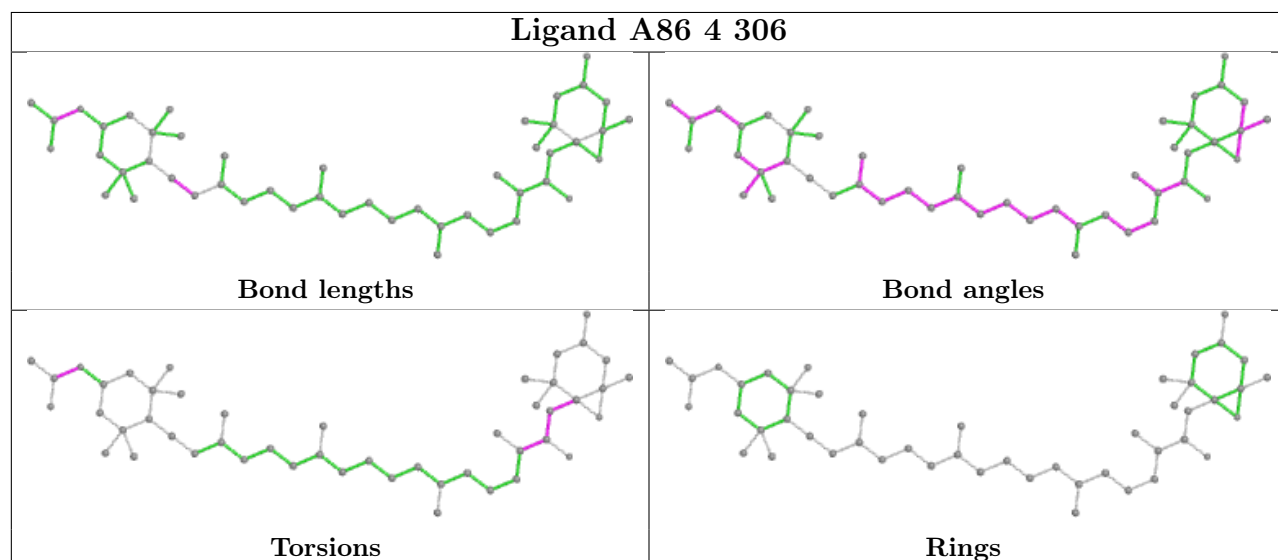


Rings

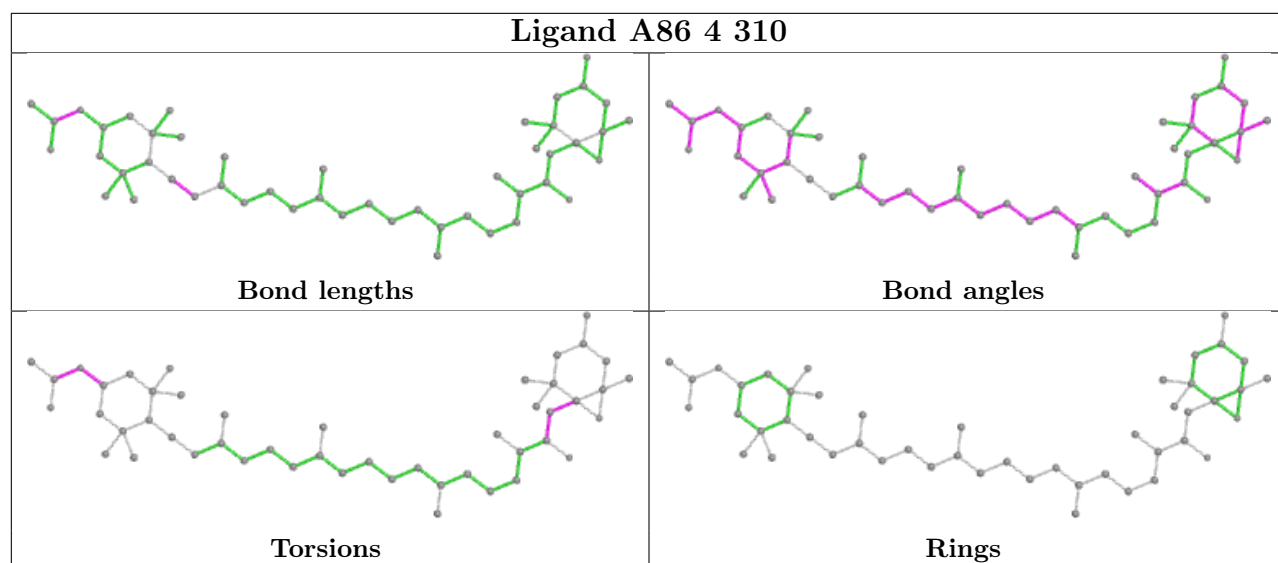
## Ligand CLA i 101



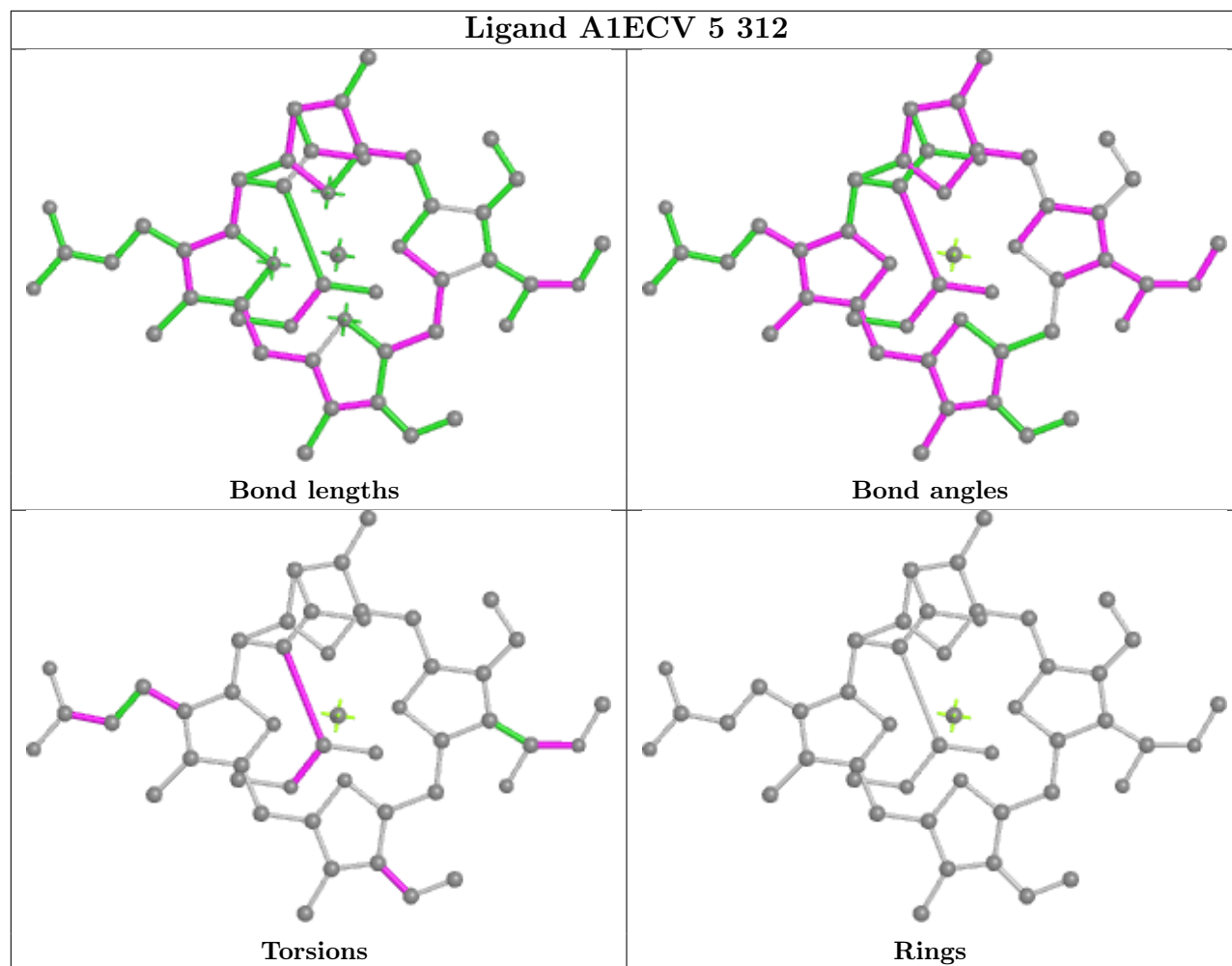
## Ligand A86 4 306



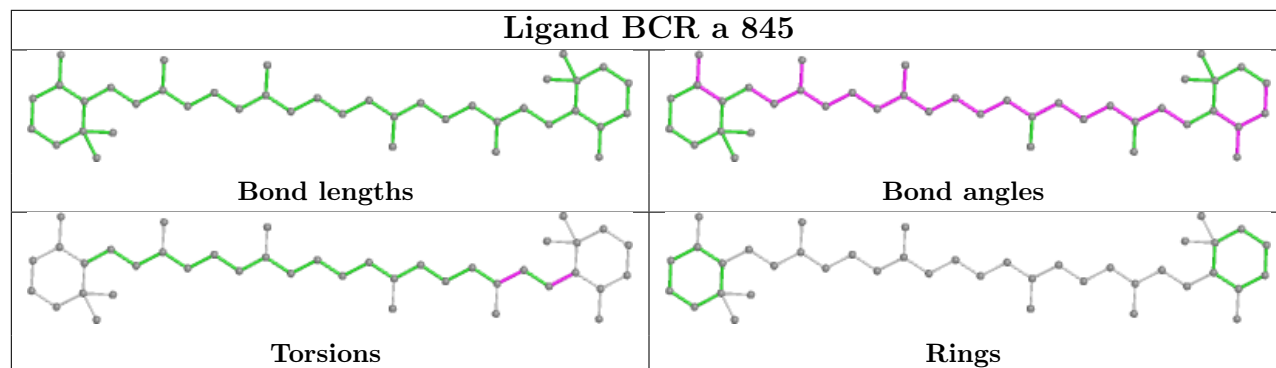
## Ligand A86 4 310



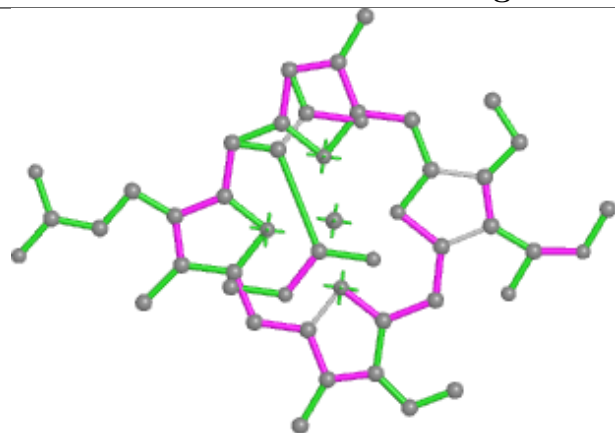
## Ligand A1ECV 5 312



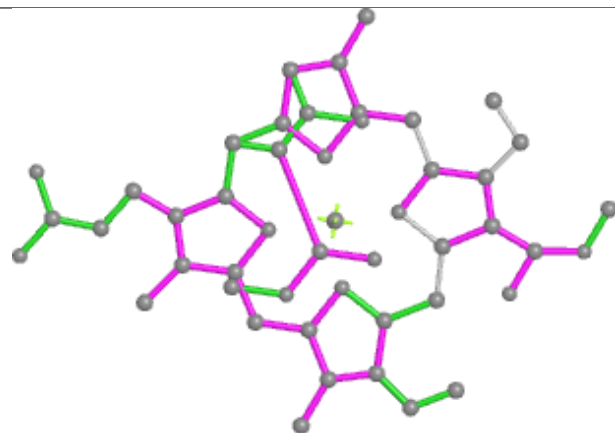
## Ligand BCR a 845



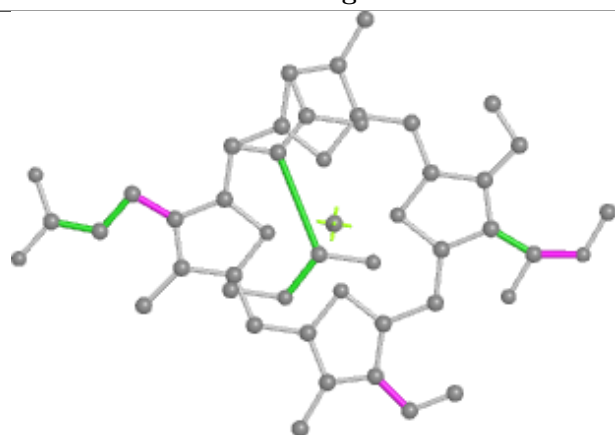
## Ligand A1ECV T 317



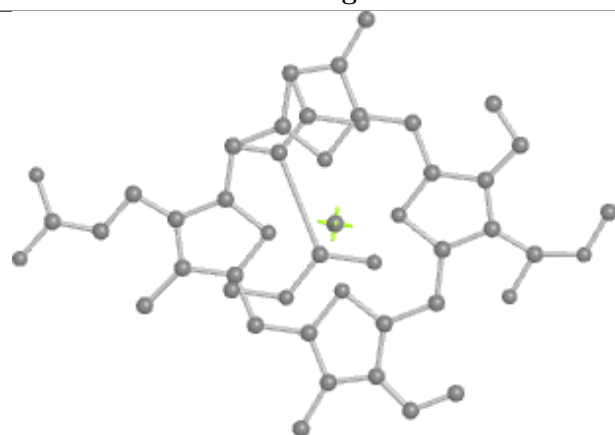
Bond lengths



Bond angles

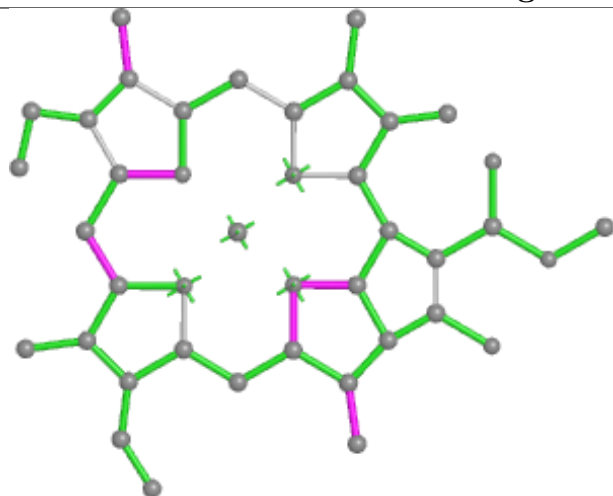


Torsions

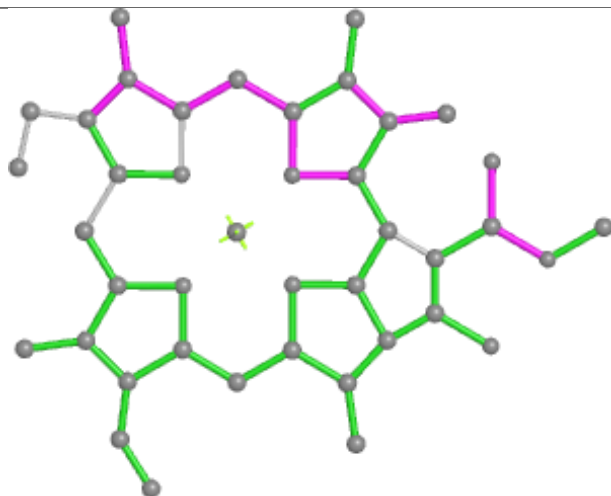


Rings

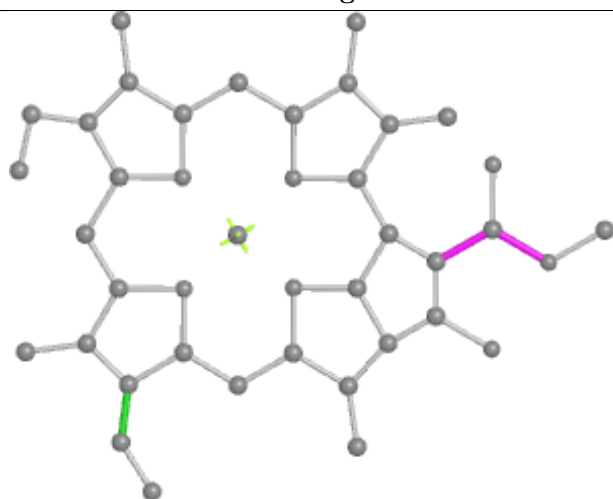
## Ligand CLA x 309



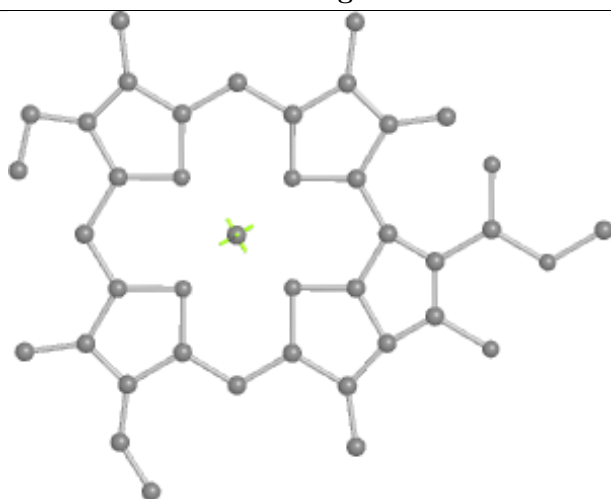
Bond lengths



Bond angles

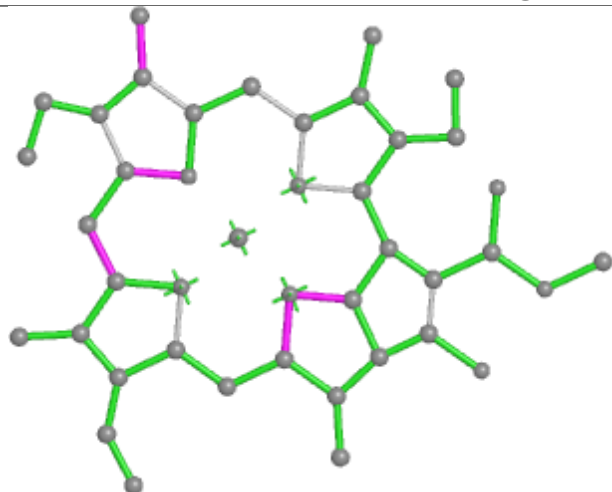


Torsions

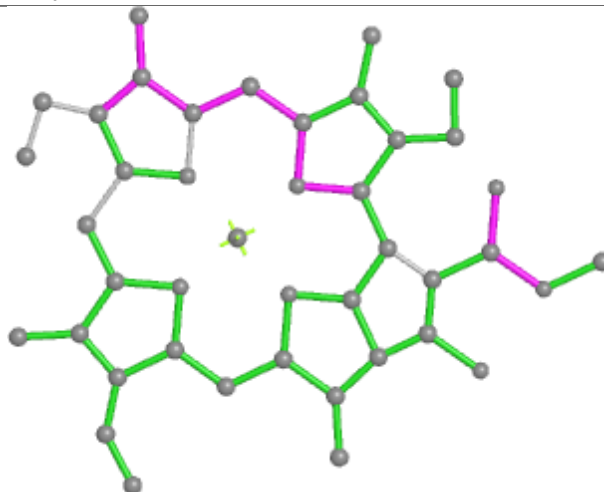


Rings

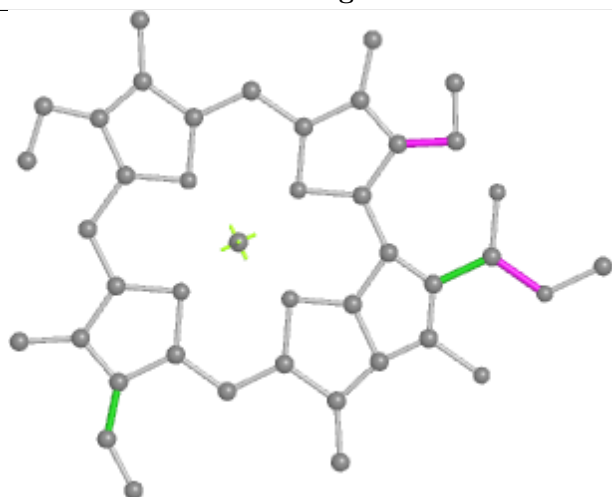
## Ligand CLA y 312



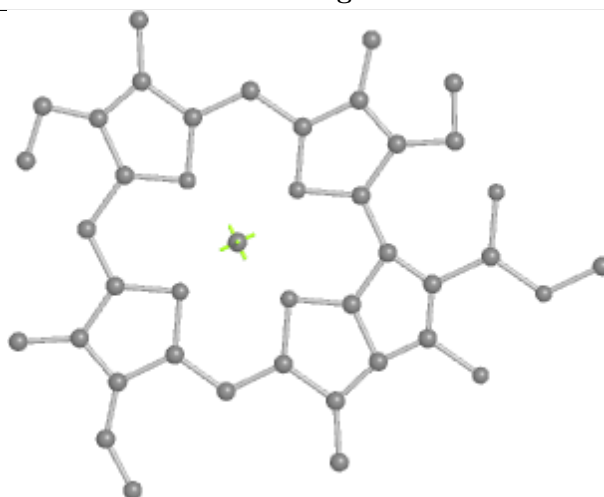
Bond lengths



Bond angles

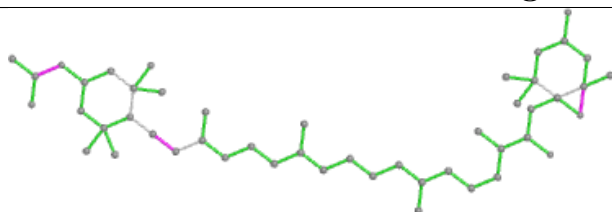


Torsions

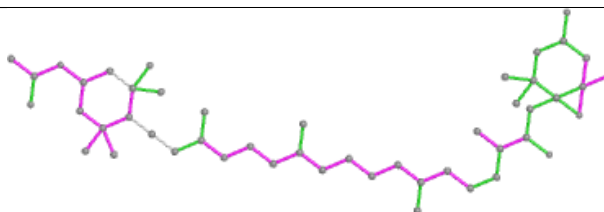


Rings

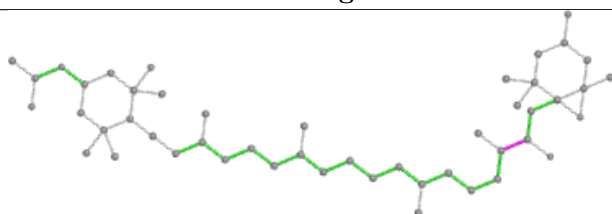
## Ligand A86 L 305



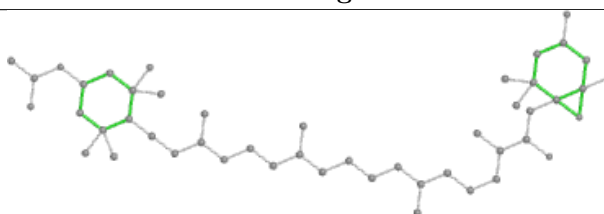
Bond lengths



Bond angles

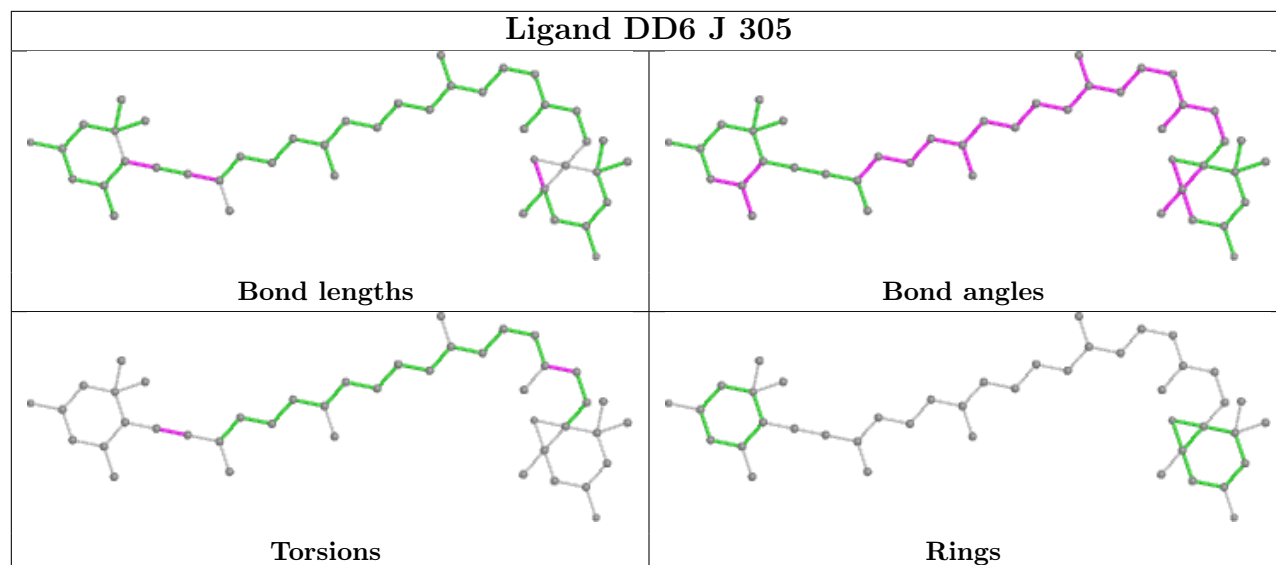


Torsions

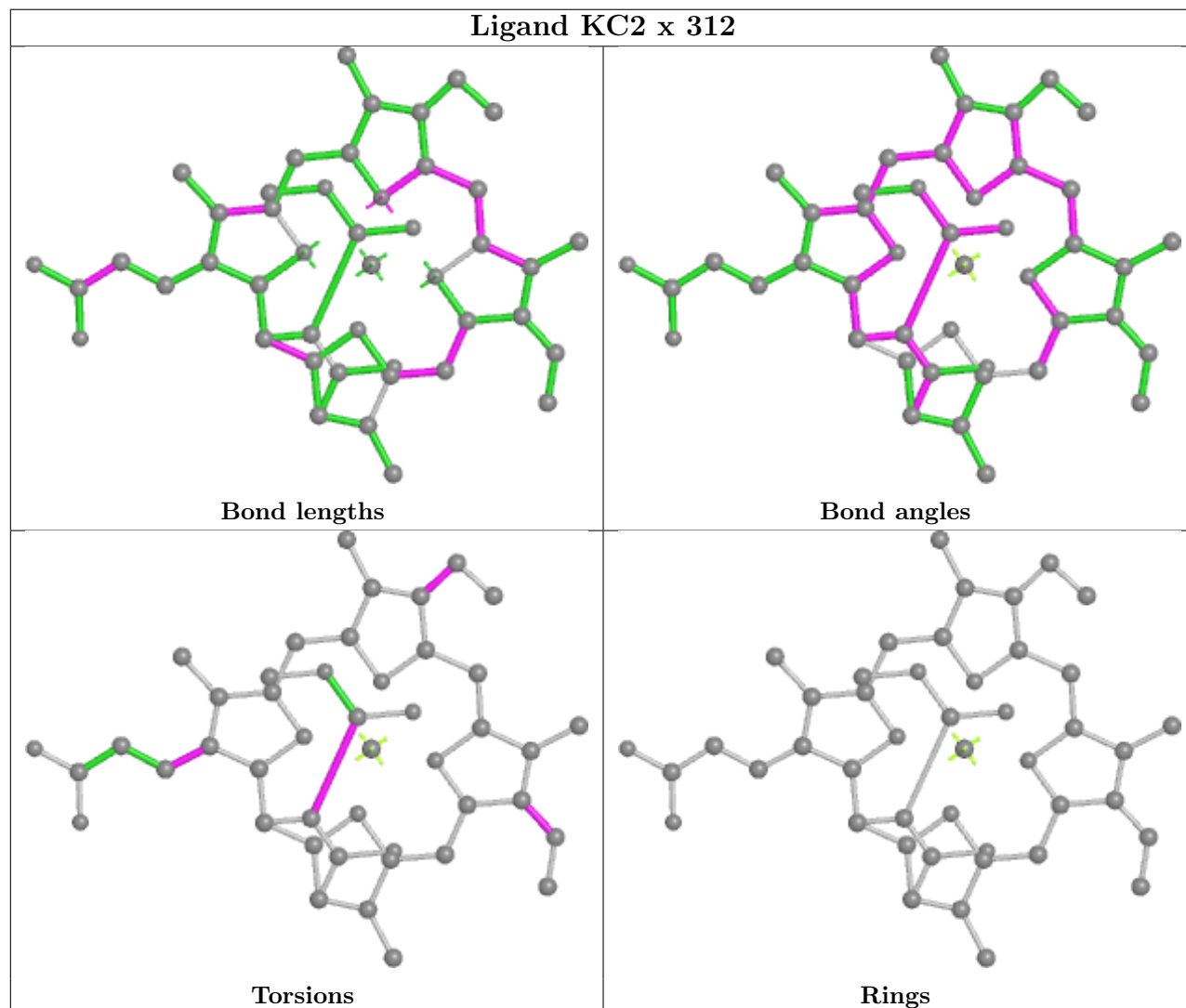


Rings

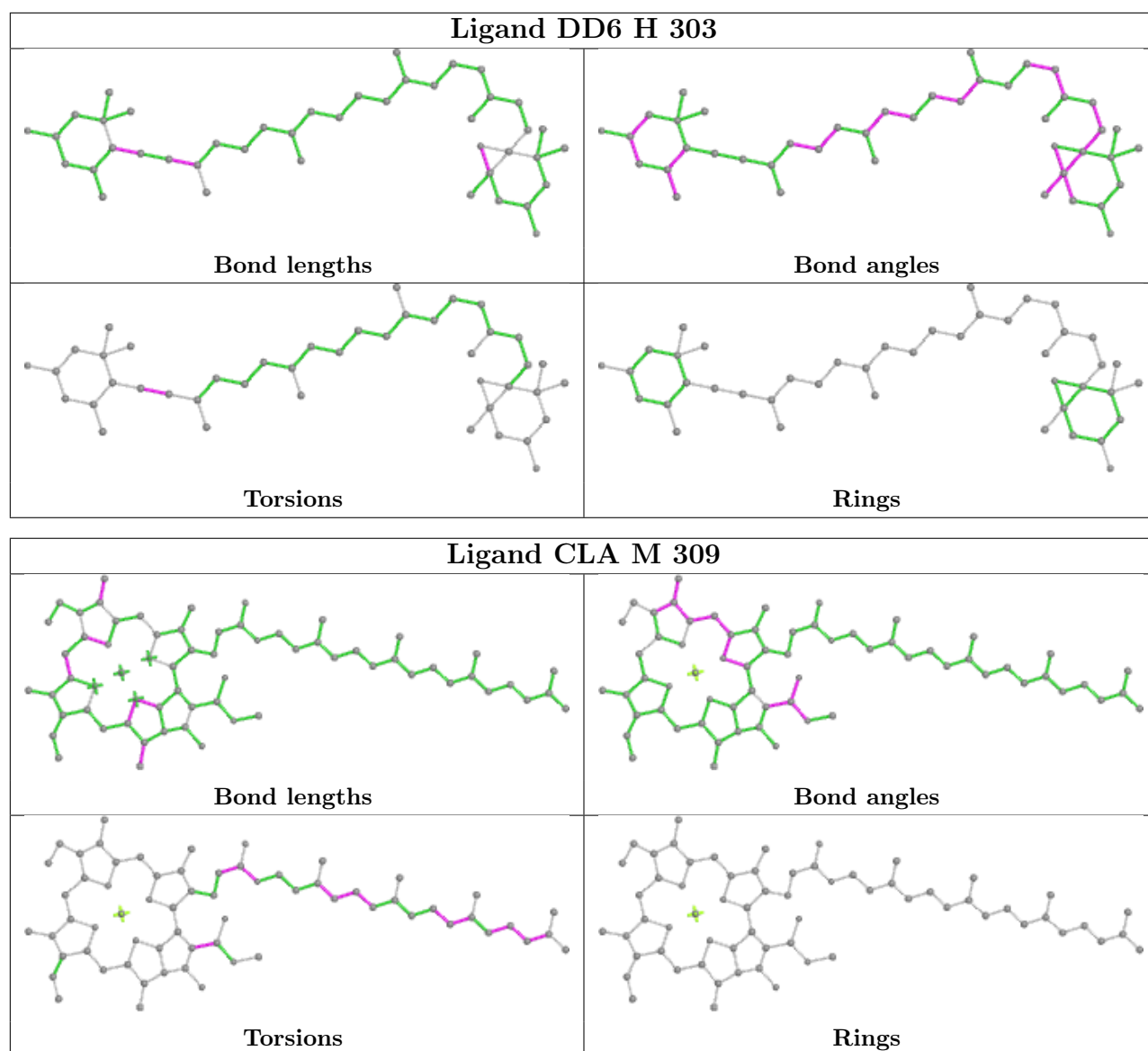
## Ligand DD6 J 305



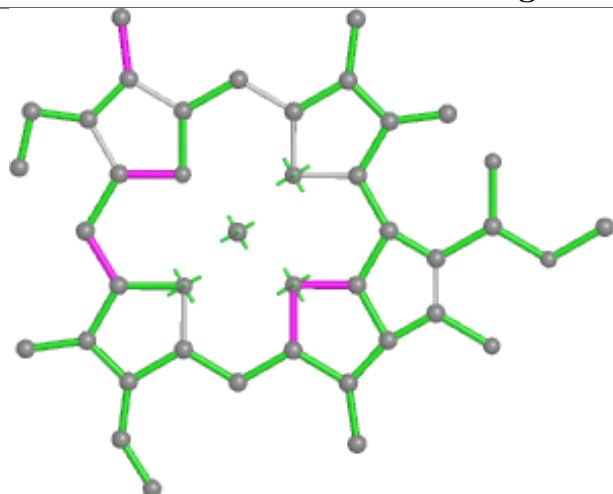
## Ligand KC2 x 312



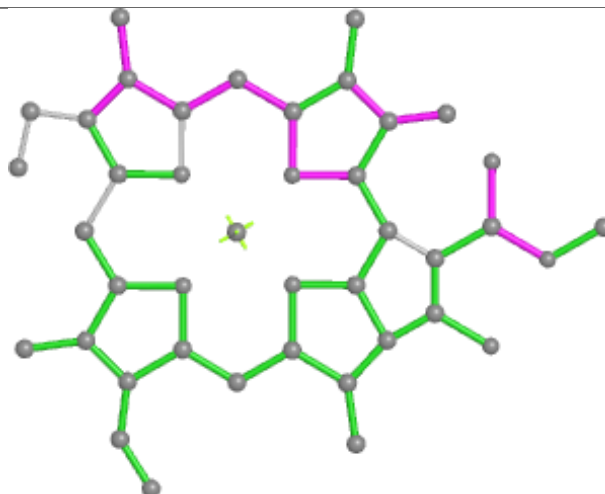




## Ligand CLA 1 308



Bond lengths



Bond angles

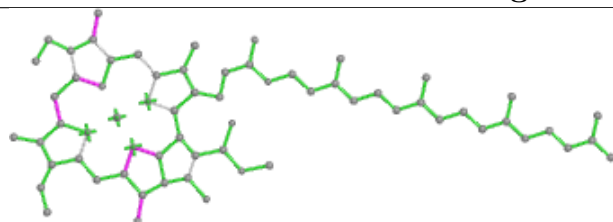


Torsions

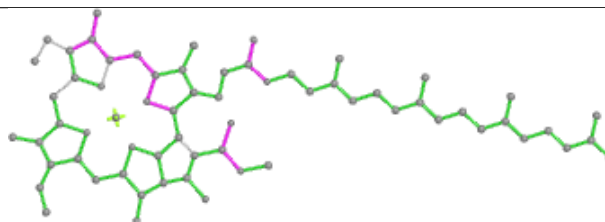


Rings

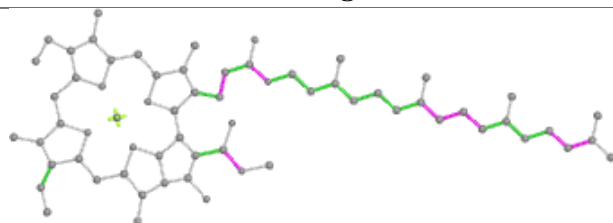
## Ligand CLA M 308



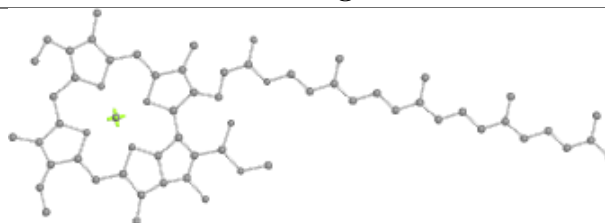
Bond lengths



Bond angles

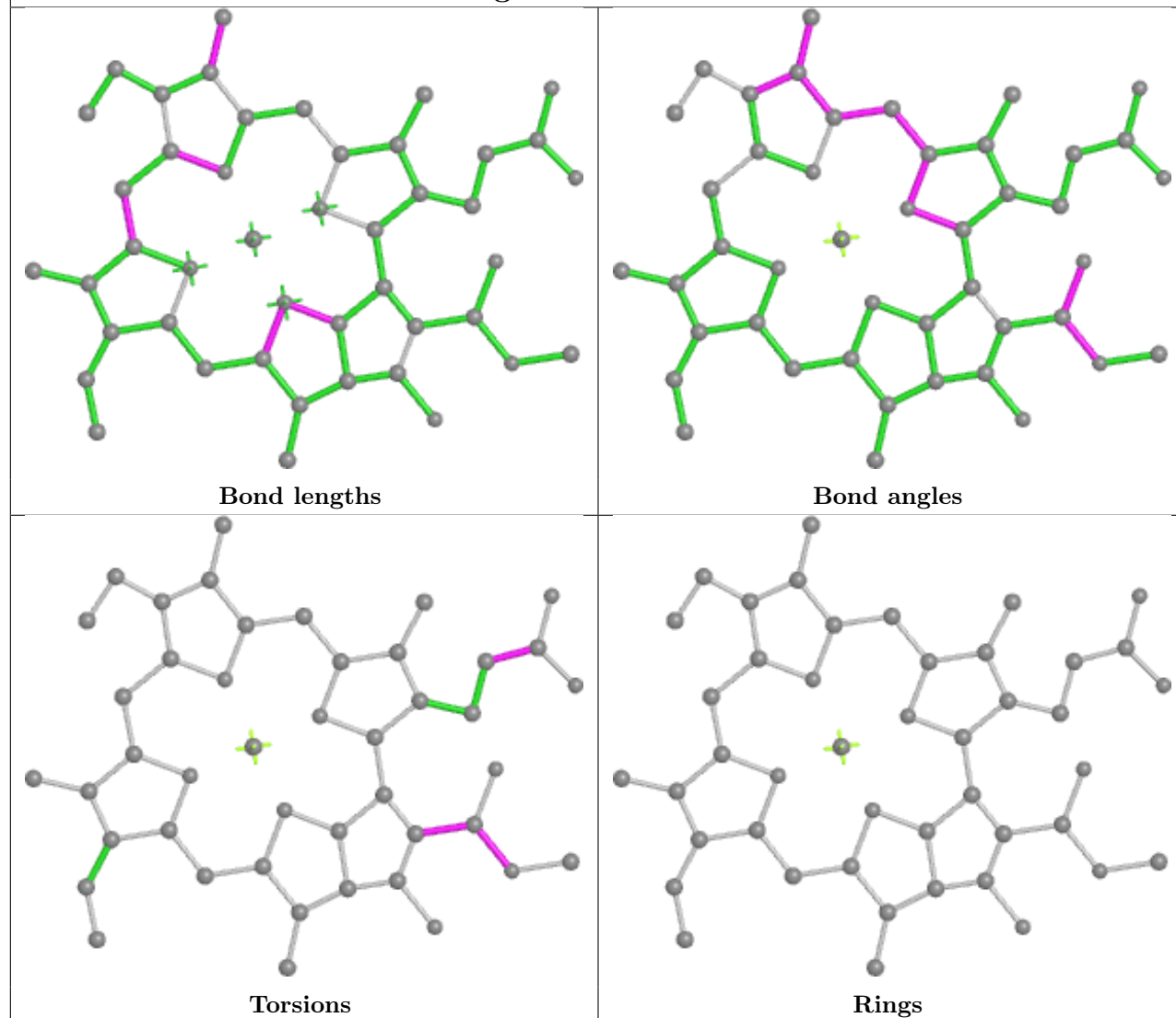


Torsions

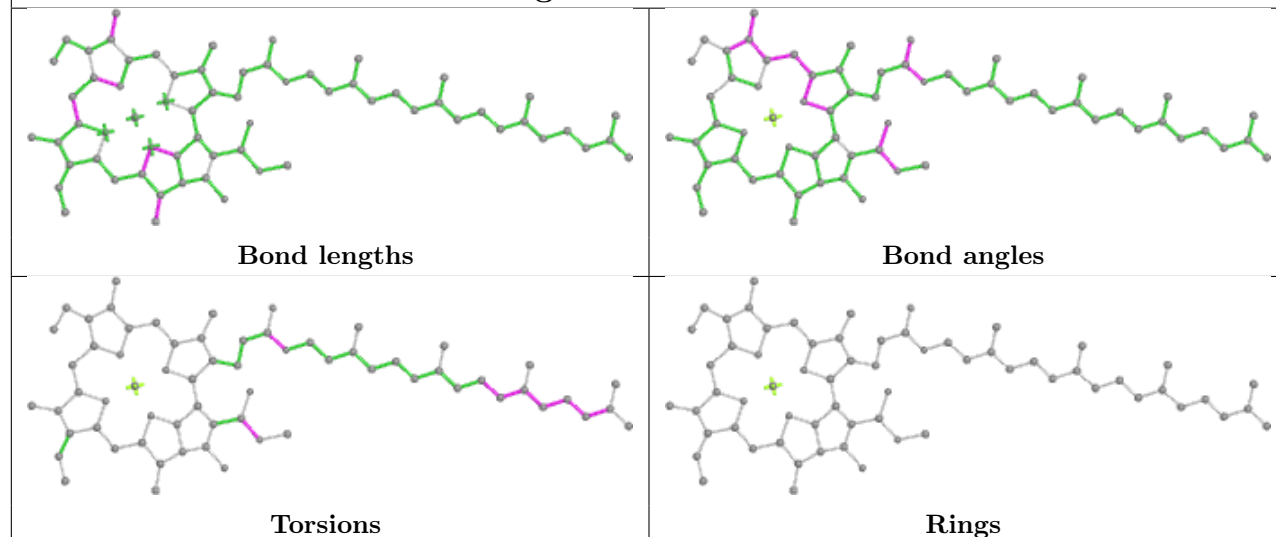


Rings

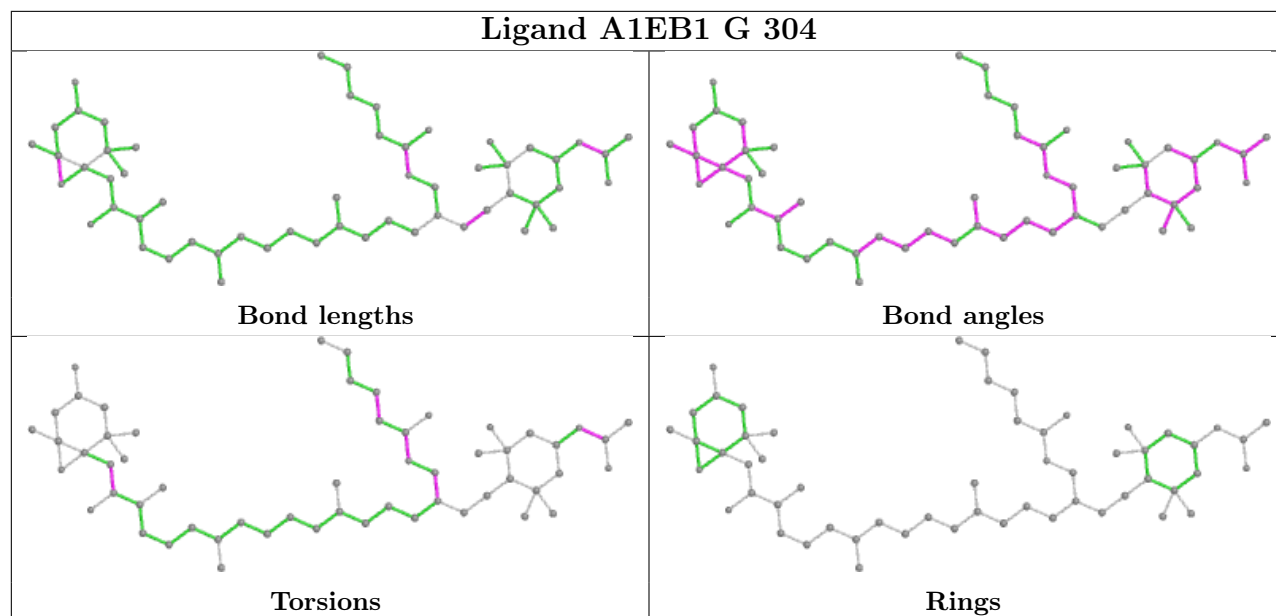
## Ligand CLA 8 312



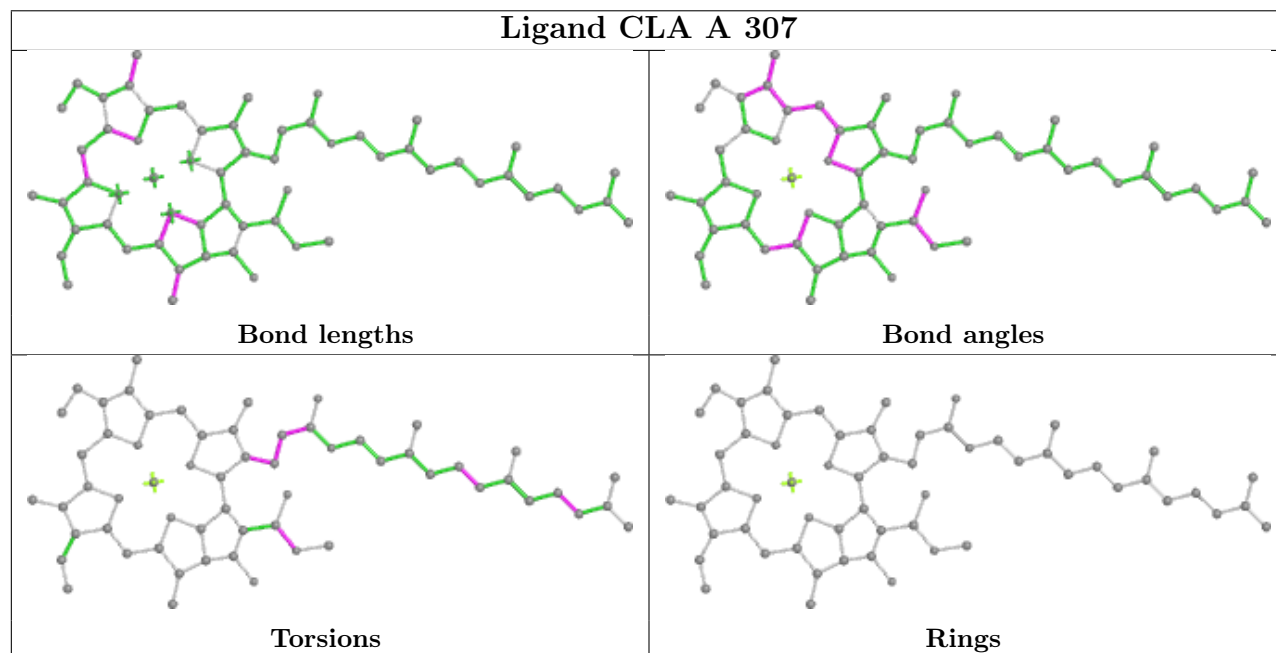
## Ligand CLA b 842

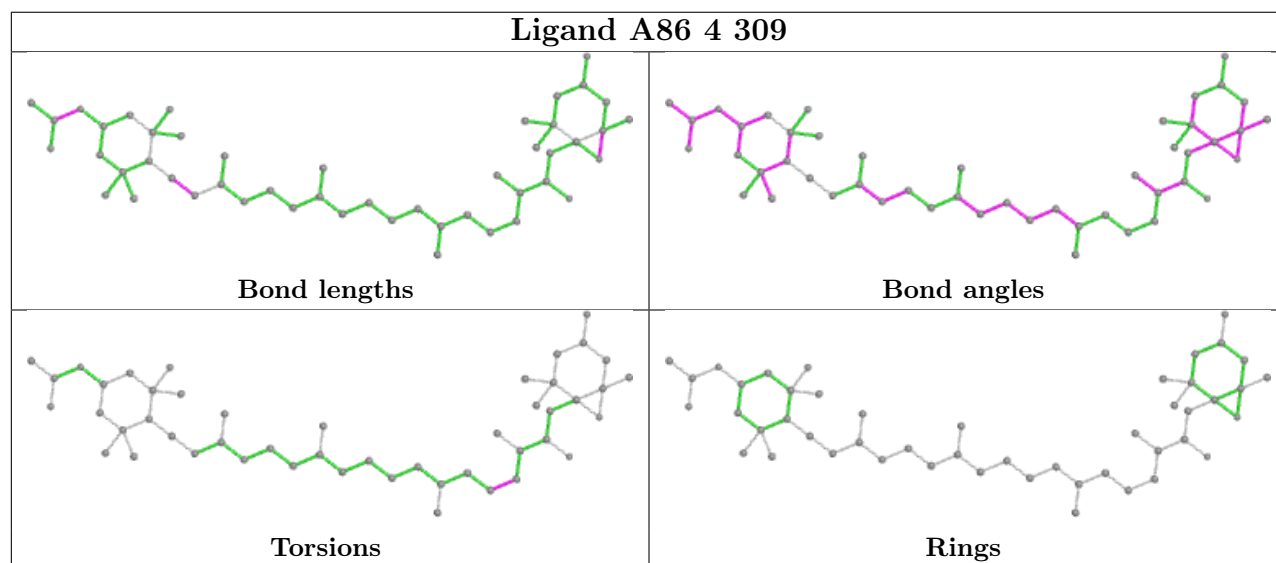
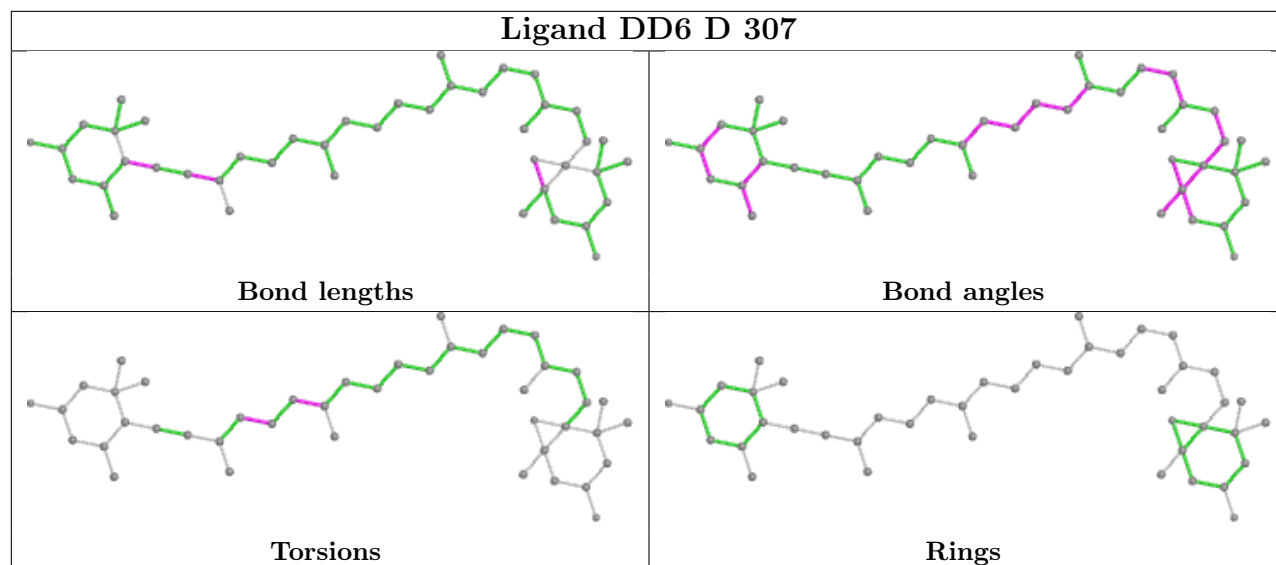


## Ligand A1EB1 G 304

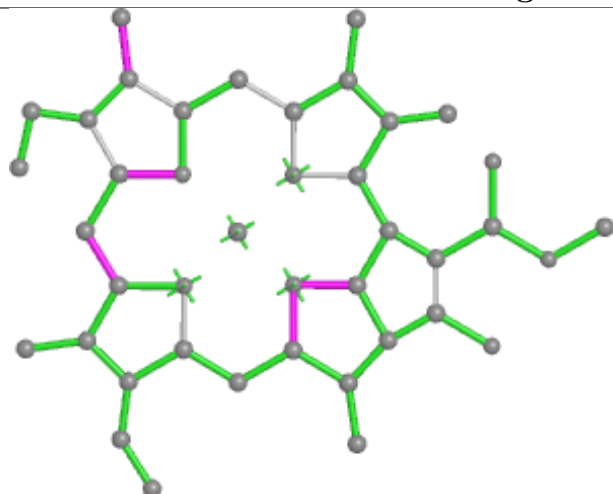


## Ligand CLA A 307

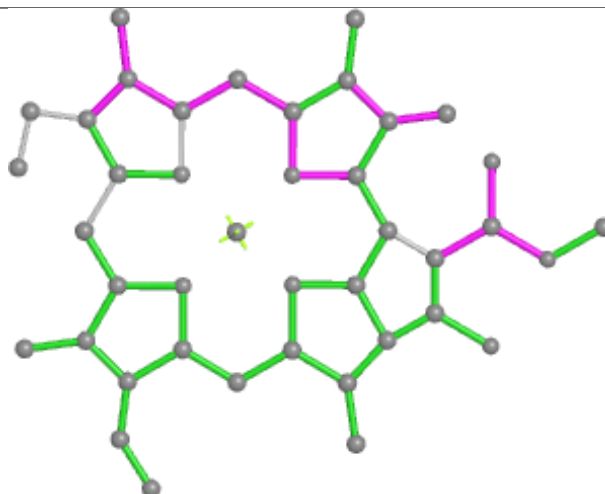




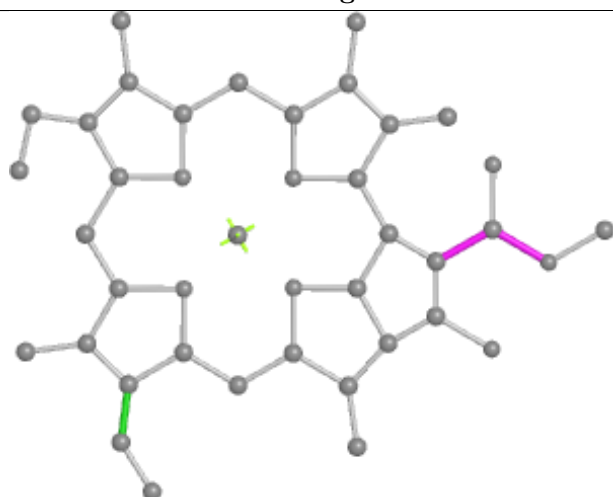
## Ligand CLA L 316



Bond lengths



Bond angles

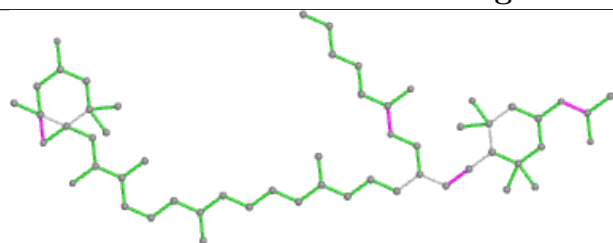


Torsions

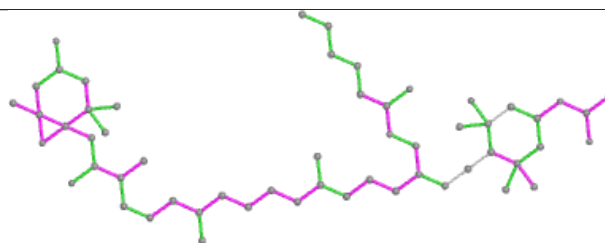


Rings

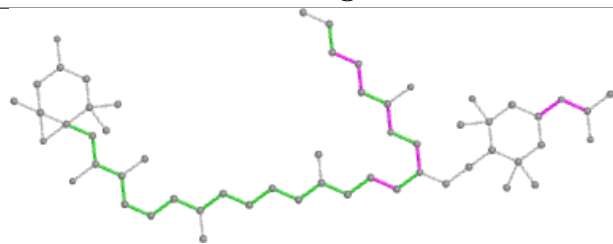
## Ligand A1EB1 U 205



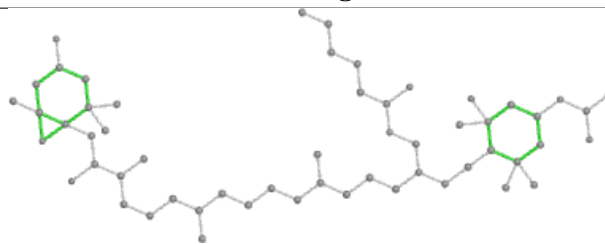
Bond lengths



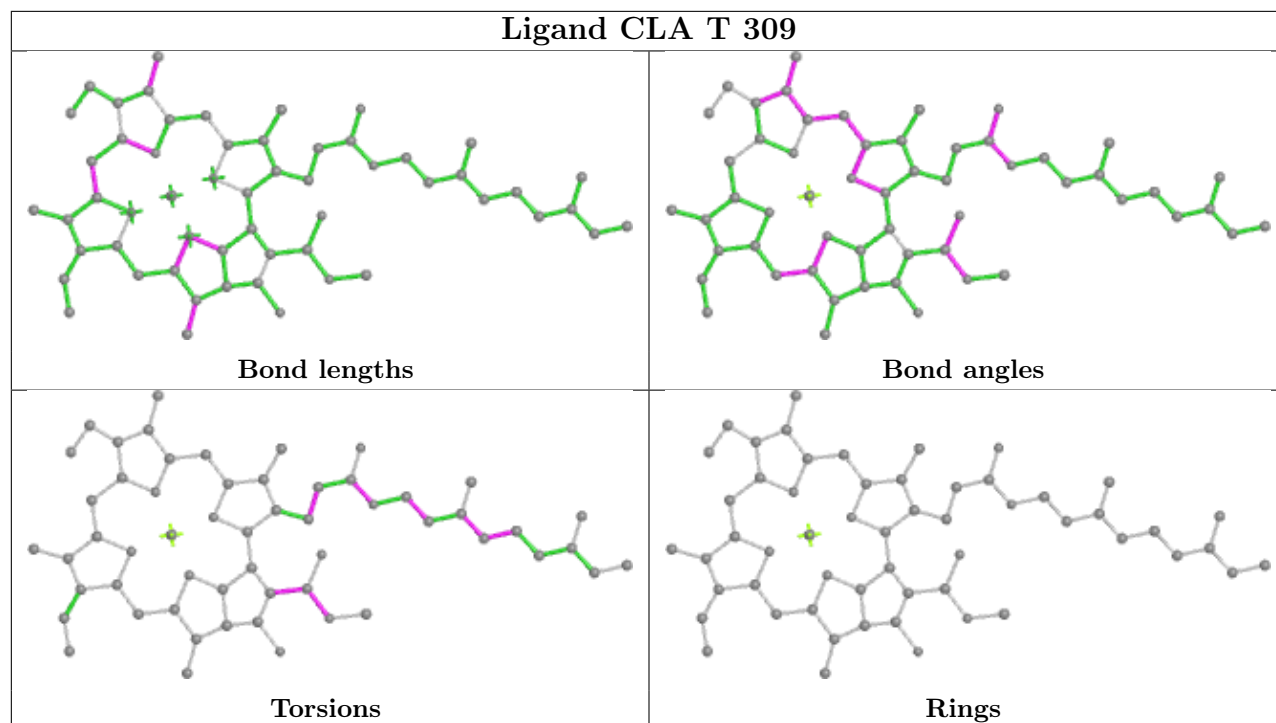
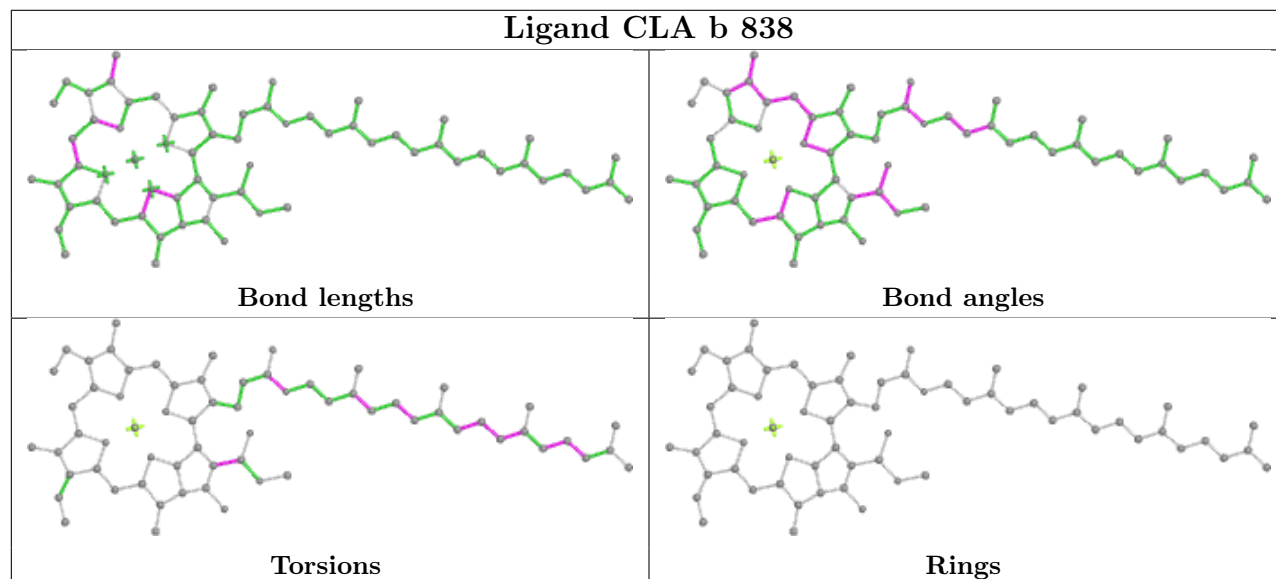
Bond angles



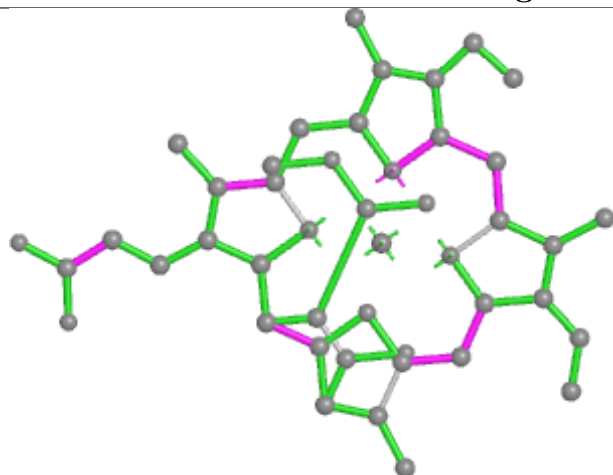
Torsions



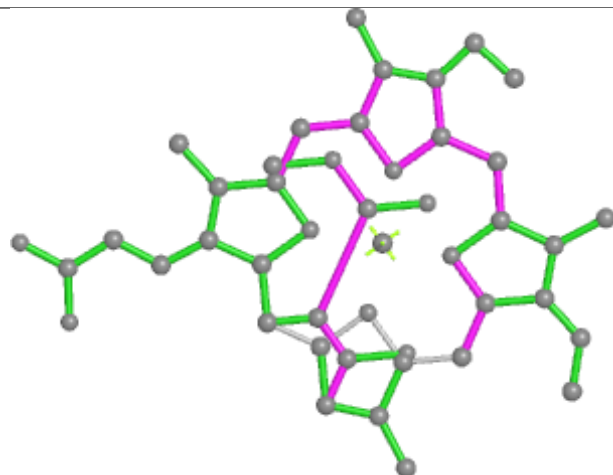
Rings

**Ligand CLA T 309****Ligand CLA b 838**

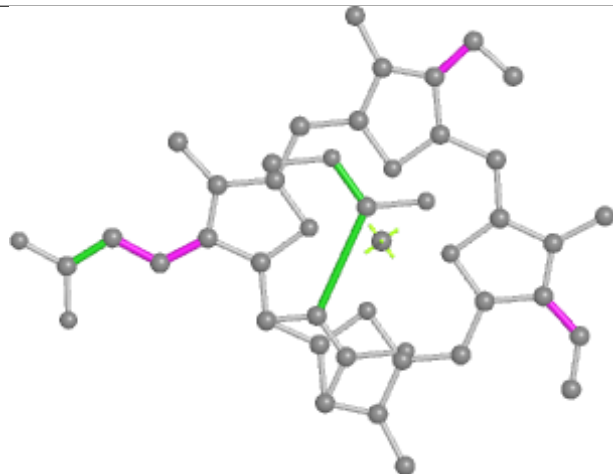
## Ligand KC2 A 310



Bond lengths



Bond angles



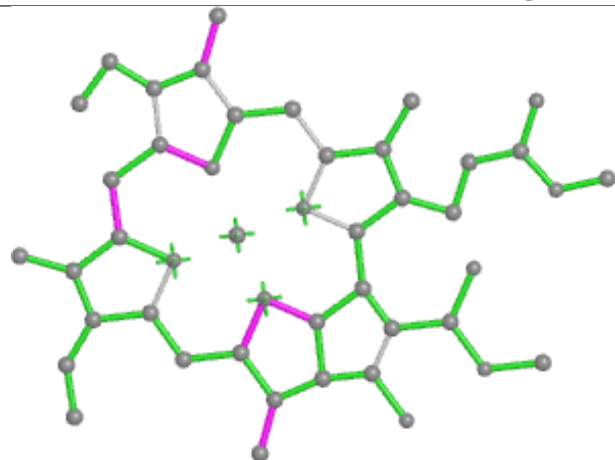
Torsions



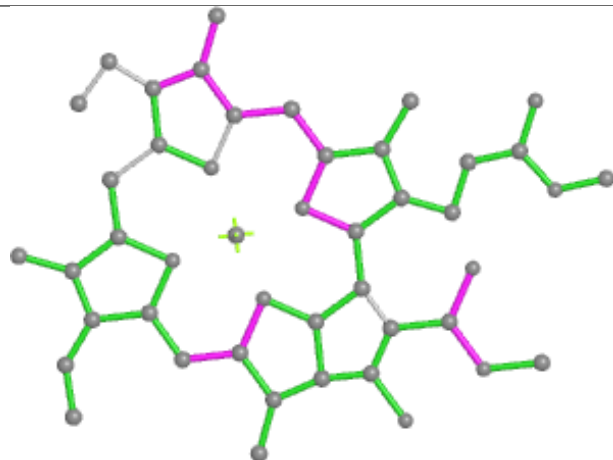
Rings



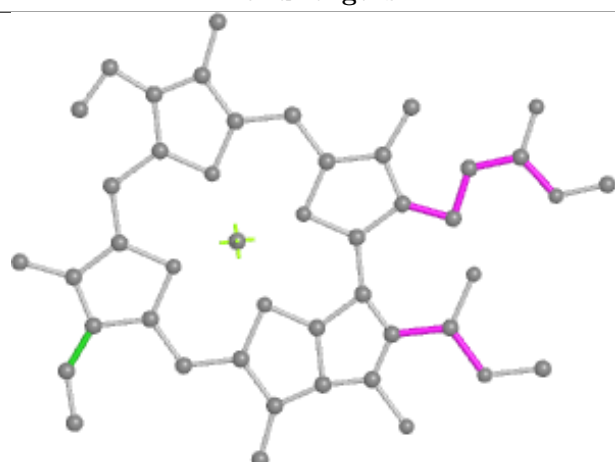
## Ligand CLA 2 308



Bond lengths



Bond angles

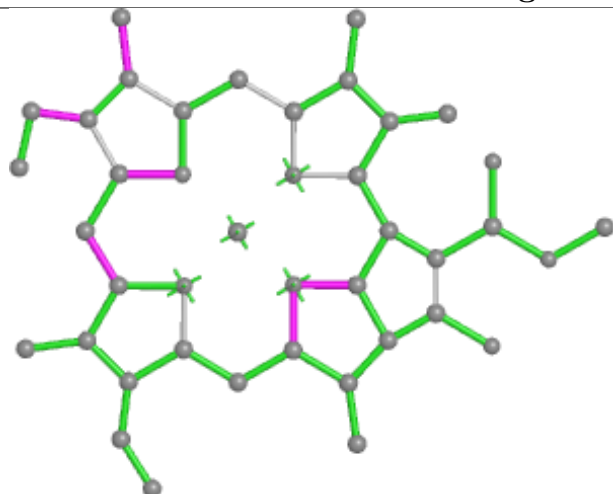


Torsions

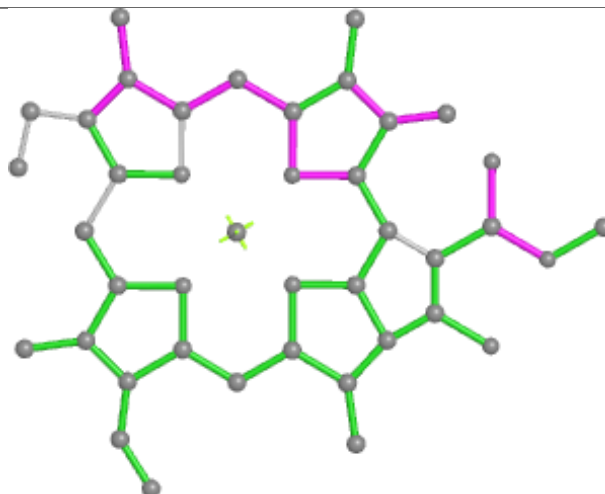


Rings

## Ligand CLA 2 316



Bond lengths



Bond angles

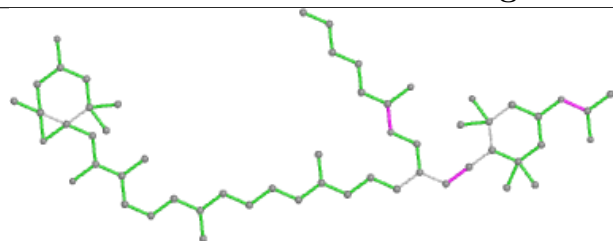


Torsions

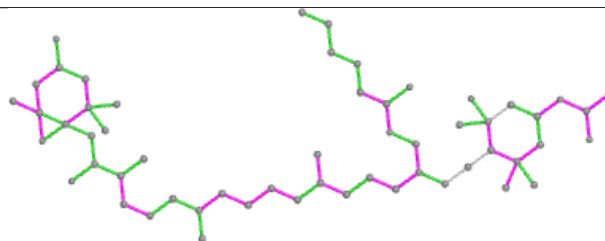


Rings

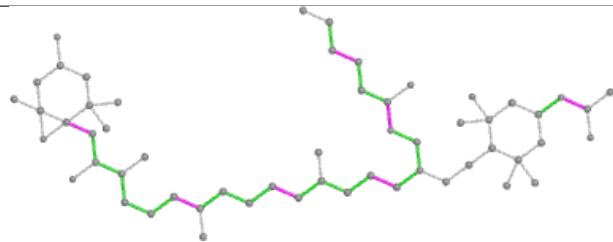
## Ligand A1EB1 0 303



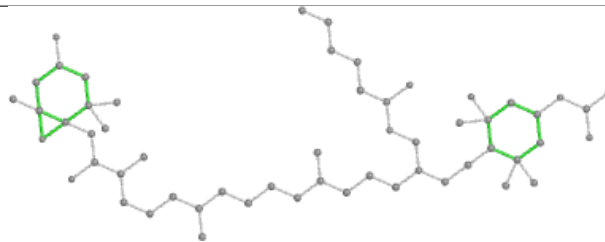
Bond lengths



Bond angles

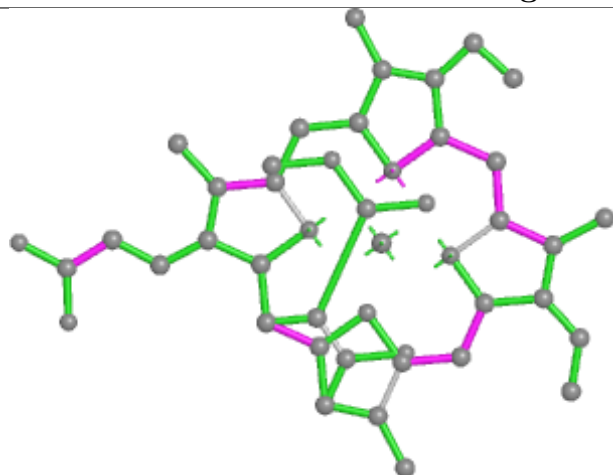


Torsions

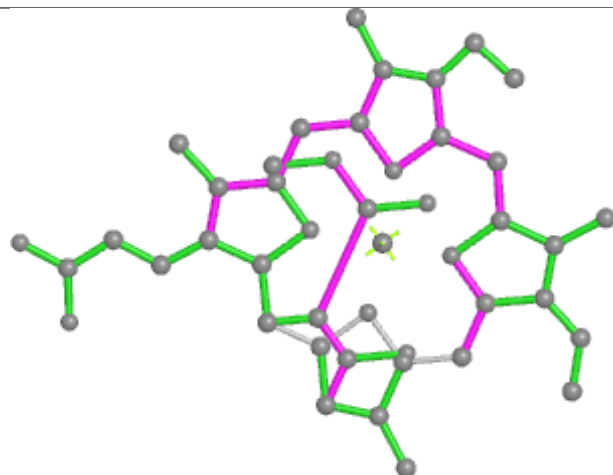


Rings

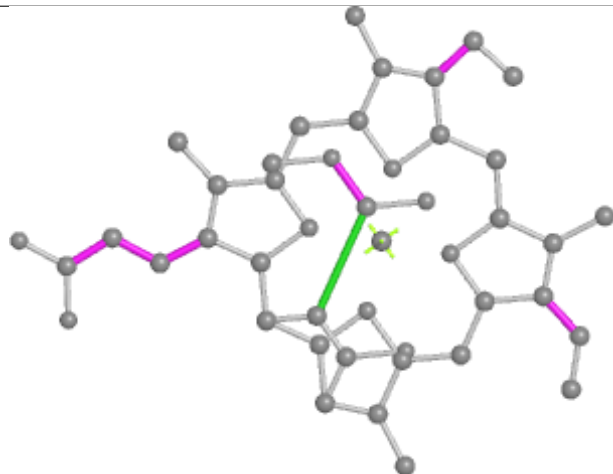
## Ligand KC2 6 319



Bond lengths



Bond angles

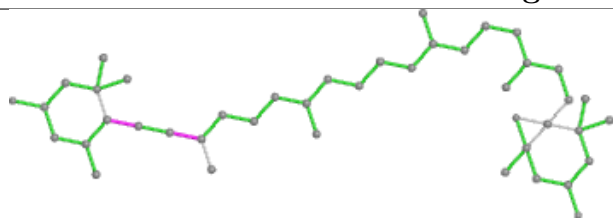


Torsions

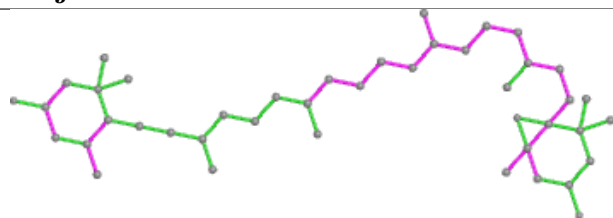


Rings

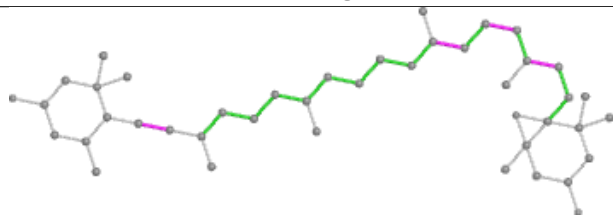
## Ligand DD6 j 102



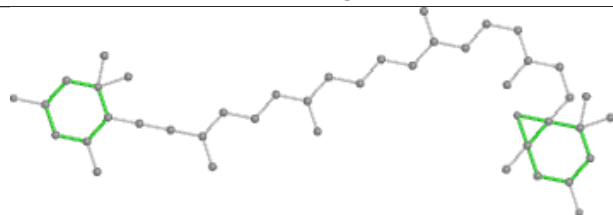
Bond lengths



Bond angles

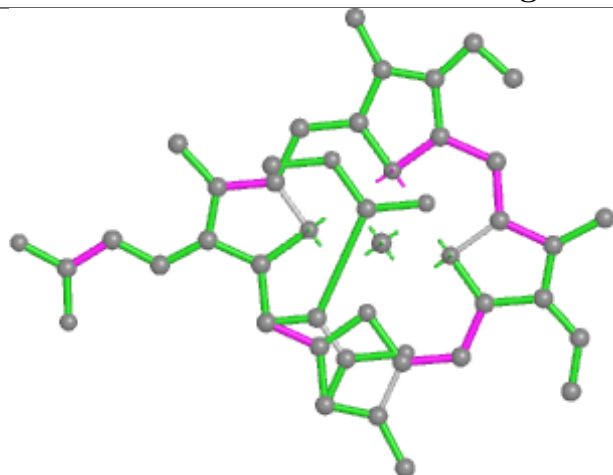


Torsions

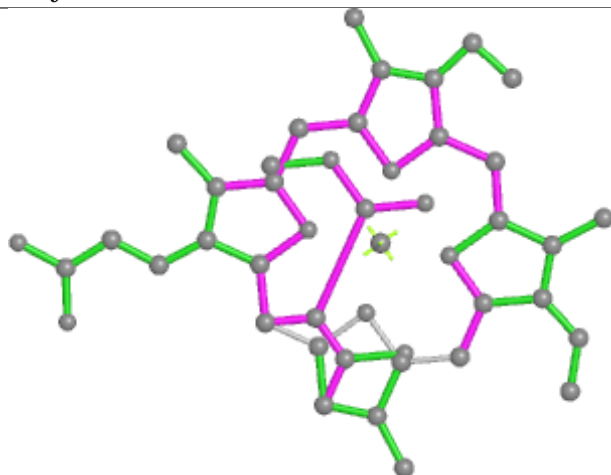


Rings

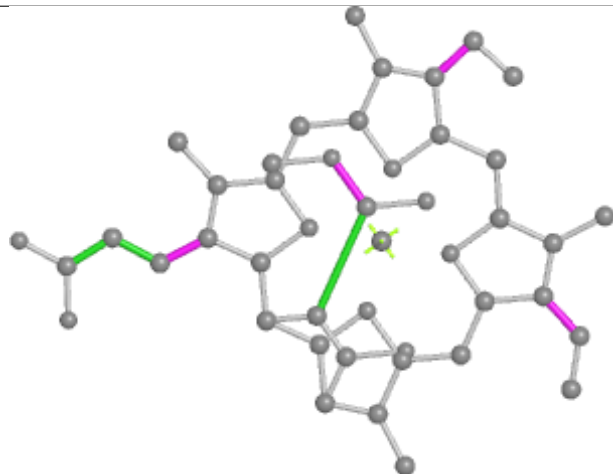
## Ligand KC2 y 316



Bond lengths



Bond angles

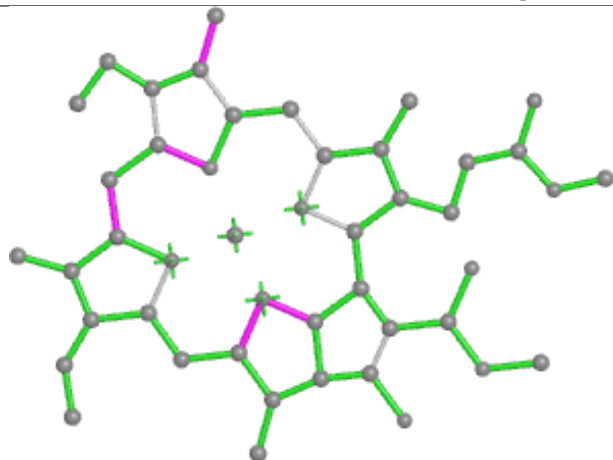


Torsions

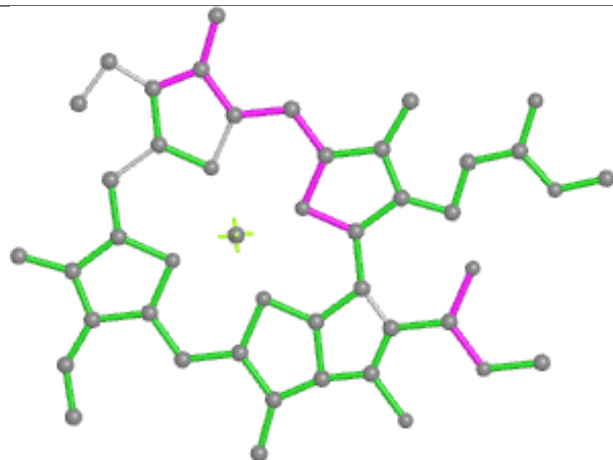


Rings

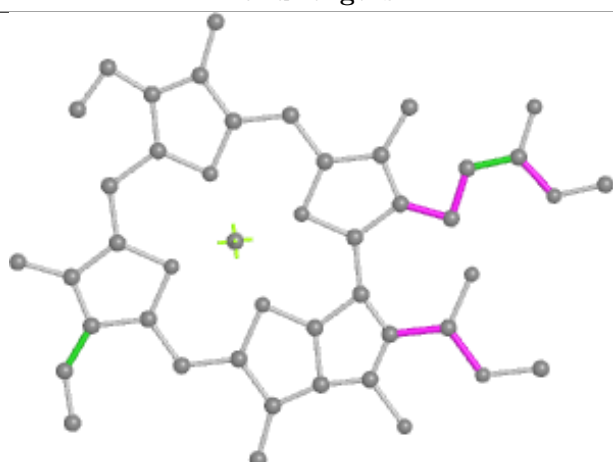
## Ligand CLA C 309



Bond lengths



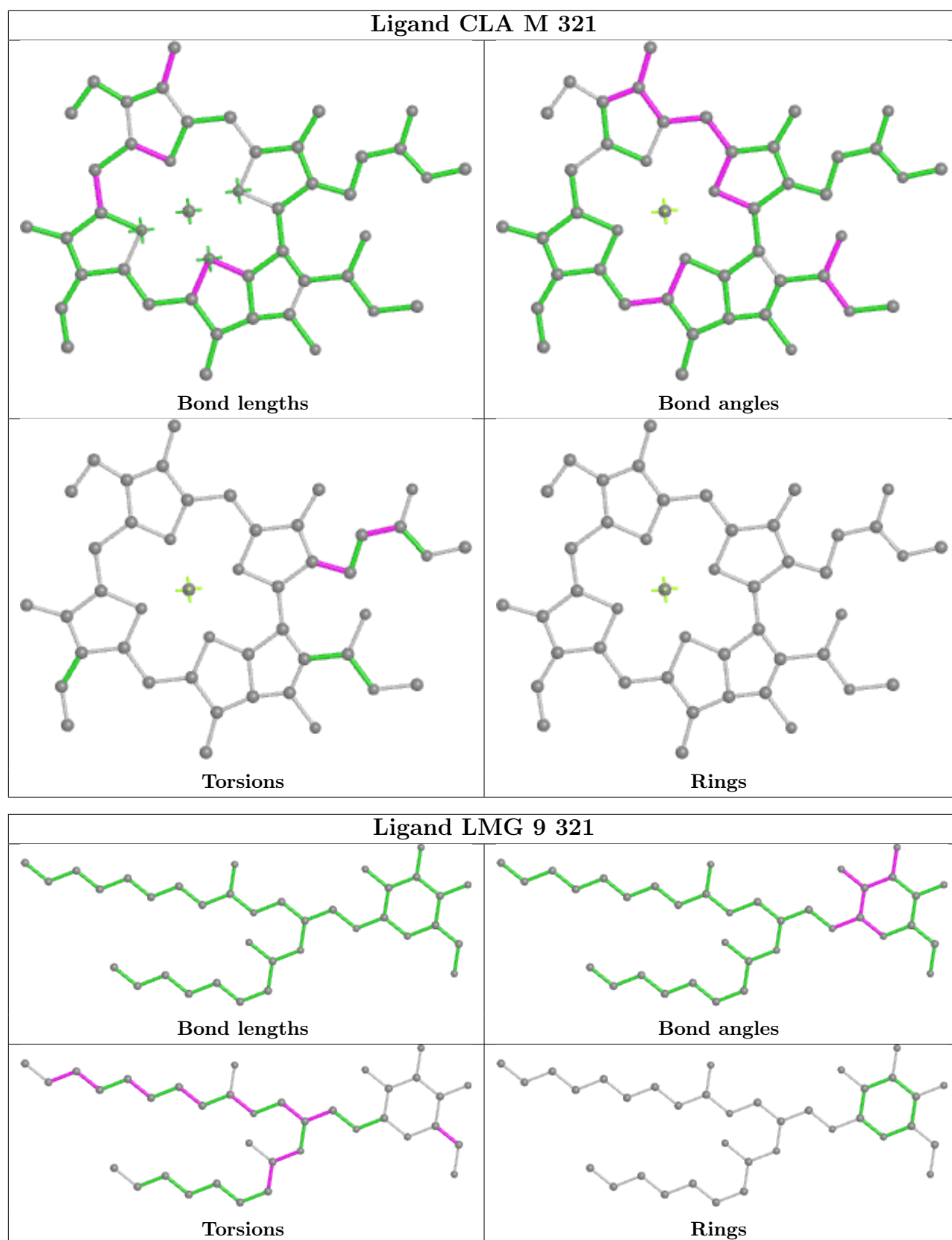
Bond angles



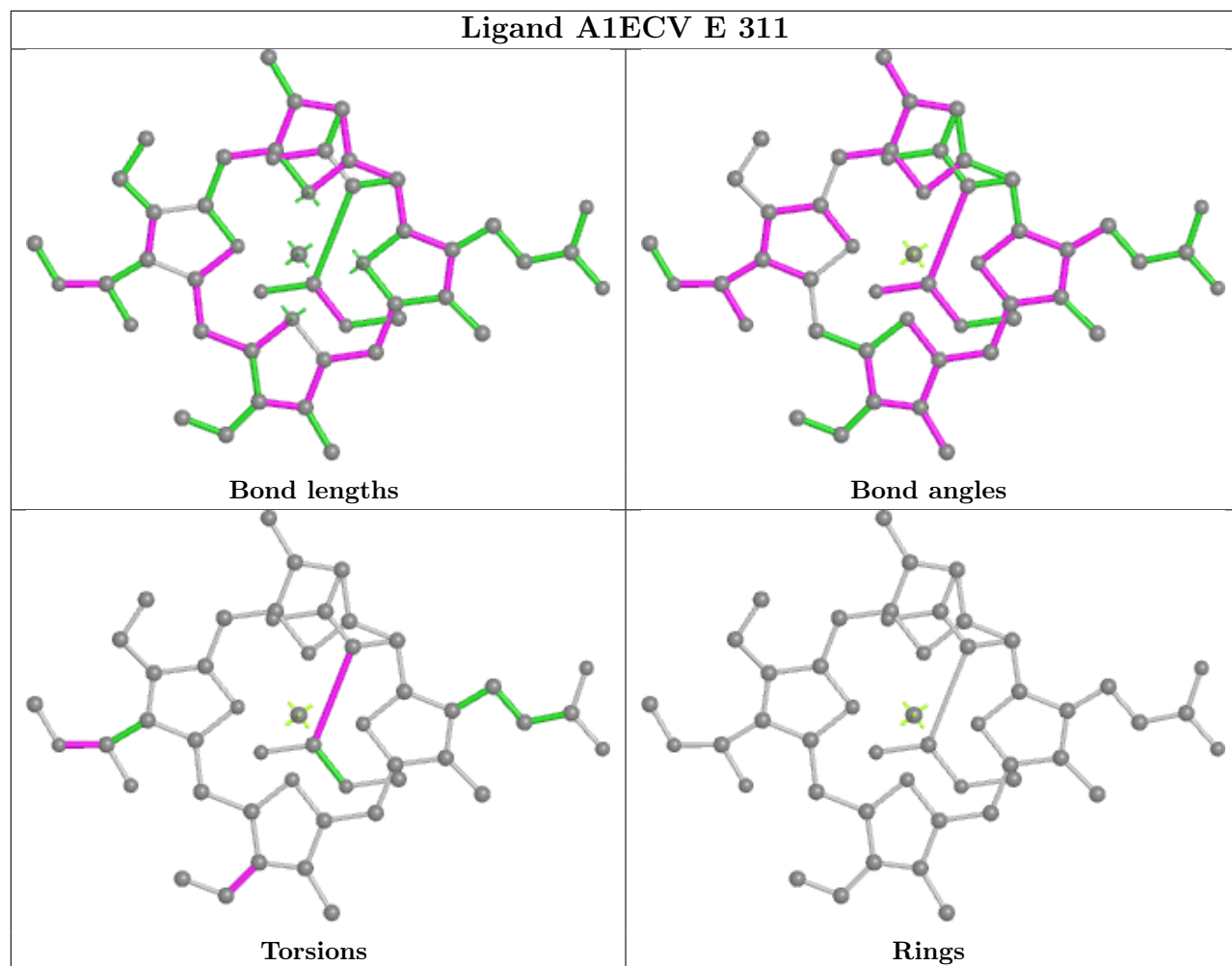
Torsions



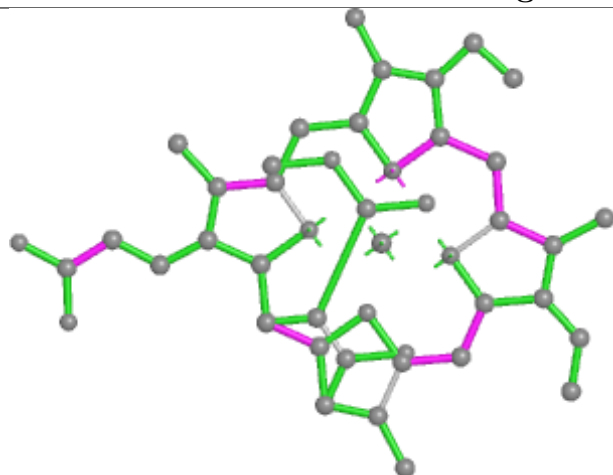
Rings



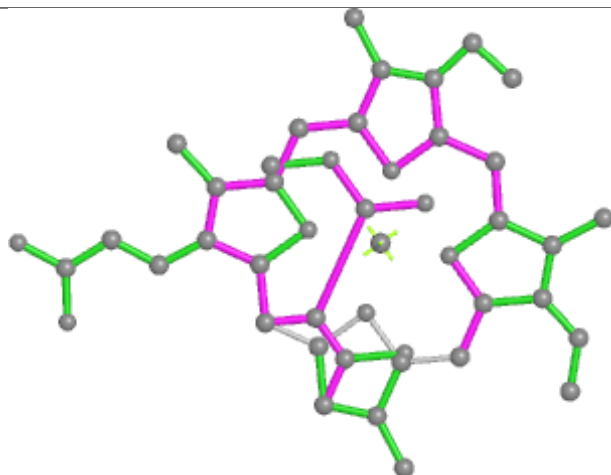
## Ligand A1ECV E 311



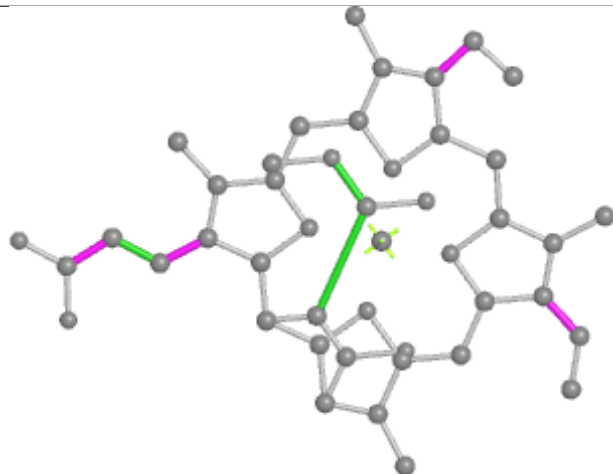
## Ligand KC2 T 315



Bond lengths



Bond angles

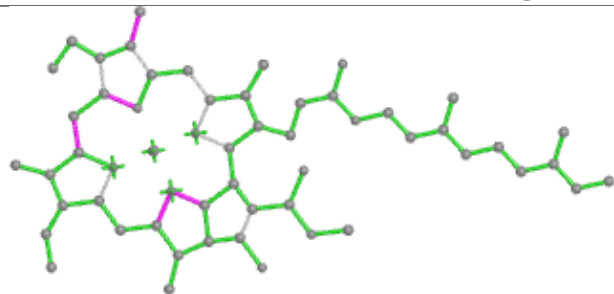


Torsions

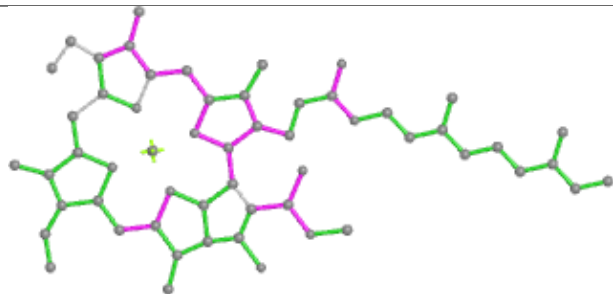


Rings

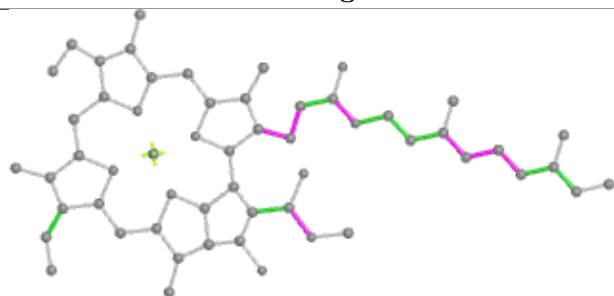


**Ligand CLA 7 314**

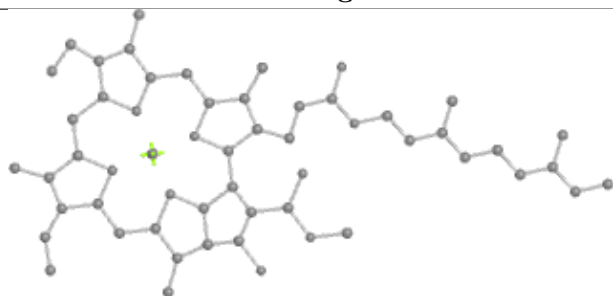
Bond lengths



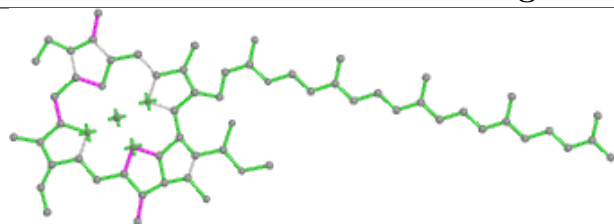
Bond angles



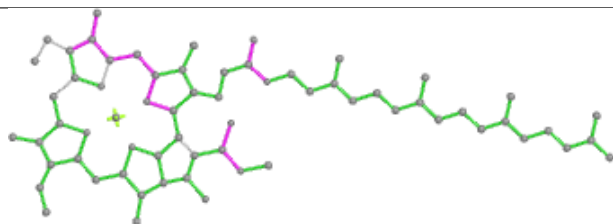
Torsions



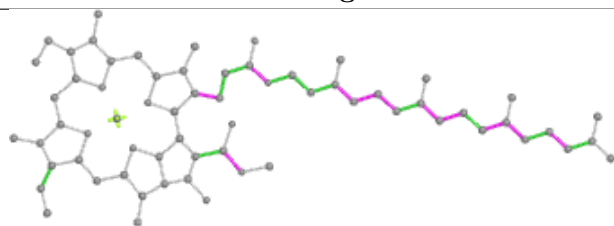
Rings

**Ligand CLA a 804**

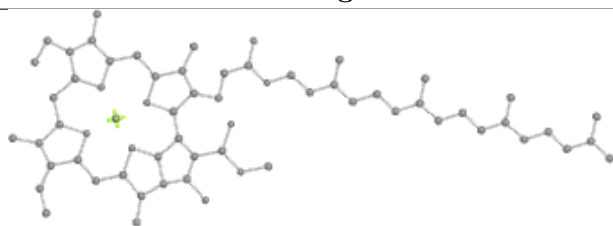
Bond lengths



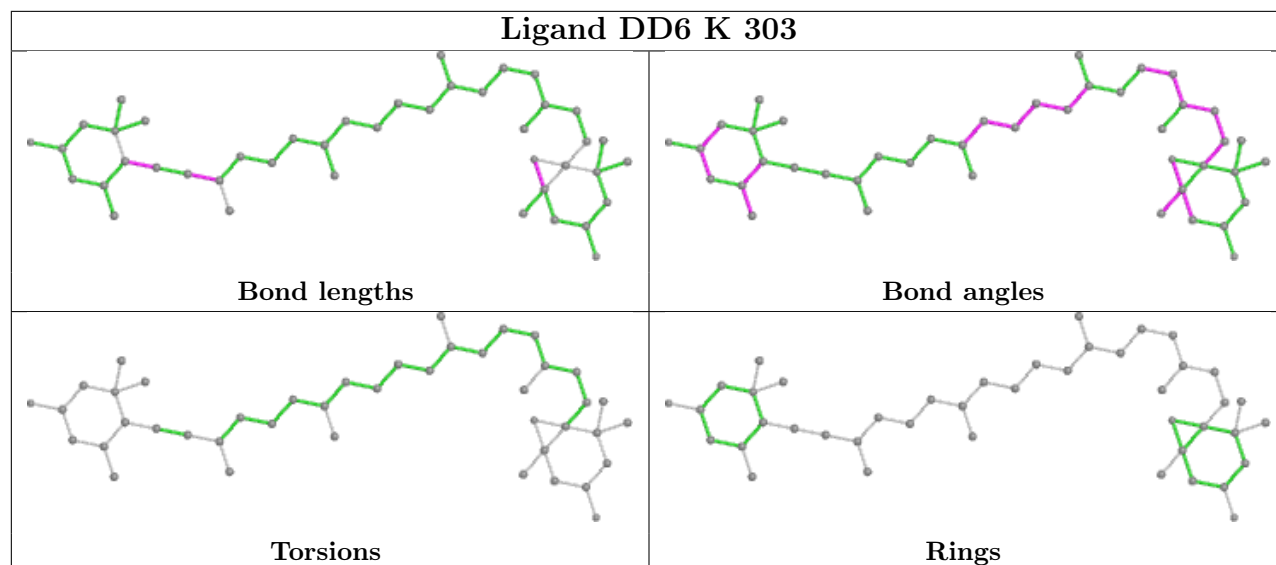
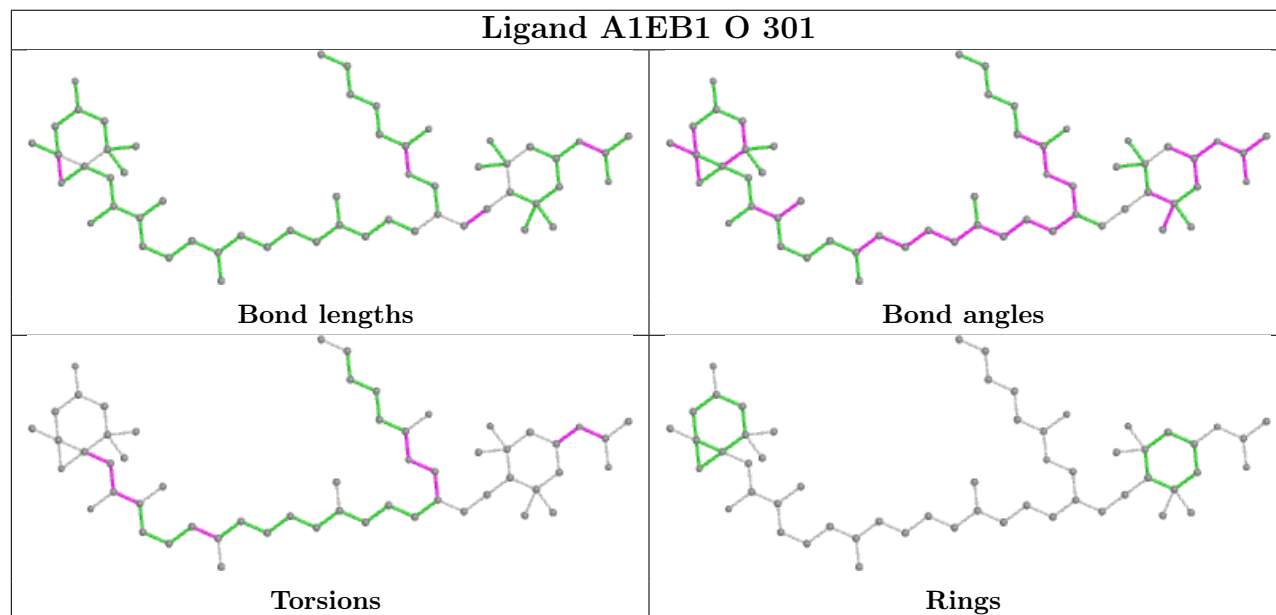
Bond angles



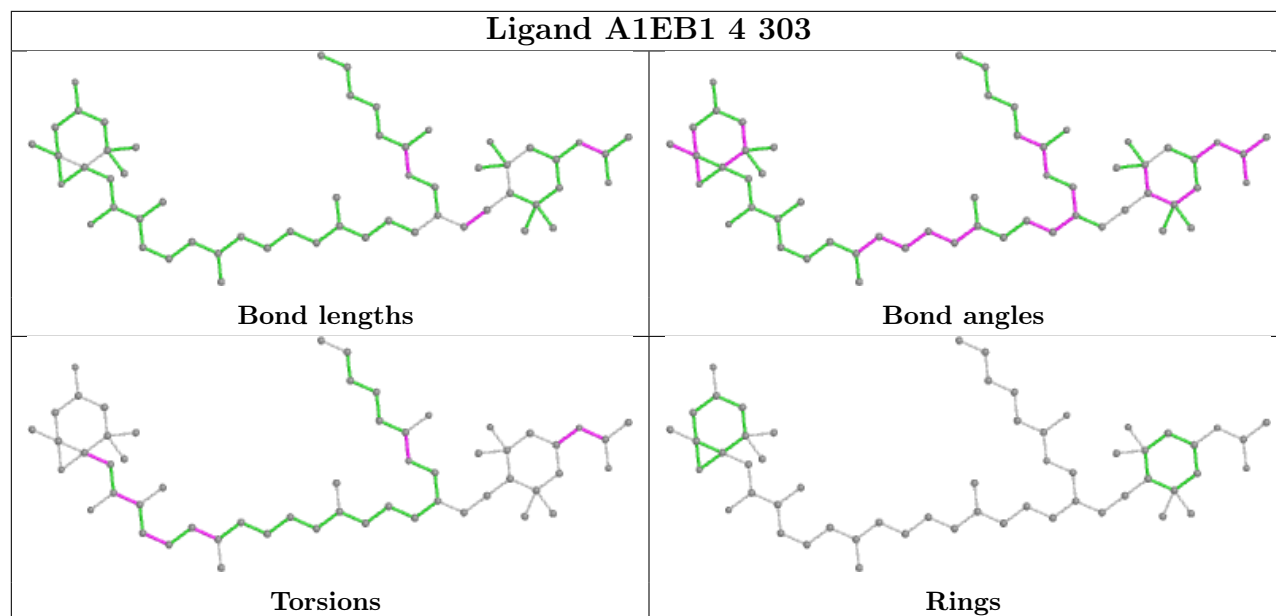
Torsions



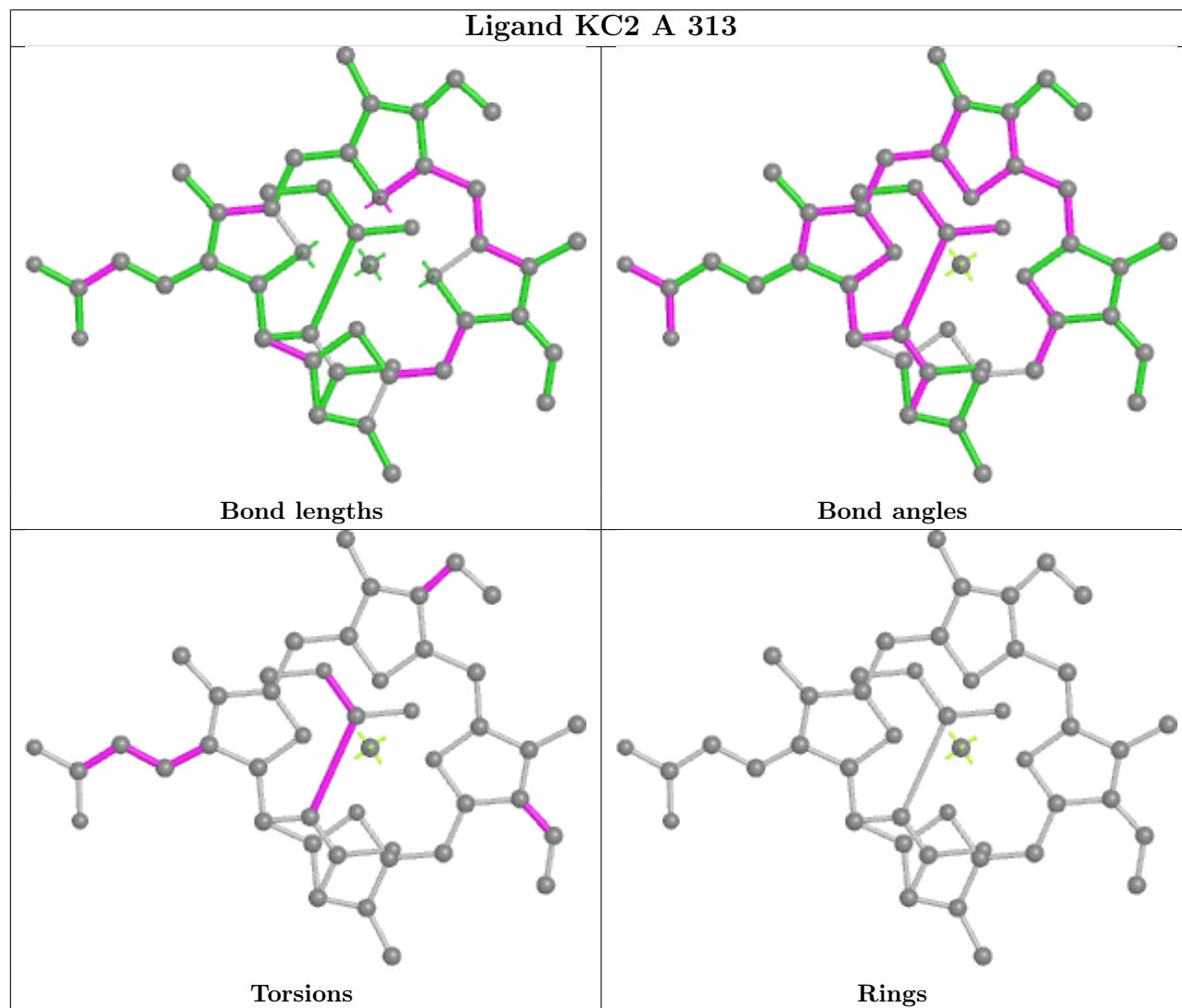
Rings

**Ligand DD6 K 303****Ligand A1EB1 O 301**

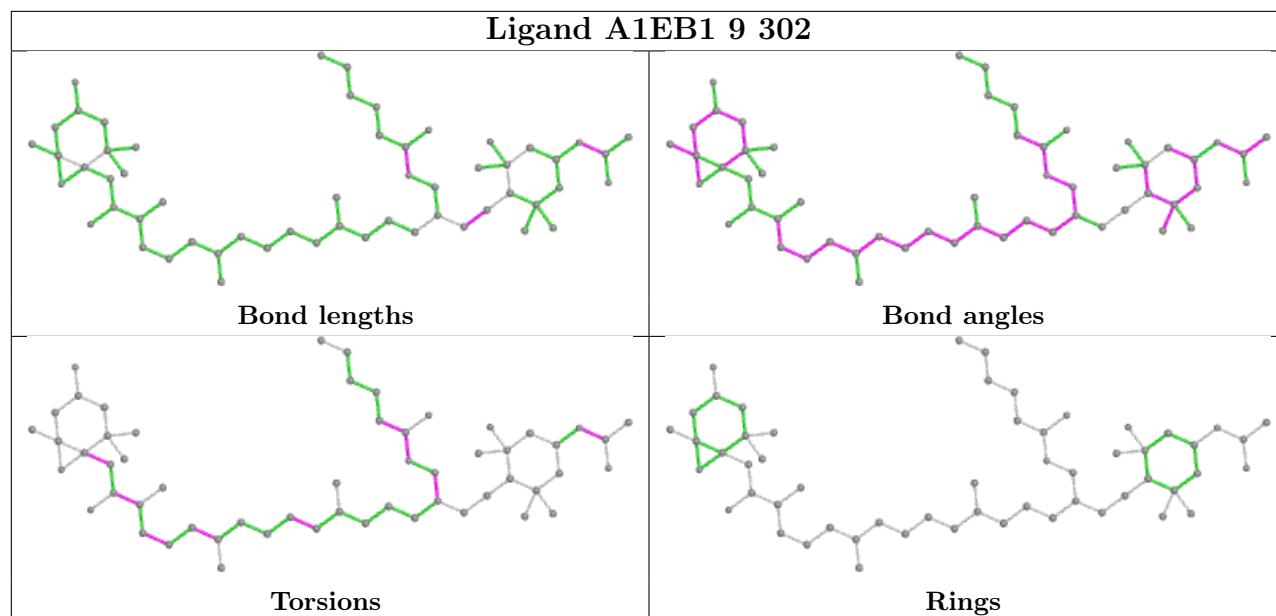
## Ligand A1EB1 4 303



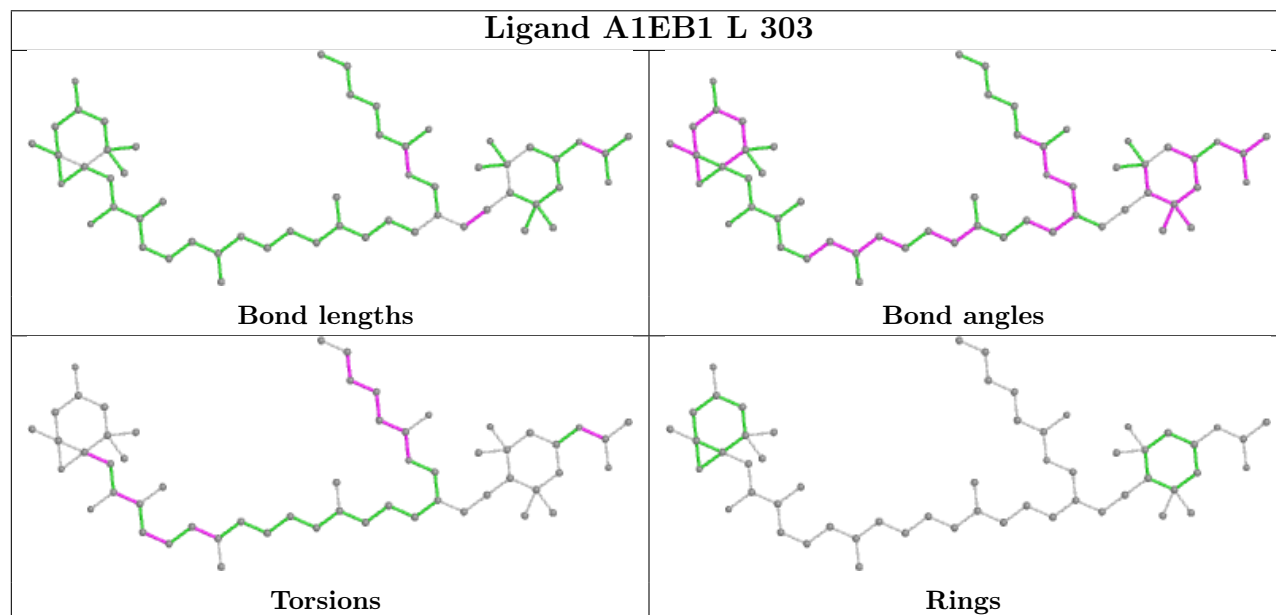
## Ligand KC2 A 313

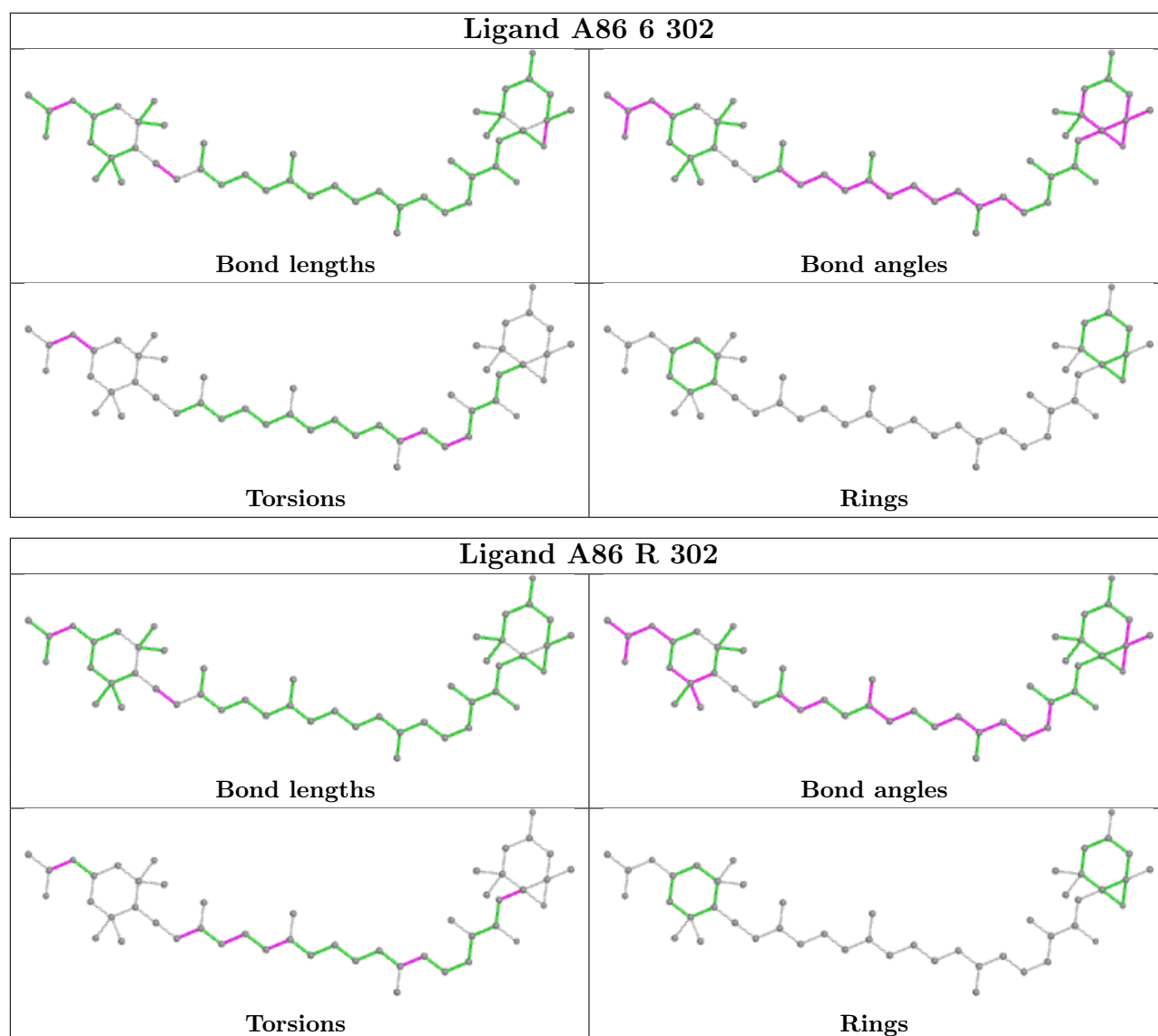


## Ligand A1EB1 9 302

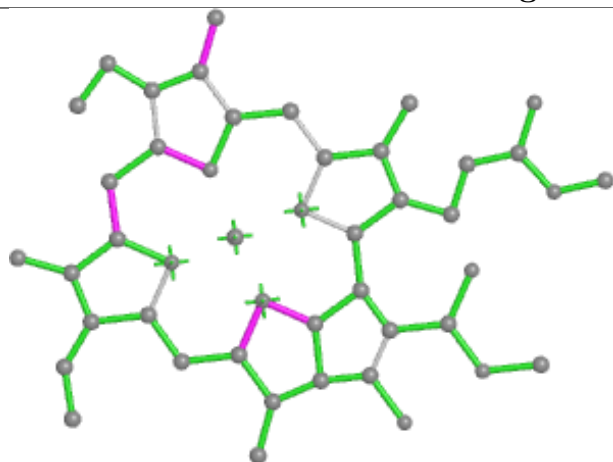


## Ligand A1EB1 L 303

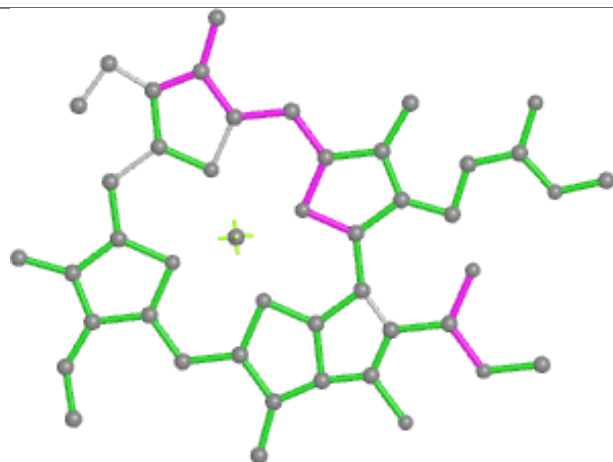




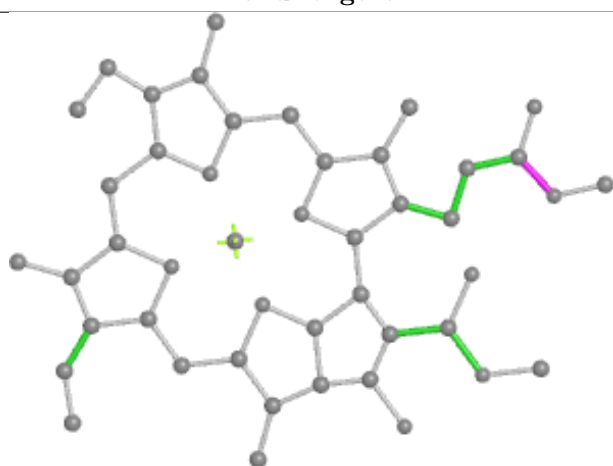
## Ligand CLA z 308



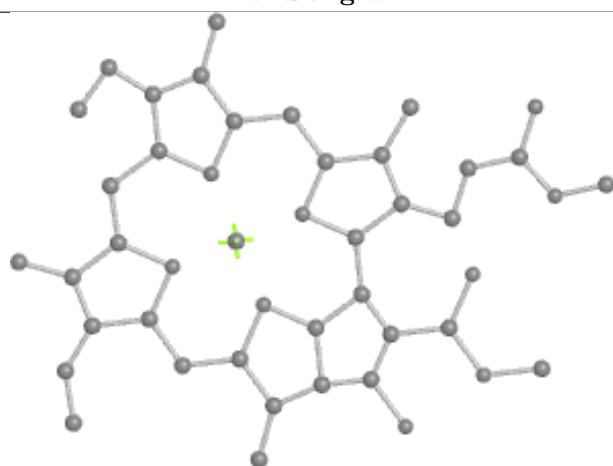
Bond lengths



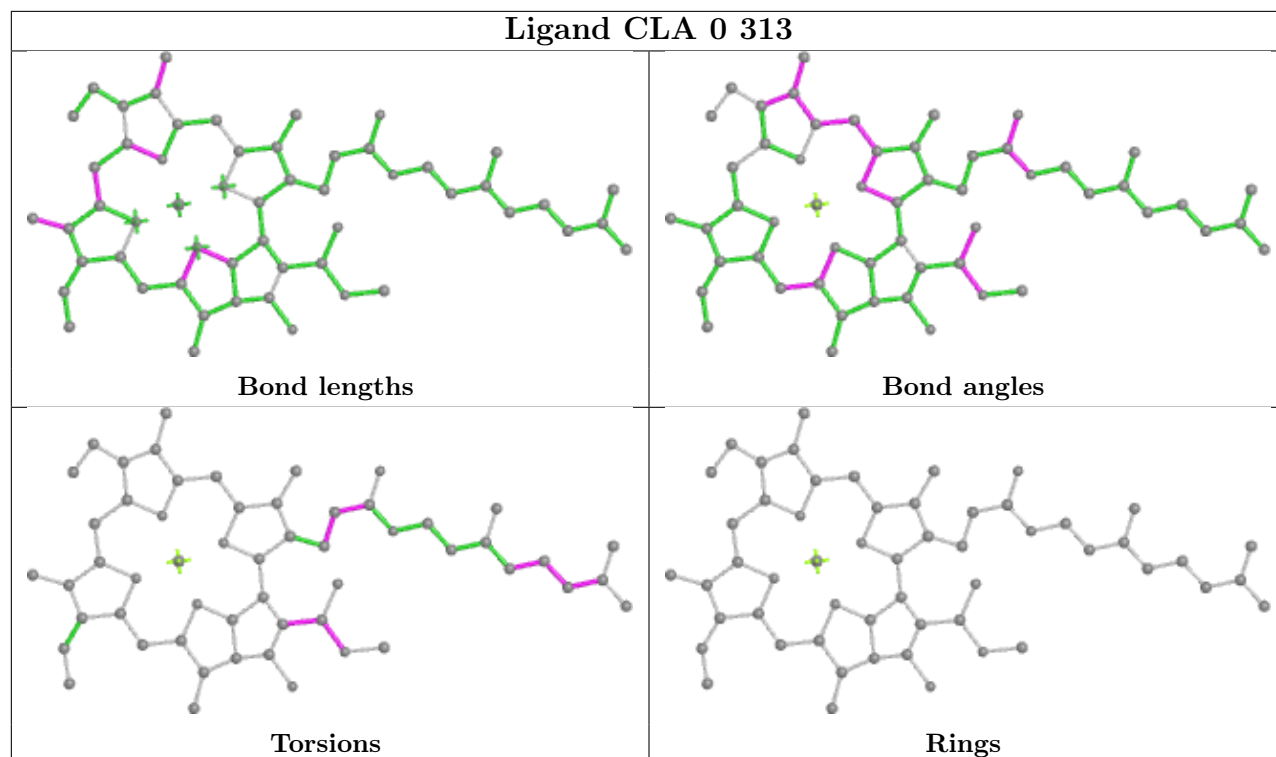
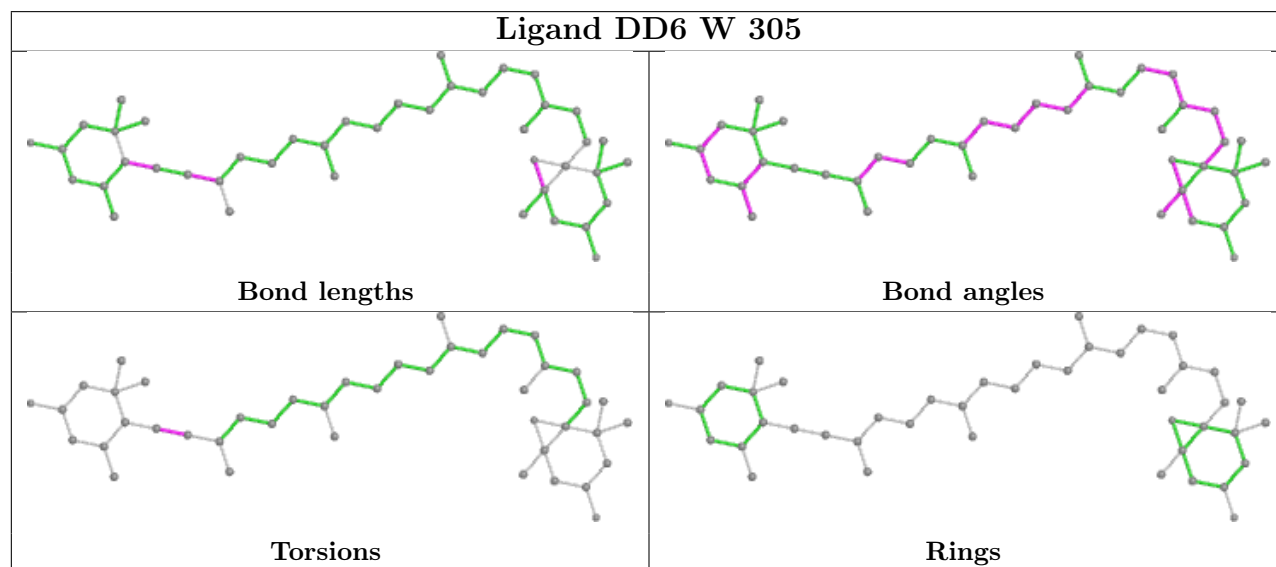
Bond angles

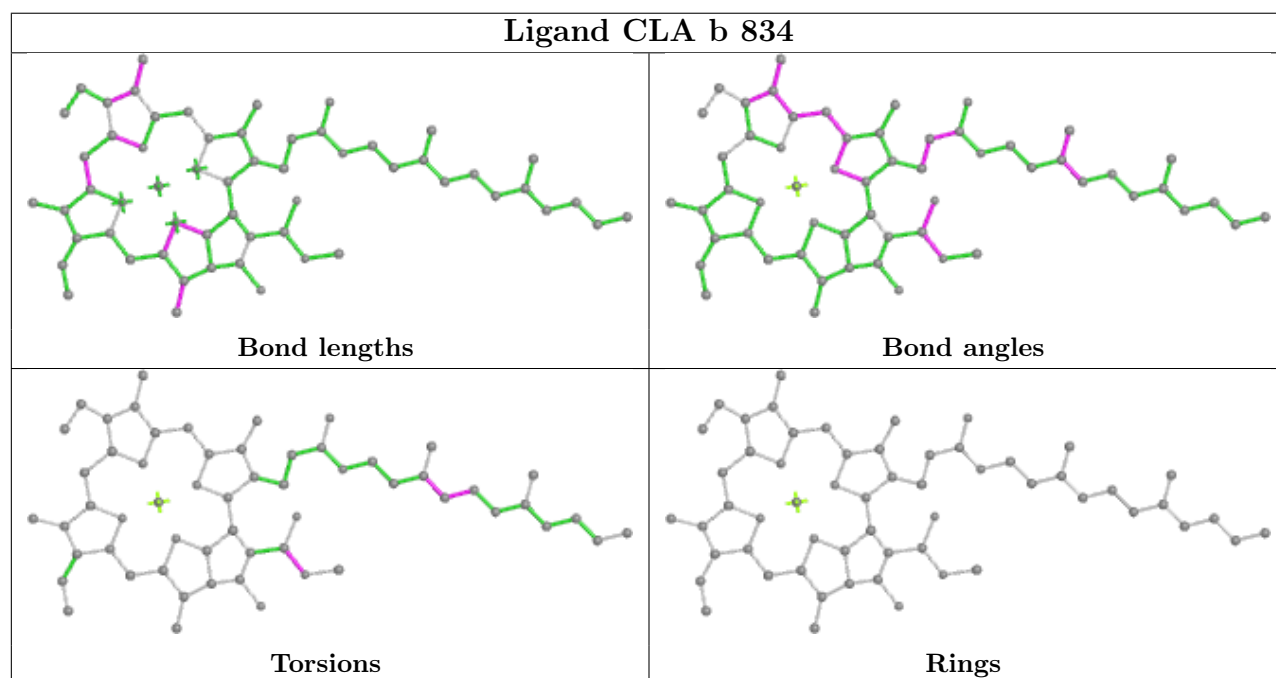
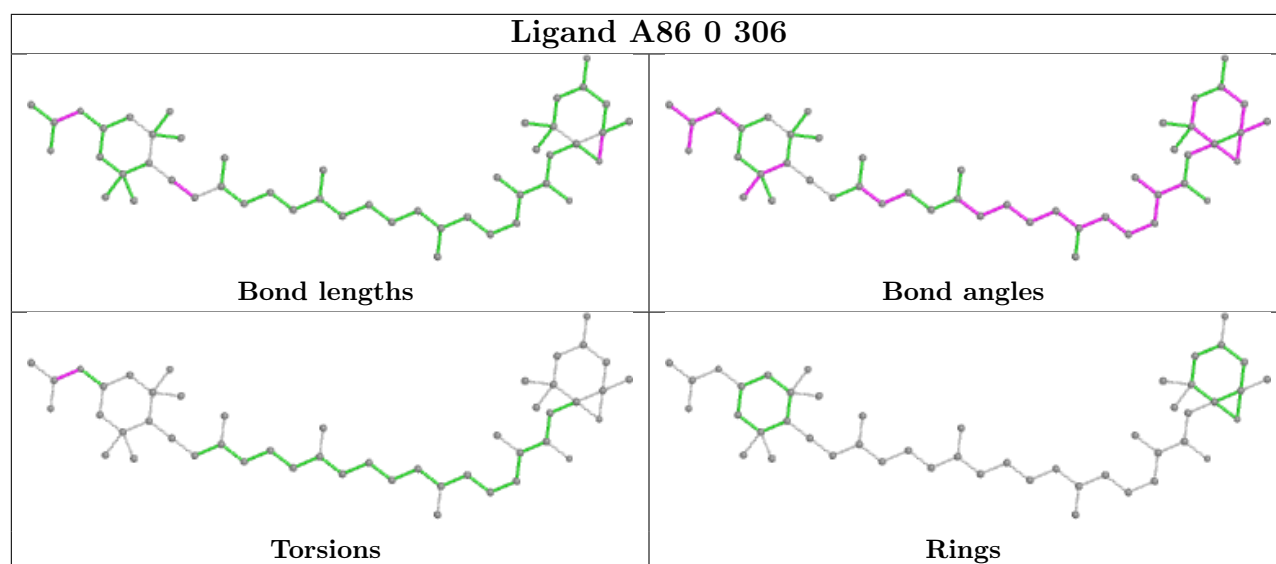


Torsions



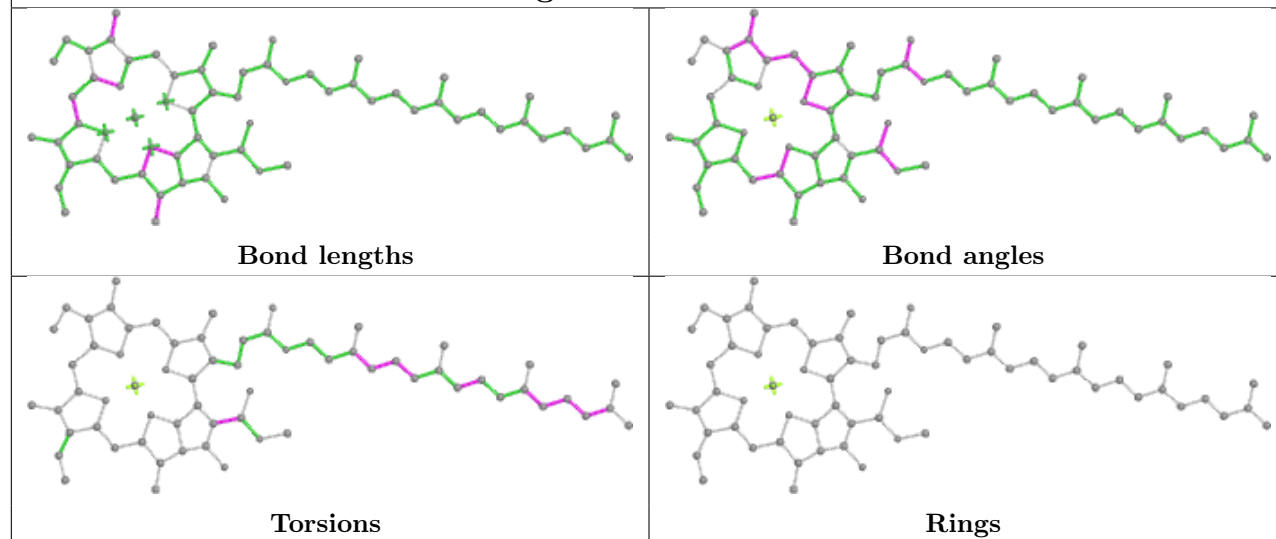
Rings

**Ligand CLA 0 313****Ligand DD6 W 305**

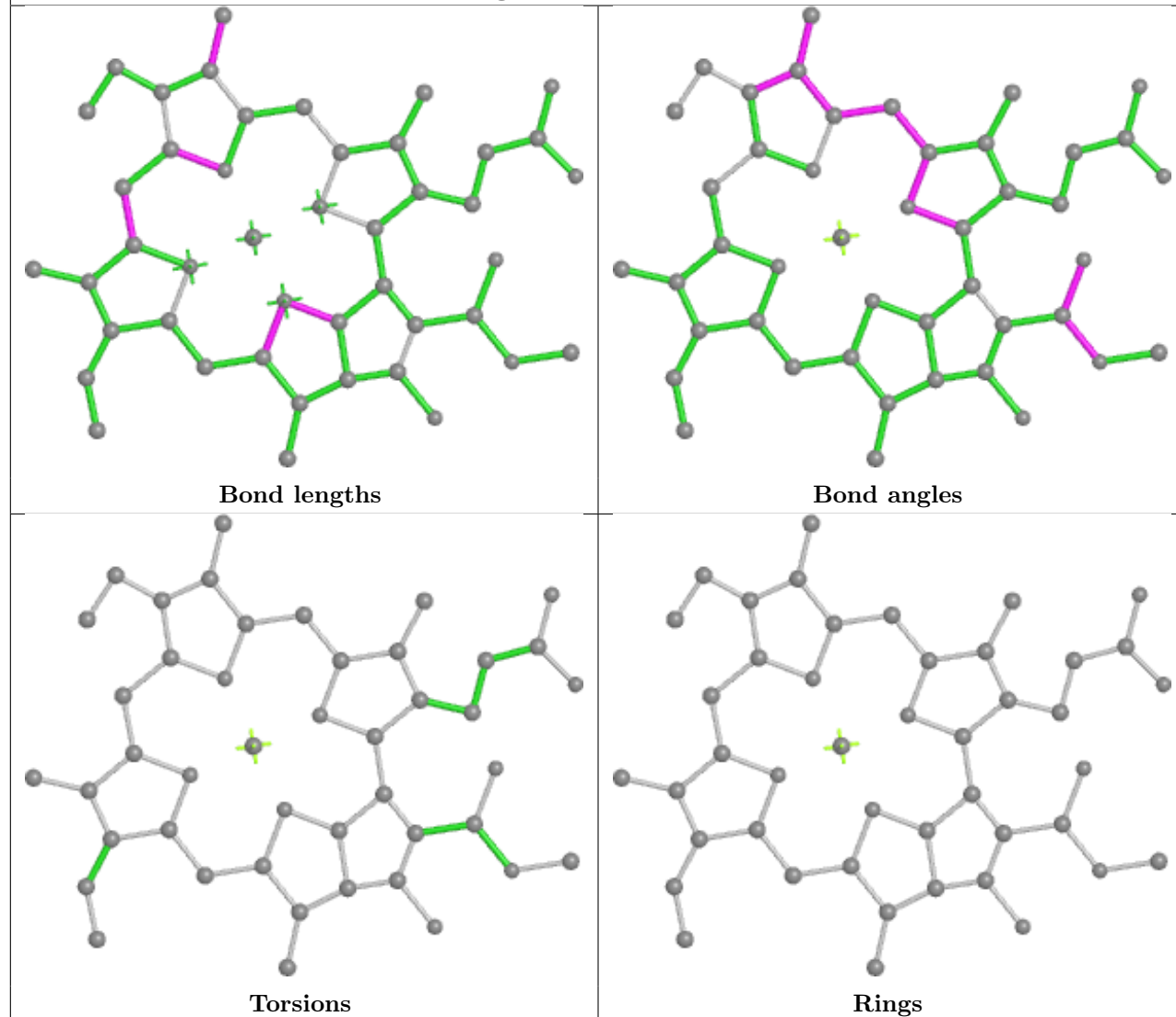


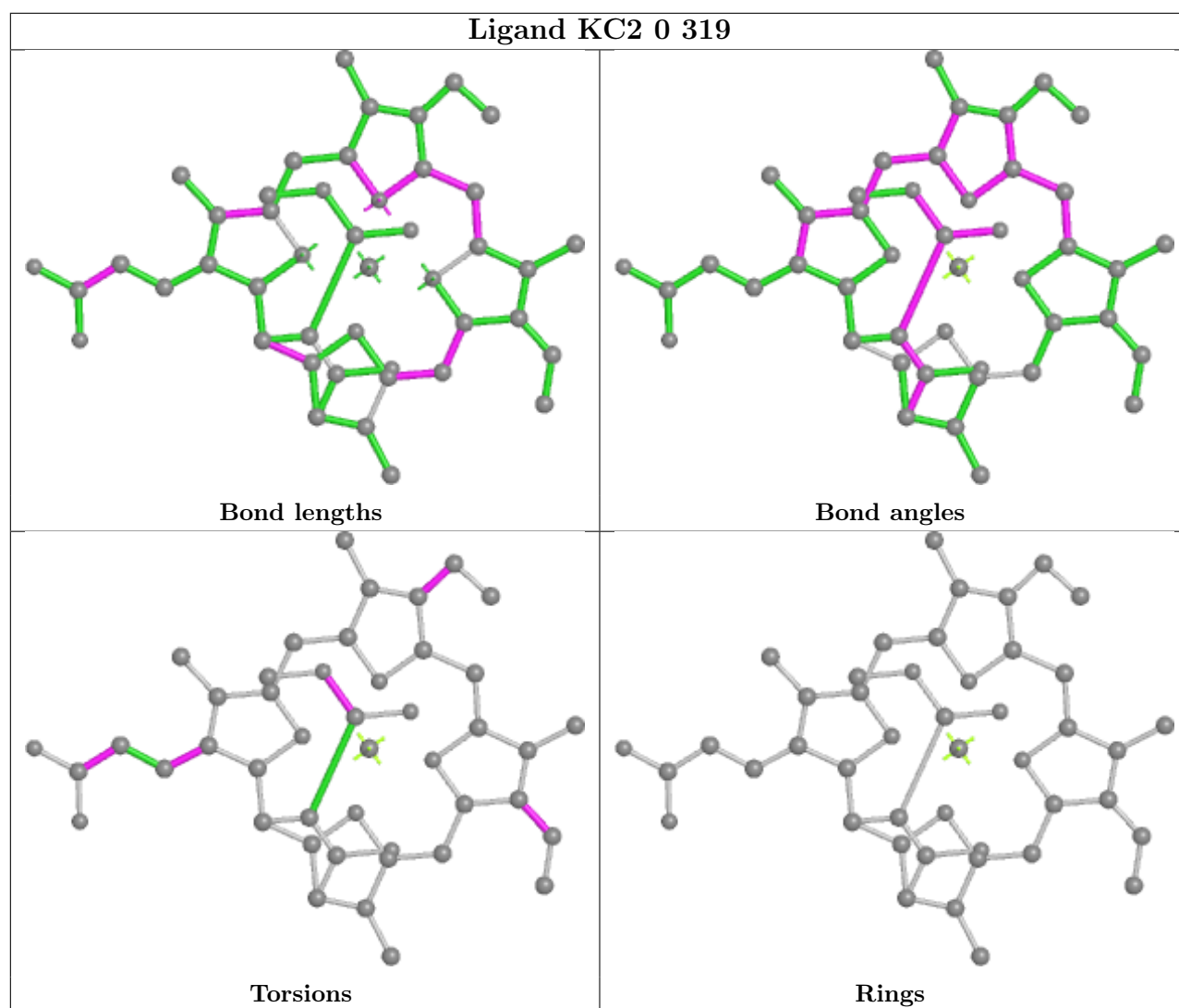
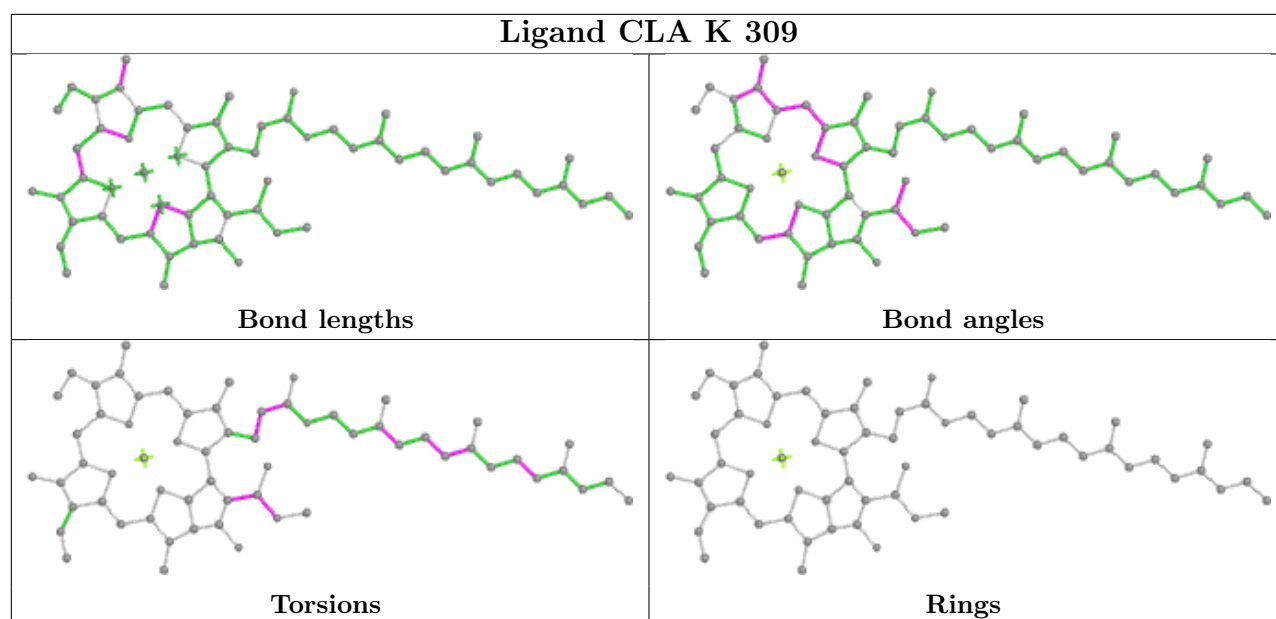


## Ligand CLA a 805

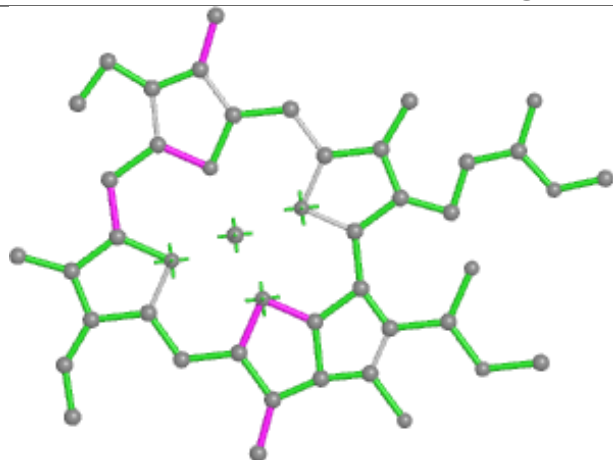


## Ligand CLA x 311

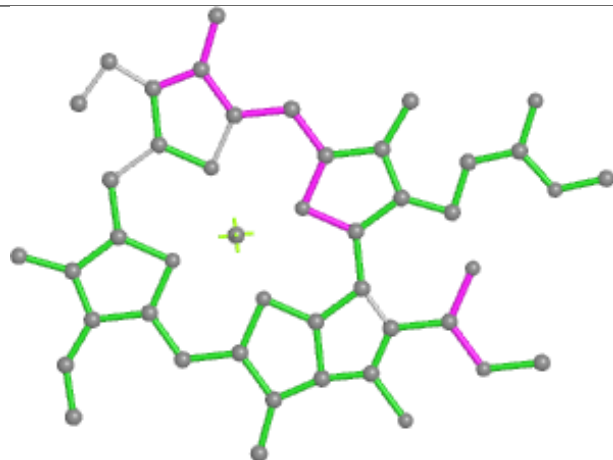




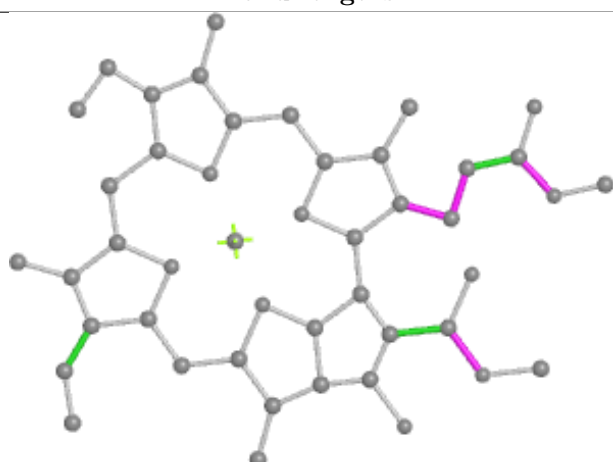
## Ligand CLA J 313



Bond lengths



Bond angles

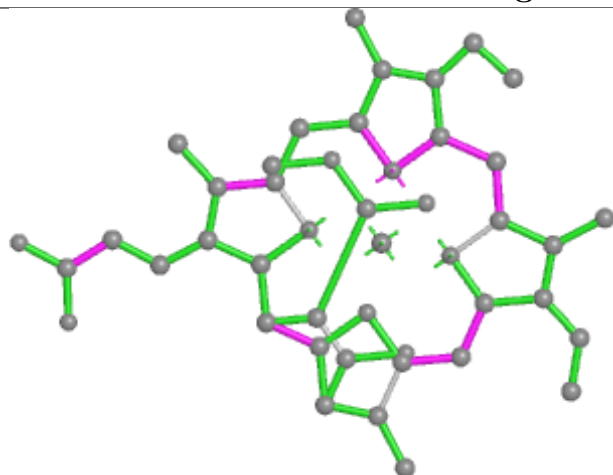


Torsions

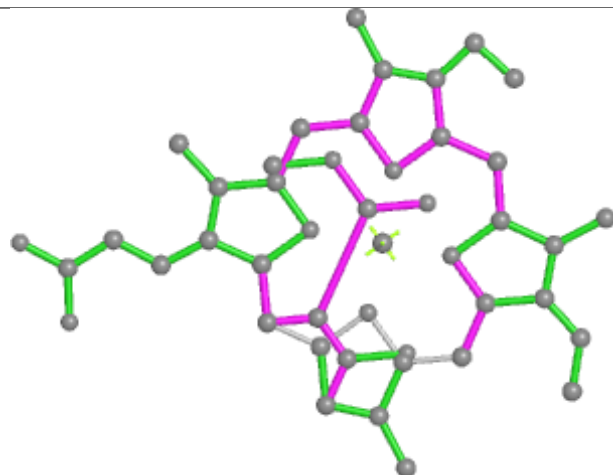


Rings

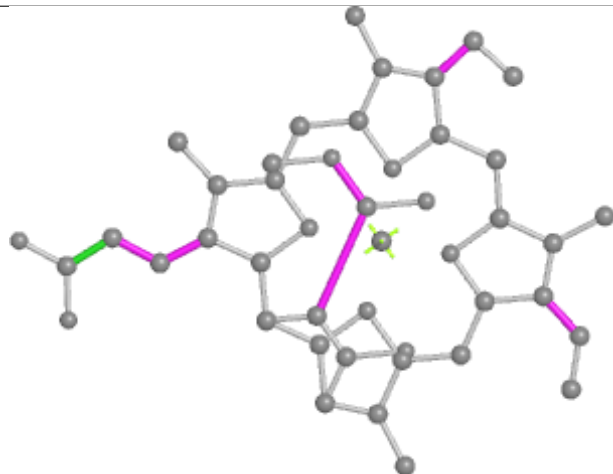
## Ligand KC2 X 306



Bond lengths



Bond angles

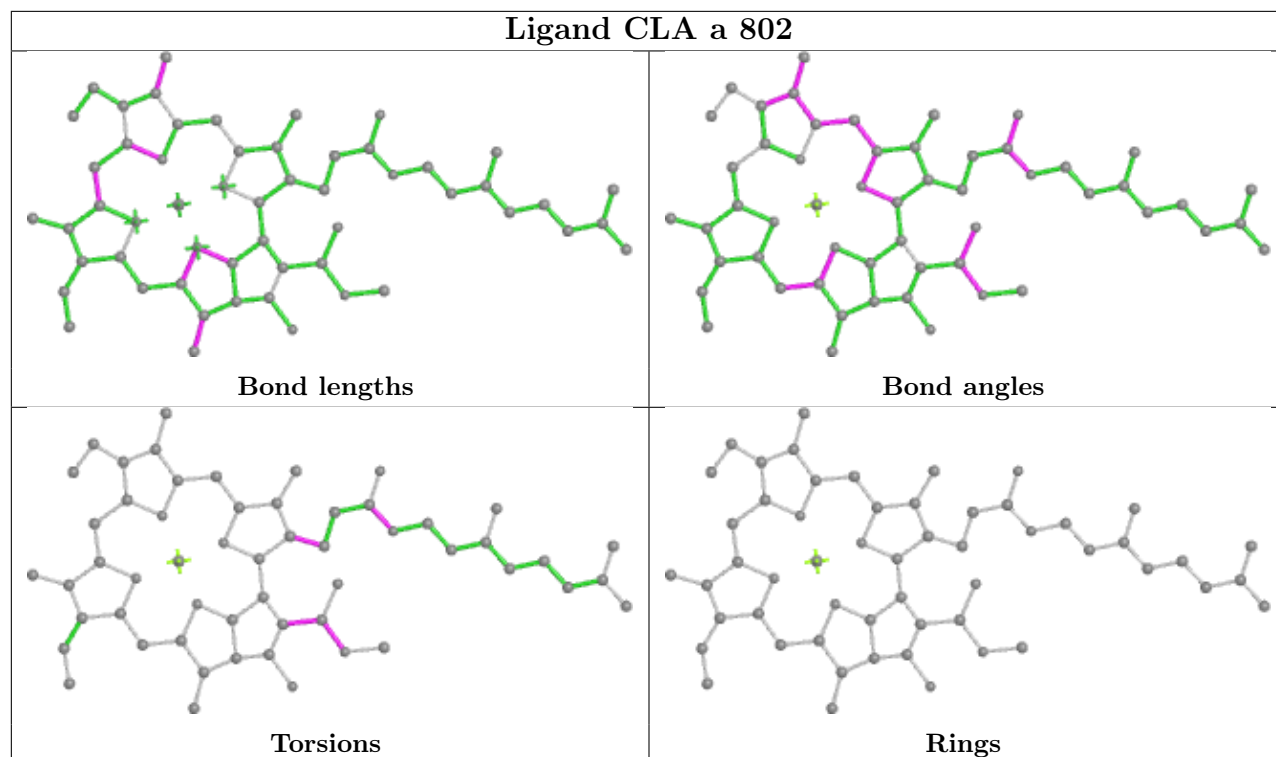


Torsions

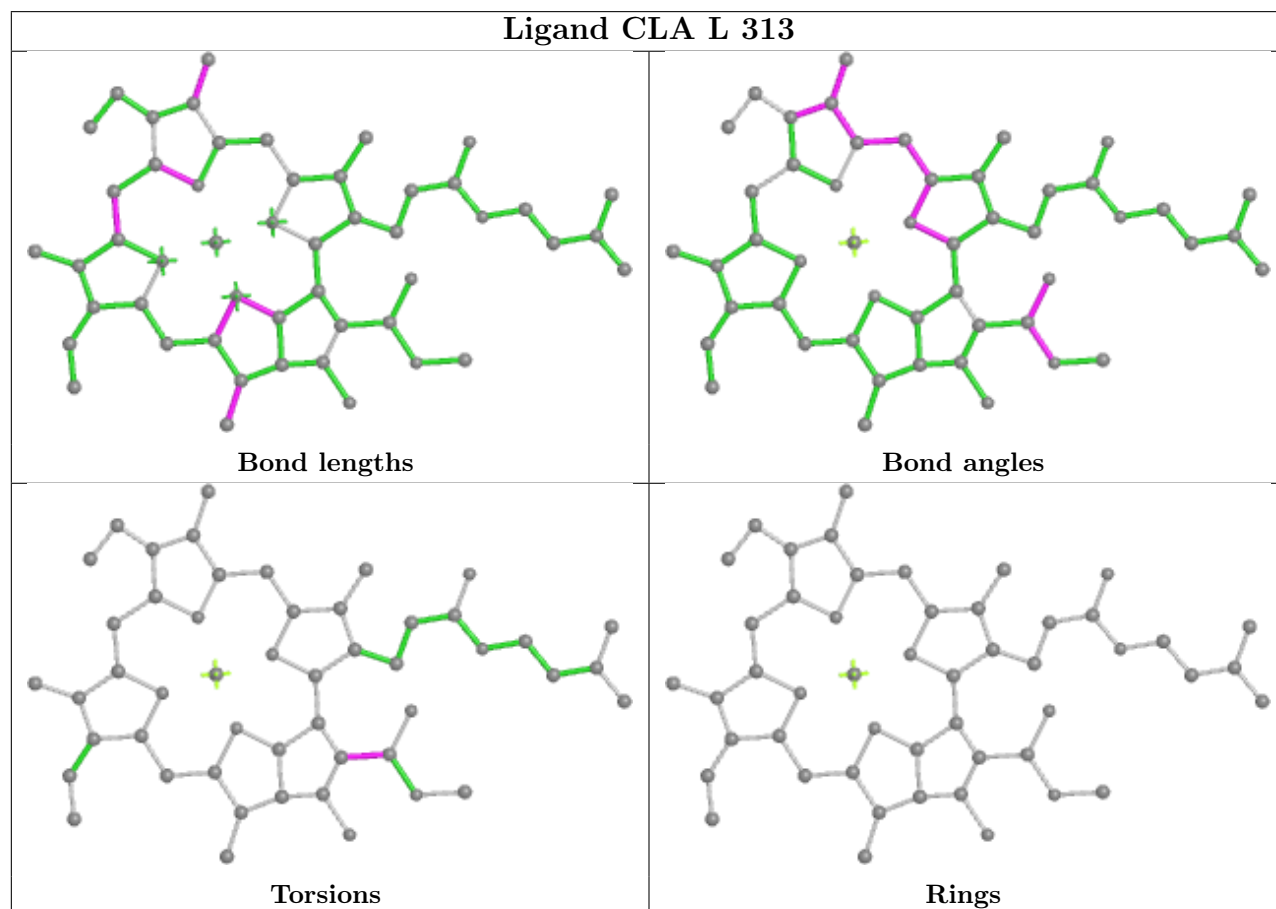


Rings

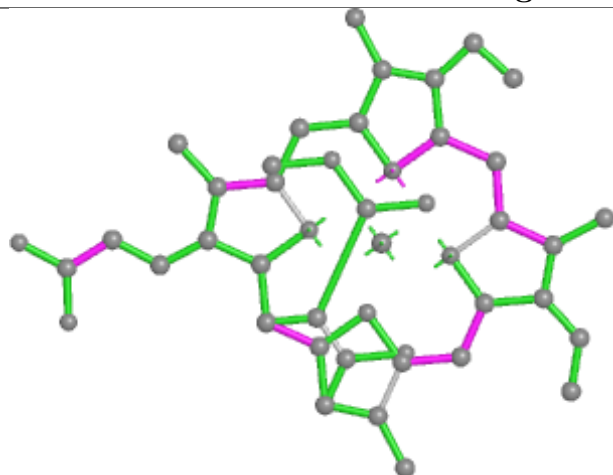
## Ligand CLA a 802



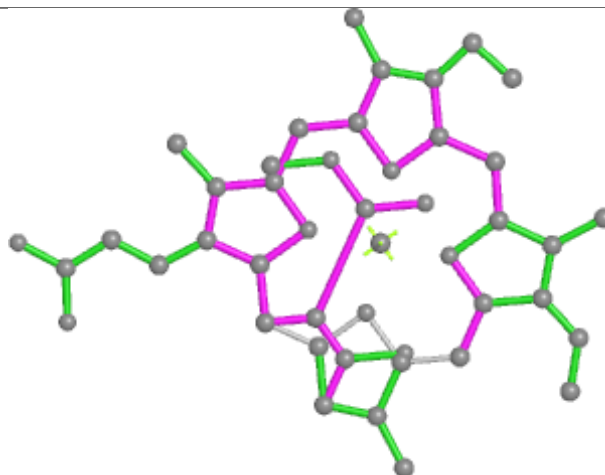
## Ligand CLA L 313



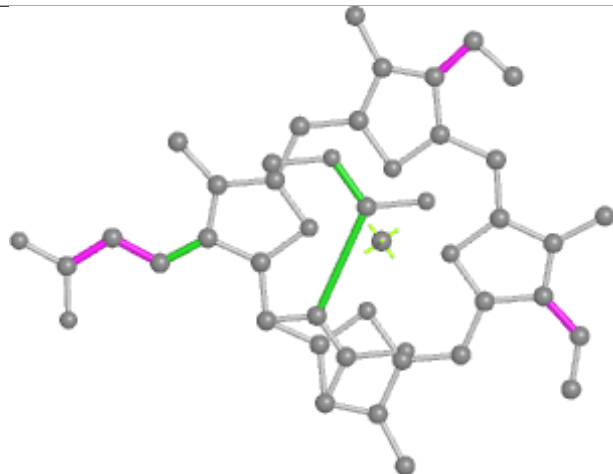
## Ligand KC2 V 312



Bond lengths



Bond angles

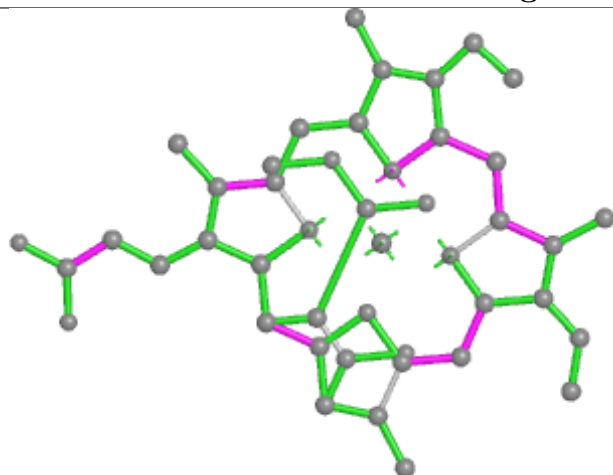


Torsions

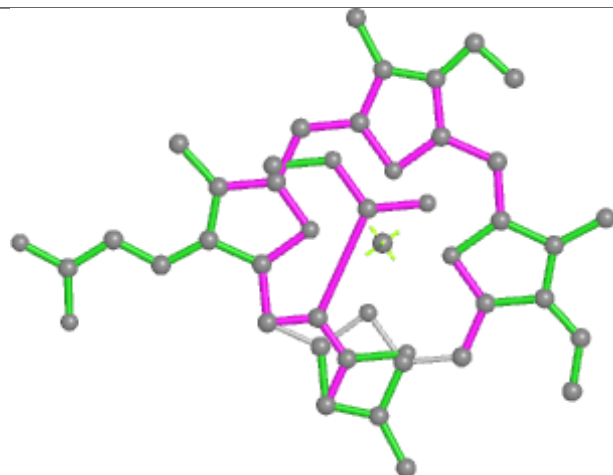


Rings

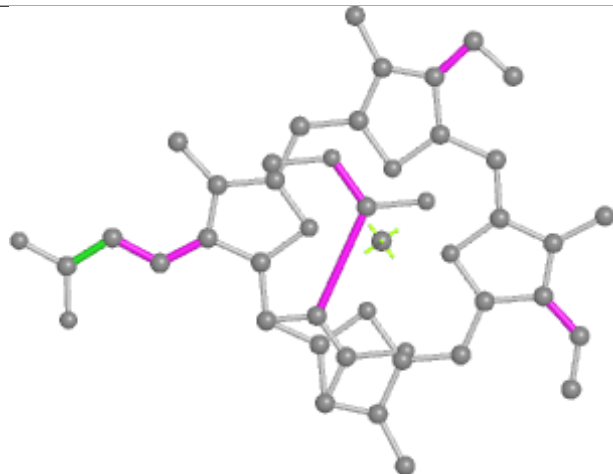
## Ligand KC2 8 316



Bond lengths



Bond angles

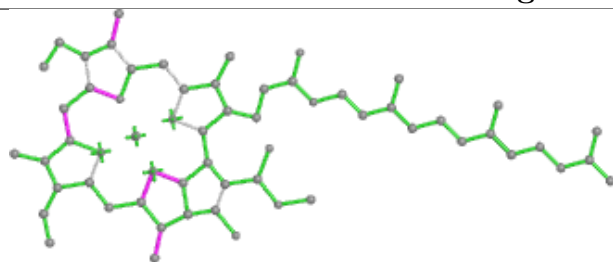


Torsions

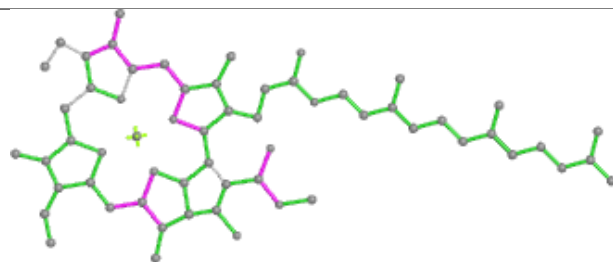


Rings

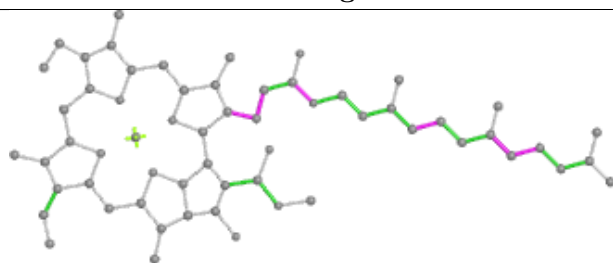
## Ligand CLA b 816



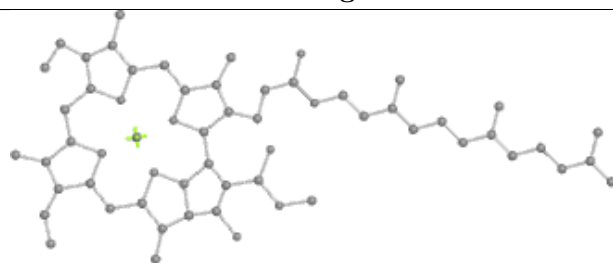
Bond lengths



Bond angles

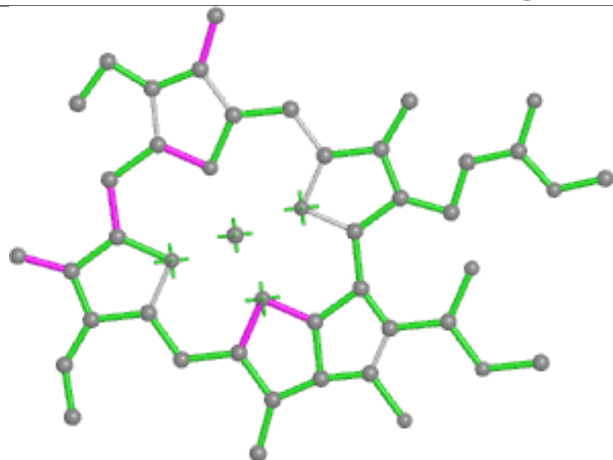


Torsions

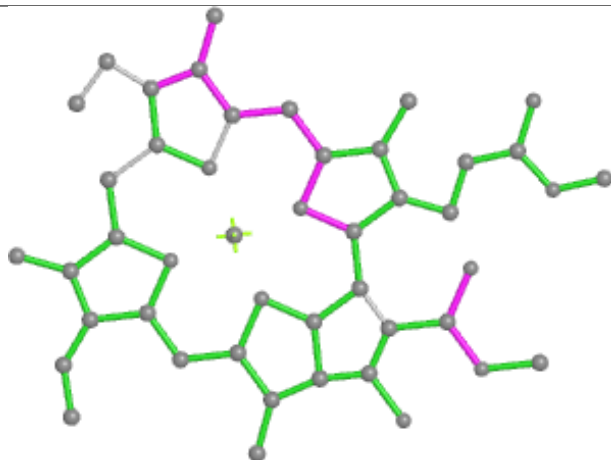


Rings

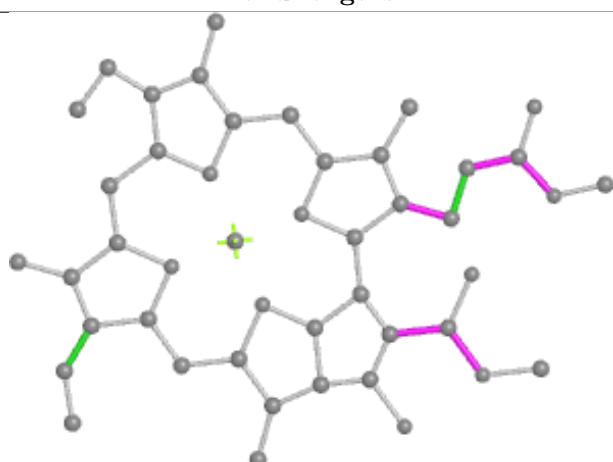
## Ligand CLA 3 323



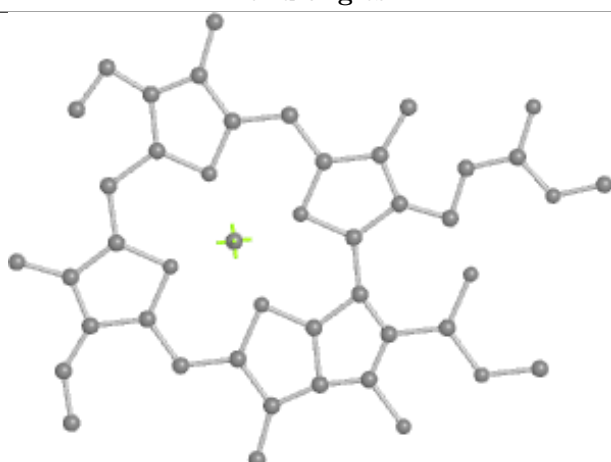
Bond lengths



Bond angles



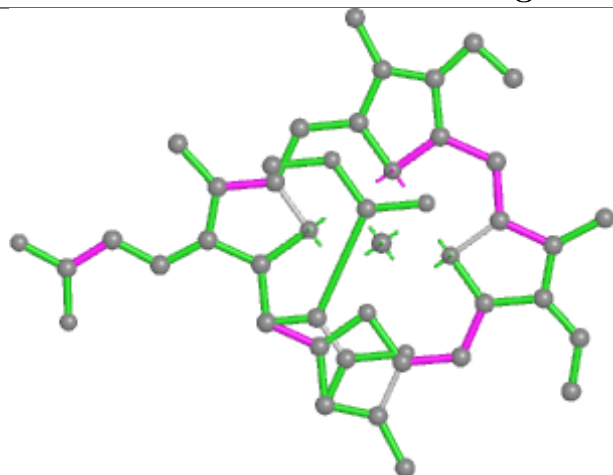
Torsions



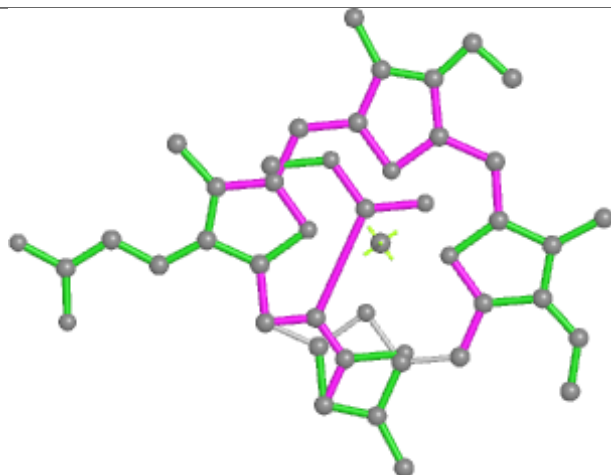
Rings



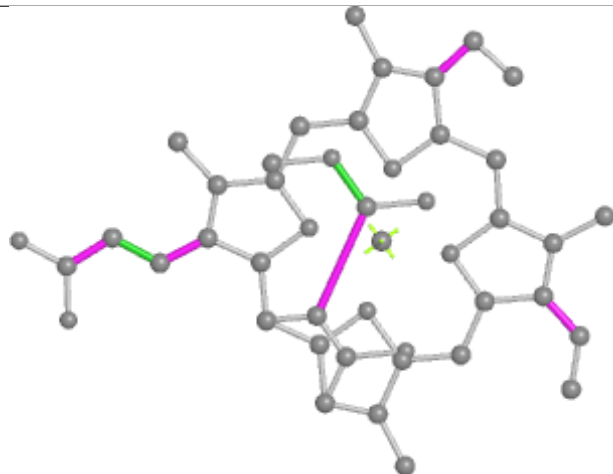
## Ligand KC2 V 320



Bond lengths



Bond angles

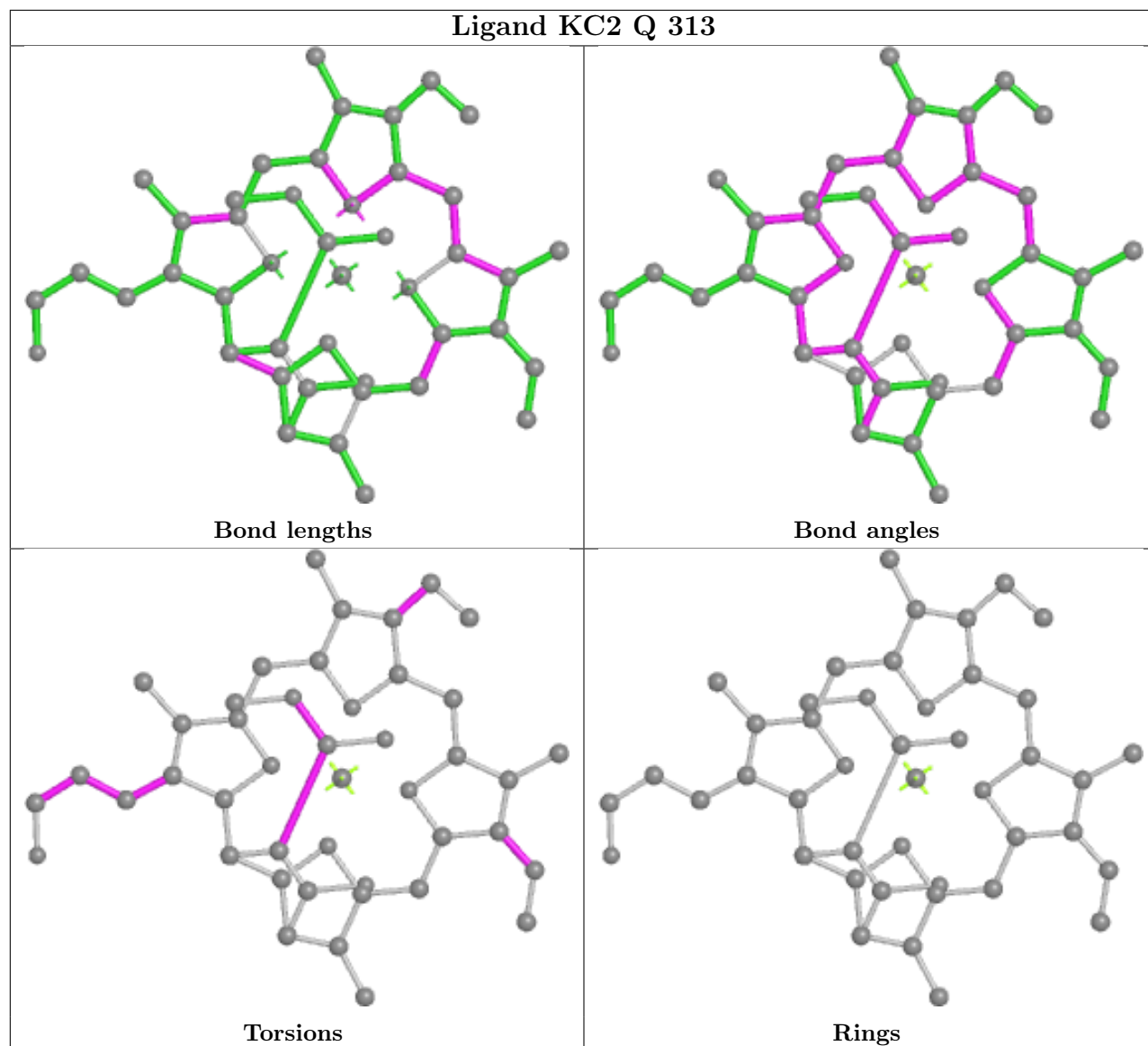


Torsions

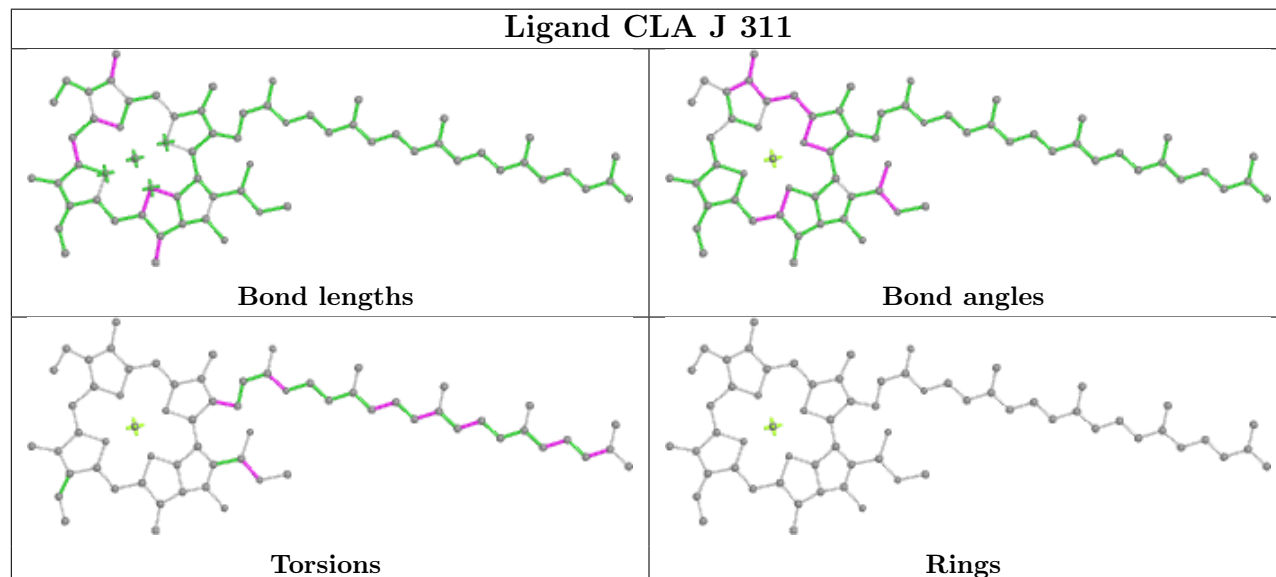


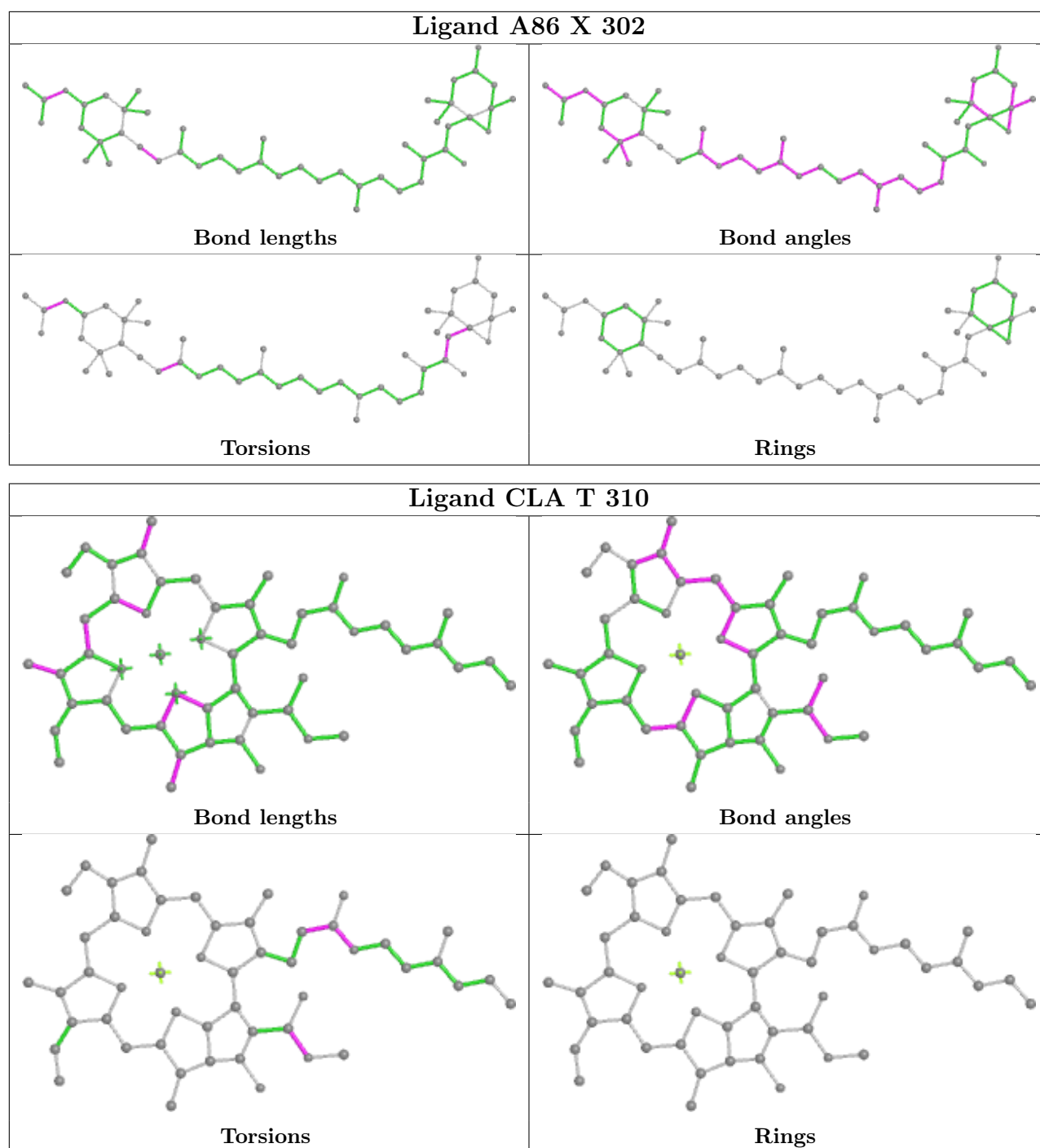
Rings

## Ligand KC2 Q 313

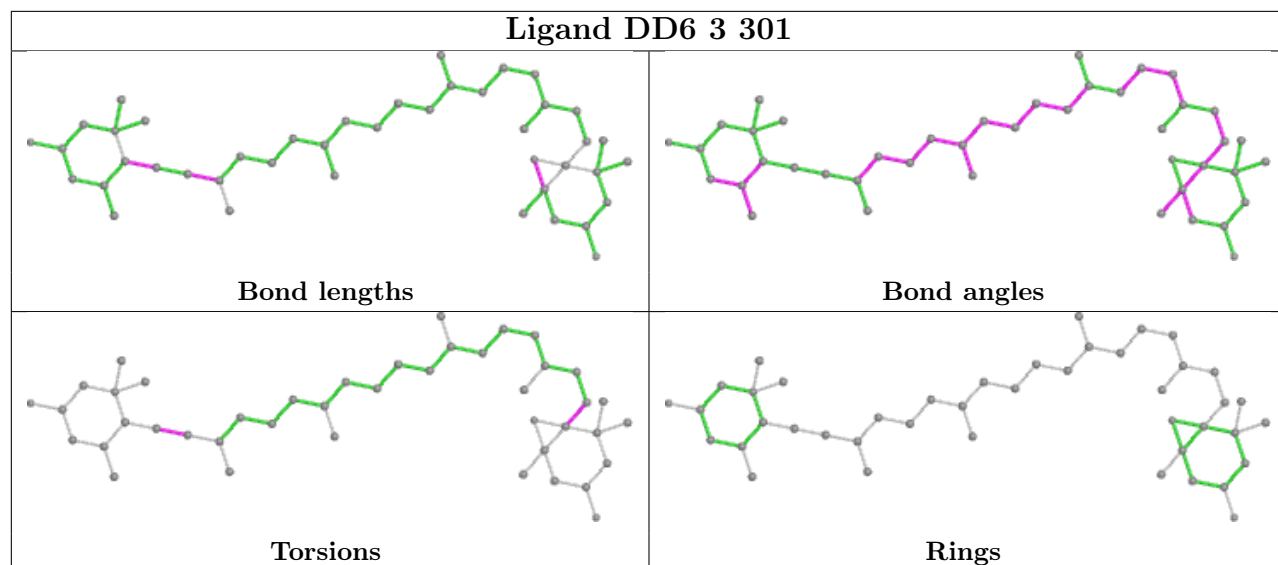


## Ligand CLA J 311

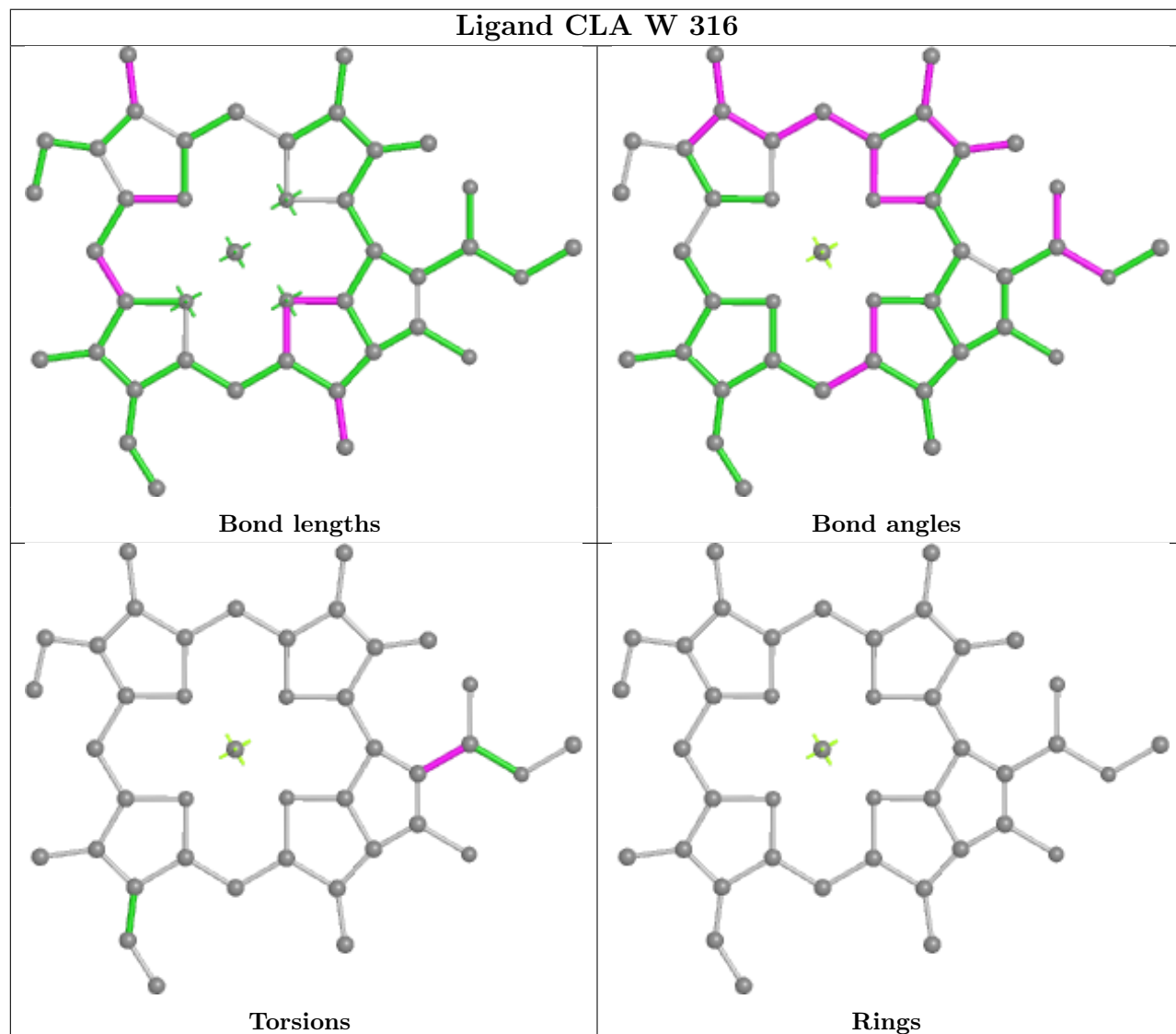


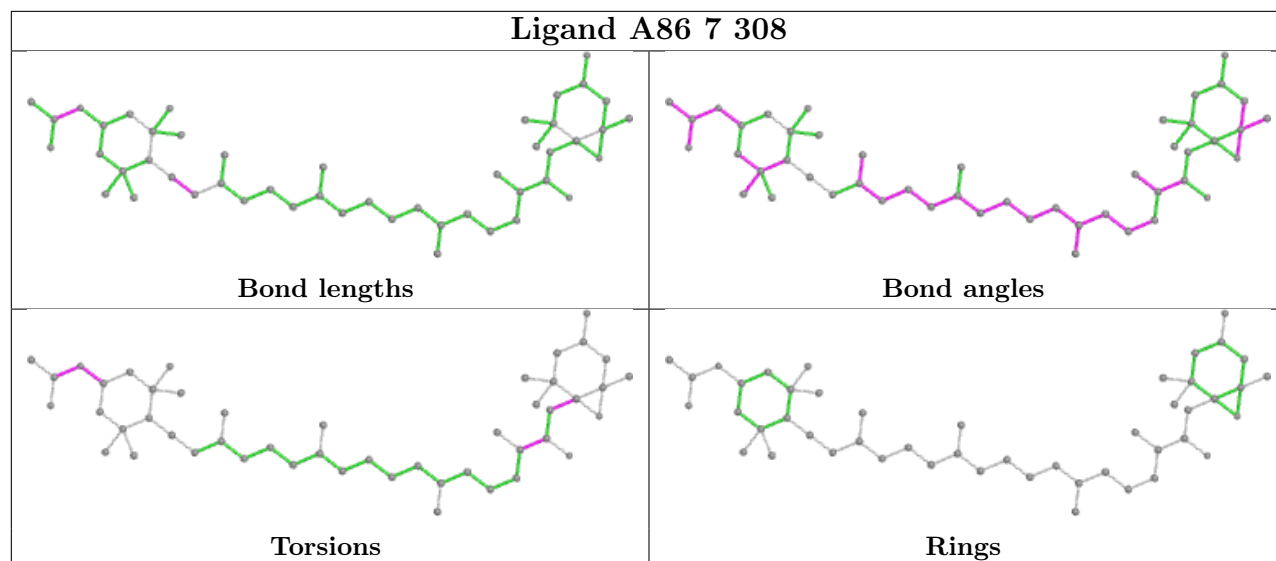
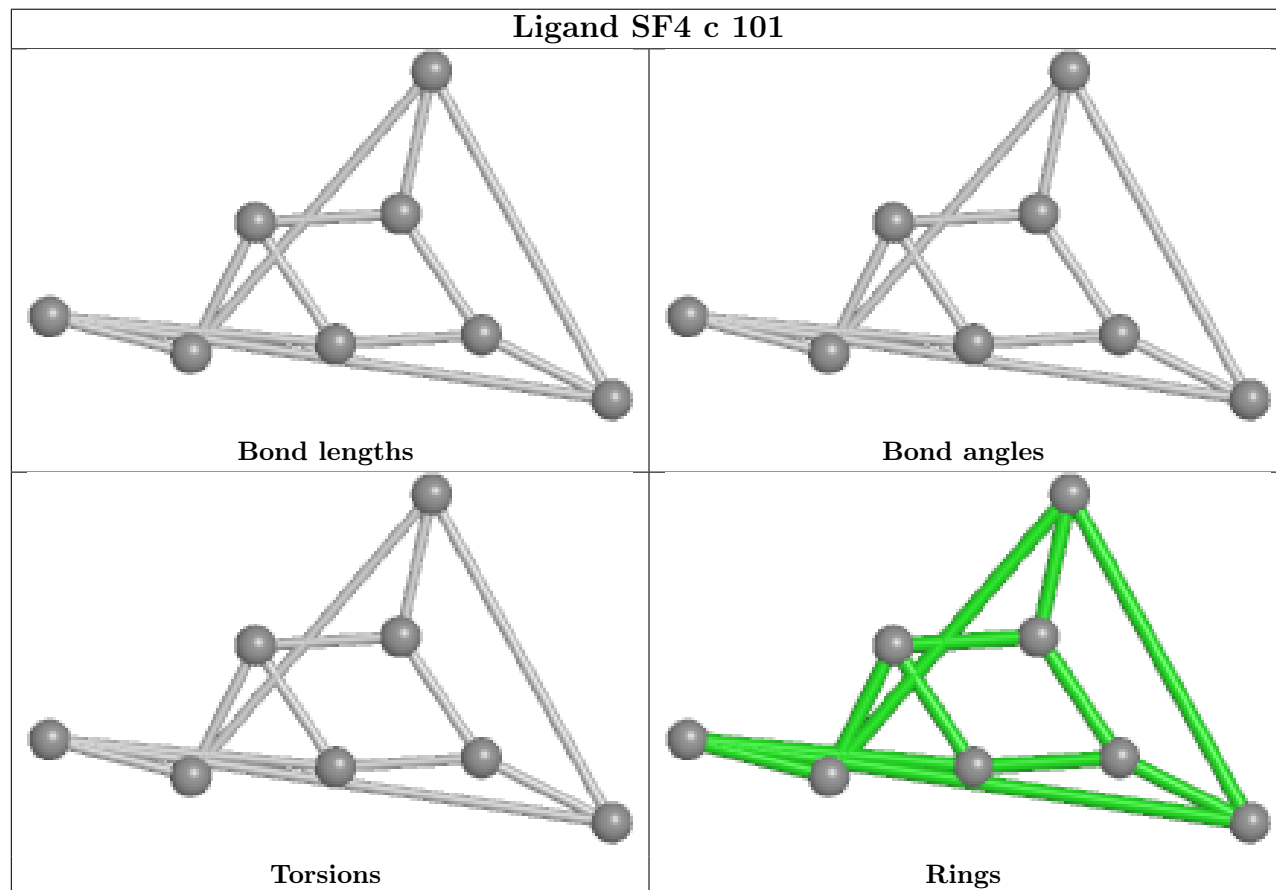


