



wwPDB EM Validation Summary Report ⓘ

Jun 17, 2025 – 11:24 AM EDT

PDB ID : 9MGW / pdb_00009mgw
EMDB ID : EMD-48262
Title : Dunaliella salina PSI-LHCI-TIDI1 supercomplex
Authors : Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.
Deposited on : 2024-12-11
Resolution : 3.00 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

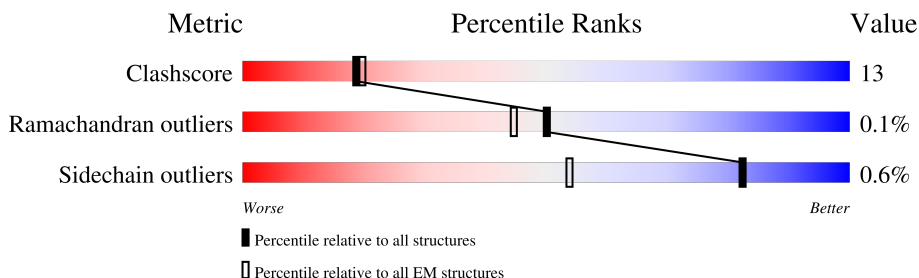
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	
1	a	228	
2	2	263	
3	3	320	
4	7	256	
4	c	256	
5	8	254	
5	b	254	

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Mol	Chain	Length	Quality of chain
6	9	222	
7	A	750	
8	B	735	
9	C	81	
10	D	202	
11	E	125	
12	F	232	
13	G	141	
14	H	135	
15	J	41	
16	L	202	
17	O	129	
18	I	109	
19	K	123	
20	T	365	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	301	X	-	-	-
21	CLA	1	302	X	-	-	-
21	CLA	1	303	X	-	-	-
21	CLA	1	304	X	-	-	-
21	CLA	1	306	X	-	-	-
21	CLA	1	307	X	-	-	-
21	CLA	1	308	X	-	-	-
21	CLA	1	309	X	-	-	-
21	CLA	1	310	X	-	-	-
21	CLA	1	311	X	-	-	-
21	CLA	1	312	X	-	-	-
21	CLA	1	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	321	X	-	-	-
21	CLA	2	602	X	-	-	-
21	CLA	2	603	X	-	-	-
21	CLA	2	604	X	-	-	-
21	CLA	2	605	X	-	-	-
21	CLA	2	607	X	-	-	-
21	CLA	2	608	X	-	-	-
21	CLA	2	609	X	-	-	-
21	CLA	2	610	X	-	-	-
21	CLA	2	611	X	-	-	-
21	CLA	2	612	X	-	-	-
21	CLA	2	613	X	-	-	-
21	CLA	3	402	X	-	-	-
21	CLA	3	403	X	-	-	-
21	CLA	3	404	X	-	-	-
21	CLA	3	405	X	-	-	-
21	CLA	3	406	X	-	-	-
21	CLA	3	407	X	-	-	-
21	CLA	3	408	X	-	-	-
21	CLA	3	409	X	-	-	-
21	CLA	3	410	X	-	-	-
21	CLA	3	411	X	-	-	-
21	CLA	3	412	X	-	-	-
21	CLA	3	413	X	-	-	-
21	CLA	3	414	X	-	-	-
21	CLA	7	304	X	-	-	-
21	CLA	7	305	X	-	-	-
21	CLA	7	306	X	-	-	-
21	CLA	7	310	X	-	-	-
21	CLA	7	311	X	-	-	-
21	CLA	7	312	X	-	-	-
21	CLA	7	313	X	-	-	-
21	CLA	7	314	X	-	-	-
21	CLA	7	315	X	-	-	-
21	CLA	7	316	X	-	-	-
21	CLA	7	323	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	604	X	-	-	-
21	CLA	8	605	X	-	-	-
21	CLA	8	609	X	-	-	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	8	612	X	-	-	-
21	CLA	8	613	X	-	-	-
21	CLA	8	614	X	-	-	-
21	CLA	8	615	X	-	-	-
21	CLA	8	622	X	-	-	-
21	CLA	9	601	X	-	-	-
21	CLA	9	602	X	-	-	-
21	CLA	9	603	X	-	-	-
21	CLA	9	604	X	-	-	-
21	CLA	9	605	X	-	-	-
21	CLA	9	607	X	-	-	-
21	CLA	9	608	X	-	-	-
21	CLA	9	609	X	-	-	-
21	CLA	9	610	X	-	-	-
21	CLA	9	611	X	-	-	-
21	CLA	9	612	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	843	X	-	-	-
21	CLA	A	856	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-
21	CLA	B	841	X	-	-	-
21	CLA	B	842	X	-	-	-
21	CLA	B	843	X	-	-	-
21	CLA	B	844	X	-	-	-
21	CLA	F	5005	X	-	-	-
21	CLA	F	5006	X	-	-	-
21	CLA	F	5007	X	-	-	-
21	CLA	G	201	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	G	204	X	-	-	-
21	CLA	G	205	X	-	-	-
21	CLA	H	203	X	-	-	-
21	CLA	H	204	X	-	-	-
21	CLA	J	5002	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	202	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	L	301	X	-	-	-
21	CLA	L	303	X	-	-	-
21	CLA	L	304	X	-	-	-
21	CLA	L	305	X	-	-	-
21	CLA	L	306	X	-	-	-
21	CLA	O	2001	X	-	-	-
21	CLA	O	2002	X	-	-	-
21	CLA	O	2003	X	-	-	-
21	CLA	T	603	X	-	-	-
21	CLA	T	604	X	-	-	-
21	CLA	T	605	X	-	-	-
21	CLA	T	607	X	-	-	-
21	CLA	T	608	X	-	-	-
21	CLA	T	609	X	-	-	-
21	CLA	T	610	X	-	-	-
21	CLA	T	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	T	612	X	-	-	-
21	CLA	T	613	X	-	-	-
21	CLA	T	614	X	-	-	-
21	CLA	a	302	X	-	-	-
21	CLA	a	303	X	-	-	-
21	CLA	a	304	X	-	-	-
21	CLA	a	305	X	-	-	-
21	CLA	a	307	X	-	-	-
21	CLA	a	308	X	-	-	-
21	CLA	a	309	X	-	-	-
21	CLA	a	310	X	-	-	-
21	CLA	a	311	X	-	-	-
21	CLA	a	312	X	-	-	-
21	CLA	a	313	X	-	-	-
21	CLA	a	314	X	-	-	-
21	CLA	b	304	X	-	-	-
21	CLA	b	305	X	-	-	-
21	CLA	b	306	X	-	-	-
21	CLA	b	310	X	-	-	-
21	CLA	b	311	X	-	-	-
21	CLA	b	312	X	-	-	-
21	CLA	b	313	X	-	-	-
21	CLA	b	314	X	-	-	-
21	CLA	b	315	X	-	-	-
21	CLA	b	316	X	-	-	-
21	CLA	c	601	X	-	-	-
21	CLA	c	602	X	-	-	-
21	CLA	c	603	X	-	-	-
21	CLA	c	604	X	-	-	-
21	CLA	c	608	X	-	-	-
21	CLA	c	609	X	-	-	-
21	CLA	c	610	X	-	-	-
21	CLA	c	611	X	-	-	-
21	CLA	c	612	X	-	-	-
21	CLA	c	613	X	-	-	-
21	CLA	c	614	X	-	-	-
22	CHL	1	305	X	-	-	-
22	CHL	2	601	X	-	-	-
22	CHL	2	606	X	-	-	-
22	CHL	3	401	X	-	-	-
22	CHL	7	303	X	-	-	-
22	CHL	7	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CHL	7	308	X	-	-	-
22	CHL	7	309	X	-	-	-
22	CHL	8	601	X	-	-	-
22	CHL	8	606	X	-	-	-
22	CHL	8	607	X	-	-	-
22	CHL	8	608	X	-	-	-
22	CHL	9	606	X	-	-	-
22	CHL	T	601	X	-	-	-
22	CHL	T	602	X	-	-	-
22	CHL	a	306	X	-	-	-
22	CHL	b	302	X	-	-	-
22	CHL	b	307	X	-	-	-
22	CHL	b	308	X	-	-	-
22	CHL	b	309	X	-	-	-
22	CHL	c	605	X	-	-	-
22	CHL	c	606	X	-	-	-
22	CHL	c	607	X	-	-	-
23	LUT	1	314	X	-	-	-
23	LUT	2	614	X	-	-	-
23	LUT	2	615	X	-	-	-
23	LUT	2	616	X	-	-	-
23	LUT	3	415	X	-	-	-
23	LUT	7	317	X	-	-	-
23	LUT	8	616	X	-	-	-
23	LUT	9	613	X	-	-	-
23	LUT	B	801	X	-	-	-
23	LUT	O	2005	X	-	-	-
23	LUT	T	615	X	-	-	-
23	LUT	a	315	X	-	-	-
23	LUT	b	317	X	-	-	-
23	LUT	c	615	X	-	-	-
36	SF4	A	845	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 53613 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
			1497	962	253	275	7		
1	a	196	Total	C	N	O	S	0	0
			1490	956	252	275	7		

- Molecule 2 is a protein called LHCA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	221	Total	C	N	O	S	0	0
			1731	1125	285	312	9		

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	230	Total	C	N	O	S	0	0
			1756	1146	287	318	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		
4	c	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		
5	b	223	Total	C	N	O	S	0	0
			1707	1103	284	314	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	98	Total	C	N	O	S	0	0
			763	482	131	149	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit IX.

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

- Molecule 16 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	159	Total	C	N	O	S	0	0
			1170	762	192	210	6		

- Molecule 17 is a protein called PSAO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	88	Total	C	N	O	S	0	0
			697	464	113	118	2		

- Molecule 18 is a protein called PSAL1.

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

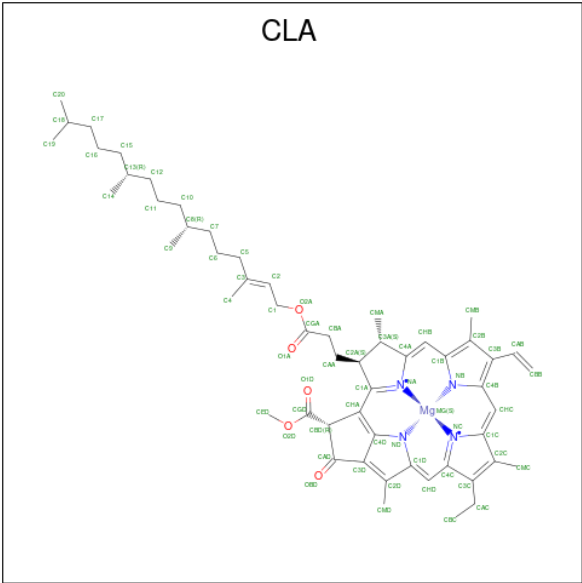
- Molecule 19 is a protein called PSAK1.

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

- Molecule 20 is a protein called TIDI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	205	Total	C	N	O	S	0	0
			1612	1048	266	290	8		

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	8	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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

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

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Mol	Chain	Residues	Atoms					AltConf
21	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	L	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	a	1	Total 46	C 36	Mg 1	N 4	O 5	0

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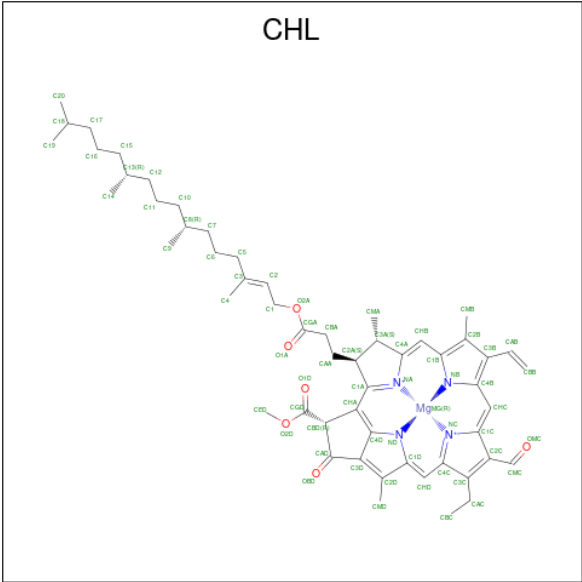
Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 22 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



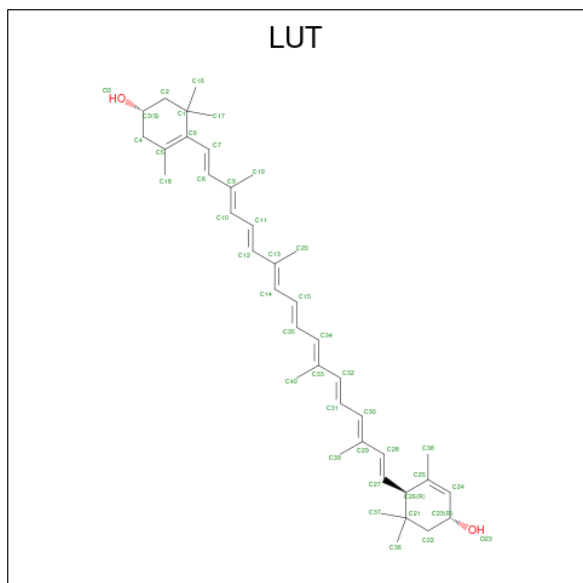
Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
22	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
22	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
22	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
22	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
22	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
22	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
22	7	1	Total 48	C 37	Mg 1	N 4	O 6	0
22	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
22	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
22	8	1	Total 47	C 36	Mg 1	N 4	O 6	0
22	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
22	9	1	Total 47	C 36	Mg 1	N 4	O 6	0
22	a	1	Total 47	C 36	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
22	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
22	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
22	b	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
22	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
22	c	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
22	c	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
22	T	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
22	T	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



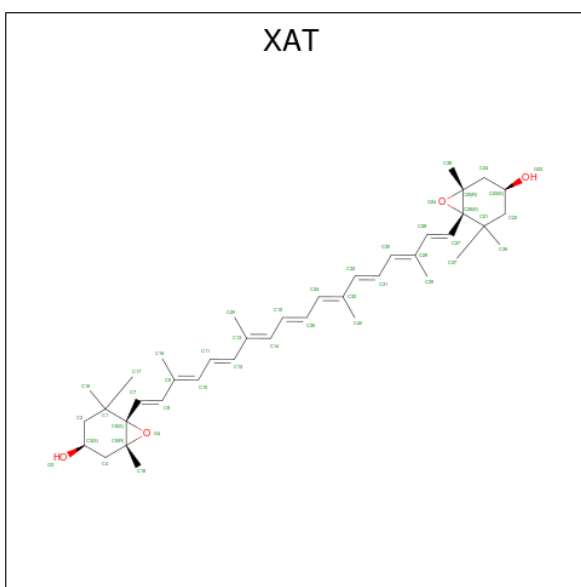
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			42	40	2	

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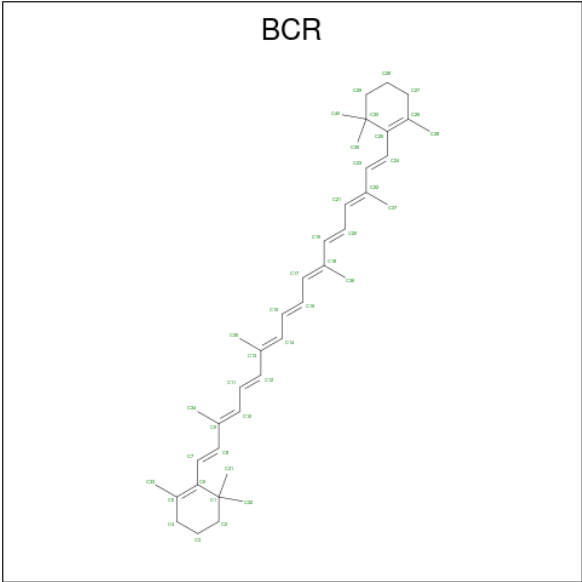
Mol	Chain	Residues	Atoms			AltConf
23	2	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	
23	3	1	Total	C	O	0
			42	40	2	
23	7	1	Total	C	O	0
			42	40	2	
23	8	1	Total	C	O	0
			42	40	2	
23	9	1	Total	C	O	0
			42	40	2	
23	B	1	Total	C	O	0
			42	40	2	
23	O	1	Total	C	O	0
			42	40	2	
23	a	1	Total	C	O	0
			42	40	2	
23	b	1	Total	C	O	0
			42	40	2	
23	c	1	Total	C	O	0
			42	40	2	
23	T	1	Total	C	O	0
			42	40	2	

- Molecule 24 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
24	1	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	7	1	Total	C	O	0
			44	40	4	
24	8	1	Total	C	O	0
			44	40	4	
24	9	1	Total	C	O	0
			44	40	4	
24	9	1	Total	C	O	0
			44	40	4	
24	a	1	Total	C	O	0
			44	40	4	
24	b	1	Total	C	O	0
			44	40	4	
24	c	1	Total	C	O	0
			44	40	4	
24	T	1	Total	C	O	0
			44	40	4	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



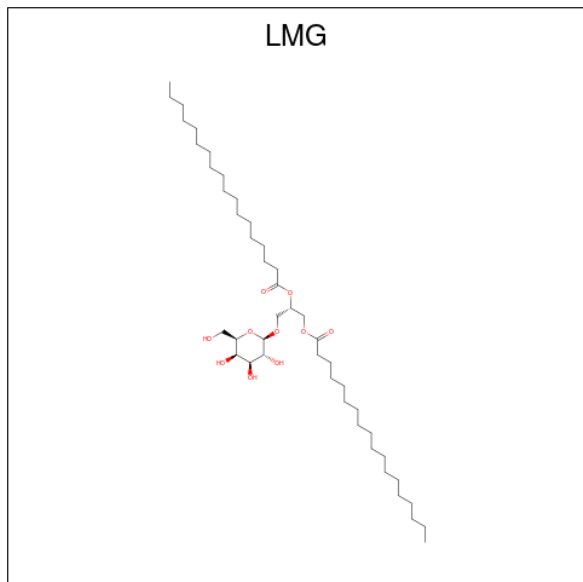
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	T	1	Total C 40 40	0

- Molecule 26 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
26	1	1	Total	C	O	0
			28	19	9	
26	3	1	Total	C	O	0
			40	30	10	
26	7	1	Total	C	O	0
			47	37	10	
26	A	1	Total	C	O	0
			32	22	10	
26	F	1	Total	C	O	0
			39	29	10	
26	G	1	Total	C	O	0
			43	34	9	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total 35	C 24	O 11	0
27	9	1	Total 35	C 24	O 11	0
27	A	1	Total 35	C 24	O 11	0
27	A	1	Total 35	C 24	O 11	0

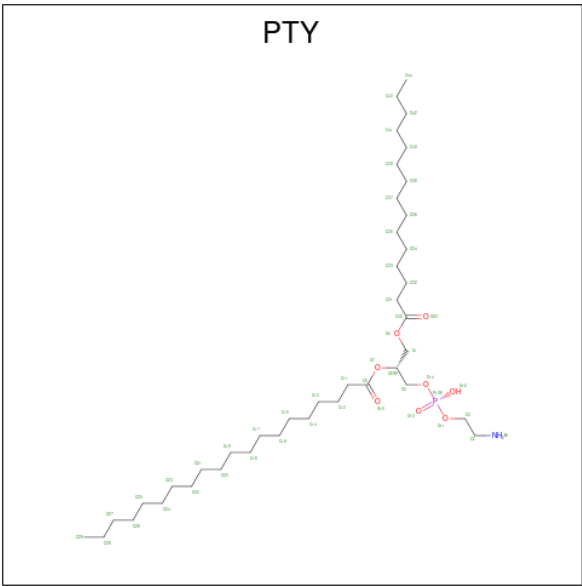
- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	1	1	Total	C	O	P	0
			25	14	10	1	
28	1	1	Total	C	O	P	0
			27	16	10	1	
28	1	1	Total	C	O	P	0
			46	35	10	1	
28	2	1	Total	C	O	P	0
			22	13	8	1	
28	3	1	Total	C	O	P	0
			17	8	8	1	
28	3	1	Total	C	O	P	0
			26	15	10	1	
28	7	1	Total	C	O	P	0
			43	32	10	1	
28	7	1	Total	C	O	P	0
			31	20	10	1	
28	8	1	Total	C	O	P	0
			40	29	10	1	
28	9	1	Total	C	O	P	0
			28	17	10	1	
28	A	1	Total	C	O	P	0
			30	20	9	1	
28	A	1	Total	C	O	P	0
			45	34	10	1	
28	B	1	Total	C	O	P	0
			32	21	10	1	
28	F	1	Total	C	O	P	0
			31	20	10	1	
28	F	1	Total	C	O	P	0
			43	32	10	1	
28	H	1	Total	C	O	P	0
			49	38	10	1	
28	a	1	Total	C	O	P	0
			22	11	10	1	
28	a	1	Total	C	O	P	0
			23	12	10	1	
28	b	1	Total	C	O	P	0
			31	20	10	1	
28	b	1	Total	C	O	P	0
			23	13	9	1	
28	c	1	Total	C	O	P	0
			29	18	10	1	

- Molecule 29 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P)

(labeled as "Ligand of Interest" by depositor).



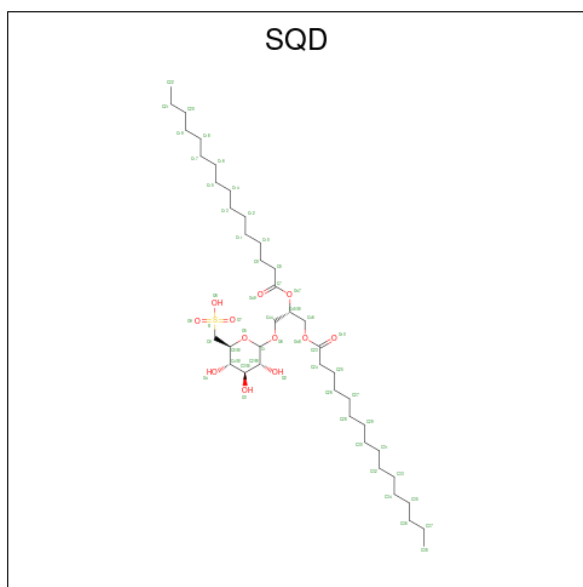
Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	N	O	P	0
			21	11	1	8	1	
29	2	1	Total	C	N	O	P	0
			32	22	1	8	1	
29	3	1	Total	C	O	P		0
			17	9	7	1		
29	7	1	Total	C	N	O	P	0
			26	16	1	8	1	
29	7	1	Total	C	N	O	P	0
			25	15	1	8	1	
29	8	1	Total	C	N	O	P	0
			21	11	1	8	1	
29	B	1	Total	C	N	O	P	0
			27	17	1	8	1	
29	B	1	Total	C	O	P		0
			26	18	7	1		
29	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
29	J	1	Total	C	N	O	P	0
			22	12	1	8	1	
29	L	1	Total	C	N	O	P	0
			20	10	1	8	1	
29	a	1	Total	C	N	O	P	0
			18	8	1	8	1	
29	c	1	Total	C	N	O	P	0
			31	21	1	8	1	

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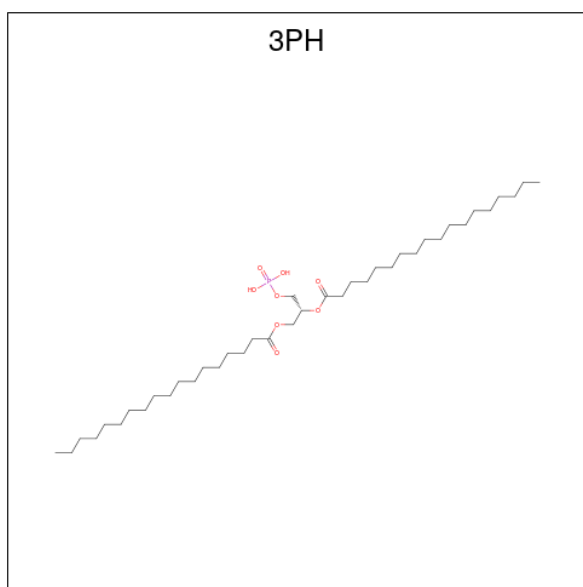
Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total	C	N	O	P	0
			26	16	1	8	1	
29	I	1	Total	C	O	P		0
			38	29	8	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



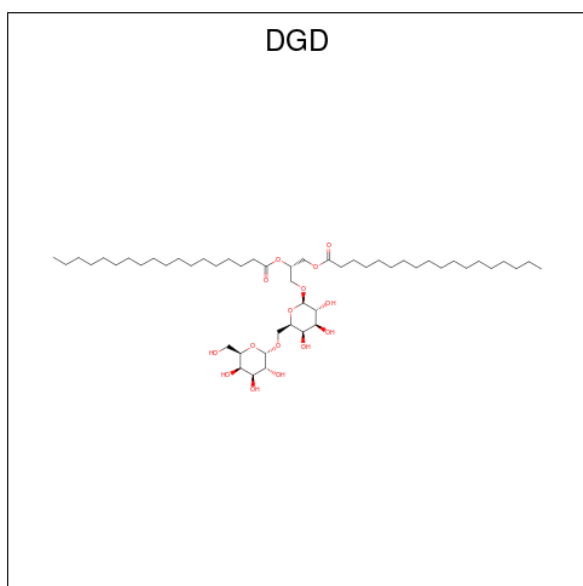
Mol	Chain	Residues	Atoms				AltConf
30	2	1	Total	C	O	S	0
			45	32	12	1	
30	3	1	Total	C	O	S	0
			35	22	12	1	

- Molecule 31 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
31	2	1	Total	C	O	P	0
			43	34	8	1	
31	F	1	Total	C	O	P	0
			26	17	8	1	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



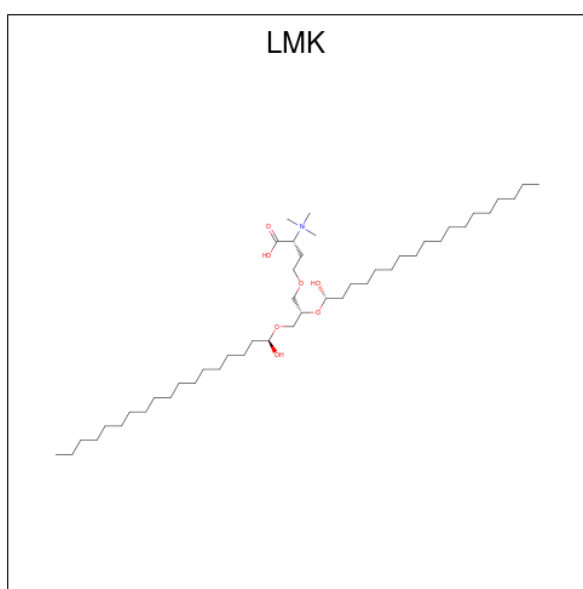
Mol	Chain	Residues	Atoms			AltConf
32	7	1	Total	C	O	0
			39	24	15	

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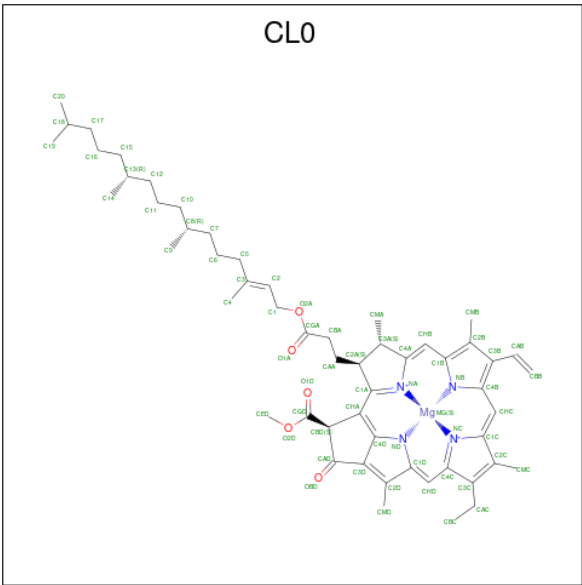
Mol	Chain	Residues	Atoms			AltConf
32	8	1	Total	C	O	0
			47	32	15	
32	A	1	Total	C	O	0
			66	51	15	
32	B	1	Total	C	O	0
			61	46	15	

- Molecule 33 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]azanium (CCD ID: LMK) (formula: C₄₆H₉₄NO₇) (labeled as "Ligand of Interest" by depositor).



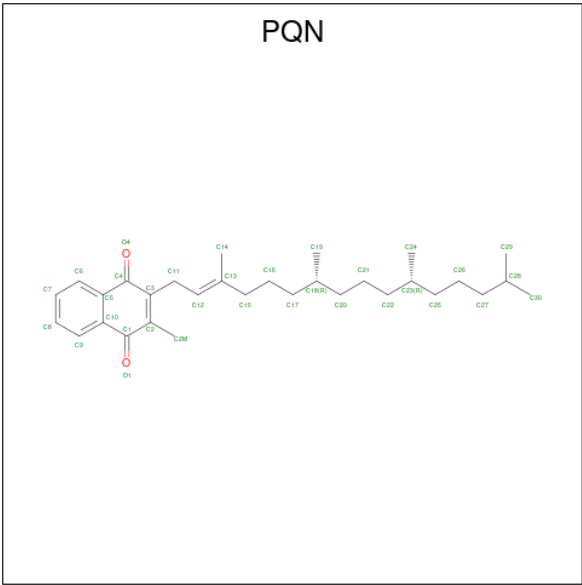
Mol	Chain	Residues	Atoms				AltConf
33	8	1	Total	C	N	O	0
			35	27	1	7	

- Molecule 34 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



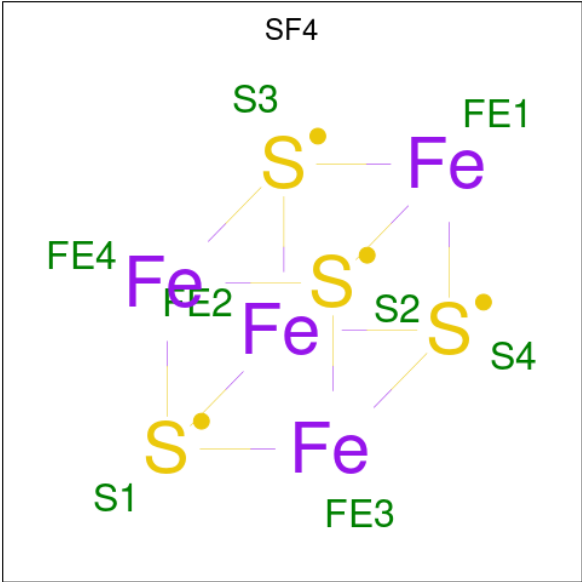
Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 35 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



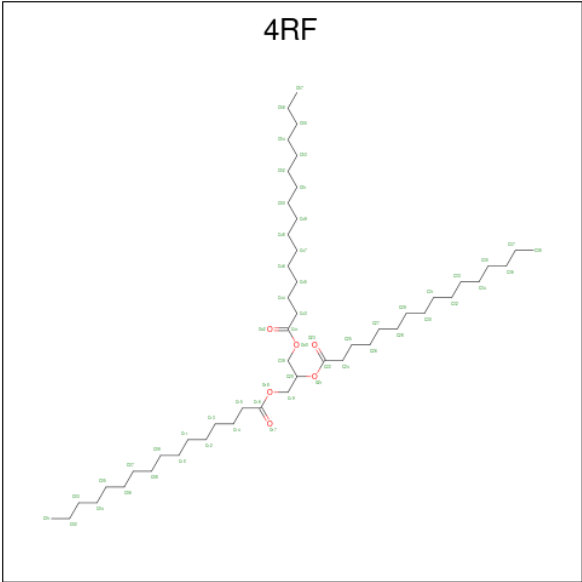
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			33	31	2	
35	B	1	Total	C	O	0
			33	31	2	

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 37 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: C₅₁H₉₈O₆) (labeled as "Ligand of Interest" by depositor).



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

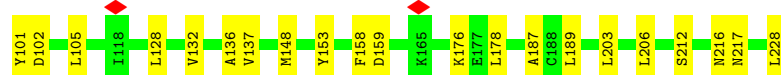
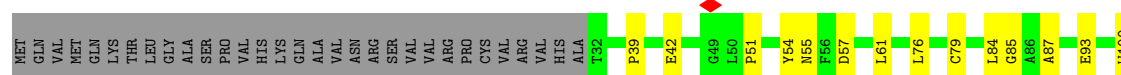
- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	1	Total	O	0
			1	1	
38	C	1	Total	O	0
			1	1	
38	F	2	Total	O	0
			2	2	
38	L	1	Total	O	0
			1	1	

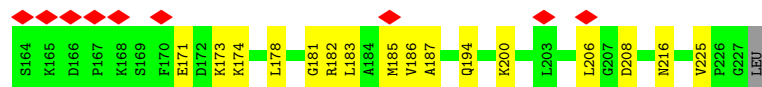
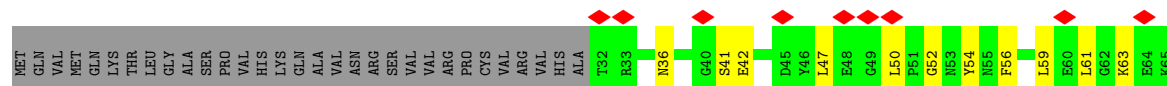
3 Residue-property plots

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.

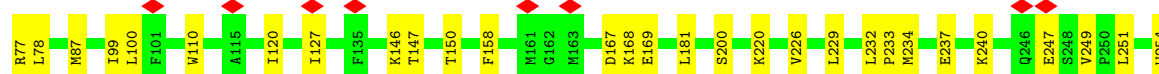
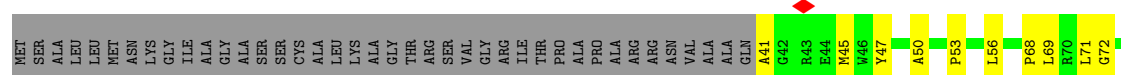
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

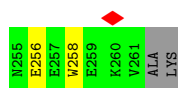


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

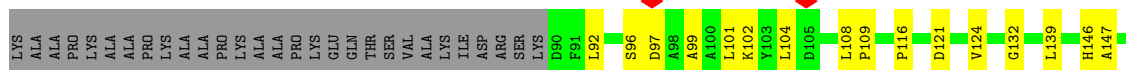
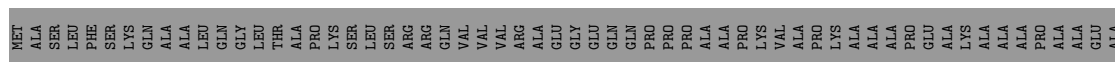


- Molecule 2: LHCA2

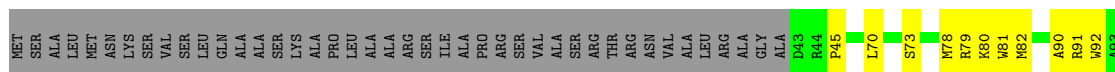




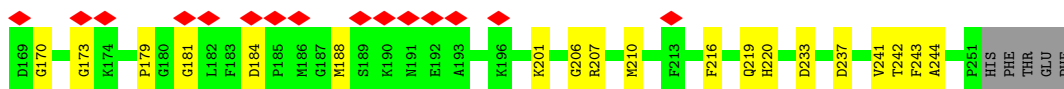
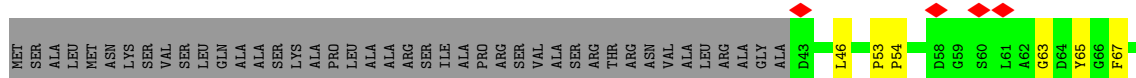
• Molecule 3: LHCA3



• Molecule 4: LHCA7

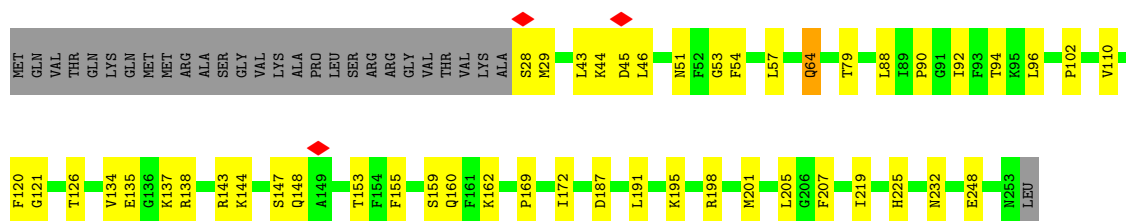


• Molecule 4: LHCA7



• Molecule 5: LHCA8

Chain 8: 



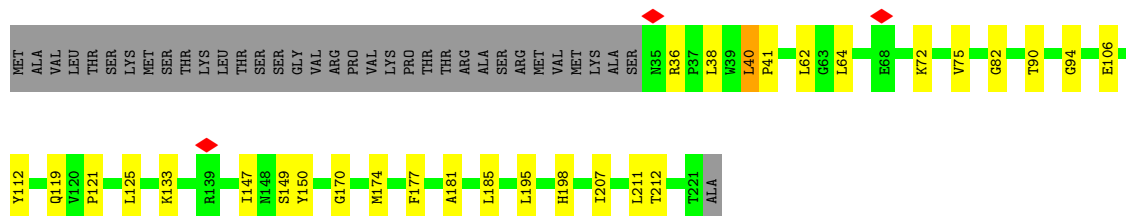
• Molecule 5: LHCA8

Chain b: 



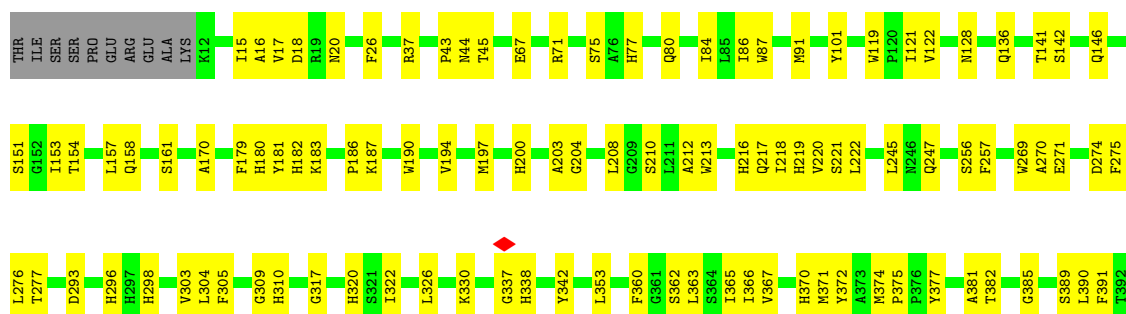
• Molecule 6: LHCA9

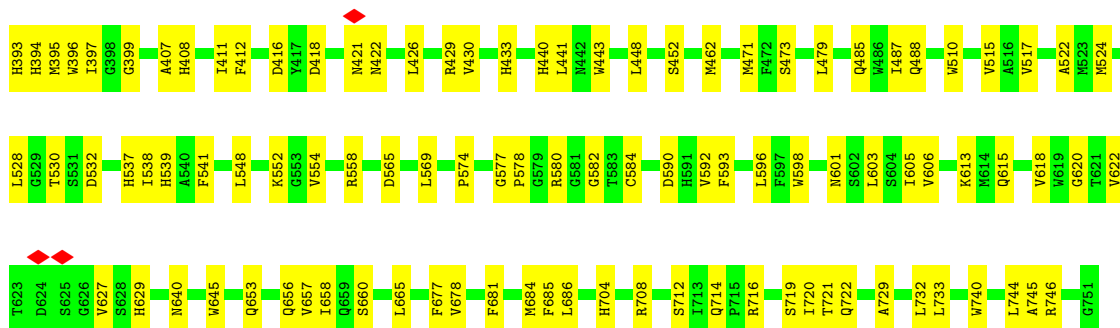
Chain 9: 



• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

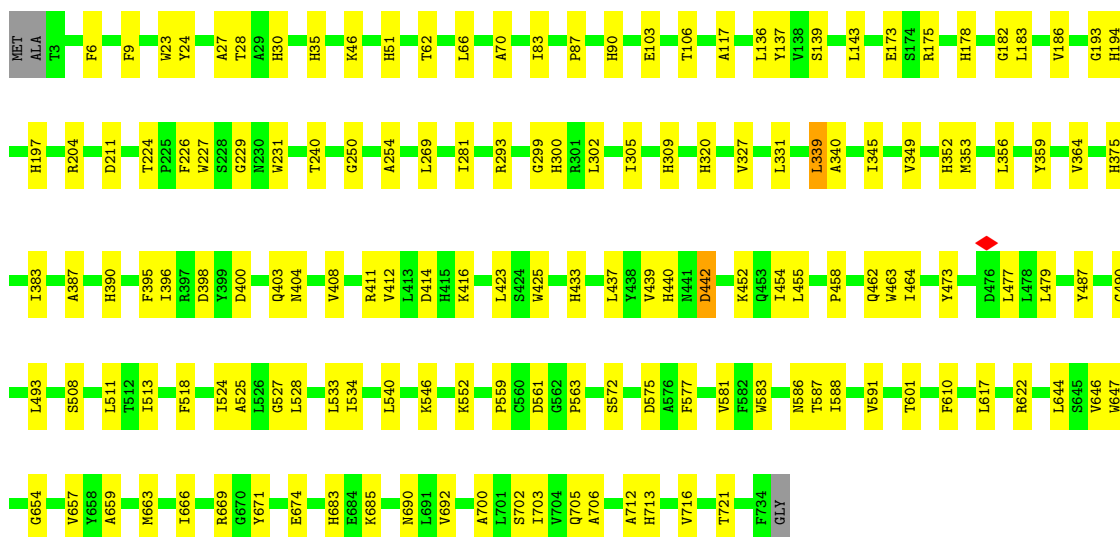
Chain A: 





- Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 79% 20%



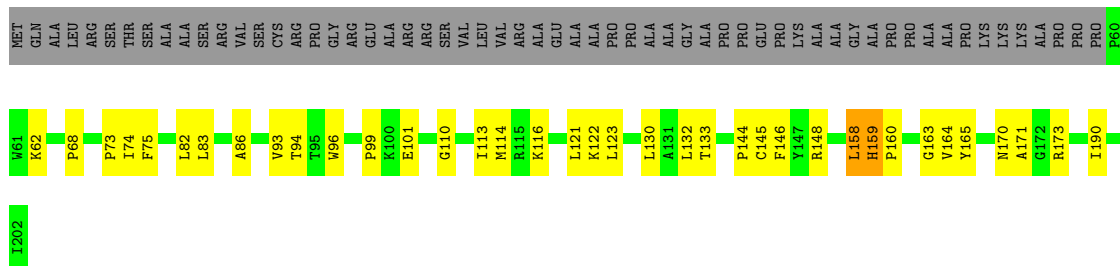
- Molecule 9: Photosystem I iron-sulfur center

Chain C: 78% 21%



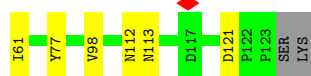
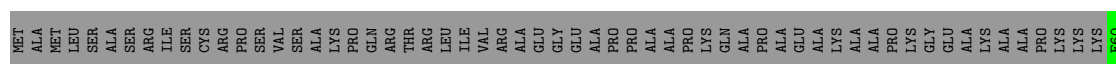
- Molecule 10: PSAD1

Chain D: 52% 17% 29%



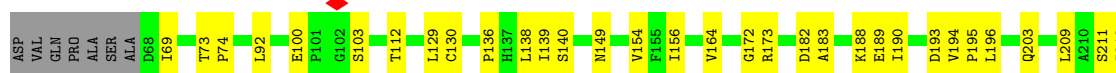
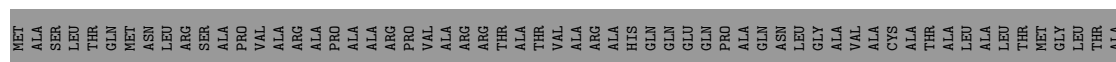
- Molecule 11: PSAE1

Chain E:  46% 5% 49%



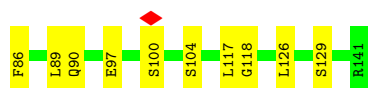
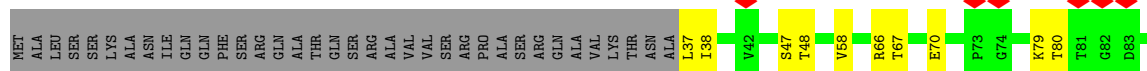
- Molecule 12: PSAF1

Chain F:  55% 16% 29%



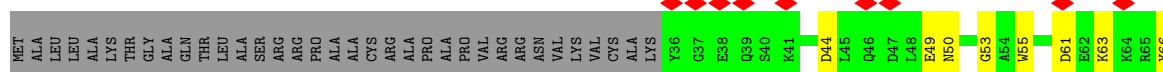
- Molecule 13: PSAG1

Chain G: 



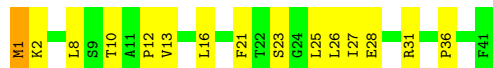
- Molecule 14: PSAH1

Chain H: 

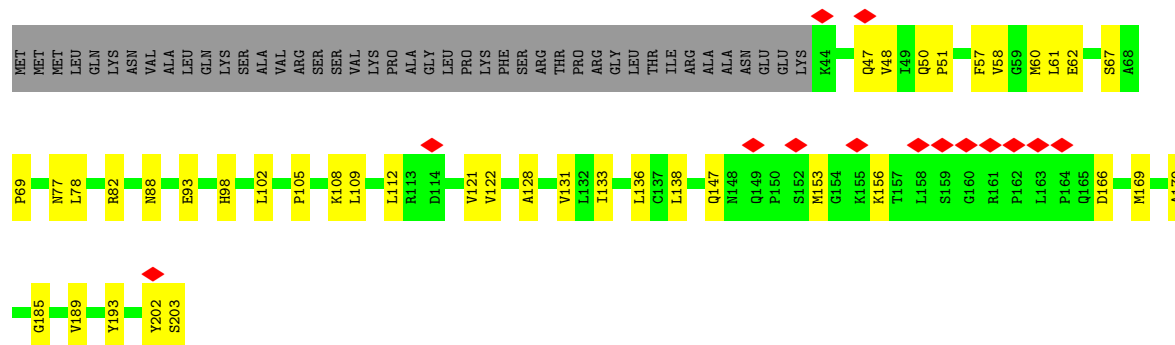


- Molecule 15: Photosystem I reaction center subunit IX

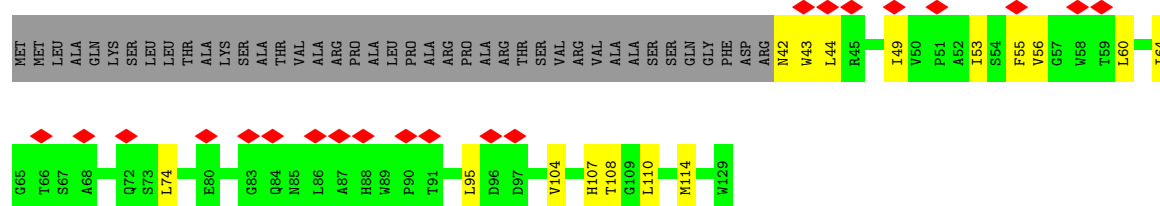
Chain J: 63% 34%



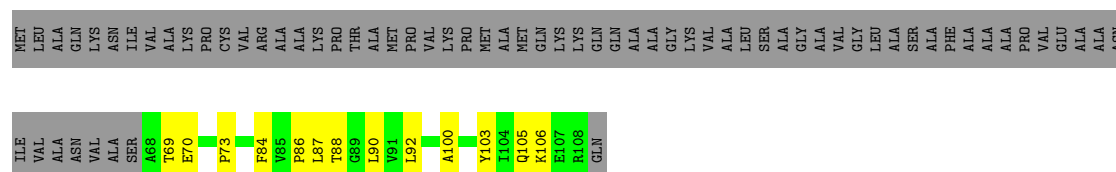
- Molecule 16: PSAL1



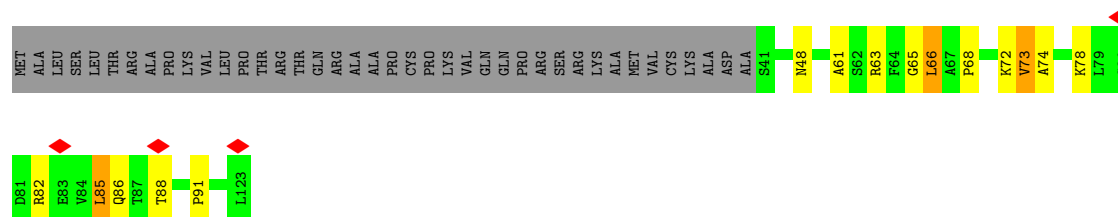
- Molecule 17: PSAO1



- Molecule 18: PSAI1

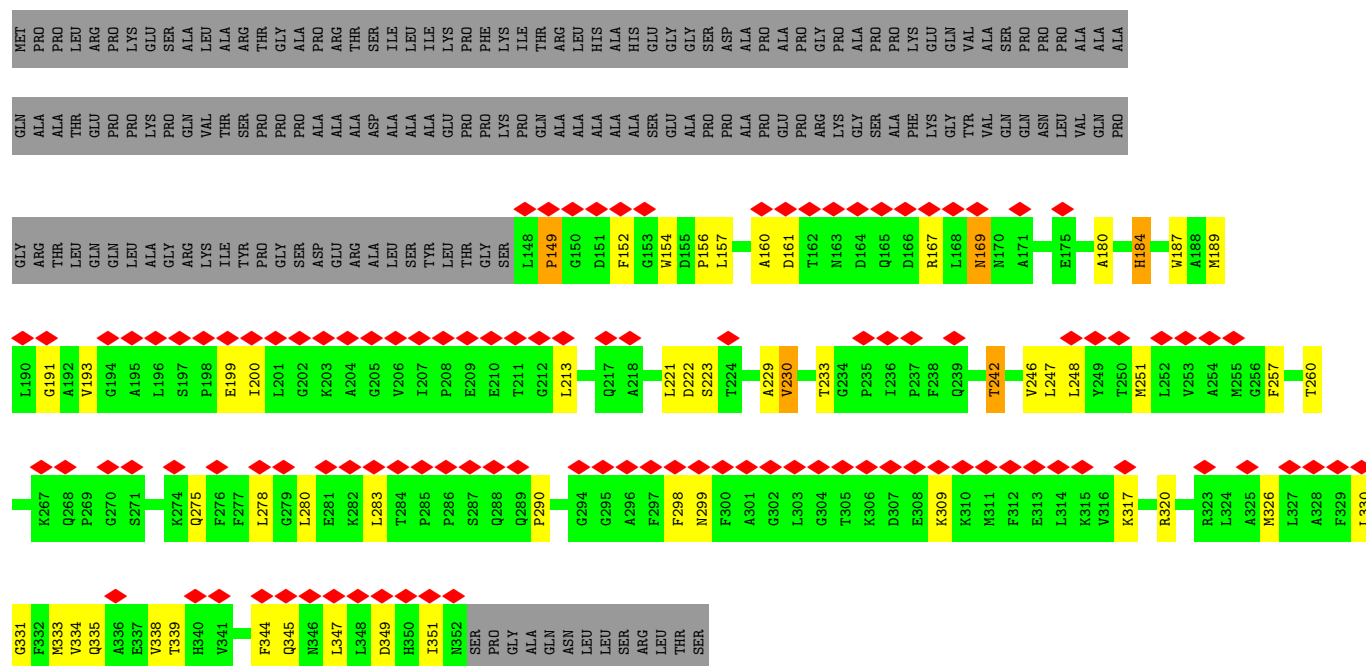


- Molecule 19: PSAK1



- Molecule 20: TIDI1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120321	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	0.083	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0128	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, LMU, DGD, LHG, PTY, CLA, SQD, LMG, BCR, LMK, LUT, 4RF, CHL, PQN, SF4, CL0, 3PH

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	0.15	0/1536	0.37	0/2082
1	a	0.19	0/1529	0.46	0/2073
2	2	0.17	0/1782	0.40	0/2418
3	3	0.17	0/1807	0.41	0/2451
4	7	0.17	0/1659	0.41	0/2254
4	c	0.18	0/1659	0.44	0/2254
5	8	0.15	0/1775	0.41	2/2406 (0.1%)
5	b	0.16	0/1756	0.38	0/2380
6	9	0.27	1/1499 (0.1%)	0.54	2/2043 (0.1%)
7	A	0.15	0/6003	0.35	0/8189
8	B	0.15	0/6016	0.38	0/8225
9	C	0.16	0/610	0.43	0/828
10	D	0.18	0/1163	0.44	0/1571
11	E	0.14	0/521	0.35	0/711
12	F	0.17	0/1332	0.46	2/1801 (0.1%)
13	G	0.19	0/815	0.47	0/1104
14	H	0.22	0/776	0.60	1/1043 (0.1%)
15	J	0.25	0/338	0.70	3/461 (0.7%)
16	L	0.20	0/1201	0.48	0/1643
17	O	0.24	0/723	0.60	0/990
18	I	0.26	0/335	0.66	0/463
19	K	0.29	0/592	0.78	2/801 (0.2%)
20	T	0.22	0/1659	0.64	5/2252 (0.2%)
All	All	0.18	1/37086 (0.0%)	0.44	17/50443 (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
10	D	0	1
12	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	40	LEU	C-N	6.30	1.42	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	149	PRO	N-CA-CB	8.12	111.78	103.25
6	9	40	LEU	CA-CB-CG	7.84	143.74	116.30
6	9	40	LEU	CB-CG-CD2	-6.57	90.98	110.70
20	T	309	LYS	CA-CB-CG	6.03	126.17	114.10
5	8	64	GLN	CB-CG-CD	5.97	122.75	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	D	159	HIS	Peptide
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	1497	0	1465	41	0
1	a	1490	0	1453	39	0
2	2	1731	0	1693	35	0
3	3	1756	0	1710	70	0
4	7	1609	0	1564	49	0
4	c	1609	0	1564	36	0
5	8	1726	0	1674	46	0
5	b	1707	0	1662	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	9	1456	0	1442	34	0
7	A	5807	0	5639	179	0
8	B	5803	0	5554	125	0
9	C	600	0	583	13	0
10	D	1133	0	1141	39	0
11	E	509	0	497	4	0
12	F	1303	0	1327	51	0
13	G	794	0	799	15	0
14	H	763	0	753	33	0
15	J	327	0	328	12	0
16	L	1170	0	1187	37	0
17	O	697	0	678	12	0
18	I	321	0	316	18	0
19	K	584	0	614	15	0
20	T	1612	0	1565	46	0
21	1	683	0	591	33	0
21	2	568	0	492	25	0
21	3	706	0	635	34	0
21	7	598	0	539	22	0
21	8	547	0	429	30	0
21	9	551	0	447	15	0
21	A	2526	0	2620	179	0
21	B	2453	0	2529	138	0
21	F	161	0	146	4	0
21	G	203	0	173	9	0
21	H	106	0	89	1	0
21	J	45	0	33	2	0
21	K	193	0	151	6	0
21	L	267	0	231	13	0
21	O	121	0	69	2	0
21	T	596	0	482	14	0
21	a	619	0	507	23	0
21	b	517	0	430	17	0
21	c	523	0	395	12	0
22	1	47	0	31	3	0
22	2	113	0	101	8	0
22	3	66	0	70	8	0
22	7	206	0	165	26	0
22	8	195	0	134	15	0
22	9	47	0	31	5	0
22	T	104	0	80	15	0
22	a	47	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	b	211	0	166	23	0
22	c	142	0	97	11	0
23	1	42	0	56	7	0
23	2	126	0	168	6	0
23	3	42	0	56	1	0
23	7	42	0	56	1	0
23	8	42	0	56	0	0
23	9	42	0	56	3	0
23	B	42	0	55	4	0
23	O	42	0	54	1	0
23	T	42	0	54	3	0
23	a	42	0	54	6	0
23	b	42	0	56	2	0
23	c	42	0	56	1	0
24	1	44	0	56	12	0
24	3	44	0	56	6	0
24	7	44	0	56	3	0
24	8	44	0	56	3	0
24	9	88	0	112	7	0
24	T	44	0	56	4	0
24	a	44	0	56	5	0
24	b	44	0	56	3	0
24	c	44	0	56	1	0
25	1	40	0	56	3	0
25	3	120	0	166	8	0
25	7	40	0	53	4	0
25	8	40	0	56	6	0
25	A	240	0	336	31	0
25	B	240	0	336	26	0
25	F	80	0	111	9	0
25	G	80	0	112	4	0
25	I	80	0	112	9	0
25	J	80	0	112	8	0
25	K	40	0	56	6	0
25	L	120	0	168	3	0
25	O	40	0	56	1	0
25	T	40	0	56	1	0
25	a	40	0	56	0	0
25	b	40	0	54	6	0
25	c	40	0	56	2	0
26	1	28	0	26	4	0
26	3	40	0	53	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	7	47	0	64	7	0
26	A	32	0	34	2	0
26	F	39	0	48	3	0
26	G	43	0	55	5	0
27	1	35	0	45	1	0
27	9	35	0	46	4	0
27	A	70	0	92	4	0
28	1	98	0	109	9	0
28	2	22	0	17	0	0
28	3	43	0	32	0	0
28	7	74	0	91	5	0
28	8	40	0	53	3	0
28	9	28	0	26	0	0
28	A	75	0	92	5	0
28	B	32	0	33	0	0
28	F	74	0	91	4	0
28	H	49	0	74	3	0
28	a	45	0	28	2	0
28	b	54	0	43	3	0
28	c	29	0	27	0	0
29	1	21	0	15	0	0
29	2	32	0	37	1	0
29	3	17	0	7	0	0
29	7	51	0	47	0	0
29	8	21	0	17	0	0
29	B	53	0	50	0	0
29	H	42	0	56	1	0
29	I	38	0	49	7	0
29	J	22	0	17	2	0
29	L	20	0	11	1	0
29	a	18	0	9	0	0
29	c	57	0	60	4	0
30	2	45	0	54	4	0
30	3	35	0	34	4	0
31	2	43	0	62	4	0
31	F	26	0	24	1	0
32	7	39	0	36	2	0
32	8	47	0	52	4	0
32	A	66	0	92	4	0
32	B	61	0	83	3	0
33	8	35	0	0	0	0
34	A	65	0	72	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	33	0	46	1	0
35	B	33	0	46	4	0
36	A	8	0	0	4	0
36	C	16	0	0	1	0
37	A	39	0	53	2	0
38	A	1	0	0	0	0
38	C	1	0	0	0	0
38	F	2	0	0	0	0
38	L	1	0	0	0	0
All	All	53613	0	52599	1344	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 13.

