



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 9MH0 / pdb_00009mh0
EMDB ID : EMD-48265
Title : Dunaliella salina PSI-LHCI supercomplex
Authors : Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.
Deposited on : 2024-12-11
Resolution : 2.90 Å(reported)
Based on initial model : 6SL5

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

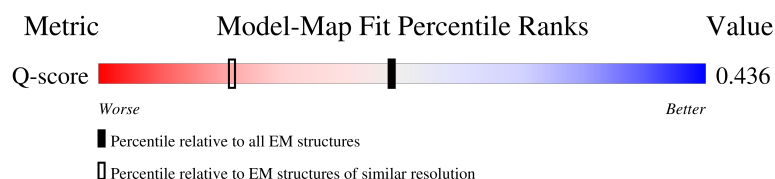
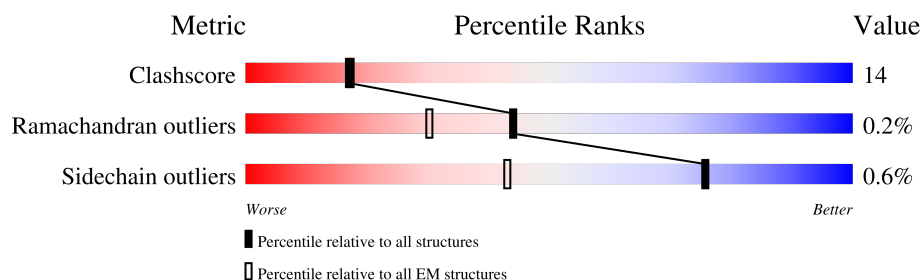
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1	228	13% 63% 24% 14%
2	2	263	41% 65% 19% 16%
3	3	320	8% 48% 17% 35%
4	7	256	7% 65% 17% 18%

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Mol	Chain	Length	Quality of chain
5	8	254	
6	9	222	
7	A	751	
8	B	735	
9	C	81	
10	D	202	
11	E	125	
12	F	232	
13	G	141	
14	H	135	
15	I	109	
16	J	41	
17	K	123	
18	L	202	

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
19	CHL	1	601	X	-	-	-
19	CHL	1	606	X	-	-	-
19	CHL	2	601	X	-	-	-
19	CHL	2	606	X	-	-	-
19	CHL	3	401	X	-	-	-
19	CHL	7	302	X	-	-	-
19	CHL	7	306	X	-	-	-
19	CHL	7	307	X	-	-	-
19	CHL	7	308	X	-	-	-
19	CHL	8	304	X	-	-	-
19	CHL	8	305	X	-	-	-
19	CHL	8	306	X	-	-	-
19	CHL	9	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	1	602	X	-	-	-
20	CLA	1	603	X	-	-	-
20	CLA	1	604	X	-	-	-
20	CLA	1	605	X	-	-	-
20	CLA	1	607	X	-	-	-
20	CLA	1	608	X	-	-	-
20	CLA	1	609	X	-	-	-
20	CLA	1	610	X	-	-	-
20	CLA	1	611	X	-	-	-
20	CLA	1	612	X	-	-	-
20	CLA	1	613	X	-	-	-
20	CLA	1	614	X	-	-	-
20	CLA	2	602	X	-	-	-
20	CLA	2	603	X	-	-	-
20	CLA	2	604	X	-	-	-
20	CLA	2	605	X	-	-	-
20	CLA	2	607	X	-	-	-
20	CLA	2	608	X	-	-	-
20	CLA	2	609	X	-	-	-
20	CLA	2	610	X	-	-	-
20	CLA	2	611	X	-	-	-
20	CLA	2	612	X	-	-	-
20	CLA	2	613	X	-	-	-
20	CLA	2	622	X	-	-	-
20	CLA	3	402	X	-	-	-
20	CLA	3	403	X	-	-	-
20	CLA	3	404	X	-	-	-
20	CLA	3	405	X	-	-	-
20	CLA	3	406	X	-	-	-
20	CLA	3	407	X	-	-	-
20	CLA	3	408	X	-	-	-
20	CLA	3	409	X	-	-	-
20	CLA	3	410	X	-	-	-
20	CLA	3	411	X	-	-	-
20	CLA	3	412	X	-	-	-
20	CLA	3	413	X	-	-	-
20	CLA	3	414	X	-	-	-
20	CLA	7	303	X	-	-	-
20	CLA	7	304	X	-	-	-
20	CLA	7	305	X	-	-	-
20	CLA	7	309	X	-	-	-
20	CLA	7	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	7	311	X	-	-	-
20	CLA	7	312	X	-	-	-
20	CLA	7	313	X	-	-	-
20	CLA	7	314	X	-	-	-
20	CLA	7	315	X	-	-	-
20	CLA	7	324	X	-	-	-
20	CLA	8	302	X	-	-	-
20	CLA	8	303	X	-	-	-
20	CLA	8	307	X	-	-	-
20	CLA	8	308	X	-	-	-
20	CLA	8	309	X	-	-	-
20	CLA	8	310	X	-	-	-
20	CLA	8	312	X	-	-	-
20	CLA	8	313	X	-	-	-
20	CLA	9	601	X	-	-	-
20	CLA	9	602	X	-	-	-
20	CLA	9	603	X	-	-	-
20	CLA	9	604	X	-	-	-
20	CLA	9	605	X	-	-	-
20	CLA	9	607	X	-	-	-
20	CLA	9	608	X	-	-	-
20	CLA	9	609	X	-	-	-
20	CLA	9	610	X	-	-	-
20	CLA	9	611	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	819	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	842	X	-	-	-
20	CLA	A	843	X	-	-	-
20	CLA	A	844	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	B	840	X	-	-	-
20	CLA	B	841	X	-	-	-
20	CLA	B	842	X	-	-	-
20	CLA	B	843	X	-	-	-
20	CLA	F	5003	X	-	-	-
20	CLA	F	5005	X	-	-	-
20	CLA	F	5006	X	-	-	-
20	CLA	F	5007	X	-	-	-
20	CLA	G	4002	X	-	-	-
20	CLA	G	4003	X	-	-	-
20	CLA	G	4004	X	-	-	-
20	CLA	H	204	X	-	-	-
20	CLA	J	4002	X	-	-	-
20	CLA	K	201	X	-	-	-
20	CLA	K	202	X	-	-	-
20	CLA	K	203	X	-	-	-
20	CLA	K	204	X	-	-	-
20	CLA	L	301	X	-	-	-
20	CLA	L	302	X	-	-	-
20	CLA	L	304	X	-	-	-
20	CLA	L	305	X	-	-	-
20	CLA	L	306	X	-	-	-
20	CLA	L	307	X	-	-	-
21	LUT	1	615	X	-	-	-
21	LUT	2	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	LUT	2	615	X	-	-	-
21	LUT	2	616	X	-	-	-
21	LUT	2	617	X	-	-	-
21	LUT	3	415	X	-	-	-
21	LUT	7	316	X	-	-	-
21	LUT	8	314	X	-	-	-
21	LUT	9	613	X	-	-	-
34	SF4	A	846	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 43016 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	197	Total	C	N	O	S	0	0
			1498	962	253	276	7		

- Molecule 2 is a protein called LHCA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1736	1128	286	313	9		

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	208	Total	C	N	O	S	0	0
			1597	1042	264	286	5		

- Molecule 4 is a protein called LHCA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	209	Total	C	N	O	S	0	0
			1609	1039	269	295	6		

- Molecule 5 is a protein called LHCA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	226	Total	C	N	O	S	0	0
			1726	1113	288	319	6		

- Molecule 6 is a protein called LHCA9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	187	Total	C	N	O	S	0	0
			1456	947	244	259	6		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	740	Total	C	N	O	S	0	0
			5807	3795	993	1001	18		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	732	Total	C	N	O	S	0	0
			5803	3813	973	1004	13		

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

- Molecule 10 is a protein called PSAD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	143	Total	C	N	O	S	0	0
			1133	726	196	205	6		

- Molecule 11 is a protein called PSAE1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	E	64	Total	C	N	O	0	0
			509	323	88	98		

- Molecule 12 is a protein called PSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	165	Total	C	N	O	S	0	0
			1303	840	223	238	2		

- Molecule 13 is a protein called PSAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	105	Total	C	N	O	S	0	0
			794	516	136	140	2		

- Molecule 14 is a protein called PSAH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	65	Total	C	N	O	S	0	0
			488	307	88	92	1		

- Molecule 15 is a protein called PSAI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	41	Total	C	N	O	S	0	0
			321	219	48	53	1		

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	41	Total	C	N	O	S	0	0
			327	223	47	56	1		

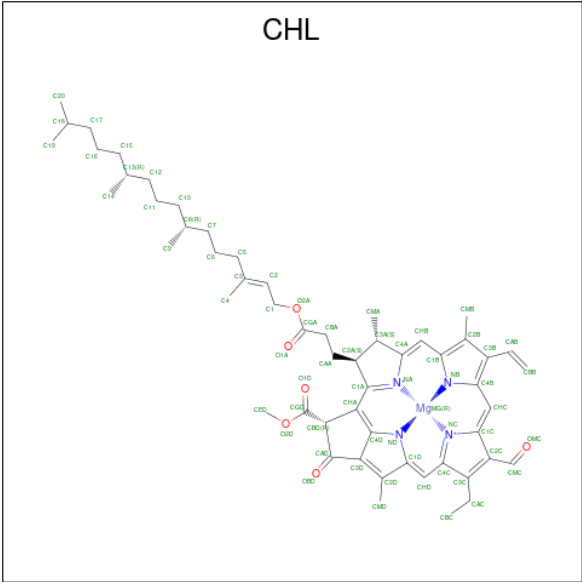
- Molecule 17 is a protein called PSAK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	83	Total	C	N	O	S	0	0
			584	373	101	107	3		

- Molecule 18 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	156	Total	C	N	O	S	0	0
			1149	749	188	206	6		

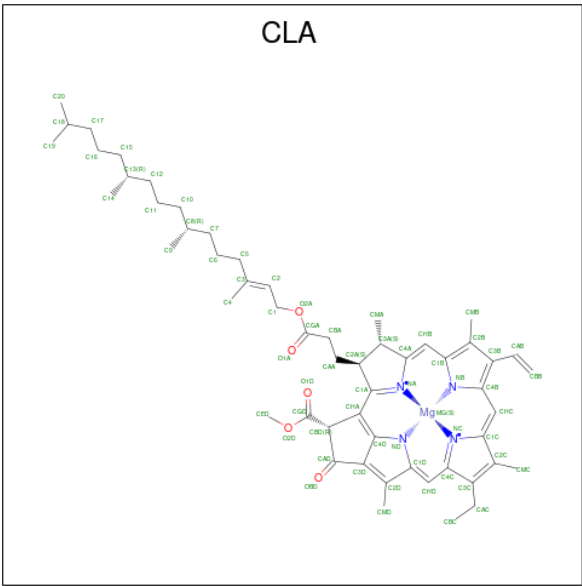
- Molecule 19 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	3	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
19	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 44	C 35	Mg 1	N 4	O 4	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	3	1	Total 57	C 47	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	7	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 48	C 38	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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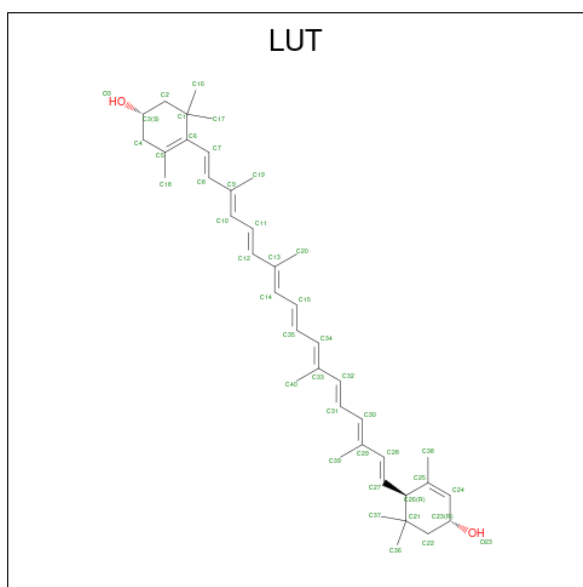
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	F	1	Total 49	C 39	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	J	1	Total 49	C 39	Mg 1	N 4	O 5	0

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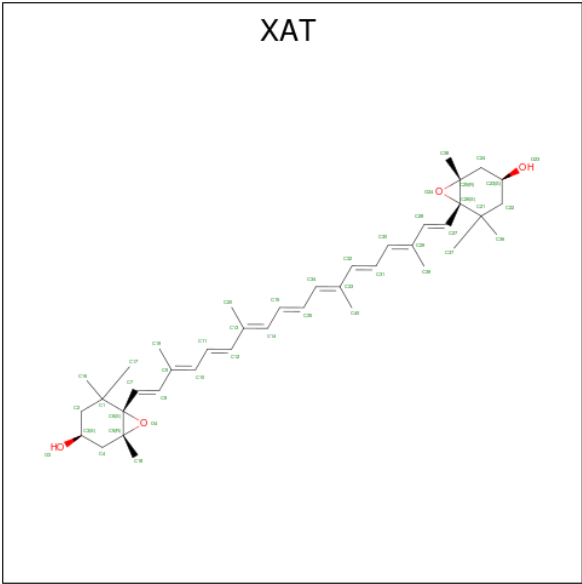
Mol	Chain	Residues	Atoms					AltConf
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	7	1	Total	C	O	0
			42	40	2	
21	8	1	Total	C	O	0
			42	40	2	
21	9	1	Total	C	O	0
			42	40	2	

- Molecule 22 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



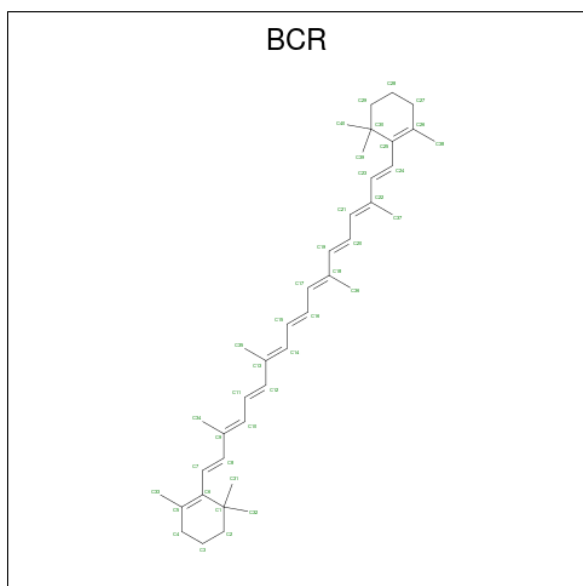
Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
22	7	1	Total	C	O	0
			44	40	4	
22	8	1	Total	C	O	0
			44	40	4	
22	9	1	Total	C	O	0
			44	40	4	
22	9	1	Total	C	O	0
			44	40	4	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
23	1	1	Total	C	0
			40	40	
23	3	1	Total	C	0
			40	40	
23	3	1	Total	C	0
			40	40	
23	3	1	Total	C	0
			40	40	
23	7	1	Total	C	0
			40	40	
23	8	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	

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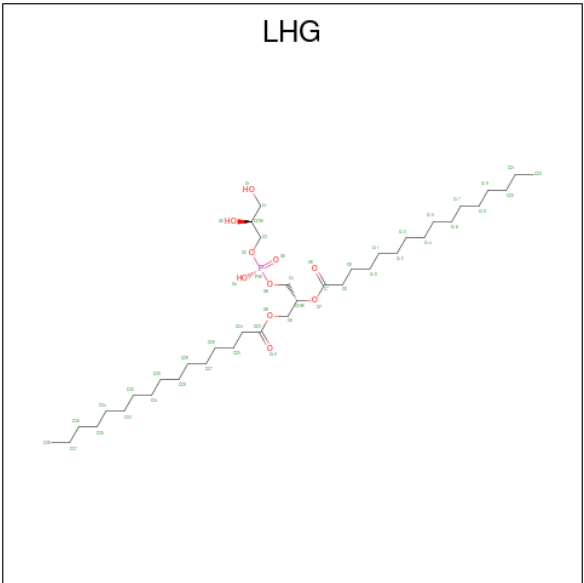
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	H	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
23	L	1	Total	C	0
			40	40	
23	L	1	Total	C	0
			40	40	
23	L	1	Total	C	0
			40	40	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



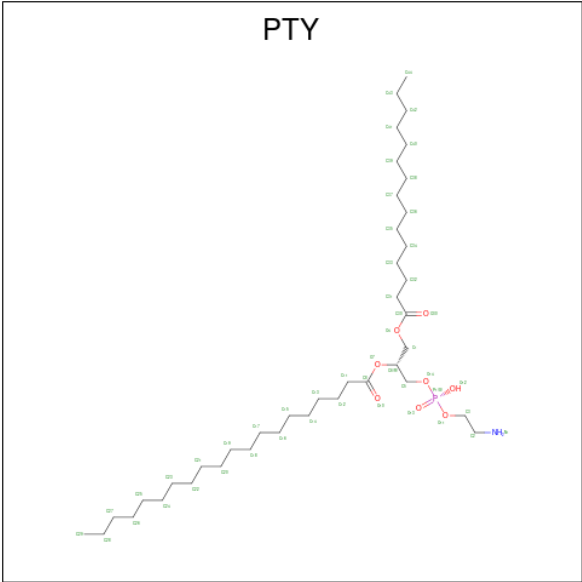
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	P	0
			25	14	10	1	
24	1	1	Total	C	O	P	0
			44	33	10	1	
24	1	1	Total	C	O	P	0
			31	20	10	1	
24	1	1	Total	C	O	P	0
			46	35	10	1	
24	2	1	Total	C	O	P	0
			44	35	8	1	
24	2	1	Total	C	O	P	0
			36	25	10	1	
24	3	1	Total	C	O	P	0
			17	8	8	1	
24	3	1	Total	C	O	P	0
			39	28	10	1	

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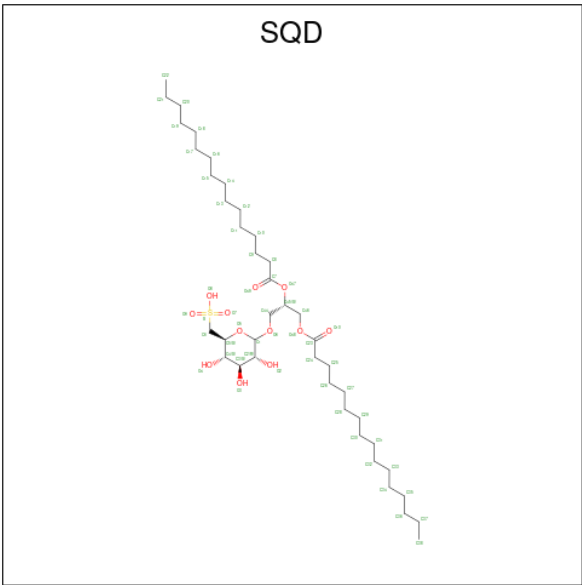
Mol	Chain	Residues	Atoms				AltConf
24	7	1	Total	C	O	P	0
			49	38	10	1	
24	7	1	Total	C	O	P	0
			22	11	10	1	
24	7	1	Total	C	O	P	0
			40	29	10	1	
24	8	1	Total	C	O	P	0
			34	23	10	1	
24	8	1	Total	C	O	P	0
			31	20	10	1	
24	9	1	Total	C	O	P	0
			41	30	10	1	
24	9	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			30	20	9	1	
24	A	1	Total	C	O	P	0
			45	34	10	1	
24	B	1	Total	C	O	P	0
			49	38	10	1	
24	F	1	Total	C	O	P	0
			43	32	10	1	
24	F	1	Total	C	O	P	0
			42	31	10	1	
24	G	1	Total	C	O	P	0
			49	38	10	1	
24	H	1	Total	C	O	P	0
			38	27	10	1	
24	I	1	Total	C	O	P	0
			49	38	10	1	
24	J	1	Total	C	O	P	0
			36	29	6	1	

- Molecule 25 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



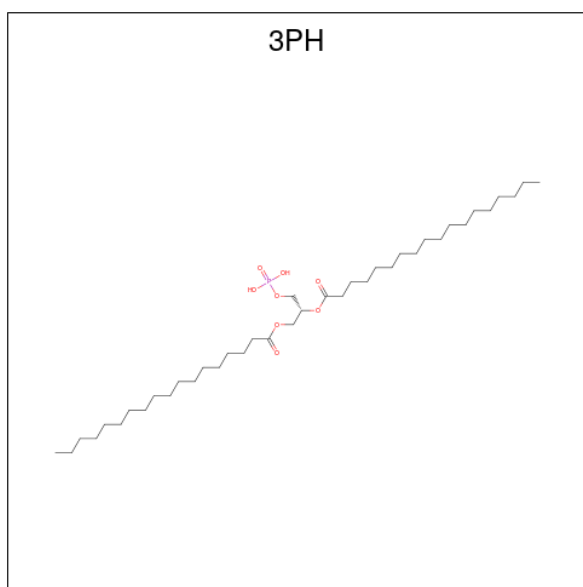
Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	N	O	P	0
			20	10	1	8	1	
25	1	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	3	1	Total	C	N	O	P	0
			26	16	1	8	1	
25	7	1	Total	C	N	O	P	0
			25	15	1	8	1	
25	8	1	Total	C	N	O	P	0
			24	14	1	8	1	
25	8	1	Total	C	N	O	P	0
			21	11	1	8	1	
25	B	1	Total	C	N	O	P	0
			27	17	1	8	1	
25	F	1	Total	C	N	O	P	0
			22	12	1	8	1	
25	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
25	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	L	1	Total	C	N	O	P	0
			20	10	1	8	1	

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



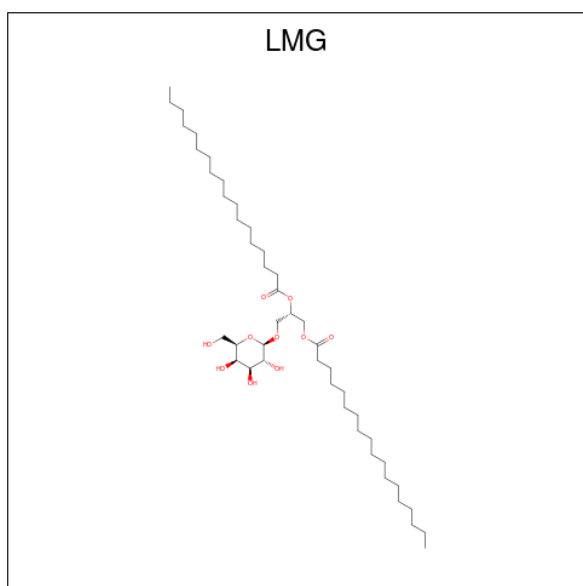
Mol	Chain	Residues	Atoms				AltConf
26	2	1	Total	C	O	S	0
			41	28	12	1	
26	3	1	Total	C	O	S	0
			35	22	12	1	
26	3	1	Total	C	O	S	0
			32	19	12	1	
26	9	1	Total	C	O	S	0
			37	24	12	1	
26	B	1	Total	C	O	S	0
			31	18	12	1	

- Molecule 27 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
27	2	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



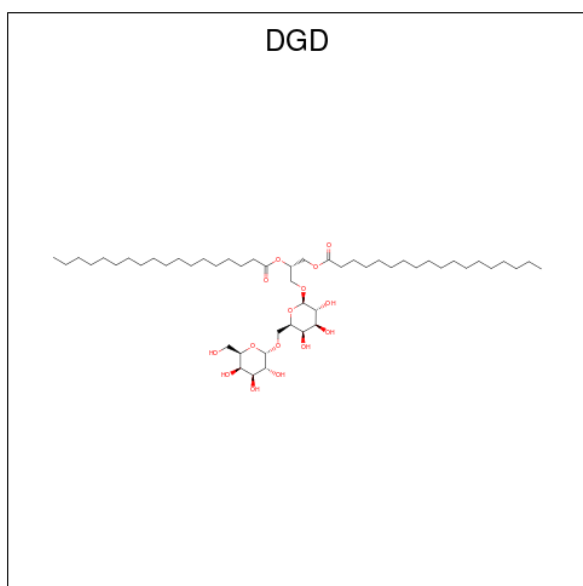
Mol	Chain	Residues	Atoms				AltConf
28	7	1	Total	C	O		0
			40	30	10		
28	7	1	Total	C	O		0
			54	44	10		

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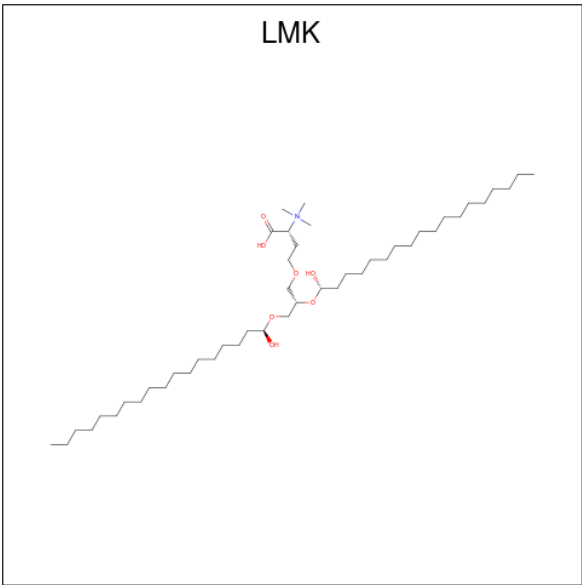
Mol	Chain	Residues	Atoms			AltConf
28	8	1	Total	C	O	0
			50	40	10	
28	A	1	Total	C	O	0
			32	22	10	
28	F	1	Total	C	O	0
			46	36	10	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



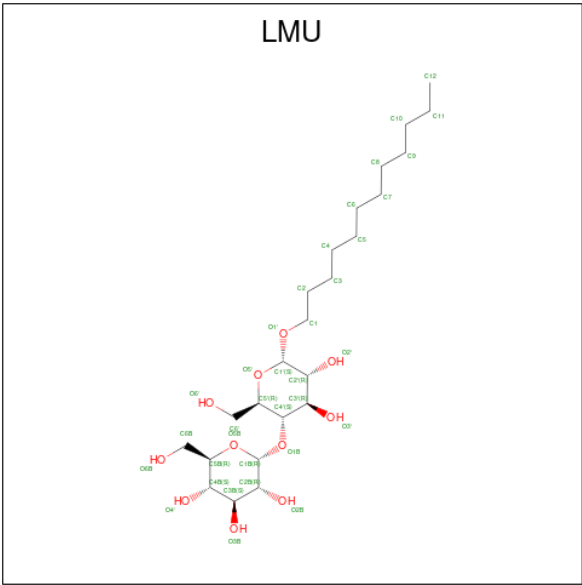
Mol	Chain	Residues	Atoms			AltConf
29	7	1	Total	C	O	0
			47	32	15	
29	A	1	Total	C	O	0
			66	51	15	
29	B	1	Total	C	O	0
			61	46	15	
29	L	1	Total	C	O	0
			58	43	15	

- Molecule 30 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanum (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$) (labeled as "Ligand of Interest" by depositor).



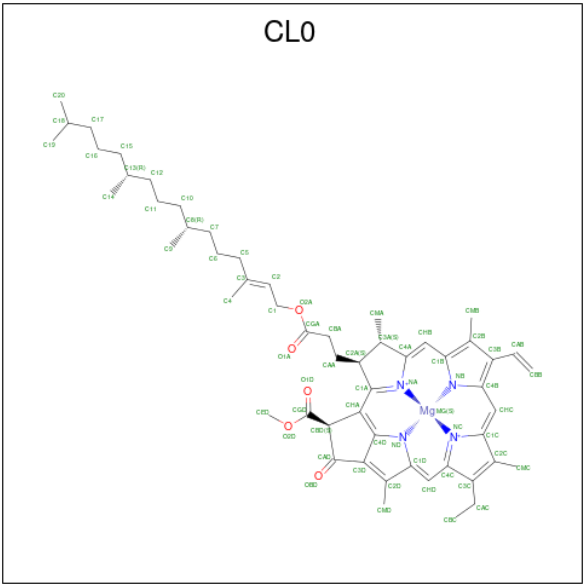
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	8	1	35	27	1	7	0

- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



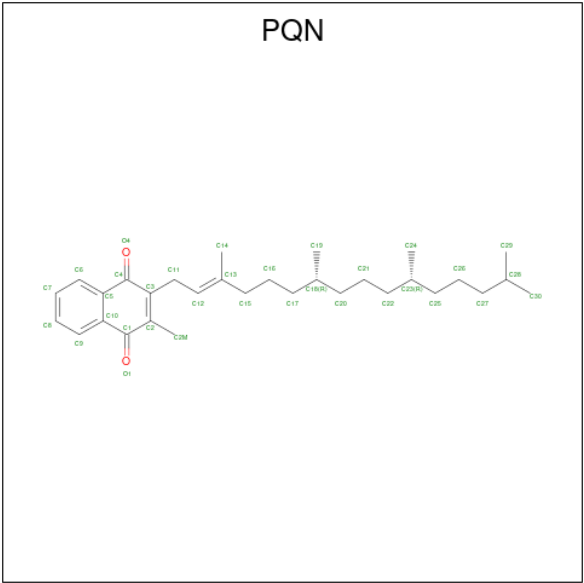
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	9	1	35	24	11	0
31	A	1	35	24	11	0
31	A	1	35	24	11	0

- Molecule 32 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 33 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



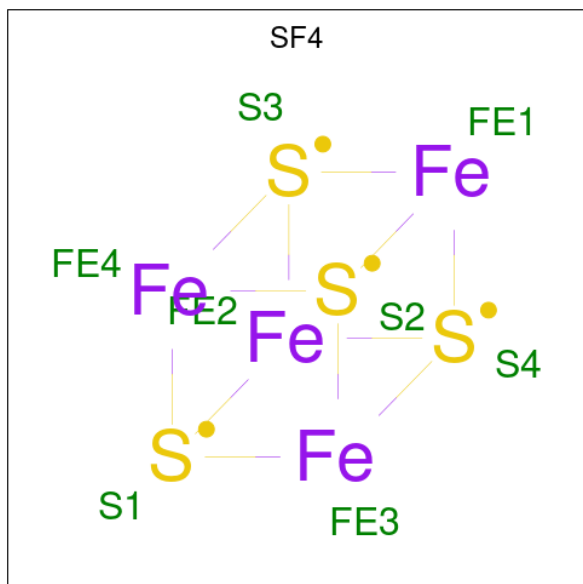
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			33	31	2	

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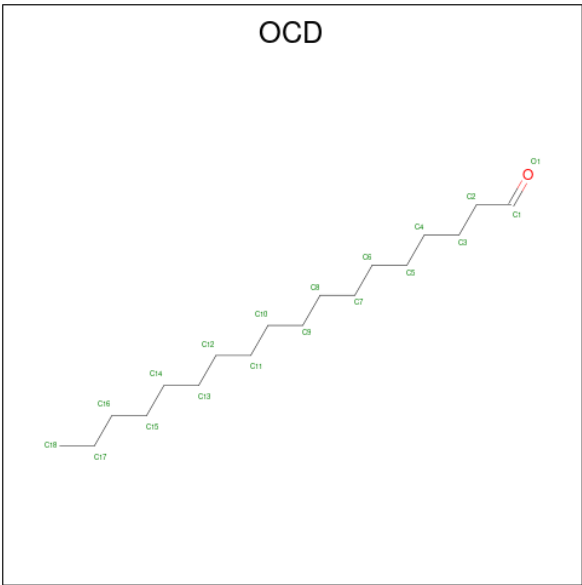
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			33	31	2	

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



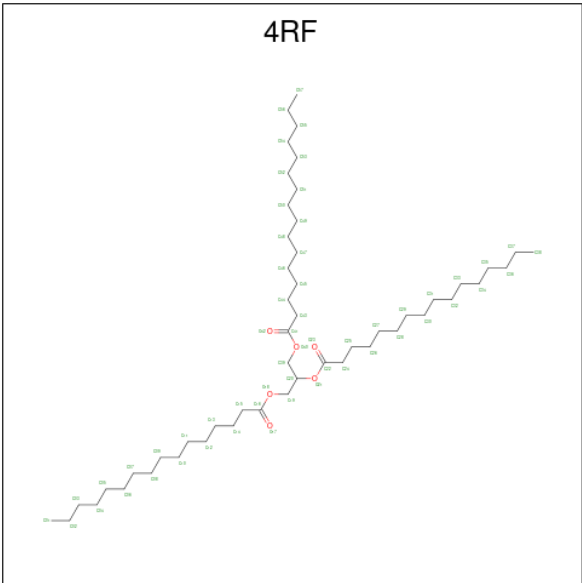
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 35 is octadecanal (CCD ID: OCD) (formula: $\text{C}_{18}\text{H}_{36}\text{O}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	C	0
			11	11	

- Molecule 36 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$) (labeled as "Ligand of Interest" by depositor).

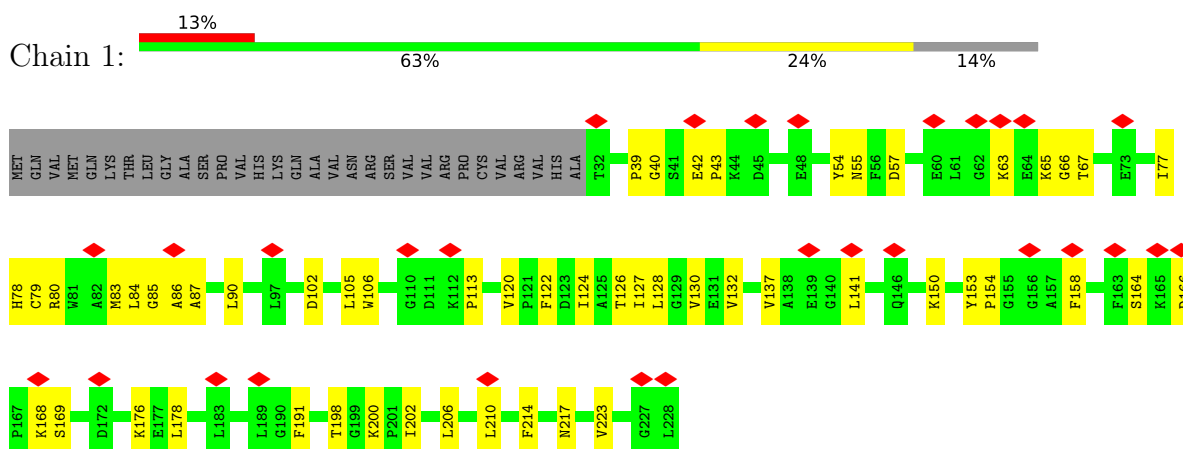


Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			39	33	6	

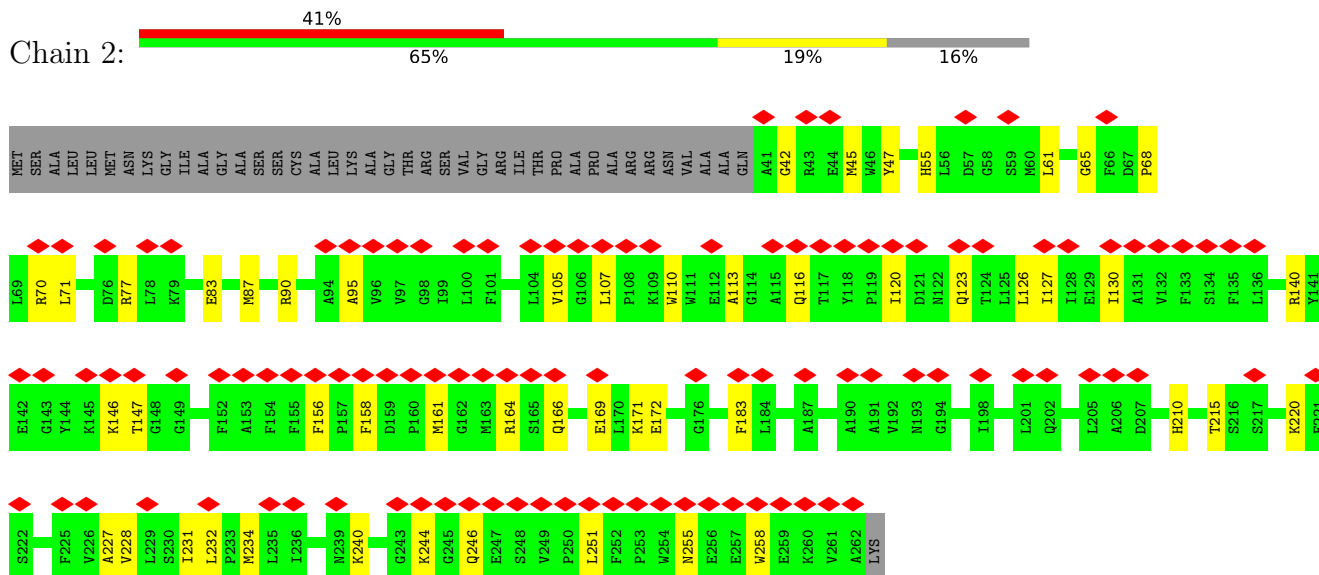
3 Residue-property plots

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: Chlorophyll a-b binding protein, chloroplastic

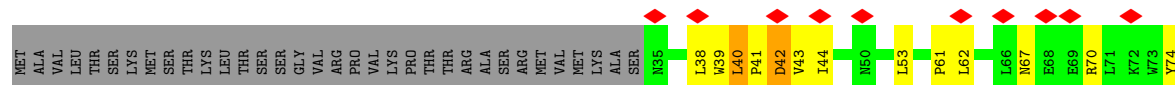


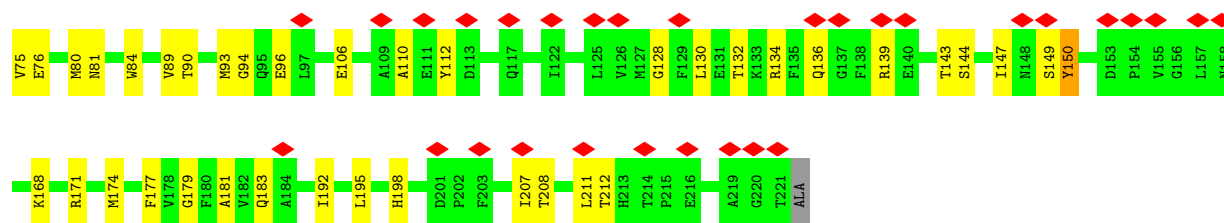
- Molecule 2: LHCA2



- Molecule 3: LHCA3

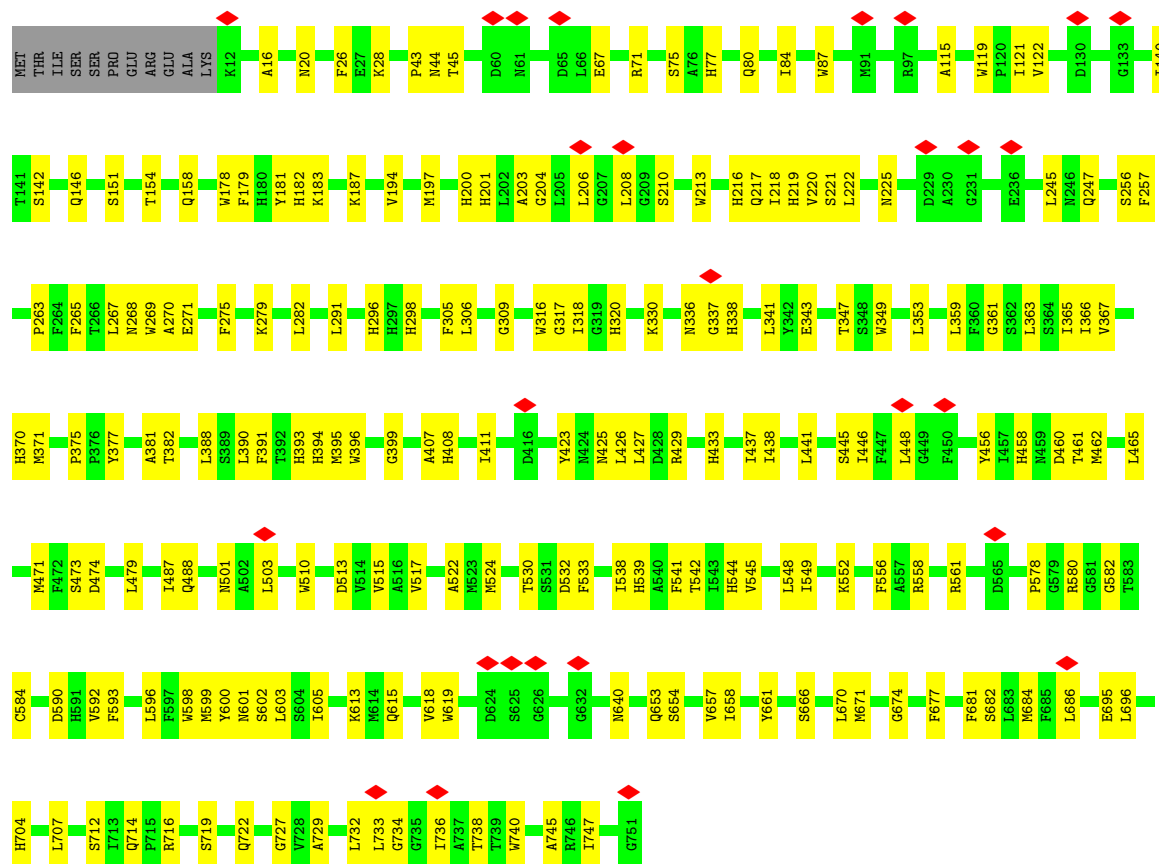






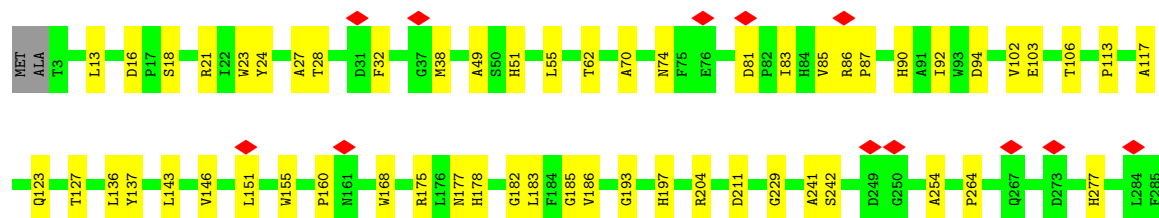
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

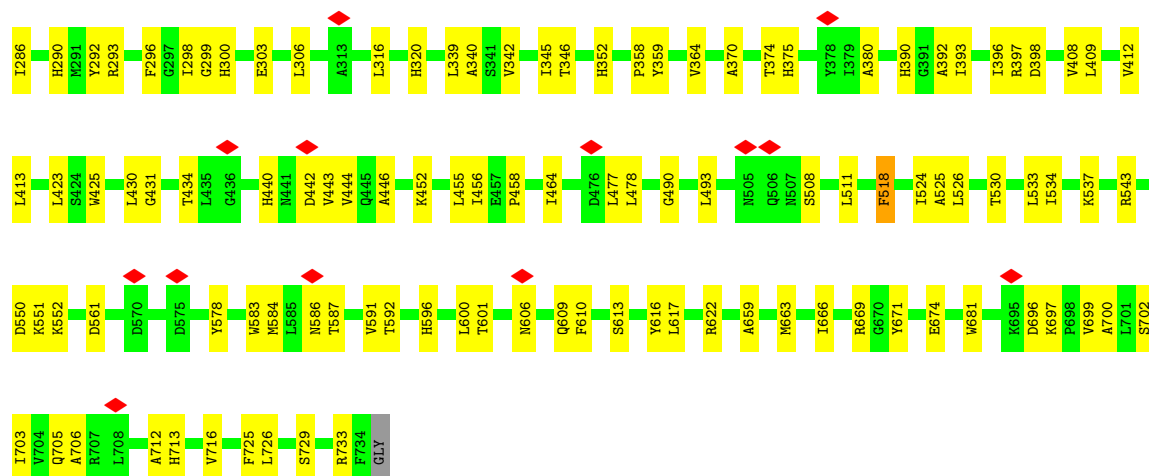
Chain A: 71% 27%



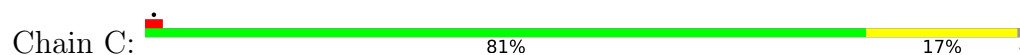
• Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 77% 22%





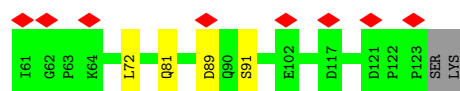
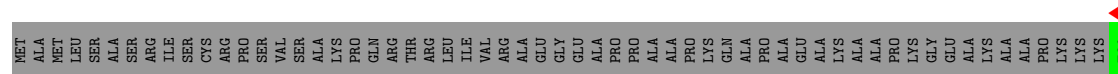
- Molecule 9: Photosystem I iron-sulfur center



- Molecule 10: PSAD1

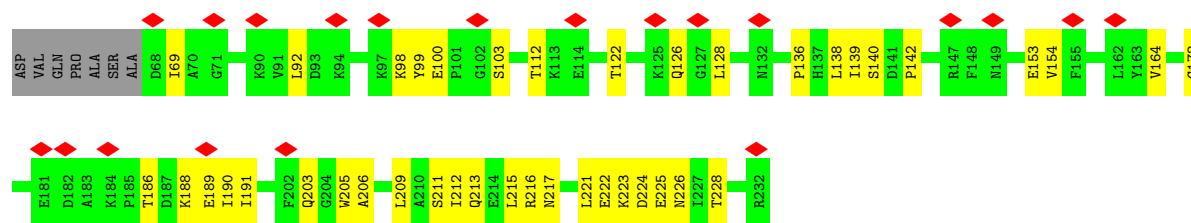


- Molecule 11: PSAE1

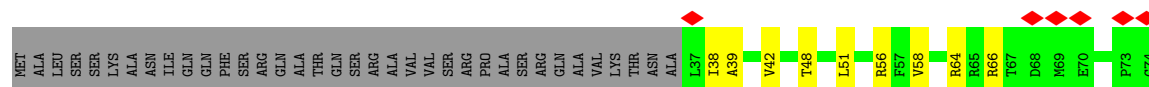


- Molecule 12: PSAF1

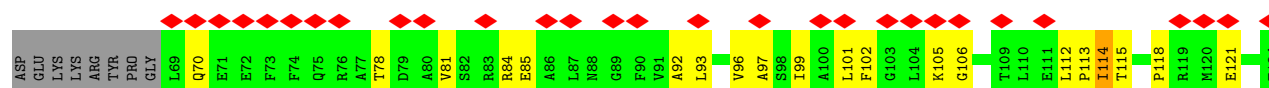
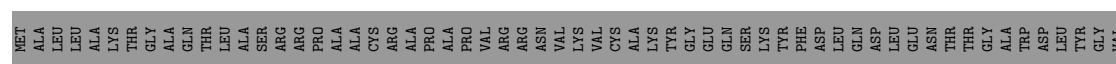
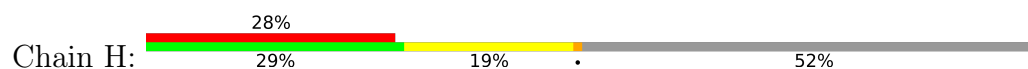




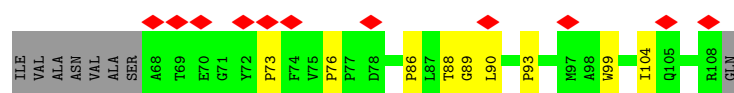
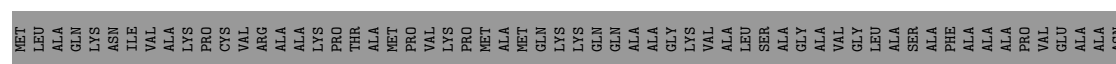
- Molecule 13: PSAG1



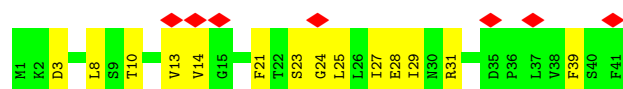
- Molecule 14: PSAH1



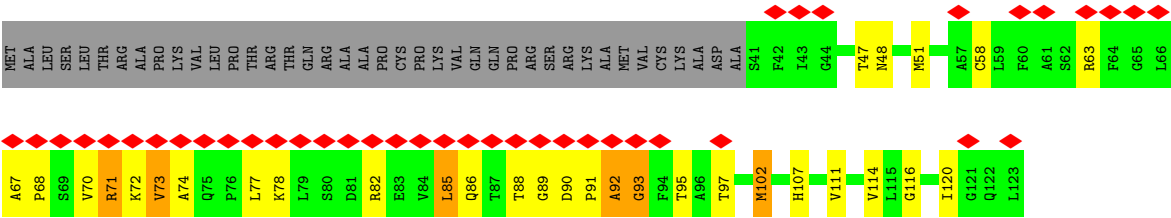
- Molecule 15: PSAI1



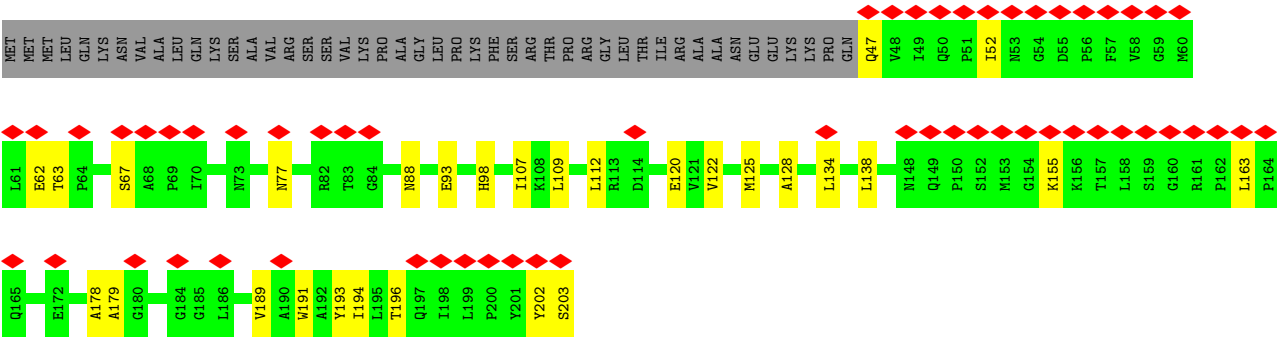
- Molecule 16: Photosystem I reaction center subunit IX



- Molecule 17: PSAK1



● Molecule 18: PSAL1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98784	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0165	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, LMU, LHG, LMG, PQN, PTY, DGD, 3PH, SF4, 4RF, OCD, CL0, LMK, SQD, LUT, CHL, 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	1	0.19	0/1537	0.47	0/2084
2	2	0.18	0/1787	0.44	0/2425
3	3	0.19	0/1644	0.42	0/2228
4	7	0.17	0/1659	0.39	0/2254
5	8	0.19	0/1775	0.44	1/2406 (0.0%)
6	9	0.29	0/1499	0.60	0/2043
7	A	0.15	0/6003	0.34	0/8189
8	B	0.16	0/6016	0.35	0/8225
9	C	0.15	0/610	0.36	0/828
10	D	0.15	0/1163	0.35	0/1571
11	E	0.12	0/521	0.28	0/711
12	F	0.19	0/1332	0.47	0/1801
13	G	0.18	0/815	0.47	0/1104
14	H	0.28	0/493	0.75	1/660 (0.2%)
15	I	0.23	0/335	0.62	0/463
16	J	0.23	0/338	0.59	0/461
17	K	0.31	0/592	0.96	4/801 (0.5%)
18	L	0.17	0/1179	0.48	0/1612
All	All	0.18	0/29298	0.44	6/39866 (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
12	F	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	71	ARG	CA-C-N	-11.03	107.45	123.11
17	K	71	ARG	C-N-CA	-11.03	107.45	123.11
17	K	85	LEU	CA-CB-CG	5.87	136.84	116.30
5	8	125	MET	CB-CG-SD	5.73	129.90	112.70
17	K	102	MET	CB-CG-SD	5.51	129.24	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	F	216	ARG	Sidechain

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	1	1498	0	1468	52	0
2	2	1736	0	1704	54	0
3	3	1597	0	1559	63	0
4	7	1609	0	1565	39	0
5	8	1726	0	1678	53	0
6	9	1456	0	1441	51	0
7	A	5807	0	5640	192	0
8	B	5803	0	5556	153	0
9	C	600	0	583	15	0
10	D	1133	0	1141	16	0
11	E	509	0	497	2	0
12	F	1303	0	1331	33	0
13	G	794	0	799	28	0
14	H	488	0	505	30	0
15	I	321	0	316	10	0
16	J	327	0	327	16	0
17	K	584	0	614	41	0
18	L	1149	0	1171	22	0
19	1	98	0	68	8	0
19	2	108	0	88	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	3	56	0	47	6	0
19	7	211	0	171	16	0
19	8	145	0	97	9	0
19	9	47	0	31	4	0
20	1	659	0	603	29	0
20	2	589	0	467	25	0
20	3	699	0	622	25	0
20	7	647	0	634	21	0
20	8	488	0	434	15	0
20	9	591	0	520	20	0
20	A	2535	0	2641	175	0
20	B	2559	0	2703	148	0
20	F	262	0	225	11	0
20	G	138	0	101	4	0
20	H	45	0	33	0	0
20	J	49	0	38	6	0
20	K	193	0	151	11	0
20	L	340	0	325	13	0
21	1	42	0	56	7	0
21	2	168	0	224	15	0
21	3	42	0	56	2	0
21	7	42	0	56	2	0
21	8	42	0	56	0	0
21	9	42	0	56	4	0
22	1	44	0	56	2	0
22	3	44	0	56	3	0
22	7	44	0	56	6	0
22	8	44	0	56	3	0
22	9	88	0	112	9	0
23	1	40	0	56	2	0
23	3	120	0	168	10	0
23	7	40	0	56	4	0
23	8	40	0	56	4	0
23	A	280	0	389	46	0
23	B	240	0	336	27	0
23	F	80	0	111	9	0
23	G	80	0	112	5	0
23	H	40	0	56	0	0
23	I	40	0	56	3	0
23	J	80	0	112	10	0
23	K	40	0	56	5	0
23	L	120	0	168	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	1	146	0	178	5	0
24	2	80	0	107	4	0
24	3	56	0	62	2	0
24	7	111	0	141	6	0
24	8	65	0	70	3	0
24	9	90	0	129	4	0
24	A	75	0	92	4	0
24	B	49	0	74	0	0
24	F	85	0	113	6	0
24	G	49	0	74	3	0
24	H	38	0	49	2	0
24	I	49	0	74	6	0
24	J	36	0	52	1	0
25	1	55	0	56	2	0
25	3	26	0	25	0	0
25	7	25	0	23	0	0
25	8	45	0	38	0	0
25	B	27	0	27	0	0
25	F	22	0	17	0	0
25	H	78	0	100	6	0
25	L	20	0	13	0	0
26	2	41	0	49	3	0
26	3	67	0	62	5	0
26	9	37	0	38	1	0
26	B	31	0	26	1	0
27	2	33	0	39	4	0
28	7	94	0	134	4	0
28	8	50	0	70	5	0
28	A	32	0	34	2	0
28	F	46	0	62	3	0
29	7	47	0	52	4	0
29	A	66	0	92	4	0
29	B	61	0	83	8	0
29	L	58	0	77	4	0
30	8	35	0	0	0	0
31	9	35	0	46	4	0
31	A	70	0	91	3	0
32	A	65	0	72	8	0
33	A	33	0	46	1	0
33	B	33	0	46	4	0
34	A	8	0	0	4	0
34	C	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	11	0	0	0	0
36	A	39	0	53	2	0
All	All	43016	0	43152	1190	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 14.

The worst 5 of 1190 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)
7:A:584:CYS:SG	34:A:846:SF4:FE4	1.05	1.49
2:2:227:ALA:O	2:2:231:ILE:HD12	1.19	1.29
8:B:431:GLY:CA	8:B:526:LEU:HD11	1.74	1.16
1:1:80:ARG:HA	1:1:83:MET:HE3	1.24	1.15
17:K:71:ARG:NH1	17:K:72:LYS:HE2	1.61	1.15

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	1	195/228 (86%)	179 (92%)	16 (8%)	0	100	100
2	2	220/263 (84%)	211 (96%)	8 (4%)	1 (0%)	24	54
3	3	206/320 (64%)	201 (98%)	4 (2%)	1 (0%)	24	54
4	7	207/256 (81%)	198 (96%)	9 (4%)	0	100	100
5	8	224/254 (88%)	218 (97%)	6 (3%)	0	100	100
6	9	185/222 (83%)	168 (91%)	15 (8%)	2 (1%)	11	36
7	A	738/751 (98%)	709 (96%)	29 (4%)	0	100	100
8	B	730/735 (99%)	704 (96%)	26 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
10	D	141/202 (70%)	134 (95%)	7 (5%)	0	100	100
11	E	62/125 (50%)	60 (97%)	2 (3%)	0	100	100
12	F	163/232 (70%)	152 (93%)	11 (7%)	0	100	100
13	G	103/141 (73%)	96 (93%)	6 (6%)	1 (1%)	12	39
14	H	63/135 (47%)	55 (87%)	7 (11%)	1 (2%)	7	27
15	I	39/109 (36%)	38 (97%)	1 (3%)	0	100	100
16	J	39/41 (95%)	33 (85%)	6 (15%)	0	100	100
17	K	81/123 (66%)	64 (79%)	15 (18%)	2 (2%)	4	17
18	L	154/202 (76%)	145 (94%)	9 (6%)	0	100	100
All	All	3628/4420 (82%)	3438 (95%)	182 (5%)	8 (0%)	44	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	120	ILE
3	3	255	PHE
6	9	40	LEU
13	G	38	ILE
17	K	92	ALA

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	1	151/178 (85%)	150 (99%)	1 (1%)	76	92
2	2	179/207 (86%)	179 (100%)	0	100	100
3	3	159/236 (67%)	158 (99%)	1 (1%)	78	93
4	7	166/201 (83%)	165 (99%)	1 (1%)	78	93
5	8	173/196 (88%)	171 (99%)	2 (1%)	63	86
6	9	153/183 (84%)	150 (98%)	3 (2%)	48	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	A	599/609 (98%)	597 (100%)	2 (0%)	86	96
8	B	593/594 (100%)	591 (100%)	2 (0%)	86	96
9	C	68/69 (99%)	68 (100%)	0	100	100
10	D	123/163 (76%)	122 (99%)	1 (1%)	73	90
11	E	57/101 (56%)	56 (98%)	1 (2%)	51	80
12	F	138/184 (75%)	137 (99%)	1 (1%)	76	92
13	G	81/110 (74%)	81 (100%)	0	100	100
14	H	50/105 (48%)	50 (100%)	0	100	100
15	I	32/77 (42%)	32 (100%)	0	100	100
16	J	36/36 (100%)	36 (100%)	0	100	100
17	K	61/94 (65%)	59 (97%)	2 (3%)	33	67
18	L	120/159 (76%)	120 (100%)	0	100	100
All	All	2939/3502 (84%)	2922 (99%)	17 (1%)	76	93

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	F	222	GLU
17	K	88	THR
6	9	150	TYR
7	A	471	MET
7	A	544	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
7	A	387	GLN
8	B	99	GLN
12	F	174	GLN
7	A	539	HIS
8	B	206	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

291 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	$\# Z > 2$
31	LMU	A	856	-	36,36,36	0.18	0	47,47,47	0.40	0
23	BCR	B	847	-	41,41,41	0.14	0	56,56,56	0.28	0
20	CLA	9	609	24	64,68,73	1.17	7 (10%)	76,107,113	1.18	4 (5%)
25	PTY	H	201	-	45,45,49	0.48	0	48,50,54	0.44	0
20	CLA	8	313	5	55,59,73	1.30	8 (14%)	64,96,113	1.20	4 (6%)
20	CLA	A	838	7	55,59,73	1.34	8 (14%)	64,96,113	1.37	4 (6%)
33	PQN	B	844	-	34,34,34	0.29	0	43,45,45	0.57	1 (2%)
23	BCR	A	848	-	41,41,41	0.43	0	56,56,56	0.99	3 (5%)
20	CLA	7	312	4	56,60,73	1.29	9 (16%)	65,97,113	1.42	5 (7%)
20	CLA	A	816	7	69,73,73	1.14	8 (11%)	82,113,113	1.30	6 (7%)
25	PTY	8	317	-	23,23,49	0.67	0	26,28,54	0.49	0
20	CLA	1	610	24	50,54,73	1.33	7 (14%)	59,90,113	1.20	4 (6%)
20	CLA	A	811	7	69,73,73	1.12	7 (10%)	82,113,113	1.10	5 (6%)
20	CLA	A	810	-	64,68,73	1.23	8 (12%)	76,107,113	1.17	7 (9%)
20	CLA	A	812	7	69,73,73	1.21	8 (11%)	82,113,113	1.33	8 (9%)
20	CLA	B	816	8	59,63,73	1.26	9 (15%)	70,101,113	1.28	4 (5%)
20	CLA	F	5006	-	51,55,73	1.34	8 (15%)	60,91,113	1.27	5 (8%)
21	LUT	9	613	-	42,43,43	0.30	0	51,60,60	0.34	0
23	BCR	B	848	-	41,41,41	0.13	0	56,56,56	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	H	203	-	37,37,48	0.34	0	40,43,54	0.35	0
23	BCR	J	4001	-	41,41,41	0.31	0	56,56,56	0.96	4 (7%)
29	DGD	L	311	-	59,59,67	0.20	0	73,73,81	0.23	0
20	CLA	G	4002	13	51,55,73	1.35	7 (13%)	60,91,113	1.35	5 (8%)
20	CLA	B	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.17	6 (7%)
20	CLA	B	835	-	64,68,73	1.19	8 (12%)	76,107,113	1.24	5 (6%)
20	CLA	B	838	-	64,68,73	1.18	7 (10%)	76,107,113	1.17	5 (6%)
20	CLA	3	409	-	54,58,73	1.31	6 (11%)	64,95,113	1.35	5 (7%)
20	CLA	A	837	7	59,63,73	1.27	8 (13%)	70,101,113	1.28	7 (10%)
20	CLA	A	828	-	69,73,73	1.18	8 (11%)	82,113,113	1.34	6 (7%)
24	LHG	7	323	-	21,21,48	0.41	0	24,27,54	0.44	0
20	CLA	7	314	4	54,58,73	1.30	7 (12%)	64,95,113	1.32	6 (9%)
20	CLA	F	5007	12	53,57,73	1.31	7 (13%)	61,93,113	1.32	5 (8%)
20	CLA	A	814	7	69,73,73	1.16	8 (11%)	82,113,113	1.09	5 (6%)
20	CLA	F	5008	12	50,54,73	1.61	8 (16%)	59,90,113	1.43	6 (10%)
25	PTY	L	310	-	19,19,49	0.71	0	22,24,54	0.56	0
20	CLA	2	604	-	54,58,73	1.28	8 (14%)	64,95,113	1.19	6 (9%)
20	CLA	B	832	8	64,68,73	1.22	8 (12%)	76,107,113	1.31	5 (6%)
20	CLA	B	817	8	64,68,73	1.23	9 (14%)	76,107,113	1.30	5 (6%)
20	CLA	L	305	18	69,73,73	1.11	7 (10%)	82,113,113	1.13	8 (9%)
19	CHL	2	601	2	55,69,74	0.80	2 (3%)	52,108,114	2.19	7 (13%)
20	CLA	L	302	-	69,73,73	1.15	7 (10%)	82,113,113	1.15	6 (7%)
20	CLA	A	813	7	59,63,73	1.28	8 (13%)	70,101,113	1.19	4 (5%)
20	CLA	7	309	4	69,73,73	1.14	6 (8%)	82,113,113	1.22	6 (7%)
24	LHG	2	621	-	35,35,48	0.38	0	38,41,54	0.34	0
20	CLA	9	605	6	49,53,73	1.63	11 (22%)	58,89,113	1.38	9 (15%)
20	CLA	B	820	-	69,73,73	1.21	10 (14%)	82,113,113	1.21	6 (7%)
20	CLA	B	809	8	69,73,73	1.14	7 (10%)	82,113,113	1.14	6 (7%)
20	CLA	1	613	1	59,63,73	1.28	8 (13%)	70,101,113	1.32	6 (8%)
20	CLA	A	842	7	65,69,73	1.23	8 (12%)	77,108,113	1.23	4 (5%)
20	CLA	B	837	8	55,59,73	1.31	8 (14%)	64,96,113	1.42	6 (9%)
23	BCR	B	802	-	41,41,41	0.23	0	56,56,56	1.02	5 (8%)
20	CLA	3	404	-	50,54,73	1.33	7 (14%)	59,90,113	1.25	4 (6%)
20	CLA	1	614	1	50,54,73	1.35	8 (16%)	59,90,113	1.51	9 (15%)
20	CLA	9	603	6	59,63,73	1.38	9 (15%)	70,101,113	1.31	6 (8%)
24	LHG	1	621	-	45,45,48	0.32	0	48,51,54	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	L	304	18	69,73,73	1.16	6 (8%)	82,113,113	1.18	5 (6%)
20	CLA	1	603	1	69,73,73	1.16	9 (13%)	82,113,113	1.18	4 (4%)
20	CLA	3	402	3	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
23	BCR	3	417	-	41,41,41	0.19	0	56,56,56	0.37	0
26	SQD	2	619	-	39,41,54	0.20	0	49,52,65	0.22	0
22	XAT	8	315	-	41,47,47	0.16	0	54,74,74	0.68	1 (1%)
24	LHG	3	420	-	16,16,48	0.90	1 (6%)	17,20,54	0.65	0
24	LHG	1	619	-	43,43,48	0.32	0	46,49,54	0.33	0
24	LHG	7	325	-	39,39,48	0.34	0	42,45,54	0.38	0
20	CLA	1	612	-	59,63,73	1.39	11 (18%)	70,101,113	1.60	17 (24%)
22	XAT	9	614	-	41,47,47	0.14	0	54,74,74	0.76	2 (3%)
24	LHG	3	424	-	38,38,48	0.34	0	41,44,54	0.34	0
20	CLA	B	840	-	69,73,73	1.20	9 (13%)	82,113,113	1.22	5 (6%)
20	CLA	B	812	-	59,63,73	1.25	7 (11%)	70,101,113	1.24	4 (5%)
20	CLA	2	605	-	49,53,73	1.37	6 (12%)	58,89,113	1.28	4 (6%)
28	LMG	A	801	-	32,32,55	0.21	0	40,40,63	0.27	0
20	CLA	B	819	8	69,73,73	1.14	7 (10%)	82,113,113	1.14	9 (10%)
31	LMU	9	616	-	36,36,36	0.27	0	47,47,47	0.59	0
20	CLA	A	823	7	69,73,73	1.13	8 (11%)	82,113,113	1.21	5 (6%)
20	CLA	B	836	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	6 (9%)
20	CLA	B	821	8	69,73,73	1.20	8 (11%)	82,113,113	1.20	6 (7%)
21	LUT	1	615	-	42,43,43	0.22	0	51,60,60	1.47	8 (15%)
20	CLA	2	608	-	49,53,73	1.33	6 (12%)	58,89,113	1.23	5 (8%)
20	CLA	9	610	6	54,58,73	1.33	7 (12%)	64,95,113	1.42	7 (10%)
20	CLA	9	607	6	69,73,73	1.15	7 (10%)	82,113,113	1.13	5 (6%)
20	CLA	3	406	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	5 (7%)
20	CLA	8	303	-	54,58,73	1.31	9 (16%)	64,95,113	1.39	5 (7%)
20	CLA	B	843	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
20	CLA	K	202	-	59,63,73	1.25	7 (11%)	70,101,113	1.15	4 (5%)
20	CLA	A	839	7	69,73,73	1.13	7 (10%)	82,113,113	1.16	5 (6%)
20	CLA	F	5005	-	59,63,73	1.24	6 (10%)	70,101,113	1.18	5 (7%)
20	CLA	B	827	8	69,73,73	1.20	9 (13%)	82,113,113	1.24	5 (6%)
21	LUT	8	314	-	42,43,43	0.26	0	51,60,60	0.39	0
28	LMG	7	319	-	54,54,55	0.23	0	62,62,63	0.28	0
25	PTY	F	5010	-	21,21,49	0.66	0	24,26,54	0.54	0
33	PQN	A	845	-	34,34,34	0.28	0	43,45,45	0.55	1 (2%)
19	CHL	8	306	-	45,59,74	0.90	2 (4%)	40,96,114	2.06	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	XAT	9	615	-	41,47,47	0.18	0	54,74,74	1.09	4 (7%)
23	BCR	F	5009	-	41,41,41	0.16	0	56,56,56	0.34	0
20	CLA	8	312	5	50,54,73	1.34	6 (12%)	59,90,113	1.23	4 (6%)
29	DGD	A	802	-	67,67,67	0.17	0	81,81,81	0.16	0
23	BCR	A	851	-	41,41,41	0.19	0	56,56,56	0.46	0
20	CLA	2	609	24	45,49,73	1.39	7 (15%)	54,84,113	1.28	5 (9%)
26	SQD	3	423	-	30,32,54	0.23	0	40,43,65	0.16	0
32	CL0	A	803	7	58,73,73	0.83	2 (3%)	60,113,113	2.17	7 (11%)
20	CLA	A	805	-	69,73,73	1.15	8 (11%)	82,113,113	1.10	4 (4%)
20	CLA	A	829	-	60,64,73	1.28	9 (15%)	71,102,113	1.25	5 (7%)
20	CLA	A	831	7	69,73,73	1.12	7 (10%)	82,113,113	1.19	6 (7%)
21	LUT	7	316	-	42,43,43	0.37	1 (2%)	51,60,60	0.55	1 (1%)
20	CLA	B	822	8	69,73,73	1.15	6 (8%)	82,113,113	1.09	6 (7%)
20	CLA	A	832	7	69,73,73	1.19	10 (14%)	82,113,113	1.25	6 (7%)
20	CLA	3	403	-	50,54,73	1.32	7 (14%)	59,90,113	1.36	4 (6%)
30	LMK	8	320	-	34,34,53	0.53	0	34,41,60	0.70	2 (5%)
20	CLA	1	607	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	5 (6%)
20	CLA	7	305	-	54,58,73	1.31	7 (12%)	64,95,113	1.36	6 (9%)
22	XAT	3	416	-	41,47,47	0.19	0	54,74,74	0.91	3 (5%)
25	PTY	3	422	-	25,25,49	0.62	0	28,30,54	0.51	0
20	CLA	1	609	1	69,73,73	1.13	7 (10%)	82,113,113	1.04	4 (4%)
20	CLA	H	204	14	49,53,73	1.35	8 (16%)	58,89,113	1.30	4 (6%)
29	DGD	7	321	-	48,48,67	0.20	0	62,62,81	0.32	0
23	BCR	A	850	-	41,41,41	0.25	0	56,56,56	0.95	3 (5%)
24	LHG	1	620	20	30,30,48	0.36	0	33,36,54	0.33	0
26	SQD	3	421	-	33,35,54	0.26	0	43,46,65	0.32	0
20	CLA	3	413	-	46,50,73	1.41	7 (15%)	53,85,113	1.30	4 (7%)
21	LUT	3	415	-	42,43,43	0.27	0	51,60,60	0.54	1 (1%)
20	CLA	B	828	-	69,73,73	1.14	7 (10%)	82,113,113	1.13	5 (6%)
20	CLA	B	839	-	59,63,73	1.22	7 (11%)	70,101,113	1.30	5 (7%)
20	CLA	K	201	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	4 (6%)
23	BCR	1	617	-	41,41,41	0.14	0	56,56,56	0.33	0
20	CLA	B	824	8	59,63,73	1.23	8 (13%)	70,101,113	1.13	6 (8%)
24	LHG	1	618	20	24,24,48	0.40	0	27,30,54	0.36	0
20	CLA	L	301	7	49,53,73	1.38	8 (16%)	58,89,113	1.30	4 (6%)
23	BCR	G	4001	-	41,41,41	0.18	0	56,56,56	0.39	0
20	CLA	2	622	-	50,54,73	1.31	6 (12%)	59,90,113	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PTY	1	623	-	34,34,49	0.55	0	37,39,54	0.43	0
20	CLA	9	602	6	64,68,73	1.20	8 (12%)	76,107,113	1.14	7 (9%)
24	LHG	2	618	20	43,43,48	0.42	0	46,48,54	0.65	2 (4%)
19	CHL	1	601	-	45,59,74	0.81	1 (2%)	40,96,114	2.39	8 (20%)
20	CLA	B	833	8	69,73,73	1.14	5 (7%)	82,113,113	1.37	9 (10%)
20	CLA	G	4004	-	49,53,73	1.34	8 (16%)	58,89,113	1.36	5 (8%)
20	CLA	A	830	7	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
20	CLA	J	4002	16	53,57,73	1.31	7 (13%)	61,93,113	1.57	7 (11%)
20	CLA	2	610	2	50,54,73	1.33	8 (16%)	59,90,113	1.43	4 (6%)
20	CLA	A	819	-	59,63,73	1.29	8 (13%)	70,101,113	1.34	5 (7%)
20	CLA	A	844	-	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
20	CLA	B	826	-	69,73,73	1.16	7 (10%)	82,113,113	1.12	6 (7%)
21	LUT	2	616	-	42,43,43	0.23	0	51,60,60	0.72	3 (5%)
19	CHL	3	401	3	50,64,74	0.87	2 (4%)	46,102,114	2.49	8 (17%)
20	CLA	A	821	7	69,73,73	1.20	8 (11%)	82,113,113	1.26	5 (6%)
19	CHL	8	304	-	41,55,74	0.97	2 (4%)	35,91,114	2.79	7 (20%)
20	CLA	7	304	4	59,63,73	1.27	7 (11%)	70,101,113	1.26	5 (7%)
20	CLA	B	829	8	69,73,73	1.17	10 (14%)	82,113,113	1.12	4 (4%)
20	CLA	K	203	17	49,53,73	1.41	9 (18%)	58,89,113	1.47	4 (6%)
23	BCR	F	5004	-	41,41,41	0.15	0	56,56,56	0.33	0
23	BCR	I	202	-	41,41,41	0.16	0	56,56,56	0.32	0
28	LMG	8	301	-	50,50,55	0.22	0	58,58,63	0.28	0
20	CLA	8	310	5	54,58,73	1.35	10 (18%)	64,95,113	1.38	7 (10%)
20	CLA	A	841	7	69,73,73	1.14	8 (11%)	82,113,113	1.16	6 (7%)
23	BCR	K	205	-	41,41,41	0.34	0	56,56,56	0.75	2 (3%)
20	CLA	A	826	7	64,68,73	1.18	7 (10%)	76,107,113	1.10	4 (5%)
23	BCR	J	4003	-	41,41,41	0.15	0	56,56,56	0.26	0
24	LHG	B	852	-	48,48,48	0.31	0	51,54,54	0.32	0
23	BCR	L	303	-	41,41,41	0.15	0	56,56,56	0.27	0
24	LHG	8	321	-	30,30,48	0.38	0	33,36,54	0.39	0
20	CLA	B	834	8	69,73,73	1.16	9 (13%)	82,113,113	1.14	5 (6%)
20	CLA	7	310	4	69,73,73	1.15	6 (8%)	82,113,113	1.08	6 (7%)
31	LMU	A	857	-	36,36,36	0.19	0	47,47,47	0.21	0
20	CLA	L	307	-	54,58,73	1.27	6 (11%)	64,95,113	1.30	6 (9%)
20	CLA	A	840	7	64,68,73	1.18	7 (10%)	76,107,113	1.12	6 (7%)
20	CLA	A	806	7	69,73,73	1.15	8 (11%)	82,113,113	1.22	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	8	302	5	64,68,73	1.21	7 (10%)	76,107,113	1.08	6 (7%)
23	BCR	L	308	-	41,41,41	0.19	0	56,56,56	0.37	0
19	CHL	7	302	-	60,74,74	0.73	3 (5%)	58,114,114	1.96	8 (13%)
20	CLA	7	311	24	64,68,73	1.24	9 (14%)	76,107,113	1.30	6 (7%)
24	LHG	8	319	20	33,33,48	0.34	0	36,39,54	0.34	0
24	LHG	F	5011	-	41,41,48	0.34	0	44,47,54	0.48	0
20	CLA	9	611	-	59,63,73	1.26	8 (13%)	70,101,113	1.30	5 (7%)
20	CLA	3	412	3	69,73,73	1.15	6 (8%)	82,113,113	1.15	6 (7%)
20	CLA	9	608	6	64,68,73	1.20	7 (10%)	76,107,113	1.19	5 (6%)
20	CLA	B	807	8	69,73,73	1.17	8 (11%)	82,113,113	1.15	6 (7%)
22	XAT	7	317	-	41,47,47	0.18	0	54,74,74	0.81	2 (3%)
24	LHG	F	5002	-	42,42,48	0.31	0	45,48,54	0.32	0
25	PTY	8	318	-	20,20,49	0.66	0	21,24,54	0.54	0
20	CLA	7	313	4	69,73,73	1.22	8 (11%)	82,113,113	1.17	5 (6%)
20	CLA	L	306	-	54,58,73	1.29	7 (12%)	64,95,113	1.33	5 (7%)
24	LHG	J	4004	-	32,35,48	0.23	0	34,37,54	0.33	0
36	4RF	A	859	-	38,38,56	0.43	0	41,41,59	0.38	0
34	SF4	C	101	9	0,12,12	-	-	-	-	-
24	LHG	G	4006	-	48,48,48	0.30	0	51,54,54	0.28	0
20	CLA	B	825	-	69,73,73	1.15	8 (11%)	82,113,113	1.30	8 (9%)
21	LUT	2	614	-	42,43,43	0.40	1 (2%)	51,60,60	1.15	2 (3%)
19	CHL	9	606	-	41,55,74	0.93	2 (4%)	35,91,114	2.59	5 (14%)
20	CLA	B	830	8	69,73,73	1.22	8 (11%)	82,113,113	1.18	8 (9%)
25	PTY	7	322	-	24,24,49	0.63	0	27,29,54	0.50	0
20	CLA	2	611	-	64,68,73	1.19	7 (10%)	76,107,113	1.23	4 (5%)
23	BCR	A	847	-	41,41,41	0.17	0	56,56,56	0.65	1 (1%)
23	BCR	3	419	-	41,41,41	0.22	0	56,56,56	0.49	0
19	CHL	7	306	-	40,54,74	0.93	2 (5%)	34,90,114	2.29	6 (17%)
23	BCR	B	846	-	41,41,41	0.38	0	56,56,56	1.31	7 (12%)
27	3PH	2	620	-	32,32,47	0.32	0	35,37,52	0.34	0
20	CLA	A	833	7	69,73,73	1.13	7 (10%)	82,113,113	1.19	5 (6%)
20	CLA	A	835	7	69,73,73	1.15	7 (10%)	82,113,113	1.23	6 (7%)
26	SQD	B	851	-	29,31,54	0.22	0	39,42,65	0.25	0
34	SF4	C	102	9	0,12,12	-	-	-	-	-
20	CLA	9	601	6	50,54,73	1.76	8 (16%)	59,90,113	1.16	4 (6%)
20	CLA	A	824	-	69,73,73	1.15	8 (11%)	82,113,113	1.10	5 (6%)
20	CLA	A	825	7	64,68,73	1.21	8 (12%)	76,107,113	1.27	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	7	324	5	64,68,73	1.24	7 (10%)	76,107,113	1.30	5 (6%)
20	CLA	7	315	4	69,73,73	1.16	7 (10%)	82,113,113	1.12	4 (4%)
23	BCR	L	309	-	41,41,41	0.15	0	56,56,56	0.24	0
20	CLA	A	809	7	69,73,73	1.15	7 (10%)	82,113,113	1.26	6 (7%)
20	CLA	B	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.14	6 (7%)
20	CLA	B	815	-	69,73,73	1.14	8 (11%)	82,113,113	1.13	5 (6%)
20	CLA	B	808	8	69,73,73	1.13	7 (10%)	82,113,113	1.18	4 (4%)
26	SQD	9	618	-	35,37,54	0.27	0	45,48,65	0.40	0
20	CLA	1	611	1	50,54,73	1.37	9 (18%)	59,90,113	1.40	6 (10%)
20	CLA	3	405	3	54,58,73	1.30	8 (14%)	64,95,113	1.31	5 (7%)
20	CLA	3	411	3	60,64,73	1.26	8 (13%)	70,101,113	1.24	5 (7%)
20	CLA	8	309	24	64,68,73	1.21	8 (12%)	76,107,113	1.23	5 (6%)
34	SF4	A	846	7,8	0,12,12	-	-	-	-	-
19	CHL	8	305	-	41,55,74	0.88	2 (4%)	35,91,114	2.39	8 (22%)
20	CLA	A	820	7	64,68,73	1.18	6 (9%)	76,107,113	1.16	4 (5%)
23	BCR	3	418	-	41,41,41	0.20	0	56,56,56	0.99	2 (3%)
23	BCR	A	849	-	41,41,41	0.29	0	56,56,56	0.95	4 (7%)
20	CLA	2	602	2	60,64,73	1.25	7 (11%)	71,102,113	1.26	4 (5%)
20	CLA	B	813	8	69,73,73	1.17	8 (11%)	82,113,113	1.18	6 (7%)
20	CLA	2	613	-	54,58,73	1.34	8 (14%)	64,95,113	1.32	9 (14%)
23	BCR	B	849	-	41,41,41	0.19	0	56,56,56	0.67	2 (3%)
23	BCR	G	4005	-	41,41,41	0.24	0	56,56,56	0.84	3 (5%)
23	BCR	H	205	-	41,41,41	0.30	0	56,56,56	0.72	2 (3%)
20	CLA	A	808	7	69,73,73	1.12	7 (10%)	82,113,113	1.09	6 (7%)
23	BCR	B	845	-	41,41,41	0.16	0	56,56,56	0.37	0
25	PTY	H	202	-	31,31,49	0.53	0	34,36,54	0.75	1 (2%)
19	CHL	7	308	-	42,56,74	0.86	1 (2%)	36,92,114	2.55	9 (25%)
24	LHG	I	201	-	48,48,48	0.30	0	51,54,54	0.31	0
20	CLA	B	831	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
20	CLA	1	602	1	65,69,73	1.20	8 (12%)	77,108,113	1.17	5 (6%)
20	CLA	3	408	3	64,68,73	1.16	6 (9%)	76,107,113	1.13	5 (6%)
20	CLA	B	818	8	69,73,73	1.15	7 (10%)	82,113,113	1.16	4 (4%)
20	CLA	1	605	-	49,53,73	1.37	6 (12%)	58,89,113	1.36	4 (6%)
20	CLA	3	407	3	69,73,73	1.17	7 (10%)	82,113,113	1.23	5 (6%)
28	LMG	F	5001	-	46,46,55	0.19	0	54,54,63	0.16	0
28	LMG	7	301	-	40,40,55	0.22	0	48,48,63	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	F	5003	5	69,73,73	1.19	7 (10%)	82,113,113	1.28	5 (6%)
24	LHG	9	619	-	48,48,48	0.31	0	51,54,54	0.32	0
20	CLA	2	607	2	50,54,73	1.35	7 (14%)	59,90,113	1.21	4 (6%)
20	CLA	A	807	7	69,73,73	1.13	6 (8%)	82,113,113	1.06	5 (6%)
20	CLA	1	608	1	64,68,73	1.19	8 (12%)	76,107,113	1.25	5 (6%)
20	CLA	G	4003	13	50,54,73	1.36	7 (14%)	59,90,113	1.35	4 (6%)
23	BCR	8	316	-	41,41,41	0.17	0	56,56,56	0.50	0
19	CHL	7	307	-	45,59,74	0.83	3 (6%)	40,96,114	2.54	6 (15%)
20	CLA	A	817	-	59,63,73	1.25	6 (10%)	70,101,113	1.33	6 (8%)
20	CLA	A	822	7	69,73,73	1.15	7 (10%)	82,113,113	1.17	7 (8%)
20	CLA	B	810	8	69,73,73	1.16	7 (10%)	82,113,113	1.19	5 (6%)
20	CLA	B	842	24	69,73,73	1.17	7 (10%)	82,113,113	1.24	4 (4%)
21	LUT	2	615	-	42,43,43	0.27	0	51,60,60	0.70	1 (1%)
20	CLA	A	834	7	59,63,73	1.26	8 (13%)	70,101,113	1.25	5 (7%)
24	LHG	A	854	-	44,44,48	0.30	0	47,50,54	0.31	0
35	OCD	A	855	-	10,10,18	0.24	0	9,9,17	0.19	0
20	CLA	A	843	24	54,58,73	1.29	8 (14%)	64,95,113	1.38	6 (9%)
20	CLA	9	612	6	49,53,73	1.56	10 (20%)	58,89,113	1.54	8 (13%)
23	BCR	A	852	-	41,41,41	0.15	0	56,56,56	0.34	0
23	BCR	A	858	-	41,41,41	0.24	0	56,56,56	0.42	1 (1%)
20	CLA	A	836	-	64,68,73	1.25	9 (14%)	76,107,113	1.26	5 (6%)
20	CLA	K	204	-	52,56,73	1.34	5 (9%)	61,92,113	1.34	5 (8%)
20	CLA	7	303	4	64,68,73	1.21	7 (10%)	76,107,113	1.15	5 (6%)
20	CLA	8	311	5	69,73,73	1.51	10 (14%)	82,113,113	1.14	5 (6%)
20	CLA	2	603	2	64,68,73	1.26	8 (12%)	76,107,113	1.37	6 (7%)
20	CLA	3	414	3	50,54,73	1.36	7 (14%)	59,90,113	1.30	4 (6%)
20	CLA	8	308	5	64,68,73	1.16	8 (12%)	76,107,113	1.08	4 (5%)
20	CLA	A	804	-	69,73,73	1.19	10 (14%)	82,113,113	1.16	4 (4%)
20	CLA	A	815	7	66,70,73	1.22	9 (13%)	78,109,113	1.13	5 (6%)
24	LHG	9	617	20	40,40,48	0.33	0	43,46,54	0.36	0
20	CLA	A	827	7	64,68,73	1.20	8 (12%)	76,107,113	1.29	7 (9%)
20	CLA	B	841	8	69,73,73	1.14	7 (10%)	82,113,113	1.08	6 (7%)
20	CLA	B	814	8	69,73,73	1.17	6 (8%)	82,113,113	1.22	4 (4%)
20	CLA	2	612	2	47,52,73	1.39	7 (14%)	55,87,113	1.29	4 (7%)
20	CLA	A	818	7	69,73,73	1.16	7 (10%)	82,113,113	1.28	6 (7%)
22	XAT	1	616	-	41,47,47	0.15	0	54,74,74	1.04	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	7	320	20	48,48,48	0.29	0	51,54,54	0.28	0
20	CLA	3	410	3	56,60,73	1.32	7 (12%)	65,97,113	1.44	7 (10%)
20	CLA	B	823	8	69,73,73	1.13	8 (11%)	82,113,113	1.22	6 (7%)
19	CHL	2	606	-	41,55,74	0.89	2 (4%)	35,91,114	2.34	8 (22%)
20	CLA	1	604	-	54,58,73	1.31	7 (12%)	64,95,113	1.32	6 (9%)
20	CLA	9	604	6	54,58,73	1.31	8 (14%)	64,95,113	1.23	5 (7%)
29	DGD	B	850	-	62,62,67	0.18	0	76,76,81	0.24	0
25	PTY	B	801	-	26,26,49	0.61	0	29,31,54	0.50	0
20	CLA	B	806	8	69,73,73	1.14	7 (10%)	82,113,113	1.33	7 (8%)
21	LUT	2	617	-	42,43,43	0.31	0	51,60,60	0.36	0
23	BCR	7	318	-	41,41,41	0.14	0	56,56,56	0.40	0
20	CLA	8	307	5	50,54,73	1.36	8 (16%)	59,90,113	1.16	4 (6%)
20	CLA	B	811	8	69,73,73	1.13	8 (11%)	82,113,113	1.19	4 (4%)
25	PTY	1	622	-	19,19,49	0.69	0	22,24,54	0.53	0
20	CLA	B	805	8	52,56,73	1.30	8 (15%)	61,92,113	1.30	5 (8%)
24	LHG	A	853	20	29,29,48	0.35	0	33,35,54	0.40	0
19	CHL	1	606	-	41,55,74	0.93	2 (4%)	35,91,114	2.24	9 (25%)

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
31	LMU	A	856	-	-	0/21/61/61	0/2/2/2
23	BCR	B	847	-	-	2/29/63/63	0/2/2/2
20	CLA	9	609	24	1/1/14/20	17/33/109/115	-
25	PTY	H	201	-	-	21/49/49/53	-
20	CLA	8	313	5	1/1/12/20	6/23/99/115	-
20	CLA	A	838	7	1/1/12/20	9/23/99/115	-
33	PQN	B	844	-	-	9/23/43/43	0/2/2/2
23	BCR	A	848	-	-	11/29/63/63	0/2/2/2
20	CLA	7	312	4	1/1/12/20	8/24/100/115	-
20	CLA	A	816	7	-	14/39/115/115	-
25	PTY	8	317	-	-	8/27/27/53	-
20	CLA	1	610	24	1/1/11/20	9/17/93/115	-
20	CLA	A	811	7	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	810	-	1/1/14/20	6/33/109/115	-
20	CLA	A	812	7	1/1/15/20	14/39/115/115	-
20	CLA	B	816	8	1/1/13/20	7/27/103/115	-
20	CLA	F	5006	-	1/1/11/20	9/18/94/115	-
21	LUT	9	613	-	3/3/12/27	2/29/67/67	0/2/2/2
23	BCR	B	848	-	-	2/29/63/63	0/2/2/2
24	LHG	H	203	-	-	8/42/42/53	-
23	BCR	J	4001	-	-	9/29/63/63	0/2/2/2
29	DGD	L	311	-	-	11/47/87/95	0/2/2/2
20	CLA	G	4002	13	1/1/11/20	8/18/94/115	-
20	CLA	B	803	-	1/1/15/20	21/39/115/115	-
20	CLA	B	835	-	1/1/14/20	12/33/109/115	-
20	CLA	B	838	-	1/1/14/20	8/33/109/115	-
20	CLA	3	409	-	1/1/12/20	7/21/97/115	-
20	CLA	A	837	7	1/1/13/20	8/27/103/115	-
20	CLA	A	828	-	1/1/15/20	9/39/115/115	-
24	LHG	7	323	-	-	5/25/25/53	-
20	CLA	7	314	4	1/1/12/20	10/21/97/115	-
20	CLA	F	5007	12	1/1/11/20	7/20/96/115	-
20	CLA	A	814	7	1/1/15/20	18/39/115/115	-
20	CLA	F	5008	12	-	10/17/93/115	-
25	PTY	L	310	-	-	9/22/22/53	-
20	CLA	2	604	-	1/1/12/20	8/21/97/115	-
20	CLA	B	832	8	1/1/14/20	10/33/109/115	-
20	CLA	B	817	8	1/1/14/20	9/33/109/115	-
20	CLA	L	305	18	1/1/15/20	7/39/115/115	-
19	CHL	2	601	2	2/2/19/26	16/33/131/137	-
20	CLA	L	302	-	1/1/15/20	21/39/115/115	-
20	CLA	A	813	7	1/1/13/20	10/27/103/115	-
20	CLA	7	309	4	1/1/15/20	11/39/115/115	-
24	LHG	2	621	-	-	6/40/40/53	-
20	CLA	9	605	6	1/1/11/20	2/15/91/115	-
20	CLA	B	820	-	1/1/15/20	14/39/115/115	-
20	CLA	B	809	8	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	613	1	1/1/13/20	9/27/103/115	-
20	CLA	A	842	7	1/1/14/20	9/35/111/115	-
20	CLA	B	837	8	1/1/12/20	4/23/99/115	-
23	BCR	B	802	-	-	6/29/63/63	0/2/2/2
20	CLA	3	404	-	1/1/11/20	7/17/93/115	-
20	CLA	1	614	1	1/1/11/20	8/17/93/115	-
20	CLA	9	603	6	1/1/13/20	6/27/103/115	-
24	LHG	1	621	-	-	10/50/50/53	-
20	CLA	L	304	18	1/1/15/20	11/39/115/115	-
20	CLA	1	603	1	1/1/15/20	20/39/115/115	-
20	CLA	3	402	3	1/1/15/20	16/39/115/115	-
23	BCR	3	417	-	-	4/29/63/63	0/2/2/2
26	SQD	2	619	-	-	13/36/56/69	0/1/1/1
22	XAT	8	315	-	-	1/31/93/93	0/4/4/4
24	LHG	3	420	-	-	5/19/19/53	-
24	LHG	1	619	-	-	9/48/48/53	-
24	LHG	7	325	-	-	6/44/44/53	-
20	CLA	1	612	-	1/1/13/20	9/27/103/115	-
22	XAT	9	614	-	-	0/31/93/93	0/4/4/4
24	LHG	3	424	-	-	15/43/43/53	-
20	CLA	B	840	-	1/1/15/20	11/39/115/115	-
20	CLA	B	812	-	1/1/13/20	8/27/103/115	-
20	CLA	2	605	-	1/1/11/20	9/15/91/115	-
28	LMG	A	801	-	-	3/26/46/70	0/1/1/1
20	CLA	B	819	8	1/1/15/20	15/39/115/115	-
31	LMU	9	616	-	-	5/21/61/61	0/2/2/2
20	CLA	A	823	7	1/1/15/20	19/39/115/115	-
20	CLA	B	836	-	1/1/12/20	11/21/97/115	-
20	CLA	B	821	8	1/1/15/20	11/39/115/115	-
21	LUT	1	615	-	3/3/12/27	11/29/67/67	0/2/2/2
20	CLA	2	608	-	1/1/11/20	5/15/91/115	-
20	CLA	9	610	6	1/1/12/20	10/21/97/115	-
20	CLA	9	607	6	1/1/15/20	11/39/115/115	-
20	CLA	3	406	-	1/1/13/20	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	8	303	-	1/1/12/20	6/21/97/115	-
20	CLA	B	843	-	1/1/15/20	15/39/115/115	-
20	CLA	K	202	-	1/1/13/20	6/27/103/115	-
20	CLA	A	839	7	1/1/15/20	11/39/115/115	-
20	CLA	F	5005	-	1/1/13/20	11/27/103/115	-
20	CLA	B	827	8	1/1/15/20	8/39/115/115	-
21	LUT	8	314	-	3/3/12/27	2/29/67/67	0/2/2/2
28	LMG	7	319	-	-	11/49/69/70	0/1/1/1
25	PTY	F	5010	-	-	7/25/25/53	-
33	PQN	A	845	-	-	0/23/43/43	0/2/2/2
19	CHL	8	306	-	2/2/17/26	9/21/119/137	-
22	XAT	9	615	-	-	5/31/93/93	0/4/4/4
23	BCR	F	5009	-	-	4/29/63/63	0/2/2/2
20	CLA	8	312	5	1/1/11/20	7/17/93/115	-
29	DGD	A	802	-	-	11/55/95/95	0/2/2/2
23	BCR	A	851	-	-	2/29/63/63	0/2/2/2
20	CLA	2	609	24	1/1/10/20	4/10/86/115	-
26	SQD	3	423	-	-	9/27/47/69	0/1/1/1
32	CL0	A	803	7	-	13/37/135/135	-
20	CLA	A	805	-	1/1/15/20	13/39/115/115	-
20	CLA	A	829	-	1/1/13/20	10/29/105/115	-
20	CLA	A	831	7	1/1/15/20	17/39/115/115	-
21	LUT	7	316	-	3/3/12/27	2/29/67/67	0/2/2/2
20	CLA	B	822	8	1/1/15/20	14/39/115/115	-
20	CLA	A	832	7	1/1/15/20	12/39/115/115	-
20	CLA	3	403	-	1/1/11/20	6/17/93/115	-
30	LMK	8	320	-	-	10/41/41/60	-
20	CLA	1	607	-	1/1/15/20	13/39/115/115	-
20	CLA	7	305	-	1/1/12/20	6/21/97/115	-
22	XAT	3	416	-	-	2/31/93/93	0/4/4/4
25	PTY	3	422	-	-	5/29/29/53	-
20	CLA	1	609	1	1/1/15/20	10/39/115/115	-
20	CLA	H	204	14	1/1/11/20	8/15/91/115	-
29	DGD	7	321	-	-	11/36/76/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A	850	-	-	12/29/63/63	0/2/2/2
24	LHG	1	620	20	-	7/35/35/53	-
26	SQD	3	421	-	-	10/30/50/69	0/1/1/1
20	CLA	3	413	-	1/1/10/20	4/12/88/115	-
21	LUT	3	415	-	3/3/12/27	4/29/67/67	0/2/2/2
20	CLA	B	828	-	1/1/15/20	17/39/115/115	-
20	CLA	B	839	-	1/1/13/20	5/27/103/115	-
20	CLA	K	201	-	1/1/11/20	6/15/91/115	-
23	BCR	1	617	-	-	4/29/63/63	0/2/2/2
20	CLA	B	824	8	1/1/13/20	13/27/103/115	-
24	LHG	1	618	20	-	4/29/29/53	-
20	CLA	L	301	7	1/1/11/20	8/15/91/115	-
23	BCR	G	4001	-	-	5/29/63/63	0/2/2/2
20	CLA	2	622	-	1/1/11/20	5/17/93/115	-
25	PTY	1	623	-	-	8/38/38/53	-
20	CLA	9	602	6	1/1/14/20	18/33/109/115	-
24	LHG	2	618	20	-	5/45/45/53	-
19	CHL	1	601	-	1/1/17/26	4/21/119/137	-
20	CLA	B	833	8	1/1/15/20	13/39/115/115	-
20	CLA	G	4004	-	1/1/11/20	6/15/91/115	-
20	CLA	A	830	7	1/1/15/20	15/39/115/115	-
20	CLA	J	4002	16	1/1/11/20	10/20/96/115	-
20	CLA	2	610	2	1/1/11/20	8/17/93/115	-
20	CLA	A	819	-	1/1/13/20	13/27/103/115	-
20	CLA	A	844	-	1/1/15/20	10/39/115/115	-
20	CLA	B	826	-	1/1/15/20	10/39/115/115	-
21	LUT	2	616	-	3/3/12/27	7/29/67/67	0/2/2/2
19	CHL	3	401	3	2/2/18/26	14/27/125/137	-
20	CLA	A	821	7	1/1/15/20	17/39/115/115	-
19	CHL	8	304	-	1/1/16/26	9/17/115/137	-
20	CLA	7	304	4	1/1/13/20	11/27/103/115	-
20	CLA	B	829	8	1/1/15/20	24/39/115/115	-
20	CLA	K	203	17	1/1/11/20	8/15/91/115	-
23	BCR	F	5004	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	I	202	-	-	4/29/63/63	0/2/2/2
28	LMG	8	301	-	-	8/45/65/70	0/1/1/1
20	CLA	8	310	5	1/1/12/20	10/21/97/115	-
20	CLA	A	841	7	1/1/15/20	17/39/115/115	-
23	BCR	K	205	-	-	9/29/63/63	0/2/2/2
20	CLA	A	826	7	1/1/14/20	15/33/109/115	-
23	BCR	J	4003	-	-	4/29/63/63	0/2/2/2
24	LHG	B	852	-	-	19/53/53/53	-
23	BCR	L	303	-	-	4/29/63/63	0/2/2/2
24	LHG	8	321	-	-	10/35/35/53	-
20	CLA	B	834	8	1/1/15/20	18/39/115/115	-
20	CLA	7	310	4	1/1/15/20	13/39/115/115	-
31	LMU	A	857	-	-	5/21/61/61	0/2/2/2
20	CLA	L	307	-	1/1/12/20	11/21/97/115	-
20	CLA	A	840	7	1/1/14/20	11/33/109/115	-
20	CLA	A	806	7	1/1/15/20	13/39/115/115	-
20	CLA	8	302	5	1/1/14/20	13/33/109/115	-
23	BCR	L	308	-	-	4/29/63/63	0/2/2/2
19	CHL	7	302	-	3/3/20/26	16/39/137/137	-
20	CLA	7	311	24	1/1/14/20	9/33/109/115	-
24	LHG	8	319	20	-	4/38/38/53	-
24	LHG	F	5011	-	-	8/46/46/53	-
20	CLA	9	611	-	1/1/13/20	8/27/103/115	-
20	CLA	3	412	3	1/1/15/20	16/39/115/115	-
20	CLA	9	608	6	1/1/14/20	11/33/109/115	-
20	CLA	B	807	8	1/1/15/20	14/39/115/115	-
22	XAT	7	317	-	-	4/31/93/93	0/4/4/4
24	LHG	F	5002	-	-	12/47/47/53	-
25	PTY	8	318	-	-	11/23/23/53	-
20	CLA	7	313	4	1/1/15/20	11/39/115/115	-
20	CLA	L	306	-	1/1/12/20	7/21/97/115	-
24	LHG	J	4004	-	-	6/35/37/53	-
36	4RF	A	859	-	-	17/41/41/59	-
34	SF4	C	101	9	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	G	4006	-	-	7/53/53/53	-
20	CLA	B	825	-	1/1/15/20	12/39/115/115	-
21	LUT	2	614	-	3/3/12/27	4/29/67/67	0/2/2/2
19	CHL	9	606	-	1/1/16/26	10/17/115/137	-
20	CLA	B	830	8	1/1/15/20	15/39/115/115	-
25	PTY	7	322	-	-	5/28/28/53	-
20	CLA	2	611	-	1/1/14/20	11/33/109/115	-
23	BCR	A	847	-	-	11/29/63/63	0/2/2/2
23	BCR	3	419	-	-	5/29/63/63	0/2/2/2
19	CHL	7	306	-	1/1/16/26	7/15/113/137	-
23	BCR	B	846	-	-	13/29/63/63	0/2/2/2
27	3PH	2	620	-	-	6/34/34/49	-
20	CLA	A	833	7	1/1/15/20	9/39/115/115	-
20	CLA	A	835	7	1/1/15/20	8/39/115/115	-
26	SQD	B	851	-	-	10/25/45/69	0/1/1/1
34	SF4	C	102	9	-	-	0/6/5/5
20	CLA	9	601	6	1/1/11/20	12/17/93/115	-
20	CLA	A	824	-	1/1/15/20	14/39/115/115	-
20	CLA	A	825	7	1/1/14/20	9/33/109/115	-
20	CLA	7	324	5	1/1/14/20	9/33/109/115	-
20	CLA	7	315	4	1/1/15/20	7/39/115/115	-
23	BCR	L	309	-	-	0/29/63/63	0/2/2/2
20	CLA	A	809	7	1/1/15/20	14/39/115/115	-
20	CLA	B	804	-	1/1/15/20	12/39/115/115	-
20	CLA	B	815	-	1/1/15/20	14/39/115/115	-
20	CLA	B	808	8	1/1/15/20	14/39/115/115	-
26	SQD	9	618	-	-	9/32/52/69	0/1/1/1
20	CLA	1	611	1	1/1/11/20	8/17/93/115	-
20	CLA	3	405	3	1/1/12/20	5/21/97/115	-
20	CLA	3	411	3	1/1/13/20	9/27/103/115	-
20	CLA	8	309	24	1/1/14/20	13/33/109/115	-
34	SF4	A	846	7,8	-	-	0/6/5/5
19	CHL	8	305	-	1/1/16/26	10/17/115/137	-
20	CLA	A	820	7	1/1/14/20	13/33/109/115	-
23	BCR	3	418	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A	849	-	-	3/29/63/63	0/2/2/2
20	CLA	2	602	2	1/1/13/20	10/29/105/115	-
20	CLA	B	813	8	1/1/15/20	13/39/115/115	-
20	CLA	2	613	-	1/1/12/20	9/21/97/115	-
23	BCR	B	849	-	-	7/29/63/63	0/2/2/2
23	BCR	G	4005	-	-	8/29/63/63	0/2/2/2
23	BCR	H	205	-	-	10/29/63/63	0/2/2/2
20	CLA	A	808	7	1/1/15/20	14/39/115/115	-
23	BCR	B	845	-	-	2/29/63/63	0/2/2/2
25	PTY	H	202	-	-	16/35/35/53	-
19	CHL	7	308	-	1/1/16/26	6/18/116/137	-
24	LHG	I	201	-	-	17/53/53/53	-
20	CLA	B	831	-	1/1/15/20	15/39/115/115	-
20	CLA	1	602	1	1/1/14/20	12/35/111/115	-
20	CLA	3	408	3	1/1/14/20	14/33/109/115	-
20	CLA	B	818	8	1/1/15/20	18/39/115/115	-
20	CLA	1	605	-	1/1/11/20	6/15/91/115	-
20	CLA	3	407	3	1/1/15/20	15/39/115/115	-
28	LMG	F	5001	-	-	6/41/61/70	0/1/1/1
28	LMG	7	301	-	-	13/35/55/70	0/1/1/1
20	CLA	F	5003	5	1/1/15/20	13/39/115/115	-
24	LHG	9	619	-	-	8/53/53/53	-
20	CLA	2	607	2	1/1/11/20	9/17/93/115	-
20	CLA	A	807	7	1/1/15/20	9/39/115/115	-
20	CLA	1	608	1	1/1/14/20	12/33/109/115	-
20	CLA	G	4003	13	1/1/11/20	8/17/93/115	-
23	BCR	8	316	-	-	4/29/63/63	0/2/2/2
19	CHL	7	307	-	2/2/17/26	10/21/119/137	-
20	CLA	A	817	-	1/1/13/20	9/27/103/115	-
20	CLA	A	822	7	1/1/15/20	13/39/115/115	-
20	CLA	B	810	8	1/1/15/20	12/39/115/115	-
20	CLA	B	842	24	1/1/15/20	11/39/115/115	-
21	LUT	2	615	-	3/3/12/27	6/29/67/67	0/2/2/2
20	CLA	A	834	7	1/1/13/20	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	A	854	-	-	11/49/49/53	-
35	OCD	A	855	-	-	0/8/8/16	-
20	CLA	A	843	24	1/1/12/20	10/21/97/115	-
20	CLA	9	612	6	-	8/15/91/115	-
23	BCR	A	852	-	-	4/29/63/63	0/2/2/2
23	BCR	A	858	-	-	6/29/63/63	0/2/2/2
20	CLA	A	836	-	1/1/14/20	14/33/109/115	-
20	CLA	K	204	-	1/1/11/20	10/19/95/115	-
20	CLA	7	303	4	1/1/14/20	11/33/109/115	-
20	CLA	A	804	-	1/1/15/20	13/39/115/115	-
20	CLA	2	603	2	1/1/14/20	13/33/109/115	-
20	CLA	3	414	3	1/1/11/20	8/17/93/115	-
20	CLA	8	308	5	1/1/14/20	11/33/109/115	-
20	CLA	A	815	7	1/1/14/20	15/36/112/115	-
20	CLA	8	311	5	-	16/39/115/115	-
24	LHG	9	617	20	-	11/45/45/53	-
20	CLA	A	827	7	1/1/14/20	11/33/109/115	-
20	CLA	B	841	8	1/1/15/20	15/39/115/115	-
20	CLA	B	814	8	1/1/15/20	17/39/115/115	-
20	CLA	2	612	2	1/1/10/20	4/14/90/115	-
20	CLA	A	818	7	1/1/15/20	13/39/115/115	-
22	XAT	1	616	-	-	3/31/93/93	0/4/4/4
24	LHG	7	320	20	-	17/53/53/53	-
20	CLA	3	410	3	1/1/12/20	9/24/100/115	-
20	CLA	B	823	8	1/1/15/20	15/39/115/115	-
19	CHL	2	606	-	2/2/16/26	10/17/115/137	-
20	CLA	1	604	-	1/1/12/20	9/21/97/115	-
20	CLA	9	604	6	1/1/12/20	7/21/97/115	-
29	DGD	B	850	-	-	7/50/90/95	0/2/2/2
25	PTY	B	801	-	-	12/30/30/53	-
20	CLA	B	806	8	1/1/15/20	14/39/115/115	-
21	LUT	2	617	-	3/3/12/27	4/29/67/67	0/2/2/2
23	BCR	7	318	-	-	6/29/63/63	0/2/2/2
20	CLA	8	307	5	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	811	8	1/1/15/20	18/39/115/115	-
25	PTY	1	622	-	-	7/22/22/53	-
20	CLA	B	805	8	1/1/11/20	6/19/95/115	-
24	LHG	A	853	20	-	7/33/33/53	-
19	CHL	1	606	-	1/1/16/26	4/17/115/137	-

The worst 5 of 1325 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	311	CLA	MG-NC	7.33	2.23	2.06
20	9	601	CLA	MG-NB	6.22	2.18	2.05
20	9	601	CLA	MG-NA	5.53	2.19	2.06
20	9	612	CLA	MG-NA	4.69	2.17	2.06
20	9	603	CLA	MG-NC	4.38	2.16	2.06

The worst 5 of 1101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	803	CL0	C1B-CHB-C4A	14.26	130.49	121.32
19	3	401	CHL	C1B-CHB-C4A	14.07	130.37	121.32
19	8	304	CHL	C1B-CHB-C4A	13.63	130.09	121.32
19	9	606	CHL	C1B-CHB-C4A	13.06	129.72	121.32
19	2	601	CHL	C1B-CHB-C4A	12.30	129.24	121.32

5 of 213 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	601	CHL	ND
19	1	606	CHL	NC
19	2	601	CHL	C8
19	2	601	CHL	NC
19	2	606	CHL	C3A

5 of 2733 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	601	CHL	C3A-C2A-CAA-CBA
19	1	606	CHL	C1A-C2A-CAA-CBA
19	1	606	CHL	C3A-C2A-CAA-CBA
19	2	606	CHL	C1A-C2A-CAA-CBA
19	2	606	CHL	CHA-CBD-CGD-O1D

There are no ring outliers.