## Ligand DD6 3 301

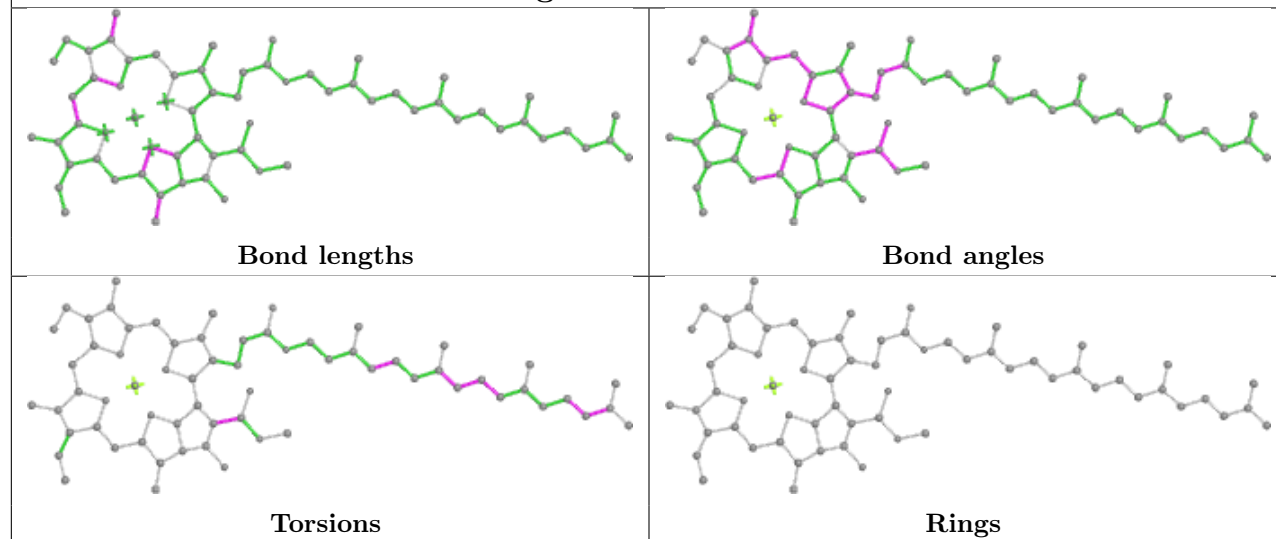


## Ligand CLA W 316

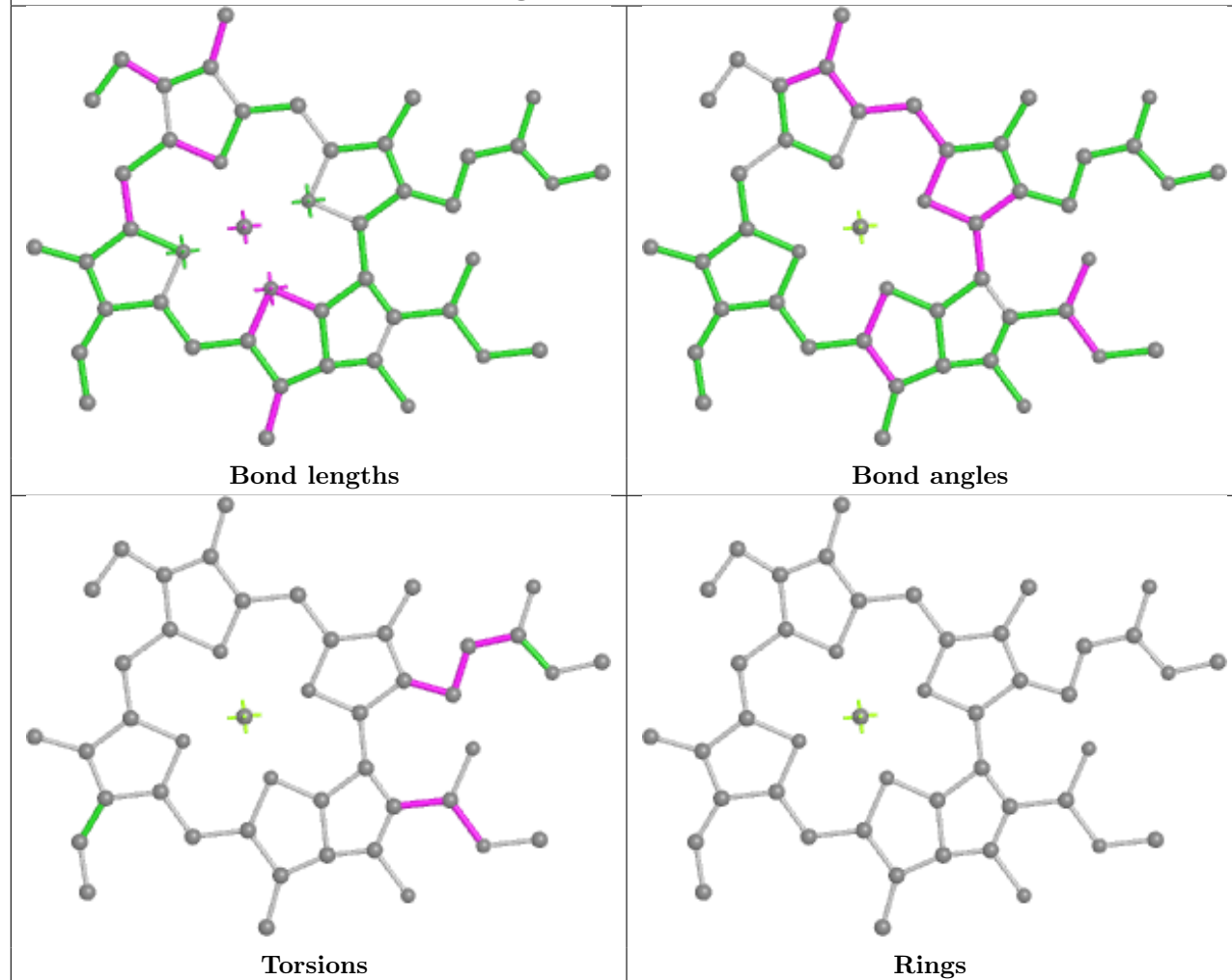


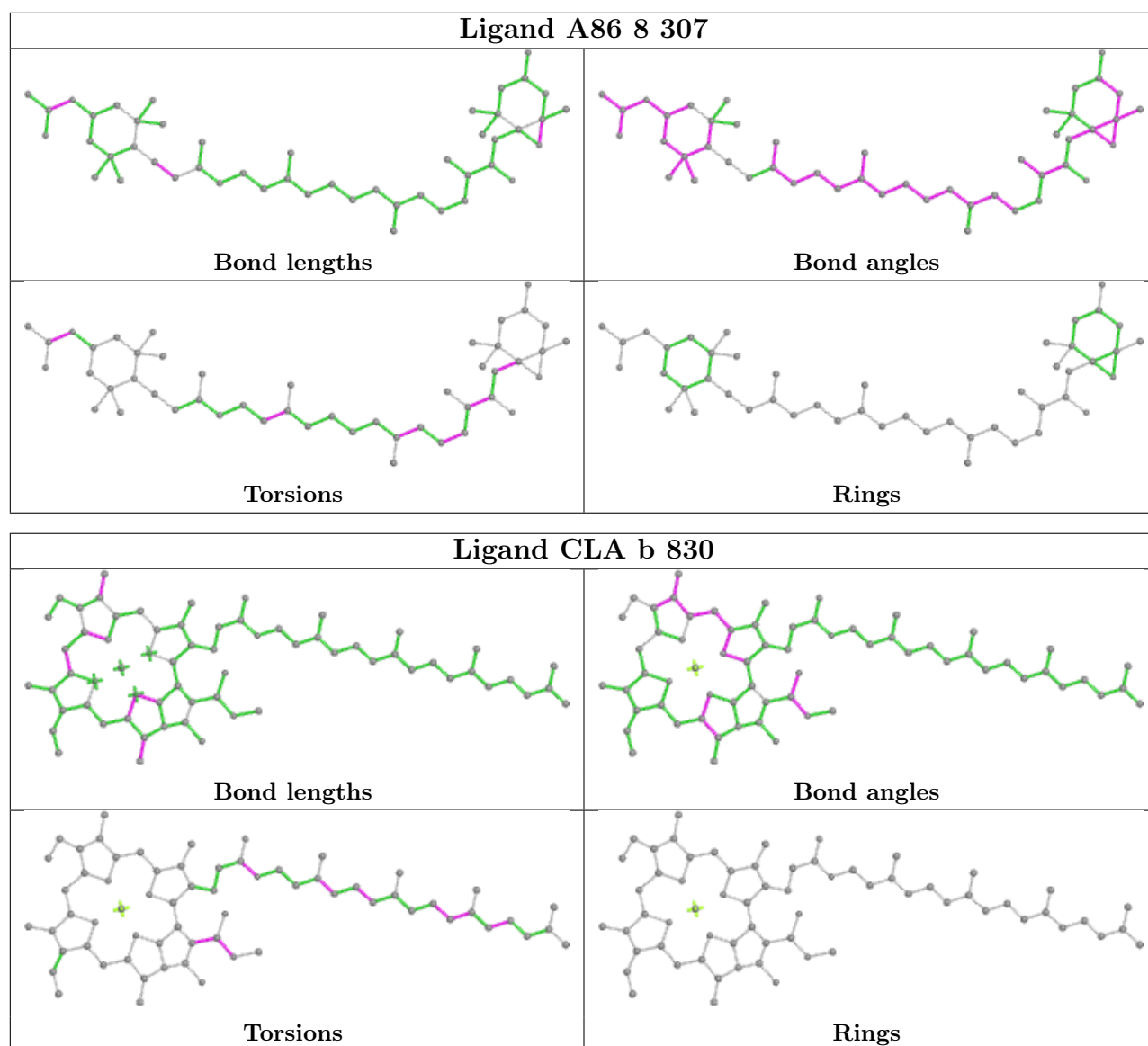
**Ligand A86 7 308****Ligand SF4 c 101**

## Ligand CLA a 823

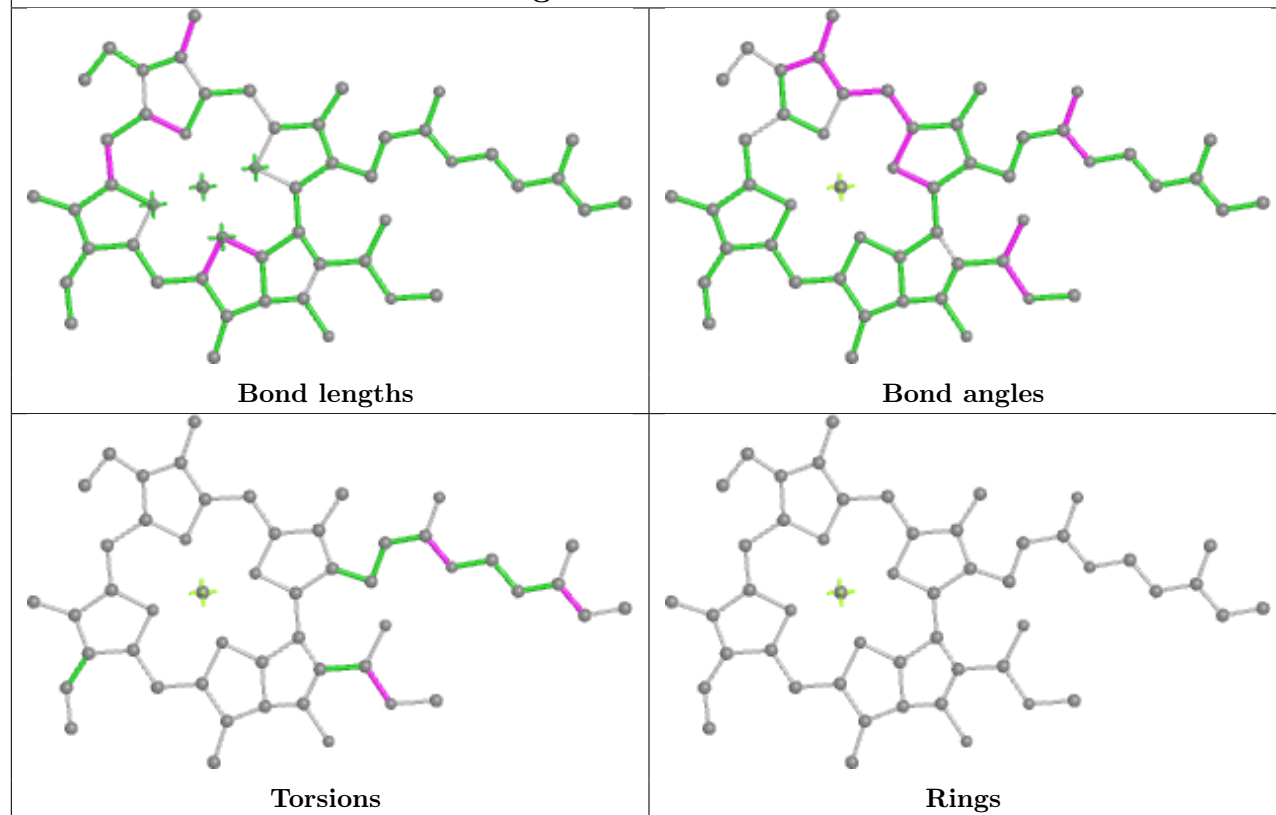


## Ligand CLA U 201

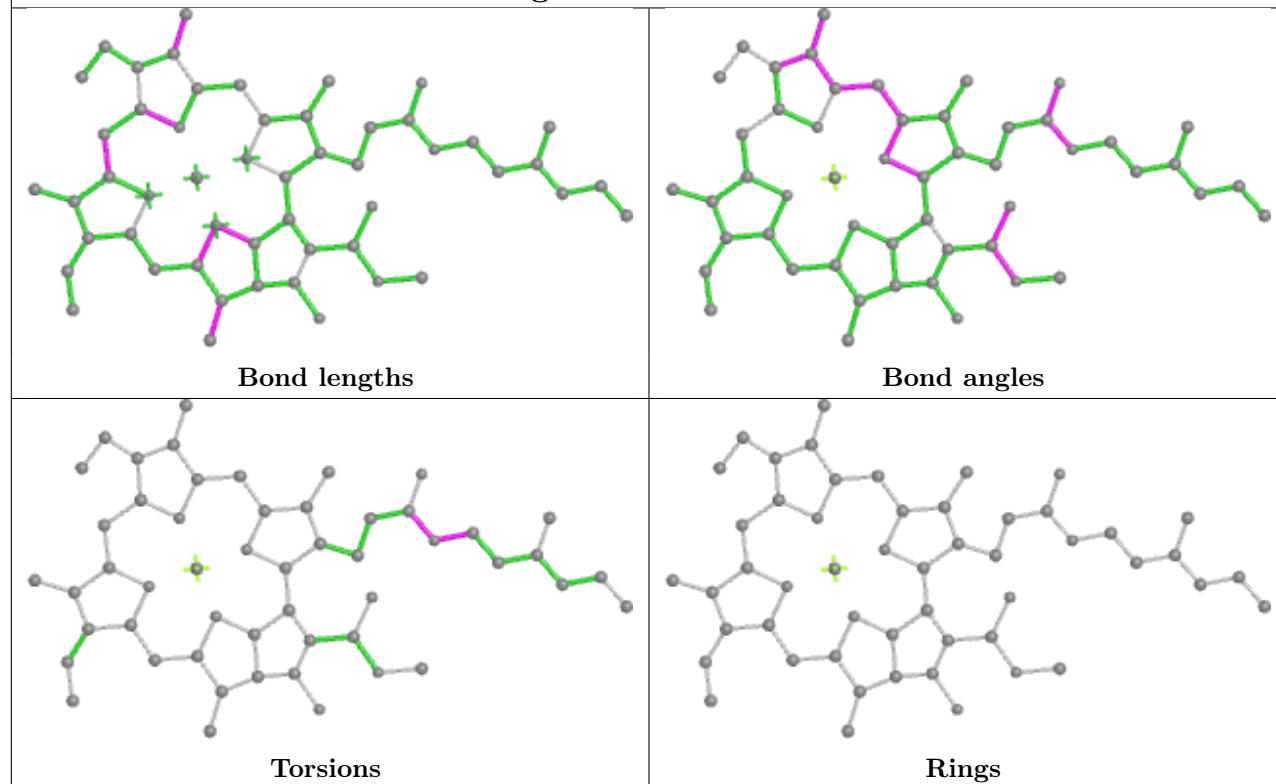




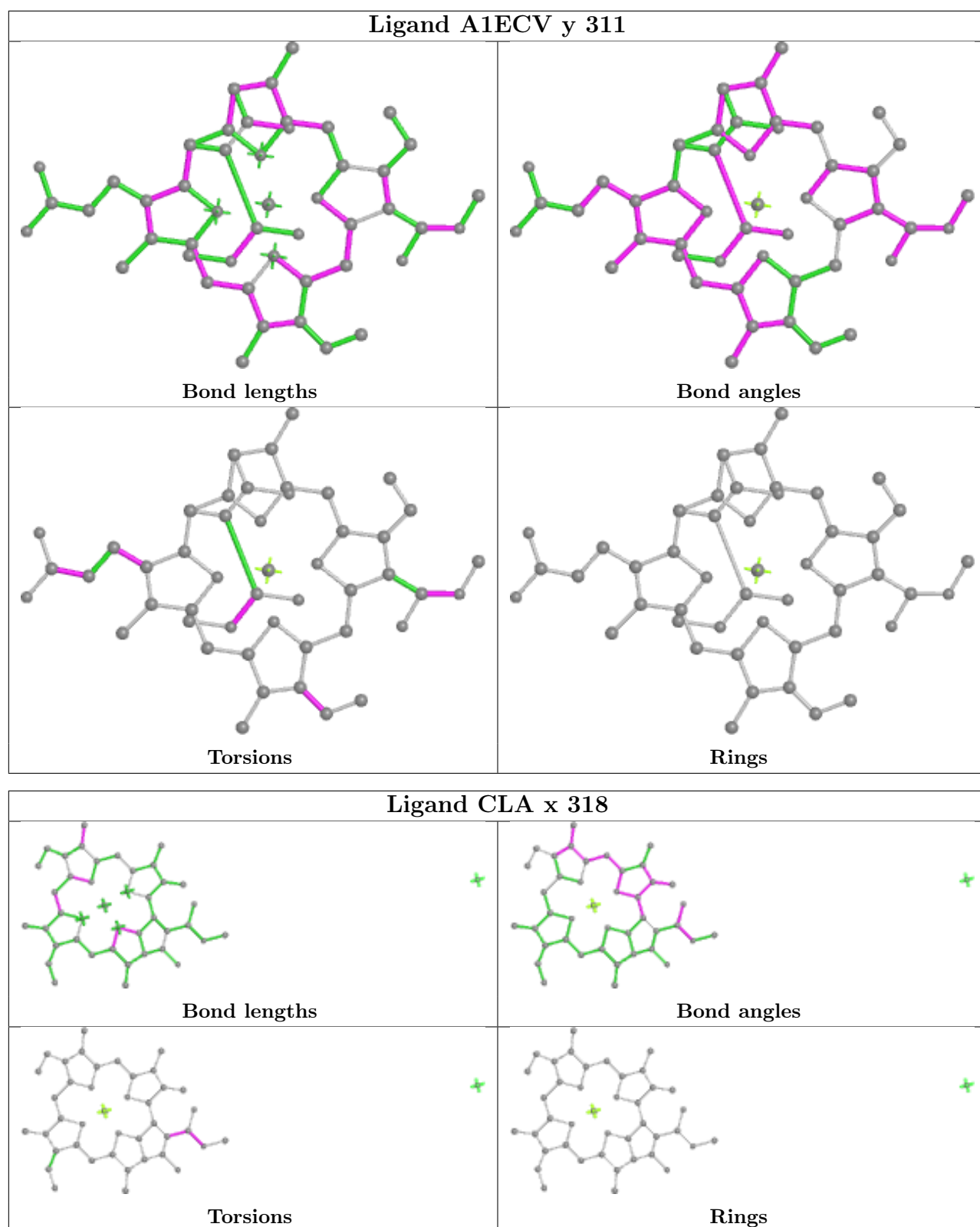
## Ligand CLA P 316

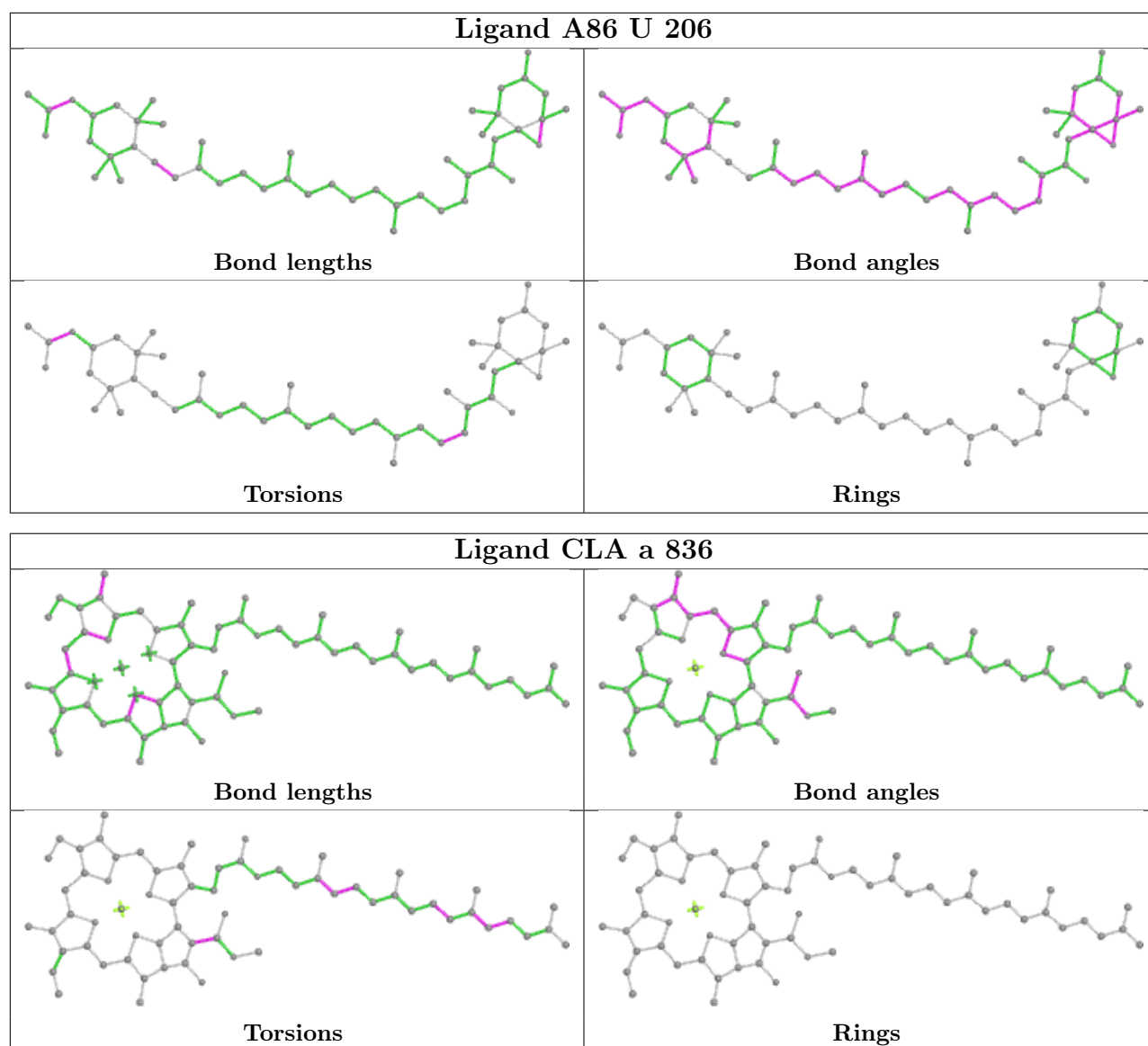


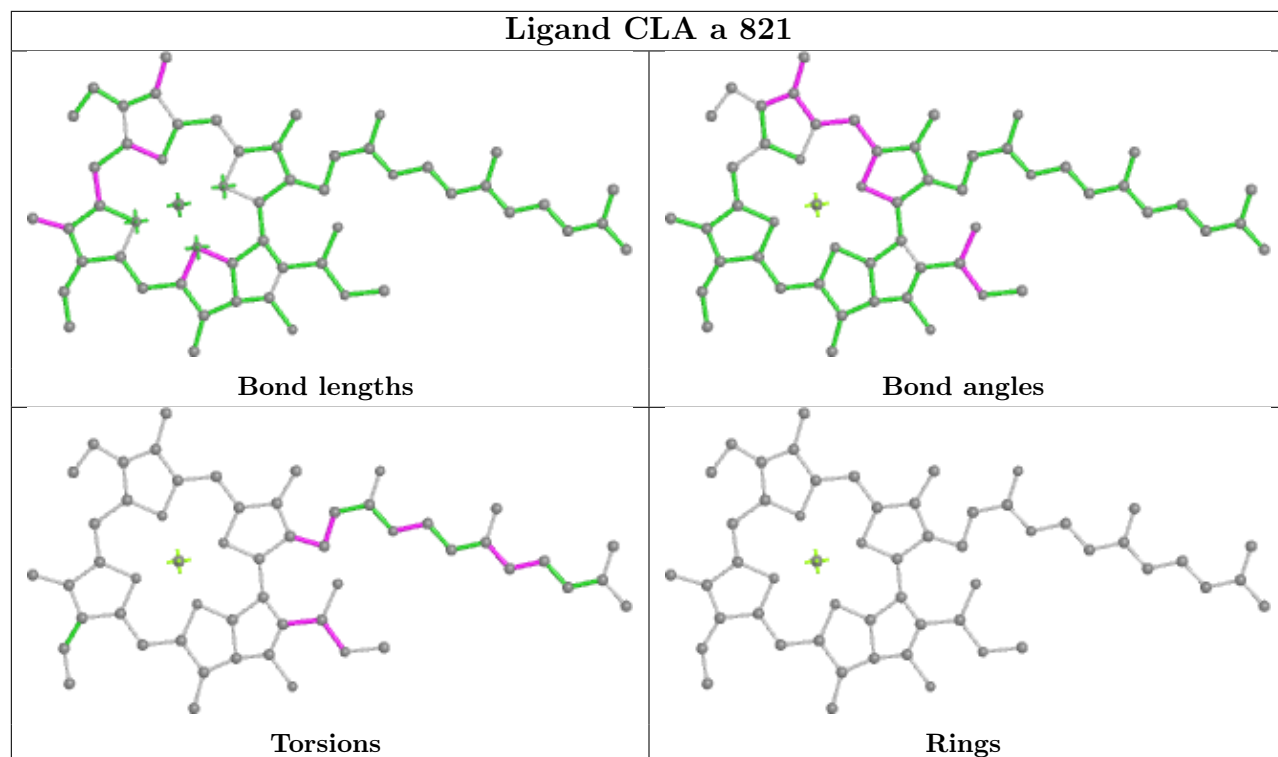
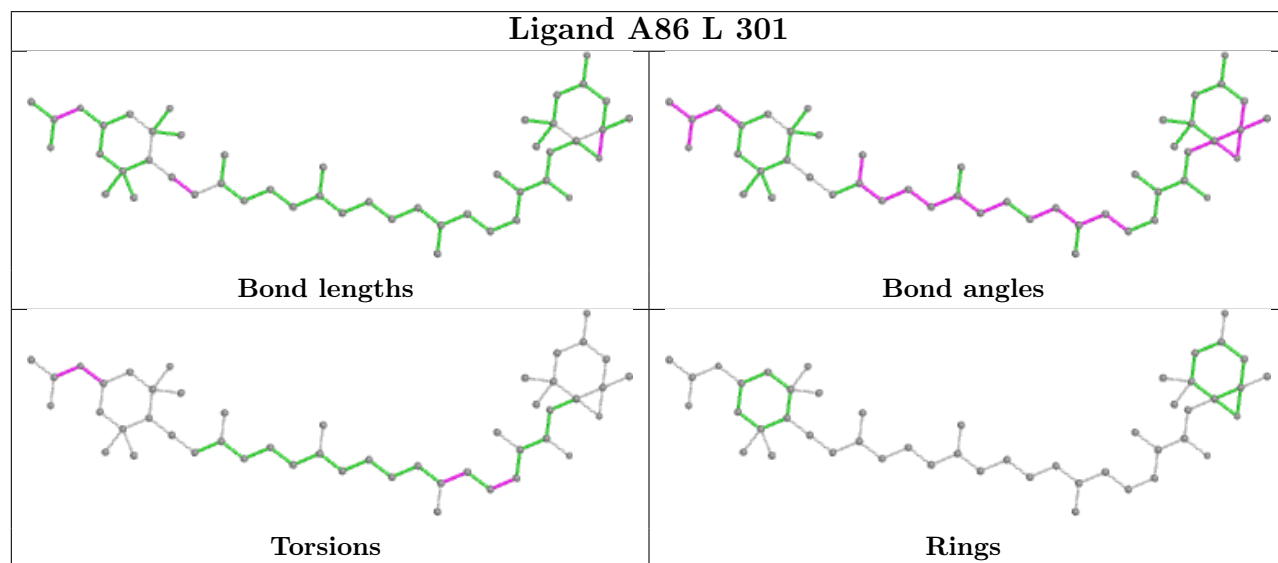
## Ligand CLA H 309



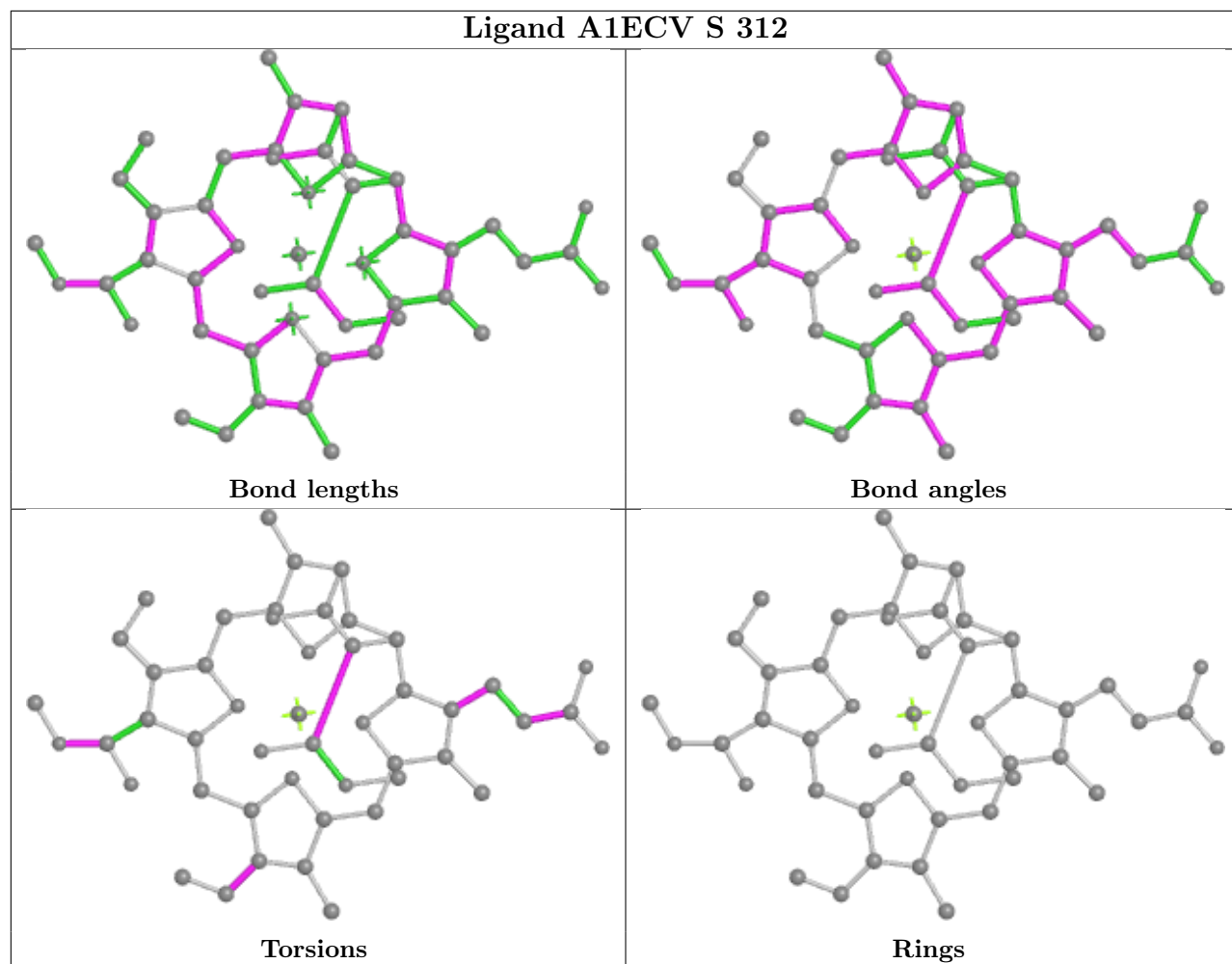




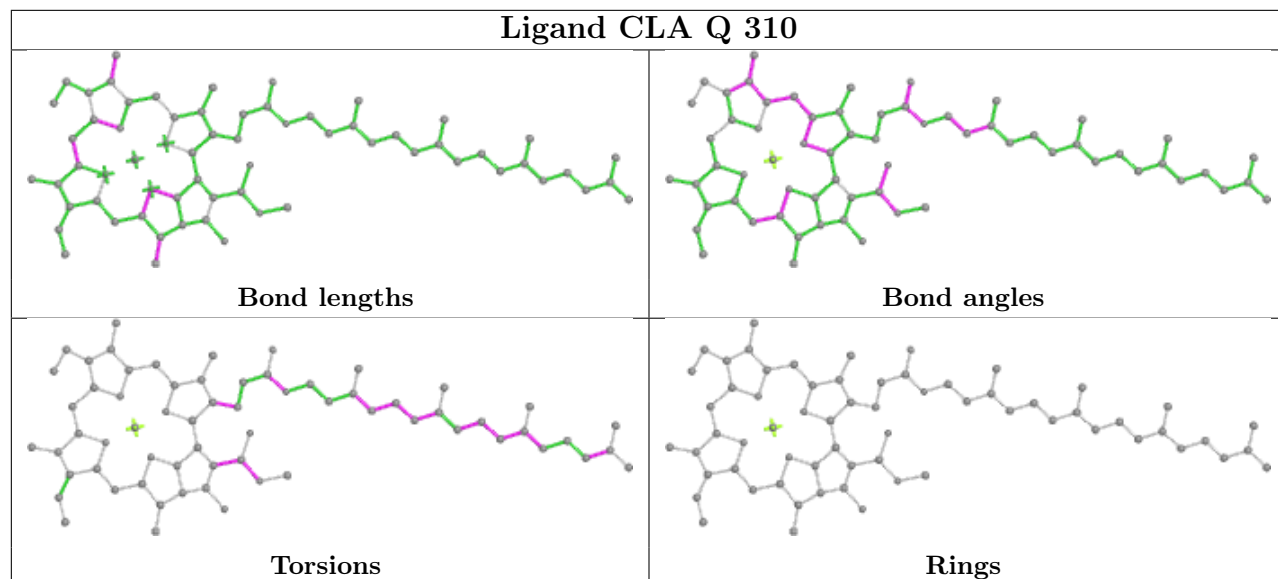


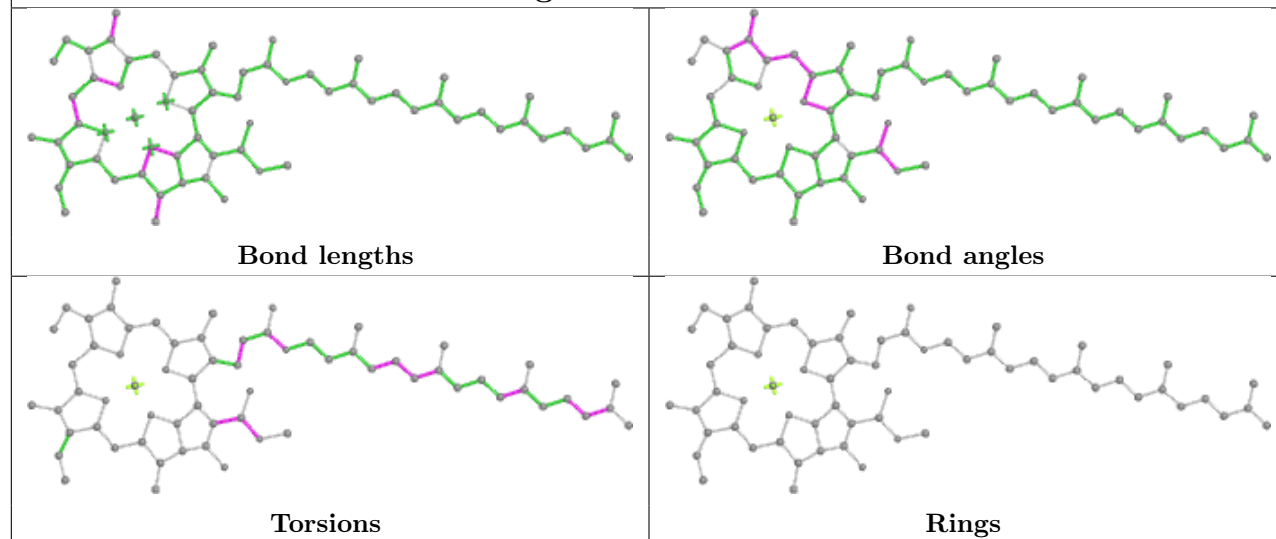
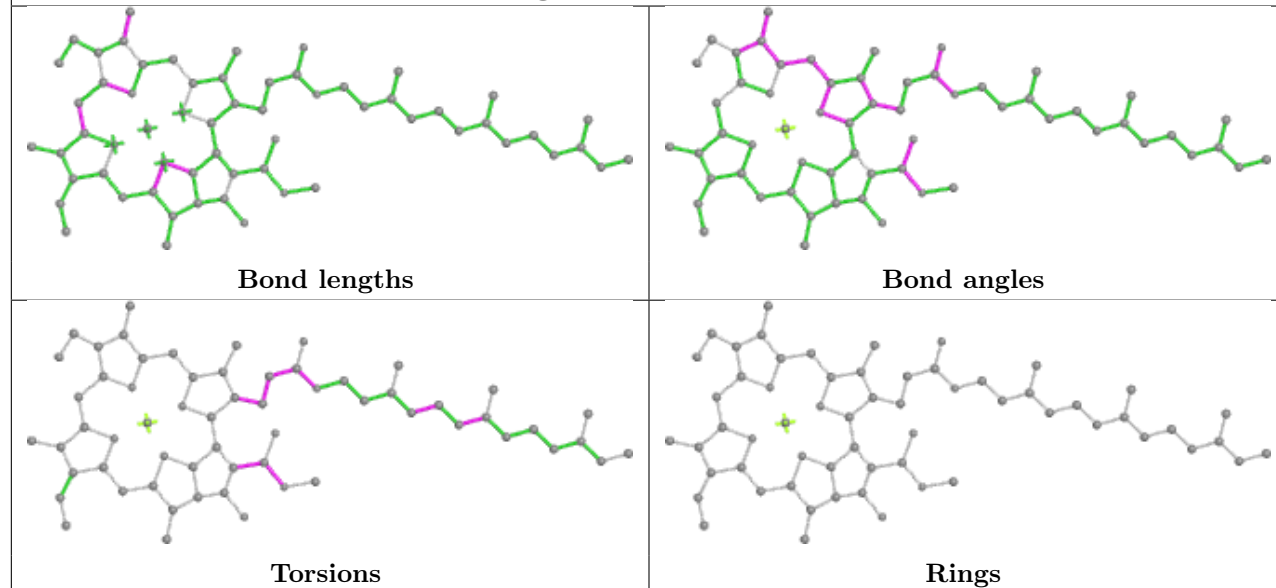
**Ligand CLA a 821****Ligand A86 L 301**

## Ligand A1ECV S 312

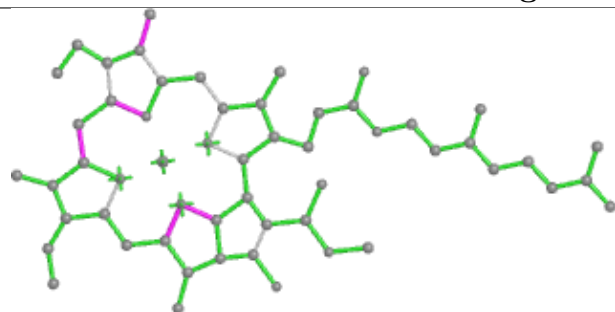


## Ligand CLA Q 310

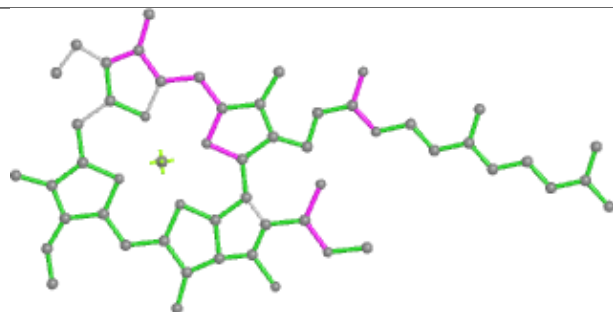


**Ligand CLA b 832****Ligand CLA L 308**

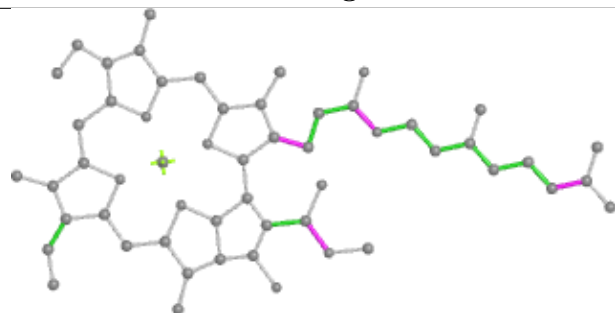
## Ligand CLA k 203



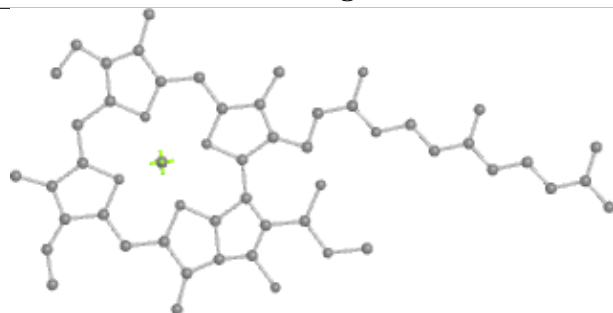
Bond lengths



Bond angles

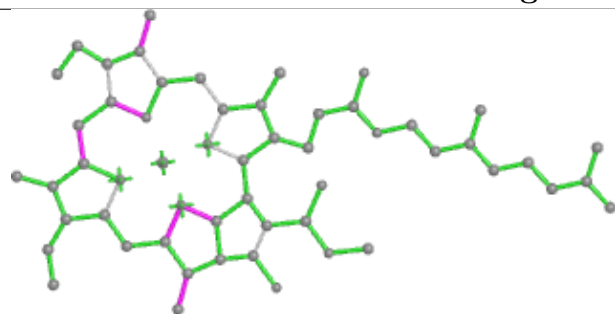


Torsions

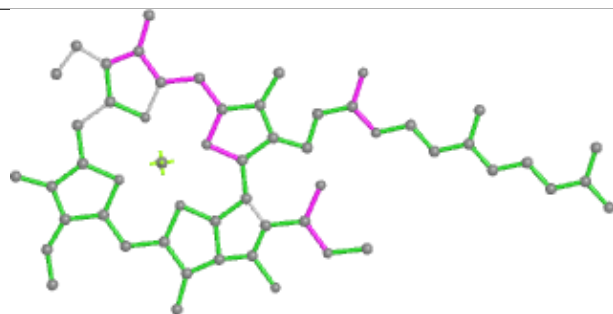


Rings

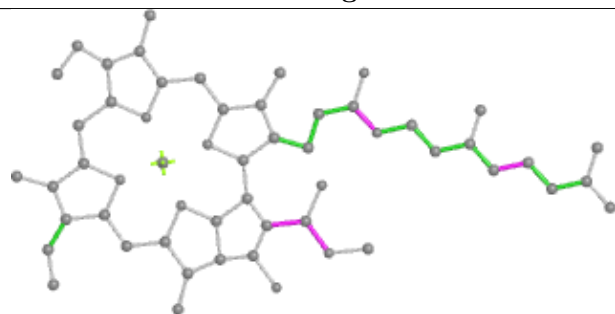
## Ligand CLA o 203



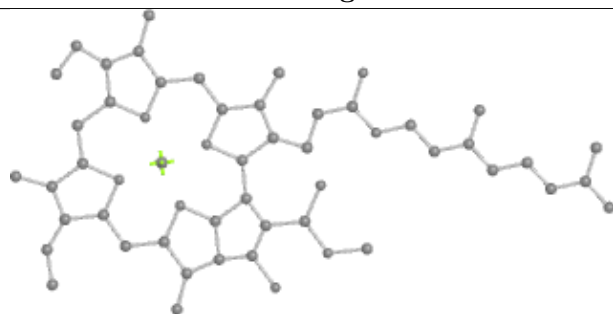
Bond lengths



Bond angles

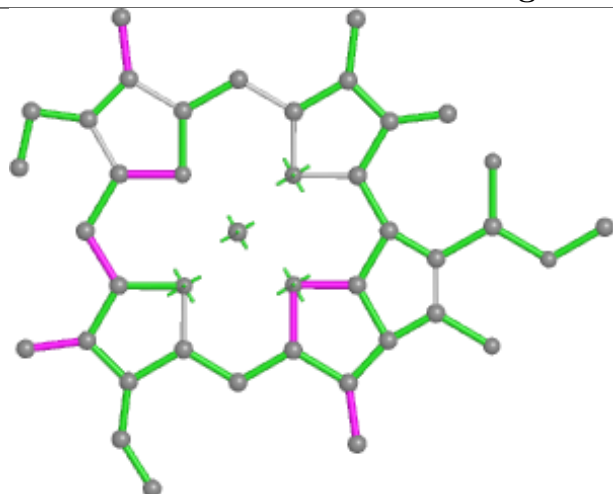


Torsions

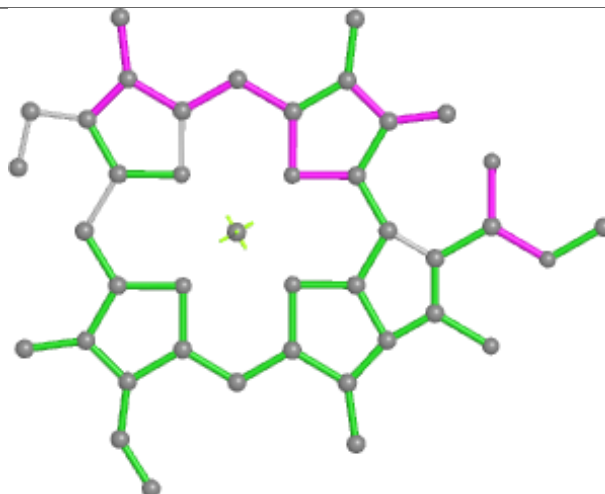


Rings

## Ligand CLA 2 315



Bond lengths



Bond angles

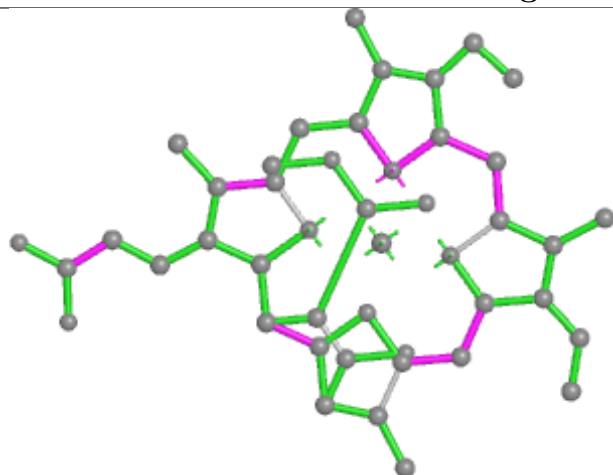


Torsions

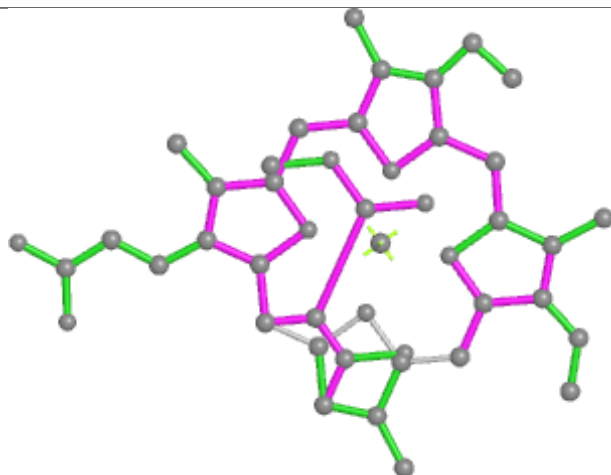


Rings

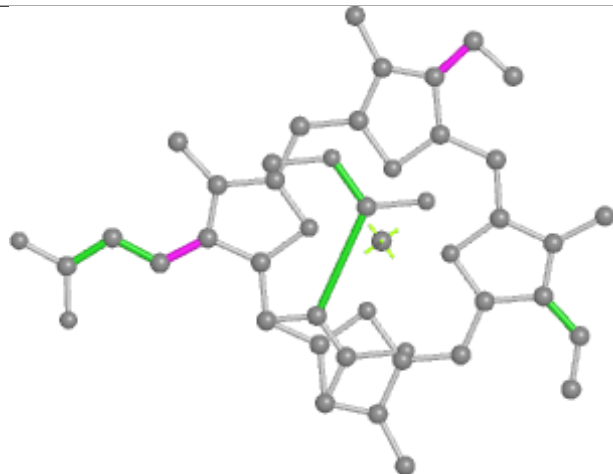
## Ligand KC2 0 317



Bond lengths



Bond angles



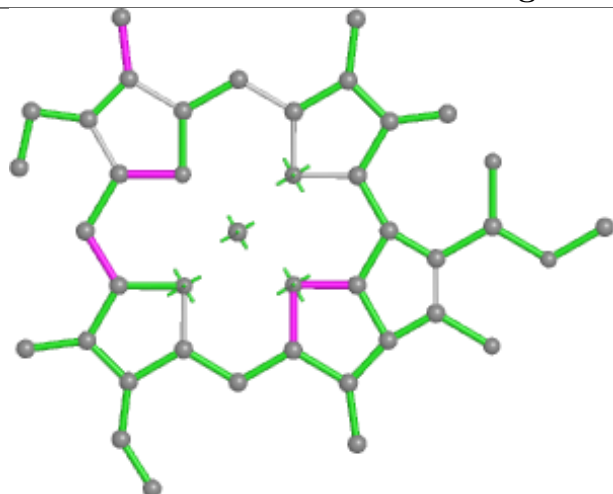
Torsions



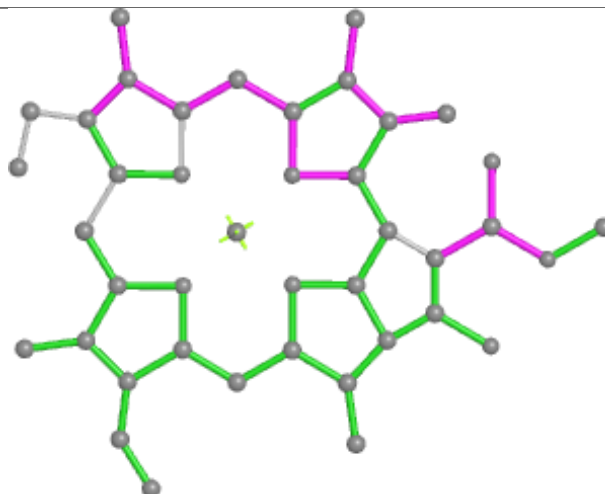
Rings



## Ligand CLA 1 320



Bond lengths



Bond angles

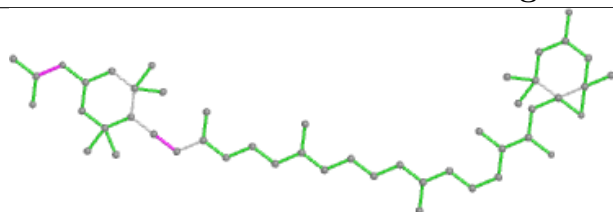


Torsions

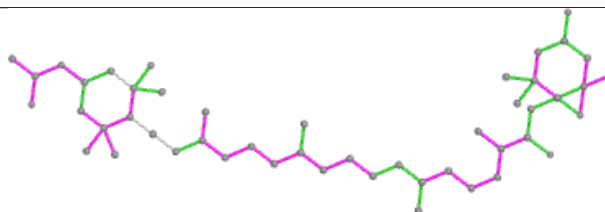


Rings

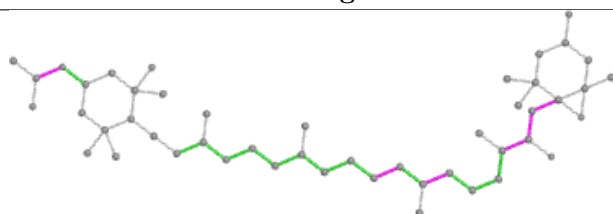
## Ligand A86 O 307



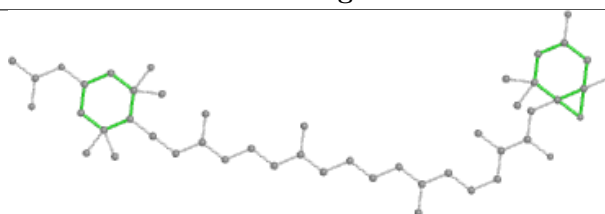
Bond lengths



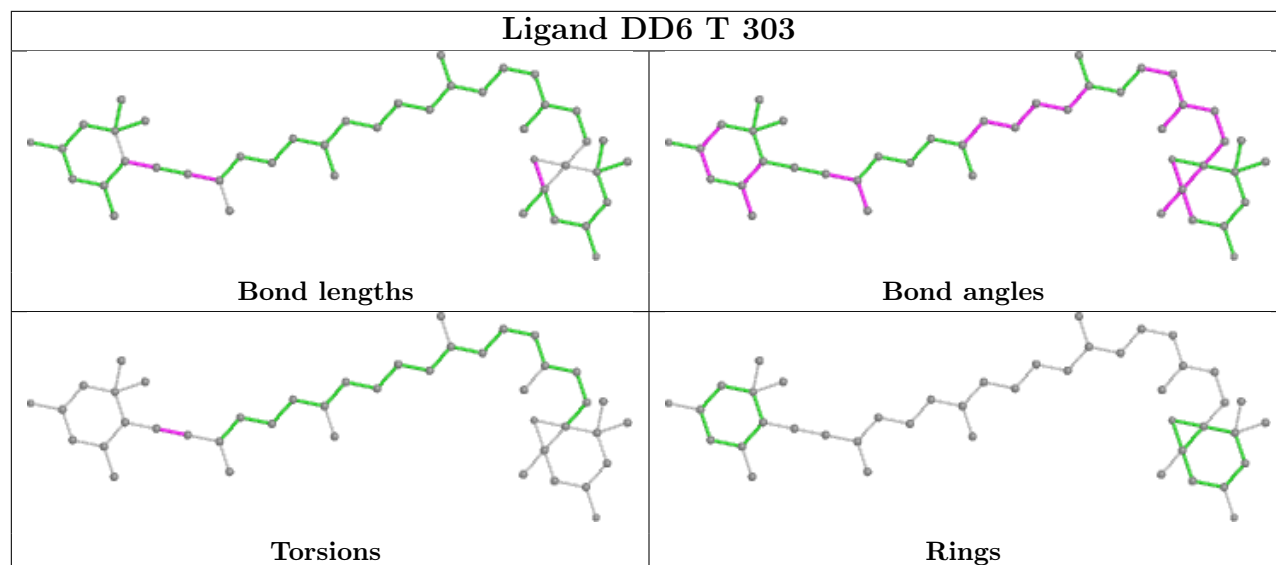
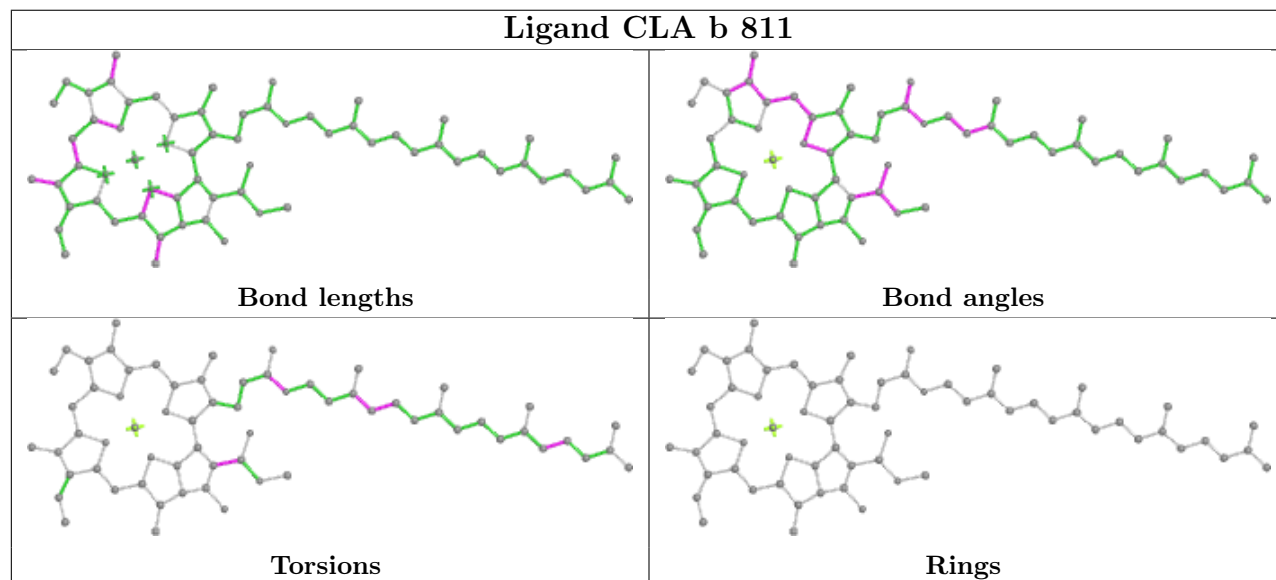
Bond angles



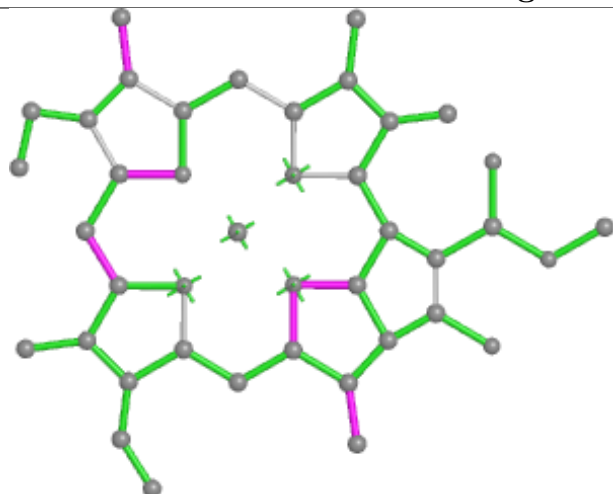
Torsions



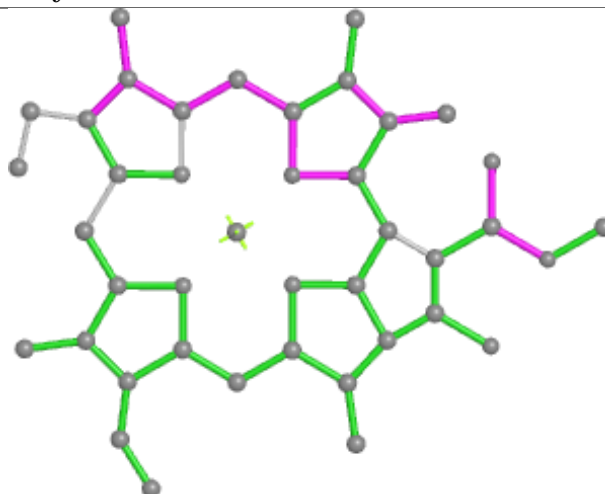
Rings

**Ligand DD6 T 303****Ligand CLA b 811**

## Ligand CLA y 315



Bond lengths



Bond angles

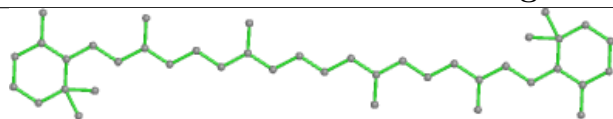


Torsions

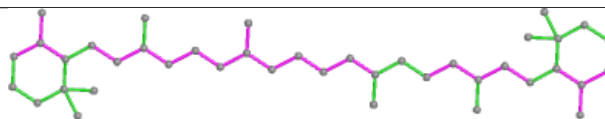


Rings

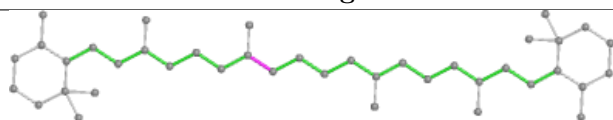
## Ligand BCR f 804



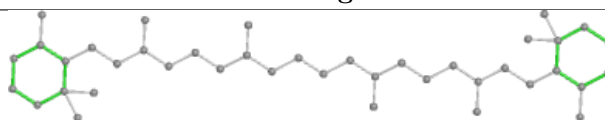
Bond lengths



Bond angles

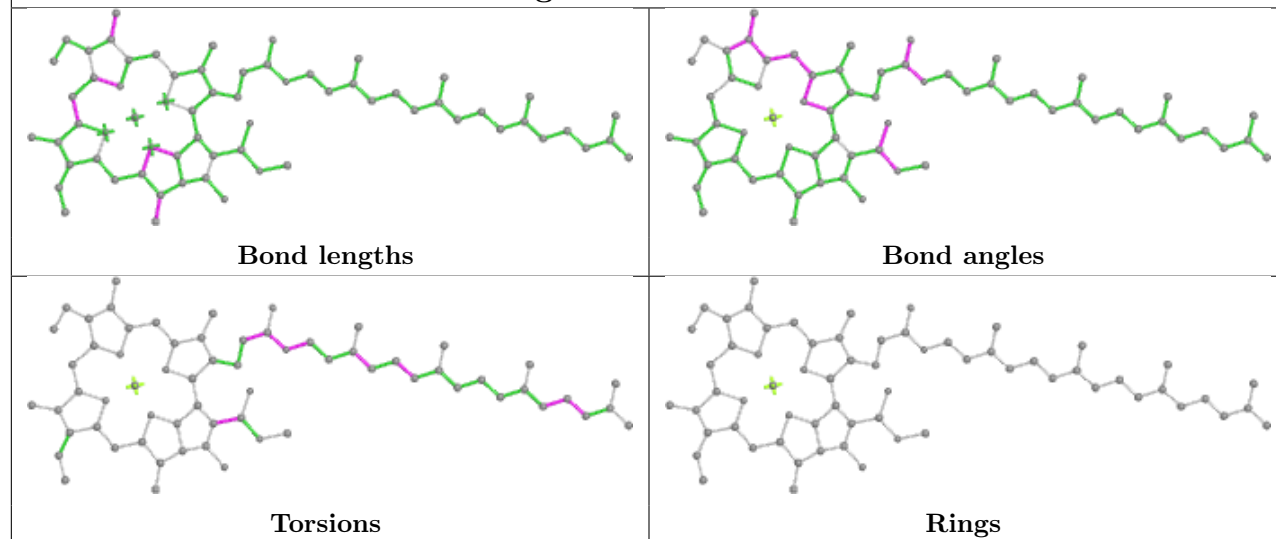


Torsions

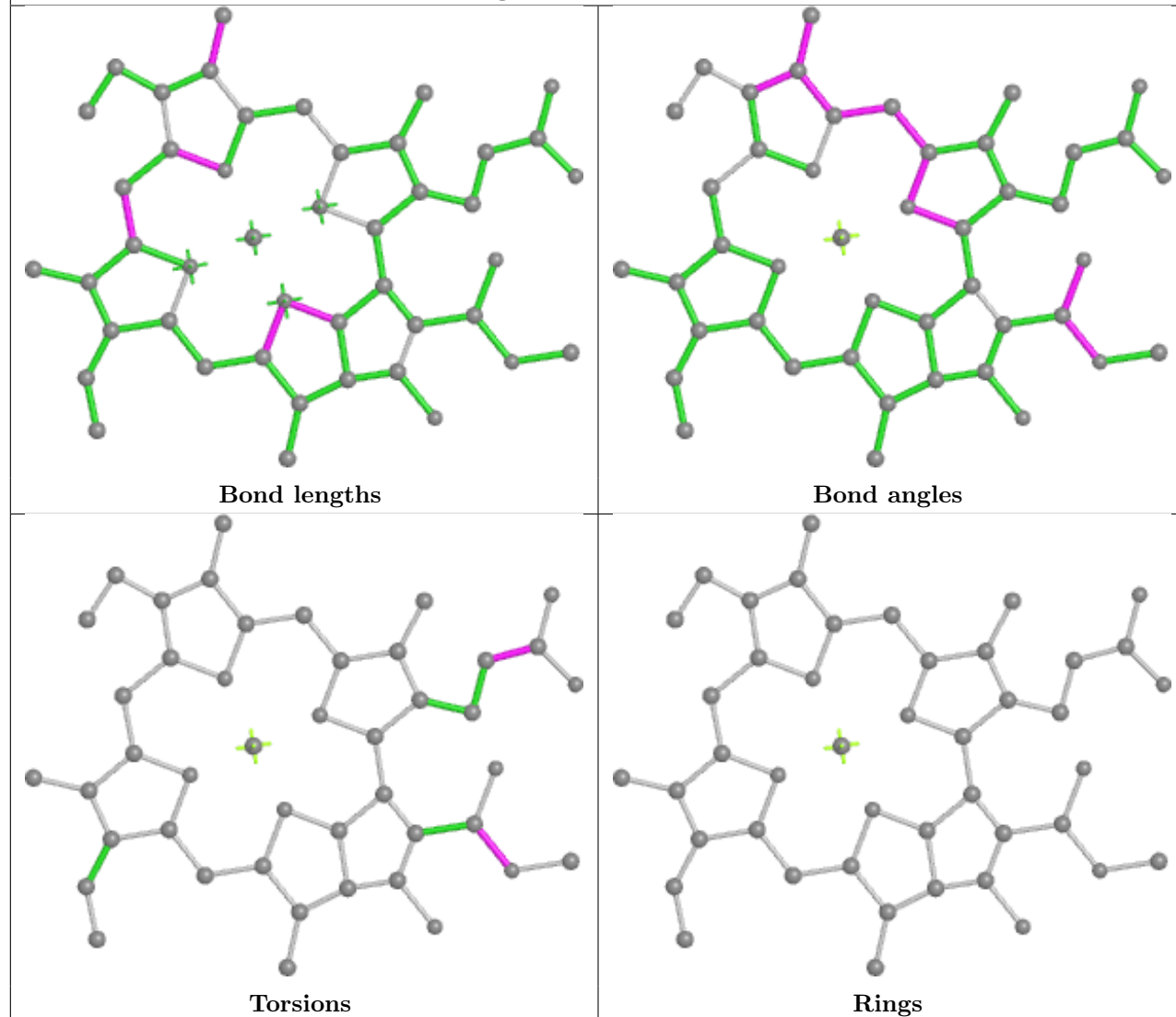


Rings

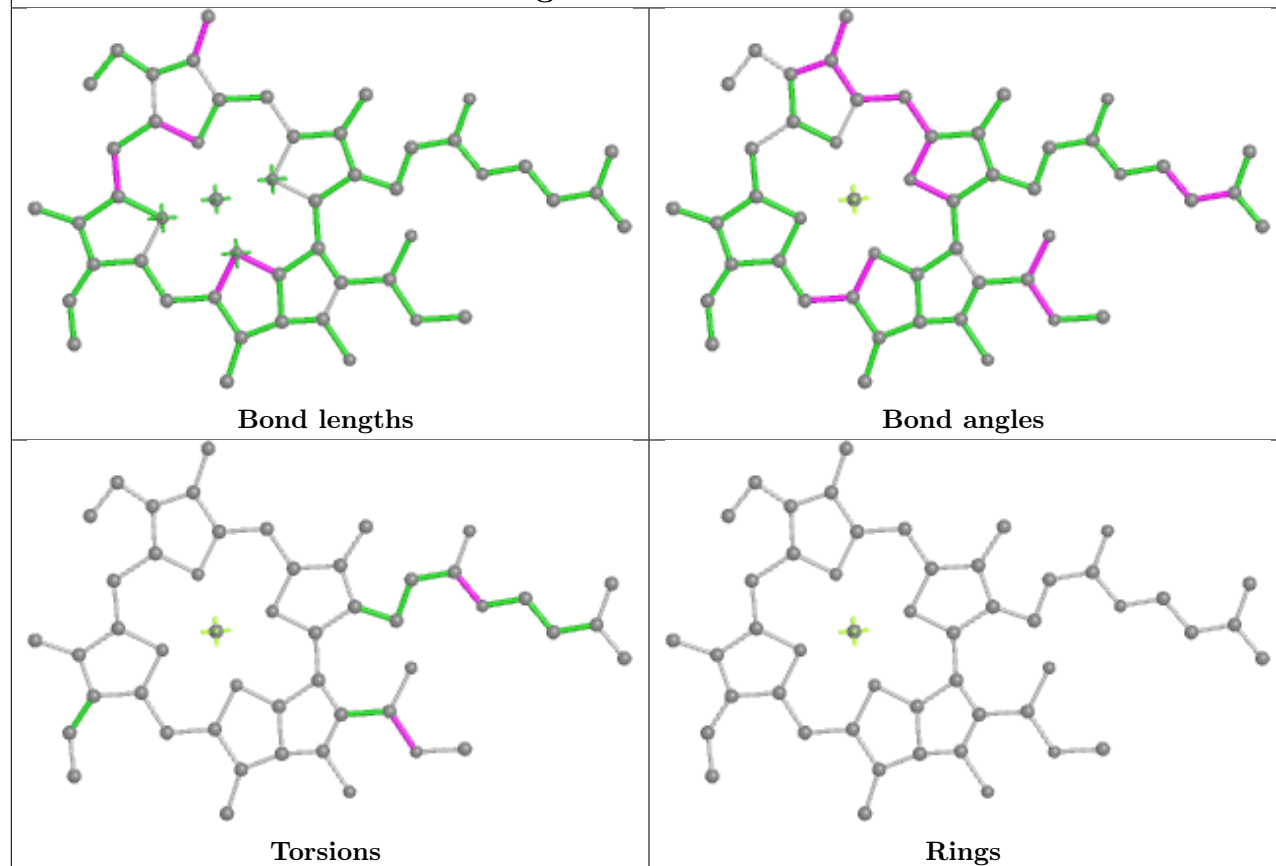
## Ligand CLA b 851



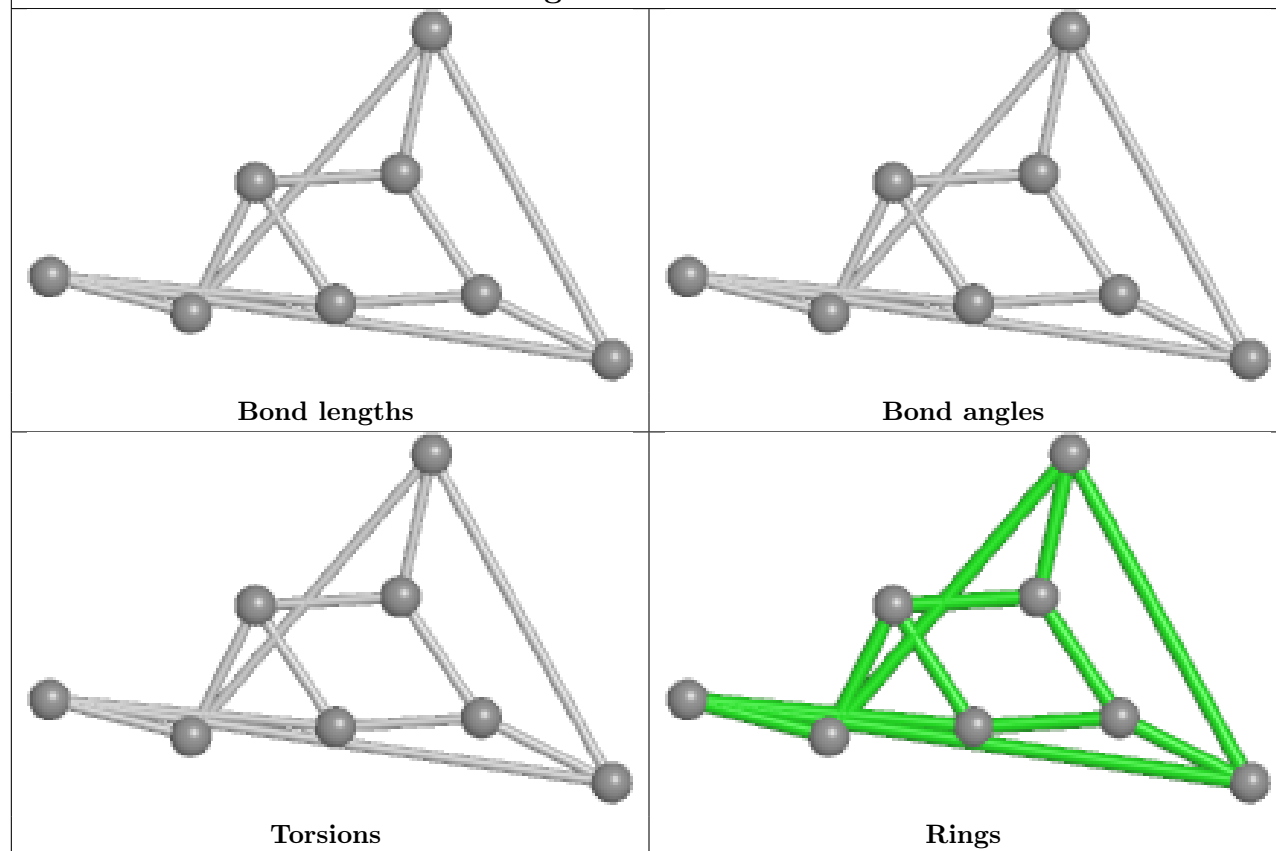
## Ligand CLA 1 310

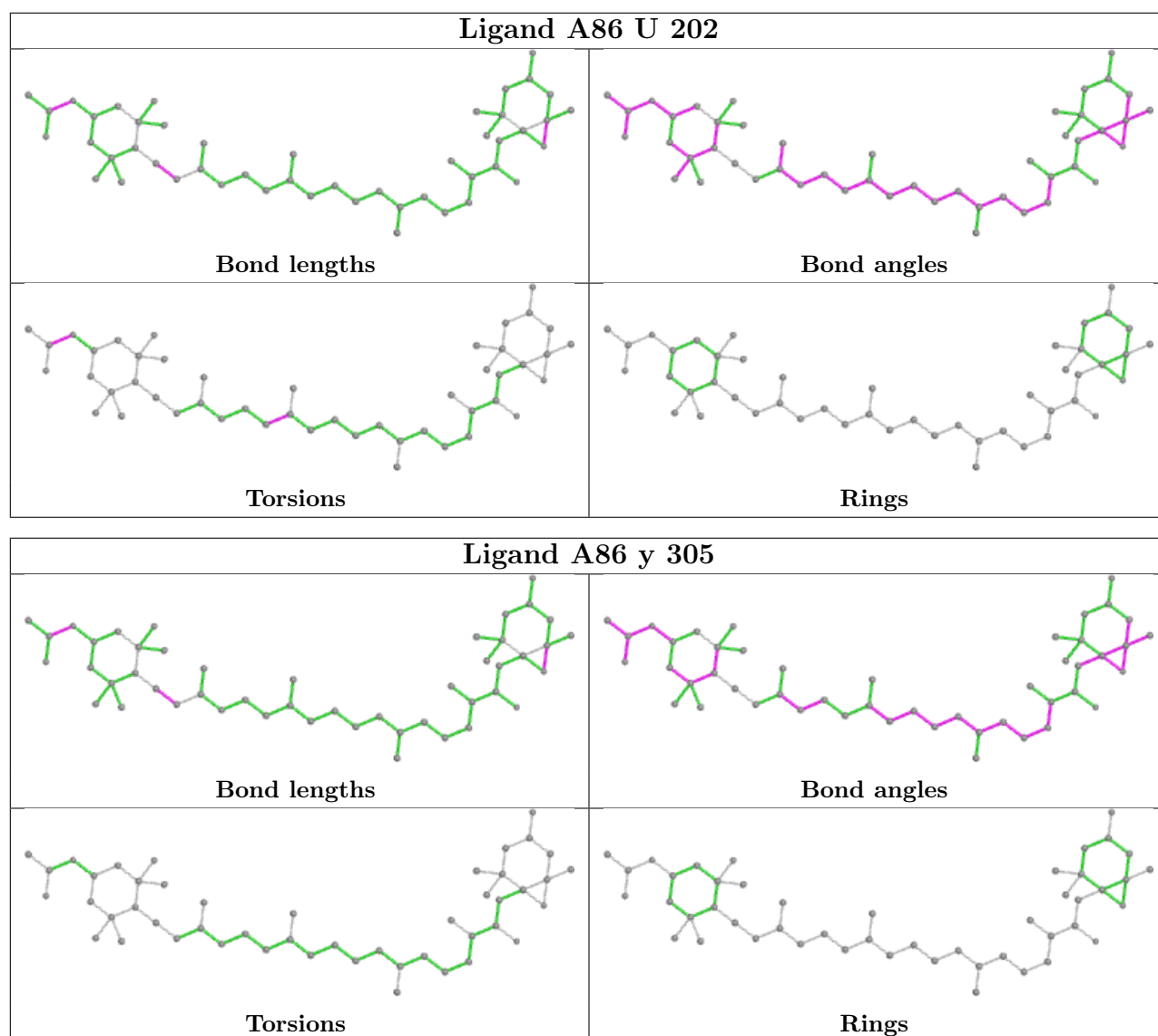


## Ligand CLA 5 310

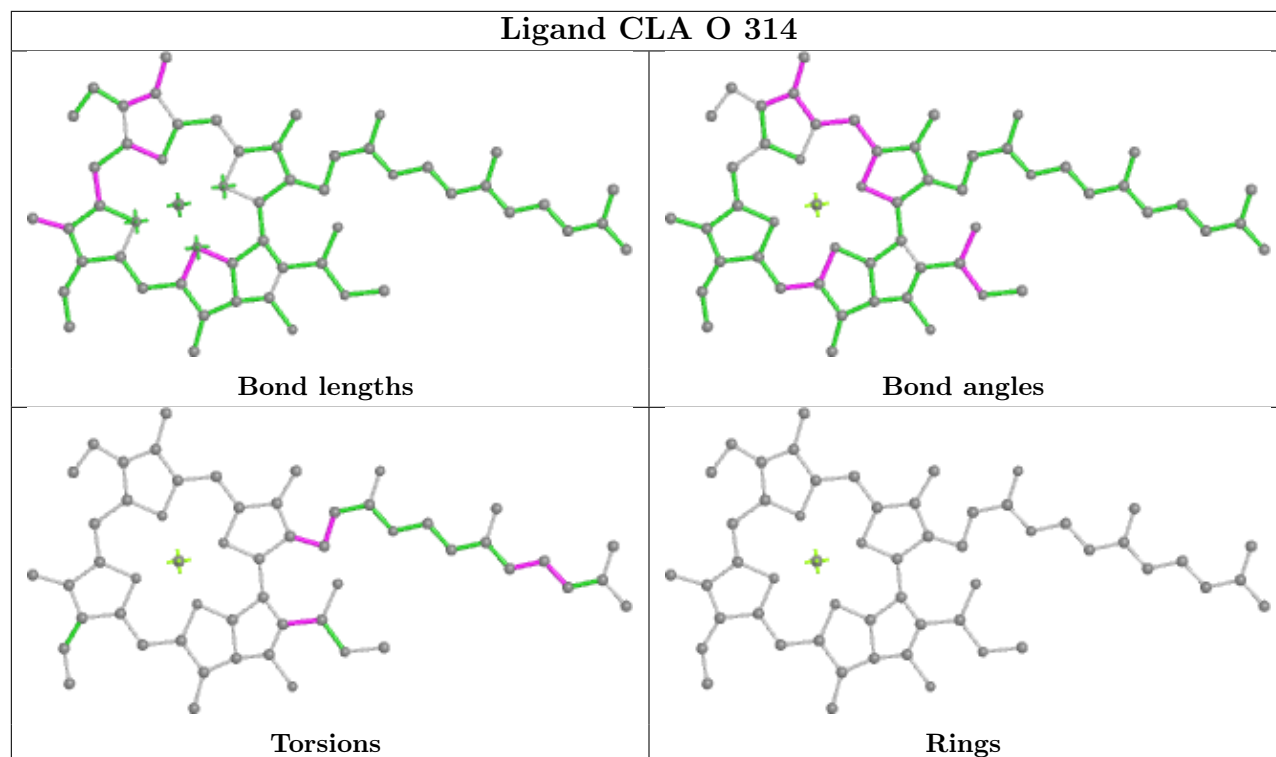


## Ligand SF4 c 102

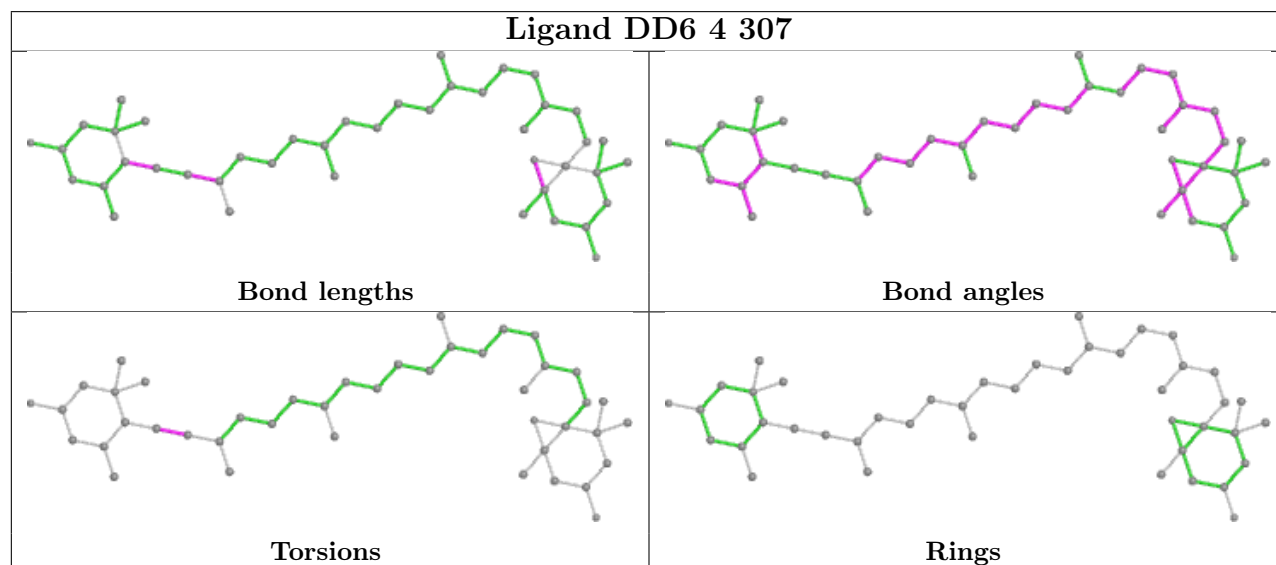




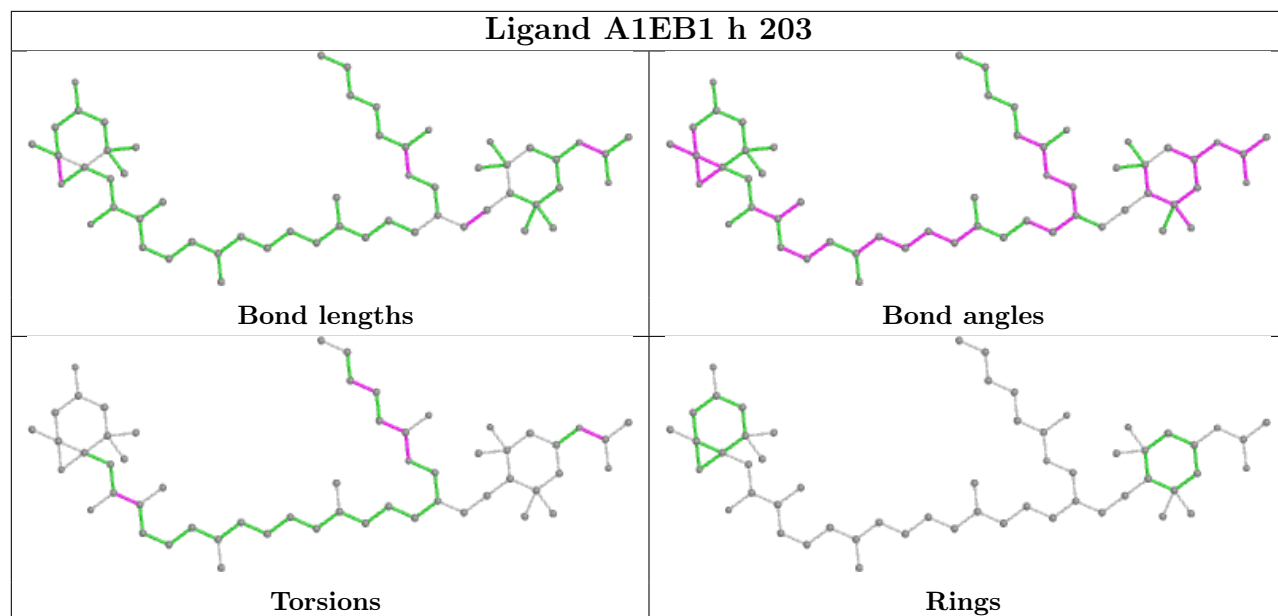
## Ligand CLA O 314



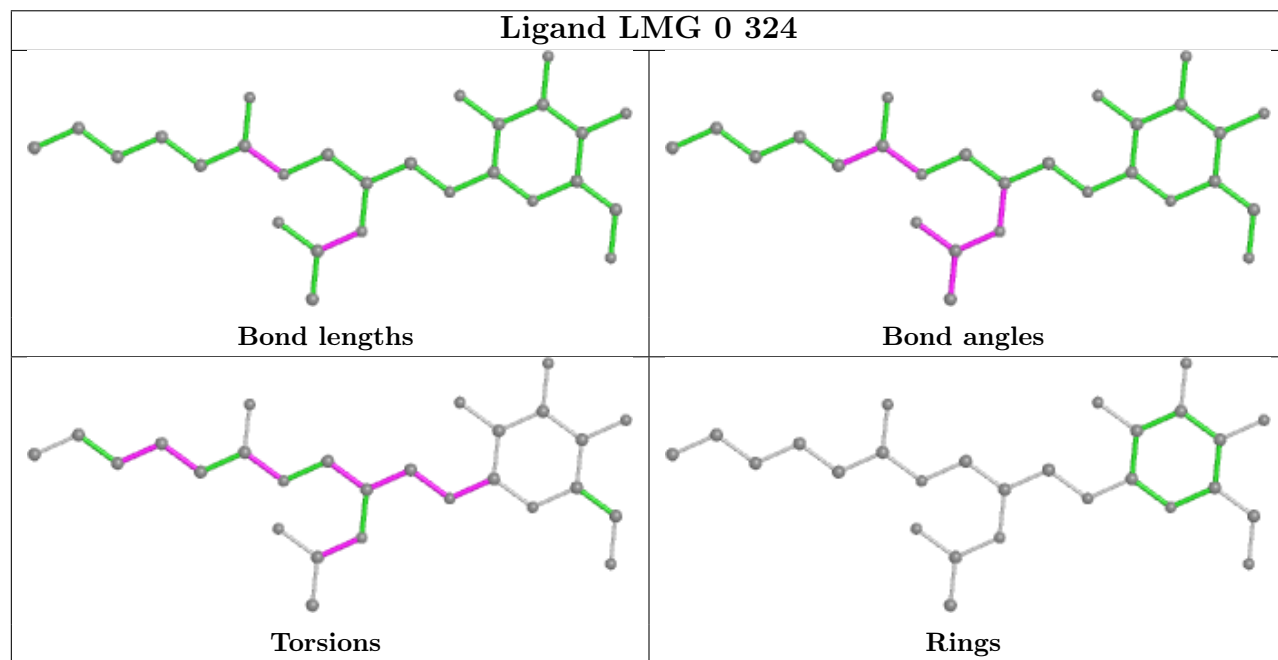
## Ligand DD6 4 307



## Ligand A1EB1 h 203

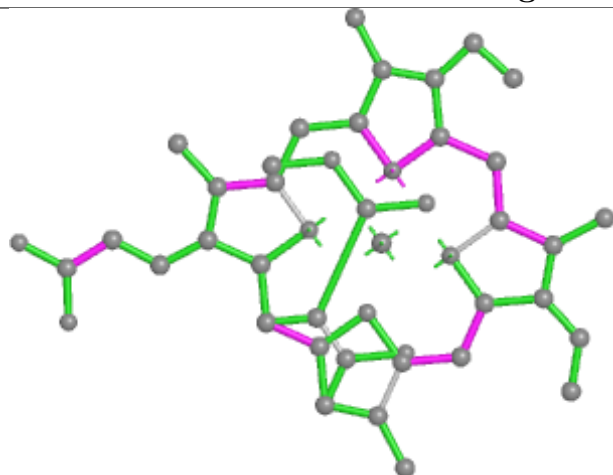


## Ligand LMG 0 324

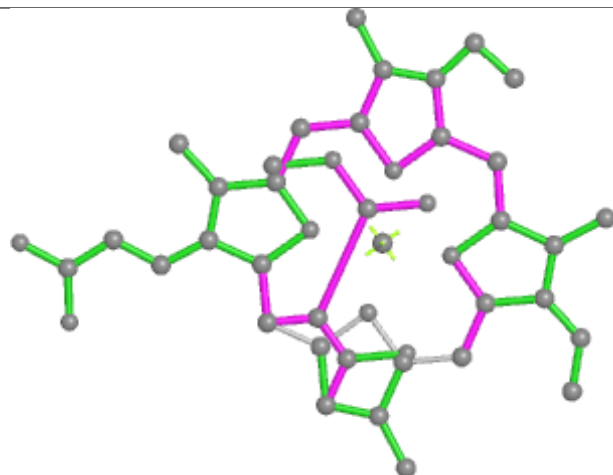




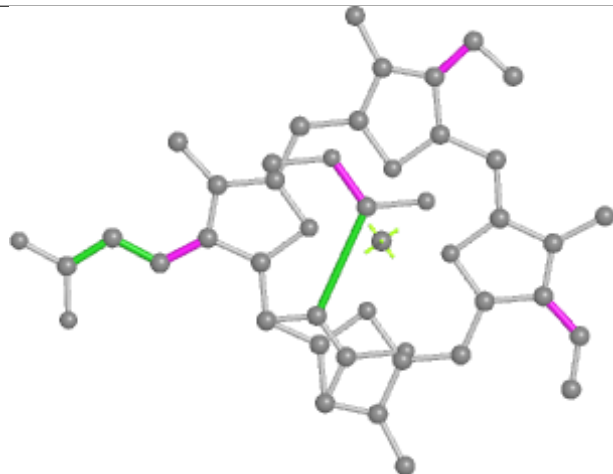
## Ligand KC2 L 321



Bond lengths



Bond angles

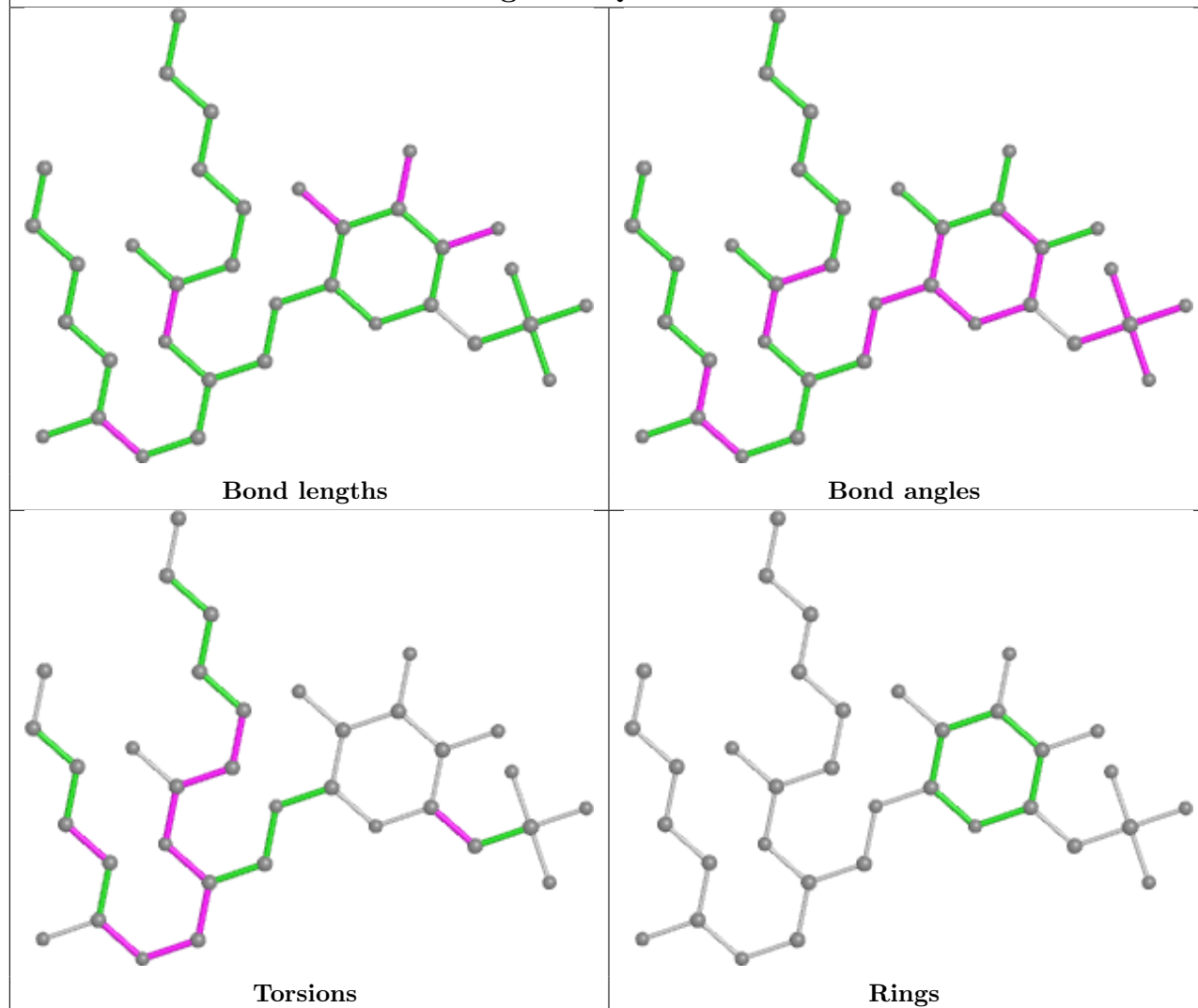


Torsions

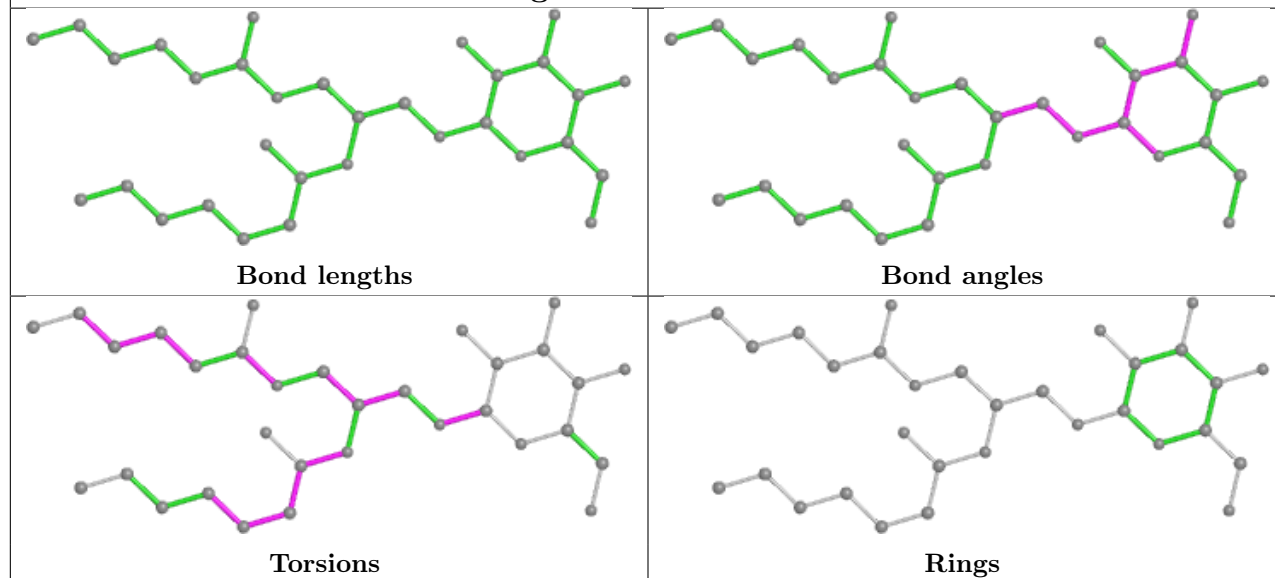


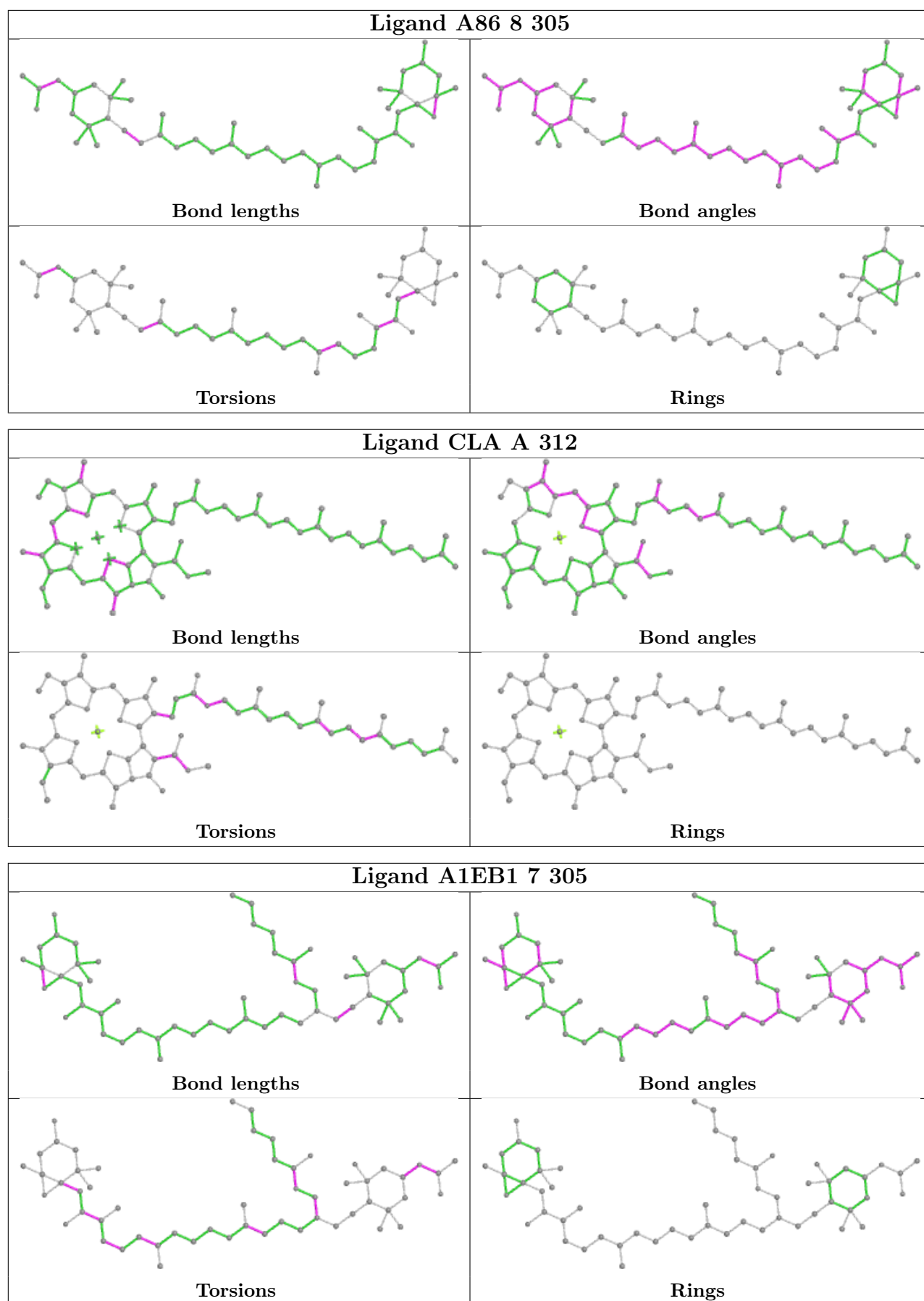
Rings

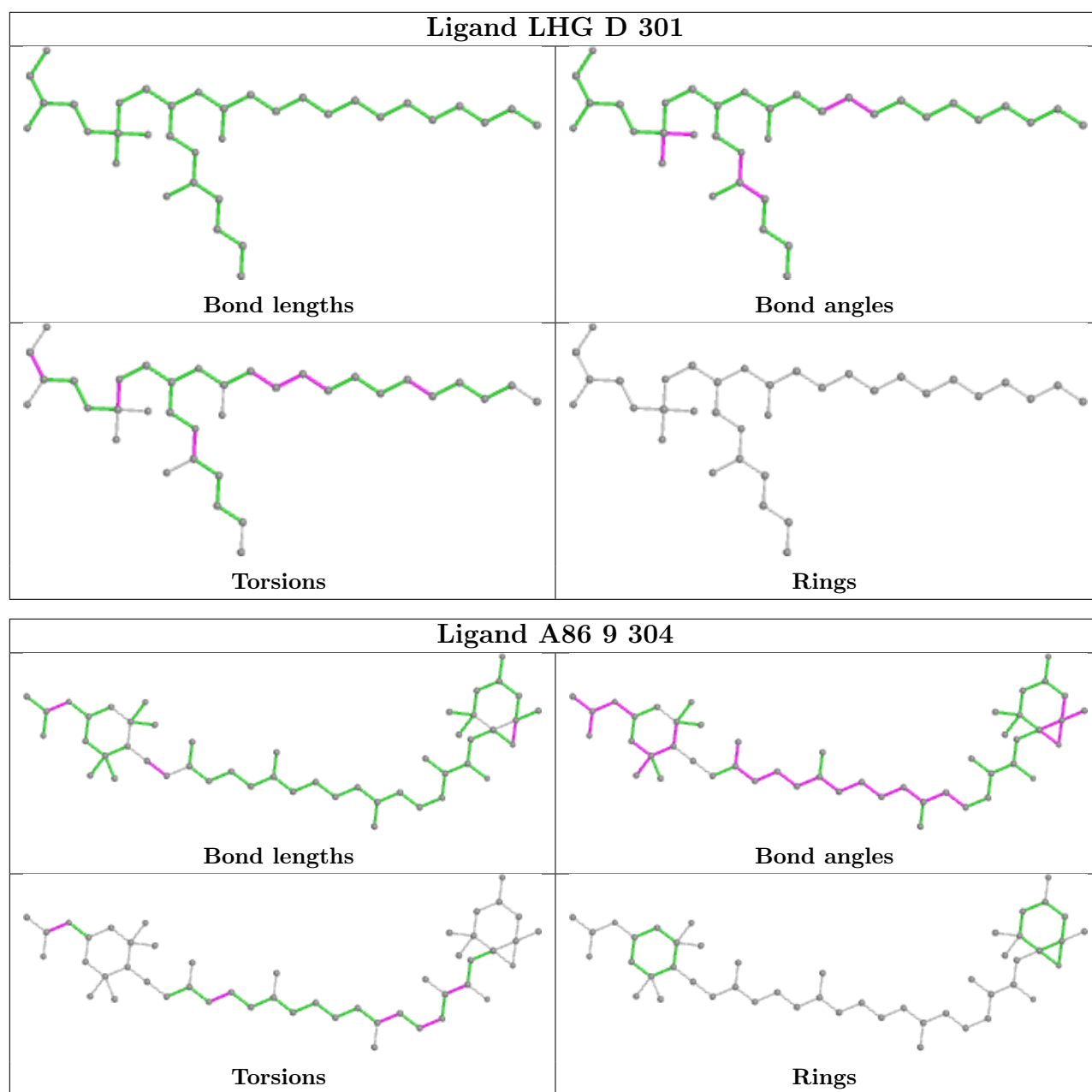
## Ligand SQD E 320



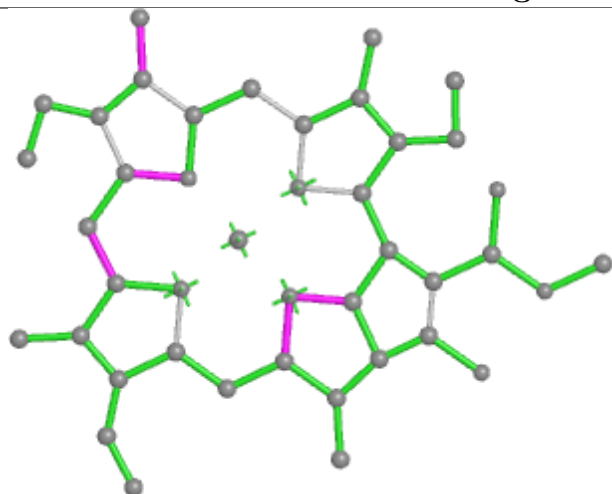
## Ligand LMG 4 325



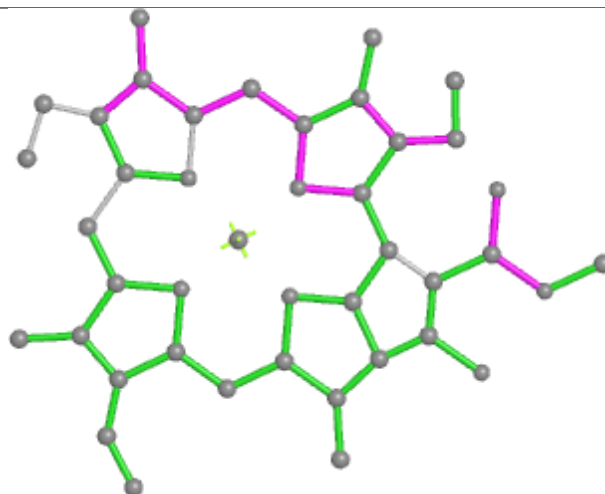




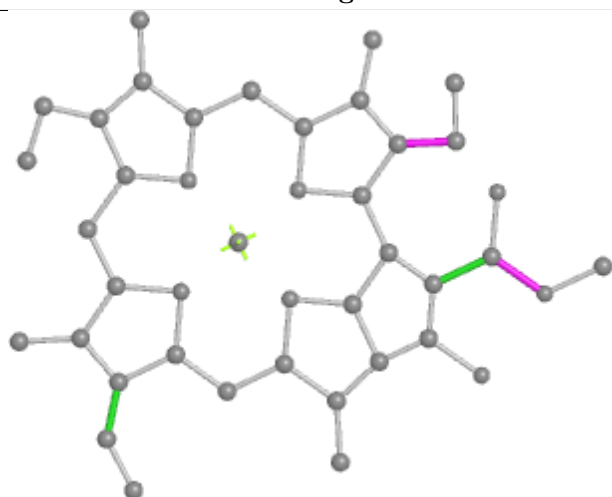
## Ligand CLA B 205



Bond lengths



Bond angles

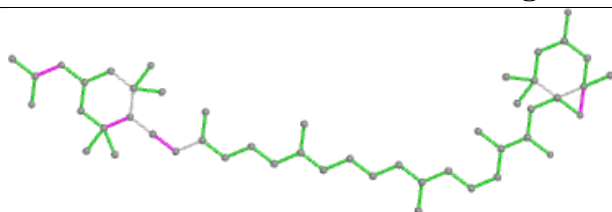


Torsions

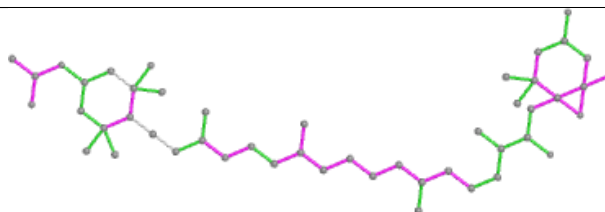


Rings

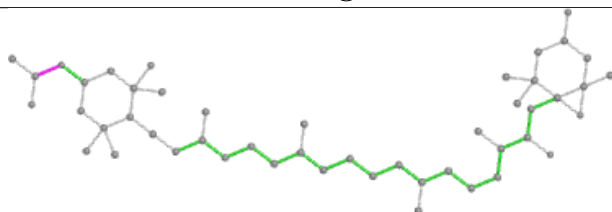
## Ligand A86 F 302



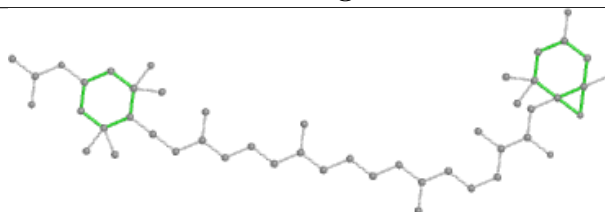
Bond lengths



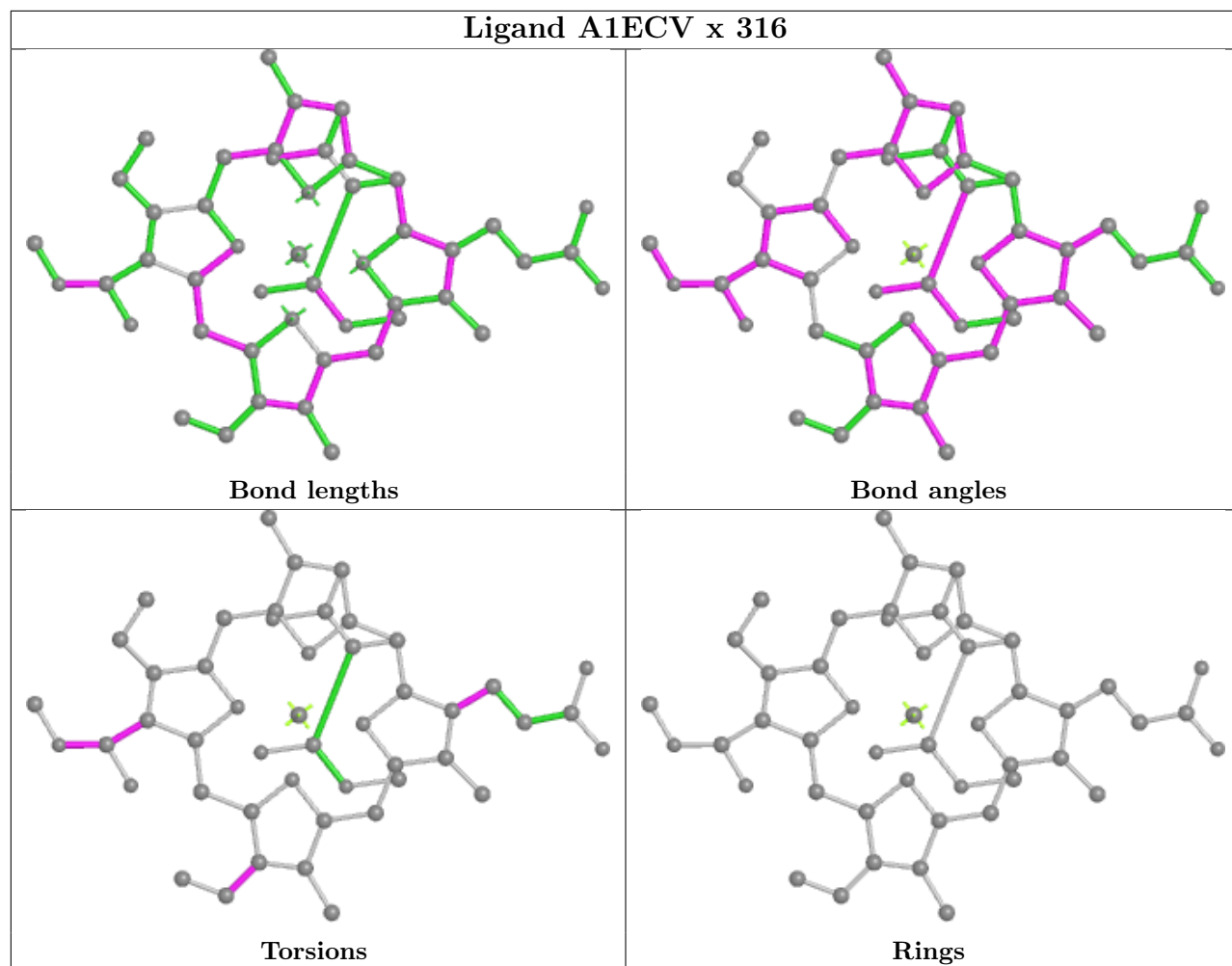
Bond angles



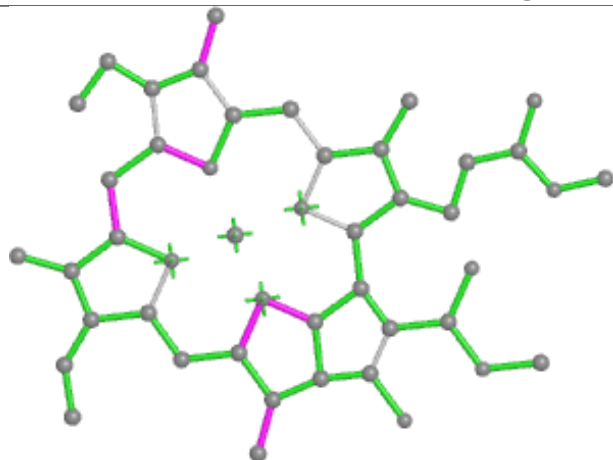
Torsions



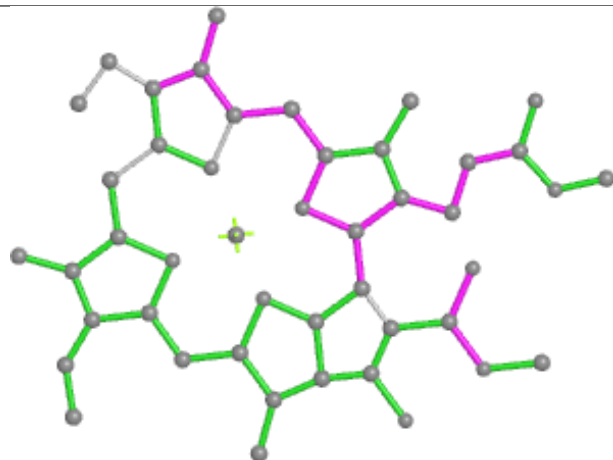
Rings



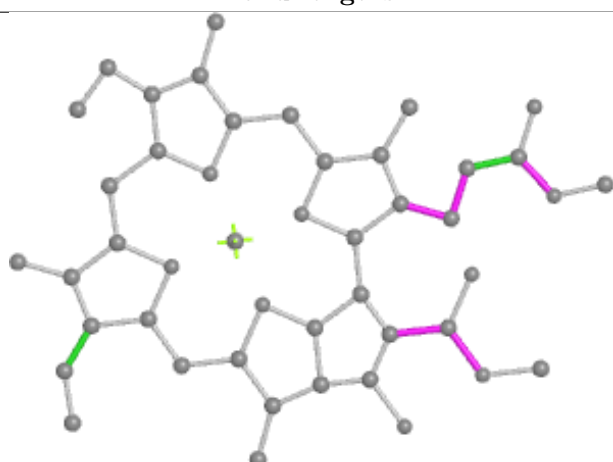
## Ligand CLA 2 319



Bond lengths



Bond angles

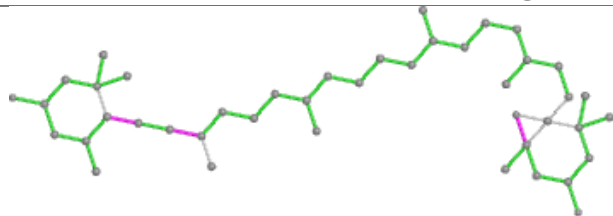


Torsions

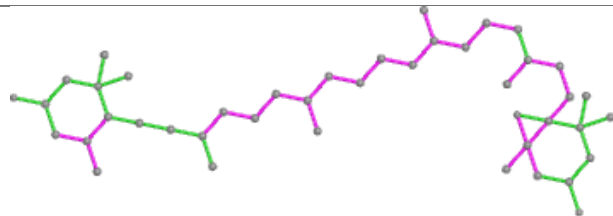


Rings

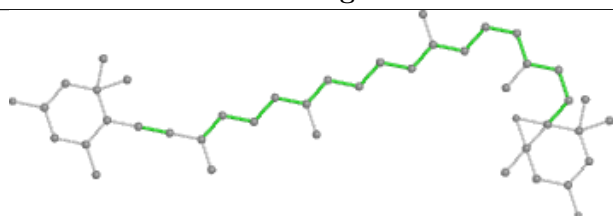
## Ligand DD6 x 304



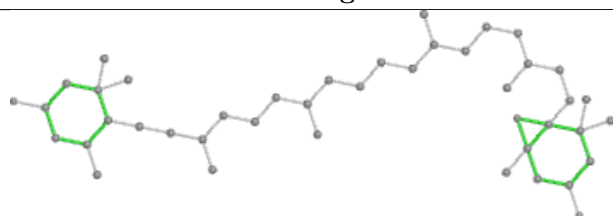
Bond lengths



Bond angles

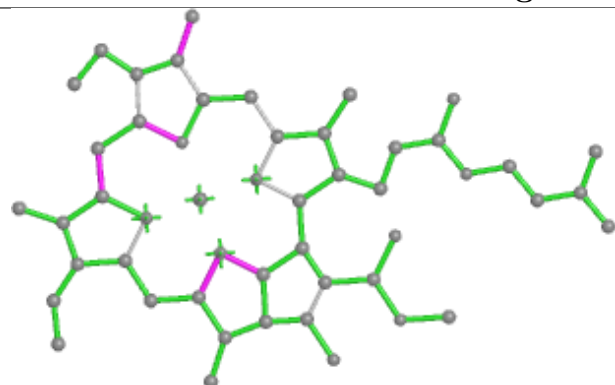


Torsions

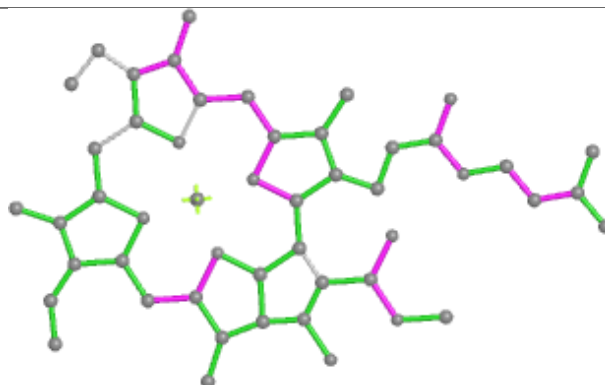


Rings

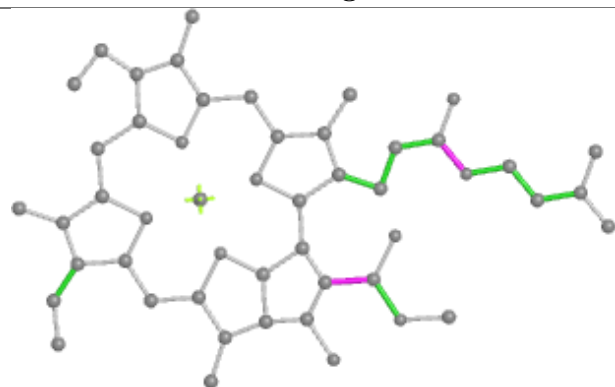
## Ligand CLA X 311



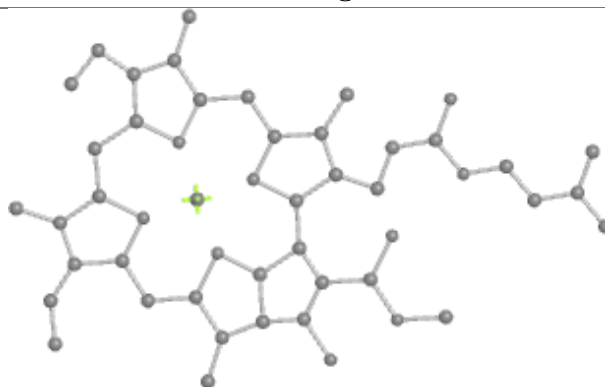
Bond lengths



Bond angles

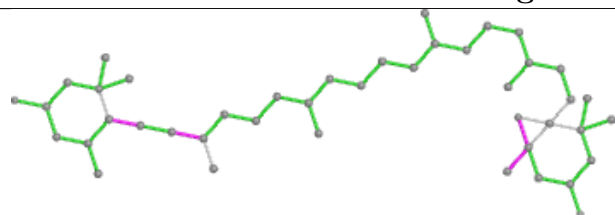


Torsions

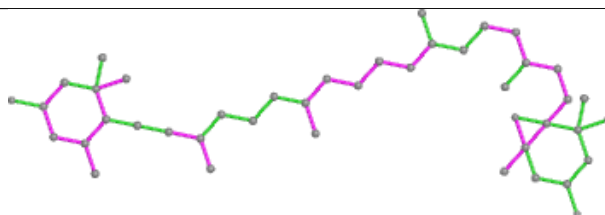


Rings

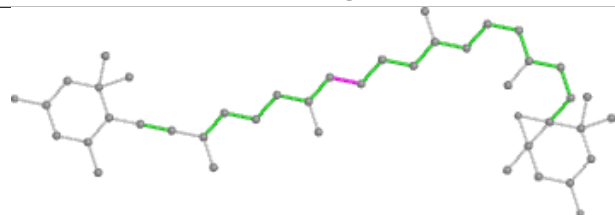
## Ligand DD6 O 304



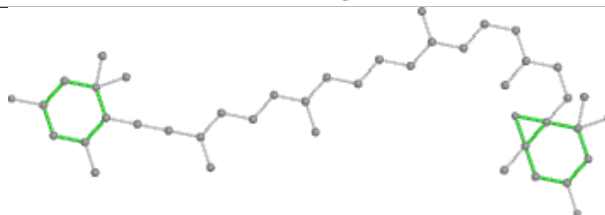
Bond lengths



Bond angles



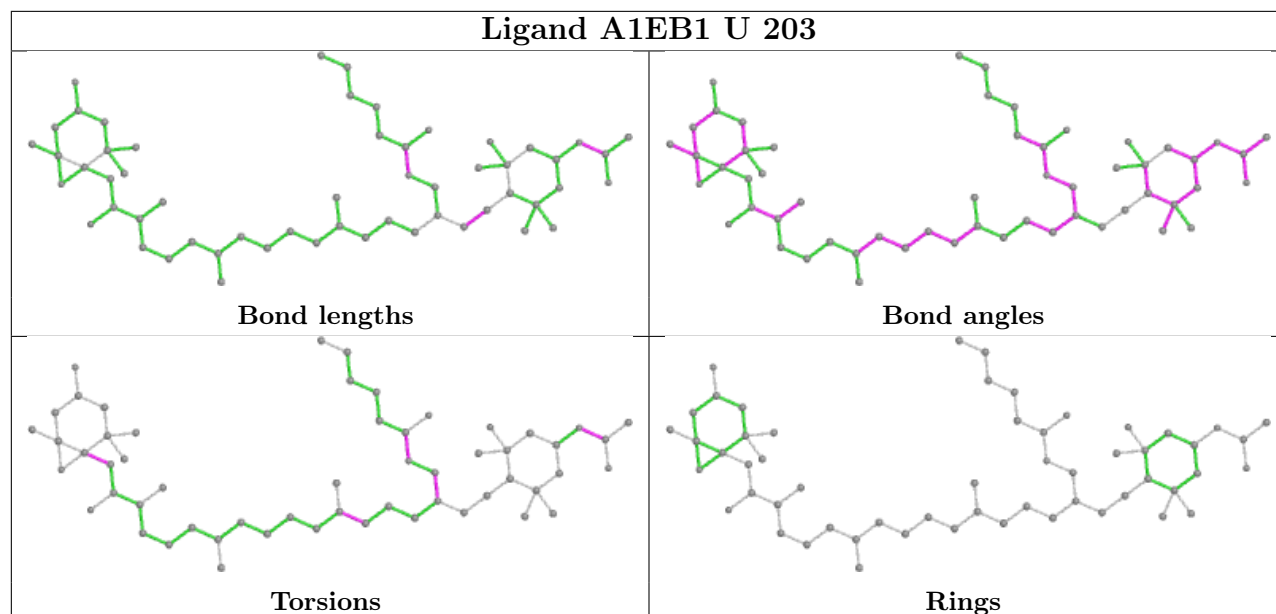
Torsions



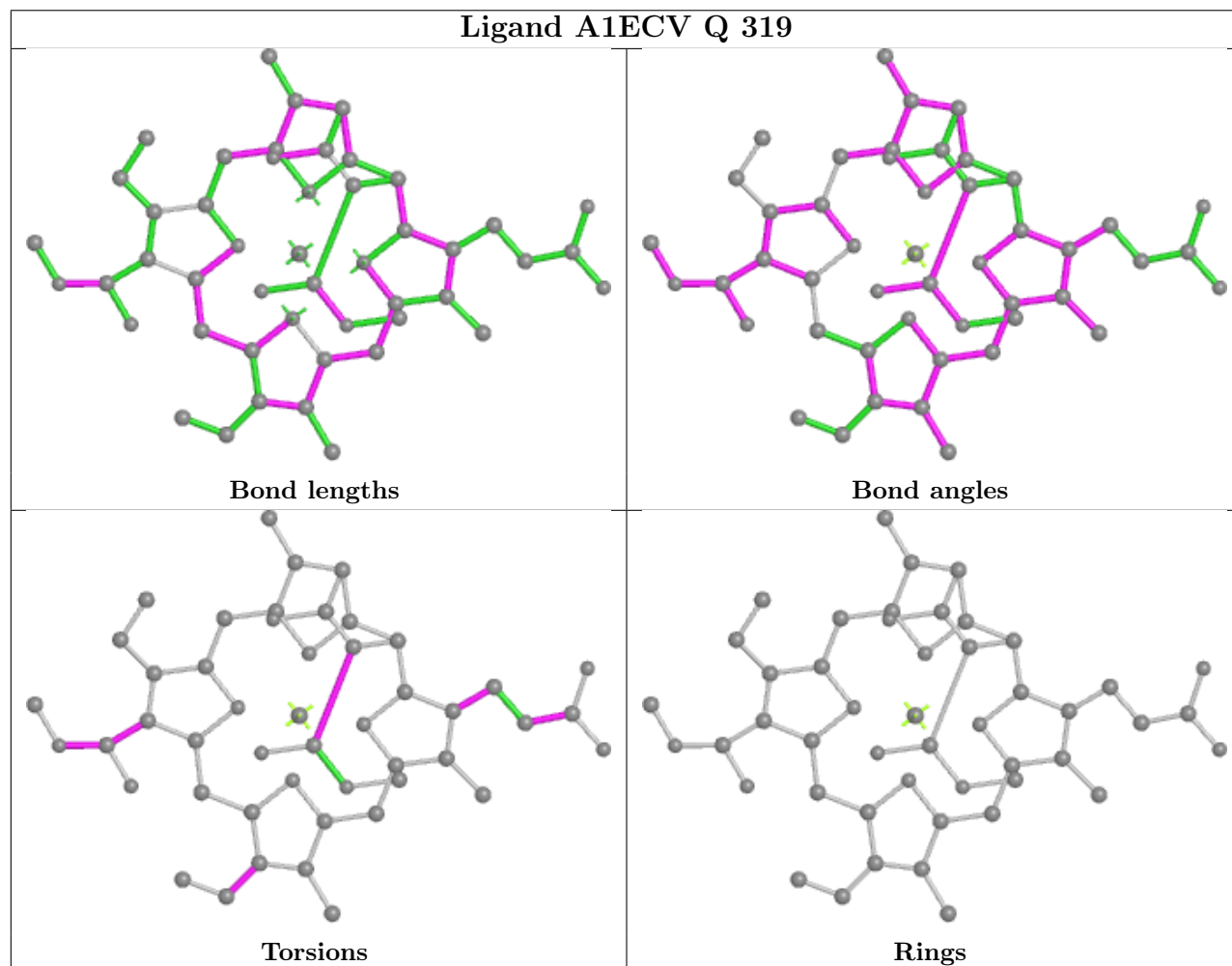
Rings

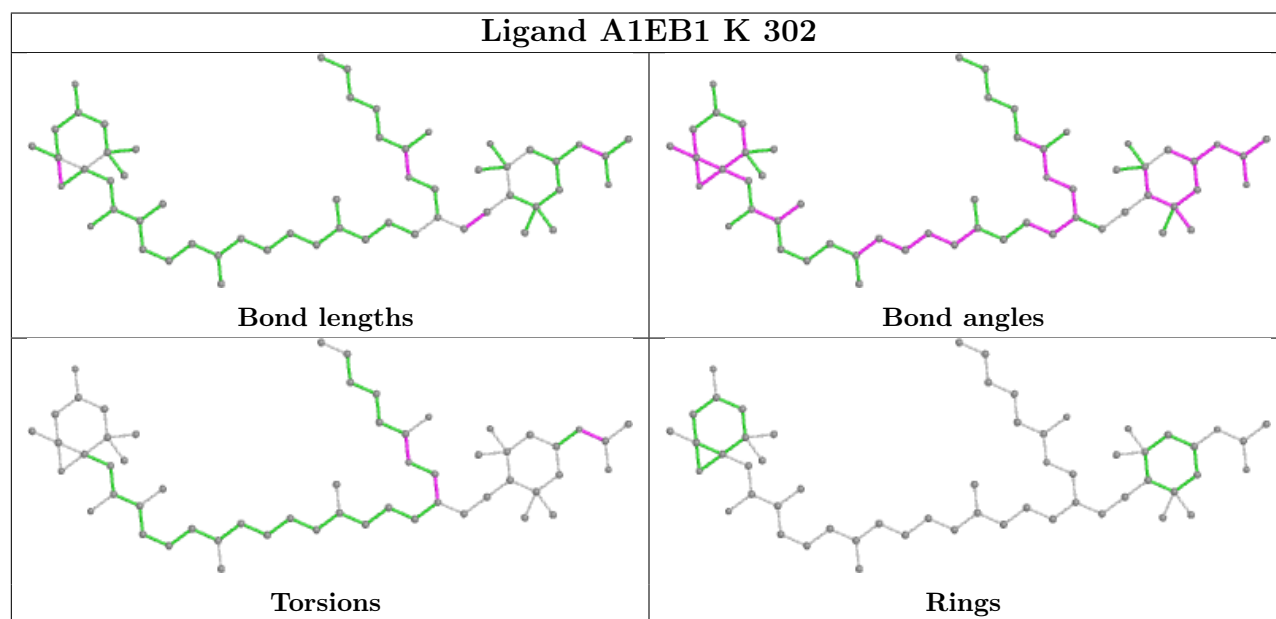
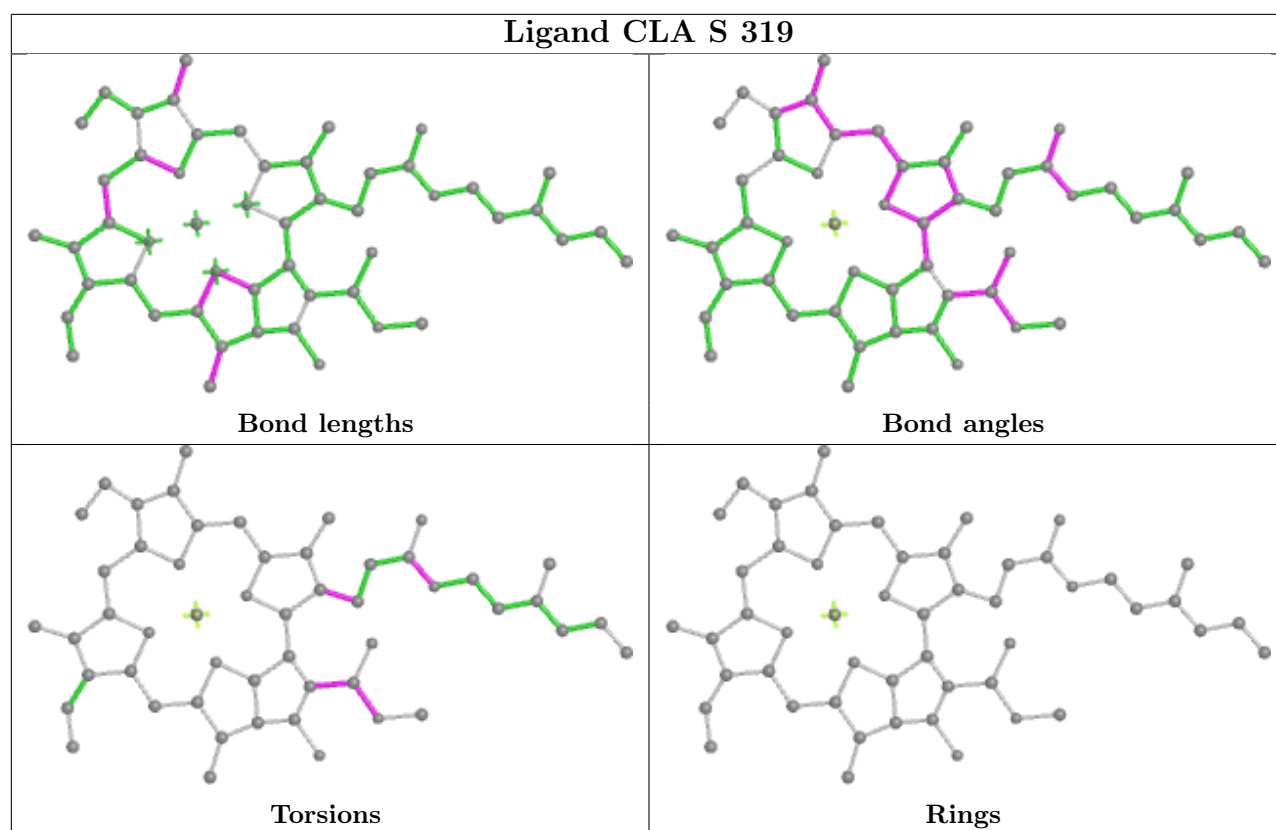


## Ligand A1EB1 U 203

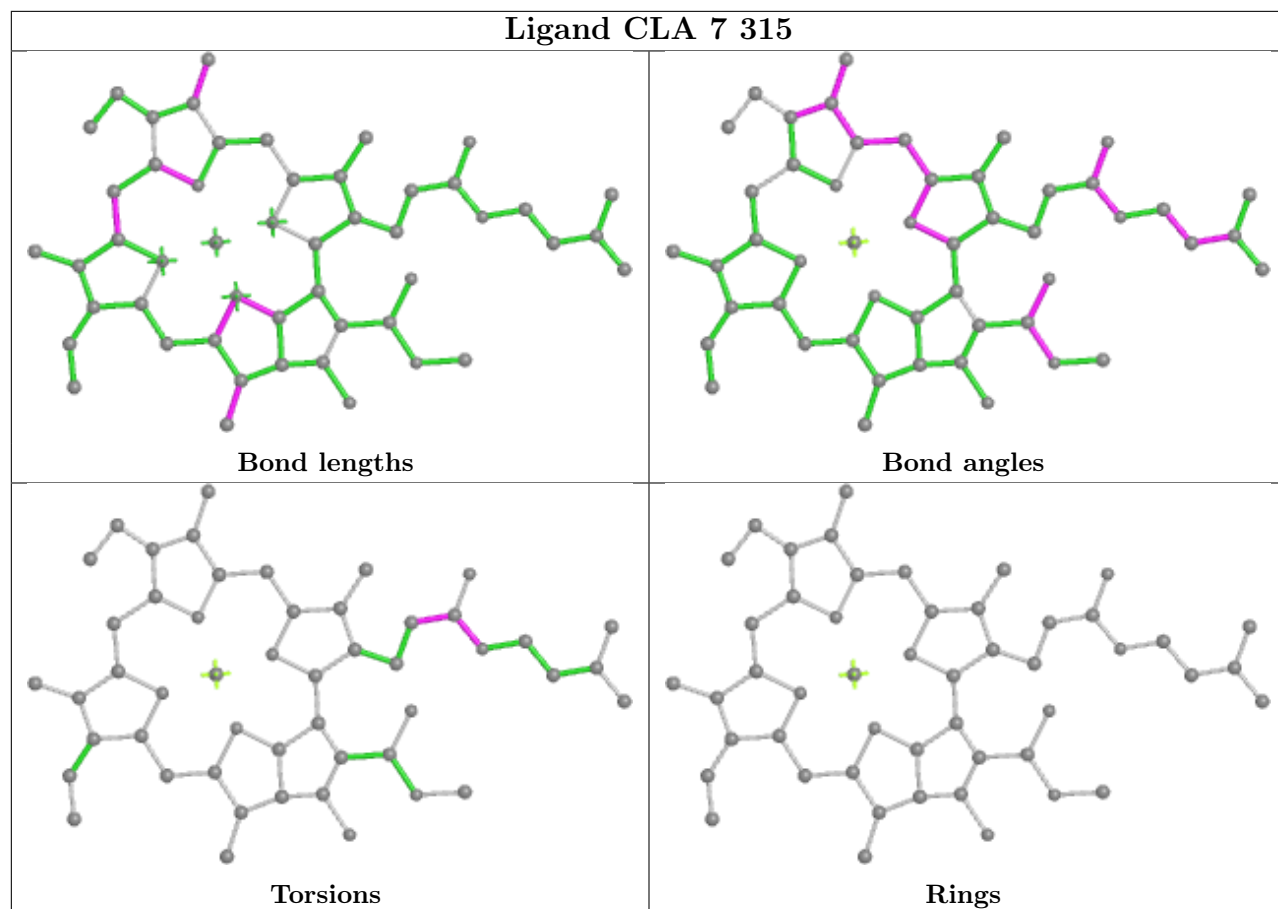


## Ligand A1ECV Q 319

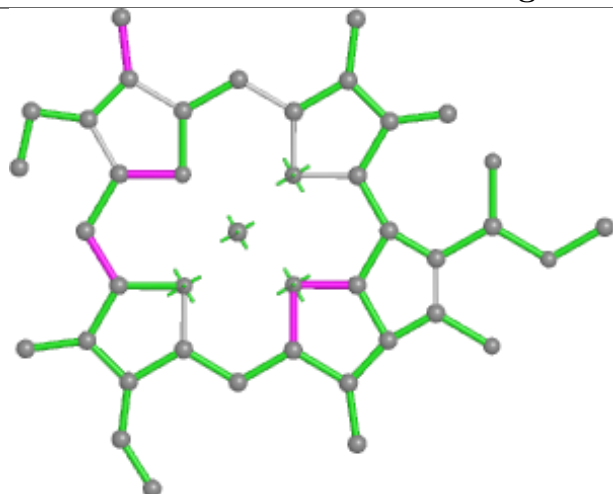




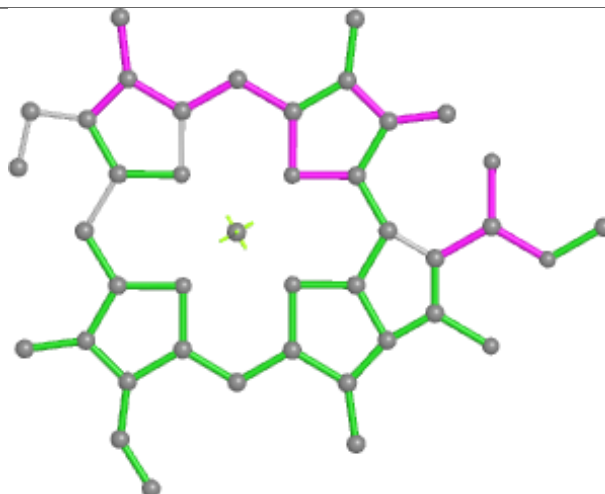
## Ligand CLA 7 315



## Ligand CLA 7 324



Bond lengths



Bond angles

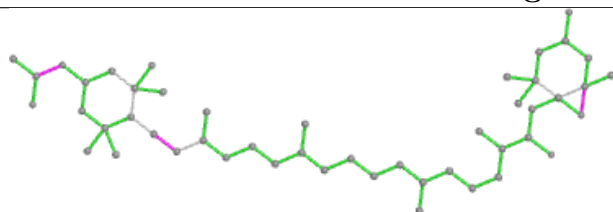


Torsions

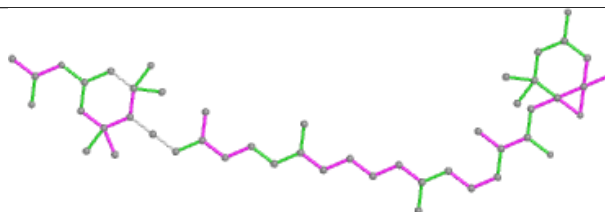


Rings

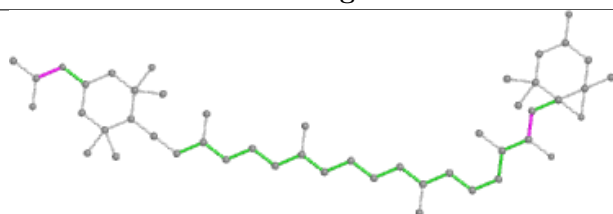
## Ligand A86 7 311



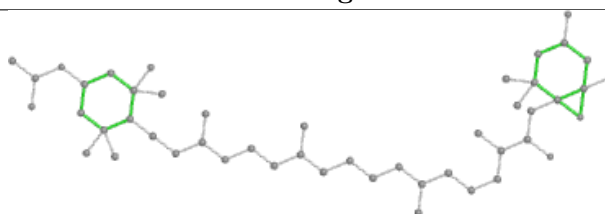
Bond lengths



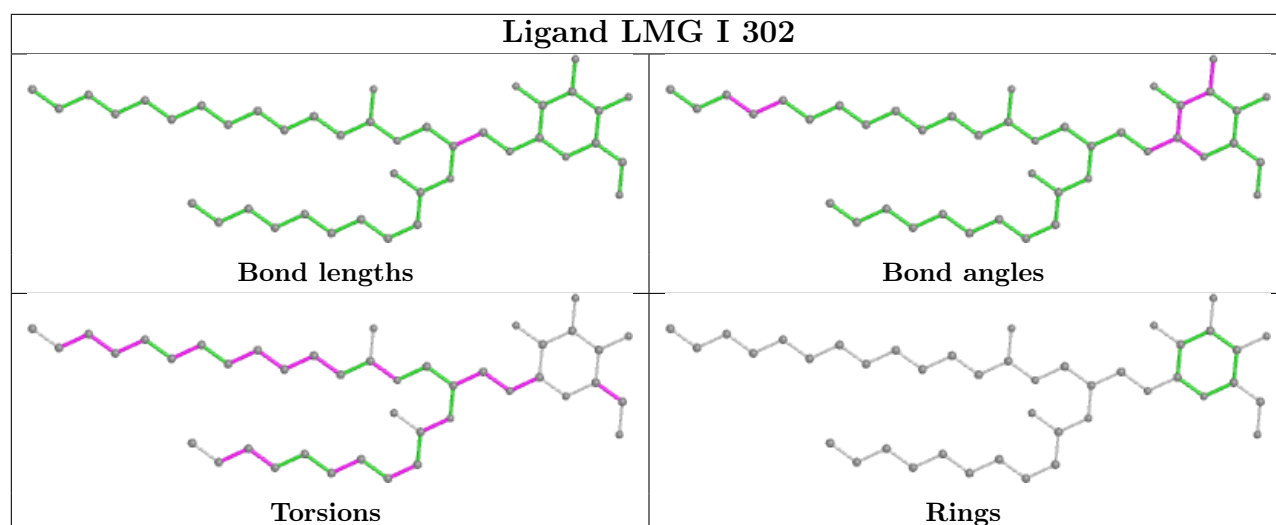
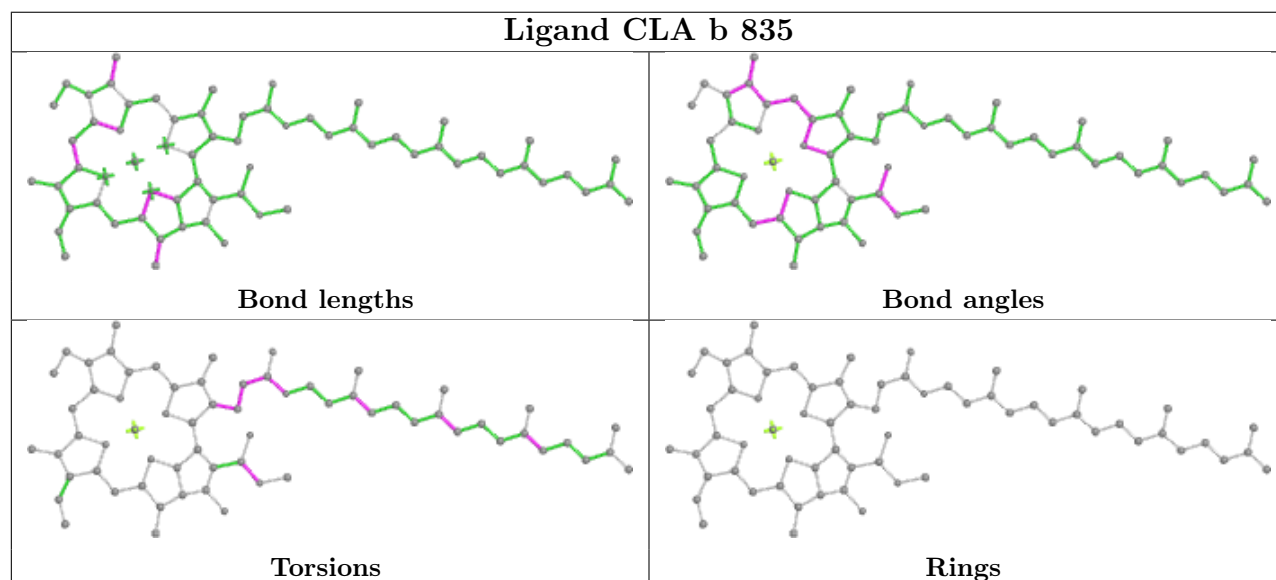
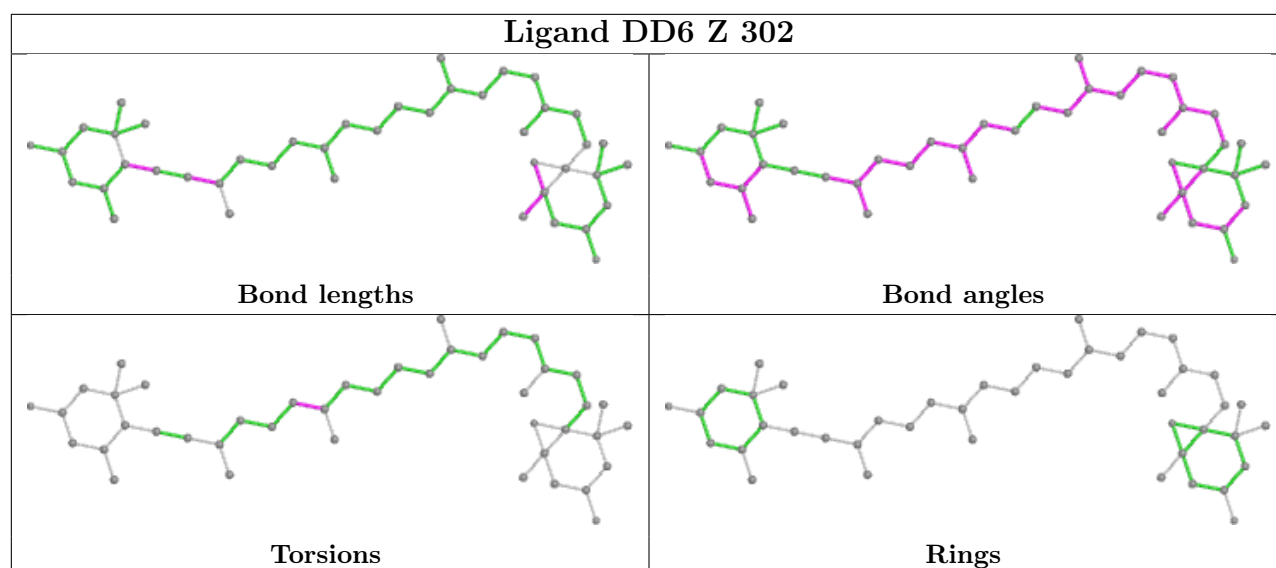
Bond angles