The worst 5 of 1344 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)
3:3:288:VAL:CG1	21:A:817:CLA:C2	1.82	1.53
3:3:288:VAL:CG1	21:A:817:CLA:H2	1.43	1.38
3:3:288:VAL:HG11	21:A:817:CLA:C2	1.46	1.36
4:7:78:MET:HE3	26:7:320:LMG:O5	1.20	1.34
7:A:584:CYS:SG	36:A:845:SF4:FE4	1.19	1.32

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%)	188 (96%)	7 (4%)	0	100	100
1	a	194/228 (85%)	182 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	219/263 (83%)	208 (95%)	10 (5%)	1 (0%)	25	61
3	3	228/320 (71%)	220 (96%)	8 (4%)	0	100	100
4	7	207/256 (81%)	196 (95%)	11 (5%)	0	100	100
4	c	207/256 (81%)	200 (97%)	7 (3%)	0	100	100
5	8	224/254 (88%)	218 (97%)	6 (3%)	0	100	100
5	b	221/254 (87%)	215 (97%)	6 (3%)	0	100	100
6	9	185/222 (83%)	171 (92%)	14 (8%)	0	100	100
7	A	738/750 (98%)	703 (95%)	35 (5%)	0	100	100
8	B	730/735 (99%)	699 (96%)	31 (4%)	0	100	100
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%)	59 (95%)	3 (5%)	0	100	100
12	F	163/232 (70%)	154 (94%)	9 (6%)	0	100	100
13	G	103/141 (73%)	95 (92%)	7 (7%)	1 (1%)	13	46
14	H	96/135 (71%)	83 (86%)	13 (14%)	0	100	100
15	J	39/41 (95%)	35 (90%)	4 (10%)	0	100	100
16	L	157/202 (78%)	147 (94%)	10 (6%)	0	100	100
17	O	86/129 (67%)	80 (93%)	6 (7%)	0	100	100
18	I	39/109 (36%)	37 (95%)	2 (5%)	0	100	100
19	K	81/123 (66%)	67 (83%)	14 (17%)	0	100	100
20	T	203/365 (56%)	181 (89%)	20 (10%)	2 (1%)	13	46
All	All	4596/5651 (81%)	4345 (94%)	247 (5%)	4 (0%)	50	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	T	149	PRO
2	2	120	ILE
13	G	38	ILE
20	T	298	PHE

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	150/178 (84%)	150 (100%)	0	100	100
1	a	150/178 (84%)	150 (100%)	0	100	100
2	2	179/207 (86%)	179 (100%)	0	100	100
3	3	174/236 (74%)	174 (100%)	0	100	100
4	7	166/201 (83%)	166 (100%)	0	100	100
4	c	166/201 (83%)	166 (100%)	0	100	100
5	8	173/196 (88%)	173 (100%)	0	100	100
5	b	171/196 (87%)	170 (99%)	1 (1%)	84	93
6	9	153/183 (84%)	153 (100%)	0	100	100
7	A	599/608 (98%)	597 (100%)	2 (0%)	91	96
8	B	593/594 (100%)	589 (99%)	4 (1%)	81	91
9	C	68/69 (99%)	67 (98%)	1 (2%)	60	83
10	D	123/163 (76%)	122 (99%)	1 (1%)	79	90
11	E	57/101 (56%)	56 (98%)	1 (2%)	54	80
12	F	138/184 (75%)	138 (100%)	0	100	100
13	G	81/110 (74%)	81 (100%)	0	100	100
14	H	78/105 (74%)	77 (99%)	1 (1%)	65	85
15	J	36/36 (100%)	36 (100%)	0	100	100
16	L	122/159 (77%)	122 (100%)	0	100	100
17	O	72/103 (70%)	70 (97%)	2 (3%)	38	70
18	I	32/77 (42%)	31 (97%)	1 (3%)	35	68
19	K	61/94 (65%)	59 (97%)	2 (3%)	33	67
20	T	165/286 (58%)	159 (96%)	6 (4%)	30	64
All	All	3707/4465 (83%)	3685 (99%)	22 (1%)	82	93

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	K	73	VAL
20	T	200	ILE
20	T	184	HIS
20	T	230	VAL
9	C	12	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
14	H	125	ASN
20	T	321	ASN
15	J	30	ASN
1	a	36	ASN
5	8	232	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

362 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
21	CLA	B	807	-	63,73,73	1.40	8 (12%)	74,113,113	1.30	7 (9%)
21	CLA	G	201	8	63,73,73	1.35	4 (6%)	74,113,113	1.26	8 (10%)
21	CLA	3	406	-	53,63,73	1.48	6 (11%)	62,101,113	1.47	8 (12%)
21	CLA	2	602	2	63,73,73	1.35	7 (11%)	74,113,113	1.28	6 (8%)
23	LUT	9	613	-	42,43,43	0.29	0	51,60,60	0.34	0
21	CLA	A	842	28	52,62,73	1.47	6 (11%)	60,99,113	1.38	8 (13%)
29	PTY	1	320	-	20,20,49	0.69	0	23,25,54	0.51	0
21	CLA	3	403	-	48,58,73	1.53	4 (8%)	56,95,113	1.49	7 (12%)
21	CLA	A	812	7	53,63,73	1.47	7 (13%)	62,101,113	1.31	6 (9%)
21	CLA	3	408	3	58,68,73	1.37	5 (8%)	68,107,113	1.28	7 (10%)
21	CLA	a	308	1	48,58,73	1.56	6 (12%)	56,95,113	1.49	10 (17%)
23	LUT	O	2005	-	42,43,43	0.34	0	51,60,60	0.68	2 (3%)
21	CLA	c	611	-	44,54,73	1.62	5 (11%)	51,90,113	1.56	6 (11%)
21	CLA	B	831	8	63,73,73	1.37	6 (9%)	74,113,113	1.27	6 (8%)
21	CLA	3	405	3	48,58,73	1.54	5 (10%)	56,95,113	1.48	7 (12%)
24	XAT	9	615	-	41,47,47	0.17	0	54,74,74	0.72	3 (5%)
21	CLA	A	839	7	63,73,73	1.29	7 (11%)	74,113,113	1.26	8 (10%)
21	CLA	3	404	-	44,54,73	1.58	5 (11%)	51,90,113	1.40	6 (11%)
21	CLA	7	306	-	48,58,73	1.59	5 (10%)	56,95,113	1.50	8 (14%)
21	CLA	c	604	-	48,58,73	1.56	6 (12%)	56,95,113	1.51	8 (14%)
21	CLA	c	603	4	49,59,73	1.54	6 (12%)	56,96,113	1.43	7 (12%)
22	CHL	c	607	-	46,56,74	1.55	4 (8%)	49,92,114	2.43	8 (16%)
21	CLA	T	607	-	48,58,73	1.53	5 (10%)	56,95,113	1.48	8 (14%)
21	CLA	A	824	7	58,68,73	1.40	5 (8%)	68,107,113	1.28	6 (8%)
28	LHG	9	617	21	27,27,48	0.40	0	30,33,54	0.39	0
22	CHL	7	303	-	64,74,74	1.40	4 (6%)	71,114,114	2.10	10 (14%)
21	CLA	b	306	-	48,58,73	1.53	5 (10%)	56,95,113	1.52	6 (10%)
27	LMU	9	616	-	36,36,36	0.27	0	47,47,47	0.63	0
25	BCR	B	848	-	41,41,41	0.15	0	56,56,56	0.26	0
21	CLA	A	838	7	49,59,73	1.53	6 (12%)	56,96,113	1.51	6 (10%)
30	SQD	3	422	-	33,35,54	0.27	0	43,46,65	0.38	0
21	CLA	8	610	5	58,68,73	1.37	6 (10%)	68,107,113	1.21	6 (8%)
21	CLA	A	837	7	45,55,73	1.61	5 (11%)	52,91,113	1.49	6 (11%)
28	LHG	3	424	-	25,25,48	0.39	0	28,31,54	0.36	0
21	CLA	a	303	1	53,63,73	1.51	6 (11%)	62,101,113	1.46	7 (11%)
22	CHL	8	606	-	44,54,74	1.39	5 (11%)	47,90,114	2.37	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	809	-	58,68,73	1.43	6 (10%)	68,107,113	1.33	9 (13%)
29	PTY	c	620	-	25,25,49	0.60	0	28,30,54	0.64	0
25	BCR	B	846	-	41,41,41	0.14	0	56,56,56	0.34	0
21	CLA	7	323	5	44,54,73	1.61	6 (13%)	51,90,113	1.52	6 (11%)
22	CHL	7	308	-	44,54,74	1.43	5 (11%)	47,90,114	2.42	11 (23%)
21	CLA	3	413	-	40,50,73	1.67	5 (12%)	45,85,113	1.34	6 (13%)
21	CLA	A	828	-	55,65,73	1.46	6 (10%)	64,103,113	1.44	8 (12%)
21	CLA	B	818	-	63,73,73	1.33	6 (9%)	74,113,113	1.24	7 (9%)
22	CHL	9	606	-	45,55,74	1.51	4 (8%)	48,91,114	2.37	8 (16%)
21	CLA	3	411	3	58,68,73	1.44	7 (12%)	68,107,113	1.33	7 (10%)
21	CLA	B	815	-	53,63,73	1.45	5 (9%)	62,101,113	1.34	6 (9%)
25	BCR	7	319	-	41,41,41	0.20	0	56,56,56	0.42	0
36	SF4	C	101	9	0,12,12	-	-	-	-	-
21	CLA	G	205	-	43,53,73	1.62	4 (9%)	50,89,113	1.42	7 (14%)
21	CLA	A	830	7	63,73,73	1.31	6 (9%)	74,113,113	1.38	9 (12%)
21	CLA	a	311	1	44,54,73	1.66	7 (15%)	51,90,113	1.59	8 (15%)
21	CLA	b	314	5	48,58,73	1.58	6 (12%)	56,95,113	1.45	8 (14%)
21	CLA	9	611	-	44,54,73	1.61	5 (11%)	51,90,113	1.55	6 (11%)
21	CLA	B	834	8	58,68,73	1.41	6 (10%)	68,107,113	1.41	7 (10%)
21	CLA	L	301	7	48,58,73	1.54	6 (12%)	56,95,113	1.45	7 (12%)
26	LMG	7	320	-	47,47,55	0.21	0	55,55,63	0.28	0
21	CLA	7	312	28	43,53,73	1.65	7 (16%)	50,89,113	1.54	6 (12%)
21	CLA	B	810	8	63,73,73	1.33	6 (9%)	74,113,113	1.31	8 (10%)
21	CLA	c	601	5	44,54,73	1.59	5 (11%)	51,90,113	1.49	6 (11%)
21	CLA	b	313	5	48,58,73	1.60	7 (14%)	56,95,113	1.53	10 (17%)
21	CLA	9	607	6	63,73,73	1.36	5 (7%)	74,113,113	1.35	8 (10%)
21	CLA	2	612	2	43,53,73	1.67	6 (13%)	50,89,113	1.46	6 (12%)
21	CLA	1	301	1	59,69,73	1.39	5 (8%)	69,108,113	1.36	7 (10%)
21	CLA	1	304	-	43,53,73	1.64	6 (13%)	50,89,113	1.53	6 (12%)
29	PTY	3	423	-	13,16,49	0.57	0	14,19,54	0.36	0
21	CLA	B	835	8	63,73,73	1.37	6 (9%)	74,113,113	1.54	9 (12%)
21	CLA	B	836	8	53,63,73	1.44	7 (13%)	62,101,113	1.36	8 (12%)
21	CLA	A	816	-	63,73,73	1.33	5 (7%)	74,113,113	1.38	8 (10%)
28	LHG	8	620	21	39,39,48	0.33	0	42,45,54	0.35	0
21	CLA	T	613	-	44,54,73	1.59	5 (11%)	51,90,113	1.37	6 (11%)
21	CLA	A	840	7	58,68,73	1.40	6 (10%)	68,107,113	1.24	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	O	2003	-	43,53,73	1.63	6 (13%)	50,89,113	1.44	6 (12%)
25	BCR	L	307	-	41,41,41	0.12	0	56,56,56	0.28	0
25	BCR	L	309	-	41,41,41	0.19	0	56,56,56	0.44	0
21	CLA	1	307	1	48,58,73	1.53	5 (10%)	56,95,113	1.48	8 (14%)
21	CLA	7	316	4	63,73,73	1.35	6 (9%)	74,113,113	1.34	7 (9%)
21	CLA	H	203	14	58,68,73	1.41	5 (8%)	68,107,113	1.35	6 (8%)
21	CLA	3	414	3	44,54,73	1.63	6 (13%)	51,90,113	1.46	6 (11%)
21	CLA	B	814	8	58,68,73	1.38	6 (10%)	68,107,113	1.39	6 (8%)
28	LHG	A	853	-	44,44,48	0.30	0	47,50,54	0.31	0
29	PTY	7	302	-	25,25,49	0.62	0	28,30,54	0.48	0
22	CHL	b	307	-	45,55,74	1.39	5 (11%)	48,91,114	2.38	8 (16%)
22	CHL	b	309	-	49,59,74	1.33	5 (10%)	53,96,114	2.40	9 (16%)
25	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.52	0
25	BCR	J	5004	-	41,41,41	0.15	0	56,56,56	0.24	0
28	LHG	7	321	21	42,42,48	0.31	0	45,48,54	0.30	0
21	CLA	T	610	-	44,54,73	1.61	5 (11%)	51,90,113	1.48	6 (11%)
21	CLA	K	204	-	46,56,73	1.57	5 (10%)	53,92,113	1.41	7 (13%)
21	CLA	L	306	-	48,58,73	1.53	5 (10%)	56,95,113	1.51	7 (12%)
21	CLA	a	310	28	44,54,73	1.65	6 (13%)	51,90,113	1.47	6 (11%)
22	CHL	b	308	-	45,55,74	1.29	4 (8%)	48,91,114	2.36	8 (16%)
23	LUT	a	315	-	42,43,43	0.21	0	51,60,60	1.48	8 (15%)
26	LMG	1	317	-	28,28,55	0.28	0	35,35,63	0.35	0
25	BCR	A	848	-	41,41,41	0.31	0	56,56,56	0.94	4 (7%)
21	CLA	c	608	-	43,53,73	1.64	4 (9%)	50,89,113	1.48	6 (12%)
21	CLA	B	840	8	58,68,73	1.43	6 (10%)	68,107,113	1.31	9 (13%)
21	CLA	A	819	7	58,68,73	1.40	6 (10%)	68,107,113	1.30	7 (10%)
21	CLA	a	312	-	58,68,73	1.39	5 (8%)	68,107,113	1.27	8 (11%)
21	CLA	2	605	-	43,53,73	1.62	5 (11%)	50,89,113	1.44	6 (12%)
35	PQN	B	845	-	34,34,34	0.29	0	43,45,45	0.57	1 (2%)
21	CLA	7	315	4	48,58,73	1.52	5 (10%)	56,95,113	1.47	8 (14%)
21	CLA	8	611	28	53,63,73	1.48	6 (11%)	62,101,113	1.41	8 (12%)
21	CLA	2	609	28	39,49,73	1.67	4 (10%)	46,84,113	1.53	7 (15%)
21	CLA	T	614	-	40,50,73	1.66	4 (10%)	45,85,113	1.37	6 (13%)
29	PTY	J	5001	-	21,21,49	0.67	0	24,26,54	0.54	0
21	CLA	c	602	4	50,60,73	1.51	7 (14%)	57,97,113	1.37	7 (12%)
22	CHL	7	309	-	46,56,74	1.57	5 (10%)	49,92,114	2.16	8 (16%)
25	BCR	1	316	-	41,41,41	0.14	0	56,56,56	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	F	5006	-	45,55,73	1.57	5 (11%)	52,91,113	1.41	7 (13%)
21	CLA	7	304	4	58,68,73	1.40	7 (12%)	68,107,113	1.29	8 (11%)
25	BCR	3	419	-	41,41,41	0.22	0	56,56,56	0.28	0
21	CLA	2	604	-	48,58,73	1.51	4 (8%)	56,95,113	1.37	8 (14%)
22	CHL	c	606	-	46,56,74	1.37	4 (8%)	49,92,114	2.05	9 (18%)
21	CLA	G	203	13	45,55,73	1.62	7 (15%)	52,91,113	1.53	7 (13%)
27	LMU	A	855	-	36,36,36	0.19	0	47,47,47	0.33	0
28	LHG	7	324	-	30,30,48	0.40	0	33,36,54	0.61	1 (3%)
28	LHG	3	420	21	16,16,48	0.89	1 (6%)	17,20,54	0.64	0
22	CHL	7	307	-	44,54,74	1.46	5 (11%)	47,90,114	2.33	8 (17%)
21	CLA	B	804	-	63,73,73	1.33	6 (9%)	74,113,113	1.20	7 (9%)
21	CLA	1	309	28	44,54,73	1.61	6 (13%)	51,90,113	1.38	6 (11%)
21	CLA	a	307	-	43,53,73	1.64	5 (11%)	50,89,113	1.49	6 (12%)
21	CLA	a	309	1	58,68,73	1.38	6 (10%)	68,107,113	1.35	7 (10%)
21	CLA	B	824	8	53,63,73	1.48	6 (11%)	62,101,113	1.39	8 (12%)
27	LMU	1	318	-	36,36,36	0.22	0	47,47,47	0.49	0
21	CLA	A	817	7	63,73,73	1.34	5 (7%)	74,113,113	1.28	6 (8%)
25	BCR	3	417	-	41,41,41	0.16	0	56,56,56	0.33	0
24	XAT	3	416	-	41,47,47	0.19	0	54,74,74	0.98	3 (5%)
21	CLA	b	304	5	58,68,73	1.38	4 (6%)	68,107,113	1.24	7 (10%)
23	LUT	T	615	-	42,43,43	0.39	0	51,60,60	0.49	0
21	CLA	L	303	16	50,60,73	1.50	5 (10%)	57,97,113	1.43	6 (10%)
25	BCR	F	5008	-	41,41,41	0.16	0	56,56,56	0.33	0
22	CHL	8	607	-	45,55,74	1.30	4 (8%)	48,91,114	2.34	9 (18%)
28	LHG	1	322	21	26,26,48	0.38	0	29,32,54	0.35	0
21	CLA	7	310	4	43,53,73	1.62	5 (11%)	50,89,113	1.46	6 (12%)
21	CLA	T	612	-	63,73,73	1.34	5 (7%)	74,113,113	1.31	7 (9%)
21	CLA	A	825	7	58,68,73	1.40	5 (8%)	68,107,113	1.23	7 (10%)
21	CLA	9	603	-	53,63,73	1.51	6 (11%)	62,101,113	1.49	8 (12%)
21	CLA	A	822	7	56,66,73	1.40	5 (8%)	65,104,113	1.40	7 (10%)
21	CLA	A	808	7	63,73,73	1.35	5 (7%)	74,113,113	1.37	8 (10%)
22	CHL	1	305	-	45,55,74	1.27	5 (11%)	48,91,114	1.96	11 (22%)
25	BCR	L	302	-	41,41,41	0.24	0	56,56,56	0.57	0
37	4RF	A	857	-	38,38,56	0.42	0	41,41,59	0.40	0
30	SQD	2	618	-	43,45,54	0.24	0	53,56,65	0.48	1 (1%)
21	CLA	c	610	28	43,53,73	1.62	5 (11%)	50,89,113	1.49	6 (12%)
29	PTY	L	308	-	19,19,49	0.71	0	22,24,54	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	823	-	58,68,73	1.44	8 (13%)	68,107,113	1.34	8 (11%)
36	SF4	C	102	9	0,12,12	-	-	-		
26	LMG	A	801	-	32,32,55	0.21	0	40,40,63	0.30	0
25	BCR	I	203	-	41,41,41	0.15	0	56,56,56	0.31	0
21	CLA	9	605	6	43,53,73	1.69	7 (16%)	50,89,113	1.69	7 (14%)
21	CLA	T	606	-	44,54,73	1.66	8 (18%)	51,90,113	1.64	8 (15%)
21	CLA	1	311	-	58,68,73	1.42	5 (8%)	68,107,113	1.33	7 (10%)
21	CLA	T	611	20	50,60,73	1.59	7 (14%)	57,97,113	1.57	9 (15%)
23	LUT	2	614	-	42,43,43	0.26	0	51,60,60	0.38	0
29	PTY	a	319	-	17,17,49	0.72	0	18,21,54	0.69	0
21	CLA	O	2002	-	36,46,73	1.86	6 (16%)	45,81,113	1.65	9 (20%)
25	BCR	8	618	-	41,41,41	0.15	0	56,56,56	0.35	0
28	LHG	F	5003	-	42,42,48	0.32	0	45,48,54	0.32	0
21	CLA	8	614	5	44,54,73	1.56	5 (11%)	51,90,113	1.37	6 (11%)
21	CLA	B	820	8	58,68,73	1.47	8 (13%)	68,107,113	1.45	8 (11%)
21	CLA	T	609	20	53,63,73	1.44	6 (11%)	62,101,113	1.43	9 (14%)
21	CLA	A	833	7	53,63,73	1.45	6 (11%)	62,101,113	1.33	7 (11%)
21	CLA	b	310	5	44,54,73	1.58	5 (11%)	51,90,113	1.38	6 (11%)
21	CLA	B	839	-	53,63,73	1.49	5 (9%)	62,101,113	1.52	6 (9%)
24	XAT	7	318	-	41,47,47	0.20	0	54,74,74	0.88	3 (5%)
21	CLA	3	402	3	63,73,73	1.34	6 (9%)	74,113,113	1.32	7 (9%)
21	CLA	9	602	6	45,55,73	1.56	5 (11%)	52,91,113	1.36	7 (13%)
21	CLA	c	612	4	45,55,73	1.67	7 (15%)	52,91,113	1.47	7 (13%)
21	CLA	8	622	-	44,54,73	2.14	10 (22%)	51,90,113	2.35	12 (23%)
21	CLA	9	601	-	44,54,73	2.66	7 (15%)	51,90,113	2.94	13 (25%)
21	CLA	A	841	7	63,73,73	1.34	5 (7%)	74,113,113	1.27	8 (10%)
29	PTY	7	322	-	24,24,49	0.63	0	27,29,54	0.51	0
25	BCR	G	202	-	41,41,41	0.24	0	56,56,56	0.42	0
21	CLA	A	829	7	63,73,73	1.40	7 (11%)	74,113,113	1.36	8 (10%)
21	CLA	B	833	-	63,73,73	1.34	5 (7%)	74,113,113	1.33	8 (10%)
28	LHG	a	301	-	21,21,48	0.44	0	24,27,54	0.52	0
35	PQN	A	844	-	34,34,34	0.28	0	43,45,45	0.57	1 (2%)
24	XAT	9	614	-	41,47,47	0.15	0	54,74,74	0.68	1 (1%)
22	CHL	8	601	-	49,59,74	1.51	4 (8%)	53,96,114	1.95	11 (20%)
25	BCR	a	317	-	41,41,41	0.19	0	56,56,56	0.40	0
28	LHG	F	5001	-	30,30,48	0.36	0	33,36,54	0.33	0
21	CLA	8	603	5	48,58,73	1.52	5 (10%)	56,95,113	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	b	315	5	44,54,73	1.58	5 (11%)	51,90,113	1.35	6 (11%)
33	LMK	8	621	-	34,34,53	0.54	0	34,41,60	0.72	1 (2%)
29	PTY	2	620	-	31,31,49	0.57	0	34,36,54	0.46	0
21	CLA	T	604	-	45,55,73	1.56	5 (11%)	52,91,113	1.35	7 (13%)
21	CLA	H	204	-	44,54,73	1.56	4 (9%)	51,90,113	1.40	6 (11%)
21	CLA	a	305	-	43,53,73	1.66	5 (11%)	50,89,113	1.53	7 (14%)
21	CLA	B	828	-	63,73,73	1.33	5 (7%)	74,113,113	1.22	8 (10%)
21	CLA	a	302	1	63,73,73	1.34	4 (6%)	74,113,113	1.25	7 (9%)
21	CLA	J	5002	15	43,53,73	1.66	5 (11%)	50,89,113	1.67	7 (14%)
31	3PH	F	5002	-	25,25,47	0.36	0	28,30,52	0.33	0
21	CLA	F	5005	-	63,73,73	1.33	5 (7%)	74,113,113	1.27	7 (9%)
25	BCR	3	418	-	41,41,41	0.13	0	56,56,56	0.28	0
21	CLA	3	409	28	58,68,73	1.41	5 (8%)	68,107,113	1.37	8 (11%)
28	LHG	b	303	-	22,22,48	0.46	0	25,27,54	0.60	0
21	CLA	1	310	1	44,54,73	1.64	7 (15%)	51,90,113	1.58	9 (17%)
21	CLA	T	603	20	54,64,73	1.45	6 (11%)	63,102,113	1.54	8 (12%)
21	CLA	8	612	5	48,58,73	1.65	8 (16%)	56,95,113	1.59	10 (17%)
31	3PH	2	619	-	42,42,47	0.30	0	45,47,52	0.34	0
21	CLA	9	604	6	48,58,73	1.54	5 (10%)	56,95,113	1.38	7 (12%)
25	BCR	A	846	-	41,41,41	0.25	0	56,56,56	1.39	9 (16%)
24	XAT	T	616	-	41,47,47	0.14	0	54,74,74	0.90	2 (3%)
23	LUT	b	317	-	42,43,43	0.24	0	51,60,60	0.41	0
21	CLA	B	841	-	48,58,73	1.51	5 (10%)	56,95,113	1.52	8 (14%)
22	CHL	2	601	2	64,74,74	1.25	4 (6%)	71,114,114	1.95	8 (11%)
21	CLA	7	314	4	63,73,73	1.41	7 (11%)	74,113,113	1.34	7 (9%)
21	CLA	b	311	5	58,68,73	1.40	7 (12%)	68,107,113	1.33	8 (11%)
21	CLA	B	821	8	63,73,73	1.34	5 (7%)	74,113,113	1.28	6 (8%)
21	CLA	A	807	7	63,73,73	1.32	6 (9%)	74,113,113	1.21	7 (9%)
21	CLA	7	313	-	50,60,73	1.53	5 (10%)	57,97,113	1.53	7 (12%)
23	LUT	1	314	-	42,43,43	0.45	1 (2%)	51,60,60	1.16	5 (9%)
24	XAT	b	318	-	41,47,47	0.16	0	54,74,74	0.65	1 (1%)
24	XAT	c	616	-	41,47,47	0.18	0	54,74,74	0.80	2 (3%)
21	CLA	L	304	16	63,73,73	1.29	5 (7%)	74,113,113	1.28	7 (9%)
21	CLA	O	2001	17	35,46,73	1.84	6 (17%)	39,80,113	1.67	7 (17%)
21	CLA	B	816	8	63,73,73	1.35	5 (7%)	74,113,113	1.19	6 (8%)
21	CLA	B	809	8	63,73,73	1.35	5 (7%)	74,113,113	1.53	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	c	617	-	41,41,41	0.16	0	56,56,56	0.25	0
21	CLA	1	312	1	43,53,73	1.64	5 (11%)	50,89,113	1.49	6 (12%)
25	BCR	F	5004	-	41,41,41	0.16	0	56,56,56	0.33	0
22	CHL	T	602	20	54,64,74	1.37	4 (7%)	59,102,114	1.86	8 (13%)
25	BCR	A	850	-	41,41,41	0.13	0	56,56,56	0.36	0
21	CLA	A	805	7	63,73,73	1.36	6 (9%)	74,113,113	1.41	8 (10%)
28	LHG	1	323	-	45,45,48	0.32	0	48,51,54	0.34	0
21	CLA	A	835	-	63,73,73	1.33	6 (9%)	74,113,113	1.25	8 (10%)
21	CLA	B	830	-	58,68,73	1.37	5 (8%)	68,107,113	1.30	7 (10%)
21	CLA	G	204	13	44,54,73	1.63	6 (13%)	51,90,113	1.45	6 (11%)
21	CLA	3	410	3	50,60,73	1.53	7 (14%)	57,97,113	1.54	8 (14%)
21	CLA	7	305	4	53,63,73	1.49	6 (11%)	62,101,113	1.46	7 (11%)
21	CLA	B	813	8	63,73,73	1.36	7 (11%)	74,113,113	1.33	7 (9%)
23	LUT	7	317	-	42,43,43	0.32	0	51,60,60	0.55	1 (1%)
26	LMG	3	421	-	40,40,55	0.19	0	48,48,63	0.17	0
21	CLA	A	806	7	58,68,73	1.39	5 (8%)	68,107,113	1.24	8 (11%)
21	CLA	9	609	28	44,54,73	1.57	4 (9%)	51,90,113	1.43	6 (11%)
29	PTY	c	619	-	30,30,49	0.58	0	33,35,54	0.46	0
21	CLA	B	826	8	53,63,73	1.44	6 (11%)	62,101,113	1.24	6 (9%)
23	LUT	c	615	-	42,43,43	0.35	0	51,60,60	0.58	1 (1%)
28	LHG	a	318	21	22,22,48	0.40	0	25,28,54	0.37	0
21	CLA	a	313	1	44,54,73	1.57	5 (11%)	51,90,113	1.43	6 (11%)
21	CLA	B	844	-	63,73,73	1.37	6 (9%)	74,113,113	1.37	6 (8%)
25	BCR	J	5003	-	41,41,41	0.17	0	56,56,56	0.26	0
21	CLA	A	818	-	53,63,73	1.50	6 (11%)	62,101,113	1.46	8 (12%)
21	CLA	1	313	1	43,53,73	1.65	6 (13%)	50,89,113	1.50	6 (12%)
23	LUT	3	415	-	42,43,43	0.29	0	51,60,60	0.54	0
21	CLA	A	815	7	63,73,73	1.32	5 (7%)	74,113,113	1.45	8 (10%)
21	CLA	c	609	4	44,54,73	1.56	5 (11%)	51,90,113	1.34	6 (11%)
25	BCR	A	851	-	41,41,41	0.17	0	56,56,56	0.35	0
21	CLA	1	306	-	48,58,73	1.55	5 (10%)	56,95,113	1.48	8 (14%)
32	DGD	7	301	-	40,40,67	0.25	0	54,54,81	0.37	0
21	CLA	A	823	-	63,73,73	1.34	5 (7%)	74,113,113	1.20	7 (9%)
21	CLA	B	819	-	63,73,73	1.32	6 (9%)	74,113,113	1.22	7 (9%)
21	CLA	A	834	7	63,73,73	1.35	5 (7%)	74,113,113	1.40	8 (10%)
21	CLA	1	308	1	58,68,73	1.37	6 (10%)	68,107,113	1.33	6 (8%)
21	CLA	8	613	5	50,60,73	1.55	6 (12%)	57,97,113	1.44	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	DGD	8	602	-	48,48,67	0.20	0	62,62,81	0.29	0
21	CLA	T	605	-	44,54,73	1.58	6 (13%)	51,90,113	1.44	6 (11%)
26	LMG	G	207	-	43,43,55	0.19	0	51,51,63	0.13	0
21	CLA	1	303	-	48,58,73	1.47	5 (10%)	56,95,113	1.37	8 (14%)
28	LHG	2	617	21	21,21,48	0.59	0	24,26,54	0.89	2 (8%)
21	CLA	A	843	-	63,73,73	1.30	5 (7%)	74,113,113	1.34	8 (10%)
23	LUT	B	801	-	42,43,43	0.39	1 (2%)	51,60,60	0.80	2 (3%)
25	BCR	B	805	-	41,41,41	0.28	0	56,56,56	1.10	7 (12%)
21	CLA	a	314	1	48,58,73	1.51	5 (10%)	56,95,113	1.51	8 (14%)
25	BCR	B	849	-	41,41,41	0.12	0	56,56,56	0.35	0
21	CLA	A	810	7	63,73,73	1.34	5 (7%)	74,113,113	1.25	8 (10%)
21	CLA	2	603	2	58,68,73	1.47	7 (12%)	68,107,113	1.43	7 (10%)
21	CLA	A	811	7	63,73,73	1.38	7 (11%)	74,113,113	1.43	8 (10%)
21	CLA	1	302	1	58,68,73	1.40	6 (10%)	68,107,113	1.38	7 (10%)
21	CLA	A	832	7	63,73,73	1.36	6 (9%)	74,113,113	1.31	7 (9%)
21	CLA	1	321	28	63,73,73	1.38	6 (9%)	74,113,113	1.50	11 (14%)
21	CLA	A	836	-	58,68,73	1.39	5 (8%)	68,107,113	1.30	7 (10%)
29	PTY	I	201	-	37,37,49	0.63	1 (2%)	40,42,54	0.99	2 (5%)
22	CHL	b	302	-	64,74,74	1.37	4 (6%)	71,114,114	1.71	10 (14%)
21	CLA	A	821	7	63,73,73	1.34	6 (9%)	74,113,113	1.30	9 (12%)
21	CLA	2	610	2	44,54,73	1.61	7 (15%)	51,90,113	1.60	6 (11%)
32	DGD	A	802	-	67,67,67	0.17	0	81,81,81	0.15	0
25	BCR	b	319	-	41,41,41	0.16	0	56,56,56	0.32	0
23	LUT	2	616	-	42,43,43	0.25	0	51,60,60	0.37	0
21	CLA	B	812	8	63,73,73	1.33	6 (9%)	74,113,113	1.21	8 (10%)
25	BCR	A	847	-	41,41,41	0.32	0	56,56,56	0.88	2 (3%)
23	LUT	8	616	-	42,43,43	0.25	0	51,60,60	0.36	0
22	CHL	3	401	3	64,74,74	1.17	4 (6%)	71,114,114	1.85	7 (9%)
21	CLA	2	613	-	63,73,73	1.34	5 (7%)	74,113,113	1.28	7 (9%)
21	CLA	A	826	7	58,68,73	1.43	6 (10%)	68,107,113	1.30	7 (10%)
21	CLA	A	814	7	60,70,73	1.40	6 (10%)	70,109,113	1.23	8 (11%)
21	CLA	L	305	-	48,58,73	1.56	6 (12%)	56,95,113	1.51	6 (10%)
21	CLA	b	312	-	44,54,73	1.60	5 (11%)	51,90,113	1.45	6 (11%)
21	CLA	3	412	3	53,63,73	1.45	6 (11%)	62,101,113	1.21	6 (9%)
21	CLA	B	806	-	63,73,73	1.37	7 (11%)	74,113,113	1.32	8 (10%)
25	BCR	I	202	-	41,41,41	0.13	0	56,56,56	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	822	8	63,73,73	1.30	5 (7%)	74,113,113	1.26	8 (10%)
21	CLA	2	608	2	43,53,73	1.61	5 (11%)	50,89,113	1.46	6 (12%)
22	CHL	T	601	4	46,56,74	1.64	4 (8%)	49,92,114	2.39	10 (20%)
21	CLA	B	811	8	53,63,73	1.47	6 (11%)	62,101,113	1.36	6 (9%)
22	CHL	c	605	-	44,54,74	1.53	5 (11%)	47,90,114	2.51	8 (17%)
21	CLA	B	832	8	63,73,73	1.39	7 (11%)	74,113,113	1.29	8 (10%)
21	CLA	B	842	-	63,73,73	1.40	7 (11%)	74,113,113	1.33	7 (9%)
21	CLA	K	202	-	53,63,73	1.46	5 (9%)	62,101,113	1.28	8 (12%)
28	LHG	B	802	-	31,31,48	0.35	0	34,37,54	0.34	0
29	PTY	H	201	-	41,41,49	0.50	0	44,46,54	0.48	0
29	PTY	8	619	-	20,20,49	0.65	0	21,24,54	0.55	0
25	BCR	T	617	-	41,41,41	0.13	0	56,56,56	0.28	0
26	LMG	F	5009	-	39,39,55	0.18	0	47,47,63	0.15	0
21	CLA	B	825	8	58,68,73	1.40	5 (8%)	68,107,113	1.35	7 (10%)
21	CLA	B	817	8	63,73,73	1.37	6 (9%)	74,113,113	1.38	7 (9%)
21	CLA	b	305	5	61,71,73	1.40	6 (9%)	71,110,113	1.42	9 (12%)
28	LHG	1	319	21	24,24,48	0.40	0	27,30,54	0.37	0
21	CLA	3	407	3	63,73,73	1.37	6 (9%)	74,113,113	1.26	7 (9%)
21	CLA	B	808	8	46,56,73	1.56	5 (10%)	53,92,113	1.39	7 (13%)
25	BCR	G	206	-	41,41,41	0.19	0	56,56,56	0.56	0
21	CLA	8	604	5	49,59,73	1.53	6 (12%)	56,96,113	1.50	8 (14%)
29	PTY	B	803	-	26,26,49	0.61	0	29,31,54	0.48	0
22	CHL	a	306	-	45,55,74	1.45	5 (11%)	48,91,114	2.06	10 (20%)
21	CLA	A	856	7	59,69,73	1.40	6 (10%)	69,108,113	1.35	7 (10%)
21	CLA	B	837	-	58,68,73	1.41	5 (8%)	68,107,113	1.37	7 (10%)
25	BCR	B	847	-	41,41,41	0.19	0	56,56,56	0.40	0
21	CLA	c	614	4	43,53,73	1.63	4 (9%)	50,89,113	1.43	6 (12%)
21	CLA	B	843	8	63,73,73	1.37	7 (11%)	74,113,113	1.17	7 (9%)
21	CLA	K	203	19	43,53,73	1.69	8 (18%)	50,89,113	1.65	8 (16%)
21	CLA	A	804	-	63,73,73	1.42	8 (12%)	74,113,113	1.26	6 (8%)
29	PTY	B	851	-	22,25,49	0.46	0	23,28,54	0.27	0
32	DGD	B	850	-	62,62,67	0.18	0	76,76,81	0.22	0
21	CLA	8	609	5	44,54,73	1.63	7 (15%)	51,90,113	1.37	6 (11%)
21	CLA	a	304	-	48,58,73	1.49	5 (10%)	56,95,113	1.41	8 (14%)
21	CLA	8	605	-	44,54,73	1.61	6 (13%)	51,90,113	1.58	6 (11%)
28	LHG	A	852	21	29,29,48	0.35	0	33,35,54	0.47	0
24	XAT	1	315	-	41,47,47	0.16	0	54,74,74	0.98	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	2	607	-	44,54,73	1.62	5 (11%)	51,90,113	1.41	6 (11%)
25	BCR	K	205	-	41,41,41	0.31	0	56,56,56	0.77	2 (3%)
28	LHG	H	202	-	48,48,48	0.29	0	51,54,54	0.29	0
21	CLA	b	316	5	43,53,73	1.65	5 (11%)	50,89,113	1.44	6 (12%)
25	BCR	B	852	-	41,41,41	0.24	0	56,56,56	1.28	6 (10%)
21	CLA	A	831	7	63,73,73	1.36	7 (11%)	74,113,113	1.31	7 (9%)
28	LHG	b	301	-	30,30,48	0.35	0	33,36,54	0.34	0
21	CLA	A	827	-	63,73,73	1.40	6 (9%)	74,113,113	1.44	7 (9%)
21	CLA	7	311	4	63,73,73	1.30	5 (7%)	74,113,113	1.22	8 (10%)
21	CLA	c	613	4	48,58,73	1.55	5 (10%)	56,95,113	1.48	8 (14%)
28	LHG	c	618	21	28,28,48	0.37	0	31,34,54	0.34	0
21	CLA	B	838	-	48,58,73	1.53	5 (10%)	56,95,113	1.49	8 (14%)
22	CHL	2	606	-	45,55,74	1.36	5 (11%)	48,91,114	2.30	8 (16%)
23	LUT	2	615	-	42,43,43	0.25	0	51,60,60	0.43	0
21	CLA	A	813	7	63,73,73	1.34	6 (9%)	74,113,113	1.20	7 (9%)
21	CLA	F	5007	-	47,57,73	1.55	5 (10%)	53,93,113	1.50	7 (13%)
24	XAT	a	316	-	41,47,47	0.20	0	54,74,74	1.09	6 (11%)
21	CLA	9	610	6	43,53,73	1.71	7 (16%)	50,89,113	1.59	8 (16%)
24	XAT	8	617	-	41,47,47	0.17	0	54,74,74	0.65	1 (1%)
21	CLA	2	611	-	58,68,73	1.40	6 (10%)	68,107,113	1.39	6 (8%)
27	LMU	A	854	-	36,36,36	0.18	0	47,47,47	0.35	0
21	CLA	K	201	-	43,53,73	1.66	6 (13%)	50,89,113	1.60	6 (12%)
21	CLA	8	615	5	43,53,73	1.63	5 (11%)	50,89,113	1.35	6 (12%)
34	CL0	A	803	7	63,73,73	1.09	4 (6%)	74,113,113	1.83	10 (13%)
36	SF4	A	845	8,7	0,12,12	-	-	-	-	-
25	BCR	O	2004	-	41,41,41	0.20	0	56,56,56	0.73	2 (3%)
21	CLA	B	827	-	63,73,73	1.31	6 (9%)	74,113,113	1.45	10 (13%)
21	CLA	B	829	8	63,73,73	1.41	6 (9%)	74,113,113	1.34	7 (9%)
21	CLA	9	608	6	58,68,73	1.38	5 (8%)	68,107,113	1.26	7 (10%)
21	CLA	A	820	7	59,69,73	1.42	6 (10%)	69,108,113	1.40	7 (10%)
21	CLA	T	608	20	43,53,73	1.67	6 (13%)	50,89,113	1.62	6 (12%)
21	CLA	9	612	6	44,54,73	1.61	6 (13%)	51,90,113	1.44	6 (11%)
22	CHL	8	608	-	49,59,74	1.35	5 (10%)	53,96,114	2.39	7 (13%)

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
21	CLA	B	807	-	1/1/15/20	15/37/115/115	-
21	CLA	G	201	8	1/1/15/20	14/37/115/115	-
21	CLA	3	406	-	1/1/13/20	6/25/103/115	-
21	CLA	2	602	2	1/1/15/20	13/37/115/115	-
23	LUT	9	613	-	3/3/12/27	1/29/67/67	0/2/2/2
21	CLA	A	842	28	1/1/12/20	7/24/102/115	-
29	PTY	1	320	-	-	9/23/23/53	-
21	CLA	3	403	-	1/1/12/20	5/19/97/115	-
21	CLA	A	812	7	1/1/13/20	7/25/103/115	-
21	CLA	3	408	3	1/1/14/20	11/31/109/115	-
21	CLA	a	308	1	1/1/12/20	11/19/97/115	-
23	LUT	O	2005	-	3/3/12/27	4/29/67/67	0/2/2/2
21	CLA	c	611	-	1/1/11/20	4/15/93/115	-
21	CLA	B	831	8	1/1/15/20	23/37/115/115	-
21	CLA	3	405	3	1/1/12/20	5/19/97/115	-
24	XAT	9	615	-	-	4/31/93/93	0/4/4/4
21	CLA	A	839	7	1/1/15/20	9/37/115/115	-
21	CLA	3	404	-	1/1/11/20	5/15/93/115	-
21	CLA	7	306	-	1/1/12/20	4/19/97/115	-
21	CLA	c	604	-	1/1/12/20	4/19/97/115	-
21	CLA	c	603	4	1/1/12/20	5/21/99/115	-
22	CHL	c	607	-	2/2/16/26	4/18/116/137	-
21	CLA	T	607	-	1/1/12/20	7/19/97/115	-
21	CLA	A	824	7	1/1/14/20	10/31/109/115	-
28	LHG	9	617	21	-	10/32/32/53	-
22	CHL	7	303	-	3/3/20/26	11/39/137/137	-
21	CLA	b	306	-	1/1/12/20	7/19/97/115	-
27	LMU	9	616	-	-	6/21/61/61	0/2/2/2
25	BCR	B	848	-	-	2/29/63/63	0/2/2/2
21	CLA	A	838	7	1/1/12/20	7/21/99/115	-
30	SQD	3	422	-	-	11/30/50/69	0/1/1/1
21	CLA	8	610	5	1/1/14/20	12/31/109/115	-
21	CLA	A	837	7	1/1/11/20	5/16/94/115	-
28	LHG	3	424	-	-	9/30/30/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	303	1	1/1/13/20	10/25/103/115	-
22	CHL	8	606	-	1/1/16/26	6/15/113/137	-
21	CLA	A	809	-	1/1/14/20	7/31/109/115	-
29	PTY	c	620	-	-	7/29/29/53	-
25	BCR	B	846	-	-	2/29/63/63	0/2/2/2
21	CLA	7	323	5	1/1/11/20	6/15/93/115	-
22	CHL	7	308	-	1/1/16/26	4/15/113/137	-
21	CLA	3	413	-	1/1/10/20	4/10/88/115	-
21	CLA	A	828	-	1/1/13/20	10/28/106/115	-
21	CLA	B	818	-	1/1/15/20	14/37/115/115	-
22	CHL	9	606	-	1/1/16/26	6/17/115/137	-
21	CLA	3	411	3	1/1/14/20	8/31/109/115	-
21	CLA	B	815	-	1/1/13/20	6/25/103/115	-
25	BCR	7	319	-	-	4/29/63/63	0/2/2/2
36	SF4	C	101	9	-	-	0/6/5/5
21	CLA	G	205	-	1/1/11/20	4/13/91/115	-
21	CLA	A	830	7	1/1/15/20	17/37/115/115	-
21	CLA	a	311	1	1/1/11/20	6/15/93/115	-
21	CLA	b	314	5	1/1/12/20	5/19/97/115	-
21	CLA	9	611	-	1/1/11/20	3/15/93/115	-
21	CLA	B	834	8	1/1/14/20	7/31/109/115	-
21	CLA	L	301	7	1/1/12/20	2/19/97/115	-
26	LMG	7	320	-	-	3/42/62/70	0/1/1/1
21	CLA	7	312	28	1/1/11/20	4/13/91/115	-
21	CLA	B	810	8	1/1/15/20	12/37/115/115	-
21	CLA	c	601	5	1/1/11/20	6/15/93/115	-
21	CLA	b	313	5	1/1/12/20	8/19/97/115	-
21	CLA	9	607	6	1/1/15/20	16/37/115/115	-
21	CLA	2	612	2	1/1/11/20	3/13/91/115	-
21	CLA	1	301	1	1/1/14/20	10/33/111/115	-
21	CLA	1	304	-	1/1/11/20	4/13/91/115	-
29	PTY	3	423	-	-	1/16/18/53	-
21	CLA	B	835	8	1/1/15/20	11/37/115/115	-
21	CLA	B	836	8	1/1/13/20	12/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	816	-	1/1/15/20	14/37/115/115	-
28	LHG	8	620	21	-	11/44/44/53	-
21	CLA	T	613	-	1/1/11/20	8/15/93/115	-
21	CLA	A	840	7	1/1/14/20	5/31/109/115	-
21	CLA	O	2003	-	1/1/11/20	9/13/91/115	-
25	BCR	L	307	-	-	0/29/63/63	0/2/2/2
25	BCR	L	309	-	-	4/29/63/63	0/2/2/2
21	CLA	1	307	1	1/1/12/20	6/19/97/115	-
21	CLA	7	316	4	1/1/15/20	8/37/115/115	-
21	CLA	H	203	14	1/1/14/20	10/31/109/115	-
21	CLA	3	414	3	1/1/11/20	3/15/93/115	-
21	CLA	B	814	8	1/1/14/20	9/31/109/115	-
28	LHG	A	853	-	-	10/49/49/53	-
29	PTY	7	302	-	-	10/29/29/53	-
22	CHL	b	307	-	1/1/16/26	7/17/115/137	-
22	CHL	b	309	-	2/2/17/26	5/21/119/137	-
25	BCR	A	849	-	-	6/29/63/63	0/2/2/2
25	BCR	J	5004	-	-	2/29/63/63	0/2/2/2
28	LHG	7	321	21	-	11/47/47/53	-
21	CLA	T	610	-	1/1/11/20	3/15/93/115	-
21	CLA	K	204	-	1/1/11/20	8/17/95/115	-
21	CLA	L	306	-	1/1/12/20	9/19/97/115	-
21	CLA	a	310	28	1/1/11/20	6/15/93/115	-
22	CHL	b	308	-	1/1/16/26	2/17/115/137	-
23	LUT	a	315	-	3/3/12/27	8/29/67/67	0/2/2/2
26	LMG	1	317	-	-	5/23/40/70	1/1/1/1
25	BCR	A	848	-	-	3/29/63/63	0/2/2/2
21	CLA	c	608	-	1/1/11/20	4/13/91/115	-
21	CLA	B	840	8	1/1/14/20	7/31/109/115	-
21	CLA	A	819	7	1/1/14/20	14/31/109/115	-
21	CLA	a	312	-	1/1/14/20	9/31/109/115	-
21	CLA	2	605	-	1/1/11/20	6/13/91/115	-
35	PQN	B	845	-	-	9/23/43/43	0/2/2/2
21	CLA	7	315	4	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	8	611	28	1/1/13/20	8/25/103/115	-
21	CLA	2	609	28	1/1/10/20	2/8/86/115	-
21	CLA	T	614	-	1/1/10/20	4/10/88/115	-
29	PTY	J	5001	-	-	6/25/25/53	-
21	CLA	c	602	4	1/1/12/20	7/22/100/115	-
22	CHL	7	309	-	2/2/16/26	7/18/116/137	-
25	BCR	1	316	-	-	4/29/63/63	0/2/2/2
21	CLA	F	5006	-	1/1/11/20	6/16/94/115	-
21	CLA	7	304	4	1/1/14/20	11/31/109/115	-
25	BCR	3	419	-	-	5/29/63/63	0/2/2/2
21	CLA	2	604	-	1/1/12/20	7/19/97/115	-
22	CHL	c	606	-	1/1/16/26	4/18/116/137	-
21	CLA	G	203	13	1/1/11/20	5/16/94/115	-
27	LMU	A	855	-	-	7/21/61/61	0/2/2/2
28	LHG	7	324	-	-	15/35/35/53	-
28	LHG	3	420	21	-	11/19/19/53	-
22	CHL	7	307	-	1/1/16/26	5/15/113/137	-
21	CLA	B	804	-	1/1/15/20	13/37/115/115	-
21	CLA	1	309	28	1/1/11/20	7/15/93/115	-
21	CLA	a	307	-	1/1/11/20	4/13/91/115	-
21	CLA	a	309	1	1/1/14/20	14/31/109/115	-
21	CLA	B	824	8	1/1/13/20	9/25/103/115	-
27	LMU	1	318	-	-	9/21/61/61	0/2/2/2
21	CLA	A	817	7	1/1/15/20	18/37/115/115	-
25	BCR	3	417	-	-	4/29/63/63	0/2/2/2
24	XAT	3	416	-	-	2/31/93/93	0/4/4/4
21	CLA	b	304	5	1/1/14/20	12/31/109/115	-
23	LUT	T	615	-	3/3/12/27	1/29/67/67	0/2/2/2
21	CLA	L	303	16	1/1/12/20	6/22/100/115	-
25	BCR	F	5008	-	-	4/29/63/63	0/2/2/2
22	CHL	8	607	-	1/1/16/26	6/17/115/137	-
28	LHG	1	322	21	-	9/31/31/53	-
21	CLA	7	310	4	1/1/11/20	4/13/91/115	-
21	CLA	T	612	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	825	7	1/1/14/20	12/31/109/115	-
21	CLA	9	603	-	1/1/13/20	5/25/103/115	-
21	CLA	A	822	7	1/1/13/20	12/29/107/115	-
21	CLA	A	808	7	1/1/15/20	14/37/115/115	-
22	CHL	1	305	-	2/2/16/26	7/17/115/137	-
25	BCR	L	302	-	-	12/29/63/63	0/2/2/2
37	4RF	A	857	-	-	10/41/41/59	-
30	SQD	2	618	-	-	13/40/60/69	0/1/1/1
21	CLA	c	610	28	1/1/11/20	5/13/91/115	-
29	PTY	L	308	-	-	11/22/22/53	-
21	CLA	B	823	-	1/1/14/20	8/31/109/115	-
36	SF4	C	102	9	-	-	0/6/5/5
26	LMG	A	801	-	-	10/26/46/70	0/1/1/1
25	BCR	I	203	-	-	4/29/63/63	0/2/2/2
21	CLA	9	605	6	1/1/11/20	4/13/91/115	-
21	CLA	T	606	-	-	6/15/93/115	-
21	CLA	1	311	-	1/1/14/20	9/31/109/115	-
21	CLA	T	611	20	1/1/12/20	5/22/100/115	-
23	LUT	2	614	-	3/3/12/27	2/29/67/67	0/2/2/2
29	PTY	a	319	-	-	12/19/19/53	-
21	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
25	BCR	8	618	-	-	4/29/63/63	0/2/2/2
28	LHG	F	5003	-	-	14/47/47/53	-
21	CLA	8	614	5	1/1/11/20	5/15/93/115	-
21	CLA	B	820	8	1/1/14/20	7/31/109/115	-
21	CLA	T	609	20	1/1/13/20	7/25/103/115	-
21	CLA	A	833	7	1/1/13/20	4/25/103/115	-
21	CLA	b	310	5	1/1/11/20	4/15/93/115	-
21	CLA	B	839	-	1/1/13/20	8/25/103/115	-
24	XAT	7	318	-	-	2/31/93/93	0/4/4/4
21	CLA	3	402	3	1/1/15/20	14/37/115/115	-
21	CLA	9	602	6	1/1/11/20	9/16/94/115	-
21	CLA	c	612	4	1/1/11/20	5/16/94/115	-
21	CLA	8	622	-	1/1/11/20	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	9	601	-	1/1/11/20	6/15/93/115	-
21	CLA	A	841	7	1/1/15/20	12/37/115/115	-
29	PTY	7	322	-	-	6/28/28/53	-
25	BCR	G	202	-	-	5/29/63/63	0/2/2/2
21	CLA	A	829	7	1/1/15/20	14/37/115/115	-
21	CLA	B	833	-	1/1/15/20	12/37/115/115	-
28	LHG	a	301	-	-	10/25/25/53	-
35	PQN	A	844	-	-	0/23/43/43	0/2/2/2
24	XAT	9	614	-	-	0/31/93/93	0/4/4/4
22	CHL	8	601	-	1/1/17/26	8/21/119/137	-
25	BCR	a	317	-	-	5/29/63/63	0/2/2/2
28	LHG	F	5001	-	-	12/35/35/53	-
21	CLA	8	603	5	1/1/12/20	7/19/97/115	-
21	CLA	b	315	5	1/1/11/20	5/15/93/115	-
33	LMK	8	621	-	-	6/41/41/60	-
29	PTY	2	620	-	-	8/35/35/53	-
21	CLA	T	604	-	1/1/11/20	9/16/94/115	-
21	CLA	H	204	-	1/1/11/20	3/15/93/115	-
21	CLA	a	305	-	1/1/11/20	3/13/91/115	-
21	CLA	B	828	-	1/1/15/20	8/37/115/115	-
21	CLA	a	302	1	1/1/15/20	12/37/115/115	-
21	CLA	J	5002	15	1/1/11/20	5/13/91/115	-
31	3PH	F	5002	-	-	1/27/27/49	-
21	CLA	F	5005	-	1/1/15/20	15/37/115/115	-
25	BCR	3	418	-	-	4/29/63/63	0/2/2/2
21	CLA	3	409	28	1/1/14/20	11/31/109/115	-
28	LHG	b	303	-	-	8/26/26/53	-
21	CLA	1	310	1	1/1/11/20	6/15/93/115	-
21	CLA	T	603	20	1/1/13/20	10/27/105/115	-
21	CLA	8	612	5	1/1/12/20	7/19/97/115	-
31	3PH	2	619	-	-	13/44/44/49	-
21	CLA	9	604	6	1/1/12/20	5/19/97/115	-
25	BCR	A	846	-	-	6/29/63/63	0/2/2/2
24	XAT	T	616	-	-	3/31/93/93	0/4/4/4
23	LUT	b	317	-	3/3/12/27	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	841	-	1/1/12/20	4/19/97/115	-
22	CHL	2	601	2	2/2/20/26	18/39/137/137	-
21	CLA	7	314	4	1/1/15/20	8/37/115/115	-
21	CLA	b	311	5	1/1/14/20	8/31/109/115	-
21	CLA	B	821	8	1/1/15/20	16/37/115/115	-
21	CLA	A	807	7	1/1/15/20	12/37/115/115	-
21	CLA	7	313	-	1/1/12/20	6/22/100/115	-
23	LUT	1	314	-	3/3/12/27	10/29/67/67	0/2/2/2
24	XAT	b	318	-	-	1/31/93/93	0/4/4/4
24	XAT	c	616	-	-	3/31/93/93	0/4/4/4
21	CLA	L	304	16	1/1/15/20	8/37/115/115	-
21	CLA	O	2001	17	1/1/9/20	1/4/78/115	-
21	CLA	B	816	8	1/1/15/20	11/37/115/115	-
21	CLA	B	809	8	1/1/15/20	17/37/115/115	-
25	BCR	c	617	-	-	4/29/63/63	0/2/2/2
21	CLA	1	312	1	1/1/11/20	5/13/91/115	-
25	BCR	F	5004	-	-	0/29/63/63	0/2/2/2
22	CHL	T	602	20	2/2/18/26	16/27/125/137	-
25	BCR	A	850	-	-	2/29/63/63	0/2/2/2
21	CLA	A	805	7	1/1/15/20	11/37/115/115	-
28	LHG	1	323	-	-	12/50/50/53	-
21	CLA	A	835	-	1/1/15/20	17/37/115/115	-
21	CLA	B	830	-	1/1/14/20	13/31/109/115	-
21	CLA	G	204	13	1/1/11/20	7/15/93/115	-
21	CLA	3	410	3	1/1/12/20	6/22/100/115	-
21	CLA	7	305	4	1/1/13/20	11/25/103/115	-
21	CLA	B	813	8	1/1/15/20	6/37/115/115	-
23	LUT	7	317	-	3/3/12/27	2/29/67/67	0/2/2/2
26	LMG	3	421	-	-	11/35/55/70	0/1/1/1
21	CLA	A	806	7	1/1/14/20	9/31/109/115	-
21	CLA	9	609	28	1/1/11/20	7/15/93/115	-
29	PTY	c	619	-	-	10/34/34/53	-
21	CLA	B	826	8	1/1/13/20	10/25/103/115	-
23	LUT	c	615	-	3/3/12/27	2/29/67/67	0/2/2/2
28	LHG	a	318	21	-	3/26/26/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	313	1	1/1/11/20	6/15/93/115	-
21	CLA	B	844	-	1/1/15/20	13/37/115/115	-
25	BCR	J	5003	-	-	4/29/63/63	0/2/2/2
21	CLA	A	818	-	1/1/13/20	11/25/103/115	-
21	CLA	1	313	1	1/1/11/20	7/13/91/115	-
23	LUT	3	415	-	3/3/12/27	5/29/67/67	0/2/2/2
21	CLA	A	815	7	-	16/37/115/115	-
21	CLA	c	609	4	1/1/11/20	5/15/93/115	-
25	BCR	A	851	-	-	4/29/63/63	0/2/2/2
21	CLA	1	306	-	1/1/12/20	8/19/97/115	-
32	DGD	7	301	-	-	10/28/68/95	0/2/2/2
21	CLA	A	823	-	1/1/15/20	11/37/115/115	-
21	CLA	B	819	-	1/1/15/20	12/37/115/115	-
21	CLA	A	834	7	1/1/15/20	4/37/115/115	-
21	CLA	1	308	1	1/1/14/20	10/31/109/115	-
21	CLA	8	613	5	1/1/12/20	7/22/100/115	-
32	DGD	8	602	-	-	10/36/76/95	0/2/2/2
21	CLA	T	605	-	1/1/11/20	6/15/93/115	-
26	LMG	G	207	-	-	5/37/57/70	0/1/1/1
21	CLA	1	303	-	1/1/12/20	7/19/97/115	-
28	LHG	2	617	21	-	3/23/23/53	-
21	CLA	A	843	-	1/1/15/20	12/37/115/115	-
23	LUT	B	801	-	3/3/12/27	5/29/67/67	0/2/2/2
25	BCR	B	805	-	-	5/29/63/63	0/2/2/2
21	CLA	a	314	1	1/1/12/20	5/19/97/115	-
25	BCR	B	849	-	-	1/29/63/63	0/2/2/2
21	CLA	A	810	7	1/1/15/20	13/37/115/115	-
21	CLA	2	603	2	1/1/14/20	10/31/109/115	-
21	CLA	A	811	7	1/1/15/20	12/37/115/115	-
21	CLA	1	302	1	1/1/14/20	14/31/109/115	-
21	CLA	A	832	7	1/1/15/20	9/37/115/115	-
21	CLA	1	321	28	1/1/15/20	9/37/115/115	-
21	CLA	A	836	-	1/1/14/20	9/31/109/115	-
29	PTY	I	201	-	-	11/39/39/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHL	b	302	-	2/2/20/26	13/39/137/137	-
21	CLA	A	821	7	1/1/15/20	11/37/115/115	-
21	CLA	2	610	2	1/1/11/20	5/15/93/115	-
32	DGD	A	802	-	-	12/55/95/95	0/2/2/2
25	BCR	b	319	-	-	2/29/63/63	0/2/2/2
23	LUT	2	616	-	3/3/12/27	4/29/67/67	0/2/2/2
21	CLA	B	812	8	1/1/15/20	8/37/115/115	-
25	BCR	A	847	-	-	7/29/63/63	0/2/2/2
23	LUT	8	616	-	3/3/12/27	1/29/67/67	0/2/2/2
22	CHL	3	401	3	2/2/20/26	17/39/137/137	-
21	CLA	2	613	-	1/1/15/20	14/37/115/115	-
21	CLA	A	826	7	1/1/14/20	8/31/109/115	-
21	CLA	A	814	7	1/1/14/20	12/34/112/115	-
21	CLA	L	305	-	1/1/12/20	0/19/97/115	-
21	CLA	b	312	-	1/1/11/20	5/15/93/115	-
21	CLA	3	412	3	1/1/13/20	8/25/103/115	-
21	CLA	B	806	-	1/1/15/20	18/37/115/115	-
25	BCR	I	202	-	-	4/29/63/63	0/2/2/2
21	CLA	B	822	8	1/1/15/20	15/37/115/115	-
21	CLA	2	608	2	1/1/11/20	3/13/91/115	-
22	CHL	T	601	4	2/2/16/26	5/18/116/137	-
21	CLA	B	811	8	1/1/13/20	7/25/103/115	-
22	CHL	c	605	-	1/1/16/26	7/15/113/137	-
21	CLA	B	832	8	1/1/15/20	16/37/115/115	-
21	CLA	B	842	-	1/1/15/20	9/37/115/115	-
21	CLA	K	202	-	1/1/13/20	7/25/103/115	-
28	LHG	B	802	-	-	7/36/36/53	-
29	PTY	H	201	-	-	16/45/45/53	-
29	PTY	8	619	-	-	4/23/23/53	-
25	BCR	T	617	-	-	4/29/63/63	0/2/2/2
26	LMG	F	5009	-	-	6/34/54/70	0/1/1/1
21	CLA	B	825	8	1/1/14/20	11/31/109/115	-
21	CLA	B	817	8	1/1/15/20	19/37/115/115	-
21	CLA	b	305	5	1/1/15/20	15/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	1	319	21	-	2/29/29/53	-
21	CLA	3	407	3	1/1/15/20	12/37/115/115	-
21	CLA	B	808	8	1/1/11/20	6/17/95/115	-
25	BCR	G	206	-	-	6/29/63/63	0/2/2/2
21	CLA	8	604	5	1/1/12/20	9/21/99/115	-
29	PTY	B	803	-	-	9/30/30/53	-
22	CHL	a	306	-	2/2/16/26	4/17/115/137	-
21	CLA	A	856	7	1/1/14/20	9/33/111/115	-
21	CLA	B	837	-	1/1/14/20	11/31/109/115	-
25	BCR	B	847	-	-	4/29/63/63	0/2/2/2
21	CLA	c	614	4	1/1/11/20	4/13/91/115	-
21	CLA	B	843	8	1/1/15/20	12/37/115/115	-
21	CLA	K	203	19	1/1/11/20	6/13/91/115	-
21	CLA	A	804	-	1/1/15/20	10/37/115/115	-
29	PTY	B	851	-	-	7/25/27/53	-
32	DGD	B	850	-	-	8/50/90/95	0/2/2/2
21	CLA	8	609	5	1/1/11/20	5/15/93/115	-
21	CLA	a	304	-	1/1/12/20	7/19/97/115	-
21	CLA	8	605	-	1/1/11/20	6/15/93/115	-
28	LHG	A	852	21	-	8/33/33/53	-
24	XAT	1	315	-	-	2/31/93/93	0/4/4/4
21	CLA	2	607	-	1/1/11/20	9/15/93/115	-
25	BCR	K	205	-	-	11/29/63/63	0/2/2/2
28	LHG	H	202	-	-	6/53/53/53	-
21	CLA	b	316	5	1/1/11/20	6/13/91/115	-
25	BCR	B	852	-	-	8/29/63/63	0/2/2/2
21	CLA	A	831	7	1/1/15/20	10/37/115/115	-
28	LHG	b	301	-	-	7/35/35/53	-
21	CLA	A	827	-	1/1/15/20	9/37/115/115	-
21	CLA	7	311	4	1/1/15/20	12/37/115/115	-
21	CLA	c	613	4	1/1/12/20	7/19/97/115	-
28	LHG	c	618	21	-	9/33/33/53	-
21	CLA	B	838	-	1/1/12/20	8/19/97/115	-
22	CHL	2	606	-	2/2/16/26	5/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LUT	2	615	-	3/3/12/27	3/29/67/67	0/2/2/2
21	CLA	A	813	7	1/1/15/20	10/37/115/115	-
21	CLA	F	5007	-	1/1/11/20	6/18/96/115	-
24	XAT	a	316	-	-	5/31/93/93	0/4/4/4
21	CLA	9	610	6	1/1/11/20	8/13/91/115	-
24	XAT	8	617	-	-	1/31/93/93	0/4/4/4
21	CLA	2	611	-	1/1/14/20	9/31/109/115	-
27	LMU	A	854	-	-	3/21/61/61	0/2/2/2
21	CLA	K	201	-	1/1/11/20	4/13/91/115	-
21	CLA	8	615	5	1/1/11/20	4/13/91/115	-
34	CL0	A	803	7	-	12/37/135/135	-
36	SF4	A	845	8,7	-	-	0/6/5/5
25	BCR	O	2004	-	-	5/29/63/63	0/2/2/2
21	CLA	B	827	-	1/1/15/20	10/37/115/115	-
21	CLA	B	829	8	1/1/15/20	3/37/115/115	-
21	CLA	9	608	6	1/1/14/20	10/31/109/115	-
21	CLA	A	820	7	1/1/14/20	11/33/111/115	-
21	CLA	T	608	20	1/1/11/20	8/13/91/115	-
21	CLA	9	612	6	1/1/11/20	7/15/93/115	-
22	CHL	8	608	-	2/2/17/26	6/21/119/137	-