258 monomers are involved in 706 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	856	LMU	2	0
23	B	847	BCR	5	0
25	H	201	PTY	4	0
20	8	313	CLA	1	0
20	A	838	CLA	4	0
33	B	844	PQN	4	0
23	A	848	BCR	7	0
20	7	312	CLA	2	0
20	A	816	CLA	7	0
20	1	610	CLA	2	0
20	A	811	CLA	3	0
20	A	810	CLA	2	0
20	A	812	CLA	12	0
20	B	816	CLA	1	0
20	F	5006	CLA	3	0
21	9	613	LUT	4	0
23	B	848	BCR	3	0
24	H	203	LHG	2	0
23	J	4001	BCR	7	0
29	L	311	DGD	4	0
20	B	803	CLA	3	0
20	B	835	CLA	2	0
20	B	838	CLA	4	0
20	A	837	CLA	4	0
20	A	828	CLA	5	0
24	7	323	LHG	1	0
20	7	314	CLA	3	0
20	F	5007	CLA	1	0
20	A	814	CLA	4	0
20	F	5008	CLA	3	0
20	2	604	CLA	1	0
20	B	832	CLA	5	0
20	B	817	CLA	2	0
20	L	305	CLA	5	0
19	2	601	CHL	4	0
20	L	302	CLA	3	0
20	A	813	CLA	3	0
24	2	621	LHG	3	0
20	9	605	CLA	2	0
20	B	820	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	809	CLA	6	0
20	1	613	CLA	1	0
20	A	842	CLA	4	0
20	B	837	CLA	1	0
23	B	802	BCR	7	0
20	3	404	CLA	1	0
20	1	614	CLA	1	0
20	9	603	CLA	2	0
24	1	621	LHG	2	0
20	L	304	CLA	5	0
20	1	603	CLA	3	0
20	3	402	CLA	2	0
26	2	619	SQD	3	0
22	8	315	XAT	3	0
24	1	619	LHG	1	0
24	7	325	LHG	2	0
20	1	612	CLA	2	0
22	9	614	XAT	5	0
24	3	424	LHG	2	0
20	B	840	CLA	6	0
20	B	812	CLA	2	0
28	A	801	LMG	2	0
20	B	819	CLA	8	0
31	9	616	LMU	4	0
20	A	823	CLA	2	0
20	B	836	CLA	1	0
20	B	821	CLA	7	0
21	1	615	LUT	7	0
20	2	608	CLA	4	0
20	9	607	CLA	2	0
20	3	406	CLA	2	0
20	8	303	CLA	3	0
20	B	843	CLA	6	0
20	K	202	CLA	4	0
20	A	839	CLA	1	0
20	F	5005	CLA	3	0
20	B	827	CLA	6	0
28	7	319	LMG	2	0
33	A	845	PQN	1	0
19	8	306	CHL	1	0
22	9	615	XAT	4	0
23	F	5009	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	802	DGD	4	0
23	A	851	BCR	8	0
20	2	609	CLA	1	0
26	3	423	SQD	1	0
32	A	803	CL0	8	0
20	A	805	CLA	10	0
20	A	829	CLA	3	0
20	A	831	CLA	8	0
21	7	316	LUT	2	0
20	B	822	CLA	4	0
20	A	832	CLA	7	0
20	3	403	CLA	1	0
20	1	607	CLA	3	0
20	7	305	CLA	1	0
22	3	416	XAT	3	0
20	1	609	CLA	3	0
29	7	321	DGD	4	0
23	A	850	BCR	5	0
24	1	620	LHG	1	0
26	3	421	SQD	5	0
21	3	415	LUT	2	0
20	B	828	CLA	4	0
20	B	839	CLA	1	0
20	K	201	CLA	1	0
23	1	617	BCR	2	0
20	B	824	CLA	10	0
24	1	618	LHG	1	0
20	L	301	CLA	1	0
23	G	4001	BCR	3	0
25	1	623	PTY	1	0
20	9	602	CLA	6	0
24	2	618	LHG	1	0
19	1	601	CHL	5	0
20	G	4004	CLA	3	0
20	A	830	CLA	6	0
20	J	4002	CLA	6	0
20	2	610	CLA	2	0
20	A	819	CLA	5	0
20	A	844	CLA	2	0
20	B	826	CLA	3	0
21	2	616	LUT	10	0
19	3	401	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	821	CLA	5	0
19	8	304	CHL	7	0
20	7	304	CLA	1	0
20	B	829	CLA	2	0
20	K	203	CLA	5	0
23	F	5004	BCR	5	0
23	I	202	BCR	3	0
28	8	301	LMG	5	0
20	8	310	CLA	2	0
20	A	841	CLA	7	0
23	K	205	BCR	5	0
20	A	826	CLA	1	0
23	J	4003	BCR	3	0
23	L	303	BCR	5	0
24	8	321	LHG	2	0
20	B	834	CLA	7	0
20	7	310	CLA	2	0
31	A	857	LMU	1	0
20	A	840	CLA	5	0
20	A	806	CLA	2	0
20	8	302	CLA	4	0
23	L	308	BCR	4	0
19	7	302	CHL	4	0
20	7	311	CLA	1	0
24	8	319	LHG	1	0
24	F	5011	LHG	2	0
20	9	611	CLA	2	0
20	3	412	CLA	2	0
20	9	608	CLA	2	0
20	B	807	CLA	5	0
22	7	317	XAT	6	0
24	F	5002	LHG	4	0
20	7	313	CLA	5	0
24	J	4004	LHG	1	0
36	A	859	4RF	2	0
34	C	101	SF4	1	0
24	G	4006	LHG	3	0
20	B	825	CLA	5	0
19	9	606	CHL	4	0
20	B	830	CLA	4	0
20	2	611	CLA	2	0
23	A	847	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	3	419	BCR	5	0
19	7	306	CHL	3	0
23	B	846	BCR	4	0
27	2	620	3PH	4	0
20	A	833	CLA	4	0
20	A	835	CLA	6	0
26	B	851	SQD	1	0
34	C	102	SF4	1	0
20	9	601	CLA	1	0
20	A	824	CLA	4	0
20	A	825	CLA	6	0
20	7	324	CLA	3	0
23	L	309	BCR	1	0
20	A	809	CLA	4	0
20	B	804	CLA	11	0
20	B	815	CLA	1	0
20	B	808	CLA	5	0
26	9	618	SQD	1	0
20	1	611	CLA	3	0
20	3	405	CLA	2	0
20	3	411	CLA	3	0
20	8	309	CLA	3	0
34	A	846	SF4	4	0
19	8	305	CHL	2	0
20	A	820	CLA	7	0
23	3	418	BCR	5	0
23	A	849	BCR	12	0
20	2	602	CLA	4	0
20	B	813	CLA	9	0
20	2	613	CLA	1	0
23	B	849	BCR	6	0
23	G	4005	BCR	2	0
20	A	808	CLA	7	0
23	B	845	BCR	2	0
25	H	202	PTY	2	0
19	7	308	CHL	5	0
24	I	201	LHG	6	0
20	B	831	CLA	6	0
20	1	602	CLA	3	0
20	3	408	CLA	2	0
20	B	818	CLA	4	0
20	1	605	CLA	3	0

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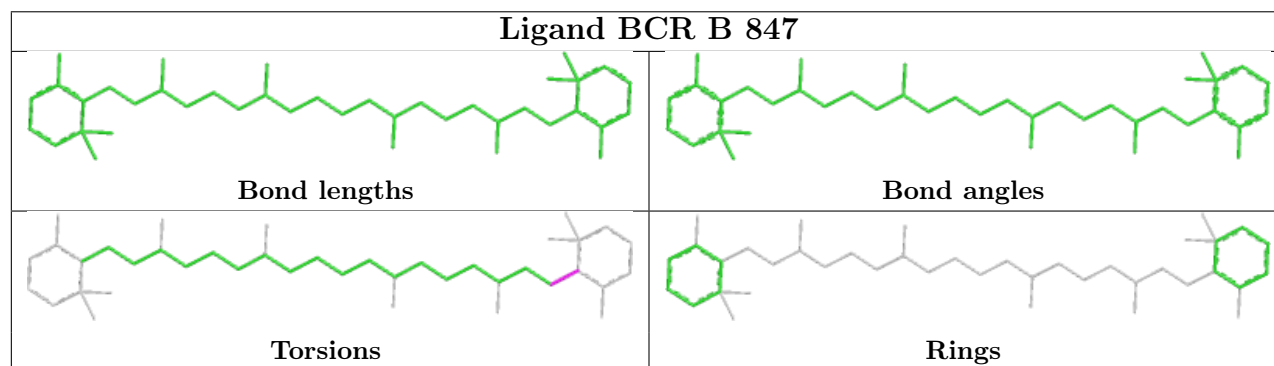
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20	3	407	CLA	8	0
28	F	5001	LMG	3	0
28	7	301	LMG	2	0
20	F	5003	CLA	1	0
24	9	619	LHG	3	0
20	2	607	CLA	1	0
20	A	807	CLA	2	0
20	1	608	CLA	5	0
20	G	4003	CLA	1	0
23	8	316	BCR	4	0
19	7	307	CHL	7	0
20	A	817	CLA	3	0
20	A	822	CLA	5	0
20	B	810	CLA	2	0
20	B	842	CLA	3	0
21	2	615	LUT	4	0
20	A	834	CLA	4	0
24	A	854	LHG	2	0
20	9	612	CLA	3	0
23	A	852	BCR	7	0
23	A	858	BCR	6	0
20	A	836	CLA	6	0
20	K	204	CLA	1	0
20	7	303	CLA	3	0
20	8	311	CLA	4	0
20	2	603	CLA	10	0
20	3	414	CLA	2	0
20	A	804	CLA	6	0
20	A	815	CLA	5	0
24	9	617	LHG	1	0
20	A	827	CLA	12	0
20	B	841	CLA	4	0
20	B	814	CLA	8	0
20	A	818	CLA	7	0
22	1	616	XAT	2	0
24	7	320	LHG	3	0
20	B	823	CLA	3	0
19	2	606	CHL	4	0
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29	B	850	DGD	8	0
20	B	806	CLA	3	0

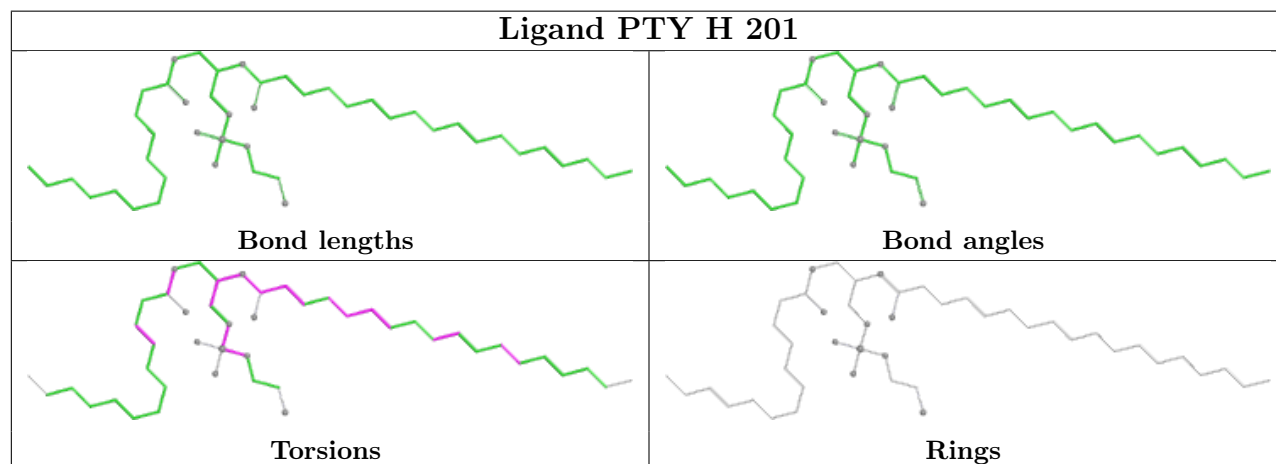
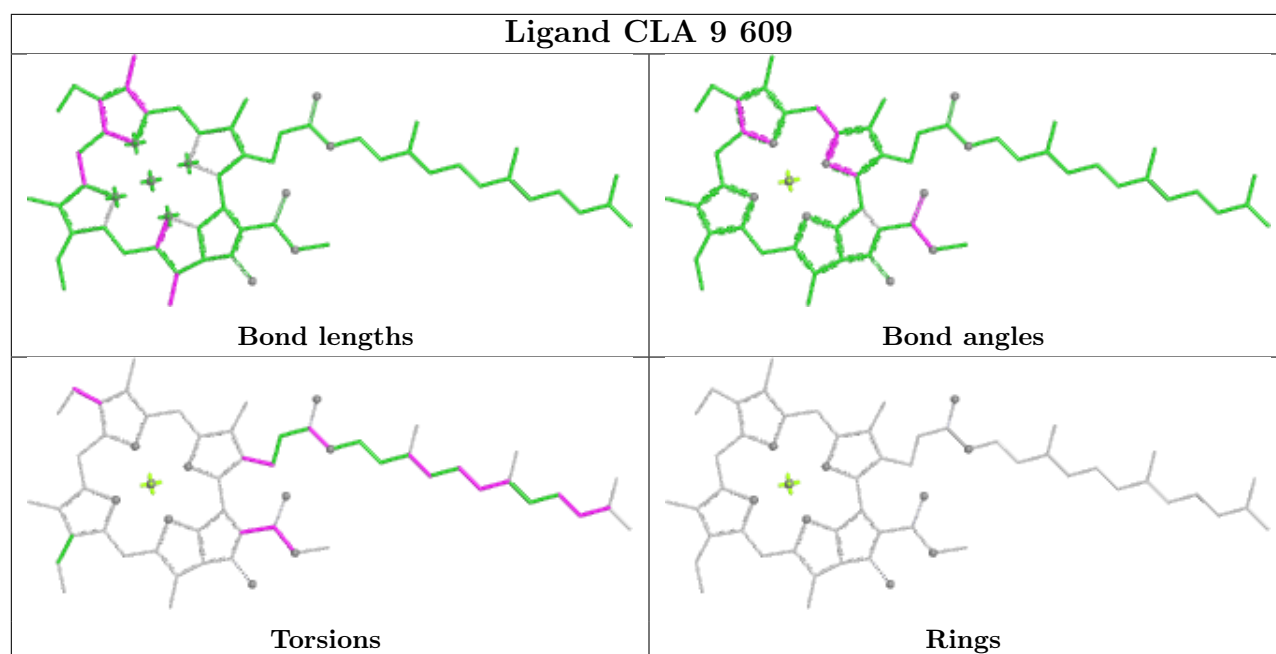
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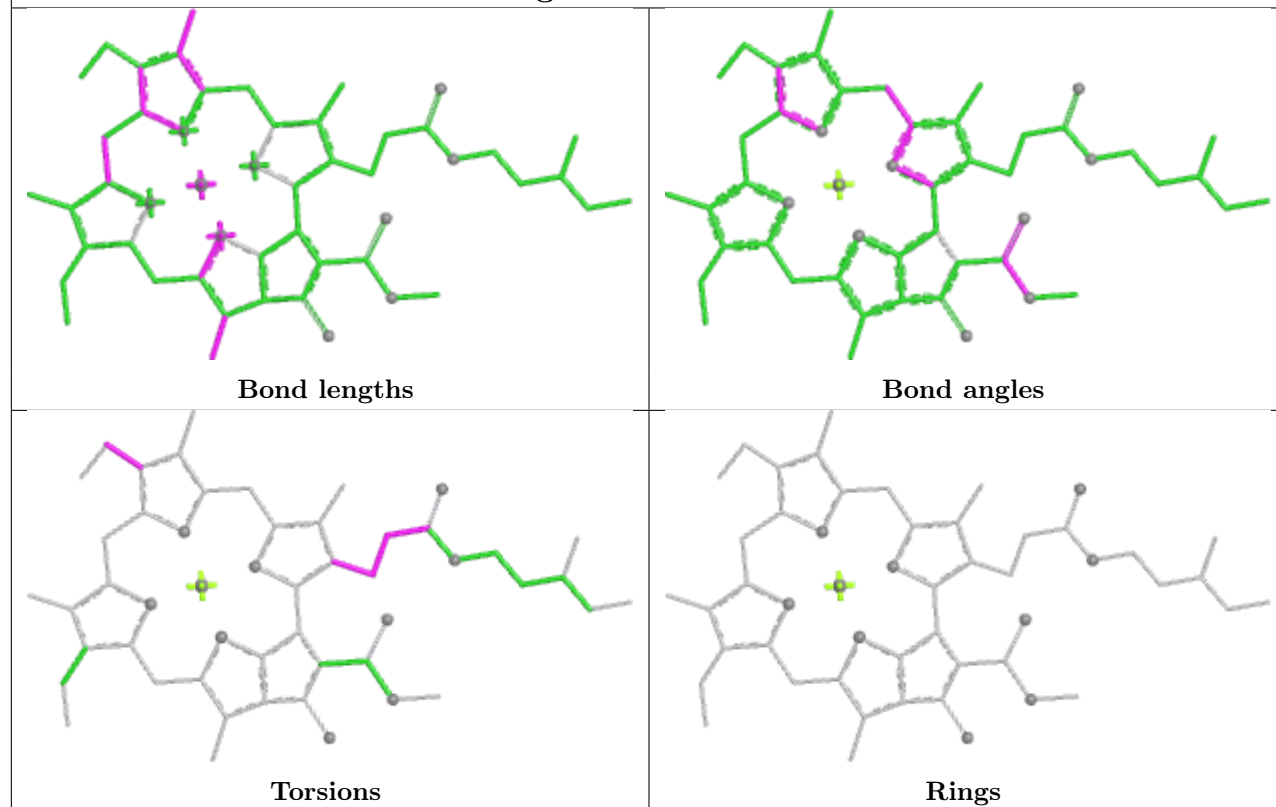
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	617	LUT	1	0
23	7	318	BCR	4	0
20	8	307	CLA	1	0
20	B	811	CLA	3	0
25	1	622	PTY	2	0
20	B	805	CLA	2	0
24	A	853	LHG	2	0
19	1	606	CHL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

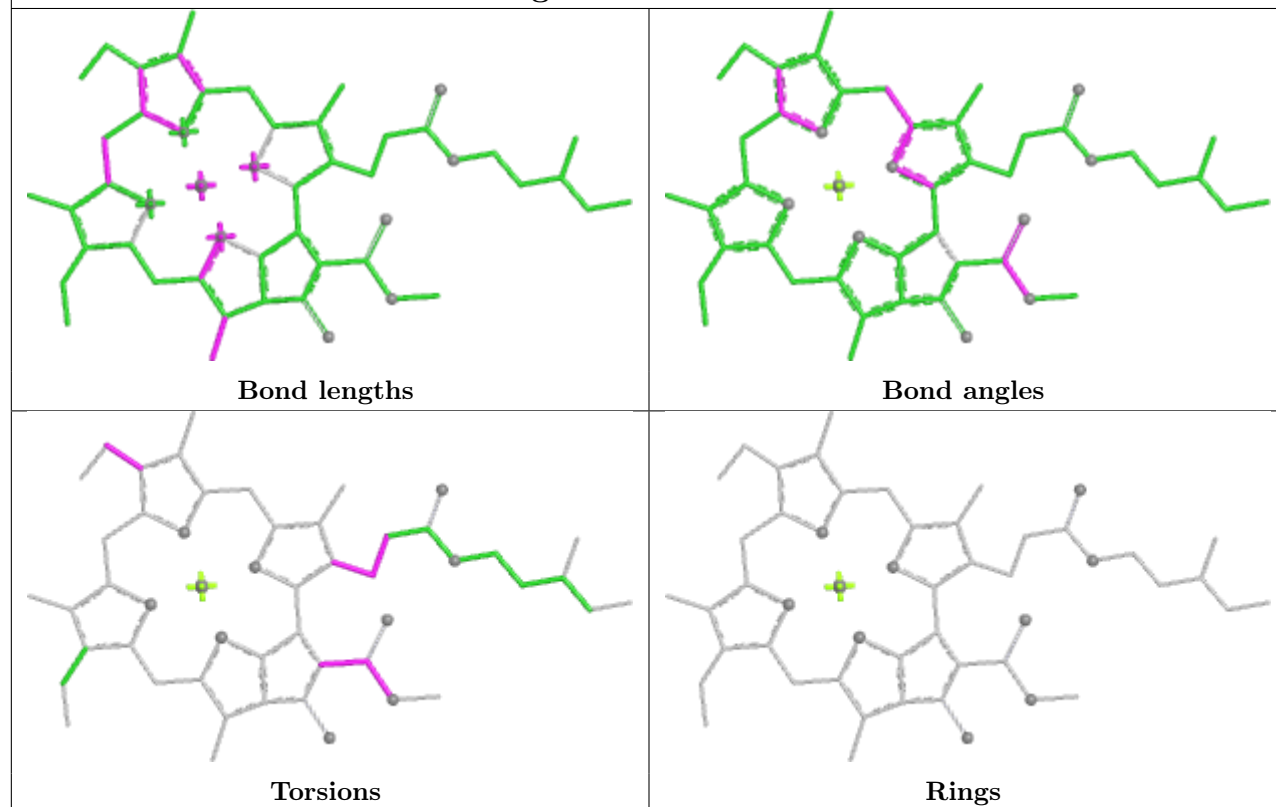


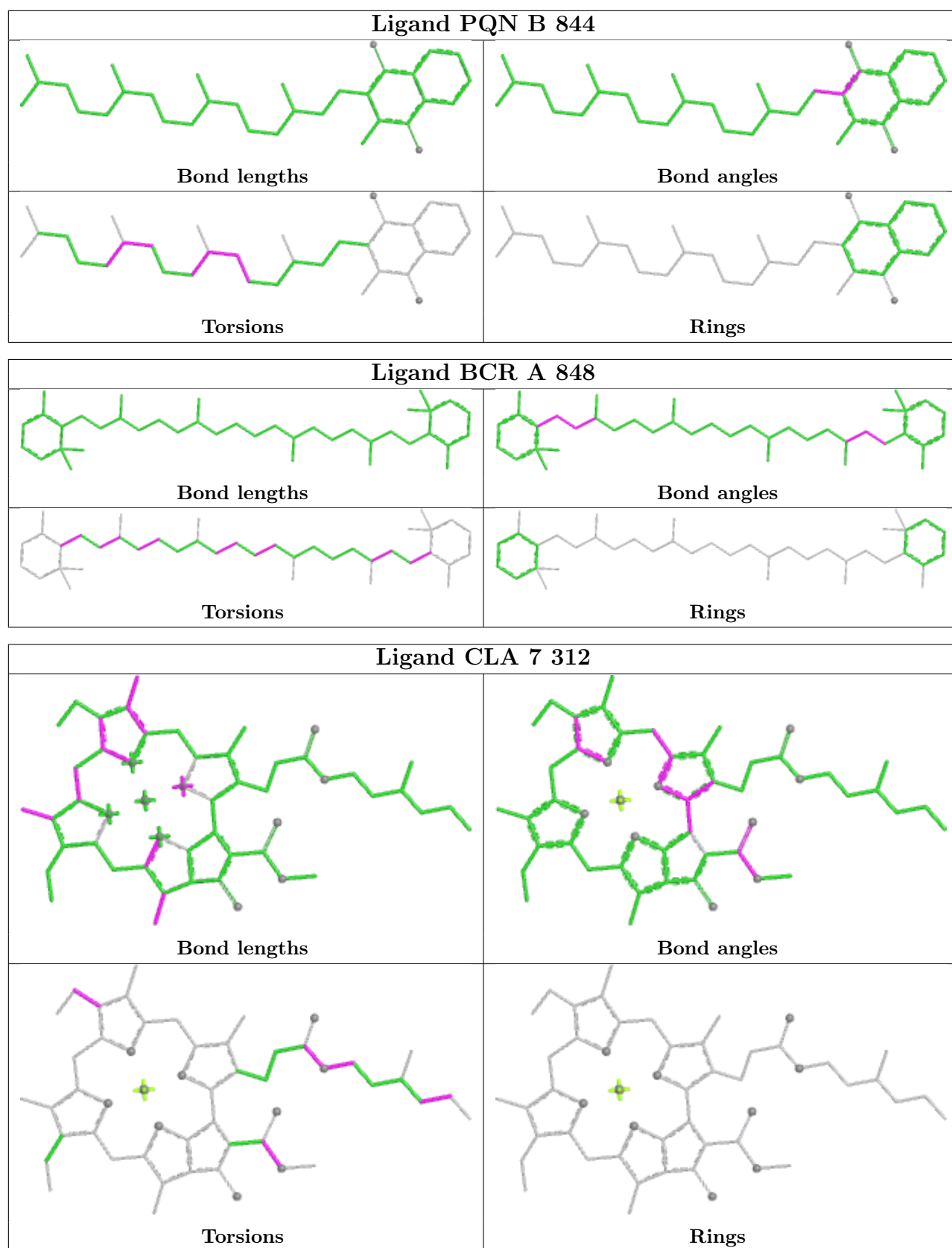


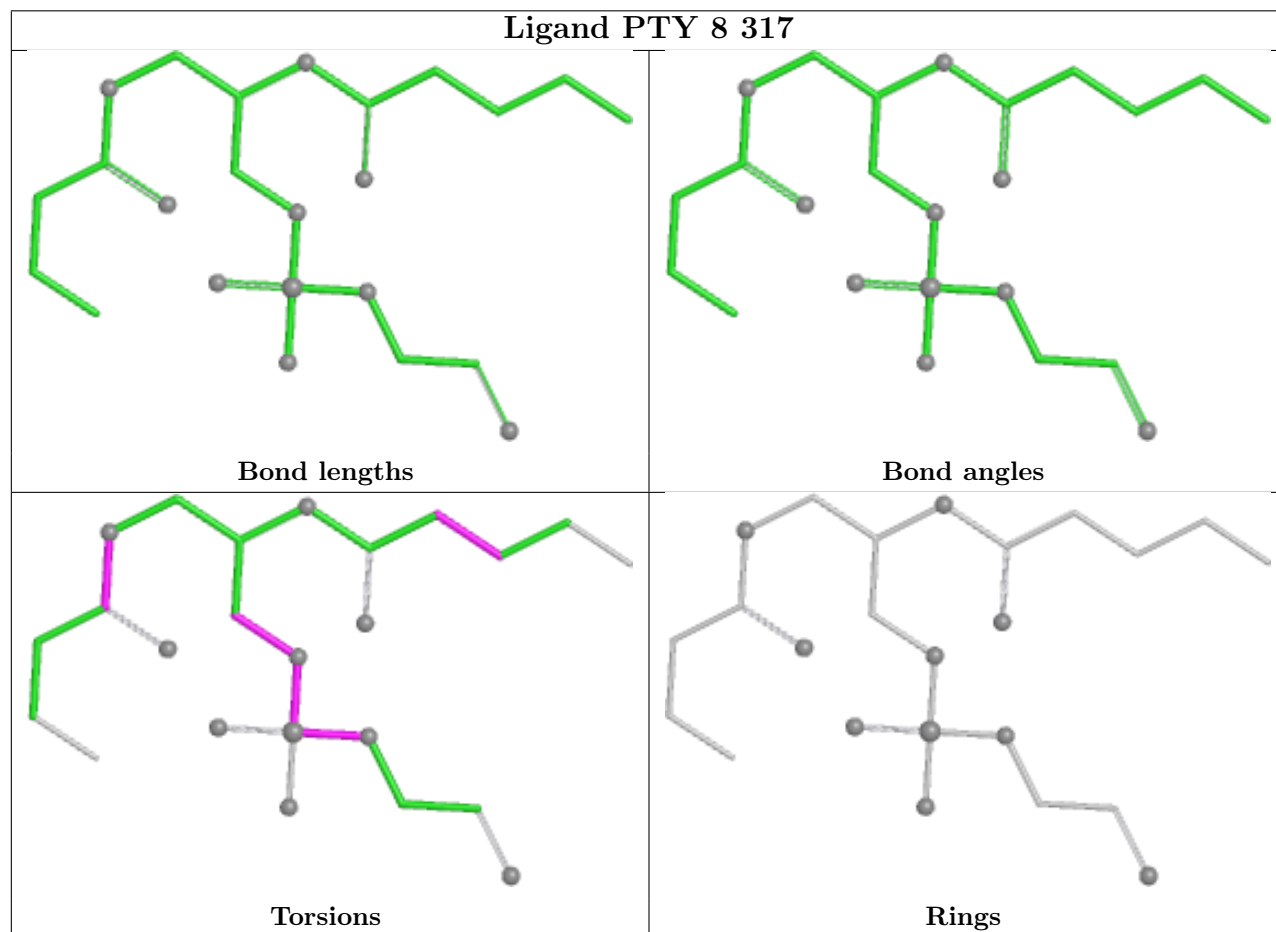
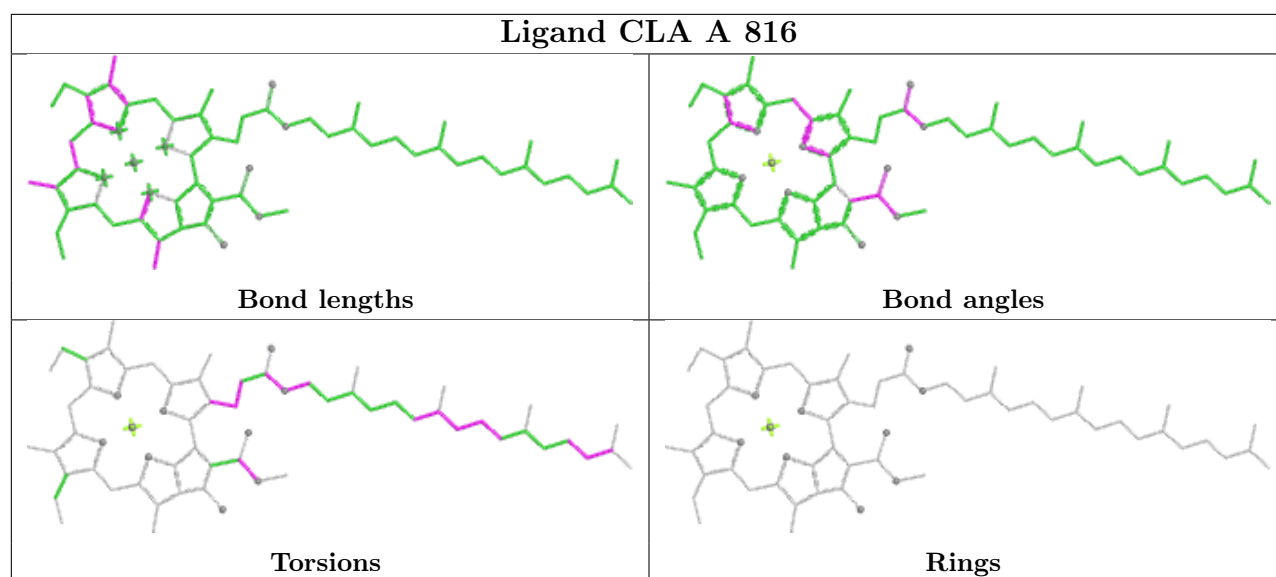
Ligand CLA 8 313



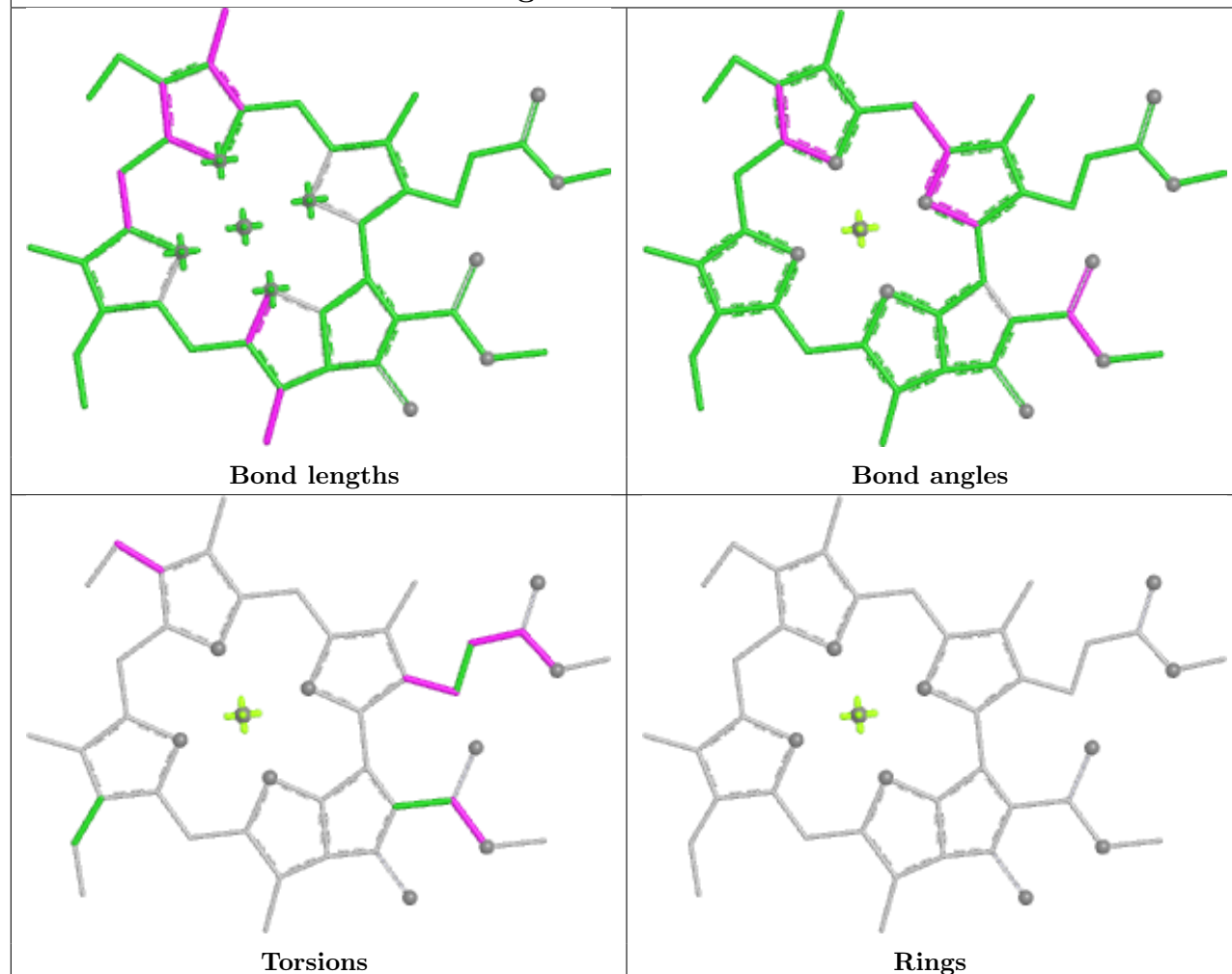
Ligand CLA A 838



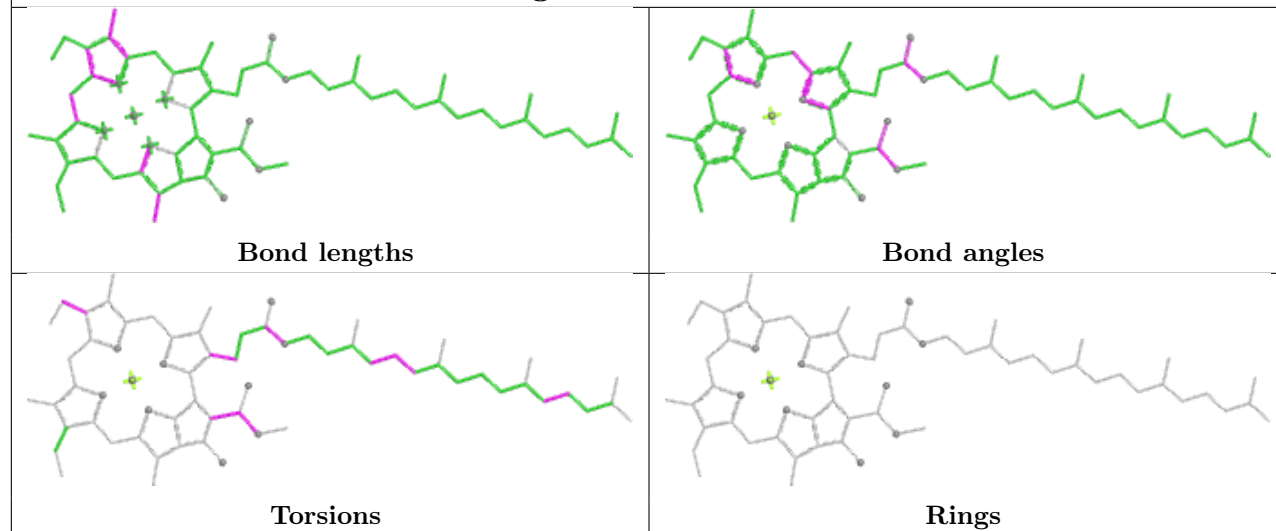


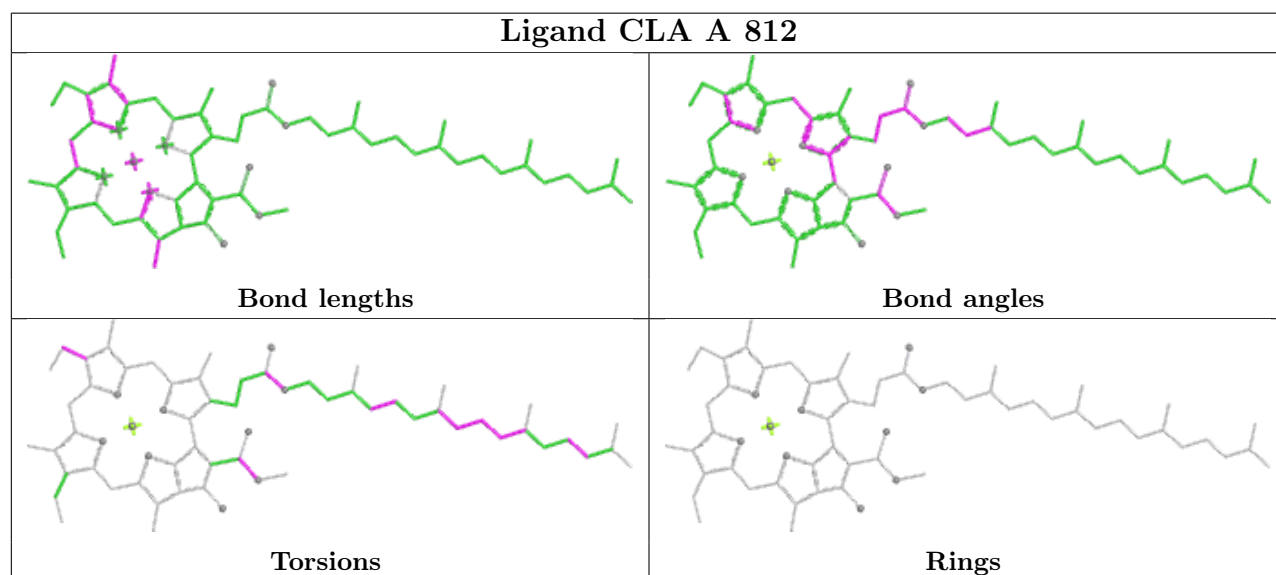
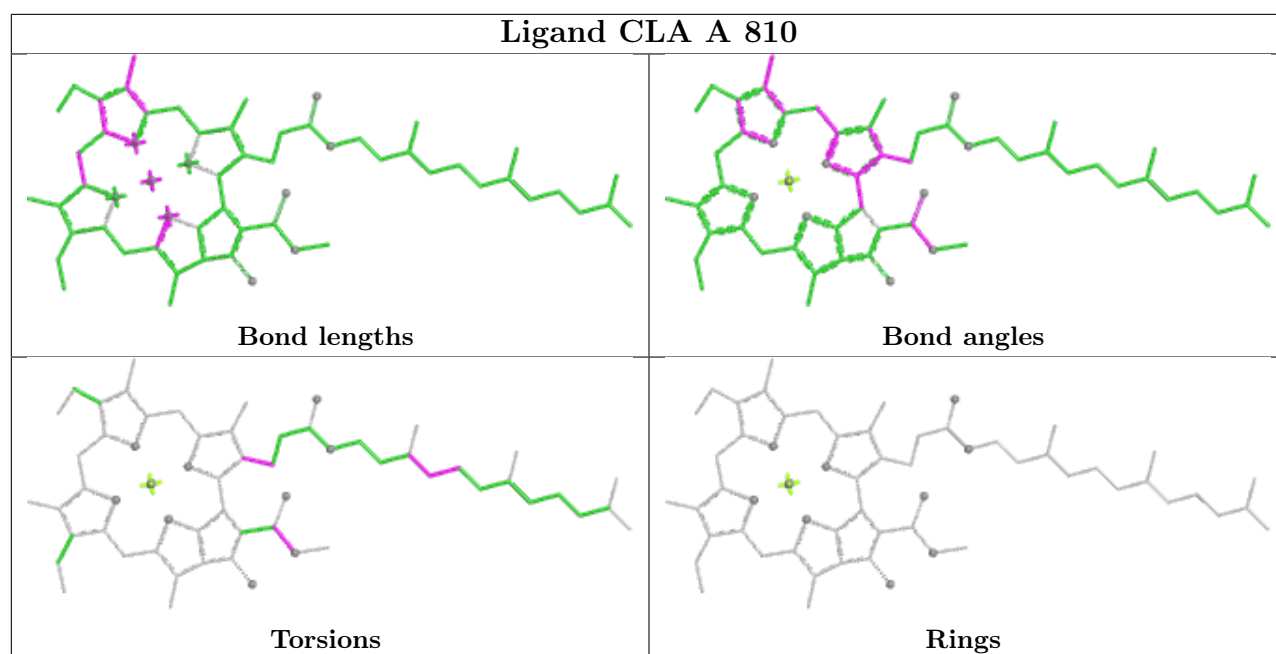


Ligand CLA 1 610

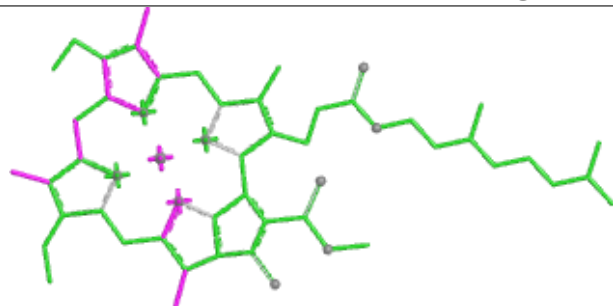


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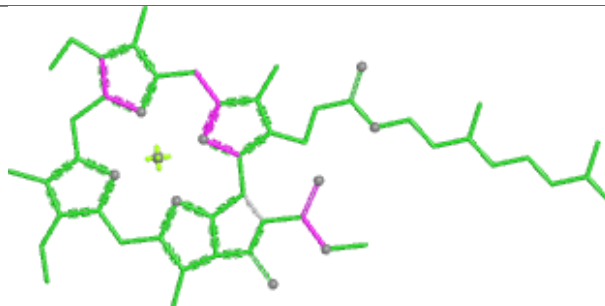




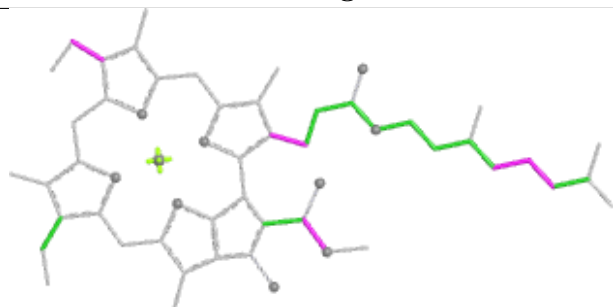
Ligand CLA B 816



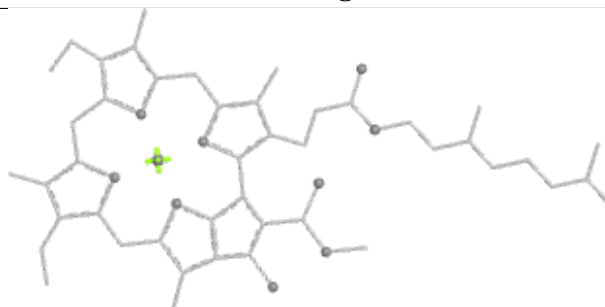
Bond lengths



Bond angles

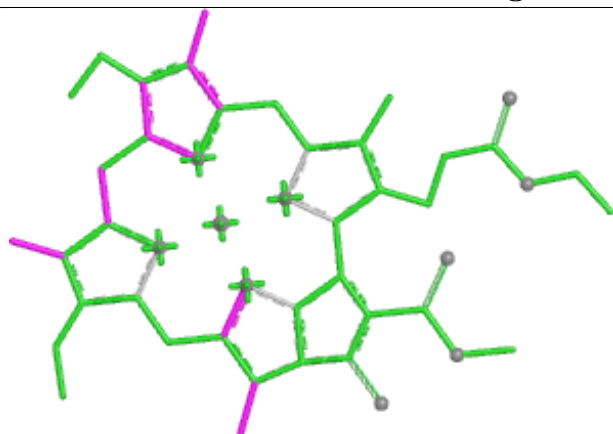


Torsions

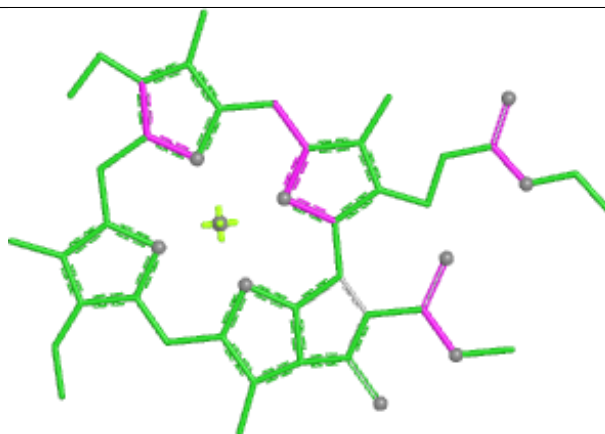


Rings

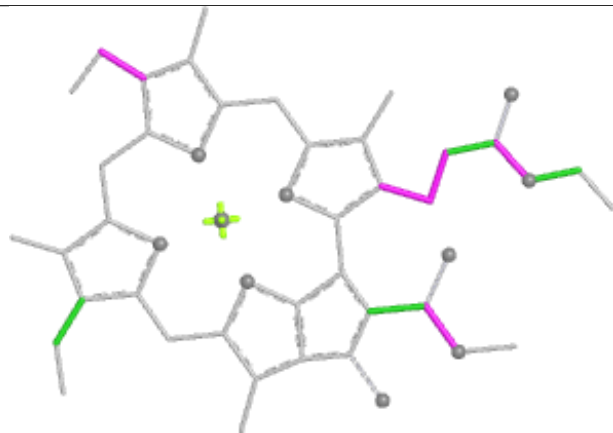
Ligand CLA F 5006



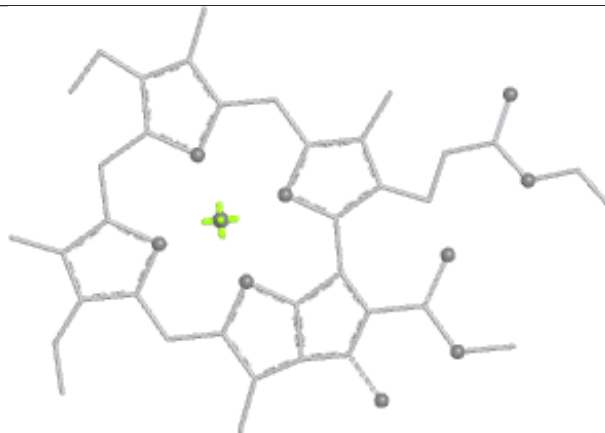
Bond lengths



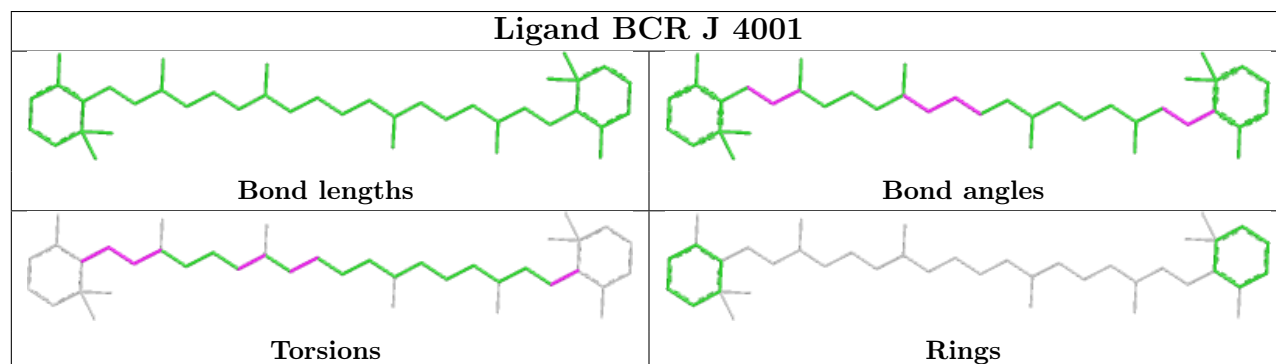
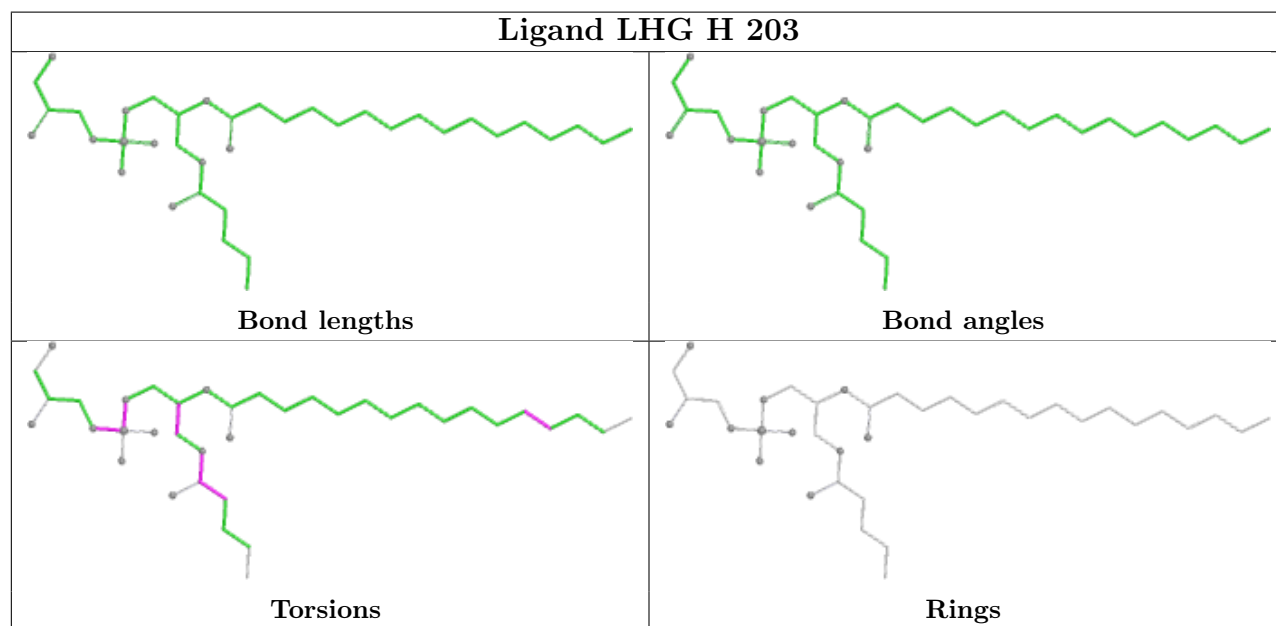
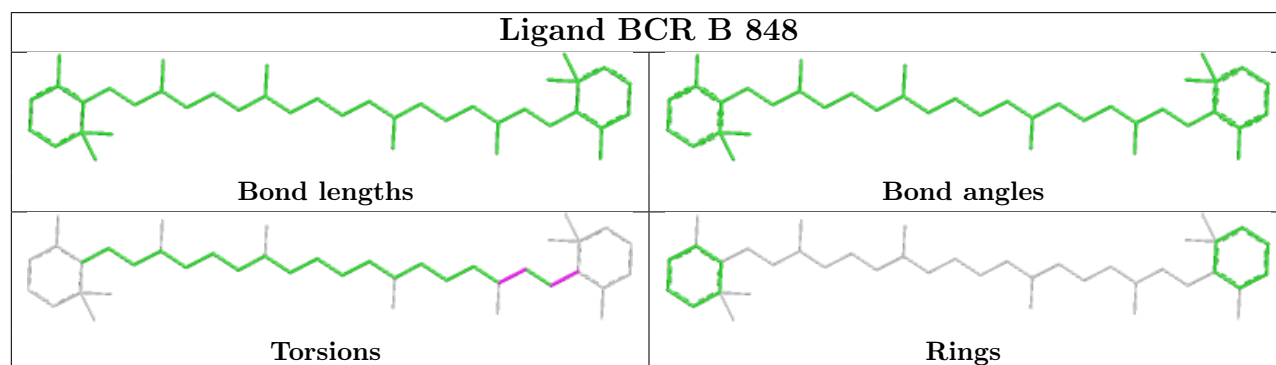
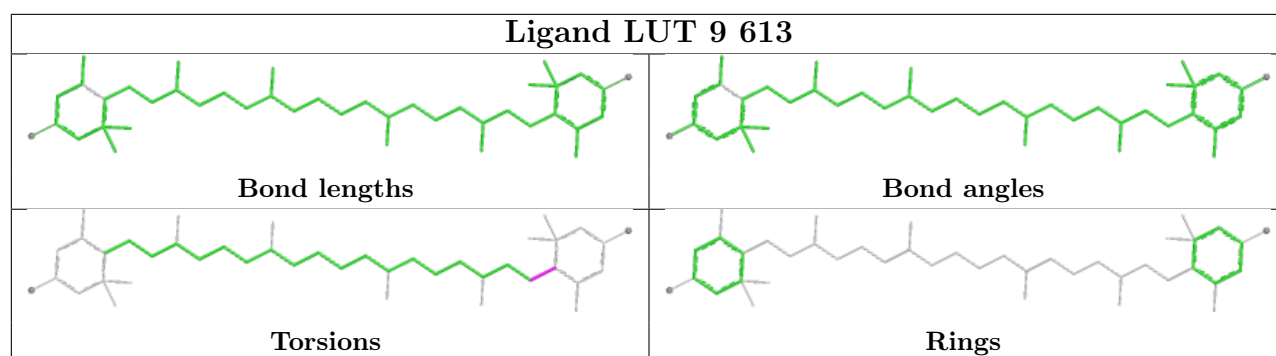
Bond angles

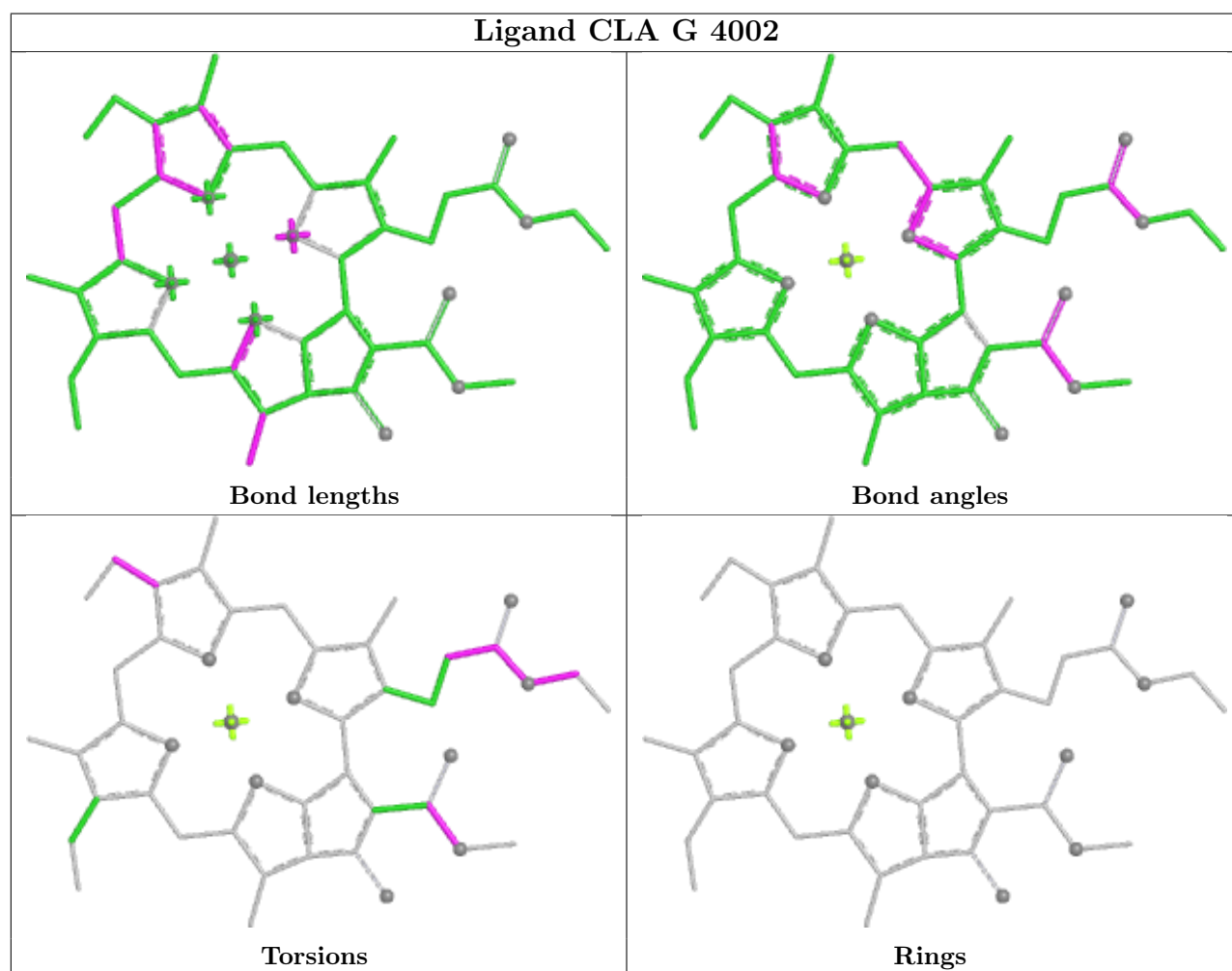
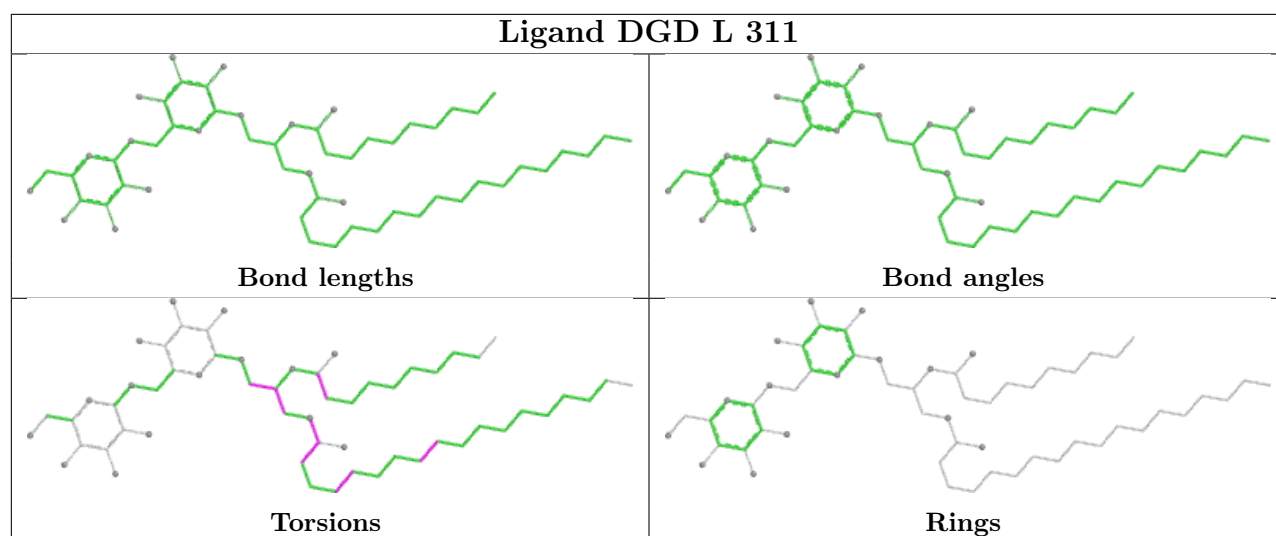


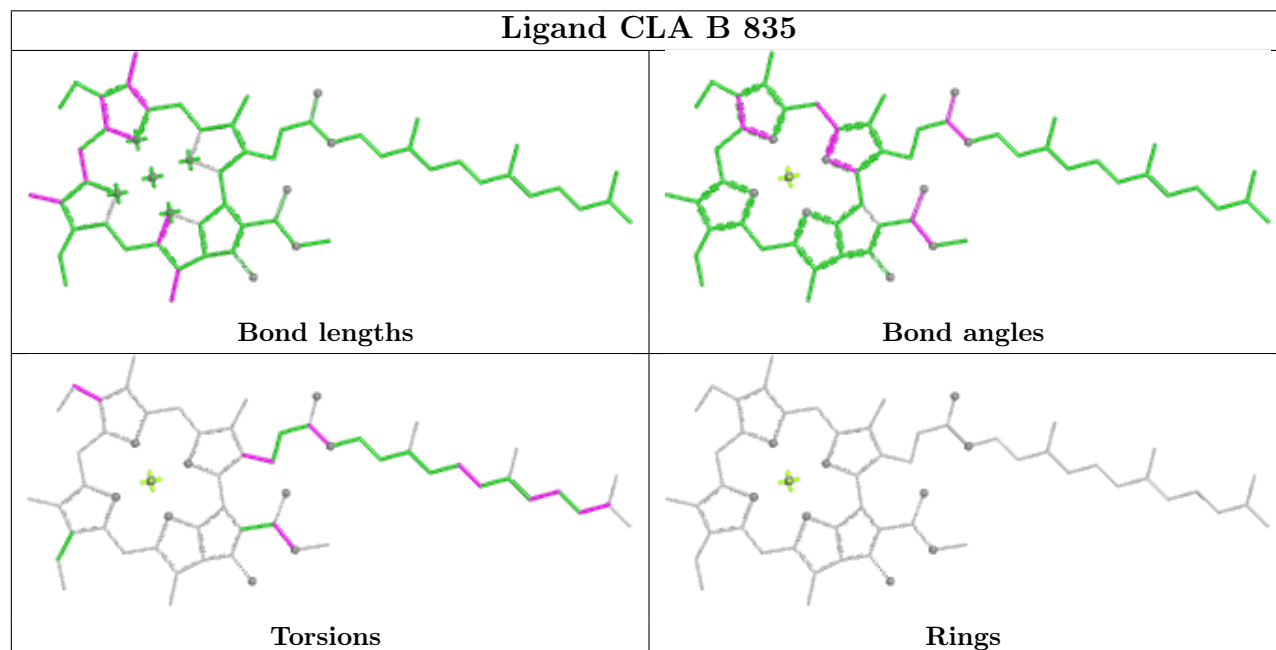
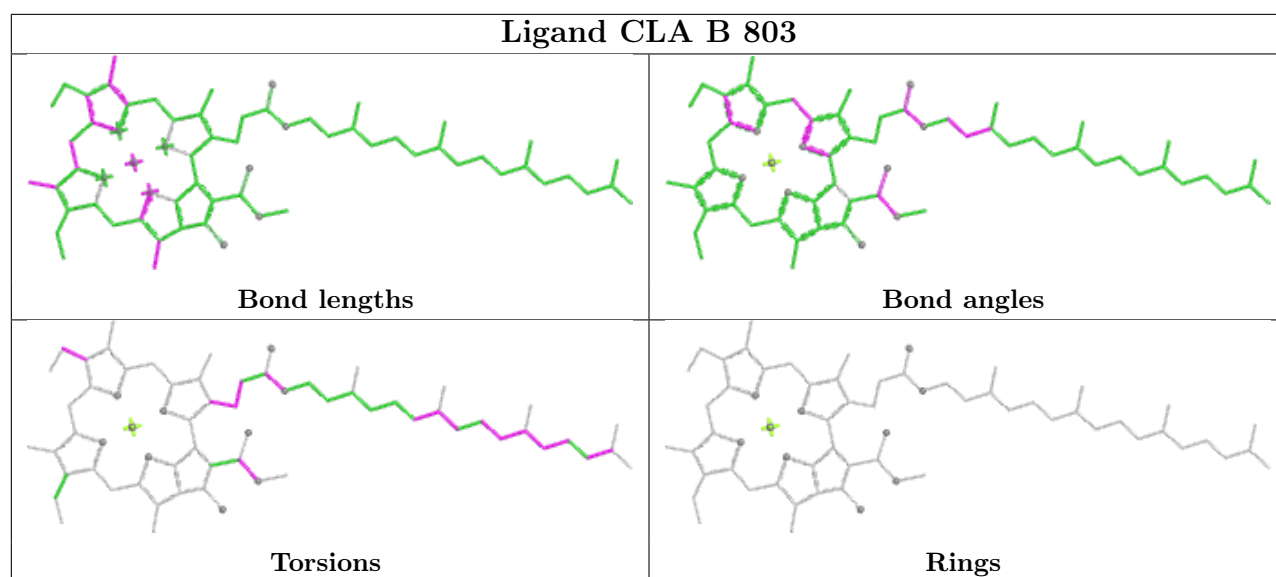
Torsions



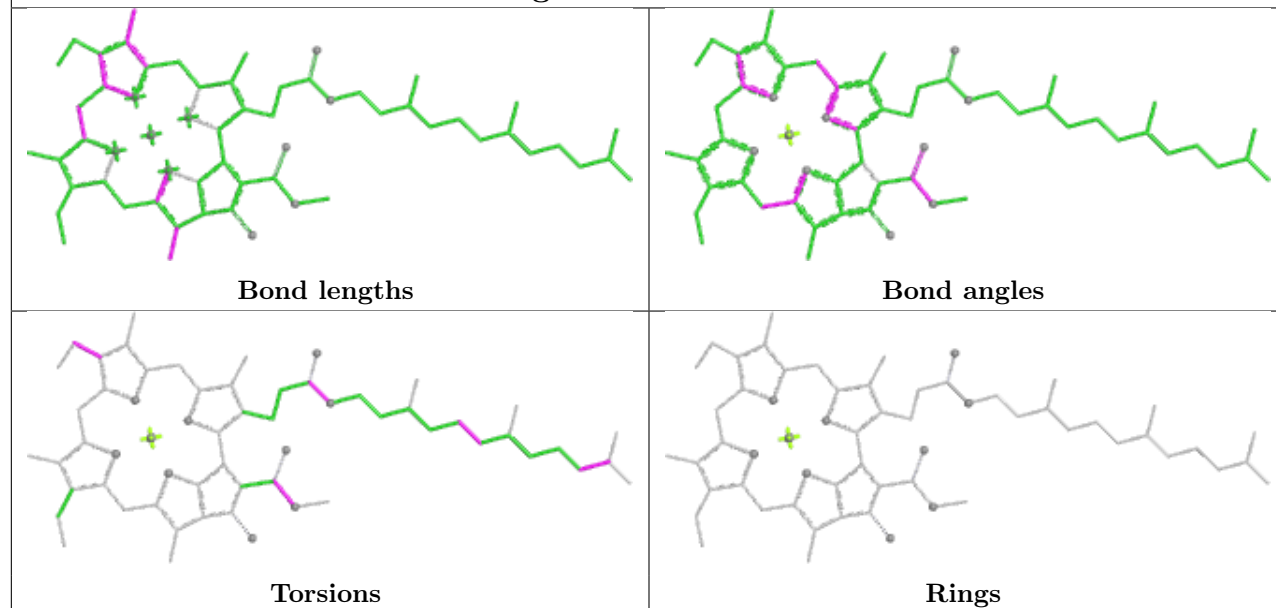
Rings



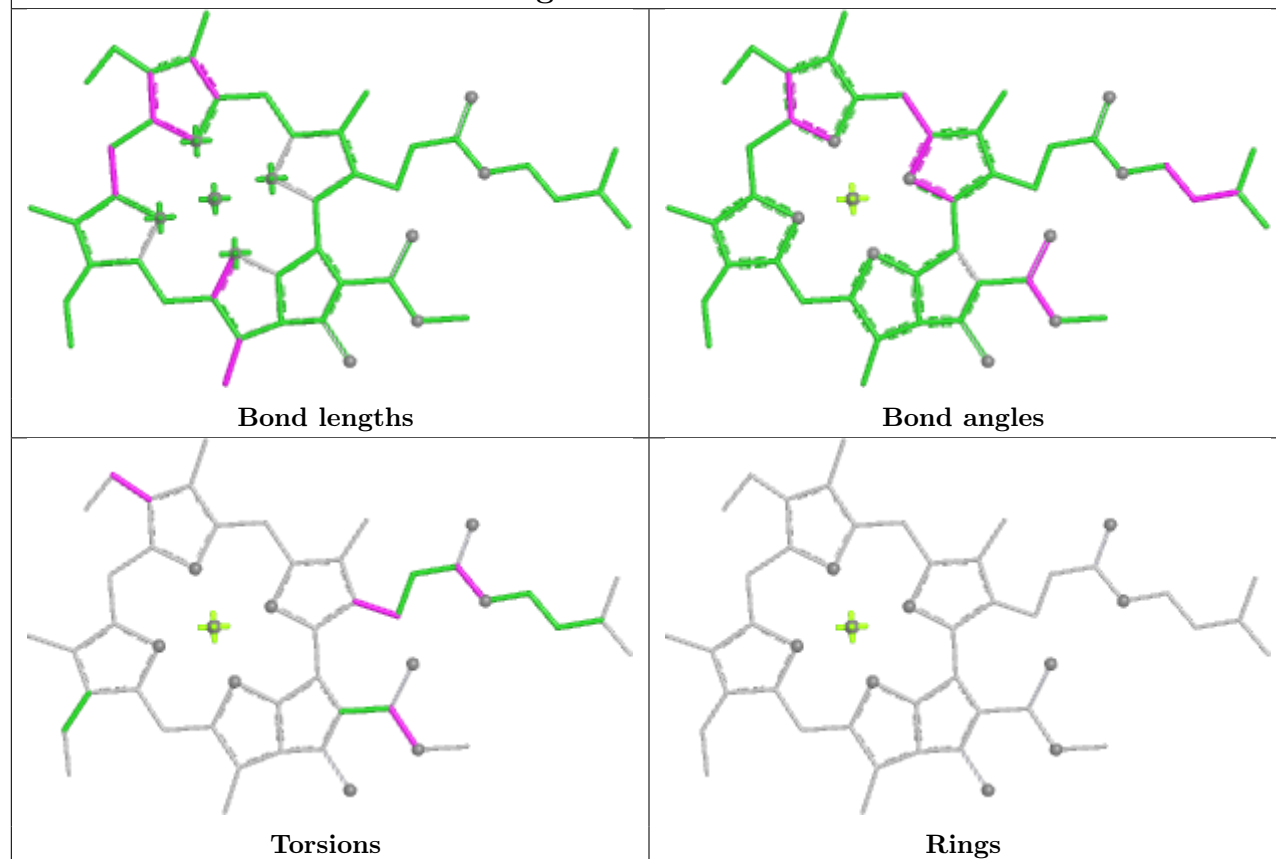


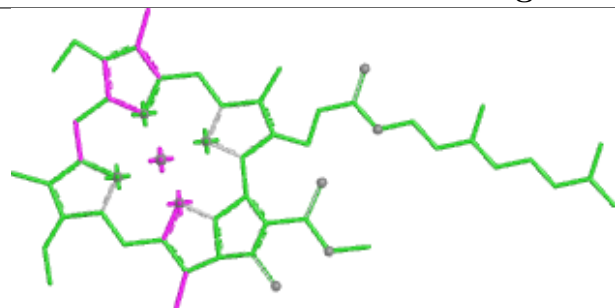


Ligand CLA B 838

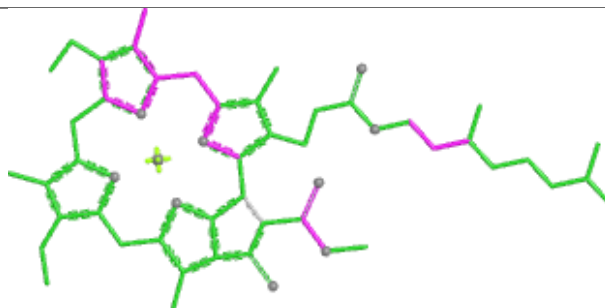


Ligand CLA 3 409

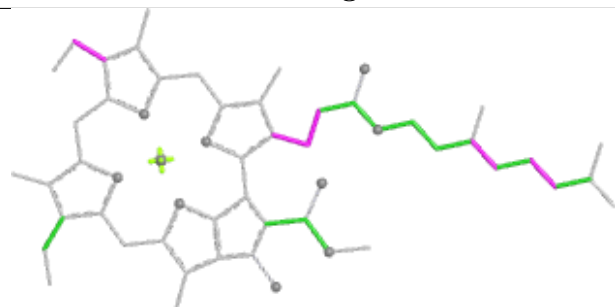


Ligand CLA A 837

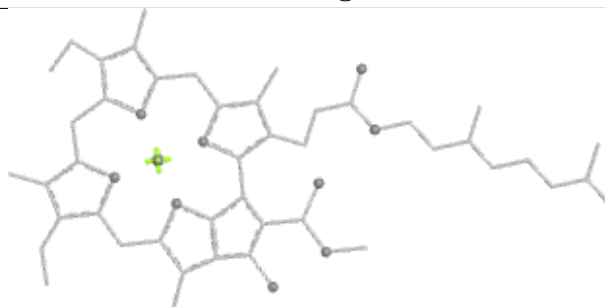
Bond lengths



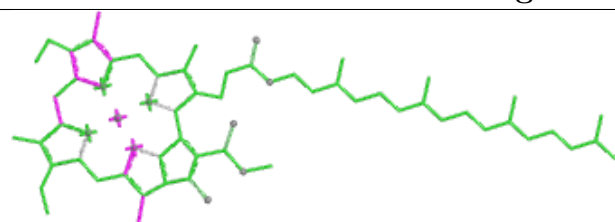
Bond angles



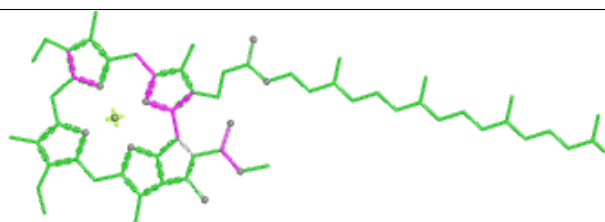
Torsions



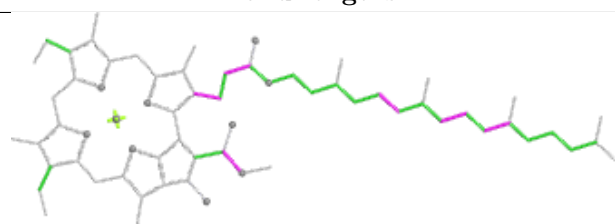
Rings

Ligand CLA A 828

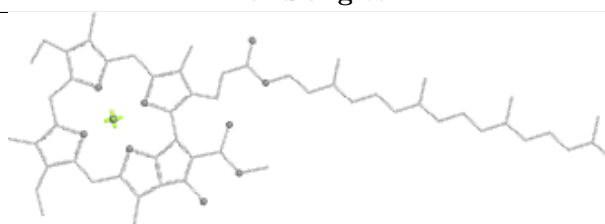
Bond lengths



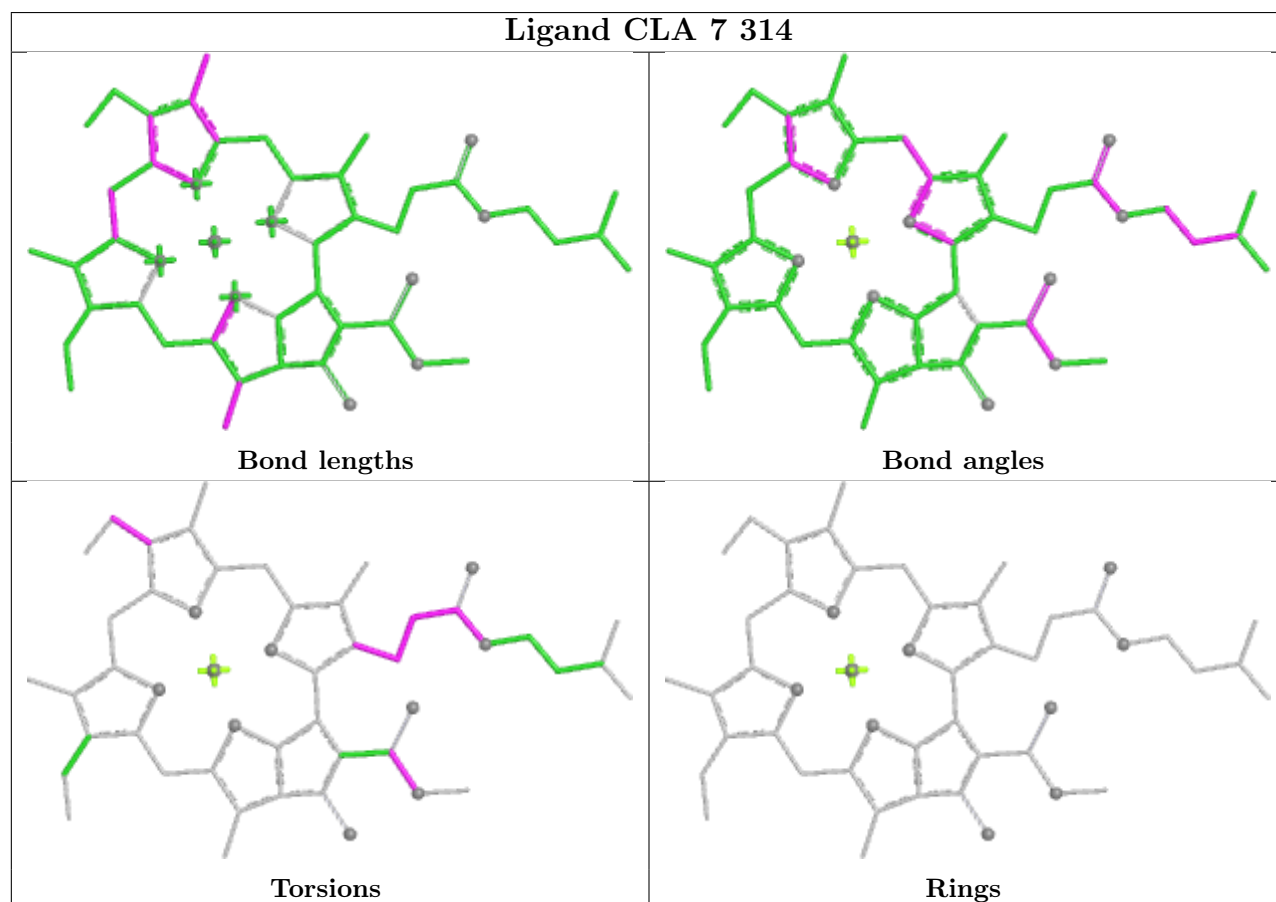
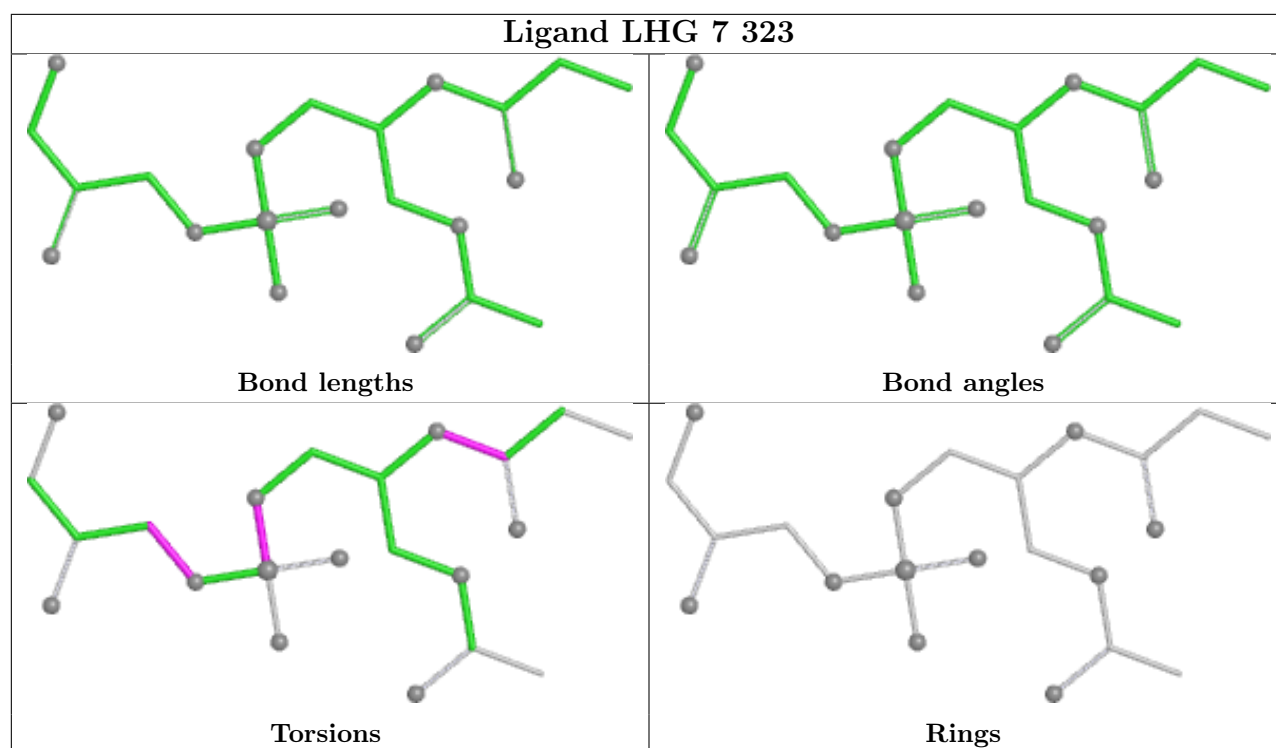
Bond angles



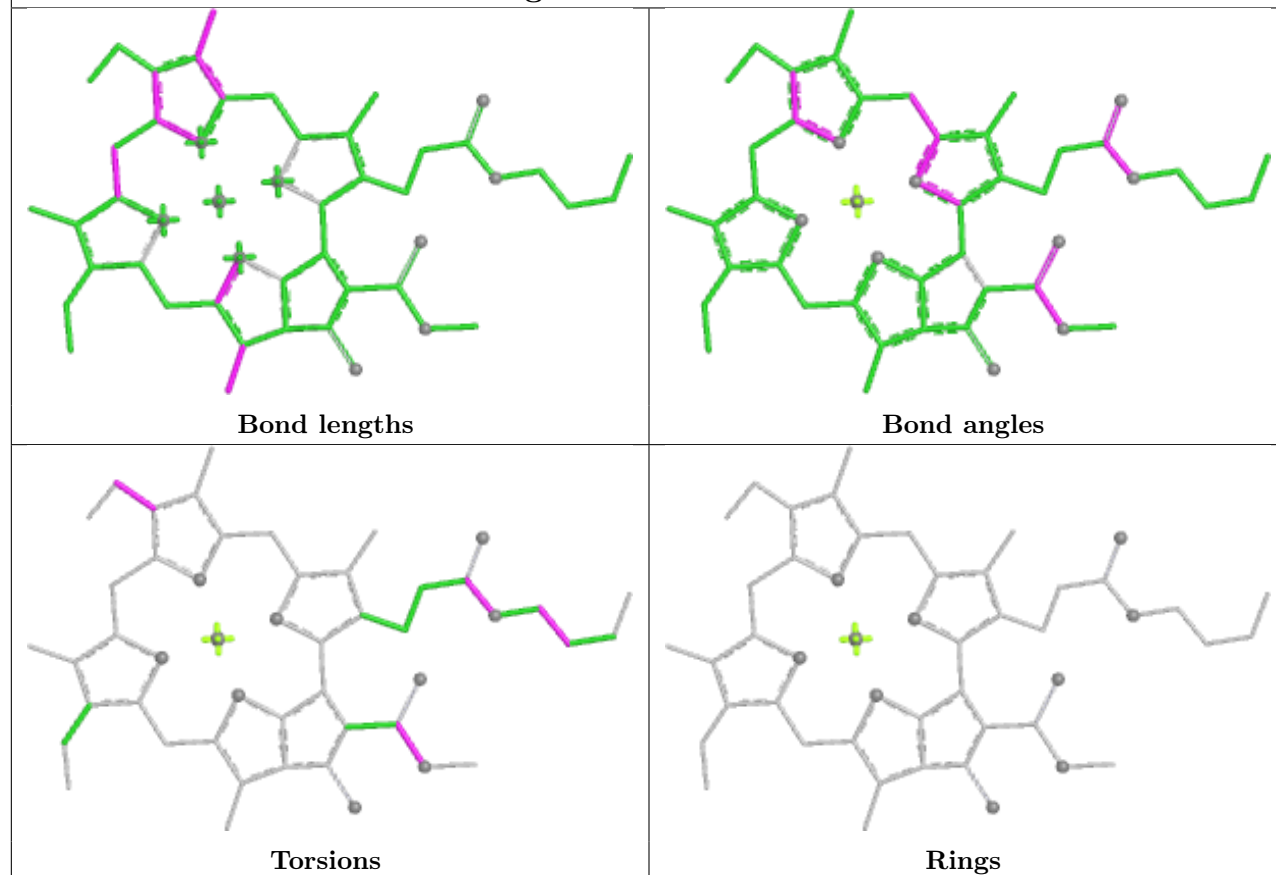
Torsions



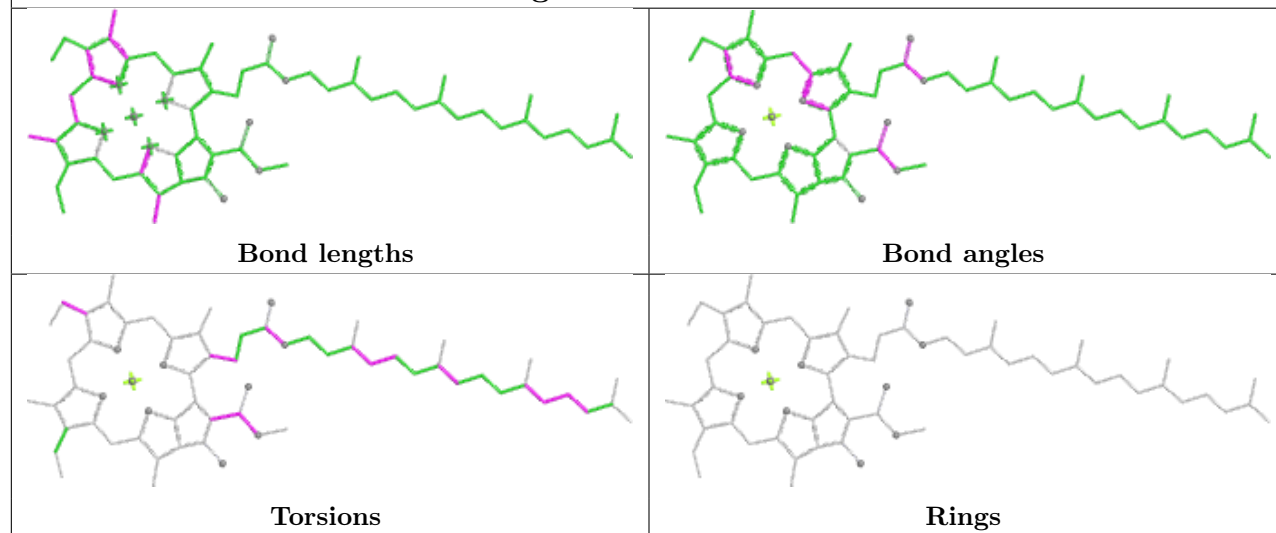
Rings

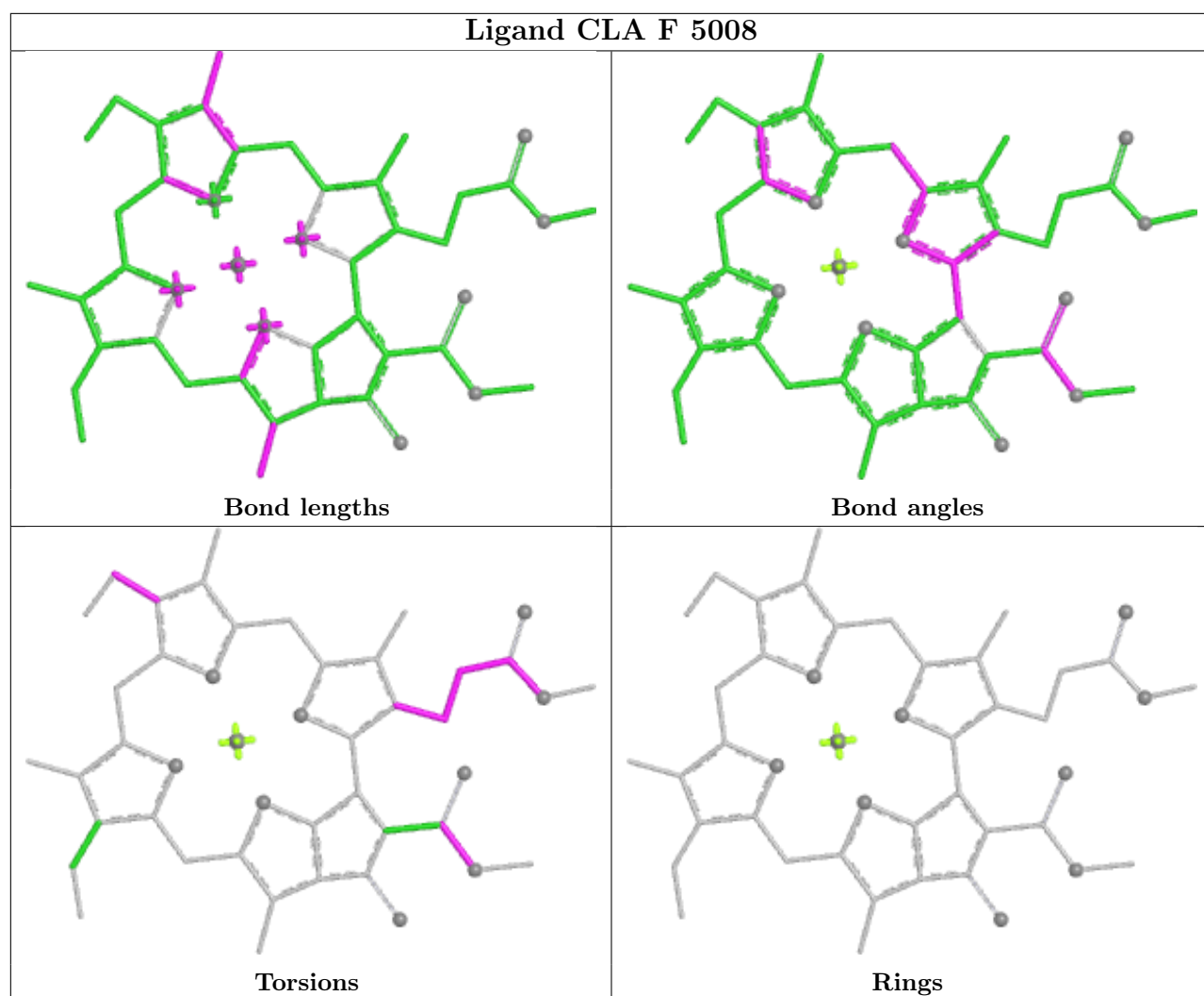


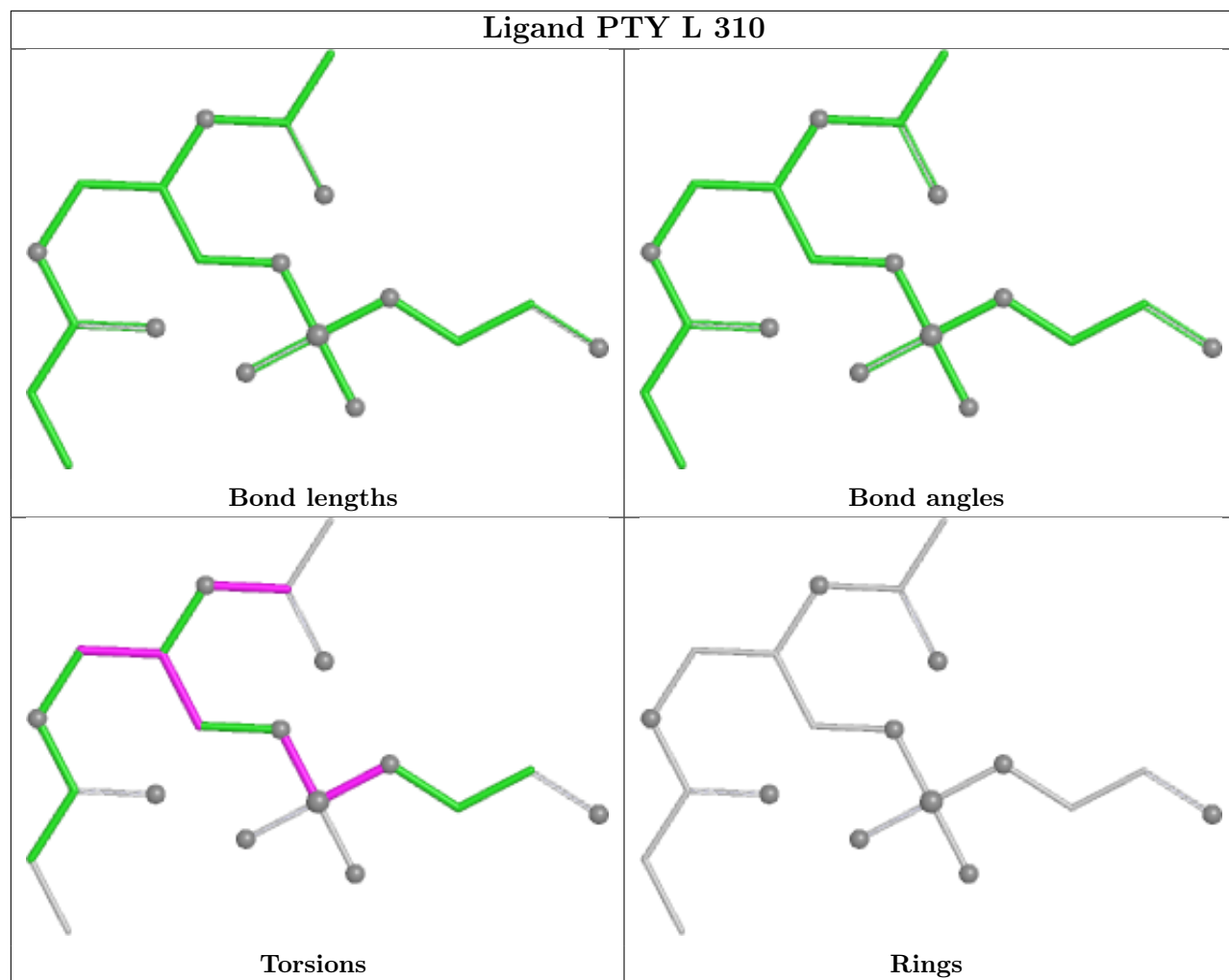
Ligand CLA F 5007



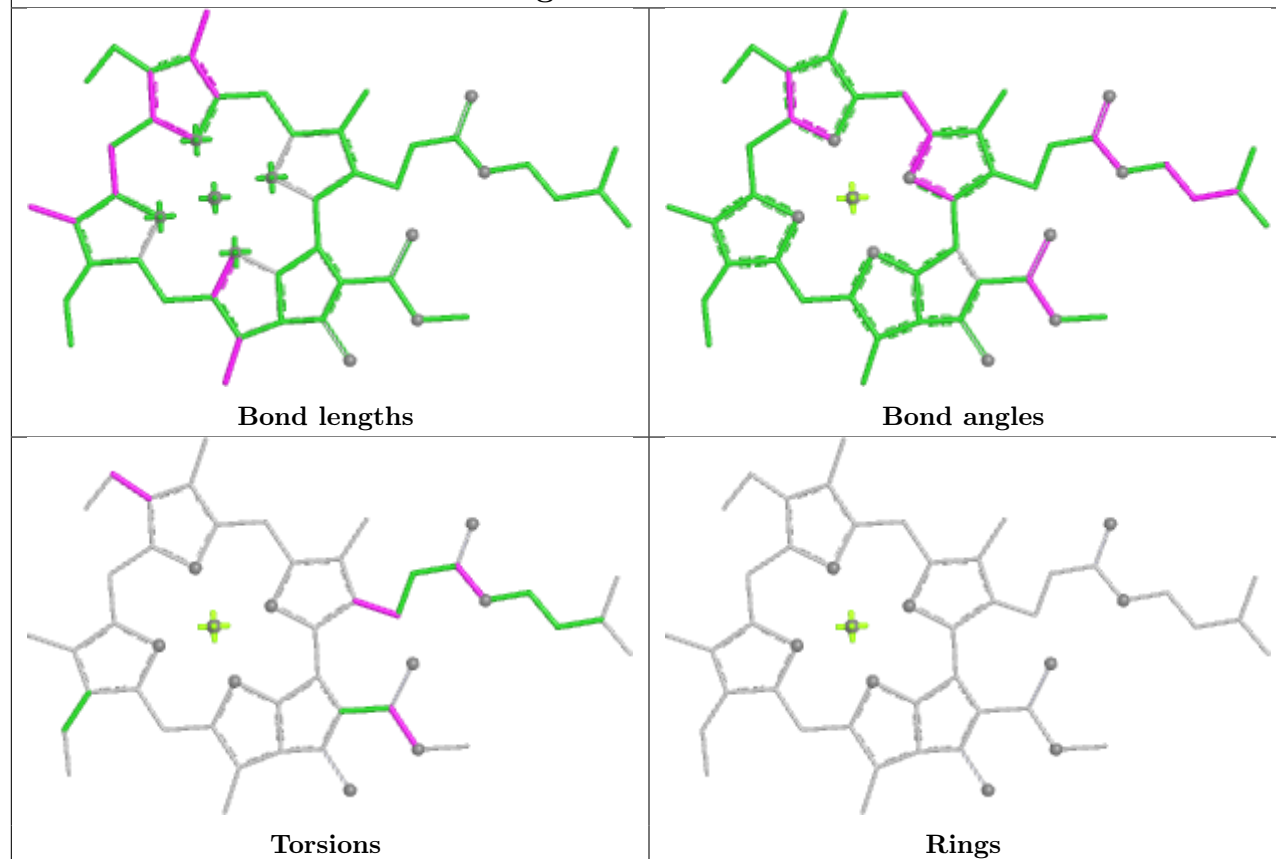
Ligand CLA A 814



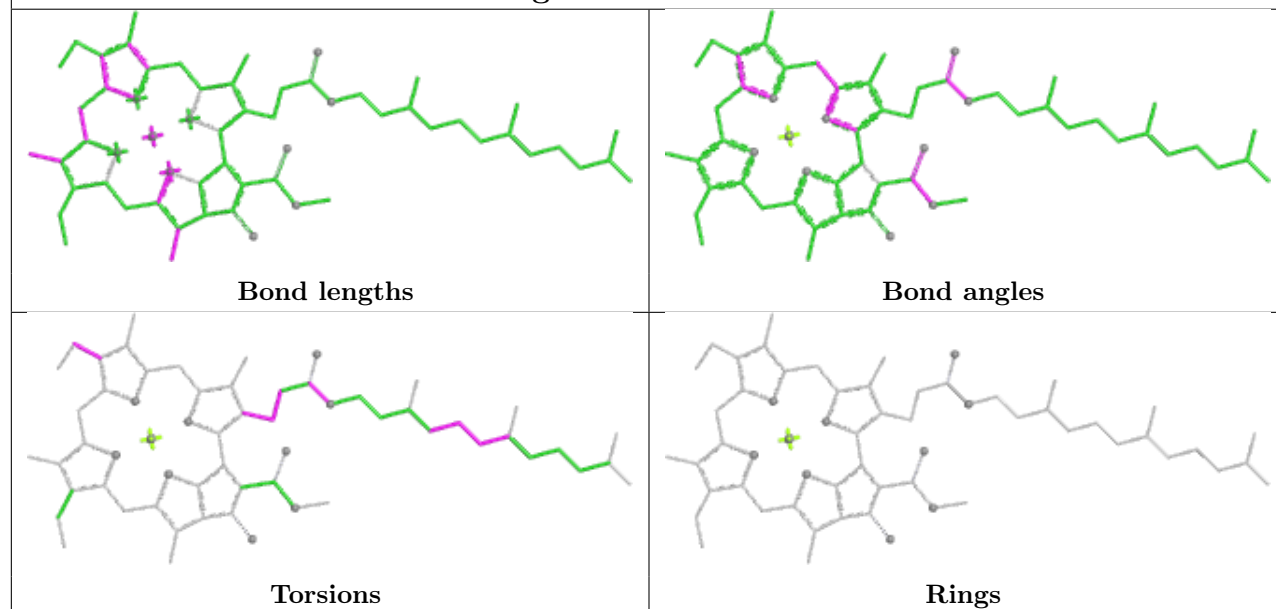


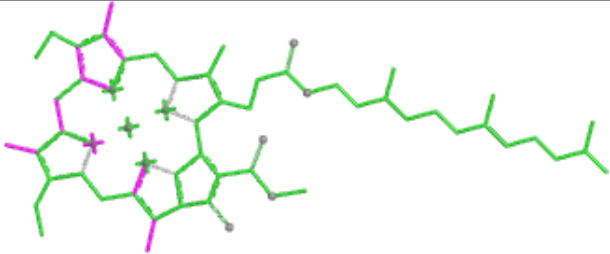
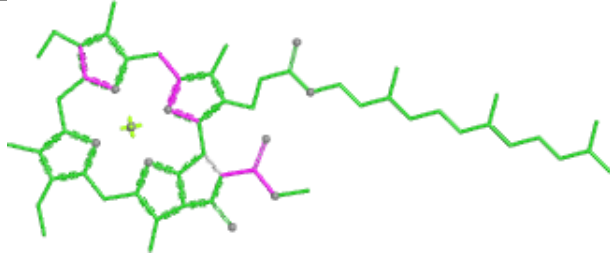
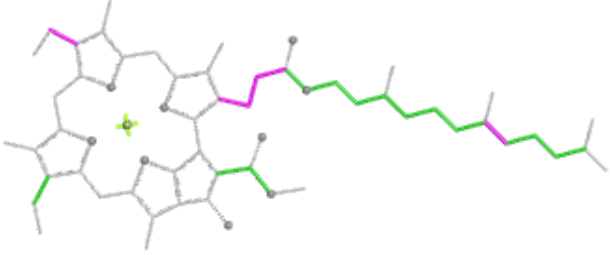
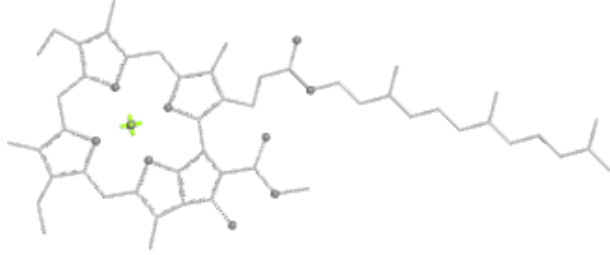
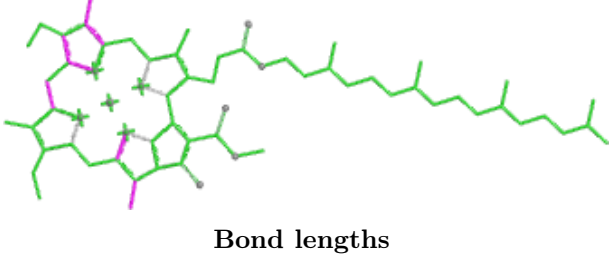
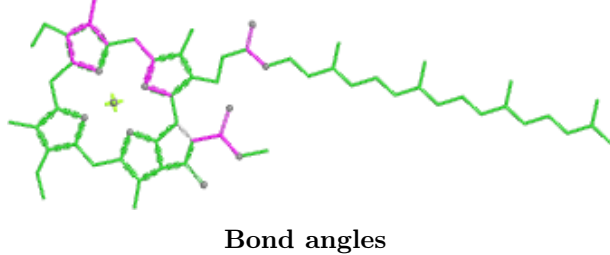
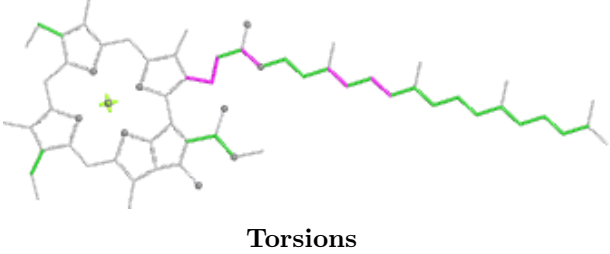
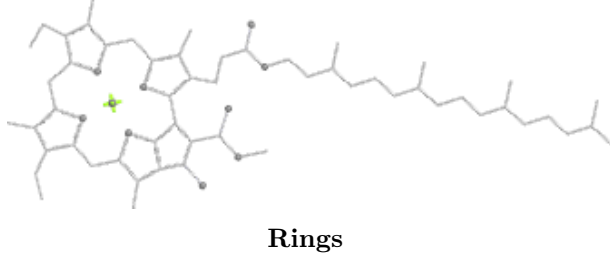