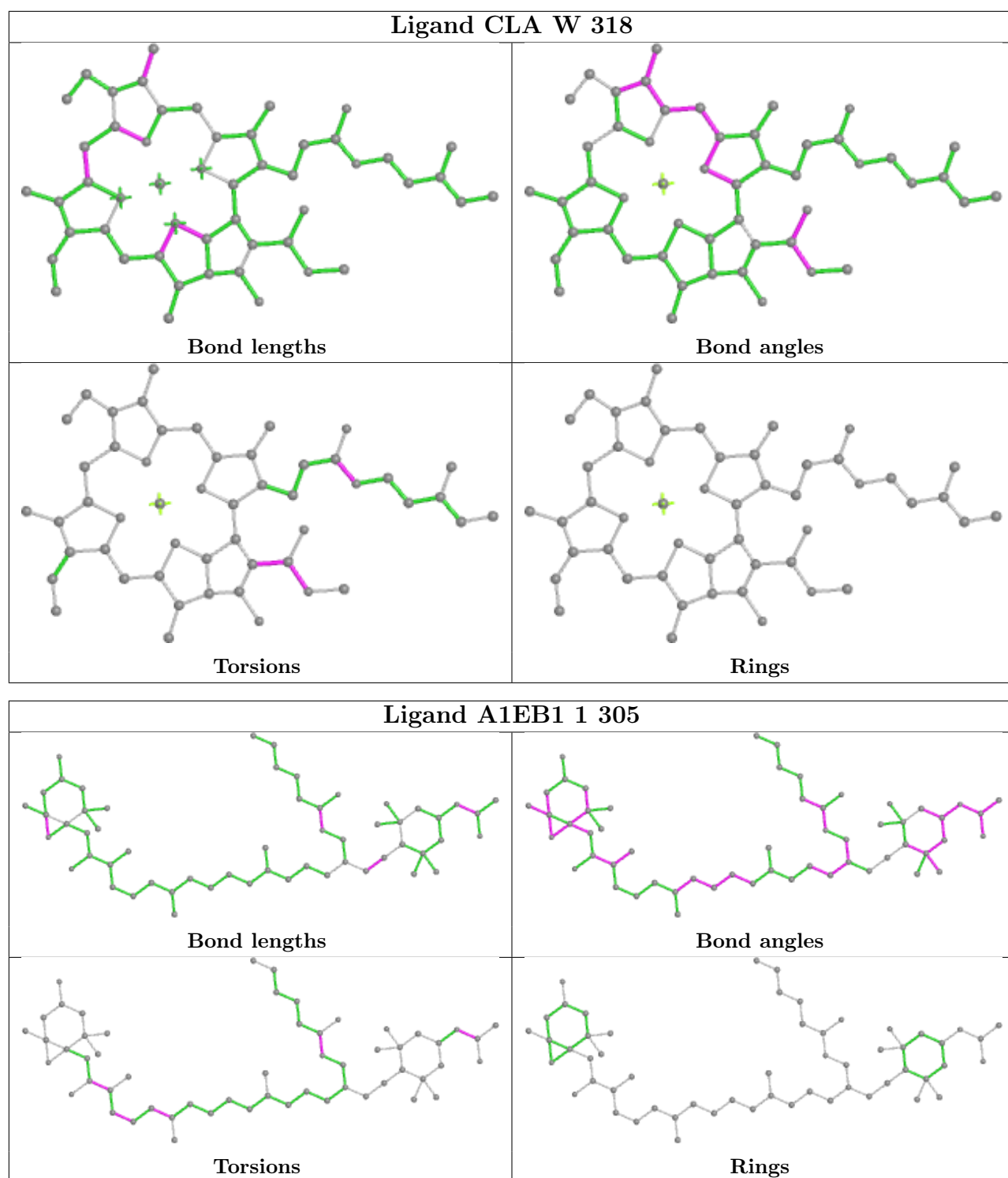


Torsions

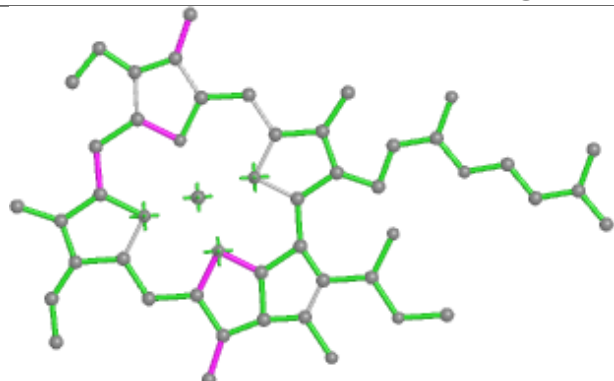


Rings

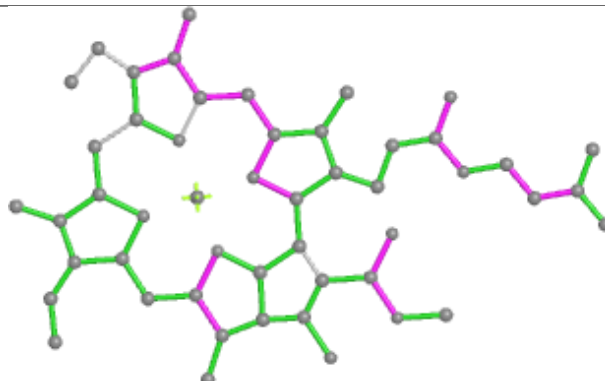




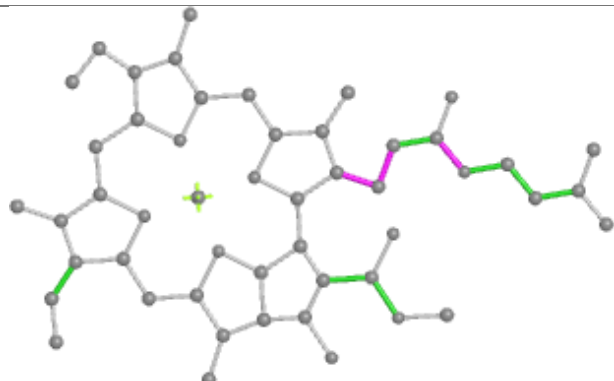
## Ligand CLA b 831



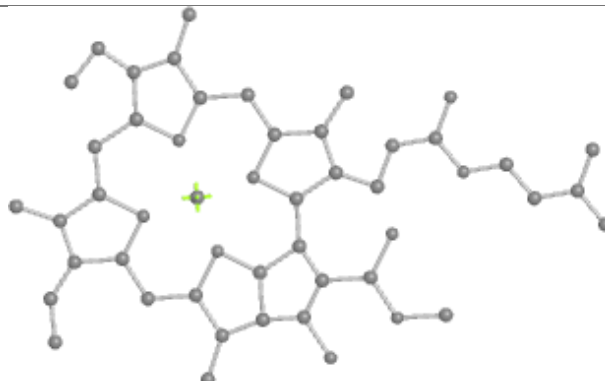
Bond lengths



Bond angles

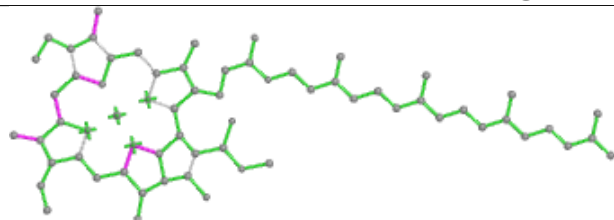


Torsions

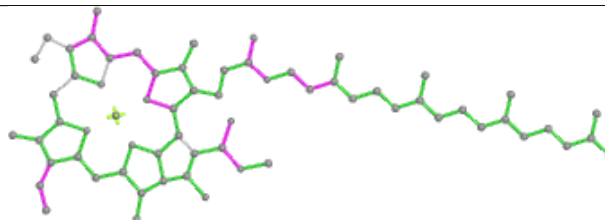


Rings

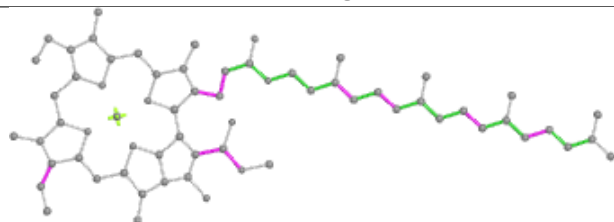
## Ligand CLA b 815



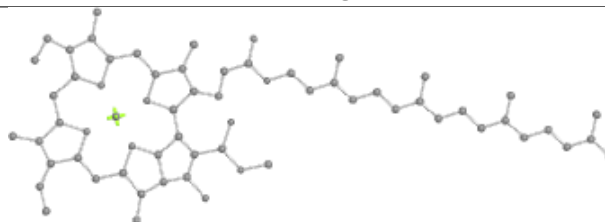
Bond lengths



Bond angles

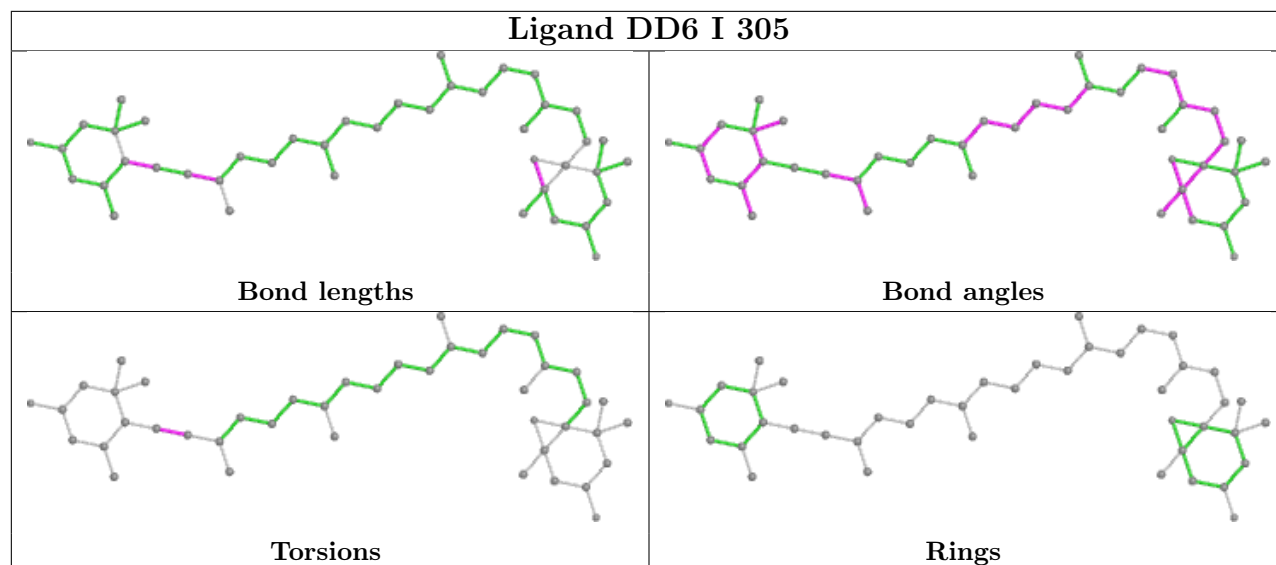


Torsions

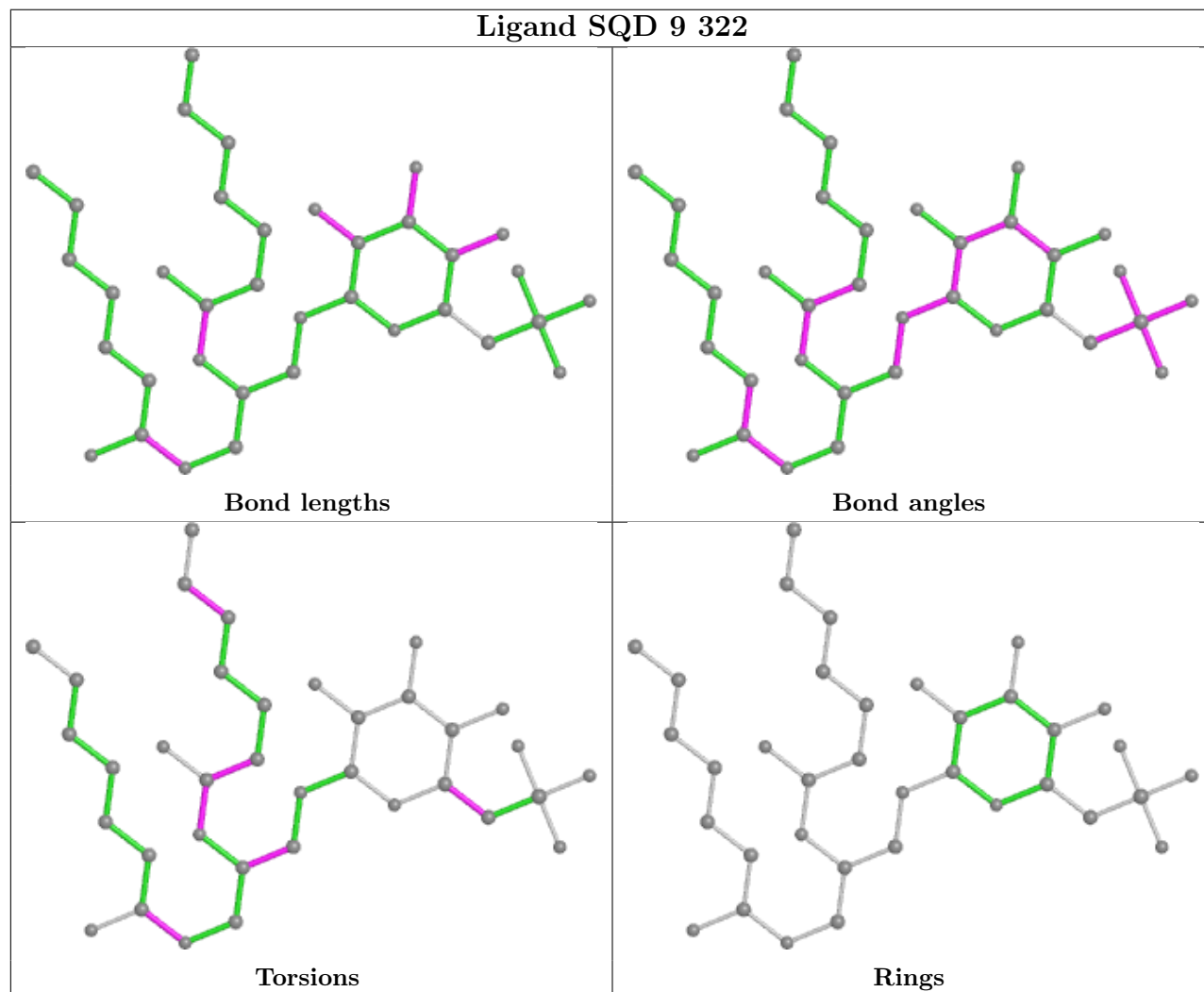


Rings

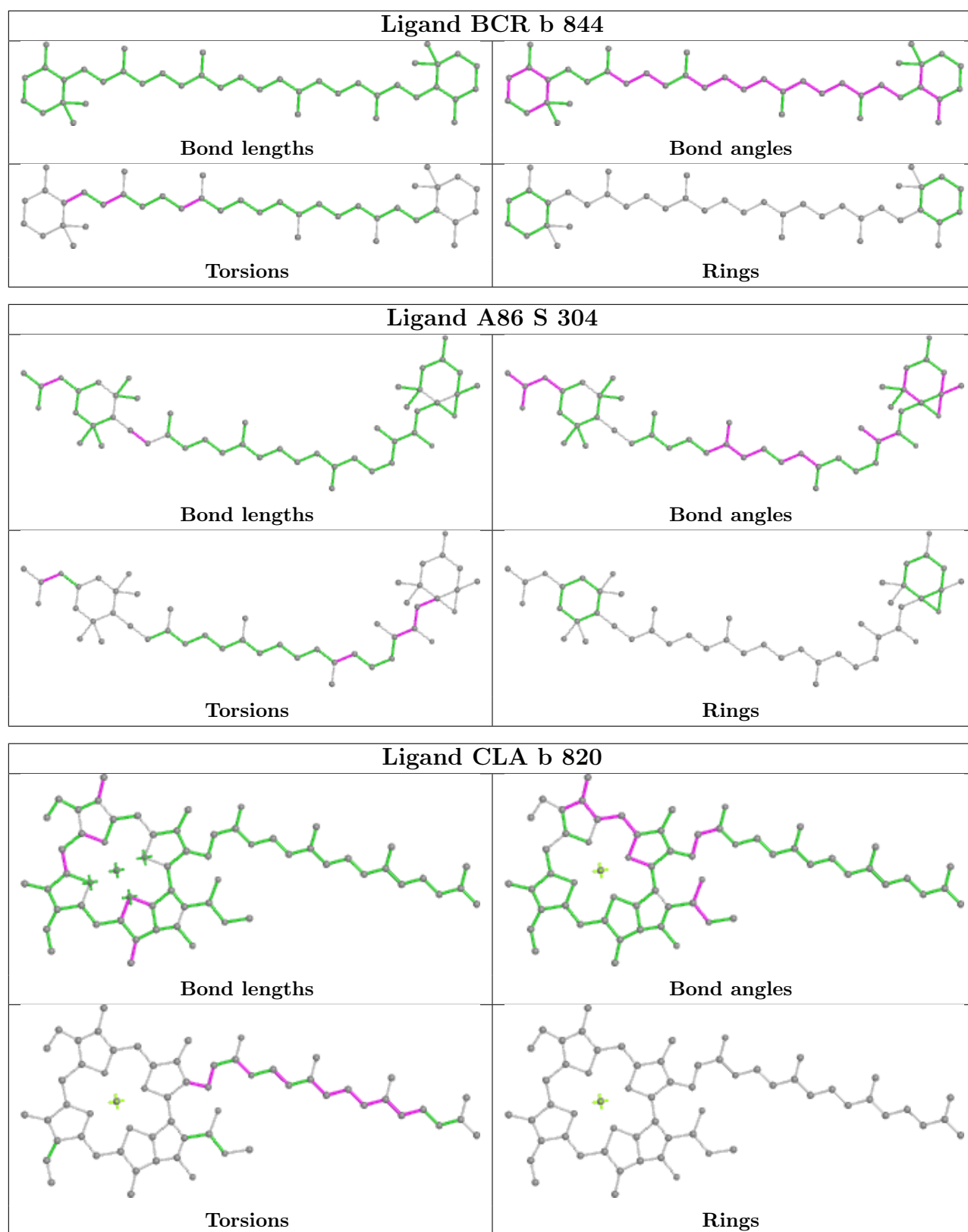
## Ligand DD6 I 305

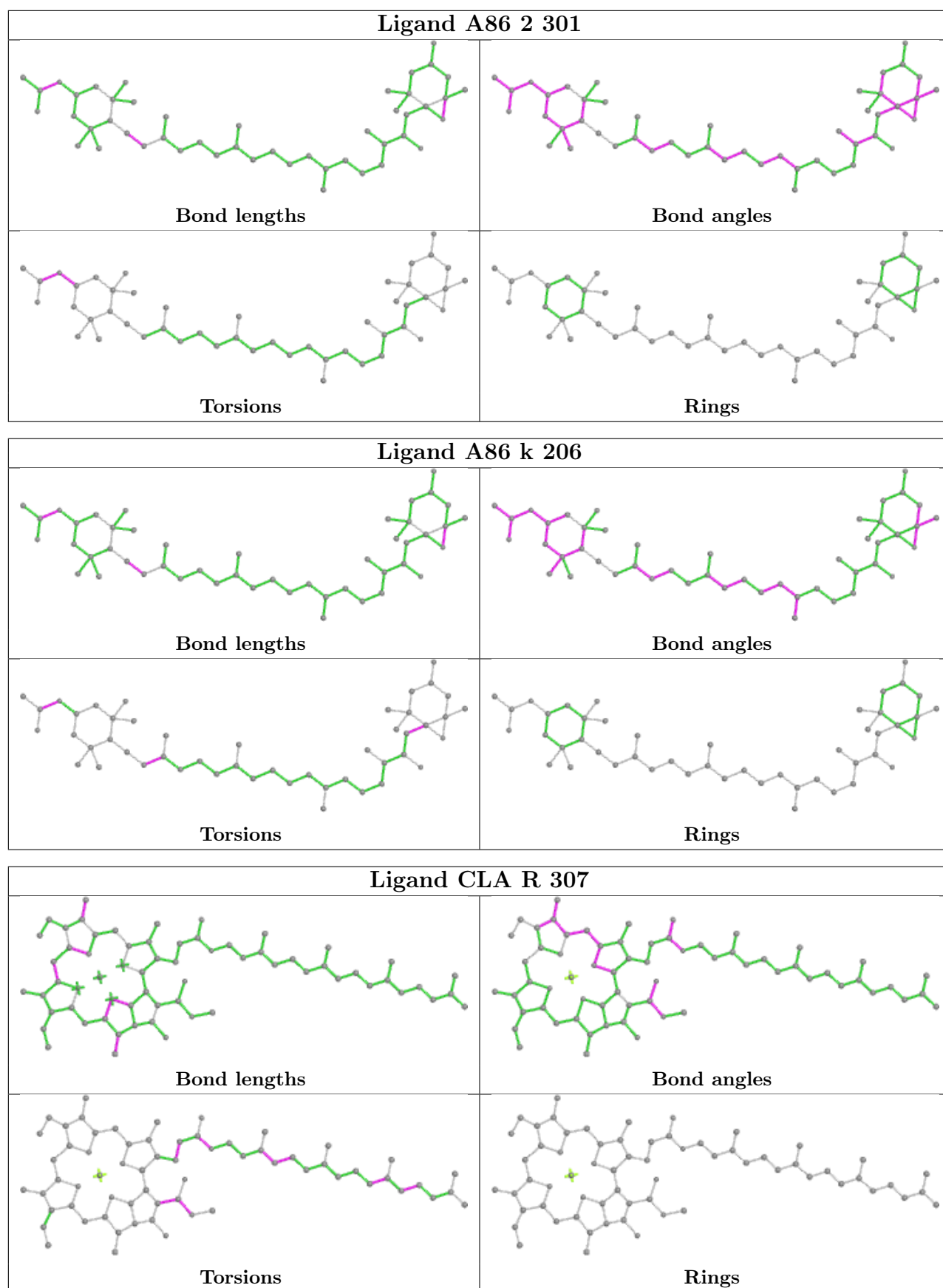


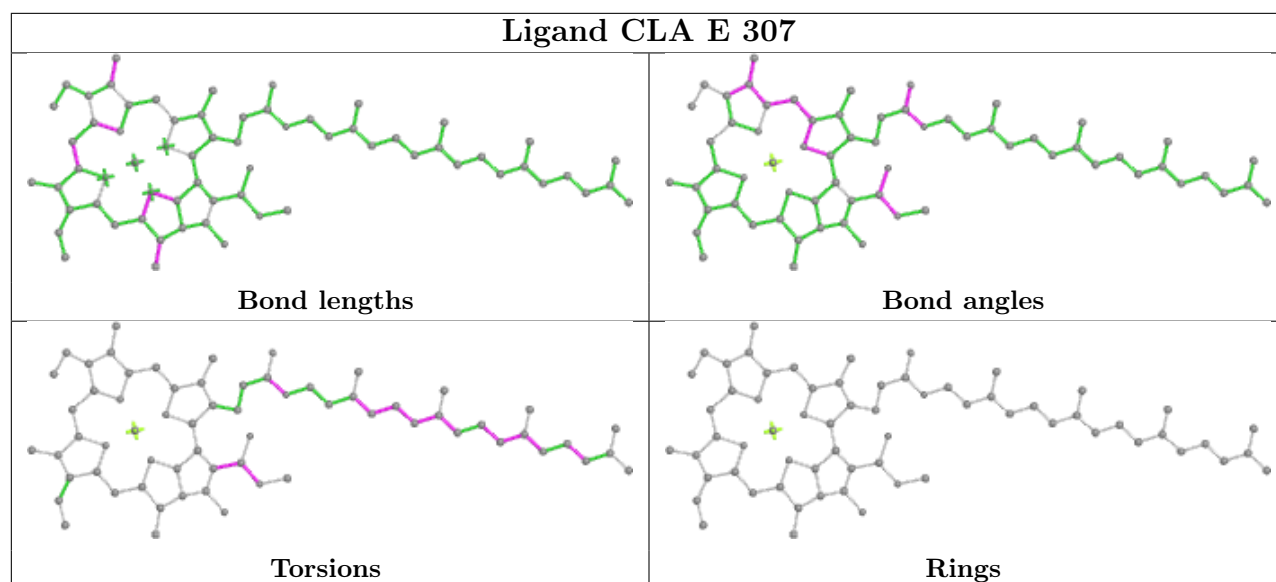
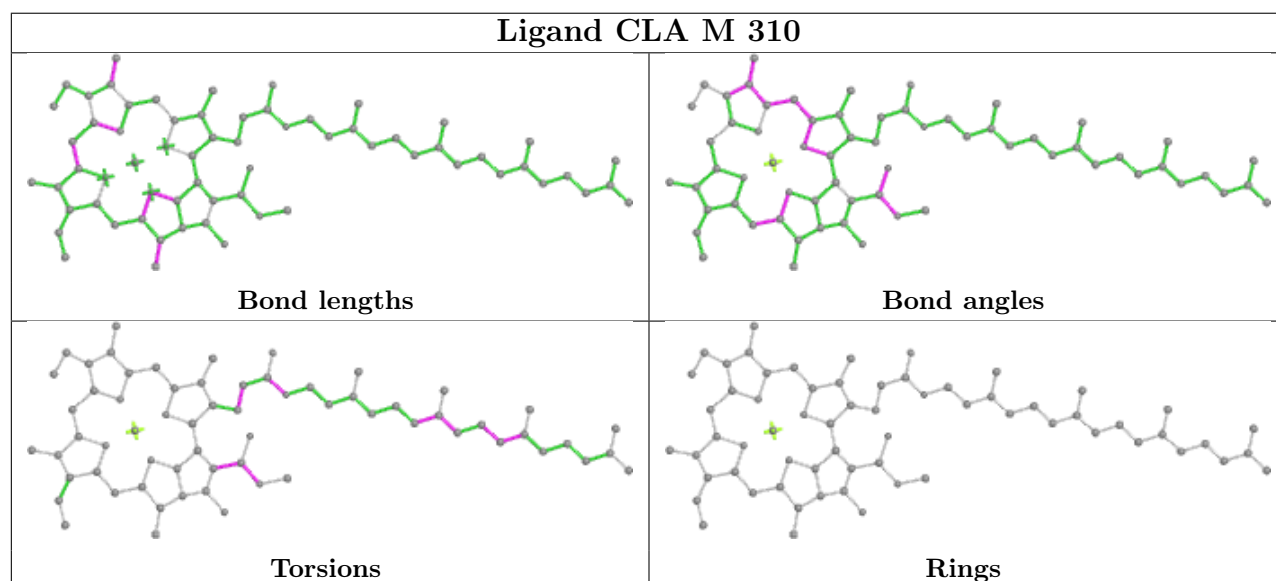
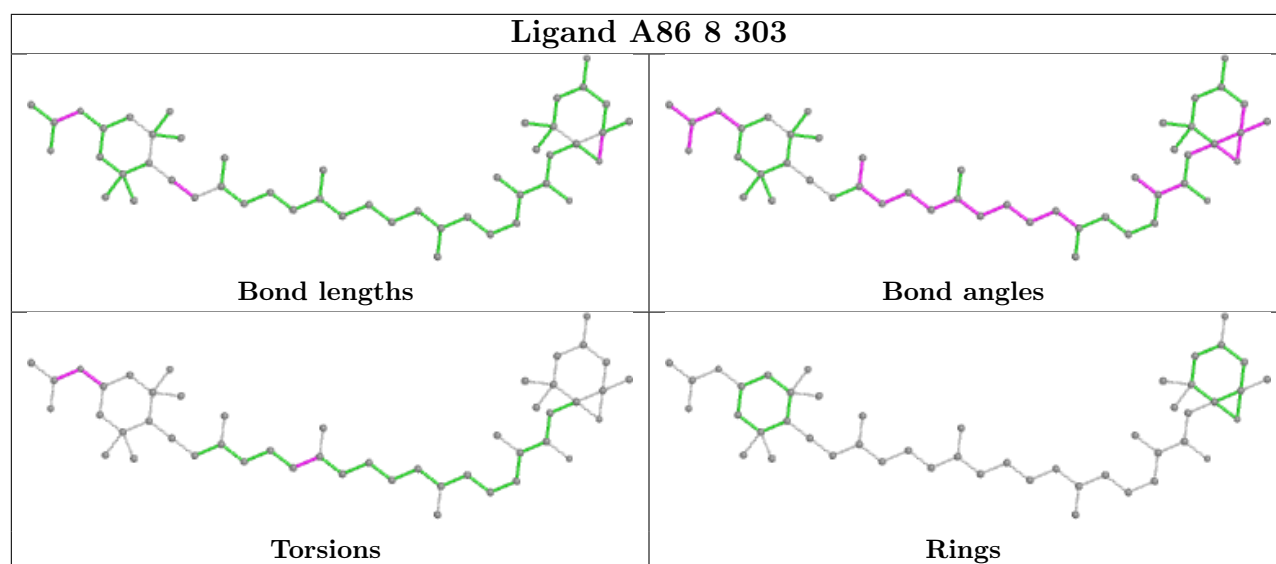
## Ligand SQD 9 322



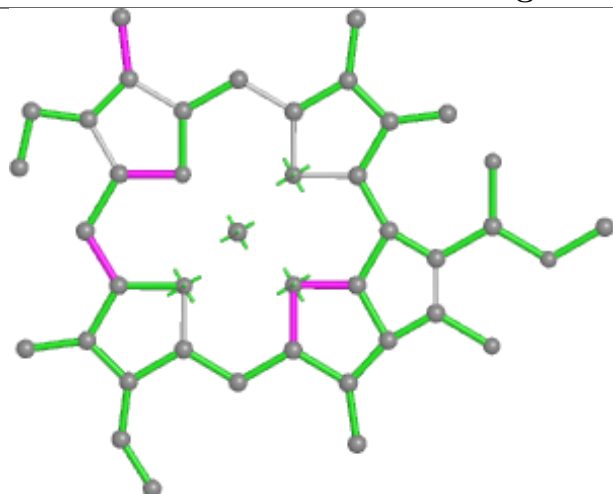




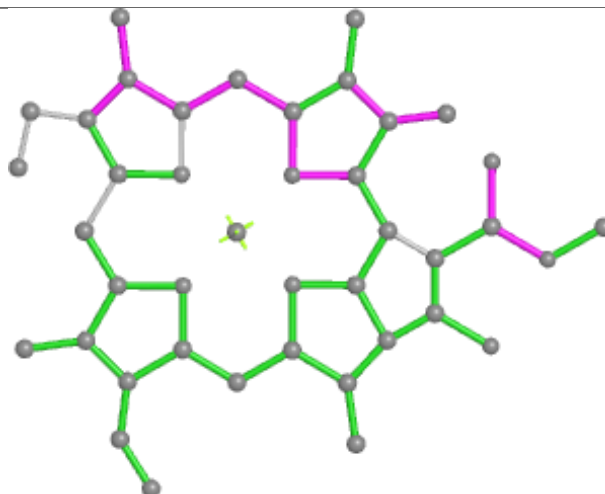




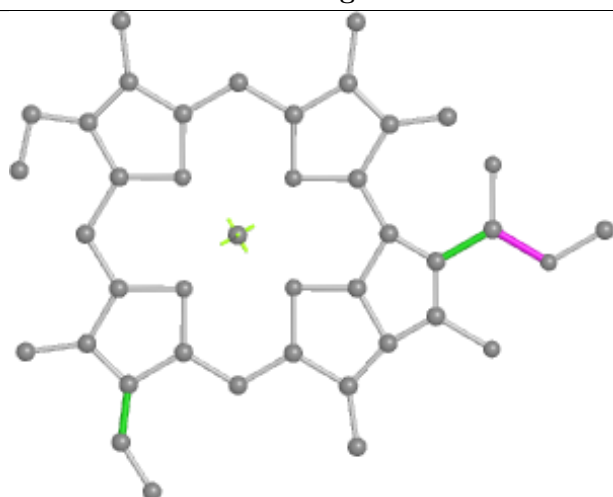
## Ligand CLA Z 315



Bond lengths



Bond angles

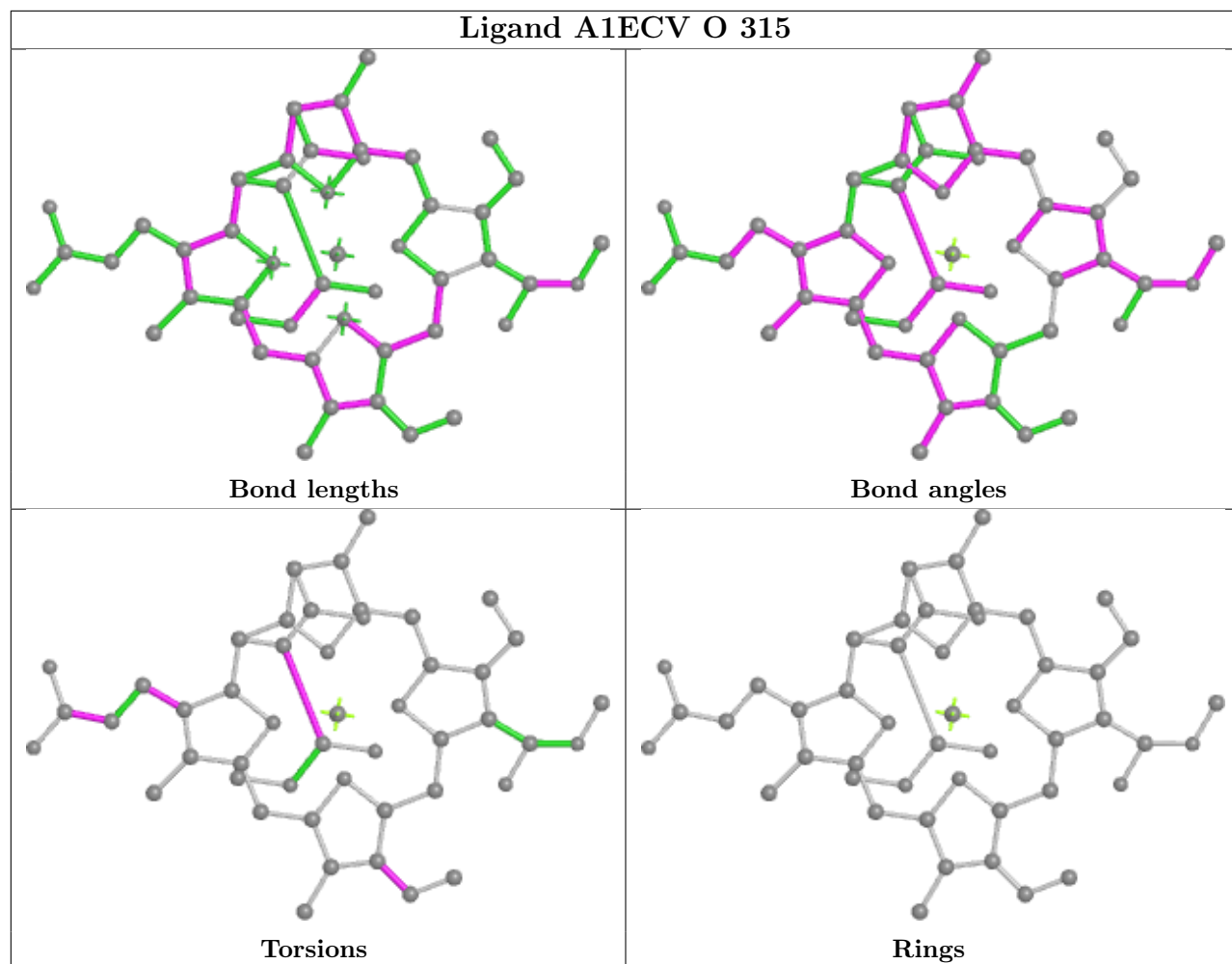


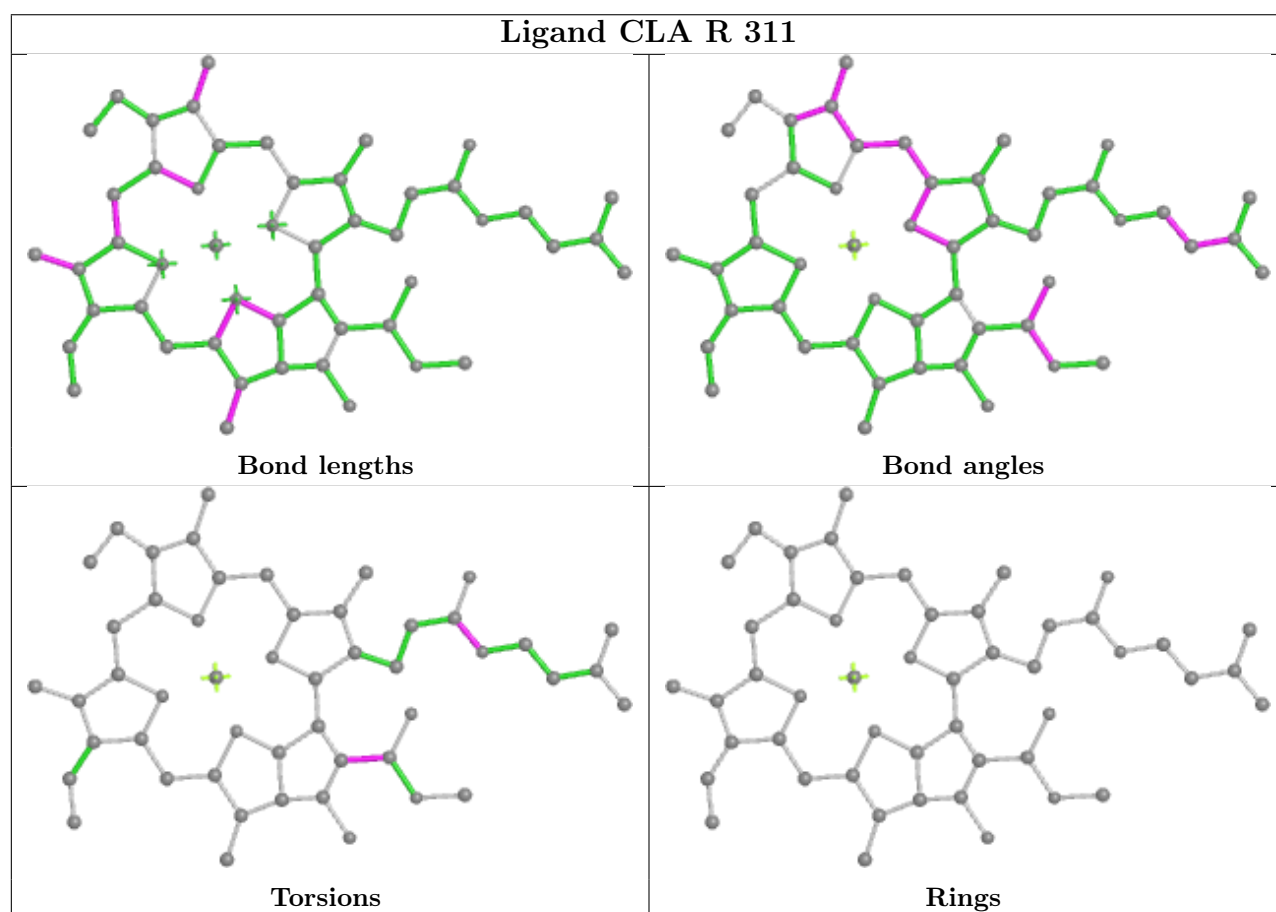
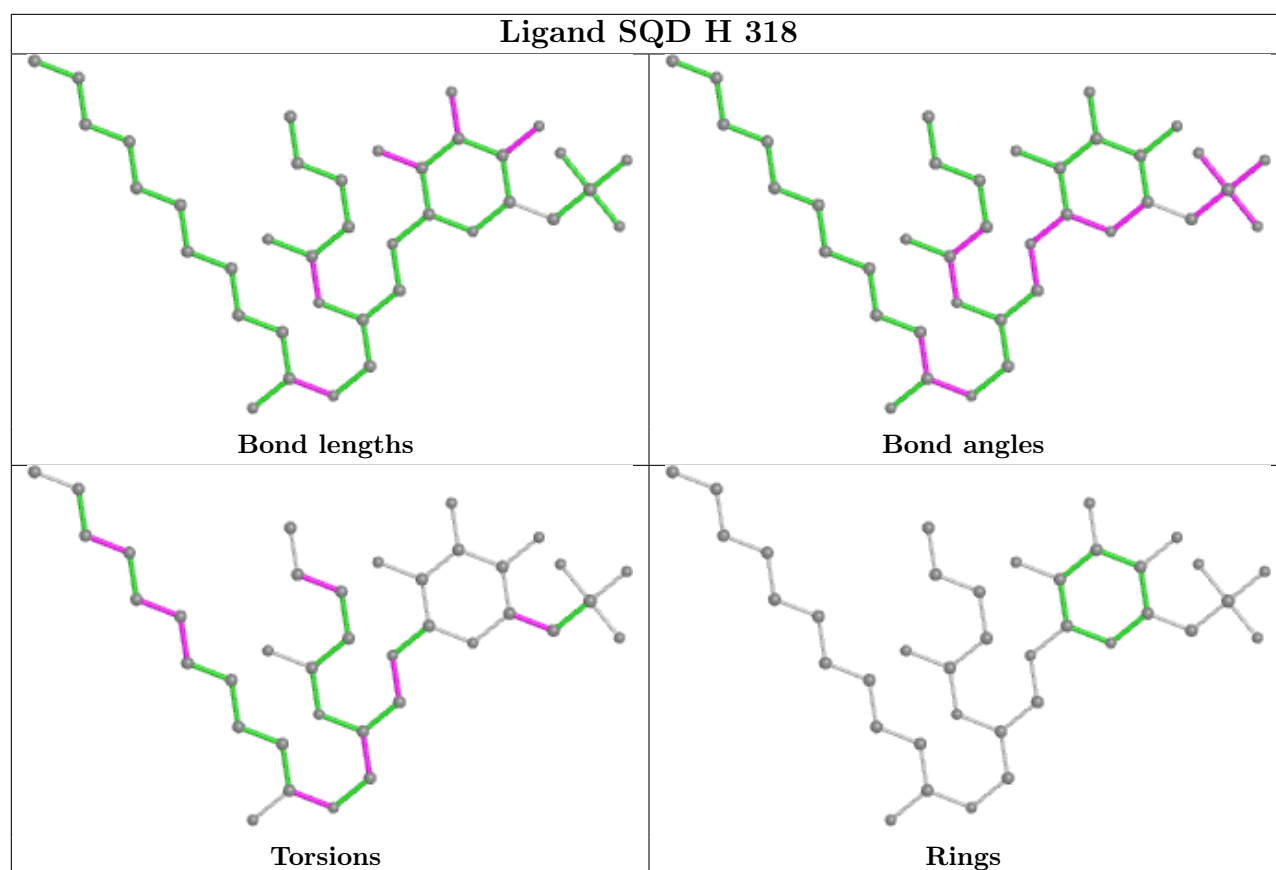
Torsions

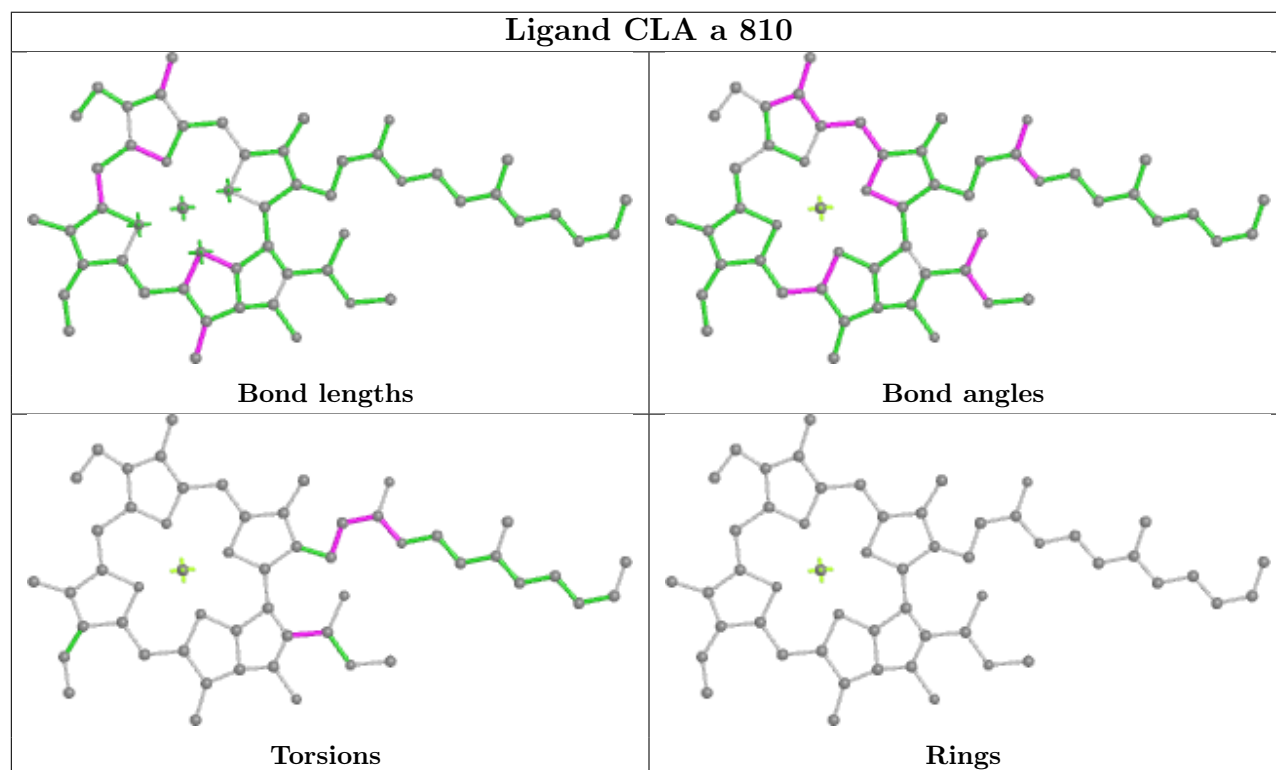
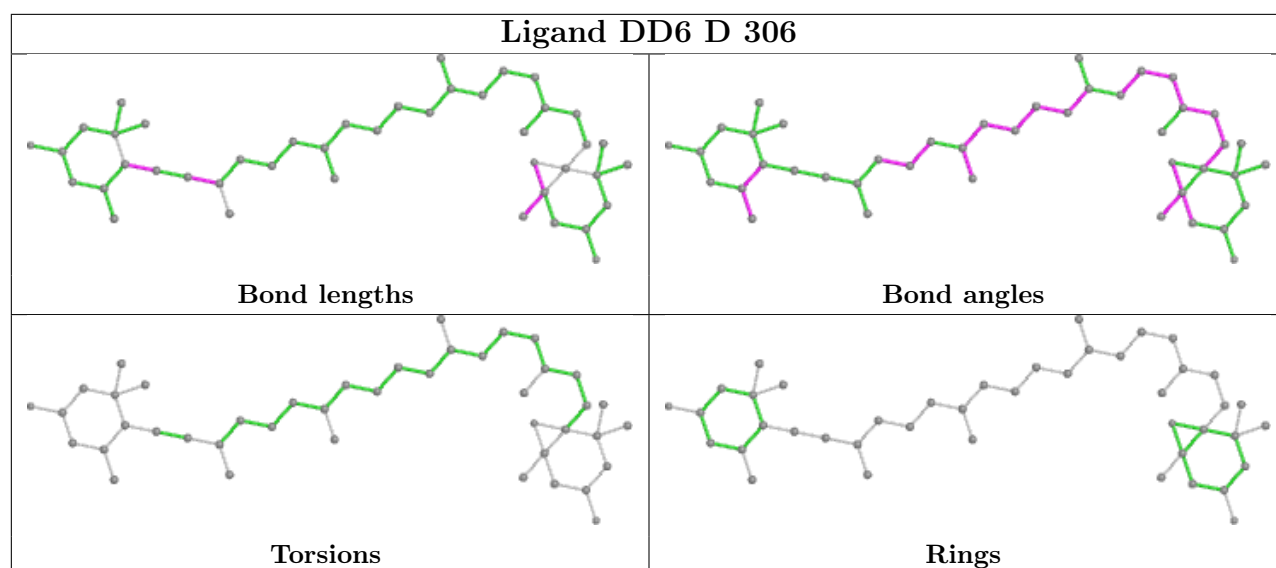


Rings

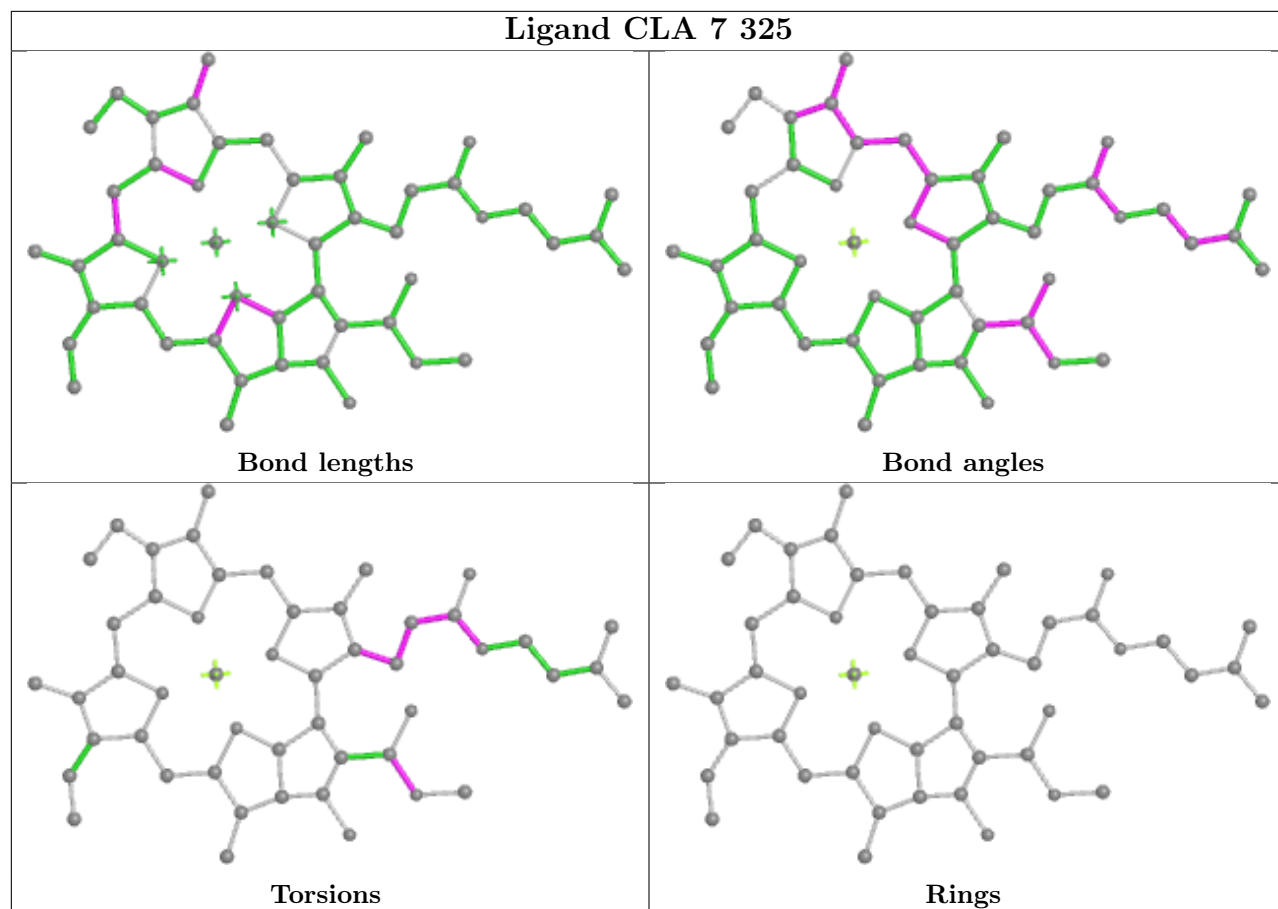
## Ligand A1ECV O 315





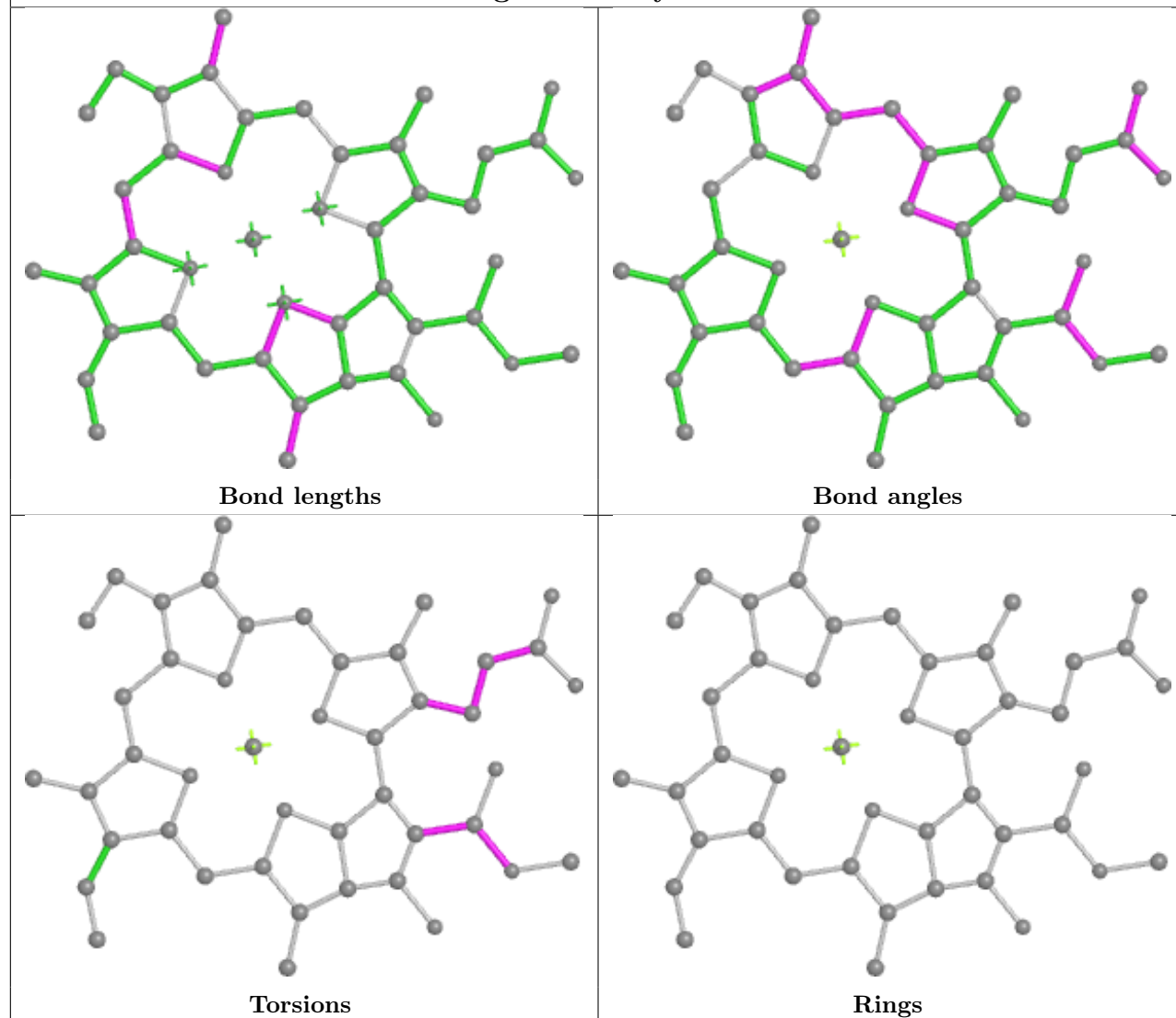


## Ligand CLA 7 325

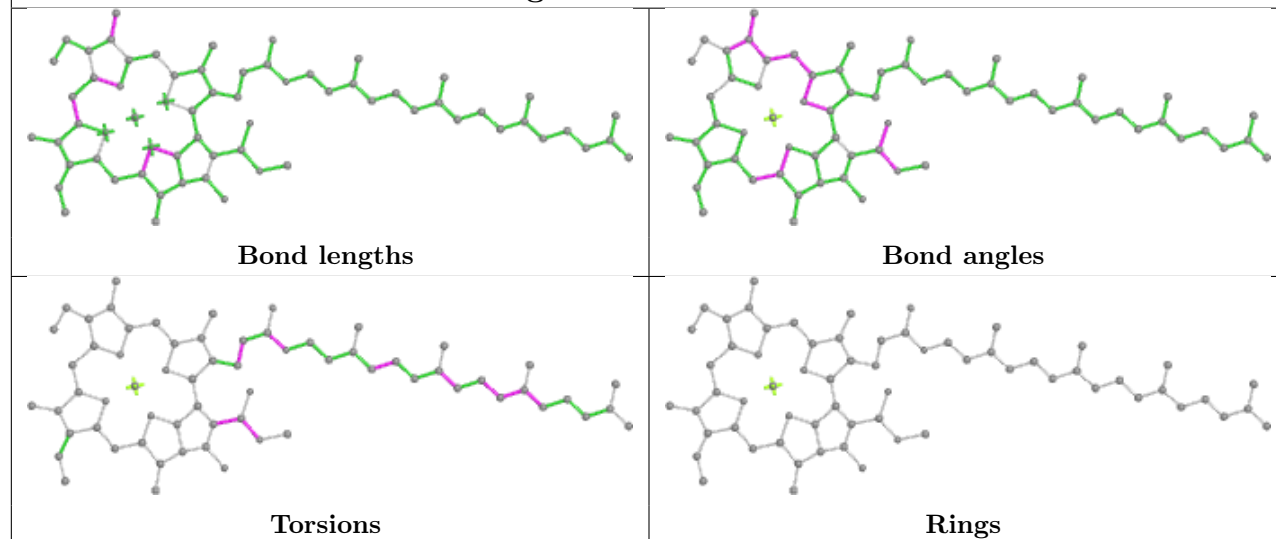




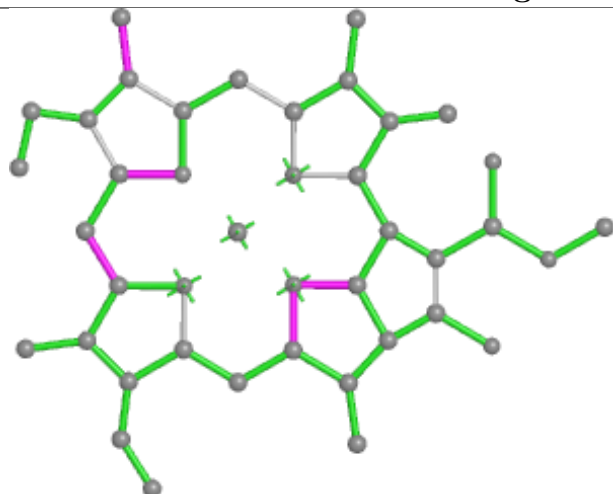
## Ligand CLA y 308



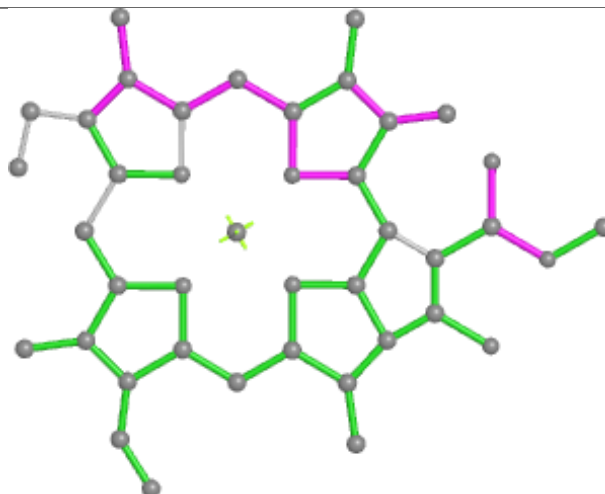
## Ligand CLA W 311



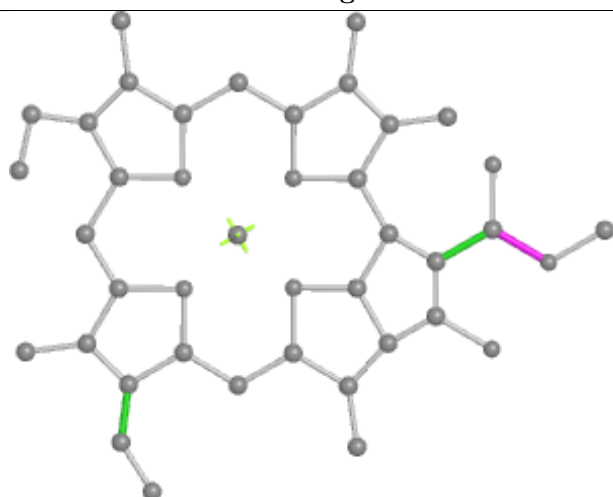
## Ligand CLA Y 310



Bond lengths



Bond angles

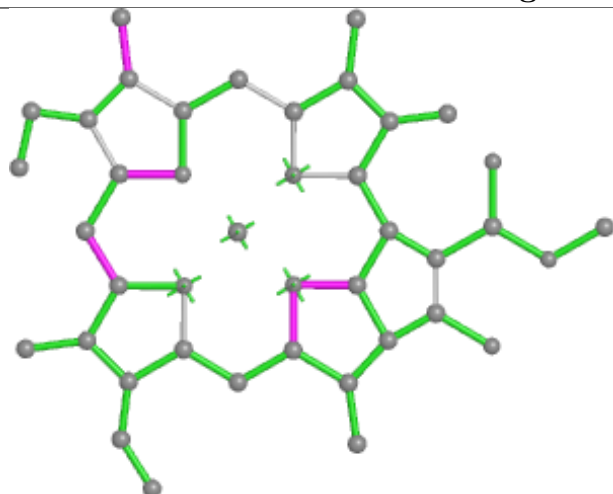


Torsions

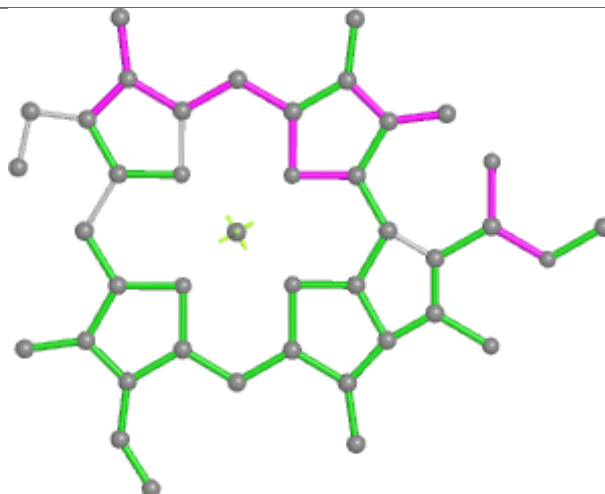


Rings

## Ligand CLA z 311



Bond lengths



Bond angles

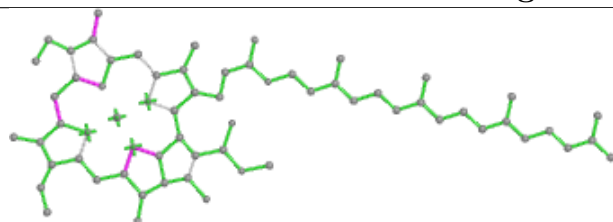


Torsions

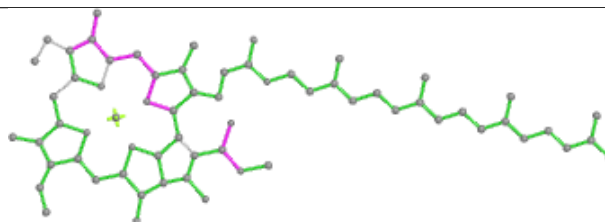


Rings

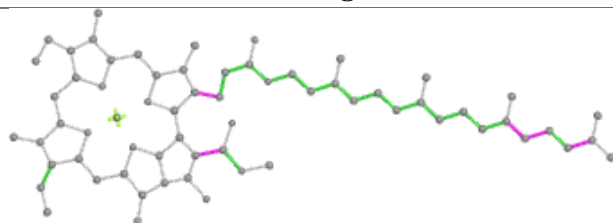
## Ligand CLA b 827



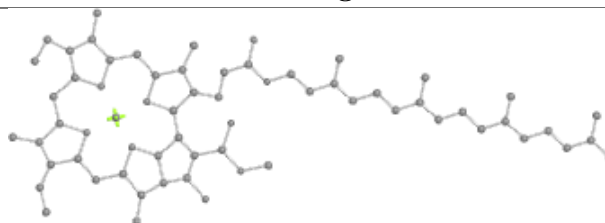
Bond lengths



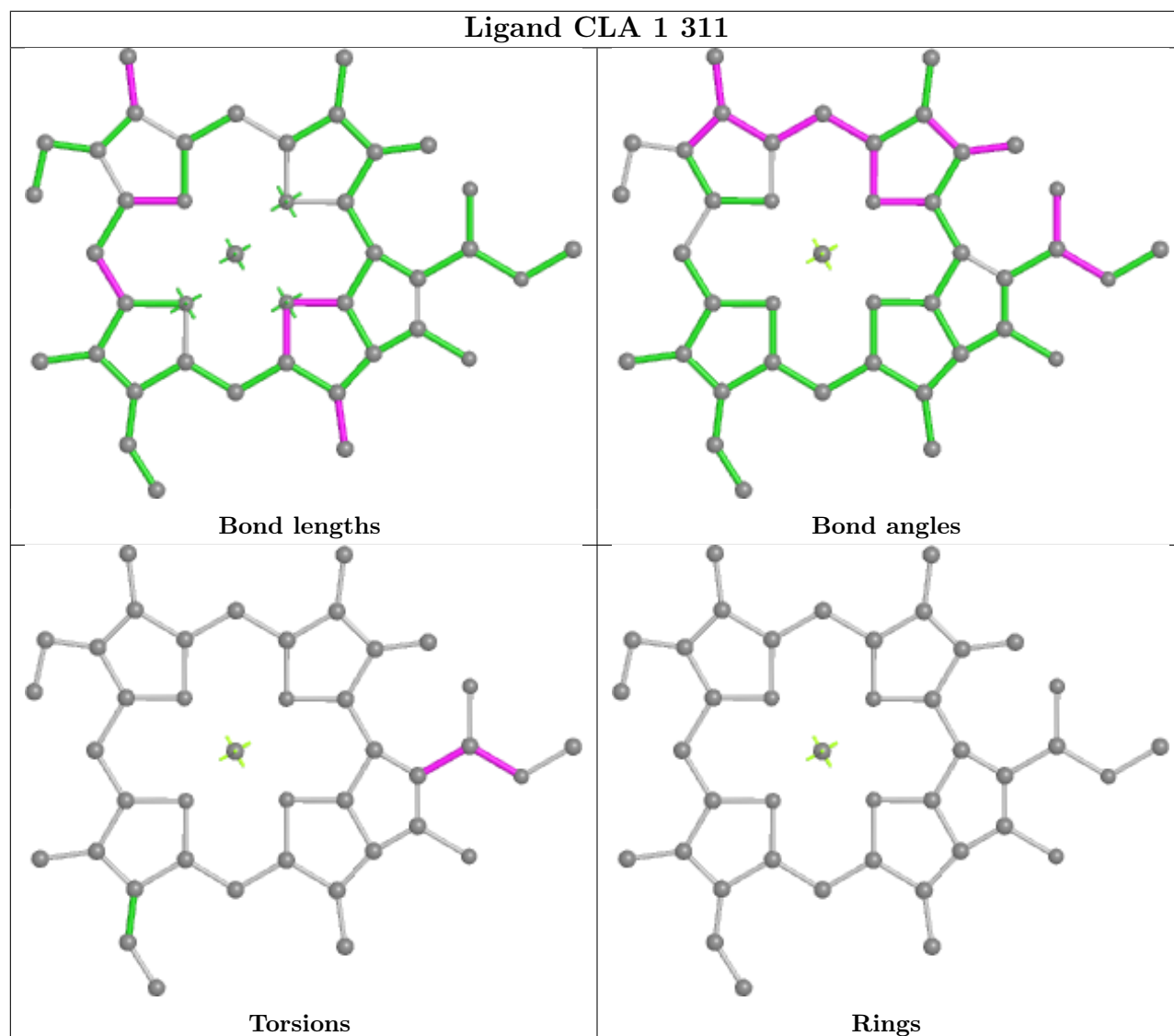
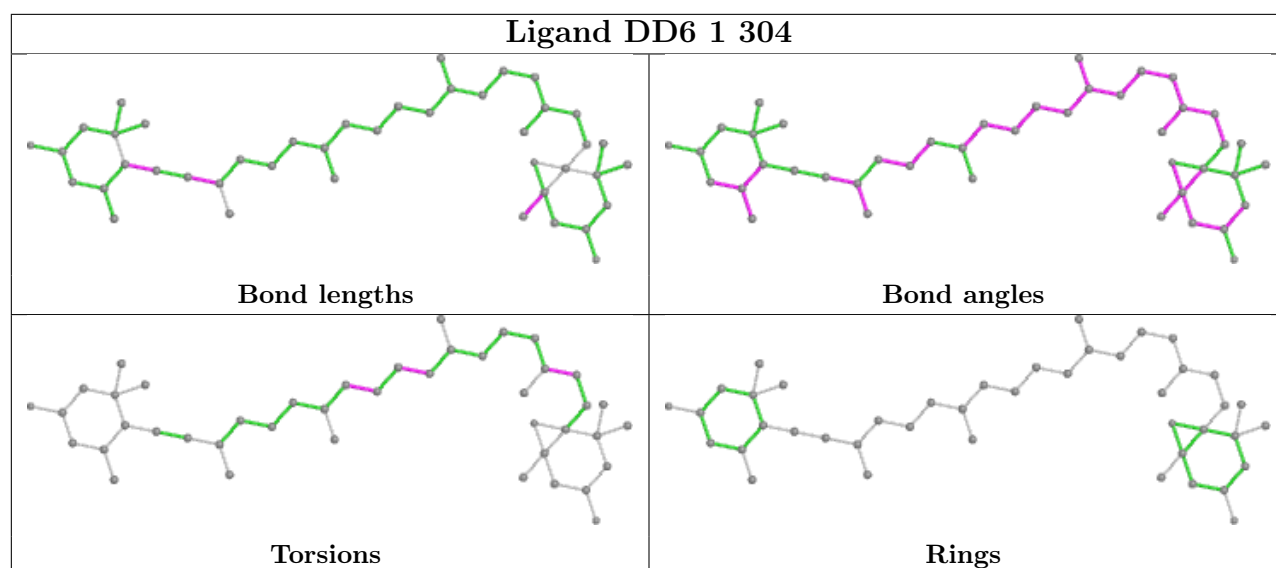
Bond angles



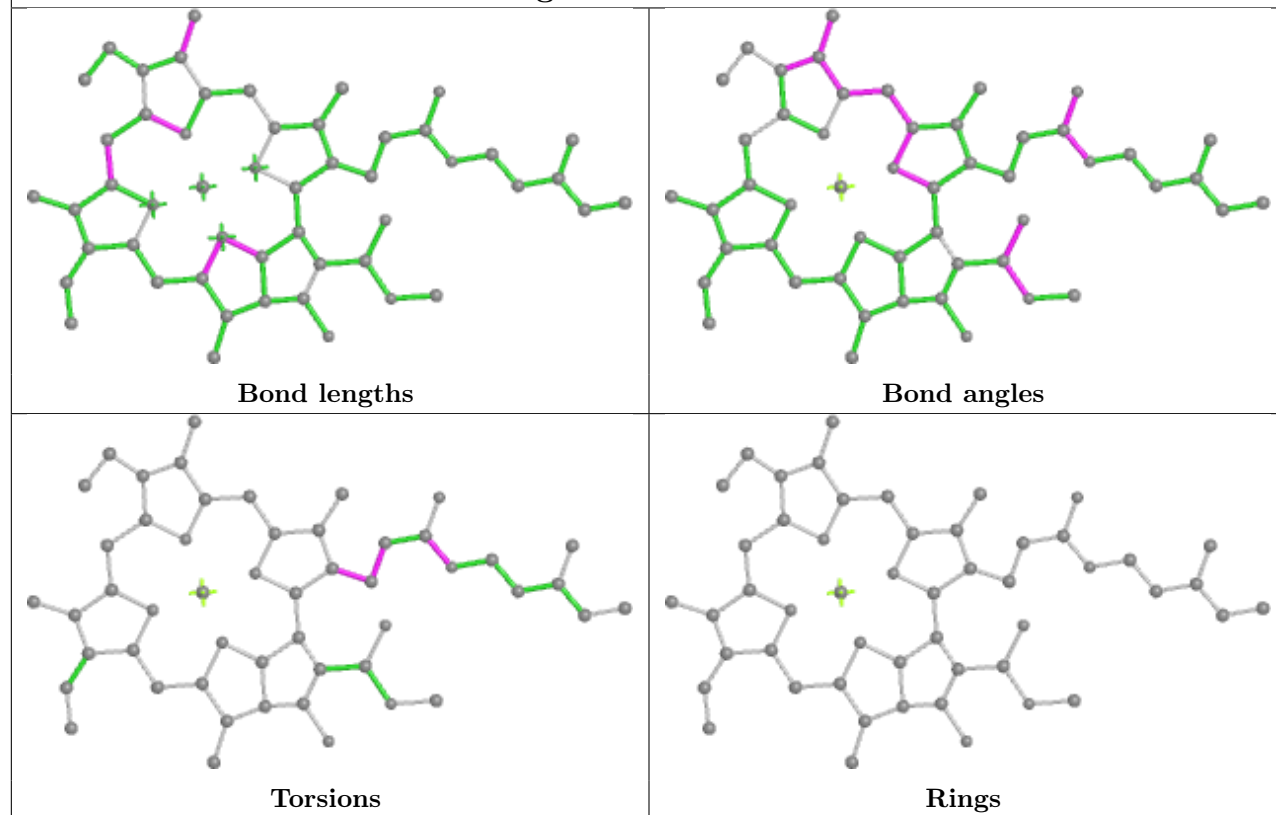
Torsions



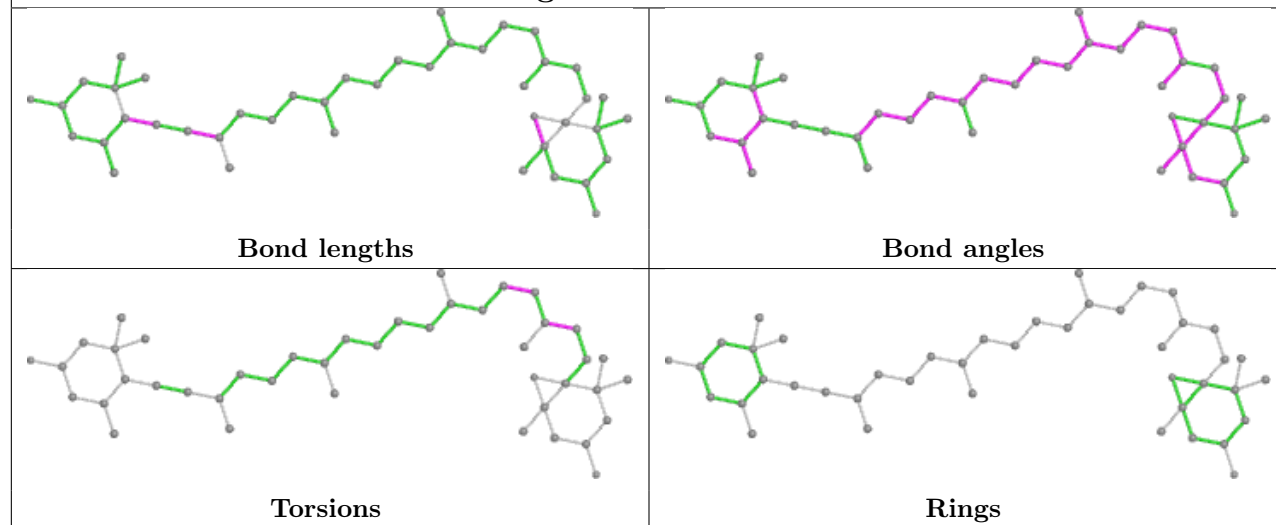
Rings

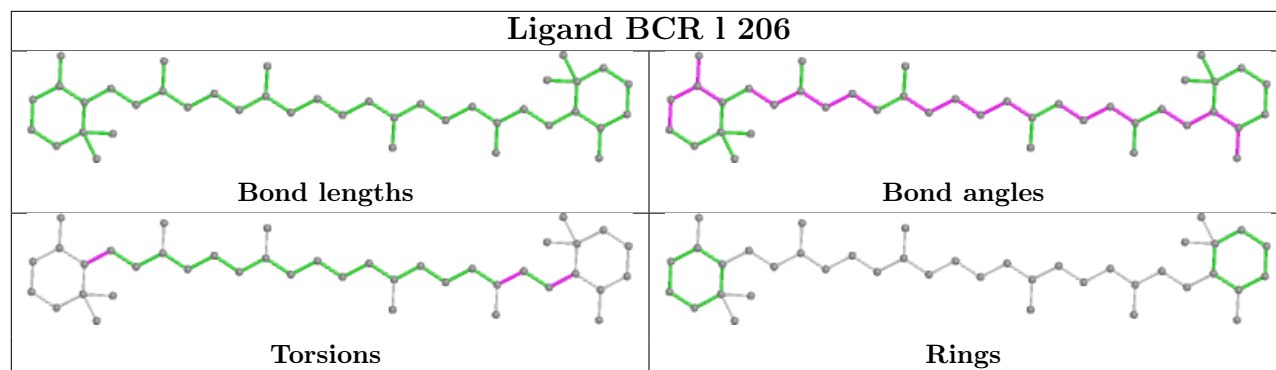
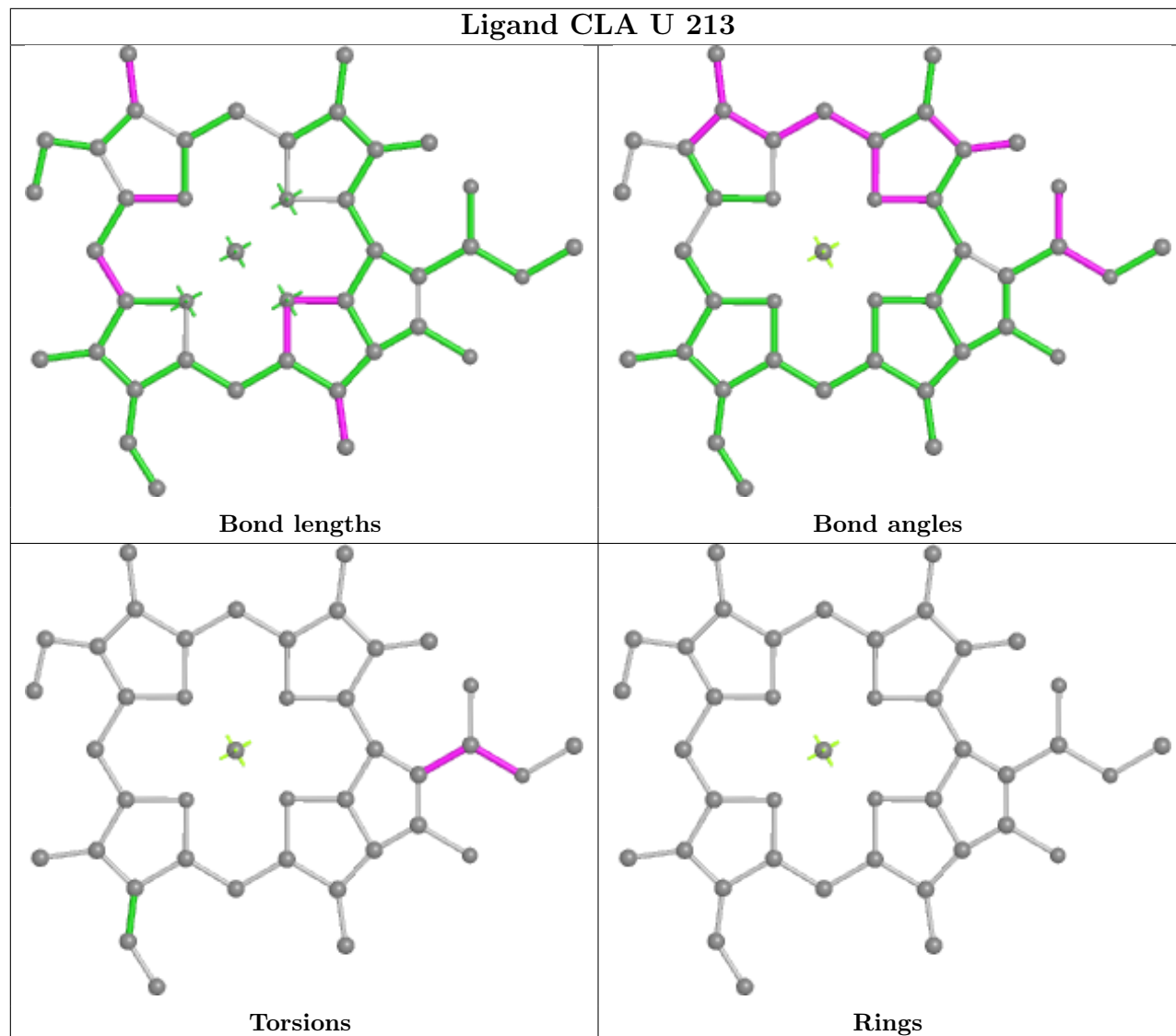


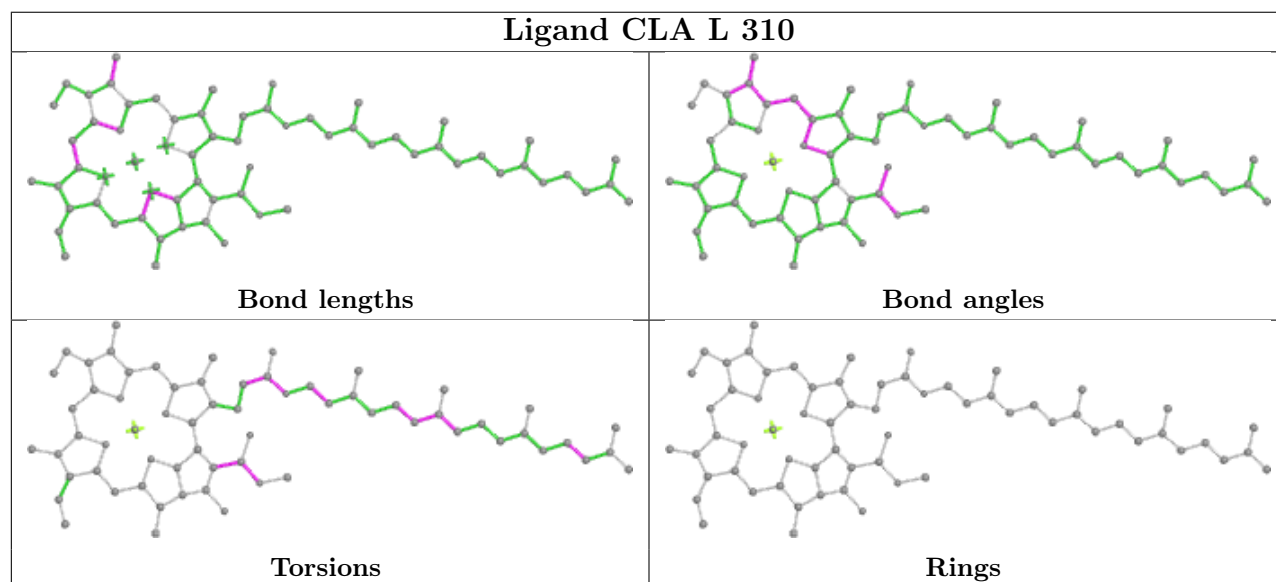
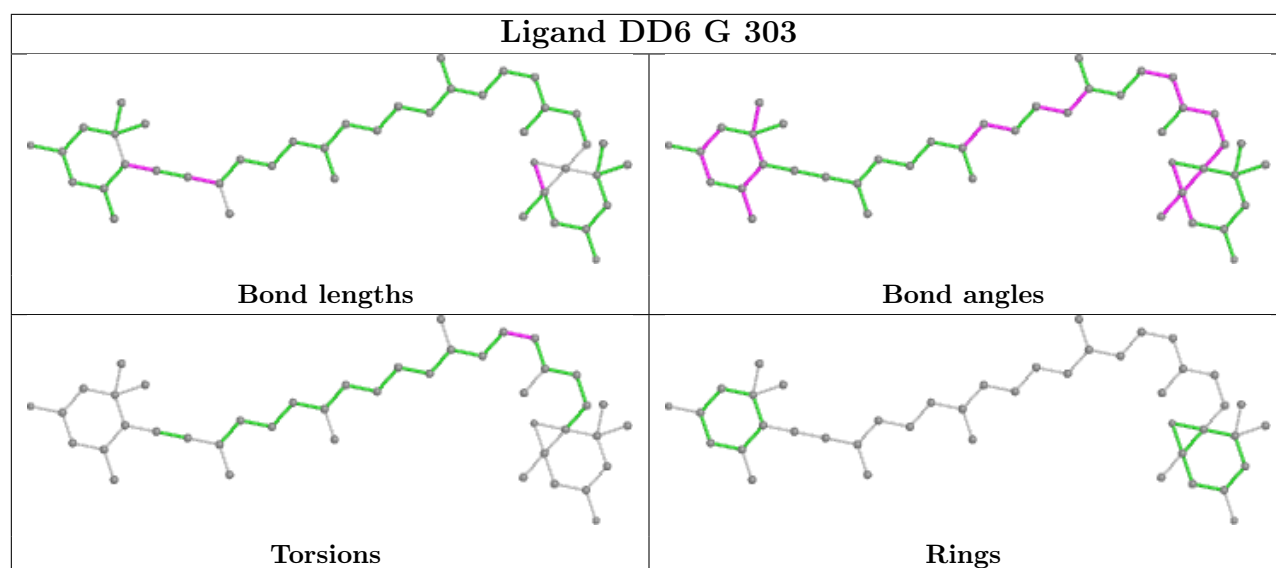
## Ligand CLA o 201



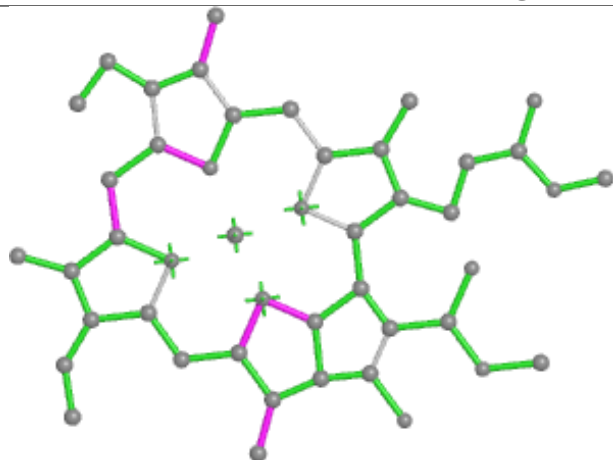
## Ligand DD6 3 304



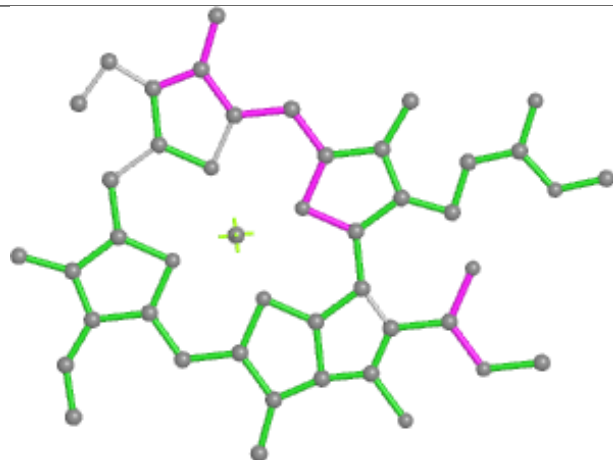
**Ligand BCR 1 206****Ligand CLA U 213**



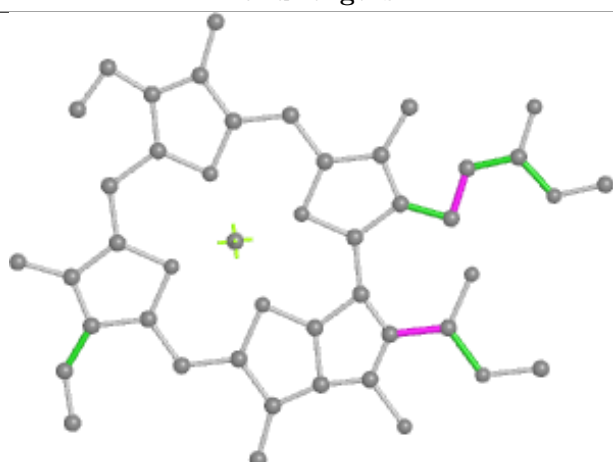
## Ligand CLA U 214



Bond lengths



Bond angles

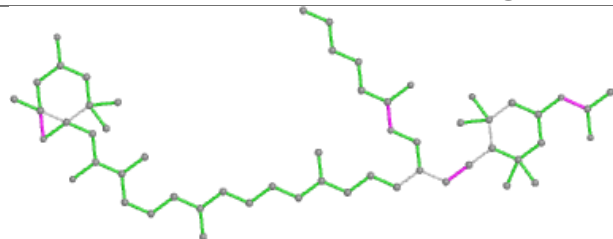


Torsions

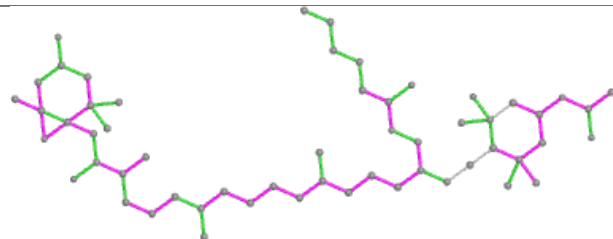


Rings

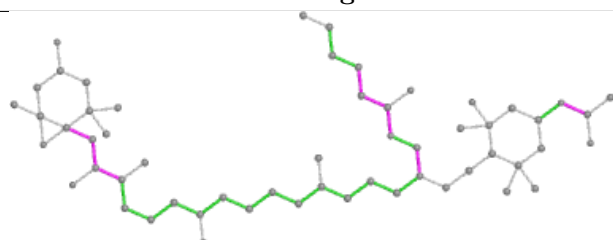
## Ligand A1EB1 7 304



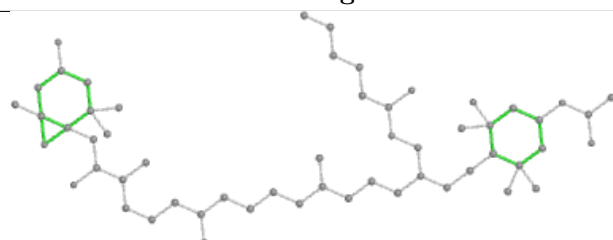
Bond lengths



Bond angles

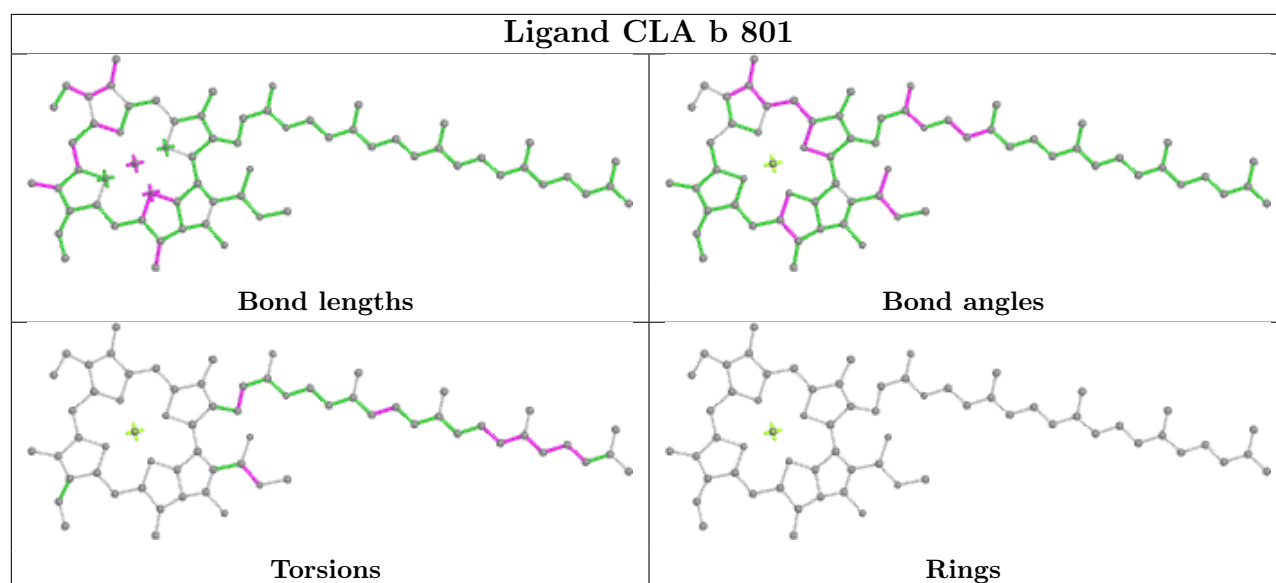
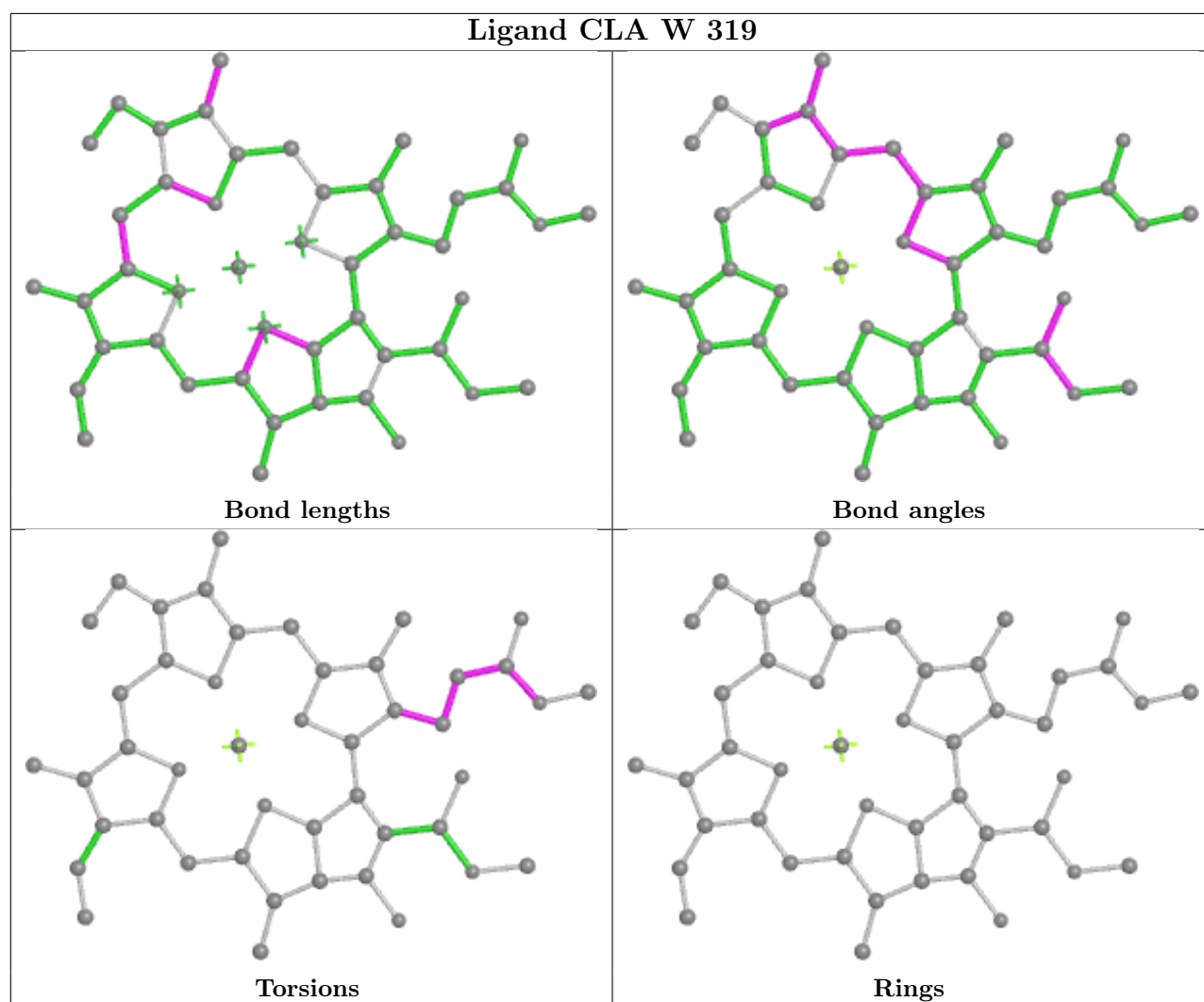


Torsions

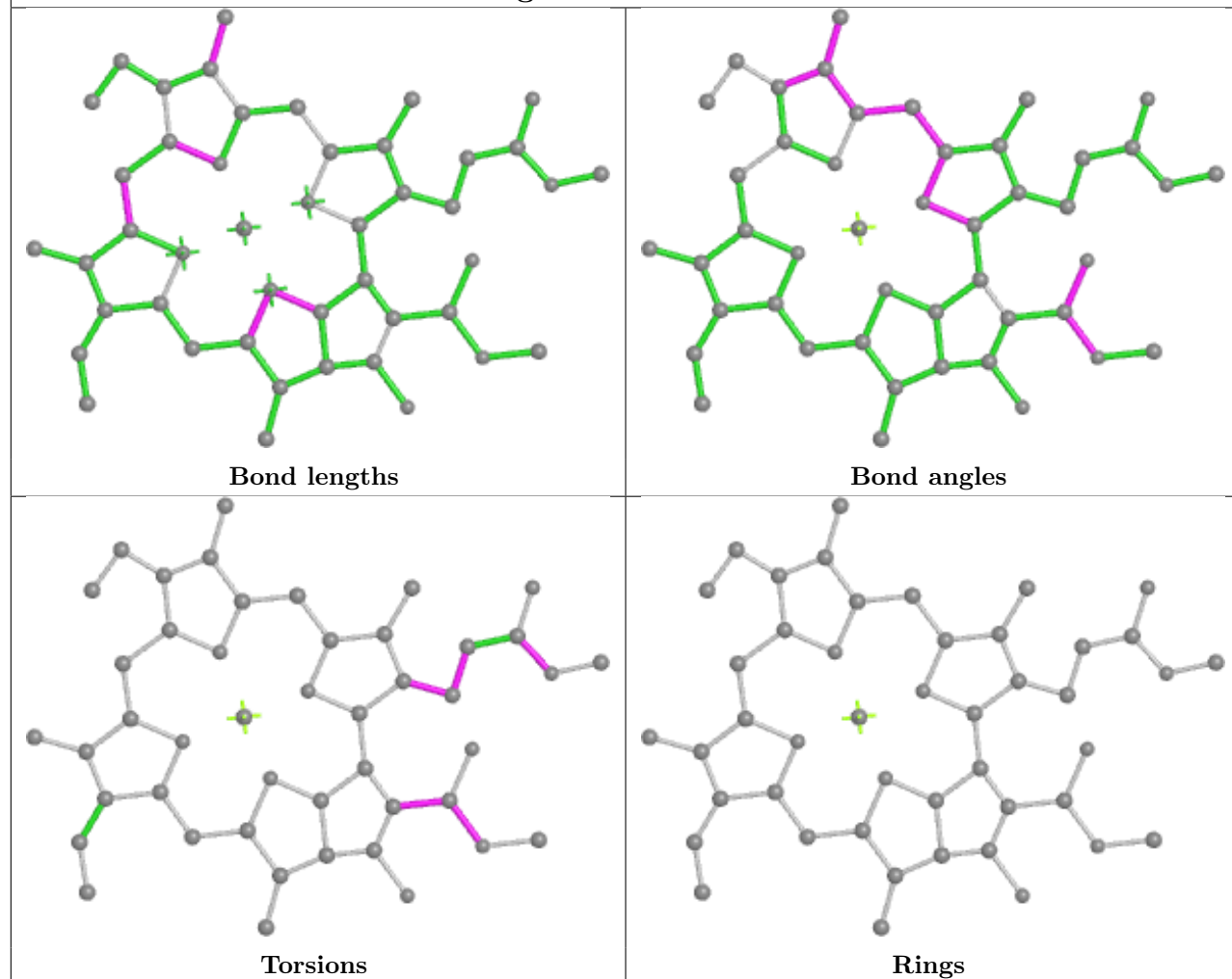


Rings

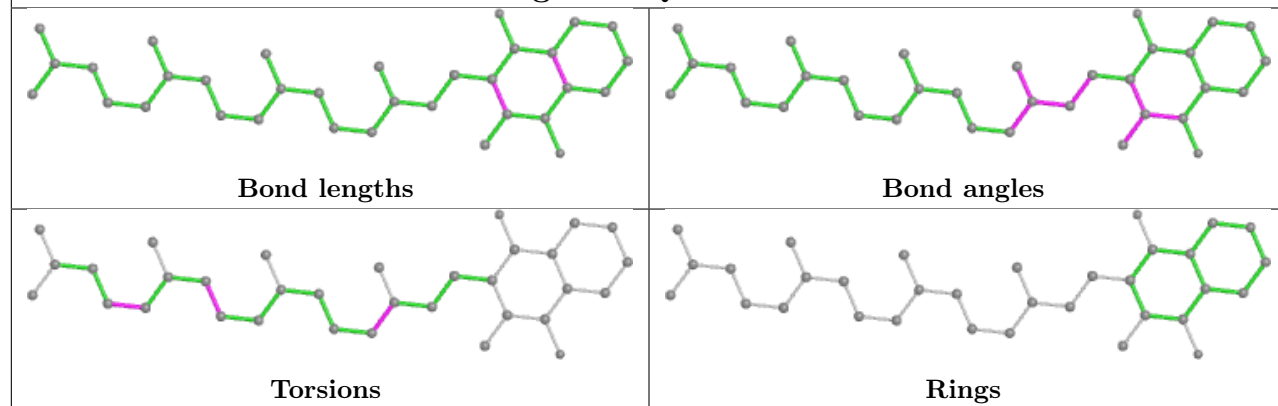


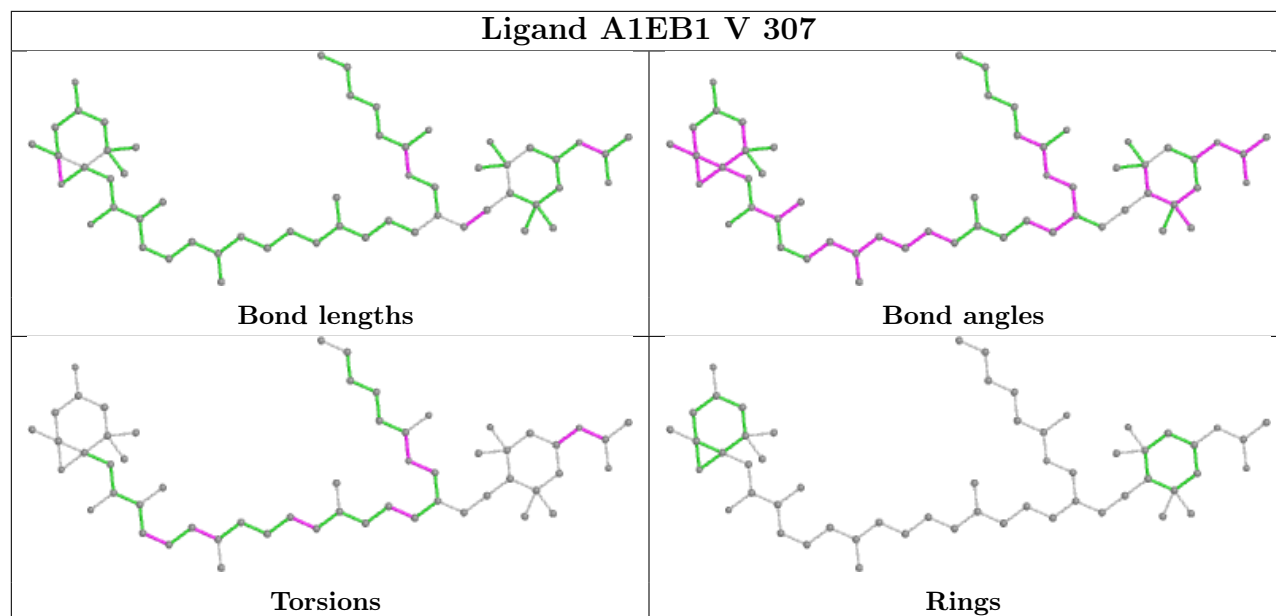
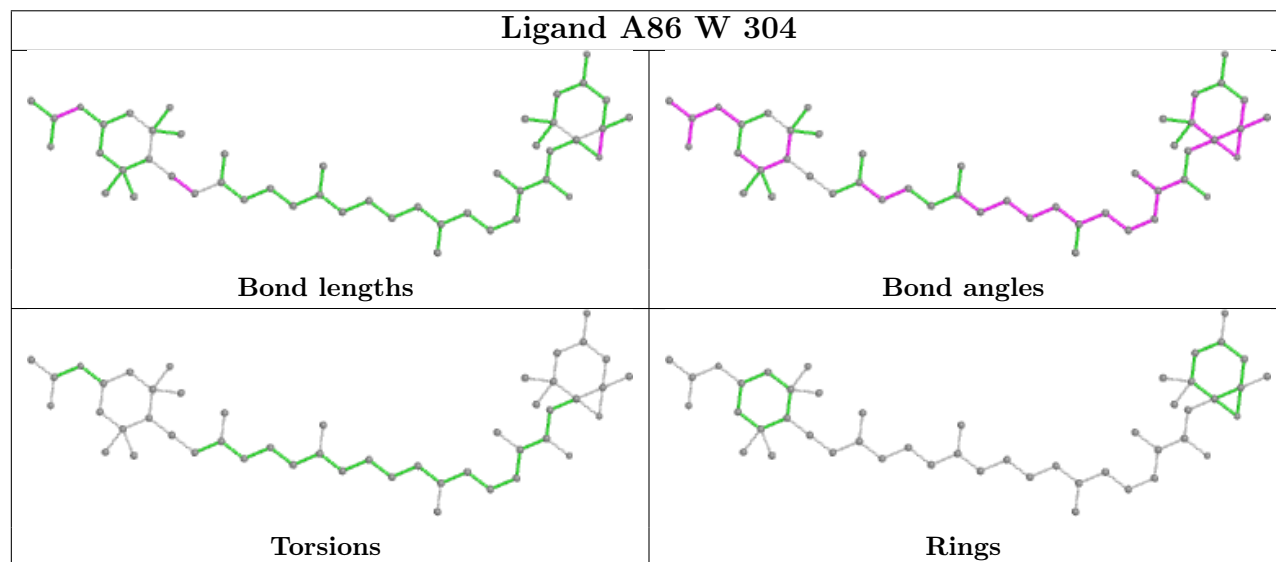


## Ligand CLA 6 322

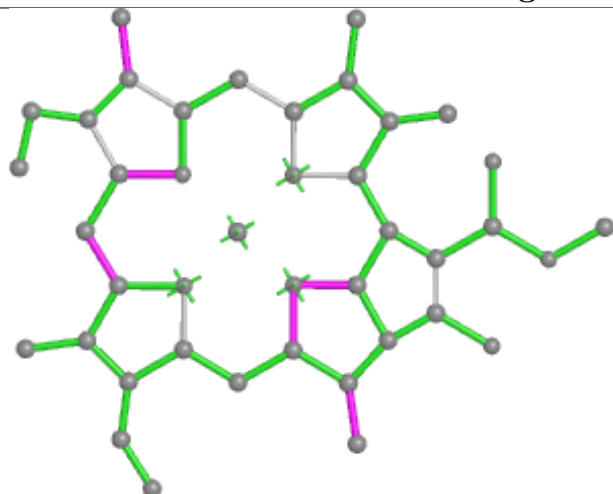


## Ligand PQN b 843

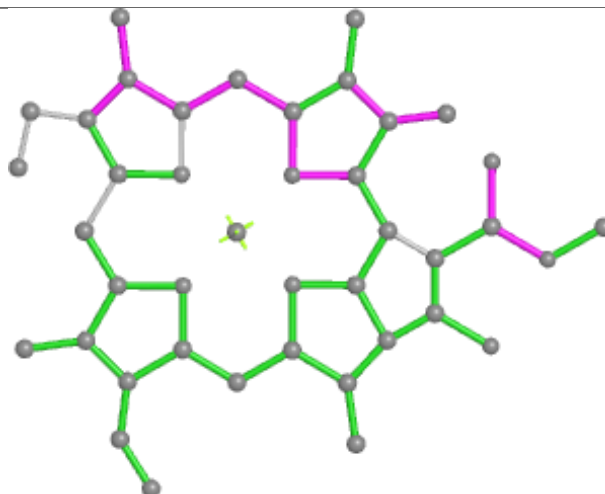


**Ligand A1EB1 V 307****Ligand A86 W 304**

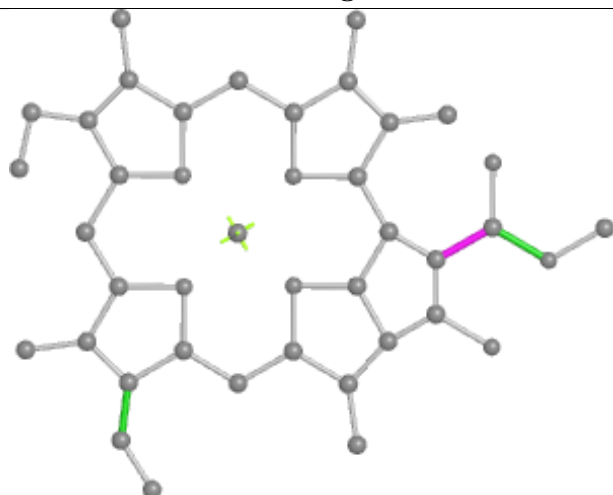
## Ligand CLA 6 315



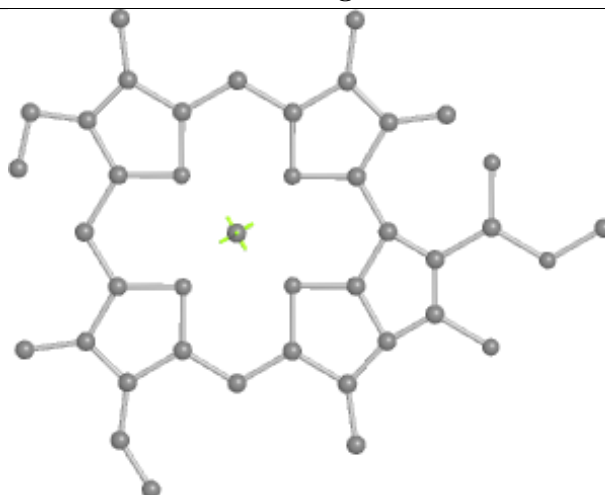
Bond lengths



Bond angles

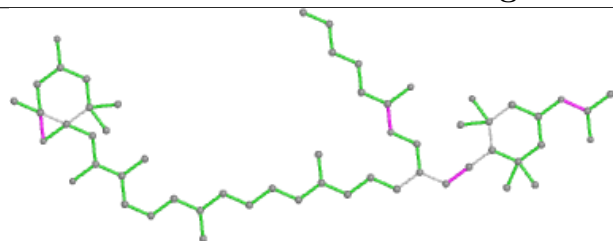


Torsions

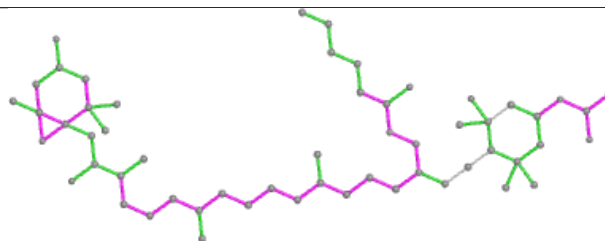


Rings

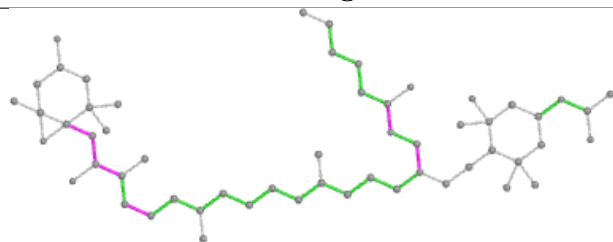
## Ligand A1EB1 3 310



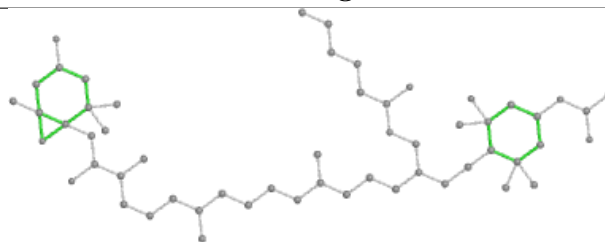
Bond lengths



Bond angles

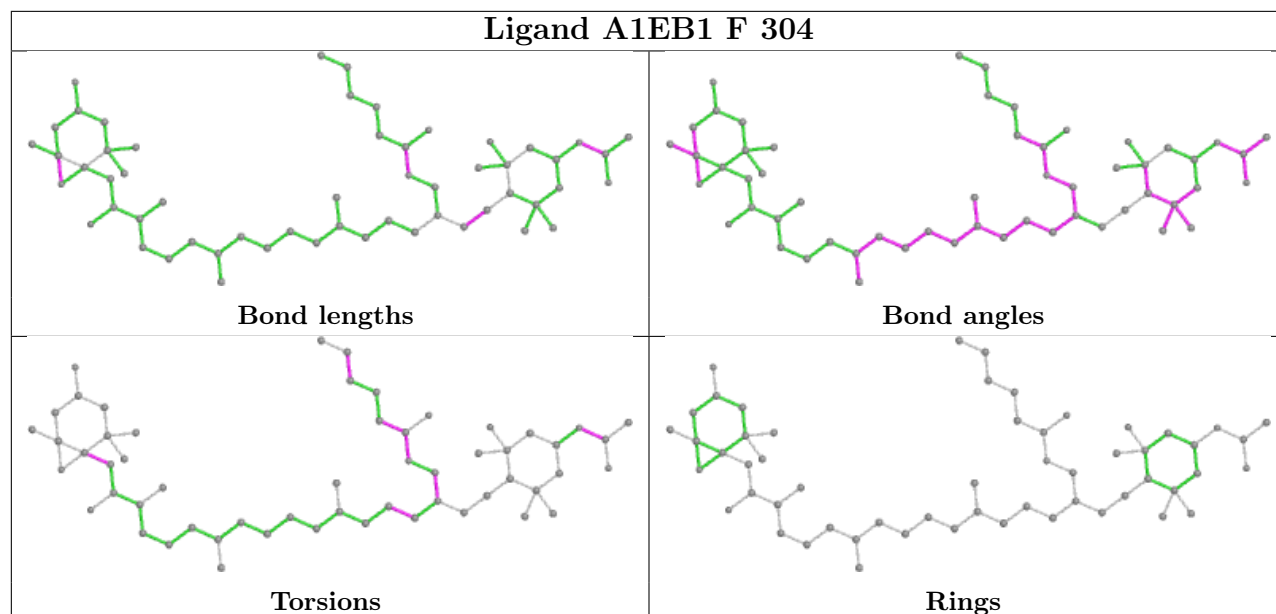


Torsions

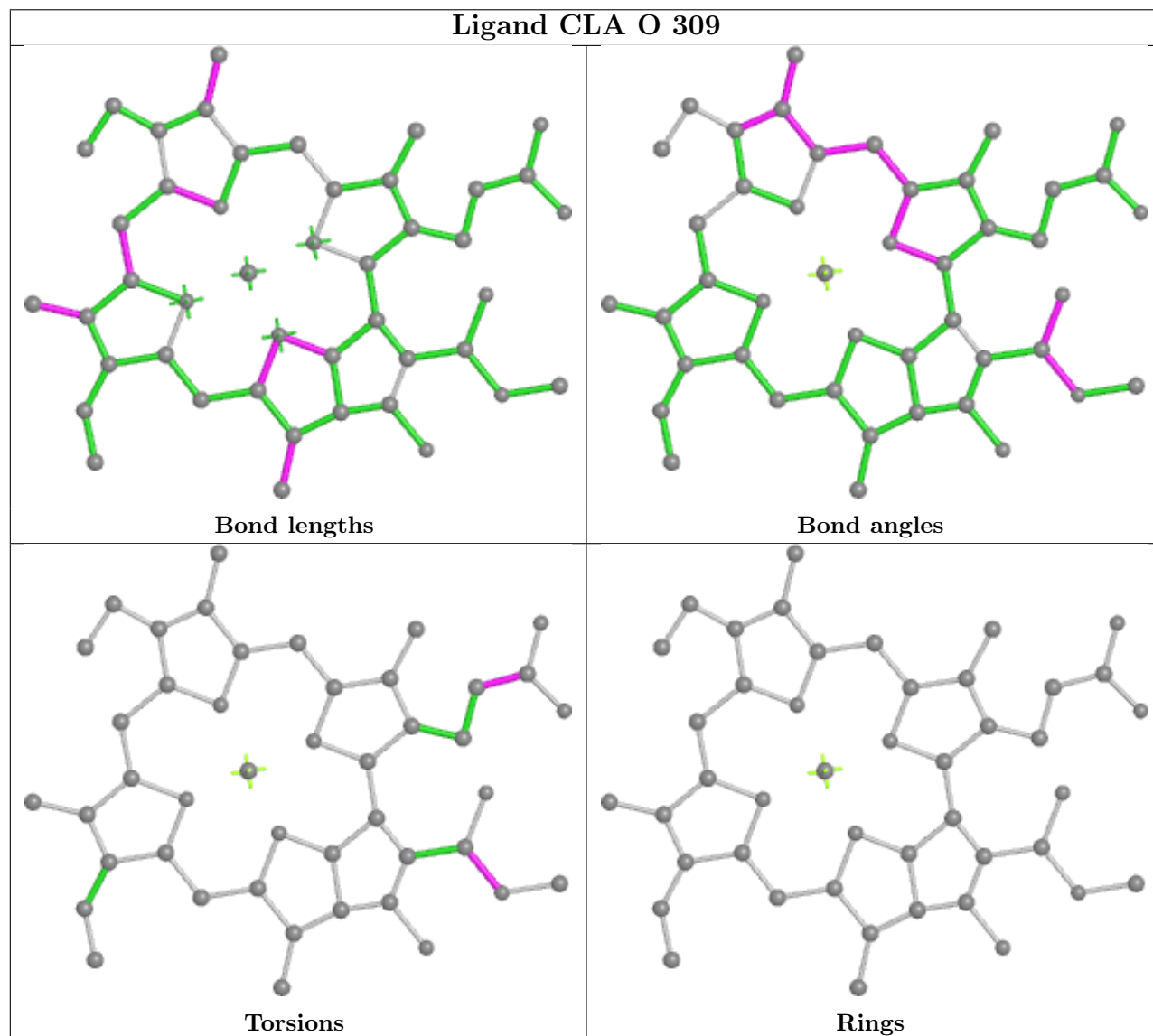


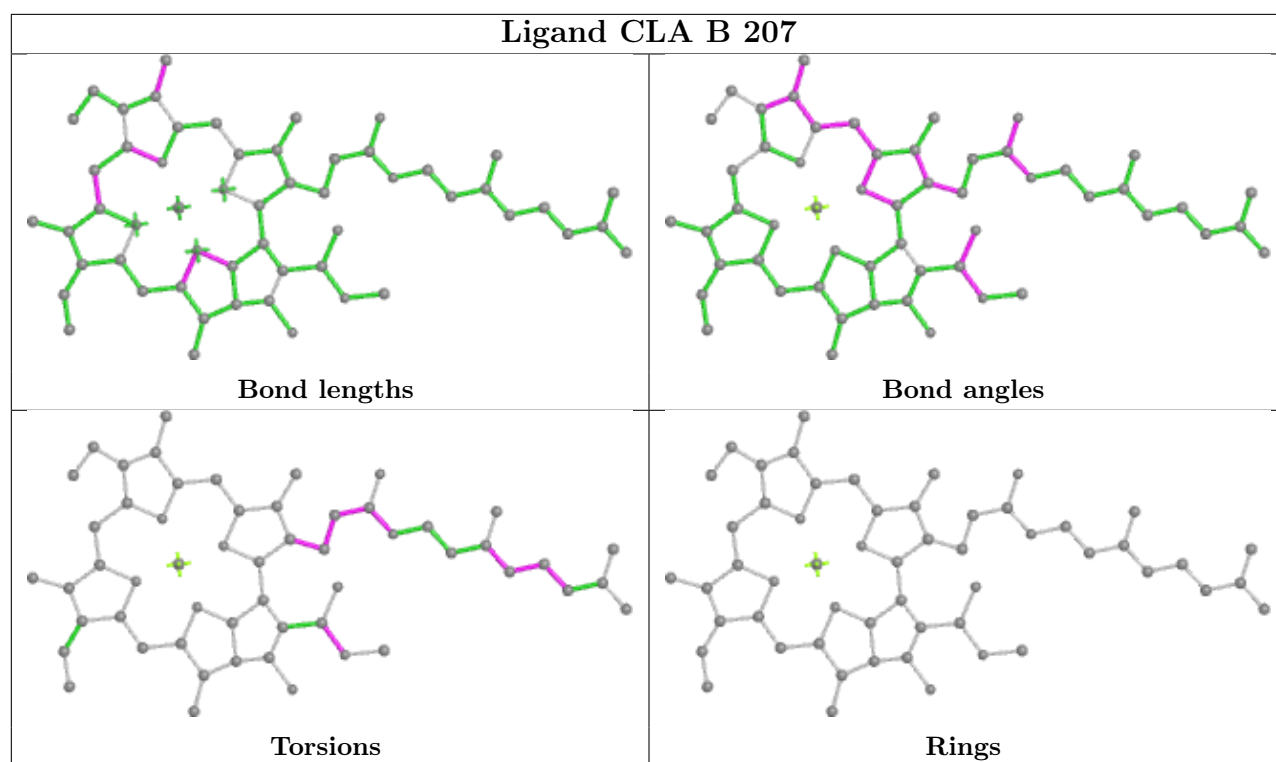
Rings

## Ligand A1EB1 F 304

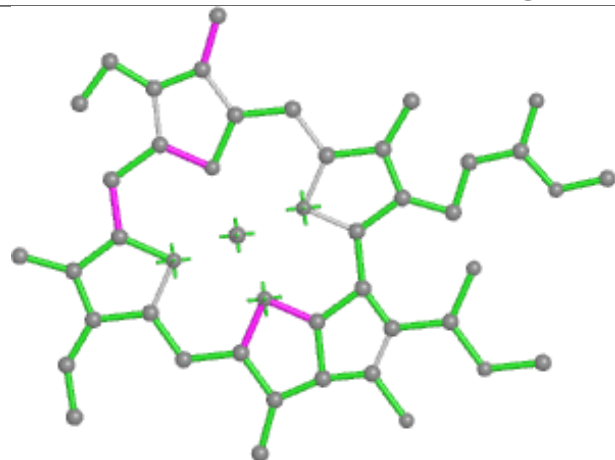


## Ligand CLA O 309

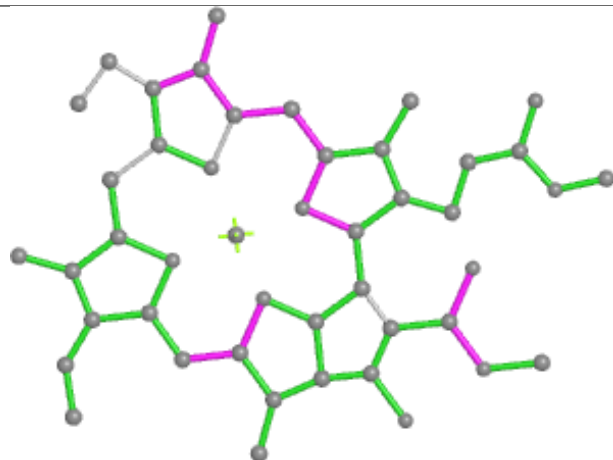




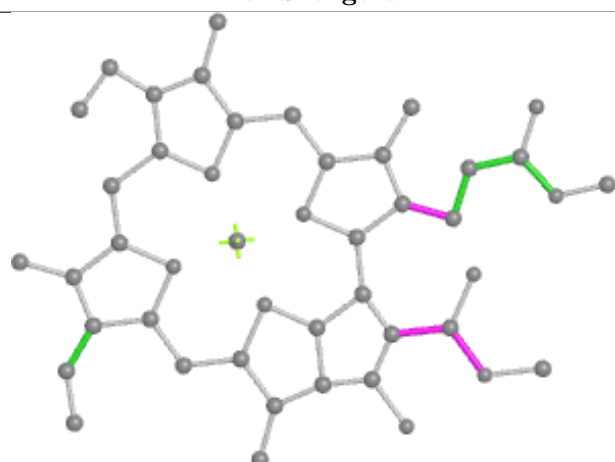
## Ligand CLA b 823



Bond lengths



Bond angles

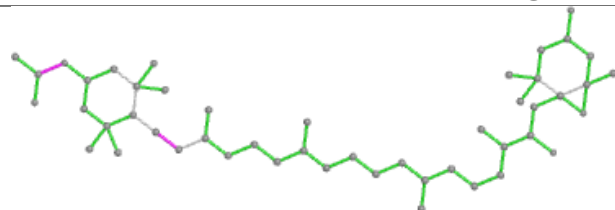


Torsions

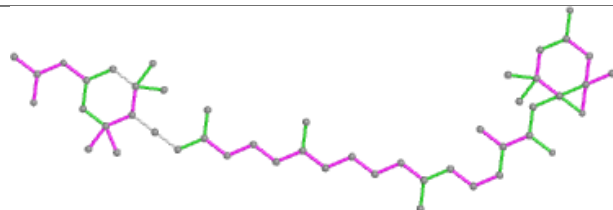


Rings

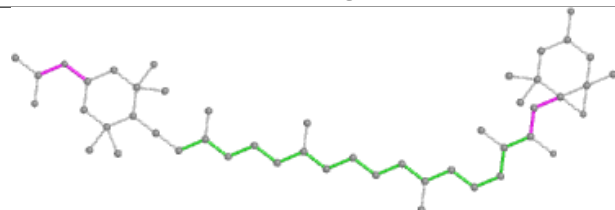
## Ligand A86 S 307



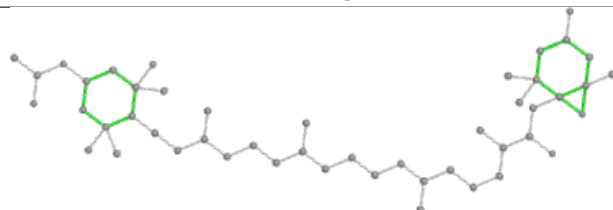
Bond lengths



Bond angles

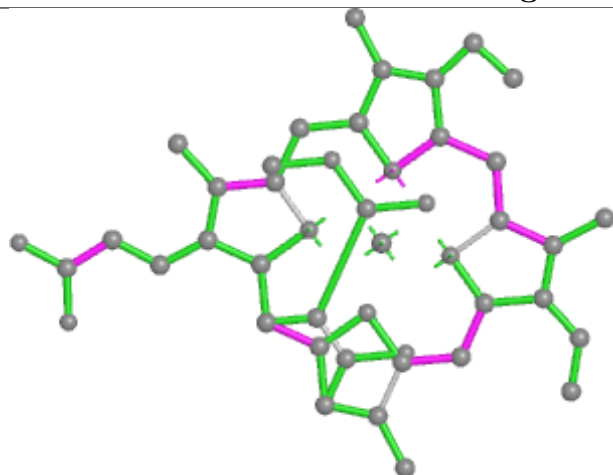


Torsions

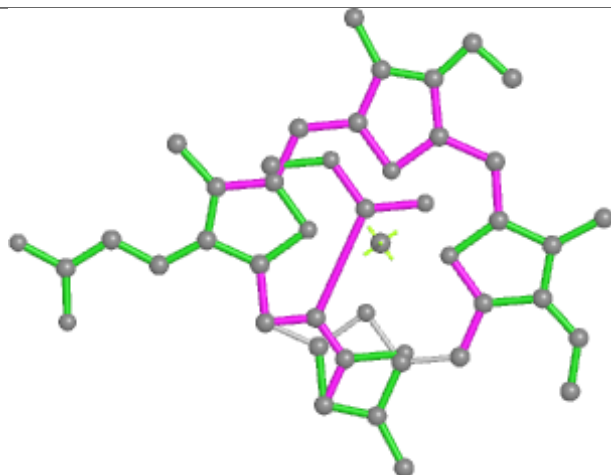


Rings

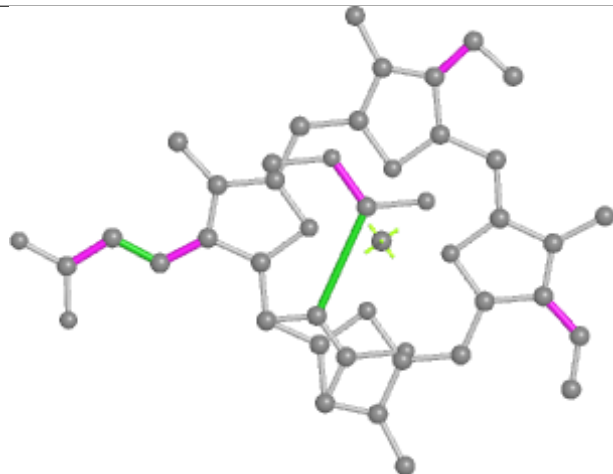
## Ligand KC2 9 316



Bond lengths



Bond angles



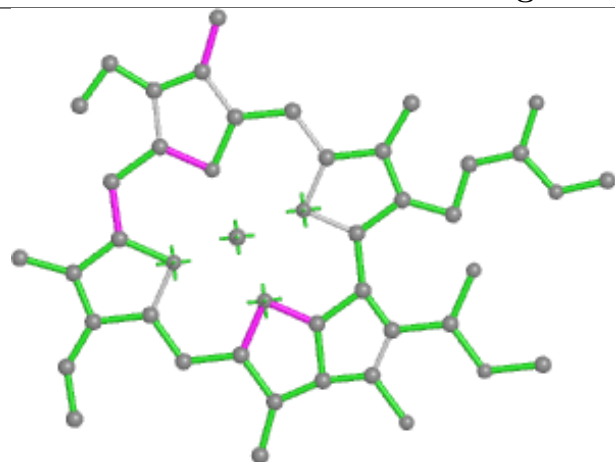
Torsions



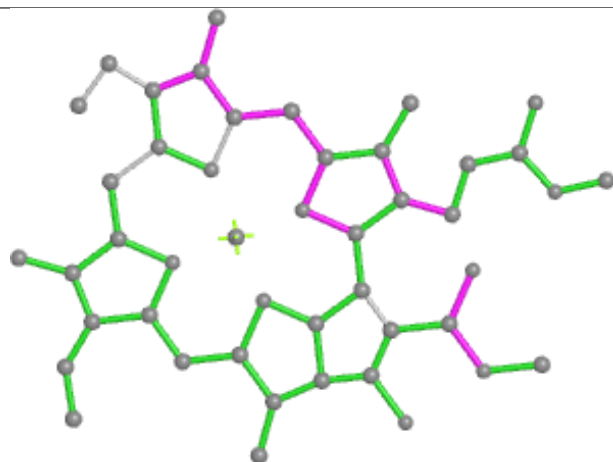
Rings



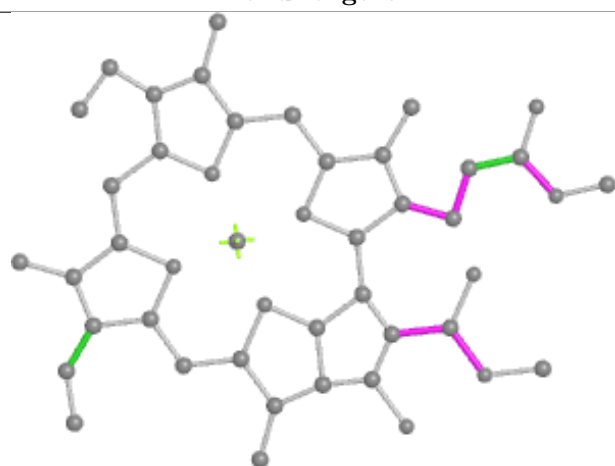
## Ligand CLA T 319



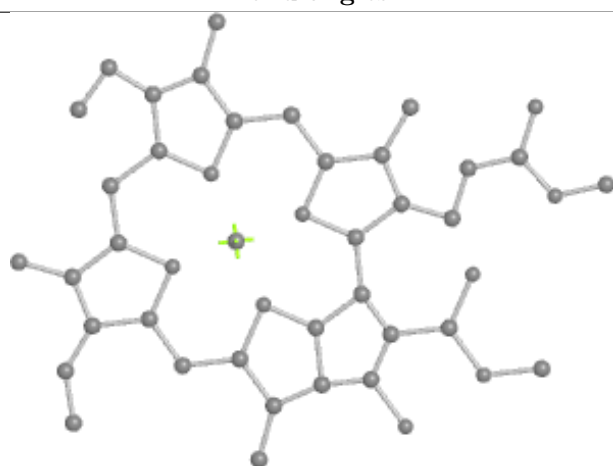
Bond lengths



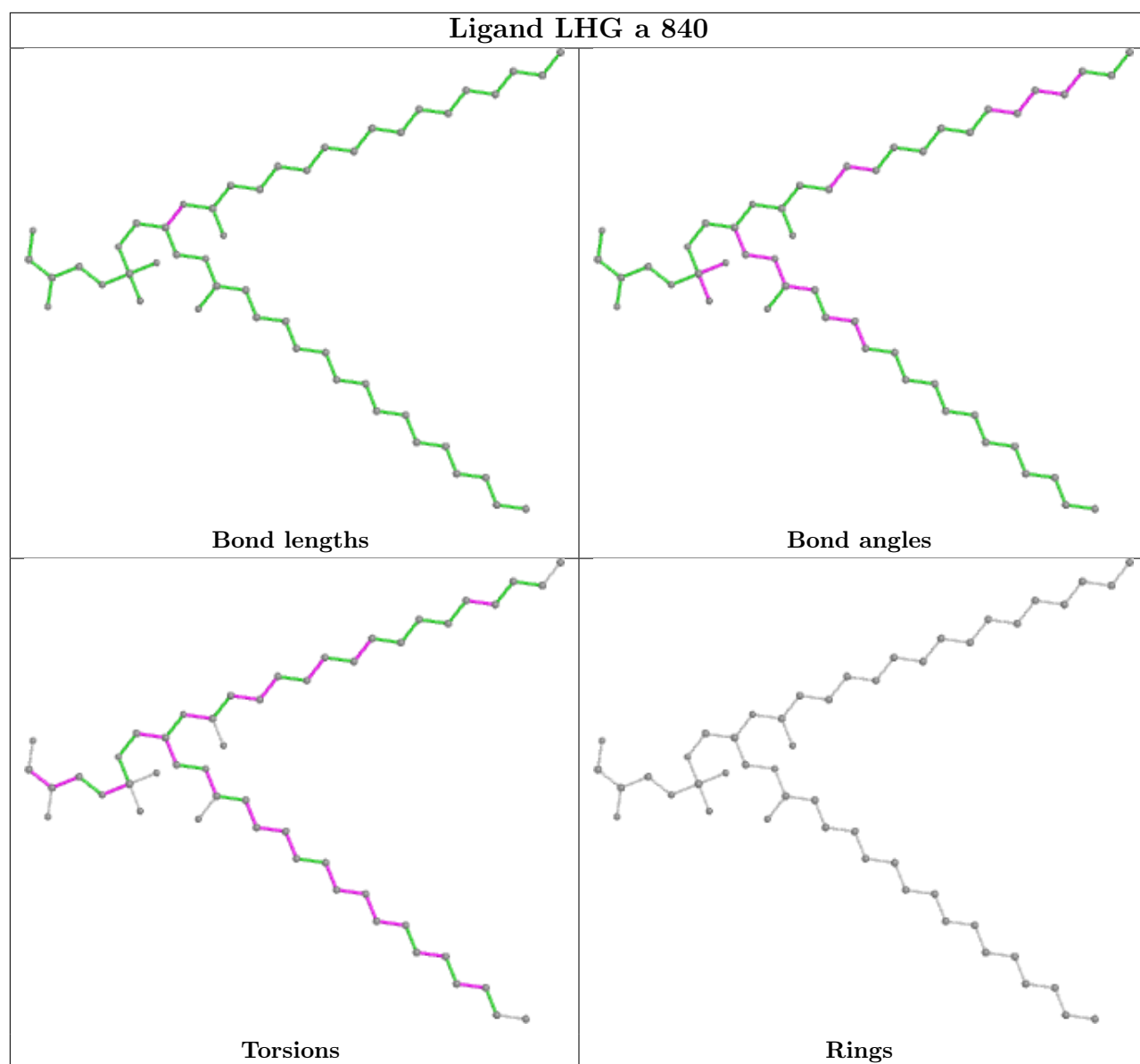
Bond angles

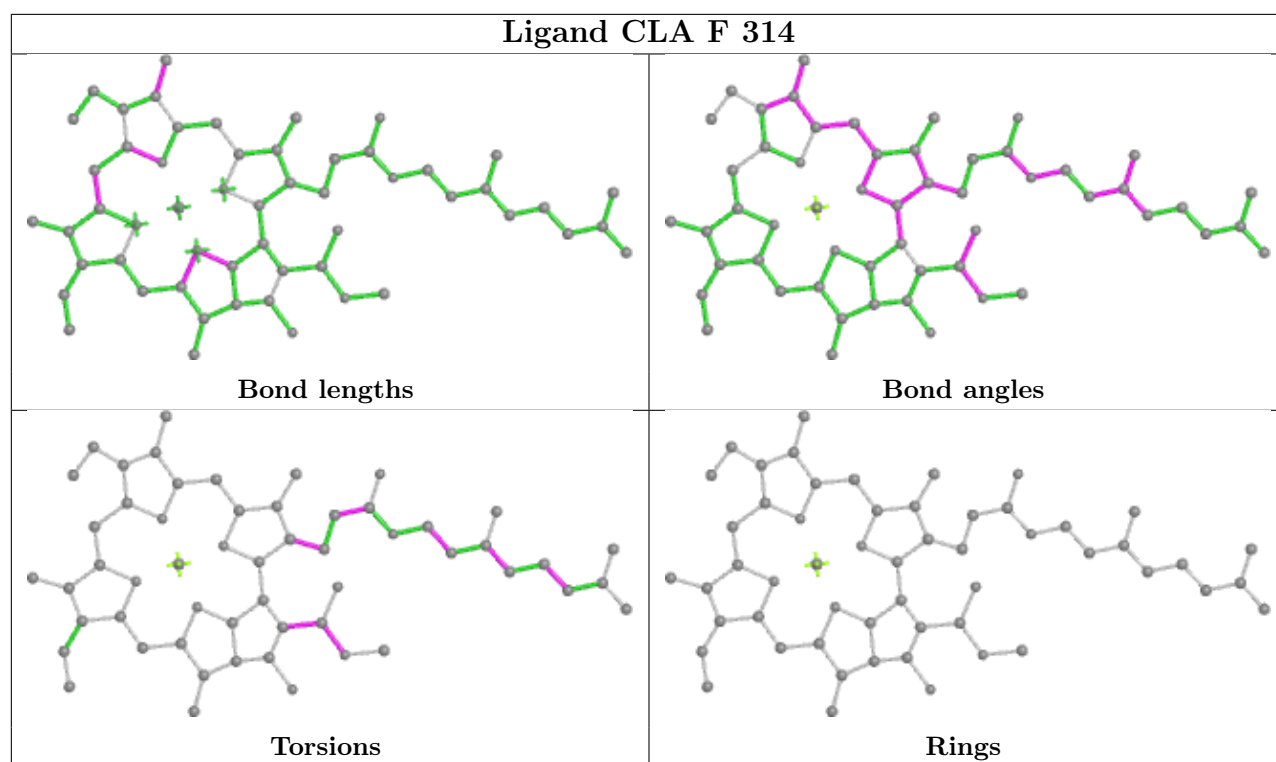
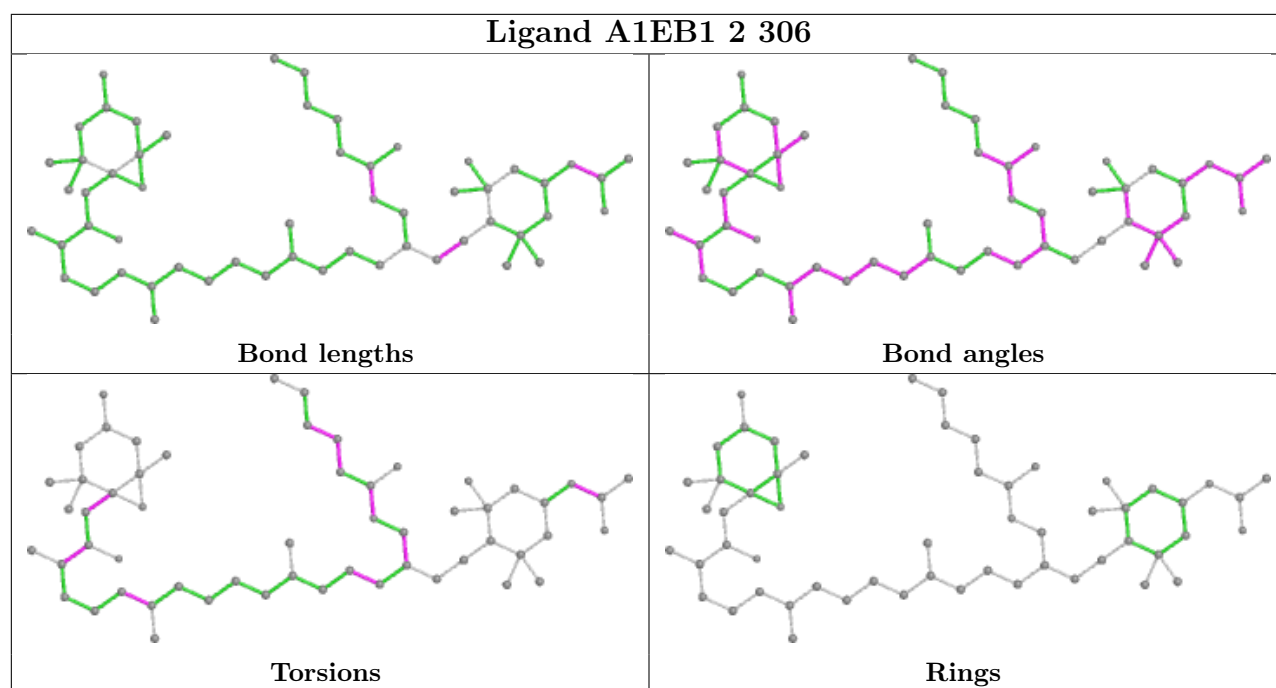


Torsions

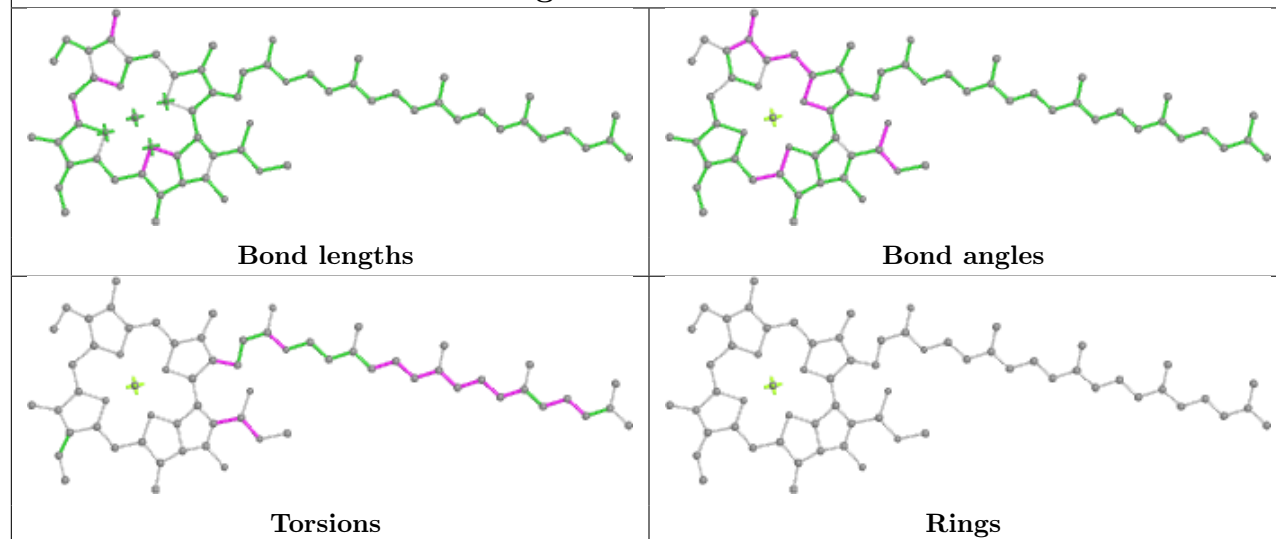


Rings

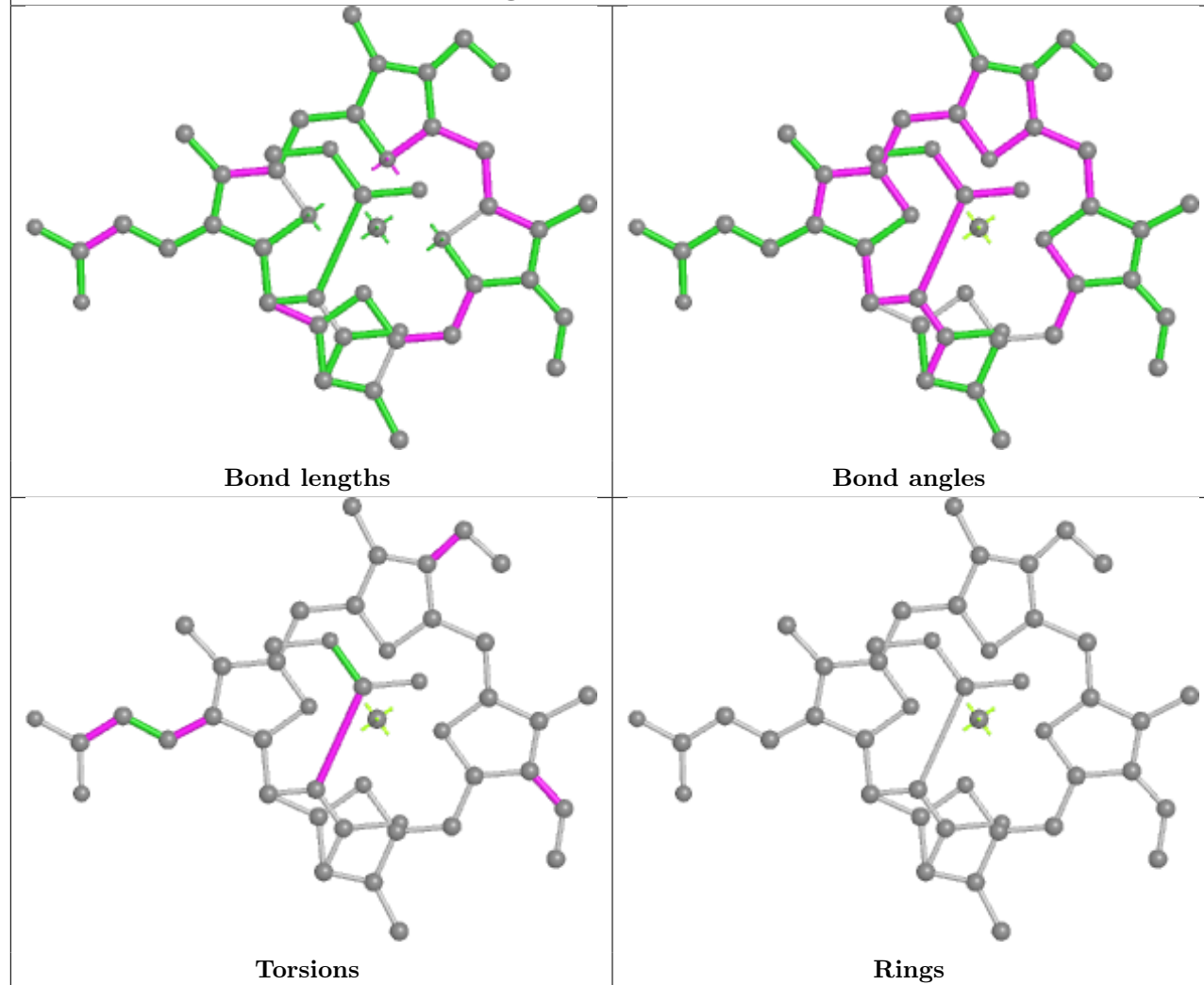




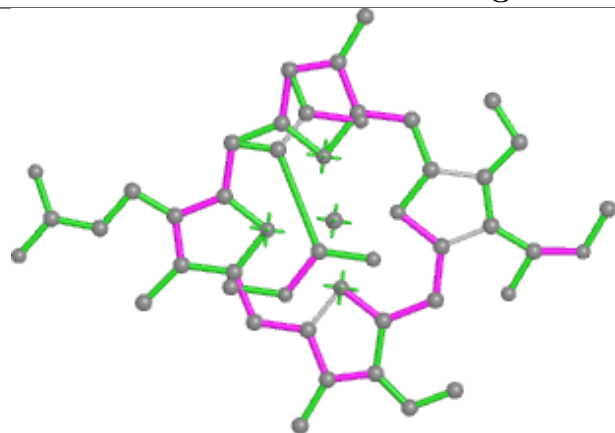
## Ligand CLA J 314



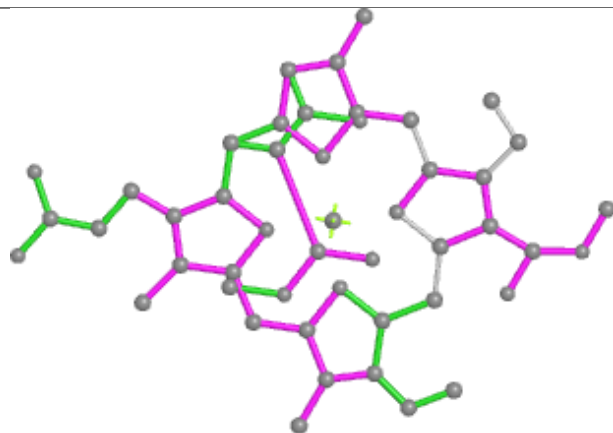
## Ligand KC2 K 313



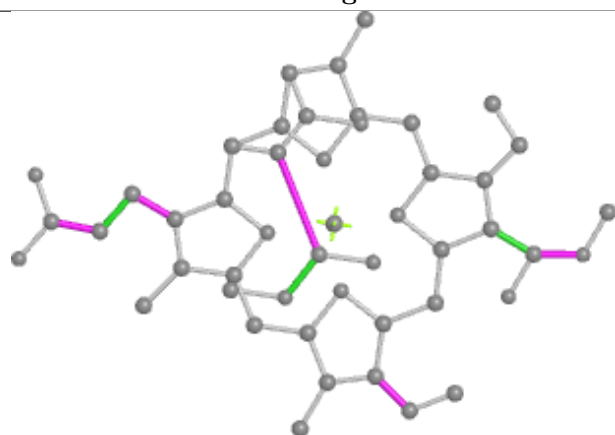
## Ligand A1ECV Y 306



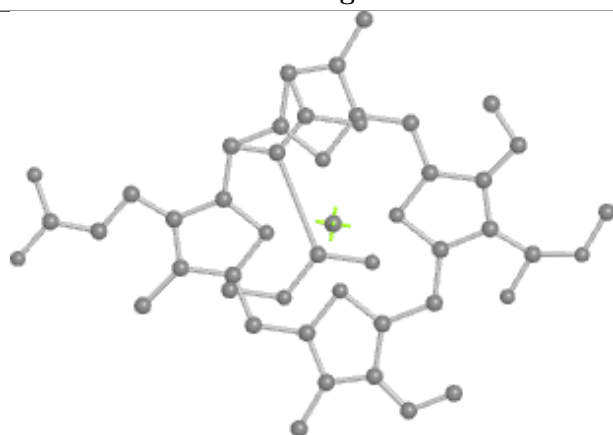
Bond lengths



Bond angles

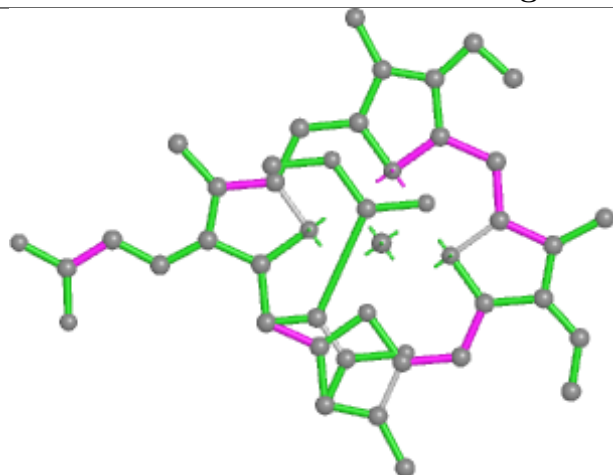


Torsions

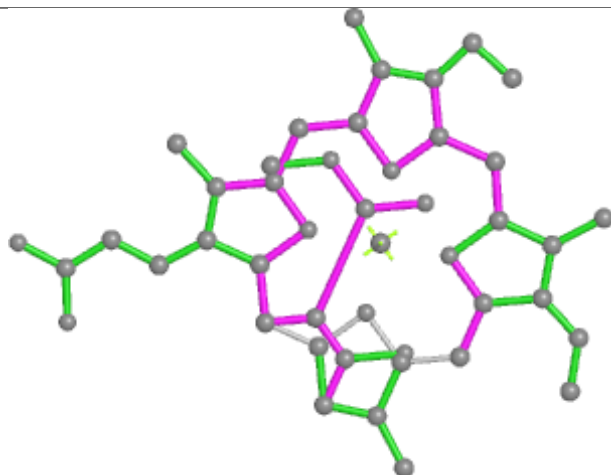


Rings

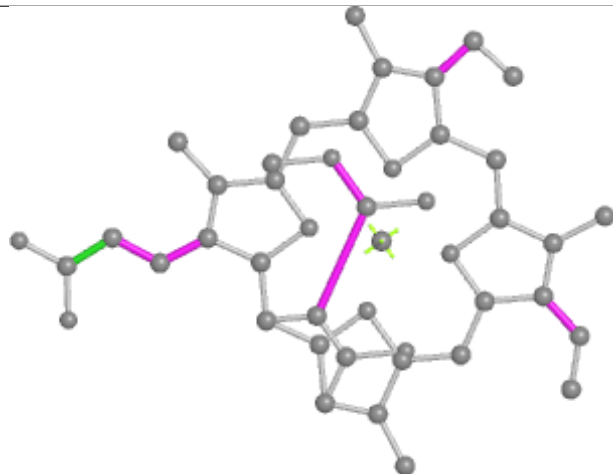
## Ligand KC2 2 314



Bond lengths



Bond angles

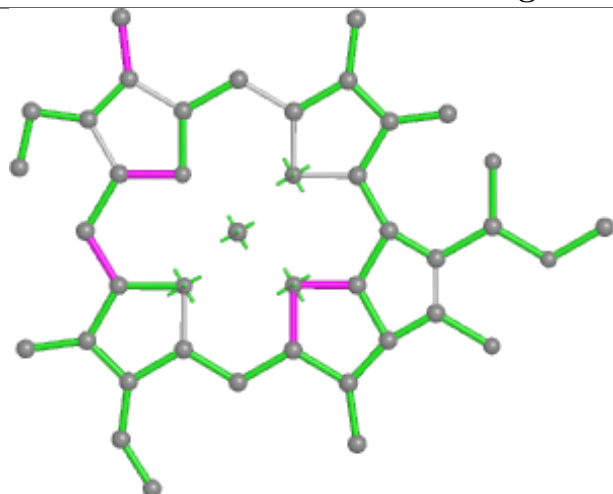


Torsions

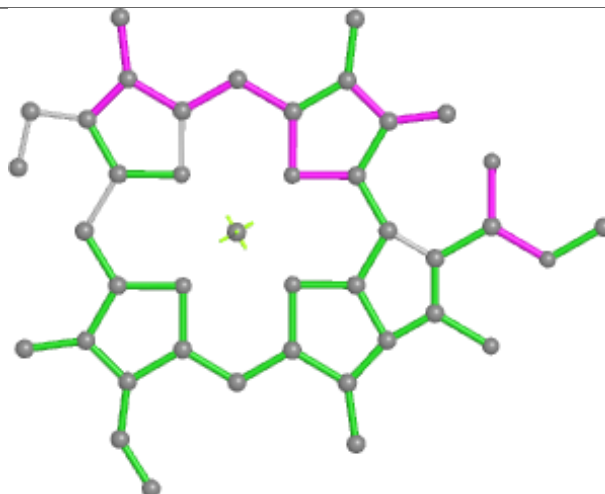


Rings

## Ligand CLA 6 321



Bond lengths



Bond angles

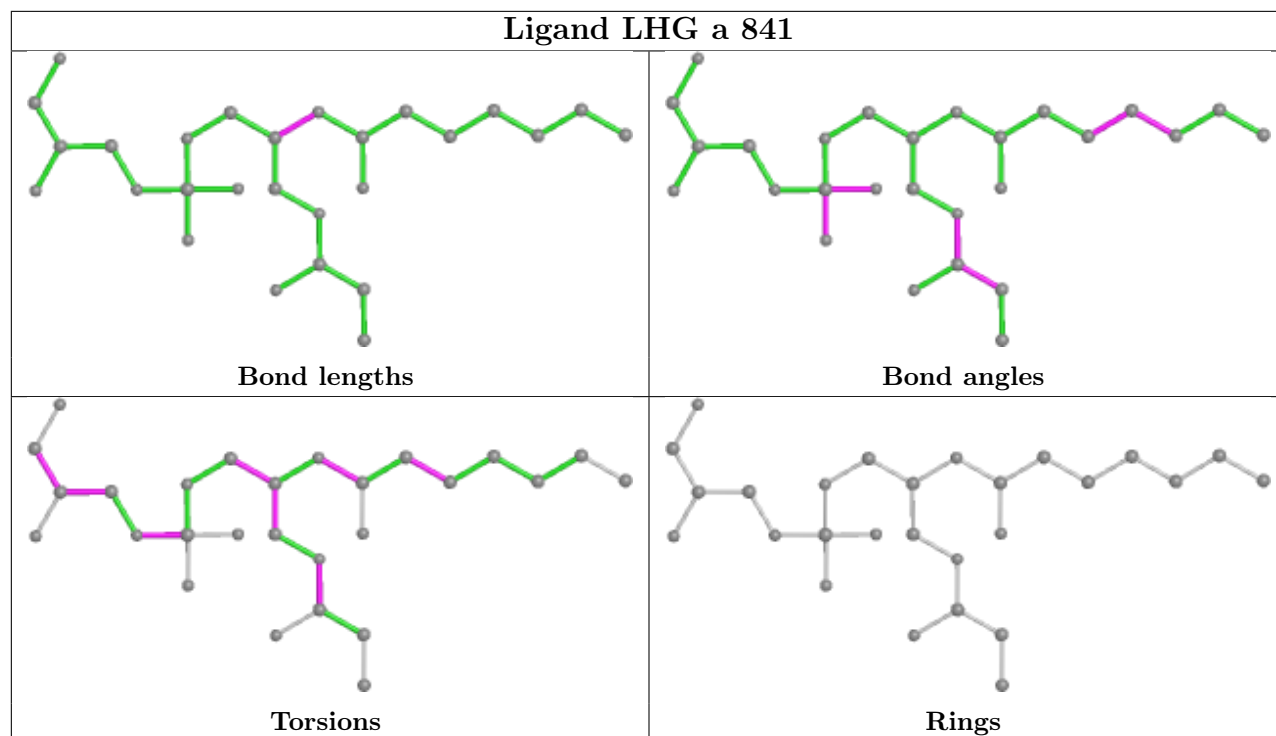


Torsions

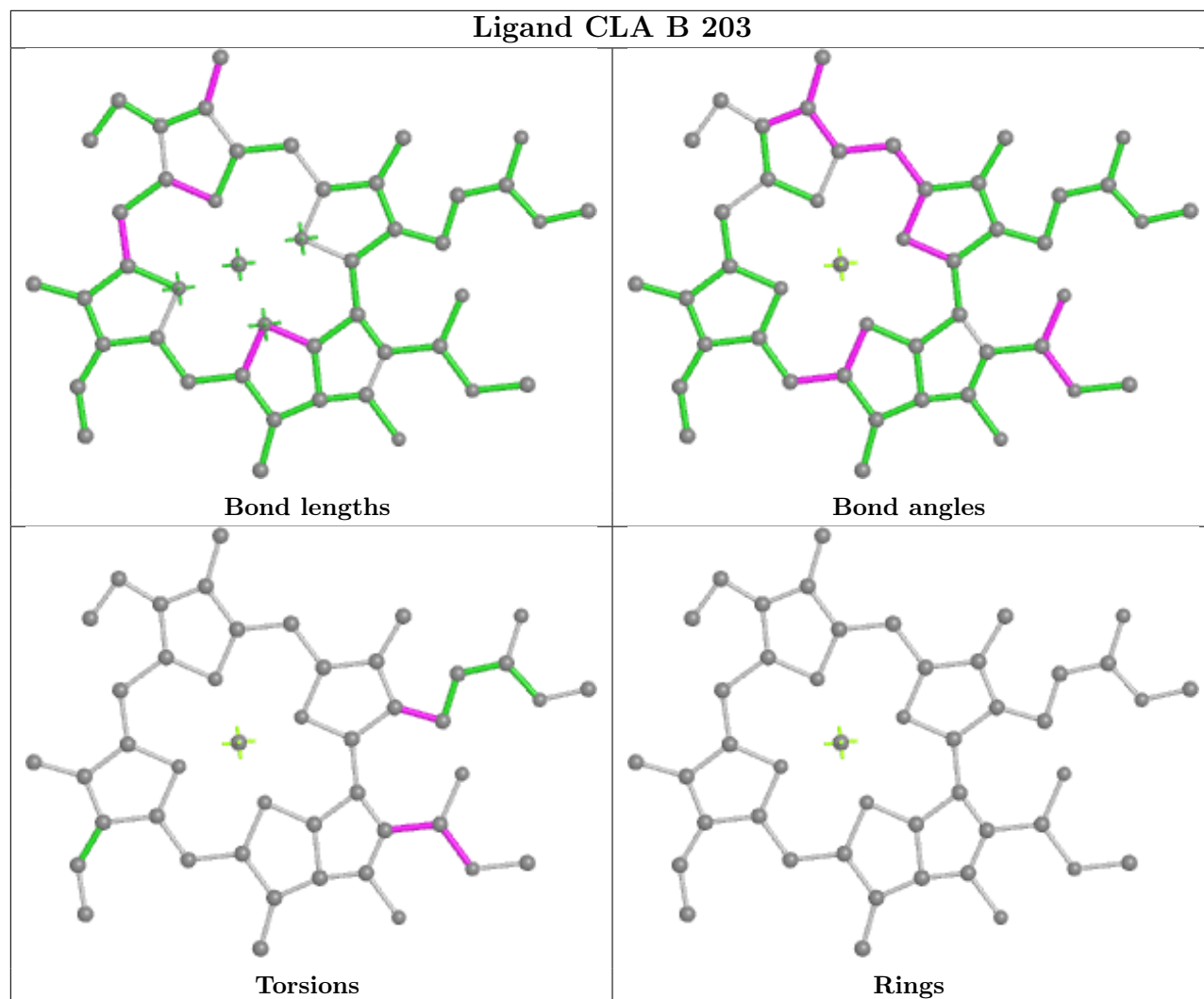


Rings

## Ligand LHG a 841

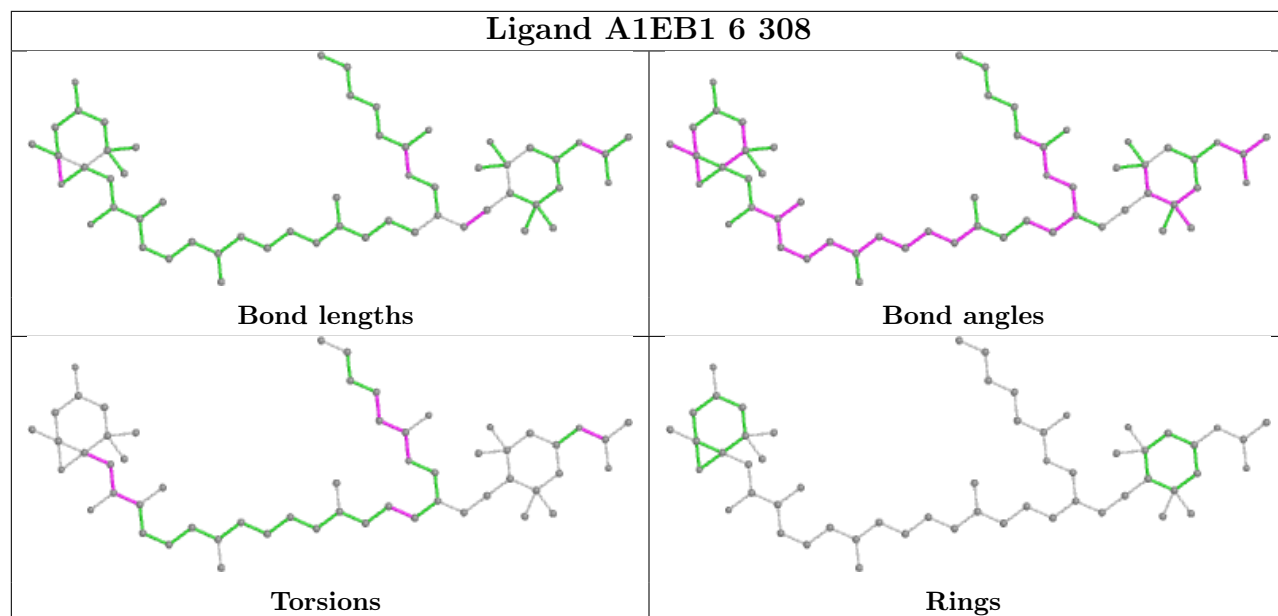


## Ligand CLA B 203

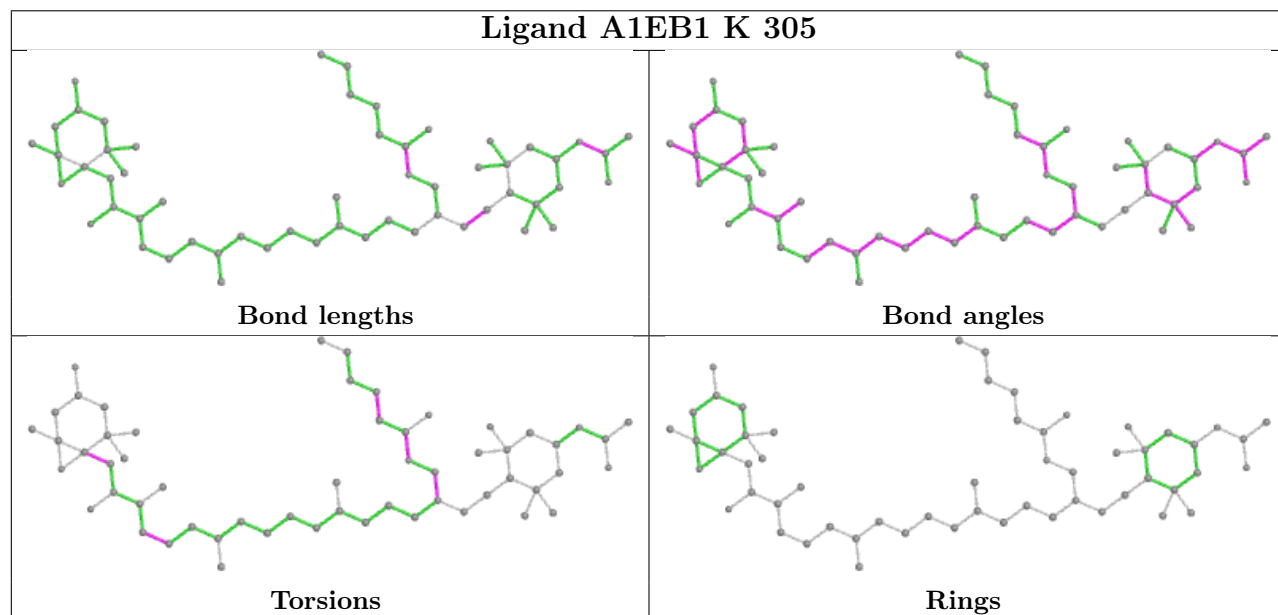




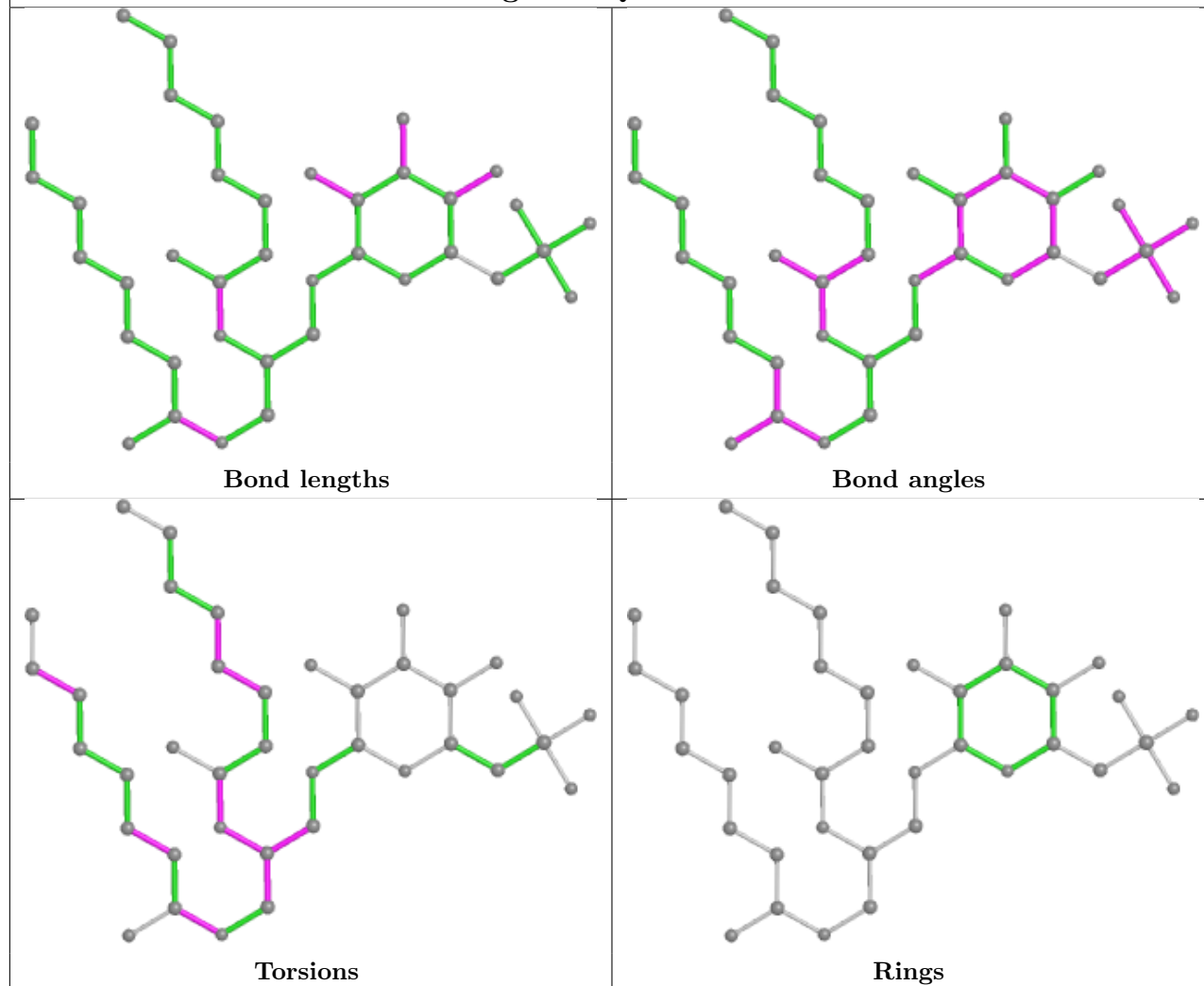
## Ligand A1EB1 6 308



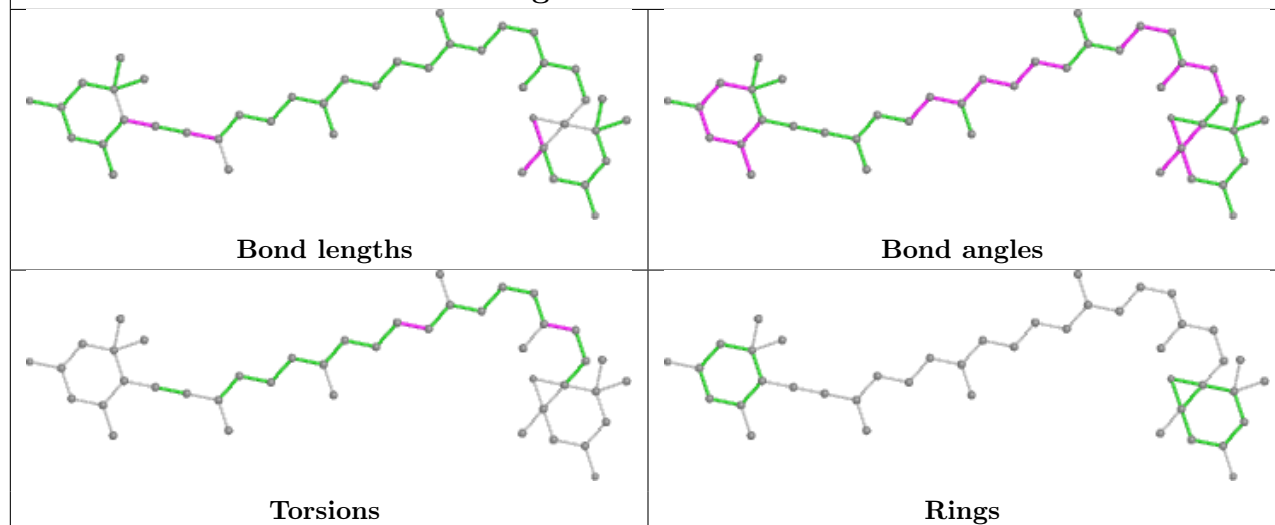
## Ligand A1EB1 K 305



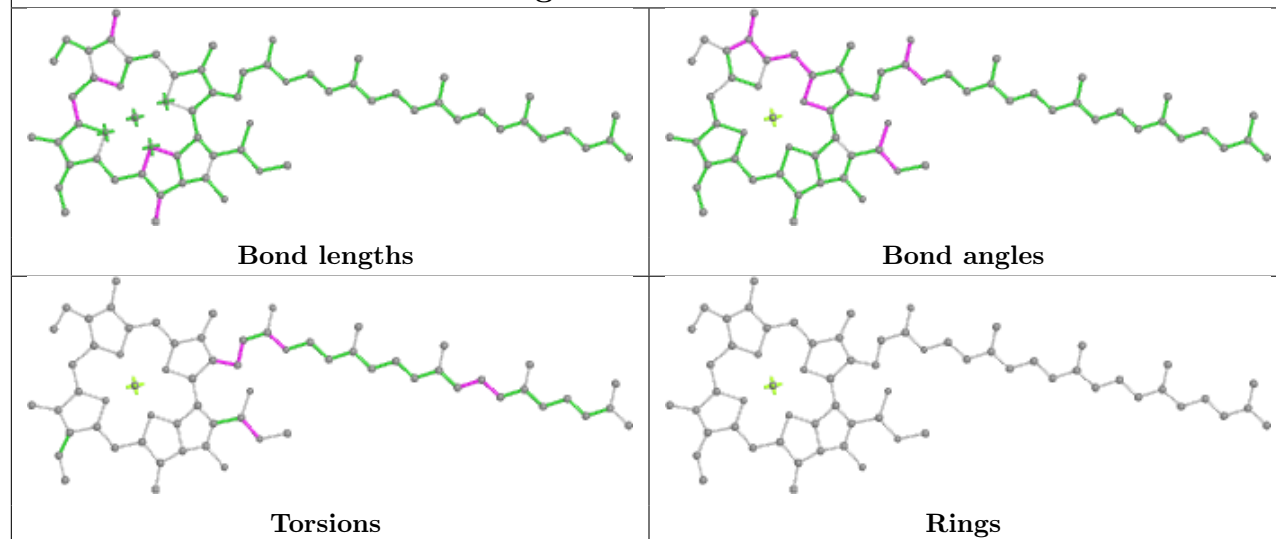
## Ligand SQD P 301



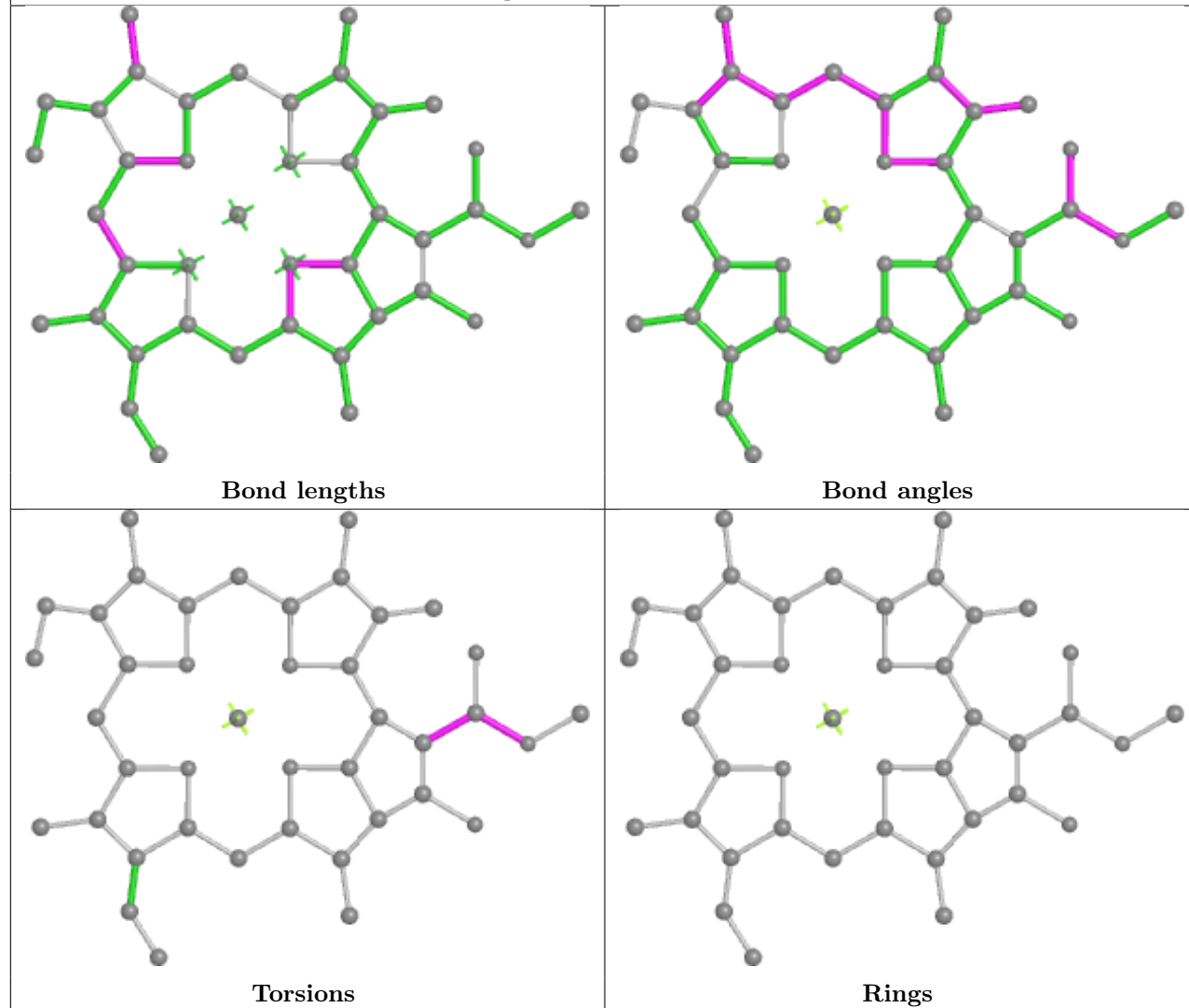
## Ligand DD6 C 301

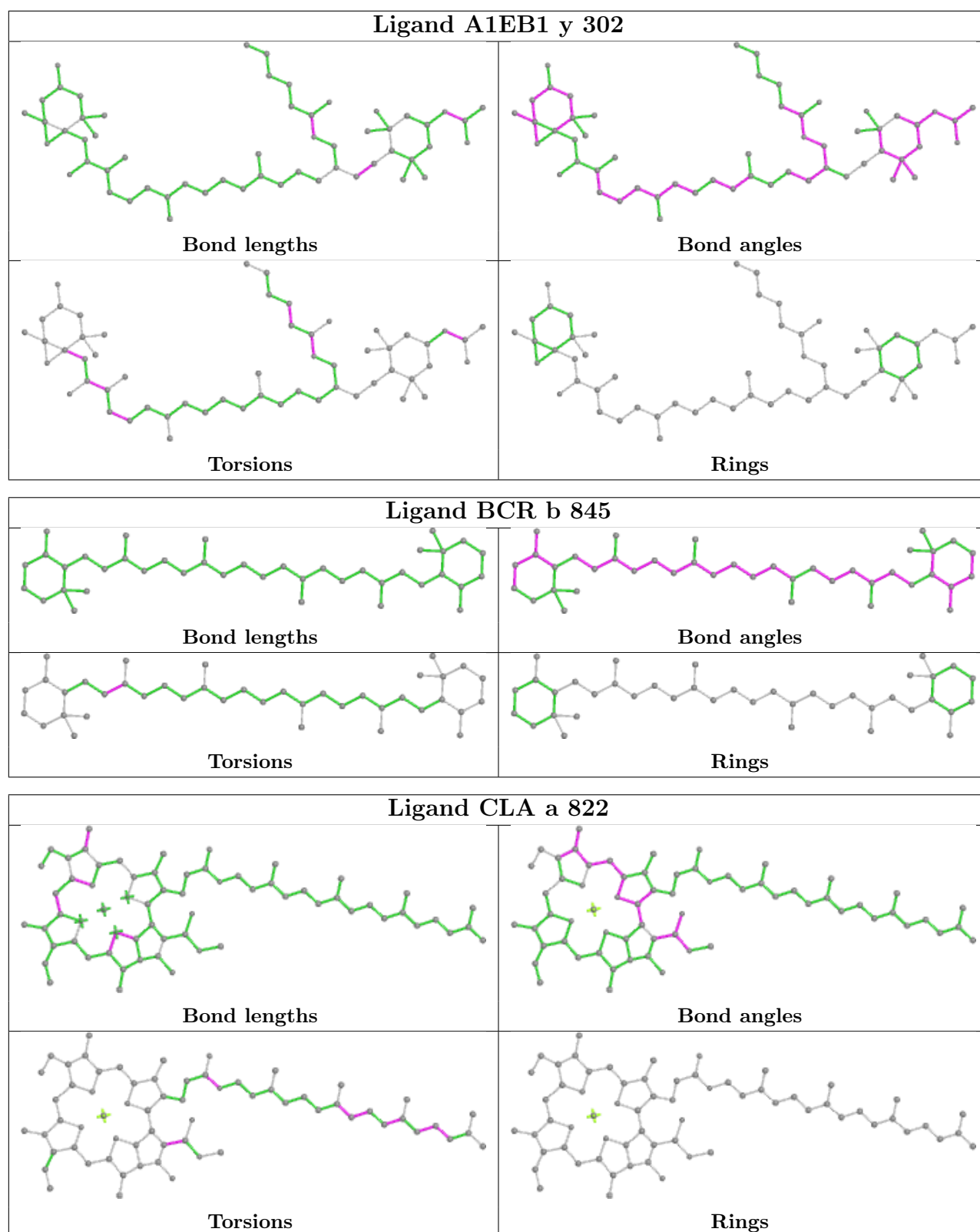


## Ligand CLA b 829

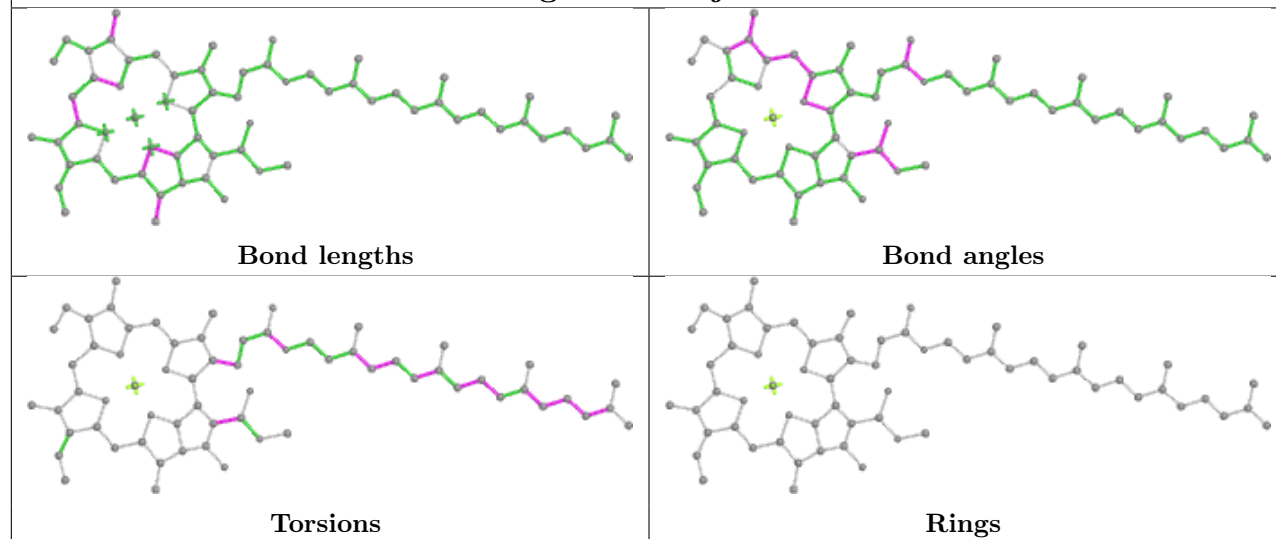


## Ligand CLA x 314

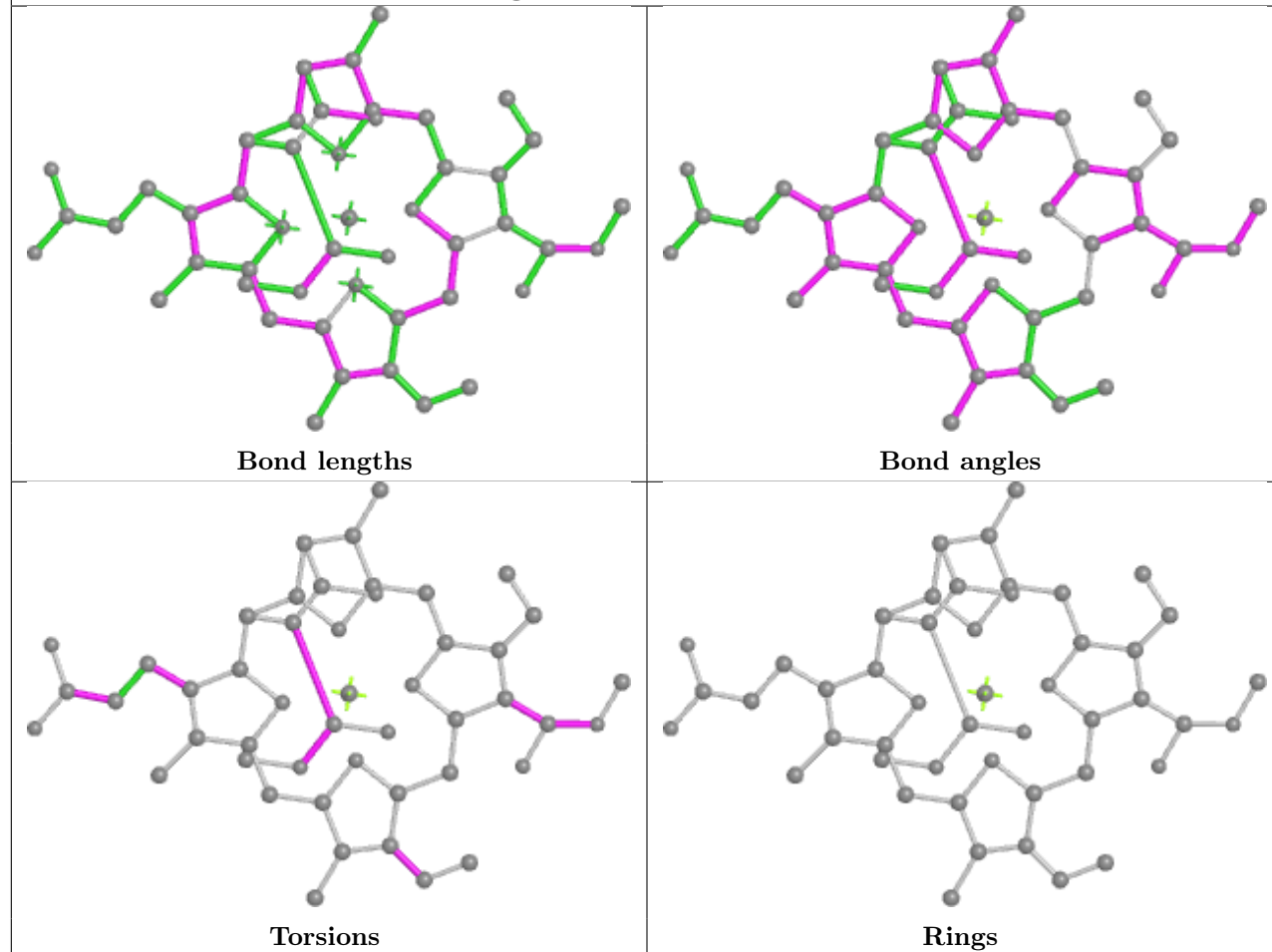




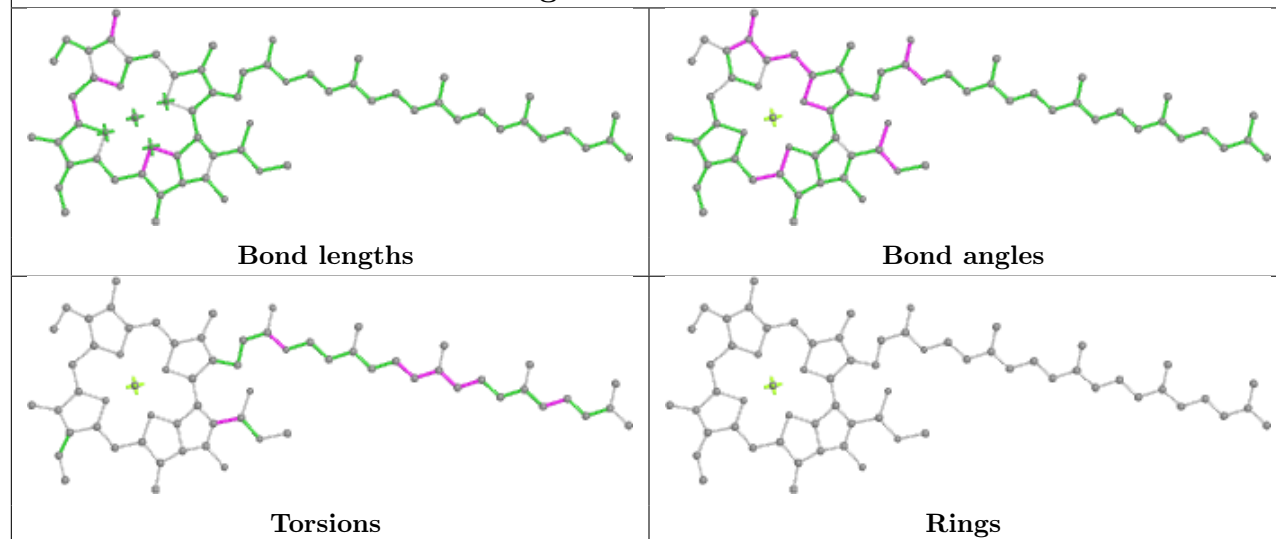
## Ligand CLA j 101



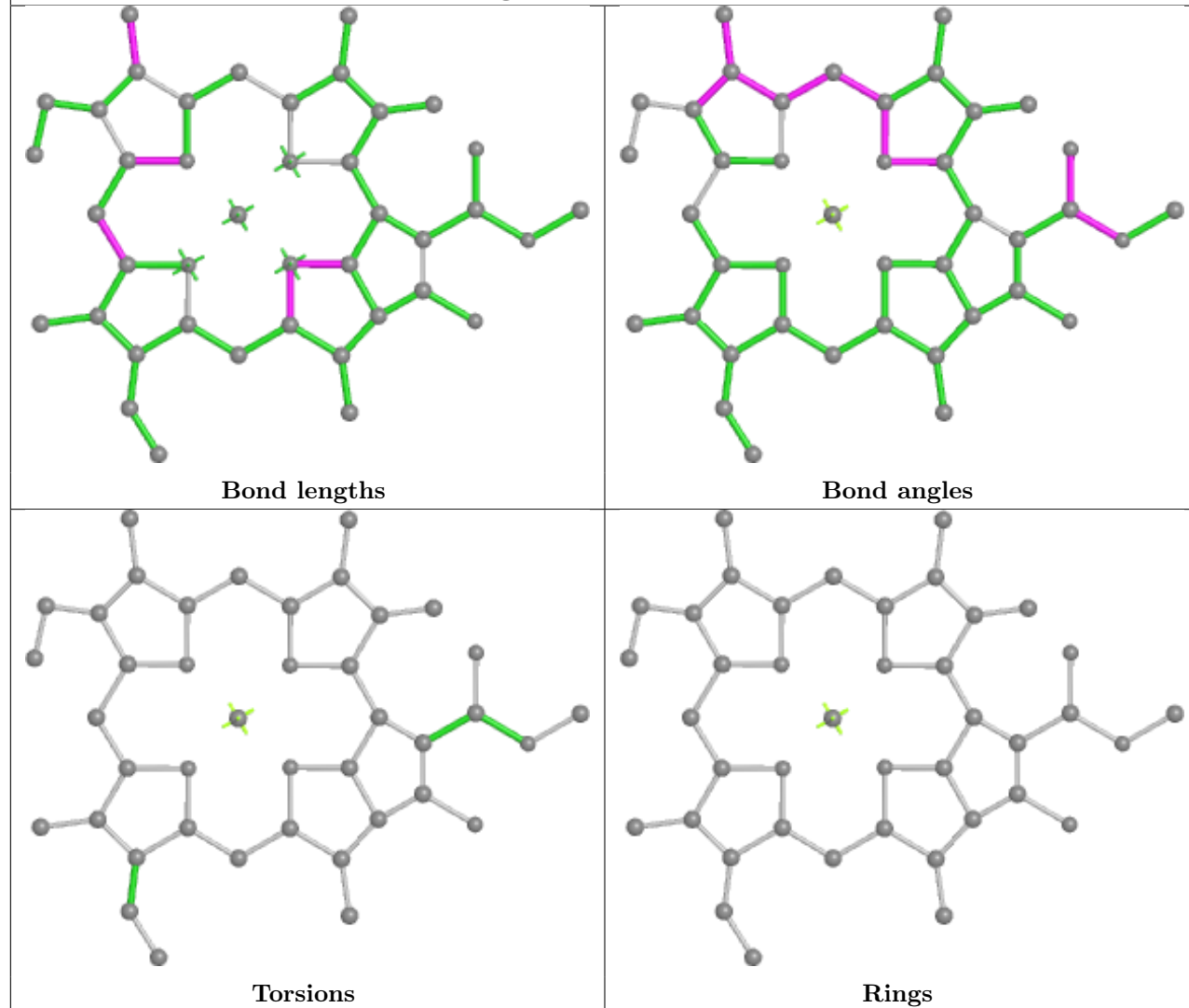
## Ligand A1ECV P 315



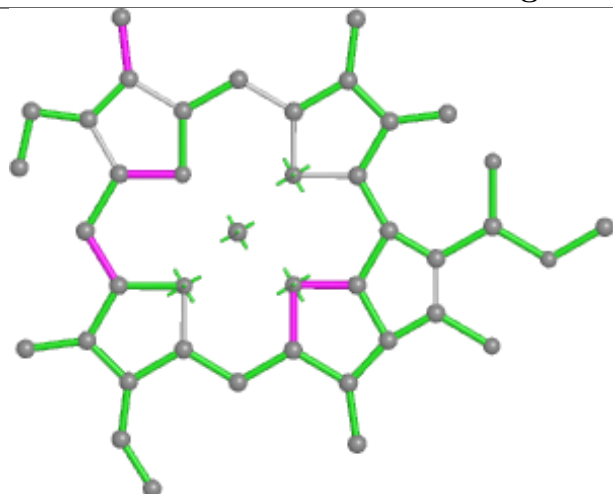
## Ligand CLA f 802



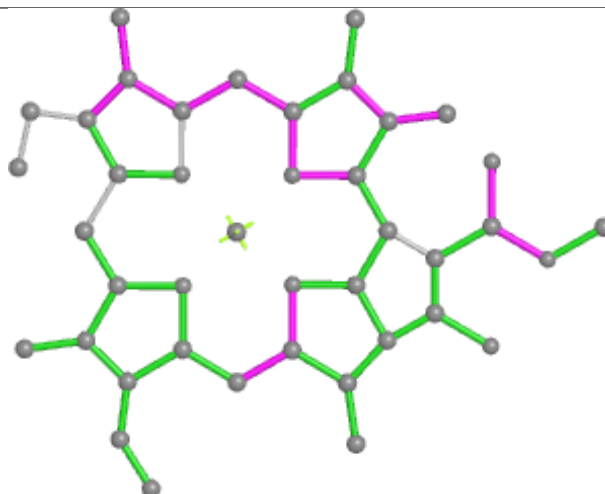
## Ligand CLA Z 309



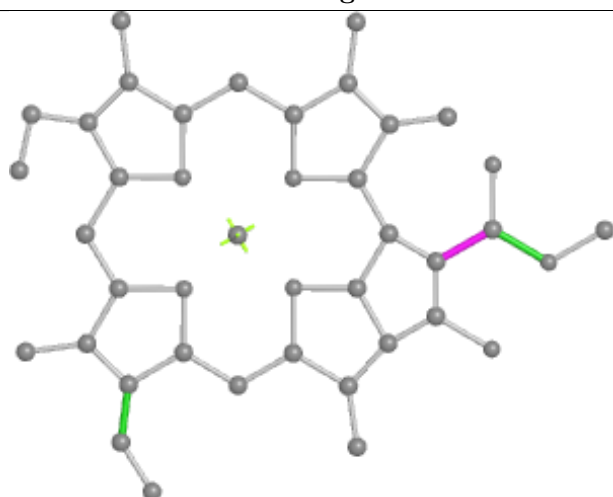
## Ligand CLA I 316



Bond lengths



Bond angles

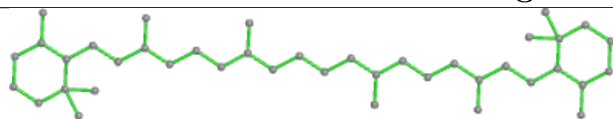


Torsions

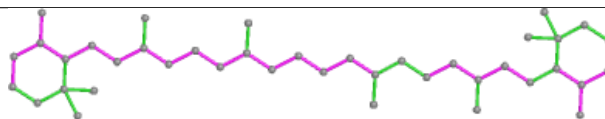


Rings

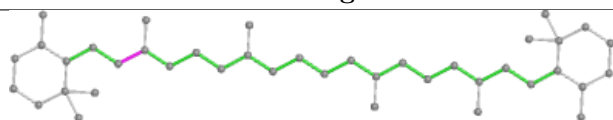
## Ligand BCR k 204



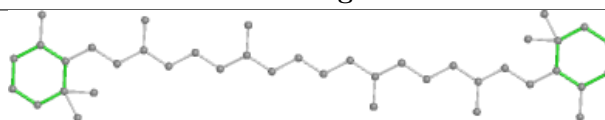
Bond lengths



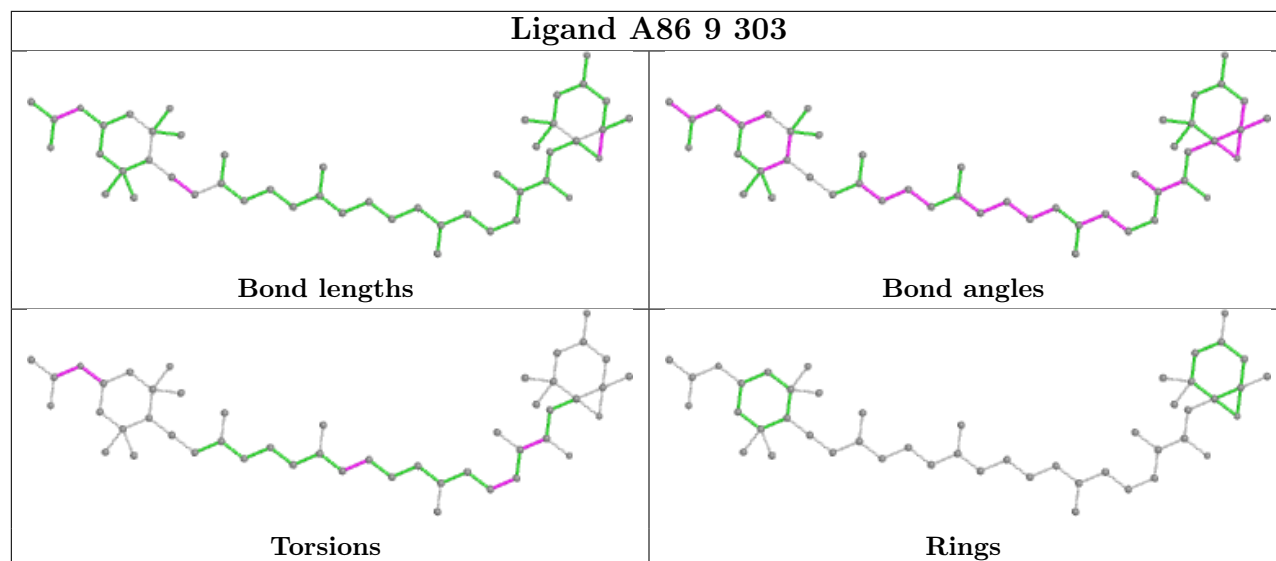
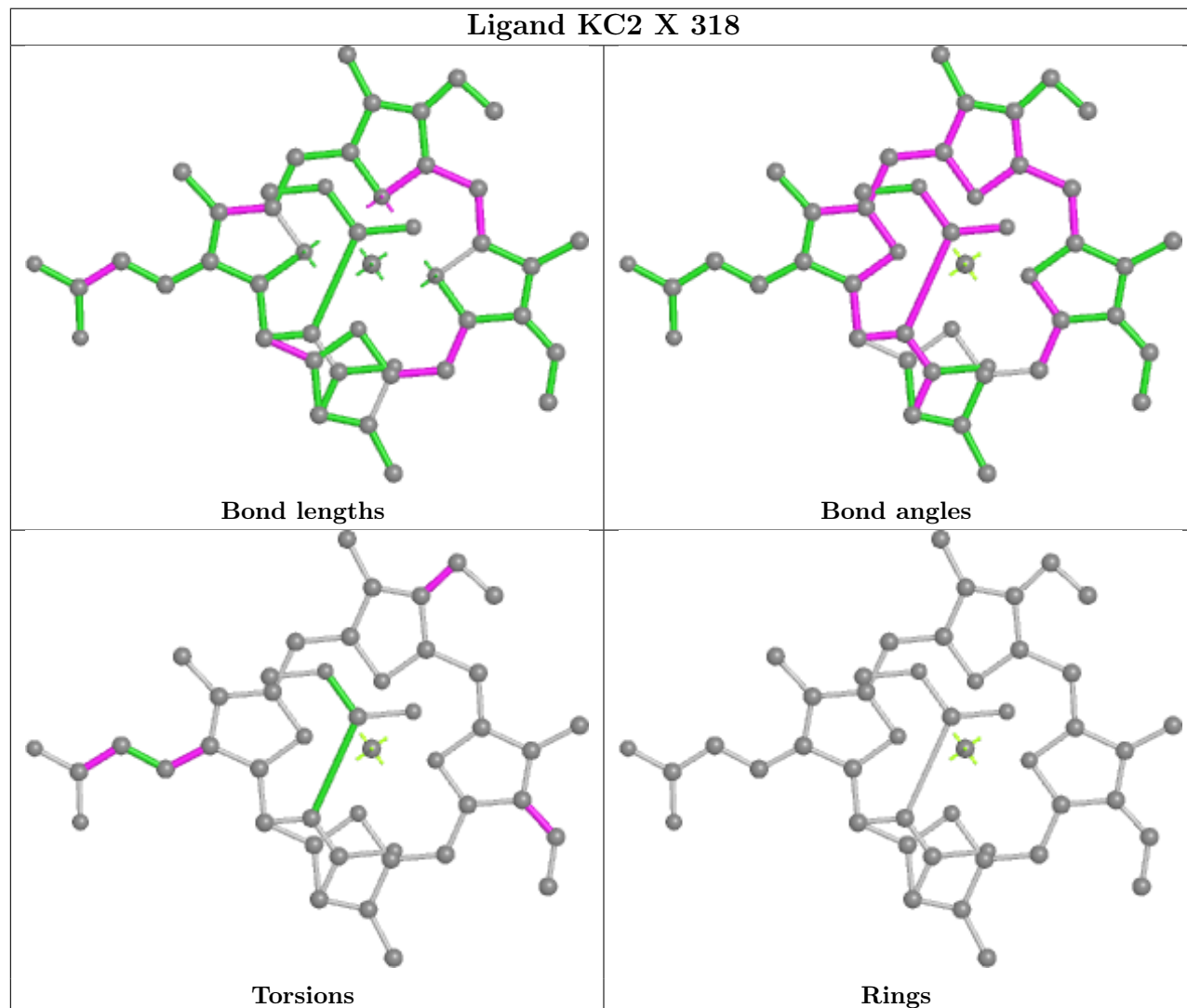
Bond angles