The worst 5 of 1356 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	601	CLA	MG-NA	12.48	2.35	2.06
22	8	601	CHL	MG-NA	7.94	2.25	2.06
21	9	601	CLA	CHB-C4A	7.85	1.40	1.33
22	b	302	CHL	MG-NA	7.80	2.24	2.06
22	7	303	CHL	MG-NA	7.18	2.23	2.06

The worst 5 of 1864 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	601	CLA	C4A-NA-C1A	-16.26	99.26	106.68
22	7	303	CHL	C4A-NA-C1A	14.84	113.45	106.68
22	8	608	CHL	C4A-NA-C1A	14.79	113.42	106.68
22	c	605	CHL	C4A-NA-C1A	14.79	113.42	106.68
22	b	309	CHL	C4A-NA-C1A	14.73	113.40	106.68

5 of 295 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1	301	CLA	ND
21	1	302	CLA	ND
21	1	303	CLA	ND
21	1	304	CLA	ND
21	1	306	CLA	ND

5 of 2724 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1	303	CLA	CAD-CBD-CGD-O1D
21	1	303	CLA	CAD-CBD-CGD-O2D
21	1	303	CLA	CBD-CGD-O2D-CED
21	1	304	CLA	CBD-CGD-O2D-CED
21	1	306	CLA	C1A-C2A-CAA-CBA

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	1	317	LMG	C1-C2-C3-C4-C5-O6

306 monomers are involved in 846 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	807	CLA	13	0
21	G	201	CLA	5	0
21	3	406	CLA	2	0
21	2	602	CLA	5	0
23	9	613	LUT	3	0
21	3	403	CLA	1	0
21	A	812	CLA	4	0
21	3	408	CLA	2	0
21	a	308	CLA	3	0
23	O	2005	LUT	1	0
21	c	611	CLA	1	0
21	B	831	CLA	6	0
21	3	405	CLA	2	0
24	9	615	XAT	2	0
21	A	839	CLA	2	0
21	3	404	CLA	1	0
21	7	306	CLA	2	0
21	c	604	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	607	CHL	4	0
21	A	824	CLA	7	0
22	7	303	CHL	9	0
21	b	306	CLA	1	0
27	9	616	LMU	4	0
25	B	848	BCR	1	0
21	A	838	CLA	4	0
30	3	422	SQD	4	0
21	a	303	CLA	1	0
22	8	606	CHL	7	0
21	A	809	CLA	4	0
29	c	620	PTY	2	0
25	B	846	BCR	1	0
21	7	323	CLA	3	0
22	7	308	CHL	5	0
21	3	413	CLA	2	0
21	A	828	CLA	4	0
21	B	818	CLA	3	0
22	9	606	CHL	5	0
21	3	411	CLA	4	0
21	B	815	CLA	1	0
25	7	319	BCR	4	0
36	C	101	SF4	1	0
21	G	205	CLA	4	0
21	A	830	CLA	9	0
21	a	311	CLA	1	0
21	b	314	CLA	1	0
21	9	611	CLA	1	0
21	B	834	CLA	3	0
21	L	301	CLA	4	0
26	7	320	LMG	7	0
21	B	810	CLA	5	0
21	c	601	CLA	3	0
21	b	313	CLA	1	0
21	9	607	CLA	1	0
21	1	301	CLA	4	0
21	1	304	CLA	3	0
21	B	835	CLA	3	0
21	B	836	CLA	4	0
21	A	816	CLA	2	0
28	8	620	LHG	3	0
21	A	840	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	L	309	BCR	3	0
21	1	307	CLA	6	0
21	H	203	CLA	1	0
21	3	414	CLA	1	0
21	B	814	CLA	3	0
28	A	853	LHG	3	0
22	b	307	CHL	7	0
22	b	309	CHL	4	0
25	A	849	BCR	4	0
25	J	5004	BCR	4	0
28	7	321	LHG	4	0
21	T	610	CLA	1	0
22	b	308	CHL	3	0
23	a	315	LUT	6	0
26	1	317	LMG	4	0
25	A	848	BCR	8	0
21	c	608	CLA	1	0
21	B	840	CLA	3	0
21	A	819	CLA	5	0
21	a	312	CLA	1	0
35	B	845	PQN	4	0
21	7	315	CLA	2	0
21	8	611	CLA	3	0
29	J	5001	PTY	2	0
21	c	602	CLA	2	0
22	7	309	CHL	10	0
25	1	316	BCR	3	0
21	F	5006	CLA	2	0
21	7	304	CLA	5	0
25	3	419	BCR	2	0
22	c	606	CHL	5	0
27	A	855	LMU	2	0
28	7	324	LHG	1	0
22	7	307	CHL	4	0
21	B	804	CLA	11	0
21	1	309	CLA	2	0
21	a	307	CLA	3	0
21	a	309	CLA	3	0
21	B	824	CLA	2	0
27	1	318	LMU	1	0
21	A	817	CLA	20	0
25	3	417	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	3	416	XAT	6	0
21	b	304	CLA	5	0
23	T	615	LUT	3	0
21	L	303	CLA	3	0
25	F	5008	BCR	4	0
22	8	607	CHL	2	0
28	1	322	LHG	2	0
21	7	310	CLA	3	0
21	T	612	CLA	2	0
21	A	825	CLA	3	0
21	9	603	CLA	1	0
21	A	822	CLA	3	0
21	A	808	CLA	2	0
22	1	305	CHL	3	0
37	A	857	4RF	2	0
30	2	618	SQD	4	0
29	L	308	PTY	1	0
21	B	823	CLA	1	0
26	A	801	LMG	2	0
25	I	203	BCR	4	0
21	9	605	CLA	3	0
21	T	606	CLA	4	0
21	1	311	CLA	4	0
21	T	611	CLA	1	0
23	2	614	LUT	1	0
21	O	2002	CLA	1	0
25	8	618	BCR	6	0
28	F	5003	LHG	3	0
21	B	820	CLA	2	0
21	T	609	CLA	2	0
21	A	833	CLA	5	0
21	b	310	CLA	1	0
21	B	839	CLA	2	0
24	7	318	XAT	3	0
21	3	402	CLA	2	0
21	9	602	CLA	2	0
21	c	612	CLA	1	0
21	8	622	CLA	10	0
21	9	601	CLA	3	0
21	A	841	CLA	5	0
25	G	202	BCR	4	0
21	A	829	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	833	CLA	6	0
28	a	301	LHG	1	0
35	A	844	PQN	1	0
24	9	614	XAT	5	0
22	8	601	CHL	2	0
28	F	5001	LHG	1	0
21	8	603	CLA	2	0
29	2	620	PTY	1	0
21	a	305	CLA	2	0
21	B	828	CLA	3	0
21	a	302	CLA	5	0
21	J	5002	CLA	2	0
31	F	5002	3PH	1	0
21	F	5005	CLA	2	0
25	3	418	BCR	4	0
21	3	409	CLA	2	0
28	b	303	LHG	3	0
21	1	310	CLA	3	0
21	T	603	CLA	2	0
21	8	612	CLA	1	0
31	2	619	3PH	4	0
21	9	604	CLA	2	0
25	A	846	BCR	6	0
24	T	616	XAT	4	0
23	b	317	LUT	2	0
21	B	841	CLA	1	0
22	2	601	CHL	6	0
21	7	314	CLA	4	0
21	b	311	CLA	4	0
21	B	821	CLA	3	0
21	A	807	CLA	6	0
21	7	313	CLA	1	0
23	1	314	LUT	7	0
24	b	318	XAT	3	0
24	c	616	XAT	1	0
21	L	304	CLA	5	0
21	O	2001	CLA	1	0
21	B	816	CLA	6	0
21	B	809	CLA	3	0
25	c	617	BCR	2	0
25	F	5004	BCR	5	0
22	T	602	CHL	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	850	BCR	5	0
21	A	805	CLA	2	0
28	1	323	LHG	5	0
21	A	835	CLA	5	0
21	B	830	CLA	5	0
21	3	410	CLA	3	0
21	B	813	CLA	3	0
23	7	317	LUT	1	0
26	3	421	LMG	2	0
21	A	806	CLA	1	0
29	c	619	PTY	2	0
21	B	826	CLA	7	0
23	c	615	LUT	1	0
28	a	318	LHG	1	0
21	a	313	CLA	3	0
21	B	844	CLA	7	0
25	J	5003	BCR	4	0
21	A	818	CLA	2	0
23	3	415	LUT	1	0
21	A	815	CLA	6	0
21	c	609	CLA	1	0
25	A	851	BCR	3	0
21	1	306	CLA	2	0
32	7	301	DGD	2	0
21	A	823	CLA	6	0
21	B	819	CLA	1	0
21	A	834	CLA	3	0
21	1	308	CLA	3	0
21	8	613	CLA	3	0
32	8	602	DGD	4	0
26	G	207	LMG	5	0
21	1	303	CLA	3	0
21	A	843	CLA	6	0
23	B	801	LUT	4	0
25	B	805	BCR	8	0
25	B	849	BCR	4	0
21	A	810	CLA	7	0
21	2	603	CLA	8	0
21	A	811	CLA	7	0
21	1	302	CLA	3	0
21	A	832	CLA	5	0
21	1	321	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	836	CLA	4	0
29	I	201	PTY	7	0
22	b	302	CHL	10	0
21	A	821	CLA	6	0
21	2	610	CLA	2	0
32	A	802	DGD	4	0
25	b	319	BCR	6	0
23	2	616	LUT	1	0
21	B	812	CLA	5	0
25	A	847	BCR	5	0
22	3	401	CHL	8	0
21	2	613	CLA	3	0
21	A	826	CLA	7	0
21	A	814	CLA	6	0
21	L	305	CLA	1	0
21	3	412	CLA	5	0
21	B	806	CLA	4	0
25	I	202	BCR	5	0
21	B	822	CLA	5	0
21	2	608	CLA	4	0
22	T	601	CHL	5	0
21	B	811	CLA	3	0
22	c	605	CHL	5	0
21	B	832	CLA	5	0
21	B	842	CLA	5	0
21	K	202	CLA	2	0
29	H	201	PTY	1	0
25	T	617	BCR	1	0
26	F	5009	LMG	3	0
21	B	825	CLA	4	0
21	B	817	CLA	6	0
21	b	305	CLA	2	0
28	1	319	LHG	2	0
21	3	407	CLA	8	0
21	B	808	CLA	2	0
21	8	604	CLA	9	0
22	a	306	CHL	2	0
21	A	856	CLA	2	0
21	B	837	CLA	7	0
25	B	847	BCR	8	0
21	c	614	CLA	1	0
21	B	843	CLA	3	0

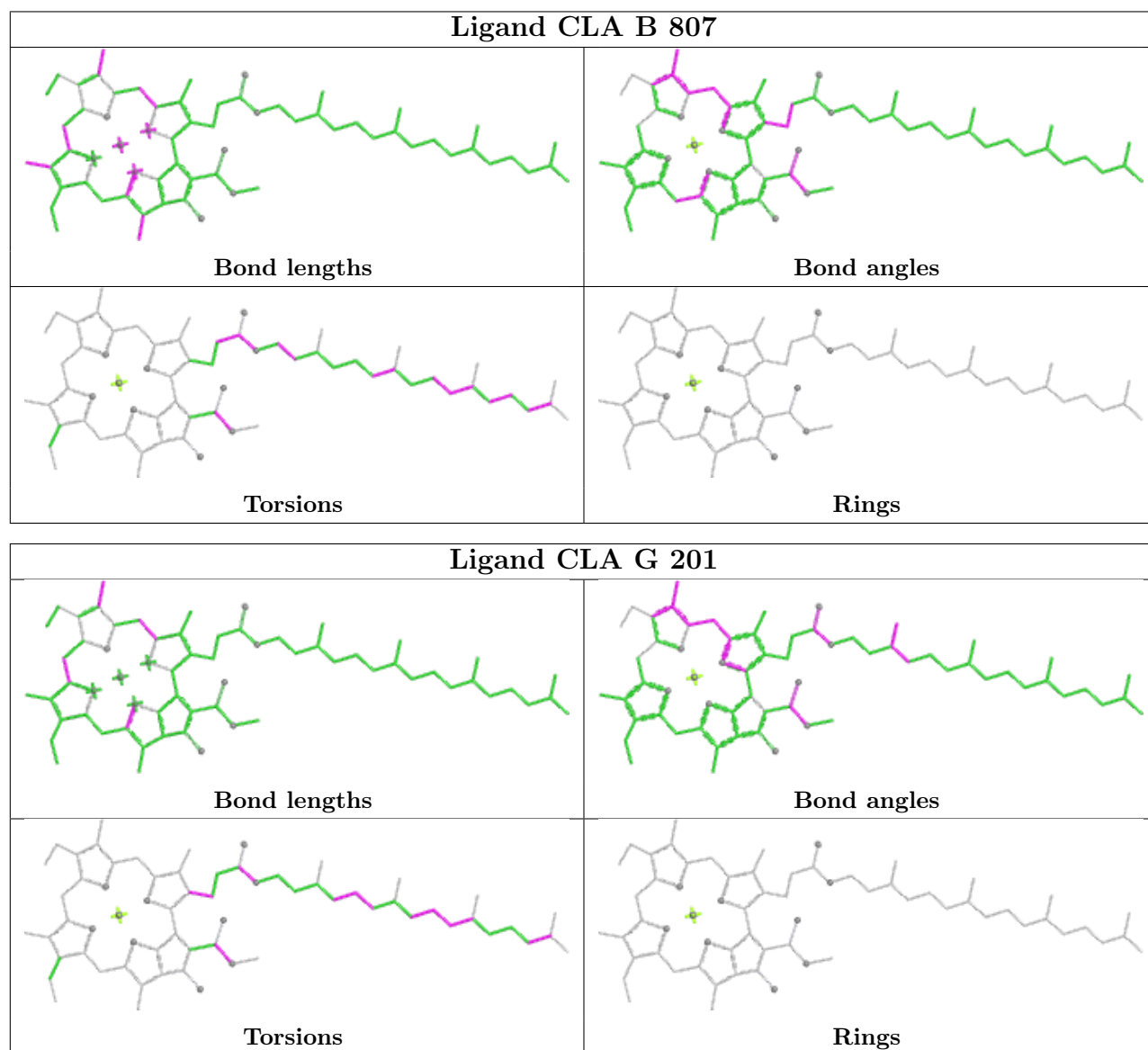
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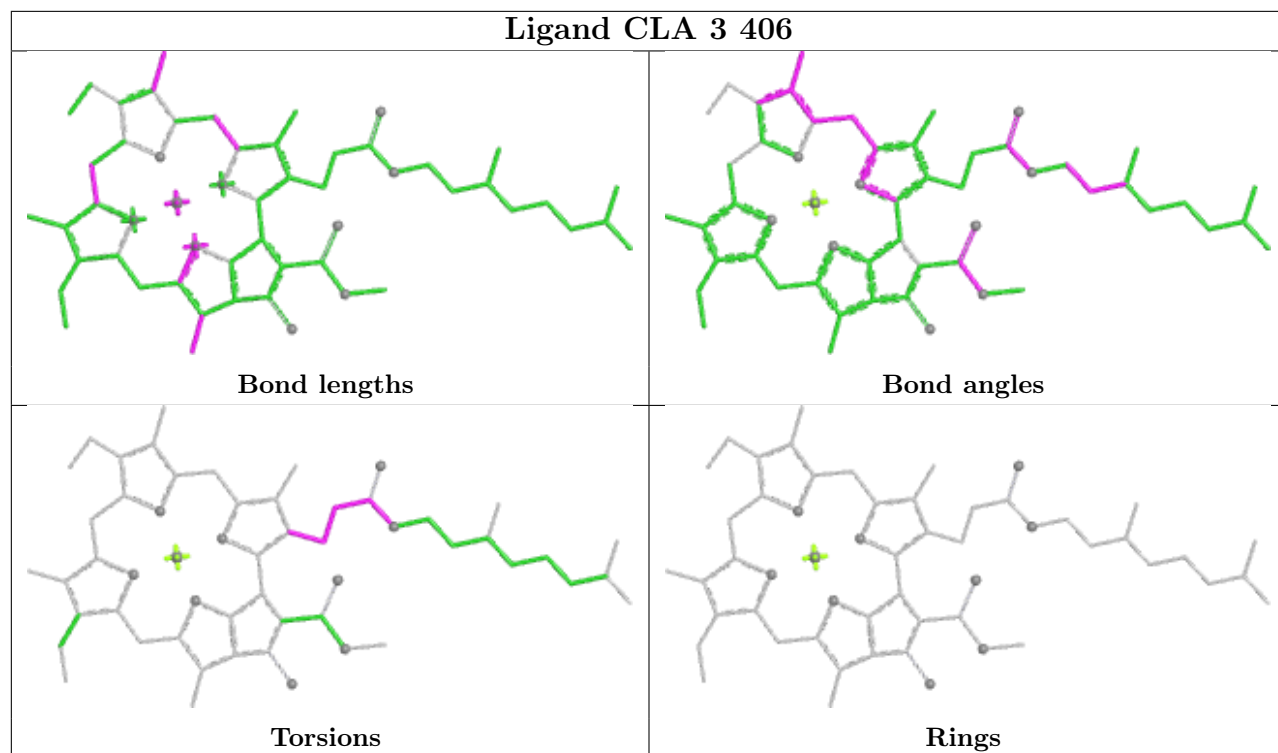
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	203	CLA	3	0
21	A	804	CLA	8	0
32	B	850	DGD	3	0
21	a	304	CLA	2	0
21	8	605	CLA	2	0
28	A	852	LHG	2	0
24	1	315	XAT	12	0
21	2	607	CLA	1	0
25	K	205	BCR	6	0
28	H	202	LHG	3	0
21	b	316	CLA	2	0
25	B	852	BCR	4	0
21	A	831	CLA	8	0
21	A	827	CLA	6	0
21	7	311	CLA	2	0
21	B	838	CLA	3	0
22	2	606	CHL	2	0
23	2	615	LUT	4	0
21	A	813	CLA	3	0
21	F	5007	CLA	1	0
24	a	316	XAT	5	0
21	9	610	CLA	1	0
24	8	617	XAT	3	0
21	2	611	CLA	3	0
27	A	854	LMU	2	0
21	K	201	CLA	1	0
21	8	615	CLA	1	0
34	A	803	CL0	8	0
36	A	845	SF4	4	0
25	O	2004	BCR	1	0
21	B	827	CLA	4	0
21	B	829	CLA	5	0
21	9	608	CLA	2	0
21	A	820	CLA	4	0
21	T	608	CLA	2	0
22	8	608	CHL	5	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

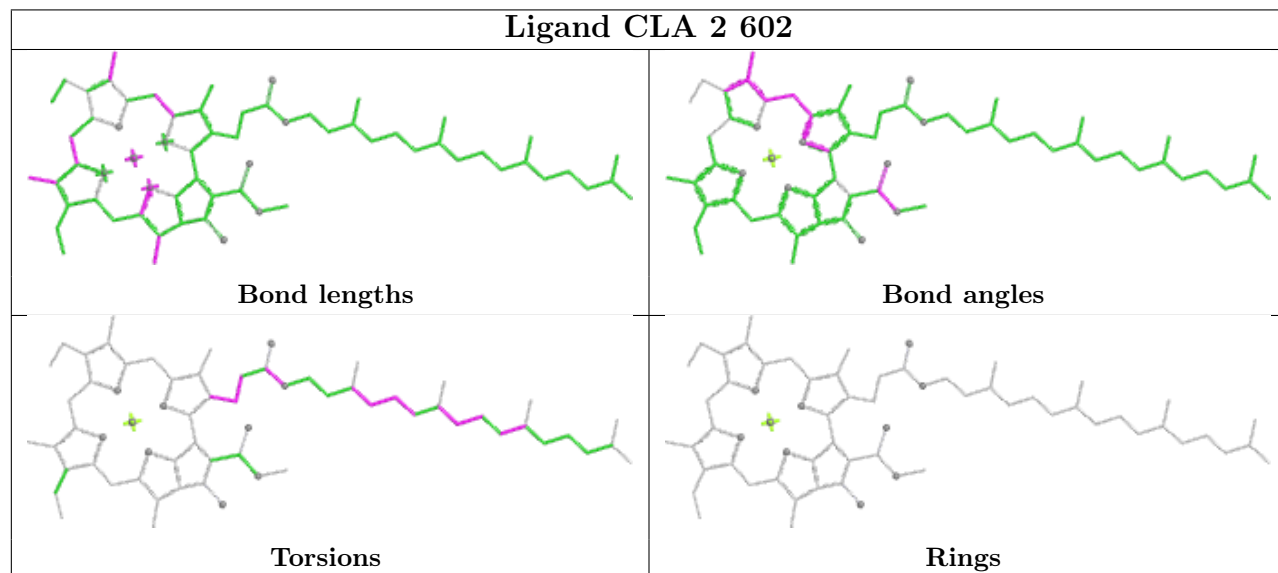
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



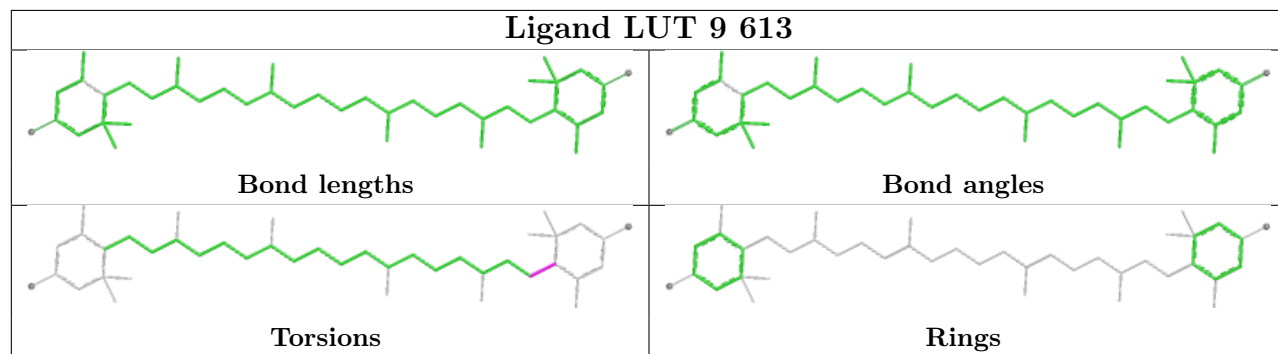
Ligand CLA 3 406



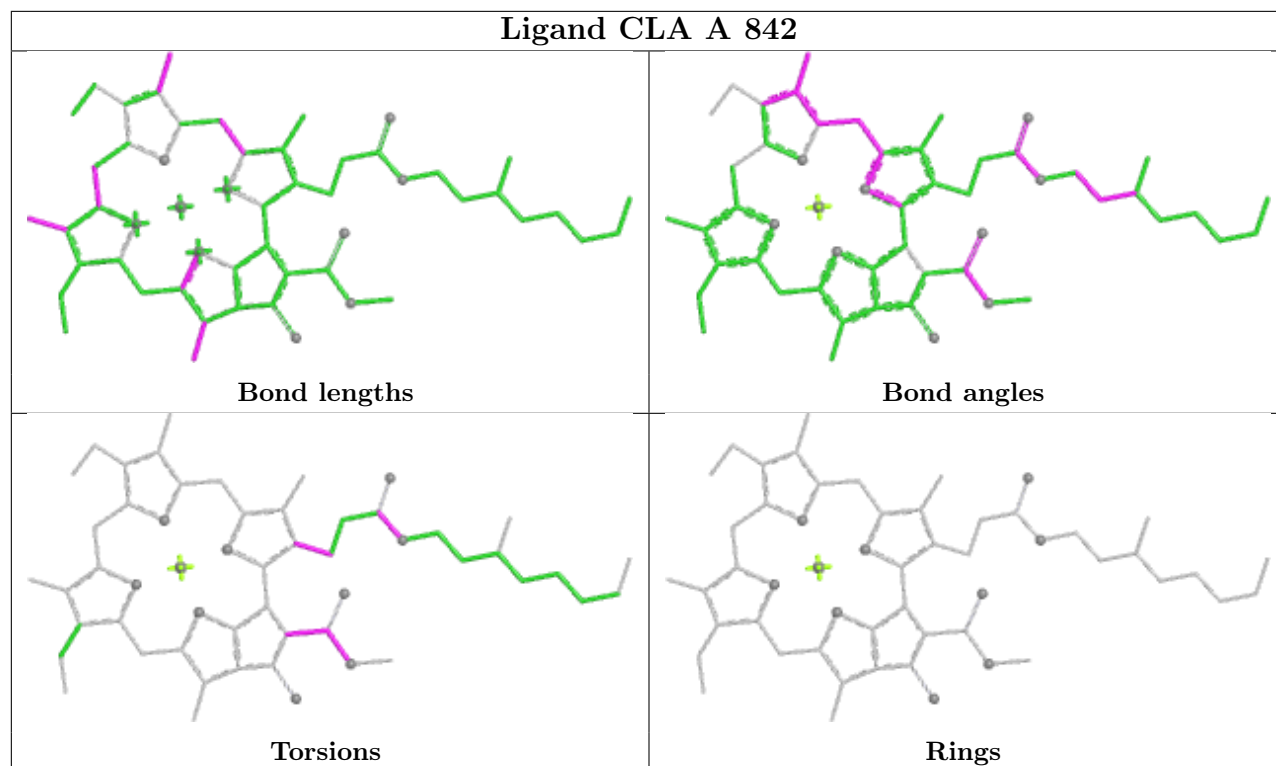
Ligand CLA 2 602



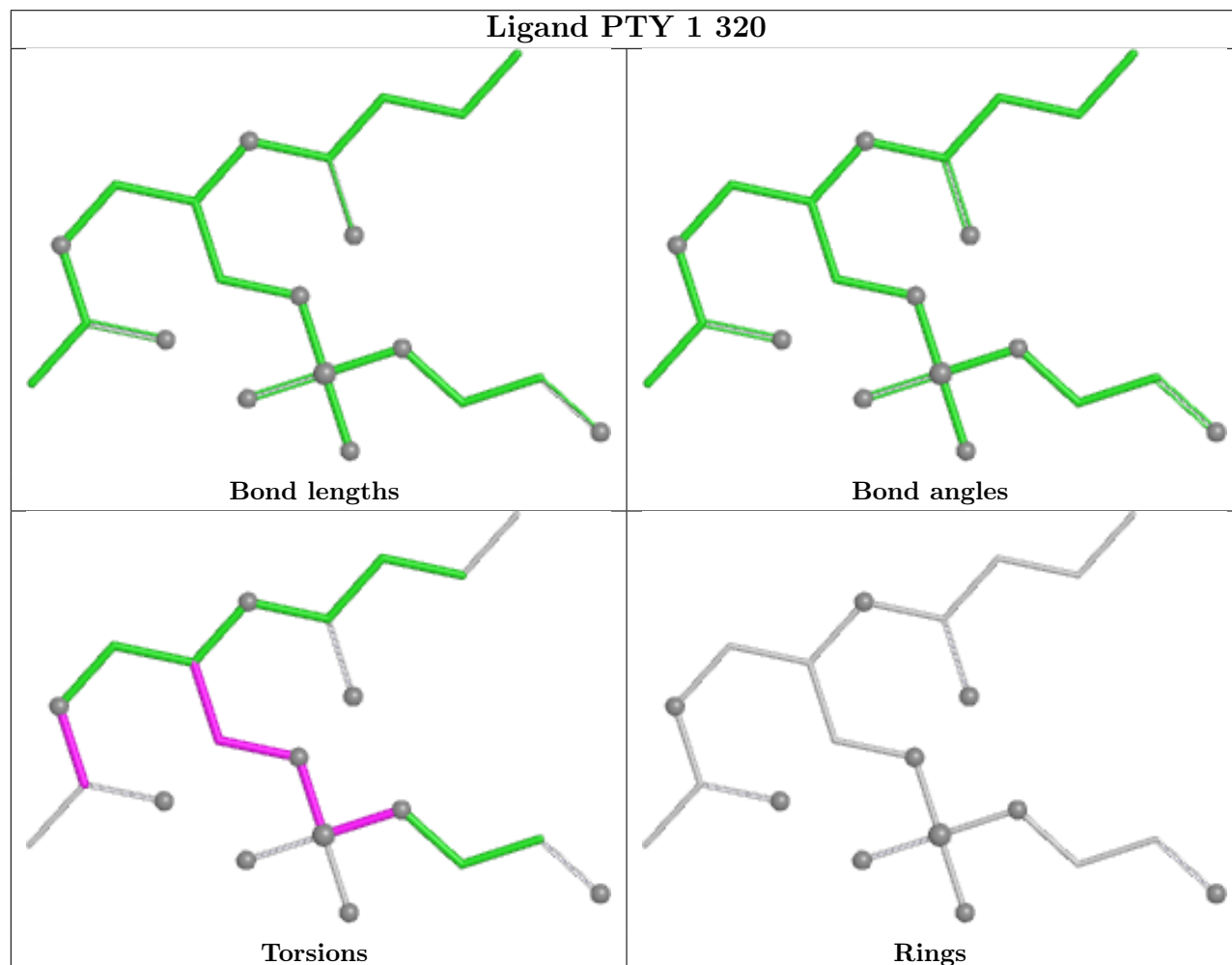
Ligand LUT 9 613



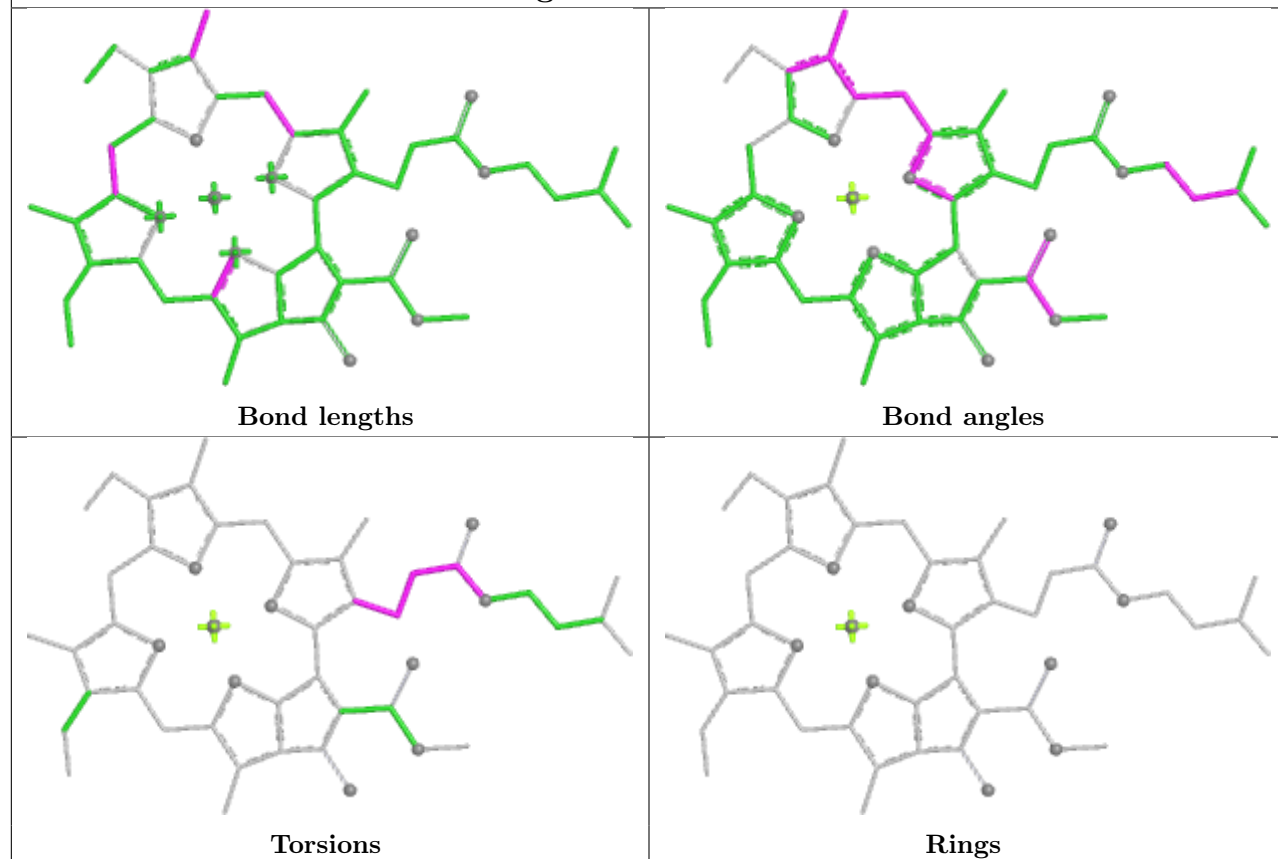
Ligand CLA A 842



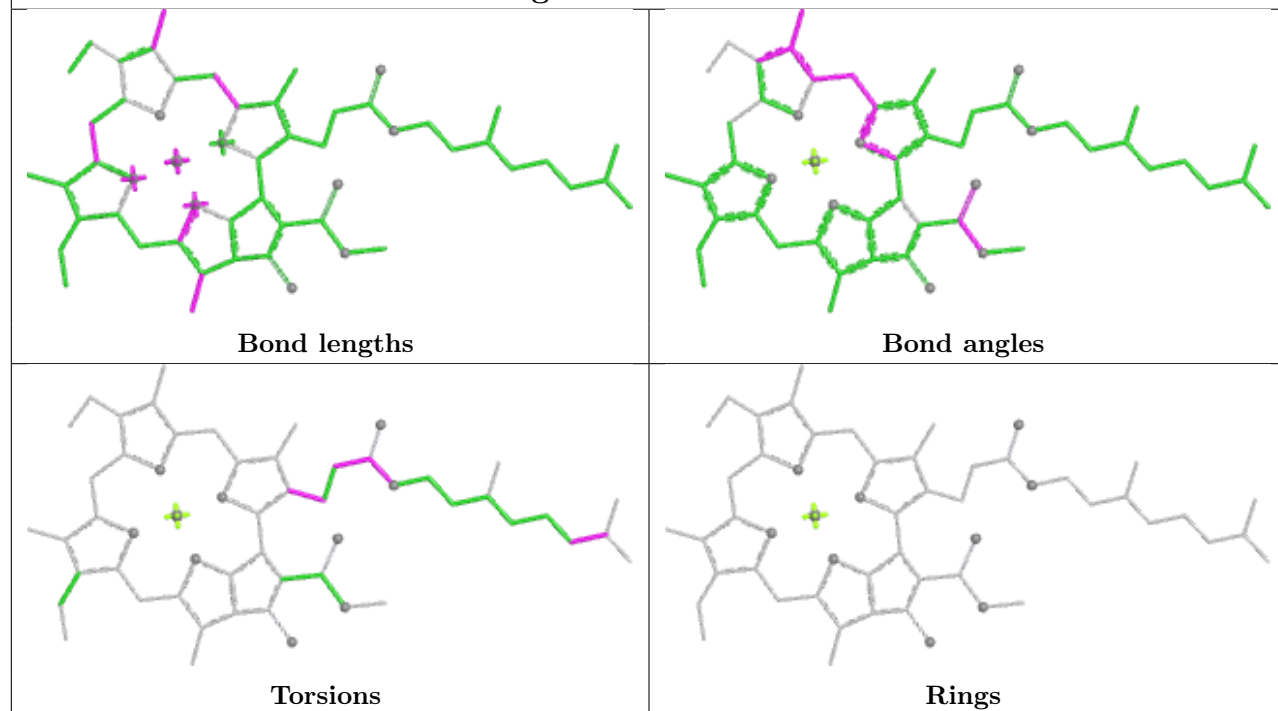
Ligand PTY 1 320



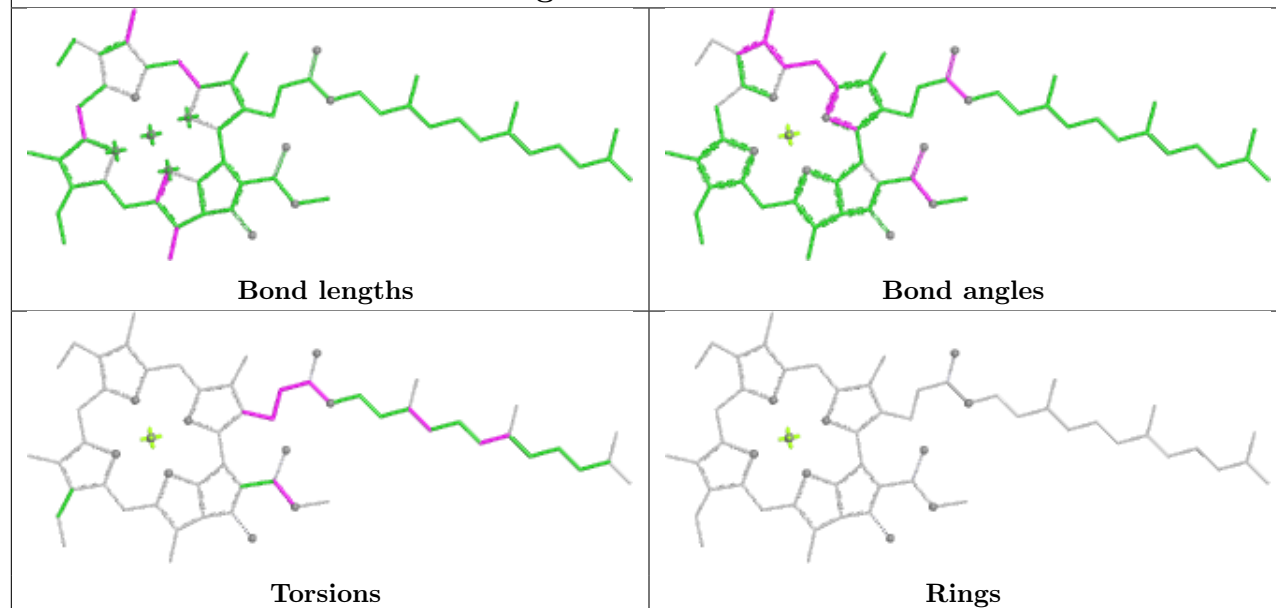
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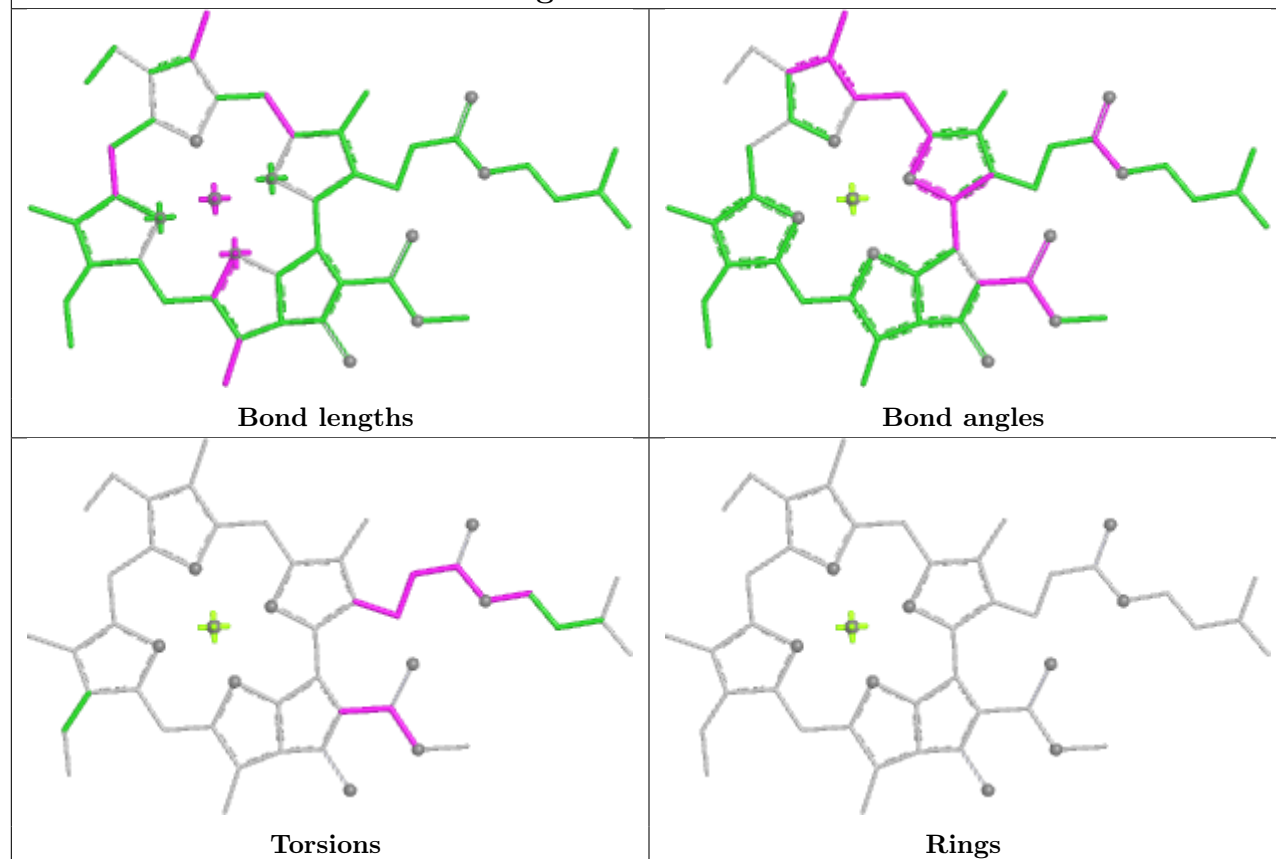
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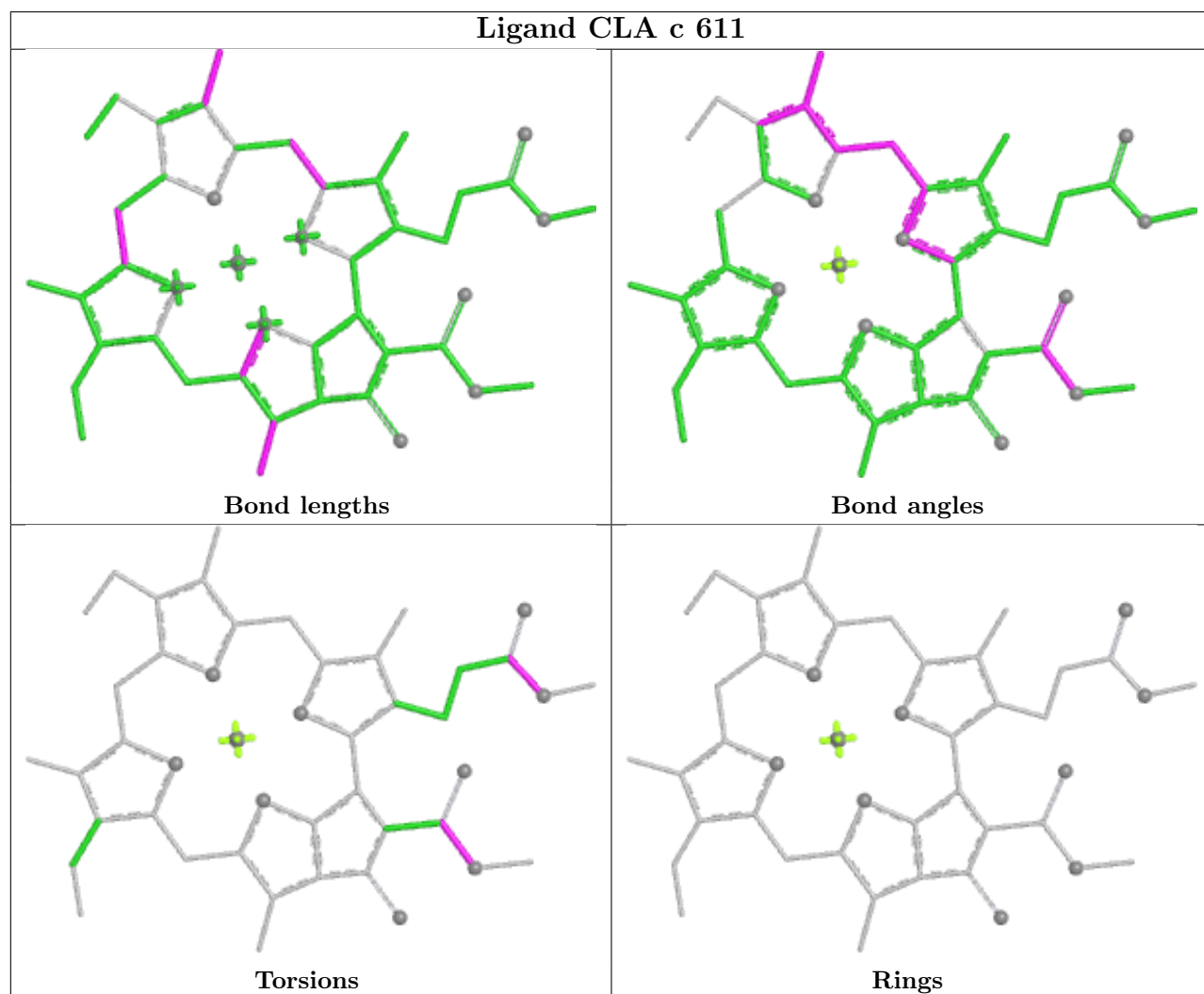
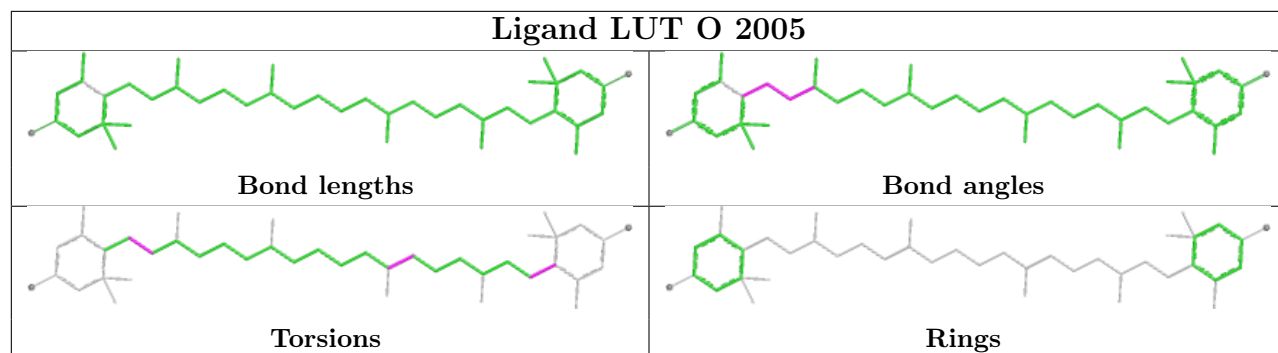


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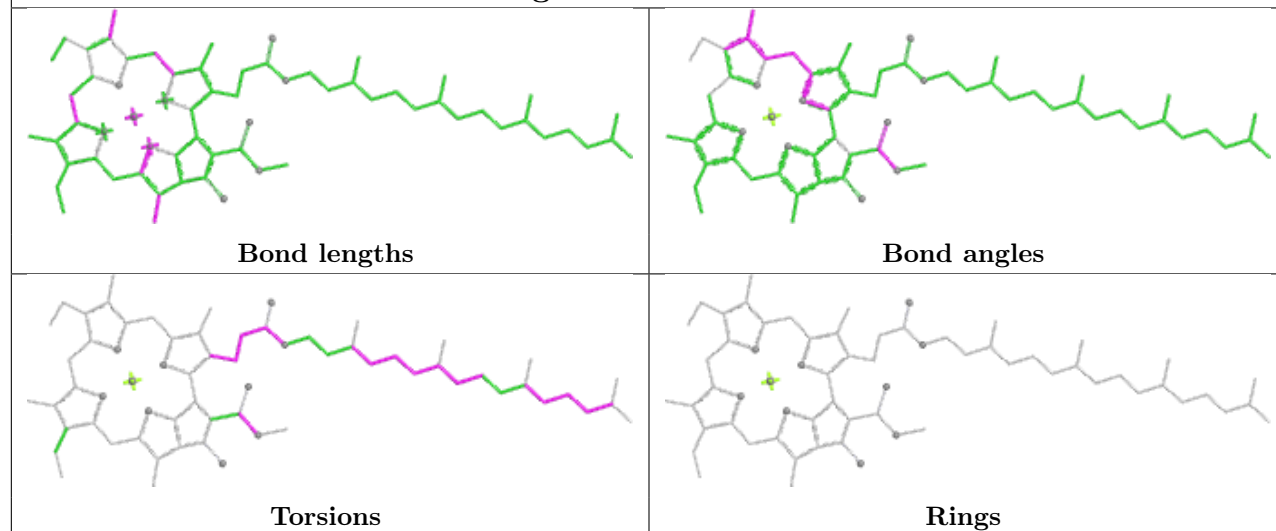


