



## wwPDB EM Validation Summary Report ⓘ

Oct 1, 2024 – 10:24 AM JST

PDB ID : 6JO5  
EMDB ID : EMD-9853  
Title : Structure of the green algal photosystem I supercomplex with light-harvesting complex I  
Authors : Suga, M.; Miyazaki, N.; Takahashi, Y.  
Deposited on : 2019-03-20  
Resolution : 2.90 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	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

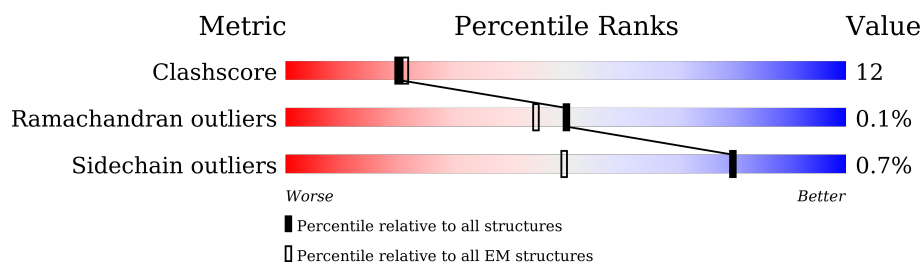
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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.






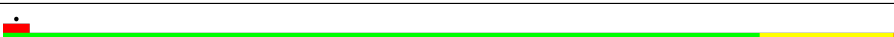
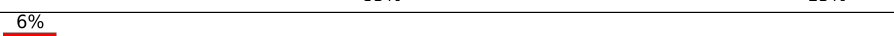
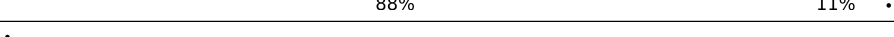





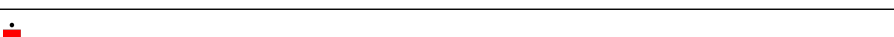
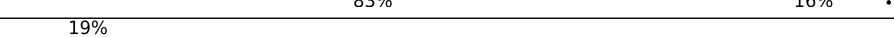
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	 83% 15% •
2	B	755	 84% 13% •
3	C	81	 85% 14% •
4	D	161	 75% 14% 11%
5	E	73	 74% 10% 16%
6	F	165	 85% 15% •
7	G	94	 60% 13% 28%
8	I	106	 31% 65% •

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Mol	Chain	Length	Quality of chain
9	J	41	
10	K	87	
11	L	156	
12	1	194	
12	Z	194	
13	3	268	
14	7	215	
15	8	217	
16	4	236	
17	5	229	
18	6	232	
19	2	221	
20	9	189	

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
21	CL0	A	801	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	606	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	609	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	1	616	X	-	-	-
22	CLA	2	601	X	-	-	-
22	CLA	2	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	606	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	609	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	611	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	3	620	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	614	X	-	-	-
22	CLA	4	616	X	-	-	-
22	CLA	5	601	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	606	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	613	X	-	-	-
22	CLA	5	616	X	-	-	-
22	CLA	5	617	X	-	-	-
22	CLA	5	621	X	-	-	-
22	CLA	6	601	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	614	X	-	-	-
22	CLA	6	616	X	-	-	-
22	CLA	6	617	X	-	-	-
22	CLA	6	622	X	-	-	-
22	CLA	7	601	X	-	-	-
22	CLA	7	602	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	606	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	610	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	614	X	-	-	-
22	CLA	7	616	X	-	-	-
22	CLA	7	620	X	-	-	-
22	CLA	8	601	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	604	X	-	-	-
22	CLA	8	606	X	-	-	-
22	CLA	8	608	X	-	-	-
22	CLA	8	609	X	-	-	-
22	CLA	8	610	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-
22	CLA	8	614	X	-	-	-
22	CLA	8	616	X	-	-	-
22	CLA	9	601	X	-	-	-
22	CLA	9	602	X	-	-	-
22	CLA	9	603	X	-	-	-
22	CLA	9	609	X	-	-	-
22	CLA	9	611	X	-	-	-
22	CLA	9	612	X	-	-	-
22	CLA	9	613	X	-	-	-
22	CLA	A	802	X	-	X	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	X	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	809	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	X	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	X	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B	852	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	J	3002	X	-	-	-
22	CLA	K	4003	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	606	X	-	-	-
22	CLA	Z	608	X	-	-	-
22	CLA	Z	609	X	-	-	-
22	CLA	Z	610	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	Z	613	X	-	-	-
22	CLA	Z	614	X	-	-	-
22	CLA	Z	616	X	-	-	-
25	BCR	4	621	-	-	X	-
29	CHL	1	601	X	-	-	-
29	CHL	1	607	X	-	-	-
29	CHL	3	608	X	-	-	-
29	CHL	4	606	X	-	-	-
29	CHL	4	607	X	-	-	-
29	CHL	4	608	X	-	-	-
29	CHL	4	618	X	-	-	-
29	CHL	5	607	X	-	-	-
29	CHL	5	608	X	-	-	-
29	CHL	5	618	X	-	-	-
29	CHL	6	606	X	-	-	-
29	CHL	6	607	X	-	-	-
29	CHL	6	608	X	-	-	-
29	CHL	6	618	X	-	-	-
29	CHL	7	607	X	-	-	-
29	CHL	8	607	X	-	-	-
29	CHL	9	606	X	-	-	-
29	CHL	9	607	X	-	-	-
29	CHL	Z	601	X	-	-	-
29	CHL	Z	607	X	-	-	-

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 48476 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	738	Total	C	N	O	S	0	0
			5800	3793	989	996	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5822	3824	978	1002	18		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	insertion	UNP P09144
B	-15	HIS	-	insertion	UNP P09144
B	-14	HIS	-	insertion	UNP P09144
B	-13	HIS	-	insertion	UNP P09144
B	-12	HIS	-	insertion	UNP P09144
B	-11	HIS	-	insertion	UNP P09144
B	-10	HIS	-	insertion	UNP P09144
B	-9	HIS	-	insertion	UNP P09144
B	-8	HIS	-	insertion	UNP P09144
B	-7	HIS	-	insertion	UNP P09144
B	-6	HIS	-	insertion	UNP P09144
B	-5	HIS	-	insertion	UNP P09144
B	-4	HIS	-	insertion	UNP P09144
B	-3	HIS	-	insertion	UNP P09144
B	-2	HIS	-	insertion	UNP P09144
B	-1	HIS	-	insertion	UNP P09144
B	0	HIS	-	insertion	UNP P09144
B	1	HIS	-	insertion	UNP P09144
B	2	HIS	-	insertion	UNP P09144
B	3	HIS	-	insertion	UNP P09144

- 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
			600	369	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1132	725	200	200	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			480	306	85	89		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	817	213	232	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	68	Total	C	N	O	0	0
			503	327	87	89		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			320	219	45	55	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	45	Total	C	N	O	S	0	0
			297	190	49	56	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			853	561	136	153	3		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
12	Z	192	Total	C	N	O	S	0	0
			1436	937	238	258	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	202	Total	C	N	O	S	0	0
			1555	1018	252	277	8		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	212	Total	C	N	O	S	0	0
			1644	1069	273	296	6		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	217	Total	C	N	O	S	0	0
			1649	1073	280	292	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	203	Total	C	N	O	S	0	0
			1570	1029	254	282	5		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	223	Total	C	N	O	S	0	0
			1744	1137	291	308	8		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	229	Total	C	N	O	S	0	0
			1765	1164	292	303	6		

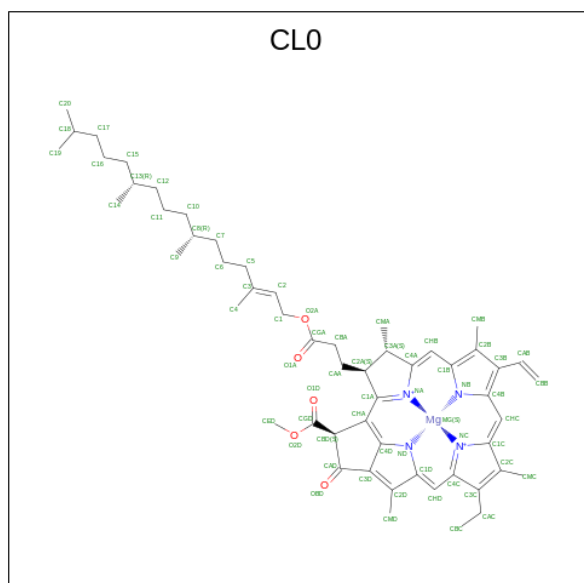
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	2	119	Total	C	N	O	S	0	0
			838	535	147	151	5		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	9	152	Total	C	N	O	S	0	0
			1180	766	195	213	6		

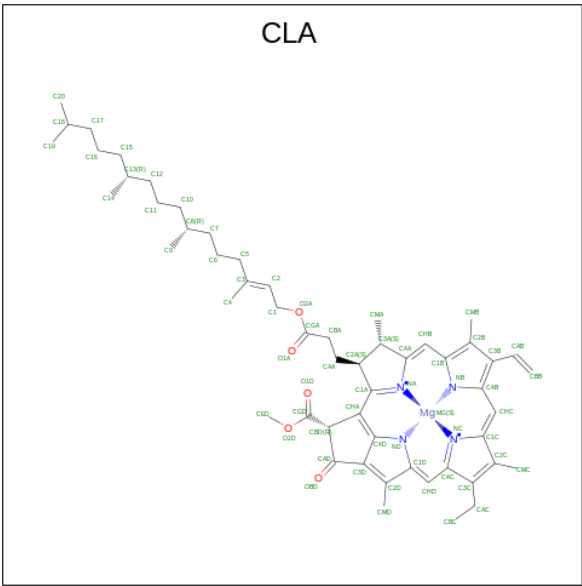
- Molecule 21 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	



- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	7	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	8	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	8	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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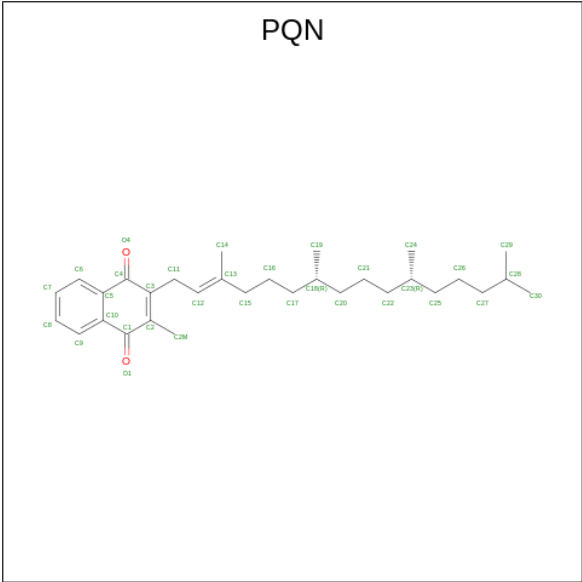
Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	6	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	2	1	Total 50	C 40	Mg 1	N 4	O 5	0

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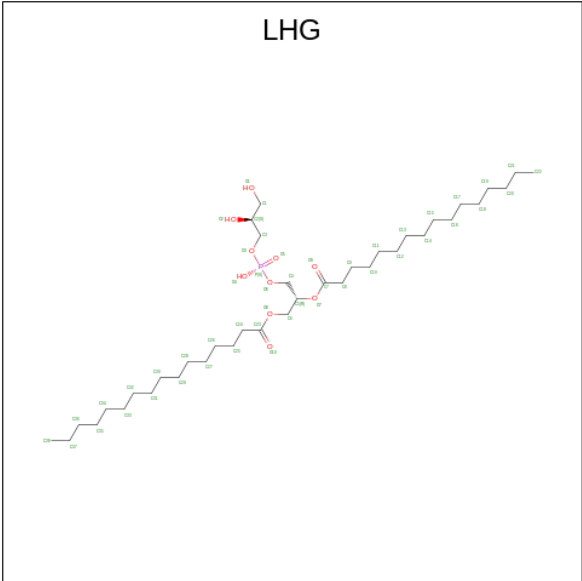
Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			33	31	2	
23	B	1	Total	C	O	0
			33	31	2	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



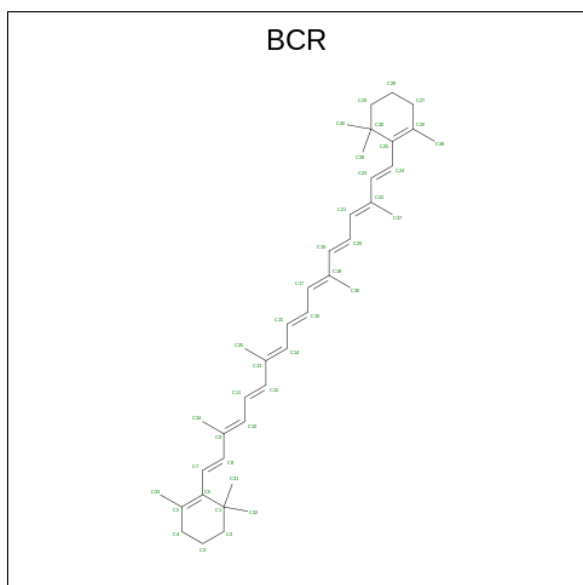
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			38	27	10	1	
24	A	1	Total	C	O	P	0
			30	19	10	1	
24	B	1	Total	C	O	P	0
			23	12	10	1	
24	1	1	Total	C	O	P	0
			43	32	10	1	
24	7	1	Total	C	O	P	0
			37	26	10	1	
24	8	1	Total	C	O	P	0
			37	26	10	1	
24	Z	1	Total	C	O	P	0
			43	32	10	1	
24	4	1	Total	C	O	P	0
			49	38	10	1	
24	4	1	Total	C	O	P	0
			32	21	10	1	
24	5	1	Total	C	O	P	0
			37	26	10	1	
24	6	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



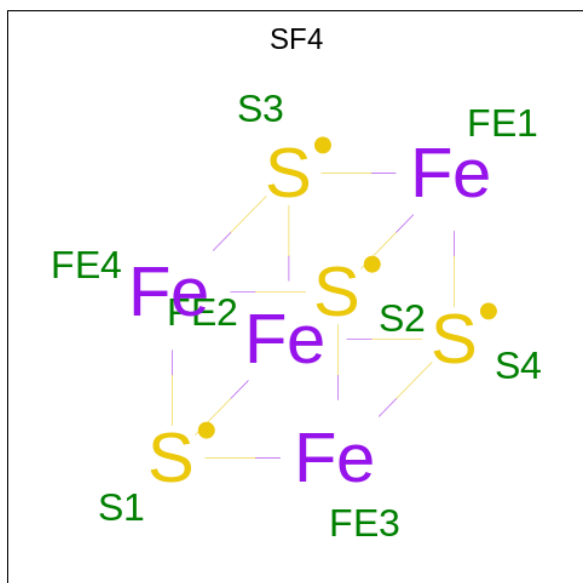
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	6	1	Total C 40 40	0

- Molecule 26 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



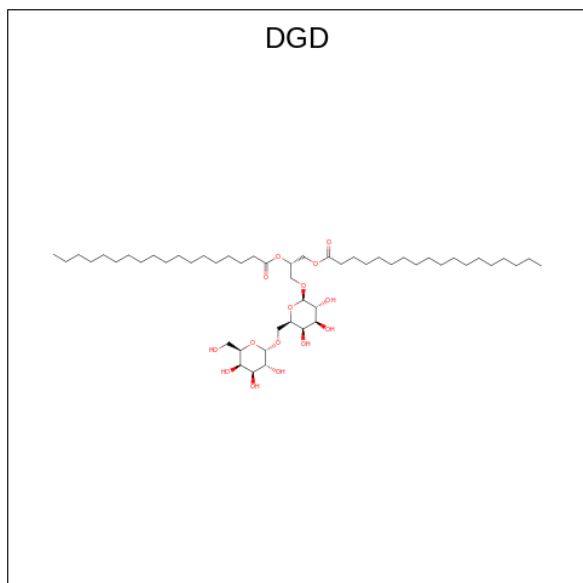
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total Fe S 8 4 4	0

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Mol	Chain	Residues	Atoms			AltConf
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

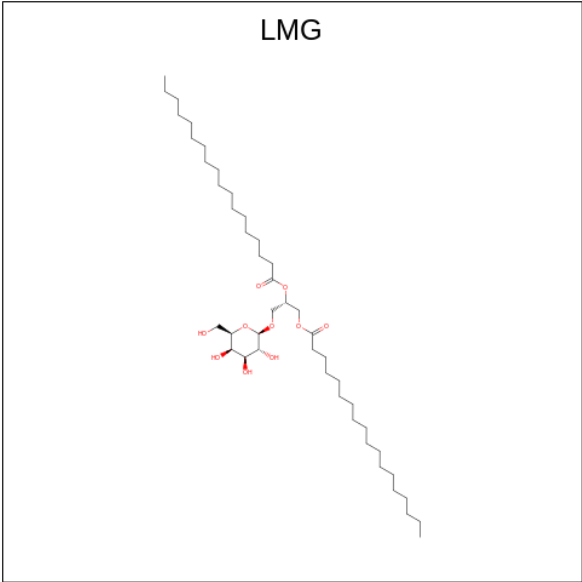
- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			66	51	15	

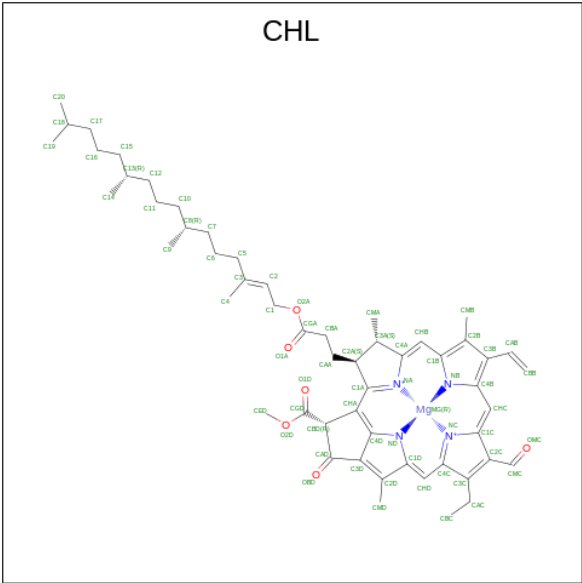
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).





Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			35	25	10	
28	9	1	Total	C	O	0
			44	34	10	

- Molecule 29 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



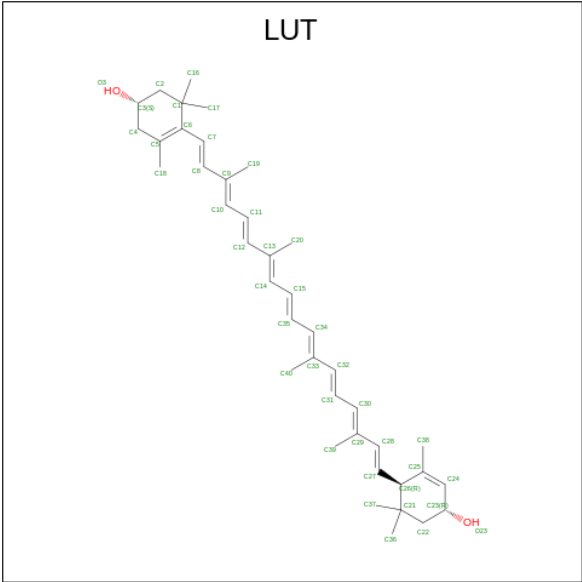
Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
29	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	Z	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	Z	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

- Molecule 30 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			42	40	2	
30	1	1	Total	C	O	0
			42	40	2	
30	1	1	Total	C	O	0
			42	40	2	
30	3	1	Total	C	O	0
			42	40	2	
30	3	1	Total	C	O	0
			42	40	2	
30	7	1	Total	C	O	0
			42	40	2	
30	7	1	Total	C	O	0
			42	40	2	
30	8	1	Total	C	O	0
			42	40	2	
30	8	1	Total	C	O	0
			42	40	2	
30	Z	1	Total	C	O	0
			42	40	2	
30	Z	1	Total	C	O	0
			42	40	2	
30	Z	1	Total	C	O	0
			42	40	2	
30	4	1	Total	C	O	0
			42	40	2	
30	4	1	Total	C	O	0
			42	40	2	

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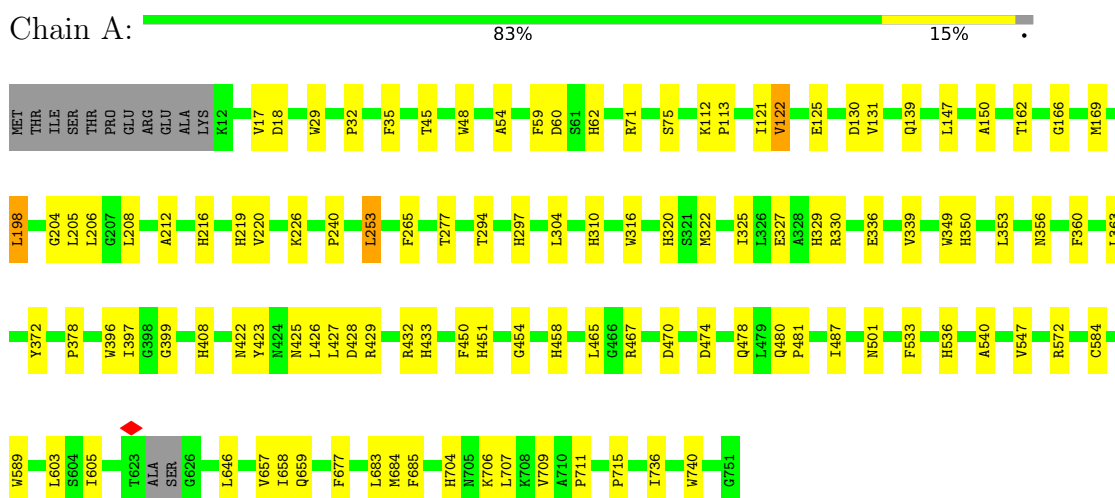
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Mol	Chain	Residues	Atoms			AltConf
30	5	1	Total	C	O	0
			42	40	2	
30	5	1	Total	C	O	0
			42	40	2	
30	6	1	Total	C	O	0
			42	40	2	
30	6	1	Total	C	O	0
			42	40	2	
30	2	1	Total	C	O	0
			42	40	2	
30	2	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	

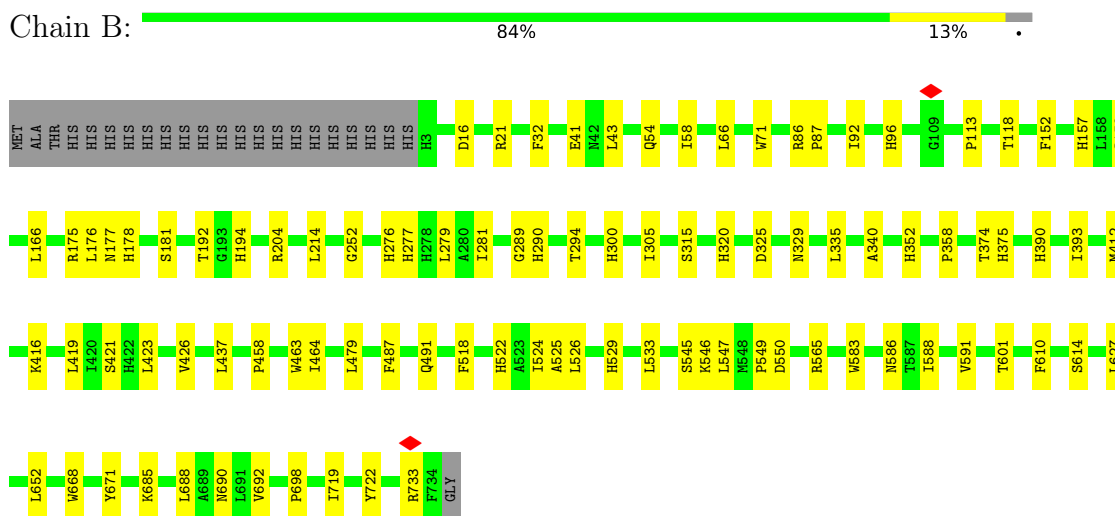
### 3 Residue-property plots [i](#)

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

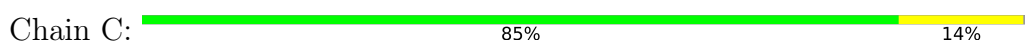
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



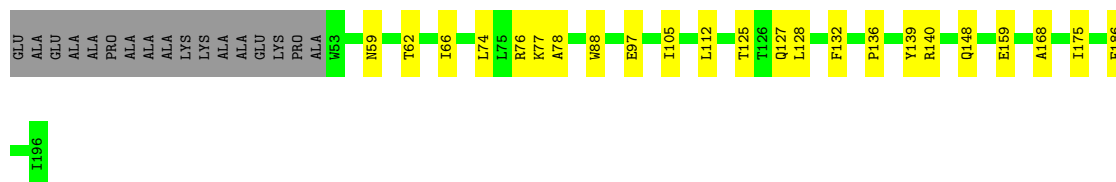
- Molecule 3: Photosystem I iron-sulfur center





- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D: 75% 14% 11%



- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E: 74% 10% 16%



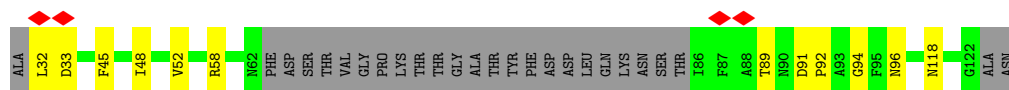
- Molecule 6: Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic

Chain F: 85% 15%



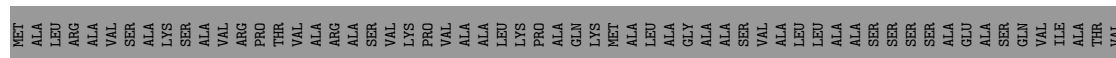
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G: 60% 13% 28%



- Molecule 8: Photosystem I reaction center subunit VIII

Chain I: 31% 65%

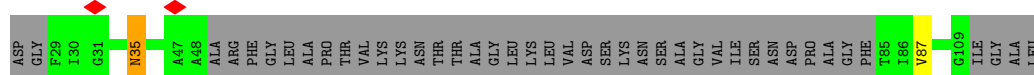


- Molecule 9: Photosystem I reaction center subunit IX

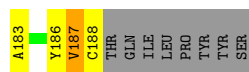
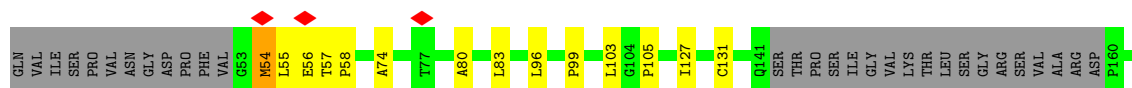
Chain J: 78% 17% 5%



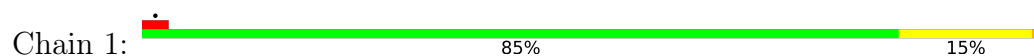
- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic



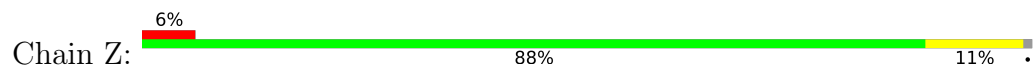
- Molecule 11: Photosystem I reaction center subunit XI



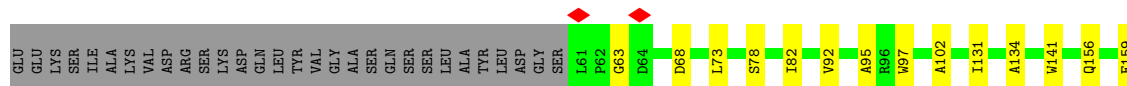
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

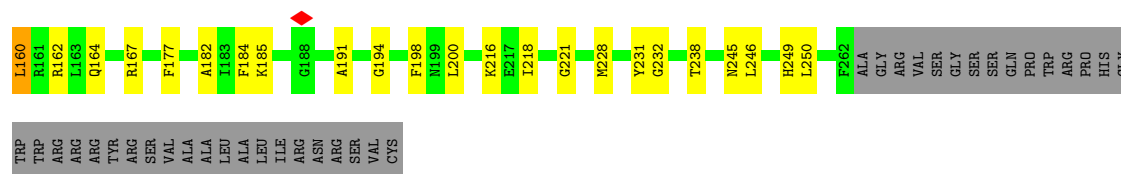


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic



- Molecule 13: Chlorophyll a-b binding protein, chloroplastic





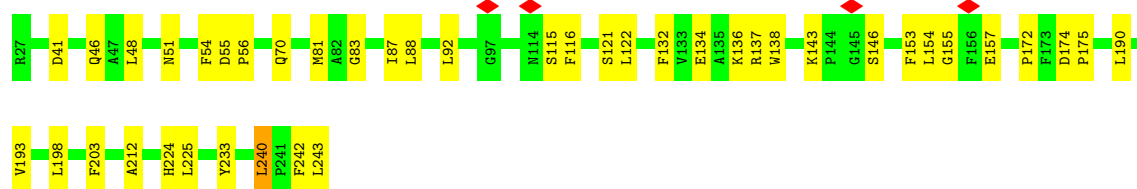
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 7: 87% 12%



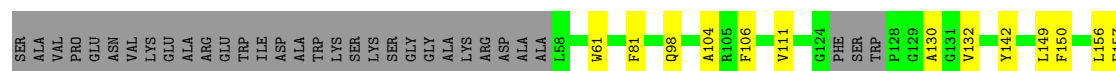
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 81% 19%



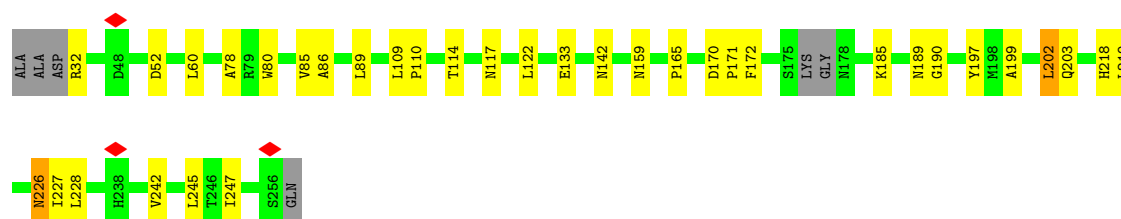
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 67% 18% 14%



- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

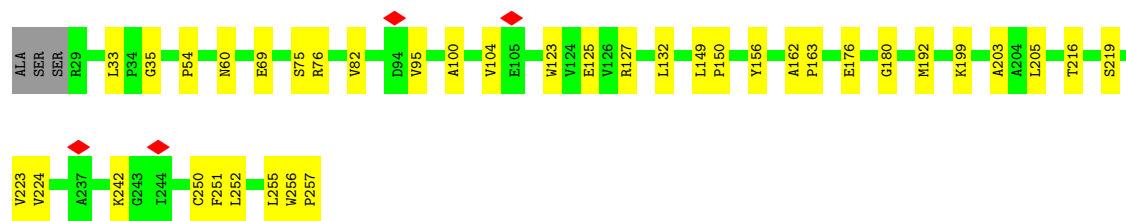
Chain 5: 82% 14%



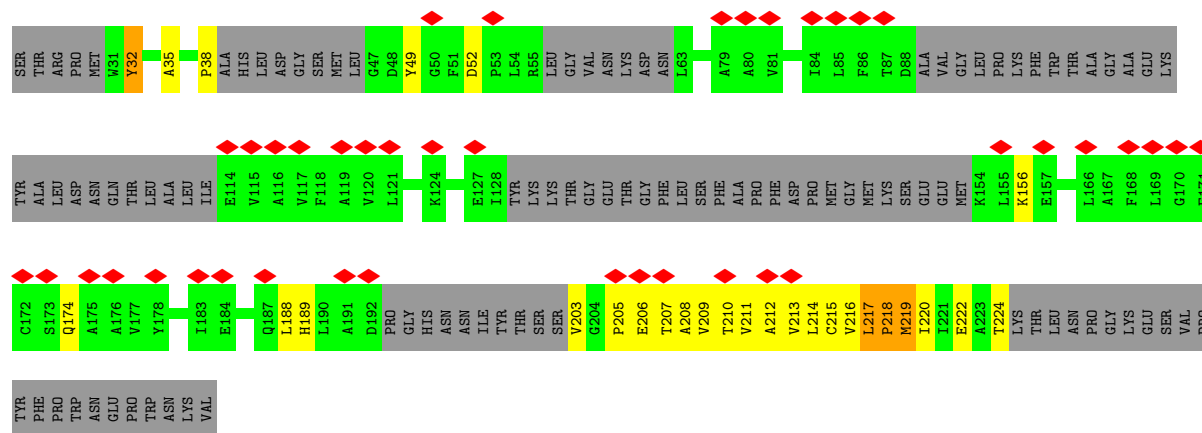
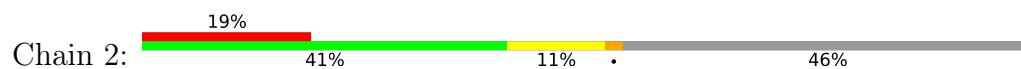
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6: 83% 16%

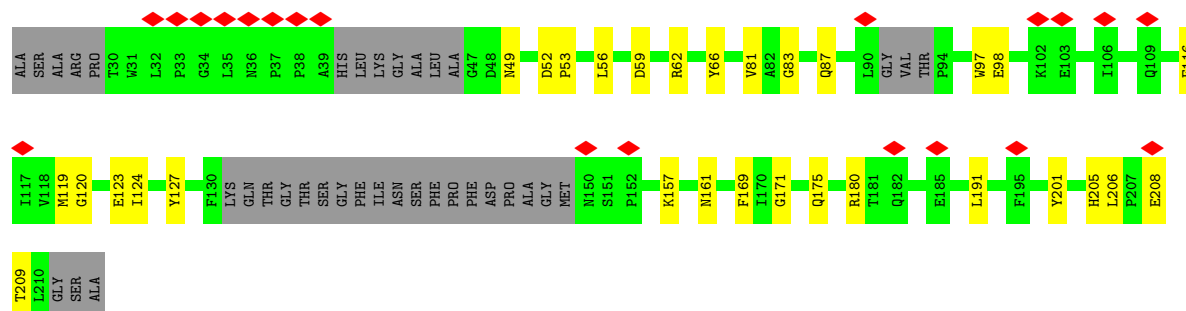




- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



- Molecule 20: Chlorophyll a-b binding protein, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	338867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.498	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	358.4, 358.4, 358.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.12, 1.12, 1.12	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, SF4, LMG, LHG, LUT, CL0, CHL, PQN, CLA, BCR

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	0.37	0/5995	0.61	4/8172 (0.0%)
2	B	0.36	0/6035	0.57	1/8240 (0.0%)
3	C	0.36	0/610	0.61	0/826
4	D	0.36	0/1160	0.55	0/1567
5	E	0.33	0/490	0.47	0/667
6	F	0.33	0/1291	0.58	0/1747
7	G	0.29	0/513	0.51	0/696
8	I	0.34	0/293	0.60	0/406
9	J	0.35	0/331	0.55	0/454
10	K	0.28	0/297	0.54	0/401
11	L	0.33	0/874	0.59	0/1194
12	1	0.31	0/1490	0.52	1/2028 (0.0%)
12	Z	0.31	0/1481	0.55	0/2015
13	3	0.36	0/1601	0.57	1/2173 (0.0%)
14	7	0.34	0/1696	0.55	0/2303
15	8	0.34	0/1700	0.67	3/2315 (0.1%)
16	4	0.33	0/1621	0.59	3/2209 (0.1%)
17	5	0.31	0/1798	0.52	0/2450
18	6	0.30	0/1827	0.54	0/2497
19	2	0.36	0/851	0.63	2/1154 (0.2%)
20	9	0.32	0/1211	0.56	0/1643
All	All	0.34	0/33165	0.58	15/45157 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
14	7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	217	LEU	C-N-CD	8.65	146.56	128.40
16	4	164	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	A	198	LEU	CA-CB-CG	7.99	133.68	115.30
15	8	137	ARG	NE-CZ-NH1	7.33	123.97	120.30
19	2	218	PRO	CA-N-CD	-6.93	101.79	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	7	150	PHE	Peptide
2	B	668	TRP	Peptide

## 5.2 Too-close contacts [i](#)

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	5800	0	5646	111	0
2	B	5822	0	5574	97	0
3	C	600	0	581	9	0
4	D	1132	0	1150	16	0
5	E	480	0	476	6	0
6	F	1265	0	1301	52	0
7	G	503	0	496	7	0
8	I	281	0	292	5	0
9	J	320	0	322	7	0
10	K	297	0	319	2	0
11	L	853	0	864	25	0
12	1	1444	0	1395	26	0
12	Z	1436	0	1388	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	3	1555	0	1522	30	0
14	7	1644	0	1582	23	0
15	8	1649	0	1628	36	0
16	4	1570	0	1526	72	0
17	5	1744	0	1715	39	0
18	6	1765	0	1767	38	0
19	2	838	0	767	65	0
20	9	1180	0	1160	35	0
21	A	65	0	72	3	0
22	1	722	0	735	34	0
22	2	540	0	426	19	0
22	3	696	0	630	26	0
22	4	576	0	490	42	0
22	5	737	0	632	34	0
22	6	696	0	620	44	0
22	7	741	0	658	32	0
22	8	680	0	592	24	0
22	9	514	0	426	19	0
22	A	2689	0	2796	204	0
22	B	2480	0	2545	122	0
22	F	175	0	177	8	0
22	G	96	0	72	0	0
22	J	42	0	31	1	0
22	K	91	0	66	2	0
22	L	115	0	111	1	0
22	Z	714	0	714	24	0
23	A	33	0	46	4	0
23	B	33	0	46	1	0
24	1	43	0	56	2	0
24	4	81	0	106	3	0
24	5	37	0	44	0	0
24	6	49	0	74	19	0
24	7	37	0	44	0	0
24	8	37	0	44	1	0
24	A	117	0	153	5	0
24	B	23	0	16	0	0
24	Z	43	0	56	1	0
25	3	120	0	163	15	0
25	4	40	0	56	39	0
25	5	80	0	112	12	0
25	6	80	0	110	11	0
25	7	80	0	112	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	8	40	0	56	6	0
25	A	240	0	336	25	0
25	B	280	0	392	29	0
25	F	40	0	56	15	0
25	G	40	0	56	3	0
25	I	40	0	56	1	0
25	J	40	0	56	2	0
25	K	80	0	112	6	0
25	L	80	0	112	9	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	66	0	96	1	0
28	9	44	0	61	1	0
28	J	35	0	40	0	0
29	1	101	0	74	4	0
29	3	66	0	70	5	0
29	4	201	0	150	25	0
29	5	145	0	101	6	0
29	6	206	0	159	11	0
29	7	54	0	43	1	0
29	8	56	0	47	0	0
29	9	93	0	64	1	0
29	Z	101	0	73	1	0
30	1	126	0	168	14	0
30	2	84	0	112	6	0
30	3	84	0	112	7	0
30	4	84	0	112	16	0
30	5	84	0	112	20	0
30	6	84	0	112	7	0
30	7	84	0	112	8	0
30	8	84	0	112	13	0
30	9	84	0	112	8	0
30	Z	126	0	168	10	0
All	All	48476	0	47944	1162	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 12.

The worst 5 of 1162 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)
16:4:257:TRP:CD1	22:4:616:CLA:CBB	1.75	1.60
19:2:32:TYR:CE2	19:2:35:ALA:HB2	1.37	1.59
22:A:802:CLA:C19	22:A:842:CLA:C4	1.79	1.53
19:2:32:TYR:CD2	19:2:35:ALA:HB2	1.41	1.50
1:A:198:LEU:HD23	1:A:322:MET:CE	1.43	1.48

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/751 (98%)	713 (97%)	20 (3%)	1 (0%)	48	77
2	B	730/755 (97%)	708 (97%)	22 (3%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	142/161 (88%)	135 (95%)	7 (5%)	0	100	100
5	E	59/73 (81%)	55 (93%)	4 (7%)	0	100	100
6	F	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
7	G	64/94 (68%)	64 (100%)	0	0	100	100
8	I	35/106 (33%)	34 (97%)	1 (3%)	0	100	100
9	J	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
10	K	41/87 (47%)	41 (100%)	0	0	100	100
11	L	114/156 (73%)	108 (95%)	5 (4%)	1 (1%)	14	43
12	1	192/194 (99%)	186 (97%)	6 (3%)	0	100	100
12	Z	188/194 (97%)	181 (96%)	7 (4%)	0	100	100
13	3	200/268 (75%)	191 (96%)	9 (4%)	0	100	100
14	7	210/215 (98%)	200 (95%)	10 (5%)	0	100	100
15	8	215/217 (99%)	206 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	4	199/236 (84%)	187 (94%)	11 (6%)	1 (0%)	25	56
17	5	219/229 (96%)	201 (92%)	18 (8%)	0	100	100
18	6	227/232 (98%)	216 (95%)	11 (5%)	0	100	100
19	2	107/221 (48%)	107 (100%)	0	0	100	100
20	9	144/189 (76%)	136 (94%)	8 (6%)	0	100	100
All	All	4098/4665 (88%)	3933 (96%)	162 (4%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	L	187	VAL
16	4	208	ILE
1	A	122	VAL

### 5.3.2 Protein sidechains ⓘ

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	599/610 (98%)	593 (99%)	6 (1%)	73	91
2	B	596/617 (97%)	595 (100%)	1 (0%)	92	98
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	121/129 (94%)	119 (98%)	2 (2%)	56	83
5	E	52/62 (84%)	52 (100%)	0	100	100
6	F	127/127 (100%)	126 (99%)	1 (1%)	79	93
7	G	48/69 (70%)	47 (98%)	1 (2%)	48	78
8	I	31/76 (41%)	31 (100%)	0	100	100
9	J	35/37 (95%)	35 (100%)	0	100	100
10	K	30/60 (50%)	29 (97%)	1 (3%)	33	68
11	L	85/119 (71%)	84 (99%)	1 (1%)	67	89
12	1	137/137 (100%)	136 (99%)	1 (1%)	81	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	137/137 (100%)	137 (100%)	0	100	100
13	3	155/209 (74%)	154 (99%)	1 (1%)	84	95
14	7	164/164 (100%)	163 (99%)	1 (1%)	84	95
15	8	163/163 (100%)	162 (99%)	1 (1%)	84	95
16	4	159/185 (86%)	158 (99%)	1 (1%)	84	95
17	5	181/184 (98%)	178 (98%)	3 (2%)	56	83
18	6	183/185 (99%)	182 (100%)	1 (0%)	86	96
19	2	70/178 (39%)	68 (97%)	2 (3%)	37	72
20	9	118/143 (82%)	118 (100%)	0	100	100
All	All	3260/3661 (89%)	3236 (99%)	24 (1%)	80	94

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	3	160	LEU
16	4	263	ARG
15	8	51	ASN
17	5	117	ASN
2	B	479	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
16	4	175	ASN
18	6	60	ASN
20	9	87	GLN
18	6	130	GLN
4	D	127	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

313 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	$\# Z  > 2$
30	LUT	8	617	-	42,43,43	0.77	0	51,60,60	1.70	13 (25%)
26	SF4	A	853	2,1	0,12,12	-	-	-		
25	BCR	B	801	-	41,41,41	0.72	0	56,56,56	1.97	14 (25%)
22	CLA	1	608	-	65,73,73	2.01	16 (24%)	76,113,113	2.71	27 (35%)
22	CLA	B	833	2	58,66,73	2.15	16 (27%)	67,104,113	2.95	28 (41%)
22	CLA	9	604	20	50,58,73	2.39	17 (34%)	58,95,113	3.07	27 (46%)
25	BCR	3	718	-	41,41,41	0.74	0	56,56,56	1.90	17 (30%)
22	CLA	7	610	14	60,68,73	2.09	14 (23%)	70,107,113	2.86	28 (40%)
22	CLA	A	823	1	49,57,73	2.33	17 (34%)	55,93,113	3.14	23 (41%)
30	LUT	Z	619	-	42,43,43	0.71	0	51,60,60	1.76	12 (23%)
22	CLA	Z	613	-	65,73,73	2.04	15 (23%)	76,113,113	2.63	27 (35%)
22	CLA	A	815	1	60,68,73	2.17	17 (28%)	70,107,113	2.88	27 (38%)
22	CLA	4	609	16	50,58,73	2.30	16 (32%)	58,95,113	3.04	28 (48%)
22	CLA	9	612	-	52,60,73	2.32	16 (30%)	60,97,113	3.00	27 (45%)
22	CLA	6	602	18	65,73,73	2.02	14 (21%)	76,113,113	2.74	26 (34%)
22	CLA	A	834	1	65,73,73	2.02	17 (26%)	76,113,113	2.79	29 (38%)
30	LUT	4	620	-	42,43,43	0.73	0	51,60,60	1.50	10 (19%)
22	CLA	2	610	19	60,68,73	2.18	16 (26%)	70,107,113	2.86	27 (38%)
22	CLA	A	808	1	65,73,73	2.02	17 (26%)	76,113,113	2.80	28 (36%)
22	CLA	A	827	-	65,73,73	2.02	15 (23%)	76,113,113	2.70	27 (35%)
22	CLA	B	829	2	65,73,73	2.05	17 (26%)	76,113,113	2.86	30 (39%)
22	CLA	5	606	-	55,63,73	2.24	17 (30%)	64,101,113	2.92	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	832	2	65,73,73	1.97	15 (23%)	76,113,113	2.76	27 (35%)
30	LUT	3	622	-	42,43,43	0.80	0	51,60,60	1.67	10 (19%)
22	CLA	5	611	24	55,63,73	2.24	17 (30%)	64,101,113	2.91	27 (42%)
22	CLA	8	612	15	52,60,73	2.26	16 (30%)	60,97,113	3.00	29 (48%)
22	CLA	9	614	20	45,53,73	2.49	16 (35%)	52,89,113	3.23	27 (51%)
22	CLA	A	805	1	55,63,73	2.22	17 (30%)	64,101,113	2.94	26 (40%)
22	CLA	B	826	2	65,73,73	1.98	15 (23%)	76,113,113	2.75	29 (38%)
22	CLA	A	813	1	54,62,73	2.22	16 (29%)	62,99,113	2.95	26 (41%)
22	CLA	4	613	16	56,64,73	2.18	15 (26%)	65,102,113	2.89	28 (43%)
25	BCR	5	622	-	41,41,41	0.66	0	56,56,56	1.87	15 (26%)
30	LUT	1	618	-	42,43,43	0.74	0	51,60,60	1.58	12 (23%)
22	CLA	9	611	-	55,63,73	2.27	16 (29%)	64,101,113	2.87	27 (42%)
22	CLA	3	617	13	46,54,73	2.41	16 (34%)	53,90,113	3.14	25 (47%)
25	BCR	B	848	-	41,41,41	0.73	0	56,56,56	1.53	10 (17%)
23	PQN	B	842	-	34,34,34	1.56	2 (5%)	42,45,45	0.94	2 (4%)
22	CLA	7	616	14	46,54,73	2.46	18 (39%)	53,90,113	3.24	24 (45%)
22	CLA	F	303	-	45,53,73	2.42	17 (37%)	52,89,113	3.21	22 (42%)
22	CLA	2	609	19	50,58,73	2.40	17 (34%)	58,95,113	3.05	29 (50%)
22	CLA	2	612	19	52,60,73	2.30	16 (30%)	60,97,113	3.01	26 (43%)
22	CLA	A	818	1	65,73,73	1.96	15 (23%)	76,113,113	2.85	26 (34%)
22	CLA	B	817	2	59,67,73	2.09	16 (27%)	68,105,113	2.83	26 (38%)
29	CHL	4	608	-	51,59,74	2.17	16 (31%)	55,96,114	3.26	24 (43%)
22	CLA	B	810	2	65,73,73	2.05	17 (26%)	76,113,113	2.74	25 (32%)
24	LHG	6	619	22	48,48,48	0.94	2 (4%)	51,54,54	0.98	2 (3%)
22	CLA	1	604	-	57,65,73	2.18	17 (29%)	66,103,113	2.82	29 (43%)
22	CLA	K	4002	-	45,53,73	2.49	17 (37%)	52,89,113	3.18	26 (50%)
22	CLA	B	804	2	45,53,73	2.40	16 (35%)	52,89,113	3.29	27 (51%)
27	DGD	B	850	-	67,67,67	0.80	2 (2%)	81,81,81	1.03	4 (4%)
24	LHG	1	620	22	42,42,48	0.99	2 (4%)	45,48,54	1.10	3 (6%)
22	CLA	5	614	17	45,53,73	2.45	16 (35%)	52,89,113	3.30	26 (50%)
24	LHG	4	623	-	31,31,48	1.14	2 (6%)	34,37,54	1.14	3 (8%)
25	BCR	6	625	-	41,41,41	0.67	0	56,56,56	2.05	16 (28%)
22	CLA	Z	604	-	57,65,73	2.18	17 (29%)	66,103,113	2.82	26 (39%)
22	CLA	5	609	17	50,58,73	2.32	17 (34%)	58,95,113	3.10	27 (46%)
24	LHG	B	851	22	22,22,48	1.15	2 (9%)	25,28,54	1.24	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	K	4004	-	41,41,41	0.70	0	56,56,56	1.74	14 (25%)
22	CLA	A	826	-	65,73,73	1.99	17 (26%)	76,113,113	2.71	26 (34%)
29	CHL	4	607	-	51,59,74	2.26	16 (31%)	55,96,114	3.33	25 (45%)
22	CLA	6	613	-	56,64,73	2.22	17 (30%)	65,102,113	2.84	27 (41%)
22	CLA	2	611	-	55,63,73	2.27	16 (29%)	64,101,113	2.88	28 (43%)
22	CLA	G	204	7	46,54,73	2.46	17 (36%)	53,90,113	3.13	24 (45%)
29	CHL	6	618	18	43,51,74	2.36	15 (34%)	45,86,114	3.52	23 (51%)
22	CLA	3	610	13	65,73,73	1.99	15 (23%)	76,113,113	2.81	31 (40%)
22	CLA	B	812	2	65,73,73	2.02	18 (27%)	76,113,113	2.72	26 (34%)
24	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
22	CLA	5	613	17	56,64,73	2.17	16 (28%)	65,102,113	2.79	24 (36%)
24	LHG	A	847	22	37,37,48	1.06	2 (5%)	40,43,54	1.26	4 (10%)
22	CLA	Z	602	12	65,73,73	2.00	18 (27%)	76,113,113	2.73	28 (36%)
22	CLA	1	614	12	65,73,73	2.05	17 (26%)	76,113,113	2.77	25 (32%)
22	CLA	6	614	18	45,53,73	2.44	16 (35%)	52,89,113	3.31	26 (50%)
22	CLA	9	603	20	46,54,73	2.42	17 (36%)	53,90,113	3.29	26 (49%)
22	CLA	3	607	13	60,68,73	2.13	18 (30%)	70,107,113	2.82	28 (40%)
22	CLA	B	823	2	60,68,73	2.11	16 (26%)	70,107,113	2.68	28 (40%)
29	CHL	6	607	-	56,64,74	2.14	18 (32%)	61,102,114	3.10	29 (47%)
22	CLA	A	820	1	65,73,73	2.01	17 (26%)	76,113,113	2.79	29 (38%)
22	CLA	B	827	2	65,73,73	2.00	17 (26%)	76,113,113	2.70	28 (36%)
22	CLA	A	836	1	50,58,73	2.33	18 (36%)	58,95,113	3.05	29 (50%)
22	CLA	6	604	-	65,73,73	2.05	18 (27%)	76,113,113	2.64	27 (35%)
22	CLA	A	807	1	65,73,73	2.03	17 (26%)	76,113,113	2.74	25 (32%)
22	CLA	L	203	11	65,73,73	1.97	18 (27%)	76,113,113	2.77	26 (34%)
22	CLA	8	602	15	62,70,73	2.02	15 (24%)	72,109,113	2.87	28 (38%)
25	BCR	A	852	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
22	CLA	B	816	2	55,63,73	2.15	15 (27%)	64,101,113	3.07	26 (40%)
22	CLA	1	602	12	65,73,73	1.99	15 (23%)	76,113,113	2.67	28 (36%)
28	LMG	J	3001	-	35,35,55	0.94	2 (5%)	43,43,63	1.23	5 (11%)
24	LHG	Z	620	22	42,42,48	0.99	2 (4%)	45,48,54	1.06	2 (4%)
22	CLA	B	802	2	65,73,73	1.92	17 (26%)	76,113,113	2.84	27 (35%)
22	CLA	6	603	18	46,54,73	2.38	16 (34%)	53,90,113	3.23	26 (49%)
22	CLA	5	602	17	65,73,73	2.00	15 (23%)	76,113,113	2.77	26 (34%)
24	LHG	5	623	22	36,36,48	1.07	2 (5%)	39,42,54	1.10	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	5	621	-	46,54,73	2.44	18 (39%)	53,90,113	2.96	25 (47%)
29	CHL	6	606	-	56,64,74	2.16	17 (30%)	61,102,114	3.15	25 (40%)
22	CLA	3	606	-	42,50,73	2.45	15 (35%)	48,85,113	3.28	23 (47%)
25	BCR	A	848	-	41,41,41	0.71	0	56,56,56	1.76	15 (26%)
24	LHG	8	620	22	36,36,48	1.02	2 (5%)	39,42,54	1.14	5 (12%)
22	CLA	6	616	18	46,54,73	2.45	17 (36%)	53,90,113	3.19	28 (52%)
22	CLA	2	613	19	50,58,73	2.39	16 (32%)	58,95,113	3.10	30 (51%)
22	CLA	B	835	-	45,53,73	2.45	17 (37%)	52,89,113	3.08	25 (48%)
22	CLA	A	841	1	65,73,73	2.01	17 (26%)	76,113,113	2.79	28 (36%)
22	CLA	Z	616	12	46,54,73	2.44	17 (36%)	53,90,113	3.09	24 (45%)
22	CLA	6	610	-	60,68,73	2.14	16 (26%)	70,107,113	2.82	30 (42%)
22	CLA	8	613	15	65,73,73	2.03	16 (24%)	76,113,113	2.60	25 (32%)
30	LUT	2	616	-	42,43,43	0.75	0	51,60,60	1.72	15 (29%)
22	CLA	7	603	14	46,54,73	2.40	17 (36%)	53,90,113	3.28	24 (45%)
22	CLA	B	803	-	65,73,73	1.93	17 (26%)	76,113,113	2.59	26 (34%)
25	BCR	K	4001	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
29	CHL	1	607	-	48,56,74	2.34	18 (37%)	51,92,114	3.13	20 (39%)
22	CLA	Z	603	12	57,65,73	2.19	16 (28%)	66,103,113	2.94	31 (46%)
22	CLA	8	610	15	60,68,73	2.10	16 (26%)	70,107,113	2.85	31 (44%)
22	CLA	A	802	-	65,73,73	2.09	17 (26%)	76,113,113	2.72	29 (38%)
25	BCR	7	624	-	41,41,41	0.67	0	56,56,56	1.75	12 (21%)
29	CHL	9	607	-	51,59,74	2.30	17 (33%)	55,96,114	3.17	24 (43%)
22	CLA	A	829	1	65,73,73	1.96	16 (24%)	76,113,113	2.73	29 (38%)
22	CLA	7	611	24	41,49,73	2.50	19 (46%)	47,84,113	3.41	26 (55%)
22	CLA	8	608	-	50,58,73	2.25	16 (32%)	58,95,113	3.14	25 (43%)
29	CHL	9	606	-	42,50,74	2.38	16 (38%)	44,85,114	3.67	23 (52%)
22	CLA	J	3002	9	42,50,73	2.46	15 (35%)	48,85,113	3.32	24 (50%)
22	CLA	A	811	1	65,73,73	2.00	15 (23%)	76,113,113	2.73	28 (36%)
22	CLA	6	612	18	52,60,73	2.26	17 (32%)	60,97,113	3.00	25 (41%)
22	CLA	B	838	2	47,55,73	2.35	17 (36%)	54,91,113	3.15	24 (44%)
25	BCR	3	719	-	41,41,41	0.69	0	56,56,56	1.64	13 (23%)
22	CLA	B	839	-	65,73,73	2.05	18 (27%)	76,113,113	2.66	26 (34%)
22	CLA	A	803	-	65,73,73	2.02	17 (26%)	76,113,113	2.88	29 (38%)
25	BCR	G	205	-	41,41,41	0.72	0	56,56,56	1.50	7 (12%)
26	SF4	C	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	822	-	65,73,73	1.99	16 (24%)	76,113,113	2.57	26 (34%)
22	CLA	B	825	-	65,73,73	2.01	16 (24%)	76,113,113	2.65	28 (36%)
22	CLA	A	812	1	65,73,73	1.99	18 (27%)	76,113,113	2.85	25 (32%)
22	CLA	2	606	-	41,49,73	2.58	16 (39%)	47,84,113	3.36	26 (55%)
22	CLA	A	825	1	55,63,73	2.18	15 (27%)	64,101,113	2.90	26 (40%)
22	CLA	3	611	-	41,49,73	2.55	16 (39%)	47,84,113	3.30	25 (53%)
22	CLA	A	819	1	65,73,73	2.02	16 (24%)	76,113,113	2.70	27 (35%)
22	CLA	A	828	1	65,73,73	1.98	17 (26%)	76,113,113	2.83	23 (30%)
22	CLA	B	807	2	65,73,73	2.04	16 (24%)	76,113,113	2.74	27 (35%)
25	BCR	4	621	-	41,41,41	0.70	0	56,56,56	2.00	18 (32%)
22	CLA	B	830	2	50,58,73	2.28	16 (32%)	58,95,113	3.14	27 (46%)
22	CLA	7	614	14	43,51,73	2.43	16 (37%)	49,86,113	3.35	26 (53%)
22	CLA	3	602	13	60,68,73	2.15	18 (30%)	70,107,113	2.87	31 (44%)
30	LUT	2	617	-	42,43,43	0.72	0	51,60,60	1.79	12 (23%)
22	CLA	9	609	-	50,58,73	2.32	16 (32%)	58,95,113	3.06	27 (46%)
29	CHL	4	618	16	43,51,74	2.38	17 (39%)	45,86,114	3.57	22 (48%)
22	CLA	8	614	15	55,63,73	2.23	17 (30%)	64,101,113	2.86	29 (45%)
29	CHL	1	601	12	53,61,74	2.20	18 (33%)	57,98,114	3.36	27 (47%)
22	CLA	4	602	16	60,68,73	2.11	17 (28%)	70,107,113	2.79	27 (38%)
25	BCR	J	3003	-	41,41,41	0.74	0	56,56,56	1.74	13 (23%)
25	BCR	L	205	-	41,41,41	0.71	0	56,56,56	1.60	12 (21%)
22	CLA	B	813	2	65,73,73	2.00	16 (24%)	76,113,113	2.73	30 (39%)
29	CHL	5	608	-	51,59,74	2.20	16 (31%)	55,96,114	3.17	25 (45%)
22	CLA	7	606	-	42,50,73	2.41	15 (35%)	48,85,113	3.48	24 (50%)
22	CLA	B	837	2	65,73,73	1.97	16 (24%)	76,113,113	2.83	28 (36%)
25	BCR	A	849	-	41,41,41	0.78	0	56,56,56	1.80	17 (30%)
29	CHL	5	607	-	51,59,74	2.25	17 (33%)	55,96,114	3.29	25 (45%)
22	CLA	2	607	-	50,58,73	2.39	16 (32%)	58,95,113	3.07	27 (46%)
22	CLA	9	601	20	46,54,73	2.47	16 (34%)	53,90,113	3.14	24 (45%)
22	CLA	6	609	18	50,58,73	2.33	17 (34%)	58,95,113	3.04	26 (44%)
22	CLA	8	601	15	65,73,73	2.03	18 (27%)	76,113,113	2.69	28 (36%)
22	CLA	7	613	14	65,73,73	1.99	16 (24%)	76,113,113	2.65	23 (30%)
22	CLA	Z	609	12	65,73,73	2.07	16 (24%)	76,113,113	2.67	27 (35%)
25	BCR	3	717	-	41,41,41	0.75	0	56,56,56	1.87	16 (28%)
29	CHL	Z	607	-	48,56,74	2.34	18 (37%)	51,92,114	3.20	23 (45%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	3	620	-	56,64,73	2.19	17 (30%)	65,102,113	2.88	26 (40%)
22	CLA	Z	606	-	52,60,73	2.31	18 (34%)	60,97,113	3.05	28 (46%)
22	CLA	1	606	-	52,60,73	2.28	17 (32%)	60,97,113	2.99	27 (45%)
22	CLA	7	620	-	60,68,73	2.15	16 (26%)	70,107,113	2.79	28 (40%)
22	CLA	B	822	2	59,67,73	2.12	17 (28%)	68,105,113	2.86	28 (41%)
22	CLA	B	821	2	46,54,73	2.41	17 (36%)	53,90,113	3.14	23 (43%)
30	LUT	6	624	-	42,43,43	0.72	0	51,60,60	1.44	8 (15%)
25	BCR	B	843	-	41,41,41	0.72	0	56,56,56	1.56	8 (14%)
22	CLA	7	601	14	65,73,73	2.02	17 (26%)	76,113,113	2.77	26 (34%)
25	BCR	B	844	-	41,41,41	0.71	0	56,56,56	1.75	11 (19%)
22	CLA	6	601	18	65,73,73	2.02	16 (24%)	76,113,113	2.75	27 (35%)
22	CLA	B	808	2	65,73,73	2.02	17 (26%)	76,113,113	2.72	27 (35%)
22	CLA	7	602	14	65,73,73	2.02	16 (24%)	76,113,113	2.80	28 (36%)
22	CLA	A	840	1	65,73,73	1.98	18 (27%)	76,113,113	2.83	27 (35%)
22	CLA	A	832	1	50,58,73	2.27	16 (32%)	58,95,113	3.00	27 (46%)
22	CLA	4	604	-	50,58,73	2.34	16 (32%)	58,95,113	3.03	27 (46%)
29	CHL	5	618	17	43,51,74	2.40	17 (39%)	45,86,114	3.62	22 (48%)
22	CLA	Z	611	24	65,73,73	2.07	17 (26%)	76,113,113	2.65	26 (34%)
22	CLA	B	815	2	57,65,73	2.14	15 (26%)	66,103,113	2.92	27 (40%)
22	CLA	A	806	1	65,73,73	2.01	15 (23%)	76,113,113	2.72	25 (32%)
22	CLA	B	818	2	60,68,73	2.09	16 (26%)	70,107,113	2.79	32 (45%)
22	CLA	B	834	2	65,73,73	2.07	15 (23%)	76,113,113	2.72	30 (39%)
22	CLA	7	609	14	50,58,73	2.32	16 (32%)	58,95,113	3.11	27 (46%)
22	CLA	4	612	16	52,60,73	2.25	18 (34%)	60,97,113	3.10	27 (45%)
26	SF4	C	102	3	0,12,12	-	-	-	-	-
25	BCR	5	625	-	41,41,41	0.71	0	56,56,56	2.25	15 (26%)
22	CLA	A	831	1	65,73,73	1.99	16 (24%)	76,113,113	2.77	29 (38%)
22	CLA	1	603	12	65,73,73	2.01	16 (24%)	76,113,113	2.76	27 (35%)
22	CLA	1	609	12	65,73,73	2.05	17 (26%)	76,113,113	2.73	26 (34%)
29	CHL	Z	601	12	53,61,74	2.26	17 (32%)	57,98,114	3.26	22 (38%)
22	CLA	A	845	24	52,60,73	2.29	16 (30%)	60,97,113	3.07	23 (38%)
22	CLA	8	616	15	46,54,73	2.41	17 (36%)	53,90,113	3.01	24 (45%)
22	CLA	3	603	13	65,73,73	1.98	17 (26%)	76,113,113	2.69	26 (34%)
22	CLA	1	616	12	46,54,73	2.42	17 (36%)	53,90,113	3.01	25 (47%)
22	CLA	3	614	13	45,53,73	2.49	16 (35%)	52,89,113	3.25	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	817	-	57,65,73	2.15	17 (29%)	66,103,113	2.94	26 (39%)
29	CHL	6	608	-	51,59,74	2.21	17 (33%)	55,96,114	3.41	26 (47%)
22	CLA	8	603	15	45,53,73	2.41	18 (40%)	52,89,113	3.21	24 (46%)
22	CLA	5	604	17	50,58,73	2.33	15 (30%)	58,95,113	2.98	27 (46%)
22	CLA	6	617	18	46,54,73	2.41	17 (36%)	53,90,113	3.13	25 (47%)
22	CLA	8	609	15	46,54,73	2.42	16 (34%)	53,90,113	3.04	26 (49%)
25	BCR	A	856	-	41,41,41	0.74	0	56,56,56	1.77	13 (23%)
22	CLA	B	820	2	56,64,73	2.24	16 (28%)	65,102,113	2.92	27 (41%)
30	LUT	1	617	-	42,43,43	0.75	0	51,60,60	1.69	13 (25%)
22	CLA	4	614	16	45,53,73	2.44	17 (37%)	52,89,113	3.14	25 (48%)
22	CLA	5	612	17	52,60,73	2.26	17 (32%)	60,97,113	3.02	27 (45%)
22	CLA	6	611	24	55,63,73	2.24	18 (32%)	64,101,113	2.82	26 (40%)
22	CLA	B	811	2	54,62,73	2.14	16 (29%)	67,100,113	3.03	32 (47%)
22	CLA	7	604	-	56,64,73	2.16	17 (30%)	65,102,113	3.03	26 (40%)
22	CLA	K	4003	10	46,54,73	2.43	15 (32%)	53,90,113	3.16	23 (43%)
25	BCR	A	851	-	41,41,41	0.81	2 (4%)	56,56,56	1.83	12 (21%)
25	BCR	7	623	-	41,41,41	0.78	1 (2%)	56,56,56	1.93	15 (26%)
22	CLA	B	841	24	65,73,73	2.09	17 (26%)	76,113,113	2.78	28 (36%)
25	BCR	B	846	-	41,41,41	0.76	0	56,56,56	2.01	15 (26%)
22	CLA	4	616	16	41,49,73	2.56	15 (36%)	47,84,113	3.46	25 (53%)
21	CL0	A	801	1	65,73,73	1.93	15 (23%)	76,113,113	2.81	30 (39%)
22	CLA	A	830	1	65,73,73	1.95	16 (24%)	76,113,113	2.63	26 (34%)
25	BCR	8	619	-	41,41,41	0.71	0	56,56,56	1.83	15 (26%)
22	CLA	4	601	16	61,69,73	2.08	16 (26%)	71,108,113	2.80	27 (38%)
22	CLA	B	819	-	65,73,73	2.02	16 (24%)	76,113,113	2.58	27 (35%)
22	CLA	A	816	1	65,73,73	2.08	17 (26%)	76,113,113	2.68	26 (34%)
30	LUT	1	619	-	42,43,43	0.76	0	51,60,60	1.83	14 (27%)
22	CLA	8	604	-	46,54,73	2.39	17 (36%)	53,90,113	3.10	24 (45%)
30	LUT	3	621	-	42,43,43	0.77	0	51,60,60	1.52	13 (25%)
29	CHL	3	608	-	66,74,74	1.89	16 (24%)	73,114,114	2.86	24 (32%)
30	LUT	8	618	-	42,43,43	0.79	0	51,60,60	1.56	11 (21%)
22	CLA	2	614	-	45,53,73	2.51	16 (35%)	52,89,113	3.21	24 (46%)
22	CLA	1	610	12	60,68,73	2.10	15 (25%)	70,107,113	2.90	31 (44%)
22	CLA	5	617	17	46,54,73	2.36	17 (36%)	53,90,113	4.43	25 (47%)
30	LUT	4	619	-	42,43,43	0.71	0	51,60,60	1.67	11 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	809	1	65,73,73	2.02	17 (26%)	76,113,113	2.80	29 (38%)
29	CHL	4	606	-	56,64,74	2.12	17 (30%)	61,102,114	3.05	24 (39%)
22	CLA	3	604	-	65,73,73	2.01	15 (23%)	76,113,113	2.67	25 (32%)
30	LUT	9	617	-	42,43,43	0.75	0	51,60,60	1.60	13 (25%)
22	CLA	L	204	-	50,58,73	2.36	16 (32%)	58,95,113	3.08	25 (43%)
22	CLA	B	831	2	49,57,73	2.29	15 (30%)	55,93,113	3.11	22 (40%)
22	CLA	G	203	7	50,58,73	2.33	17 (34%)	58,95,113	3.19	28 (48%)
22	CLA	2	601	19	46,54,73	2.45	16 (34%)	53,90,113	3.14	25 (47%)
22	CLA	A	842	1	65,73,73	1.99	16 (24%)	76,113,113	2.80	27 (35%)
22	CLA	3	609	13	50,58,73	2.32	17 (34%)	58,95,113	3.03	26 (44%)
22	CLA	A	835	1	65,73,73	2.09	17 (26%)	76,113,113	2.75	26 (34%)
22	CLA	B	824	-	65,73,73	1.99	16 (24%)	76,113,113	2.65	28 (36%)
28	LMG	9	620	-	44,44,55	0.85	2 (4%)	52,52,63	1.23	2 (3%)
22	CLA	A	854	-	65,73,73	2.02	15 (23%)	76,113,113	2.81	28 (36%)
30	LUT	Z	618	-	42,43,43	0.71	0	51,60,60	1.58	12 (23%)
22	CLA	1	612	12	52,60,73	2.26	16 (30%)	60,97,113	2.99	28 (46%)
22	CLA	F	301	-	65,73,73	2.02	16 (24%)	76,113,113	2.78	29 (38%)
22	CLA	B	828	2	65,73,73	2.01	16 (24%)	76,113,113	2.58	27 (35%)
22	CLA	5	616	17	46,54,73	2.40	18 (39%)	53,90,113	3.07	26 (49%)
22	CLA	B	814	2	60,68,73	2.09	16 (26%)	70,107,113	2.76	29 (41%)
23	PQN	A	844	-	34,34,34	1.52	2 (5%)	42,45,45	1.04	2 (4%)
22	CLA	5	601	17	65,73,73	2.06	17 (26%)	76,113,113	2.72	29 (38%)
22	CLA	6	622	18	45,53,73	2.42	17 (37%)	52,89,113	3.20	25 (48%)
30	LUT	7	621	-	42,43,43	0.73	0	51,60,60	1.53	10 (19%)
30	LUT	Z	617	-	42,43,43	0.77	0	51,60,60	1.69	15 (29%)
22	CLA	3	613	13	55,63,73	2.18	17 (30%)	64,101,113	2.77	24 (37%)
22	CLA	4	610	16	60,68,73	2.11	16 (26%)	70,107,113	2.81	30 (42%)
22	CLA	5	603	17	46,54,73	2.38	17 (36%)	53,90,113	3.18	26 (49%)
22	CLA	2	602	19	45,53,73	2.49	16 (35%)	52,89,113	3.19	24 (46%)
22	CLA	1	611	24	65,73,73	2.06	17 (26%)	76,113,113	2.65	25 (32%)
22	CLA	Z	608	-	65,73,73	2.04	17 (26%)	76,113,113	2.69	26 (34%)
22	CLA	9	602	20	60,68,73	2.12	15 (25%)	70,107,113	2.83	28 (40%)
22	CLA	B	805	2	65,73,73	1.99	16 (24%)	76,113,113	2.79	26 (34%)
22	CLA	A	821	1	45,53,73	2.41	16 (35%)	52,89,113	3.12	25 (48%)
25	BCR	B	845	-	41,41,41	0.73	0	56,56,56	1.84	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	836	2	60,68,73	2.13	17 (28%)	70,107,113	2.89	29 (41%)
22	CLA	8	611	24	46,54,73	2.42	17 (36%)	53,90,113	3.13	26 (49%)
29	CHL	7	607	-	54,62,74	2.20	17 (31%)	58,99,114	3.03	23 (39%)
24	LHG	7	625	22	36,36,48	1.02	2 (5%)	39,42,54	1.13	3 (7%)
22	CLA	Z	614	12	65,73,73	2.07	16 (24%)	76,113,113	2.71	28 (36%)
25	BCR	F	305	-	41,41,41	0.69	0	56,56,56	1.88	13 (23%)
22	CLA	B	806	2	65,73,73	2.01	15 (23%)	76,113,113	2.73	29 (38%)
30	LUT	5	624	-	42,43,43	0.77	0	51,60,60	1.54	11 (21%)
22	CLA	A	843	-	65,73,73	2.01	18 (27%)	76,113,113	2.61	27 (35%)
22	CLA	A	838	1	51,59,73	2.28	16 (31%)	59,96,113	3.13	30 (50%)
22	CLA	A	839	1	65,73,73	2.00	16 (24%)	76,113,113	2.77	27 (35%)
22	CLA	Z	610	12	60,68,73	2.09	15 (25%)	70,107,113	2.92	28 (40%)
22	CLA	3	612	13	46,54,73	2.39	17 (36%)	53,90,113	3.26	24 (45%)
25	BCR	6	623	-	41,41,41	0.65	0	56,56,56	1.98	18 (32%)
24	LHG	4	622	22	48,48,48	0.96	2 (4%)	51,54,54	1.09	3 (5%)
30	LUT	5	620	-	42,43,43	0.78	0	51,60,60	1.72	14 (27%)
29	CHL	8	607	-	56,64,74	2.12	17 (30%)	61,102,114	3.10	24 (39%)
22	CLA	F	304	6	65,73,73	2.06	18 (27%)	76,113,113	2.72	25 (32%)
22	CLA	A	810	1	65,73,73	1.98	17 (26%)	76,113,113	2.74	30 (39%)
22	CLA	B	840	2	65,73,73	2.06	16 (24%)	76,113,113	2.82	25 (32%)
22	CLA	A	833	1	65,73,73	2.05	16 (24%)	76,113,113	2.67	27 (35%)
25	BCR	A	850	-	41,41,41	0.70	0	56,56,56	1.90	12 (21%)
25	BCR	I	172	-	41,41,41	0.67	0	56,56,56	1.97	15 (26%)
22	CLA	2	603	19	46,54,73	2.43	16 (34%)	53,90,113	3.24	25 (47%)
22	CLA	Z	612	12	52,60,73	2.27	17 (32%)	60,97,113	3.07	26 (43%)
22	CLA	4	611	24	55,63,73	2.25	18 (32%)	64,101,113	2.83	28 (43%)
22	CLA	A	804	1	65,73,73	1.96	16 (24%)	76,113,113	2.81	30 (39%)
22	CLA	B	809	2	65,73,73	1.97	14 (21%)	76,113,113	2.67	28 (36%)
25	BCR	B	847	-	41,41,41	0.76	0	56,56,56	1.71	14 (25%)
22	CLA	A	814	1	65,73,73	2.00	17 (26%)	76,113,113	2.78	26 (34%)
22	CLA	5	610	17	60,68,73	2.11	16 (26%)	70,107,113	2.85	30 (42%)
22	CLA	B	852	-	65,73,73	2.07	17 (26%)	76,113,113	2.60	27 (35%)
30	LUT	6	621	-	42,43,43	0.73	0	51,60,60	1.62	11 (21%)
22	CLA	7	612	14	52,60,73	2.25	16 (30%)	60,97,113	3.06	26 (43%)
22	CLA	9	613	-	50,58,73	2.35	17 (34%)	58,95,113	3.00	27 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	7	608	-	50,58,73	2.28	16 (32%)	58,95,113	3.12	25 (43%)
22	CLA	8	606	-	42,50,73	2.46	17 (40%)	48,85,113	3.25	22 (45%)
22	CLA	9	610	20	60,68,73	2.15	16 (26%)	70,107,113	2.84	27 (38%)
22	CLA	1	613	-	65,73,73	2.00	17 (26%)	76,113,113	2.61	25 (32%)
30	LUT	9	616	-	42,43,43	0.73	0	51,60,60	1.52	11 (21%)
25	BCR	L	201	-	41,41,41	0.72	0	56,56,56	1.73	12 (21%)
22	CLA	A	837	1	45,53,73	2.49	17 (37%)	52,89,113	3.08	26 (50%)
22	CLA	4	603	16	46,54,73	2.38	16 (34%)	53,90,113	3.18	25 (47%)
22	CLA	A	824	1	51,59,73	2.27	18 (35%)	59,96,113	3.07	25 (42%)
30	LUT	7	622	-	42,43,43	0.75	0	51,60,60	1.49	10 (19%)
24	LHG	A	855	-	29,29,48	1.20	2 (6%)	32,35,54	1.17	3 (9%)

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
30	LUT	8	617	-	-	2/29/67/67	0/2/2/2
26	SF4	A	853	2,1	-	-	0/6/5/5
25	BCR	B	801	-	-	9/29/63/63	0/2/2/2
22	CLA	1	608	-	1/1/15/20	11/37/115/115	-
22	CLA	B	833	2	1/1/13/20	8/29/107/115	-
22	CLA	9	604	20	-	6/19/97/115	-
25	BCR	3	718	-	-	4/29/63/63	0/2/2/2
22	CLA	7	610	14	1/1/14/20	6/31/109/115	-
22	CLA	A	823	1	-	10/18/96/115	-
30	LUT	Z	619	-	-	4/29/67/67	0/2/2/2
22	CLA	Z	613	-	1/1/15/20	11/37/115/115	-
22	CLA	A	815	1	1/1/14/20	11/31/109/115	-
22	CLA	4	609	16	1/1/12/20	7/19/97/115	-
22	CLA	9	612	-	1/1/12/20	4/22/100/115	-
22	CLA	6	602	18	1/1/15/20	13/37/115/115	-
22	CLA	A	834	1	1/1/15/20	10/37/115/115	-
30	LUT	4	620	-	-	3/29/67/67	0/2/2/2
22	CLA	2	610	19	-	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	808	1	1/1/15/20	10/37/115/115	-
22	CLA	A	827	-	1/1/15/20	6/37/115/115	-
22	CLA	B	829	2	1/1/15/20	9/37/115/115	-
22	CLA	5	606	-	1/1/13/20	5/25/103/115	-
22	CLA	B	832	2	1/1/15/20	9/37/115/115	-
30	LUT	3	622	-	-	2/29/67/67	0/2/2/2
22	CLA	5	611	24	1/1/13/20	7/25/103/115	-
22	CLA	8	612	15	1/1/12/20	6/22/100/115	-
22	CLA	9	614	20	-	4/13/91/115	-
22	CLA	A	805	1	1/1/13/20	8/25/103/115	-
22	CLA	B	826	2	1/1/15/20	9/37/115/115	-
22	CLA	A	813	1	1/1/12/20	7/24/102/115	-
22	CLA	4	613	16	-	10/27/105/115	-
25	BCR	5	622	-	-	7/29/63/63	0/2/2/2
30	LUT	1	618	-	-	3/29/67/67	0/2/2/2
22	CLA	9	611	-	1/1/13/20	10/25/103/115	-
22	CLA	3	617	13	1/1/11/20	3/15/93/115	-
25	BCR	B	848	-	-	3/29/63/63	0/2/2/2
23	PQN	B	842	-	-	4/23/43/43	0/2/2/2
22	CLA	7	616	14	1/1/11/20	5/15/93/115	-
22	CLA	F	303	-	1/1/11/20	4/13/91/115	-
22	CLA	2	609	19	1/1/12/20	4/19/97/115	-
22	CLA	2	612	19	1/1/12/20	5/22/100/115	-
22	CLA	A	818	1	-	14/37/115/115	-
22	CLA	B	817	2	1/1/13/20	12/30/108/115	-
29	CHL	4	608	-	3/3/17/26	6/21/119/137	-
22	CLA	B	810	2	1/1/15/20	11/37/115/115	-
24	LHG	6	619	22	-	11/53/53/53	-
22	CLA	1	604	-	1/1/13/20	8/28/106/115	-
22	CLA	K	4002	-	-	6/13/91/115	-
22	CLA	B	804	2	1/1/11/20	4/13/91/115	-
27	DGD	B	850	-	-	17/55/95/95	0/2/2/2
24	LHG	1	620	22	-	14/47/47/53	-
22	CLA	5	614	17	-	1/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	4	623	-	-	9/36/36/53	-
25	BCR	6	625	-	-	9/29/63/63	0/2/2/2
22	CLA	Z	604	-	1/1/13/20	9/28/106/115	-
22	CLA	5	609	17	1/1/12/20	4/19/97/115	-
24	LHG	B	851	22	-	12/26/26/53	-
25	BCR	K	4004	-	-	5/29/63/63	0/2/2/2
22	CLA	A	826	-	1/1/15/20	16/37/115/115	-
29	CHL	4	607	-	3/3/17/26	7/21/119/137	-
22	CLA	6	613	-	1/1/13/20	4/27/105/115	-
22	CLA	2	611	-	-	7/25/103/115	-
22	CLA	G	204	7	1/1/11/20	5/15/93/115	-
29	CHL	6	618	18	3/3/15/26	6/12/110/137	-
22	CLA	3	610	13	1/1/15/20	14/37/115/115	-
22	CLA	B	812	2	1/1/15/20	14/37/115/115	-
24	LHG	A	846	-	-	16/53/53/53	-
22	CLA	5	613	17	1/1/13/20	8/27/105/115	-
24	LHG	A	847	22	-	14/42/42/53	-
22	CLA	Z	602	12	-	10/37/115/115	-
22	CLA	1	614	12	1/1/15/20	13/37/115/115	-
22	CLA	6	614	18	1/1/11/20	4/13/91/115	-
22	CLA	9	603	20	1/1/11/20	1/15/93/115	-
22	CLA	3	607	13	1/1/14/20	15/31/109/115	-
22	CLA	B	823	2	1/1/14/20	8/31/109/115	-
29	CHL	6	607	-	2/2/18/26	12/27/125/137	-
22	CLA	A	820	1	1/1/15/20	14/37/115/115	-
22	CLA	B	827	2	1/1/15/20	16/37/115/115	-
22	CLA	6	604	-	1/1/15/20	11/37/115/115	-
22	CLA	A	836	1	-	2/19/97/115	-
22	CLA	A	807	1	1/1/15/20	18/37/115/115	-
22	CLA	L	203	11	-	10/37/115/115	-
22	CLA	8	602	15	1/1/14/20	10/34/112/115	-
25	BCR	A	852	-	-	7/29/63/63	0/2/2/2
22	CLA	B	816	2	1/1/13/20	8/25/103/115	-
22	CLA	1	602	12	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	J	3001	-	-	12/30/50/70	0/1/1/1
24	LHG	Z	620	22	-	15/47/47/53	-
22	CLA	B	802	2	1/1/15/20	9/37/115/115	-
22	CLA	6	603	18	1/1/11/20	1/15/93/115	-
22	CLA	5	602	17	-	10/37/115/115	-
24	LHG	5	623	22	-	10/41/41/53	-
22	CLA	5	621	-	1/1/11/20	3/15/93/115	-
29	CHL	6	606	-	3/3/18/26	8/27/125/137	-
22	CLA	3	606	-	1/1/10/20	0/10/88/115	-
25	BCR	A	848	-	-	4/29/63/63	0/2/2/2
24	LHG	8	620	22	-	14/41/41/53	-
22	CLA	6	616	18	1/1/11/20	2/15/93/115	-
22	CLA	2	613	19	-	3/19/97/115	-
22	CLA	B	835	-	1/1/11/20	5/13/91/115	-
22	CLA	A	841	1	1/1/15/20	9/37/115/115	-
22	CLA	Z	616	12	1/1/11/20	4/15/93/115	-
22	CLA	6	610	-	1/1/14/20	9/31/109/115	-
30	LUT	2	616	-	-	0/29/67/67	0/2/2/2
22	CLA	7	603	14	1/1/11/20	2/15/93/115	-
22	CLA	B	803	-	1/1/15/20	6/37/115/115	-
25	BCR	K	4001	-	-	5/29/63/63	0/2/2/2
29	CHL	1	607	-	3/3/16/26	7/18/116/137	-
22	CLA	Z	603	12	1/1/13/20	9/28/106/115	-
22	CLA	8	610	15	1/1/14/20	12/31/109/115	-
22	CLA	A	802	-	1/1/15/20	5/37/115/115	-
25	BCR	7	624	-	-	4/29/63/63	0/2/2/2
29	CHL	9	607	-	3/3/17/26	7/21/119/137	-
22	CLA	A	829	1	1/1/15/20	19/37/115/115	-
22	CLA	7	611	24	1/1/10/20	2/8/86/115	-
22	CLA	8	608	-	1/1/12/20	1/19/97/115	-
29	CHL	9	606	-	3/3/15/26	4/10/108/137	-
22	CLA	J	3002	9	1/1/10/20	3/10/88/115	-
22	CLA	A	811	1	1/1/15/20	8/37/115/115	-
22	CLA	6	612	18	1/1/12/20	5/22/100/115	-
22	CLA	B	838	2	1/1/11/20	4/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	3	719	-	-	4/29/63/63	0/2/2/2
22	CLA	B	839	-	1/1/15/20	7/37/115/115	-
22	CLA	A	803	-	1/1/15/20	4/37/115/115	-
25	BCR	G	205	-	-	2/29/63/63	0/2/2/2
26	SF4	C	101	3	-	-	0/6/5/5
22	CLA	A	822	-	1/1/15/20	13/37/115/115	-
22	CLA	B	825	-	1/1/15/20	7/37/115/115	-
22	CLA	A	812	1	1/1/15/20	13/37/115/115	-
22	CLA	2	606	-	1/1/10/20	1/8/86/115	-
22	CLA	A	825	1	-	7/25/103/115	-
22	CLA	3	611	-	1/1/10/20	2/8/86/115	-
22	CLA	A	819	1	1/1/15/20	12/37/115/115	-
22	CLA	A	828	1	1/1/15/20	11/37/115/115	-
22	CLA	B	807	2	1/1/15/20	11/37/115/115	-
25	BCR	4	621	-	-	3/29/63/63	0/2/2/2
22	CLA	B	830	2	-	3/19/97/115	-
22	CLA	7	614	14	1/1/10/20	2/11/89/115	-
22	CLA	3	602	13	1/1/14/20	8/31/109/115	-
30	LUT	2	617	-	-	3/29/67/67	0/2/2/2
22	CLA	9	609	-	1/1/12/20	0/19/97/115	-
24	LHG	A	855	-	-	10/34/34/53	-
29	CHL	4	618	16	3/3/15/26	4/12/110/137	-
22	CLA	8	614	15	1/1/13/20	6/25/103/115	-
29	CHL	1	601	12	3/3/17/26	11/24/122/137	-
22	CLA	4	602	16	-	12/31/109/115	-
25	BCR	J	3003	-	-	8/29/63/63	0/2/2/2
25	BCR	L	205	-	-	9/29/63/63	0/2/2/2
22	CLA	B	813	2	1/1/15/20	13/37/115/115	-
29	CHL	5	608	-	3/3/17/26	8/21/119/137	-
22	CLA	7	606	-	1/1/10/20	7/10/88/115	-
22	CLA	B	837	2	1/1/15/20	11/37/115/115	-
25	BCR	A	849	-	-	3/29/63/63	0/2/2/2
29	CHL	5	607	-	3/3/17/26	10/21/119/137	-
22	CLA	2	607	-	-	5/19/97/115	-
22	CLA	9	601	20	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	609	18	1/1/12/20	4/19/97/115	-
22	CLA	8	601	15	1/1/15/20	13/37/115/115	-
22	CLA	7	613	14	-	10/37/115/115	-
22	CLA	Z	609	12	1/1/15/20	4/37/115/115	-
29	CHL	Z	607	-	3/3/16/26	4/18/116/137	-
25	BCR	3	717	-	-	5/29/63/63	0/2/2/2
22	CLA	3	620	-	1/1/13/20	8/27/105/115	-
22	CLA	Z	606	-	1/1/12/20	4/22/100/115	-
22	CLA	1	606	-	1/1/12/20	5/22/100/115	-
22	CLA	7	620	-	1/1/14/20	8/31/109/115	-
22	CLA	B	822	2	-	8/30/108/115	-
22	CLA	B	821	2	-	4/15/93/115	-
30	LUT	6	624	-	-	3/29/67/67	0/2/2/2
25	BCR	B	843	-	-	10/29/63/63	0/2/2/2
22	CLA	7	601	14	1/1/15/20	16/37/115/115	-
25	BCR	B	844	-	-	7/29/63/63	0/2/2/2
22	CLA	6	601	18	1/1/15/20	14/37/115/115	-
22	CLA	B	808	2	1/1/15/20	10/37/115/115	-
22	CLA	7	602	14	1/1/15/20	12/37/115/115	-
22	CLA	A	840	1	1/1/15/20	8/37/115/115	-
22	CLA	A	832	1	1/1/12/20	2/19/97/115	-
22	CLA	4	604	-	-	4/19/97/115	-
29	CHL	5	618	17	3/3/15/26	4/12/110/137	-
22	CLA	Z	611	24	1/1/15/20	16/37/115/115	-
22	CLA	B	815	2	1/1/13/20	6/28/106/115	-
22	CLA	A	806	1	1/1/15/20	16/37/115/115	-
22	CLA	B	818	2	1/1/14/20	12/31/109/115	-
22	CLA	B	834	2	1/1/15/20	13/37/115/115	-
22	CLA	7	609	14	1/1/12/20	5/19/97/115	-
22	CLA	4	612	16	1/1/12/20	3/22/100/115	-
26	SF4	C	102	3	-	-	0/6/5/5
25	BCR	5	625	-	-	7/29/63/63	0/2/2/2
22	CLA	A	831	1	1/1/15/20	14/37/115/115	-
22	CLA	1	603	12	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	609	12	1/1/15/20	7/37/115/115	-
29	CHL	Z	601	12	3/3/17/26	11/24/122/137	-
22	CLA	A	845	24	1/1/12/20	15/22/100/115	-
22	CLA	8	616	15	1/1/11/20	2/15/93/115	-
22	CLA	3	603	13	1/1/15/20	7/37/115/115	-
22	CLA	1	616	12	1/1/11/20	3/15/93/115	-
22	CLA	3	614	13	-	2/13/91/115	-
22	CLA	A	817	-	1/1/13/20	6/28/106/115	-
29	CHL	6	608	-	3/3/17/26	4/21/119/137	-
22	CLA	8	603	15	1/1/11/20	2/13/91/115	-
22	CLA	5	604	17	-	5/19/97/115	-
22	CLA	6	617	18	1/1/11/20	3/15/93/115	-
22	CLA	8	609	15	1/1/11/20	3/15/93/115	-
25	BCR	A	856	-	-	7/29/63/63	0/2/2/2
22	CLA	B	820	2	1/1/13/20	6/27/105/115	-
30	LUT	1	617	-	-	2/29/67/67	0/2/2/2
22	CLA	4	614	16	1/1/11/20	2/13/91/115	-
22	CLA	5	612	17	1/1/12/20	3/22/100/115	-
22	CLA	6	611	24	1/1/13/20	7/25/103/115	-
22	CLA	B	811	2	1/1/13/20	5/25/101/115	-
22	CLA	7	604	-	1/1/13/20	9/27/105/115	-
22	CLA	K	4003	10	1/1/11/20	3/15/93/115	-
25	BCR	A	851	-	-	4/29/63/63	0/2/2/2
25	BCR	7	623	-	-	7/29/63/63	0/2/2/2
22	CLA	B	841	24	1/1/15/20	5/37/115/115	-
25	BCR	B	846	-	-	5/29/63/63	0/2/2/2
22	CLA	4	616	16	1/1/10/20	0/8/86/115	-
21	CL0	A	801	1	2/2/20/25	6/37/135/135	-
22	CLA	A	830	1	1/1/15/20	8/37/115/115	-
25	BCR	8	619	-	-	6/29/63/63	0/2/2/2
22	CLA	4	601	16	1/1/14/20	11/33/111/115	-
22	CLA	B	819	-	1/1/15/20	9/37/115/115	-
22	CLA	A	816	1	1/1/15/20	10/37/115/115	-
30	LUT	1	619	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	8	604	-	1/1/11/20	3/15/93/115	-
30	LUT	3	621	-	-	5/29/67/67	0/2/2/2
29	CHL	3	608	-	3/3/20/26	22/39/137/137	-
30	LUT	8	618	-	-	4/29/67/67	0/2/2/2
22	CLA	2	614	-	-	2/13/91/115	-
22	CLA	1	610	12	1/1/14/20	12/31/109/115	-
22	CLA	5	617	17	1/1/11/20	4/15/93/115	-
30	LUT	4	619	-	-	2/29/67/67	0/2/2/2
22	CLA	A	809	1	1/1/15/20	17/37/115/115	-
29	CHL	4	606	-	3/3/18/26	3/27/125/137	-
22	CLA	3	604	-	1/1/15/20	9/37/115/115	-
30	LUT	9	617	-	-	2/29/67/67	0/2/2/2
22	CLA	L	204	-	-	5/19/97/115	-
22	CLA	B	831	2	1/1/11/20	5/18/96/115	-
22	CLA	G	203	7	1/1/12/20	3/19/97/115	-
22	CLA	2	601	19	1/1/11/20	7/15/93/115	-
22	CLA	A	842	1	1/1/15/20	16/37/115/115	-
22	CLA	3	609	13	1/1/12/20	5/19/97/115	-
22	CLA	A	835	1	1/1/15/20	4/37/115/115	-
22	CLA	B	824	-	1/1/15/20	9/37/115/115	-
28	LMG	9	620	-	-	16/39/59/70	0/1/1/1
22	CLA	A	854	-	1/1/15/20	12/37/115/115	-
30	LUT	Z	618	-	-	4/29/67/67	0/2/2/2
22	CLA	1	612	12	1/1/12/20	8/22/100/115	-
22	CLA	F	301	-	1/1/15/20	10/37/115/115	-
22	CLA	B	828	2	1/1/15/20	9/37/115/115	-
22	CLA	5	616	17	1/1/11/20	7/15/93/115	-
22	CLA	B	814	2	1/1/14/20	11/31/109/115	-
23	PQN	A	844	-	-	12/23/43/43	0/2/2/2
22	CLA	5	601	17	1/1/15/20	9/37/115/115	-
22	CLA	6	622	18	1/1/11/20	3/13/91/115	-
30	LUT	7	621	-	-	3/29/67/67	0/2/2/2
30	LUT	Z	617	-	-	4/29/67/67	0/2/2/2
22	CLA	3	613	13	-	14/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	610	16	1/1/14/20	9/31/109/115	-
22	CLA	5	603	17	1/1/11/20	1/15/93/115	-
22	CLA	2	602	19	-	4/13/91/115	-
22	CLA	1	611	24	1/1/15/20	10/37/115/115	-
22	CLA	Z	608	-	1/1/15/20	17/37/115/115	-
22	CLA	9	602	20	1/1/14/20	9/31/109/115	-
22	CLA	B	805	2	1/1/15/20	14/37/115/115	-
22	CLA	A	821	1	1/1/11/20	2/13/91/115	-
25	BCR	B	845	-	-	10/29/63/63	0/2/2/2
22	CLA	B	836	2	1/1/14/20	5/31/109/115	-
22	CLA	8	611	24	1/1/11/20	3/15/93/115	-
29	CHL	7	607	-	3/3/17/26	9/25/123/137	-
24	LHG	7	625	22	-	10/41/41/53	-
22	CLA	Z	614	12	1/1/15/20	9/37/115/115	-
25	BCR	F	305	-	-	2/29/63/63	0/2/2/2
22	CLA	B	806	2	1/1/15/20	13/37/115/115	-
30	LUT	5	624	-	-	3/29/67/67	0/2/2/2
22	CLA	A	843	-	1/1/15/20	17/37/115/115	-
22	CLA	A	838	1	1/1/12/20	5/21/99/115	-
22	CLA	A	839	1	1/1/15/20	11/37/115/115	-
22	CLA	Z	610	12	1/1/14/20	14/31/109/115	-
22	CLA	3	612	13	1/1/11/20	2/15/93/115	-
25	BCR	6	623	-	-	9/29/63/63	0/2/2/2
24	LHG	4	622	22	-	19/53/53/53	-
30	LUT	5	620	-	-	0/29/67/67	0/2/2/2
29	CHL	8	607	-	3/3/18/26	11/27/125/137	-
22	CLA	F	304	6	1/1/15/20	9/37/115/115	-
22	CLA	A	810	1	-	11/37/115/115	-
22	CLA	B	840	2	-	6/37/115/115	-
22	CLA	A	833	1	1/1/15/20	10/37/115/115	-
25	BCR	A	850	-	-	4/29/63/63	0/2/2/2
25	BCR	I	172	-	-	6/29/63/63	0/2/2/2
22	CLA	2	603	19	1/1/11/20	6/15/93/115	-
22	CLA	Z	612	12	1/1/12/20	6/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	611	24	1/1/13/20	8/25/103/115	-
22	CLA	A	804	1	1/1/15/20	12/37/115/115	-
22	CLA	B	809	2	1/1/15/20	12/37/115/115	-
25	BCR	B	847	-	-	7/29/63/63	0/2/2/2
22	CLA	A	814	1	1/1/15/20	15/37/115/115	-
22	CLA	5	610	17	1/1/14/20	7/31/109/115	-
22	CLA	B	852	-	1/1/15/20	5/37/115/115	-
30	LUT	6	621	-	-	2/29/67/67	0/2/2/2
22	CLA	7	612	14	1/1/12/20	7/22/100/115	-
22	CLA	9	613	-	1/1/12/20	8/19/97/115	-
22	CLA	7	608	-	-	3/19/97/115	-
22	CLA	8	606	-	1/1/10/20	4/10/88/115	-
22	CLA	9	610	20	-	4/31/109/115	-
22	CLA	1	613	-	1/1/15/20	7/37/115/115	-
30	LUT	9	616	-	-	2/29/67/67	0/2/2/2
25	BCR	L	201	-	-	8/29/63/63	0/2/2/2
22	CLA	A	837	1	1/1/11/20	9/13/91/115	-
22	CLA	4	603	16	1/1/11/20	2/15/93/115	-
22	CLA	A	824	1	1/1/12/20	8/21/99/115	-
30	LUT	7	622	-	-	3/29/67/67	0/2/2/2
22	CLA	8	613	15	-	12/37/115/115	-

The worst 5 of 3969 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	842	PQN	C3-C2	7.50	1.48	1.35
23	A	844	PQN	C3-C2	7.35	1.48	1.35
22	B	836	CLA	C3B-C2B	6.40	1.49	1.40
22	3	602	CLA	C3B-C2B	6.31	1.49	1.40
22	5	621	CLA	C3B-C2B	6.19	1.49	1.40

The worst 5 of 7074 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	617	CLA	O2A-CGA-O1A	-13.94	79.44	123.14
22	5	617	CLA	O2A-CGA-CBA	12.13	160.18	112.23
29	6	608	CHL	C4A-NA-C1A	-11.78	101.41	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	617	CLA	O1A-CGA-CBA	-11.02	80.75	123.73
29	Z	601	CHL	C4A-NA-C1A	-10.94	101.79	106.71

5 of 246 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	801	CL0	ND
21	A	801	CL0	NC
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND

5 of 2298 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	804	CLA	CAD-CBD-CGD-O1D
22	A	809	CLA	C3A-C2A-CAA-CBA
22	A	809	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

274 monomers are involved in 852 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	8	617	LUT	8	0
25	B	801	BCR	6	0
22	1	608	CLA	5	0
22	B	833	CLA	3	0
25	3	718	BCR	5	0
22	7	610	CLA	2	0
22	A	823	CLA	3	0
30	Z	619	LUT	2	0
22	Z	613	CLA	5	0
22	A	815	CLA	21	0
22	9	612	CLA	1	0
22	6	602	CLA	1	0
22	A	834	CLA	3	0
30	4	620	LUT	4	0
22	2	610	CLA	2	0
22	A	808	CLA	2	0
22	A	827	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	829	CLA	4	0
22	5	606	CLA	4	0
22	B	832	CLA	5	0
30	3	622	LUT	3	0
22	8	612	CLA	1	0
22	9	614	CLA	2	0
22	A	805	CLA	22	0
22	B	826	CLA	2	0
22	A	813	CLA	2	0
22	4	613	CLA	3	0
25	5	622	BCR	5	0
30	1	618	LUT	5	0
22	9	611	CLA	1	0
22	3	617	CLA	3	0
25	B	848	BCR	3	0
23	B	842	PQN	1	0
22	7	616	CLA	1	0
22	F	303	CLA	2	0
22	2	612	CLA	1	0
22	A	818	CLA	3	0
22	B	817	CLA	3	0
29	4	608	CHL	8	0
24	6	619	LHG	19	0
22	1	604	CLA	1	0
27	B	850	DGD	1	0
24	1	620	LHG	2	0
22	5	614	CLA	5	0
25	6	625	BCR	3	0
22	Z	604	CLA	1	0
22	5	609	CLA	6	0
25	K	4004	BCR	1	0
22	A	826	CLA	2	0
29	4	607	CHL	1	0
22	6	613	CLA	2	0
22	2	611	CLA	1	0
29	6	618	CHL	2	0
22	3	610	CLA	3	0
22	B	812	CLA	8	0
24	A	846	LHG	2	0
22	5	613	CLA	3	0
24	A	847	LHG	3	0
22	Z	602	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	614	CLA	3	0
22	6	614	CLA	2	0
22	9	603	CLA	1	0
22	3	607	CLA	4	0
22	B	823	CLA	4	0
29	6	607	CHL	5	0
22	A	820	CLA	4	0
22	B	827	CLA	4	0
22	A	836	CLA	2	0
22	6	604	CLA	4	0
22	A	807	CLA	9	0
22	L	203	CLA	1	0
22	8	602	CLA	3	0
25	A	852	BCR	3	0
22	B	816	CLA	5	0
22	1	602	CLA	9	0
24	Z	620	LHG	1	0
22	B	802	CLA	2	0
22	5	602	CLA	4	0
22	5	621	CLA	1	0
29	6	606	CHL	4	0
22	3	606	CLA	3	0
25	A	848	BCR	5	0
24	8	620	LHG	1	0
22	6	616	CLA	8	0
22	2	613	CLA	9	0
22	B	835	CLA	2	0
22	A	841	CLA	11	0
22	6	610	CLA	5	0
22	8	613	CLA	3	0
30	2	616	LUT	3	0
22	B	803	CLA	4	0
25	K	4001	BCR	5	0
29	1	607	CHL	3	0
22	Z	603	CLA	1	0
22	8	610	CLA	6	0
22	A	802	CLA	26	0
25	7	624	BCR	1	0
29	9	607	CHL	1	0
22	A	829	CLA	7	0
22	7	611	CLA	1	0
22	8	608	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	J	3002	CLA	1	0
22	A	811	CLA	4	0
22	6	612	CLA	2	0
22	B	838	CLA	3	0
25	3	719	BCR	6	0
22	B	839	CLA	4	0
22	A	803	CLA	2	0
25	G	205	BCR	3	0
22	A	822	CLA	2	0
22	B	825	CLA	5	0
22	A	812	CLA	15	0
22	A	825	CLA	3	0
22	A	819	CLA	3	0
22	A	828	CLA	1	0
22	B	807	CLA	2	0
25	4	621	BCR	39	0
22	B	830	CLA	3	0
22	7	614	CLA	1	0
22	3	602	CLA	1	0
30	2	617	LUT	3	0
22	9	609	CLA	11	0
29	4	618	CHL	7	0
22	8	614	CLA	5	0
29	1	601	CHL	1	0
22	4	602	CLA	1	0
25	J	3003	BCR	2	0
25	L	205	BCR	2	0
22	B	813	CLA	5	0
29	5	608	CHL	3	0
22	7	606	CLA	2	0
22	B	837	CLA	4	0
25	A	849	BCR	5	0
29	5	607	CHL	3	0
22	6	609	CLA	2	0
22	8	601	CLA	1	0
22	7	613	CLA	3	0
22	Z	609	CLA	1	0
25	3	717	BCR	4	0
22	3	620	CLA	1	0
22	Z	606	CLA	2	0
22	1	606	CLA	3	0
22	7	620	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	822	CLA	1	0
22	B	821	CLA	1	0
30	6	624	LUT	3	0
25	B	843	BCR	5	0
22	7	601	CLA	4	0
25	B	844	BCR	2	0
22	6	601	CLA	7	0
22	B	808	CLA	1	0
22	7	602	CLA	2	0
22	A	840	CLA	3	0
22	A	832	CLA	5	0
22	4	604	CLA	6	0
22	Z	611	CLA	2	0
22	B	815	CLA	3	0
22	A	806	CLA	5	0
22	B	818	CLA	4	0
22	B	834	CLA	1	0
22	7	609	CLA	3	0
22	4	612	CLA	1	0
25	5	625	BCR	7	0
22	A	831	CLA	8	0
22	1	603	CLA	3	0
22	1	609	CLA	2	0
29	Z	601	CHL	1	0
22	A	845	CLA	1	0
22	8	616	CLA	1	0
22	3	603	CLA	4	0
22	1	616	CLA	1	0
22	3	614	CLA	3	0
22	A	817	CLA	5	0
29	6	608	CHL	1	0
22	5	604	CLA	2	0
22	8	609	CLA	2	0
25	A	856	BCR	5	0
22	B	820	CLA	15	0
30	1	617	LUT	7	0
22	4	614	CLA	4	0
22	5	612	CLA	2	0
22	6	611	CLA	1	0
22	B	811	CLA	3	0
22	7	604	CLA	1	0
22	K	4003	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	851	BCR	3	0
25	7	623	BCR	5	0
22	B	841	CLA	13	0
25	B	846	BCR	6	0
22	4	616	CLA	6	0
21	A	801	CL0	3	0
22	A	830	CLA	3	0
25	8	619	BCR	6	0
22	4	601	CLA	6	0
22	B	819	CLA	2	0
22	A	816	CLA	7	0
30	1	619	LUT	2	0
22	8	604	CLA	1	0
30	3	621	LUT	4	0
29	3	608	CHL	5	0
30	8	618	LUT	5	0
22	1	610	CLA	5	0
22	5	617	CLA	6	0
30	4	619	LUT	12	0
22	A	809	CLA	4	0
29	4	606	CHL	10	0
22	3	604	CLA	3	0
30	9	617	LUT	4	0
22	B	831	CLA	6	0
22	2	601	CLA	5	0
22	A	842	CLA	10	0
22	3	609	CLA	1	0
22	A	835	CLA	23	0
22	B	824	CLA	1	0
28	9	620	LMG	1	0
22	A	854	CLA	5	0
30	Z	618	LUT	4	0
22	F	301	CLA	4	0
22	B	828	CLA	3	0
22	5	616	CLA	1	0
22	B	814	CLA	5	0
23	A	844	PQN	4	0
22	5	601	CLA	1	0
22	6	622	CLA	14	0
30	7	621	LUT	6	0
30	Z	617	LUT	4	0
22	3	613	CLA	2	0

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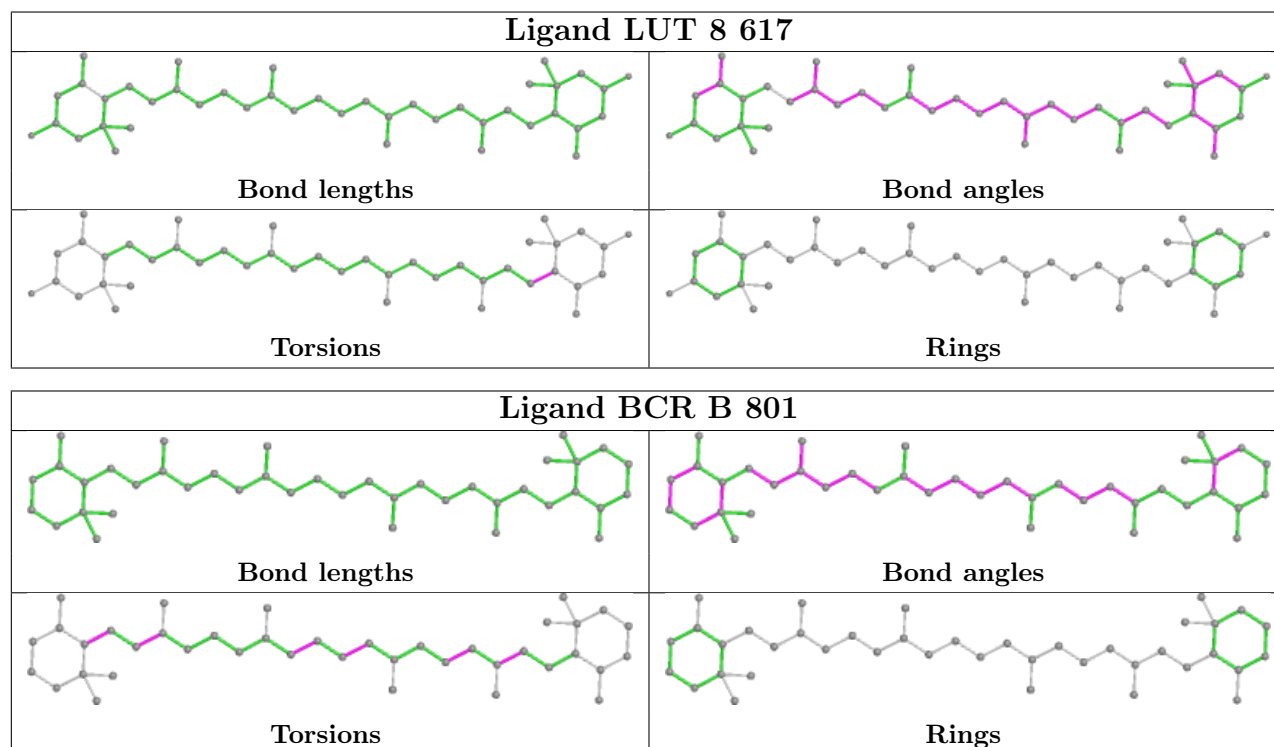
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	610	CLA	10	0
22	5	603	CLA	1	0
22	2	602	CLA	2	0
22	1	611	CLA	1	0
22	Z	608	CLA	4	0
22	9	602	CLA	3	0
22	B	805	CLA	5	0
22	A	821	CLA	1	0
25	B	845	BCR	3	0
22	B	836	CLA	2	0
29	7	607	CHL	1	0
22	Z	614	CLA	2	0
25	F	305	BCR	15	0
22	B	806	CLA	2	0
30	5	624	LUT	5	0
22	A	843	CLA	7	0
22	A	838	CLA	1	0
22	A	839	CLA	4	0
22	Z	610	CLA	3	0
22	3	612	CLA	2	0
25	6	623	BCR	8	0
24	4	622	LHG	3	0
30	5	620	LUT	15	0
22	F	304	CLA	2	0
22	B	840	CLA	4	0
22	A	833	CLA	4	0
25	A	850	BCR	5	0
25	I	172	BCR	1	0
22	Z	612	CLA	1	0
22	4	611	CLA	6	0
22	A	804	CLA	2	0
22	B	809	CLA	1	0
25	B	847	BCR	4	0
22	A	814	CLA	2	0
22	5	610	CLA	1	0
30	6	621	LUT	4	0
22	7	612	CLA	1	0
22	9	613	CLA	1	0
22	7	608	CLA	2	0
22	8	606	CLA	2	0
22	9	610	CLA	1	0
22	1	613	CLA	2	0

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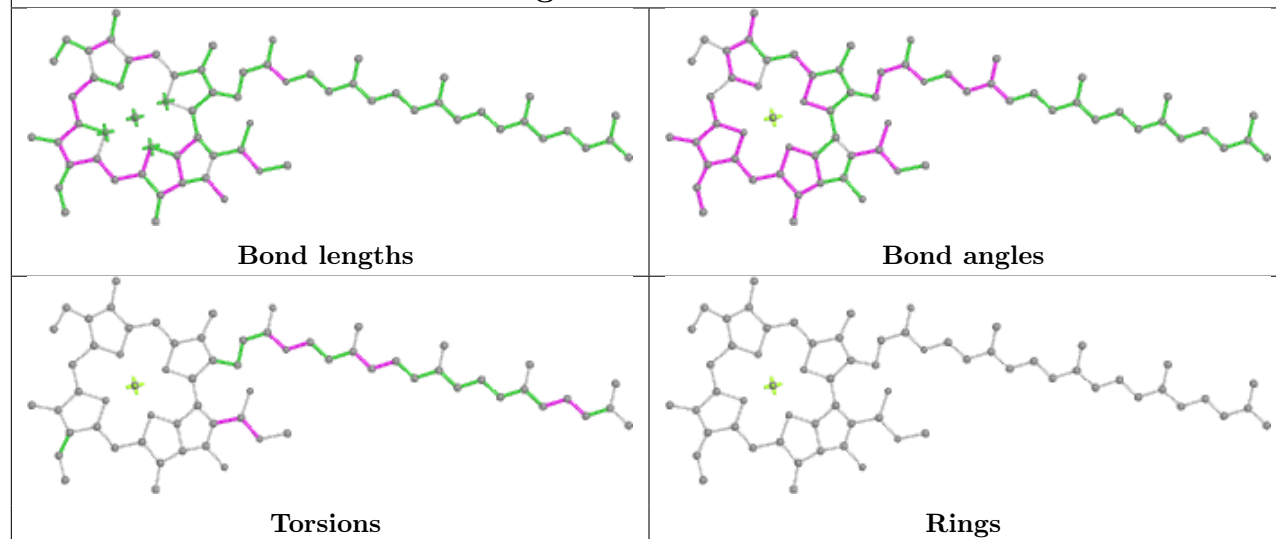
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	9	616	LUT	4	0
25	L	201	BCR	7	0
22	A	837	CLA	1	0
22	A	824	CLA	1	0
30	7	622	LUT	2	0

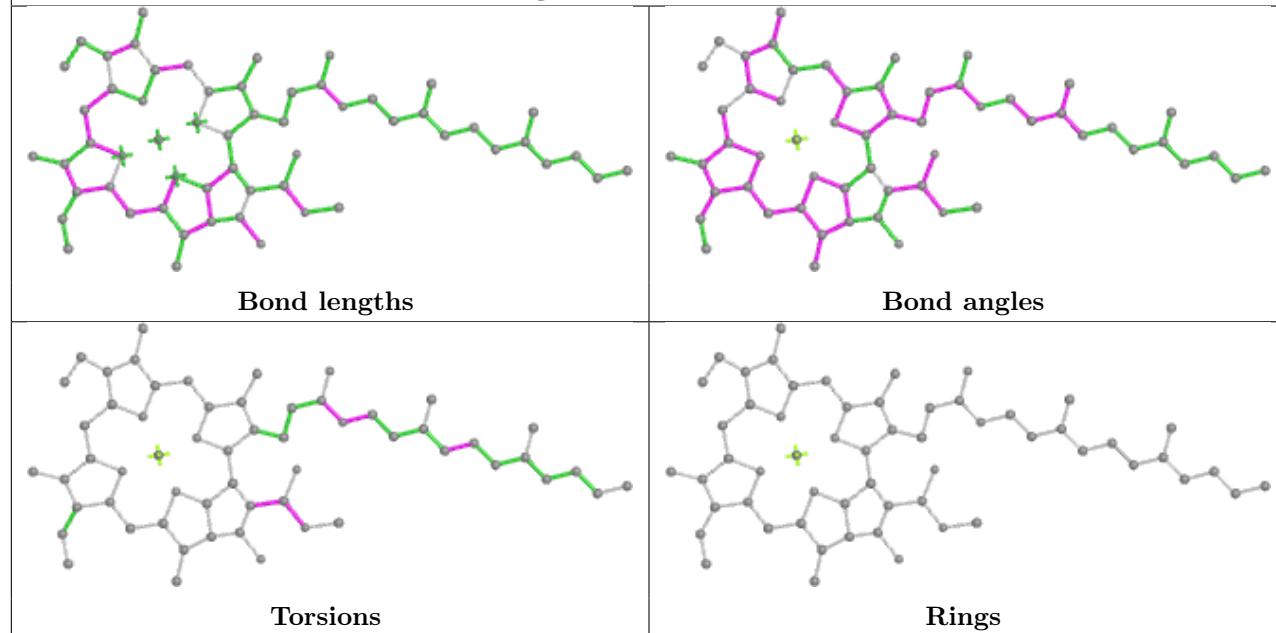
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