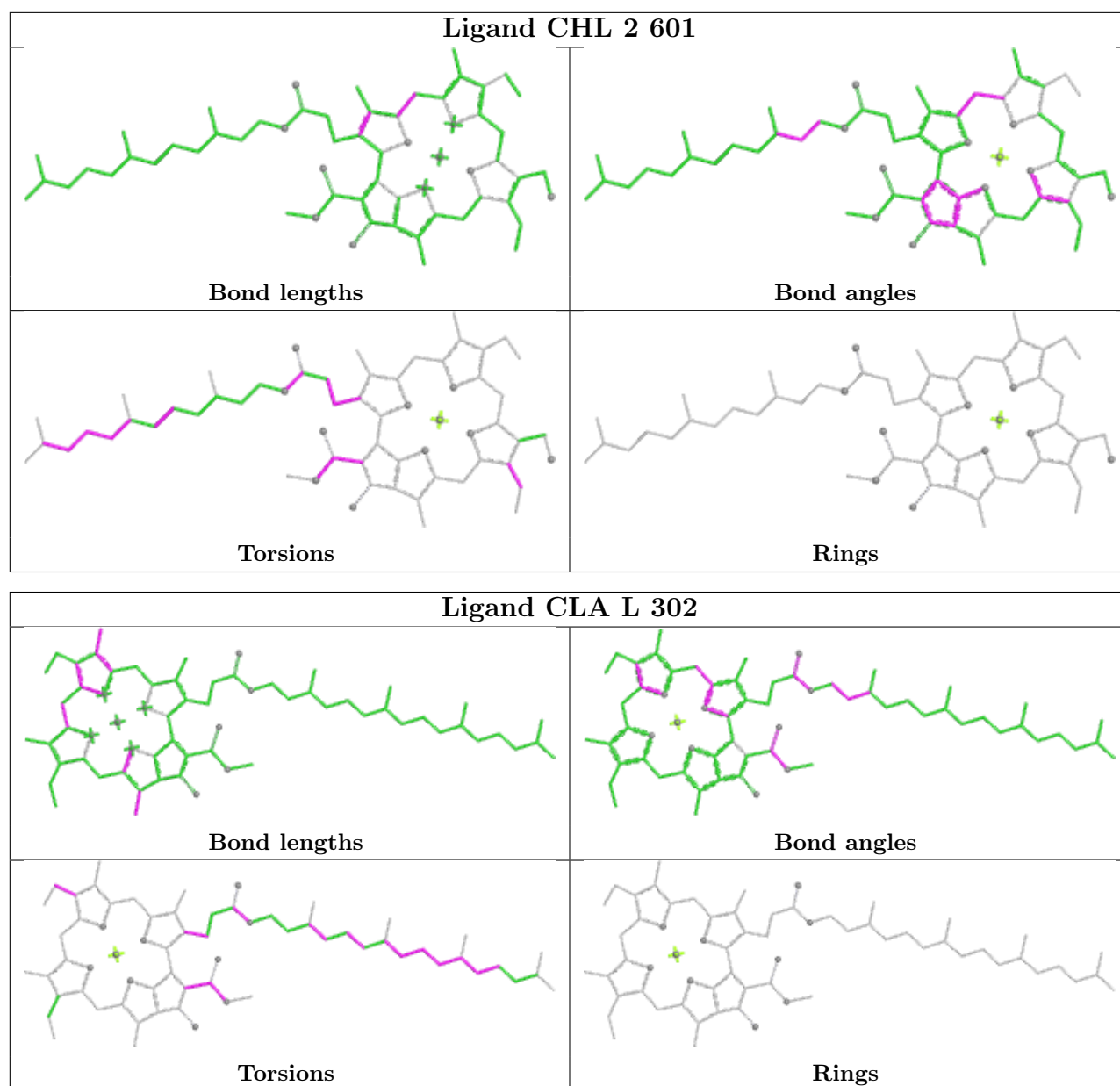
Ligand CLA 2 604



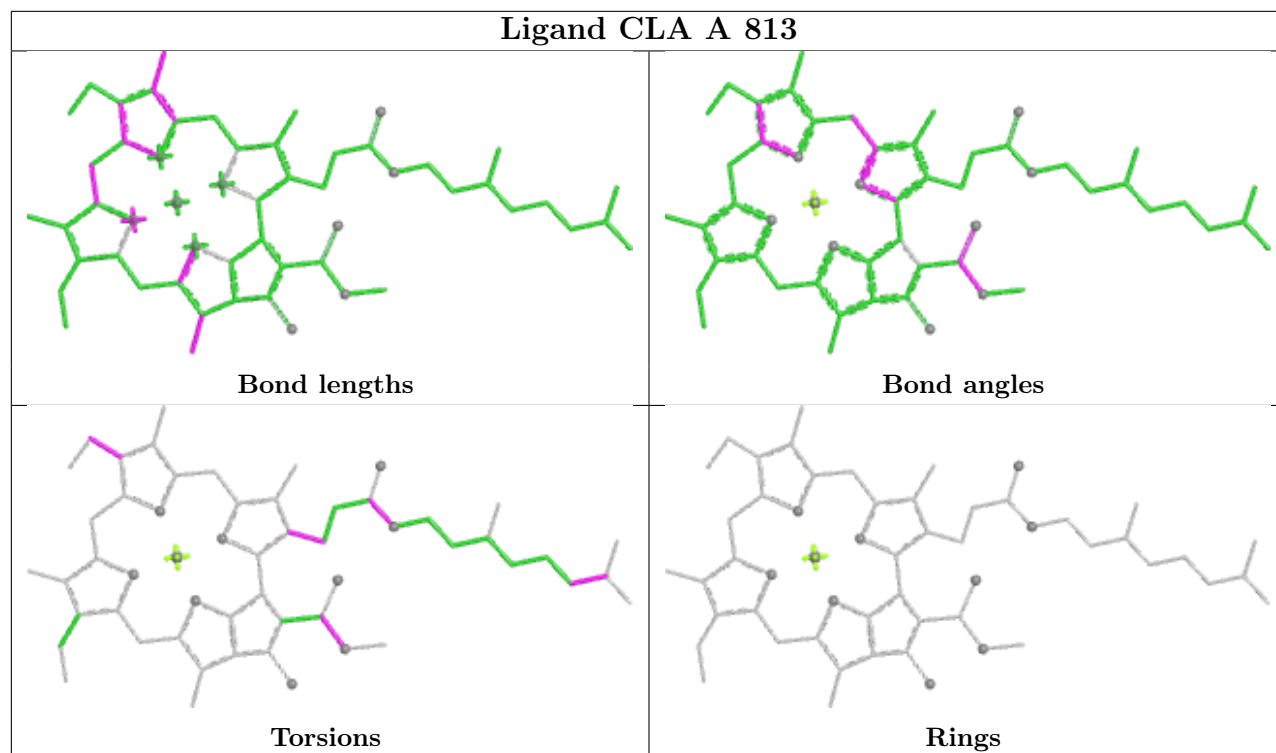
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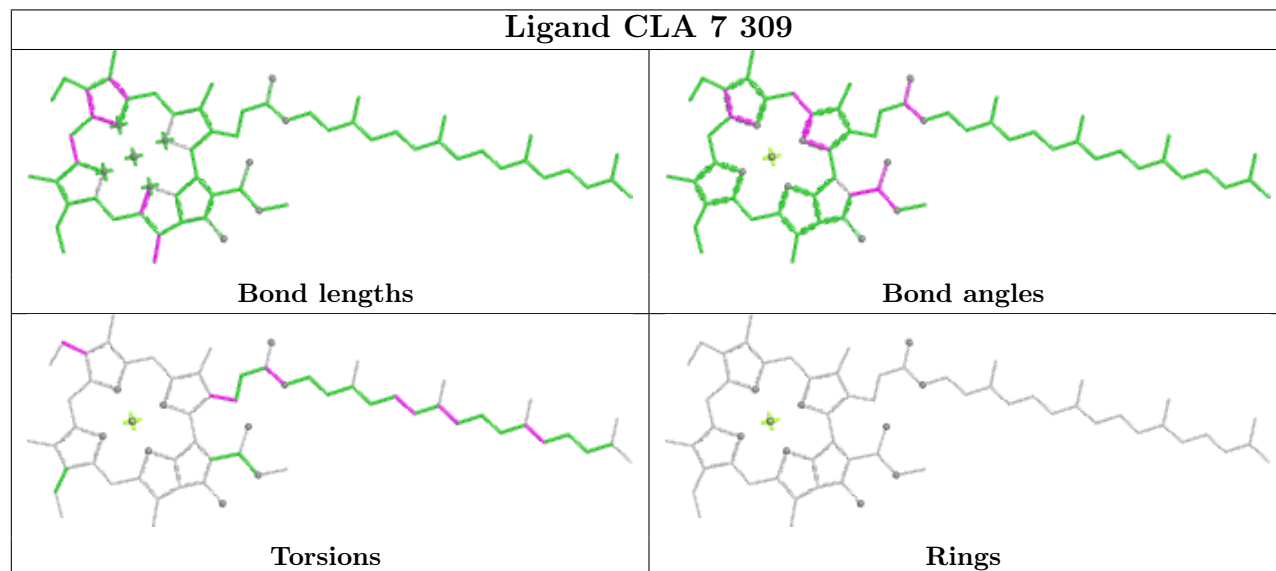
Ligand CLA B 817	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA L 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

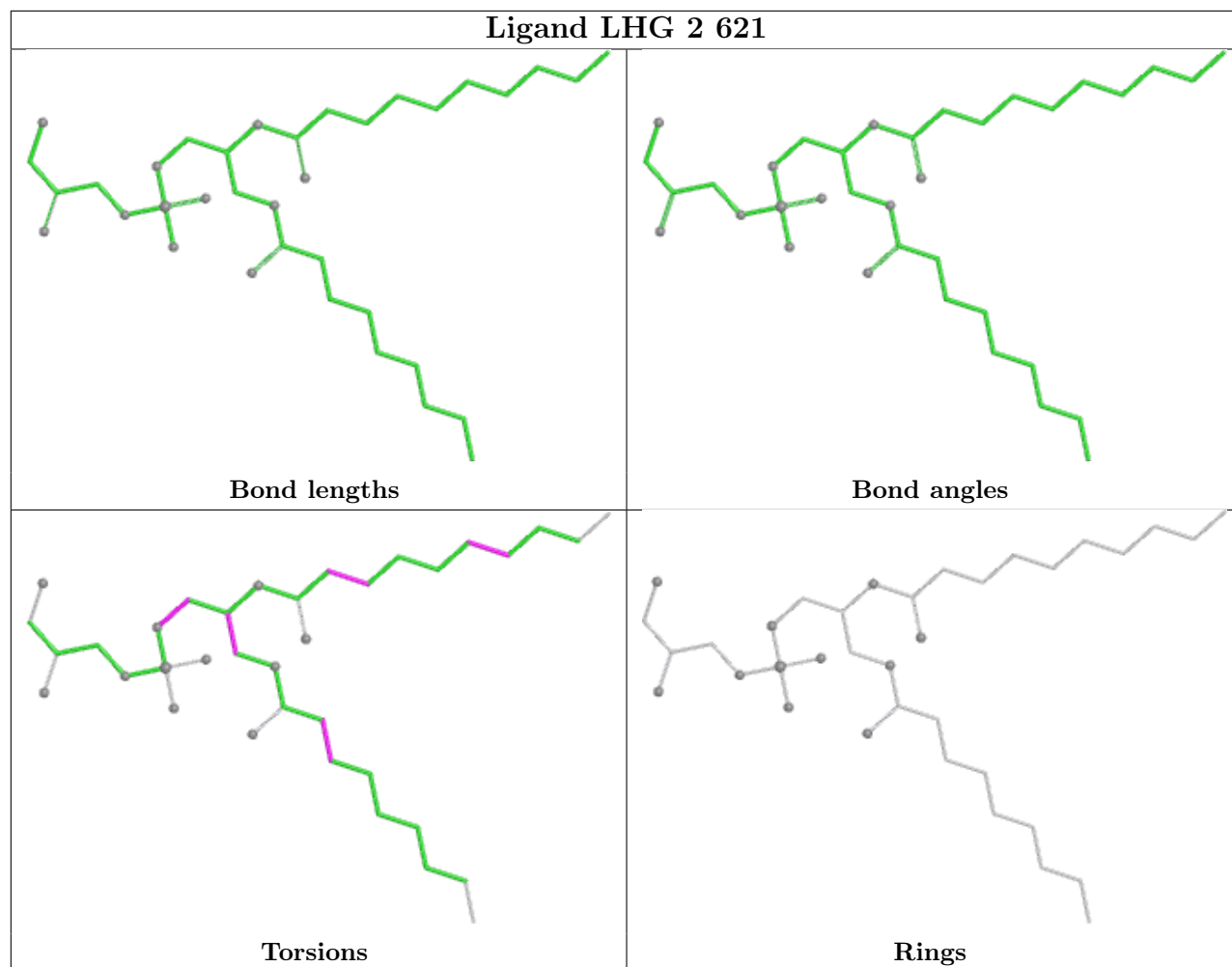


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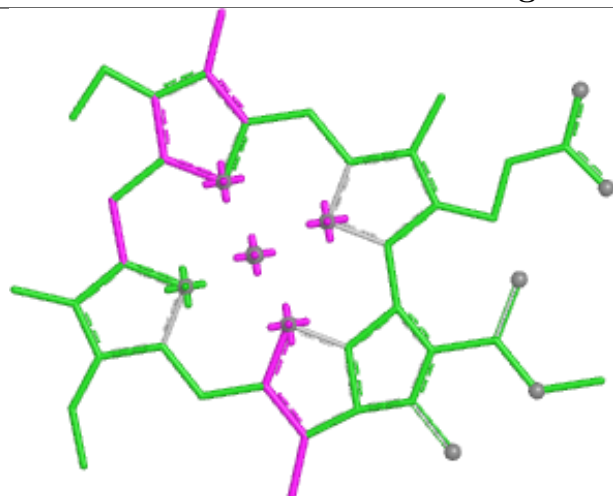


Ligand CLA 7 309

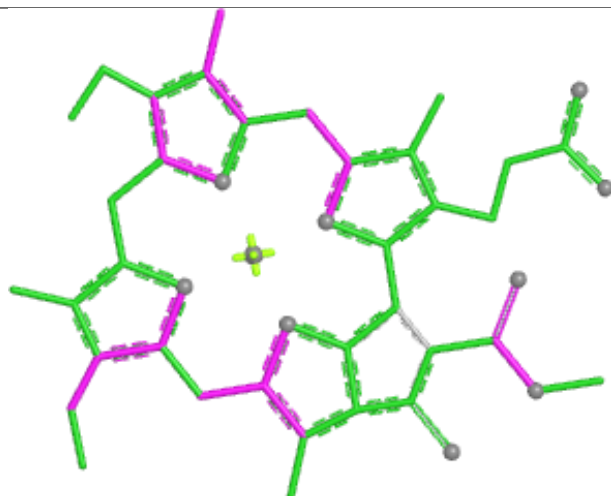




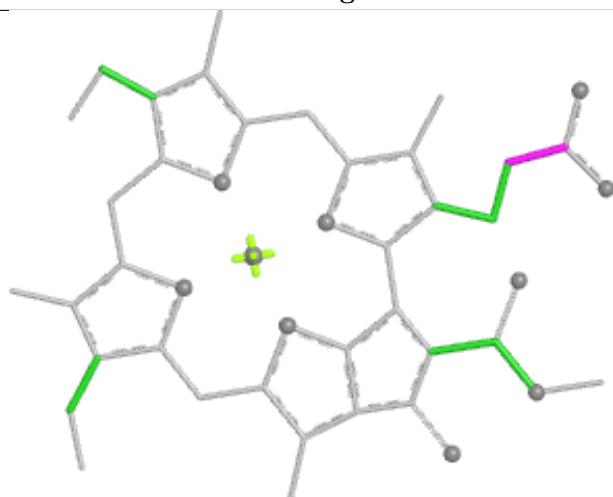
Ligand CLA 9 605



Bond lengths



Bond angles

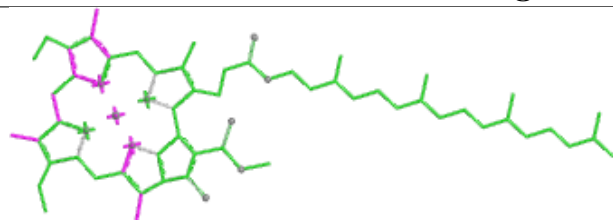


Torsions

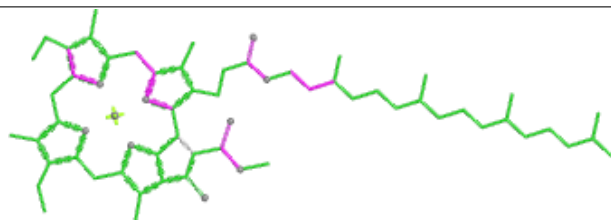


Rings

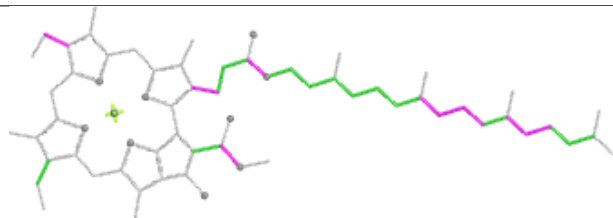
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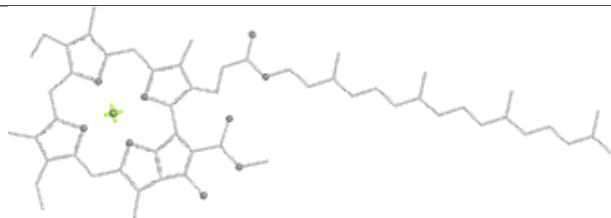
Bond lengths



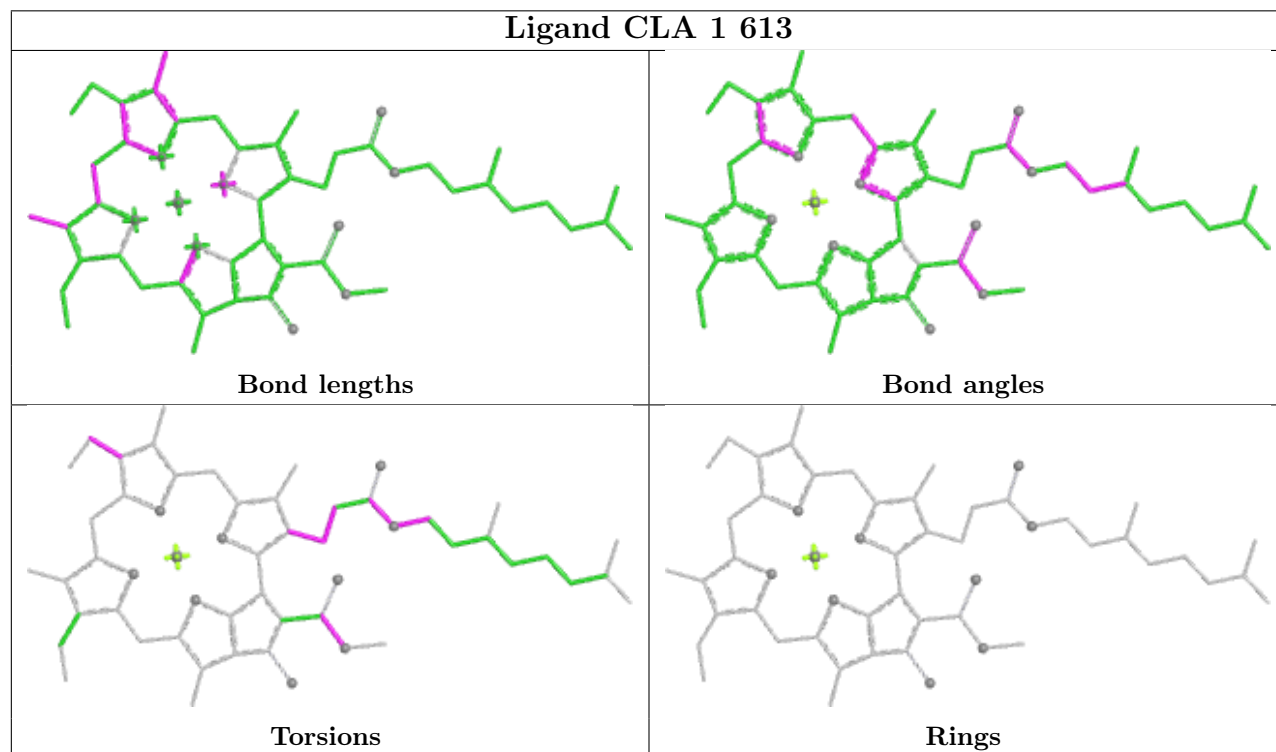
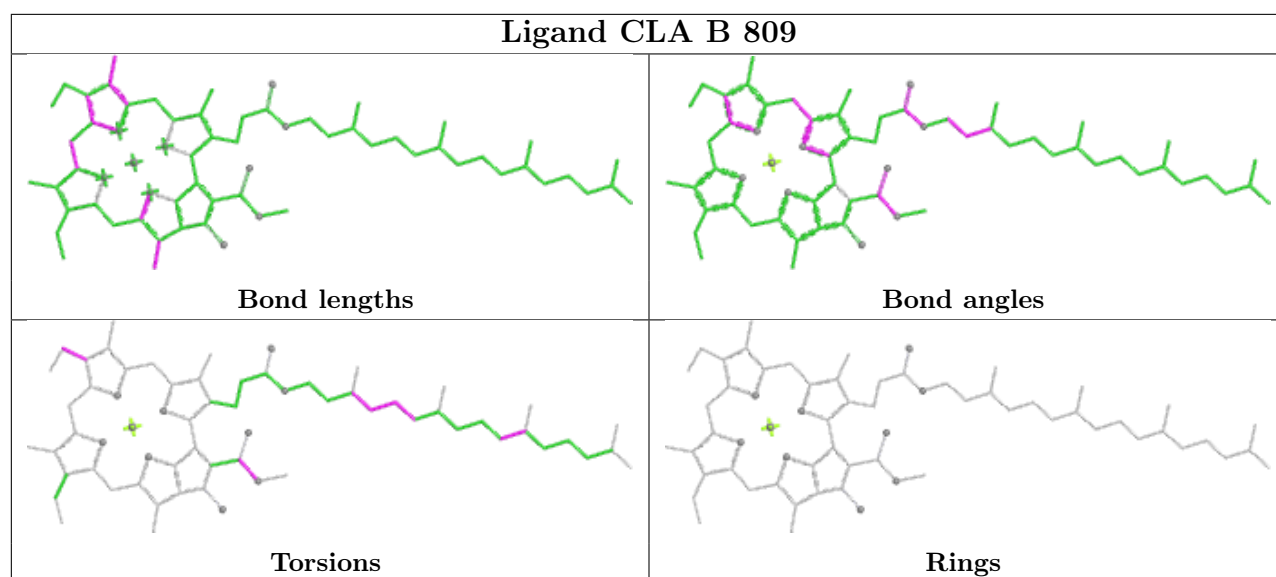
Bond angles



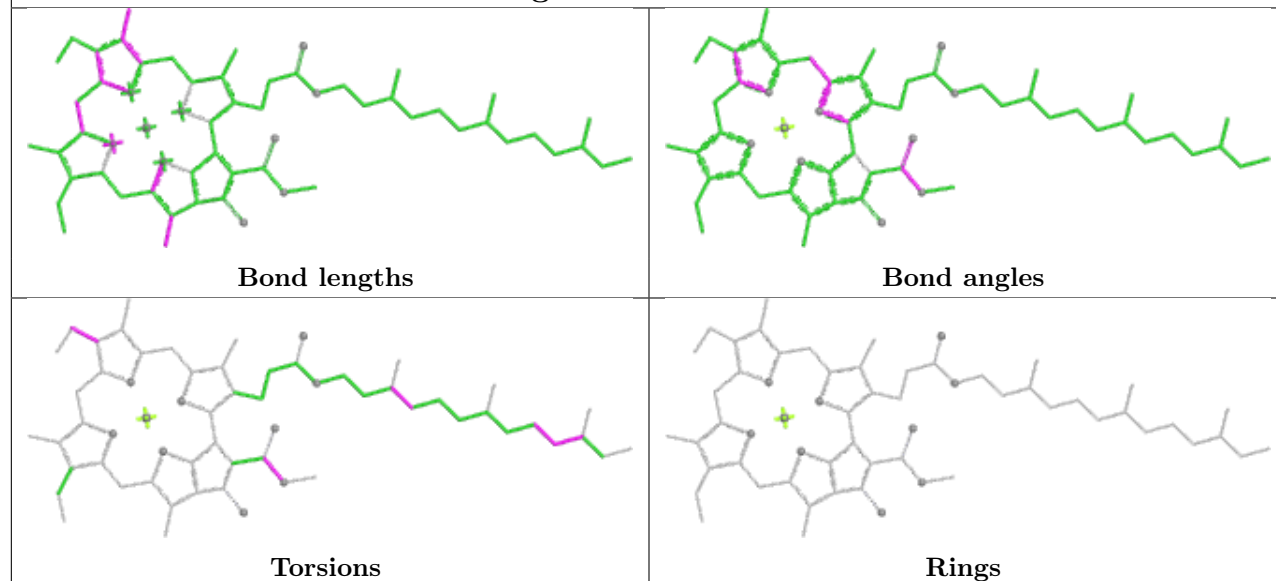
Torsions



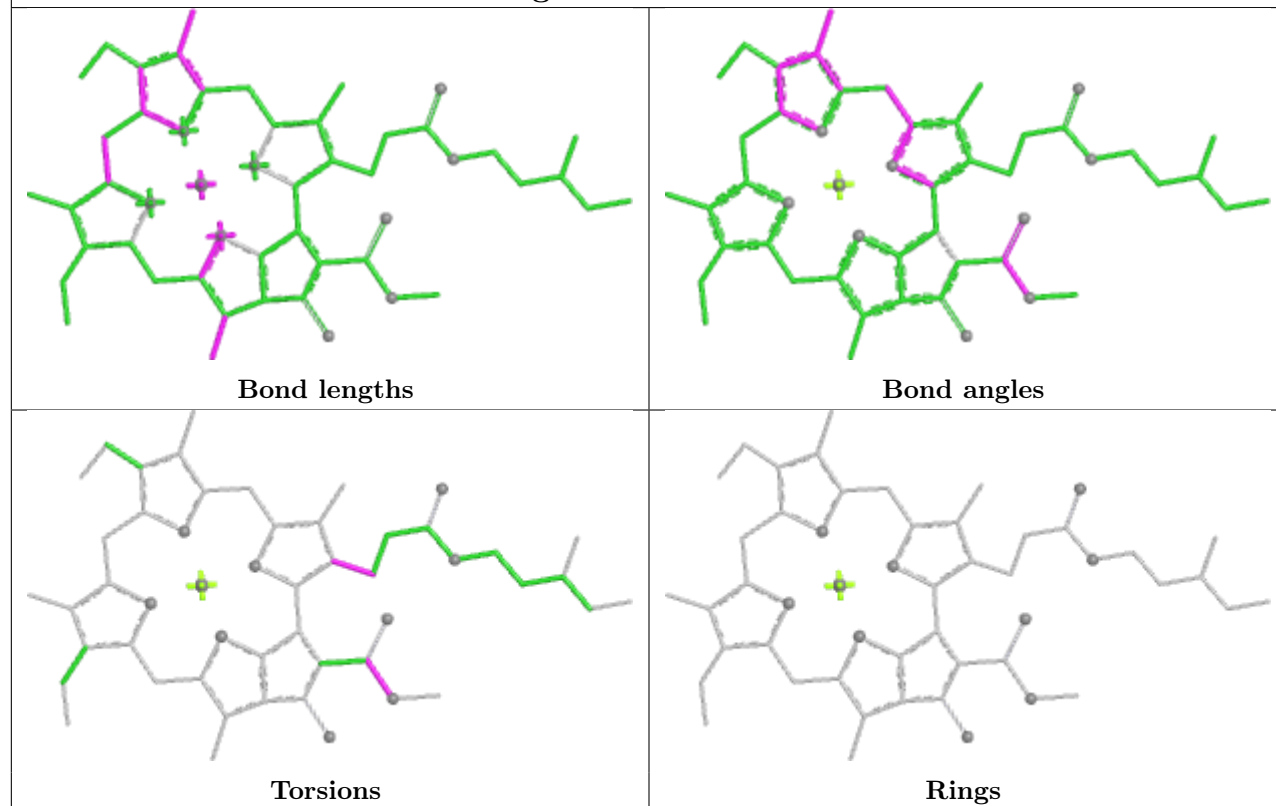
Rings

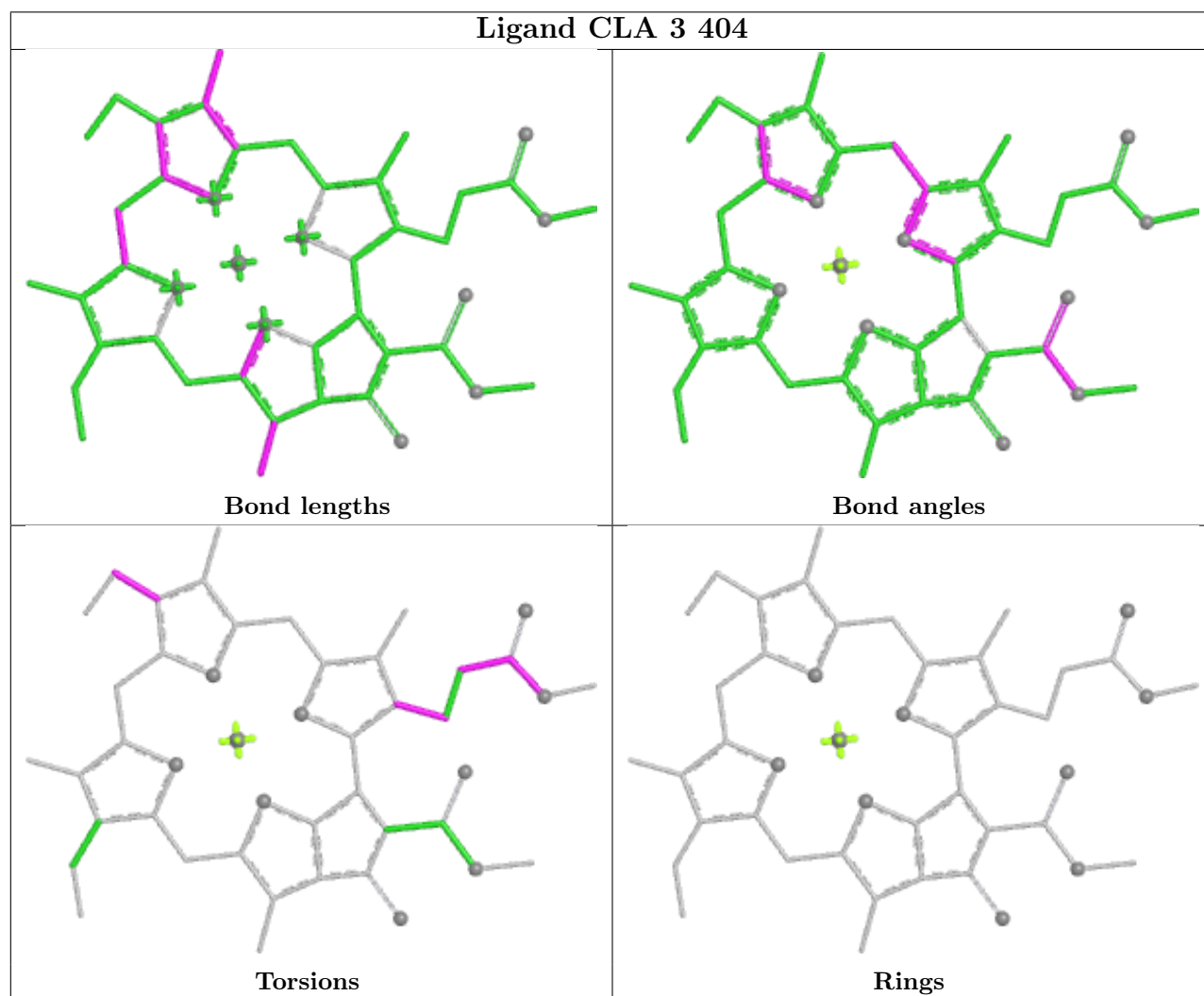
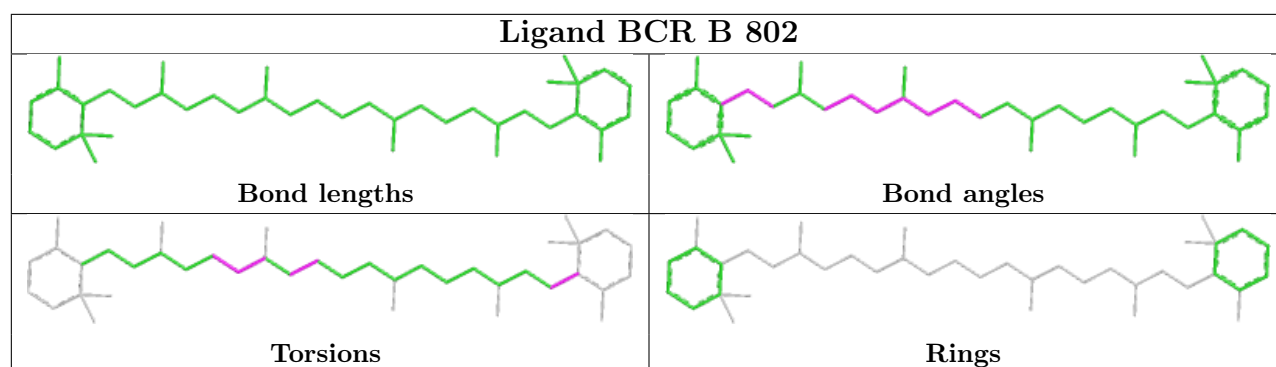


Ligand CLA A 842

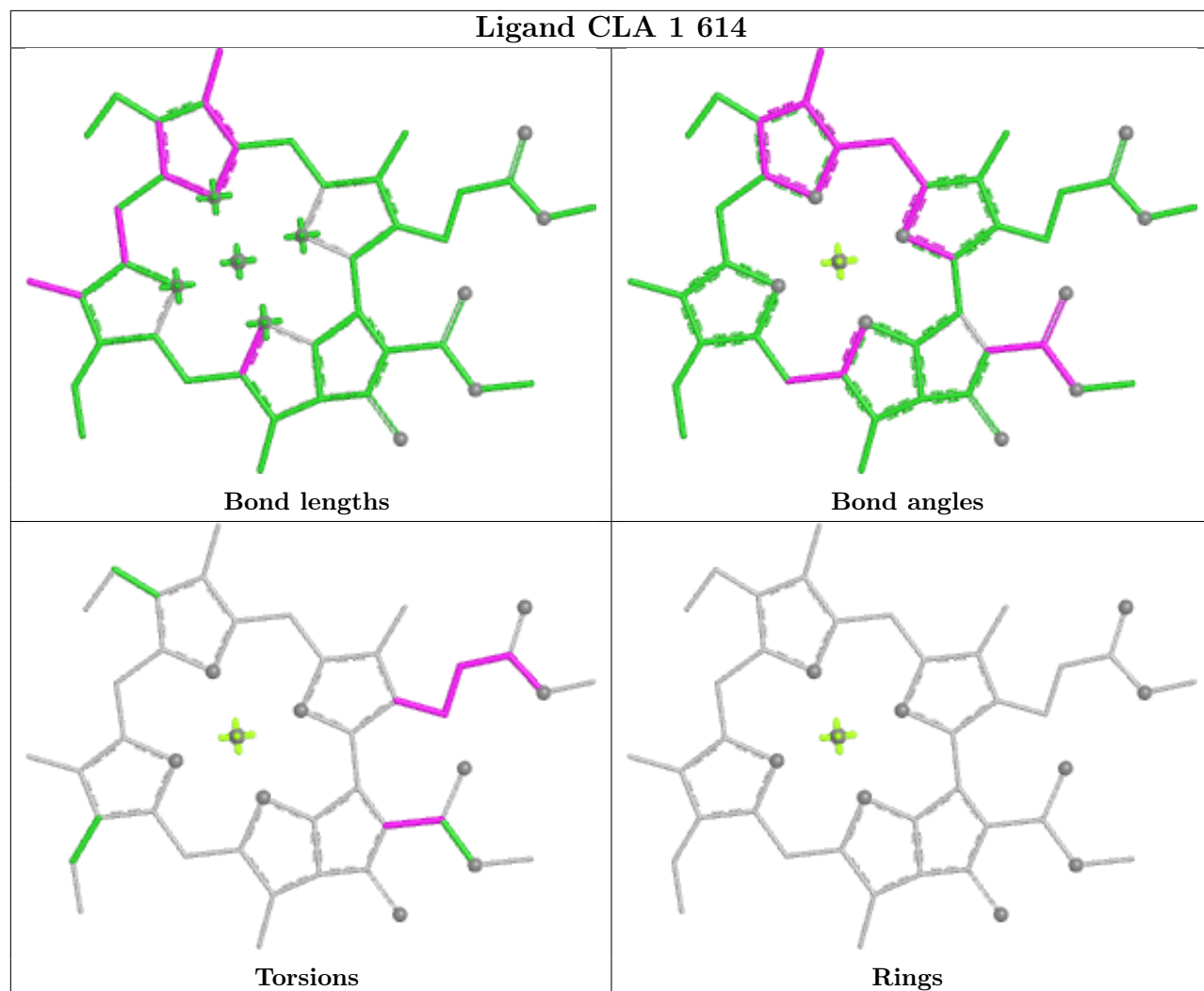


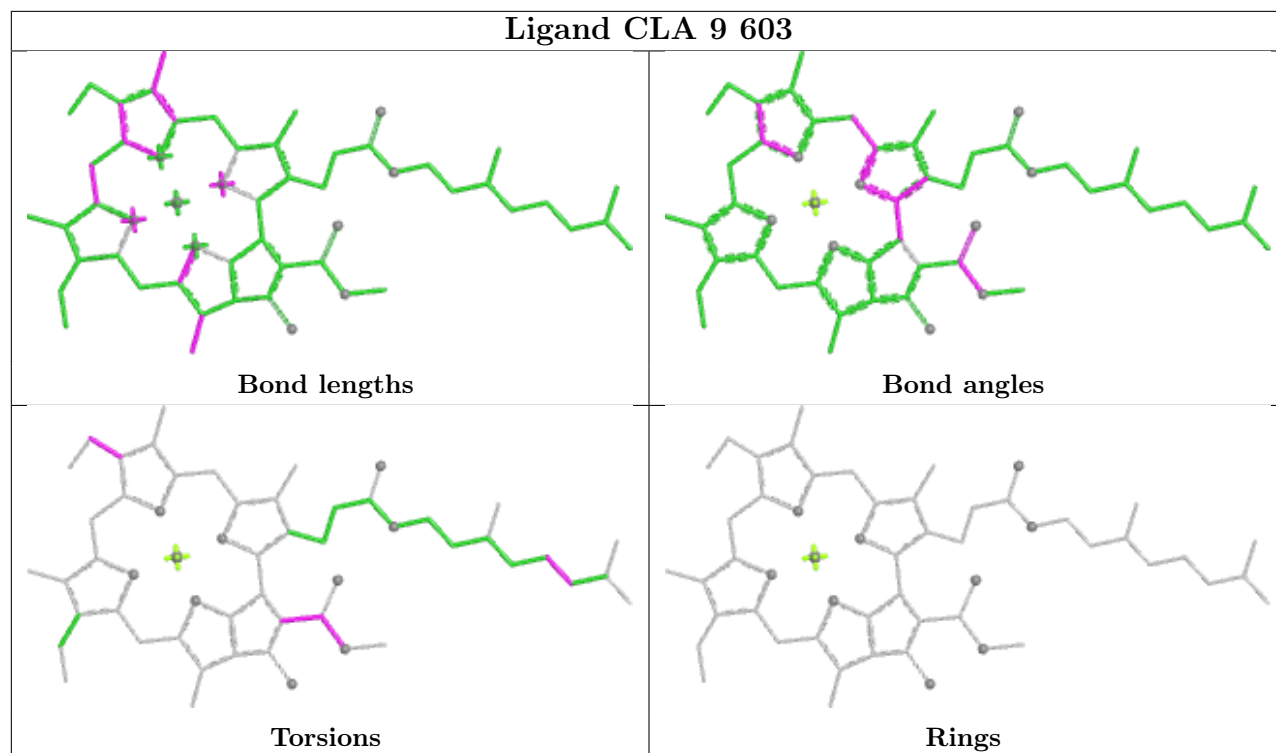
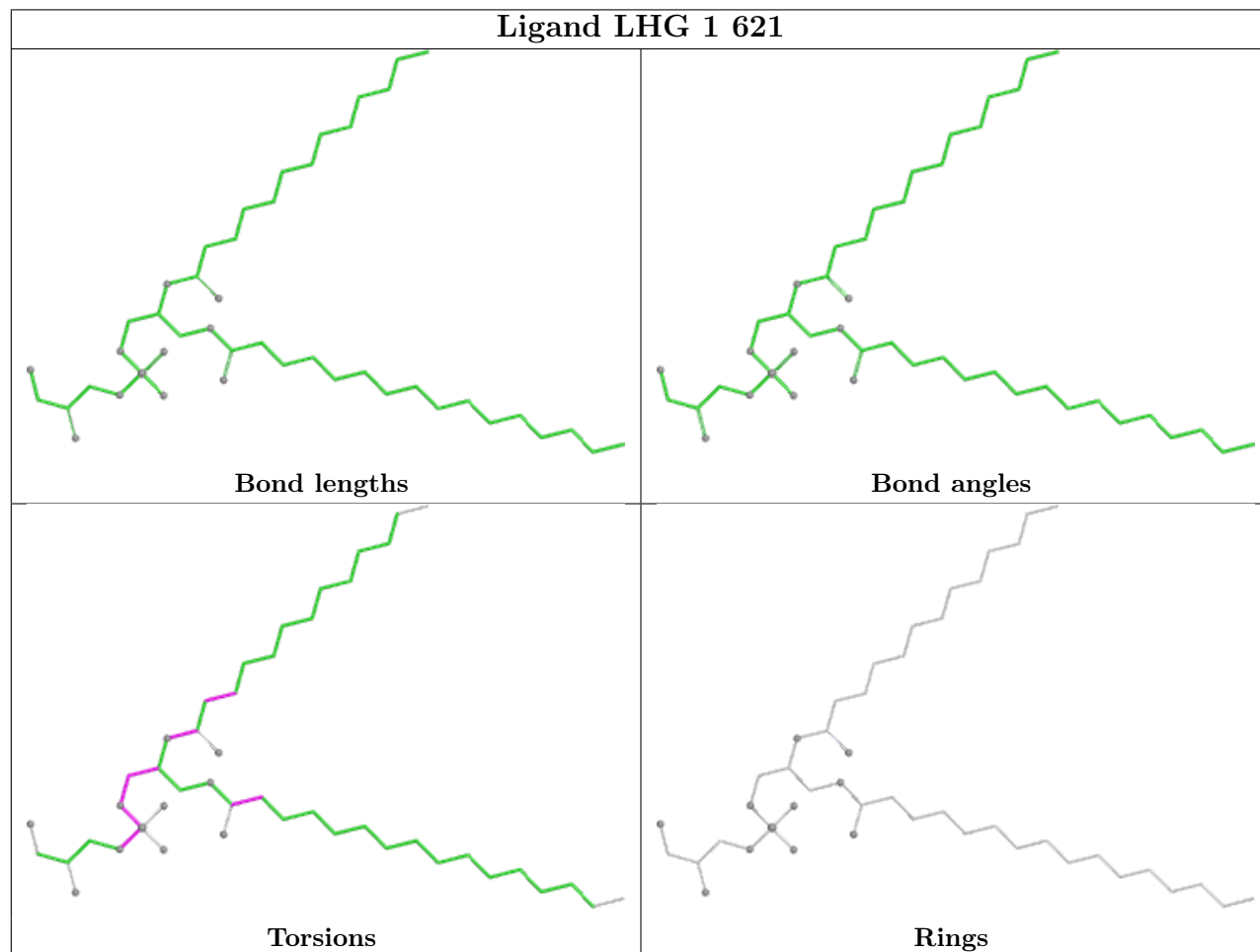
Ligand CLA B 837

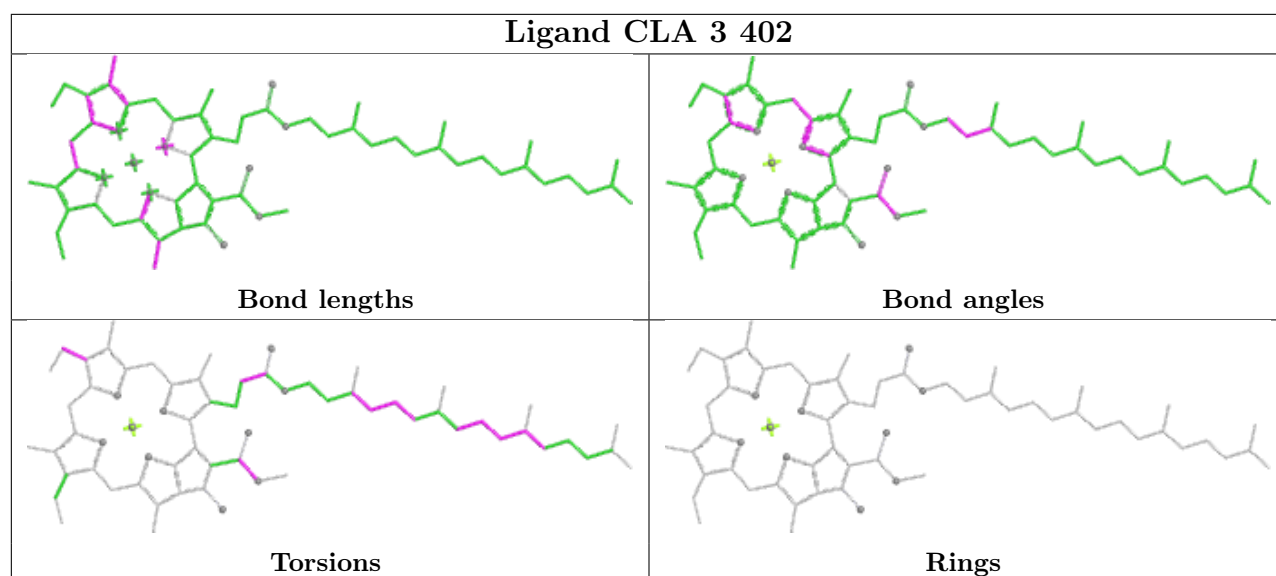
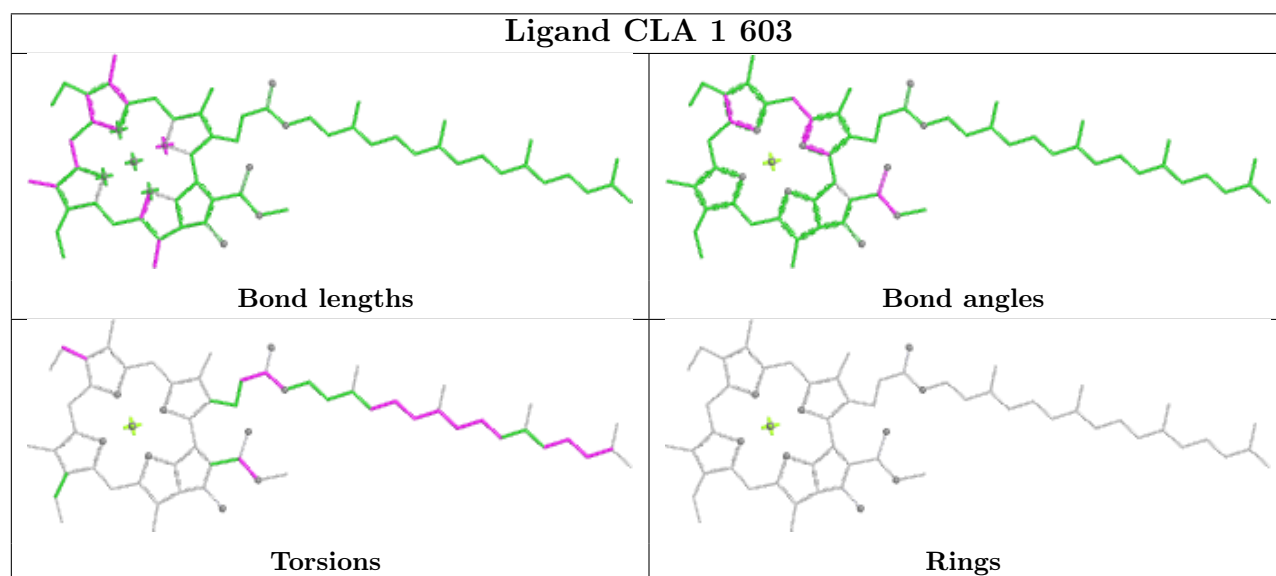
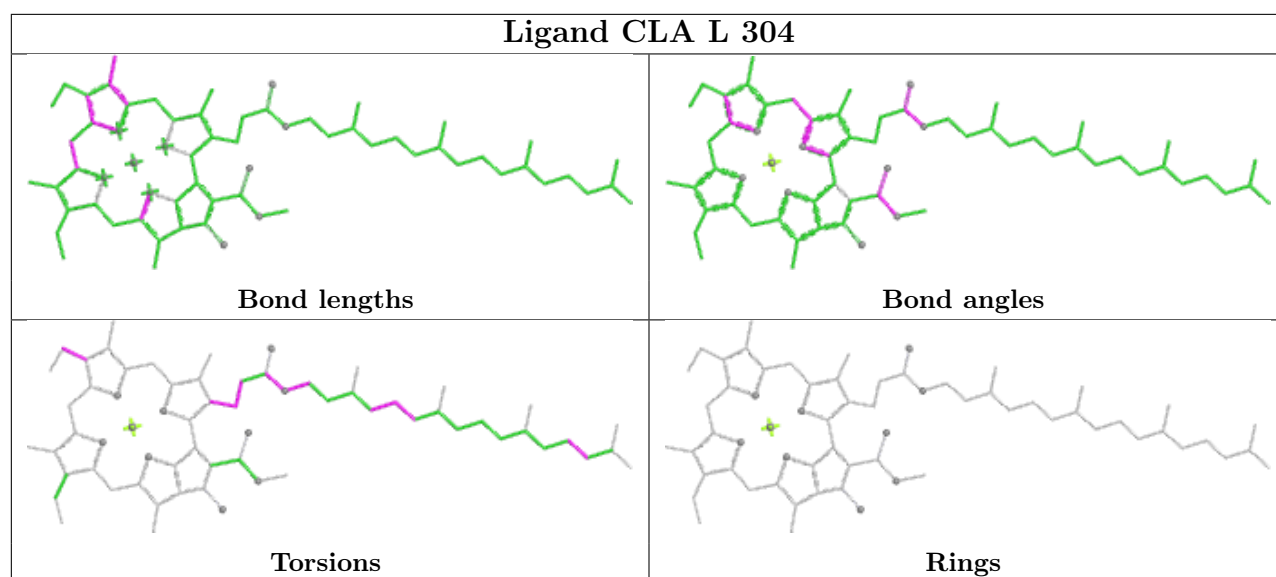


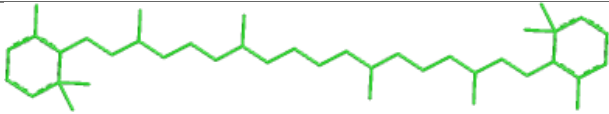
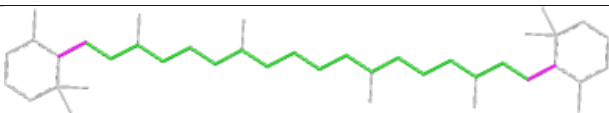
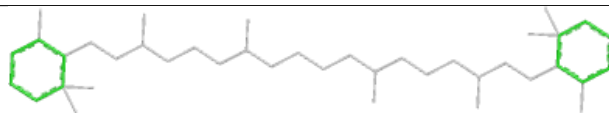


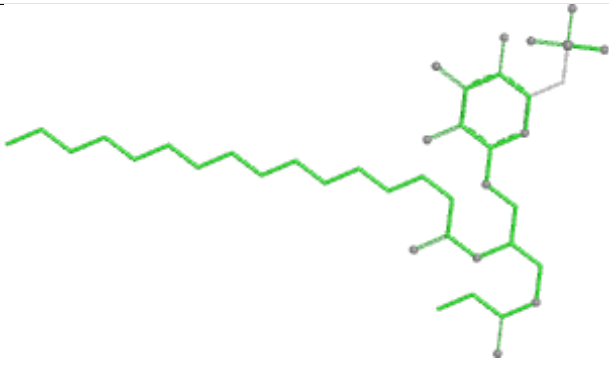
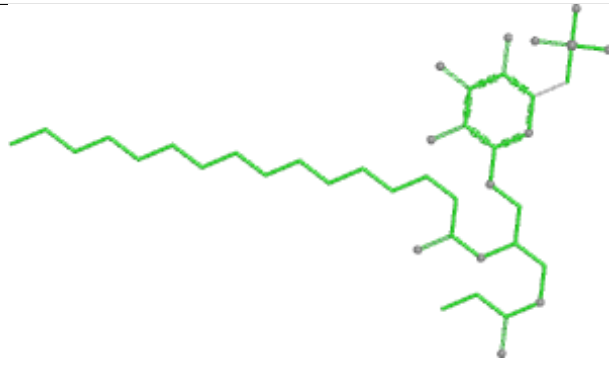
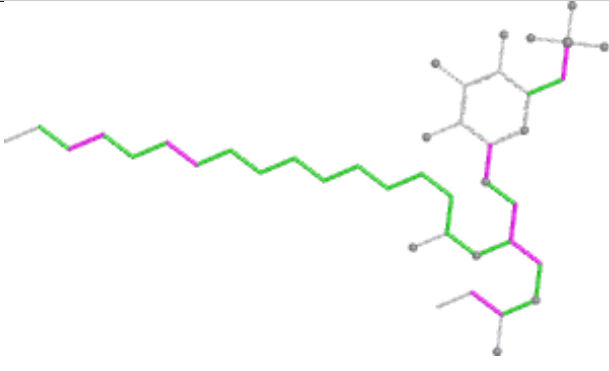
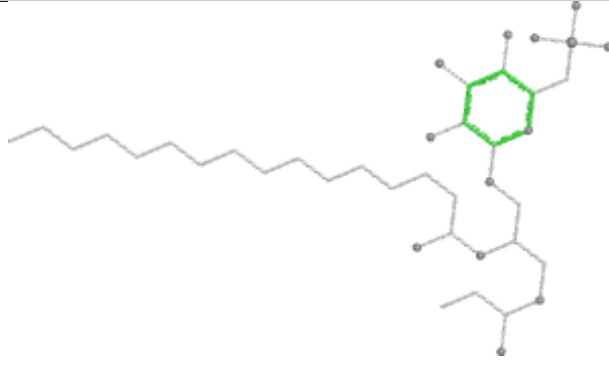
Ligand CLA 1 614

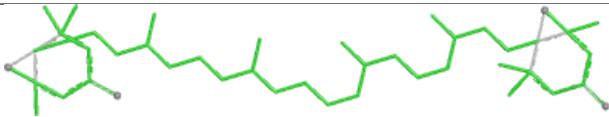
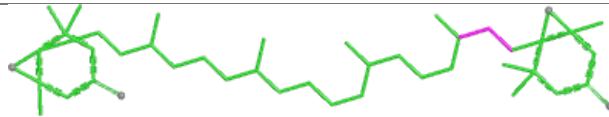
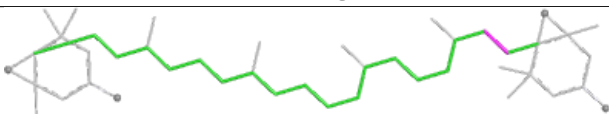
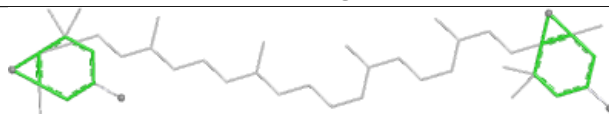


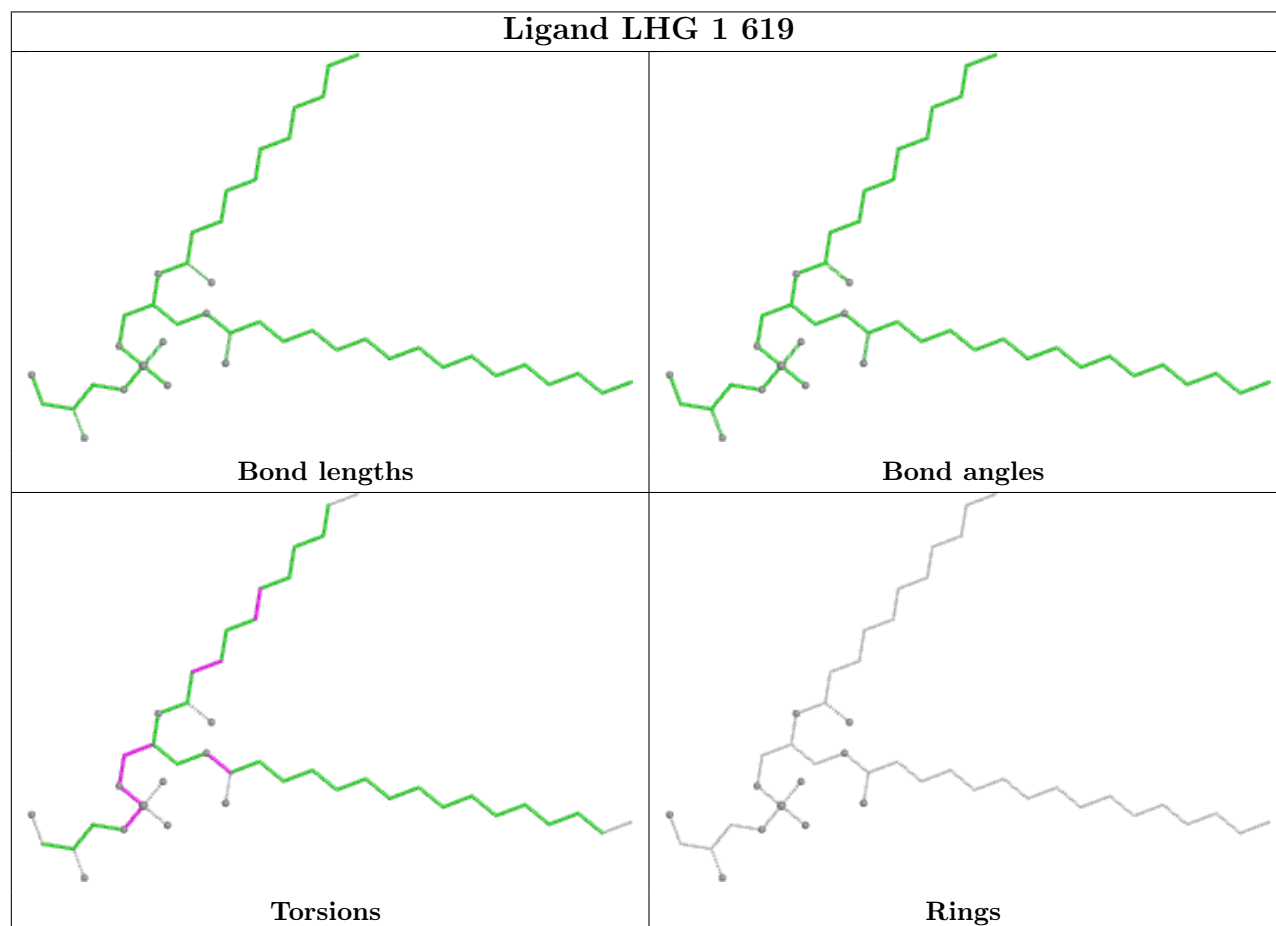
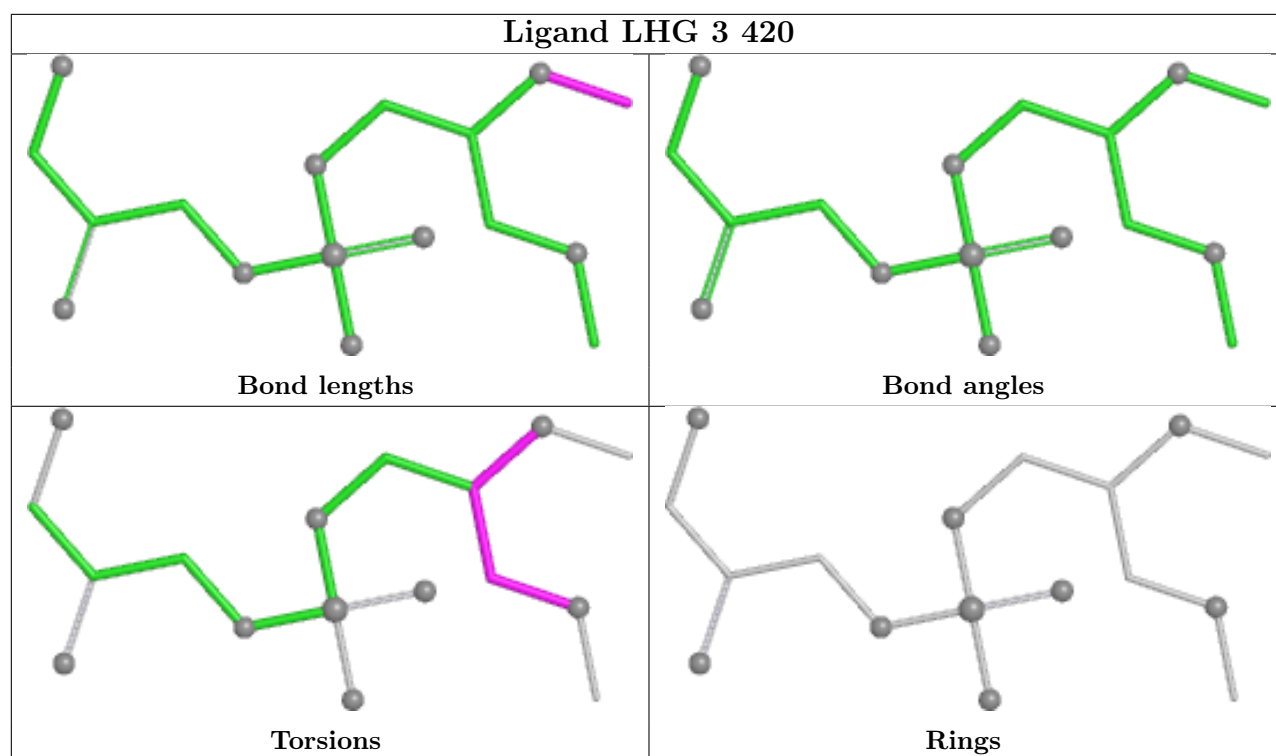
Ligand CLA 9 603**Ligand LHG 1 621**

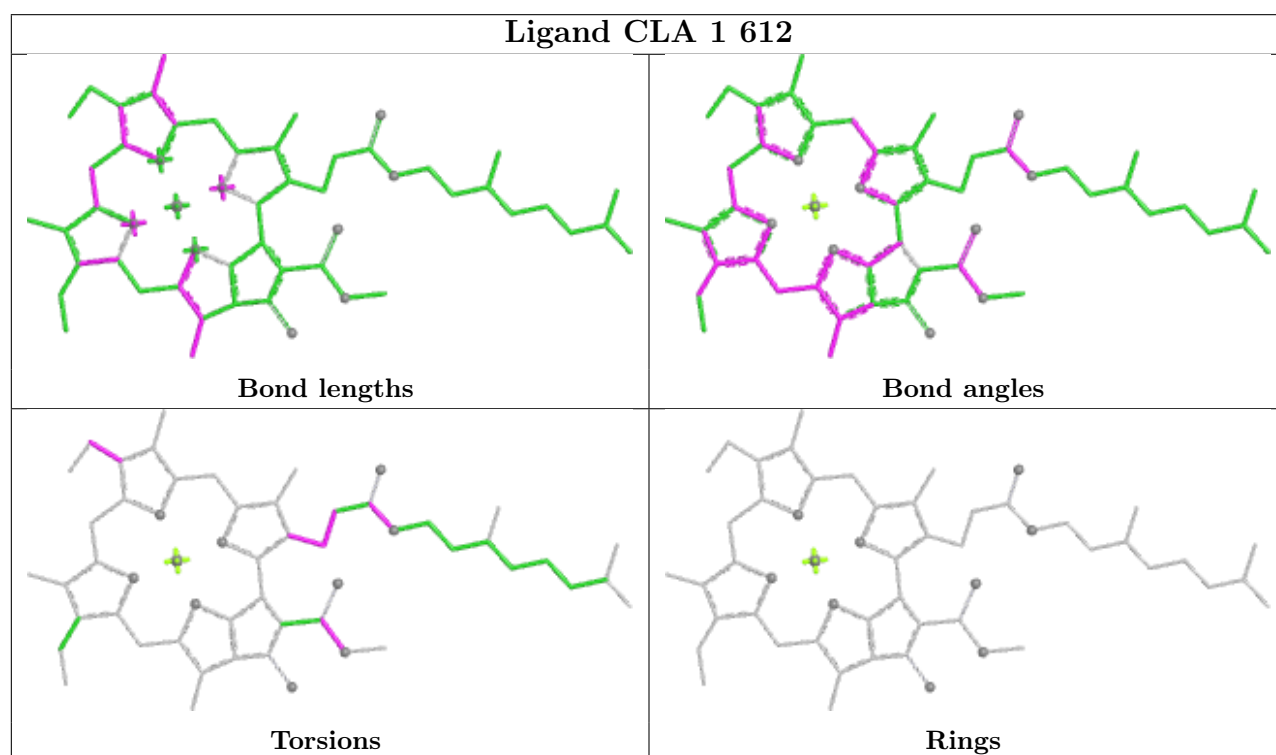
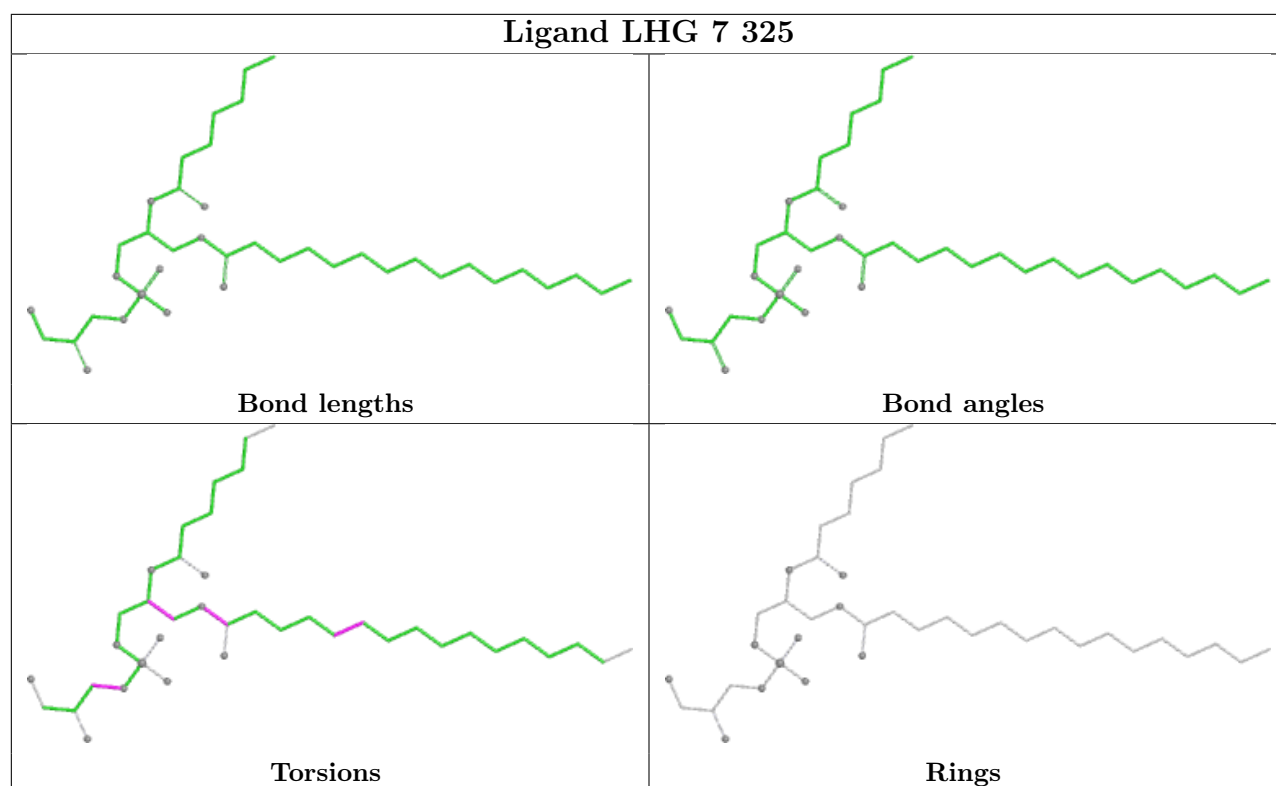


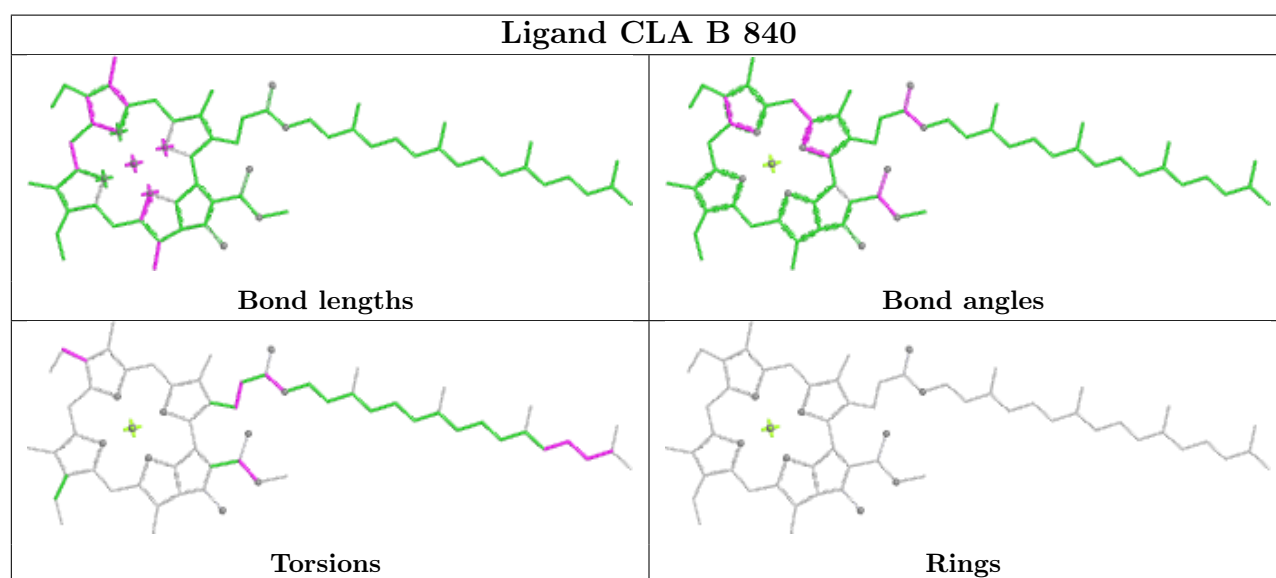
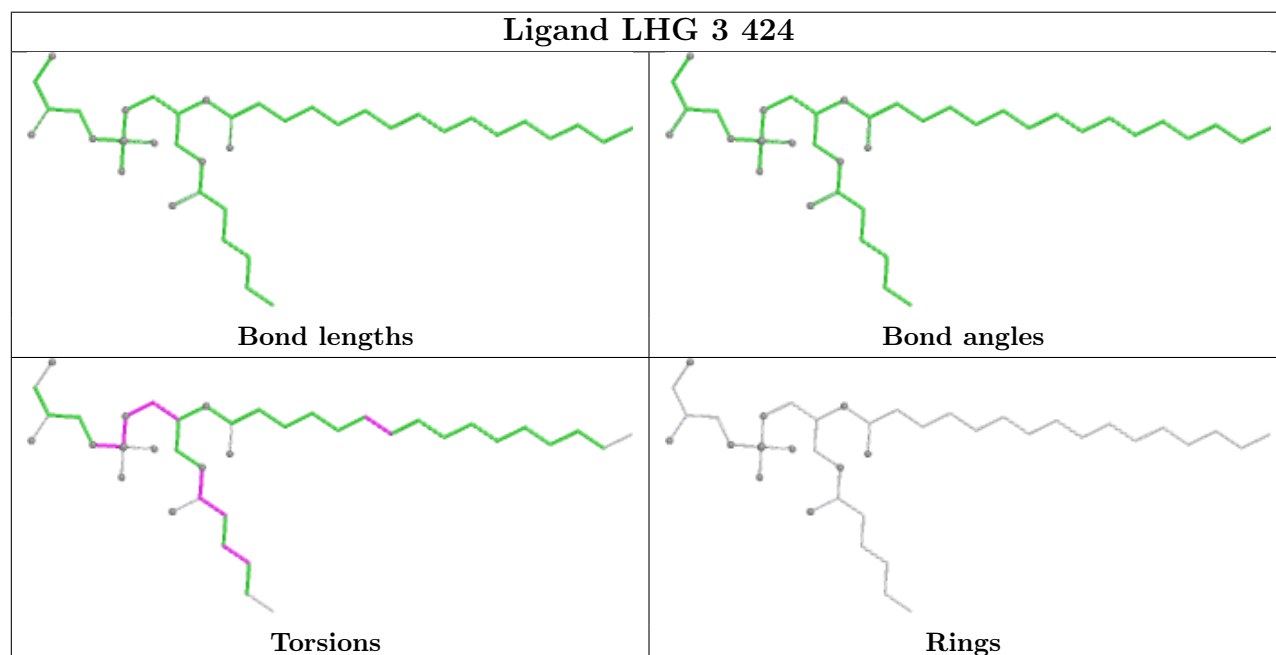
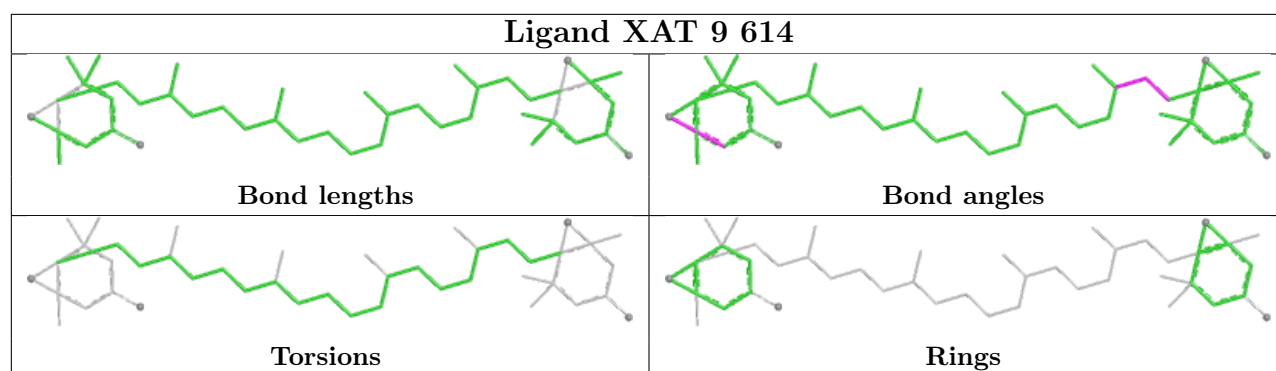
Ligand BCR 3 417	
	
Bond lengths	Bond angles
	
Torsions	Rings

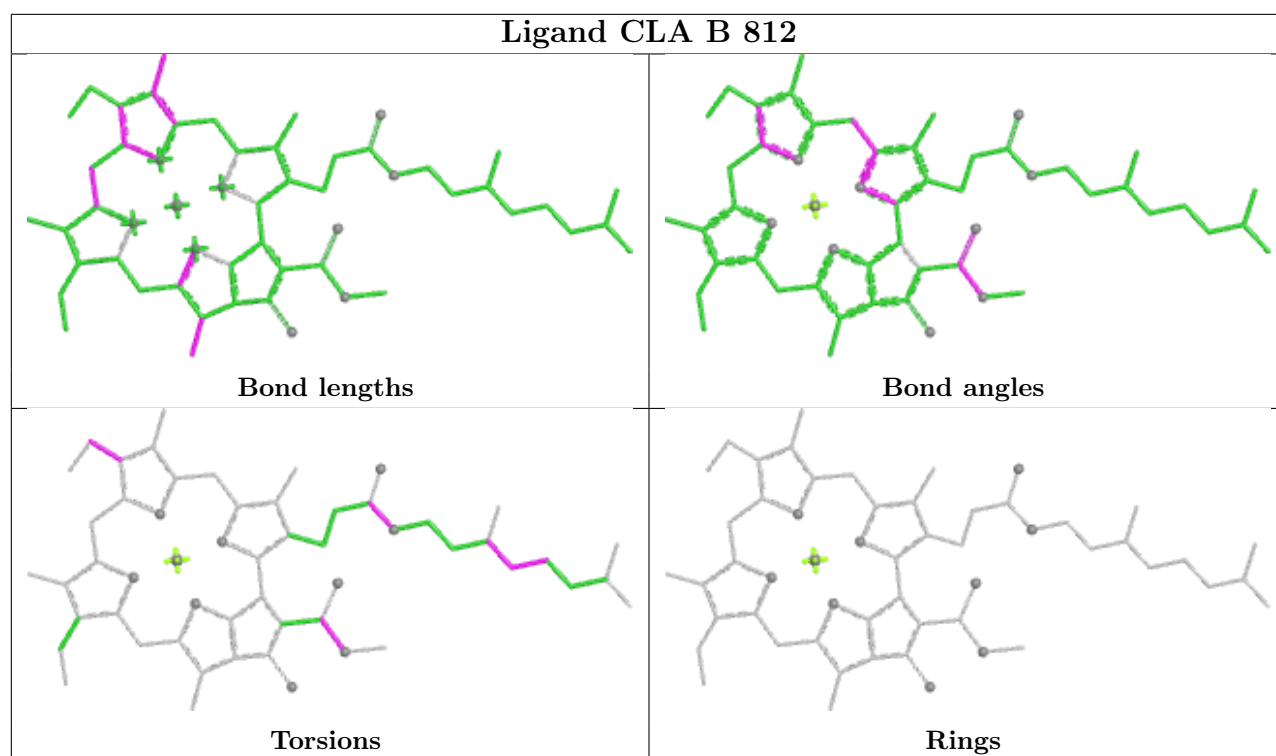
Ligand SQD 2 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 8 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

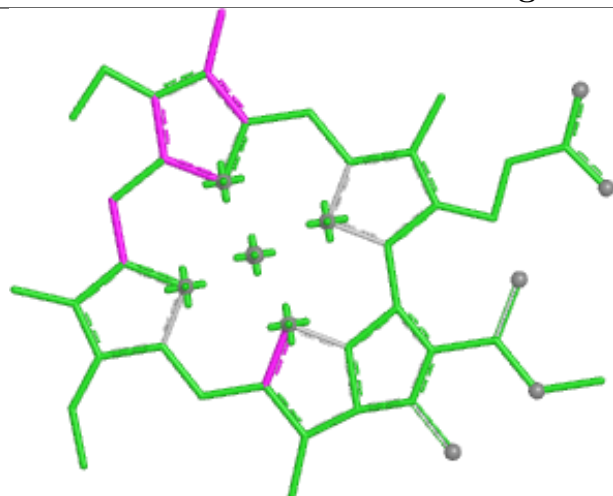




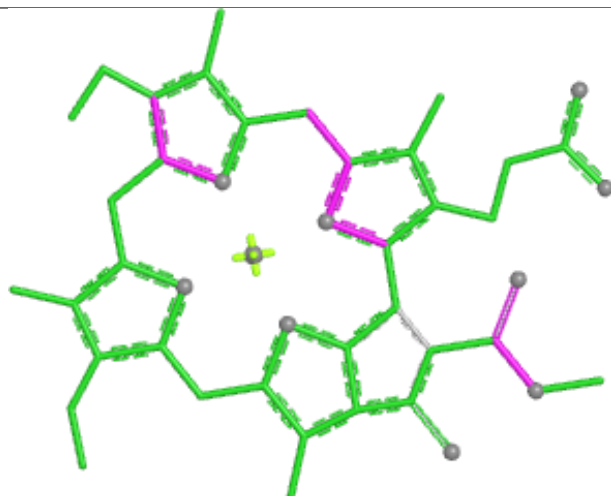




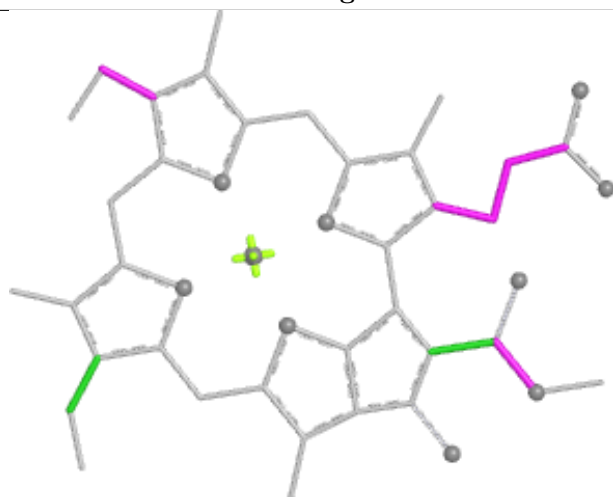
Ligand CLA 2 605



Bond lengths



Bond angles

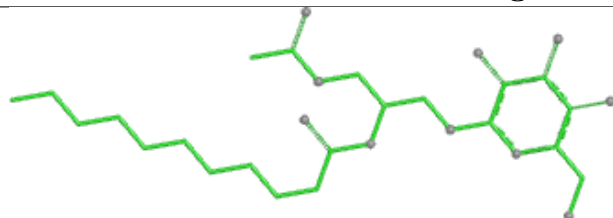


Torsions

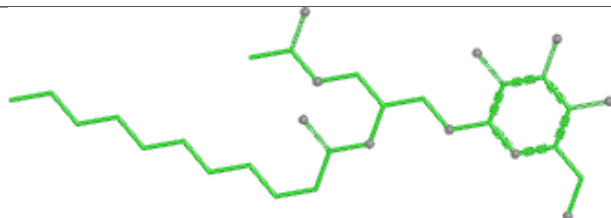


Rings

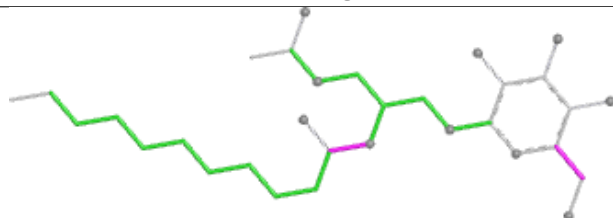
Ligand LMG A 801



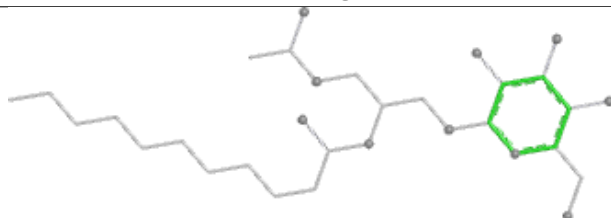
Bond lengths



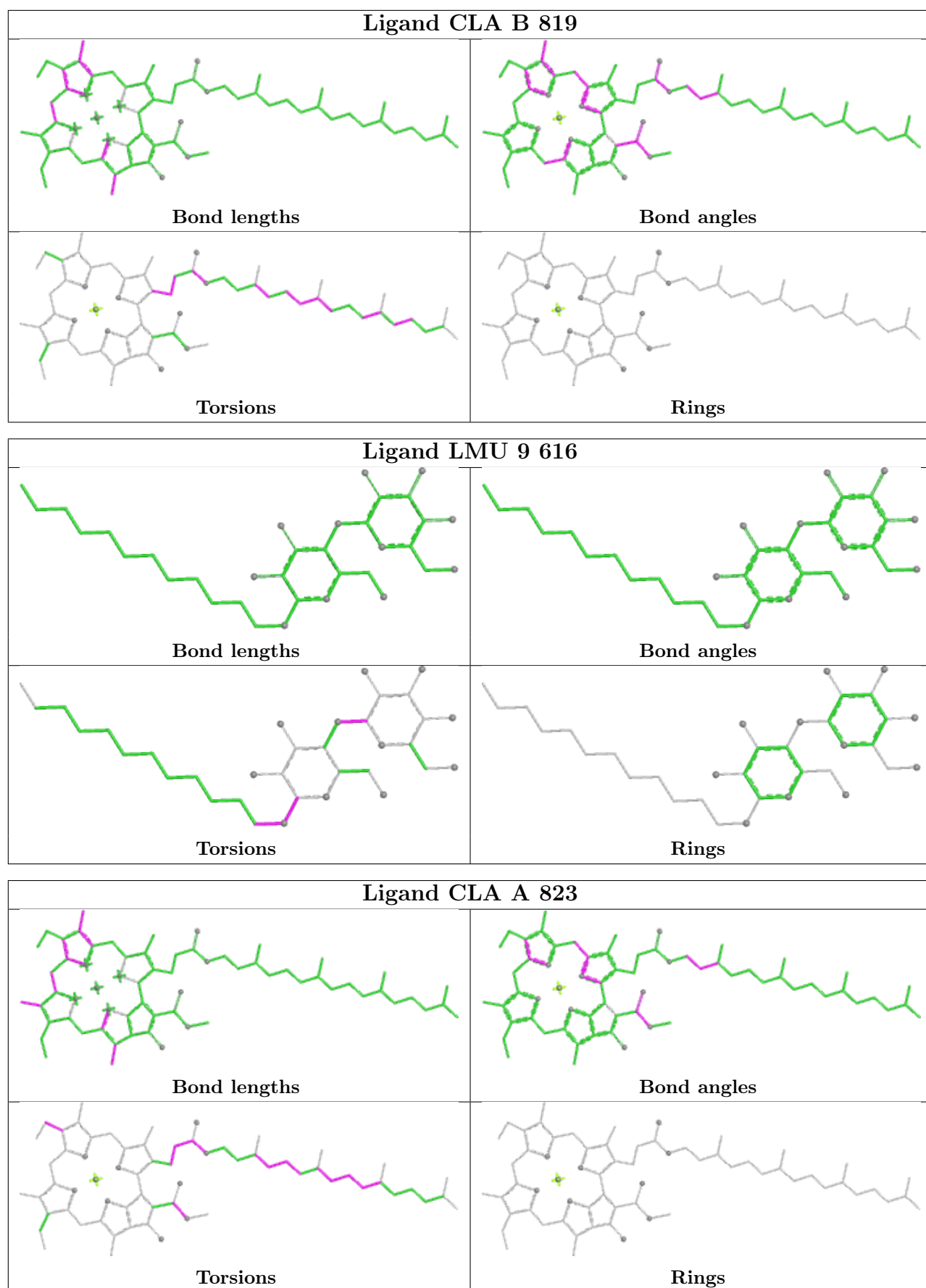
Bond angles



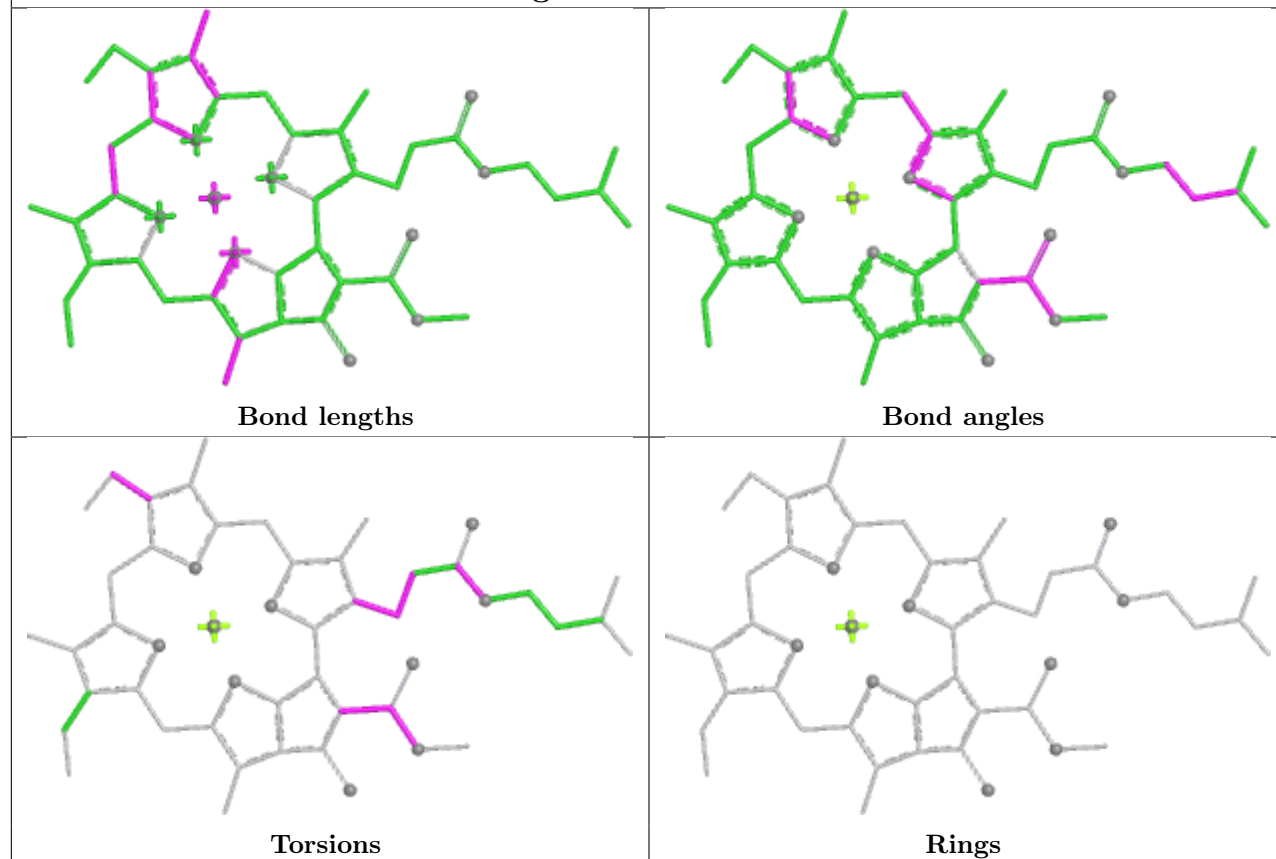
Torsions



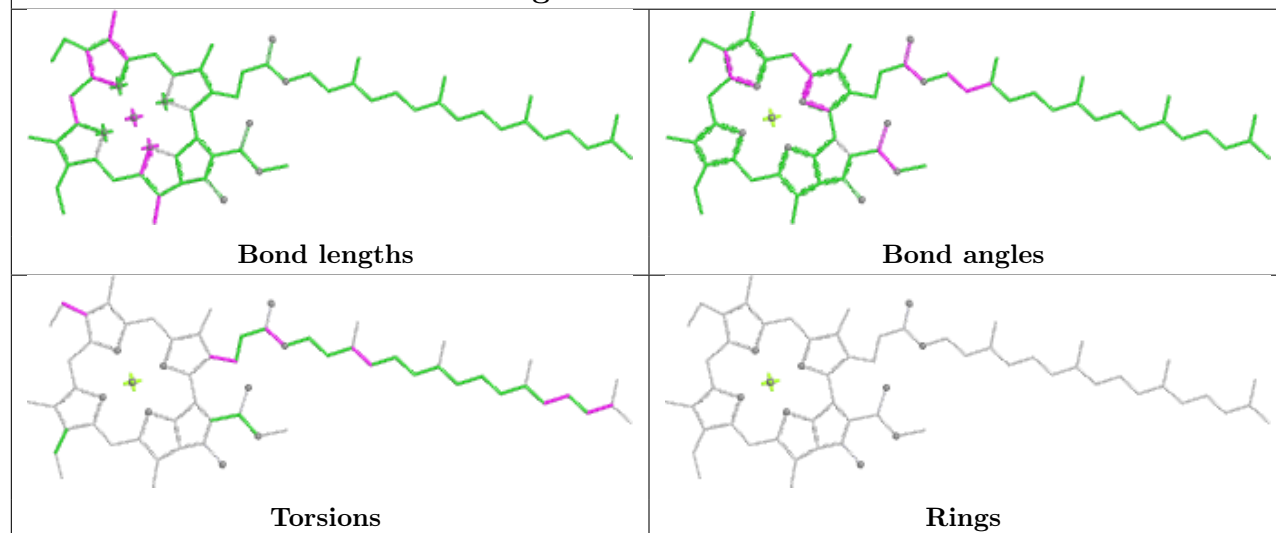
Rings



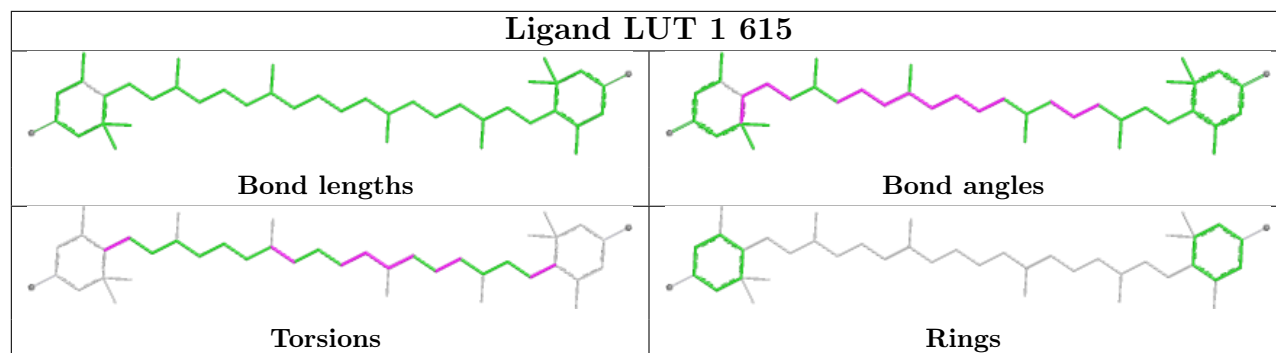
Ligand CLA B 836



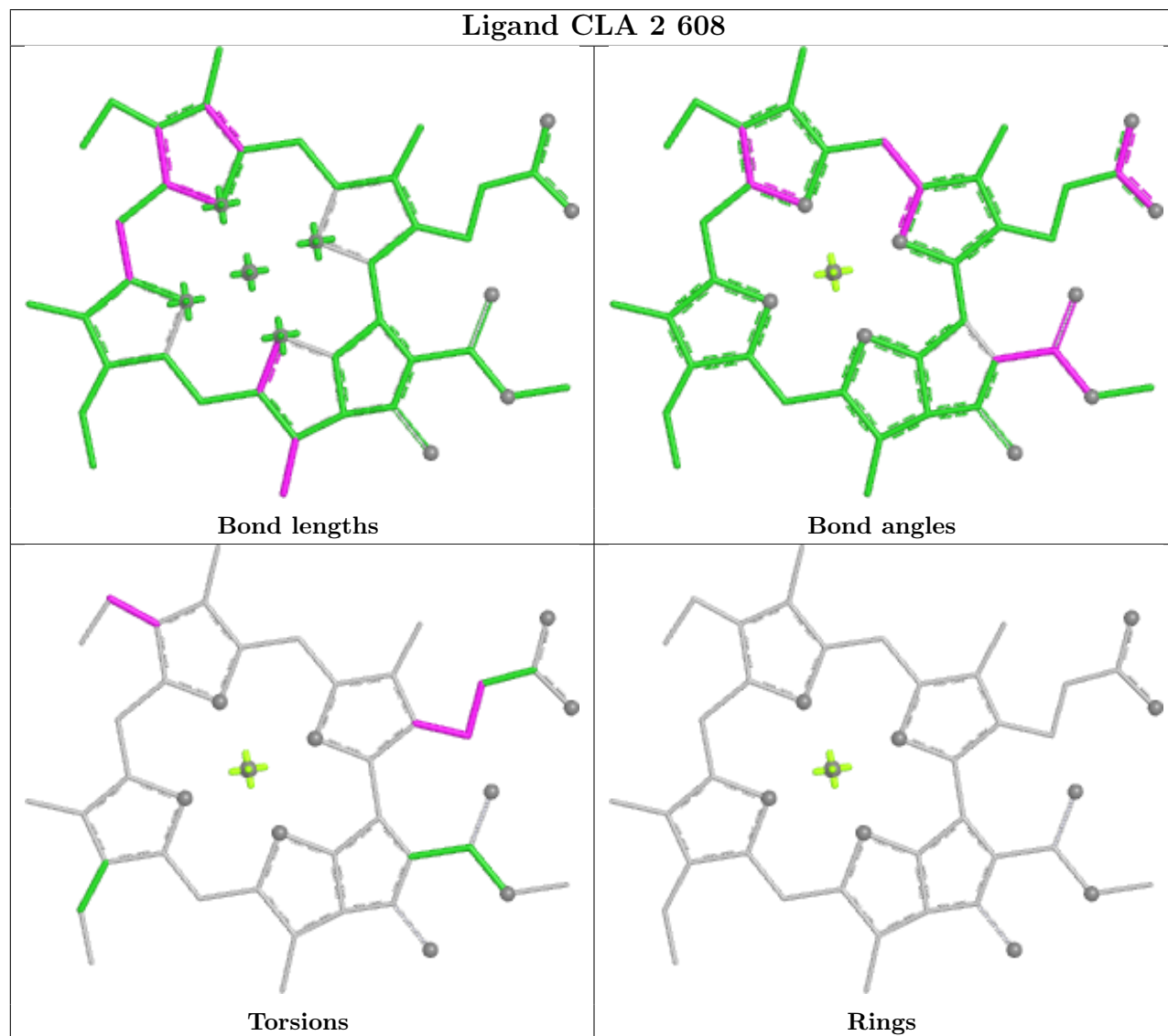
Ligand CLA B 821



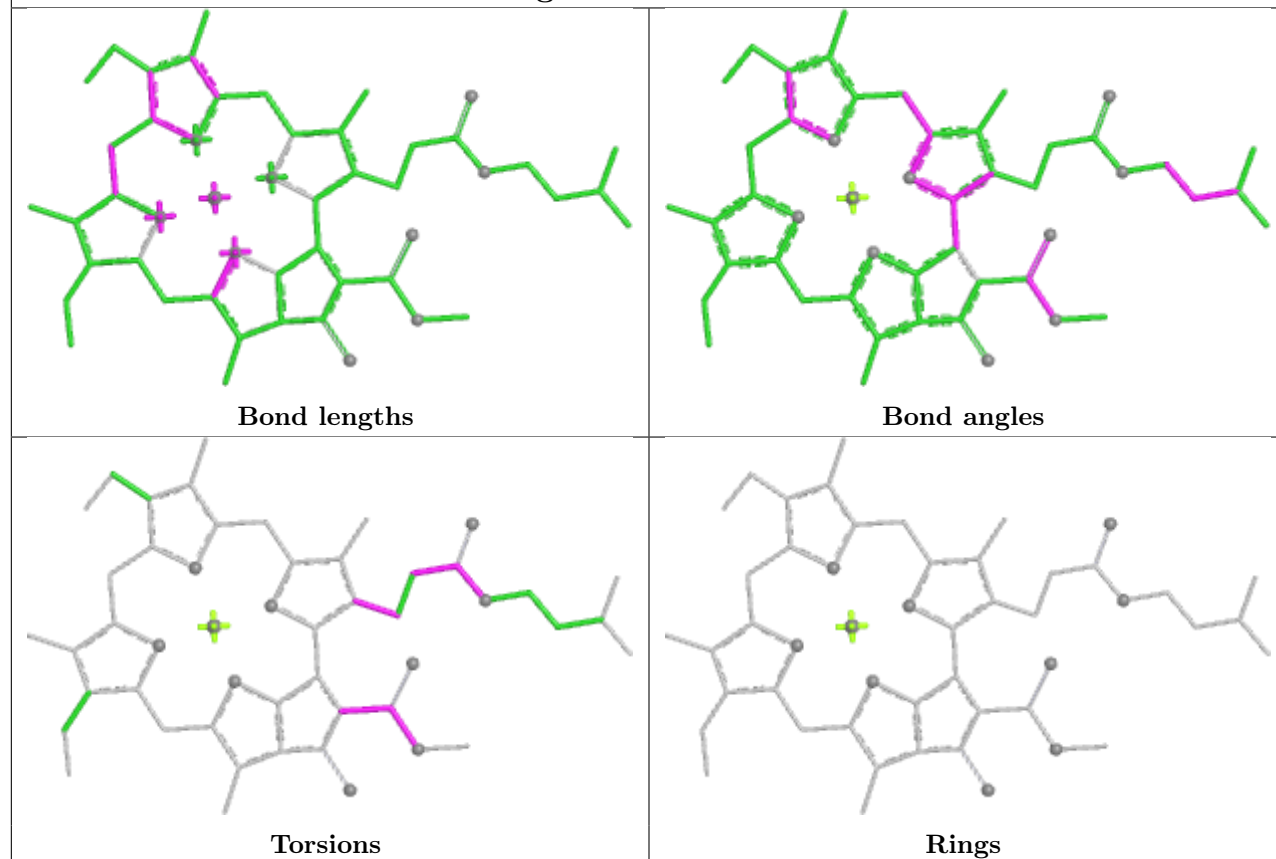
Ligand LUT 1 615



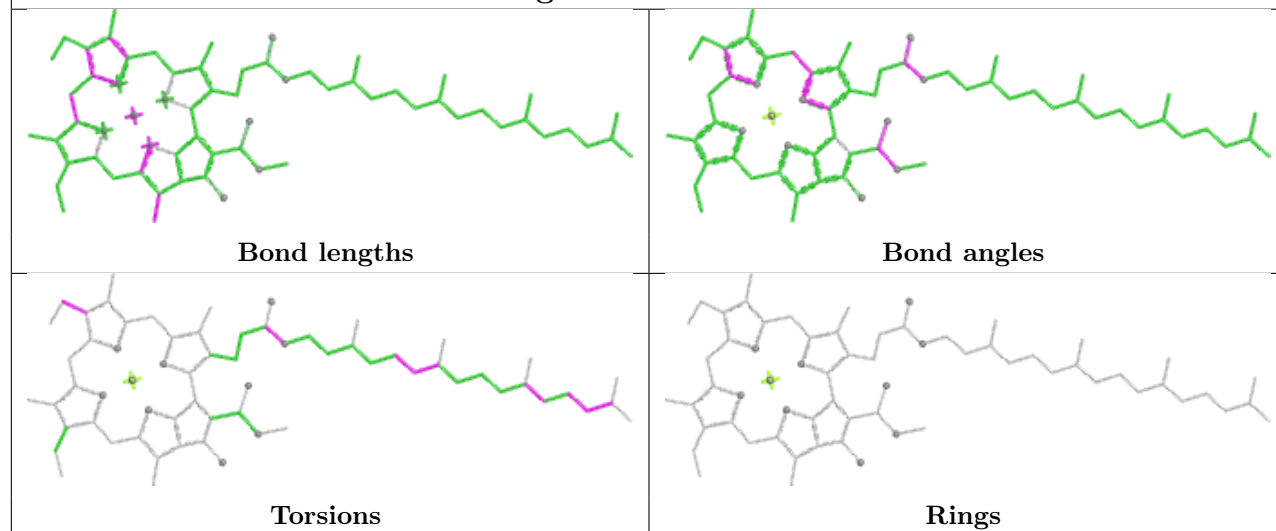
Ligand CLA 2 608



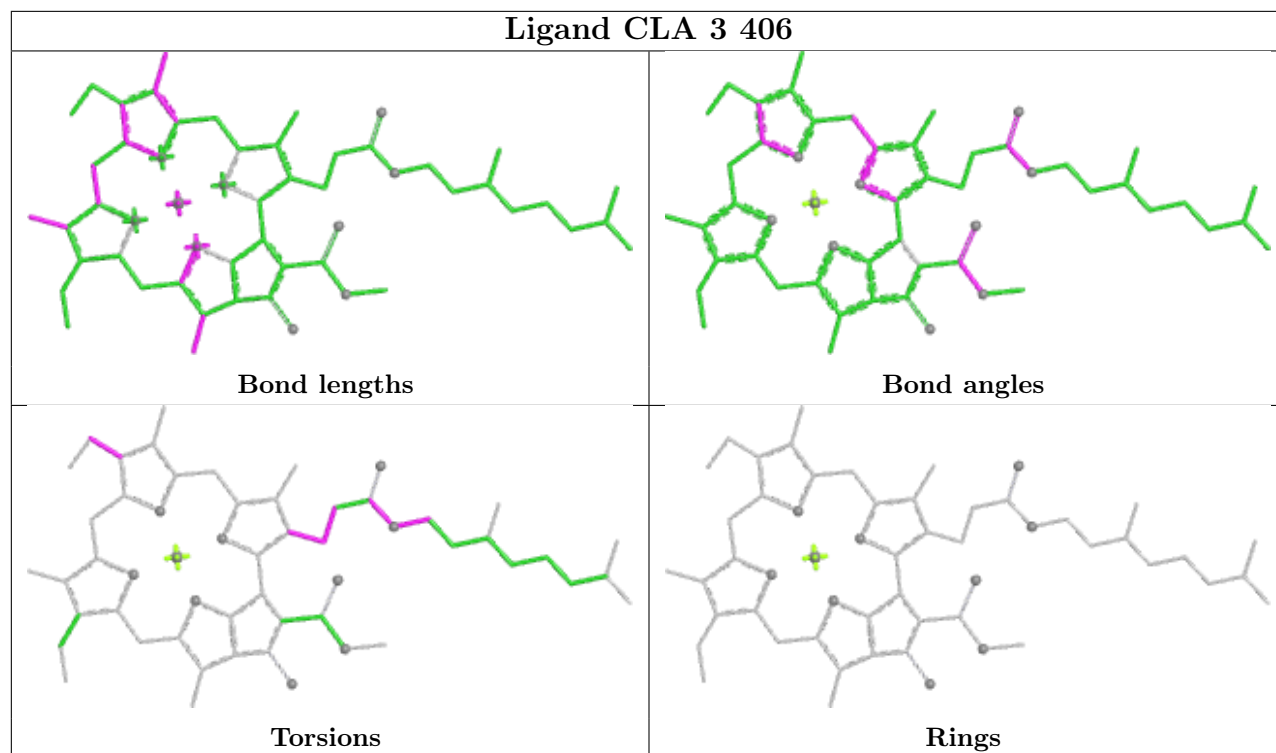
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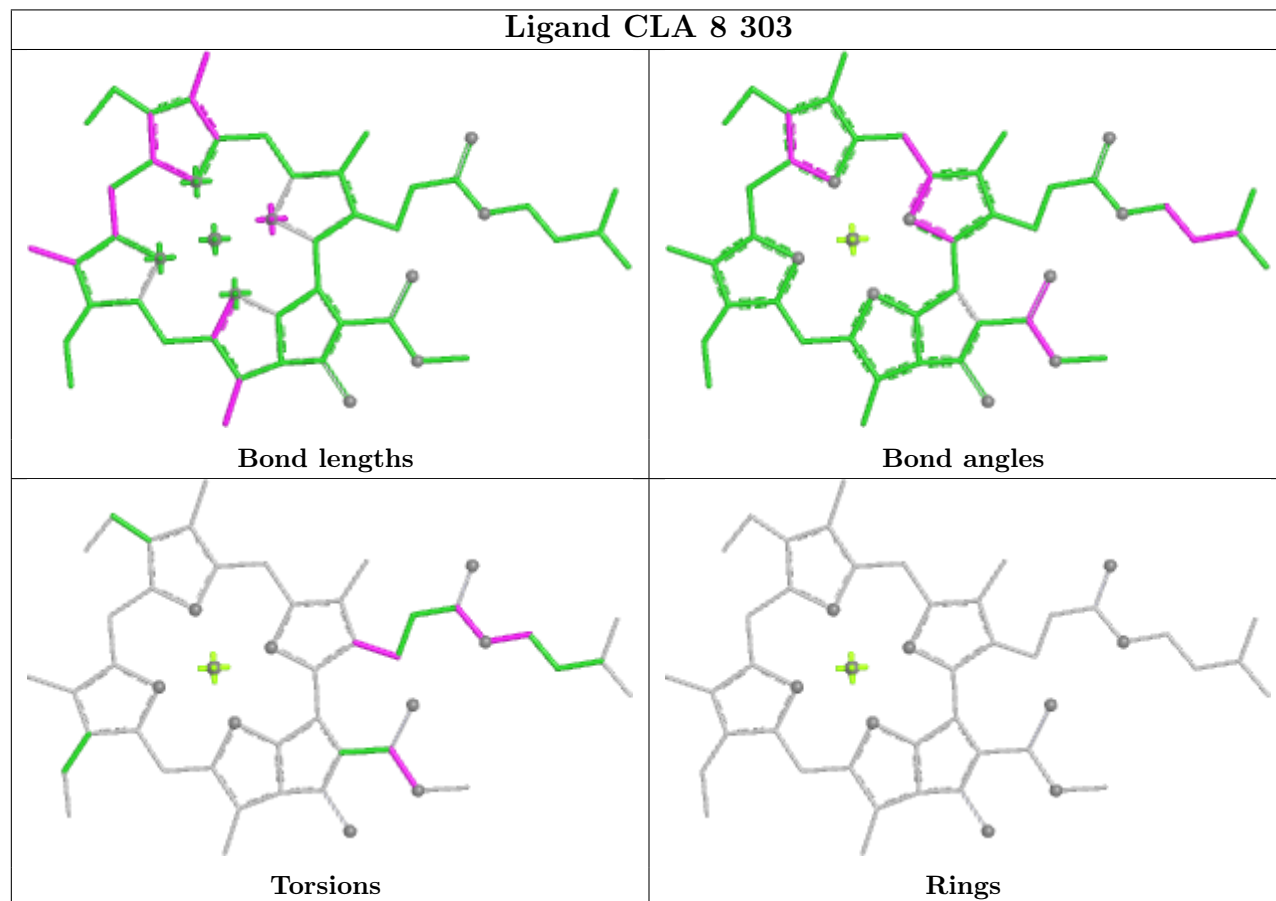
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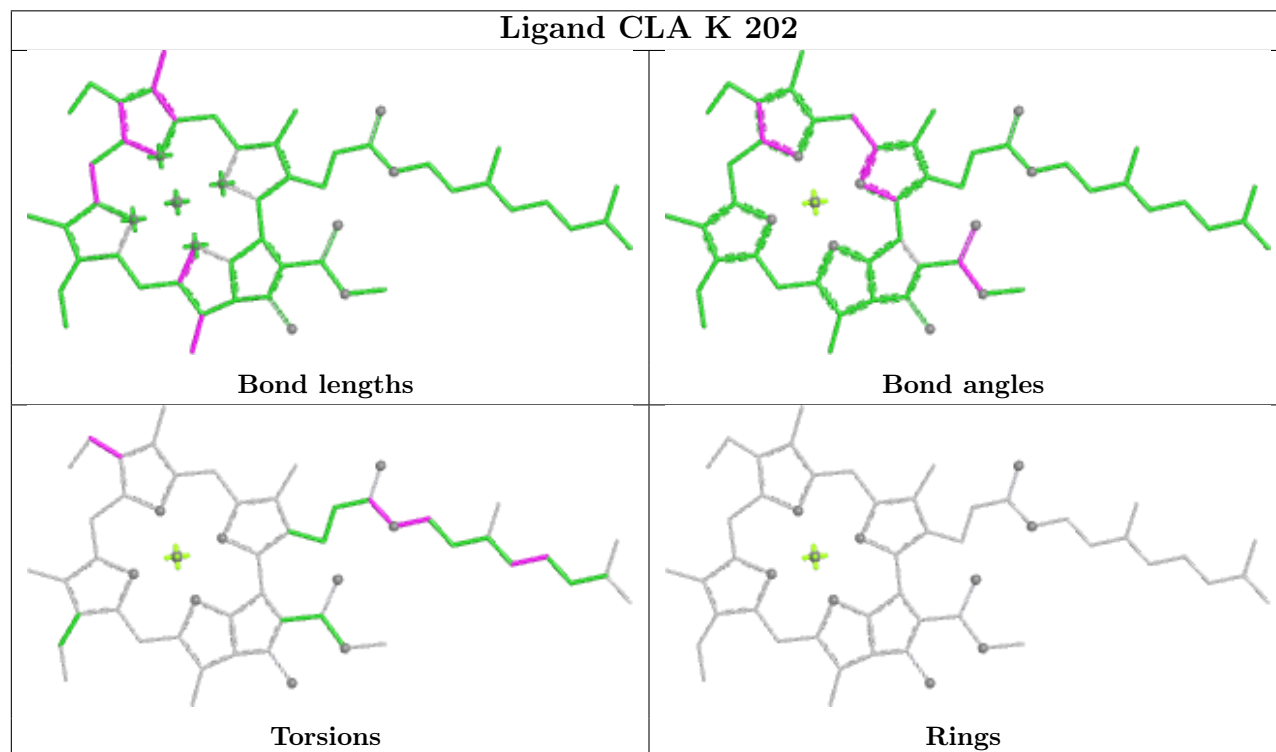
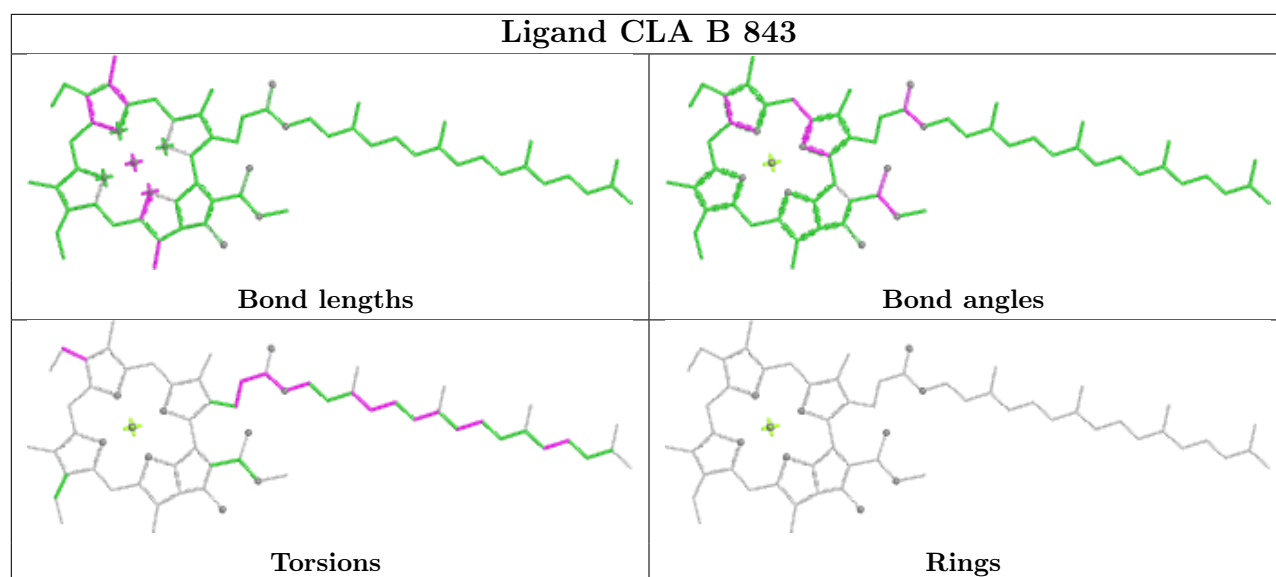