Torsions

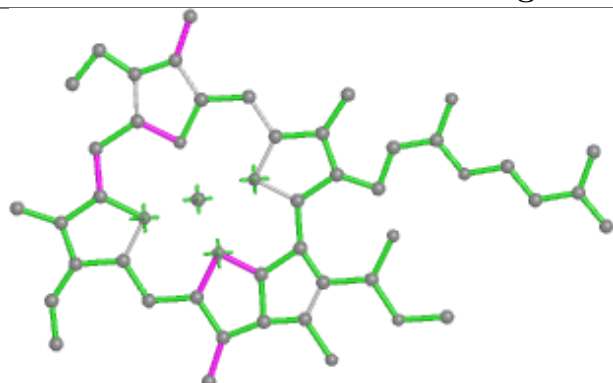


Rings

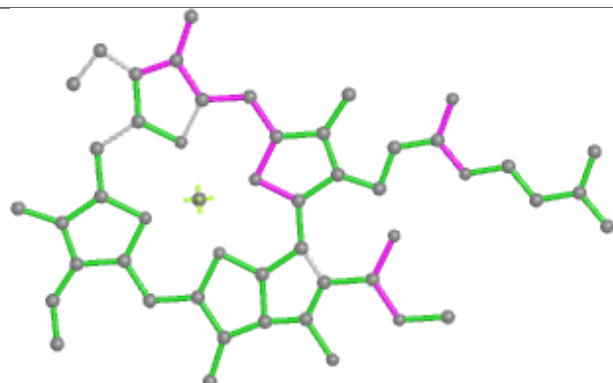
**Ligand A86 9 303****Ligand KC2 X 318**



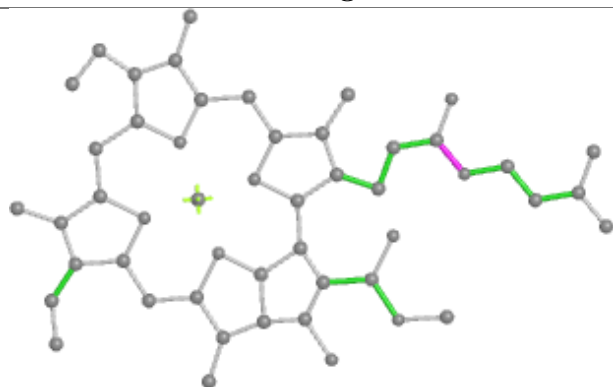
## Ligand CLA b 822



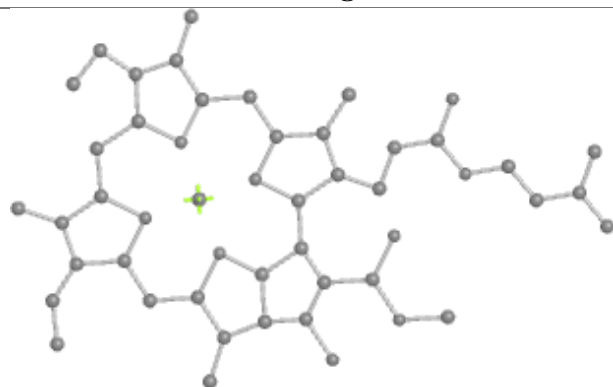
Bond lengths



Bond angles

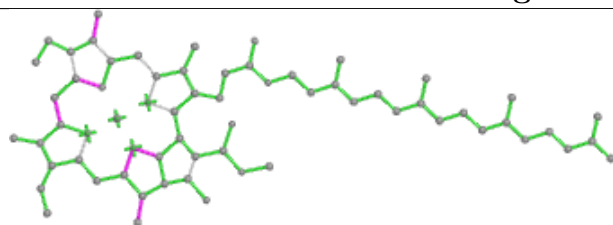


Torsions

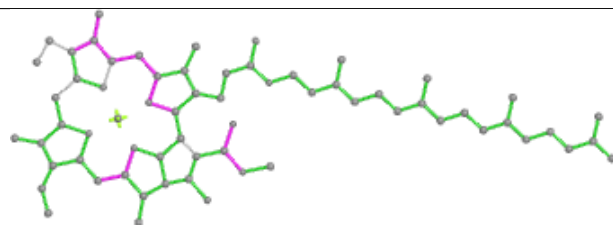


Rings

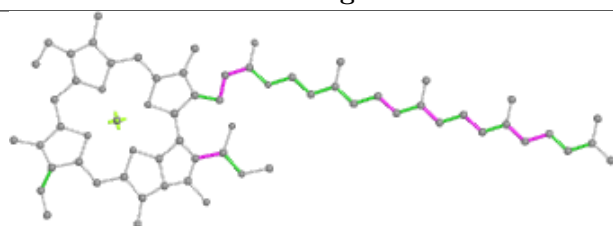
## Ligand CLA D 313



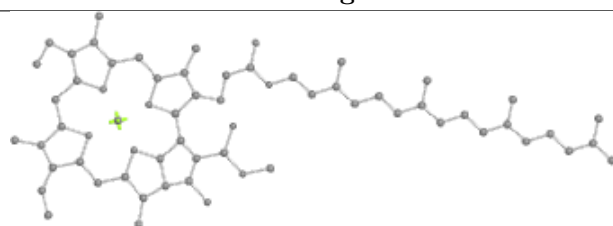
Bond lengths



Bond angles

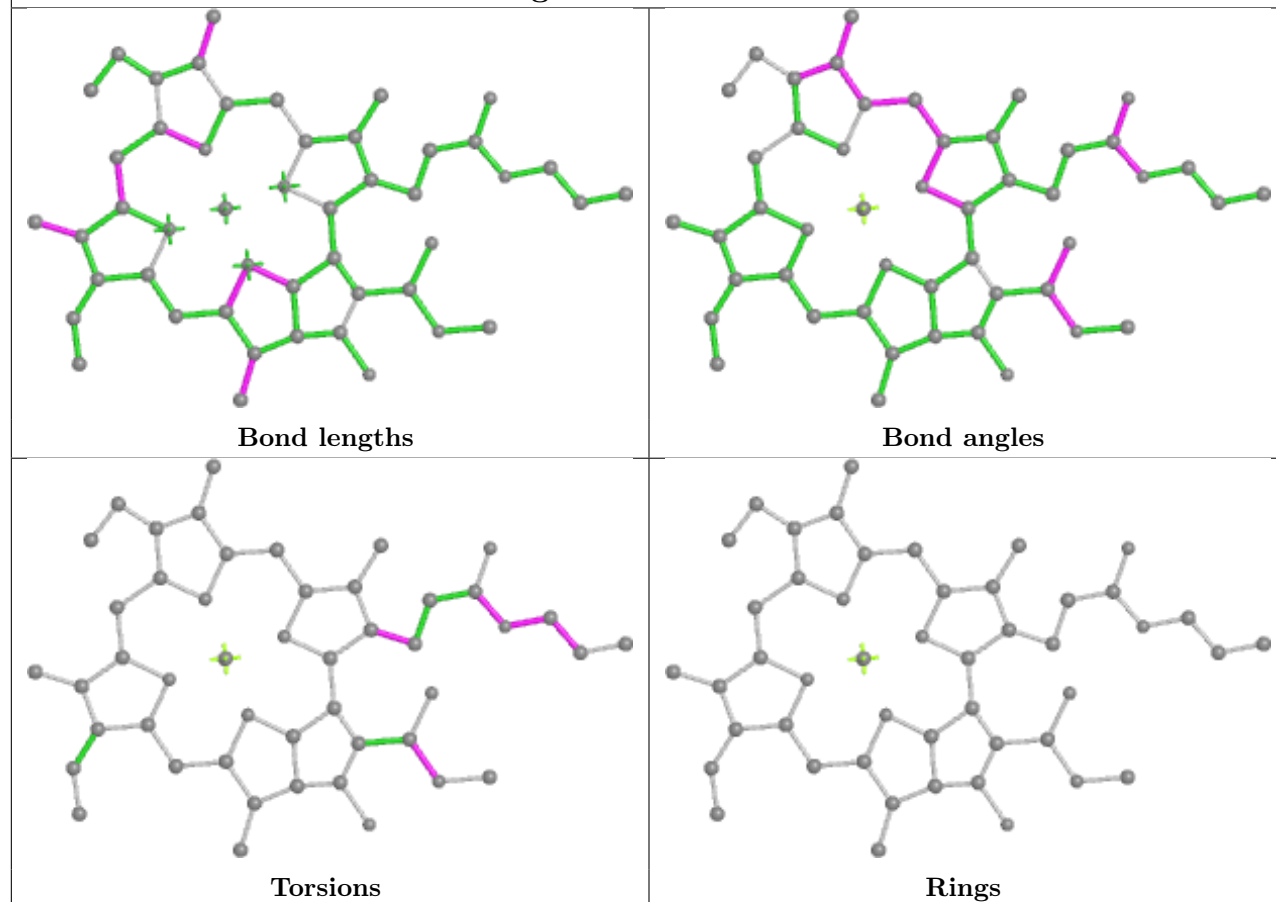


Torsions

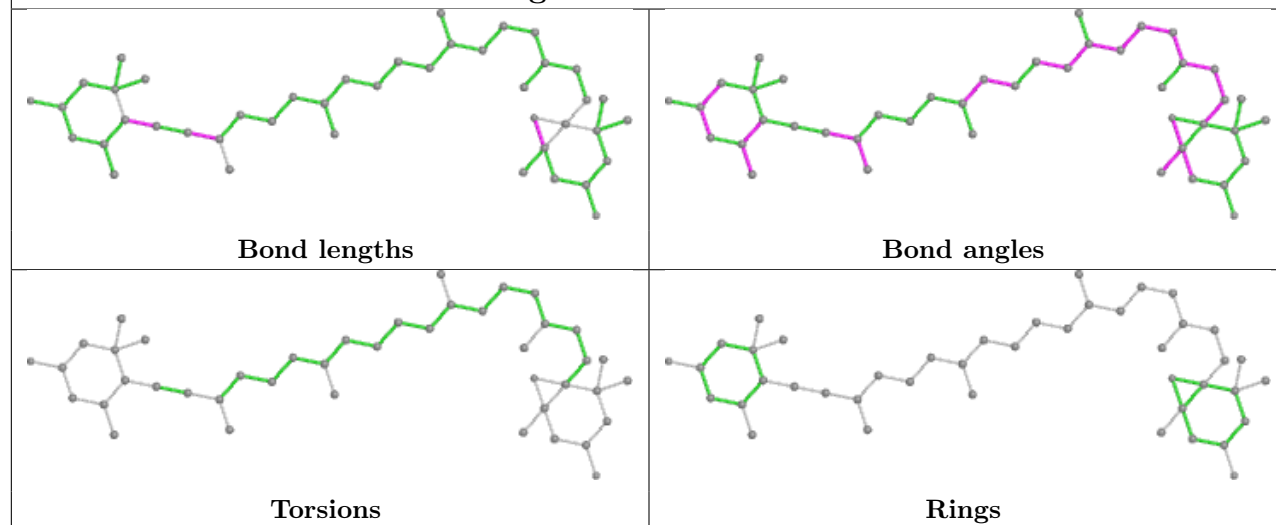


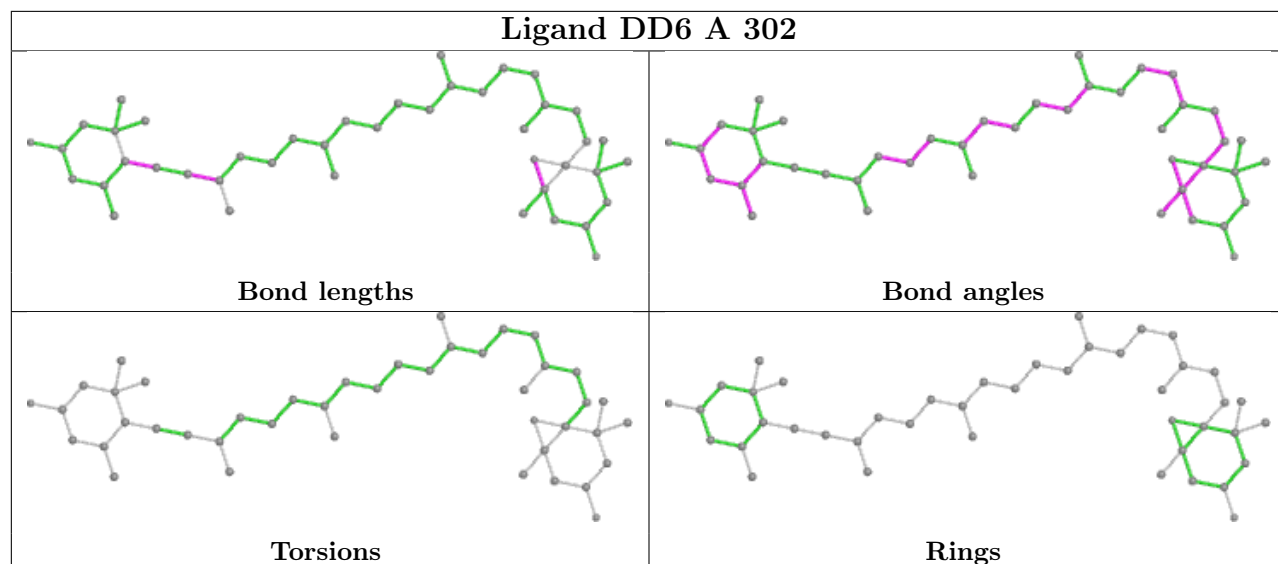
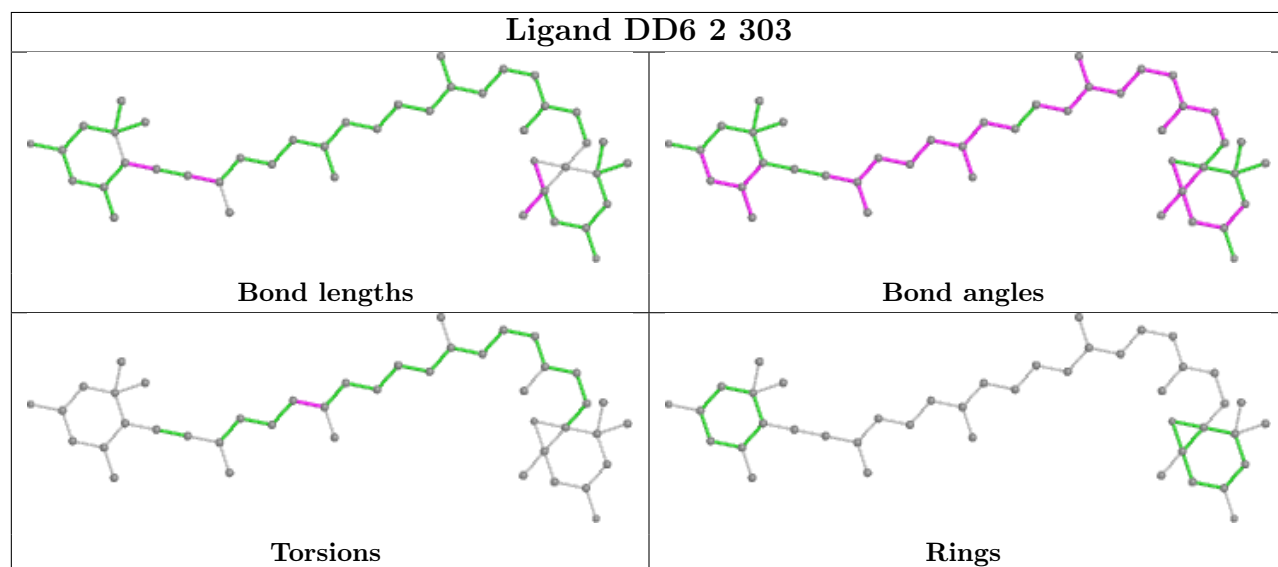
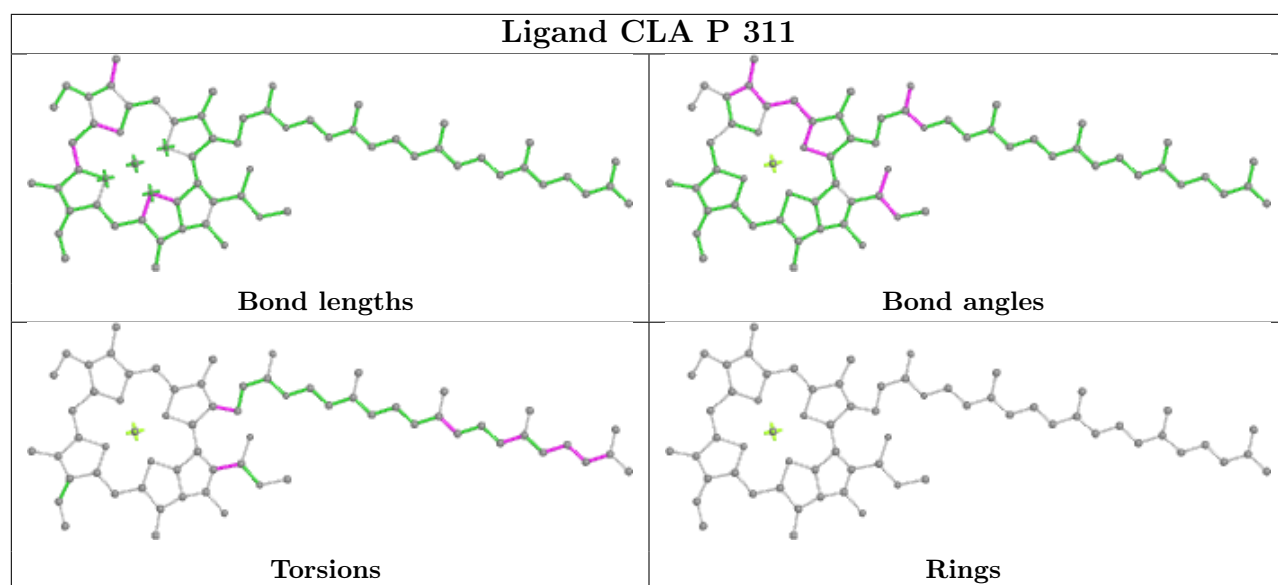
Rings

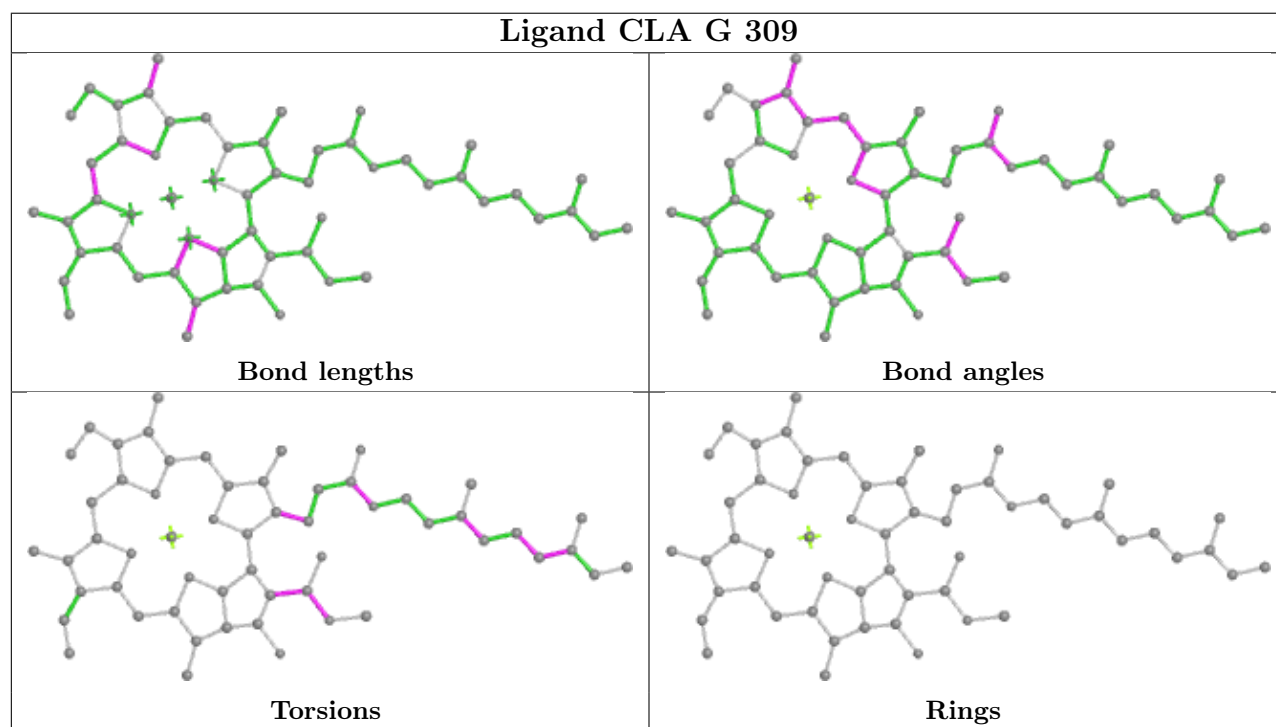
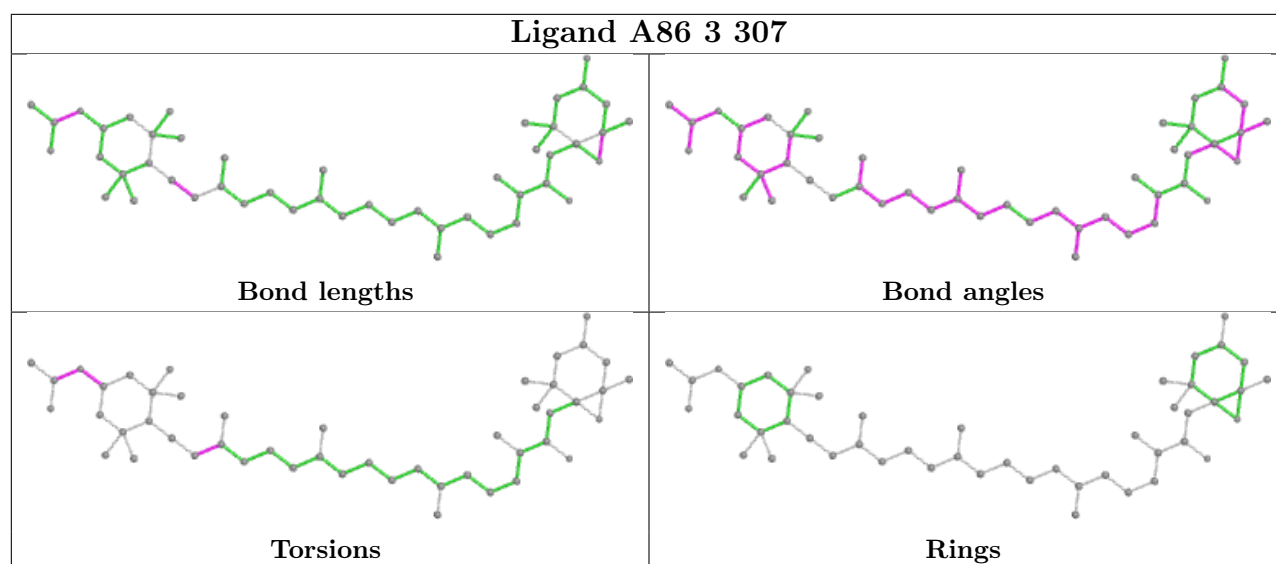
## Ligand CLA H 306

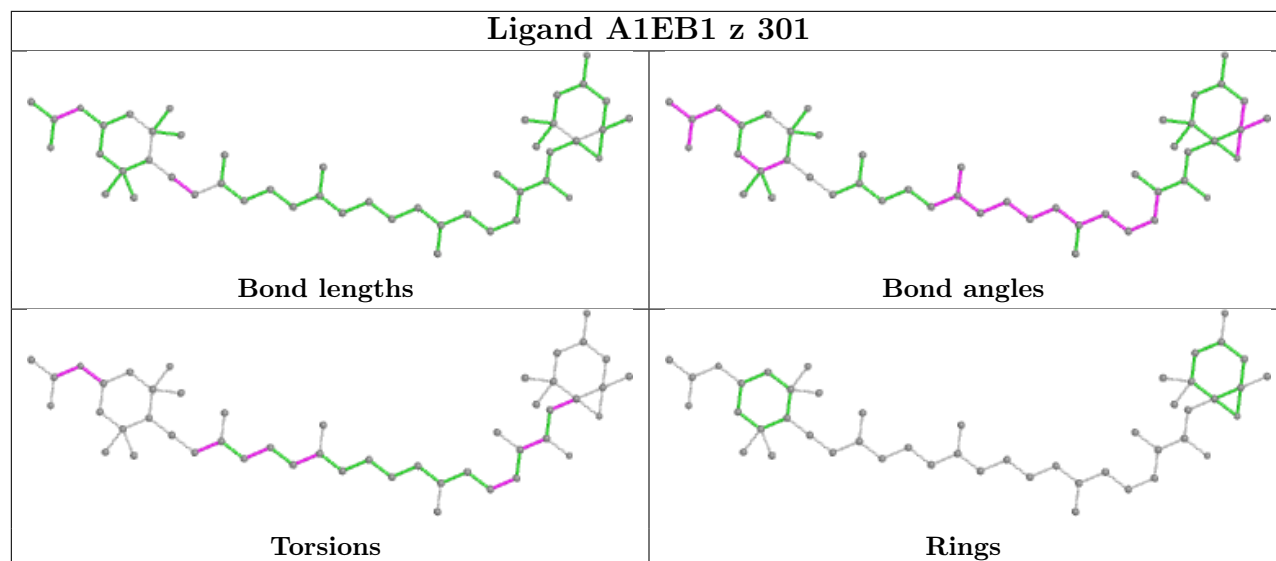
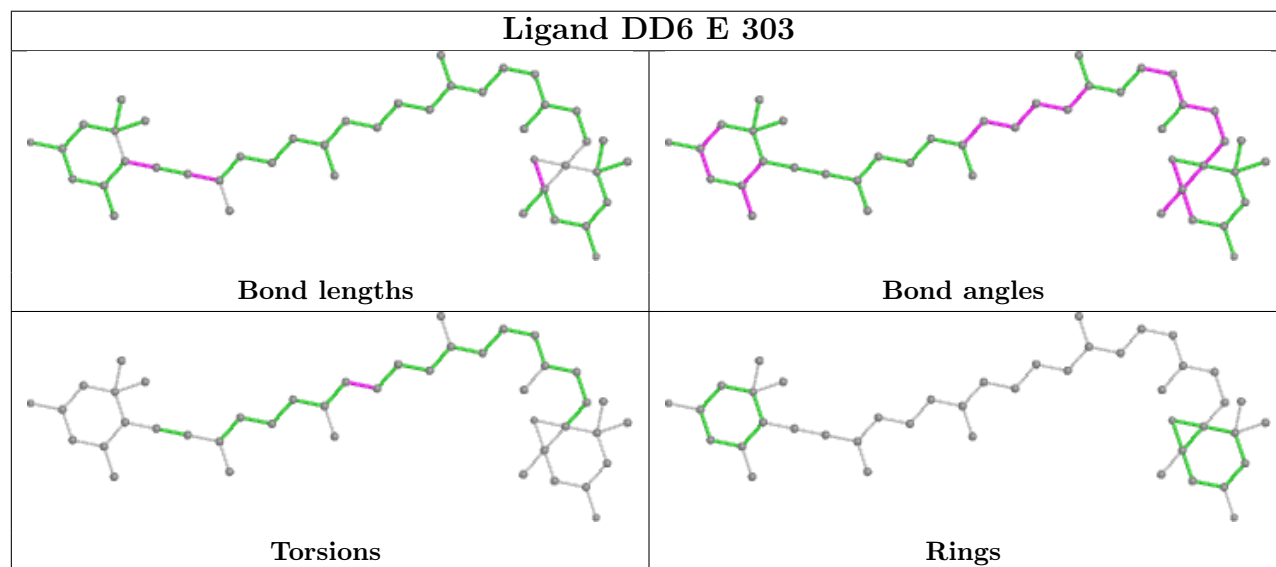


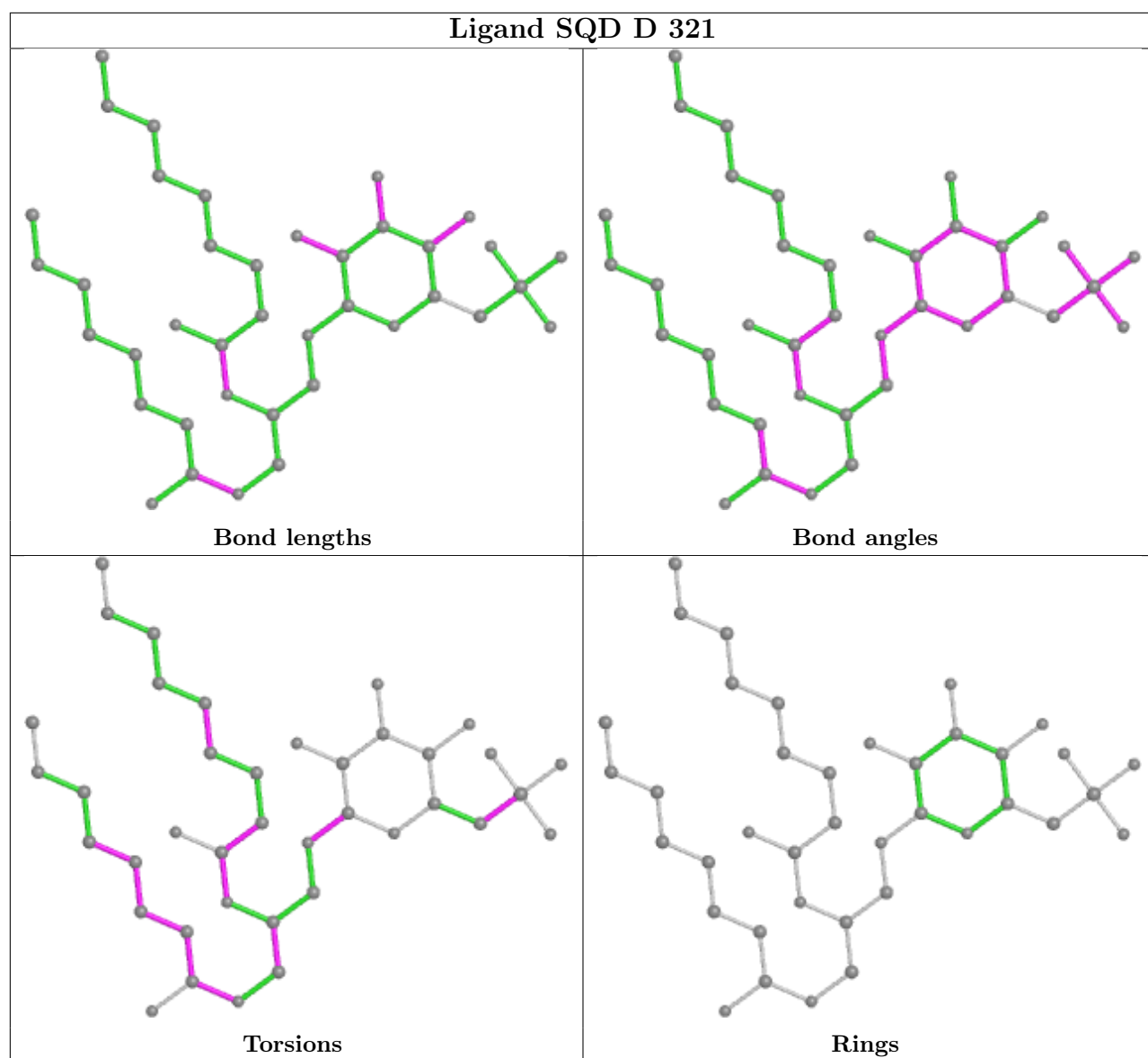
## Ligand DD6 M 304



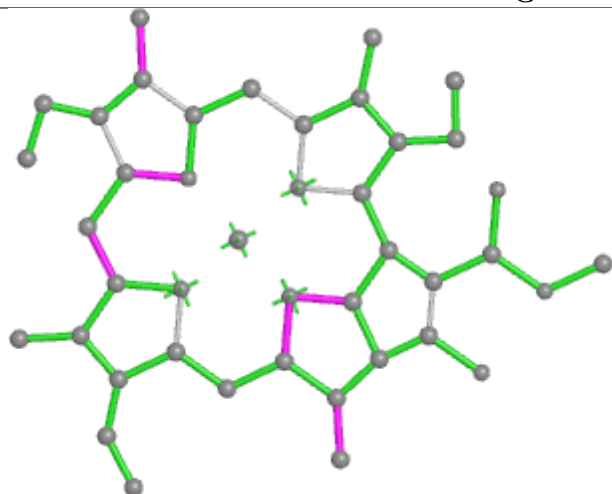




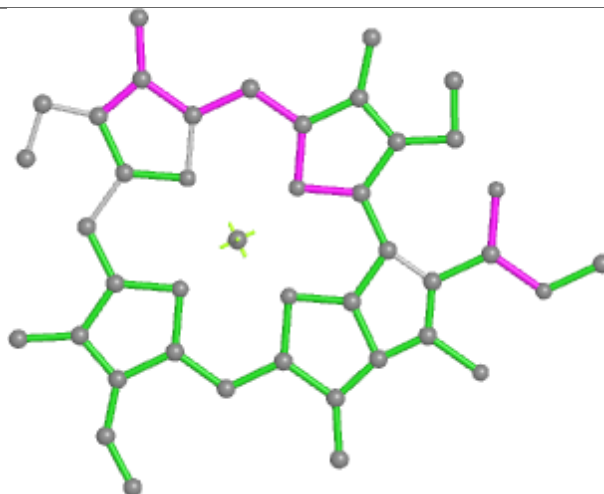
**Ligand A1EB1 z 301****Ligand DD6 E 303**



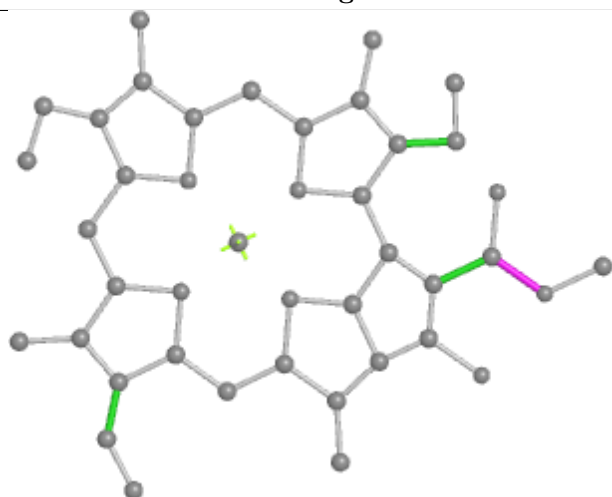
## Ligand CLA J 317



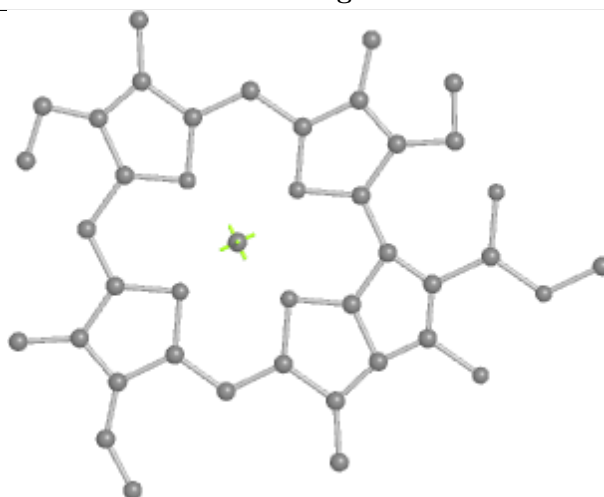
Bond lengths



Bond angles

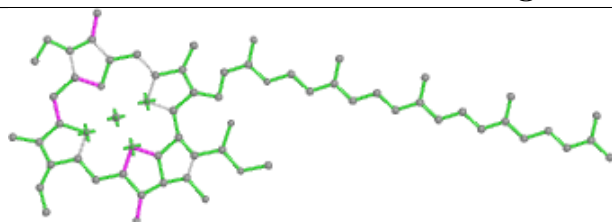


Torsions

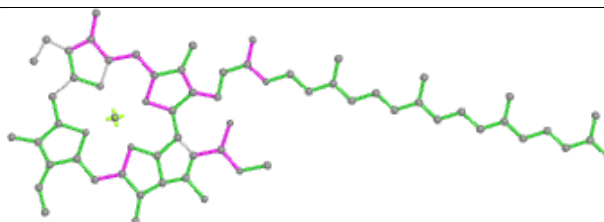


Rings

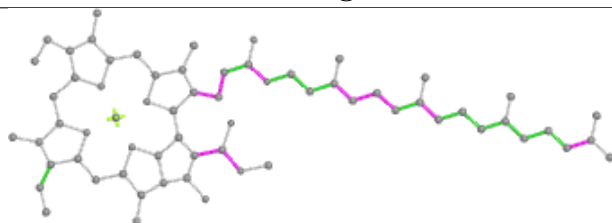
## Ligand CLA 4 312



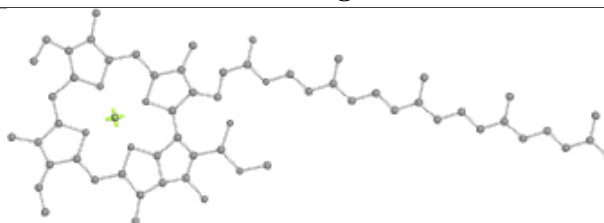
Bond lengths



Bond angles

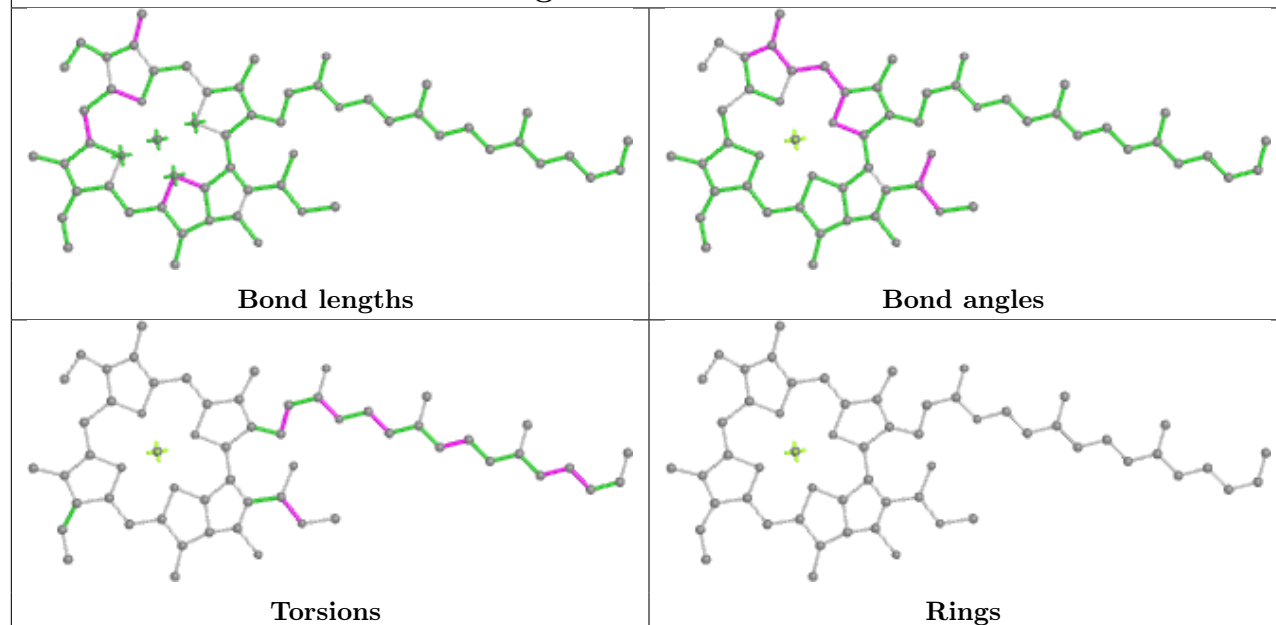


Torsions

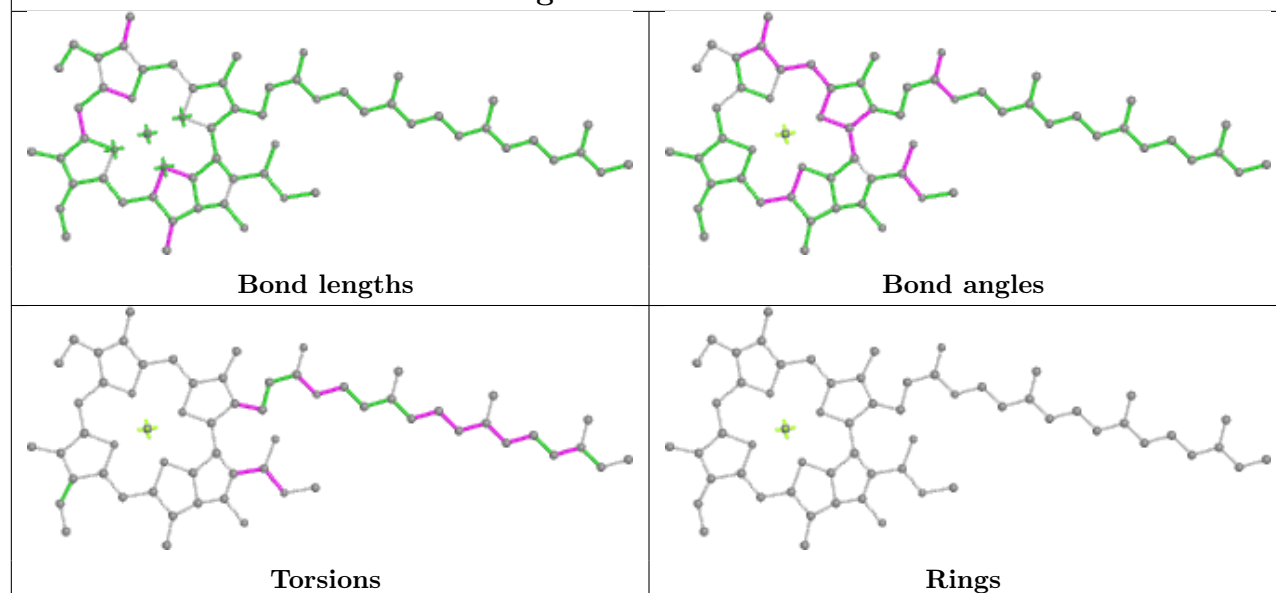


Rings

## Ligand CLA b 819

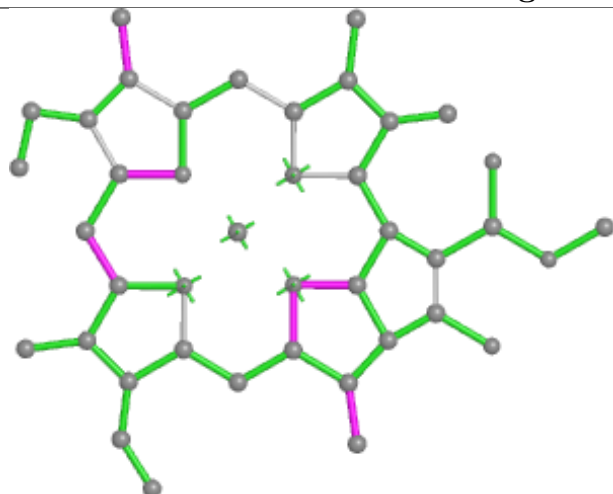


## Ligand CLA 4 311

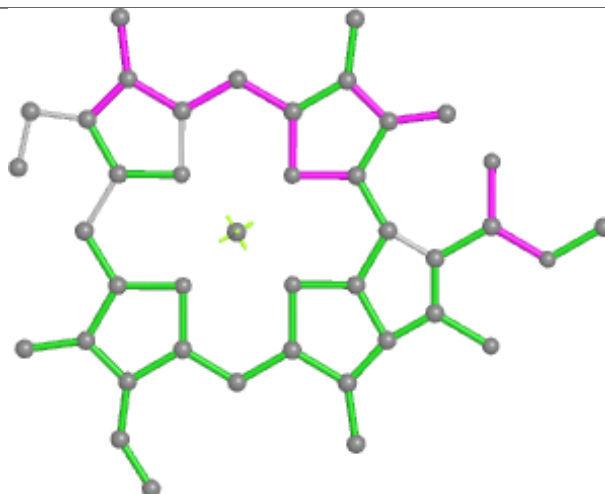




## Ligand CLA 6 318



Bond lengths



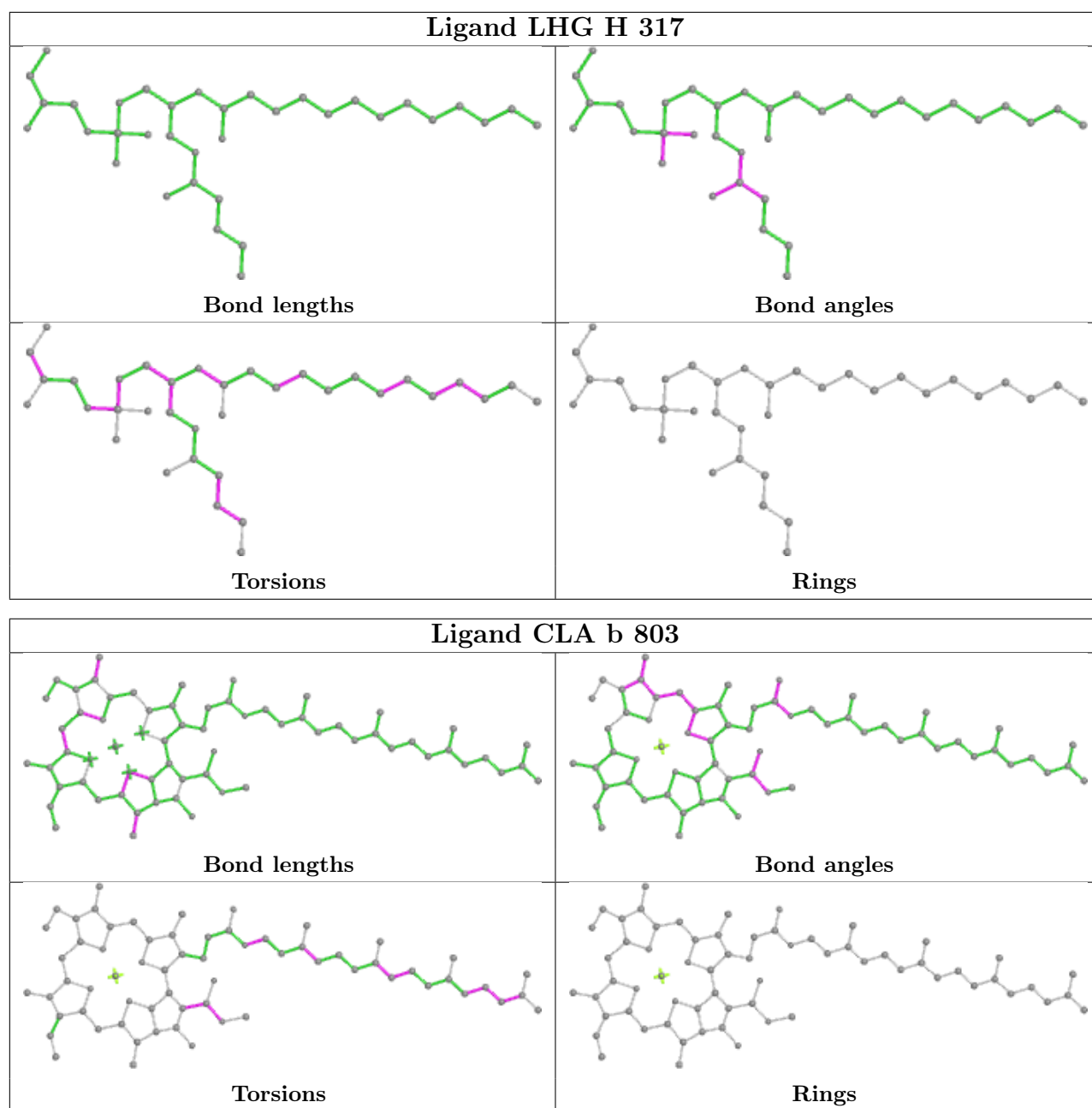
Bond angles



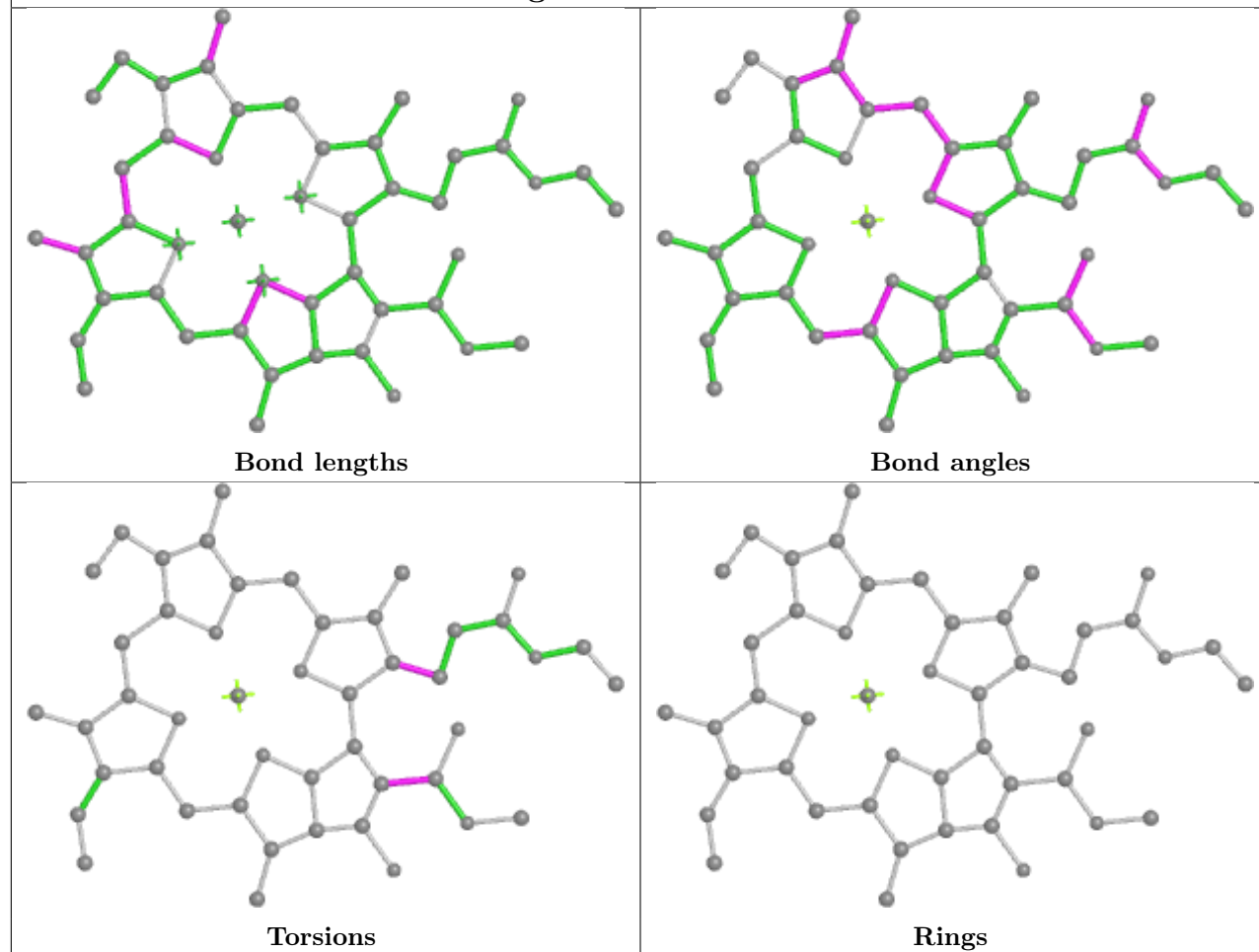
Torsions



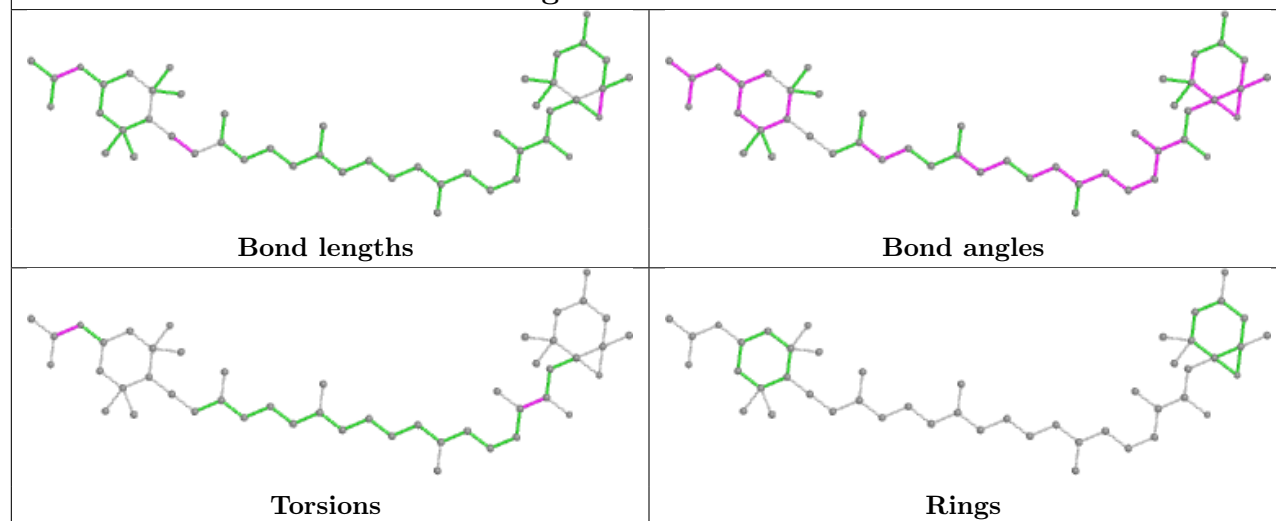
Rings



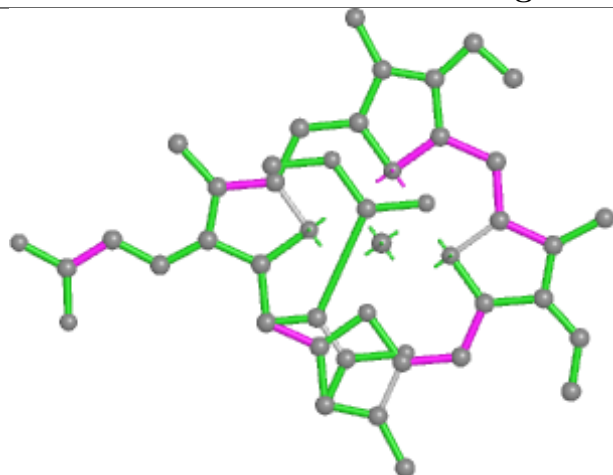
## Ligand CLA b 839



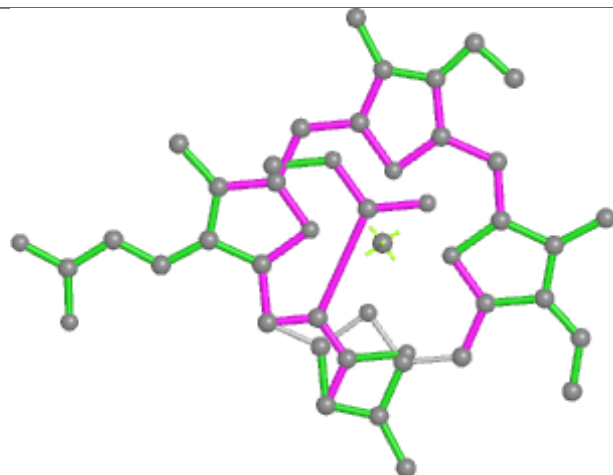
## Ligand A86 J 303



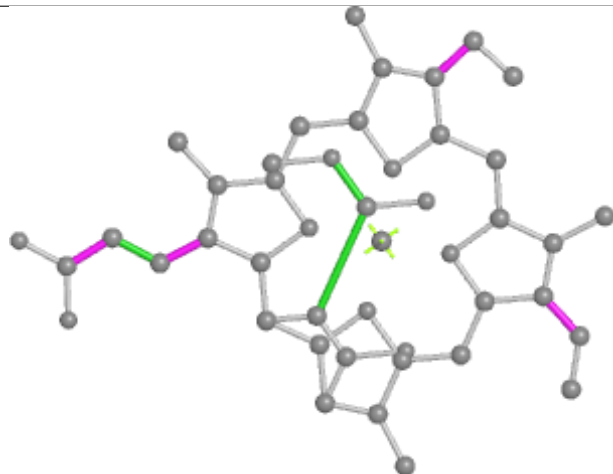
## Ligand KC2 G 317



Bond lengths



Bond angles

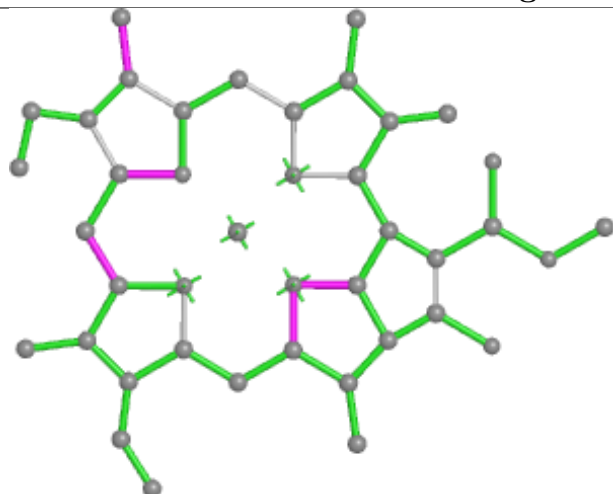


Torsions

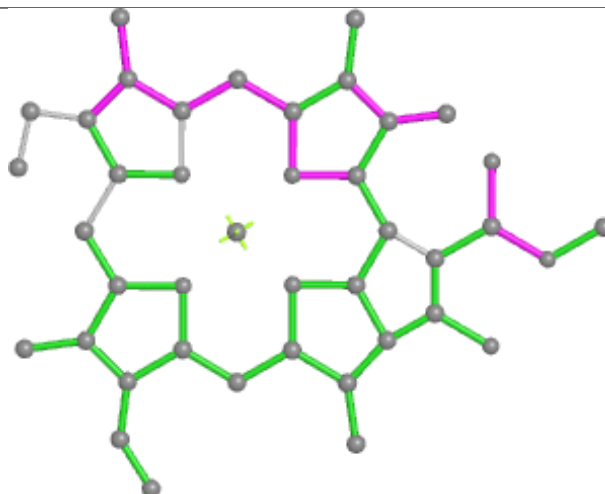


Rings

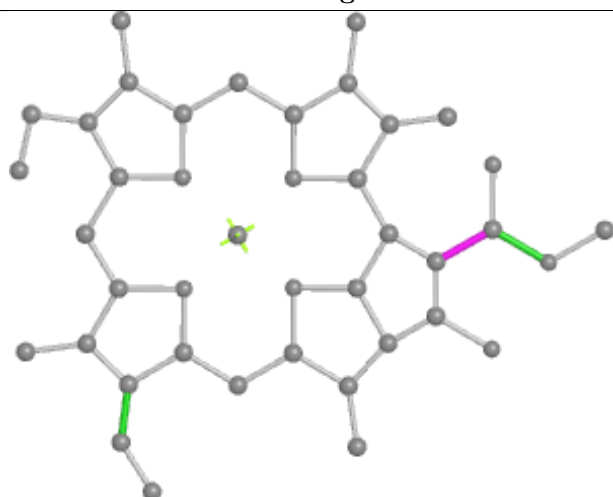
## Ligand CLA z 314



Bond lengths



Bond angles

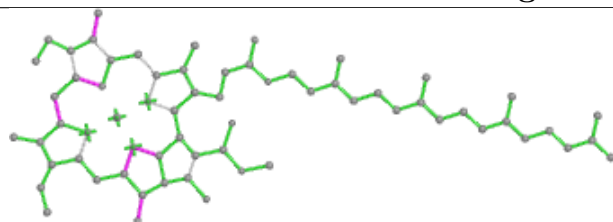


Torsions

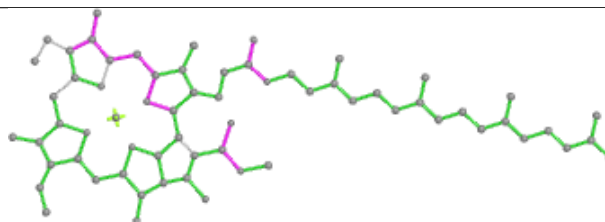


Rings

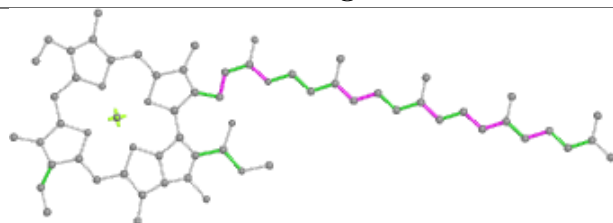
## Ligand CLA 5 306



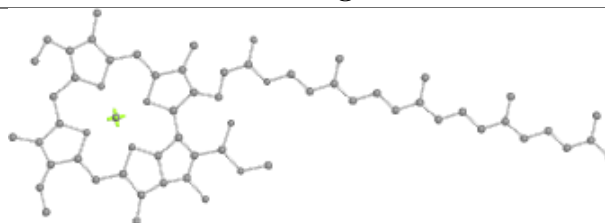
Bond lengths



Bond angles

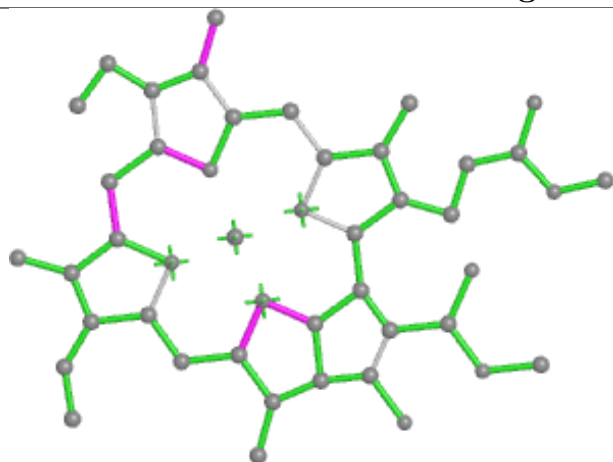


Torsions

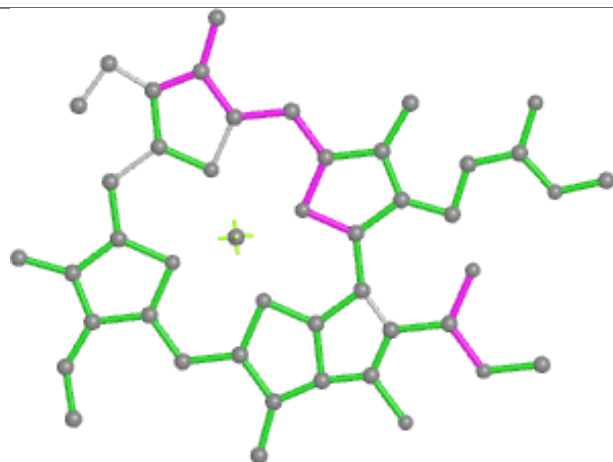


Rings

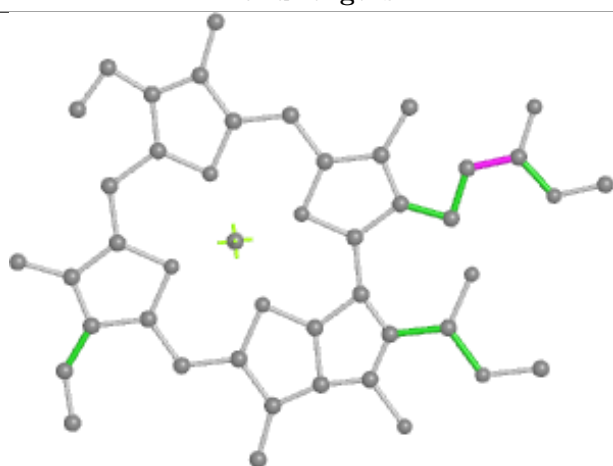
## Ligand CLA 4 313



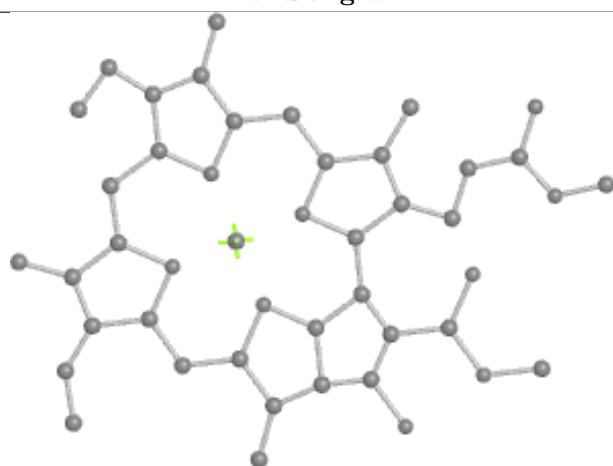
Bond lengths



Bond angles

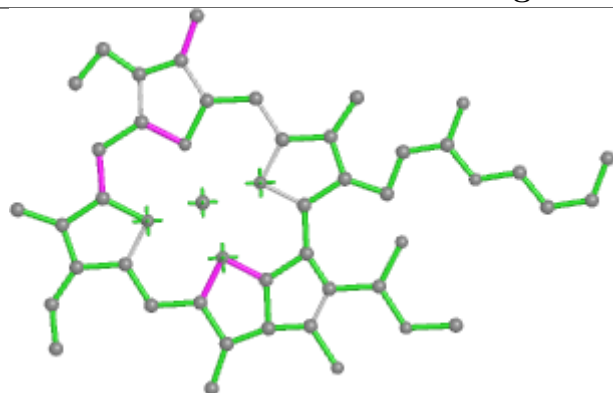


Torsions

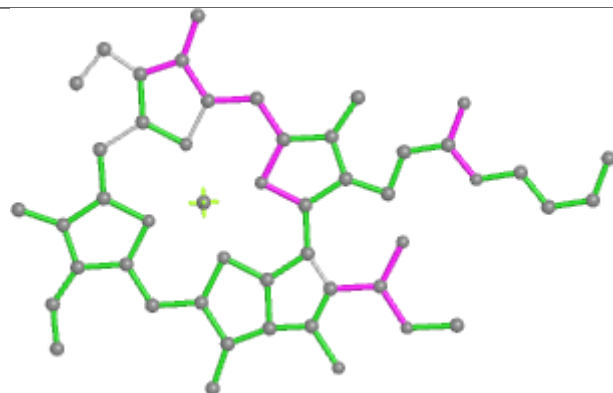


Rings

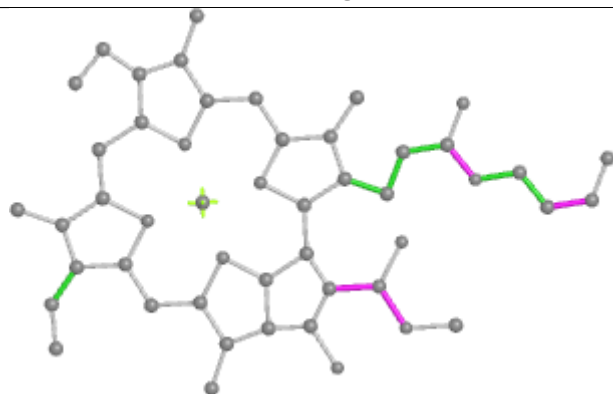
## Ligand CLA D 309



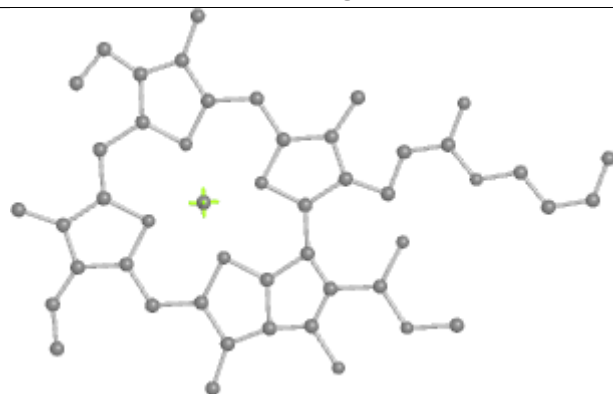
Bond lengths



Bond angles

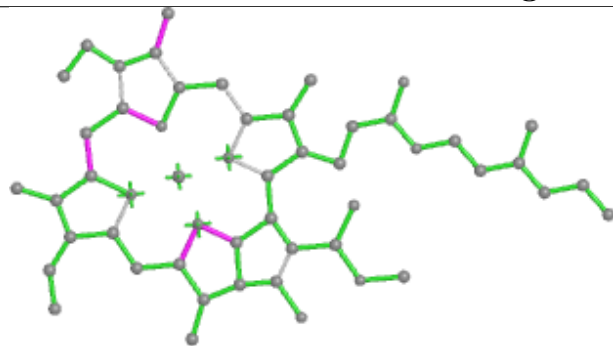


Torsions

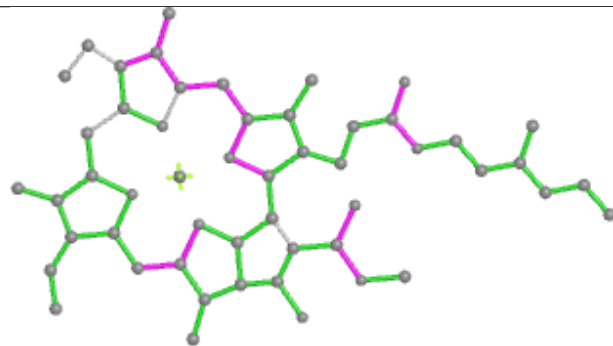


Rings

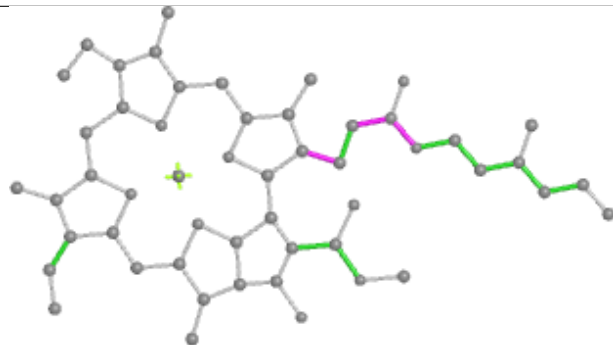
## Ligand CLA I 301



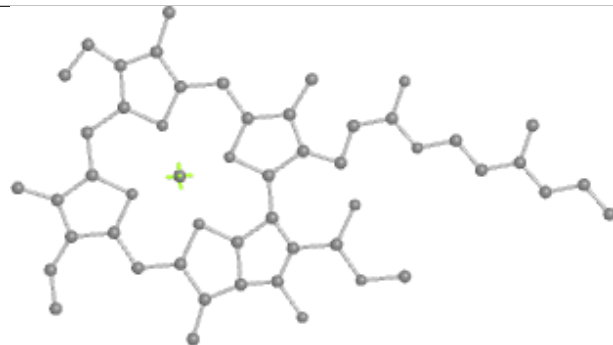
Bond lengths



Bond angles

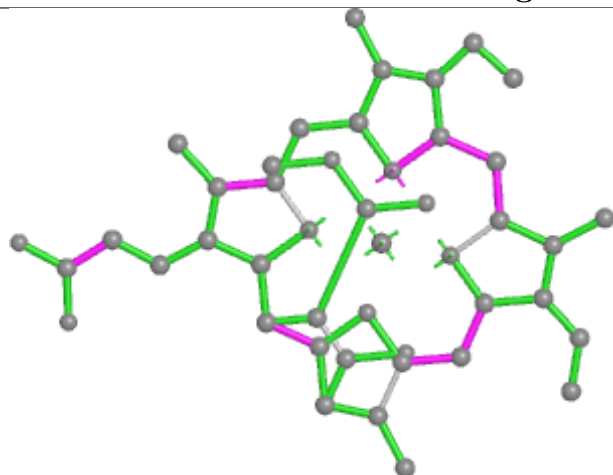


Torsions

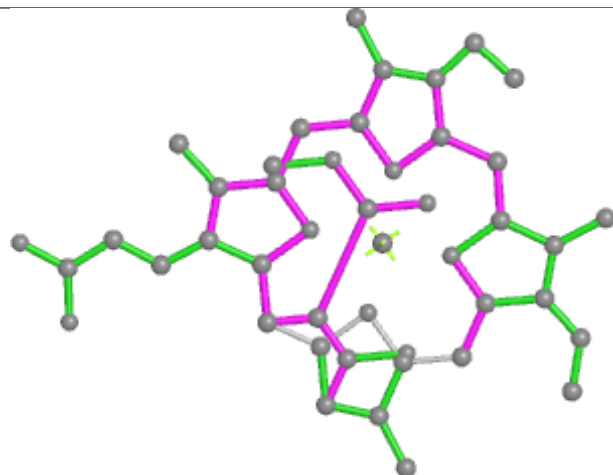


Rings

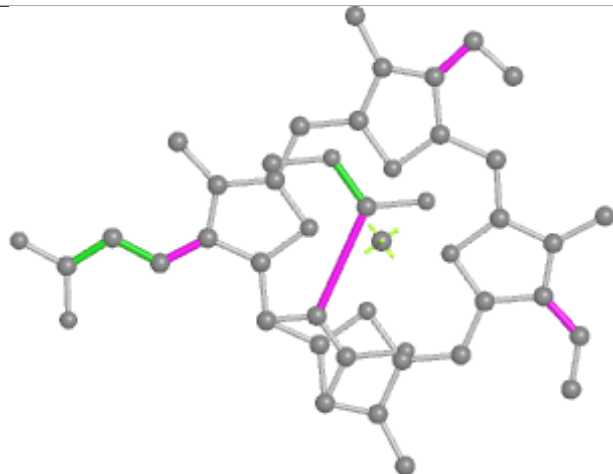
## Ligand KC2 X 312



Bond lengths



Bond angles

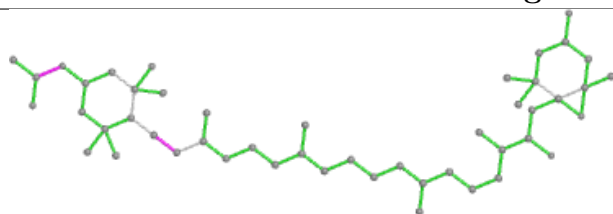


Torsions

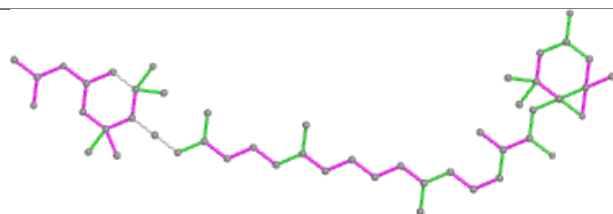


Rings

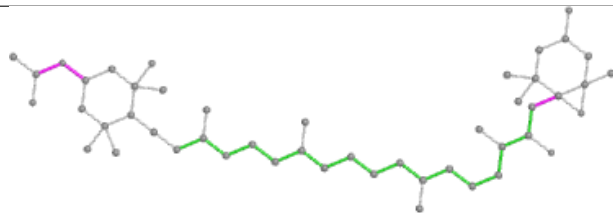
## Ligand A86 7 312



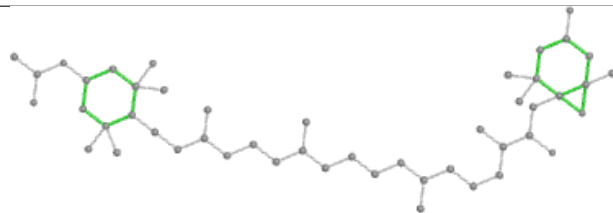
Bond lengths



Bond angles

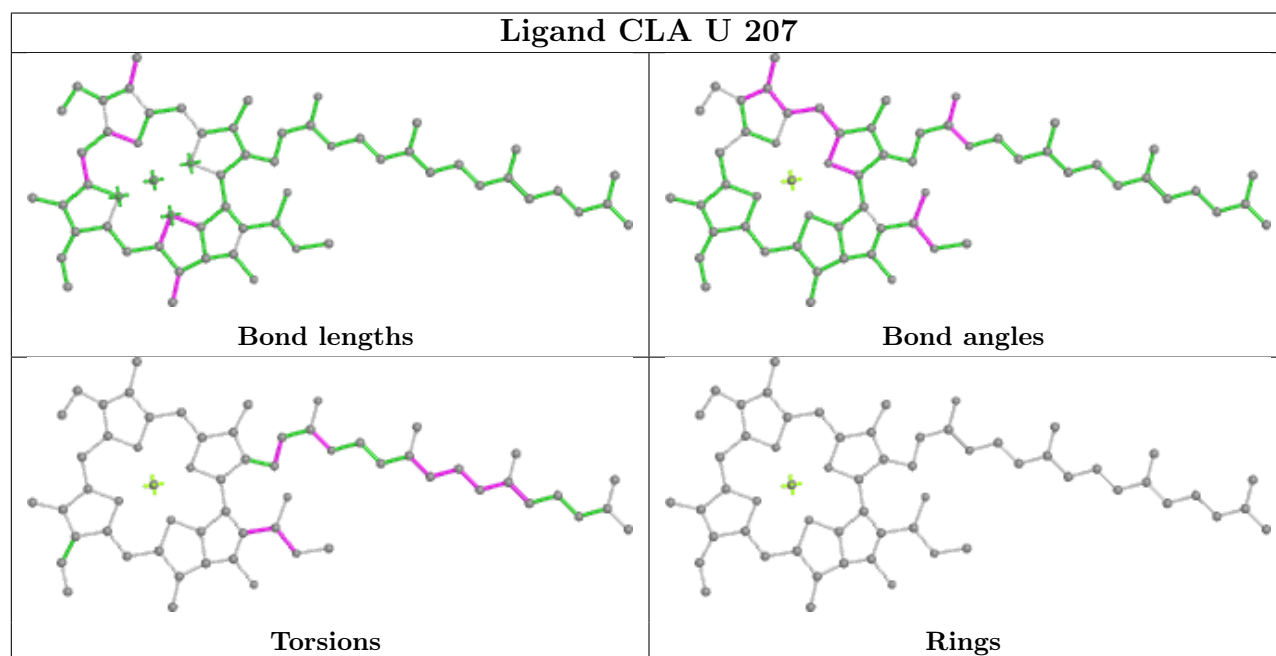
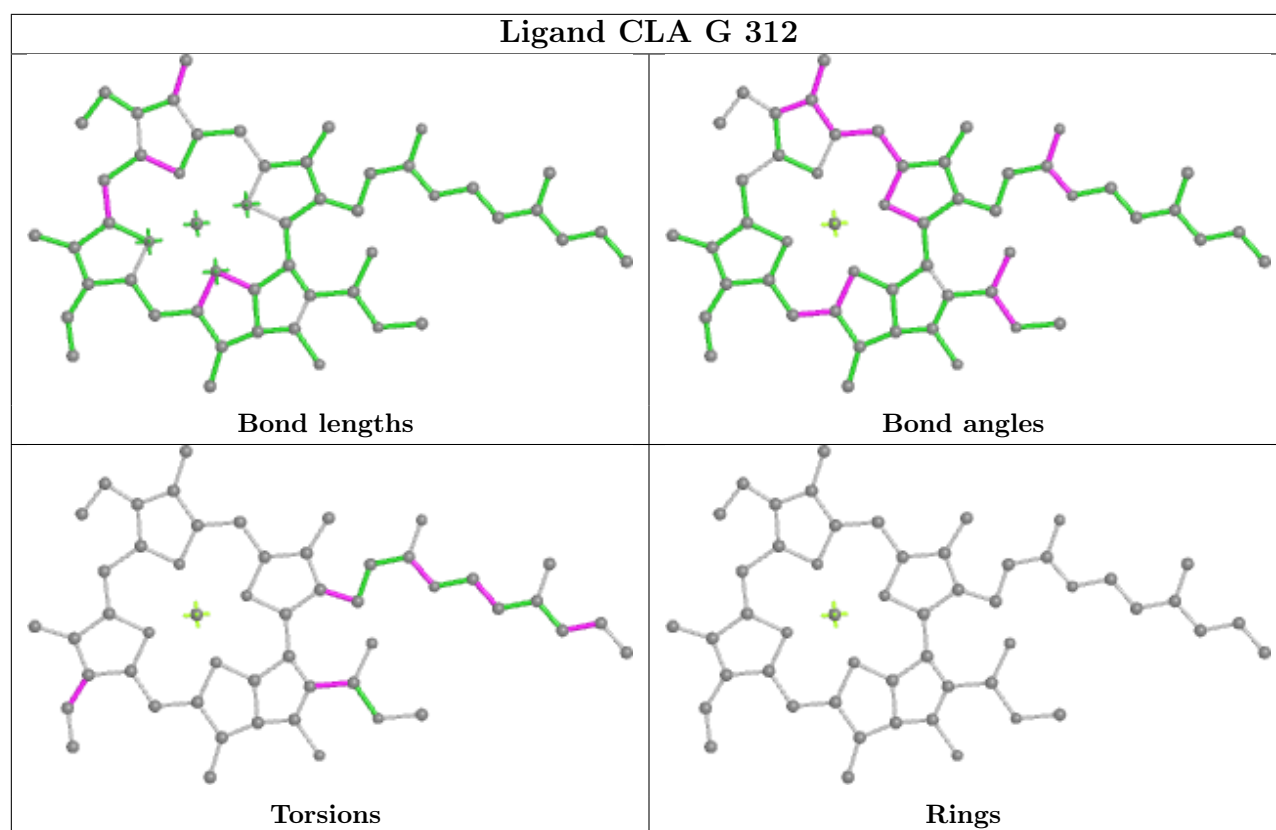


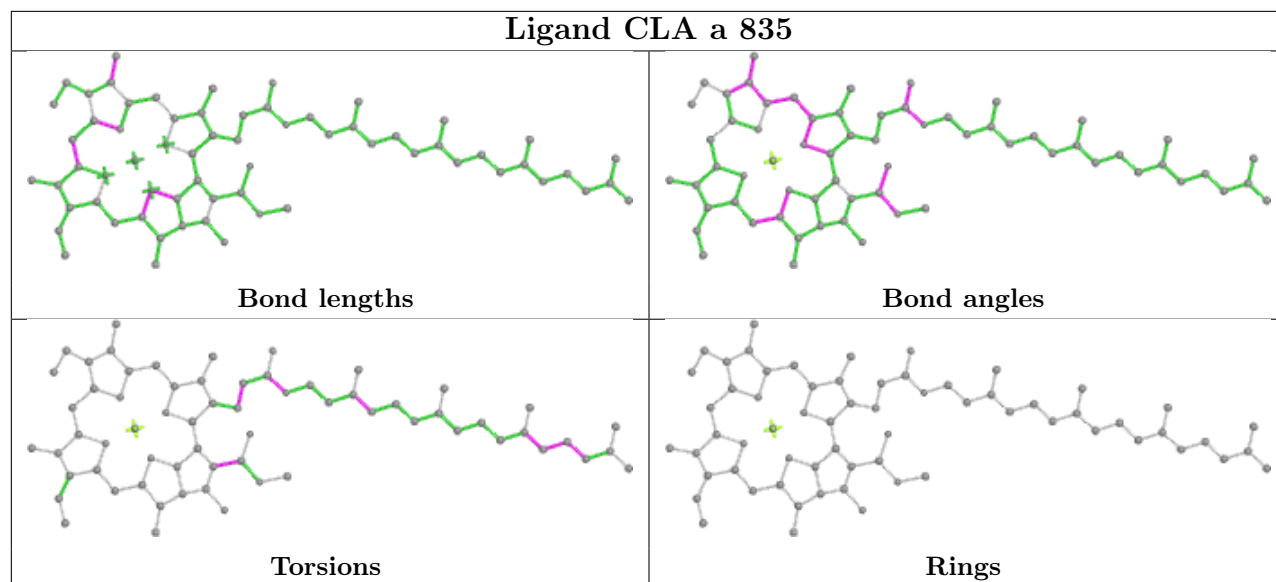
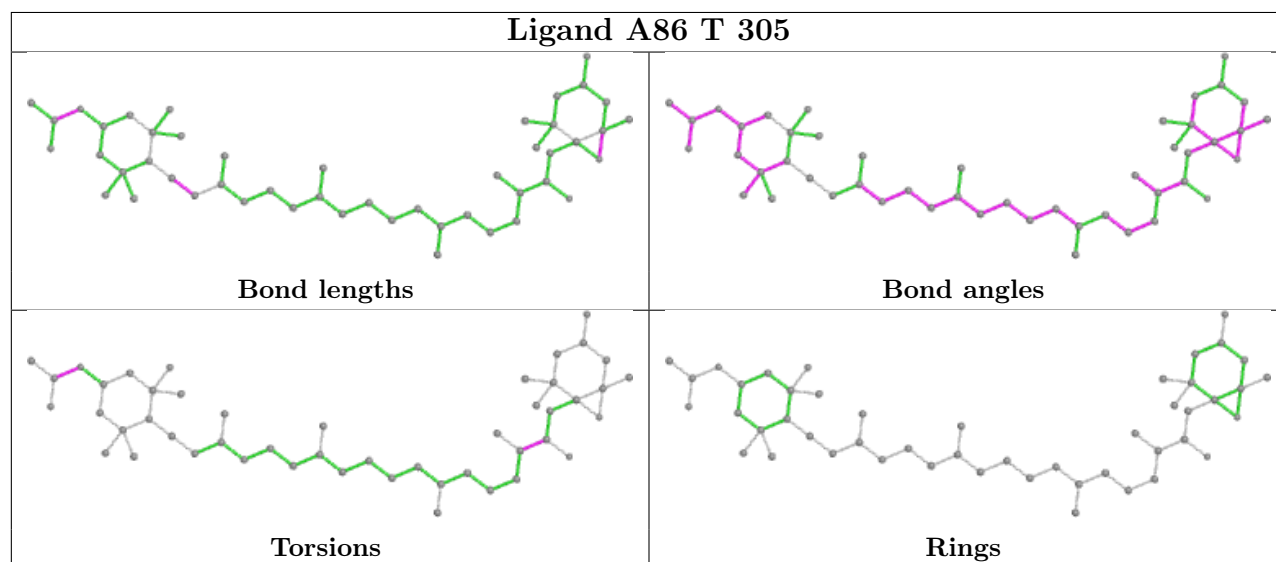
Torsions

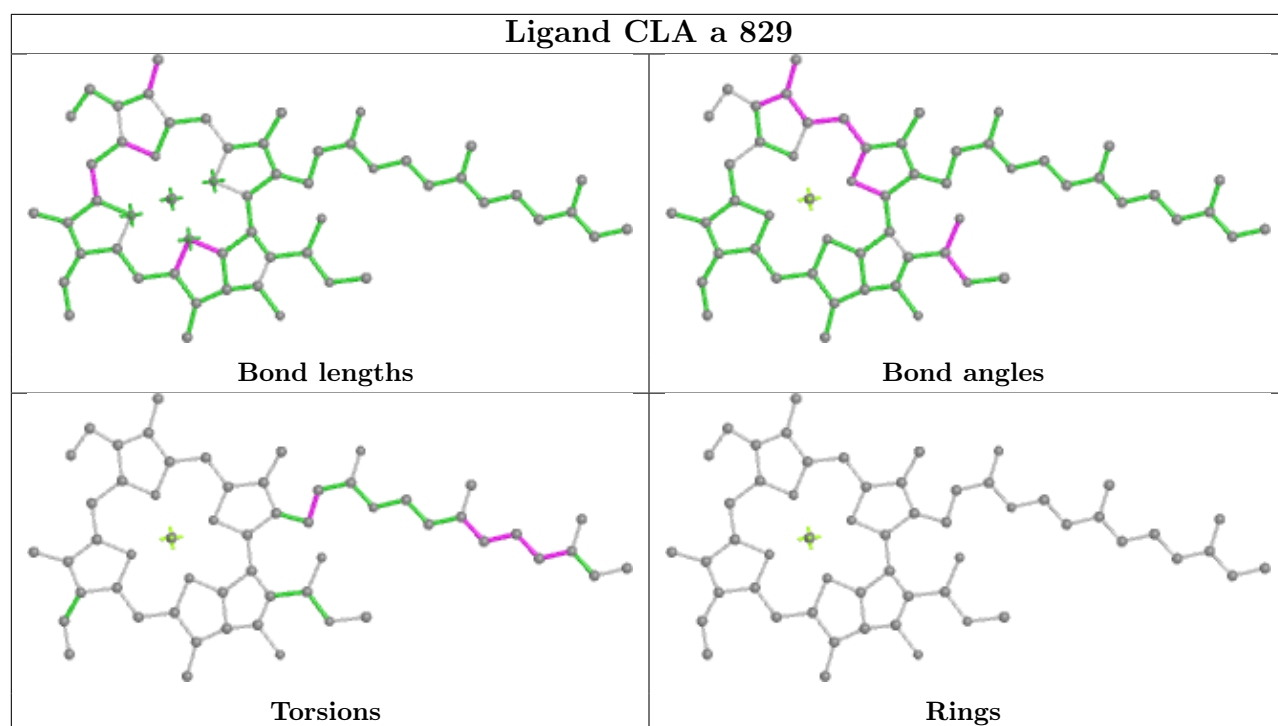


Rings

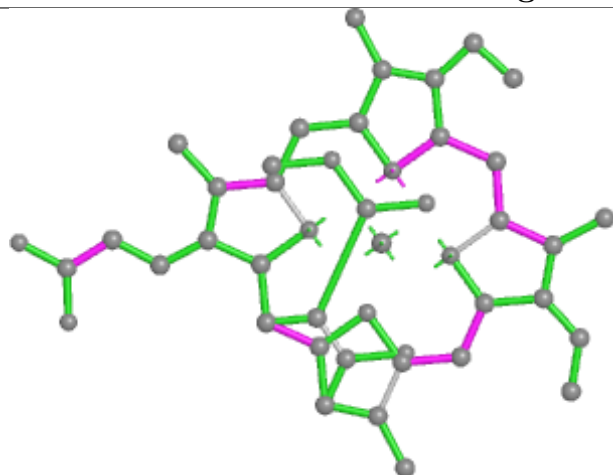




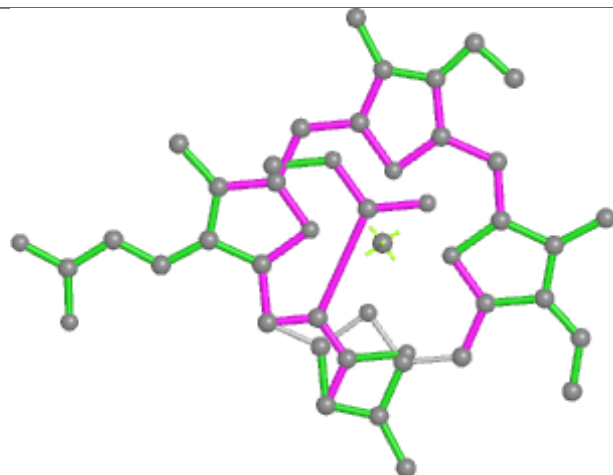
**Ligand CLA a 835****Ligand A86 T 305**



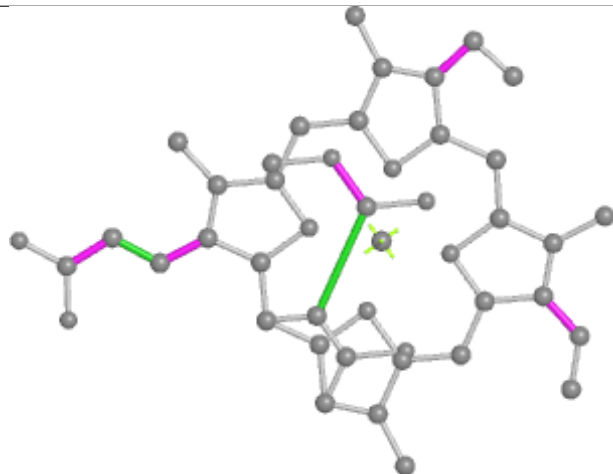
## Ligand KC2 F 307



Bond lengths



Bond angles

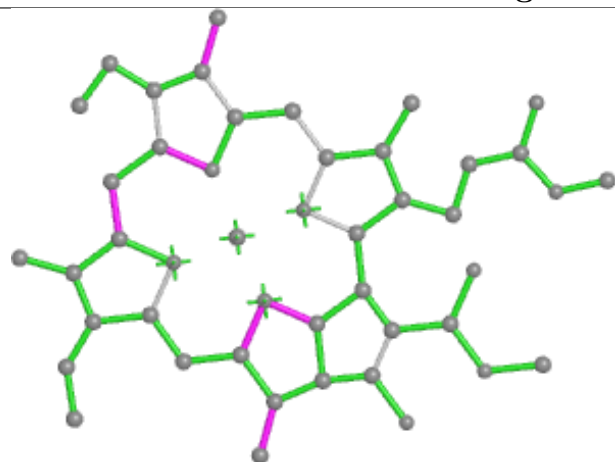


Torsions

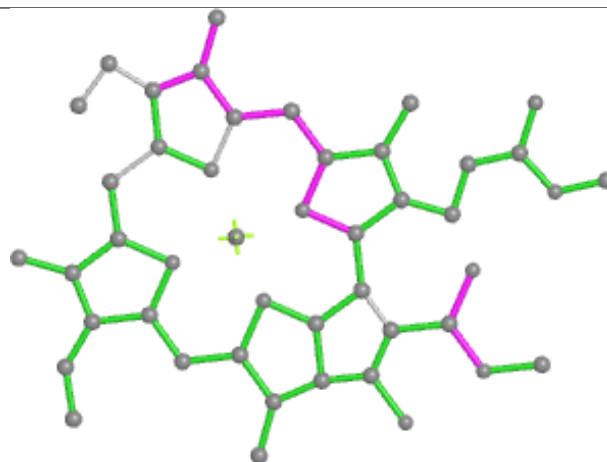


Rings

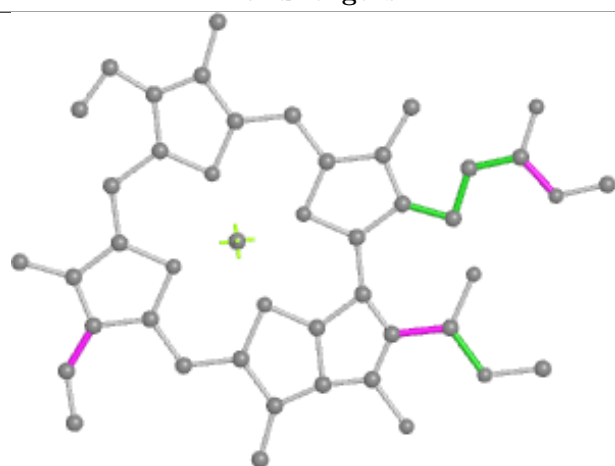
## Ligand CLA O 312



Bond lengths



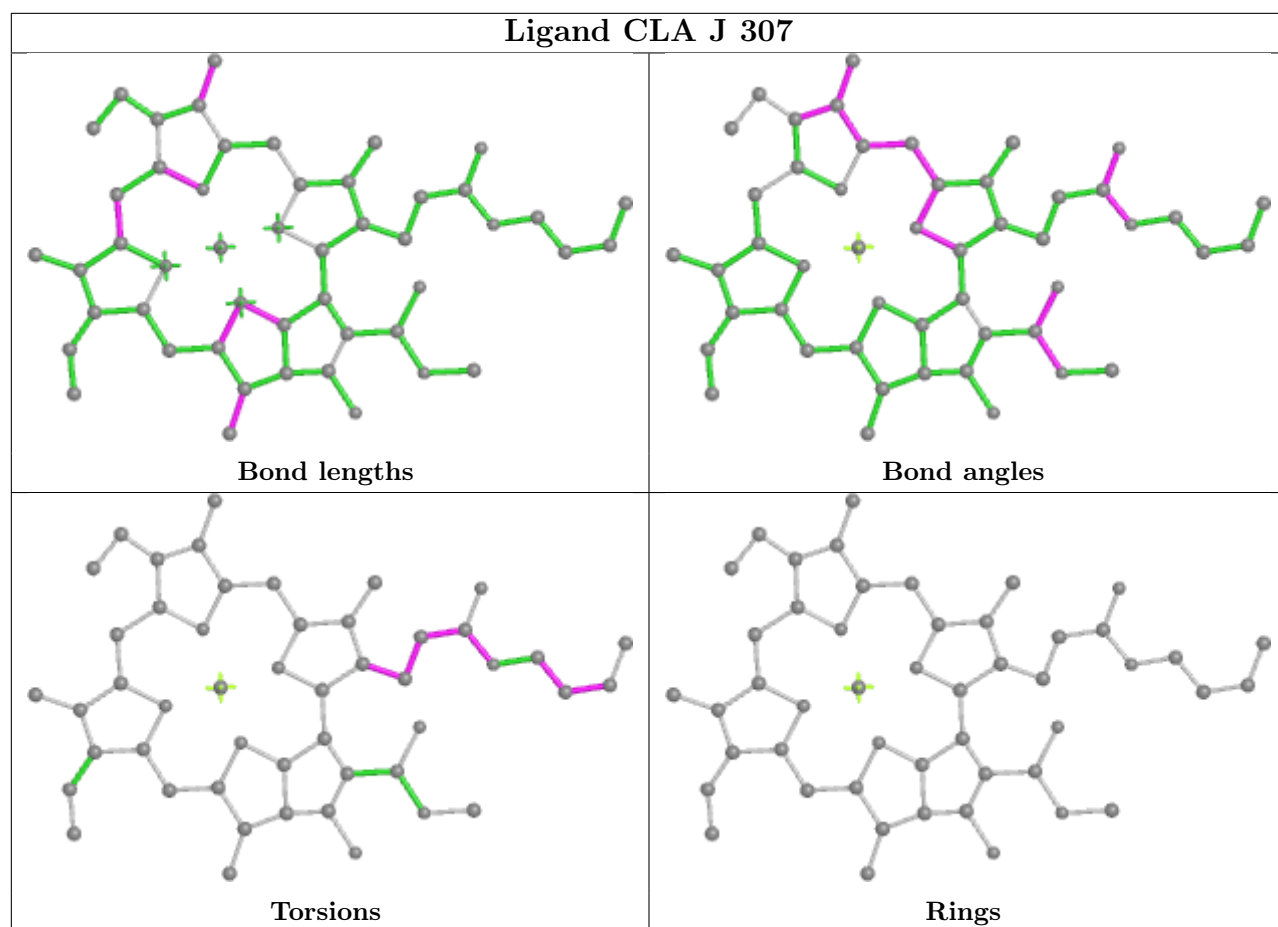
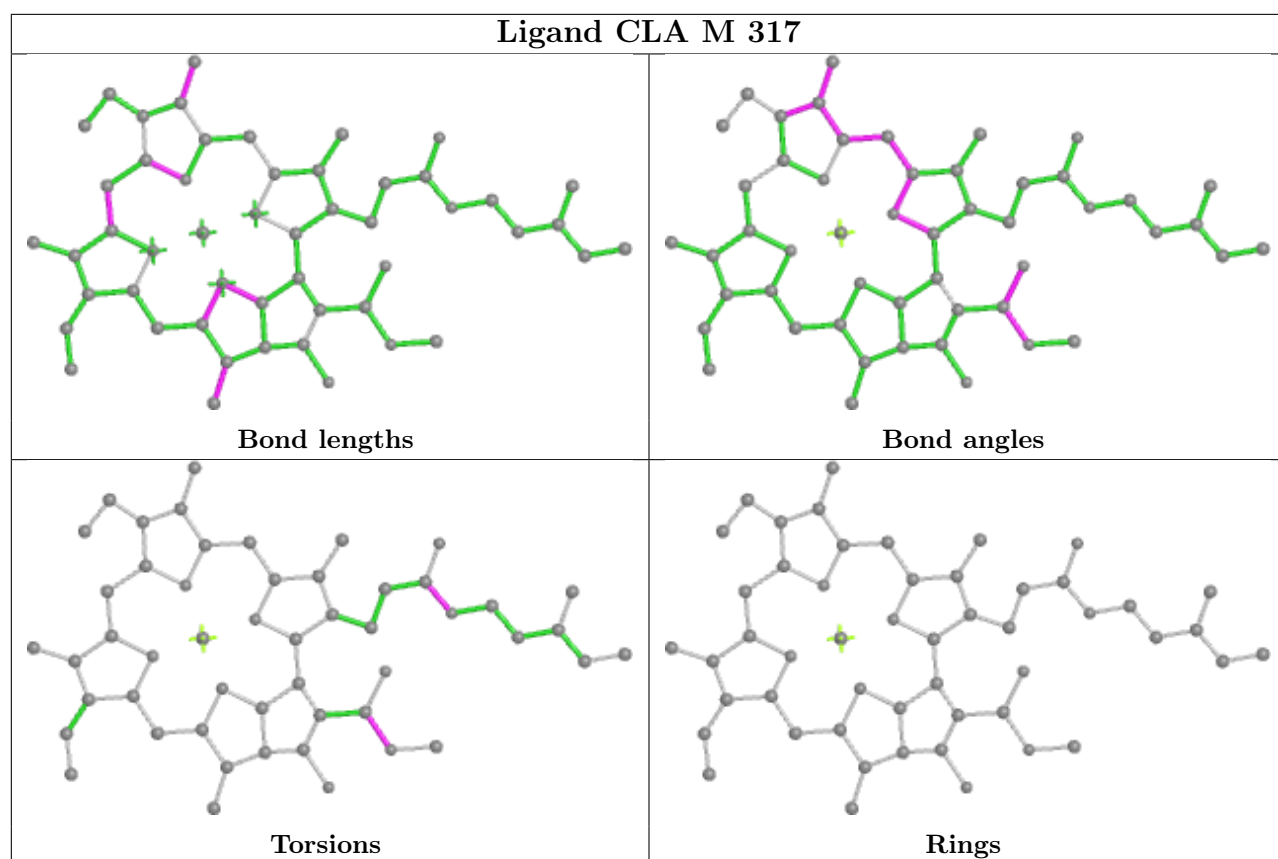
Bond angles

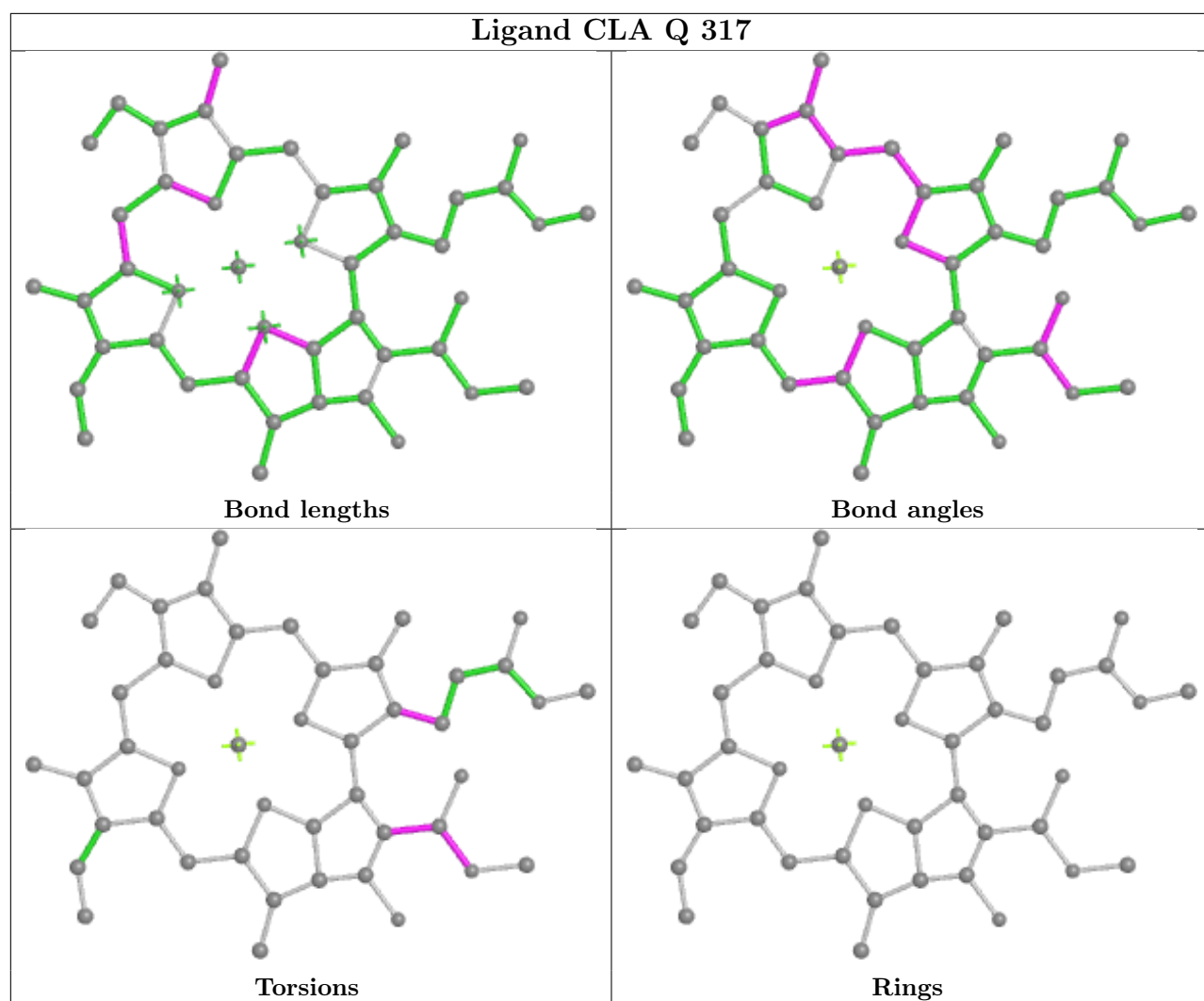


Torsions

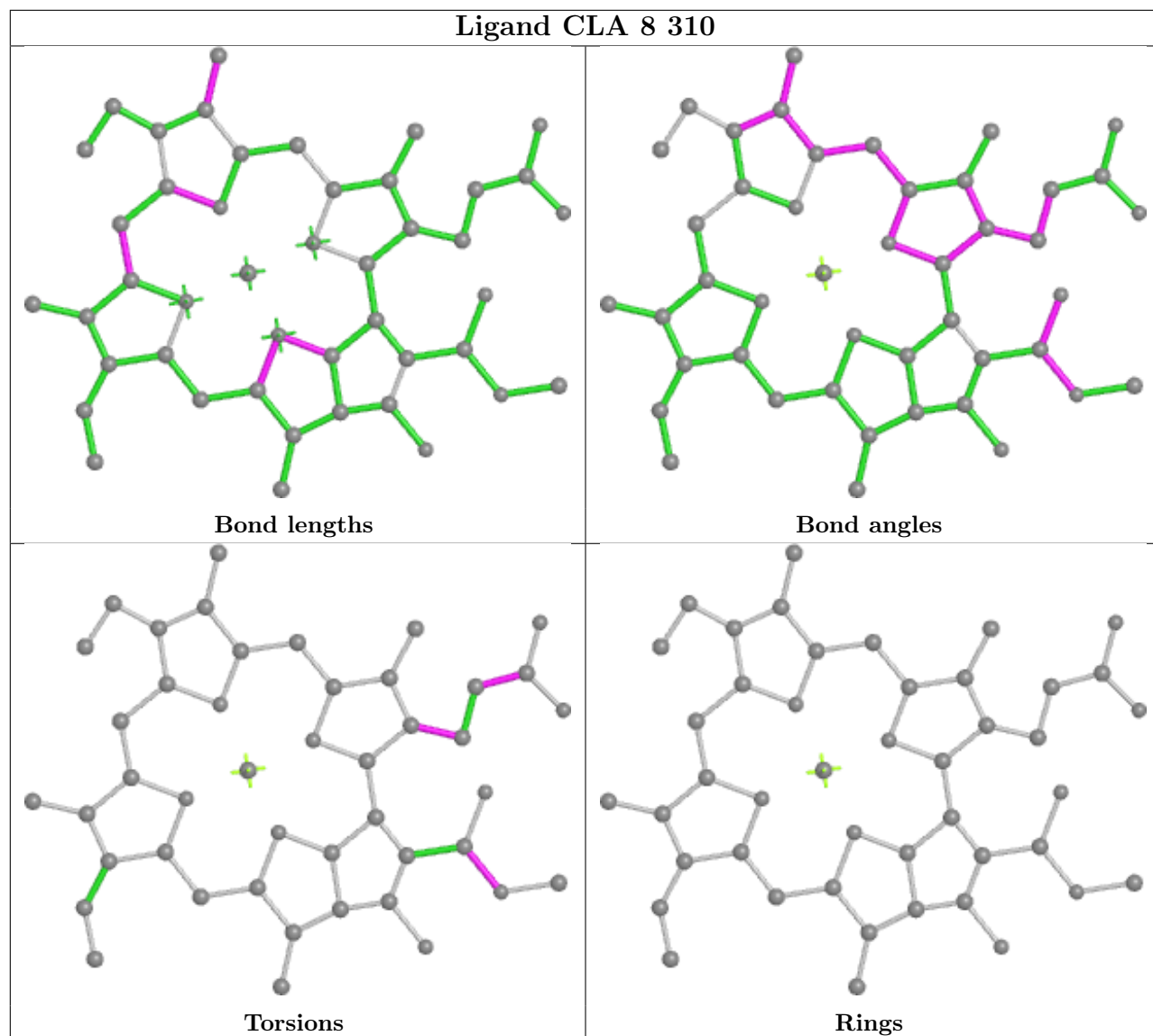


Rings

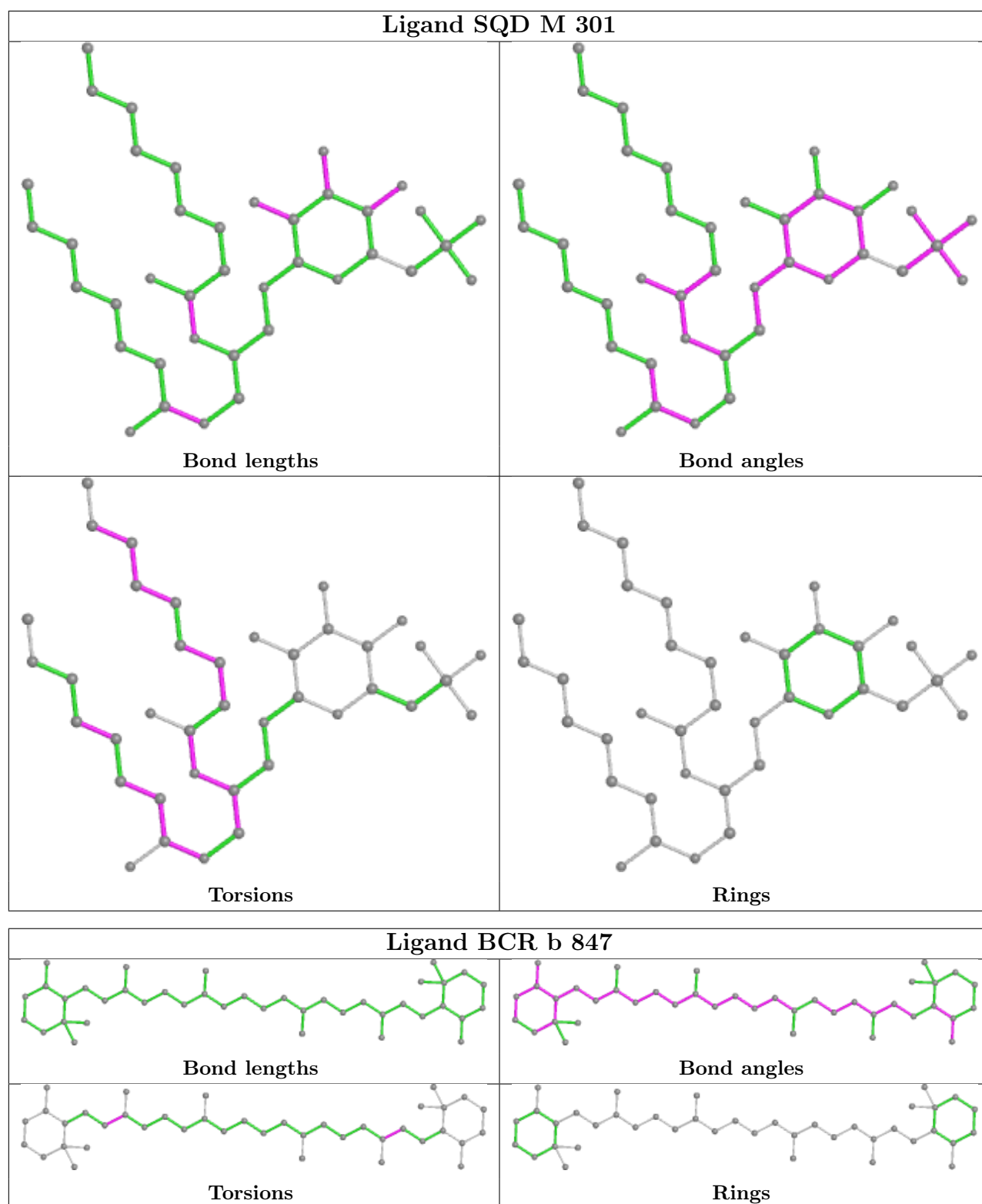




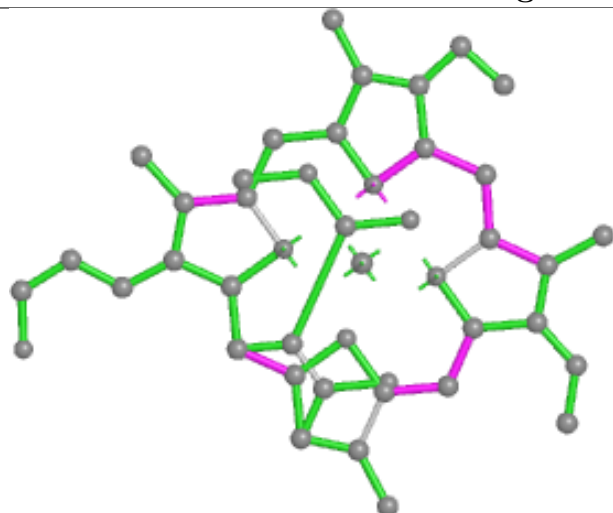
## Ligand CLA 8 310



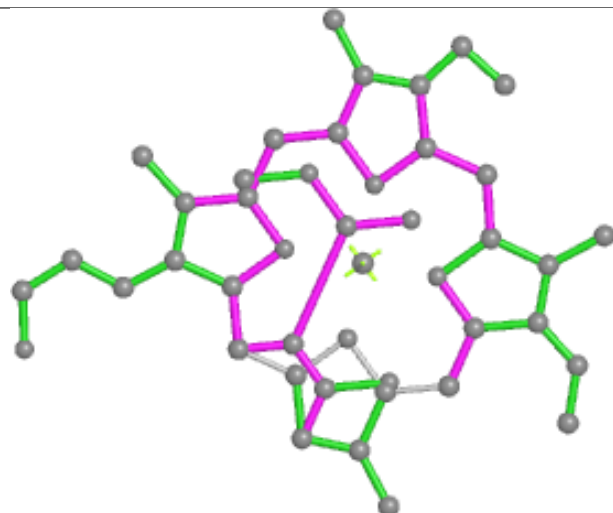




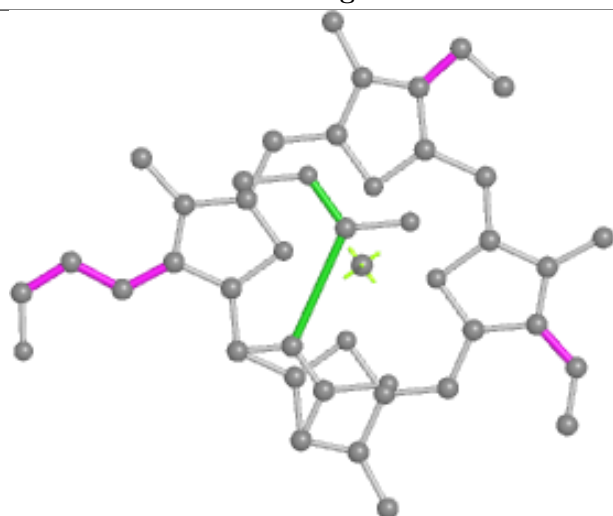
## Ligand KC2 P 310



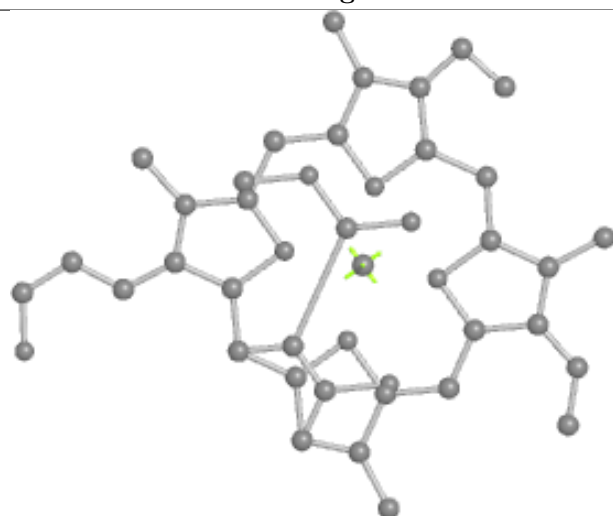
Bond lengths



Bond angles

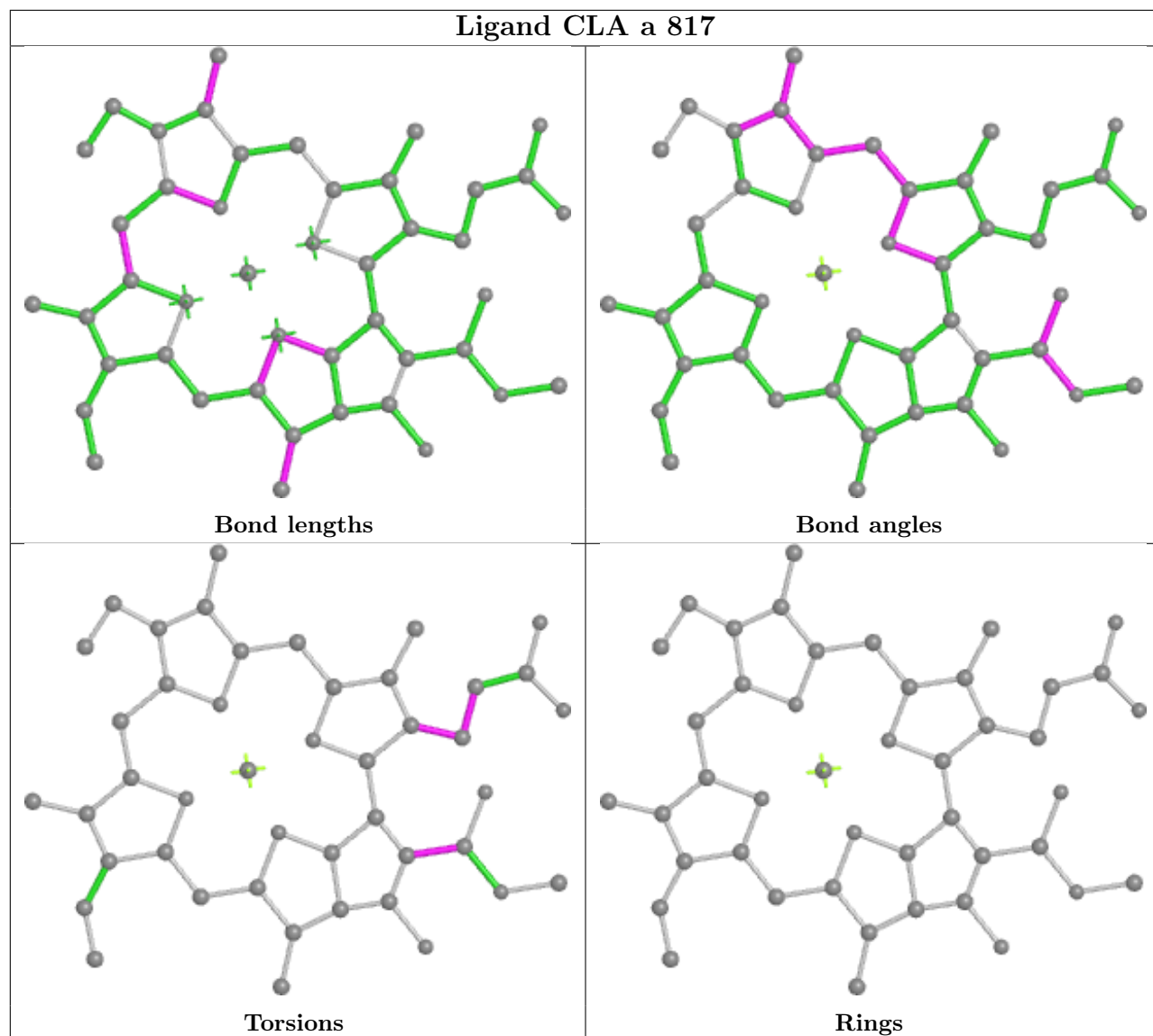


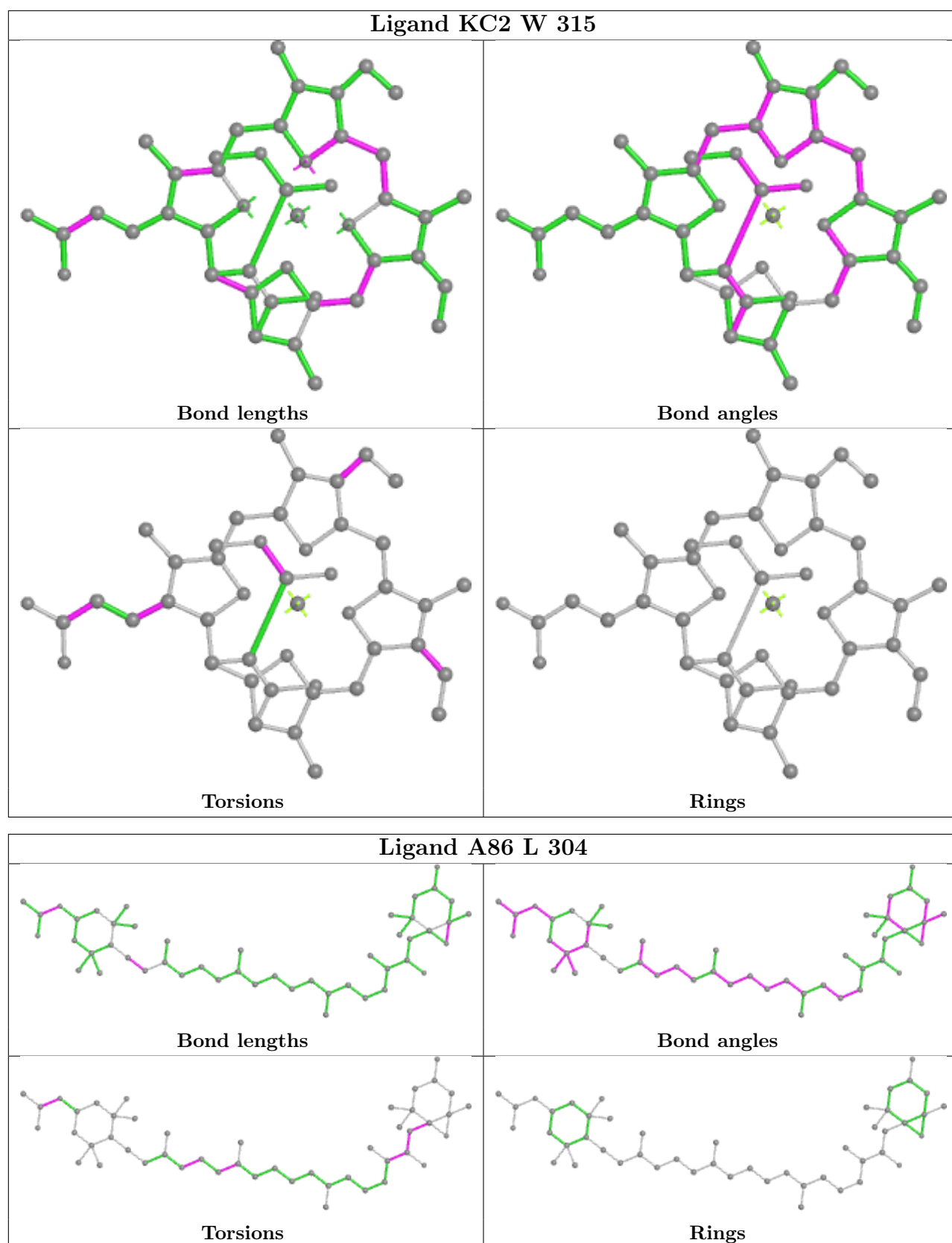
Torsions



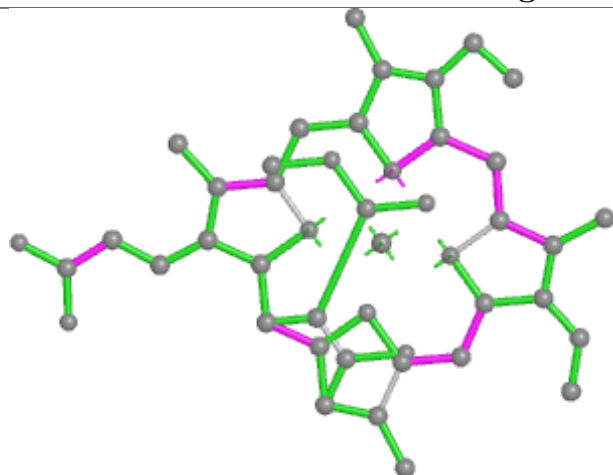
Rings

## Ligand CLA a 817

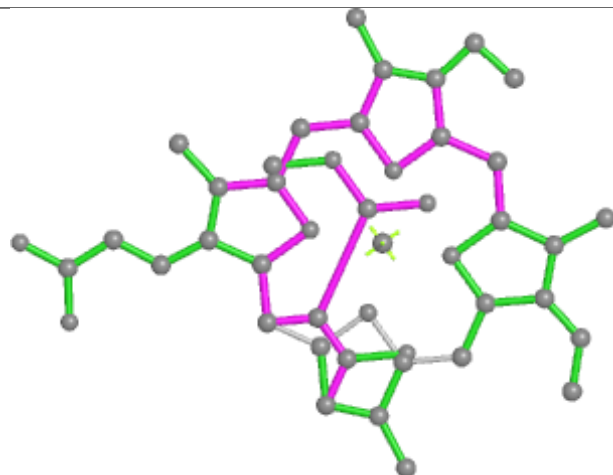




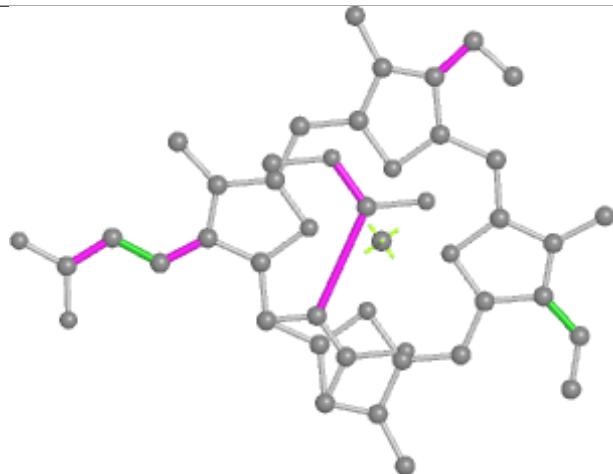
## Ligand KC2 L 315



Bond lengths



Bond angles

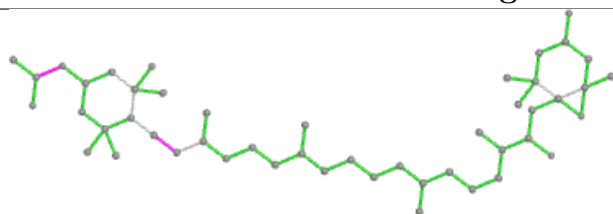


Torsions

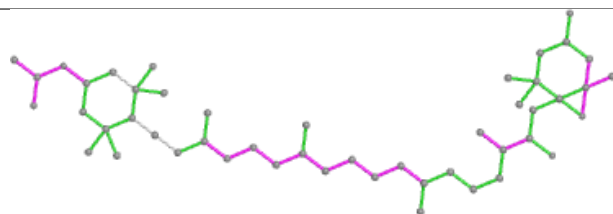


Rings

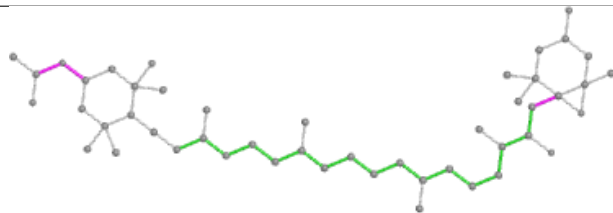
## Ligand A1EB1 6 306



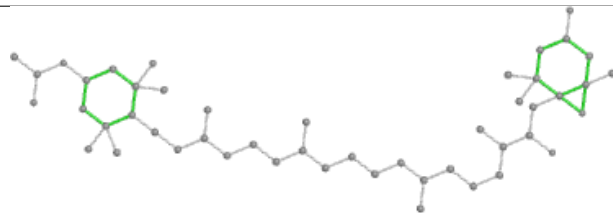
Bond lengths



Bond angles

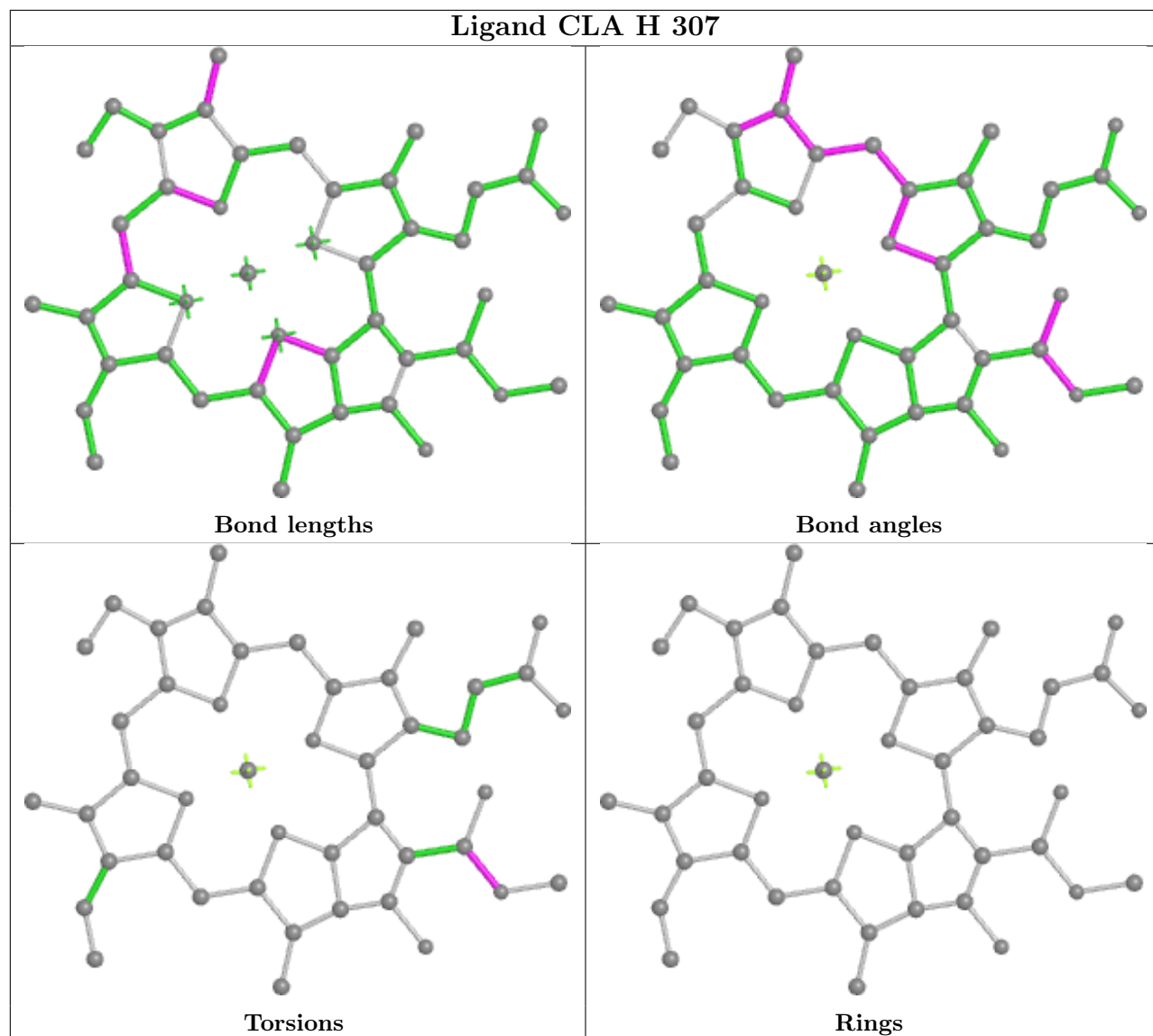


Torsions

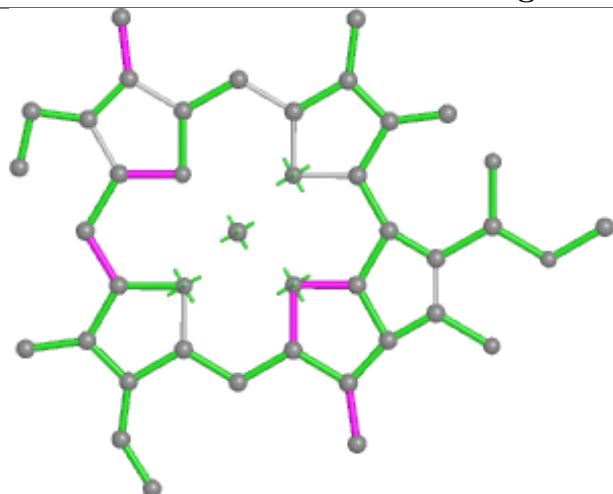


Rings

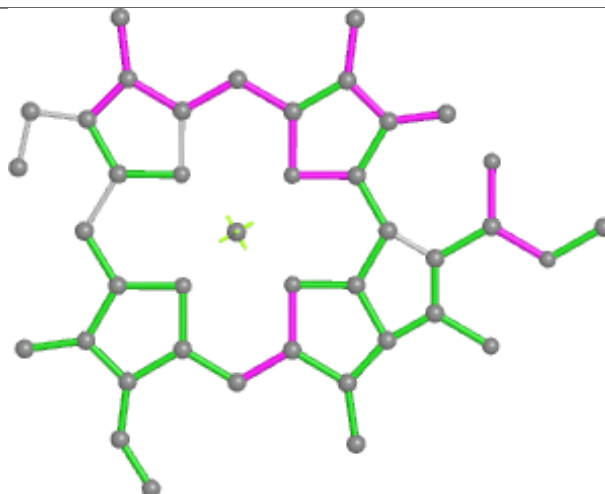
## Ligand CLA H 307



## Ligand CLA x 307



Bond lengths



Bond angles

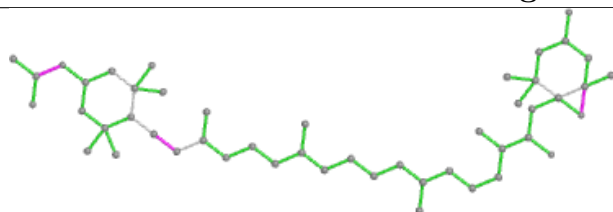


Torsions

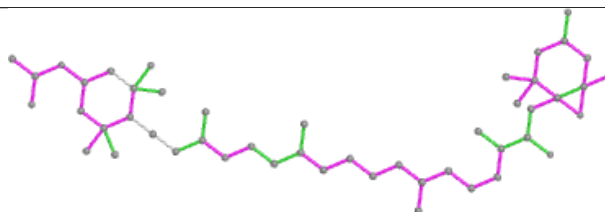


Rings

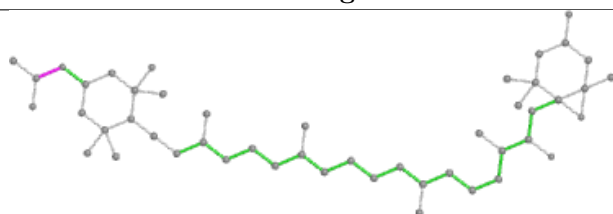
## Ligand A86 O 302



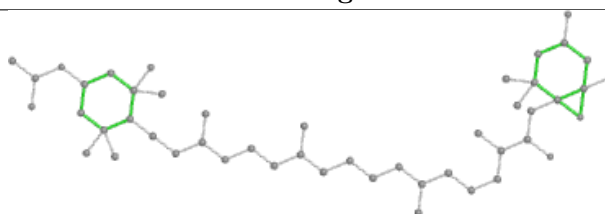
Bond lengths



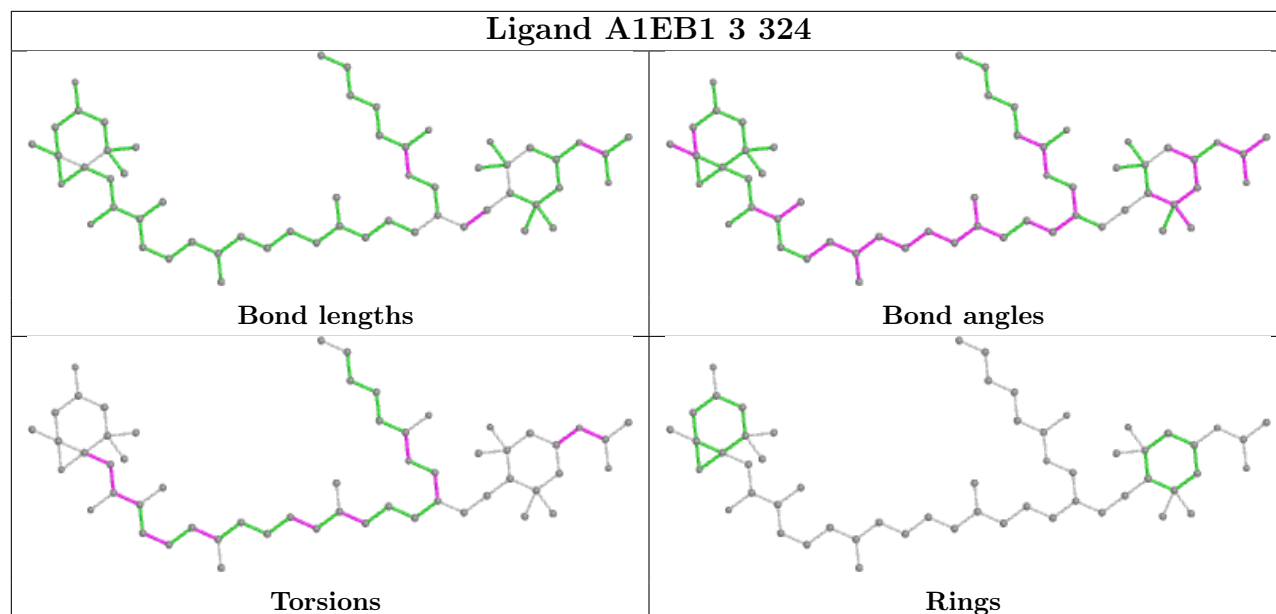
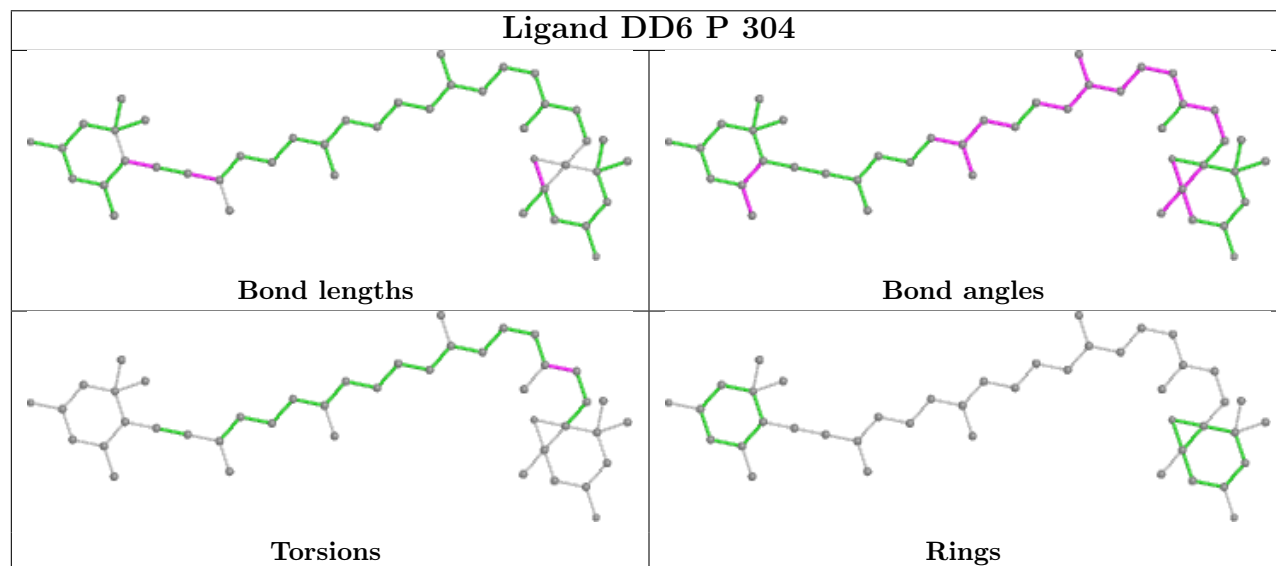
Bond angles



Torsions

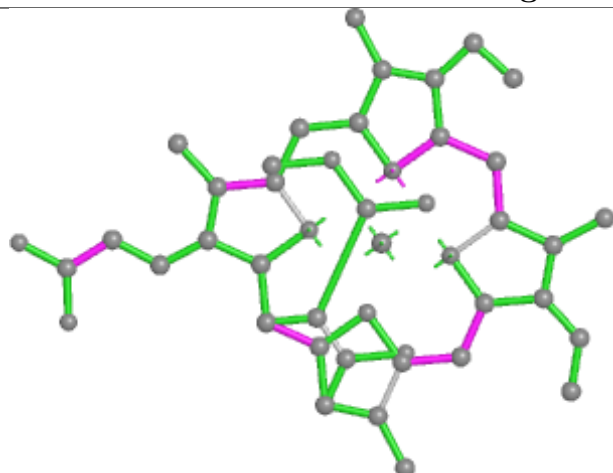


Rings

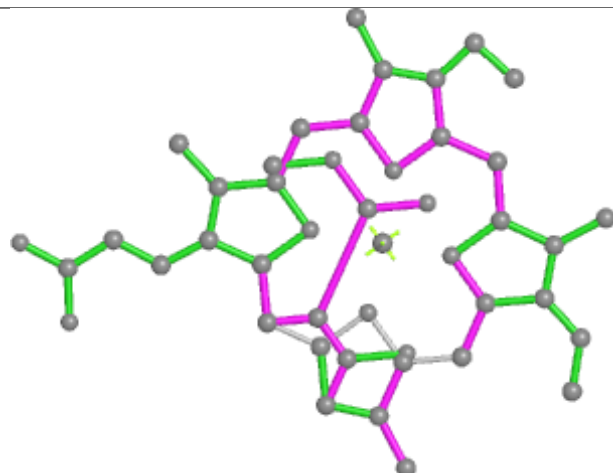
**Ligand A1EB1 3 324****Ligand DD6 P 304**



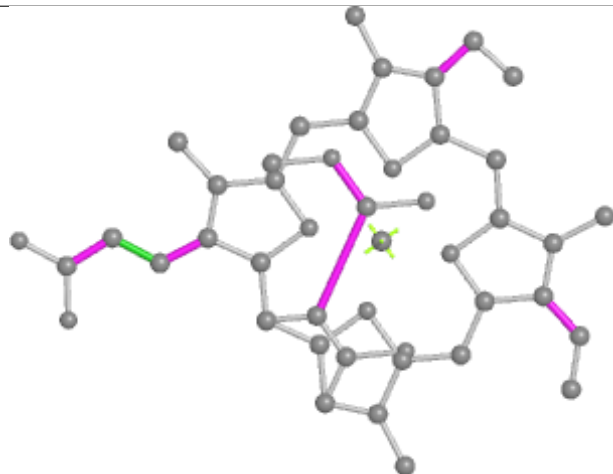
## Ligand KC2 8 314



Bond lengths



Bond angles

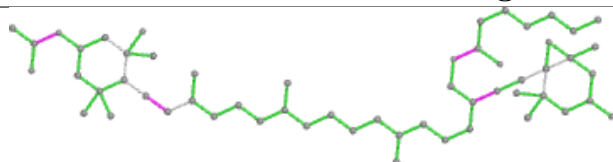


Torsions

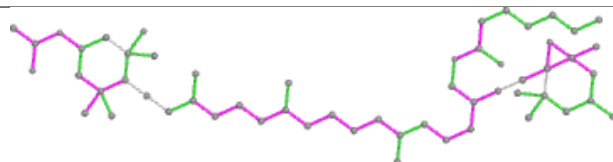


Rings

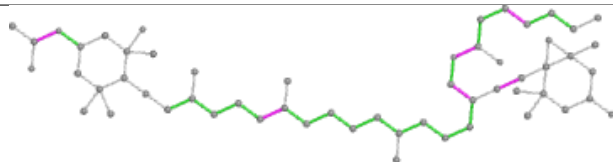
## Ligand A1EB4 P 305



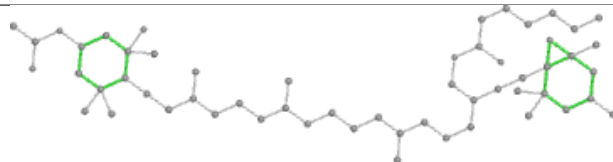
Bond lengths



Bond angles

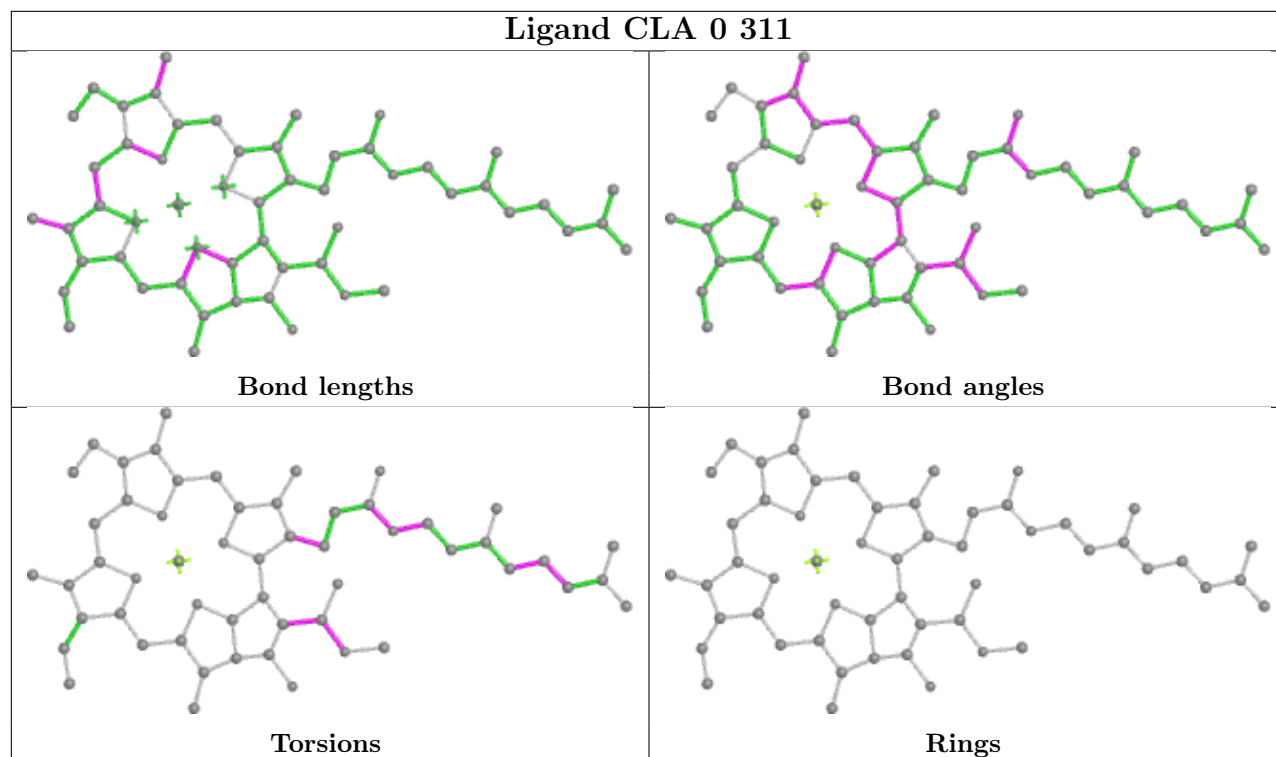


Torsions

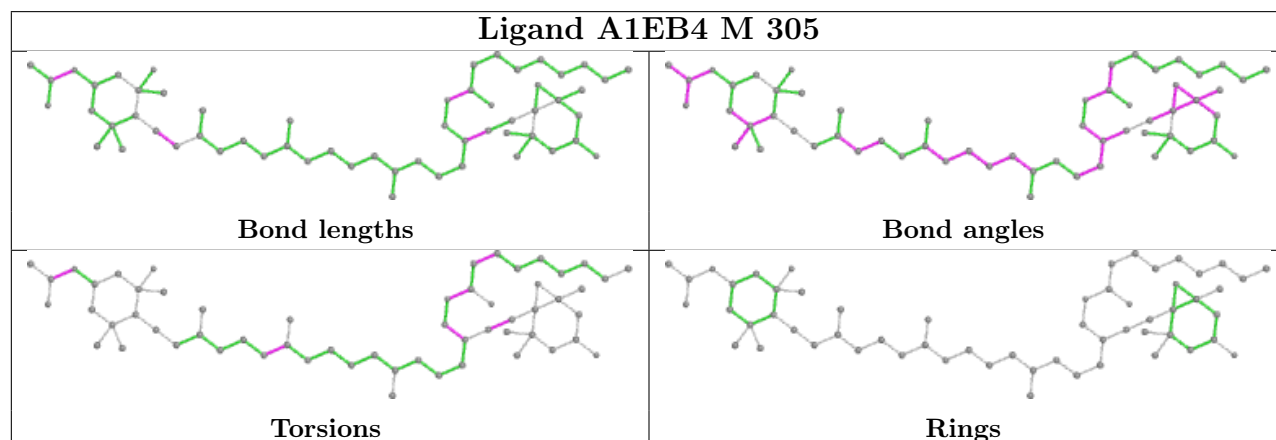


Rings

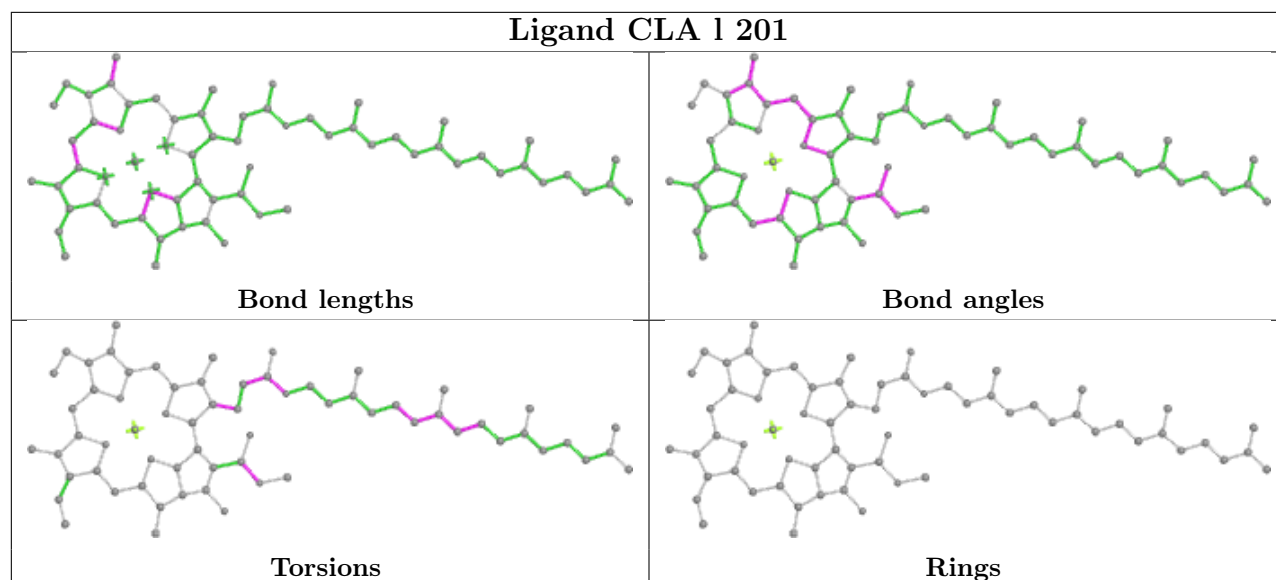
## Ligand CLA 0 311



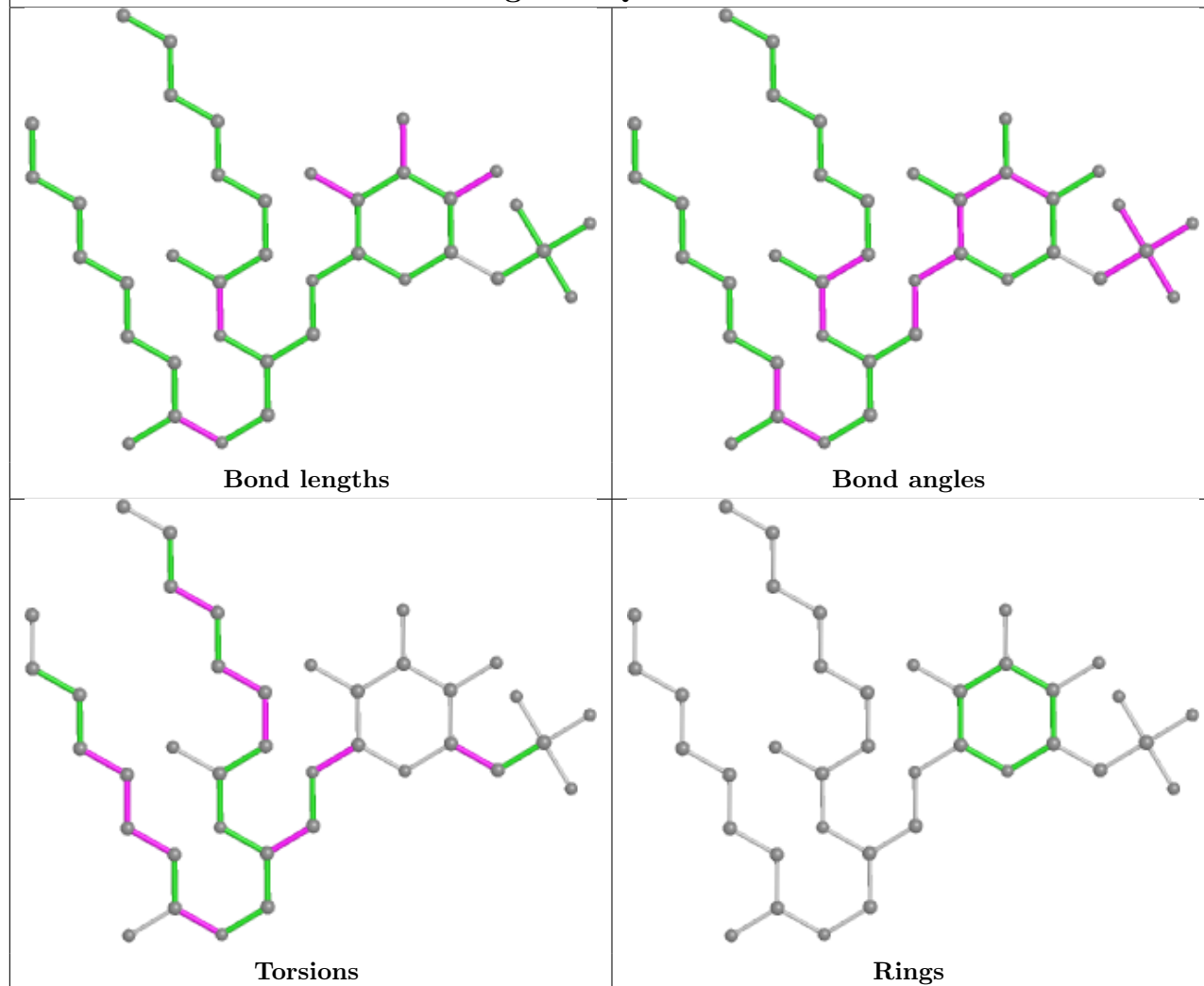
## Ligand A1EB4 M 305



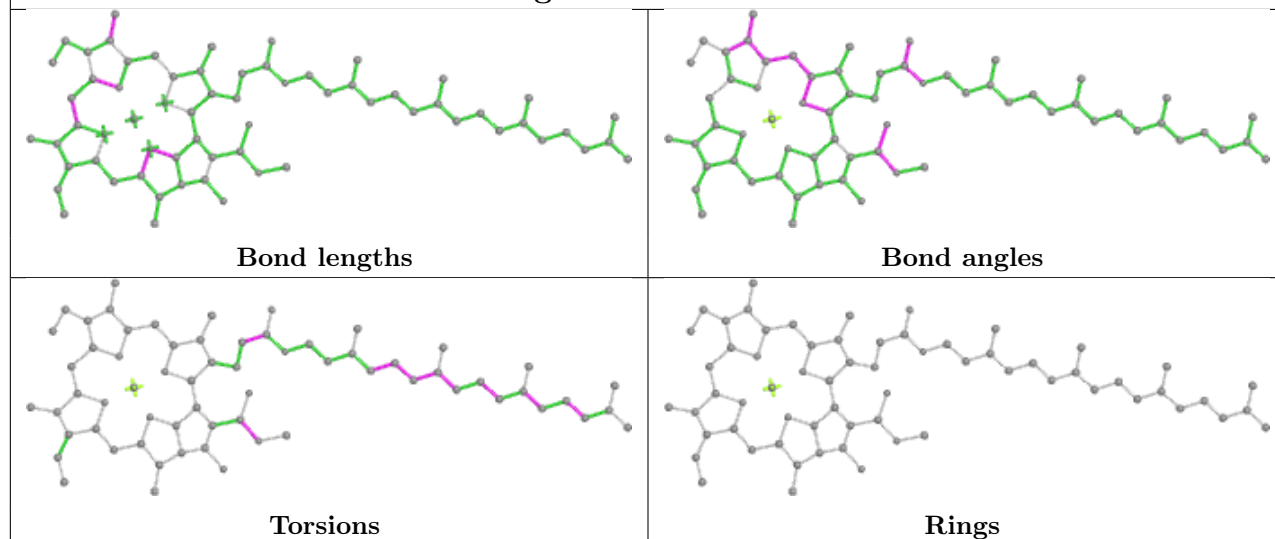
## Ligand CLA 1 201



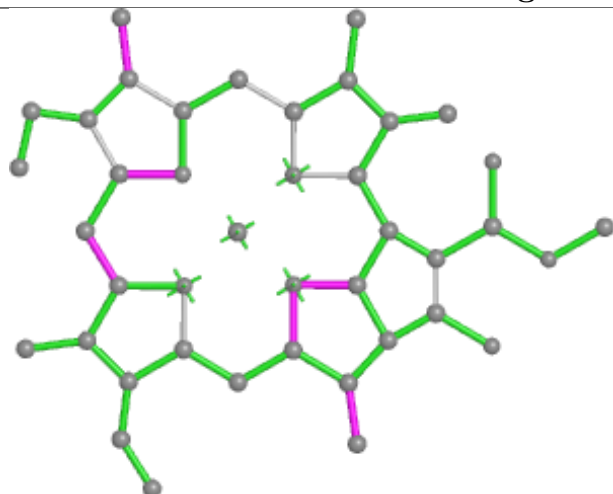
## Ligand SQD k 205



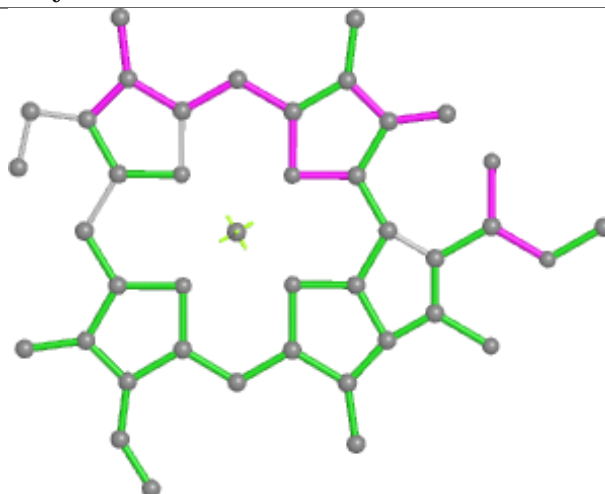
## Ligand CLA b 810



## Ligand CLA y 310



Bond lengths



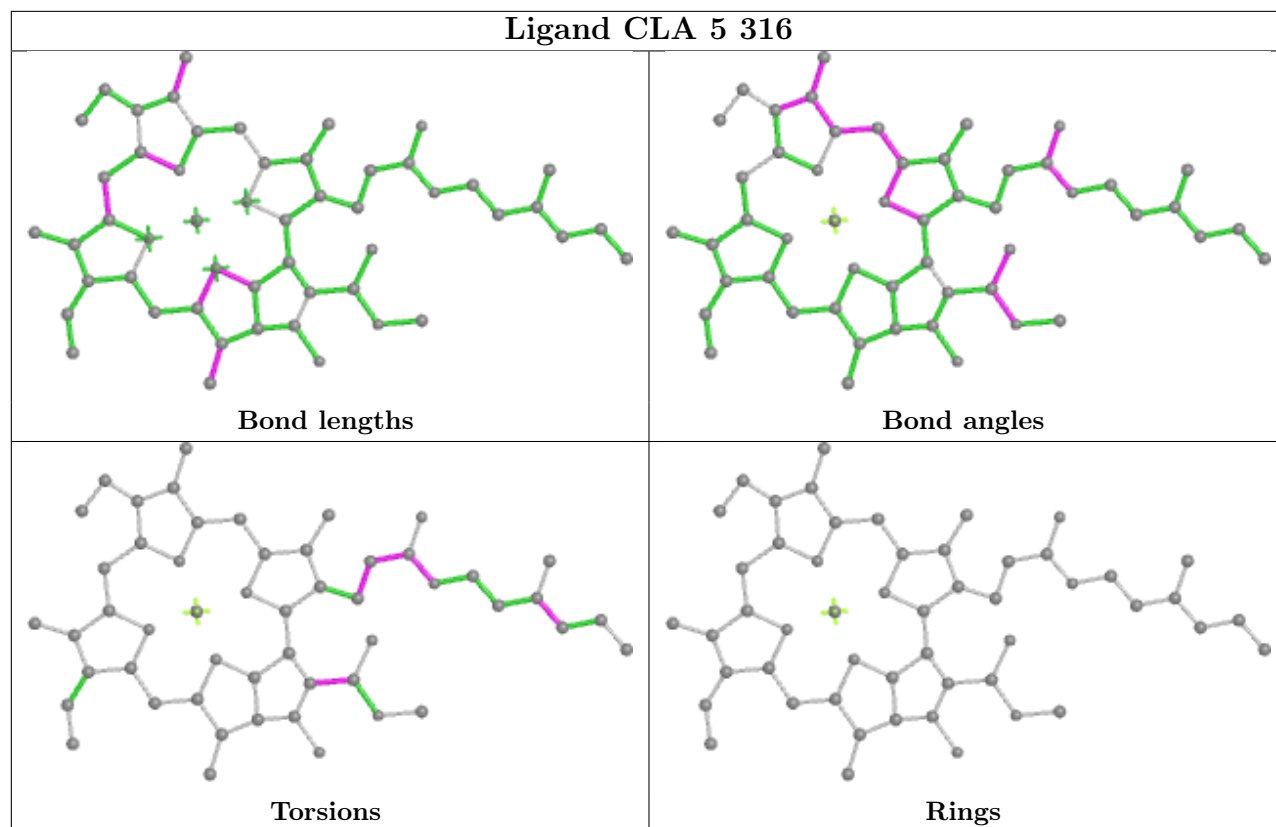
Bond angles



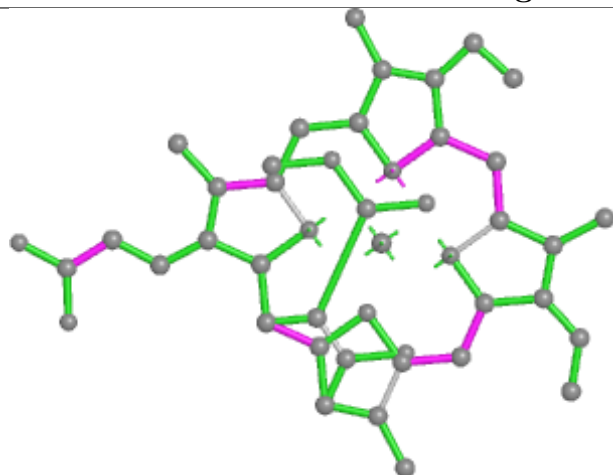
Torsions



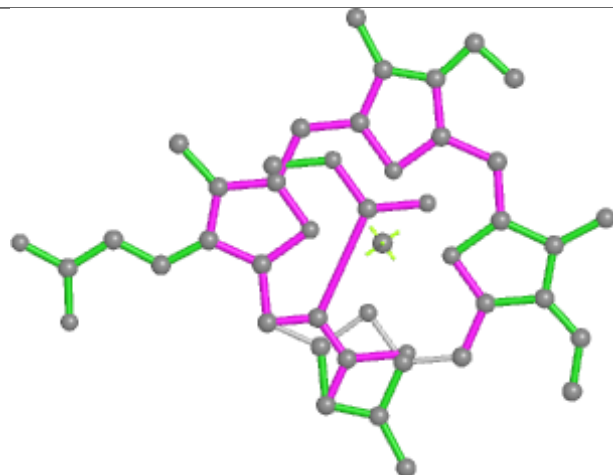
Rings



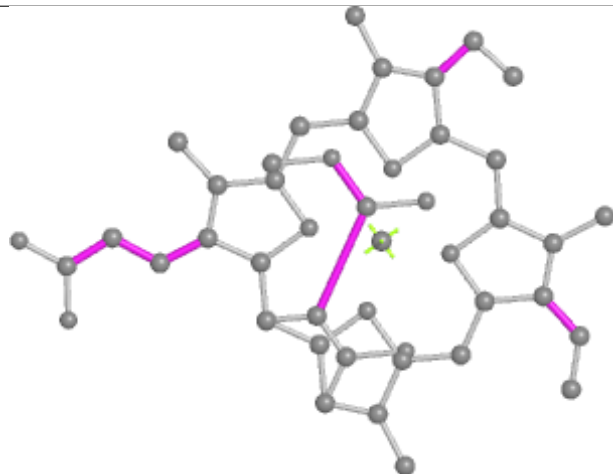
## Ligand KC2 G 315



Bond lengths



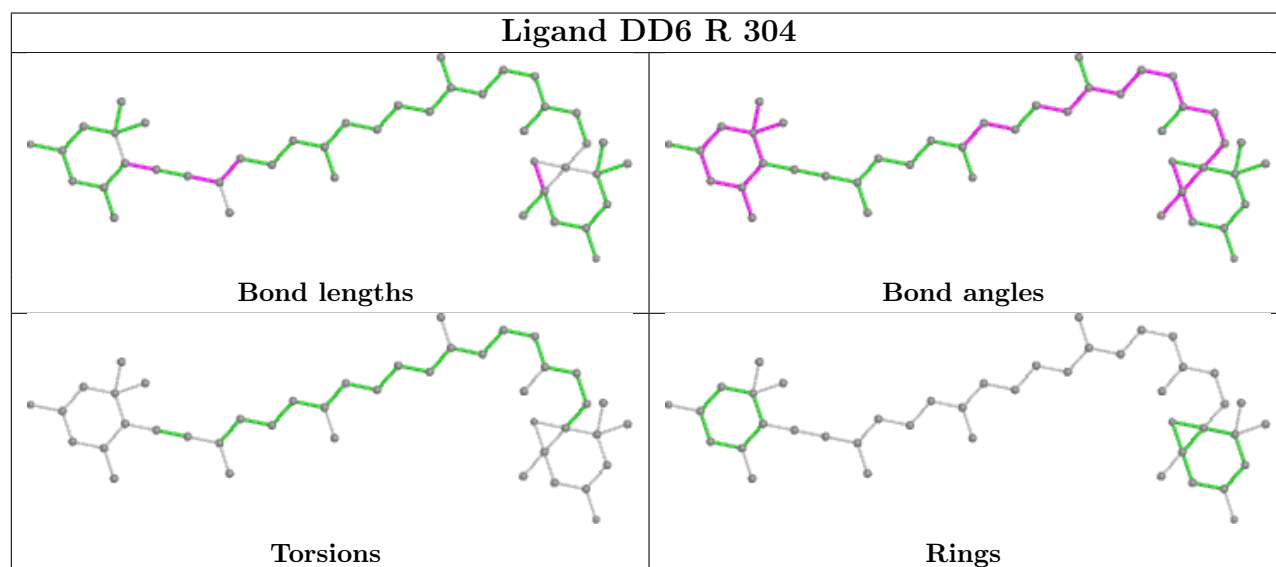
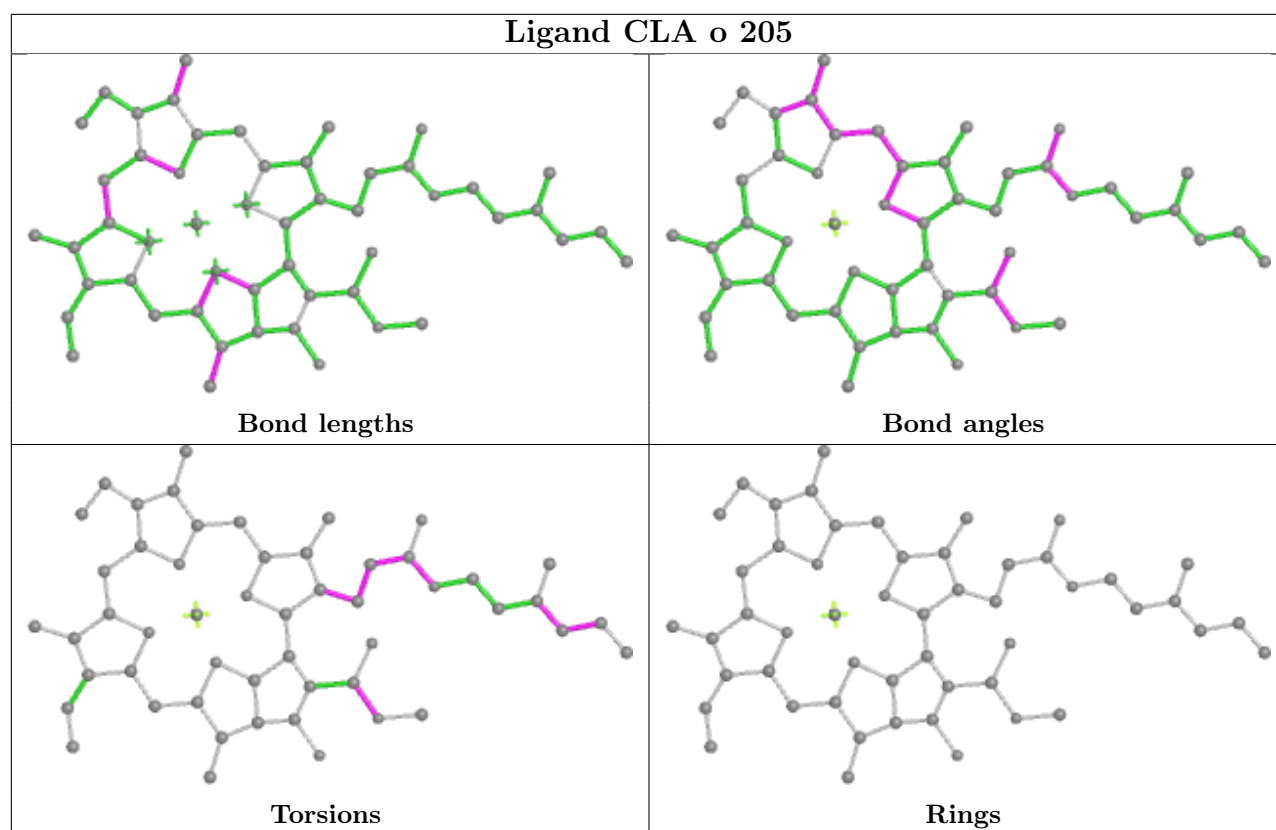
Bond angles