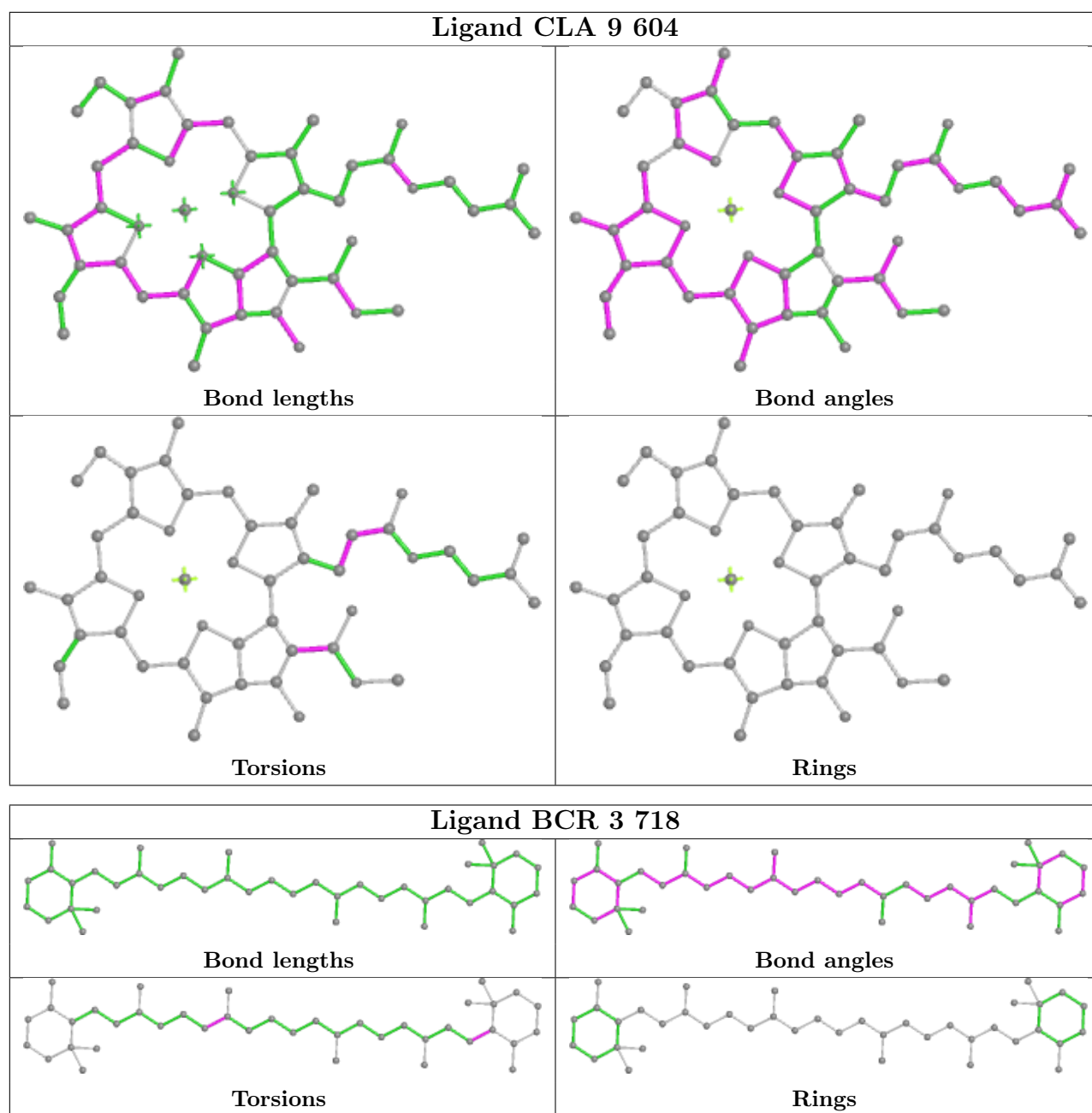


## Ligand CLA 1 608

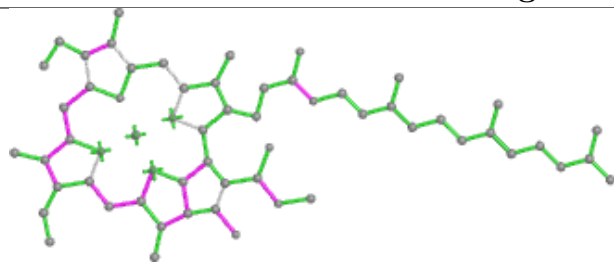


## Ligand CLA B 833

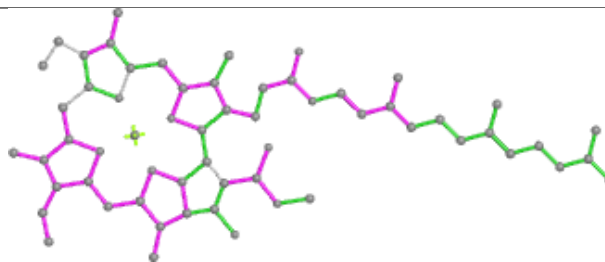




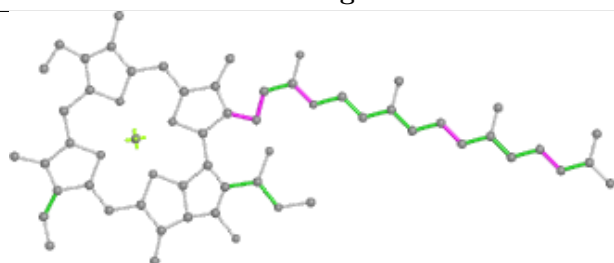
## Ligand CLA 7 610



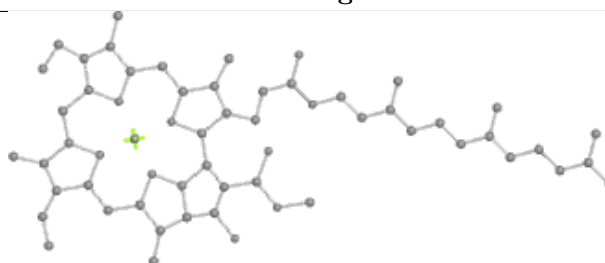
Bond lengths



Bond angles

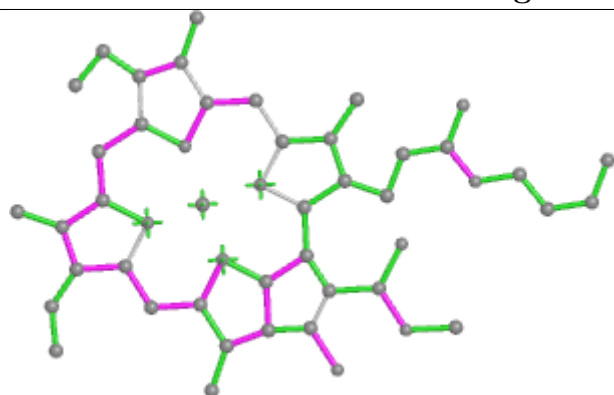


Torsions

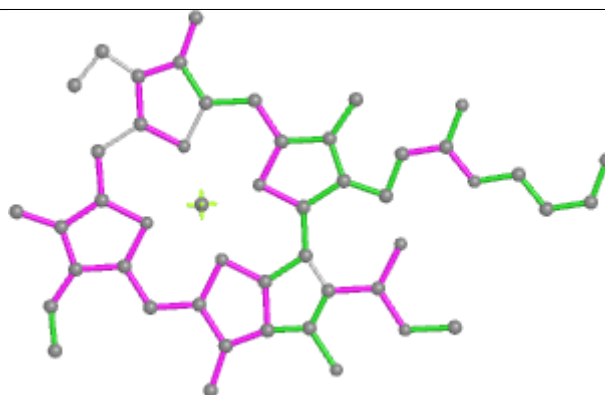


Rings

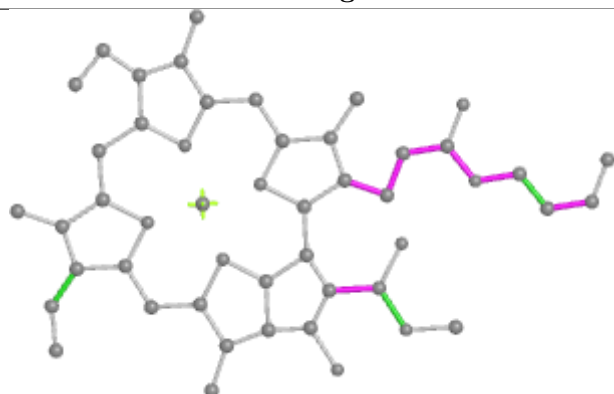
## Ligand CLA A 823



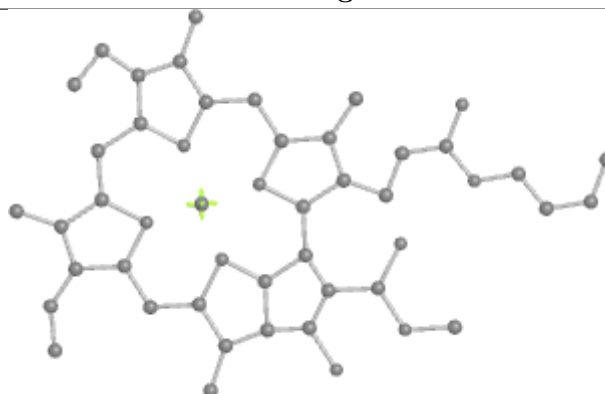
Bond lengths



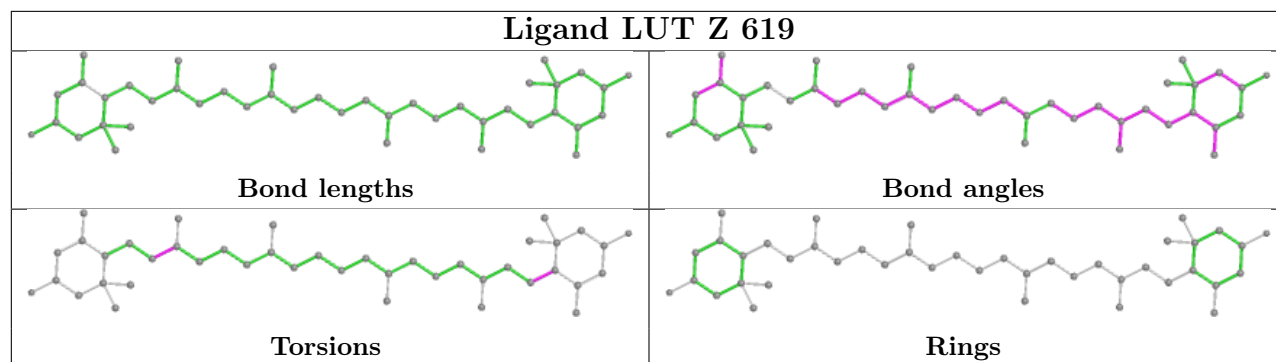
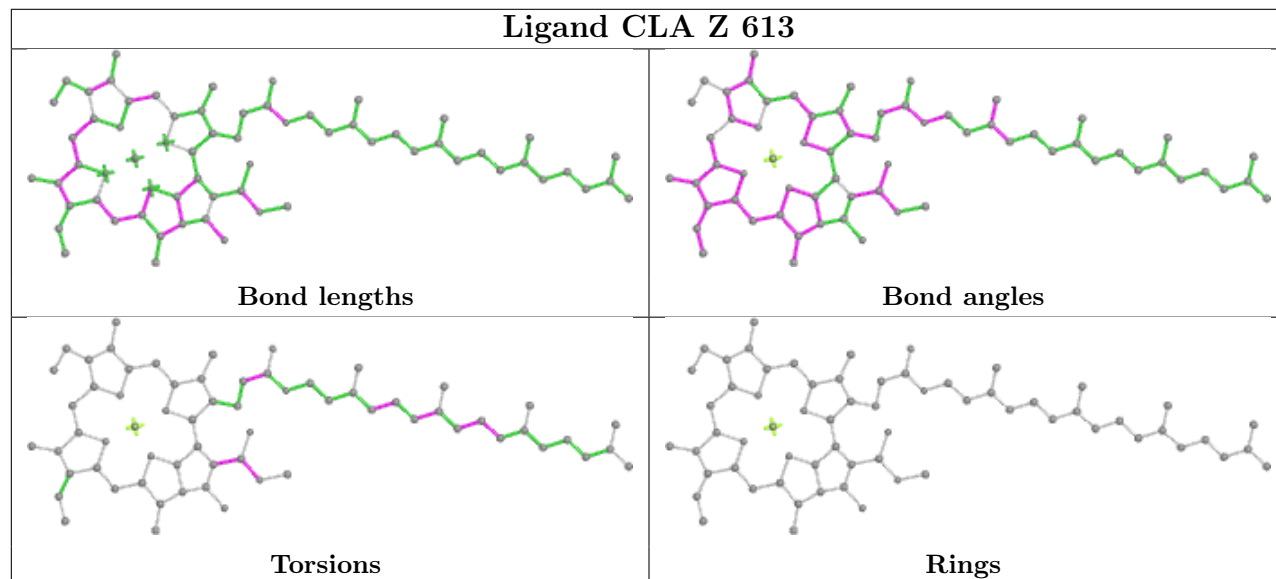
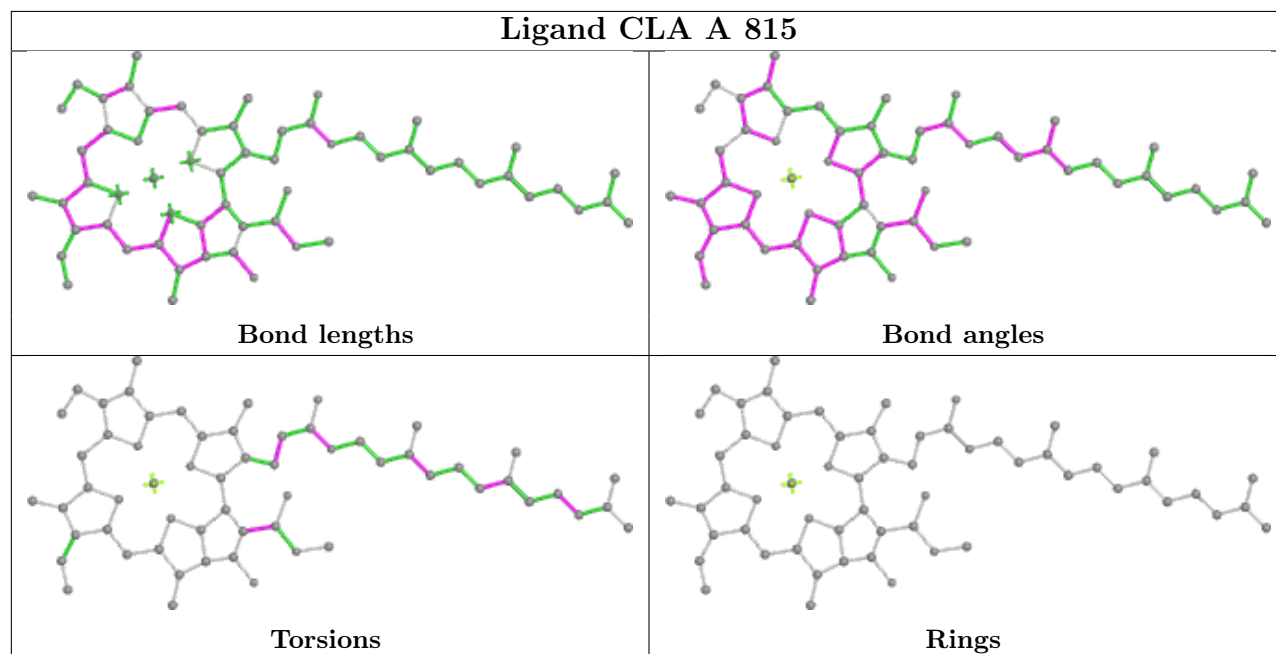
Bond angles



Torsions

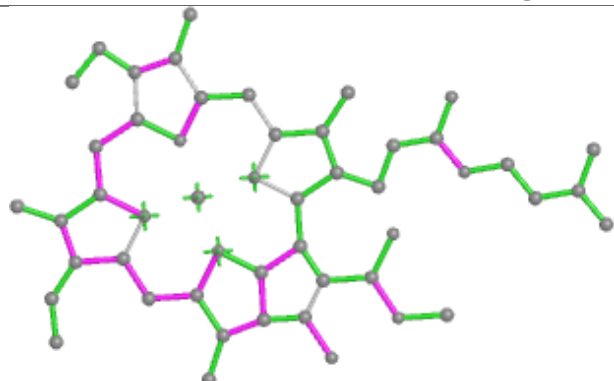


Rings

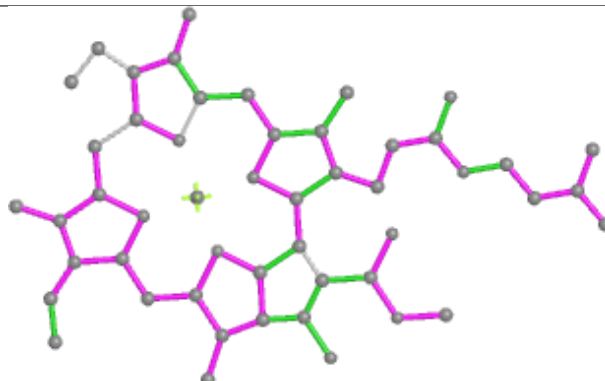
**Ligand LUT Z 619****Ligand CLA Z 613****Ligand CLA A 815**



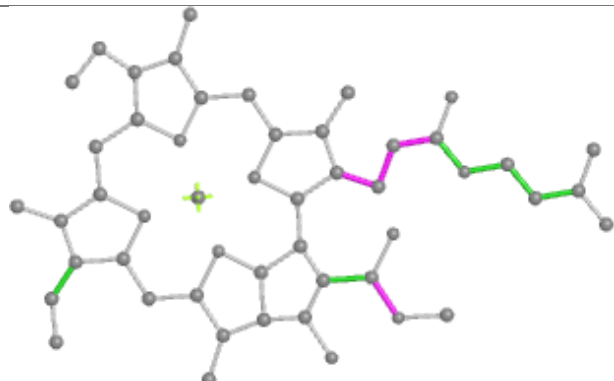
## Ligand CLA 4 609



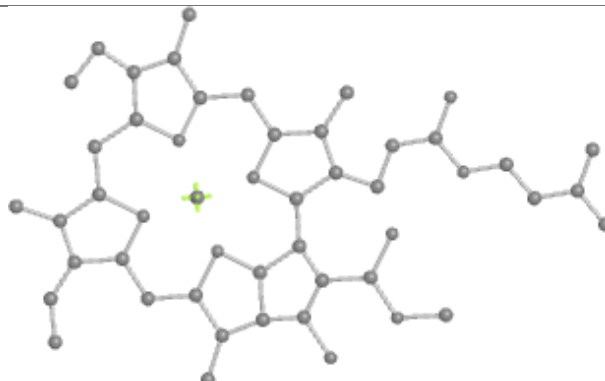
Bond lengths



Bond angles

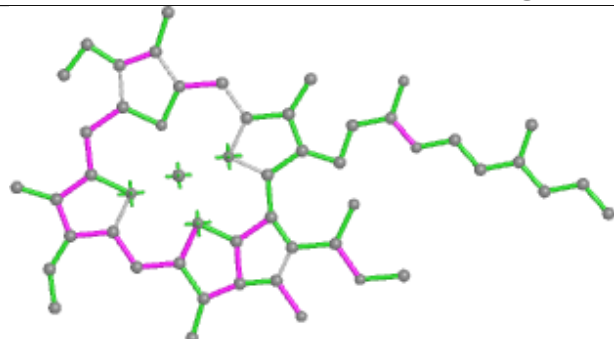


Torsions

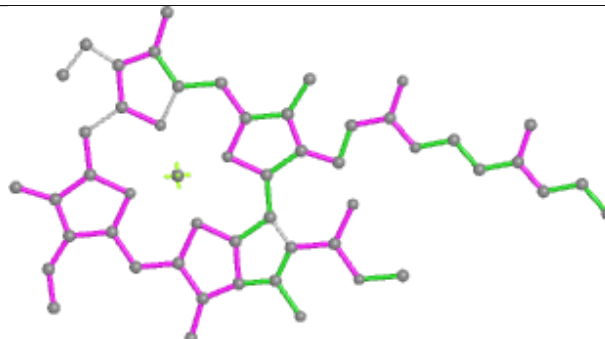


Rings

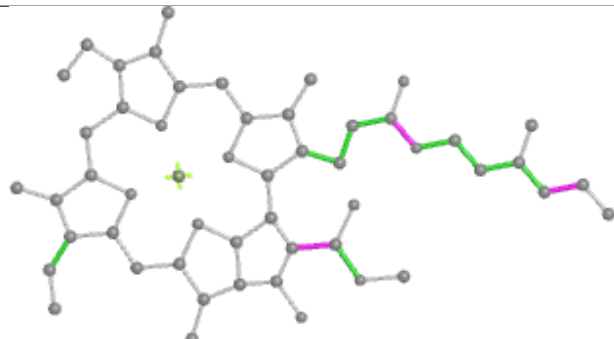
## Ligand CLA 9 612



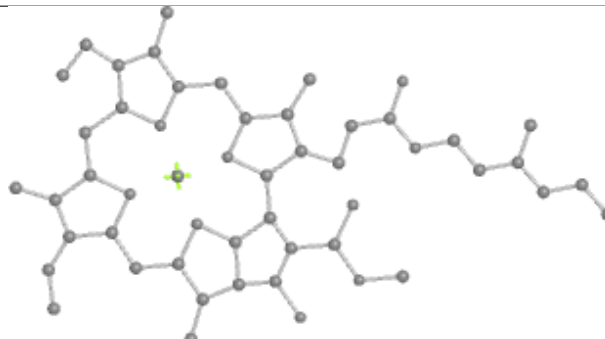
Bond lengths



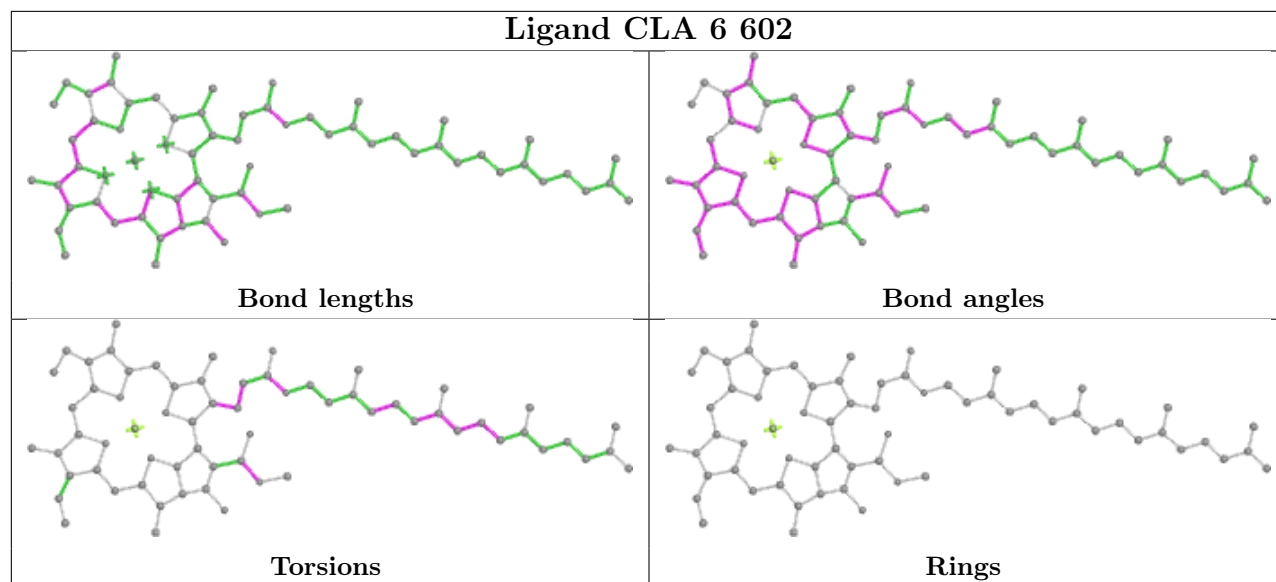
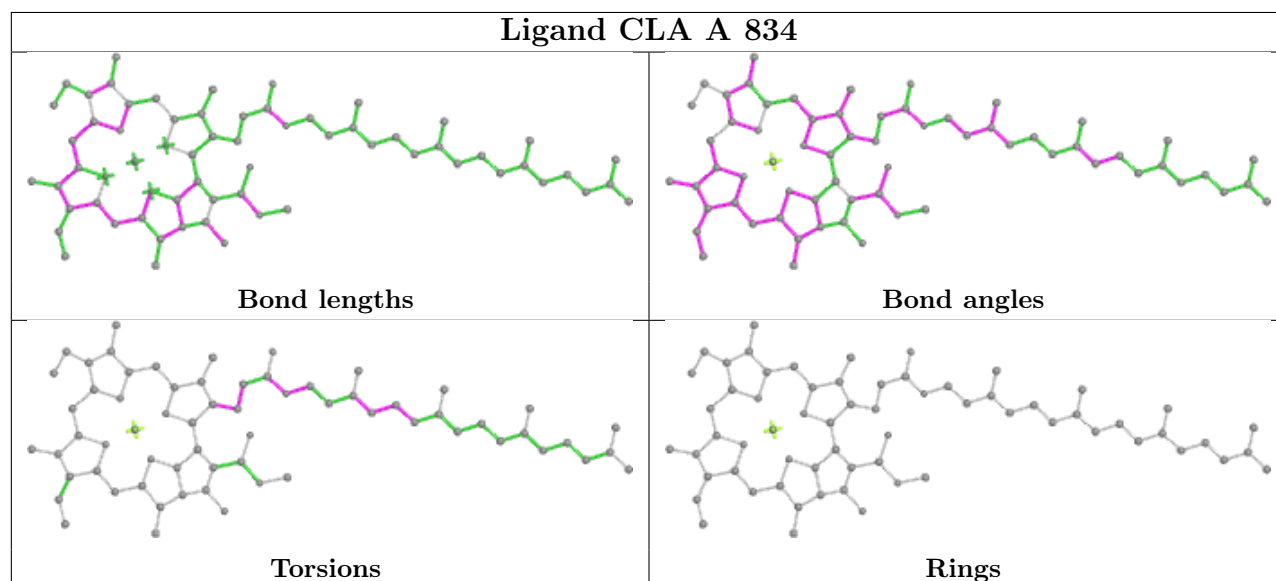
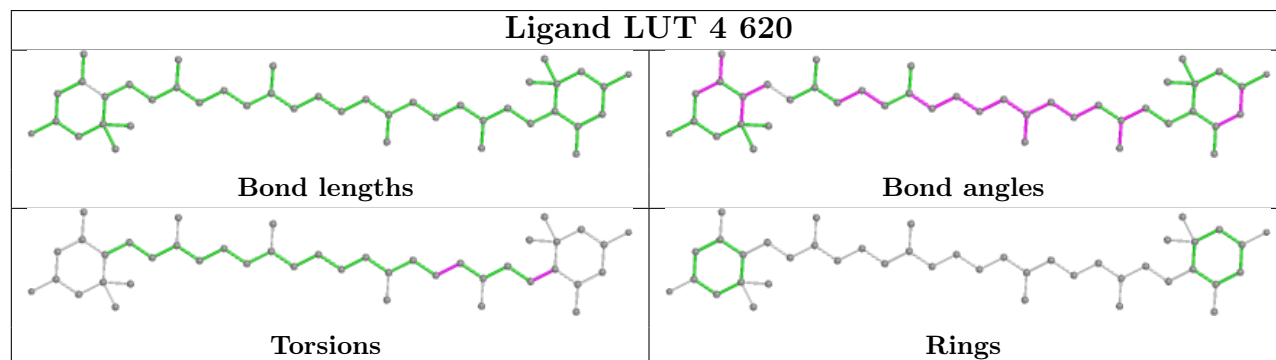
Bond angles

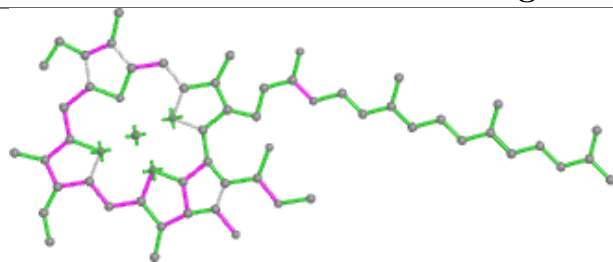
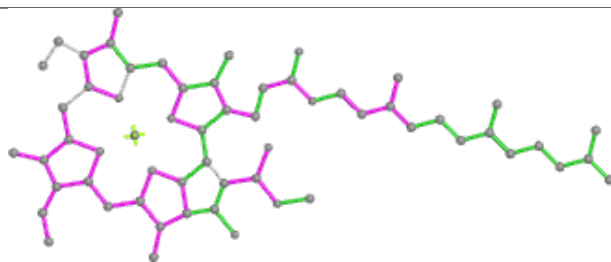
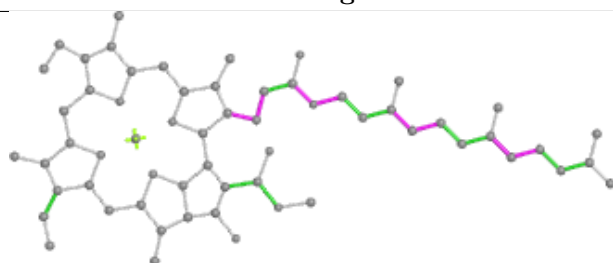
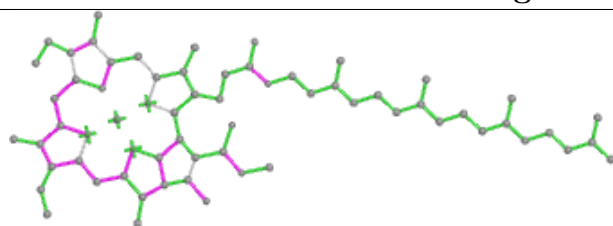
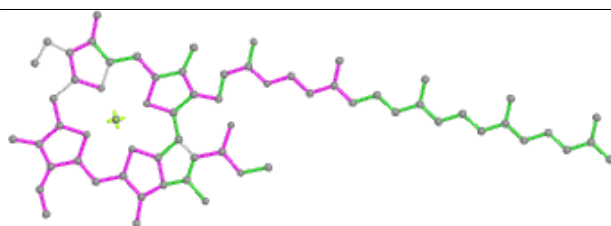
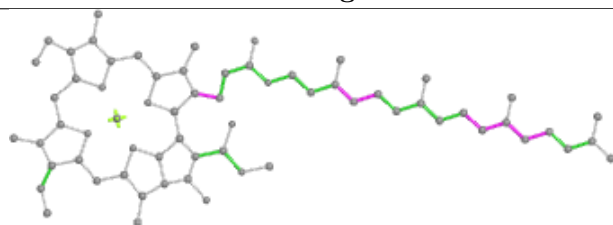
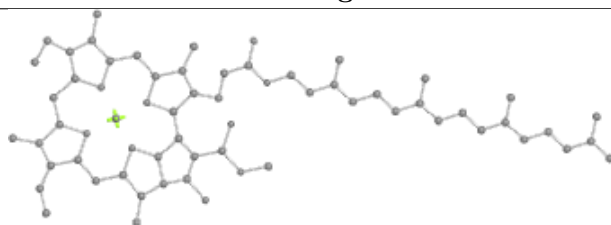


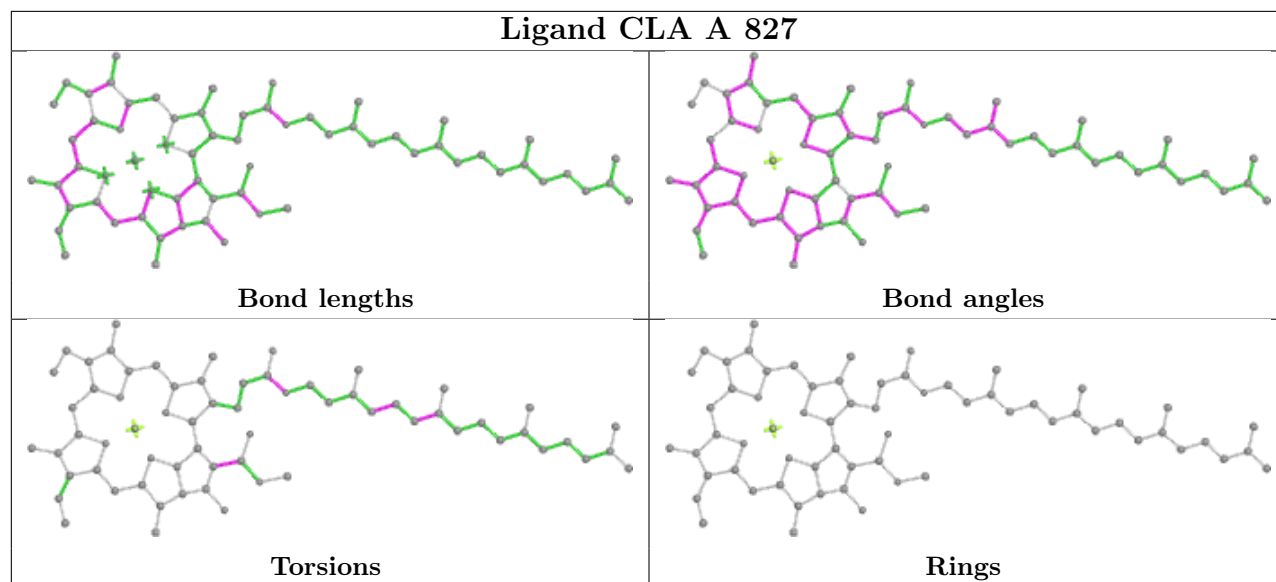
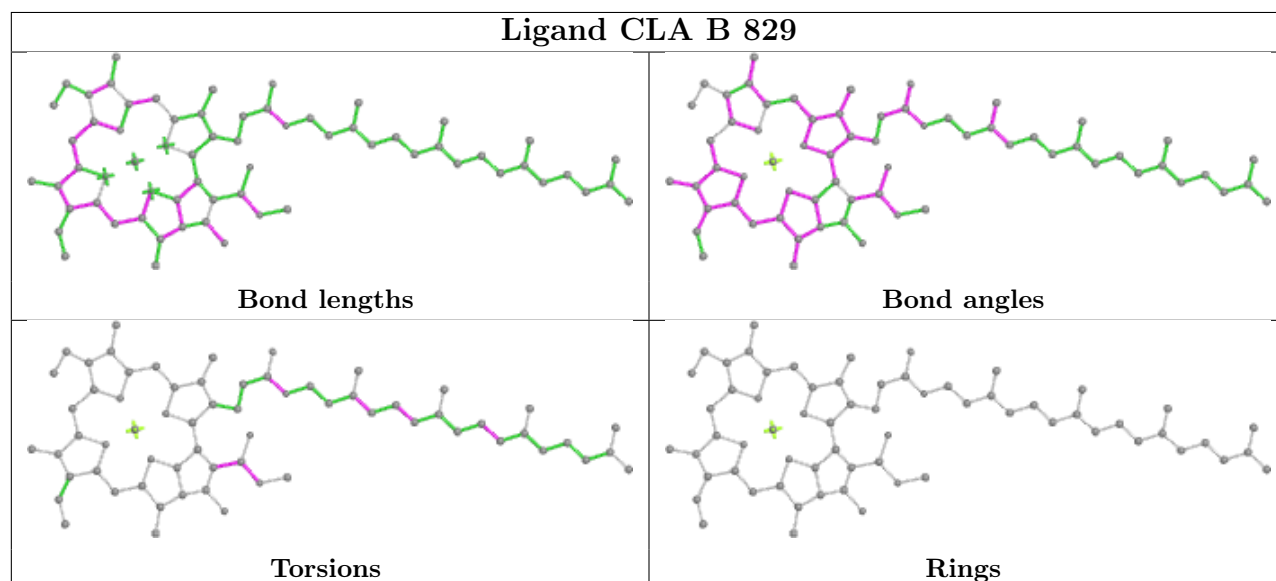
Torsions

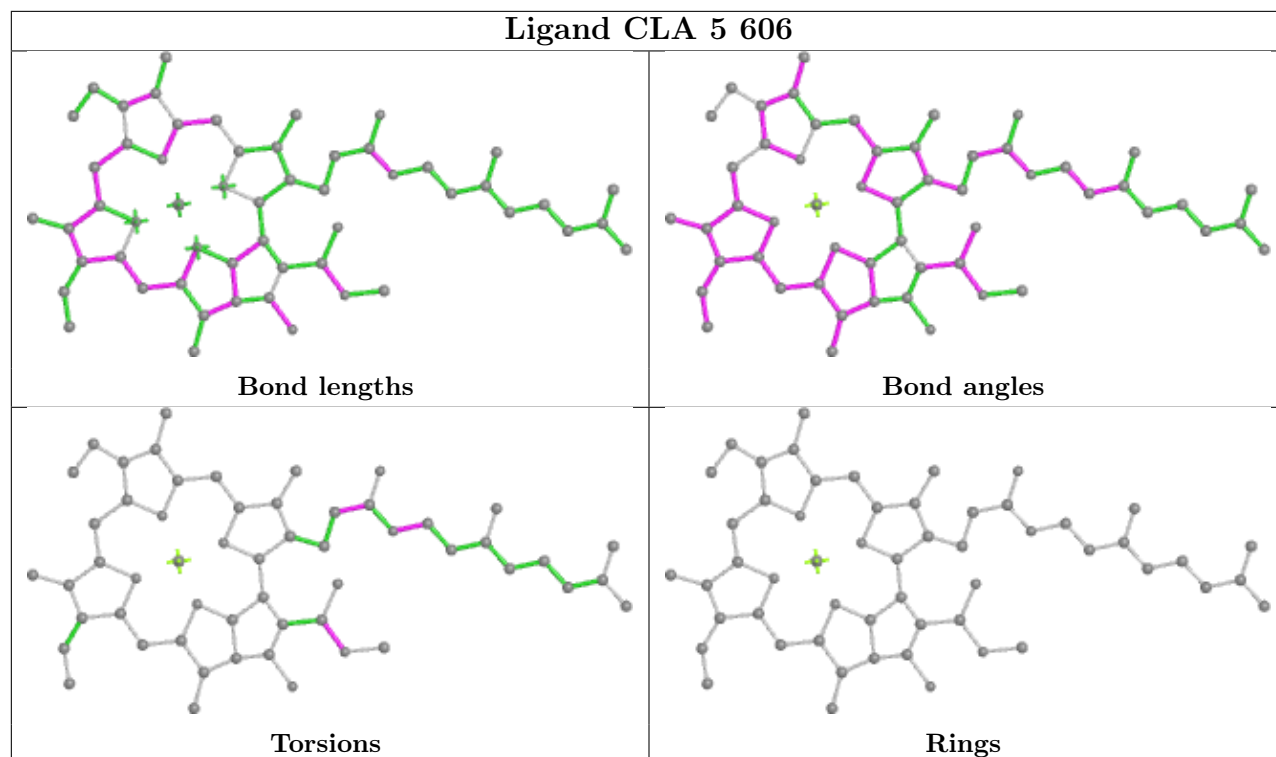
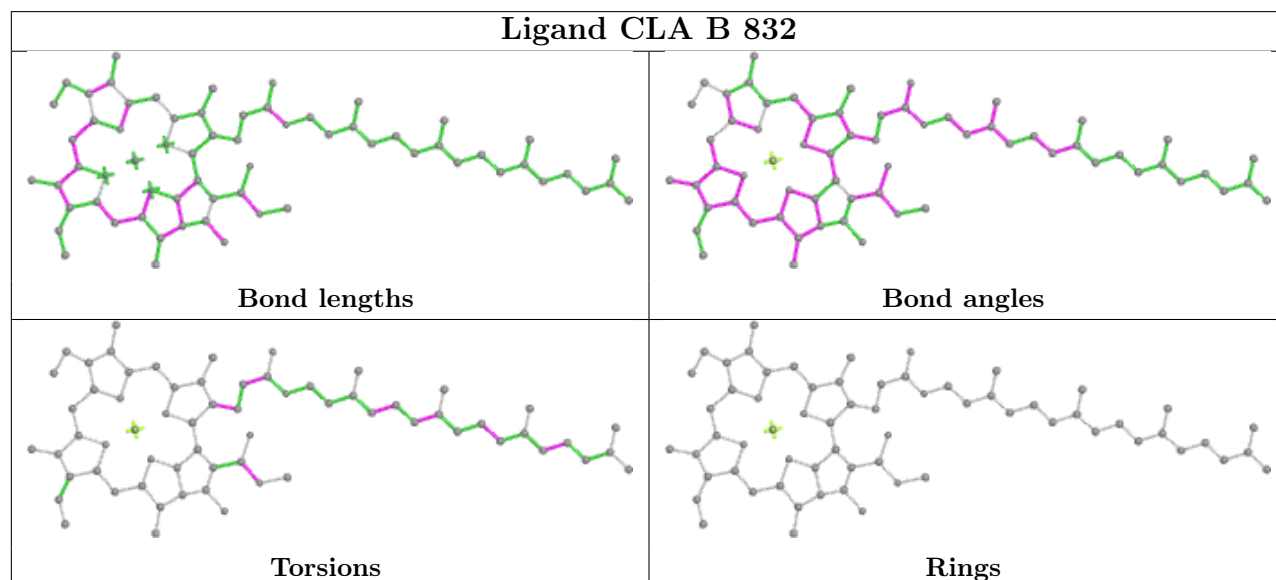
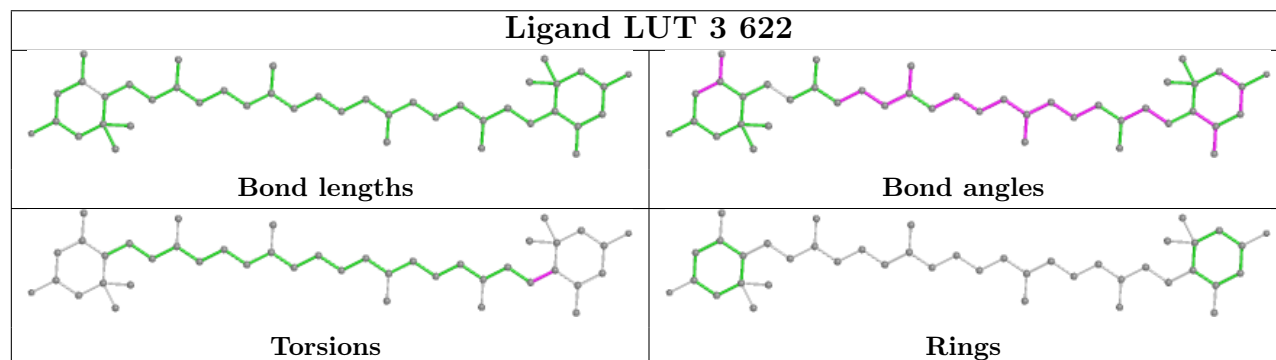


Rings

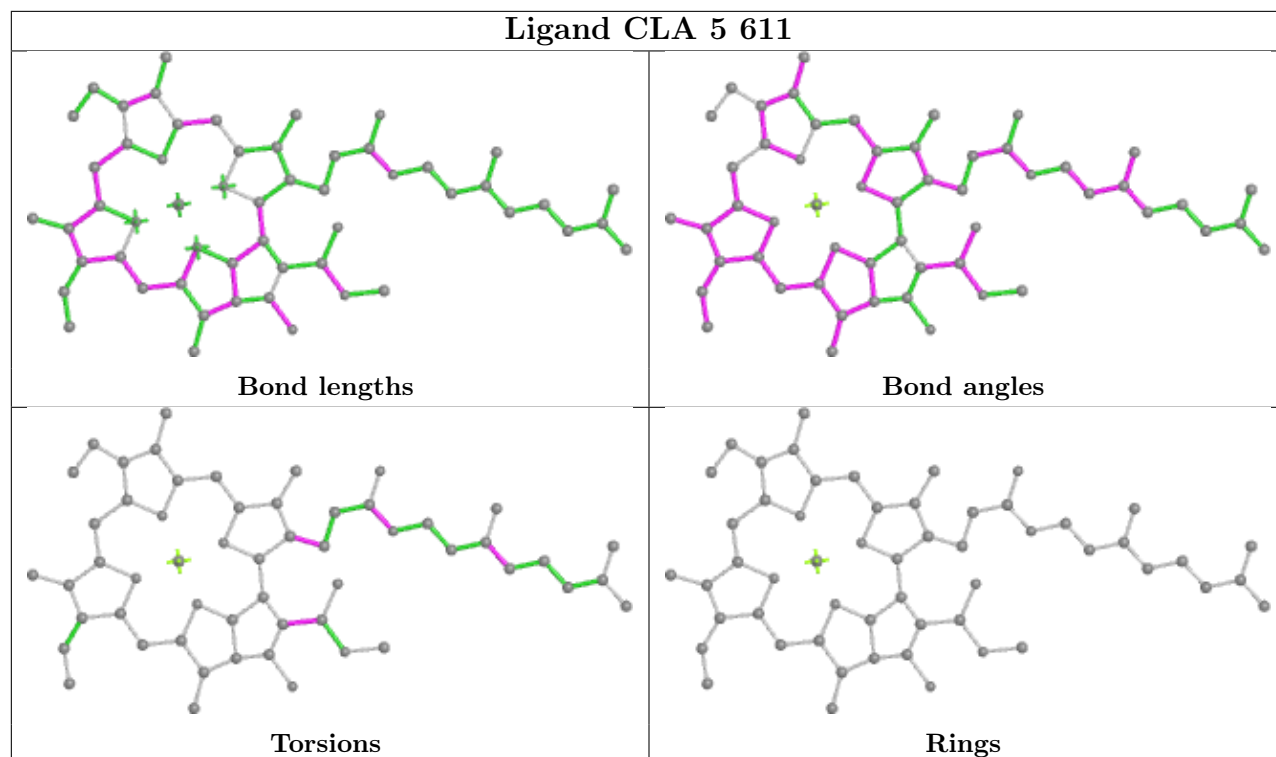
**Ligand CLA 6 602****Ligand CLA A 834****Ligand LUT 4 620**

**Ligand CLA 2 610****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 808****Bond lengths****Bond angles****Torsions****Rings**

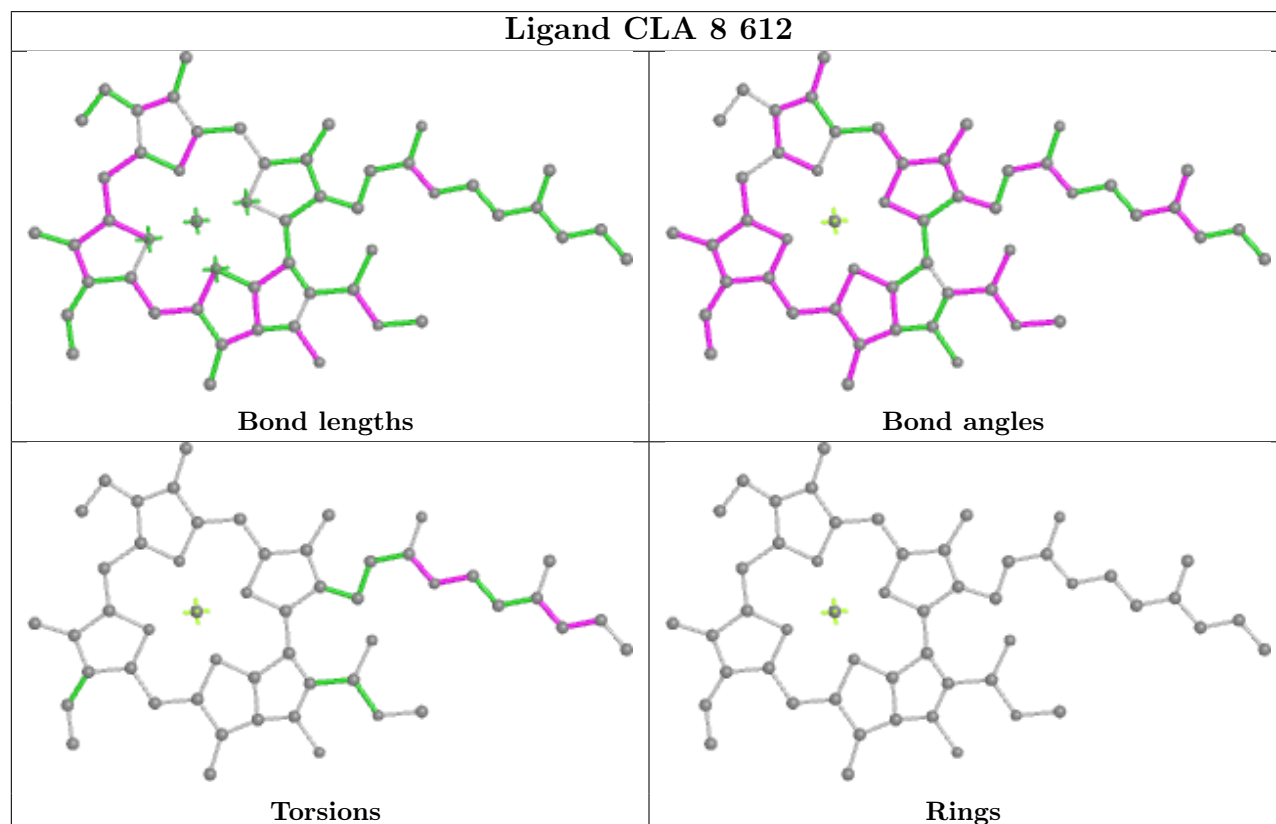
**Ligand CLA A 827****Ligand CLA B 829**

**Ligand CLA 5 606****Ligand CLA B 832****Ligand LUT 3 622**

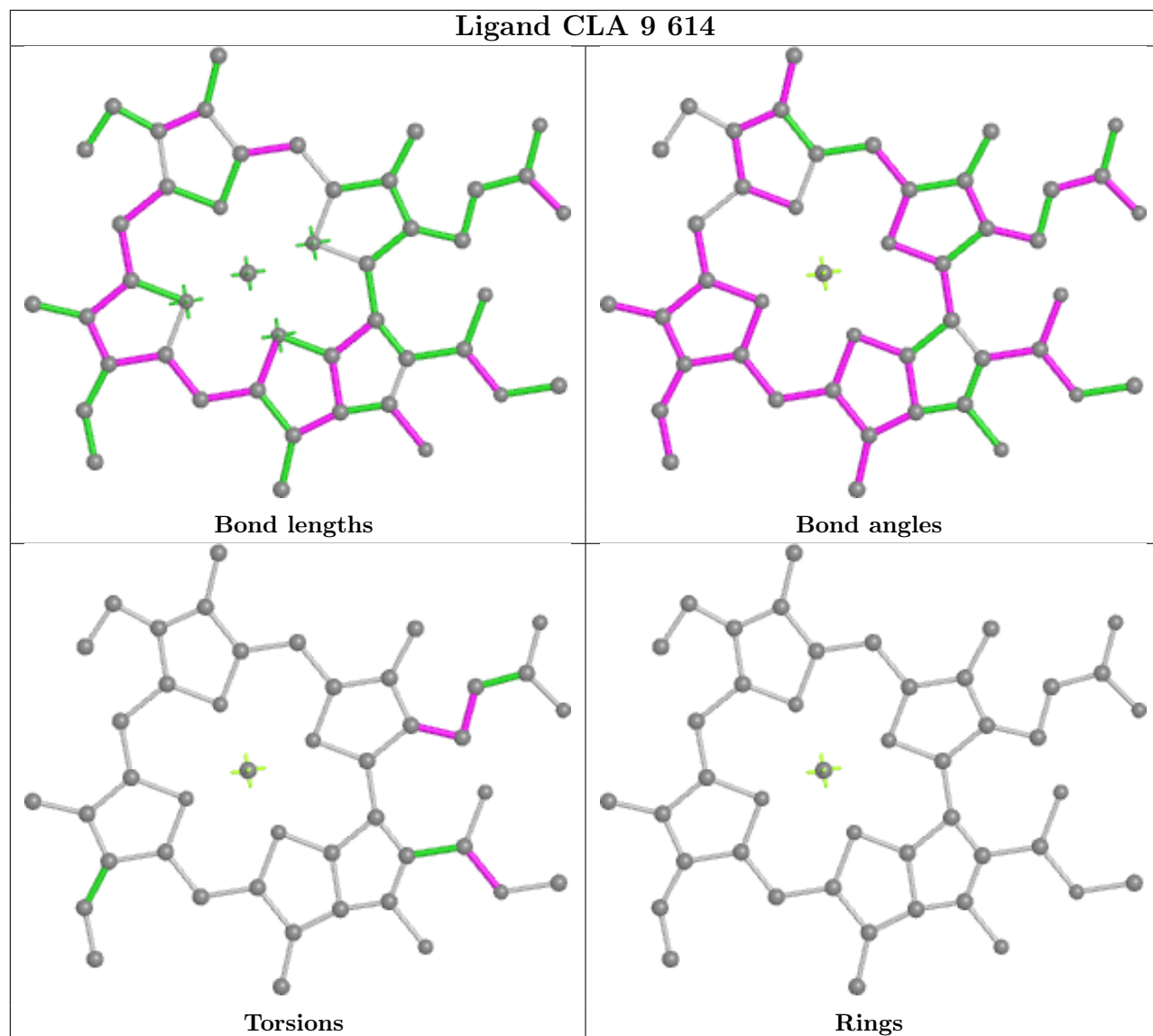
## Ligand CLA 5 611

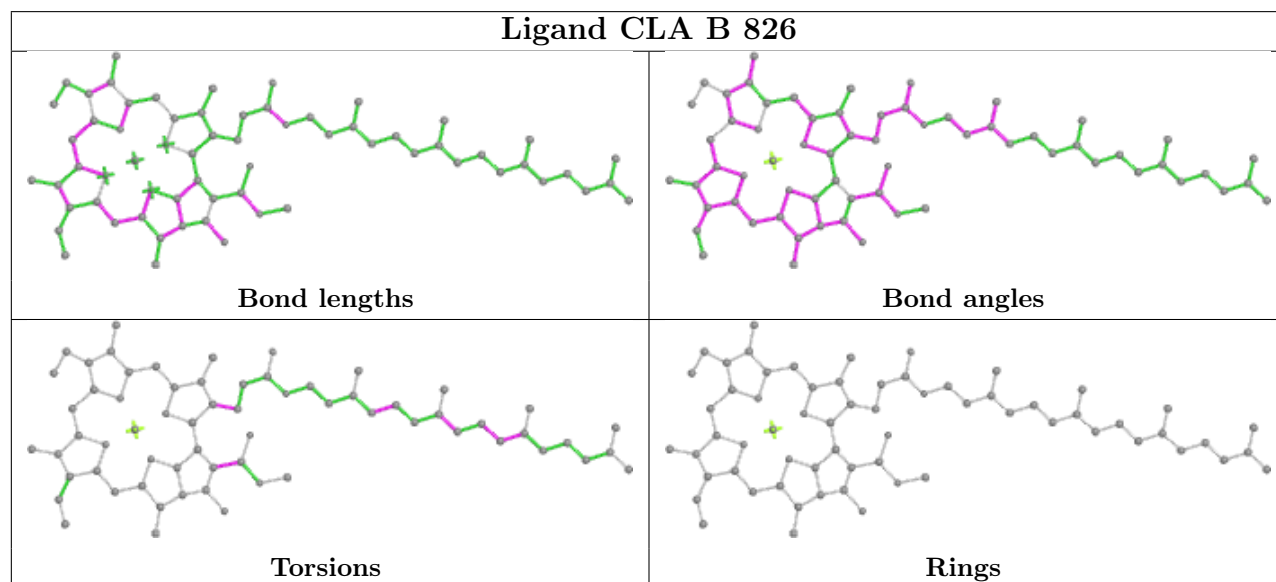
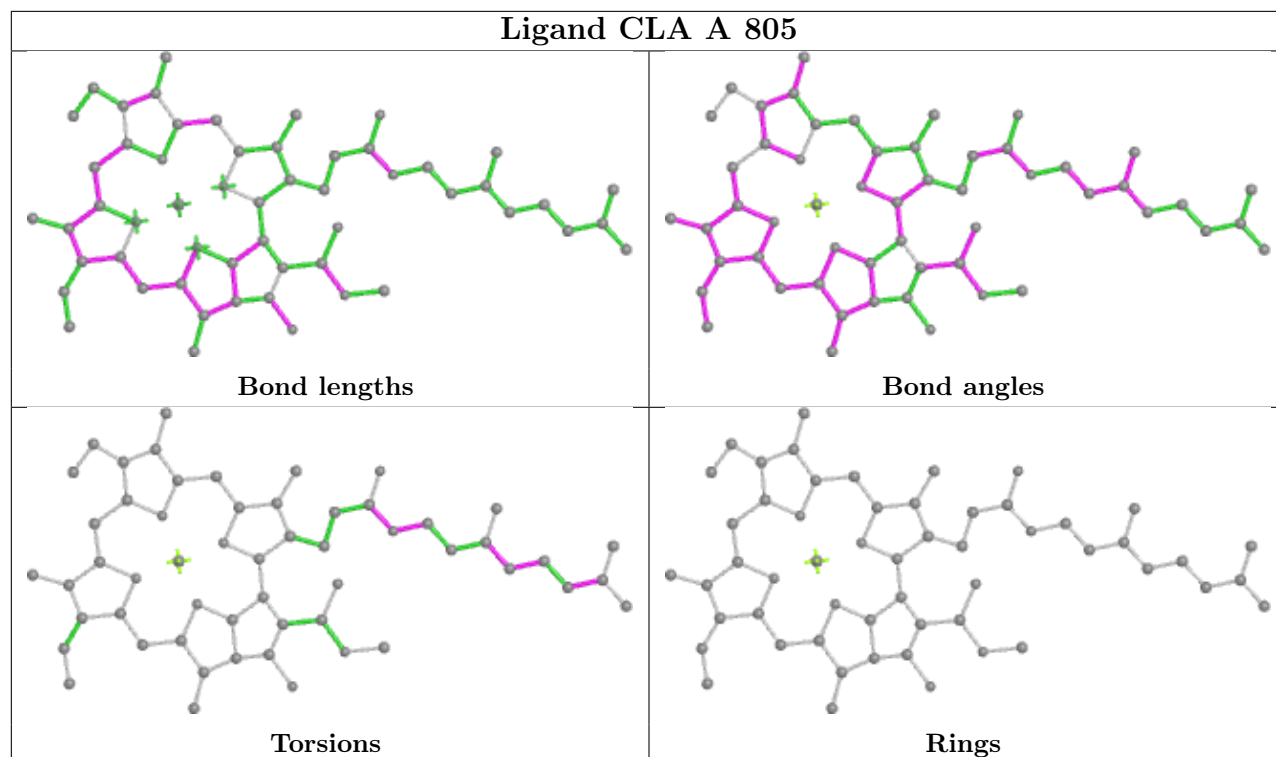


## Ligand CLA 8 612



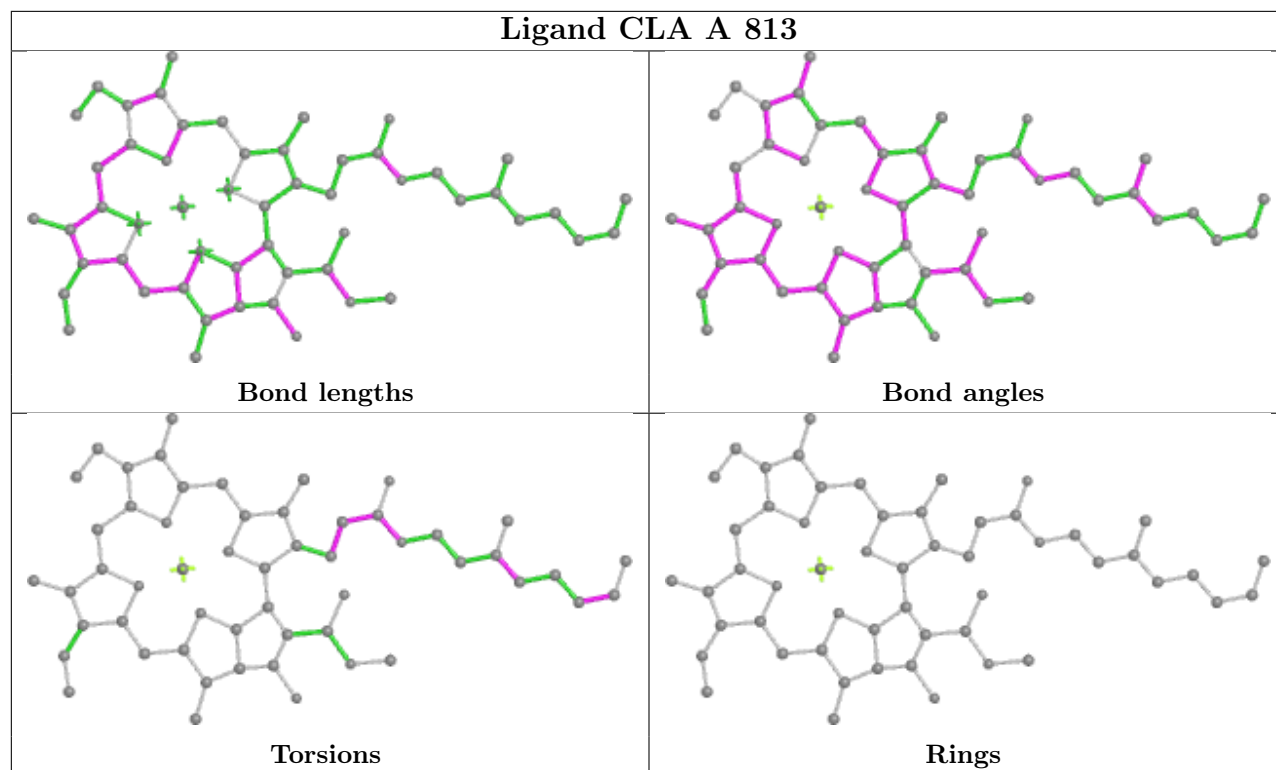
## Ligand CLA 9 614



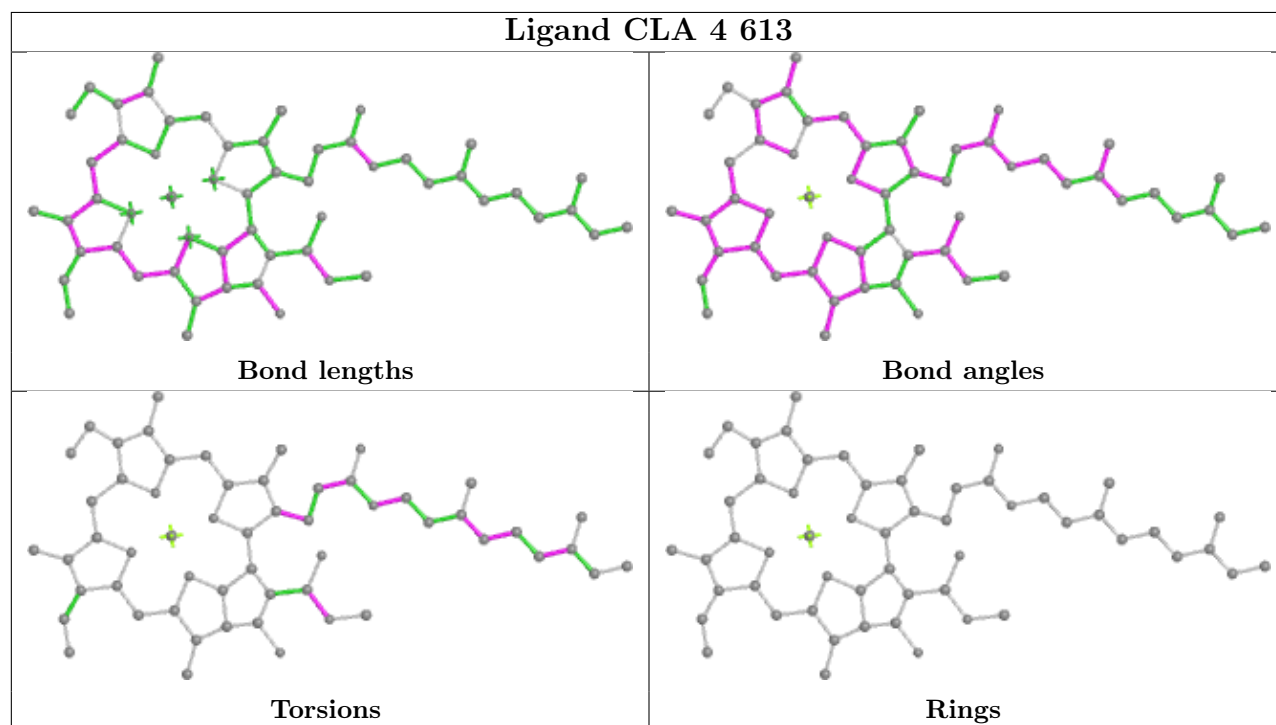


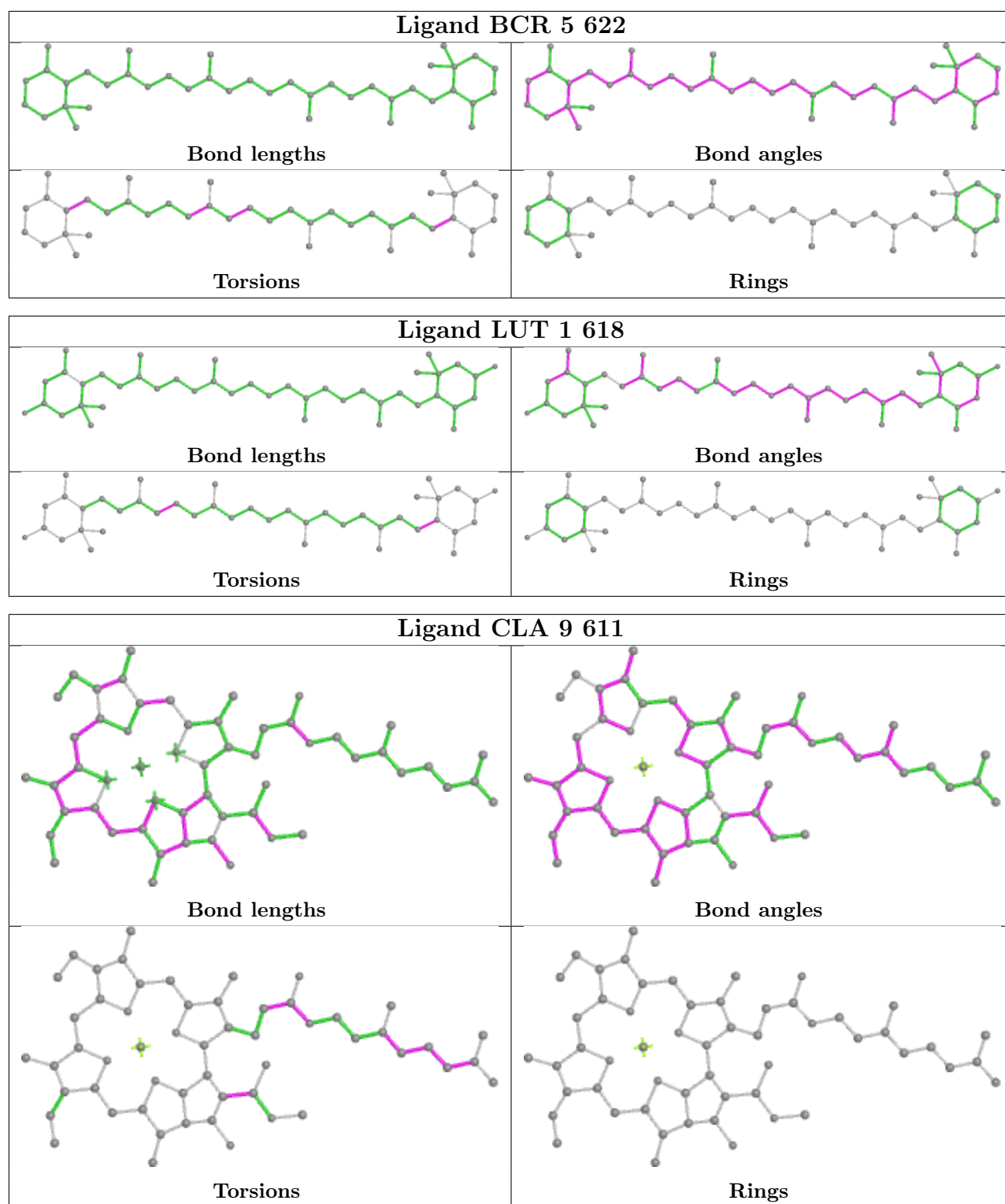


## Ligand CLA A 813

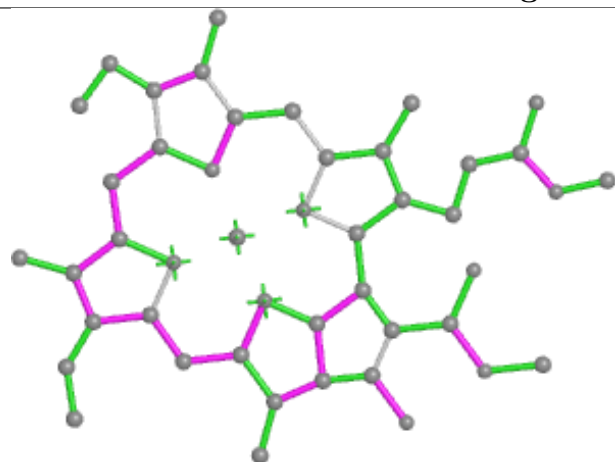


## Ligand CLA 4 613

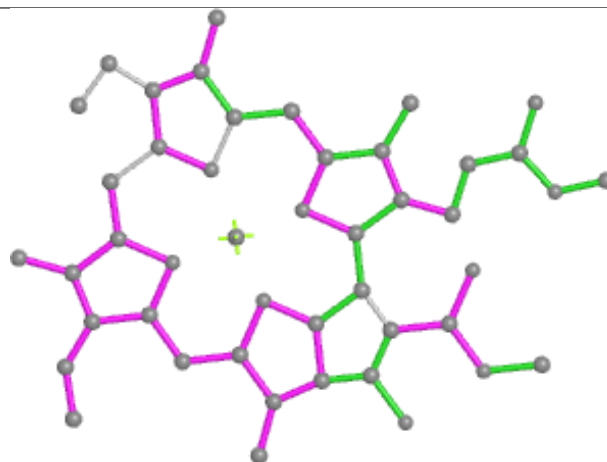




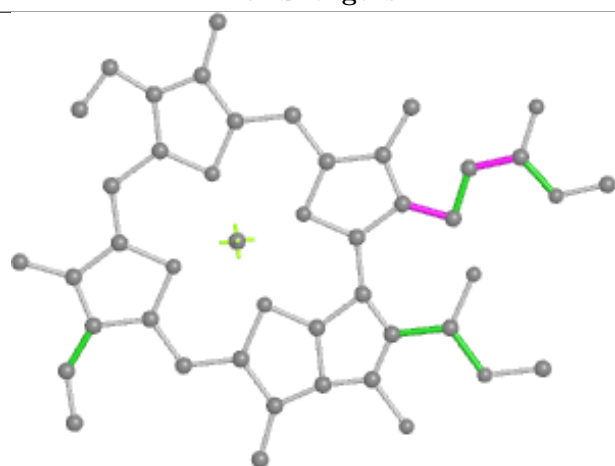
## Ligand CLA 3 617



Bond lengths



Bond angles

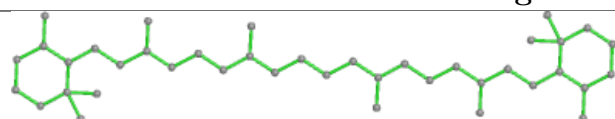


Torsions

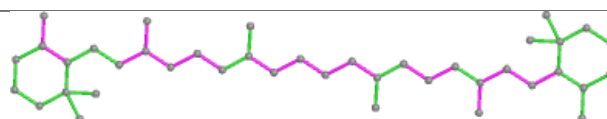


Rings

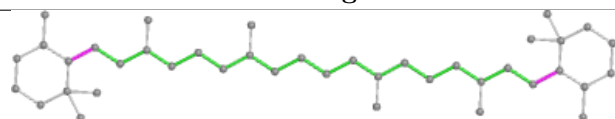
## Ligand BCR B 848



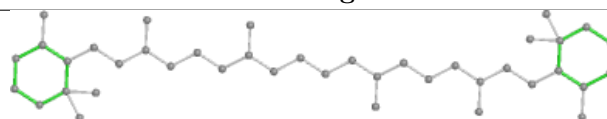
Bond lengths



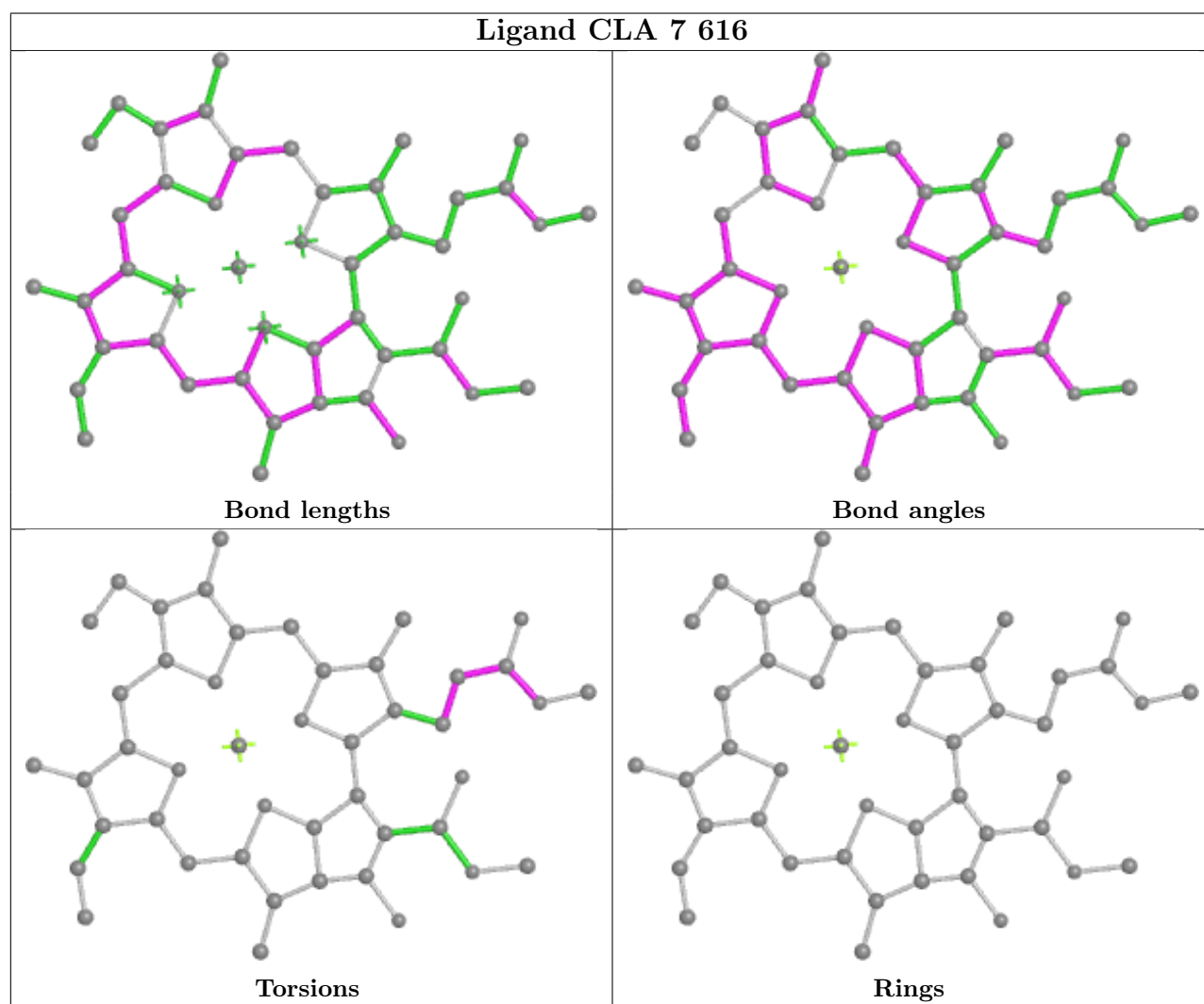
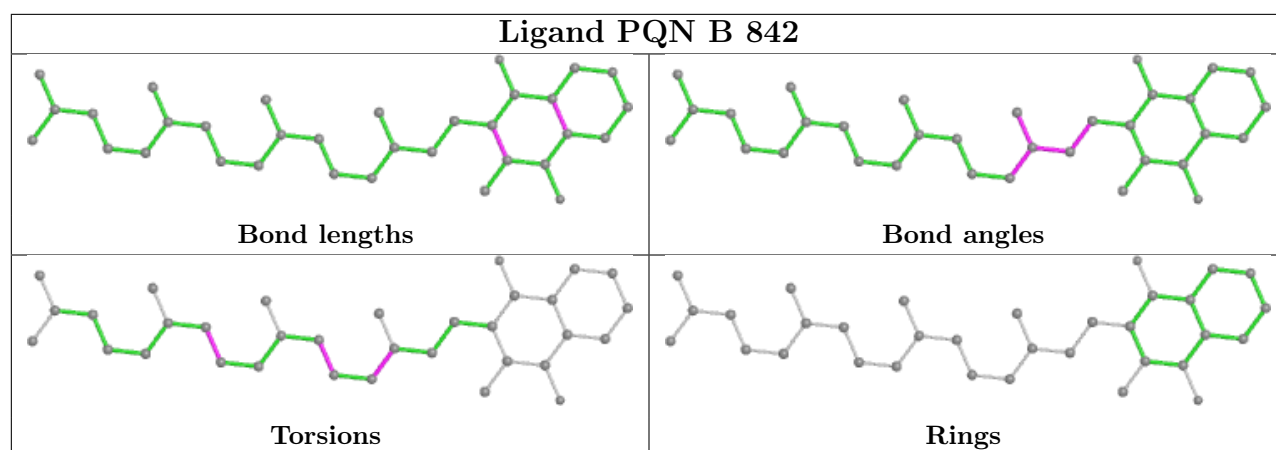
Bond angles



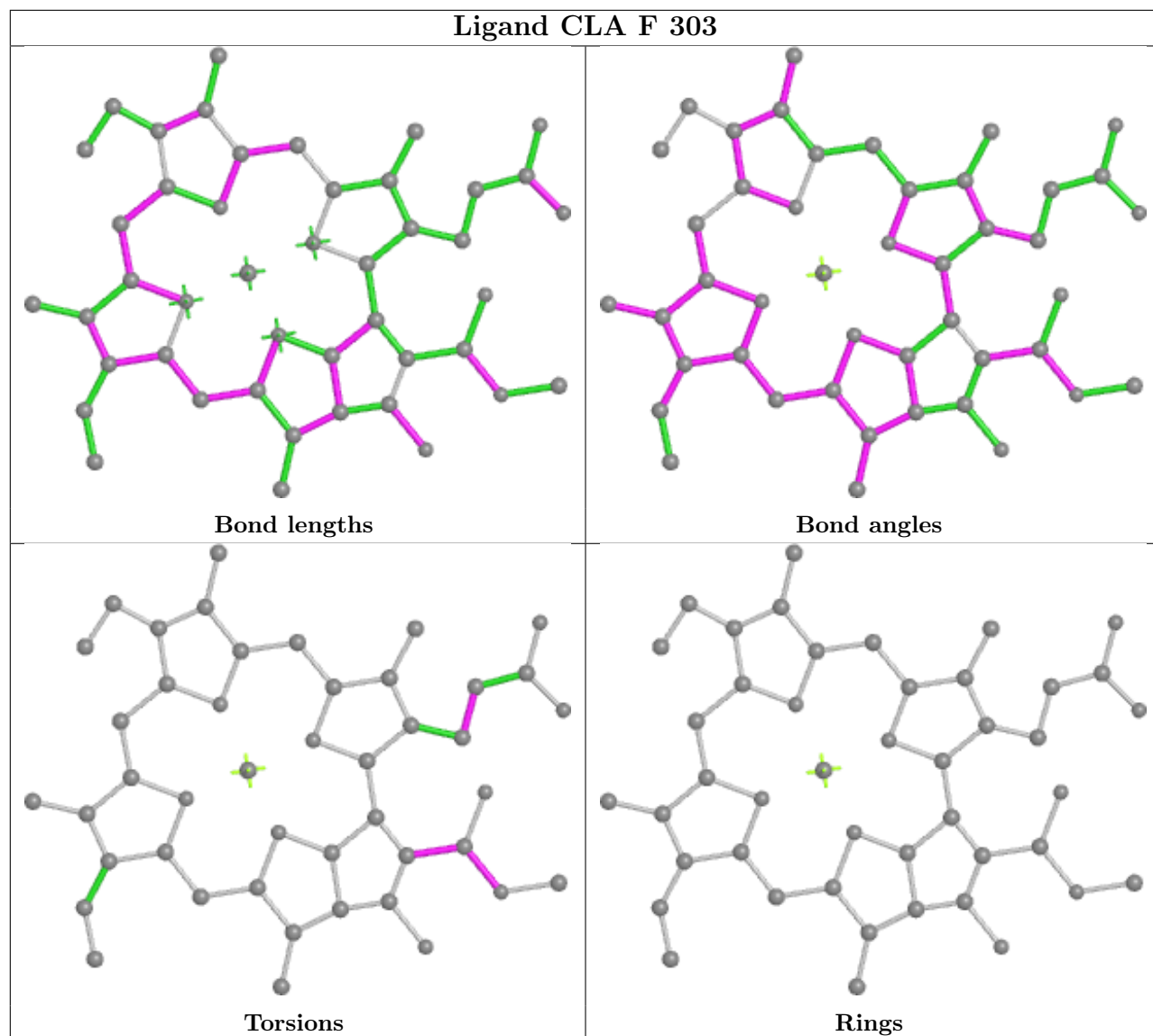
Torsions



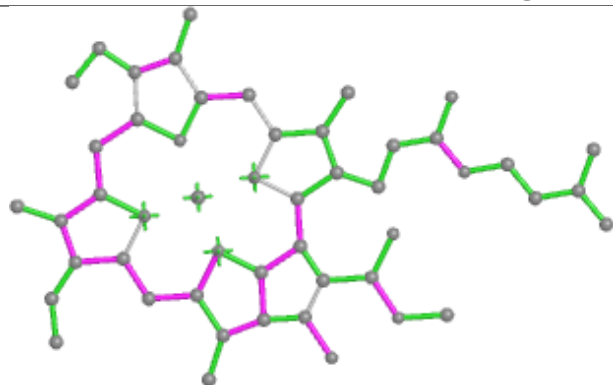
Rings



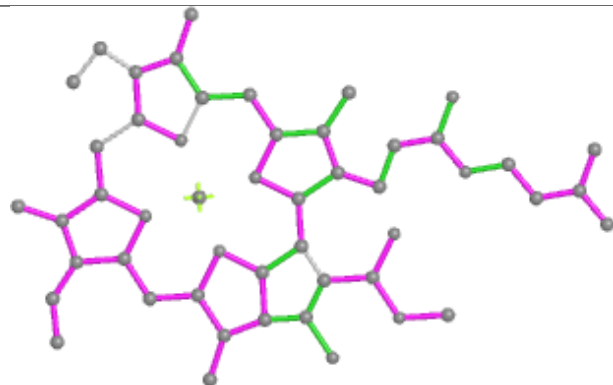
## Ligand CLA F 303



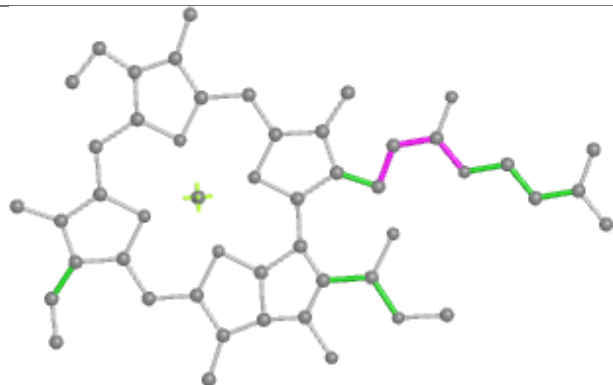
## Ligand CLA 2 609



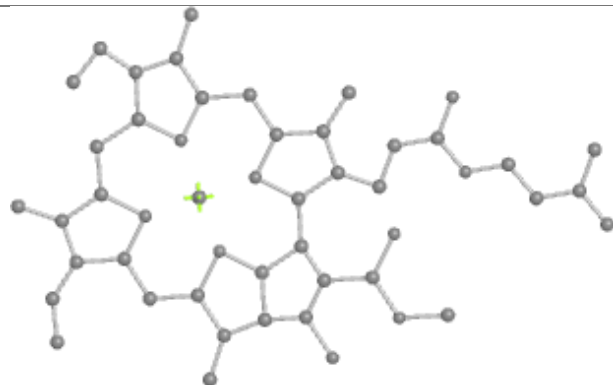
Bond lengths



Bond angles

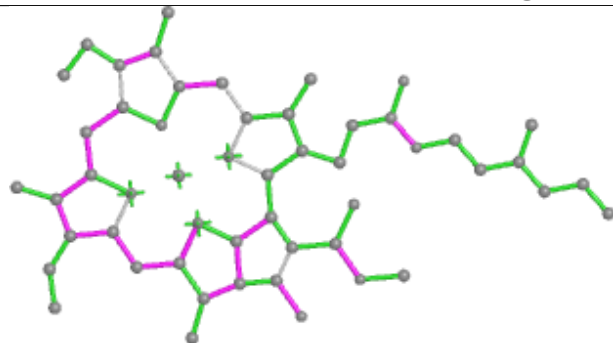


Torsions

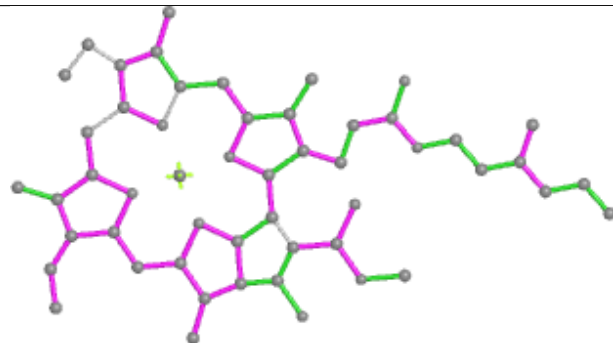


Rings

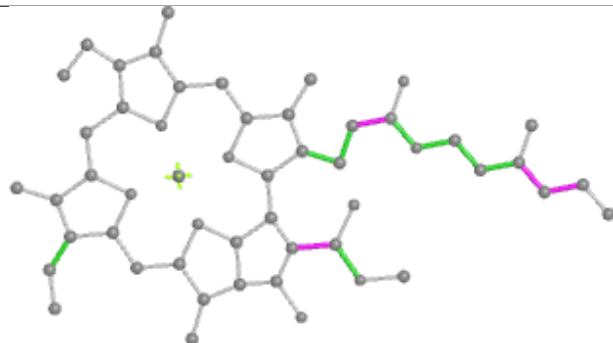
## Ligand CLA 2 612



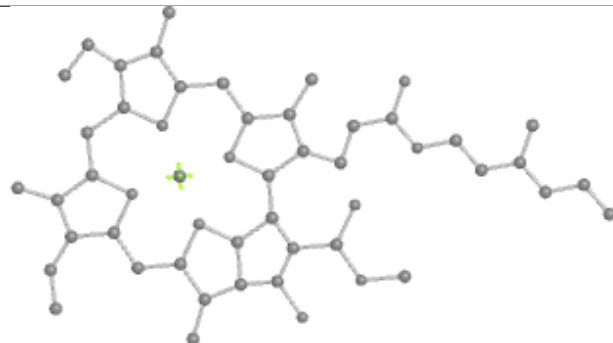
Bond lengths



Bond angles

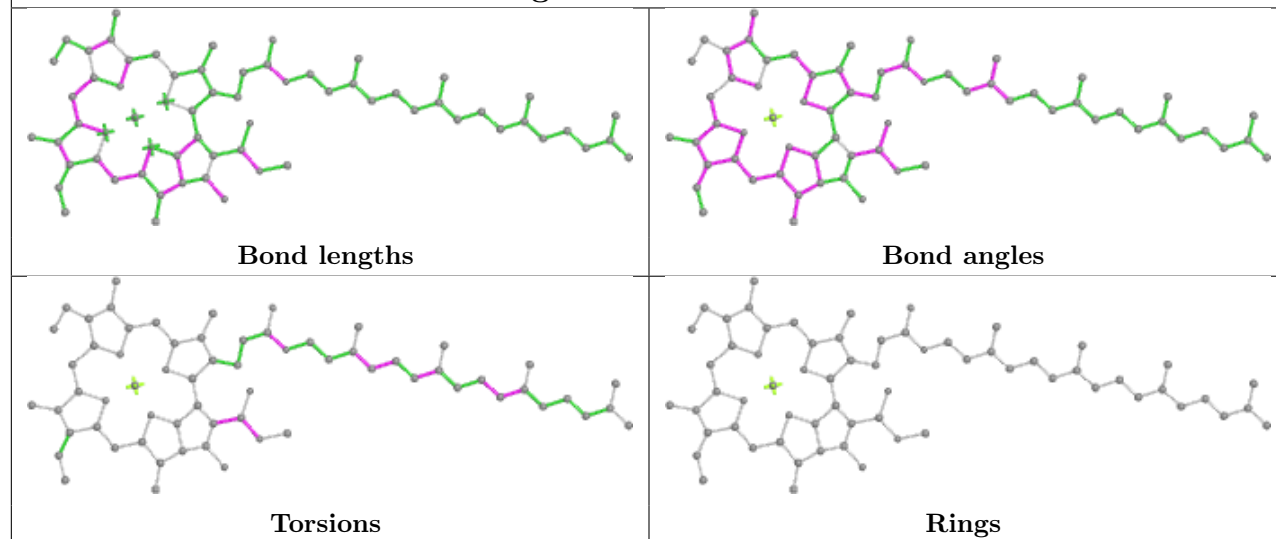


Torsions

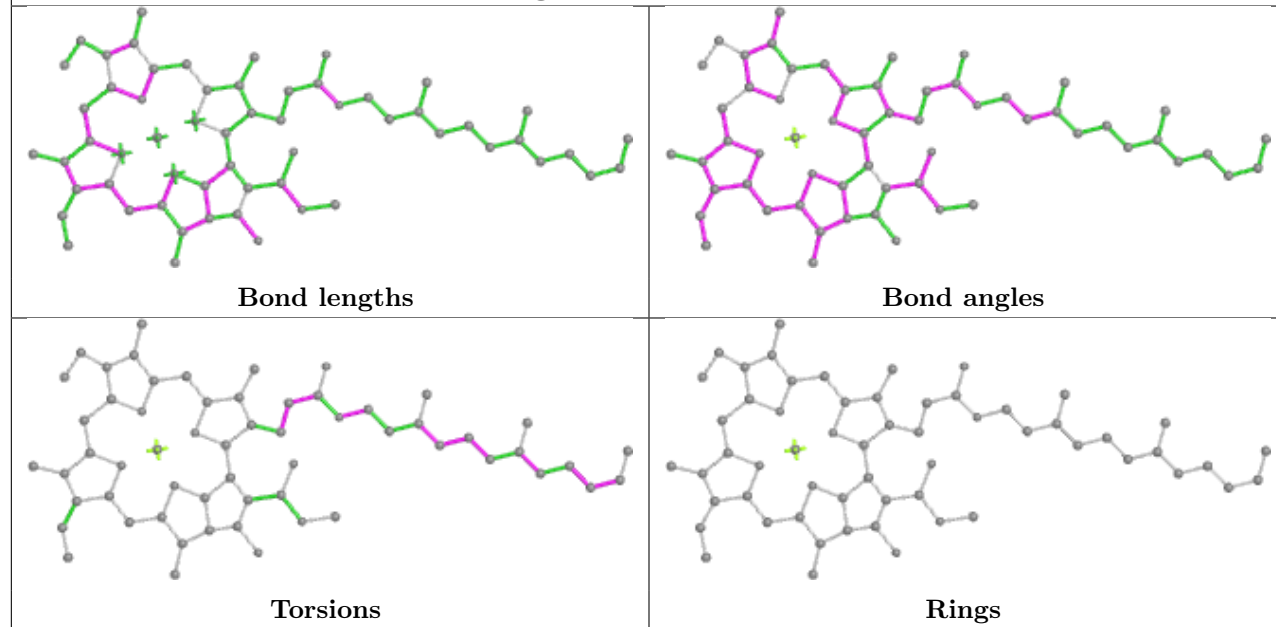


Rings

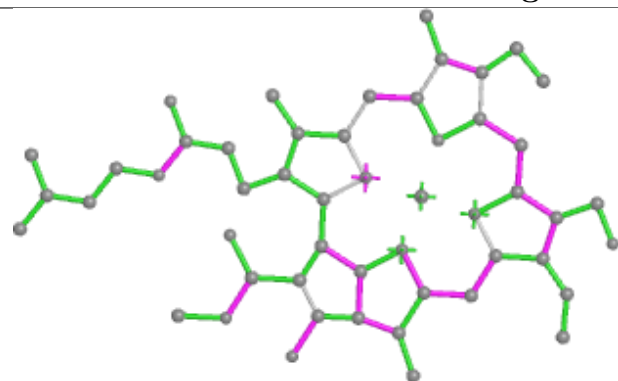
## Ligand CLA A 818



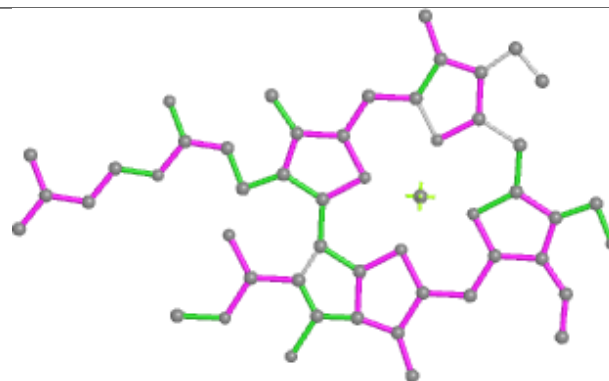
## Ligand CLA B 817



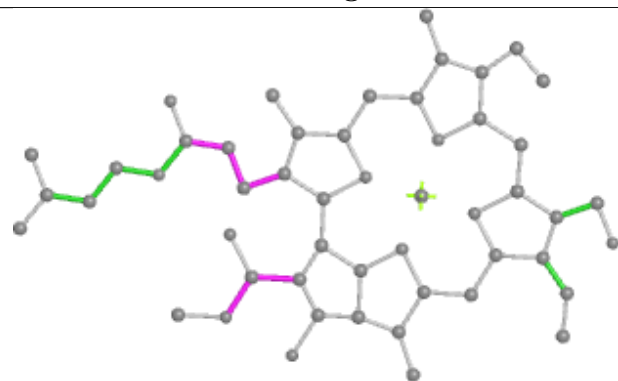
## Ligand CHL 4 608



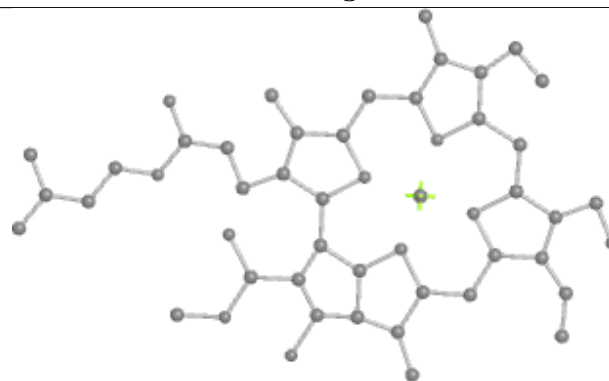
Bond lengths



Bond angles

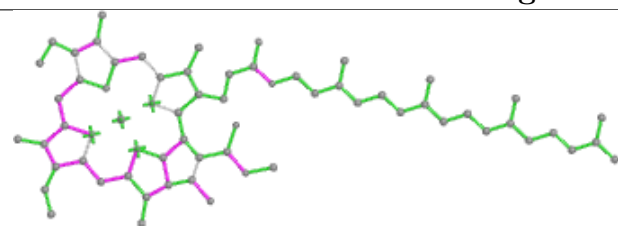


Torsions

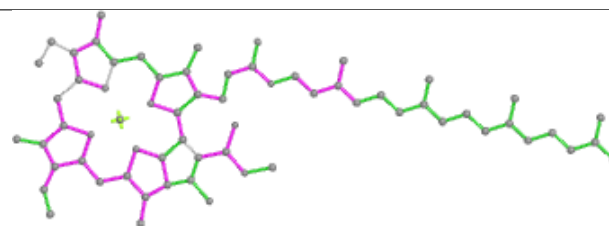


Rings

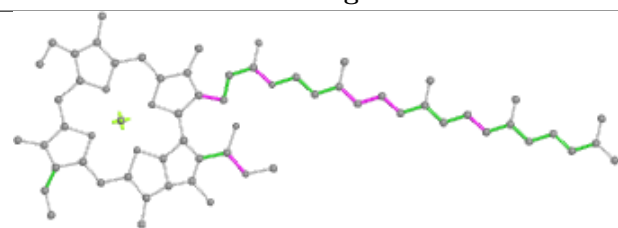
## Ligand CLA B 810



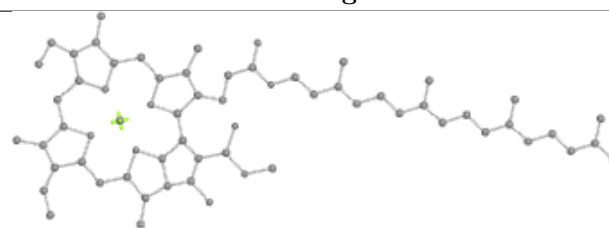
Bond lengths



Bond angles

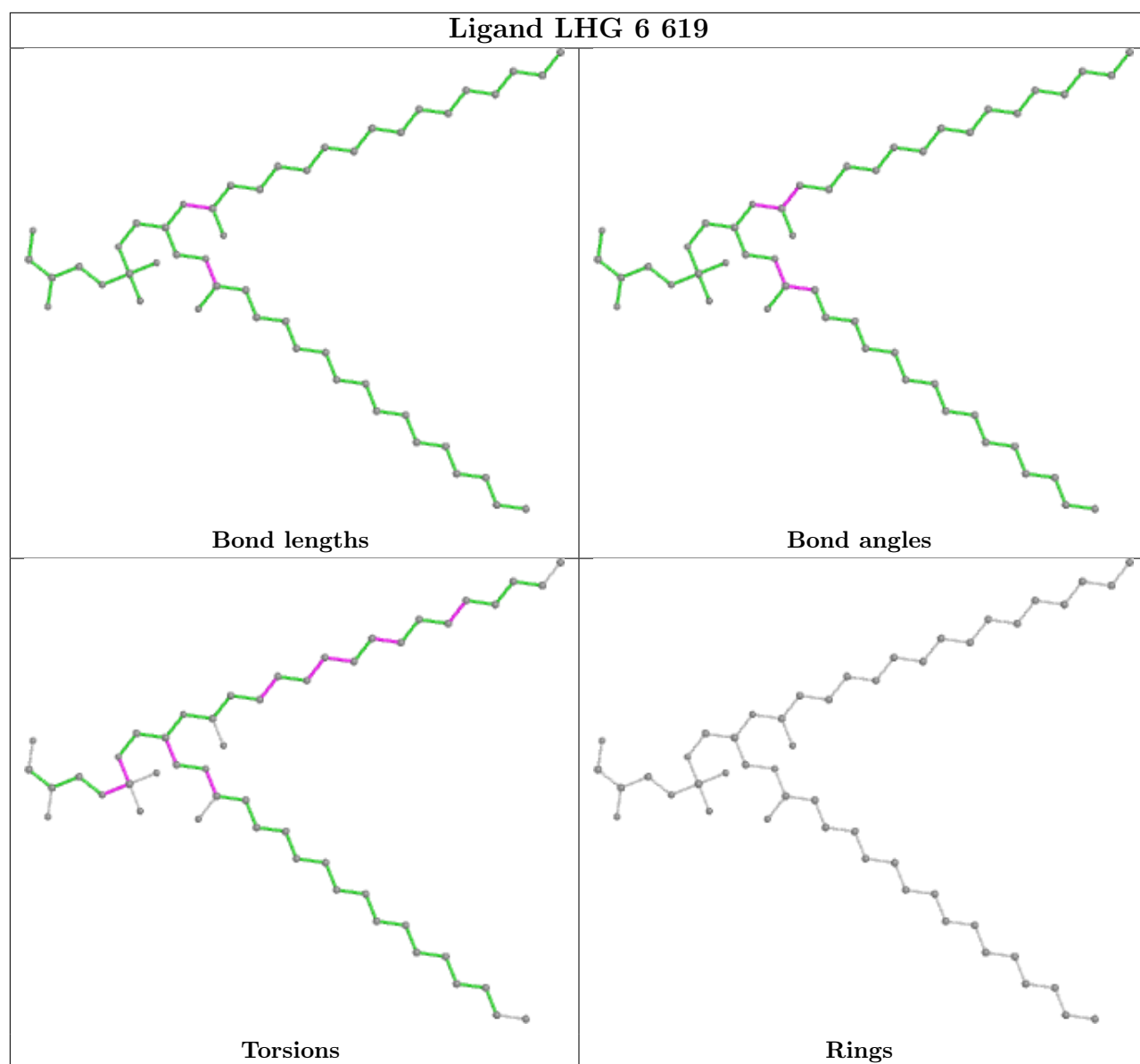


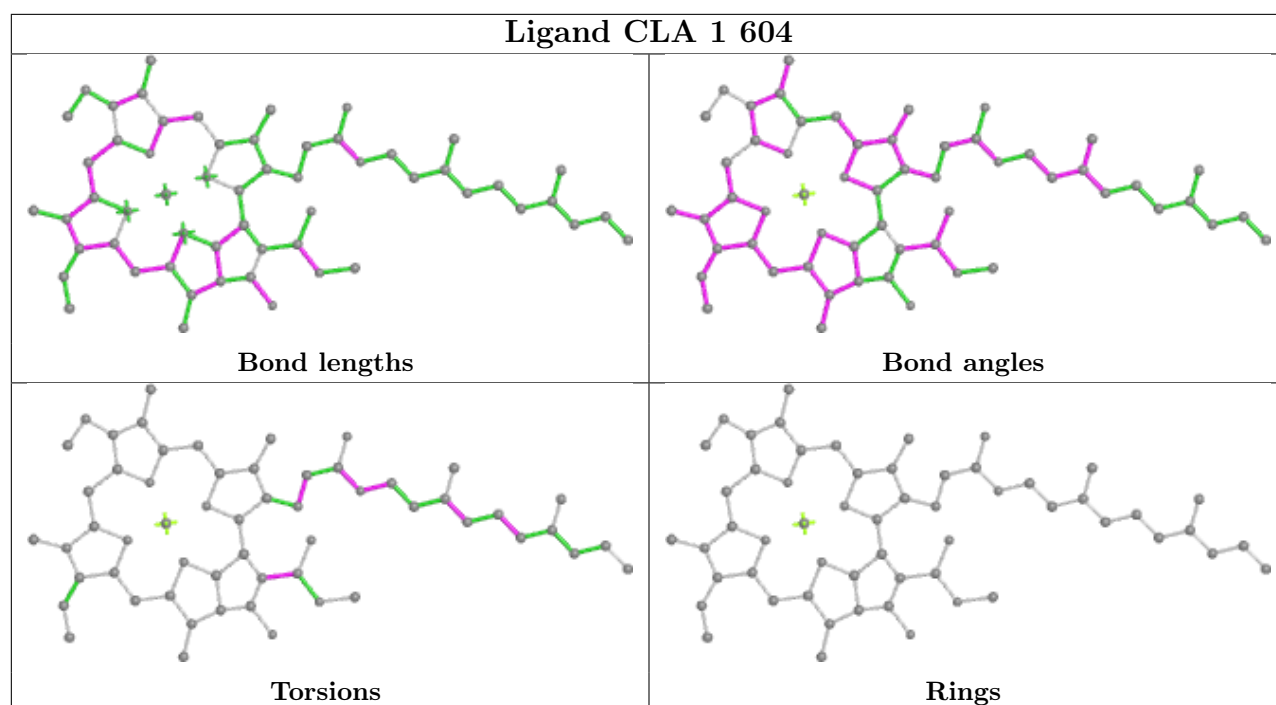
Torsions



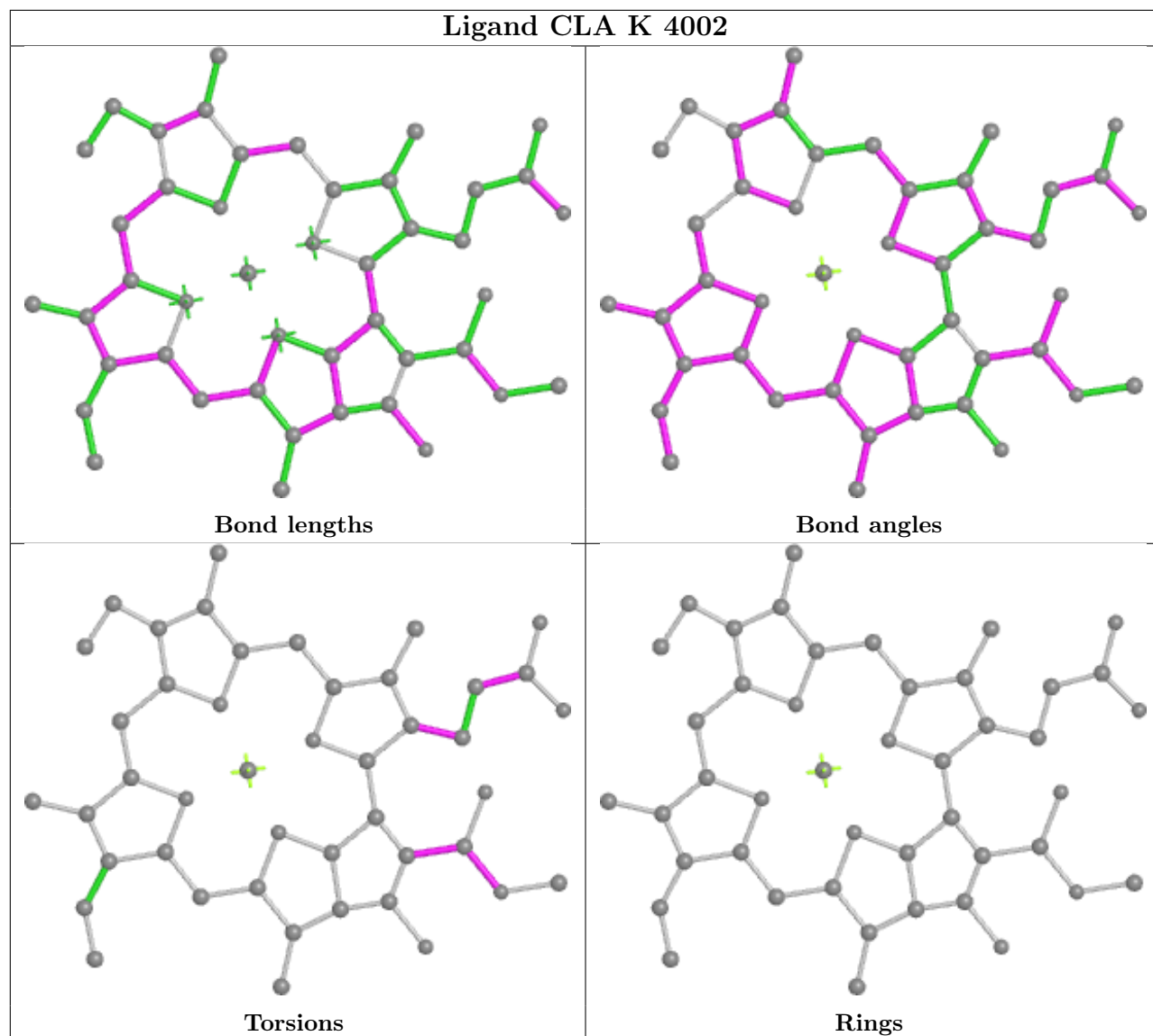
Rings



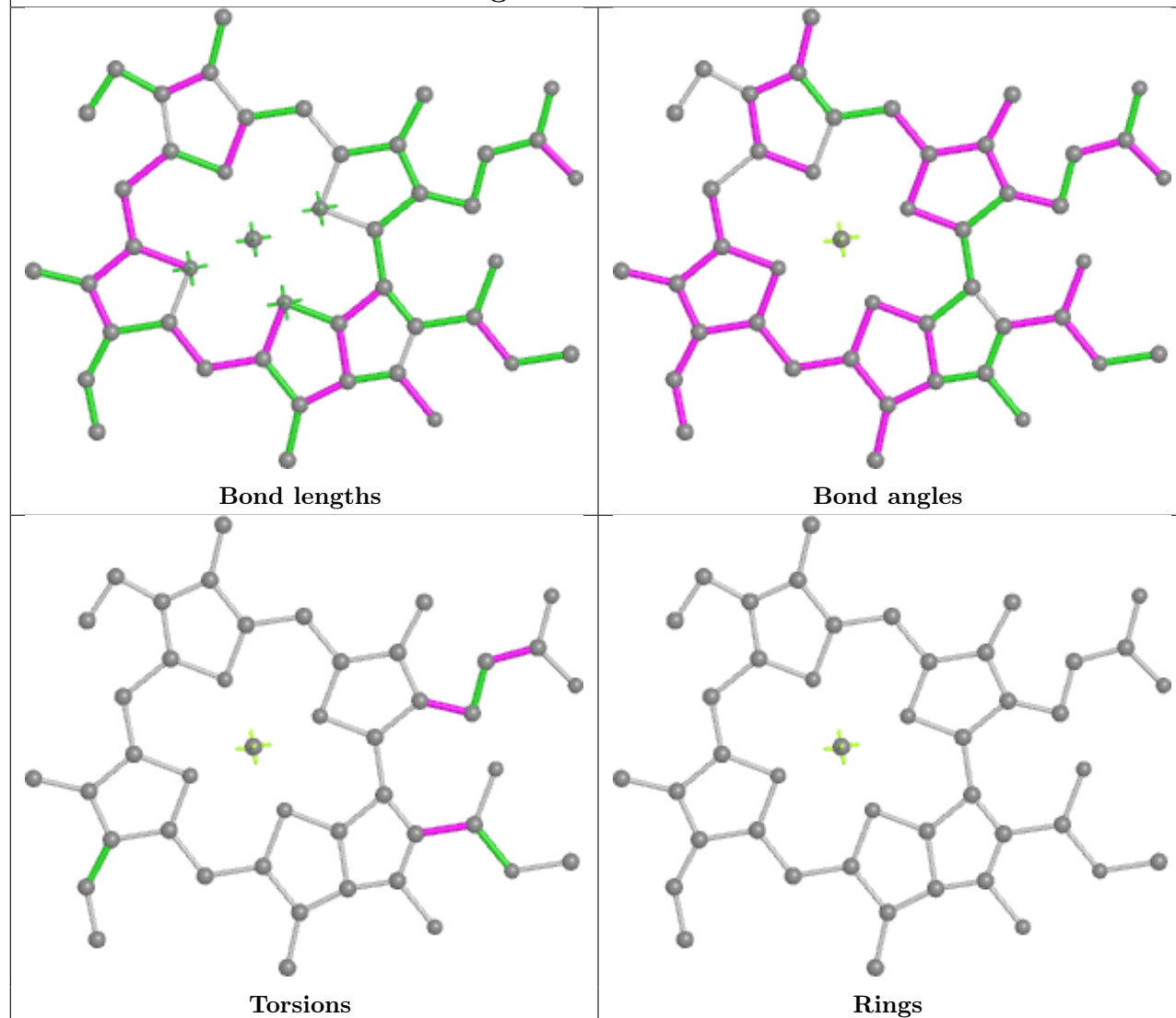




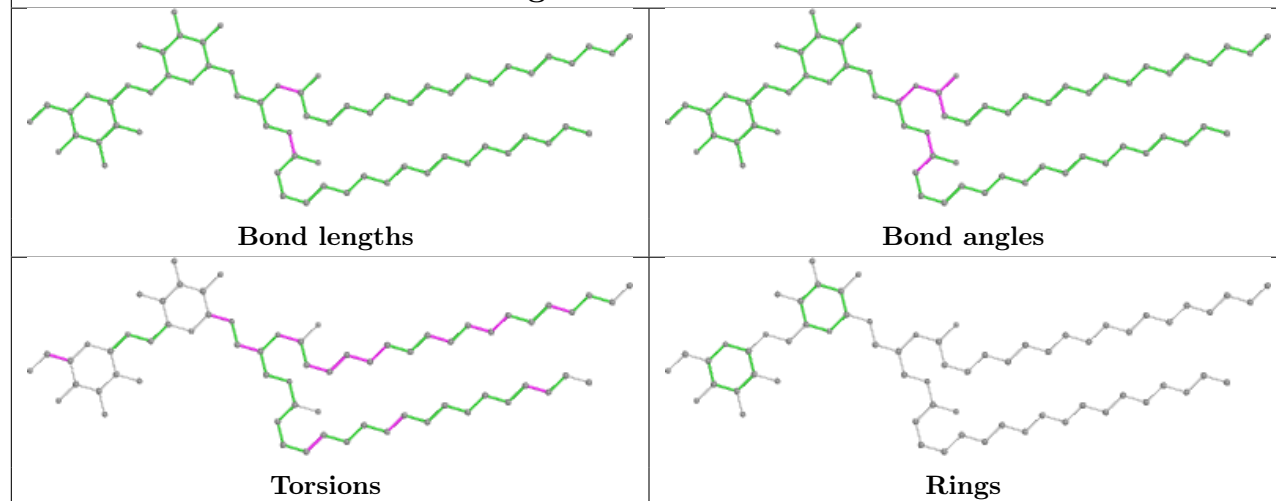
## Ligand CLA K 4002

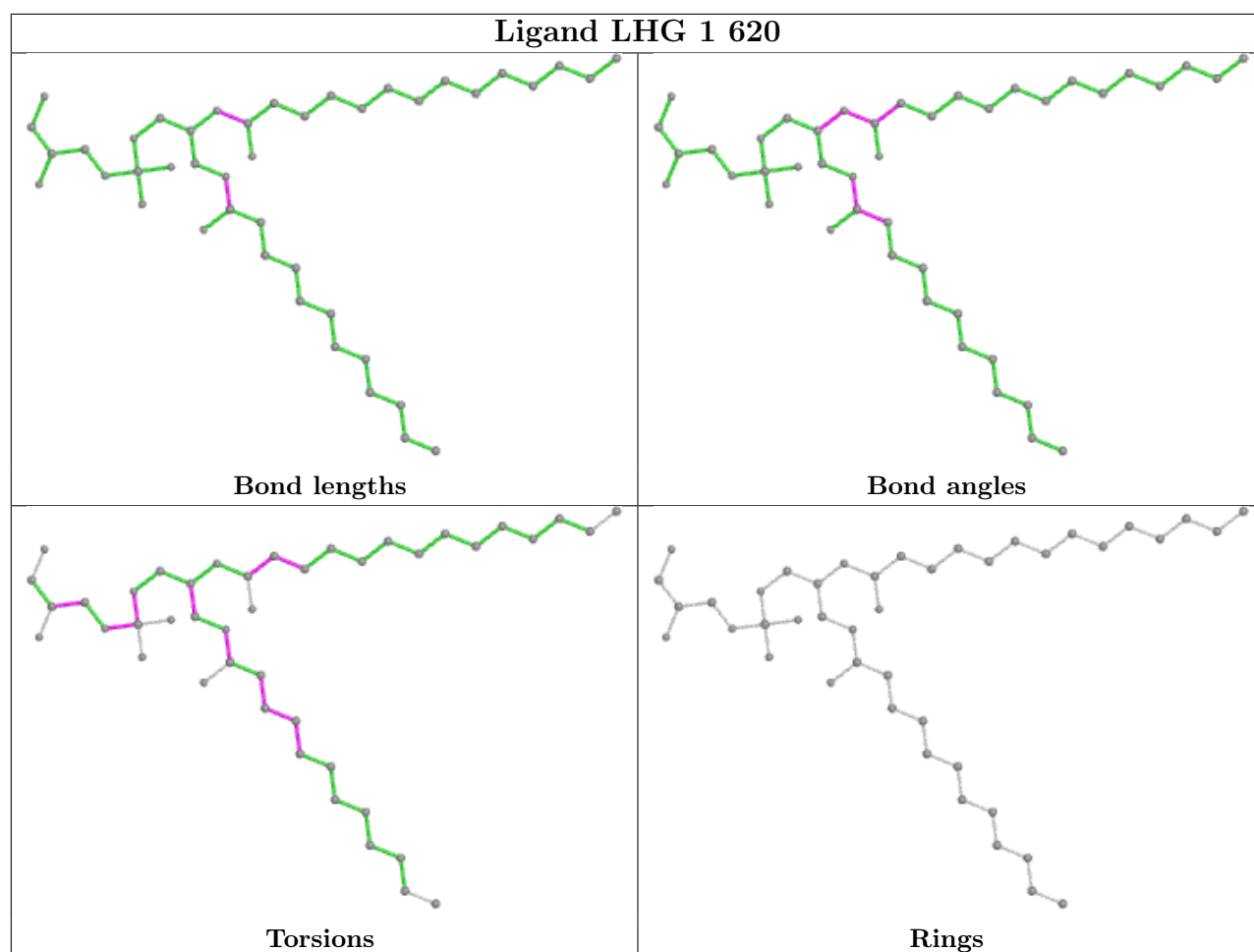


## Ligand CLA B 804

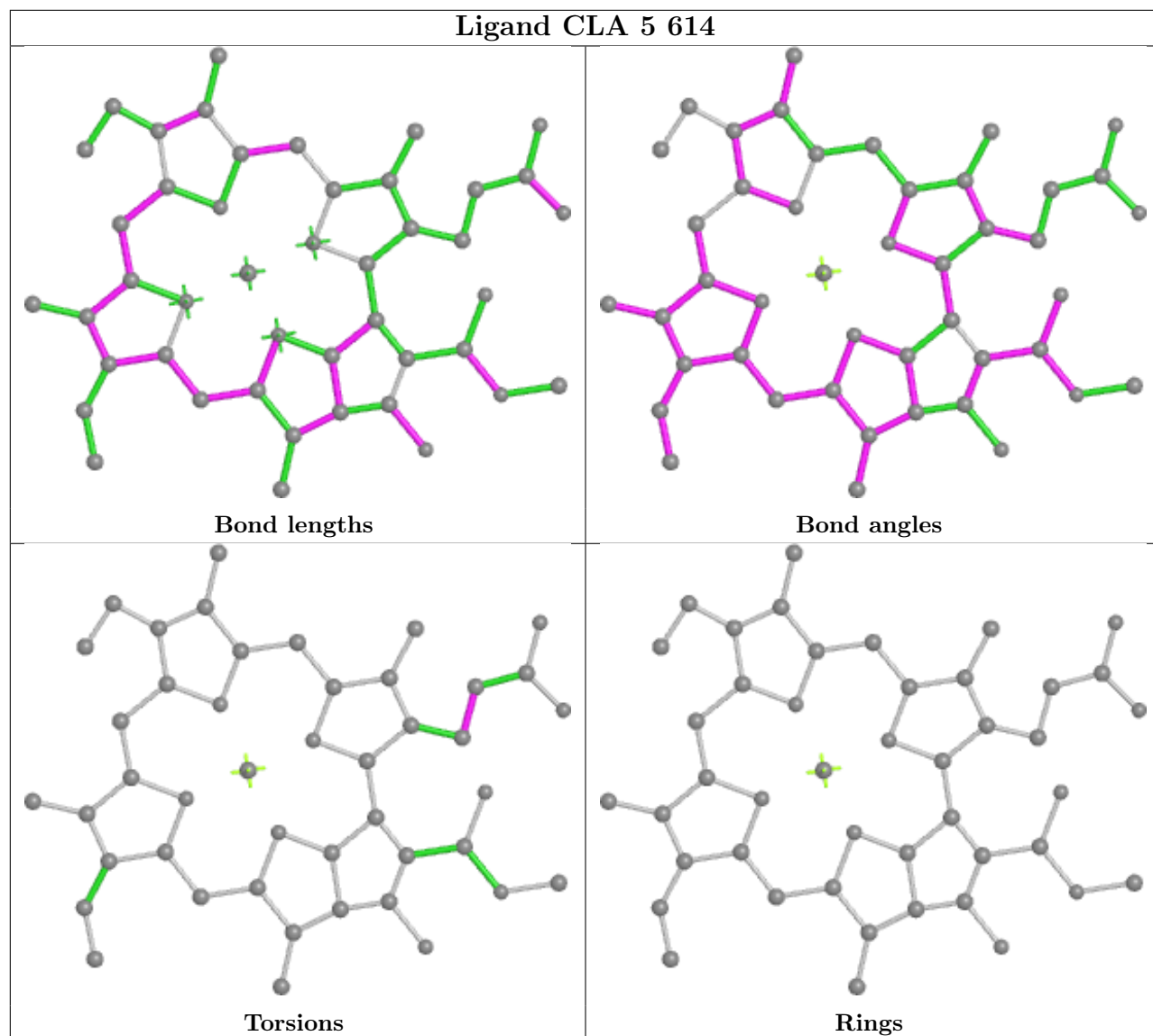


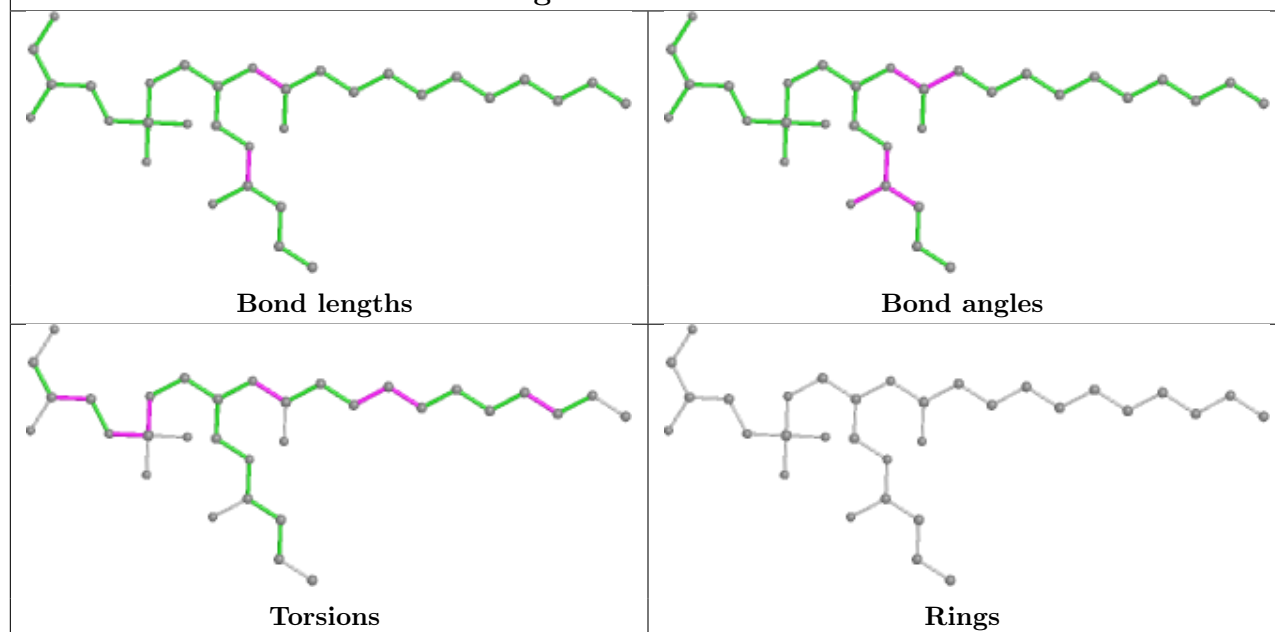
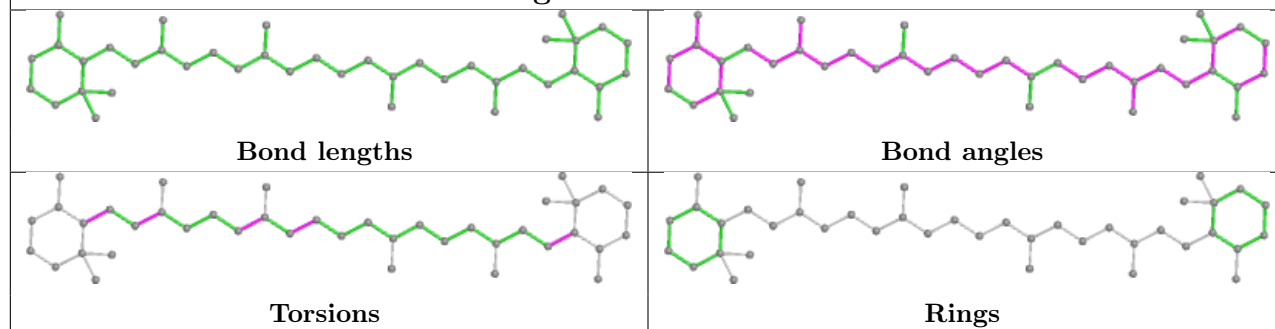
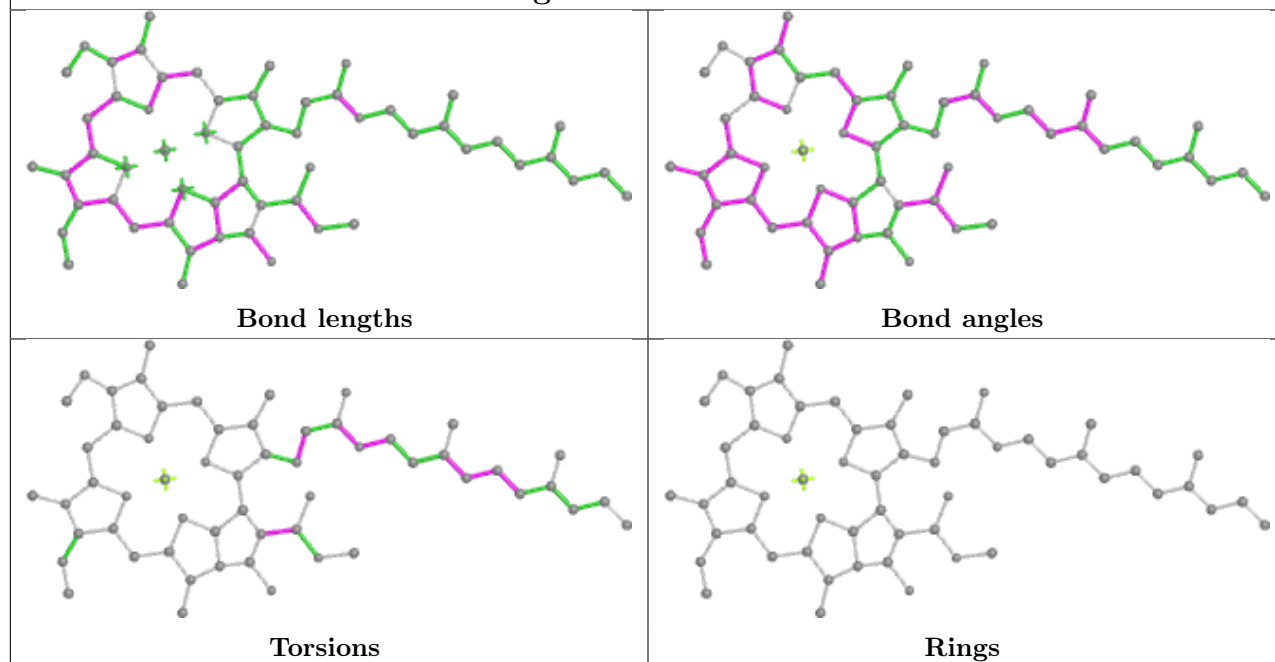
## Ligand DGD B 850