Ligand CLA a 308

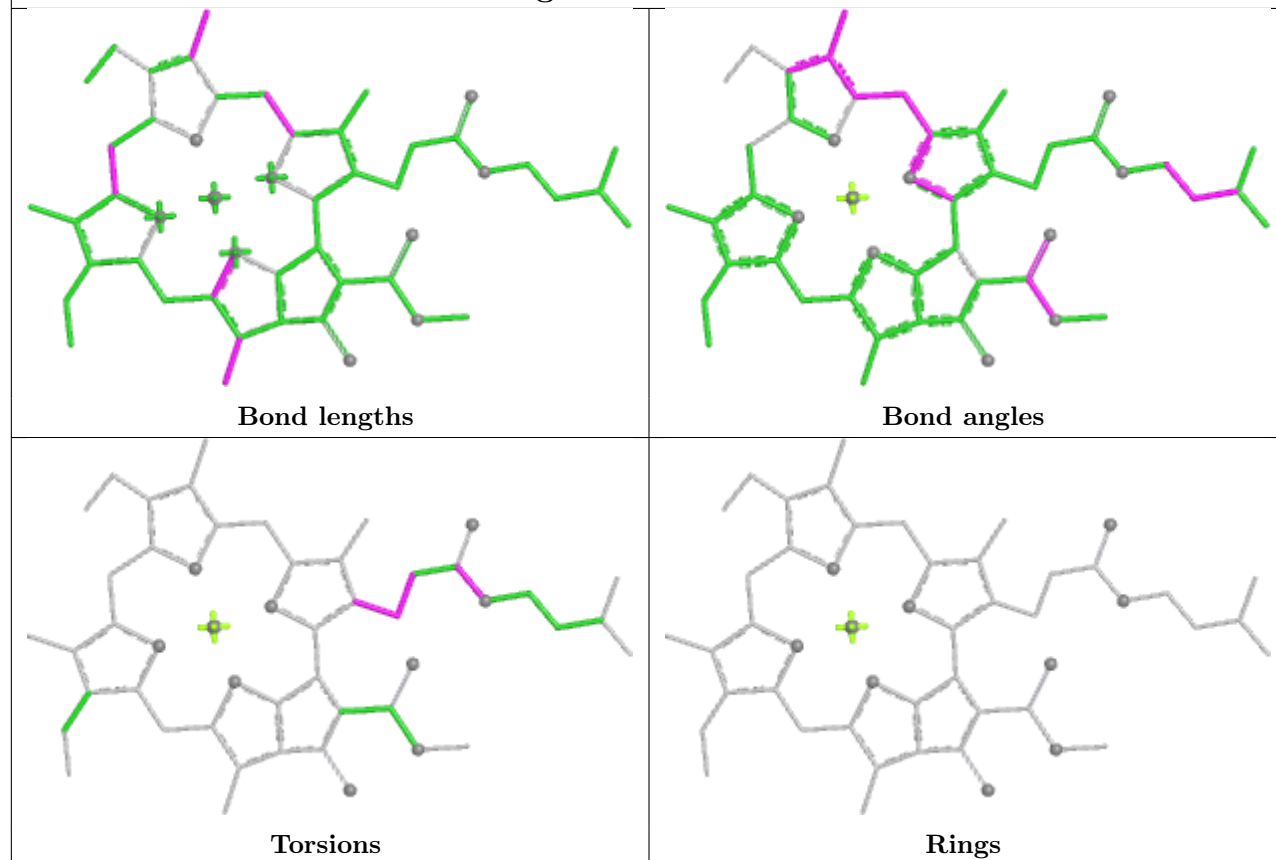


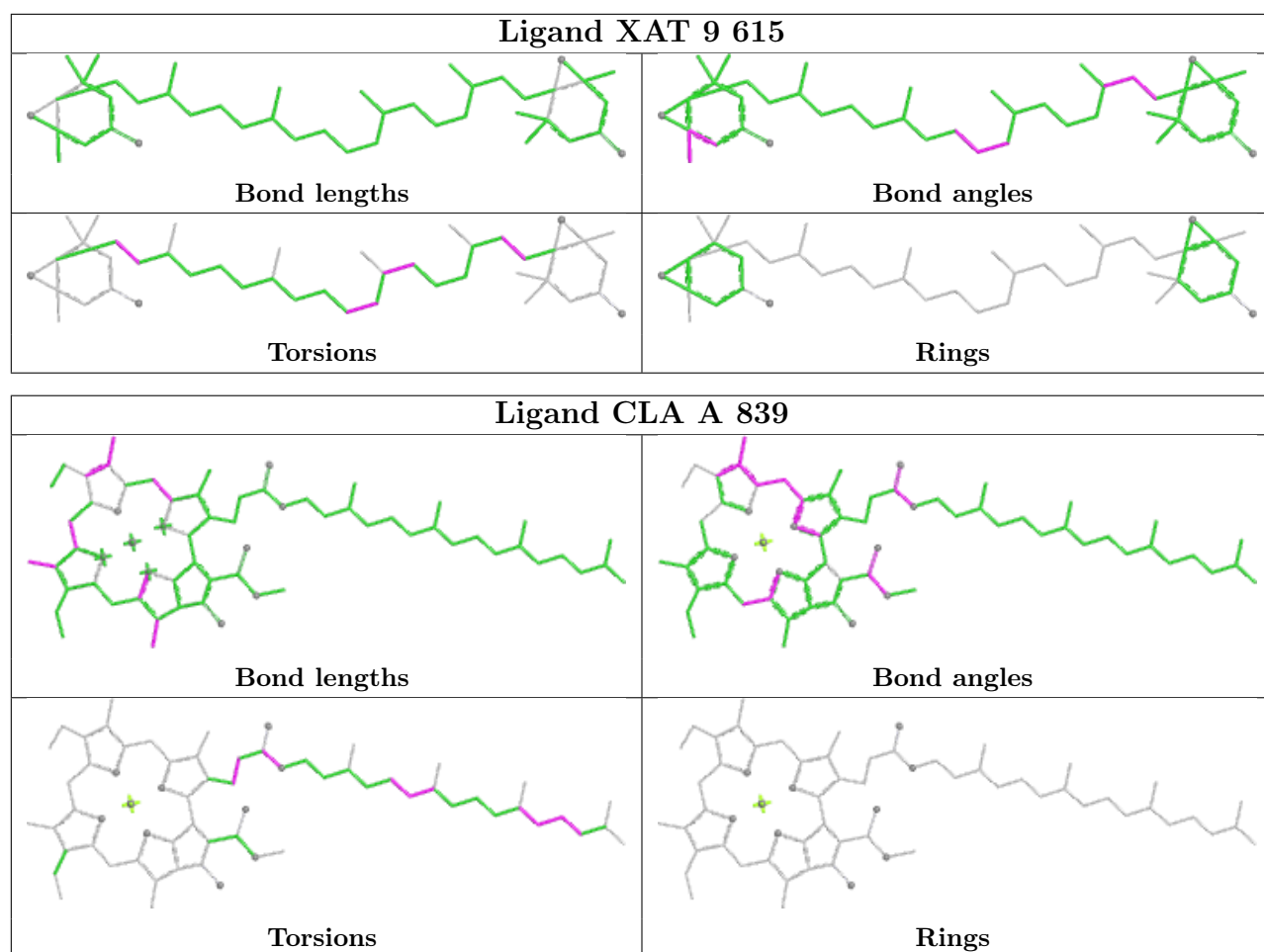


Ligand CLA B 831

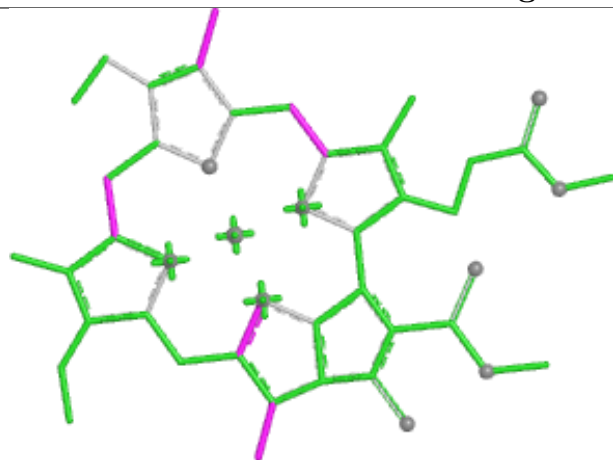


Ligand CLA 3 405

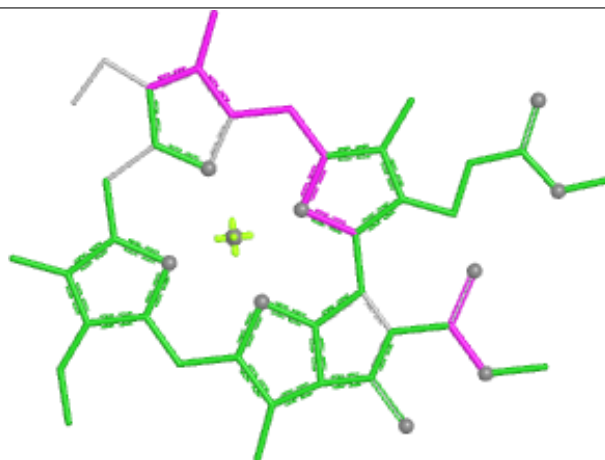




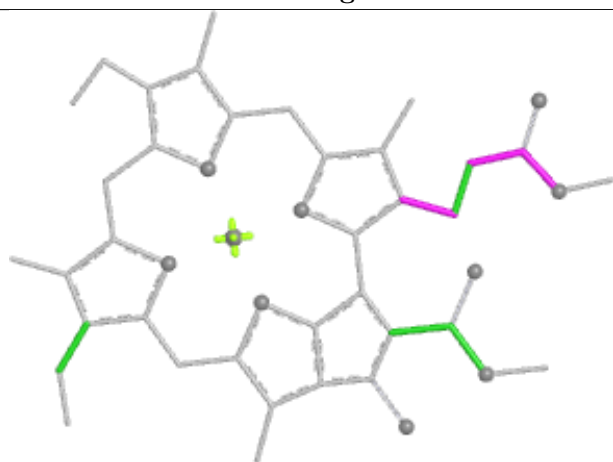
Ligand CLA 3 404



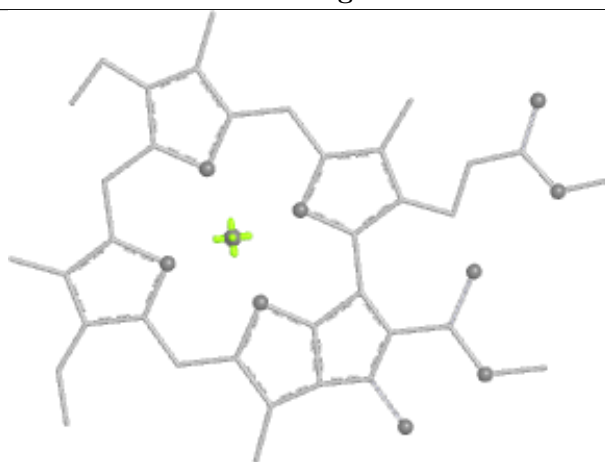
Bond lengths



Bond angles

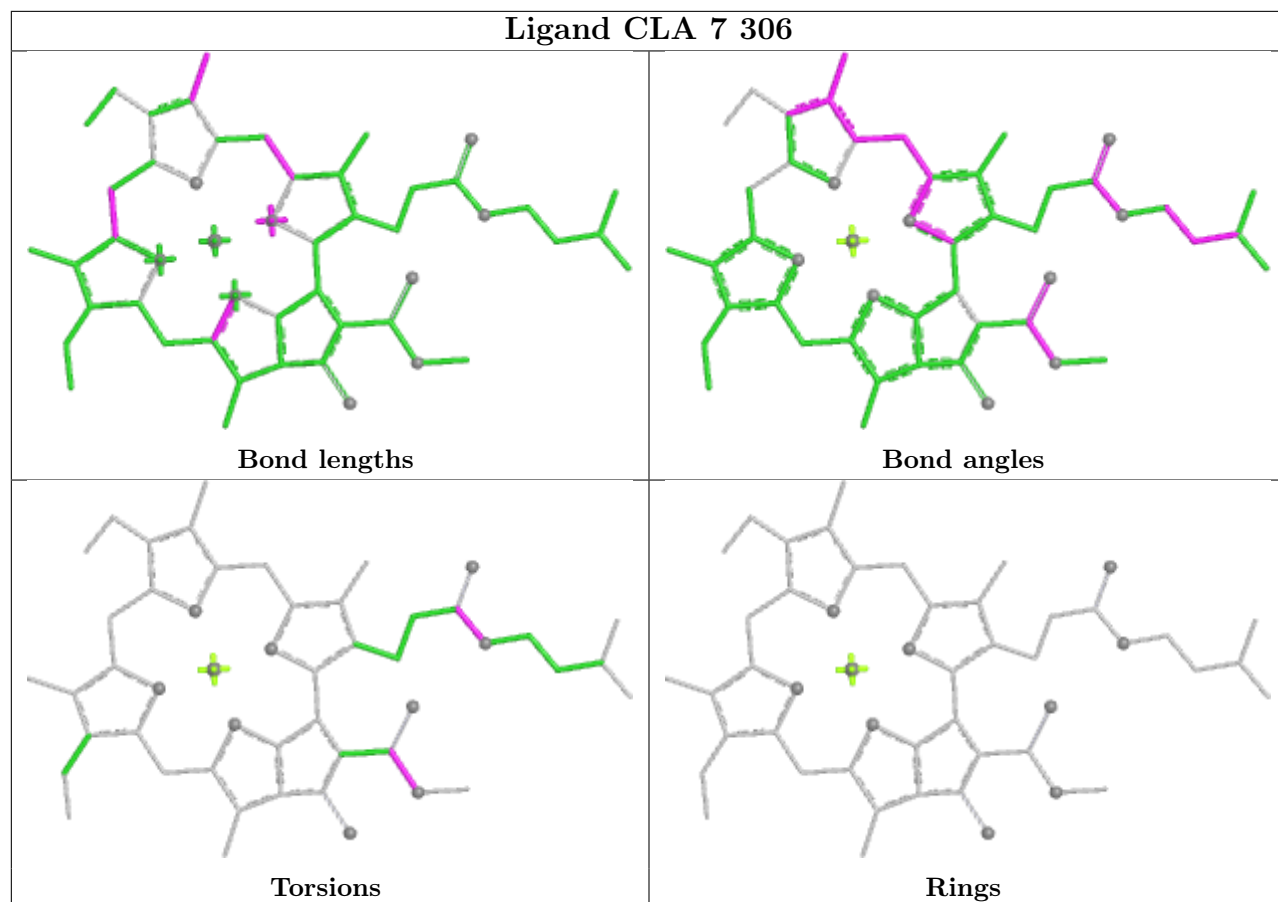


Torsions

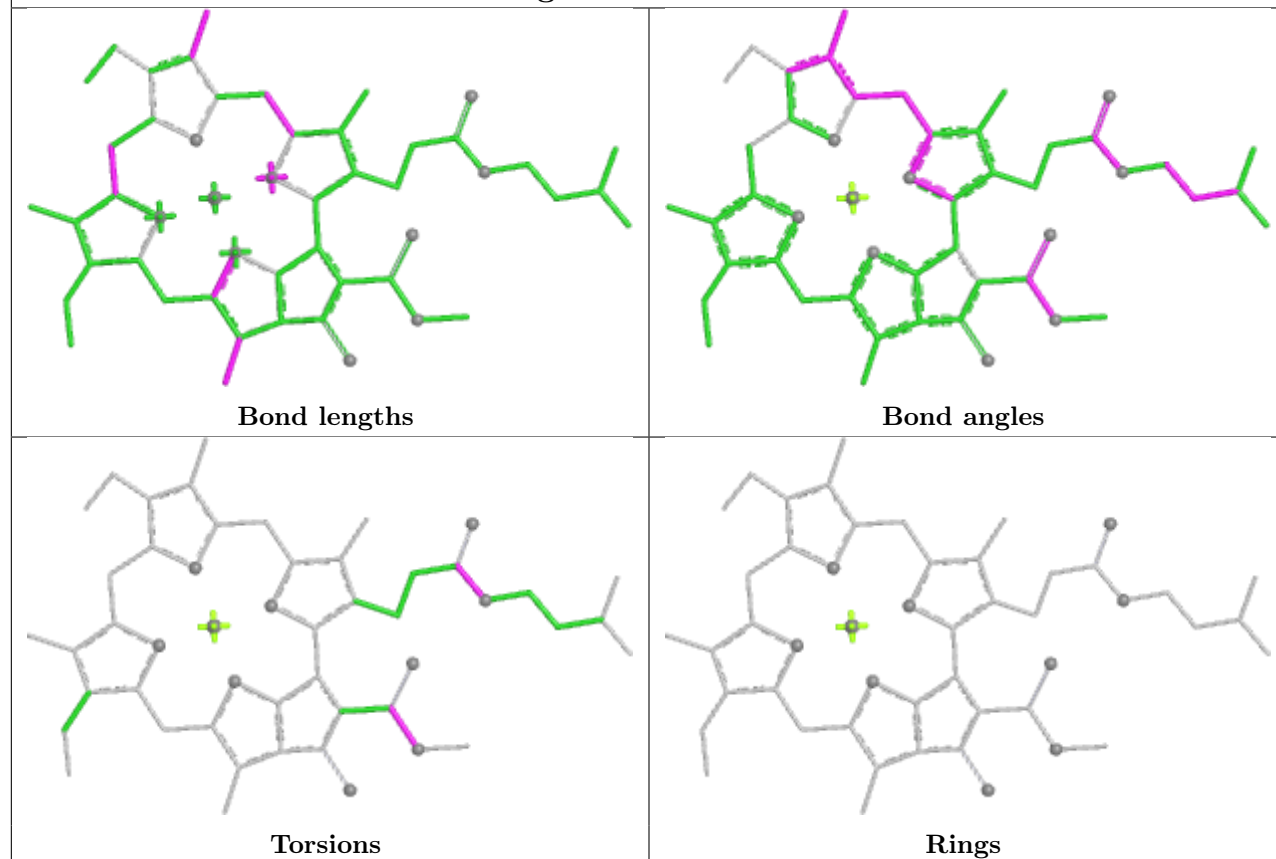


Rings

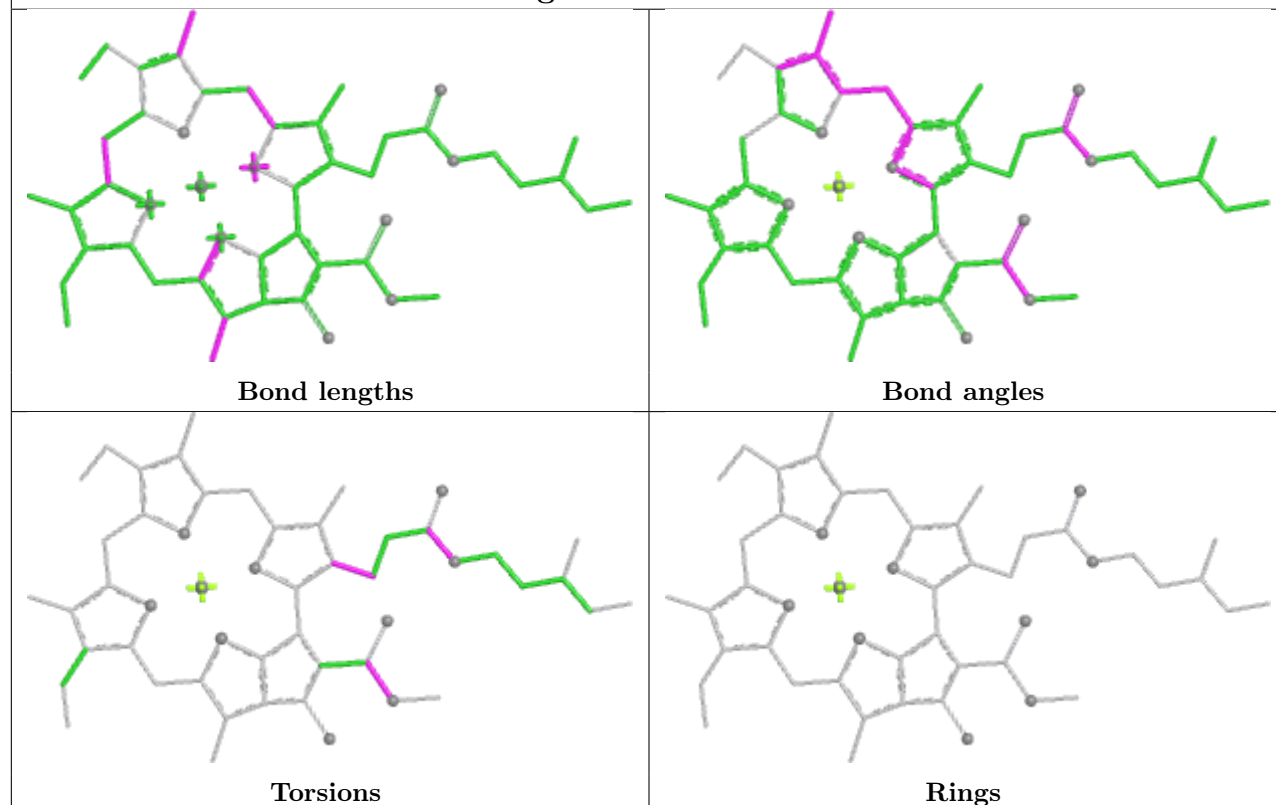
Ligand CLA 7 306



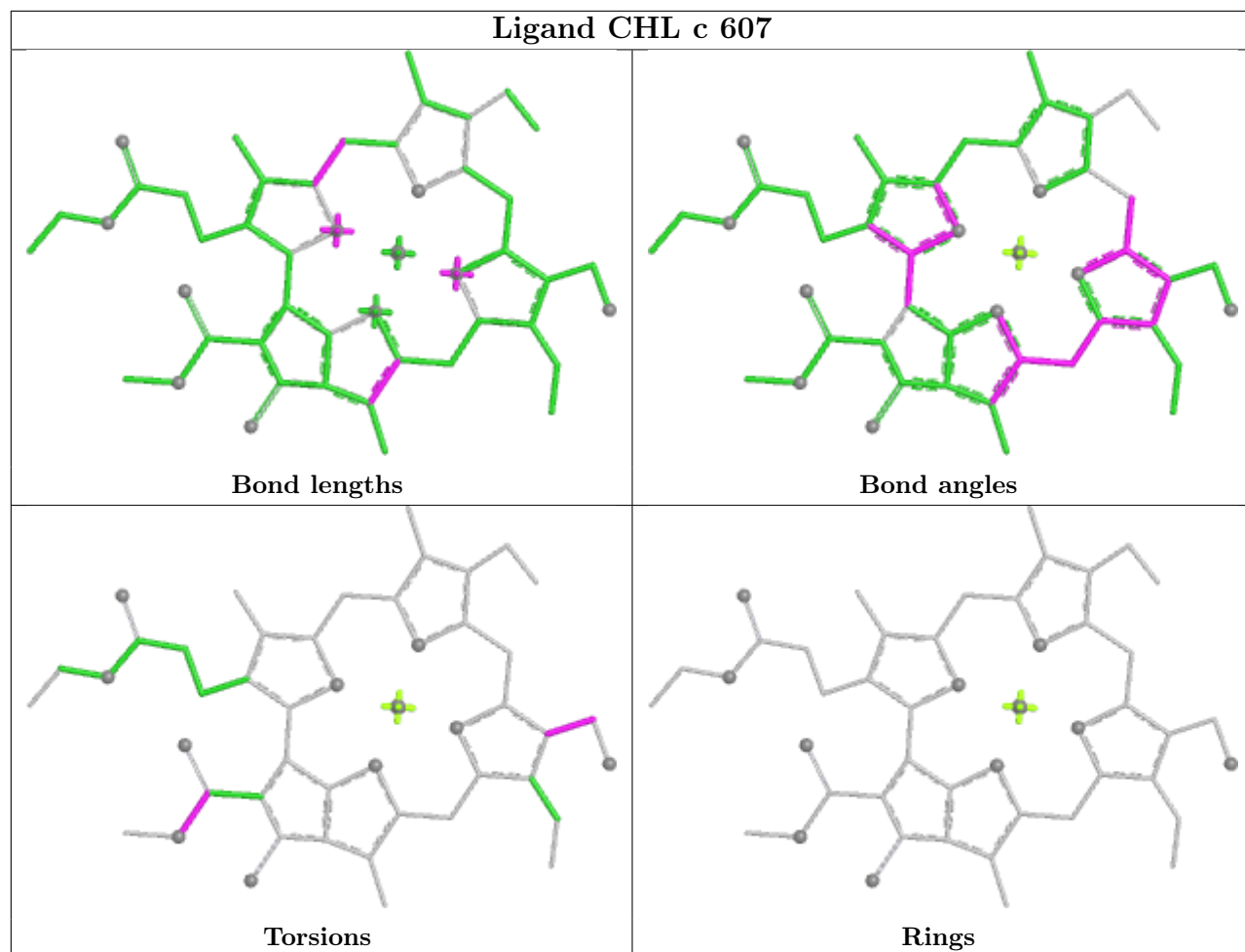
Ligand CLA c 604



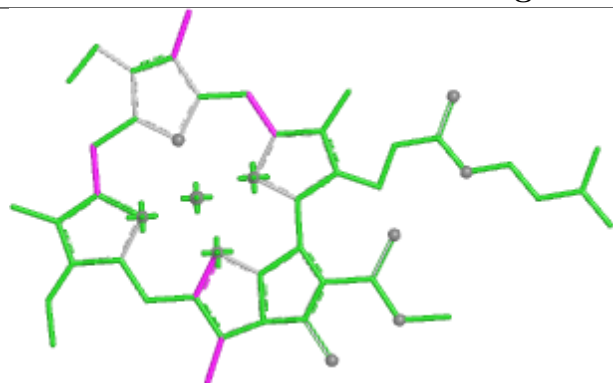
Ligand CLA c 603



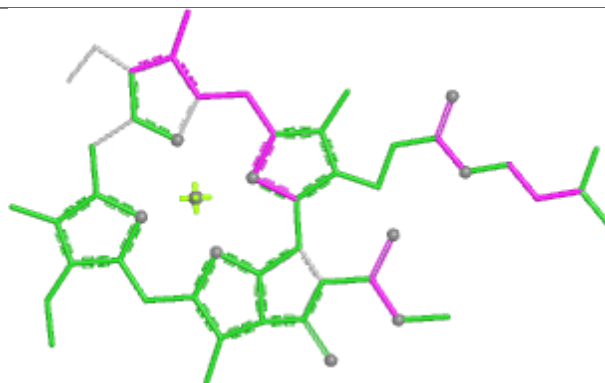
Ligand CHL c 607



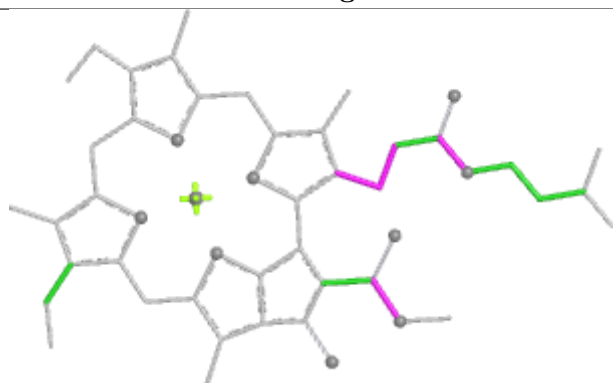
Ligand CLA T 607



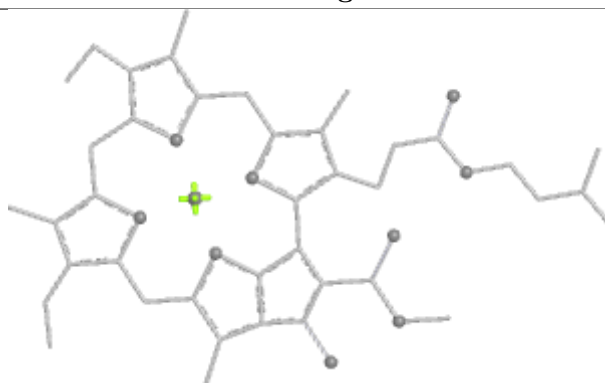
Bond lengths



Bond angles

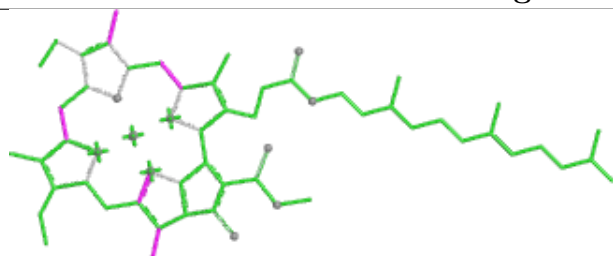


Torsions

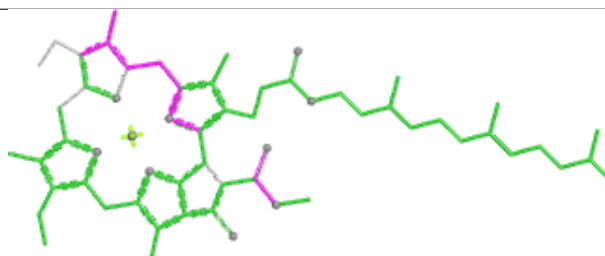


Rings

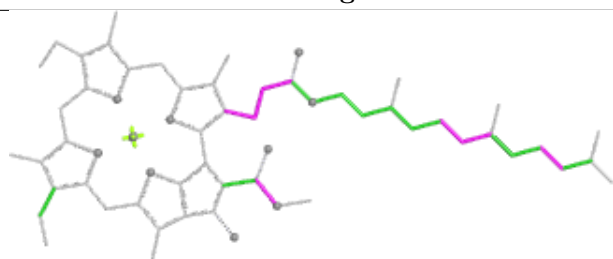
Ligand CLA A 824



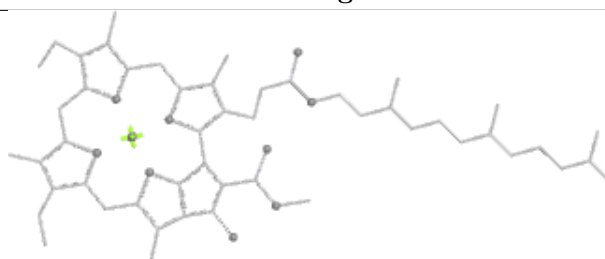
Bond lengths



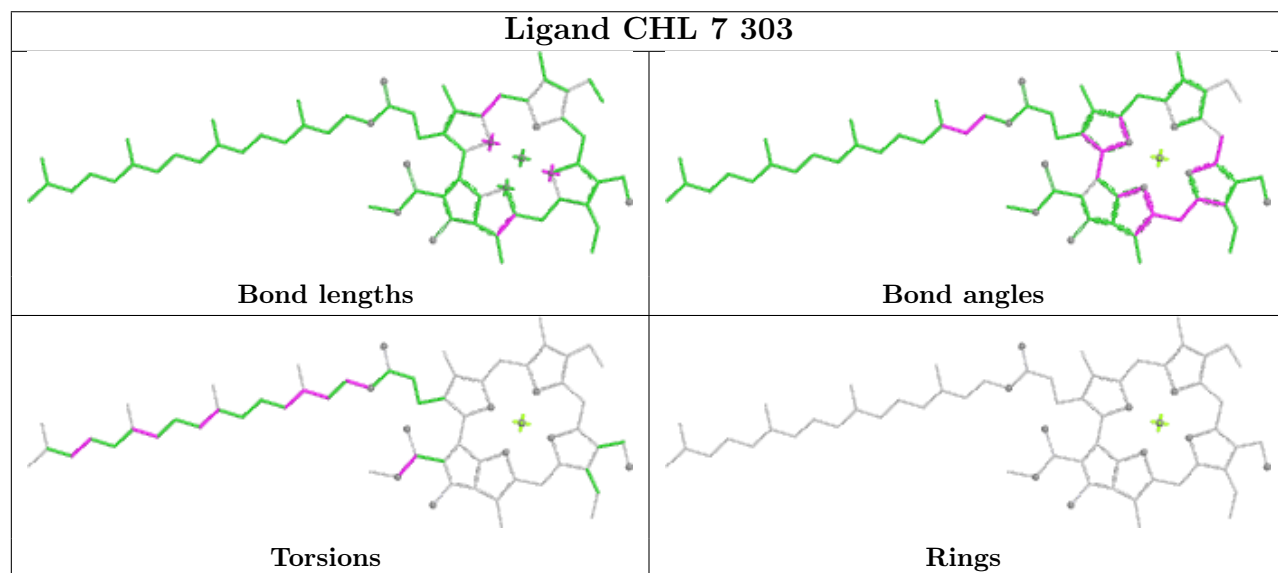
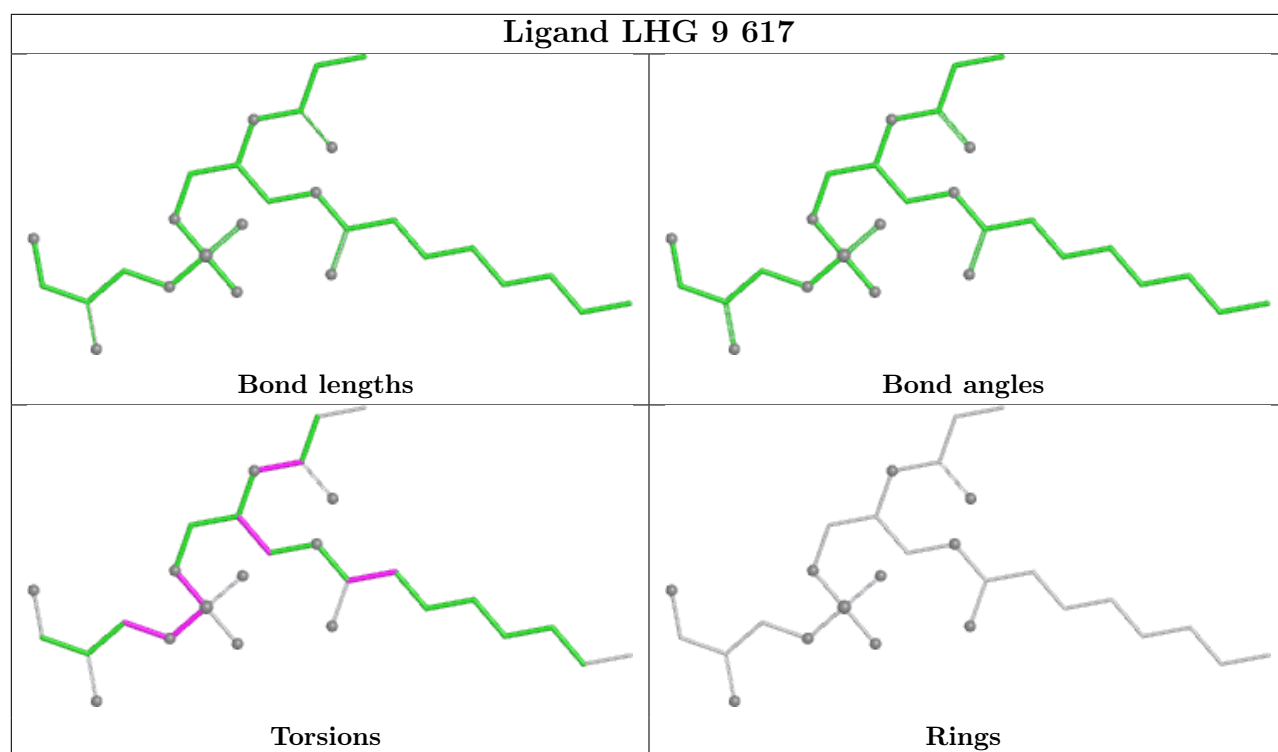
Bond angles



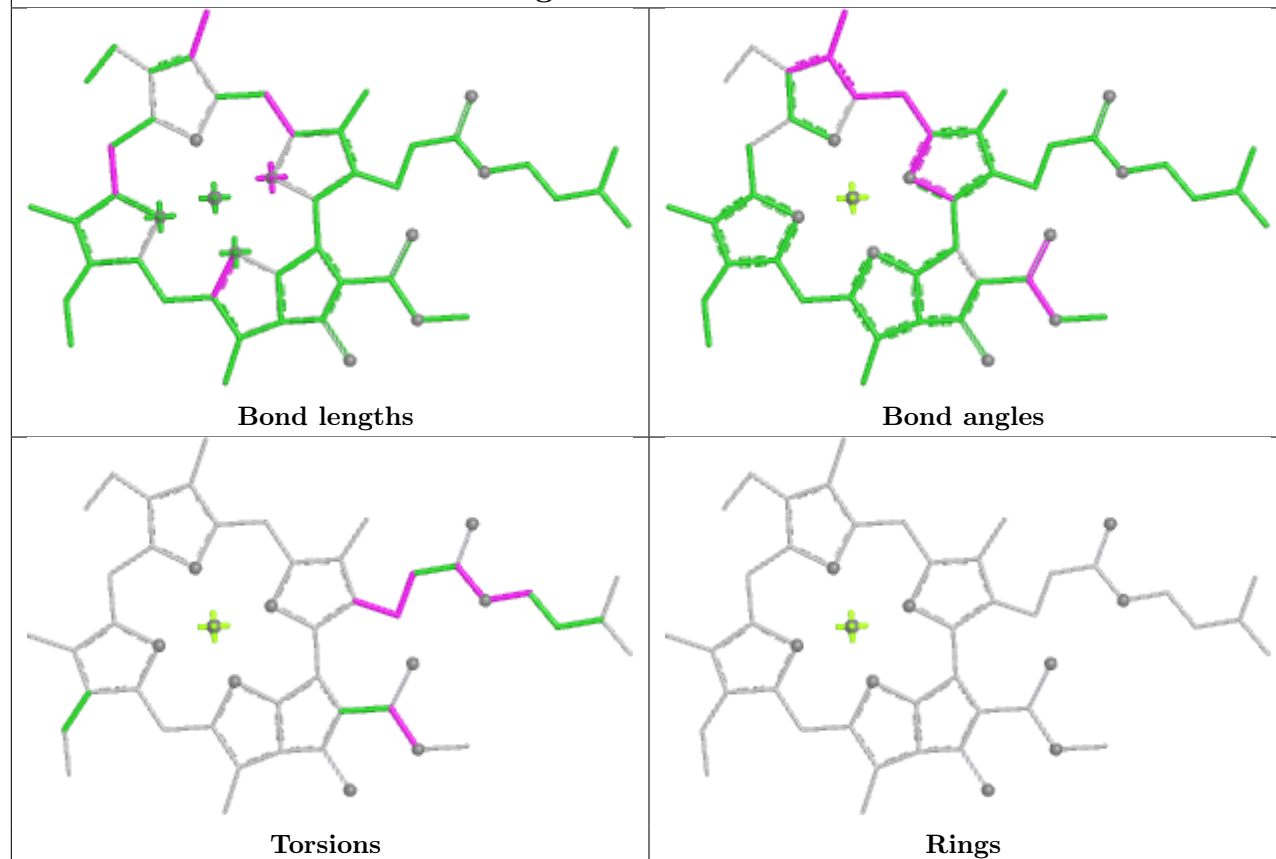
Torsions



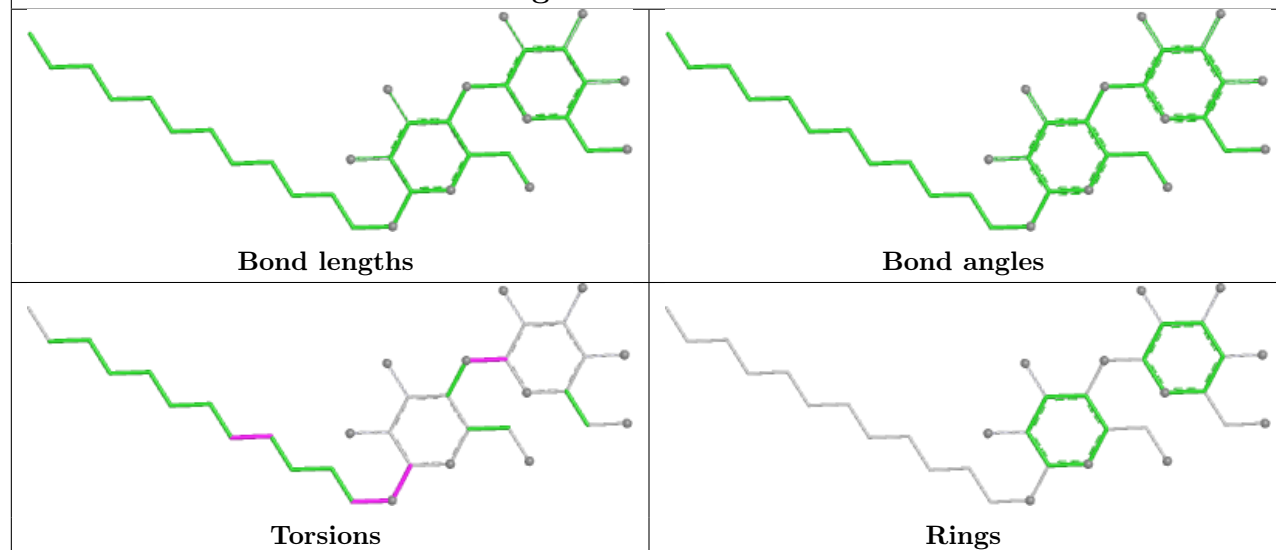
Rings

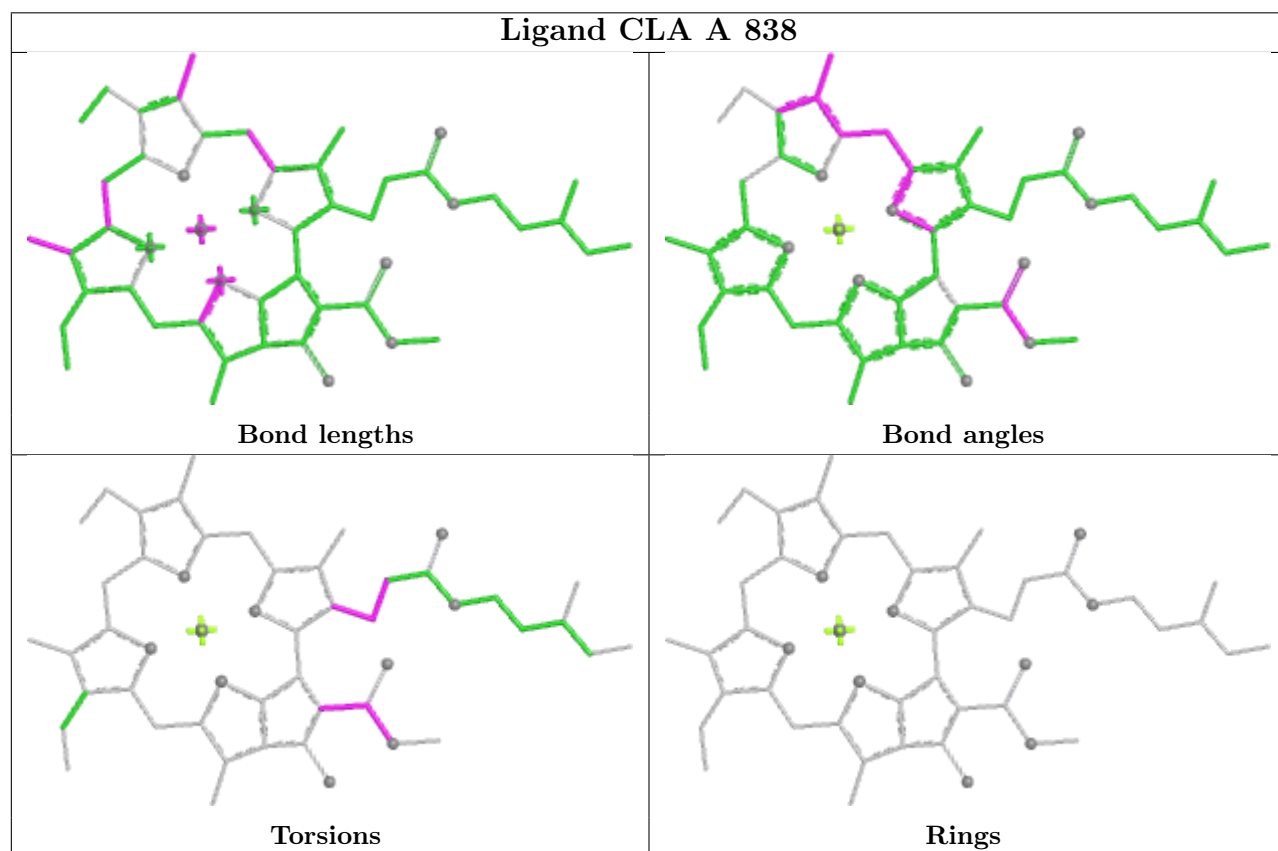
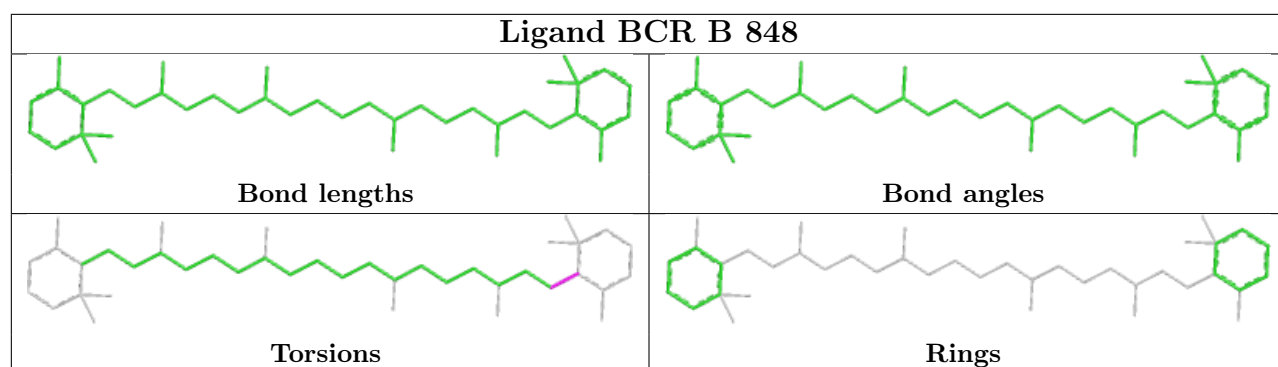


Ligand CLA b 306

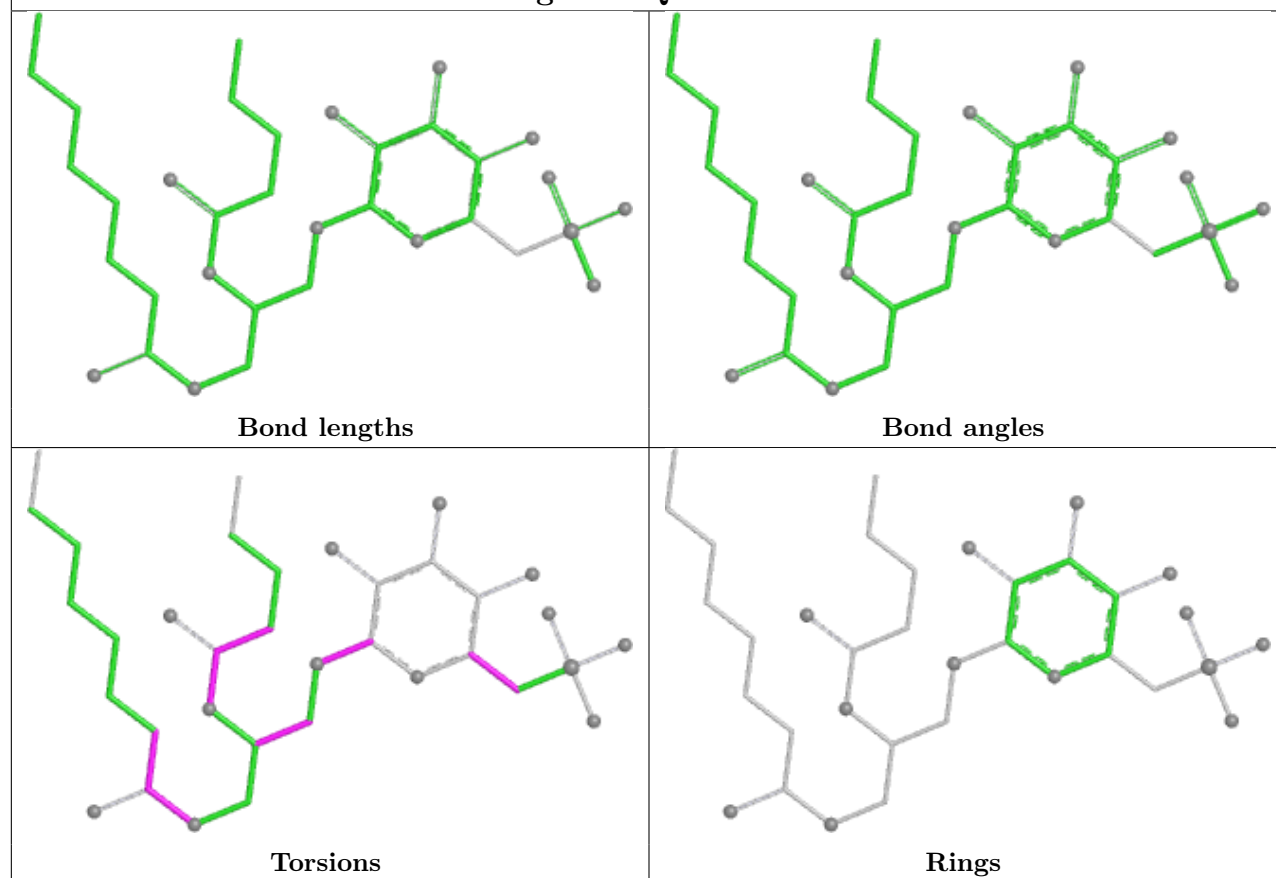


Ligand LMU 9 616

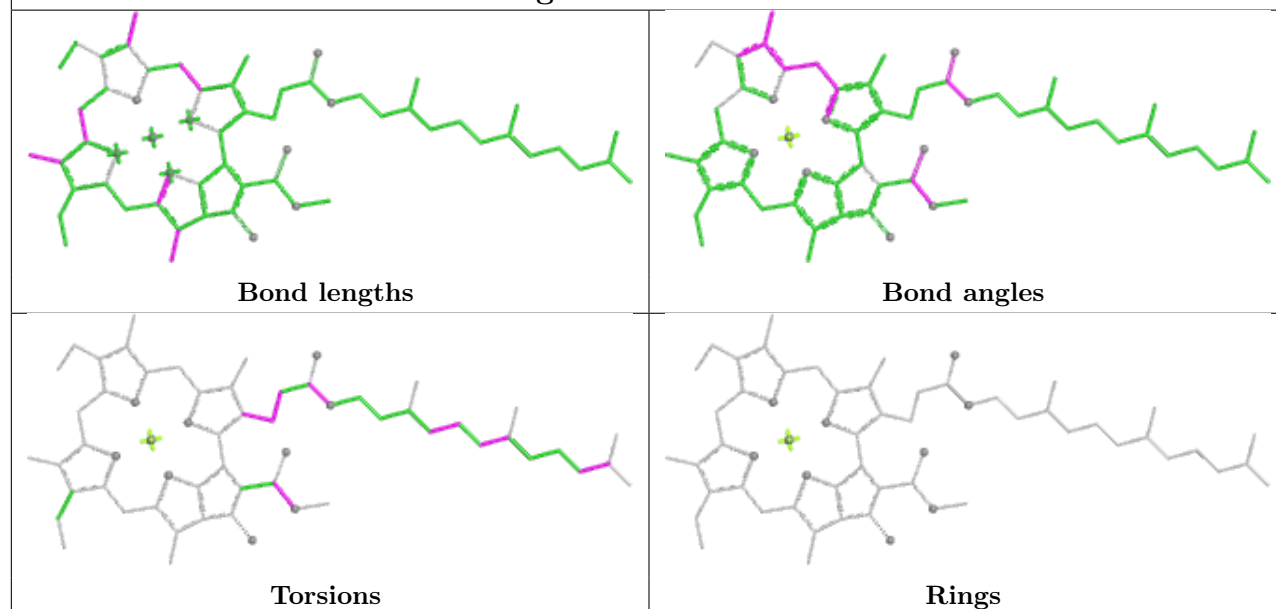




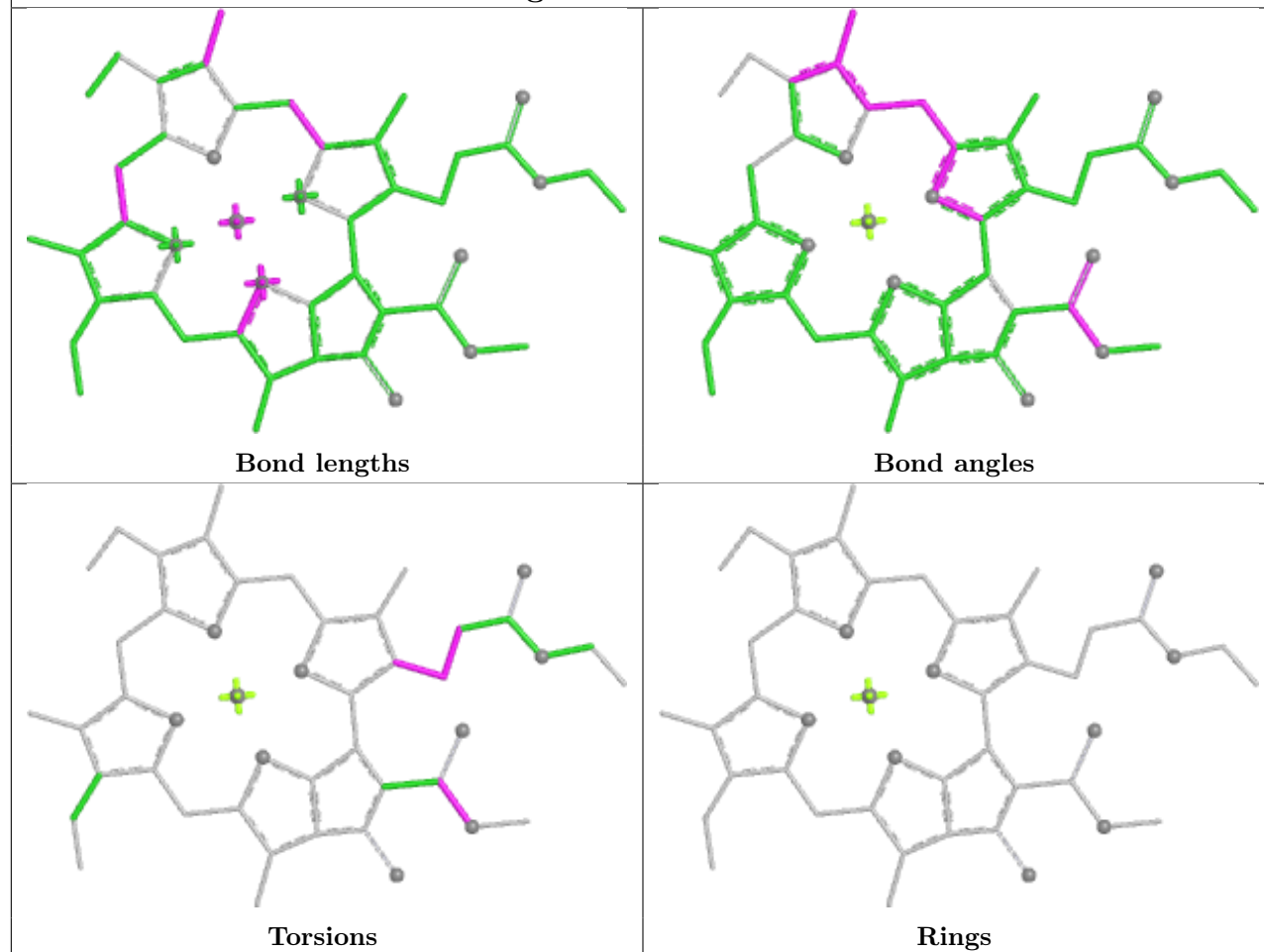
Ligand SQD 3 422



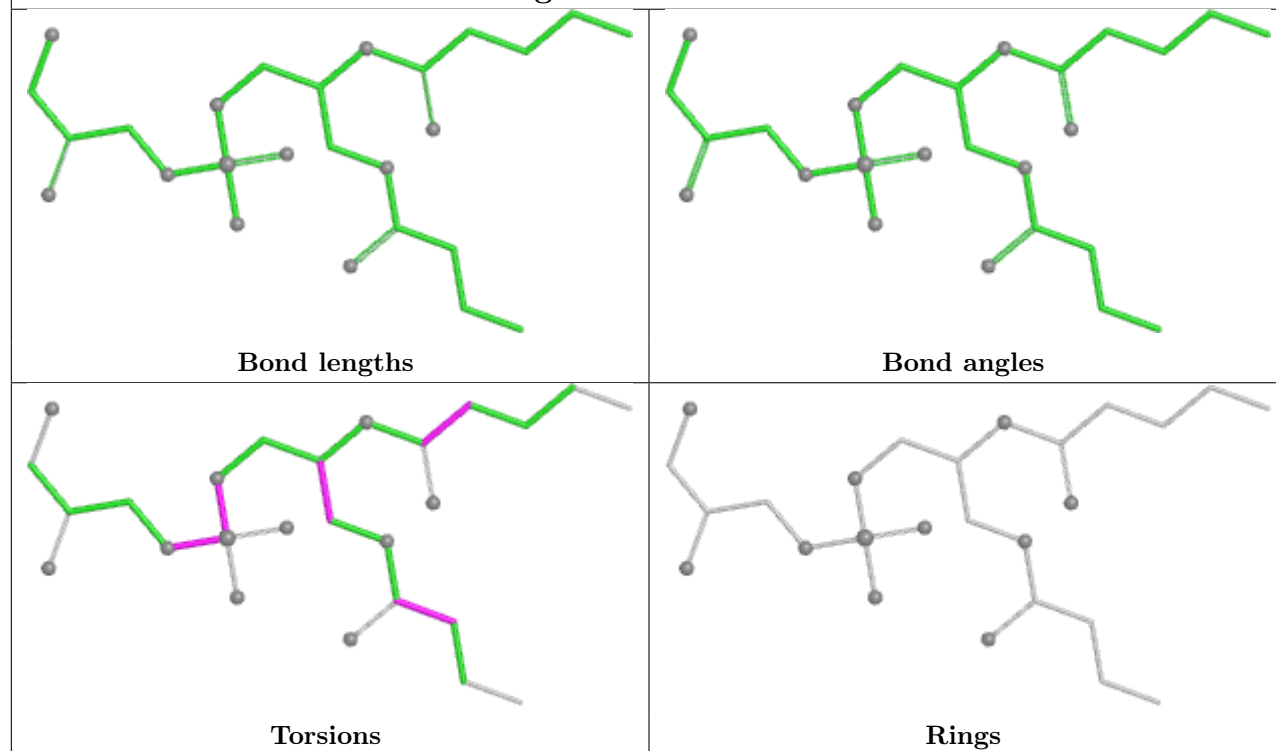
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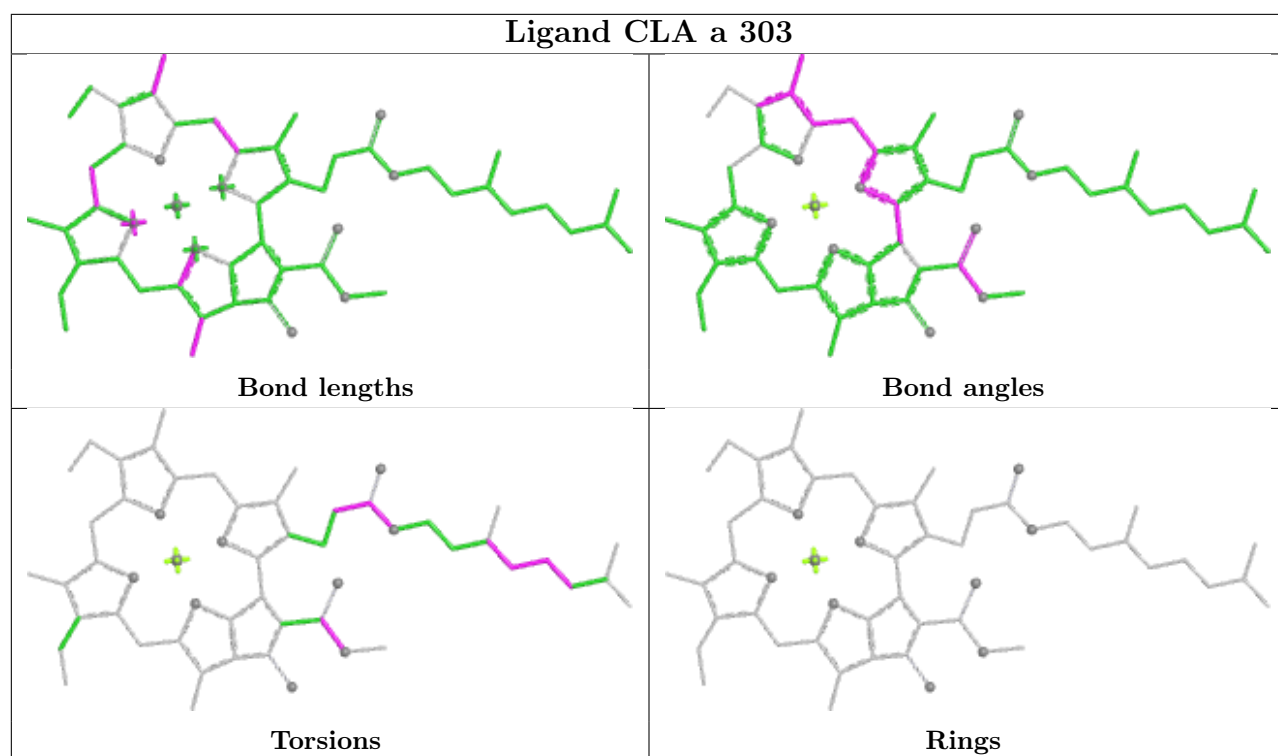