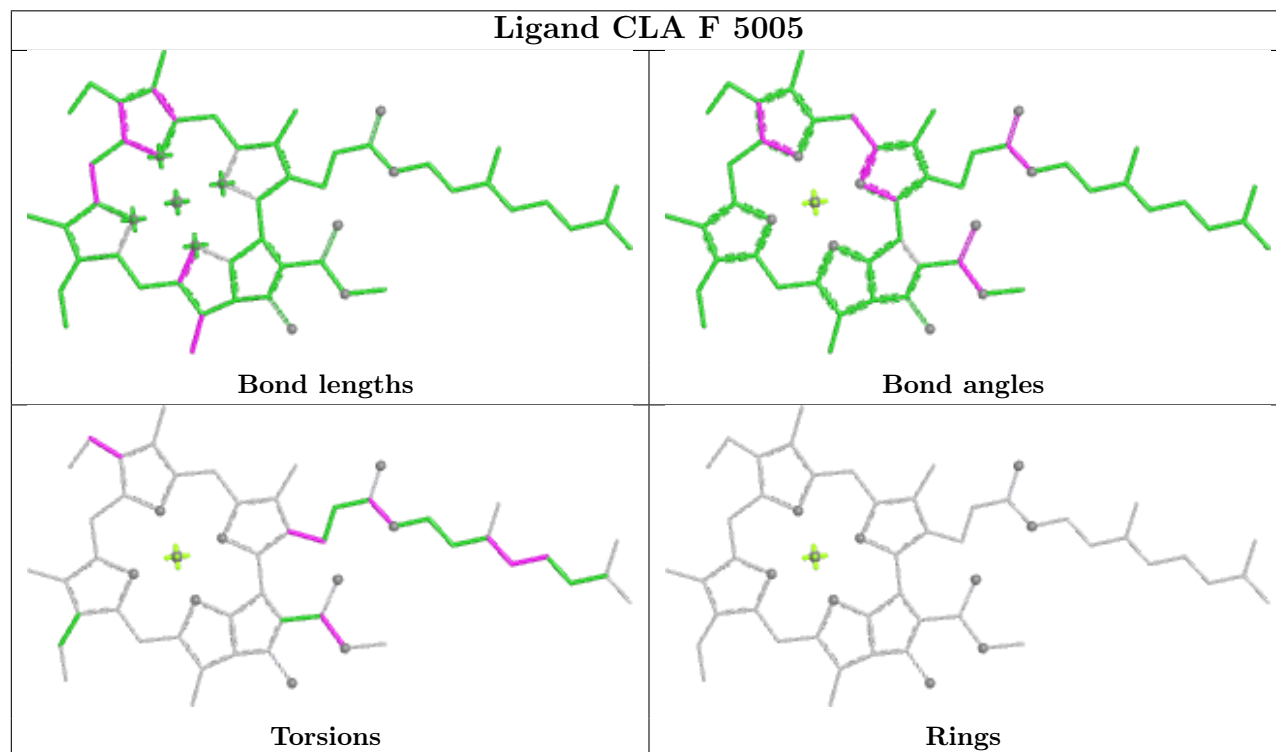
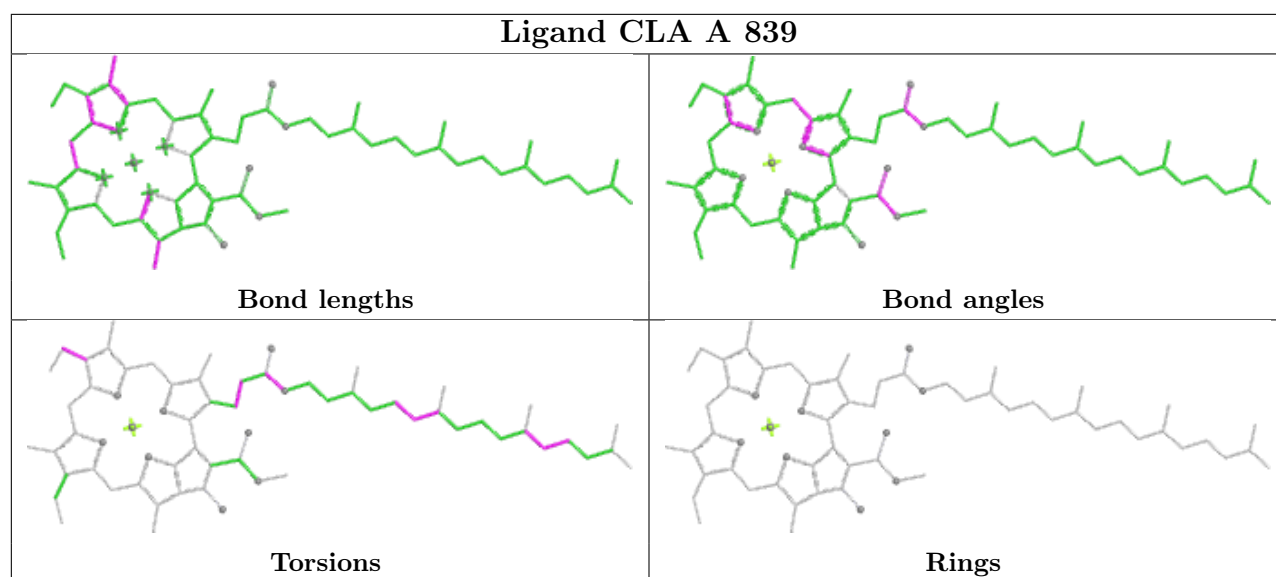
Ligand CLA 3 406

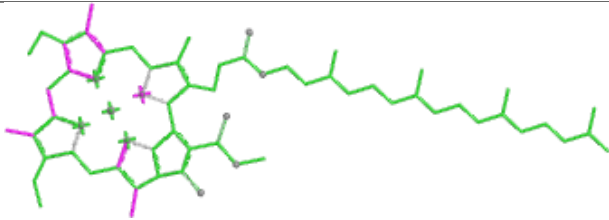
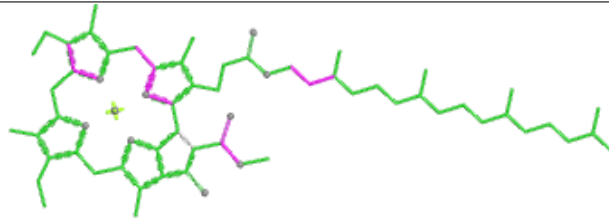
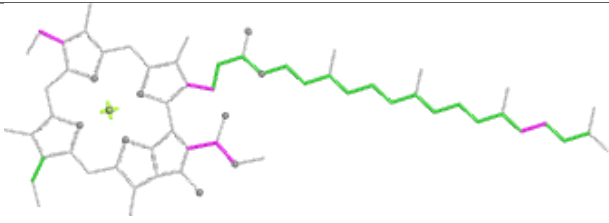
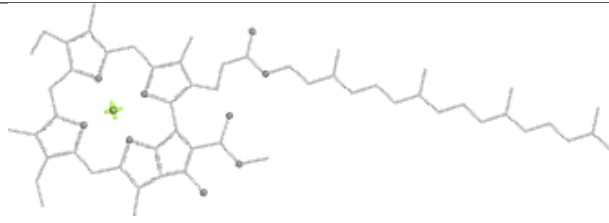


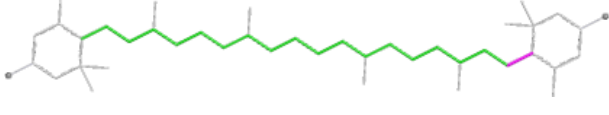
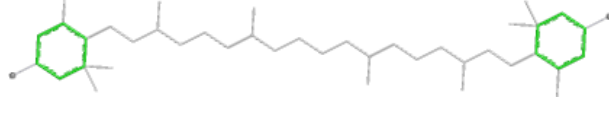
Ligand CLA 8 303

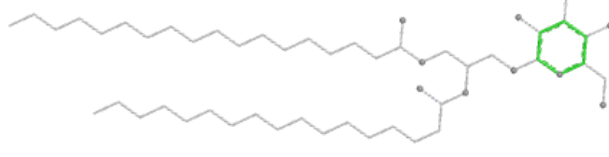


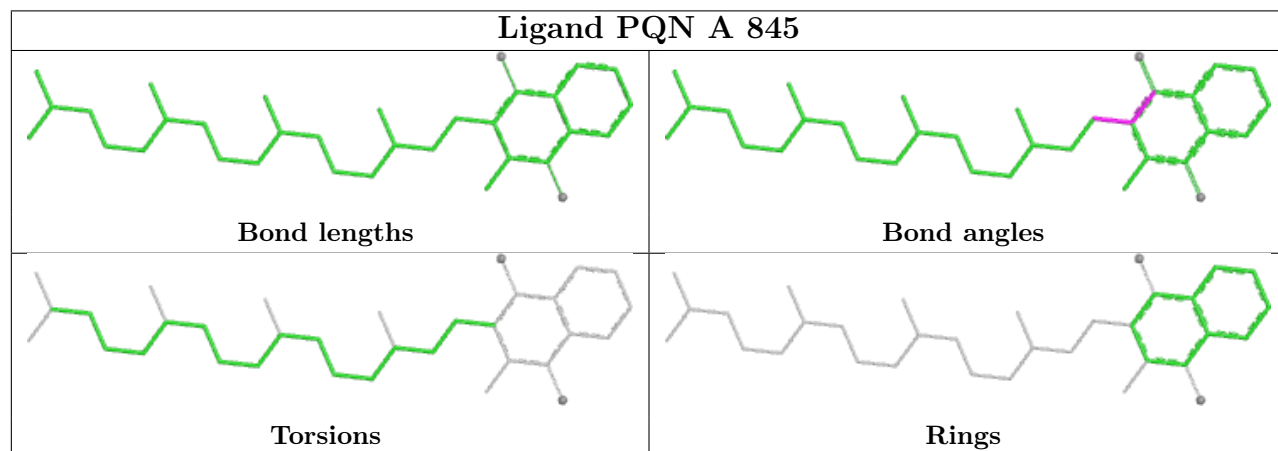
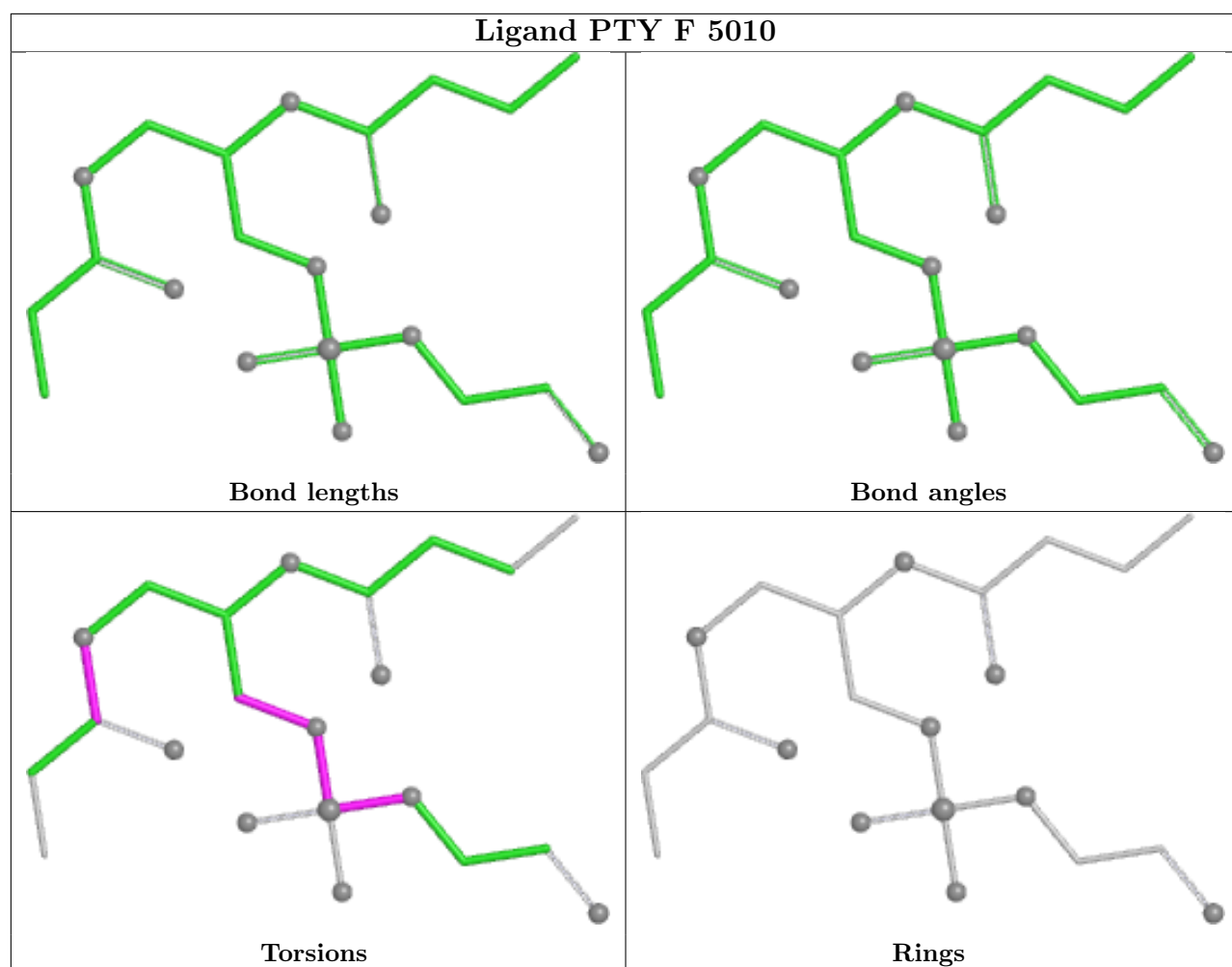


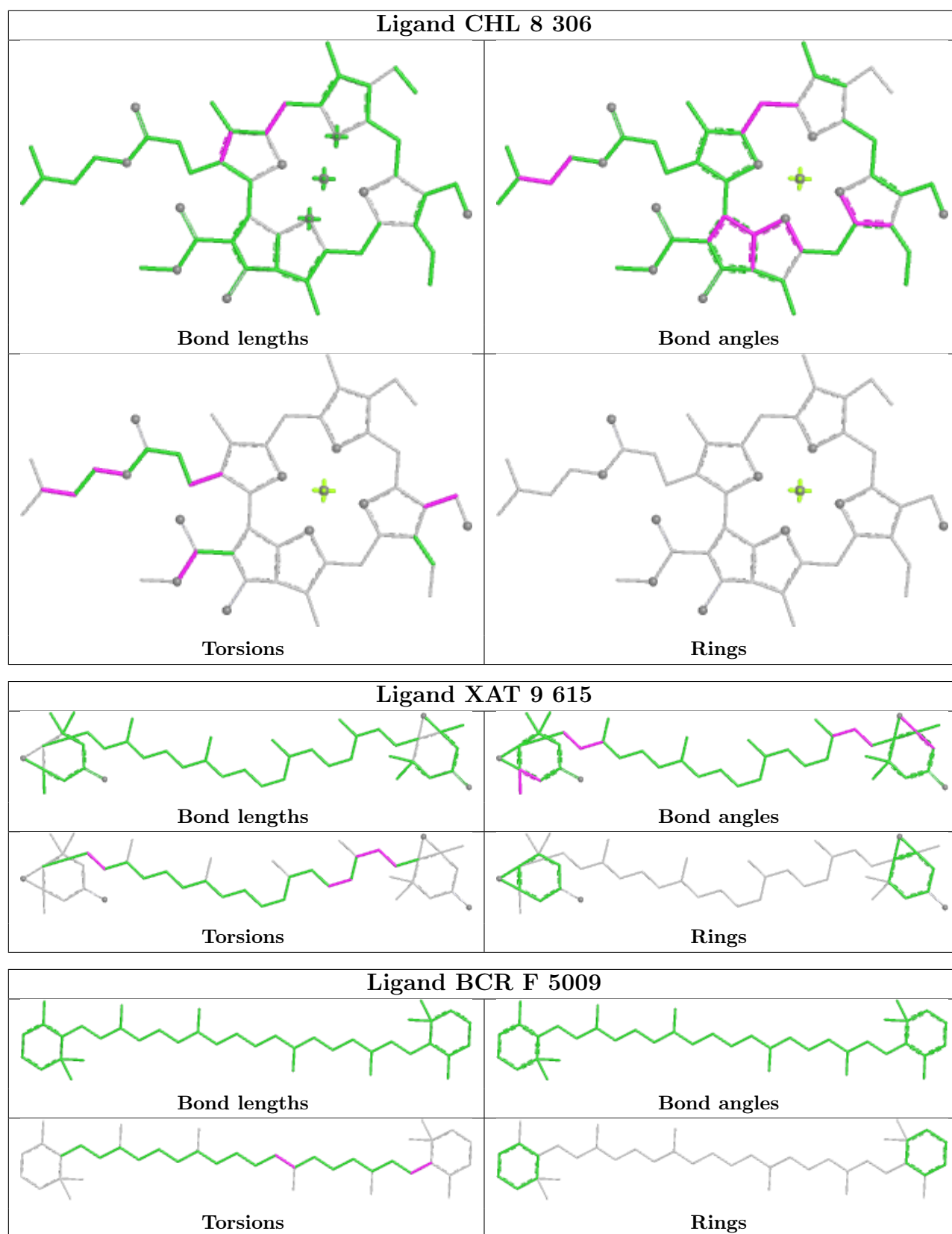


Ligand CLA B 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

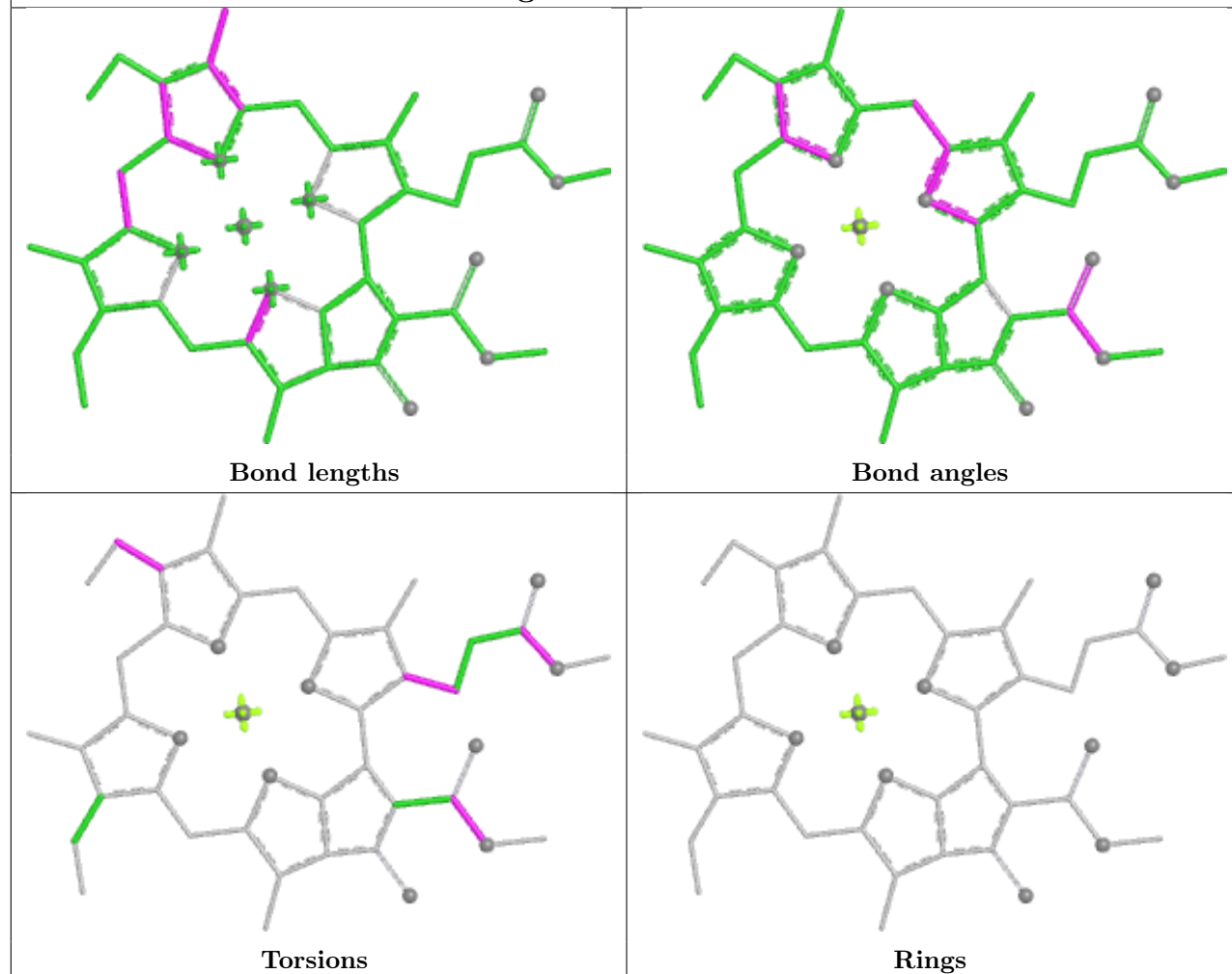
Ligand LUT 8 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG 7 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

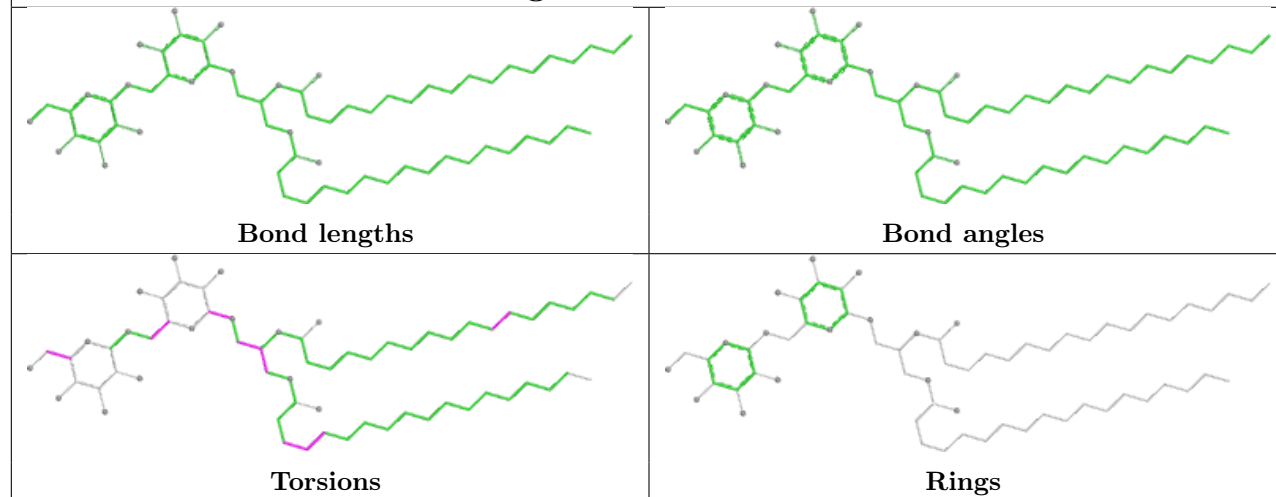


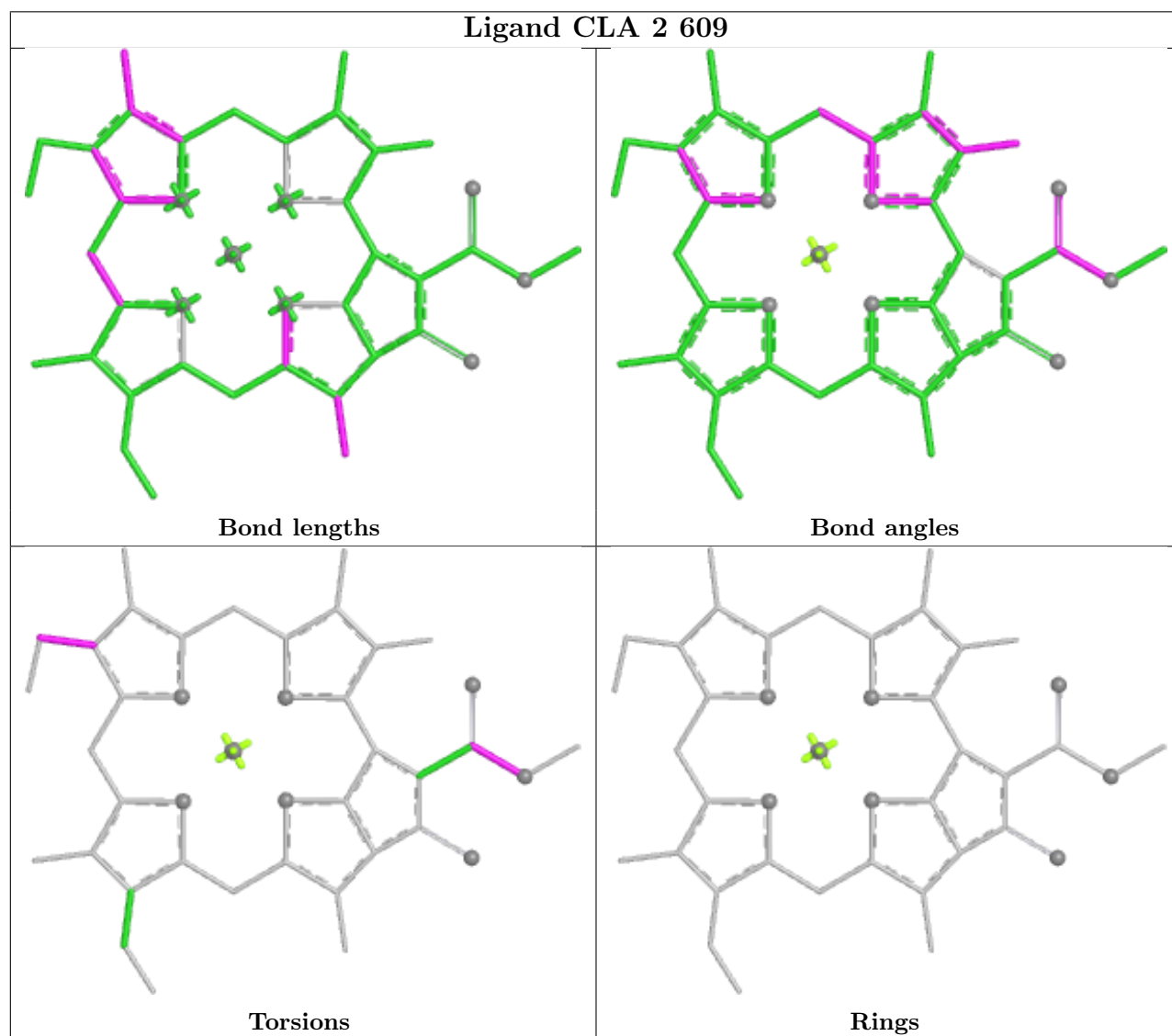
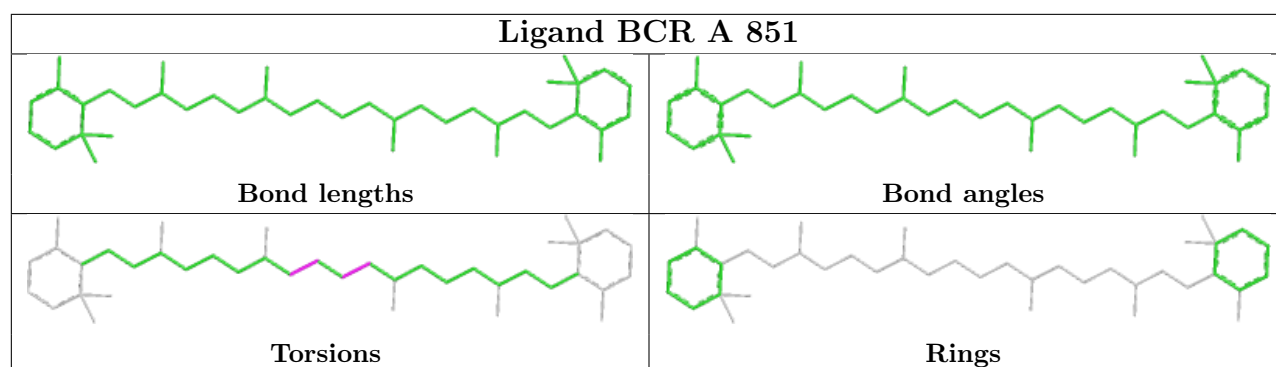


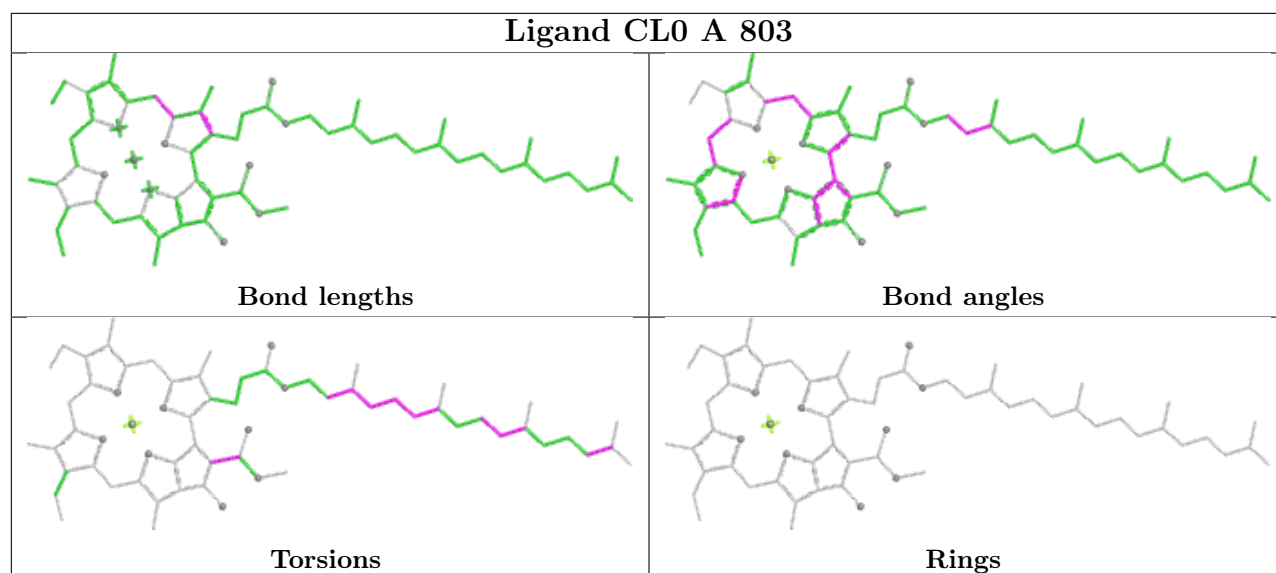
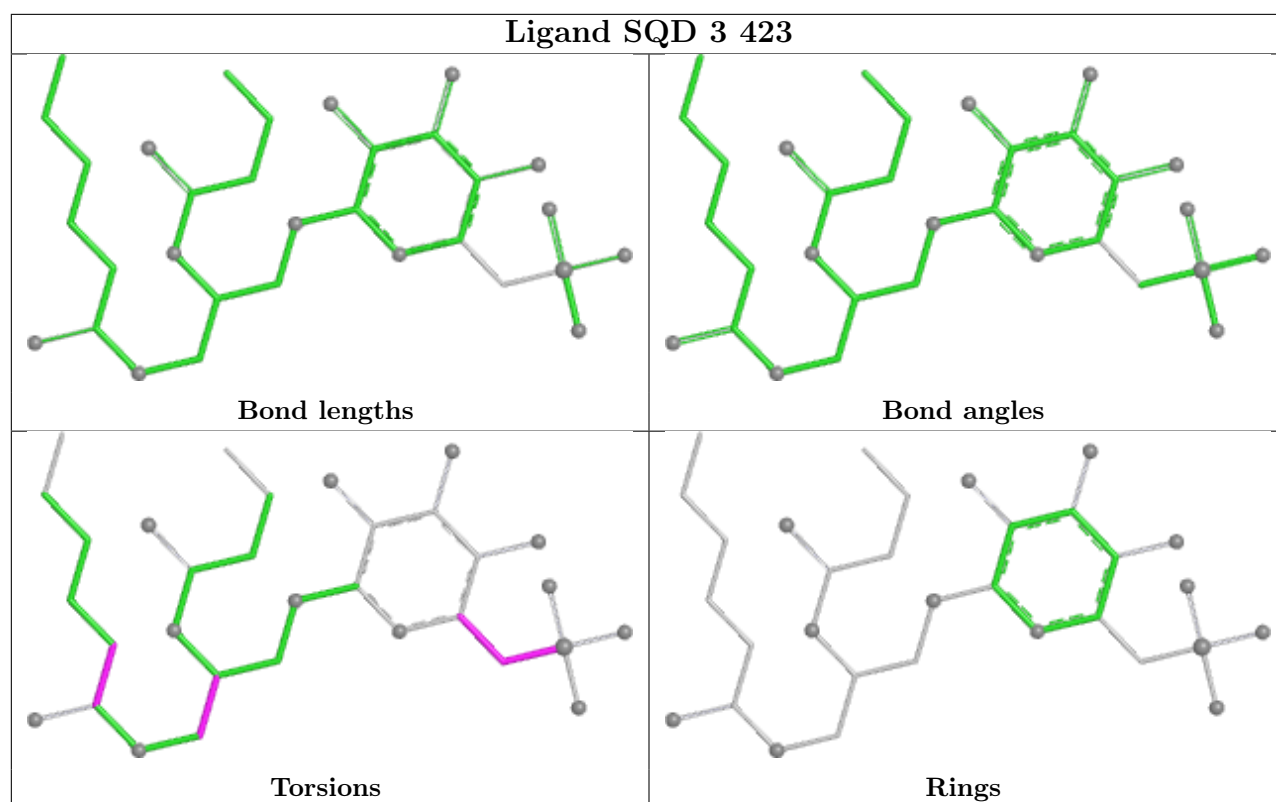
Ligand CLA 8 312

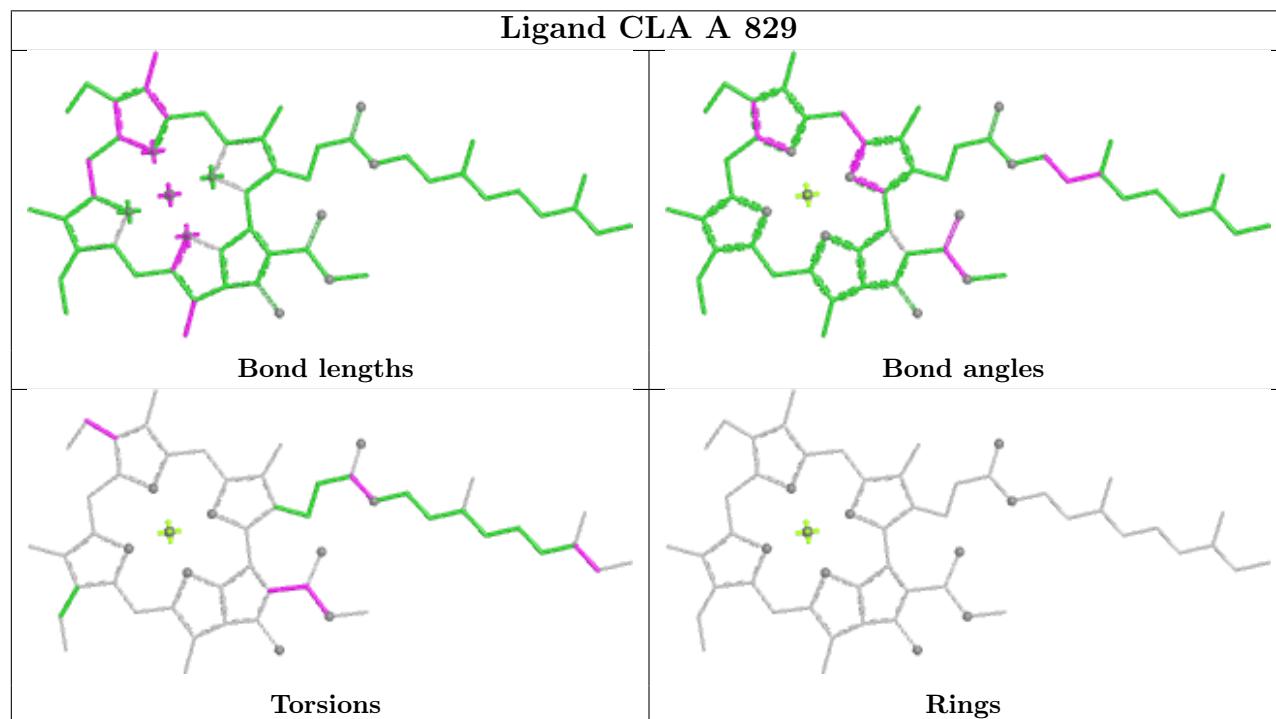
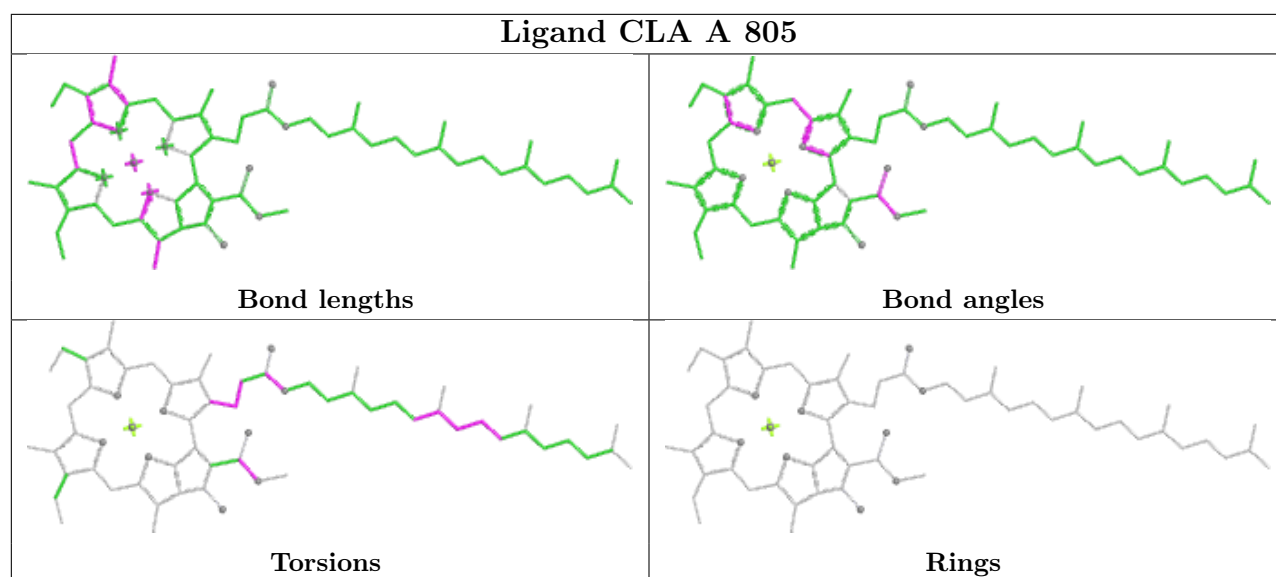


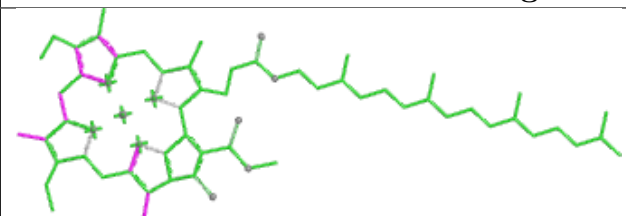
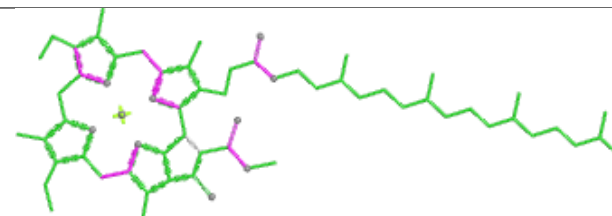
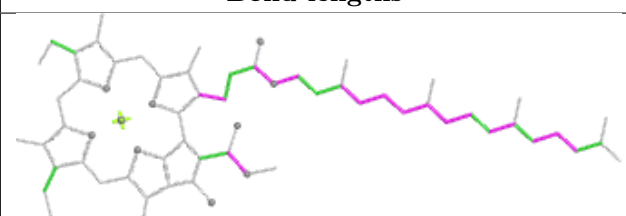
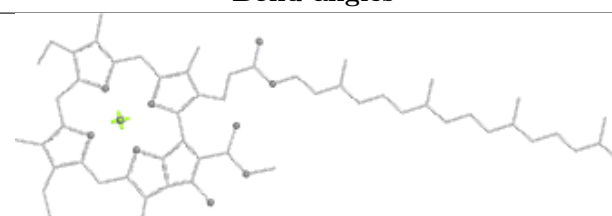
Ligand DGD A 802

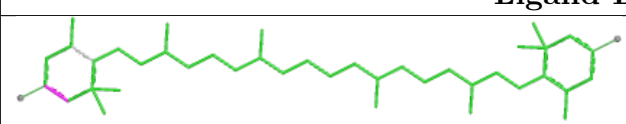
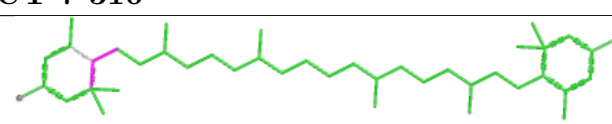
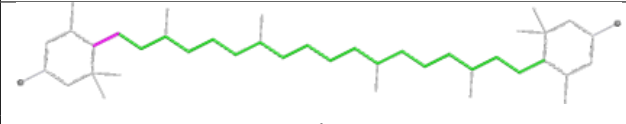
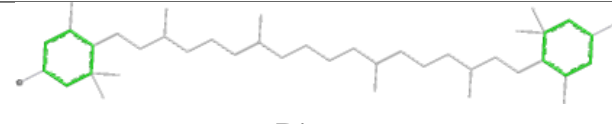


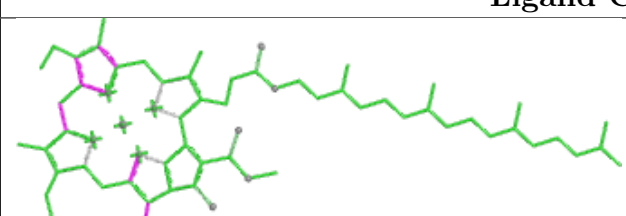
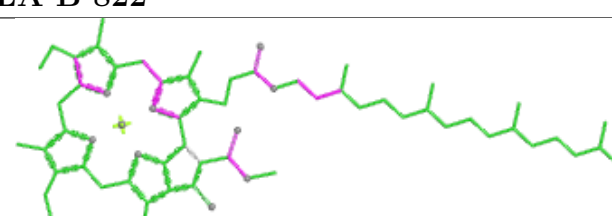
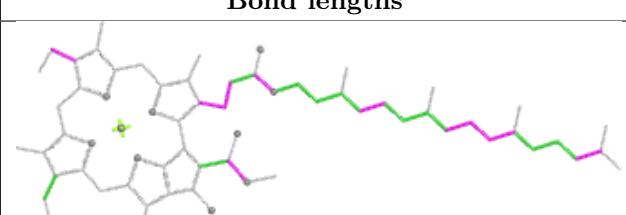
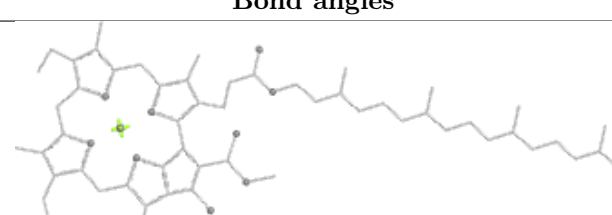


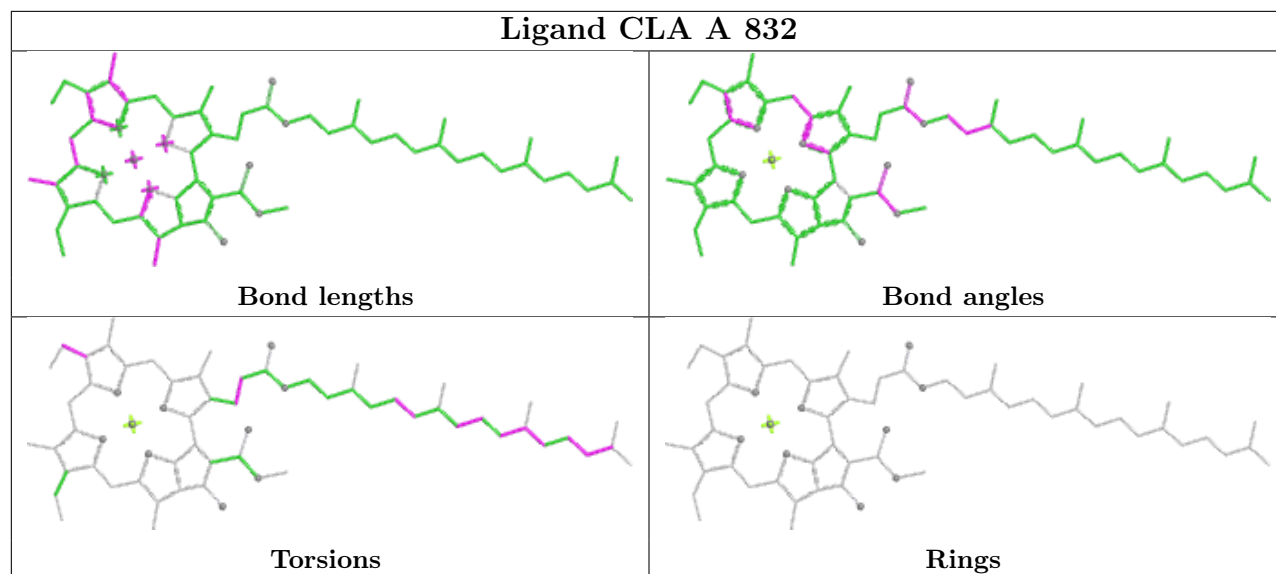
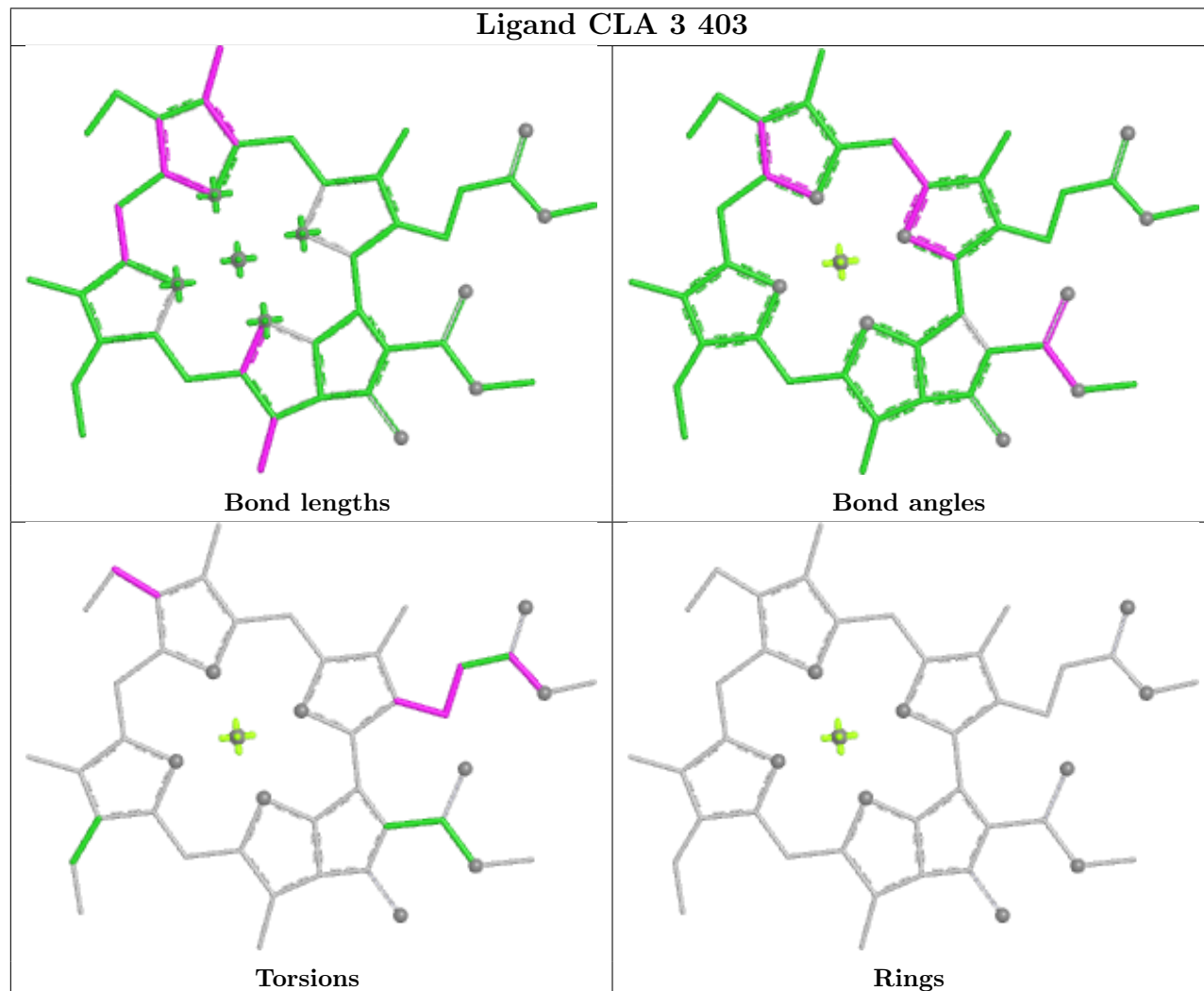


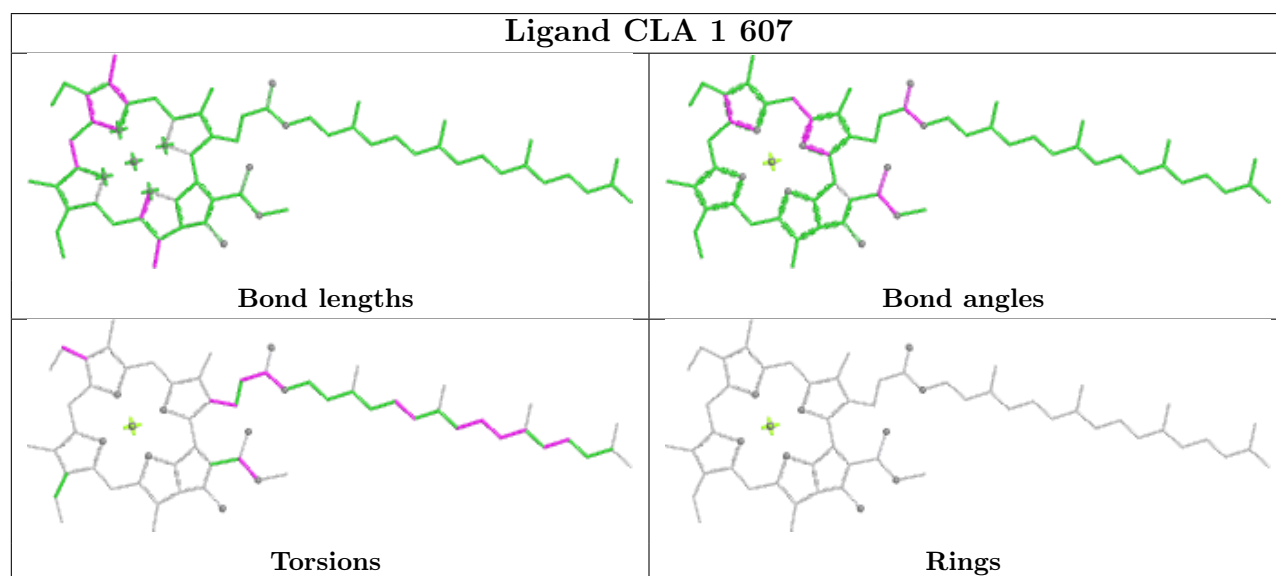
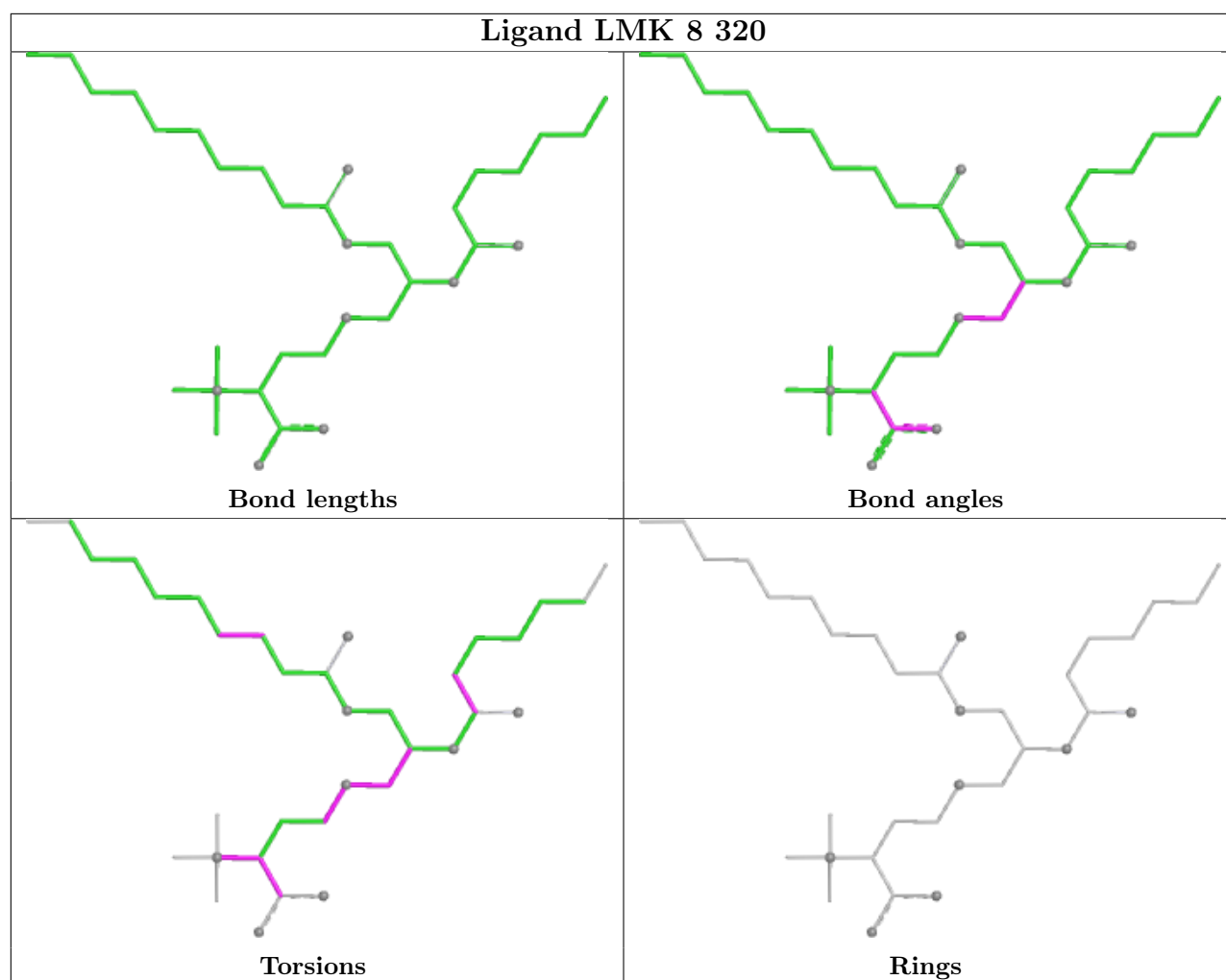


Ligand CLA A 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

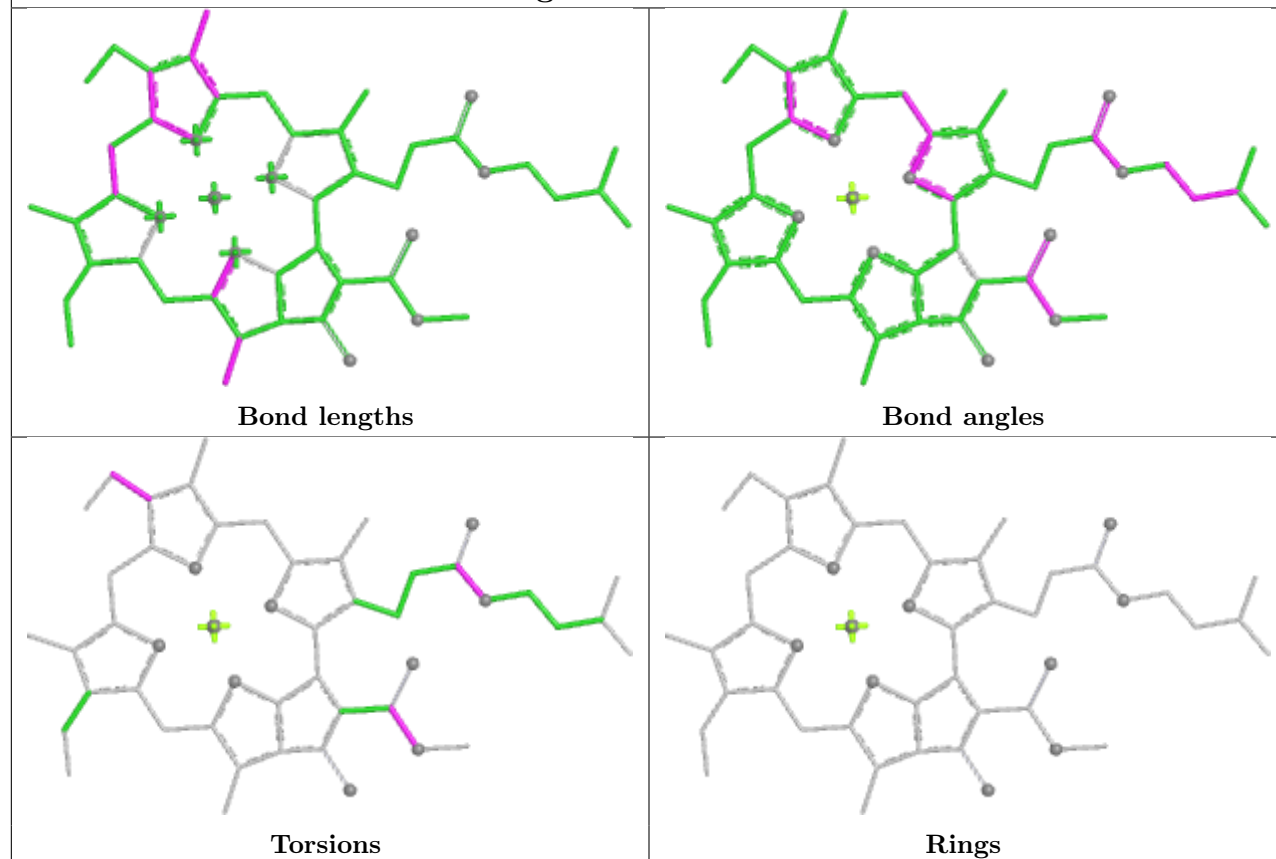
Ligand LUT 7 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

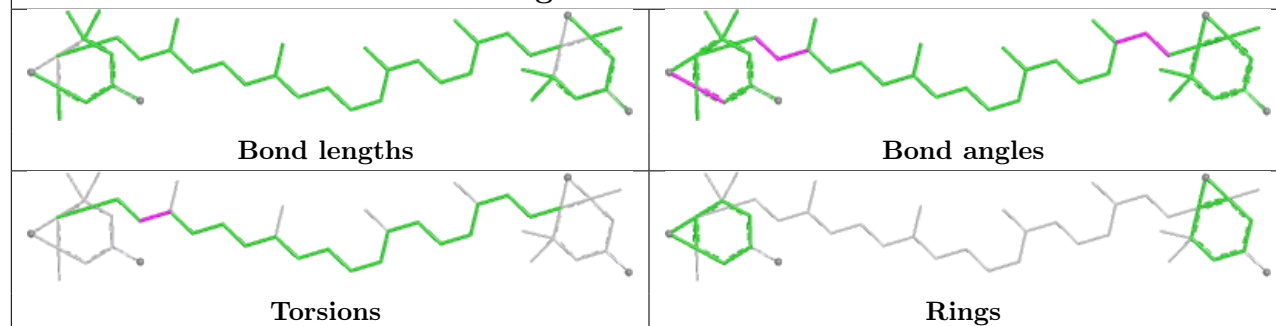
Ligand CLA A 832**Ligand CLA 3 403**



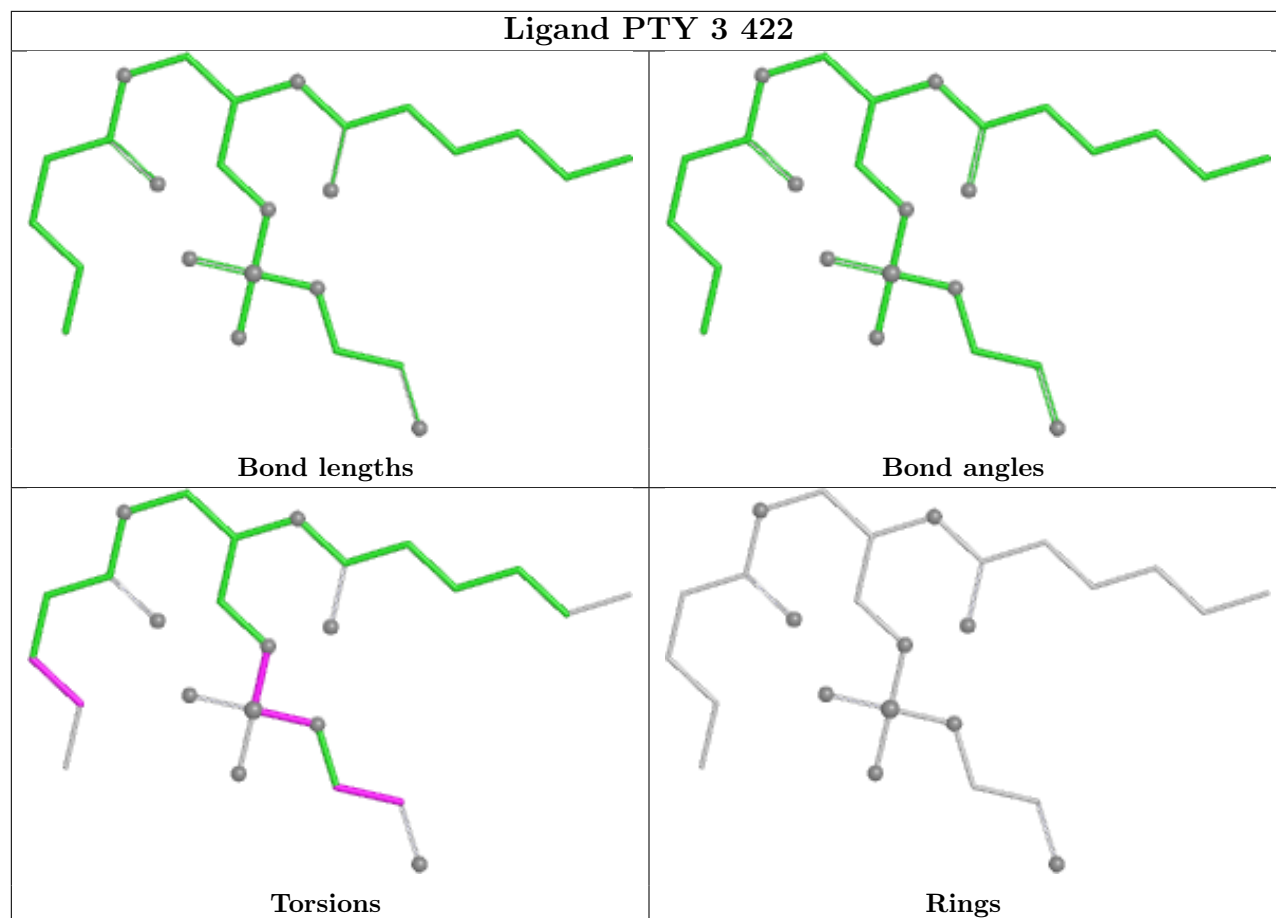
Ligand CLA 7 305



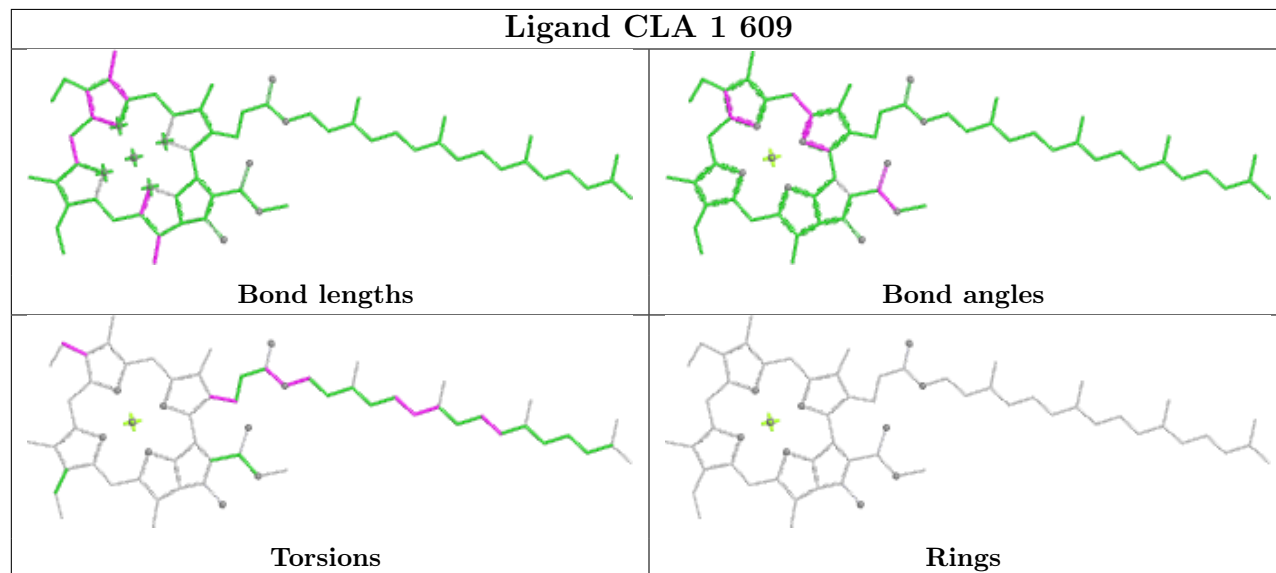
Ligand XAT 3 416



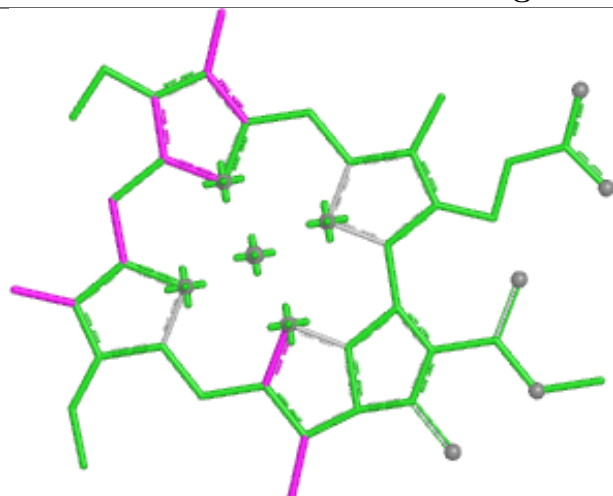
Ligand PTY 3 422



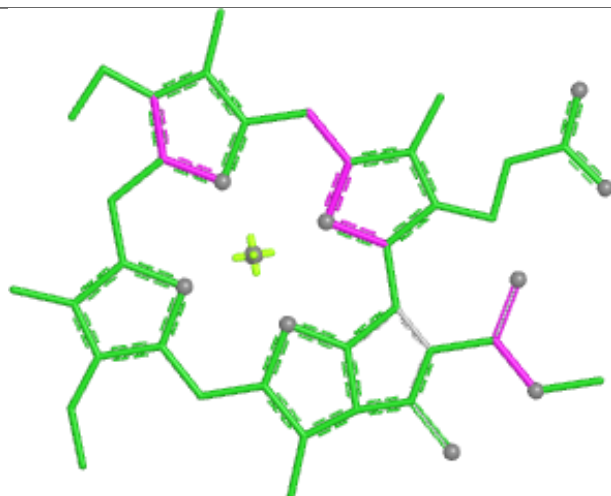
Ligand CLA 1 609



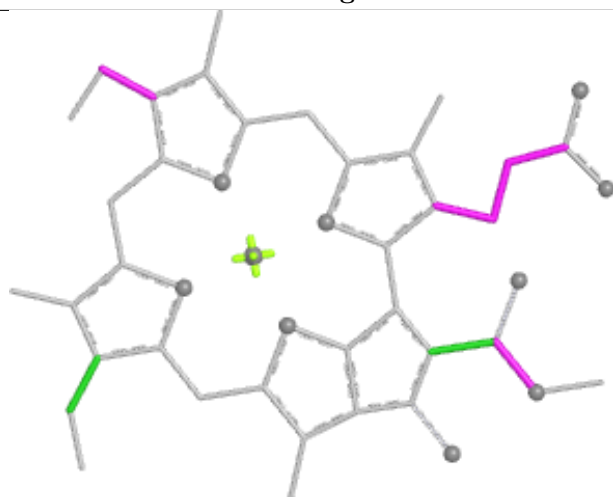
Ligand CLA H 204



Bond lengths



Bond angles

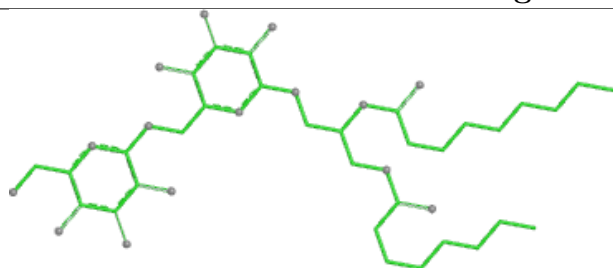


Torsions

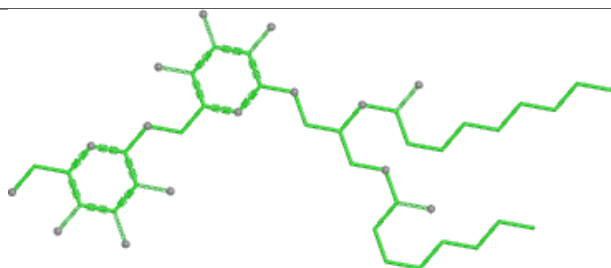


Rings

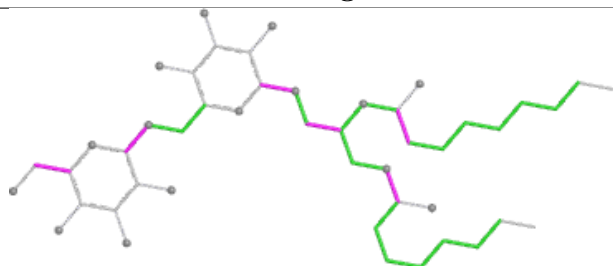
Ligand DGD 7 321



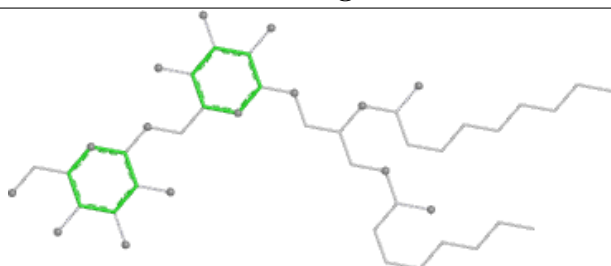
Bond lengths



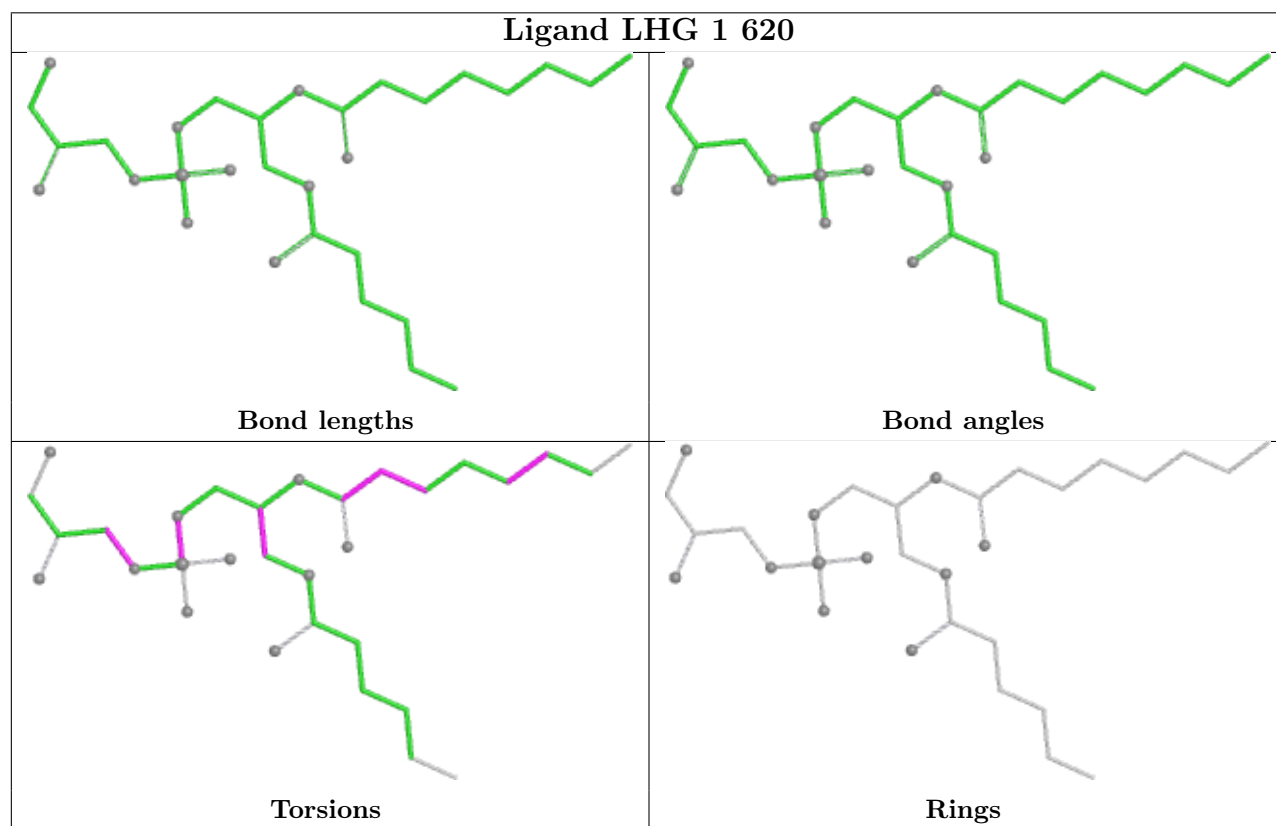
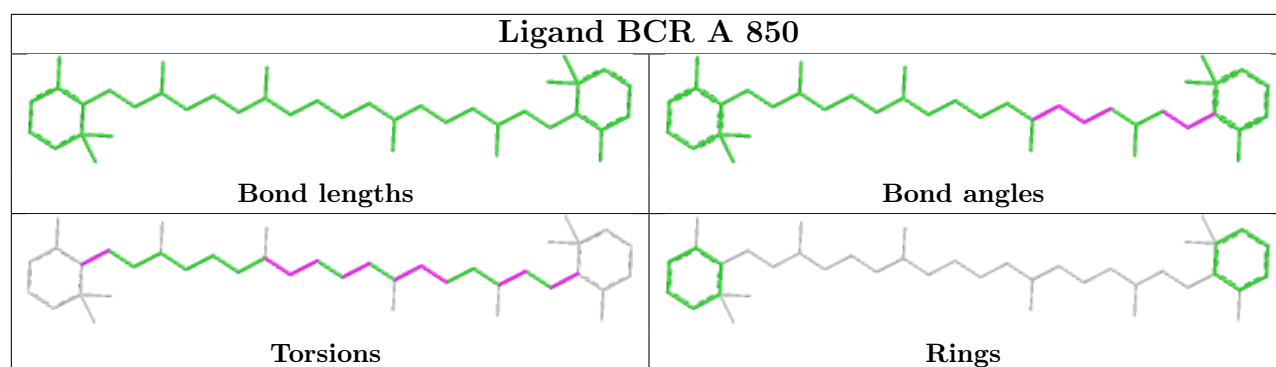
Bond angles

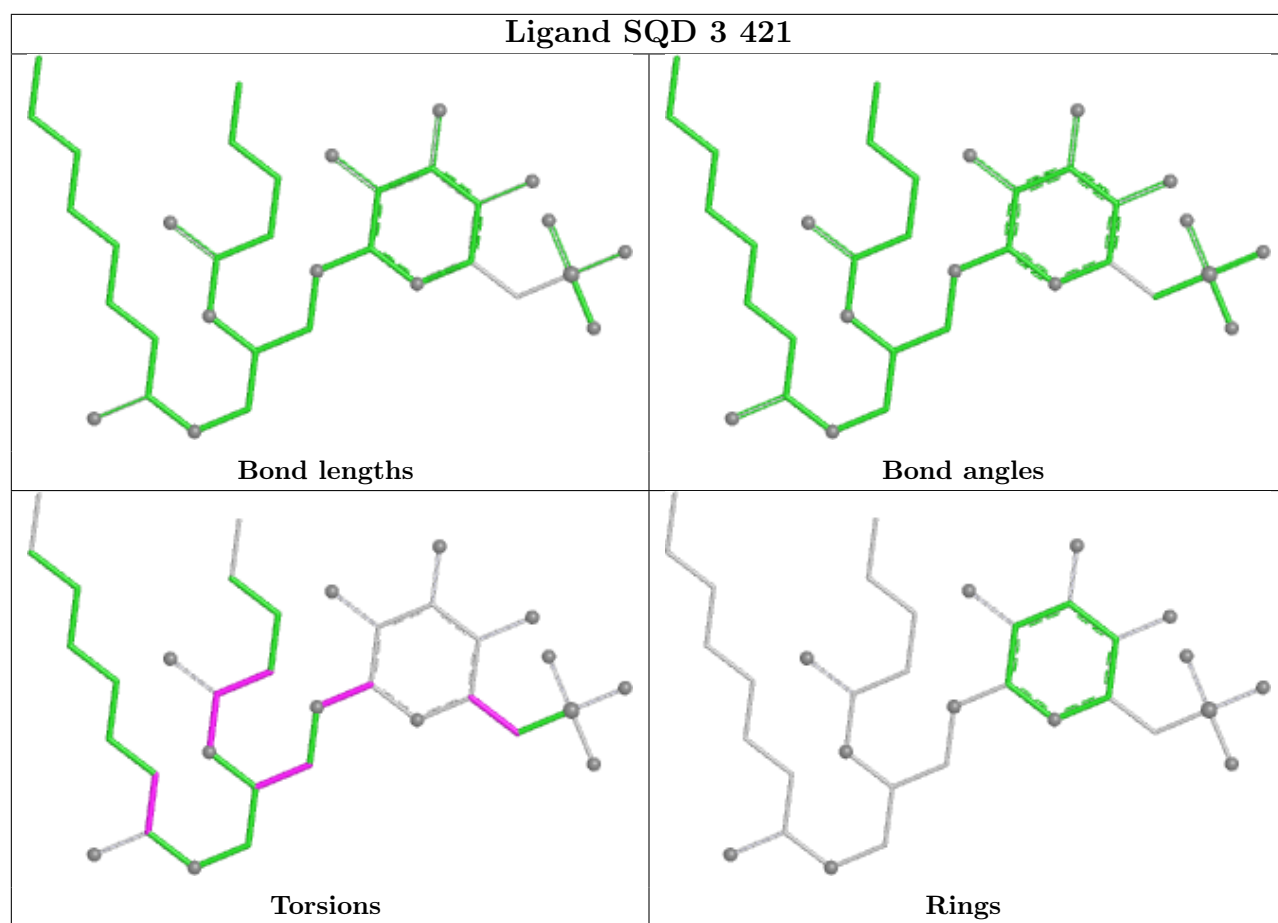


Torsions

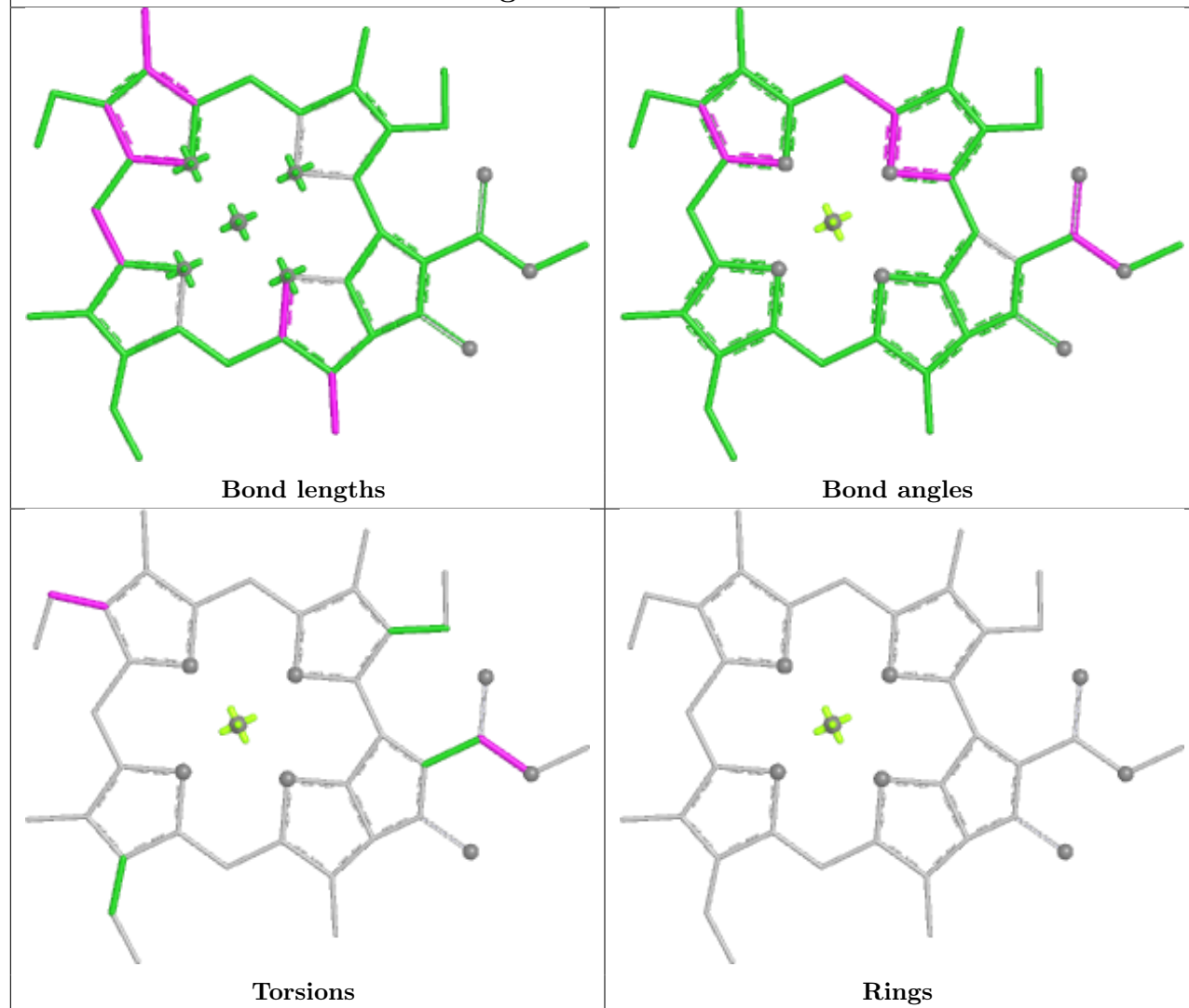


Rings

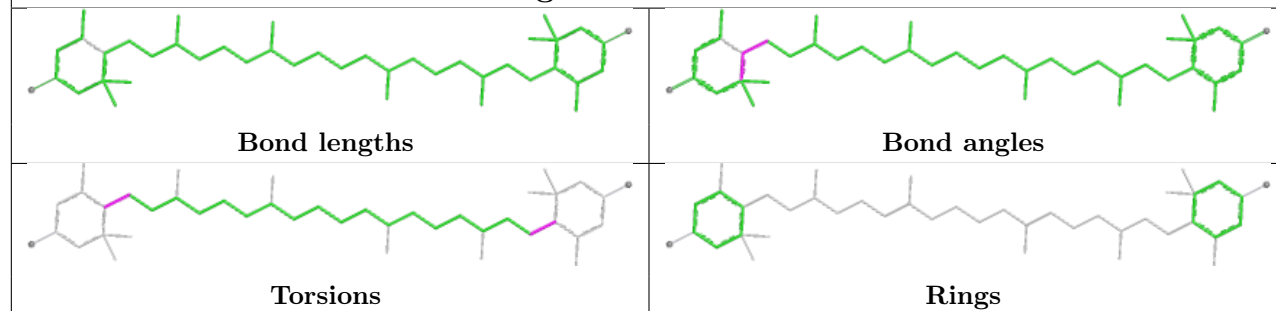


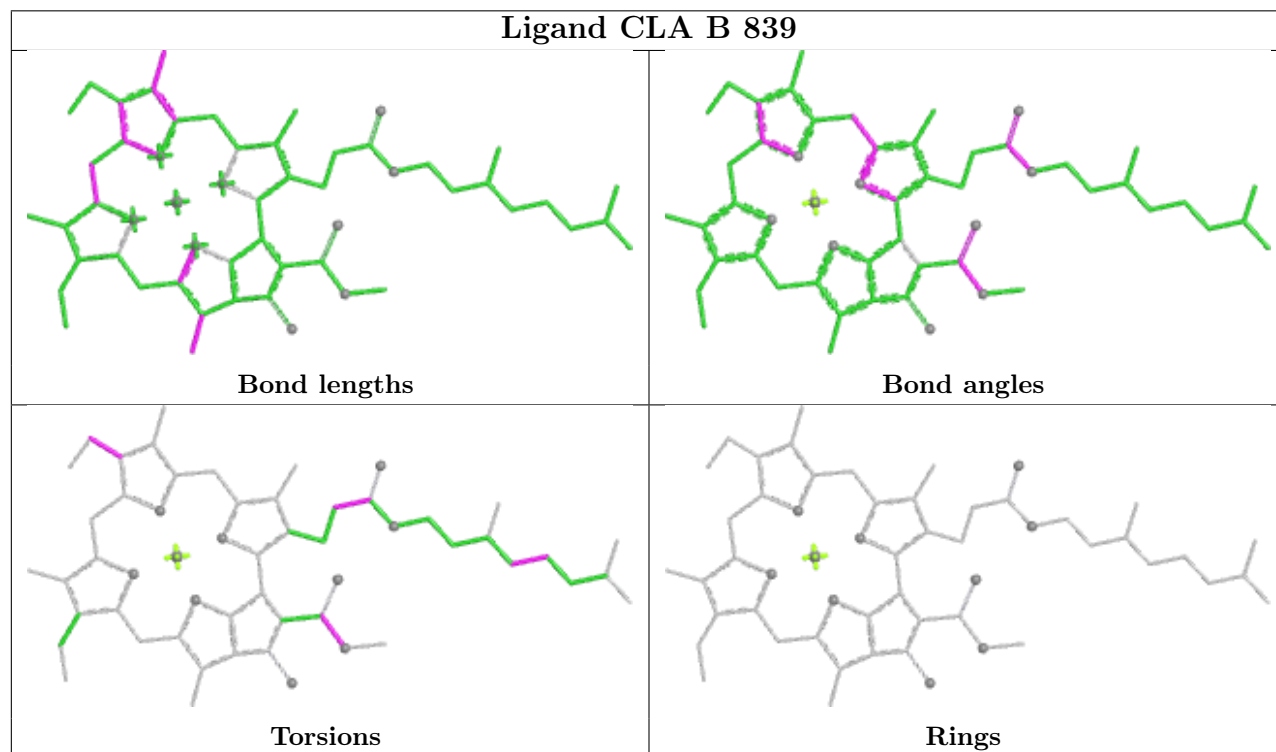
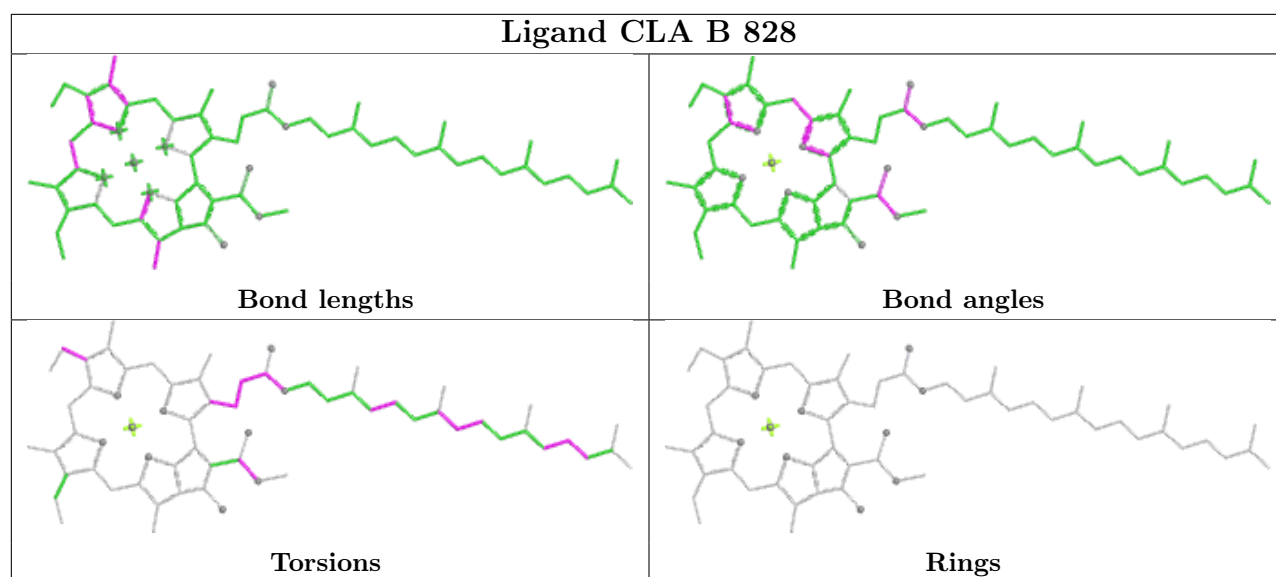


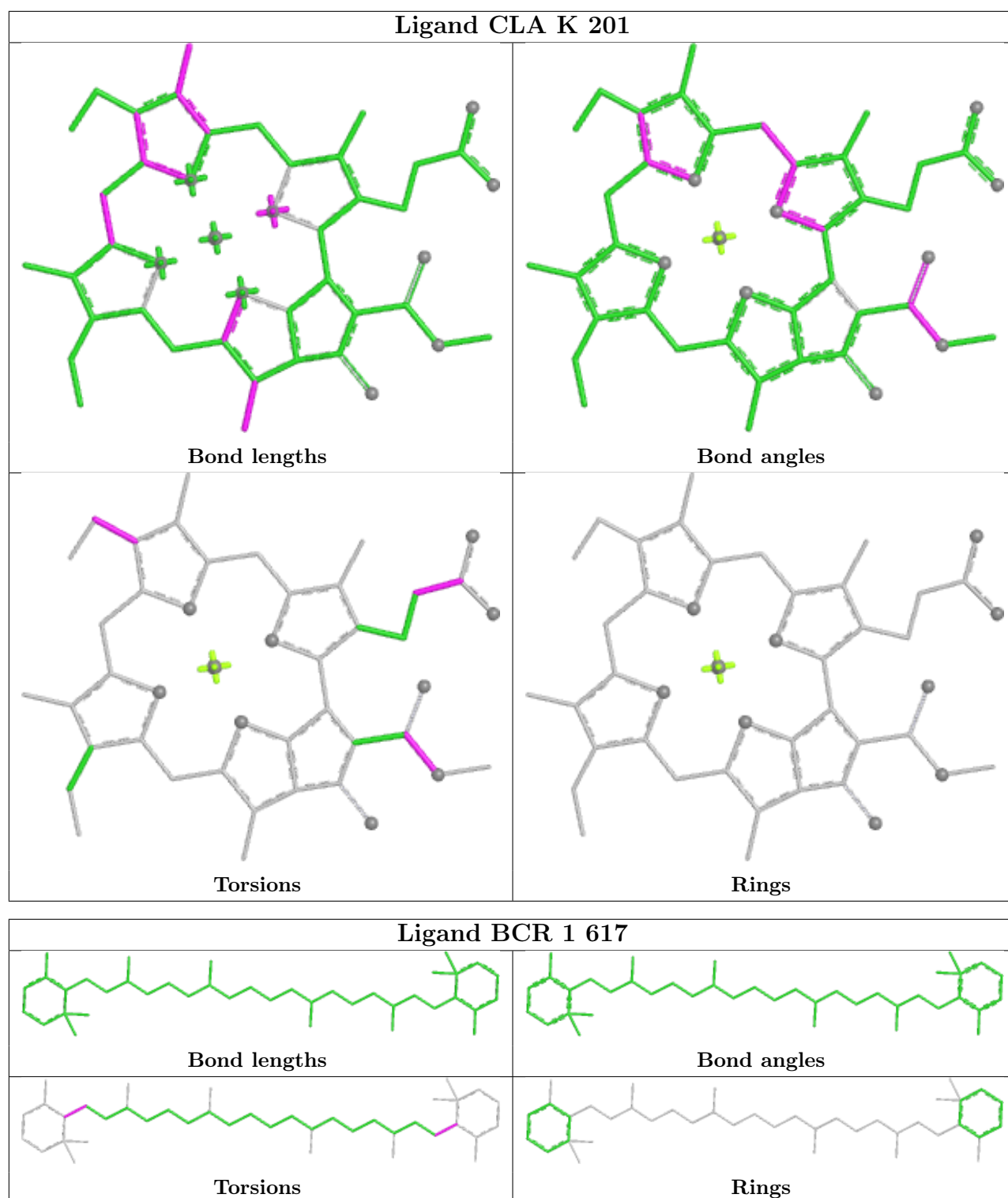
Ligand CLA 3 413

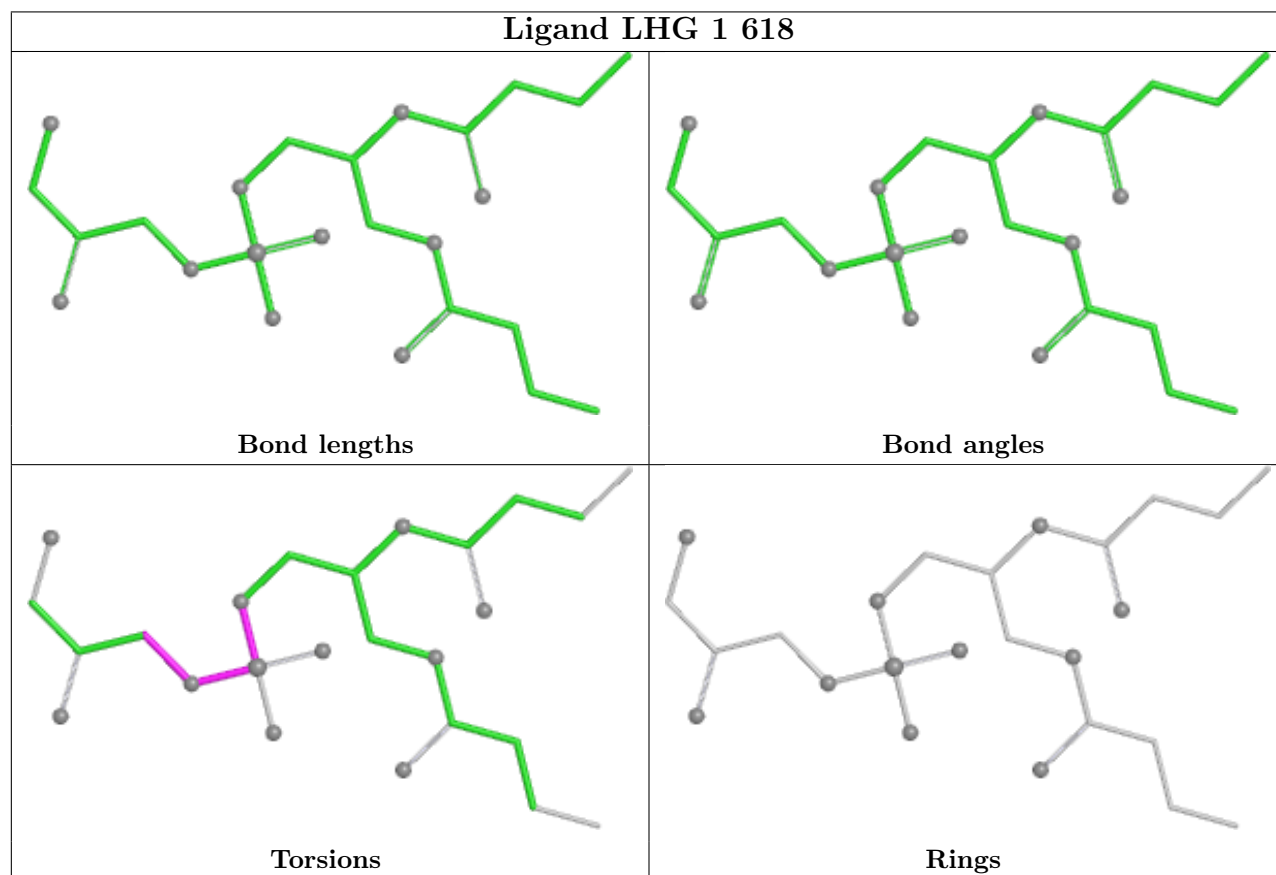
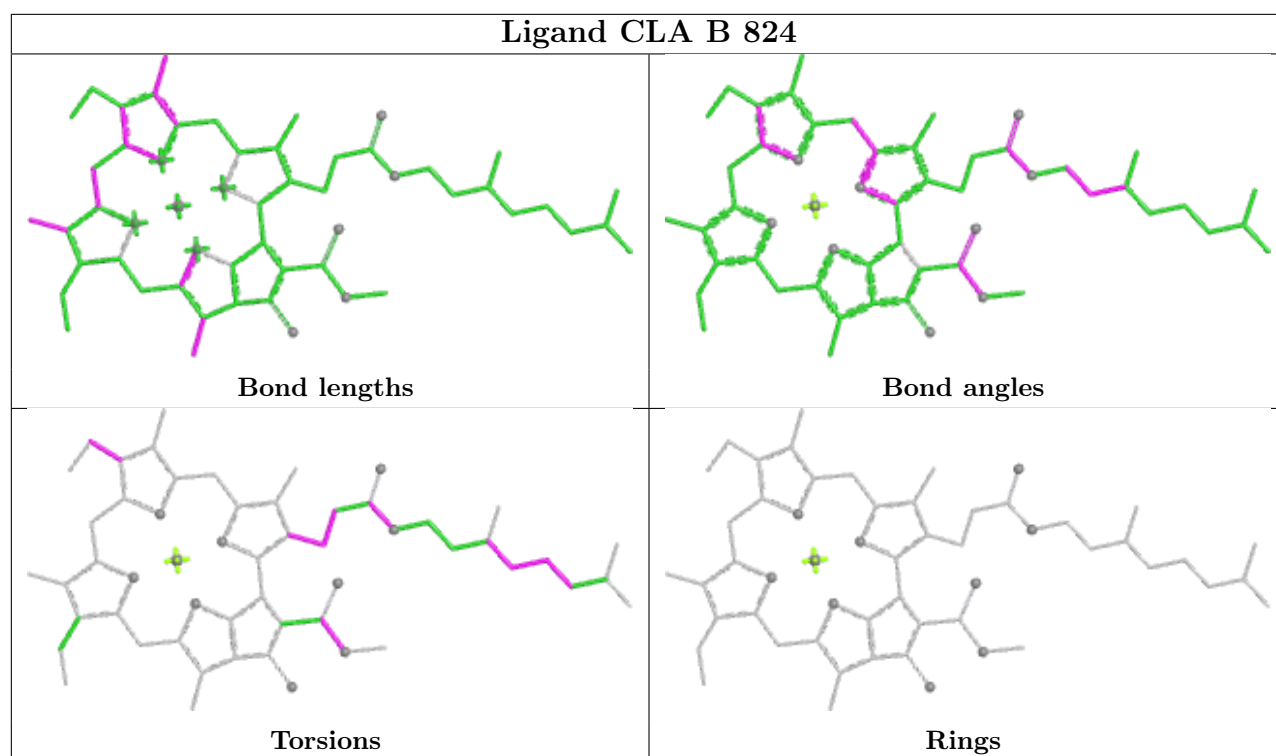