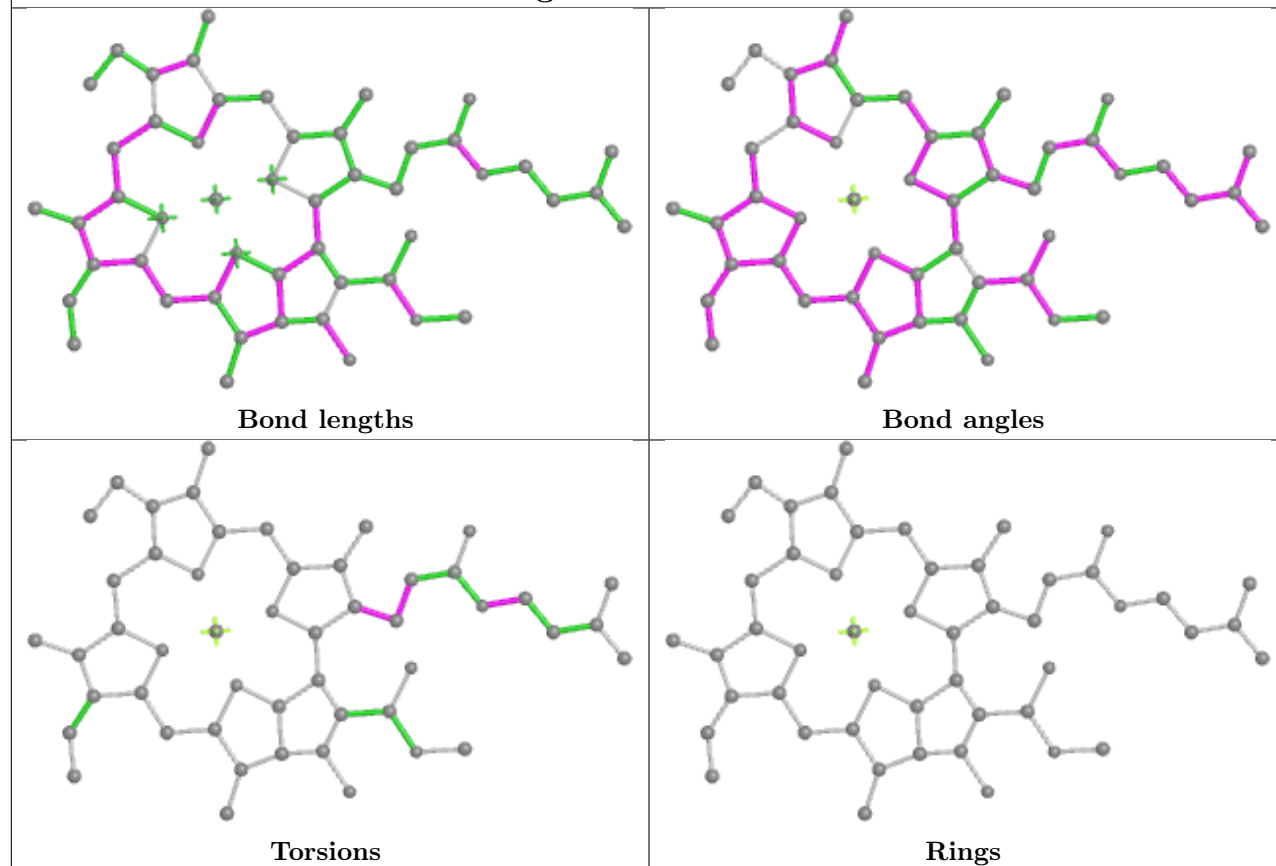


## Ligand CLA 5 614

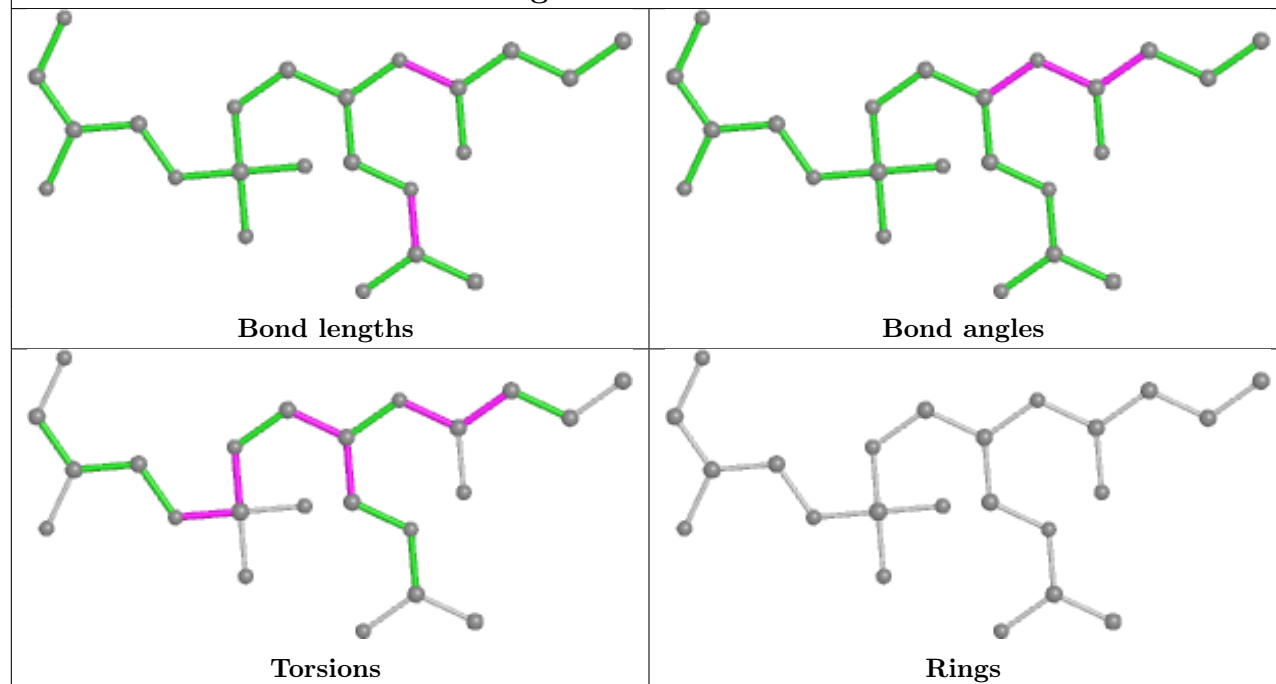


**Ligand LHG 4 623****Ligand BCR 6 625****Ligand CLA Z 604**

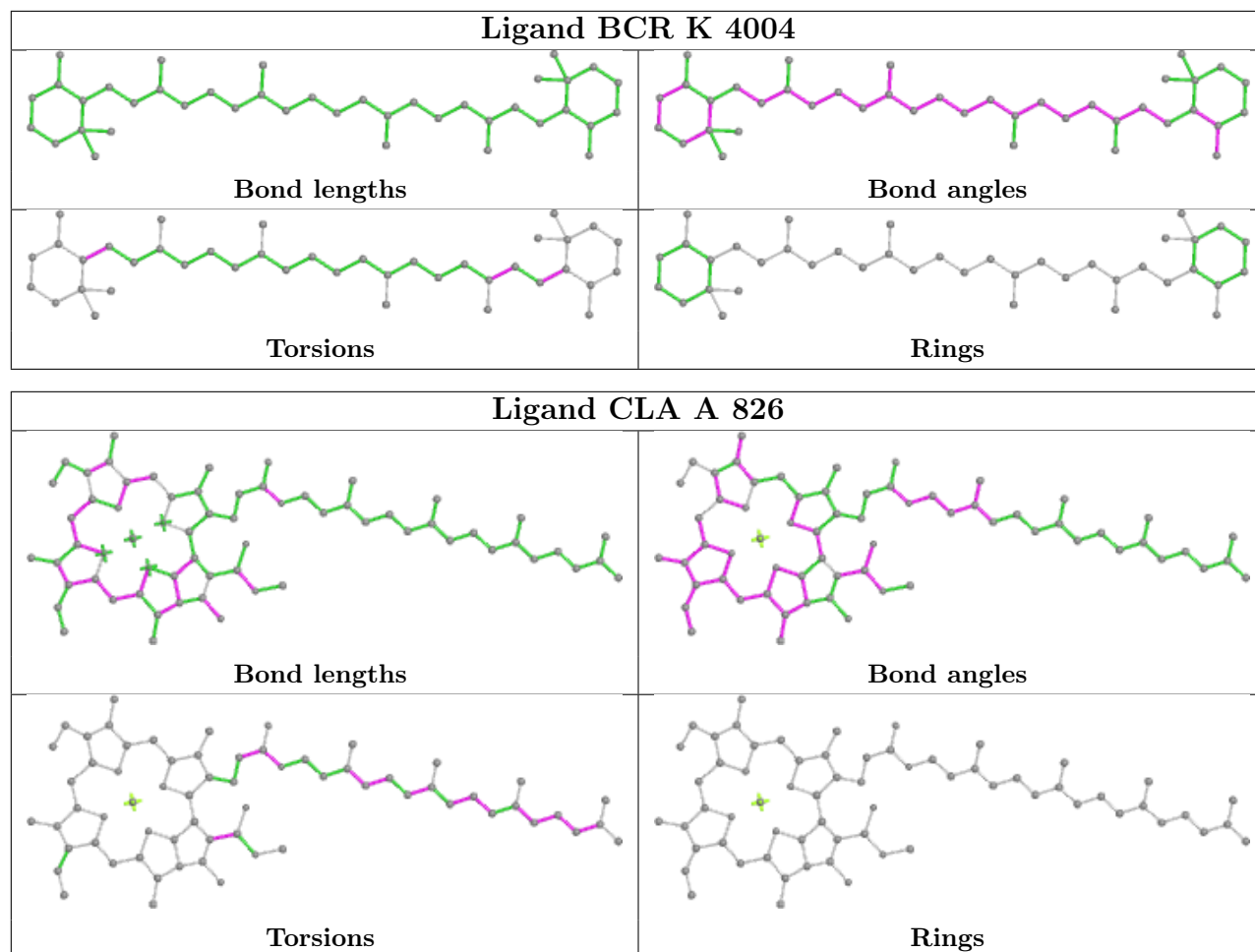
## Ligand CLA 5 609



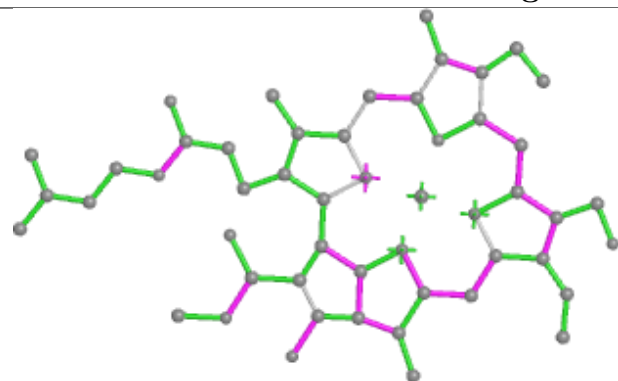
## Ligand LHG B 851



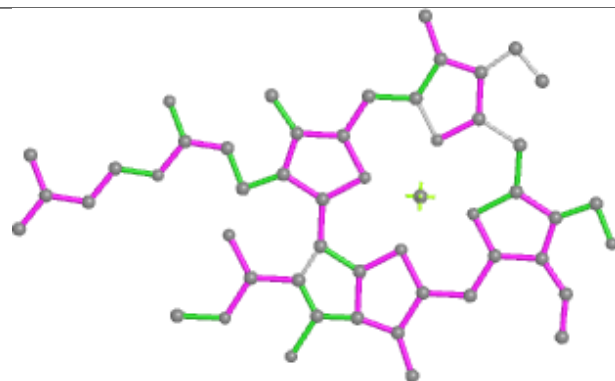




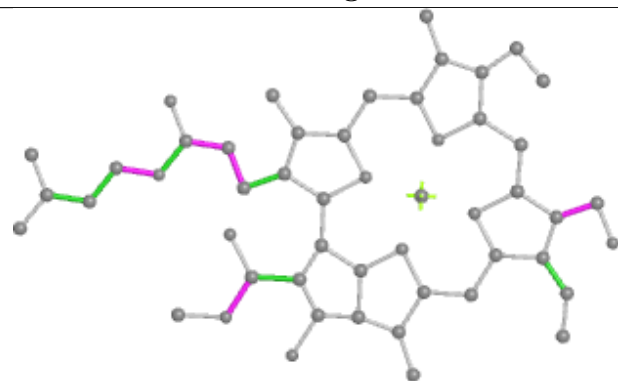
## Ligand CHL 4 607



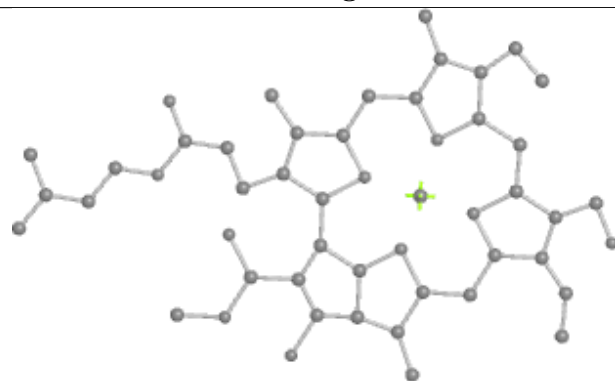
Bond lengths



Bond angles

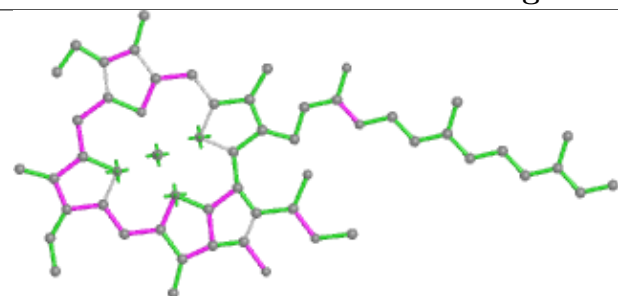


Torsions

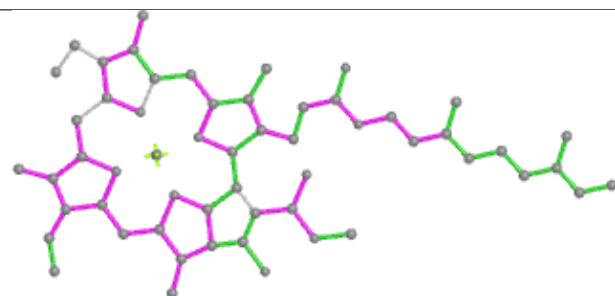


Rings

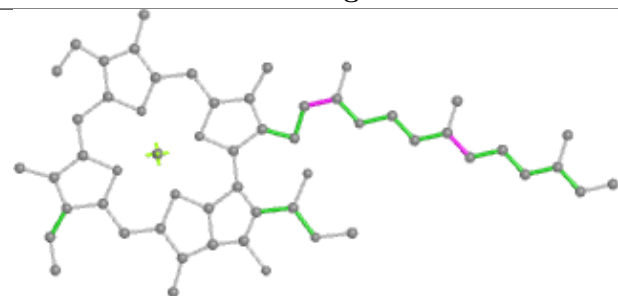
## Ligand CLA 6 613



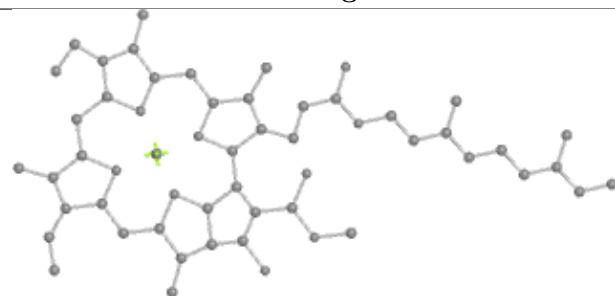
Bond lengths



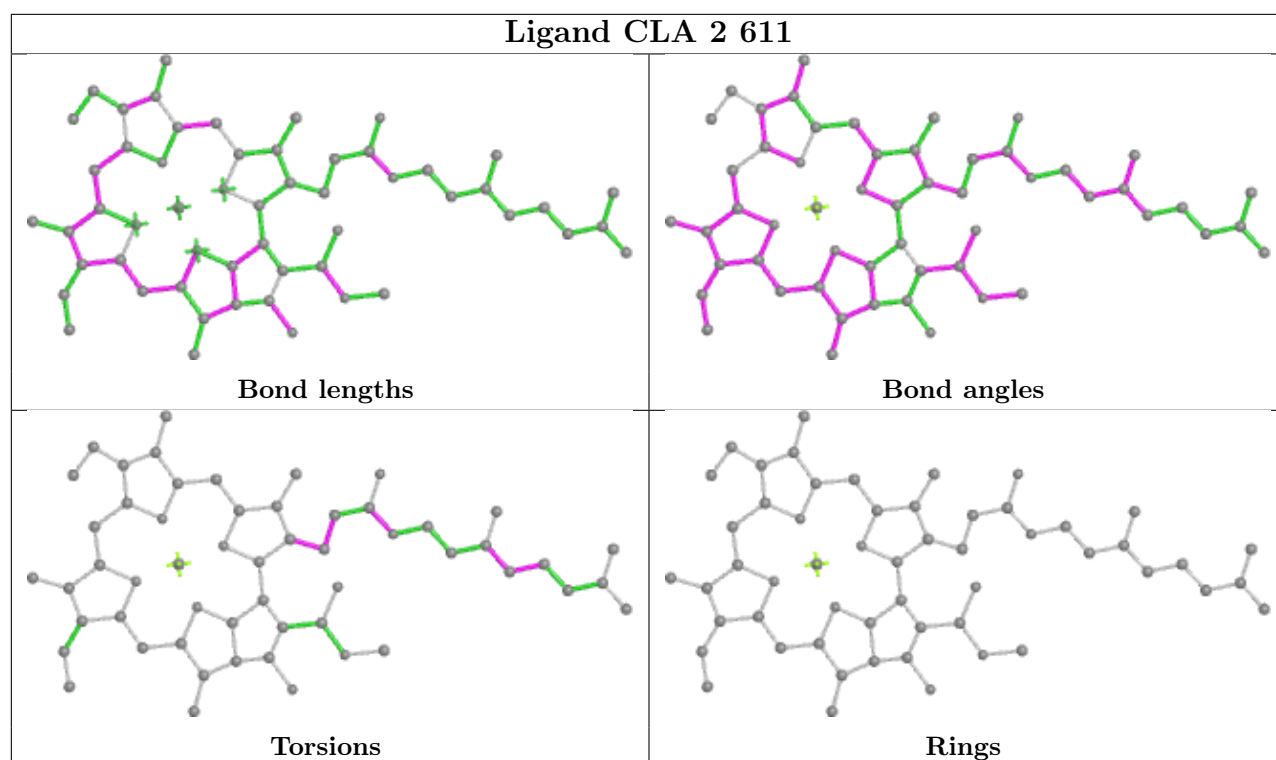
Bond angles



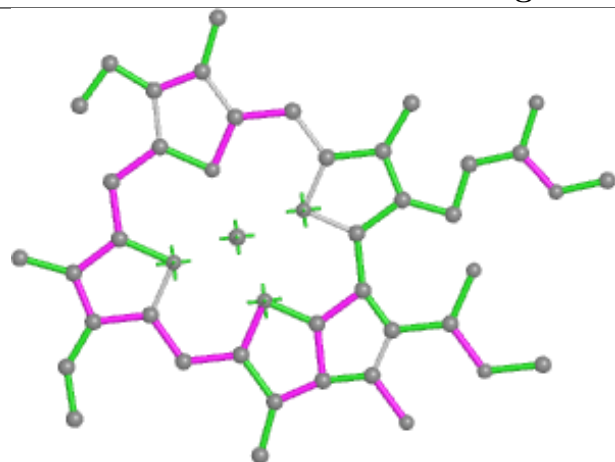
Torsions



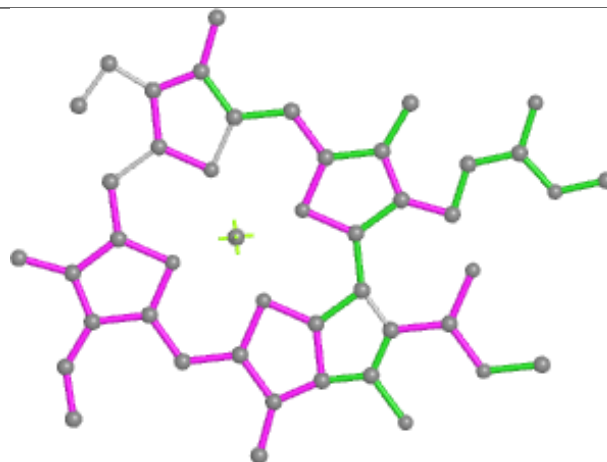
Rings



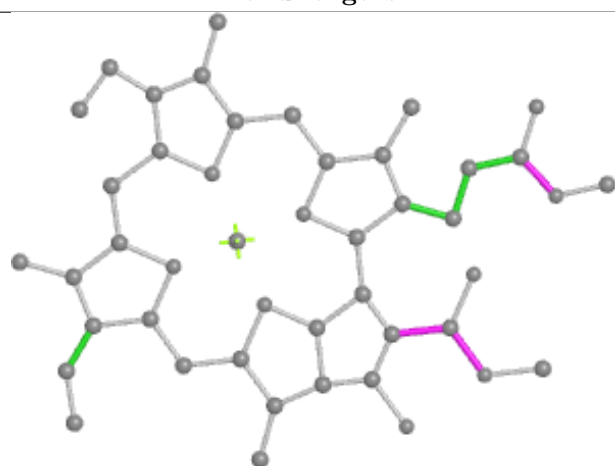
## Ligand CLA G 204



Bond lengths



Bond angles

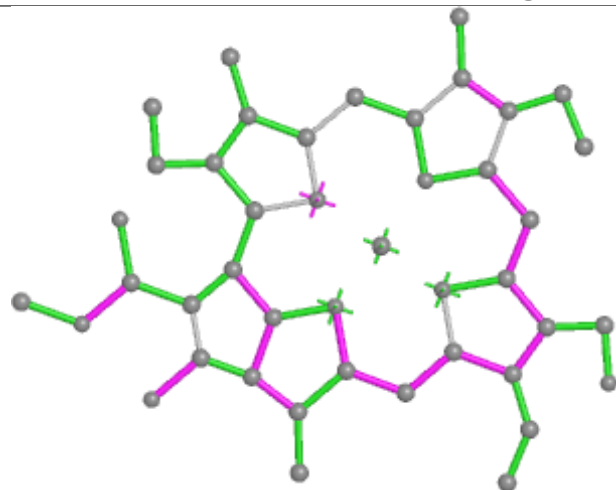


Torsions

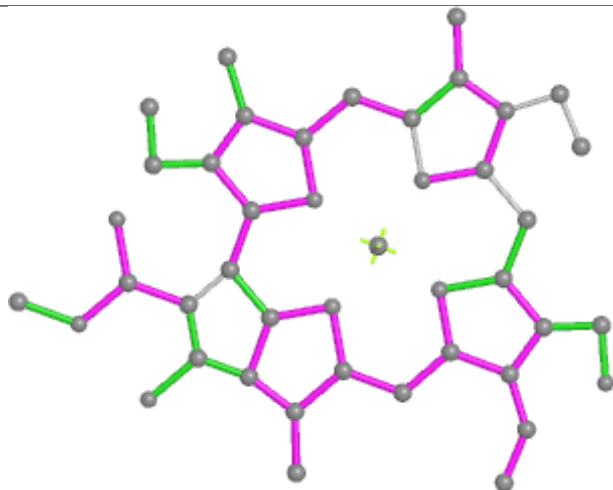


Rings

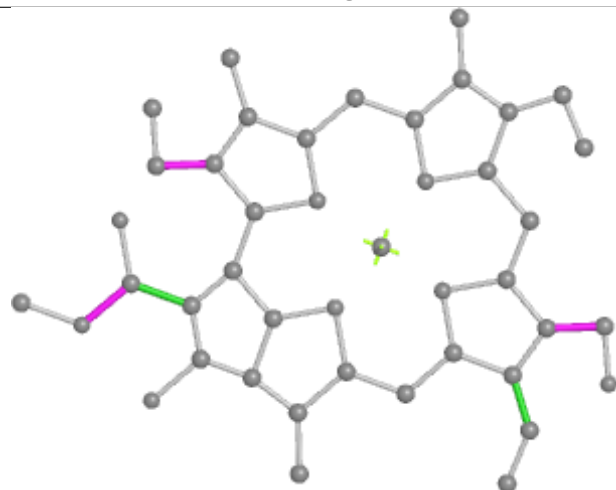
## Ligand CHL 6 618



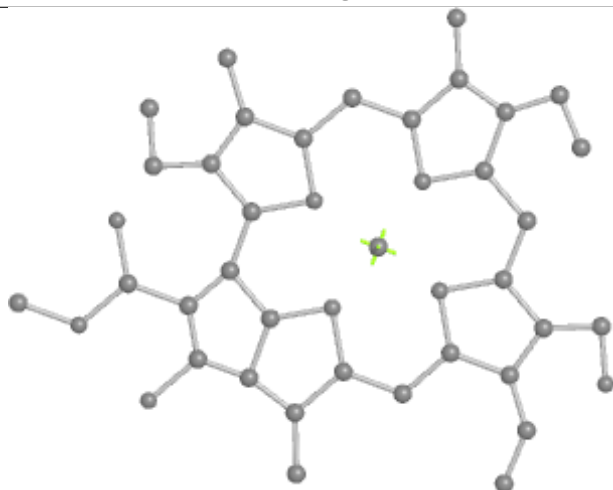
Bond lengths



Bond angles

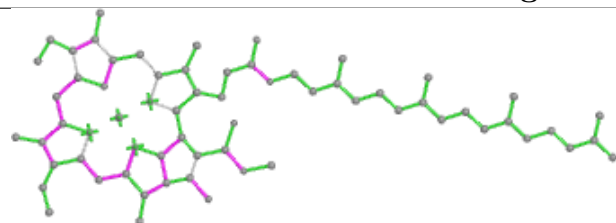


Torsions

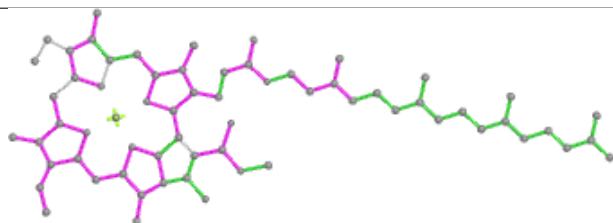


Rings

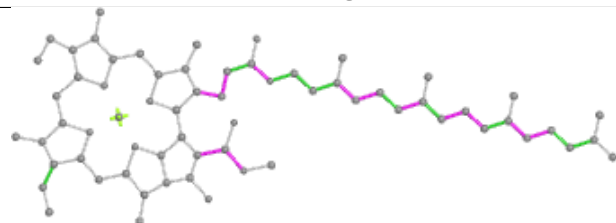
## Ligand CLA 3 610



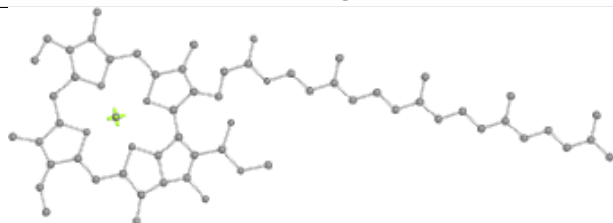
Bond lengths



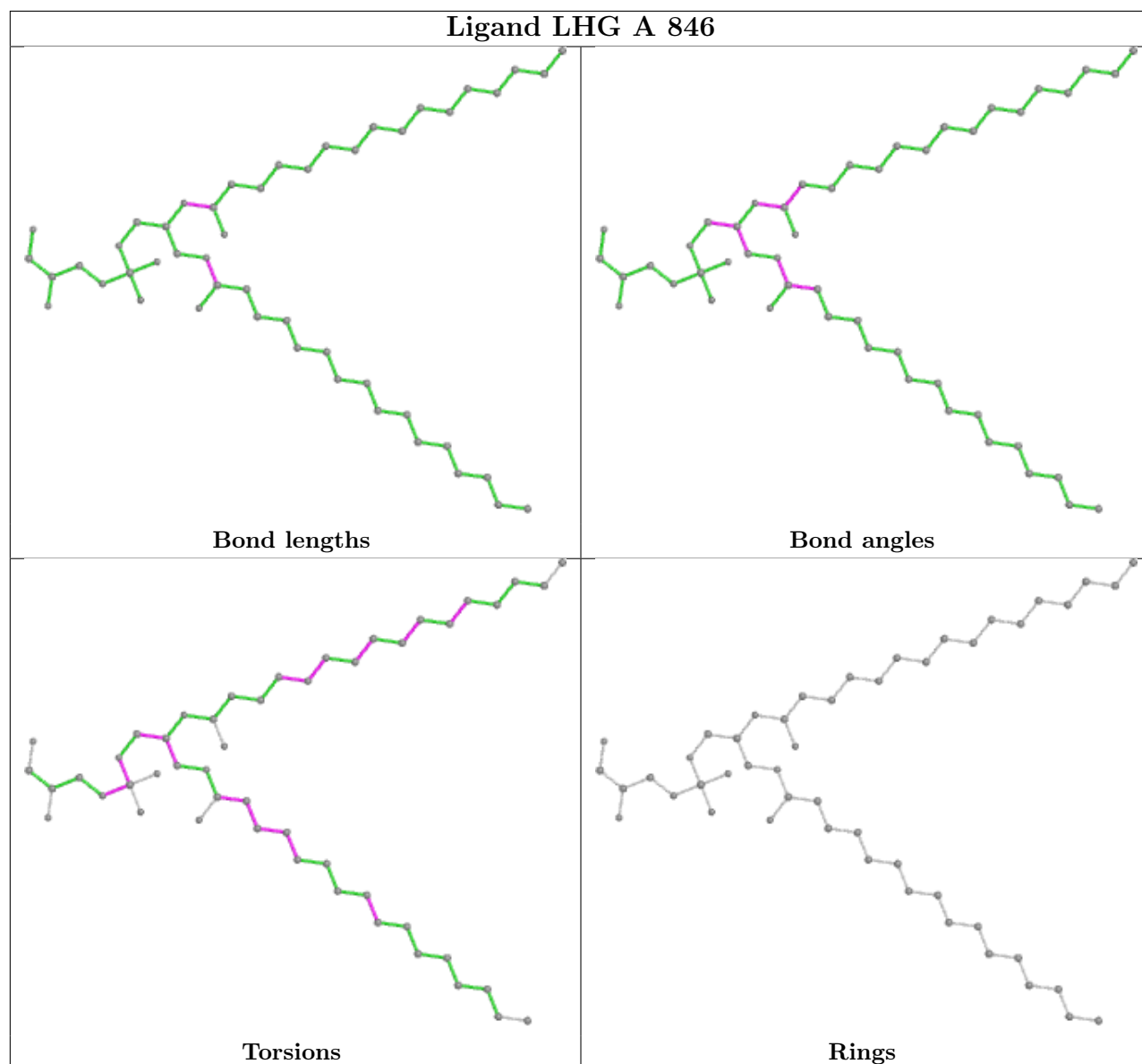
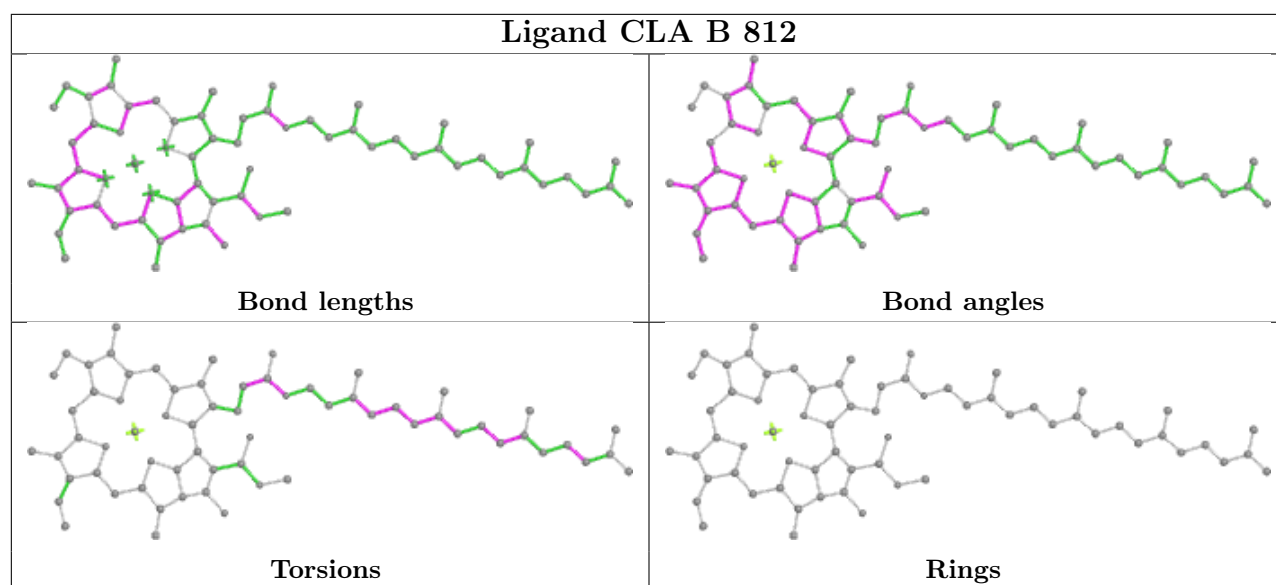
Bond angles

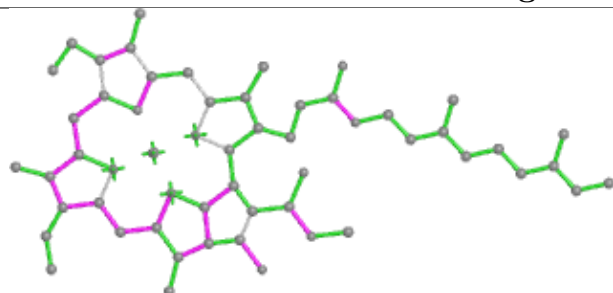


Torsions

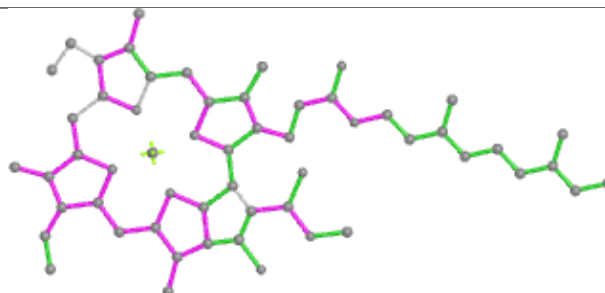


Rings

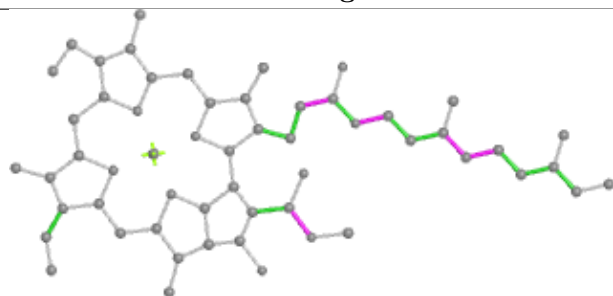


**Ligand CLA 5 613**

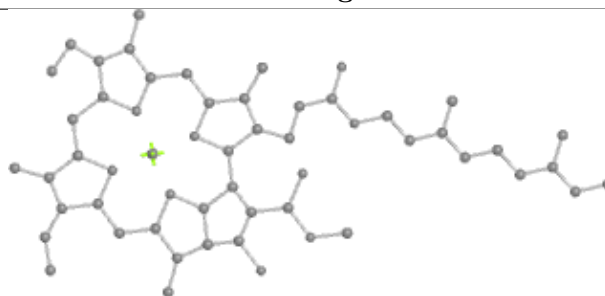
Bond lengths



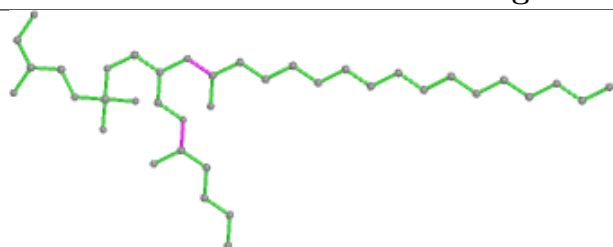
Bond angles



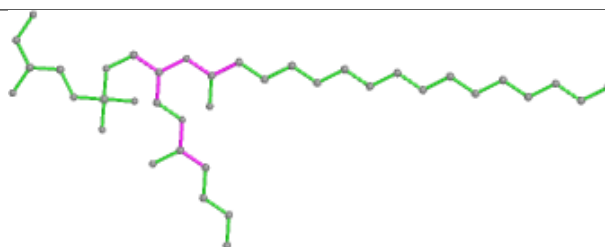
Torsions



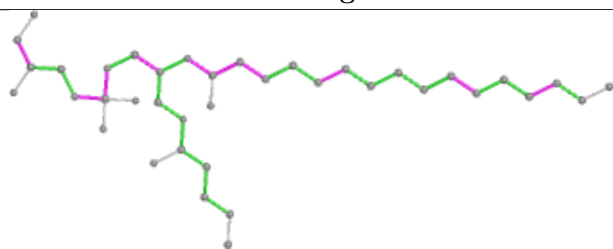
Rings

**Ligand LHG A 847**

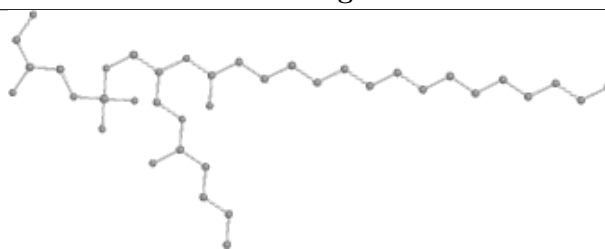
Bond lengths



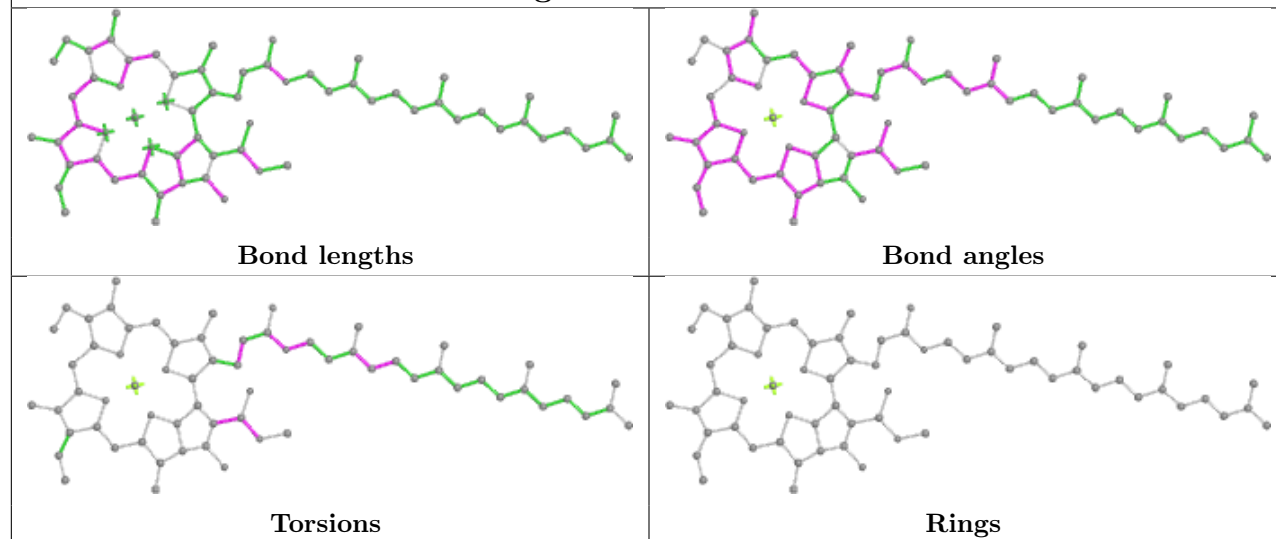
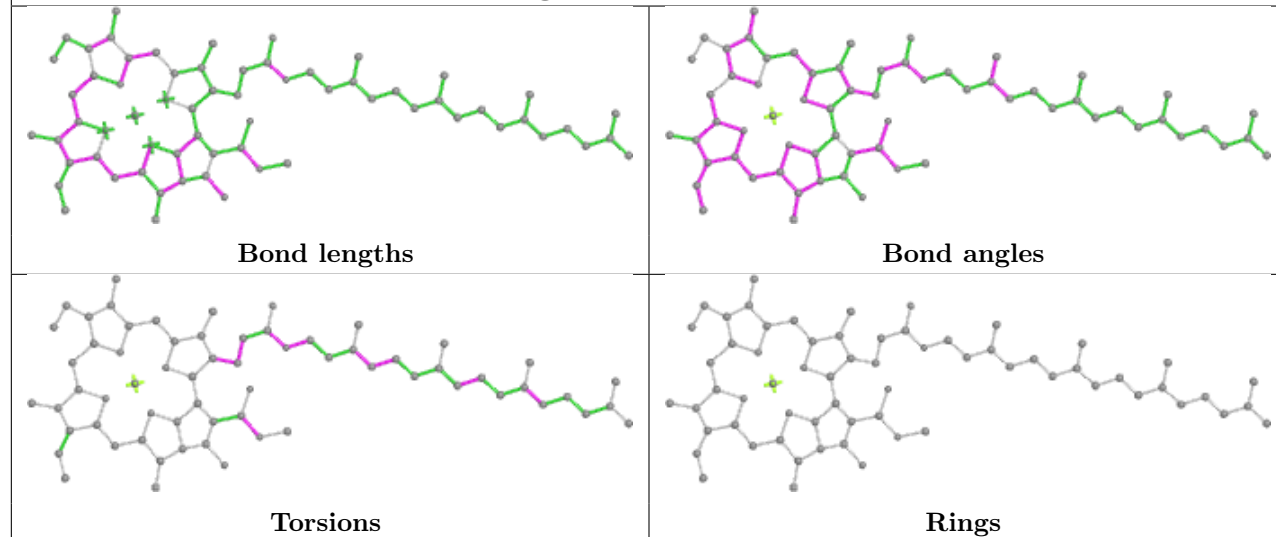
Bond angles



Torsions

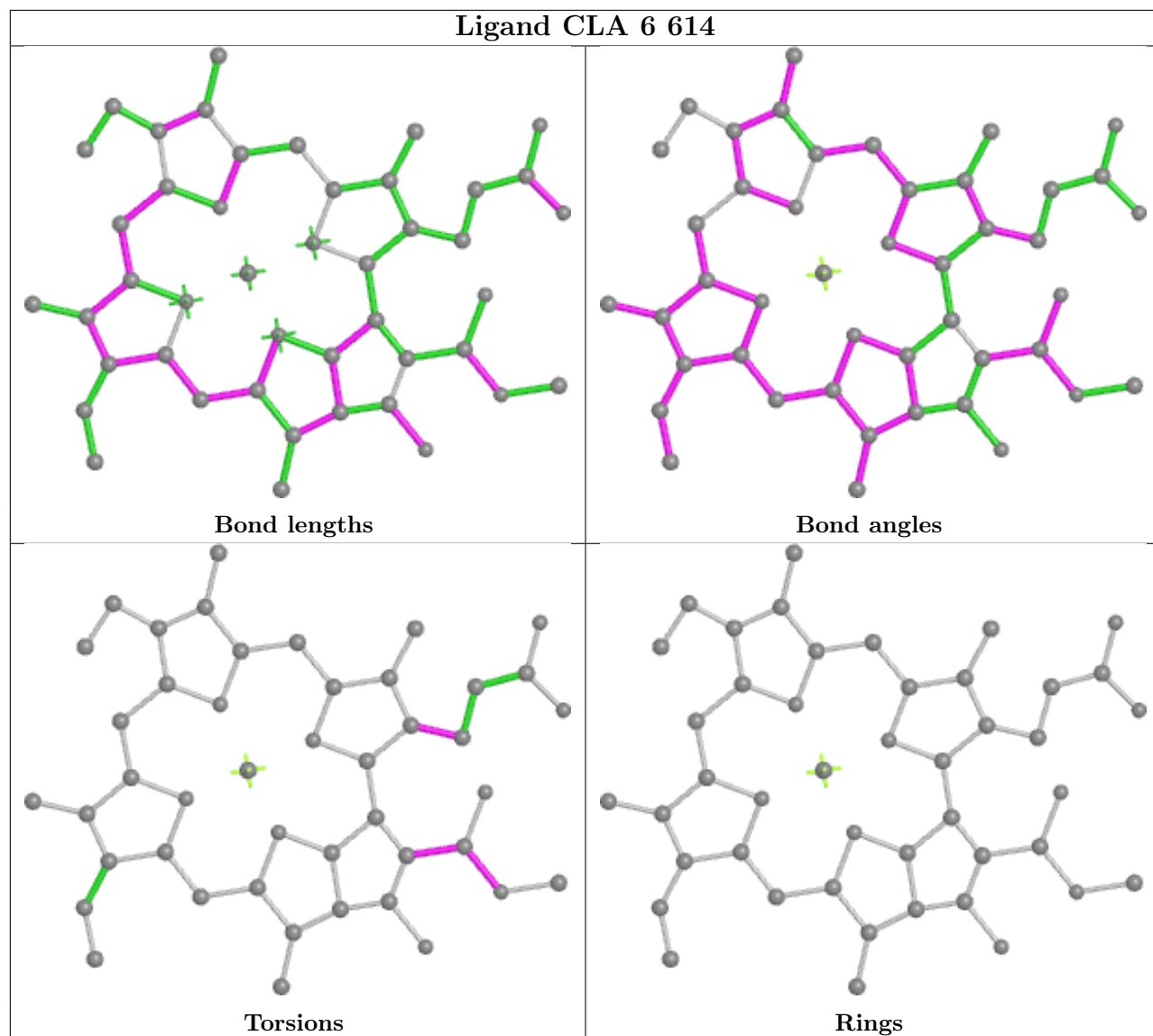


Rings

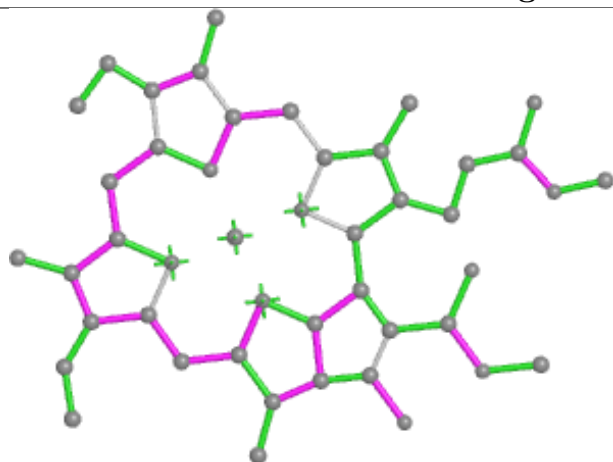
**Ligand CLA Z 602****Ligand CLA 1 614**



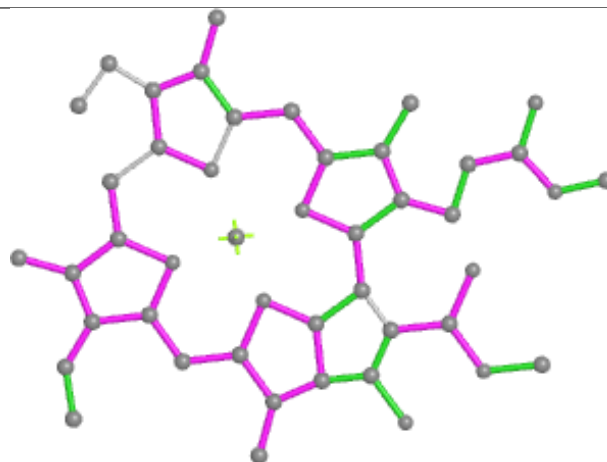
## Ligand CLA 6 614



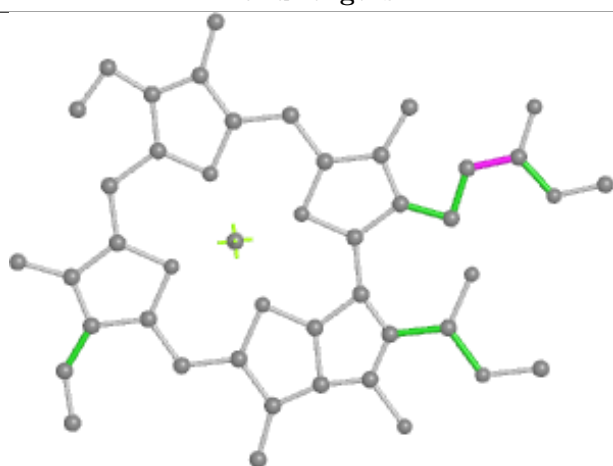
## Ligand CLA 9 603



Bond lengths



Bond angles

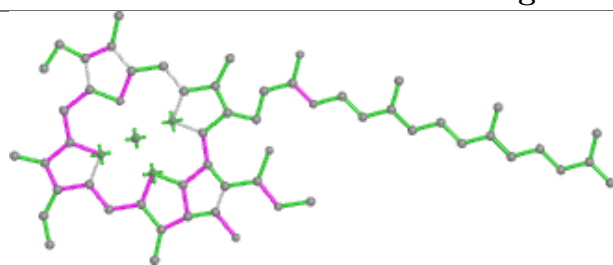


Torsions

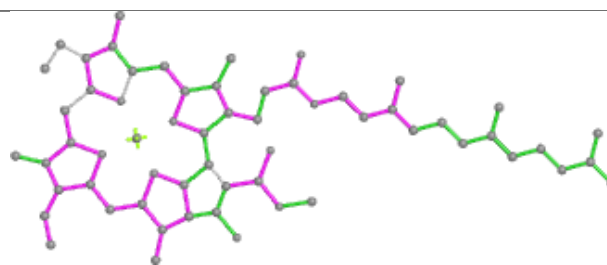


Rings

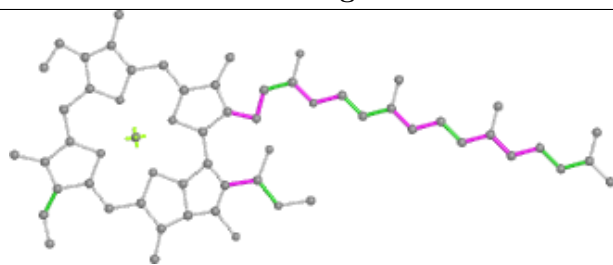
## Ligand CLA 3 607



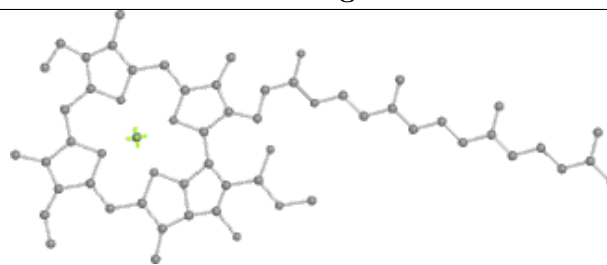
Bond lengths



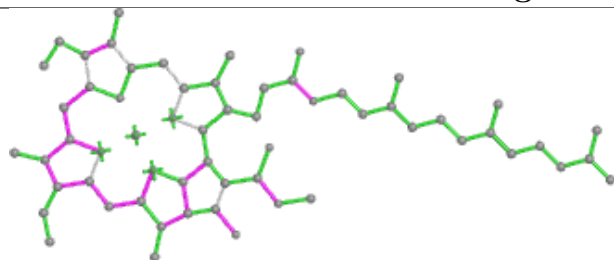
Bond angles



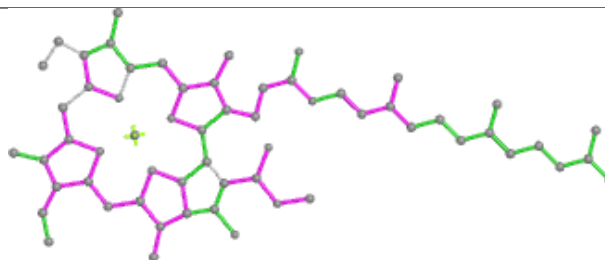
Torsions



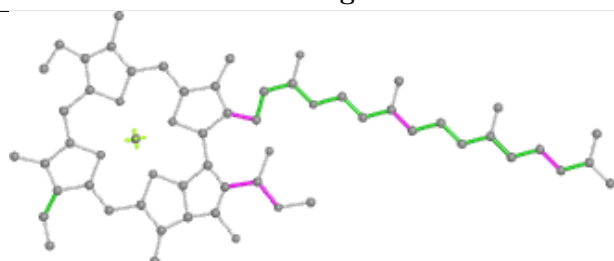
Rings

**Ligand CLA B 823**

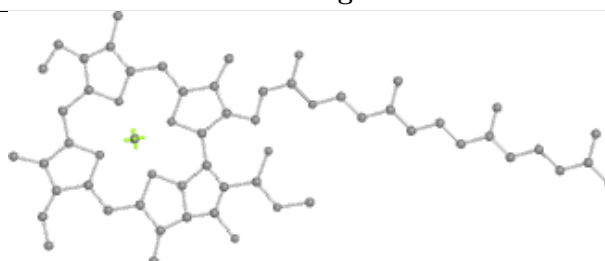
Bond lengths



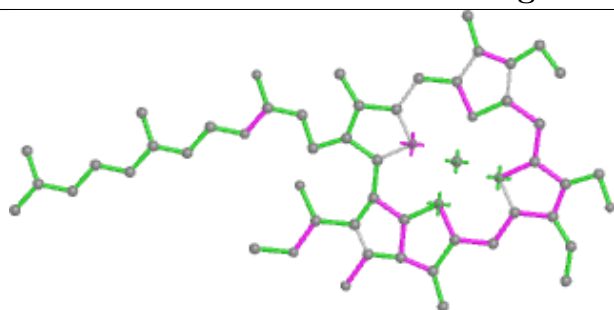
Bond angles



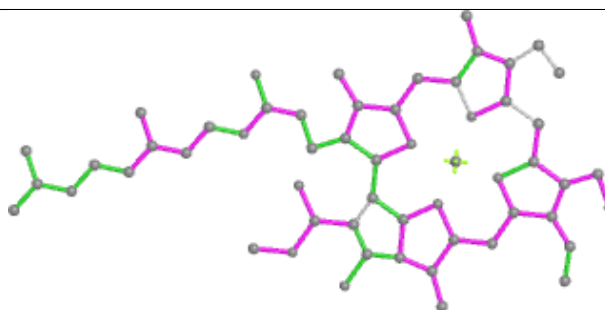
Torsions



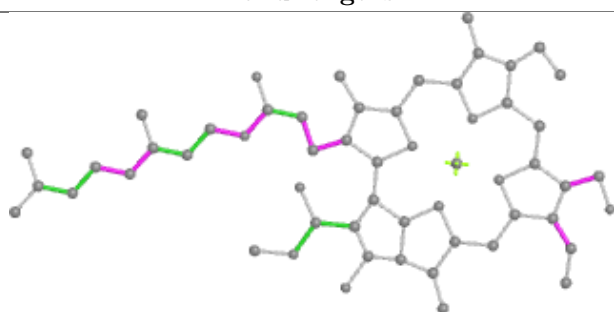
Rings

**Ligand CHL 6 607**

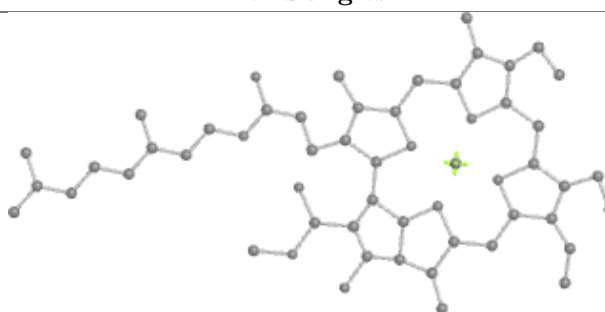
Bond lengths



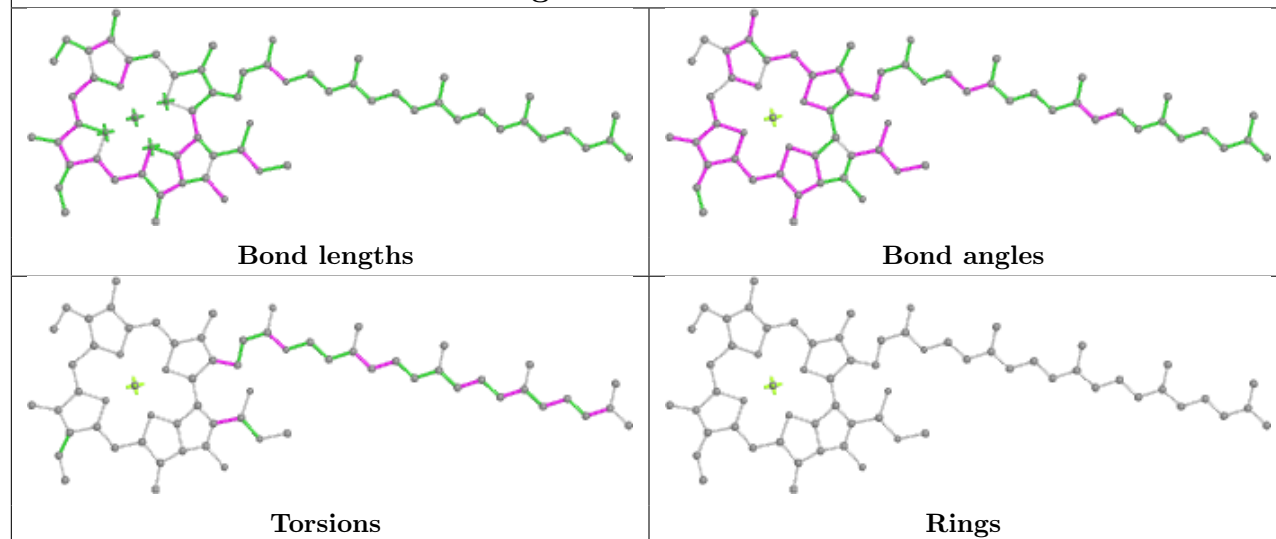
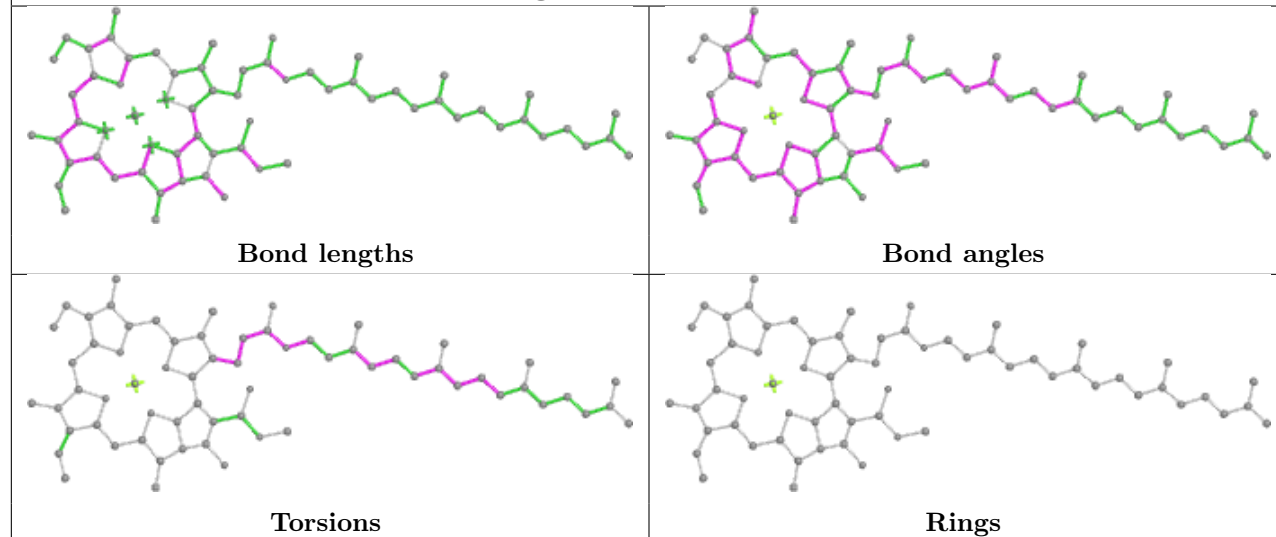
Bond angles



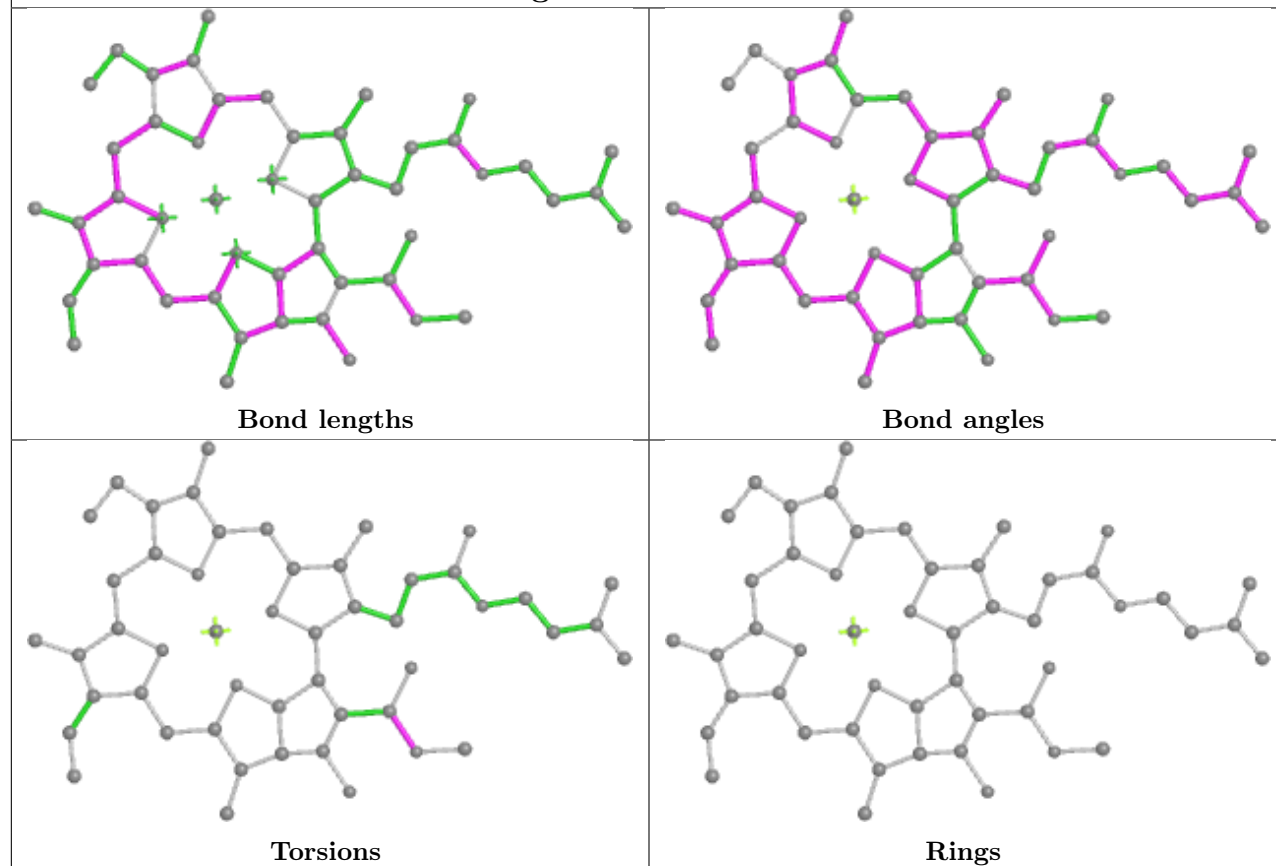
Torsions



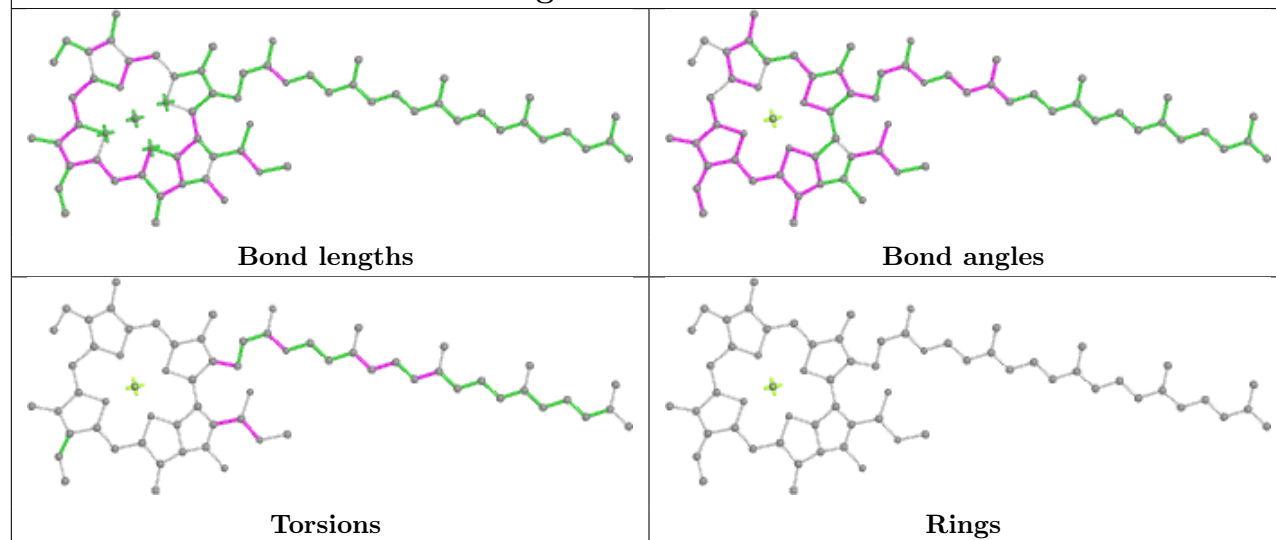
Rings

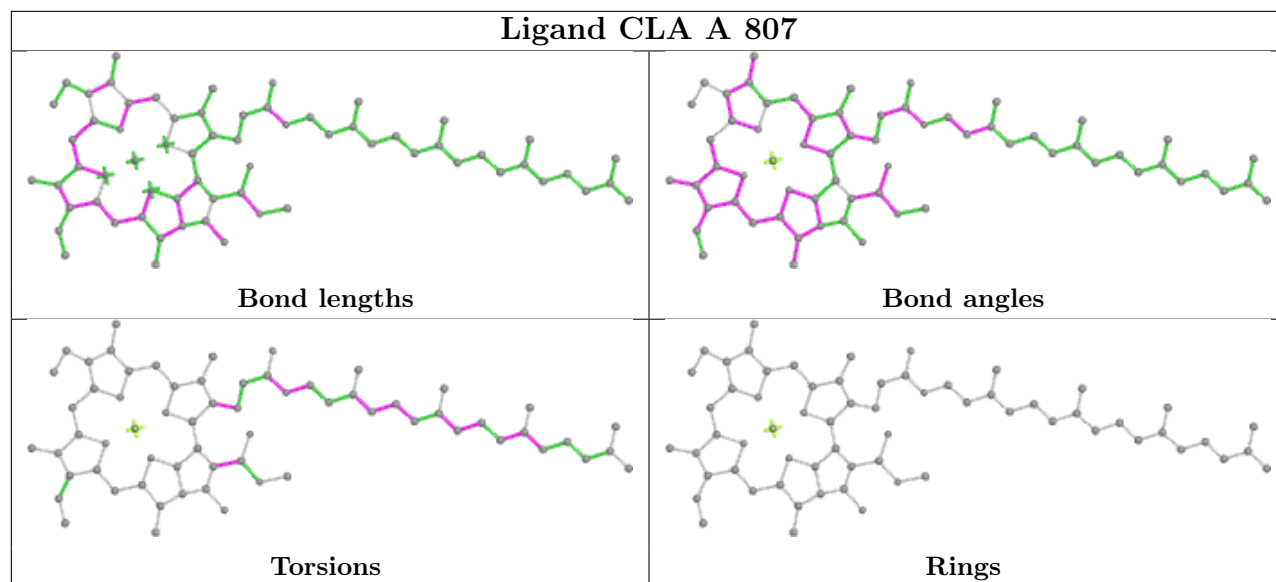
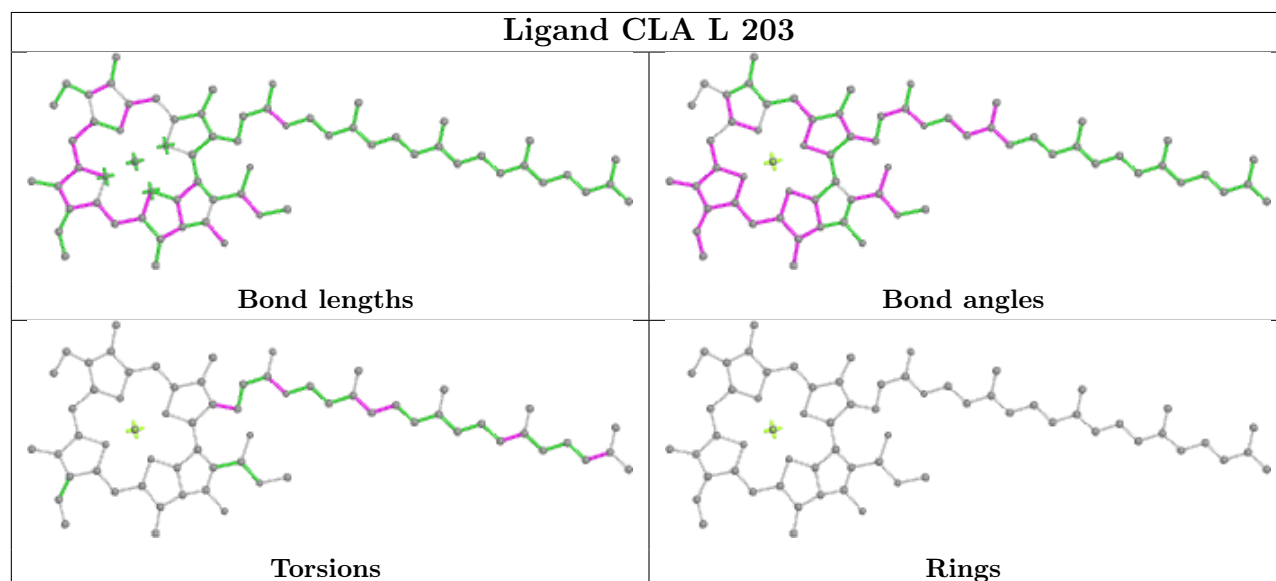
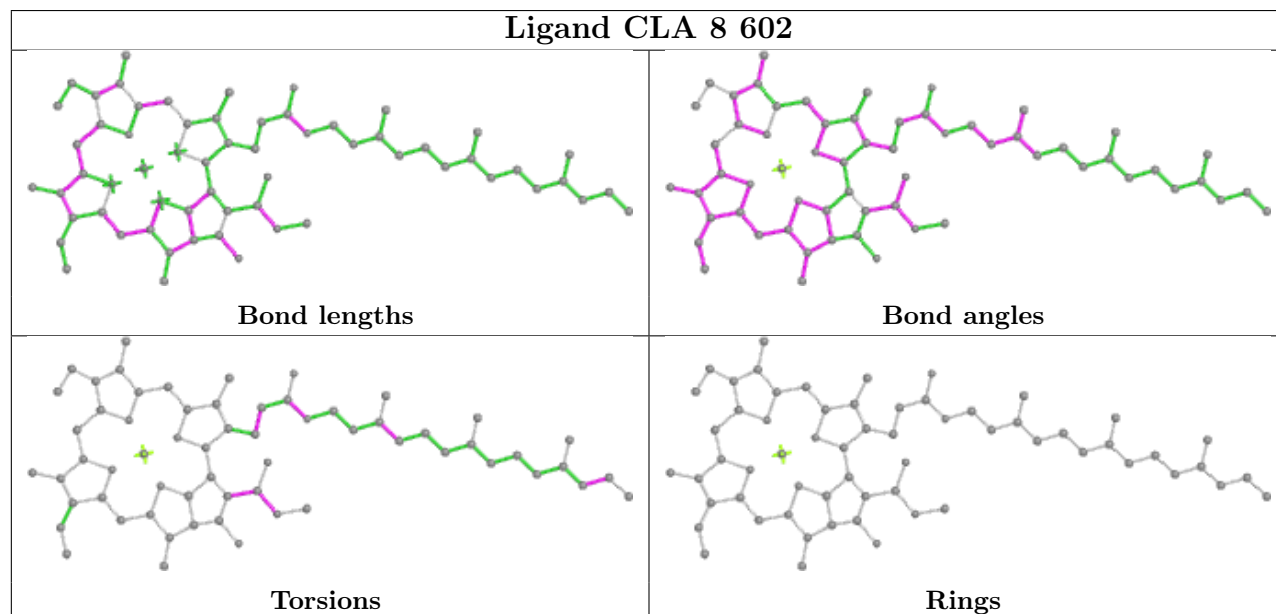
**Ligand CLA A 820****Ligand CLA B 827**

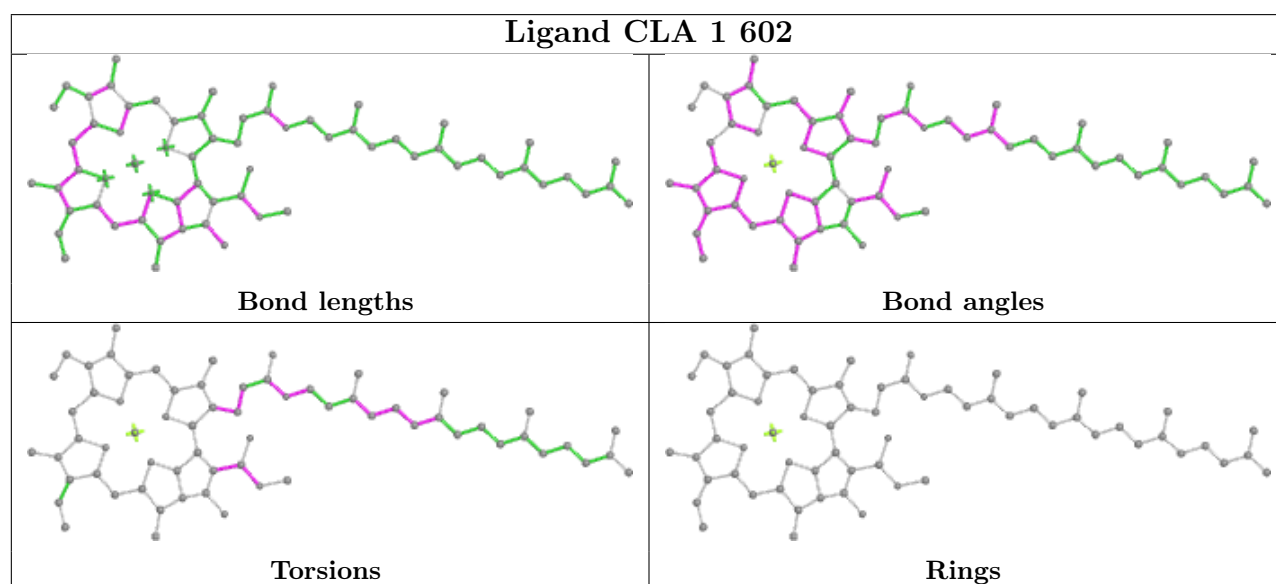
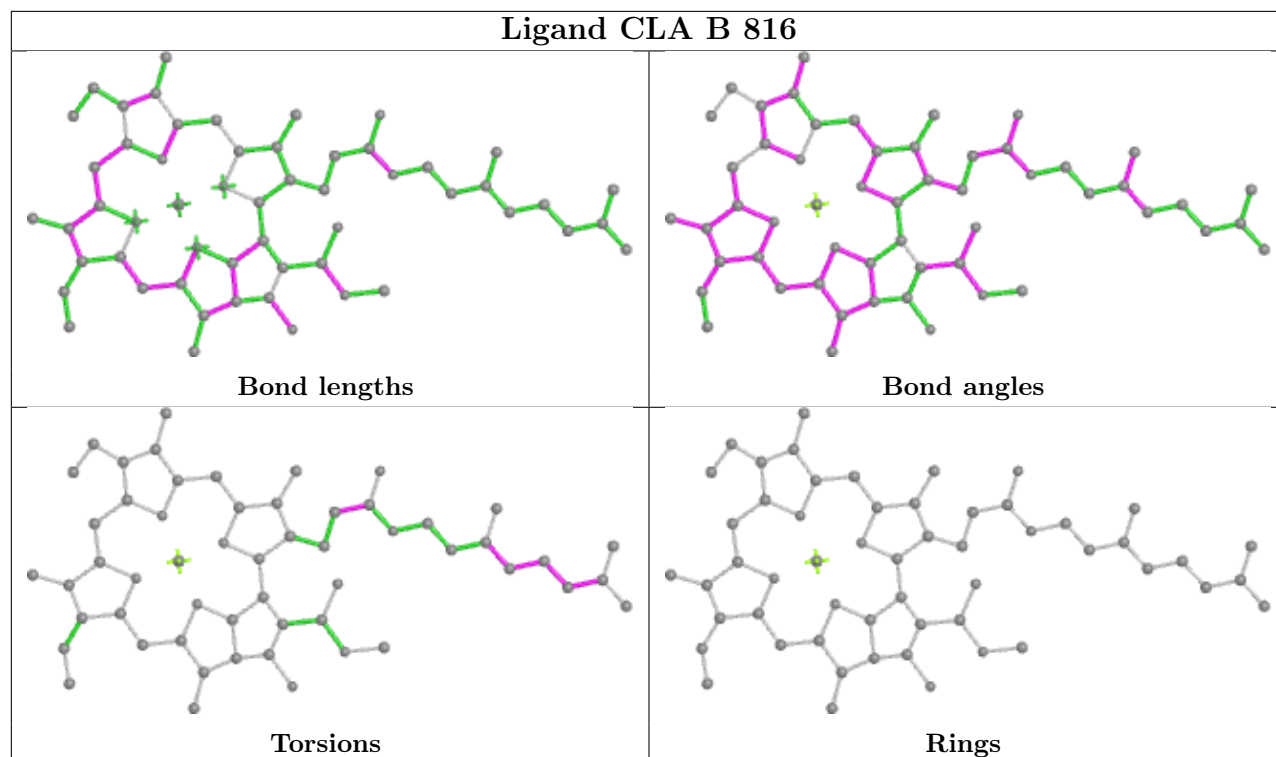
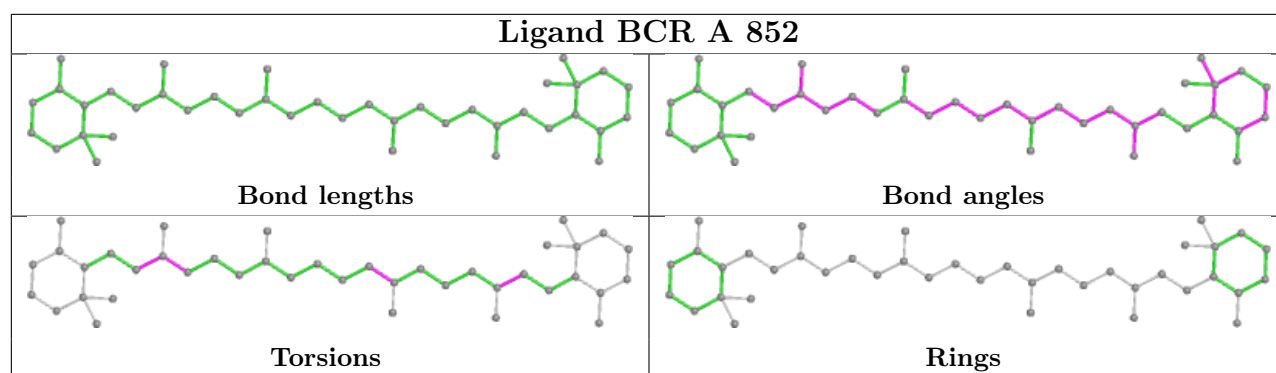
## Ligand CLA A 836

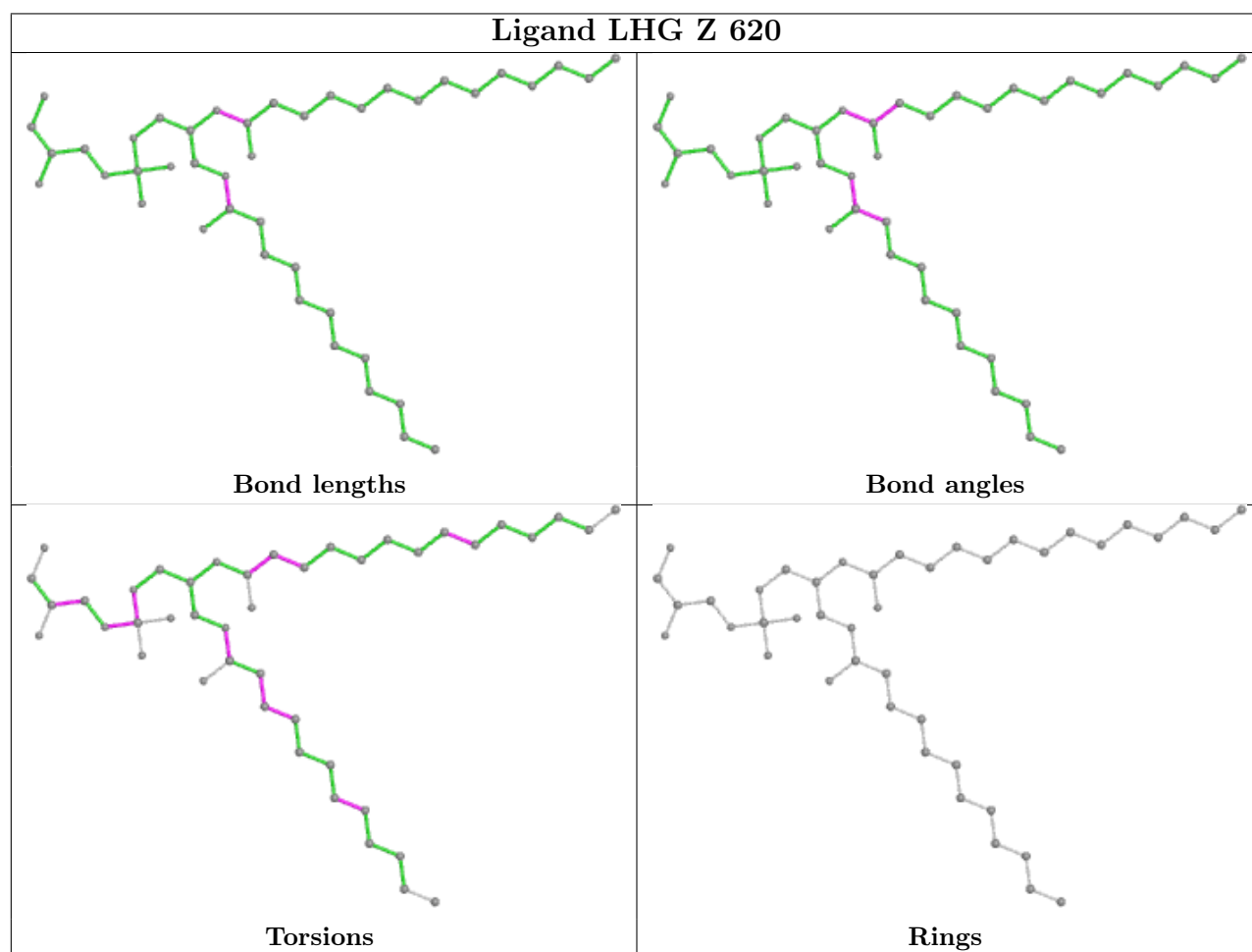
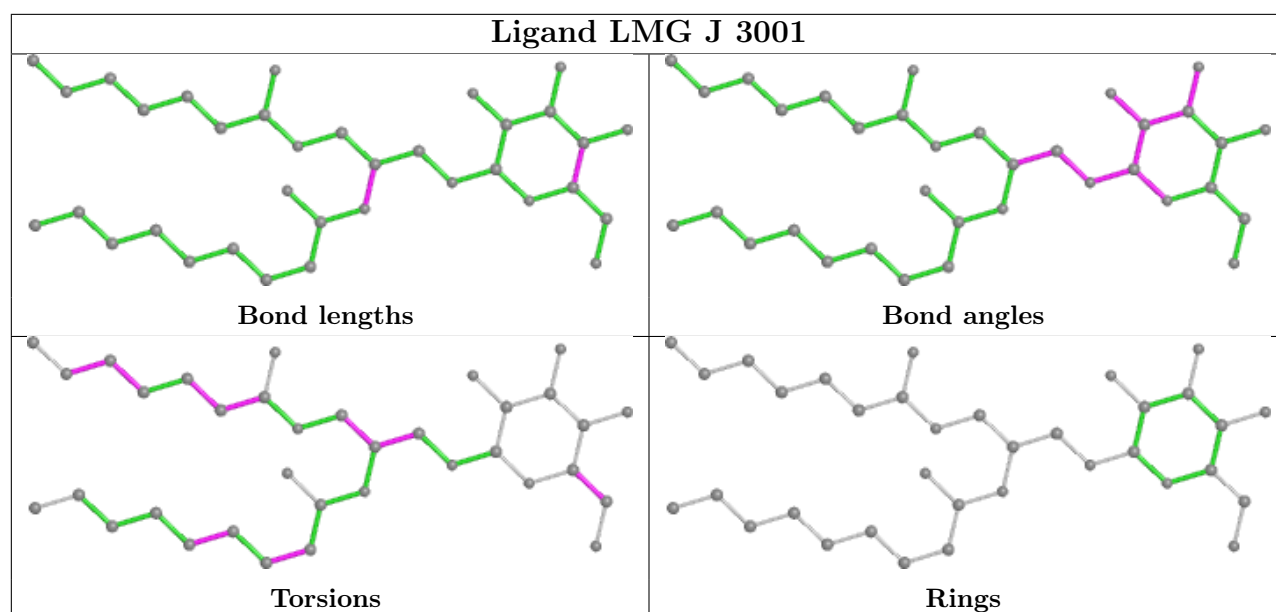


## Ligand CLA 6 604



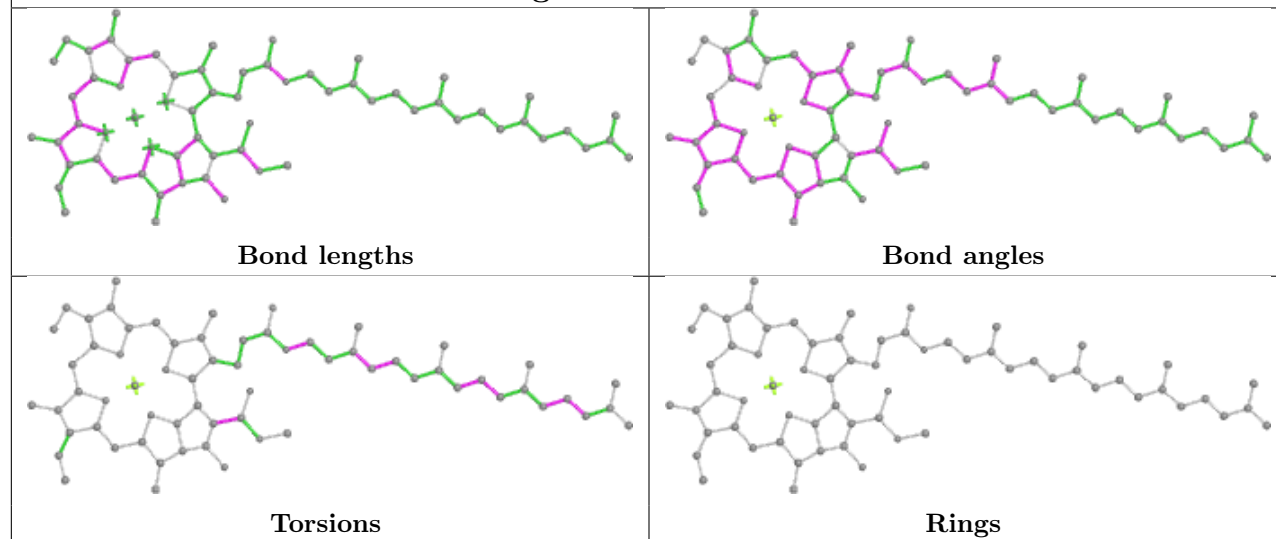
**Ligand CLA A 807****Ligand CLA L 203****Ligand CLA 8 602**



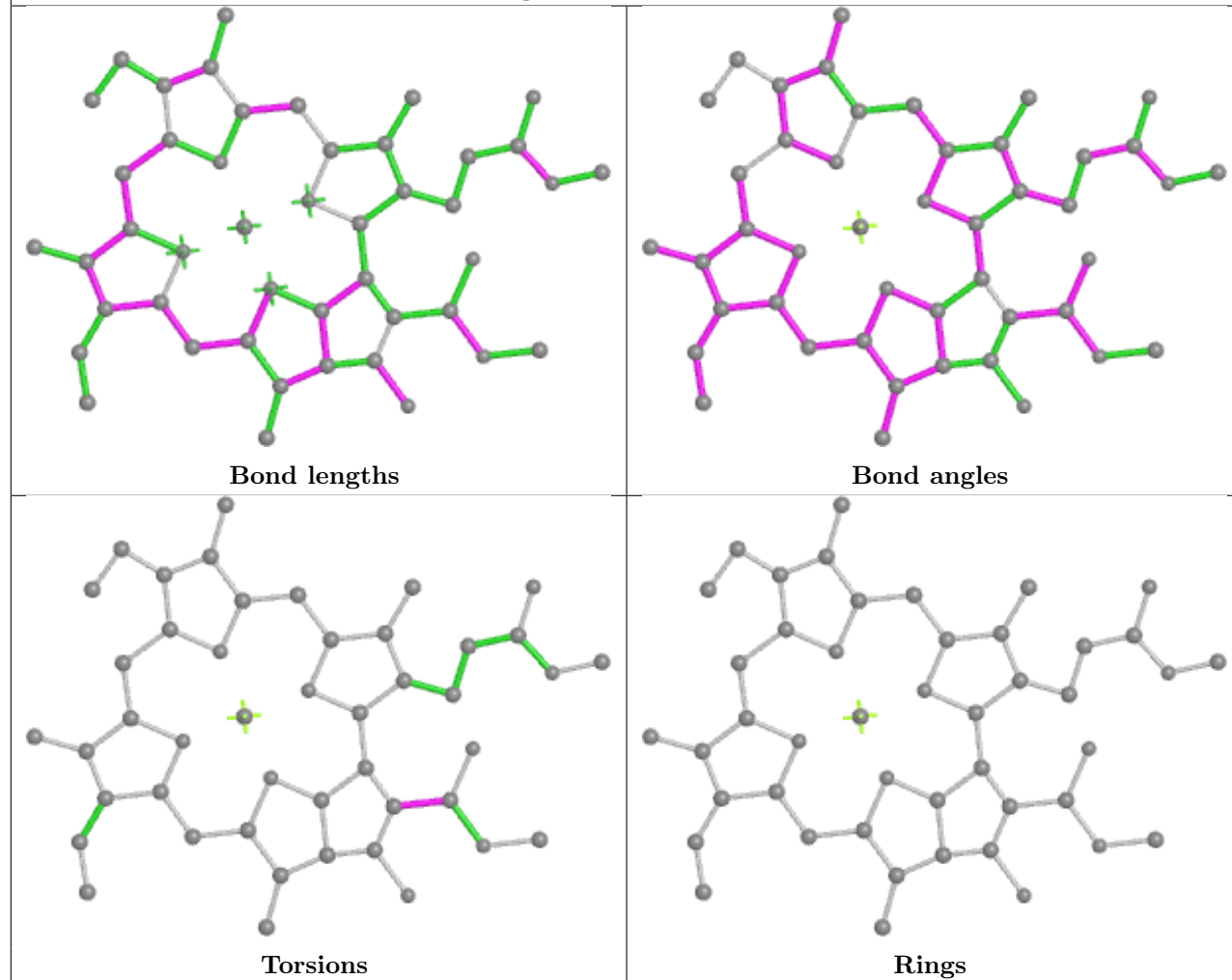


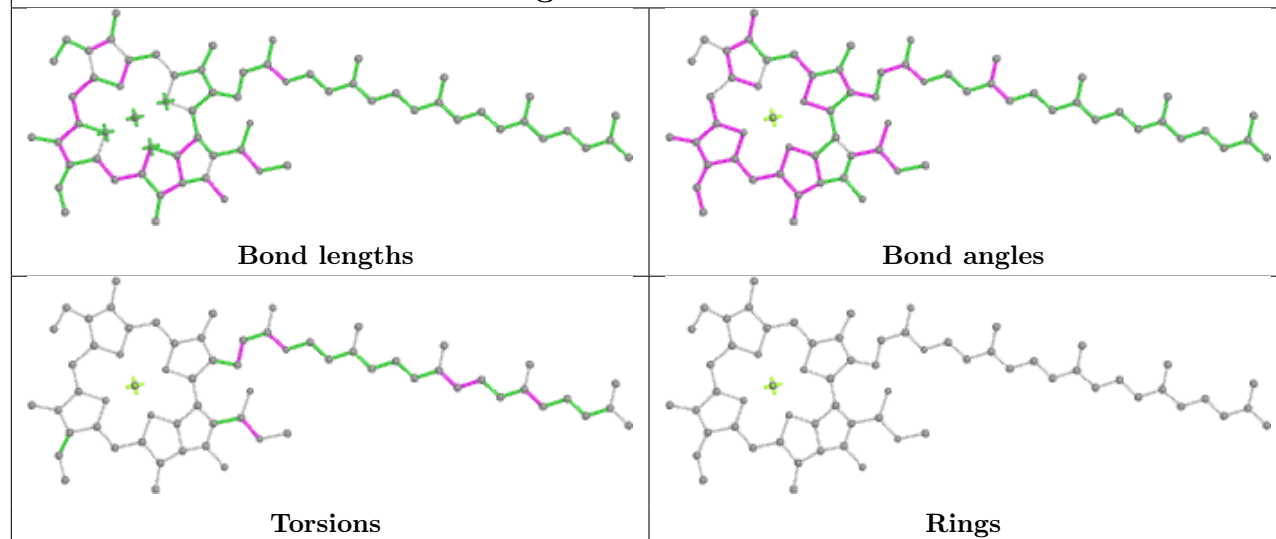
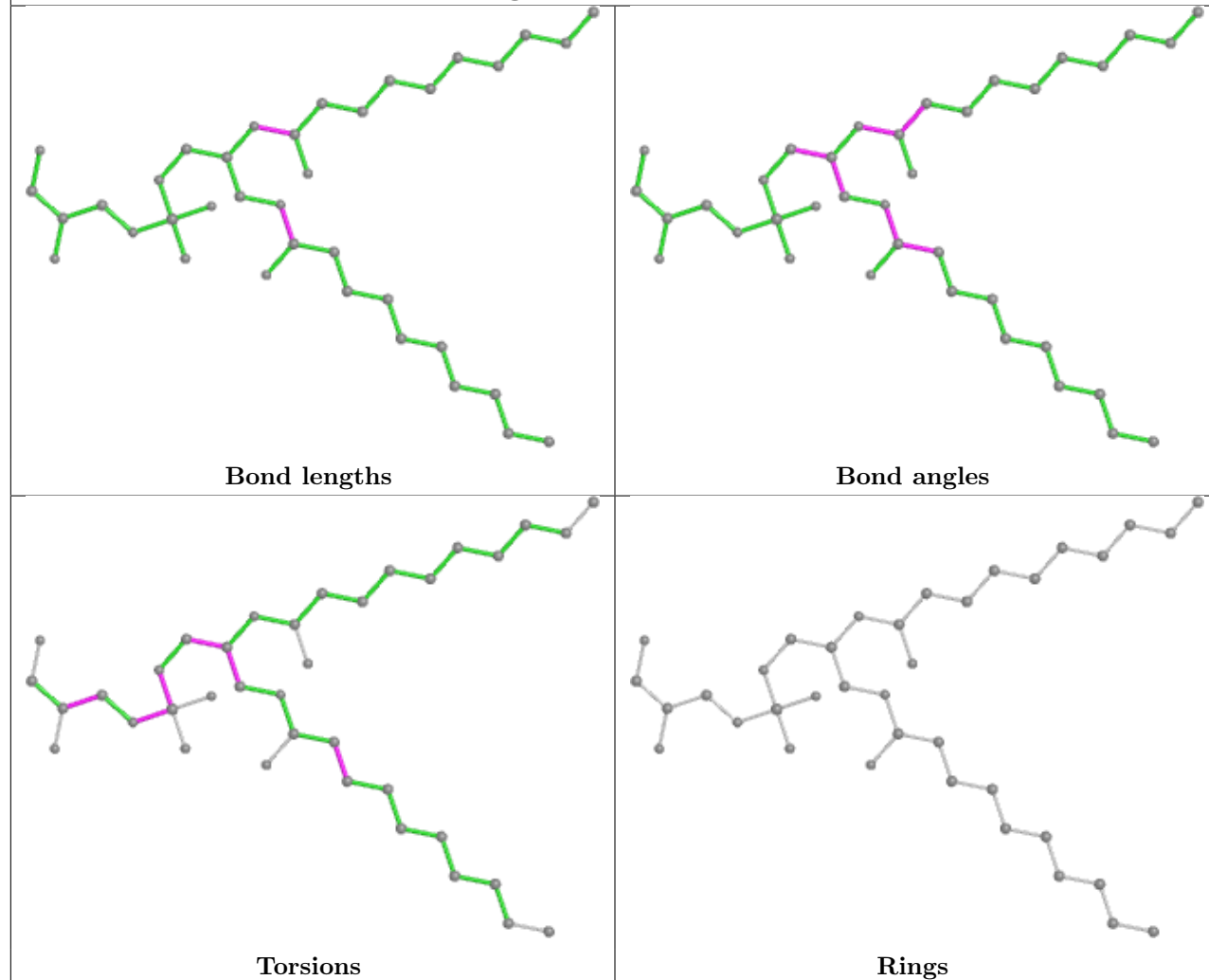