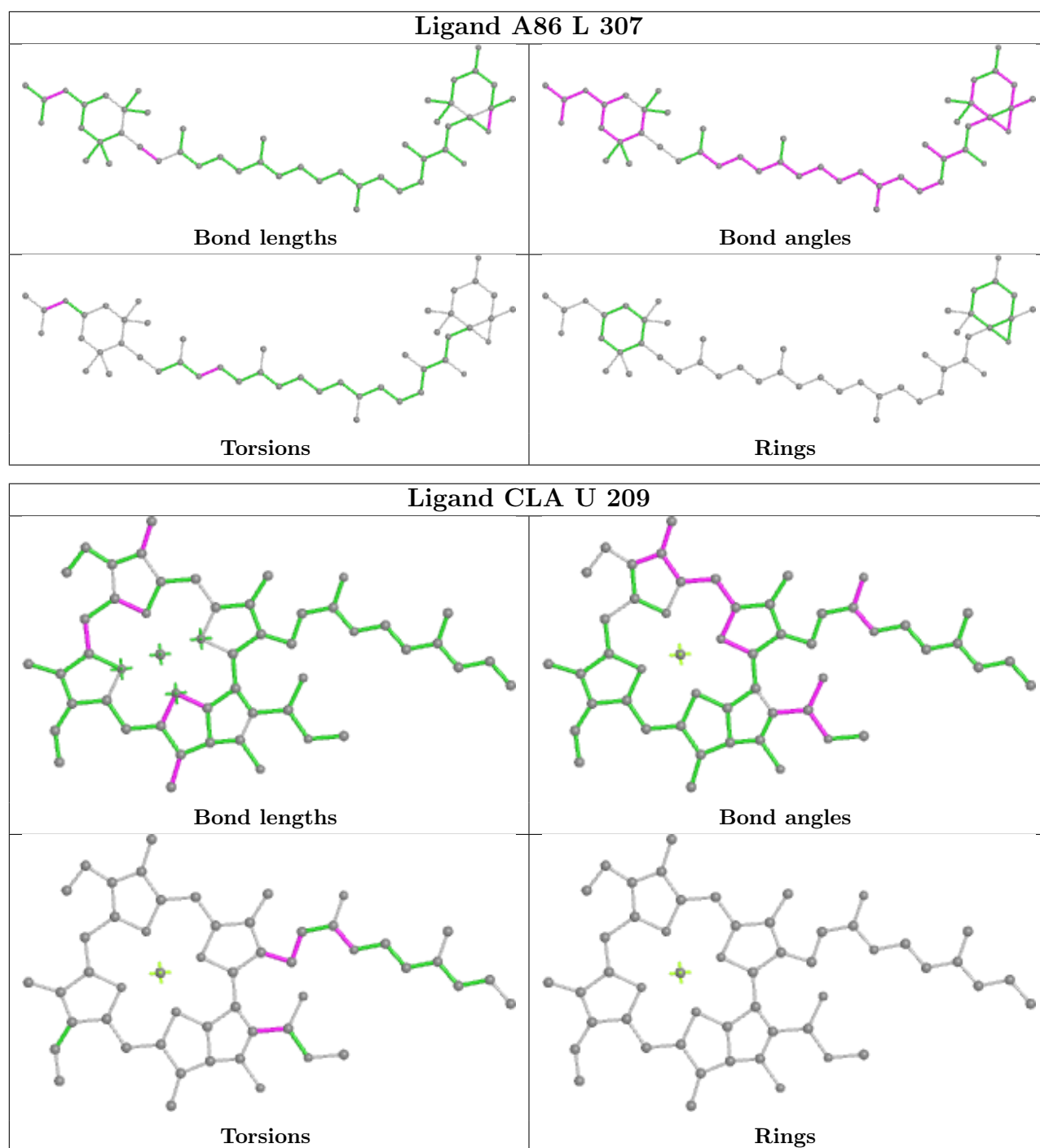


Torsions



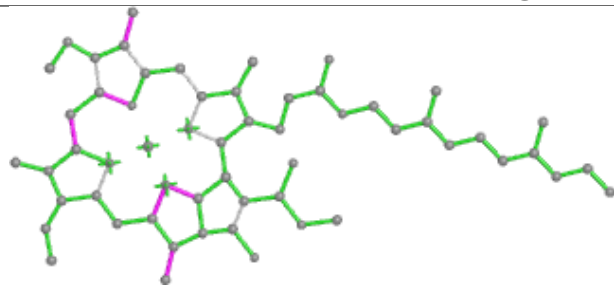
Rings



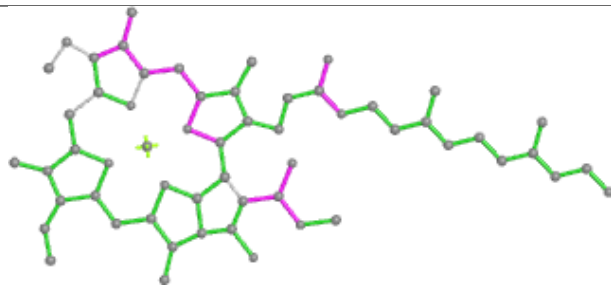




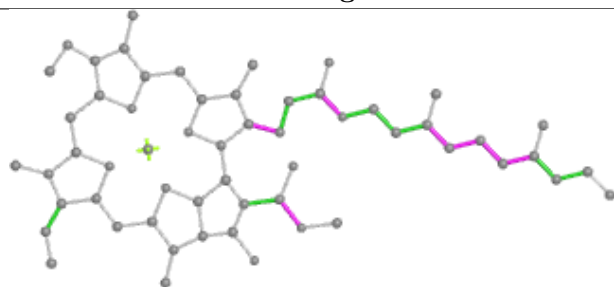
## Ligand CLA F 313



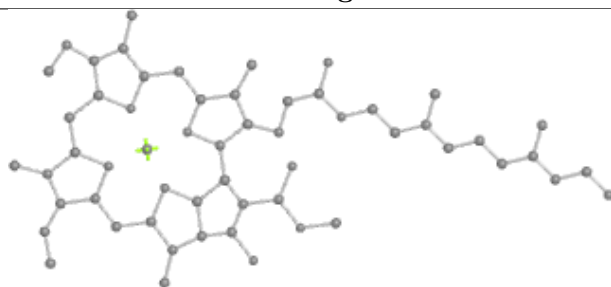
Bond lengths



Bond angles

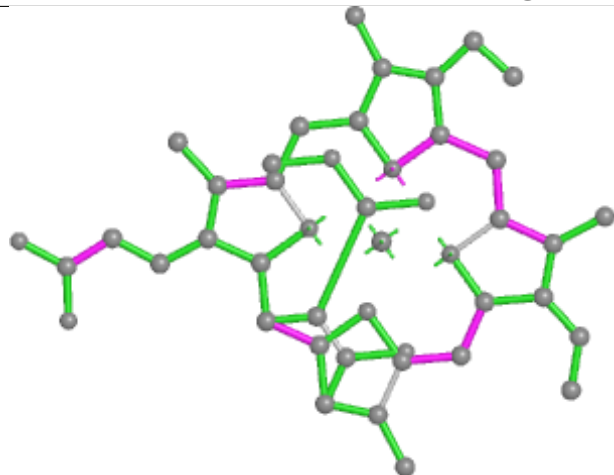


Torsions

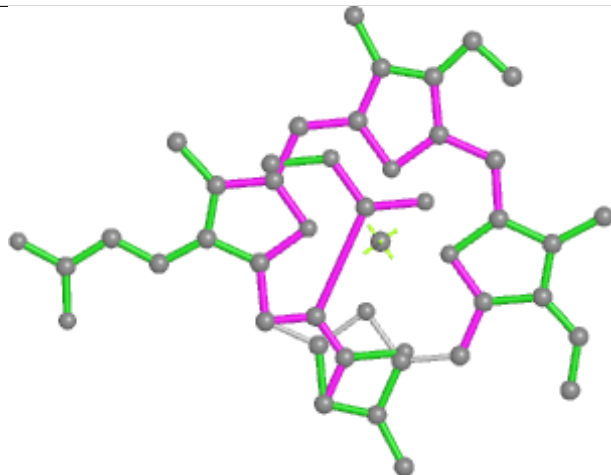


Rings

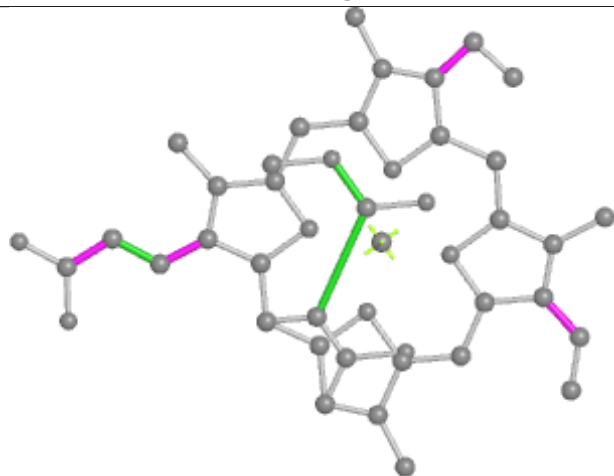
## Ligand KC2 S 317



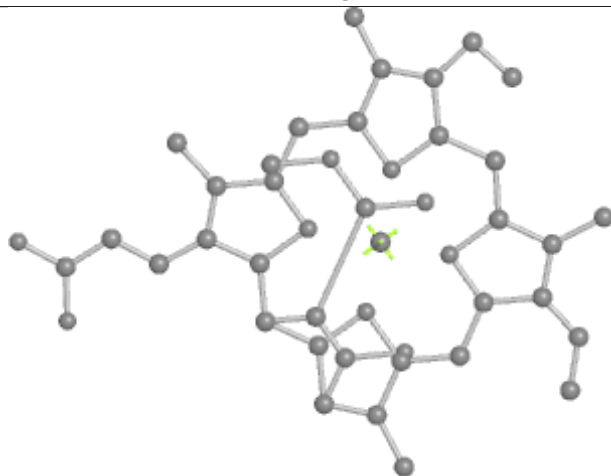
Bond lengths



Bond angles

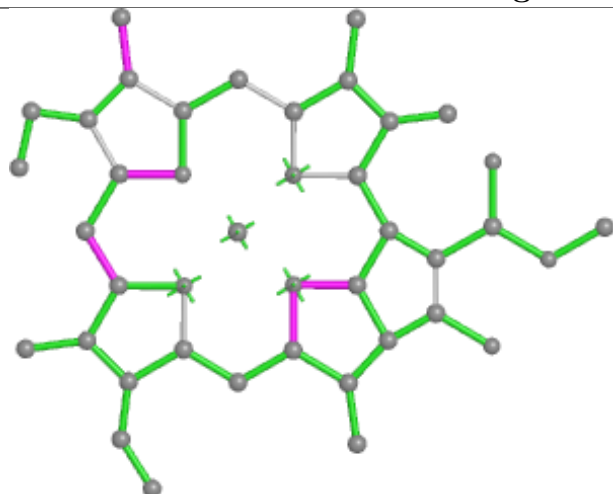


Torsions

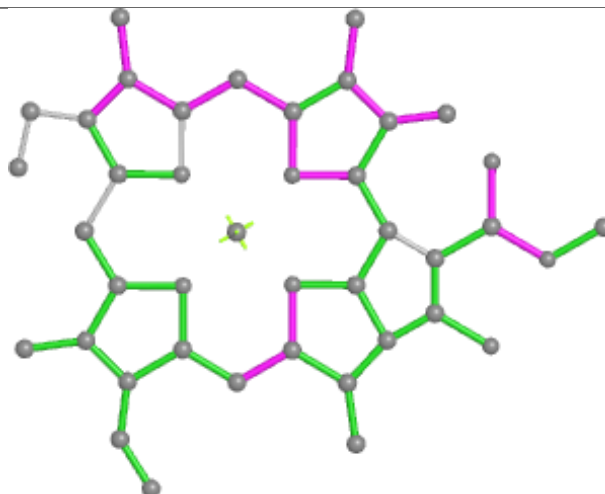


Rings

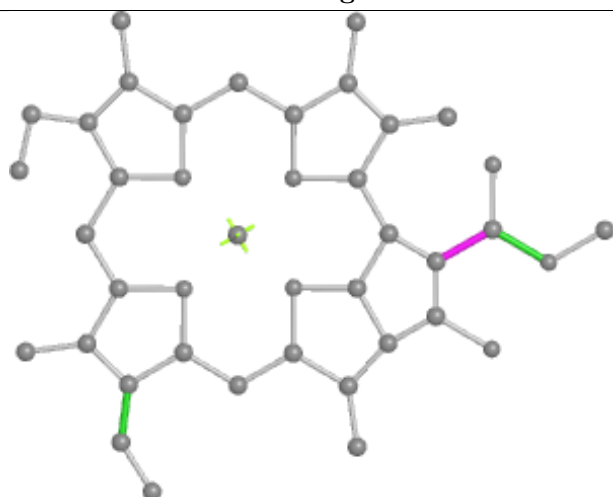
## Ligand CLA K 314



Bond lengths



Bond angles

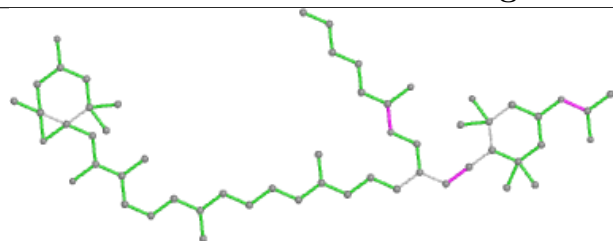


Torsions

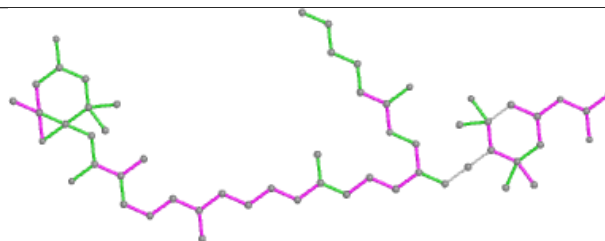


Rings

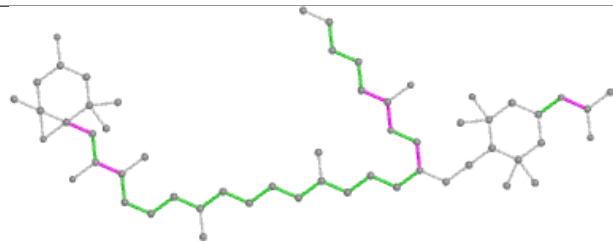
## Ligand A1EB1 4 301



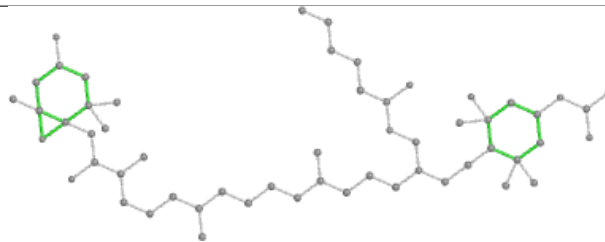
Bond lengths



Bond angles

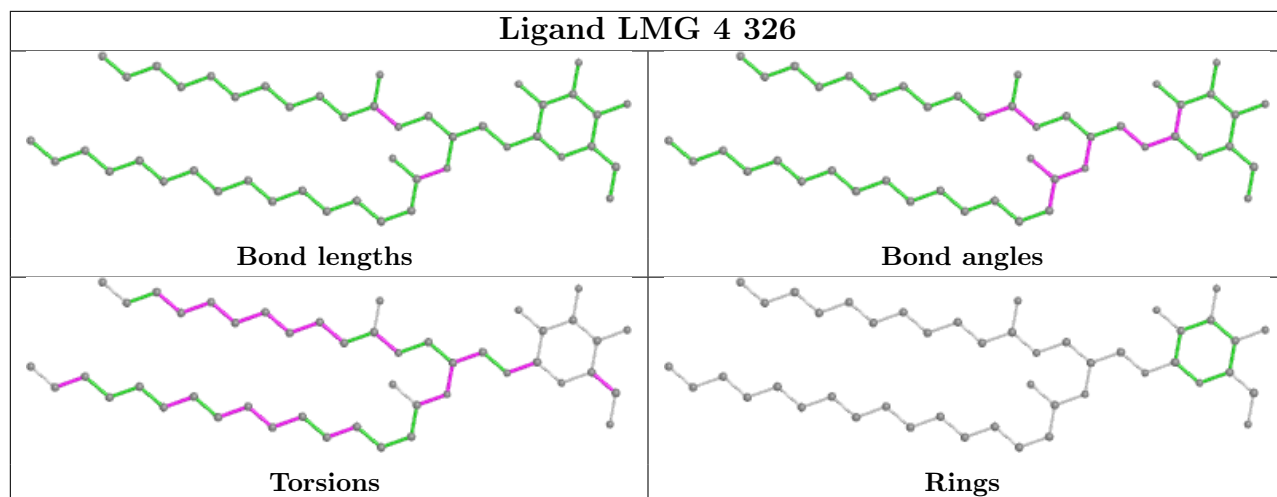


Torsions

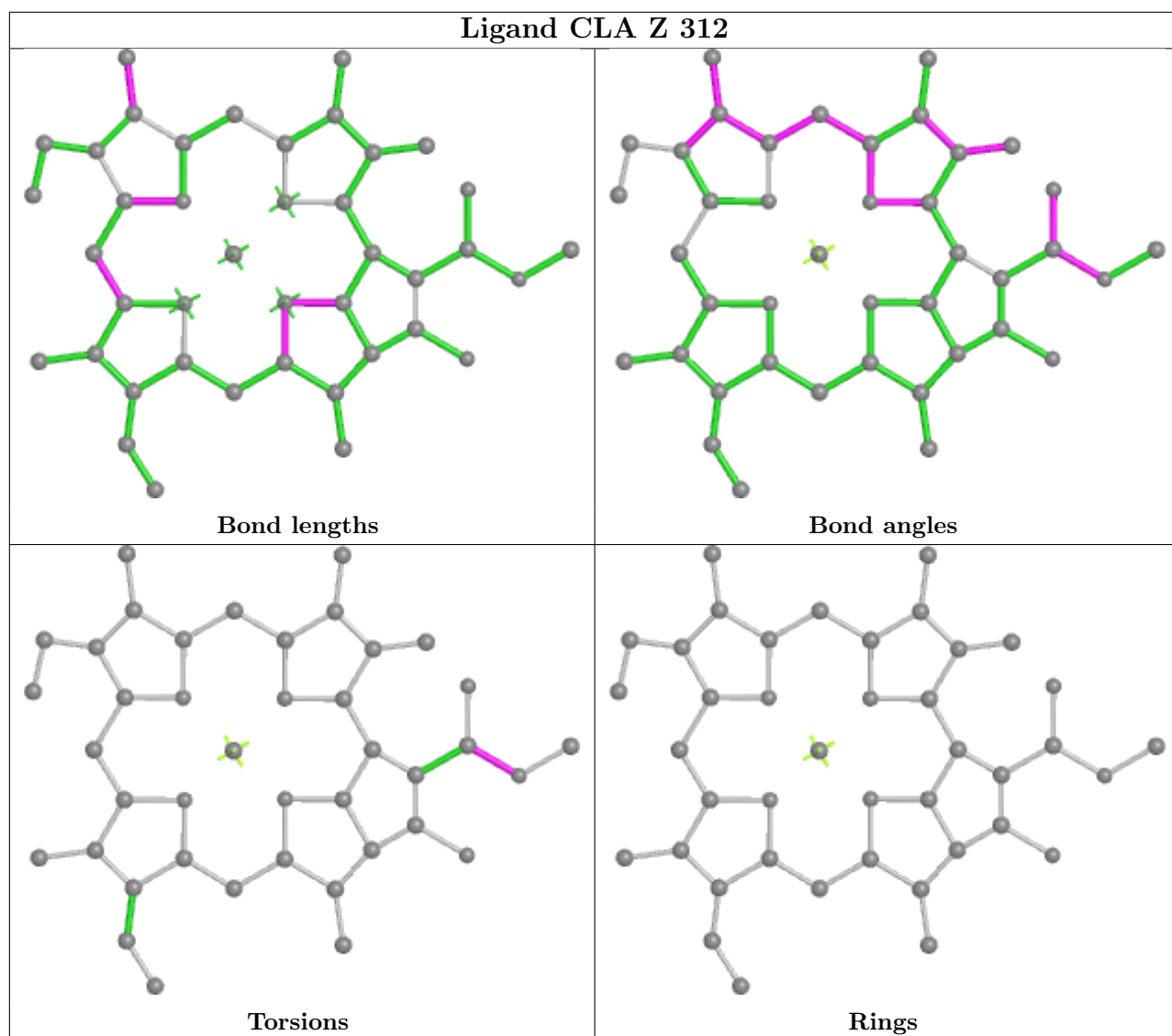


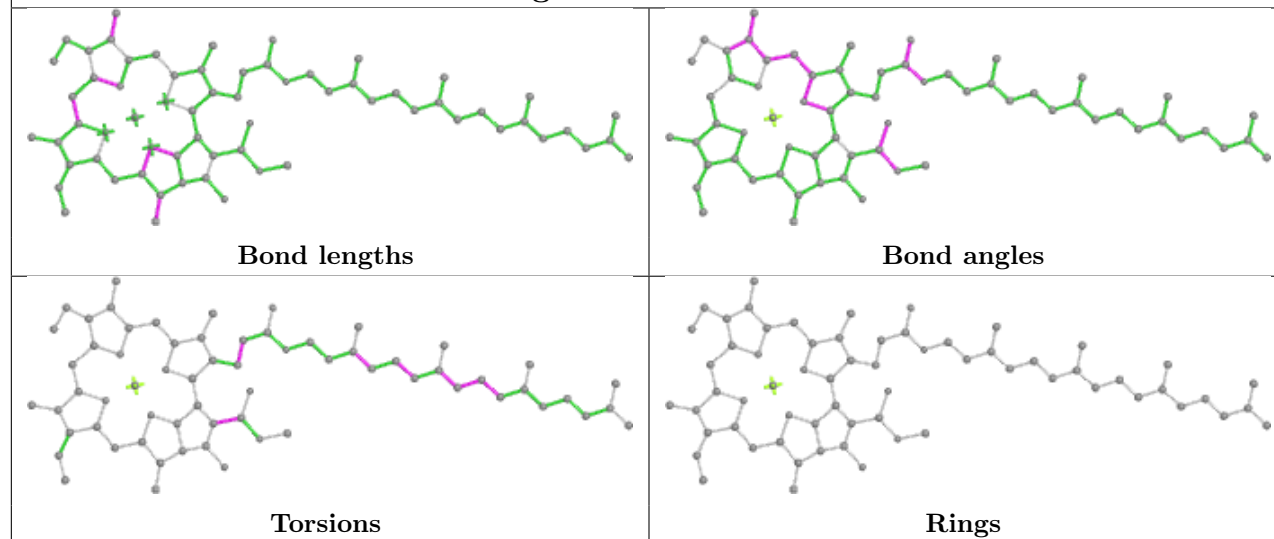
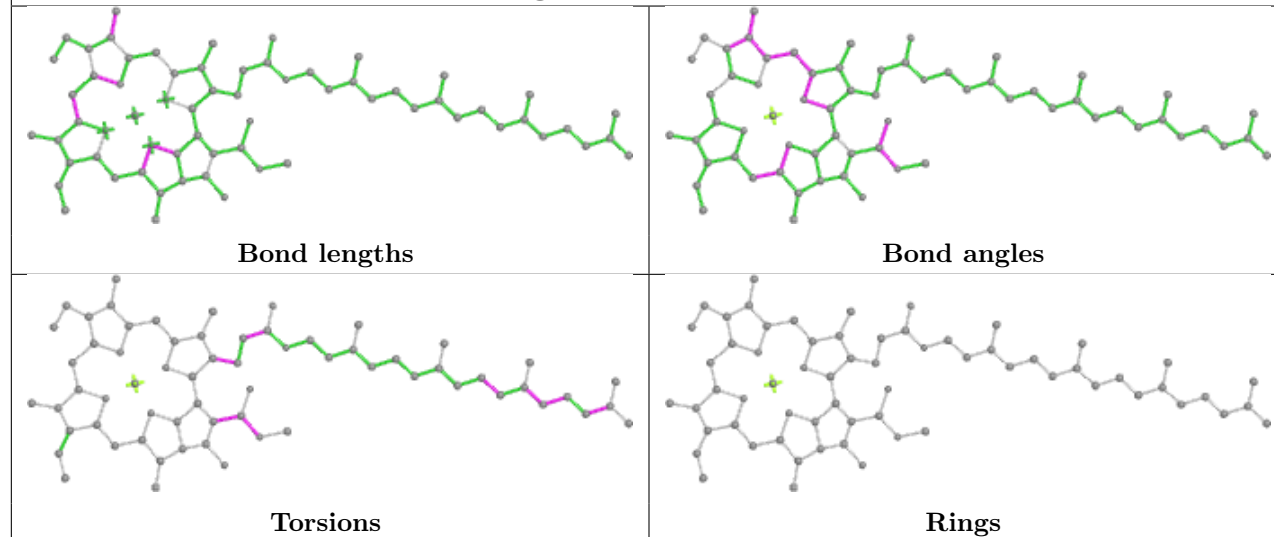
Rings

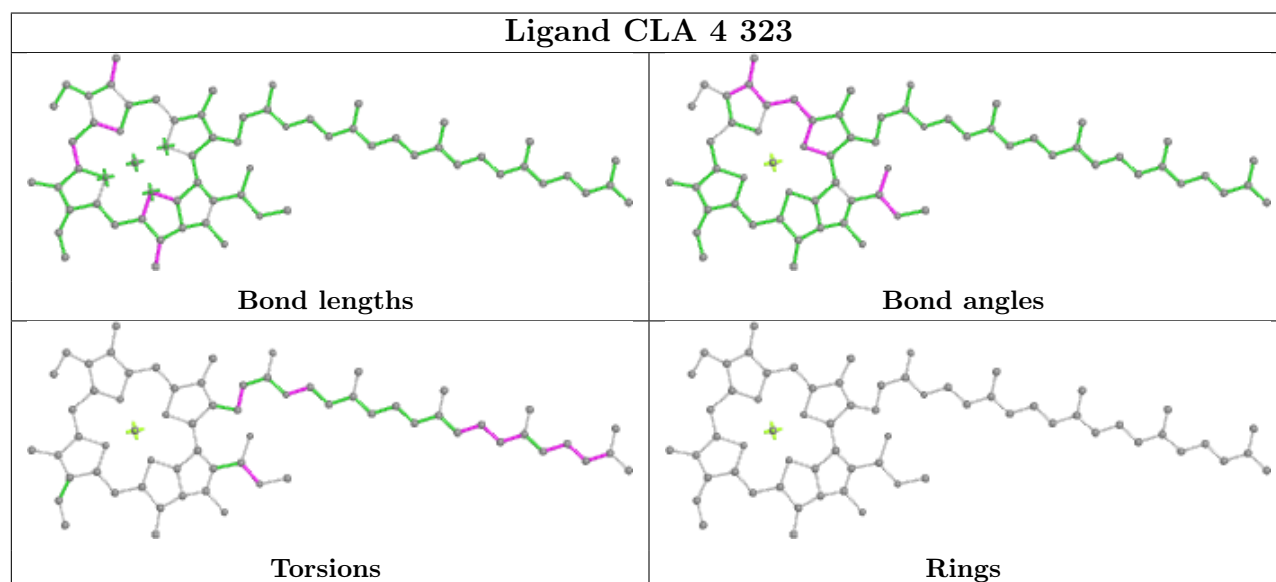
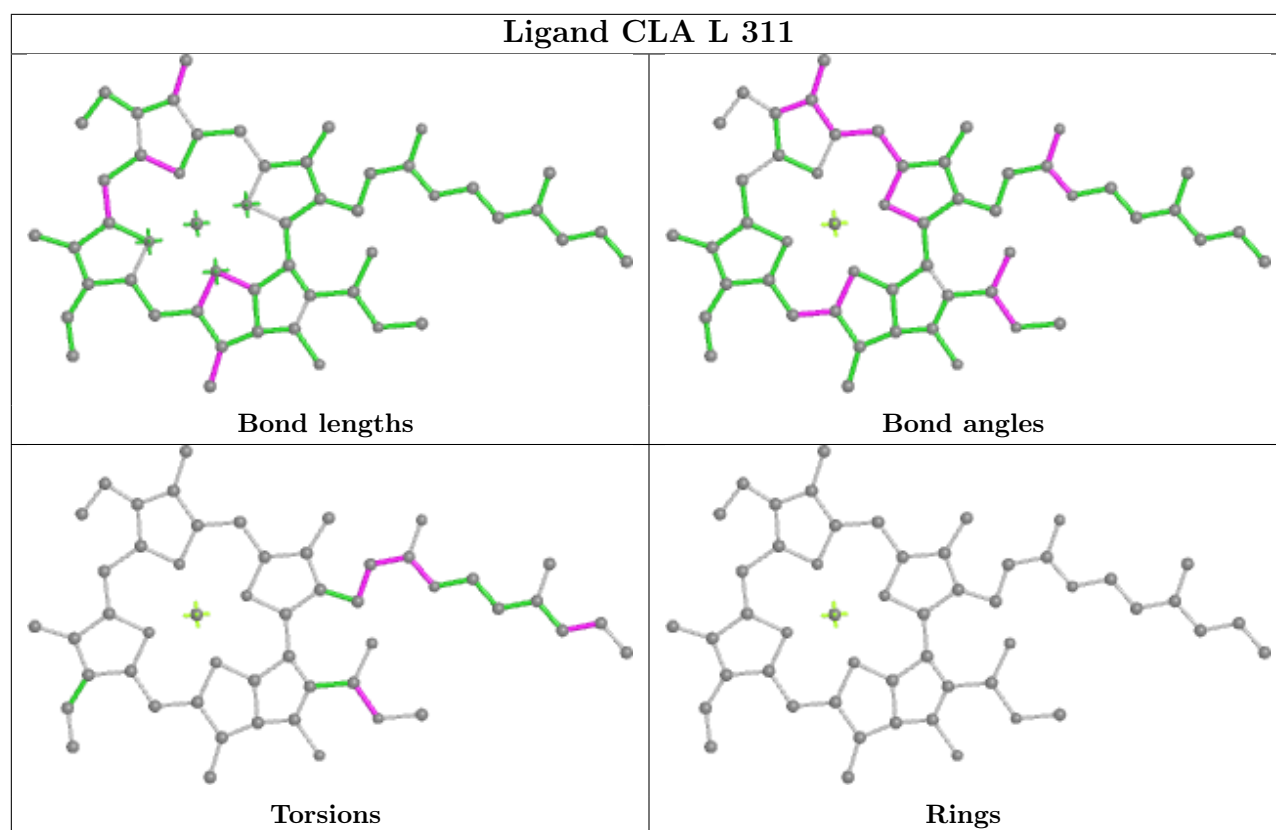
## Ligand LMG 4 326

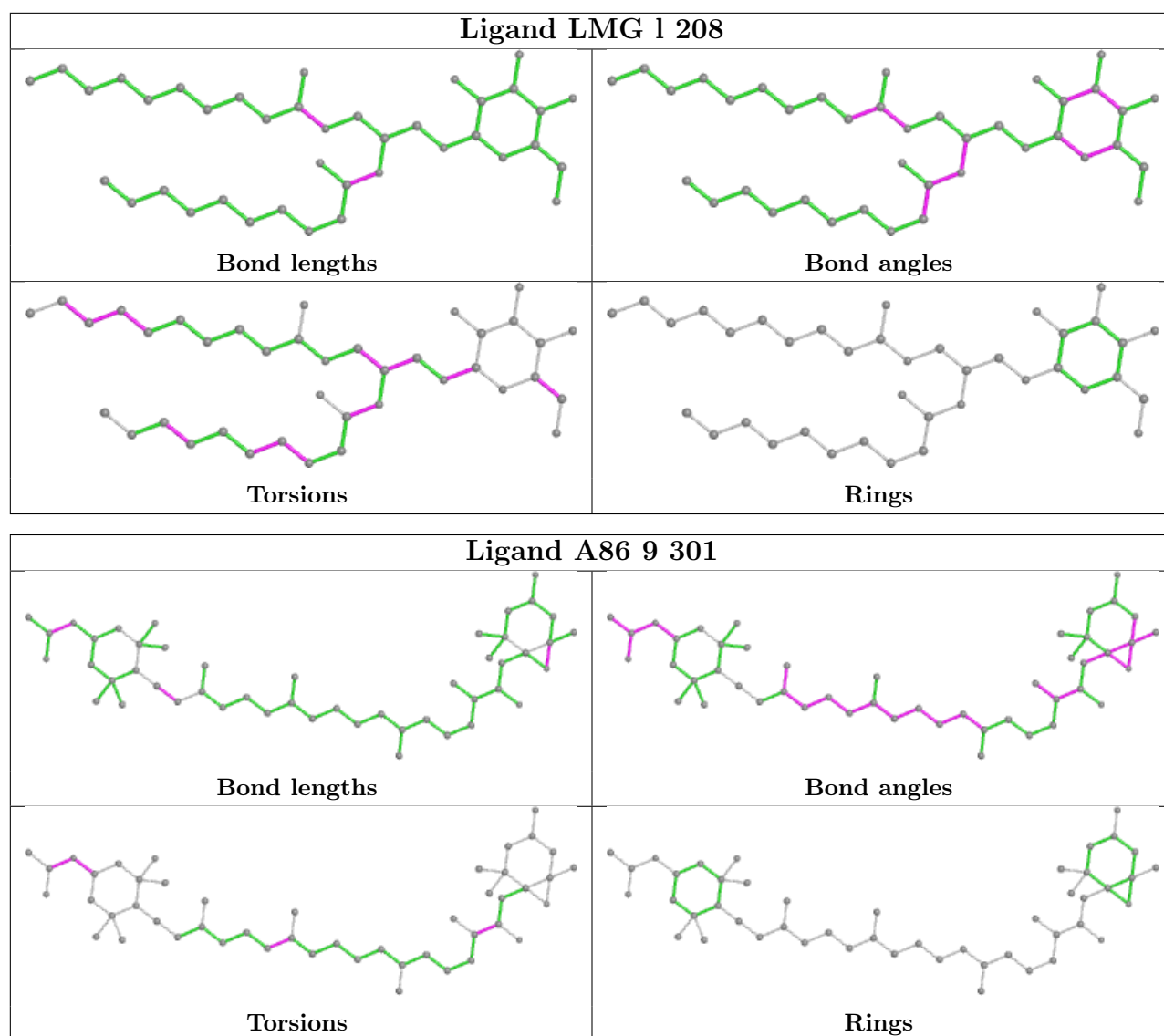


## Ligand CLA Z 312

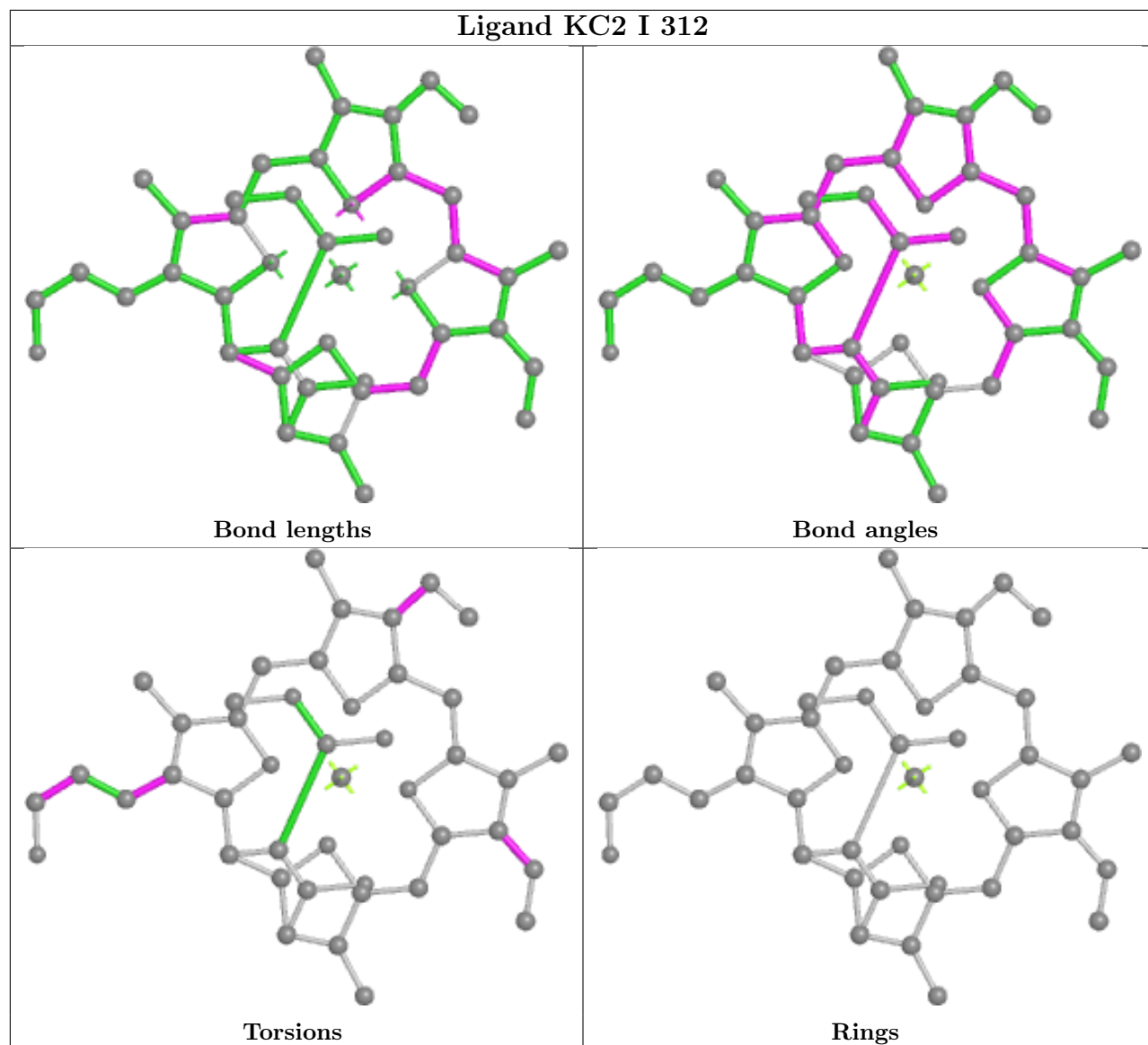


**Ligand CLA C 306****Ligand CLA D 318**

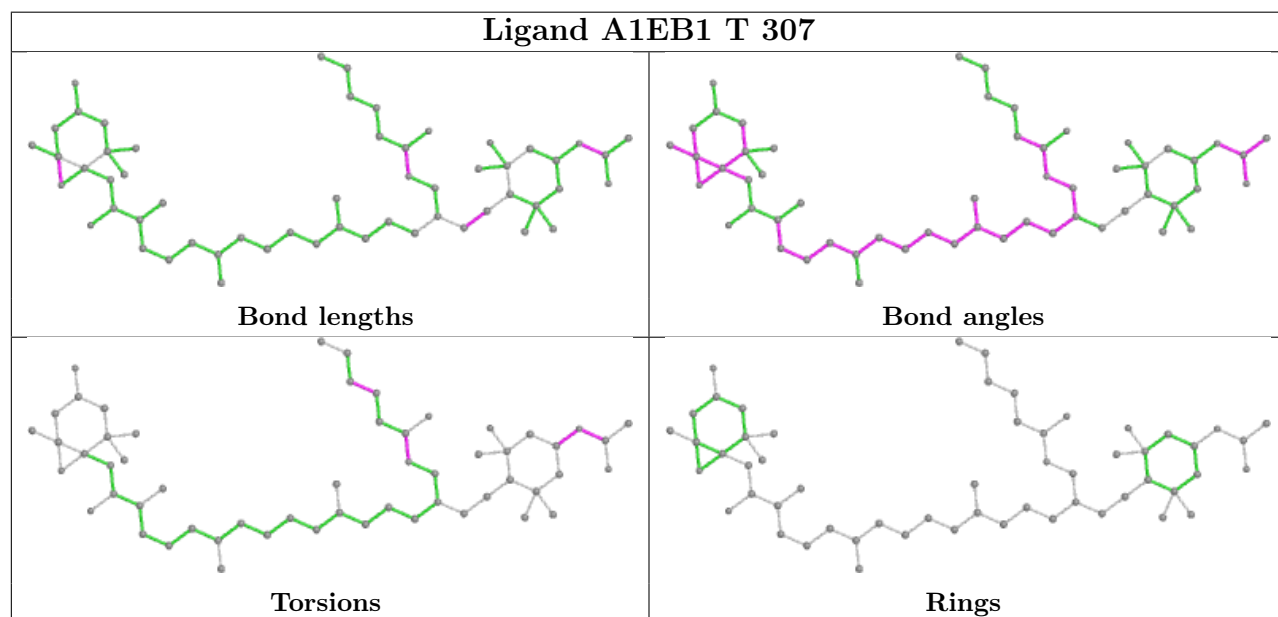




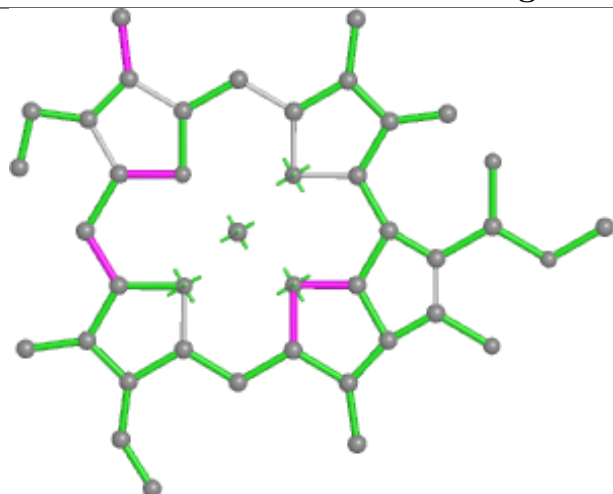
## Ligand KC2 I 312



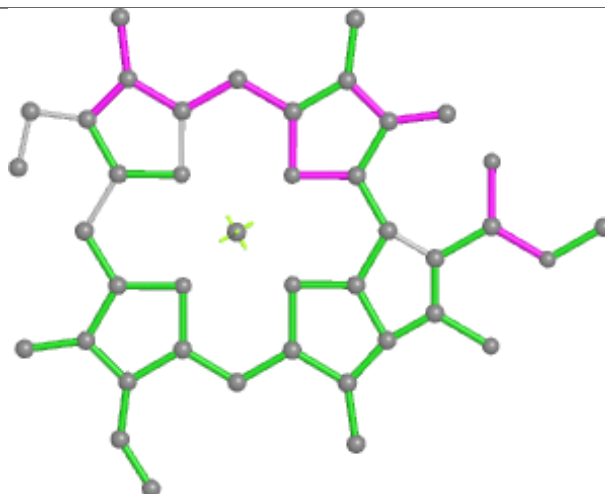
## Ligand A1EB1 T 307



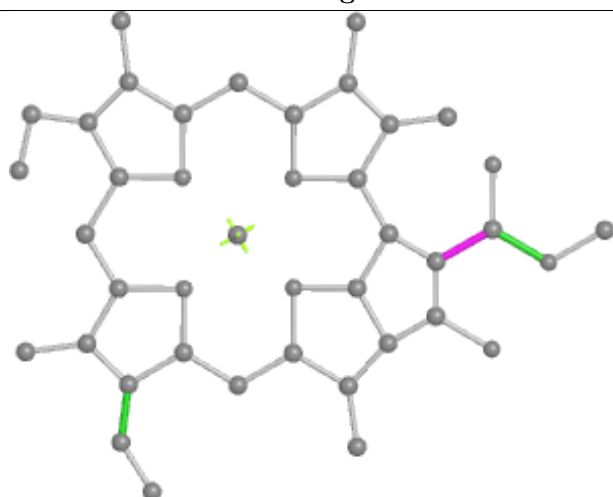
## Ligand CLA 0 318



Bond lengths



Bond angles

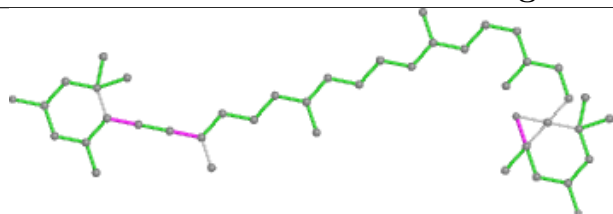


Torsions

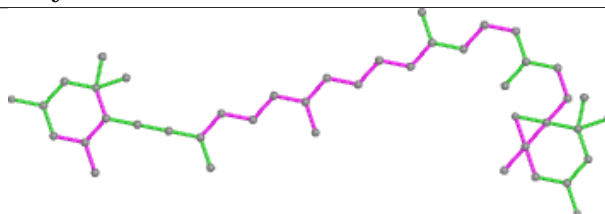


Rings

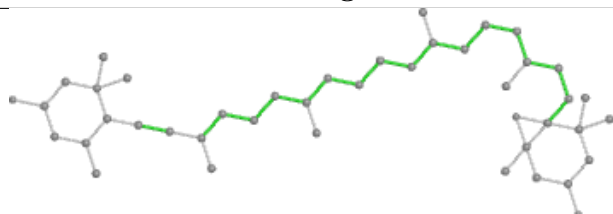
## Ligand DD6 y 304



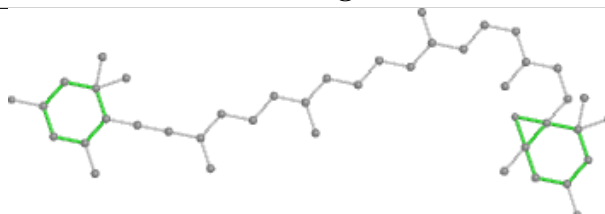
Bond lengths



Bond angles



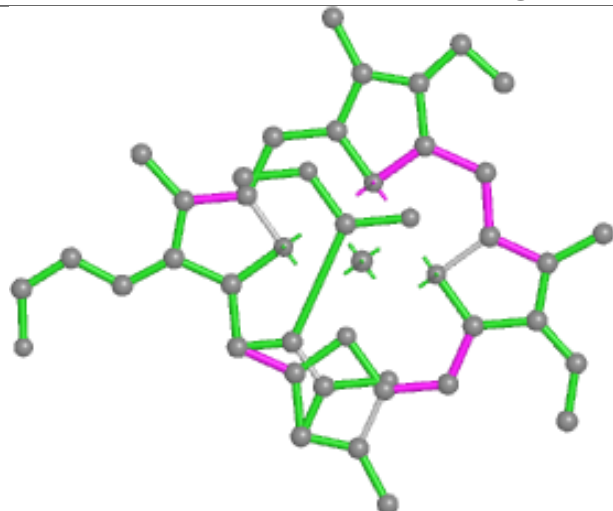
Torsions



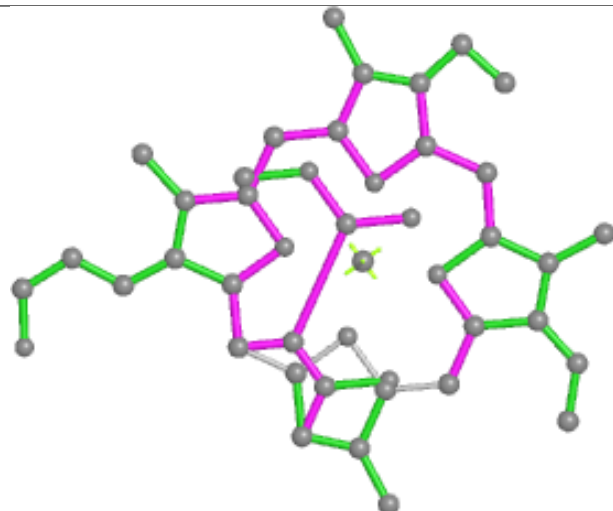
Rings



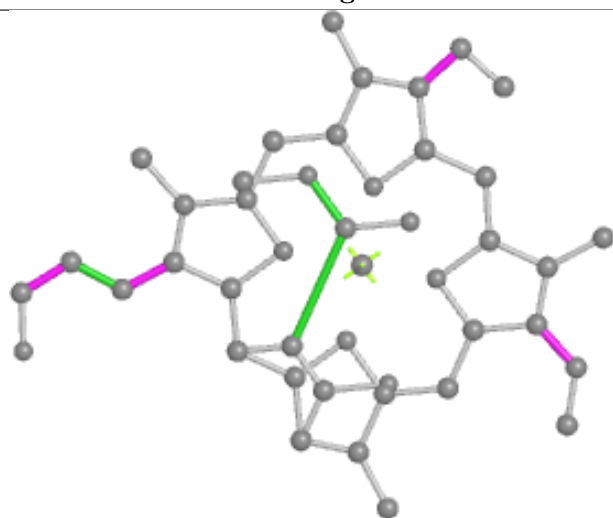
## Ligand KC2 M 311



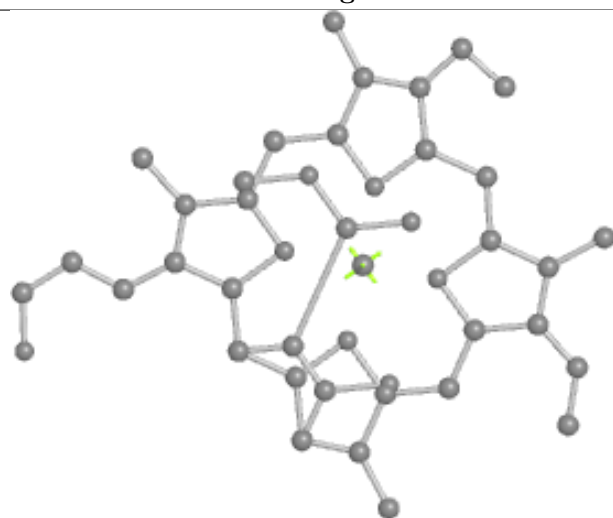
Bond lengths



Bond angles

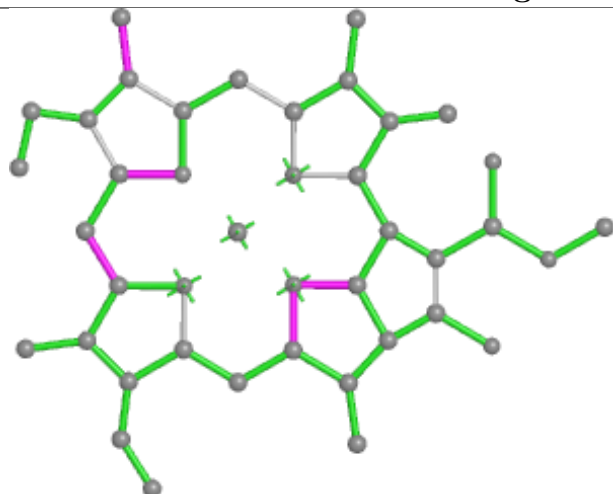


Torsions

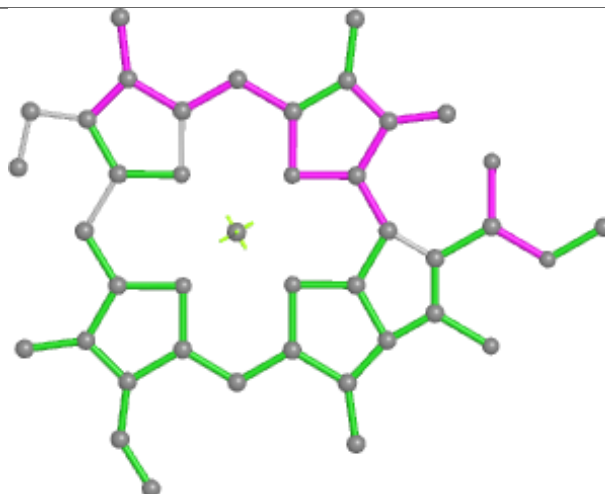


Rings

## Ligand CLA Y 314



Bond lengths



Bond angles

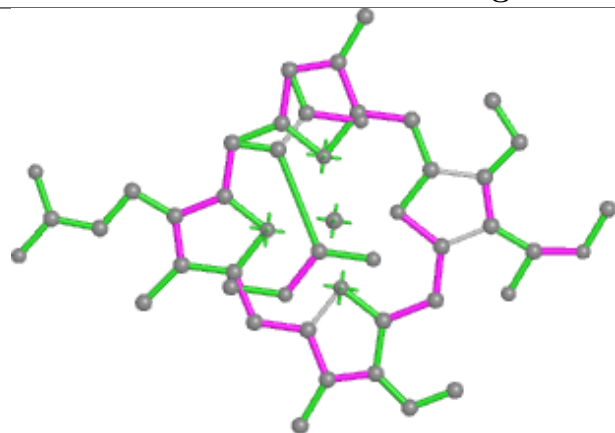


Torsions

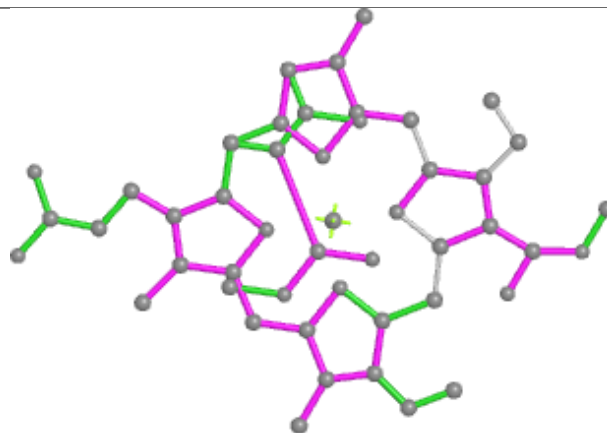


Rings

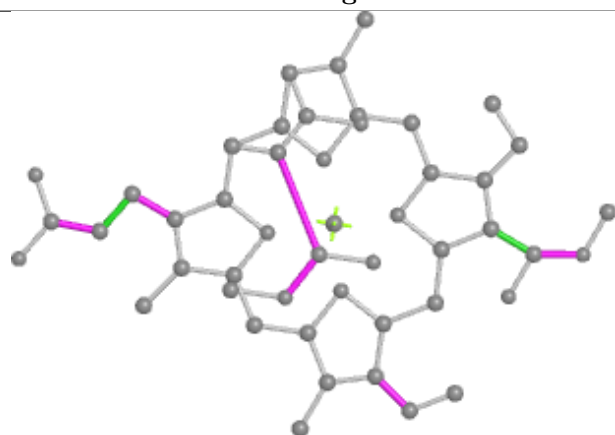
## Ligand A1ECV V 317



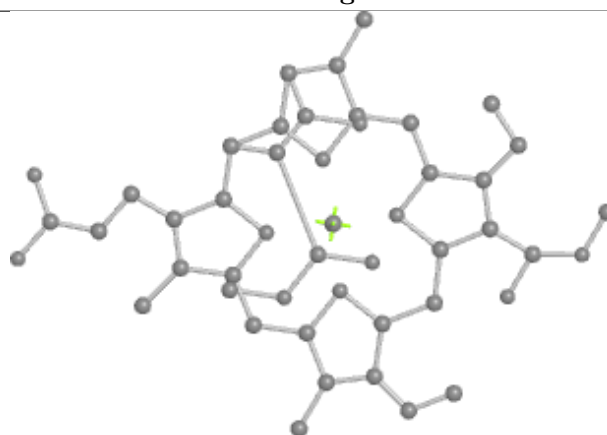
Bond lengths



Bond angles

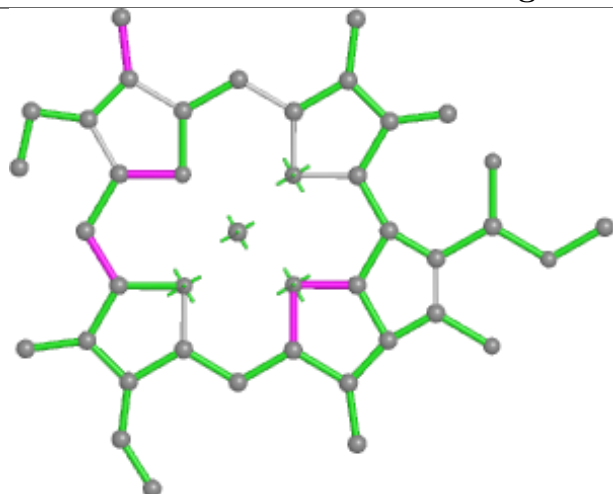


Torsions

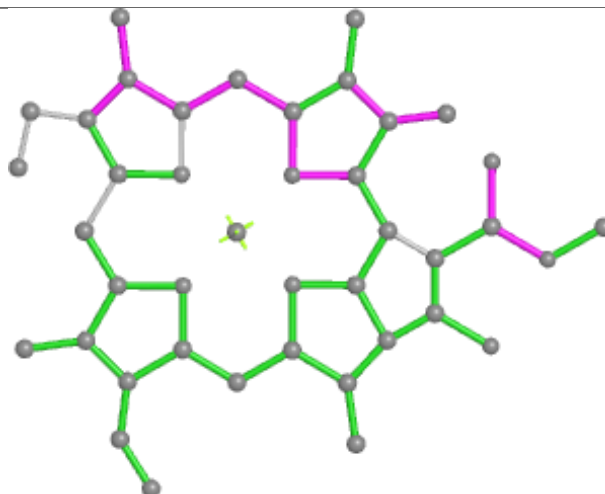


Rings

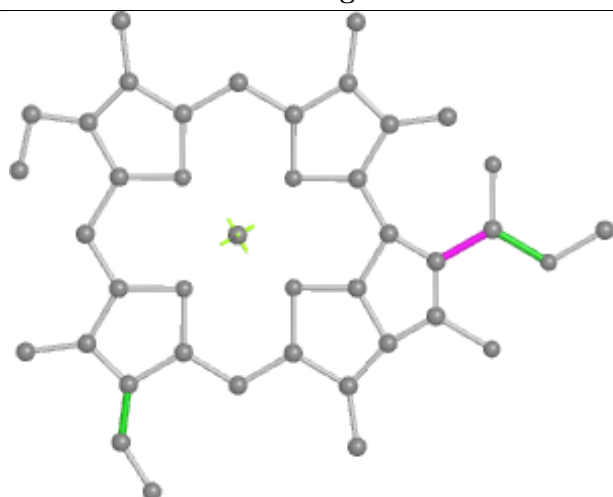
## Ligand CLA 9 315



Bond lengths



Bond angles

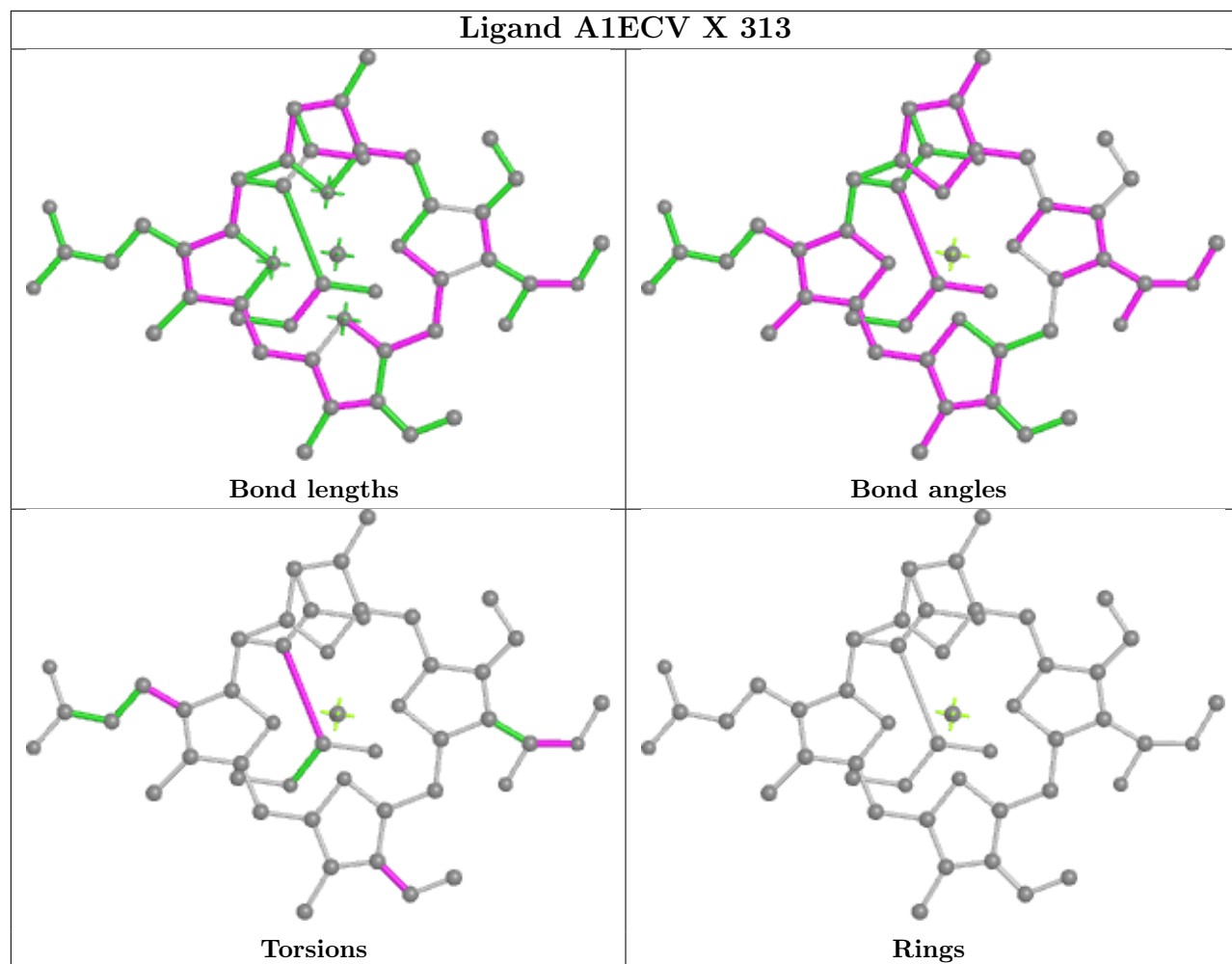


Torsions

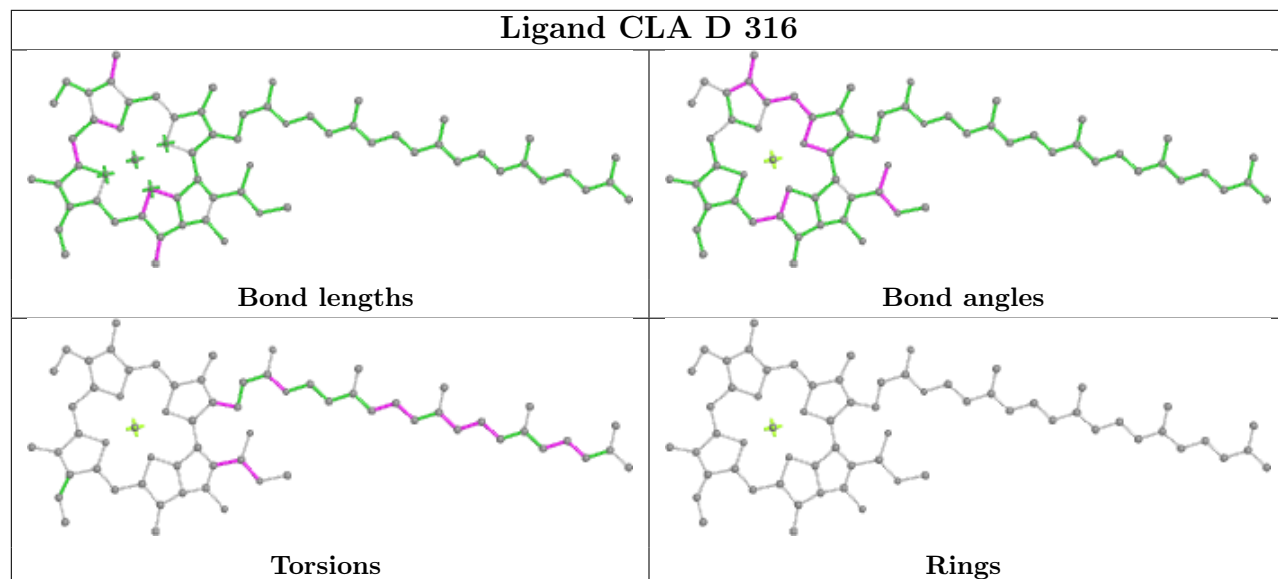


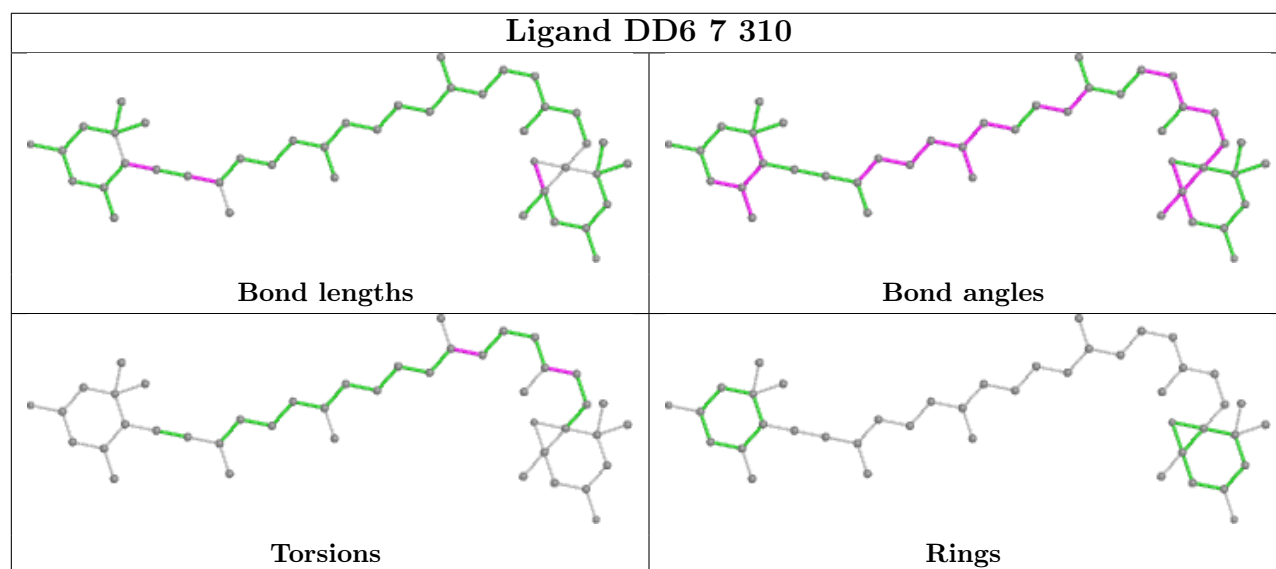
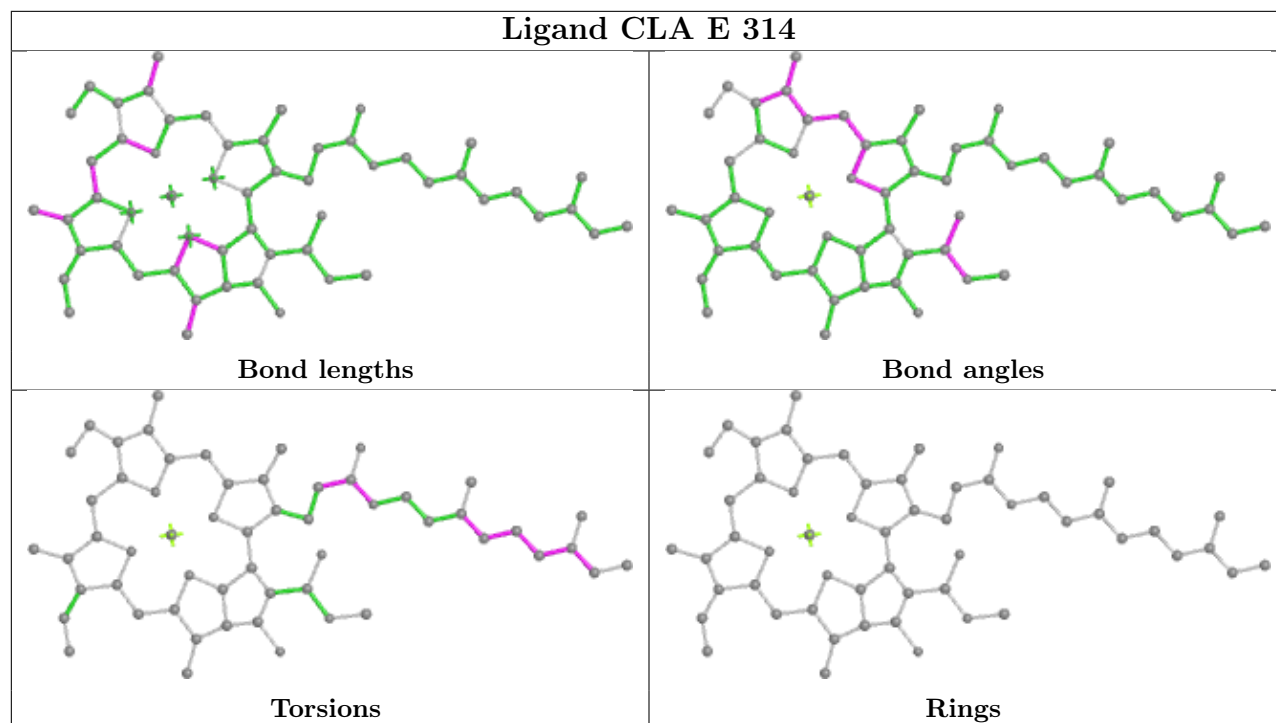
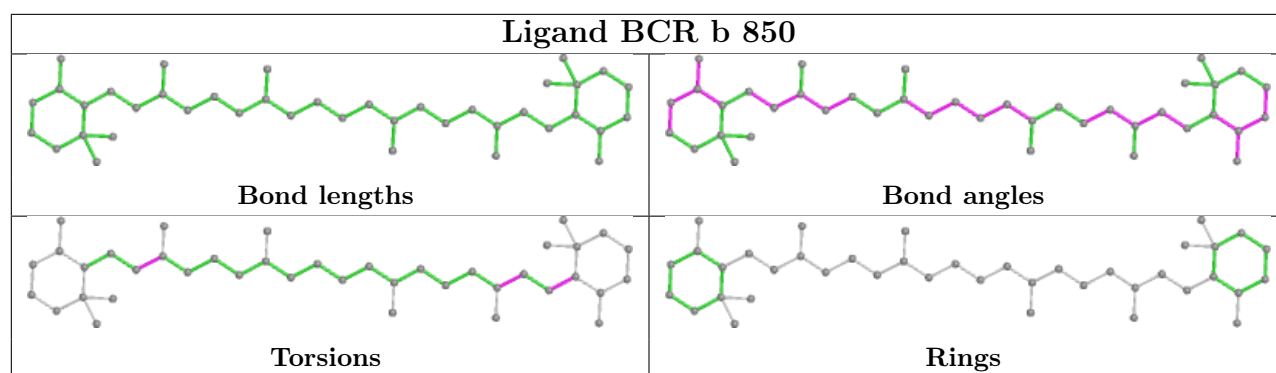
Rings

## Ligand A1ECV X 313

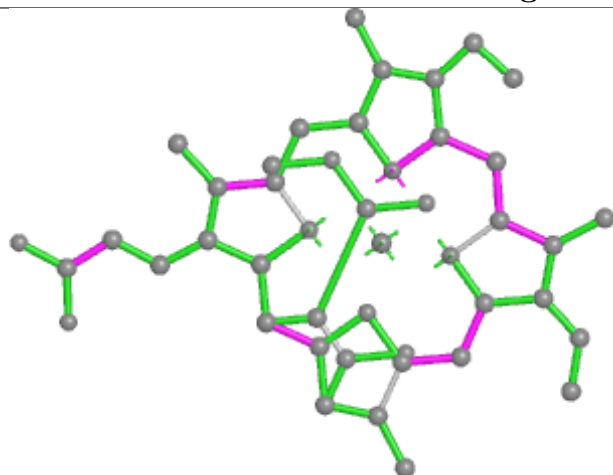


## Ligand CLA D 316

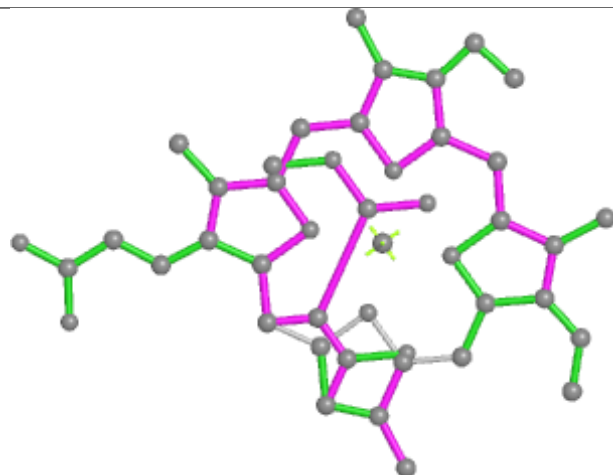




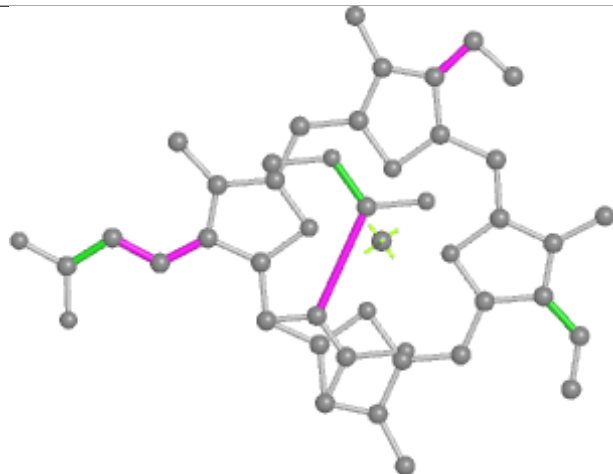
## Ligand KC2 5 311



Bond lengths



Bond angles

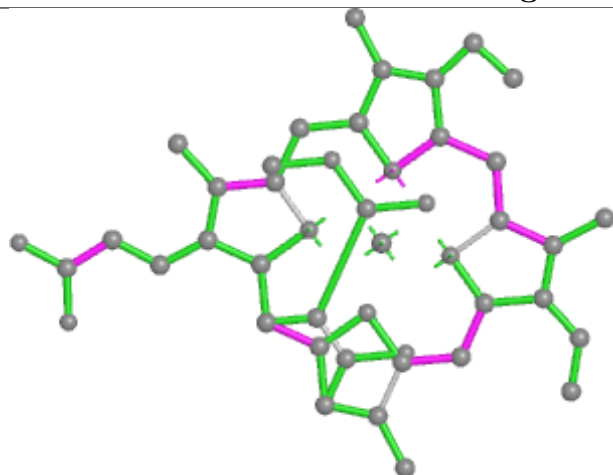


Torsions

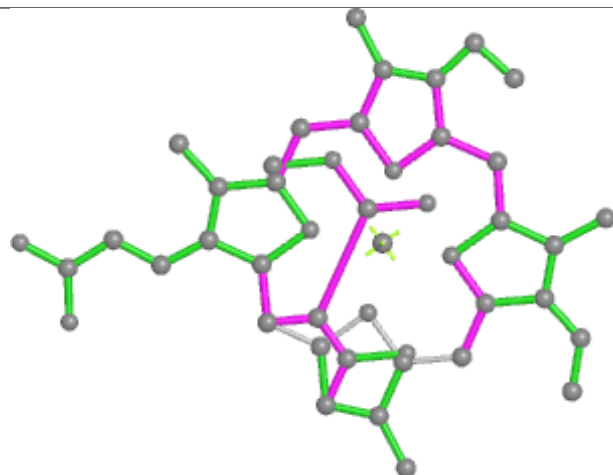


Rings

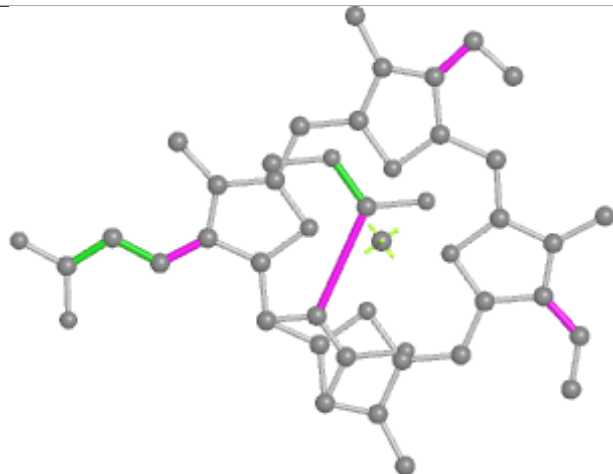
## Ligand KC2 9 311



Bond lengths



Bond angles

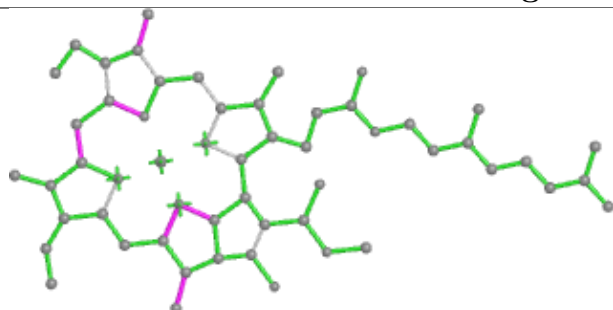
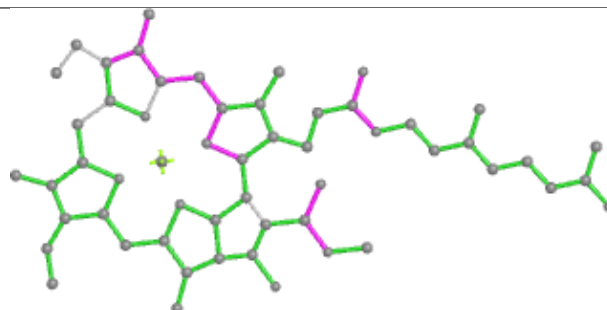
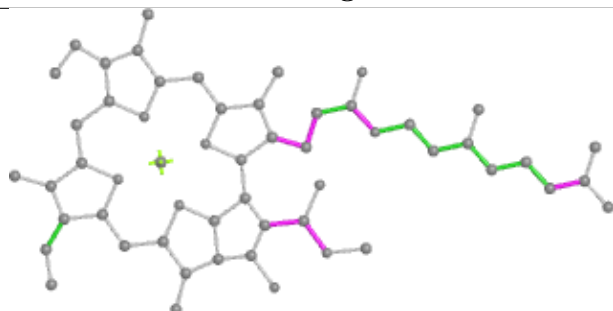
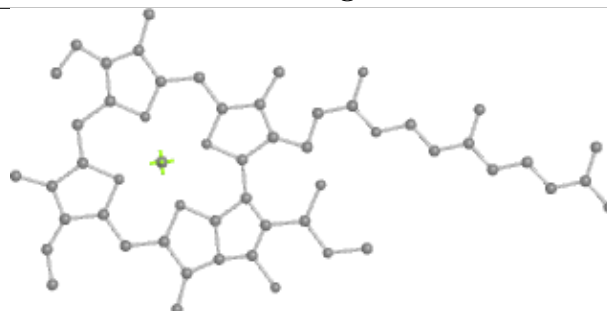
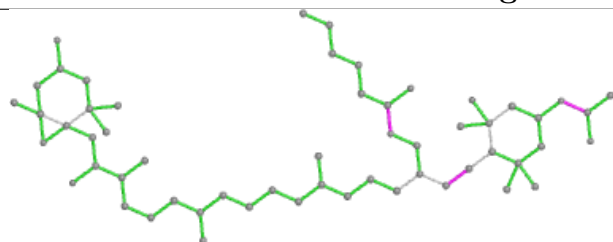
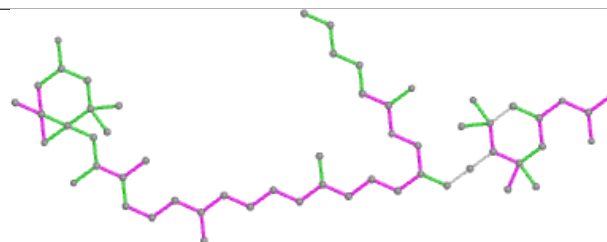
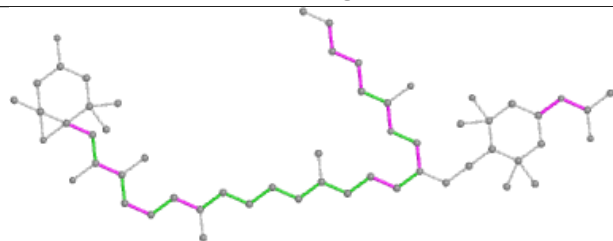
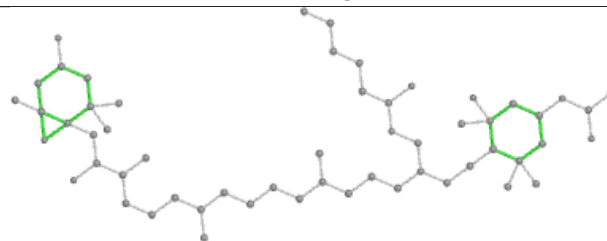


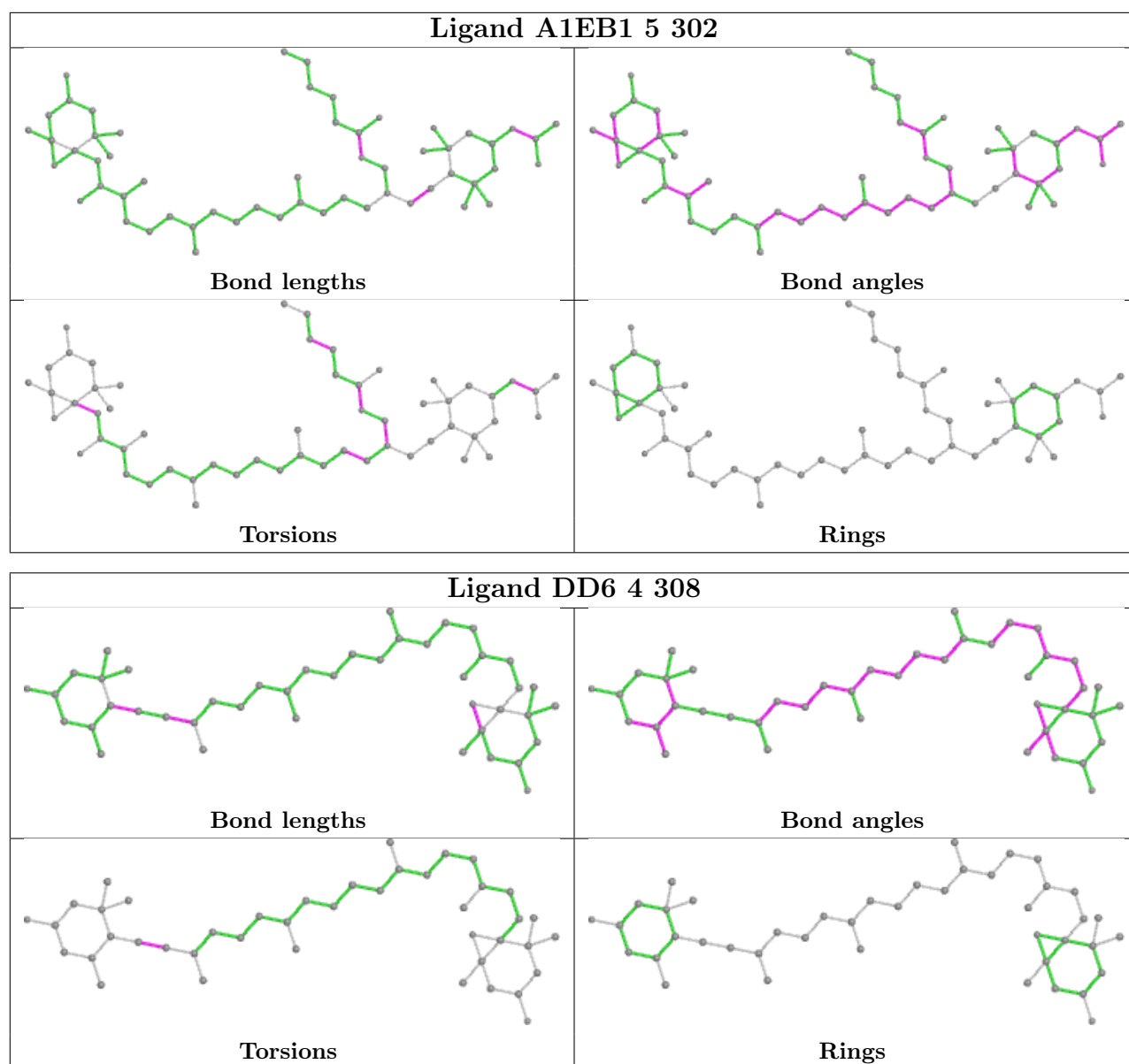
Torsions



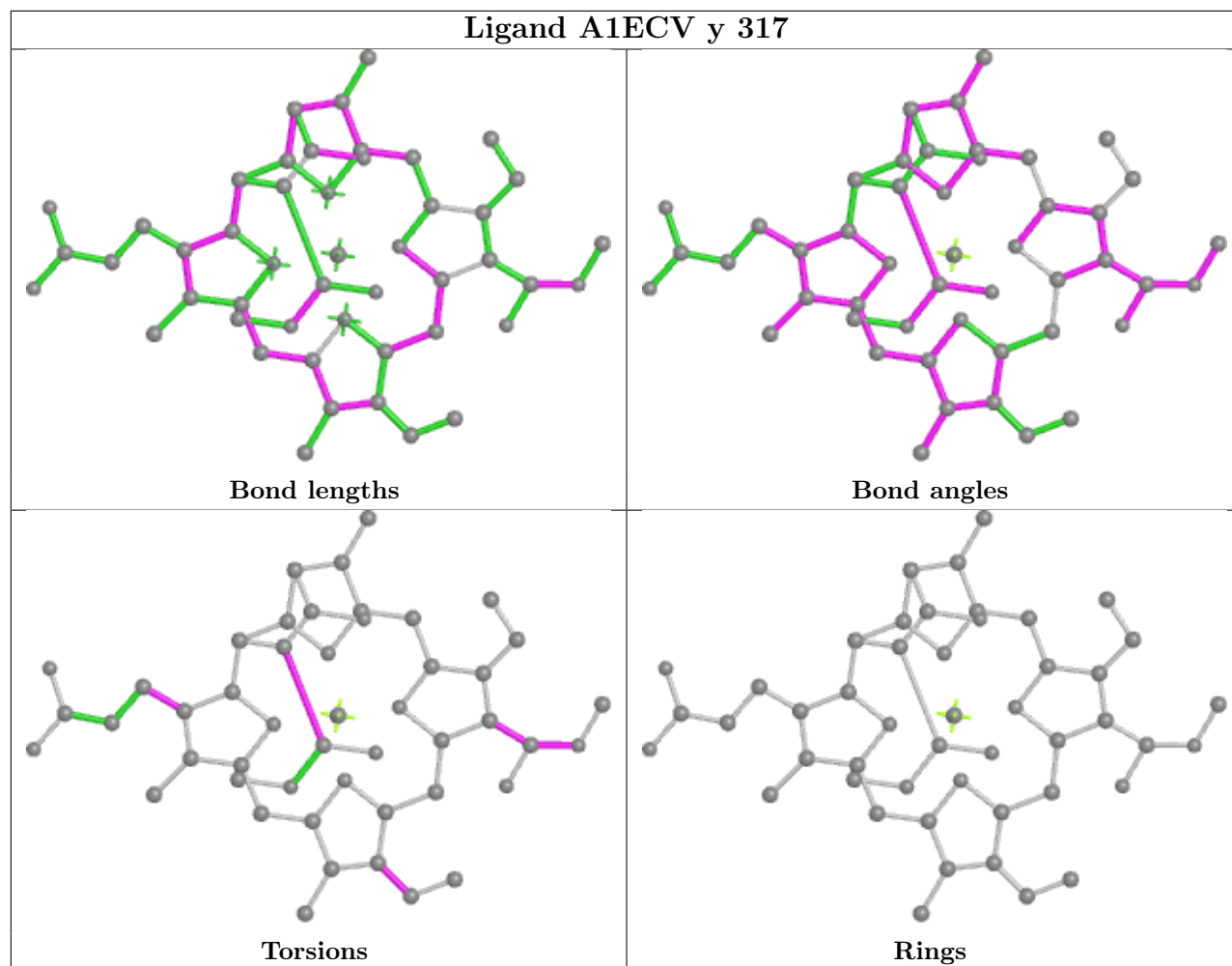
Rings



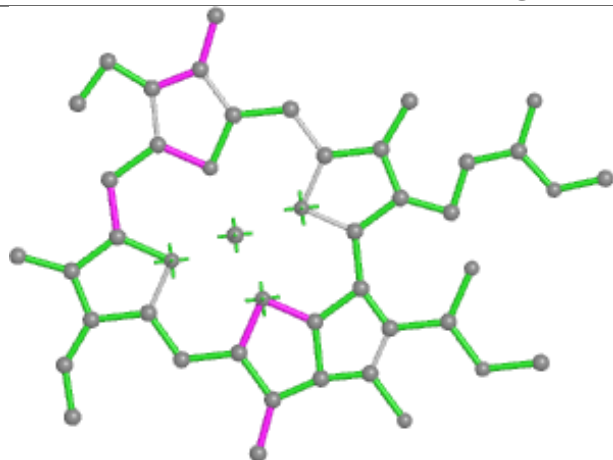
**Ligand CLA f 803****Bond lengths****Bond angles****Torsions****Rings****Ligand A1EB1 7 303****Bond lengths****Bond angles****Torsions****Rings**



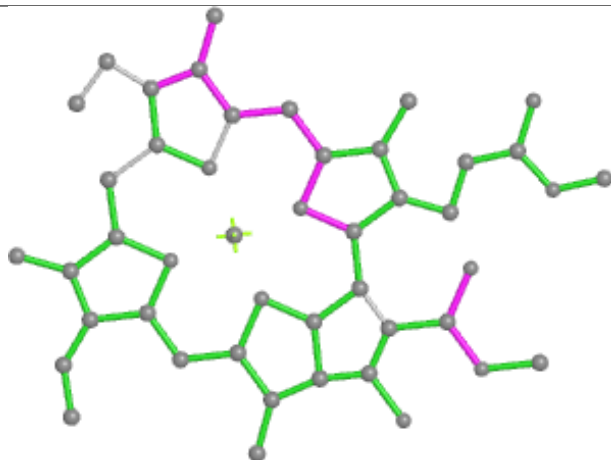
## Ligand A1ECV y 317



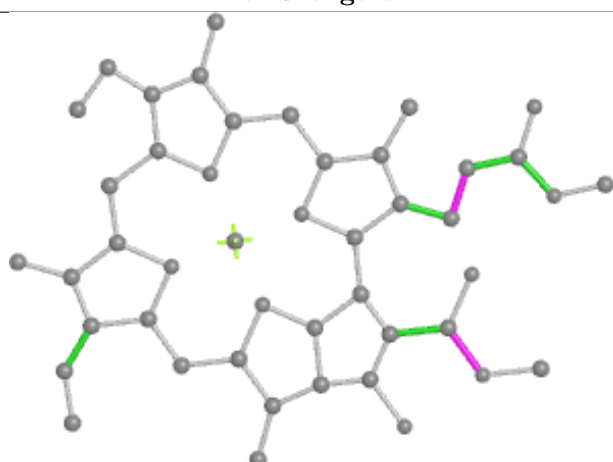
## Ligand CLA U 208



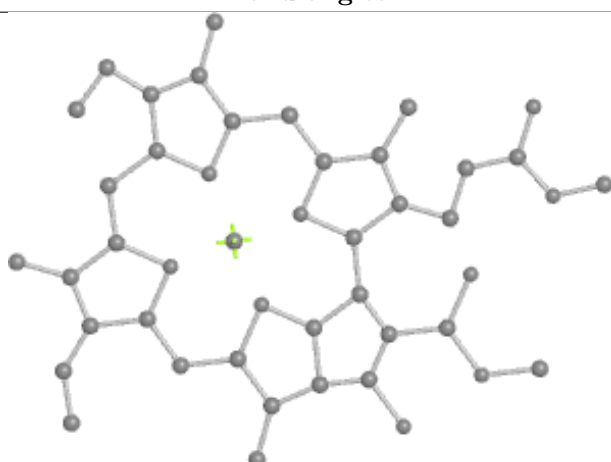
Bond lengths



Bond angles

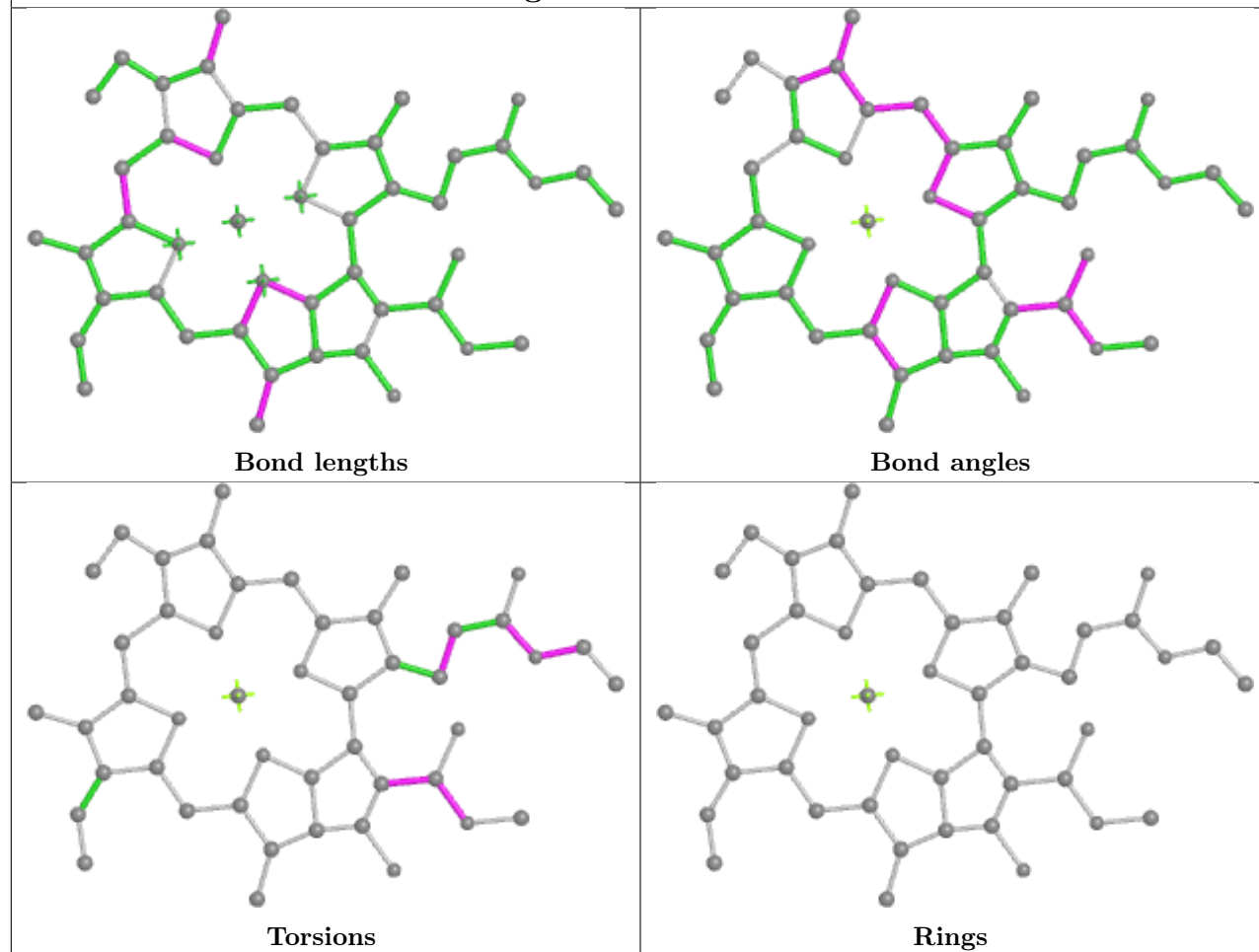


Torsions

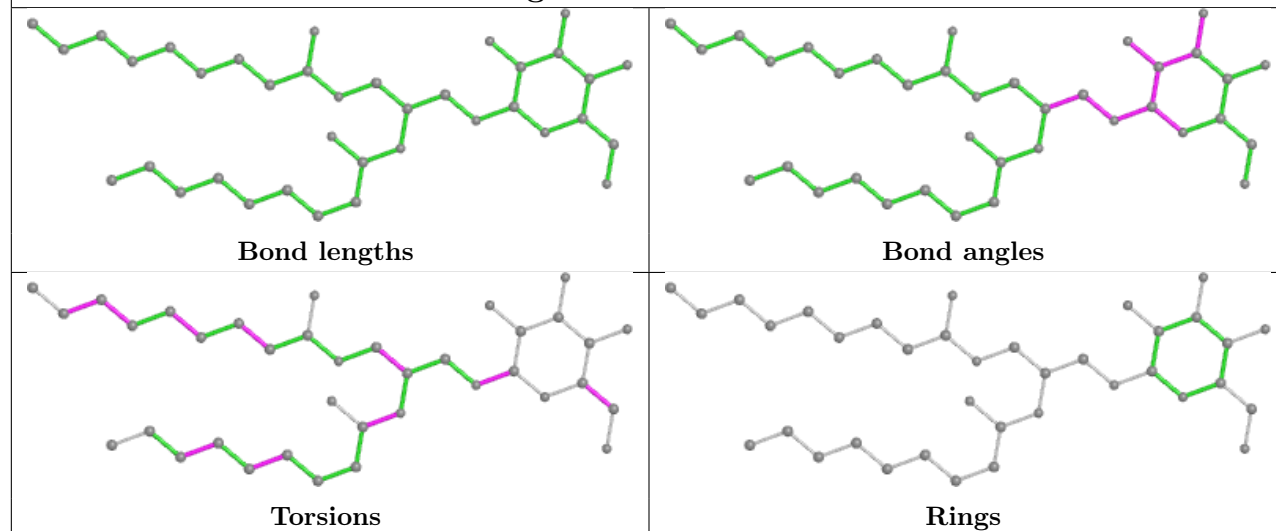


Rings

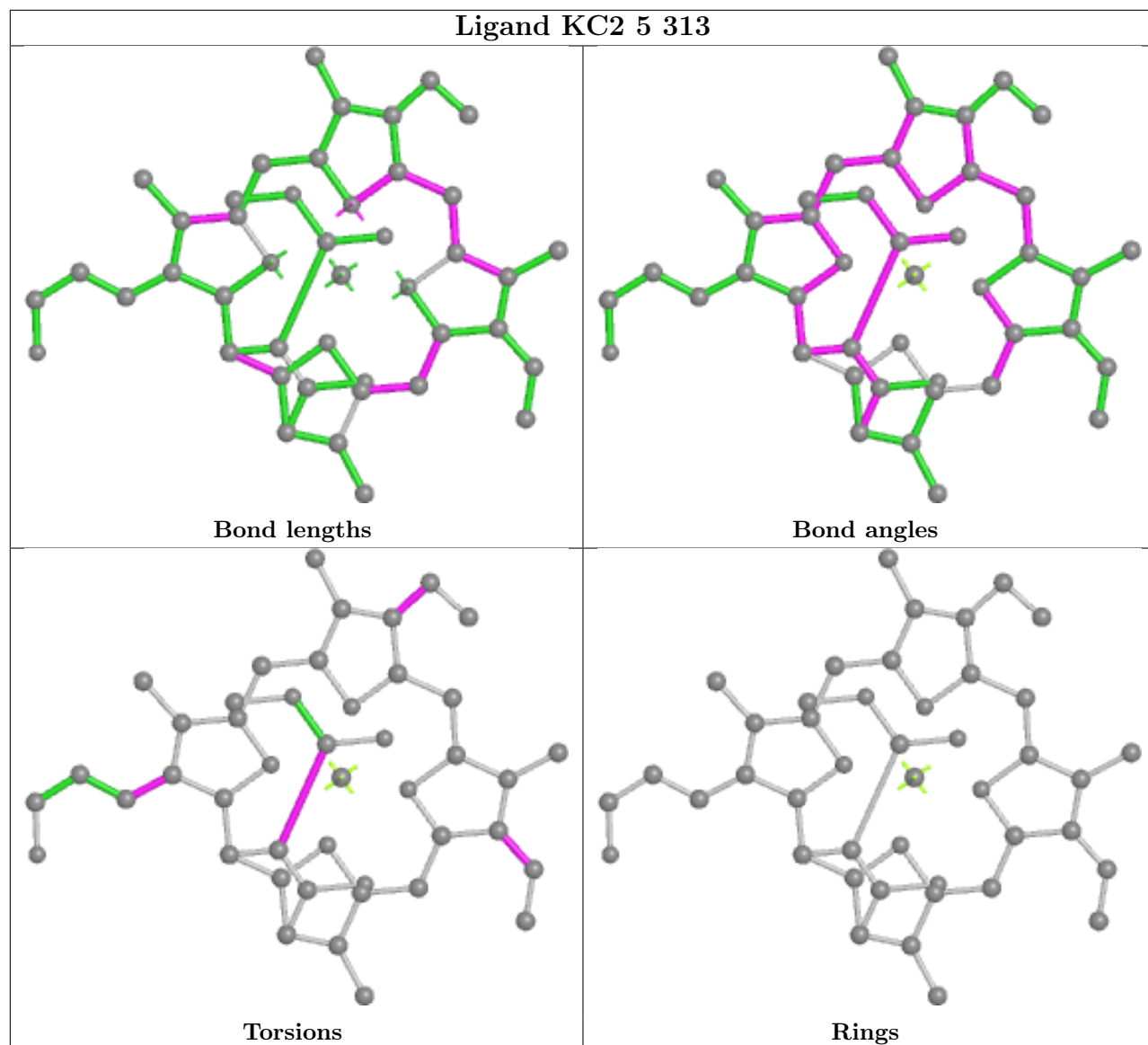
## Ligand CLA X 316



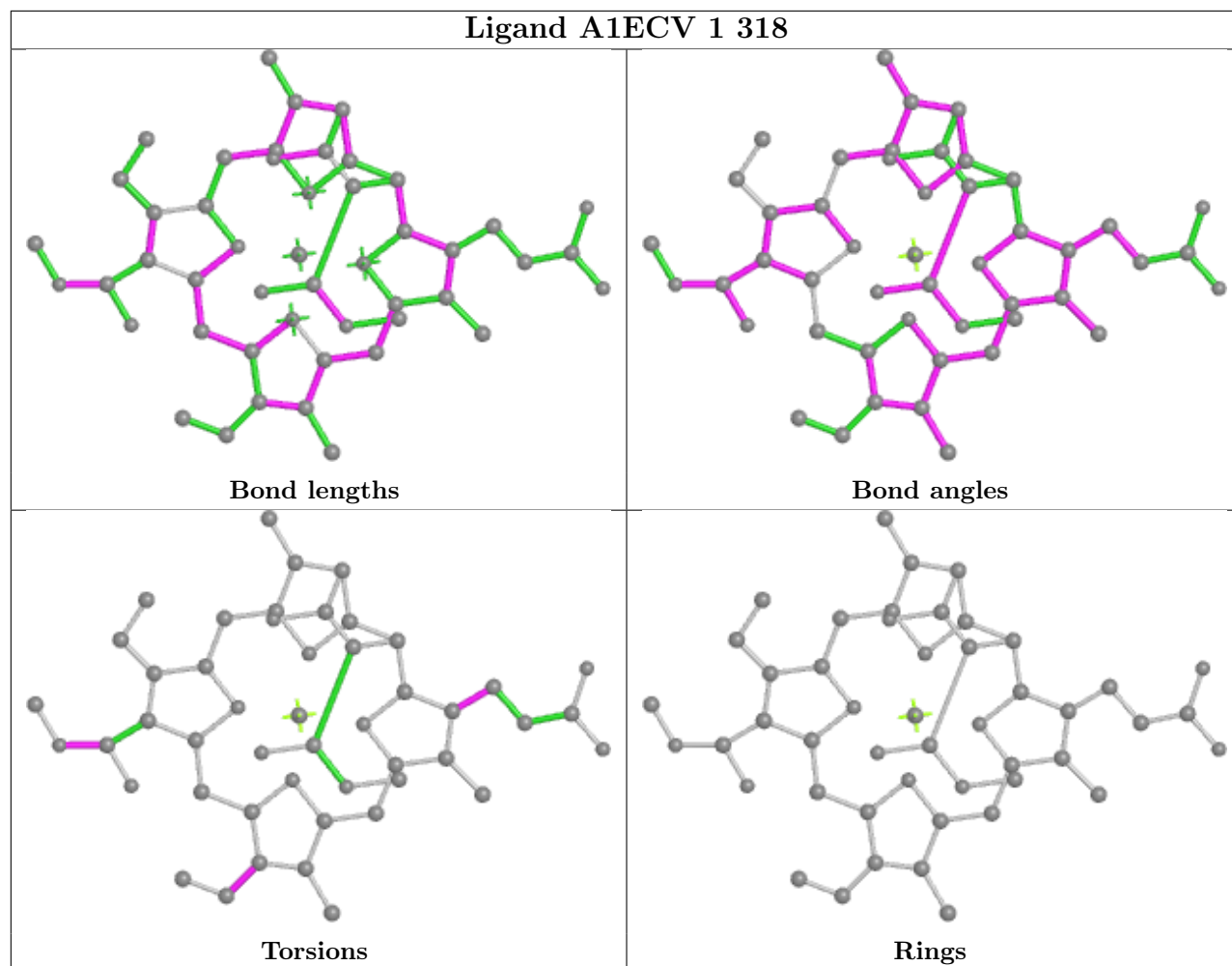
## Ligand LMG D 322



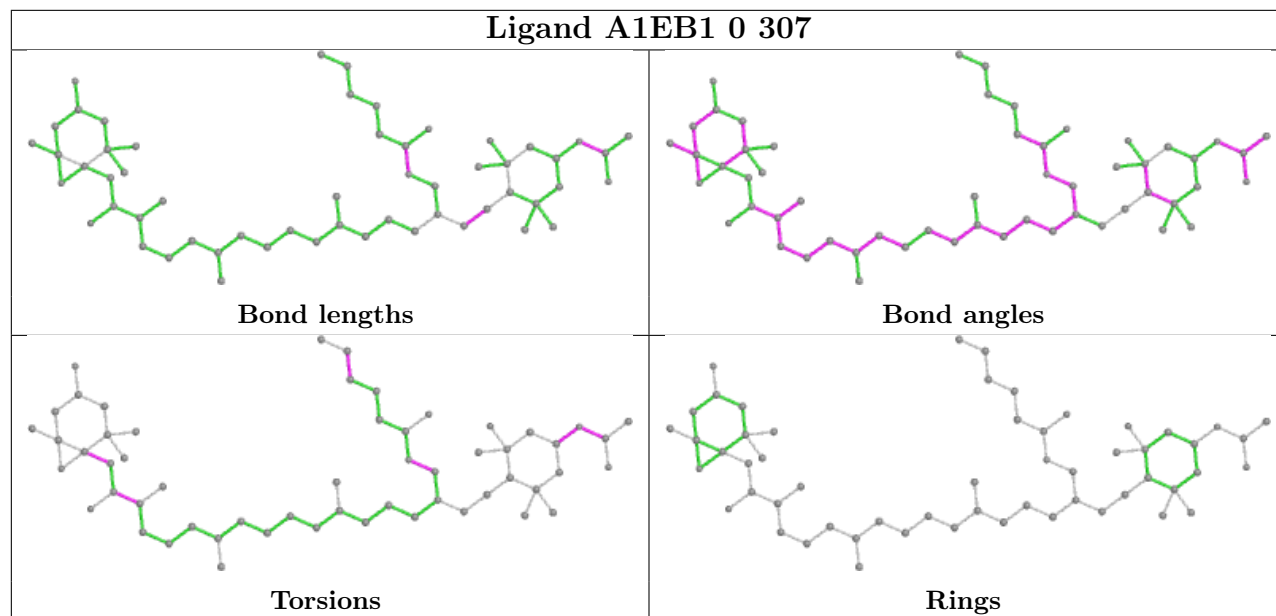
## Ligand KC2 5 313



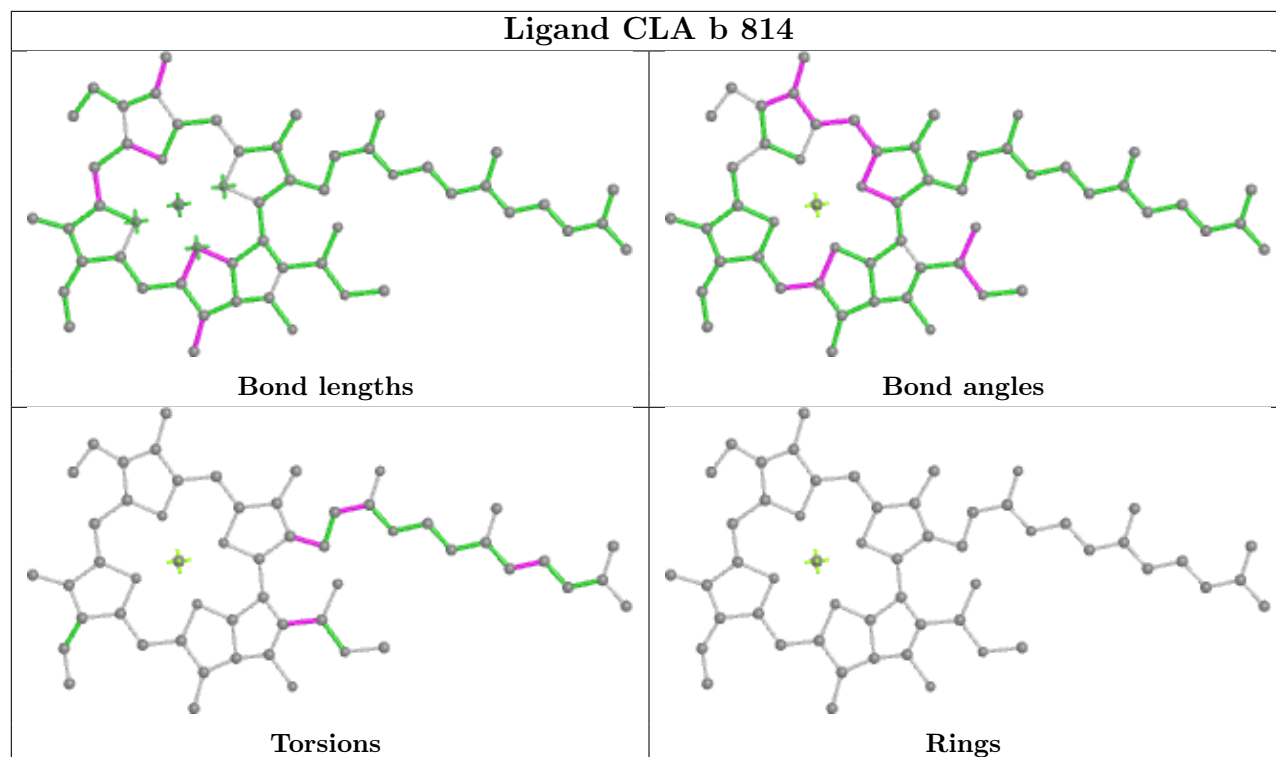
## Ligand A1ECV 1 318



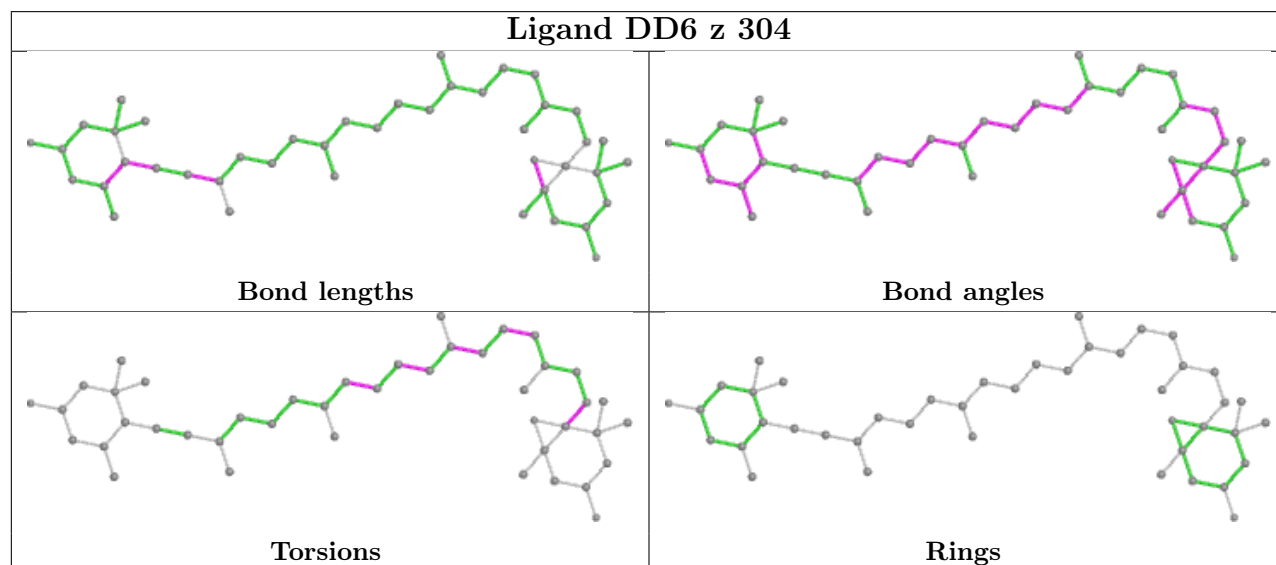
## Ligand A1EB1 0 307



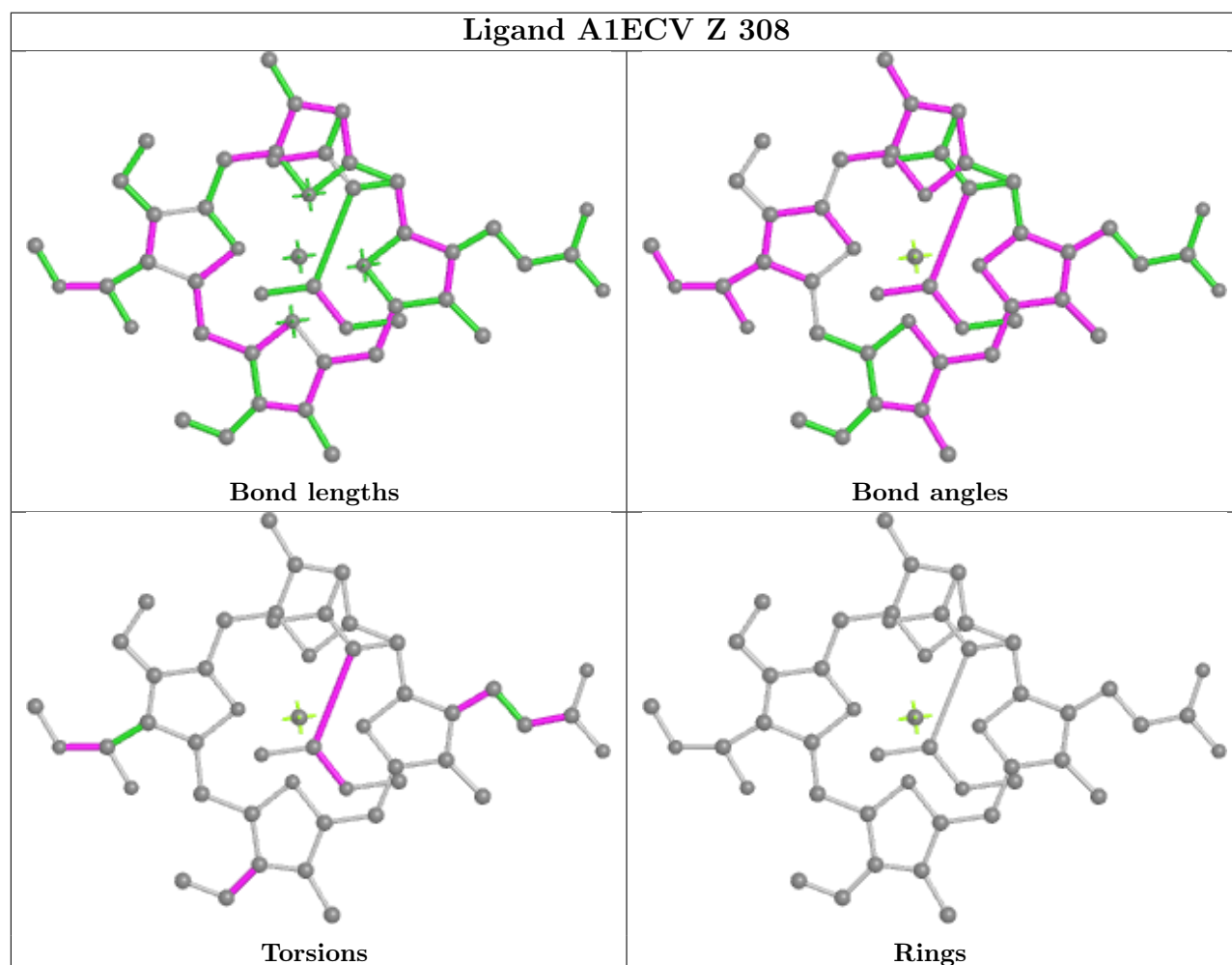
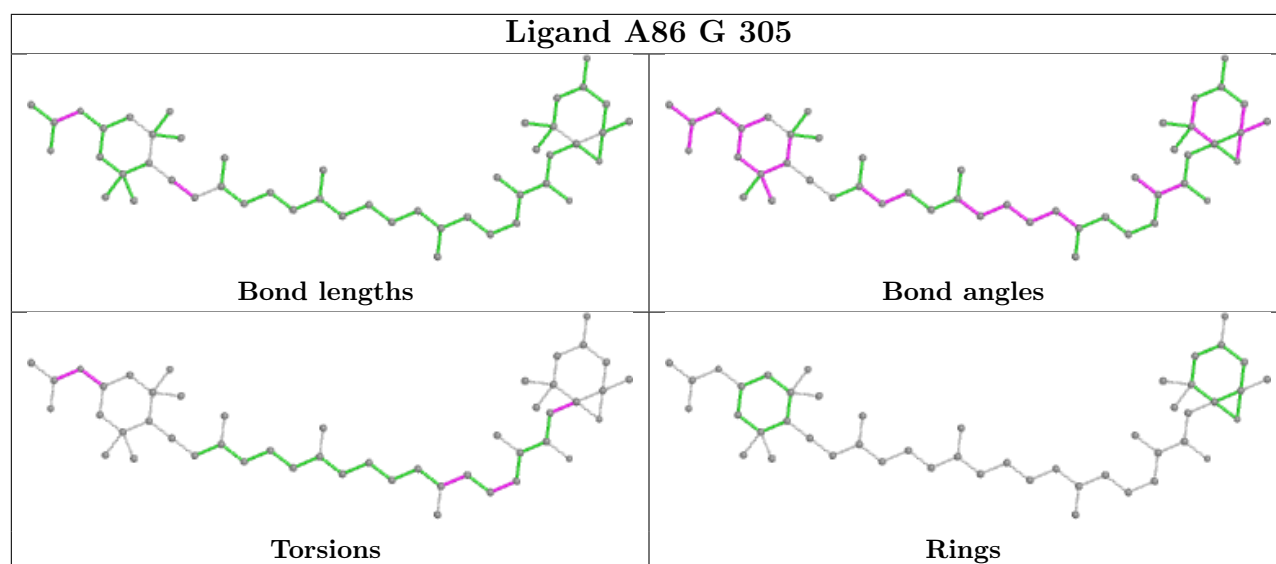
## Ligand CLA b 814



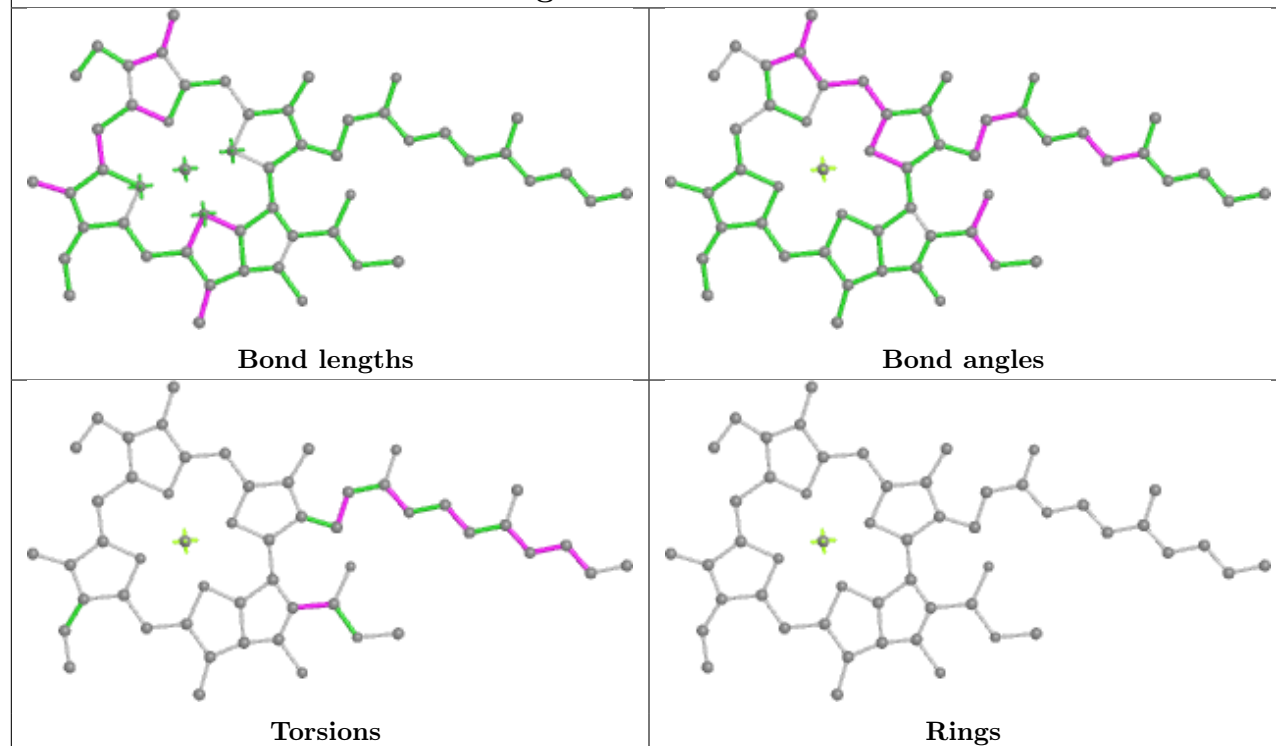
## Ligand DD6 z 304



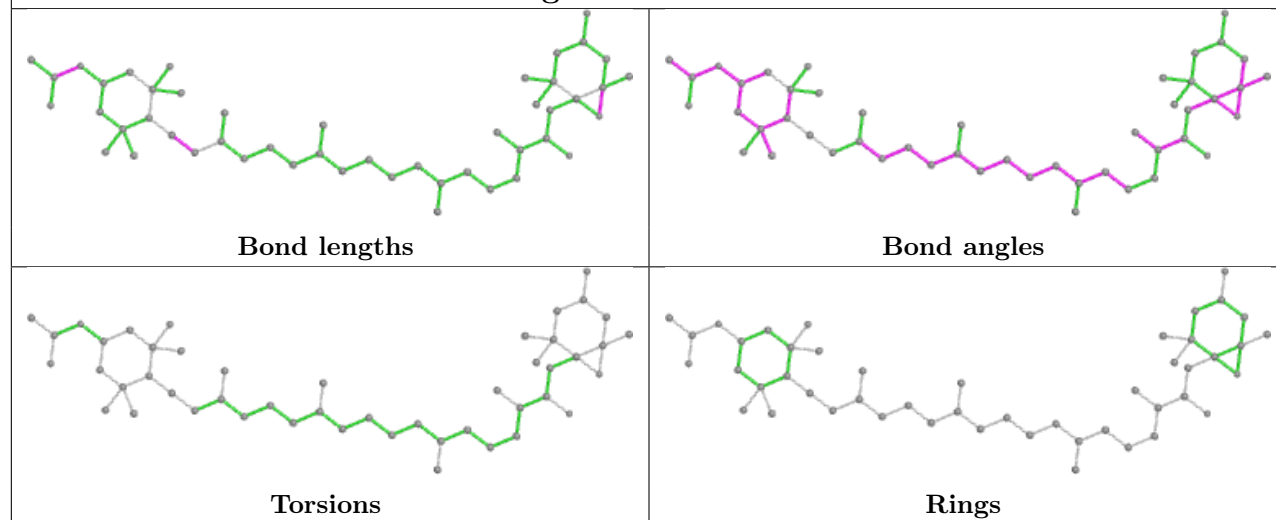




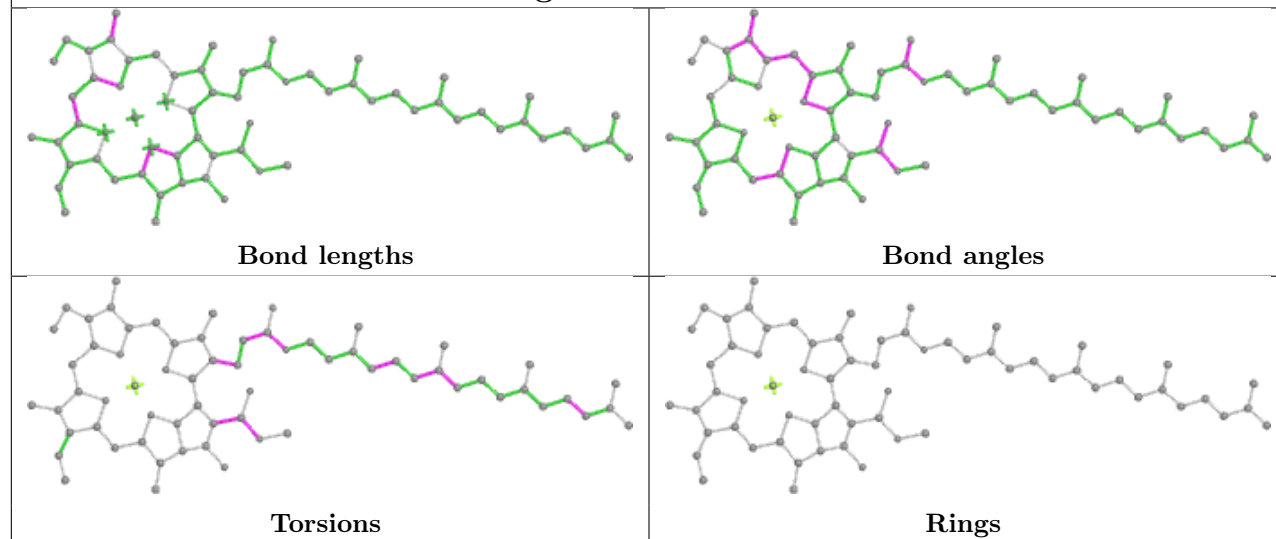
## Ligand CLA 0 312



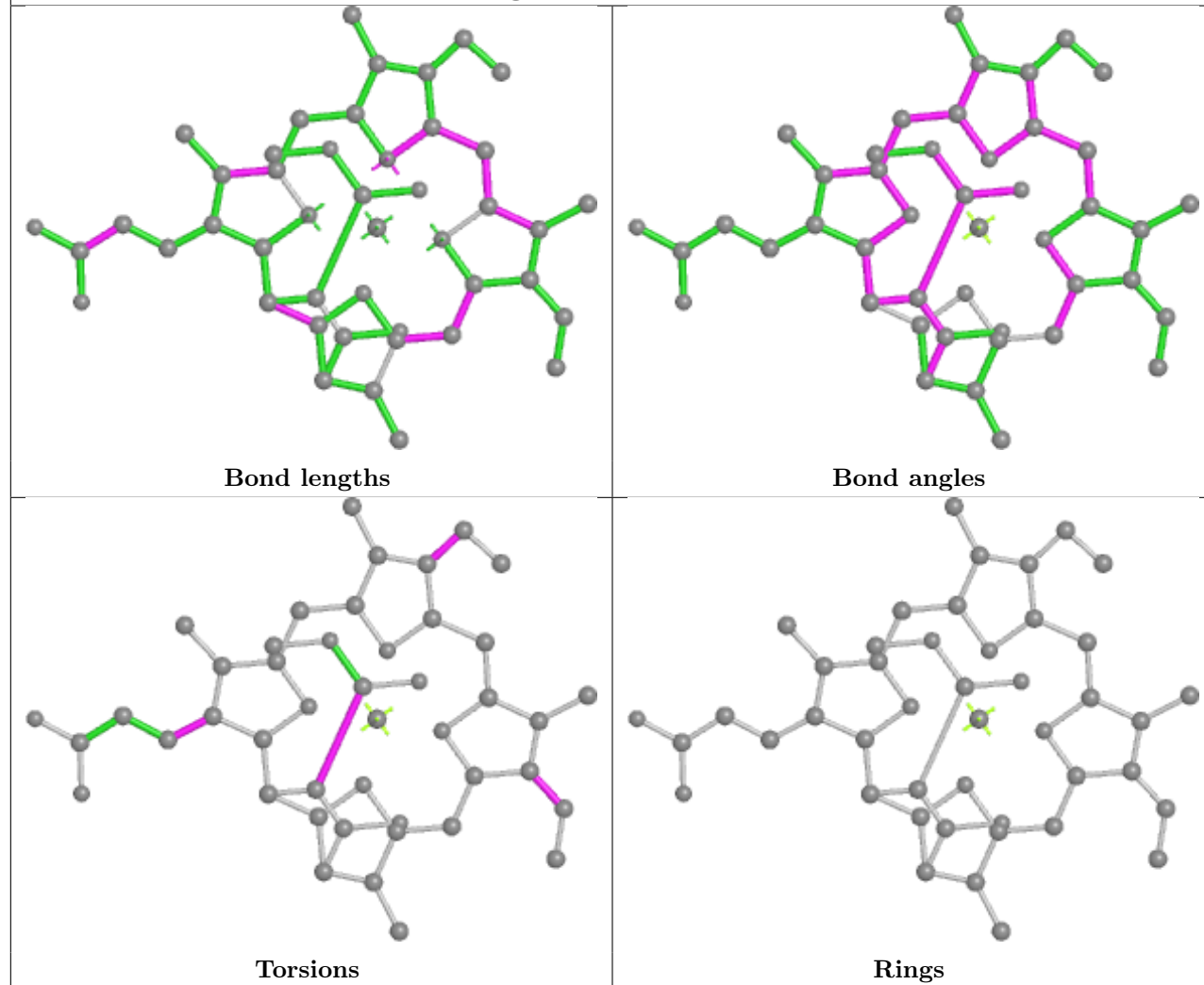
## Ligand A86 1 307



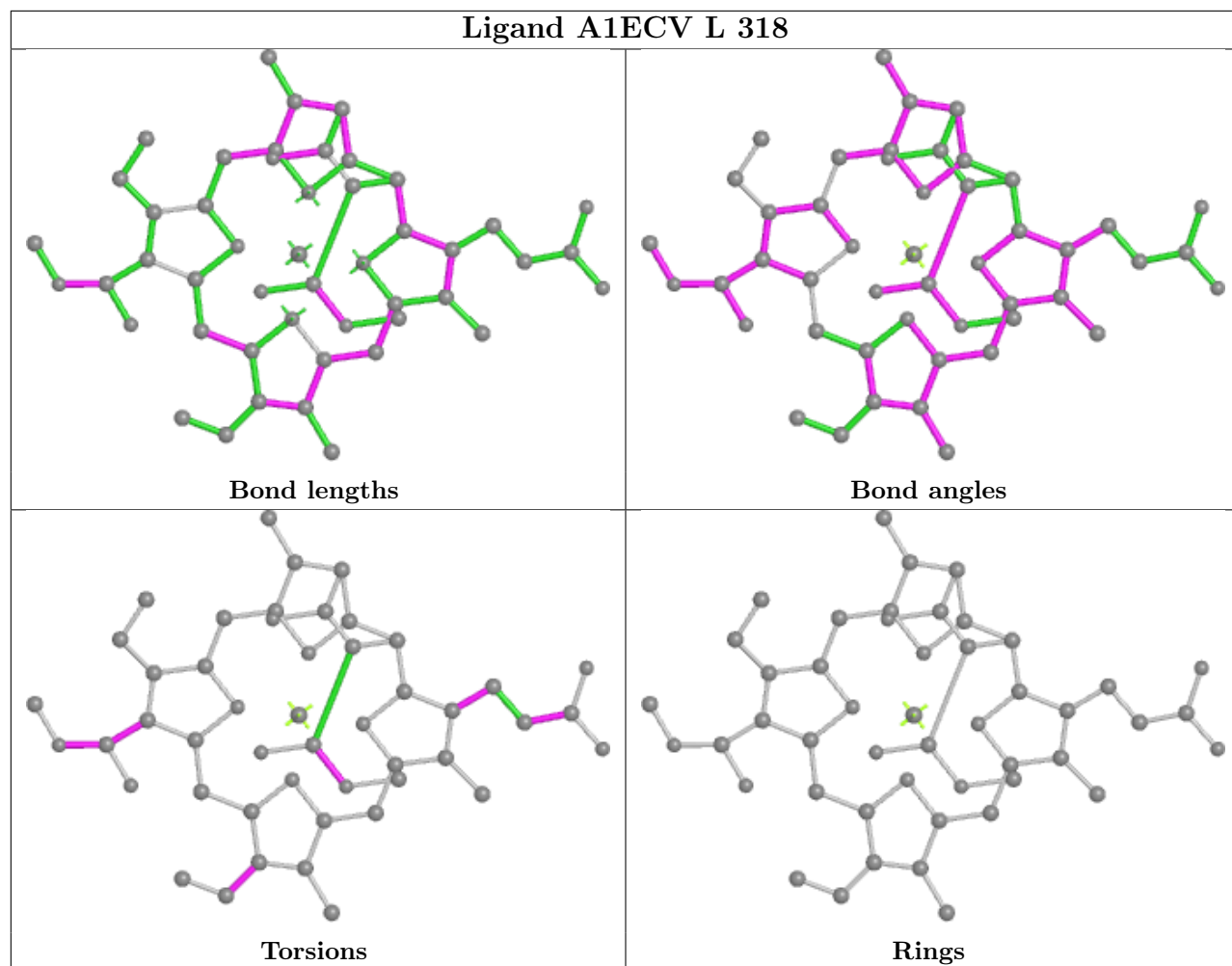
## Ligand CLA b 809



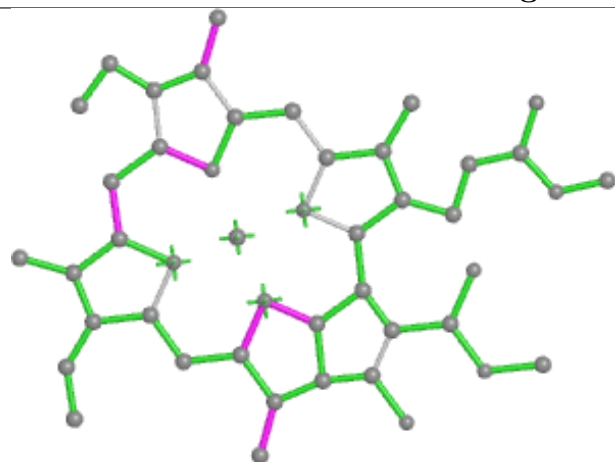
## Ligand KC2 7 319



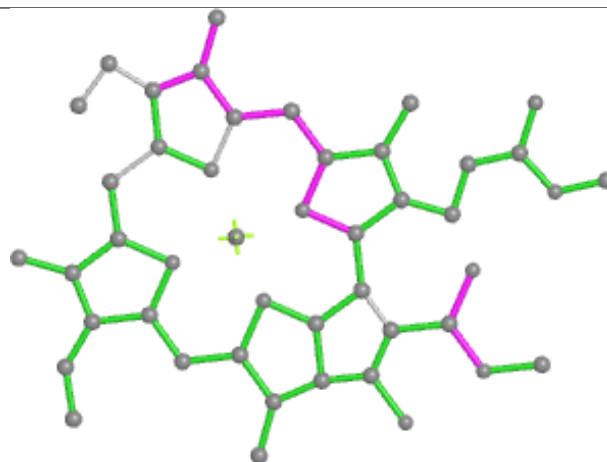
## Ligand A1ECV L 318



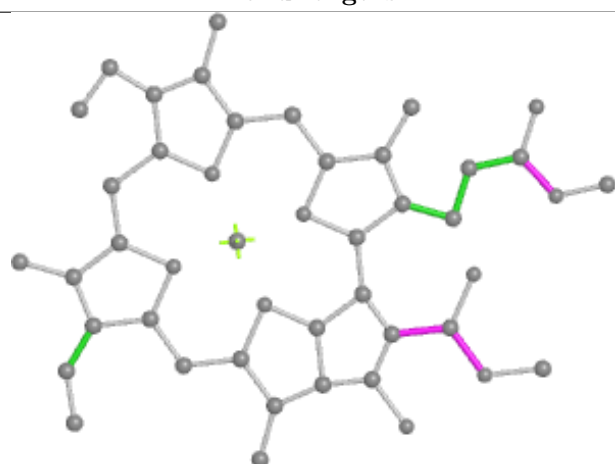
## Ligand CLA J 312



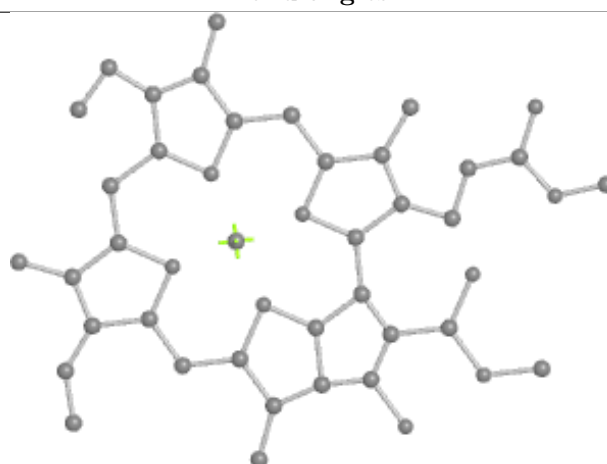
Bond lengths



Bond angles

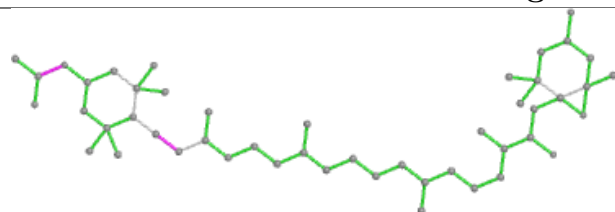


Torsions

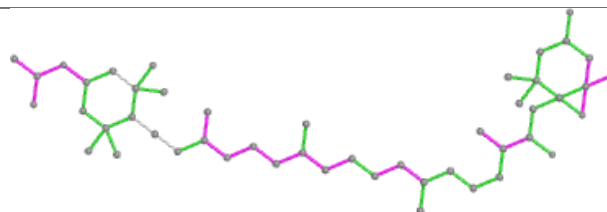


Rings

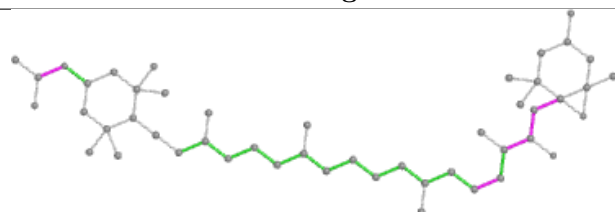
## Ligand A86 z 303



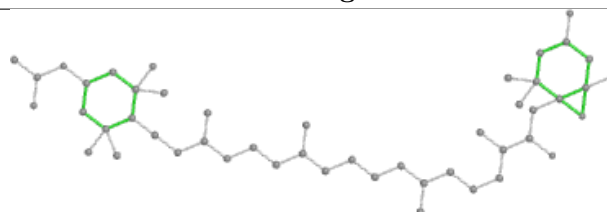
Bond lengths



Bond angles

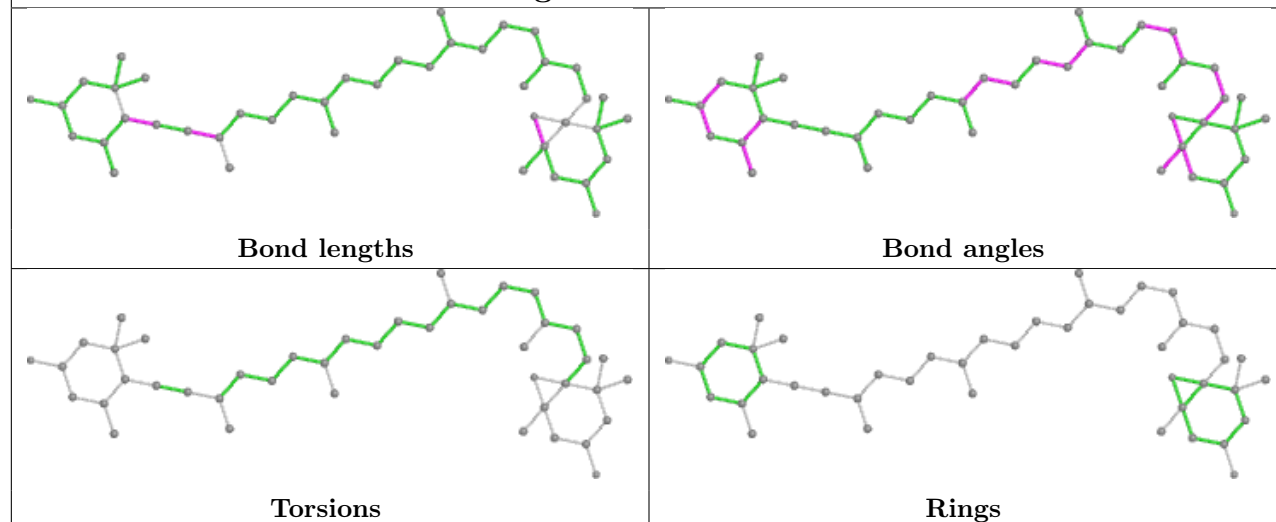


Torsions

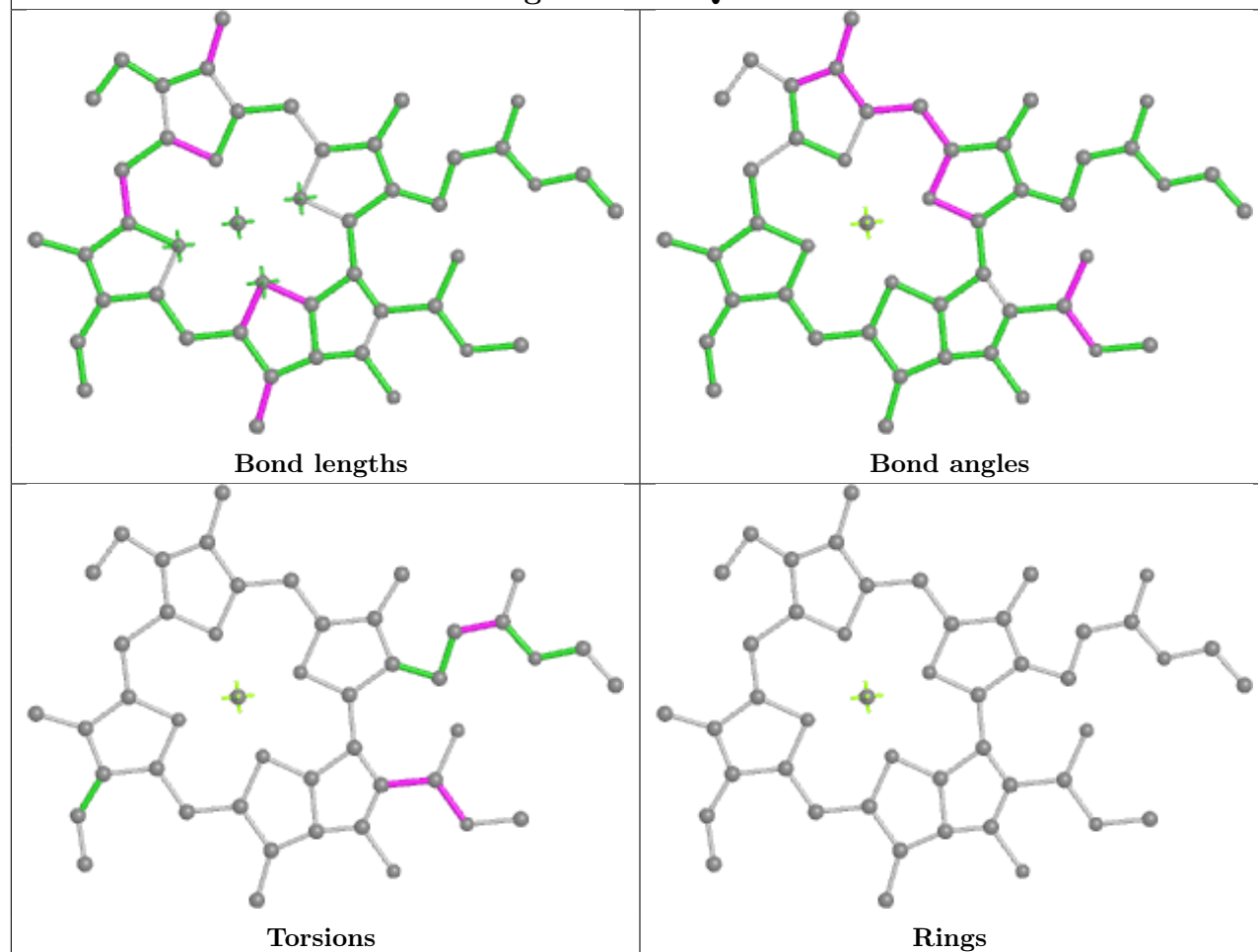


Rings

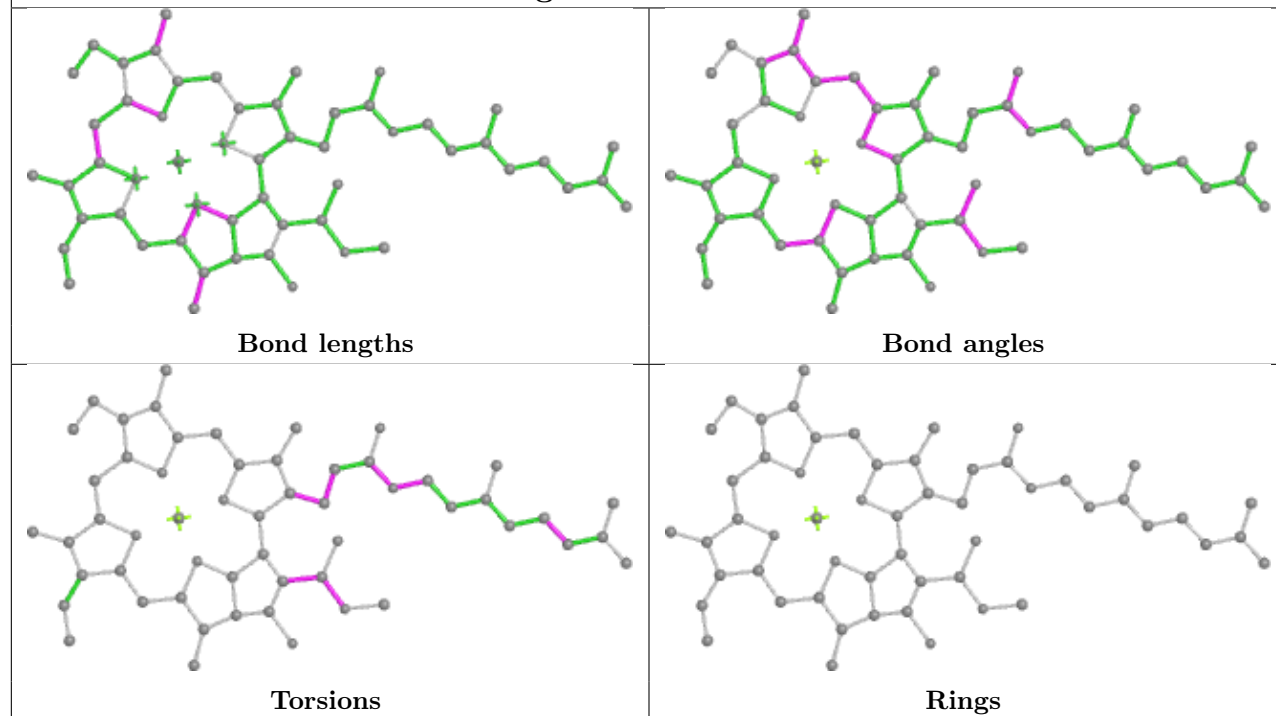
## Ligand DD6 E 302



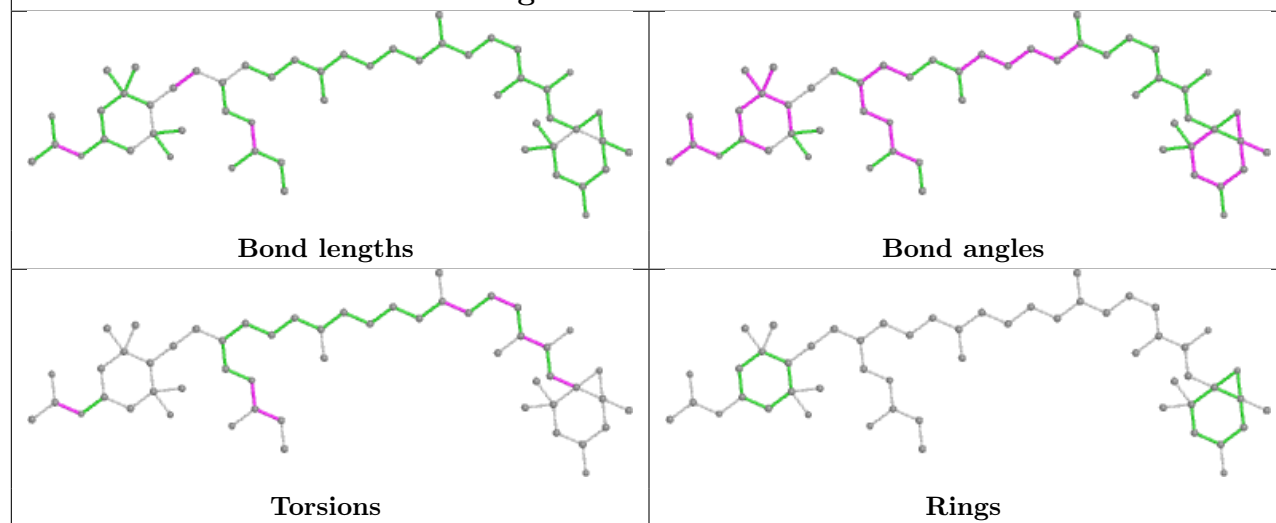
## Ligand CLA Q 320



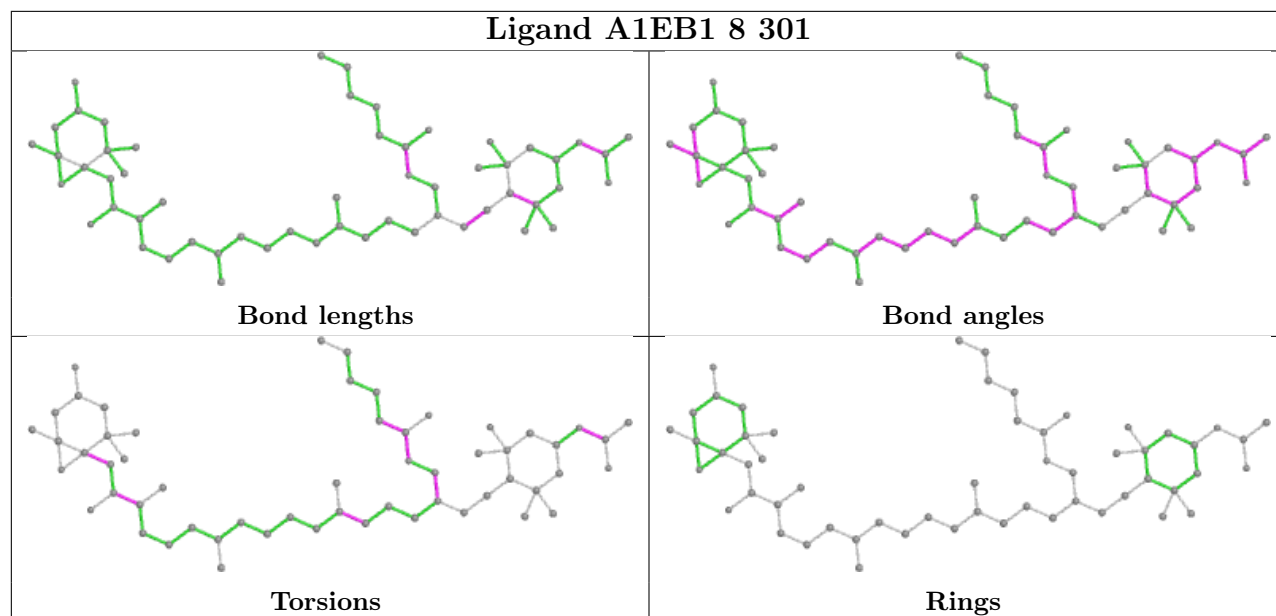
## Ligand CLA k 202



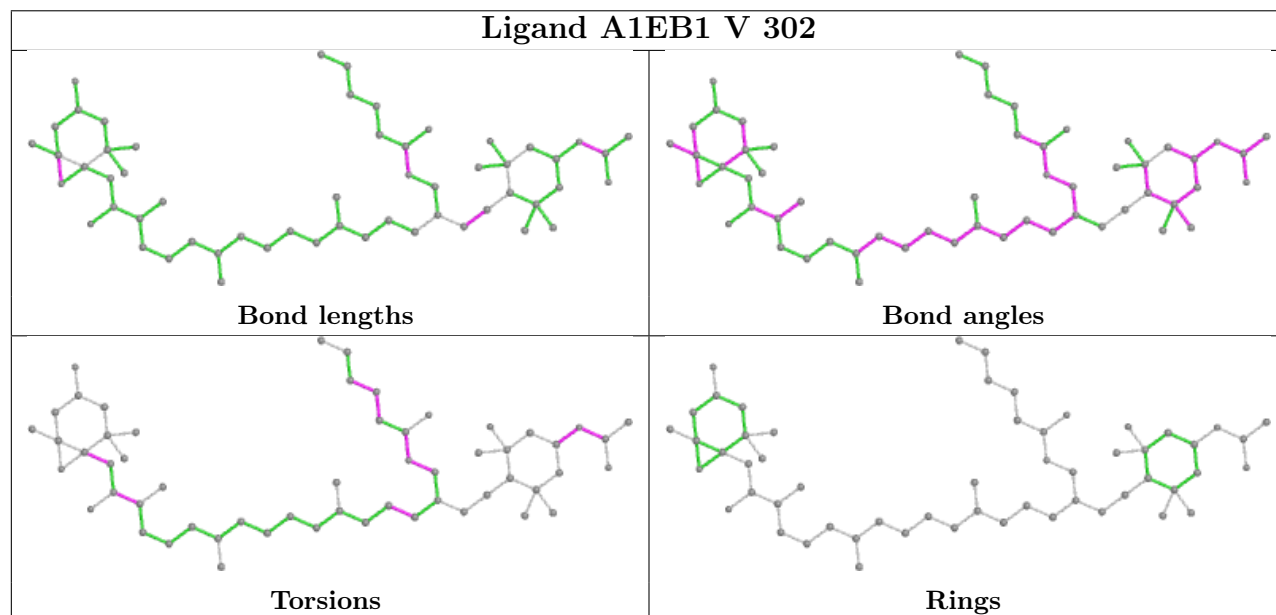
## Ligand A1EB1 6 304



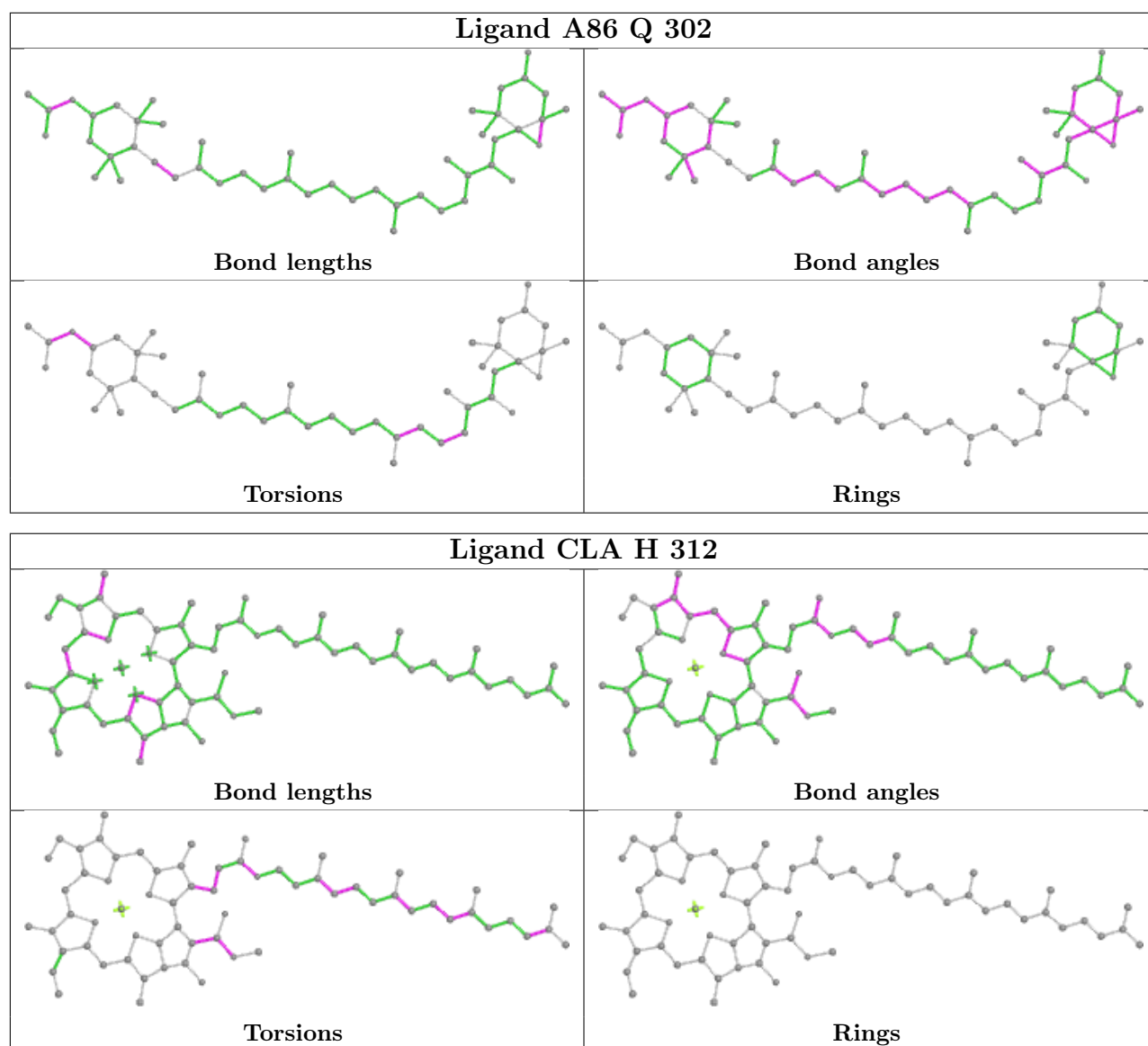
## Ligand A1EB1 8 301



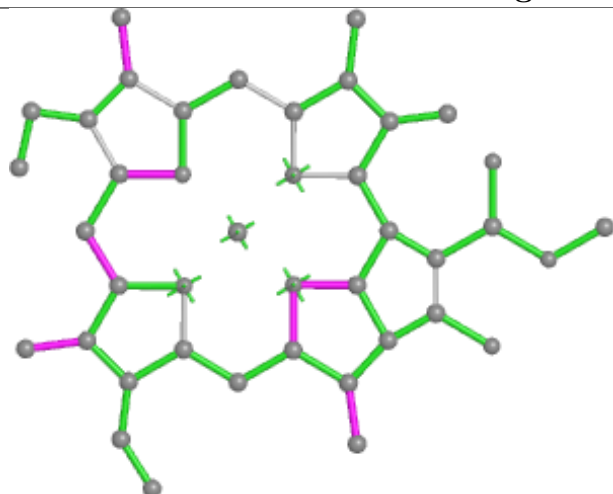
## Ligand A1EB1 V 302



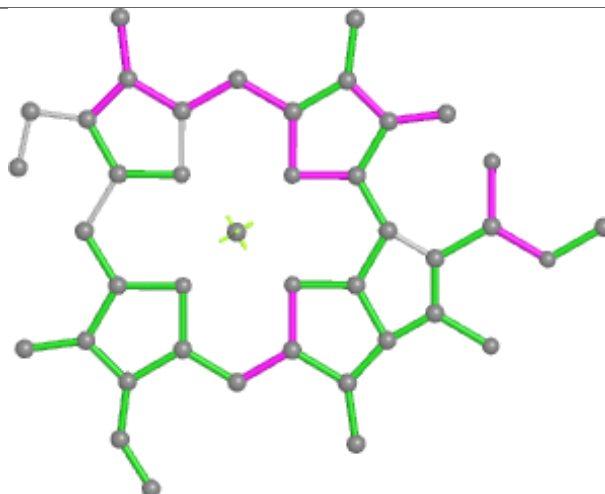




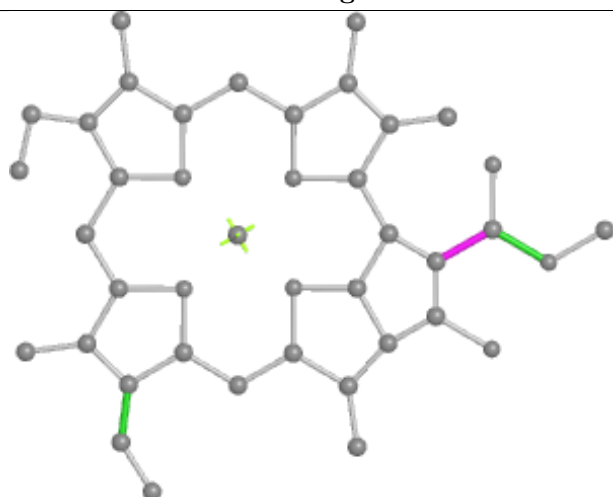
## Ligand CLA P 314



Bond lengths



Bond angles

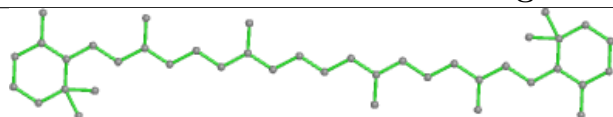


Torsions

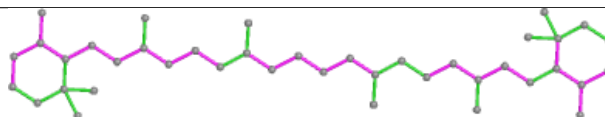


Rings

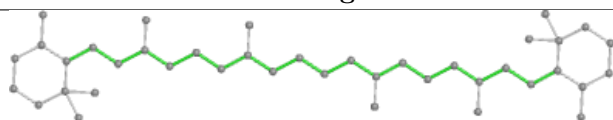
## Ligand BCR a 843



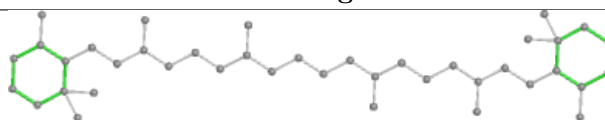
Bond lengths



Bond angles

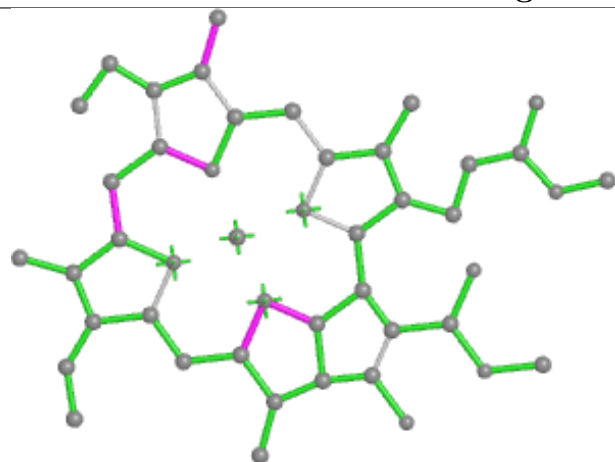


Torsions

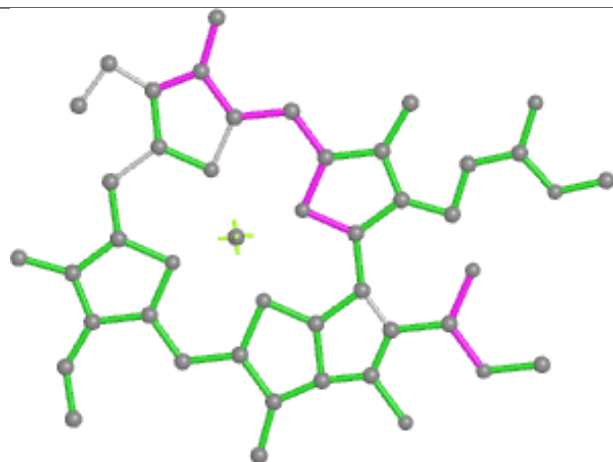


Rings

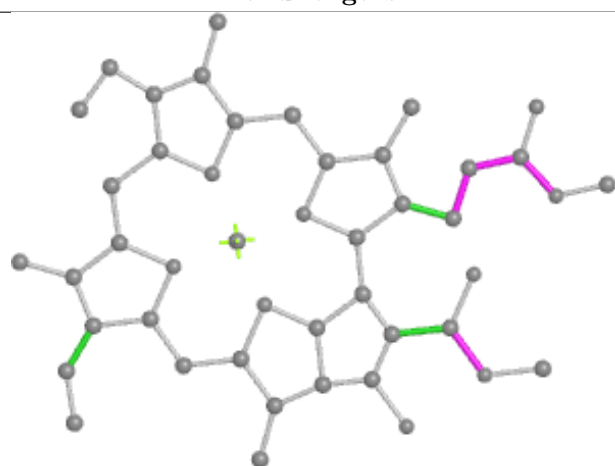
## Ligand CLA Y 304



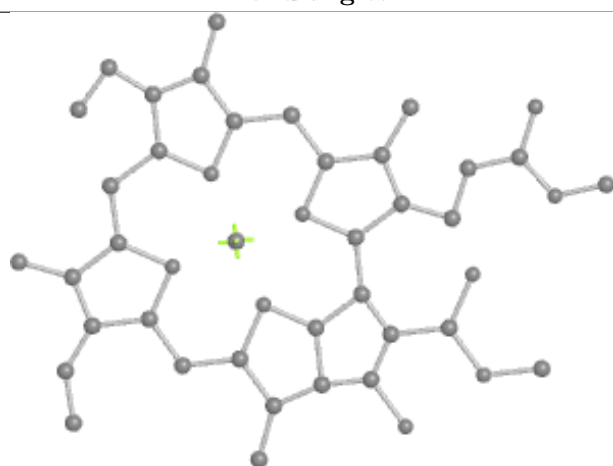
Bond lengths



Bond angles

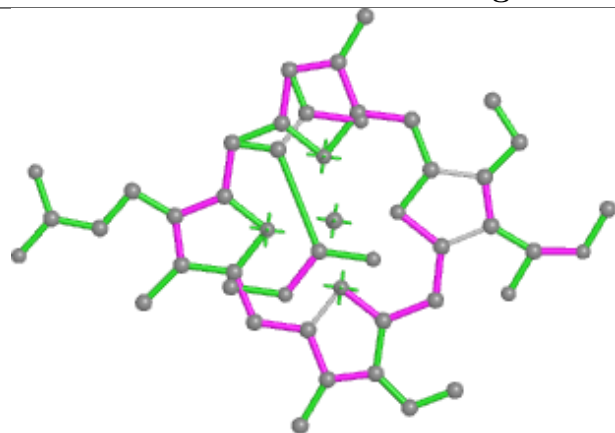


Torsions

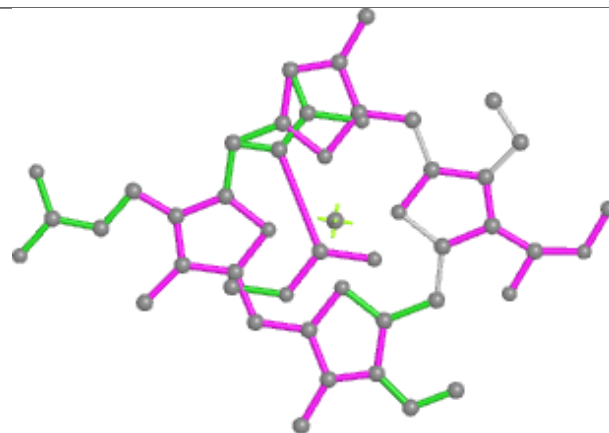


Rings

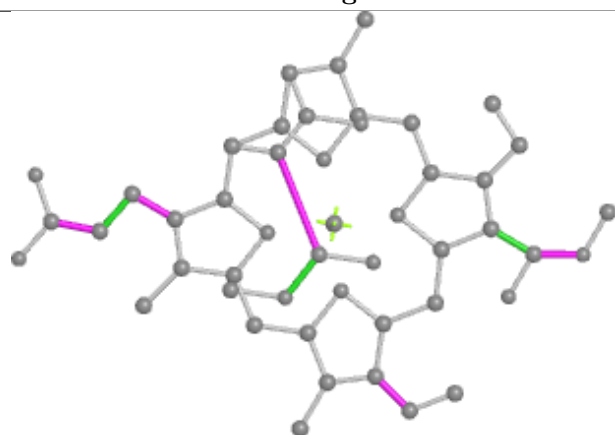
## Ligand A1ECV R 313



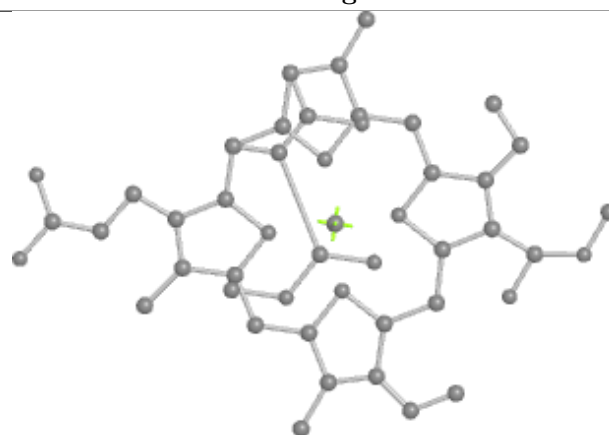
Bond lengths



Bond angles

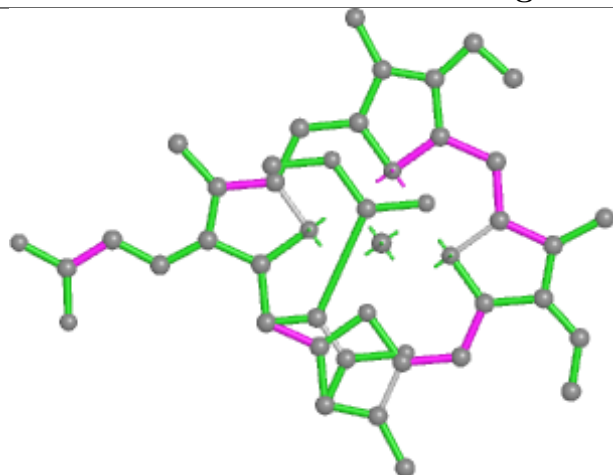


Torsions

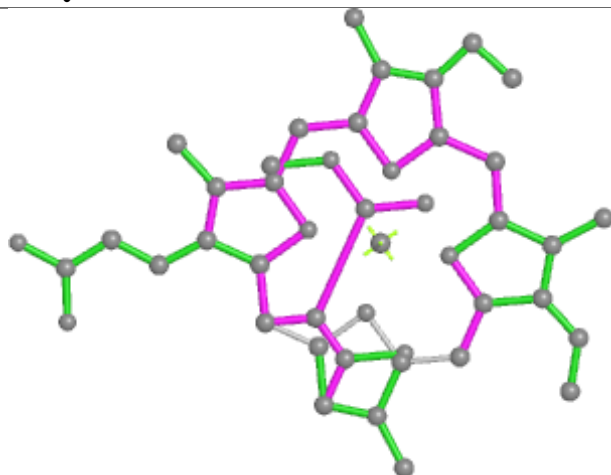


Rings

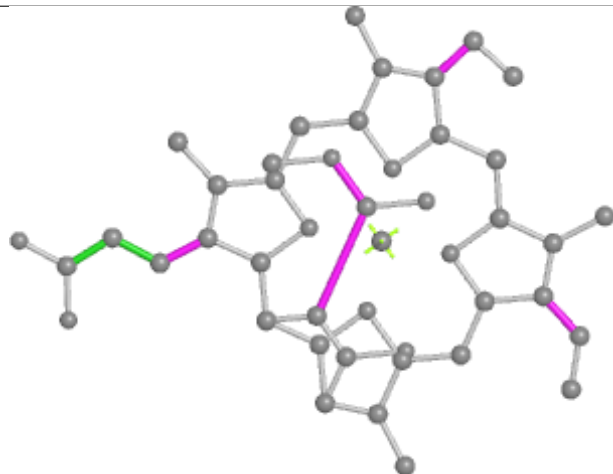
## Ligand KC2 Q 315



Bond lengths



Bond angles

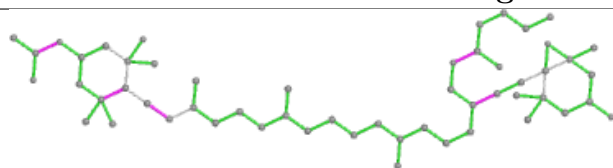


Torsions

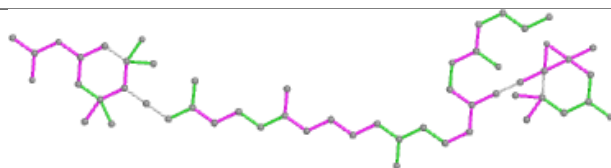


Rings

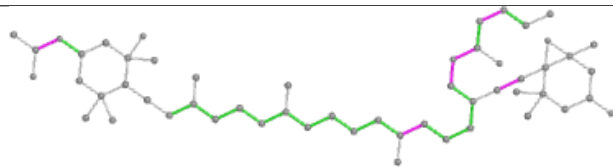
## Ligand A1EB4 P 318



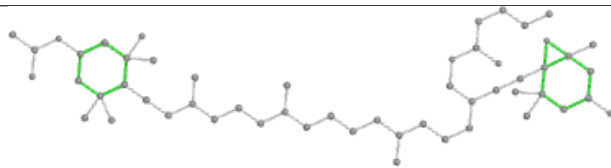
Bond lengths



Bond angles

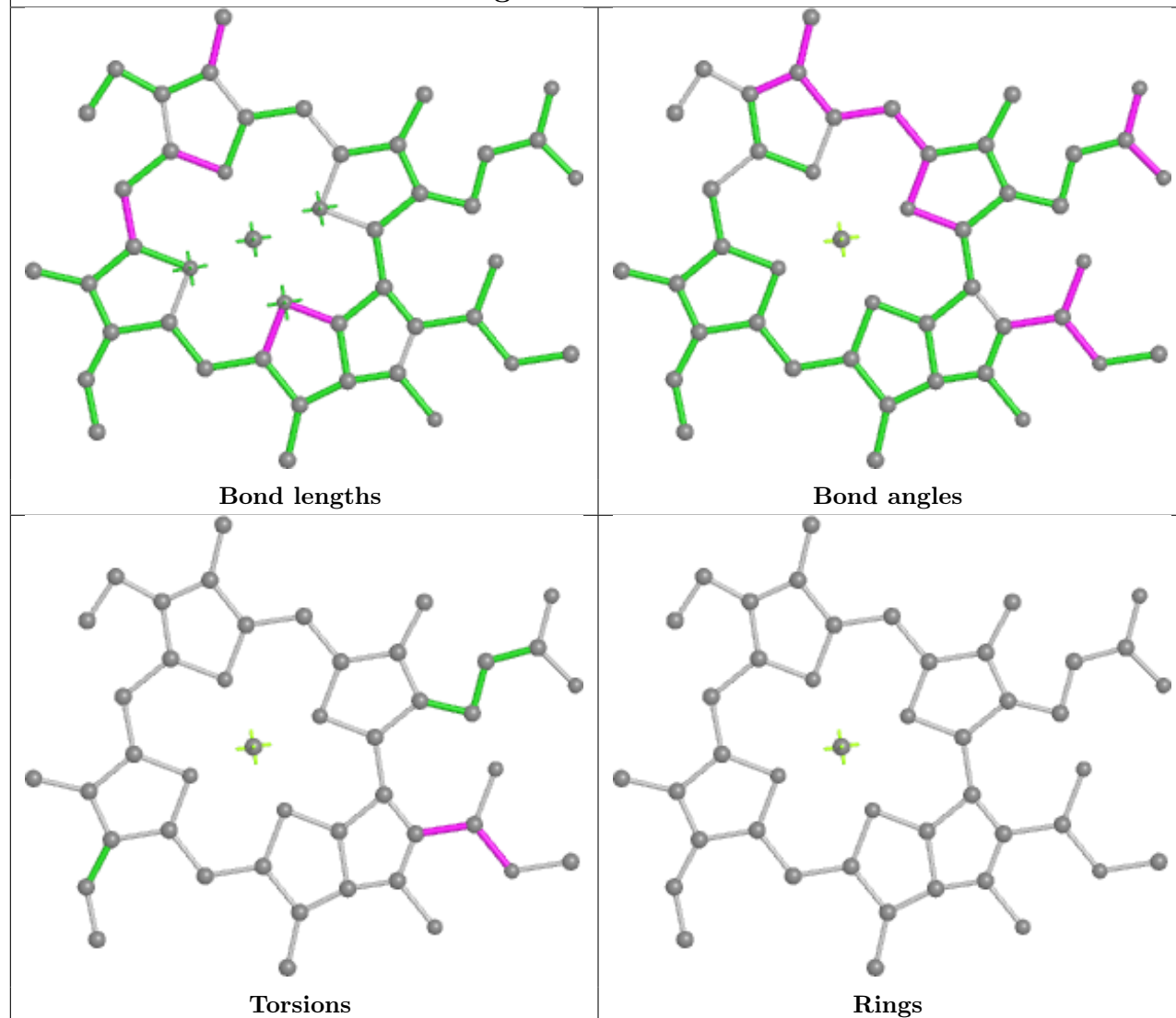


Torsions

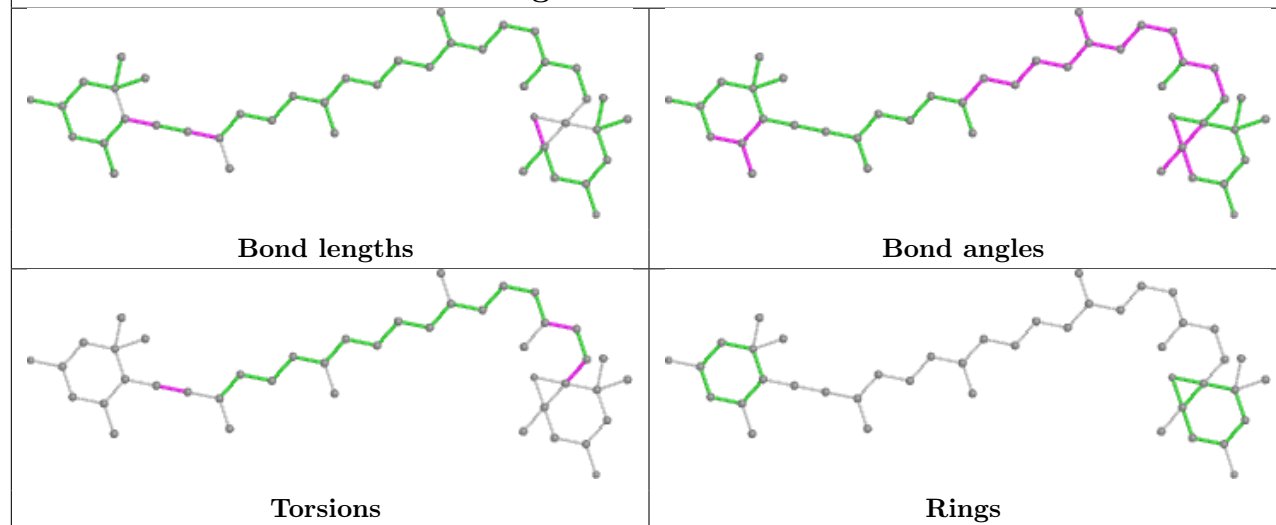


Rings

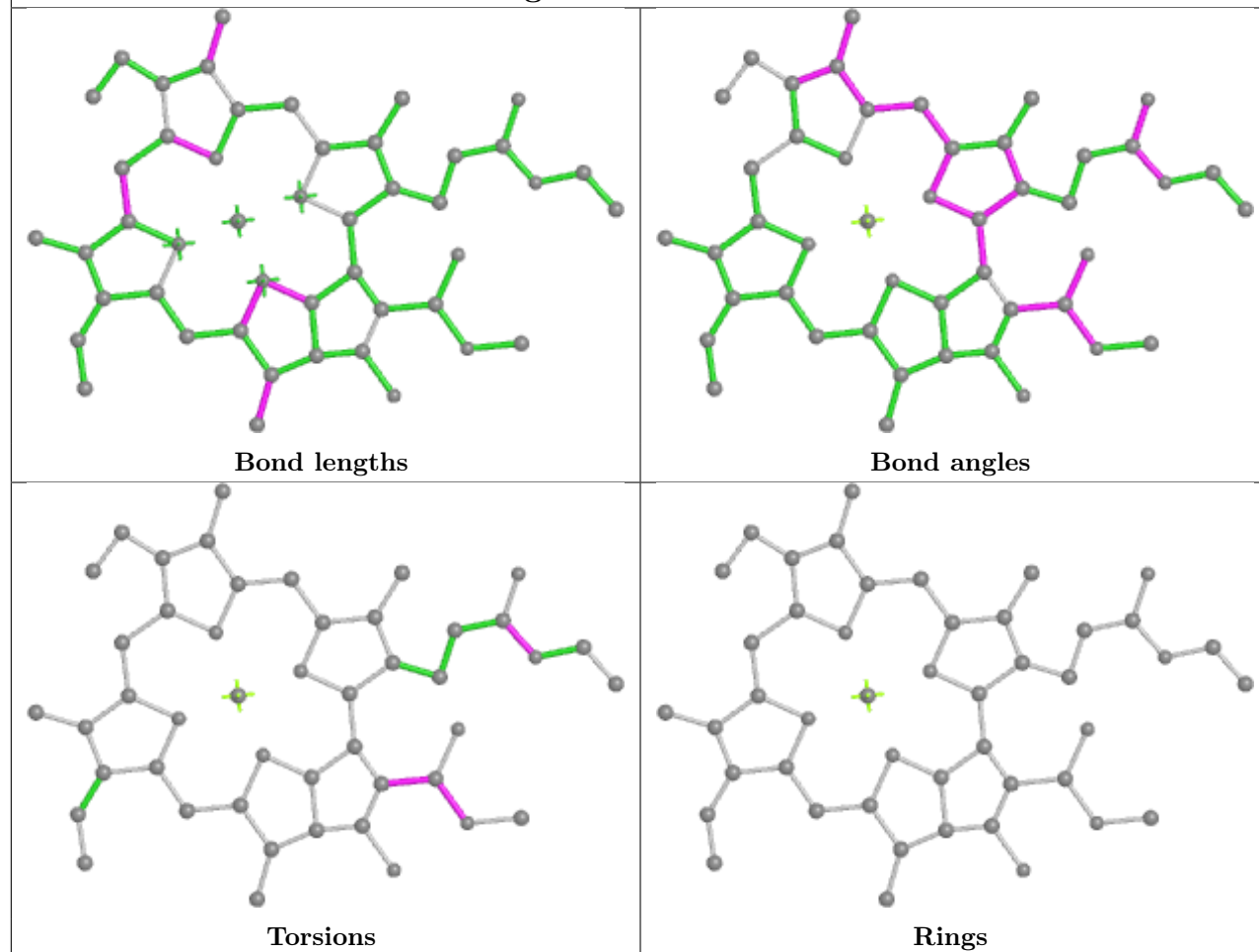
## Ligand CLA 3 320



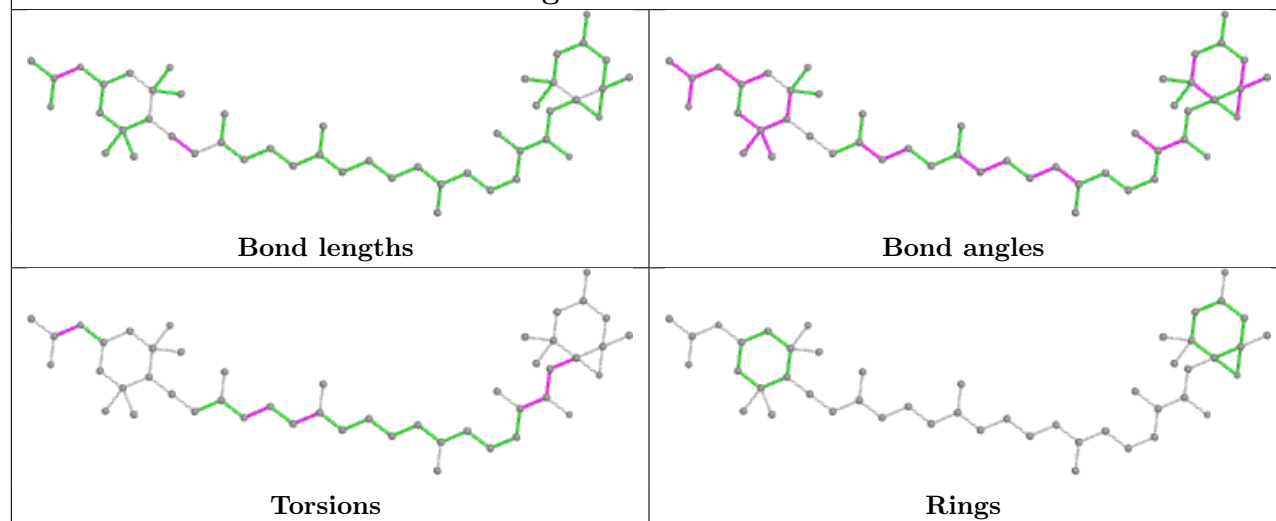
## Ligand DD6 G 306

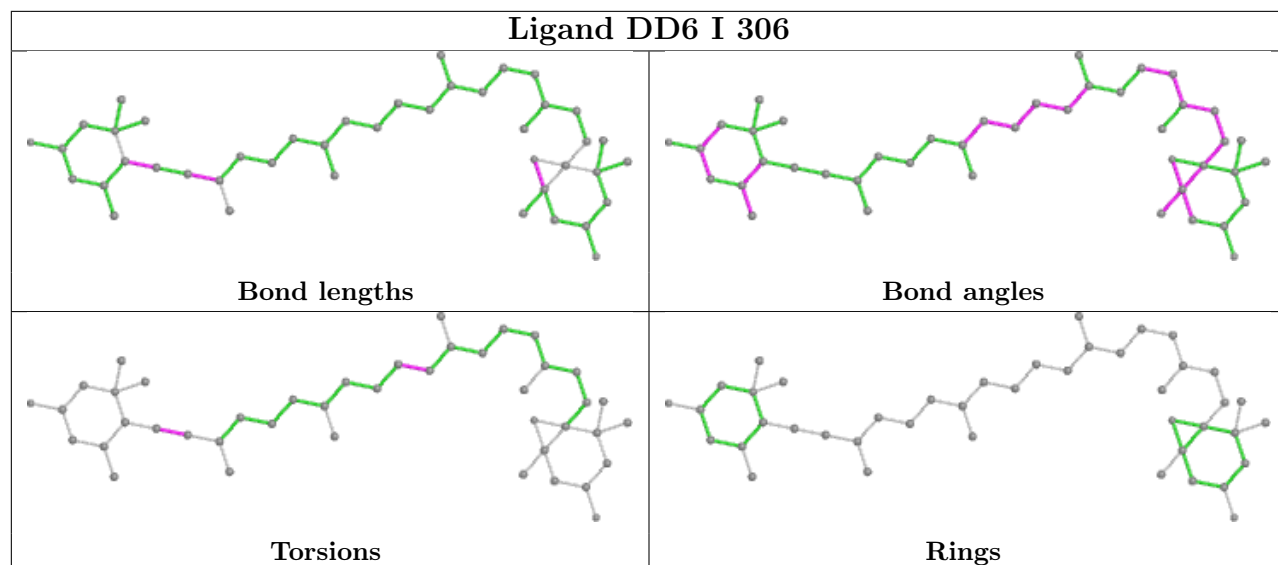
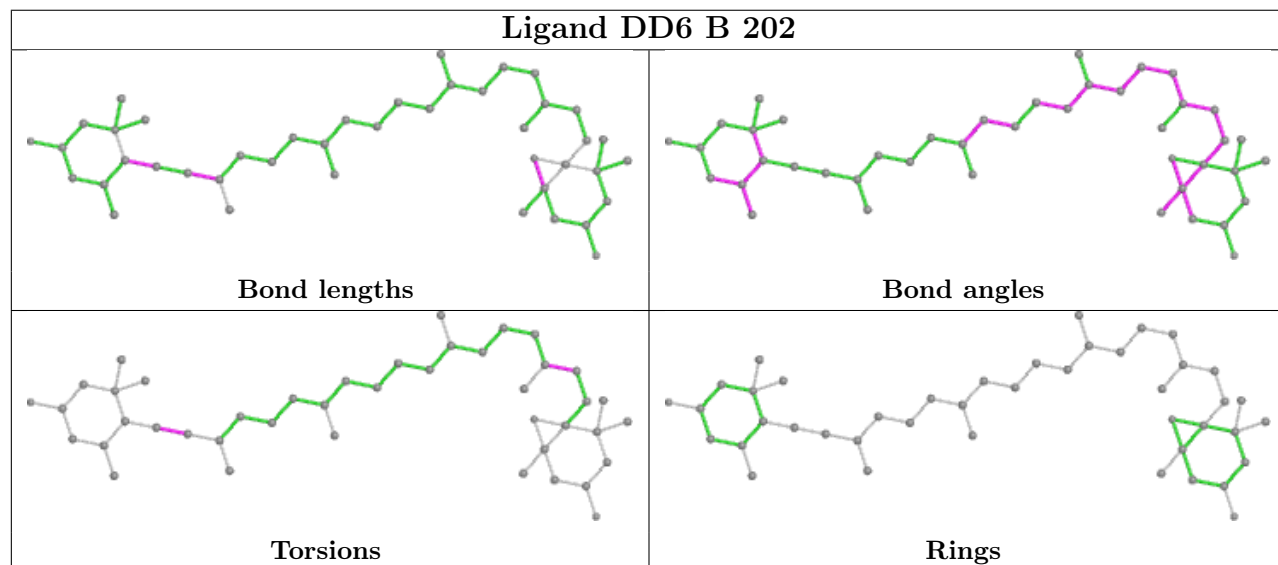