Ligand LUT 3 415

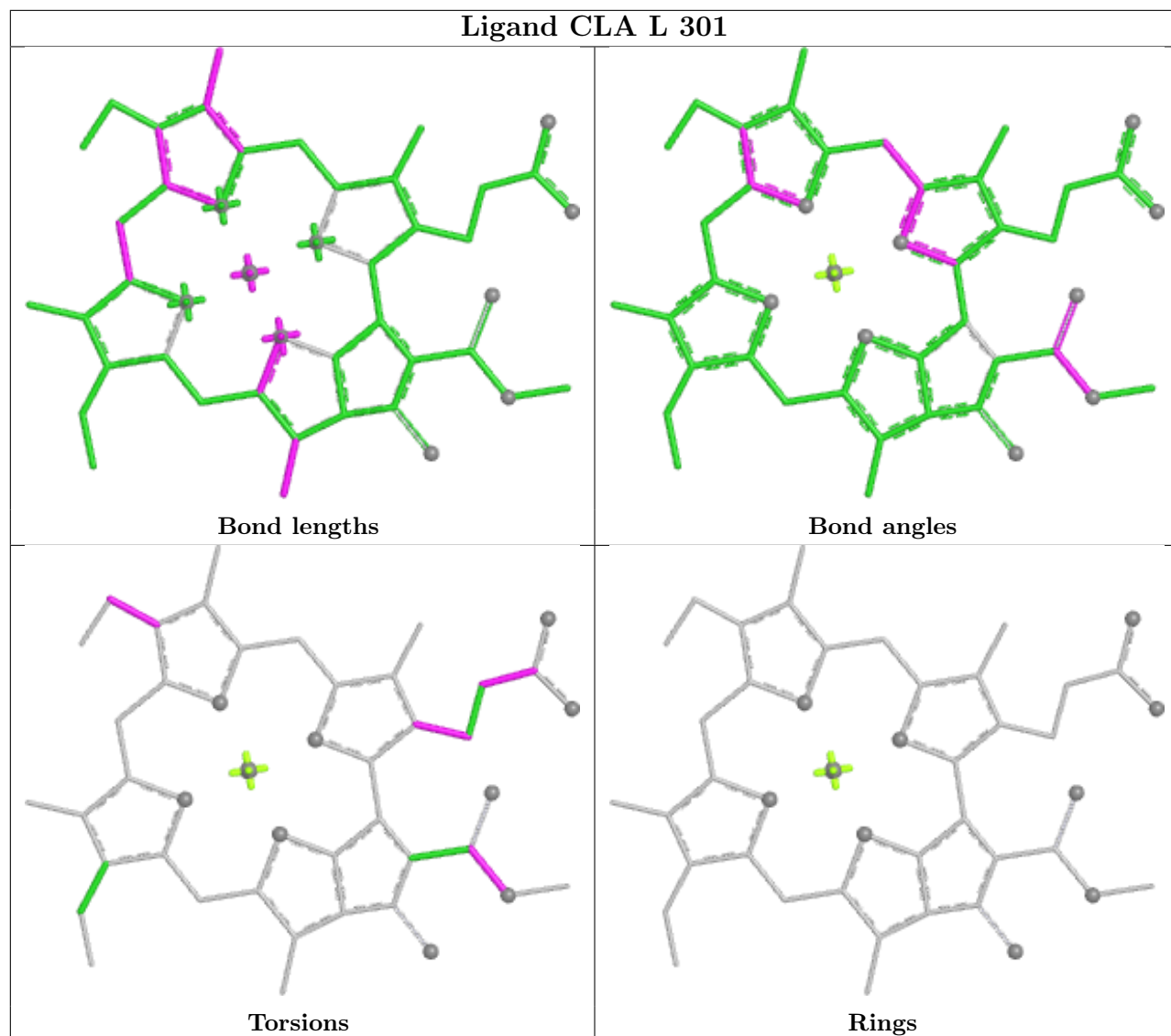




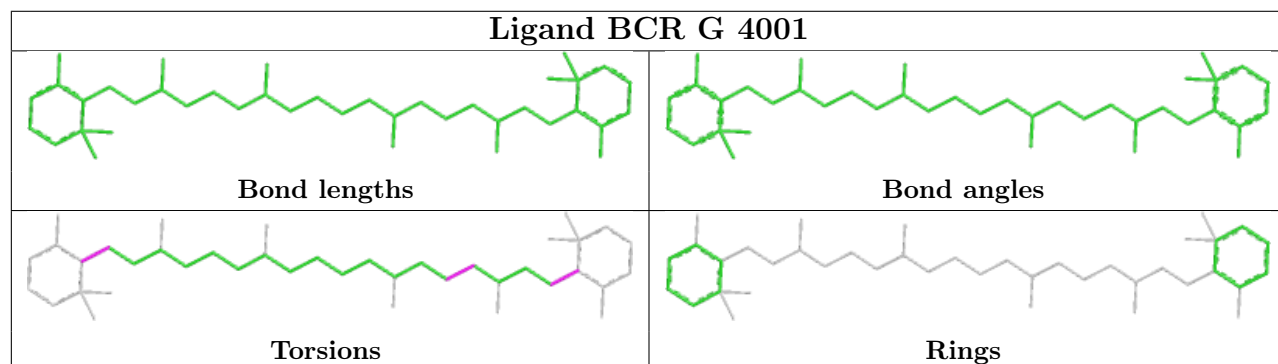




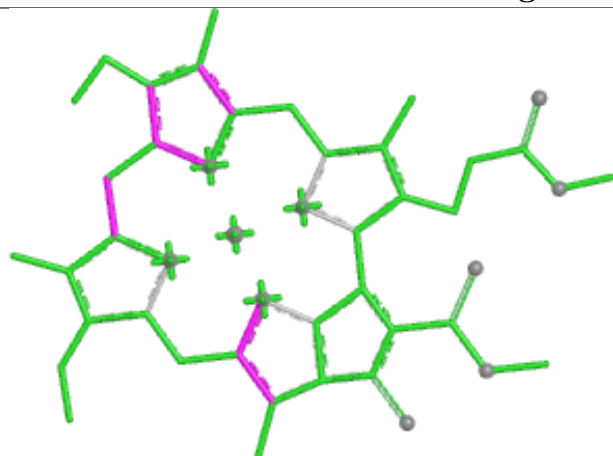
Ligand CLA L 301



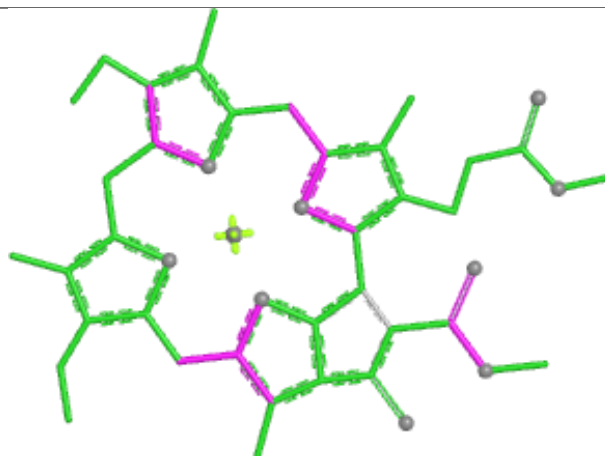
Ligand BCR G 4001



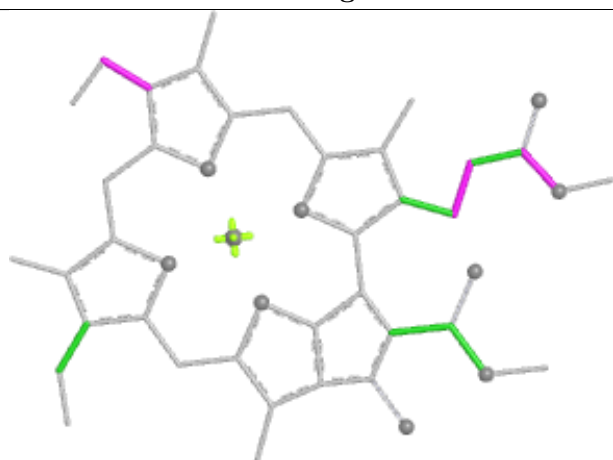
Ligand CLA 2 622



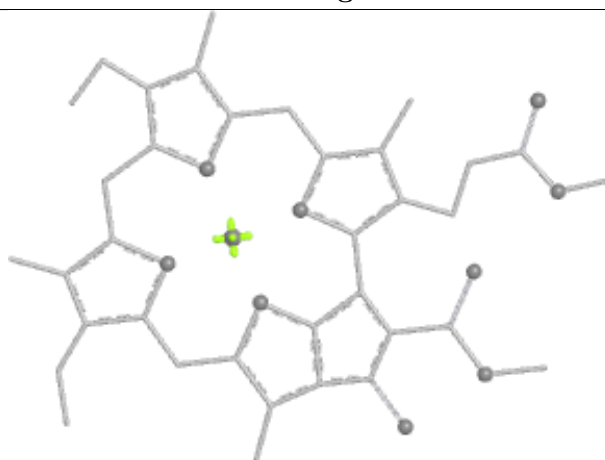
Bond lengths



Bond angles

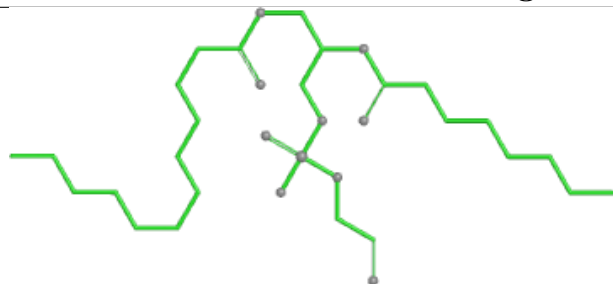


Torsions

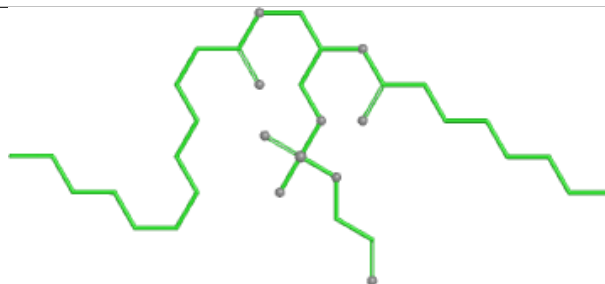


Rings

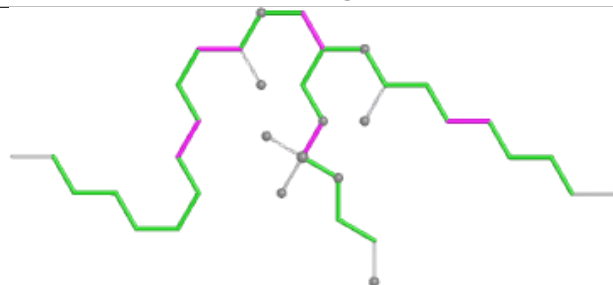
Ligand PTY 1 623



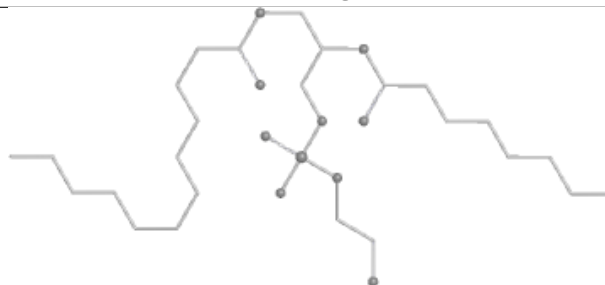
Bond lengths



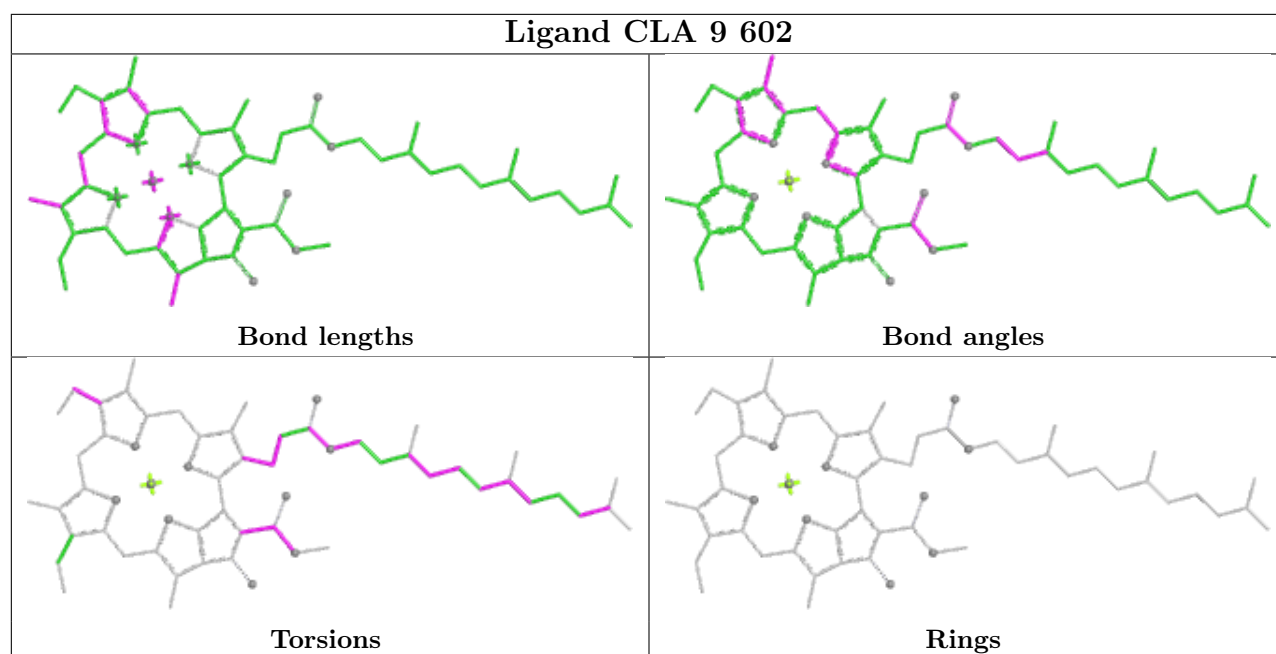
Bond angles

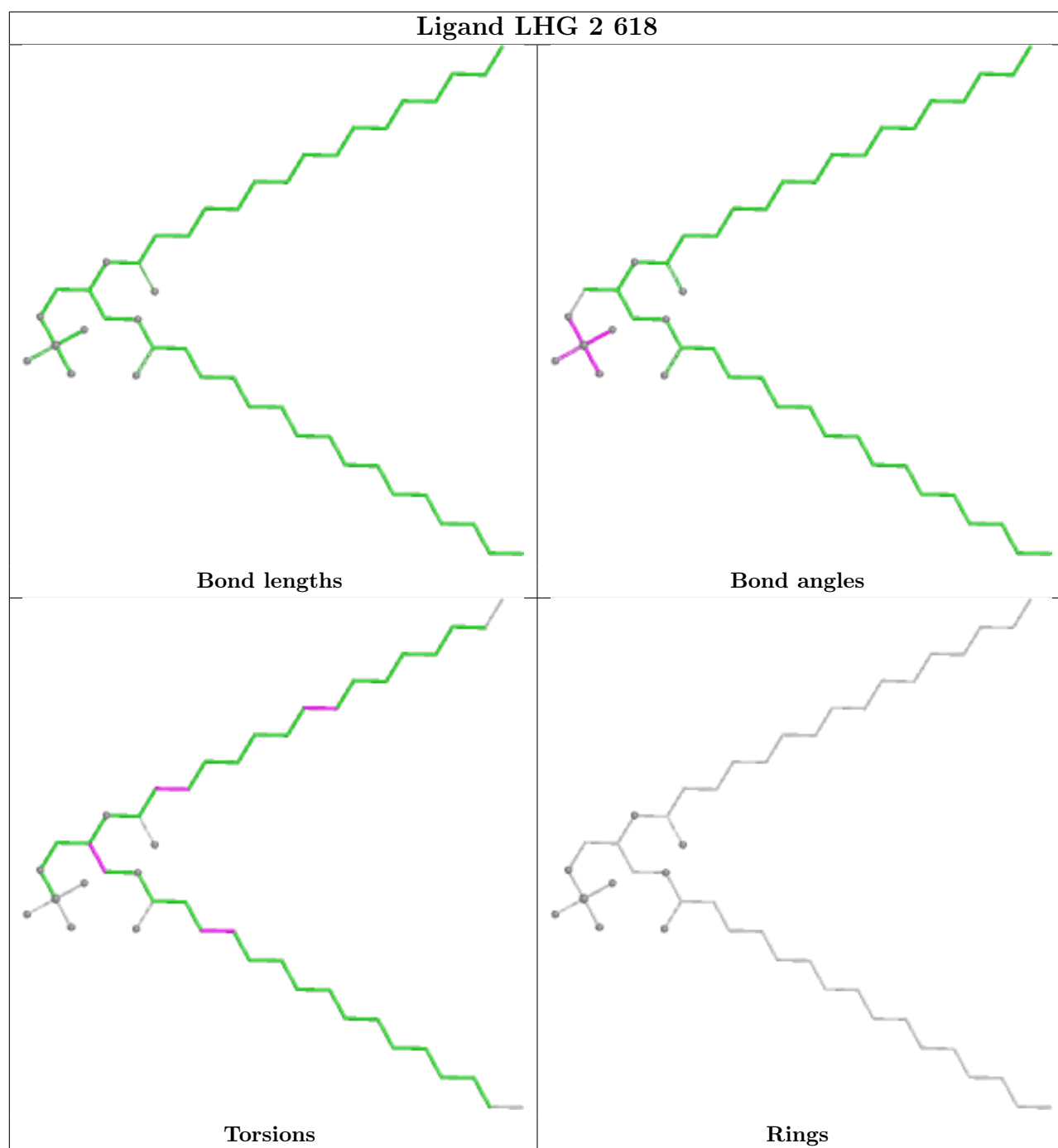


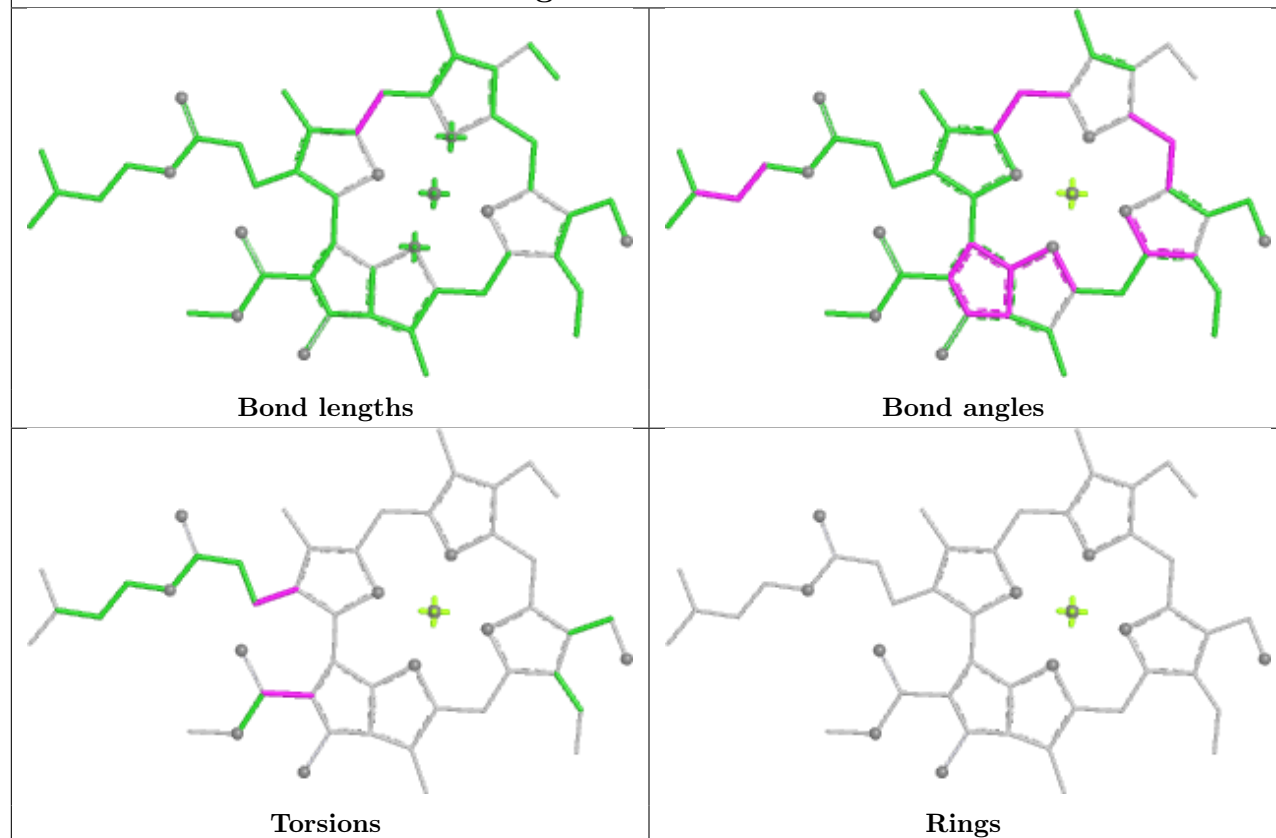
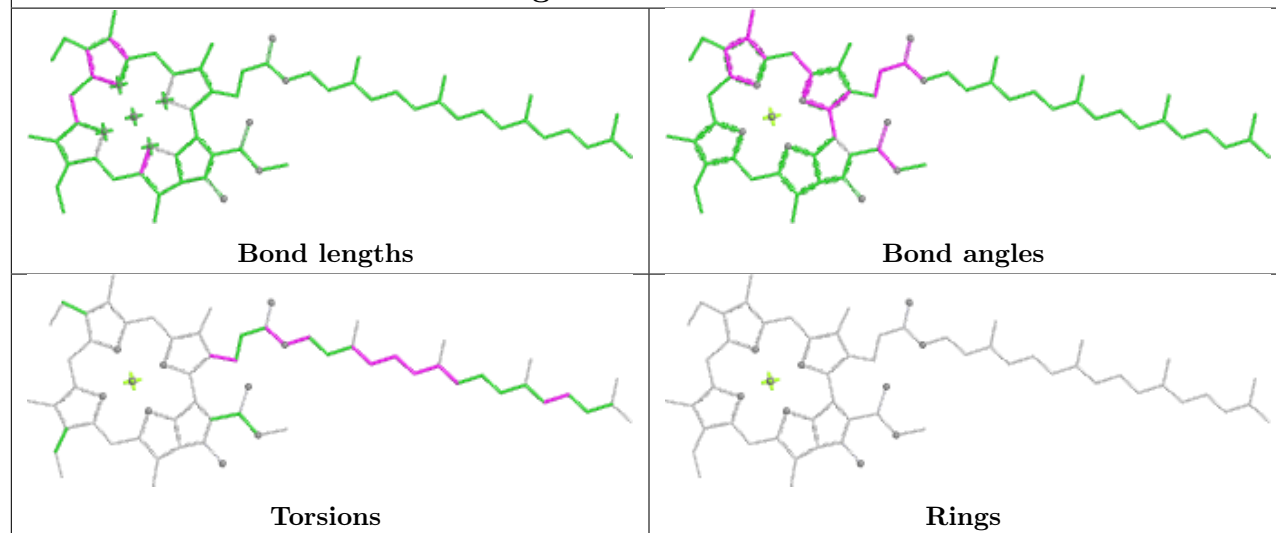
Torsions



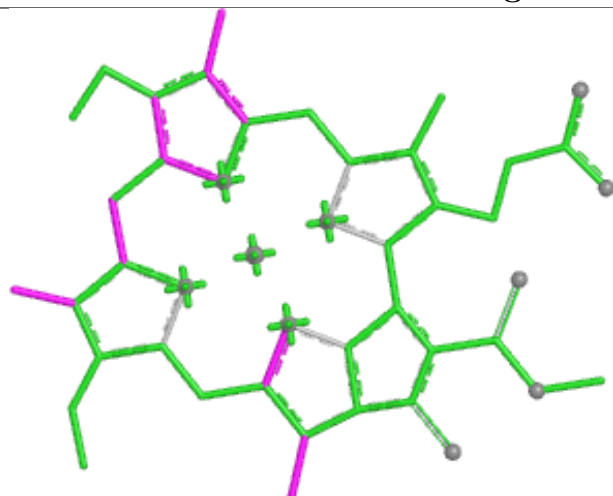
Rings



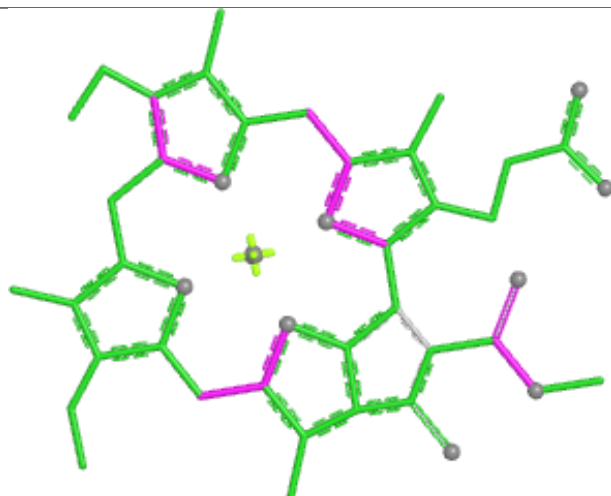


Ligand CHL 1 601**Ligand CLA B 833**

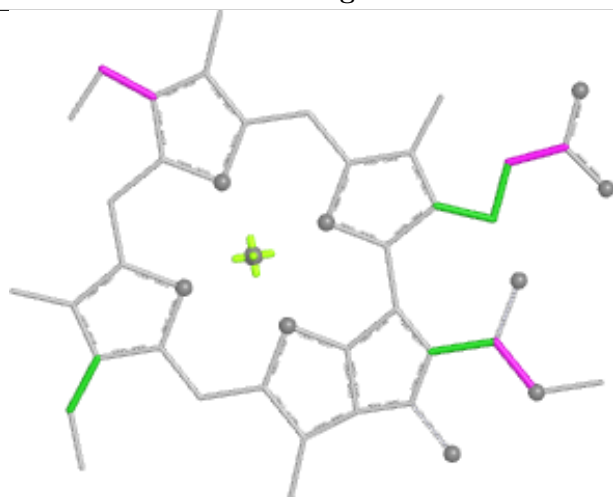
Ligand CLA G 4004



Bond lengths



Bond angles

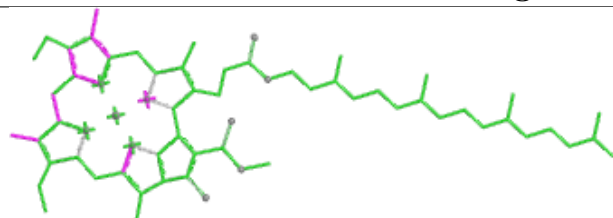


Torsions

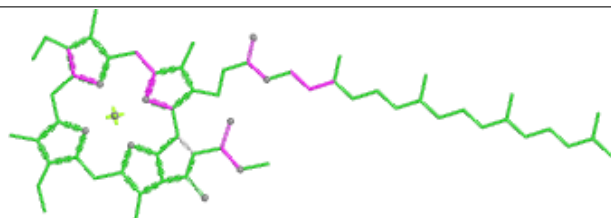


Rings

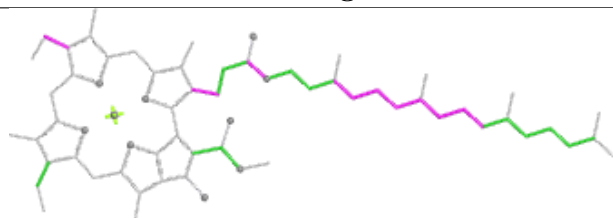
Ligand CLA A 830



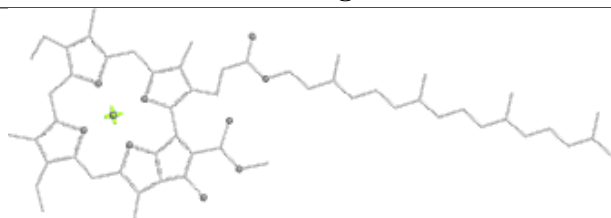
Bond lengths



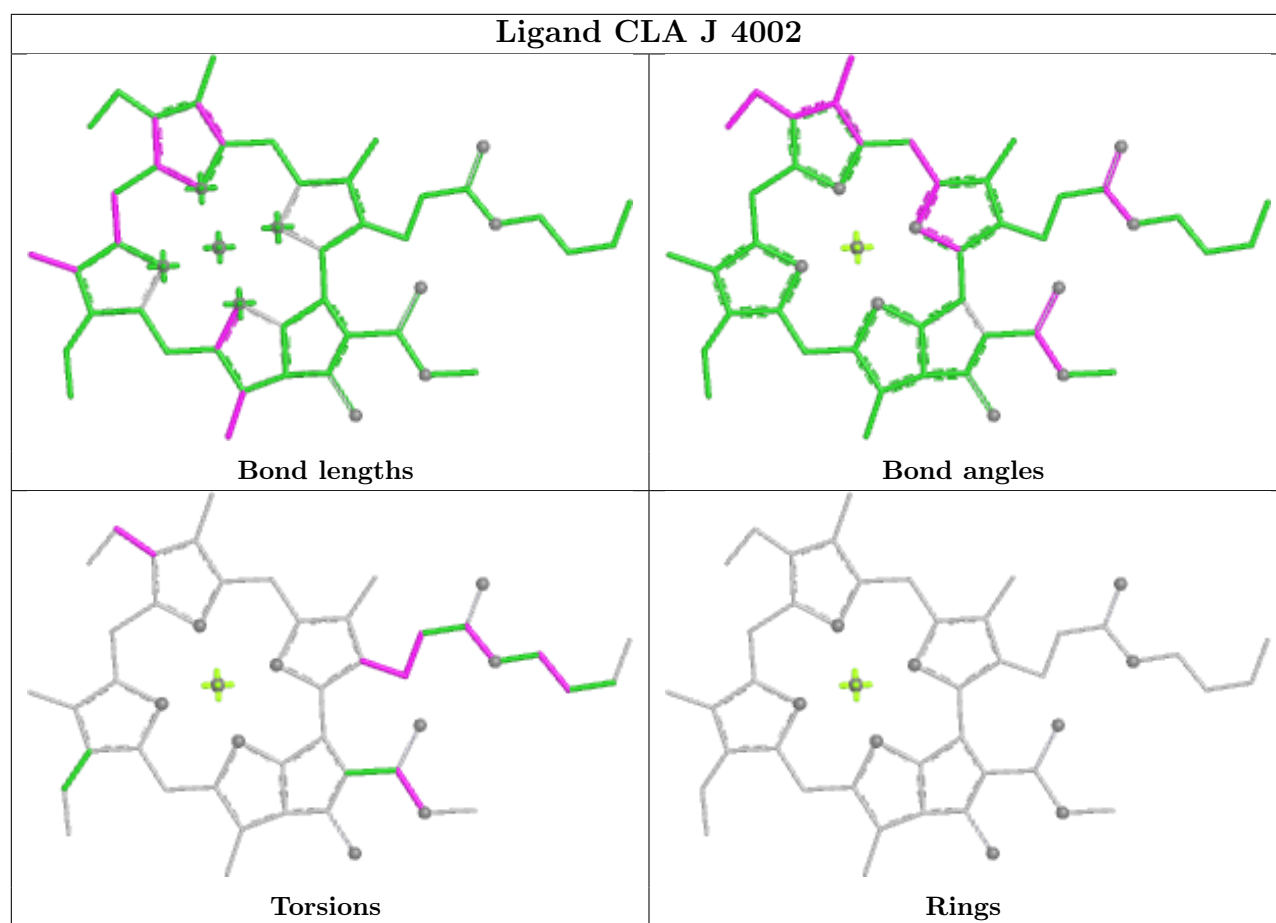
Bond angles



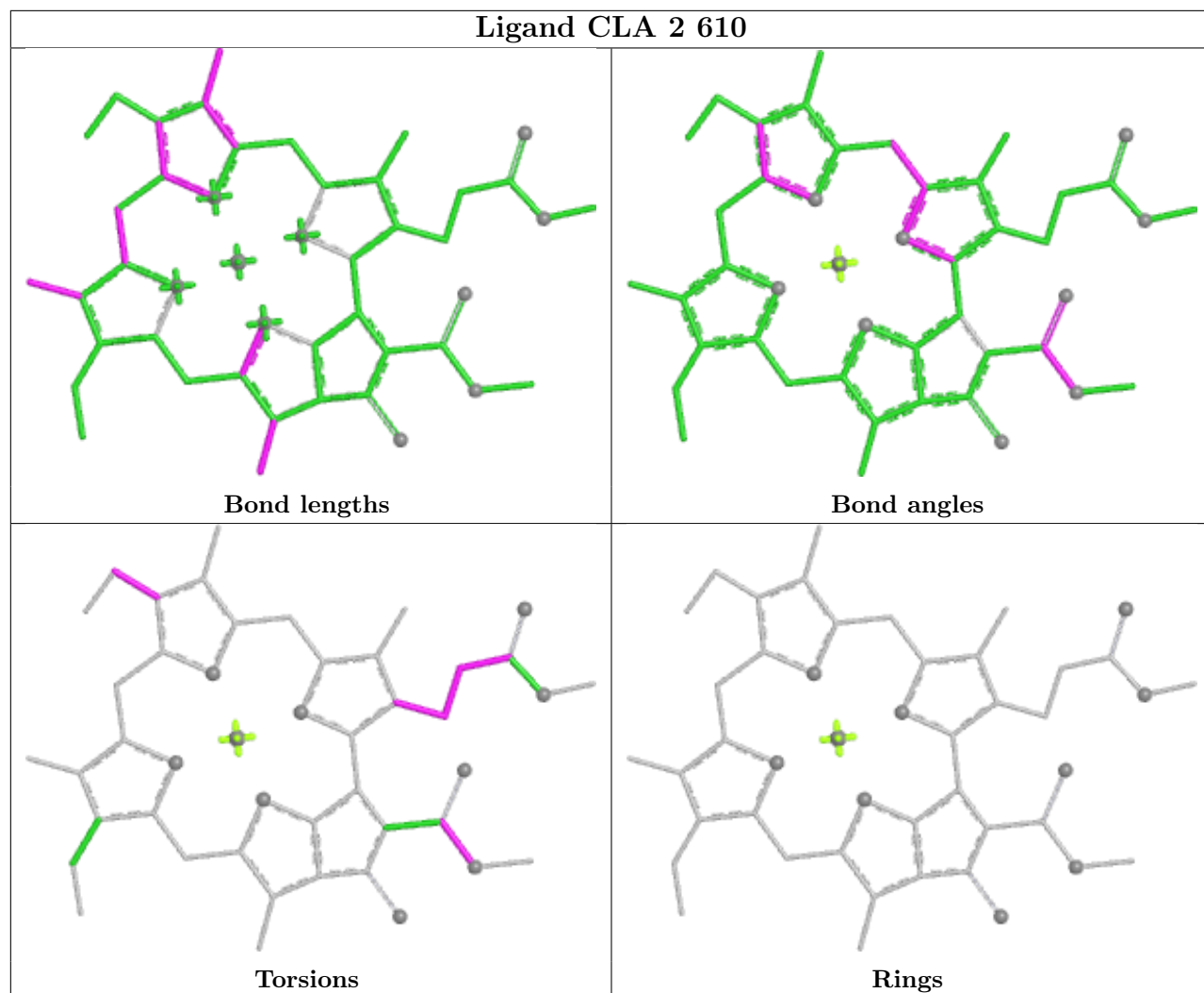
Torsions



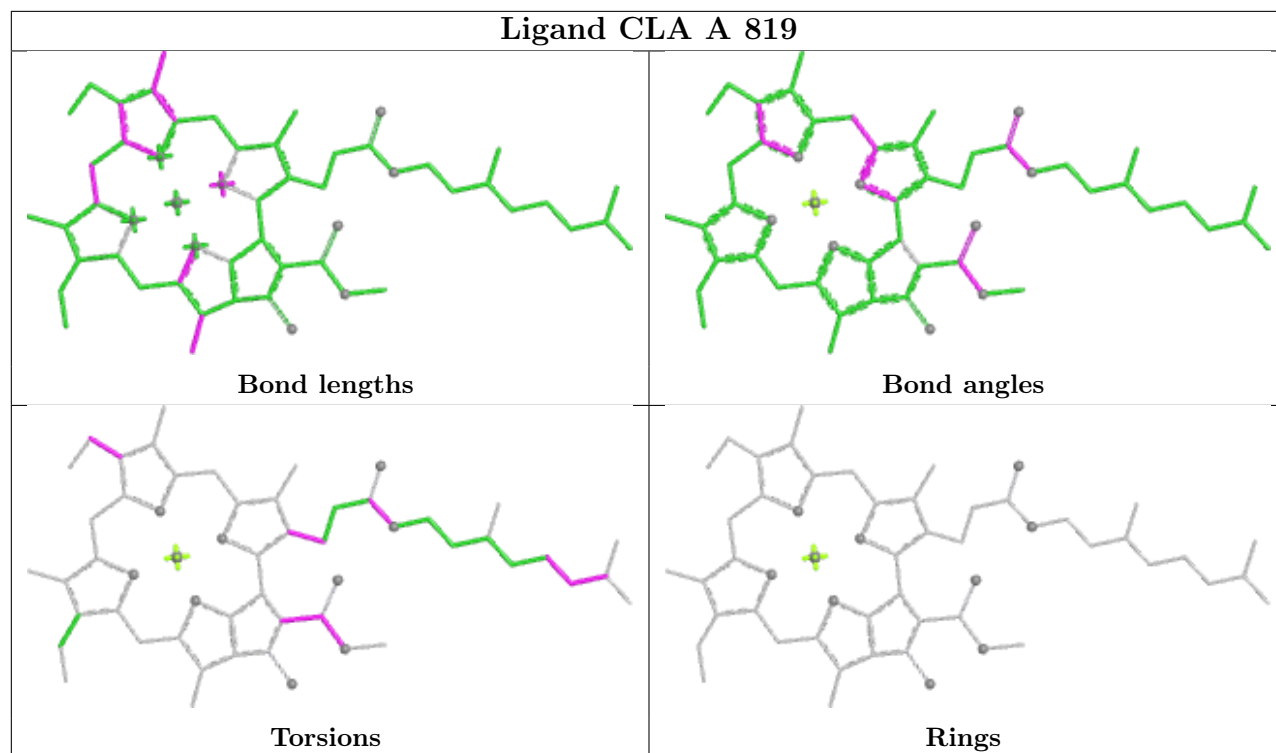
Rings



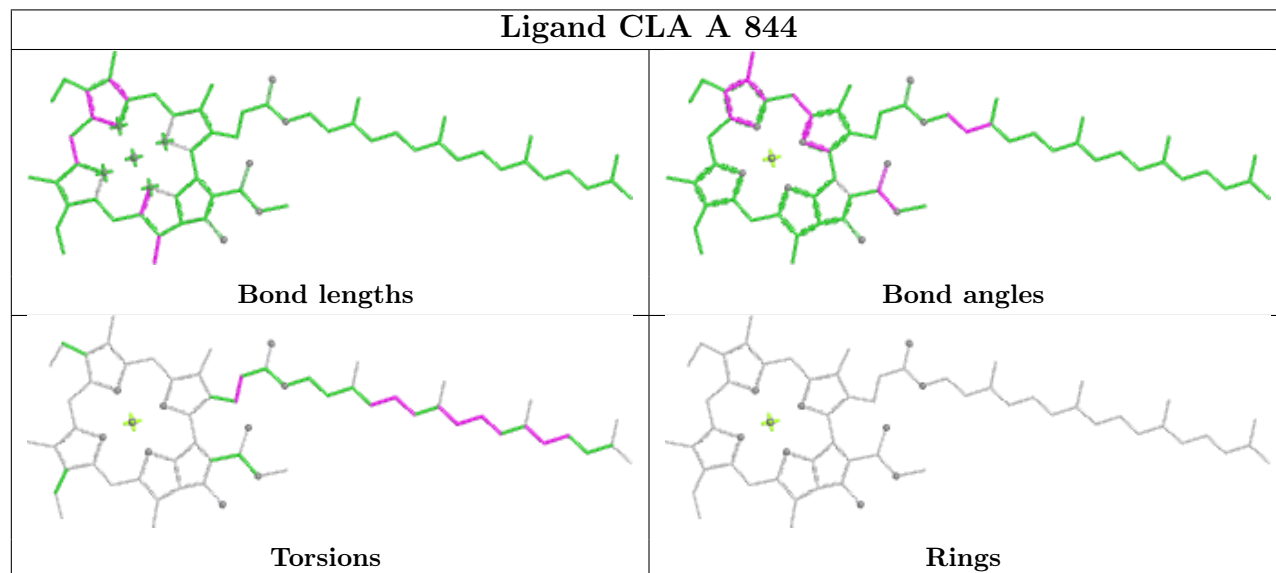
Ligand CLA 2 610

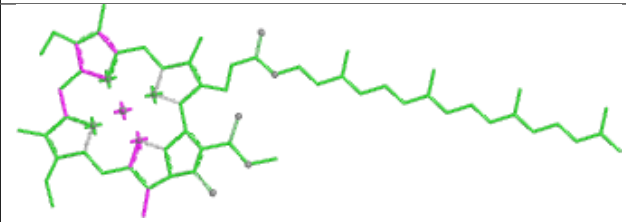
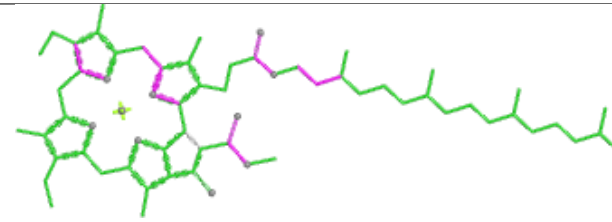
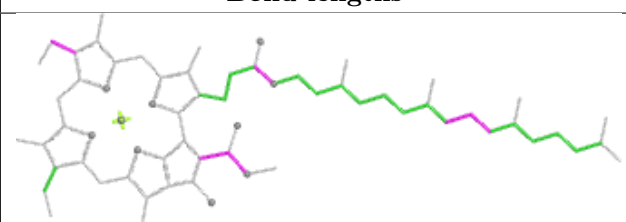
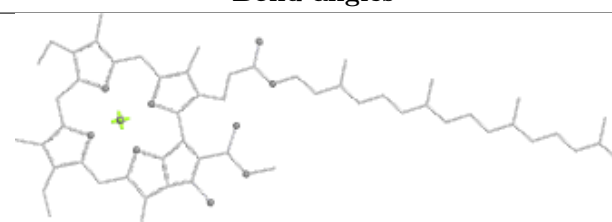


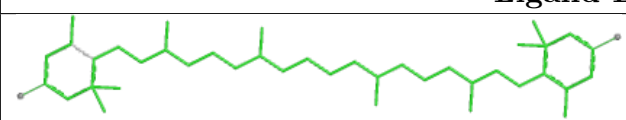
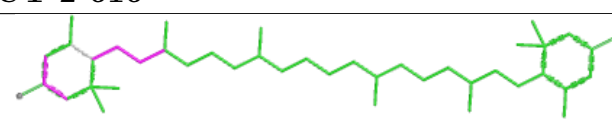
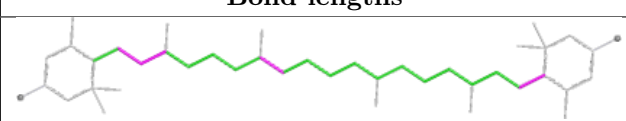
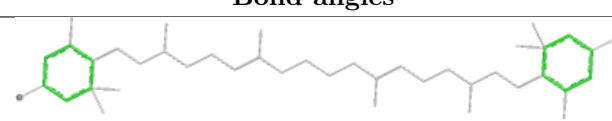
Ligand CLA A 819

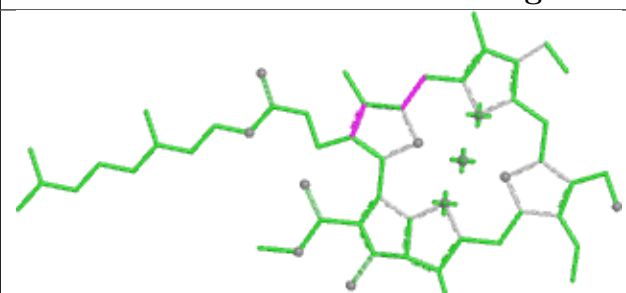
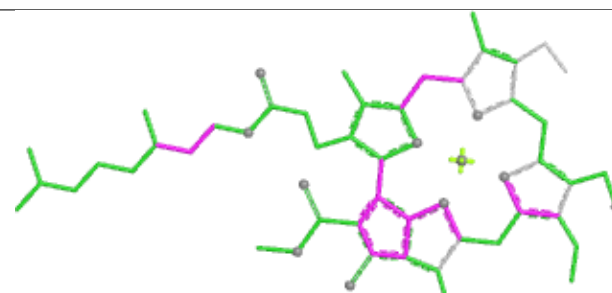
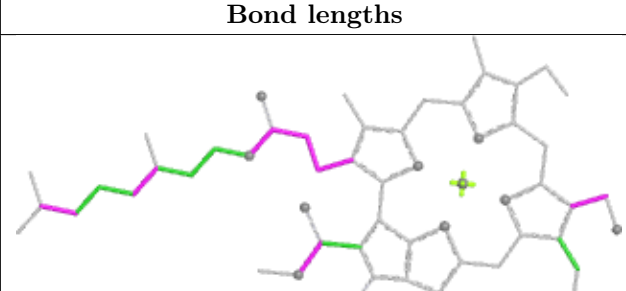
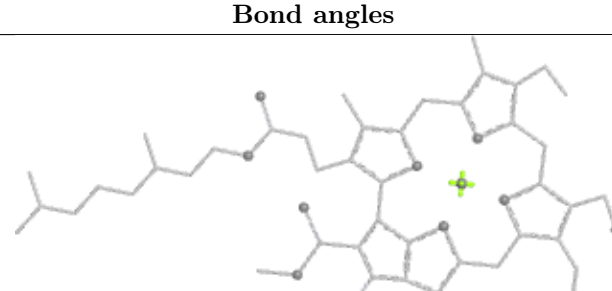


Ligand CLA A 844

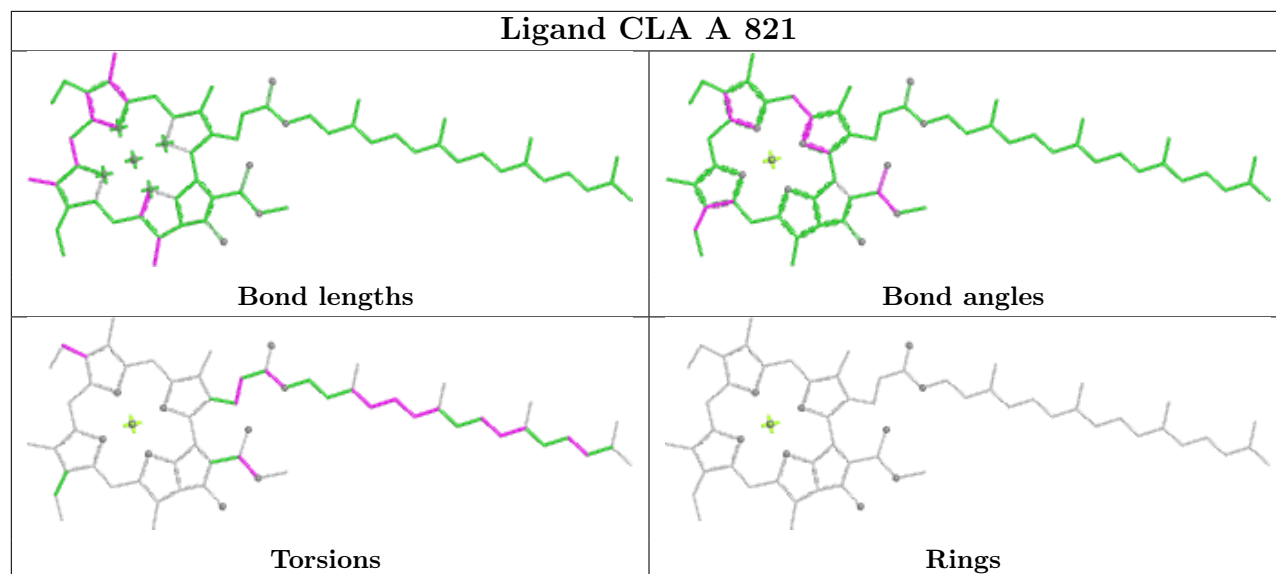


Ligand CLA B 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

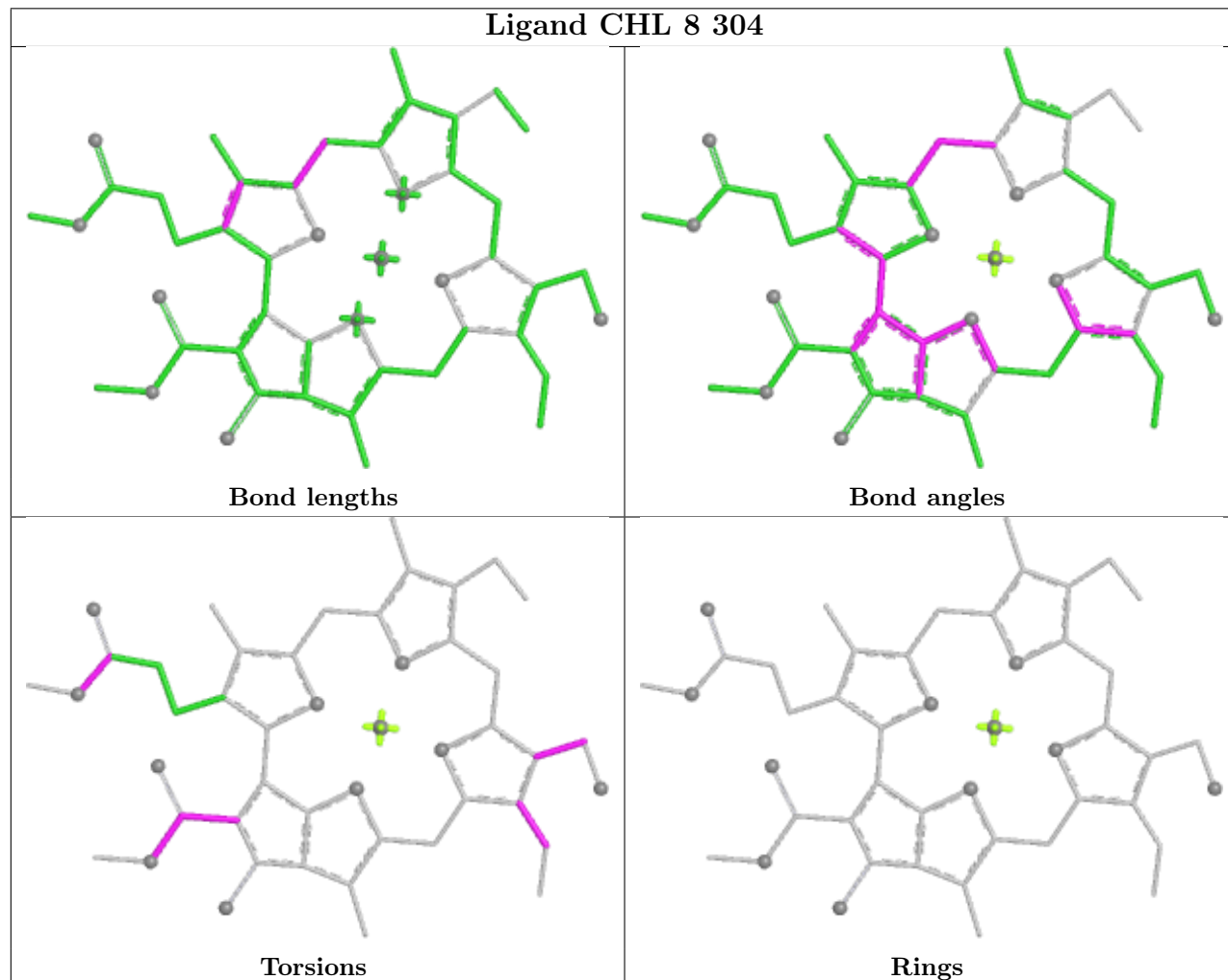
Ligand LUT 2 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 3 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

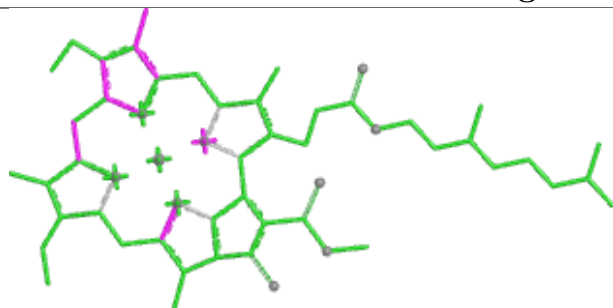
Ligand CLA A 821



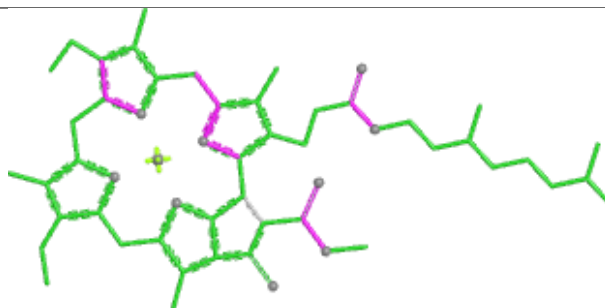
Ligand CHL 8 304



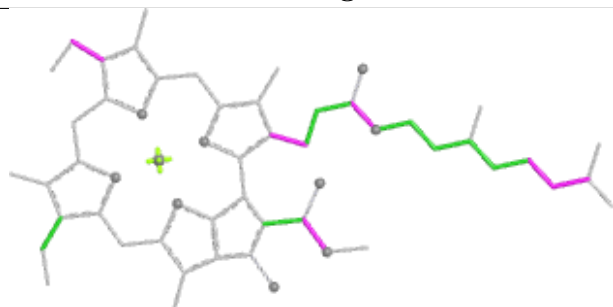
Ligand CLA 7 304



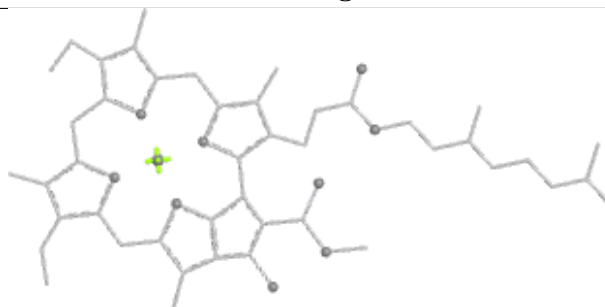
Bond lengths



Bond angles

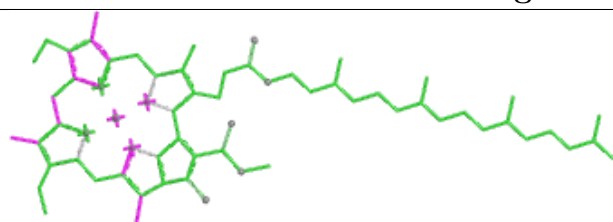


Torsions

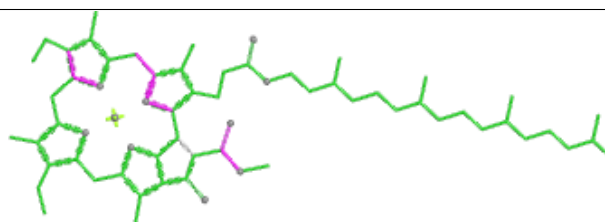


Rings

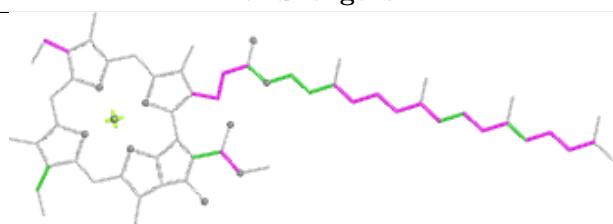
Ligand CLA B 829



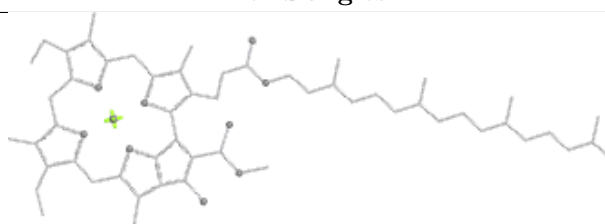
Bond lengths



Bond angles

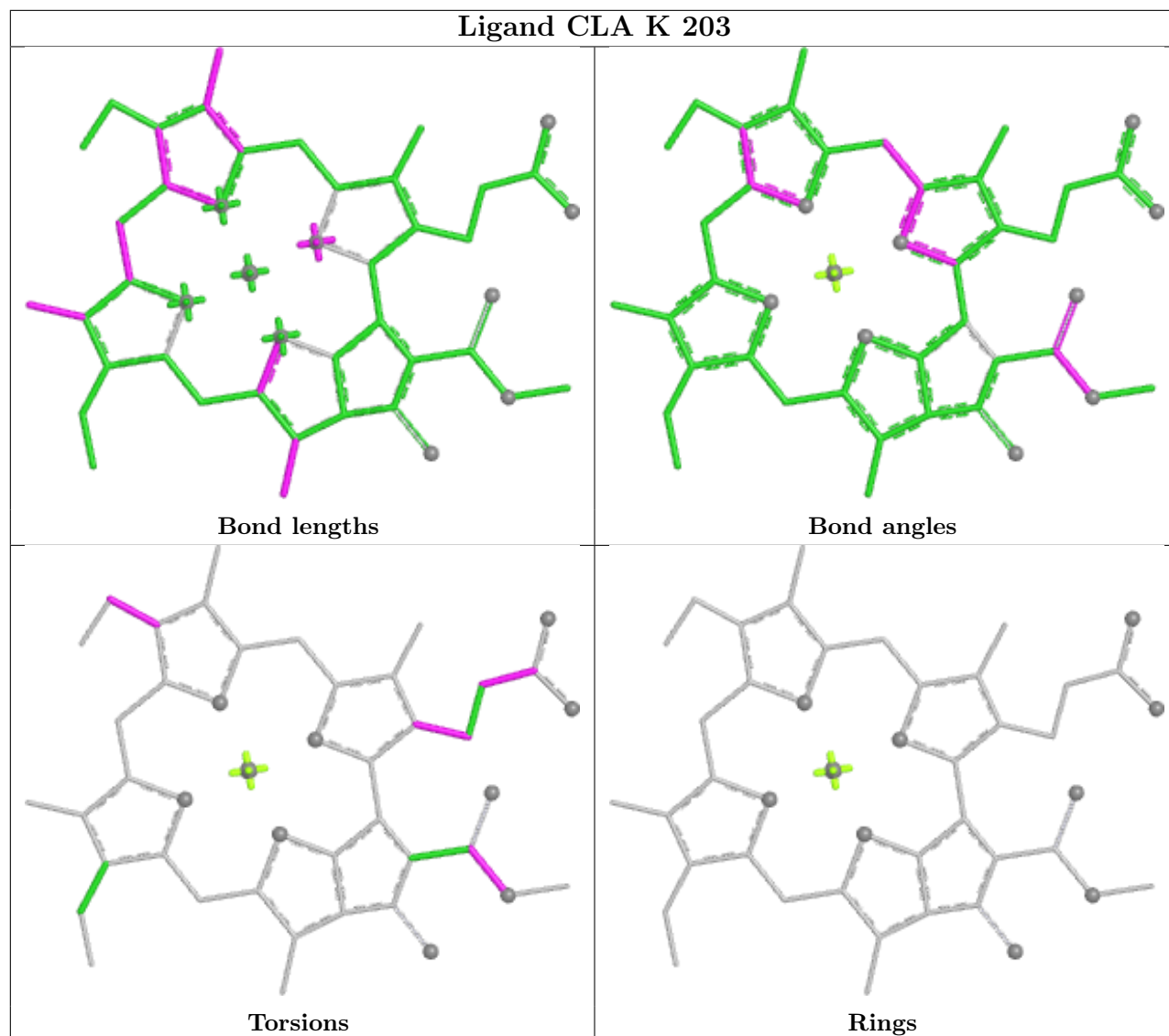


Torsions

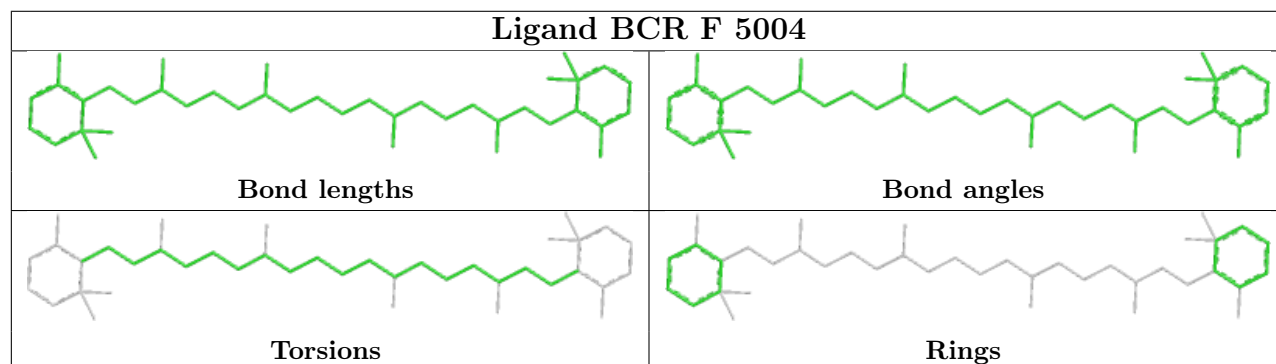


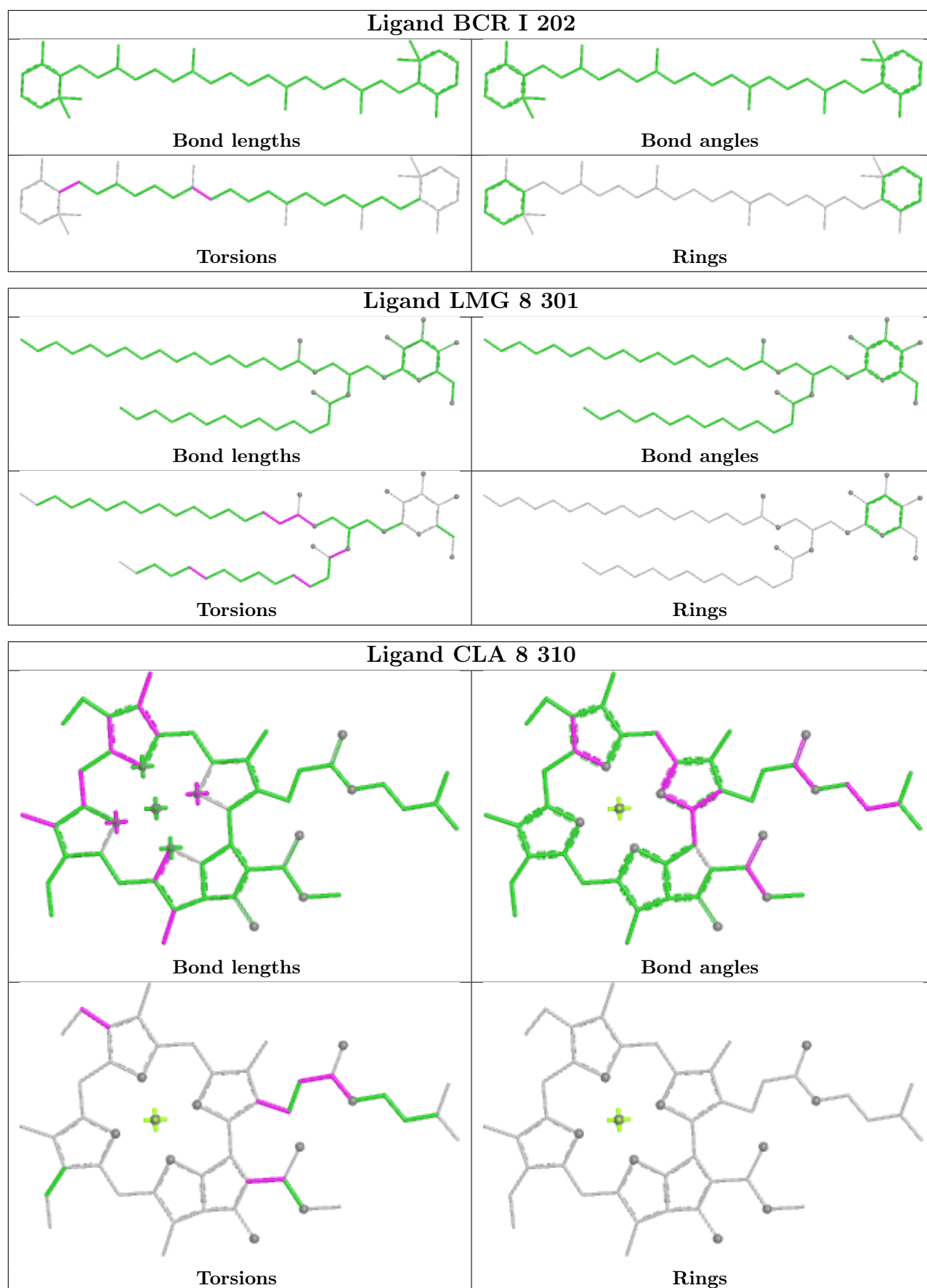
Rings

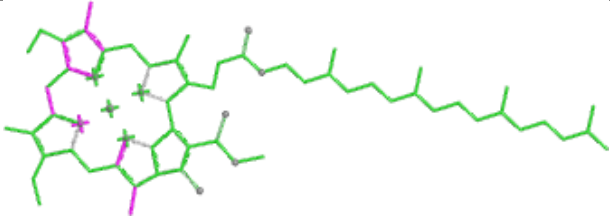
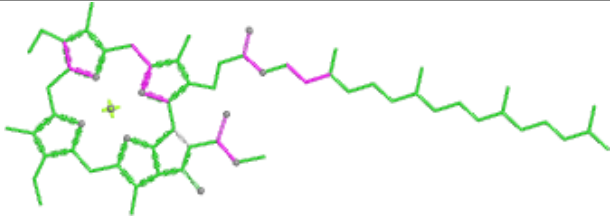
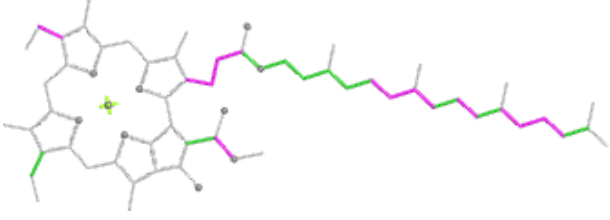
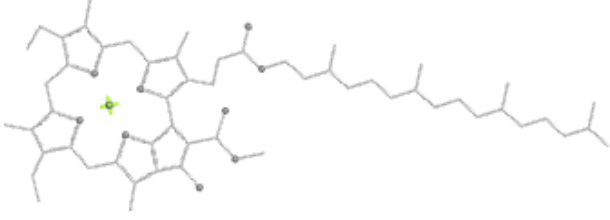
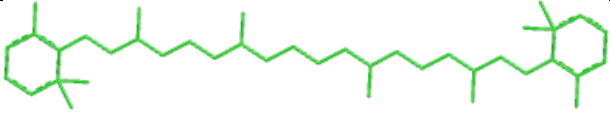
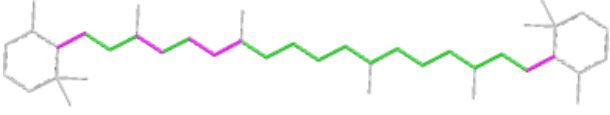
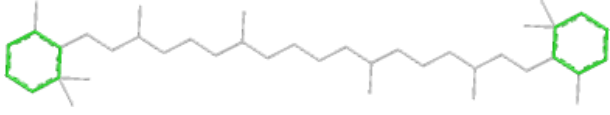
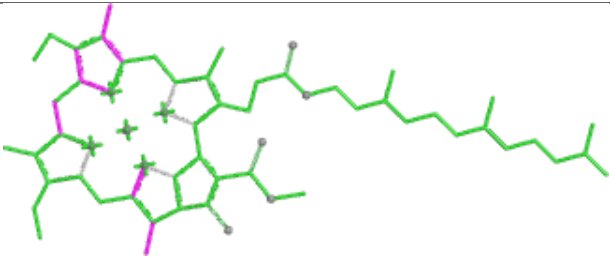
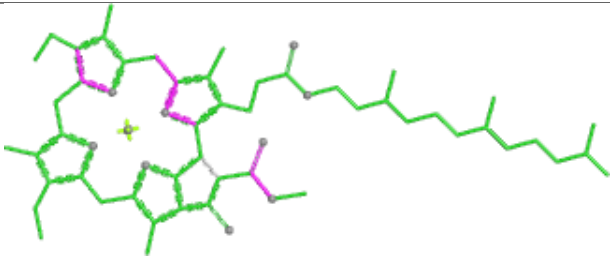
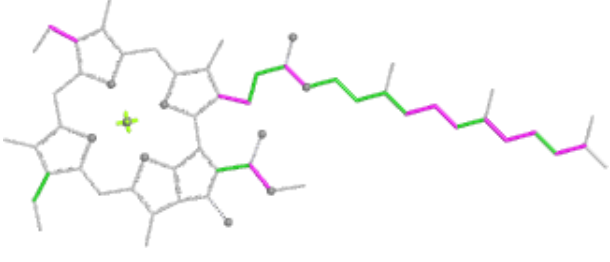
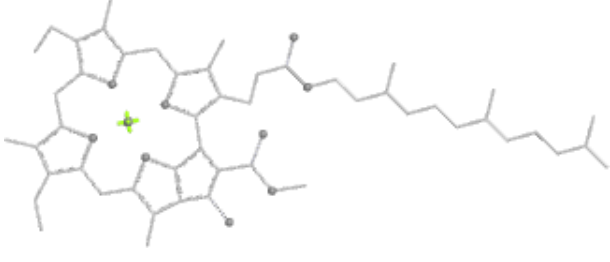
Ligand CLA K 203

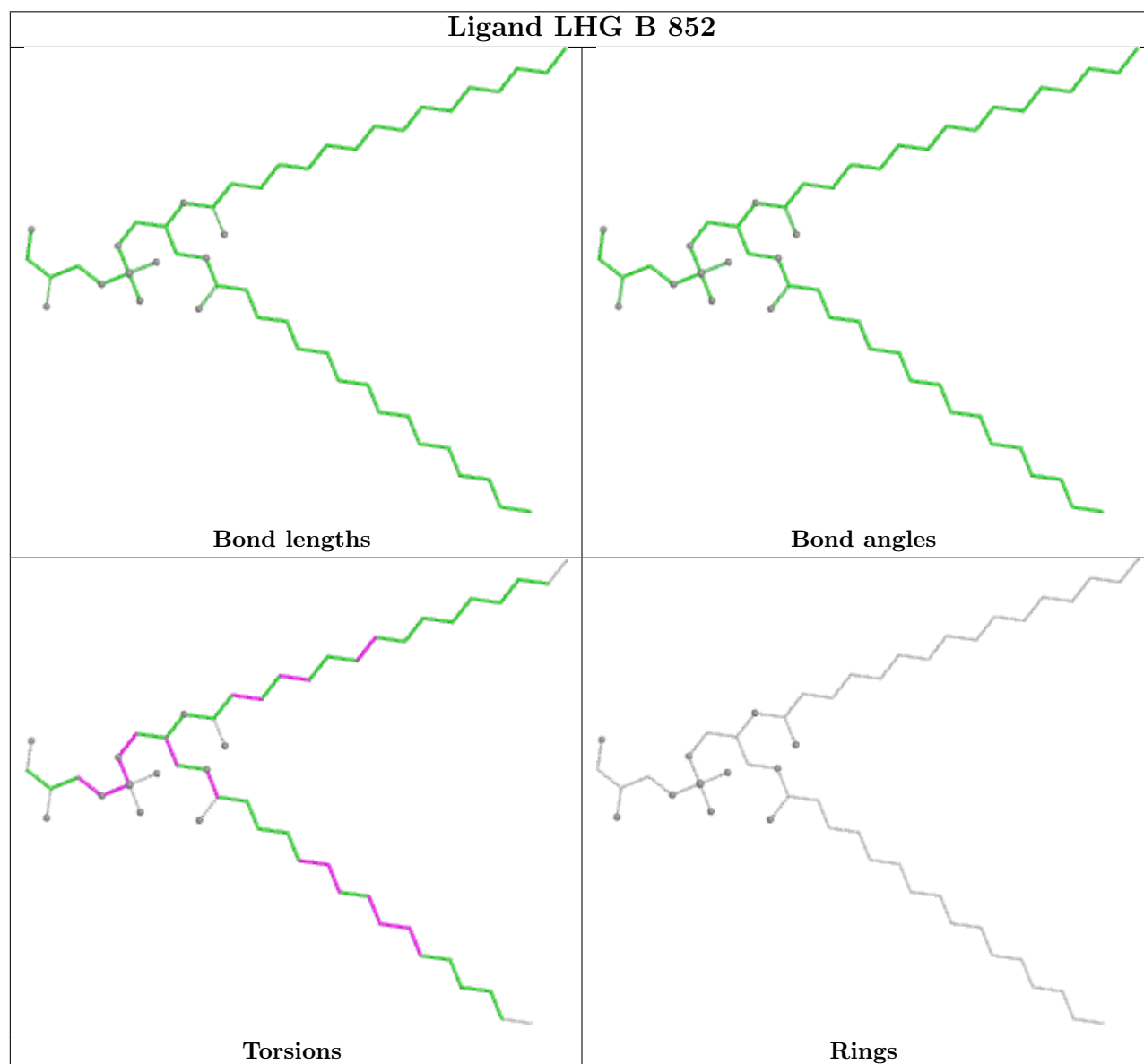
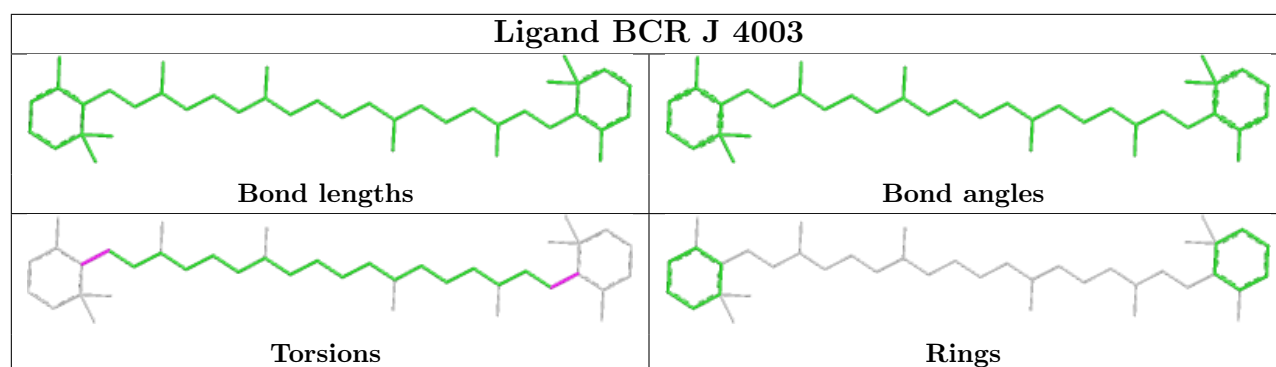


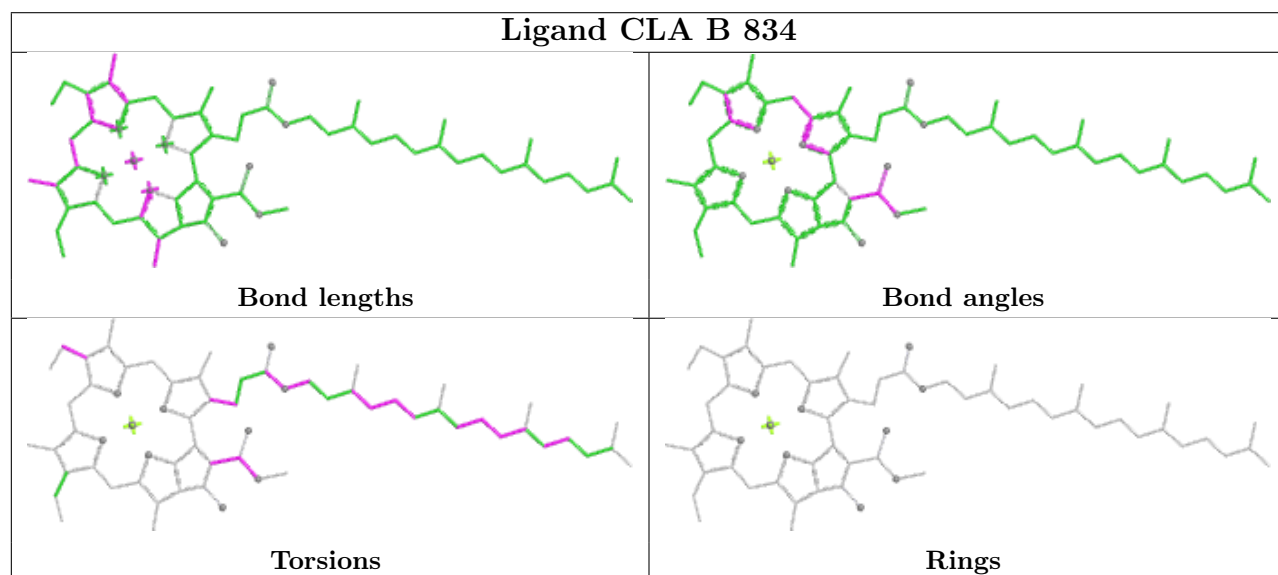
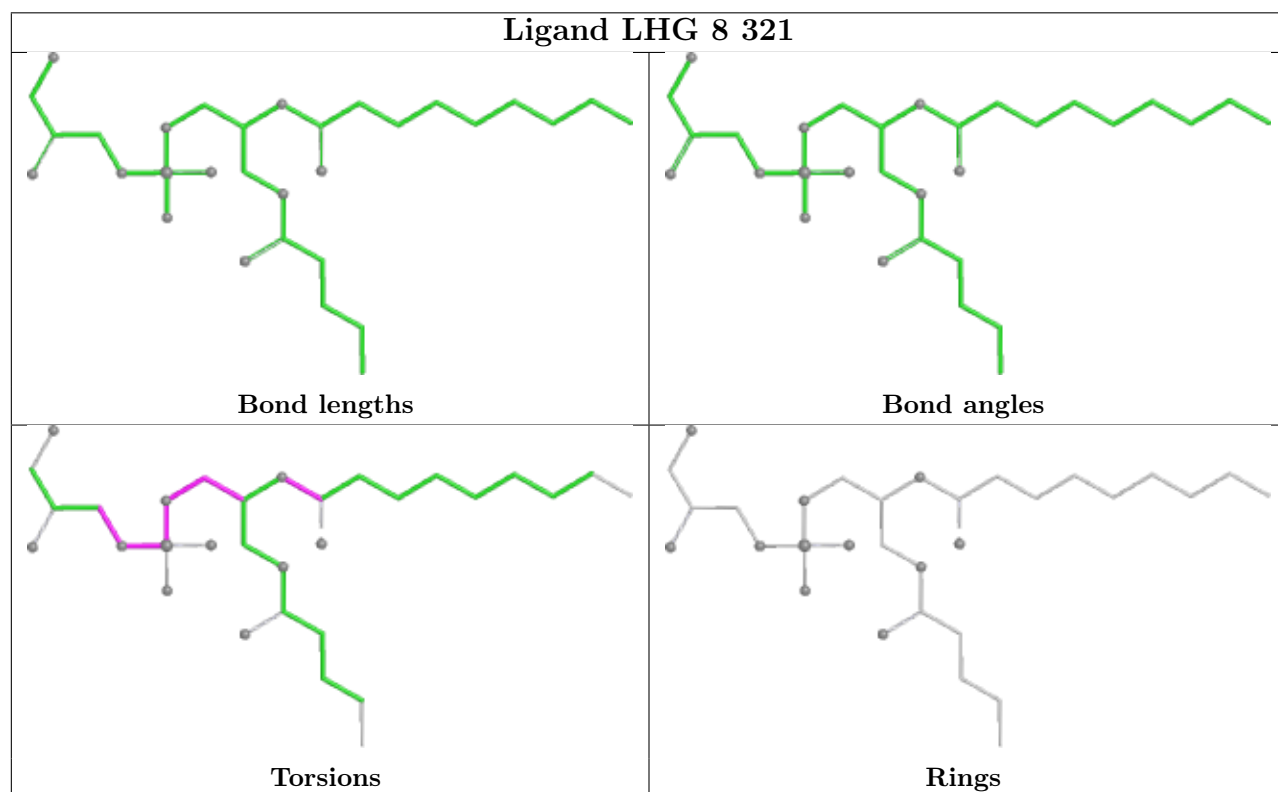
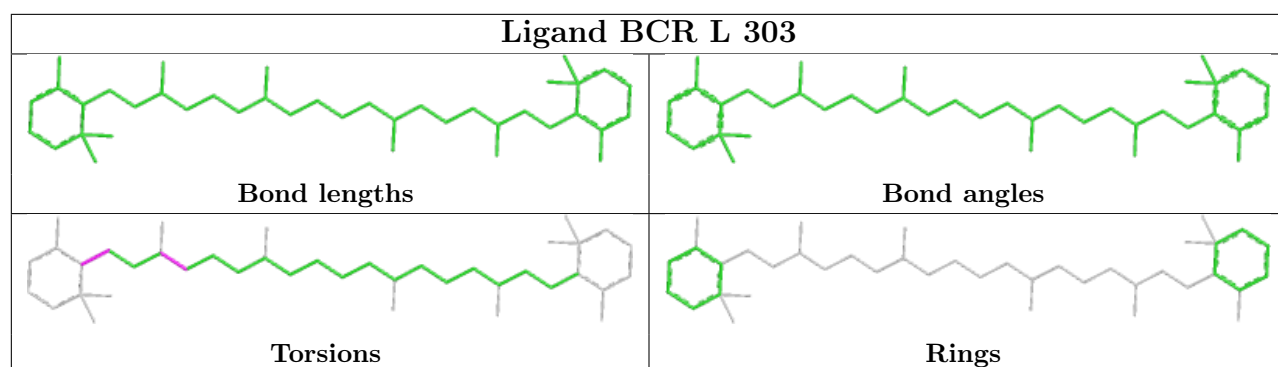
Ligand BCR F 5004

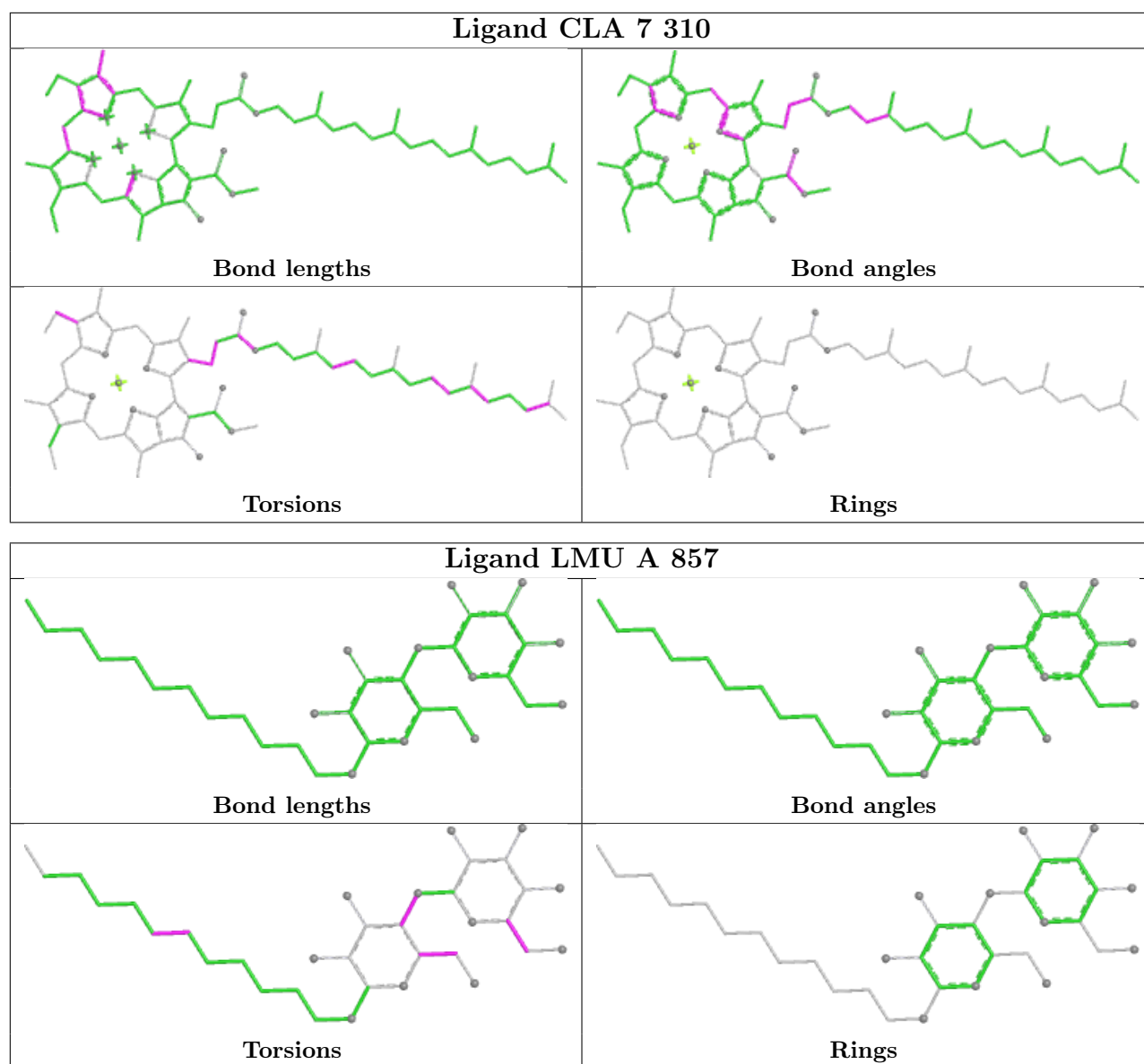




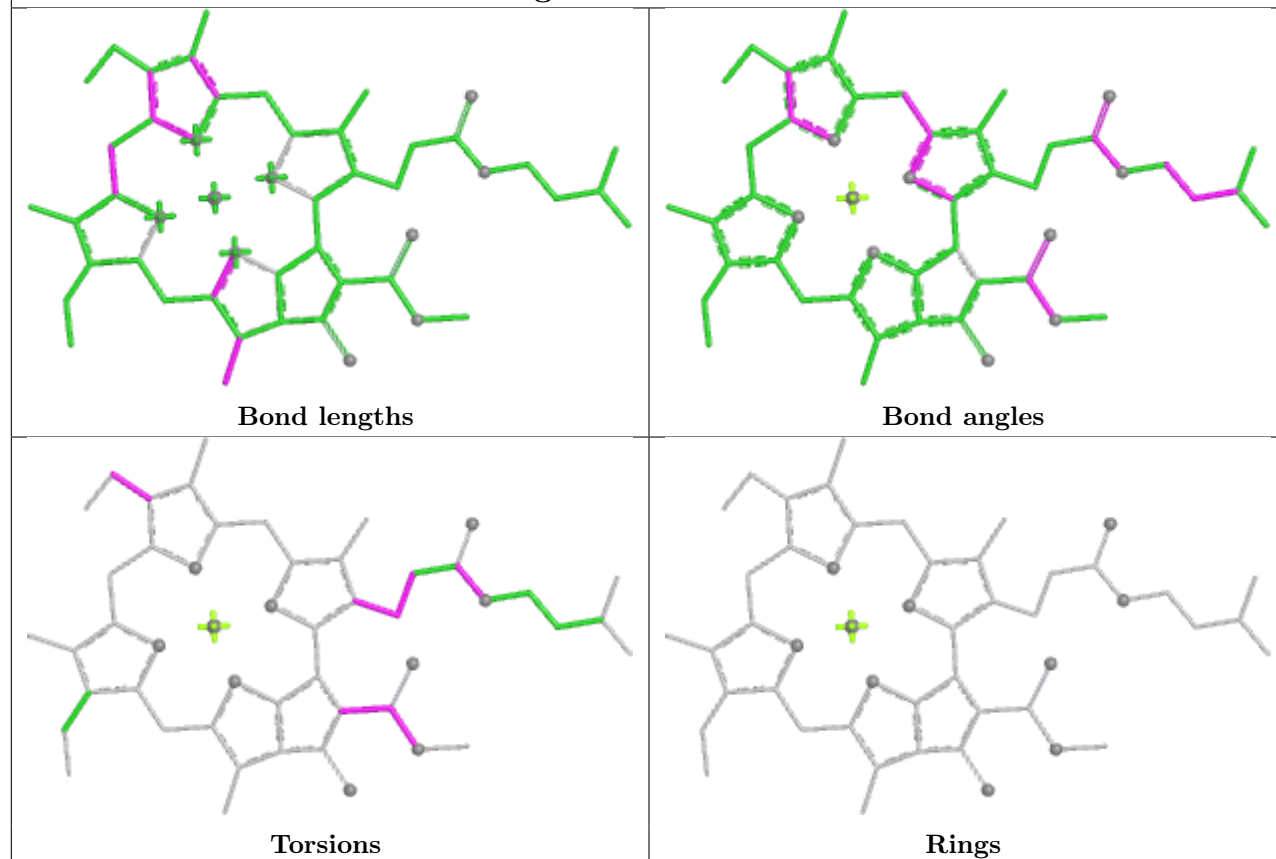
Ligand CLA A 841	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 826	
 Bond lengths	 Bond angles
 Torsions	 Rings



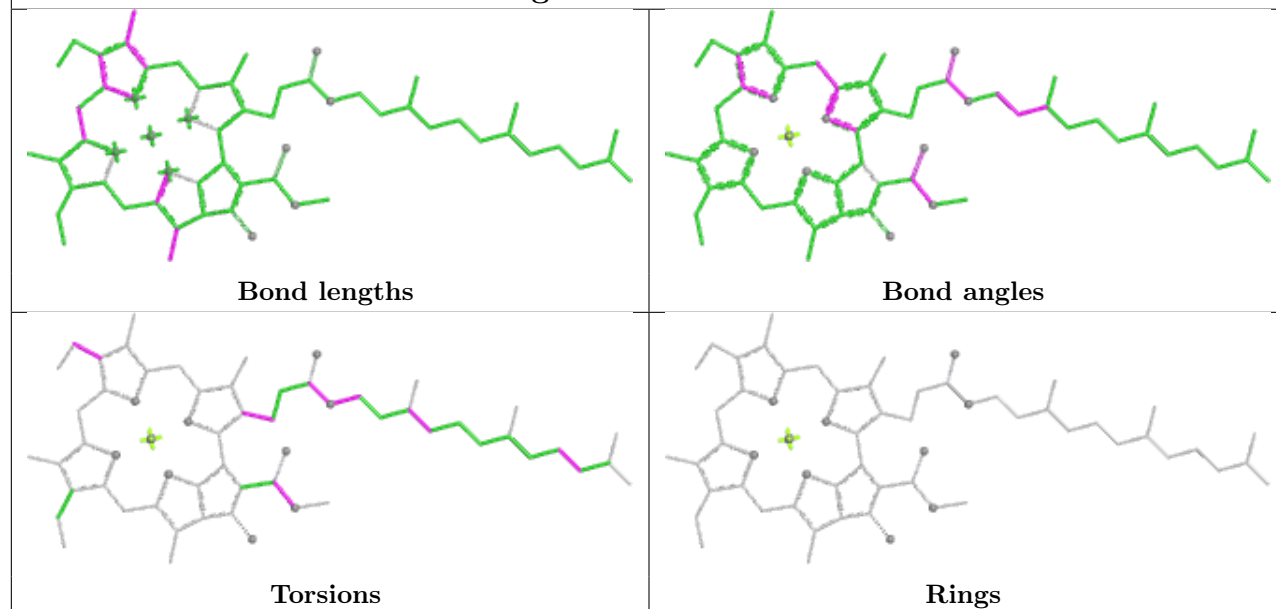


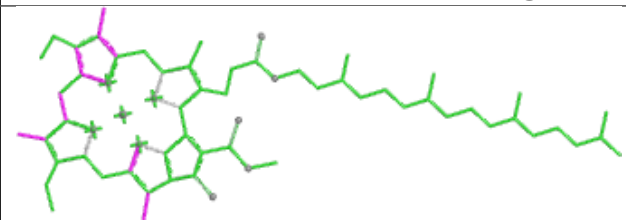
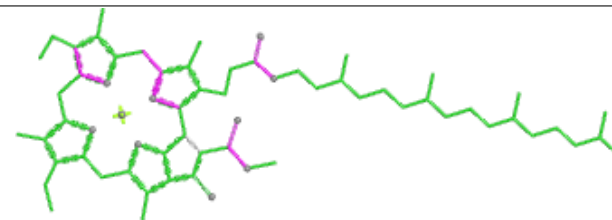
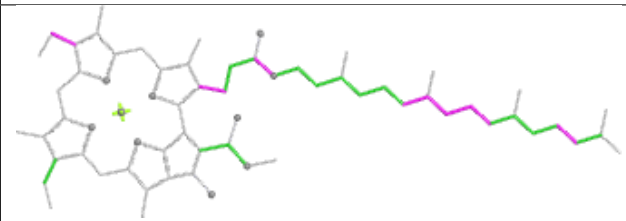
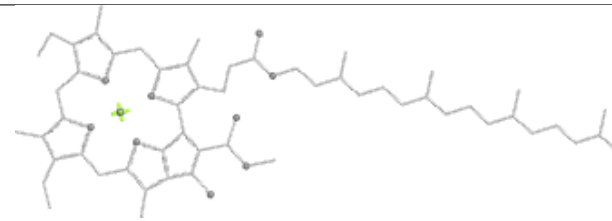
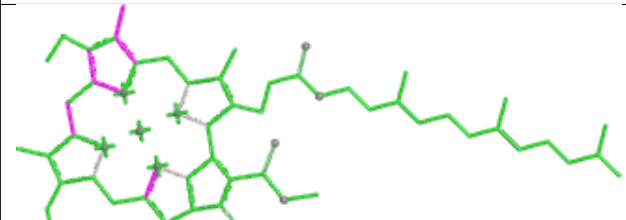
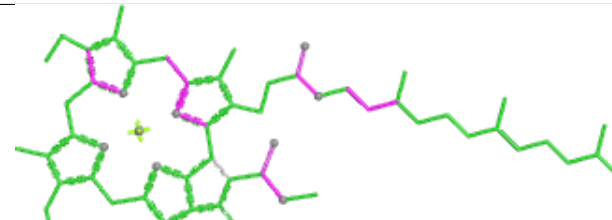
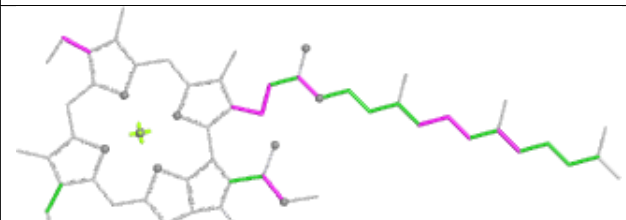
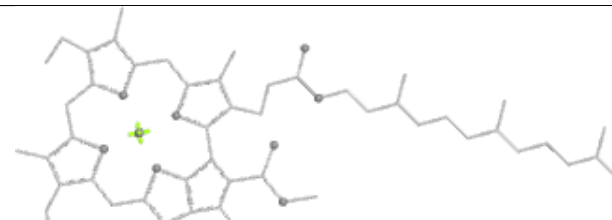
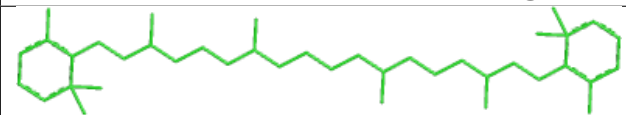
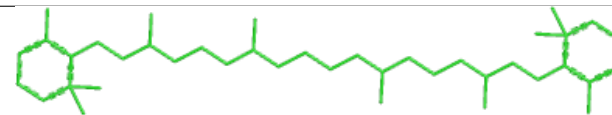
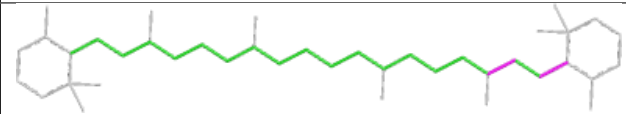
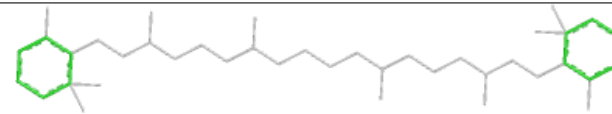


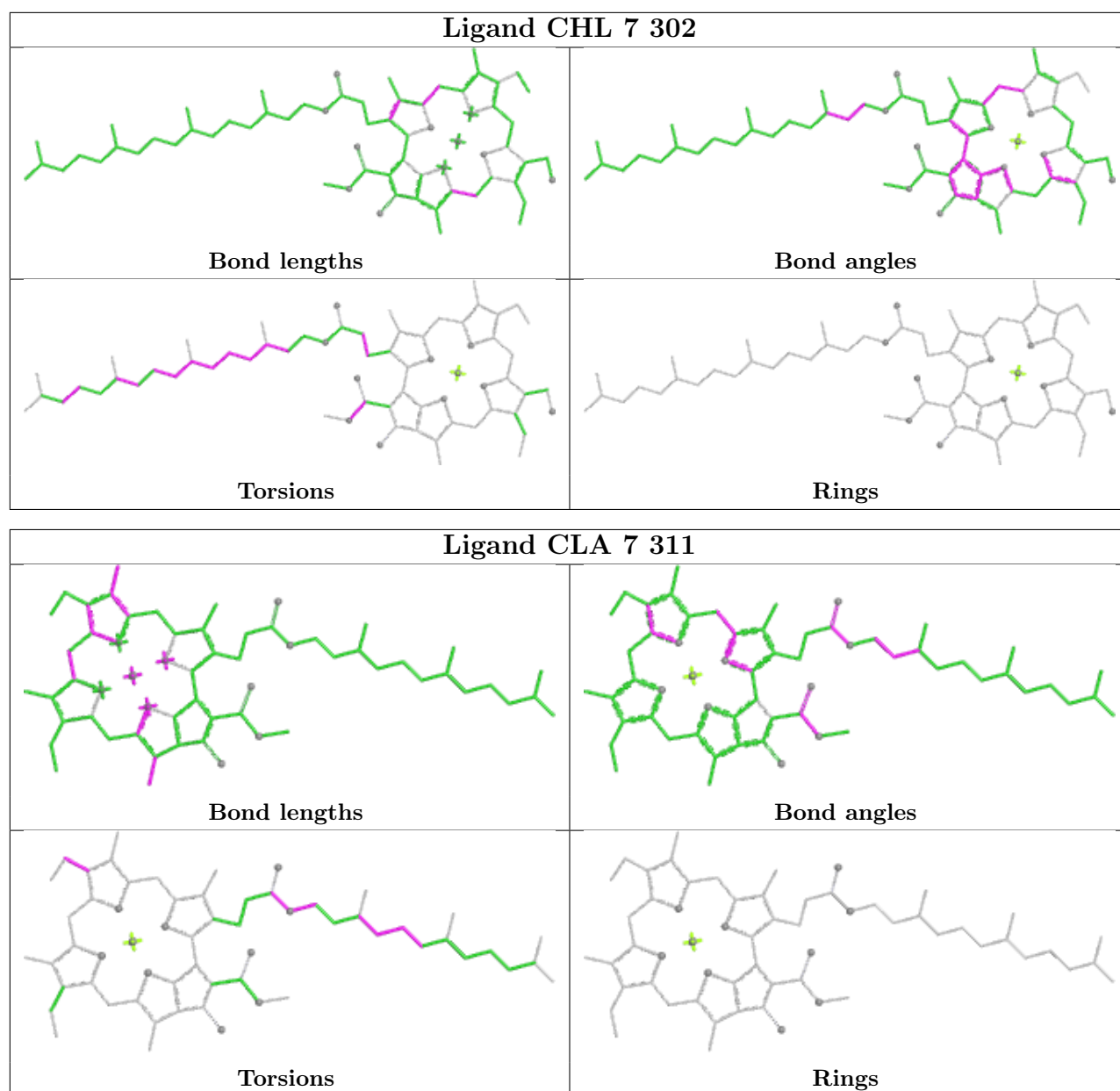
Ligand CLA L 307

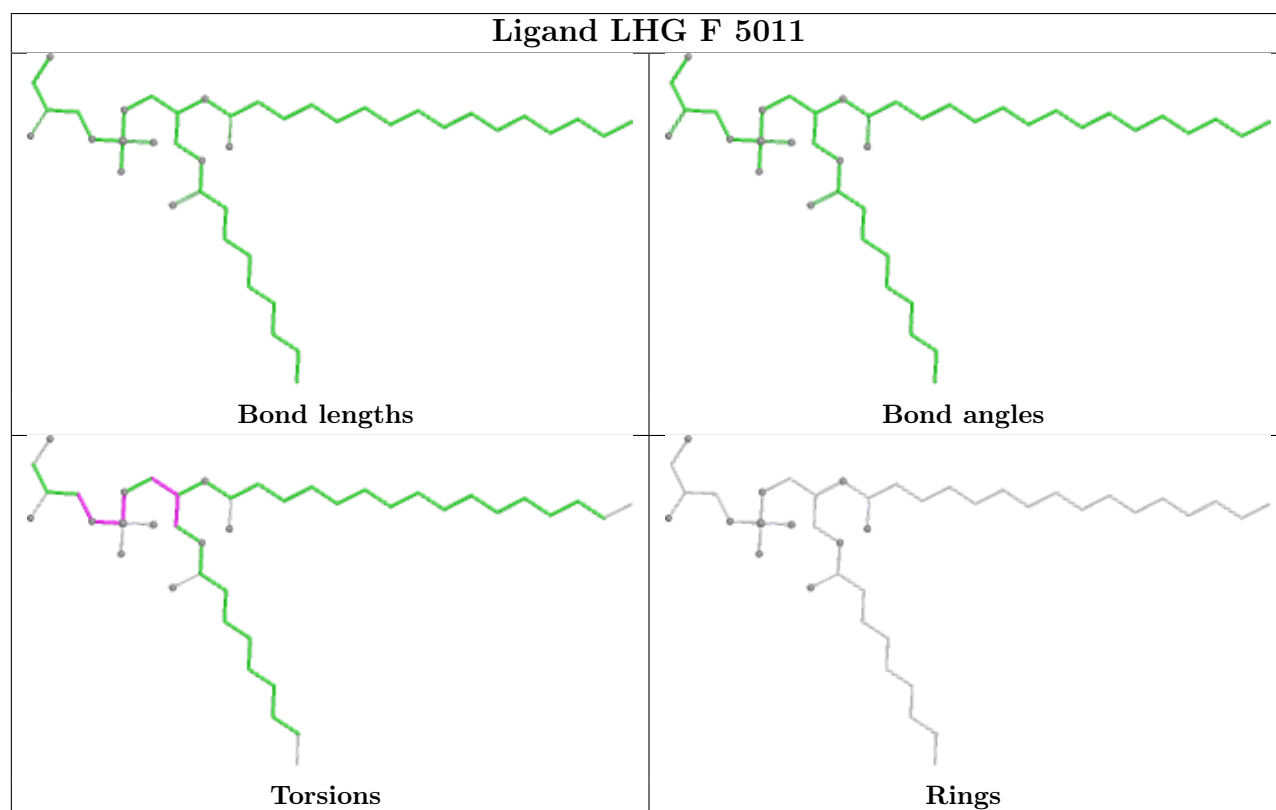
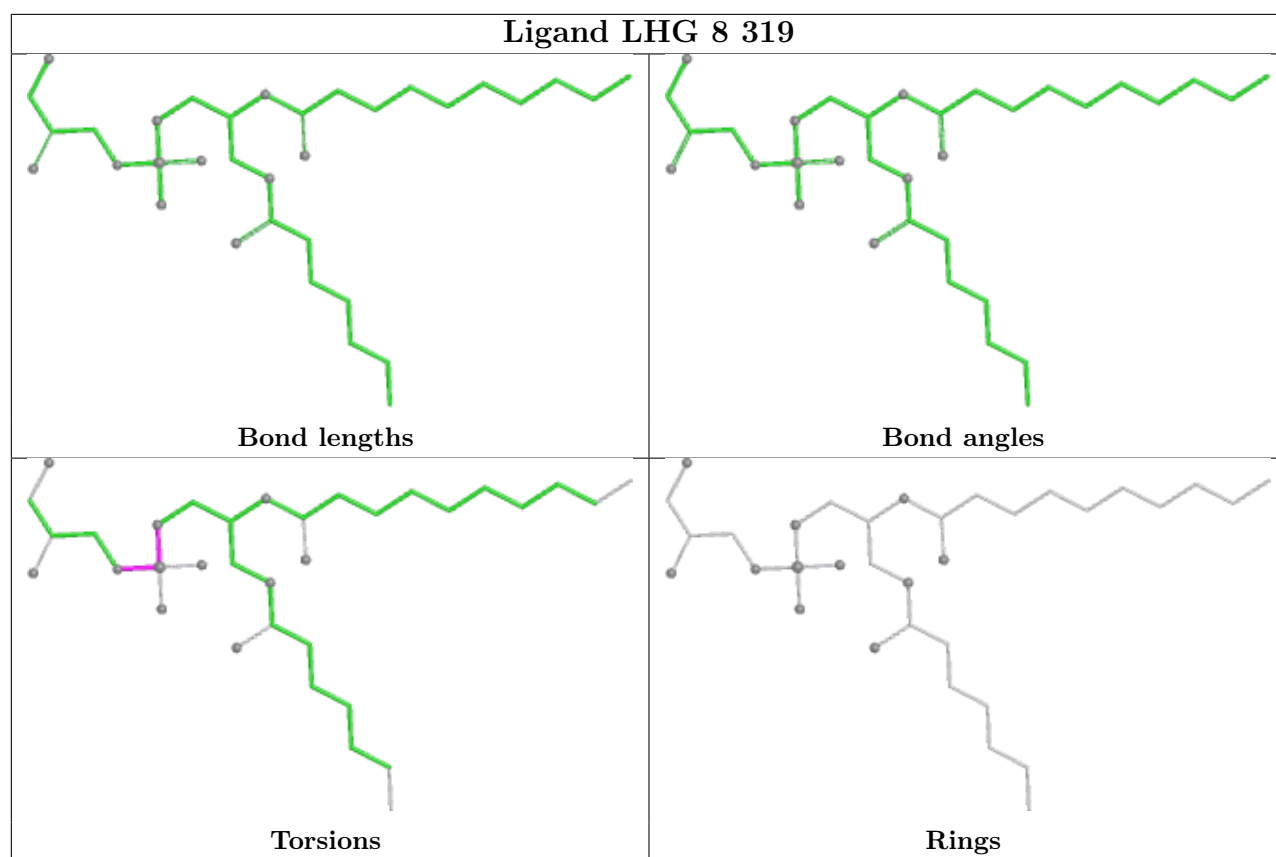


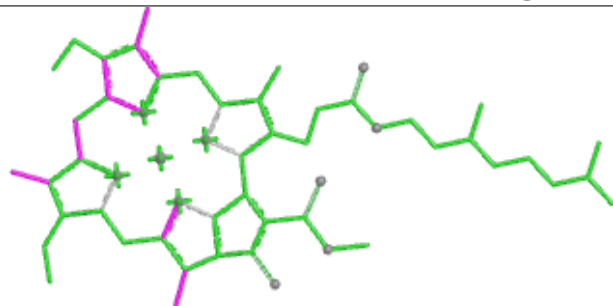
Ligand CLA A 840



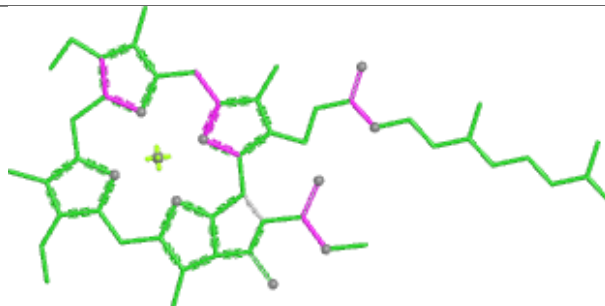
Ligand CLA A 806	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA 8 302	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR L 308	
	
Bond lengths	Bond angles
	
Torsions	Rings



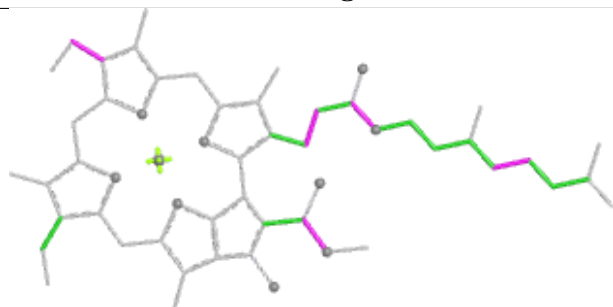


Ligand CLA 9 611

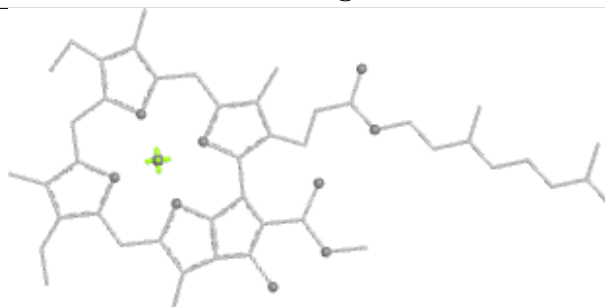
Bond lengths



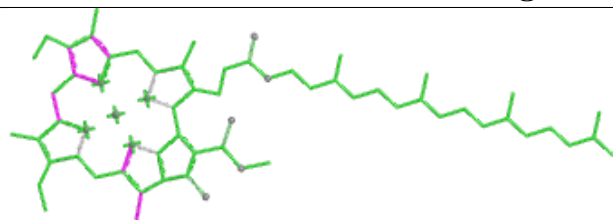
Bond angles



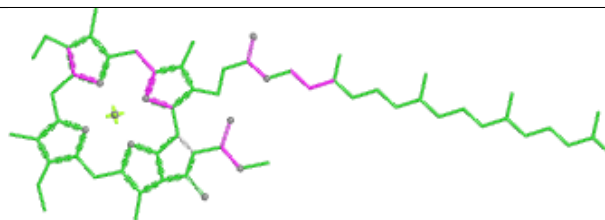
Torsions



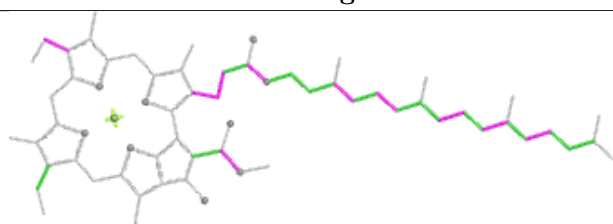
Rings

Ligand CLA 3 412

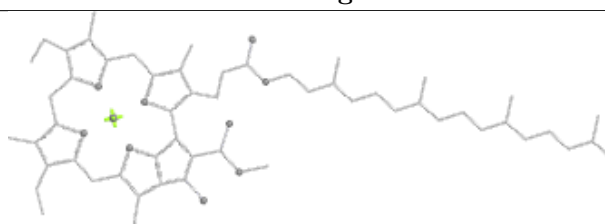
Bond lengths



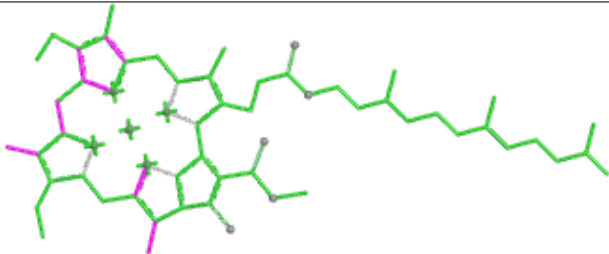
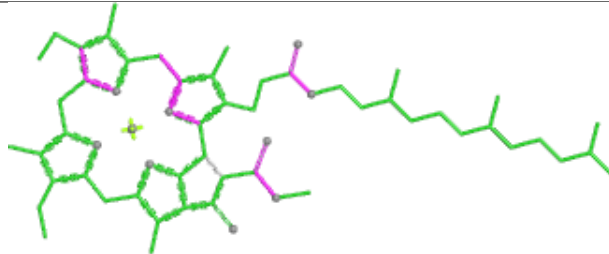
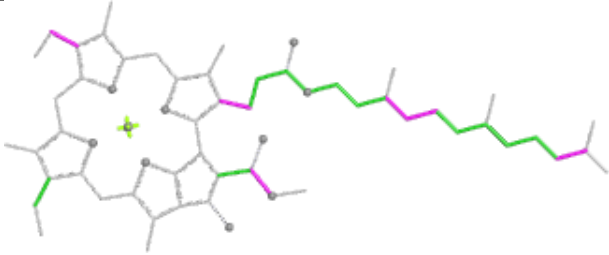
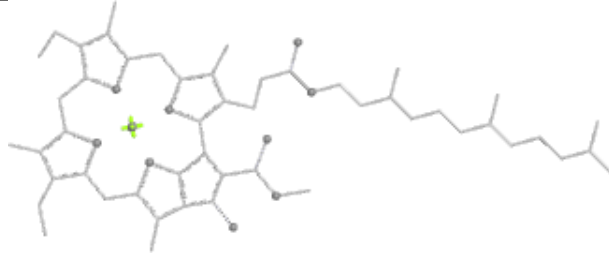
Bond angles