## Ligand CLA B 802

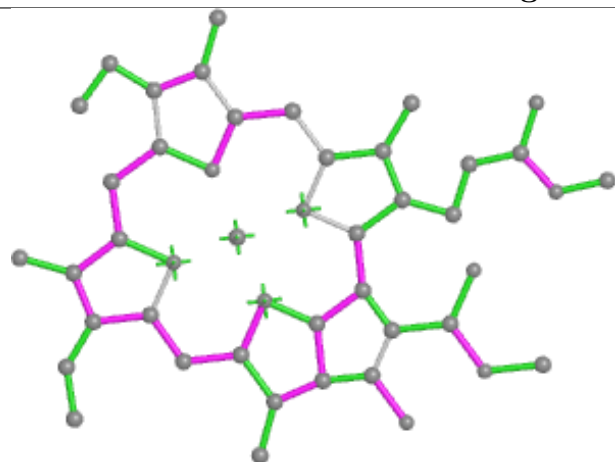


## Ligand CLA 6 603

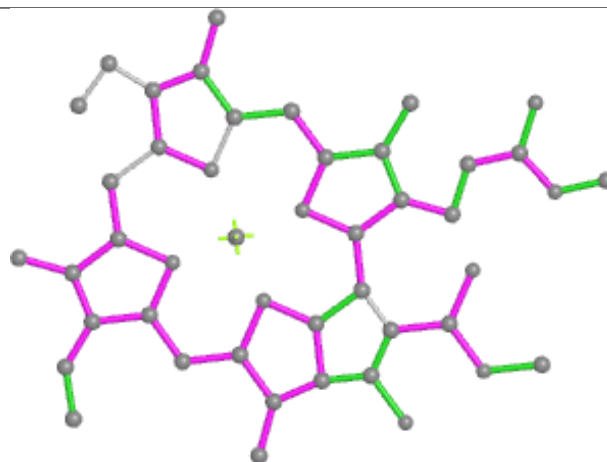


**Ligand CLA 5 602****Ligand LHG 5 623**

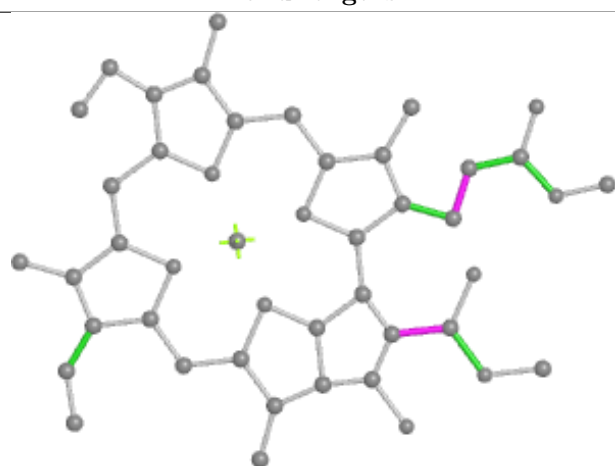
## Ligand CLA 5 621



Bond lengths



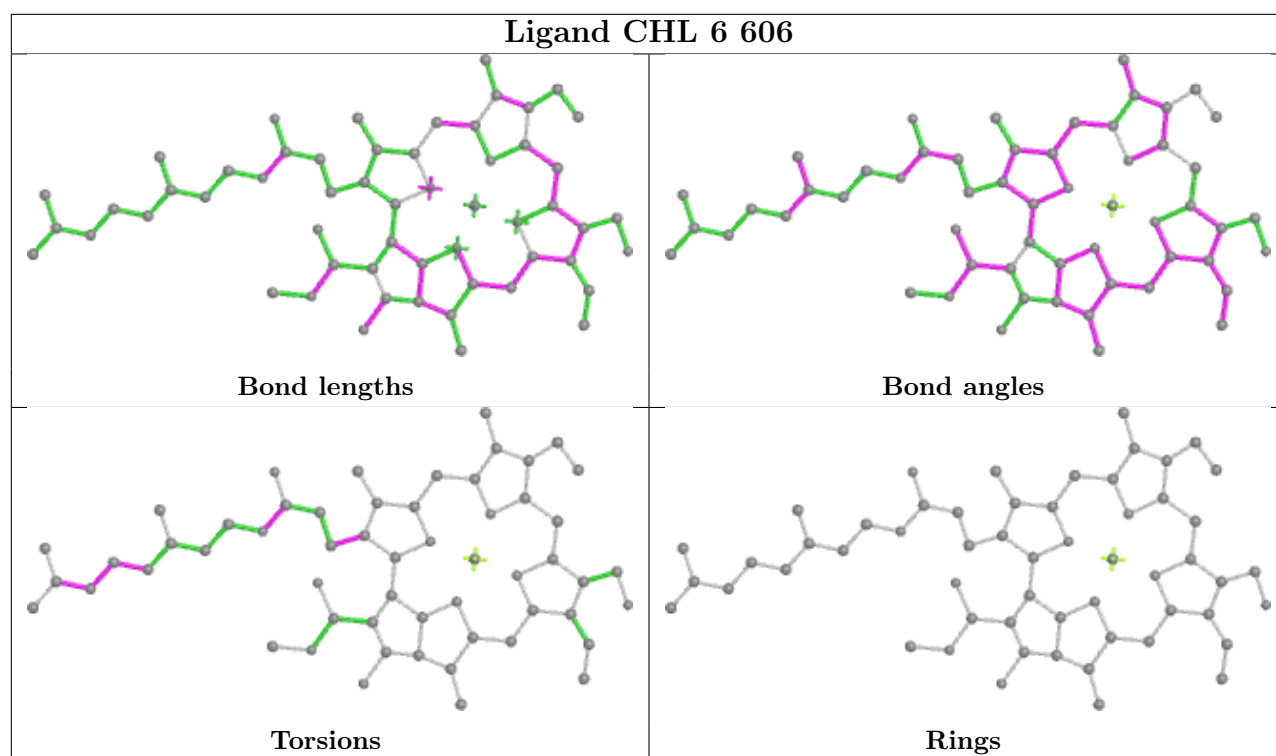
Bond angles



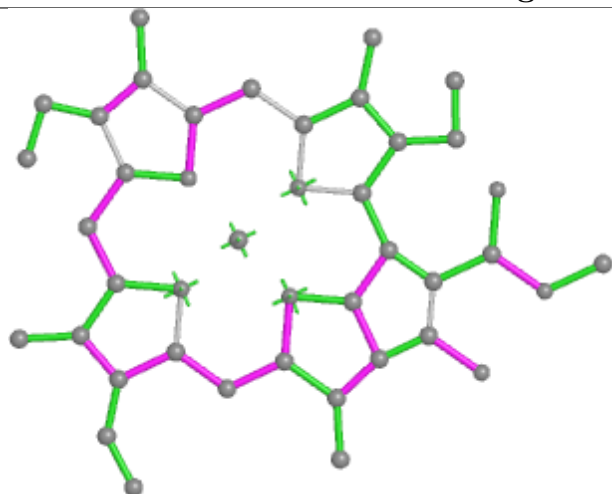
Torsions



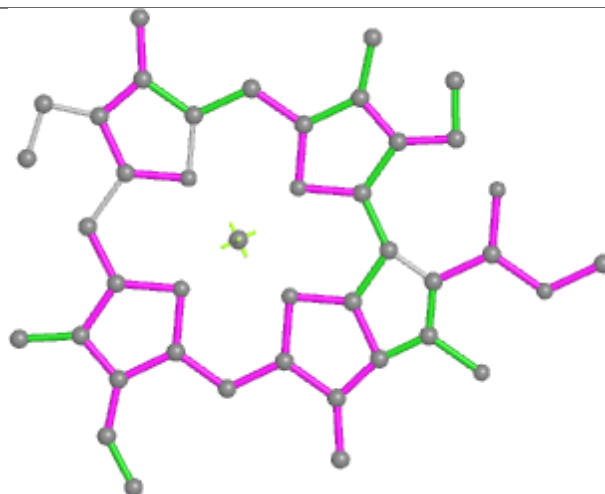
Rings



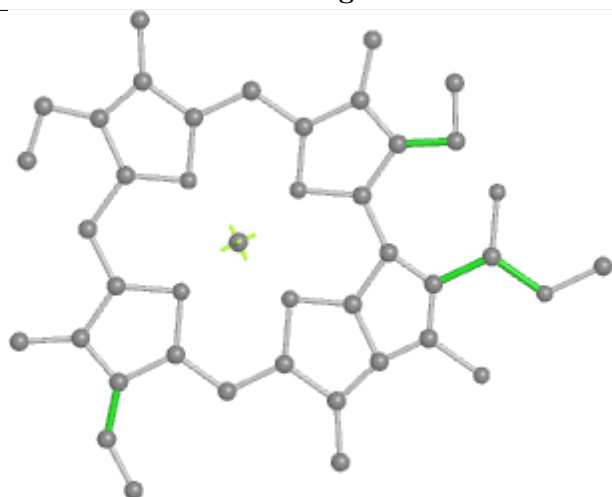
## Ligand CLA 3 606



Bond lengths



Bond angles

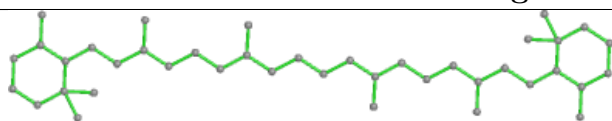


Torsions

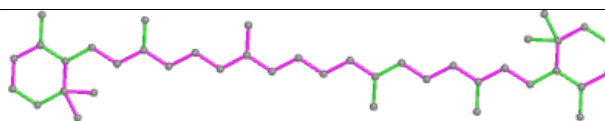


Rings

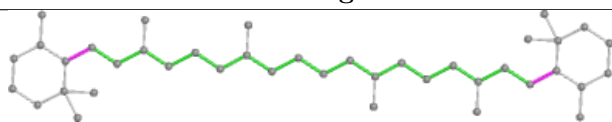
## Ligand BCR A 848



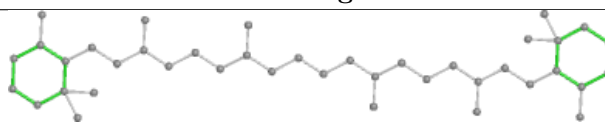
Bond lengths



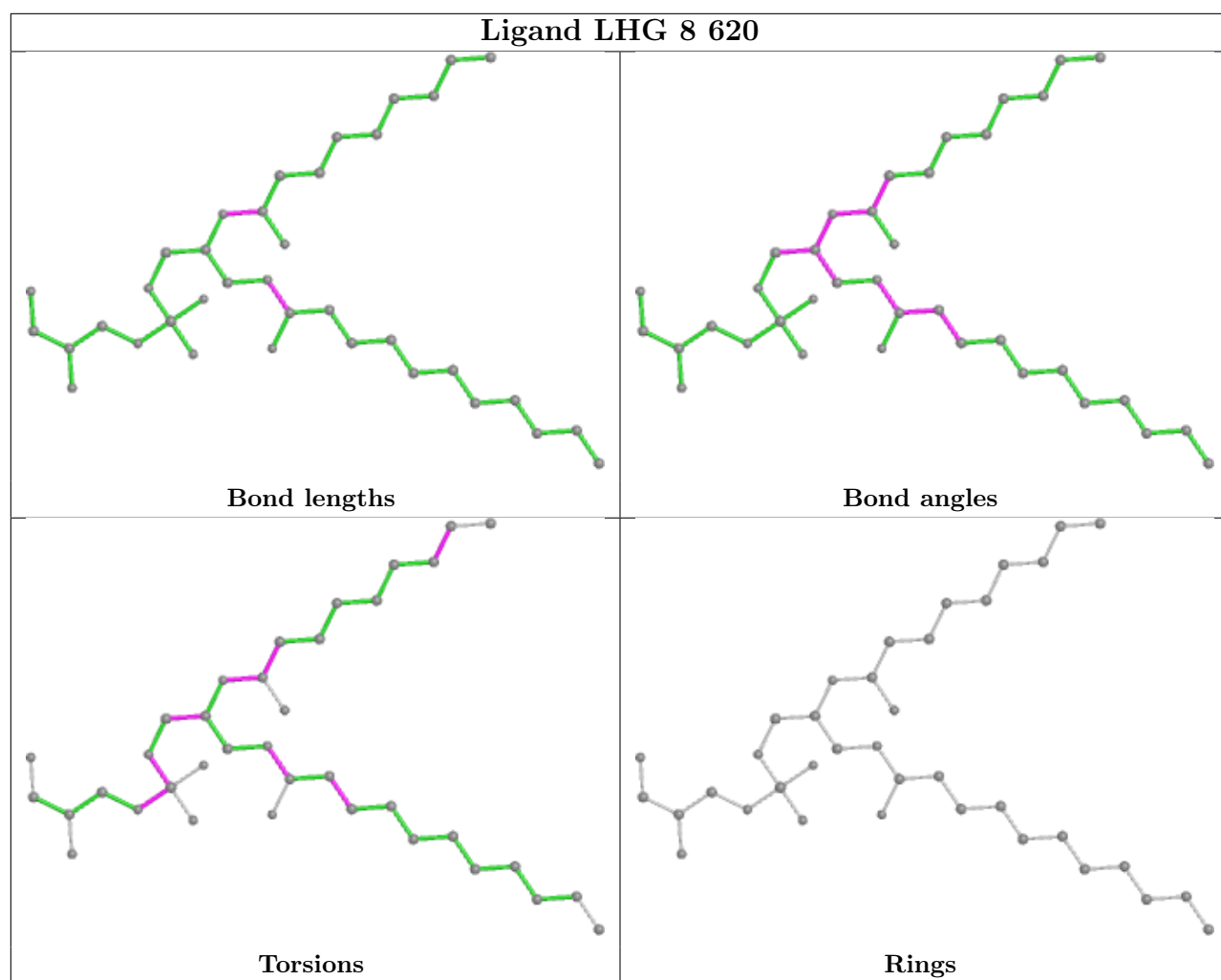
Bond angles



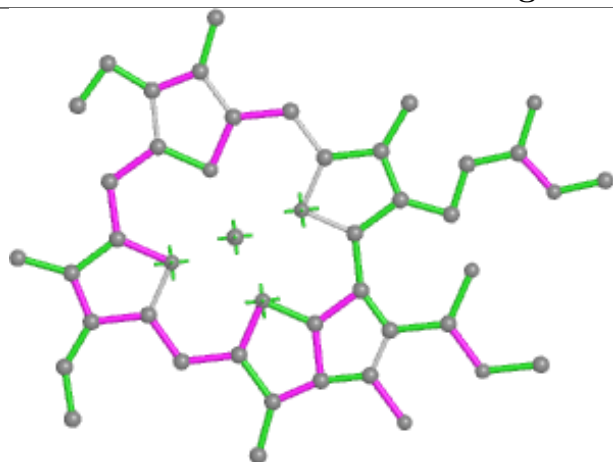
Torsions



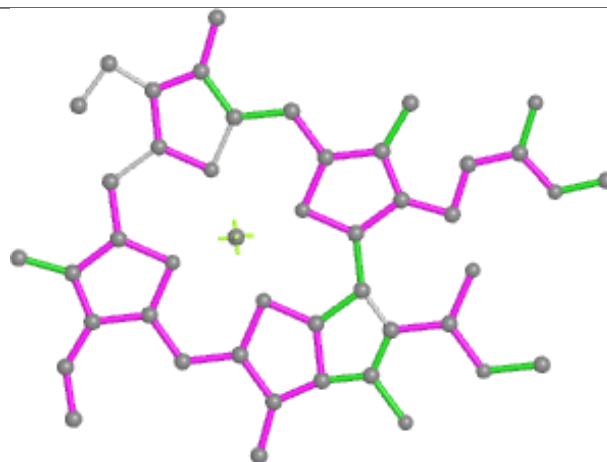
Rings



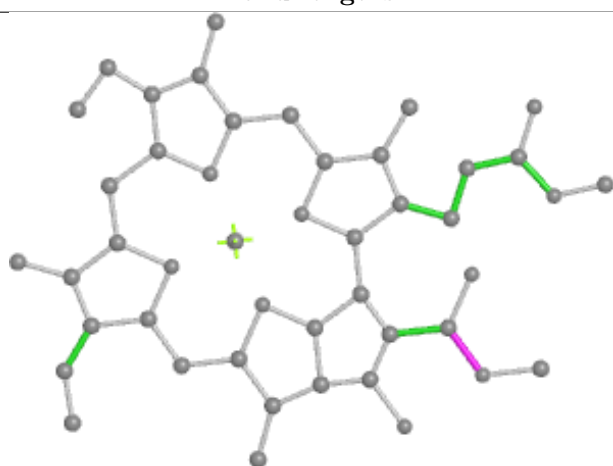
## Ligand CLA 6 616



Bond lengths



Bond angles

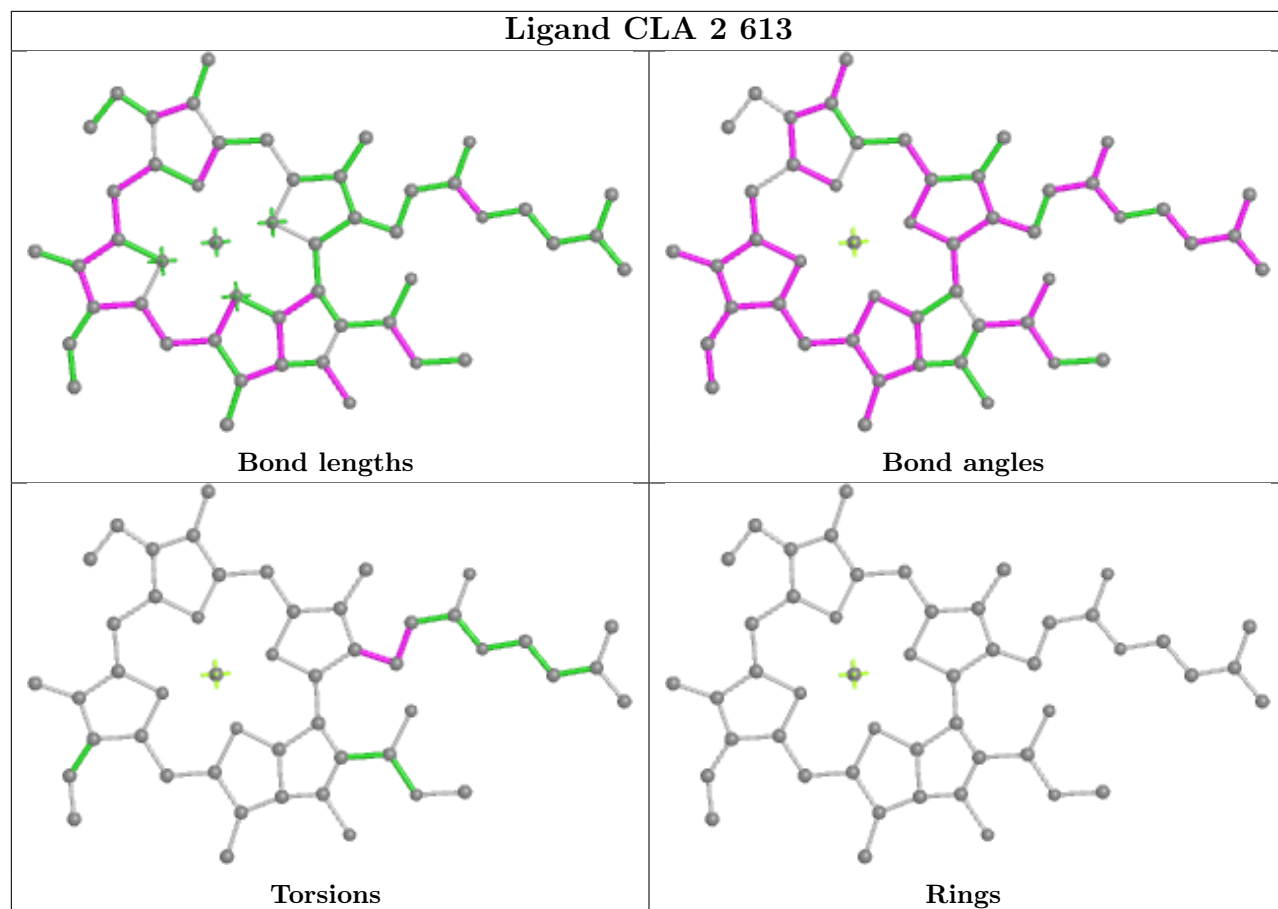


Torsions



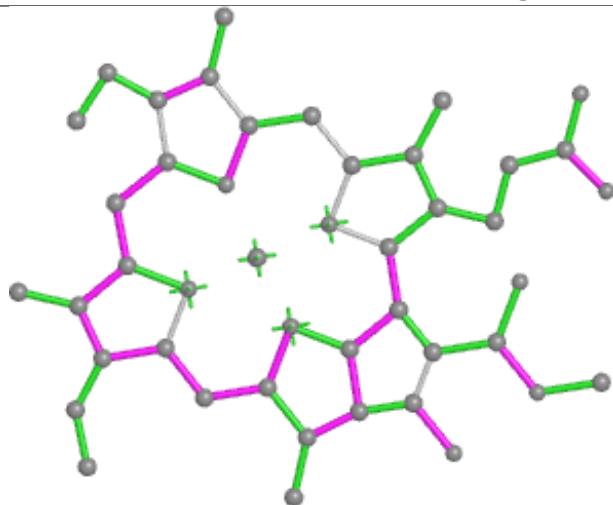
Rings

## Ligand CLA 2 613

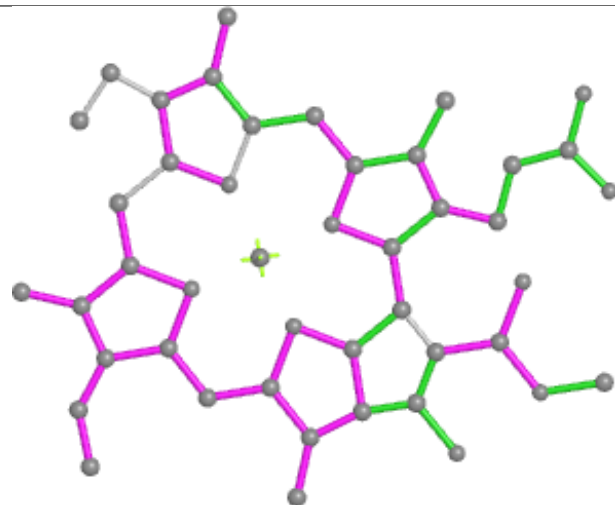




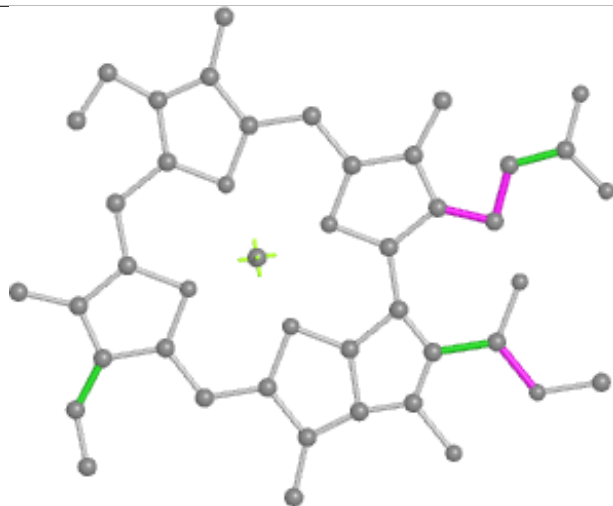
## Ligand CLA B 835



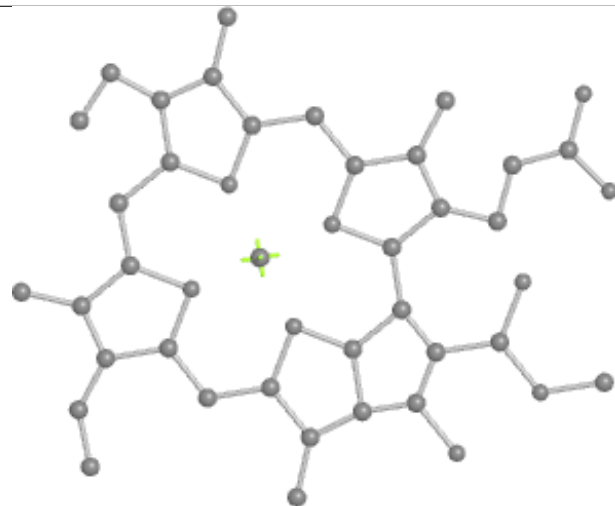
Bond lengths



Bond angles

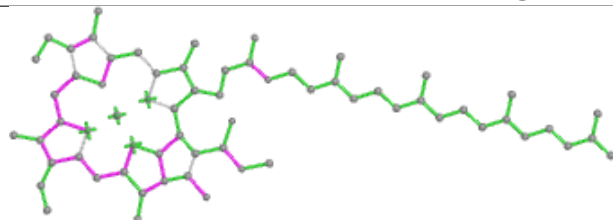


Torsions

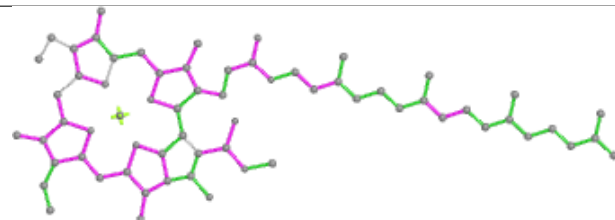


Rings

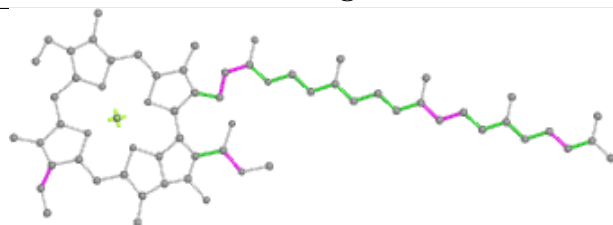
## Ligand CLA A 841



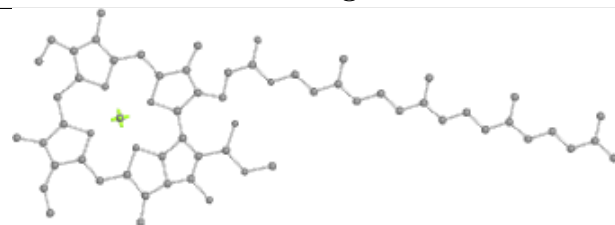
Bond lengths



Bond angles

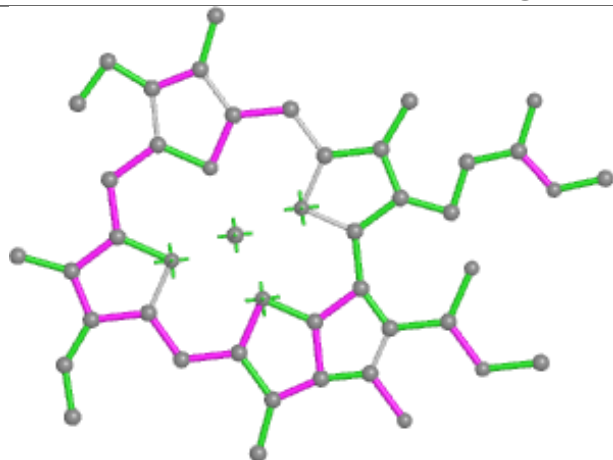


Torsions

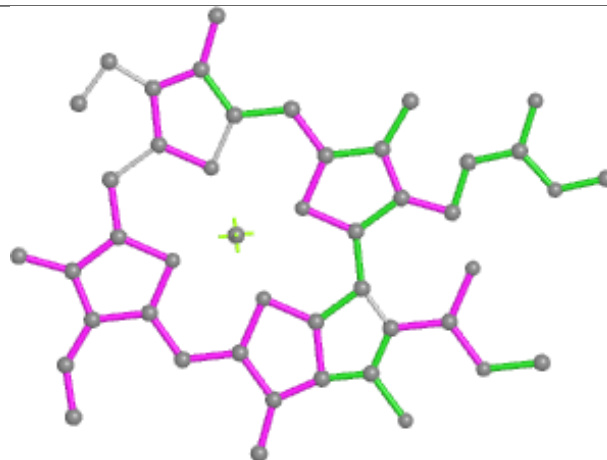


Rings

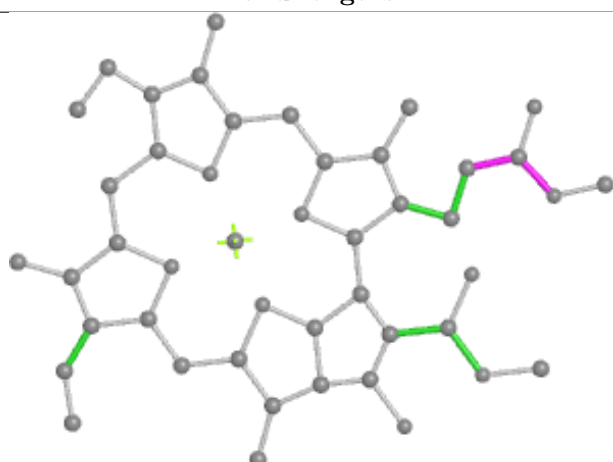
## Ligand CLA Z 616



Bond lengths



Bond angles

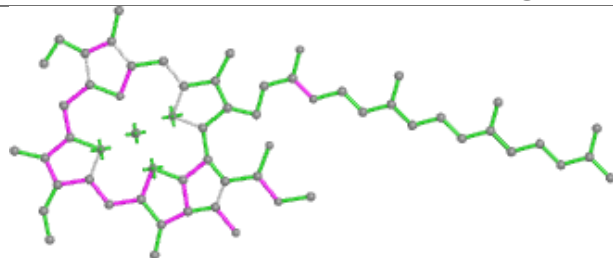


Torsions

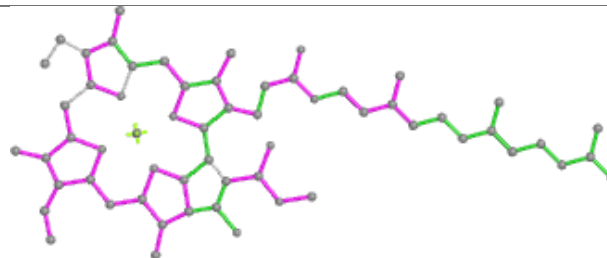


Rings

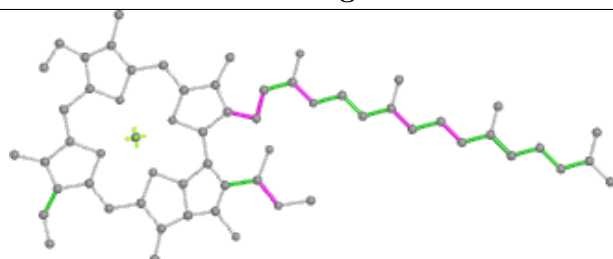
## Ligand CLA 6 610



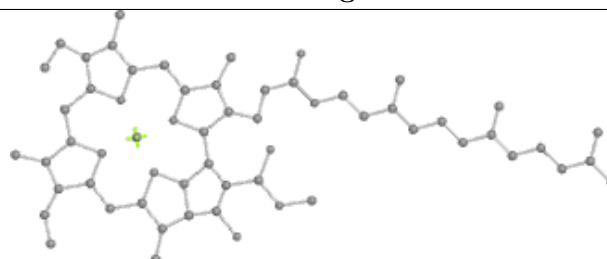
Bond lengths



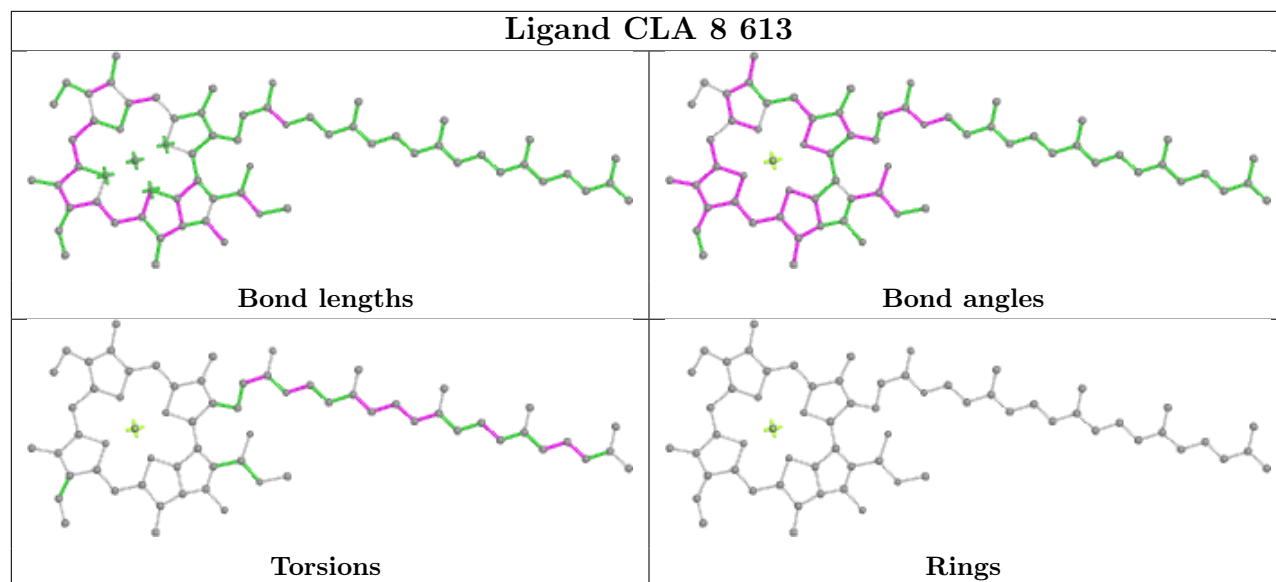
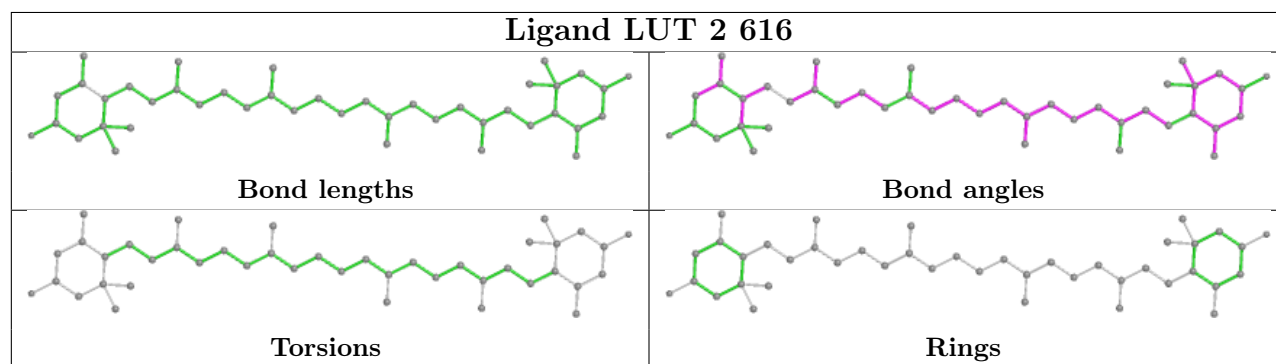
Bond angles



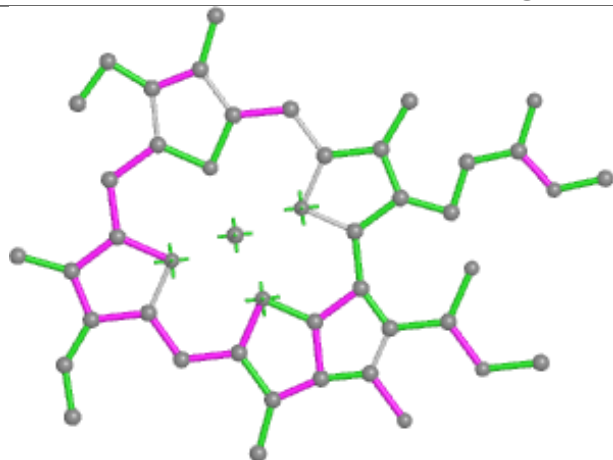
Torsions



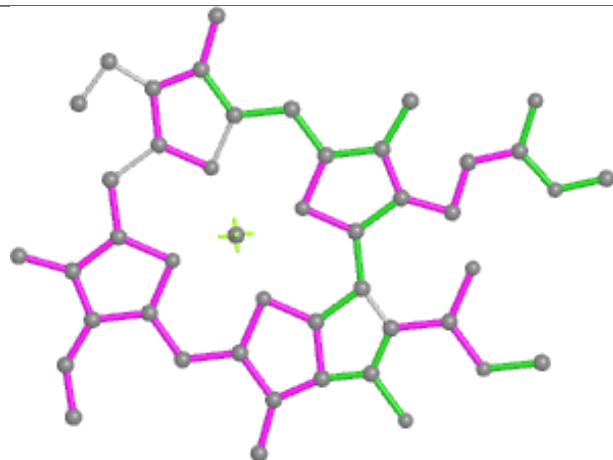
Rings

**Ligand CLA 8 613****Ligand LUT 2 616**

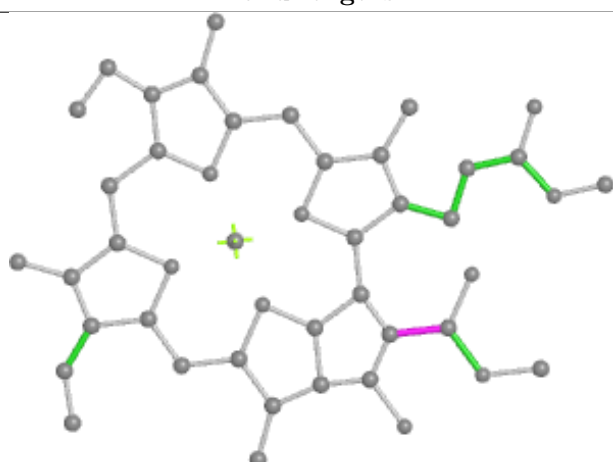
## Ligand CLA 7 603



Bond lengths



Bond angles

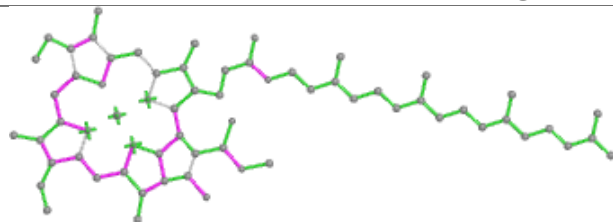


Torsions

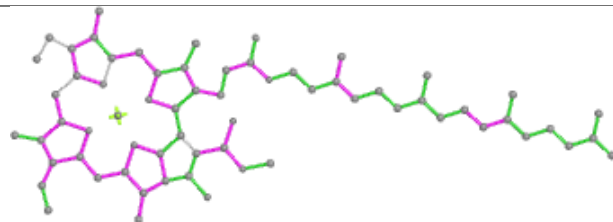


Rings

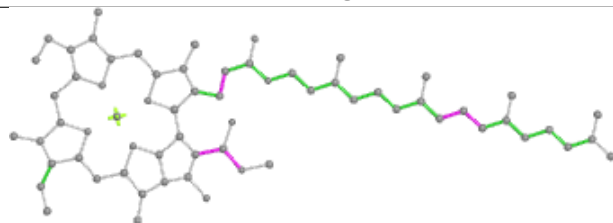
## Ligand CLA B 803



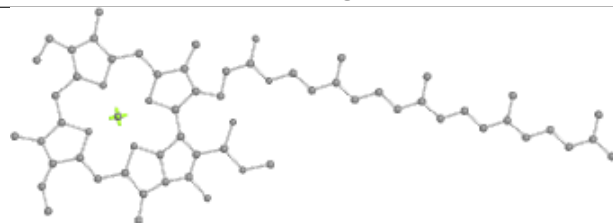
Bond lengths



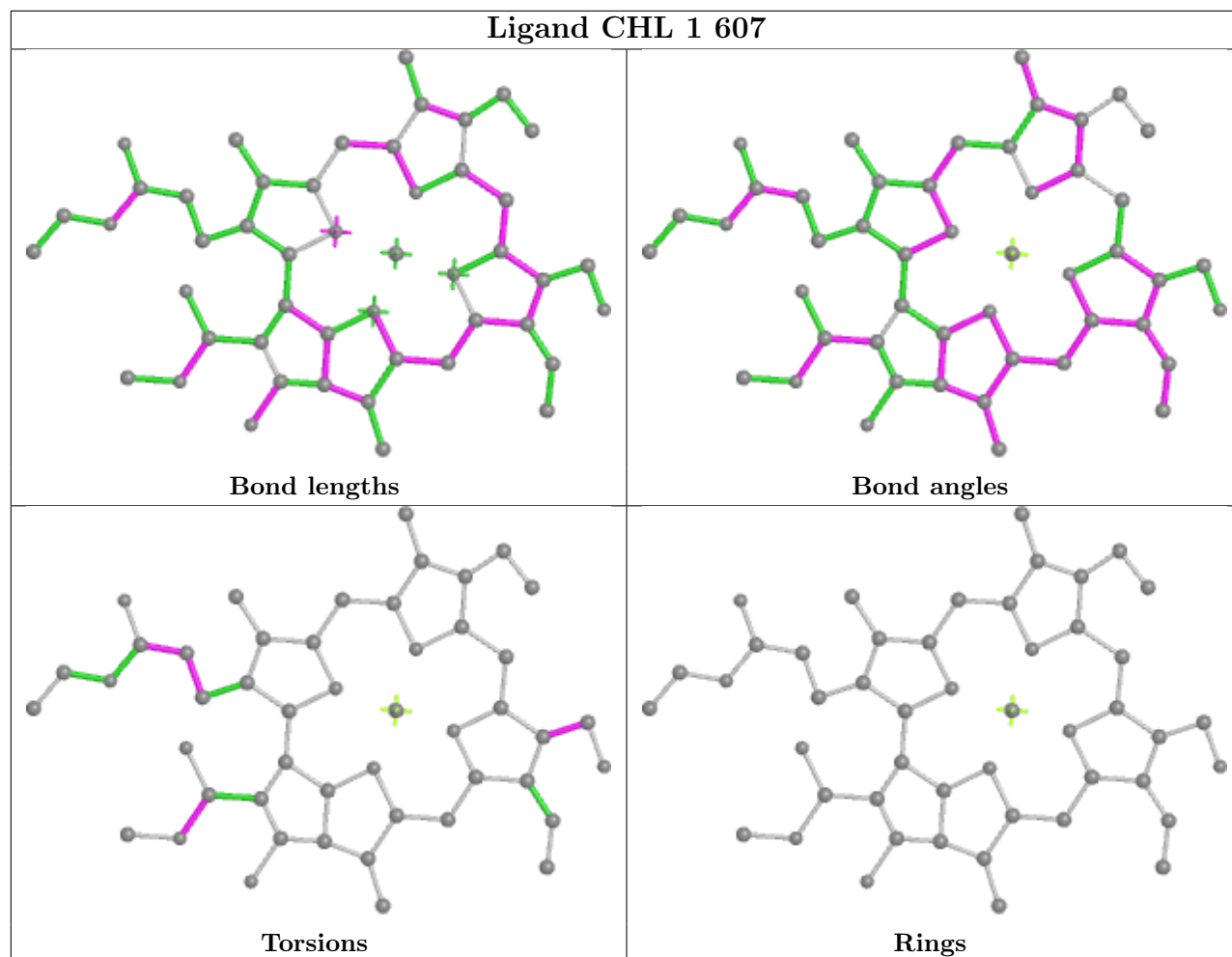
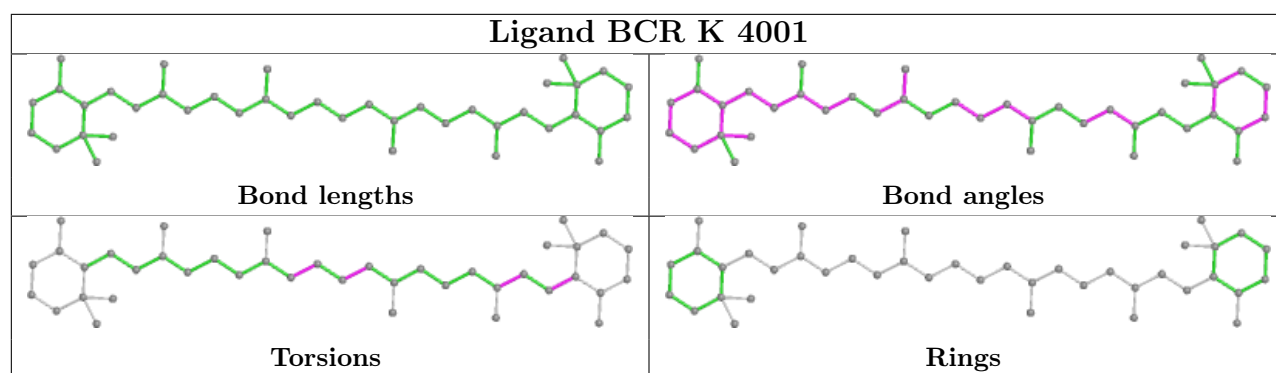
Bond angles



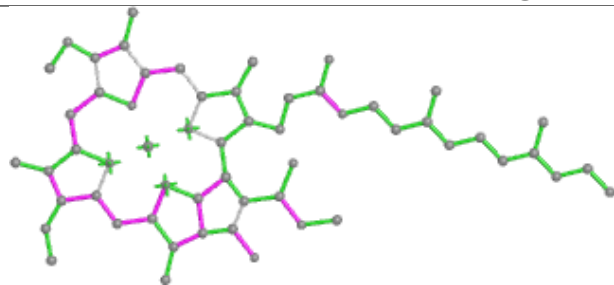
Torsions



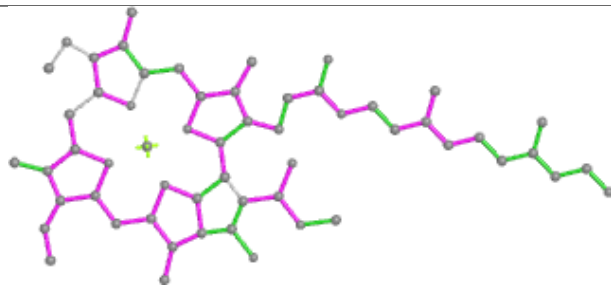
Rings



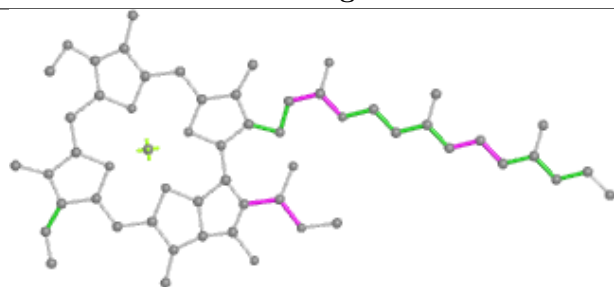
## Ligand CLA Z 603



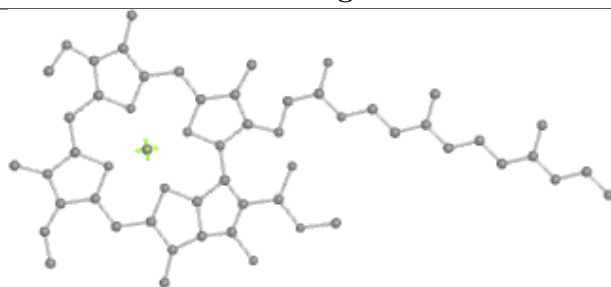
Bond lengths



Bond angles

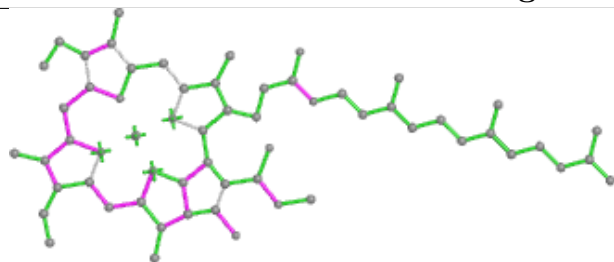


Torsions

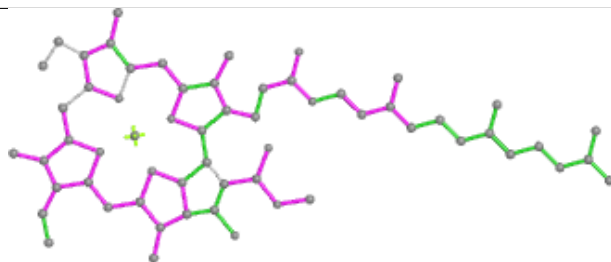


Rings

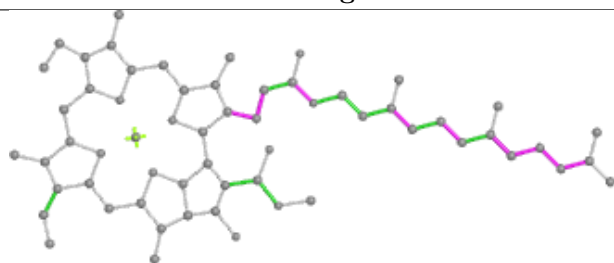
## Ligand CLA 8 610



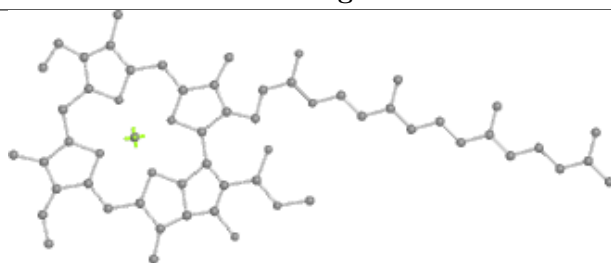
Bond lengths



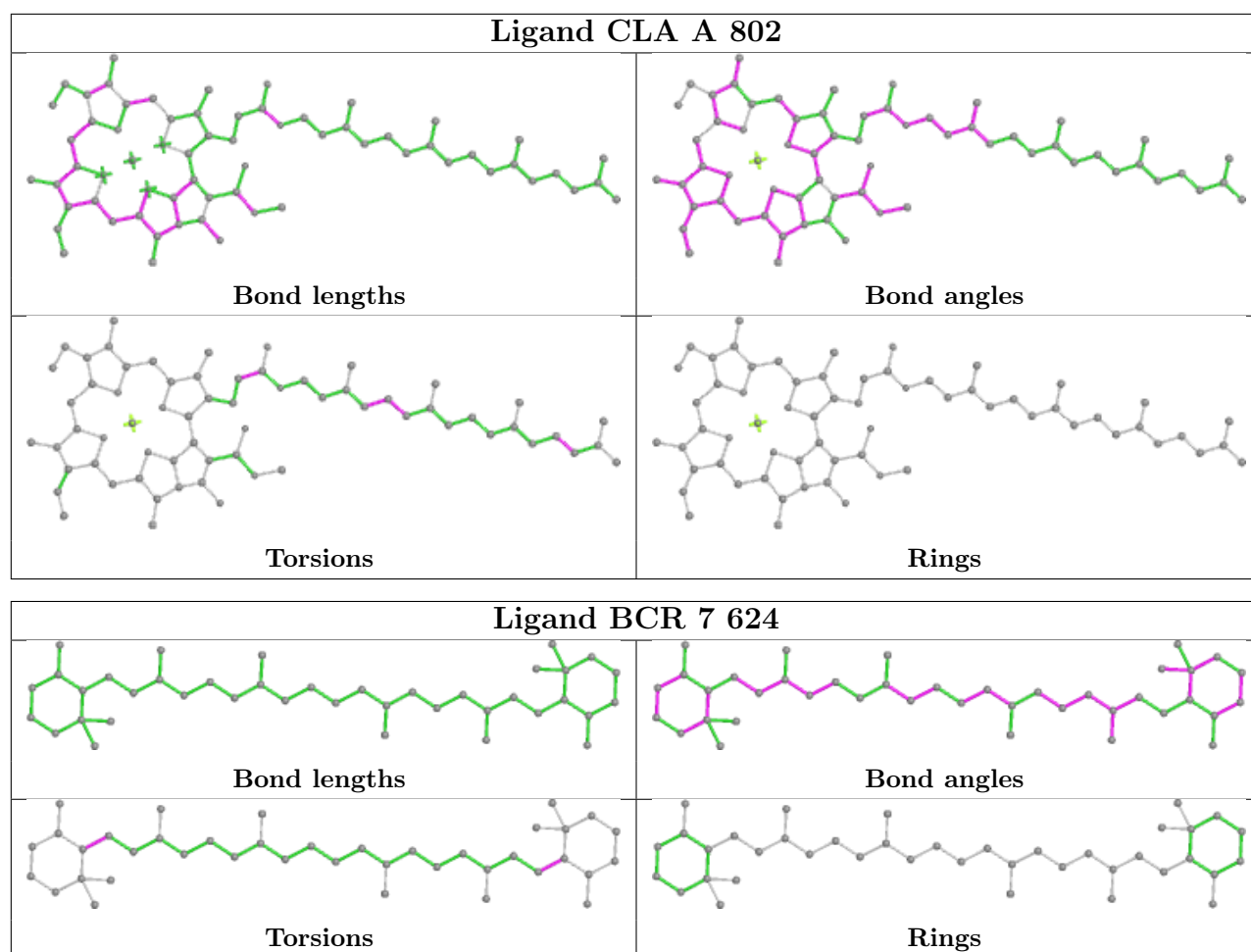
Bond angles



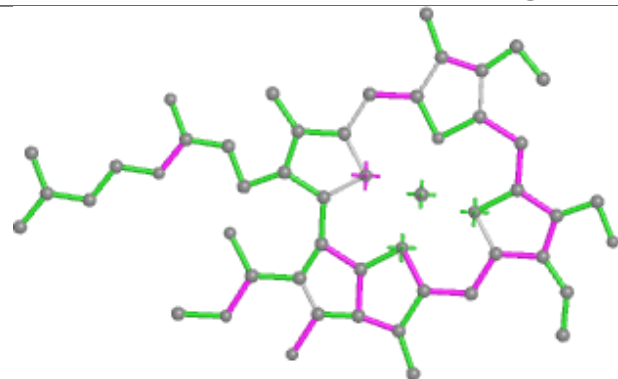
Torsions



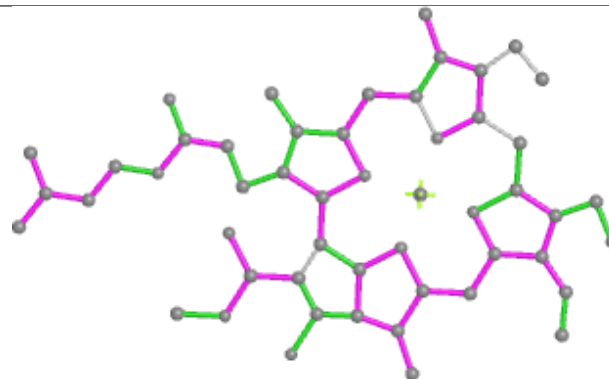
Rings



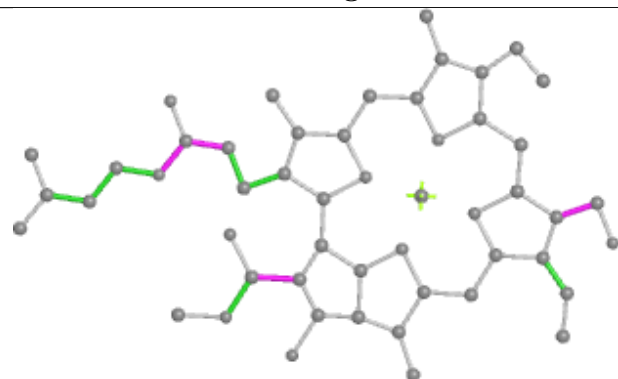
## Ligand CHL 9 607



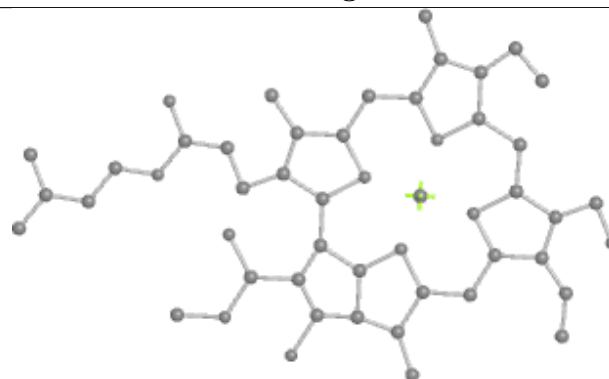
Bond lengths



Bond angles

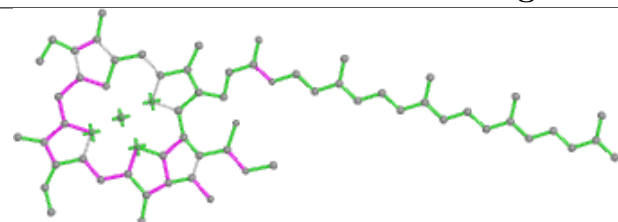


Torsions

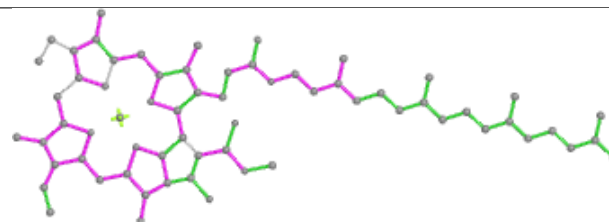


Rings

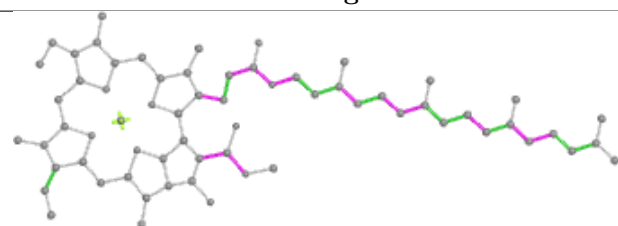
## Ligand CLA A 829



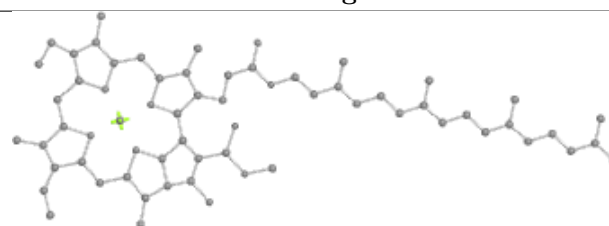
Bond lengths



Bond angles



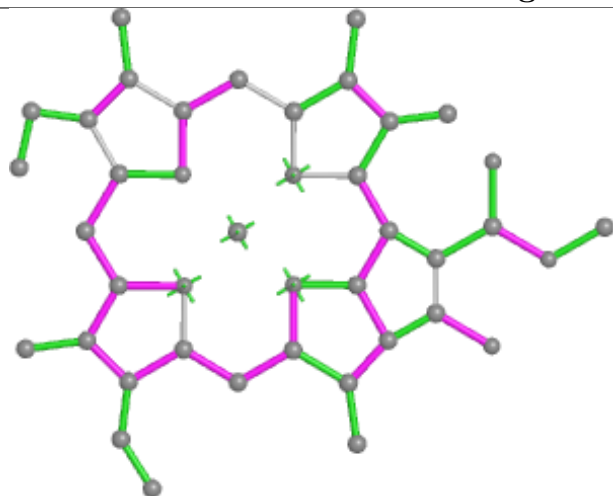
Torsions



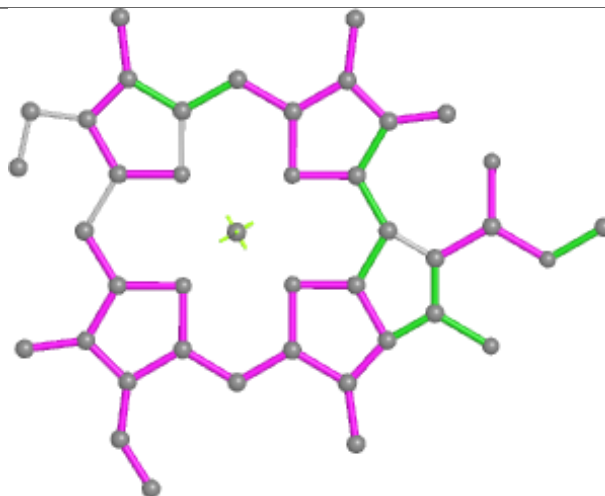
Rings



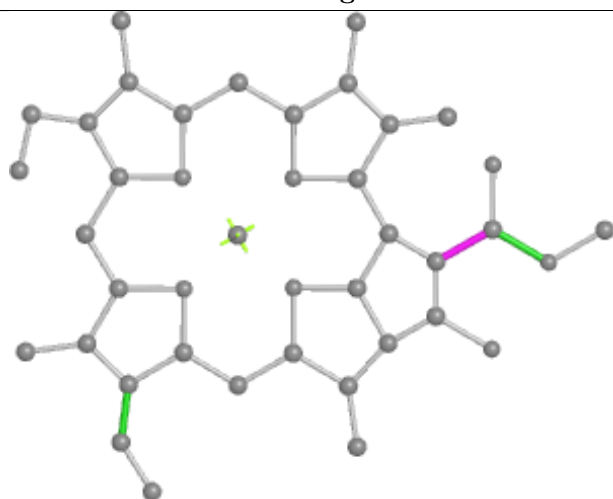
## Ligand CLA 7 611



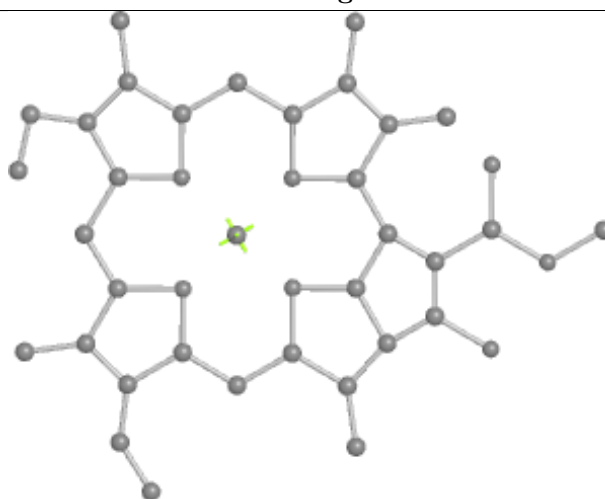
Bond lengths



Bond angles

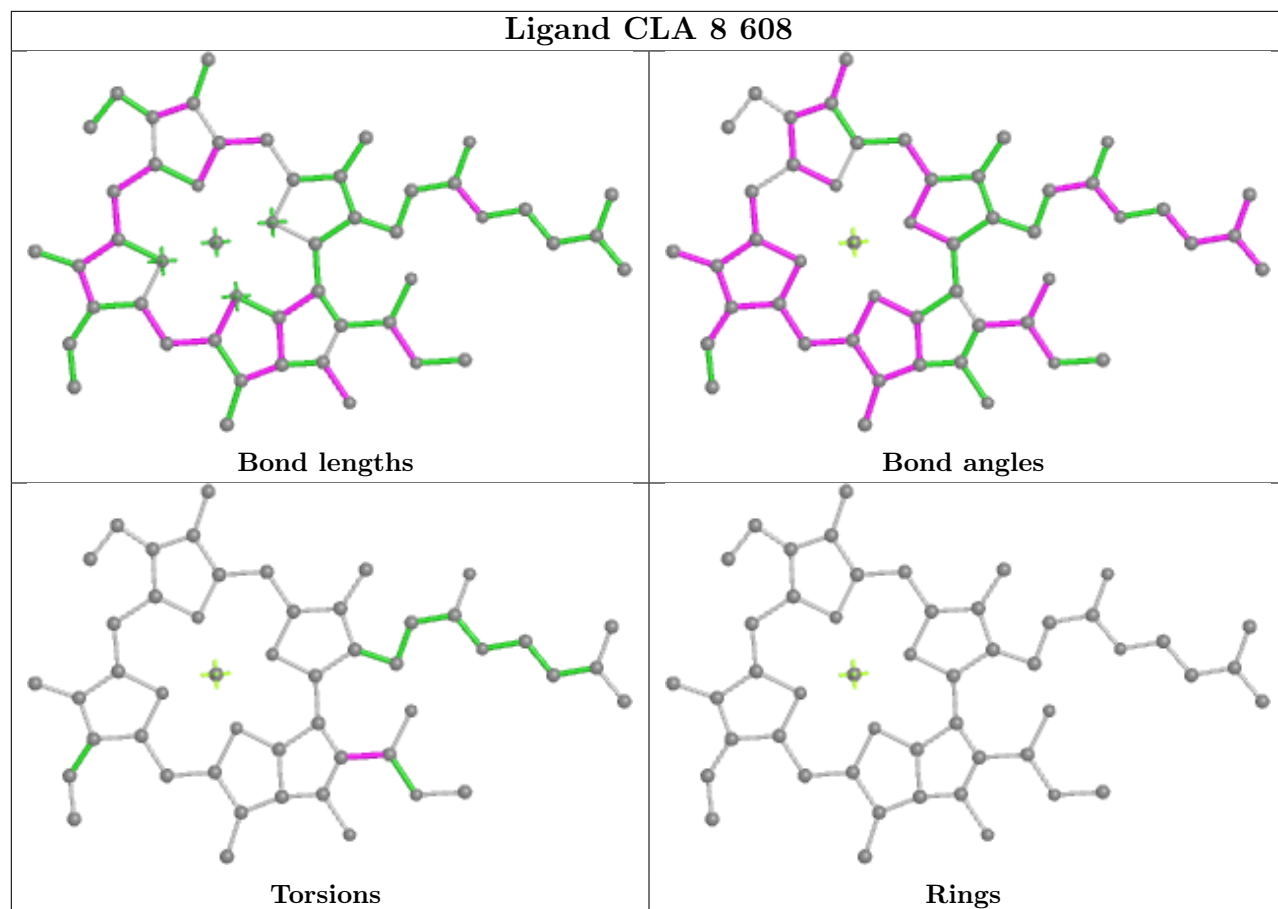


Torsions

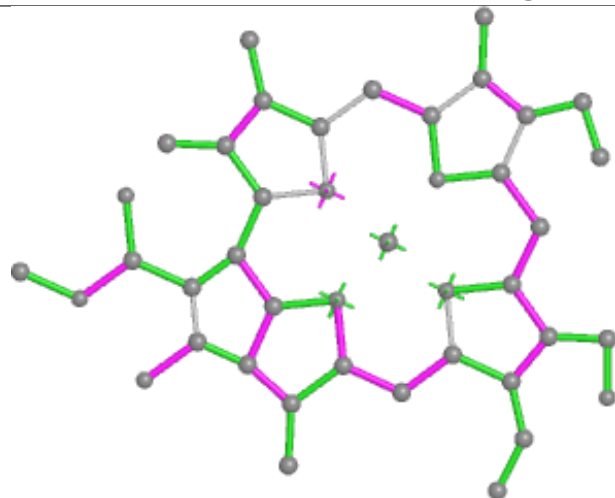


Rings

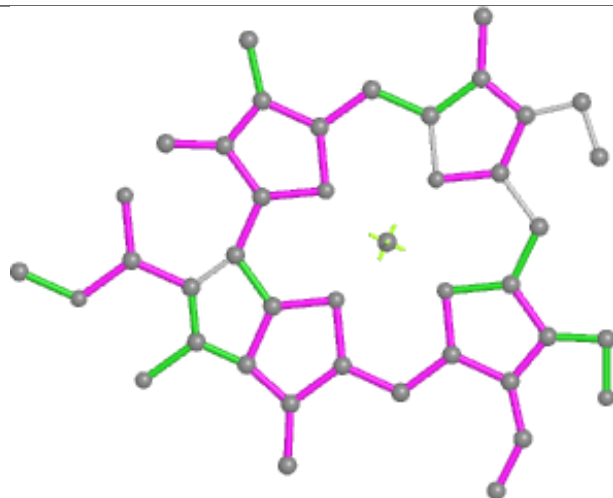
## Ligand CLA 8 608



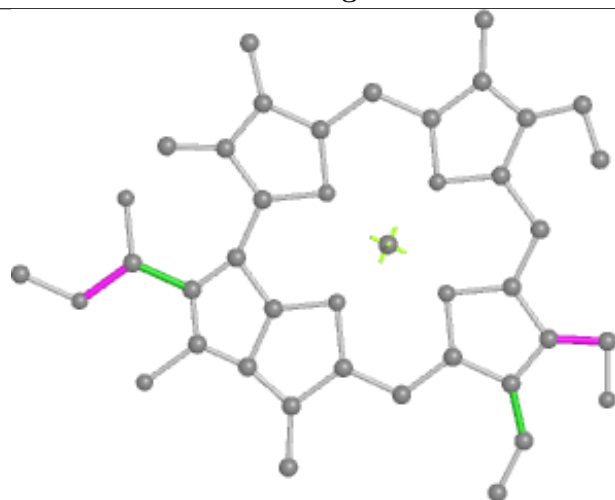
## Ligand CHL 9 606



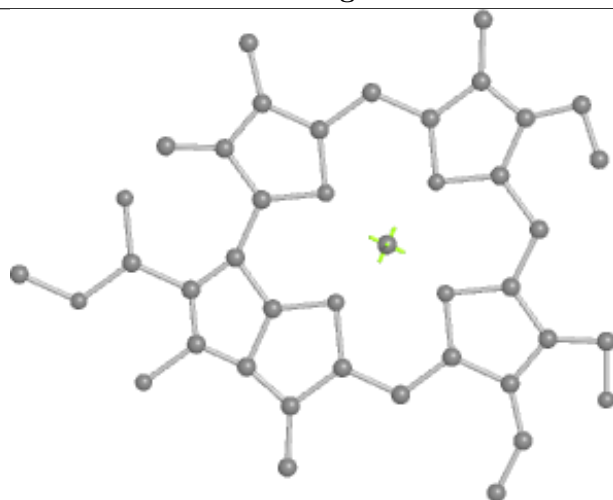
Bond lengths



Bond angles

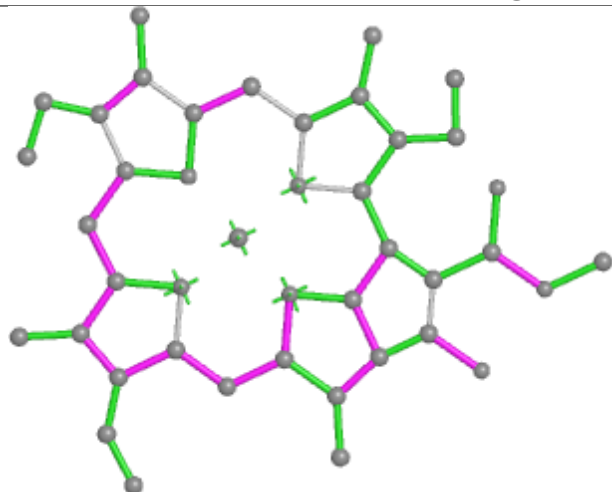


Torsions

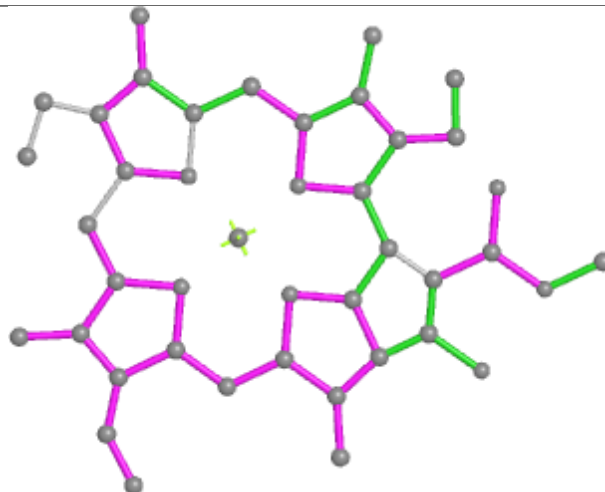


Rings

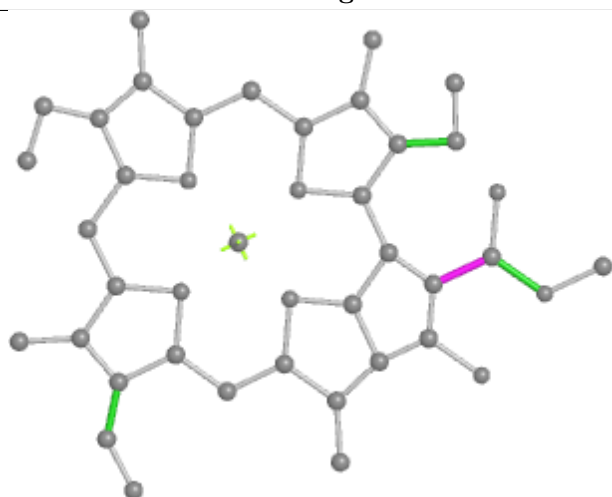
## Ligand CLA J 3002



Bond lengths



Bond angles

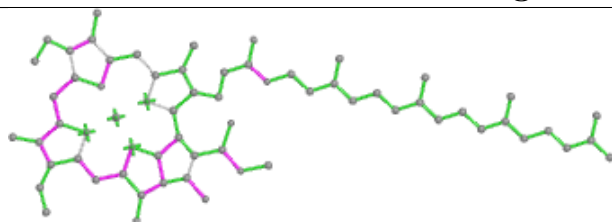


Torsions

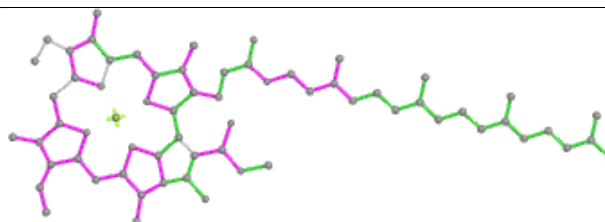


Rings

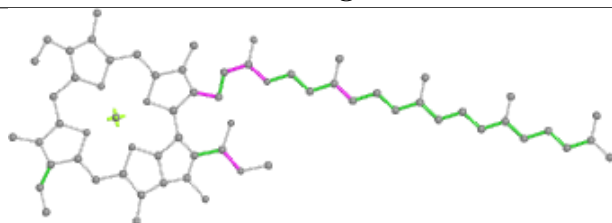
## Ligand CLA A 811



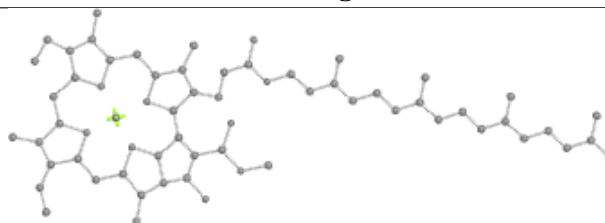
Bond lengths



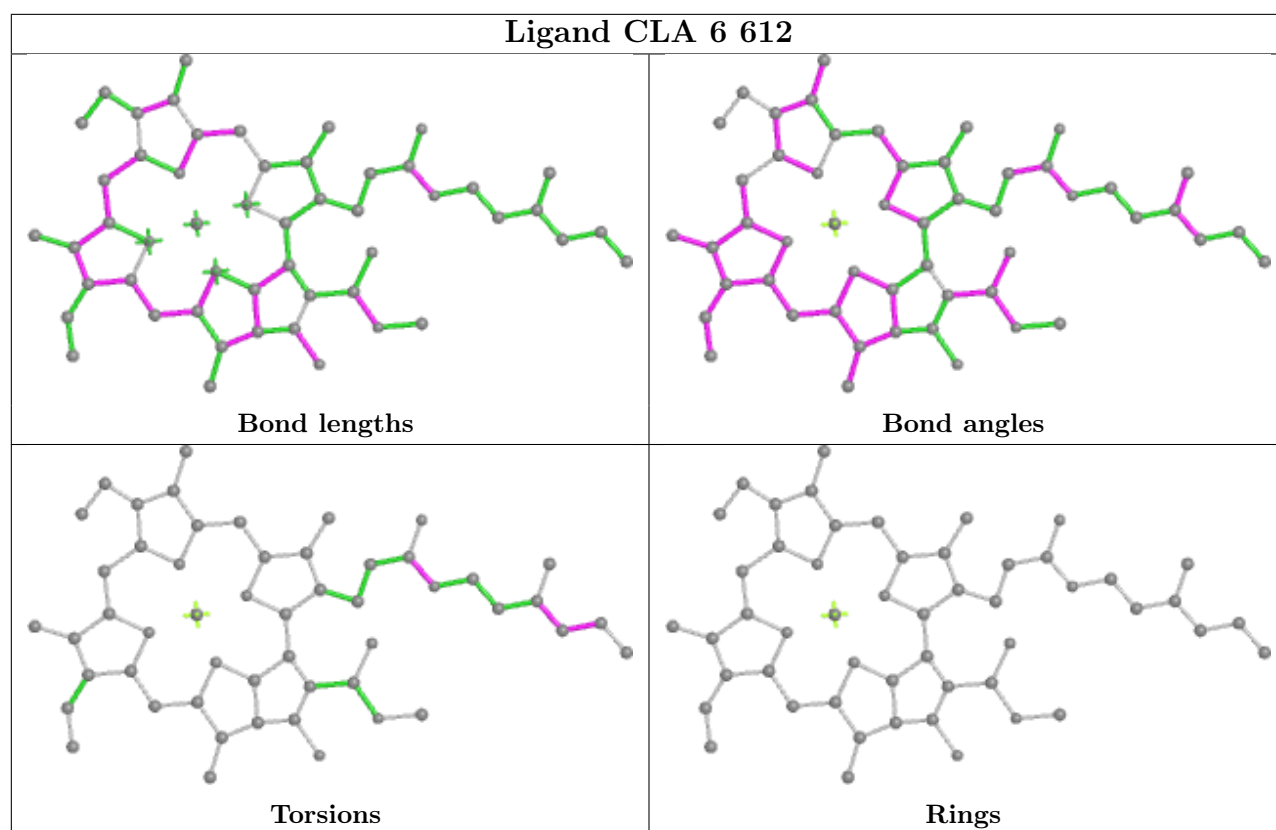
Bond angles



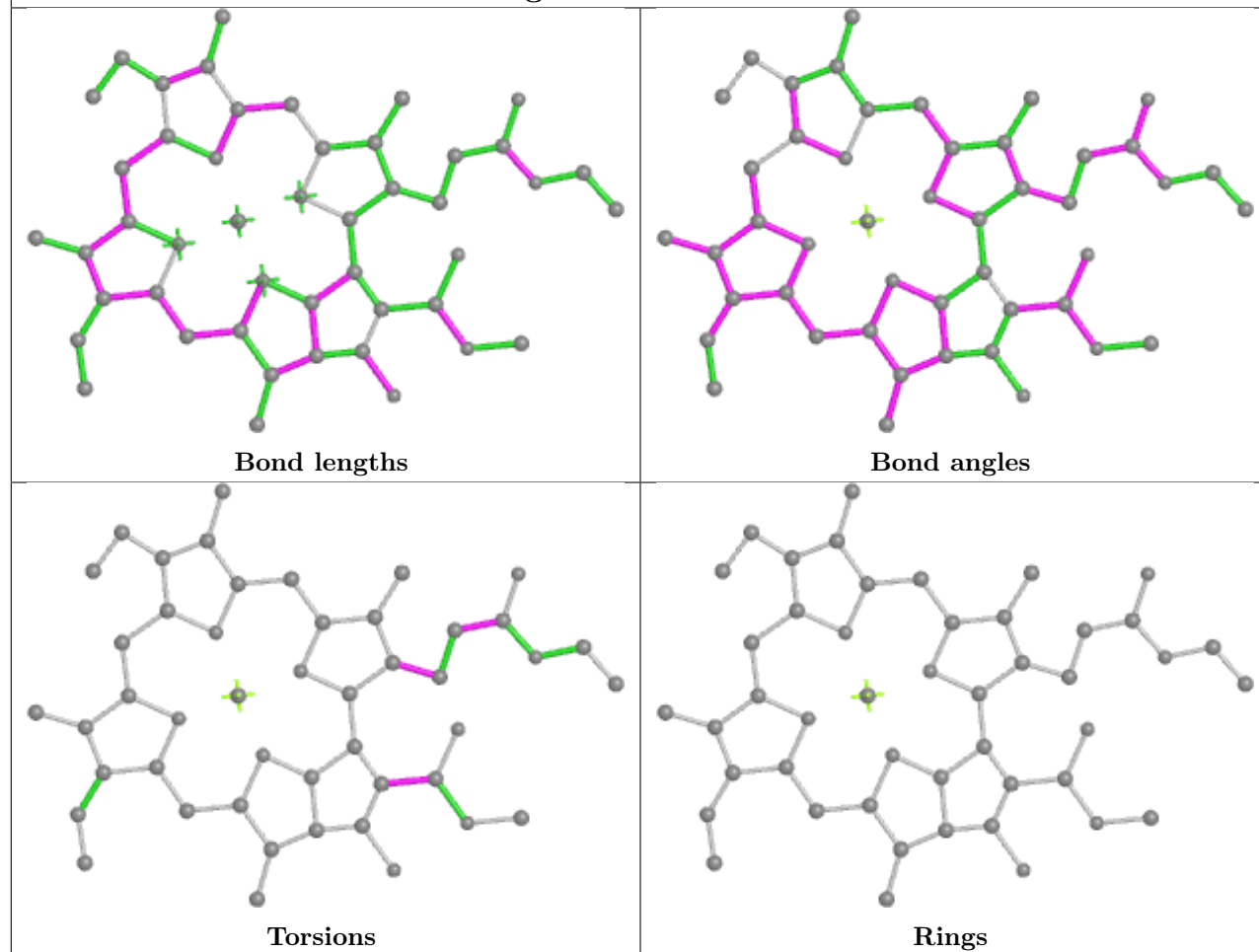
Torsions



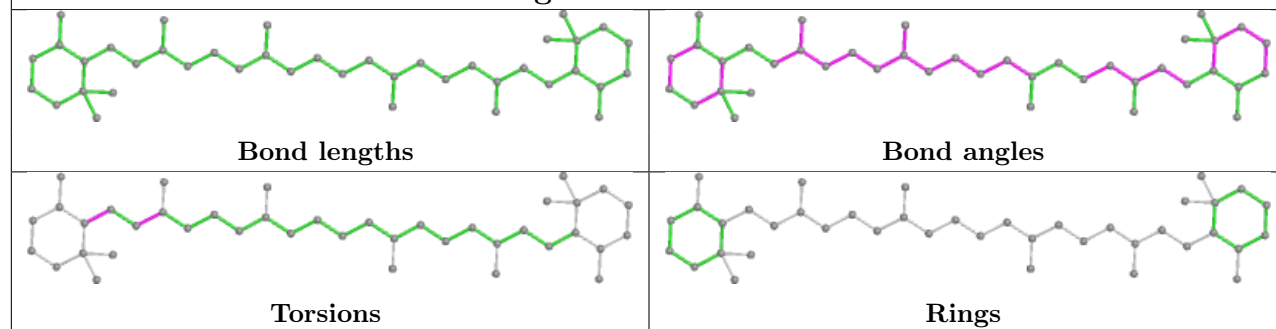
Rings

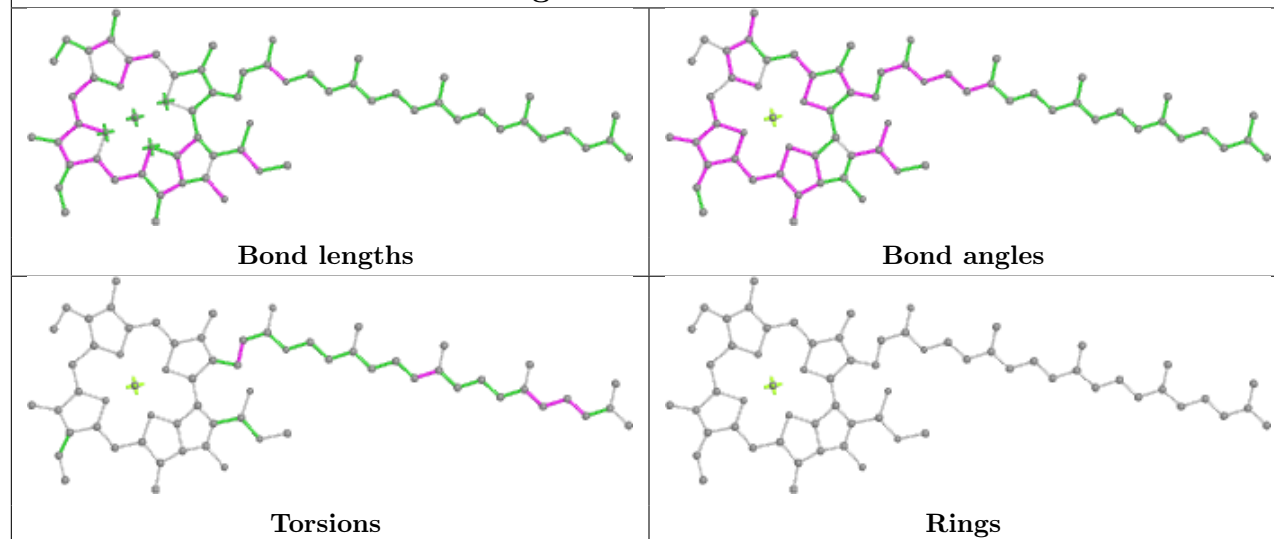
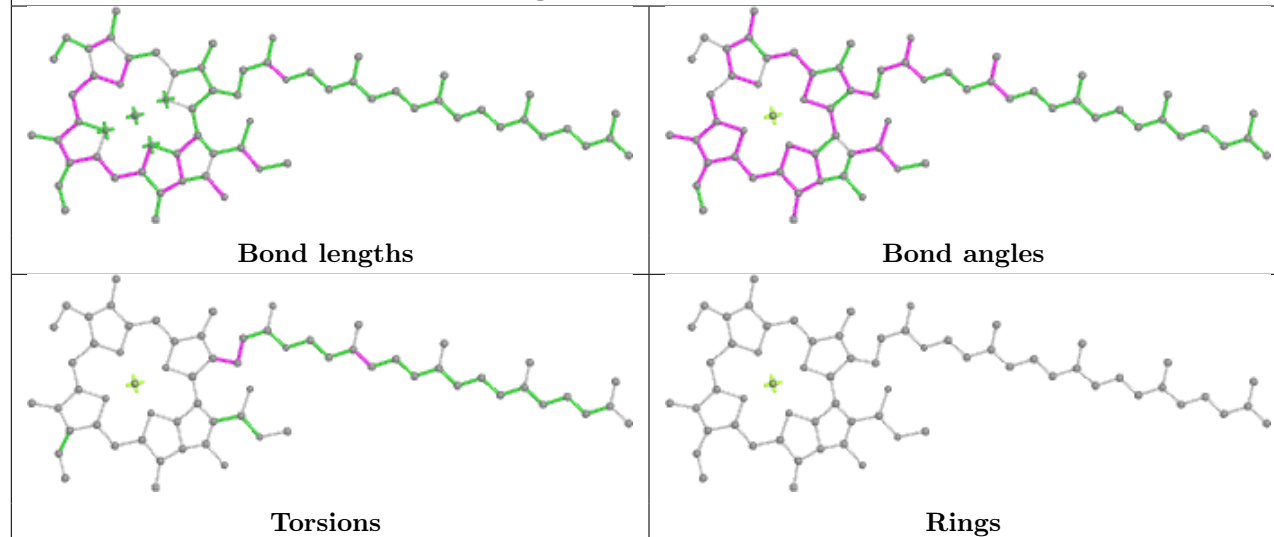
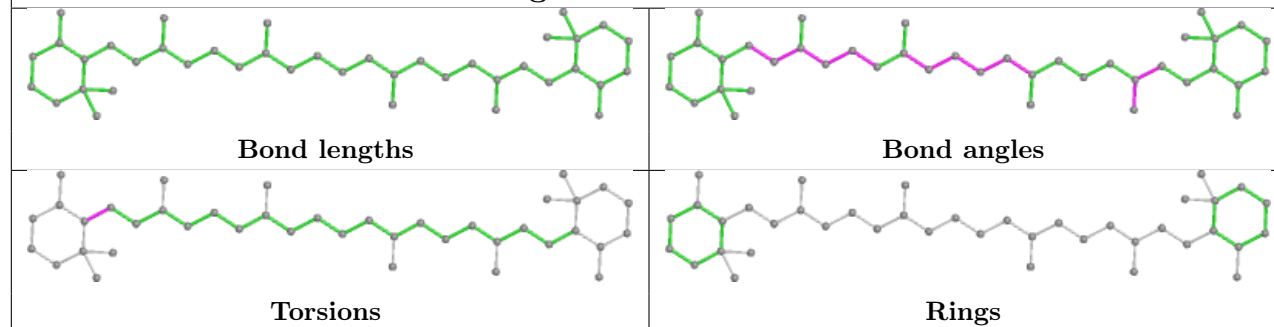


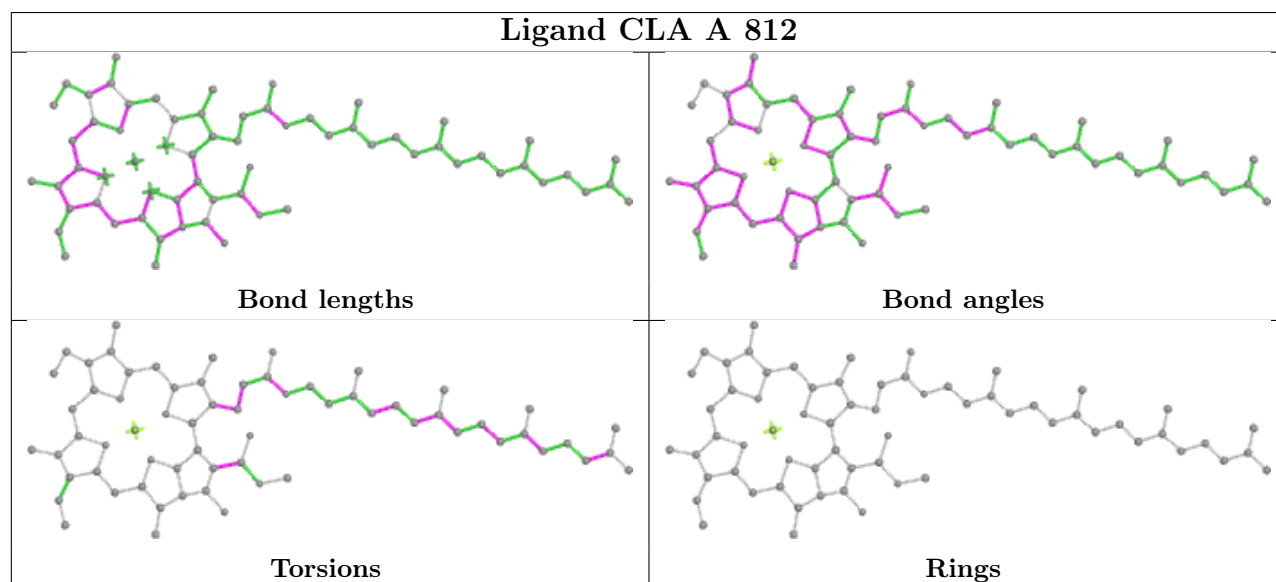
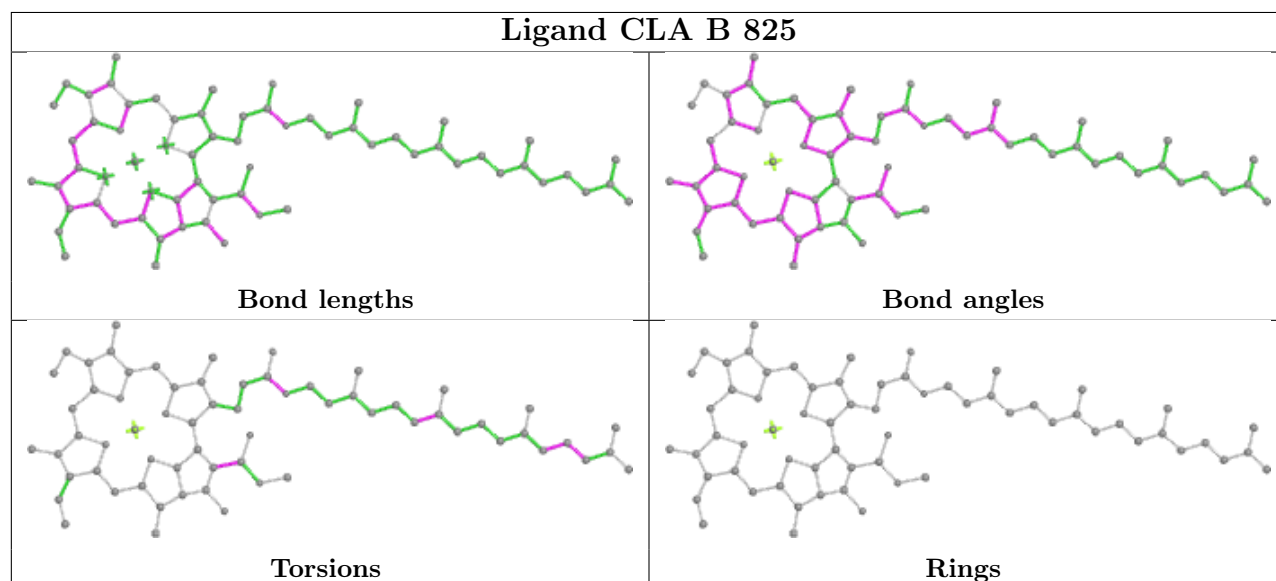
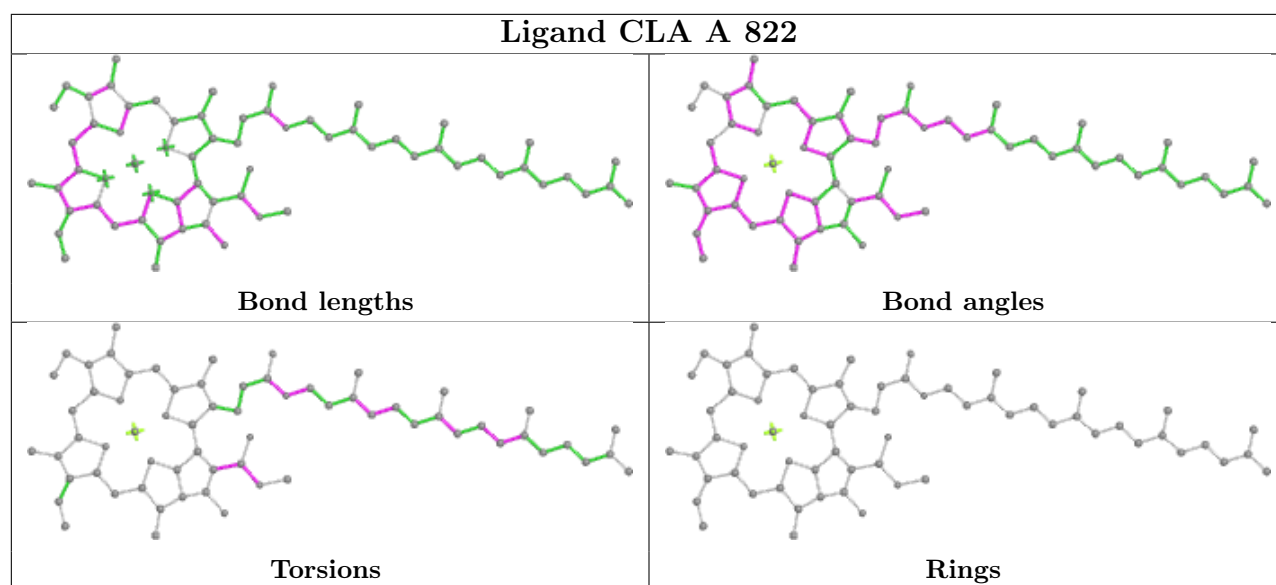
## Ligand CLA B 838



## Ligand BCR 3 719

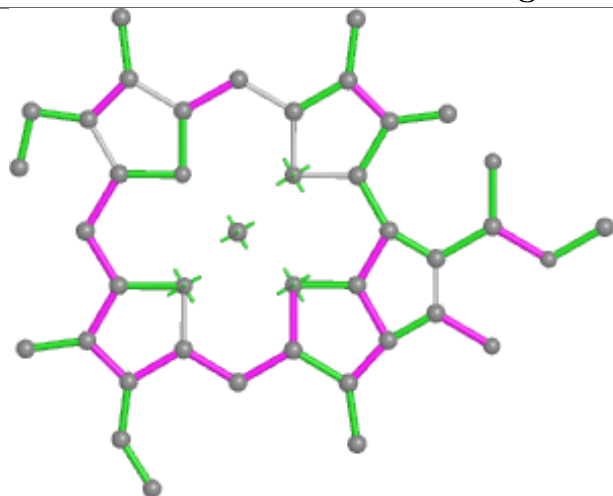


**Ligand CLA B 839****Ligand CLA A 803****Ligand BCR G 205**

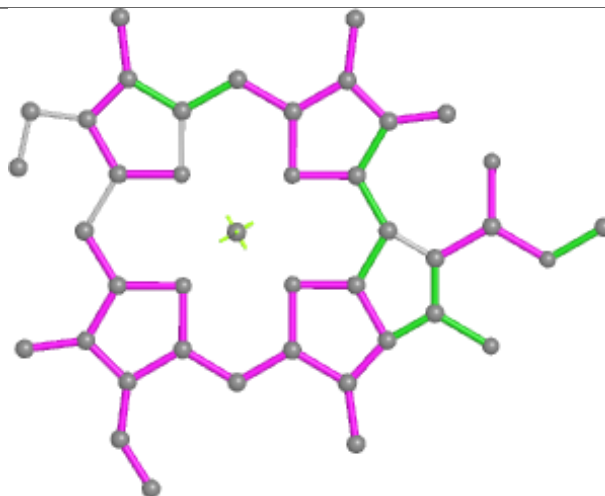




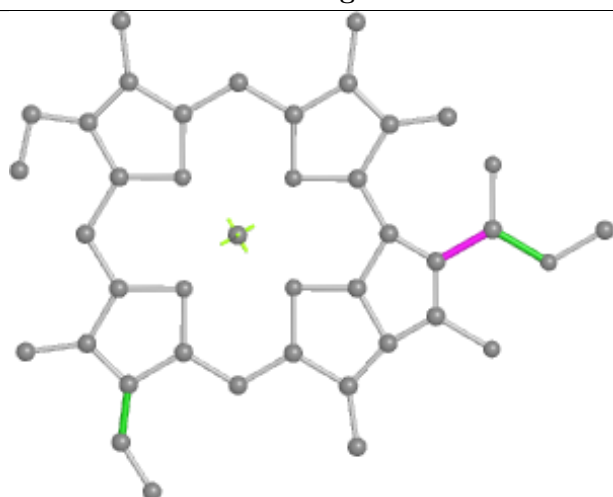
## Ligand CLA 2 606



Bond lengths



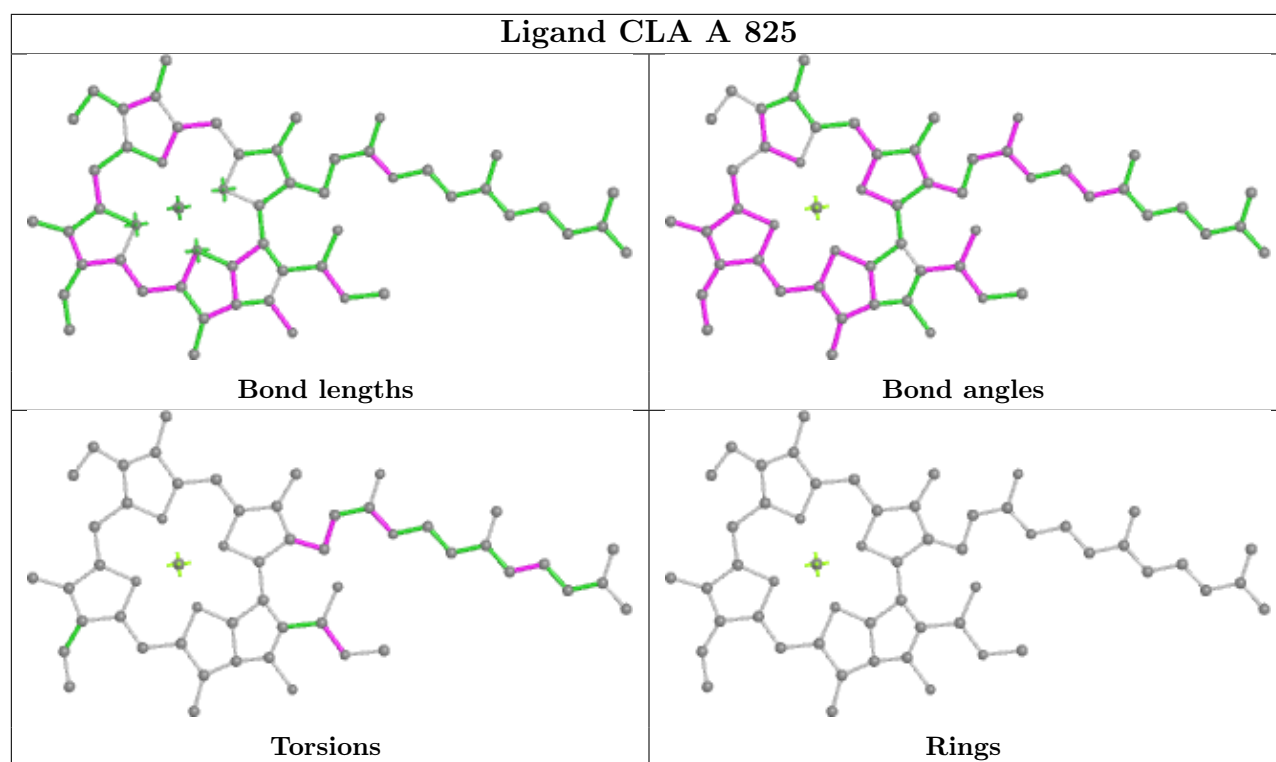
Bond angles



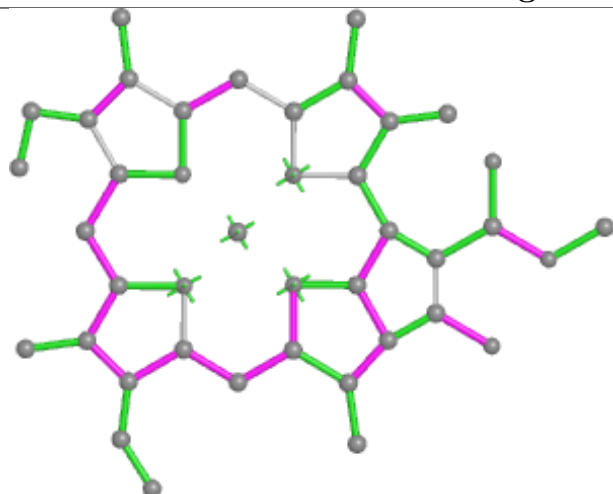
Torsions



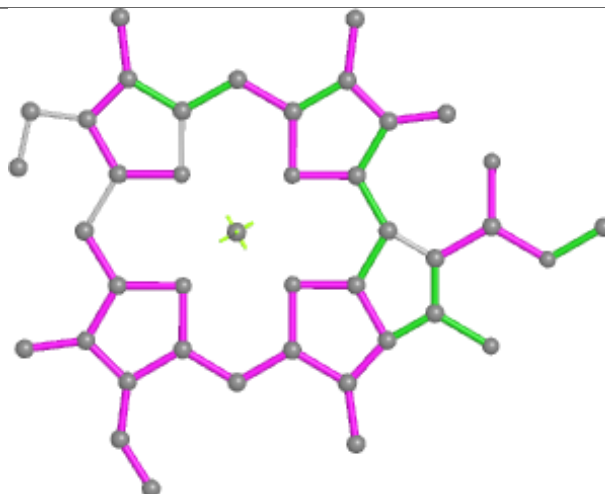
Rings



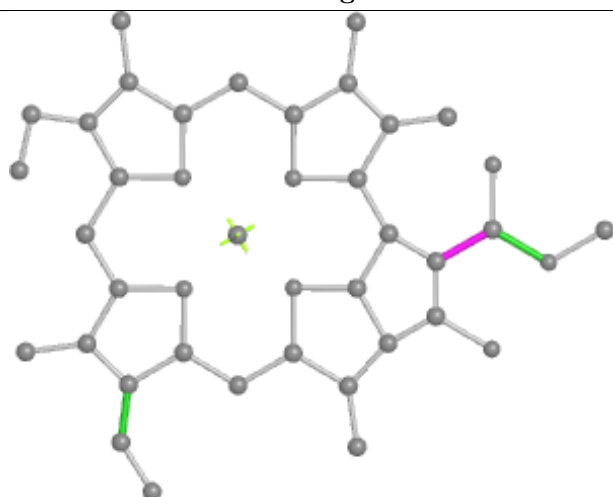
## Ligand CLA 3 611



Bond lengths



Bond angles

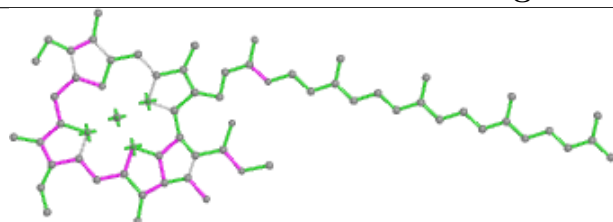


Torsions

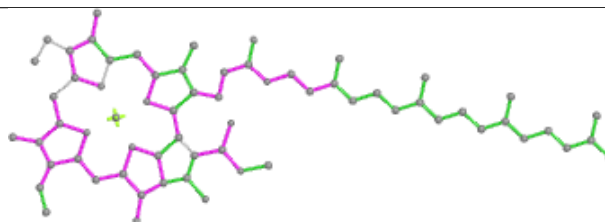


Rings

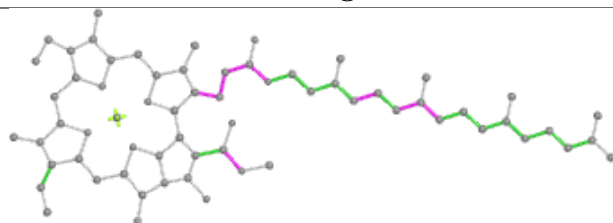
## Ligand CLA A 819



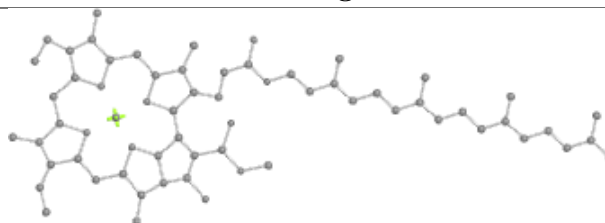
Bond lengths



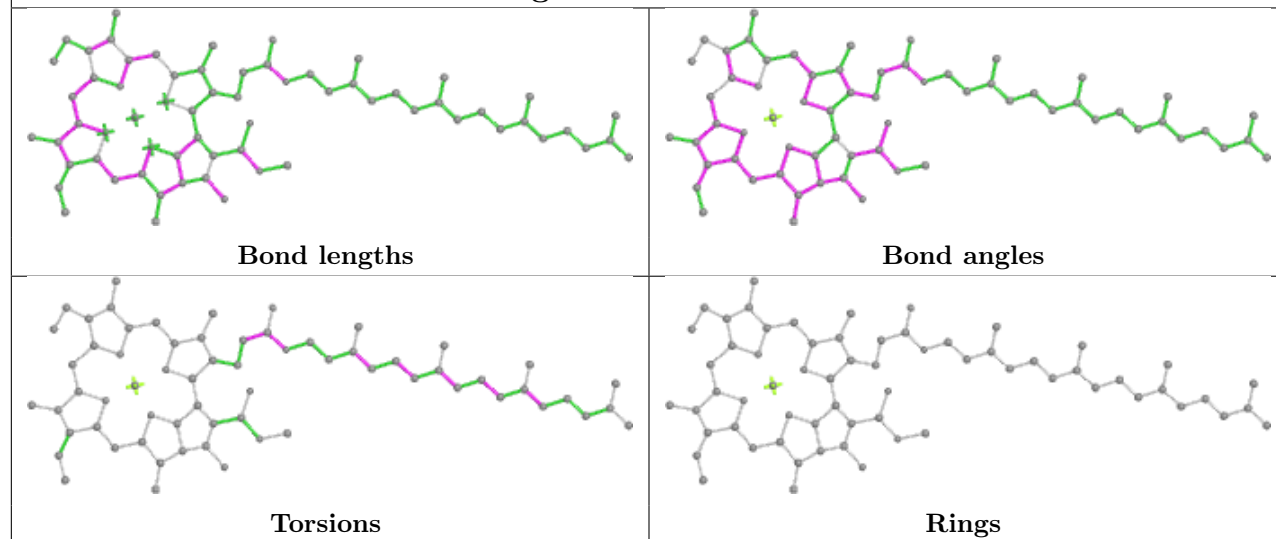
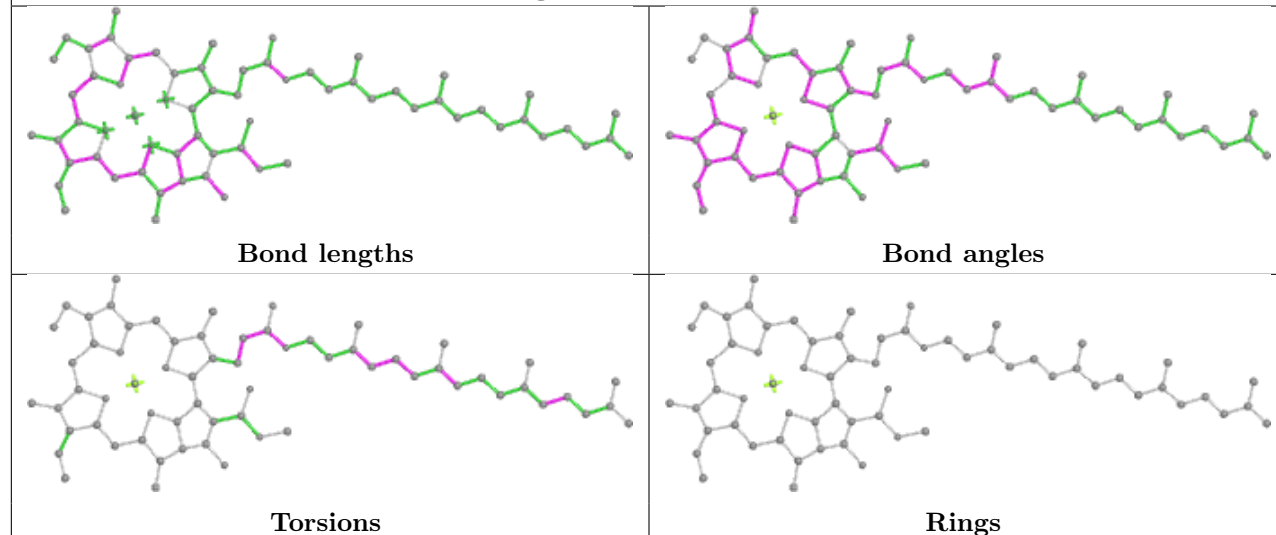
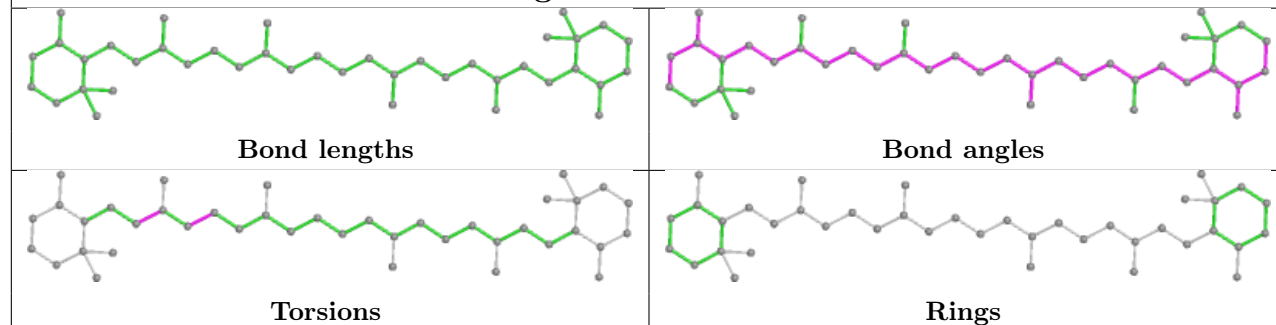
Bond angles

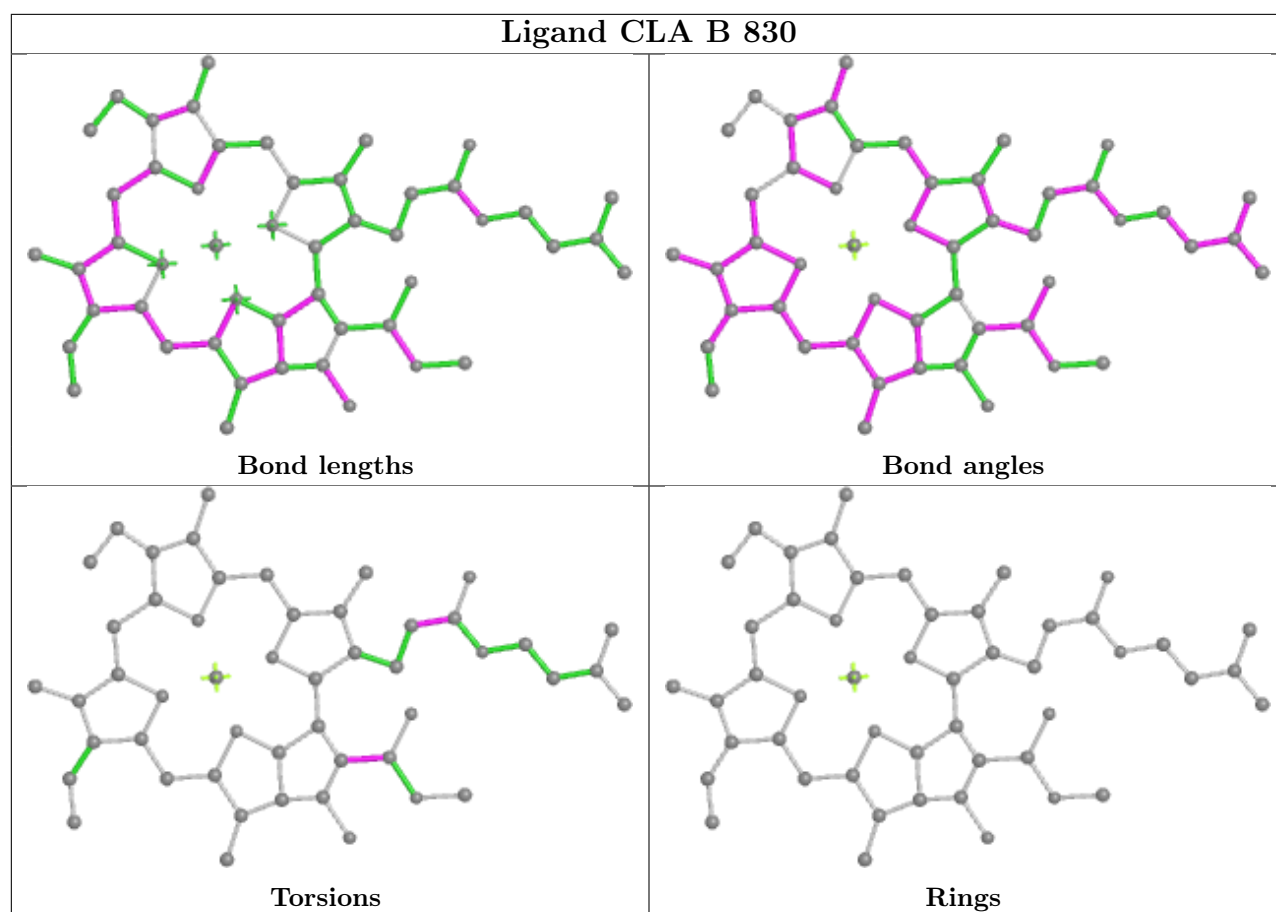


Torsions

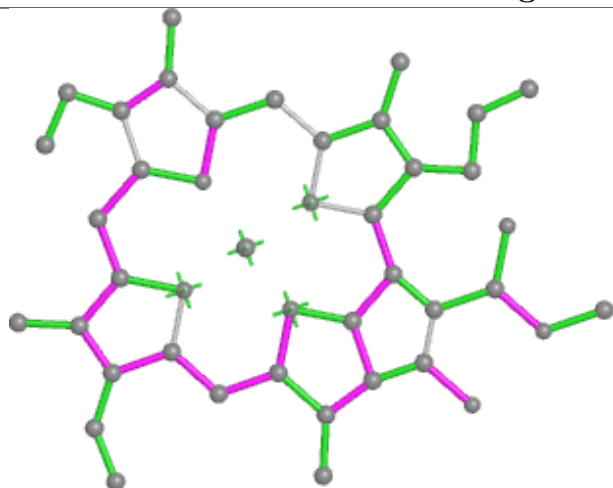


Rings

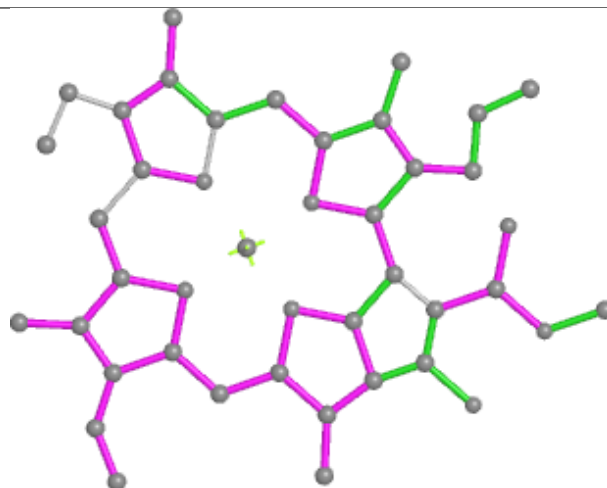
**Ligand CLA A 828****Ligand CLA B 807****Ligand BCR 4 621**