## Ligand CLA R 315

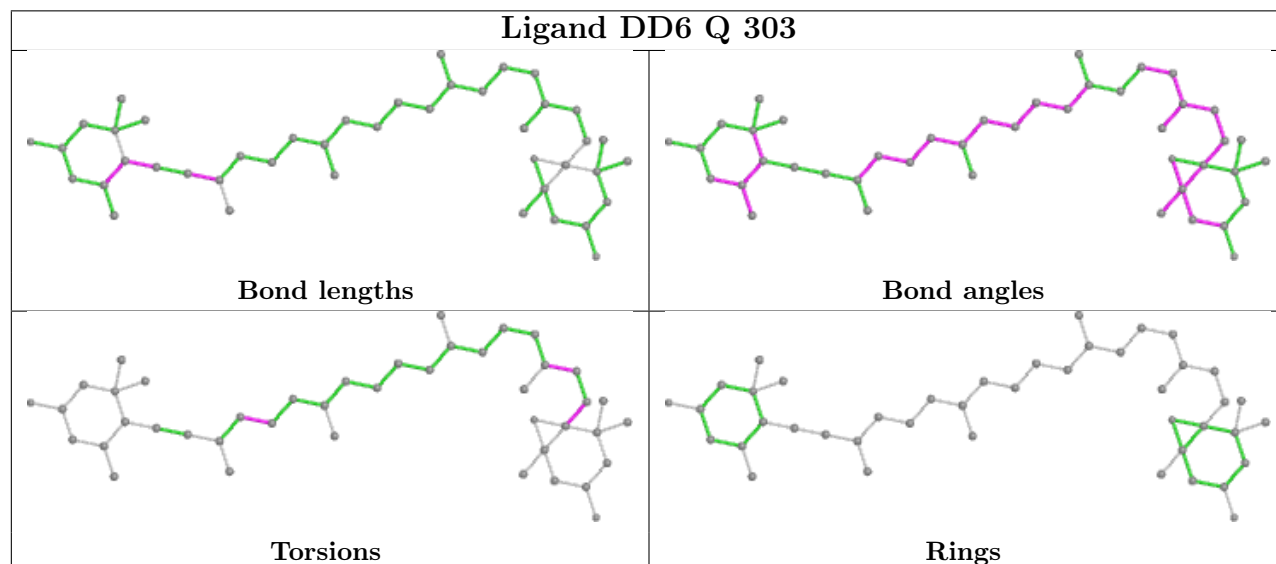
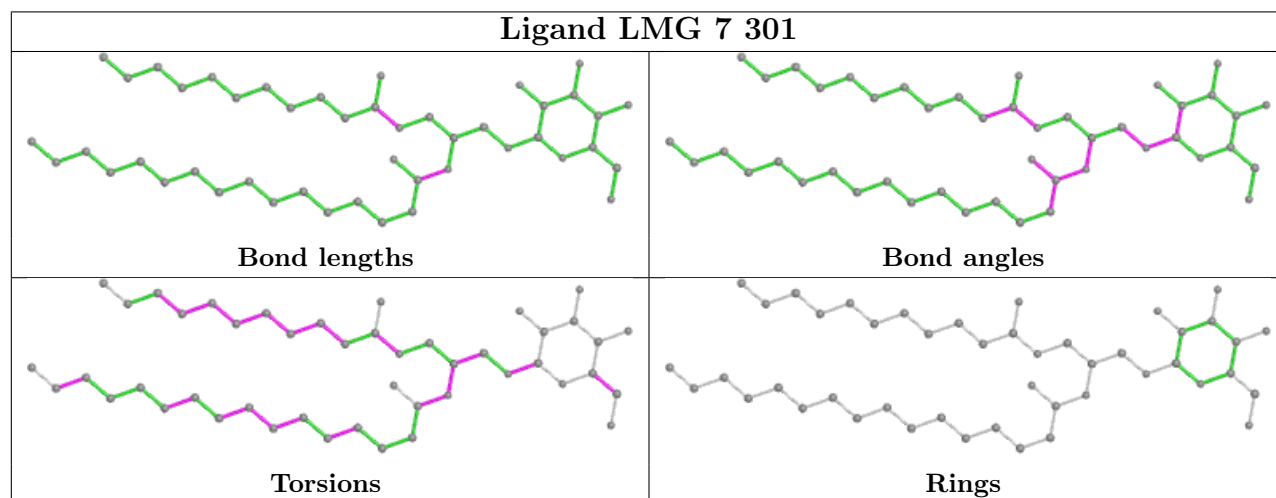
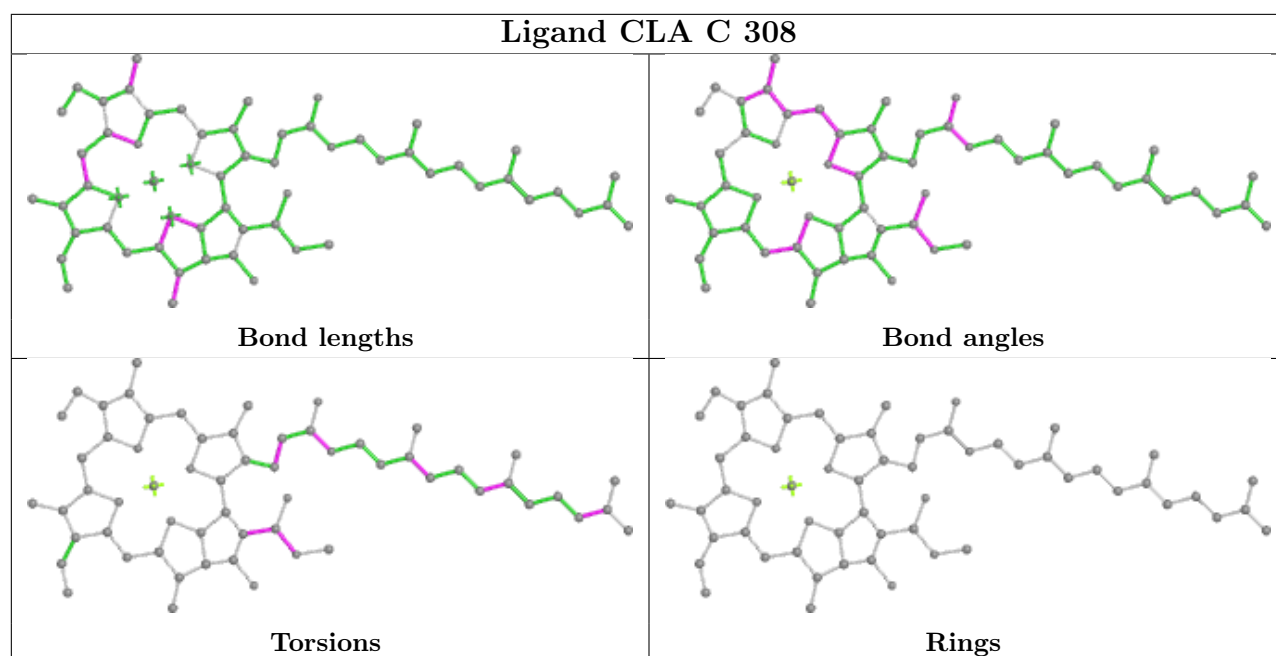


## Ligand A86 6 305

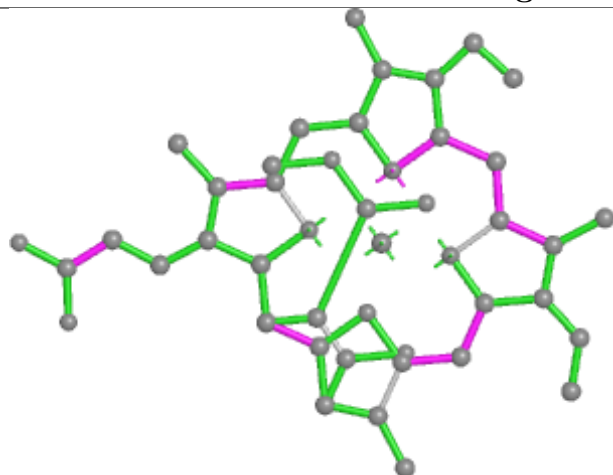


**Ligand DD6 I 306****Ligand DD6 B 202**

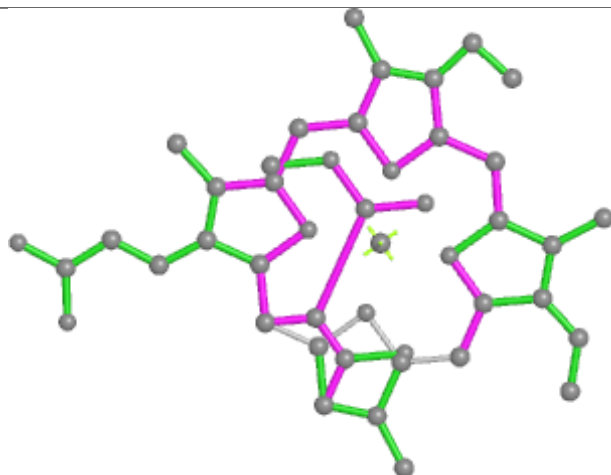




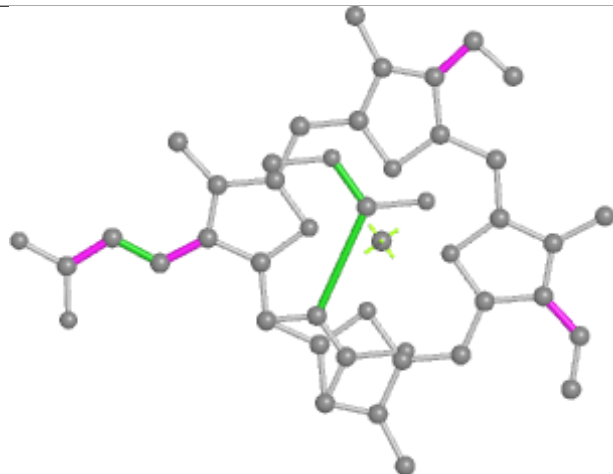
## Ligand KC2 R 318



Bond lengths



Bond angles

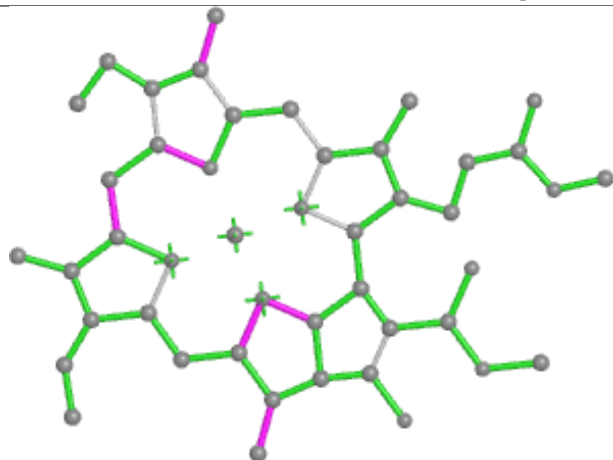


Torsions

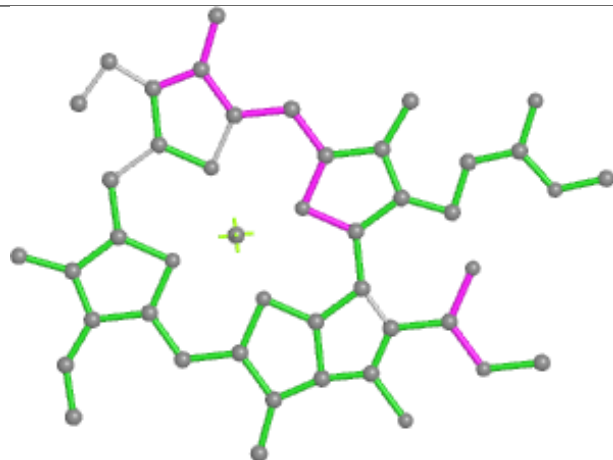


Rings

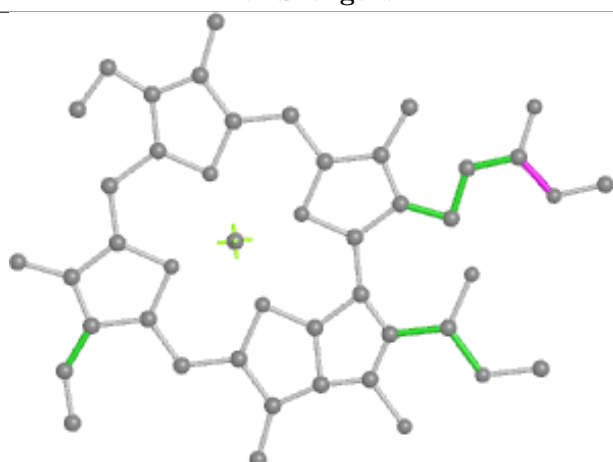
## Ligand CLA B 204



Bond lengths



Bond angles

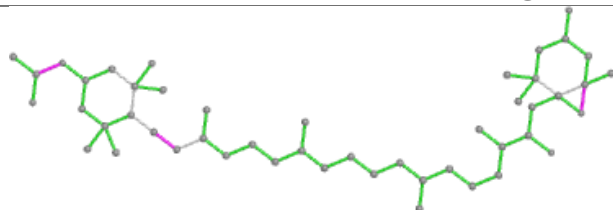


Torsions

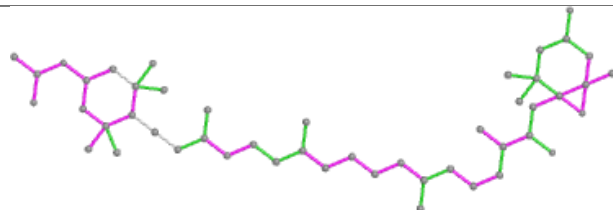


Rings

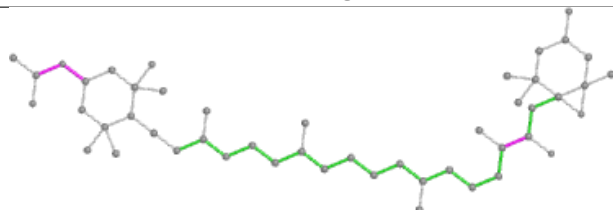
## Ligand A86 K 301



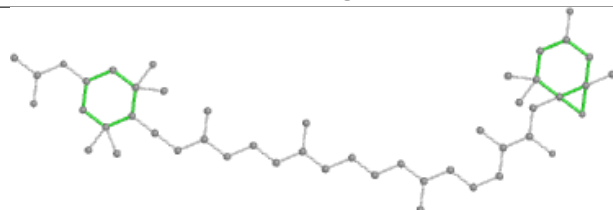
Bond lengths



Bond angles

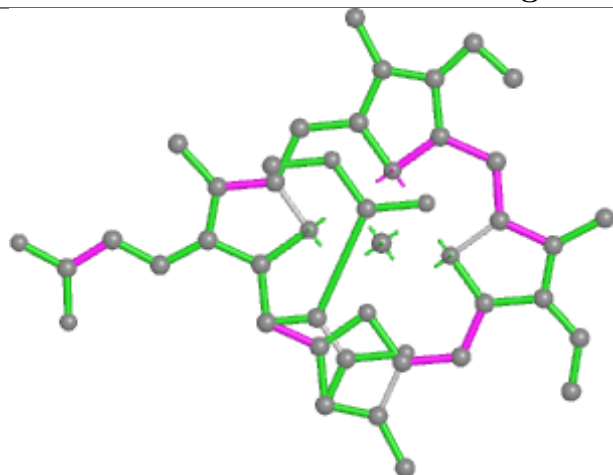


Torsions

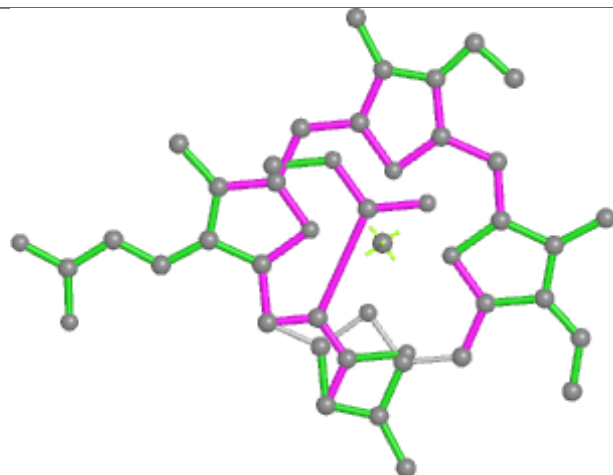


Rings

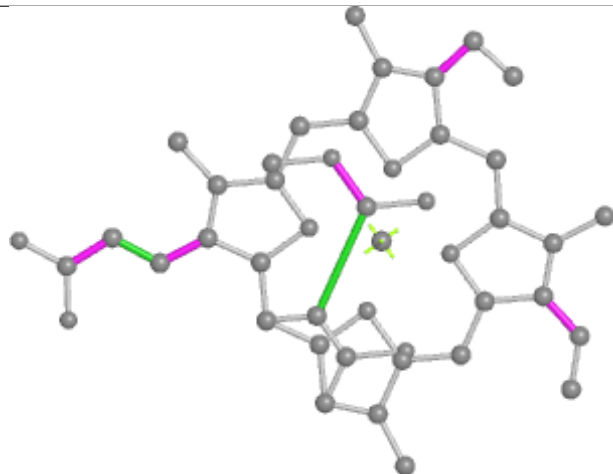
## Ligand KC2 z 315



Bond lengths



Bond angles

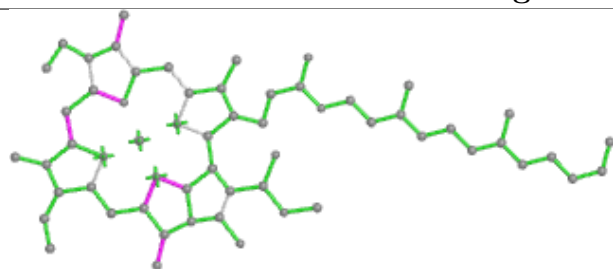


Torsions

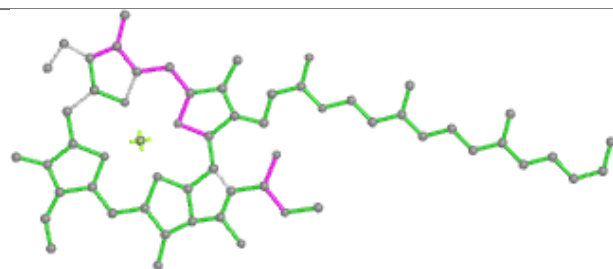


Rings

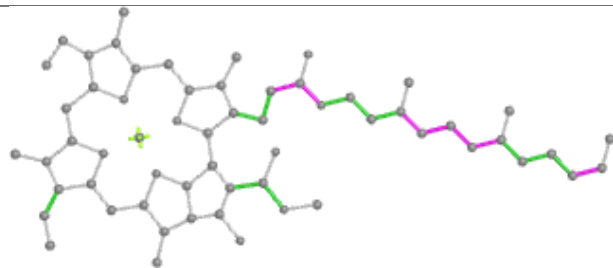
## Ligand CLA K 308



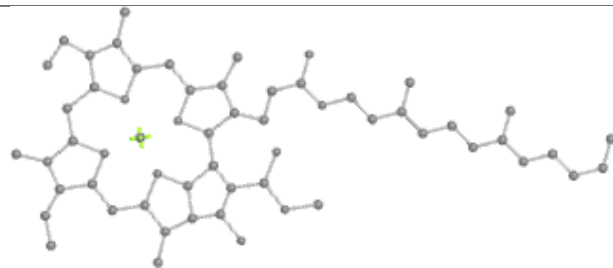
Bond lengths



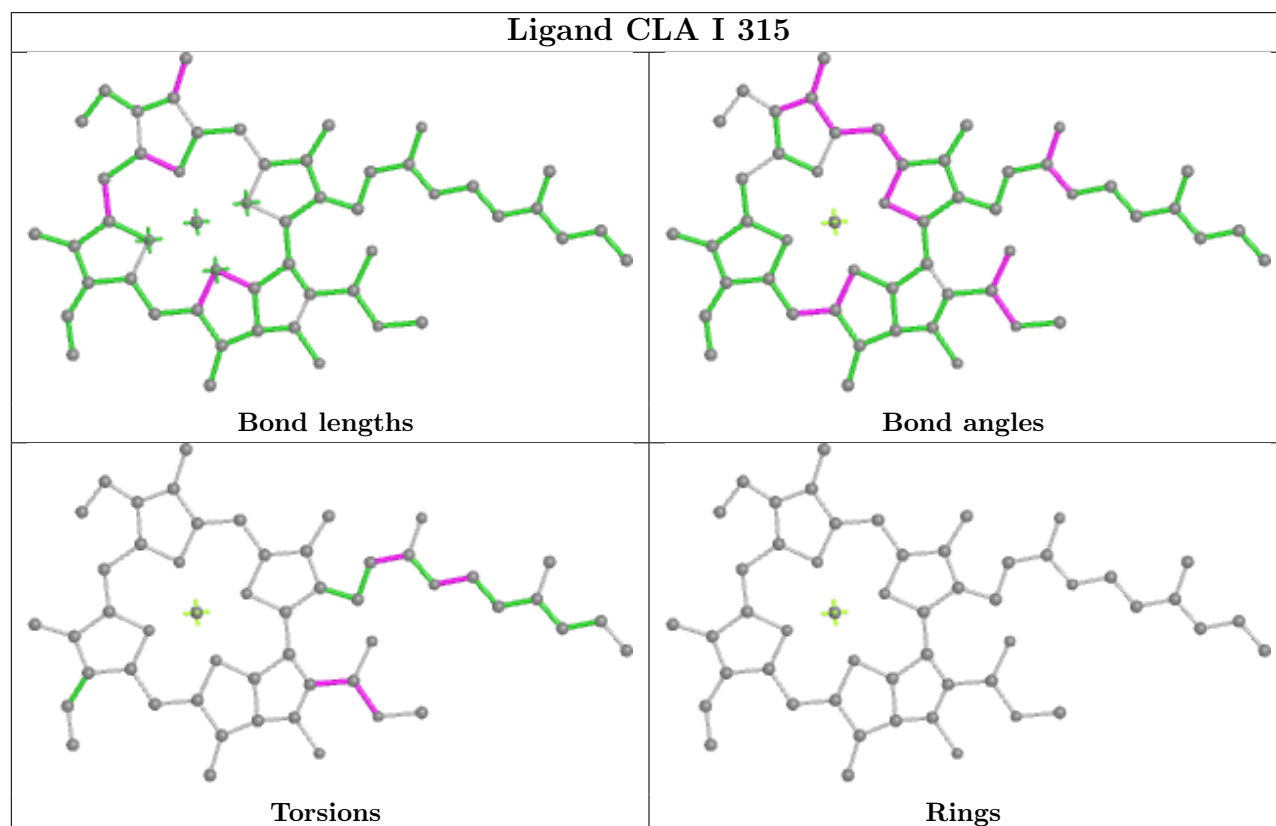
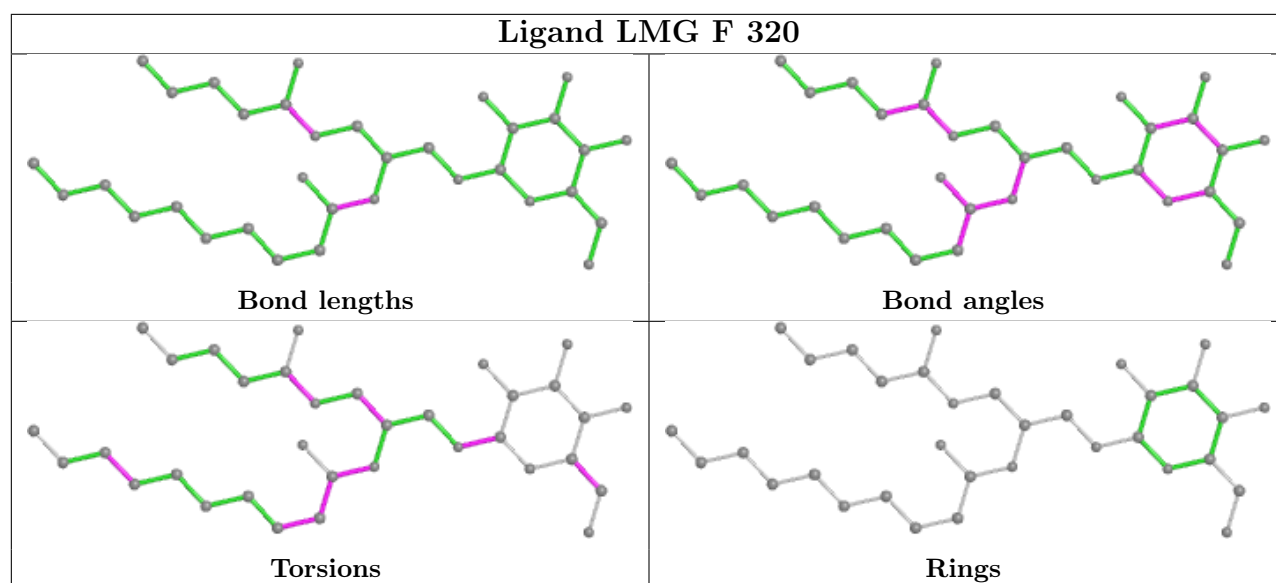
Bond angles

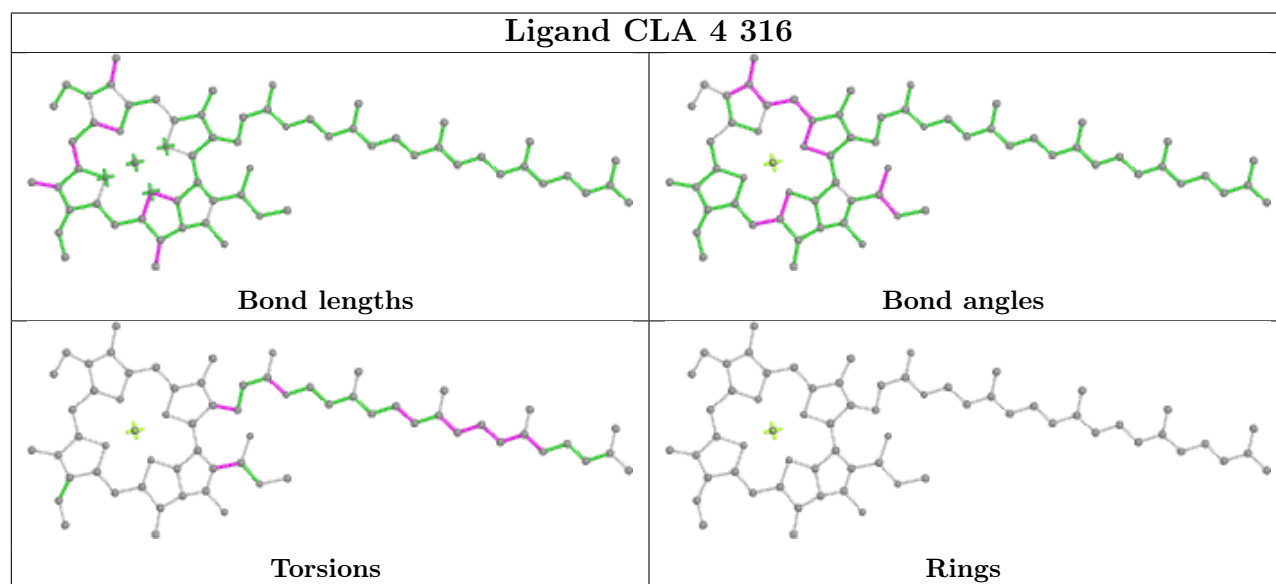
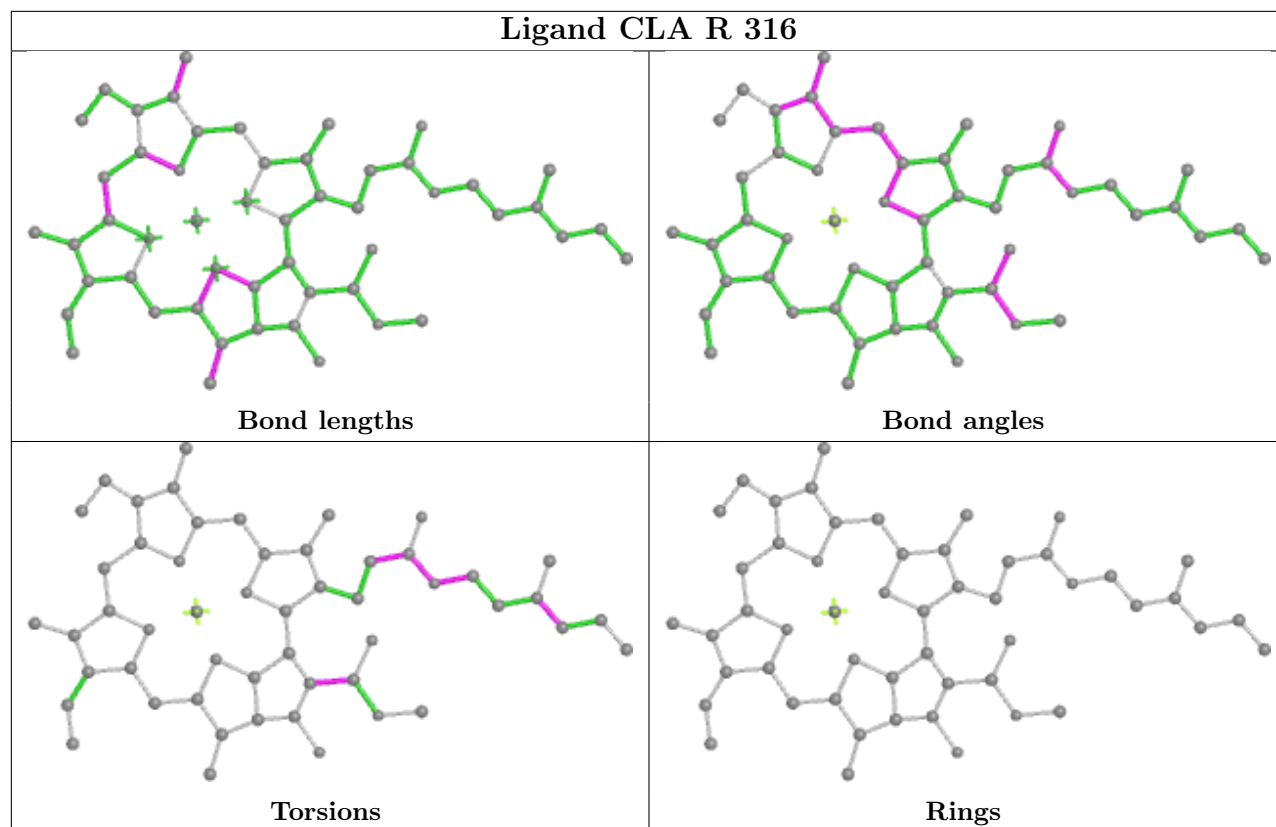


Torsions

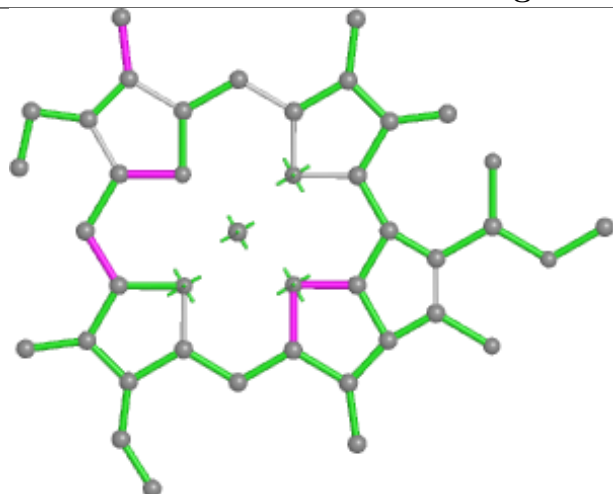


Rings

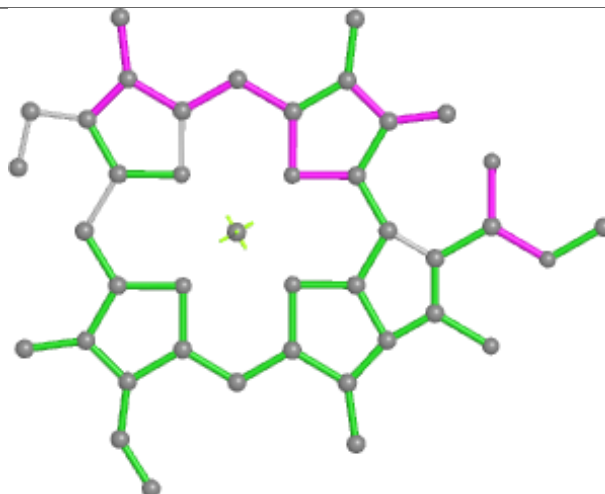




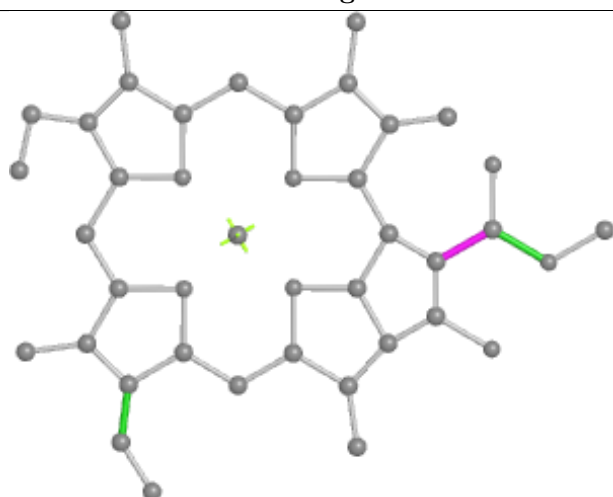
## Ligand CLA Y 307



Bond lengths



Bond angles

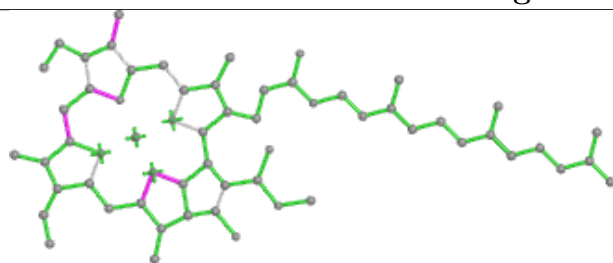


Torsions

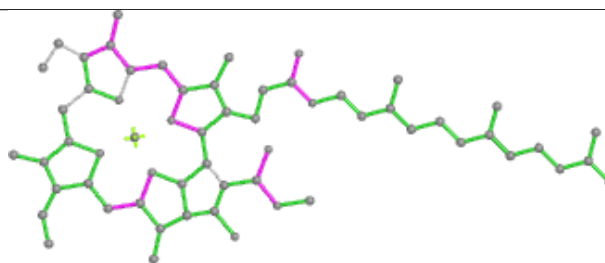


Rings

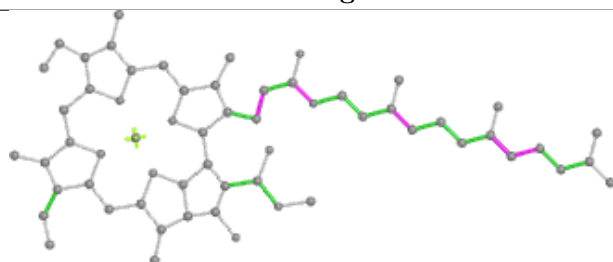
## Ligand CLA H 308



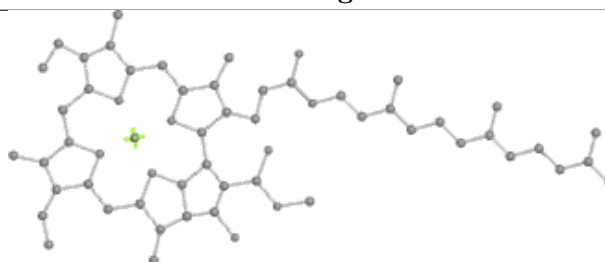
Bond lengths



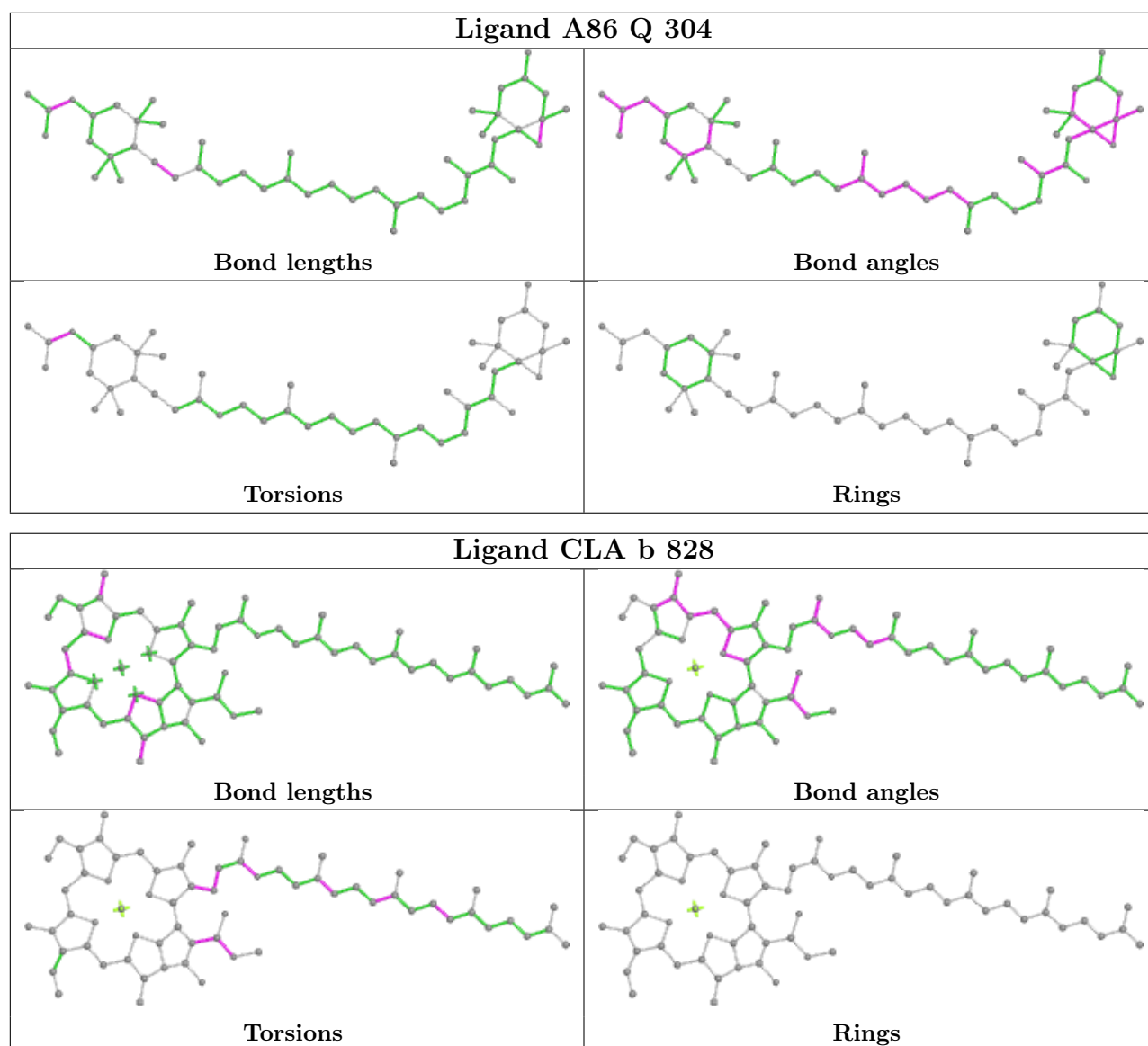
Bond angles



Torsions

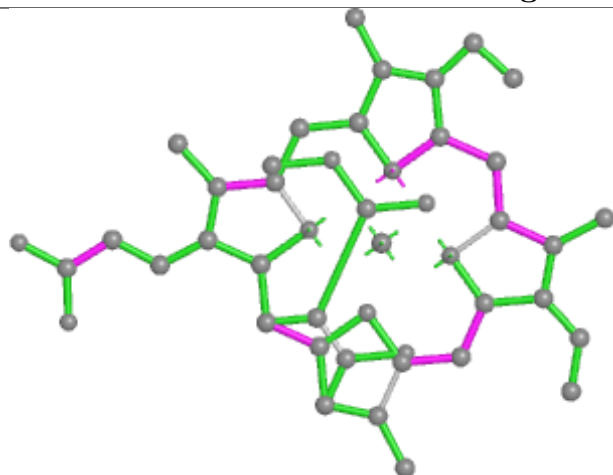


Rings

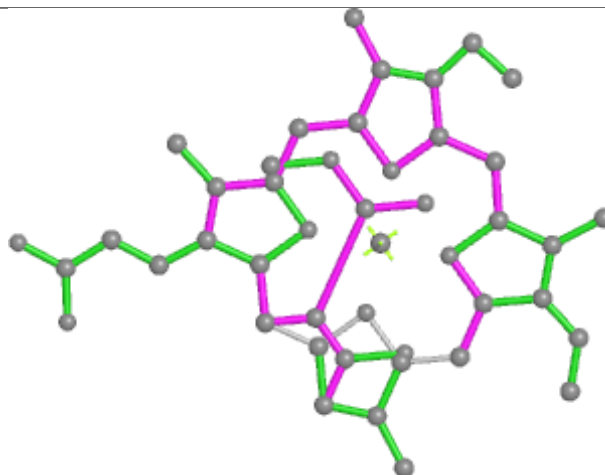




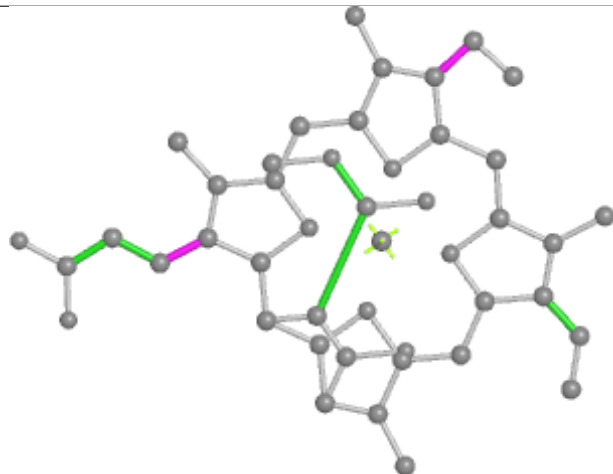
## Ligand KC2 0 316



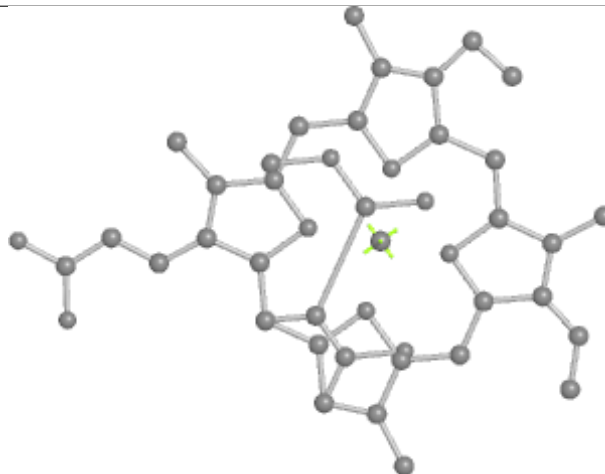
Bond lengths



Bond angles

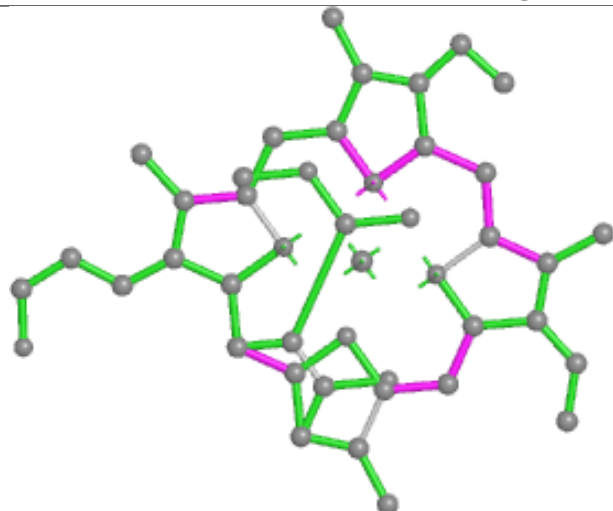


Torsions

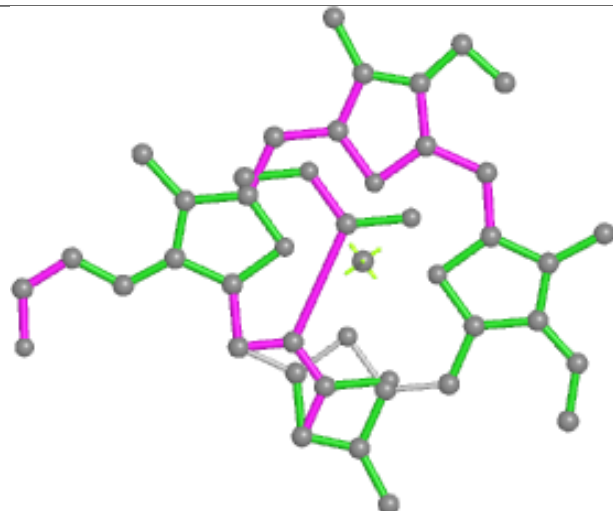


Rings

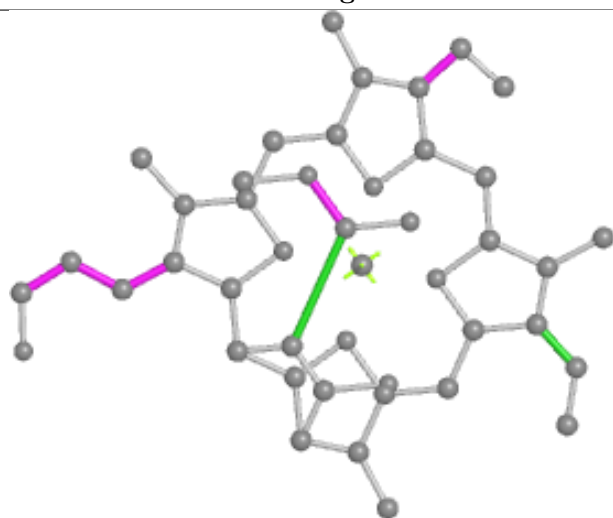
## Ligand KC2 O 317



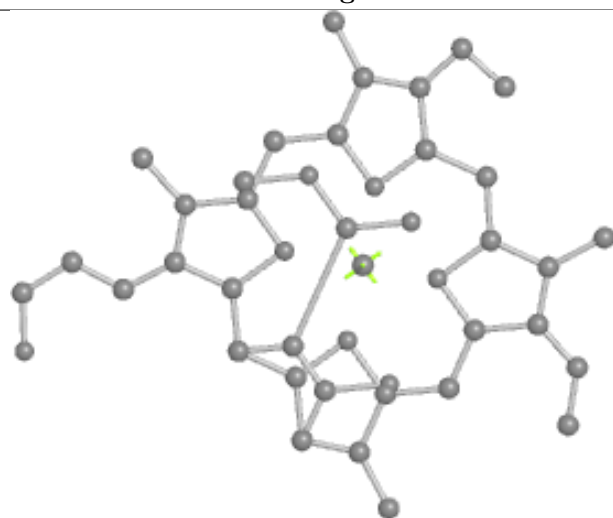
Bond lengths



Bond angles

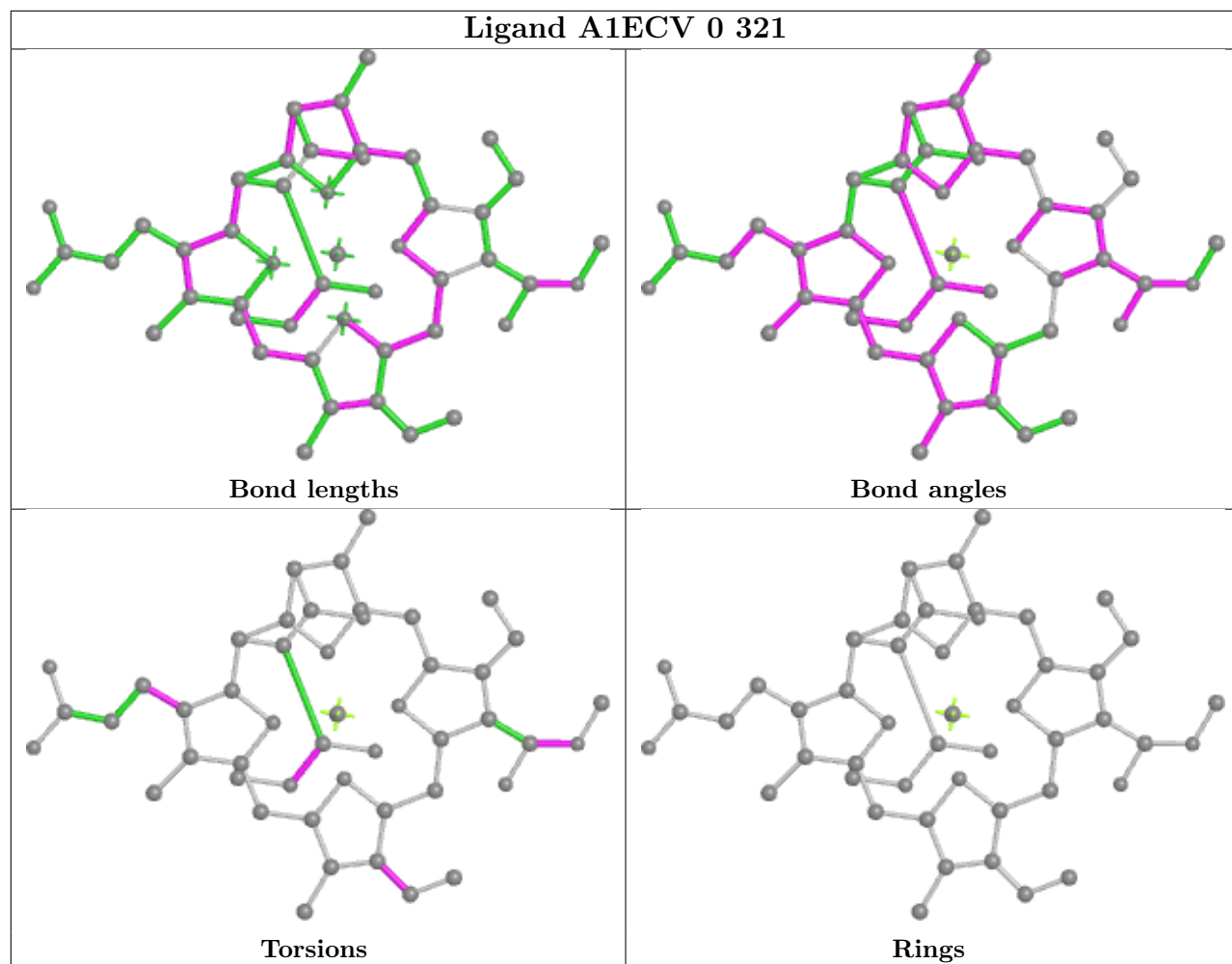


Torsions

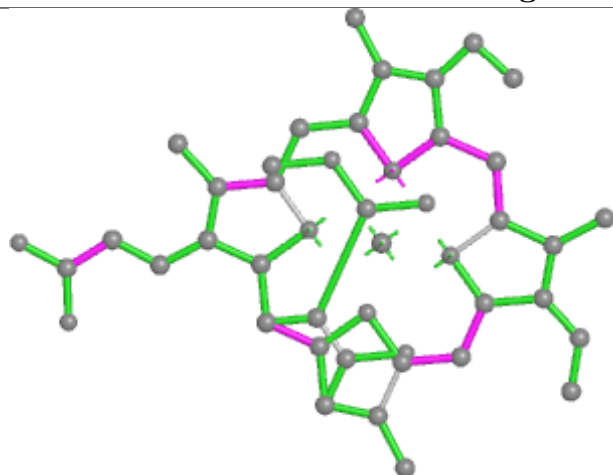


Rings

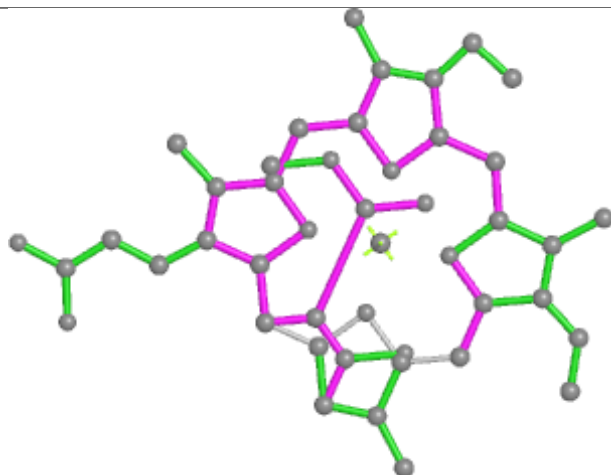
## Ligand A1ECV 0 321



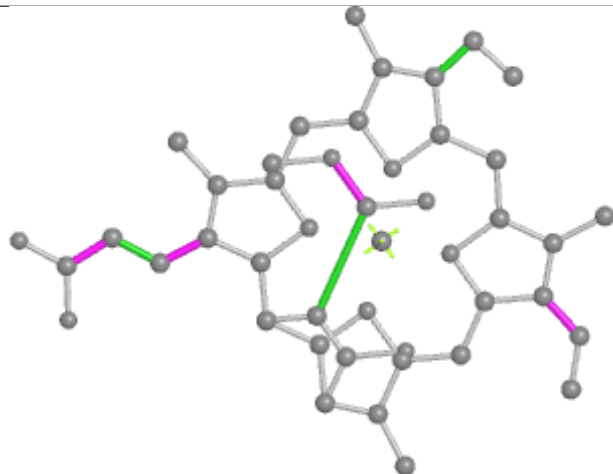
## Ligand KC2 S 315



Bond lengths



Bond angles

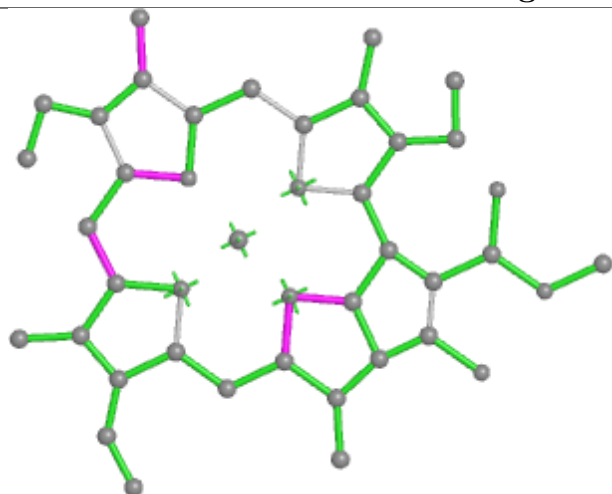


Torsions

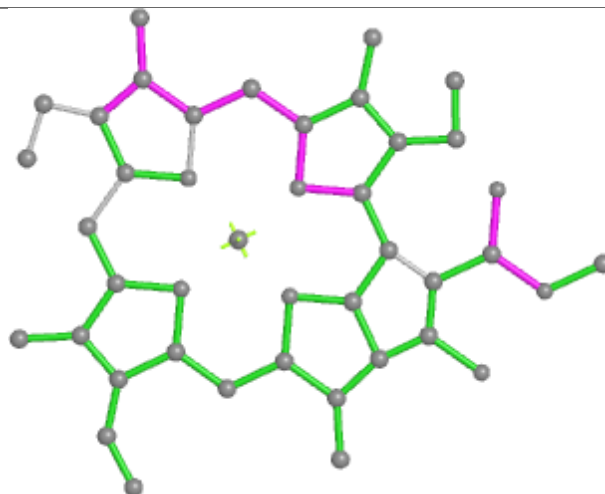


Rings

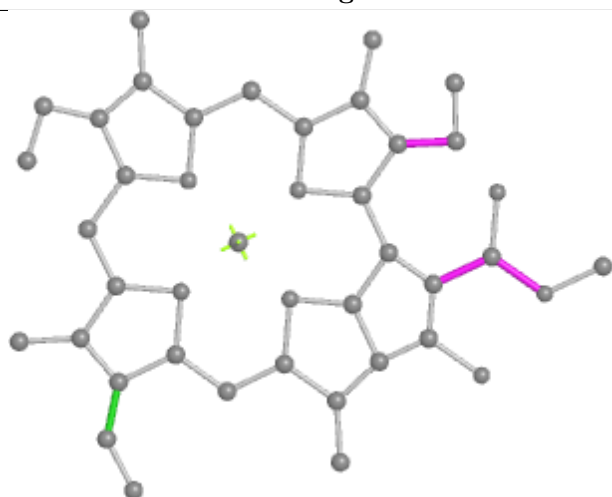
## Ligand CLA z 317



Bond lengths



Bond angles

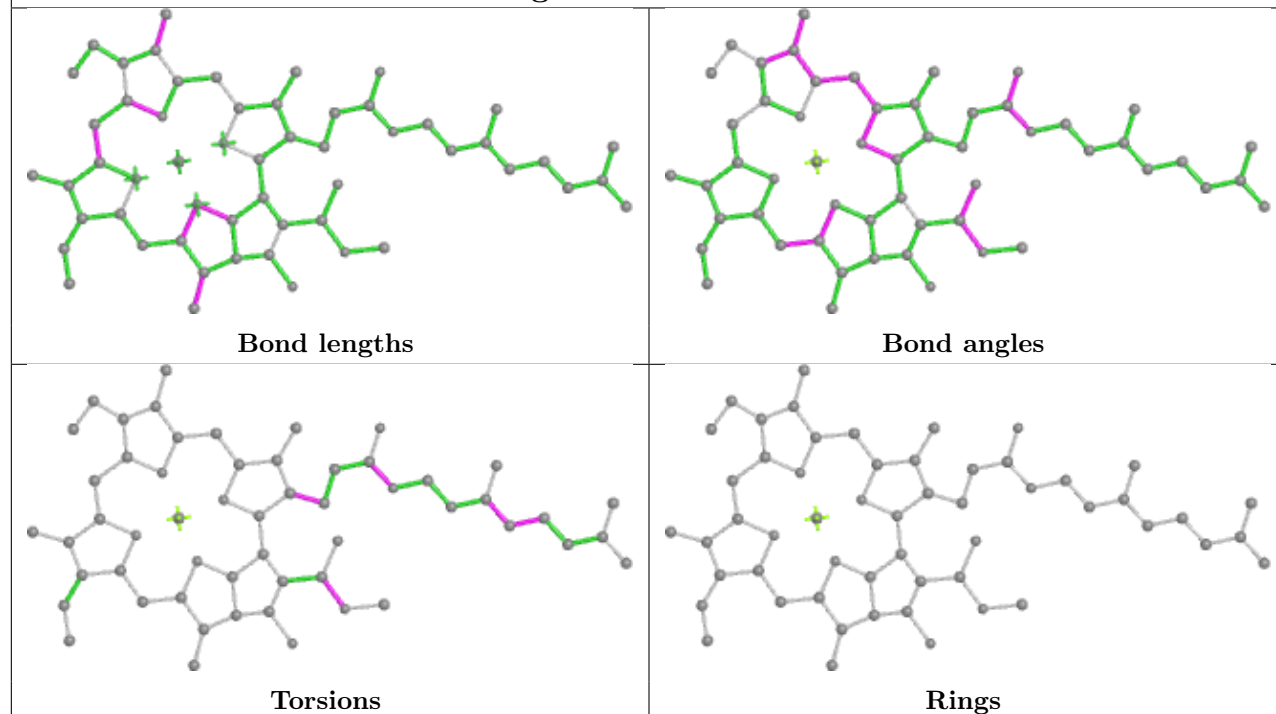


Torsions

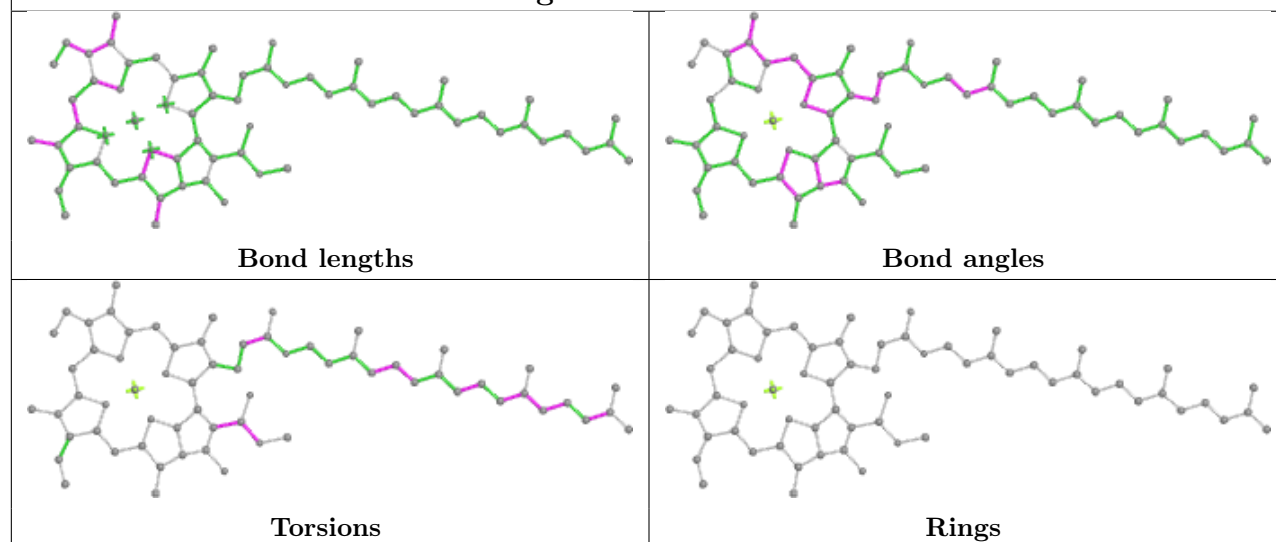


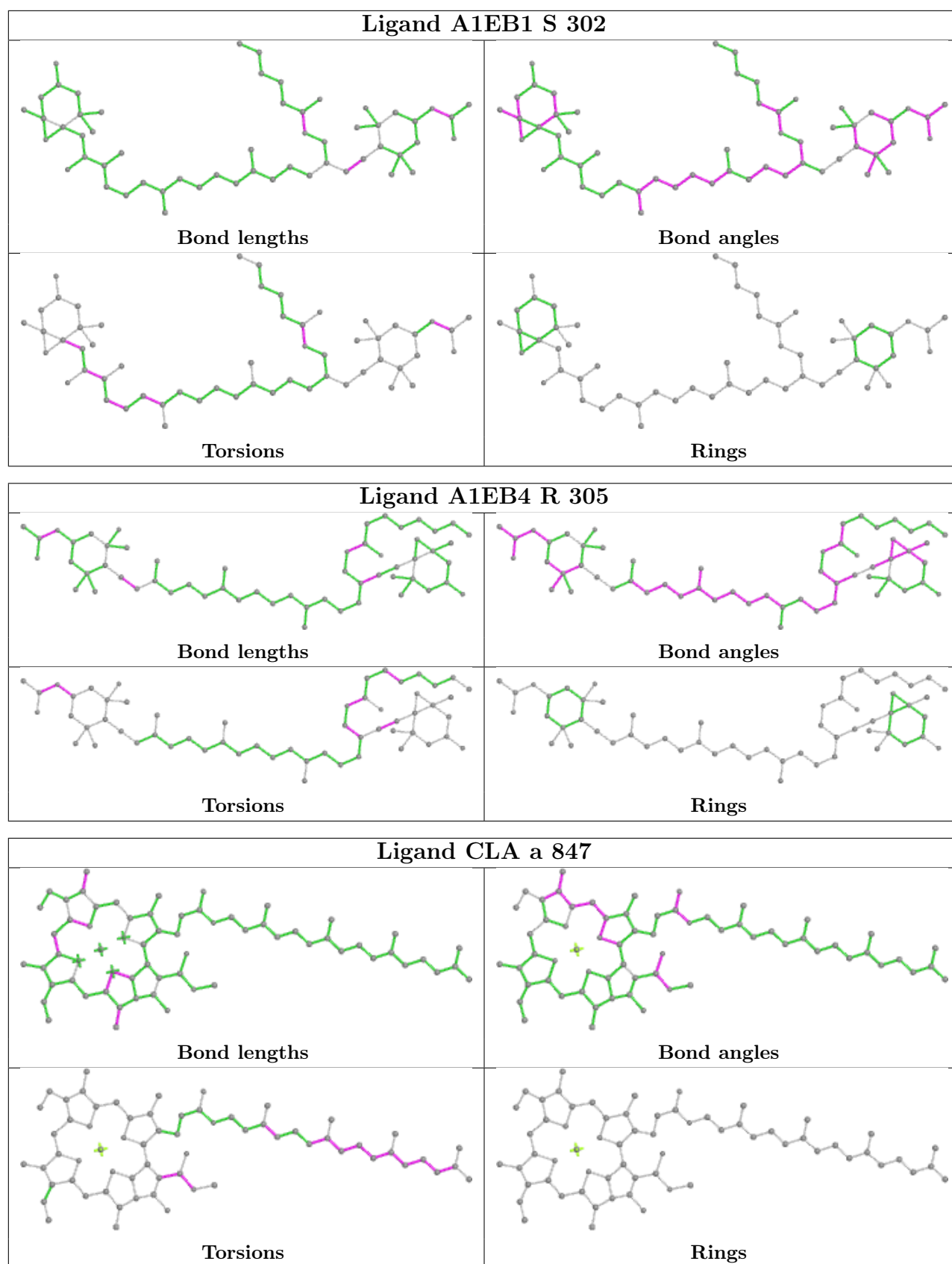
Rings

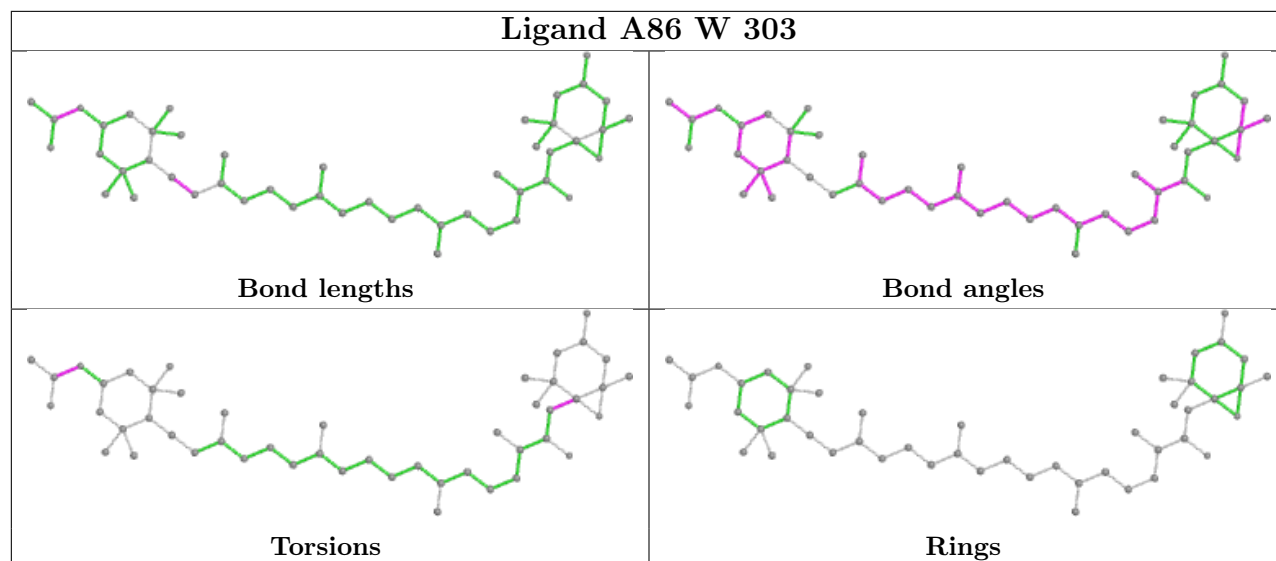
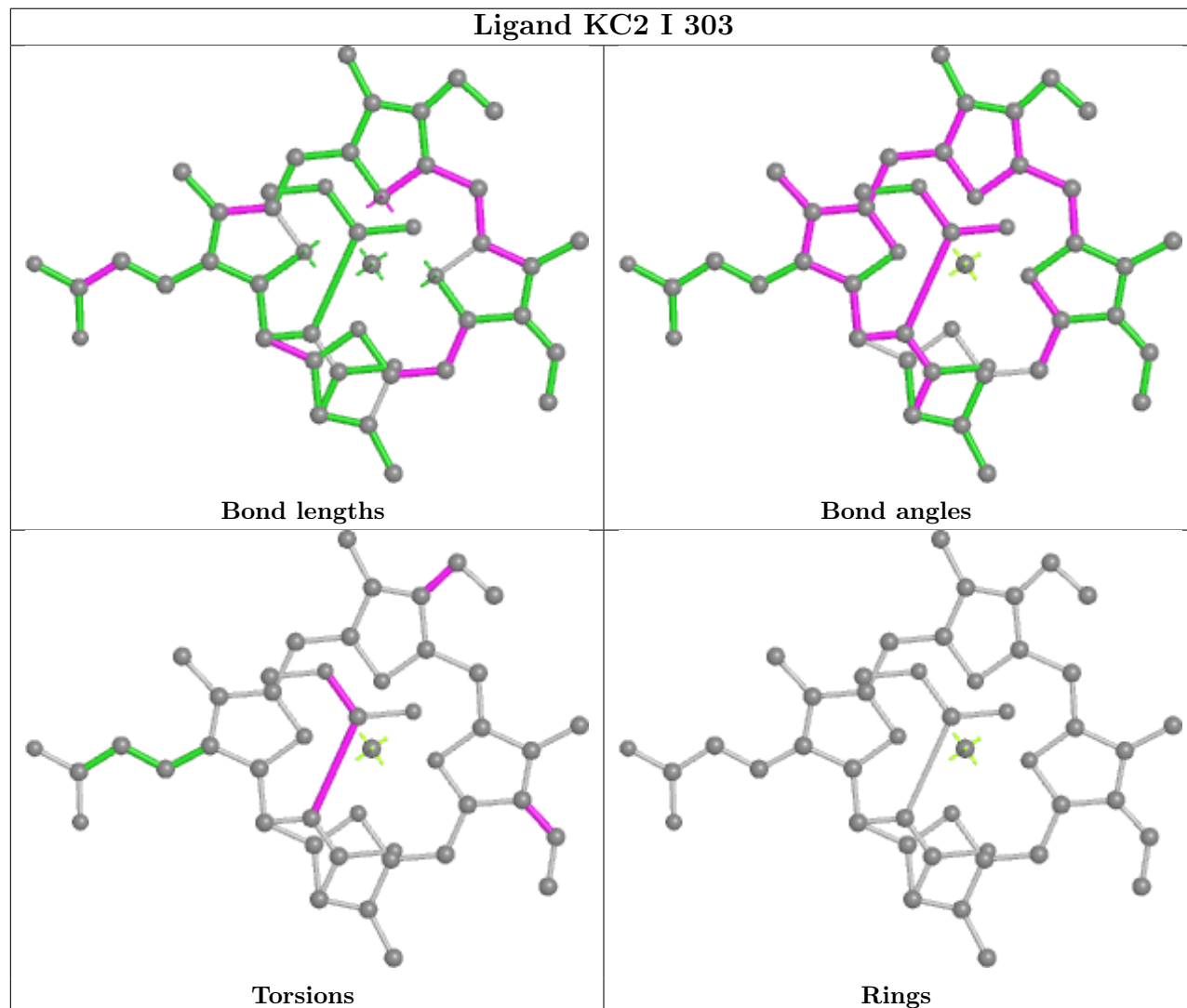
## Ligand CLA D 312



## Ligand CLA a 801

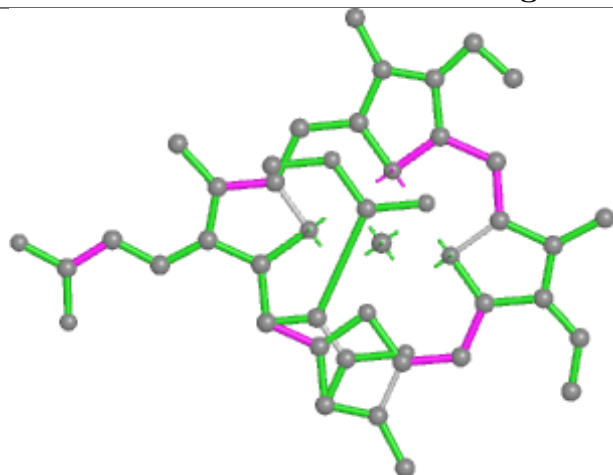




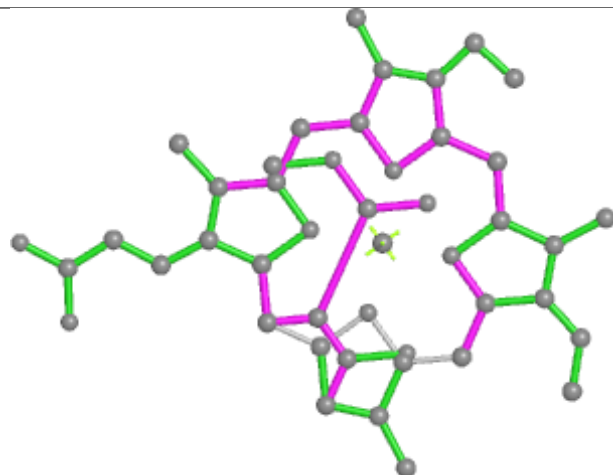
**Ligand A86 W 303****Ligand KC2 I 303**



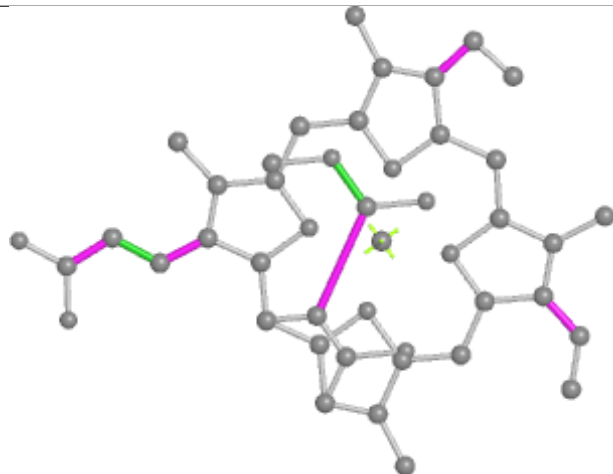
## Ligand KC2 8 320



Bond lengths



Bond angles

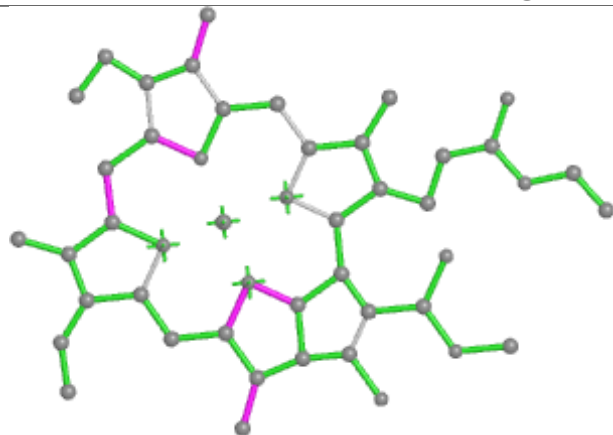


Torsions

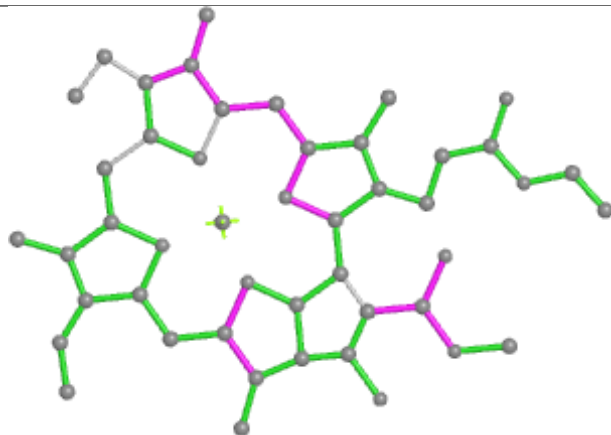


Rings

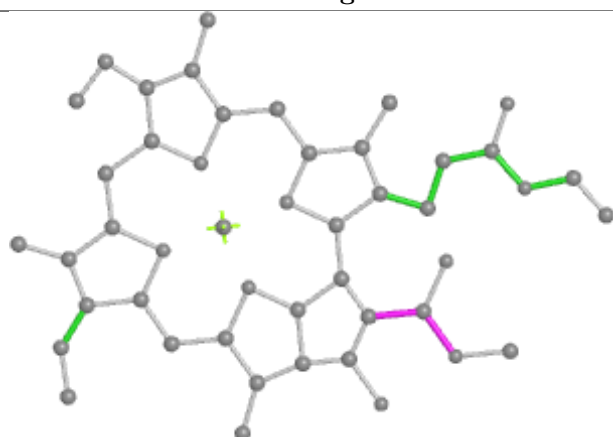
## Ligand CLA 5 315



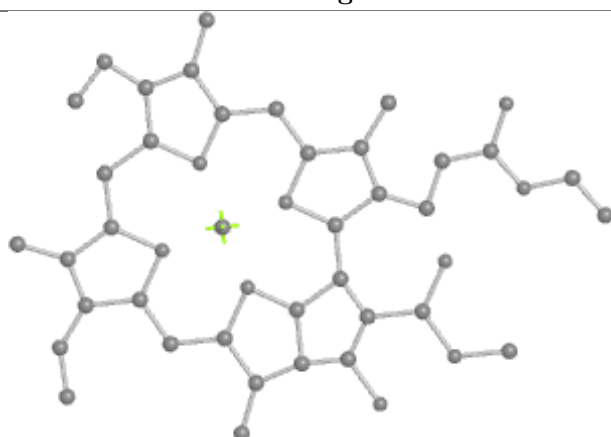
Bond lengths



Bond angles

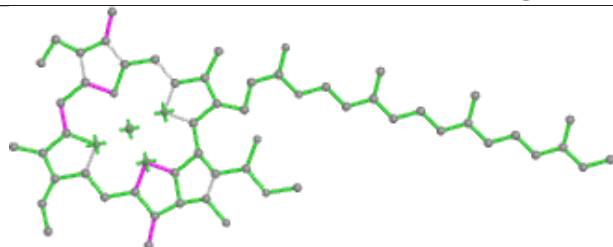


Torsions

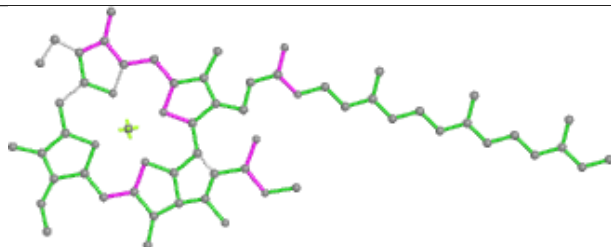


Rings

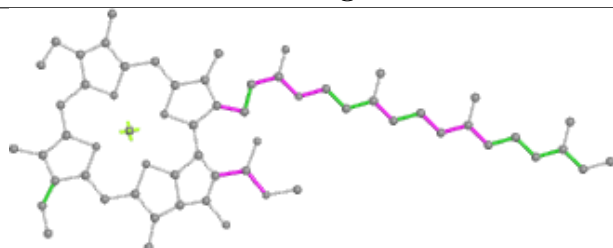
## Ligand CLA S 308



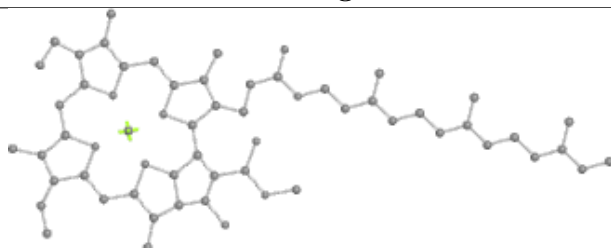
Bond lengths



Bond angles

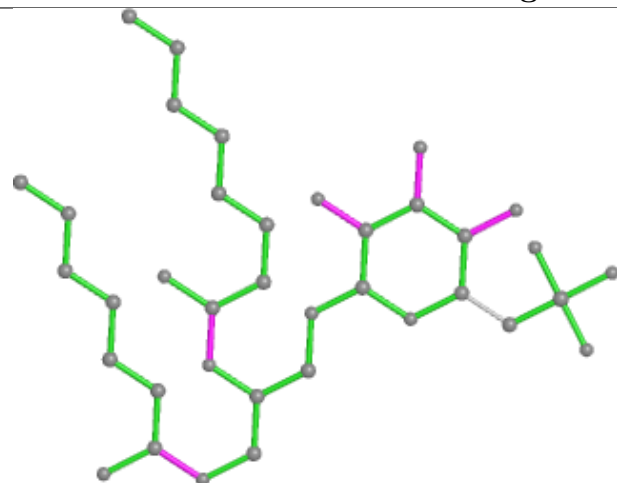


Torsions

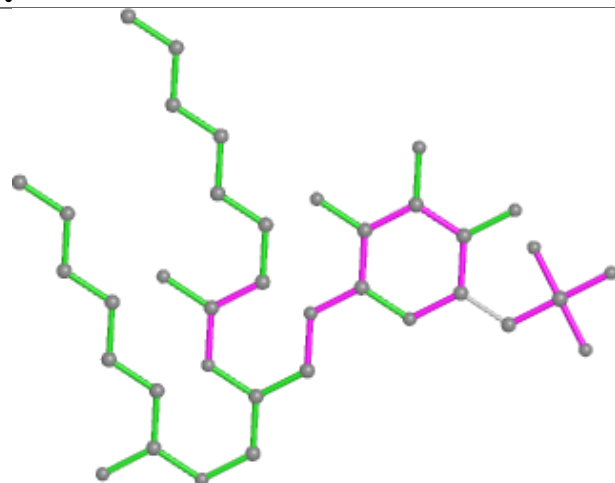


Rings

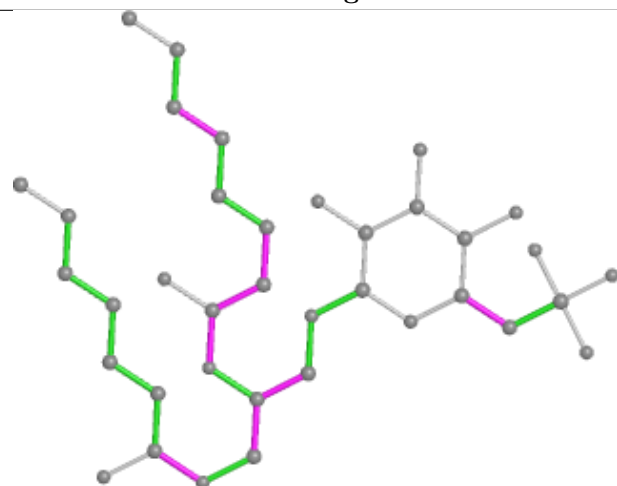
## Ligand SQD F 319



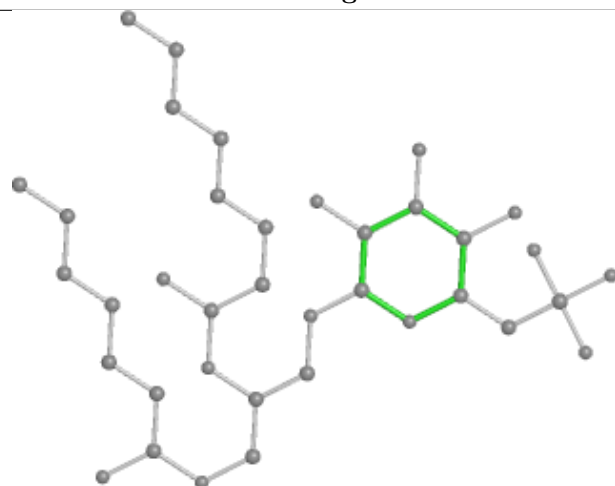
Bond lengths



Bond angles

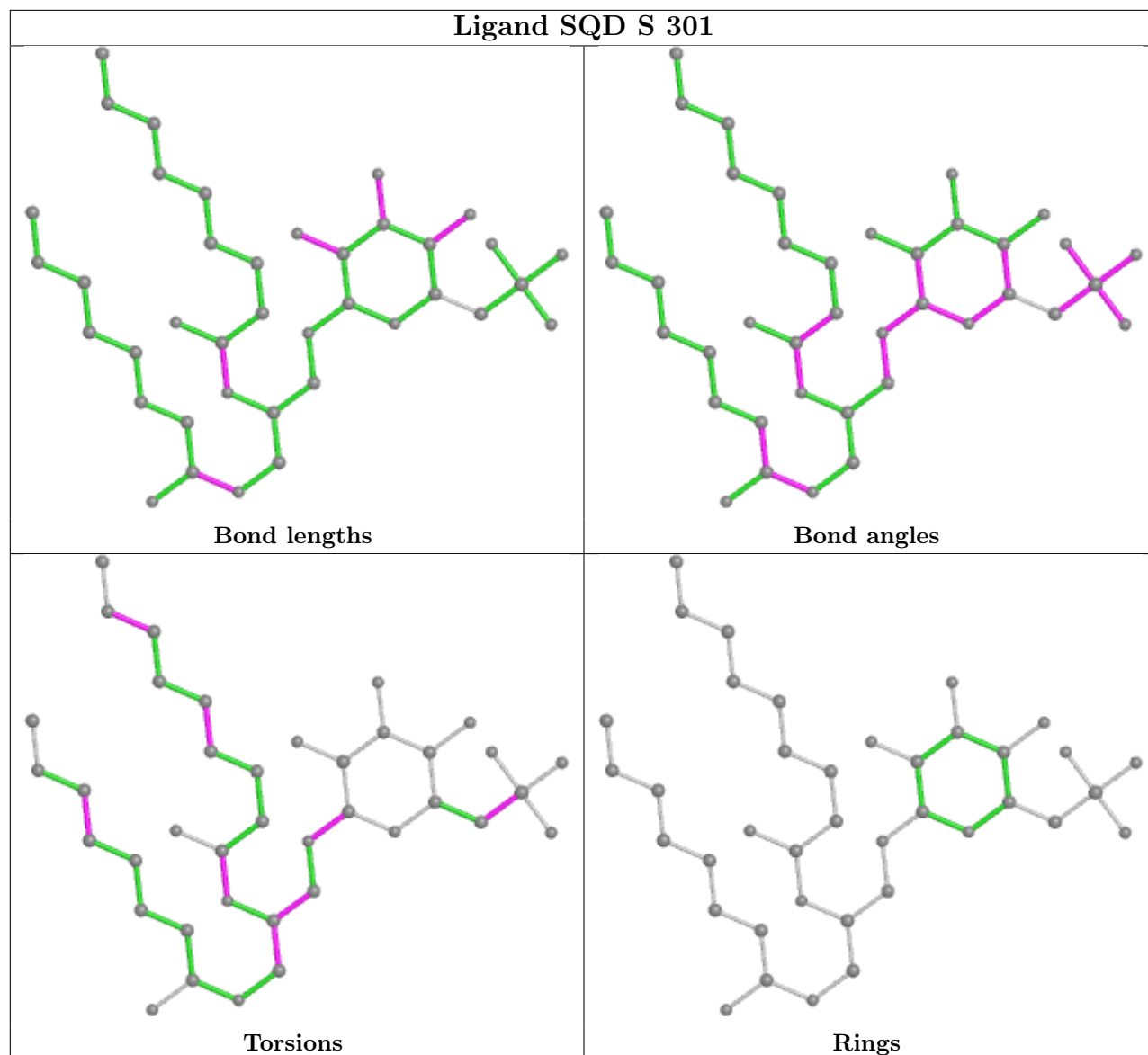


Torsions

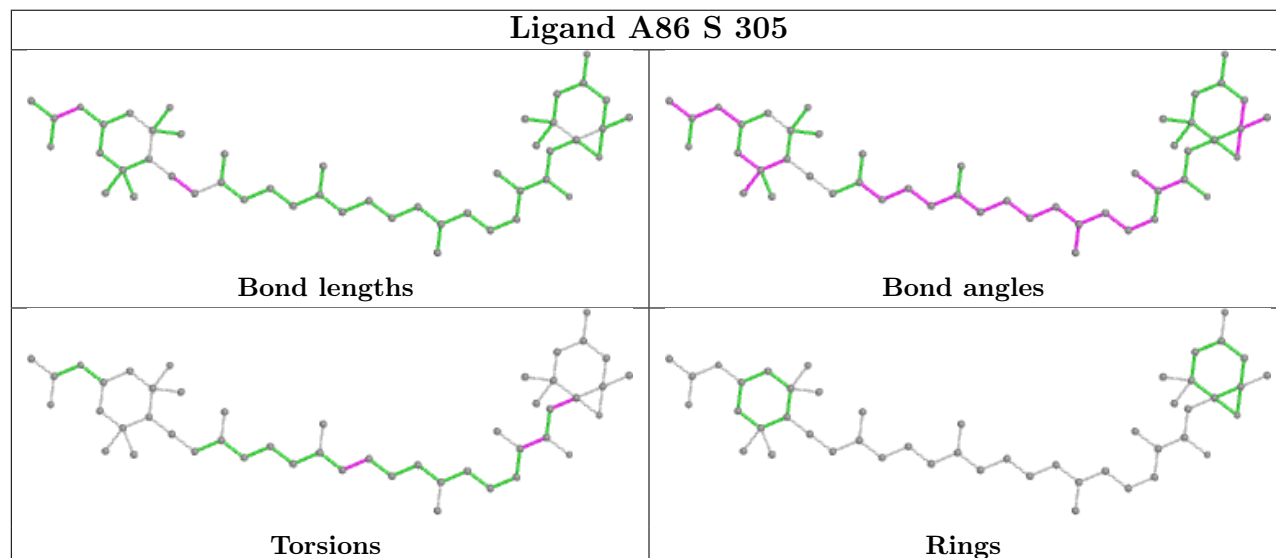


Rings

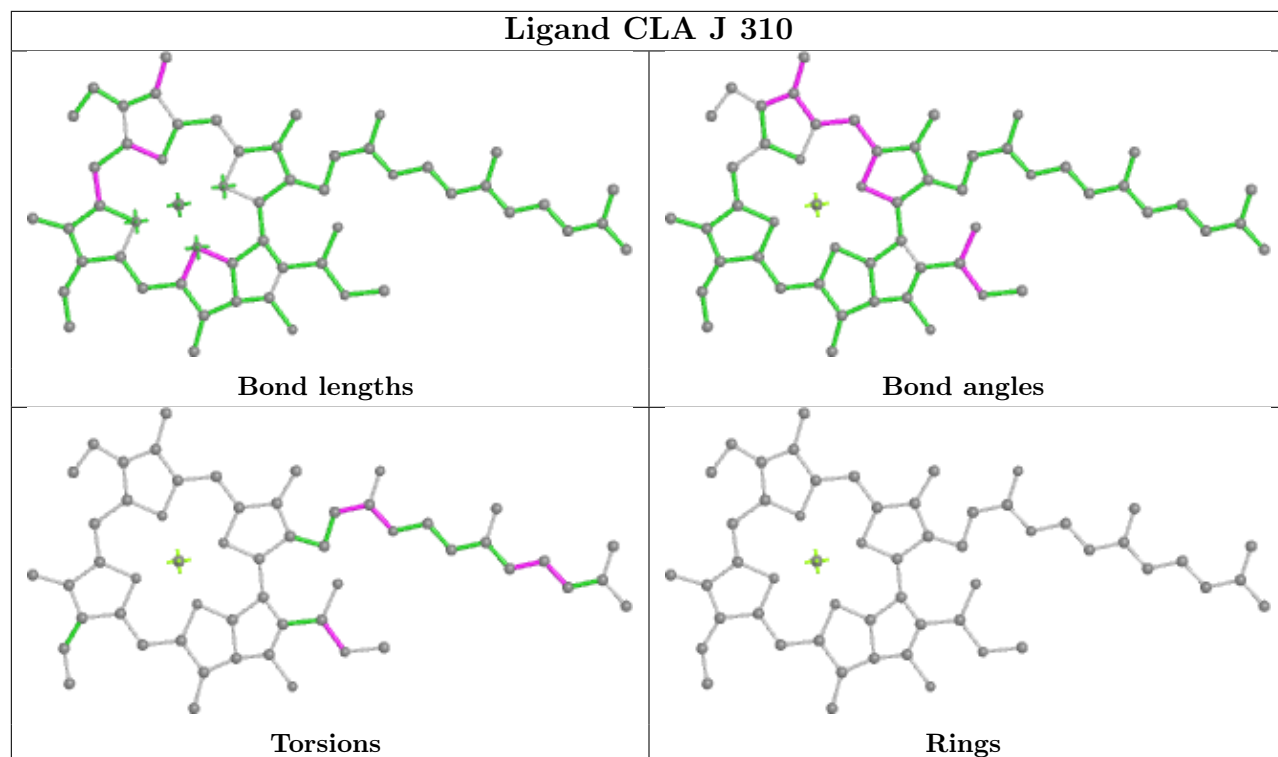
## Ligand SQD S 301



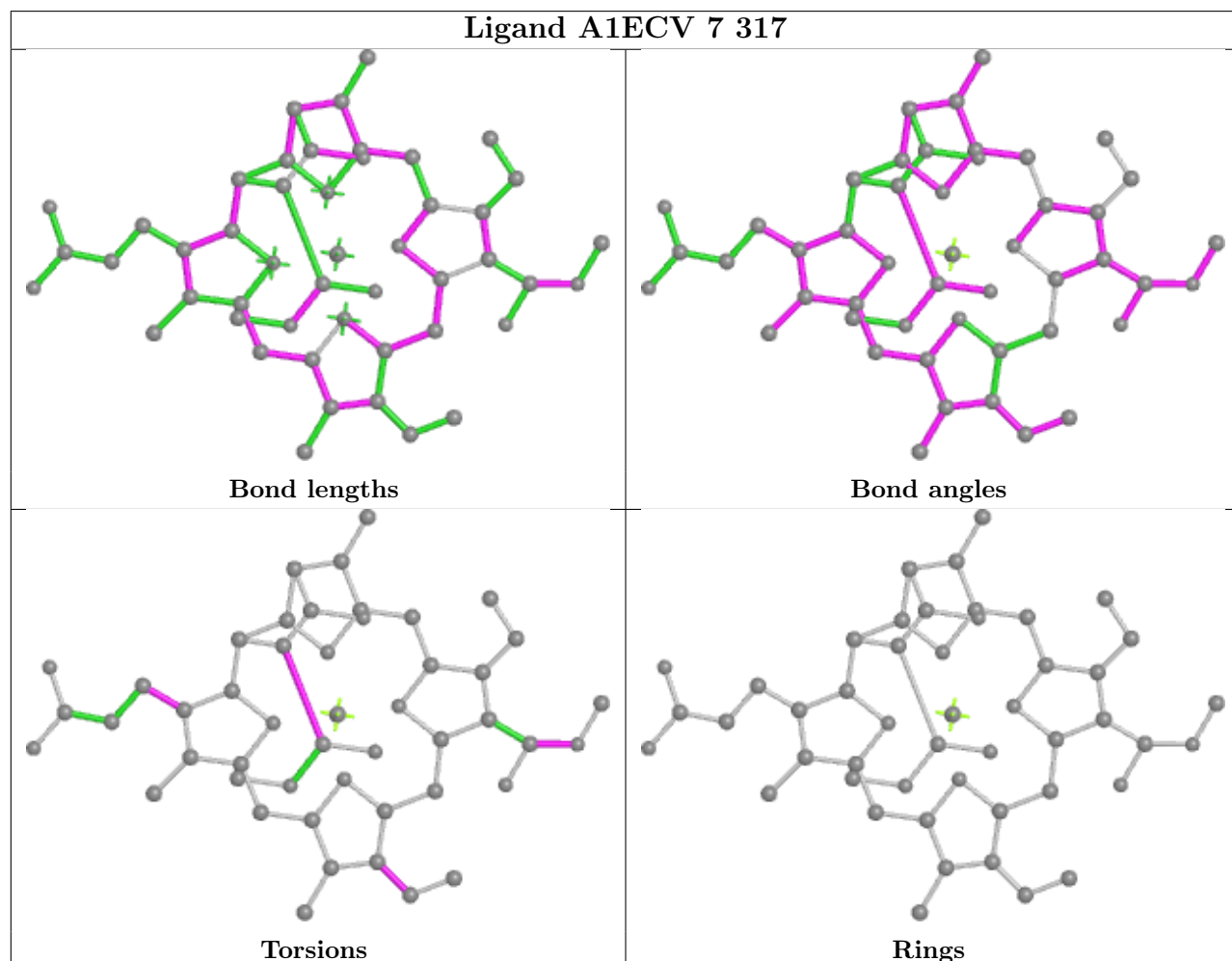
## Ligand A86 S 305



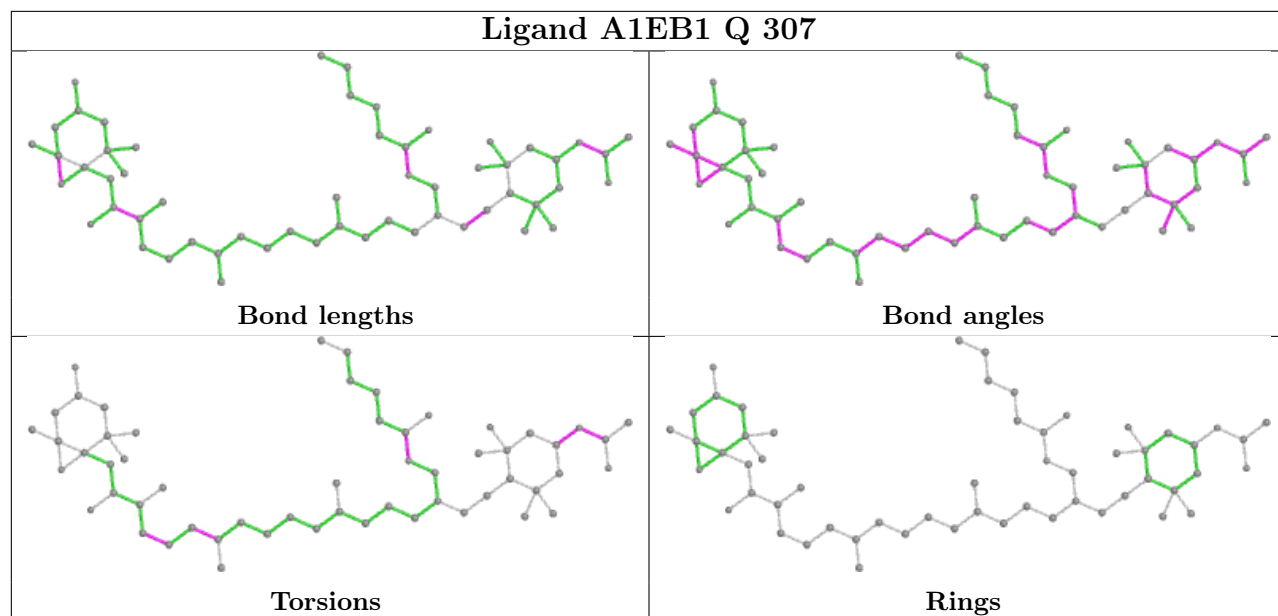
## Ligand CLA J 310



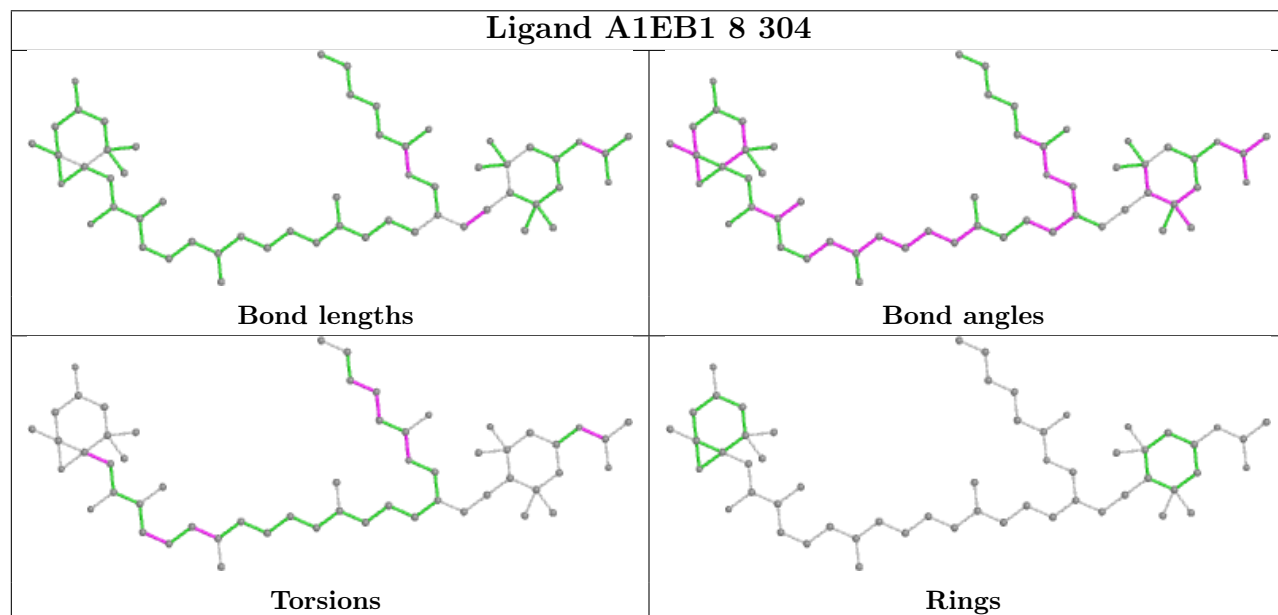
## Ligand A1ECV 7 317

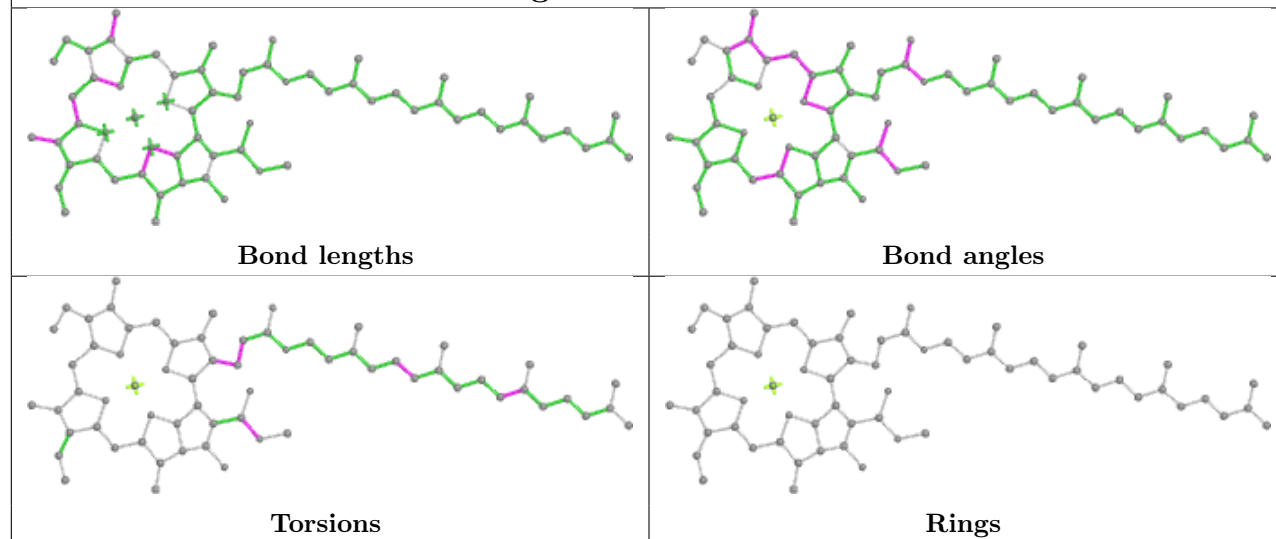
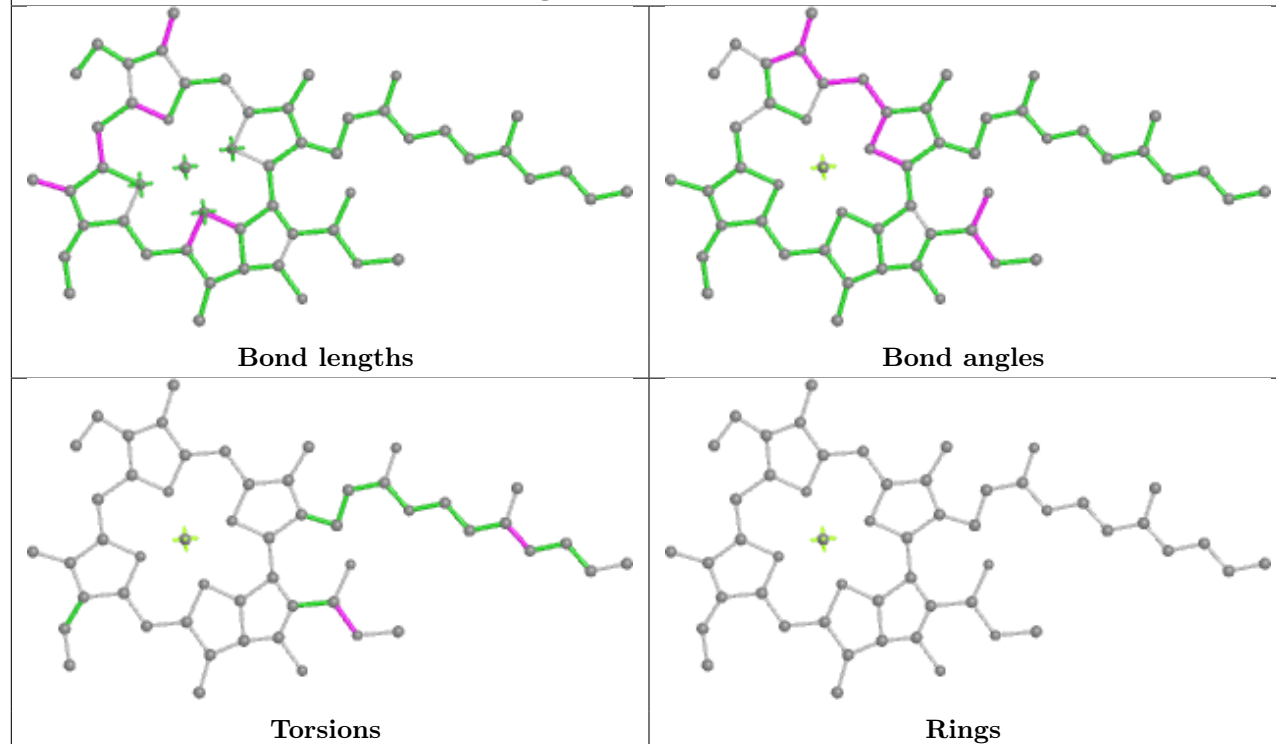


## Ligand A1EB1 Q 307

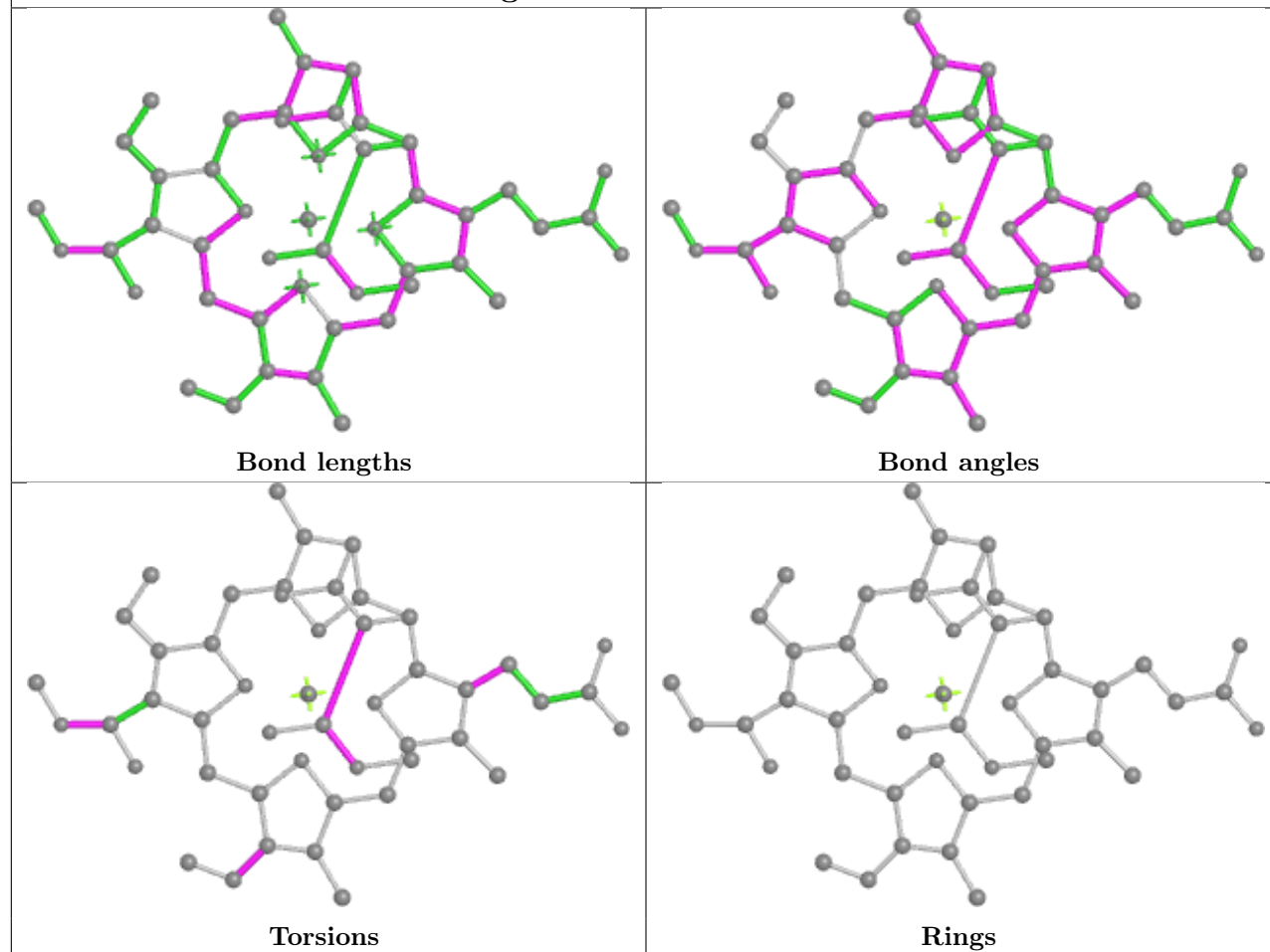


## Ligand A1EB1 8 304

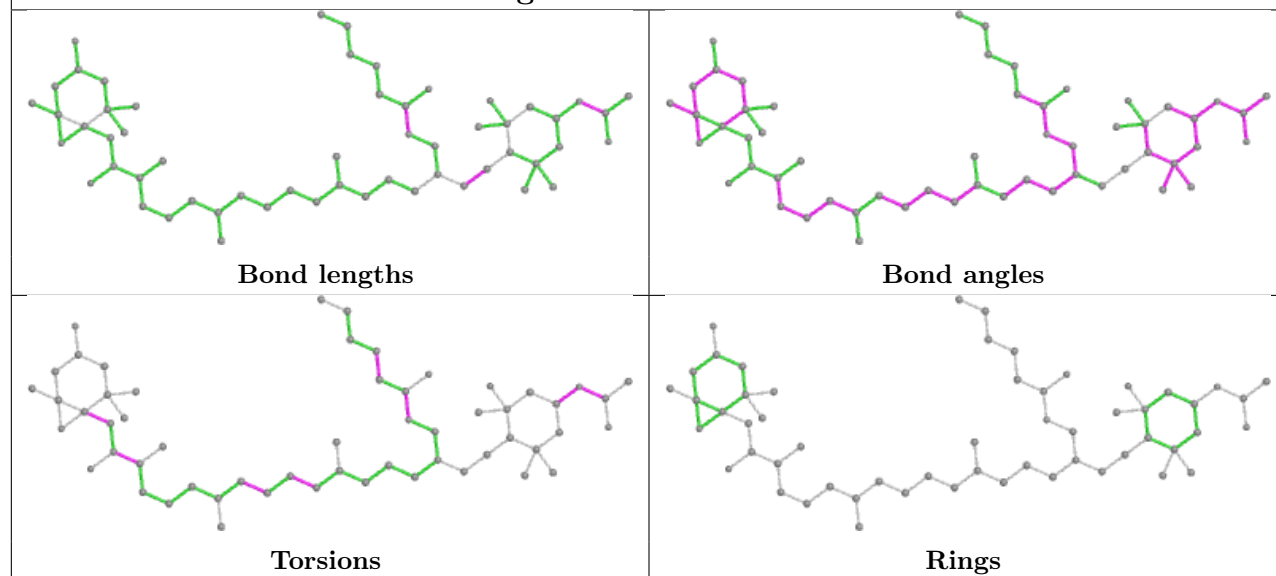


**Ligand CLA H 313****Ligand CLA 3 313**

## Ligand A1ECV W 317

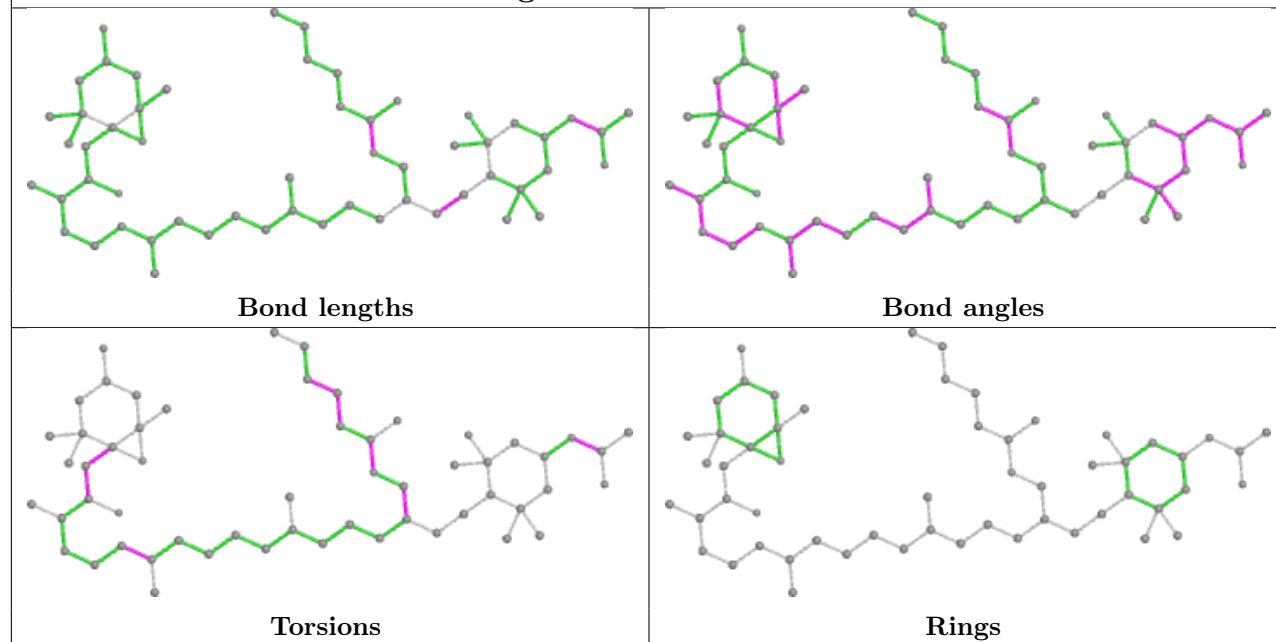


## Ligand A1EB1 S 303

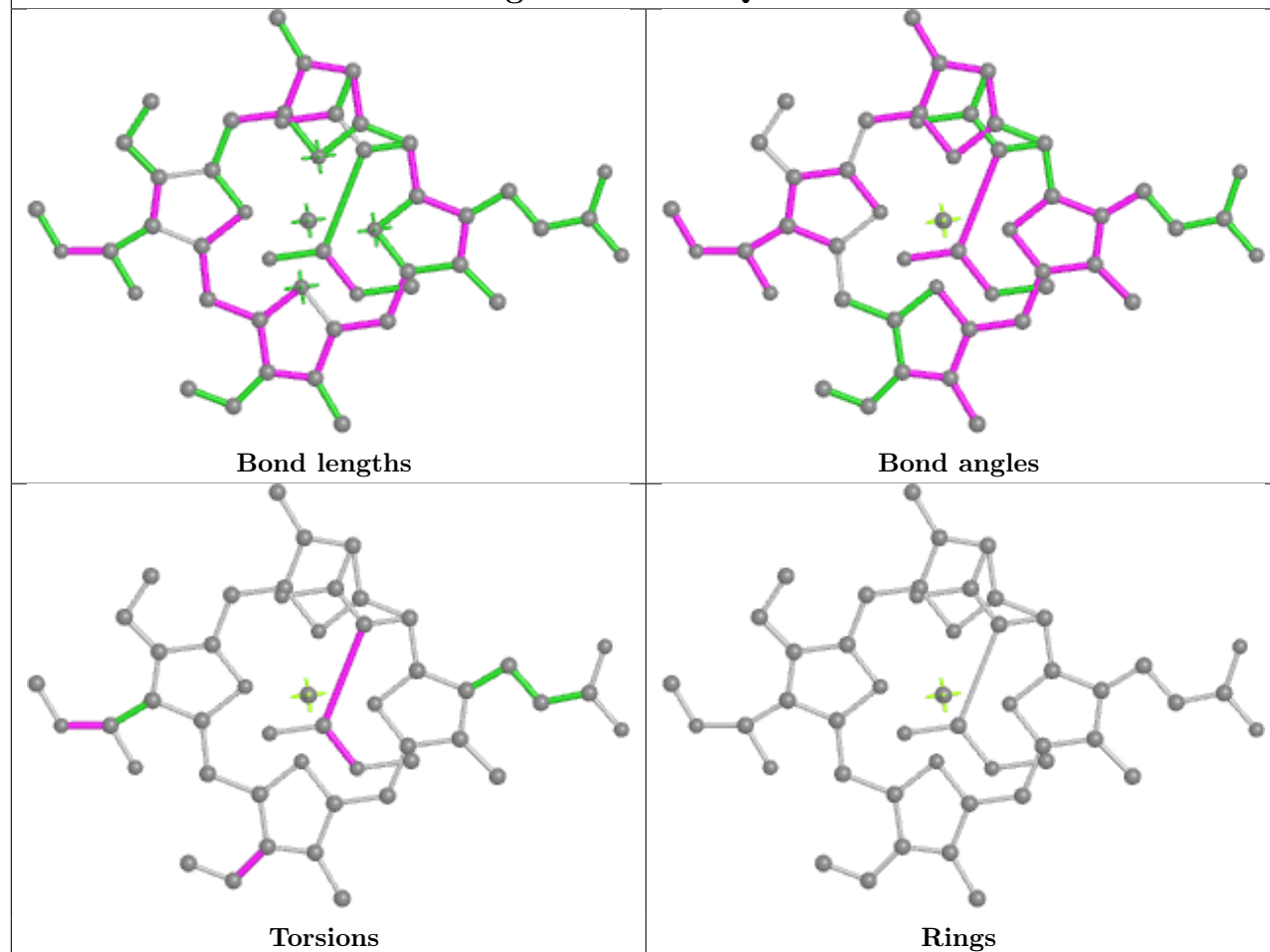




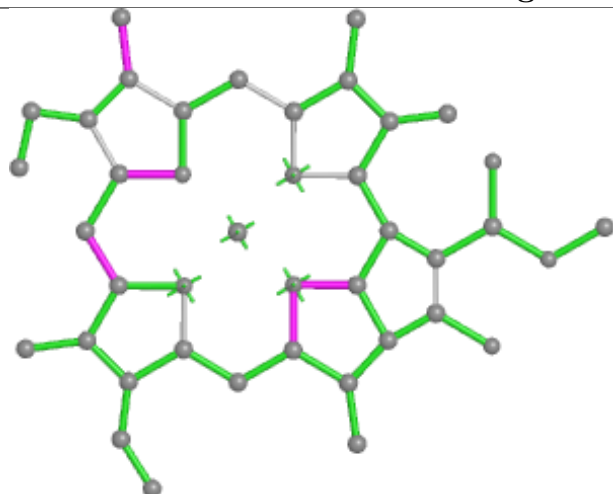
## Ligand A1EB1 6 301



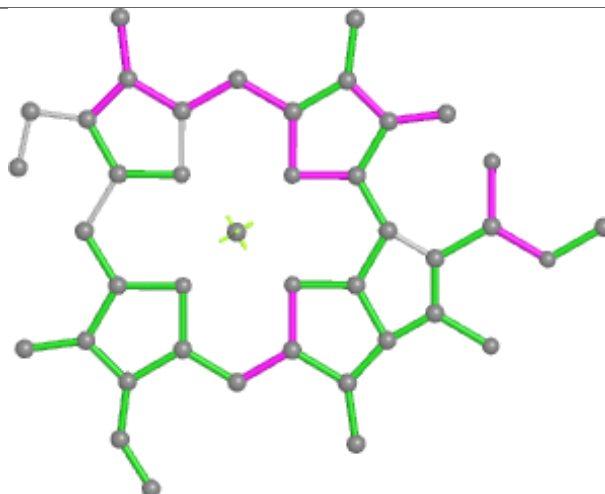
## Ligand A1ECV Q 316



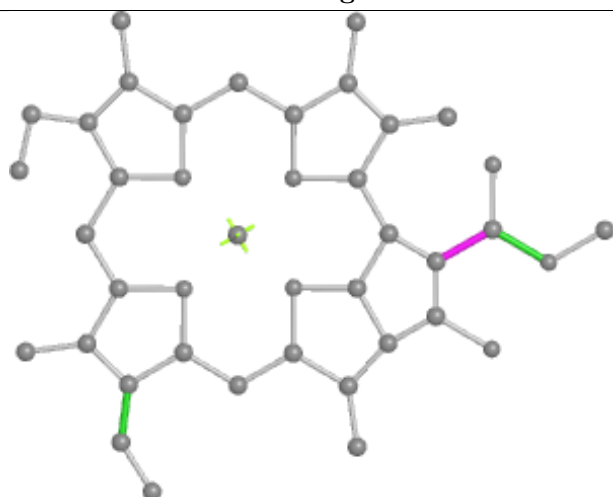
## Ligand CLA S 316



Bond lengths



Bond angles

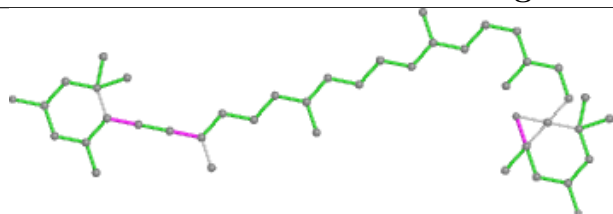


Torsions

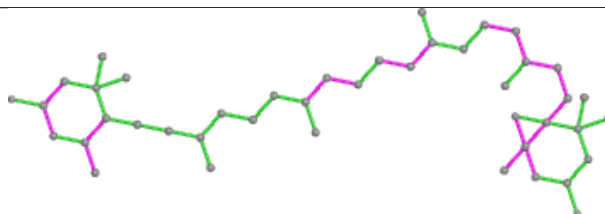


Rings

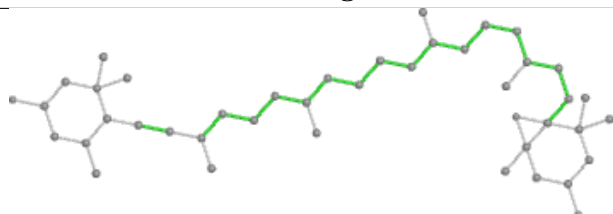
## Ligand DD6 V 303



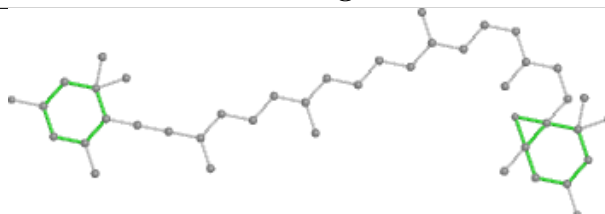
Bond lengths



Bond angles

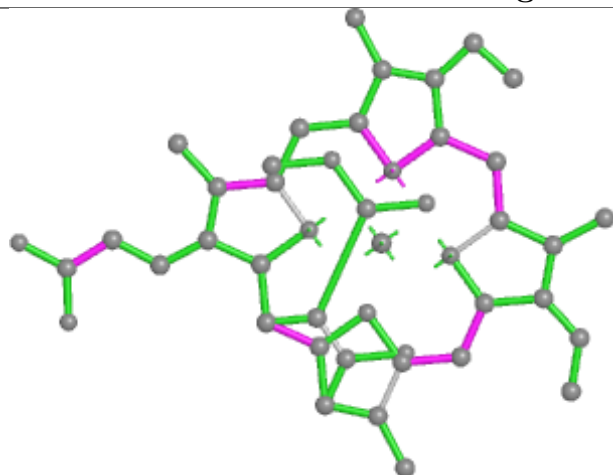


Torsions

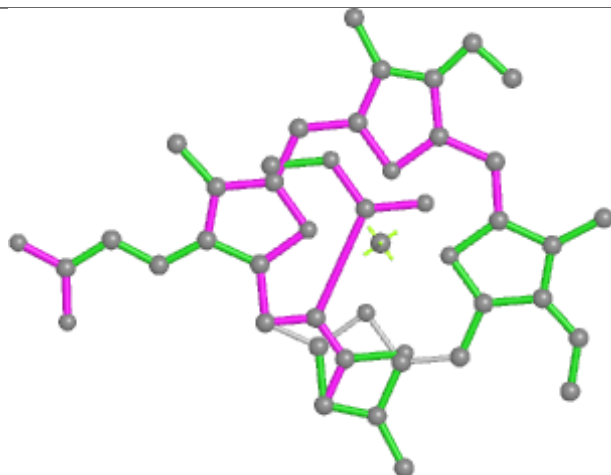


Rings

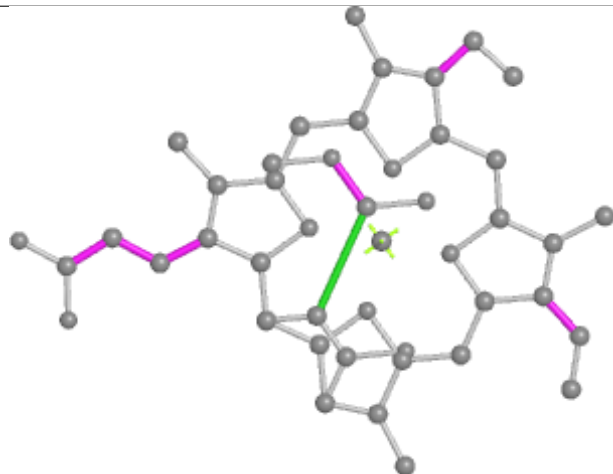
## Ligand KC2 P 313



Bond lengths



Bond angles

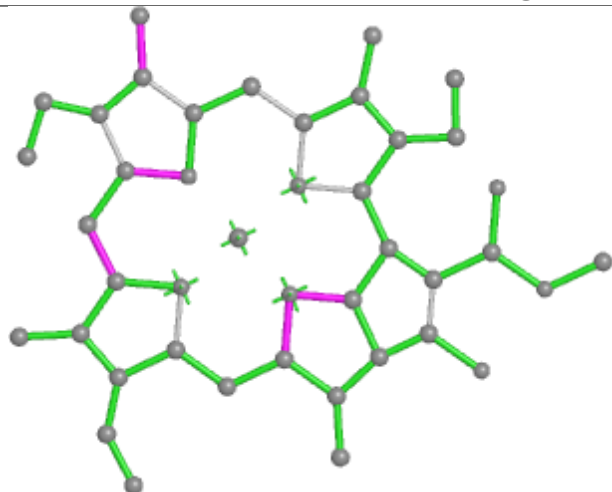


Torsions

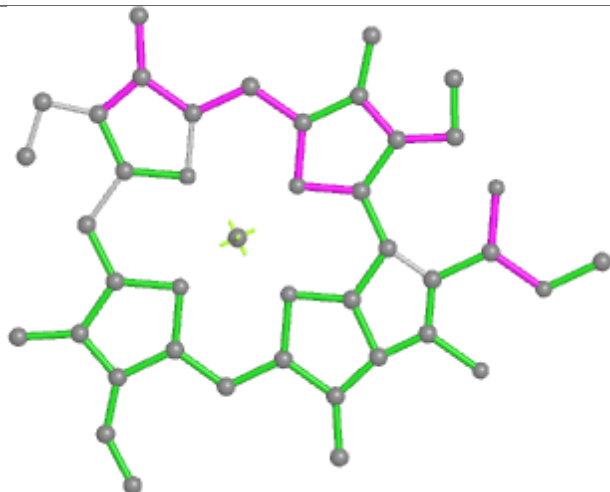


Rings

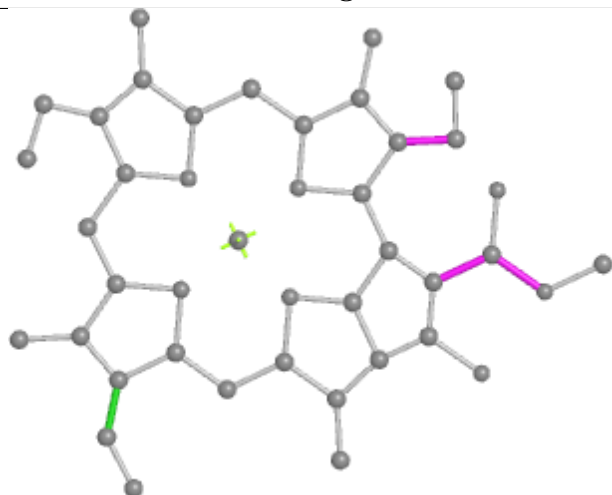
## Ligand CLA 2 310



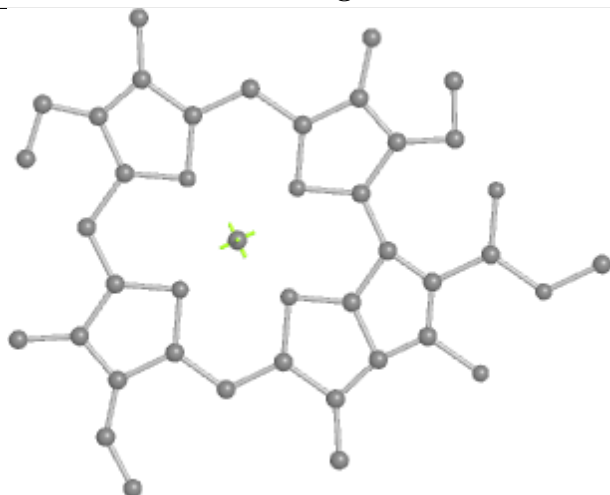
Bond lengths



Bond angles

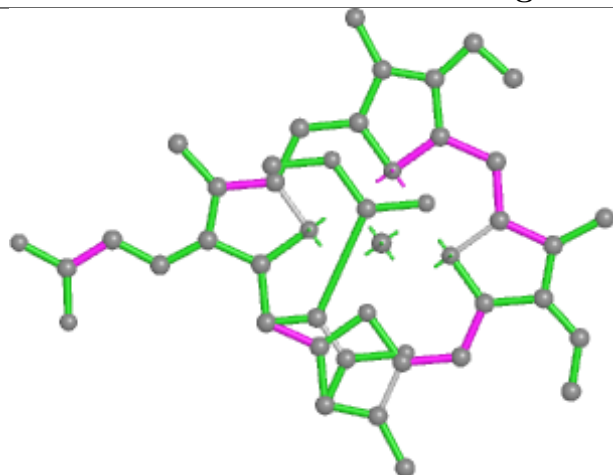


Torsions

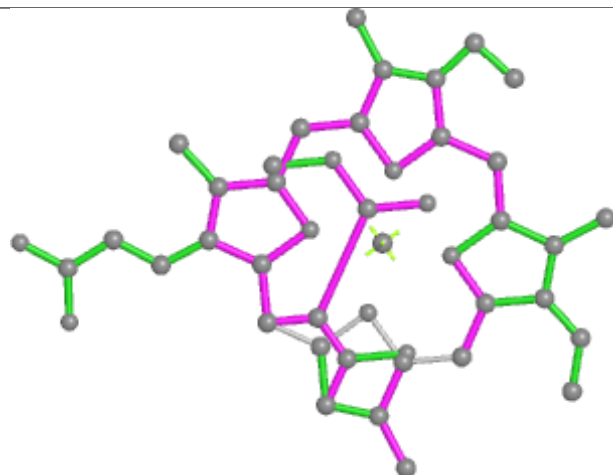


Rings

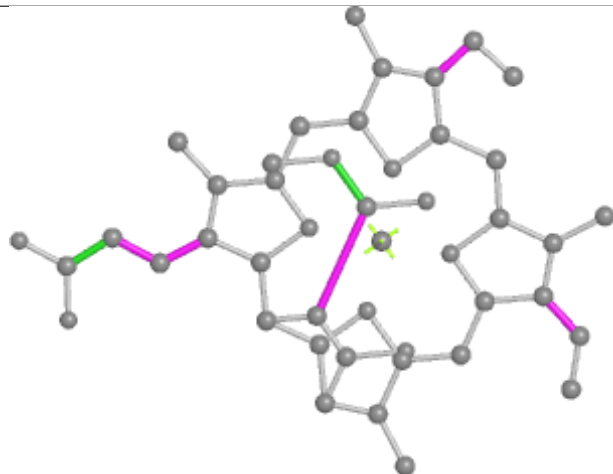
## Ligand KC2 R 312



Bond lengths



Bond angles

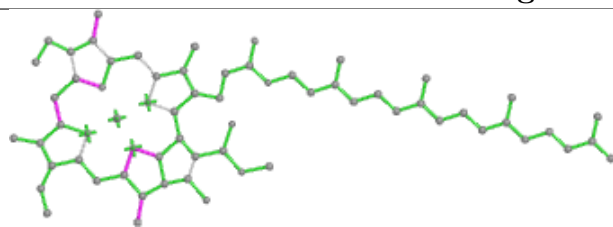


Torsions

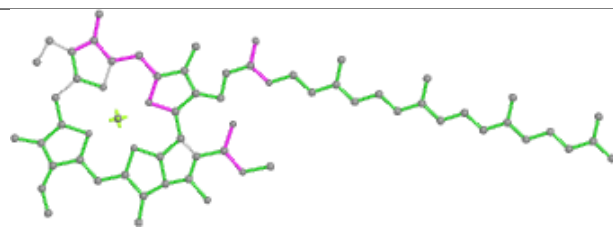


Rings

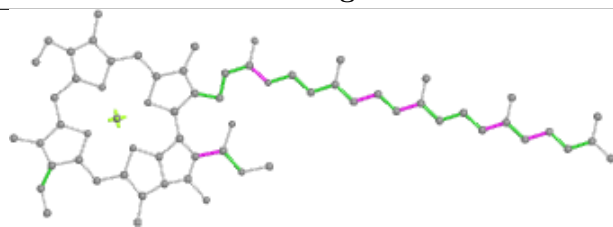
## Ligand CLA b 812



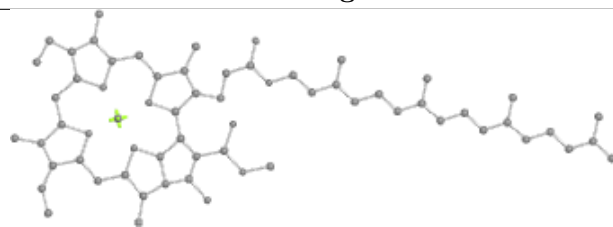
Bond lengths



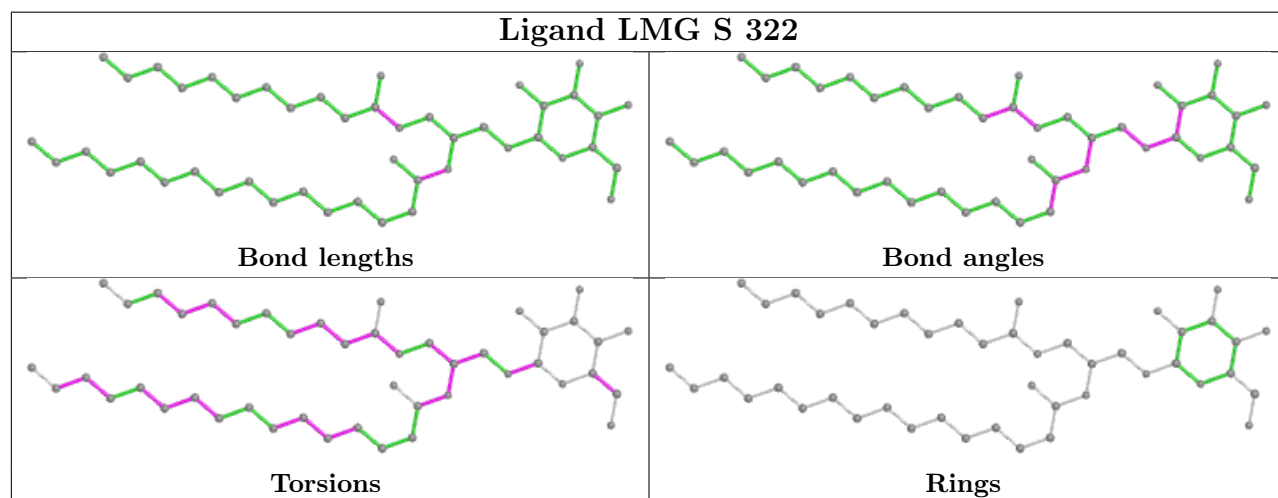
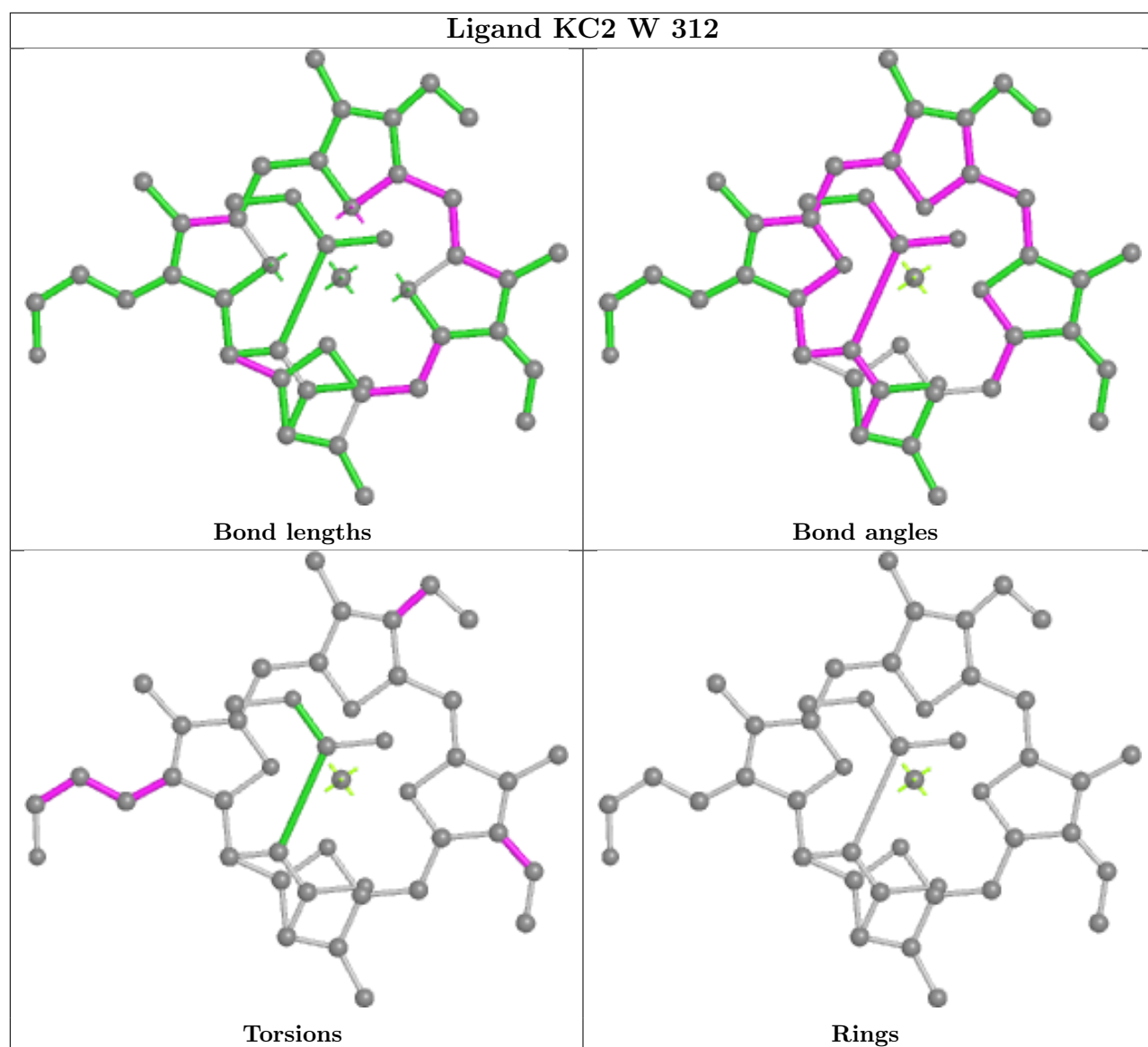
Bond angles