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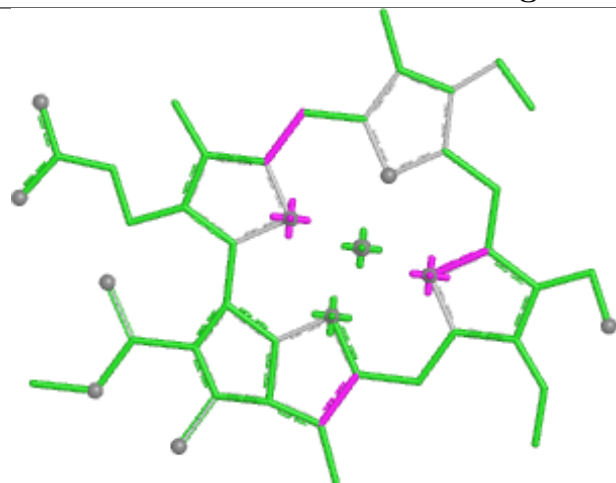


Ligand LHG 3 424

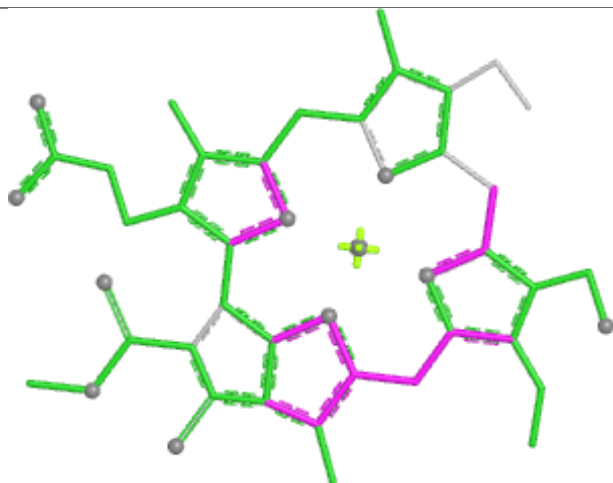




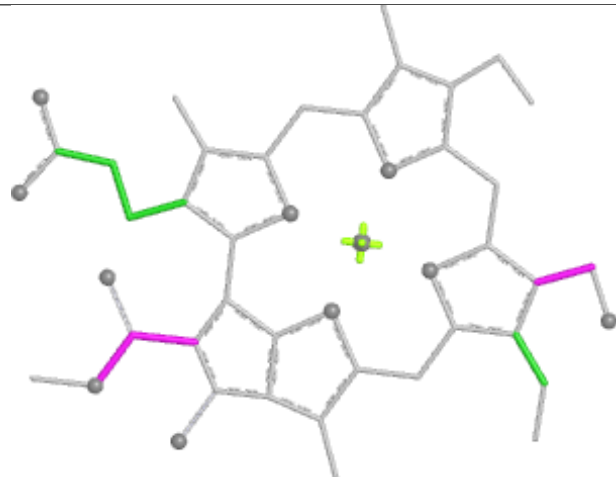
Ligand CHL 8 606



Bond lengths



Bond angles

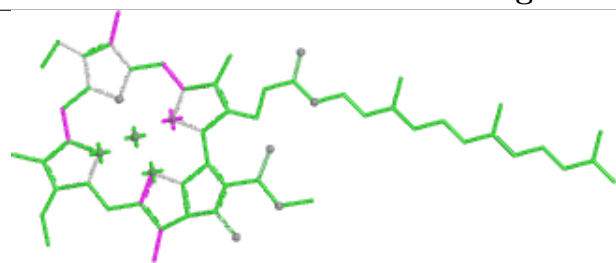


Torsions

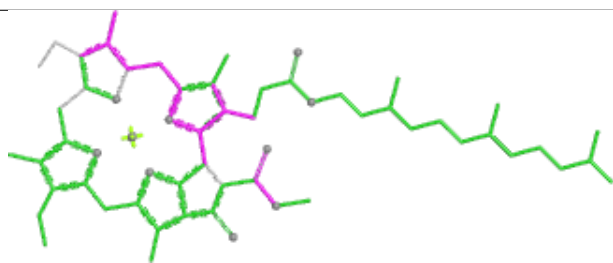


Rings

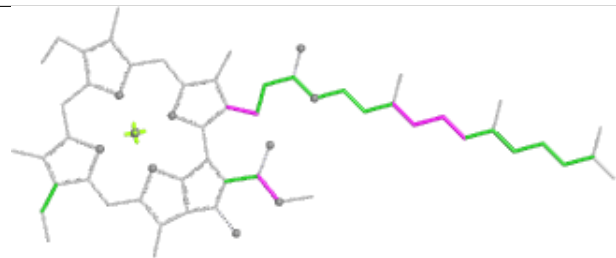
Ligand CLA A 809



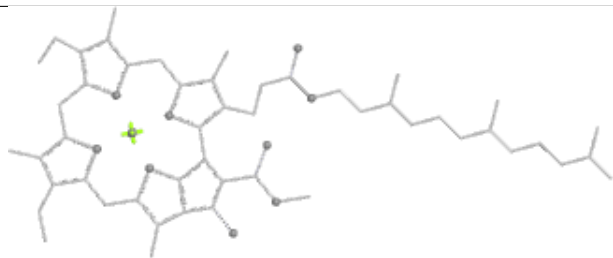
Bond lengths



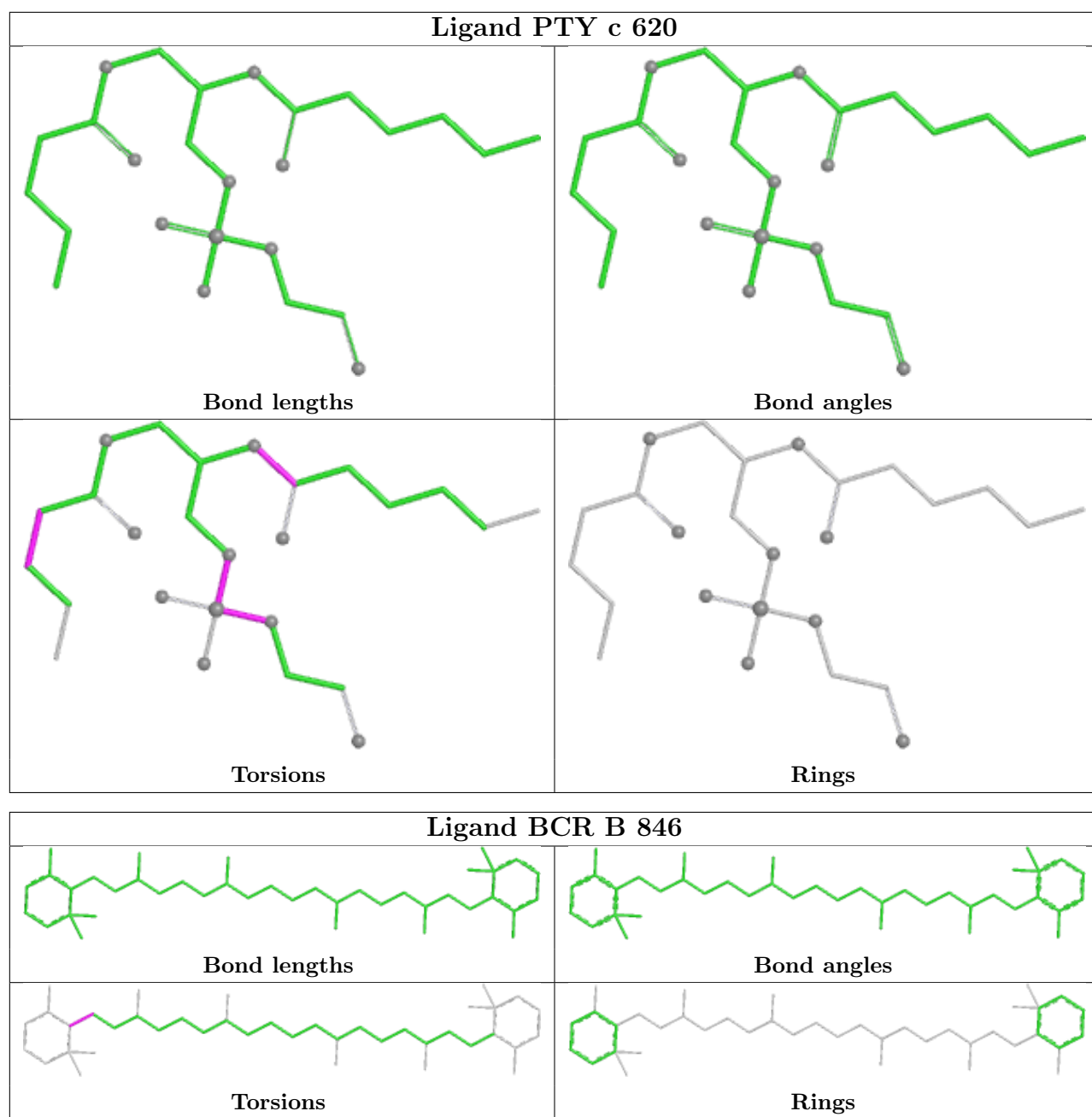
Bond angles



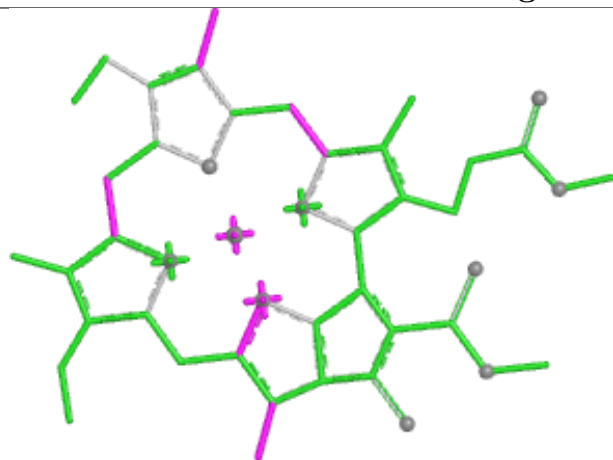
Torsions



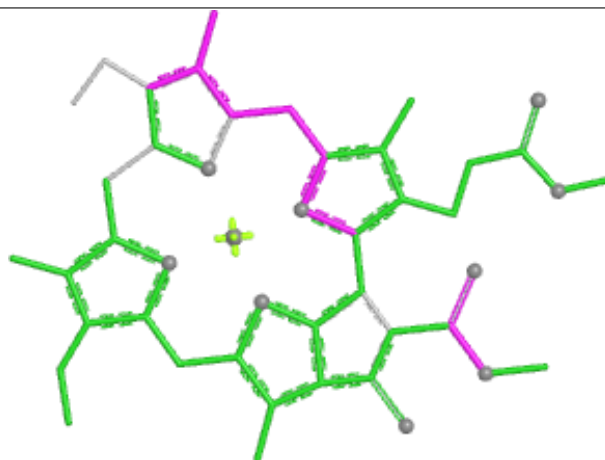
Rings



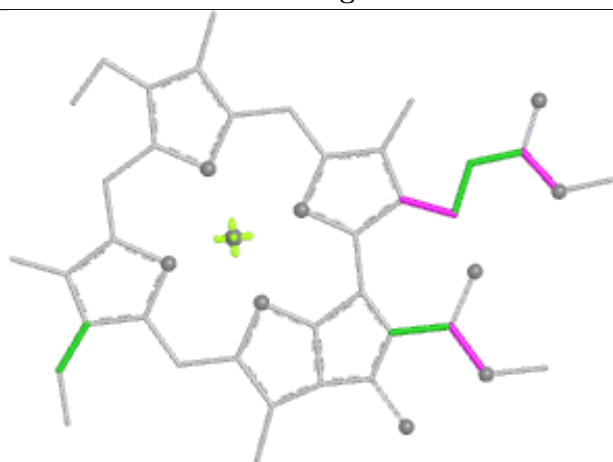
Ligand CLA 7 323



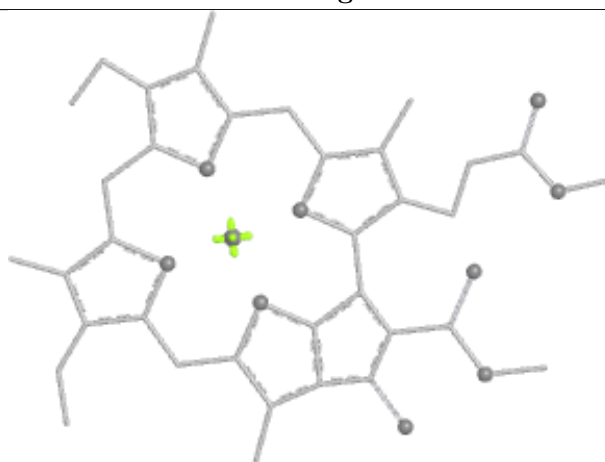
Bond lengths



Bond angles

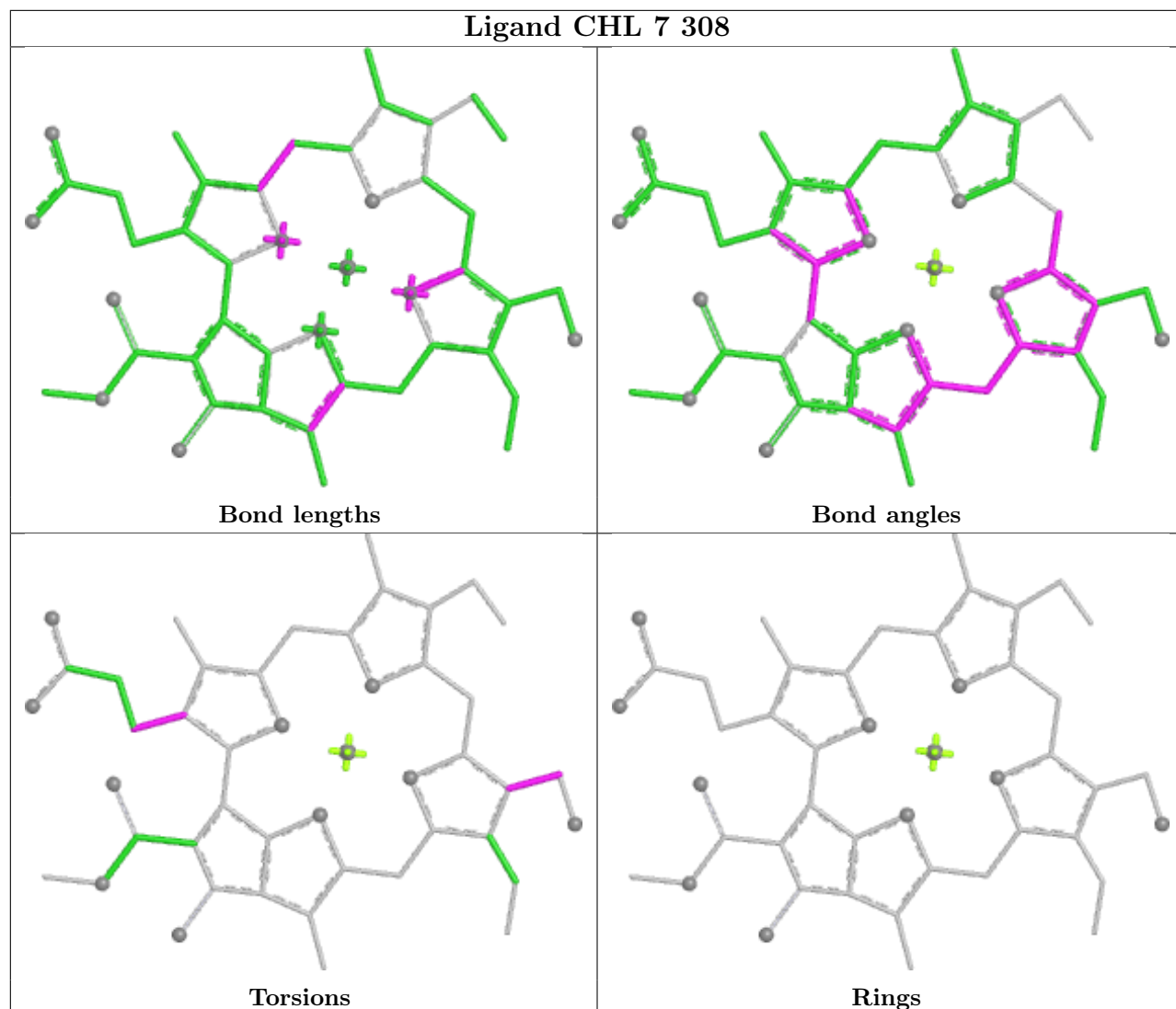


Torsions

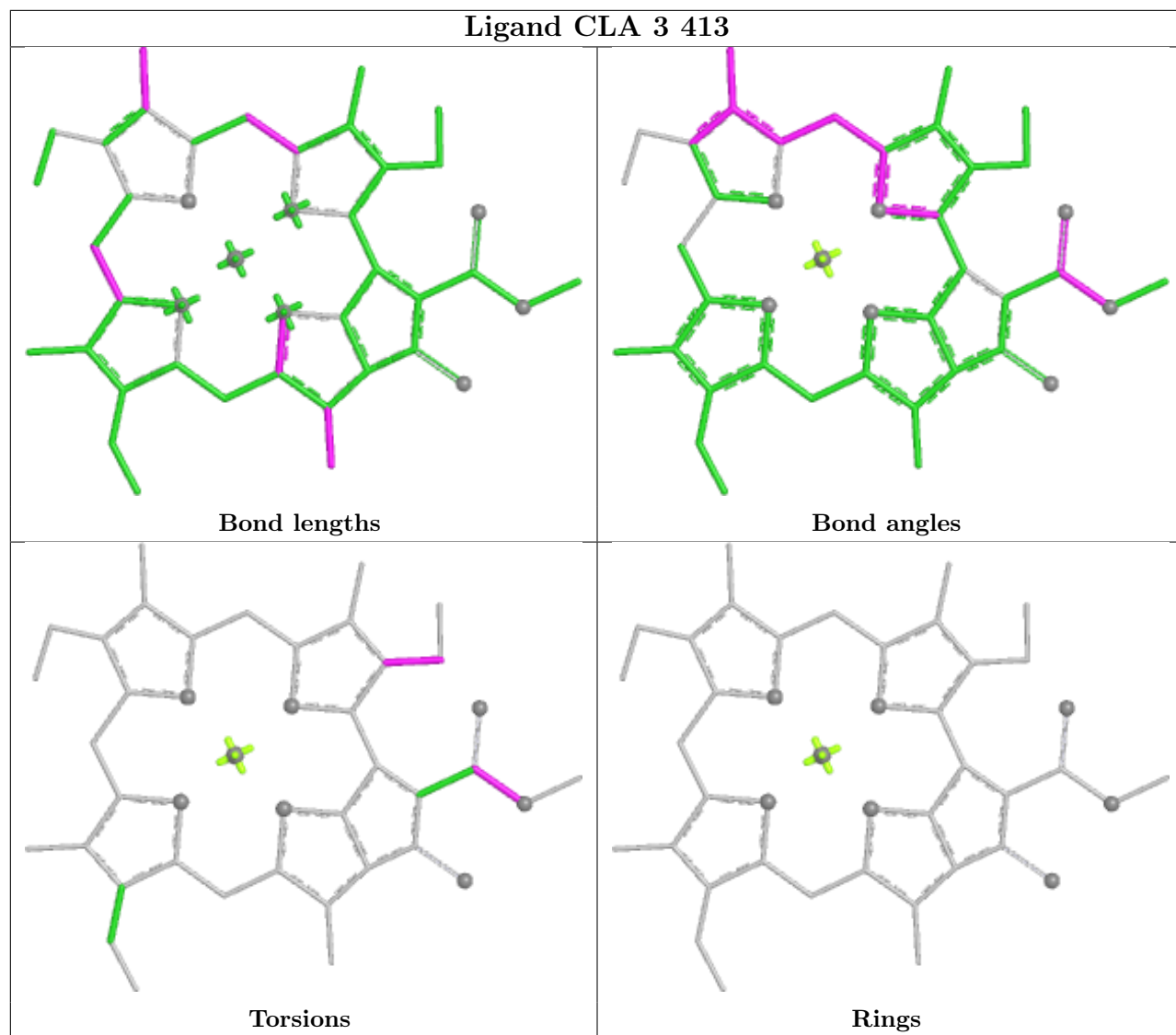


Rings

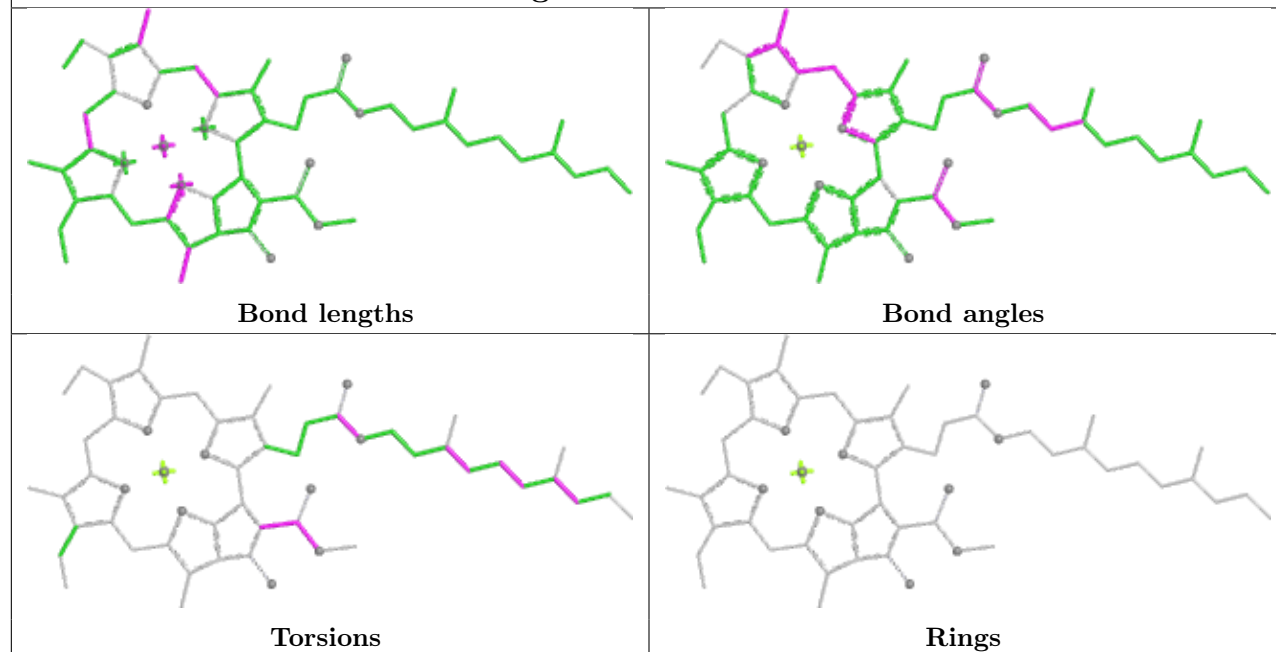
Ligand CHL 7 308



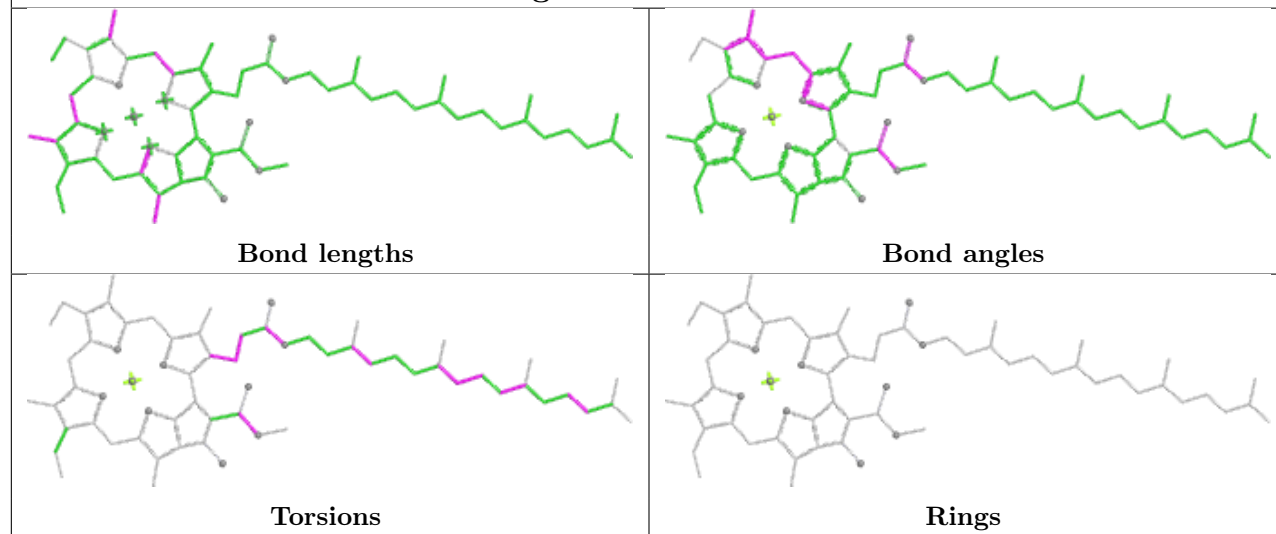
Ligand CLA 3 413



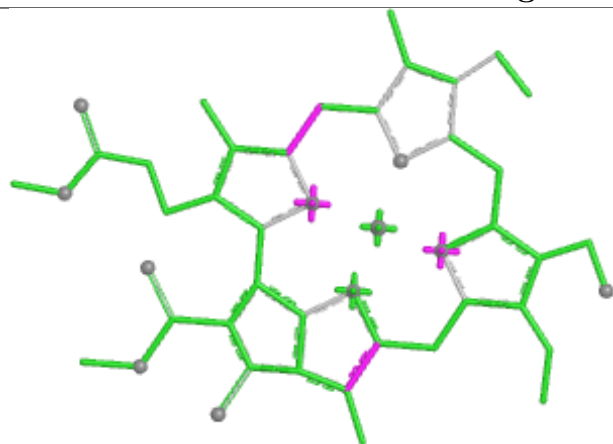
Ligand CLA A 828



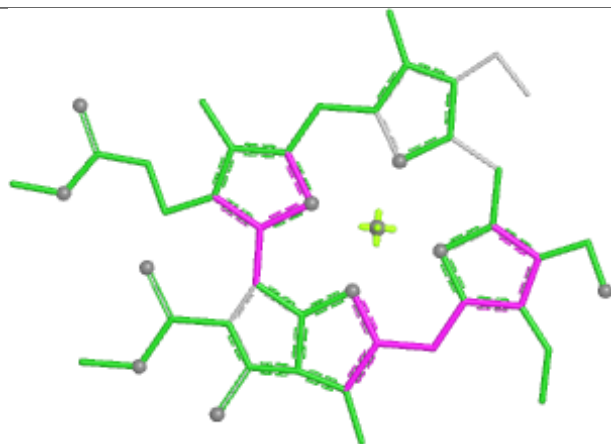
Ligand CLA B 818



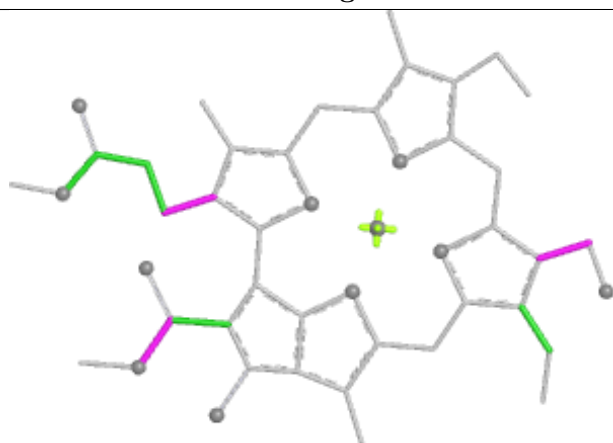
Ligand CHL 9 606



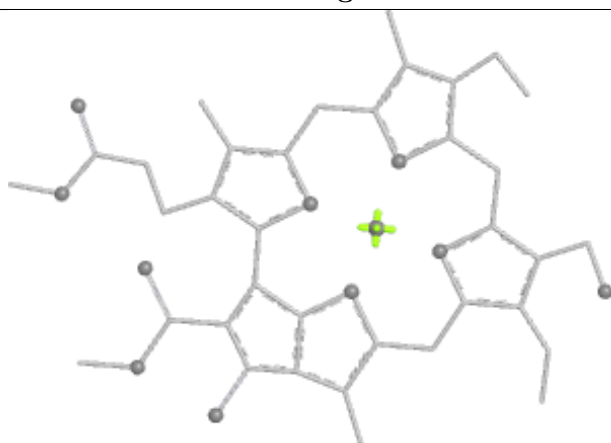
Bond lengths



Bond angles

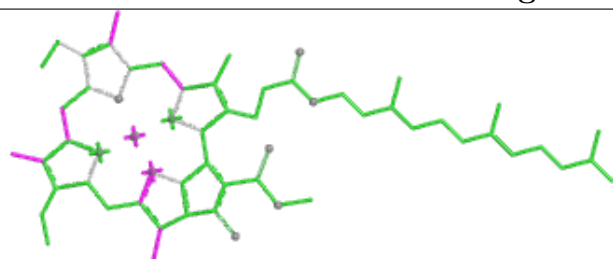


Torsions

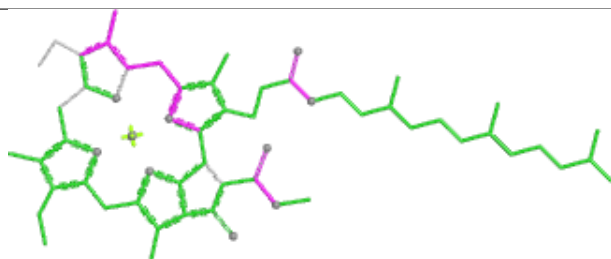


Rings

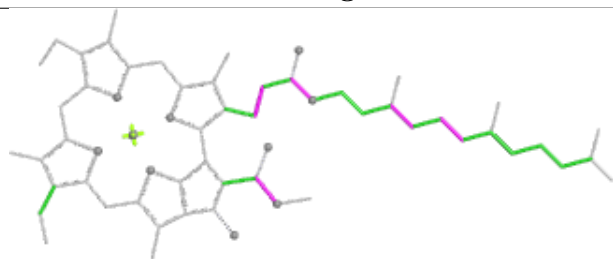
Ligand CLA 3 411



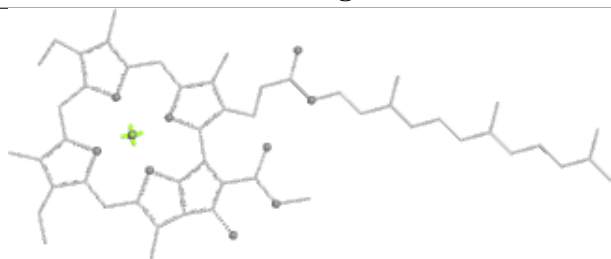
Bond lengths



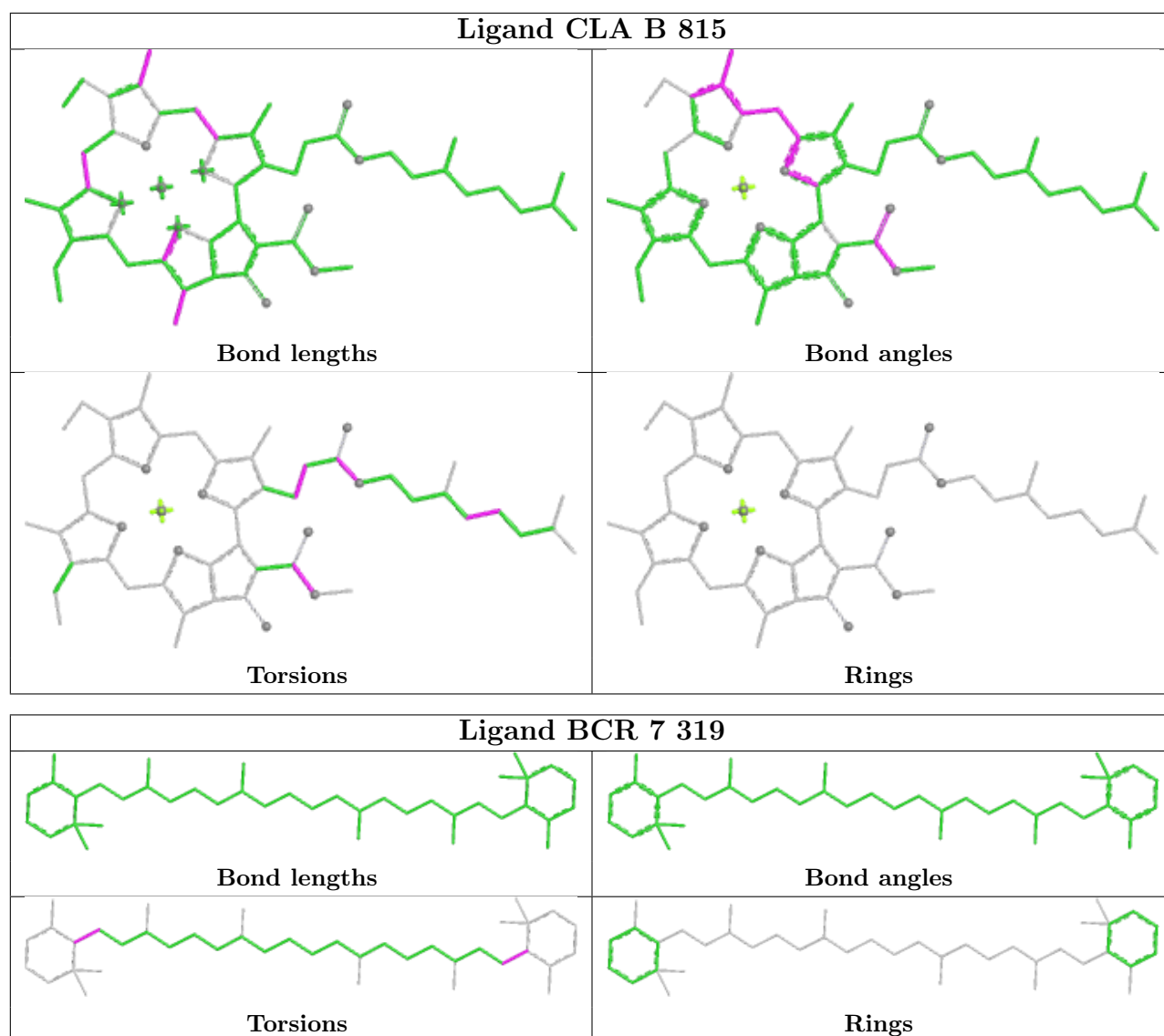
Bond angles



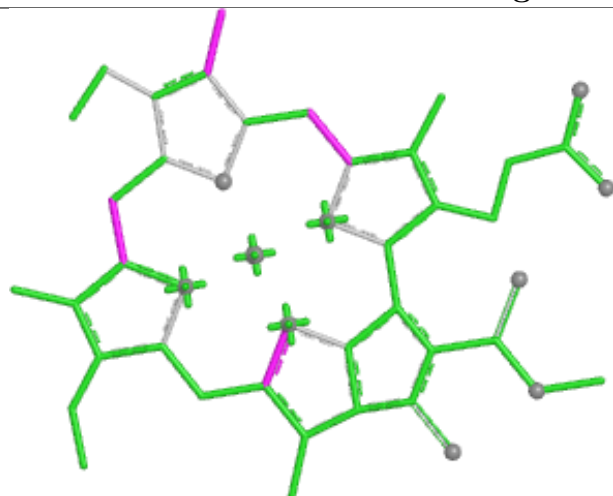
Torsions



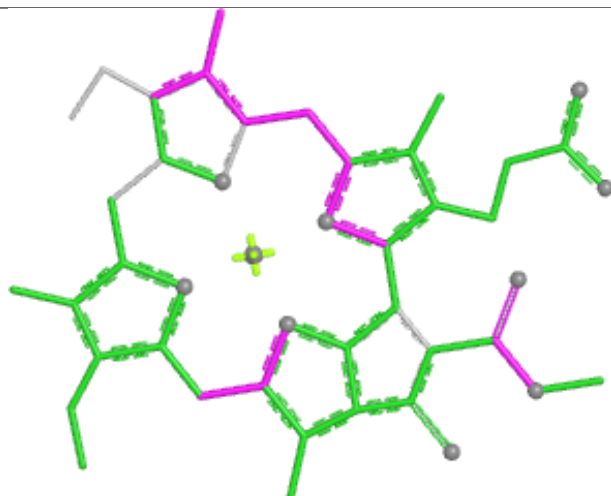
Rings



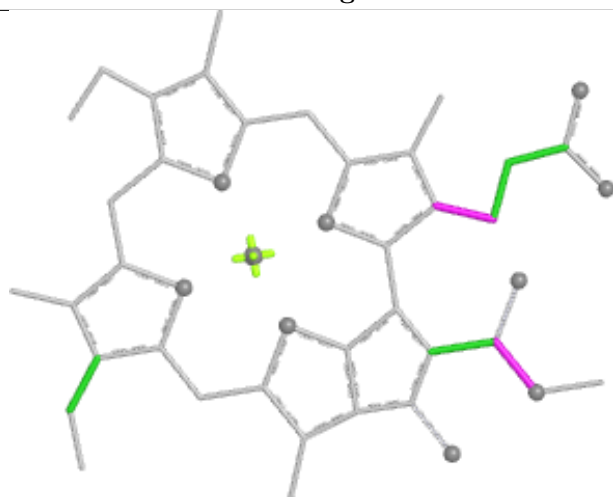
Ligand CLA G 205



Bond lengths



Bond angles

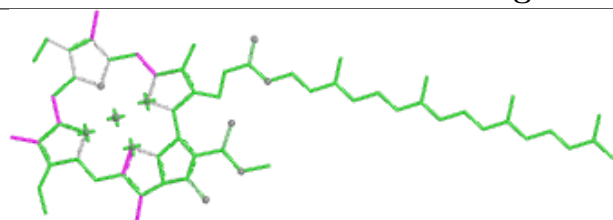


Torsions

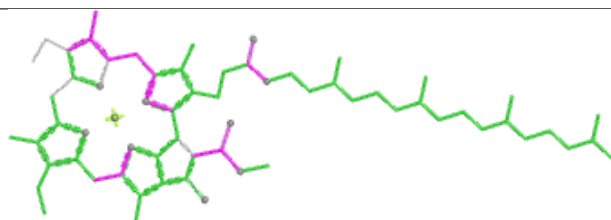


Rings

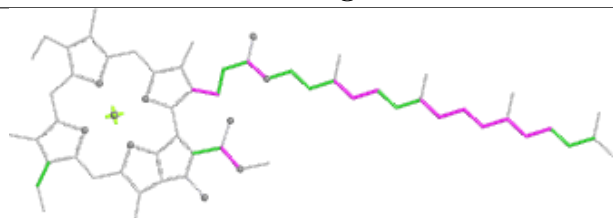
Ligand CLA A 830



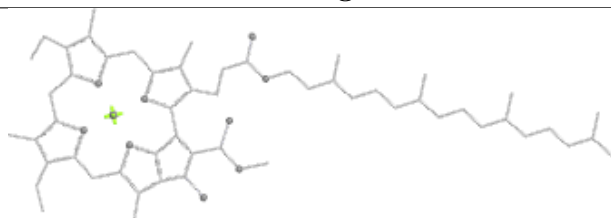
Bond lengths



Bond angles

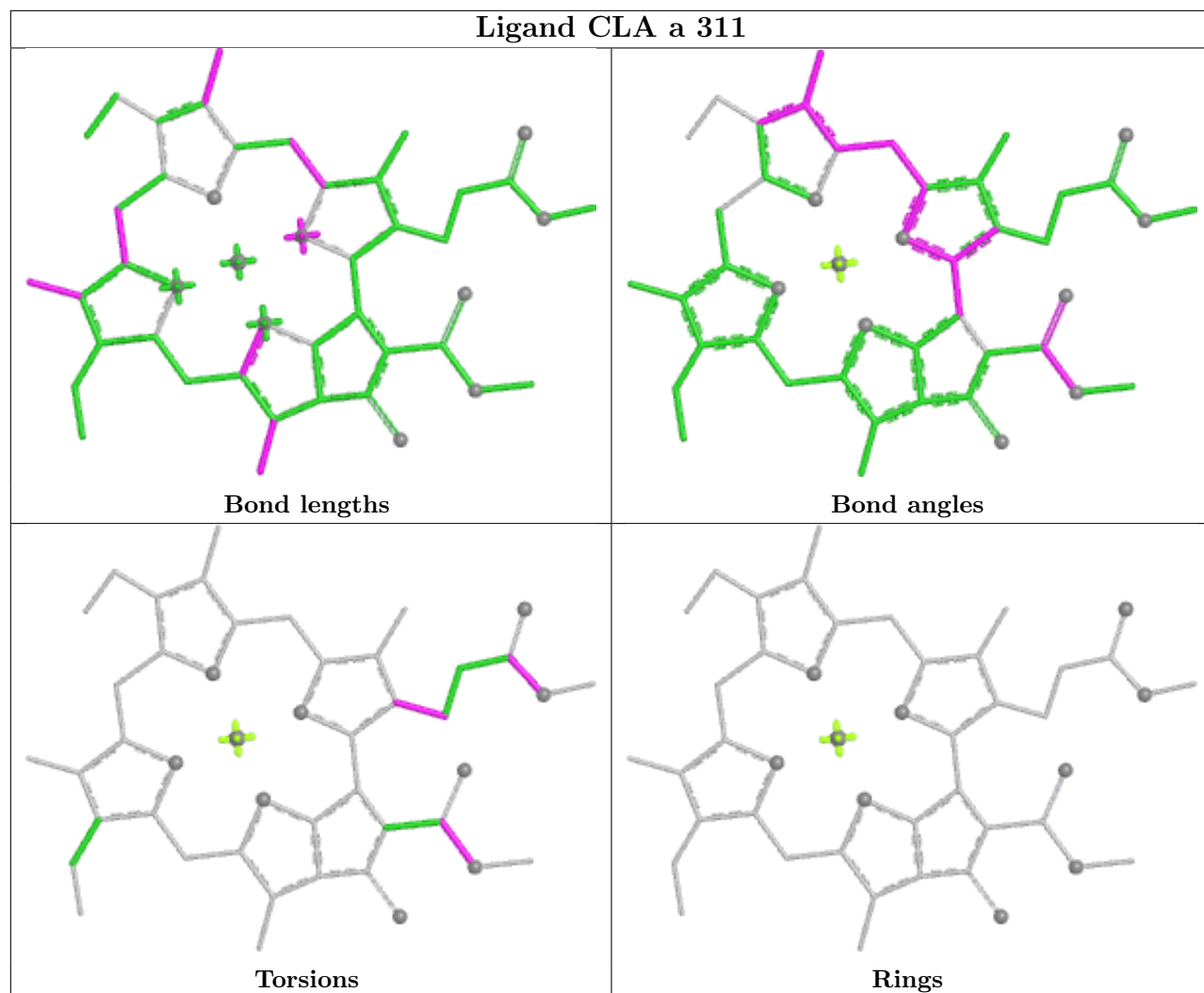


Torsions

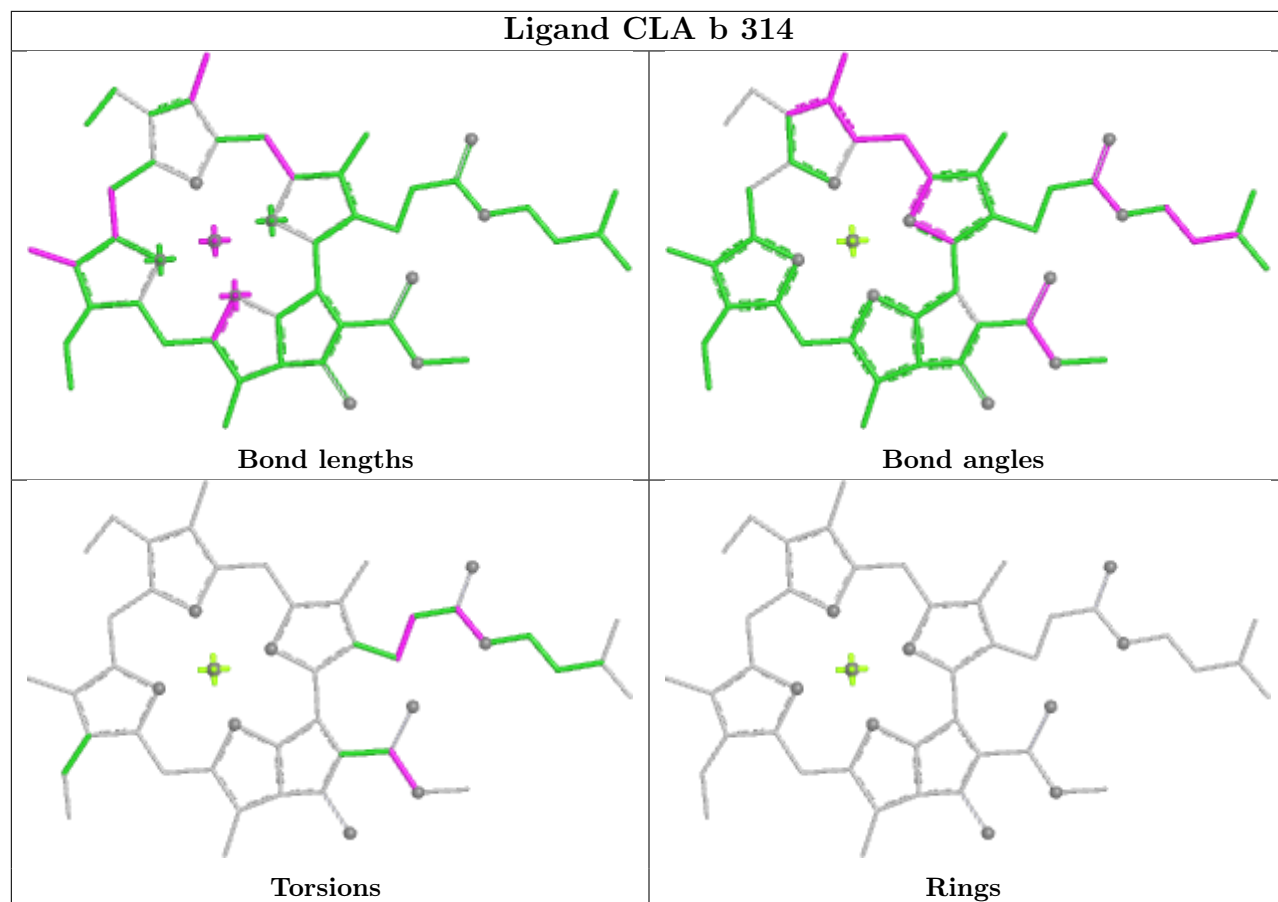


Rings

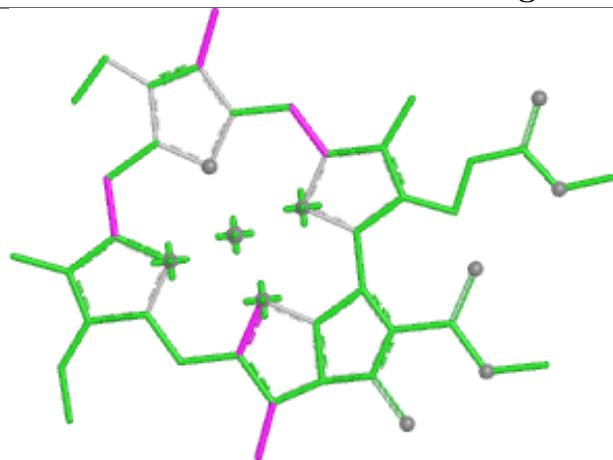
Ligand CLA a 311



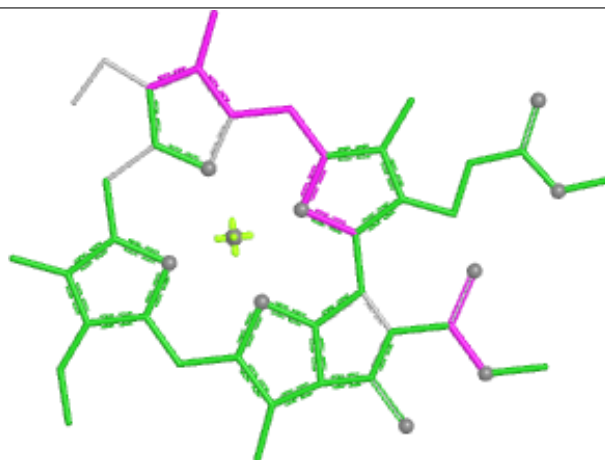
Ligand CLA b 314



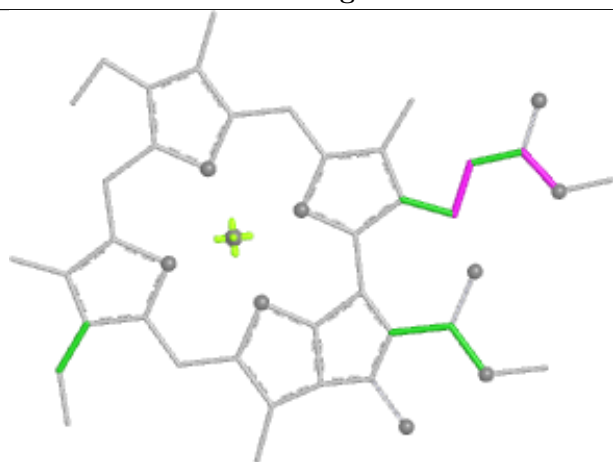
Ligand CLA 9 611