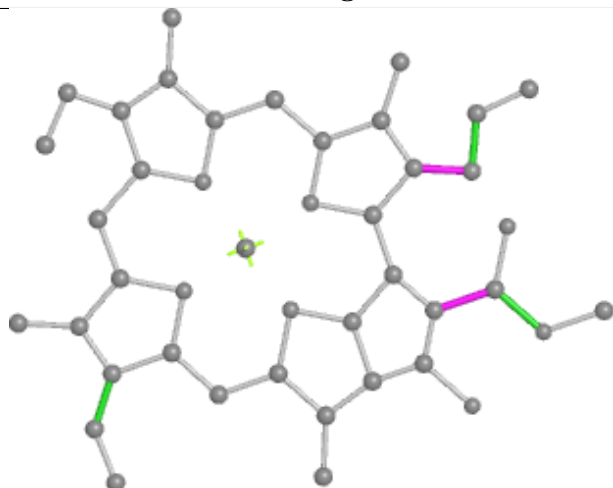
## Ligand CLA 7 614



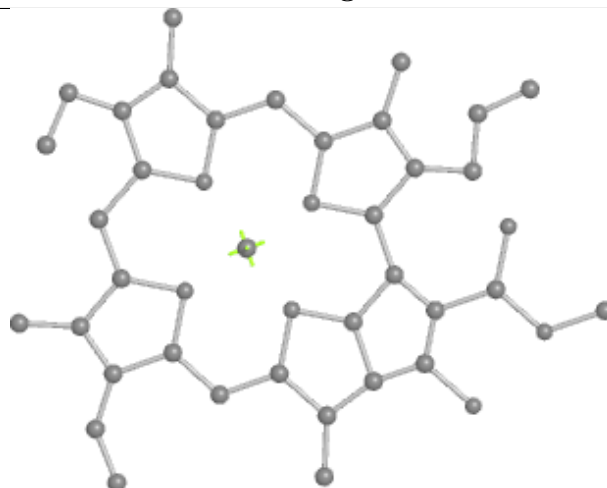
Bond lengths



Bond angles

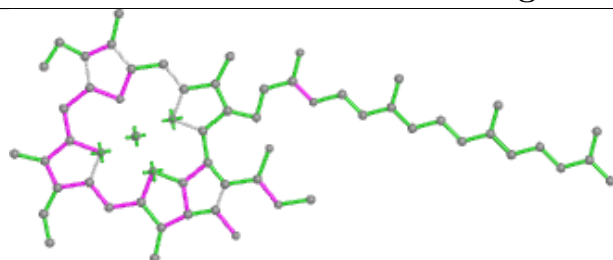


Torsions

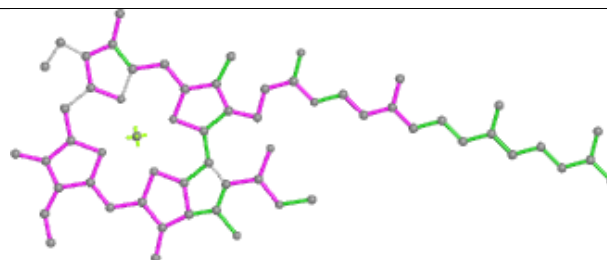


Rings

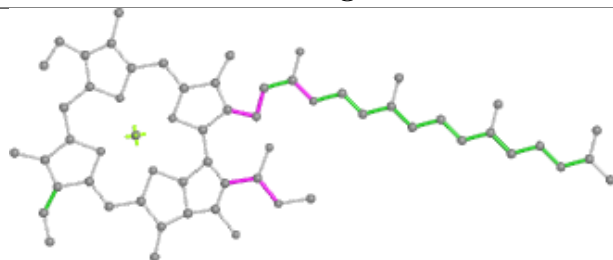
## Ligand CLA 3 602



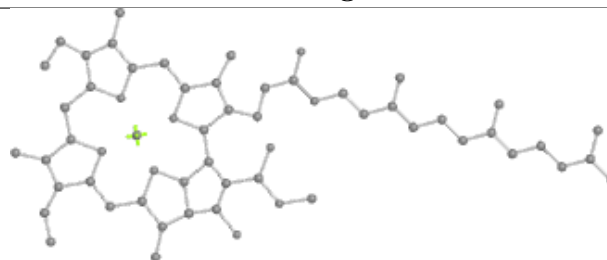
Bond lengths



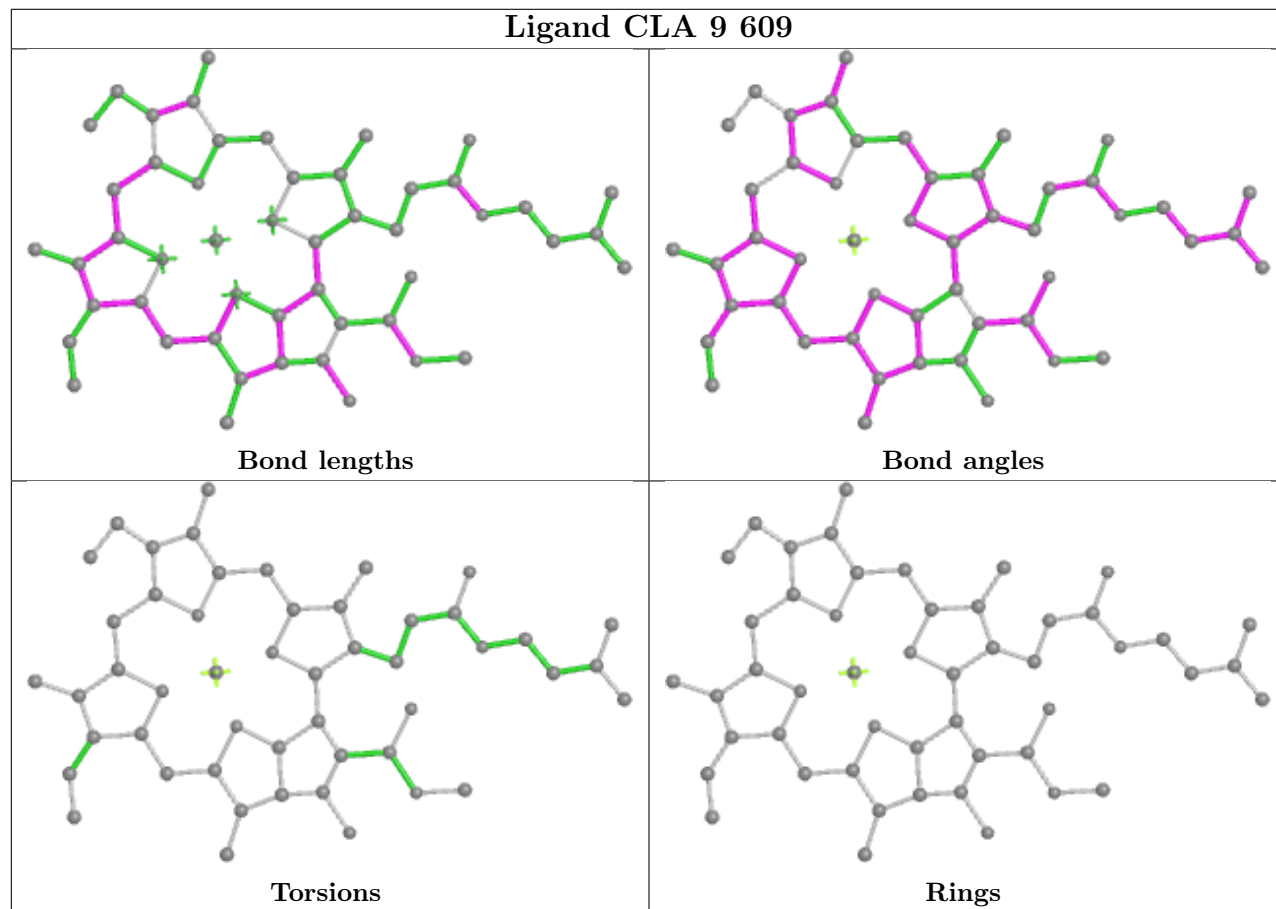
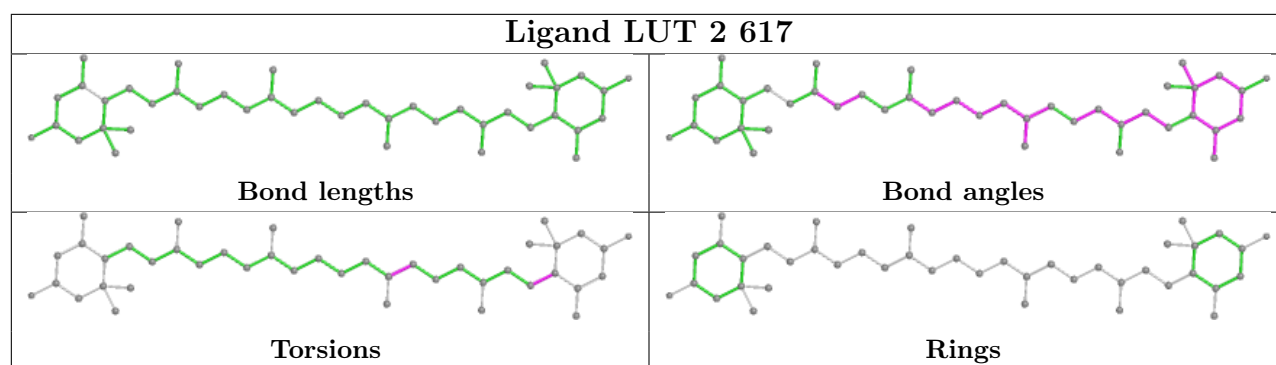
Bond angles



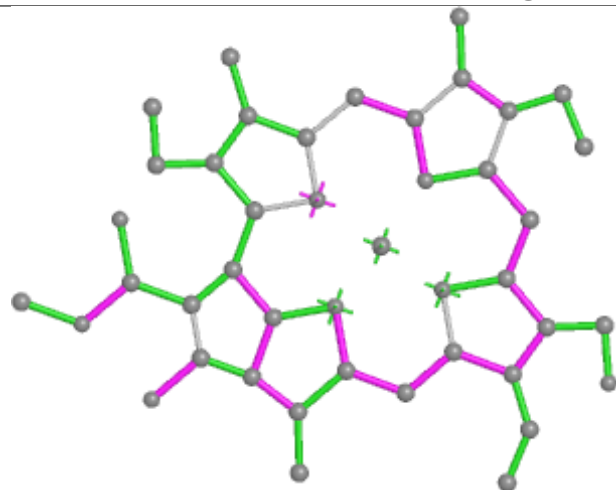
Torsions



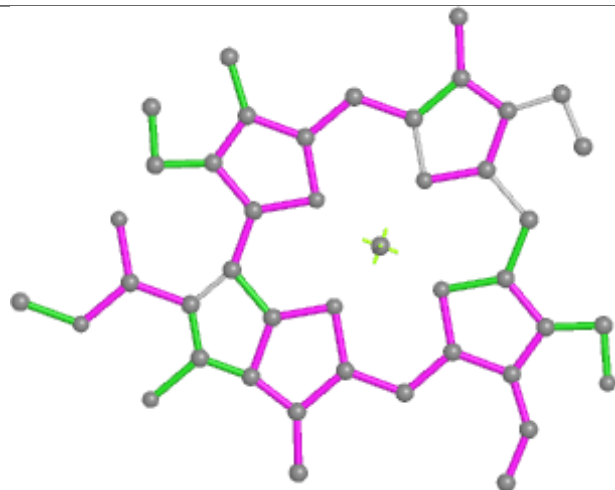
Rings



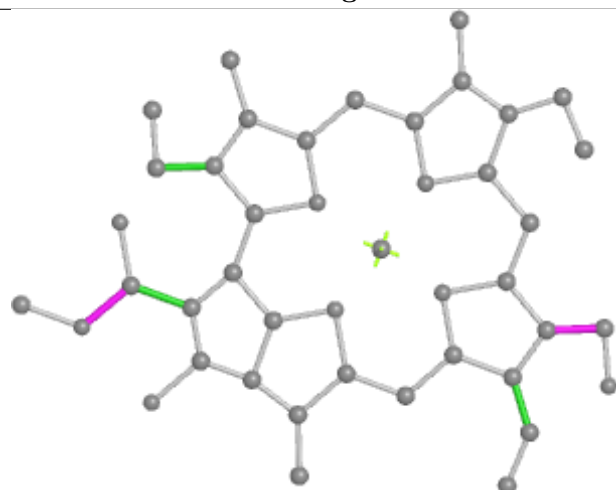
## Ligand CHL 4 618



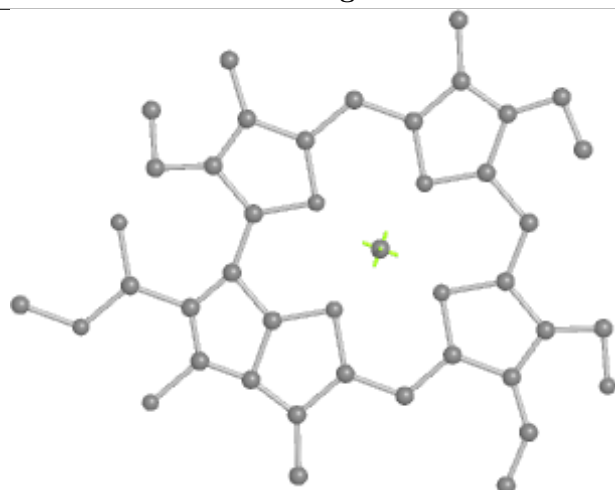
Bond lengths



Bond angles



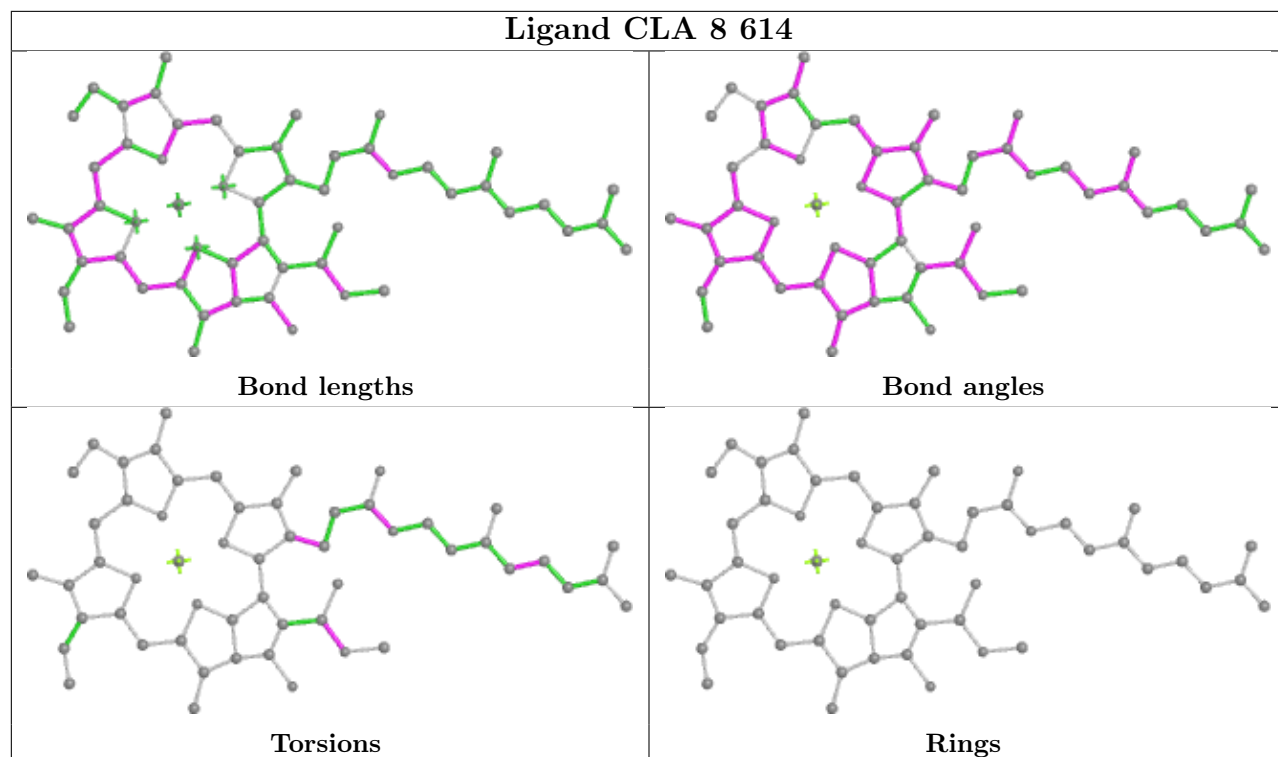
Torsions



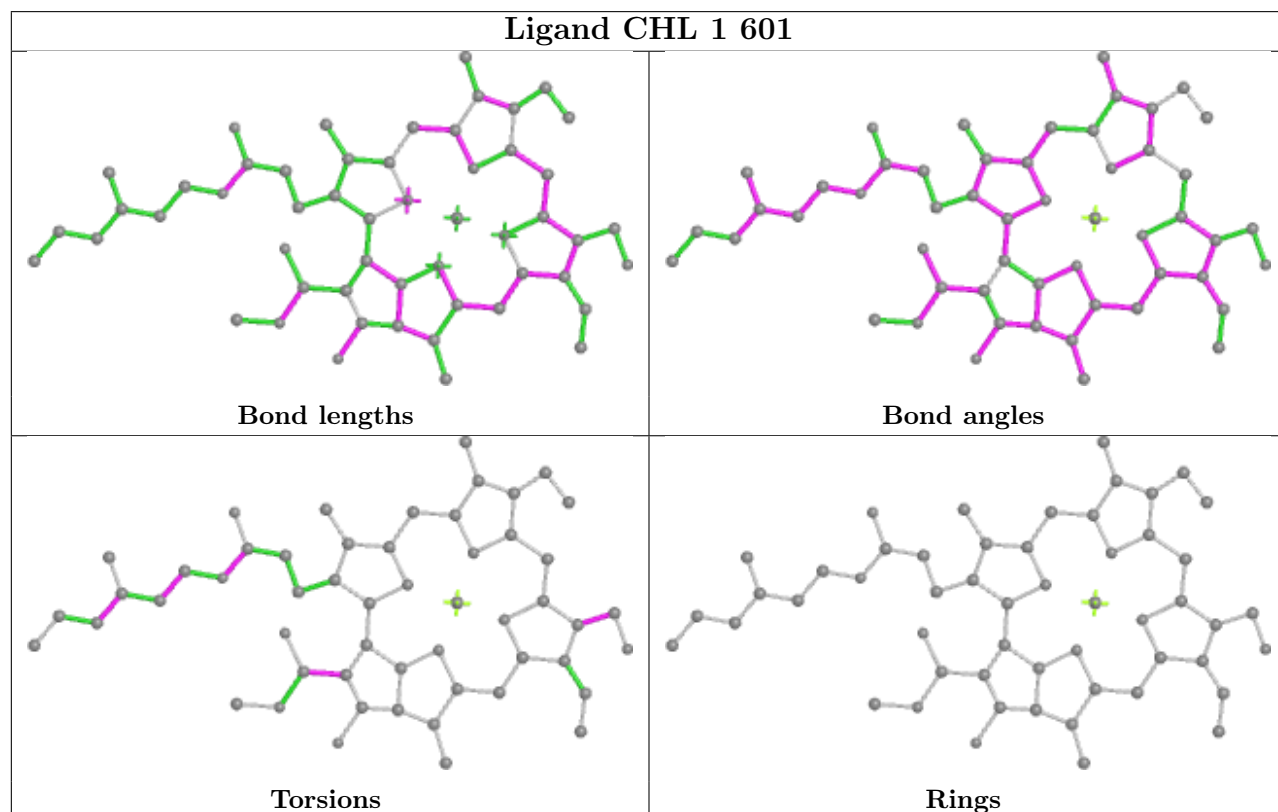
Rings

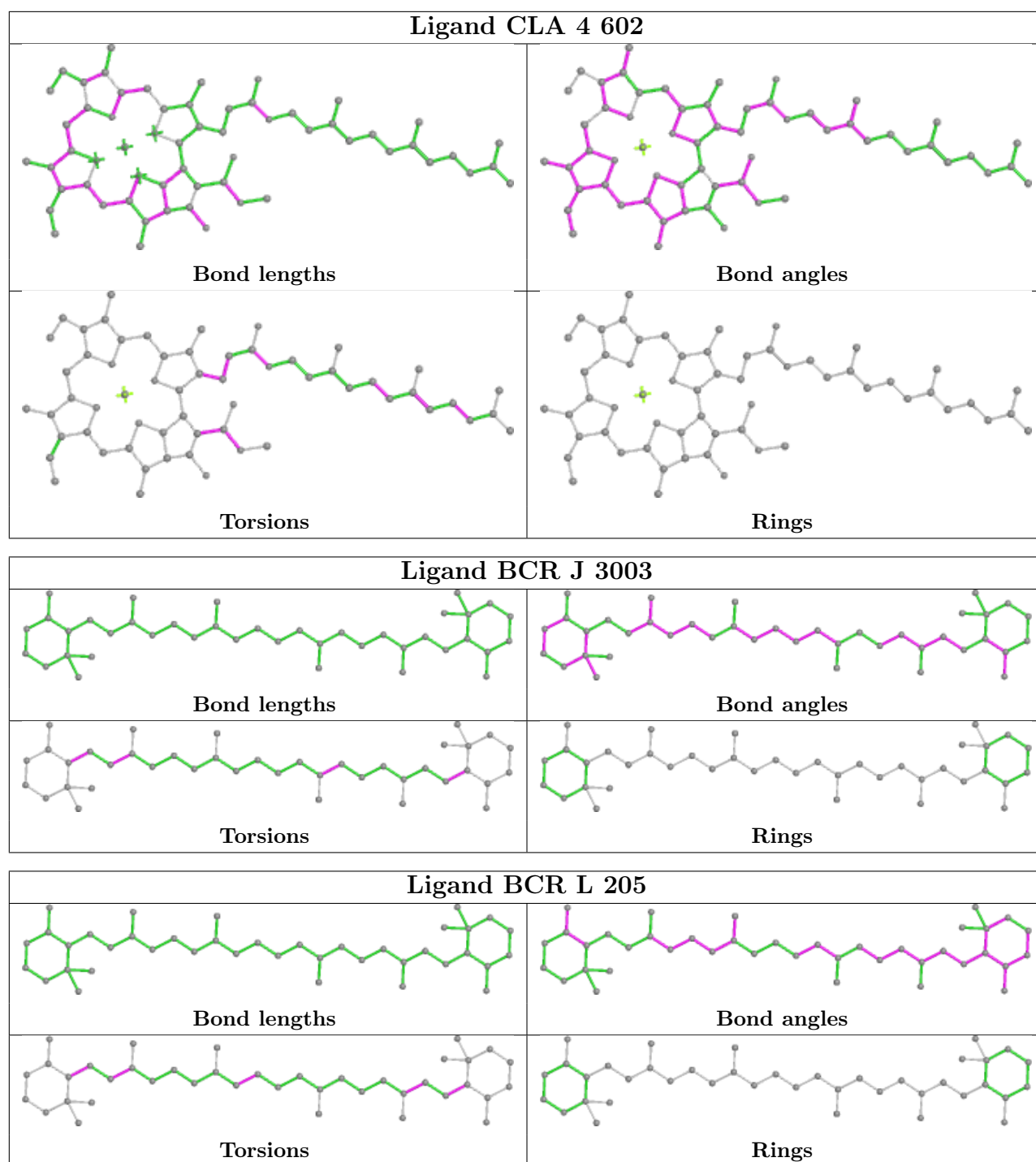


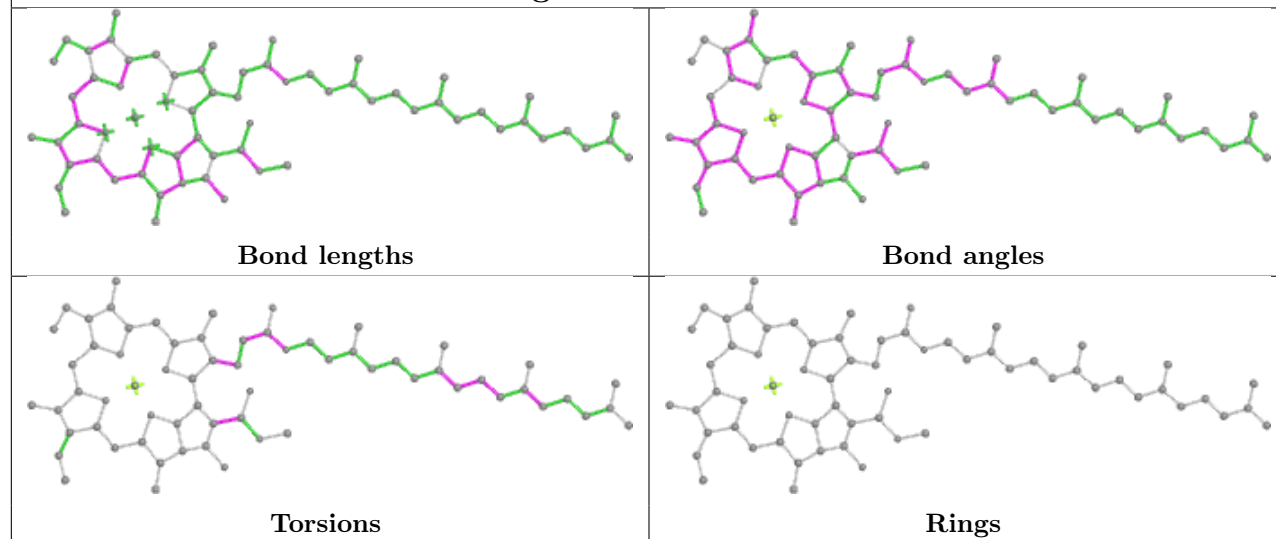
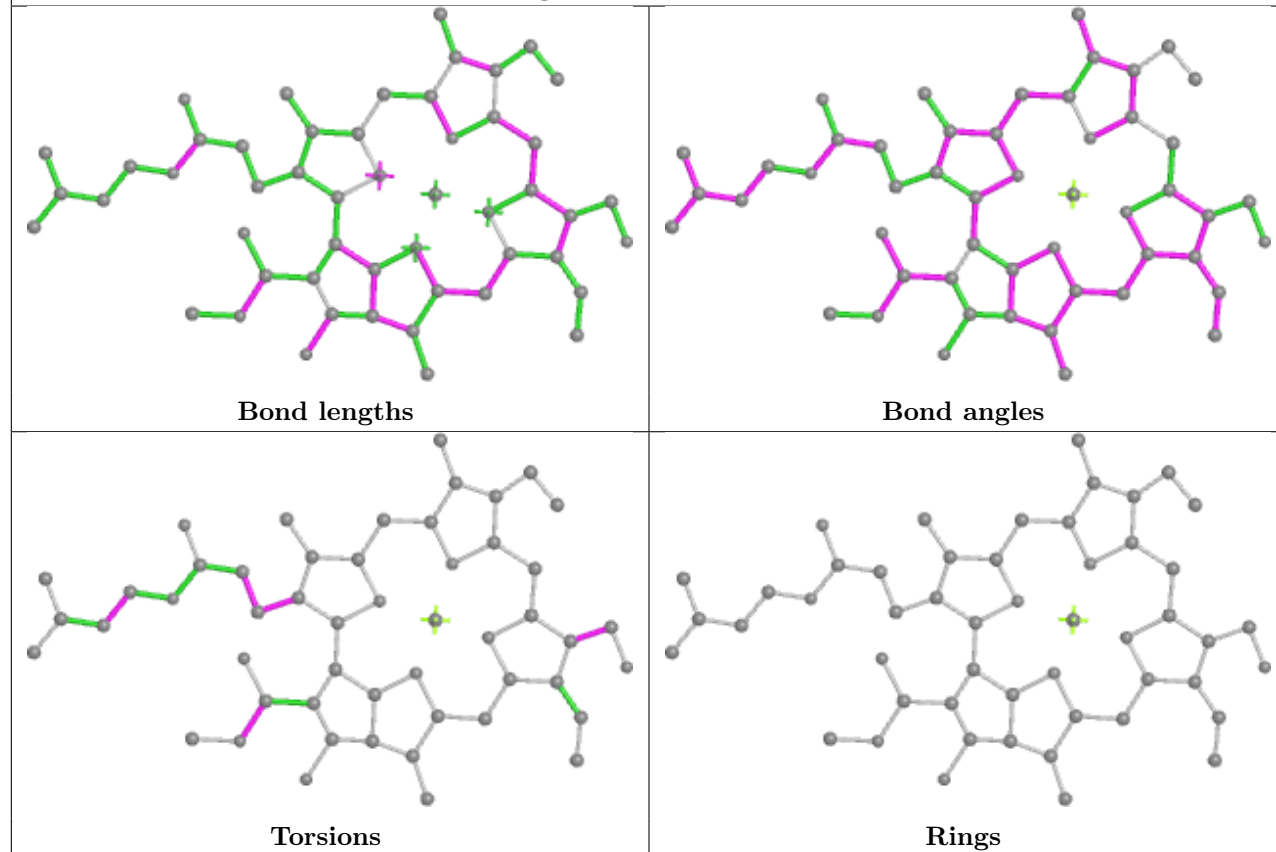
## Ligand CLA 8 614



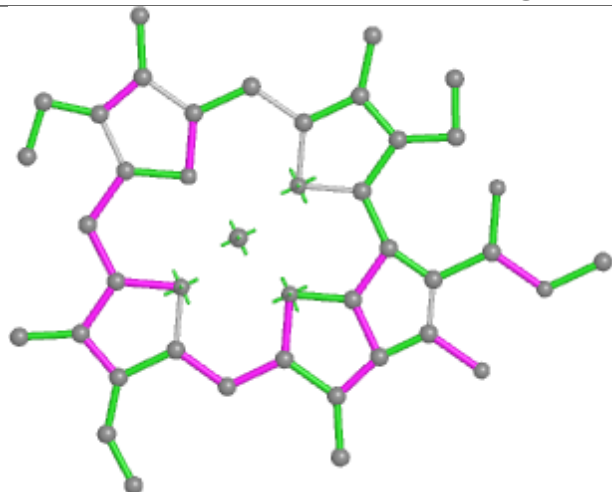
## Ligand CHL 1 601



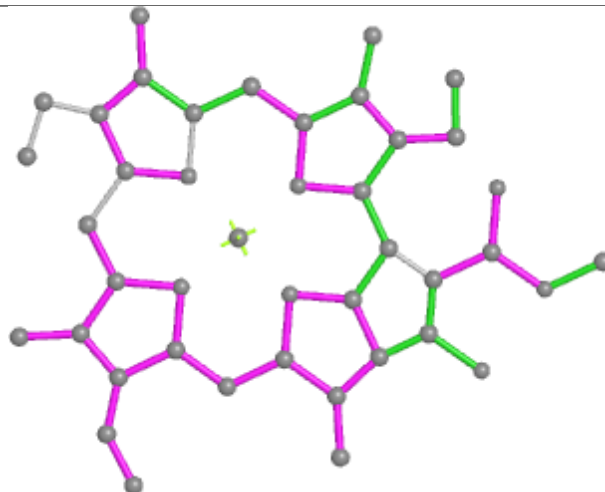


**Ligand CLA B 813****Ligand CHL 5 608**

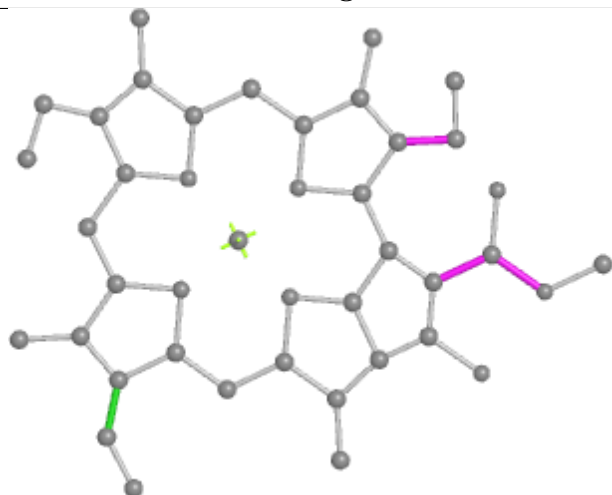
## Ligand CLA 7 606



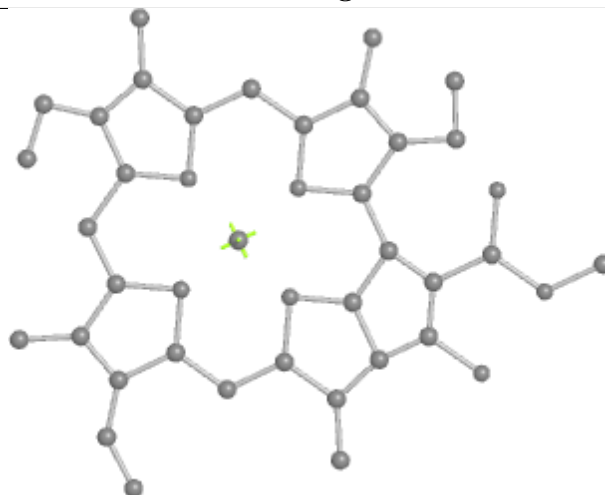
Bond lengths



Bond angles

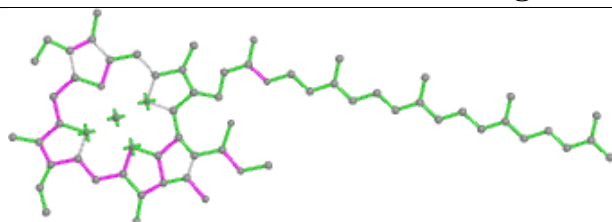


Torsions

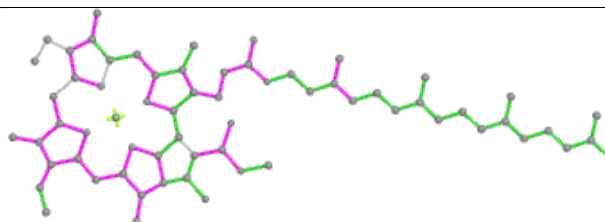


Rings

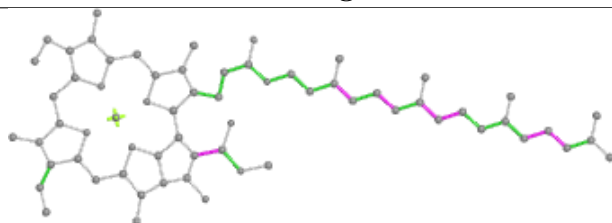
## Ligand CLA B 837



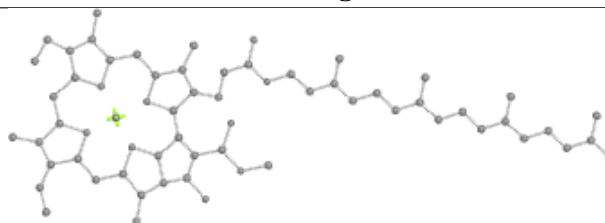
Bond lengths



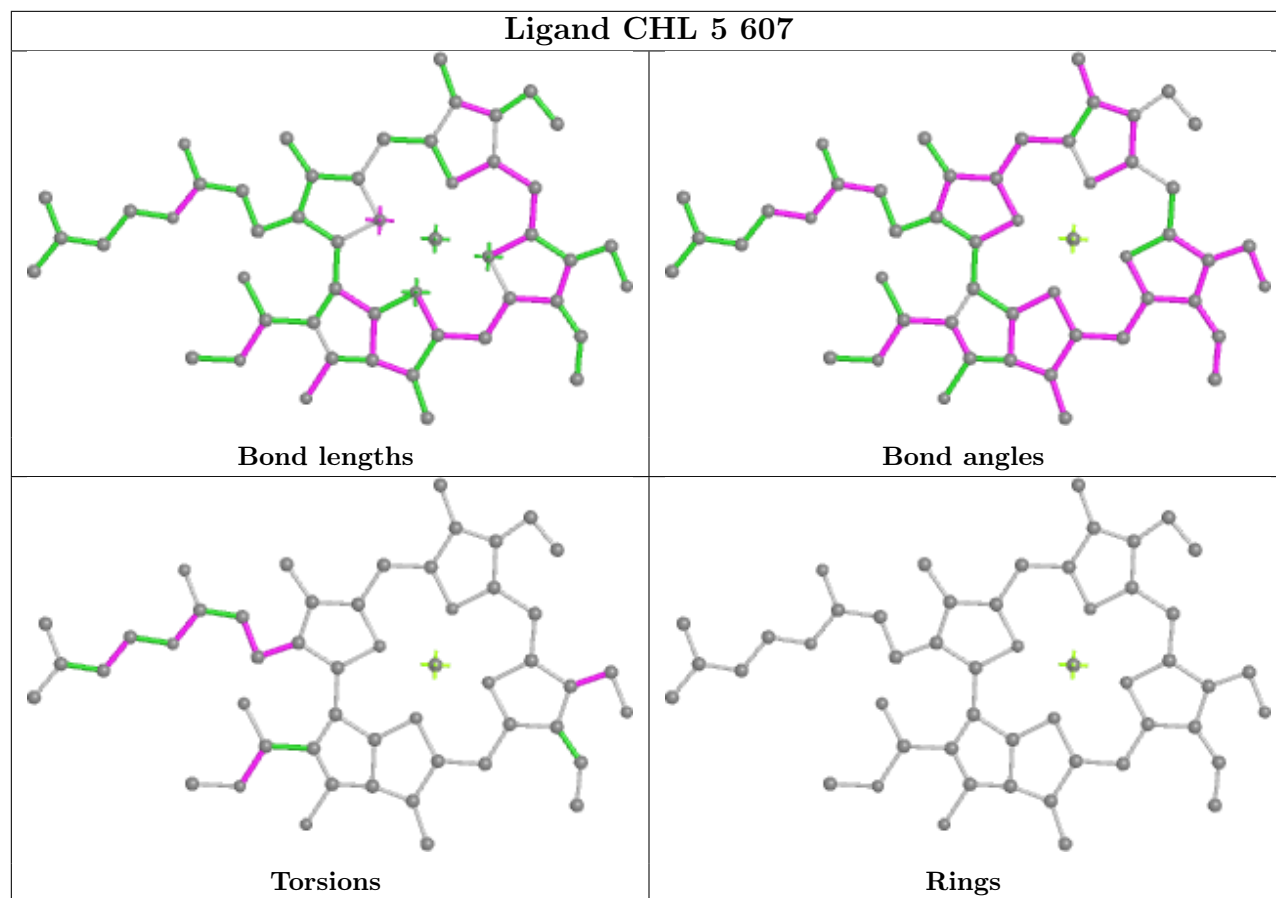
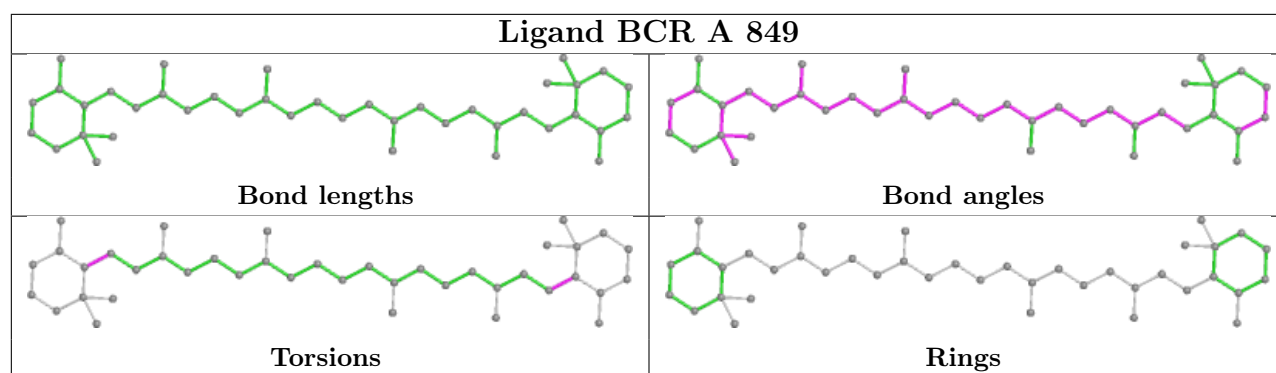
Bond angles



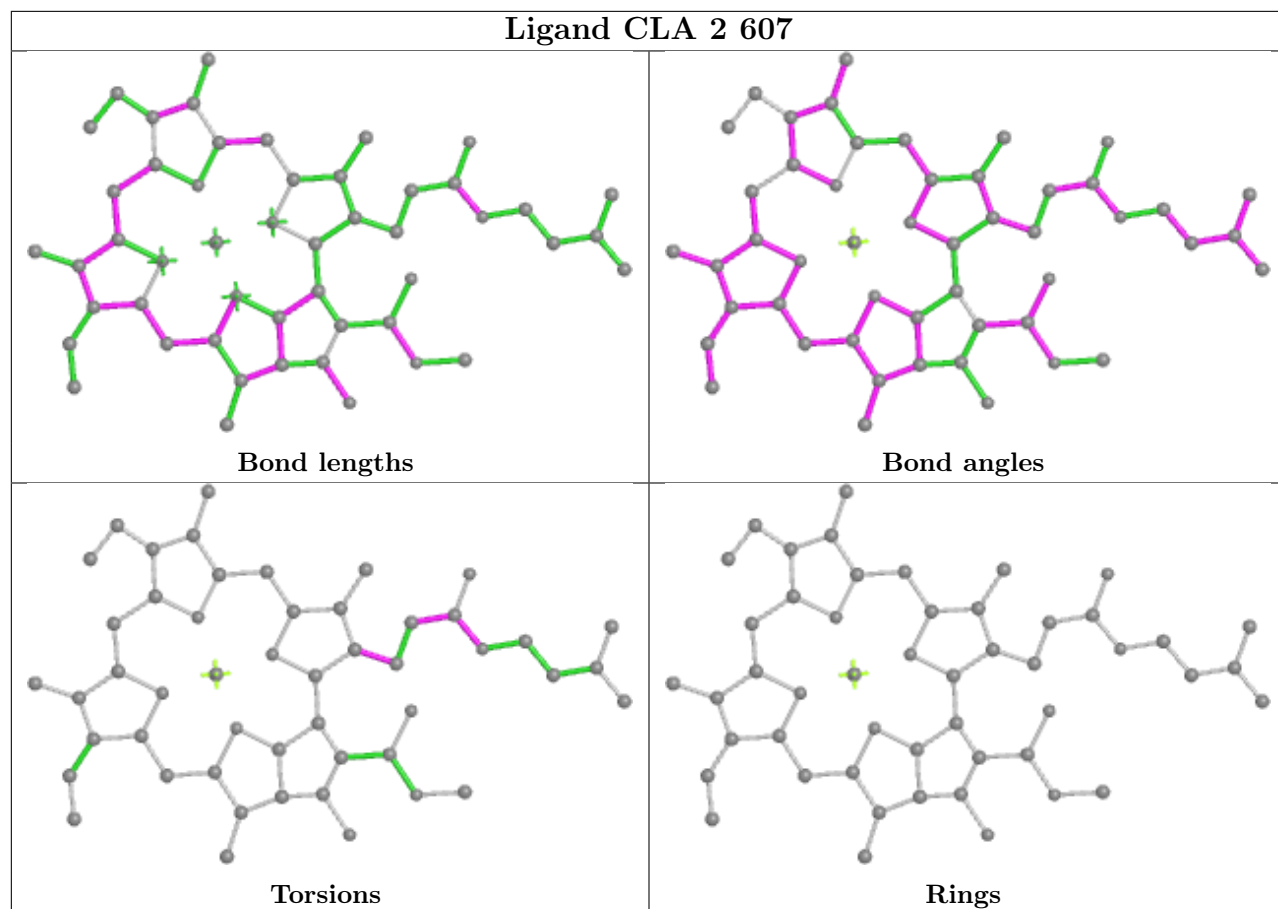
Torsions



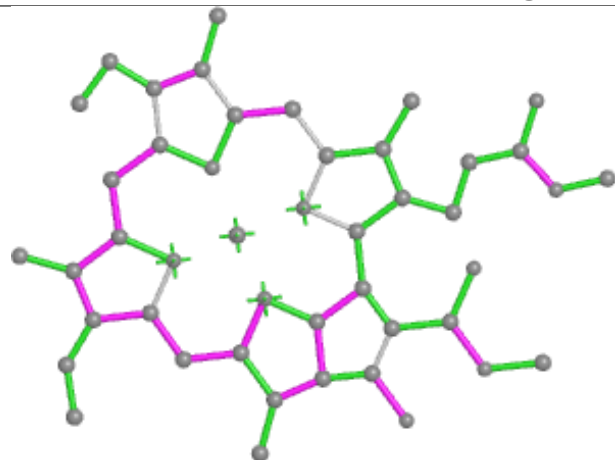
Rings



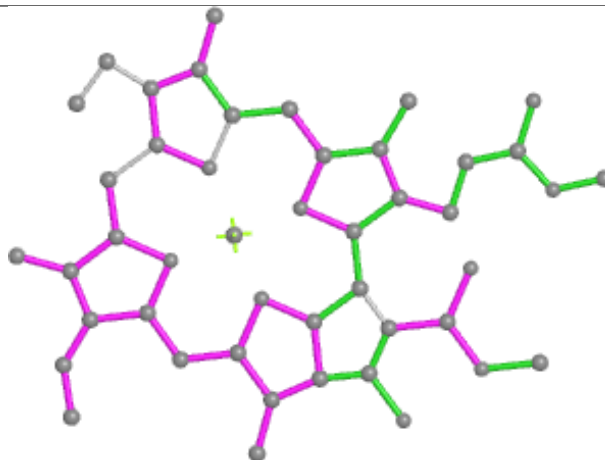
## Ligand CLA 2 607



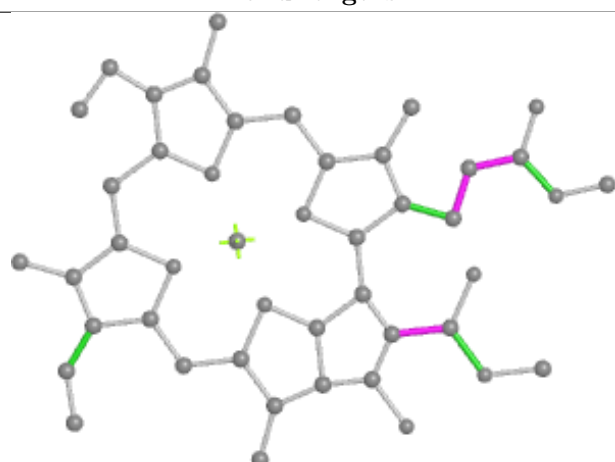
## Ligand CLA 9 601



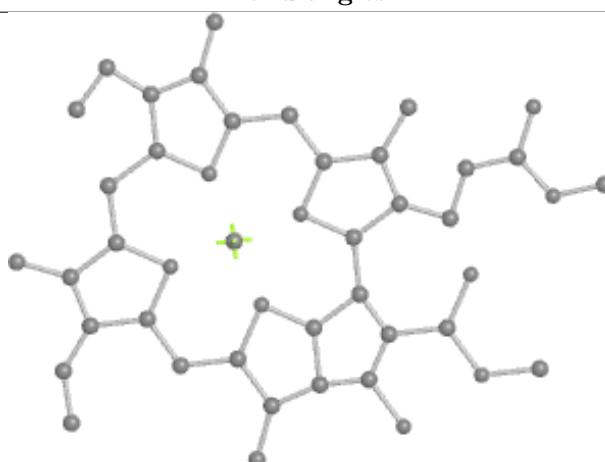
Bond lengths



Bond angles

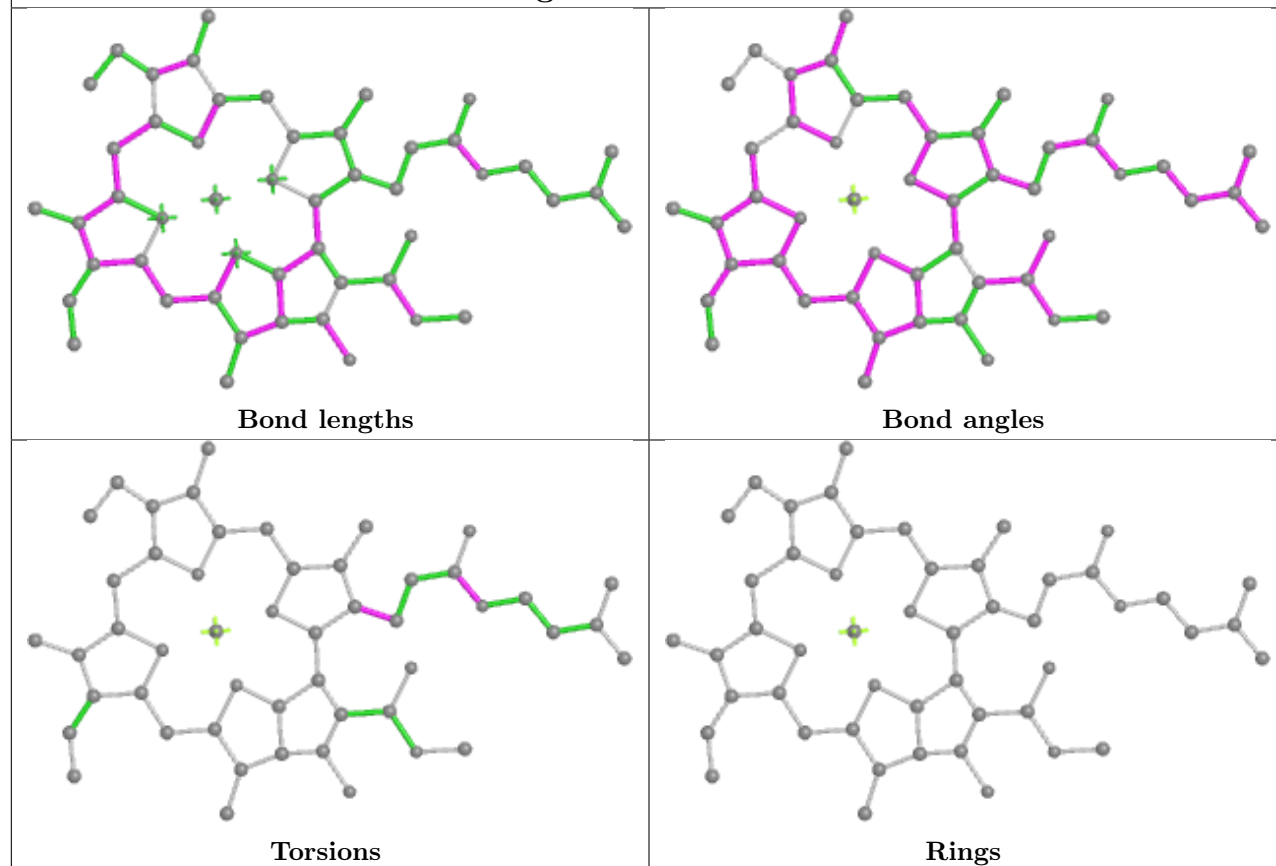


Torsions

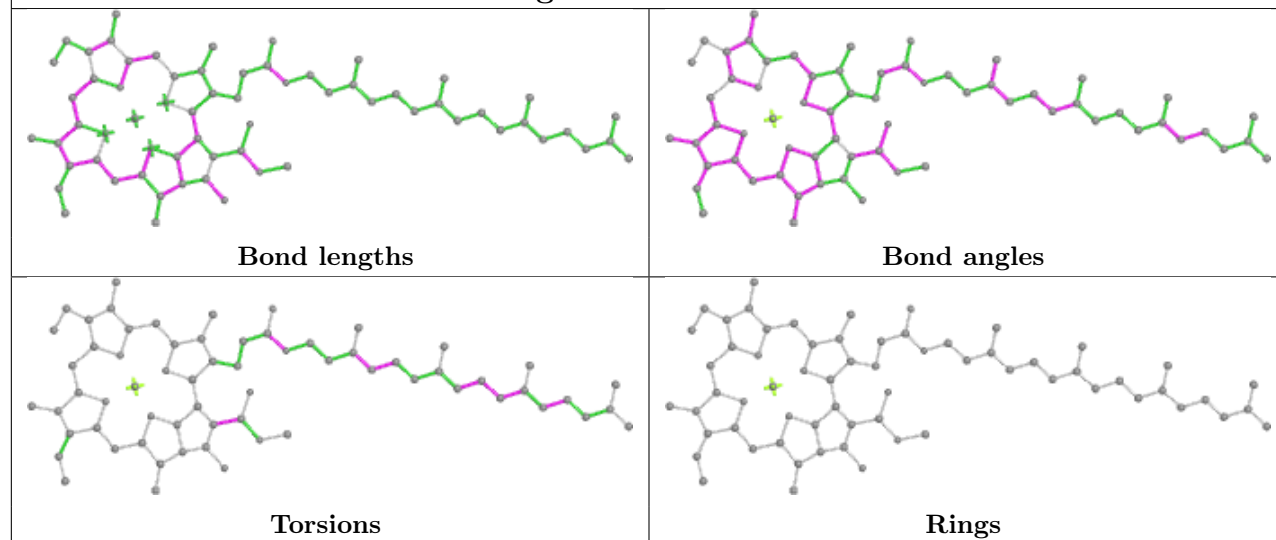


Rings

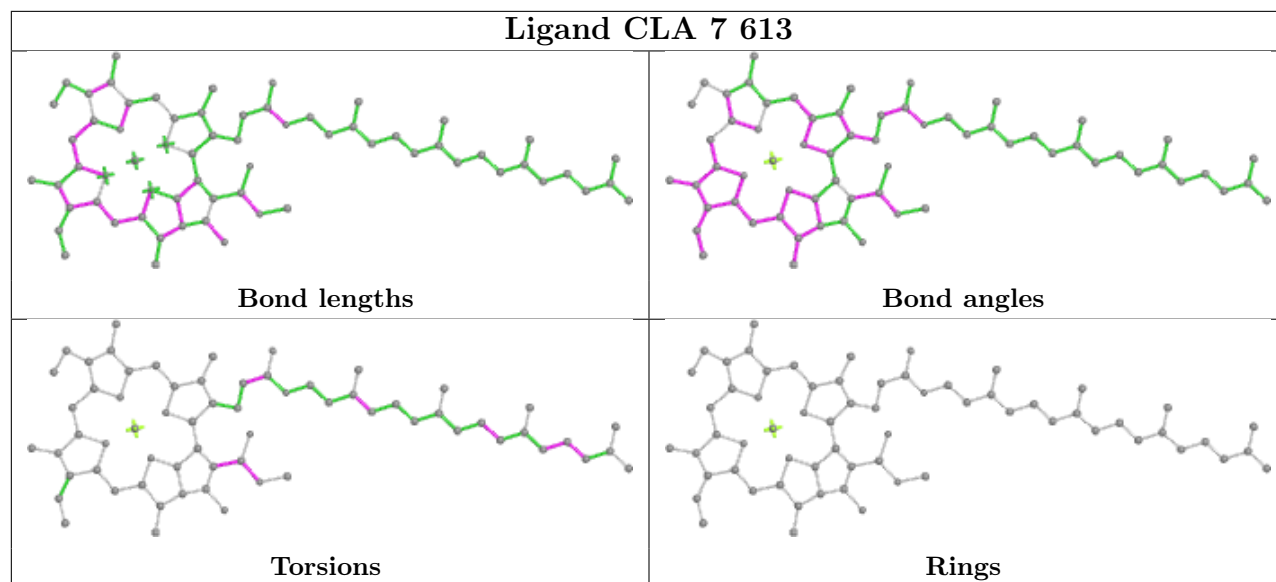
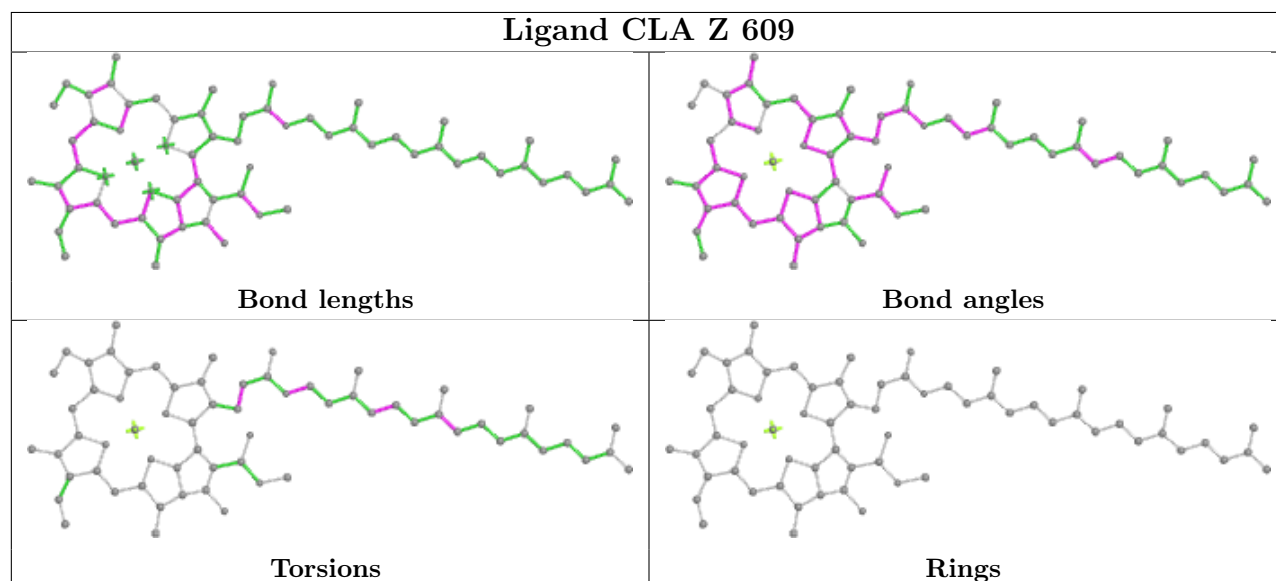
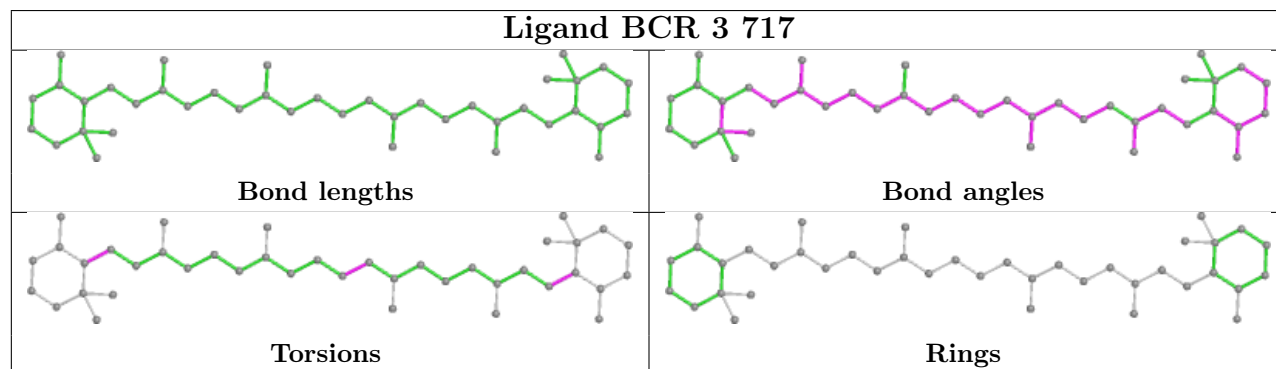
## Ligand CLA 6 609



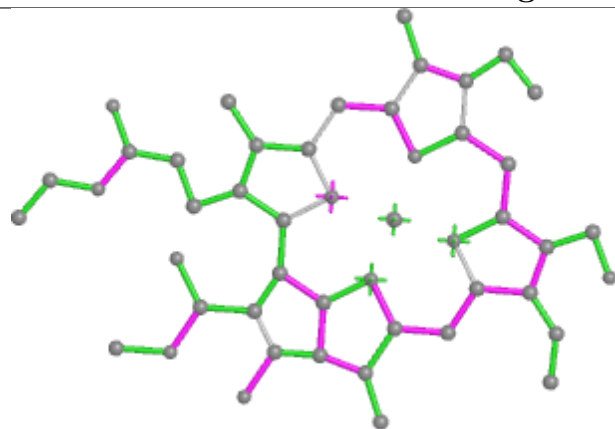
## Ligand CLA 8 601



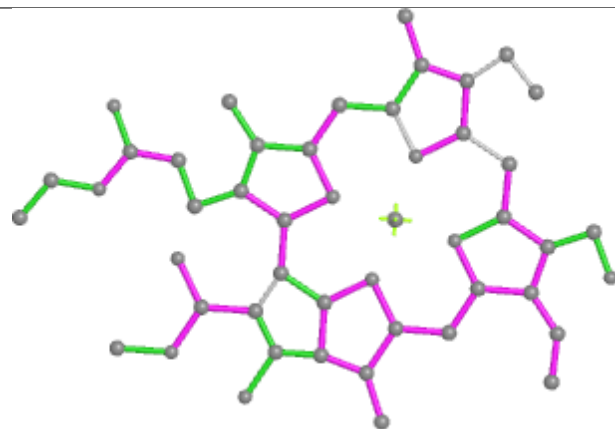


**Ligand CLA 7 613****Ligand CLA Z 609****Ligand BCR 3 717**

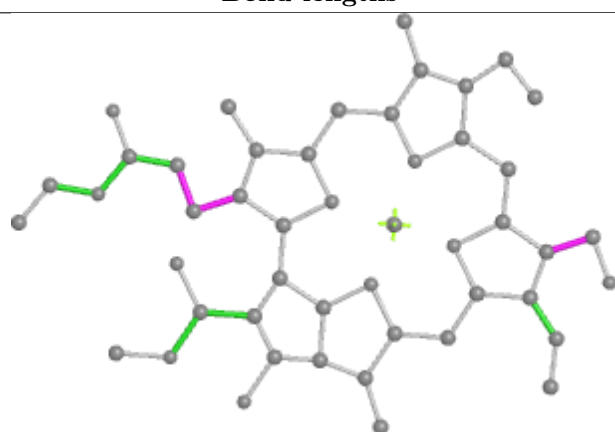
## Ligand CHL Z 607



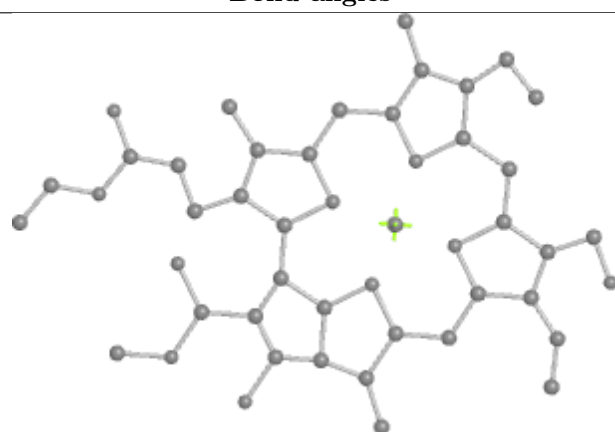
Bond lengths



Bond angles

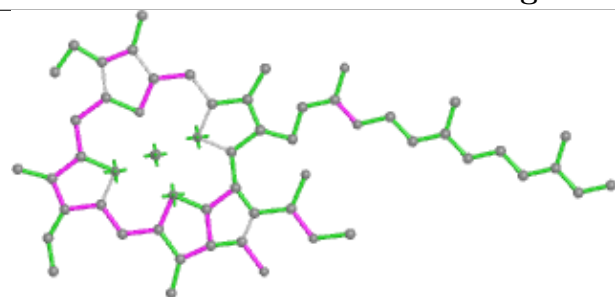


Torsions

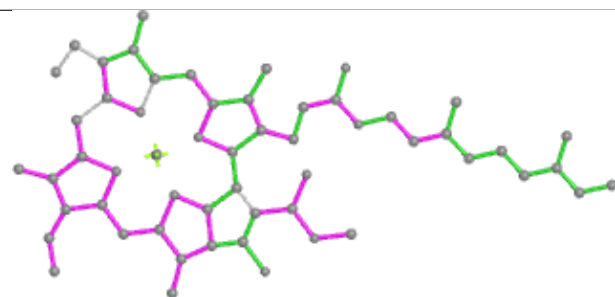


Rings

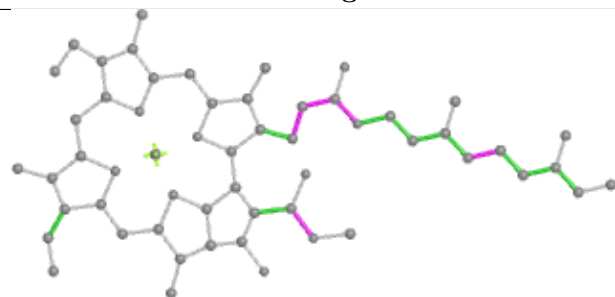
## Ligand CLA 3 620



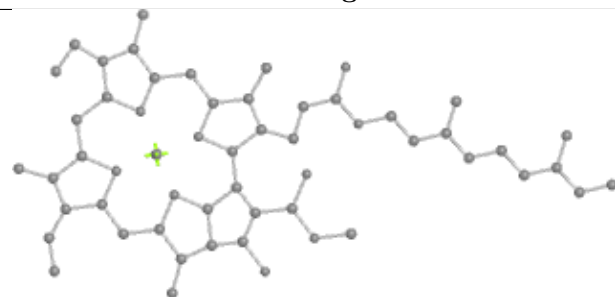
Bond lengths



Bond angles

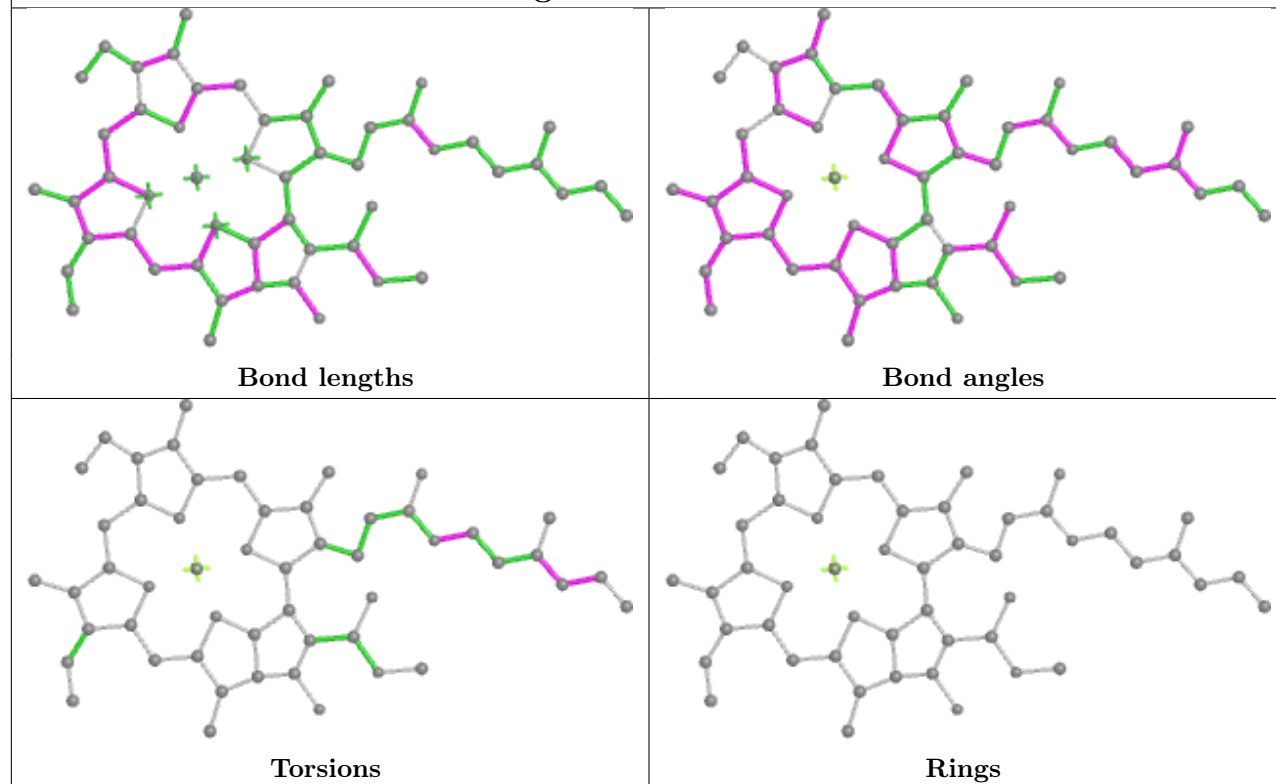


Torsions

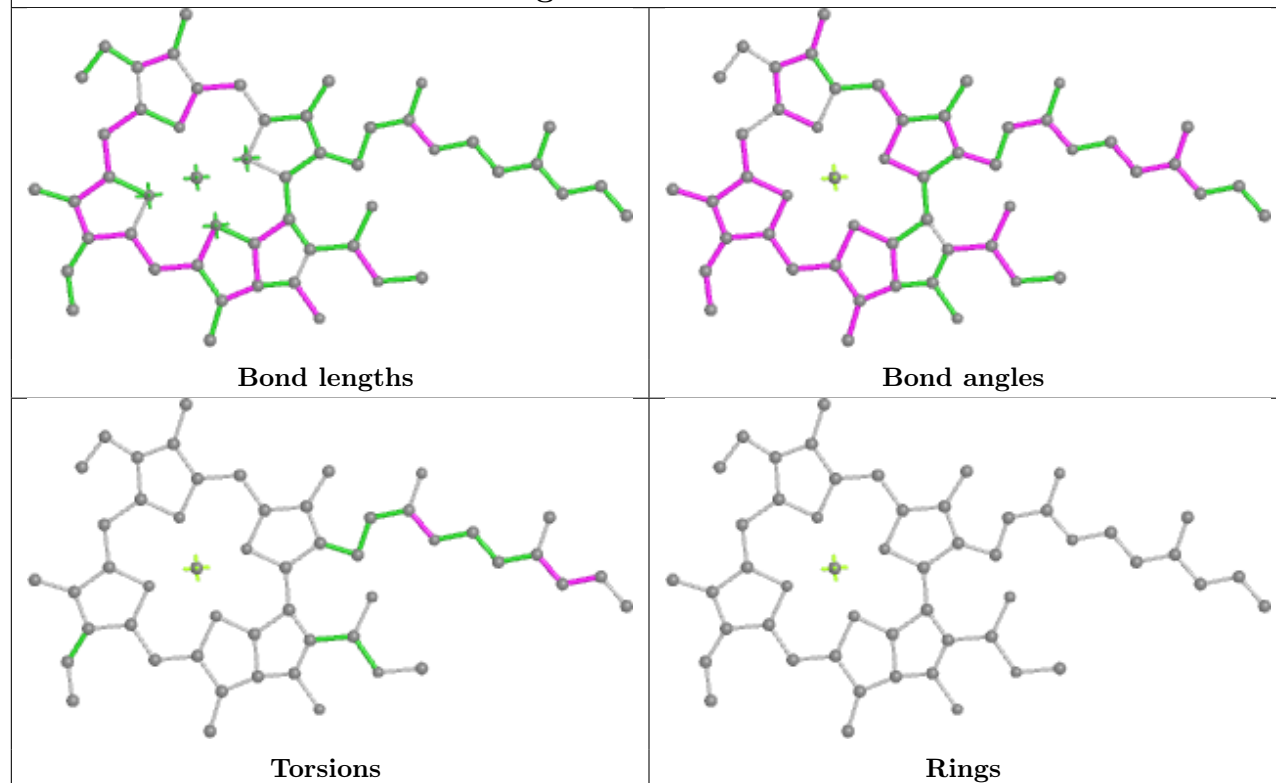


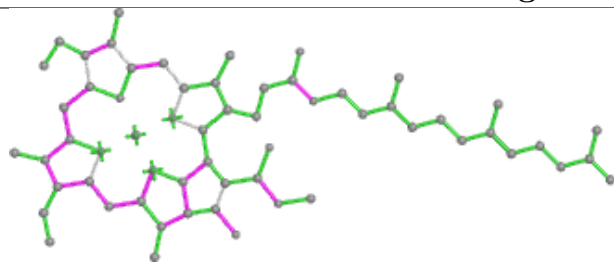
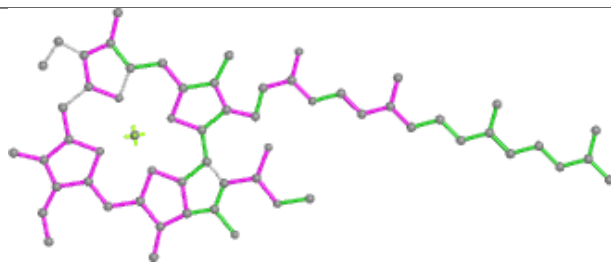
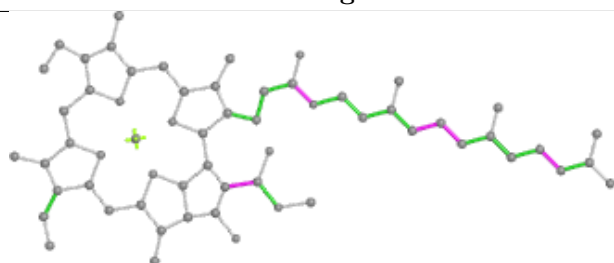
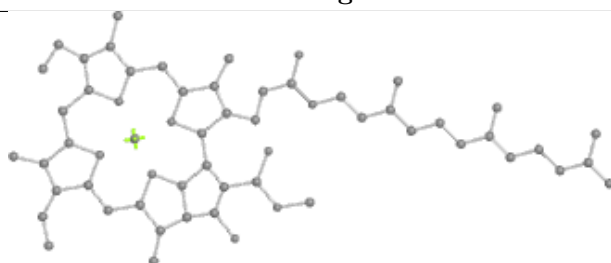
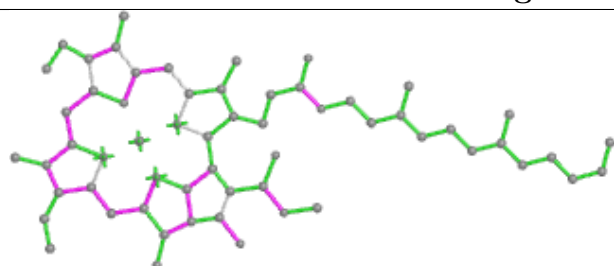
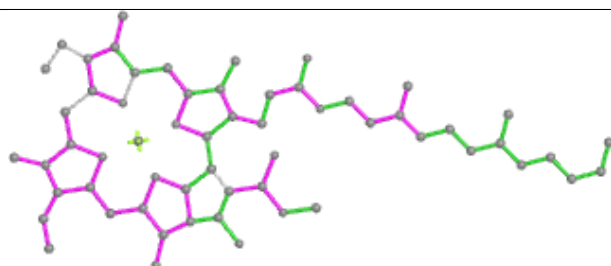
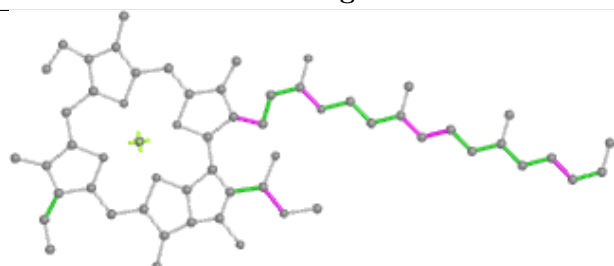
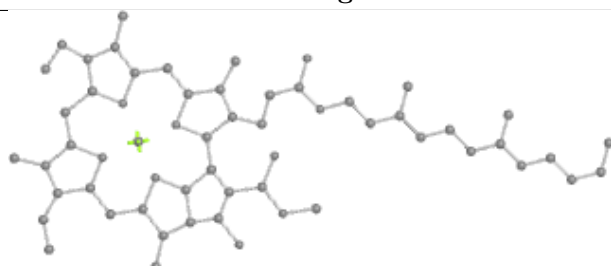
Rings

## Ligand CLA Z 606

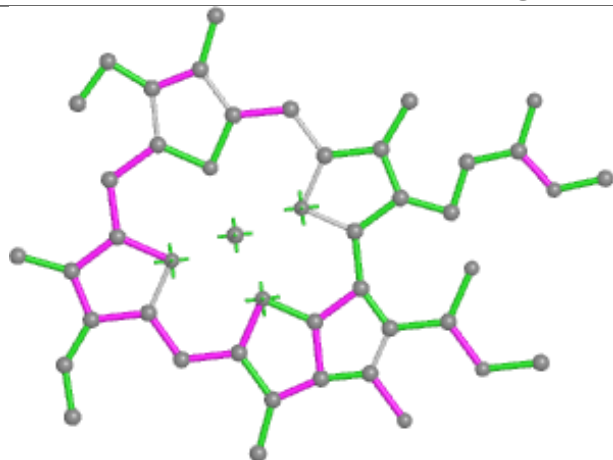


## Ligand CLA 1 606

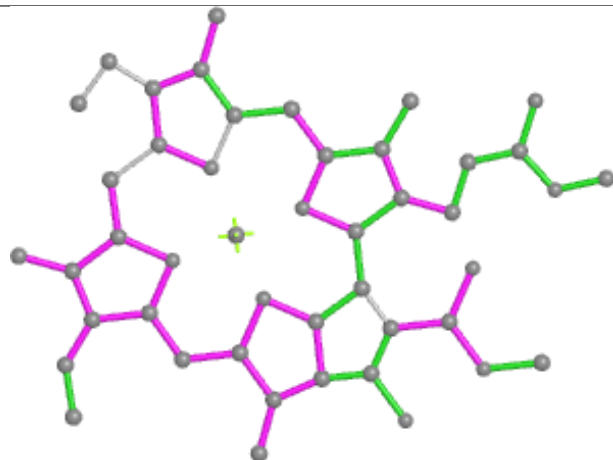


**Ligand CLA 7 620****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 822****Bond lengths****Bond angles****Torsions****Rings**

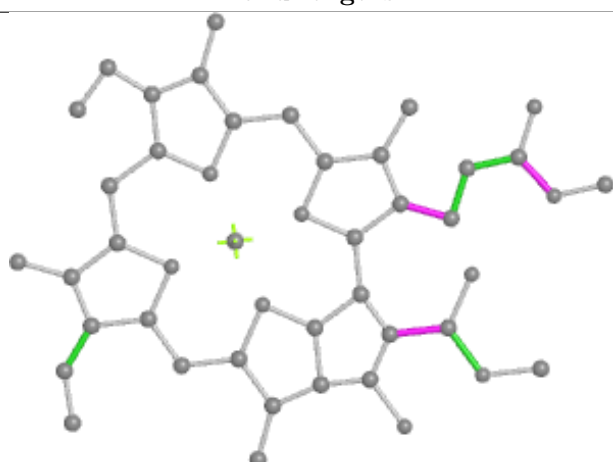
## Ligand CLA B 821



Bond lengths



Bond angles

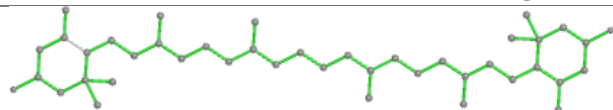


Torsions

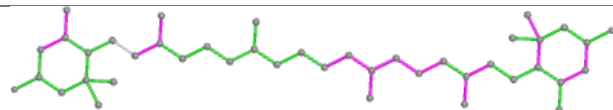


Rings

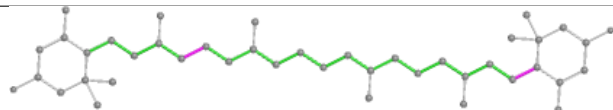
## Ligand LUT 6 624



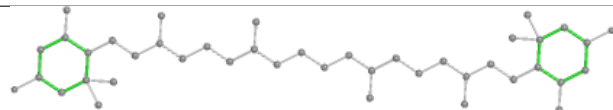
Bond lengths



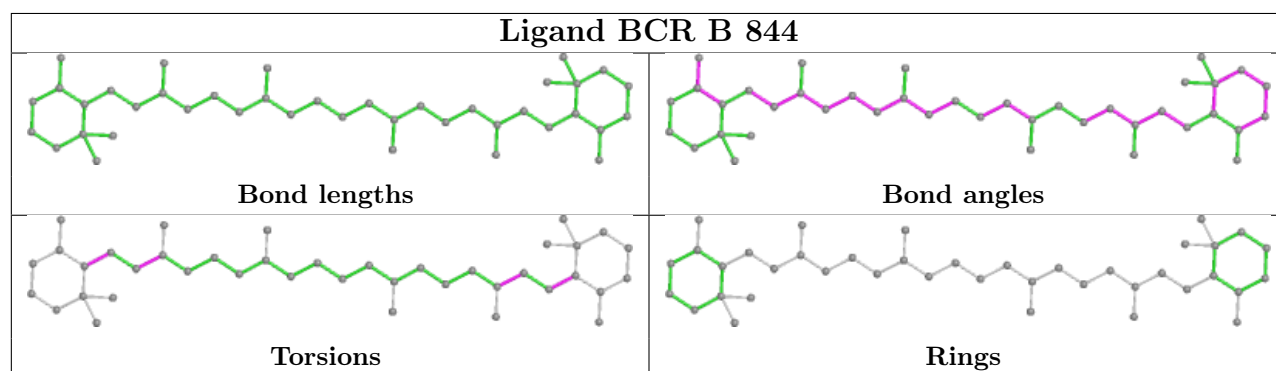
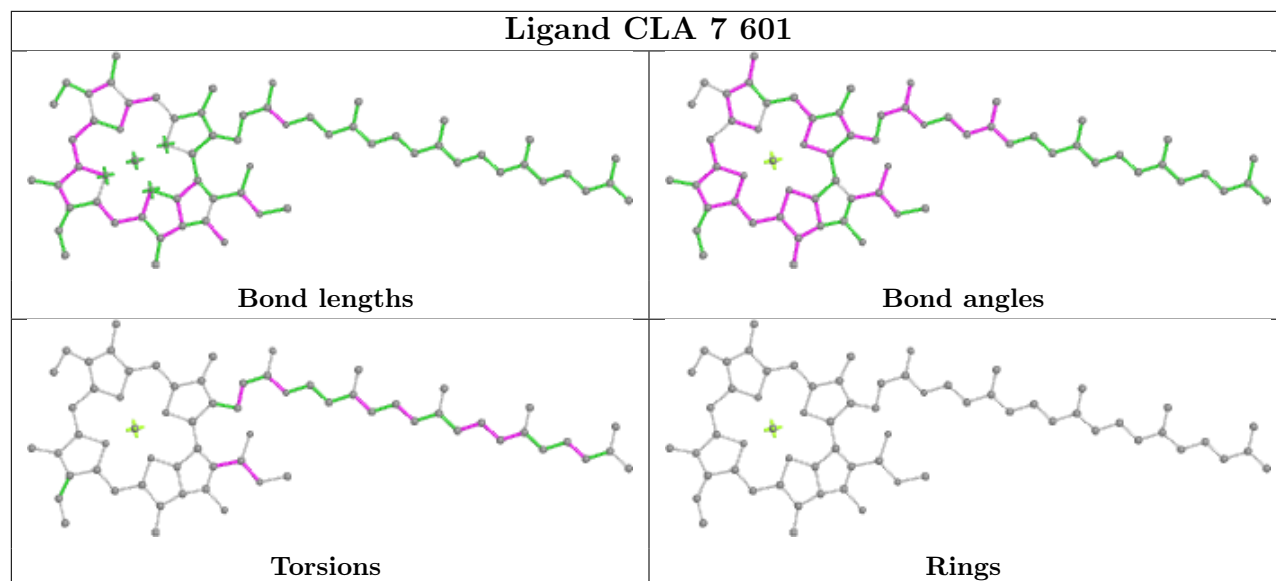
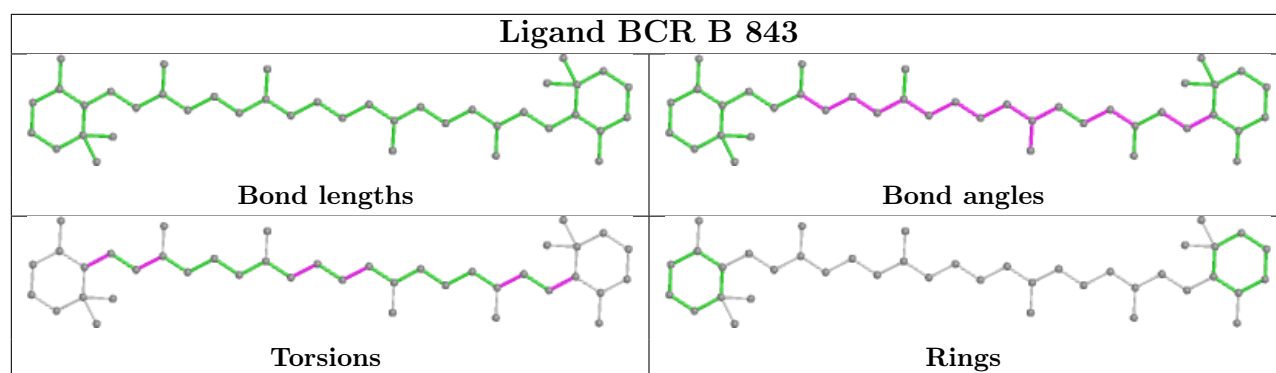
Bond angles

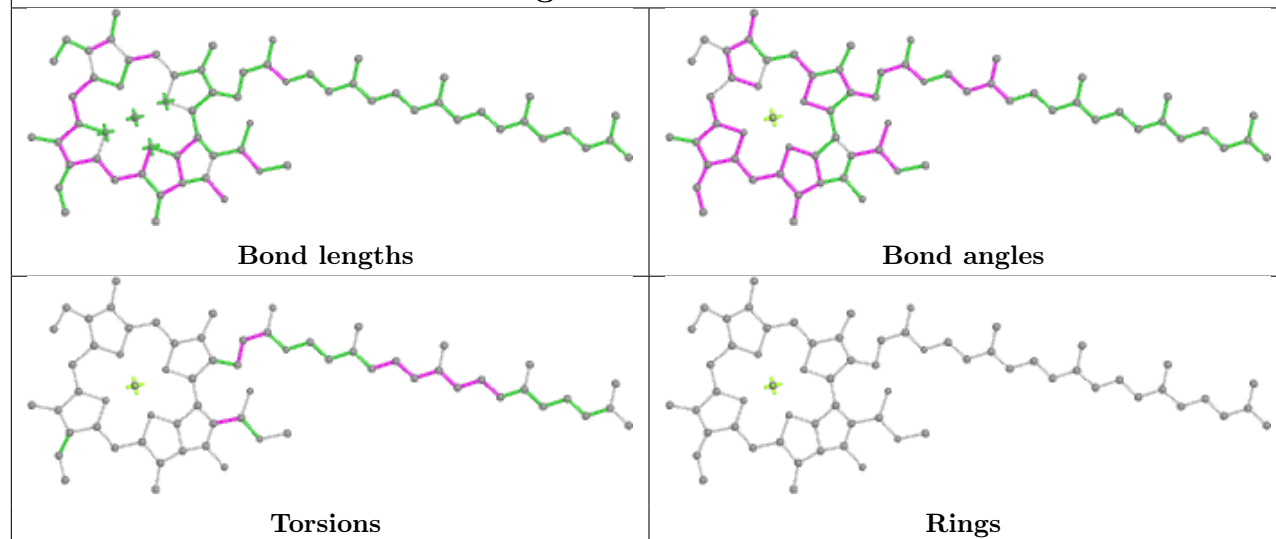
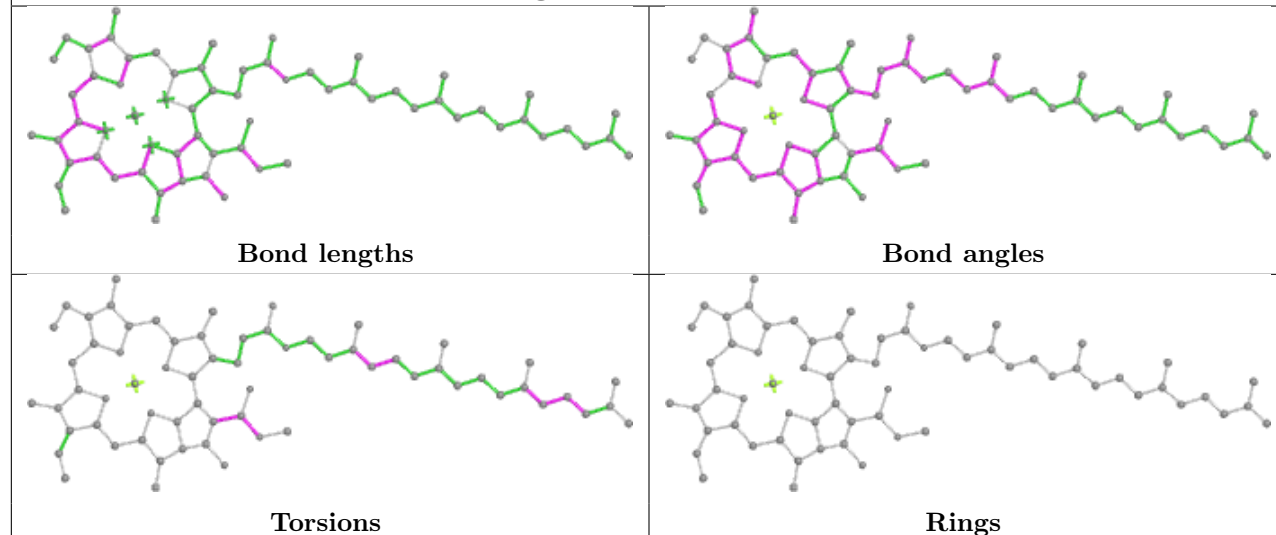
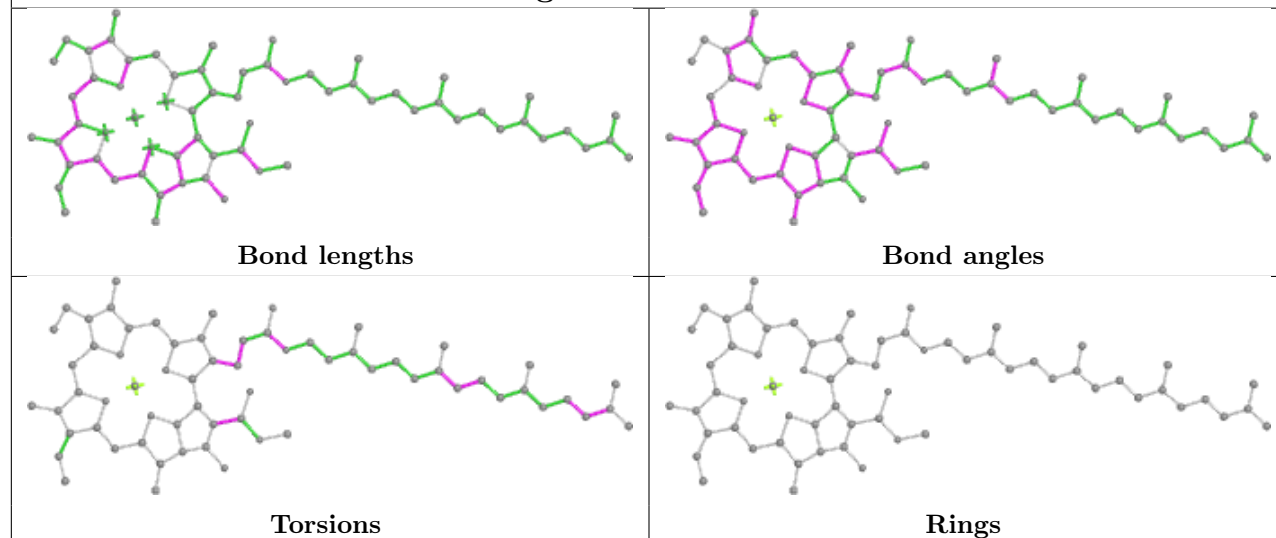


Torsions

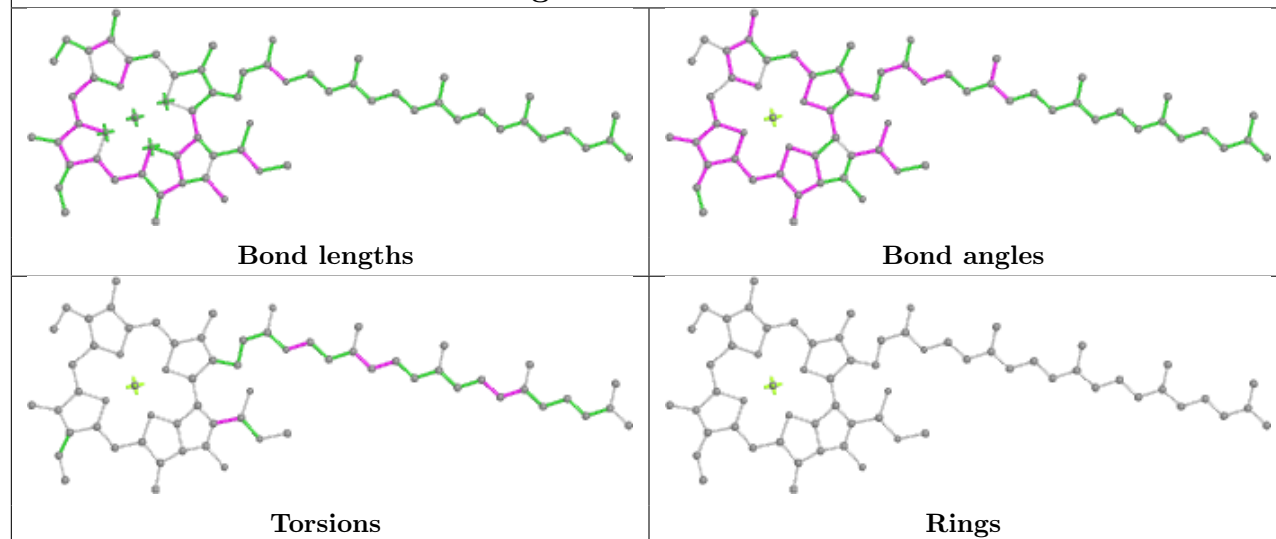


Rings

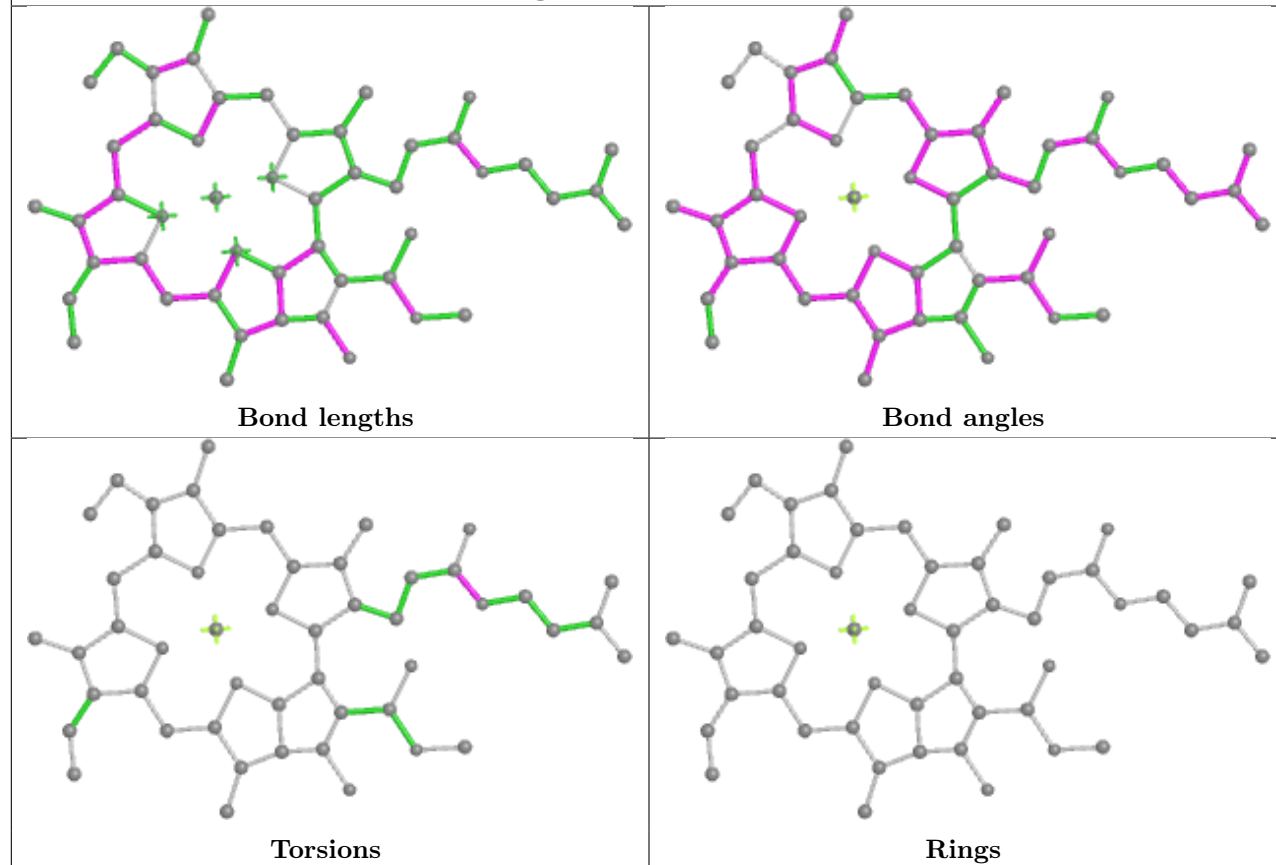


**Ligand CLA 6 601****Ligand CLA B 808****Ligand CLA 7 602**

## Ligand CLA A 840

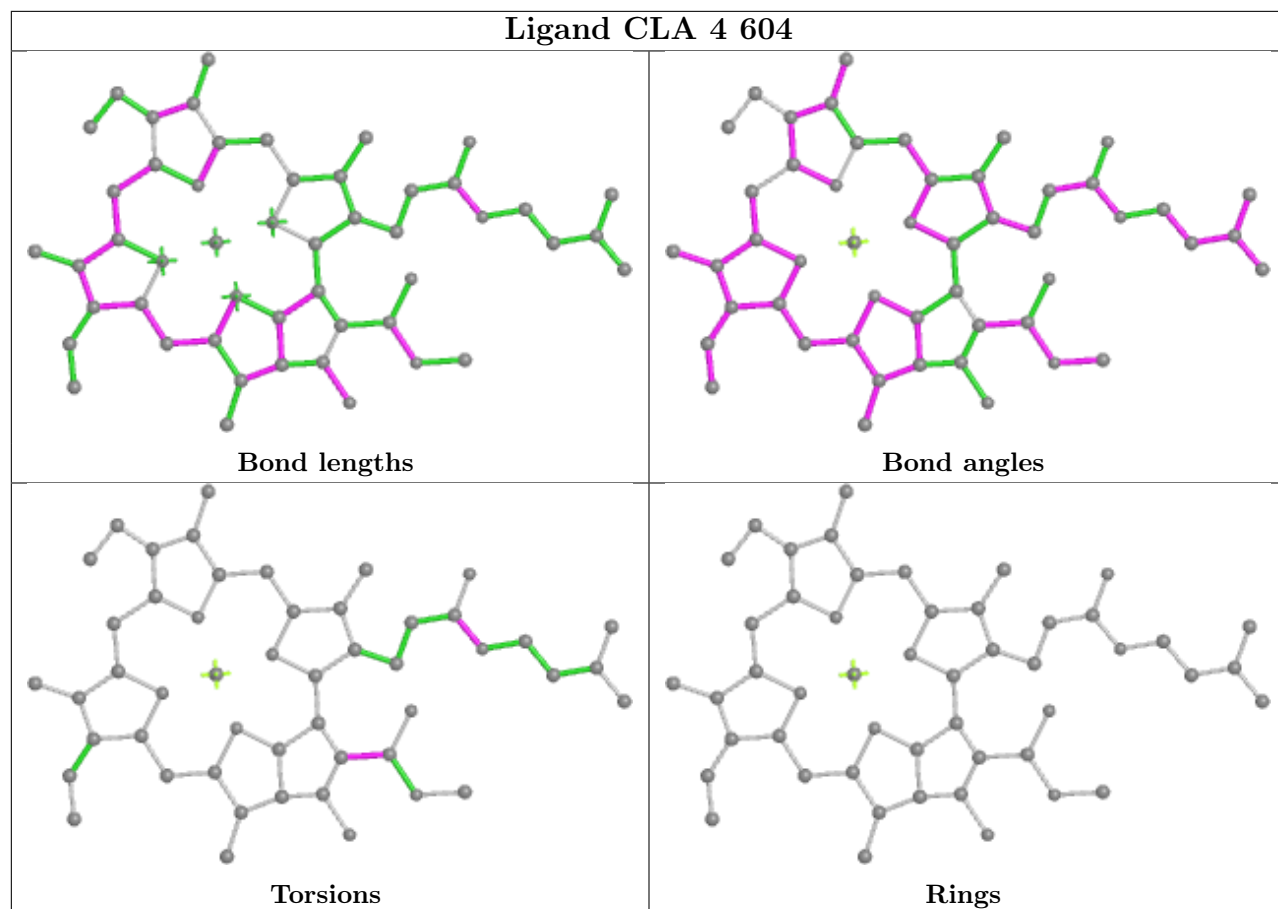


## Ligand CLA A 832

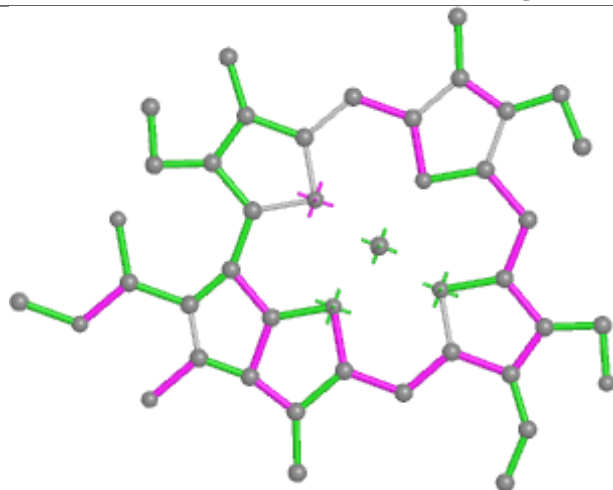




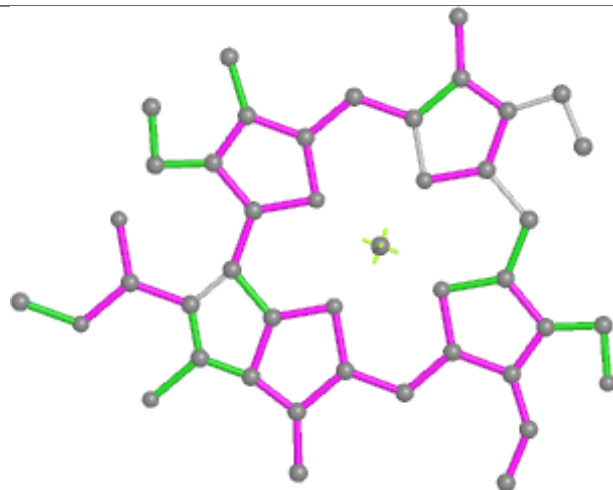
## Ligand CLA 4 604



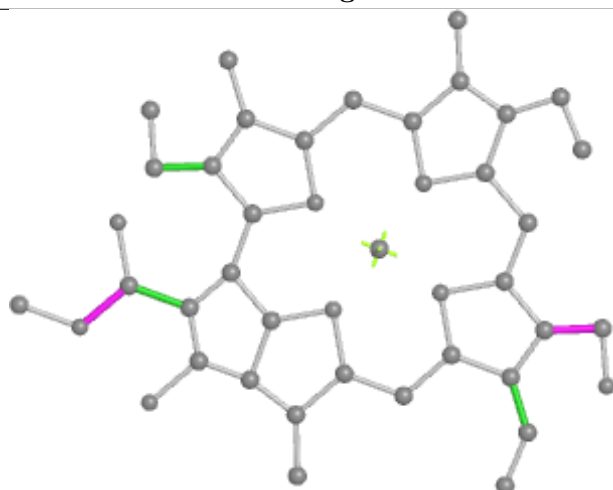
## Ligand CHL 5 618



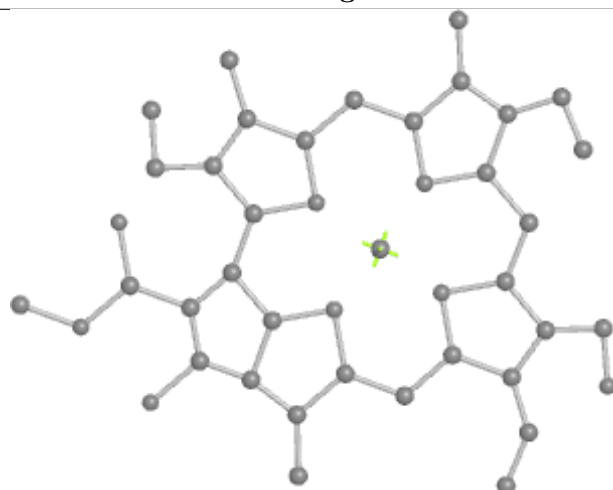
Bond lengths



Bond angles

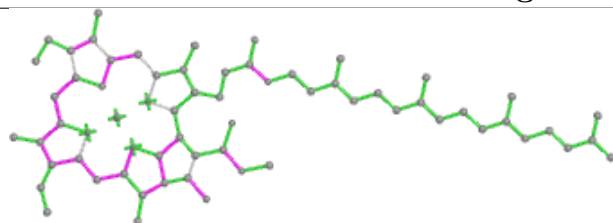


Torsions

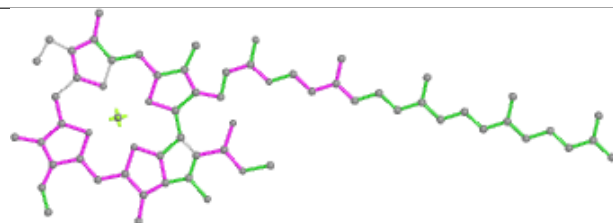


Rings

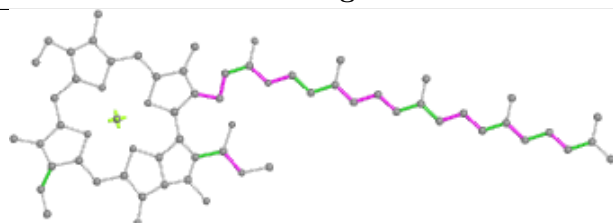
## Ligand CLA Z 611



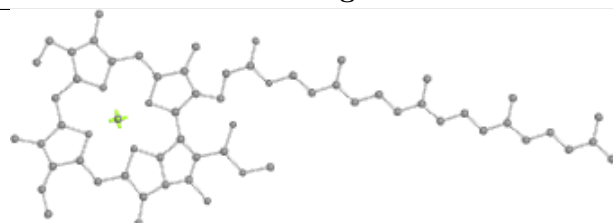
Bond lengths



Bond angles

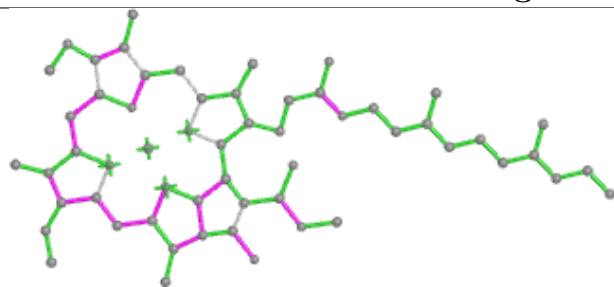


Torsions

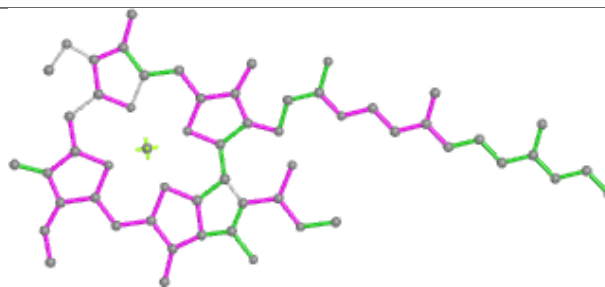


Rings

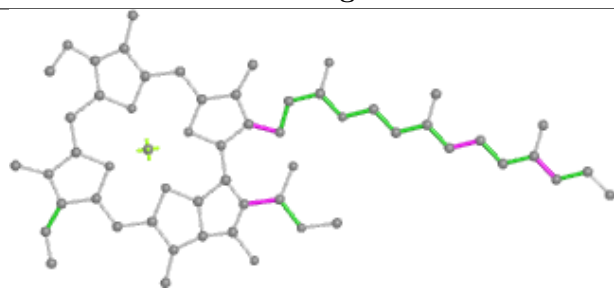
## Ligand CLA B 815



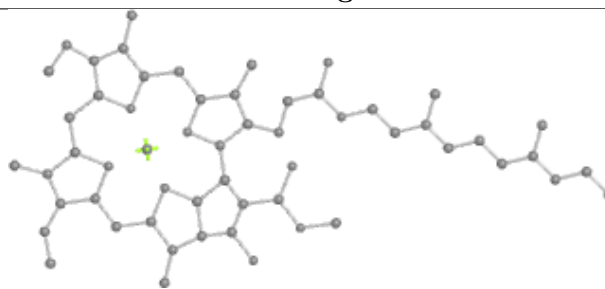
Bond lengths



Bond angles

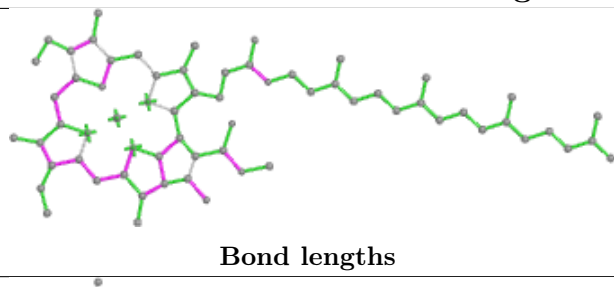


Torsions

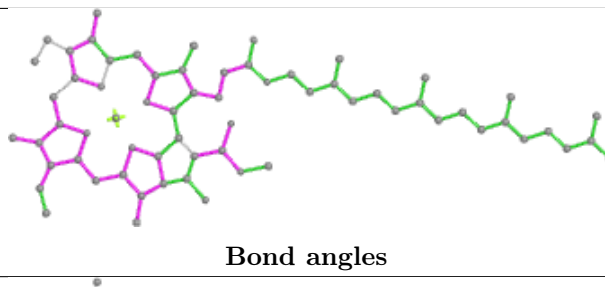


Rings

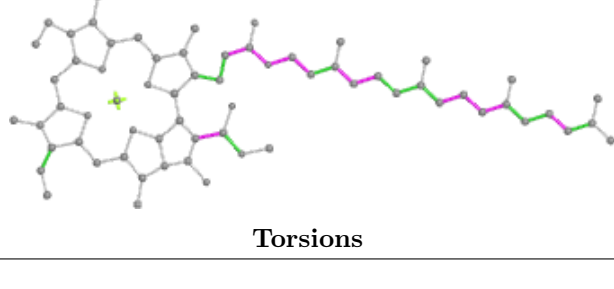
## Ligand CLA A 806



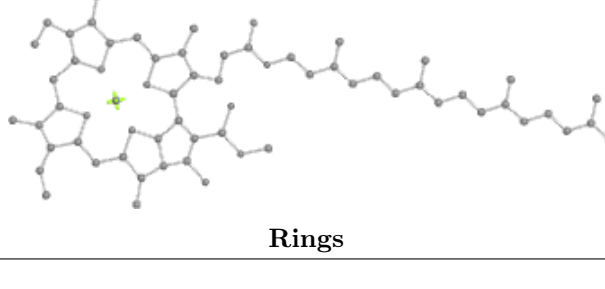
Bond lengths



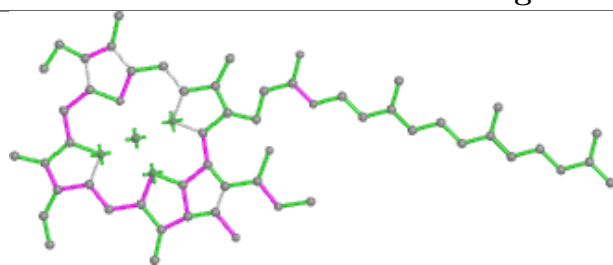
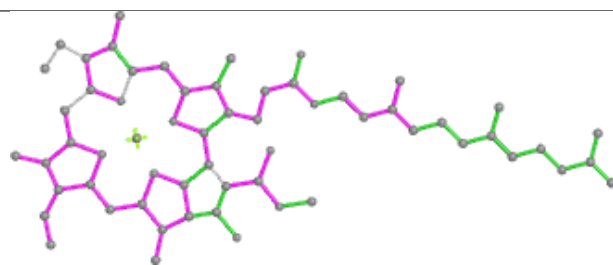
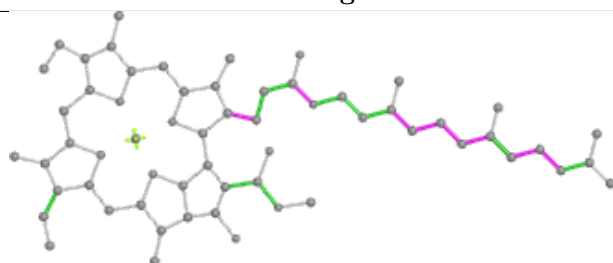
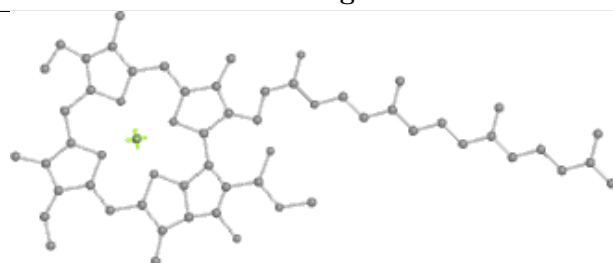
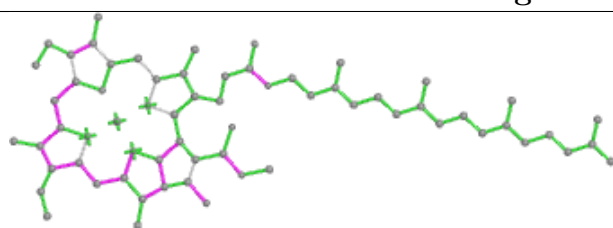
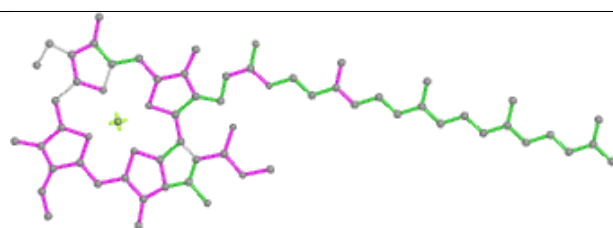
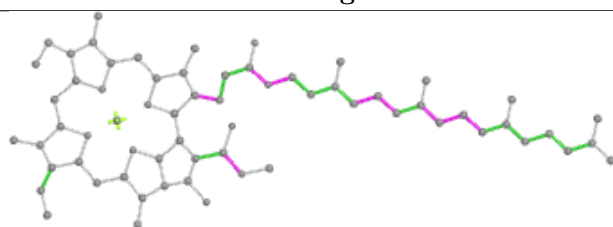
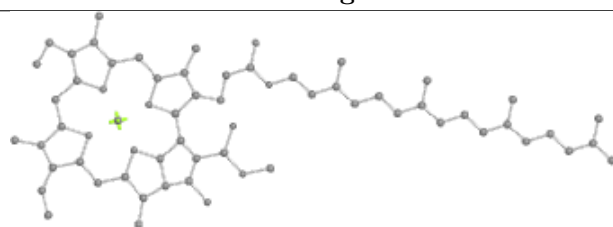
Bond angles