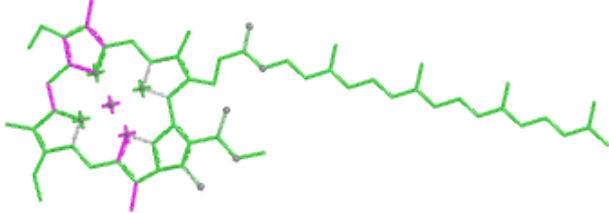
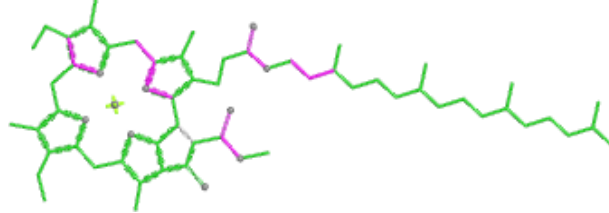
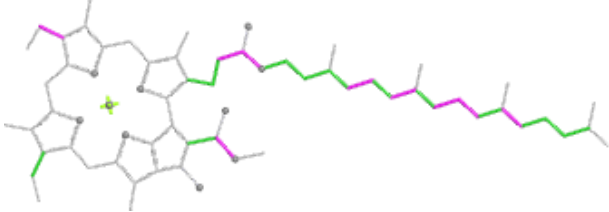
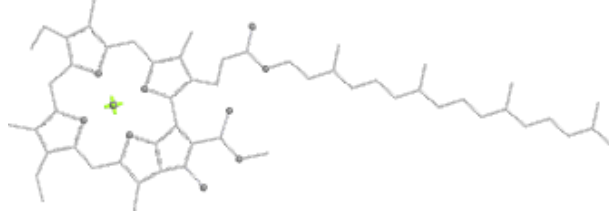


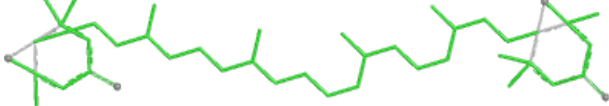
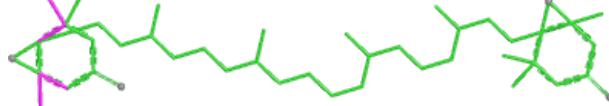
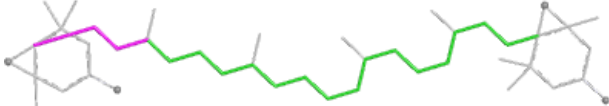
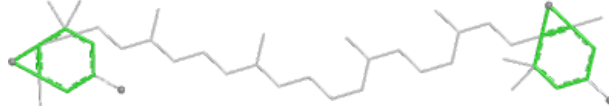
Torsions

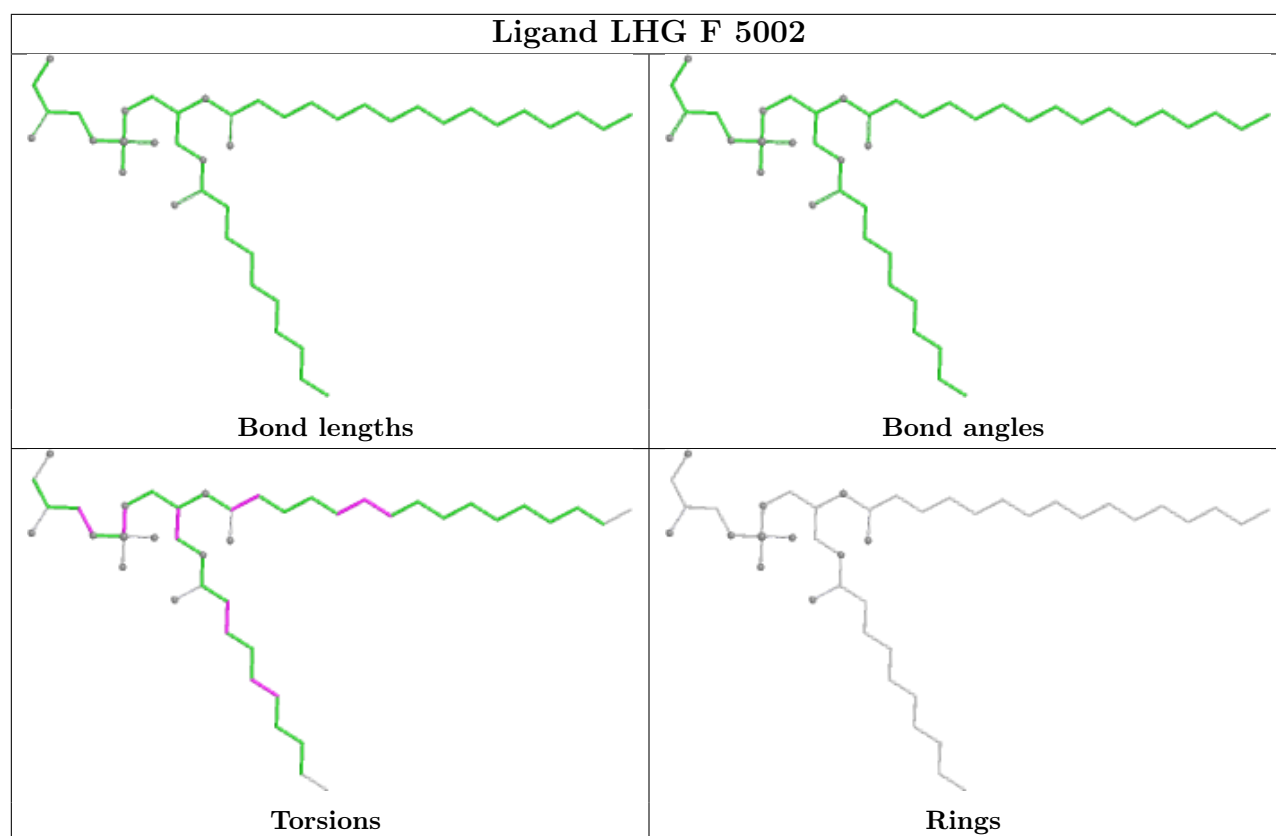


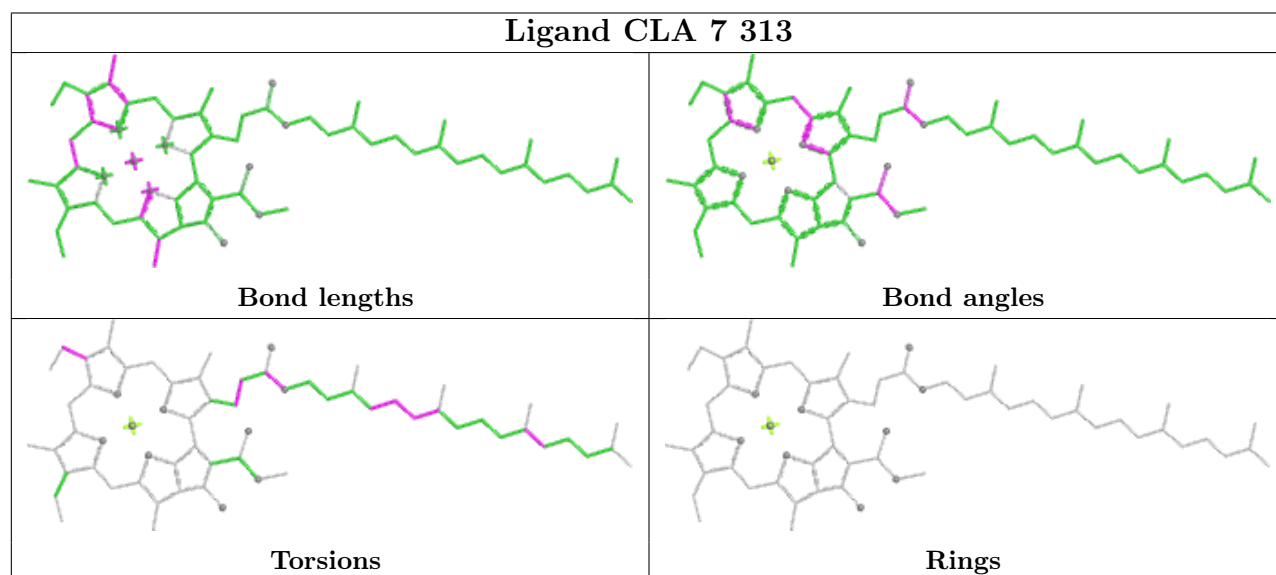
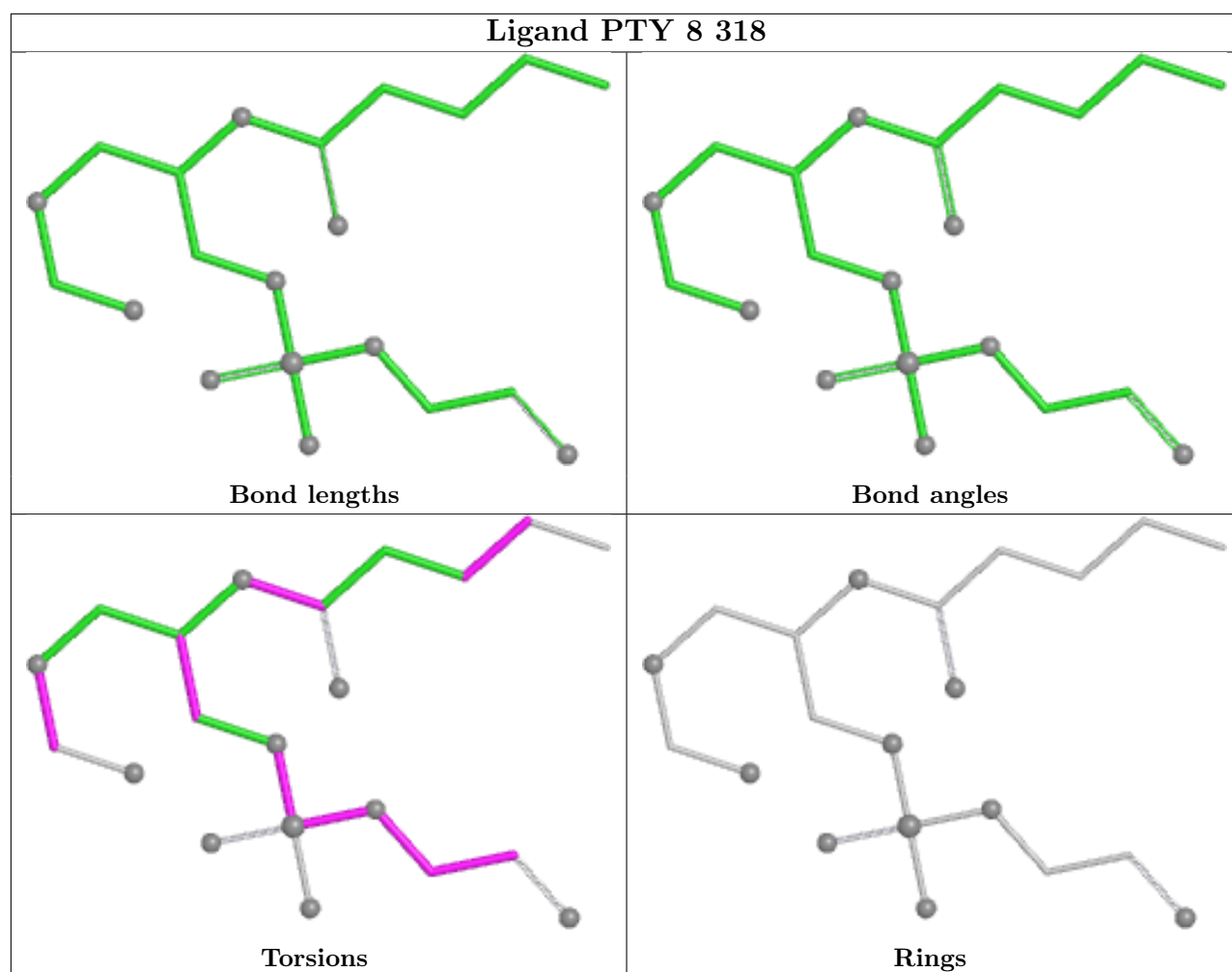
Rings

Ligand CLA 9 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

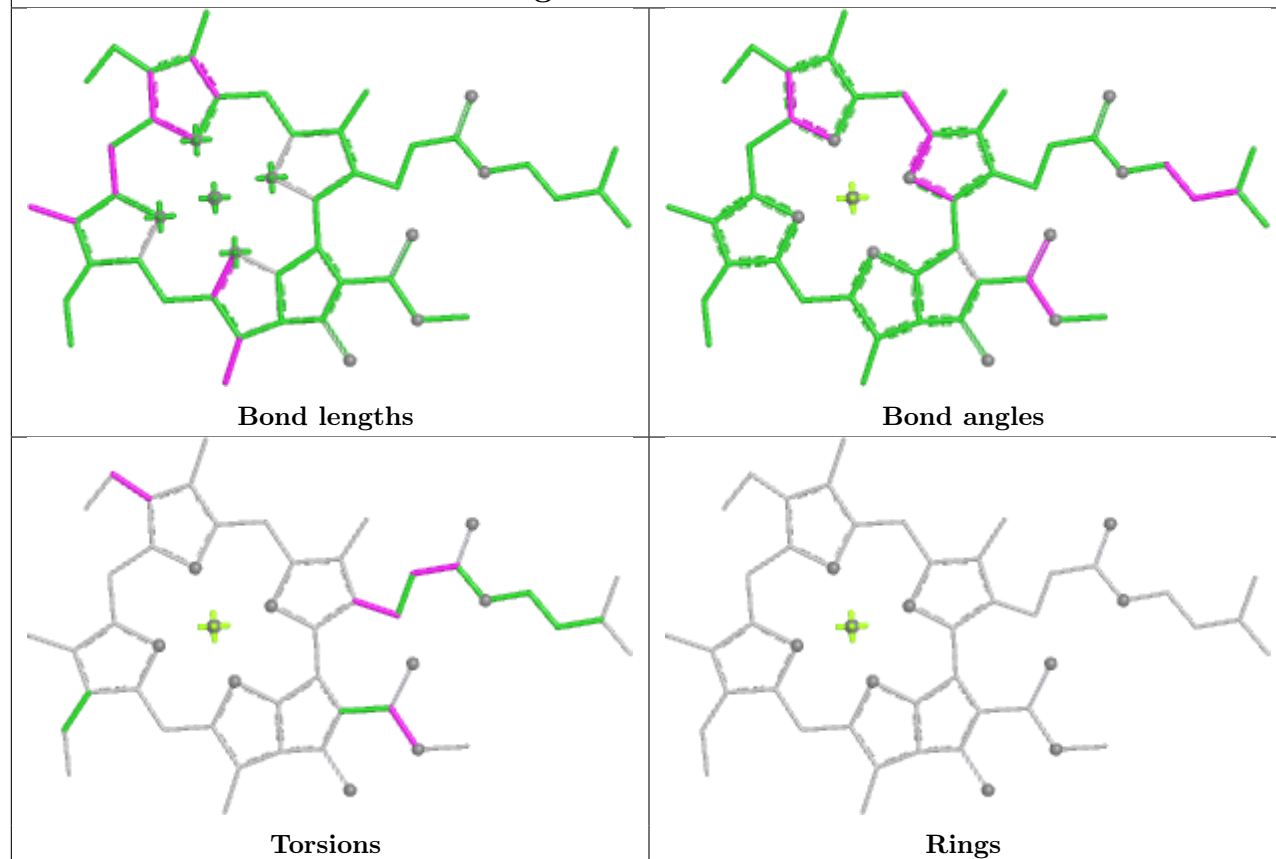
Ligand CLA B 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 7 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

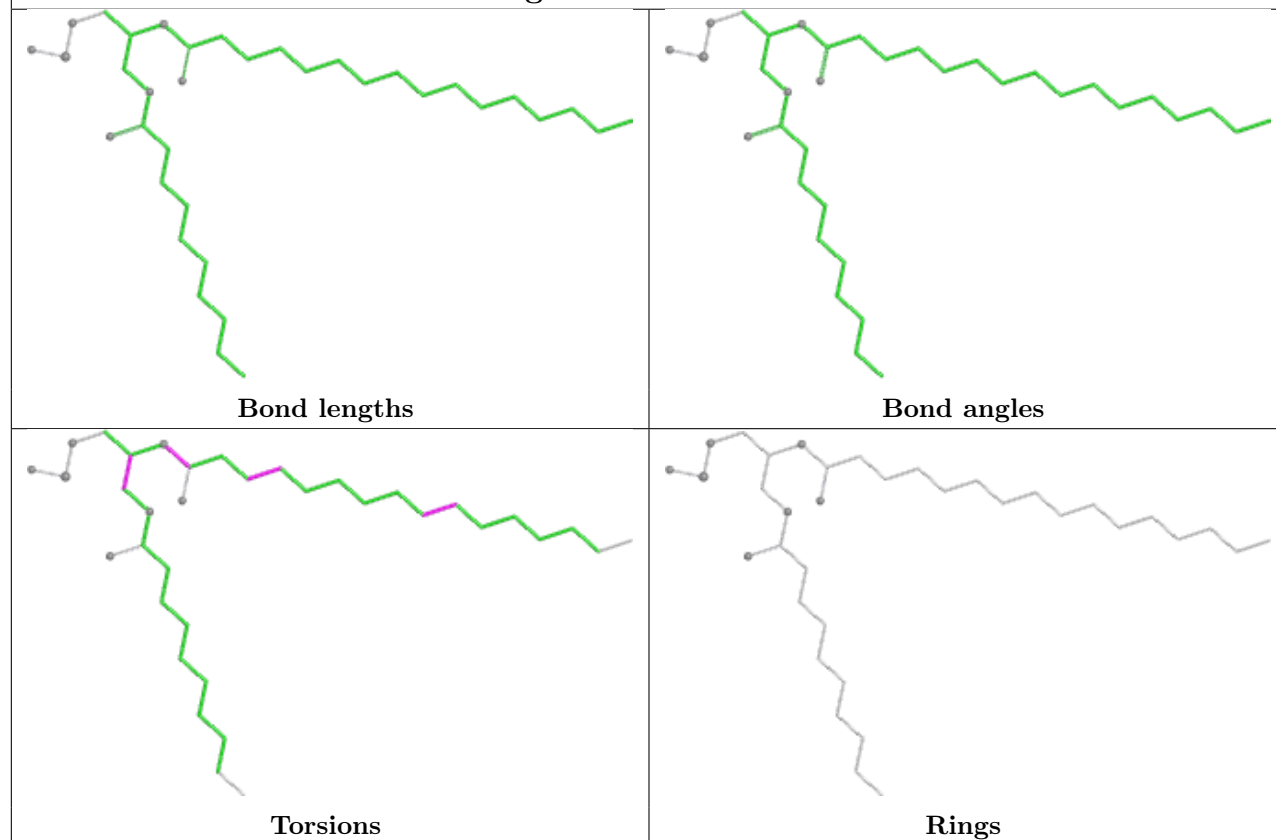


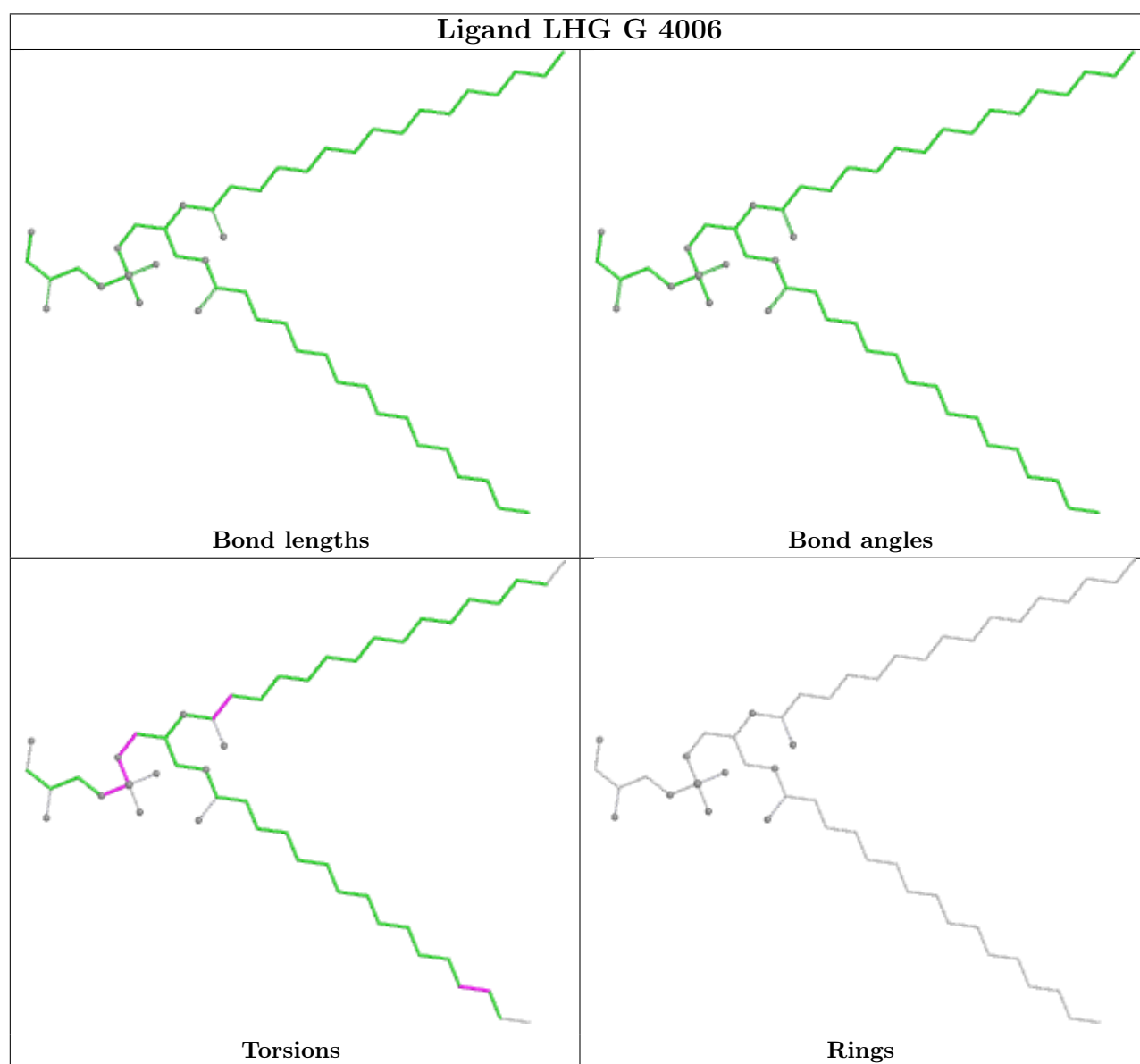
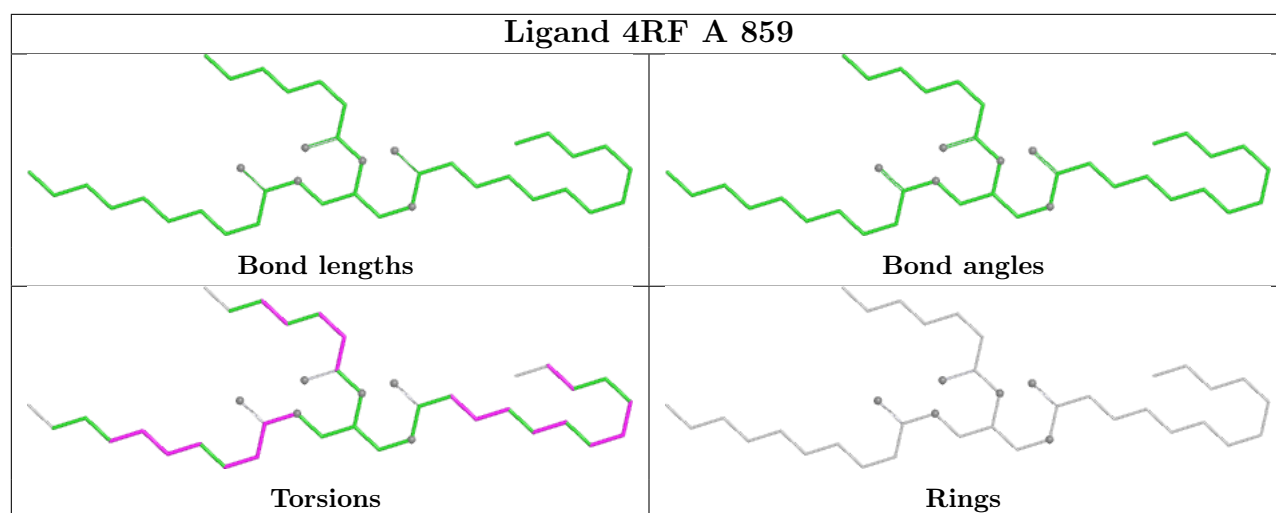


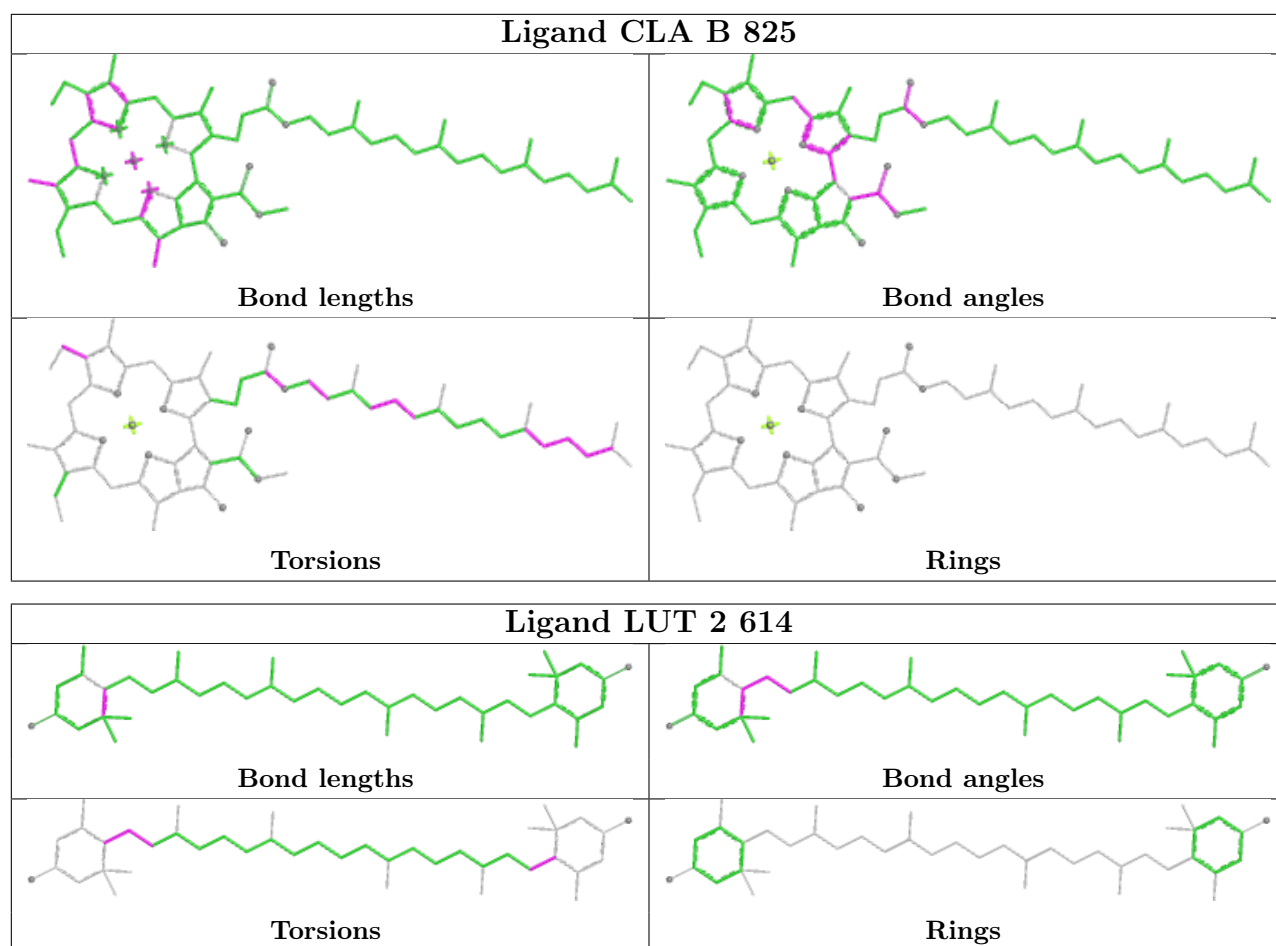
Ligand CLA L 306



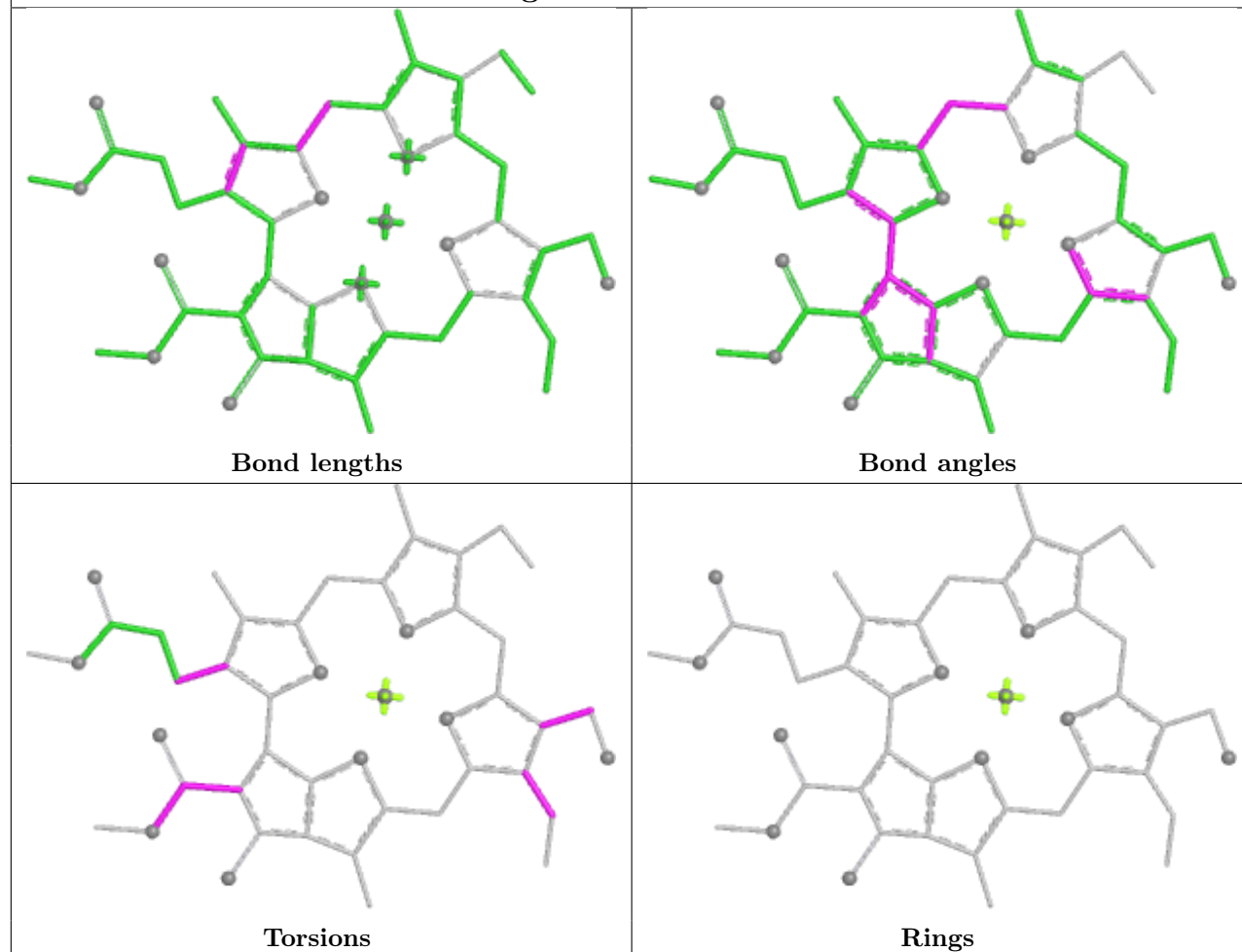
Ligand LHG J 4004



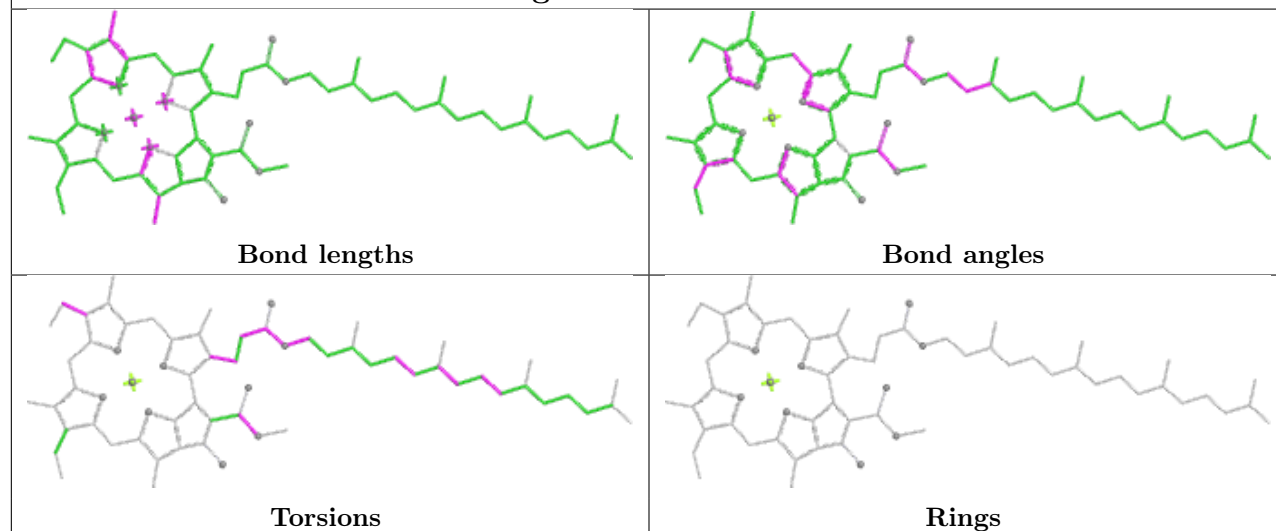




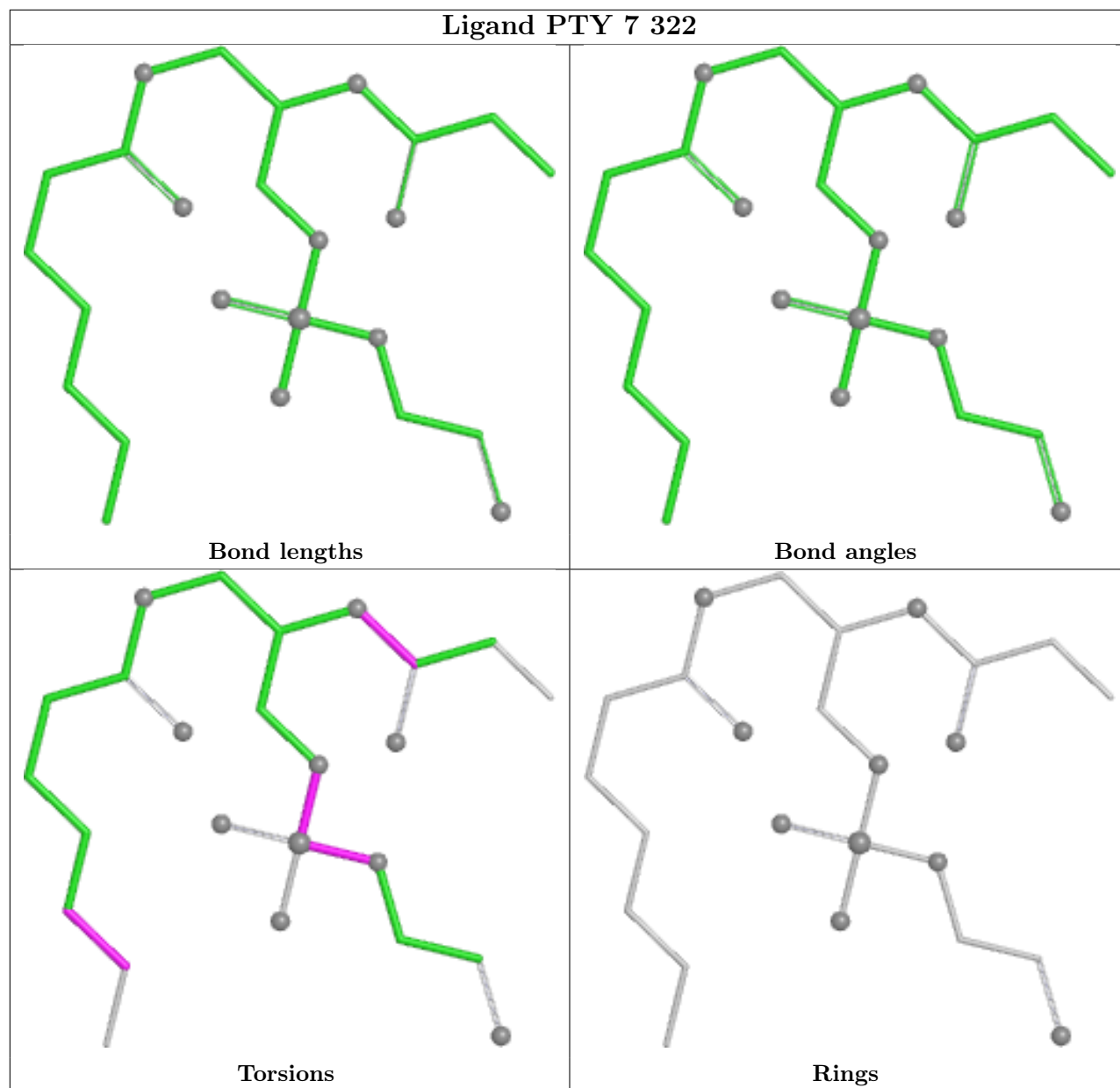
Ligand CHL 9 606

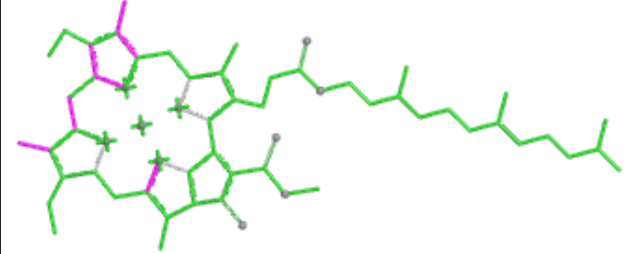
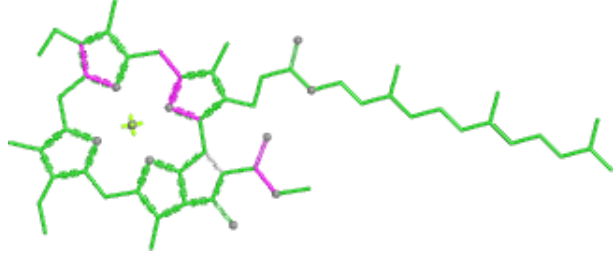
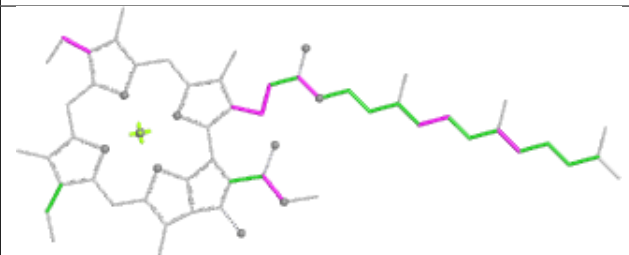
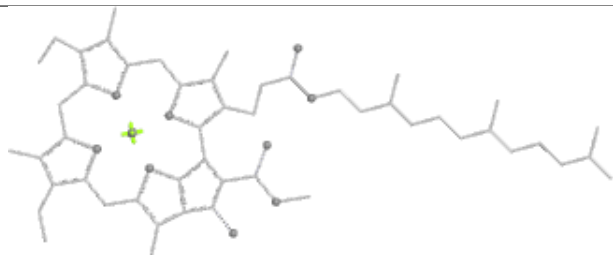
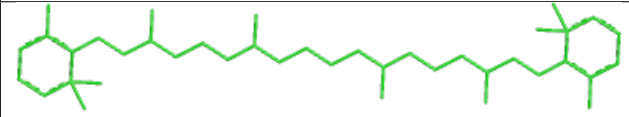
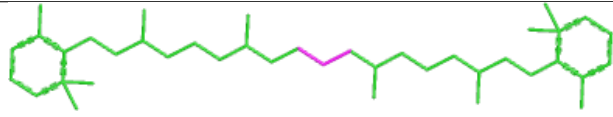
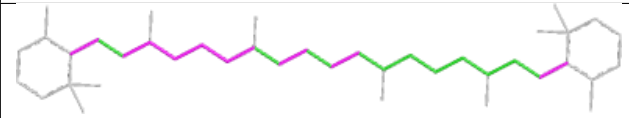
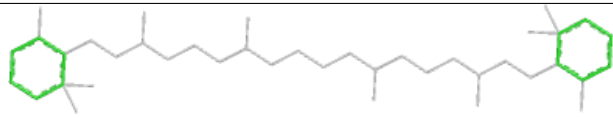
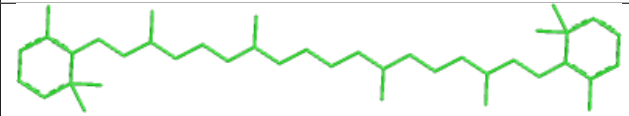
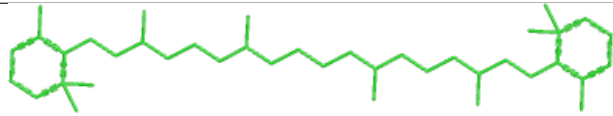
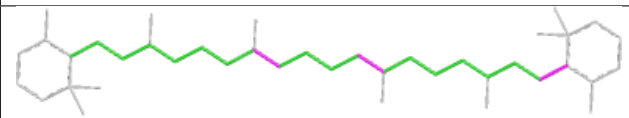
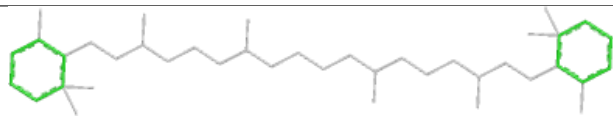


Ligand CLA B 830

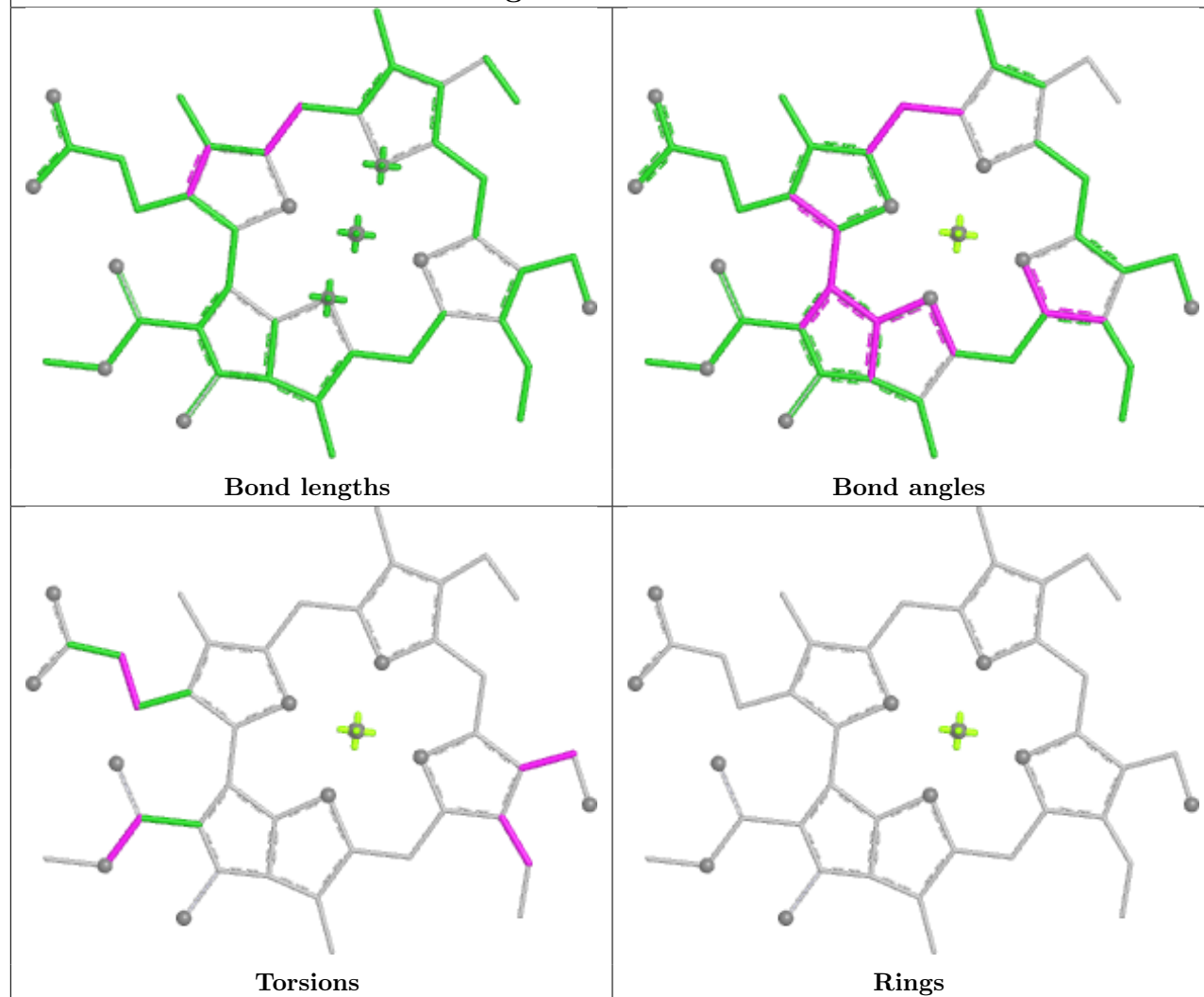


Ligand PTY 7 322

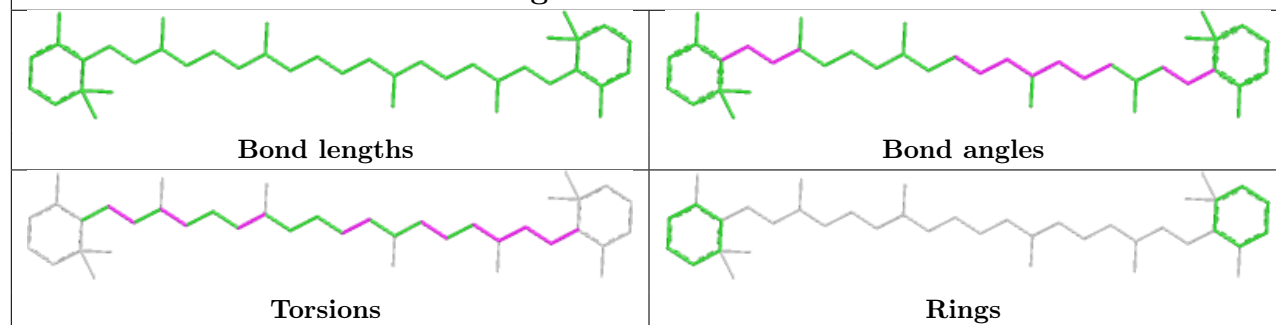


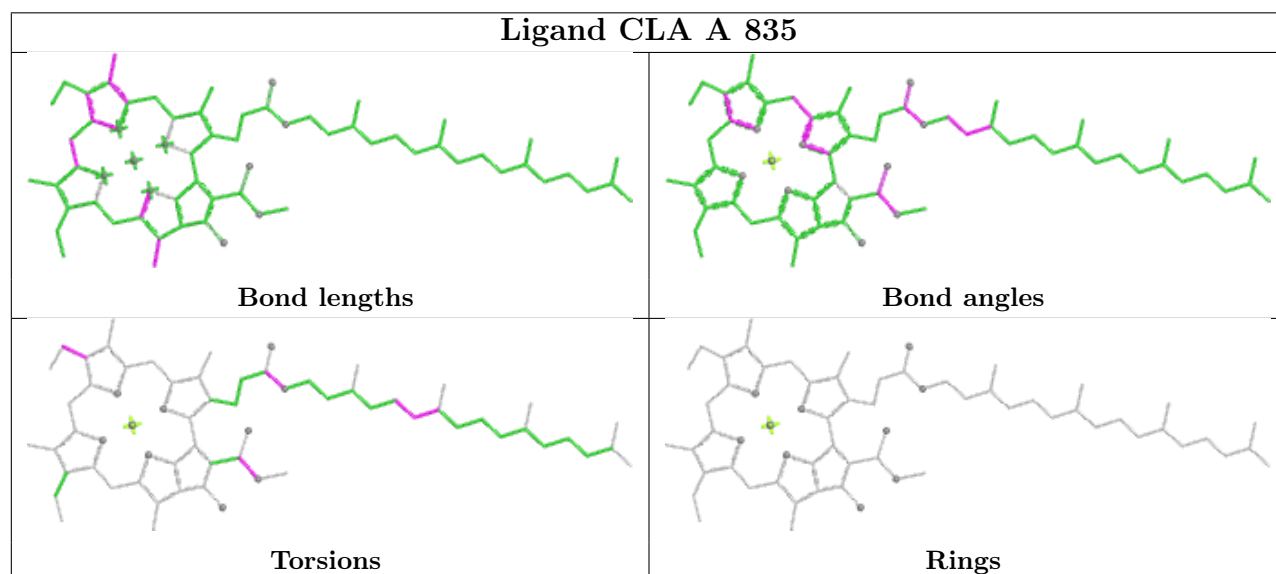
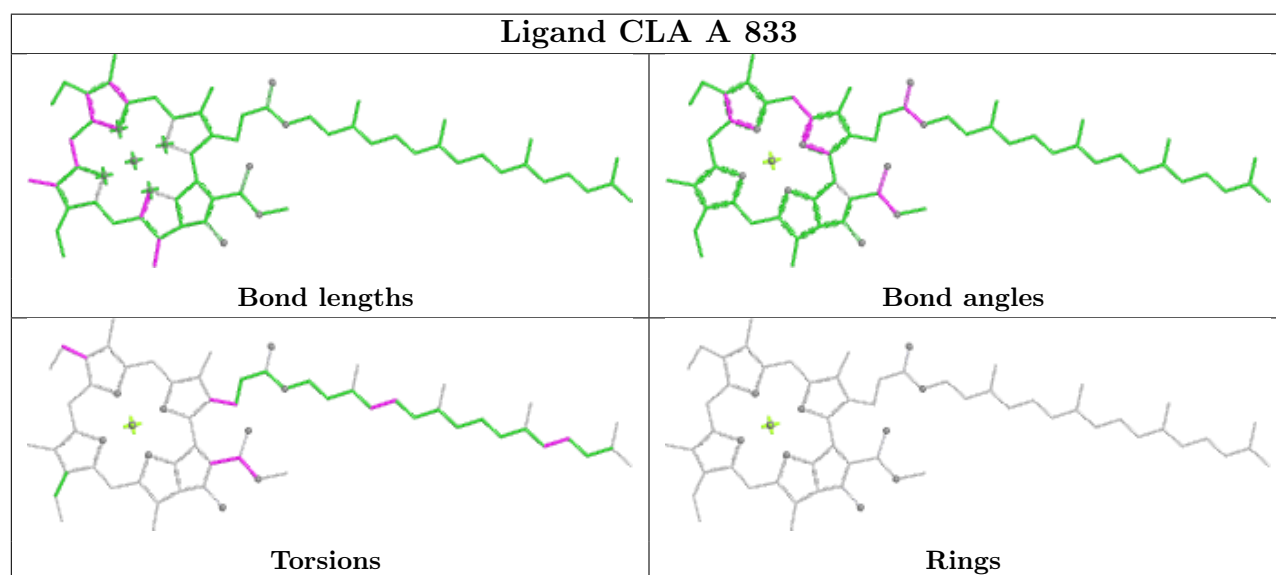
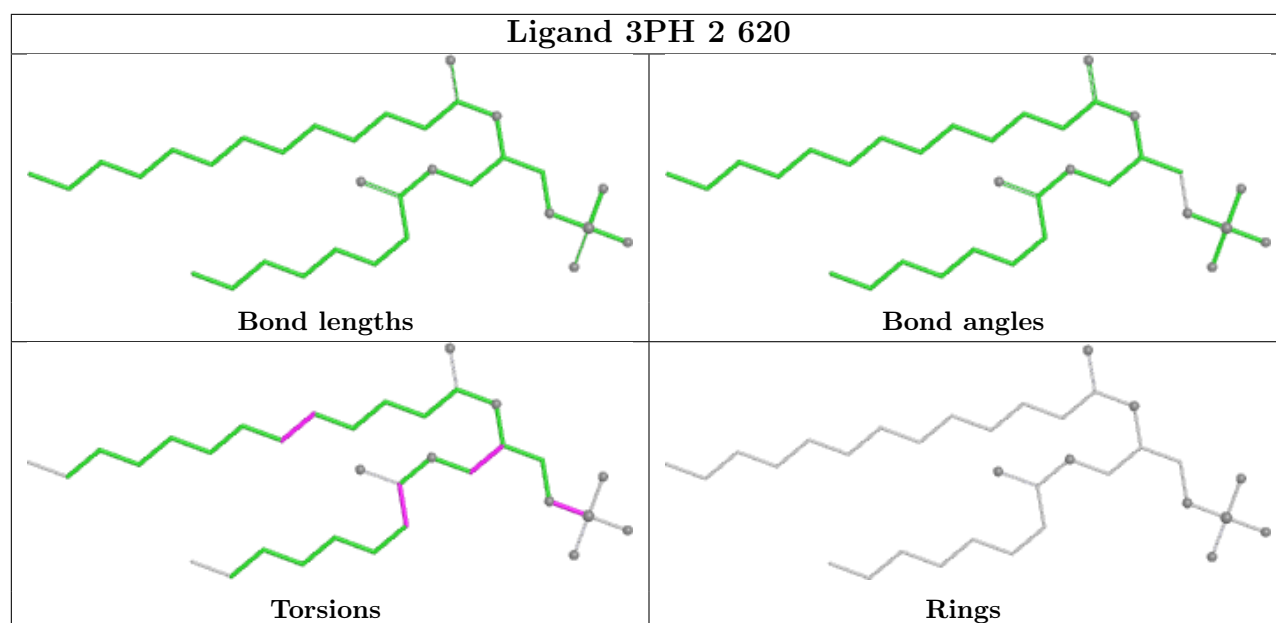
Ligand CLA 2 611	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 3 419	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 7 306

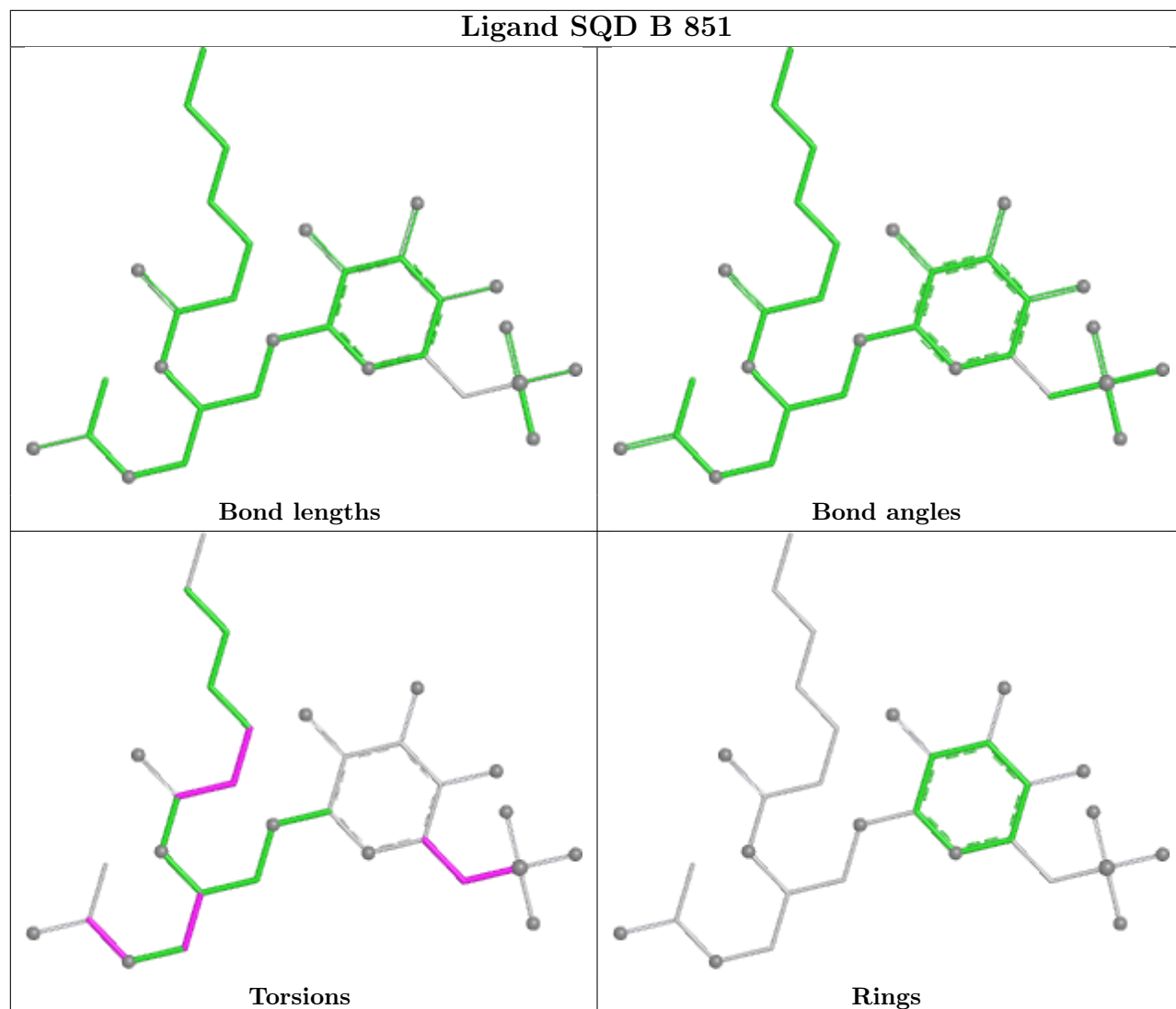


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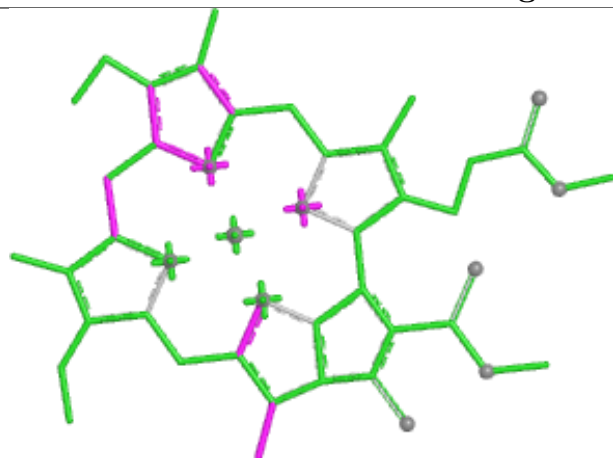




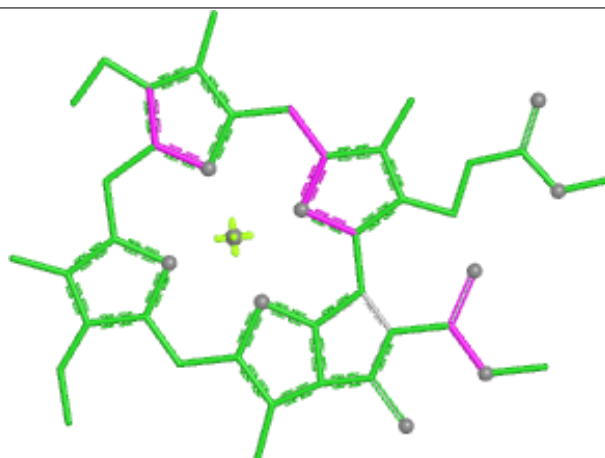
Ligand SQD B 851



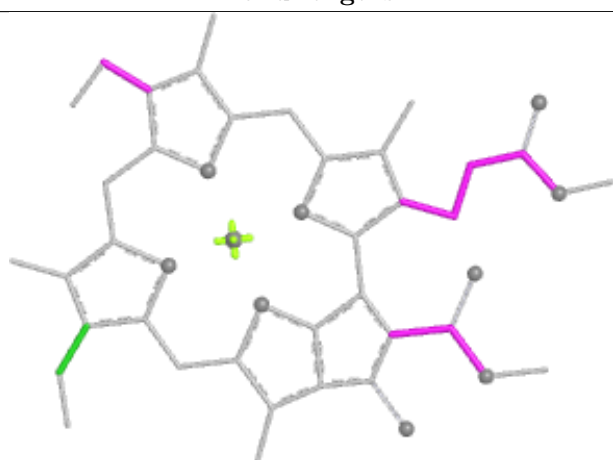
Ligand CLA 9 601



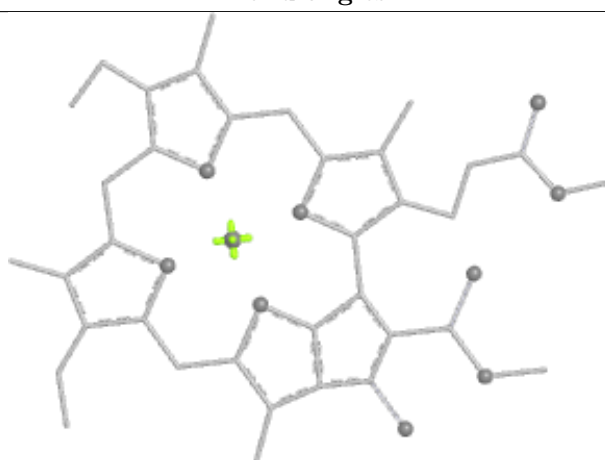
Bond lengths



Bond angles

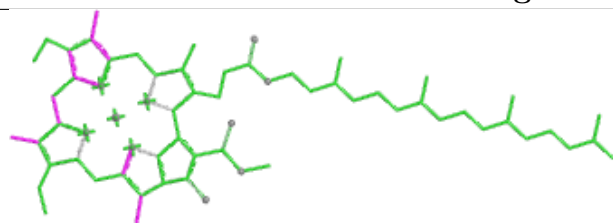


Torsions

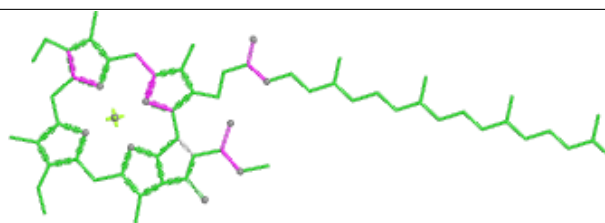


Rings

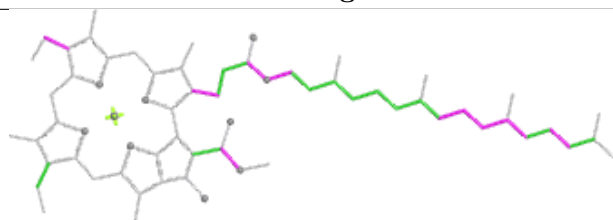
Ligand CLA A 824



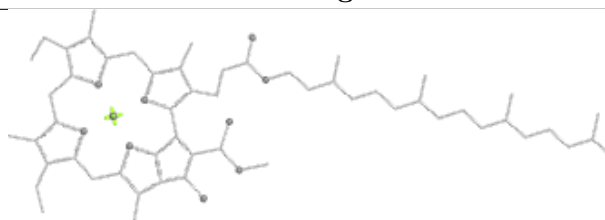
Bond lengths



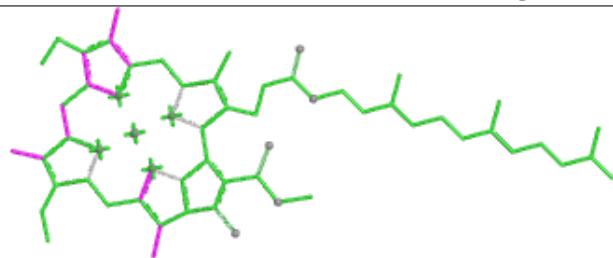
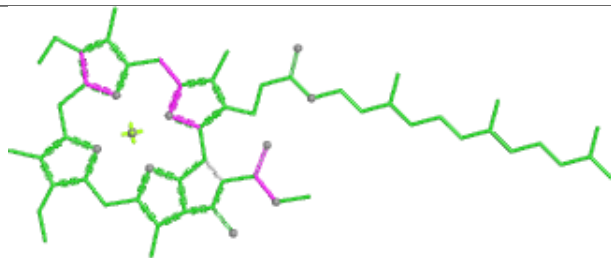
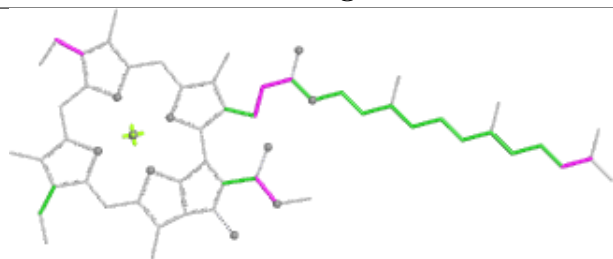
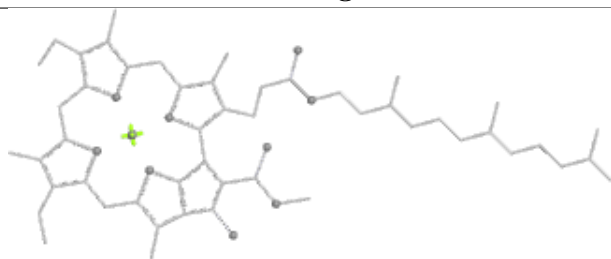
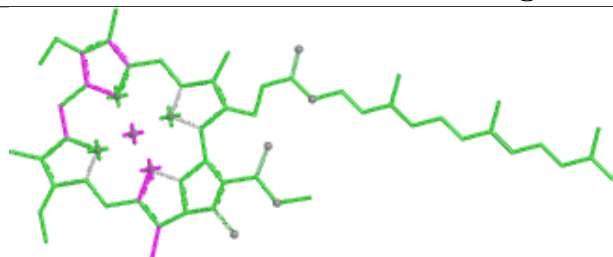
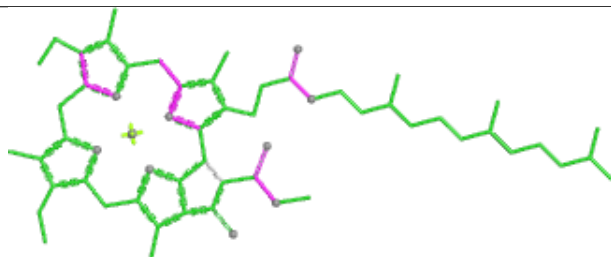
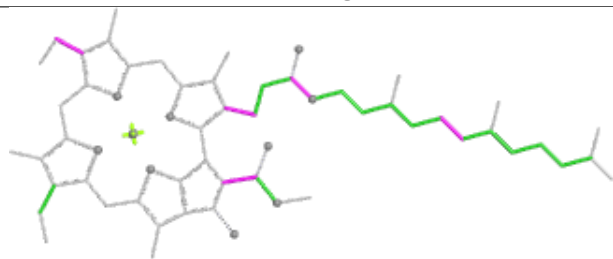
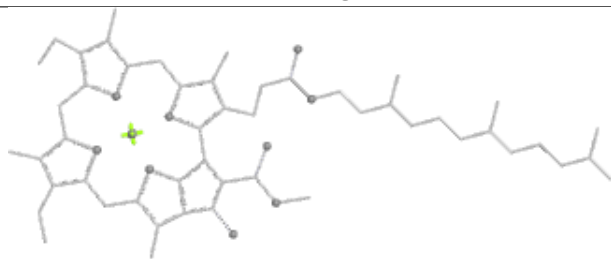
Bond angles

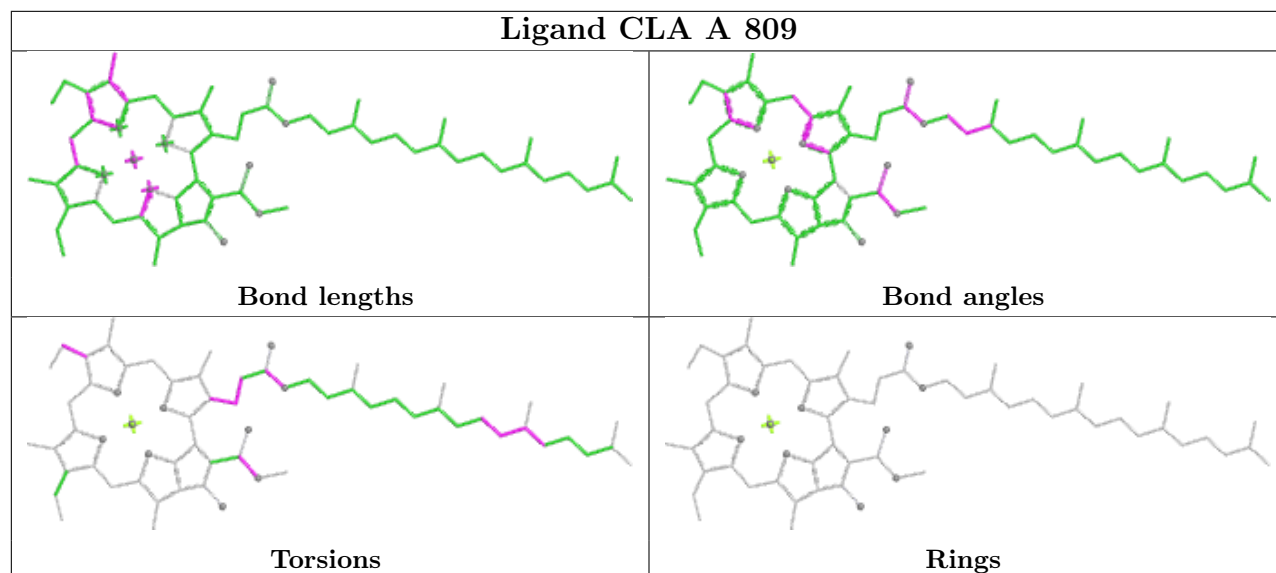
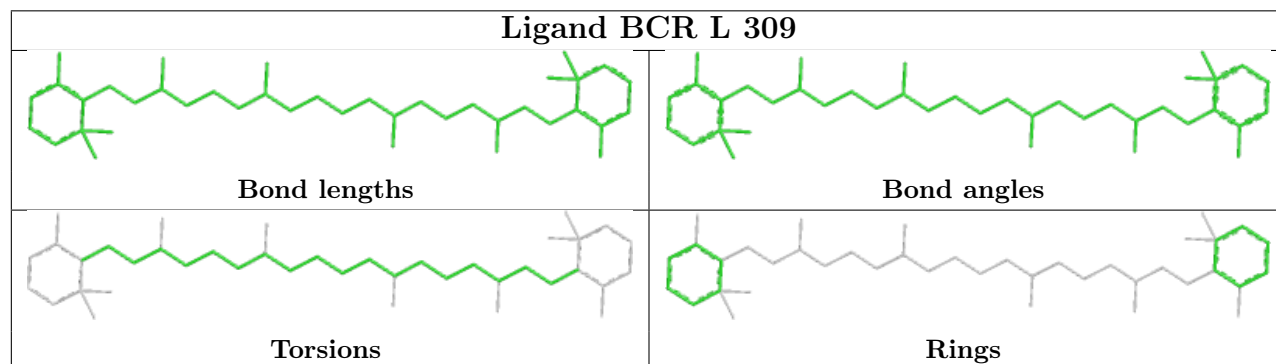
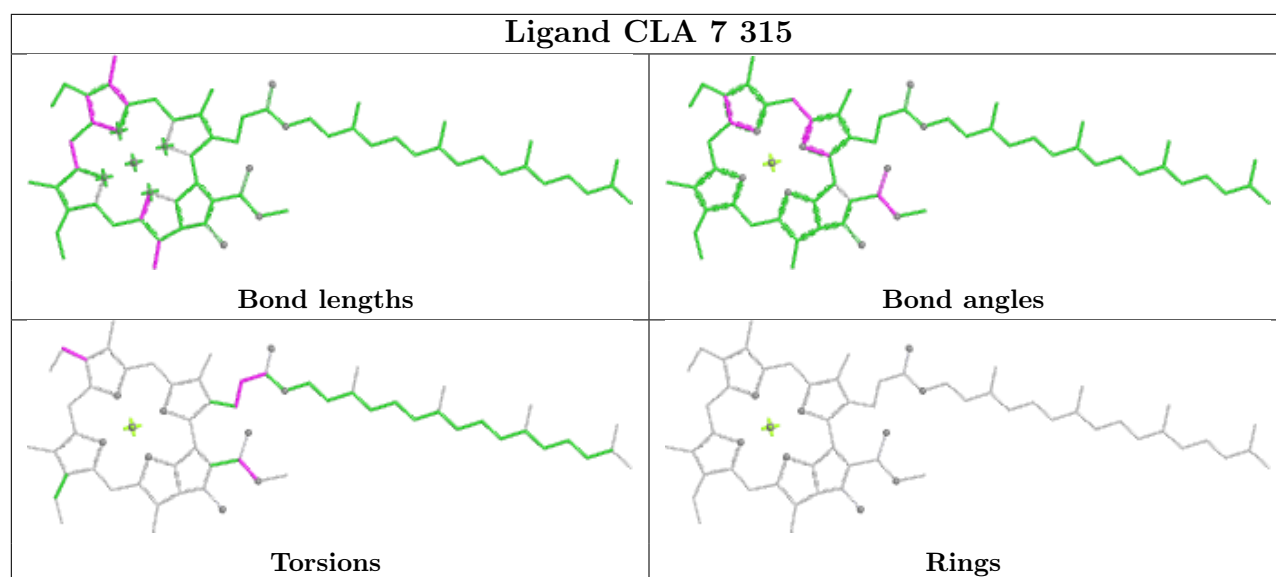


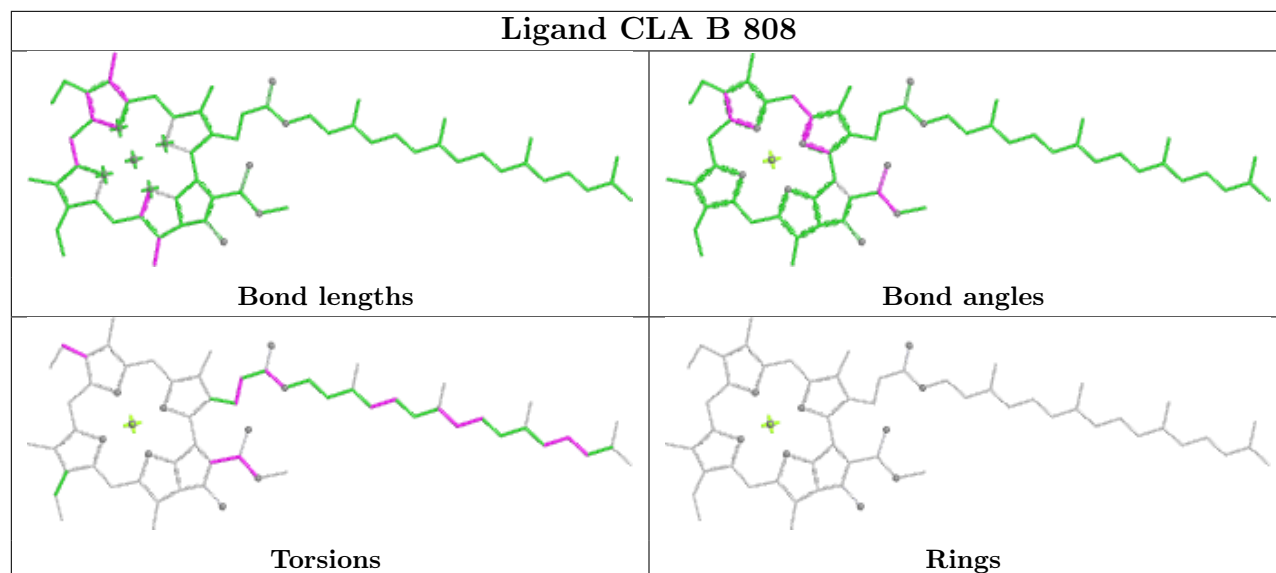
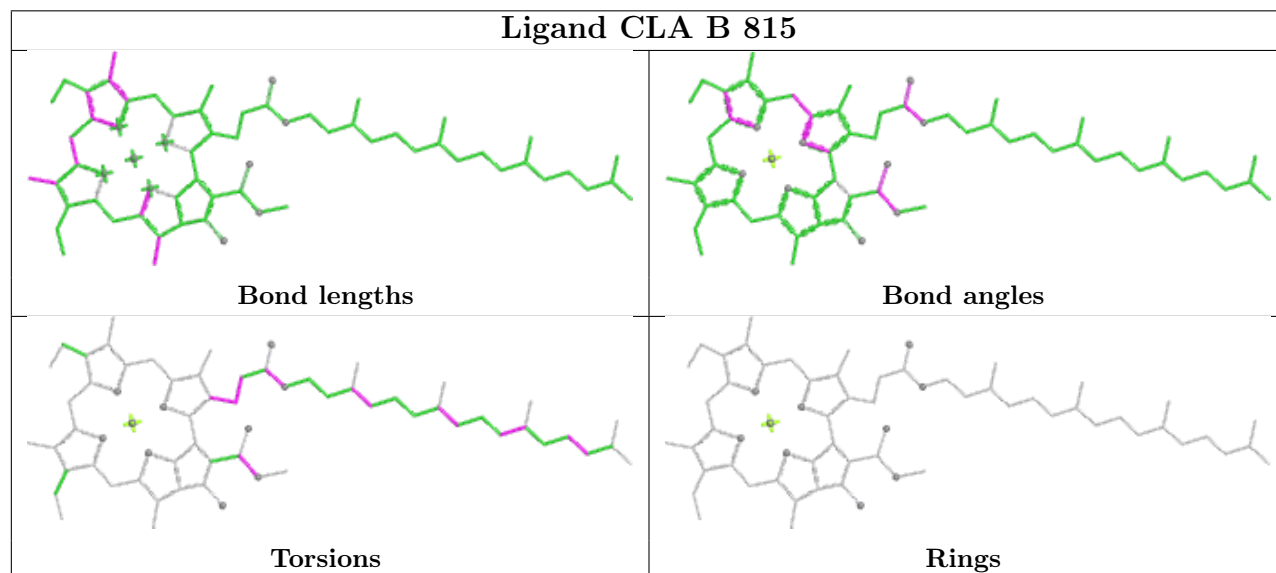
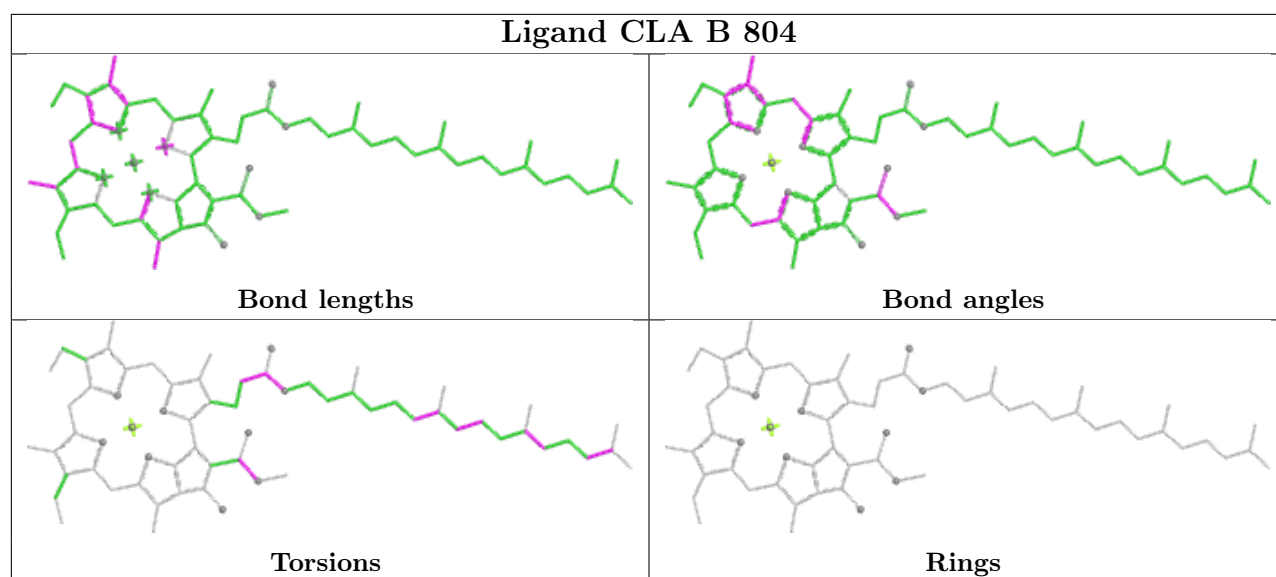
Torsions



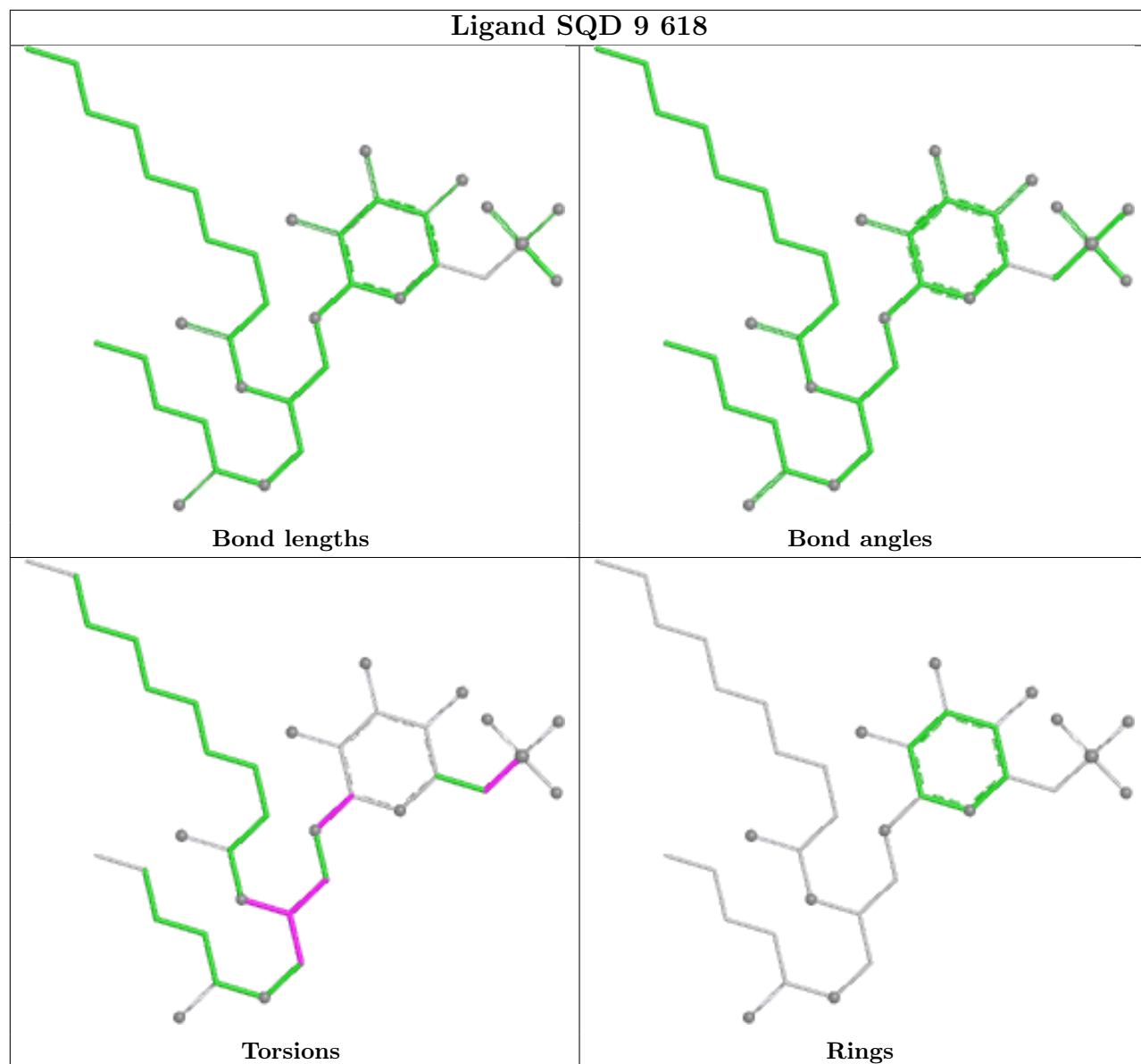
Rings

Ligand CLA A 825**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 7 324****Bond lengths****Bond angles****Torsions****Rings**

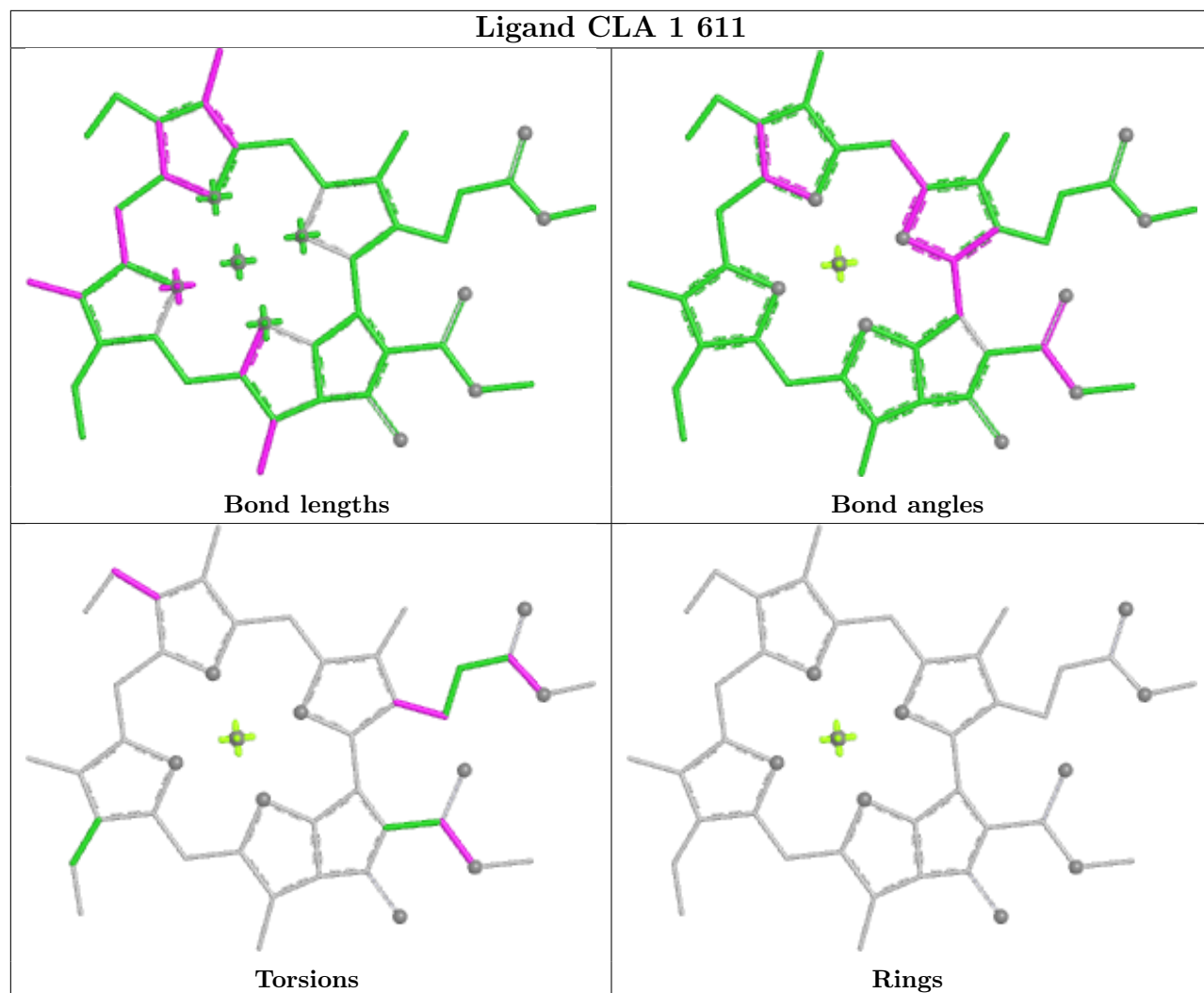




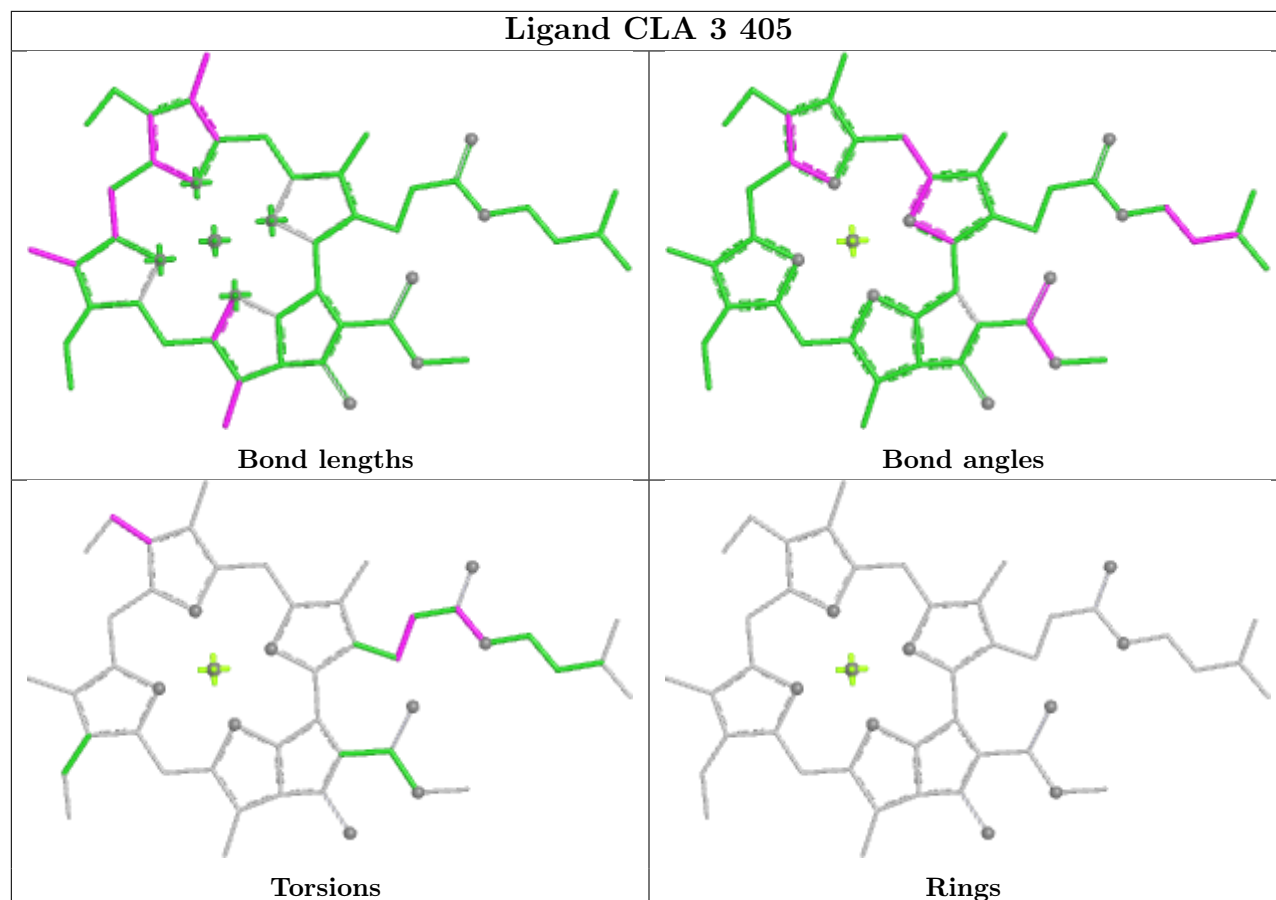
Ligand SQD 9 618



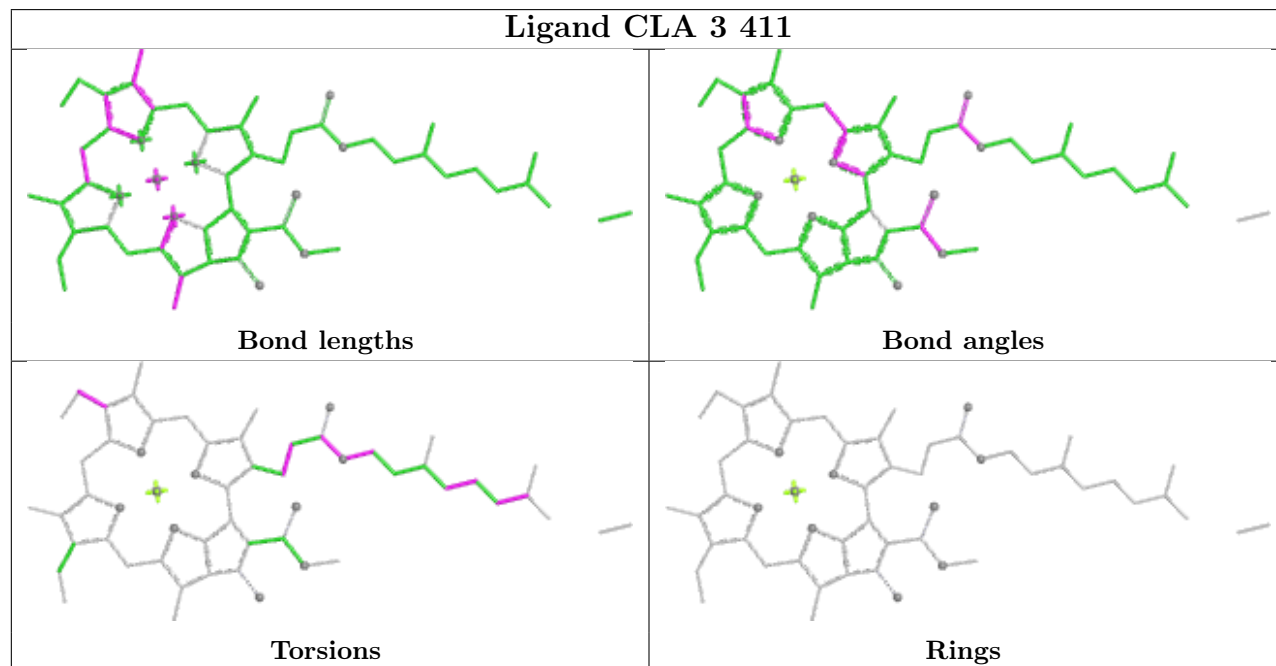
Ligand CLA 1 611



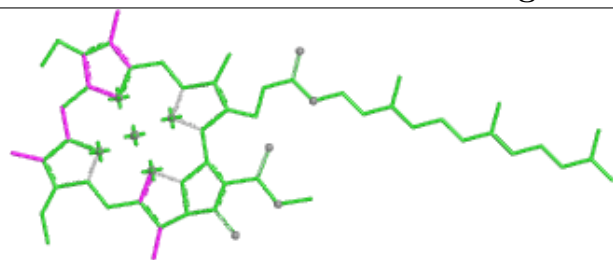
Ligand CLA 3 405



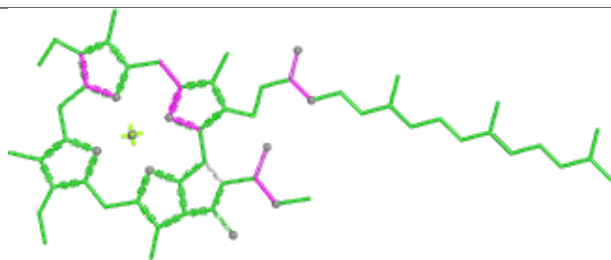
Ligand CLA 3 411



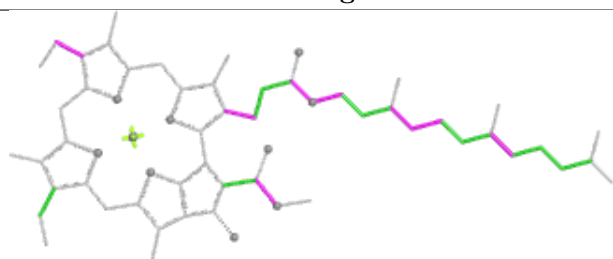
Ligand CLA 8 309



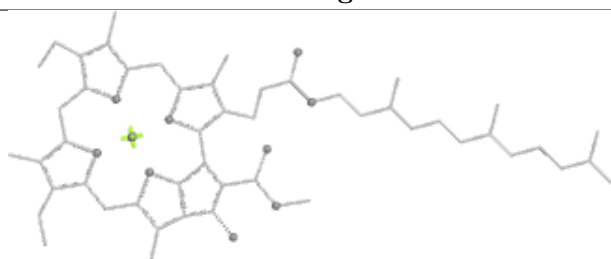
Bond lengths



Bond angles

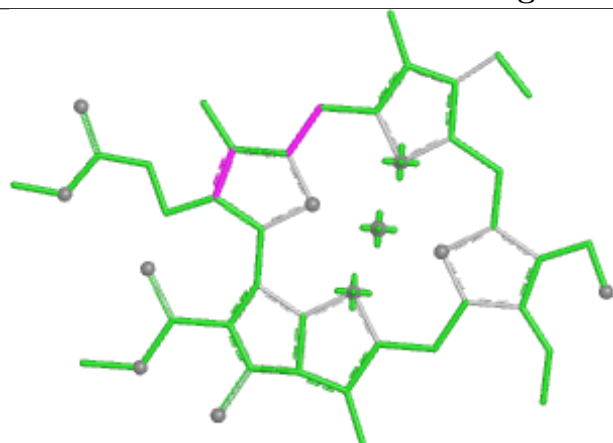


Torsions

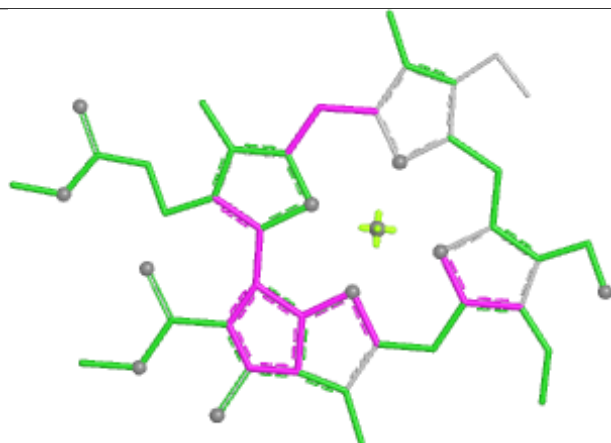


Rings

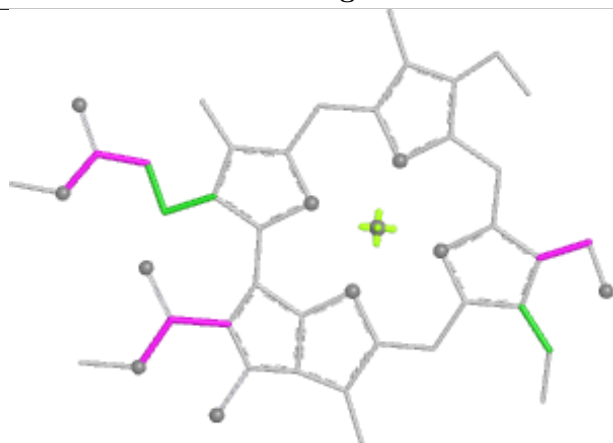
Ligand CHL 8 305



Bond lengths



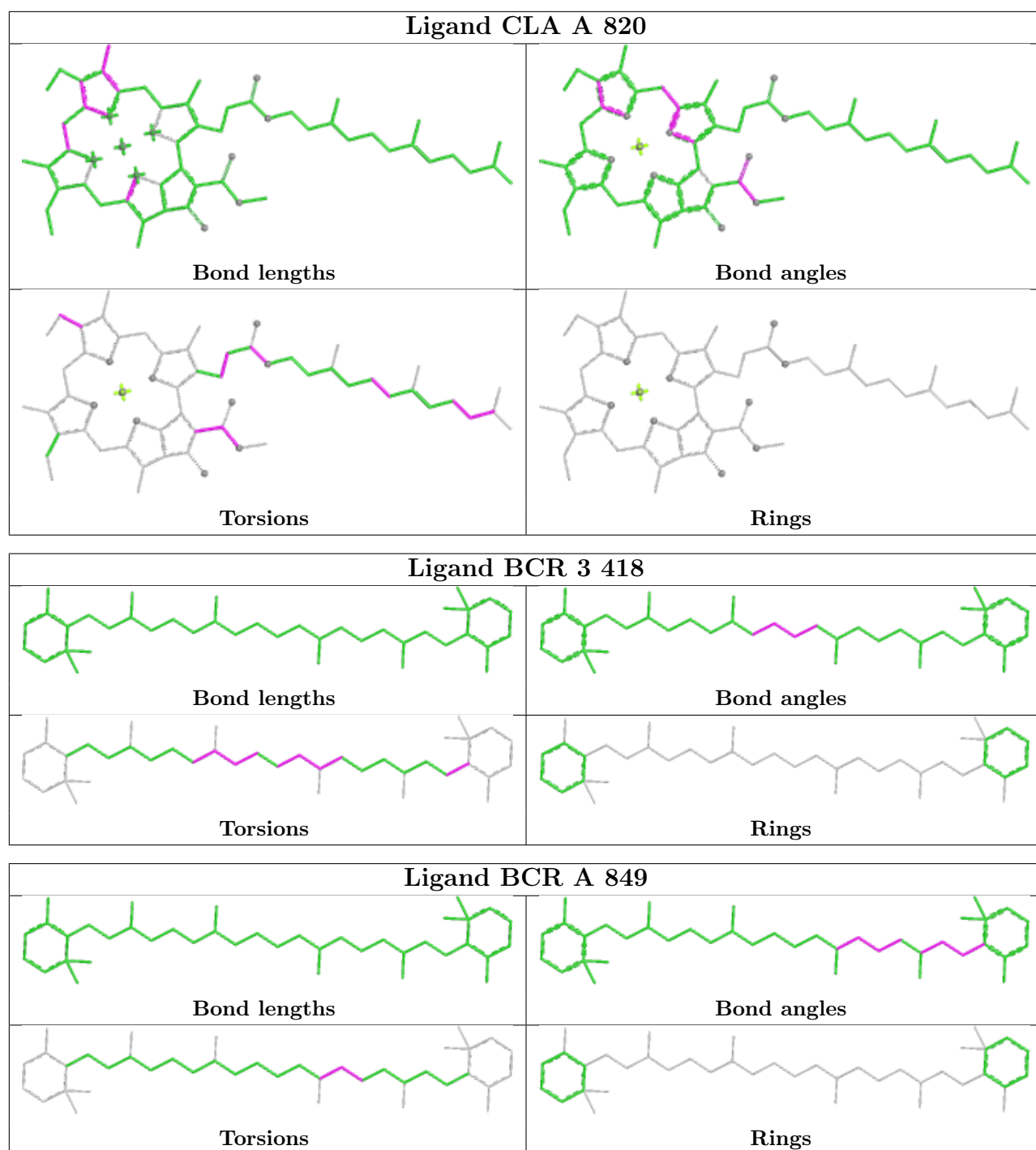
Bond angles

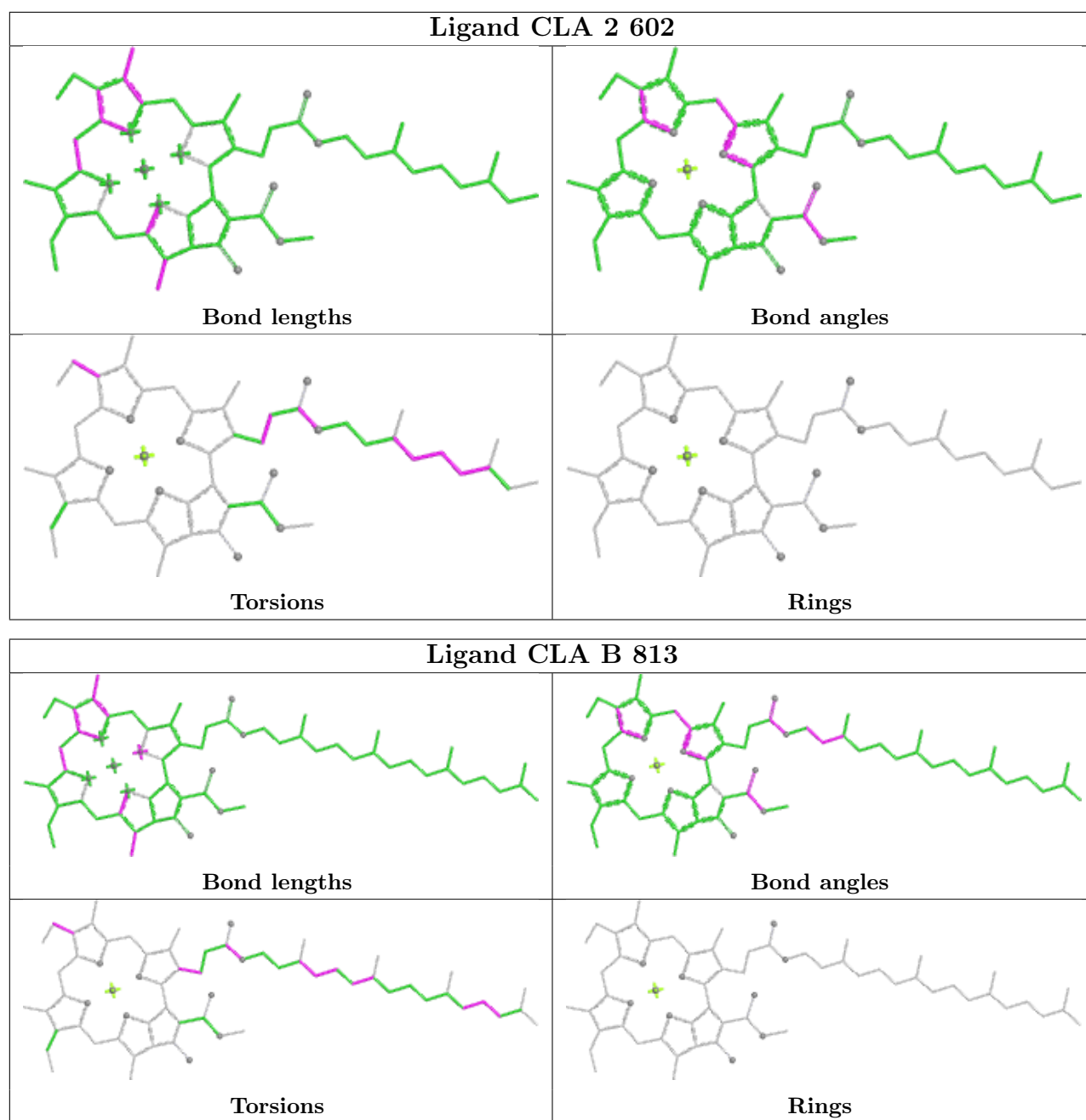


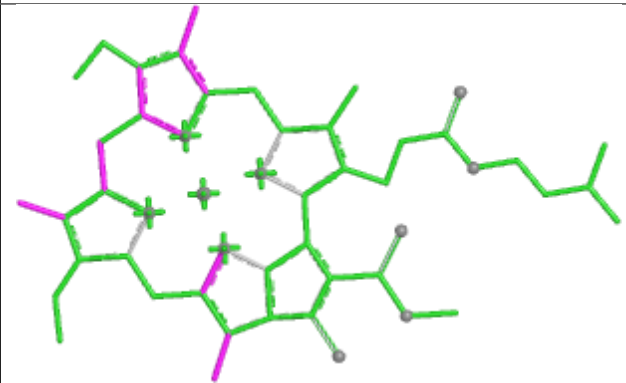
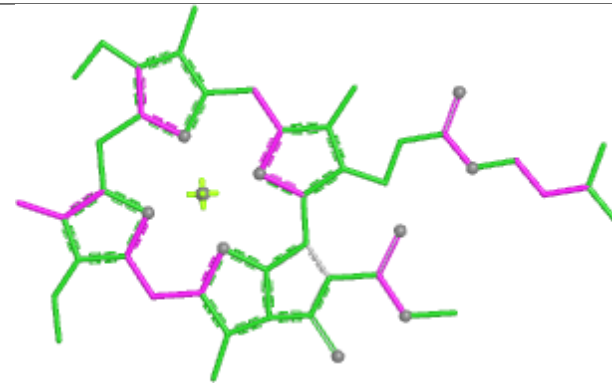
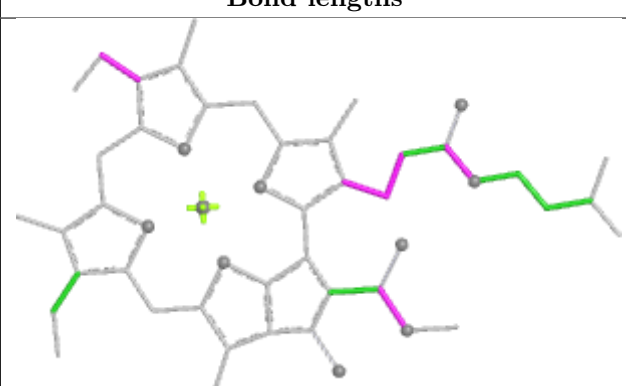
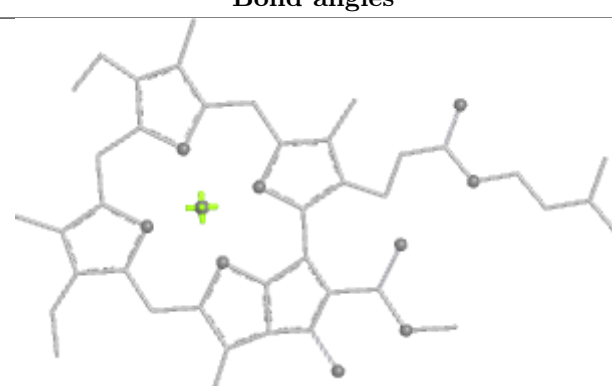
Torsions