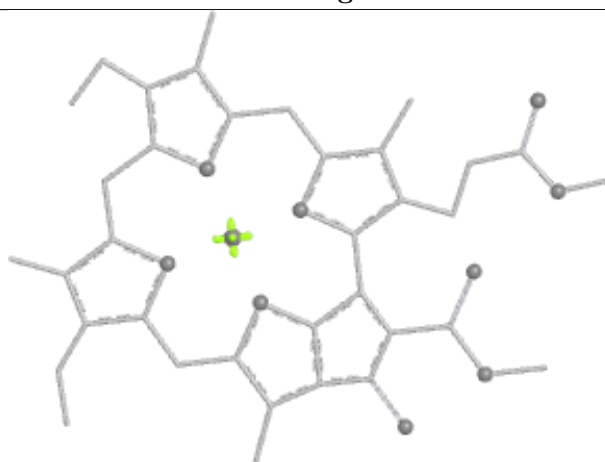
Bond lengths



Bond angles

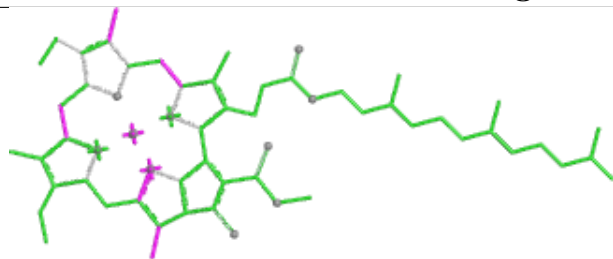


Torsions

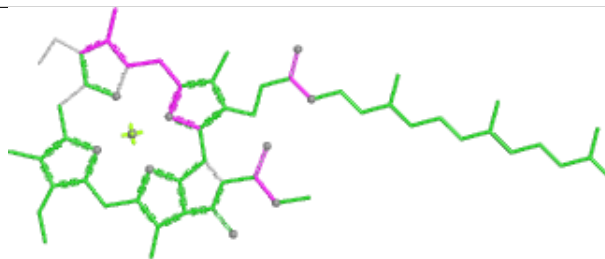


Rings

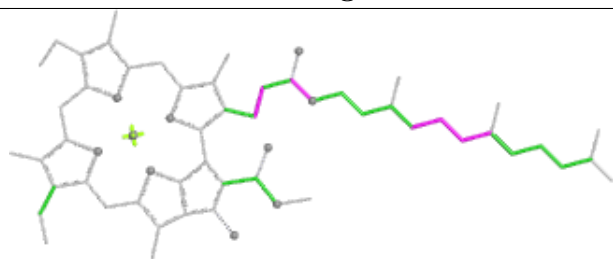
Ligand CLA B 834



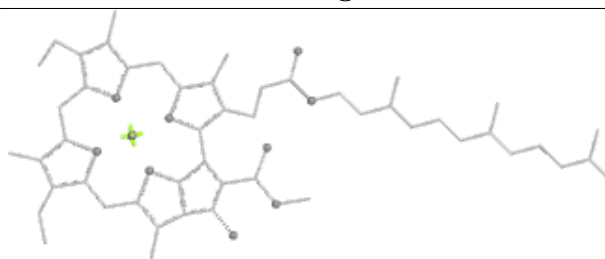
Bond lengths



Bond angles

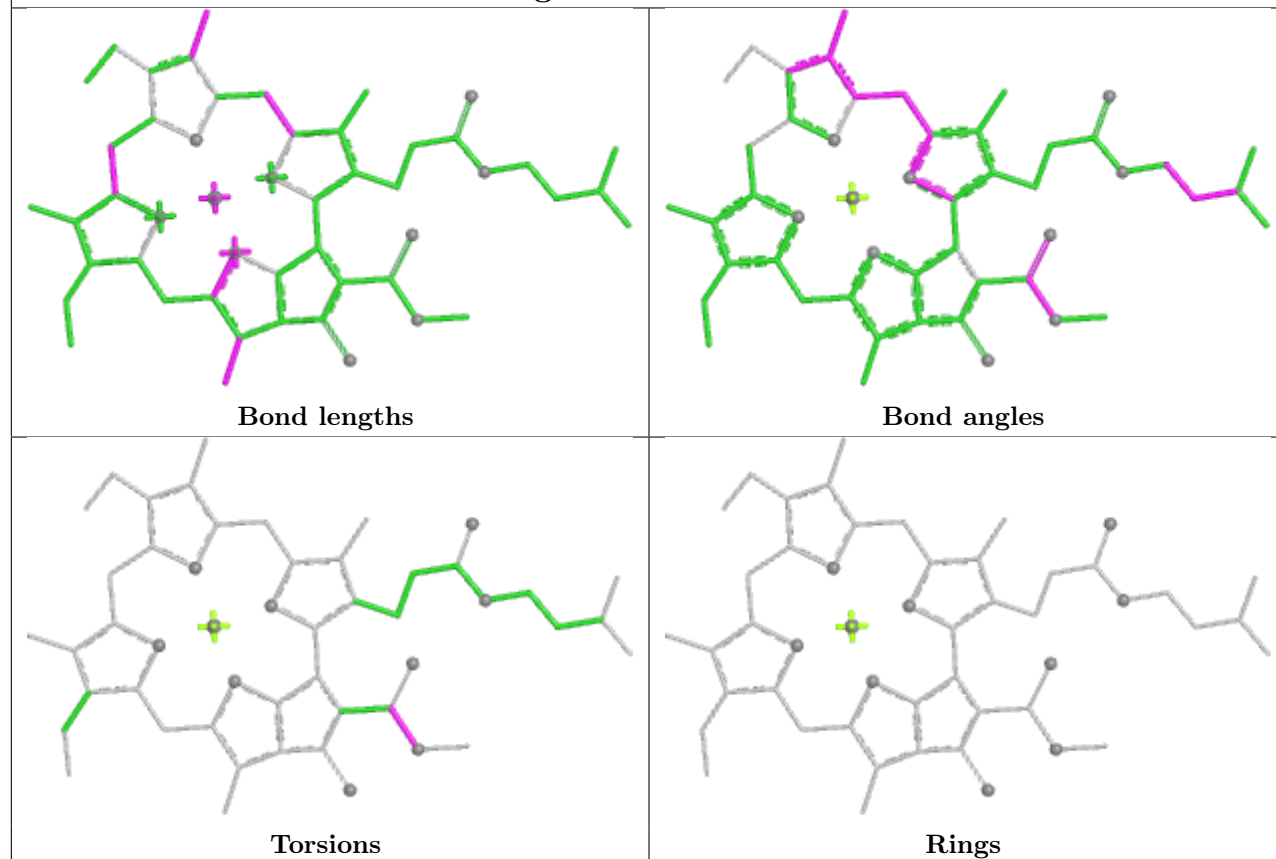


Torsions

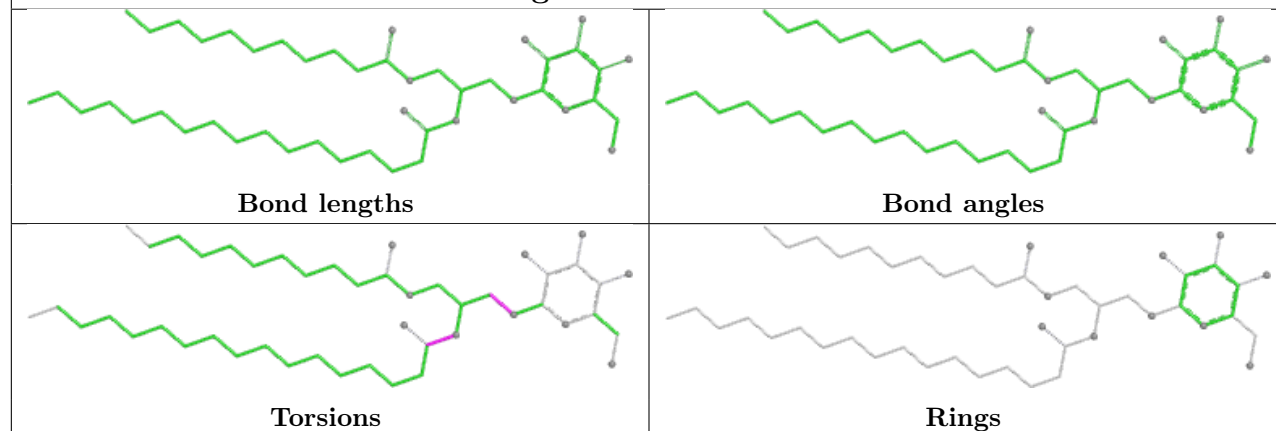


Rings

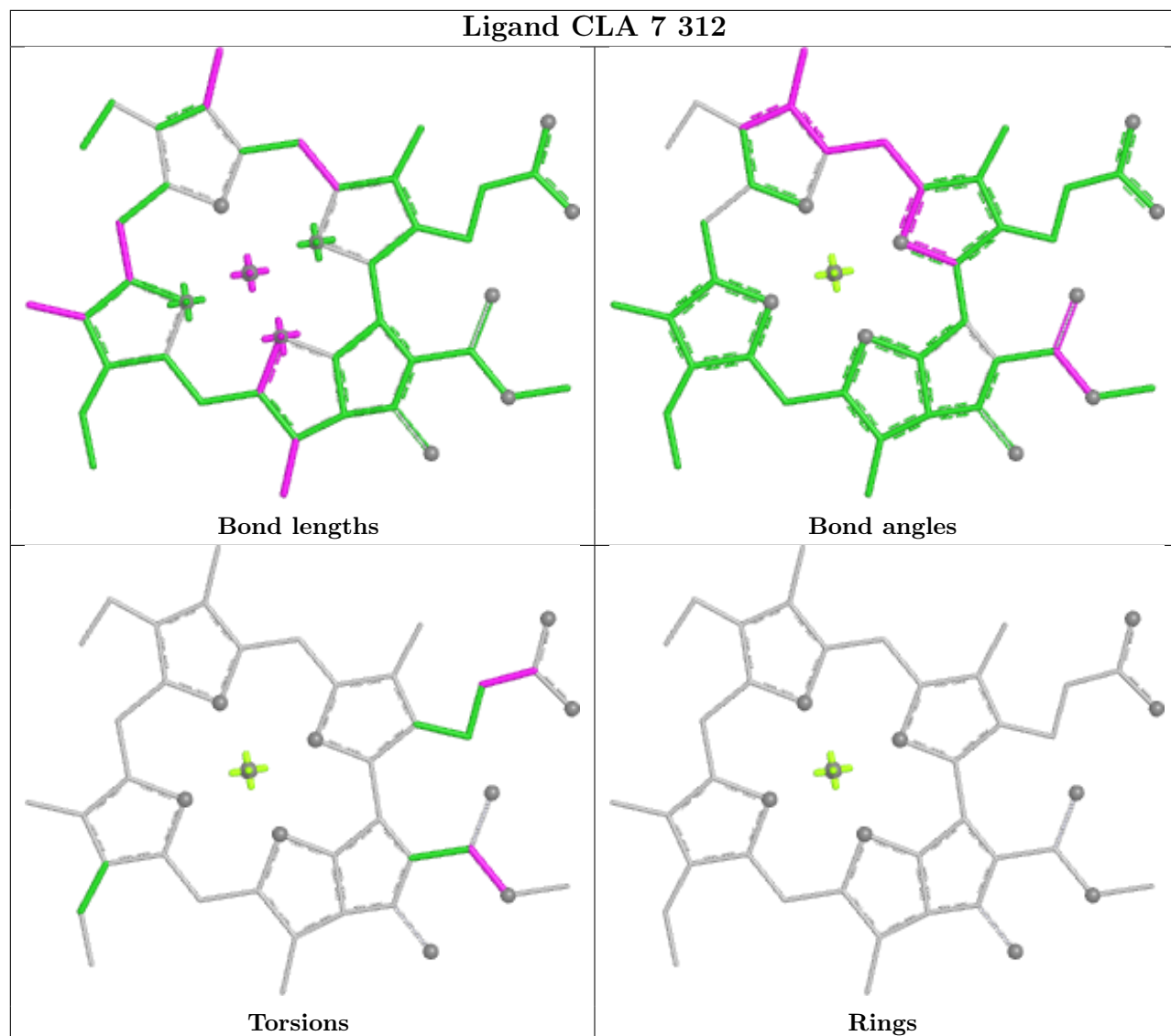
Ligand CLA L 301



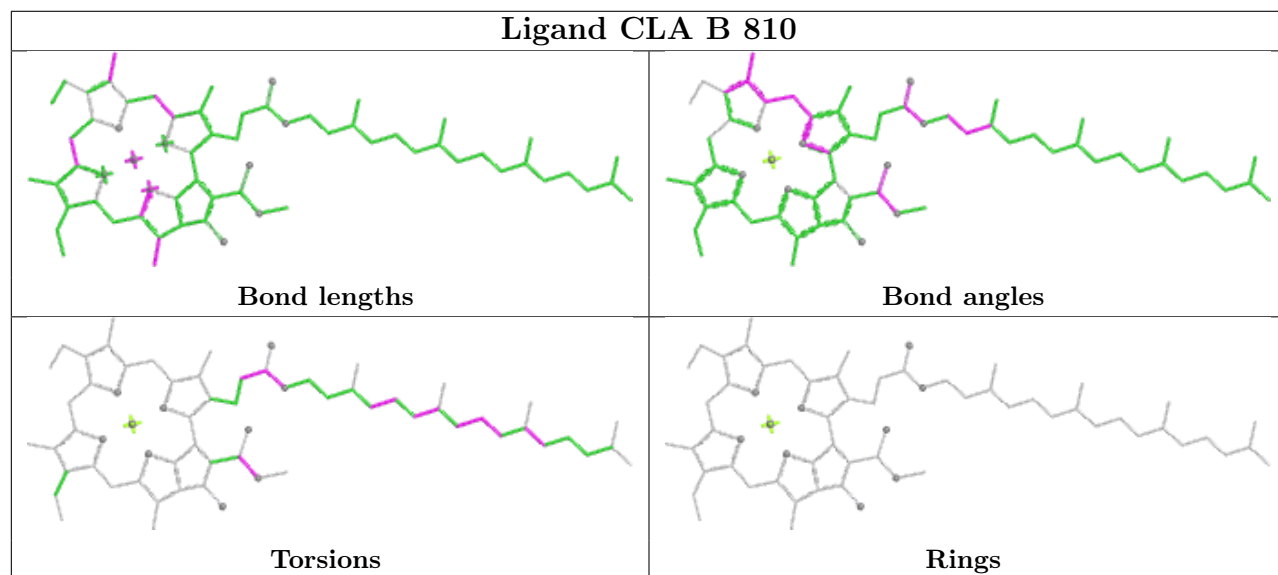
Ligand LMG 7 320



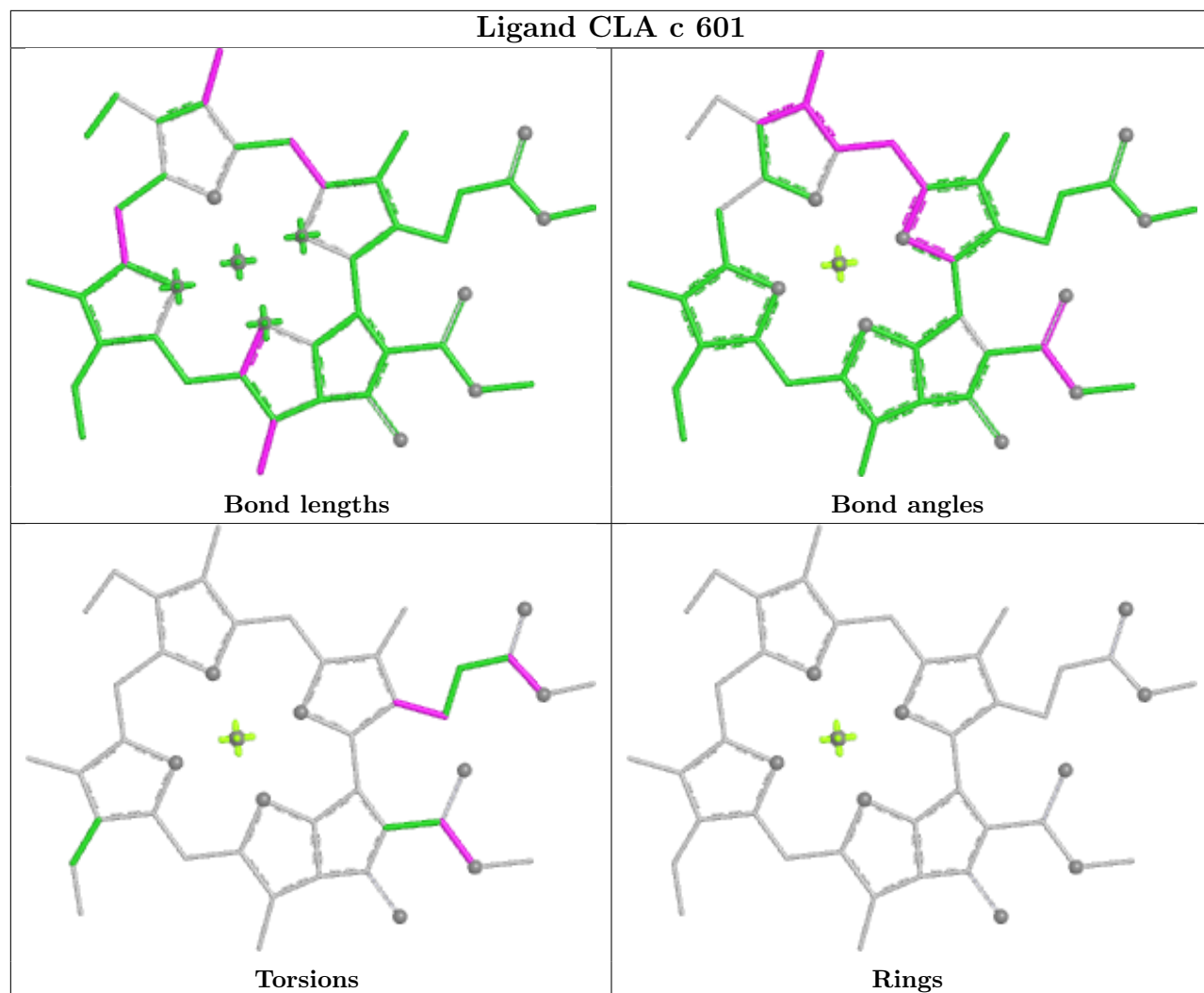
Ligand CLA 7 312



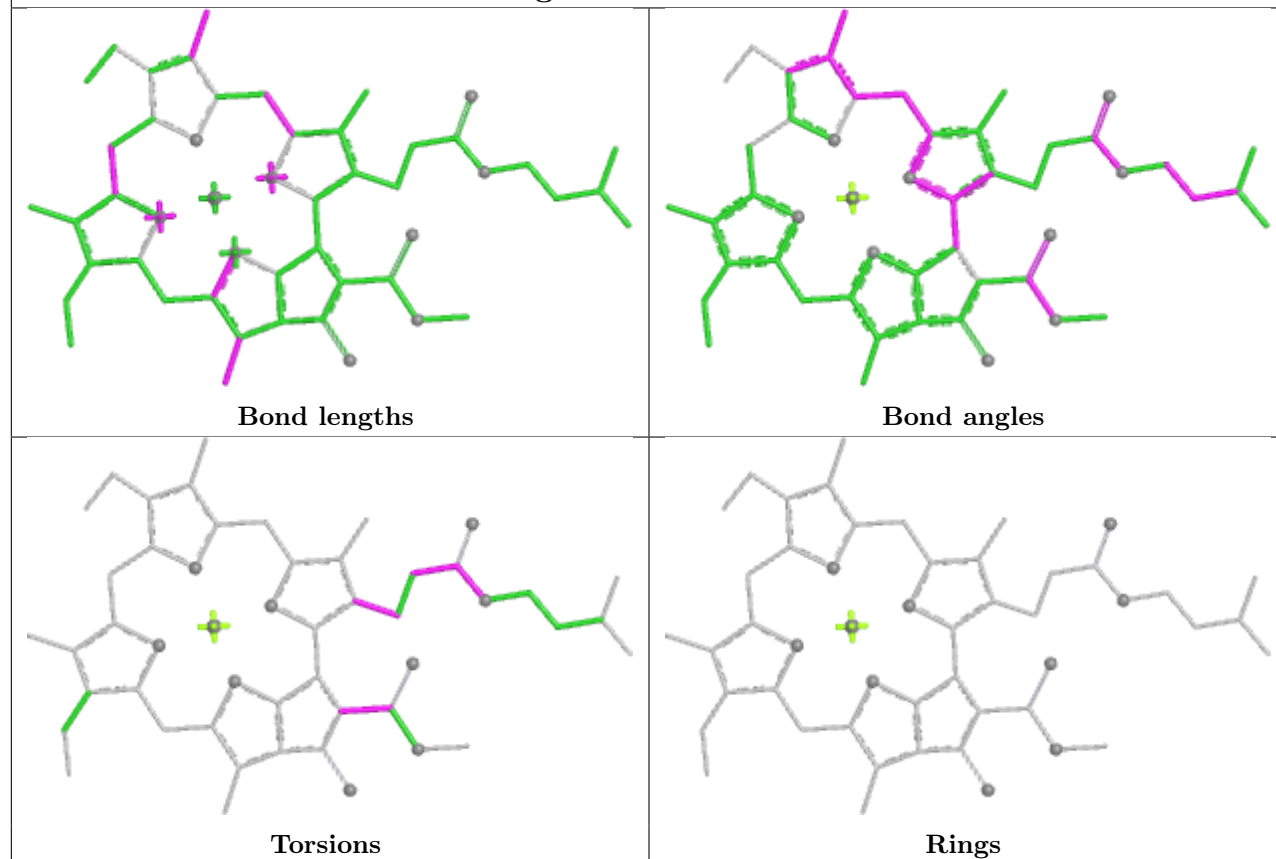
Ligand CLA B 810



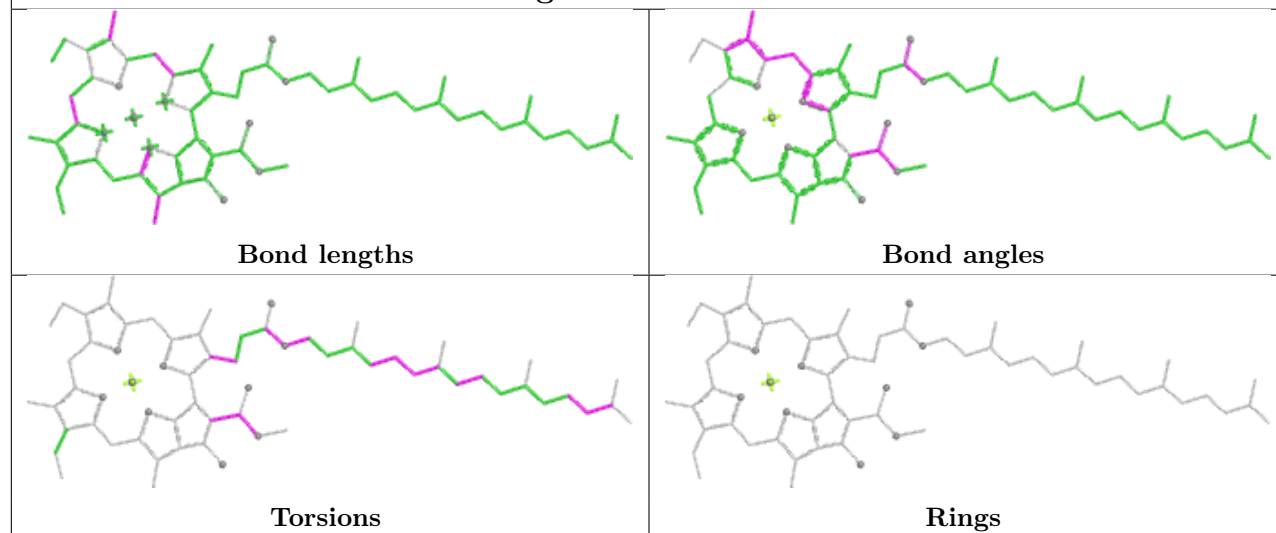
Ligand CLA c 601



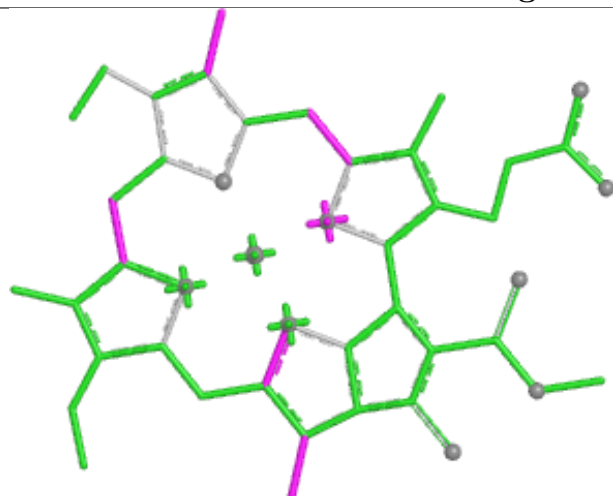
Ligand CLA b 313



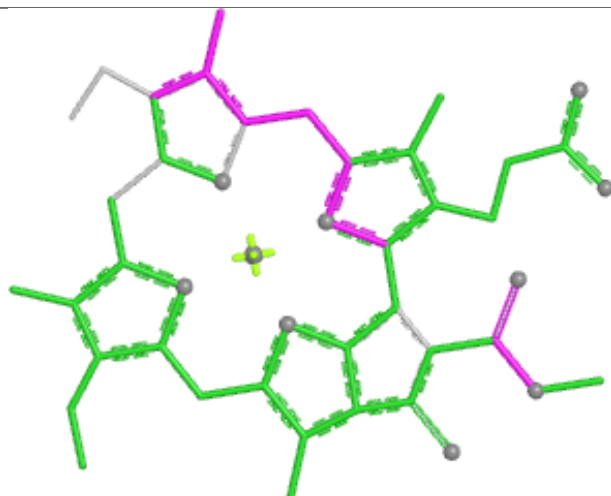
Ligand CLA 9 607



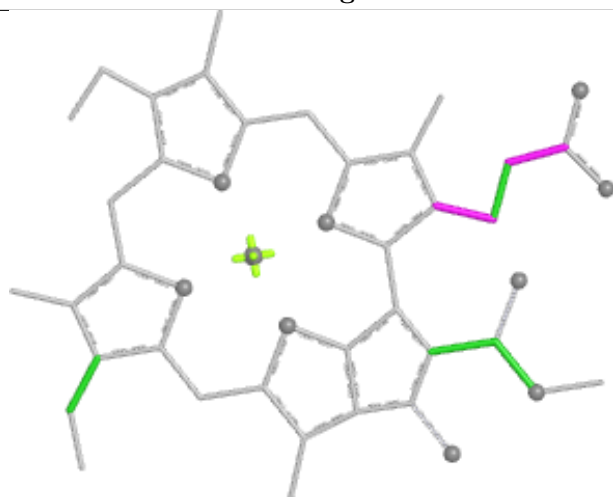
Ligand CLA 2 612



Bond lengths



Bond angles

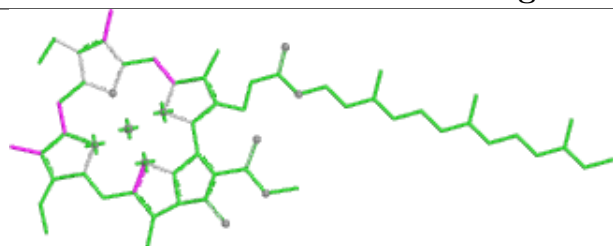


Torsions

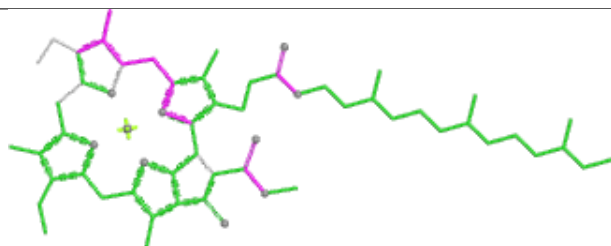


Rings

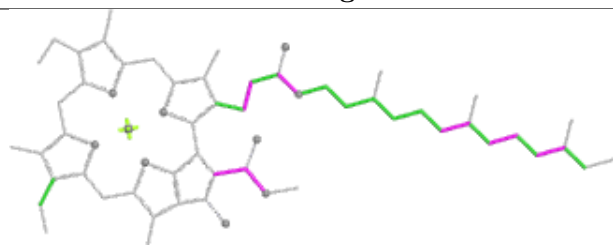
Ligand CLA 1 301



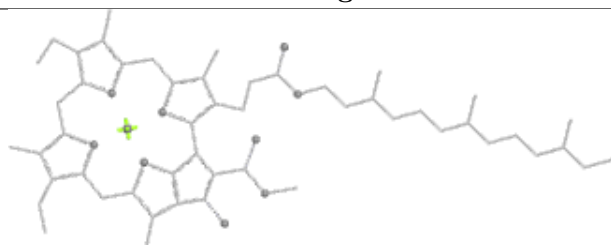
Bond lengths



Bond angles

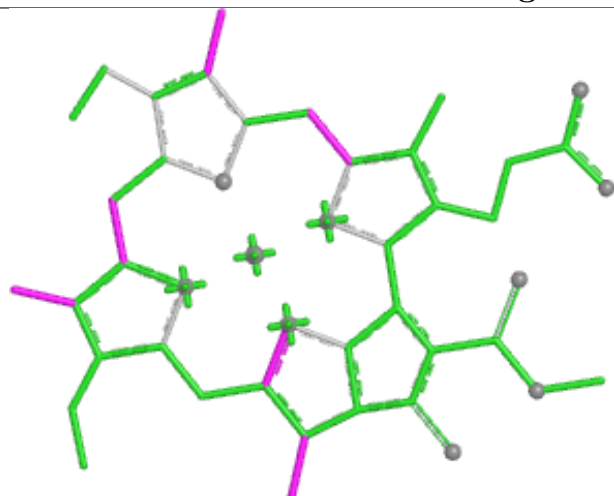


Torsions

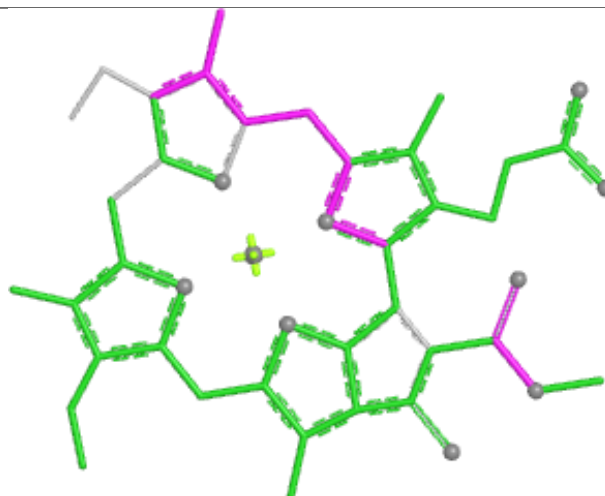


Rings

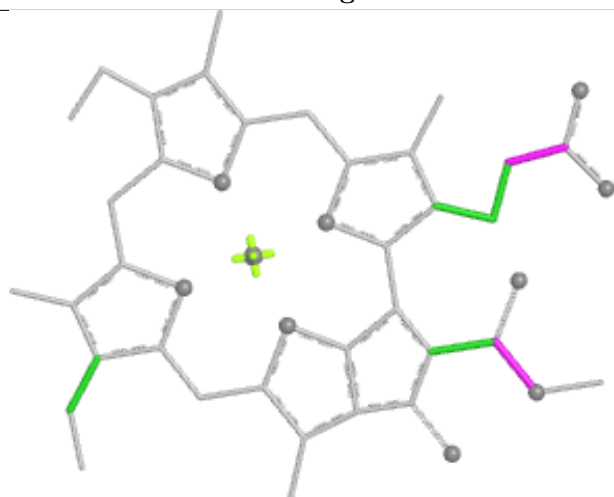
Ligand CLA 1 304



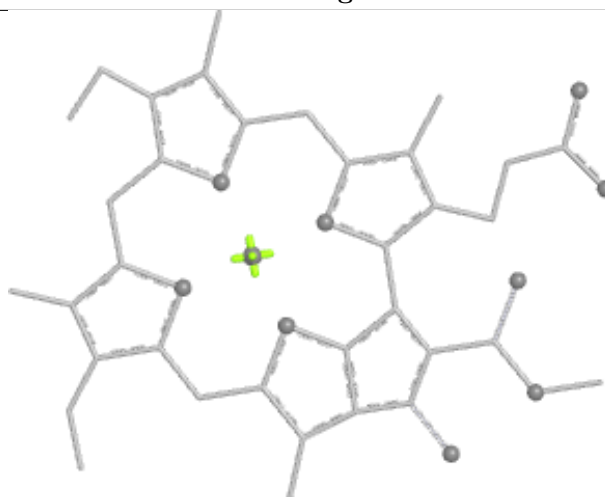
Bond lengths



Bond angles

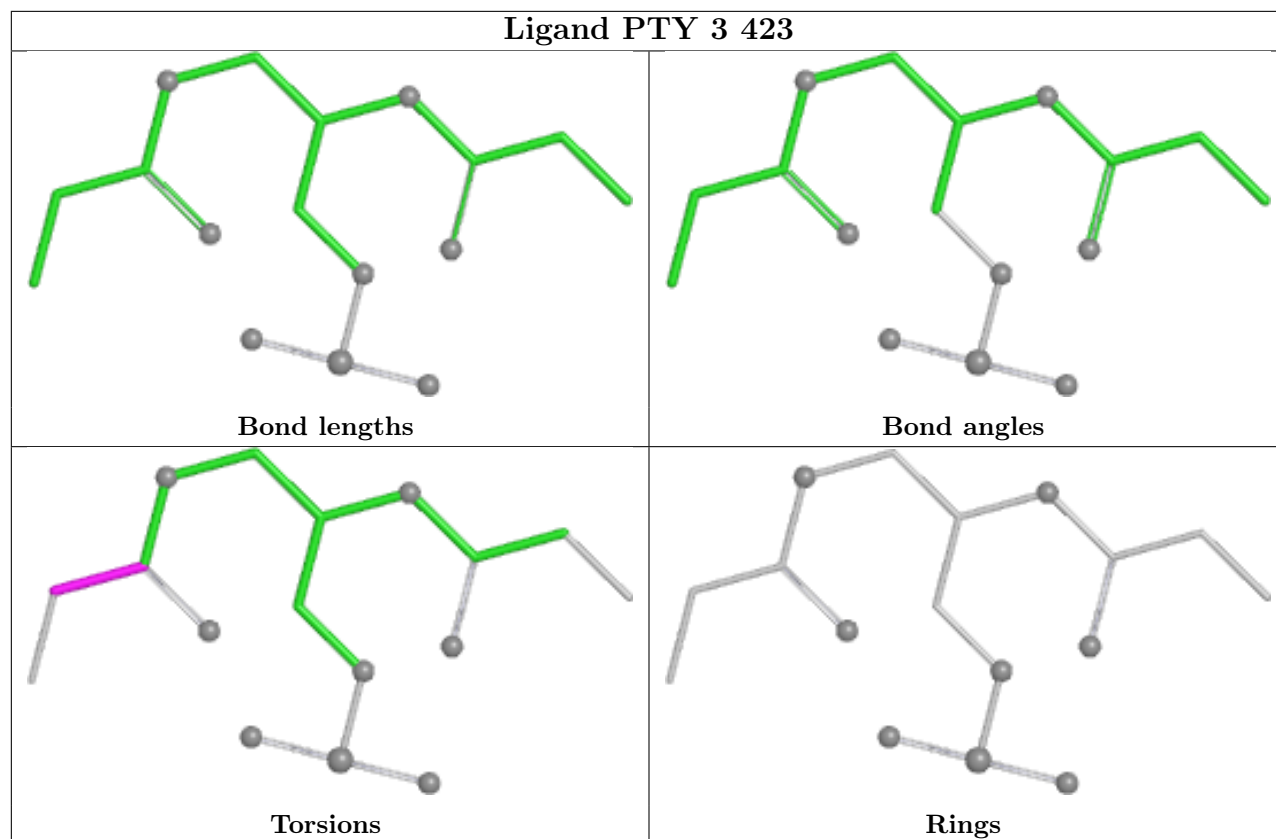


Torsions

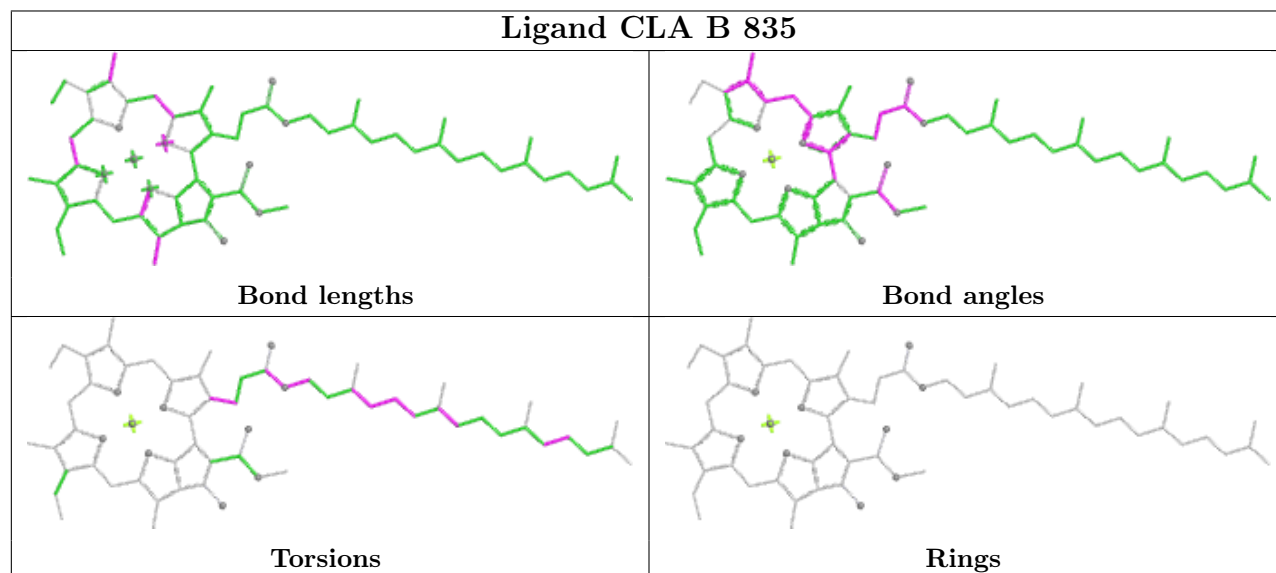


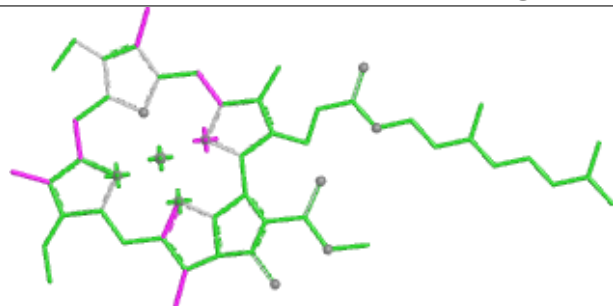
Rings

Ligand PTY 3 423

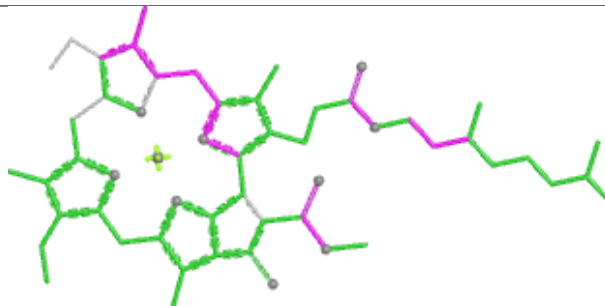


Ligand CLA B 835

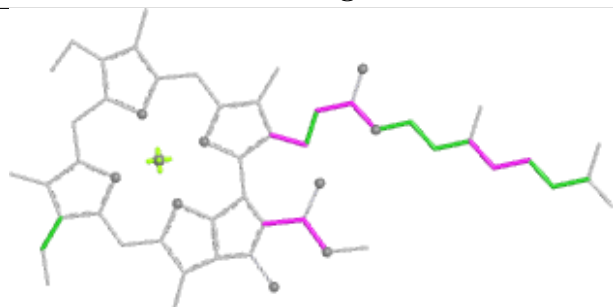


Ligand CLA B 836

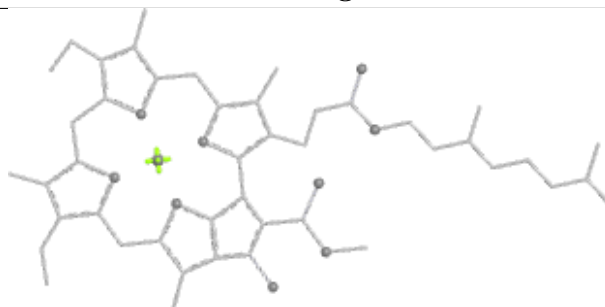
Bond lengths



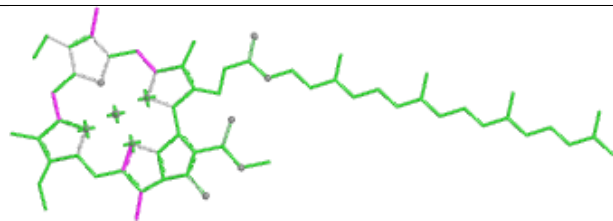
Bond angles



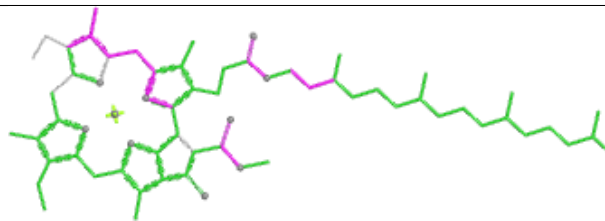
Torsions



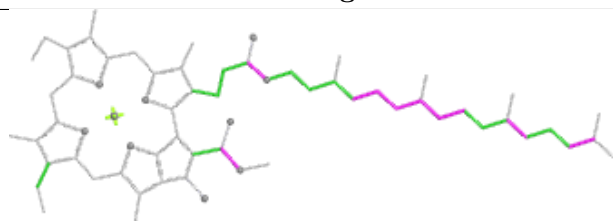
Rings

Ligand CLA A 816

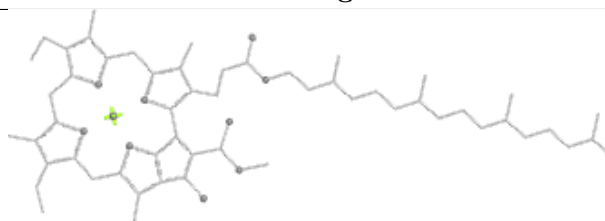
Bond lengths



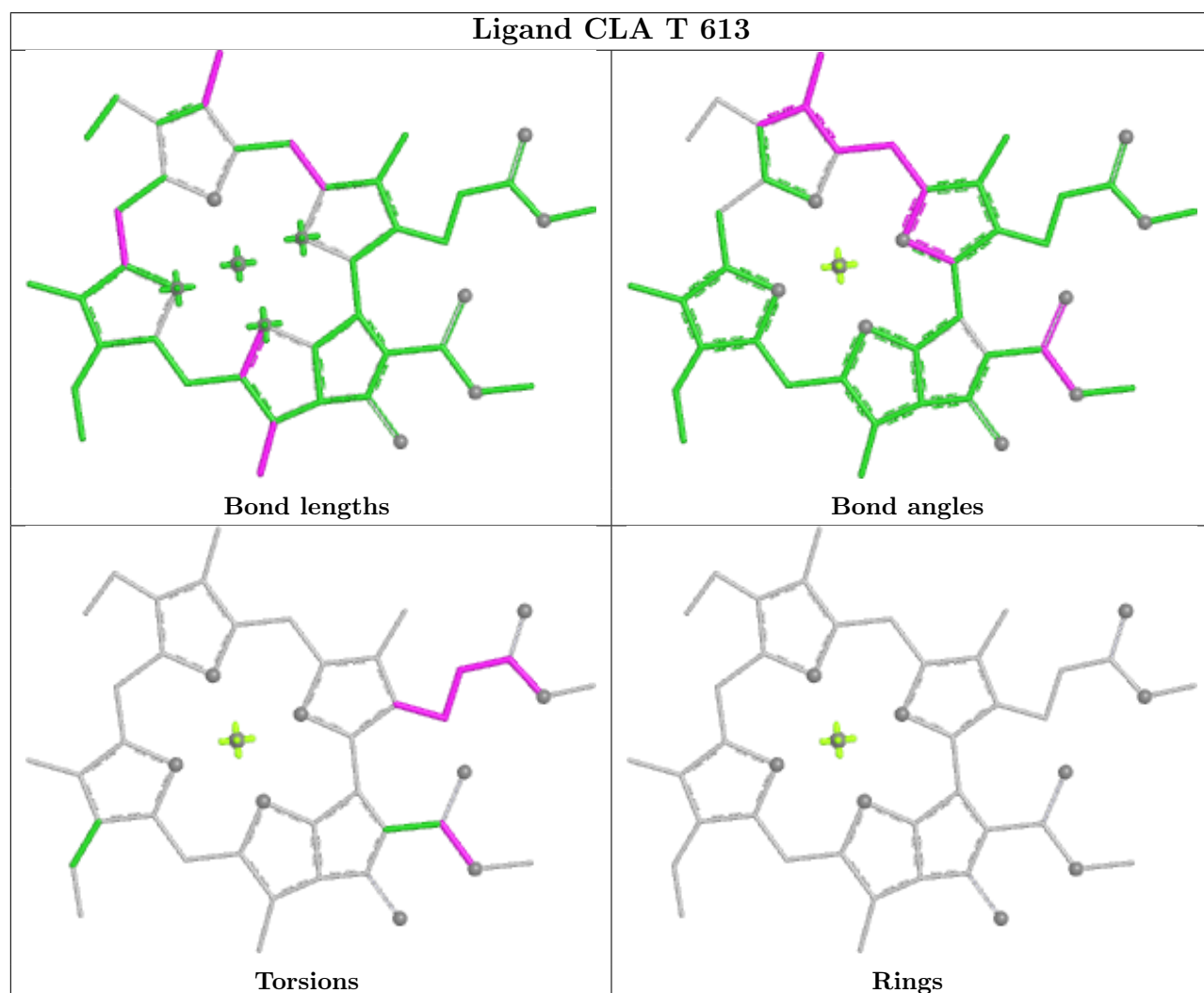
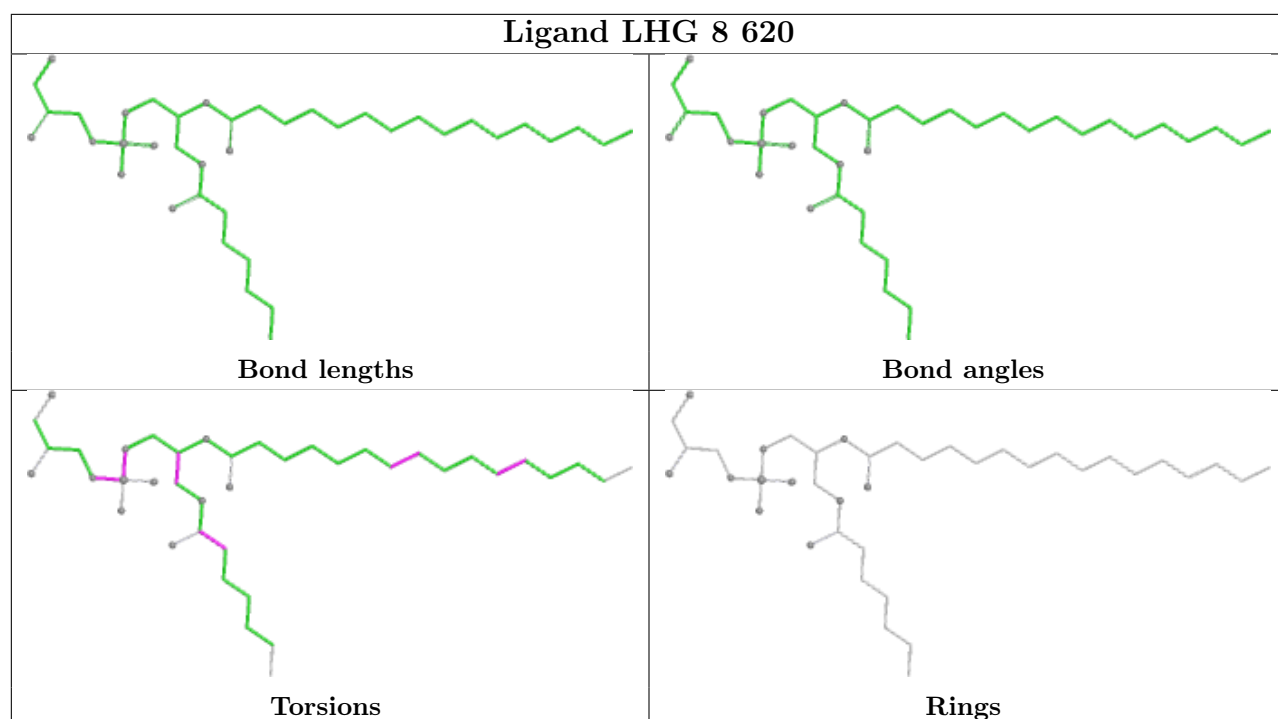
Bond angles



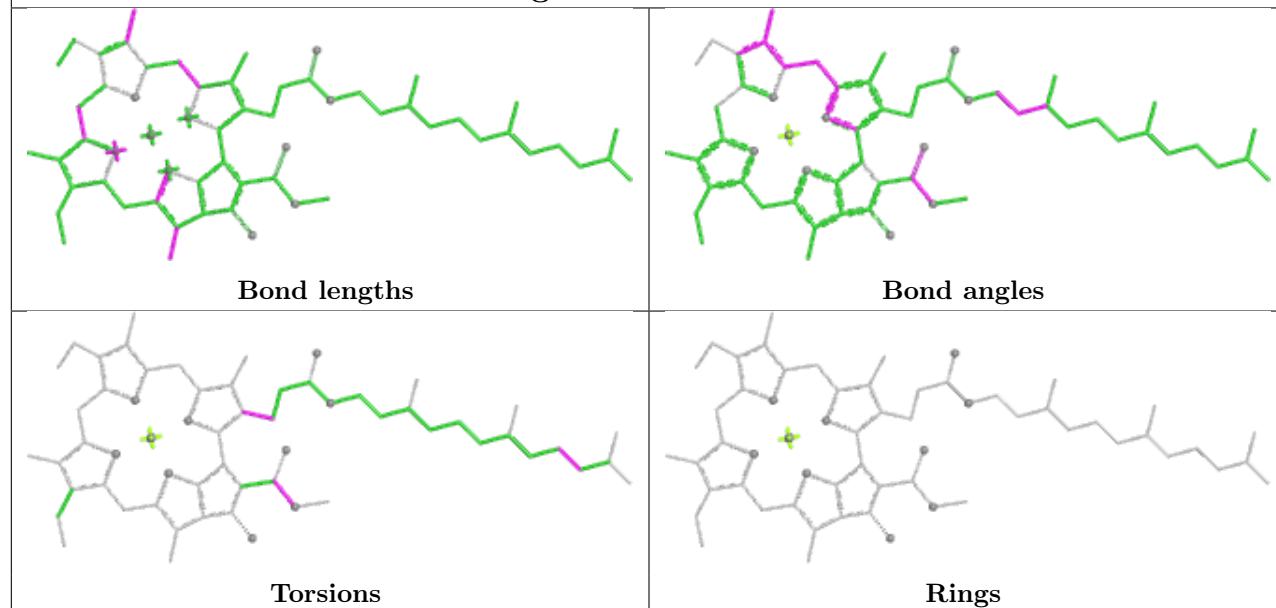
Torsions



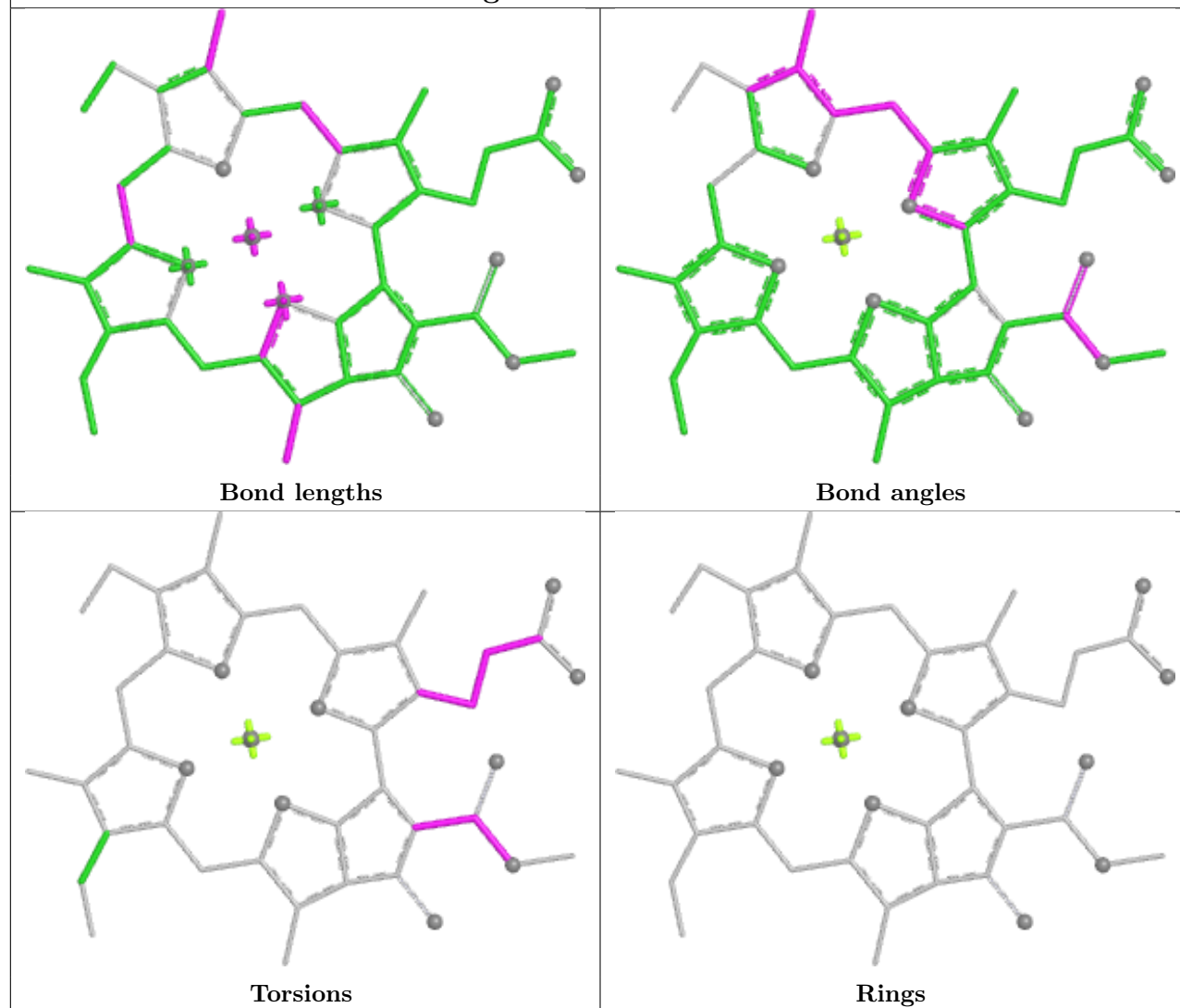
Rings

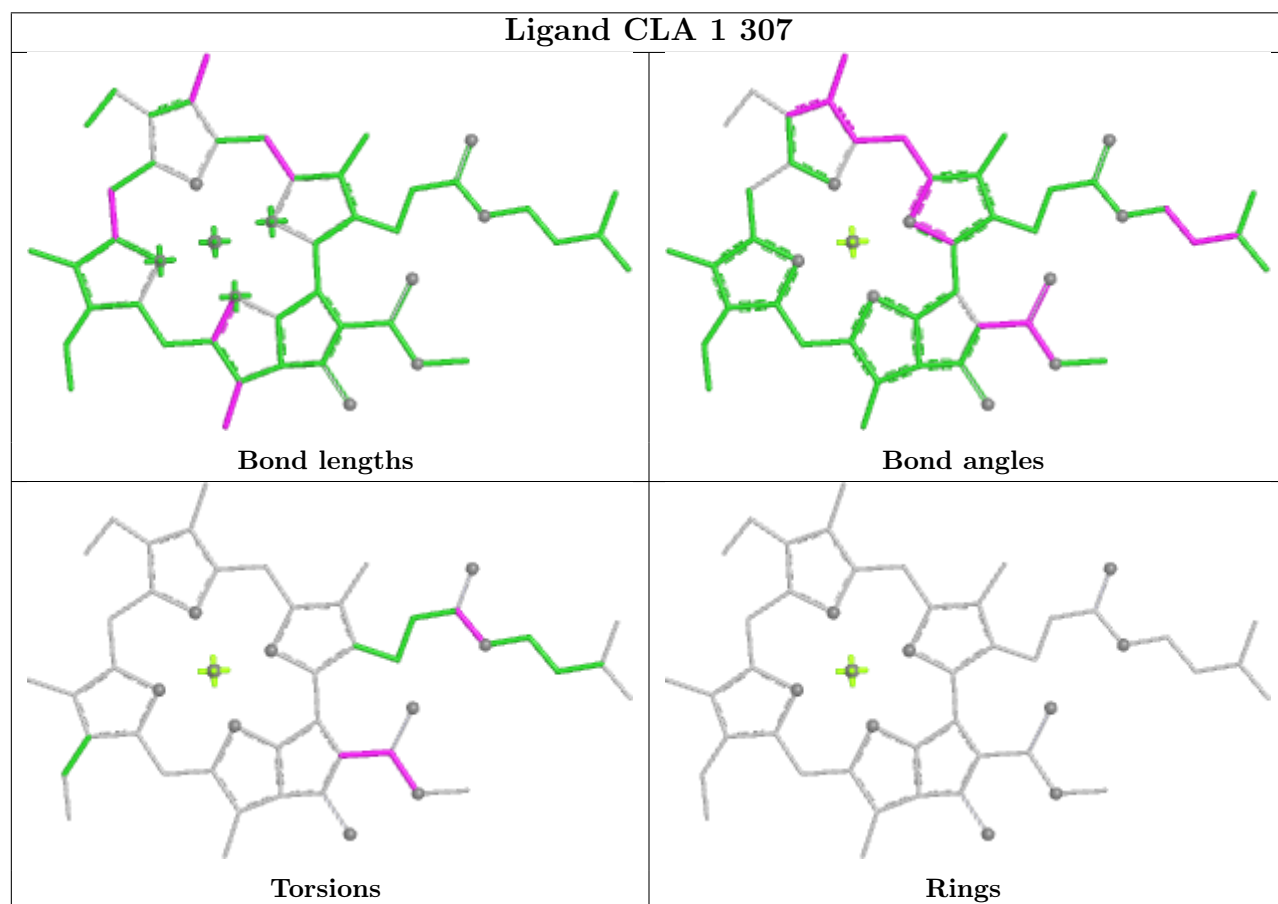
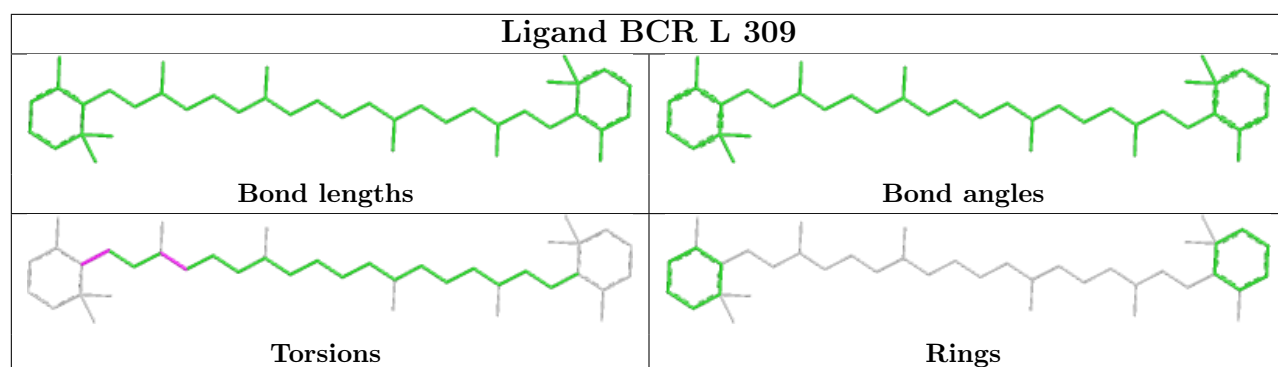