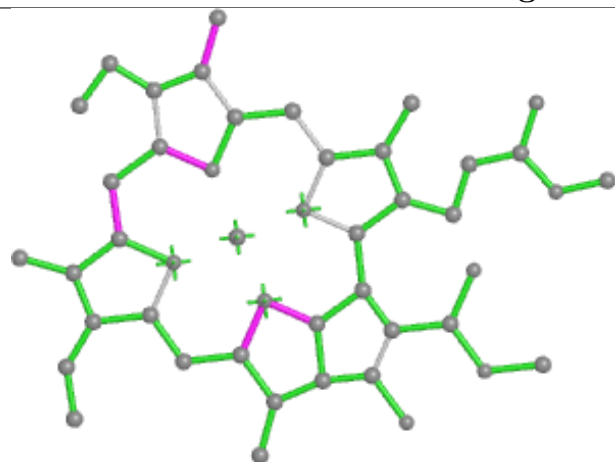
Torsions



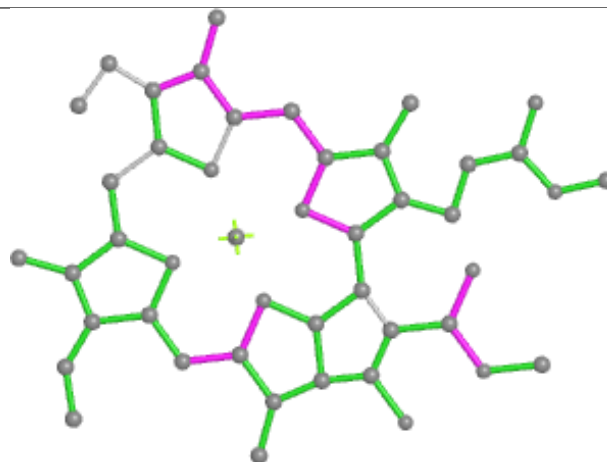
Rings



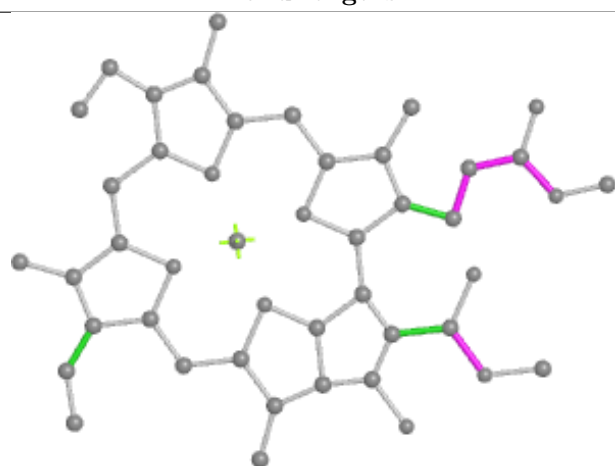
## Ligand CLA Z 306



Bond lengths



Bond angles

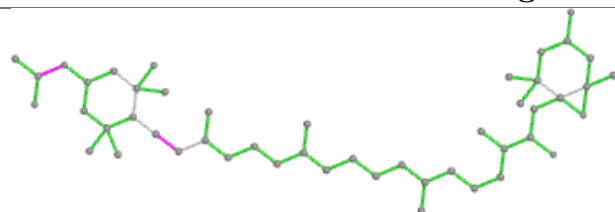


Torsions

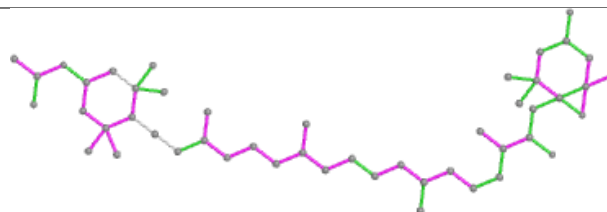


Rings

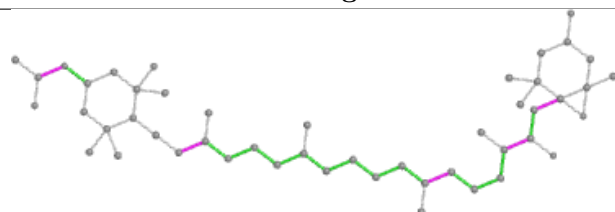
## Ligand A86 M 302



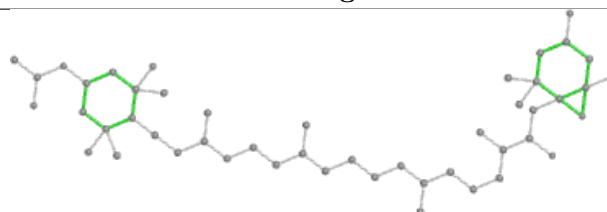
Bond lengths



Bond angles

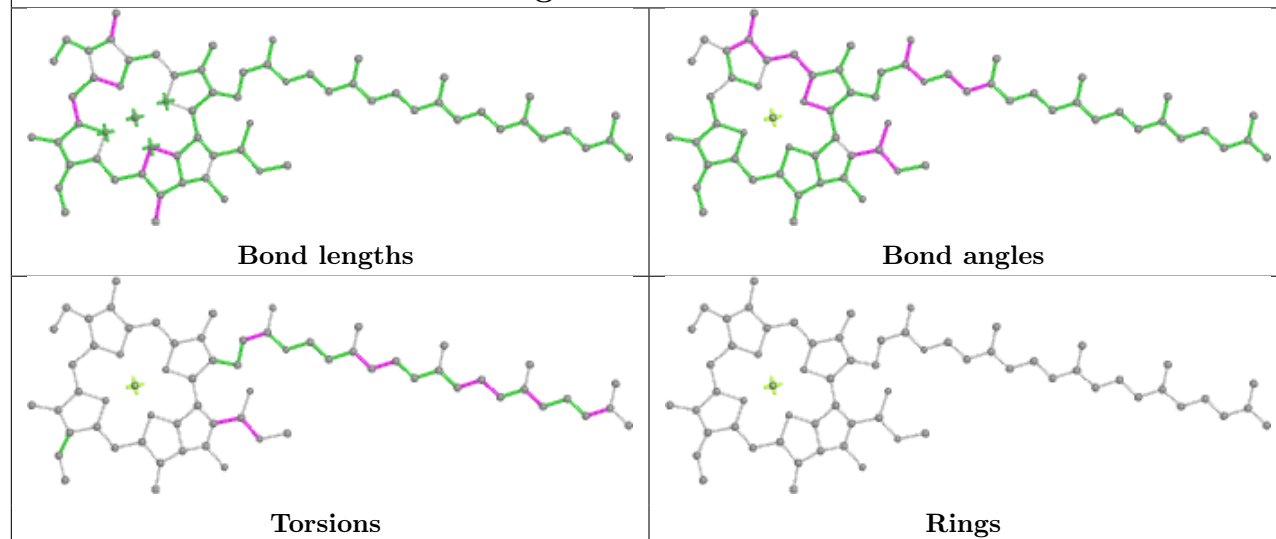


Torsions

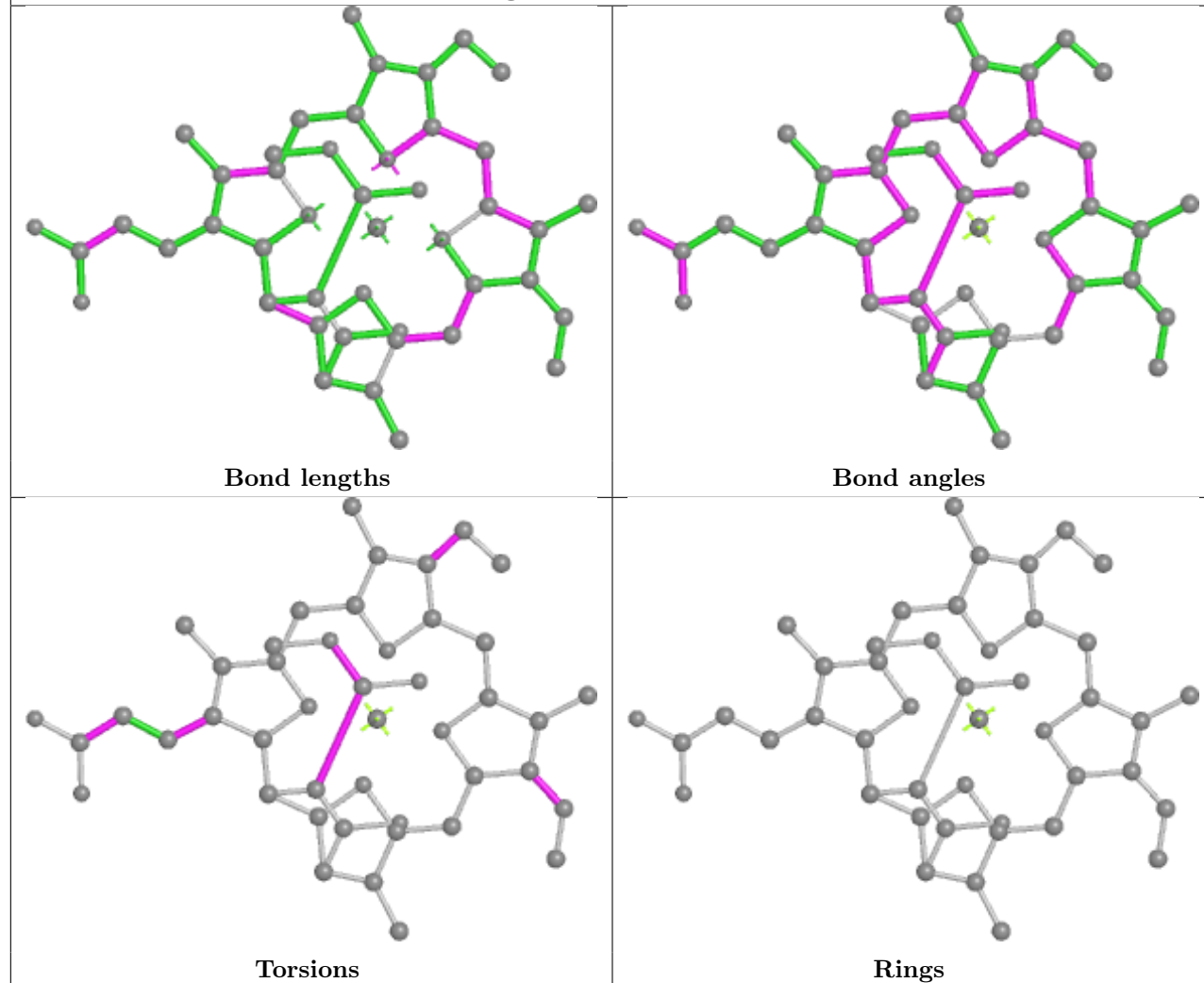


Rings

## Ligand CLA b 806

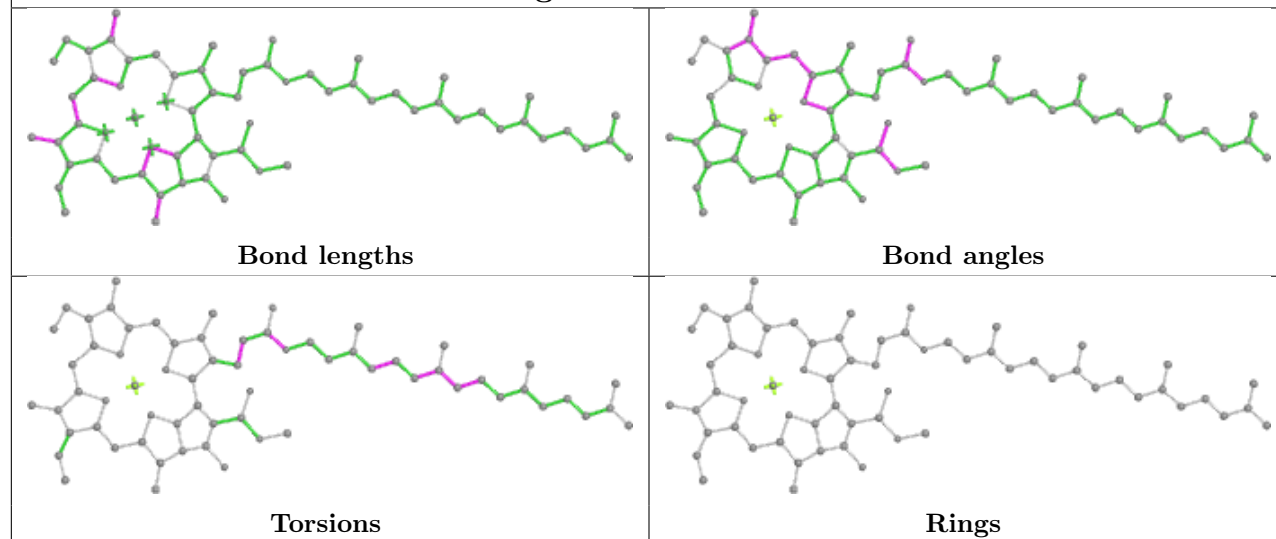


## Ligand KC2 H 314

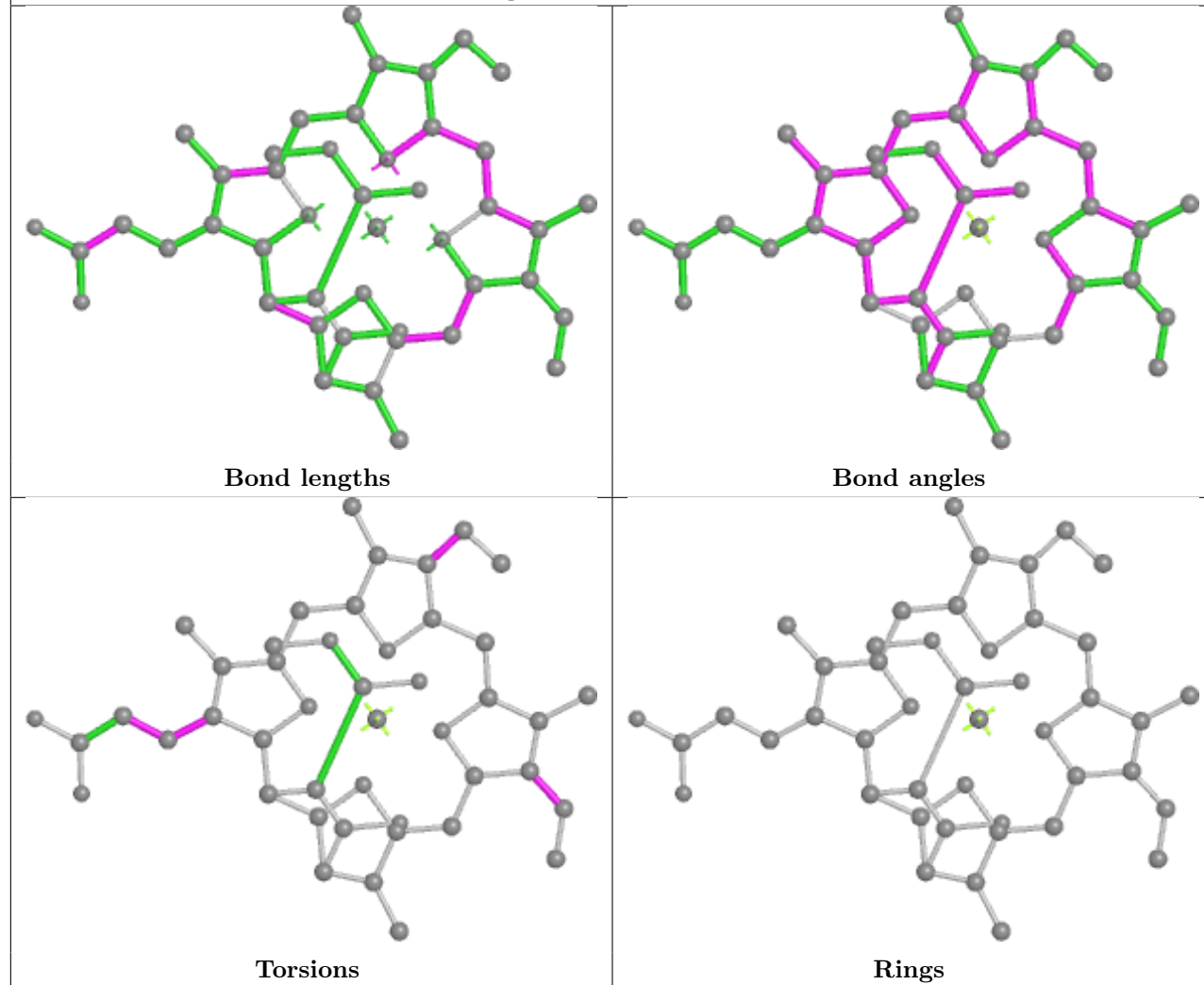




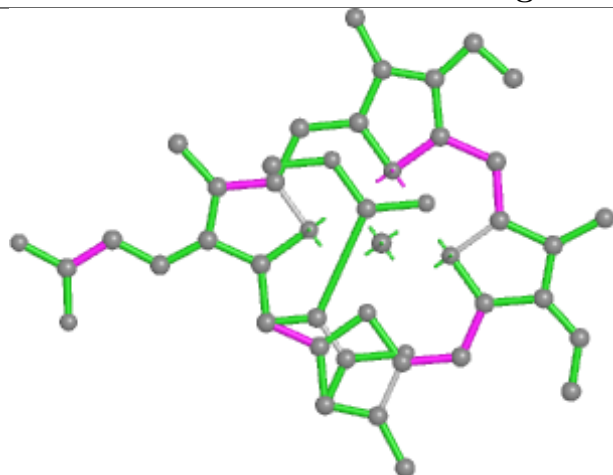
## Ligand CLA b 840



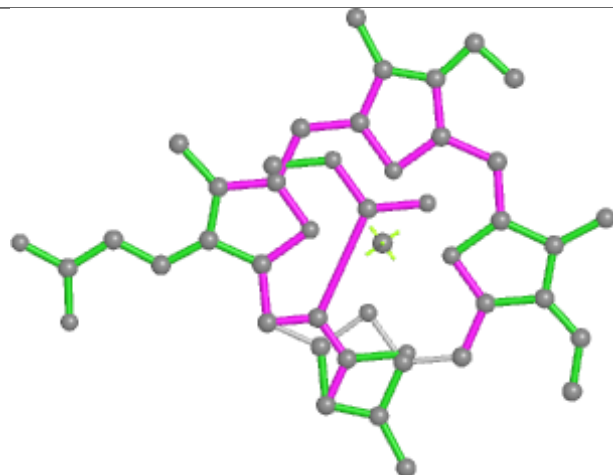
## Ligand KC2 G 313



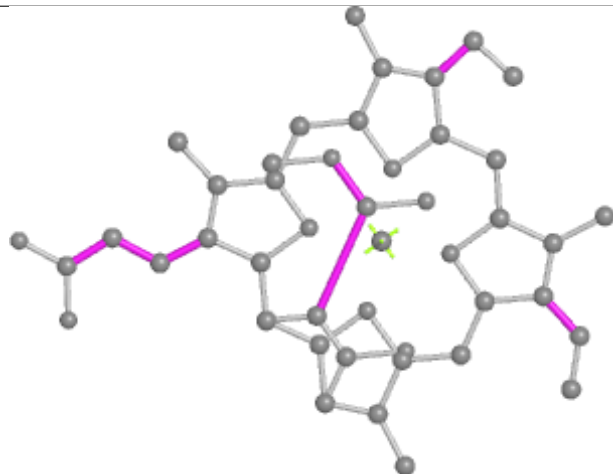
## Ligand KC2 C 313



Bond lengths



Bond angles

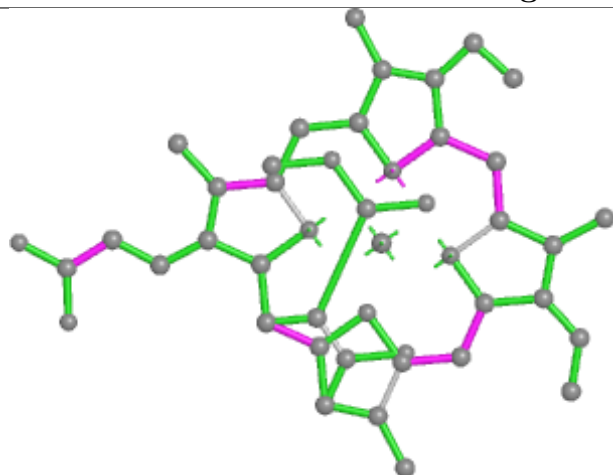


Torsions

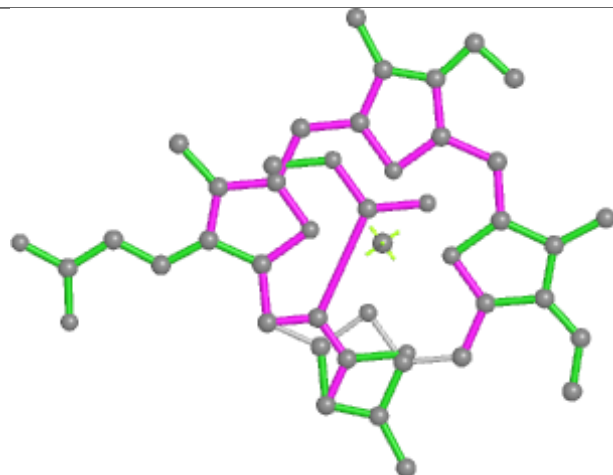


Rings

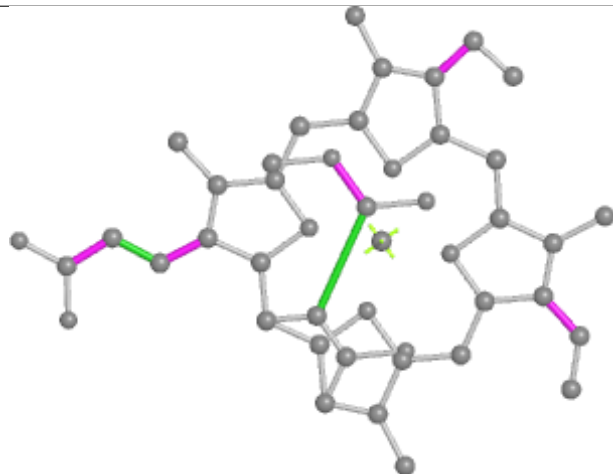
## Ligand KC2 6 316



Bond lengths



Bond angles

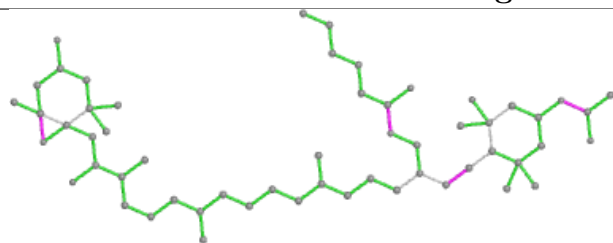


Torsions

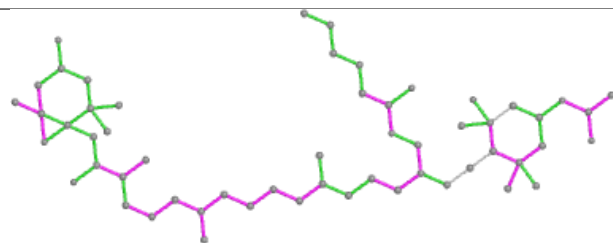


Rings

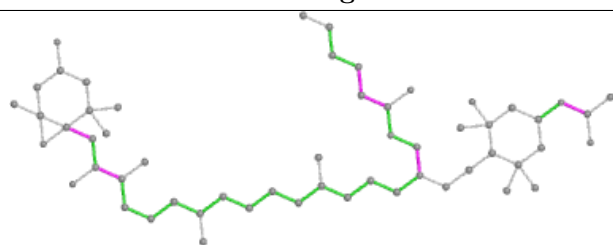
## Ligand A1EB1 V 305



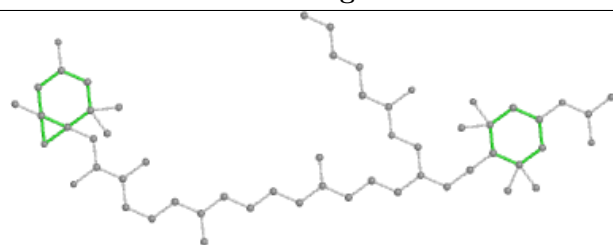
Bond lengths



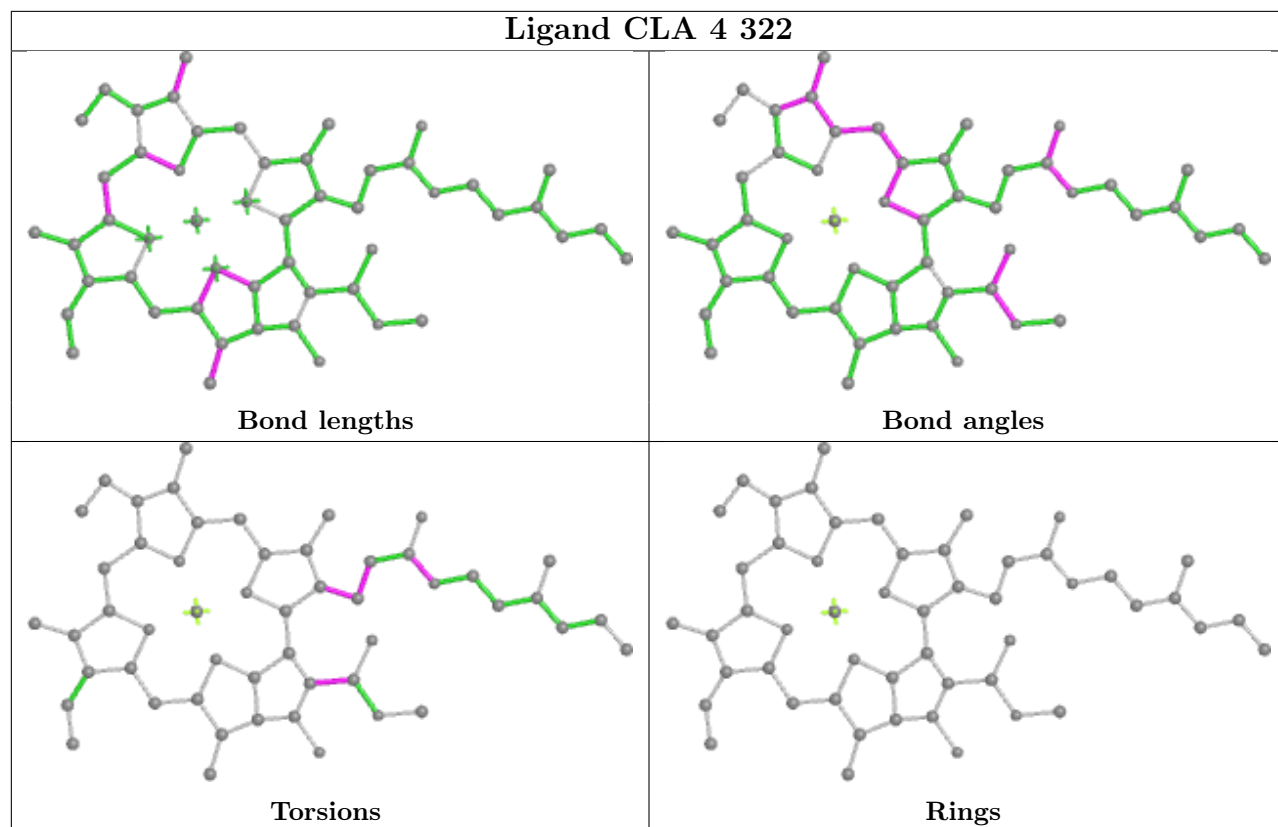
Bond angles



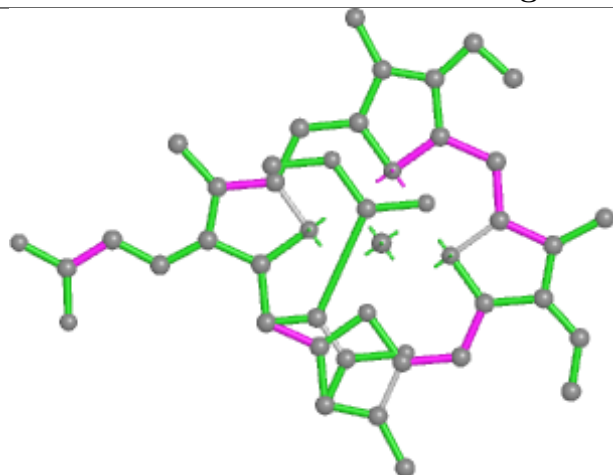
Torsions



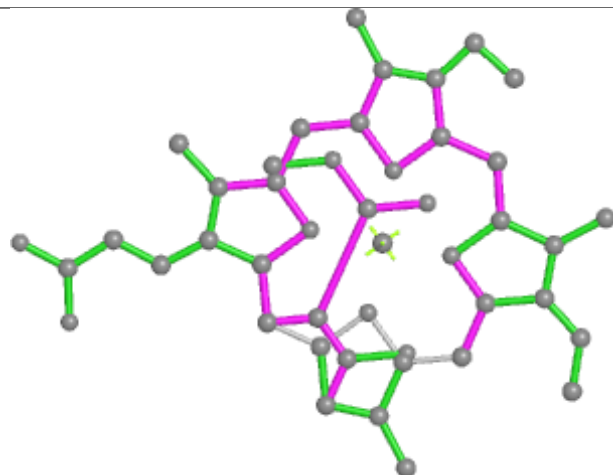
Rings



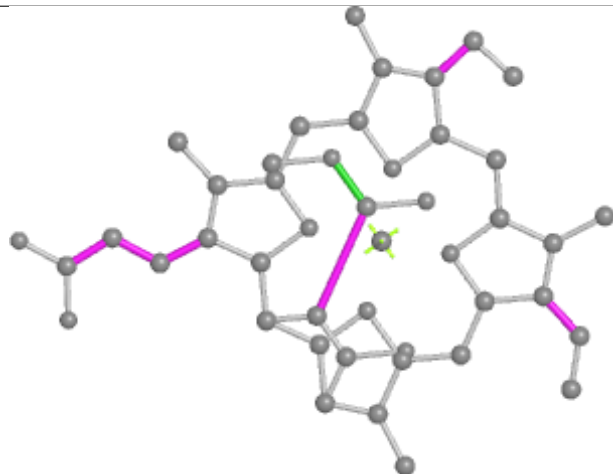
## Ligand KC2 4 318



Bond lengths



Bond angles

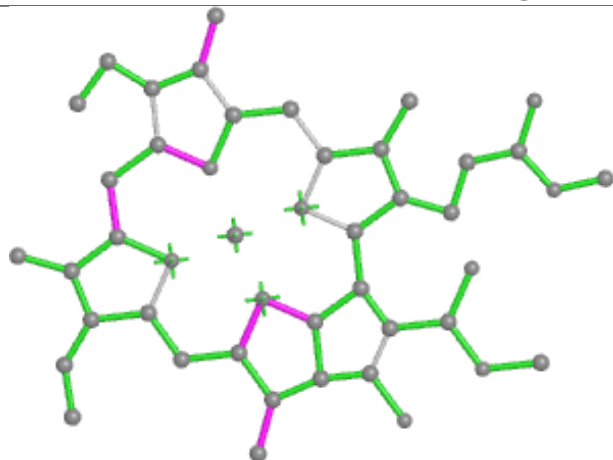


Torsions

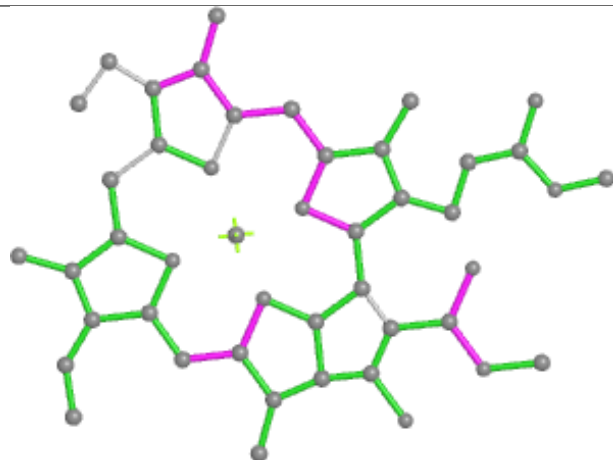


Rings

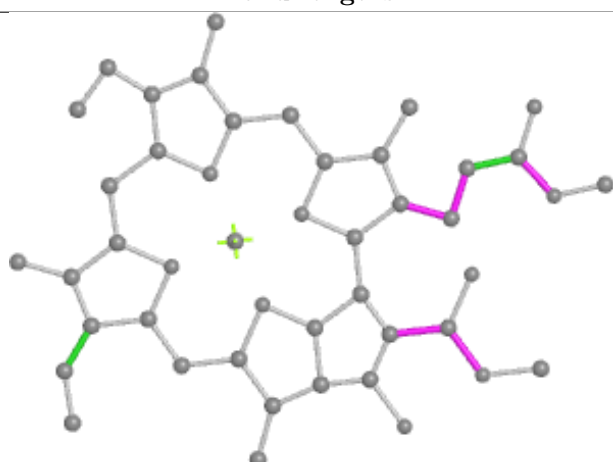
## Ligand CLA E 318



Bond lengths



Bond angles

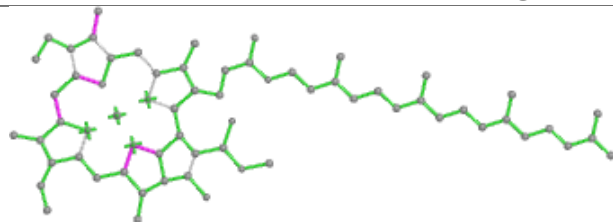


Torsions

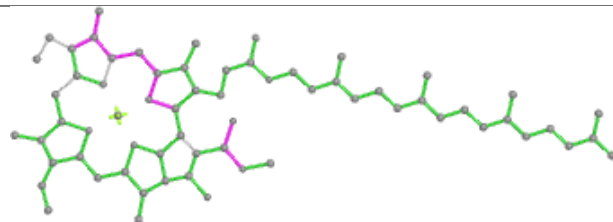


Rings

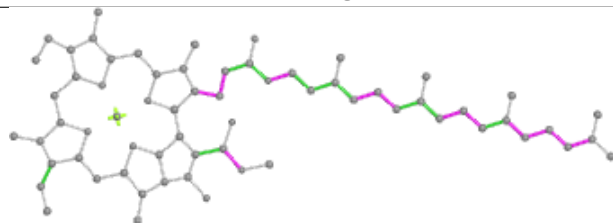
## Ligand CLA C 311



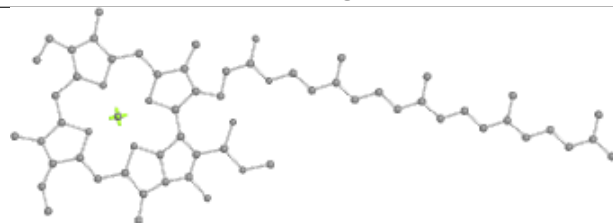
Bond lengths



Bond angles

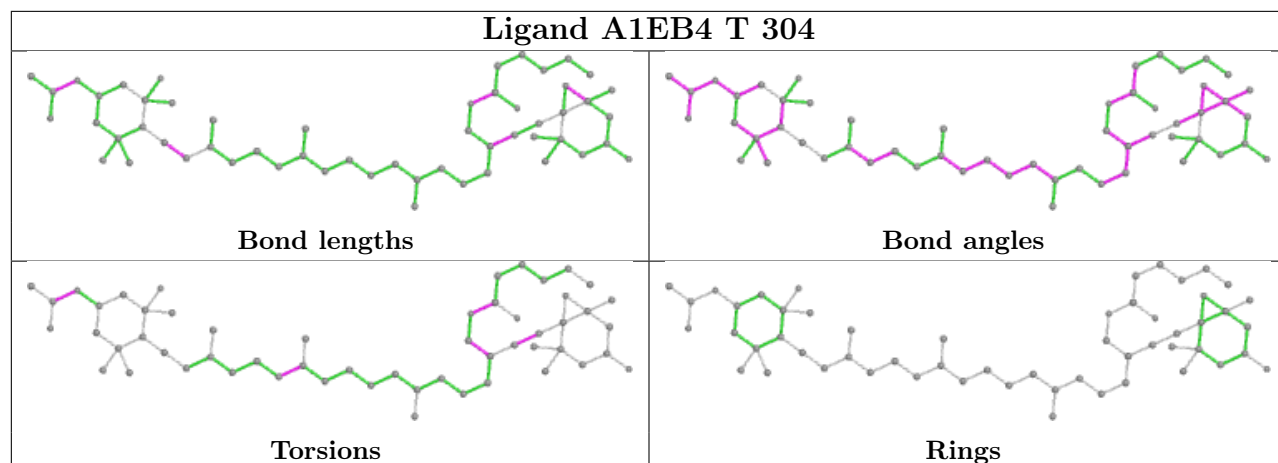


Torsions

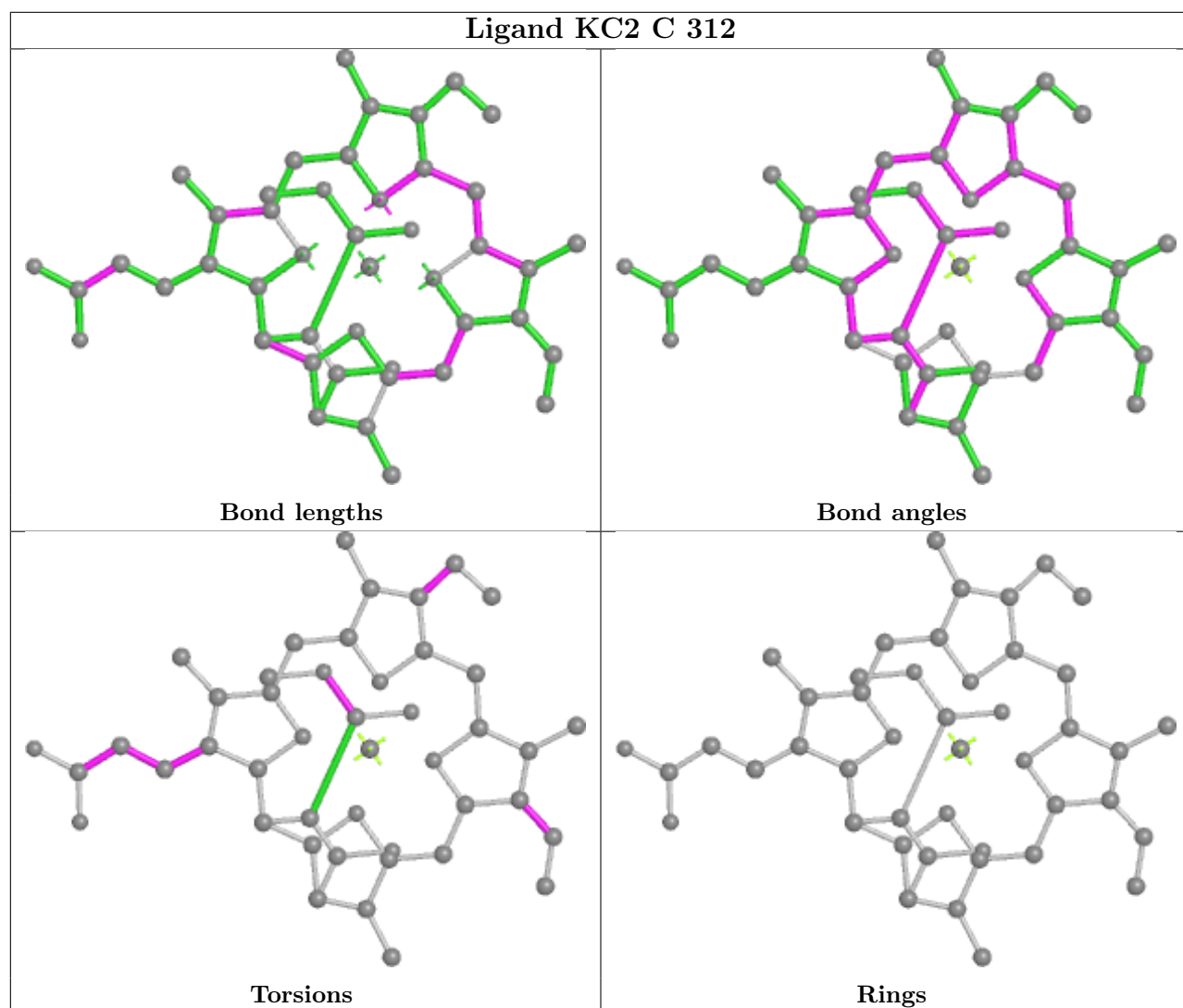


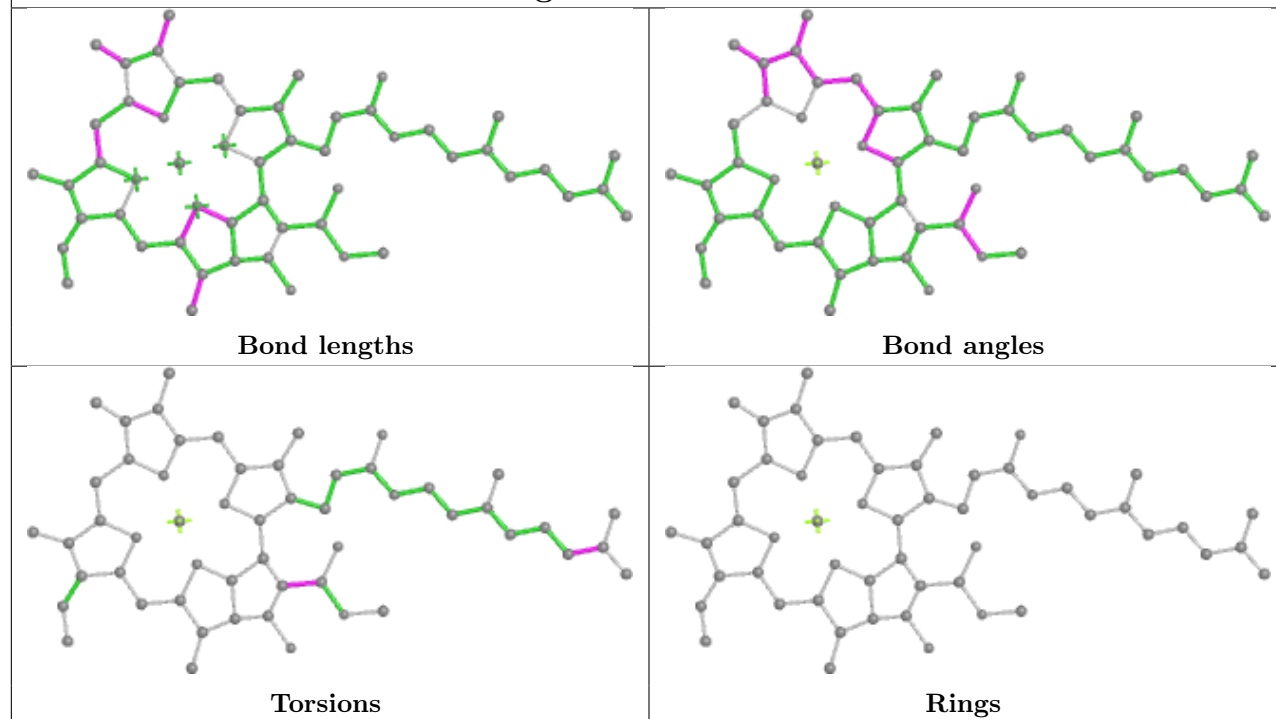
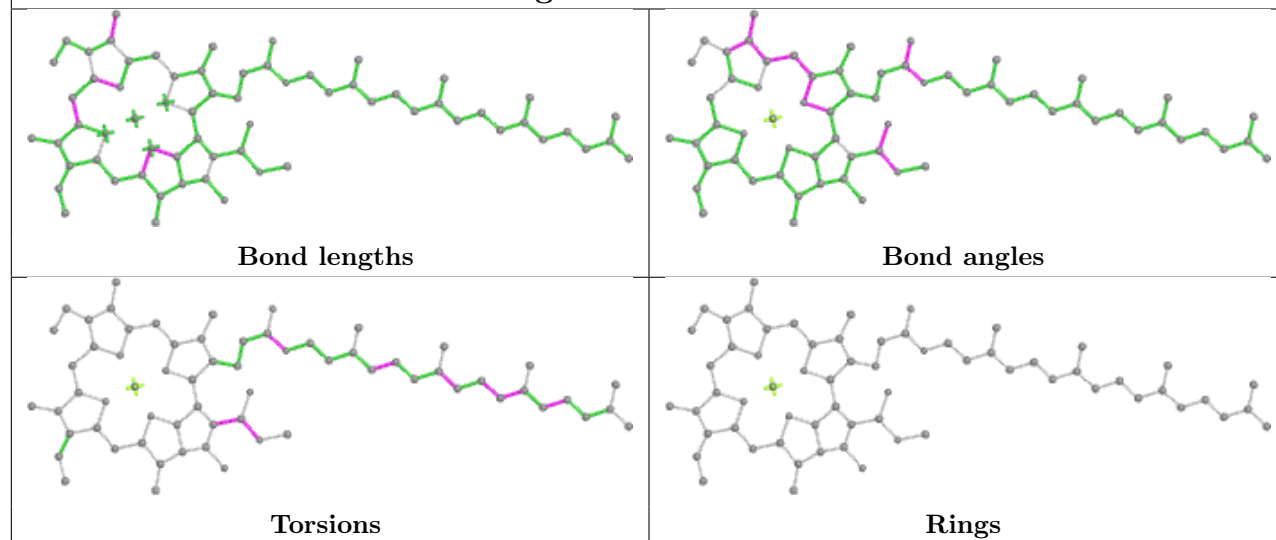
Rings

## Ligand A1EB4 T 304



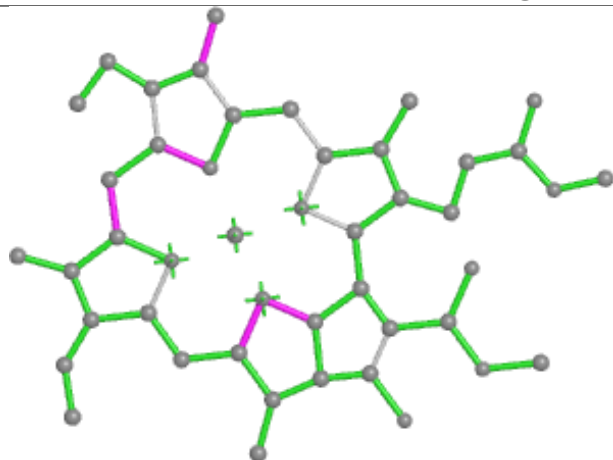
## Ligand KC2 C 312



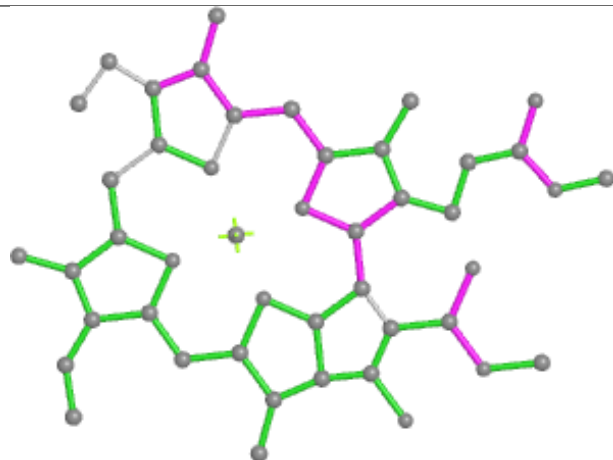
**Ligand CLA b 813****Ligand CLA b 841**



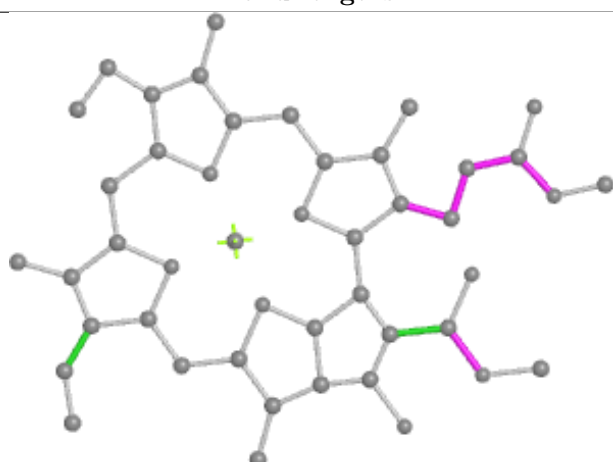
## Ligand CLA L 320



Bond lengths



Bond angles

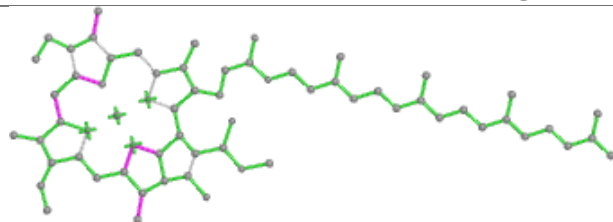


Torsions

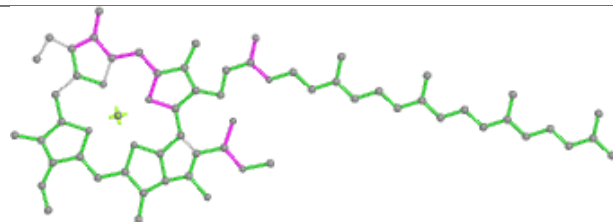


Rings

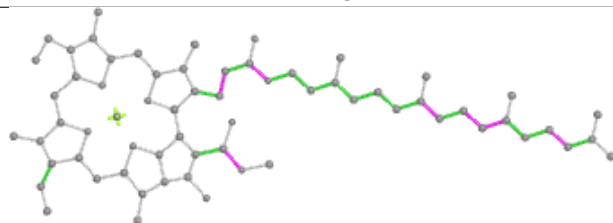
## Ligand CLA P 307



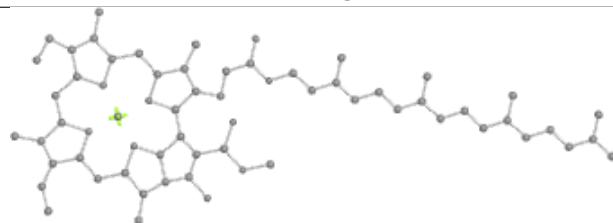
Bond lengths



Bond angles

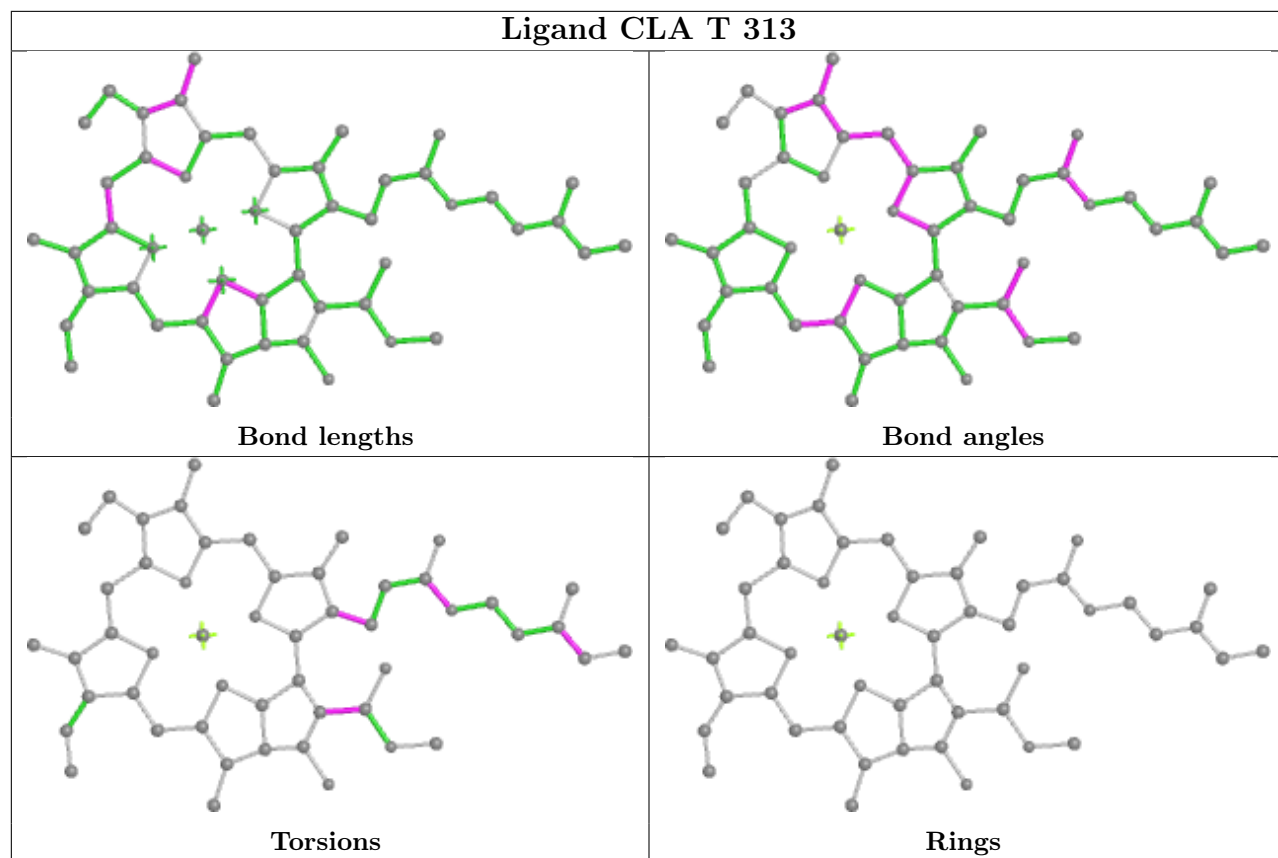


Torsions

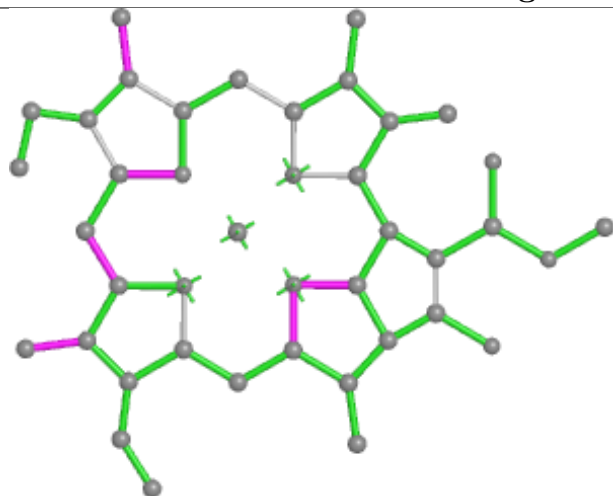


Rings

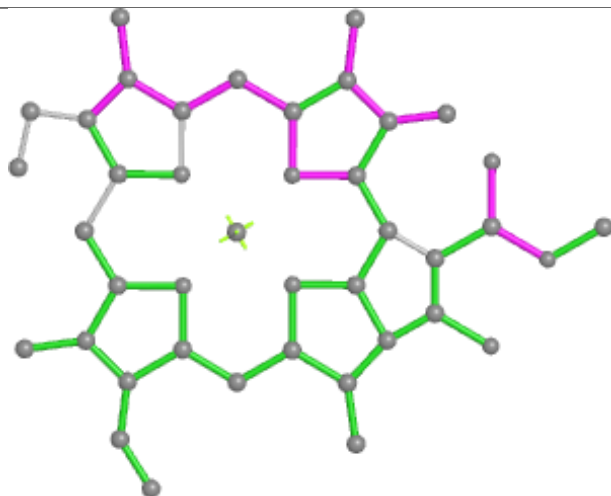
## Ligand CLA T 313



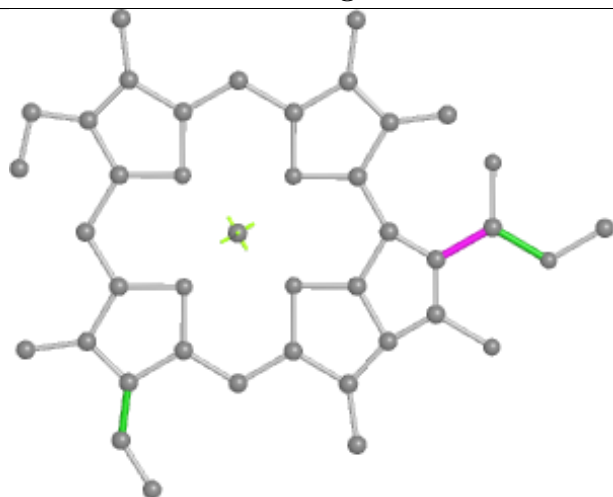
## Ligand CLA 9 310



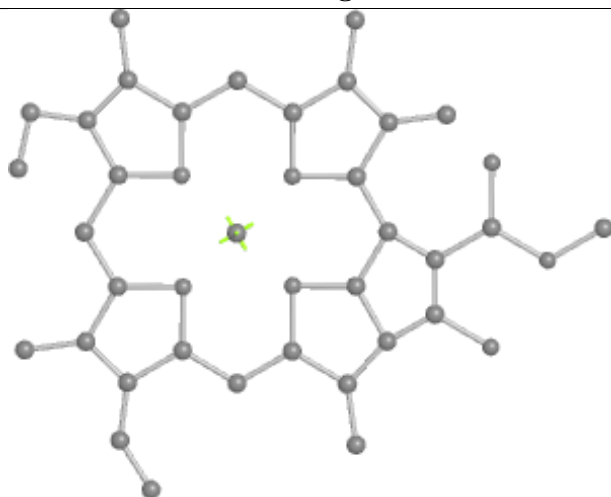
Bond lengths



Bond angles

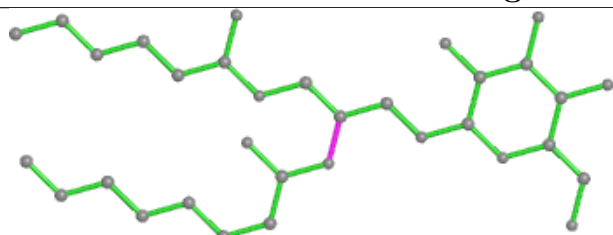


Torsions

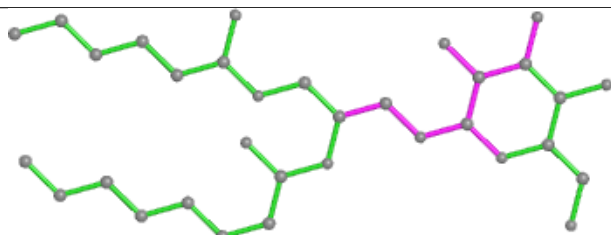


Rings

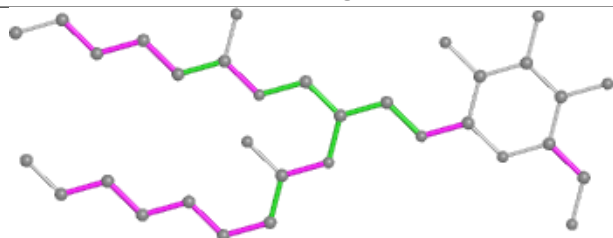
## Ligand LMG W 320



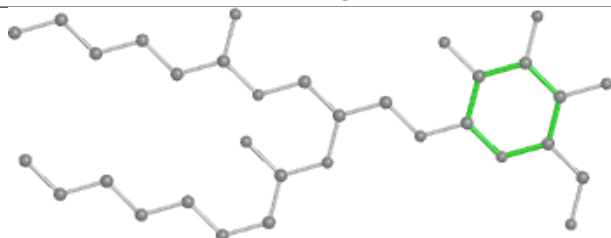
Bond lengths



Bond angles

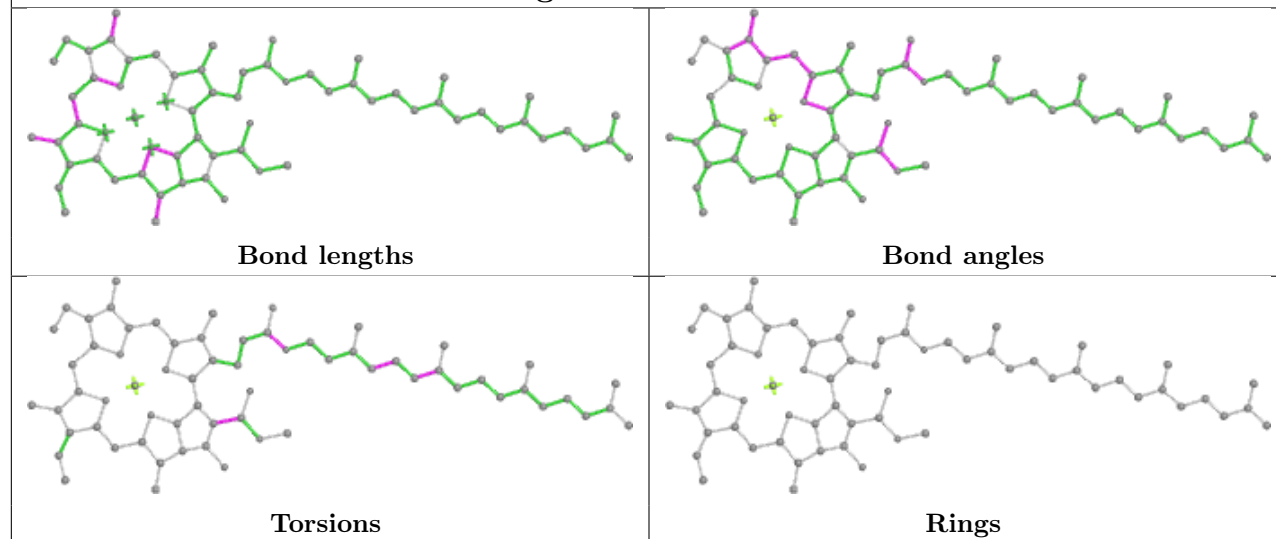


Torsions

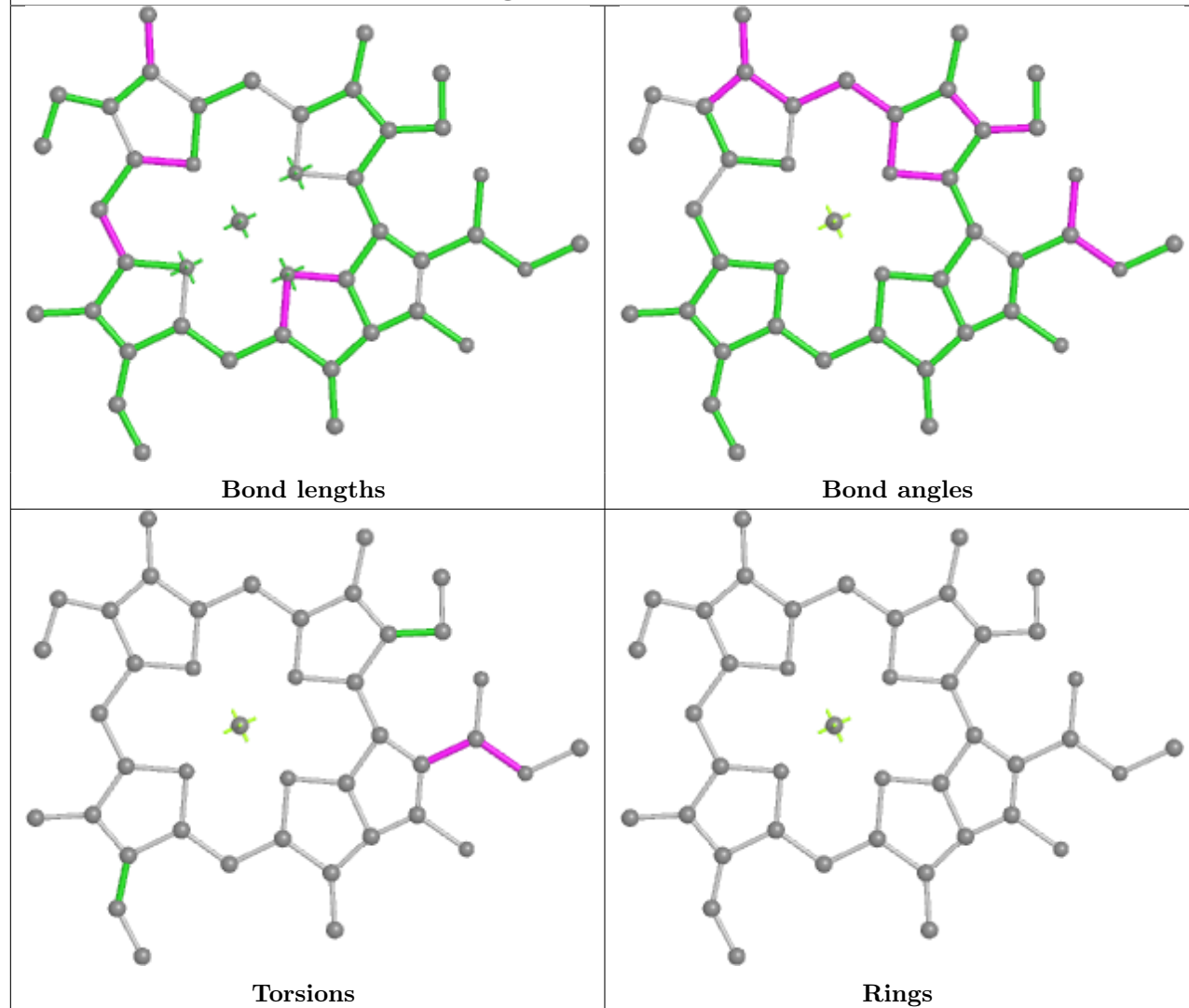


Rings

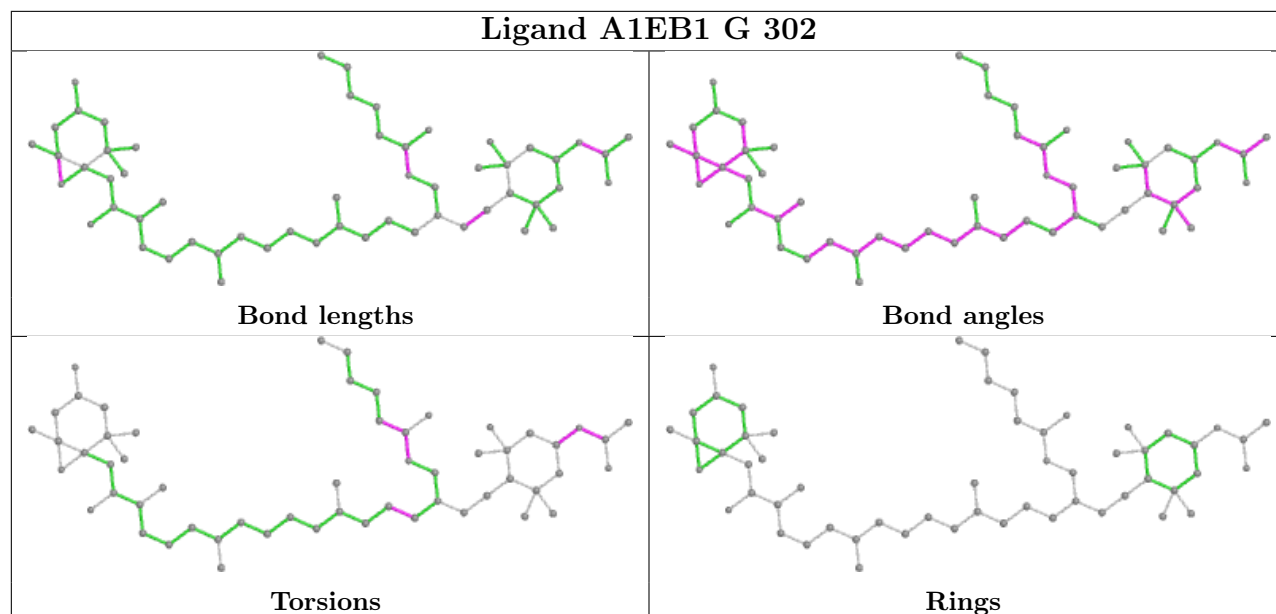
## Ligand CLA a 824



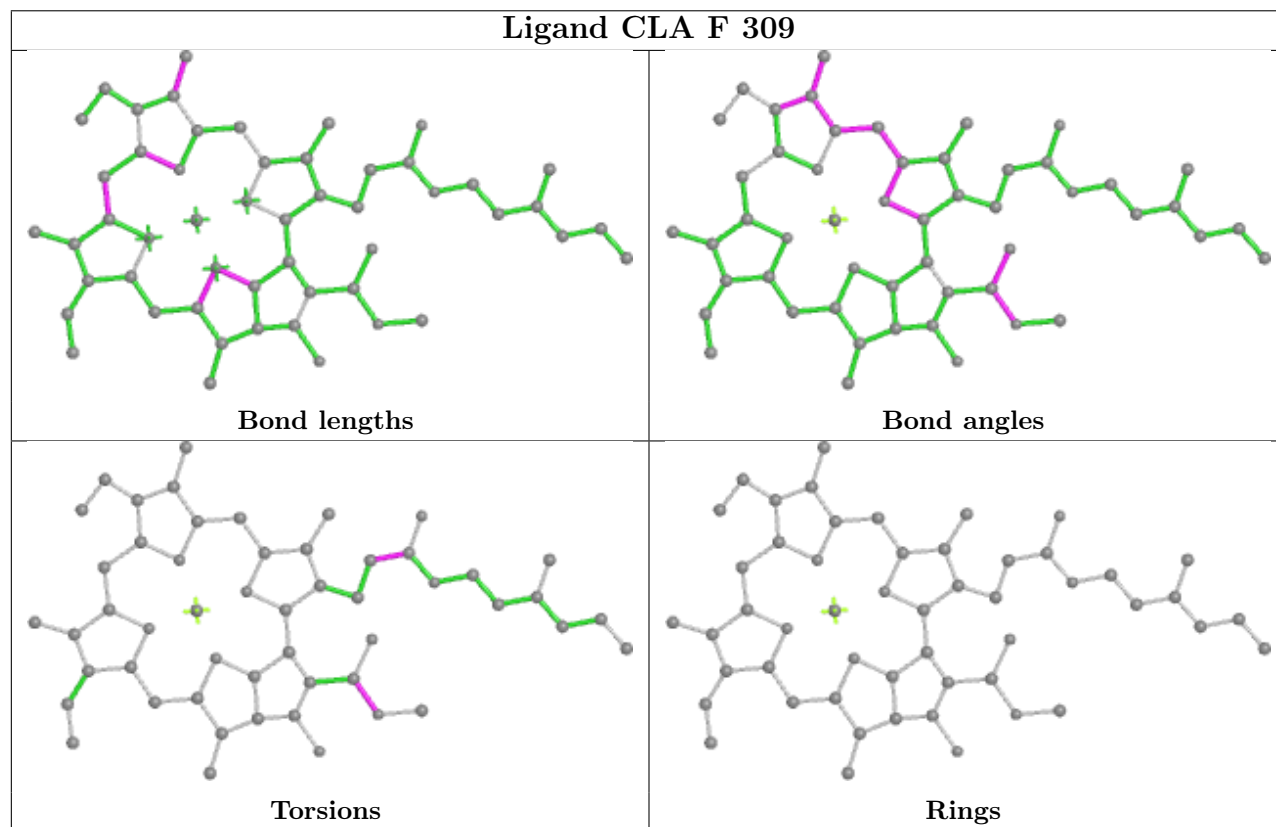
## Ligand CLA o 202

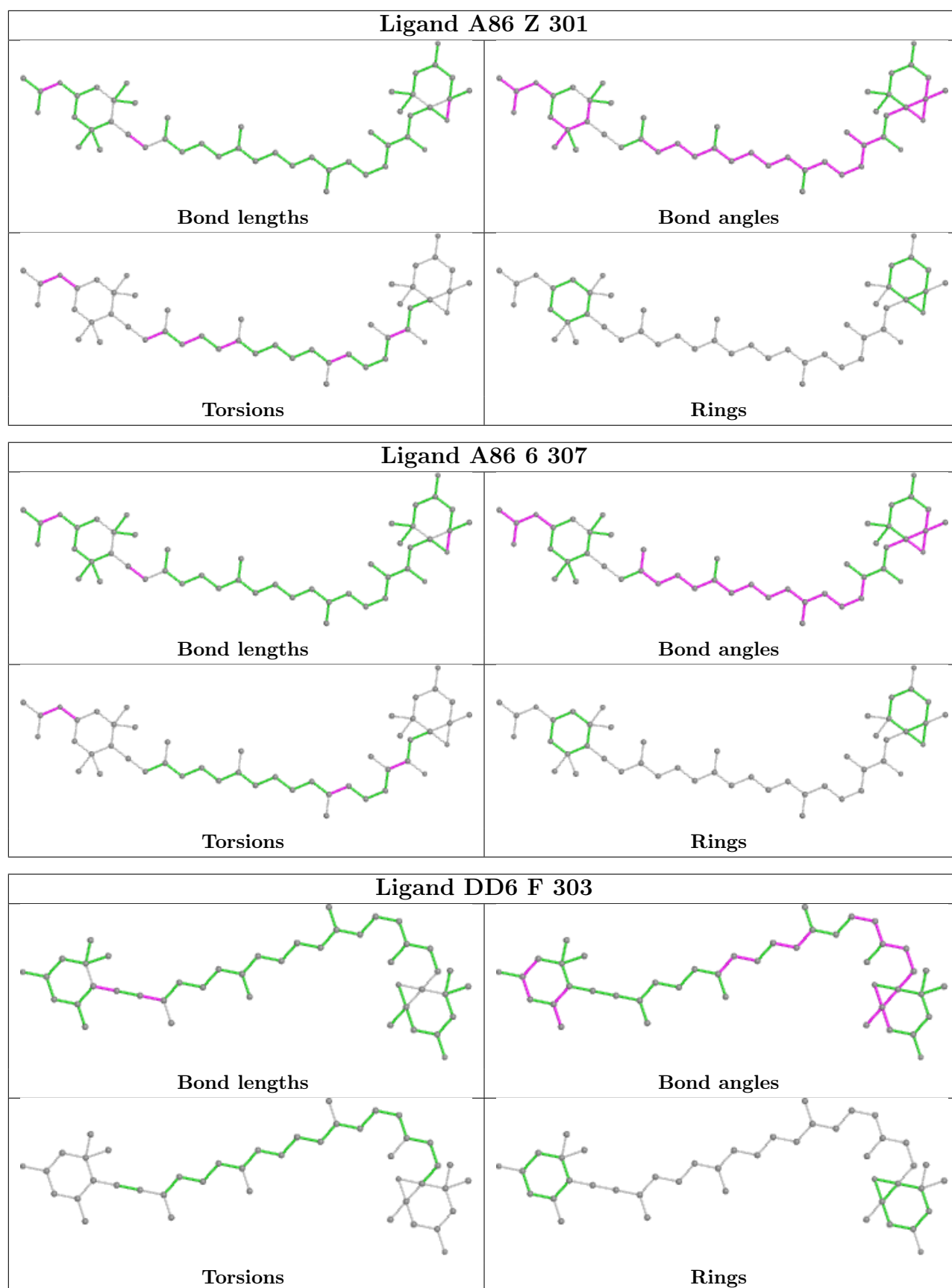


## Ligand A1EB1 G 302

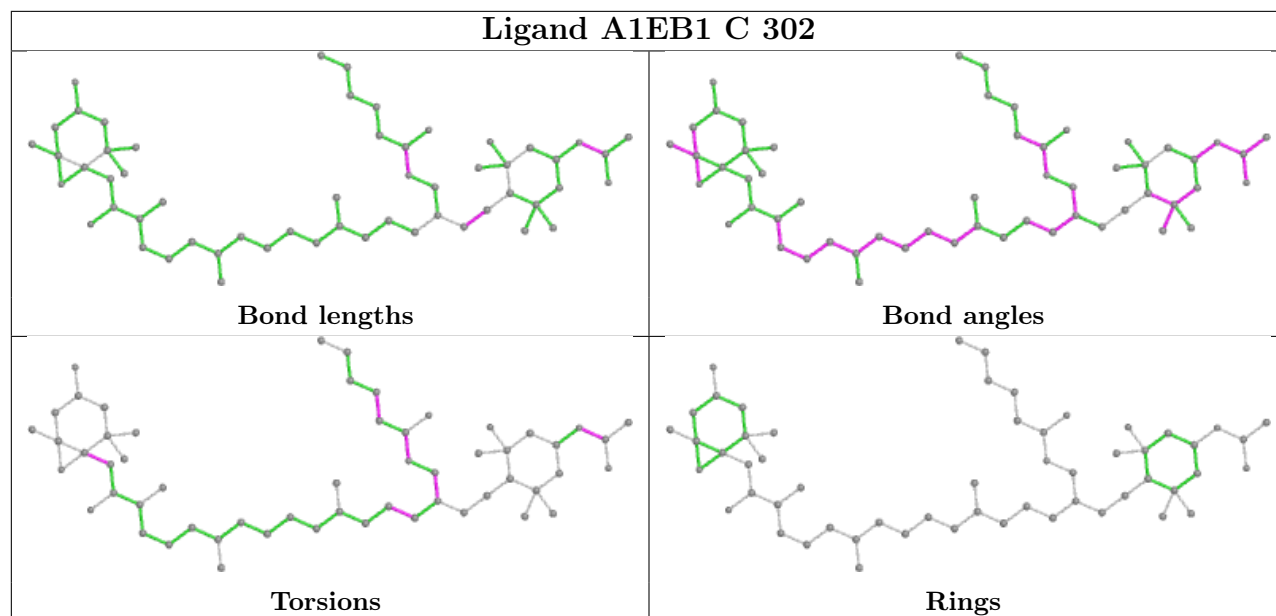


## Ligand CLA F 309

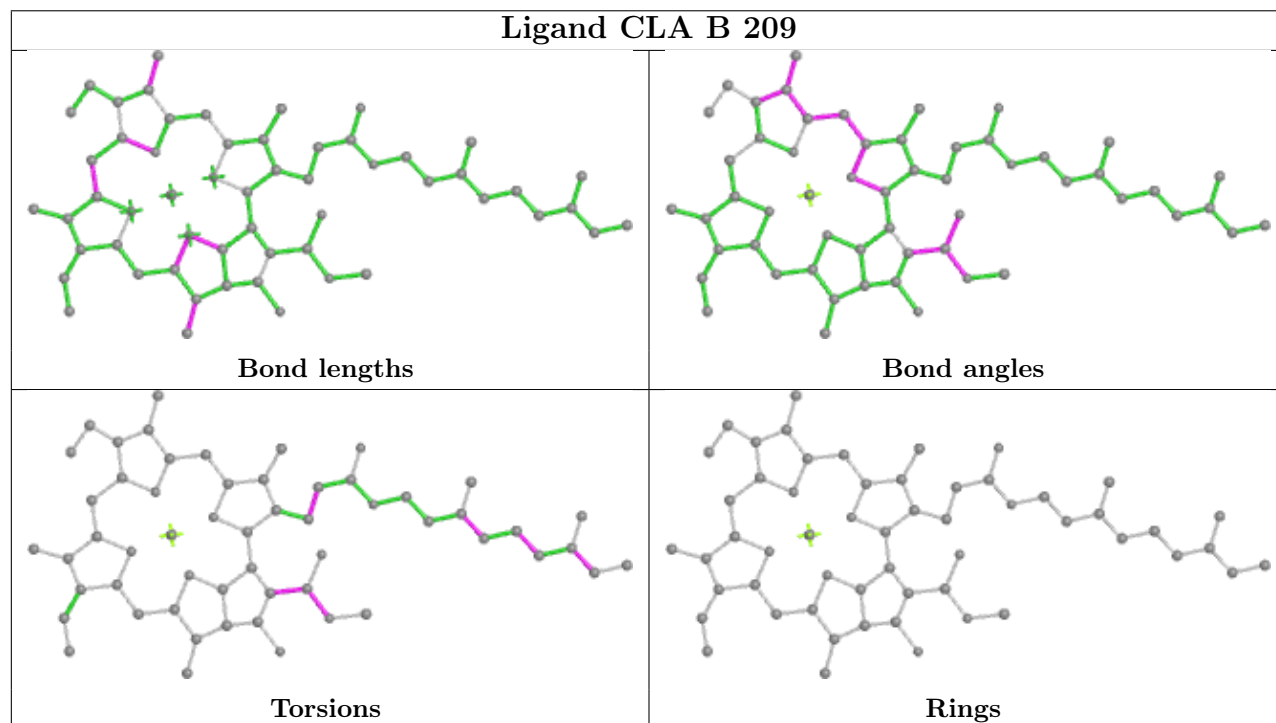




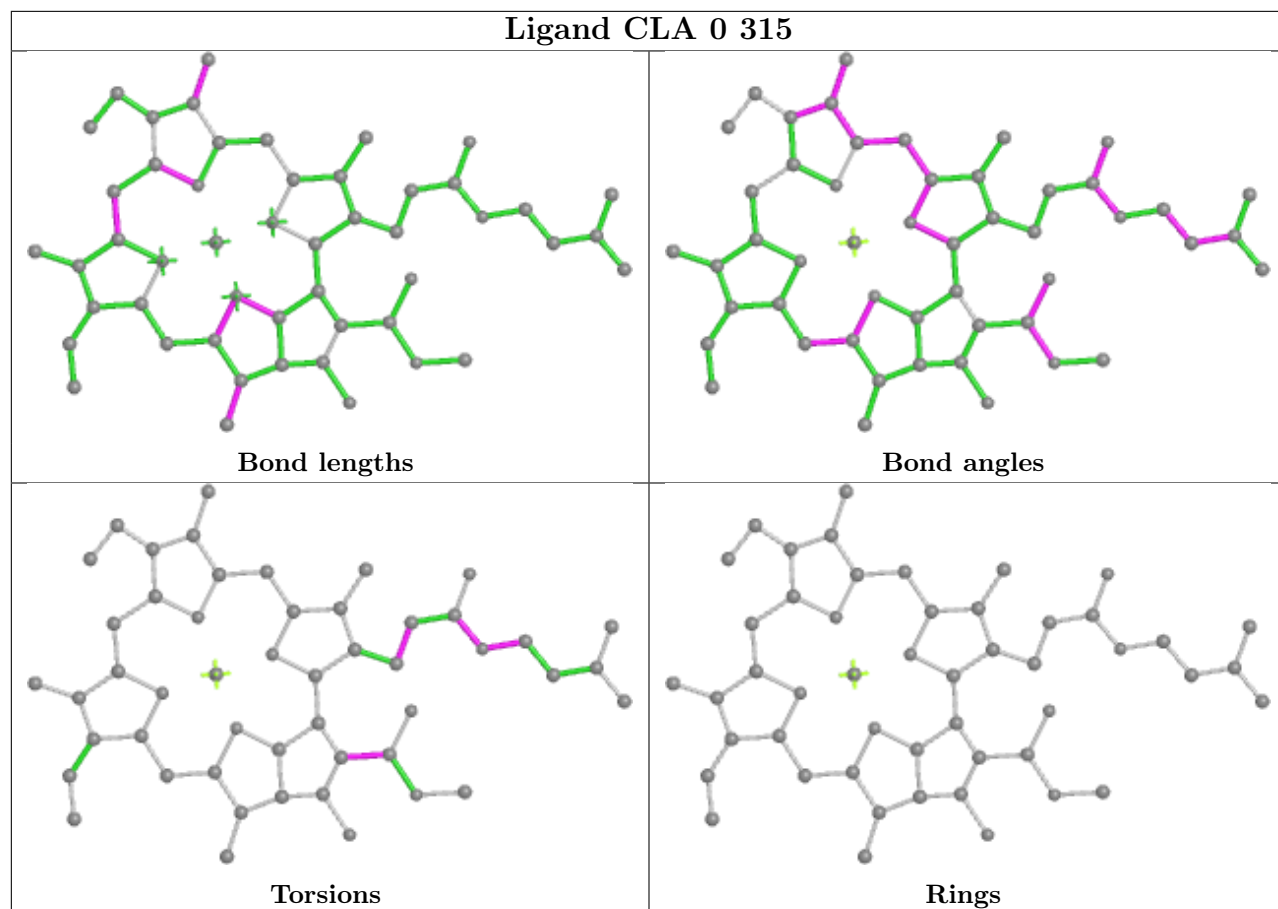
## Ligand A1EB1 C 302



## Ligand CLA B 209

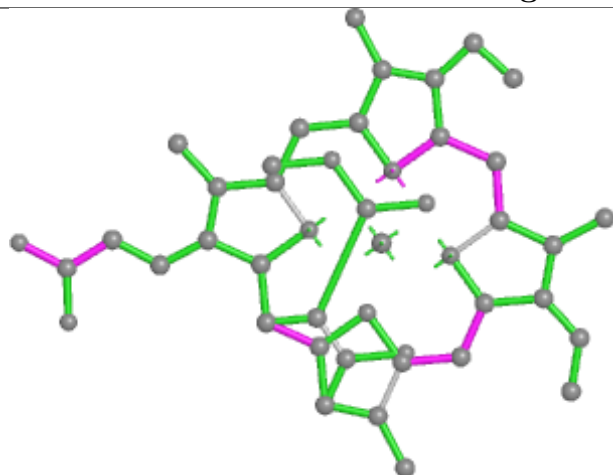


## Ligand CLA 0 315

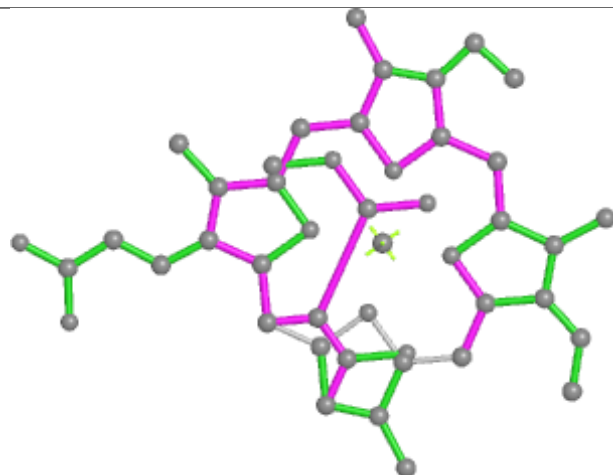




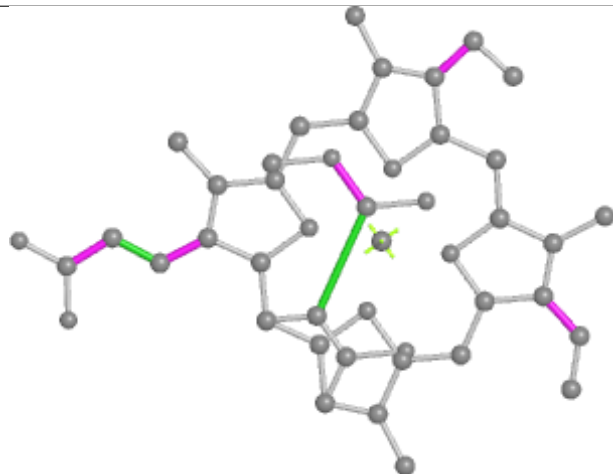
## Ligand KC2 3 321



Bond lengths



Bond angles

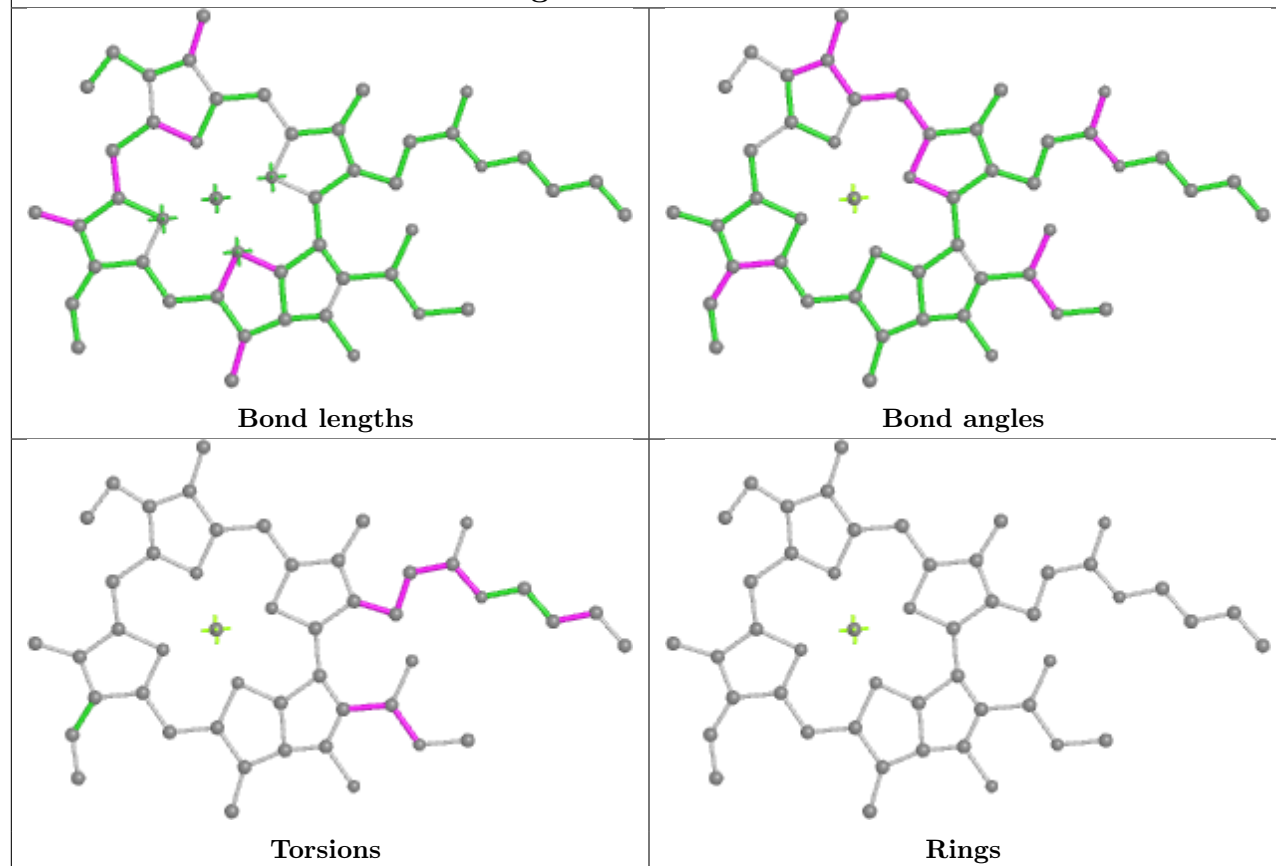


Torsions

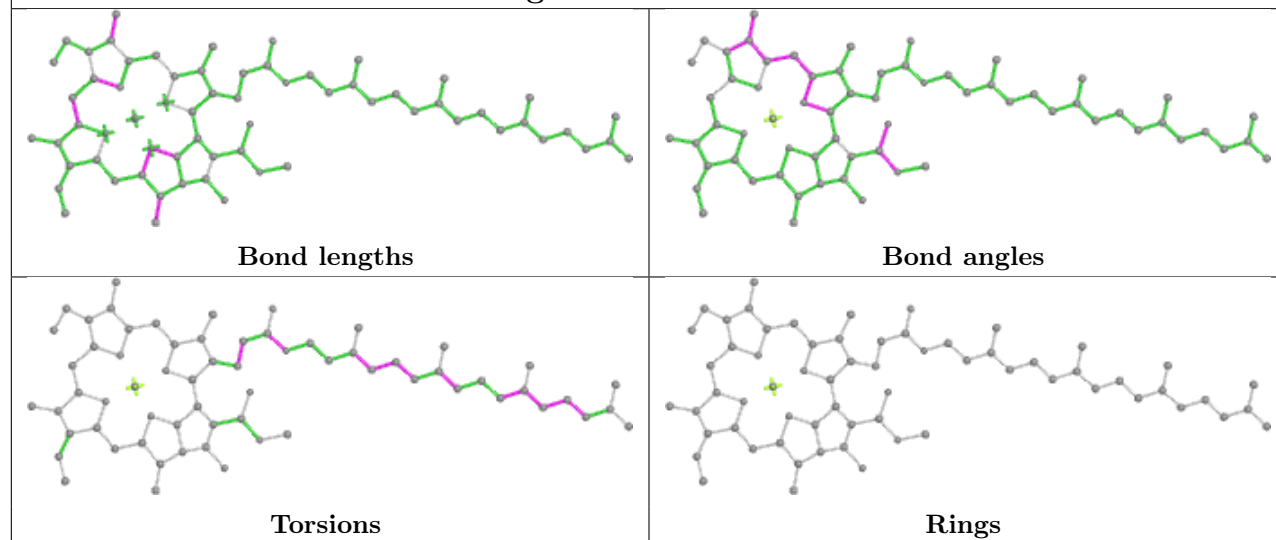


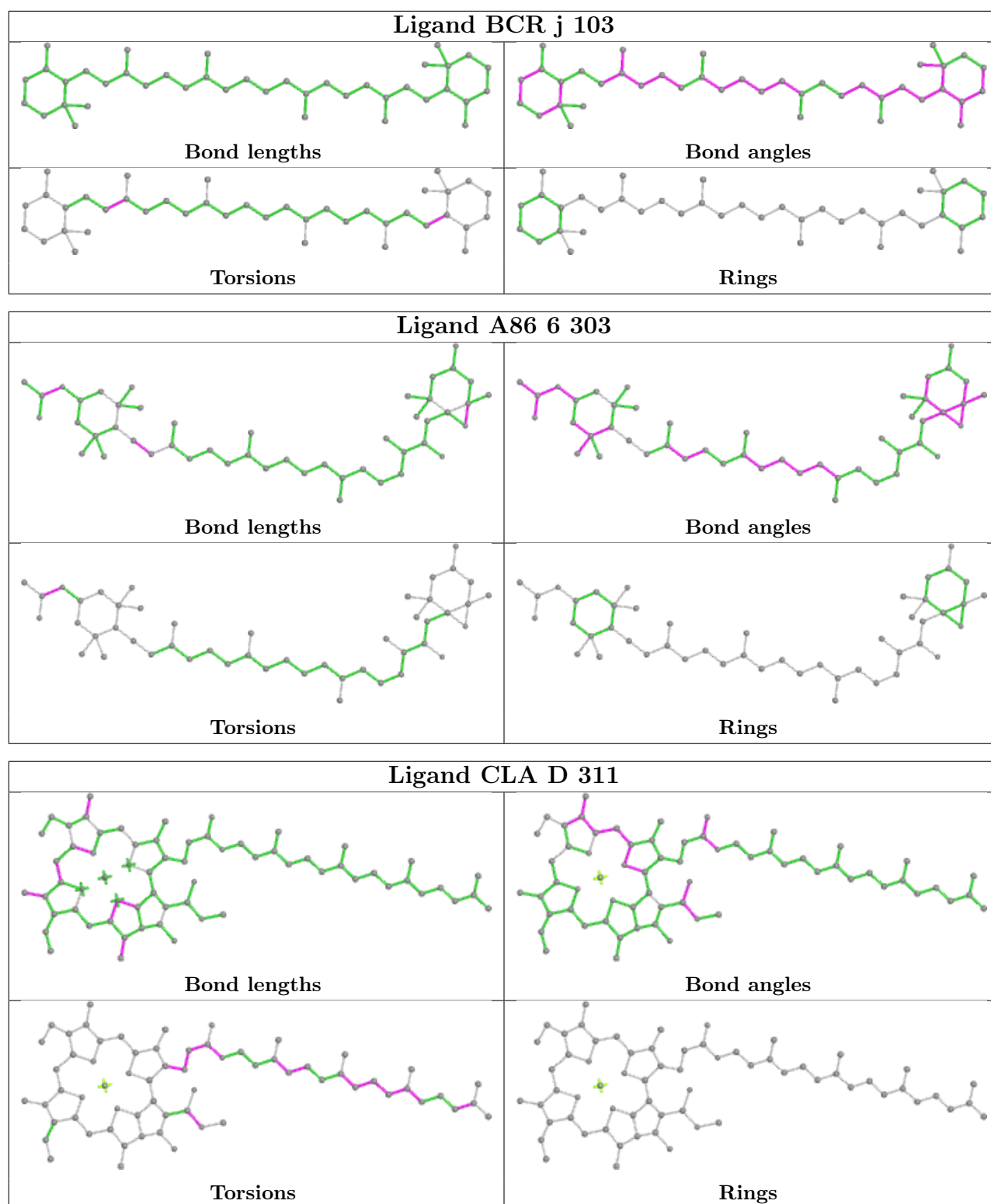
Rings

## Ligand CLA G 318

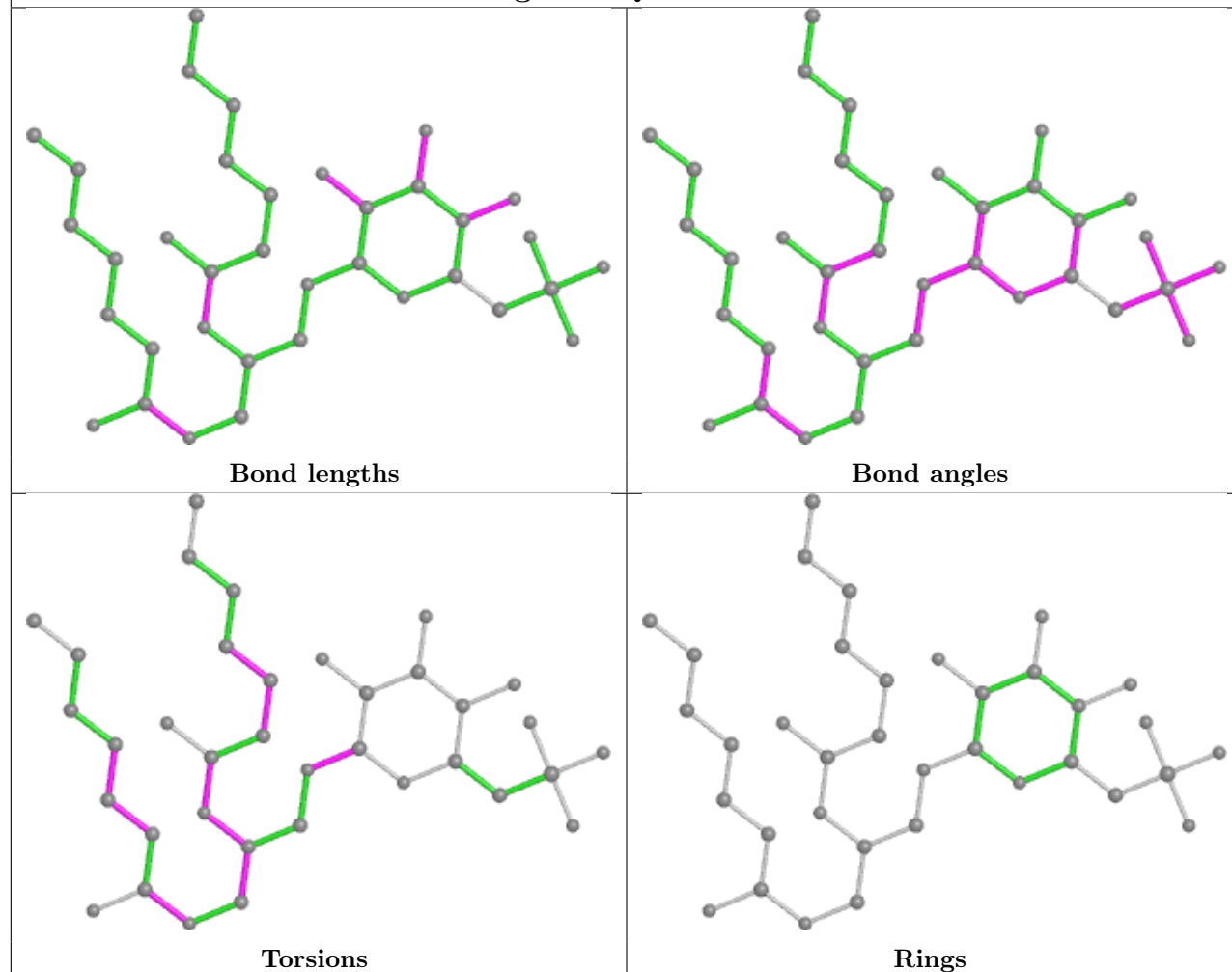


## Ligand CLA W 310

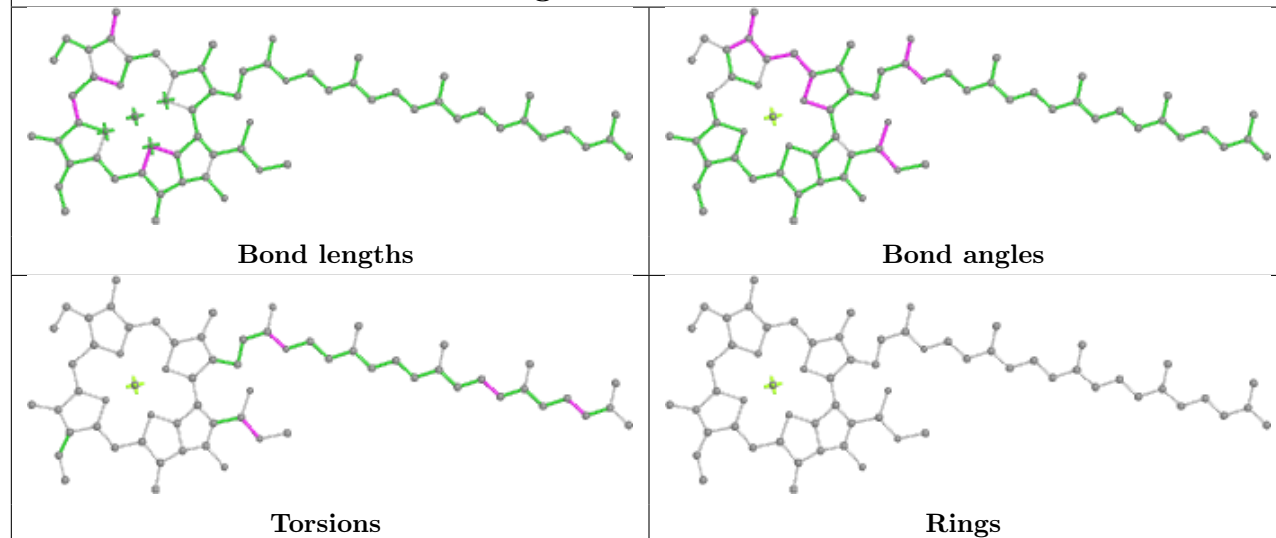




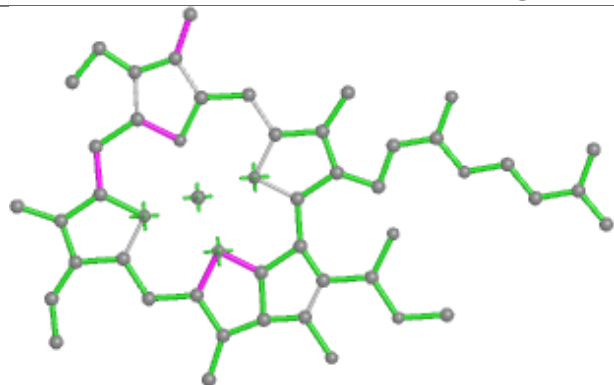
## Ligand SQD T 321



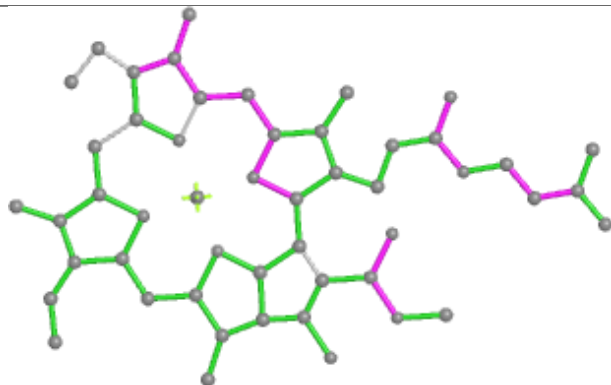
## Ligand CLA F 312



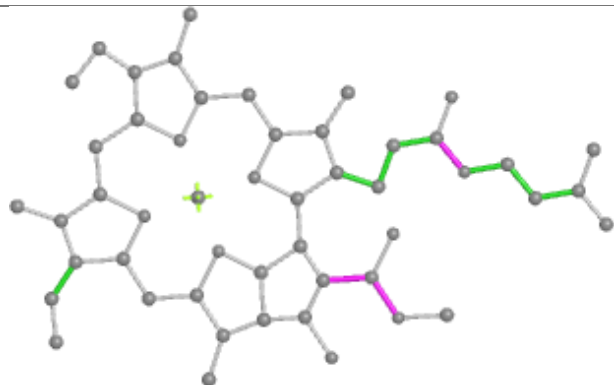
## Ligand CLA V 316



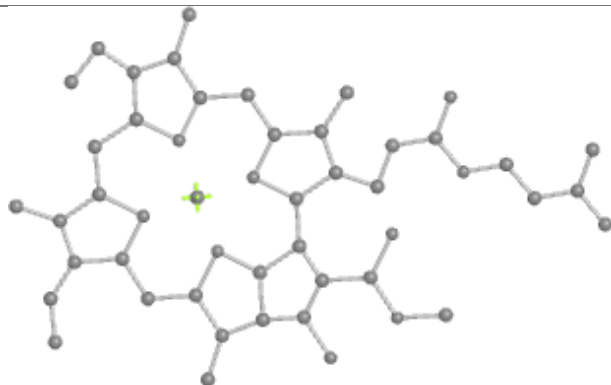
Bond lengths



Bond angles

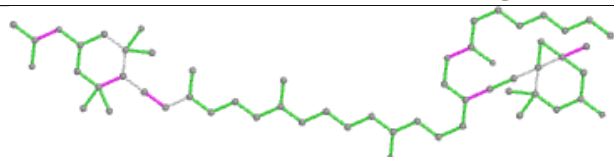


Torsions

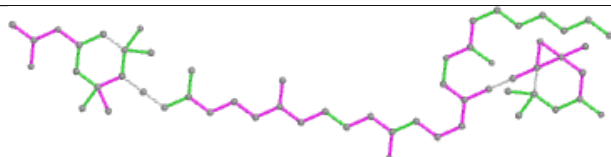


Rings

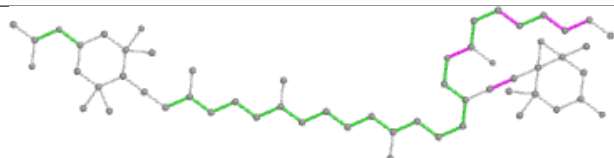
## Ligand A1EB4 P 319



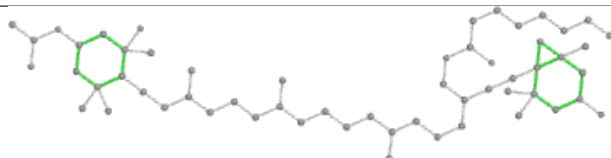
Bond lengths



Bond angles

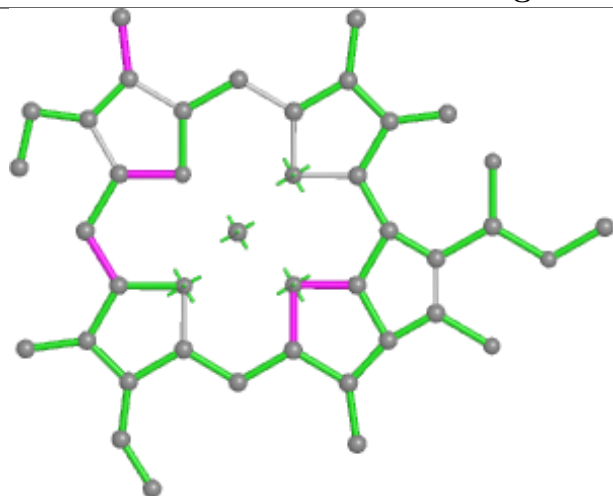


Torsions

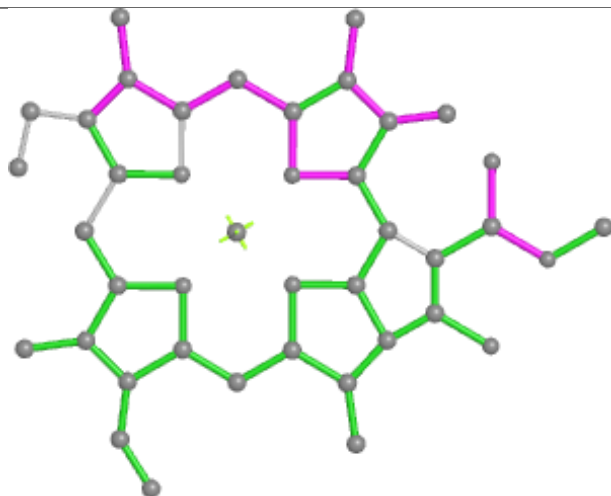


Rings

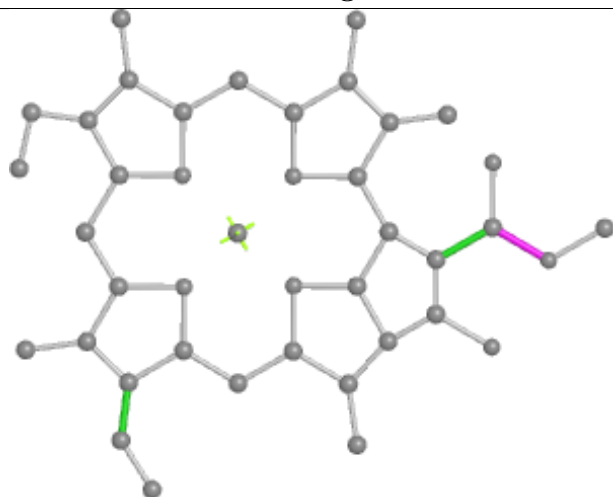
## Ligand CLA Y 303



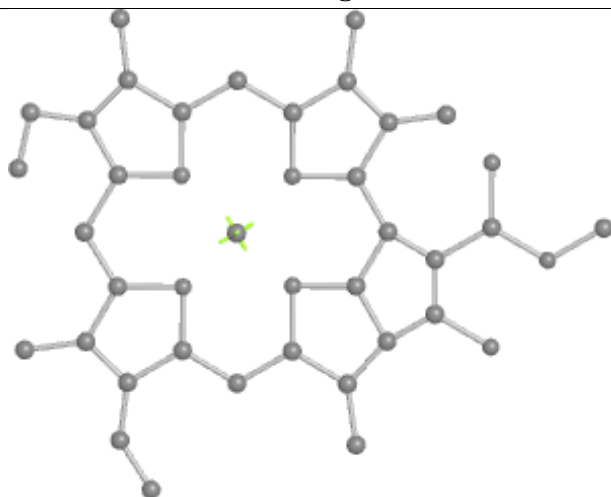
Bond lengths



Bond angles

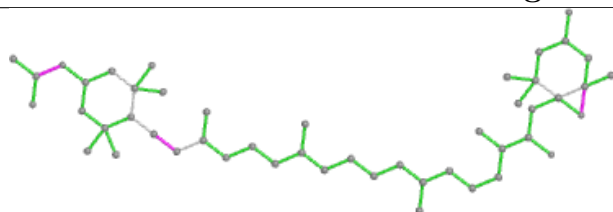


Torsions

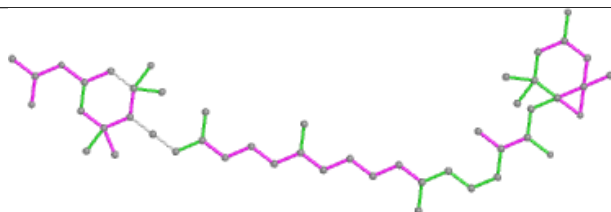


Rings

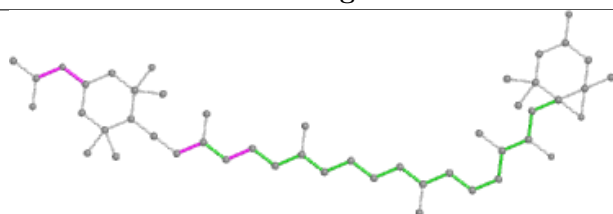
## Ligand A86 3 308



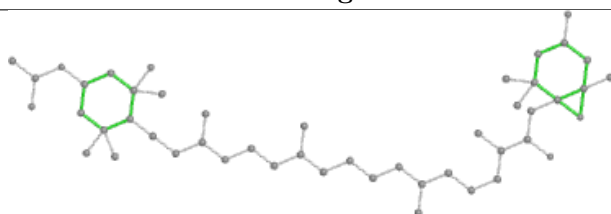
Bond lengths



Bond angles

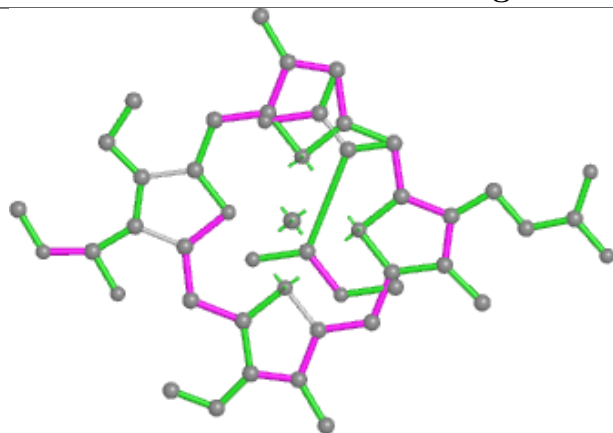


Torsions

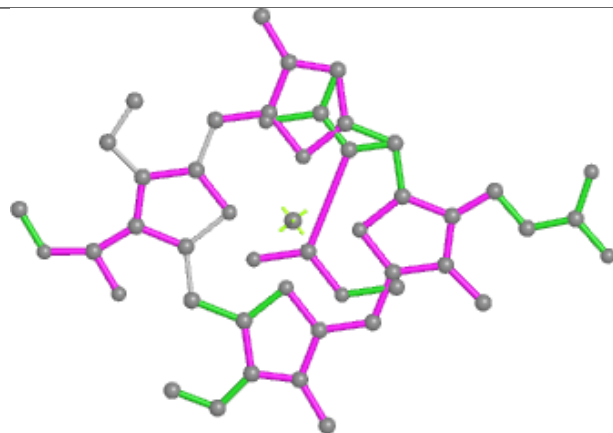


Rings

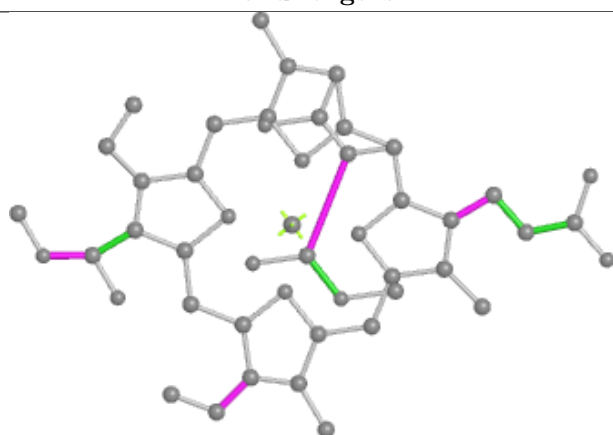
## Ligand A1ECV Z 314



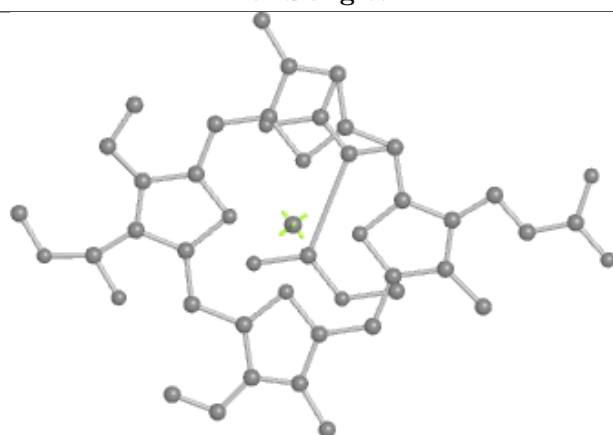
Bond lengths



Bond angles

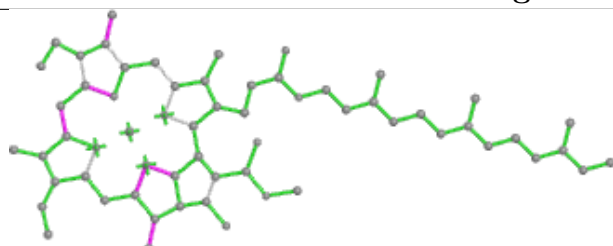


Torsions

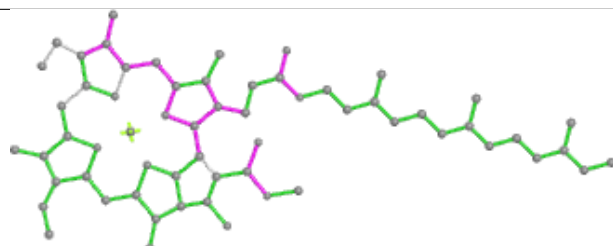


Rings

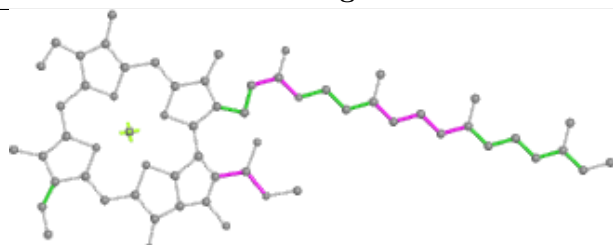
## Ligand CLA K 306



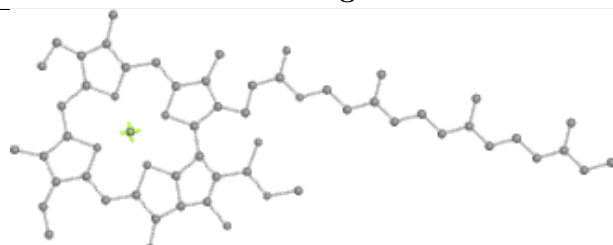
Bond lengths



Bond angles

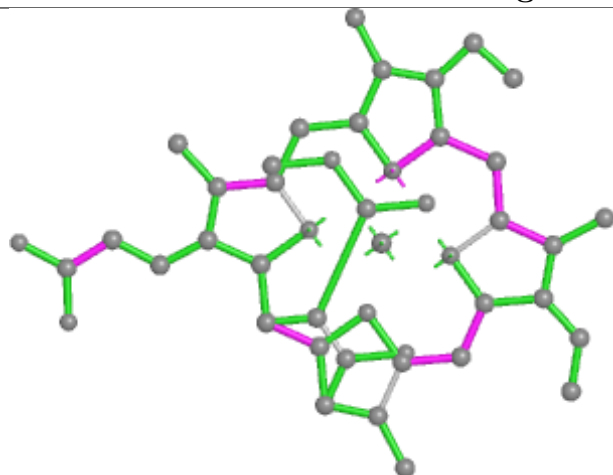


Torsions

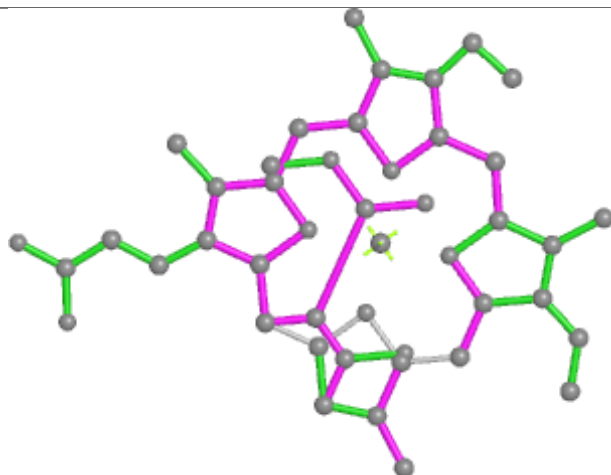


Rings

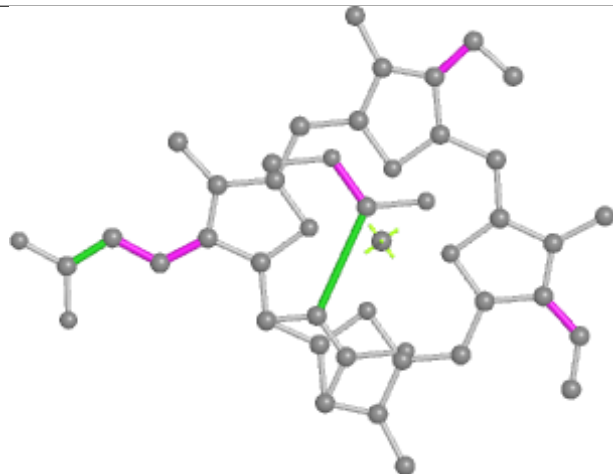
## Ligand KC2 T 314



Bond lengths



Bond angles

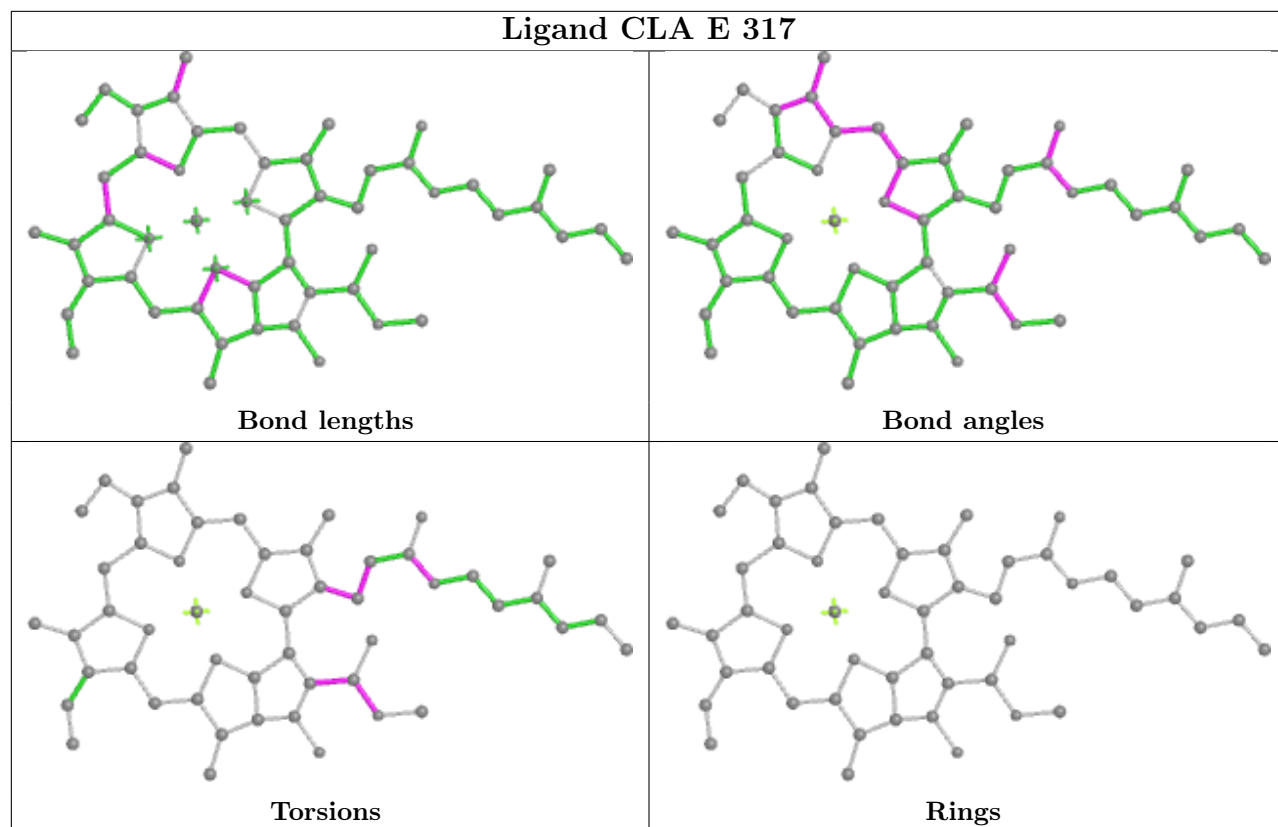


Torsions

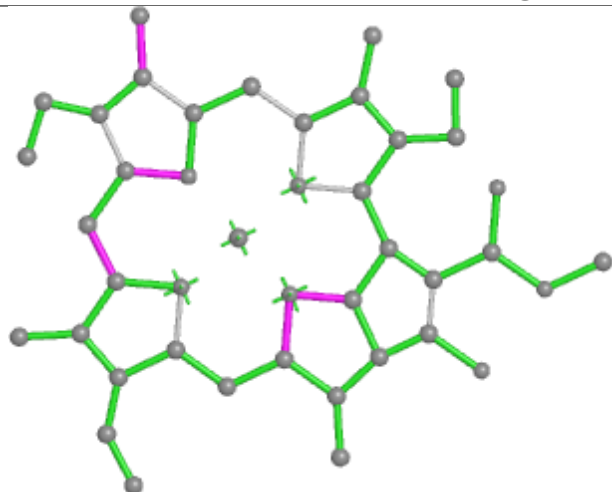


Rings

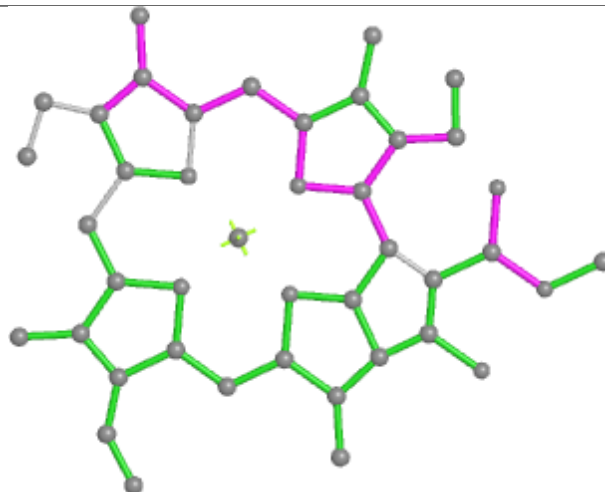




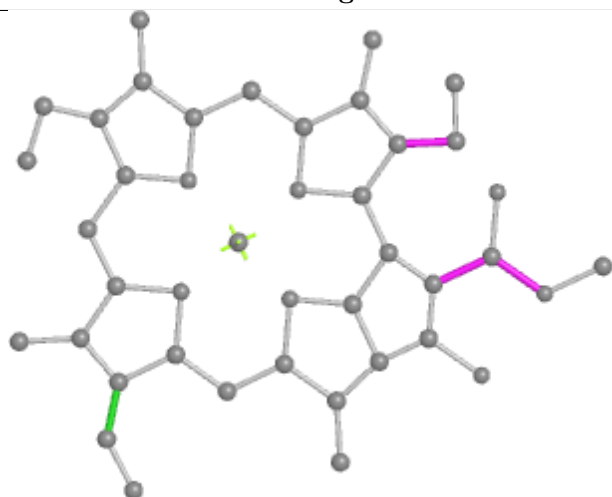
## Ligand CLA S 310



Bond lengths



Bond angles

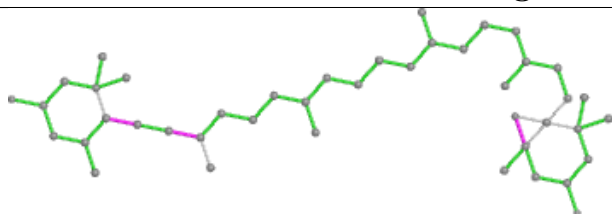


Torsions

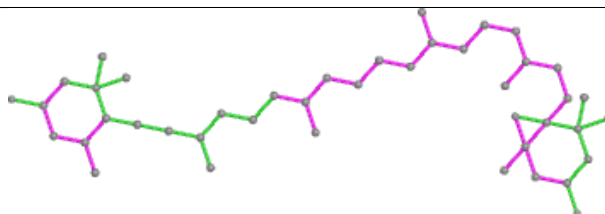


Rings

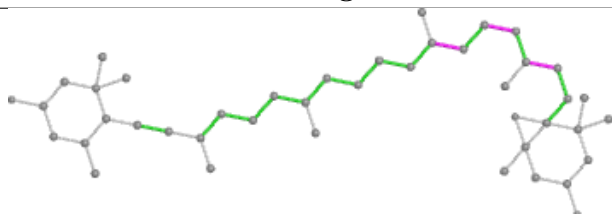
## Ligand DD6 A 303



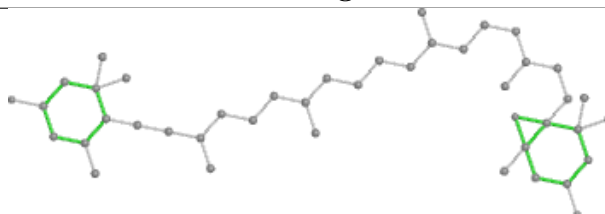
Bond lengths



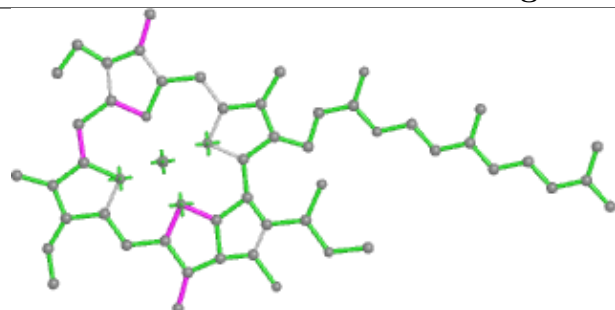
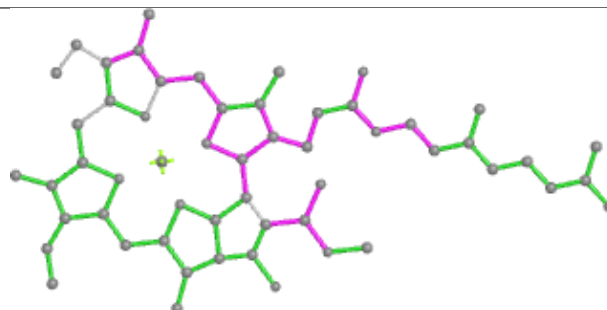
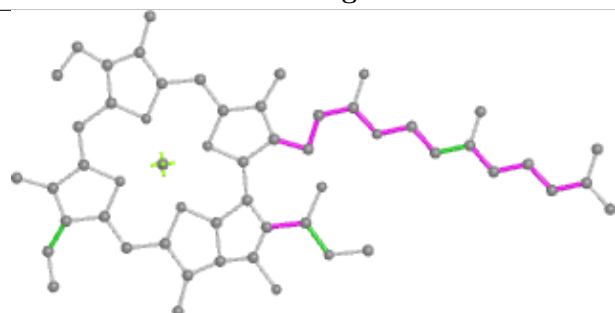
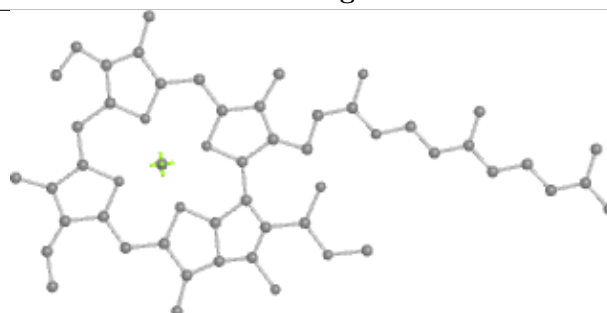
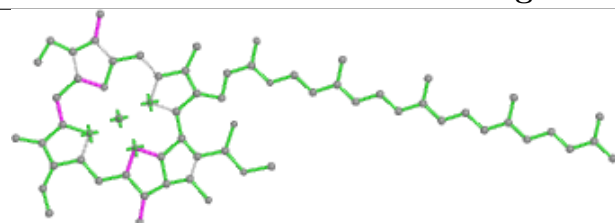
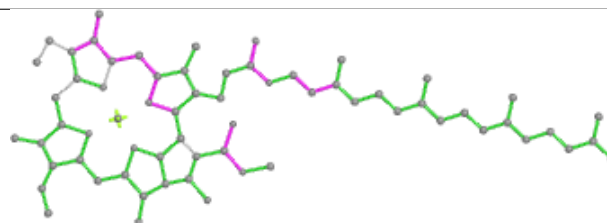
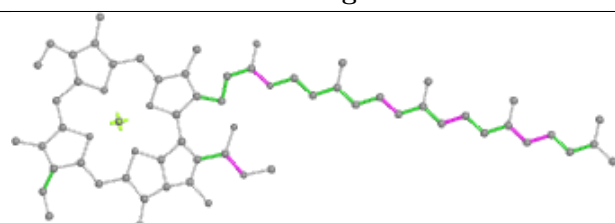
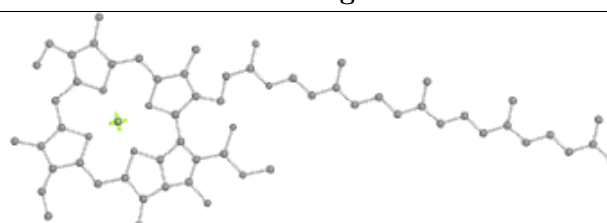
Bond angles



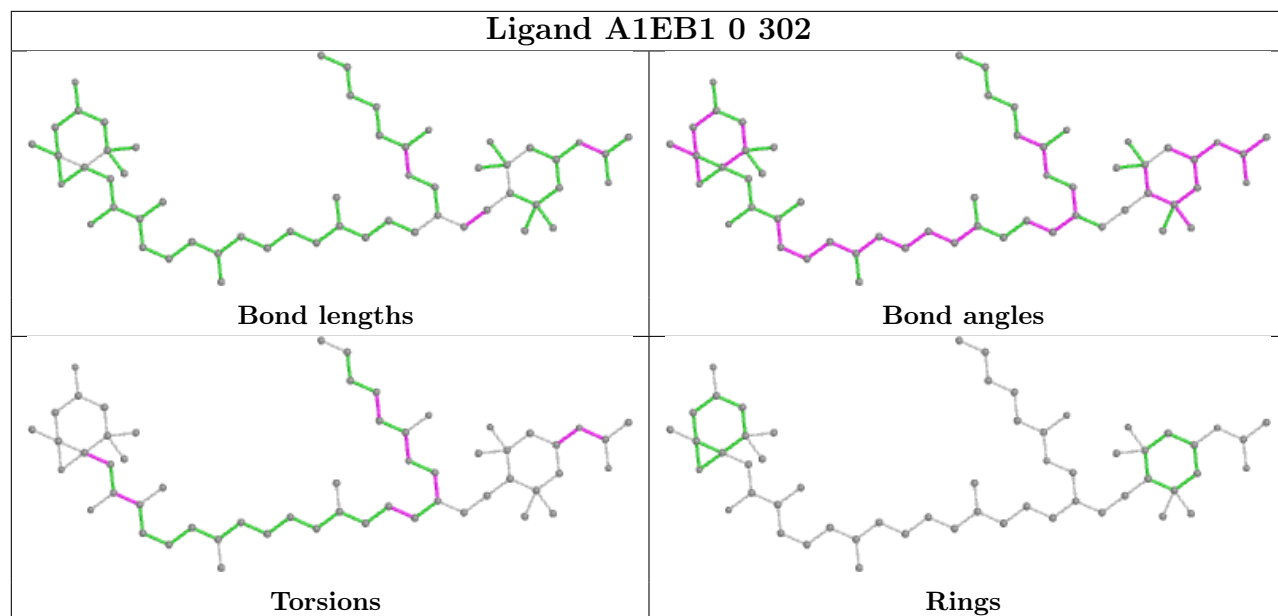
Torsions



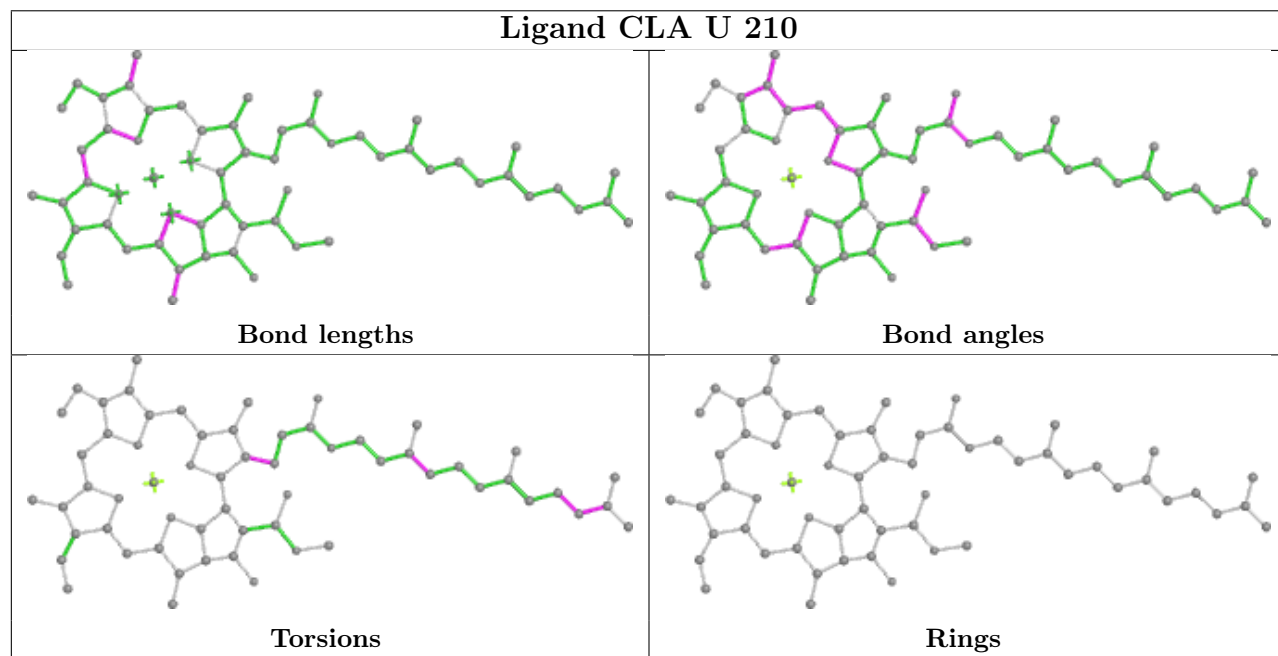
Rings

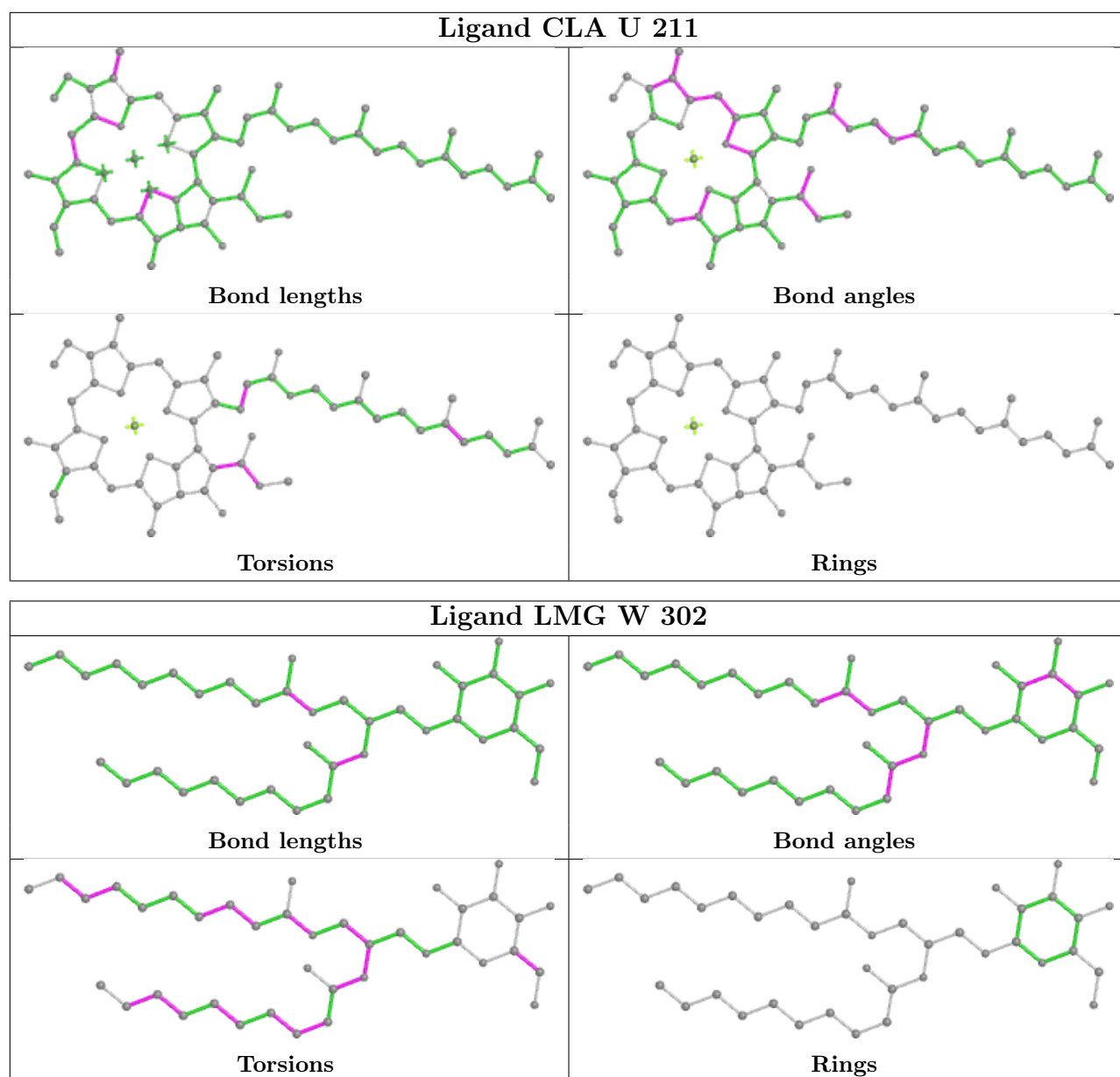
**Ligand CLA 9 308****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA D 314****Bond lengths****Bond angles****Torsions****Rings**

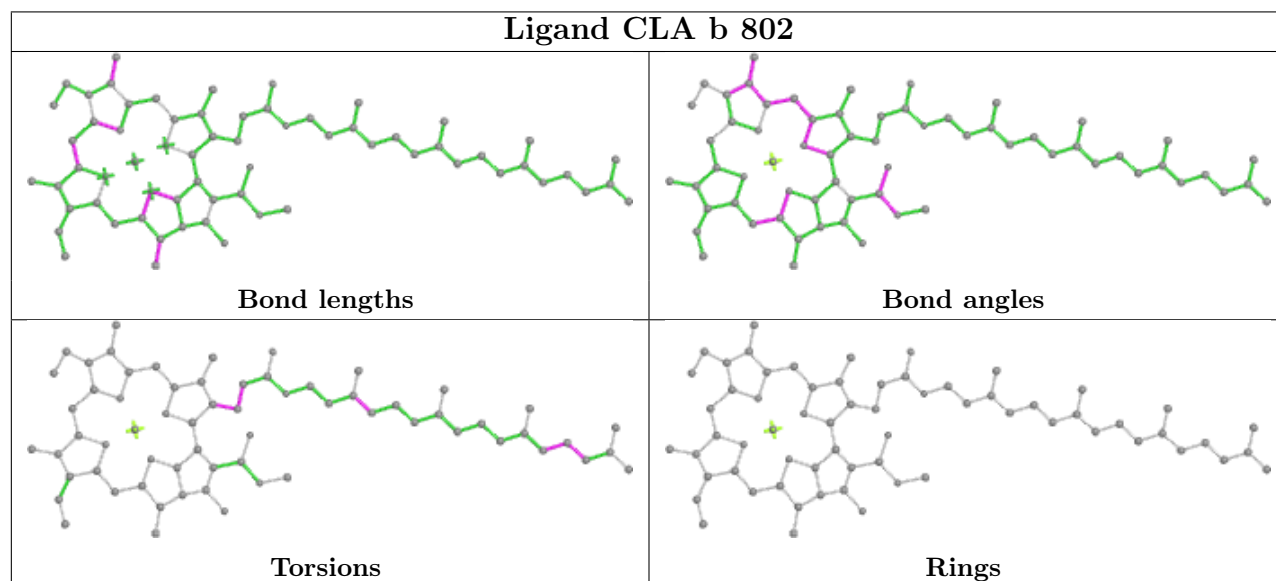
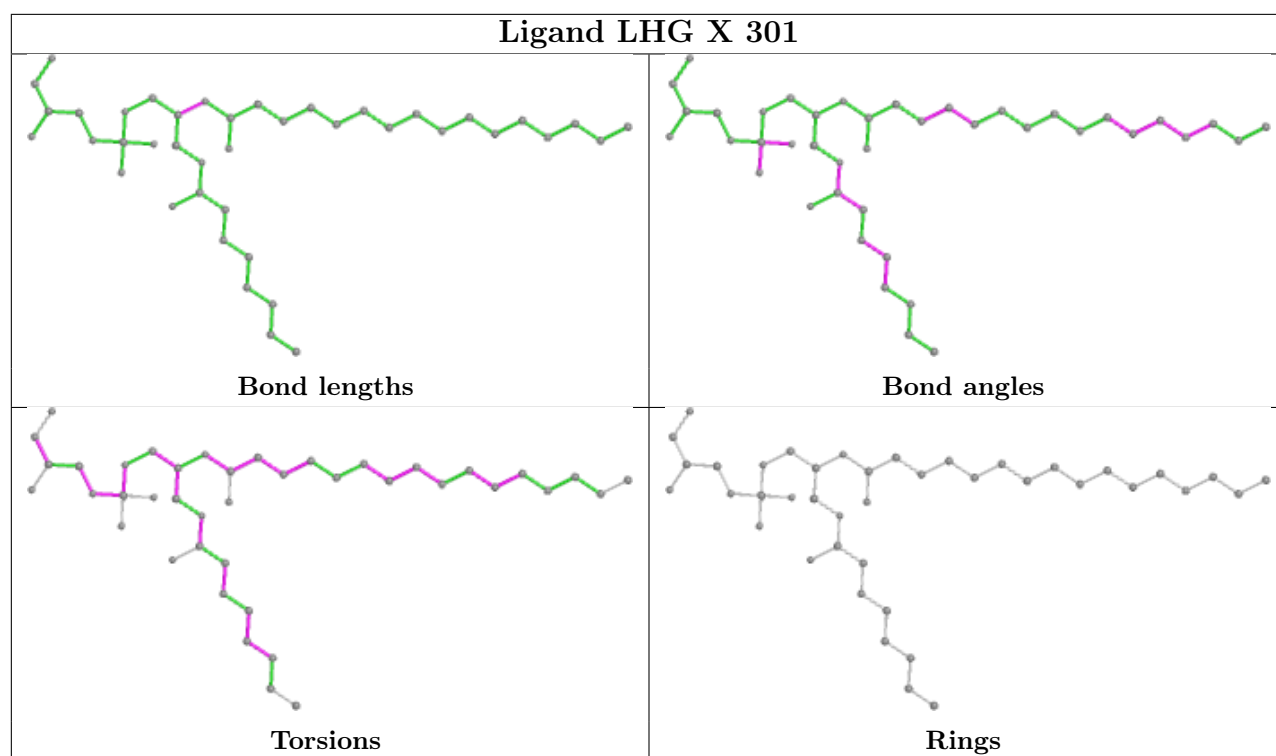
## Ligand A1EB1 0 302



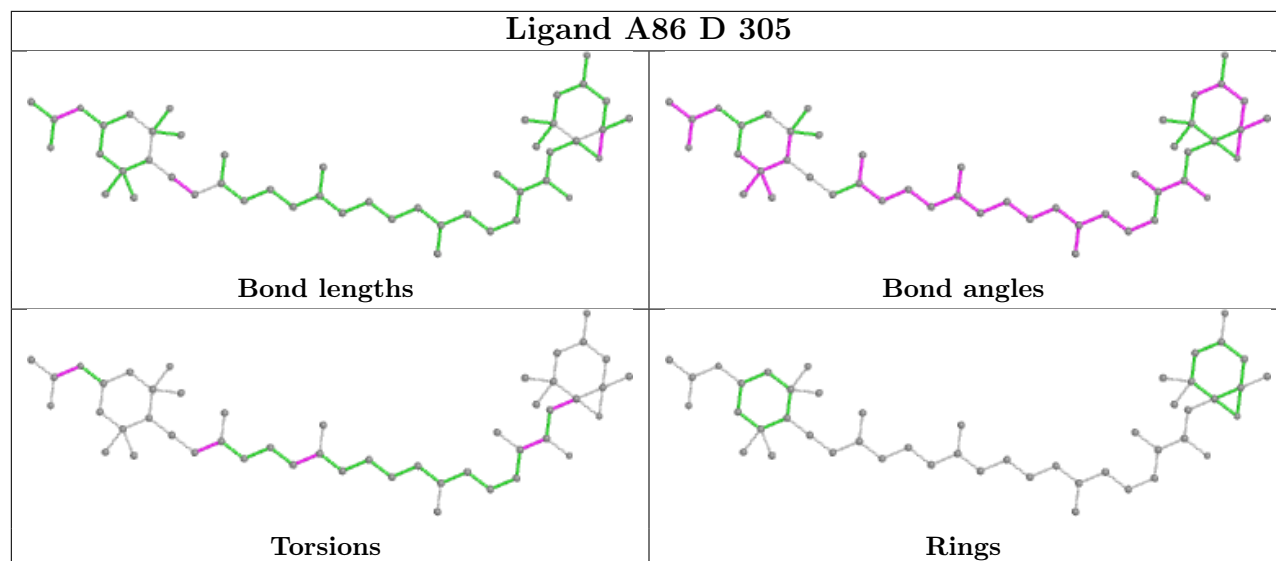
## Ligand CLA U 210



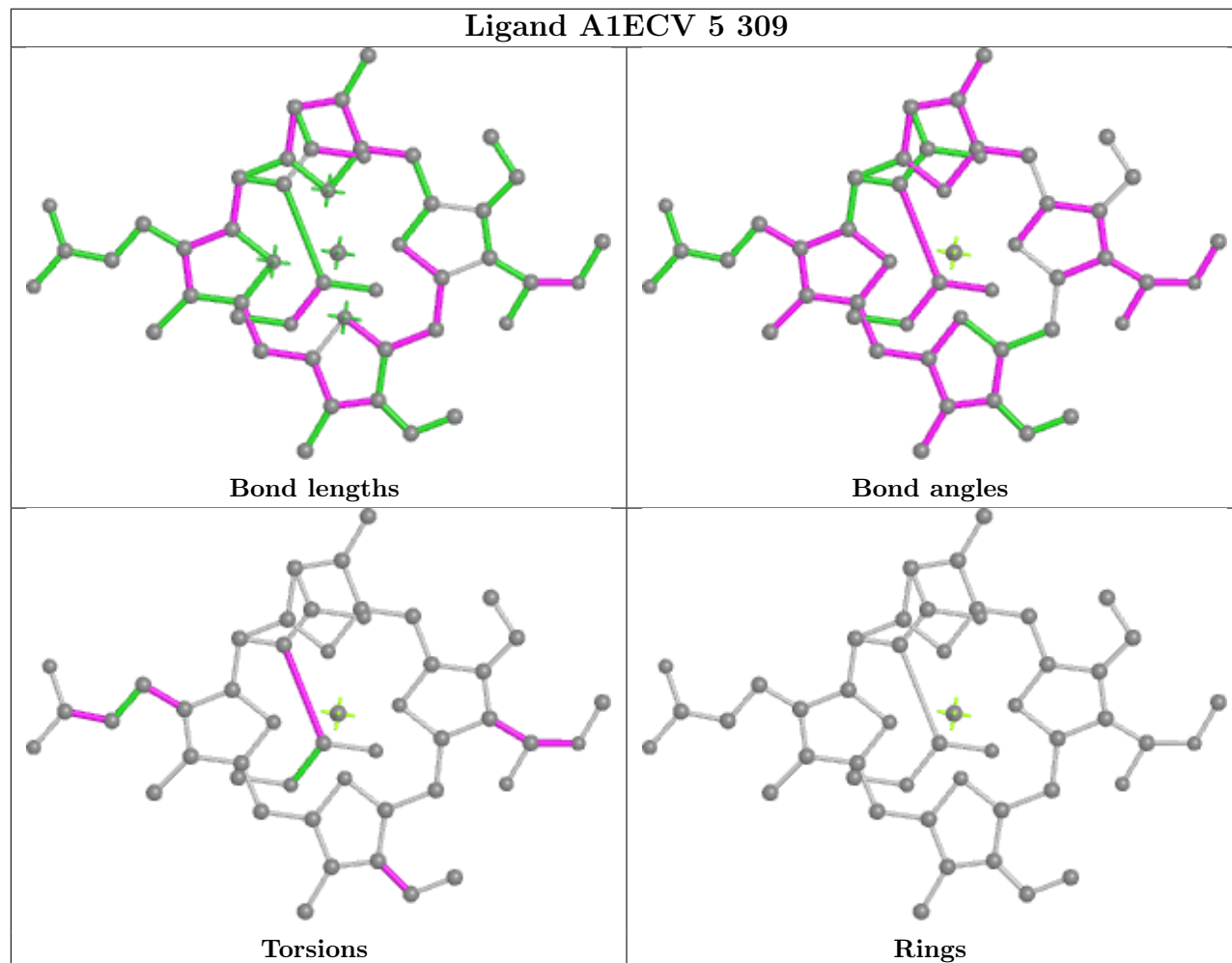




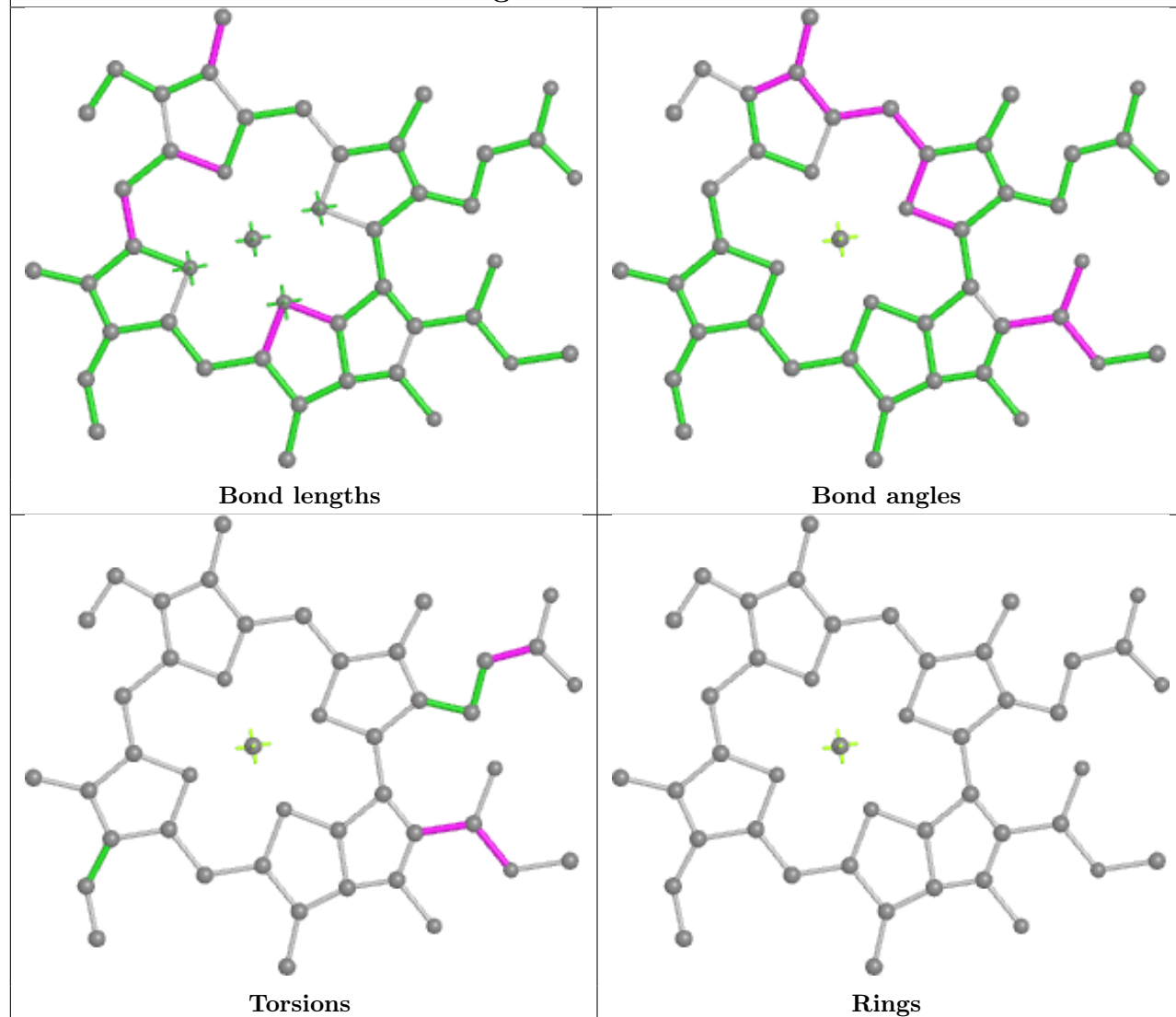
## Ligand A86 D 305



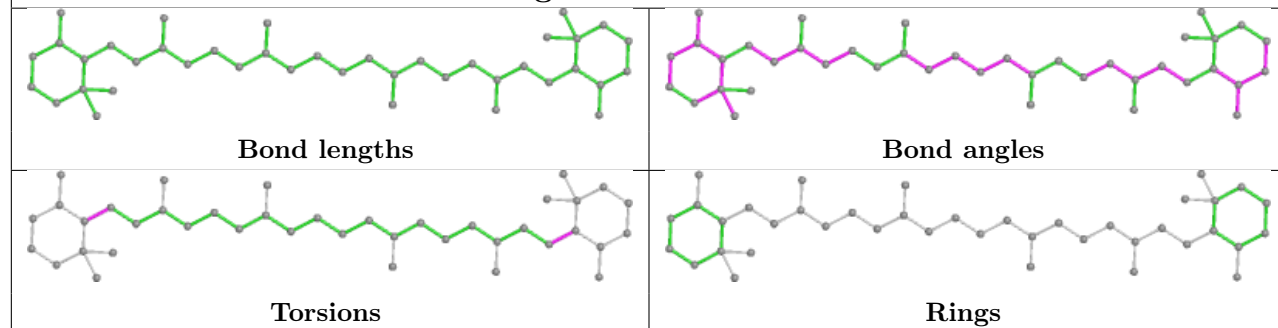
## Ligand A1ECV 5 309



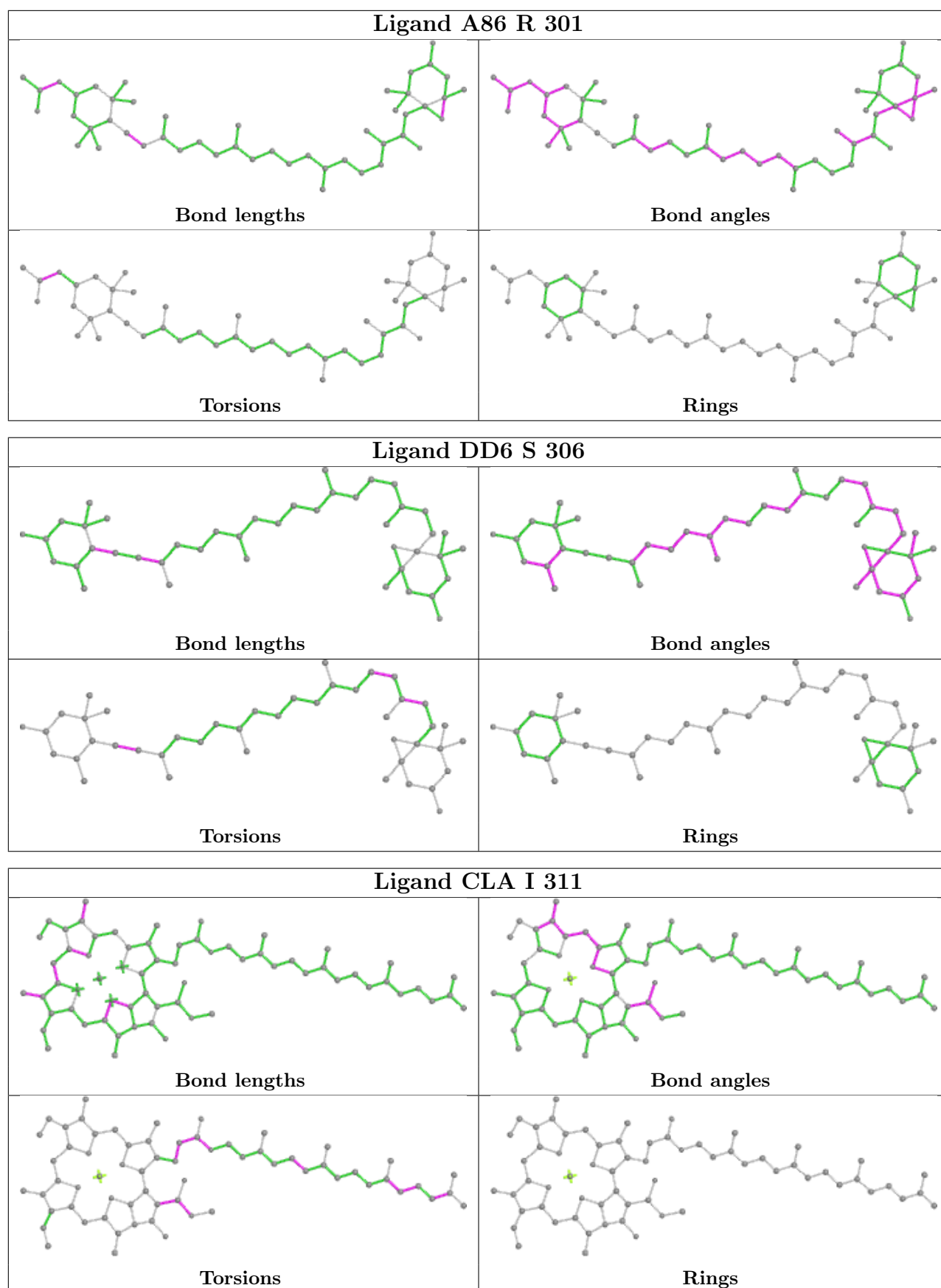
## Ligand CLA 0 320

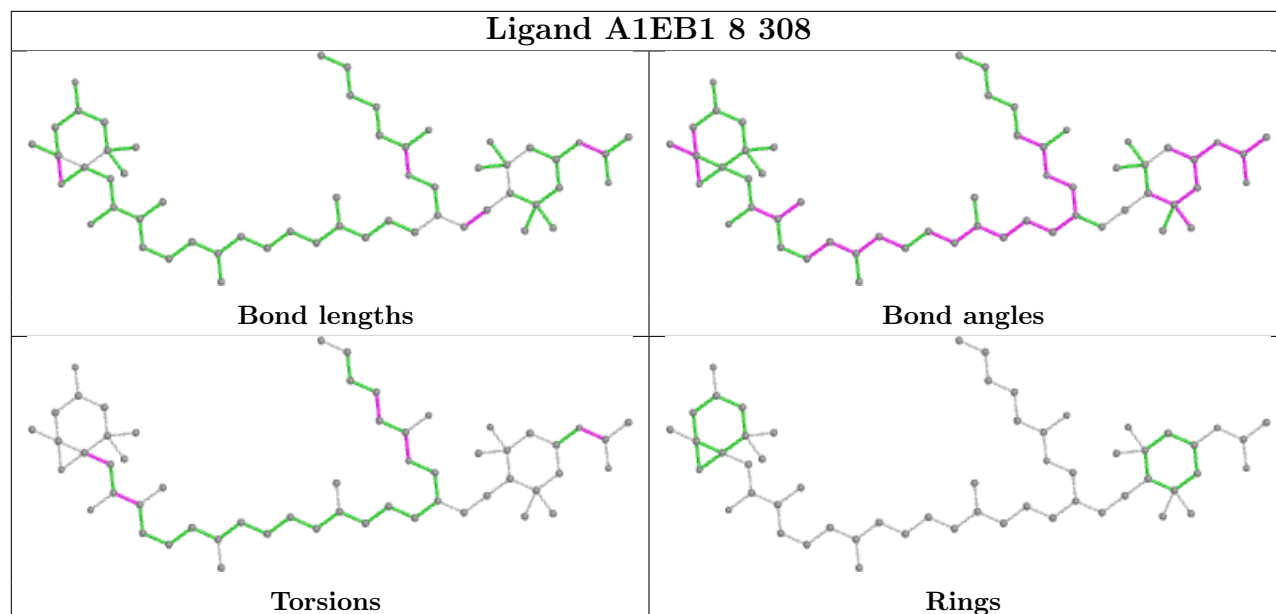
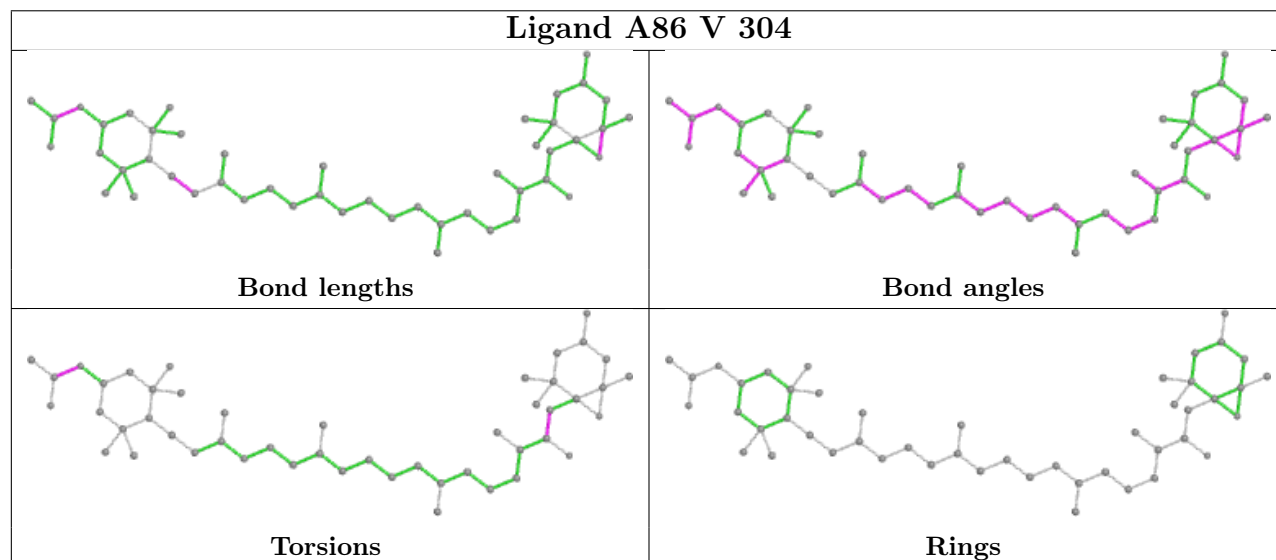


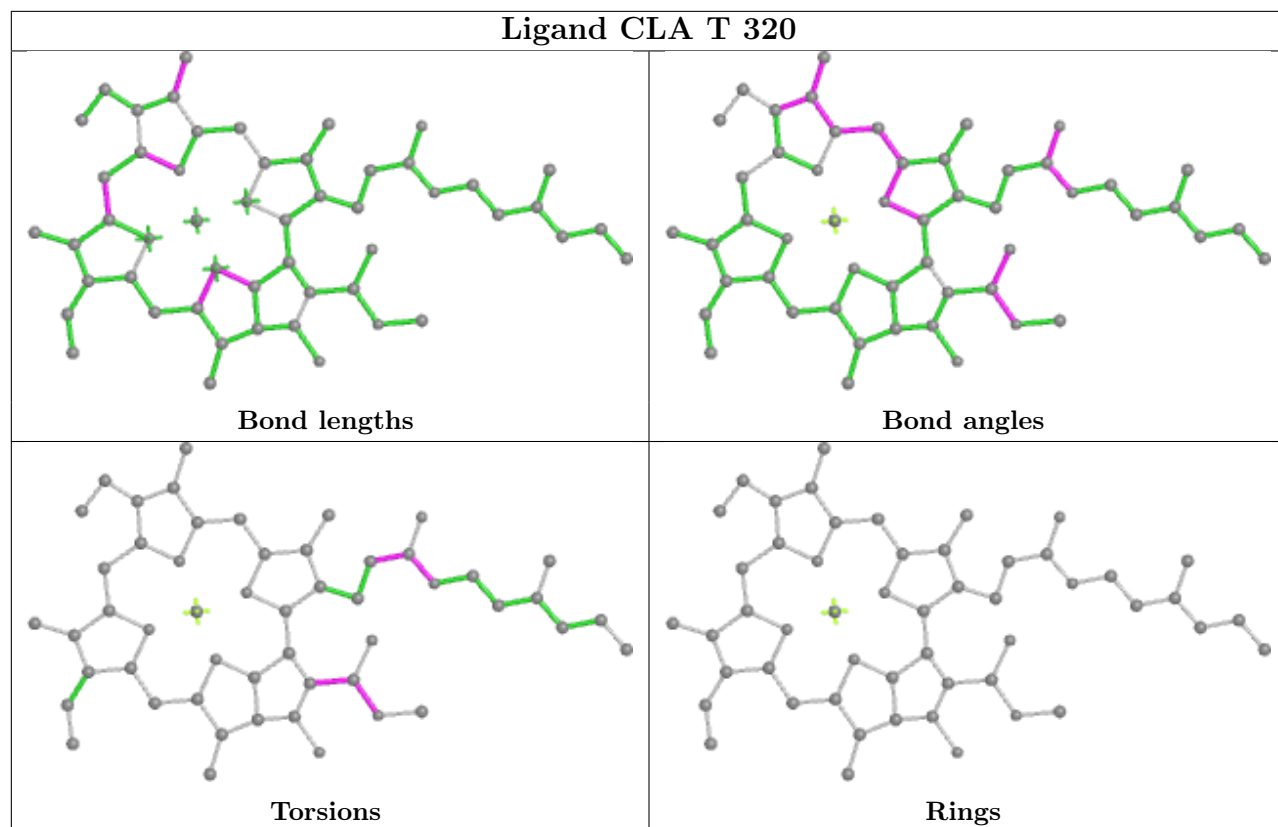
## Ligand BCR a 842



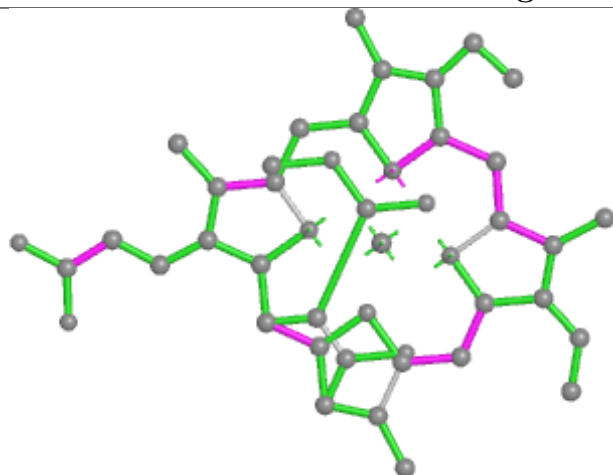




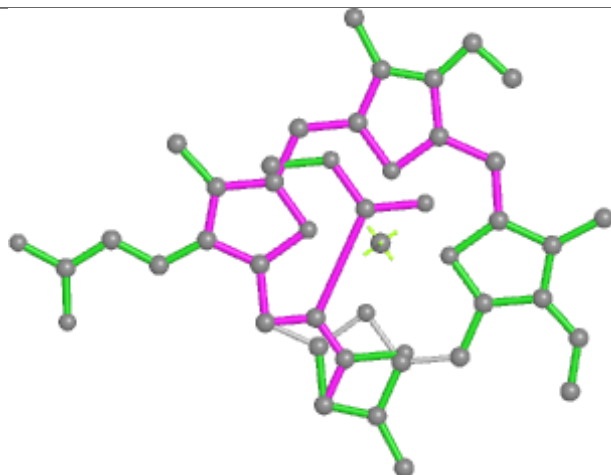
**Ligand A1EB1 8 308****Ligand A86 V 304**



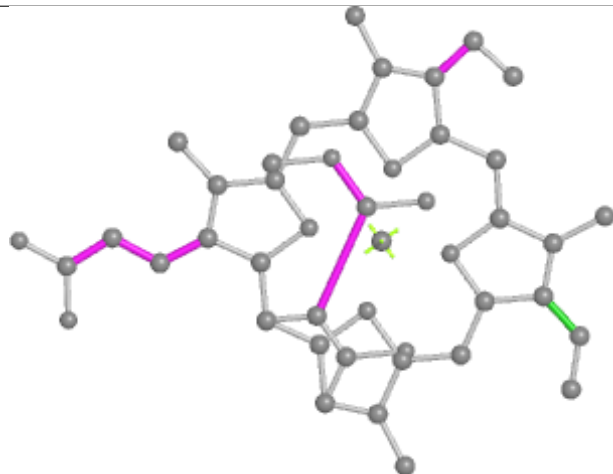
## Ligand KC2 T 312



Bond lengths



Bond angles

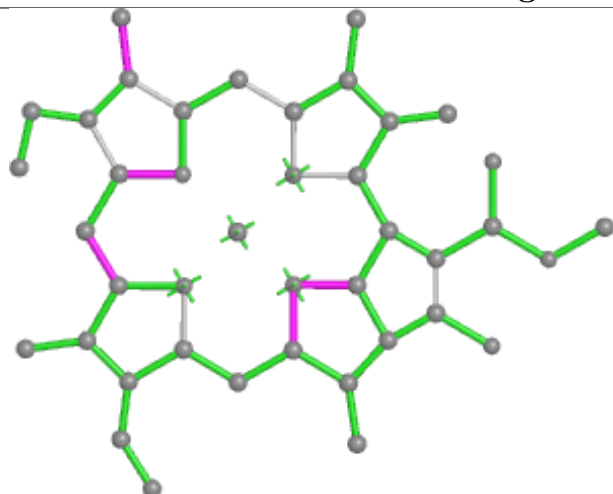


Torsions

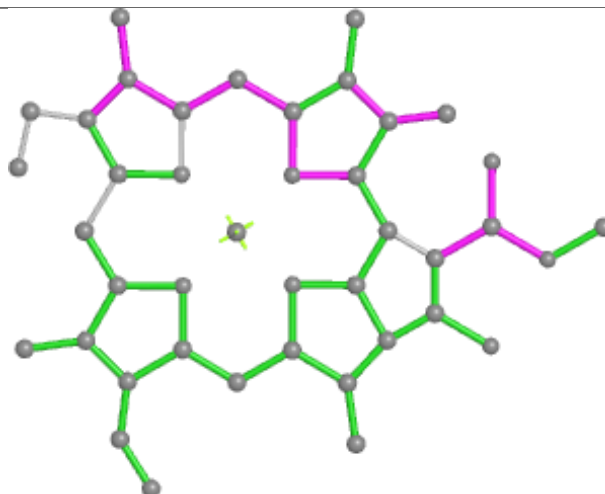


Rings

## Ligand CLA 3 319



Bond lengths



Bond angles

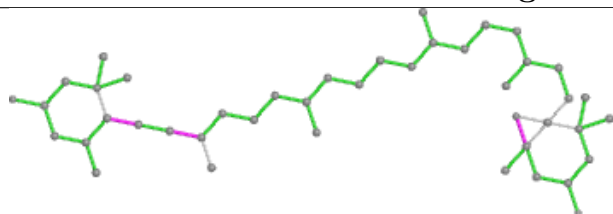


Torsions

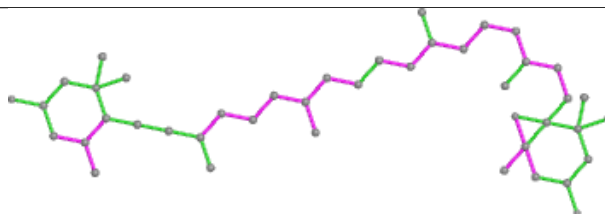


Rings

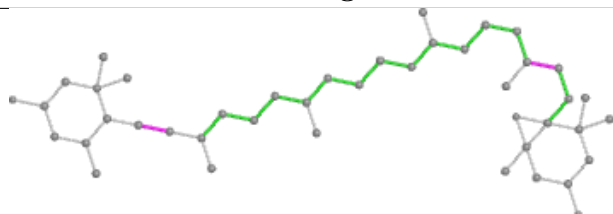
## Ligand DD6 J 306



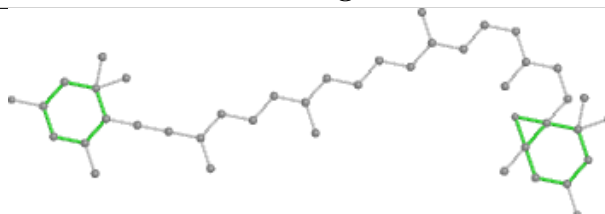
Bond lengths



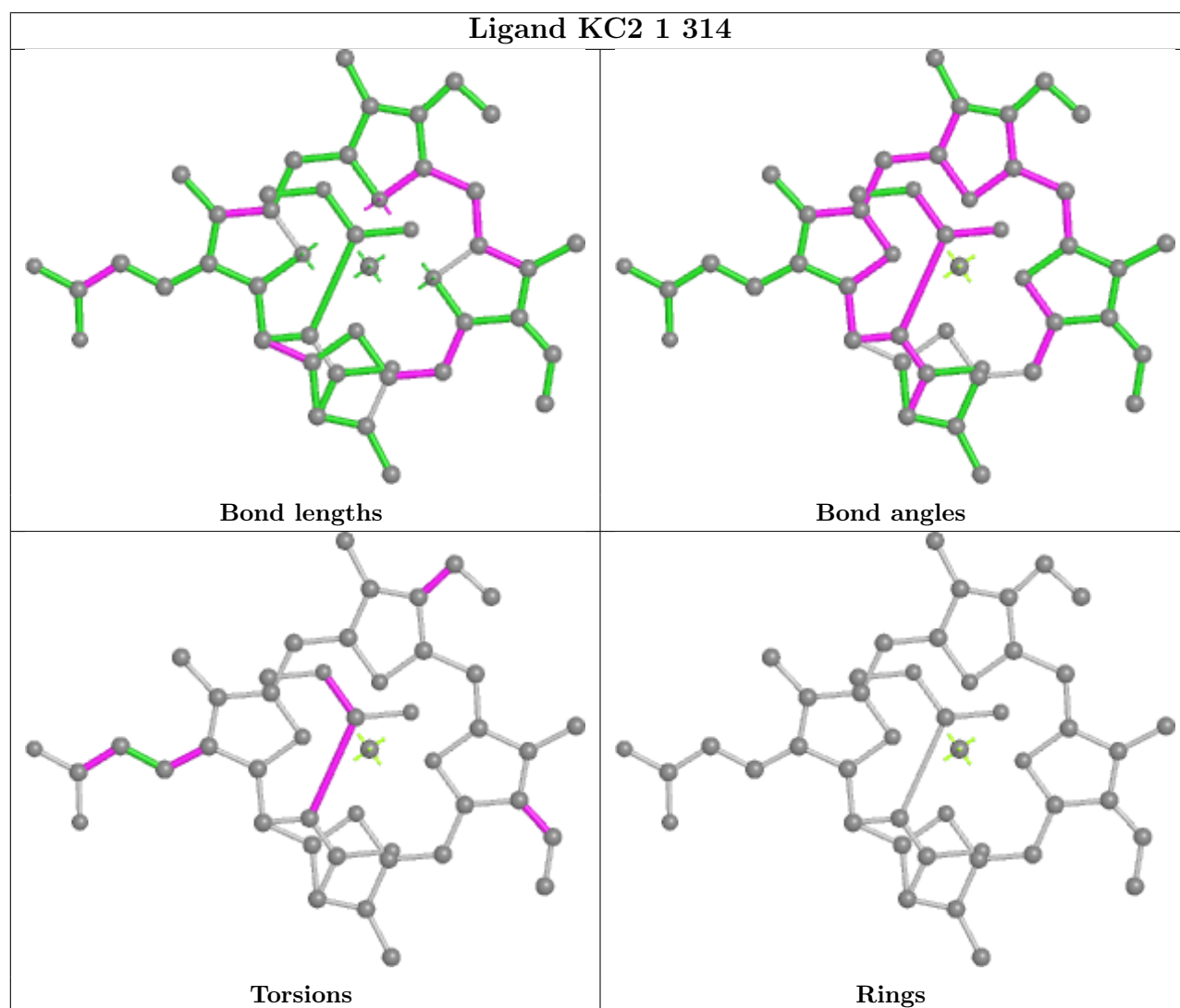
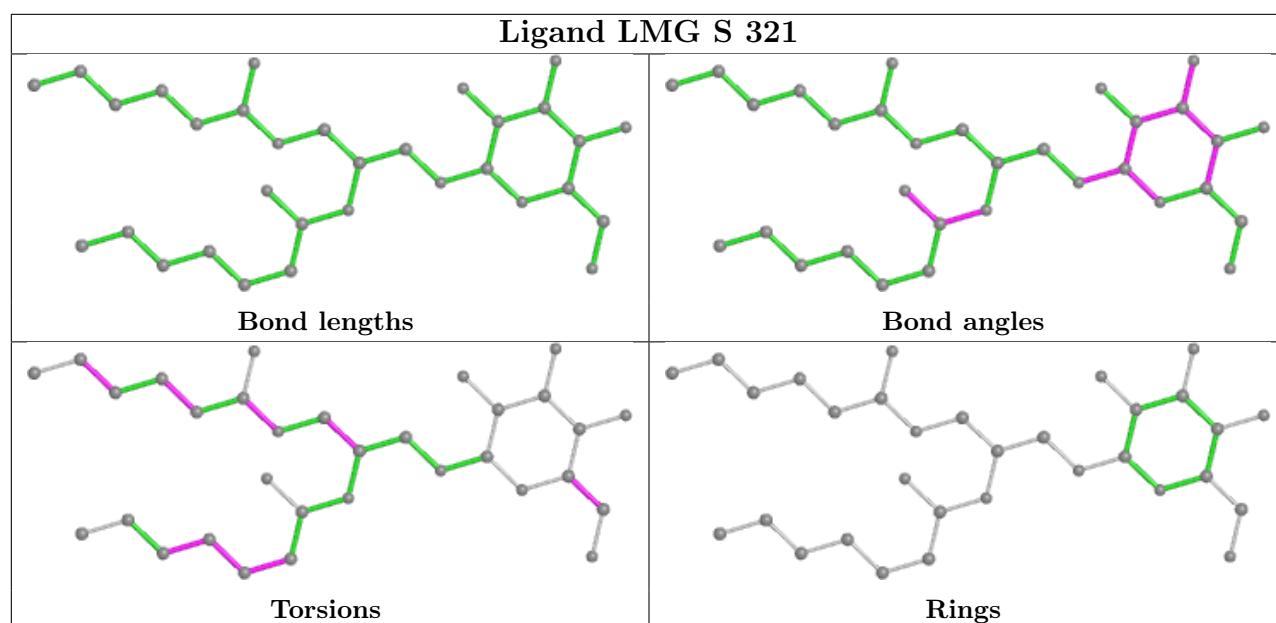
Bond angles

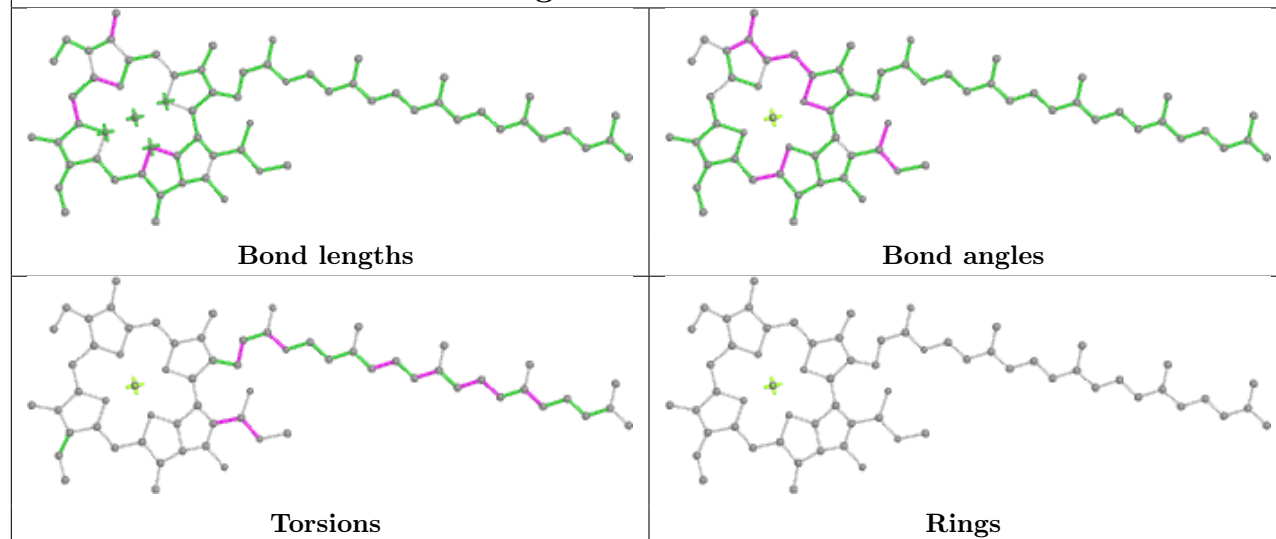
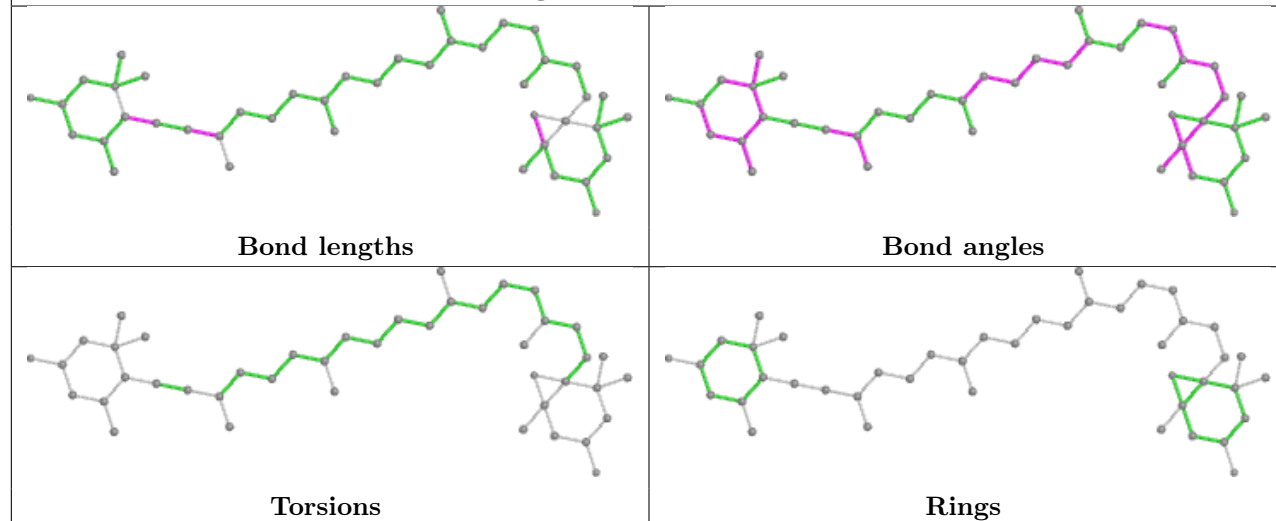
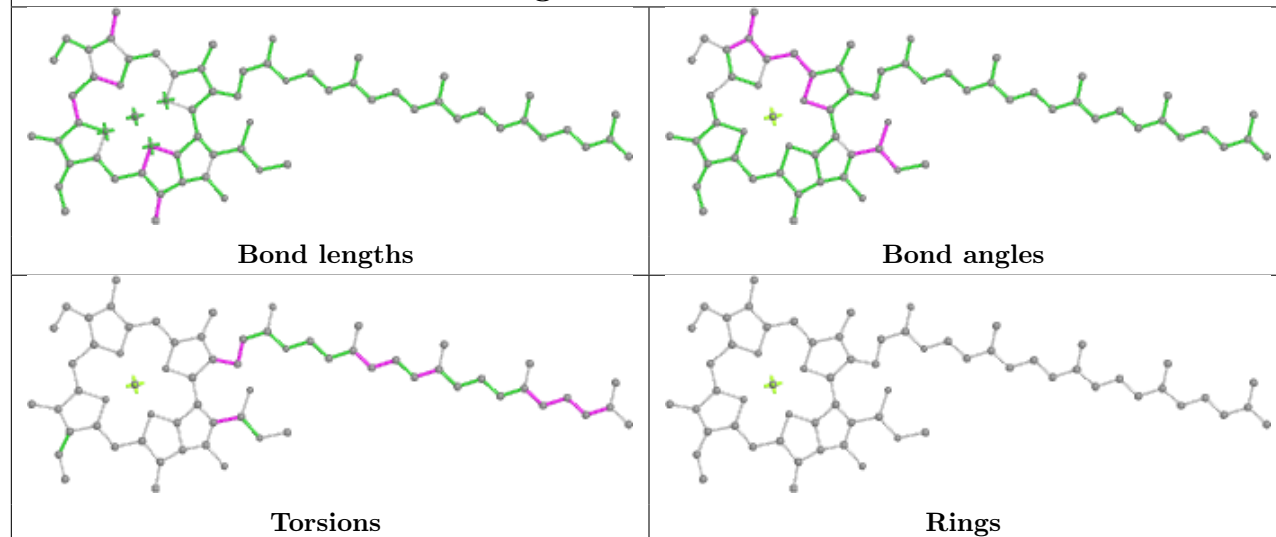