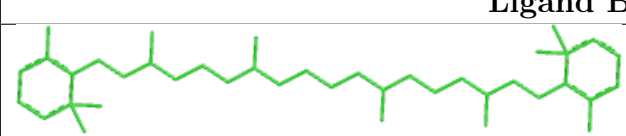
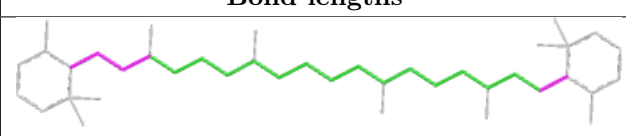
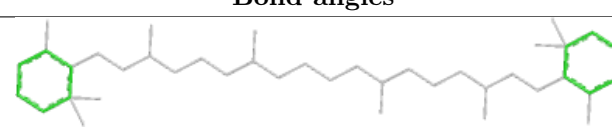


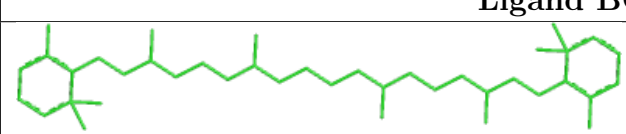
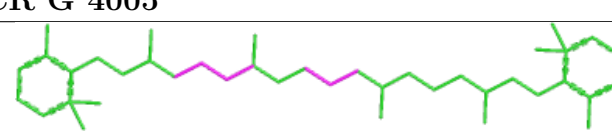
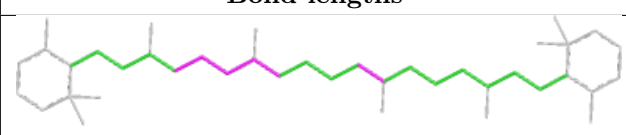
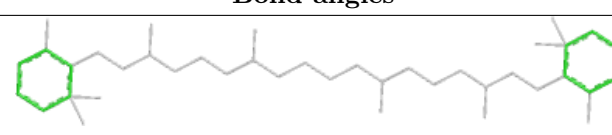
Rings

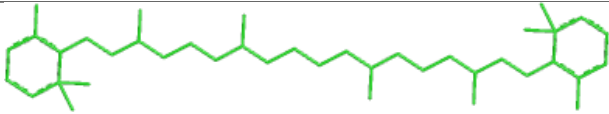
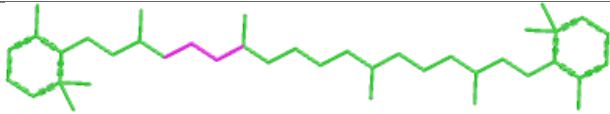
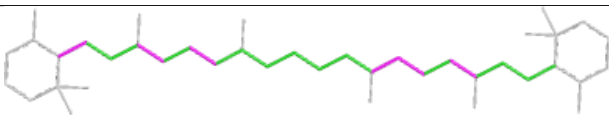
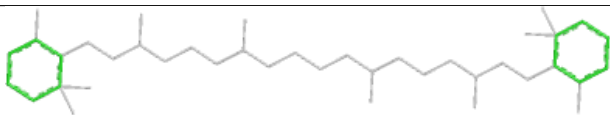


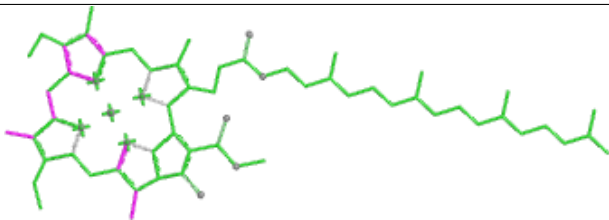
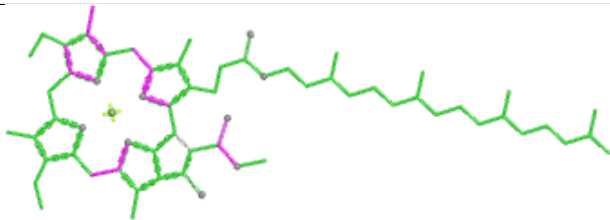
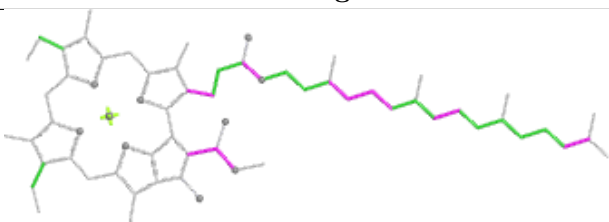
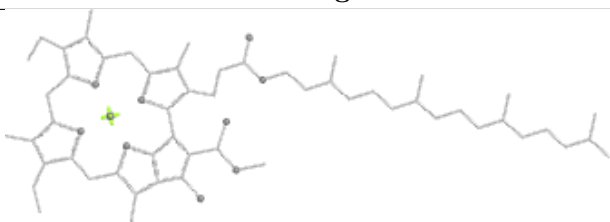


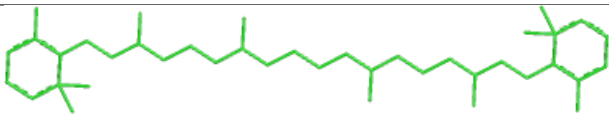
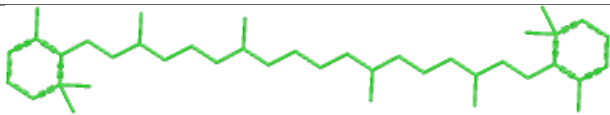
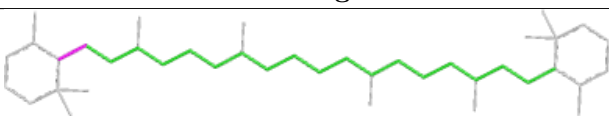
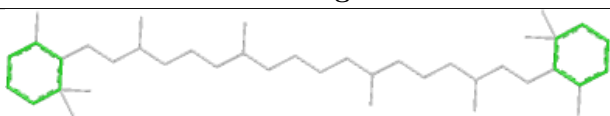
Ligand CLA 2 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

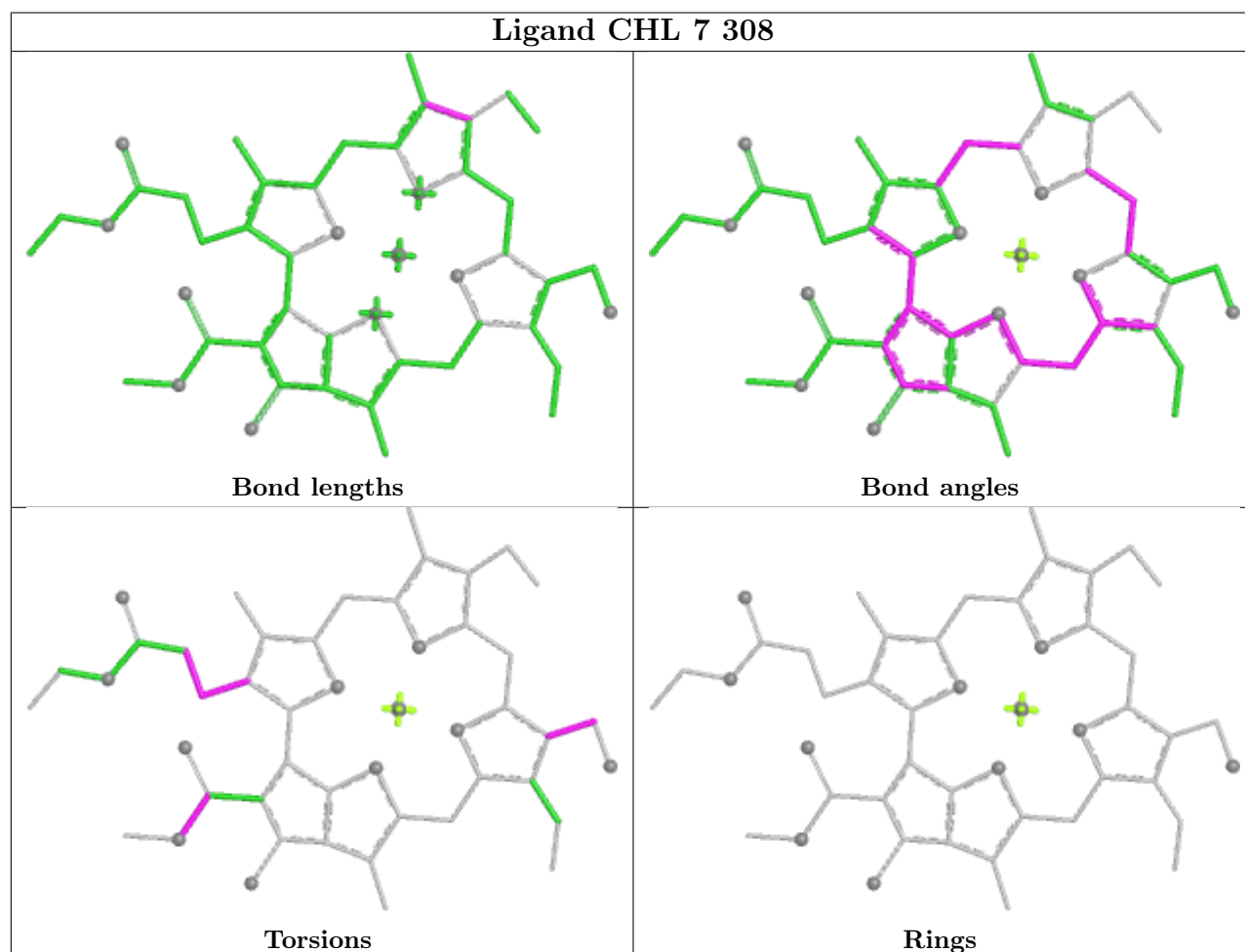
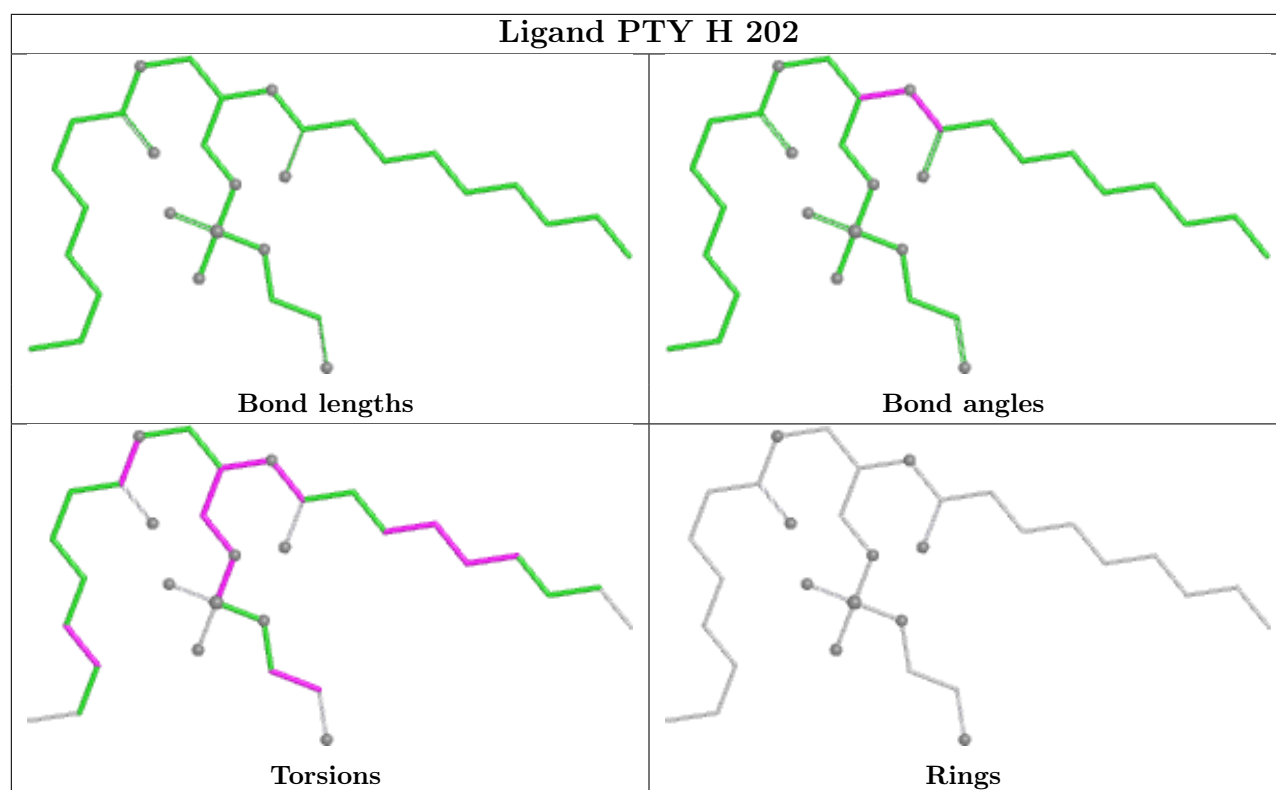
Ligand BCR B 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

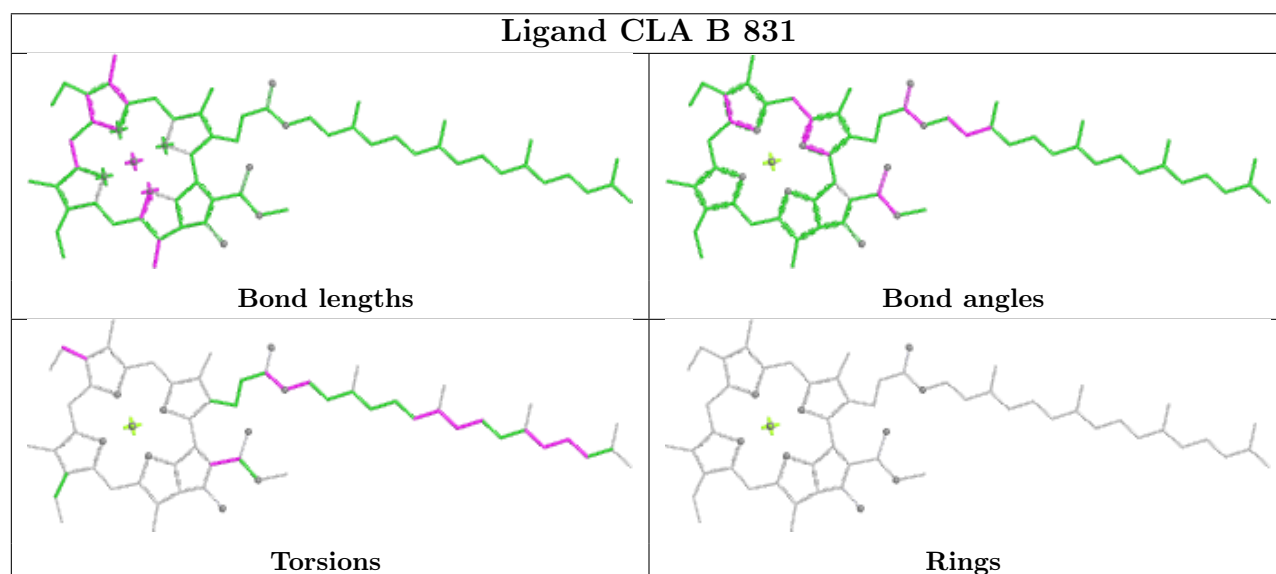
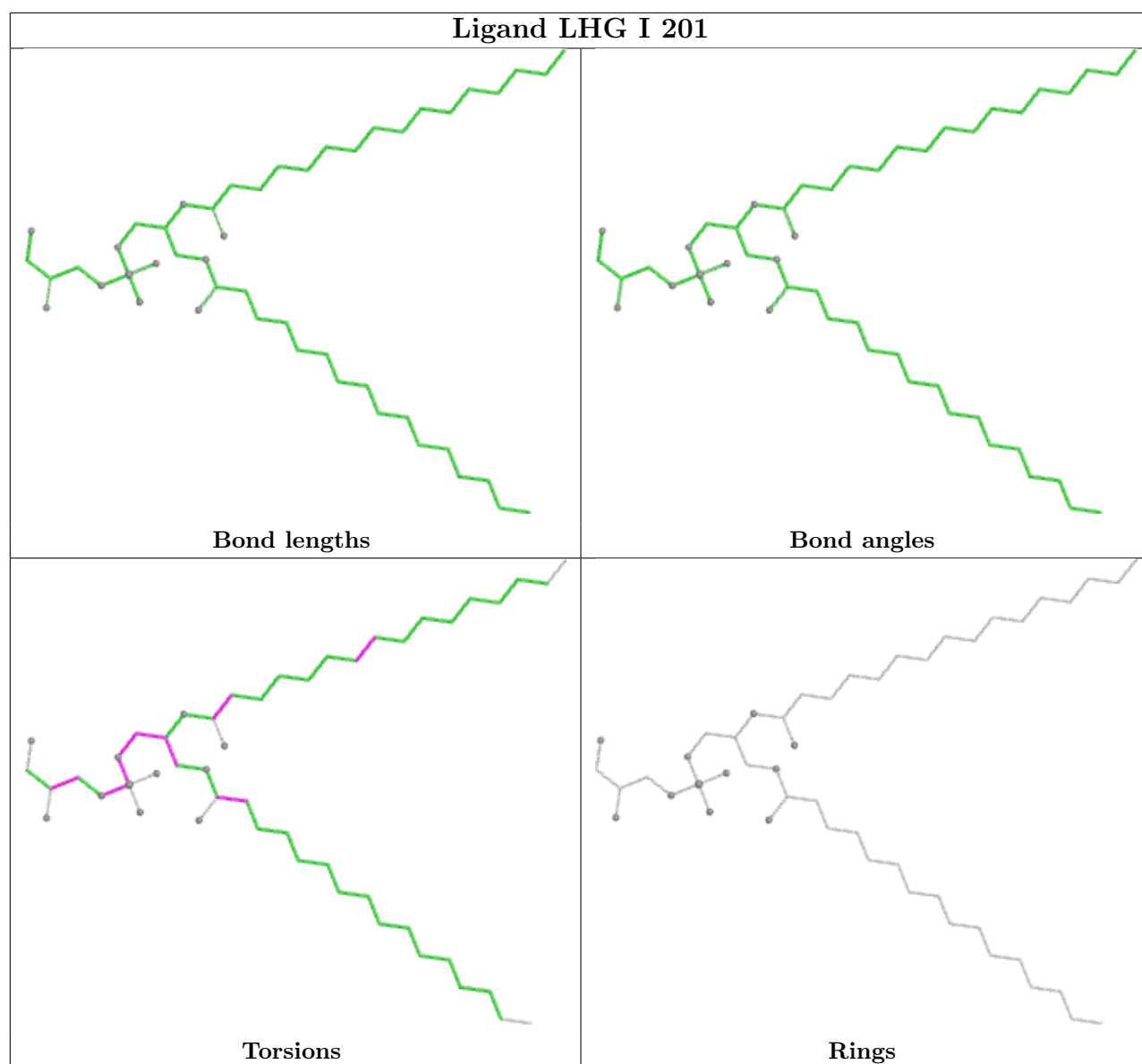
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Bond lengths	Bond angles
	
Torsions	Rings

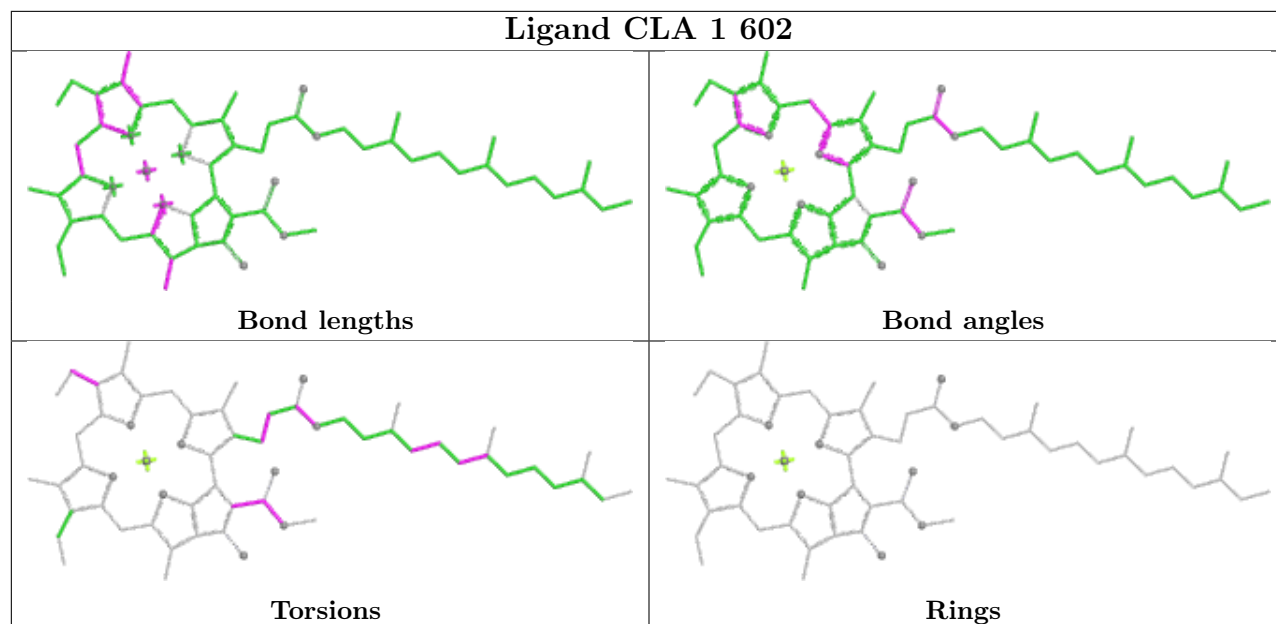
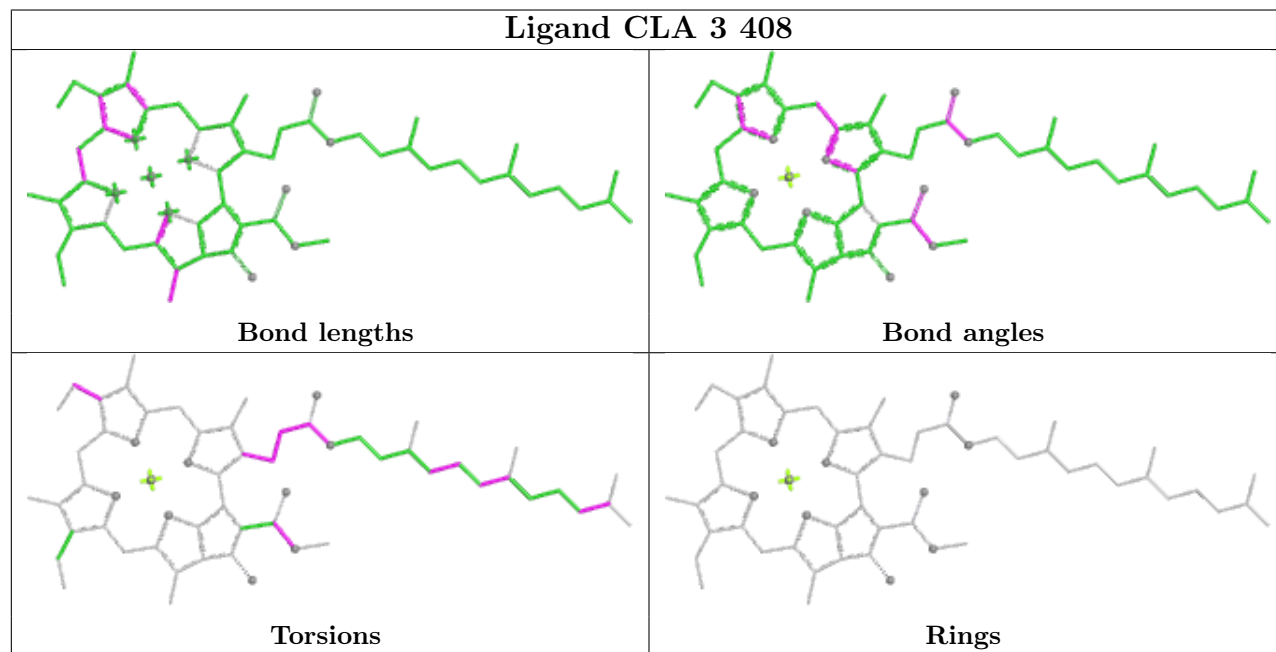
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Bond lengths	Bond angles
	
Torsions	Rings

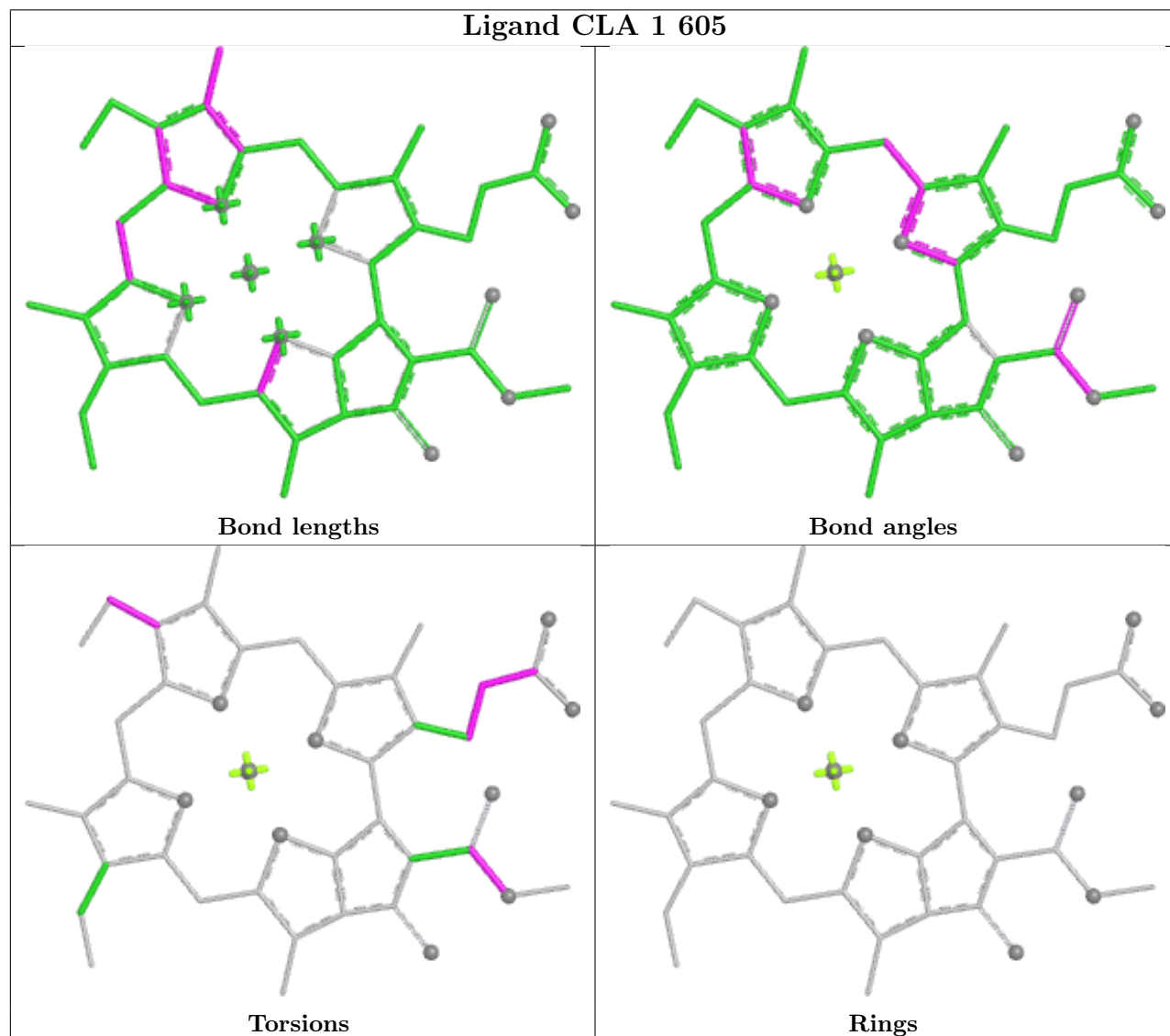
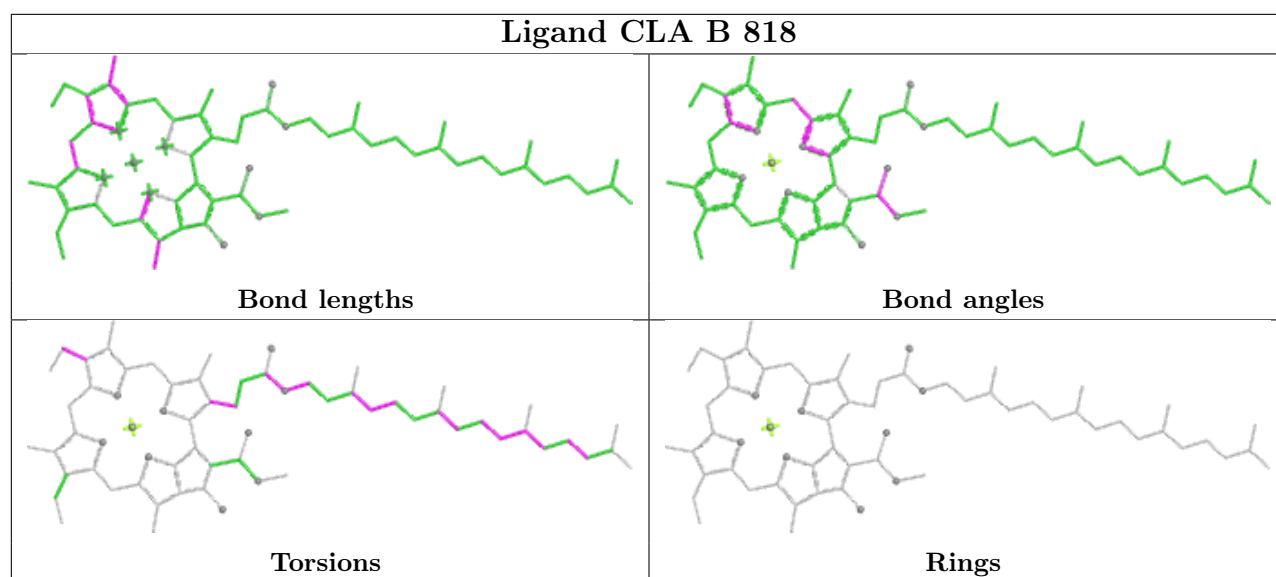
Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

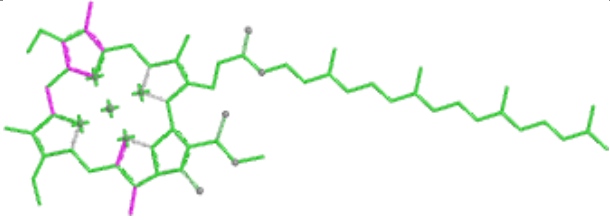
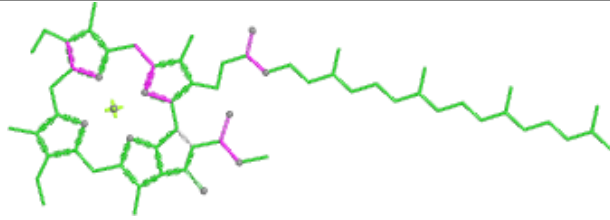
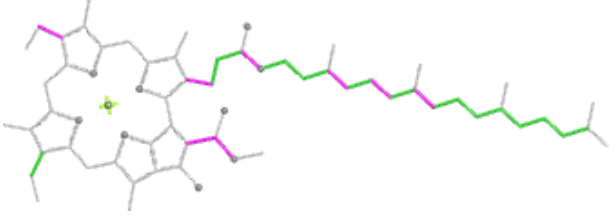
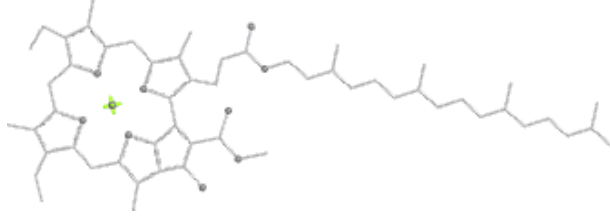
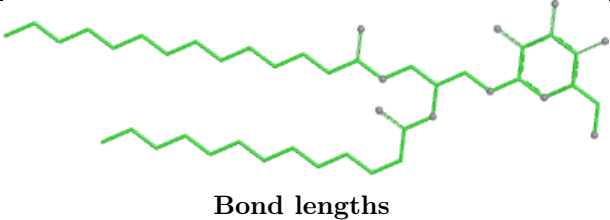
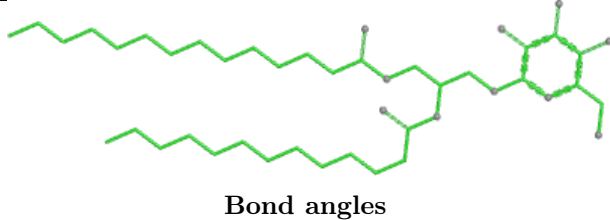
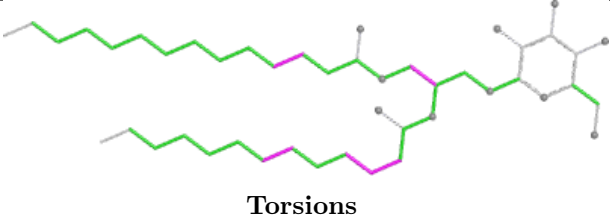
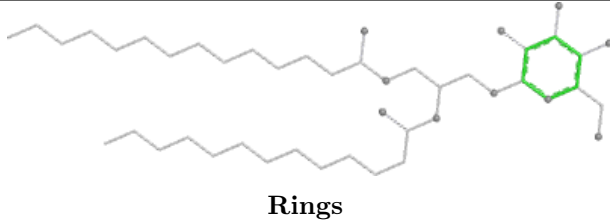
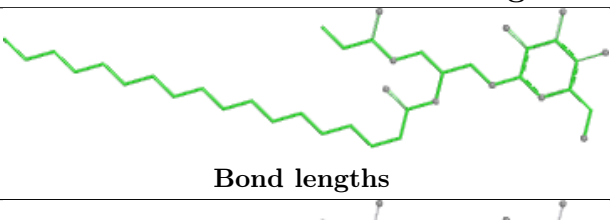
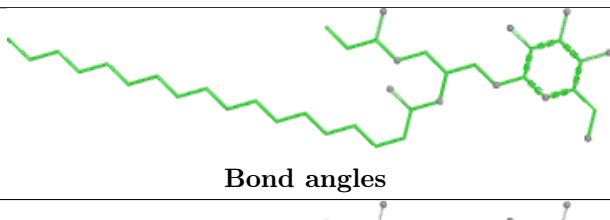
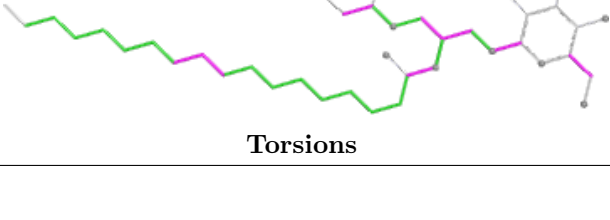
Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

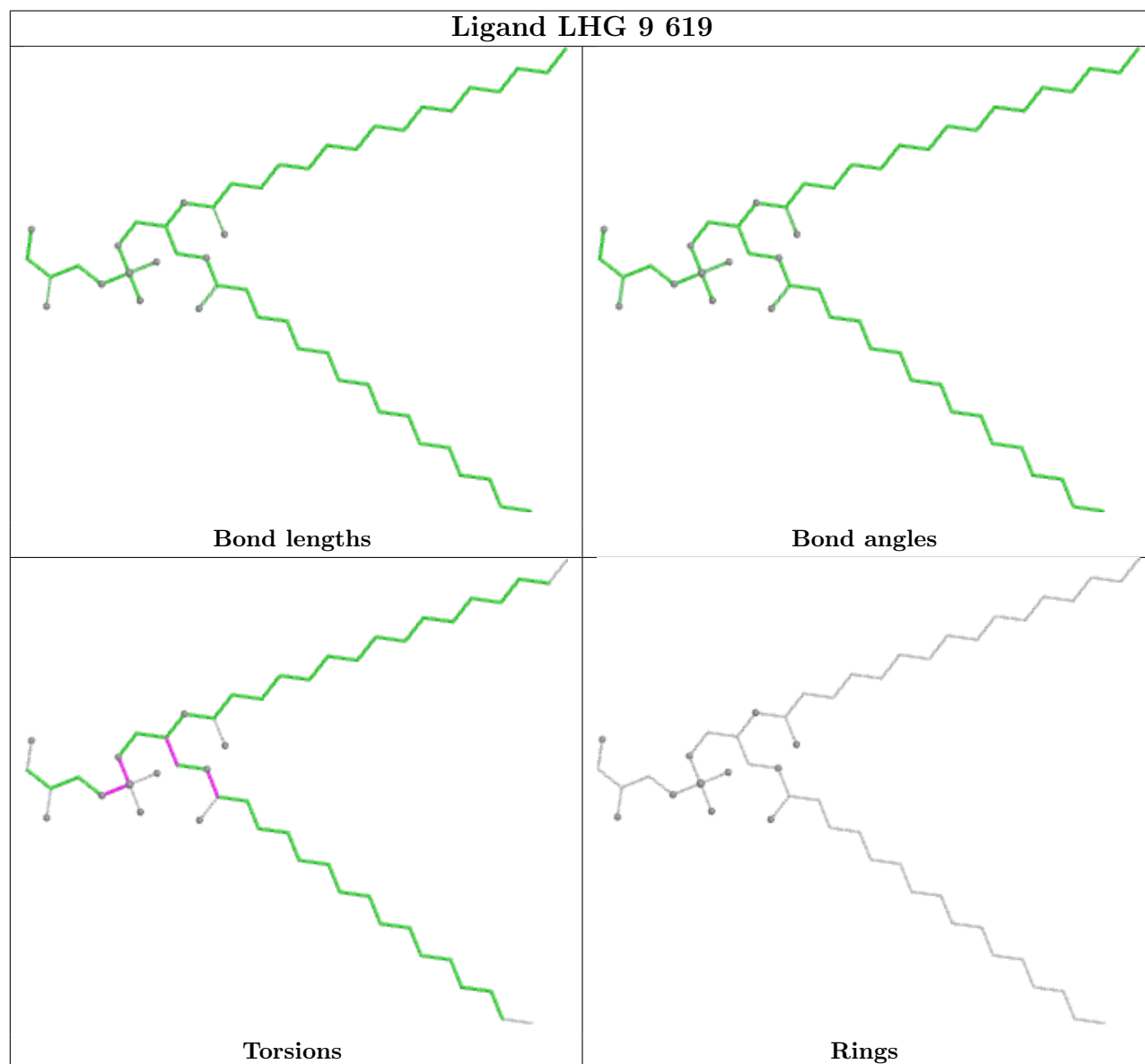
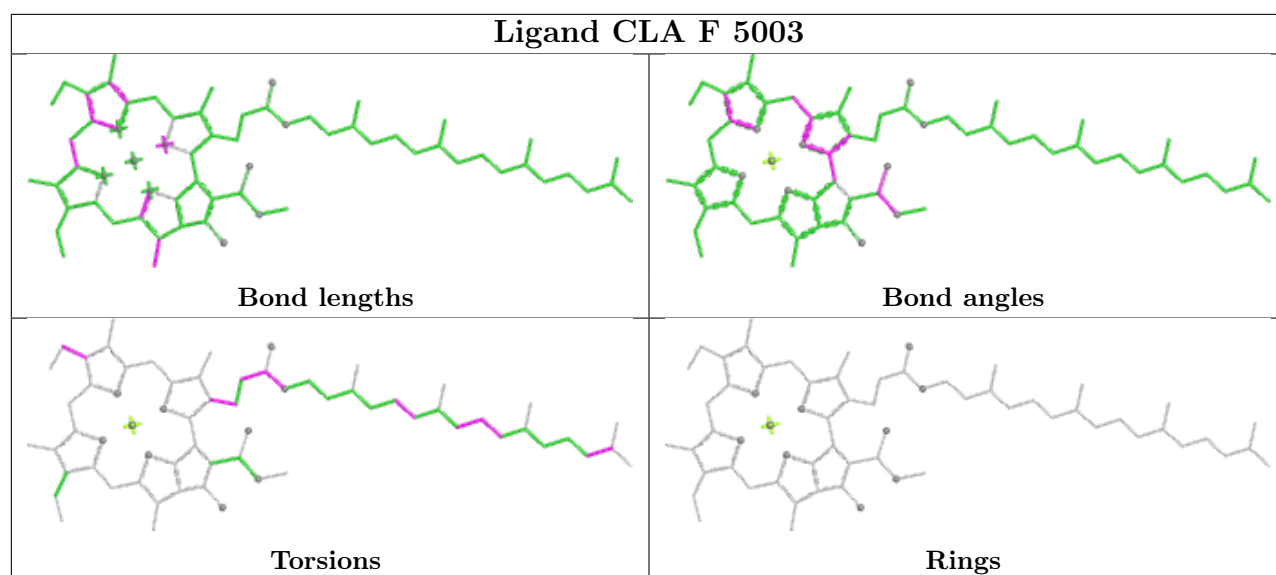




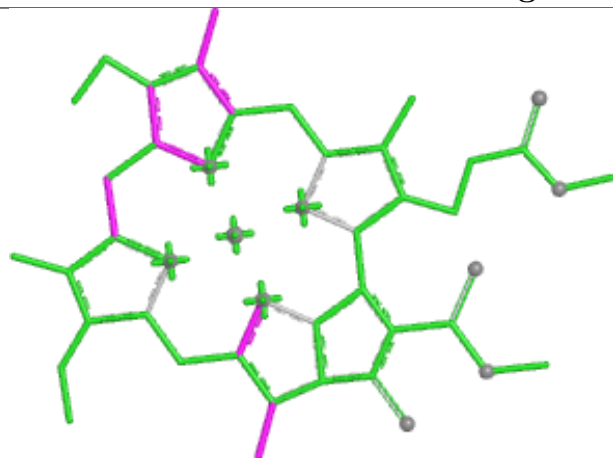
Ligand CLA 1 602**Ligand CLA 3 408**



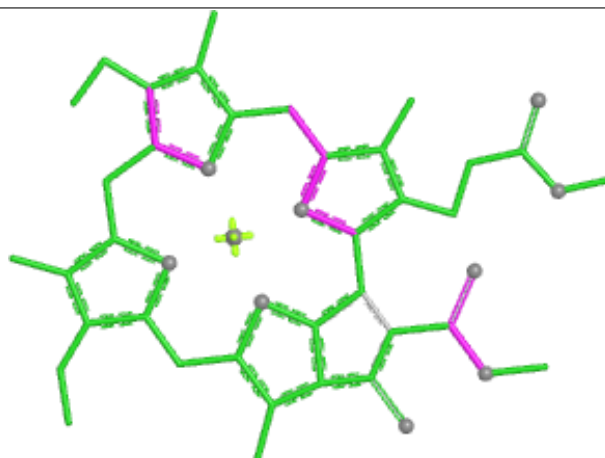
Ligand CLA 3 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG F 5001	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG 7 301	
 Bond lengths	 Bond angles
 Torsions	 Rings



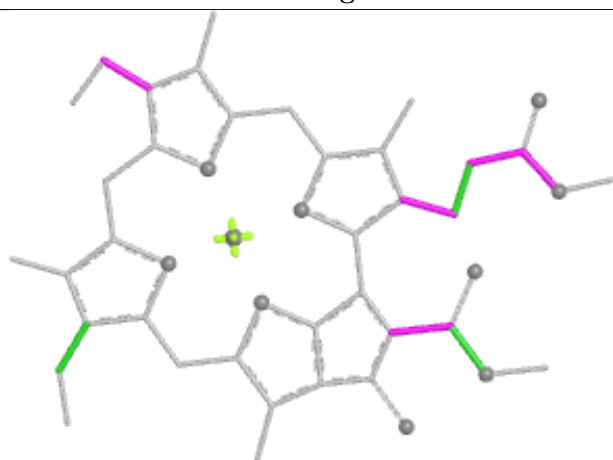
Ligand CLA 2 607



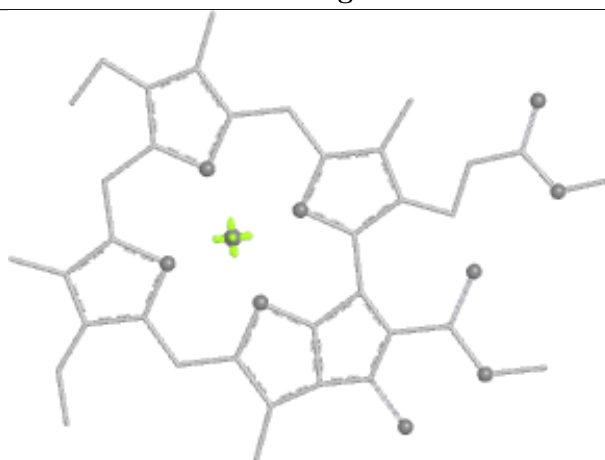
Bond lengths



Bond angles

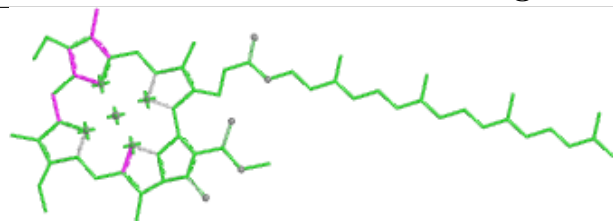


Torsions

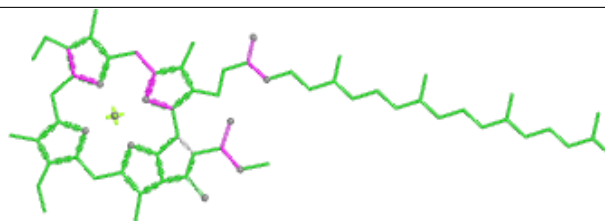


Rings

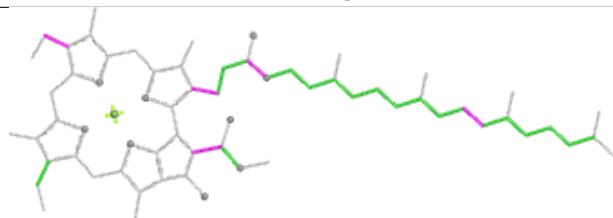
Ligand CLA A 807



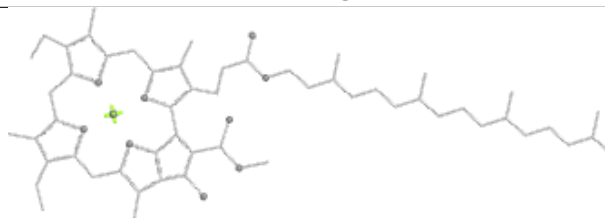
Bond lengths



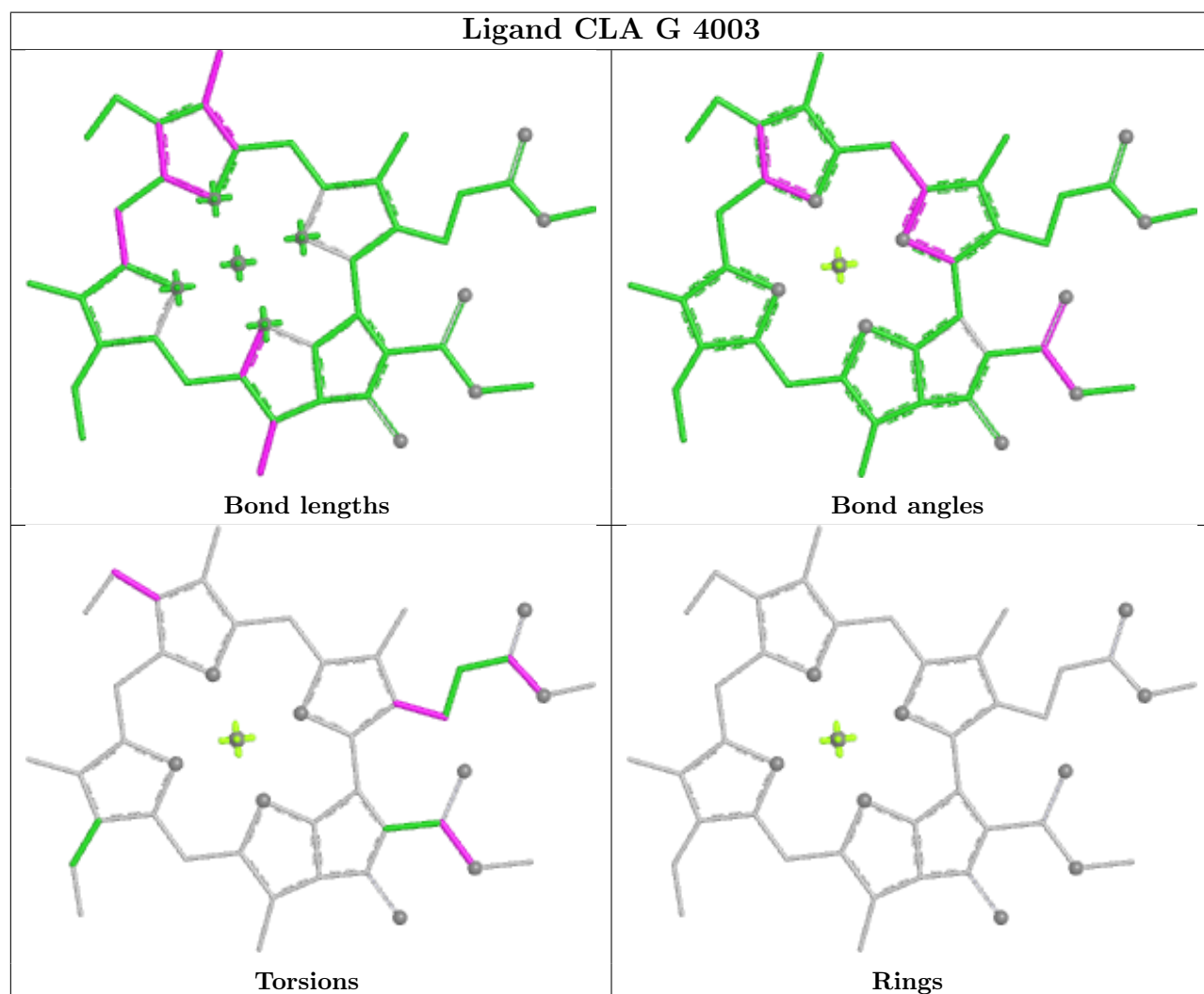
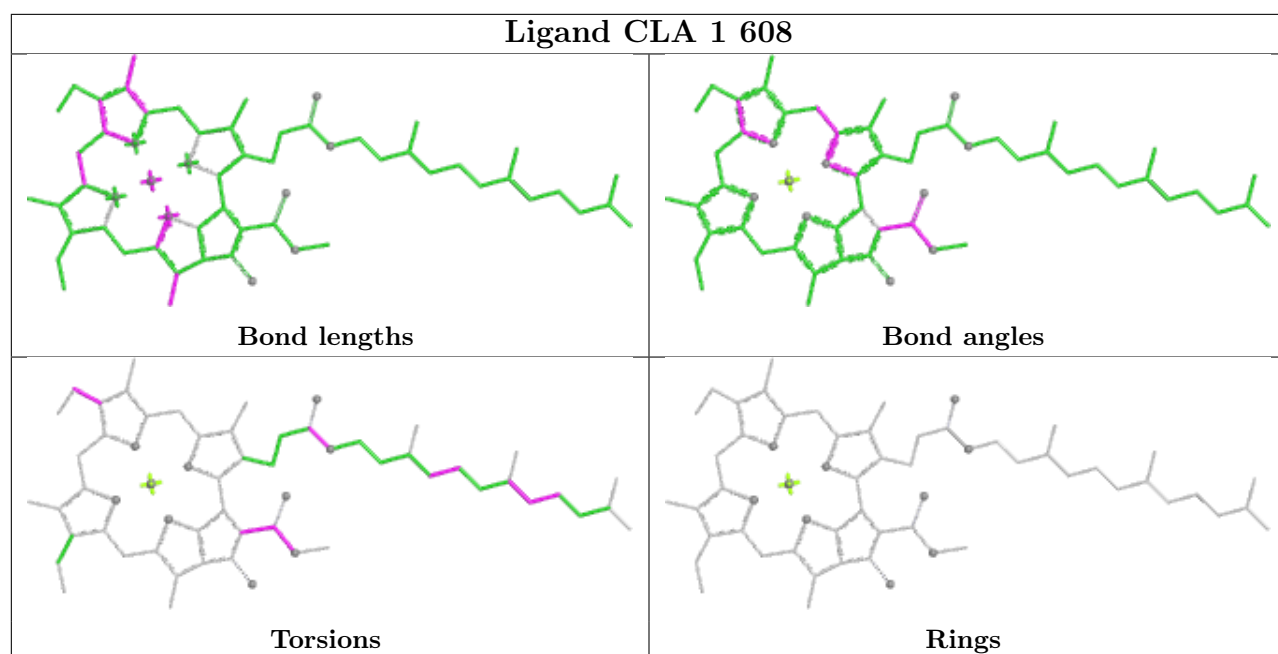
Bond angles

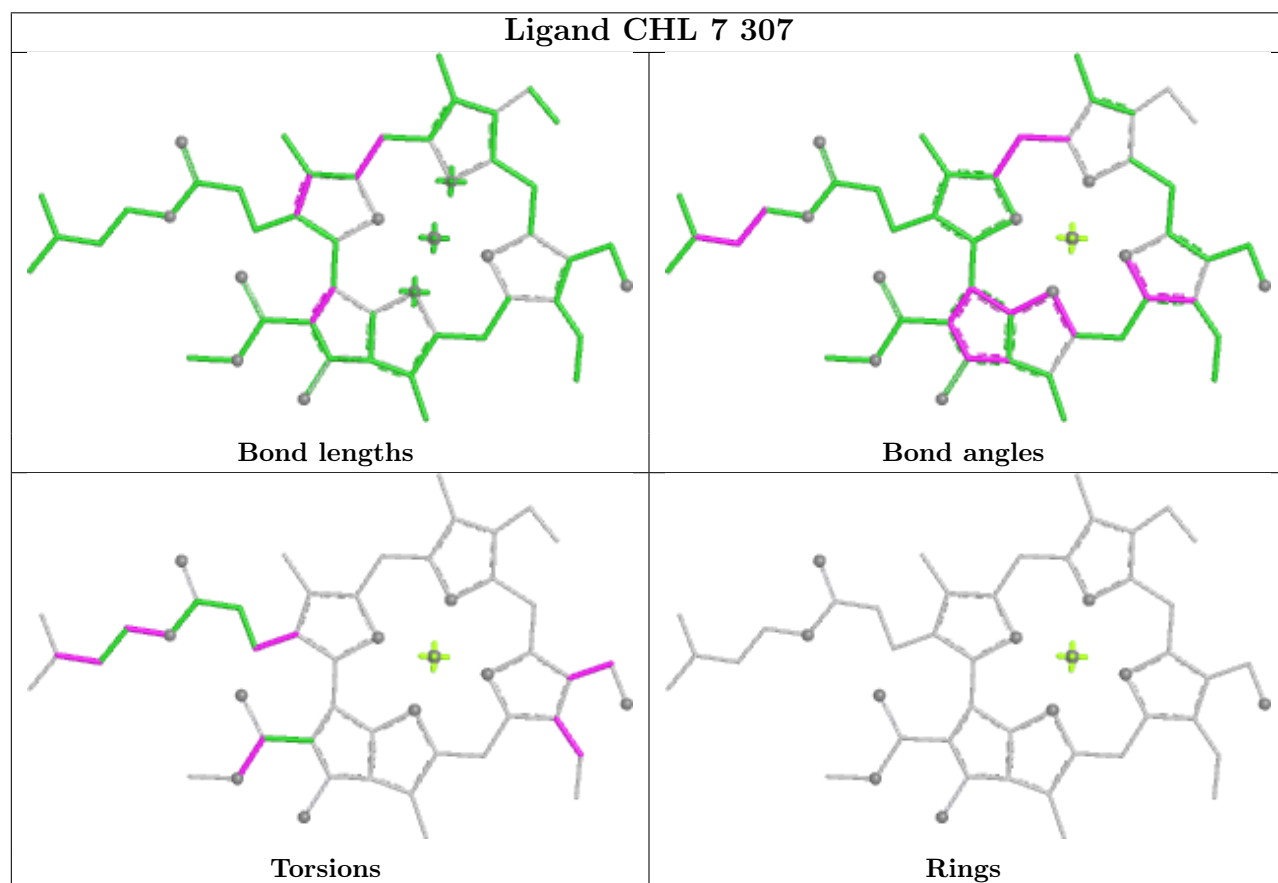
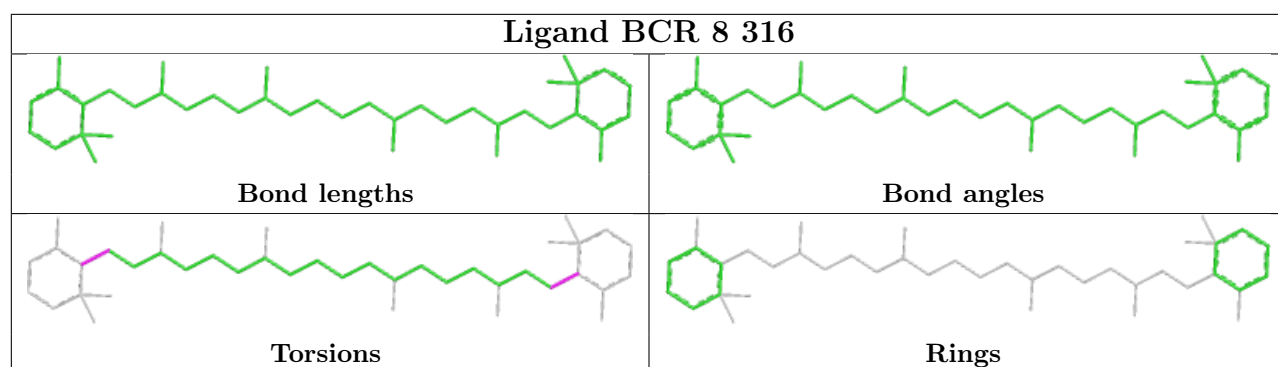


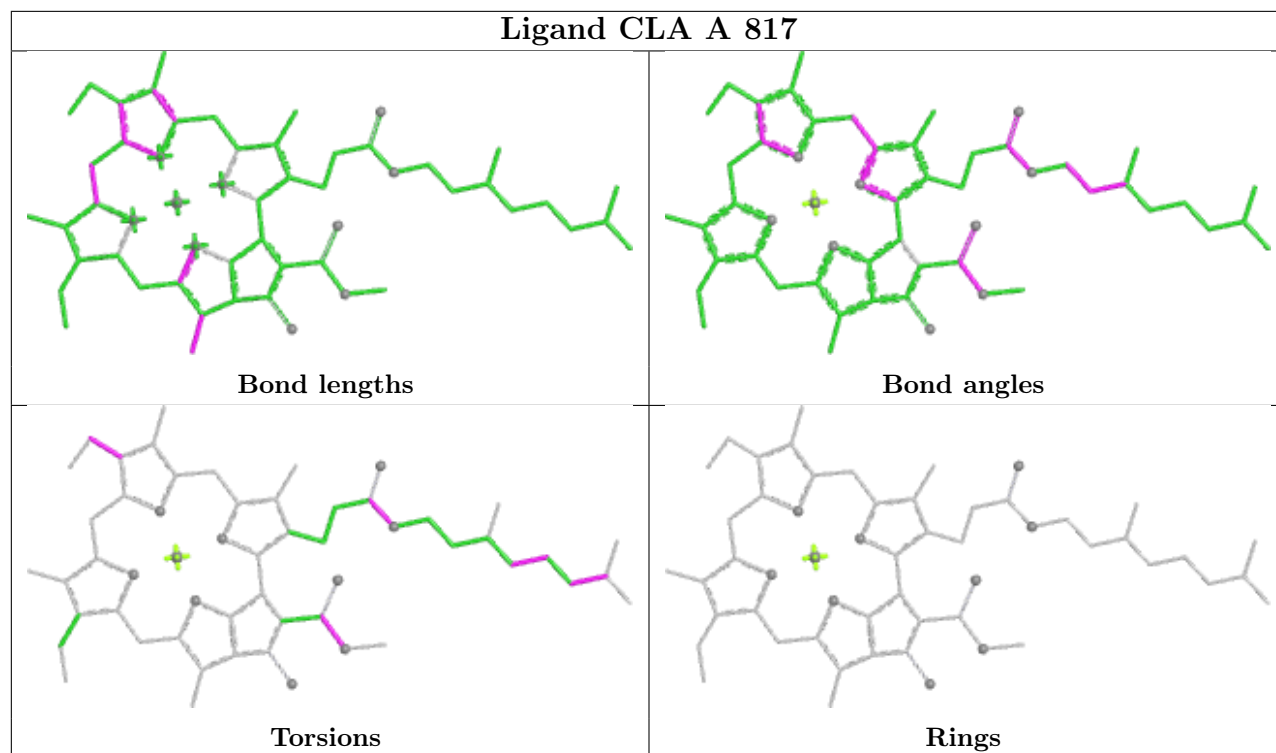
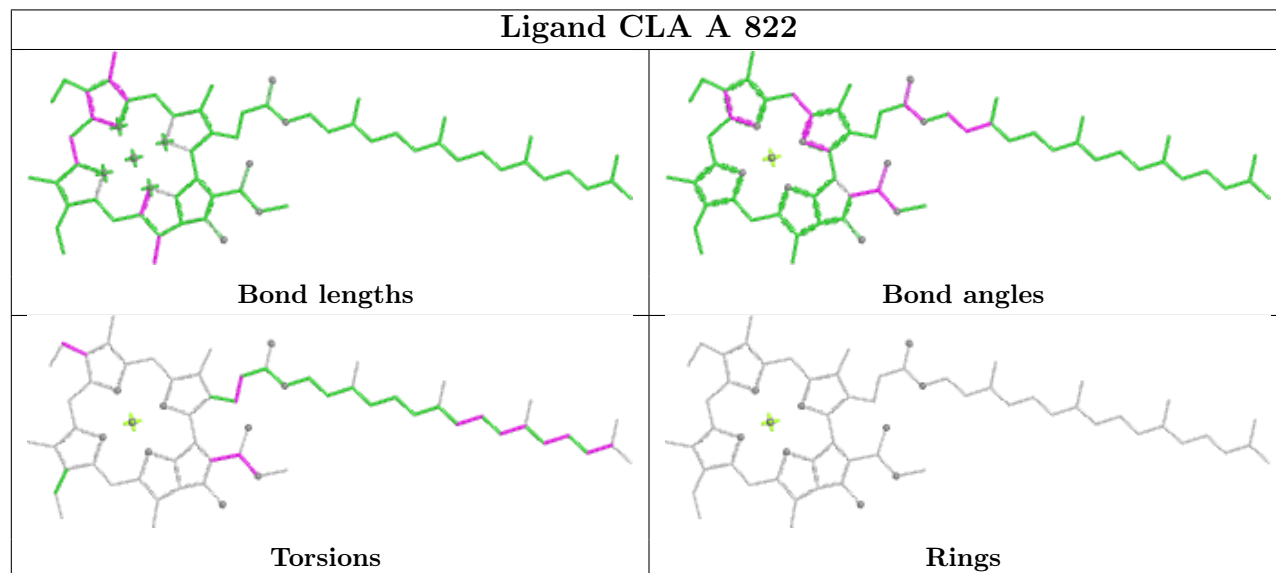
Torsions

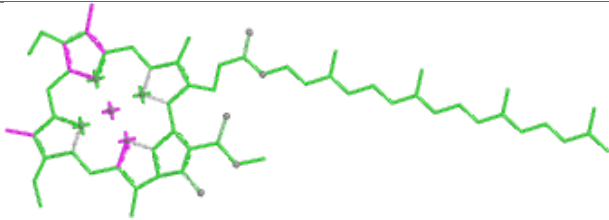
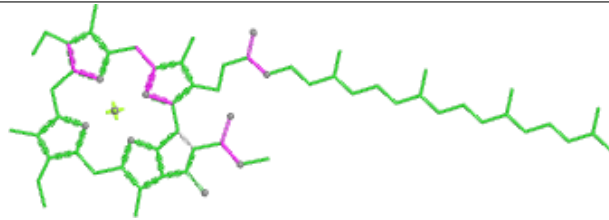
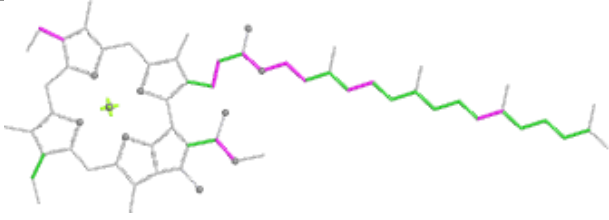
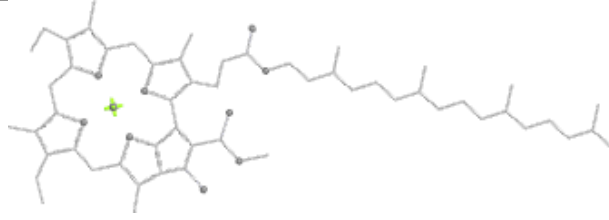


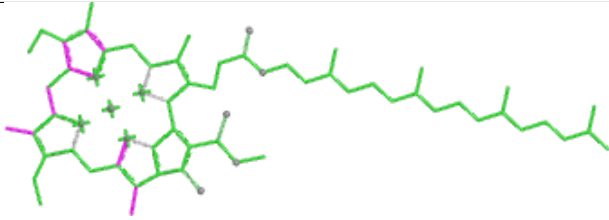
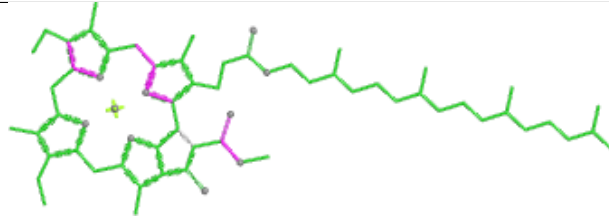
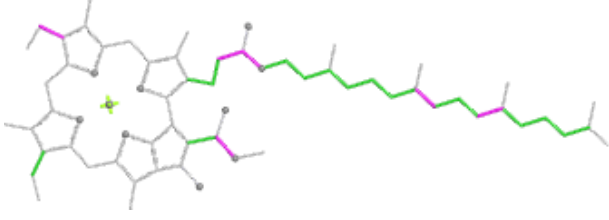
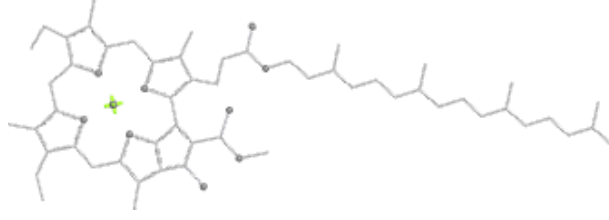
Rings

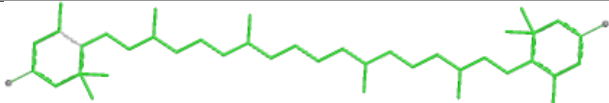
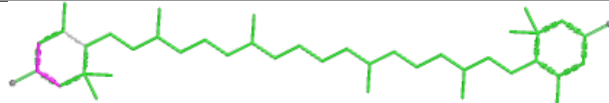
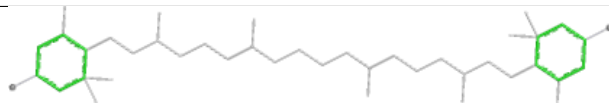




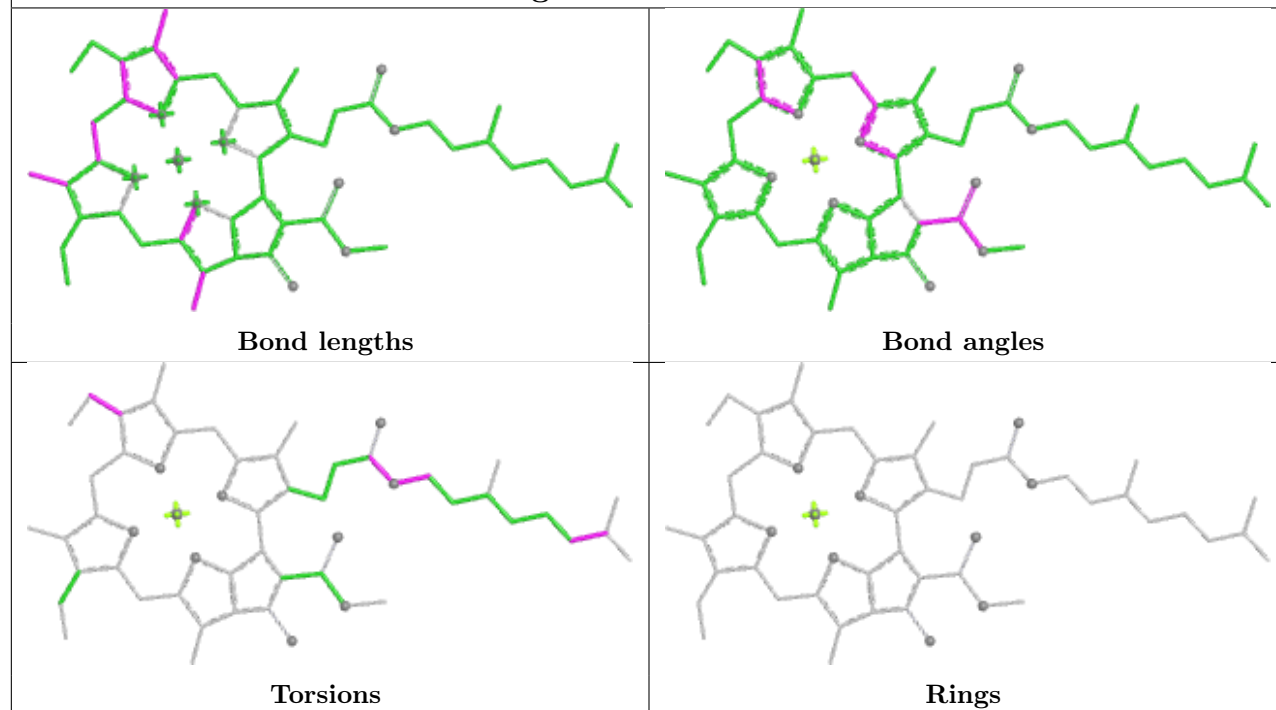
Ligand CLA A 817**Ligand CLA A 822**

Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

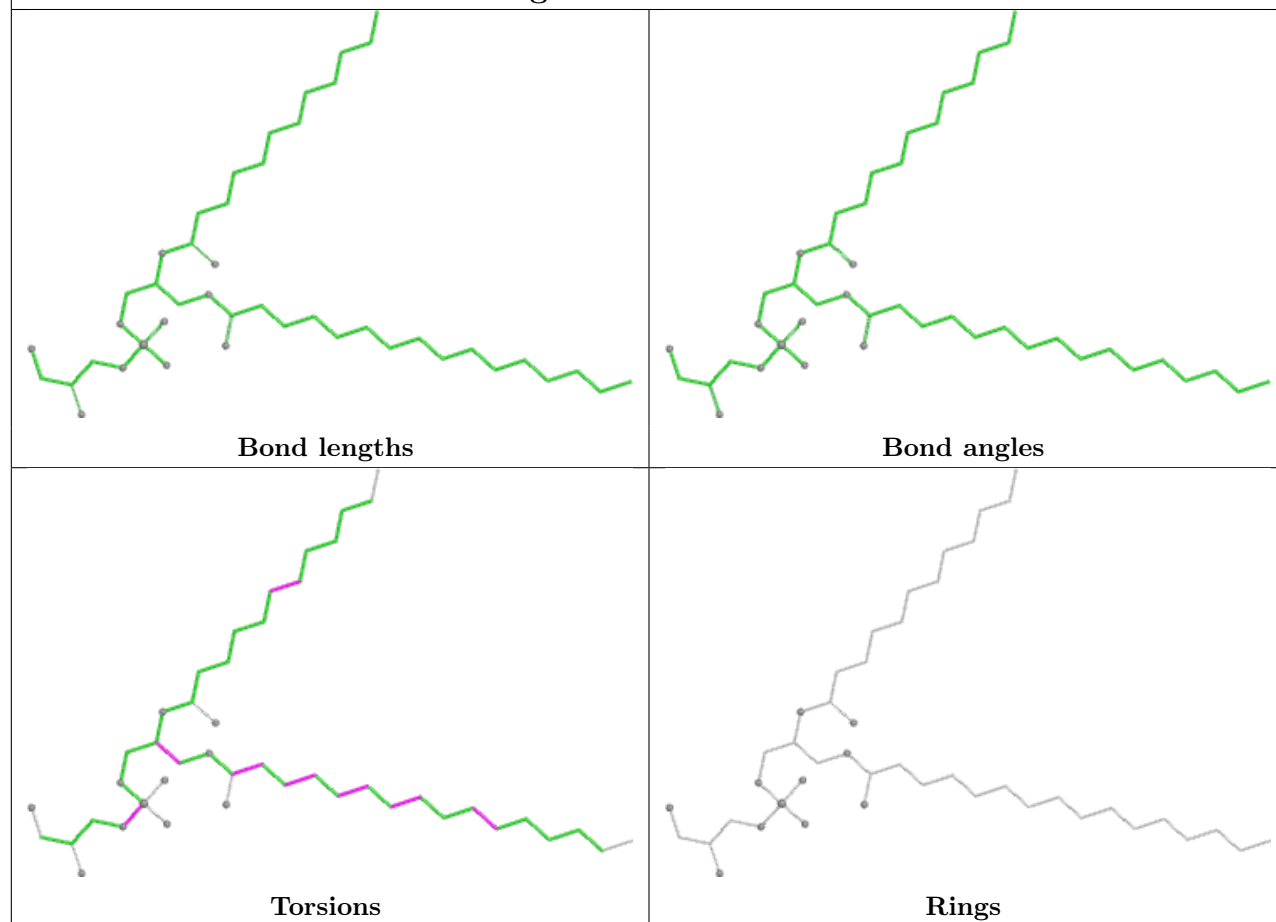
Ligand CLA B 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

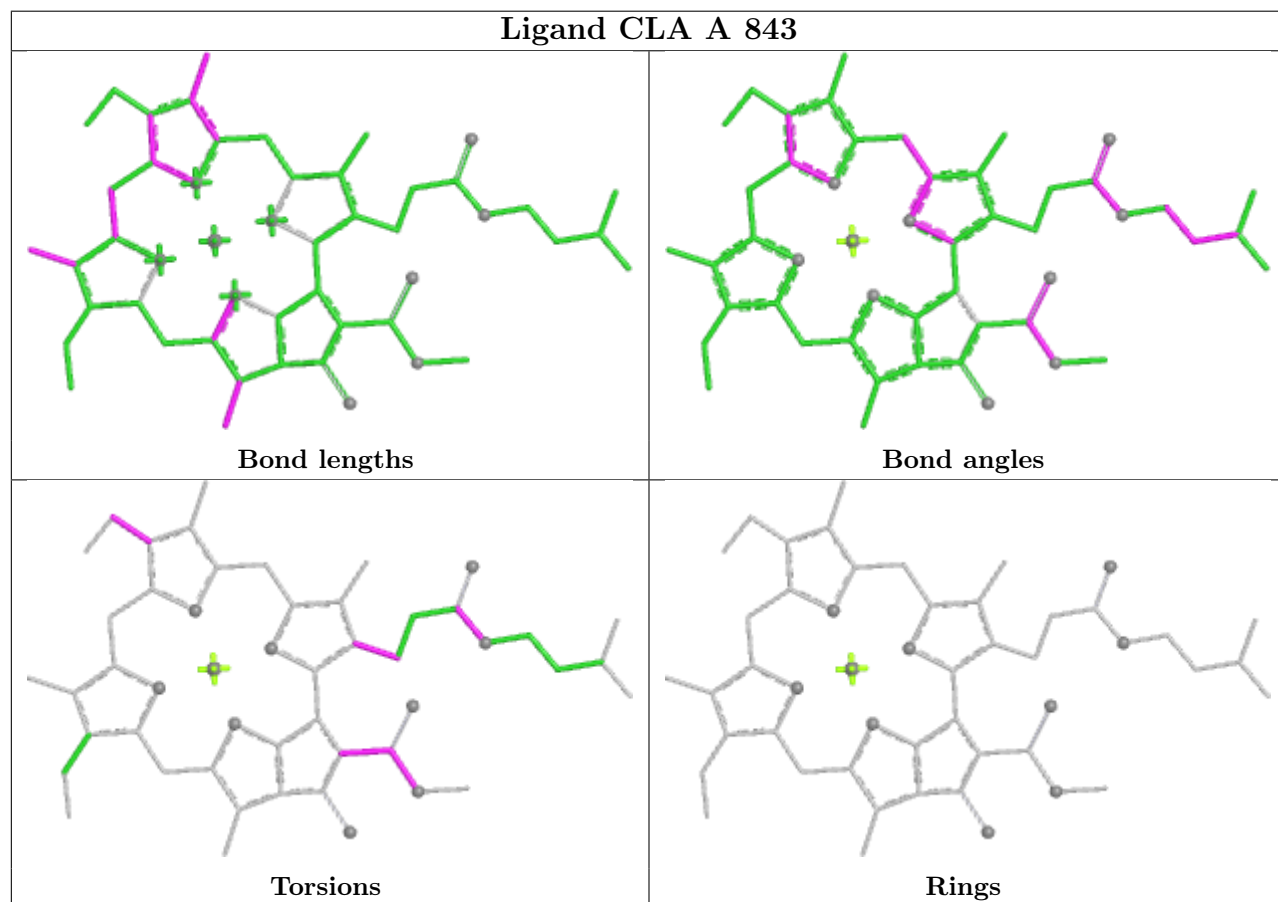
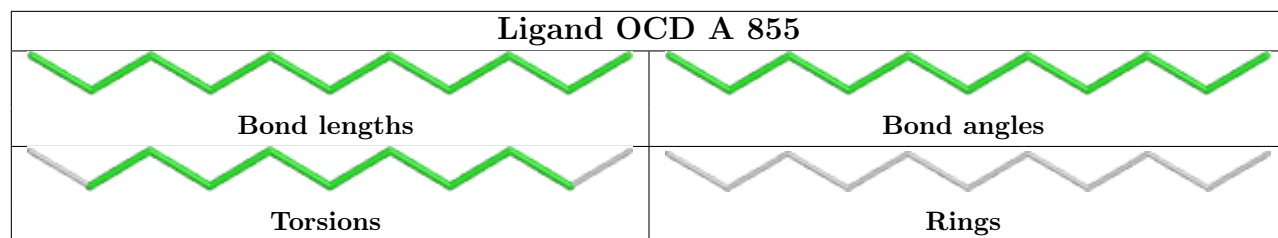
Ligand LUT 2 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 834

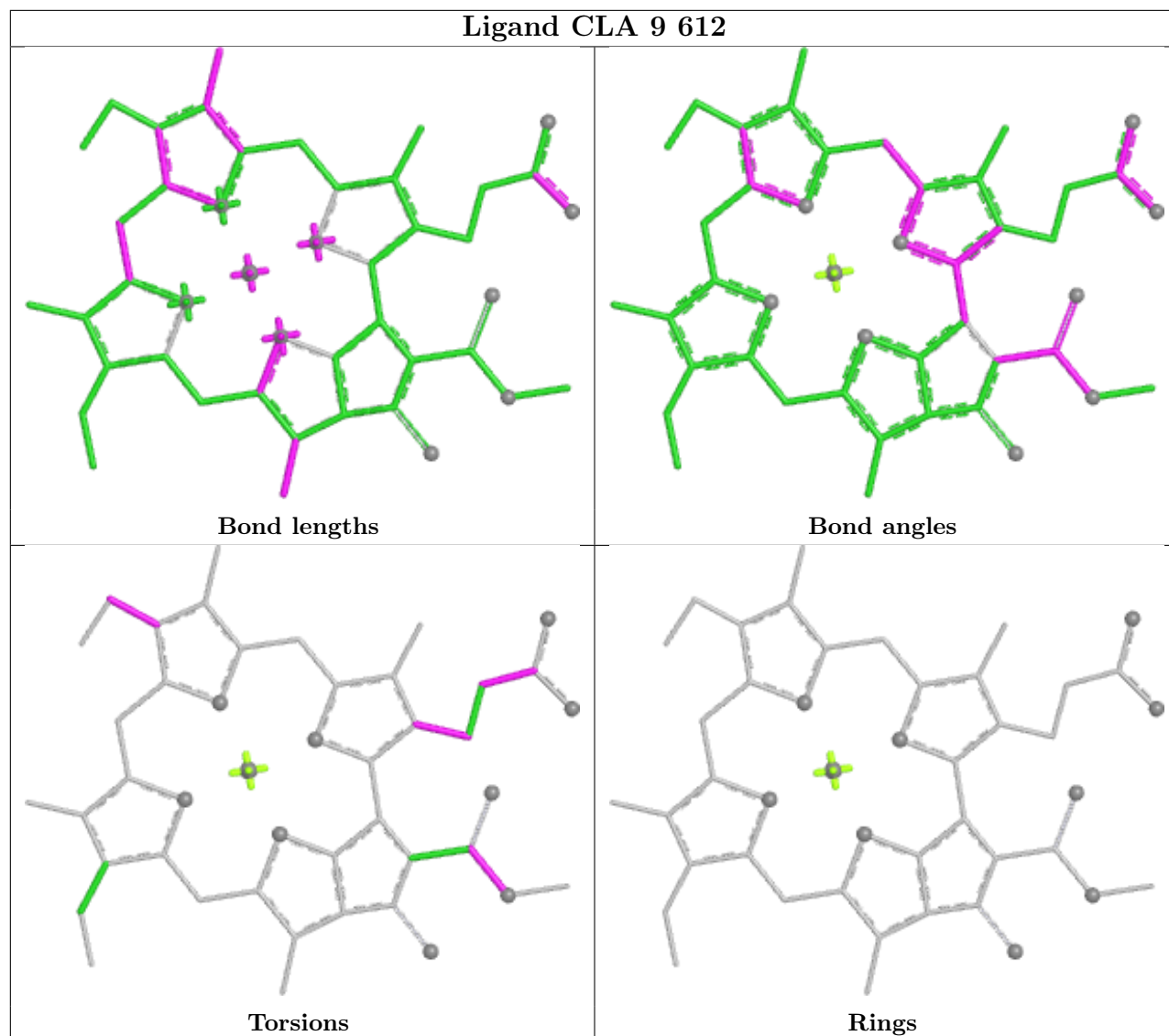


Ligand LHG A 854

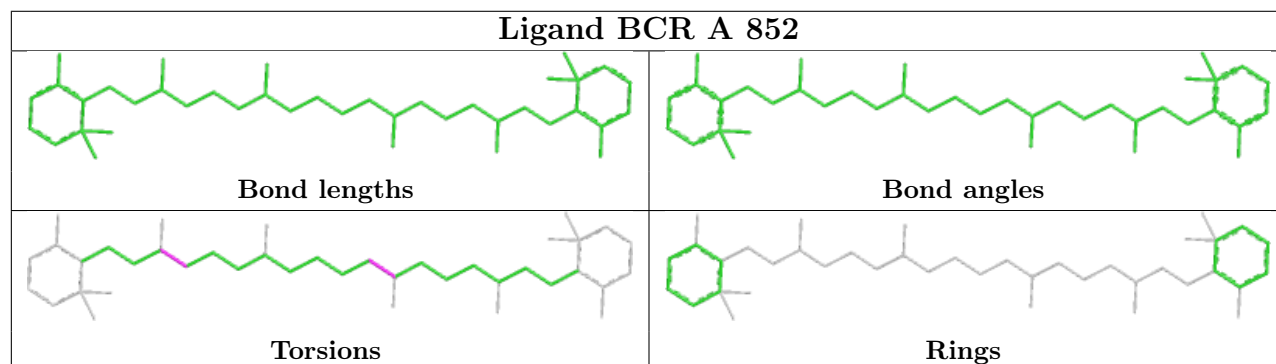


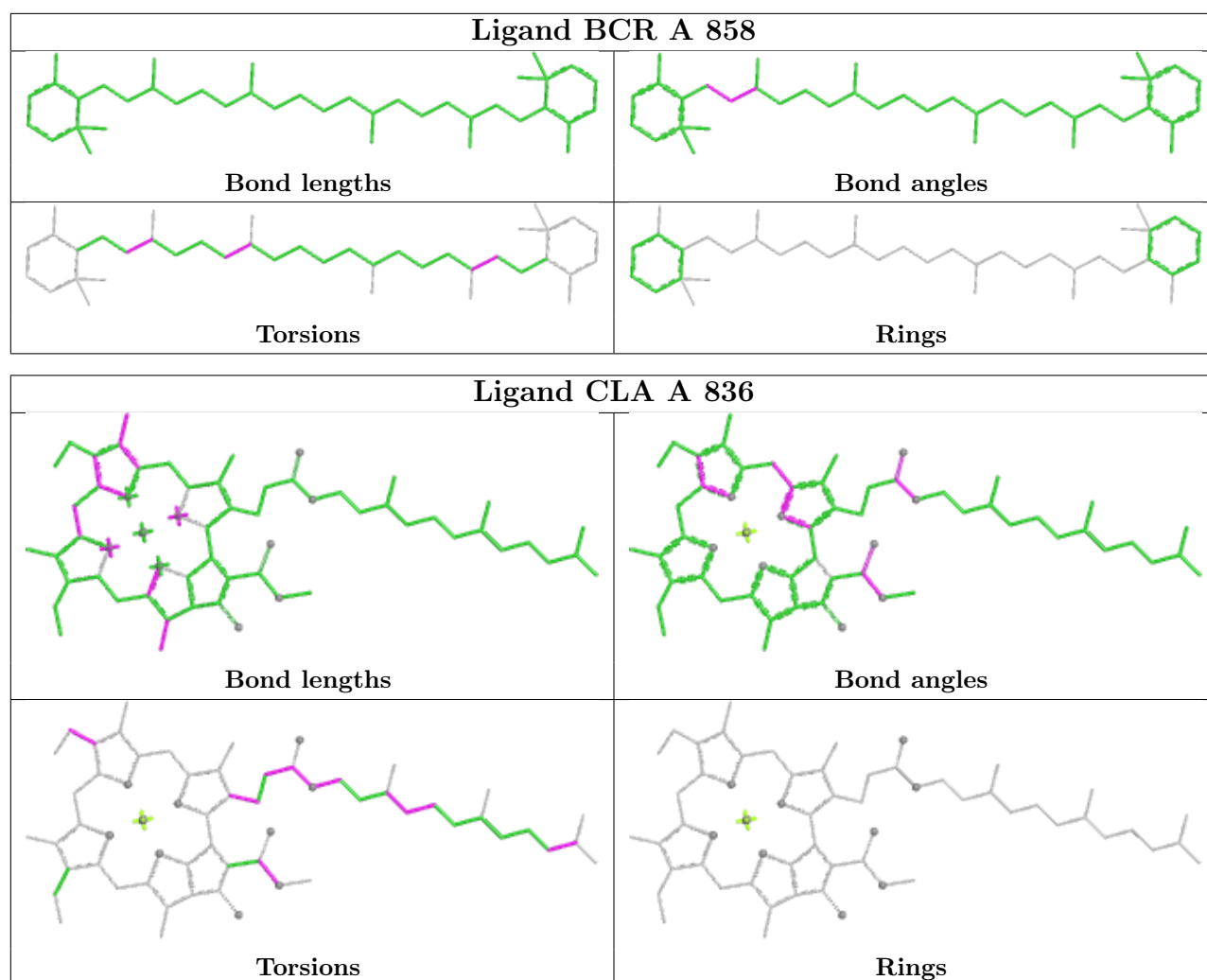


Ligand CLA 9 612

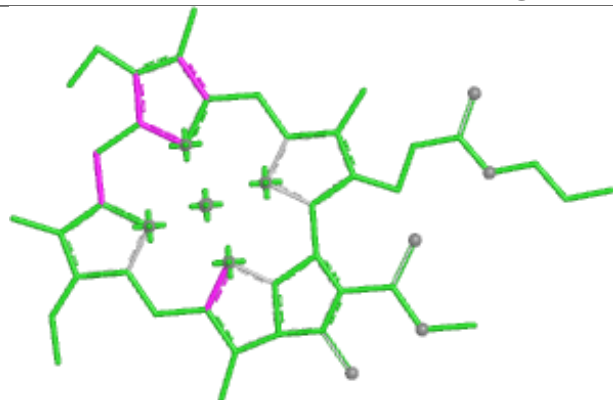


Ligand BCR A 852

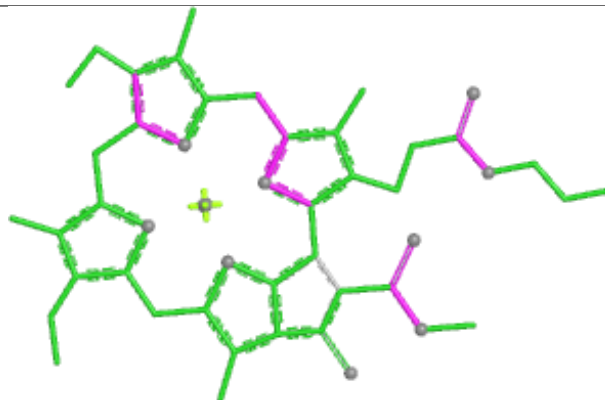




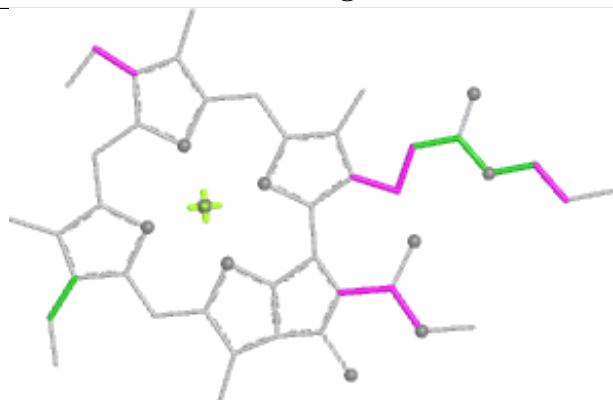
Ligand CLA K 204



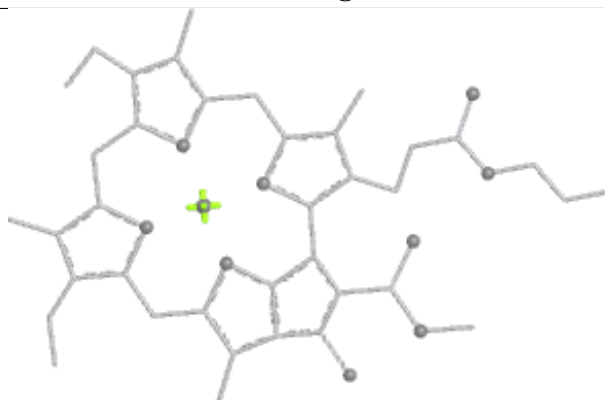
Bond lengths



Bond angles

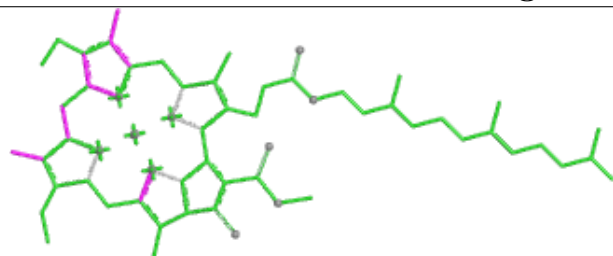


Torsions

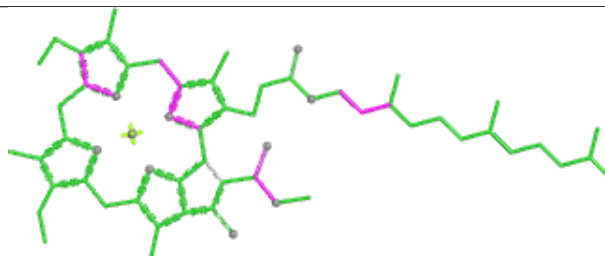


Rings

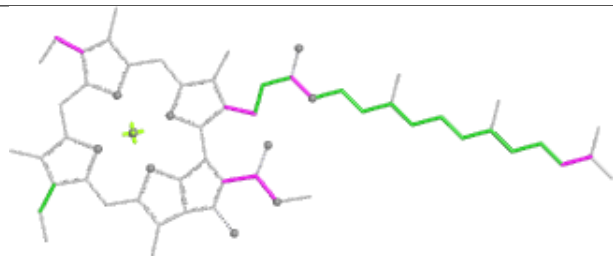
Ligand CLA 7 303



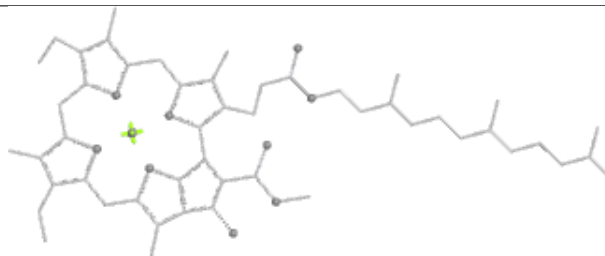
Bond lengths



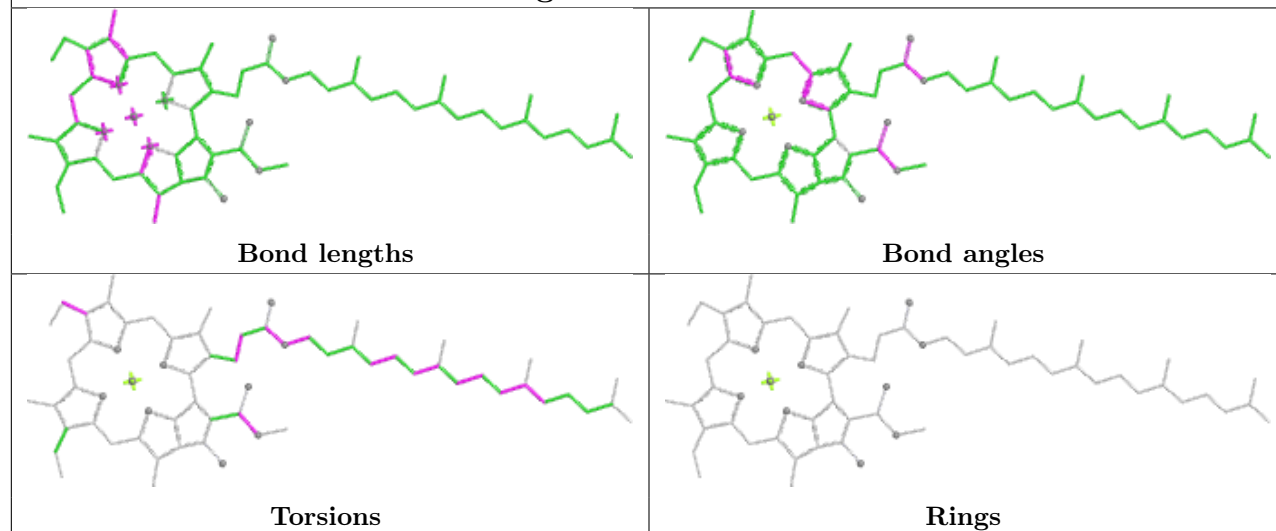
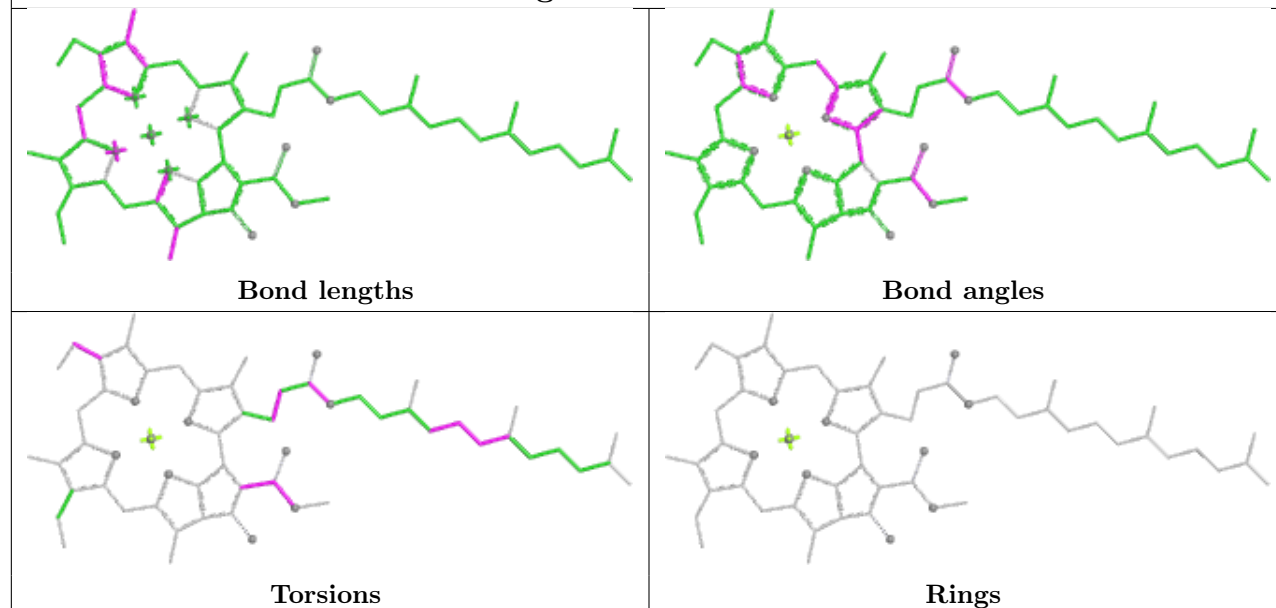
Bond angles



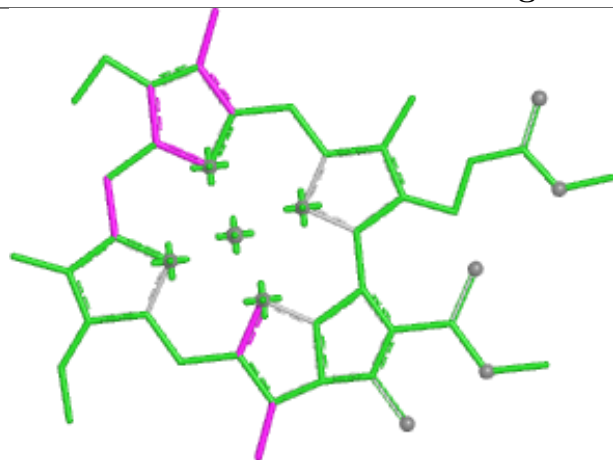
Torsions



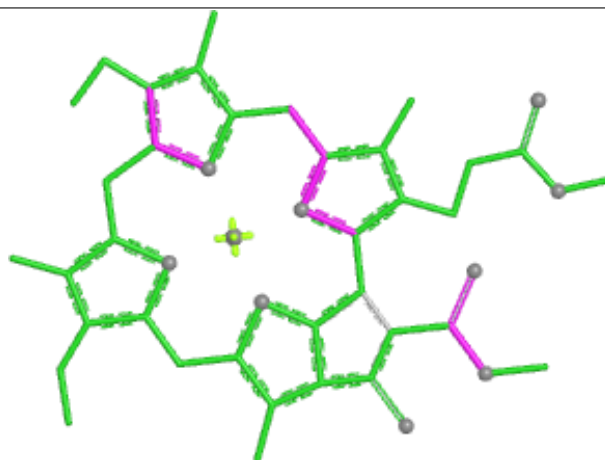
Rings

Ligand CLA 8 311**Ligand CLA 2 603**

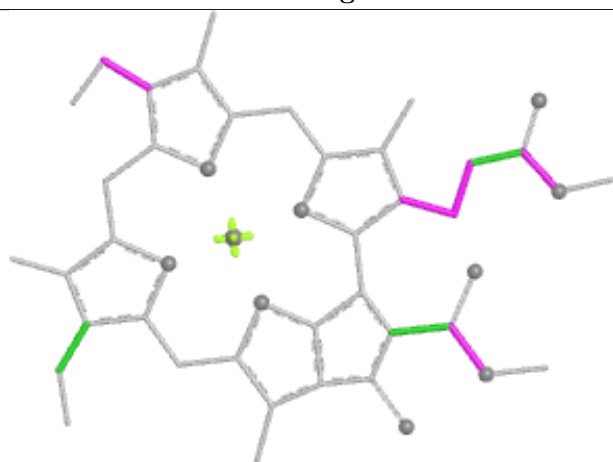
Ligand CLA 3 414



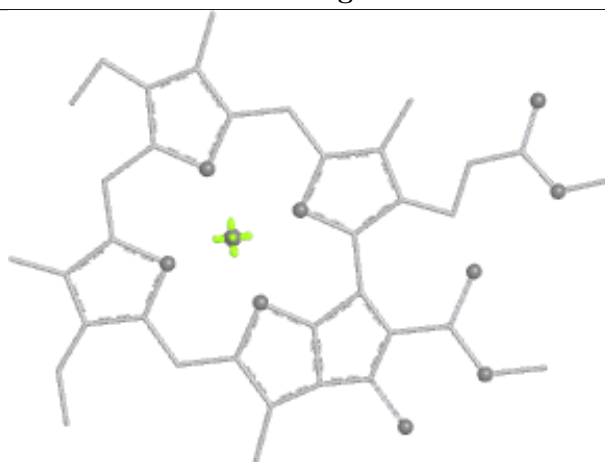
Bond lengths



Bond angles

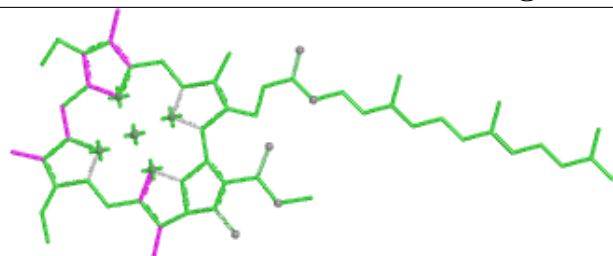


Torsions

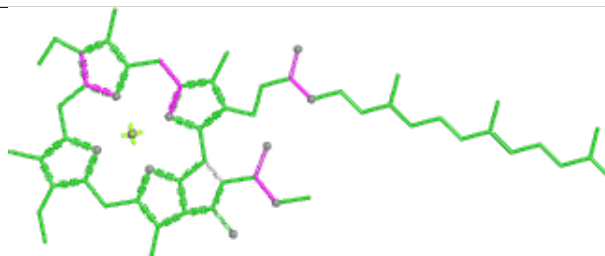


Rings

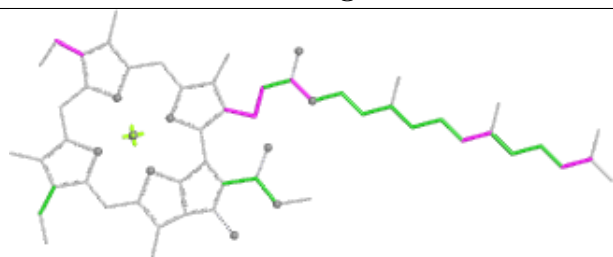
Ligand CLA 8 308



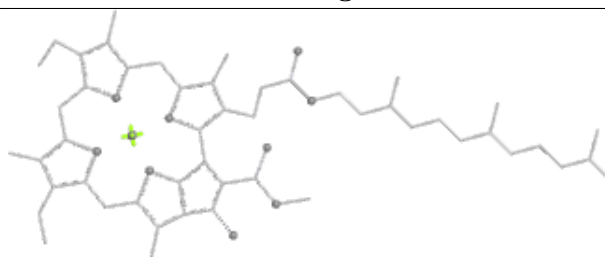
Bond lengths



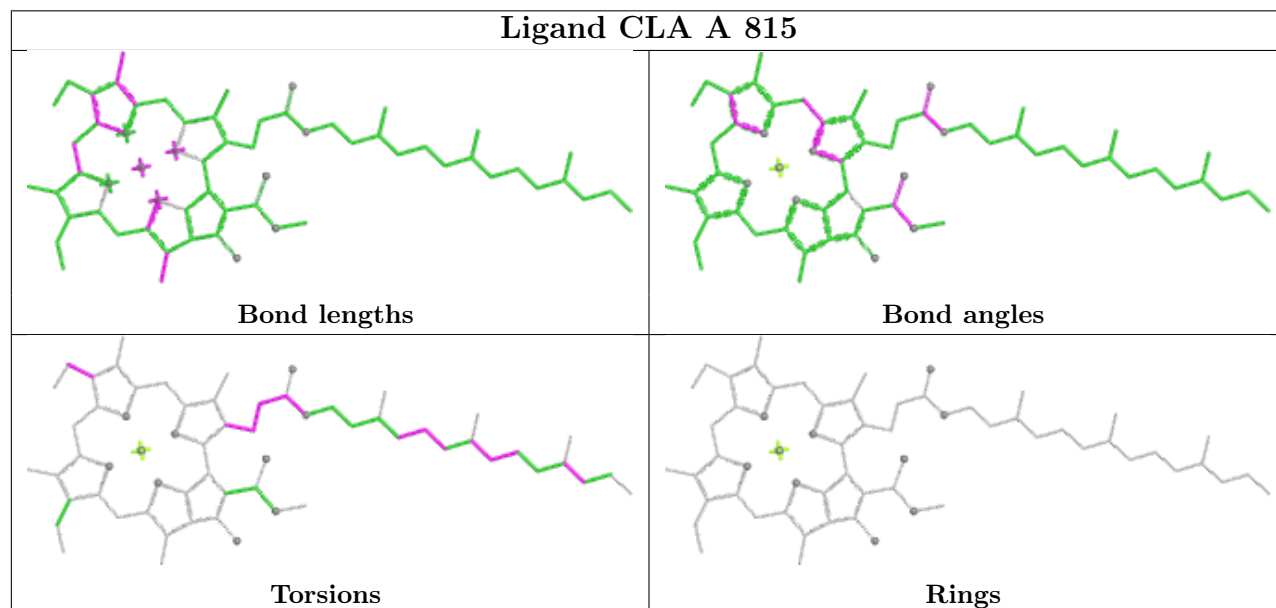
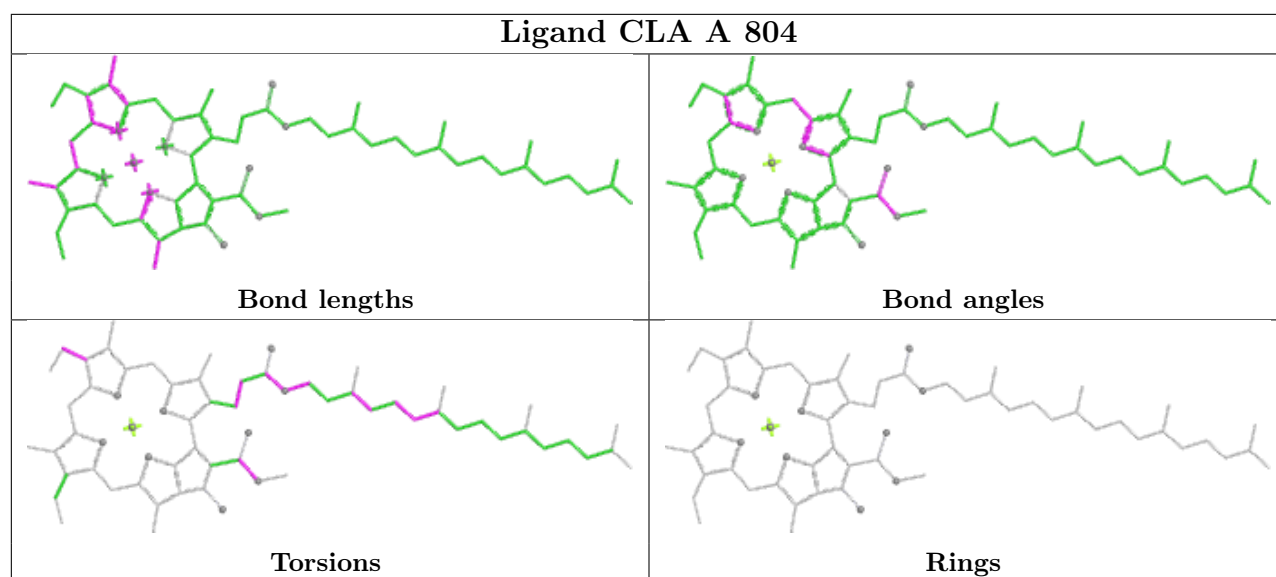
Bond angles