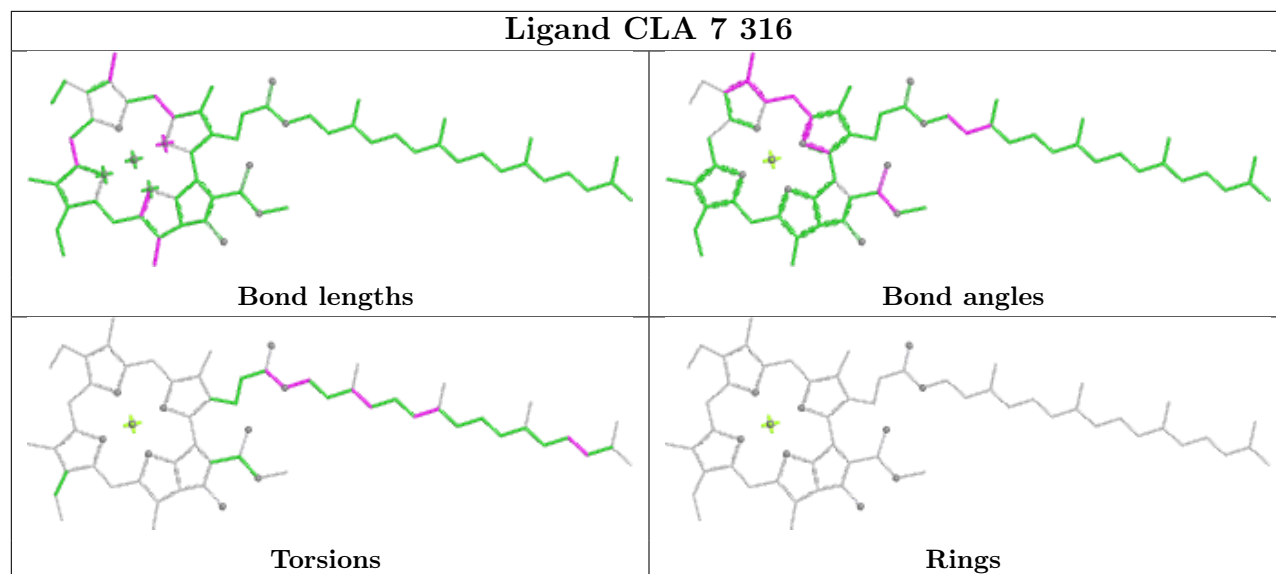
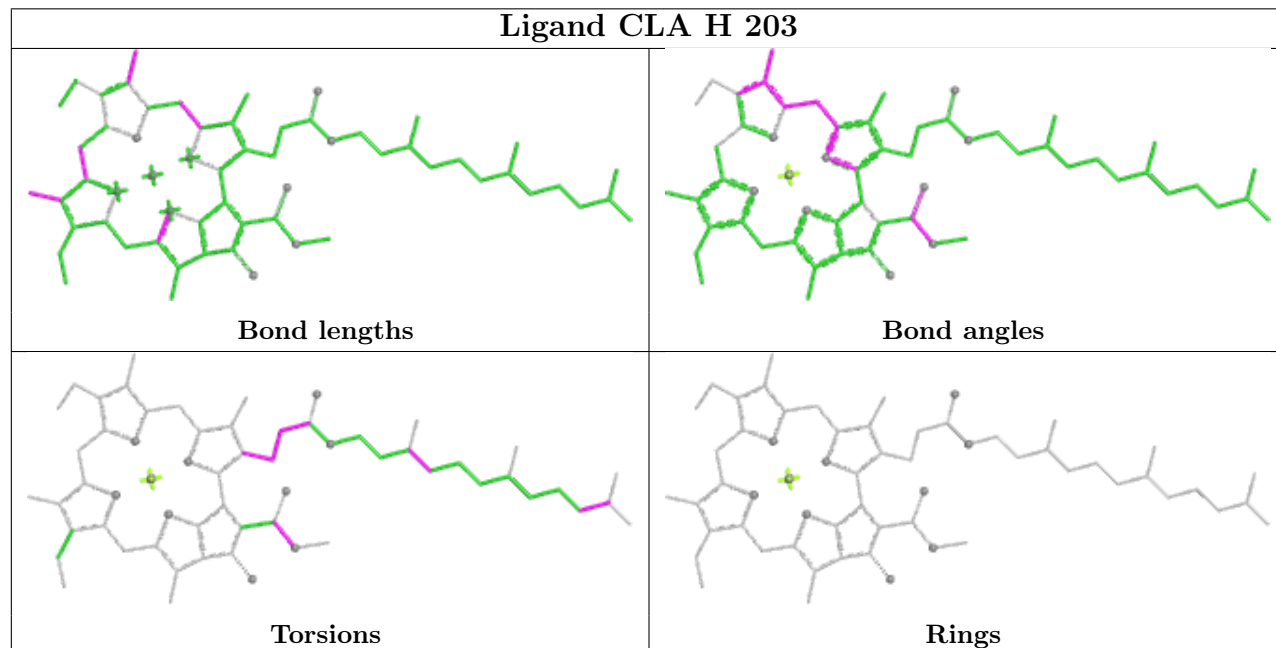
Ligand CLA A 840



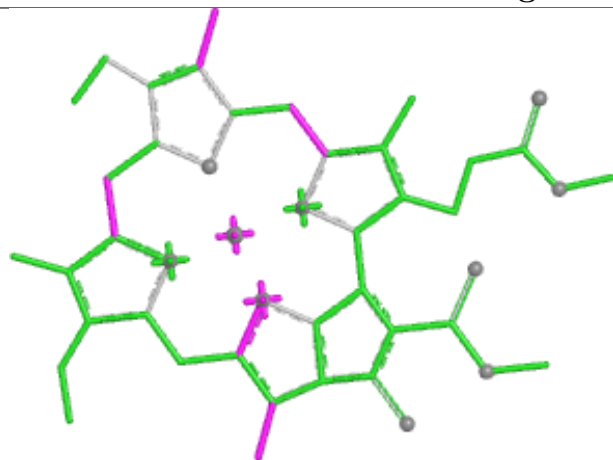
Ligand CLA O 2003



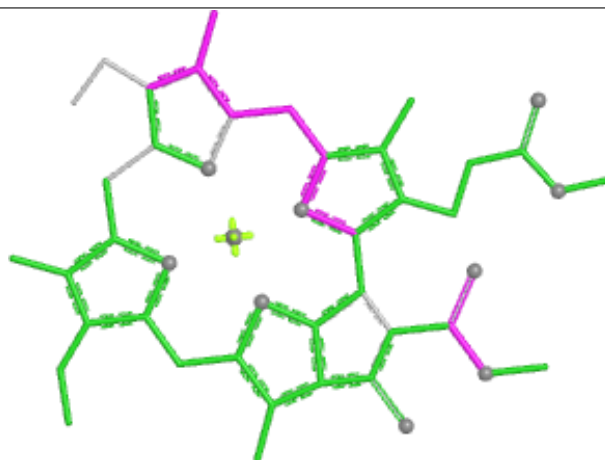


Ligand CLA 7 316**Ligand CLA H 203**

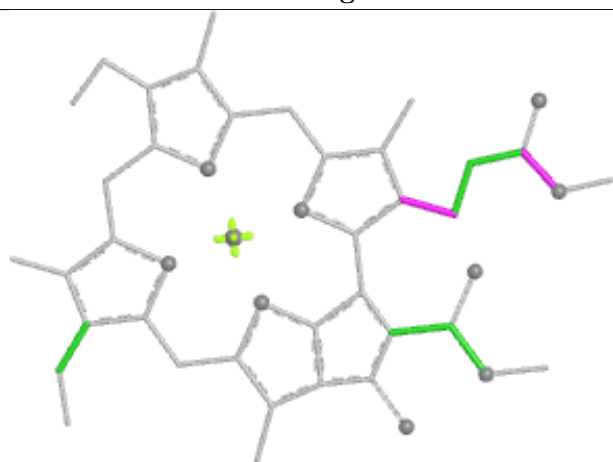
Ligand CLA 3 414



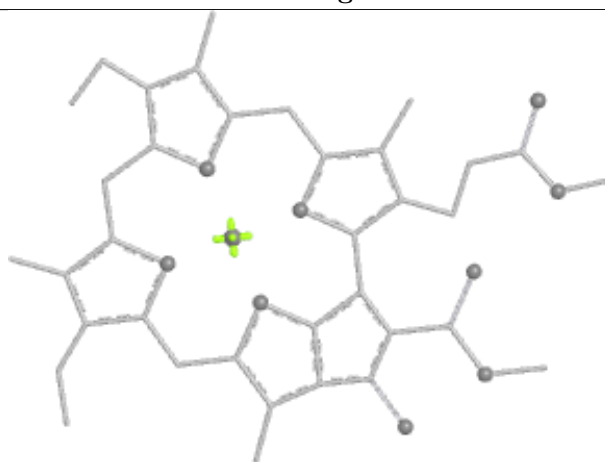
Bond lengths



Bond angles

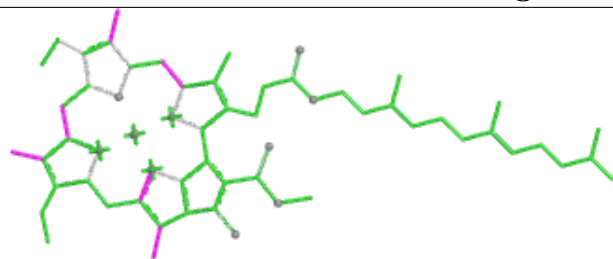


Torsions

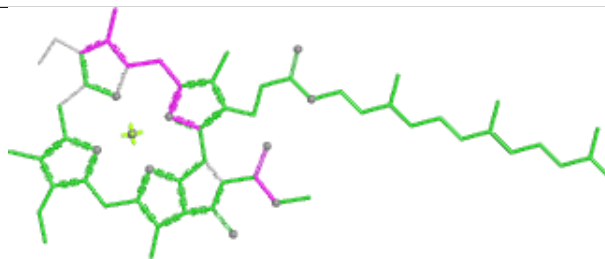


Rings

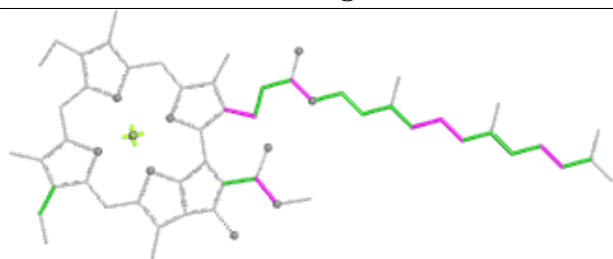
Ligand CLA B 814



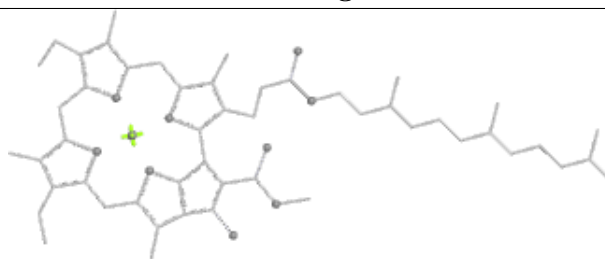
Bond lengths



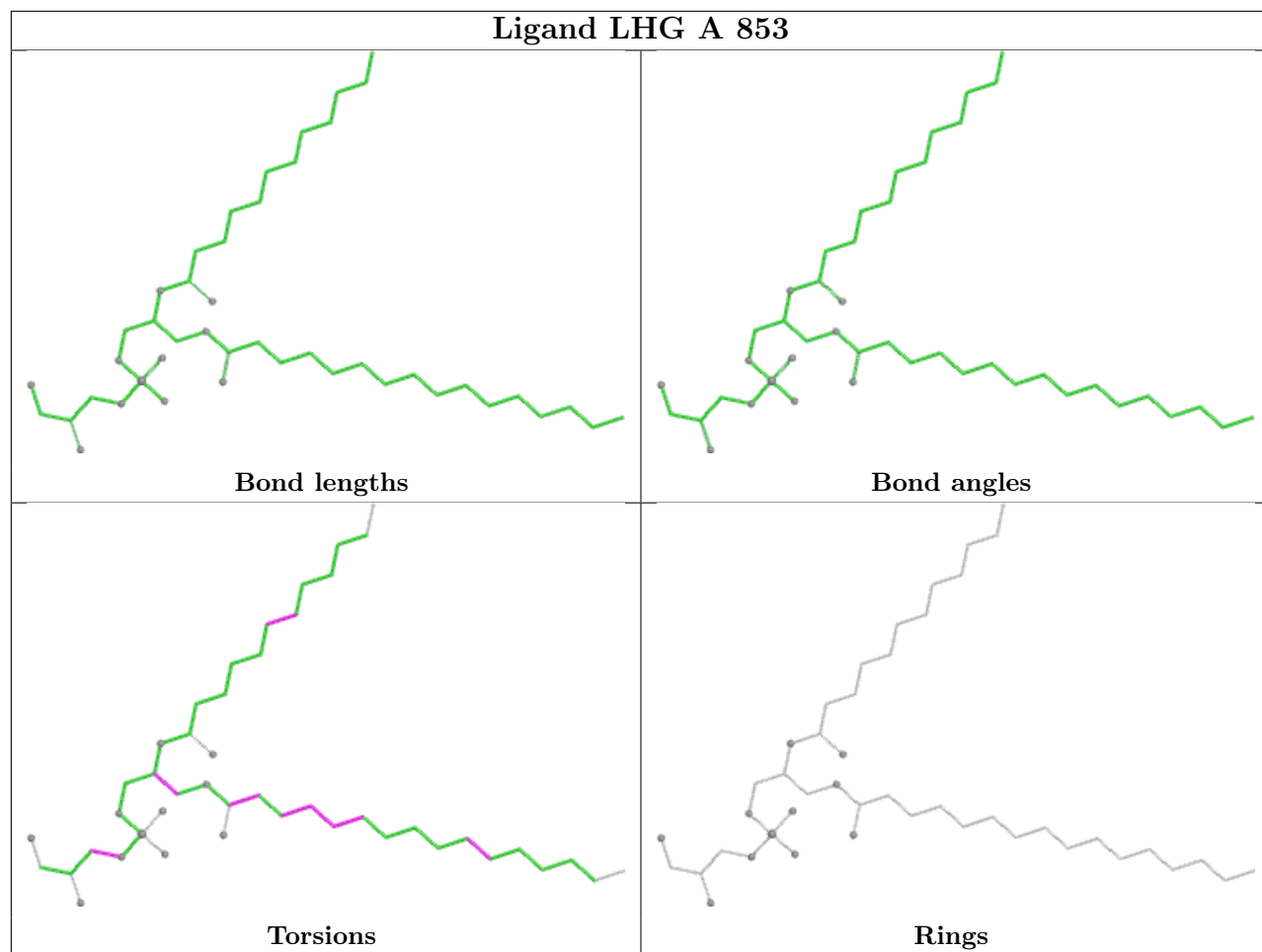
Bond angles

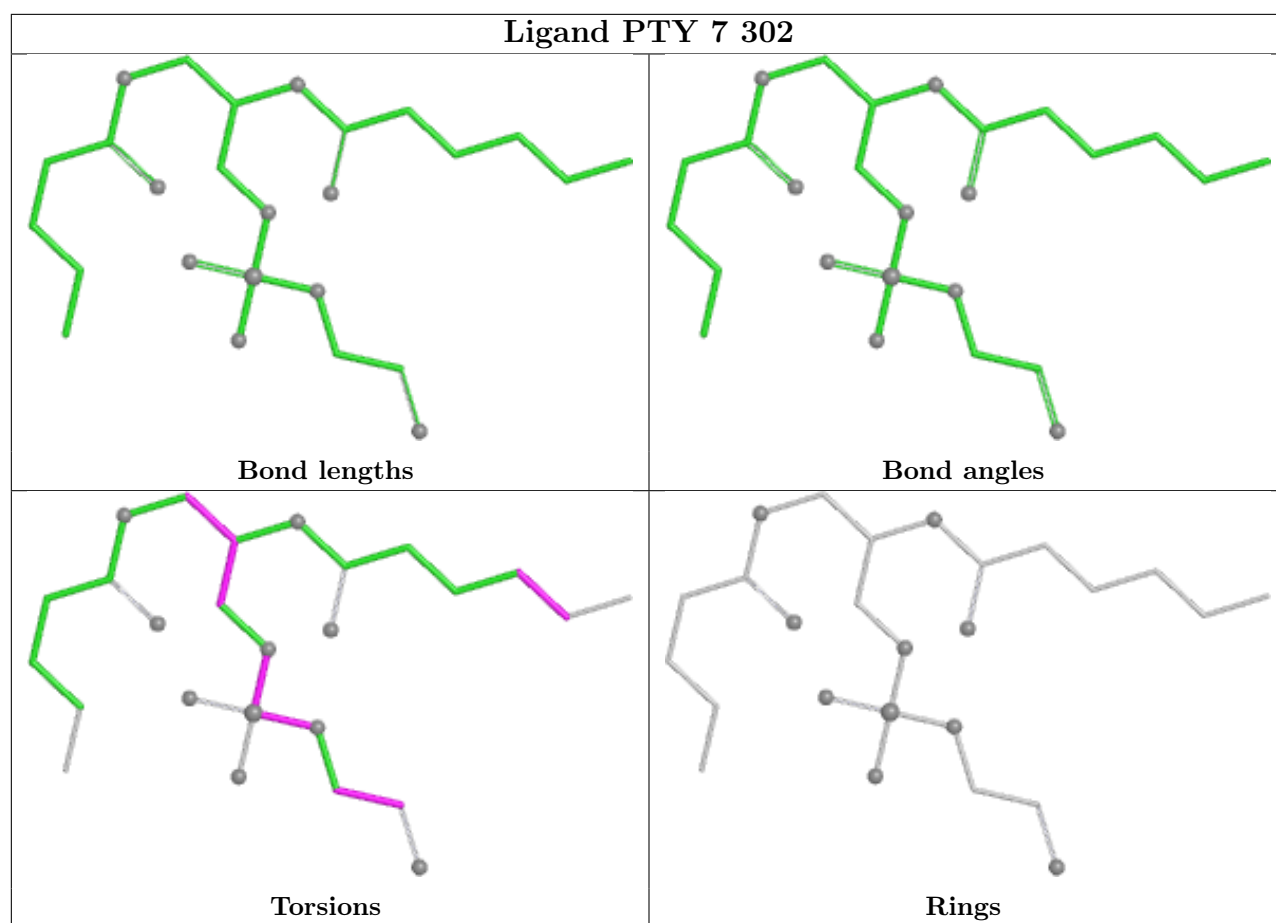


Torsions

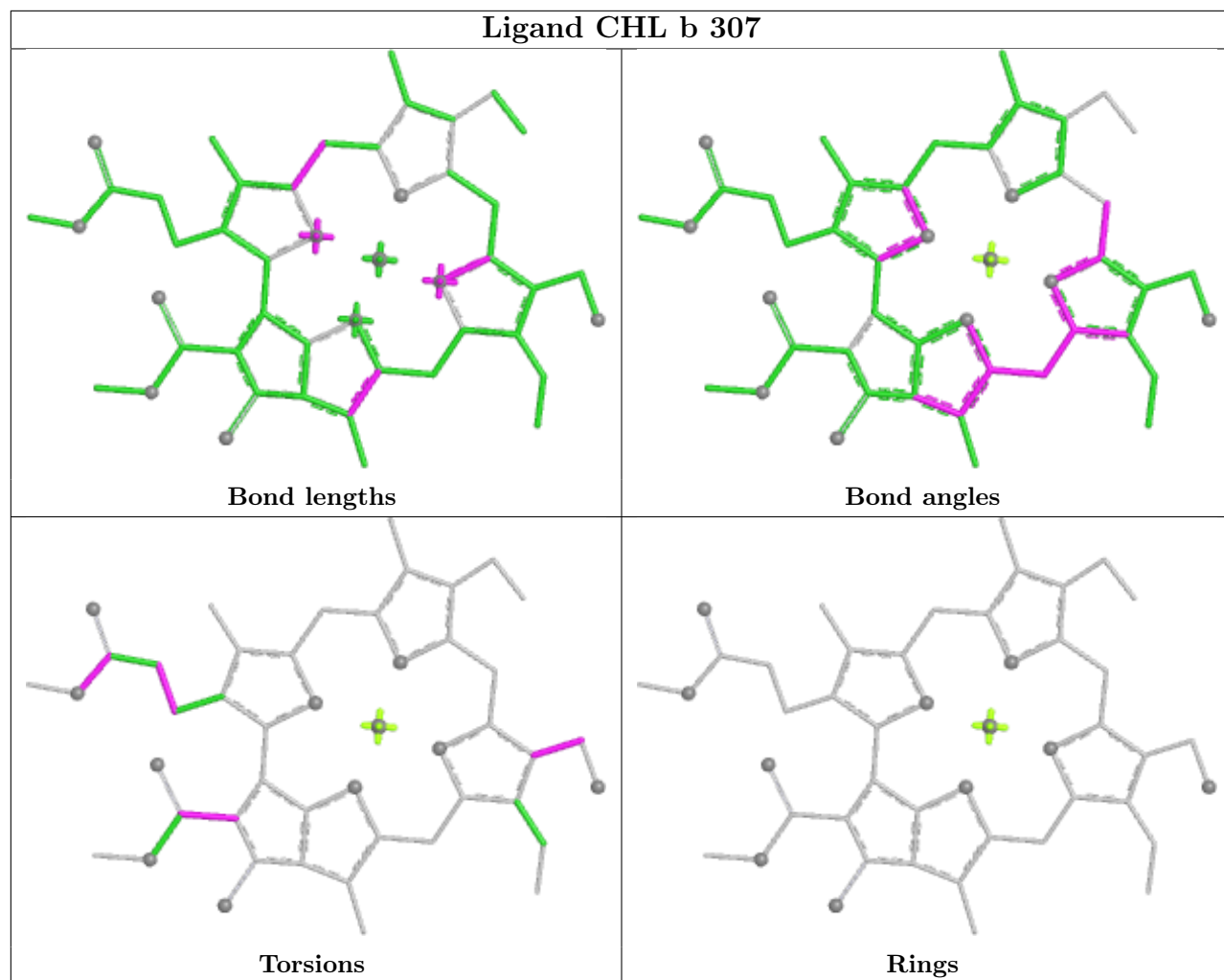


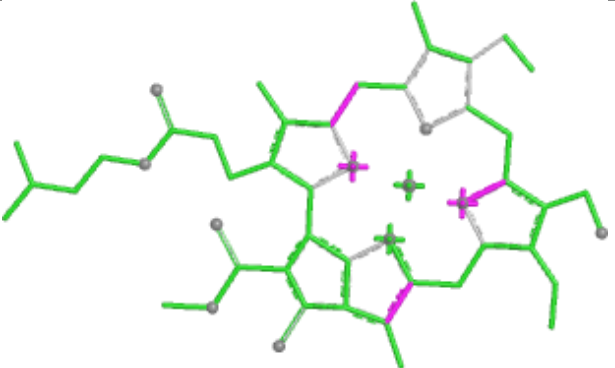
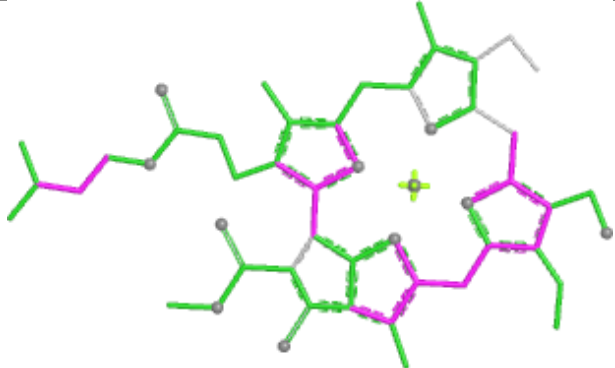
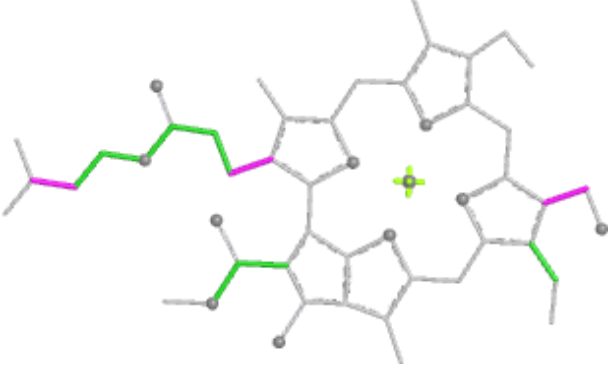
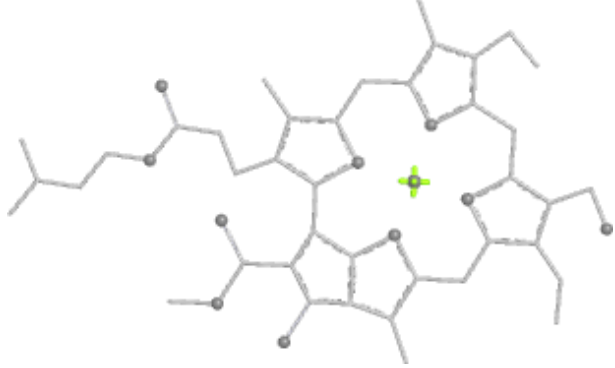
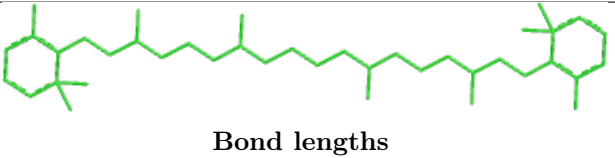
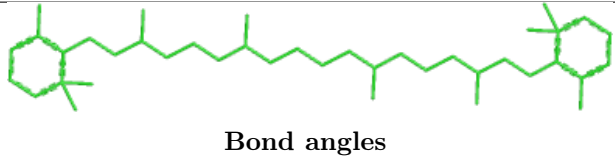
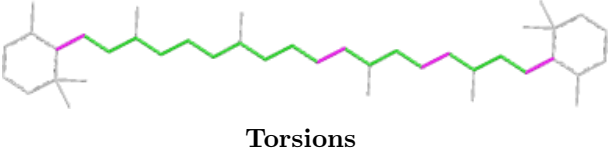
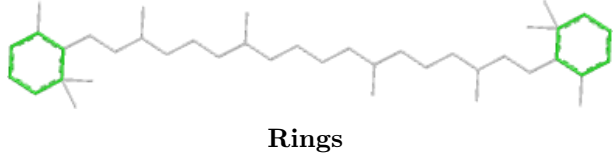
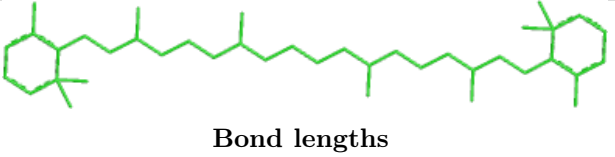
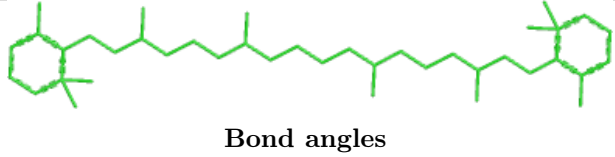
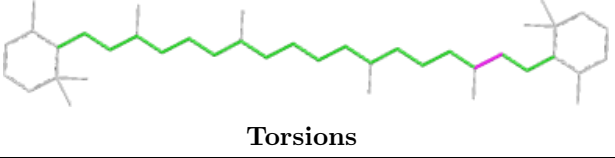
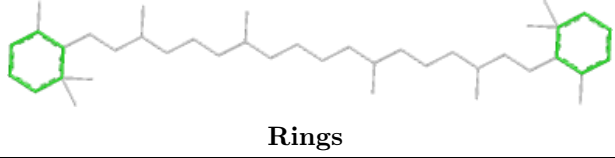
Rings

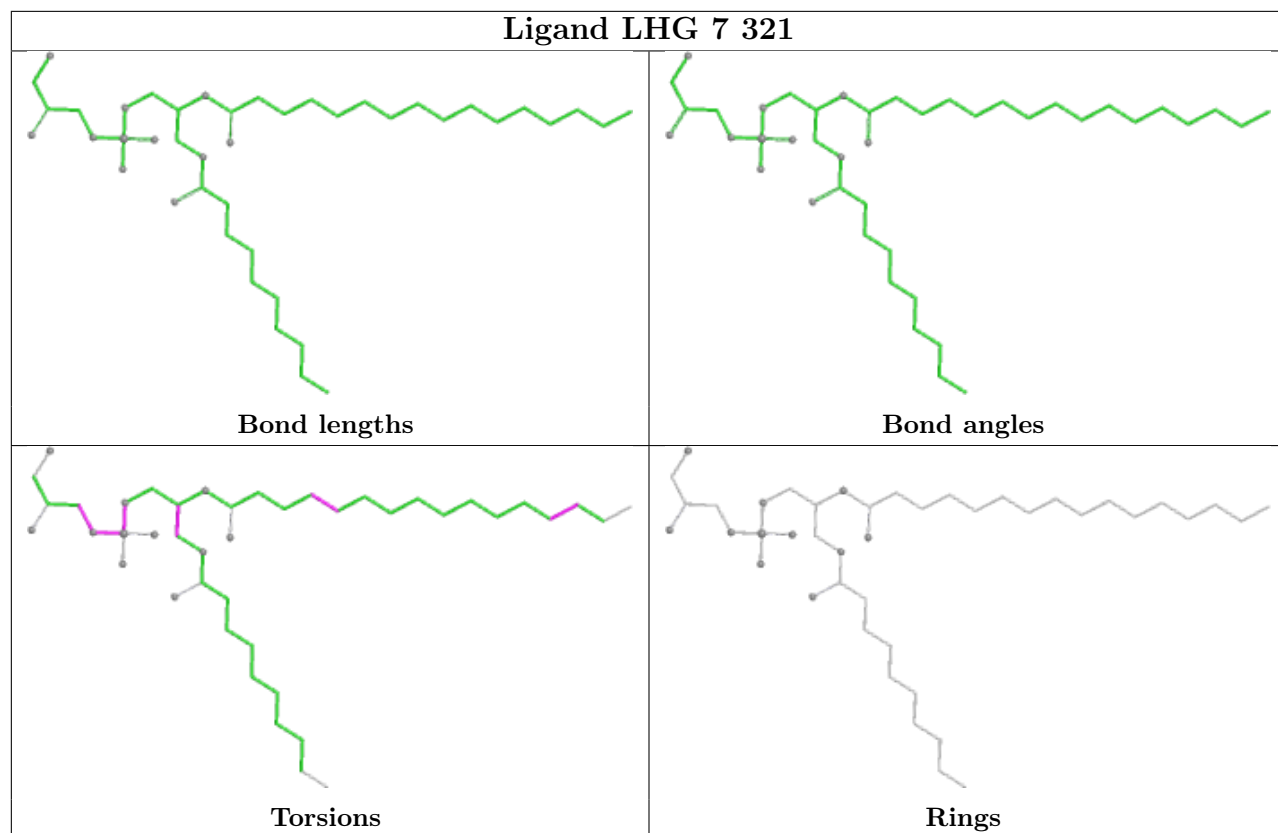




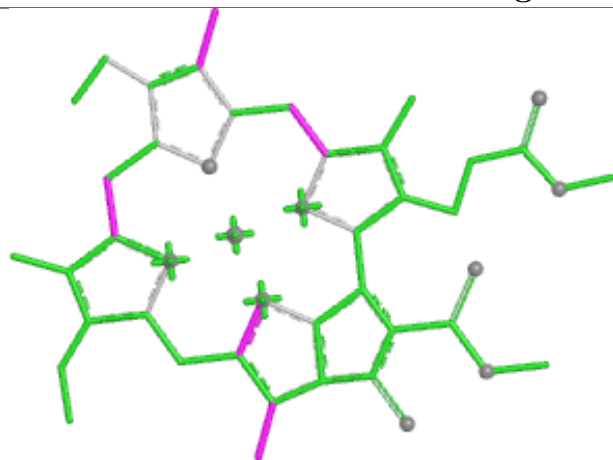
Ligand CHL b 307



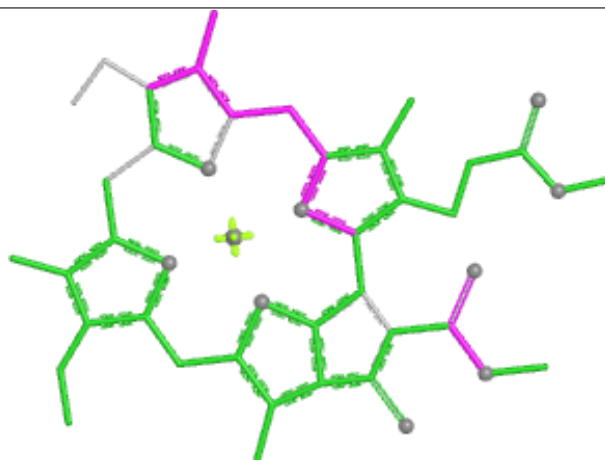
Ligand CHL b 309	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 849	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR J 5004	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