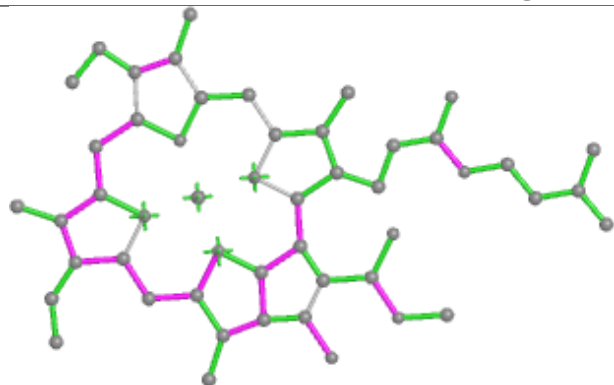
Torsions



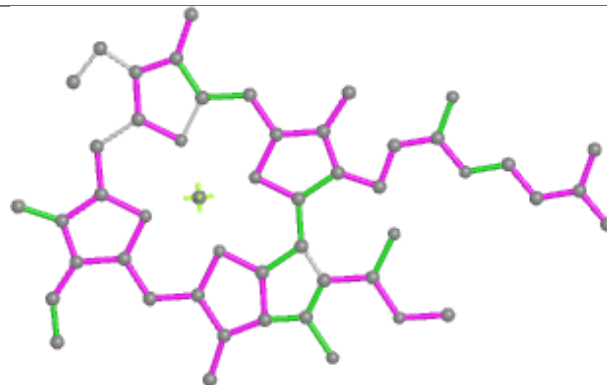
Rings

**Ligand CLA B 818****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 834****Bond lengths****Bond angles****Torsions****Rings**

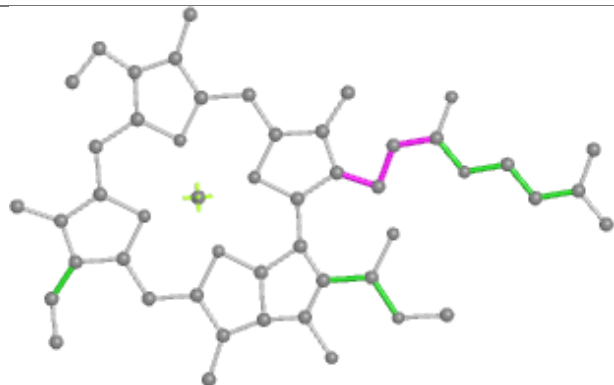
## Ligand CLA 7 609



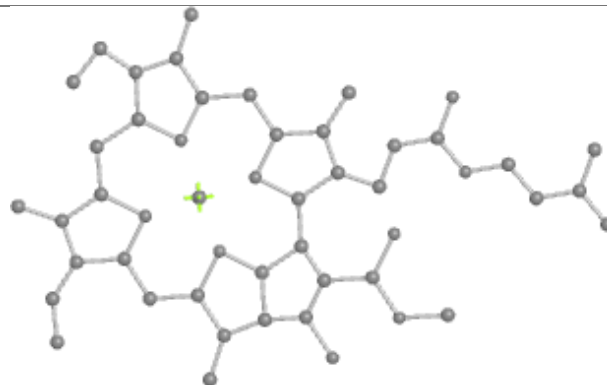
Bond lengths



Bond angles

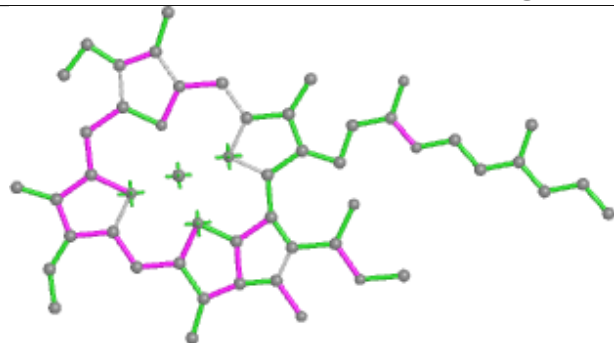


Torsions

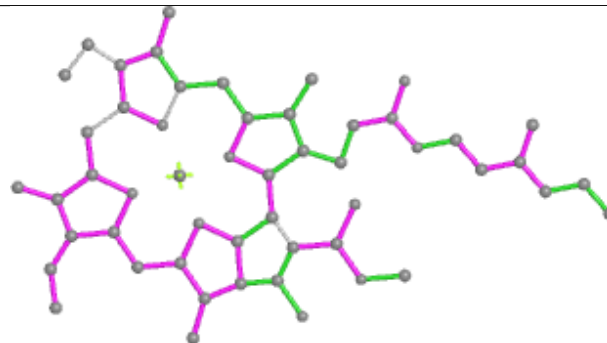


Rings

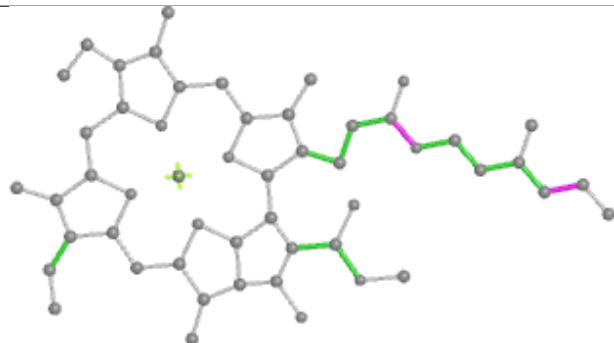
## Ligand CLA 4 612



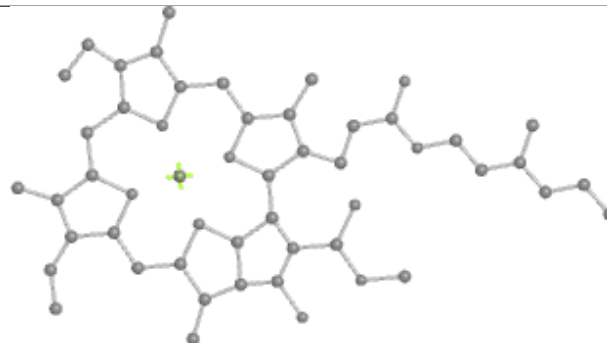
Bond lengths



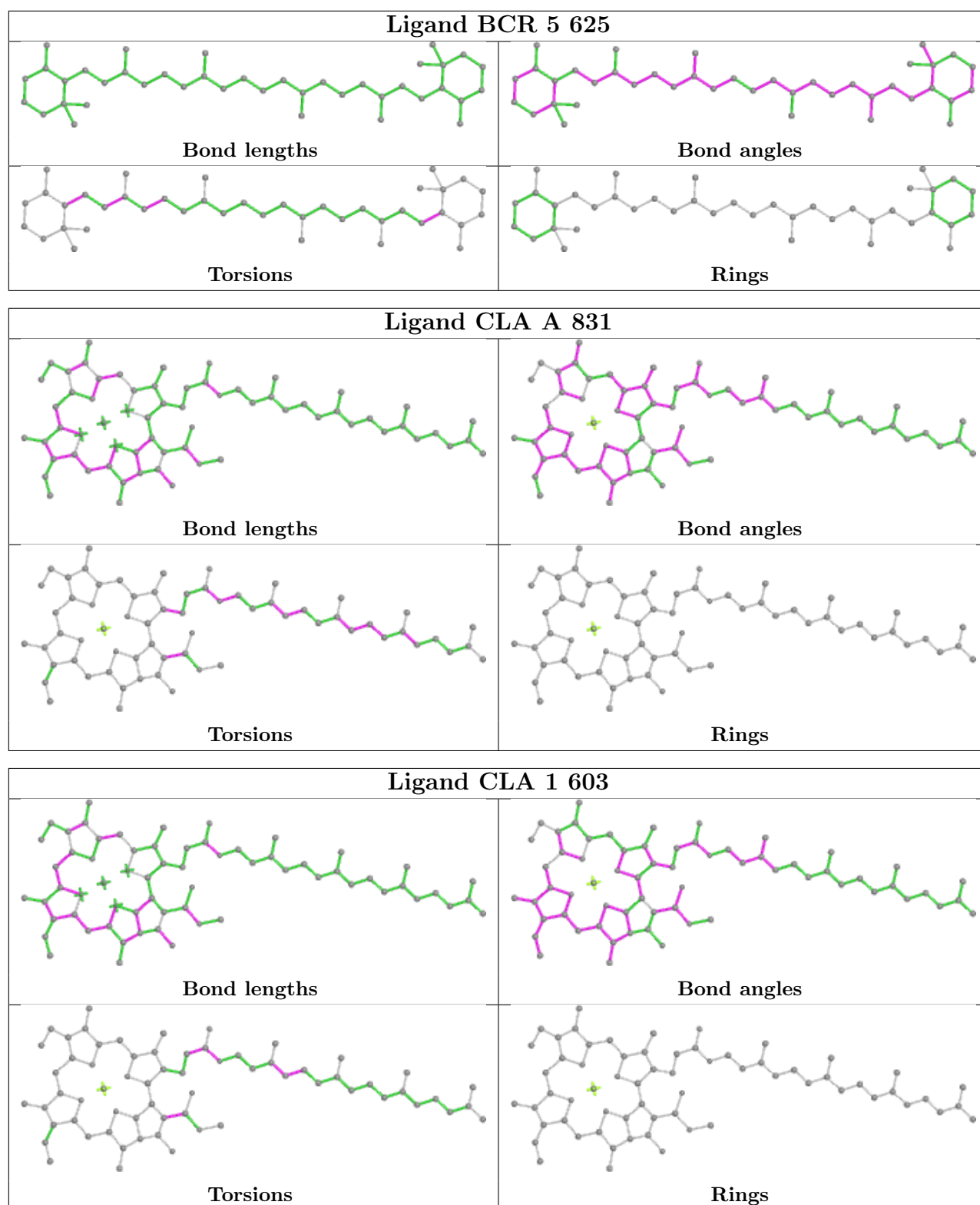
Bond angles



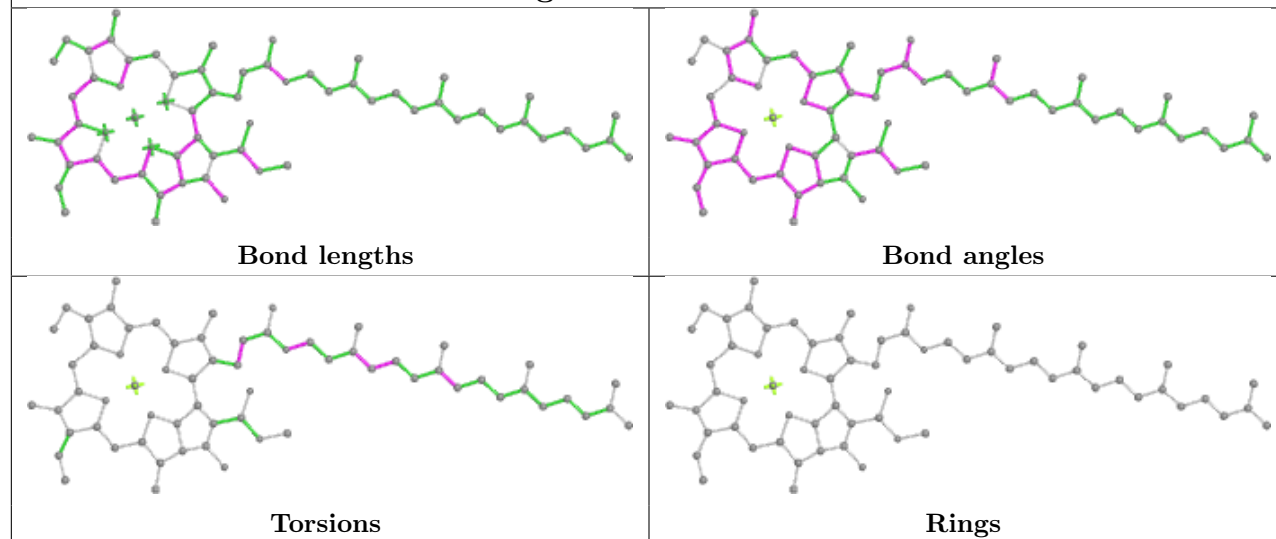
Torsions



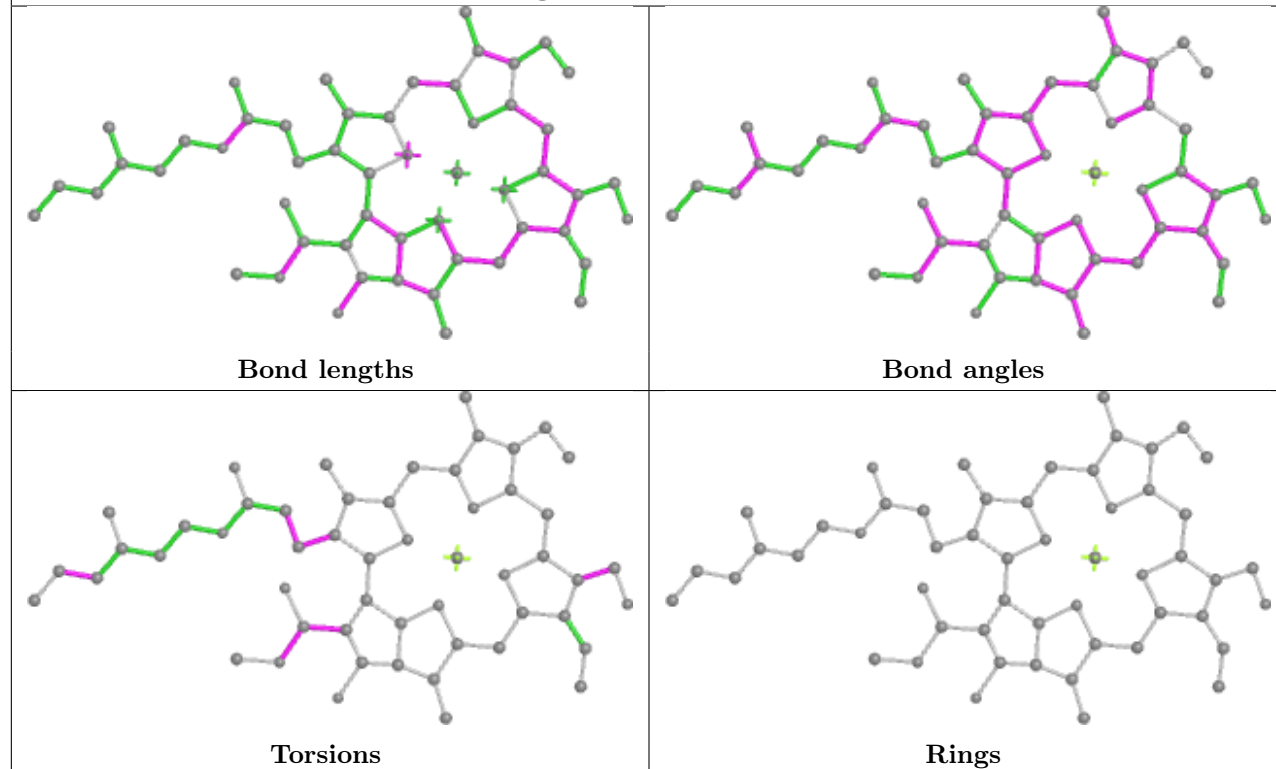
Rings

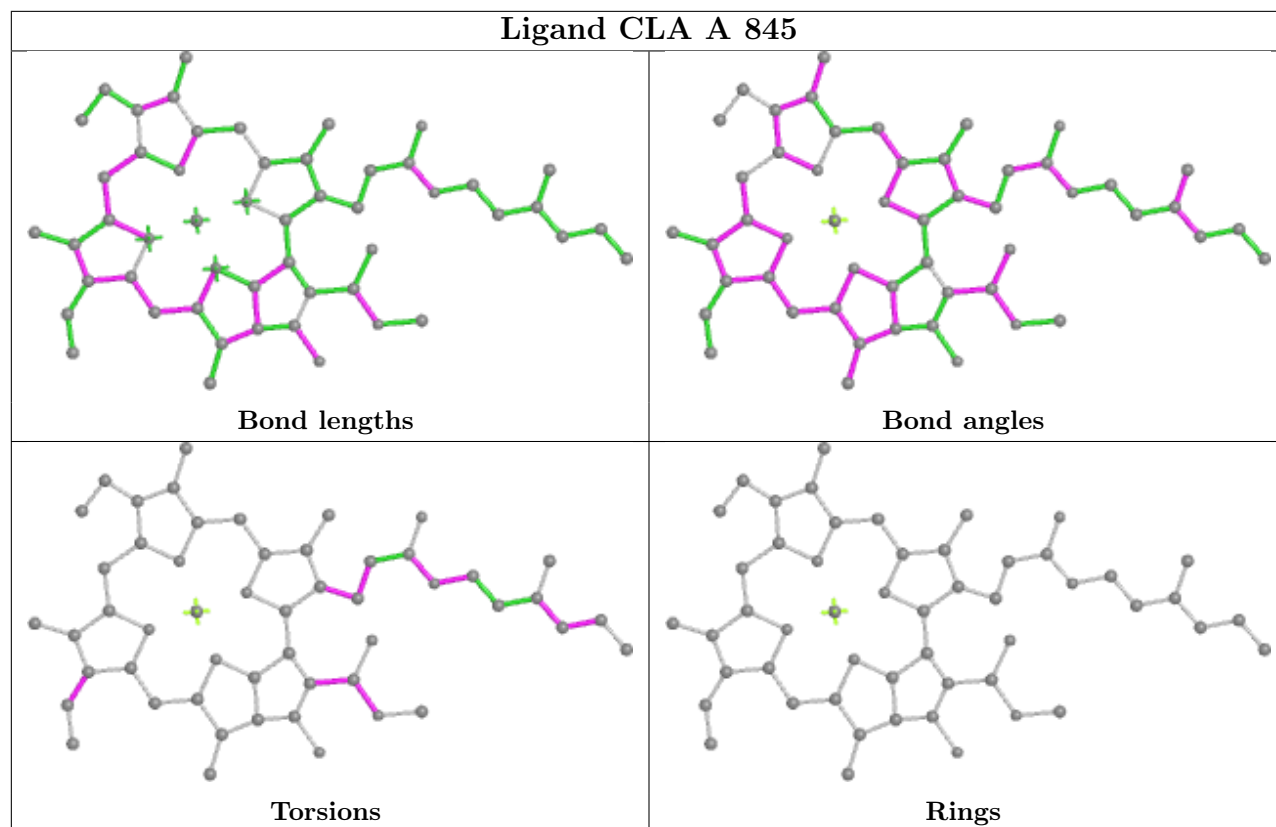


## Ligand CLA 1 609



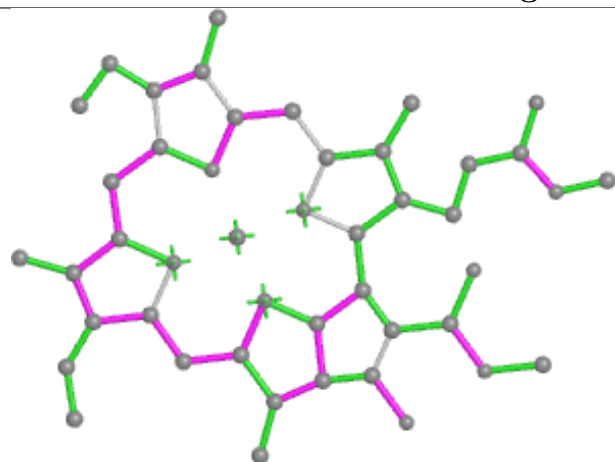
## Ligand CHL Z 601



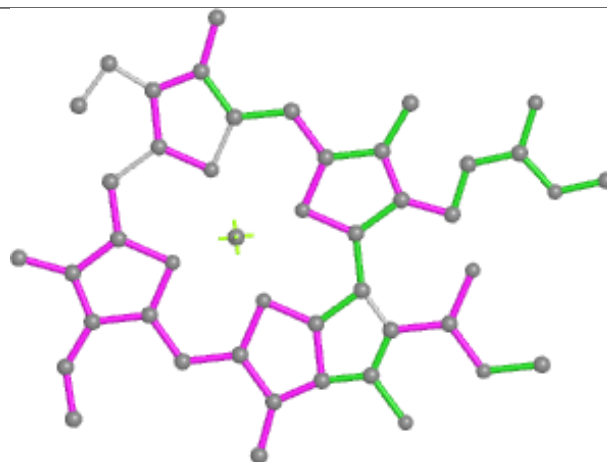




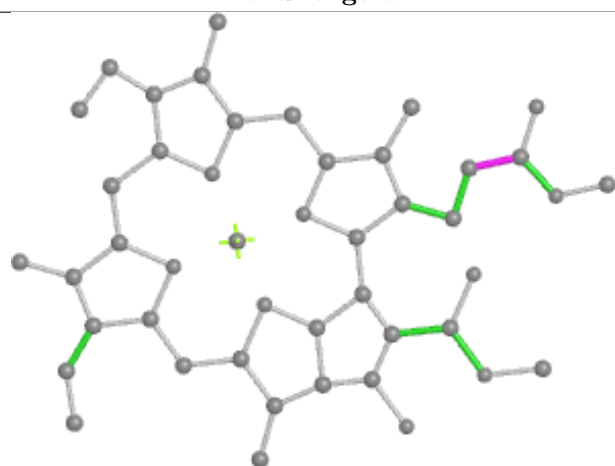
## Ligand CLA 8 616



Bond lengths



Bond angles

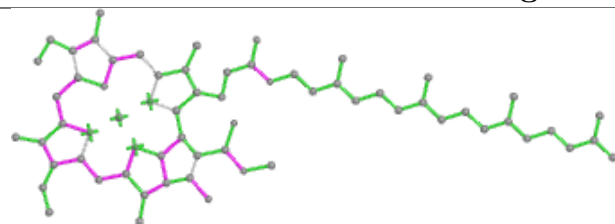


Torsions

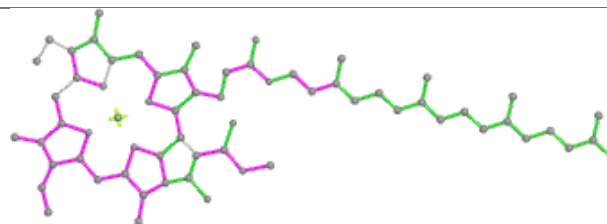


Rings

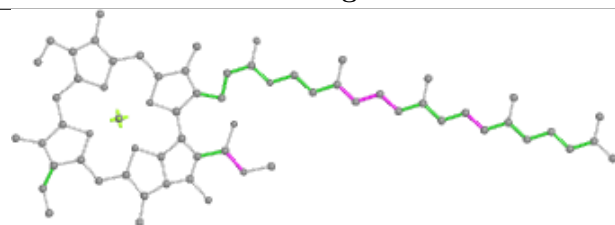
## Ligand CLA 3 603



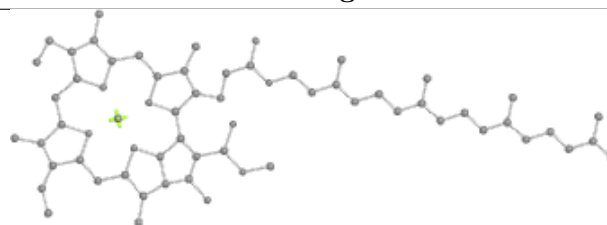
Bond lengths



Bond angles

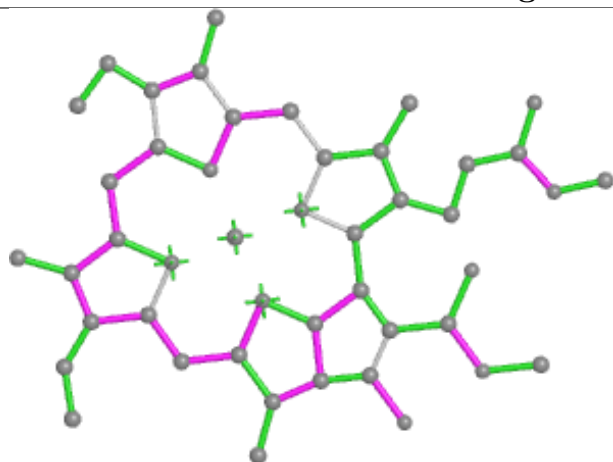


Torsions

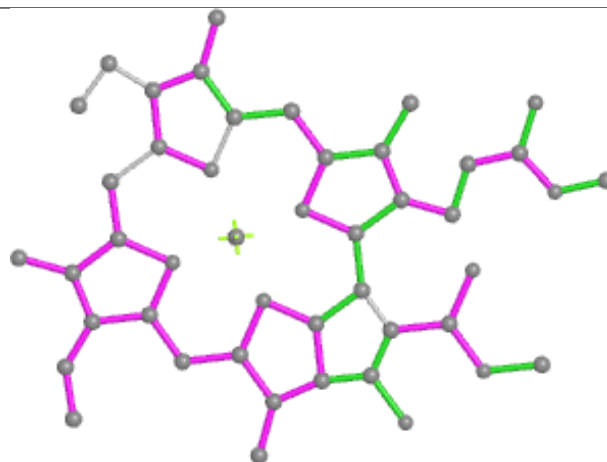


Rings

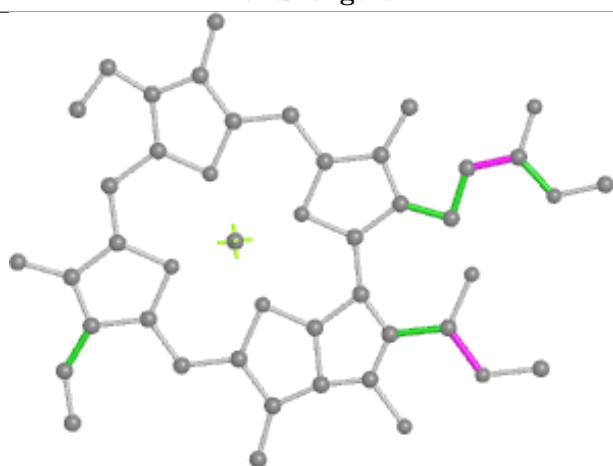
## Ligand CLA 1 616



Bond lengths



Bond angles

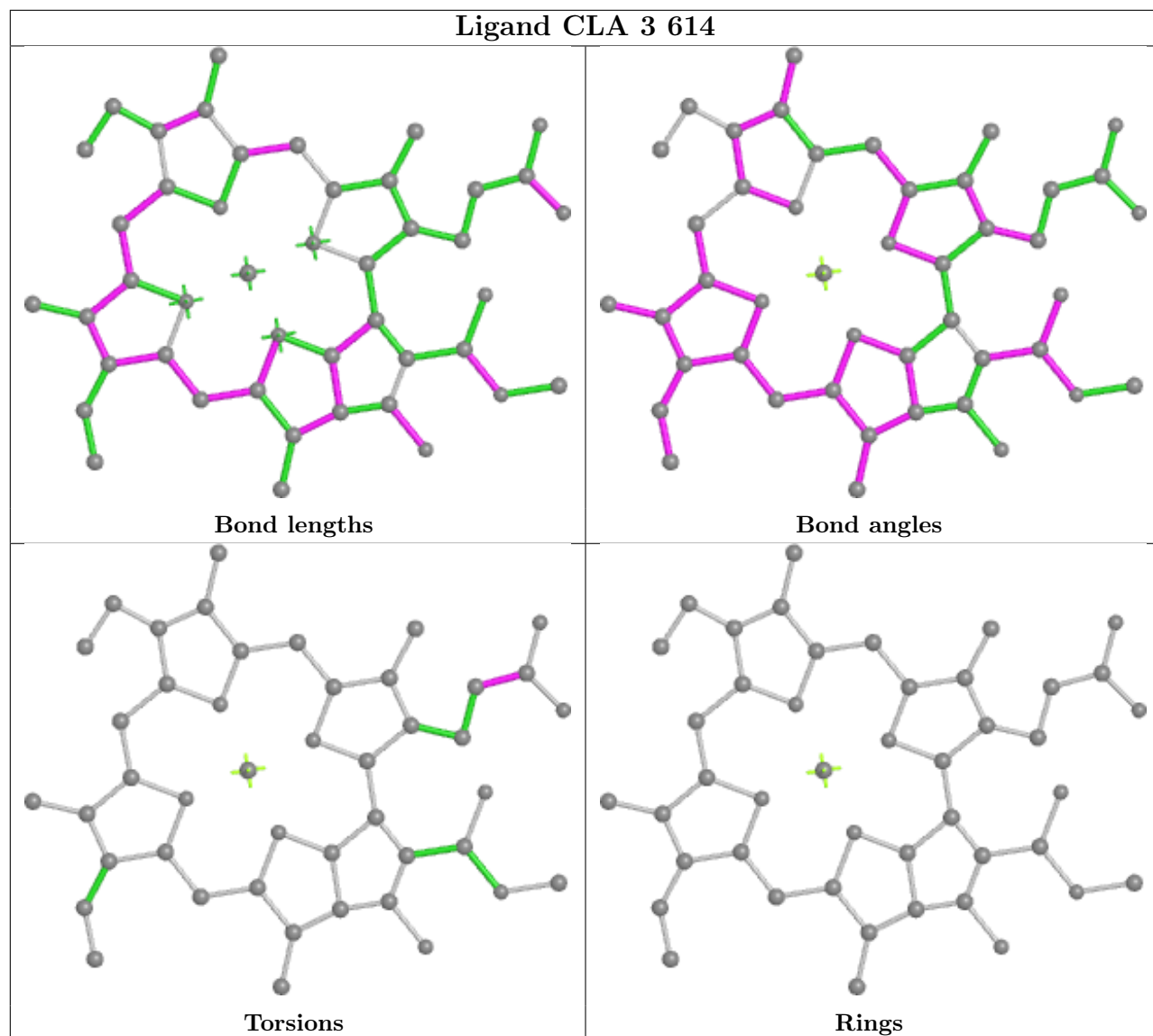


Torsions

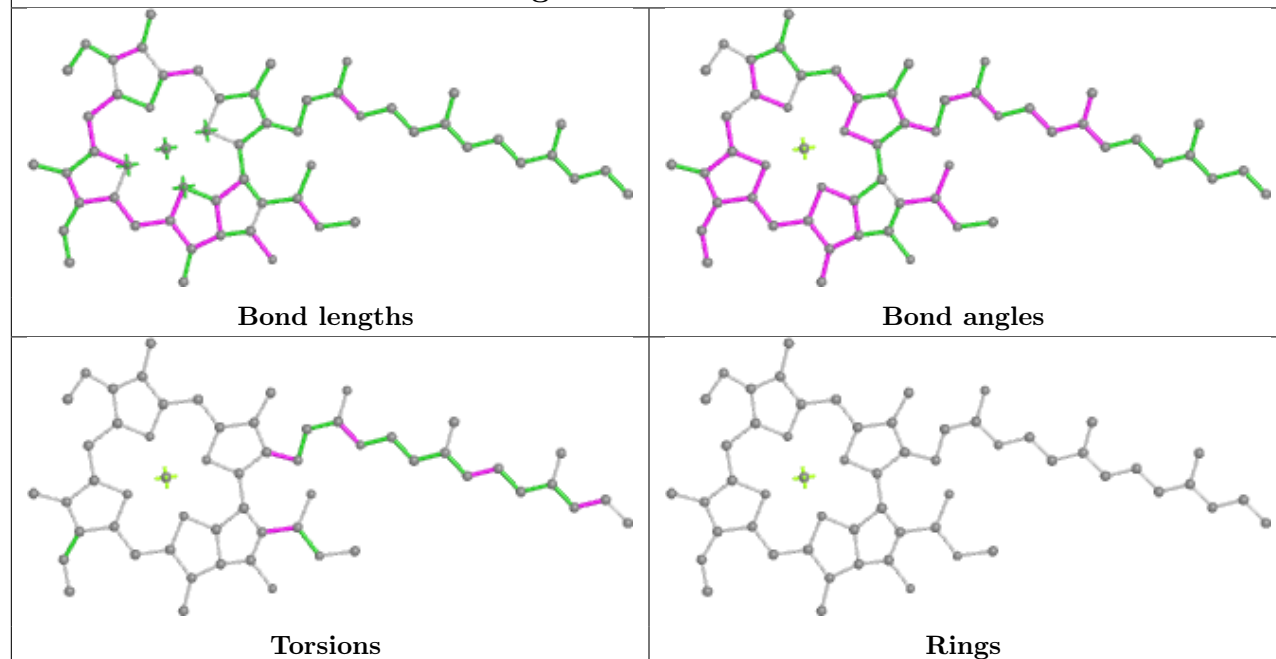


Rings

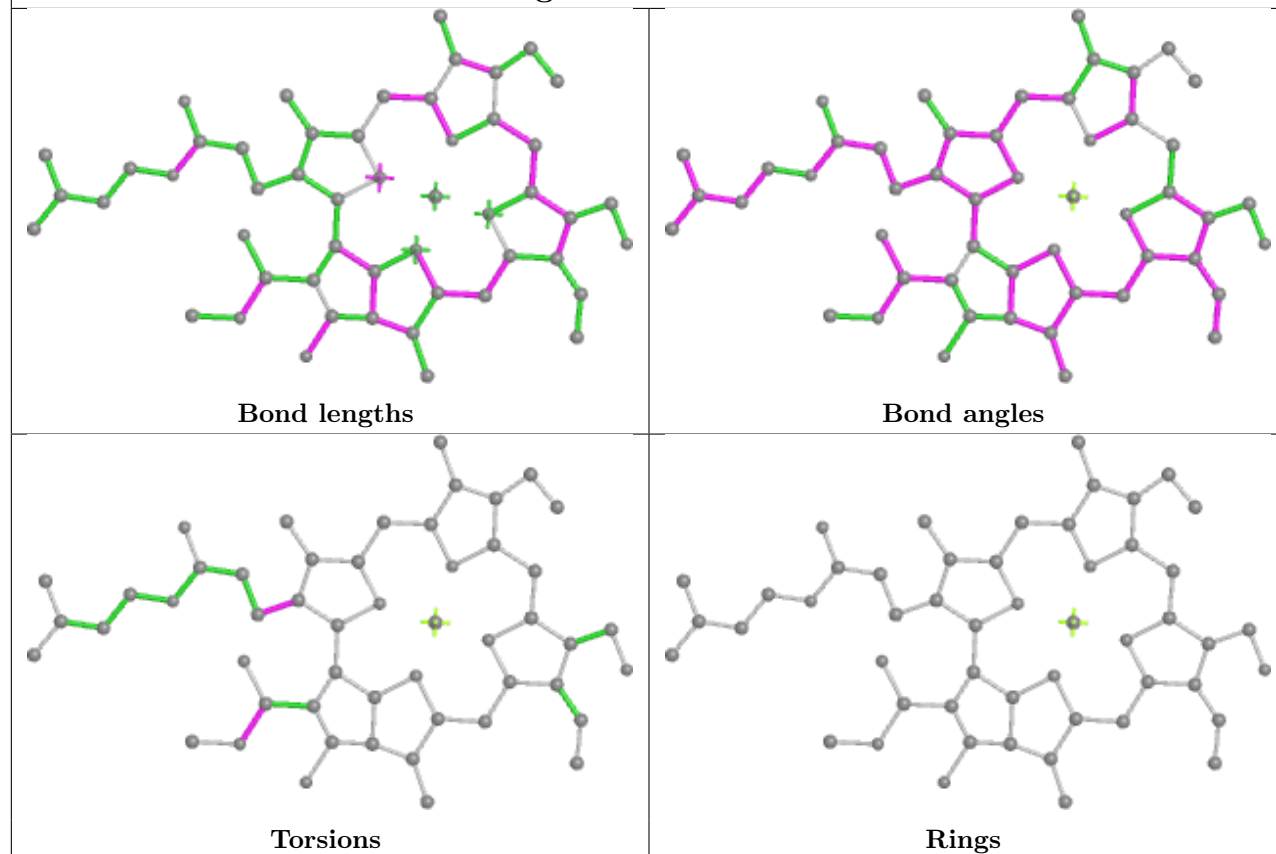
## Ligand CLA 3 614



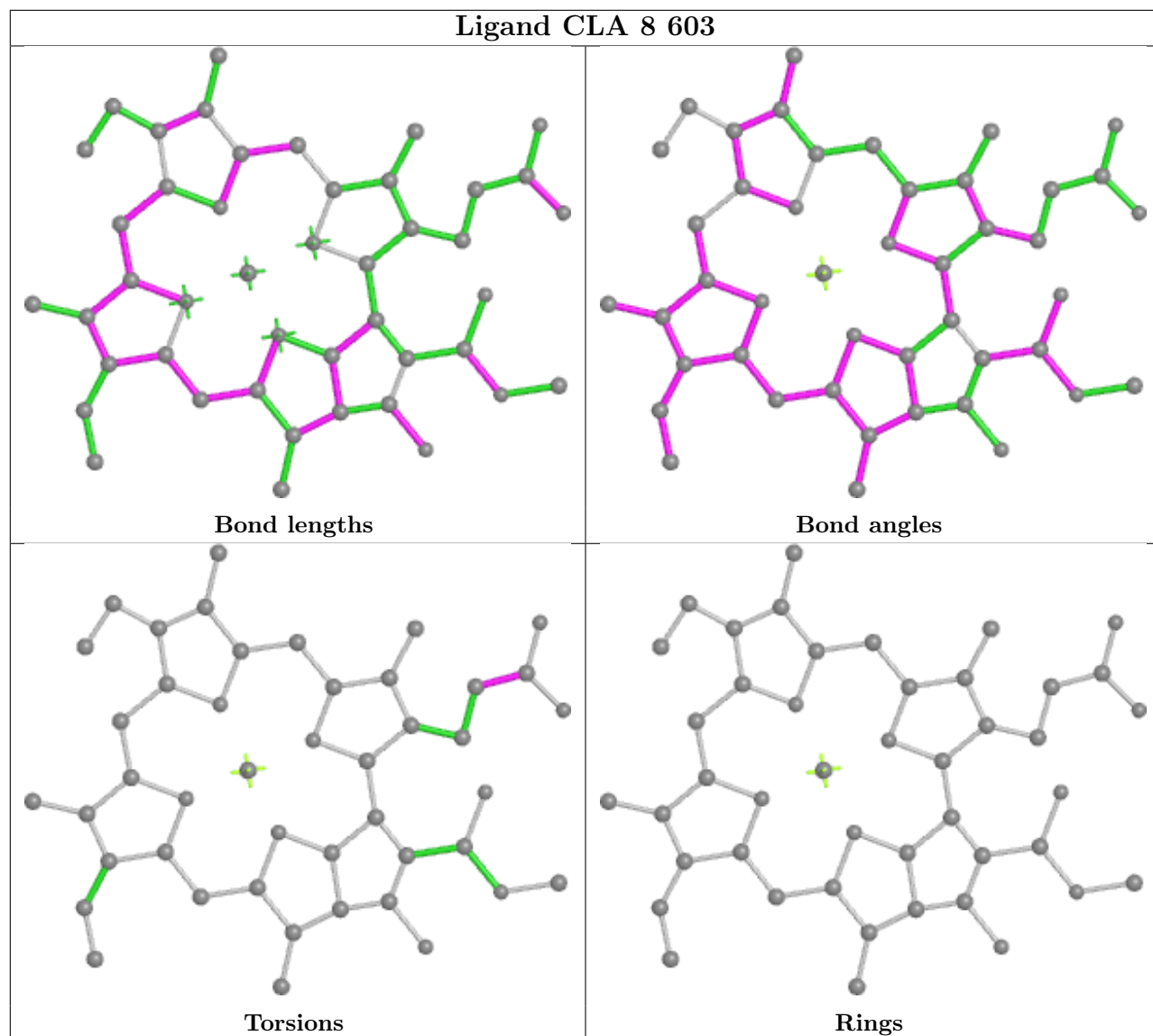
## Ligand CLA A 817



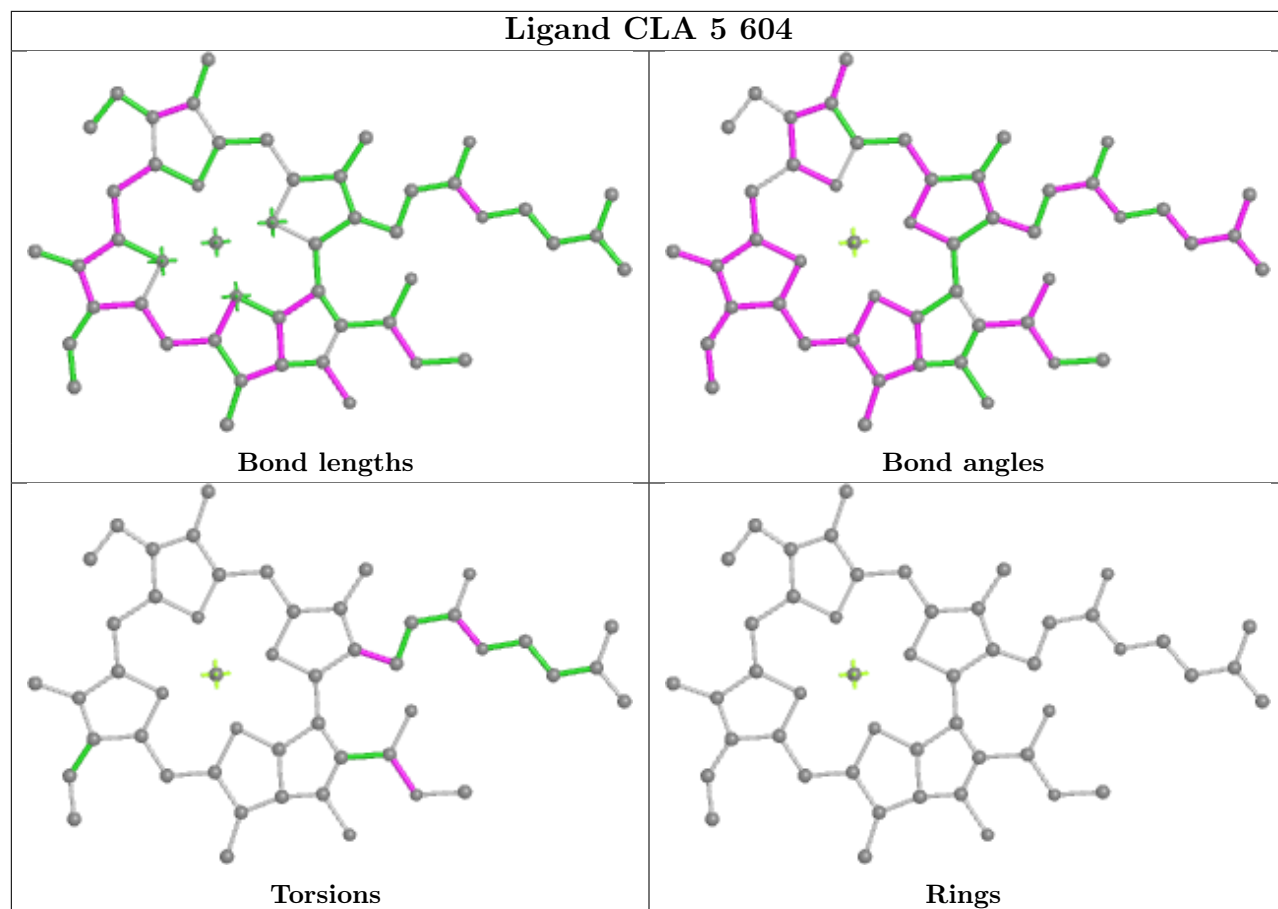
## Ligand CHL 6 608



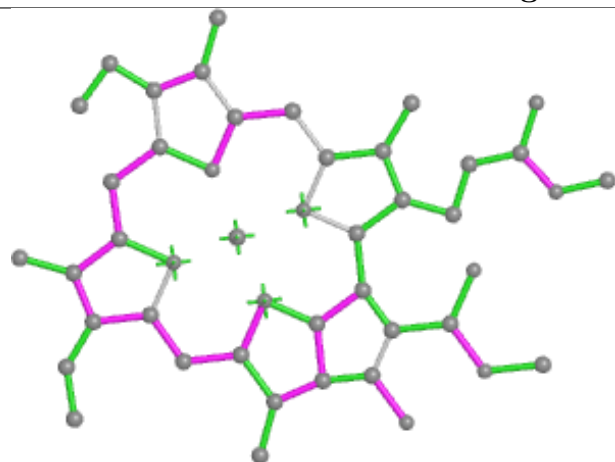
## Ligand CLA 8 603



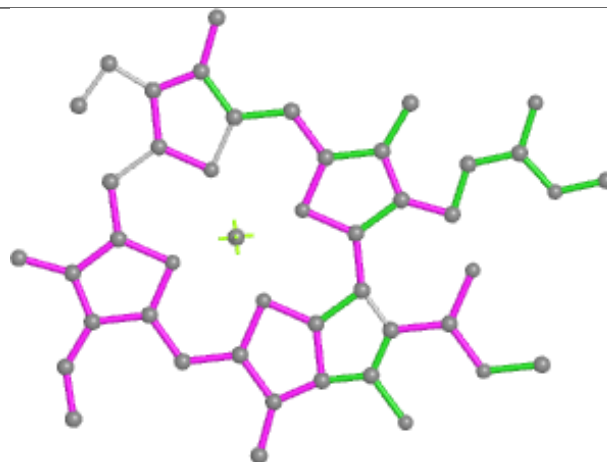
## Ligand CLA 5 604



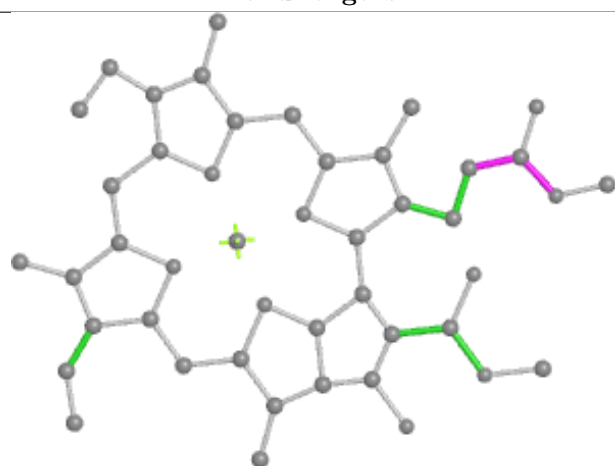
## Ligand CLA 6 617



Bond lengths



Bond angles

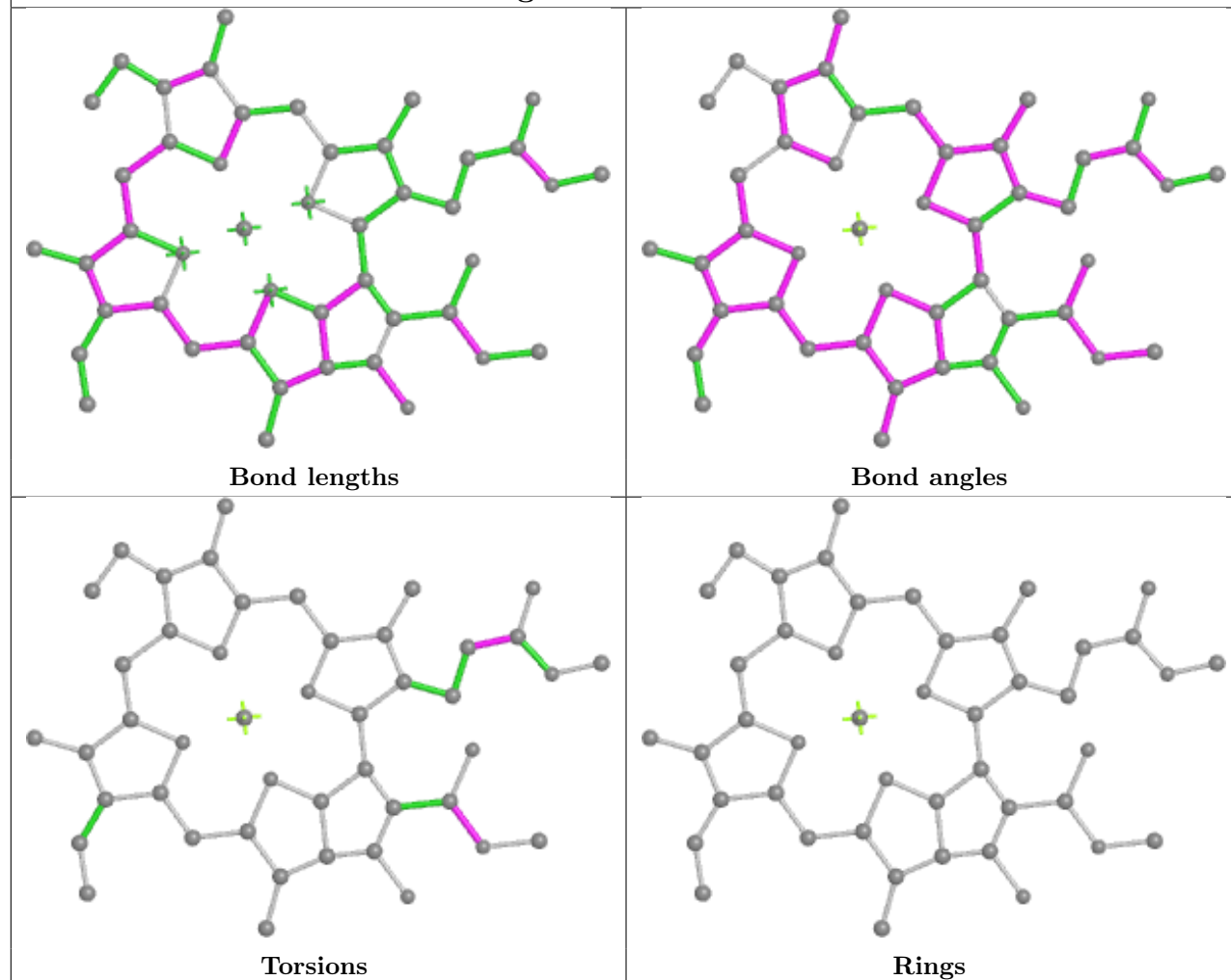


Torsions

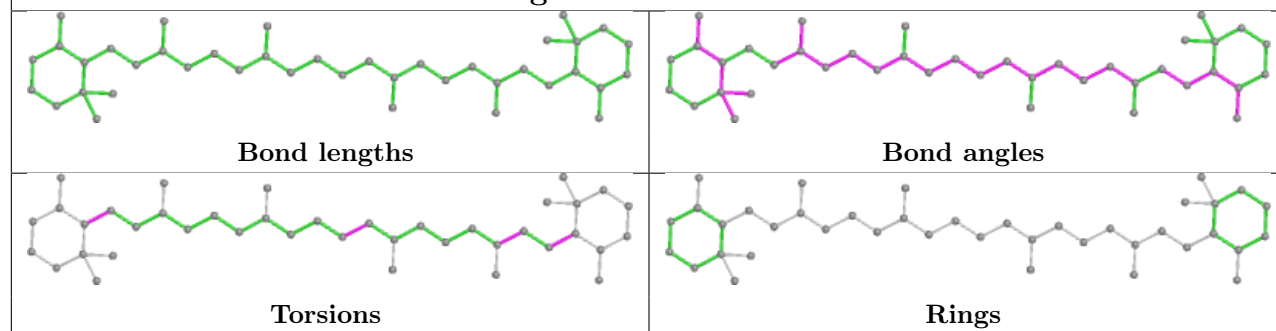


Rings

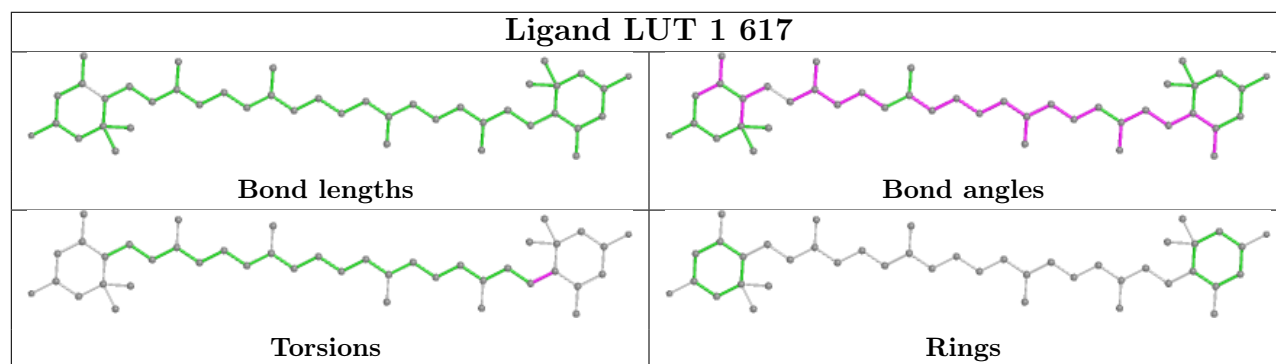
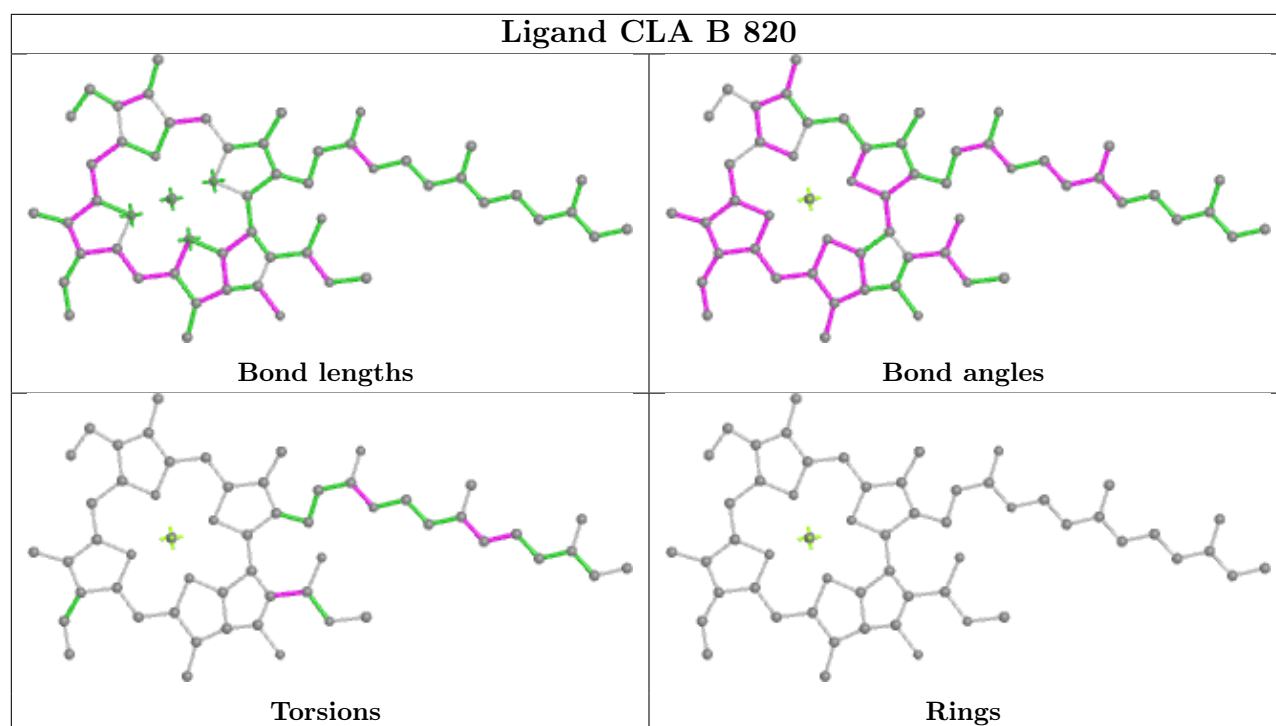
## Ligand CLA 8 609



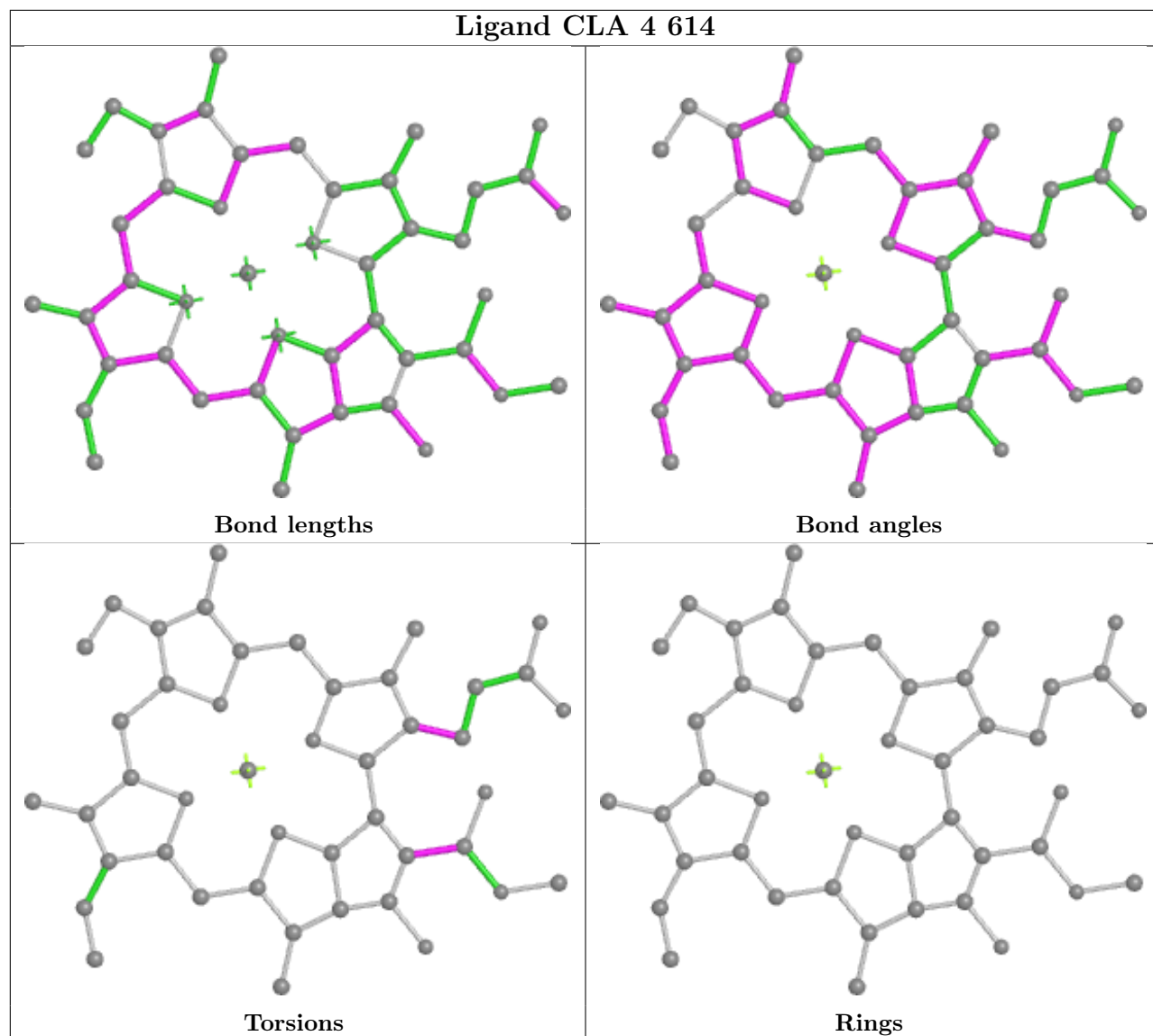
## Ligand BCR A 856



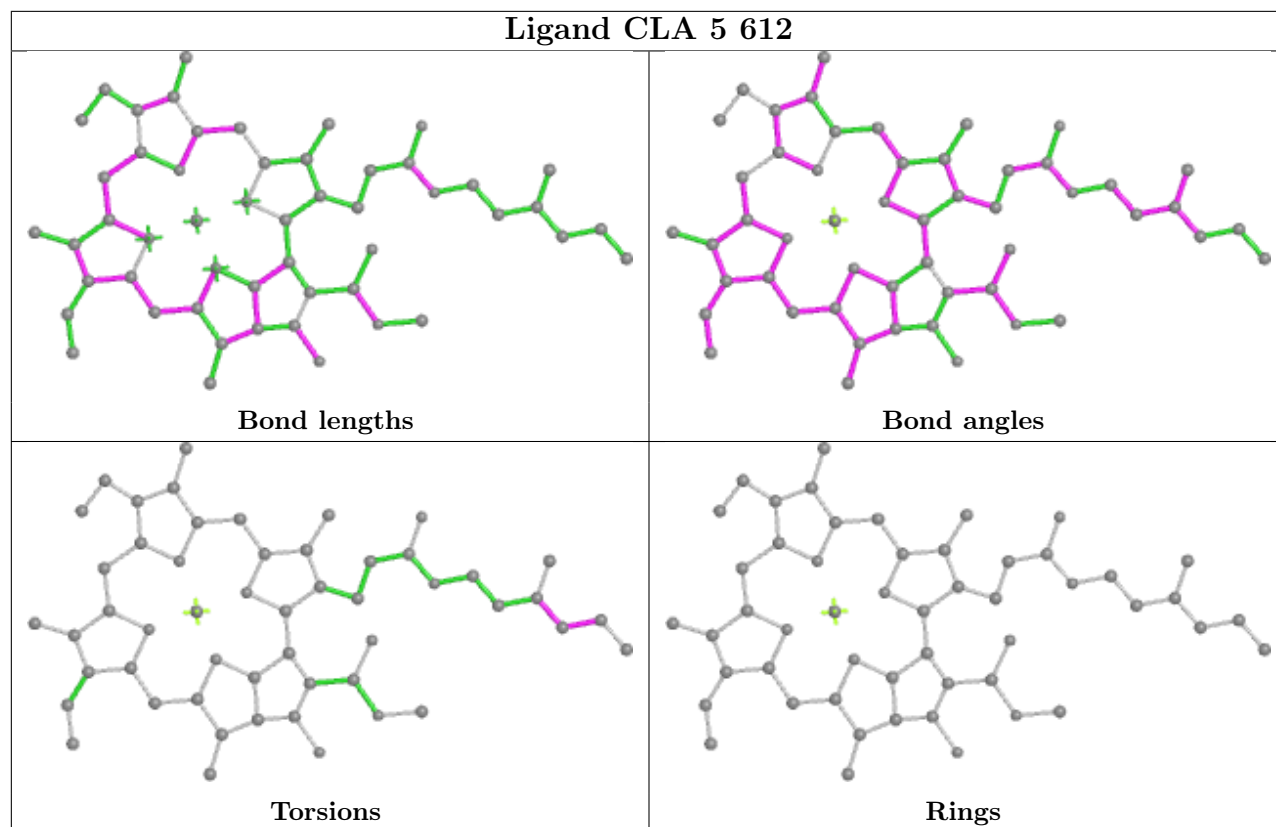




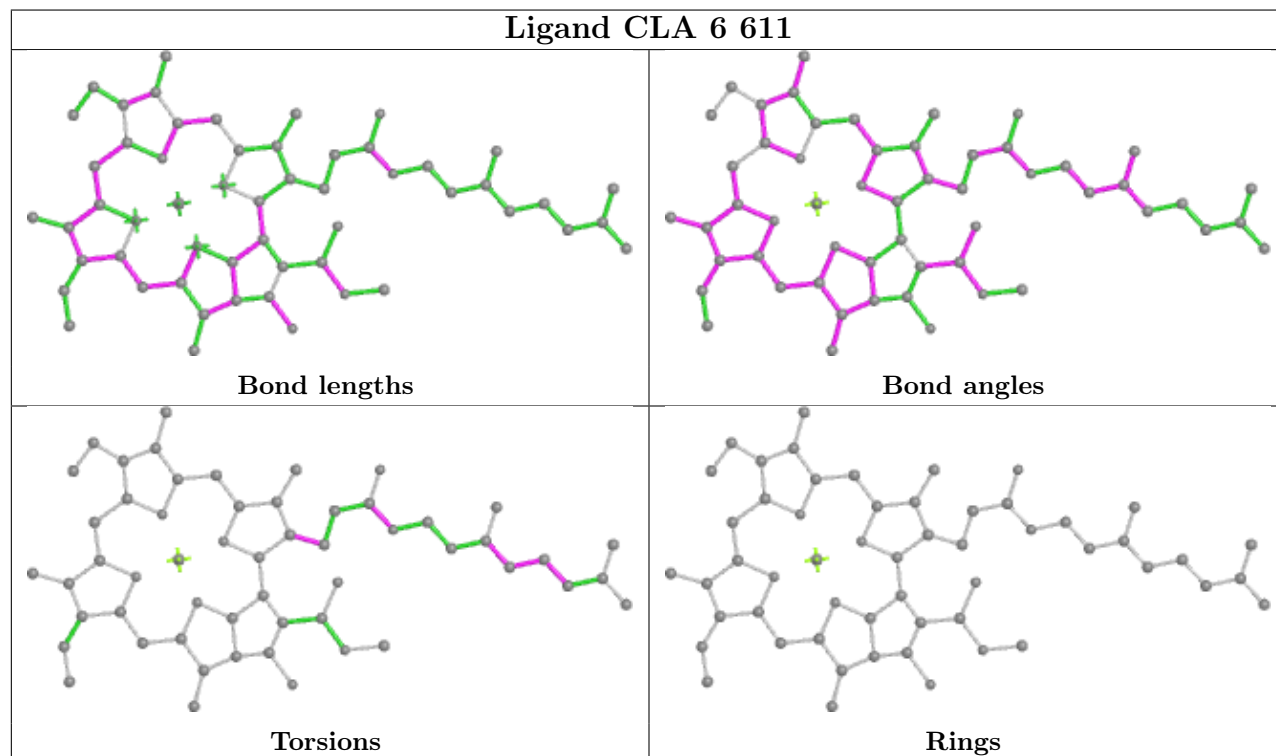
## Ligand CLA 4 614



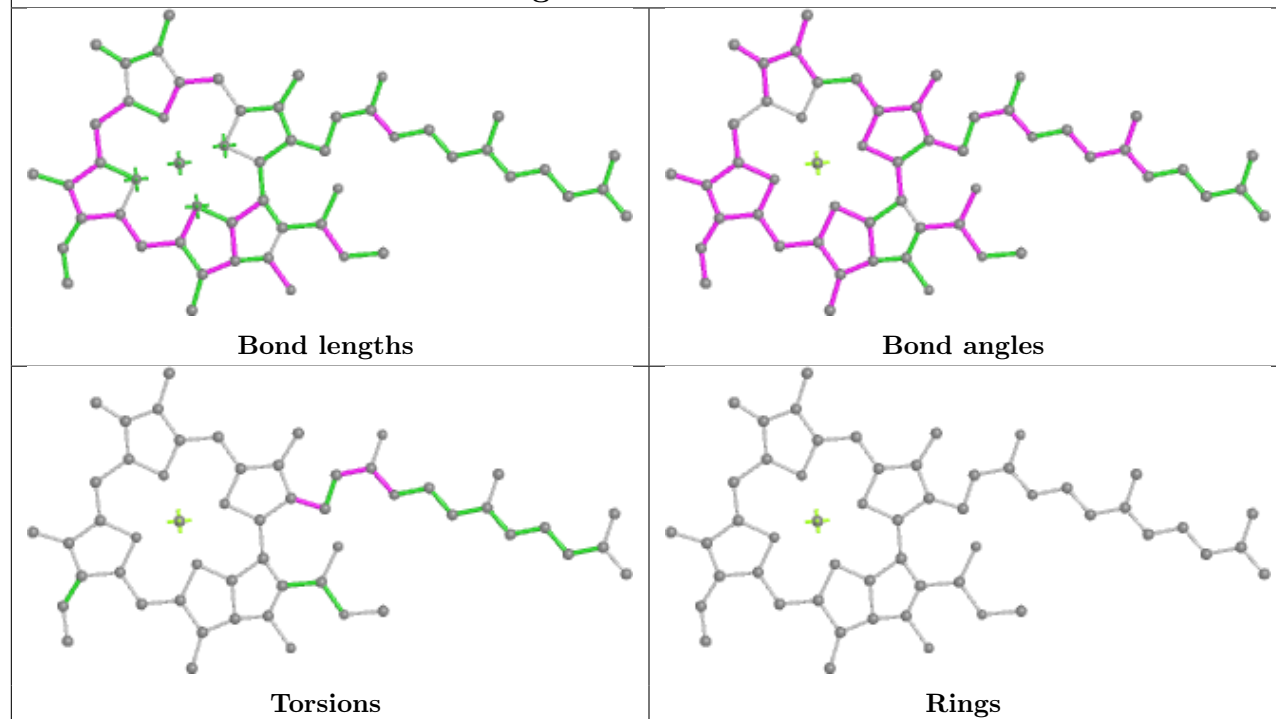
## Ligand CLA 5 612



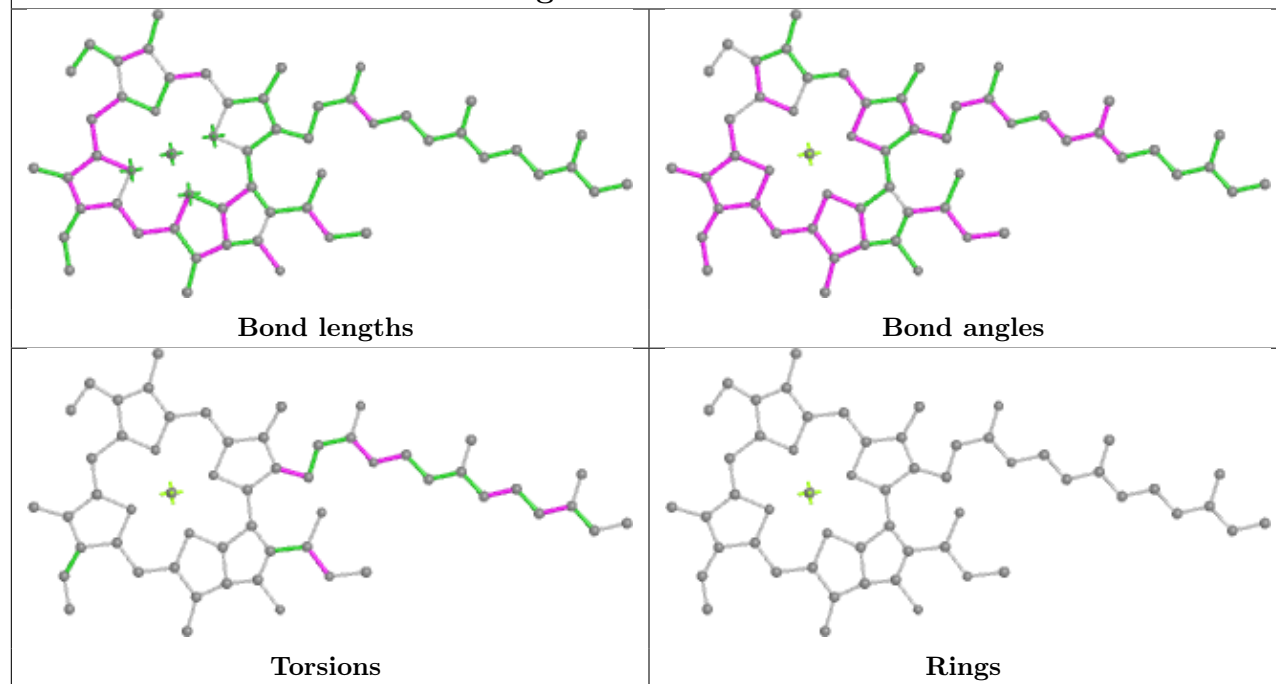
## Ligand CLA 6 611



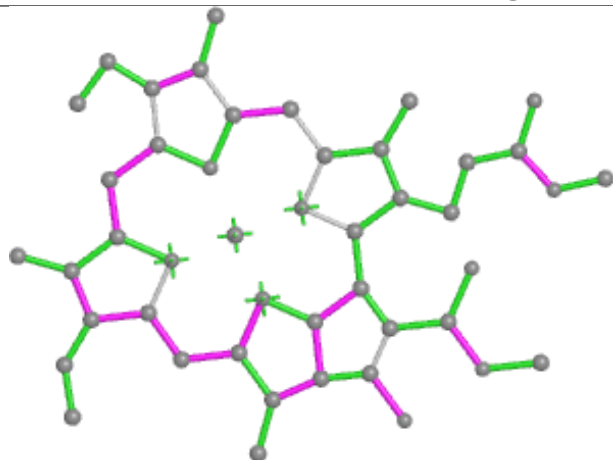
## Ligand CLA B 811



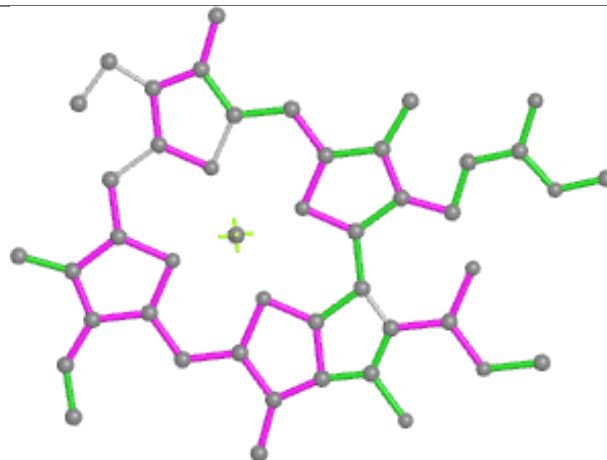
## Ligand CLA 7 604



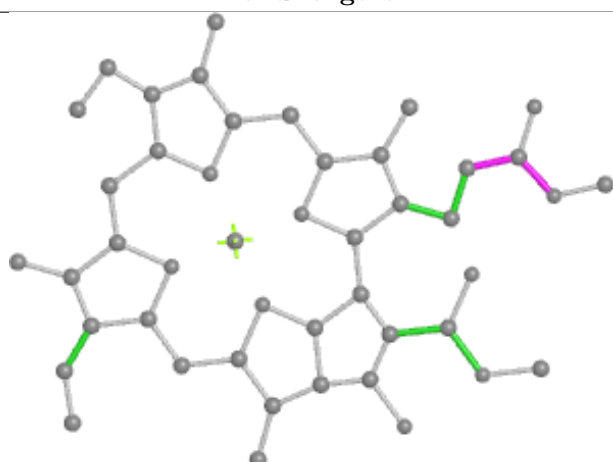
## Ligand CLA K 4003



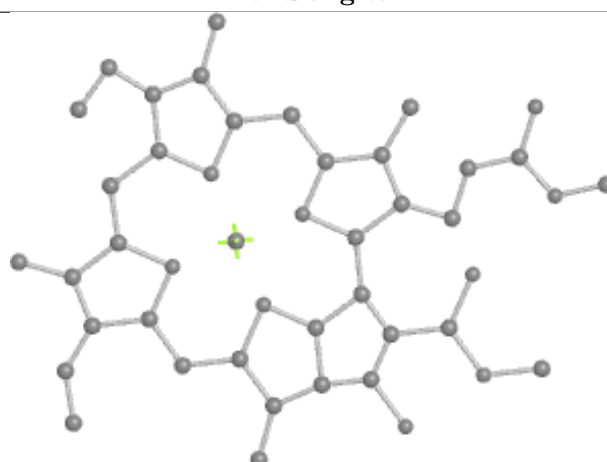
Bond lengths



Bond angles

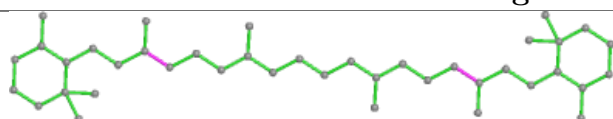


Torsions

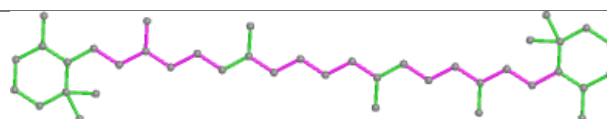


Rings

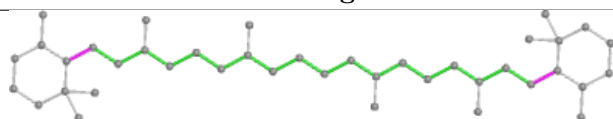
## Ligand BCR A 851



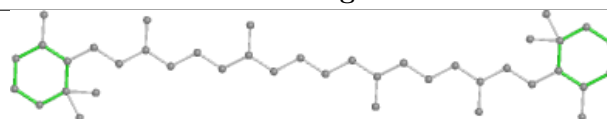
Bond lengths



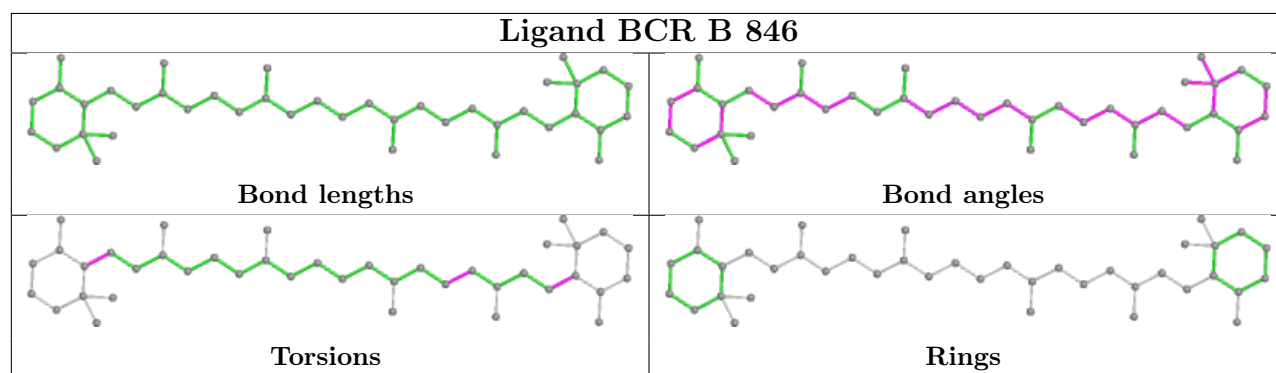
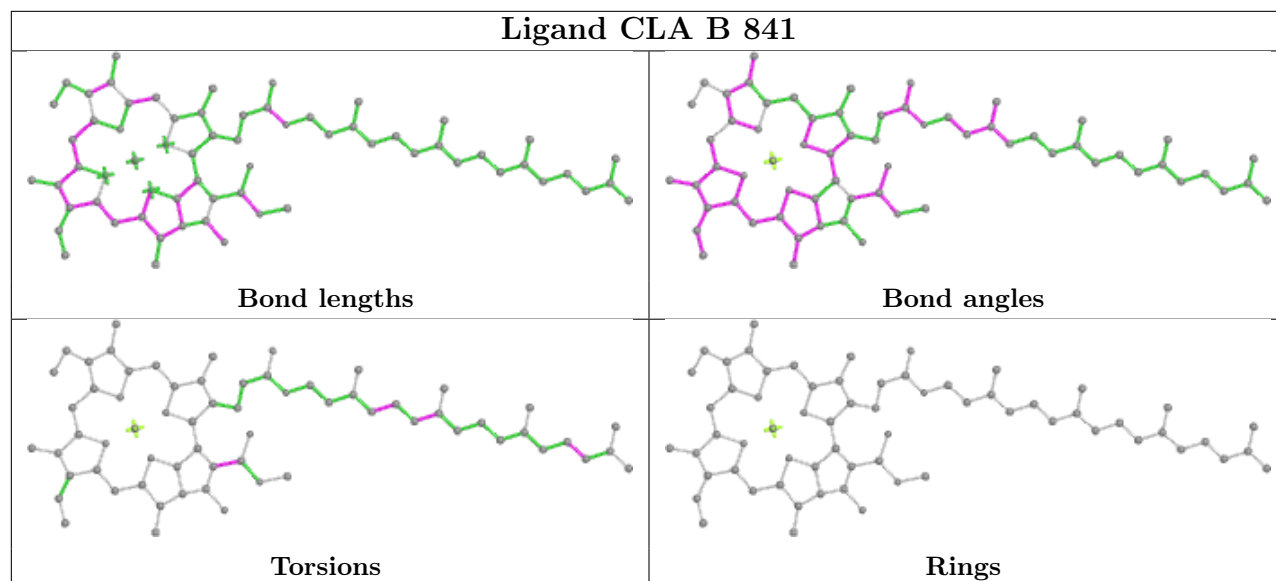
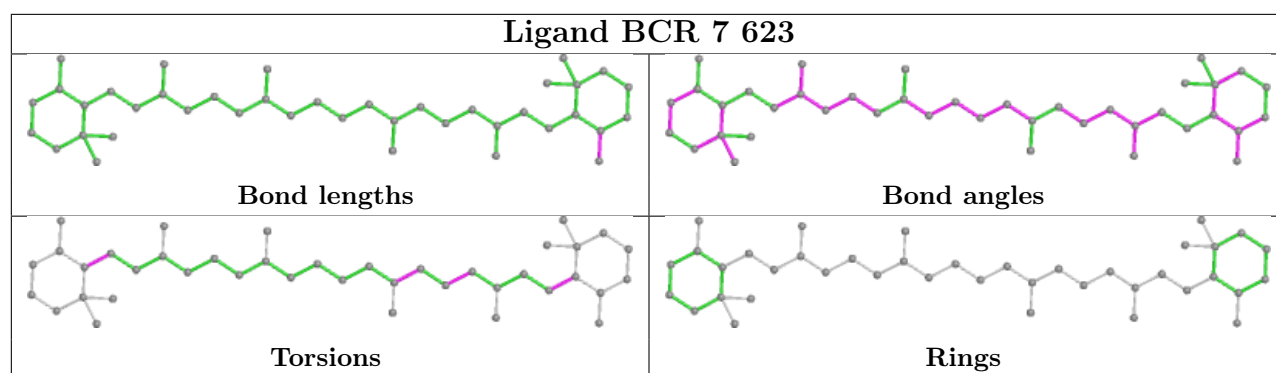
Bond angles



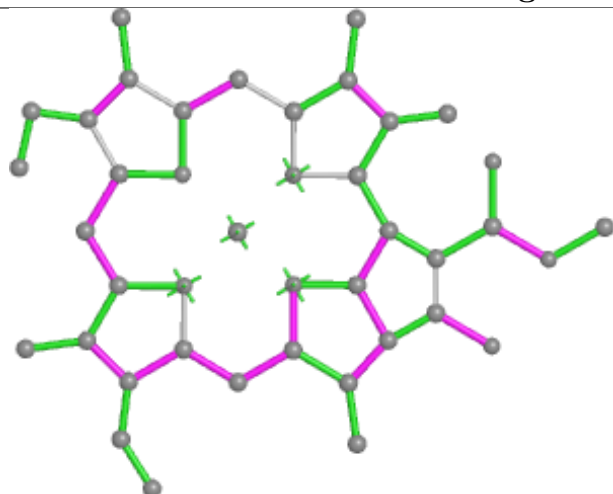
Torsions



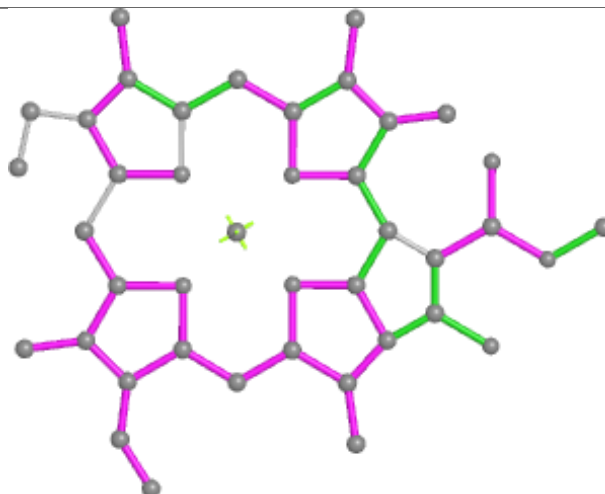
Rings



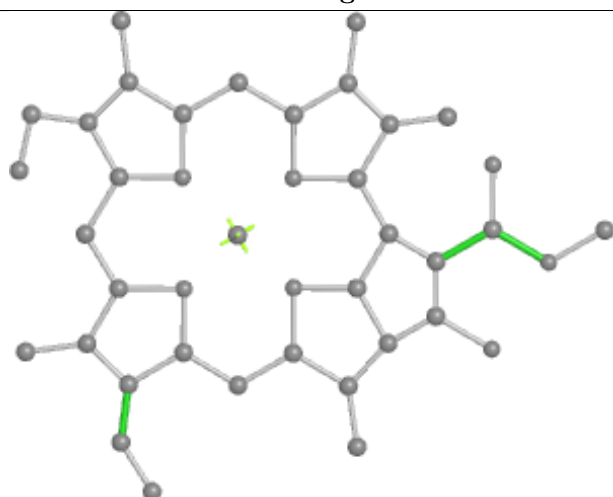
## Ligand CLA 4 616



Bond lengths



Bond angles

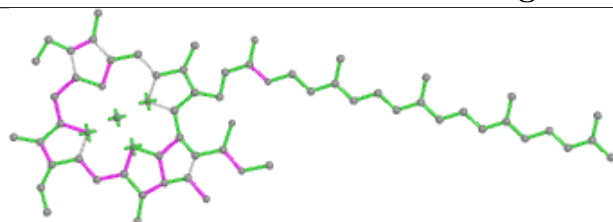


Torsions

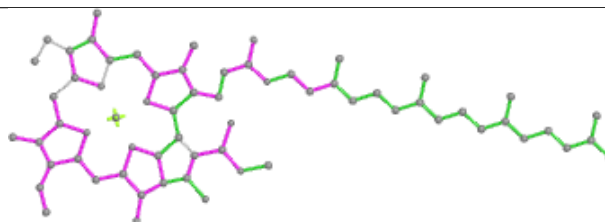


Rings

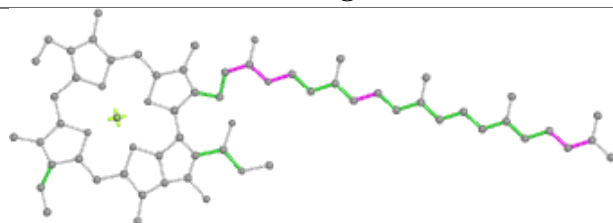
## Ligand CL0 A 801



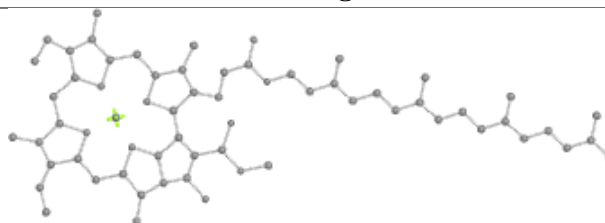
Bond lengths



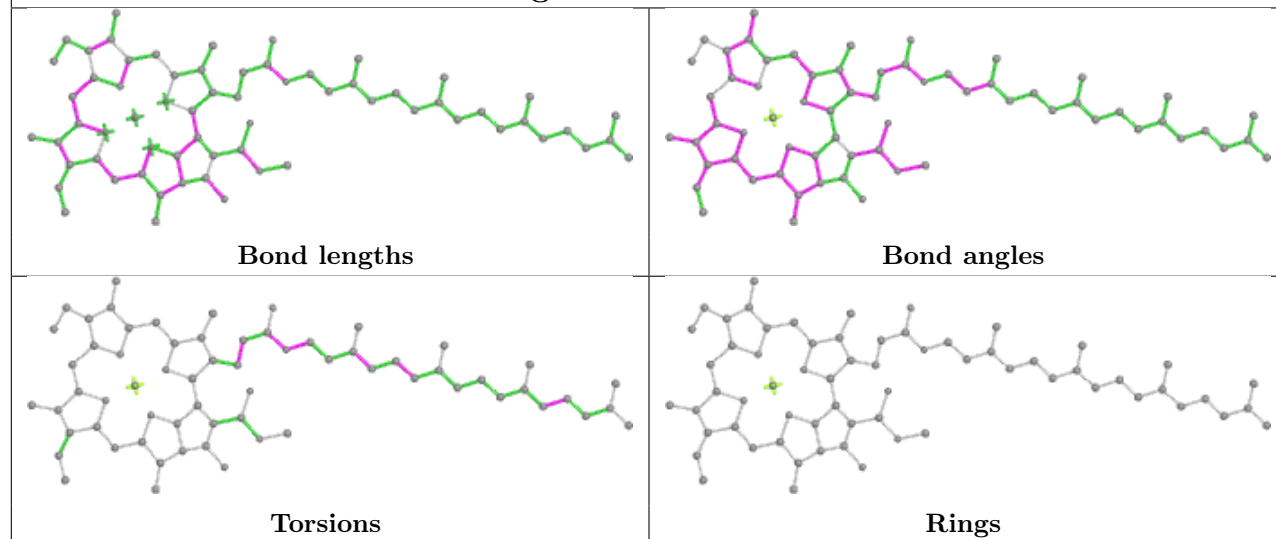
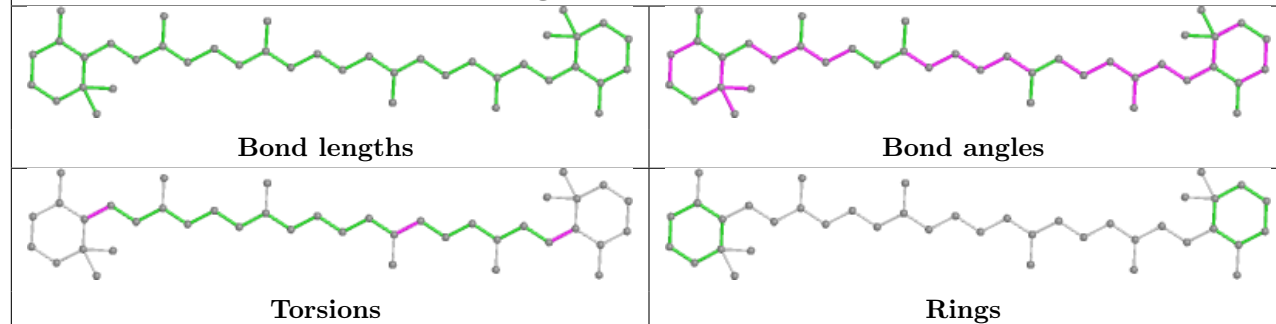
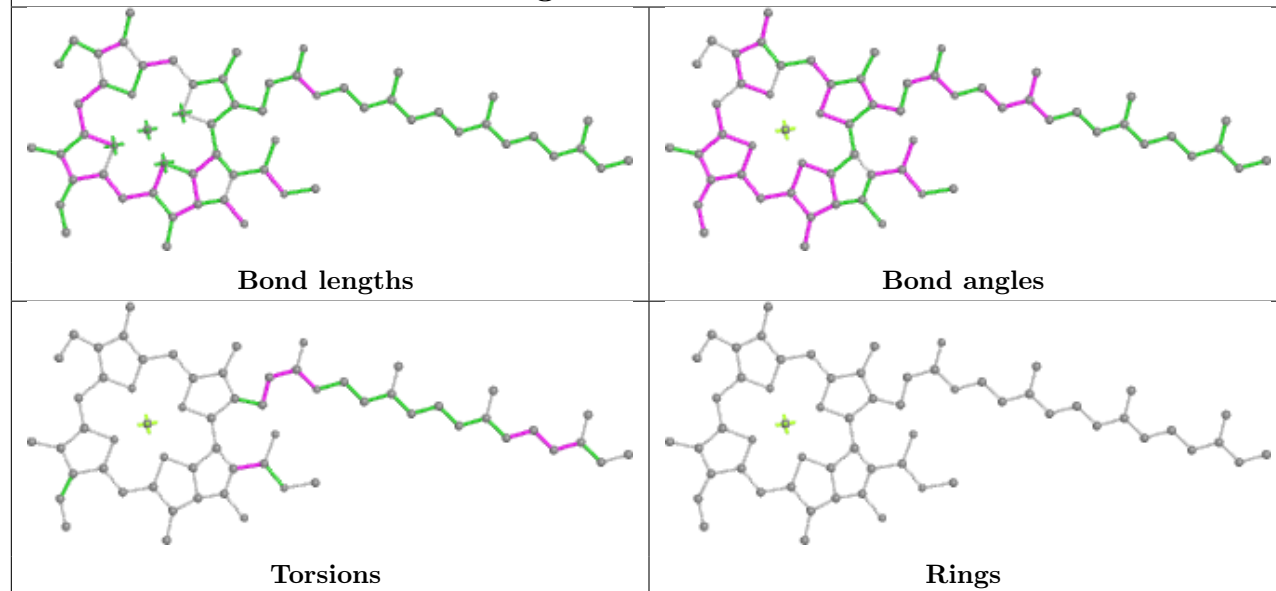
Bond angles



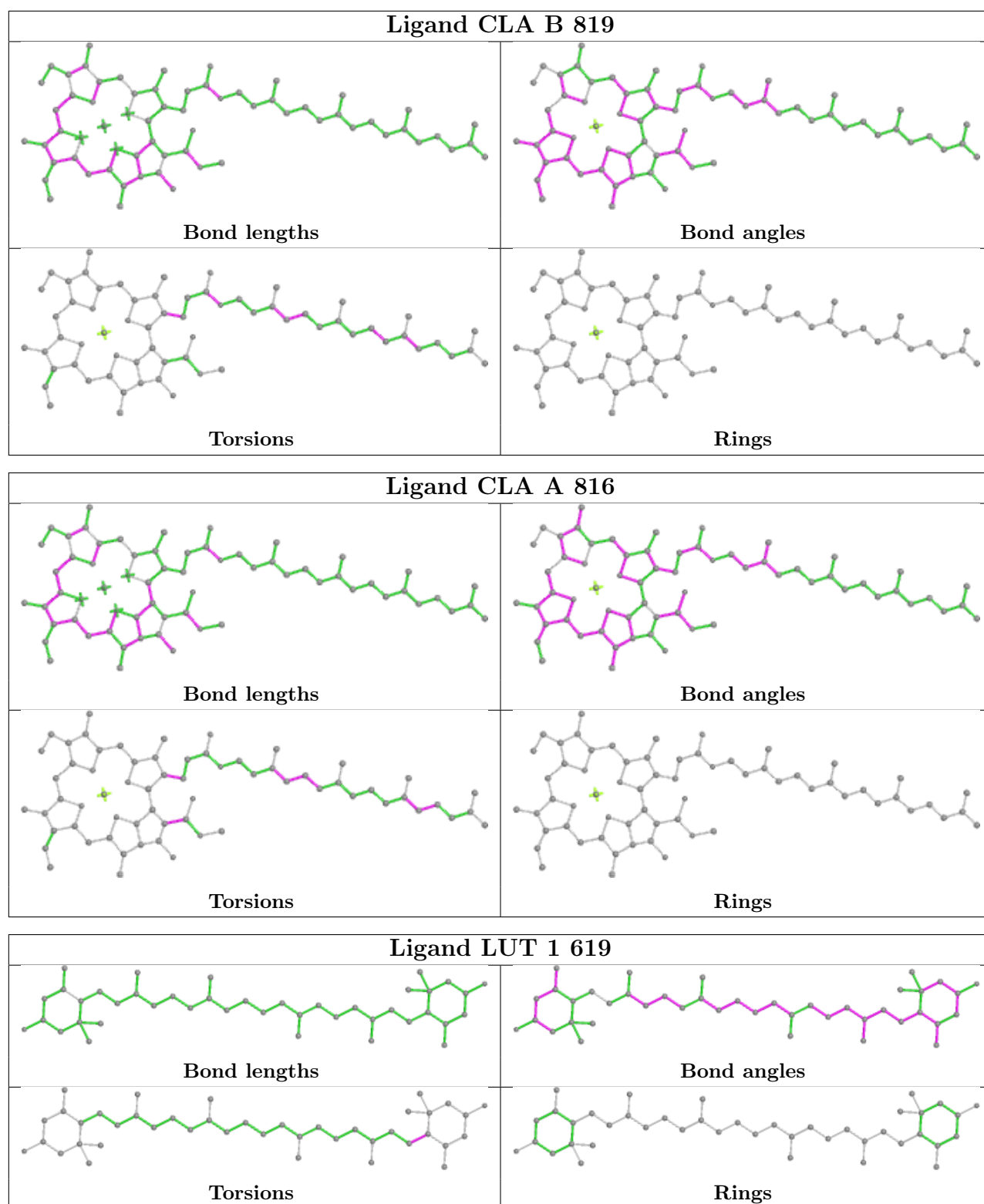
Torsions



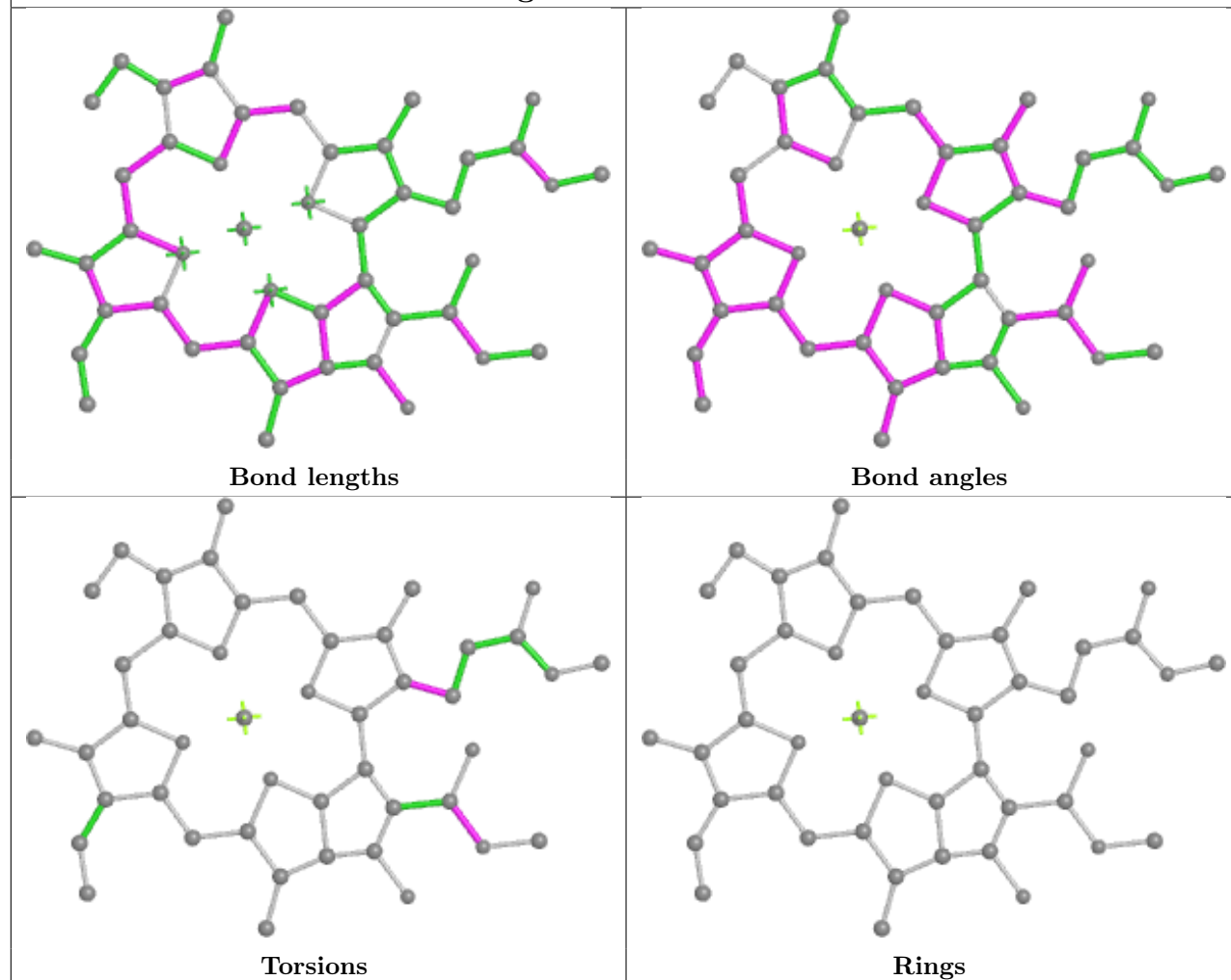
Rings

**Ligand CLA A 830****Ligand BCR 8 619****Ligand CLA 4 601**

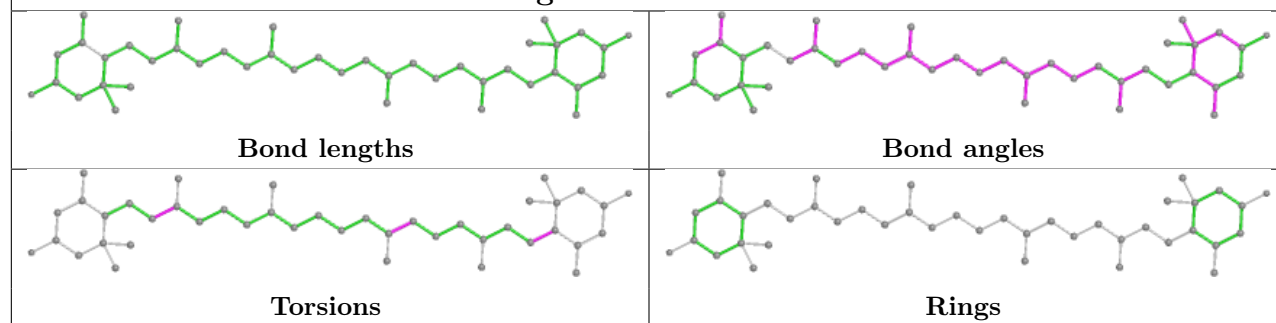


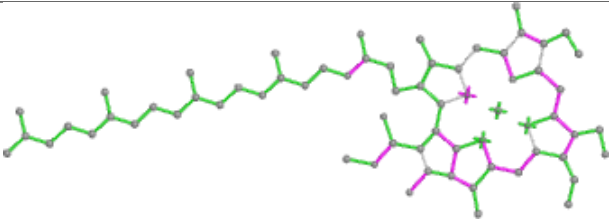
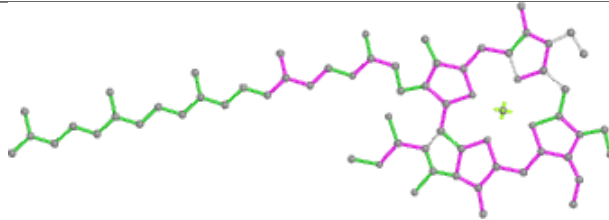
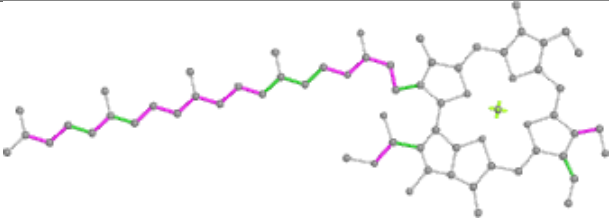
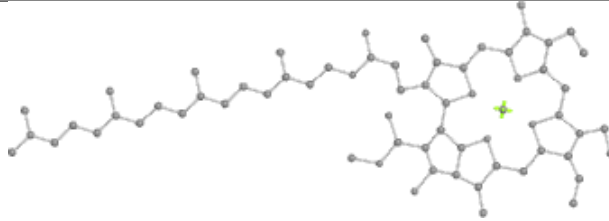


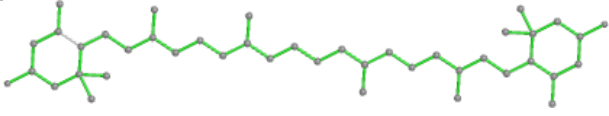
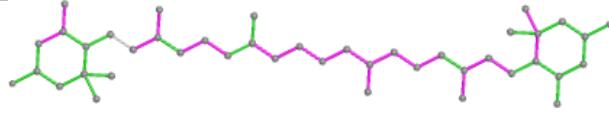
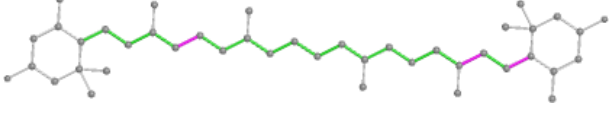
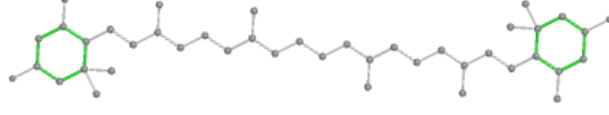
## Ligand CLA 8 604



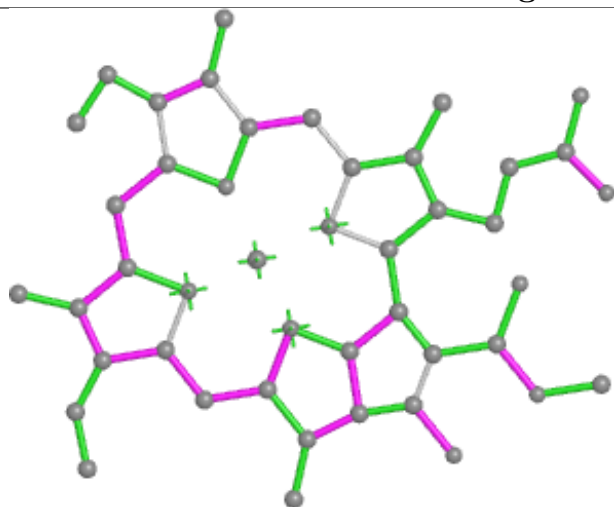
## Ligand LUT 3 621



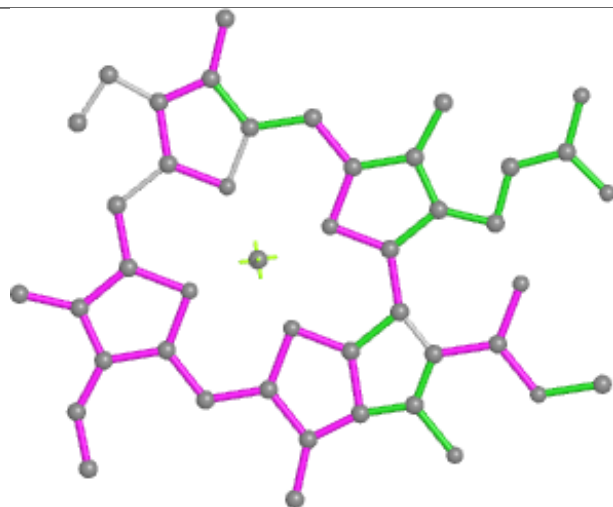
Ligand CHL 3 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 8 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

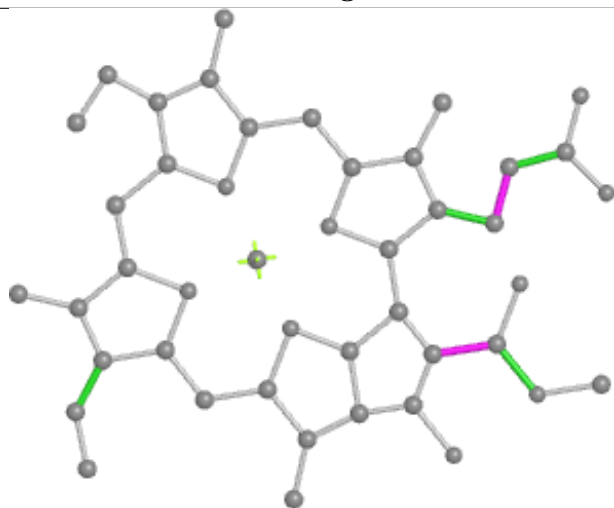
## Ligand CLA 2 614



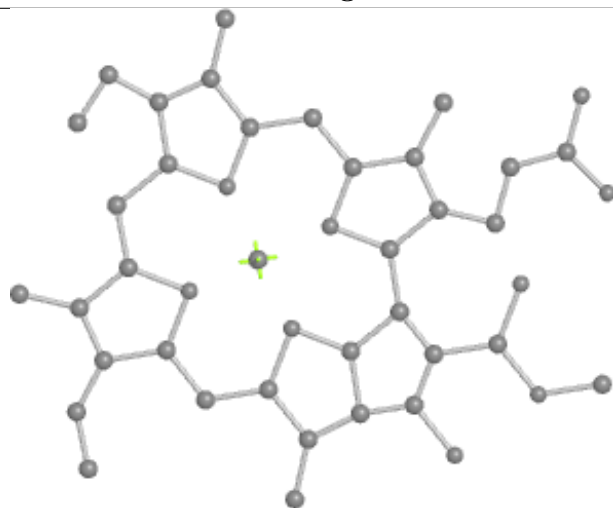
Bond lengths



Bond angles

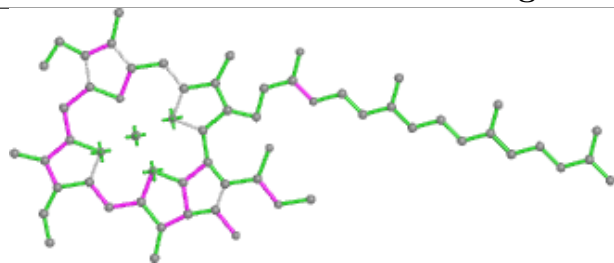


Torsions

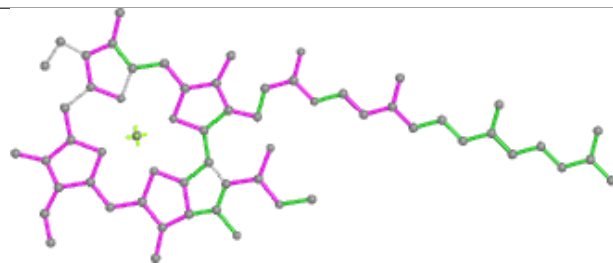


Rings

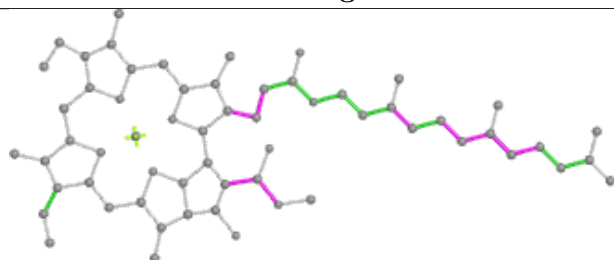
## Ligand CLA 1 610



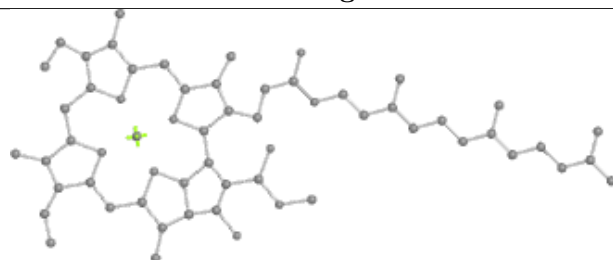
Bond lengths



Bond angles

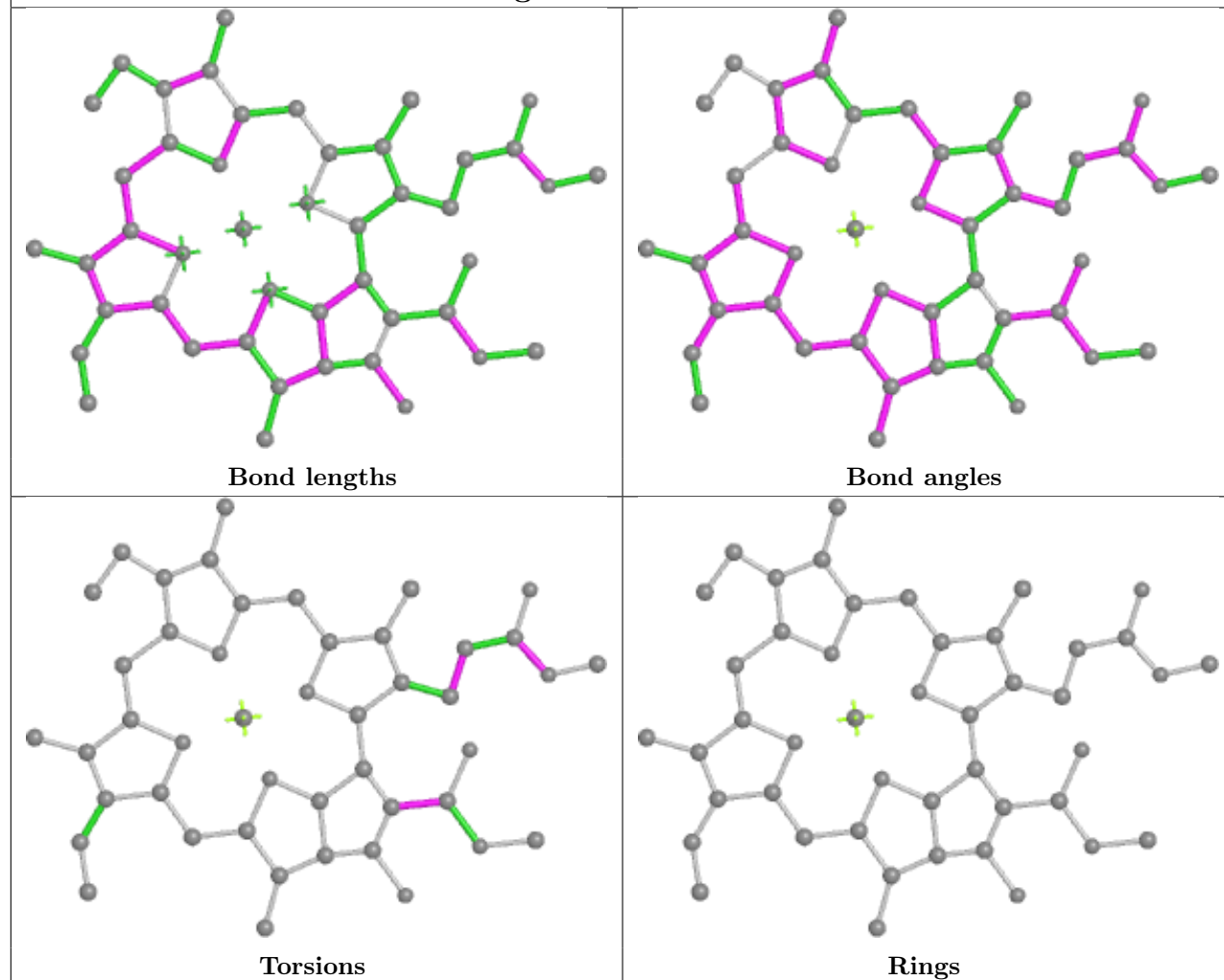


Torsions

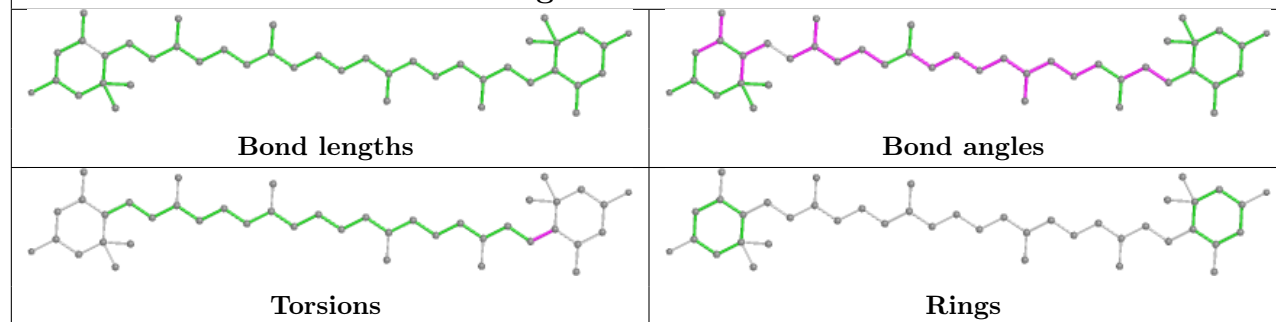


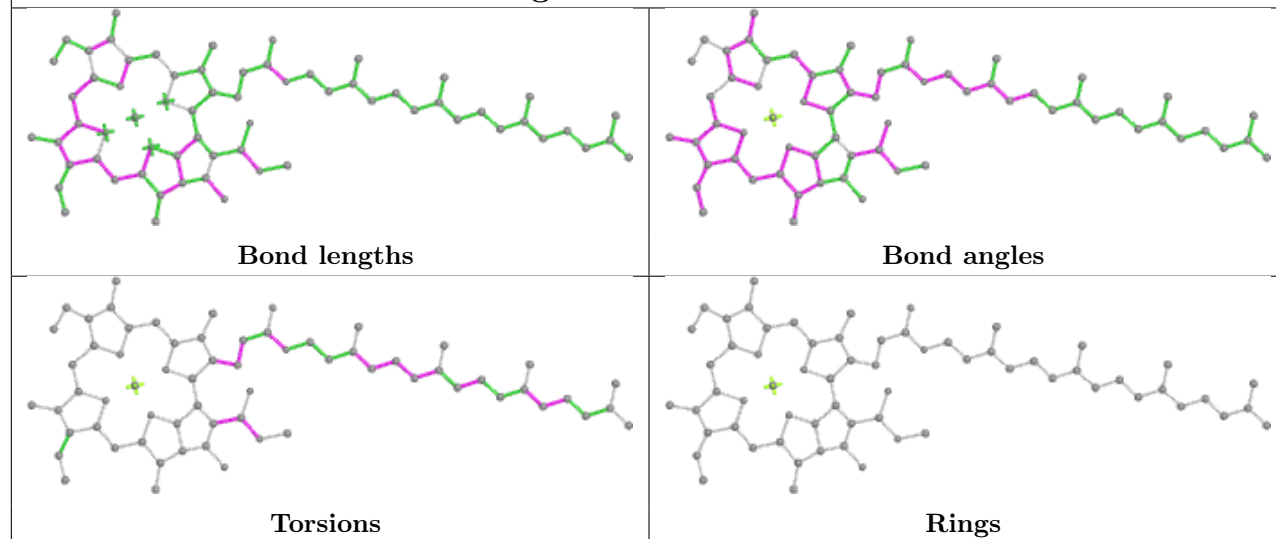
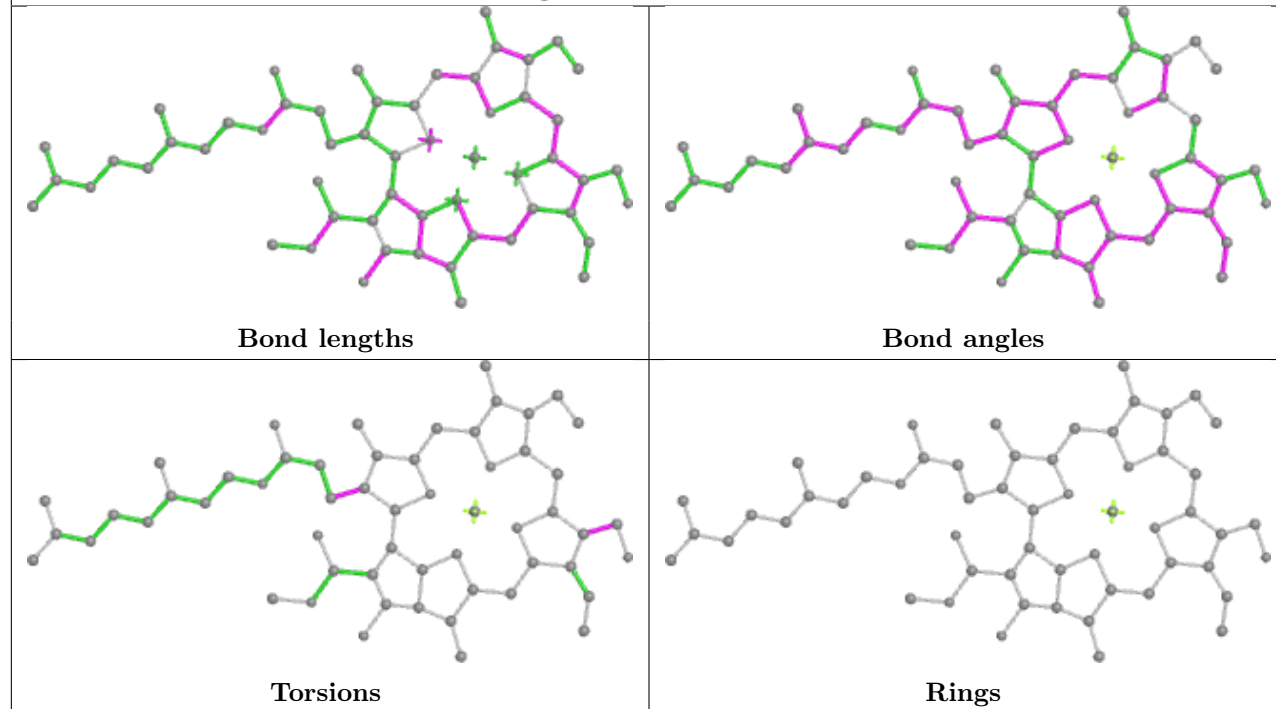
Rings