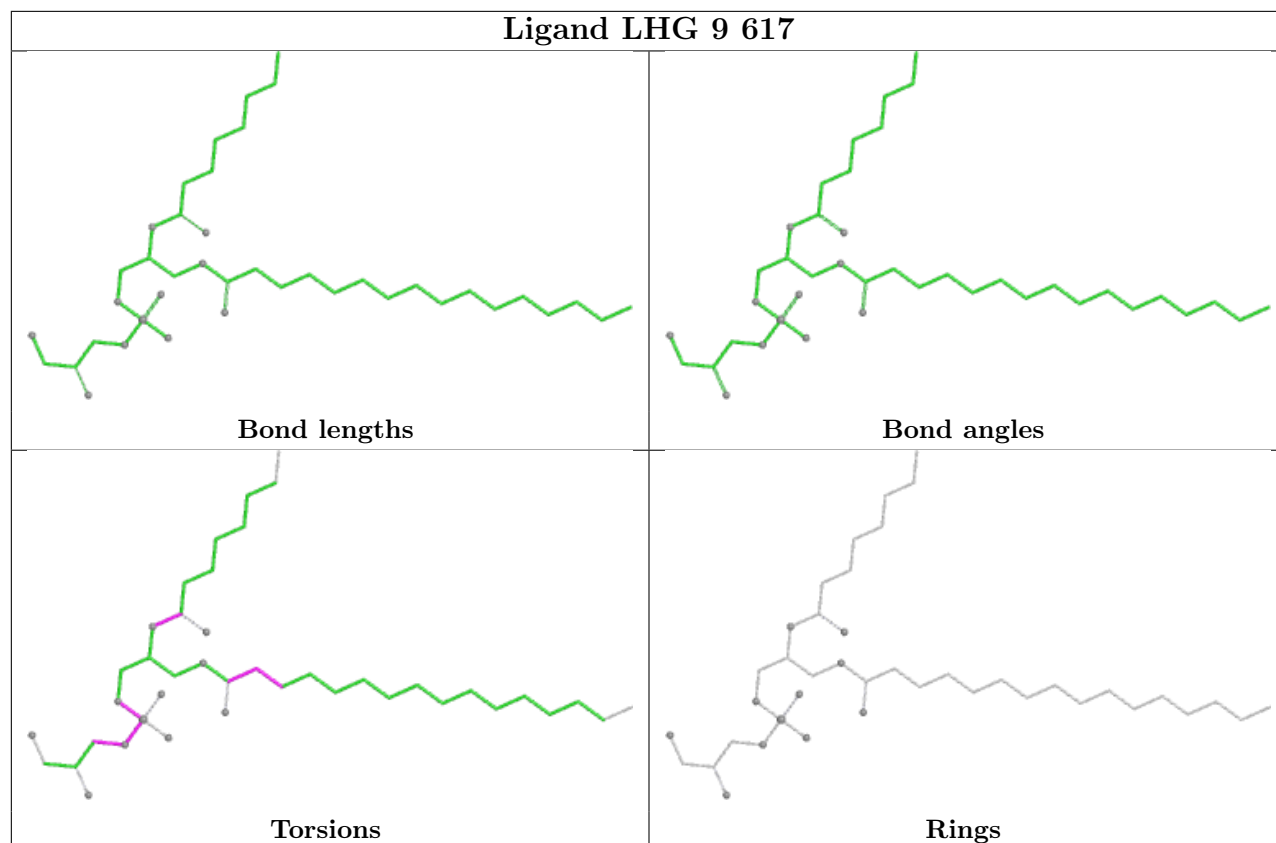
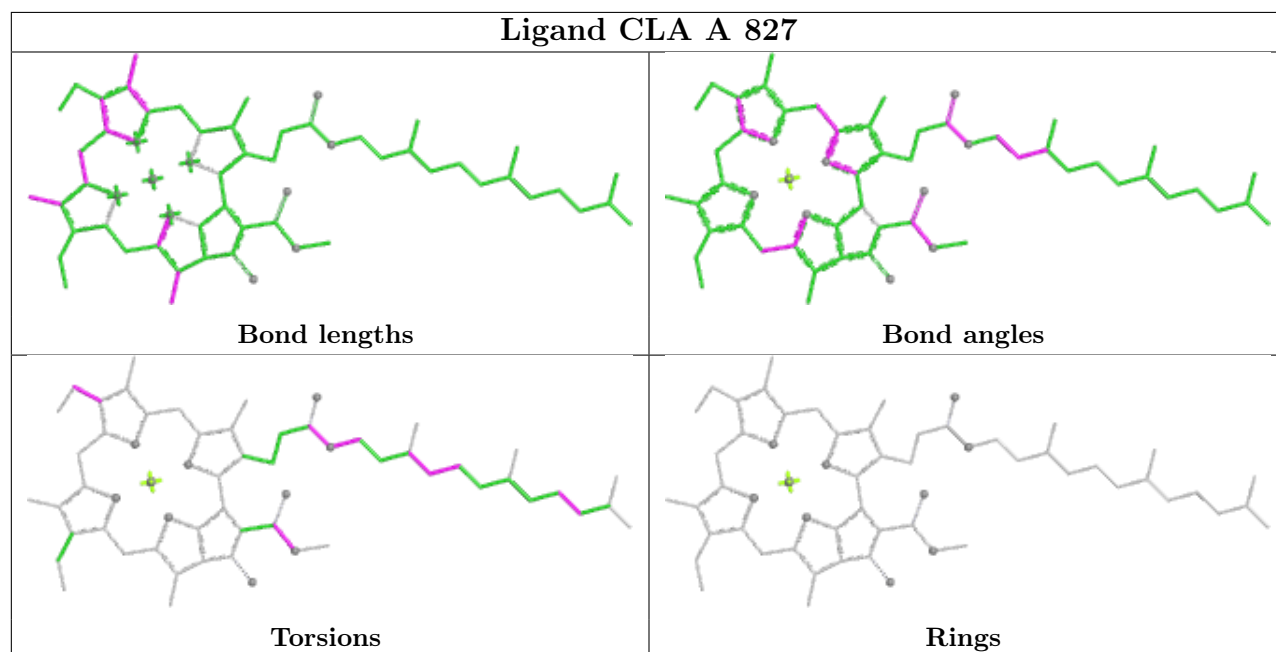


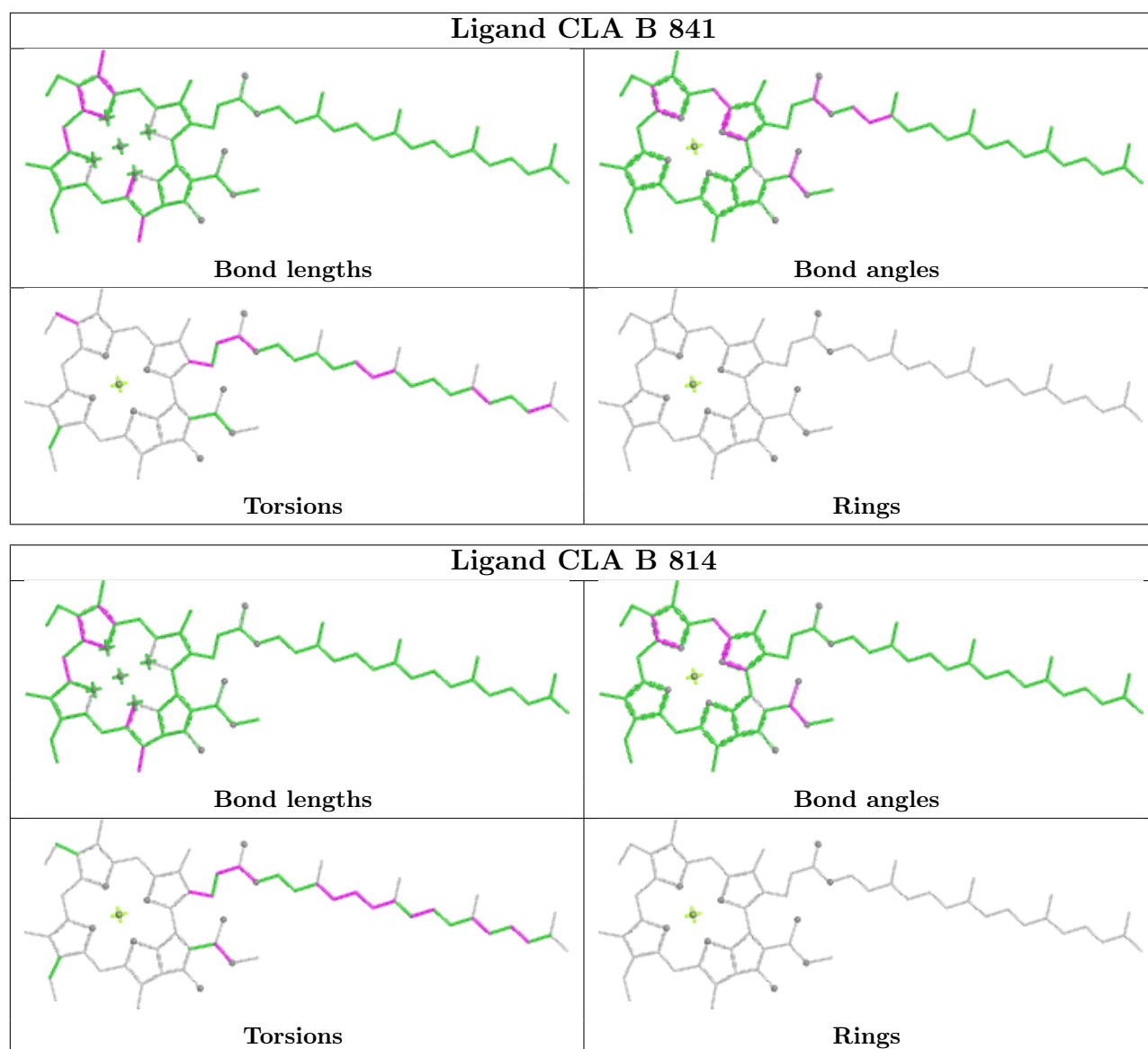
Torsions



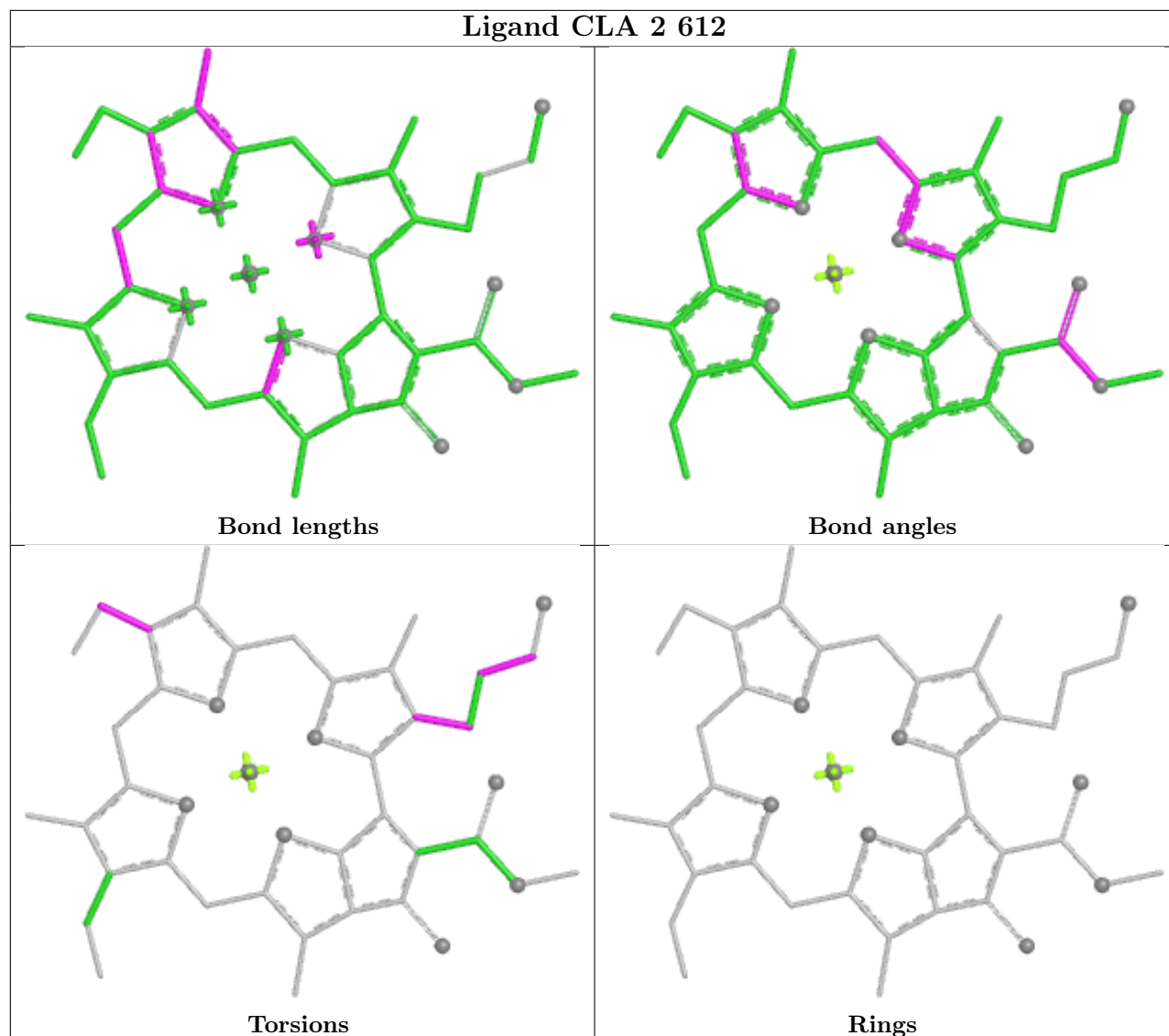
Rings



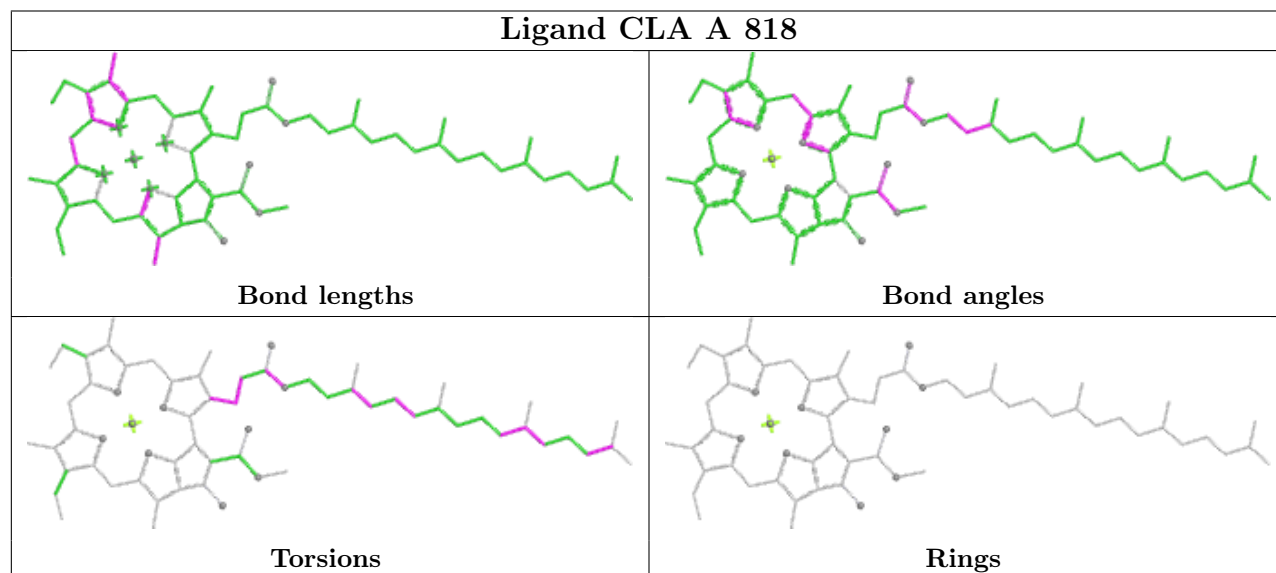
Ligand LHG 9 617**Ligand CLA A 827**

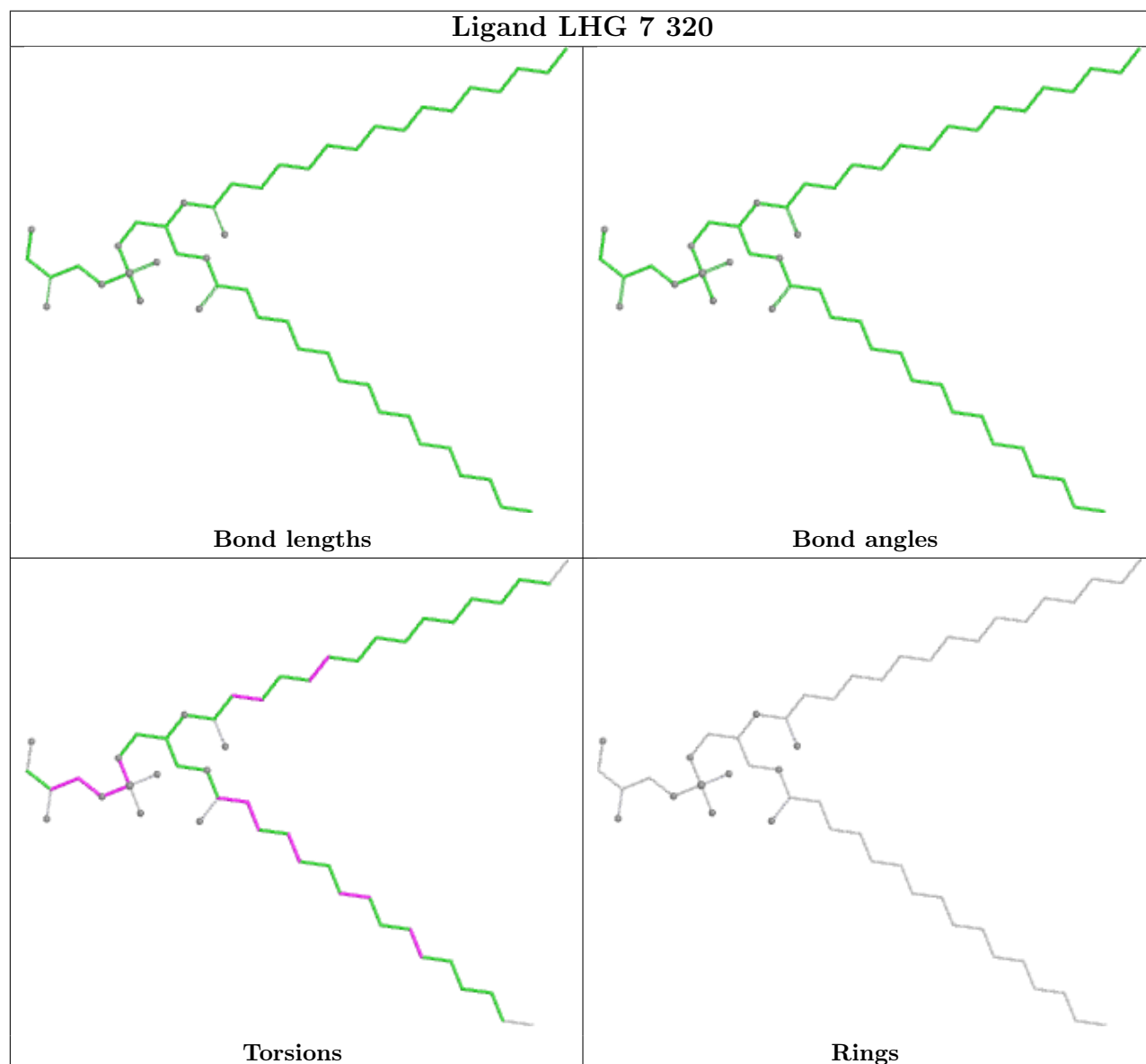
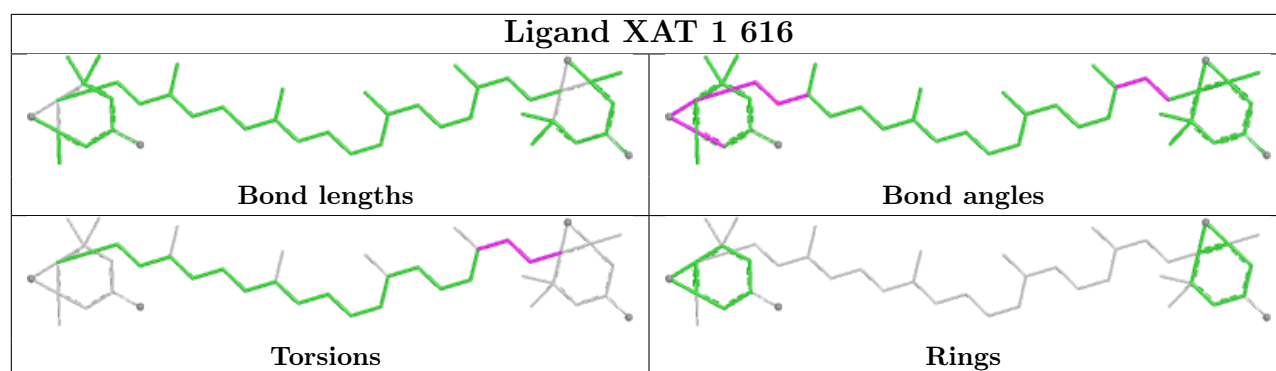


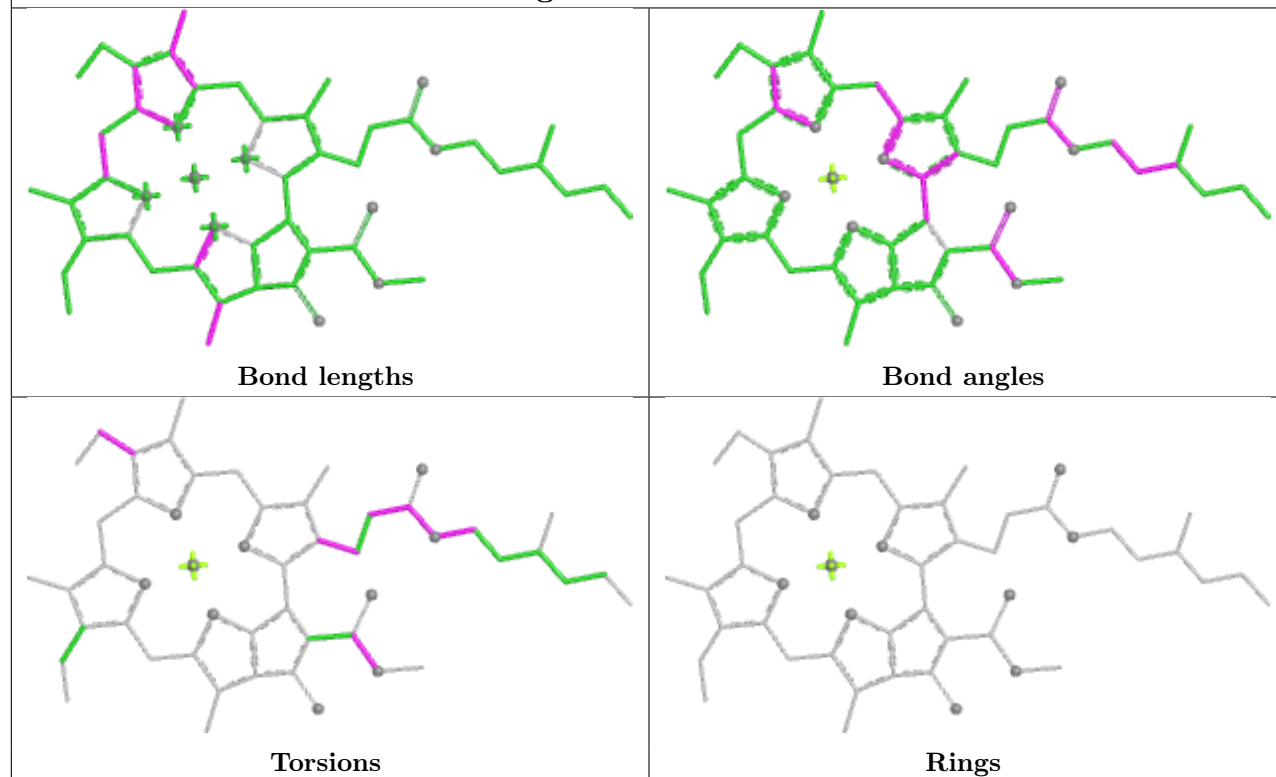
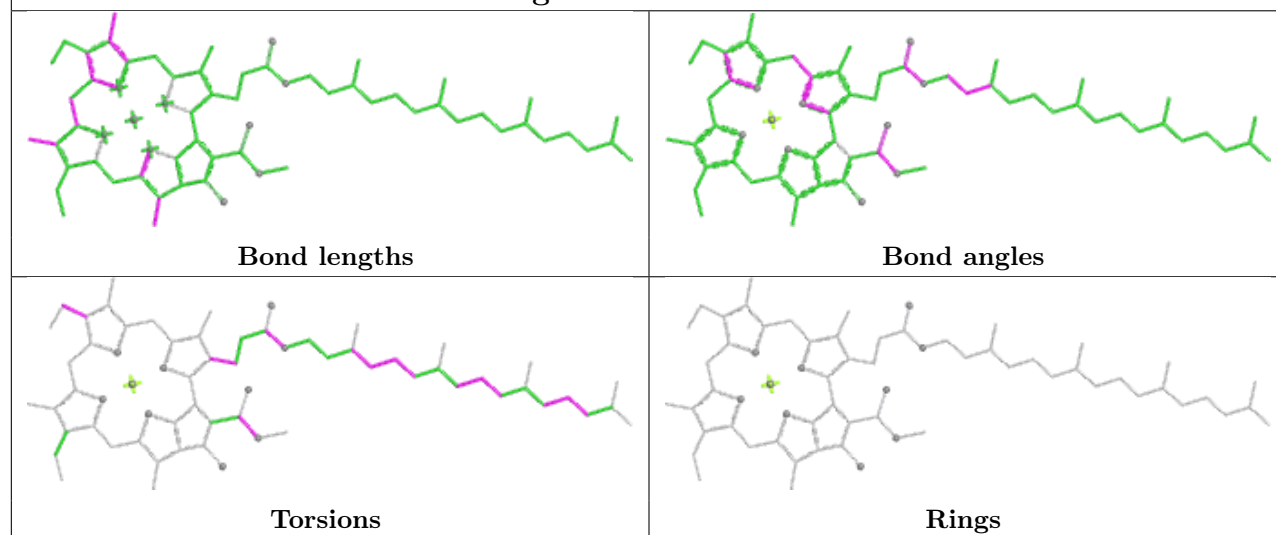
Ligand CLA 2 612



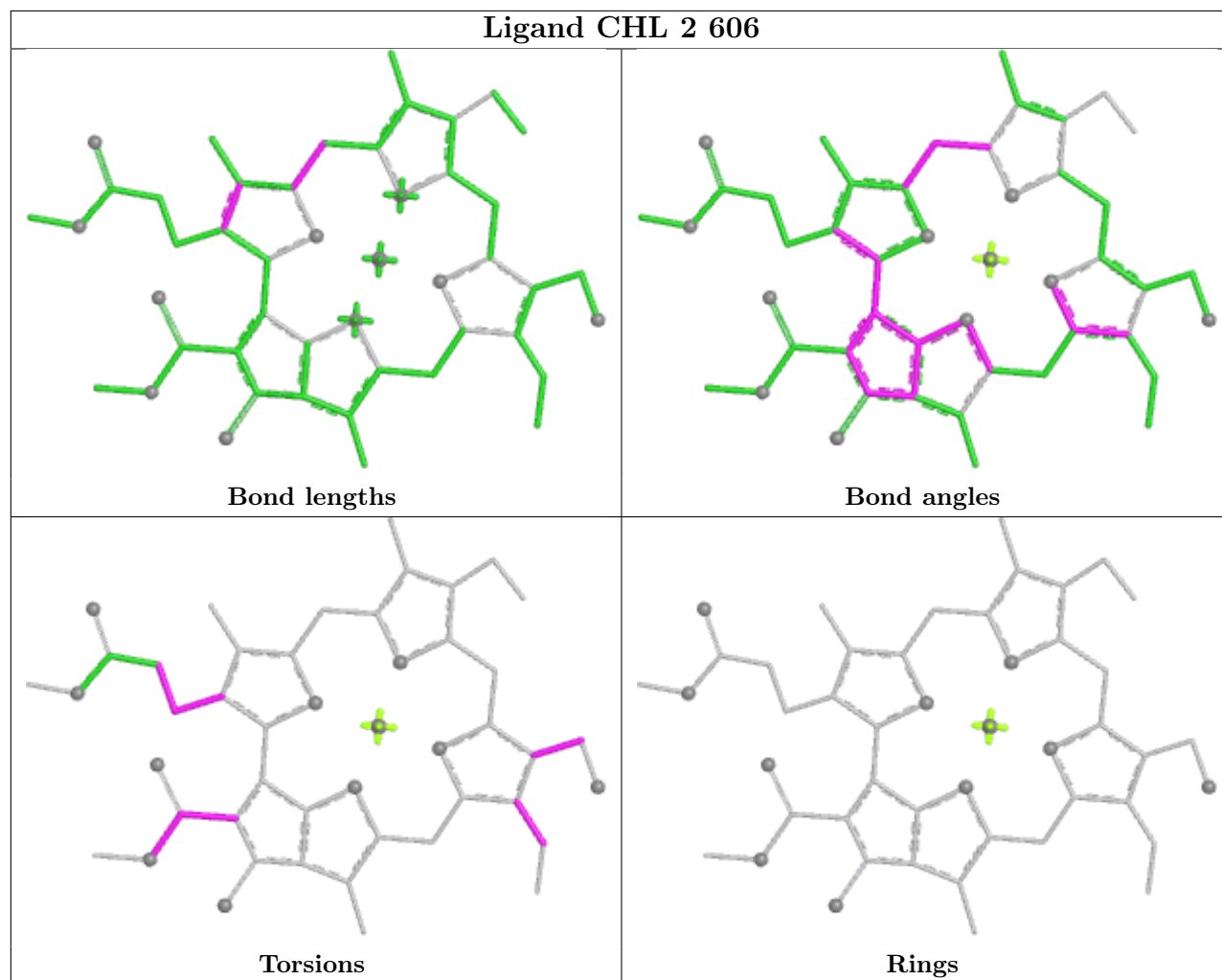
Ligand CLA A 818



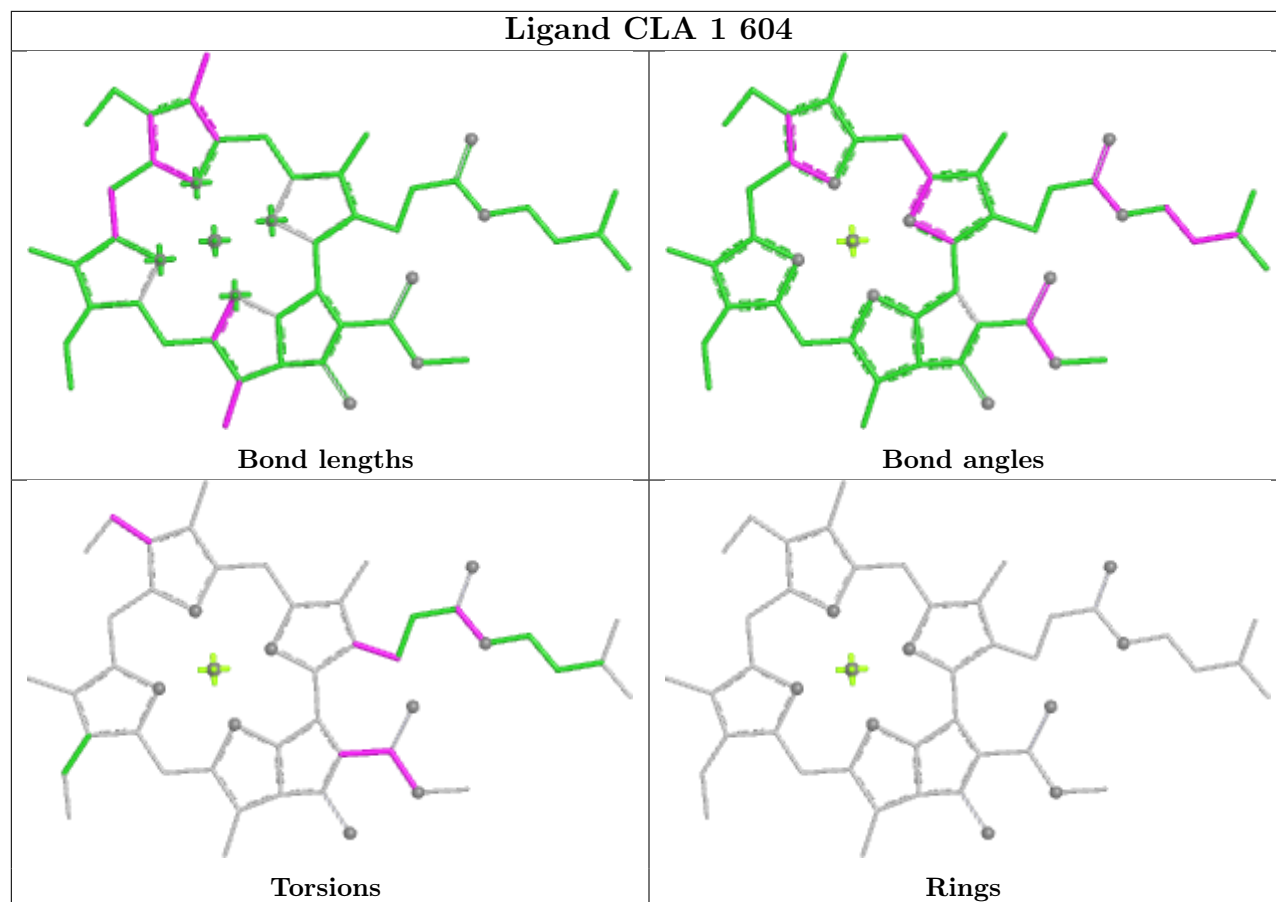


Ligand CLA 3 410**Ligand CLA B 823**

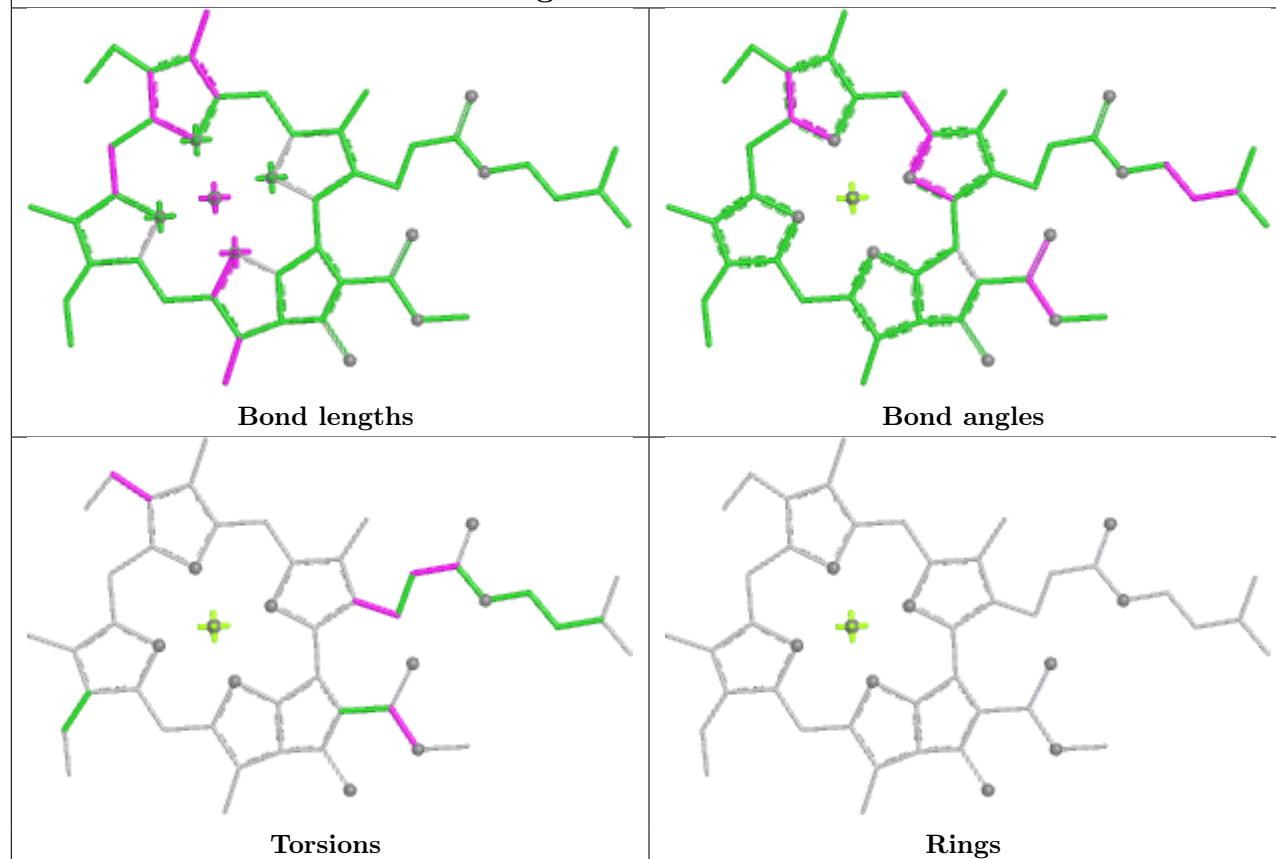
Ligand CHL 2 606



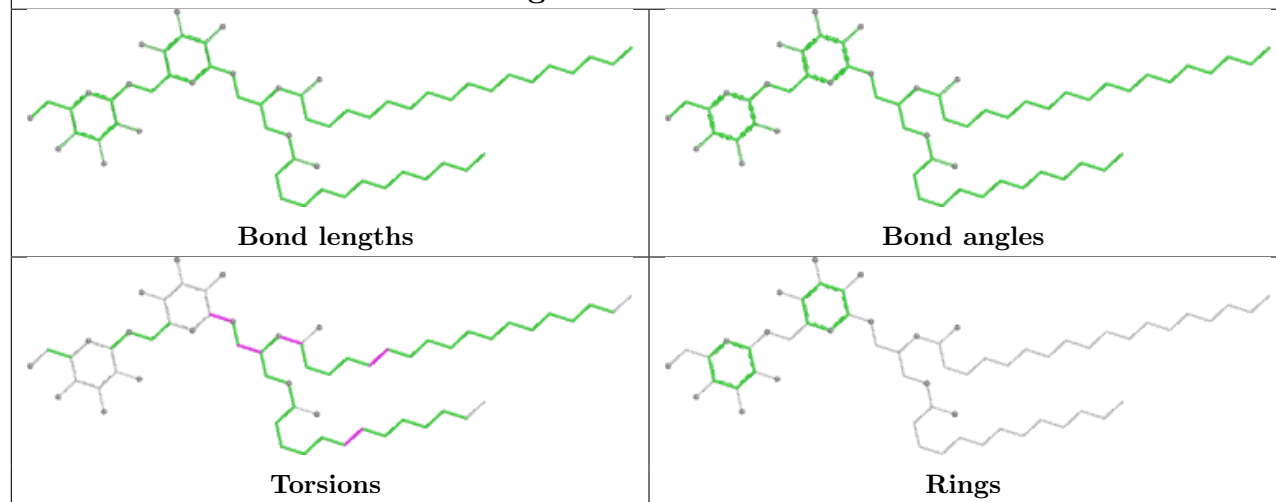
Ligand CLA 1 604

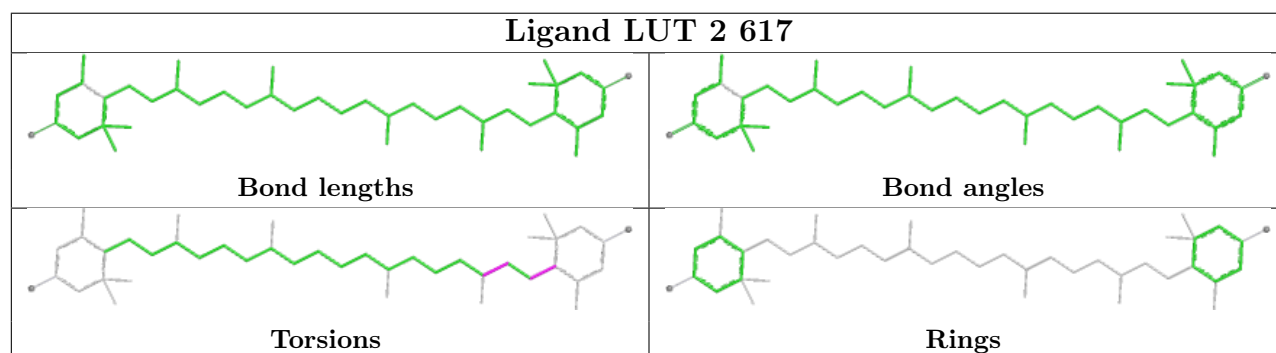
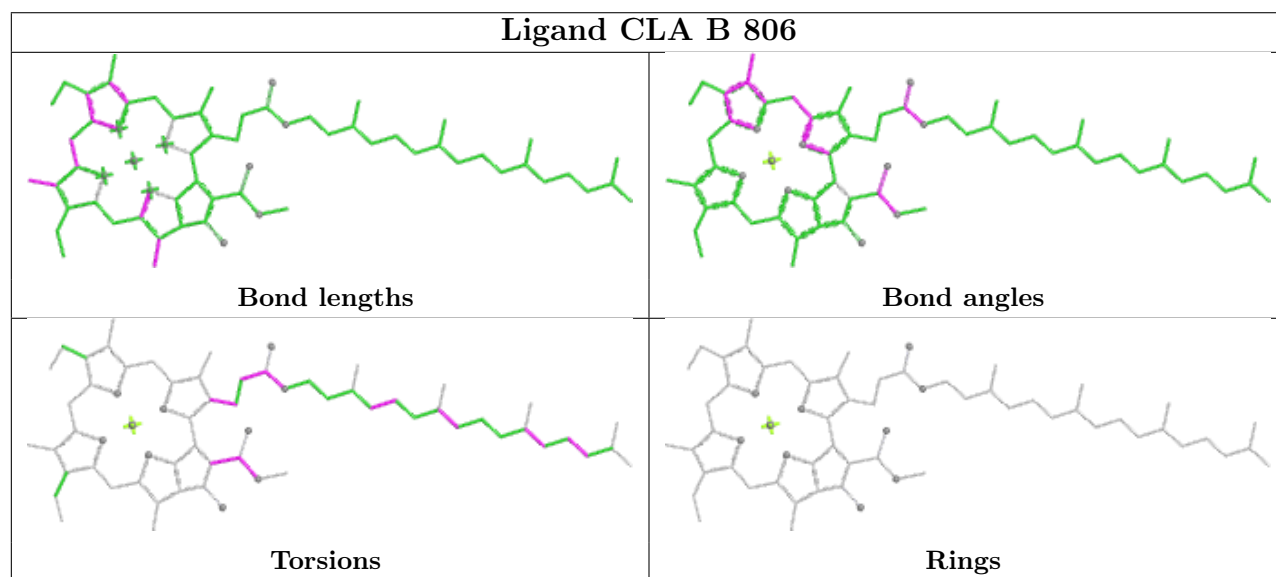
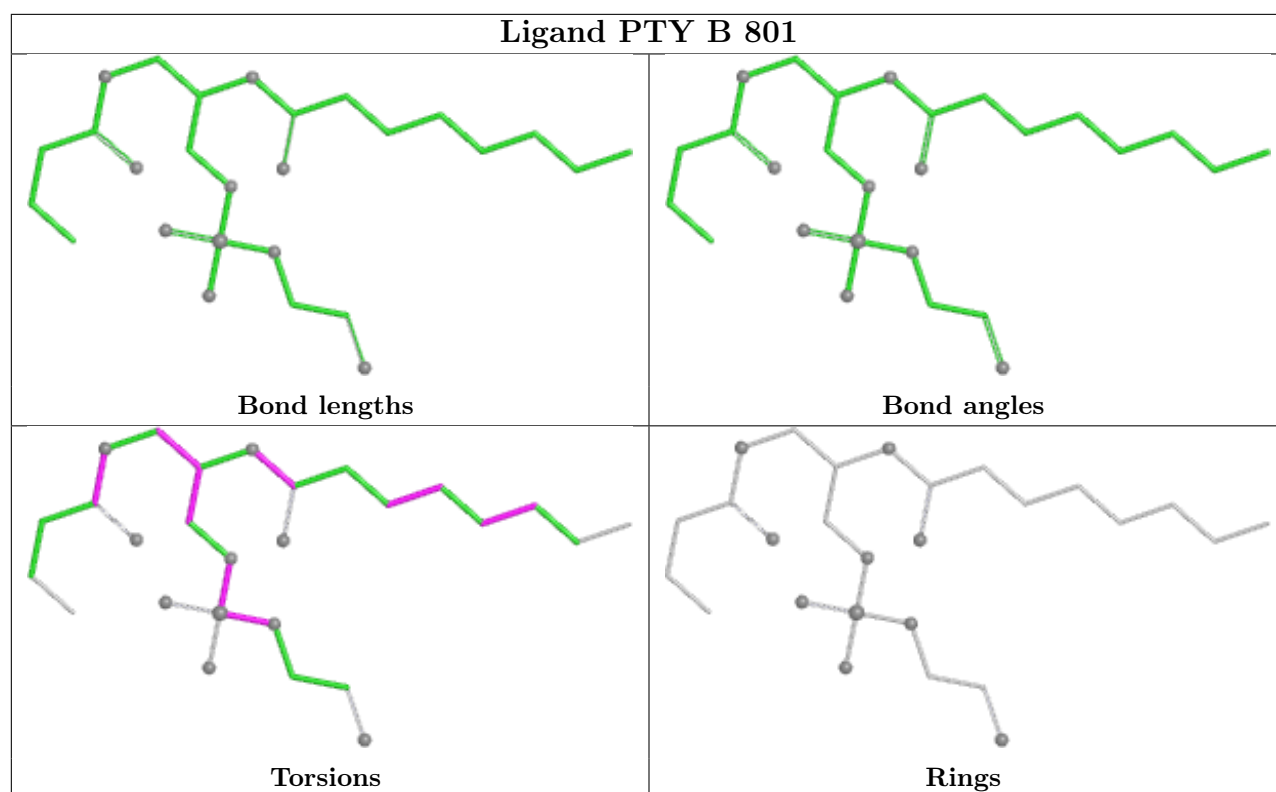


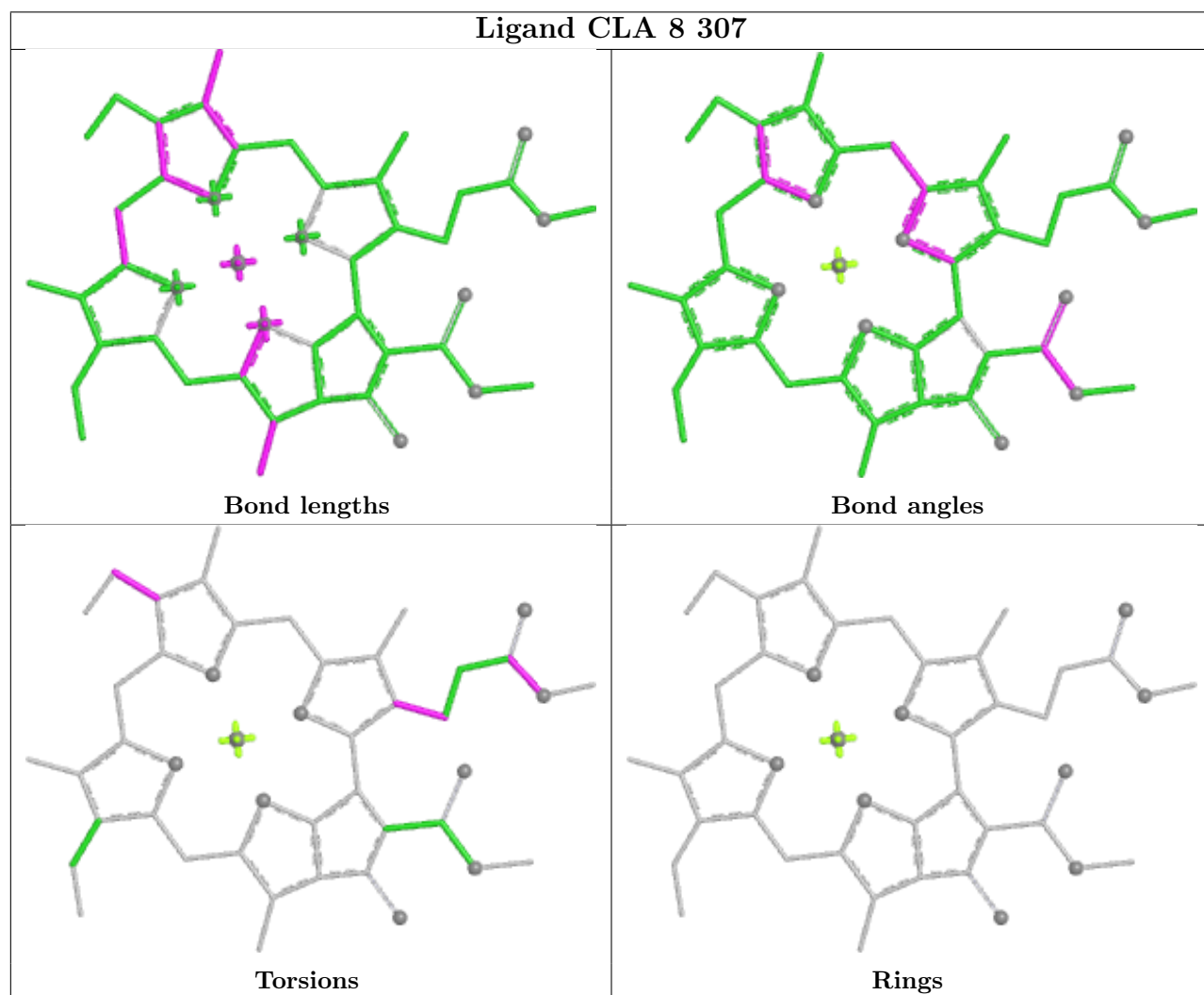
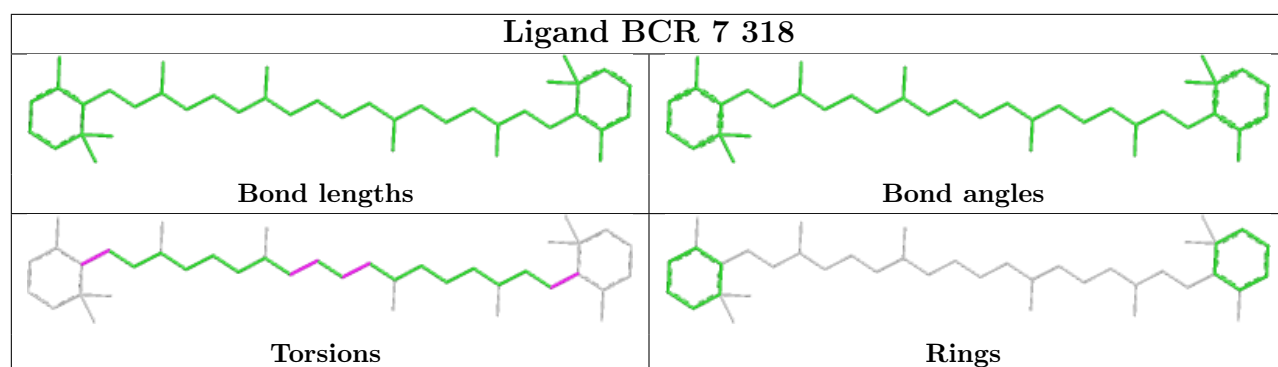
Ligand CLA 9 604



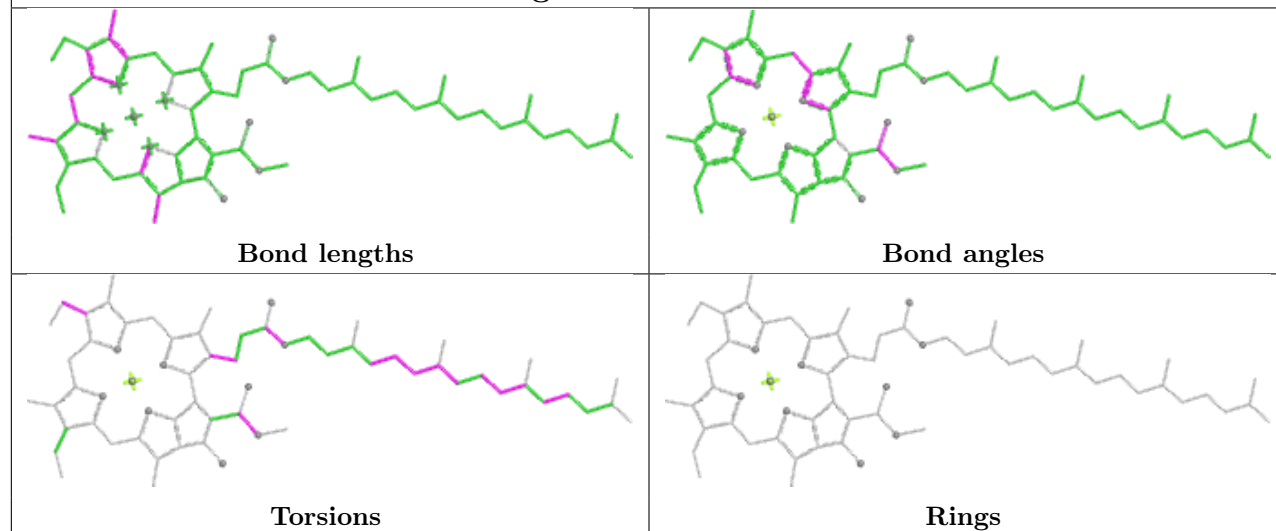
Ligand DGD B 850



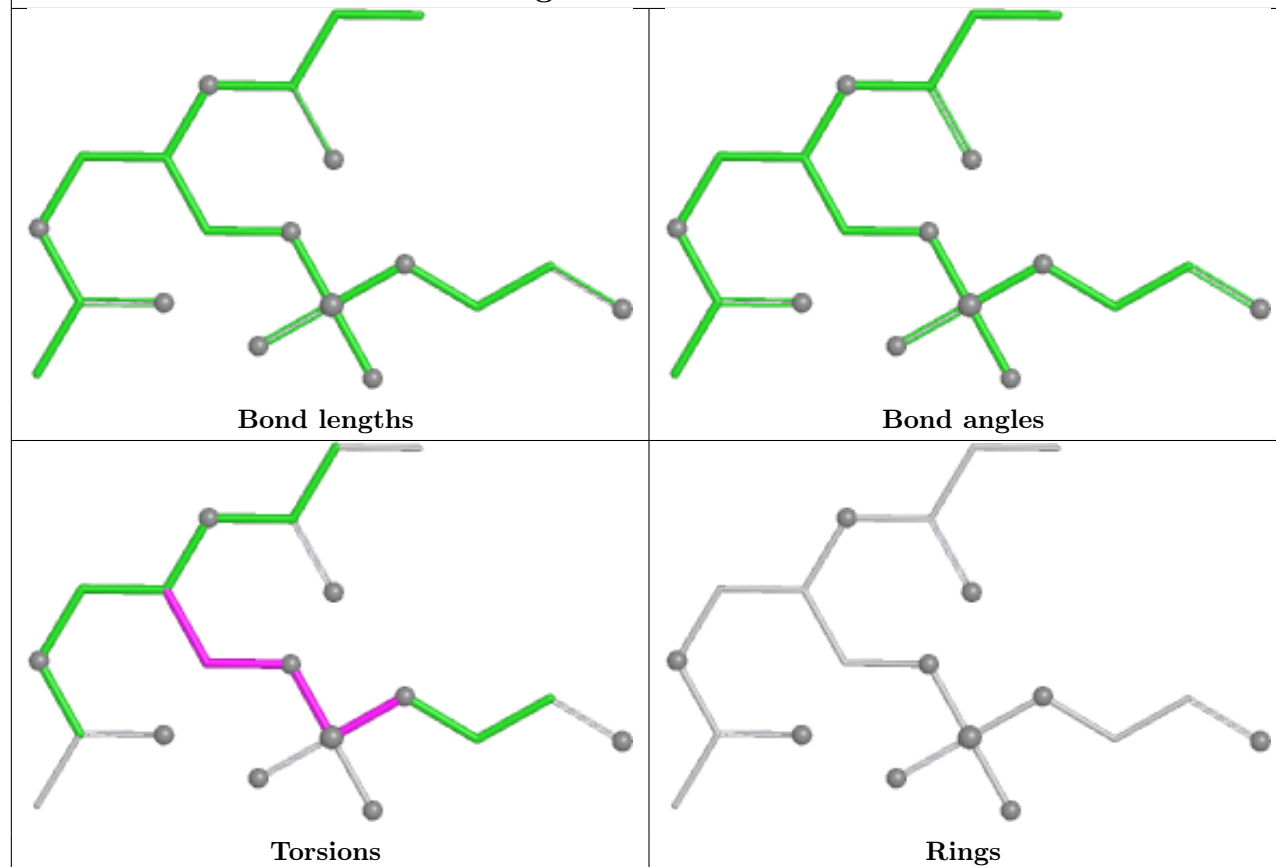




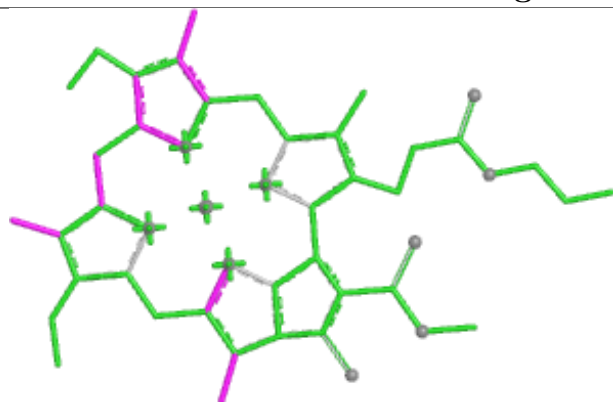
Ligand CLA B 811



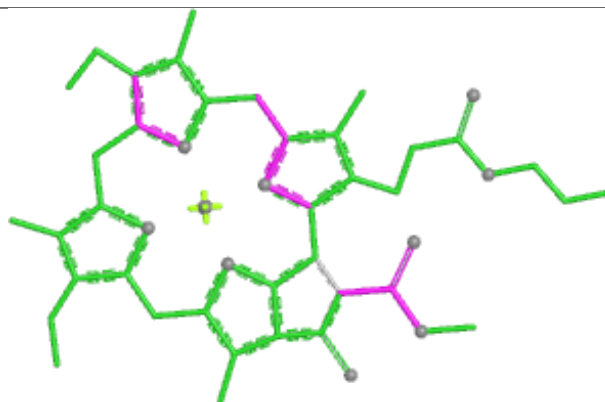
Ligand PTY 1 622



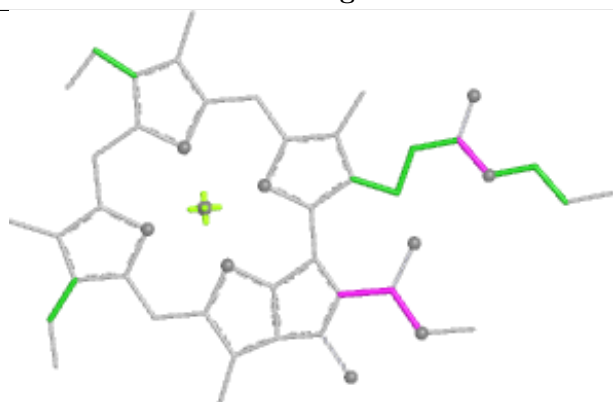
Ligand CLA B 805



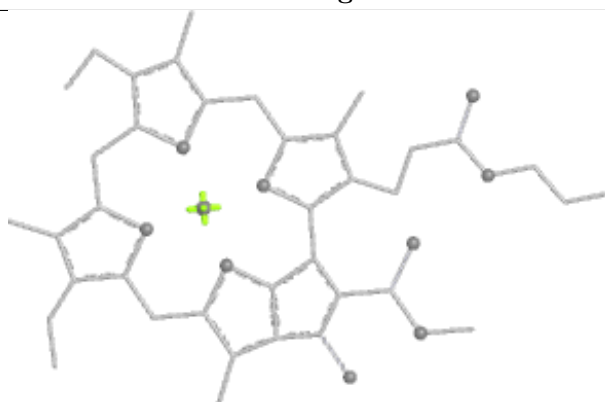
Bond lengths



Bond angles

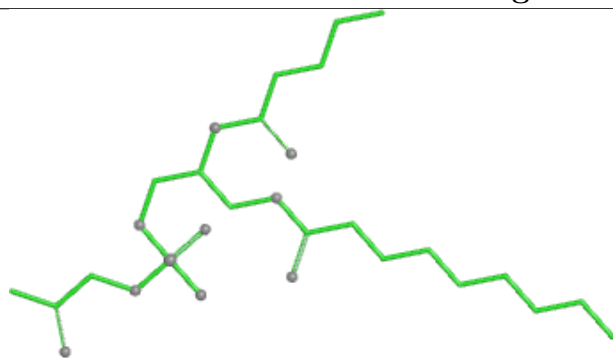


Torsions

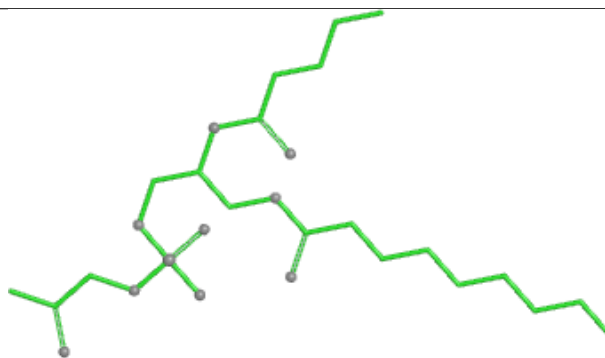


Rings

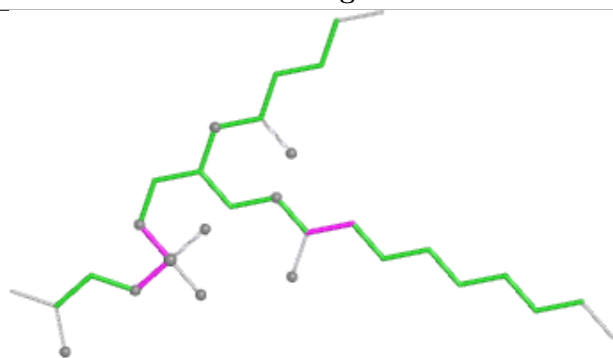
Ligand LHG A 853



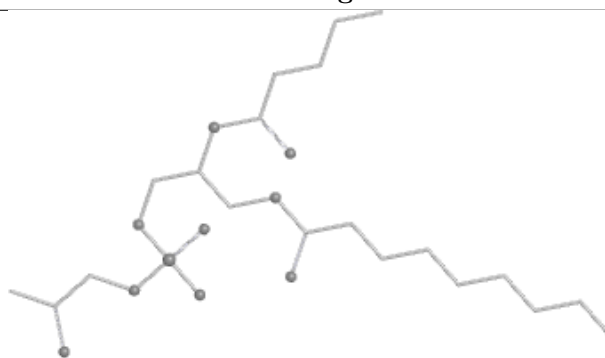
Bond lengths



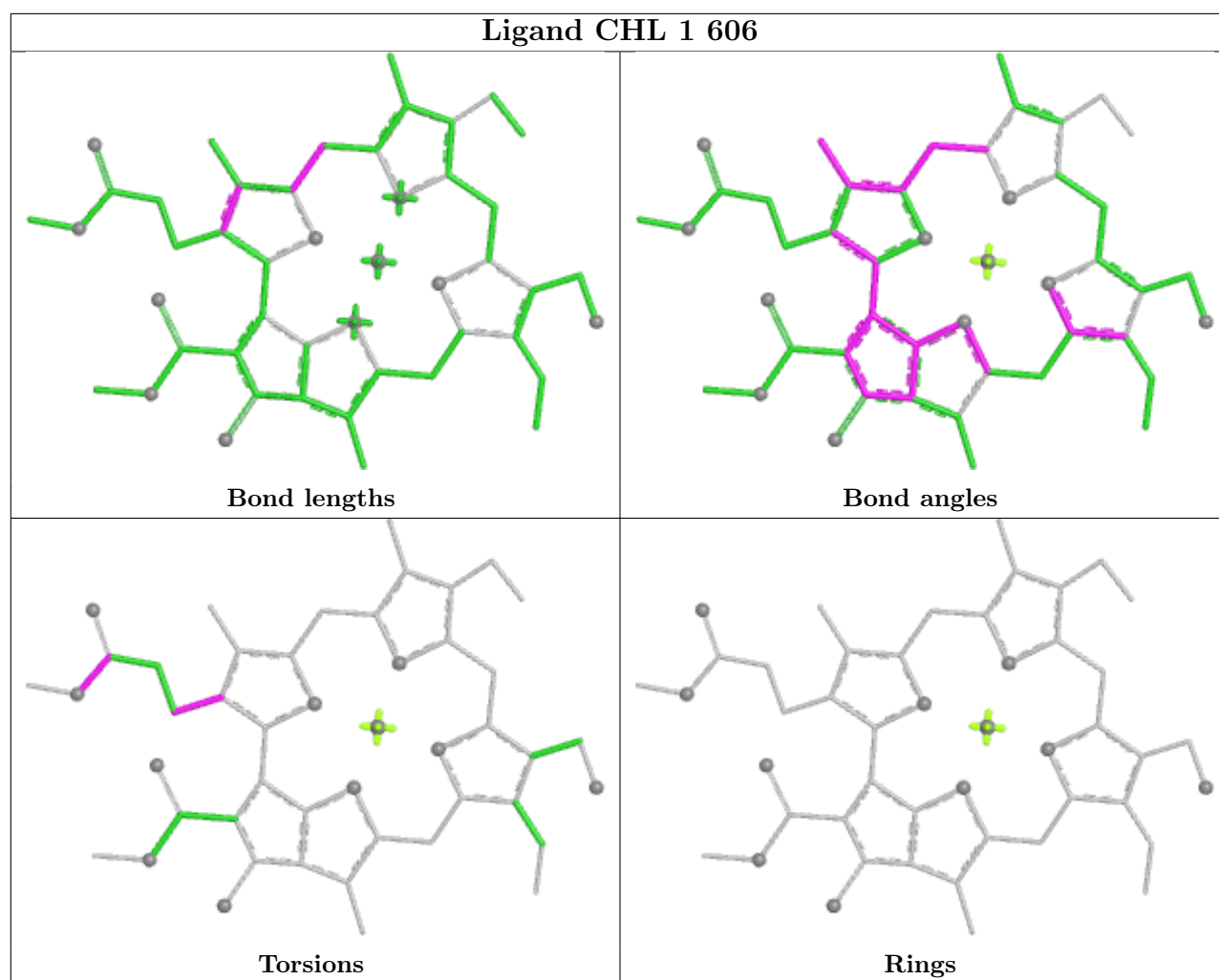
Bond angles



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.

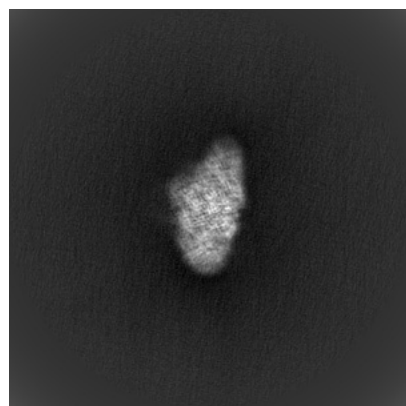
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48265. These allow visual inspection of the internal detail of the map and identification of artifacts.

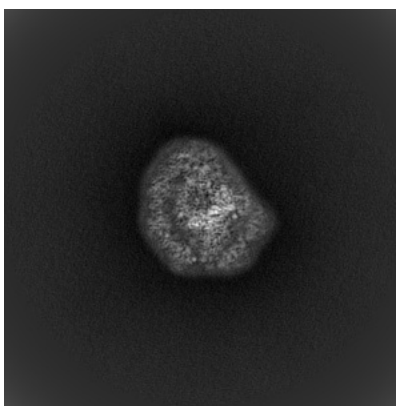
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

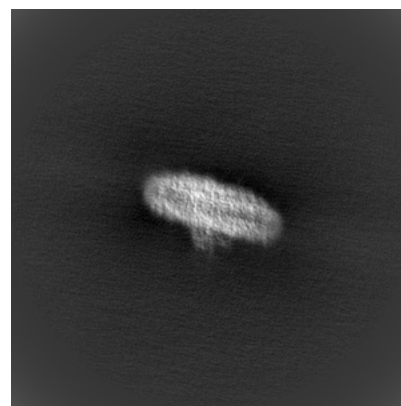
6.1.1 Primary map



X

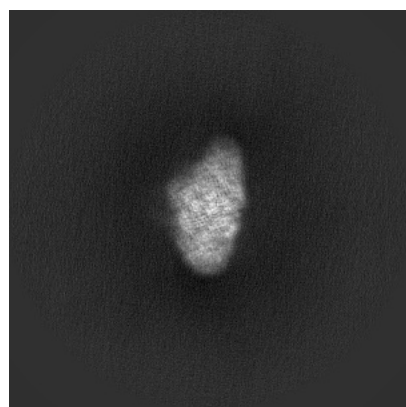


Y

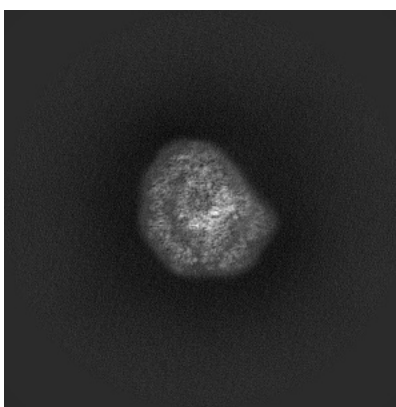


Z

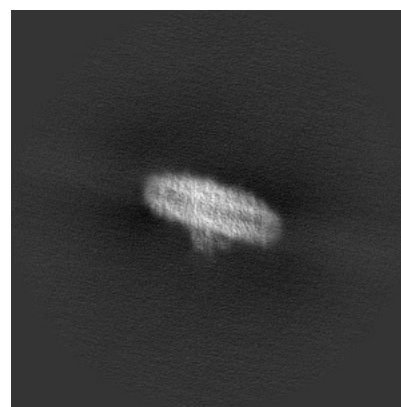
6.1.2 Raw map



X



Y

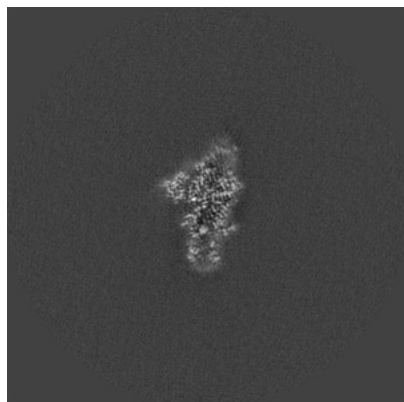


Z

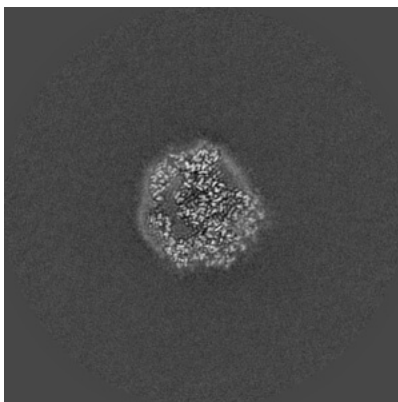
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

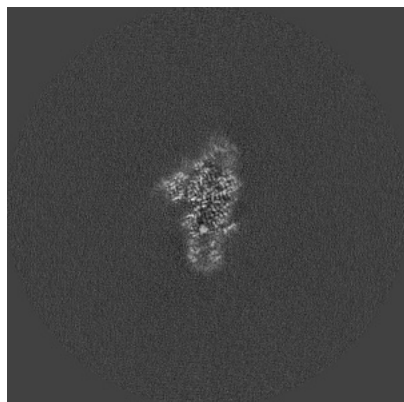


Y Index: 240

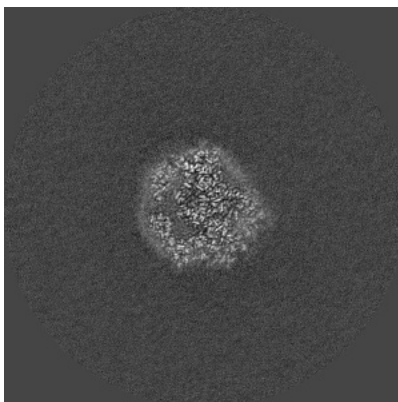


Z Index: 240

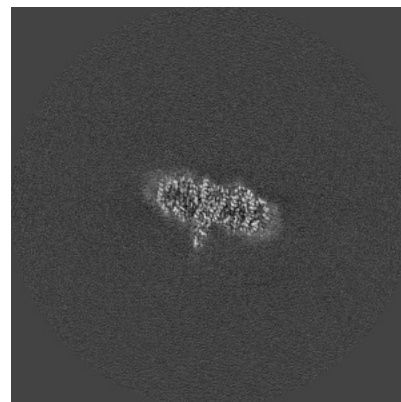
6.2.2 Raw map



X Index: 240



Y Index: 240

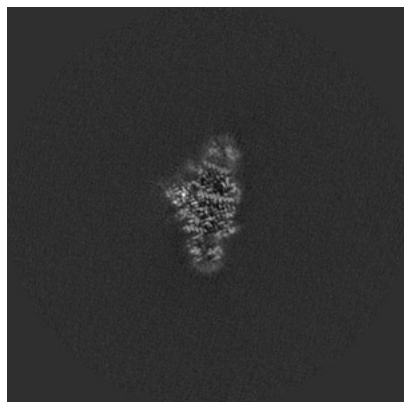


Z Index: 240

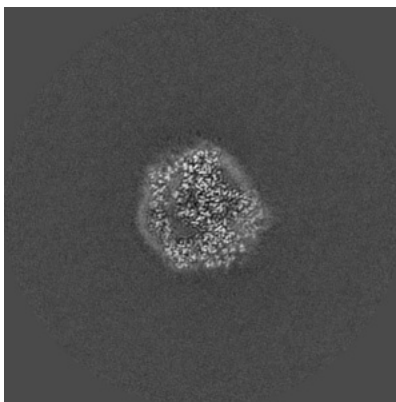
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

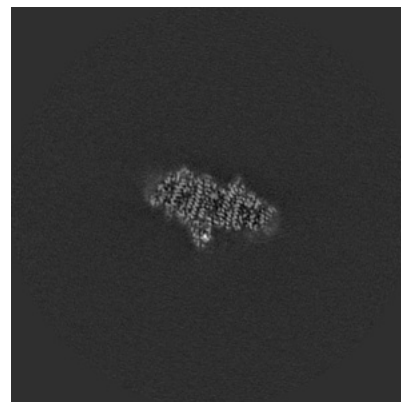
6.3.1 Primary map



X Index: 235

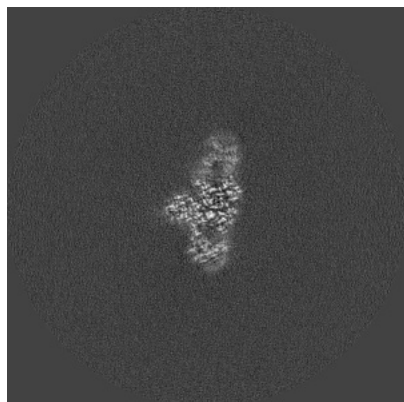


Y Index: 242

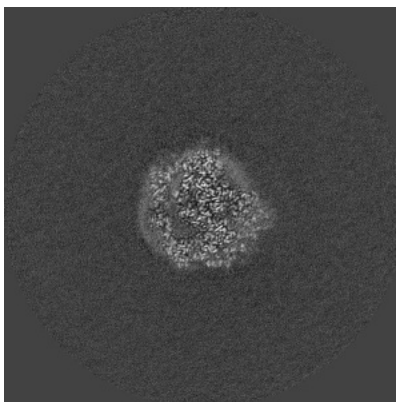


Z Index: 246

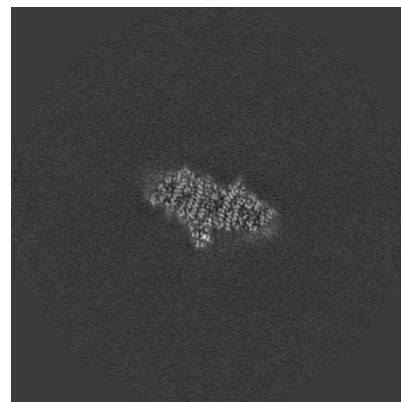
6.3.2 Raw map



X Index: 221



Y Index: 242

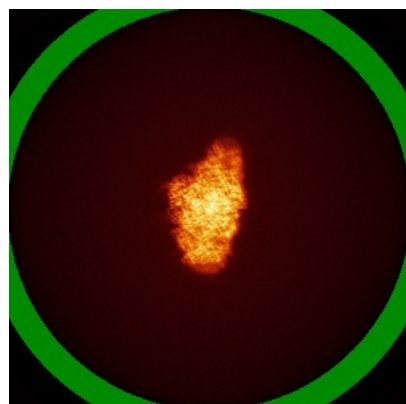


Z Index: 247

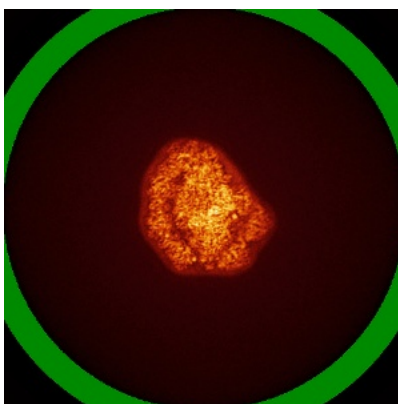
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

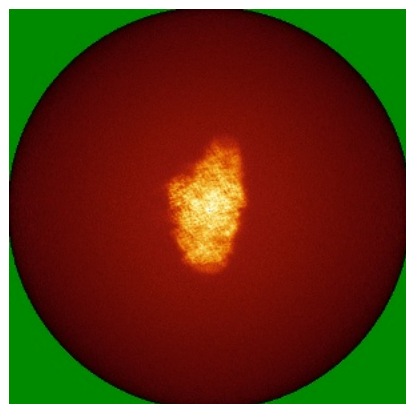


Y

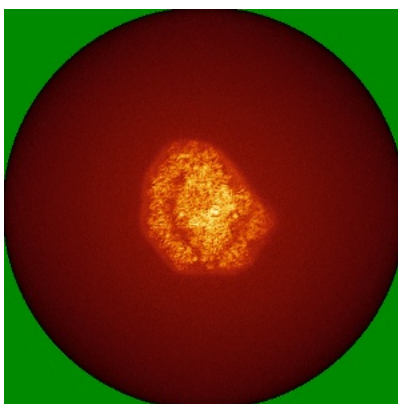


Z

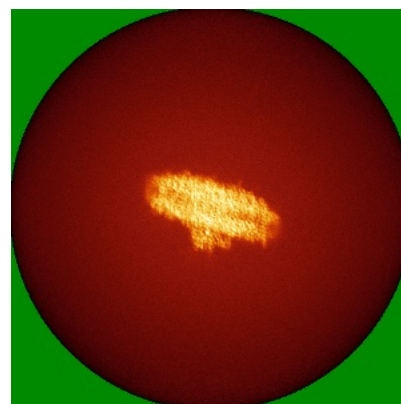
6.4.2 Raw map



X



Y

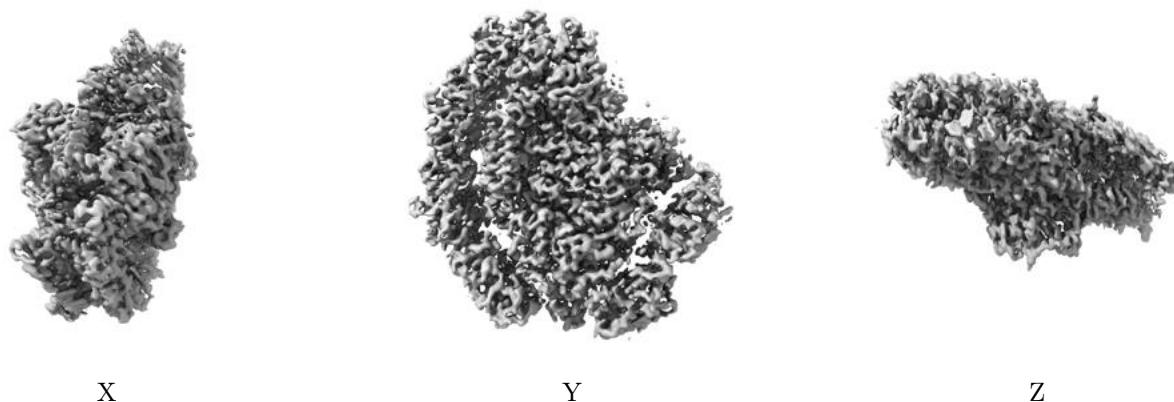


Z

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

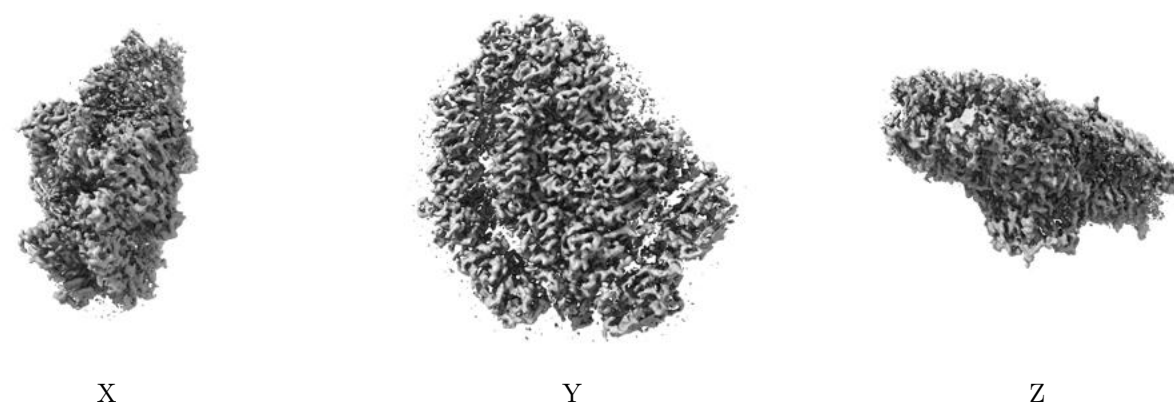
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

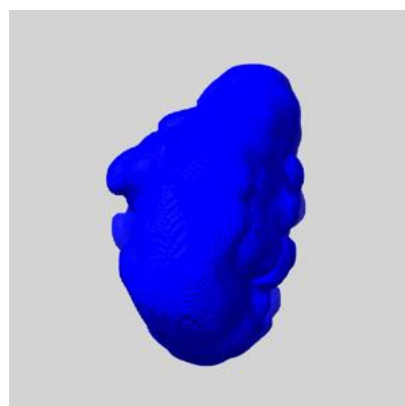
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

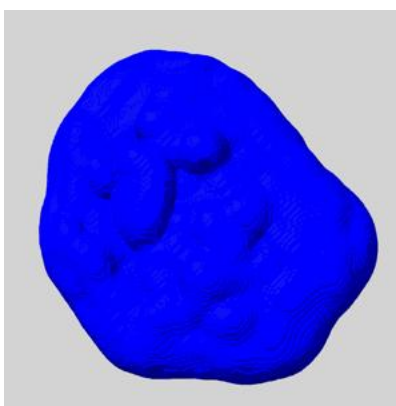
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

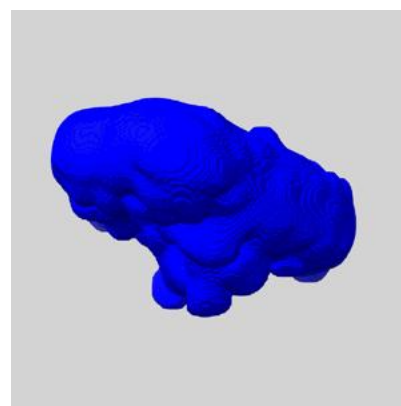
6.6.1 emd_48265_msk_1.map [i](#)



X



Y

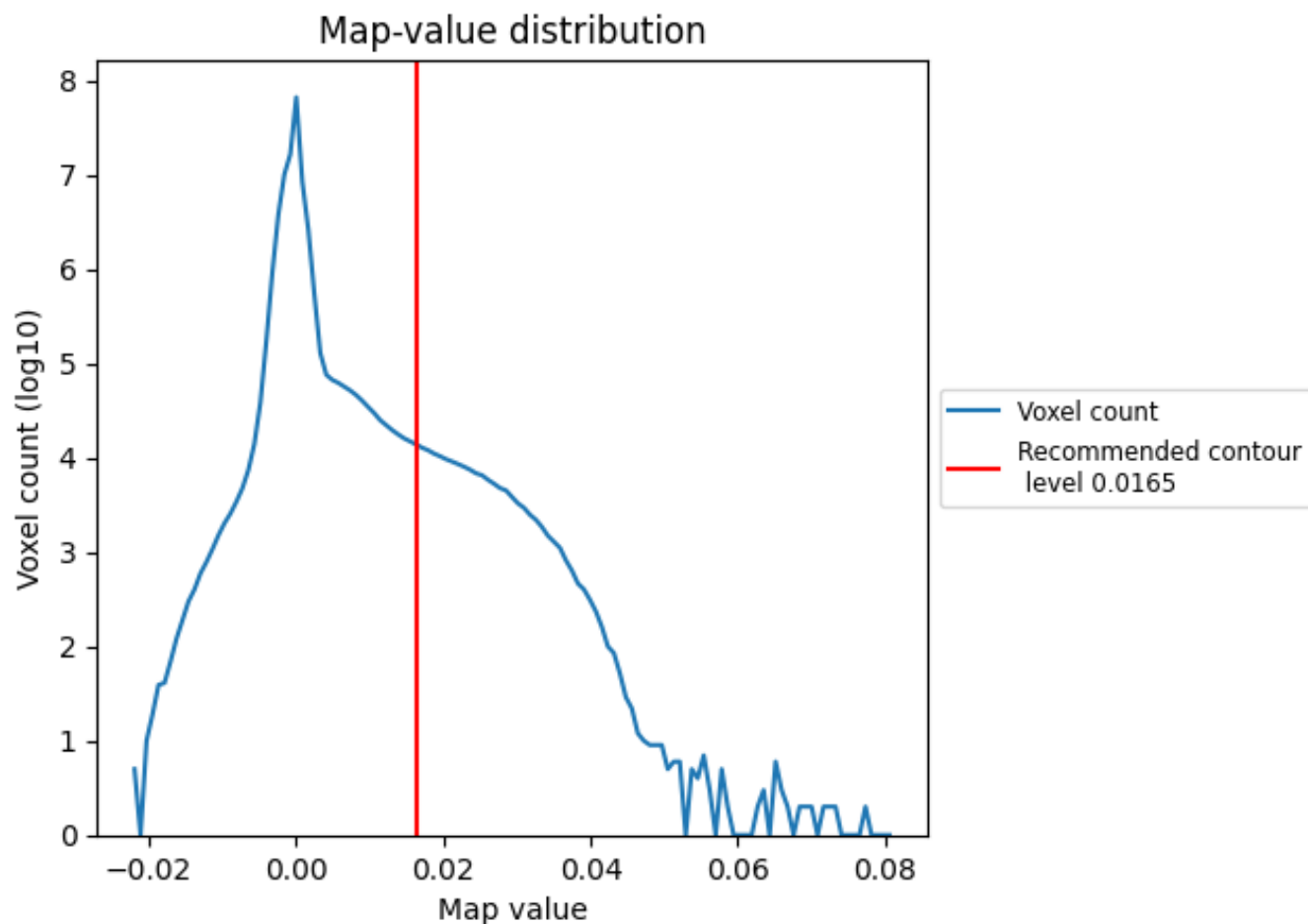


Z

7 Map analysis [i](#)

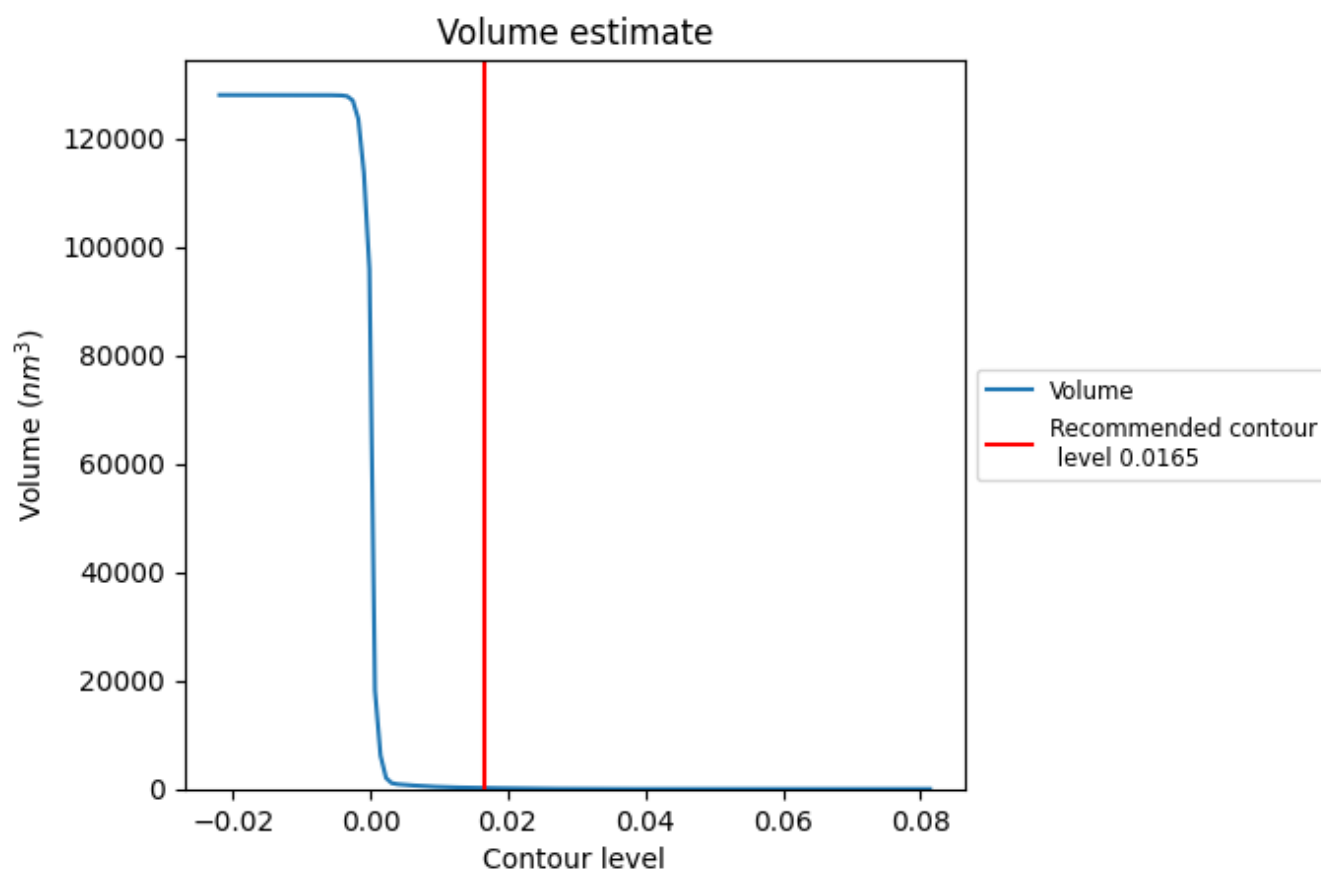
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

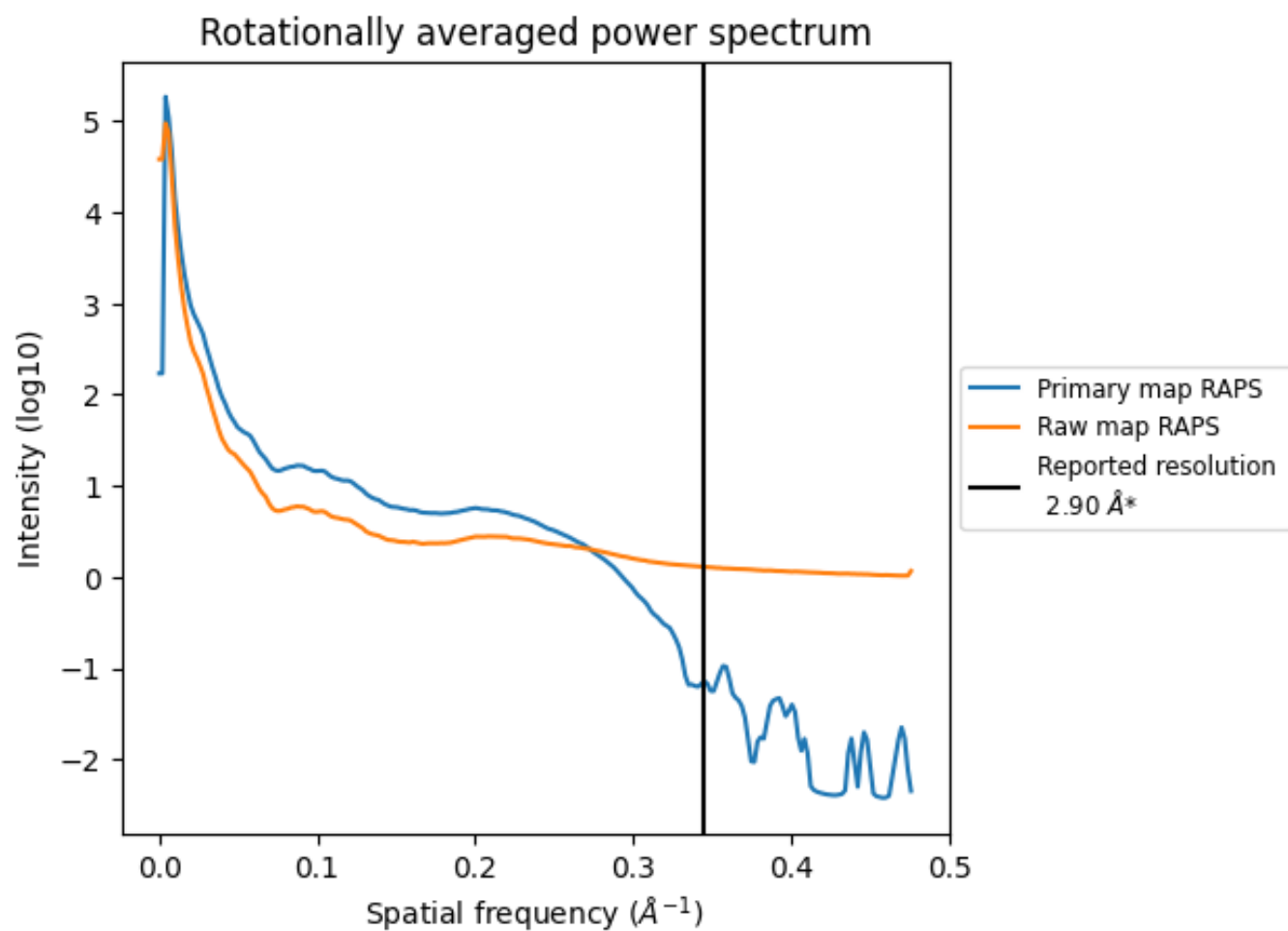
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183 nm^3 ; this corresponds to an approximate mass of 165 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 ⓘ

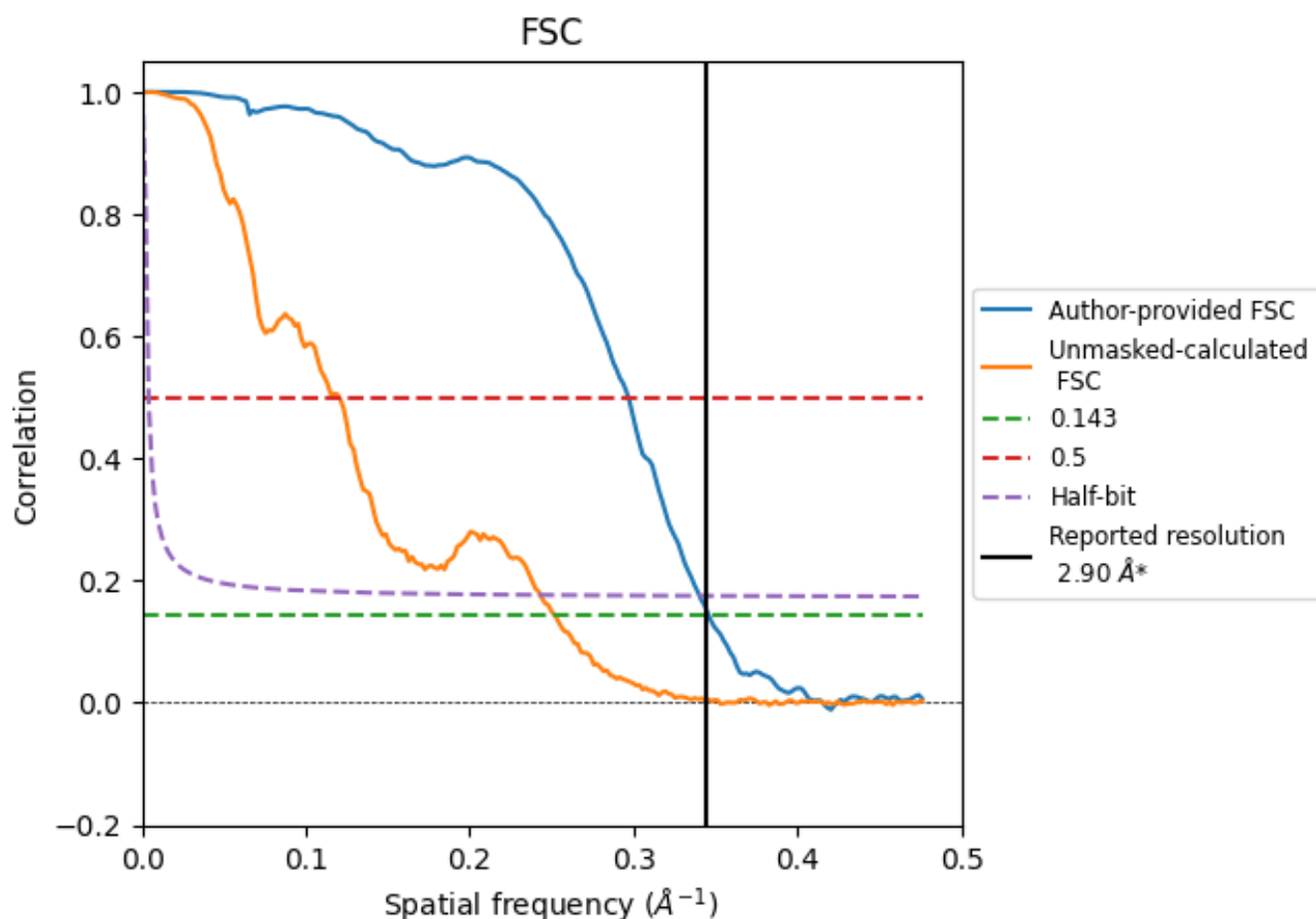


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

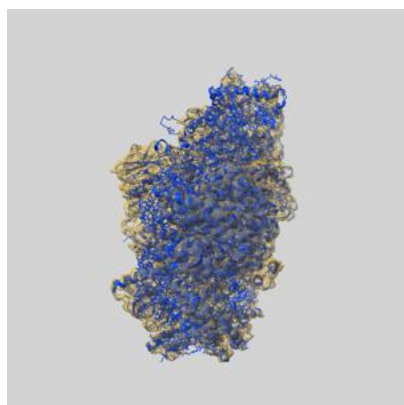
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.37	2.94
Unmasked-calculated*	3.97	8.32	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 2.9 by more than 10 %

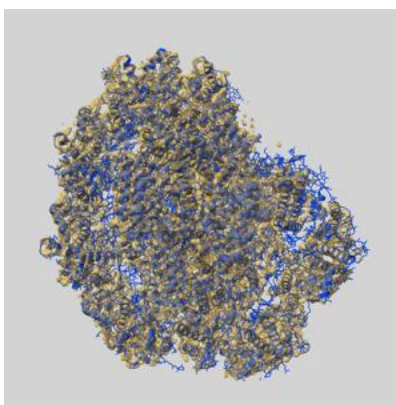
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48265 and PDB model 9MH0. Per-residue inclusion information can be found in section [3](#) on page [35](#).

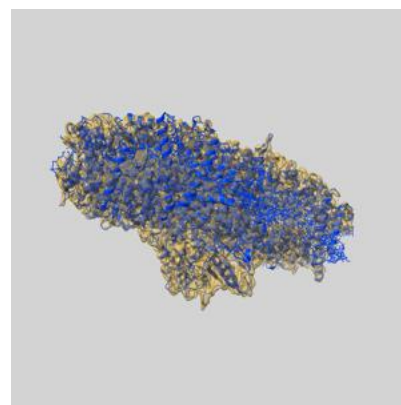
9.1 Map-model overlay [i](#)



X



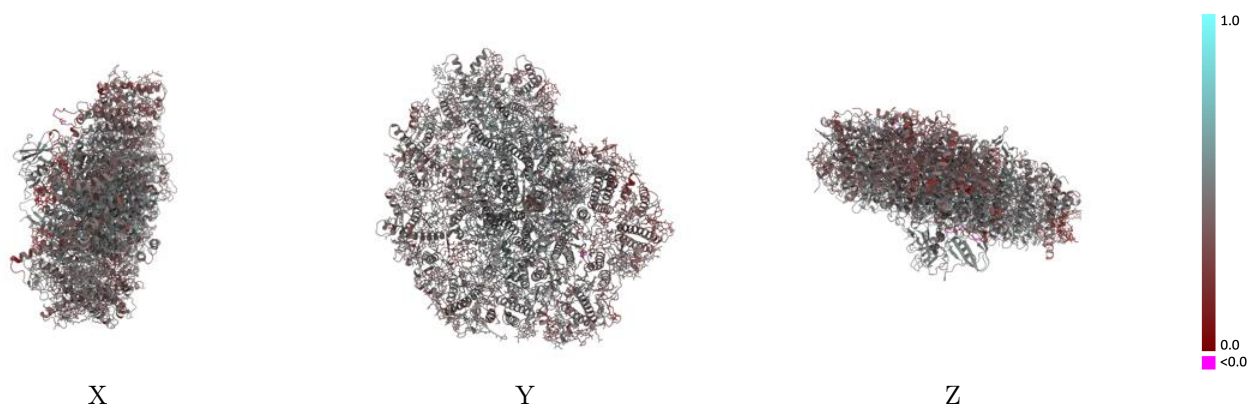
Y



Z

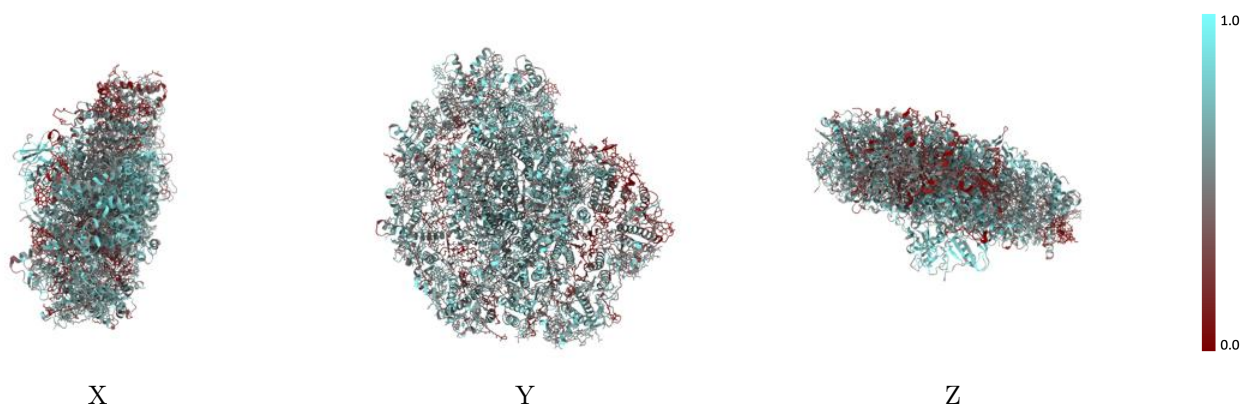
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



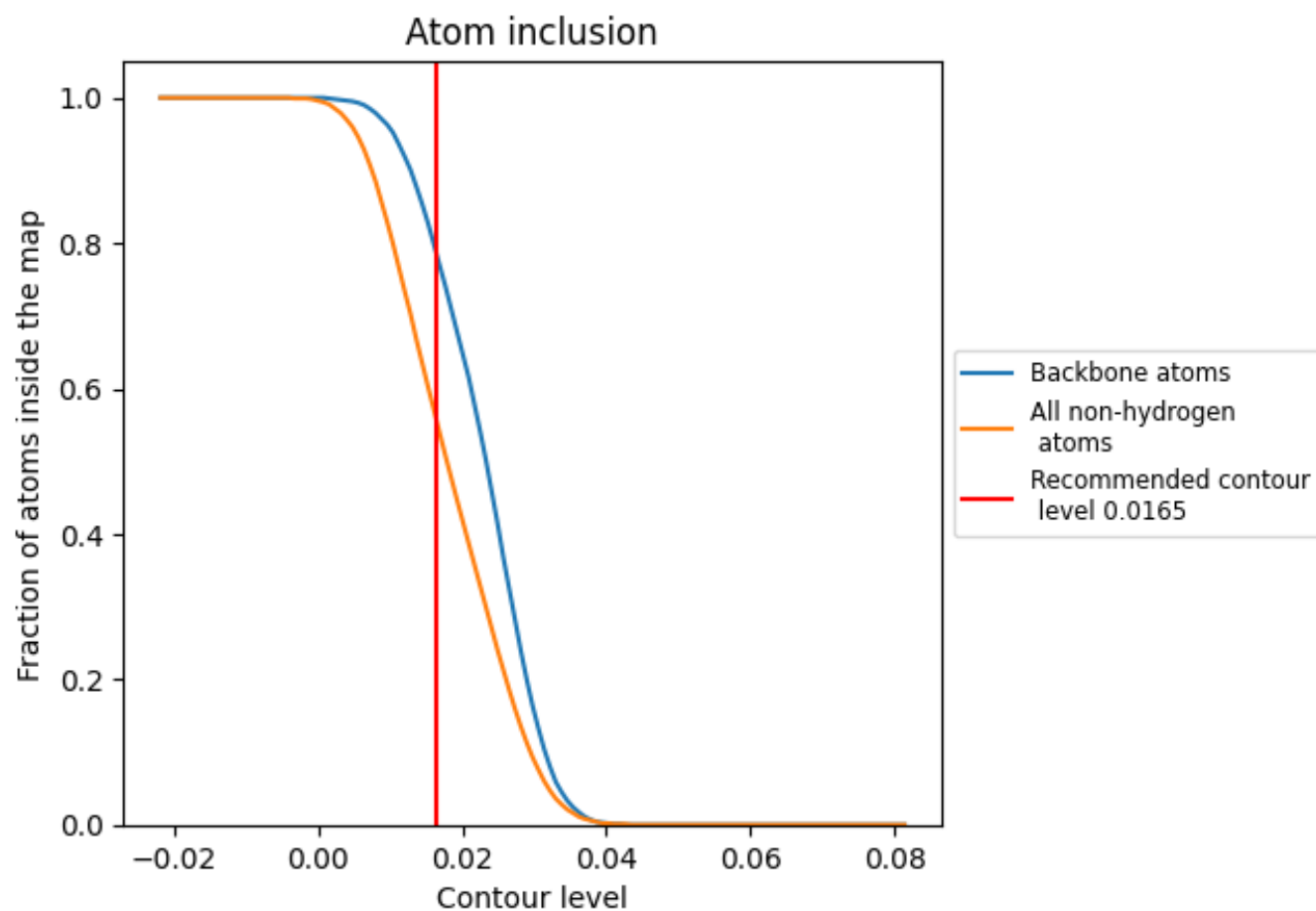
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0165).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 55% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5520	 0.4360
1	 0.5350	 0.4200
2	 0.3820	 0.3660
3	 0.5090	 0.4240
7	 0.5390	 0.4240
8	 0.5410	 0.4220
9	 0.5120	 0.3960
A	 0.6160	 0.4740
B	 0.6130	 0.4740
C	 0.7690	 0.4800
D	 0.7210	 0.4760
E	 0.6830	 0.4800
F	 0.5400	 0.4330
G	 0.5270	 0.4380
H	 0.2550	 0.3310
I	 0.4580	 0.3700
J	 0.4670	 0.4080
K	 0.3270	 0.3070
L	 0.4200	 0.3670