Torsions

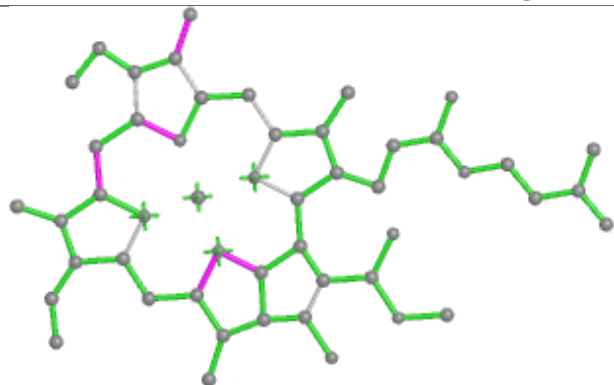


Rings

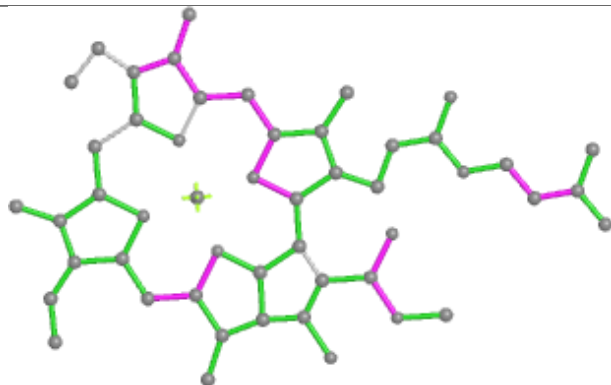


**Ligand CLA b 833****Ligand DD6 X 304****Ligand CLA F 308**

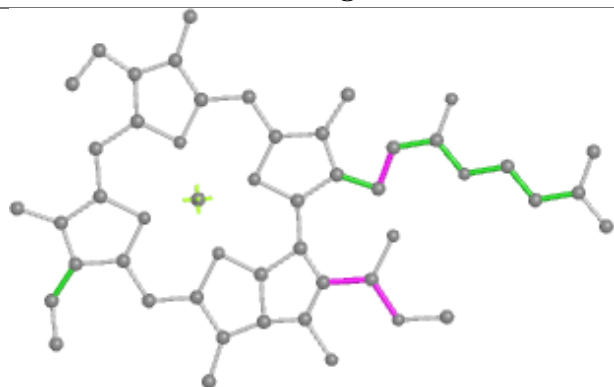
## Ligand CLA J 308



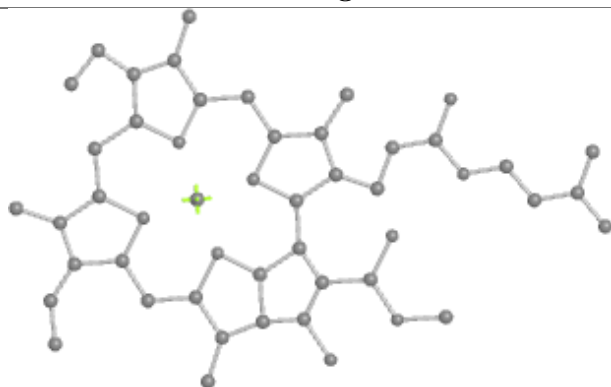
Bond lengths



Bond angles



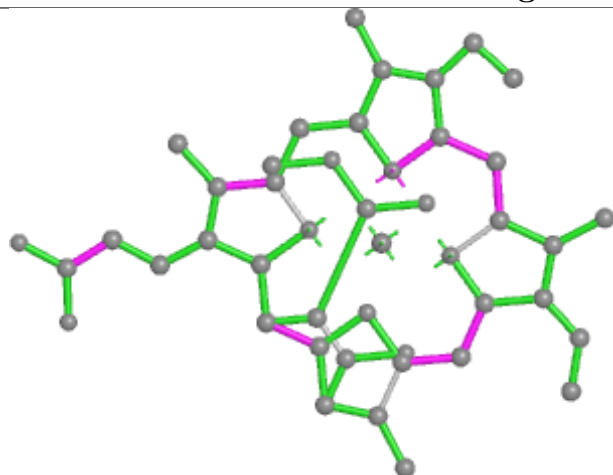
Torsions



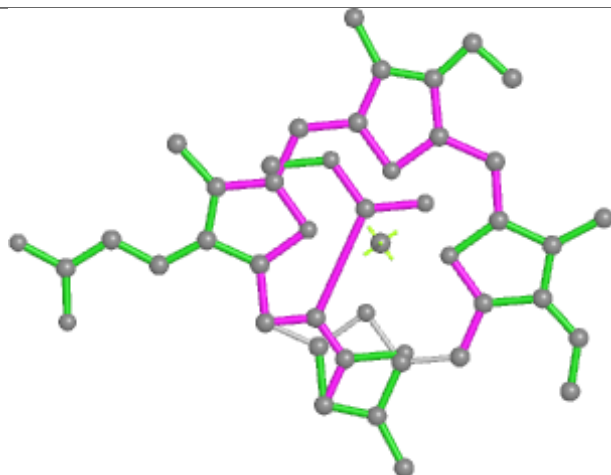
Rings



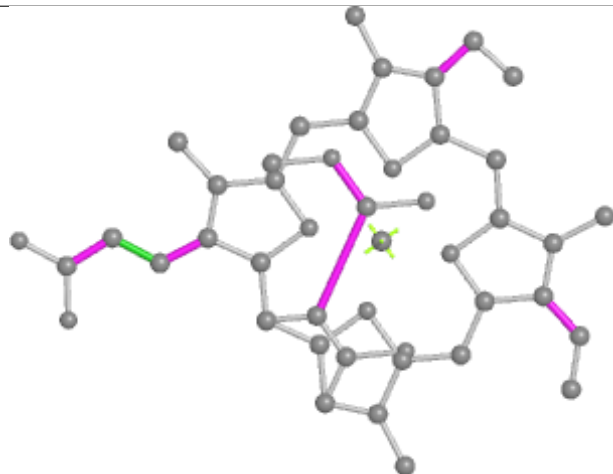
## Ligand KC2 Z 311



Bond lengths



Bond angles

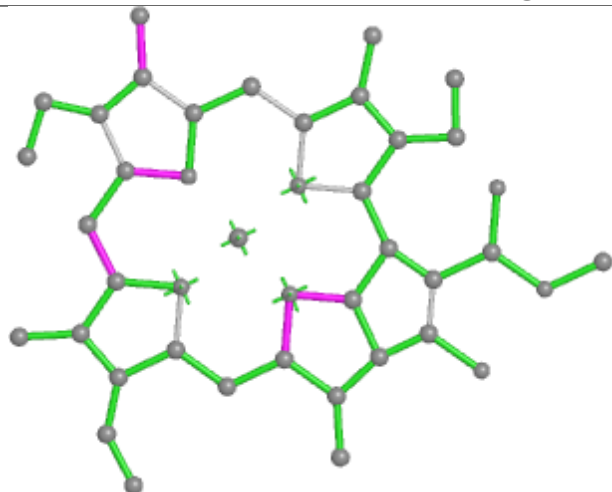


Torsions

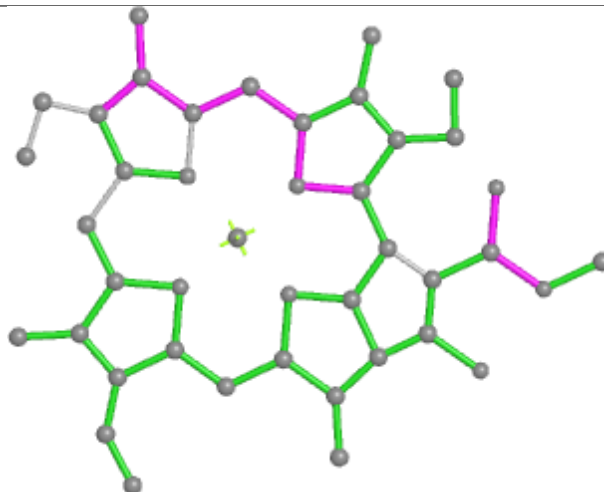


Rings

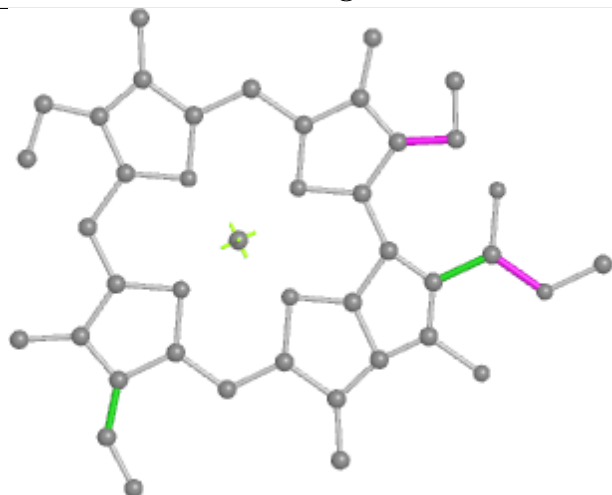
## Ligand CLA z 307



Bond lengths



Bond angles

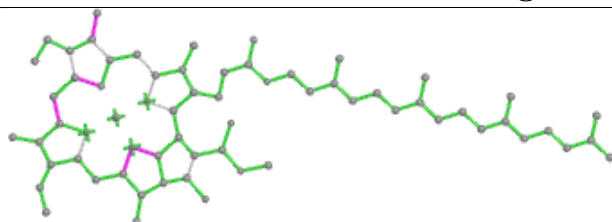


Torsions

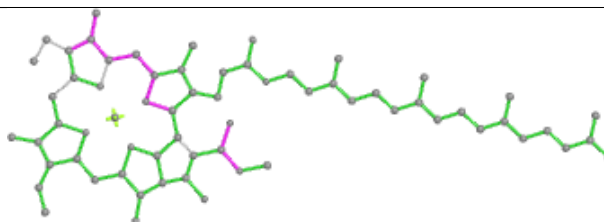


Rings

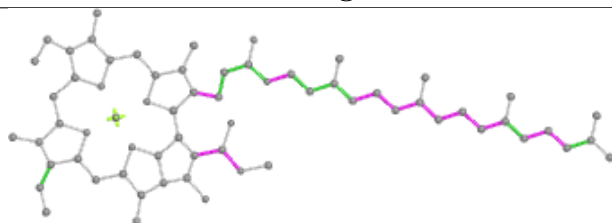
## Ligand CLA a 830



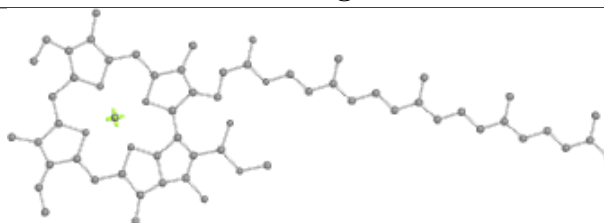
Bond lengths



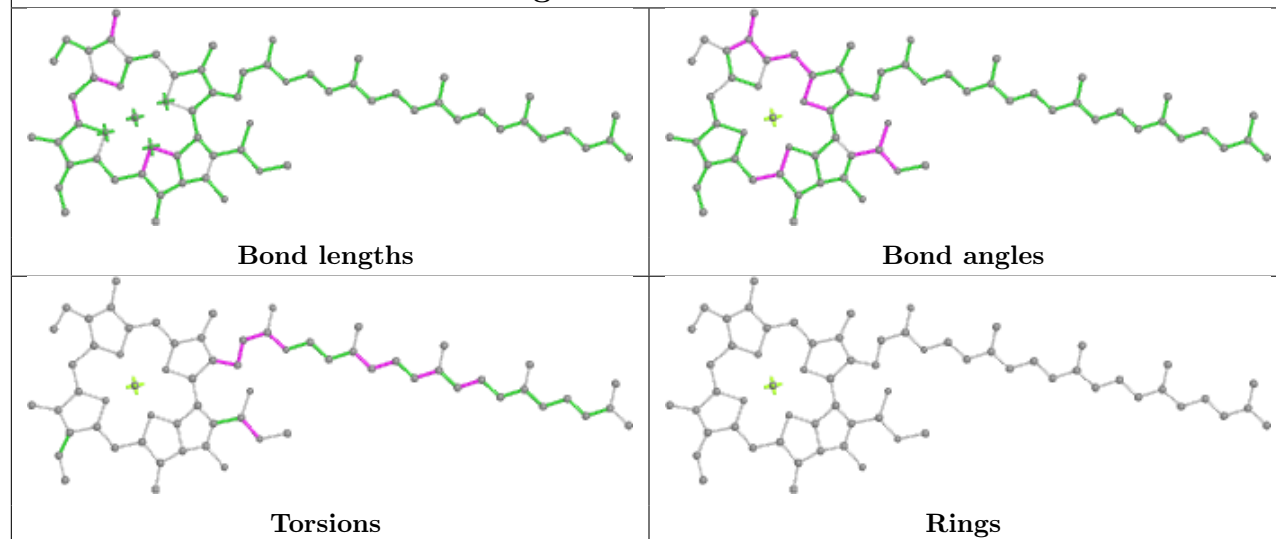
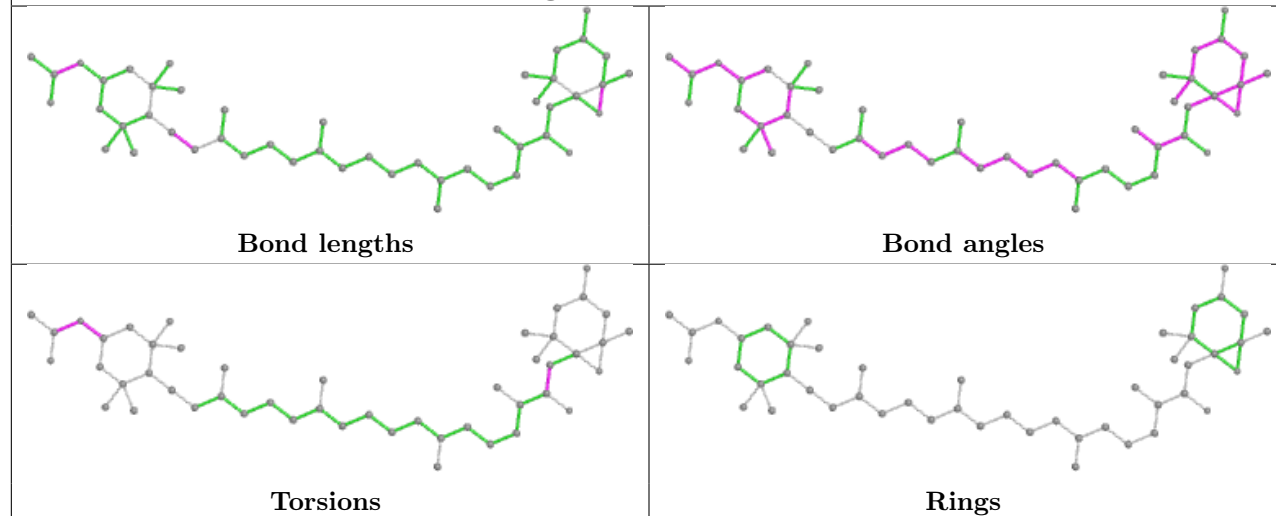
Bond angles



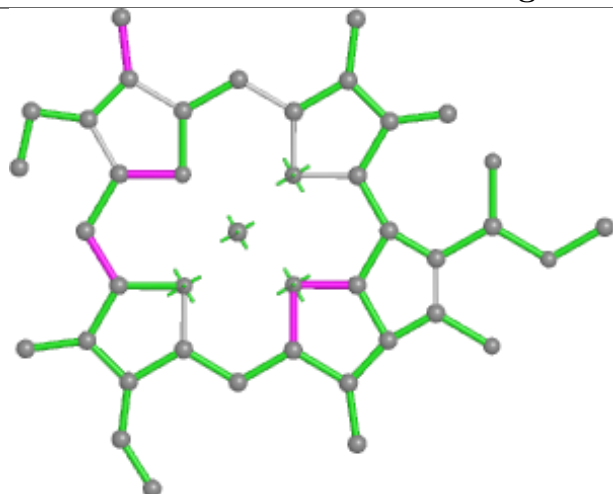
Torsions



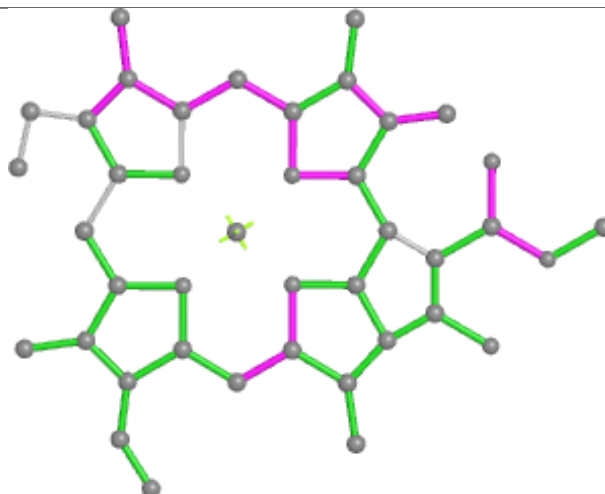
Rings

**Ligand CLA E 313****Ligand A86 0 301**

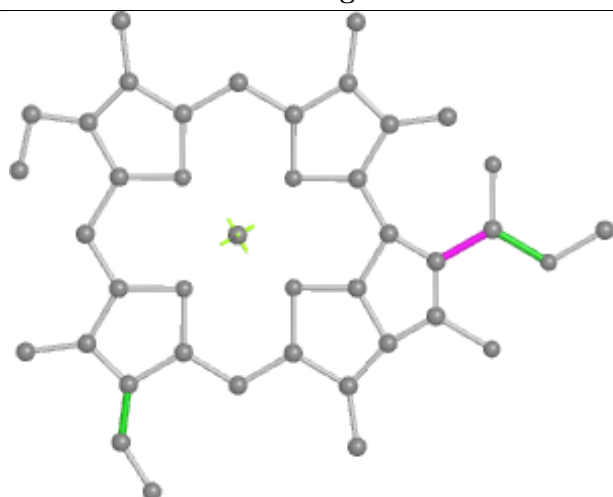
## Ligand CLA 7 321



Bond lengths



Bond angles

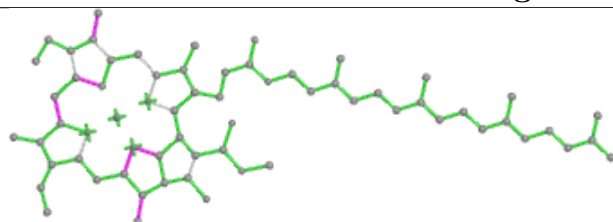


Torsions

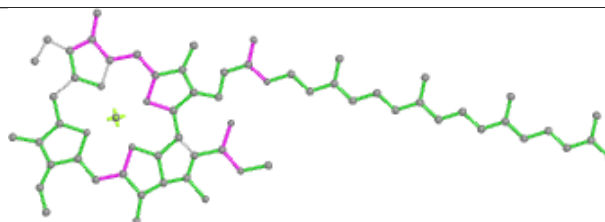


Rings

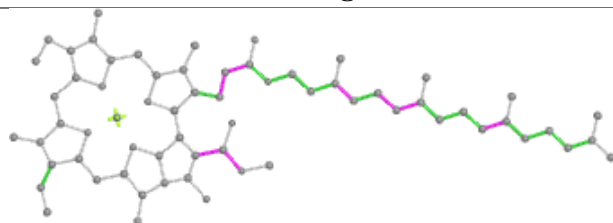
## Ligand CLA A 309



Bond lengths



Bond angles

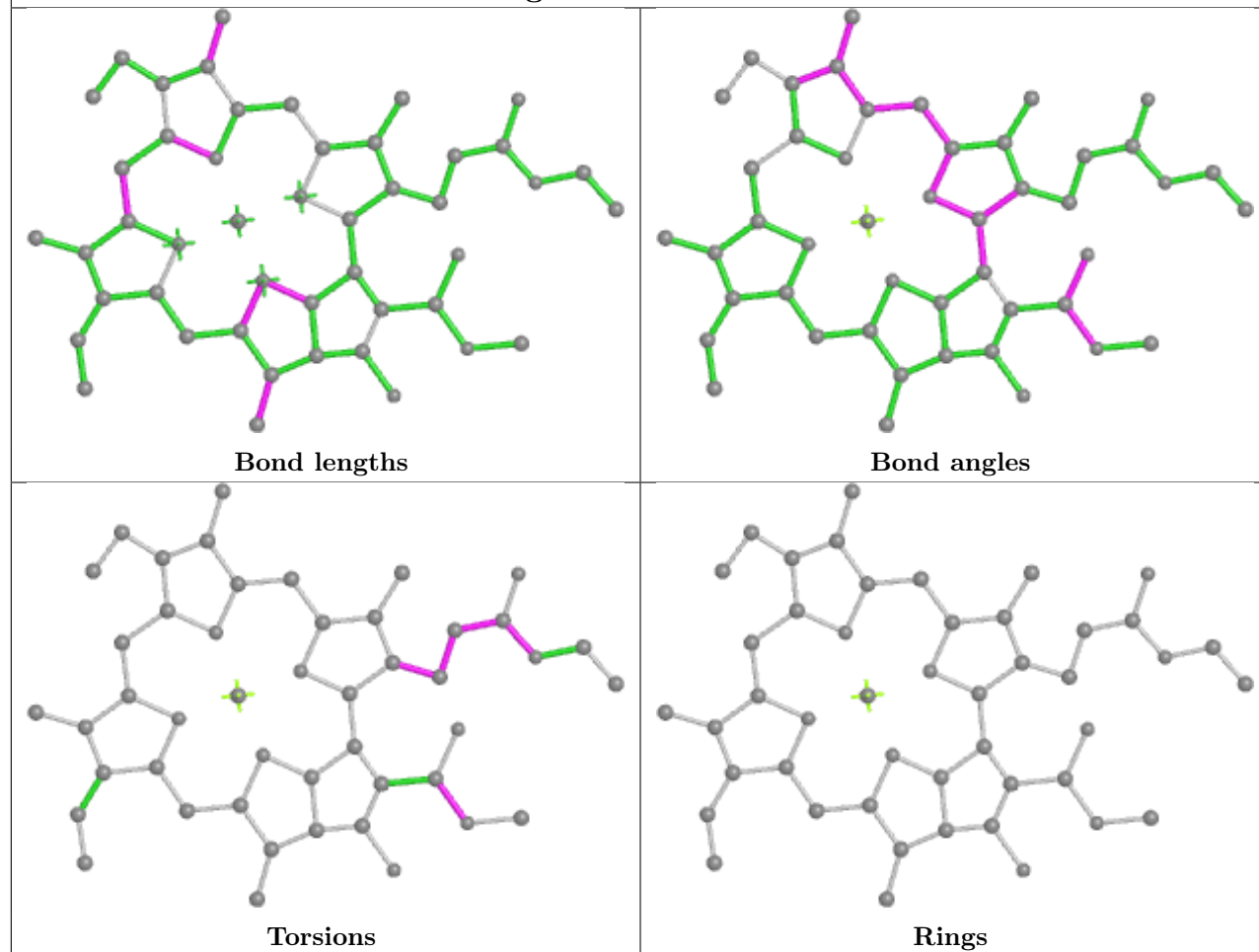


Torsions

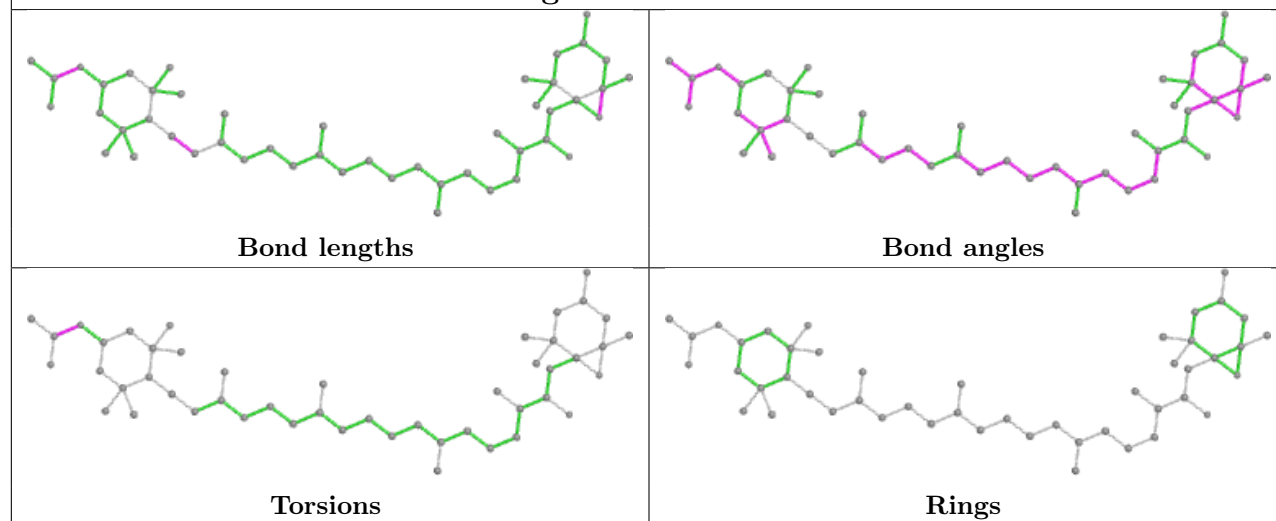


Rings

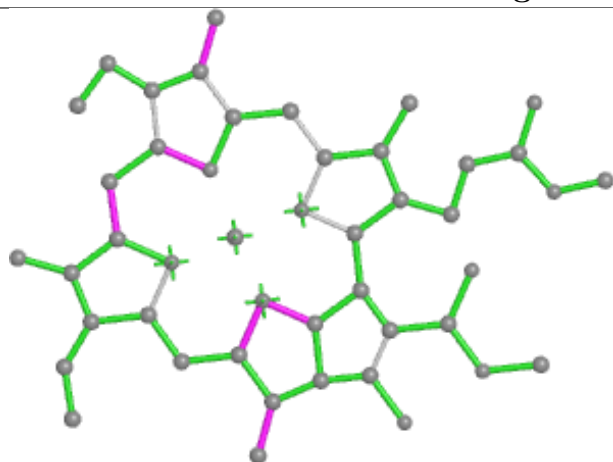
## Ligand CLA T 318



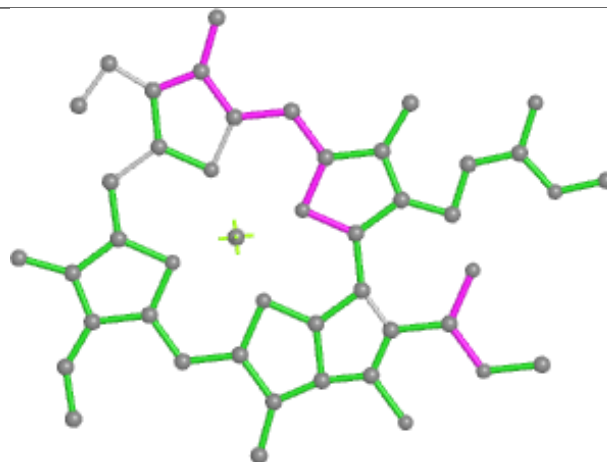
## Ligand A86 J 301



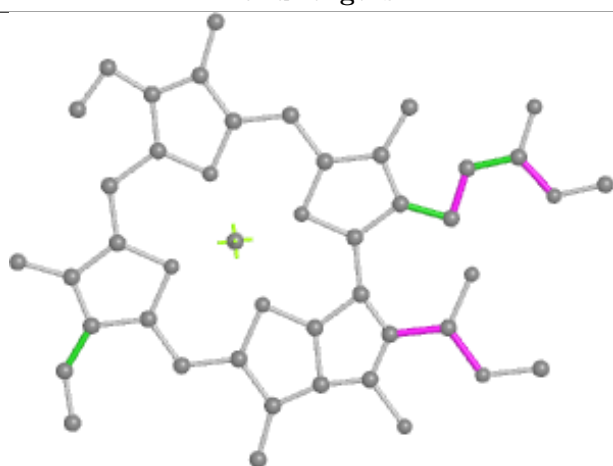
## Ligand CLA H 316



Bond lengths



Bond angles

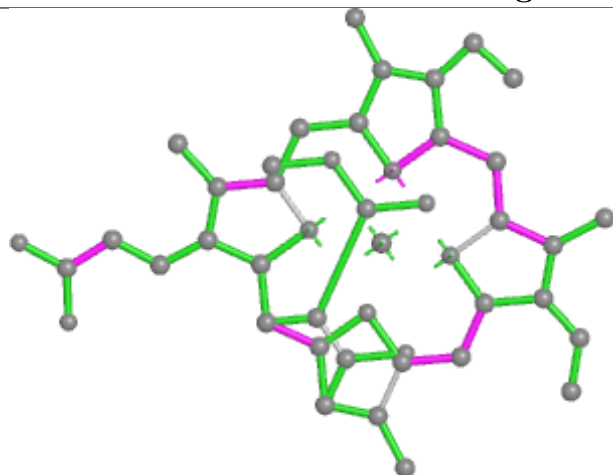


Torsions

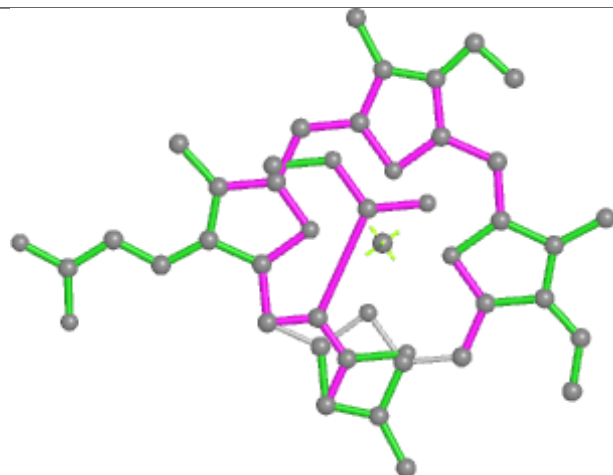


Rings

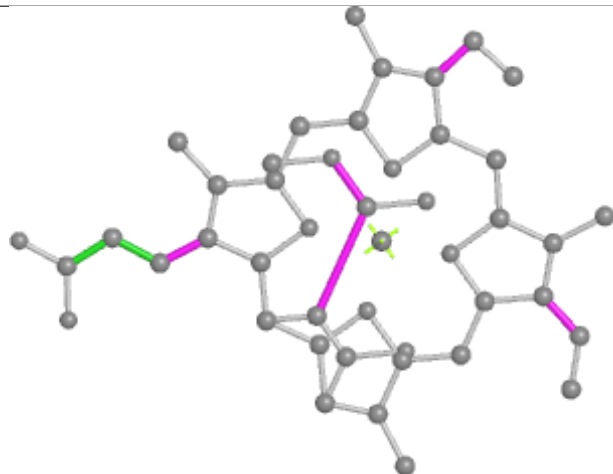
## Ligand KC2 V 308



Bond lengths



Bond angles

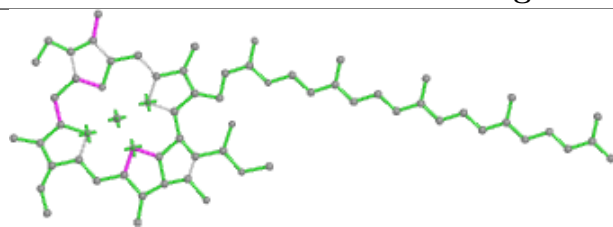


Torsions

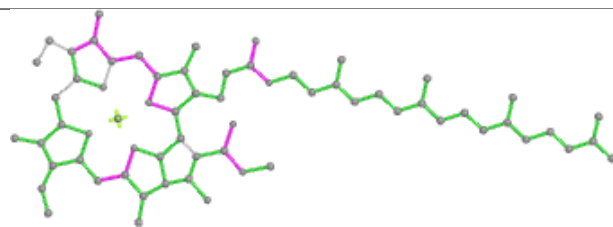


Rings

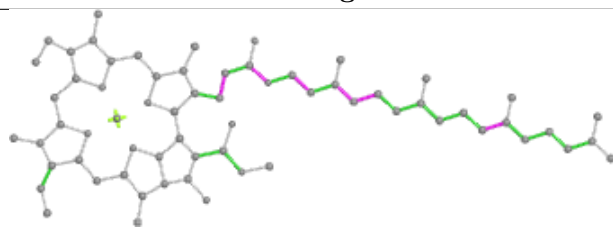
## Ligand CLA X 307



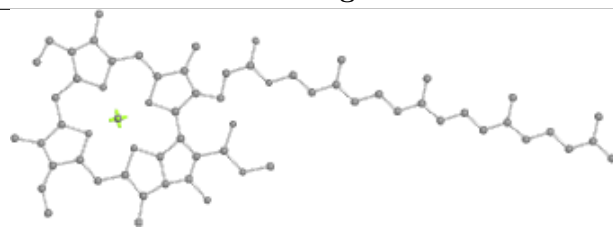
Bond lengths



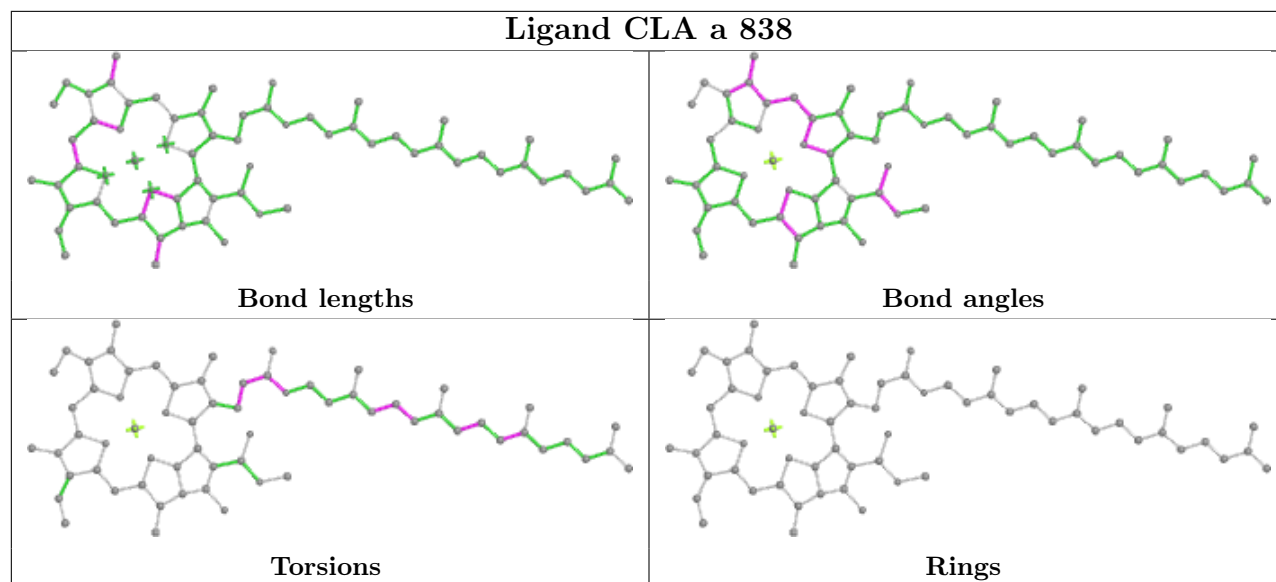
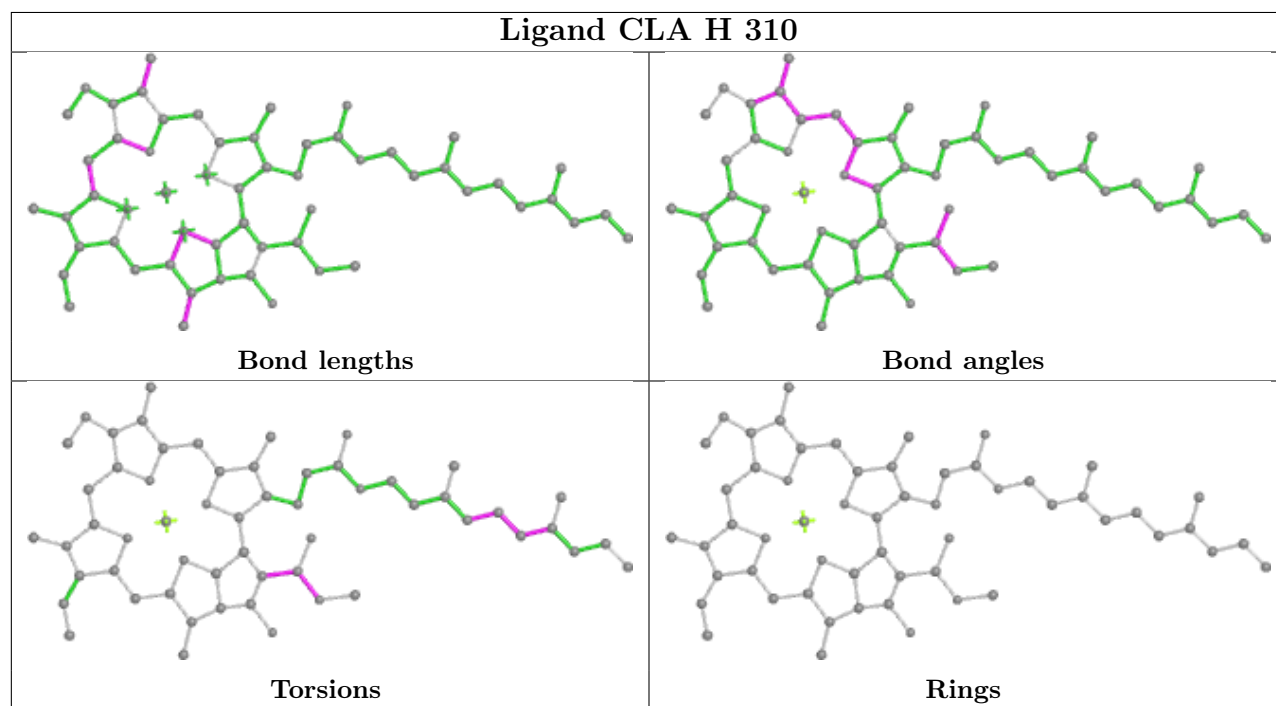
Bond angles



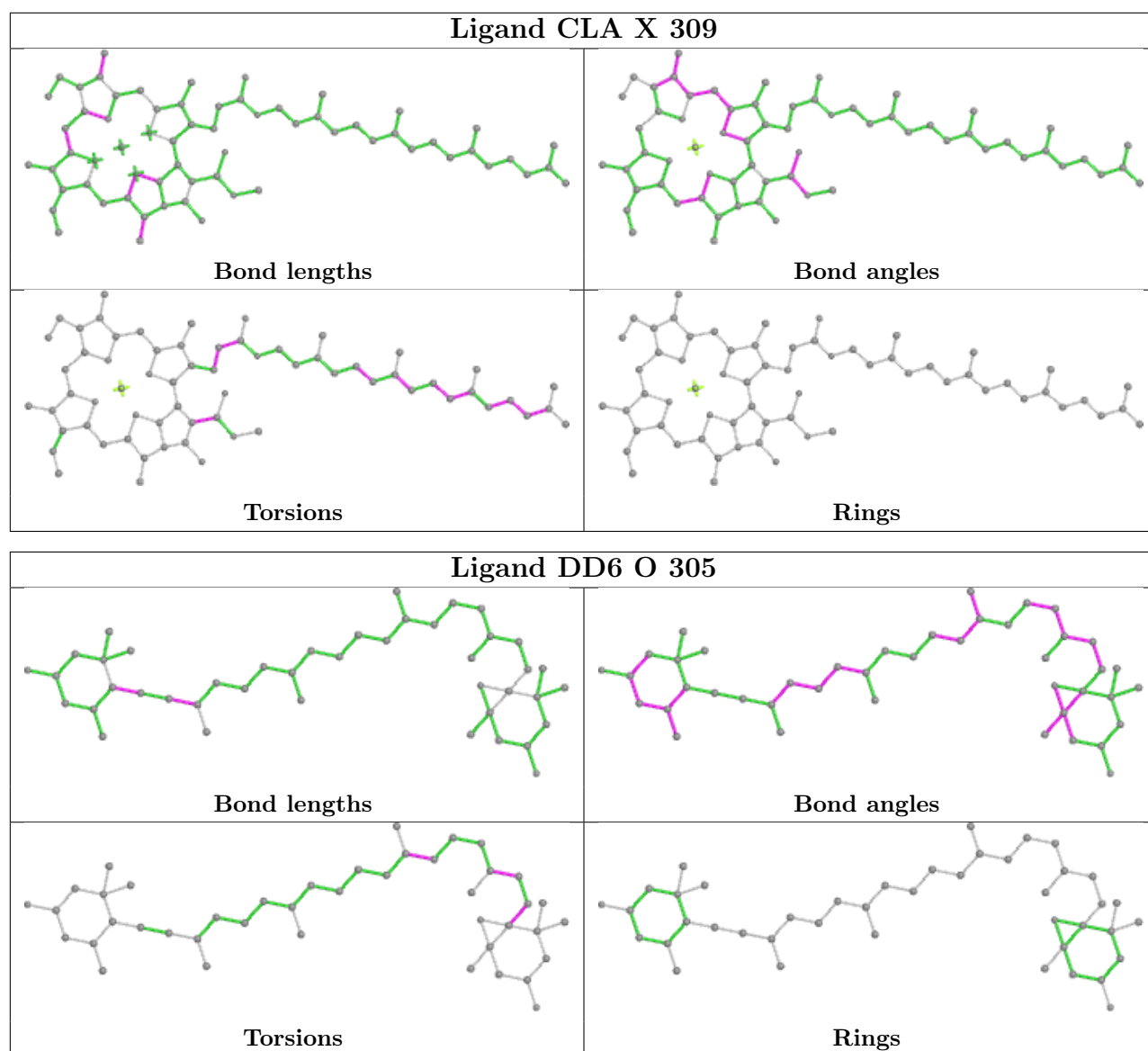
Torsions

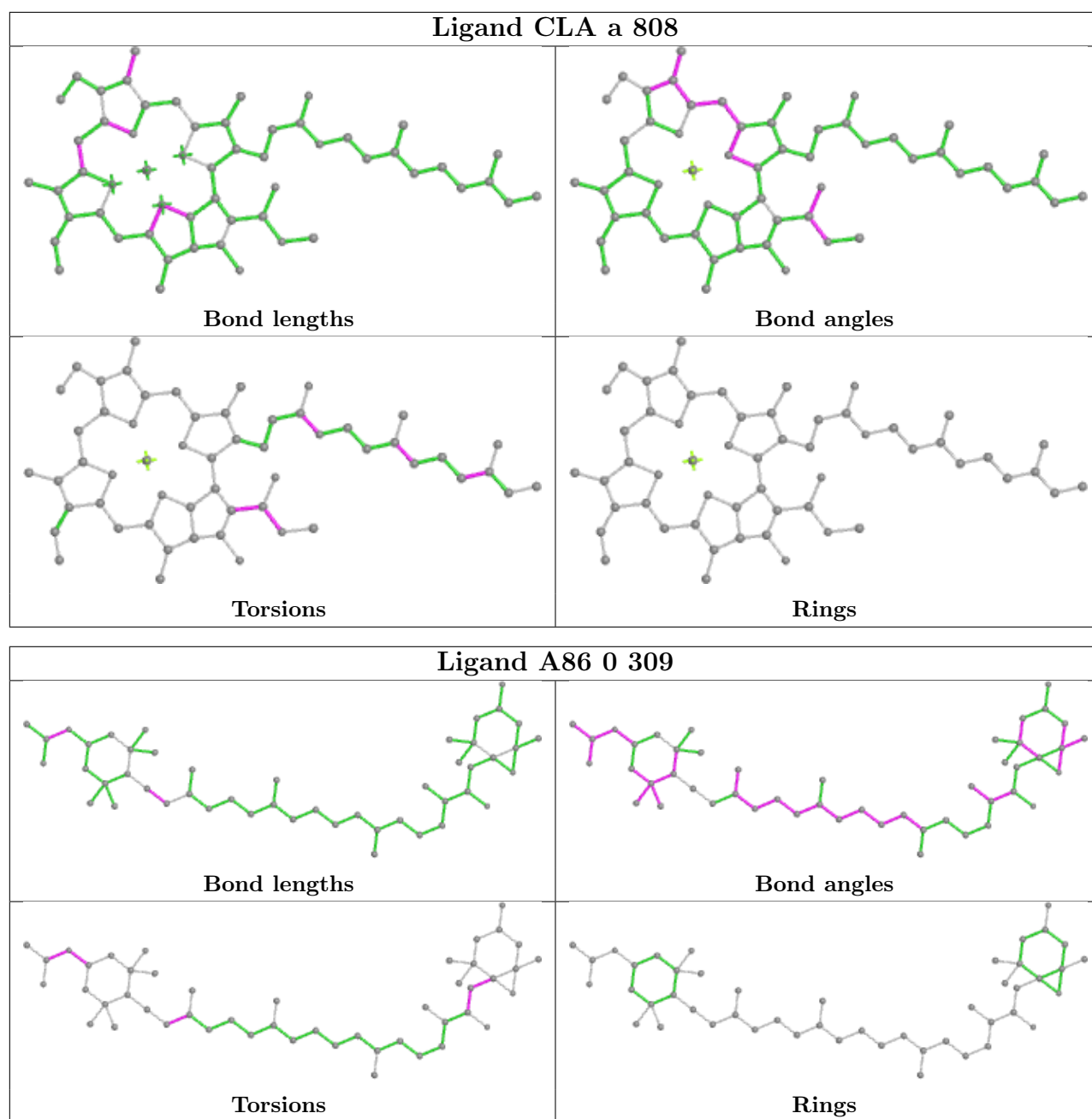


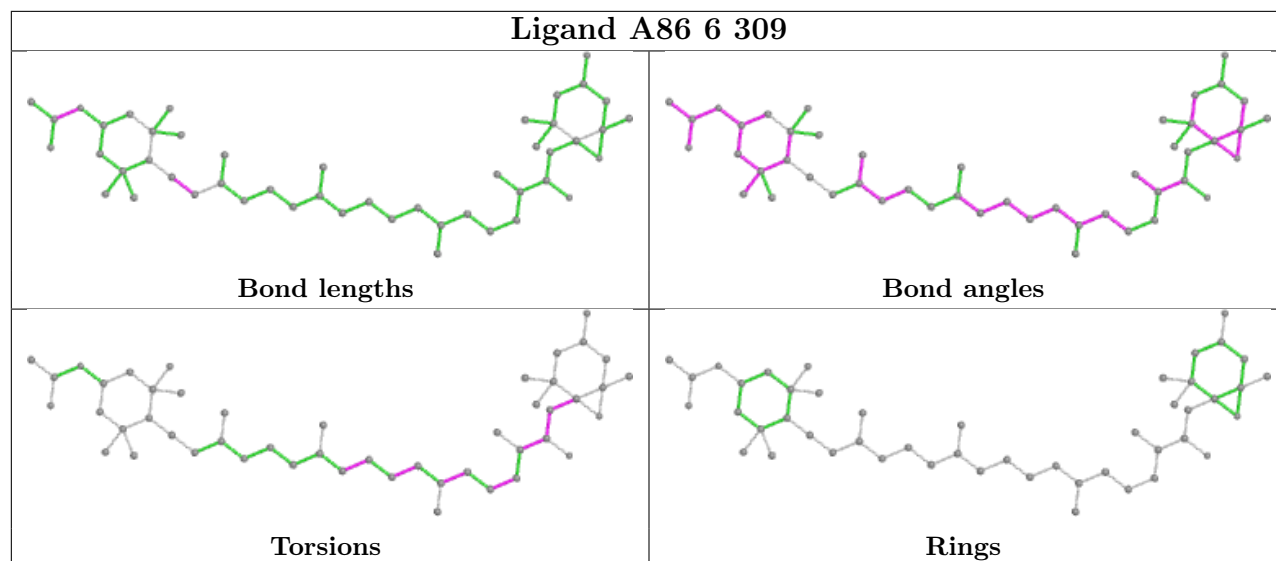
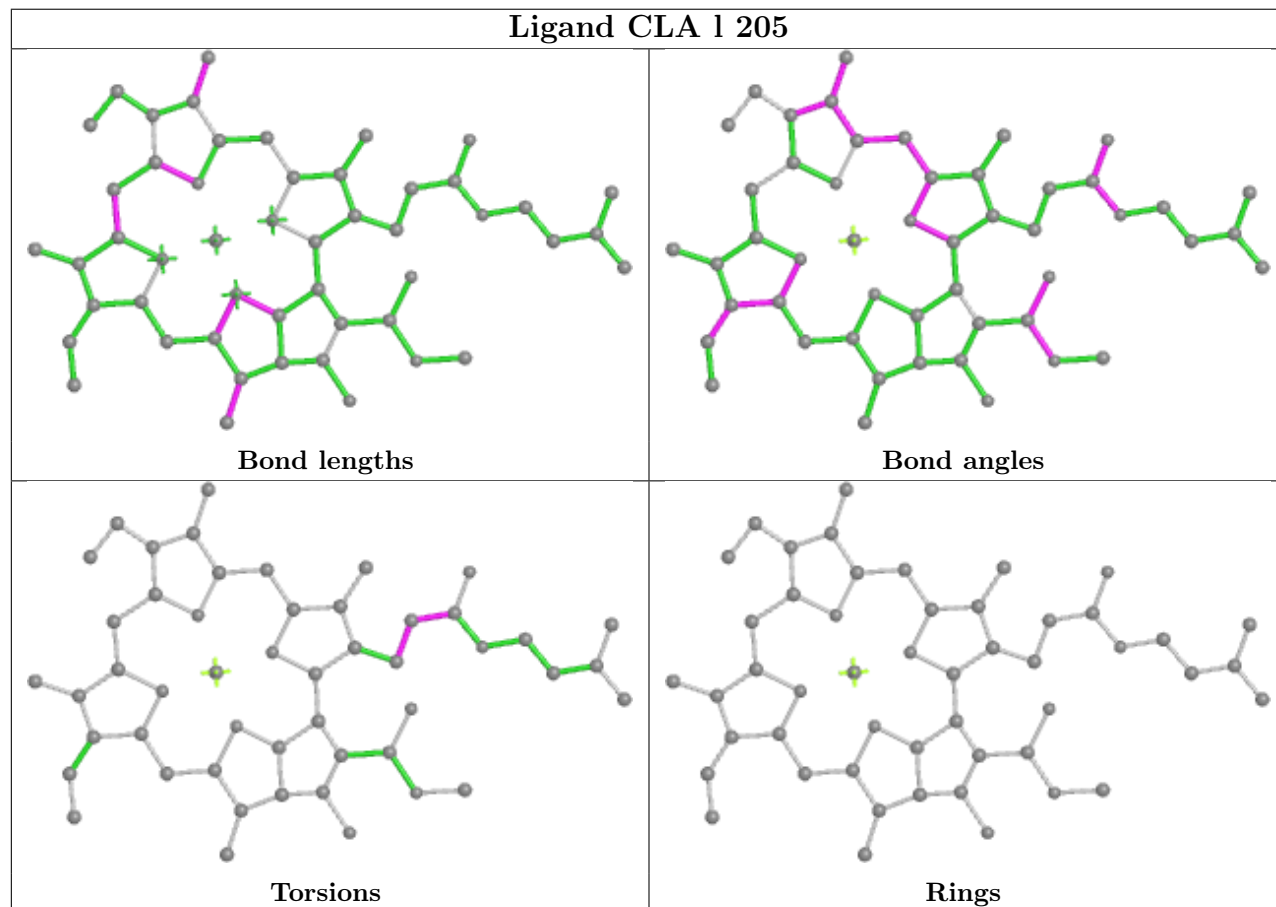
Rings

**Ligand CLA a 838****Ligand CLA H 310**

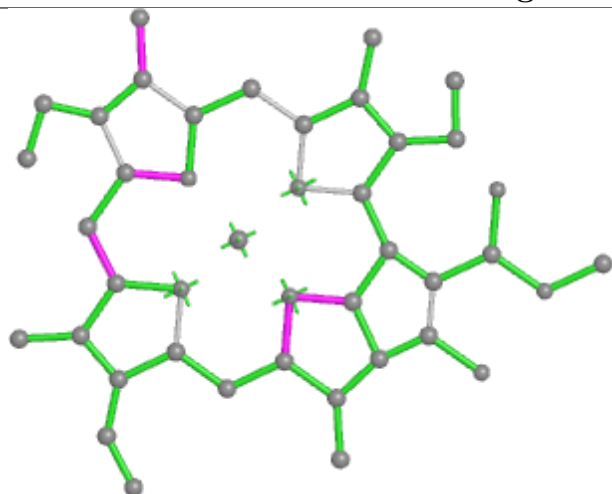




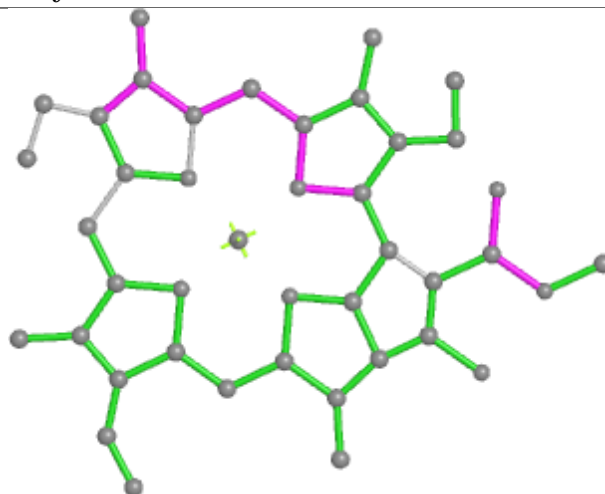


**Ligand A86 6 309****Ligand CLA 1 205**

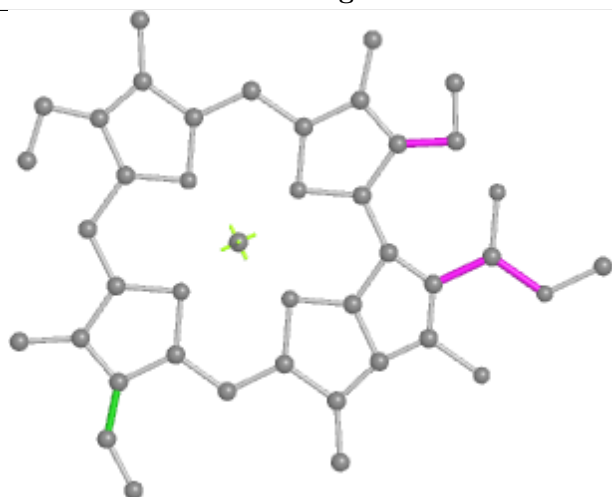
## Ligand CLA y 318



Bond lengths



Bond angles

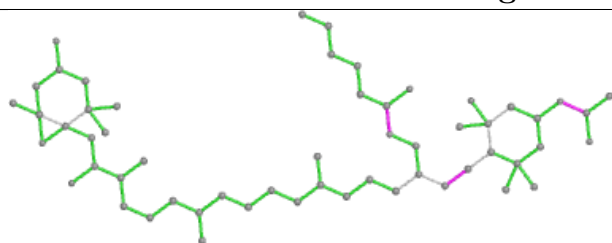


Torsions

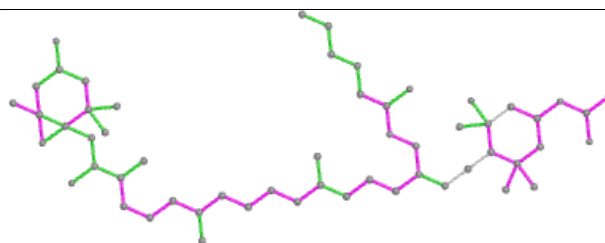


Rings

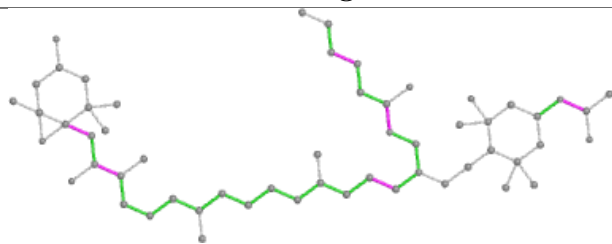
## Ligand A1EB1 7 306



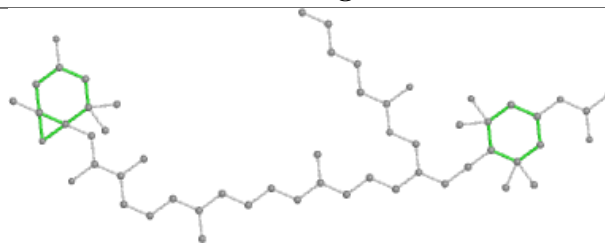
Bond lengths



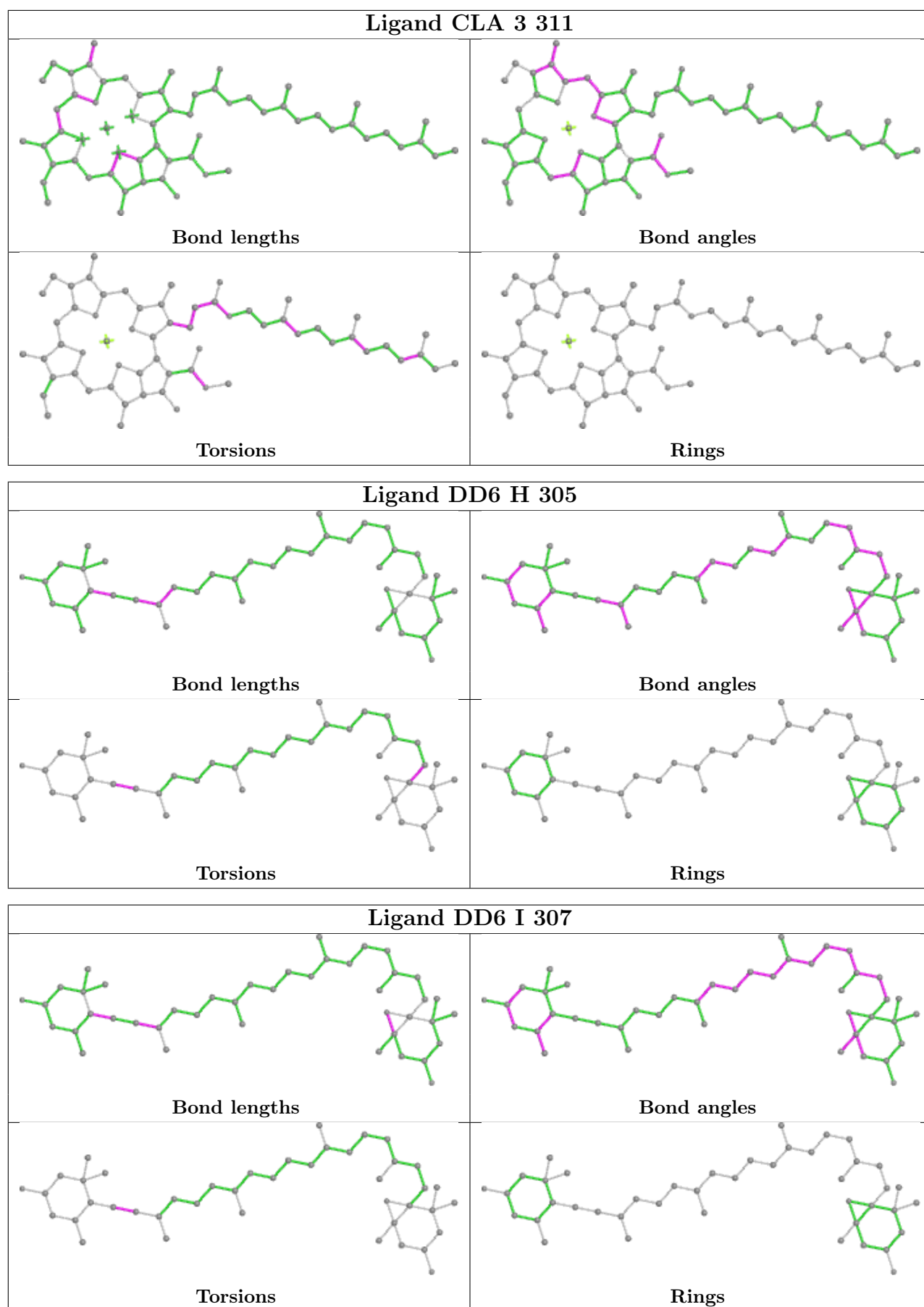
Bond angles



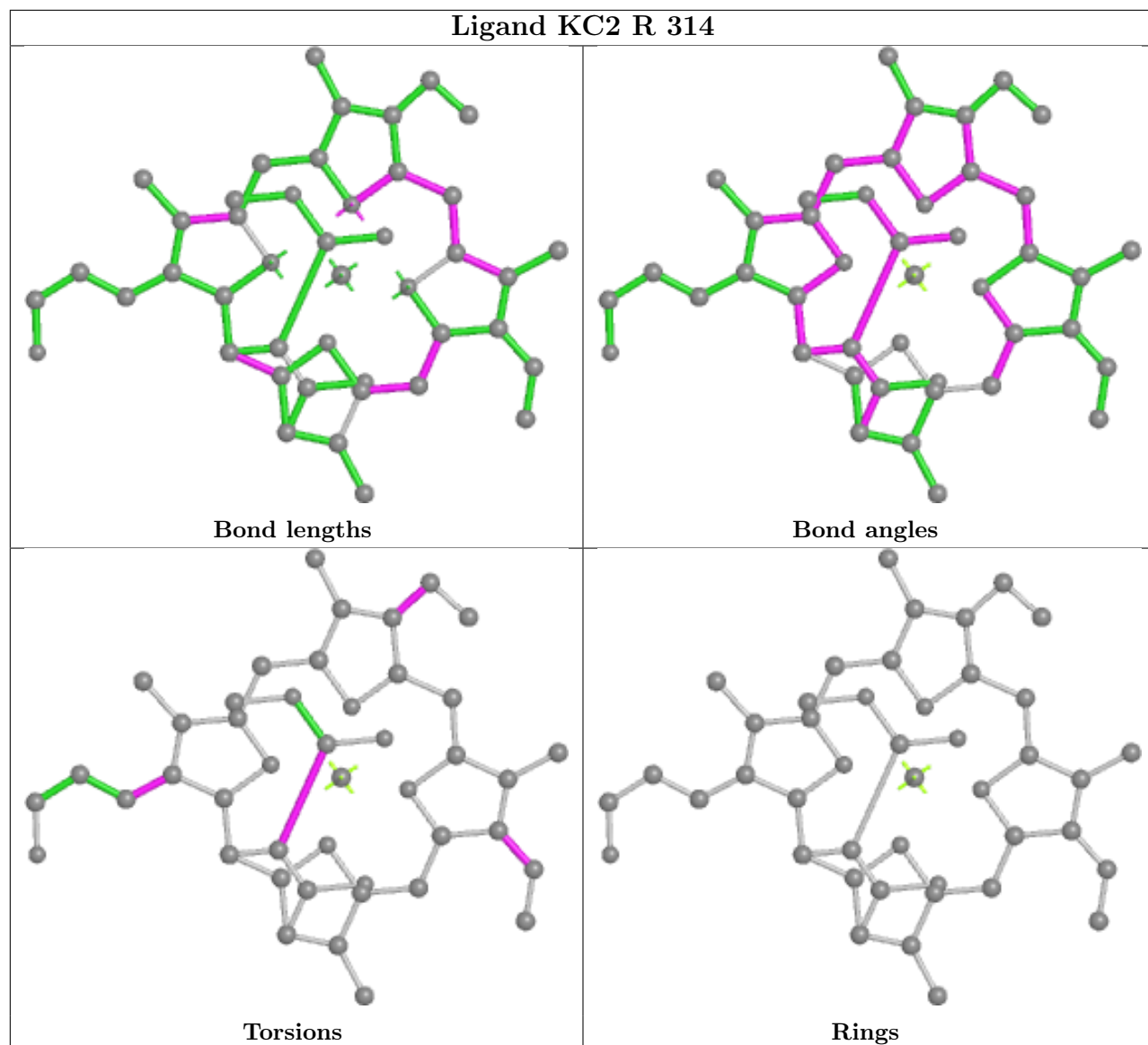
Torsions



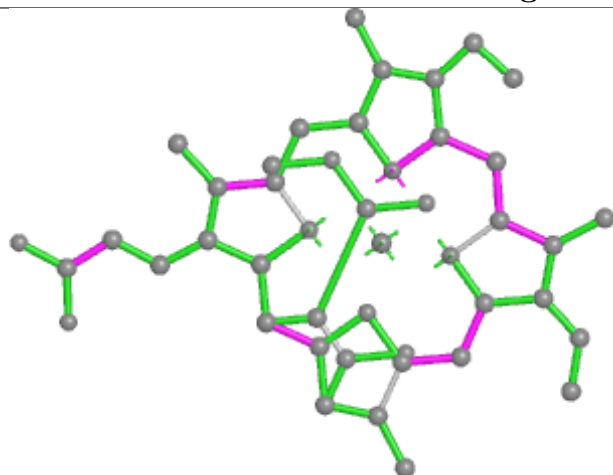
Rings



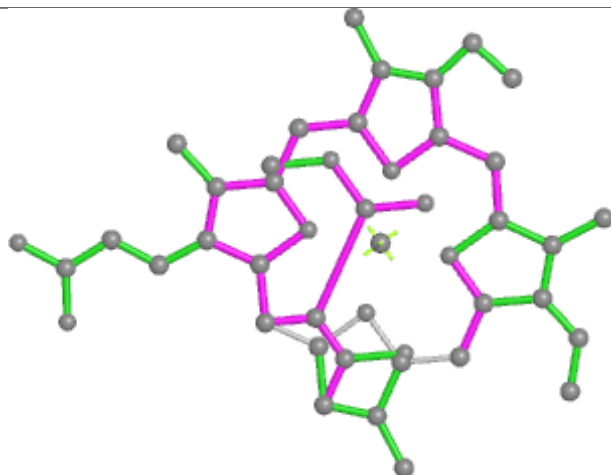
## Ligand KC2 R 314



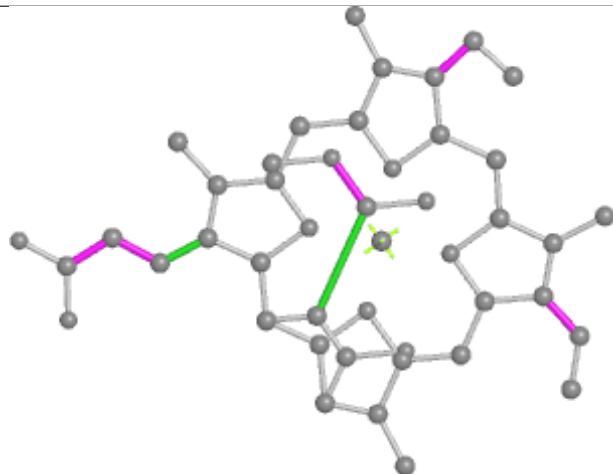
## Ligand KC2 6 314



Bond lengths



Bond angles

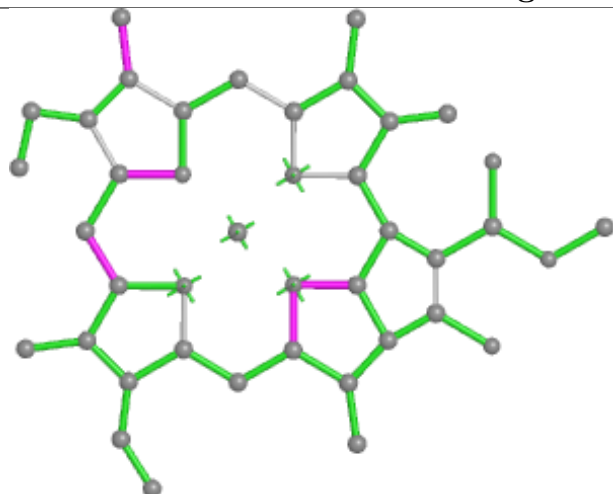


Torsions

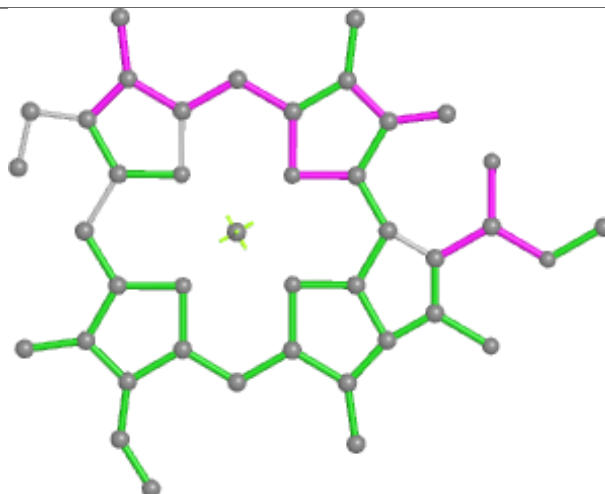


Rings

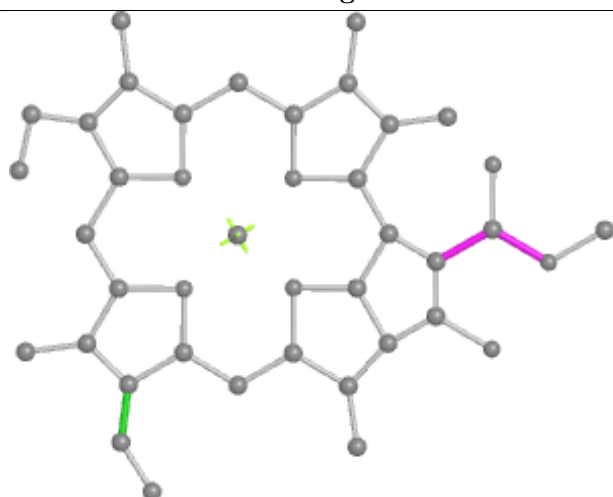
## Ligand CLA x 317



Bond lengths



Bond angles

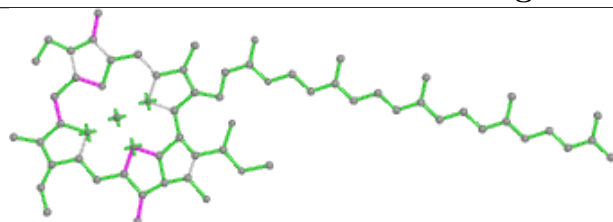


Torsions

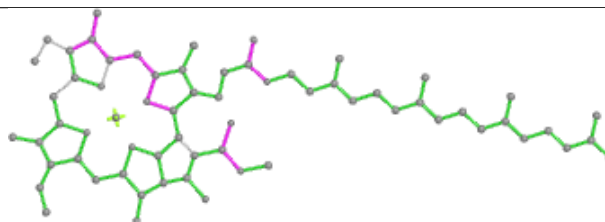


Rings

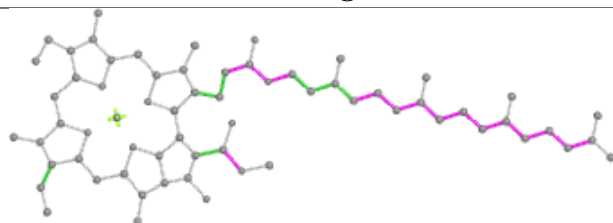
## Ligand CLA P 308



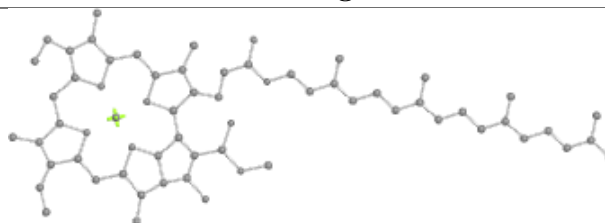
Bond lengths



Bond angles



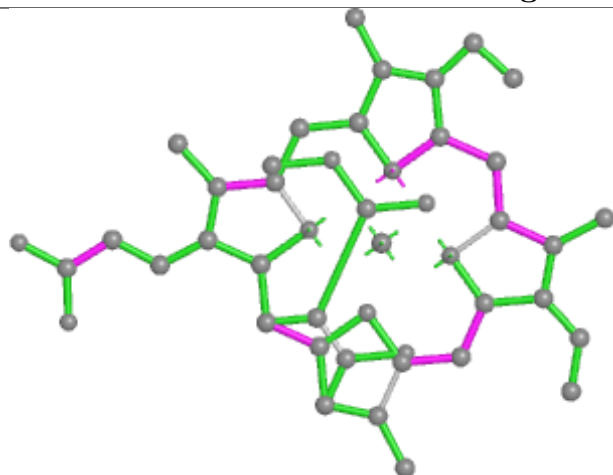
Torsions



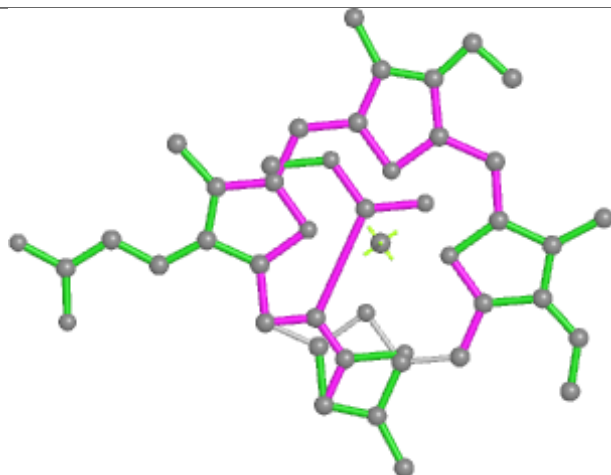
Rings



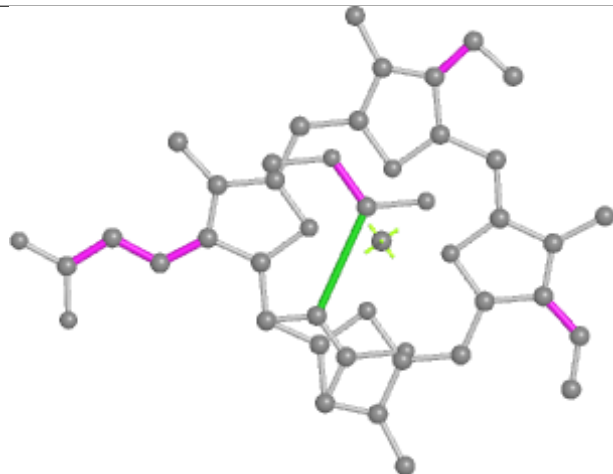
## Ligand KC2 4 320



Bond lengths



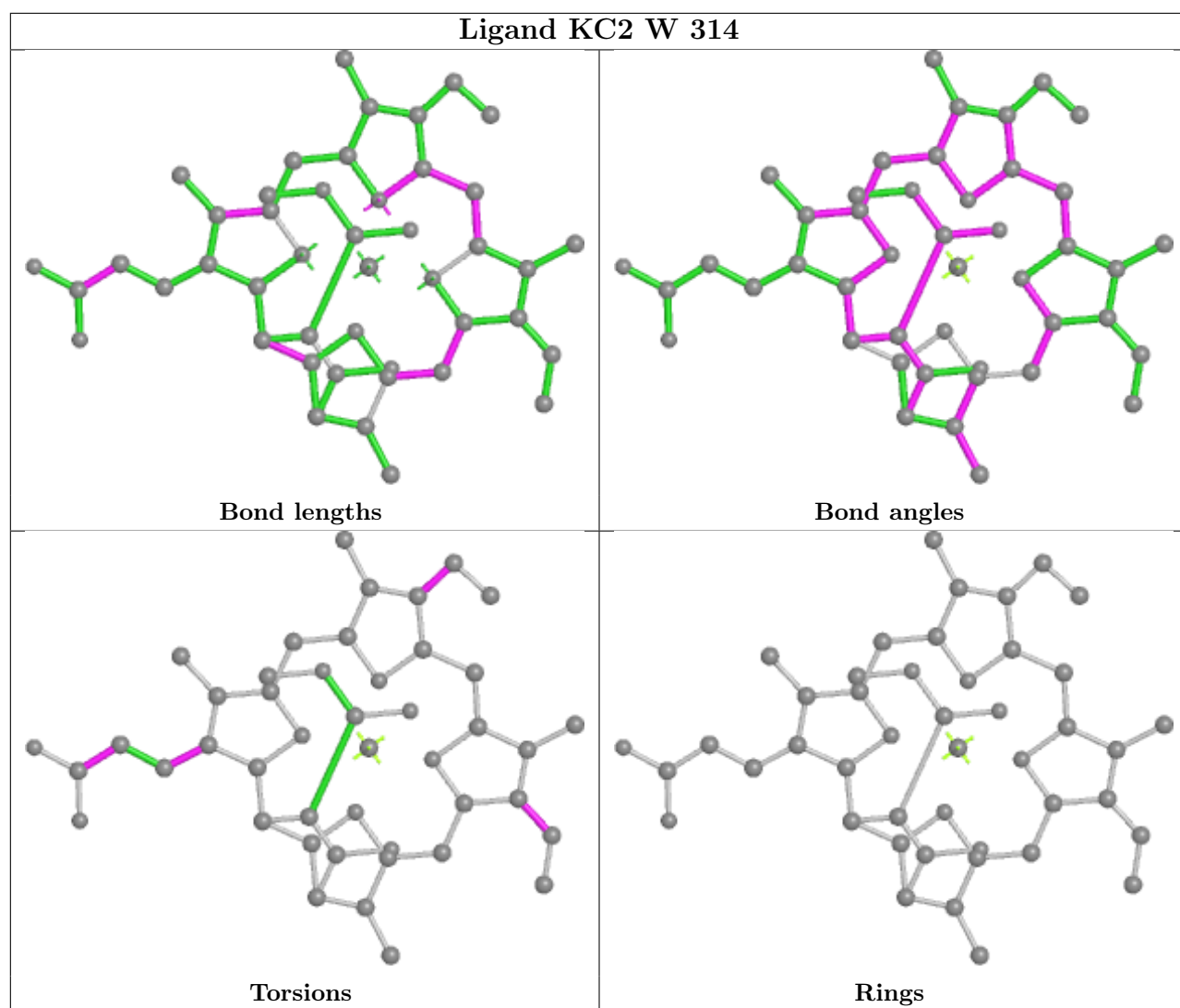
Bond angles



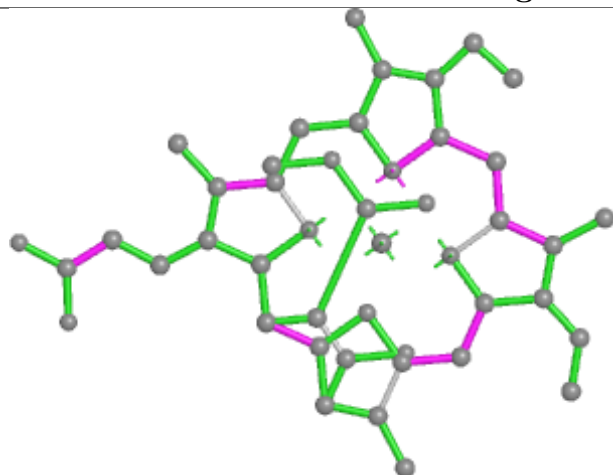
Torsions



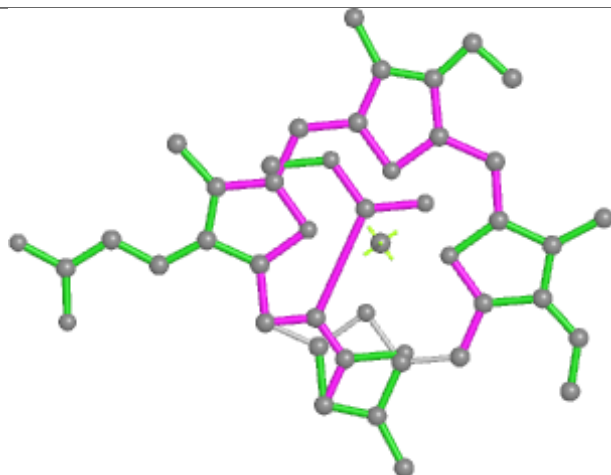
Rings



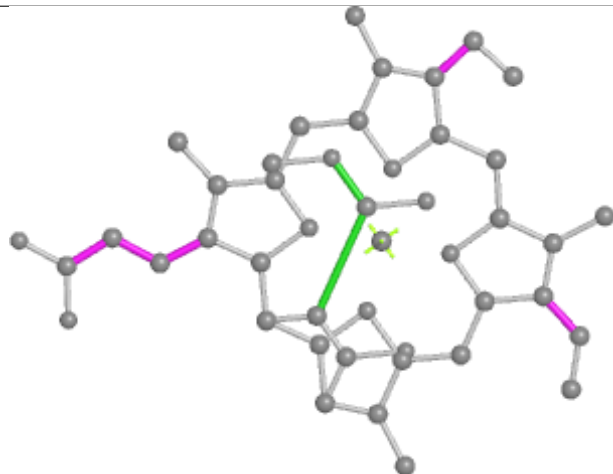
## Ligand KC2 X 315



Bond lengths



Bond angles

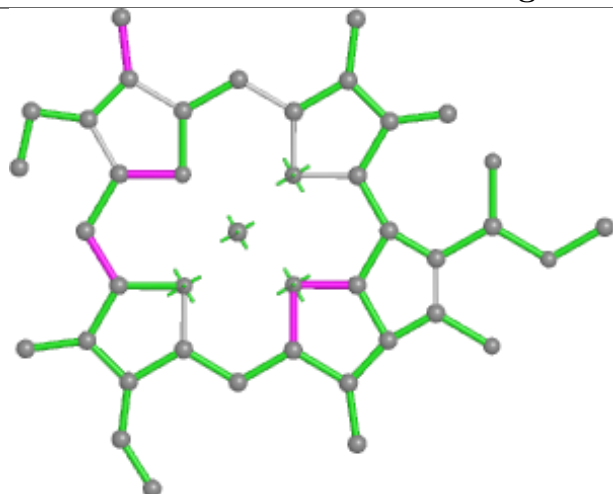


Torsions

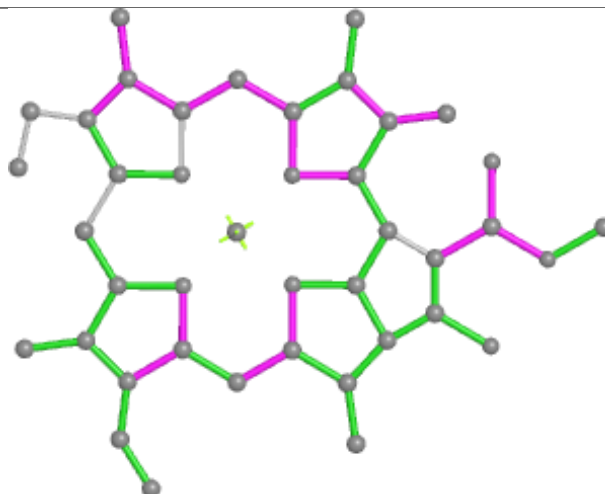


Rings

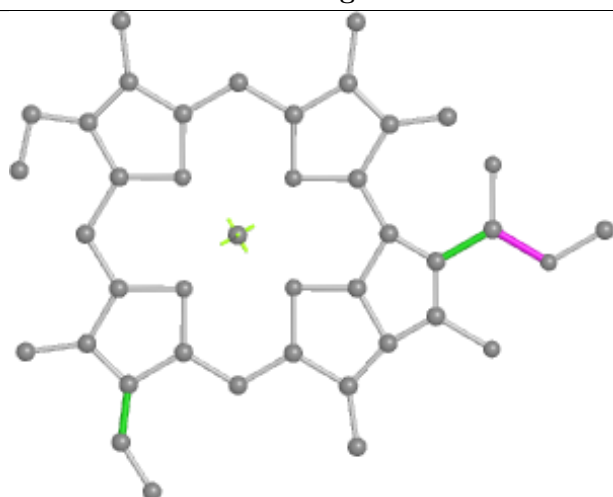
## Ligand CLA 8 322



Bond lengths



Bond angles

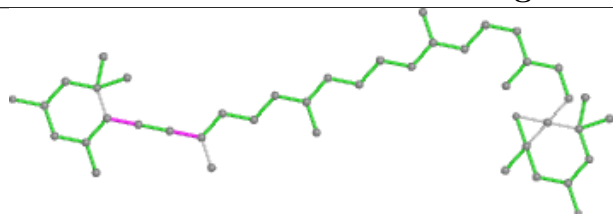


Torsions

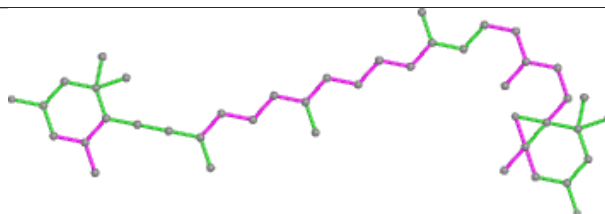


Rings

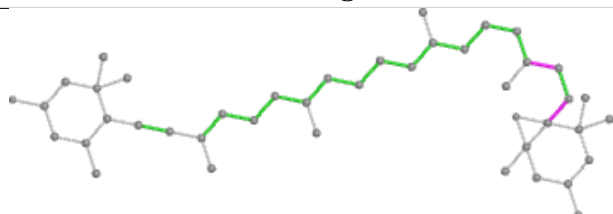
## Ligand DD6 A 304



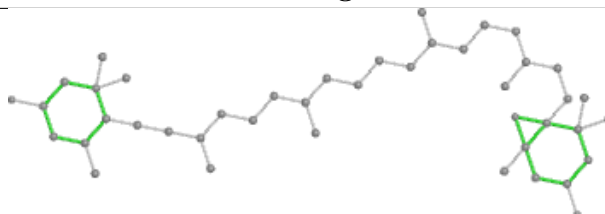
Bond lengths



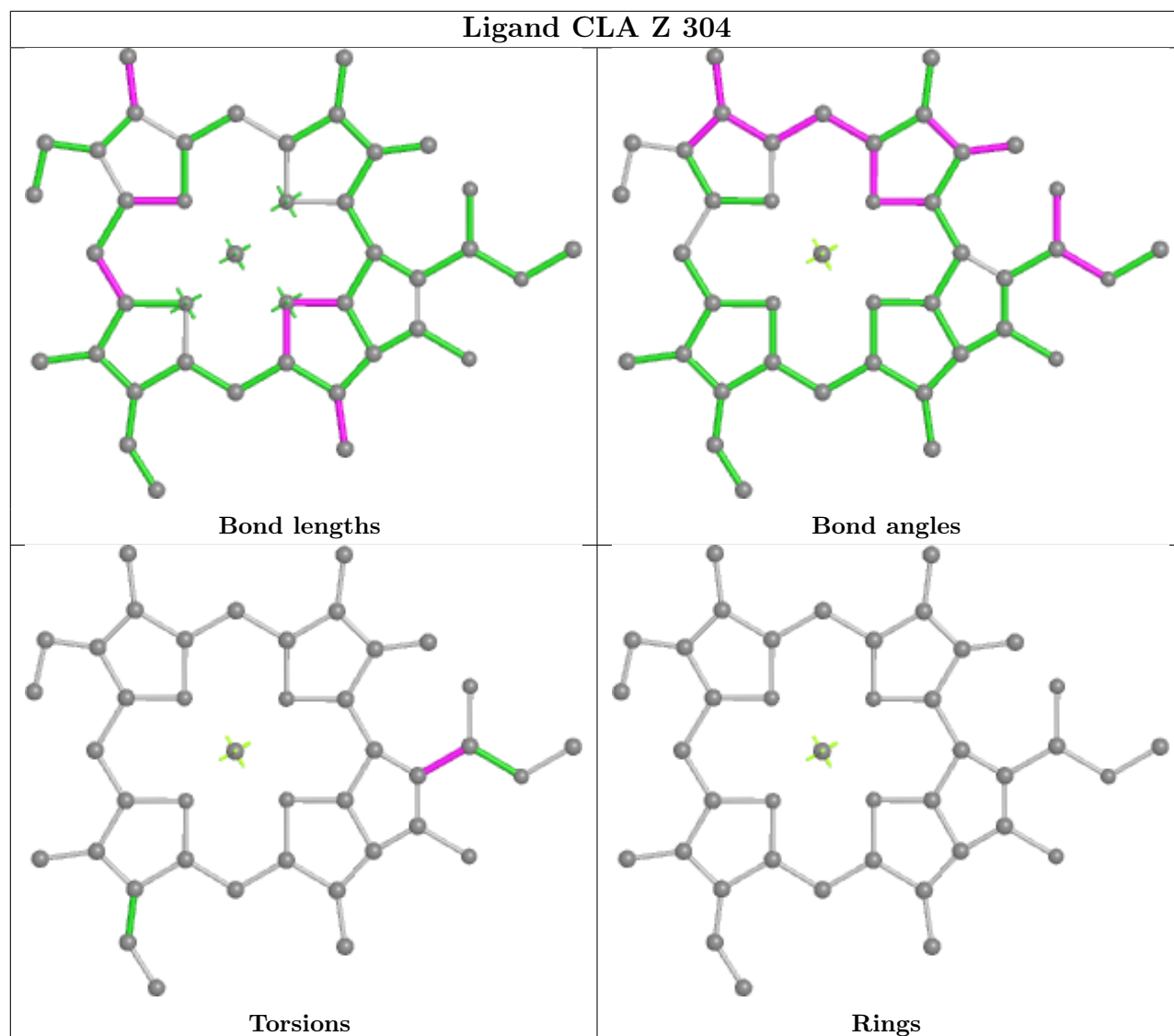
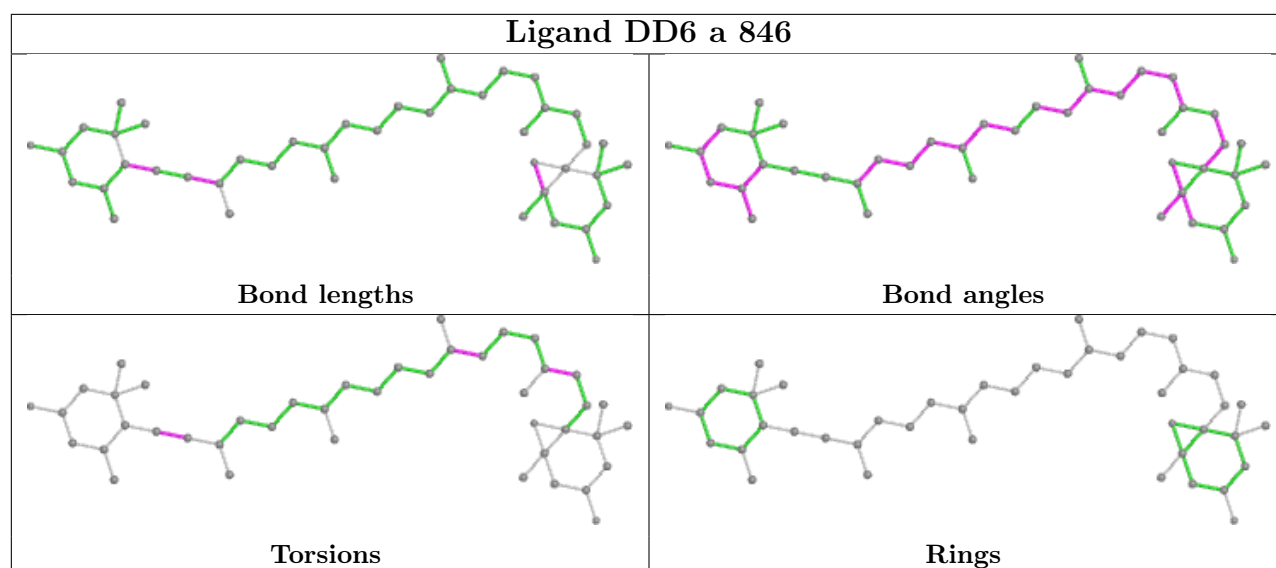
Bond angles



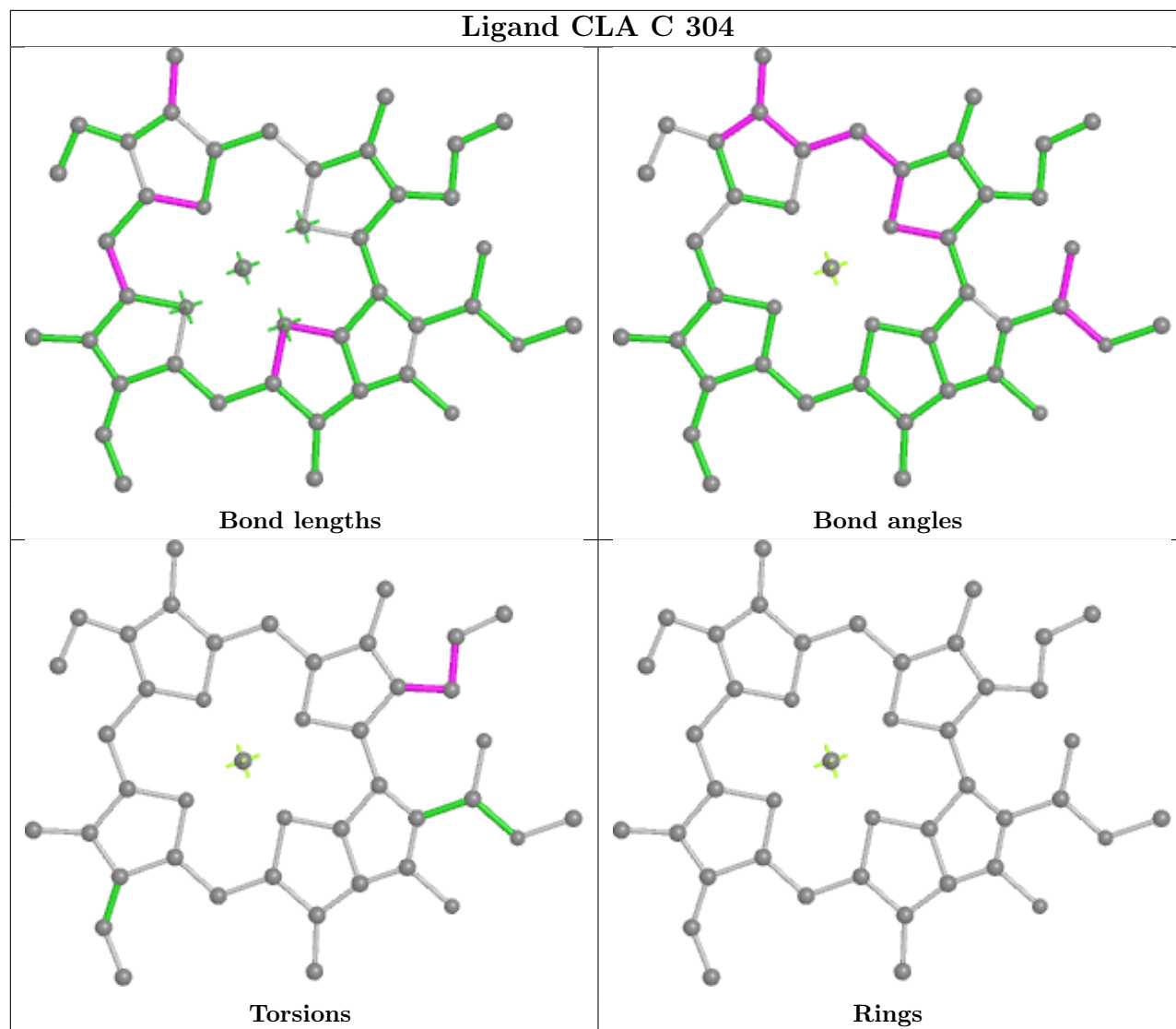
Torsions



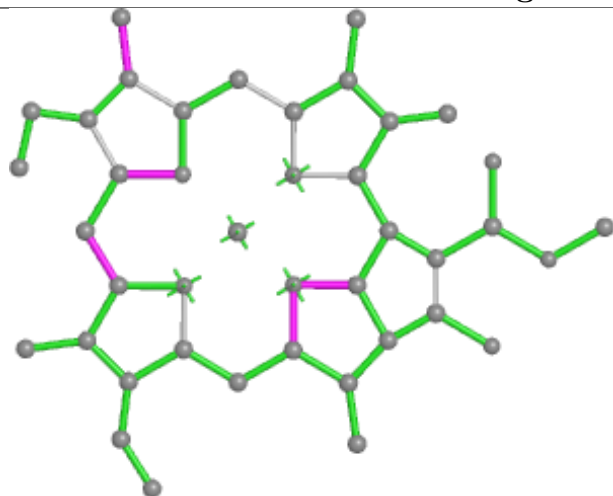
Rings



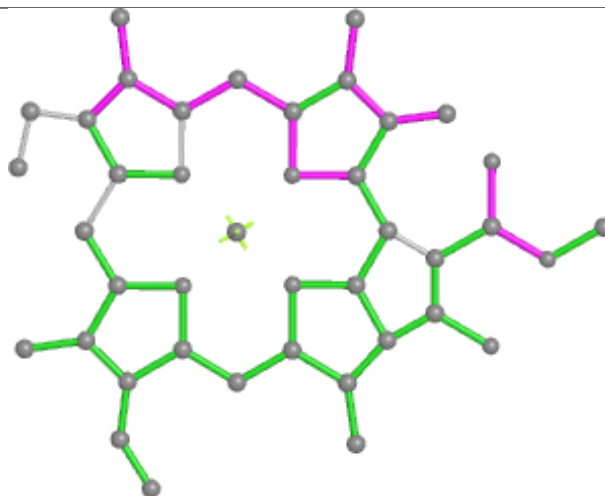
## Ligand CLA C 304



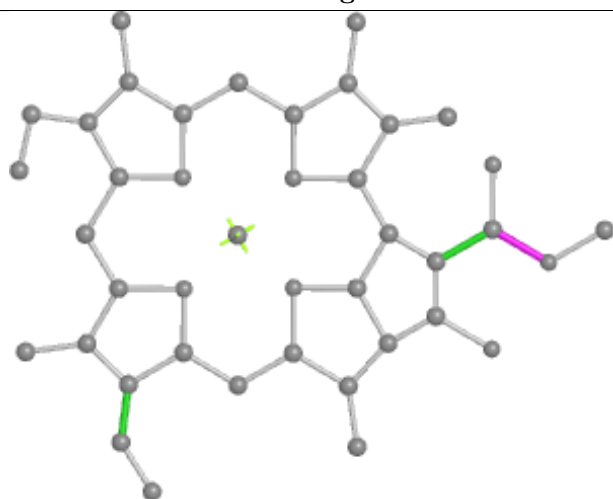
## Ligand CLA Z 305



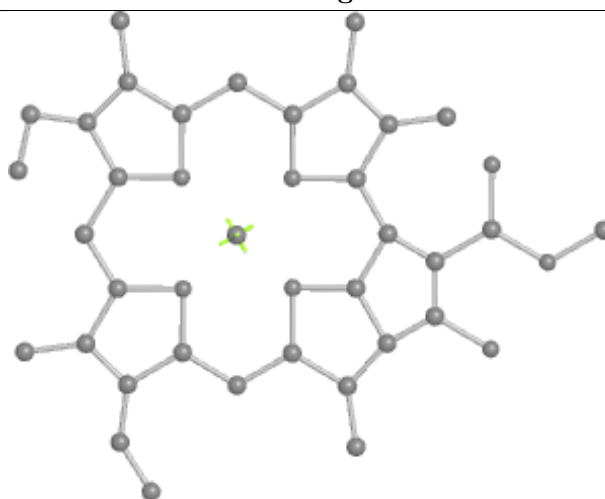
Bond lengths



Bond angles

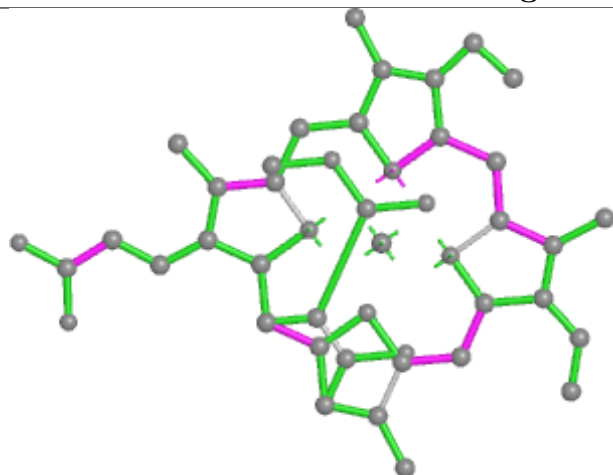


Torsions

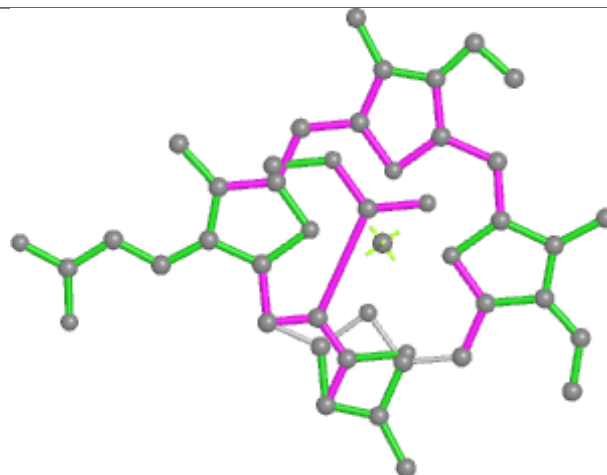


Rings

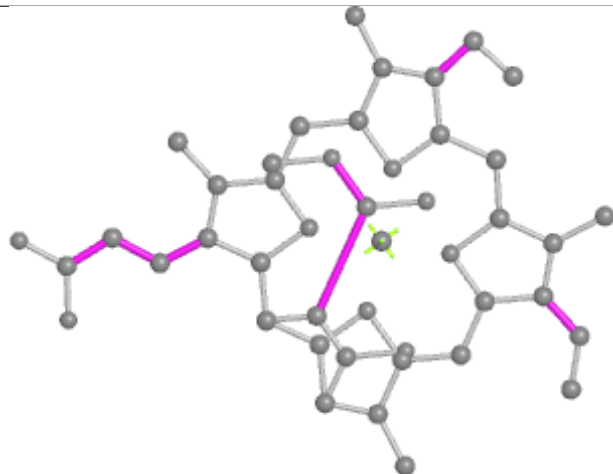
## Ligand KC2 7 322



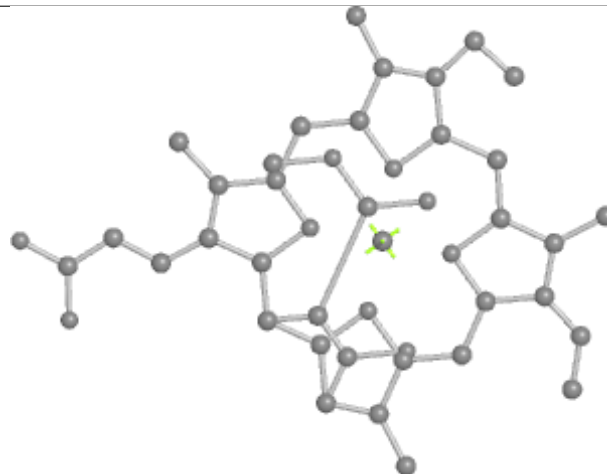
Bond lengths



Bond angles

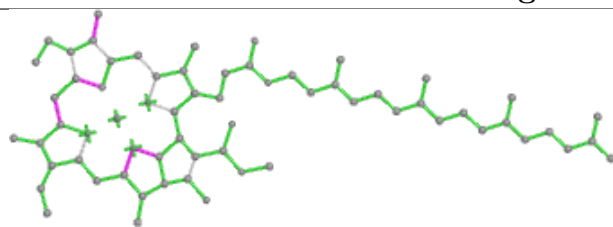


Torsions

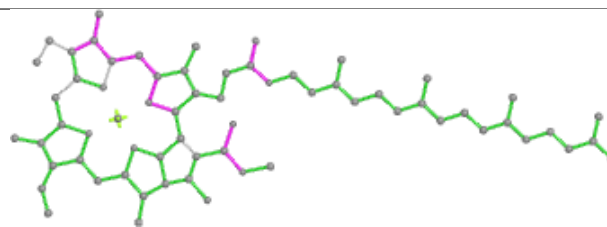


Rings

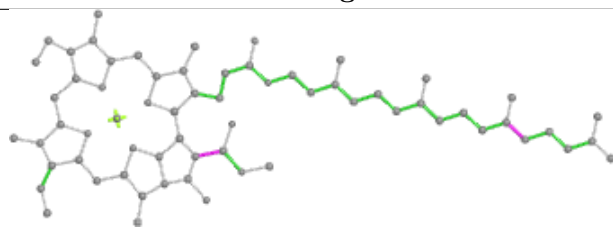
## Ligand CLA a 837



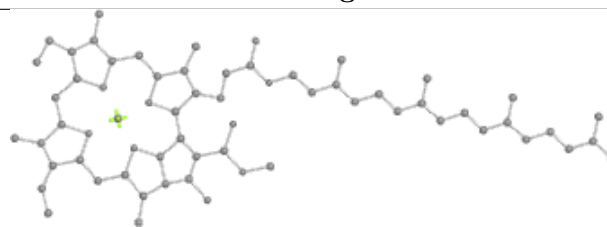
Bond lengths



Bond angles



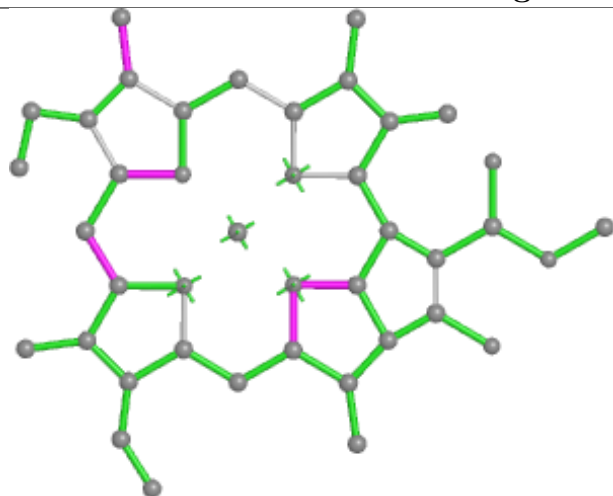
Torsions



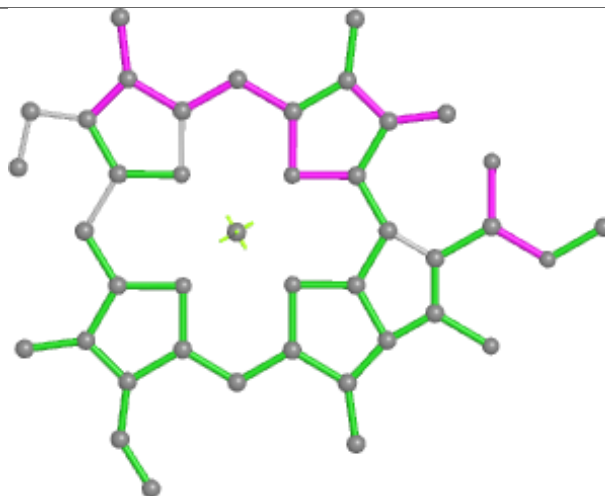
Rings



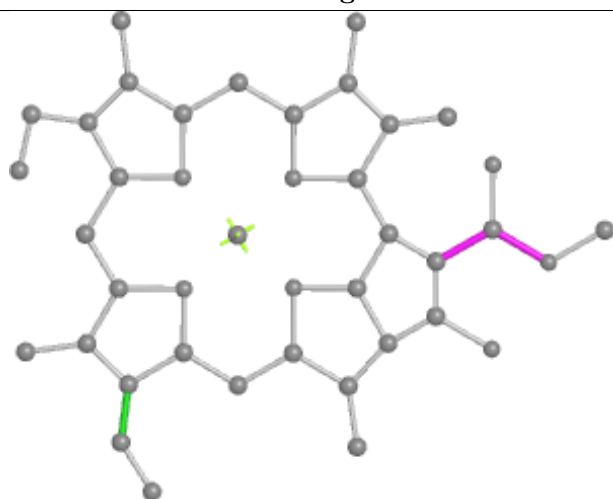
## Ligand CLA U 215



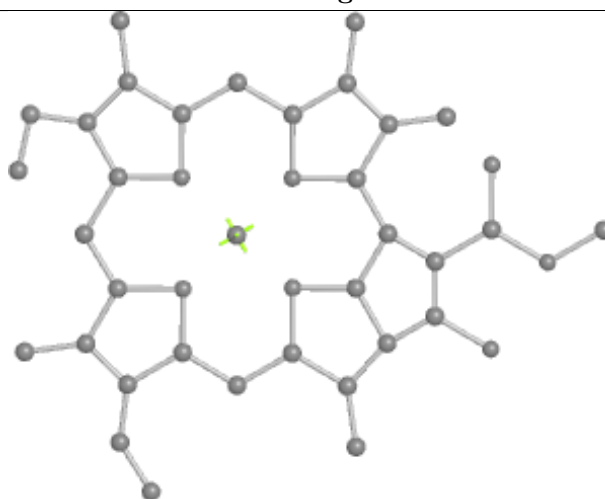
Bond lengths



Bond angles

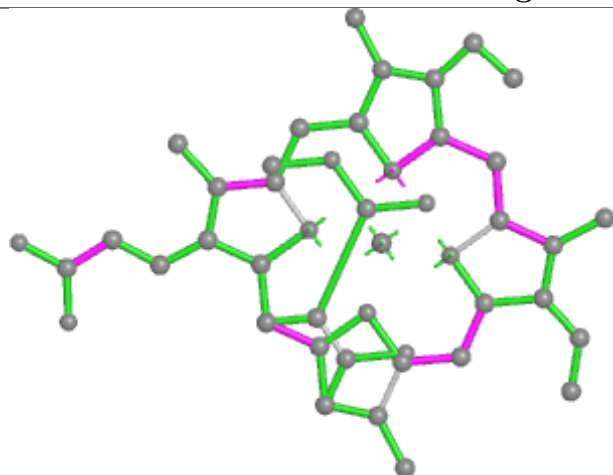


Torsions

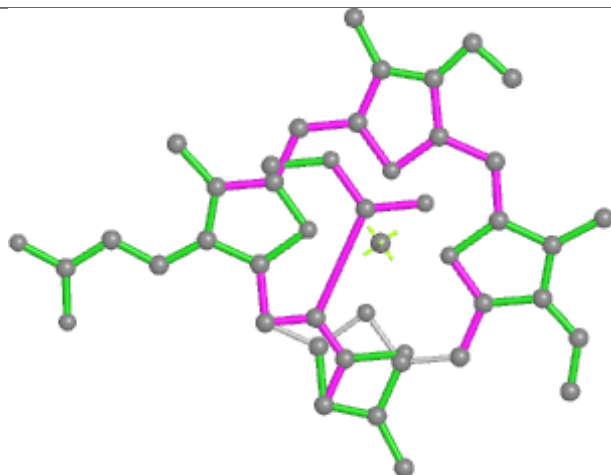


Rings

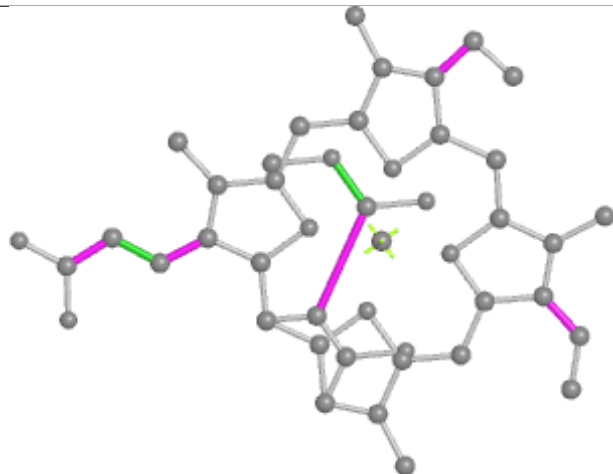
## Ligand KC2 H 311



Bond lengths



Bond angles

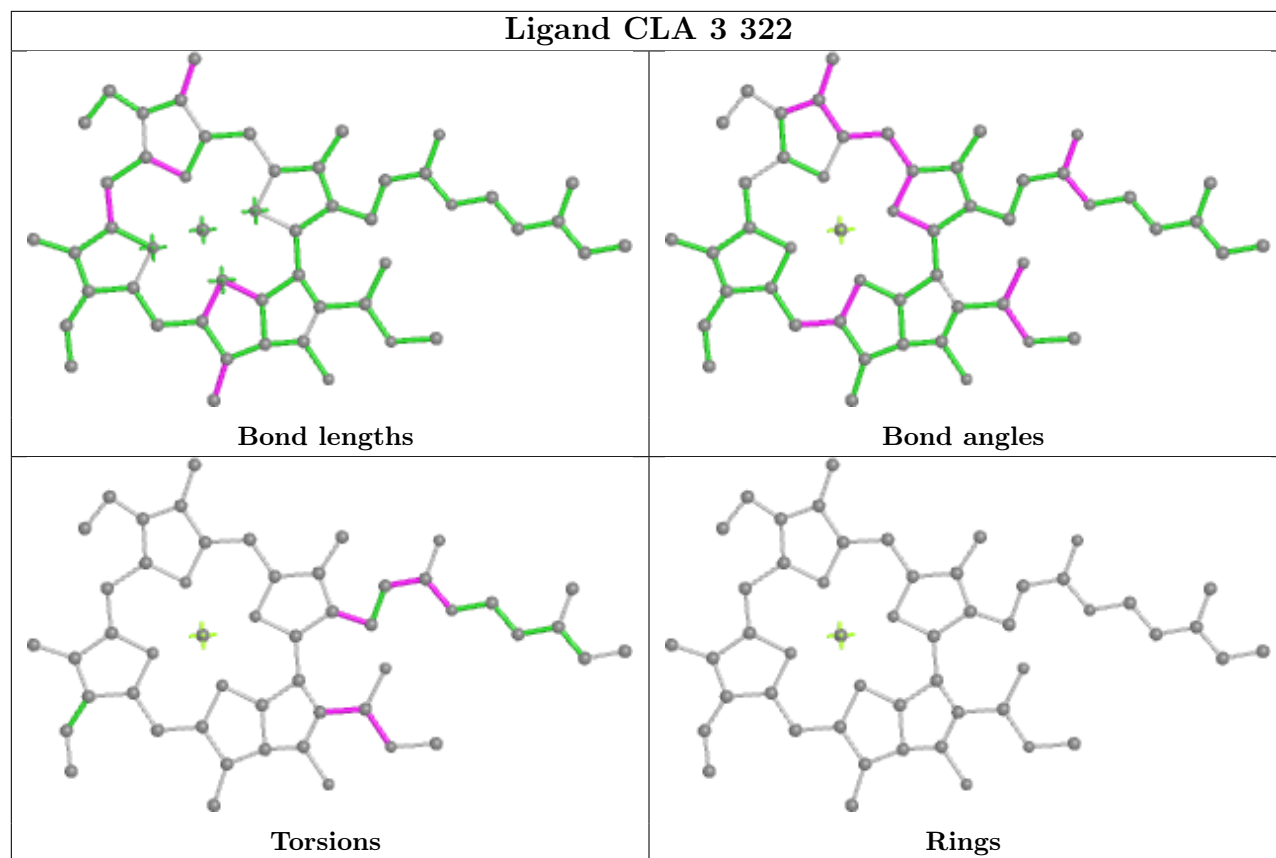


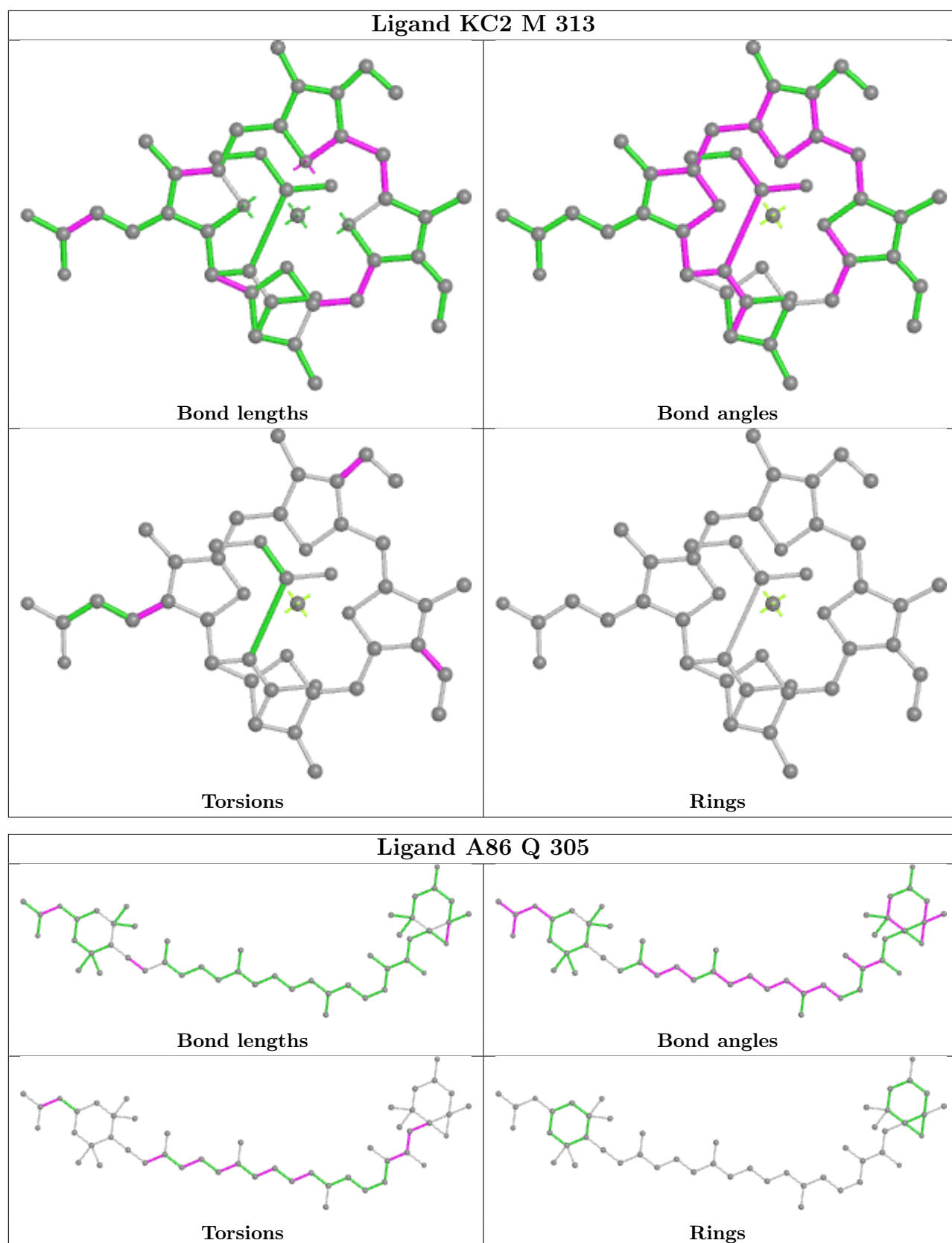
Torsions



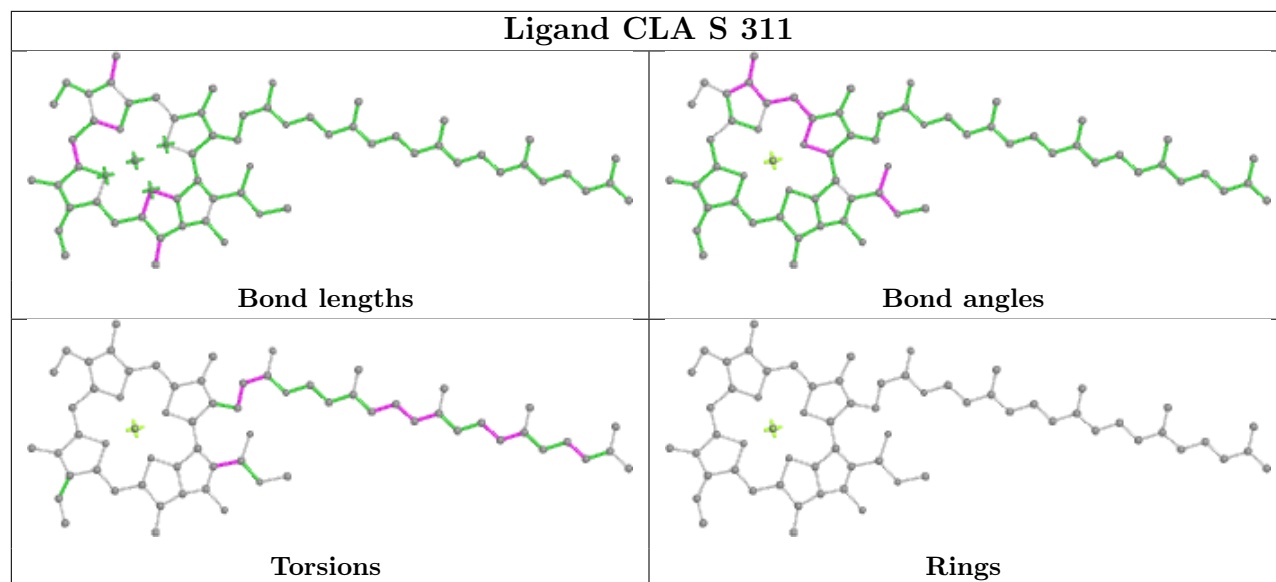
Rings

## Ligand CLA 3 322

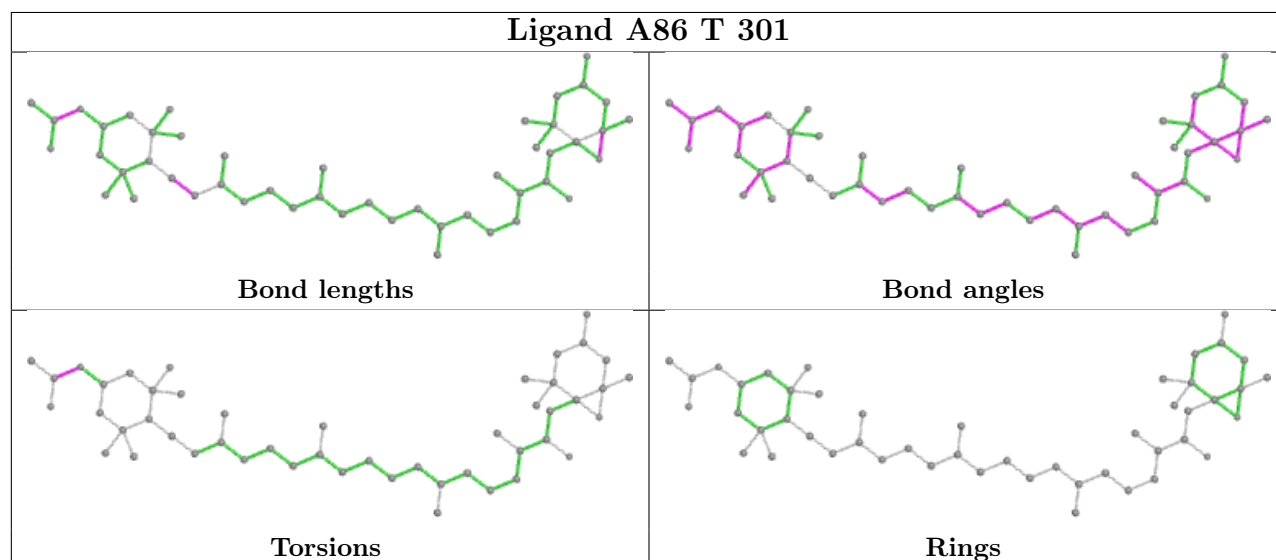




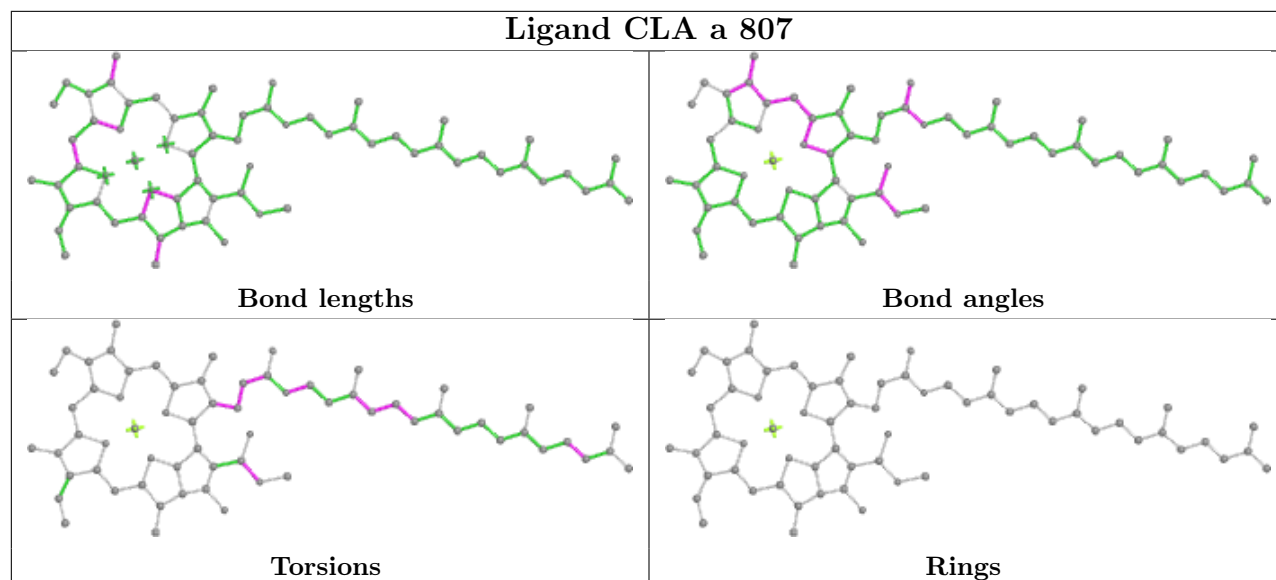
## Ligand CLA S 311



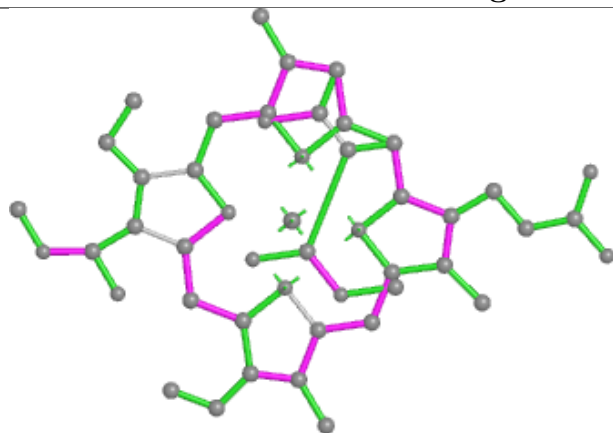
## Ligand A86 T 301



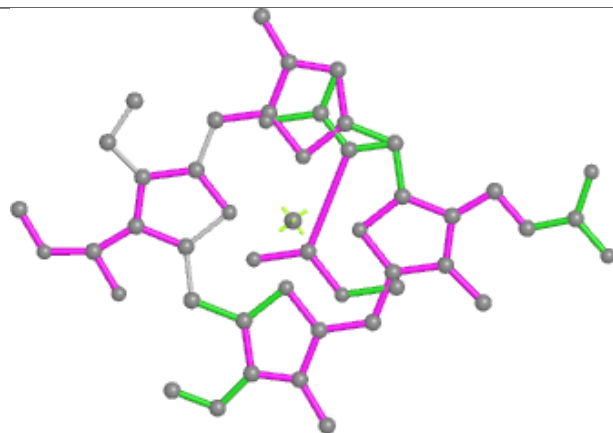
## Ligand CLA a 807



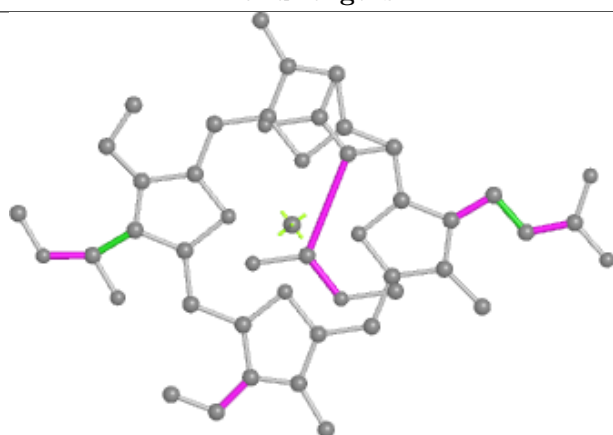
## Ligand A1ECV G 316



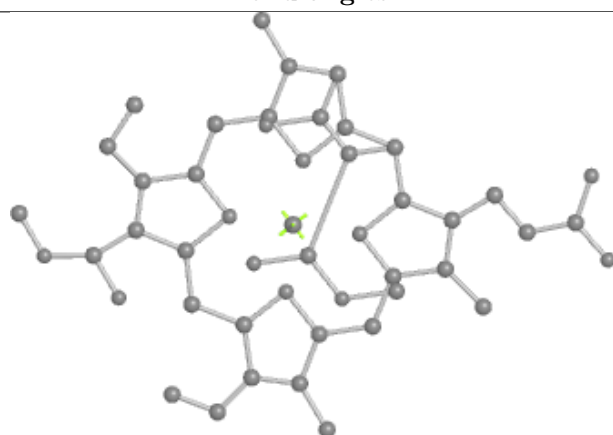
Bond lengths



Bond angles

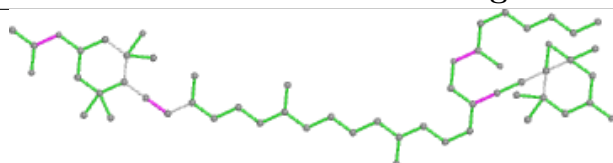


Torsions

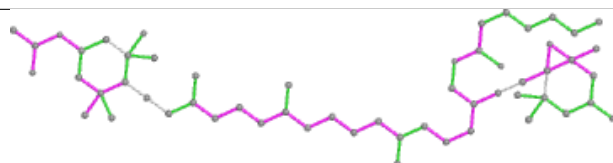


Rings

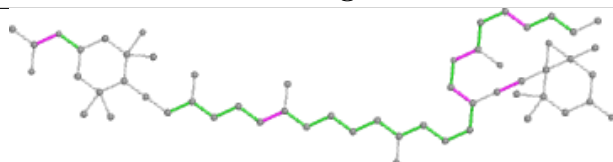
## Ligand A1EB4 W 306



Bond lengths



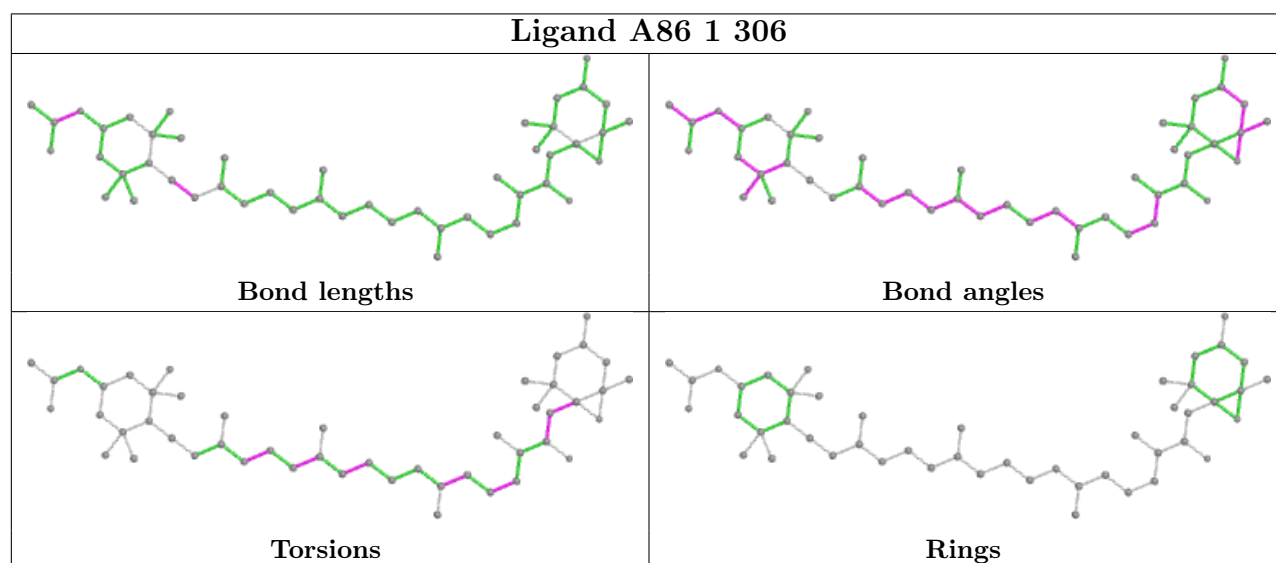
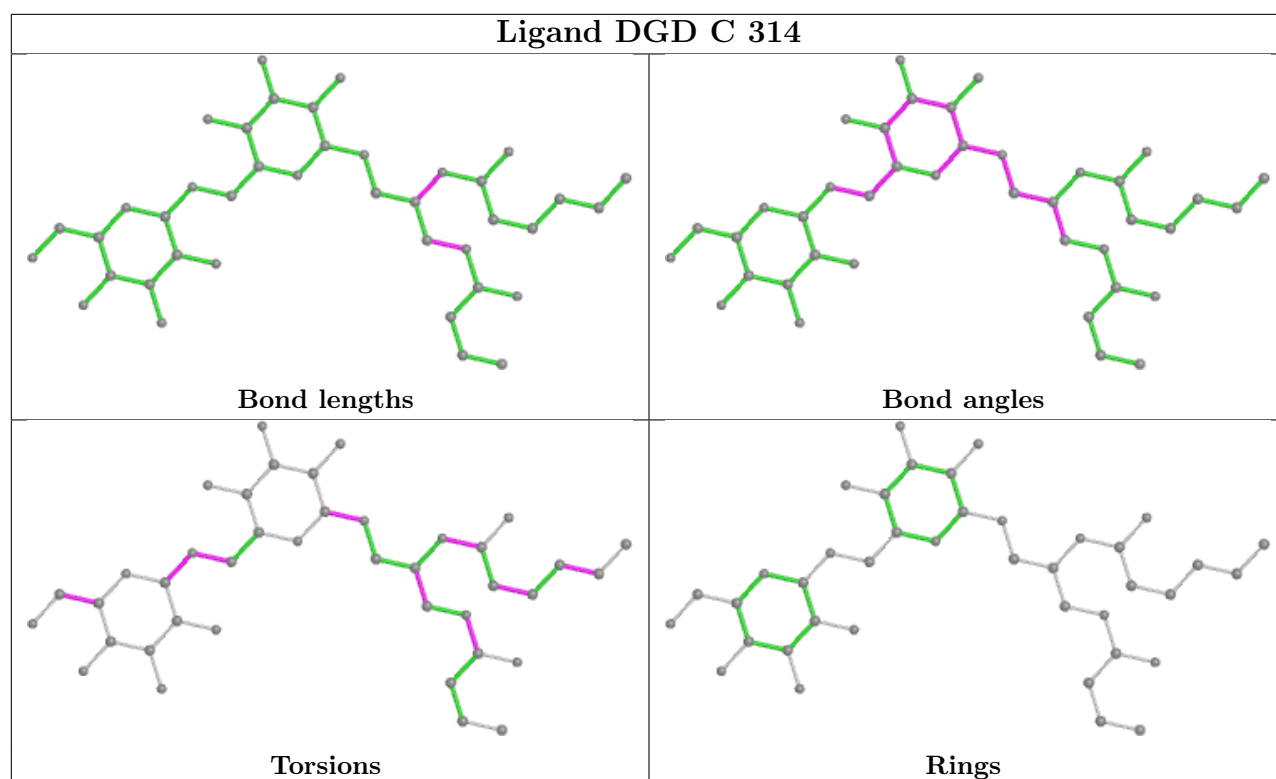
Bond angles

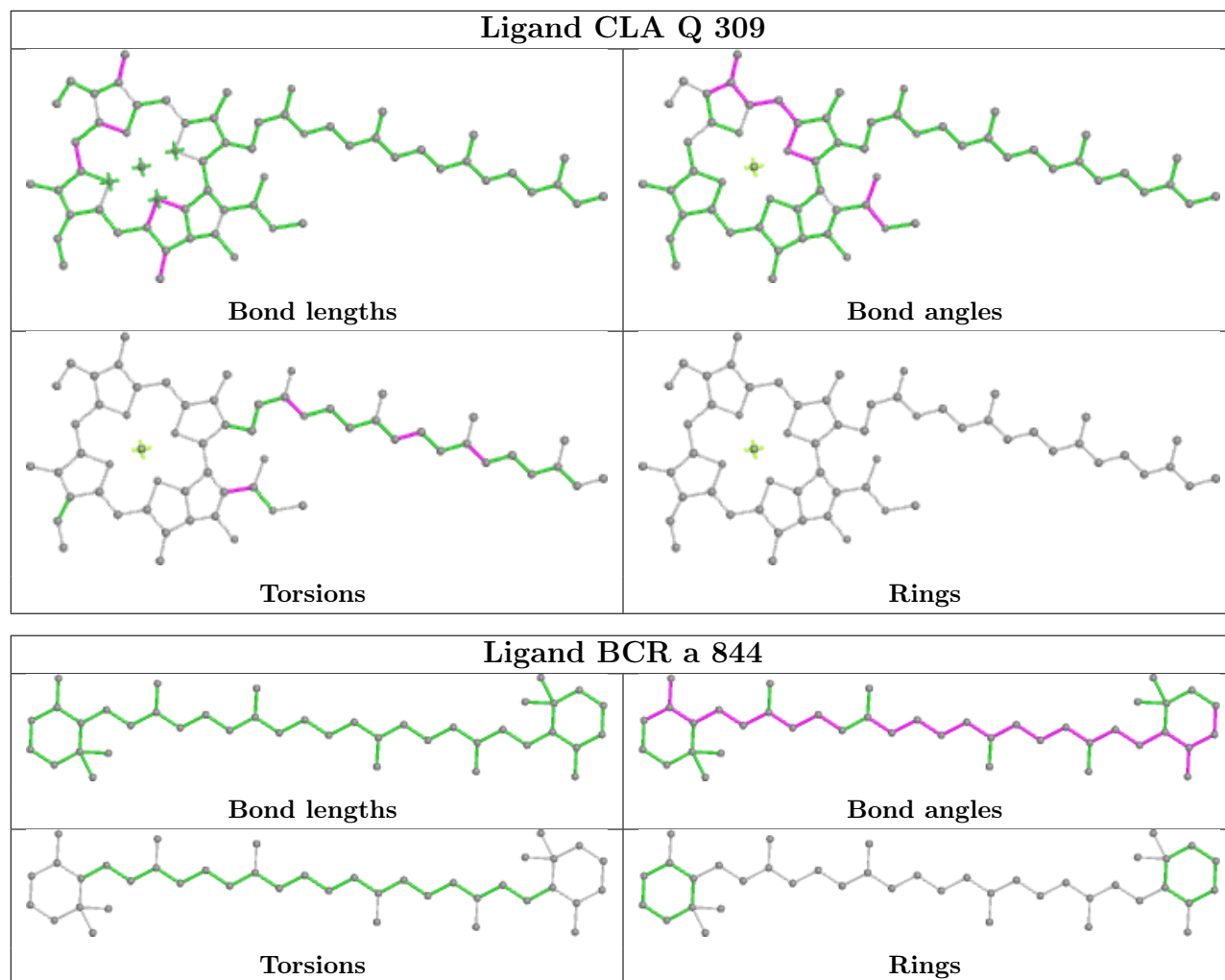


Torsions



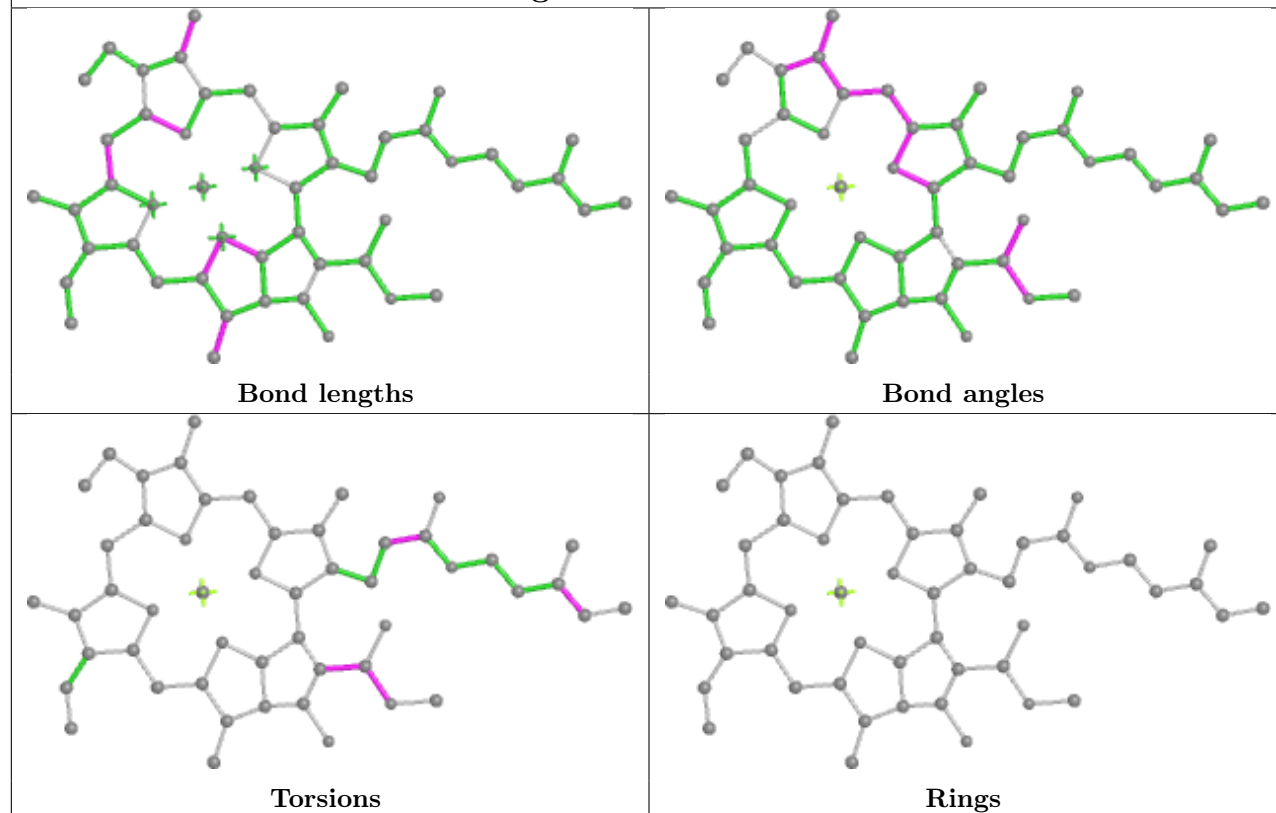
Rings



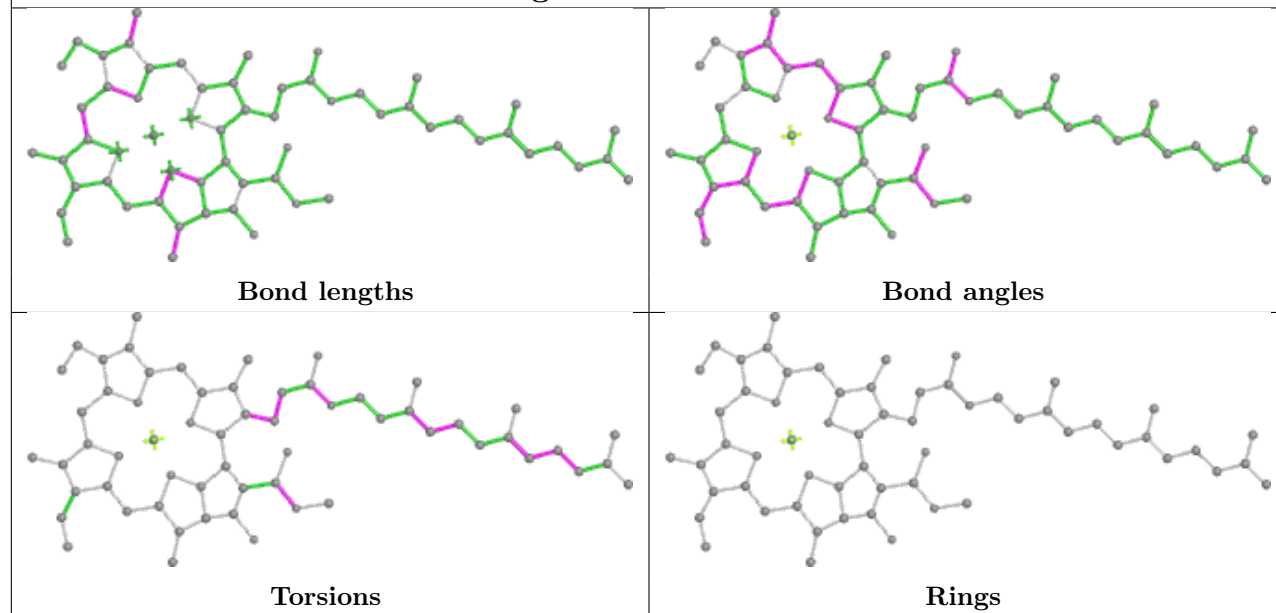




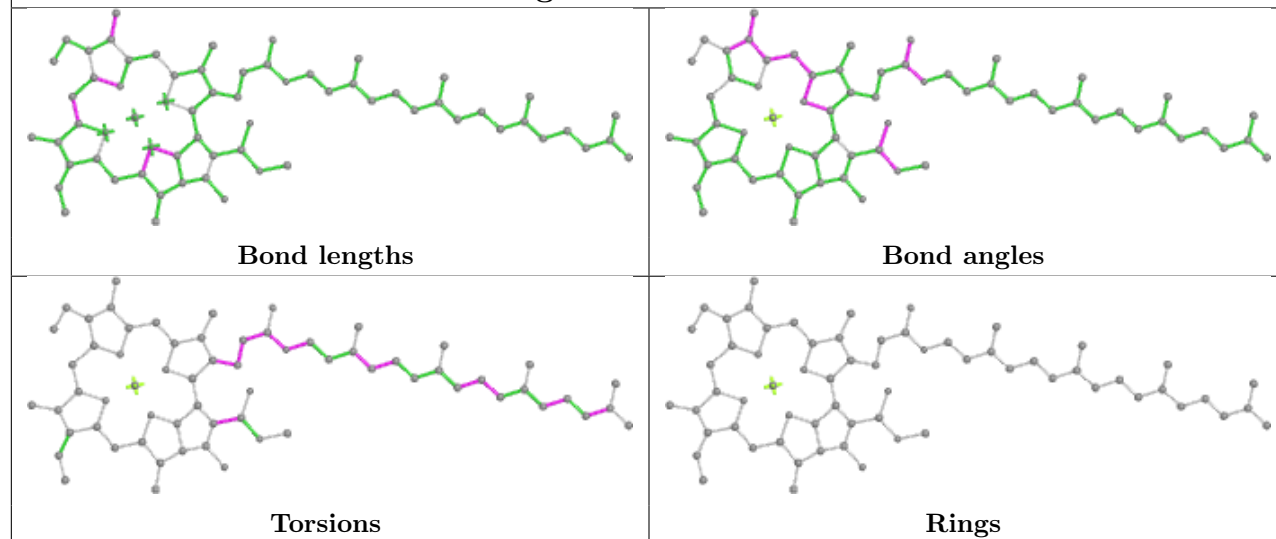
## Ligand CLA A 308



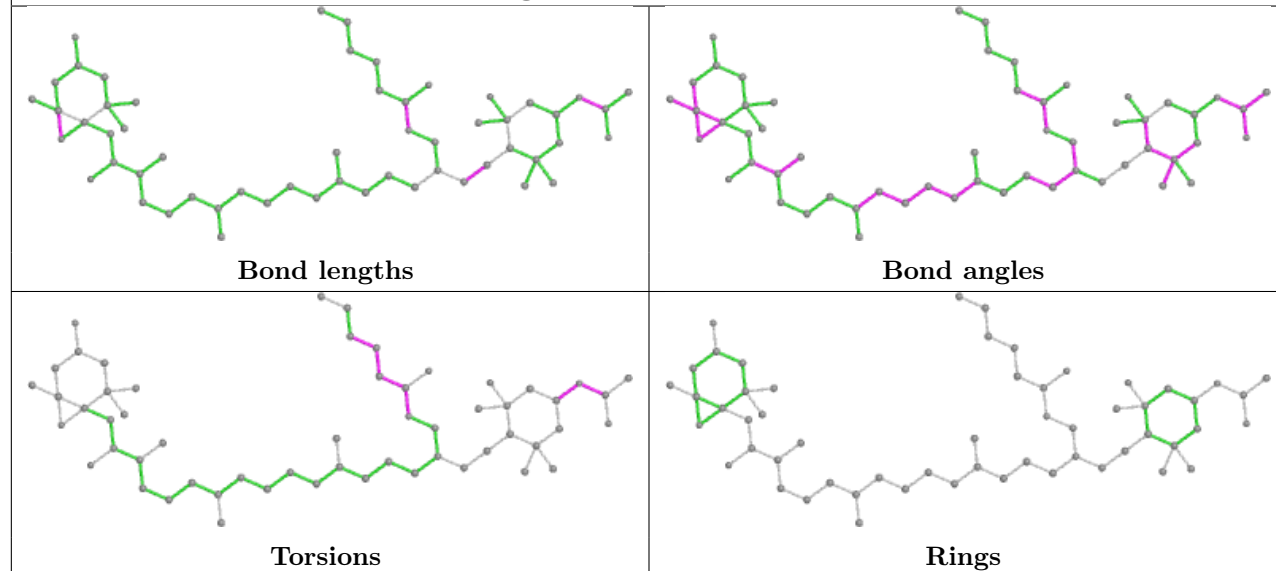
## Ligand CLA O 310



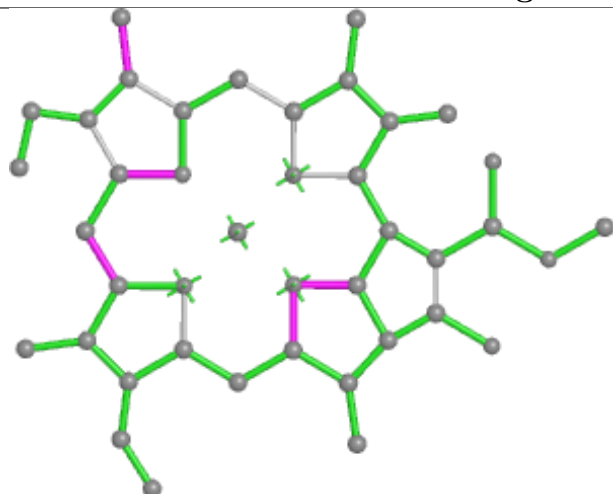
## Ligand CLA J 309



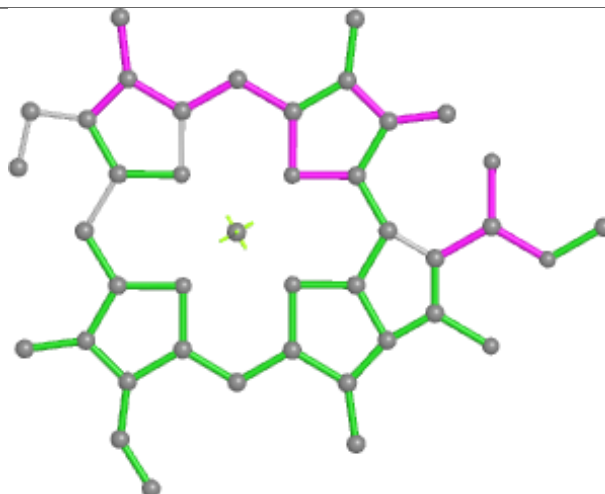
## Ligand A1EB1 3 309



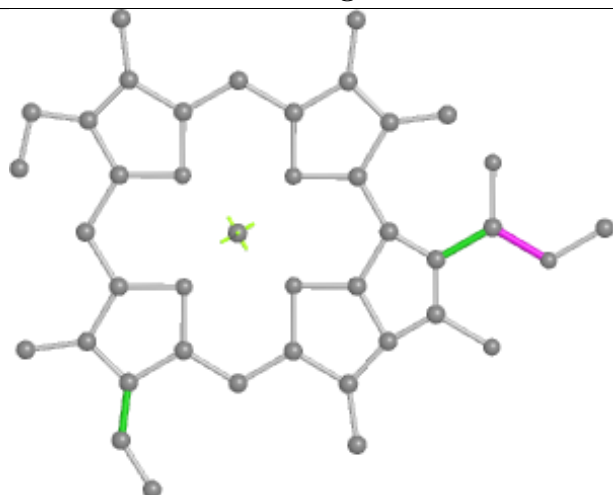
## Ligand CLA F 315



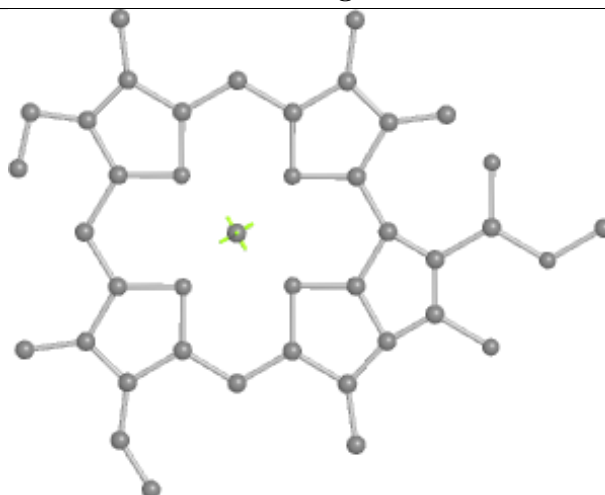
Bond lengths



Bond angles

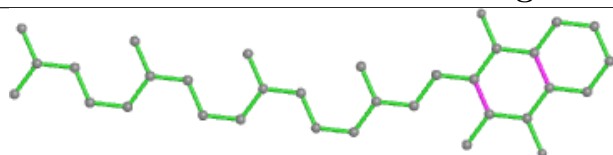


Torsions

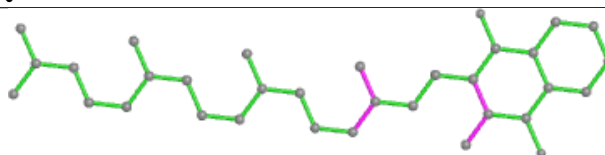


Rings

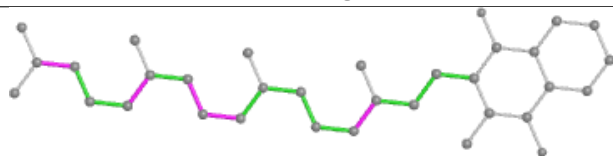
## Ligand PQN a 839



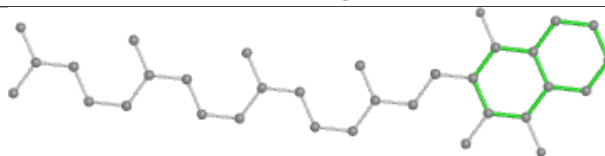
Bond lengths



Bond angles

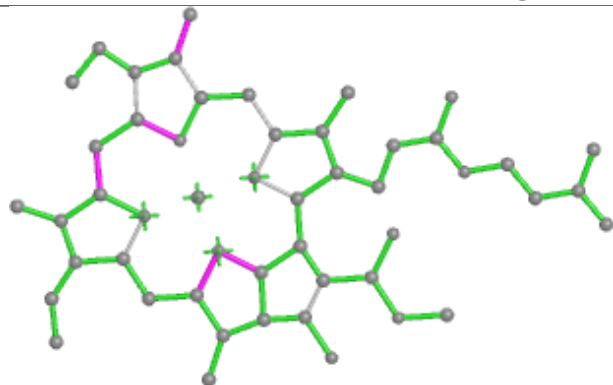


Torsions

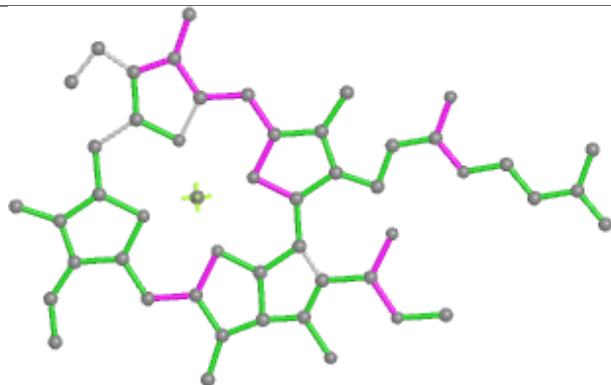


Rings

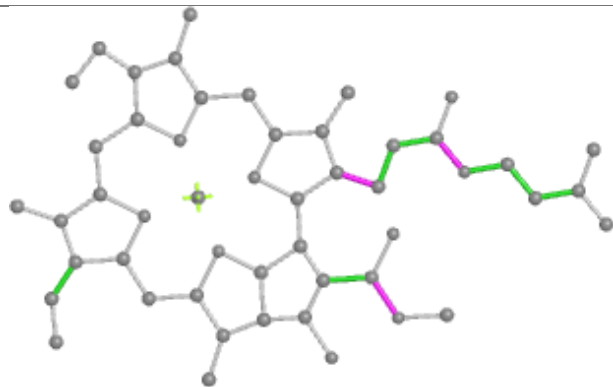
## Ligand CLA A 315



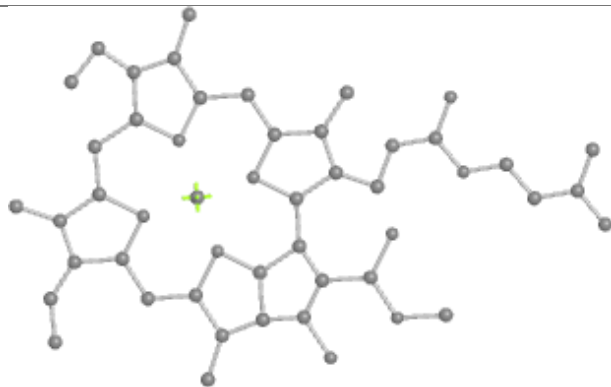
Bond lengths



Bond angles

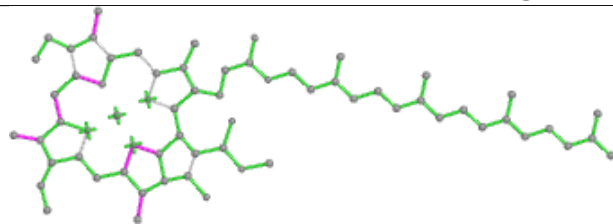


Torsions

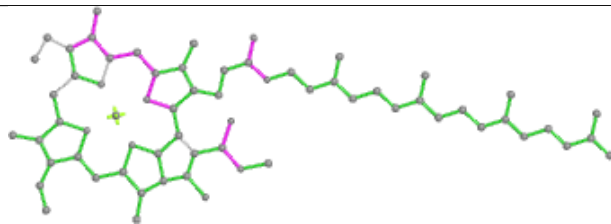


Rings

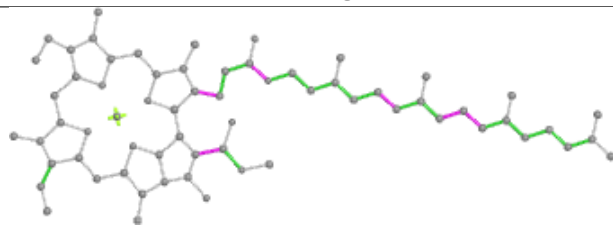
## Ligand CLA S 313



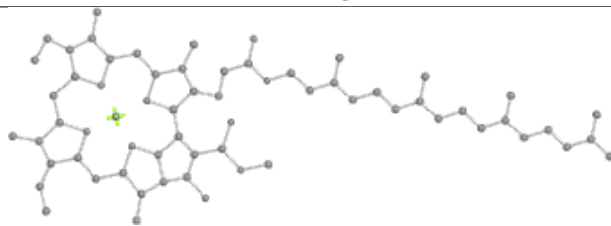
Bond lengths



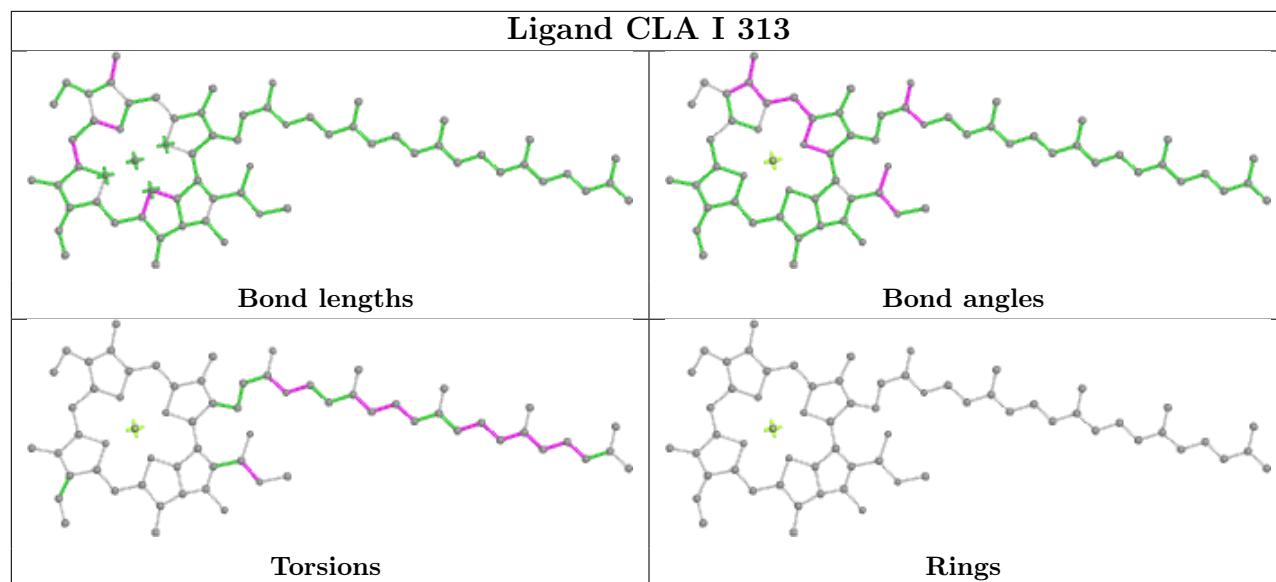
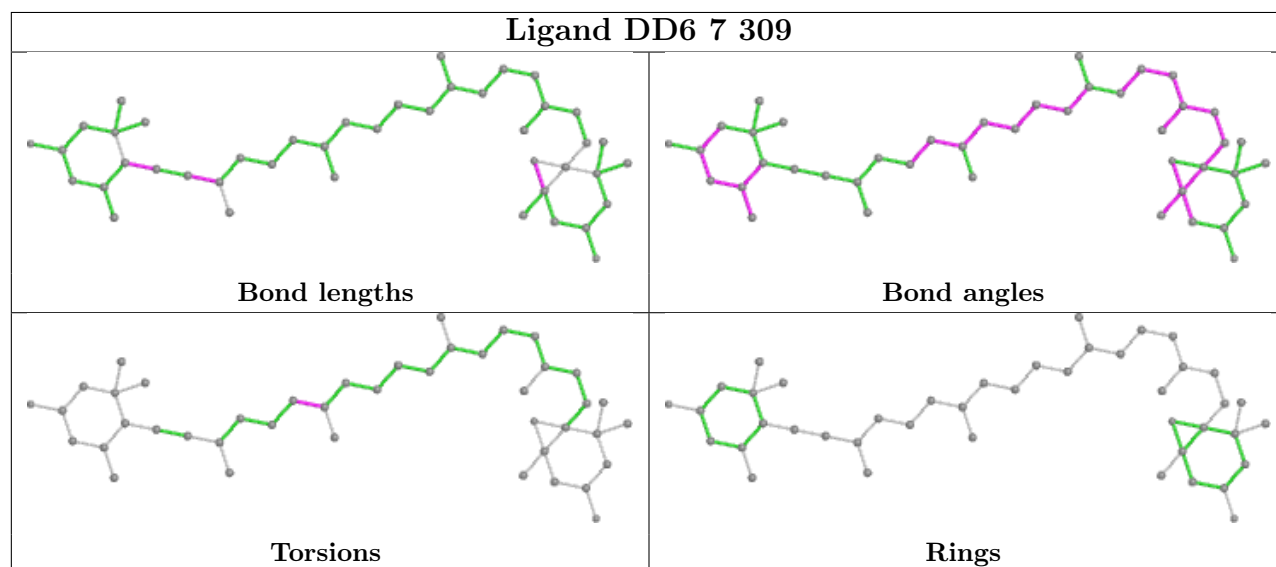
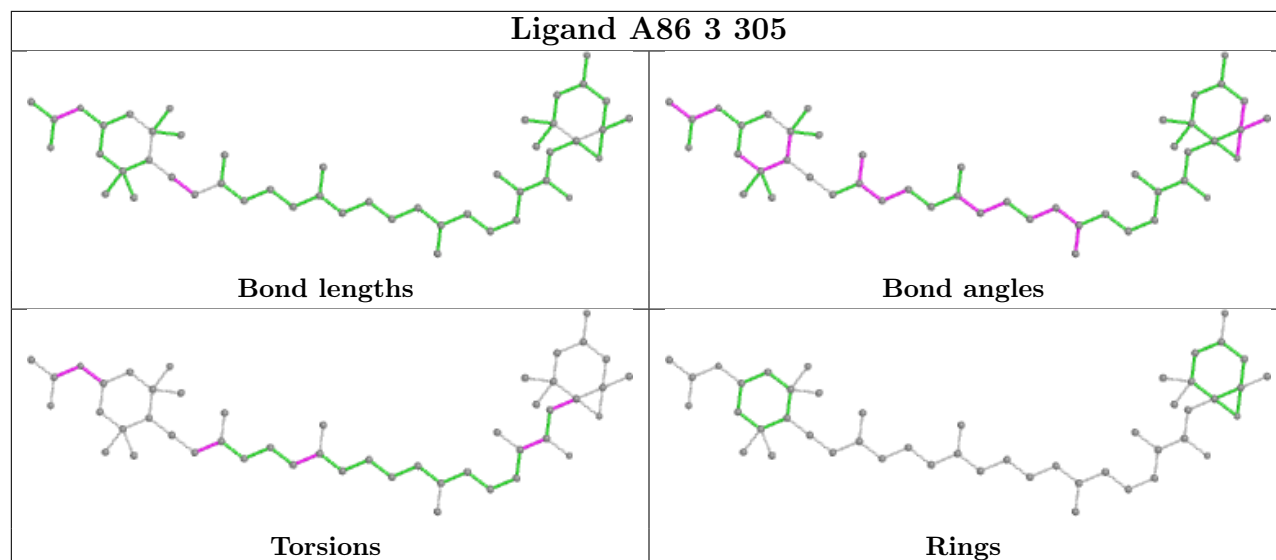
Bond angles



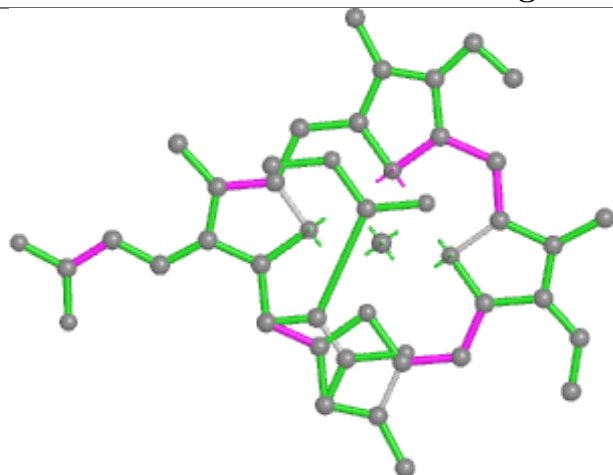
Torsions



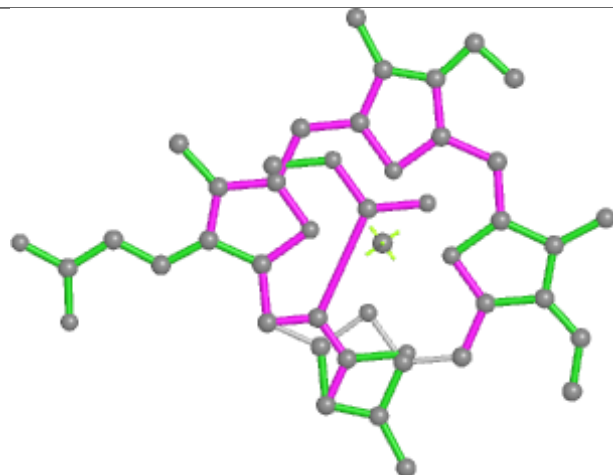
Rings

**Ligand CLA I 313****Ligand DD6 7 309****Ligand A86 3 305**

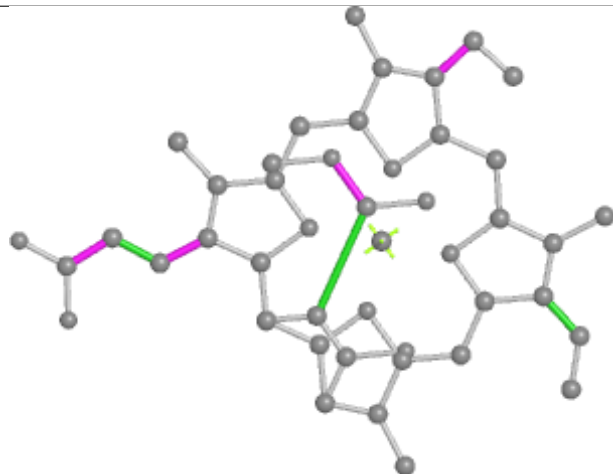
## Ligand KC2 L 314



Bond lengths



Bond angles

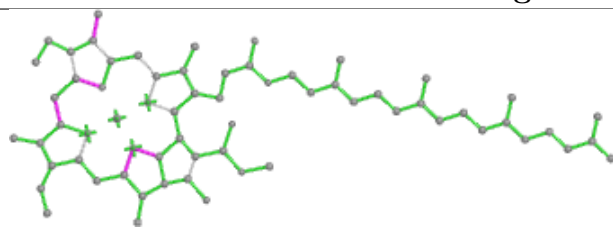


Torsions

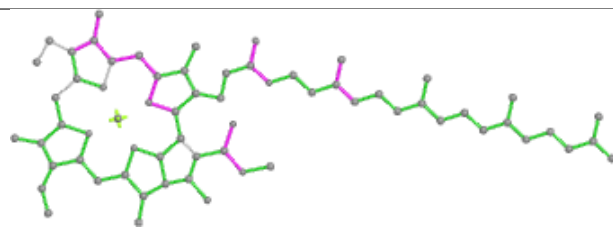


Rings

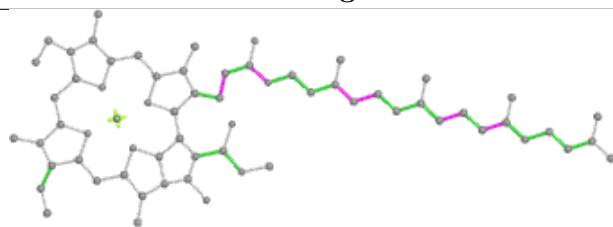
## Ligand CLA V 309



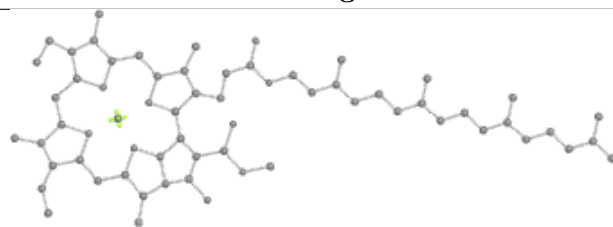
Bond lengths



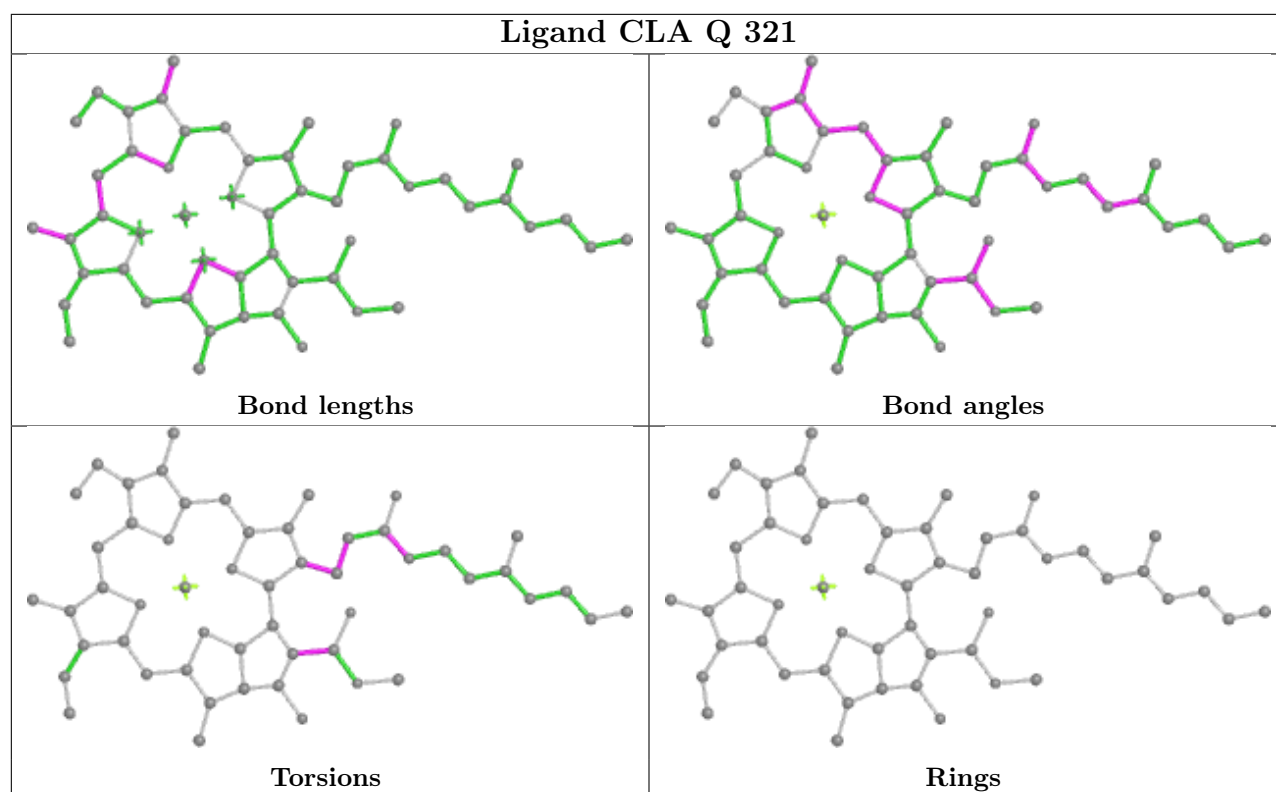
Bond angles



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.