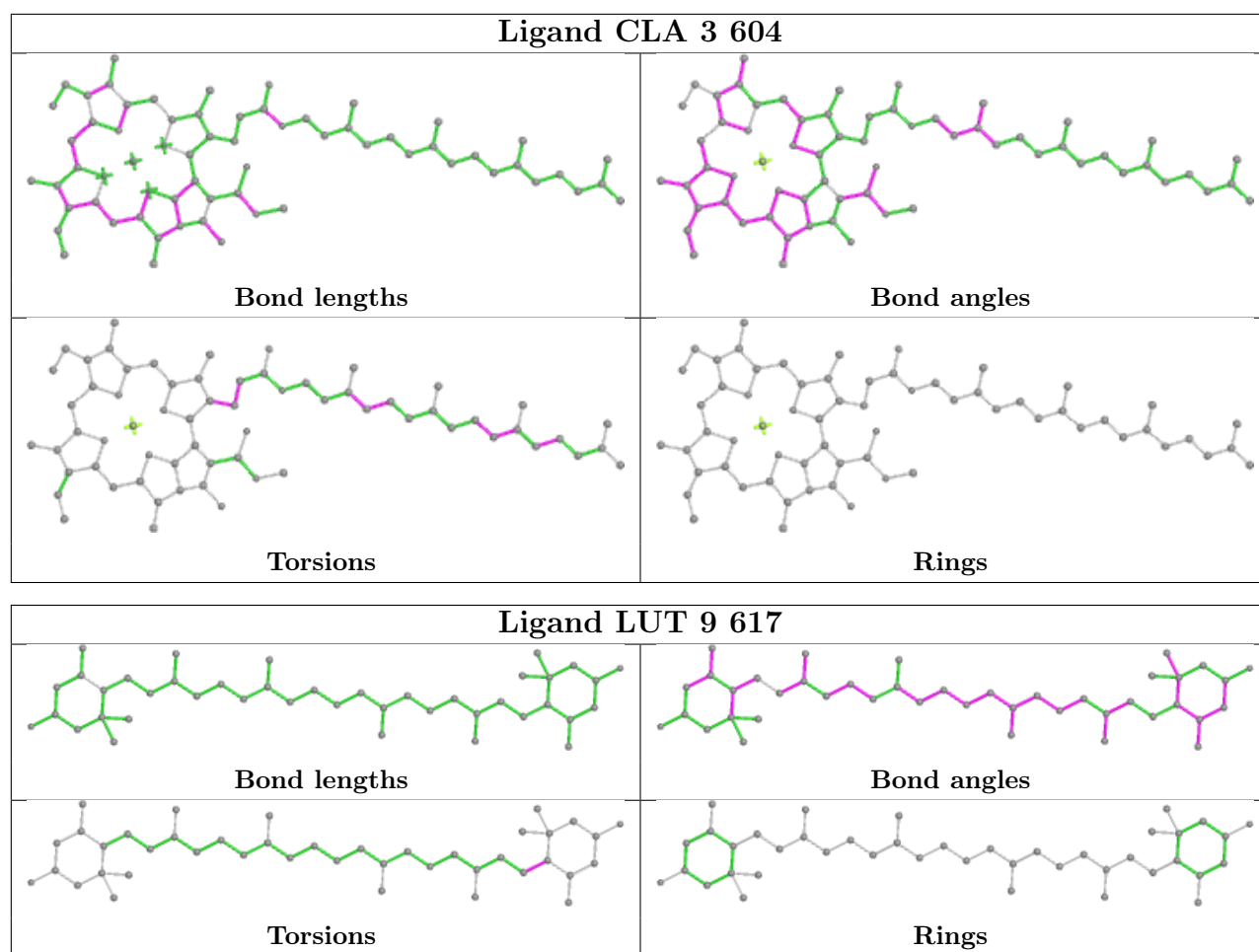
## Ligand CLA 5 617



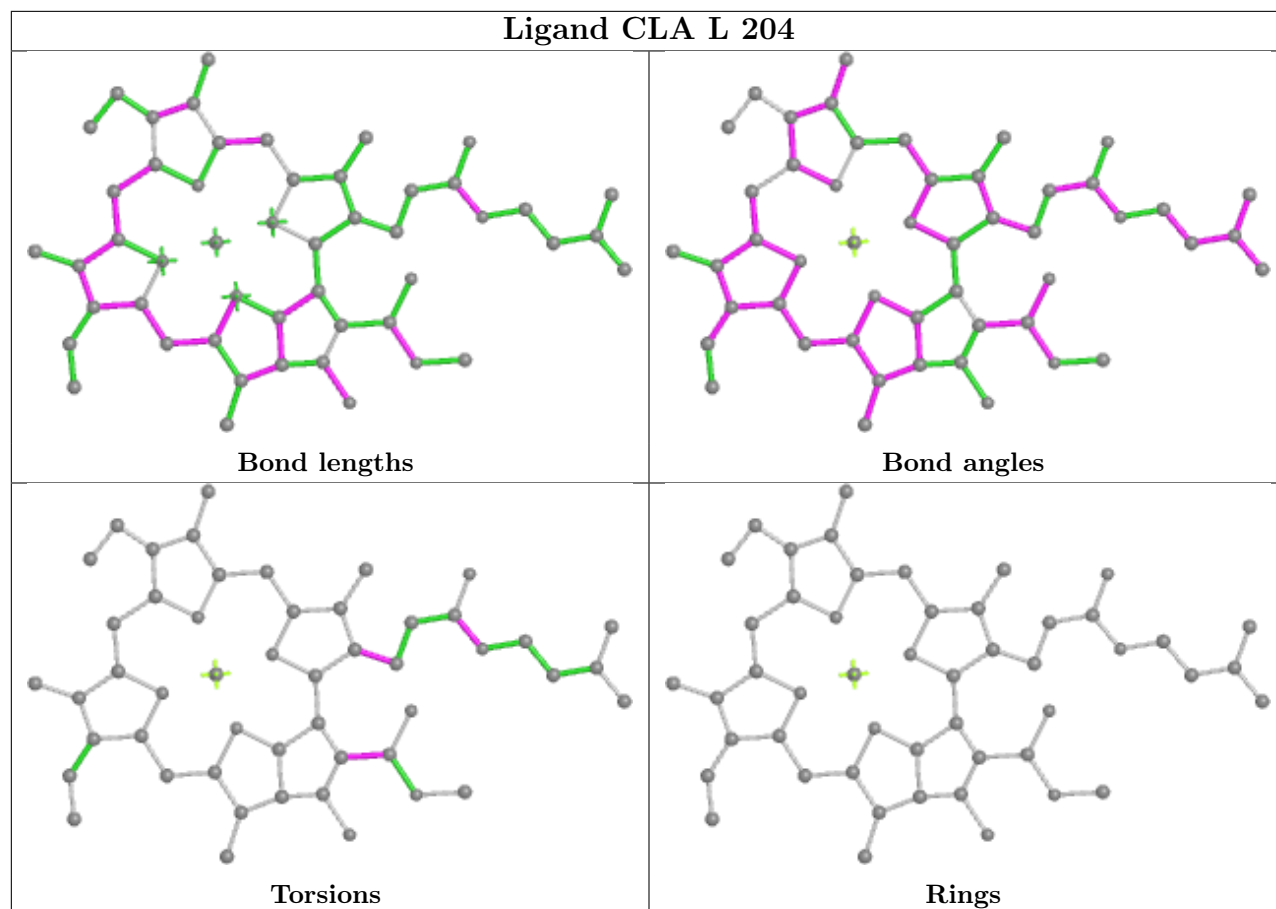
## Ligand LUT 4 619



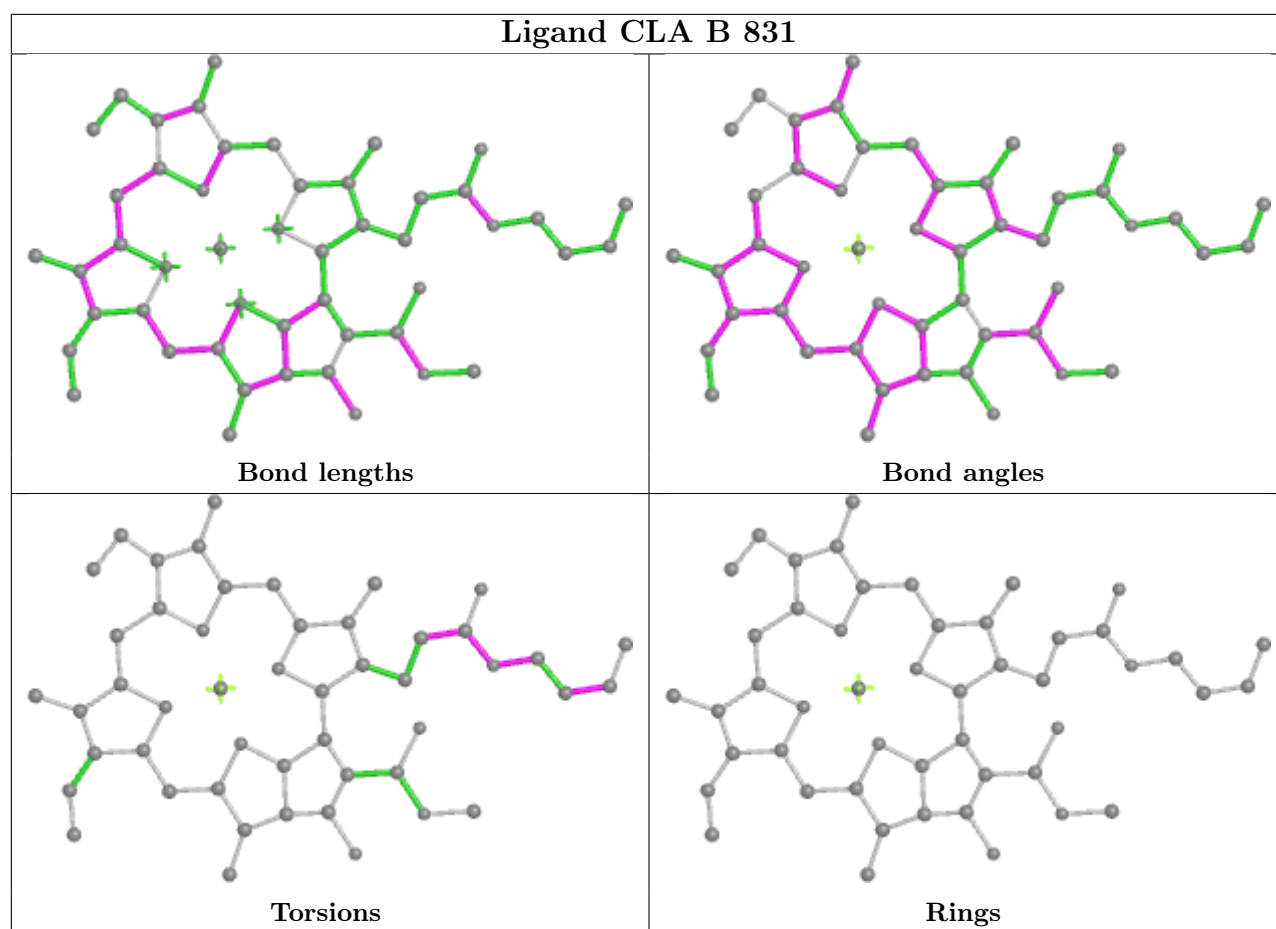
**Ligand CLA A 809****Ligand CHL 4 606**

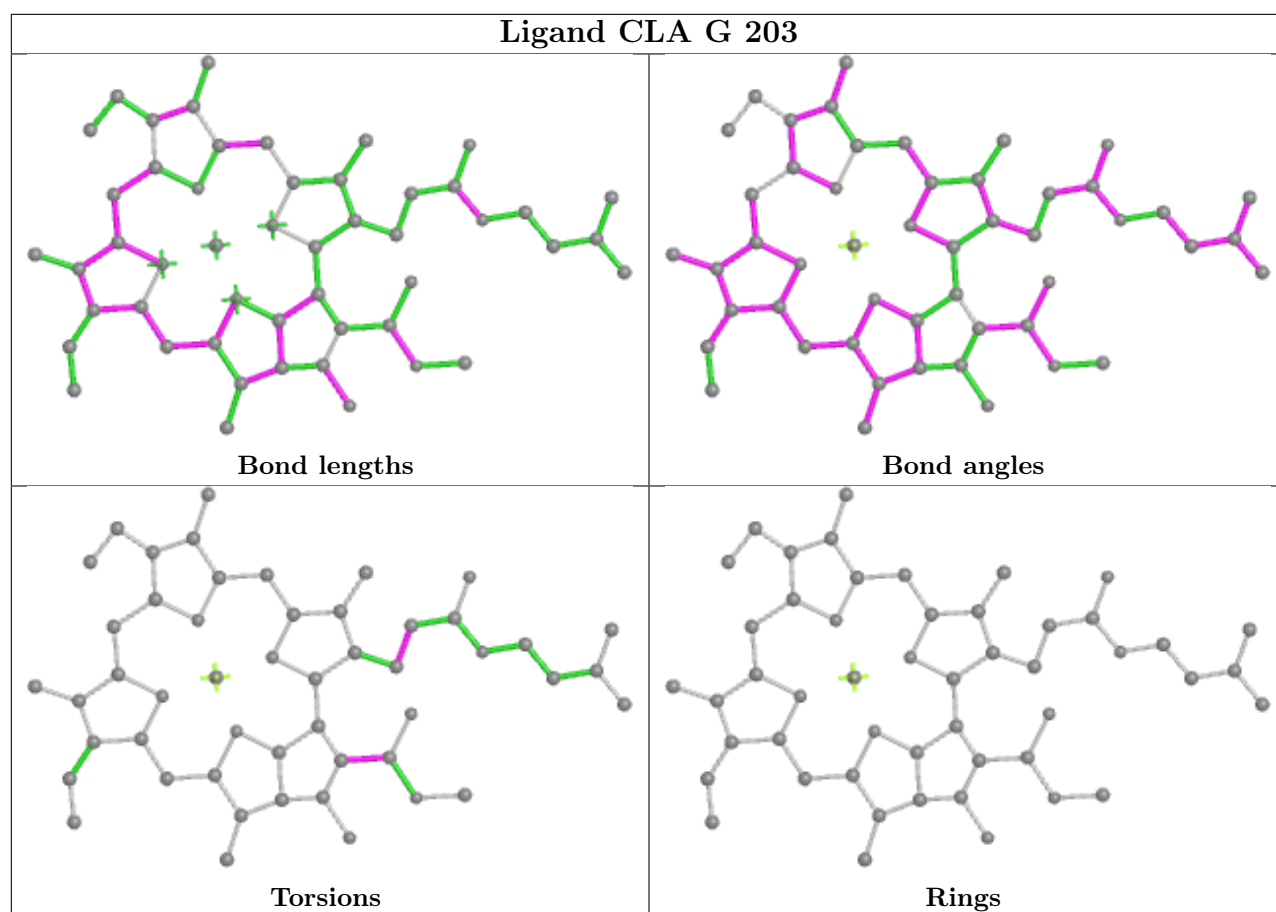


## Ligand CLA L 204

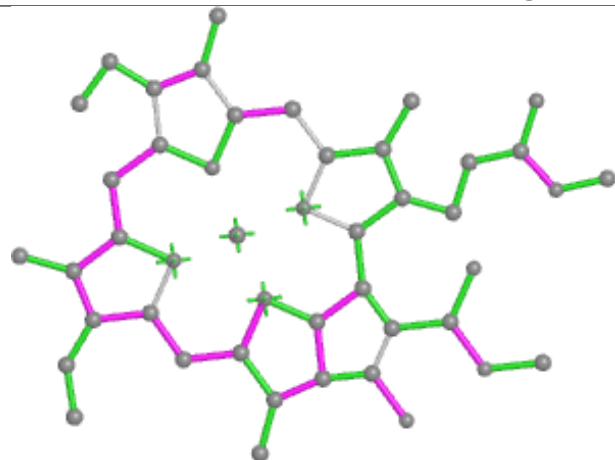




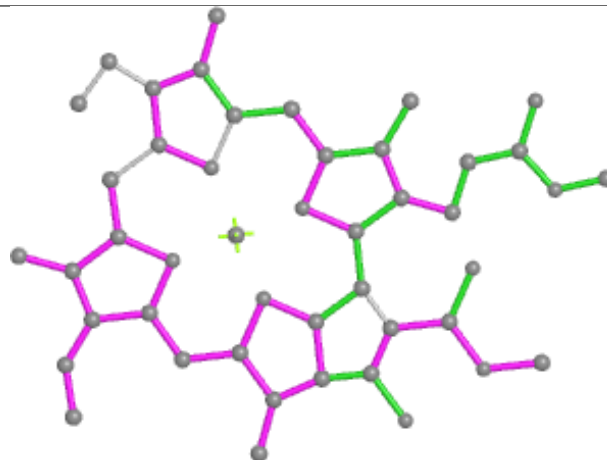




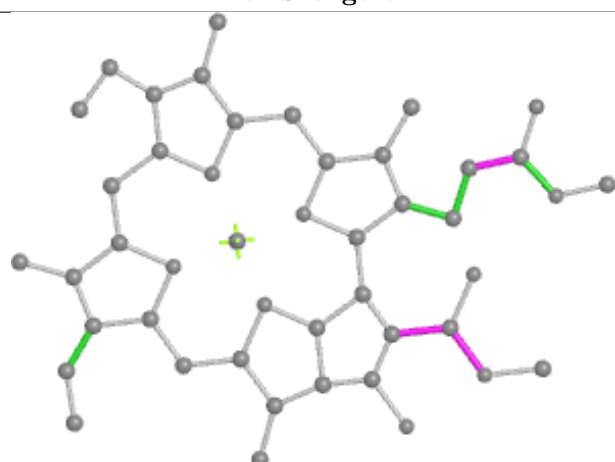
## Ligand CLA 2 601



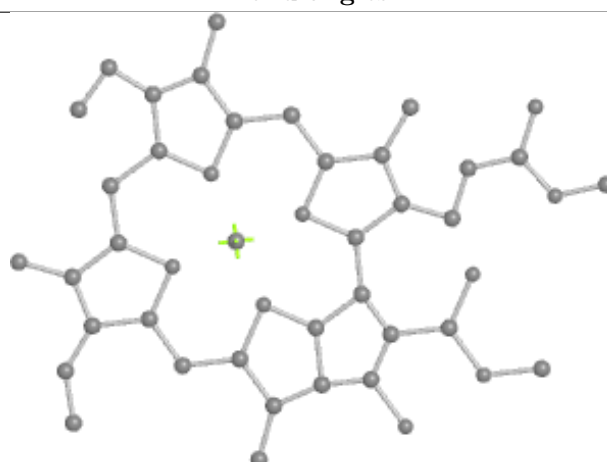
Bond lengths



Bond angles

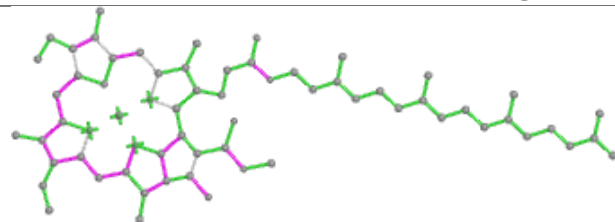


Torsions

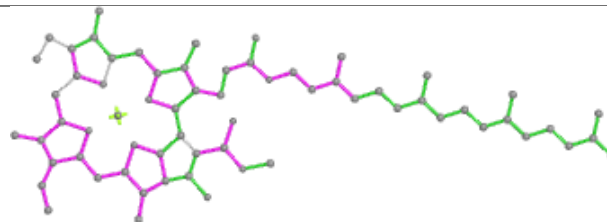


Rings

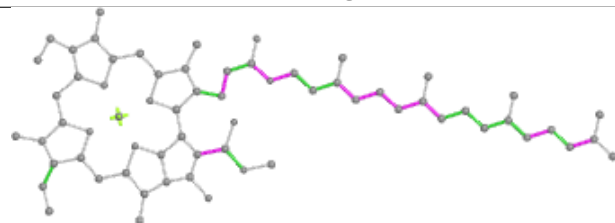
## Ligand CLA A 842



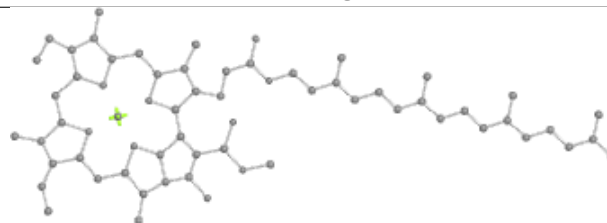
Bond lengths



Bond angles

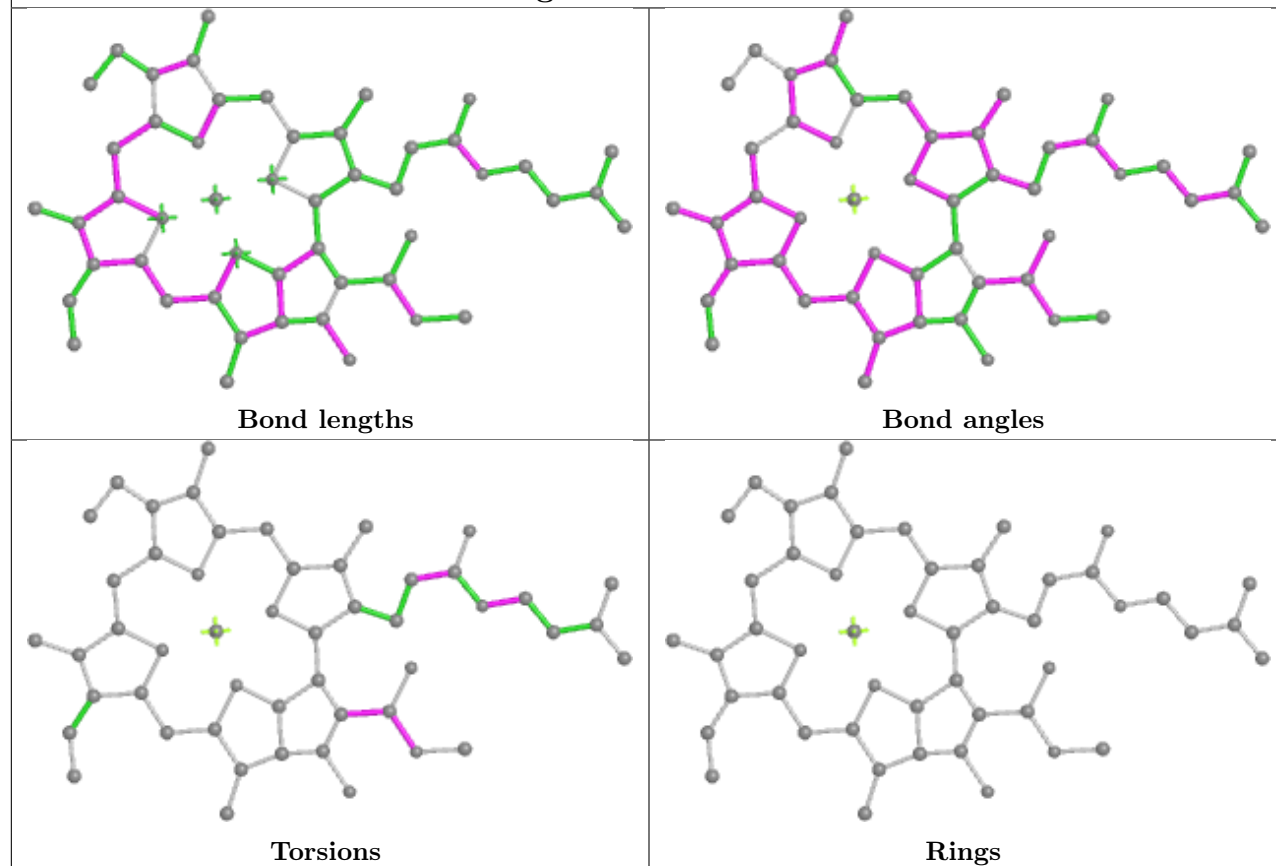


Torsions

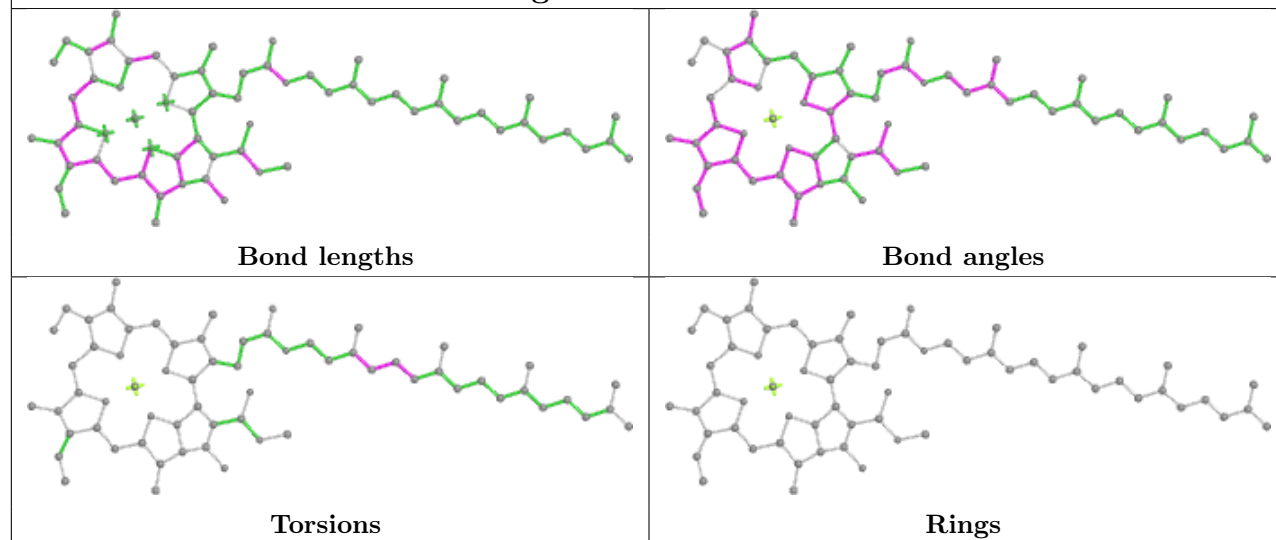


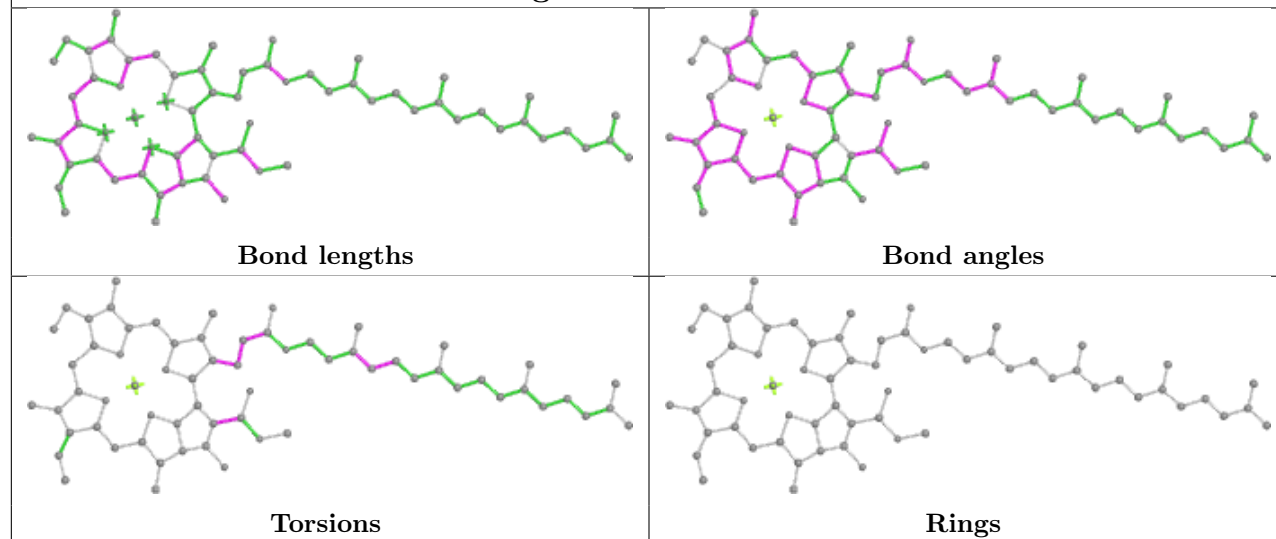
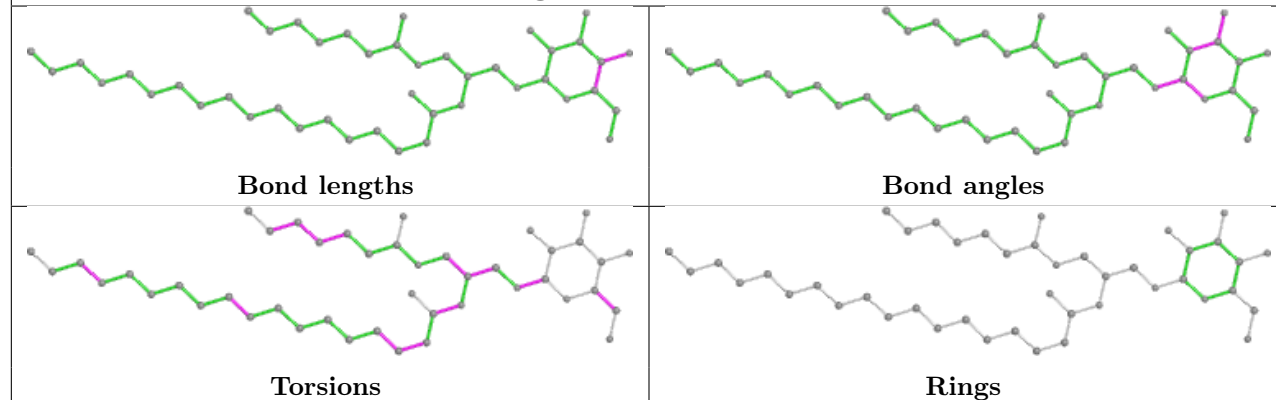
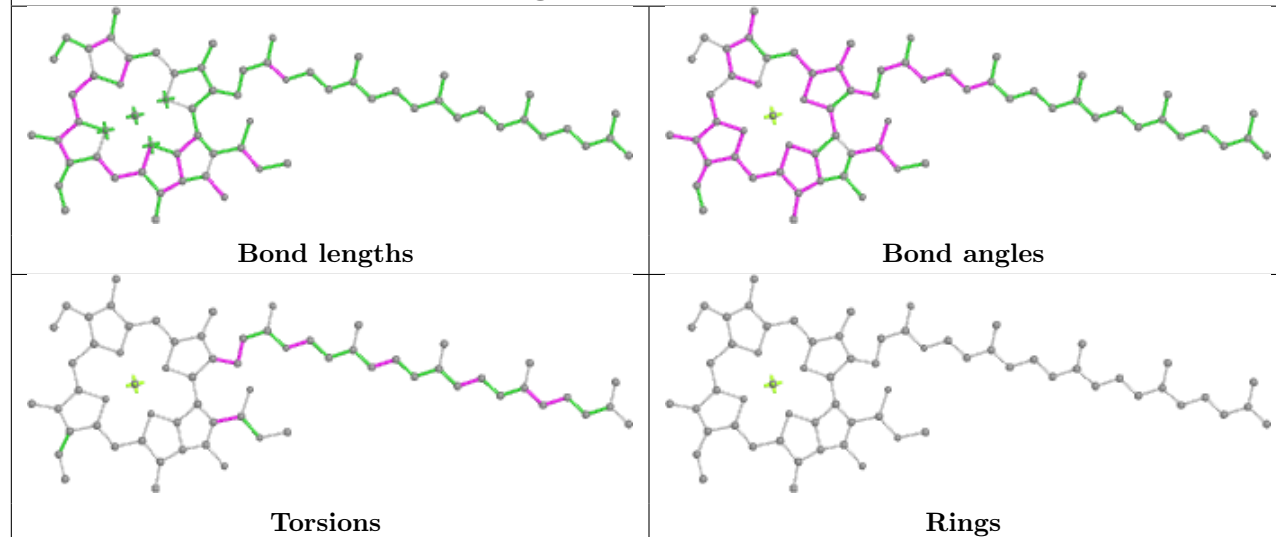
Rings

## Ligand CLA 3 609

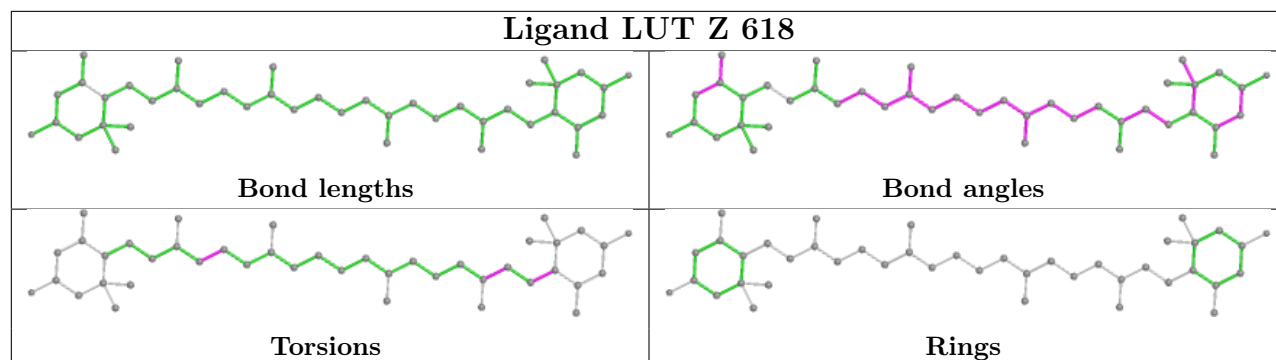


## Ligand CLA A 835

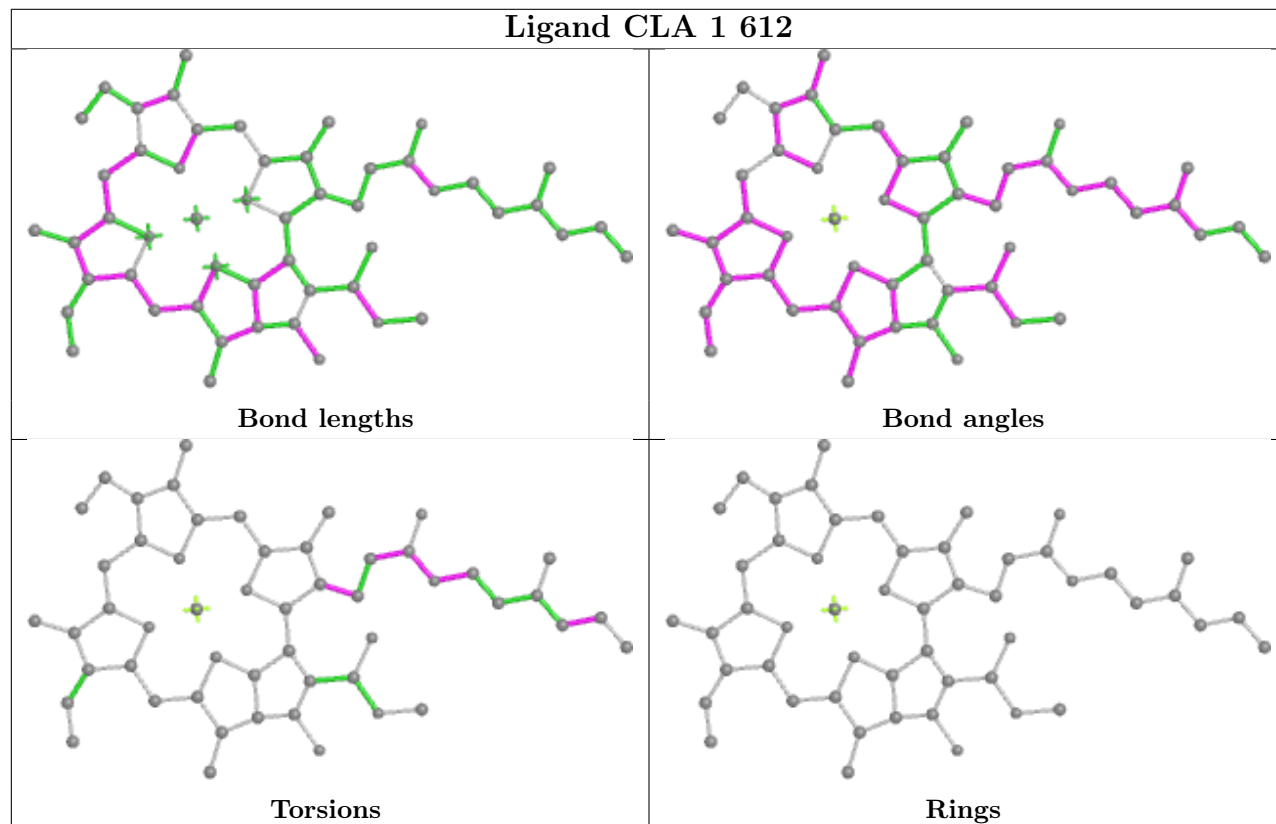


**Ligand CLA B 824****Ligand LMG 9 620****Ligand CLA A 854**

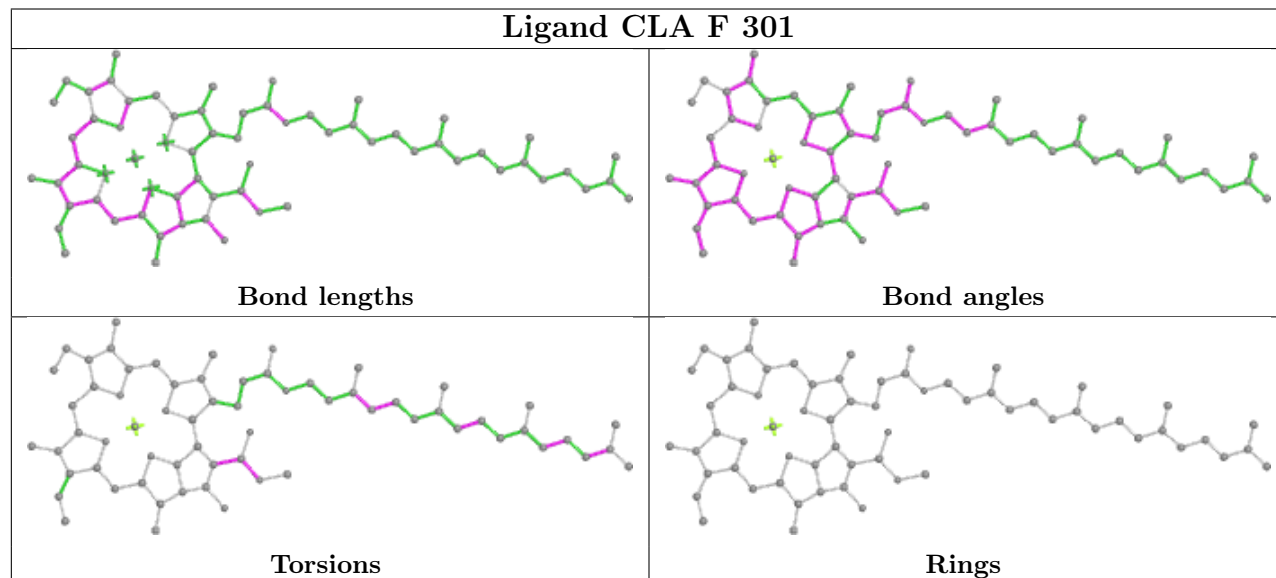
## Ligand LUT Z 618



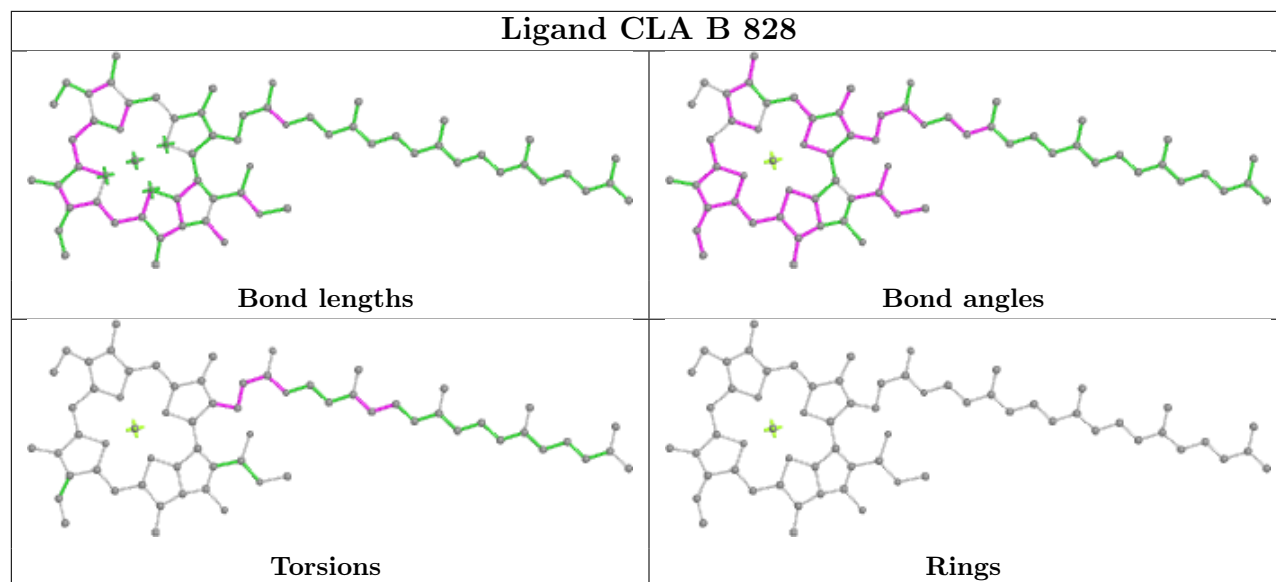
## Ligand CLA 1 612



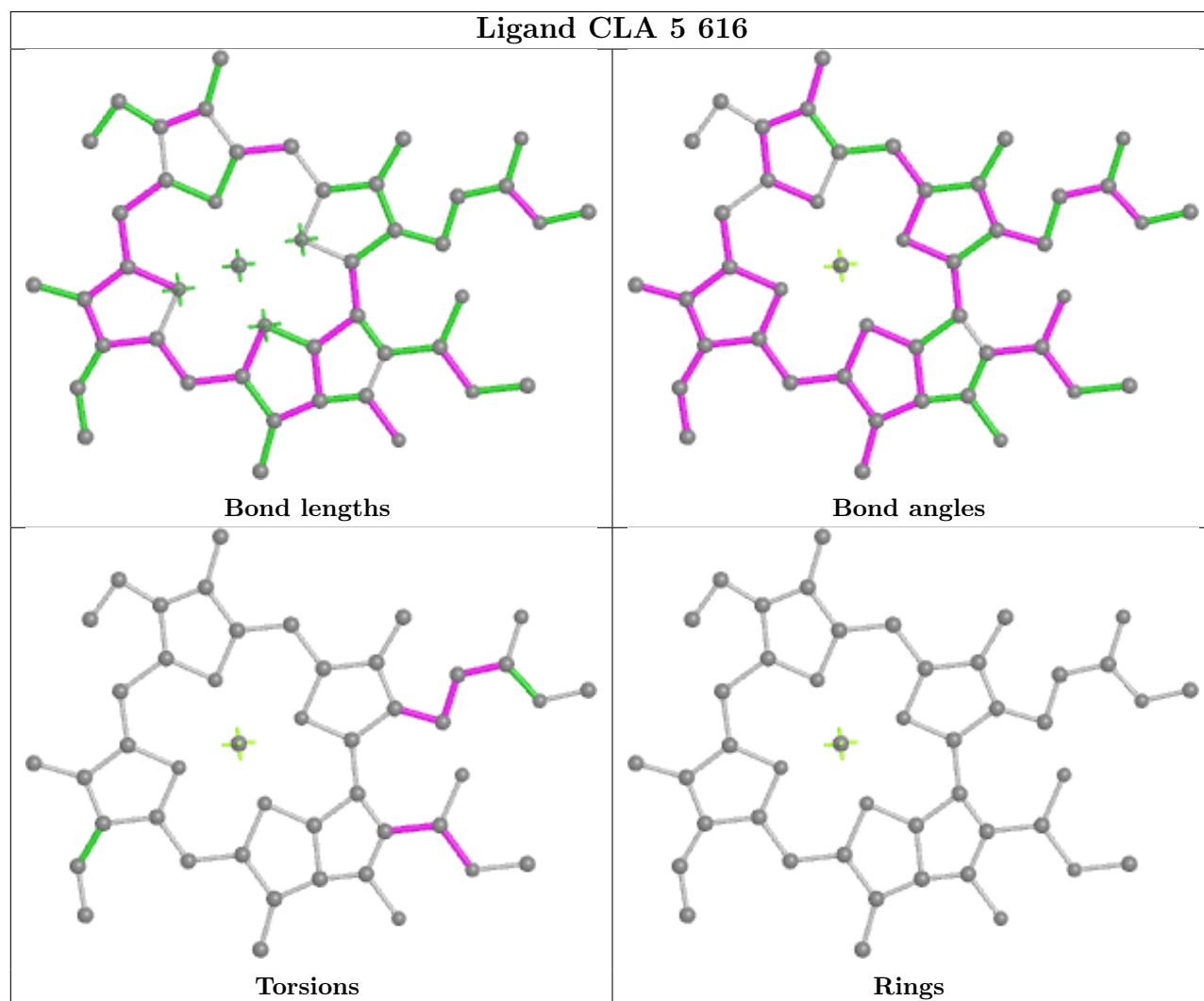
## Ligand CLA F 301

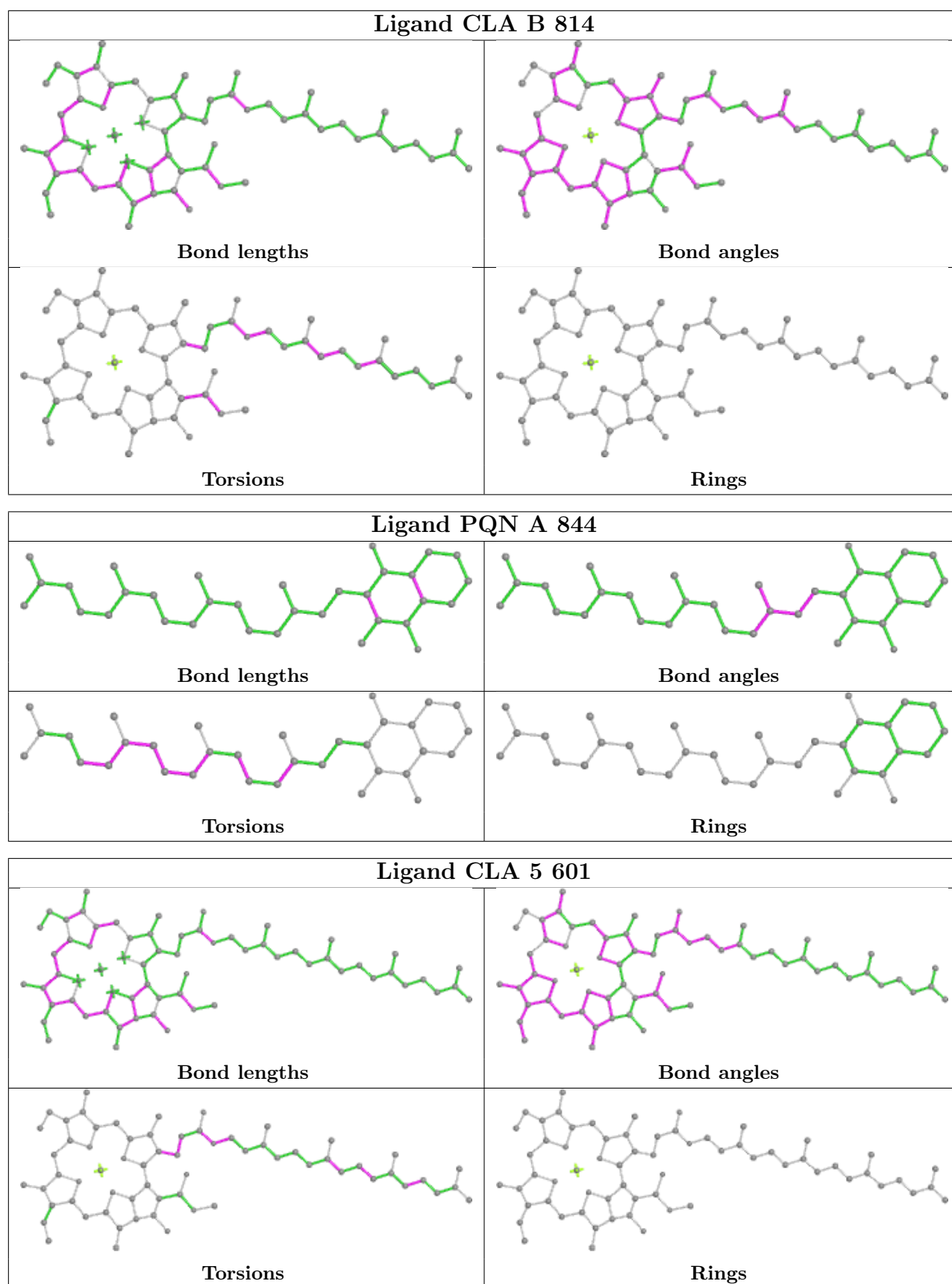


## Ligand CLA B 828



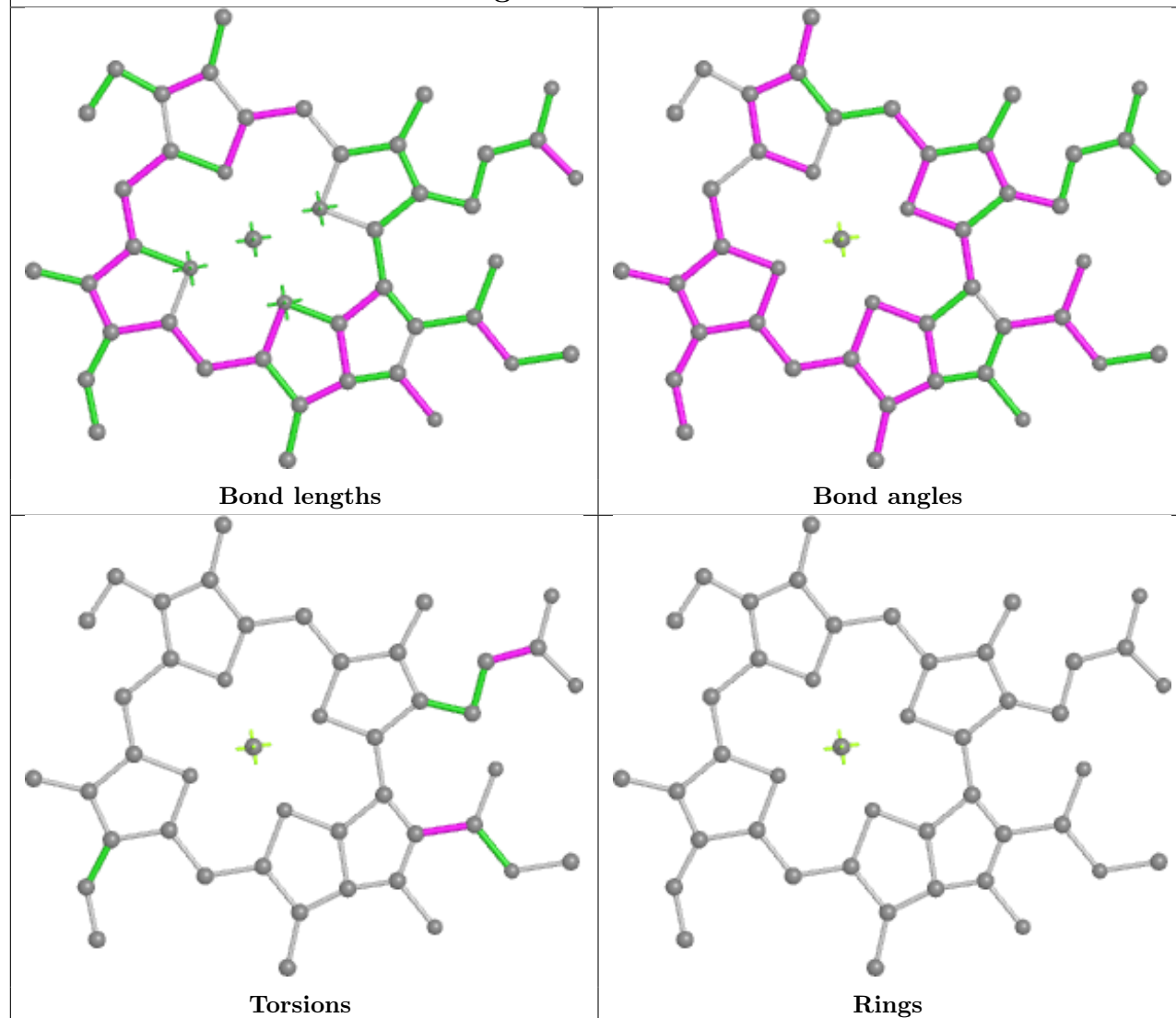
## Ligand CLA 5 616



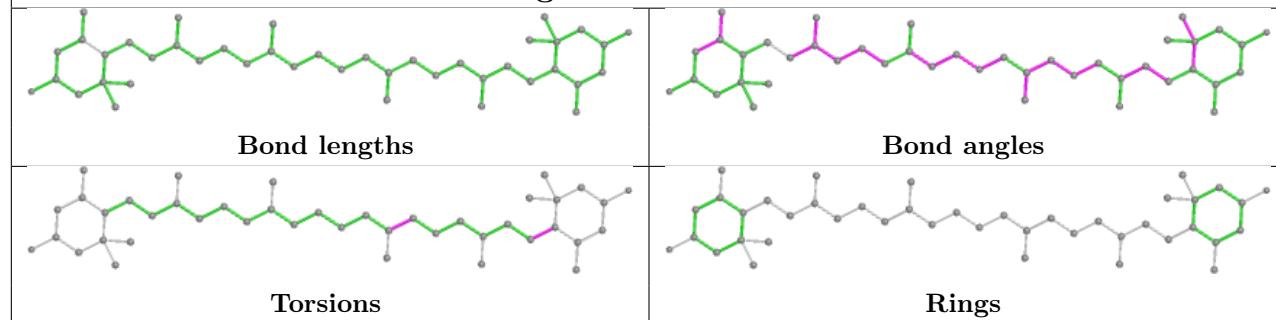




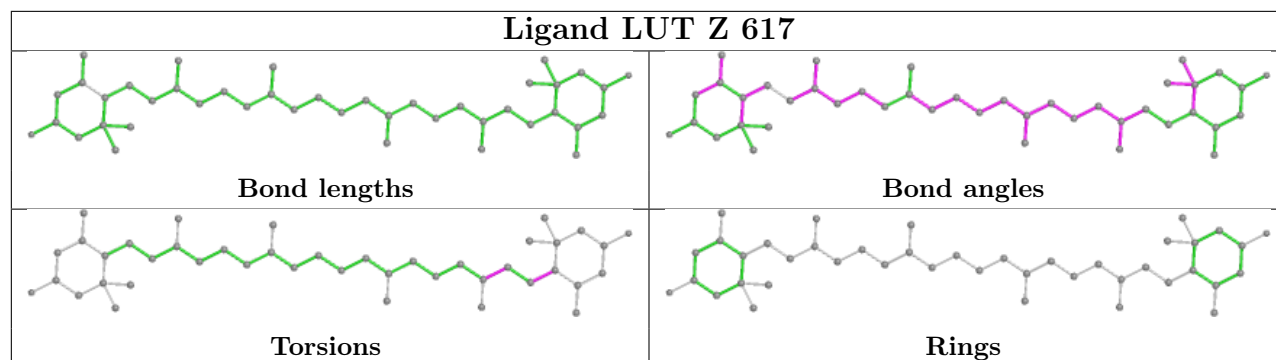
## Ligand CLA 6 622



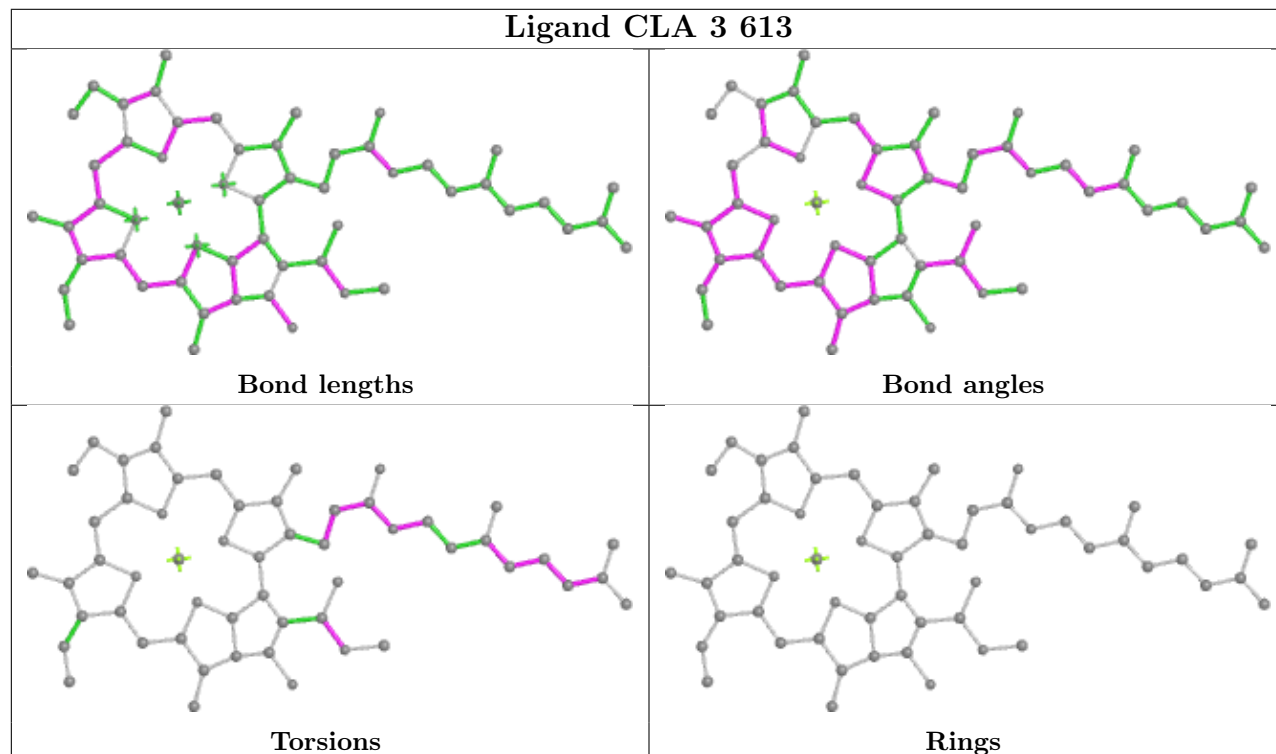
## Ligand LUT 7 621



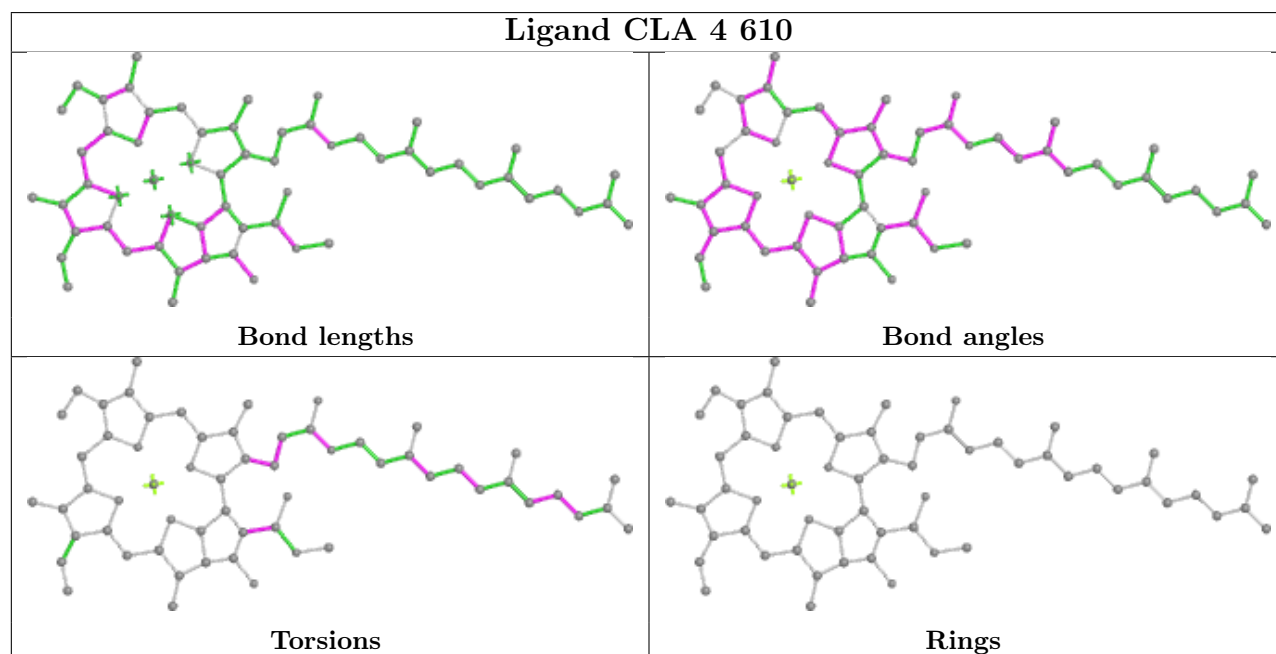
## Ligand LUT Z 617



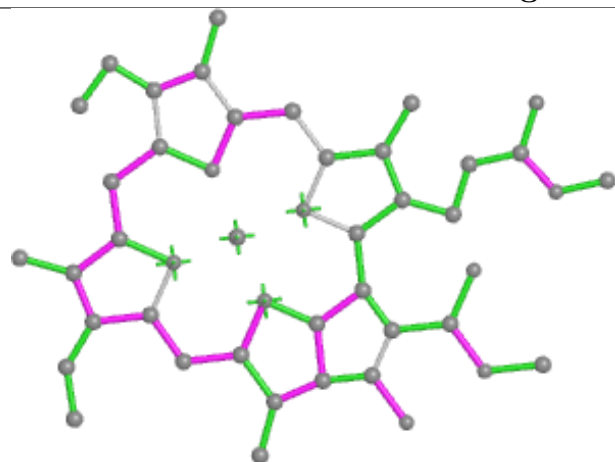
## Ligand CLA 3 613



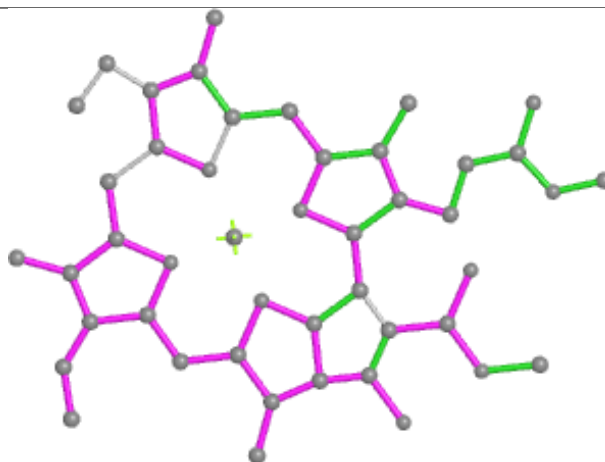
## Ligand CLA 4 610



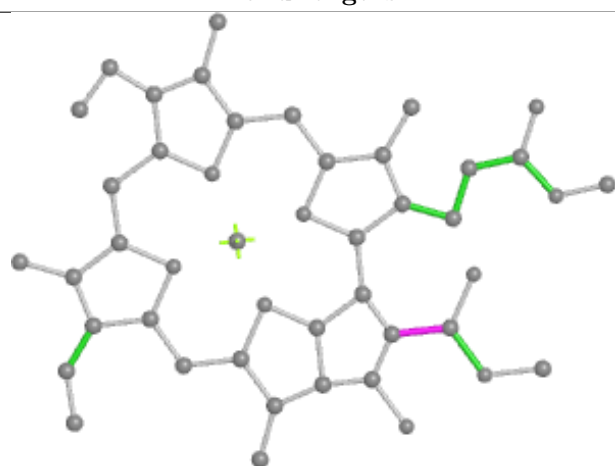
## Ligand CLA 5 603



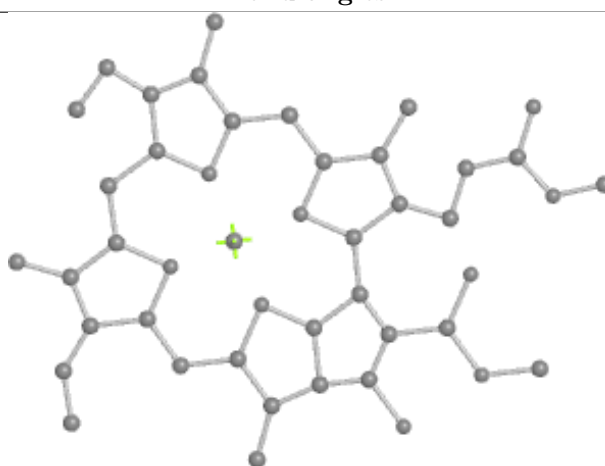
Bond lengths



Bond angles

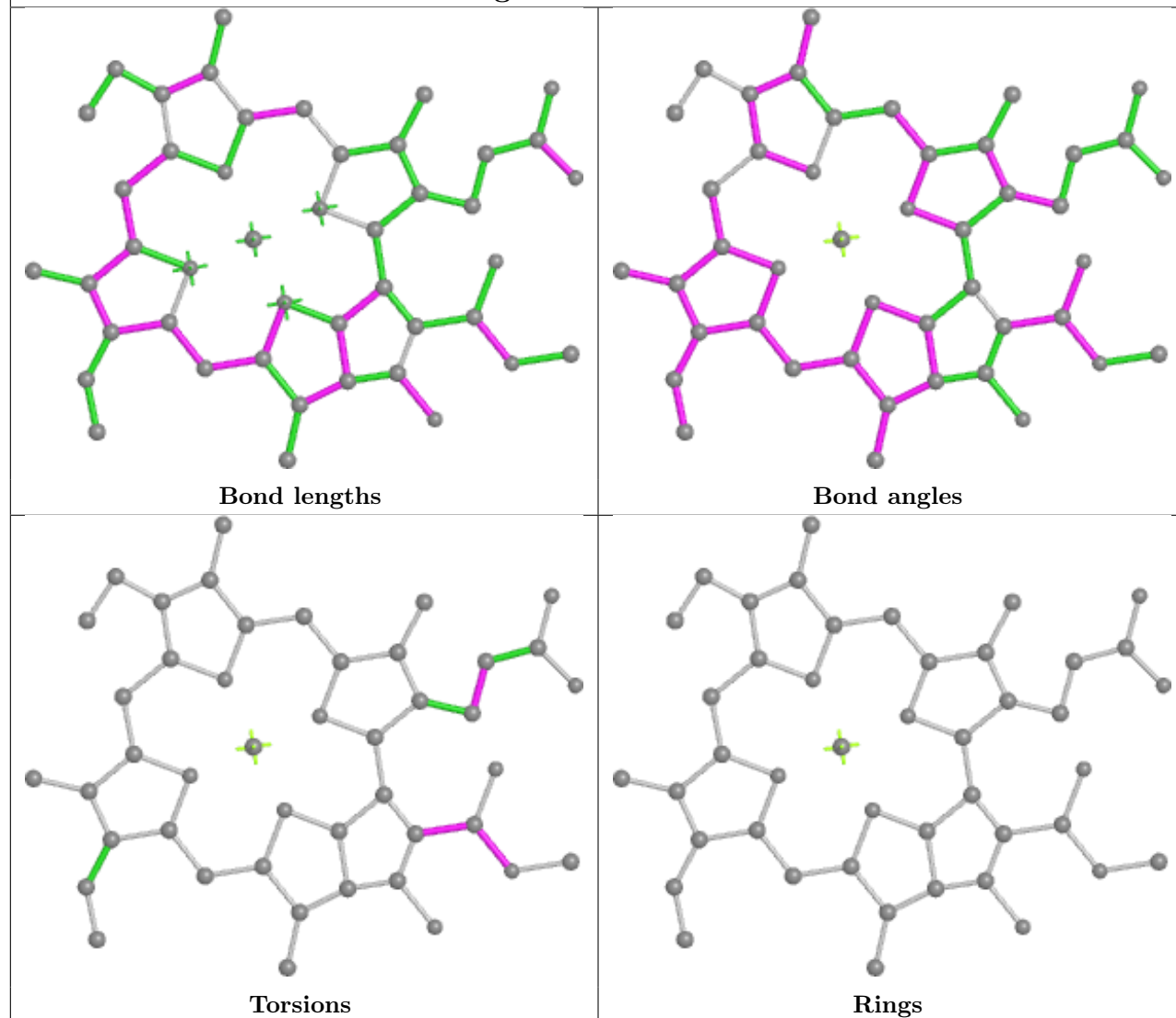


Torsions

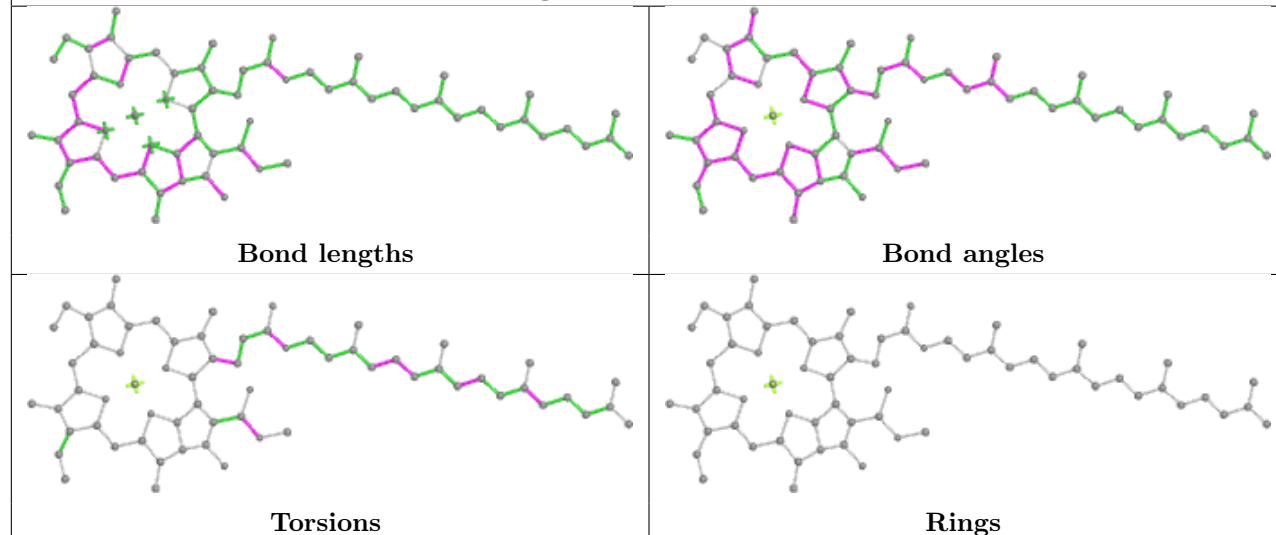


Rings

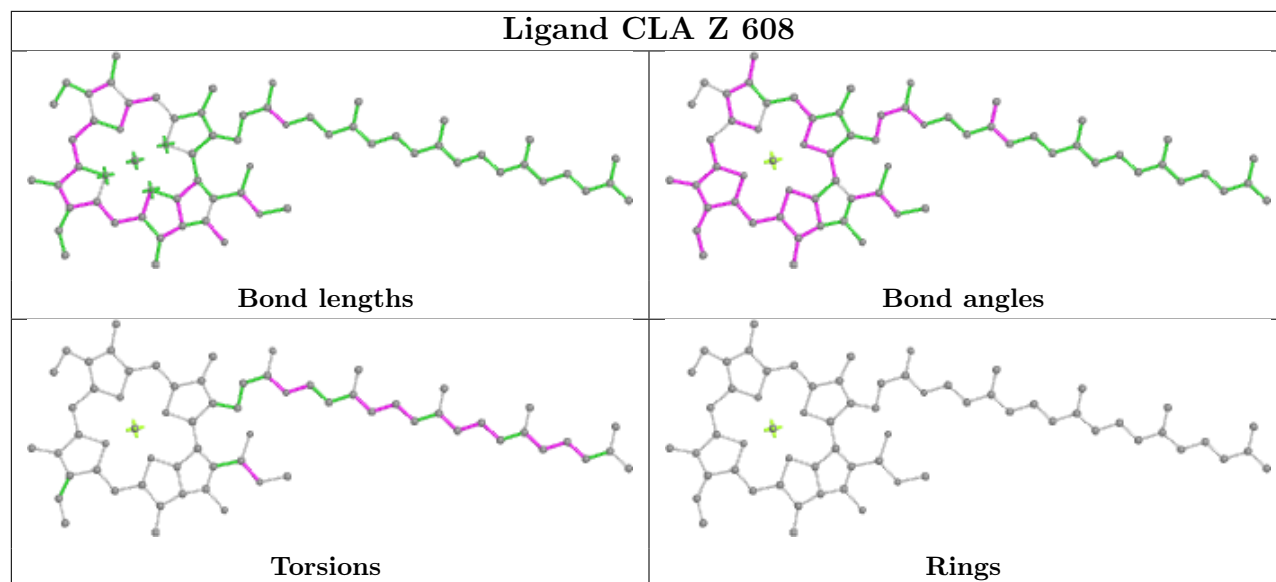
## Ligand CLA 2 602



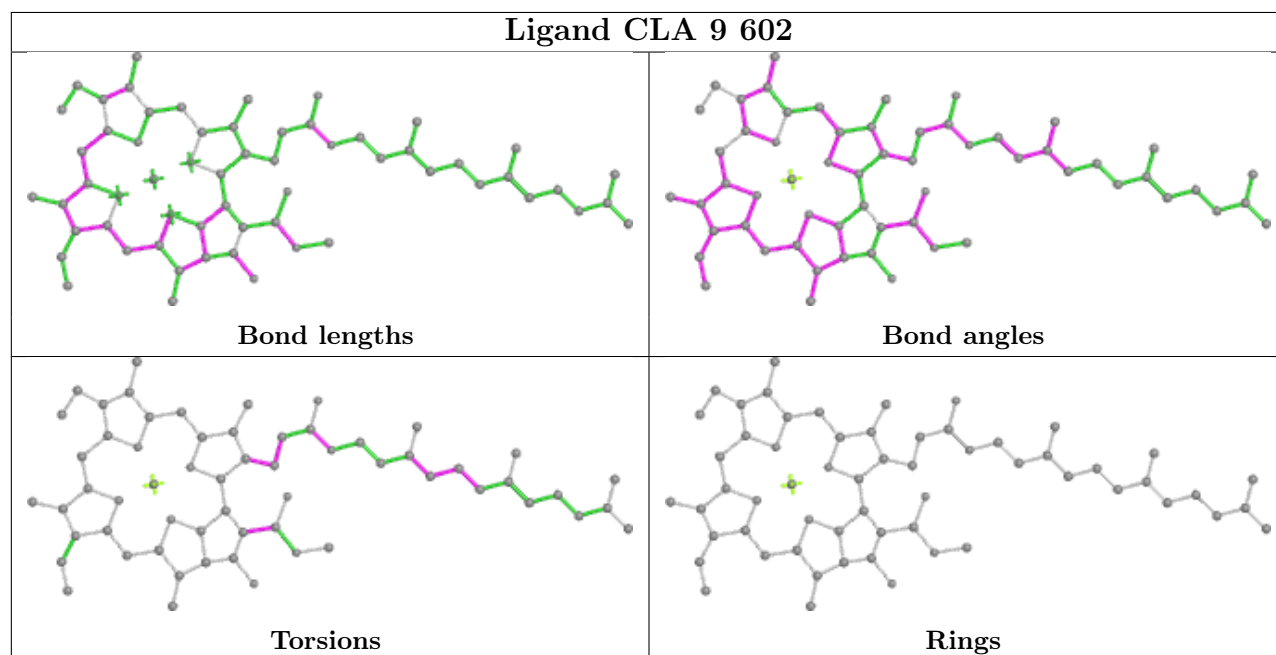
## Ligand CLA 1 611



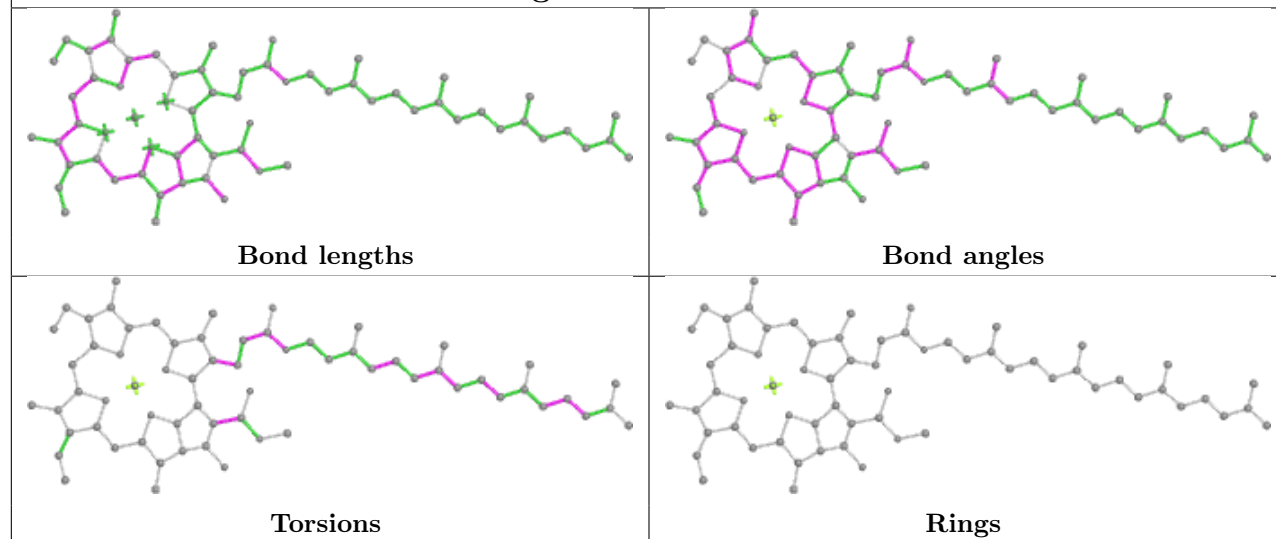
## Ligand CLA Z 608



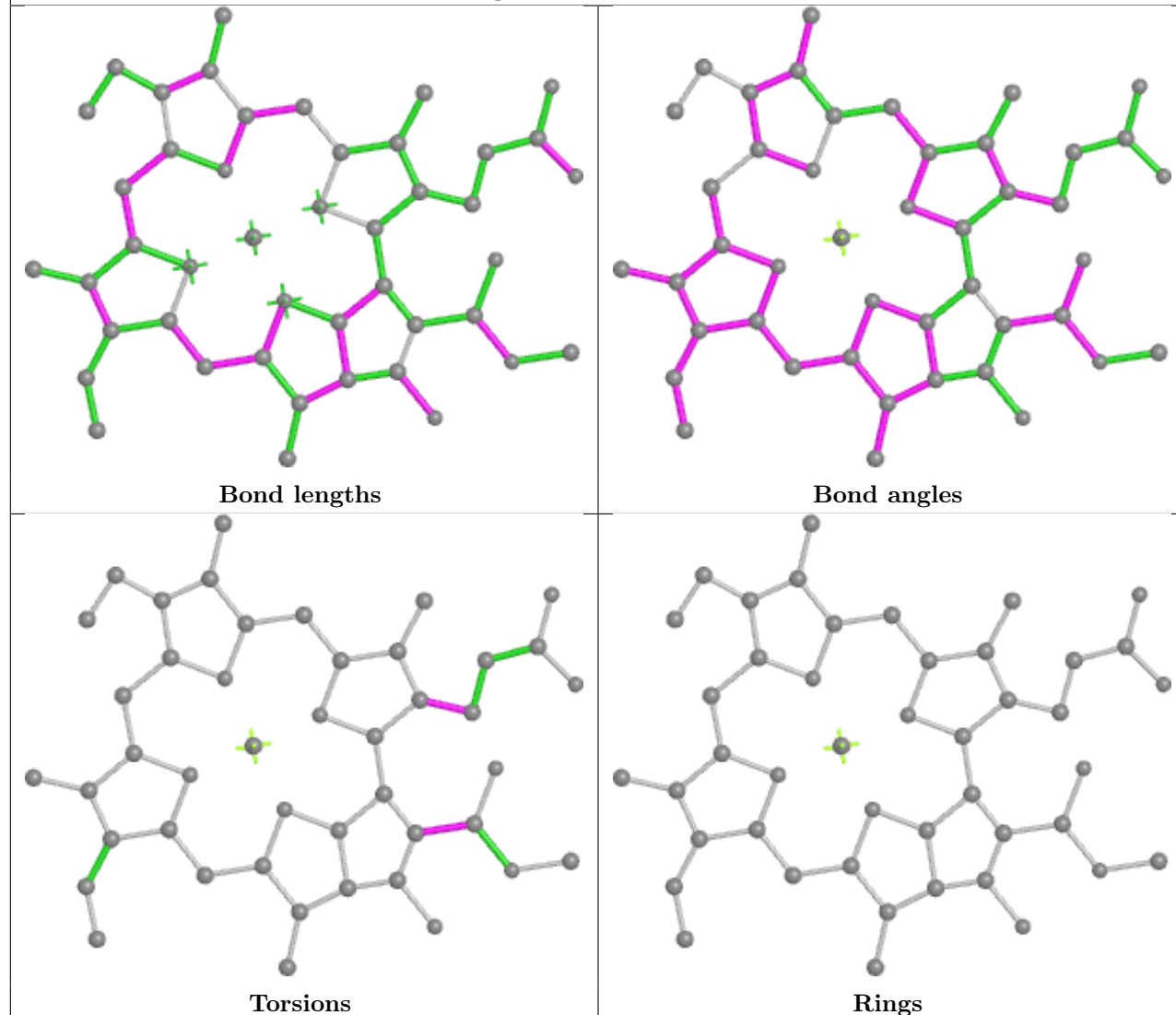
## Ligand CLA 9 602

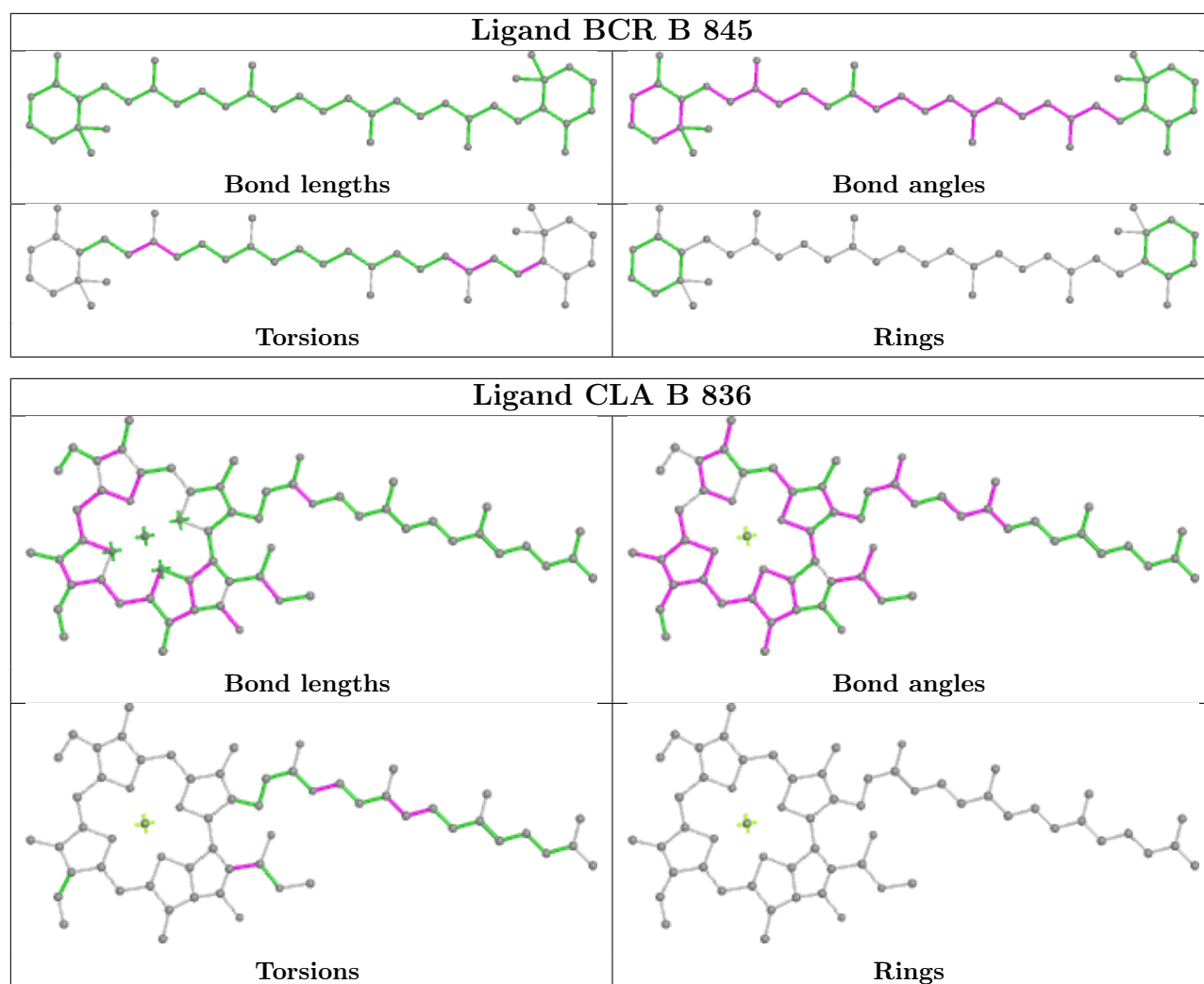


## Ligand CLA B 805

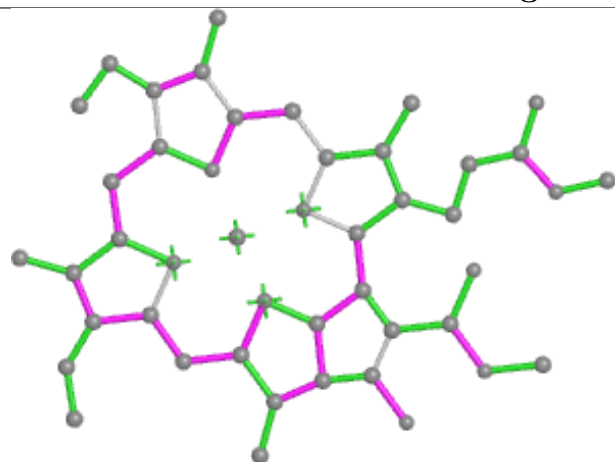


## Ligand CLA A 821

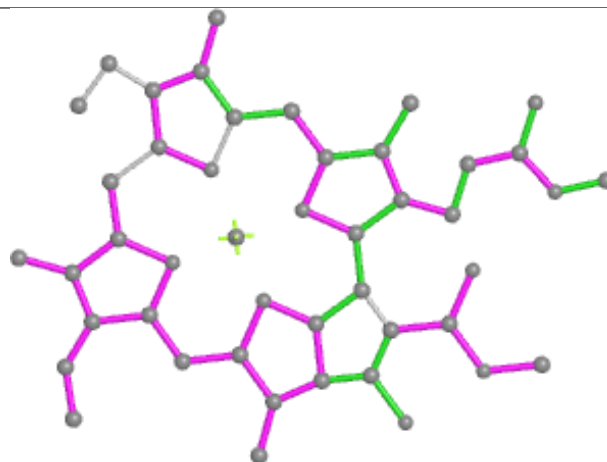




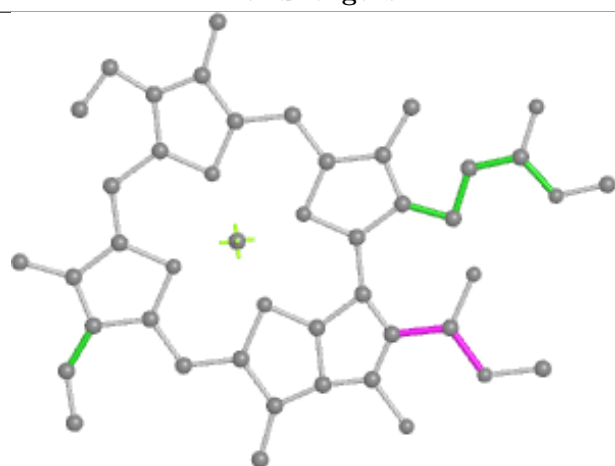
## Ligand CLA 8 611



Bond lengths



Bond angles

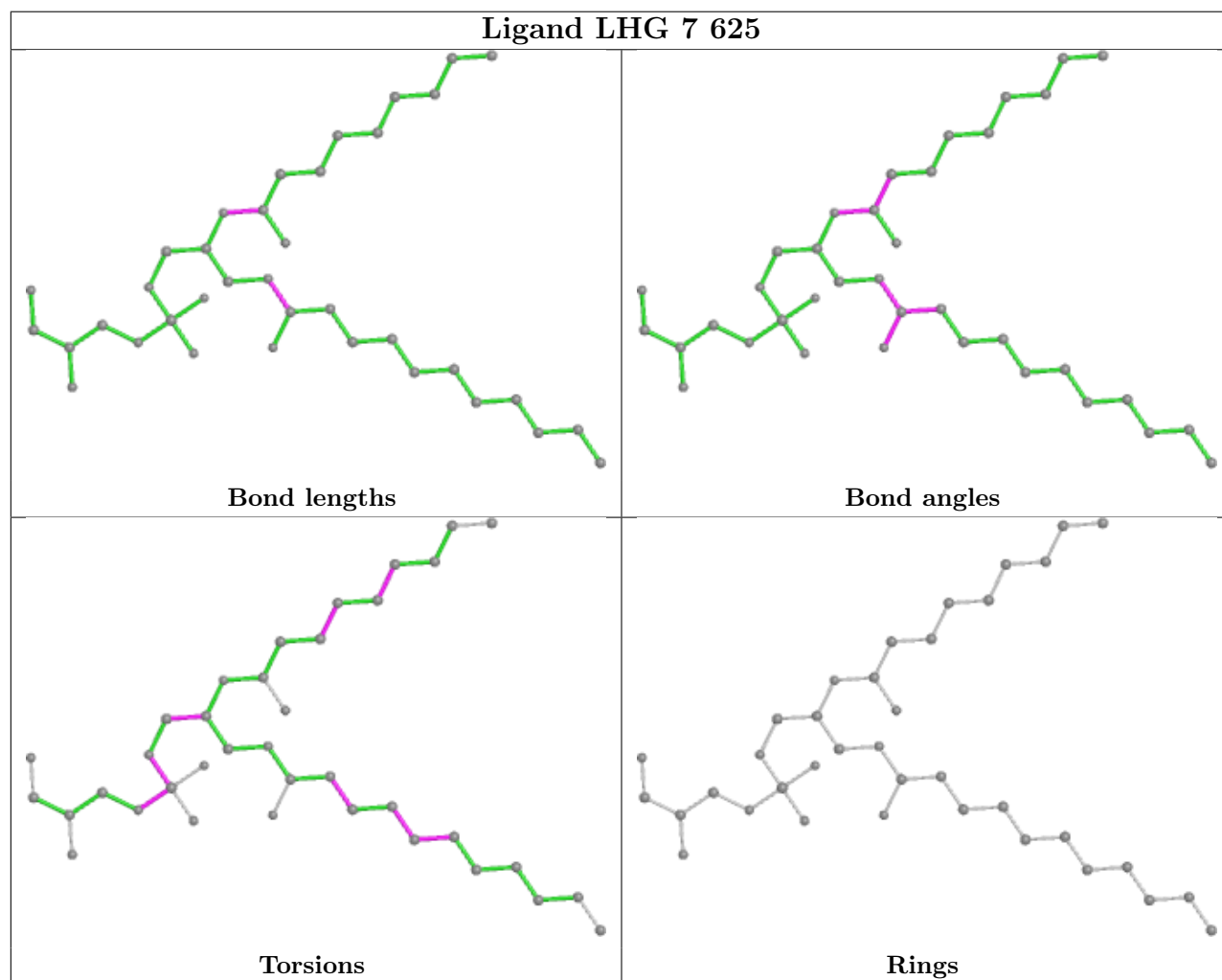
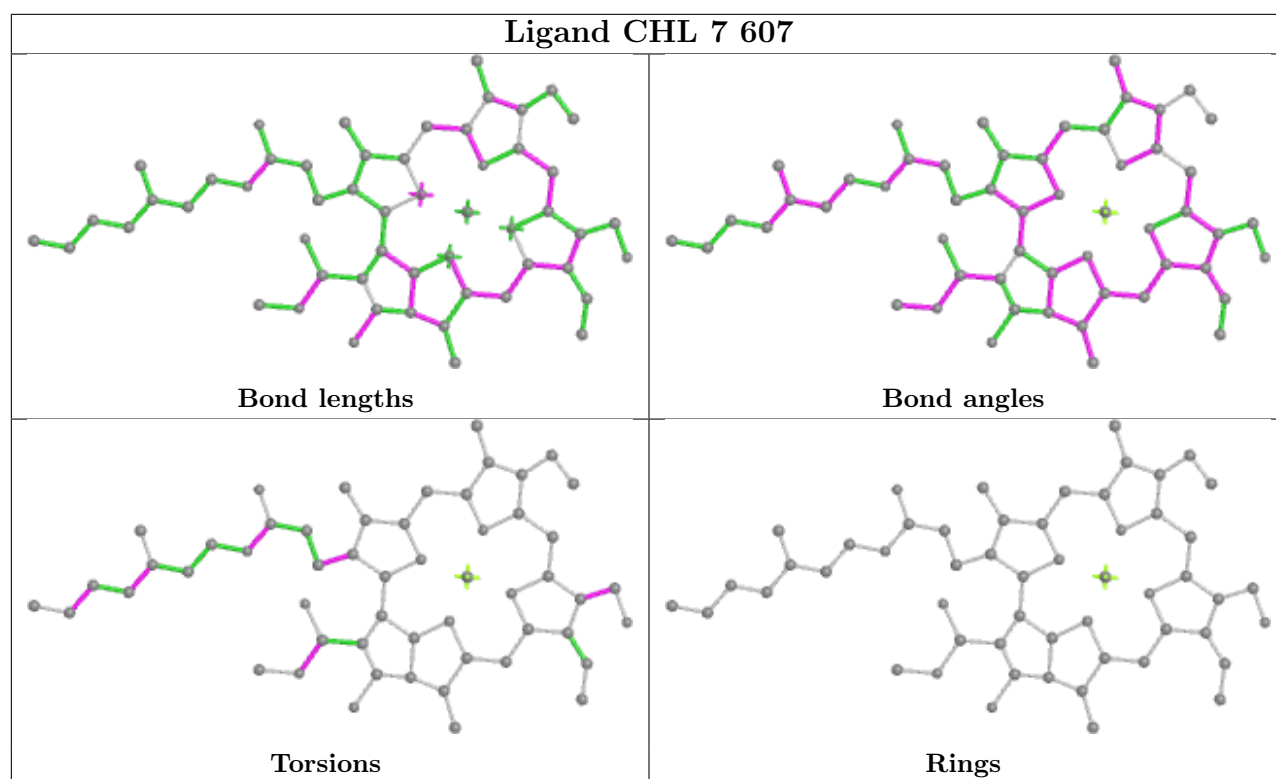


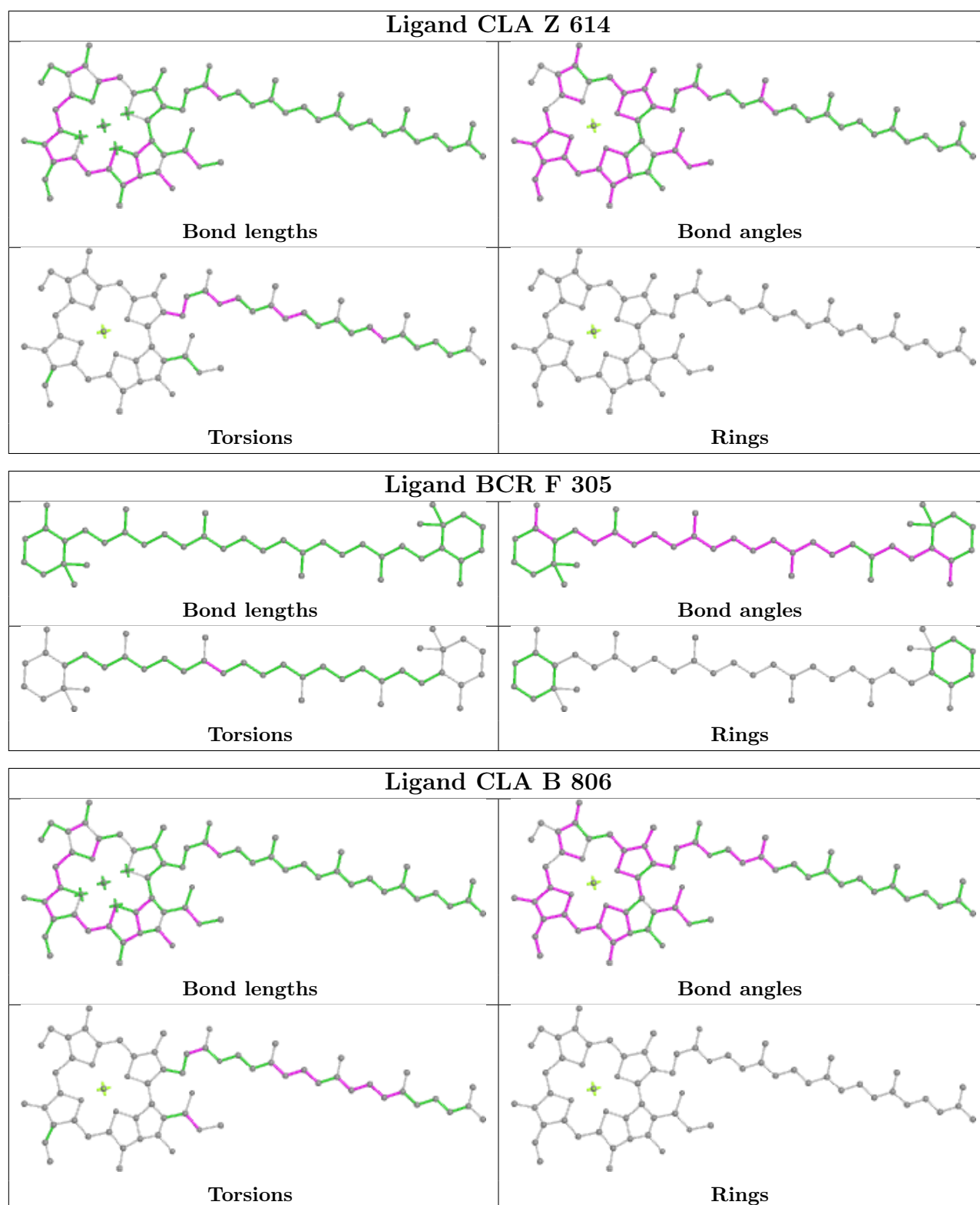
Torsions

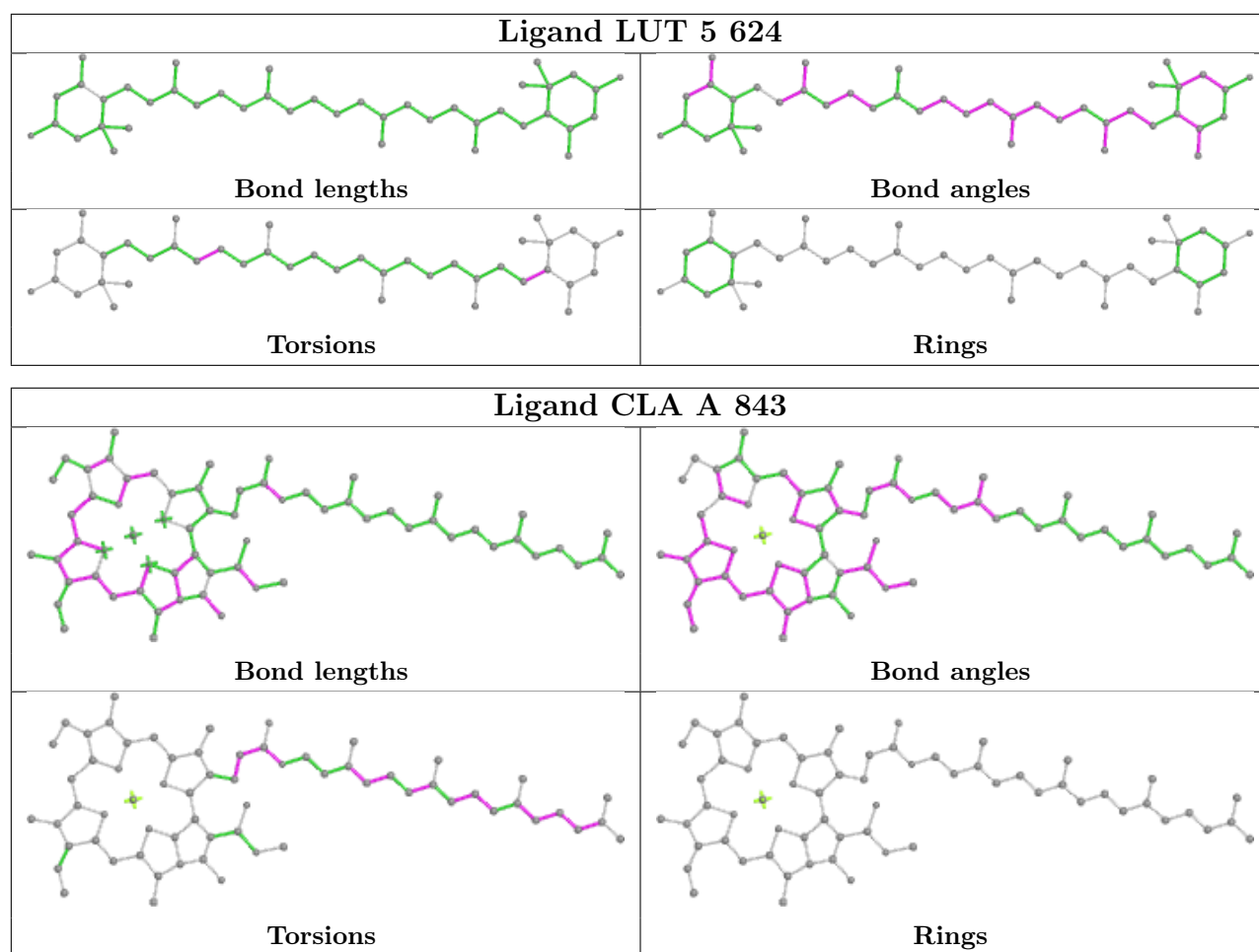


Rings

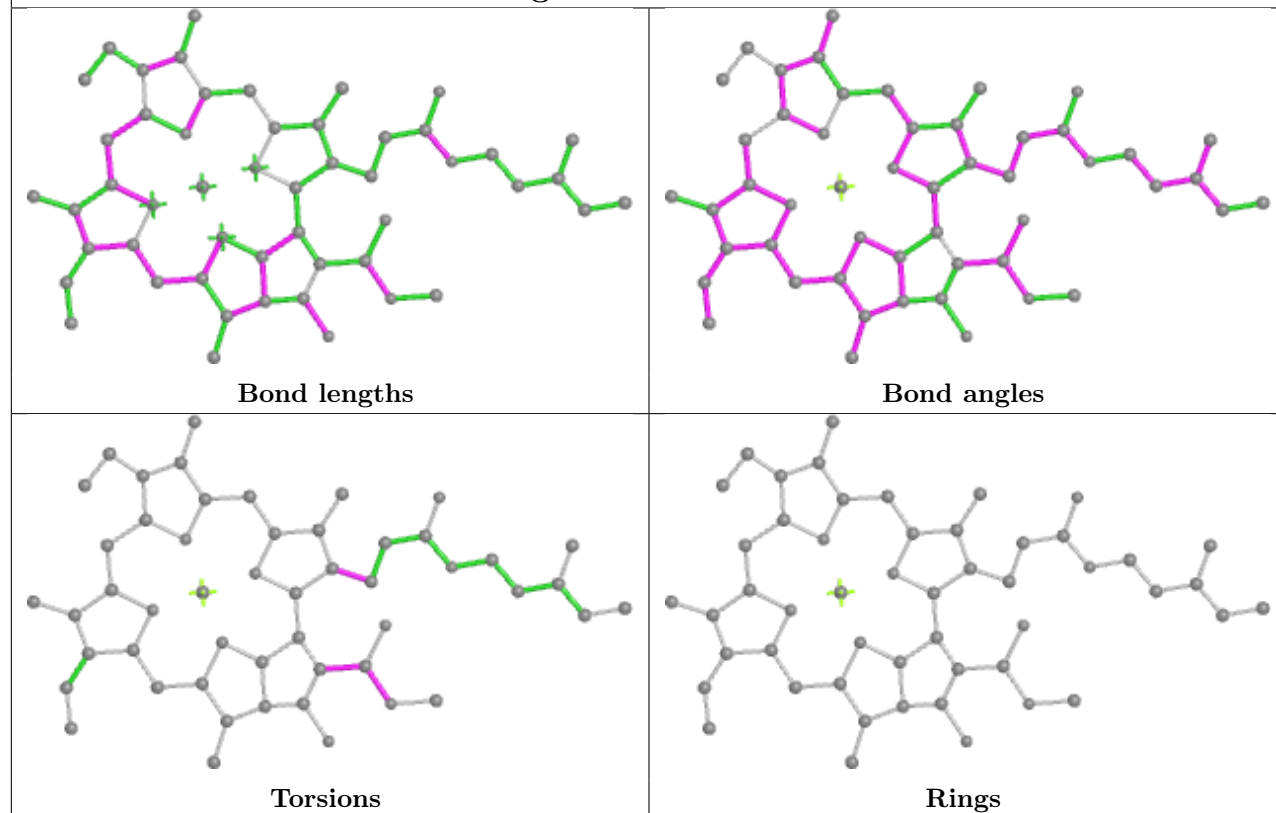




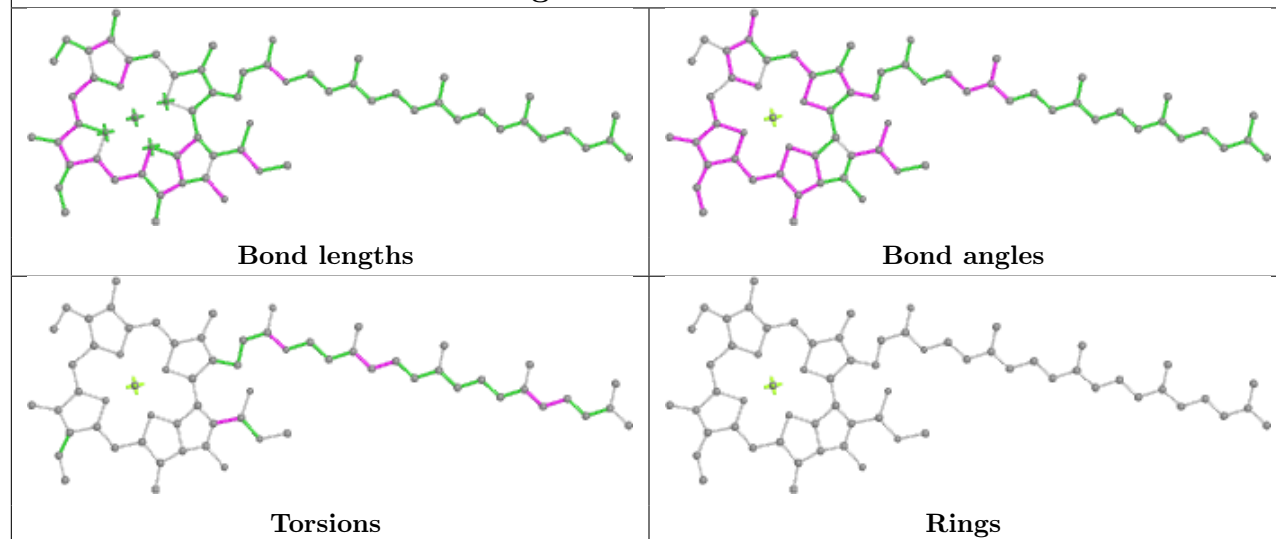


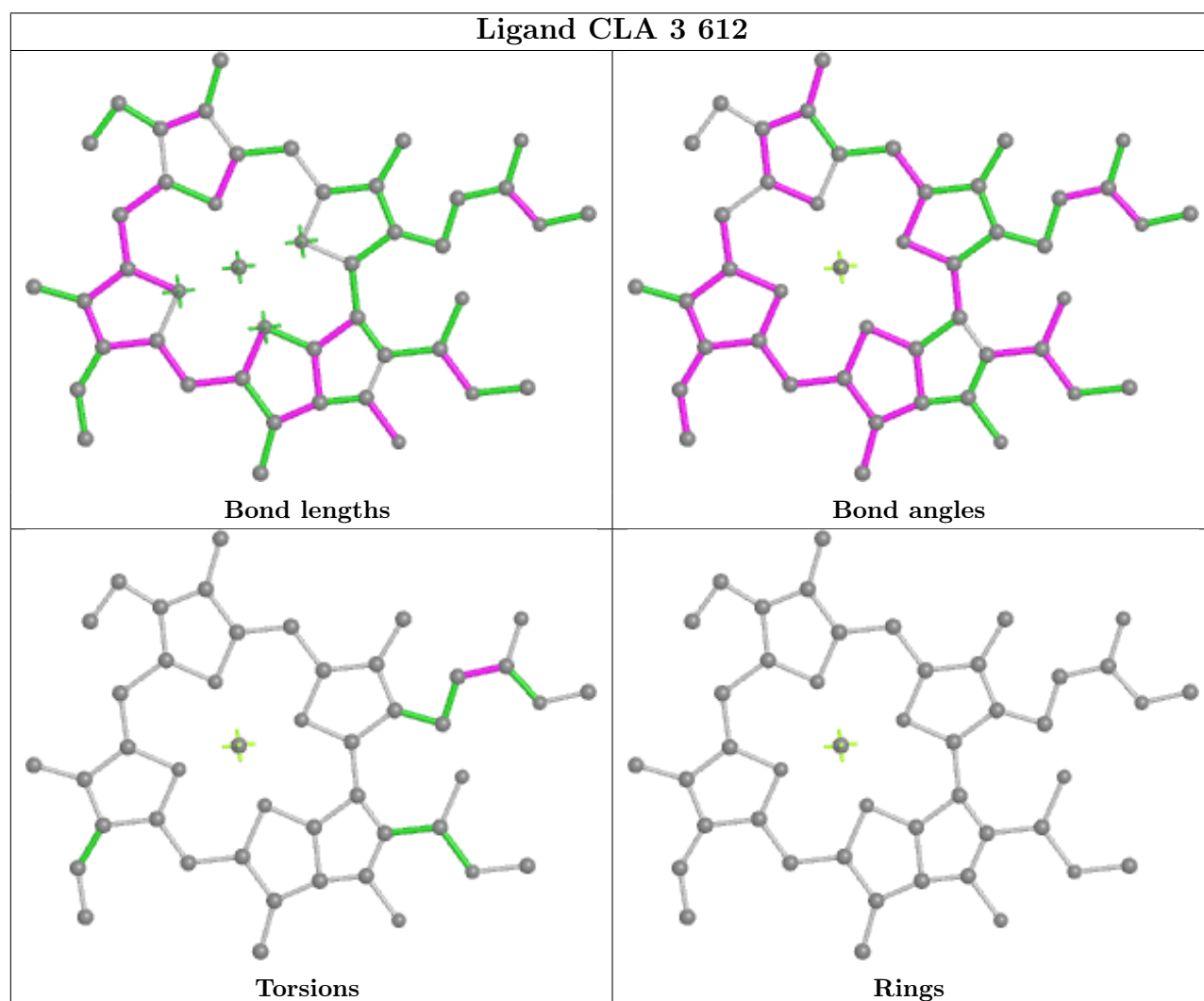
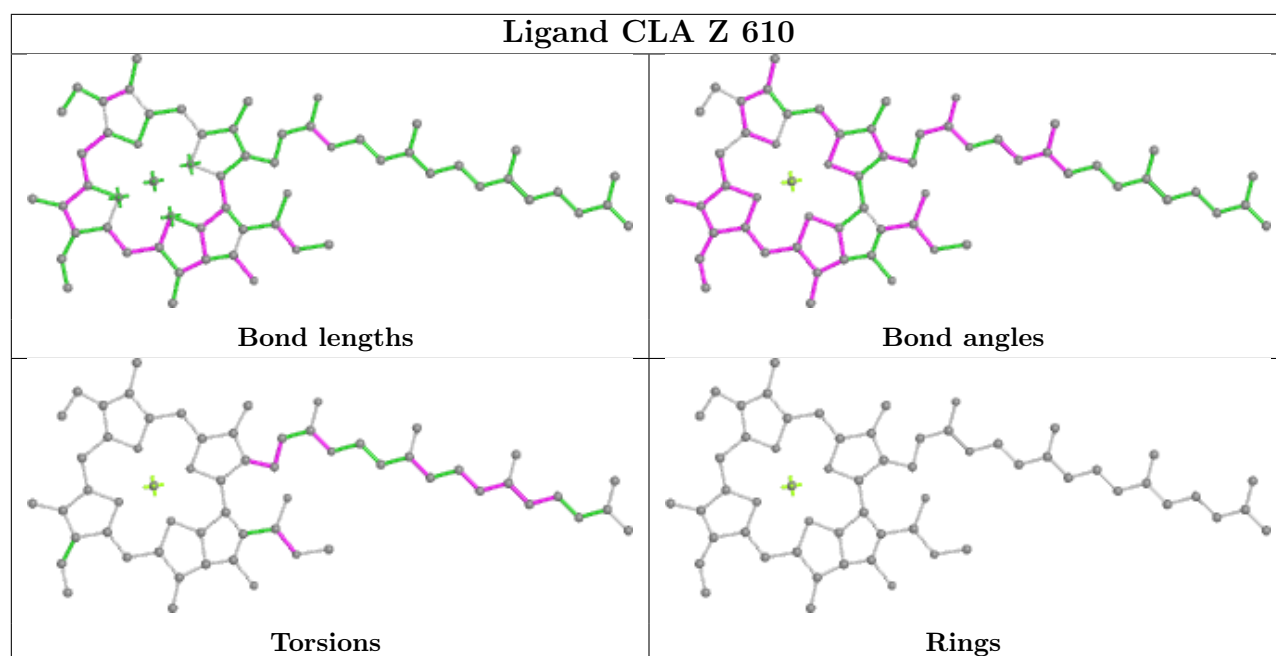


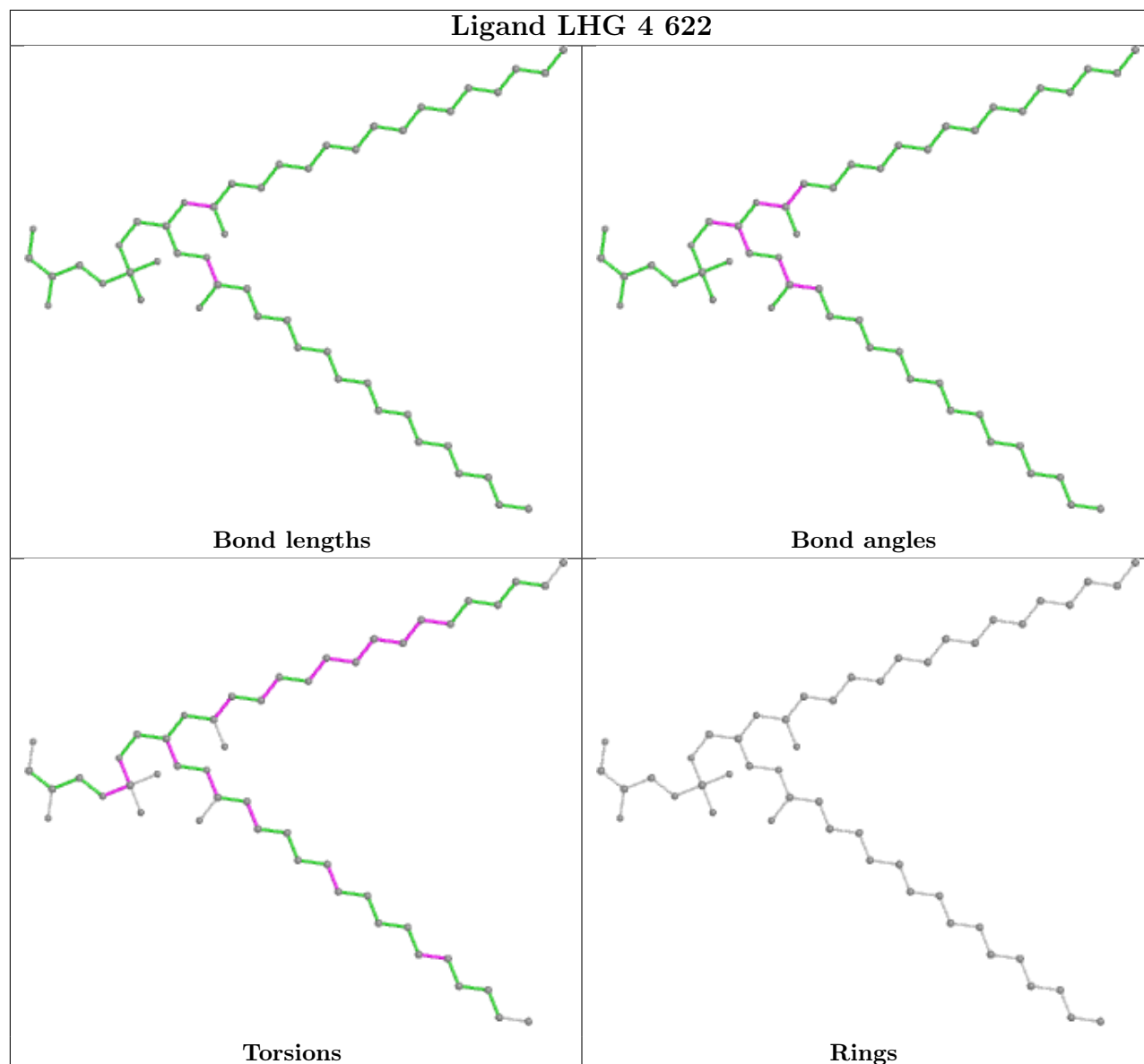
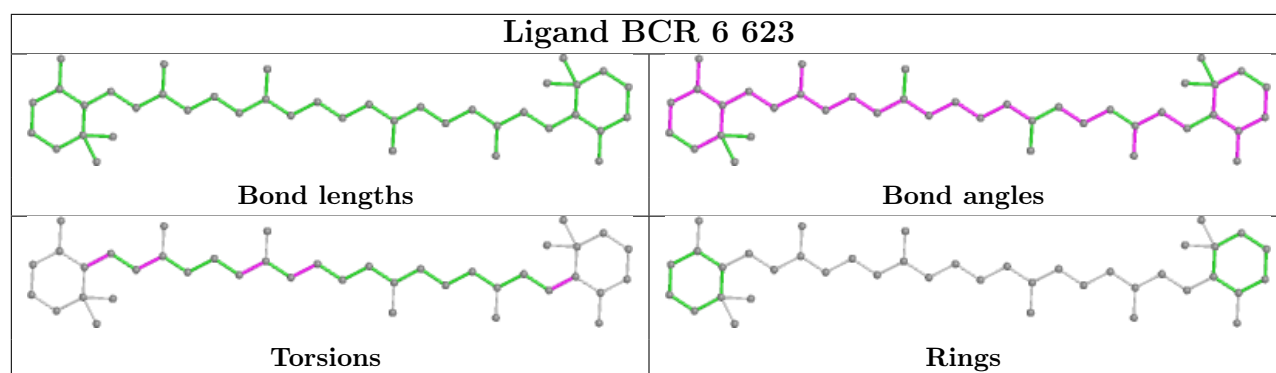
## Ligand CLA A 838

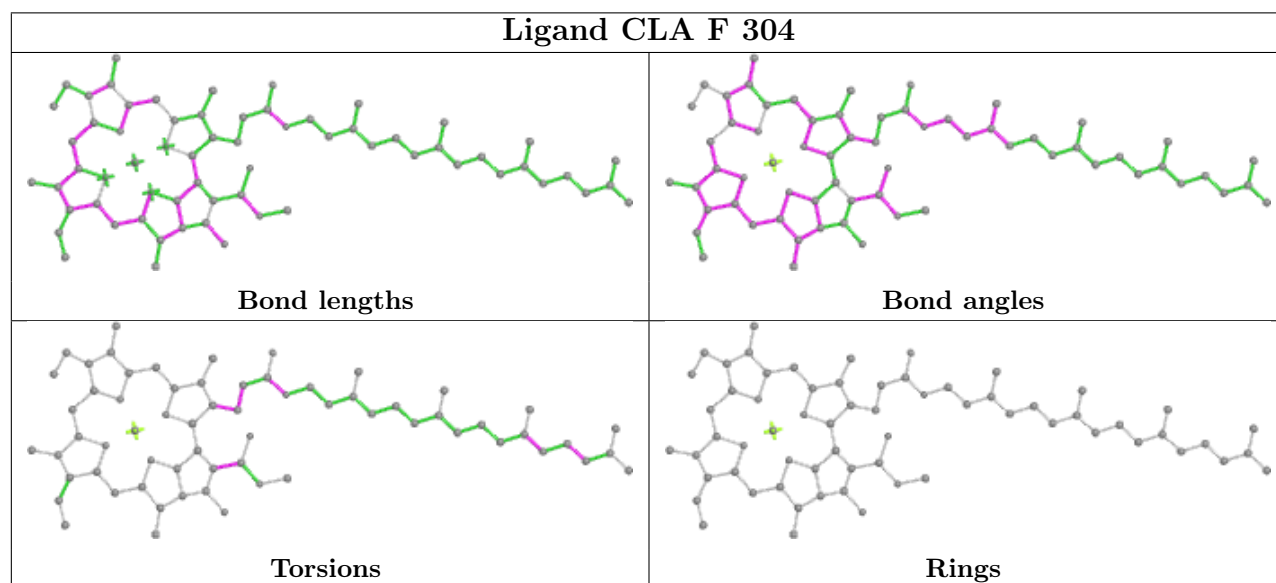
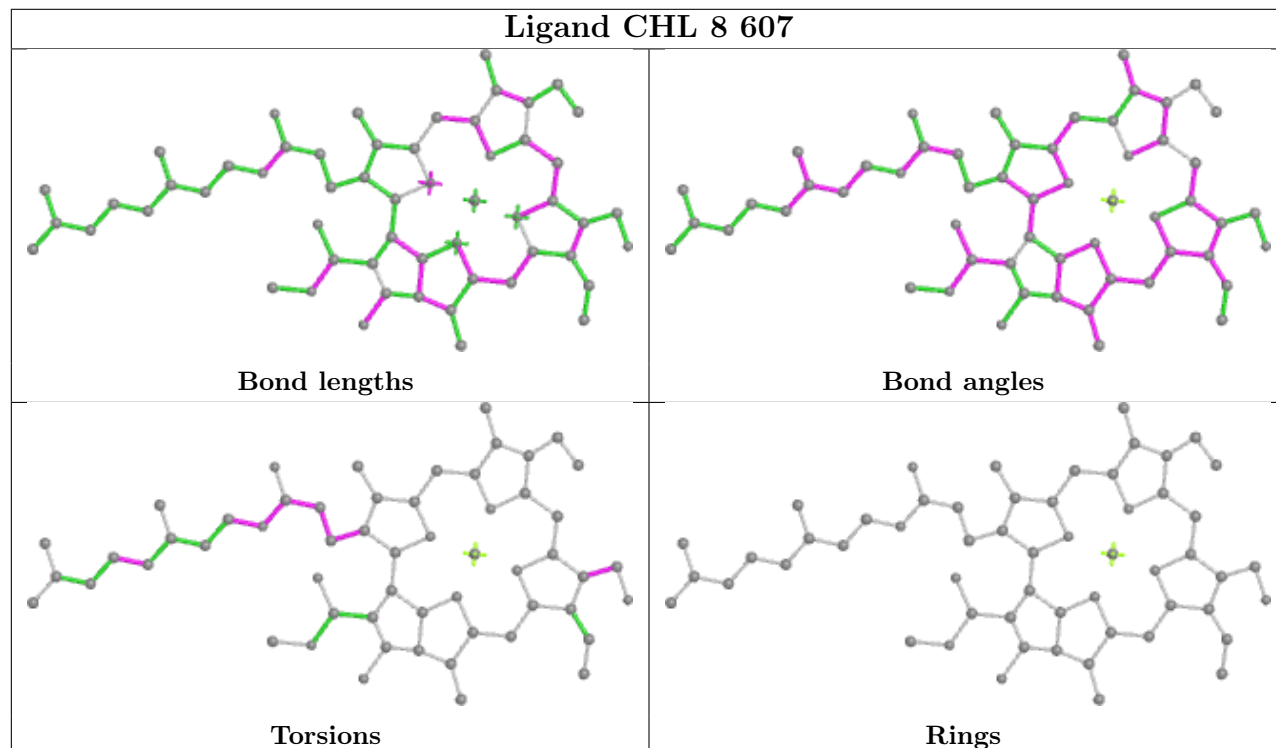
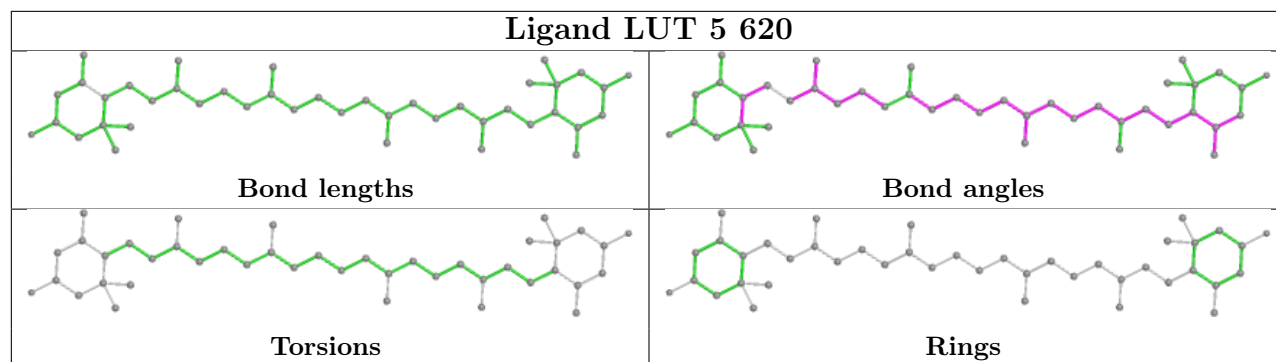


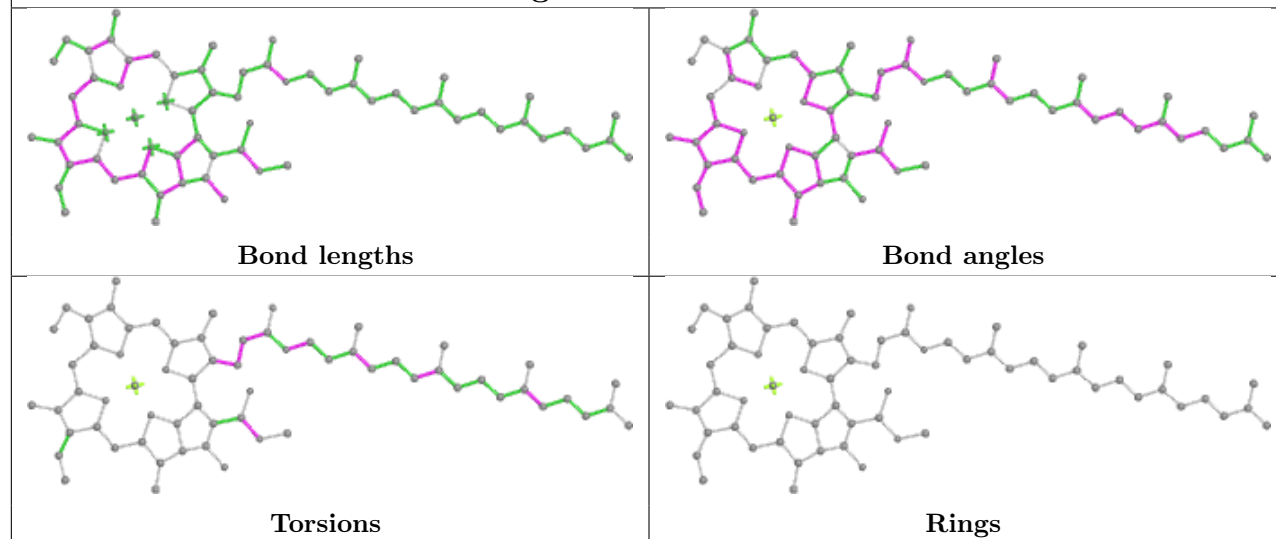
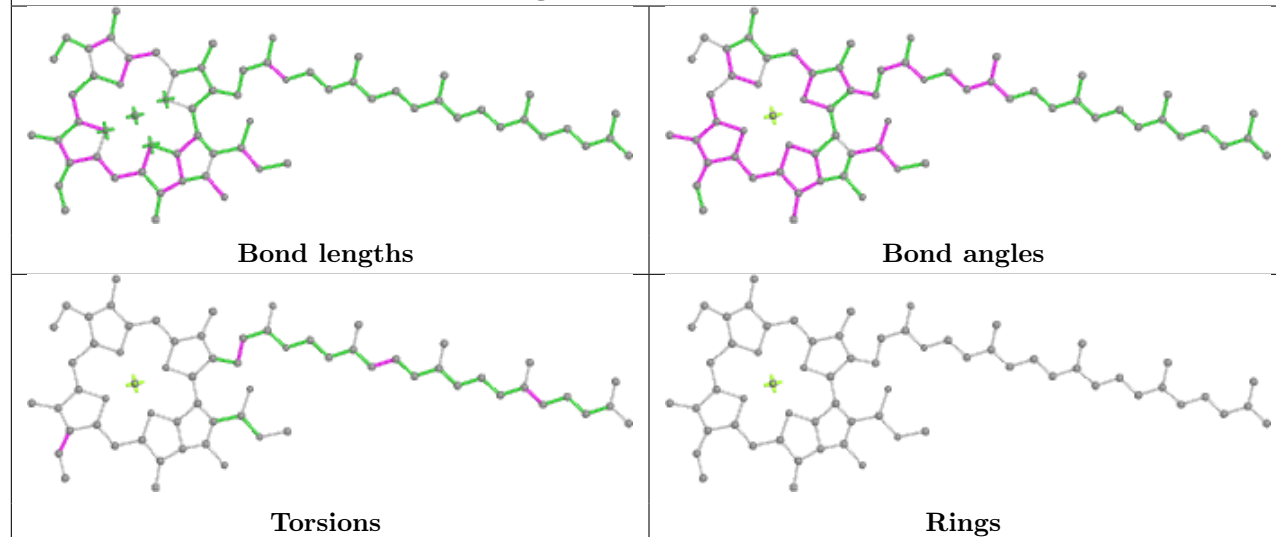
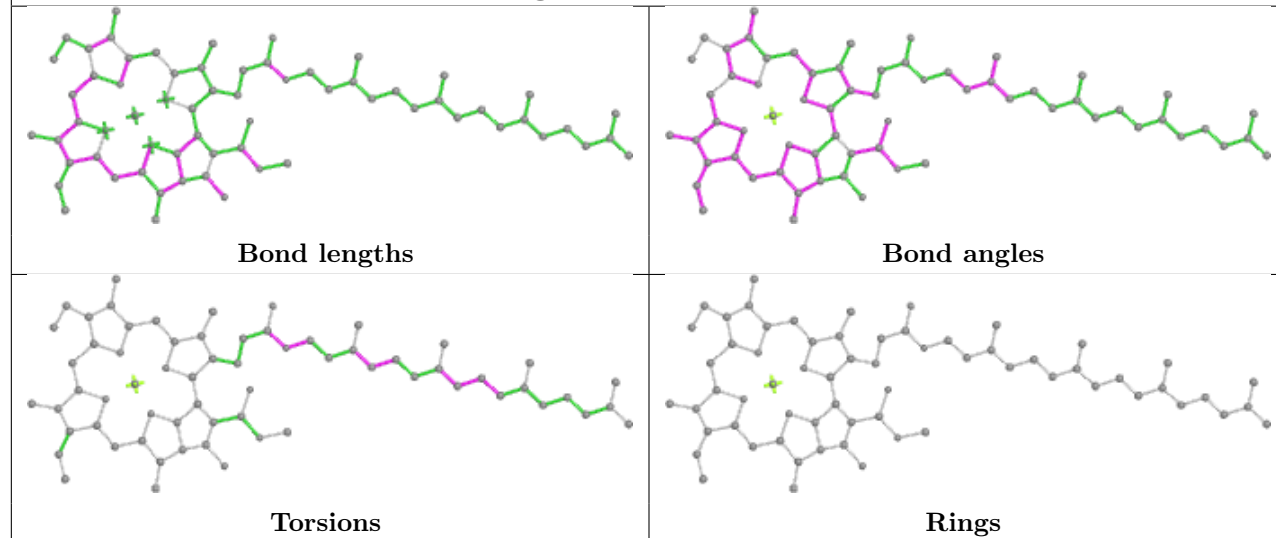
## Ligand CLA A 839



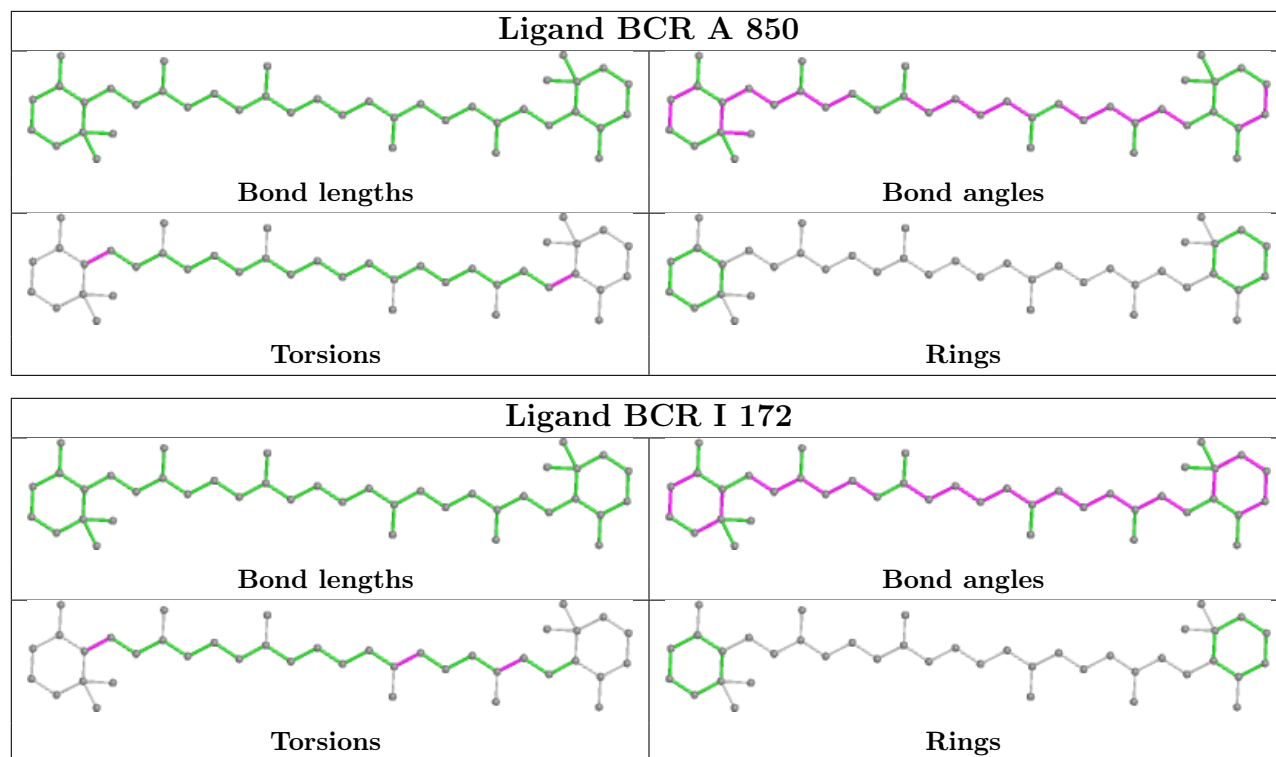




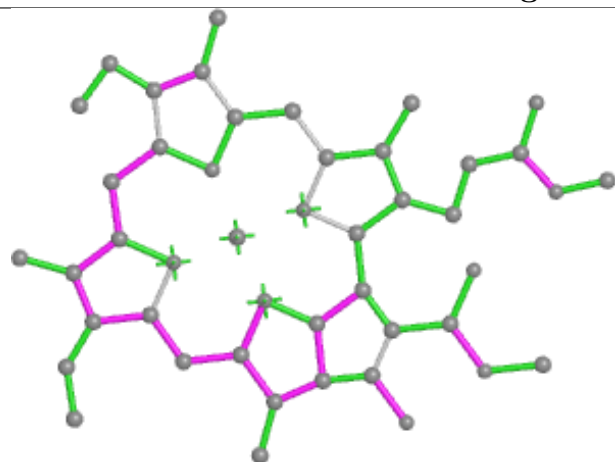


**Ligand CLA A 810****Ligand CLA B 840****Ligand CLA A 833**

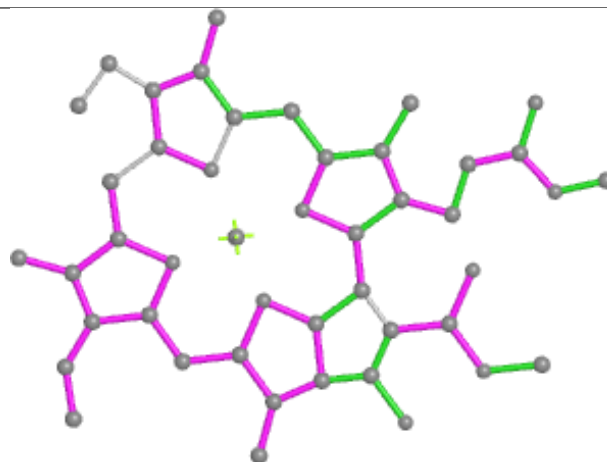




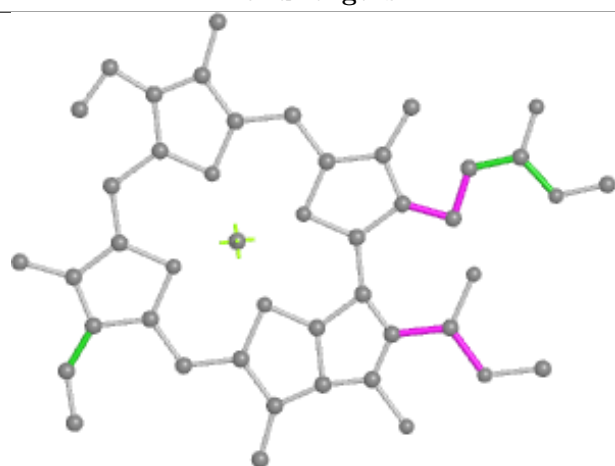
## Ligand CLA 2 603



Bond lengths



Bond angles

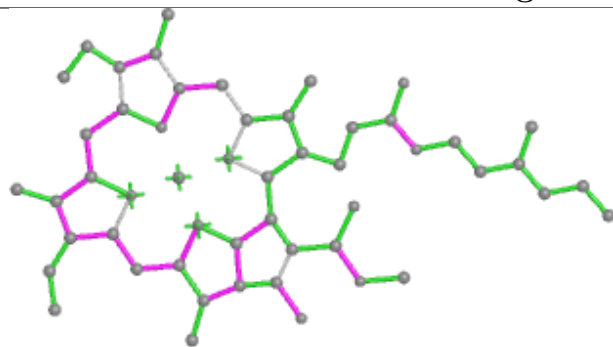


Torsions

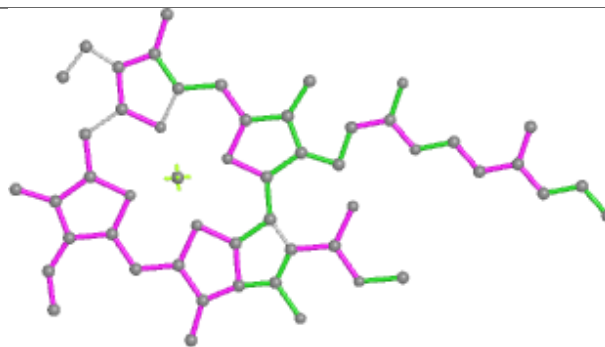


Rings

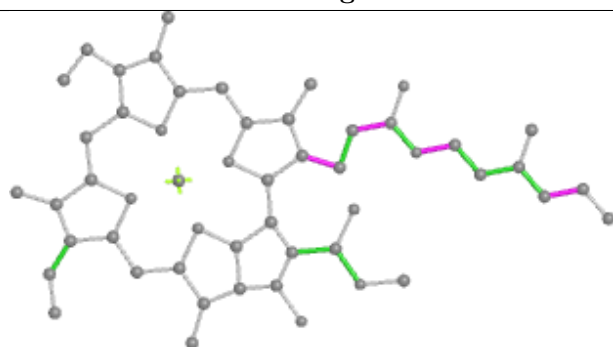
## Ligand CLA Z 612



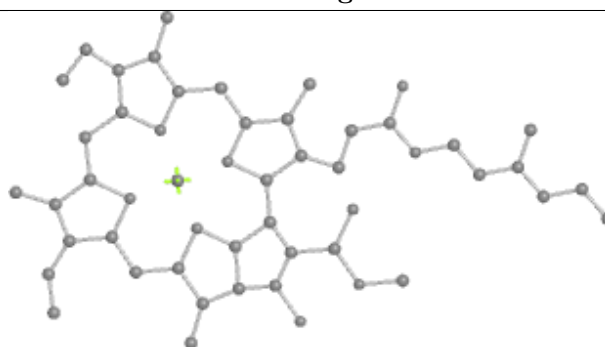
Bond lengths



Bond angles

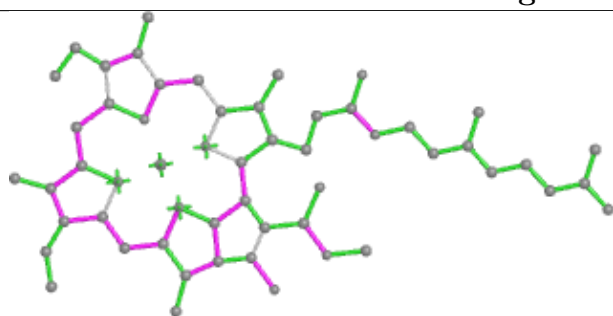


Torsions

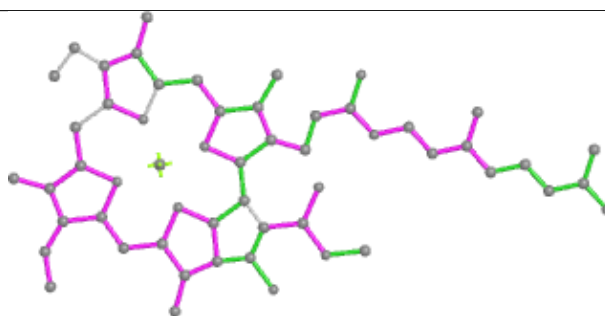


Rings

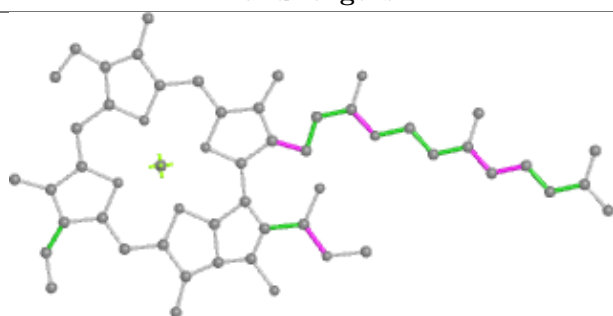
## Ligand CLA 4 611



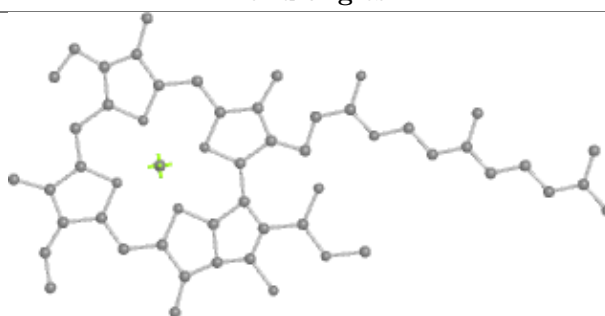
Bond lengths



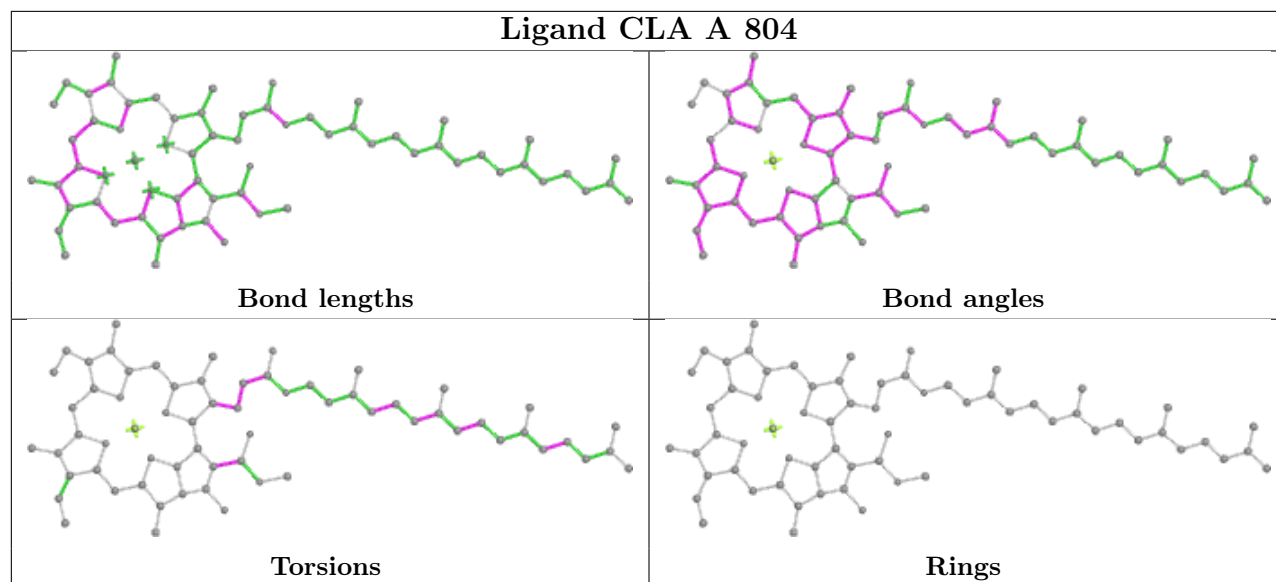
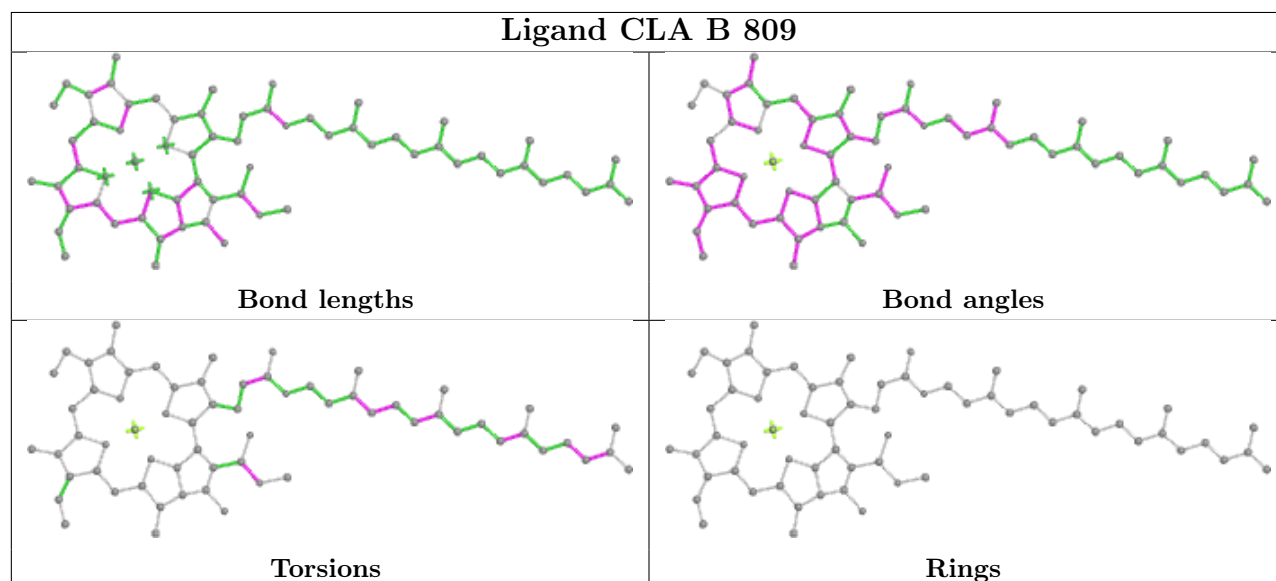
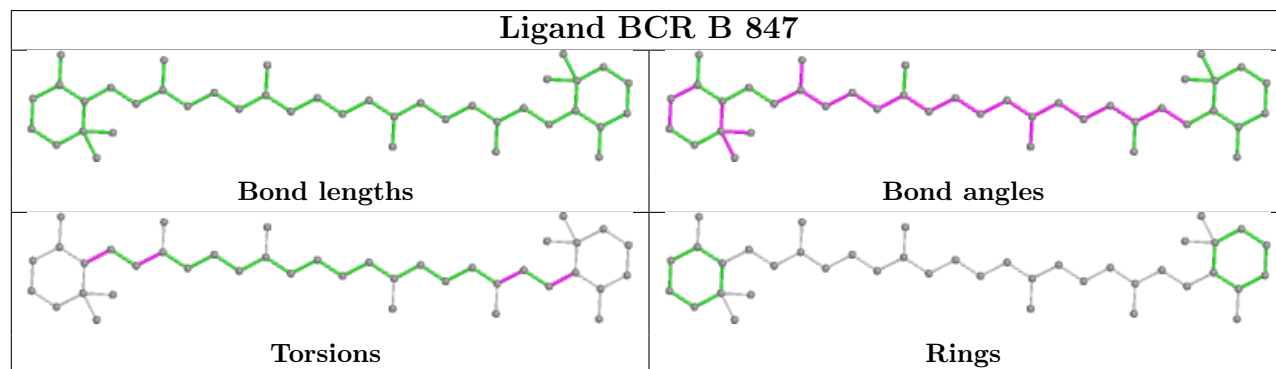
Bond angles



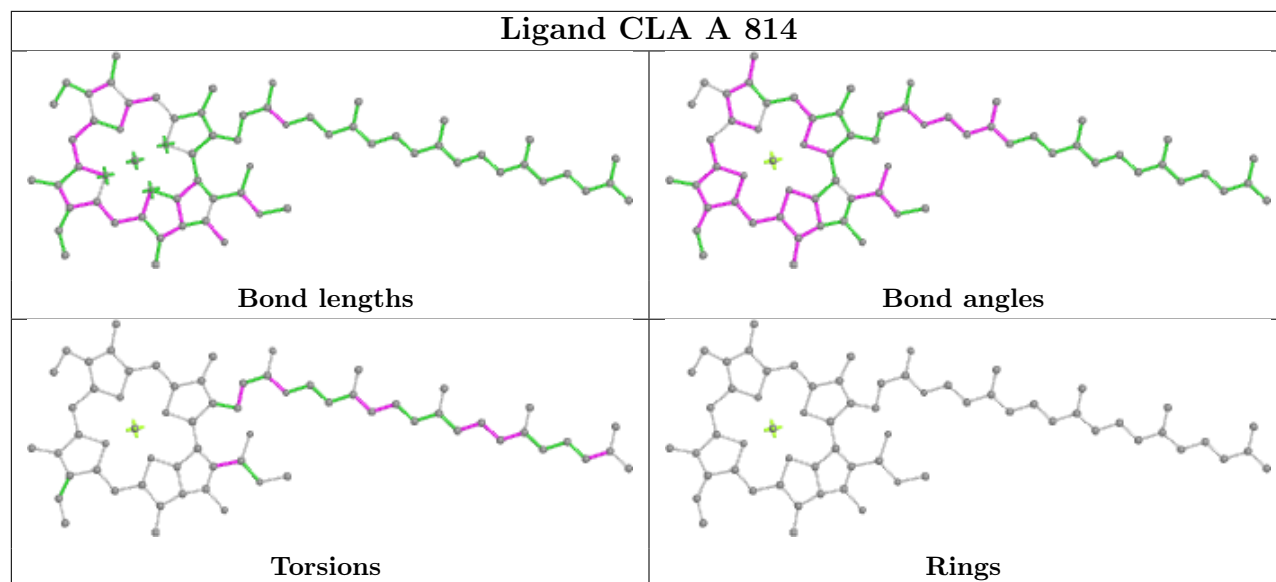
Torsions



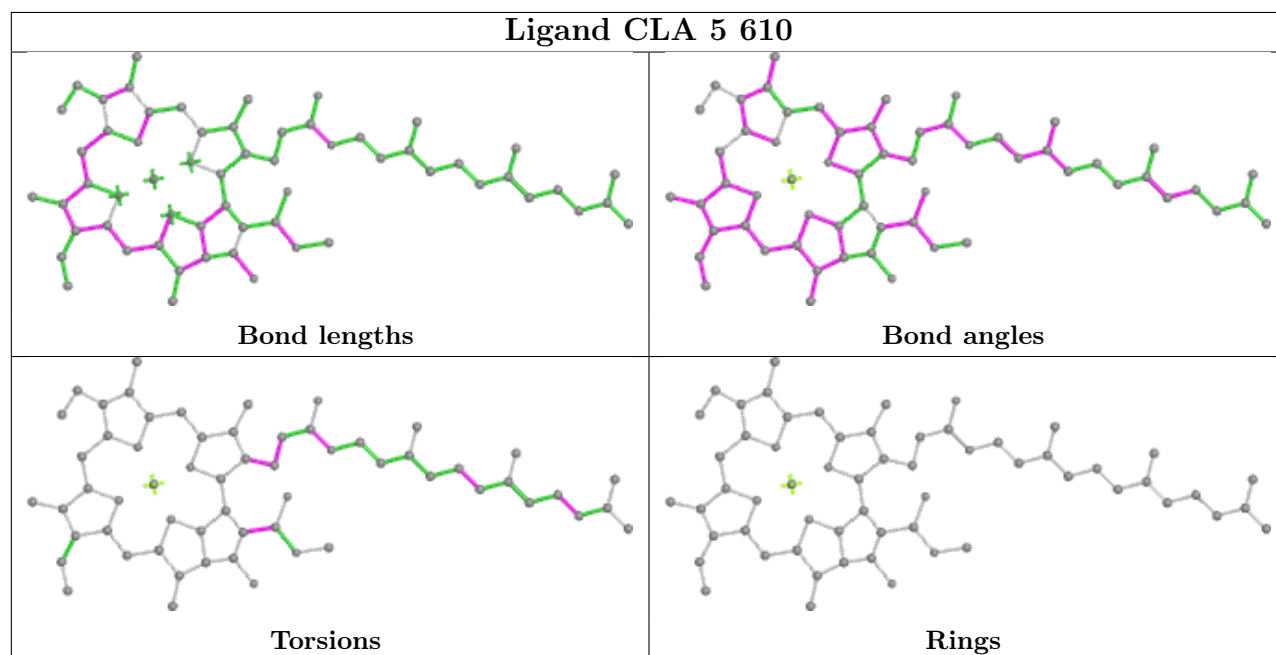
Rings

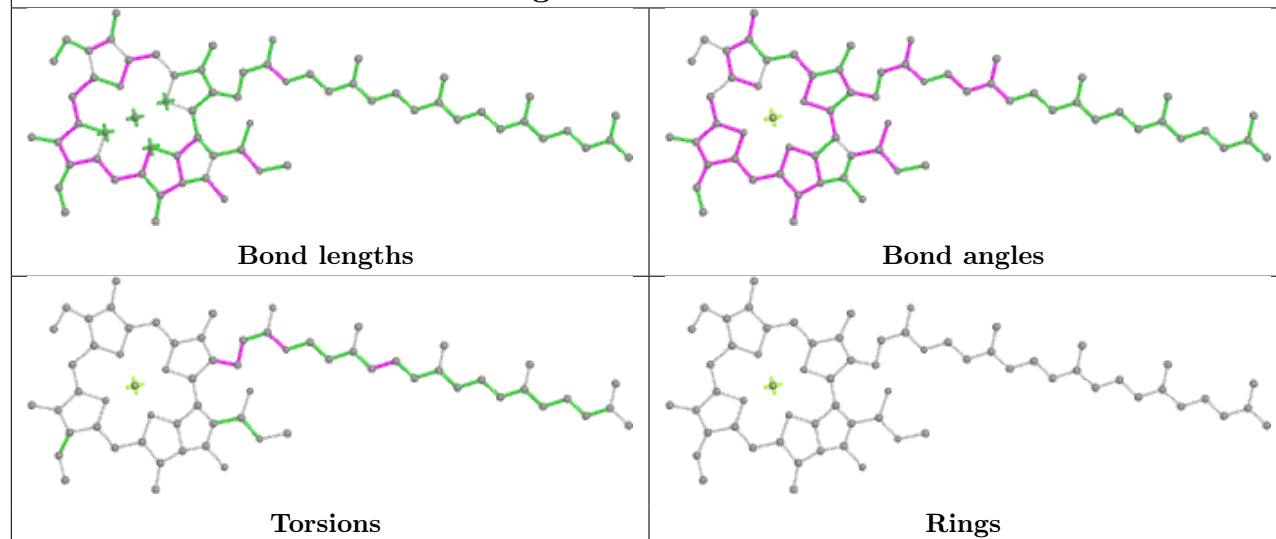
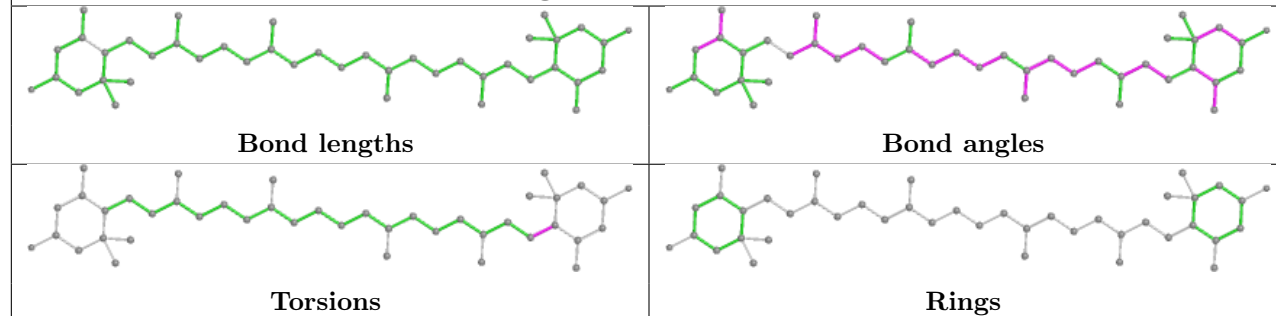
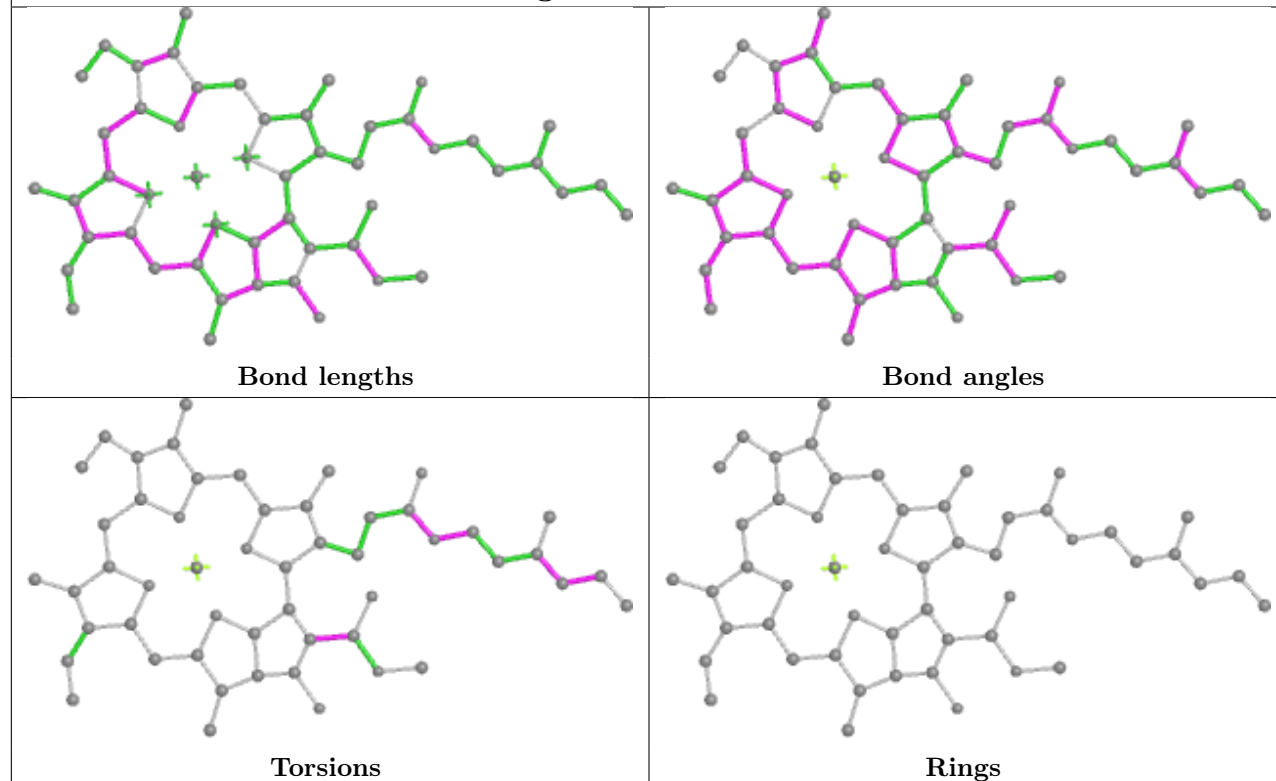
**Ligand CLA A 804****Ligand CLA B 809****Ligand BCR B 847**

## Ligand CLA A 814

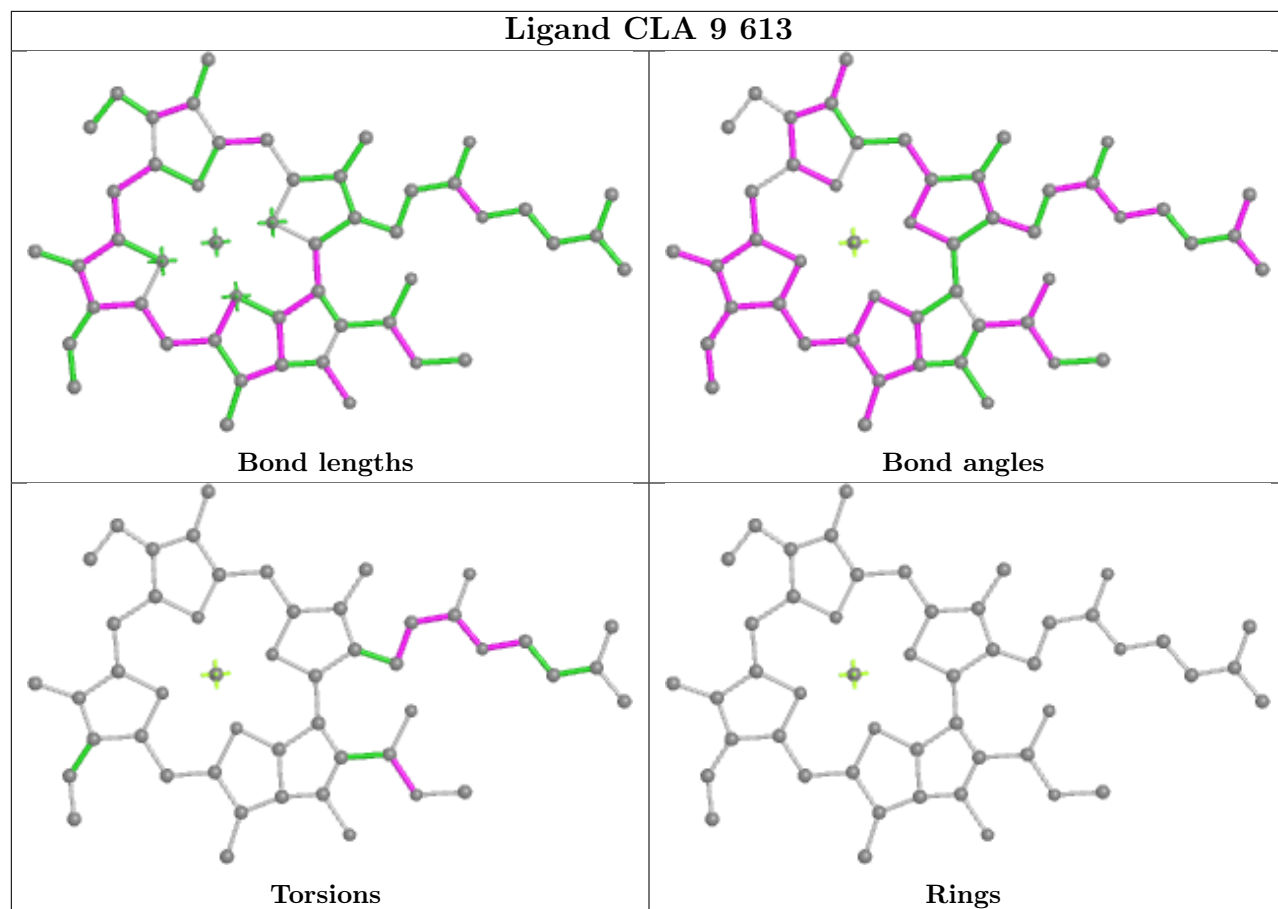


## Ligand CLA 5 610

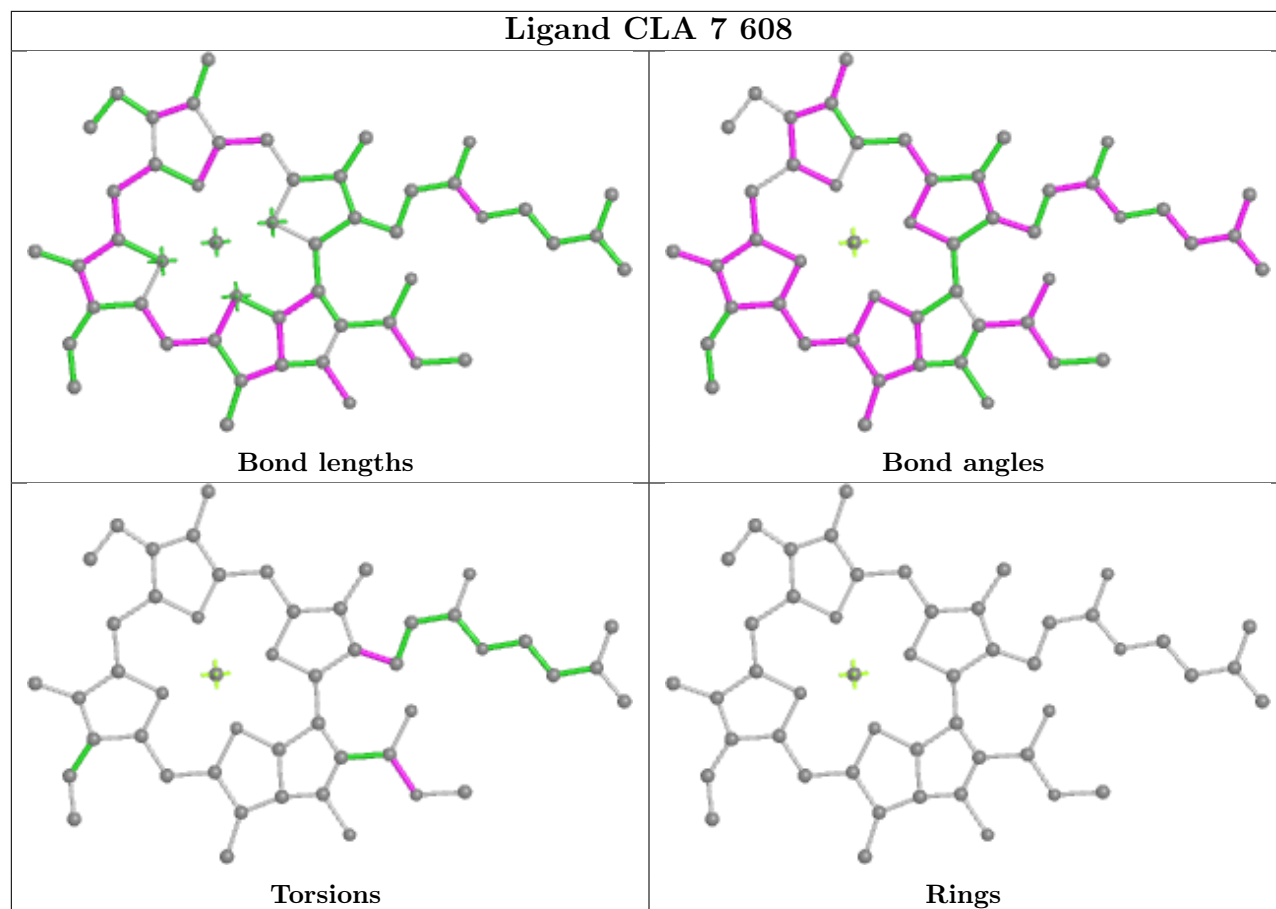


**Ligand CLA B 852****Ligand LUT 6 621****Ligand CLA 7 612**

## Ligand CLA 9 613

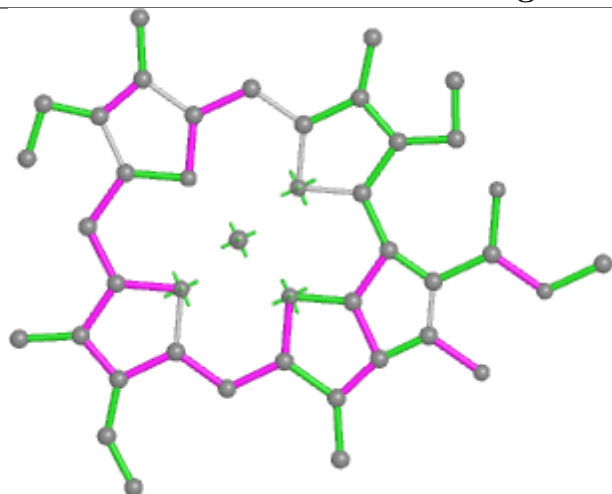


## Ligand CLA 7 608

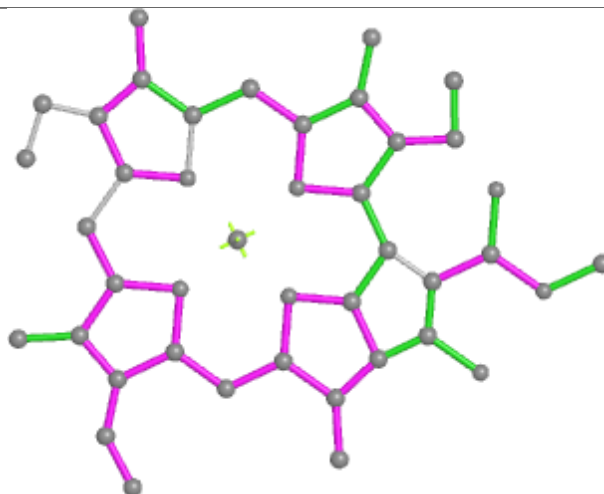




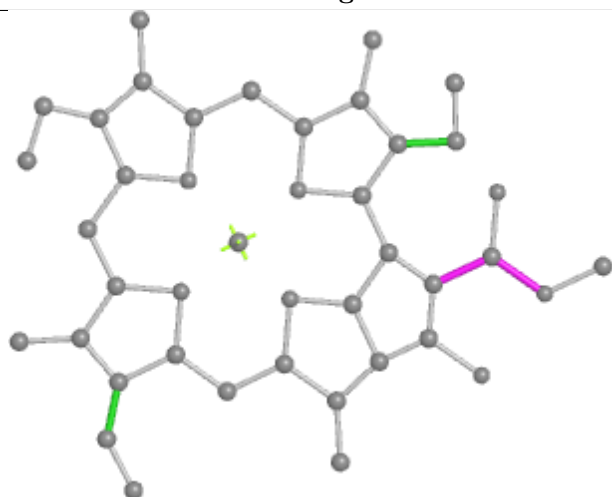
## Ligand CLA 8 606



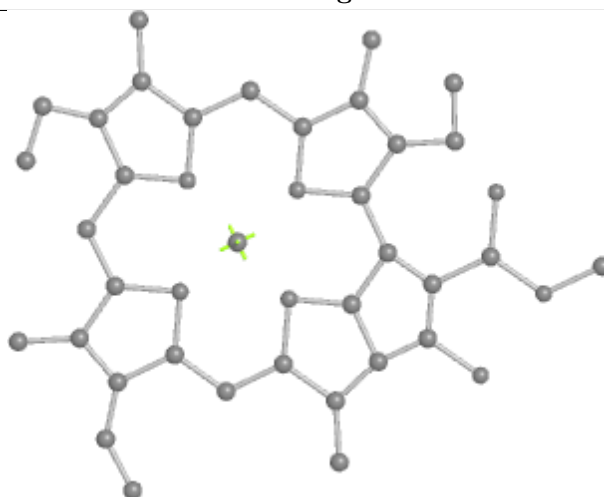
Bond lengths



Bond angles

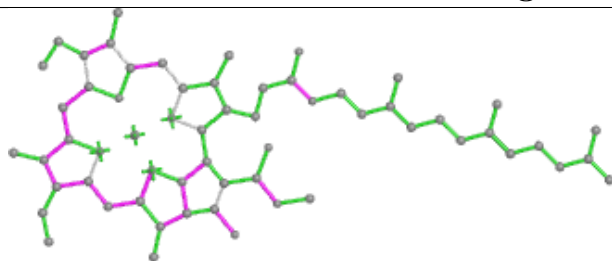


Torsions

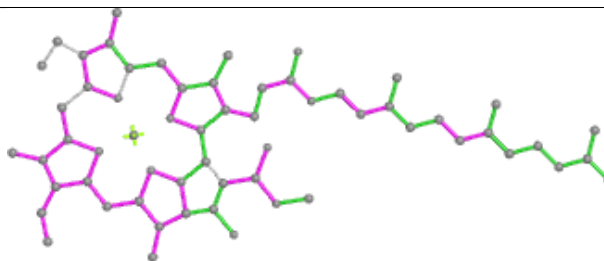


Rings

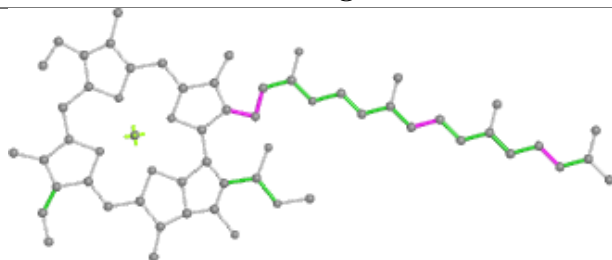
## Ligand CLA 9 610



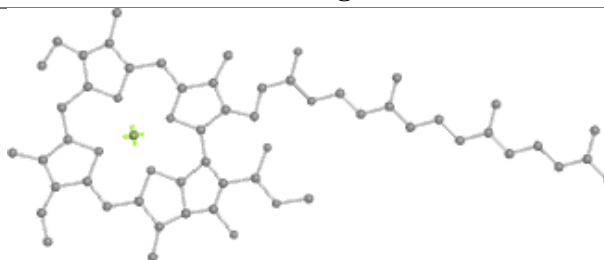
Bond lengths



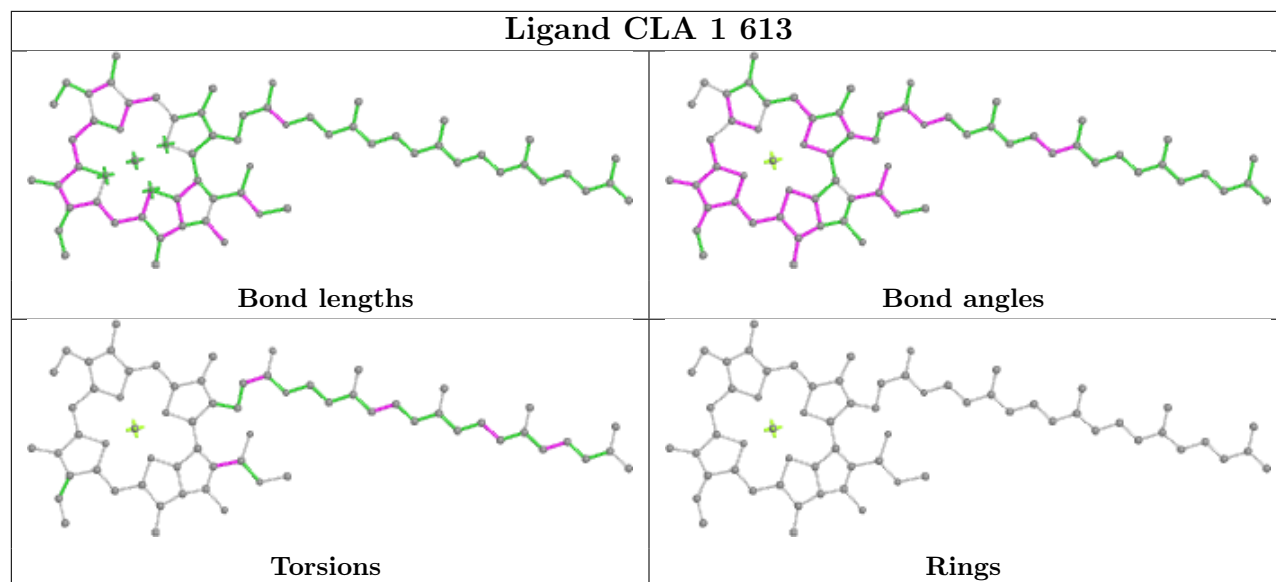
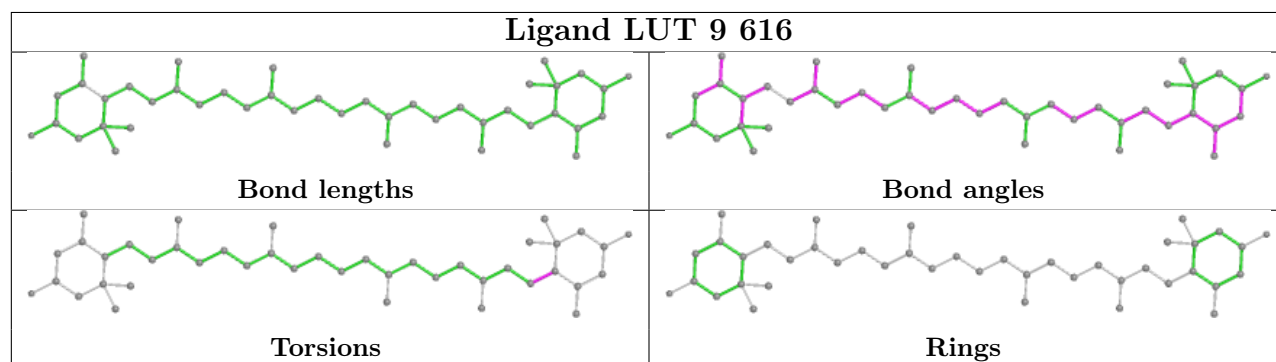
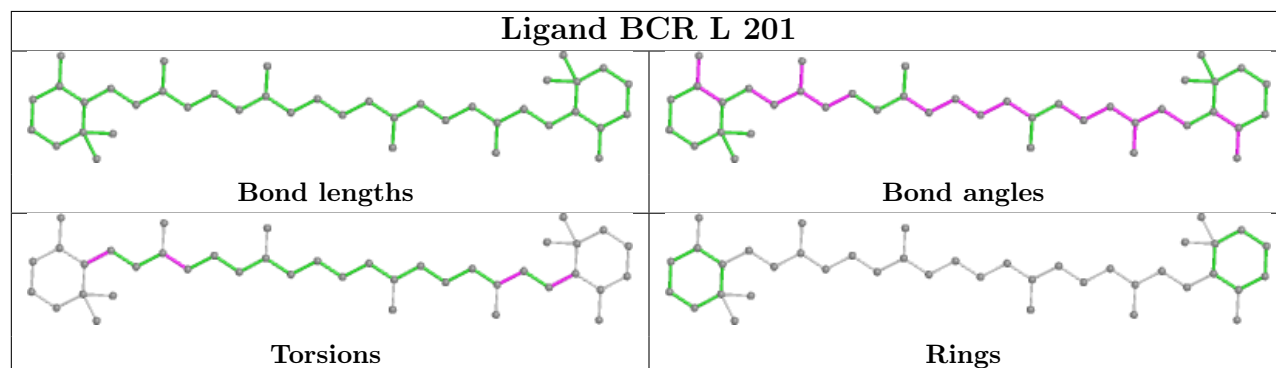
Bond angles



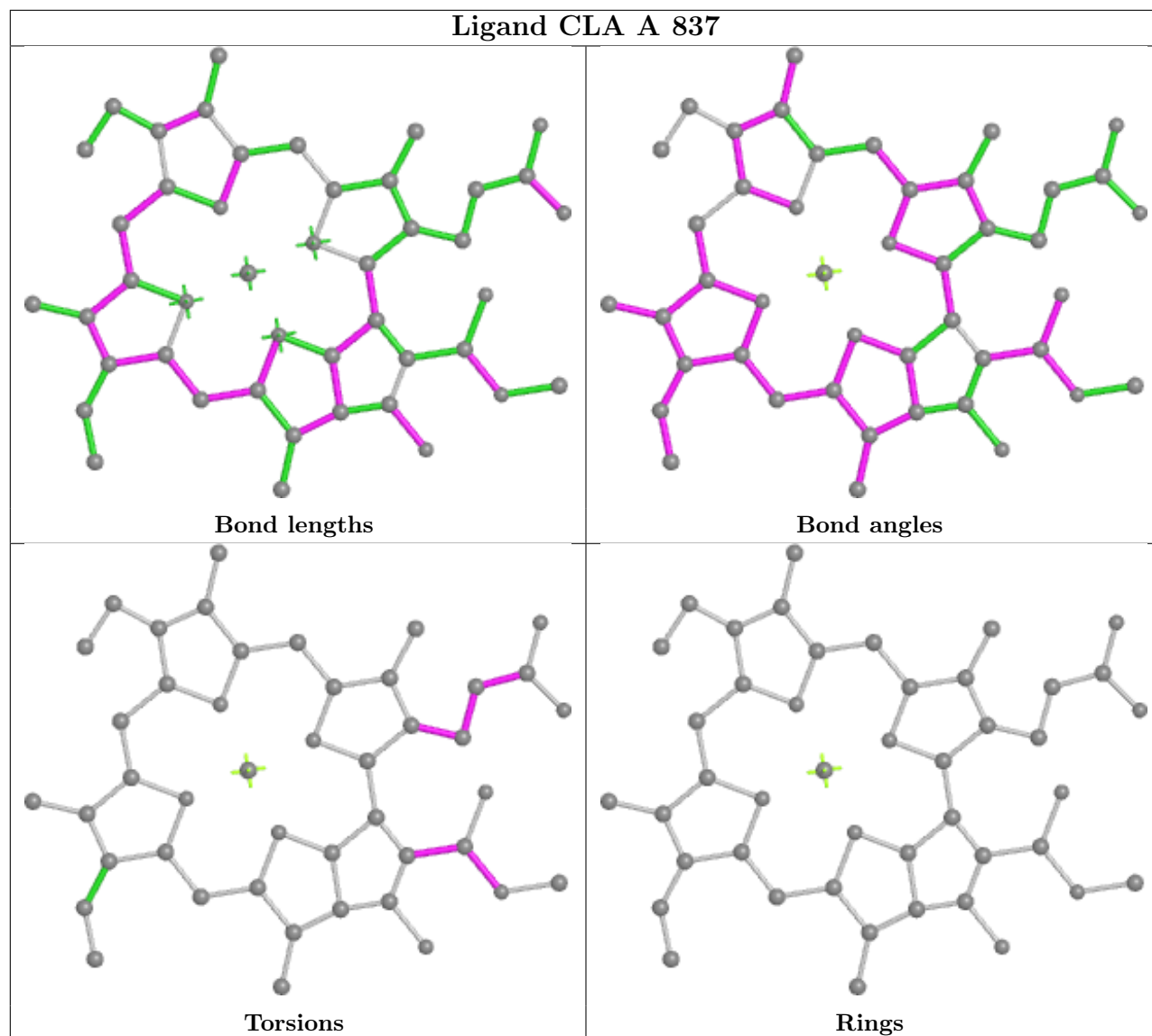
Torsions



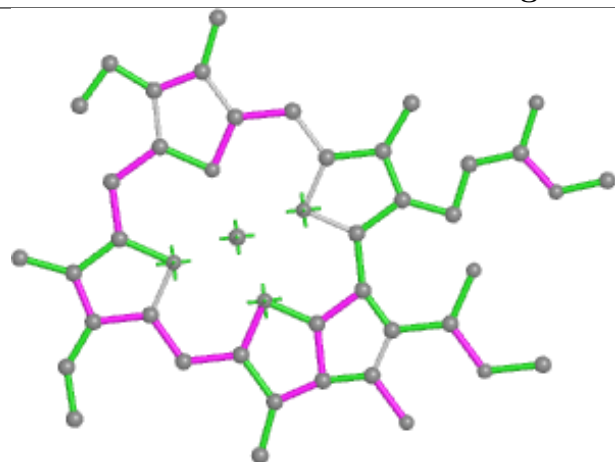
Rings

**Ligand CLA 1 613****Ligand LUT 9 616****Ligand BCR L 201**

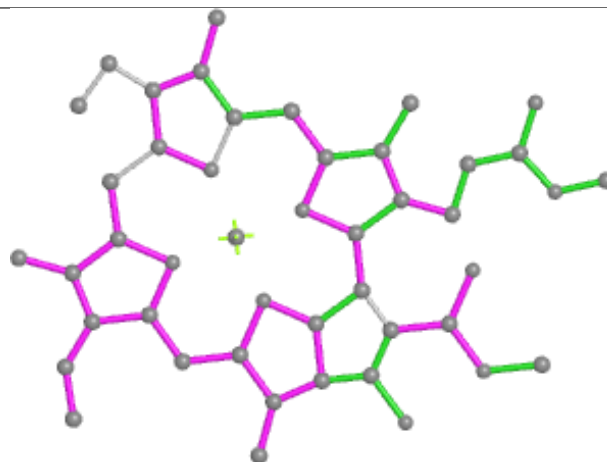
## Ligand CLA A 837



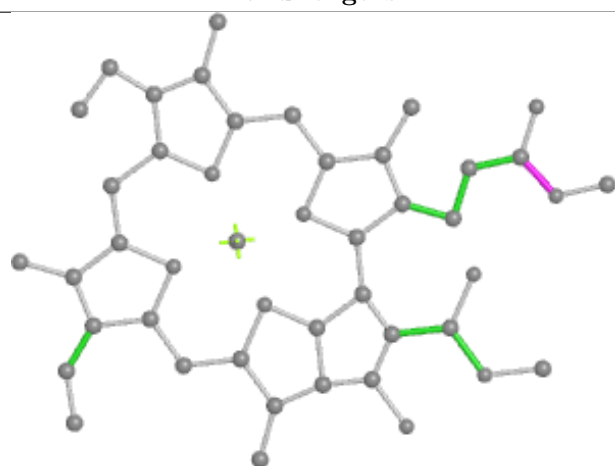
## Ligand CLA 4 603



Bond lengths



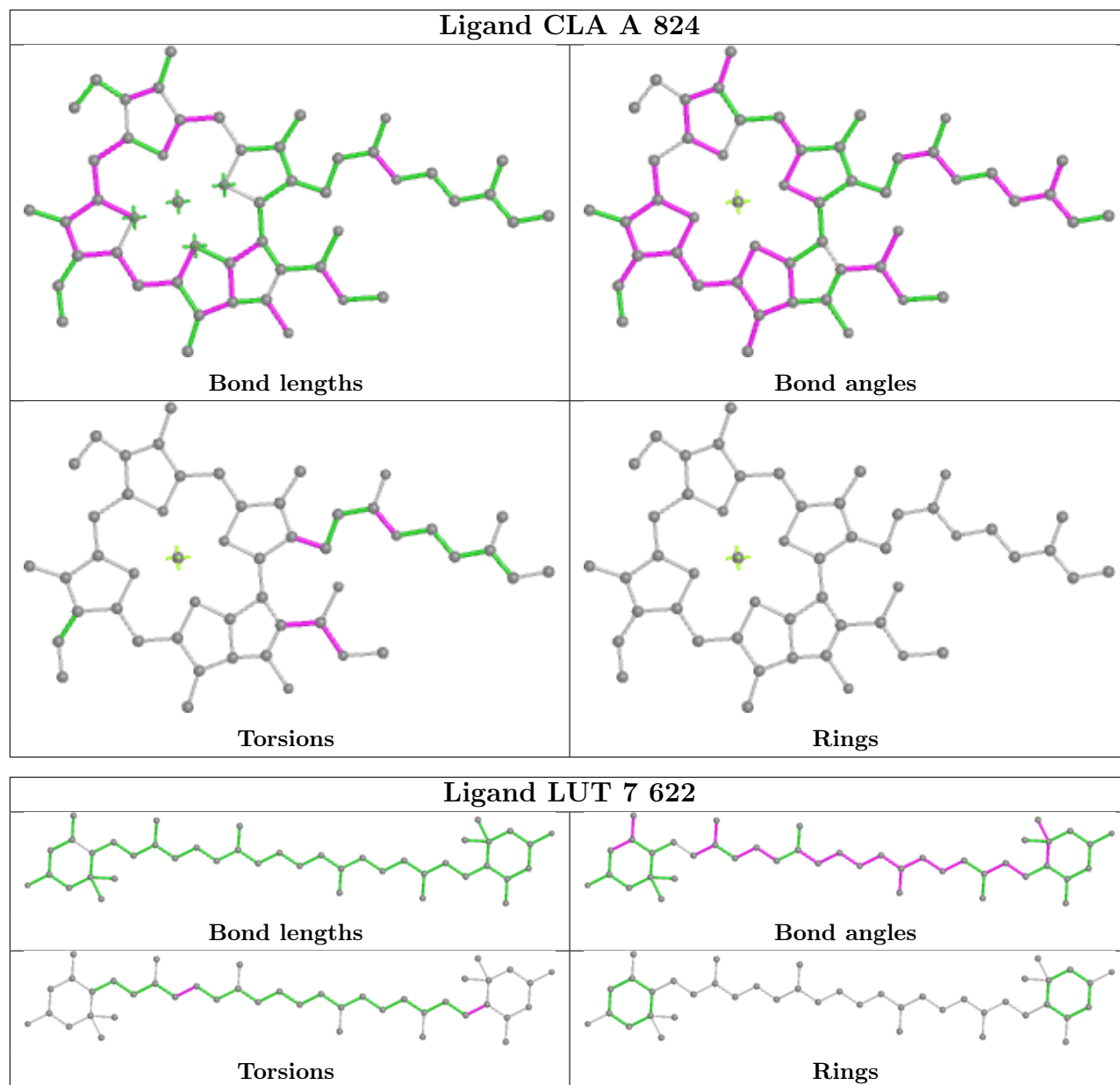
Bond angles

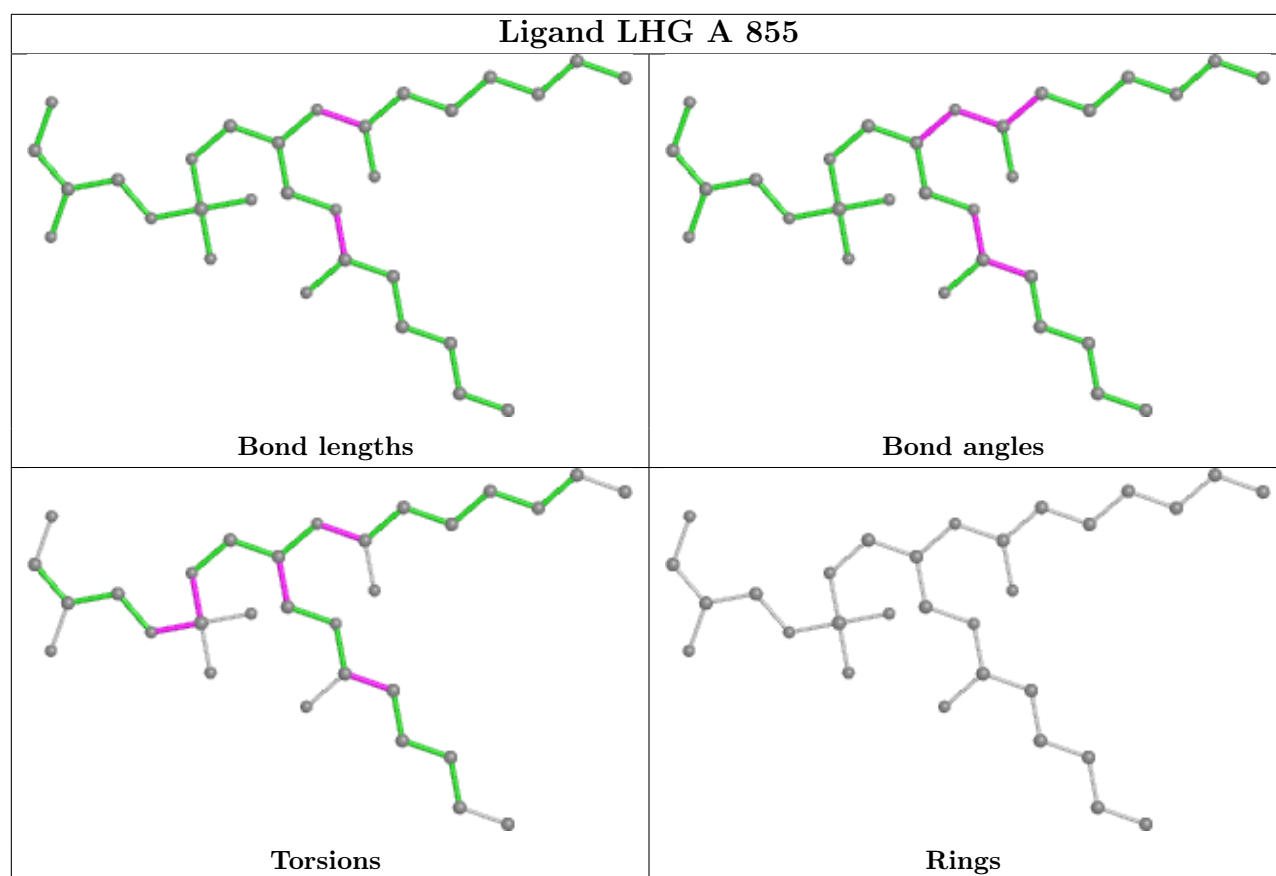


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

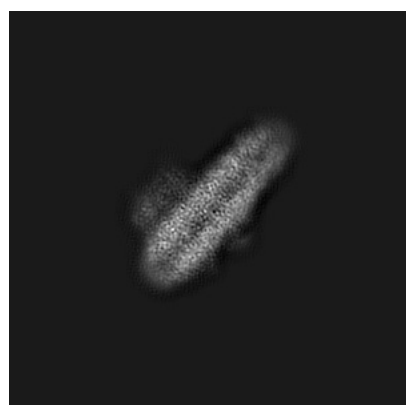
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9853. These allow visual inspection of the internal detail of the map and identification of artifacts.

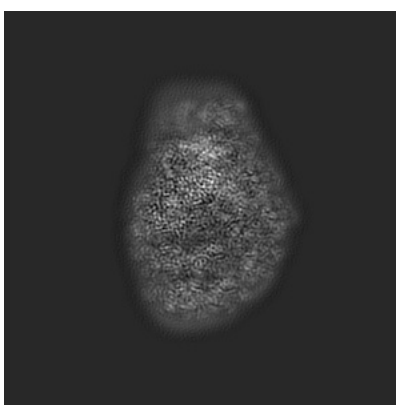
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

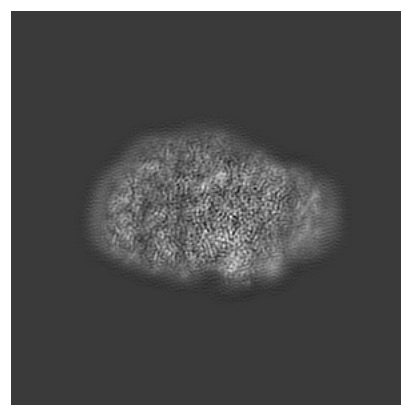
#### 6.1.1 Primary map



X



Y

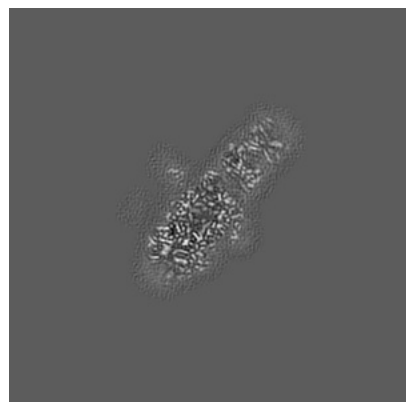


Z

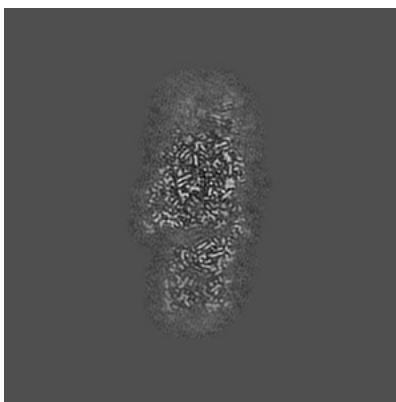
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

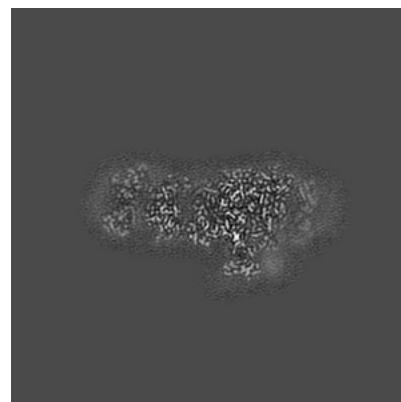
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

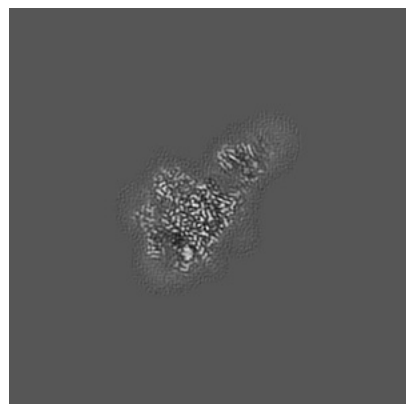


Z Index: 160

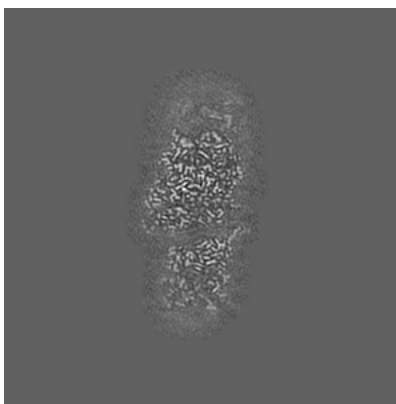
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

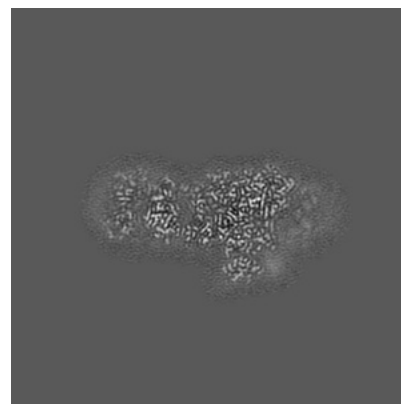
### 6.3.1 Primary map



X Index: 175



Y Index: 158

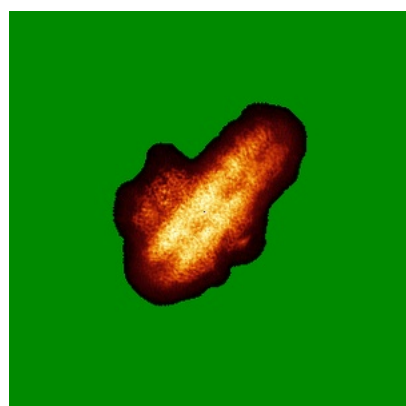


Z Index: 157

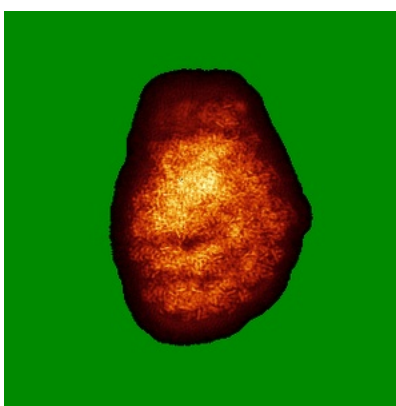
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

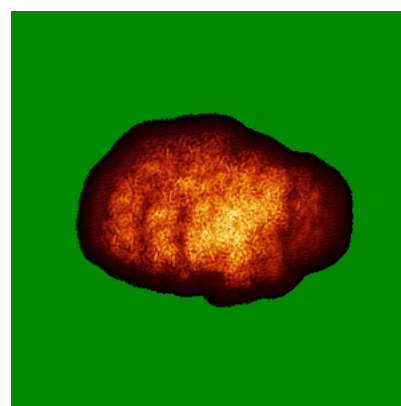
### 6.4.1 Primary map



X



Y



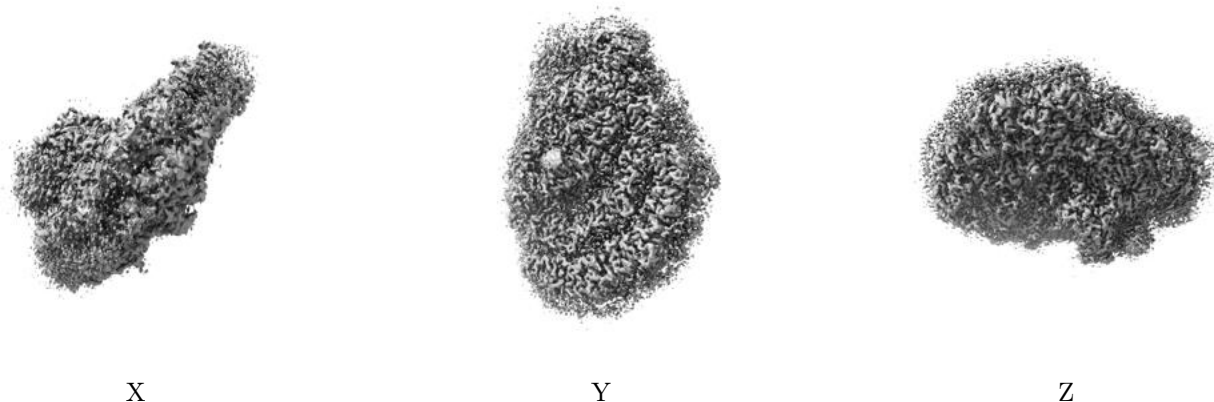
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

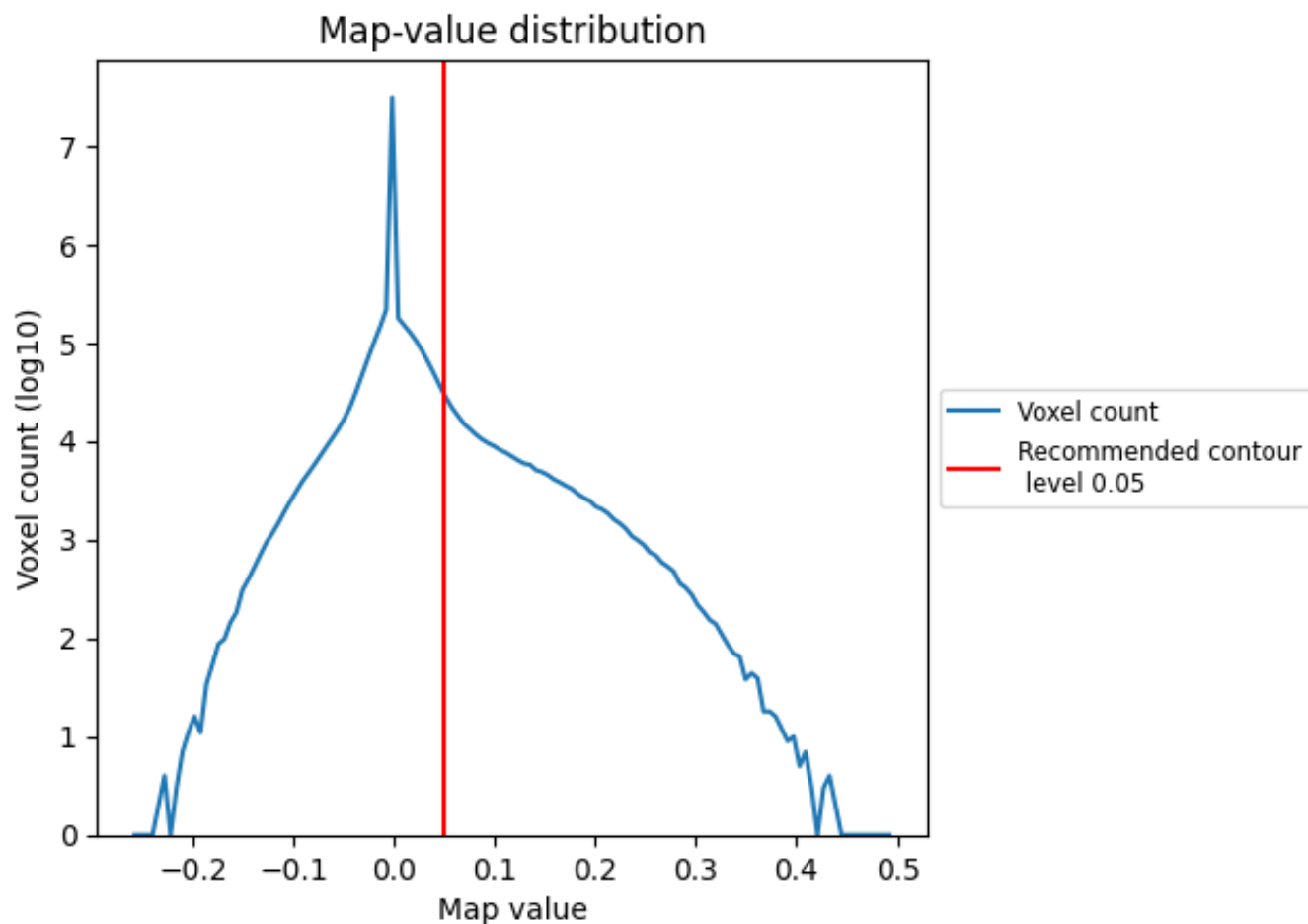
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

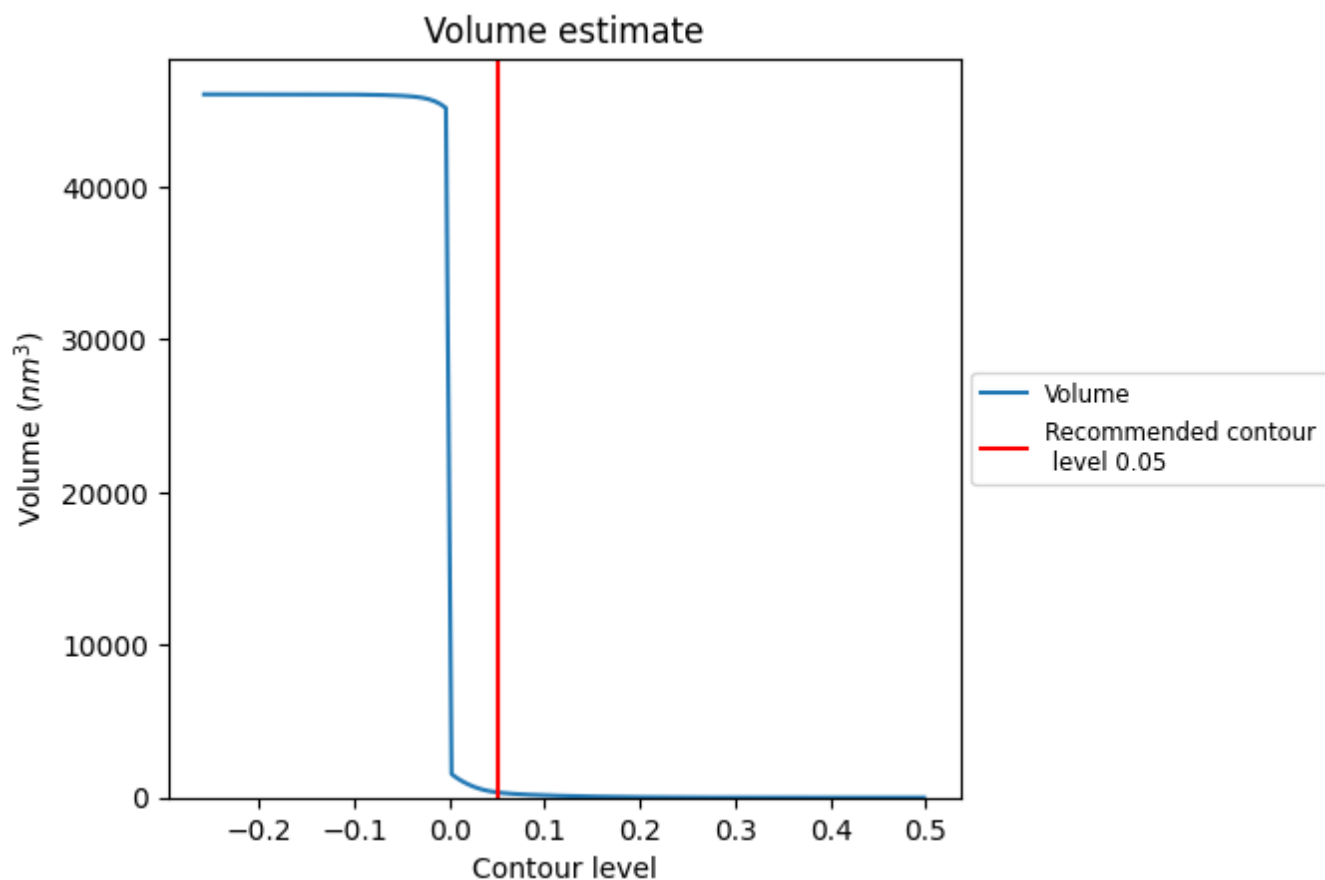
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

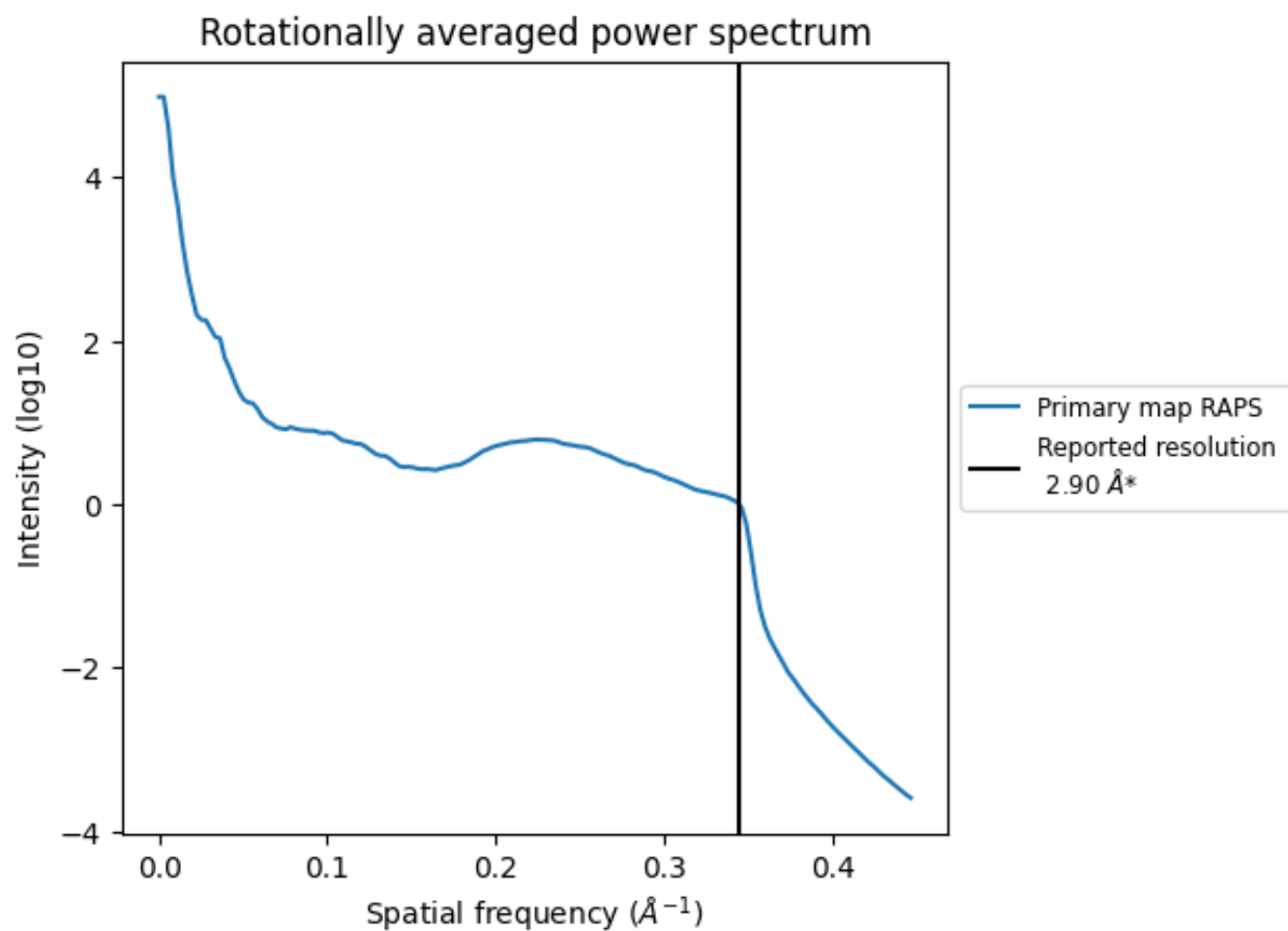
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342  $\text{nm}^3$ ; this corresponds to an approximate mass of 309 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

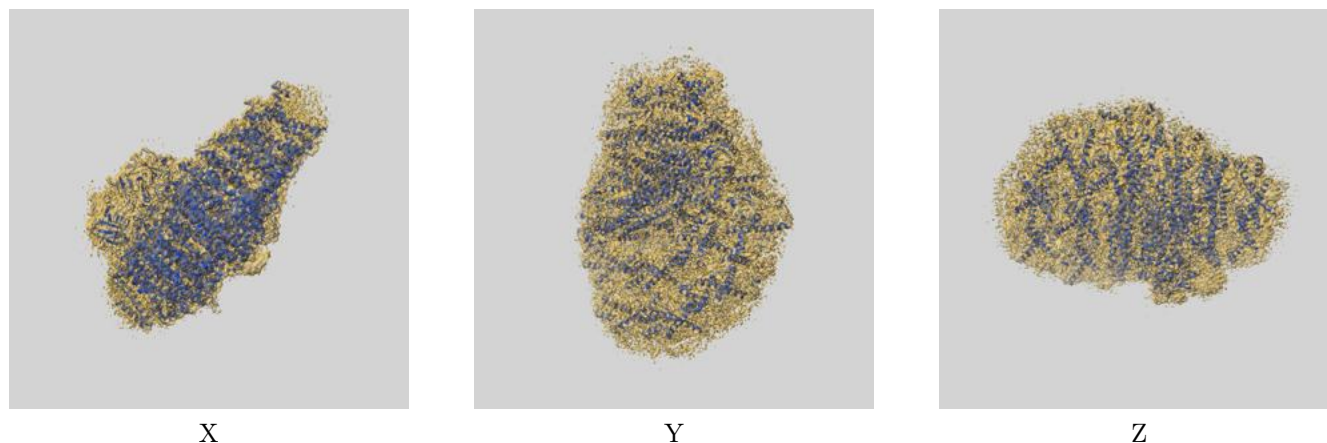
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

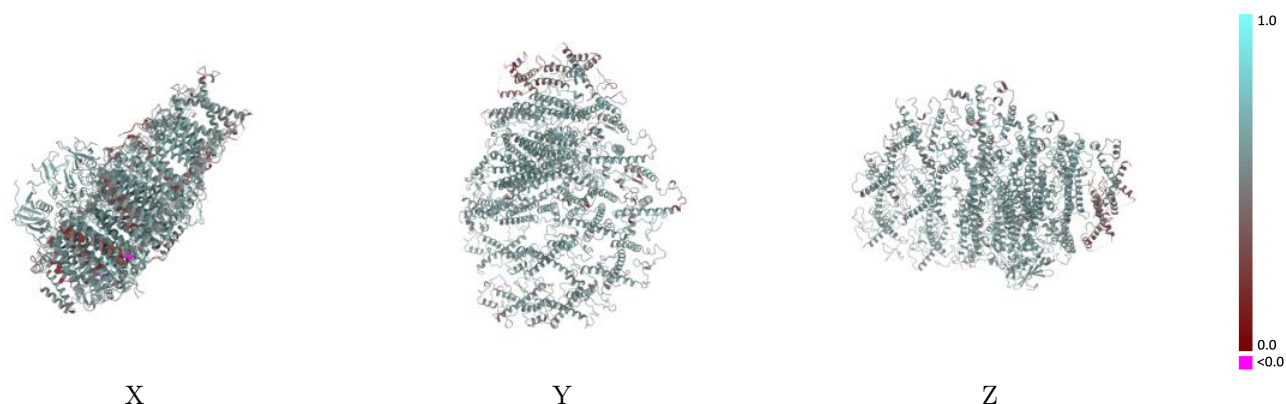
This section contains information regarding the fit between EMDB map EMD-9853 and PDB model 6JO5. Per-residue inclusion information can be found in section [3](#) on page [33](#).

### 9.1 Map-model overlay [i](#)



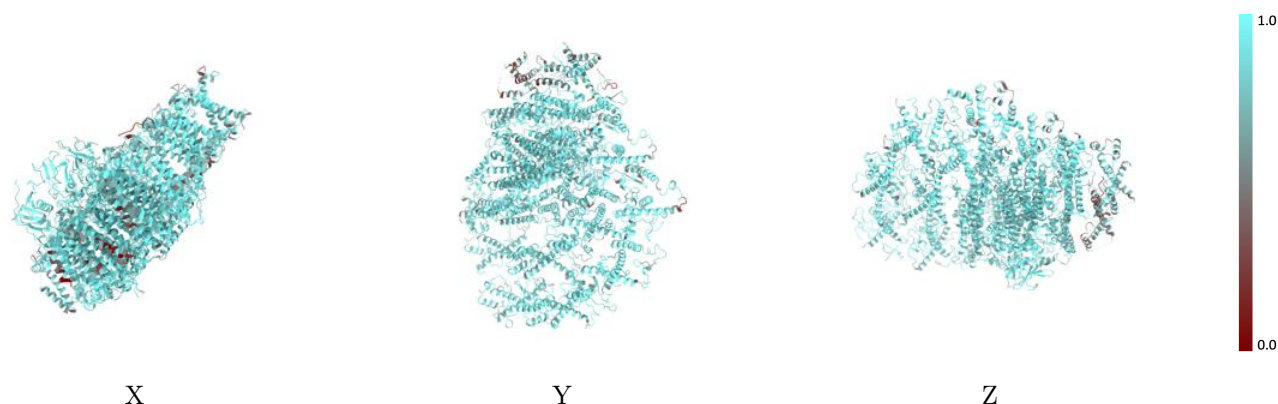
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



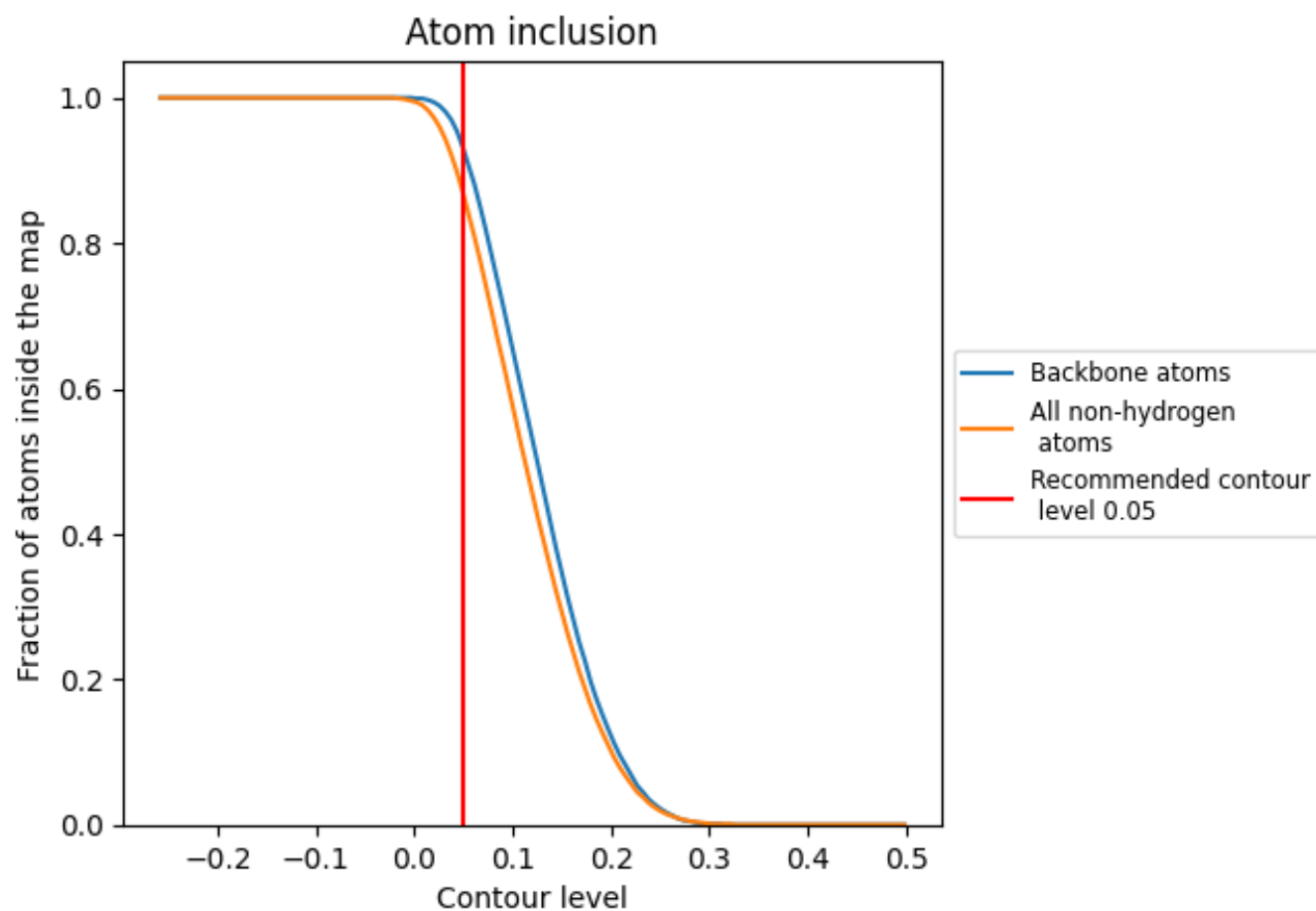
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

## 9.4 Atom inclusion [i](#)















































At the recommended contour level, 93% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.5670
1	 0.8540	 0.5660
2	 0.5380	 0.3290
3	 0.8920	 0.5820
4	 0.8490	 0.5440
5	 0.8520	 0.5470
6	 0.8490	 0.5510
7	 0.8850	 0.5860
8	 0.8910	 0.5830
9	 0.6950	 0.4490
A	 0.9280	 0.6080
B	 0.9220	 0.6090
C	 0.9550	 0.6010
D	 0.9040	 0.5730
E	 0.8910	 0.5830
F	 0.8660	 0.5660
G	 0.8300	 0.5500
I	 0.8680	 0.5680
J	 0.9140	 0.6010
K	 0.7800	 0.5270
L	 0.8370	 0.5420
Z	 0.7810	 0.5190