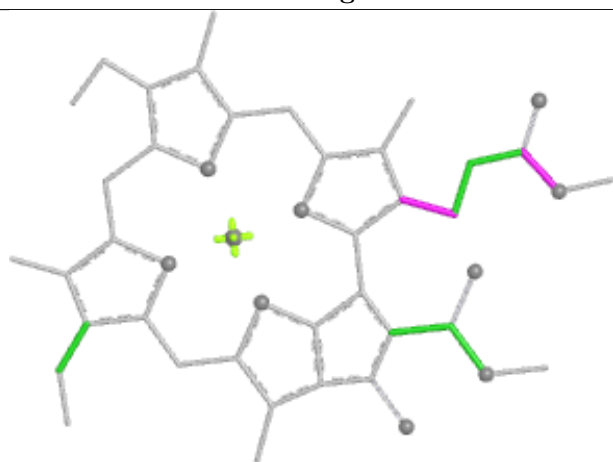
Ligand CLA T 610



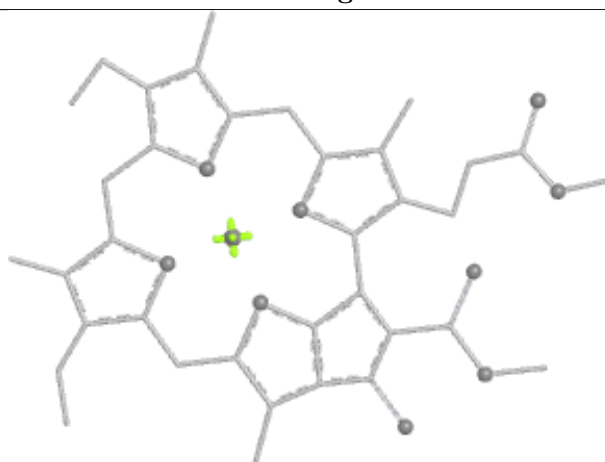
Bond lengths



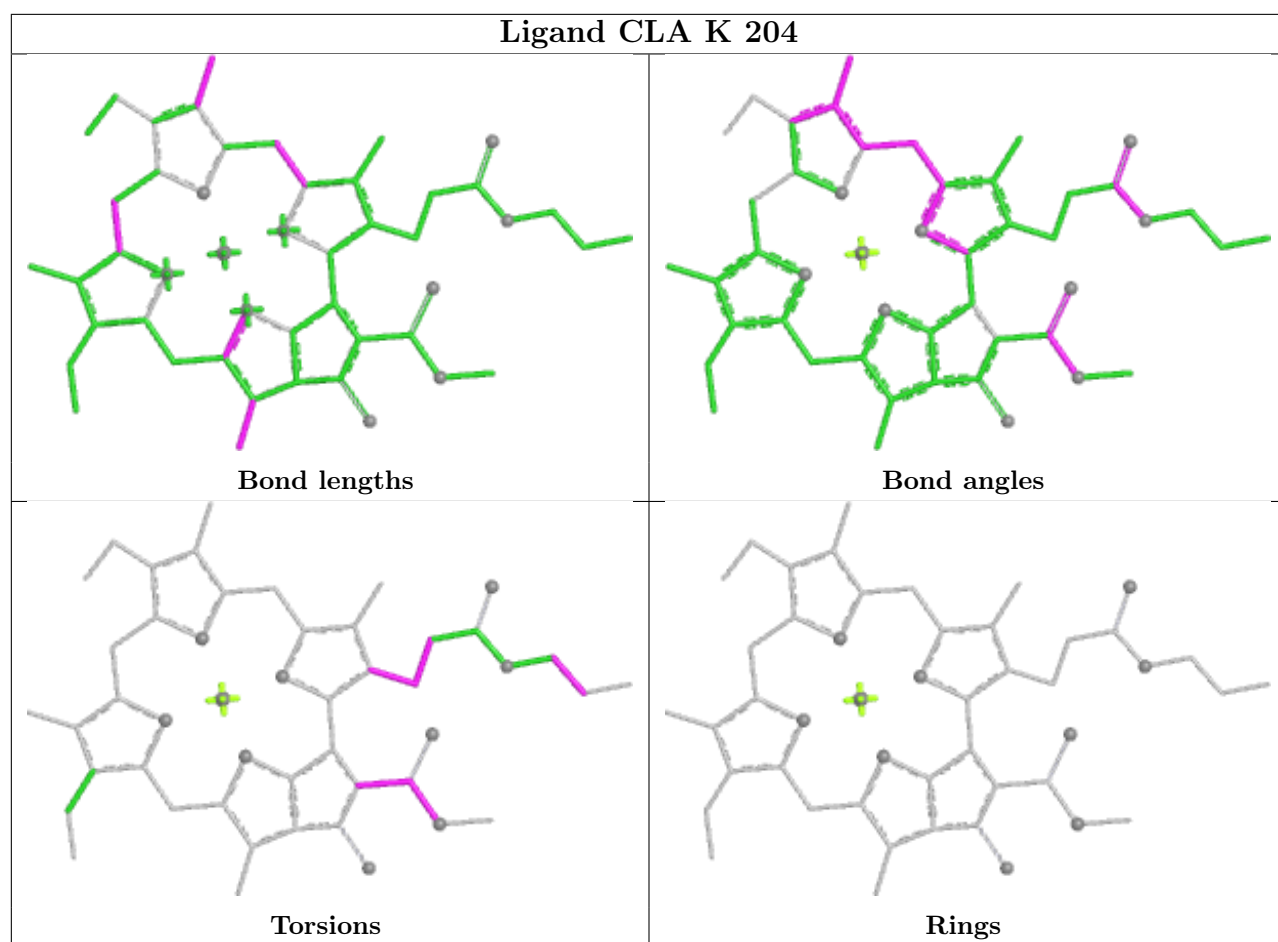
Bond angles



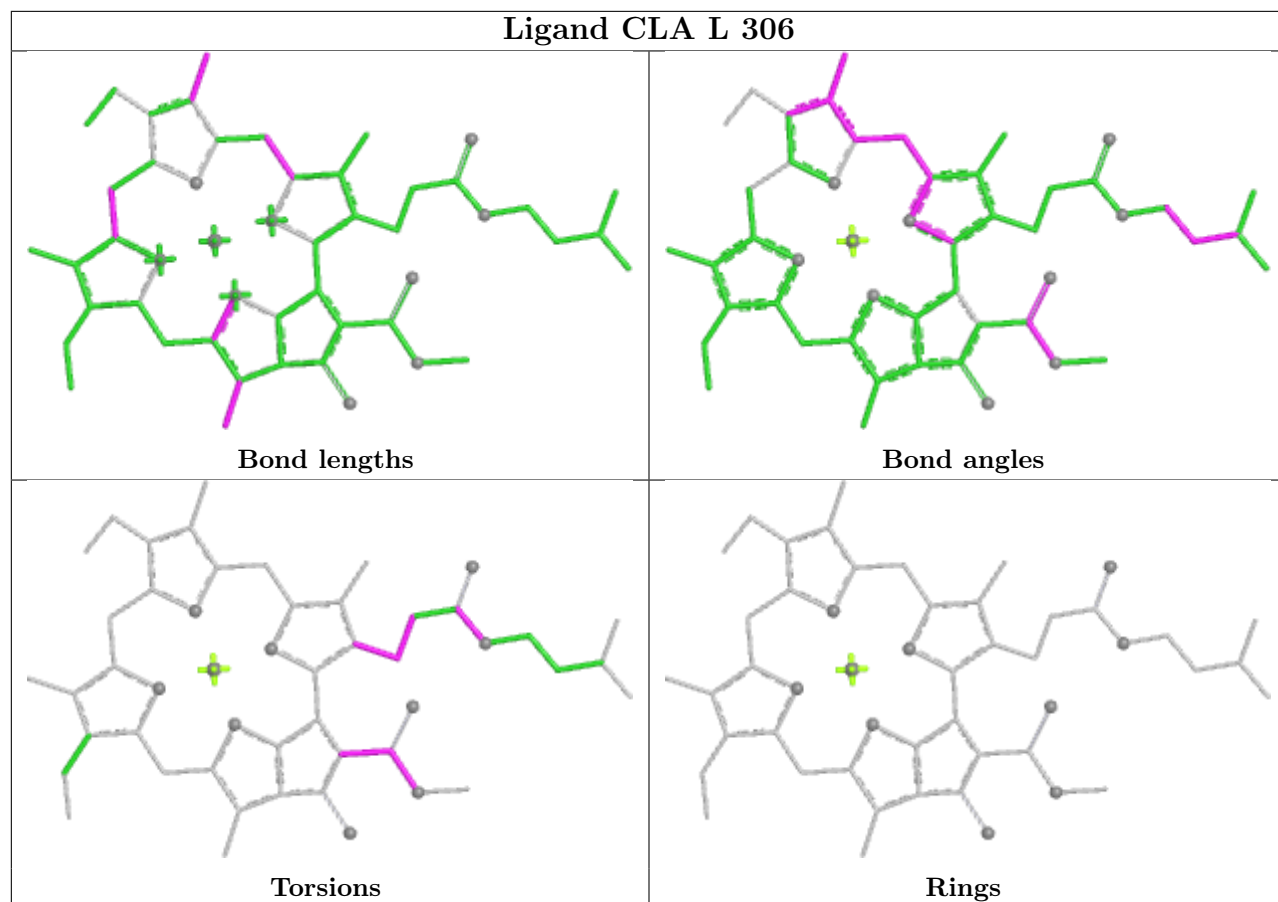
Torsions



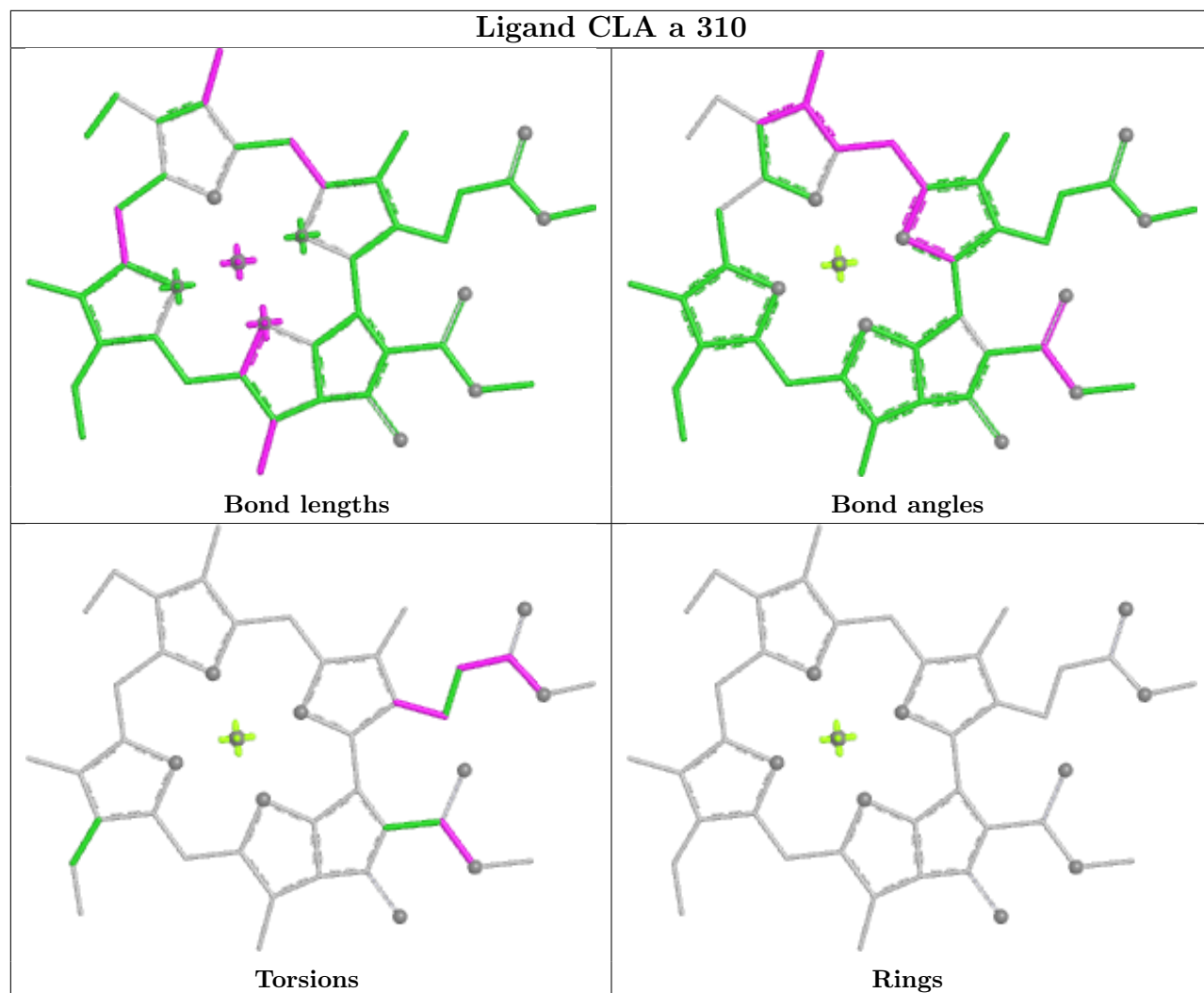
Rings

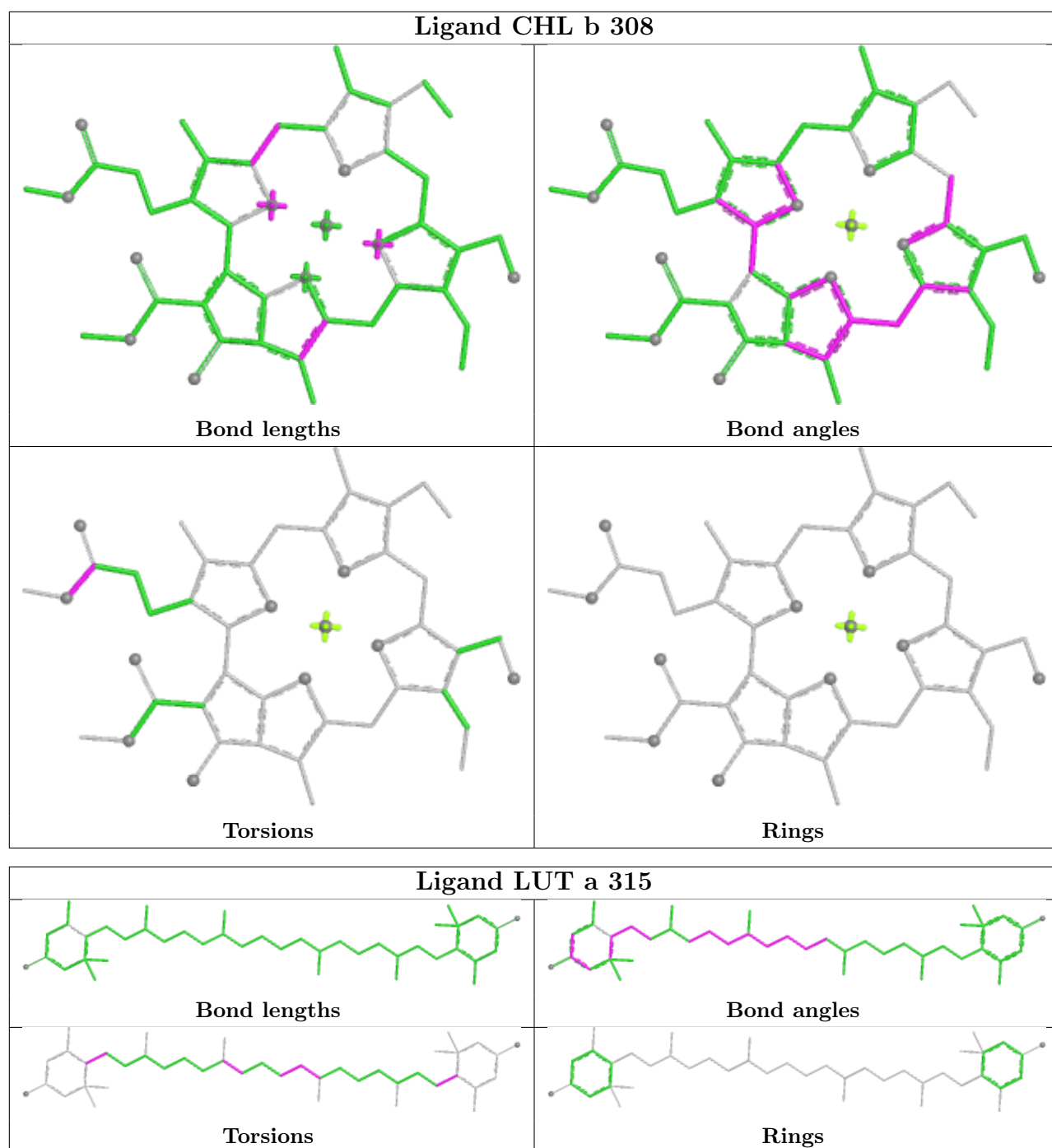


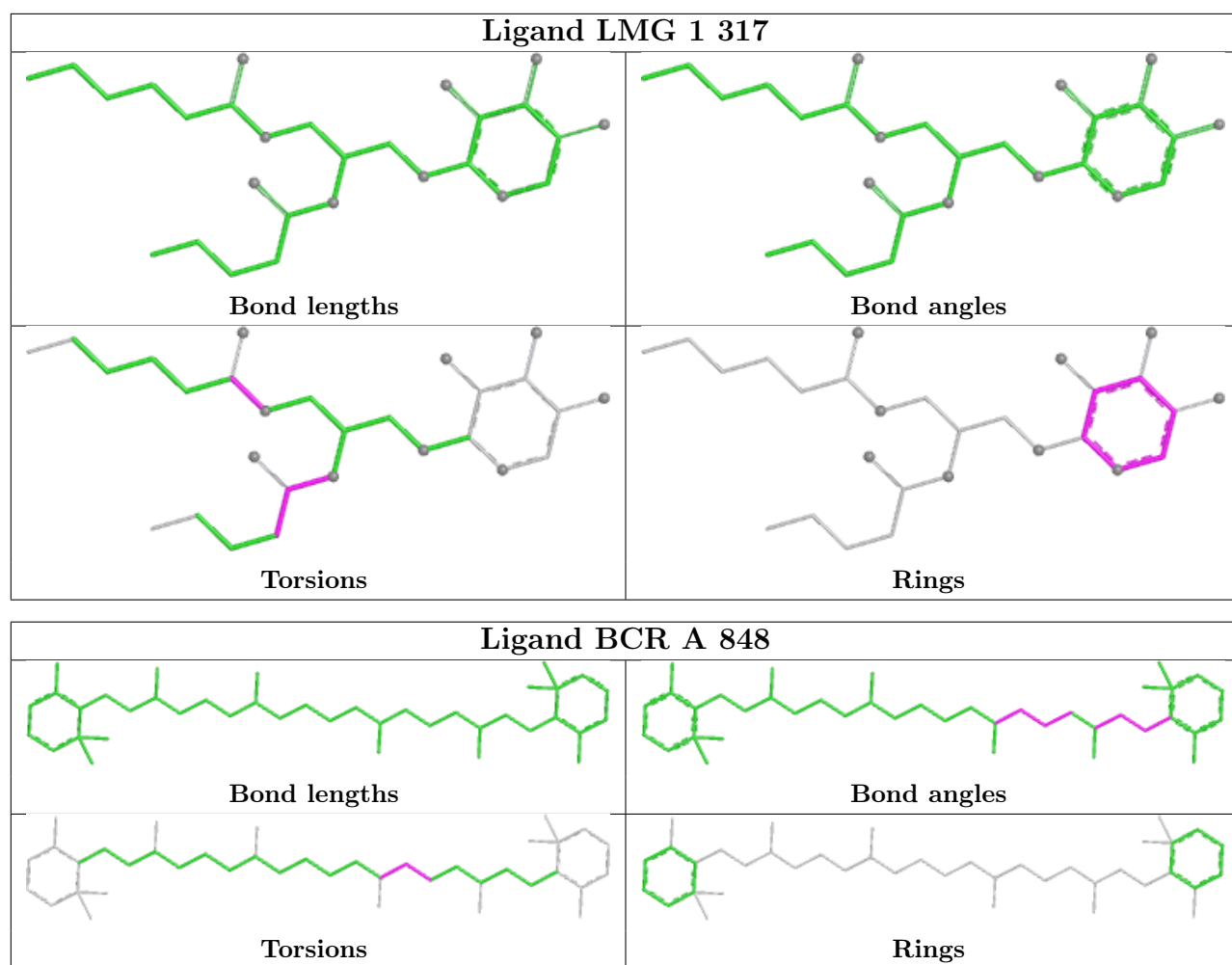
Ligand CLA L 306



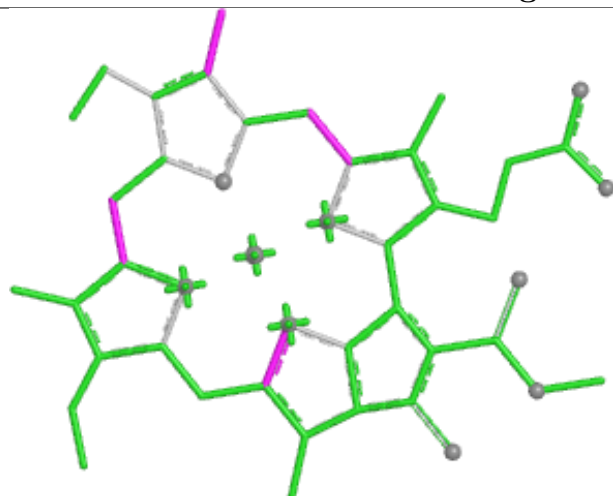
Ligand CLA a 310



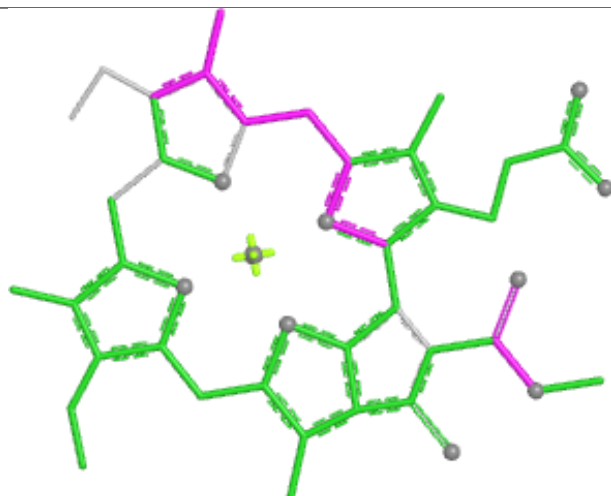




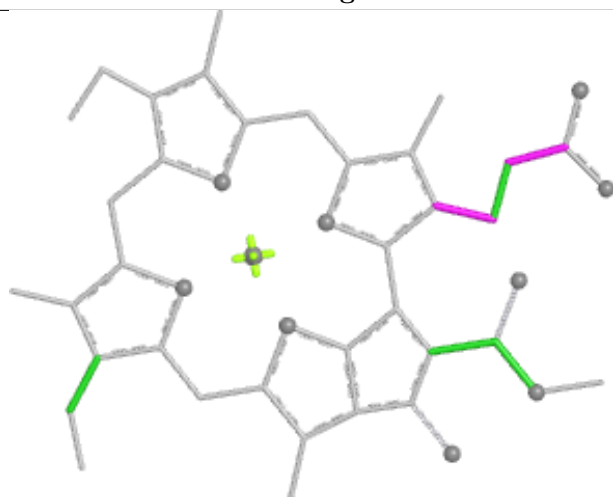
Ligand CLA c 608



Bond lengths



Bond angles

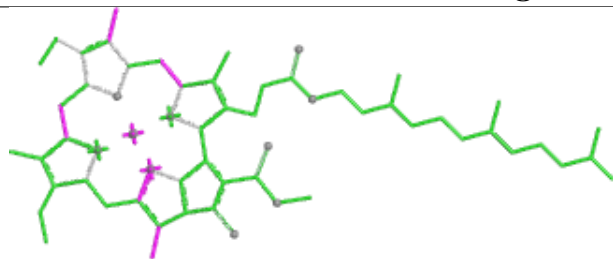


Torsions

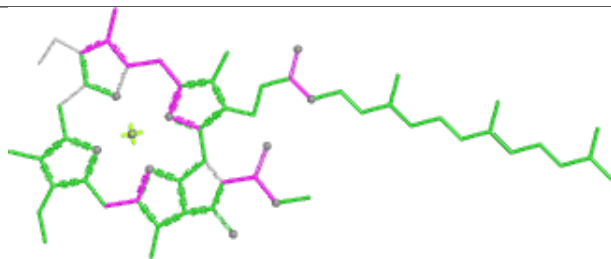


Rings

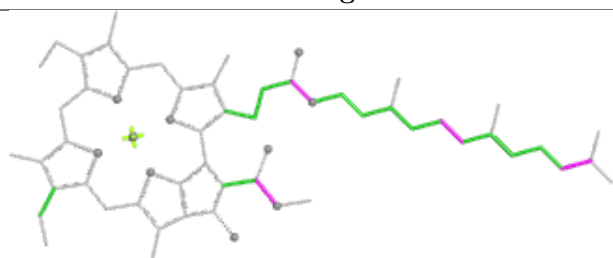
Ligand CLA B 840



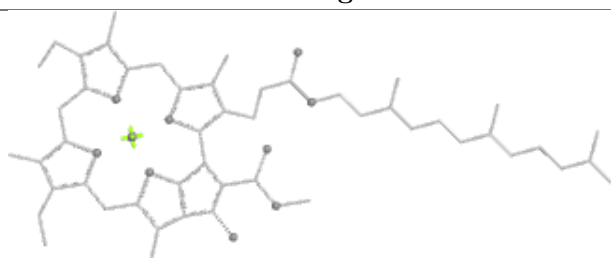
Bond lengths



Bond angles

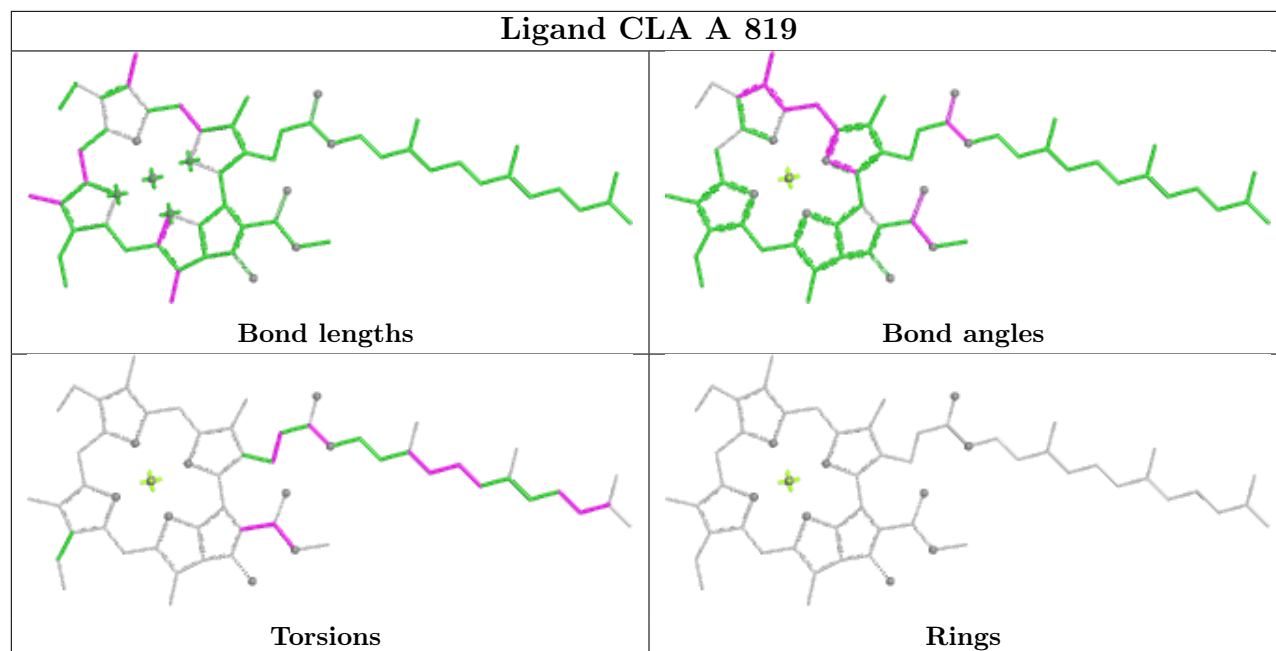


Torsions

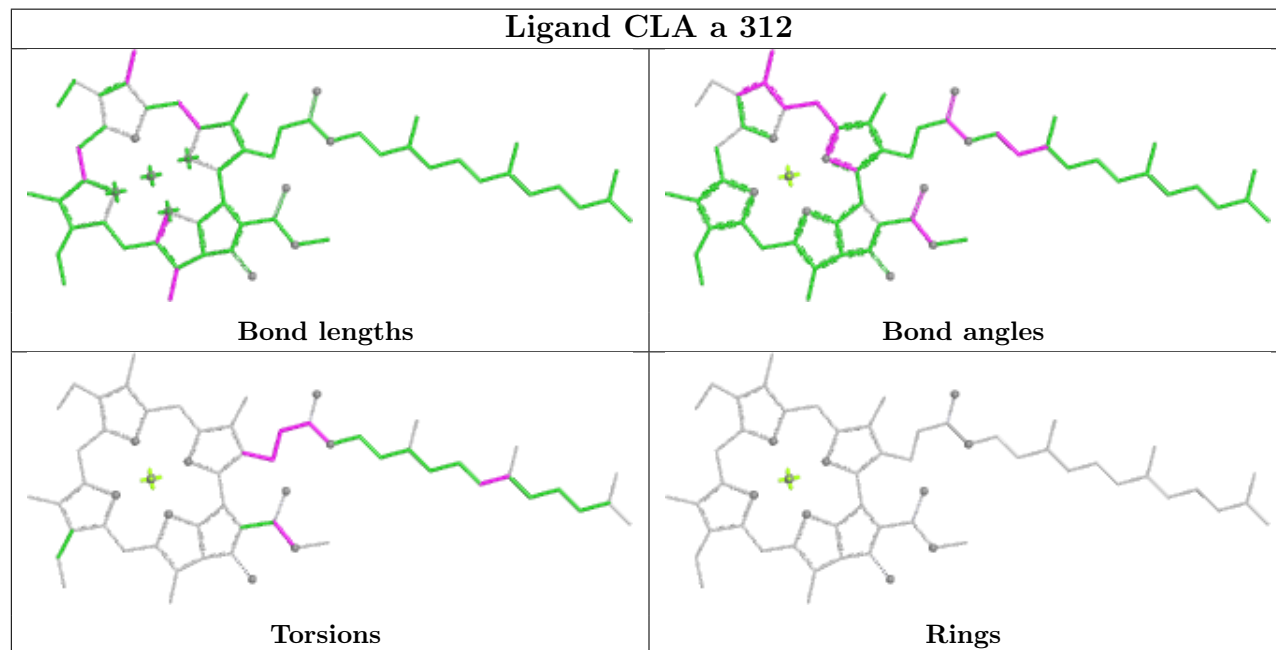


Rings

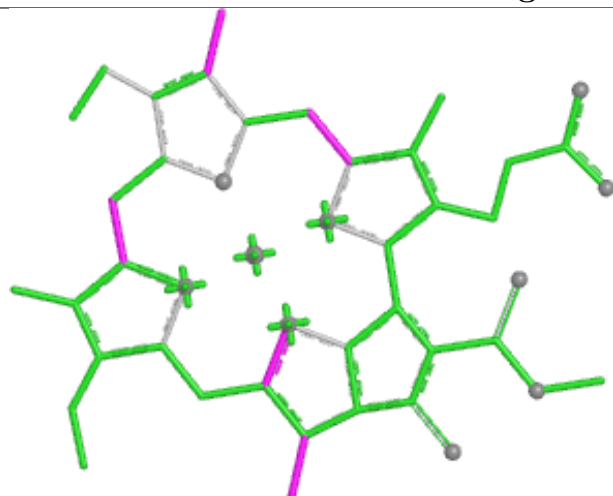
Ligand CLA A 819



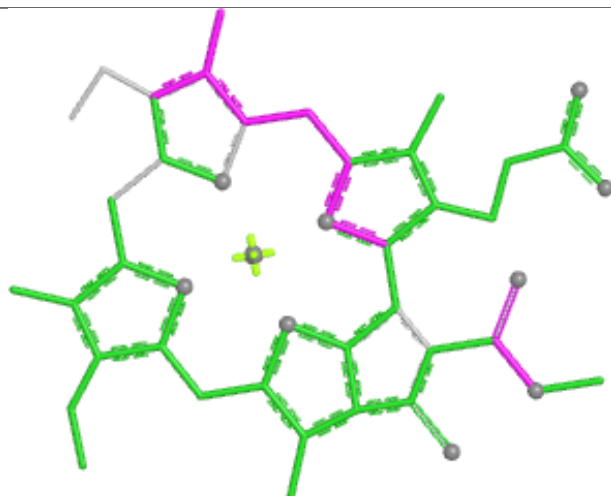
Ligand CLA a 312



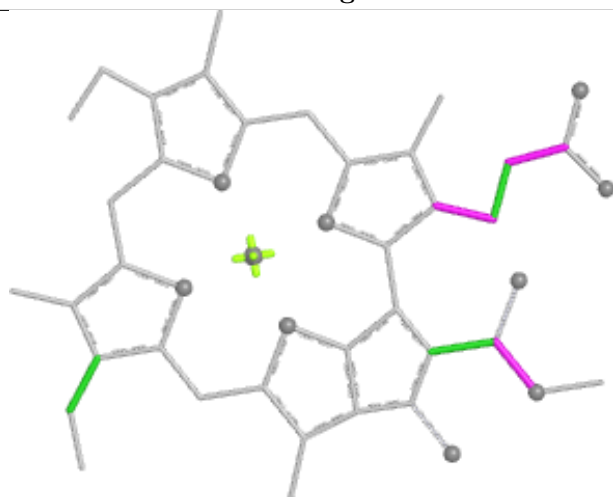
Ligand CLA 2 605



Bond lengths



Bond angles

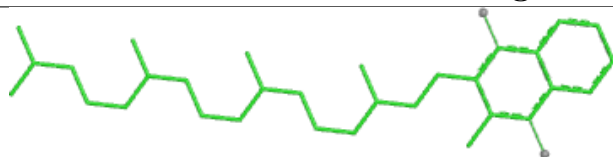


Torsions

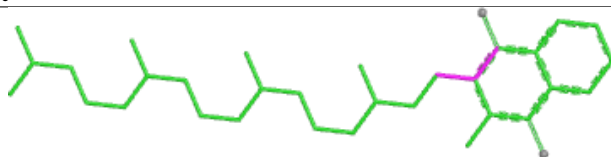


Rings

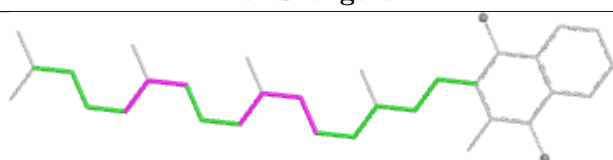
Ligand PQN B 845



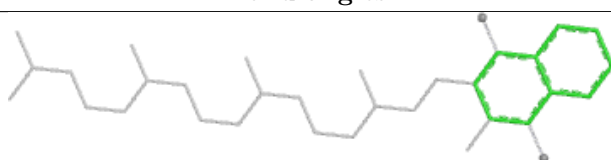
Bond lengths



Bond angles

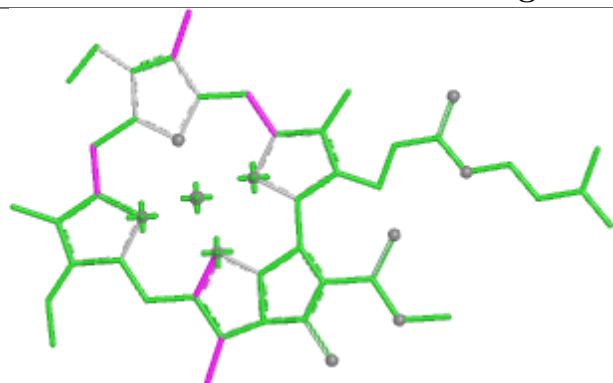


Torsions

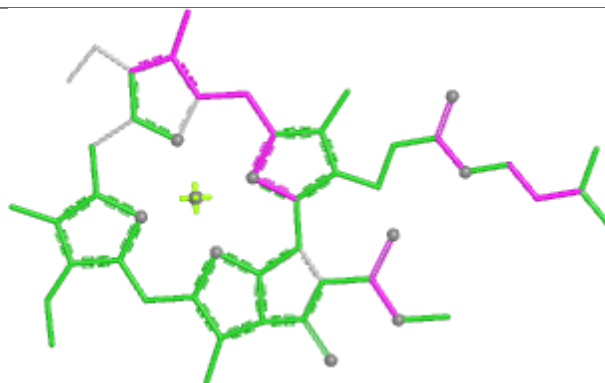


Rings

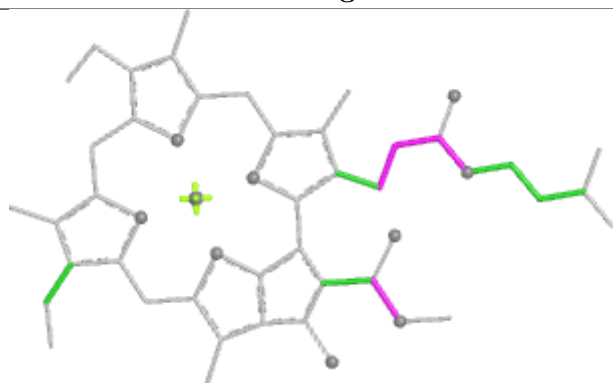
Ligand CLA 7 315



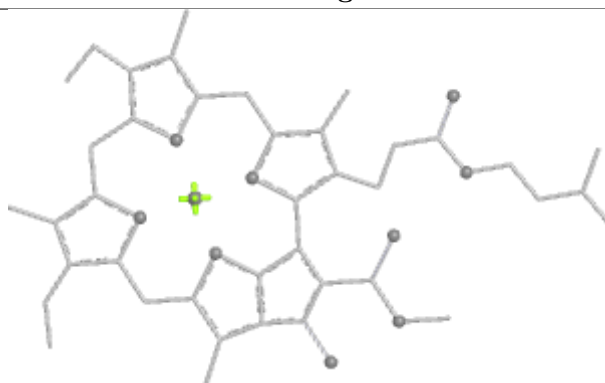
Bond lengths



Bond angles

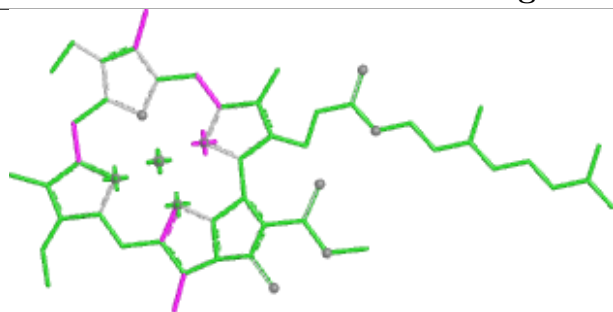


Torsions

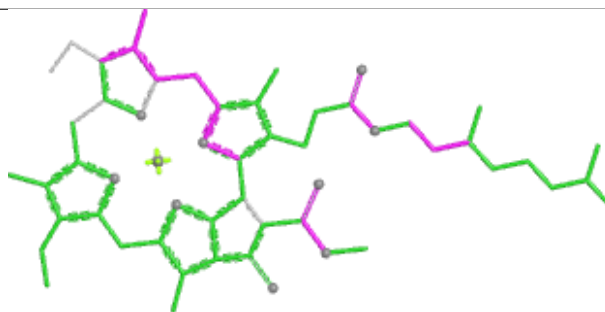


Rings

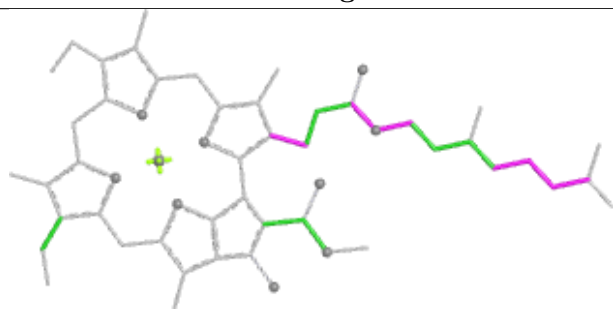
Ligand CLA 8 611



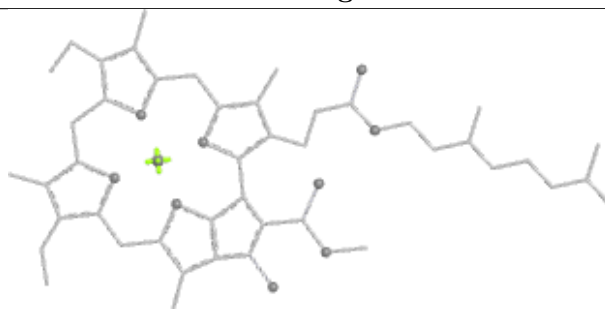
Bond lengths



Bond angles

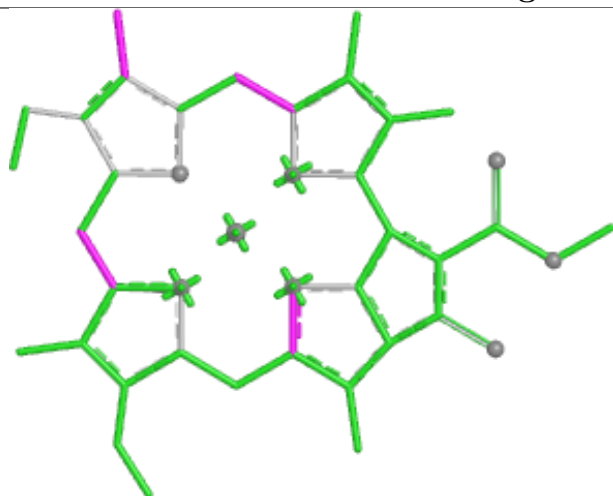


Torsions

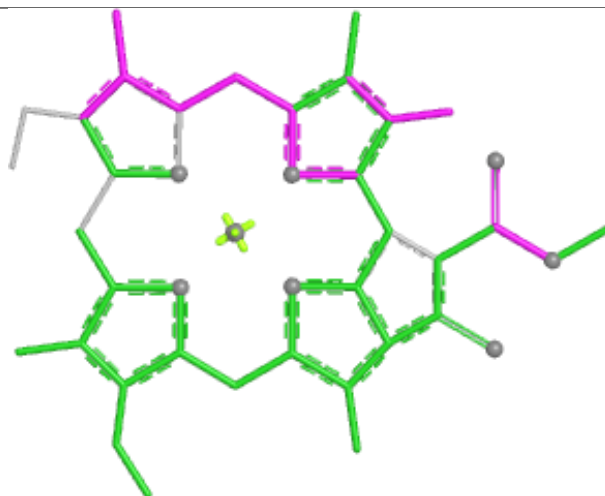


Rings

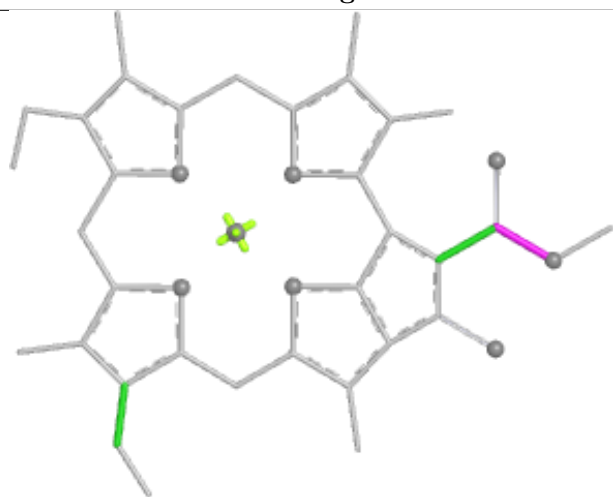
Ligand CLA 2 609



Bond lengths



Bond angles

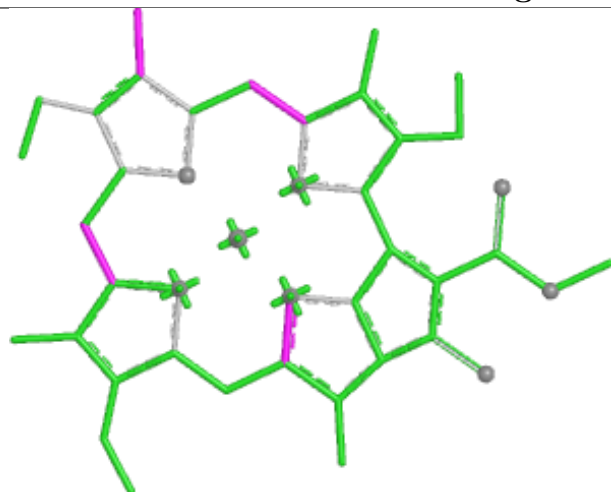


Torsions



Rings

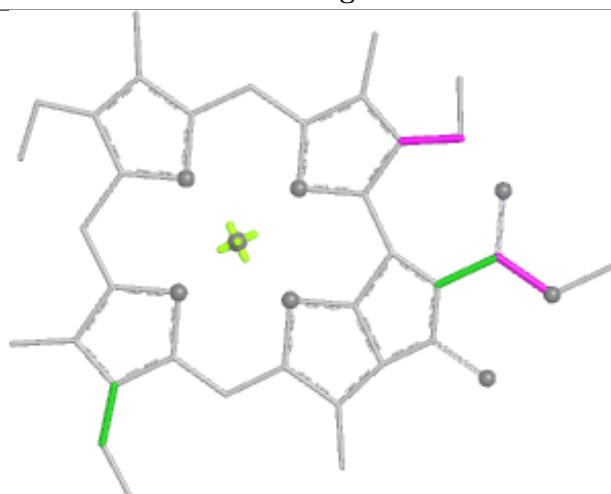
Ligand CLA T 614



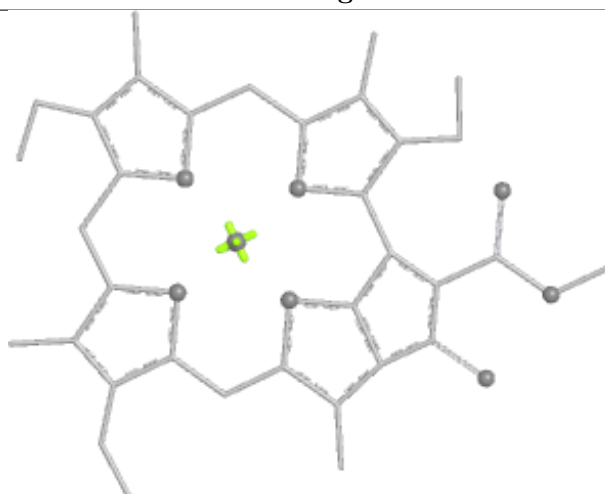
Bond lengths



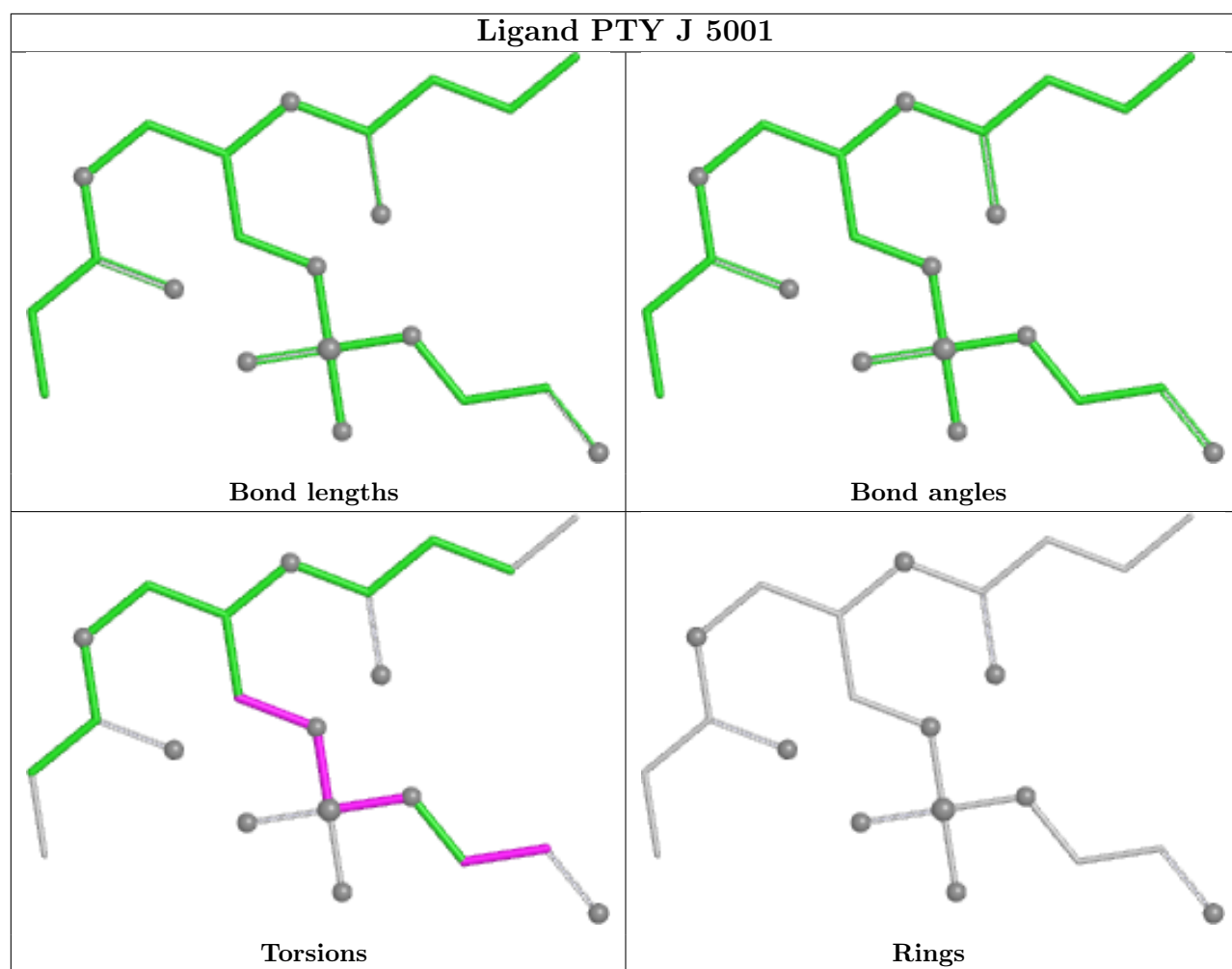
Bond angles



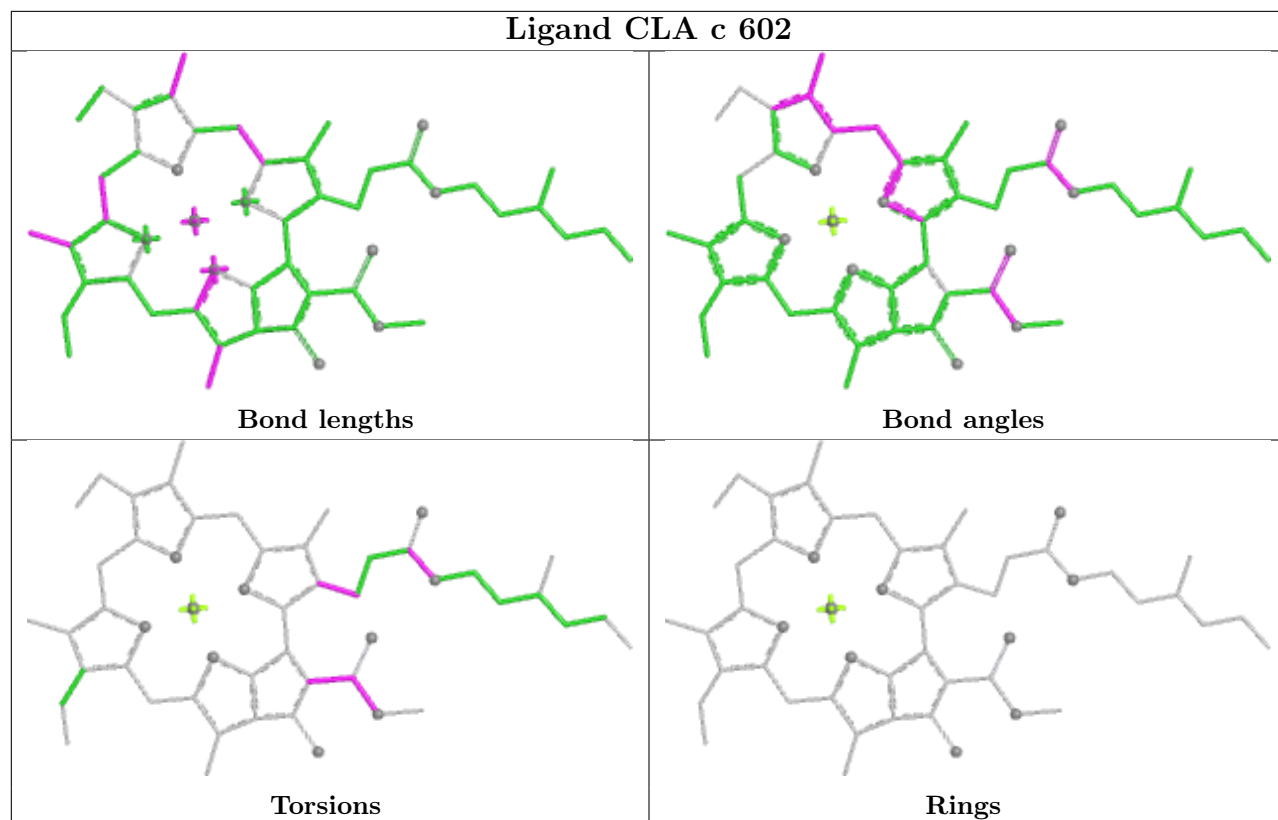
Torsions



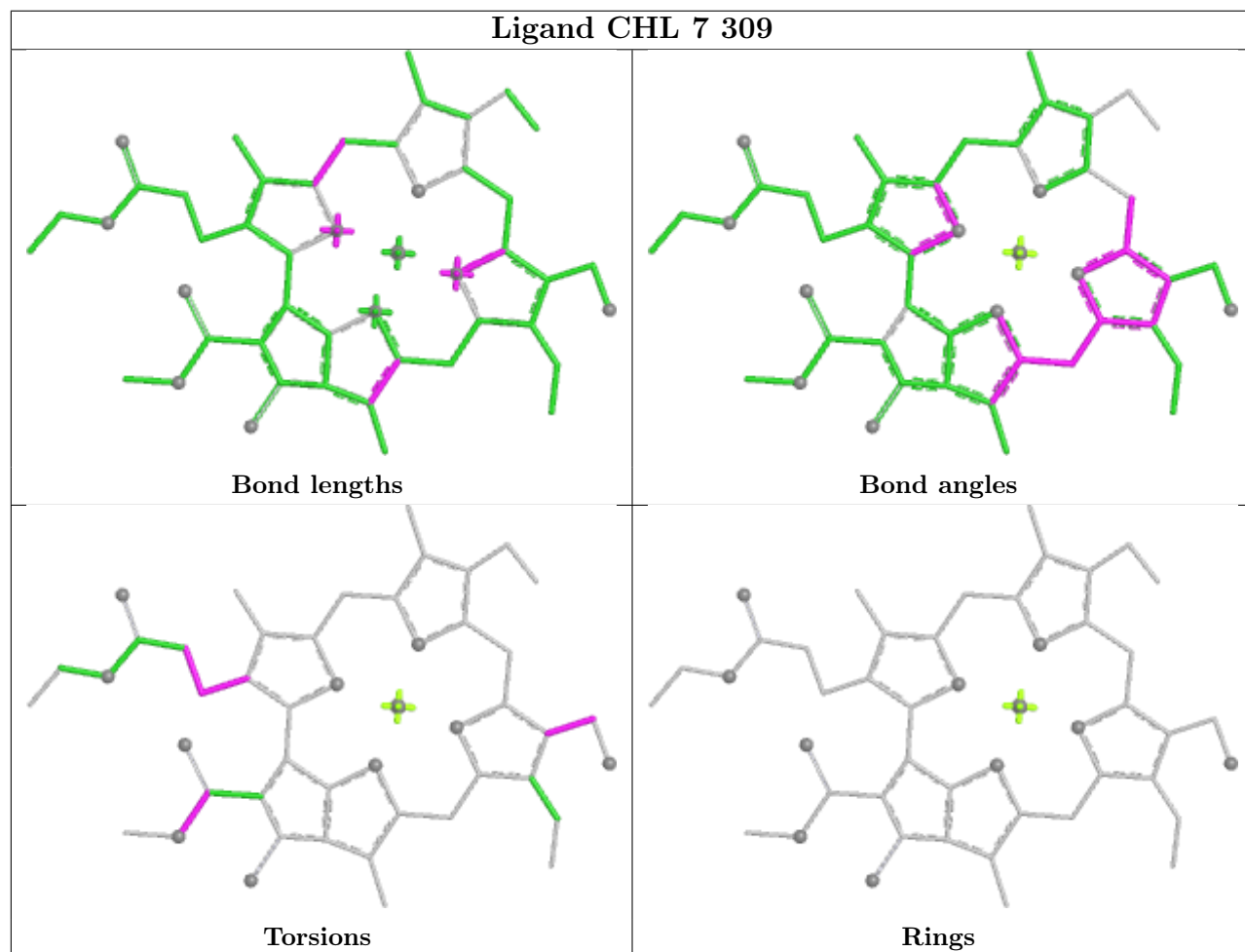
Rings

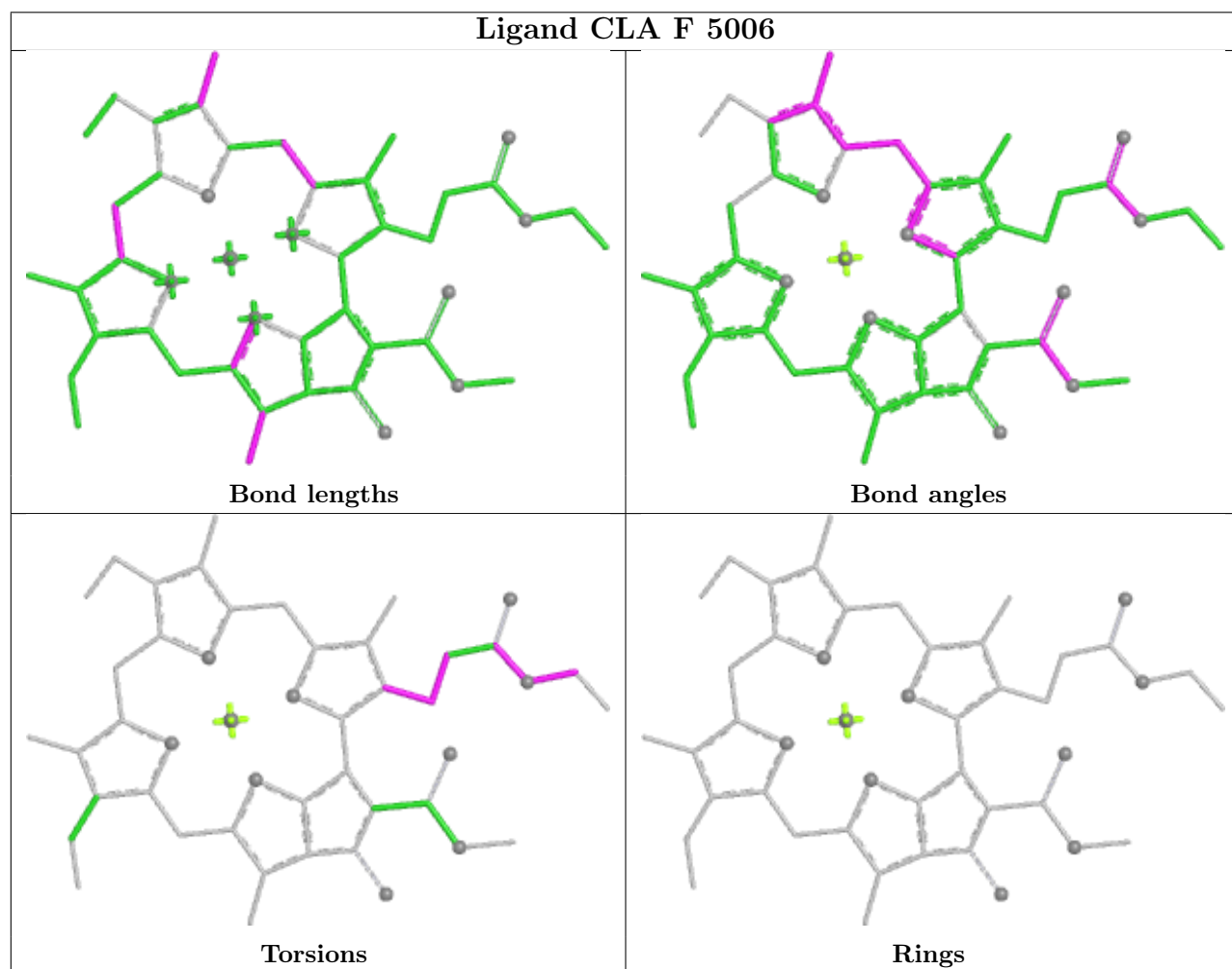
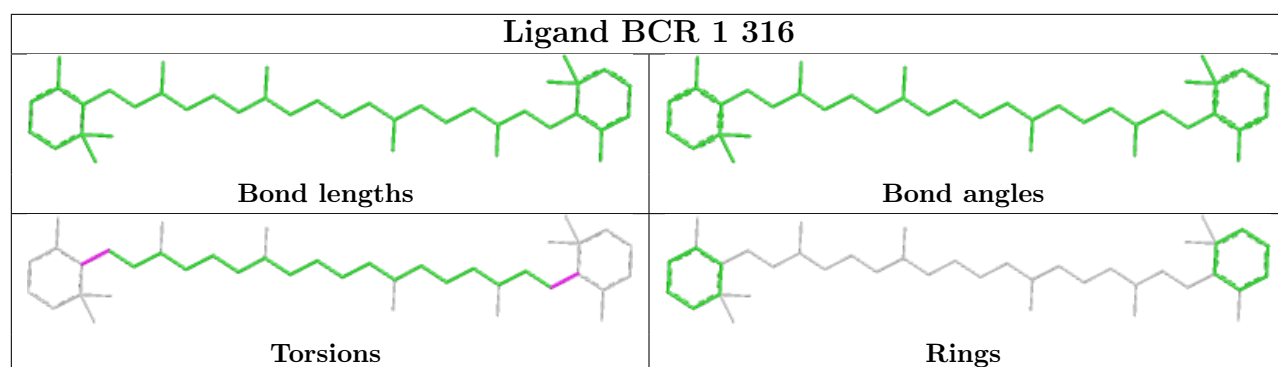


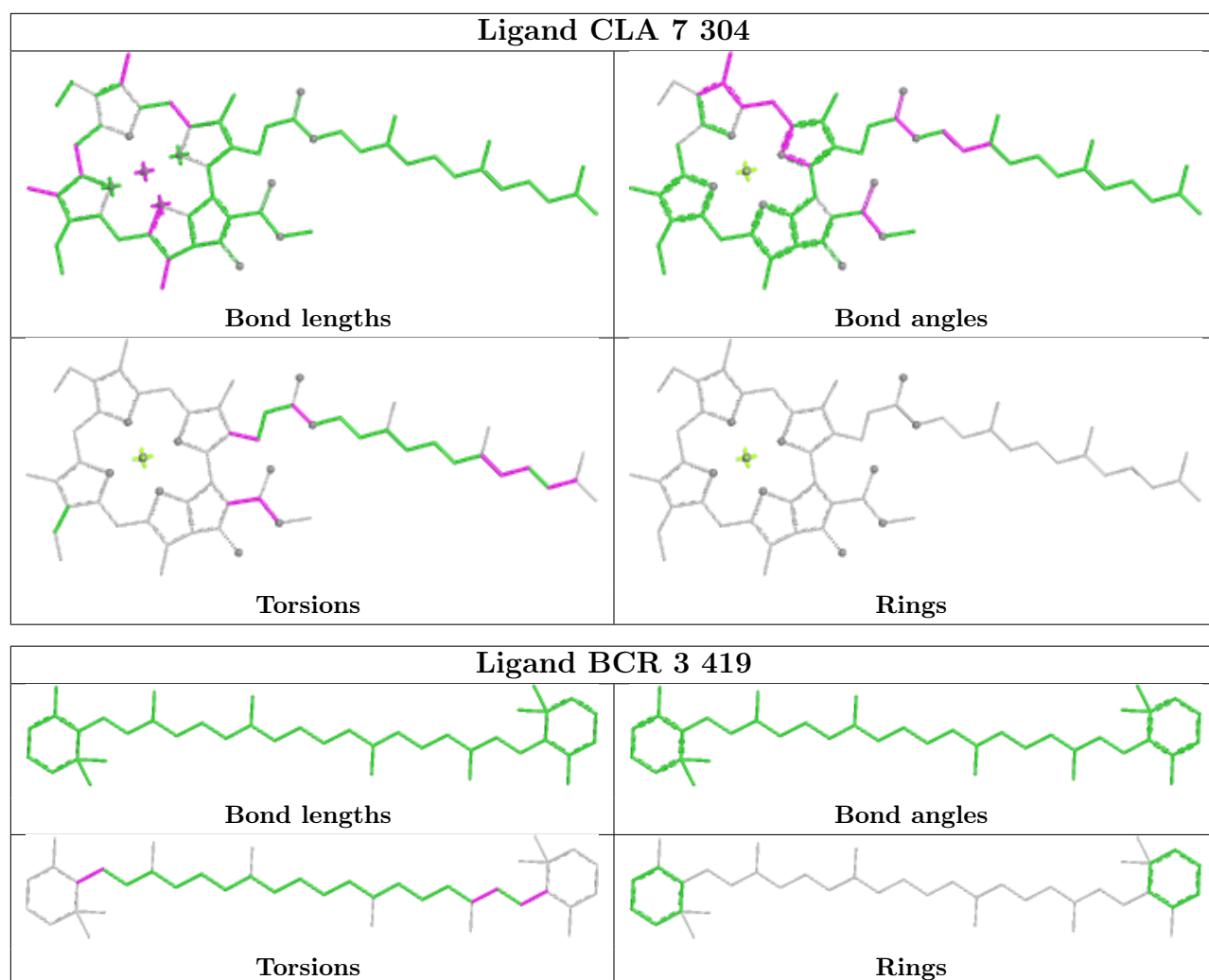
Ligand CLA c 602

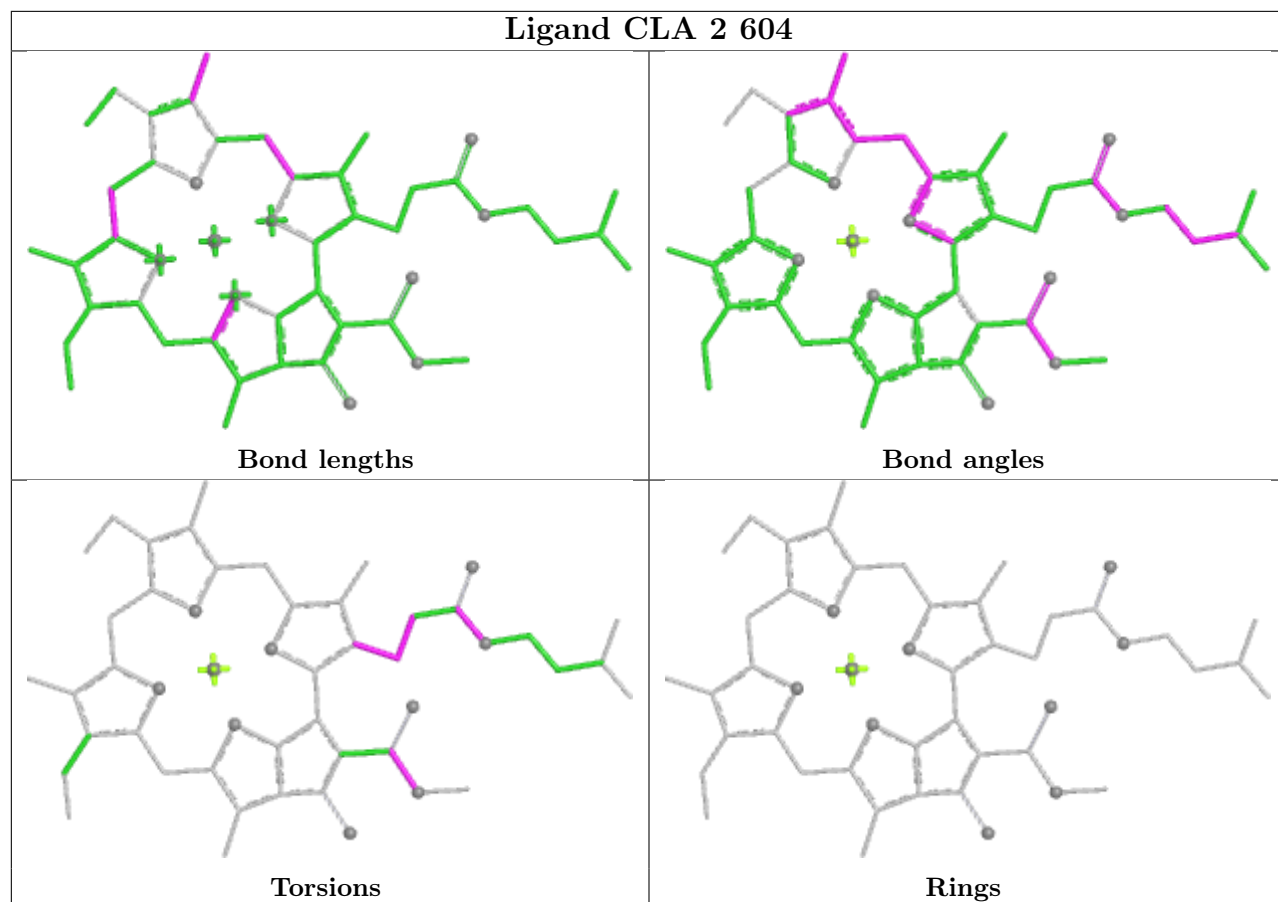


Ligand CHL 7 309

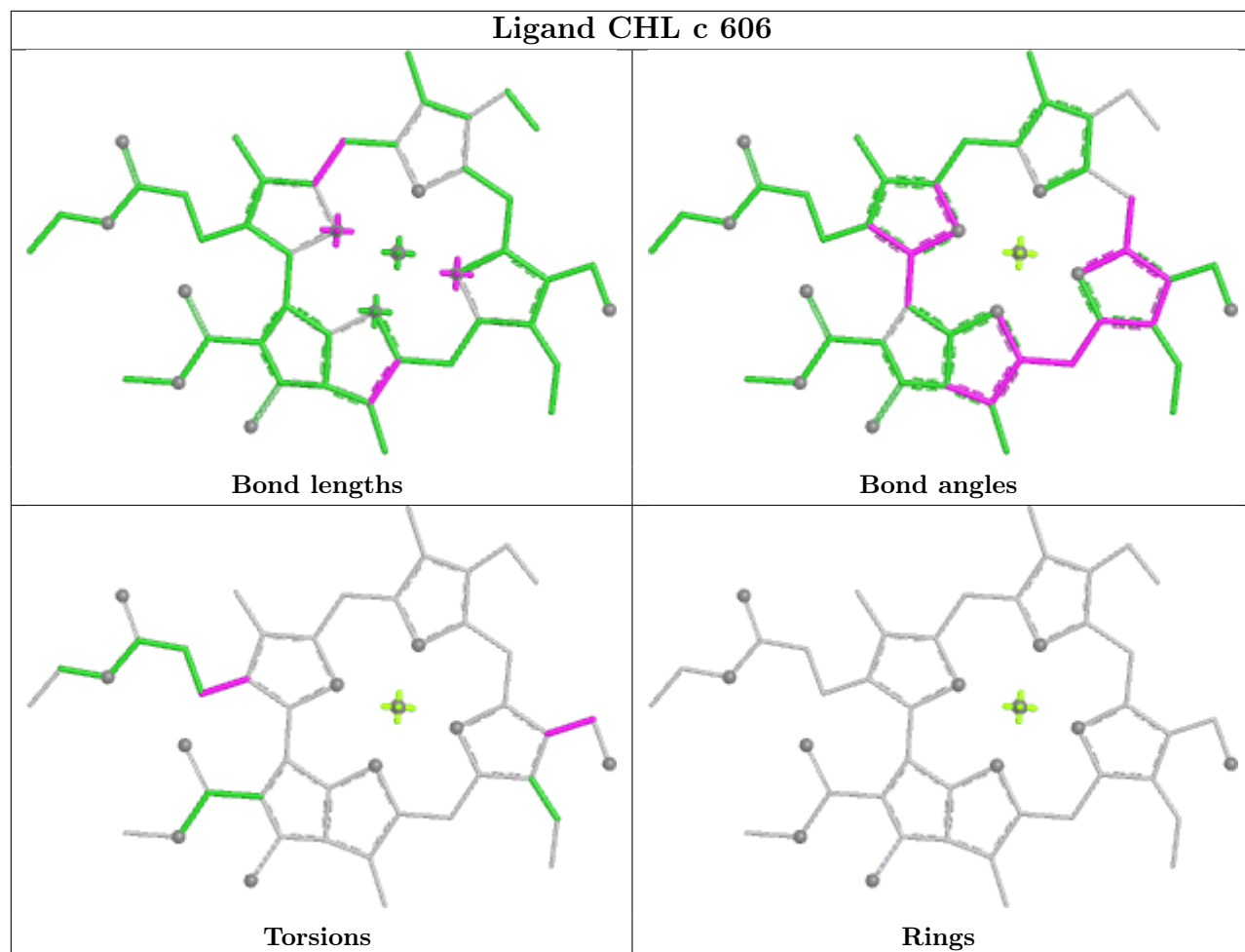




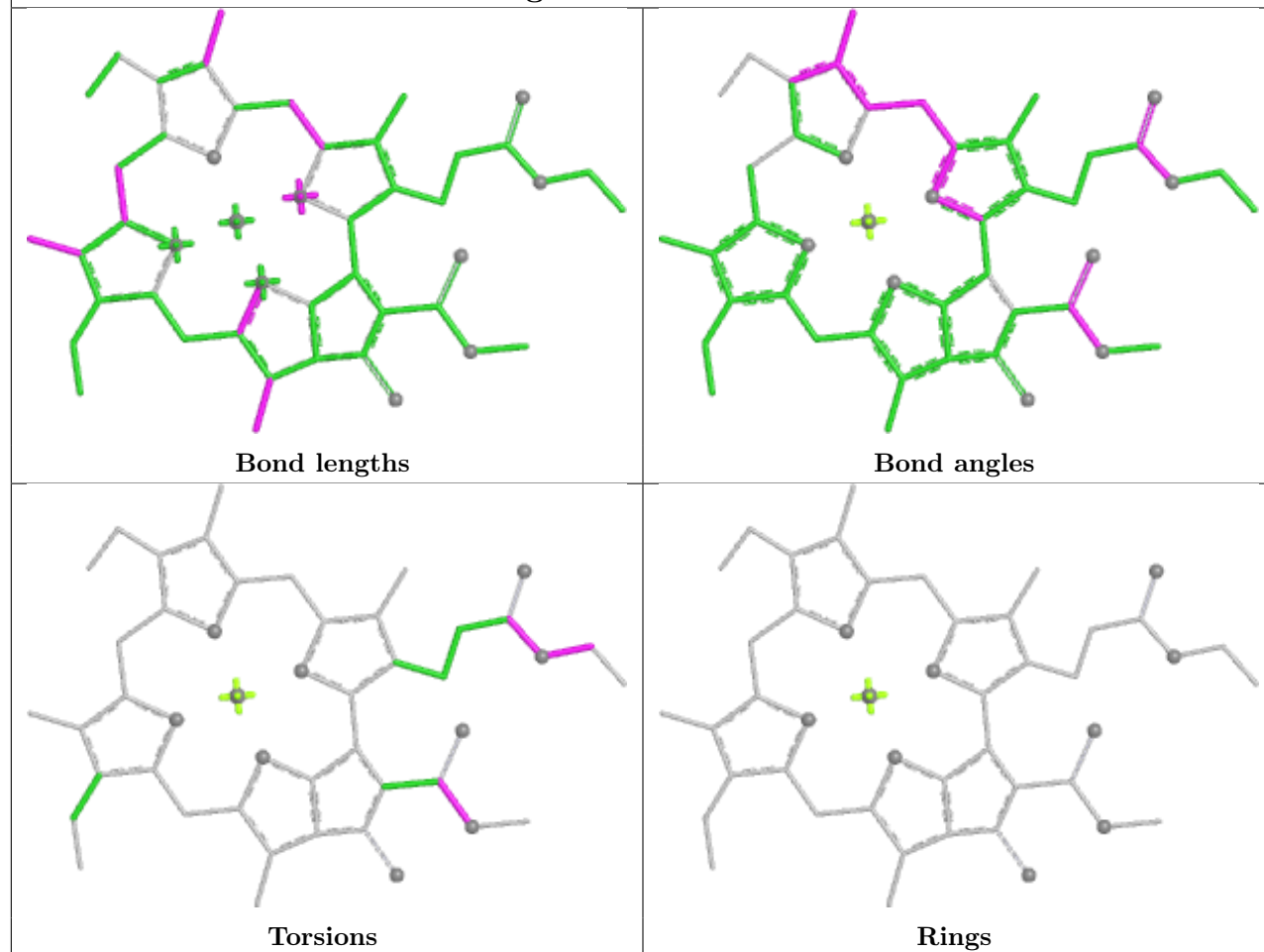




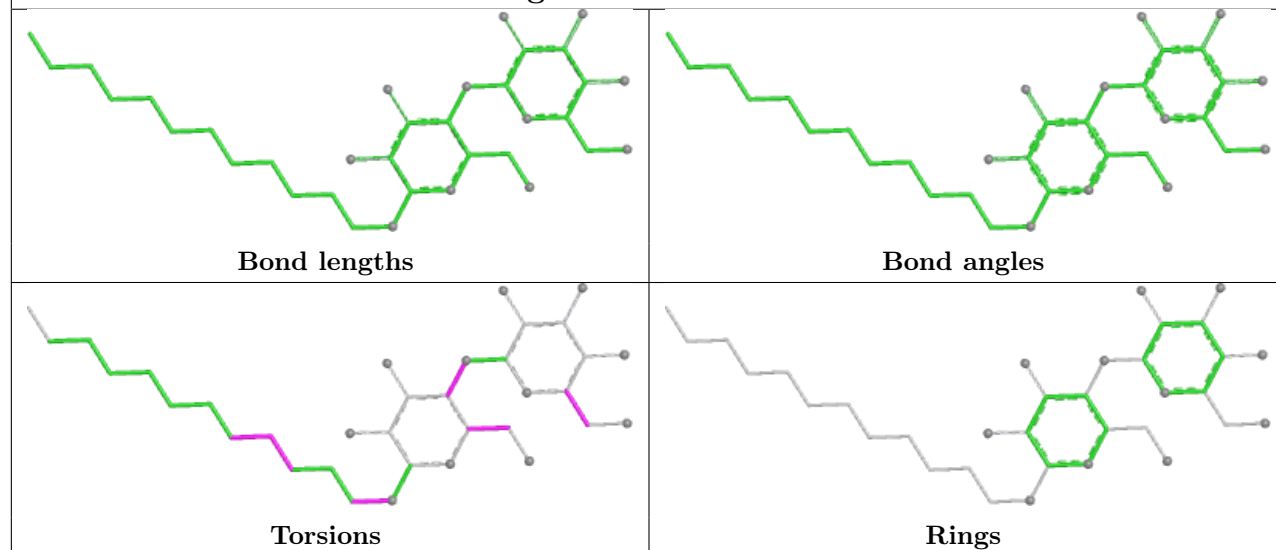
Ligand CHL c 606

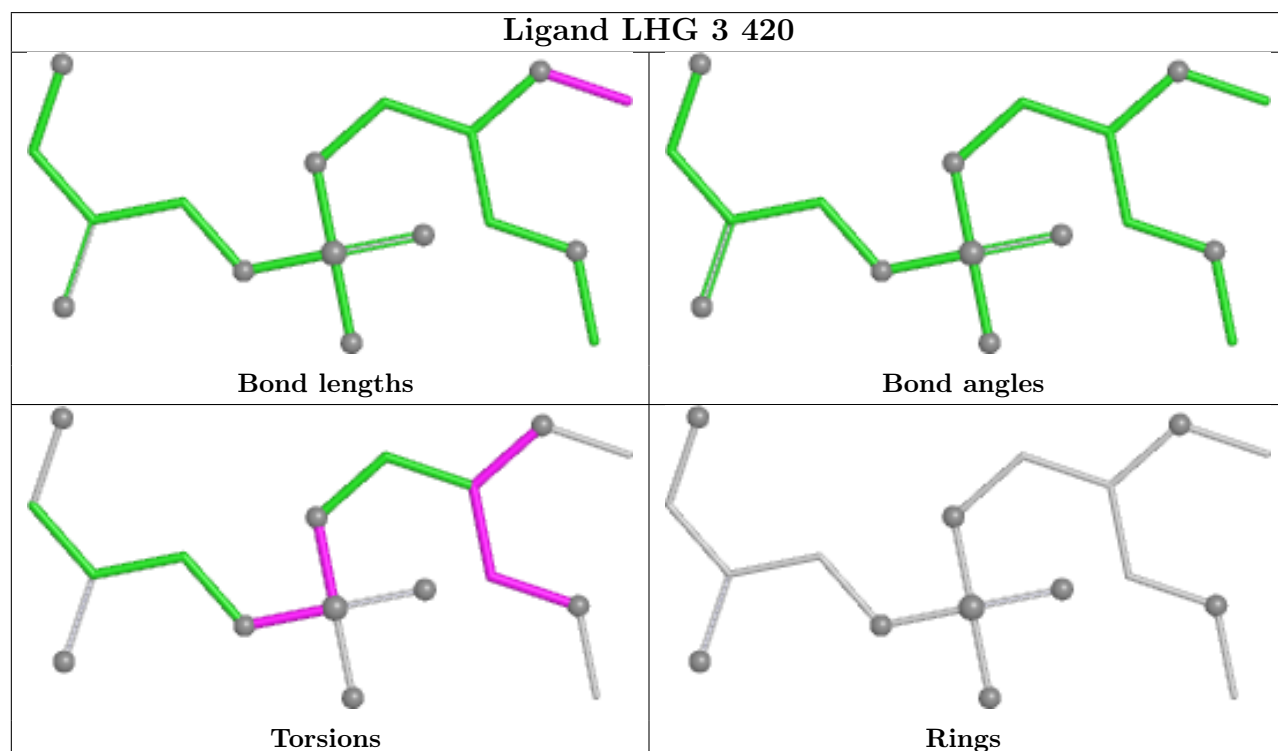
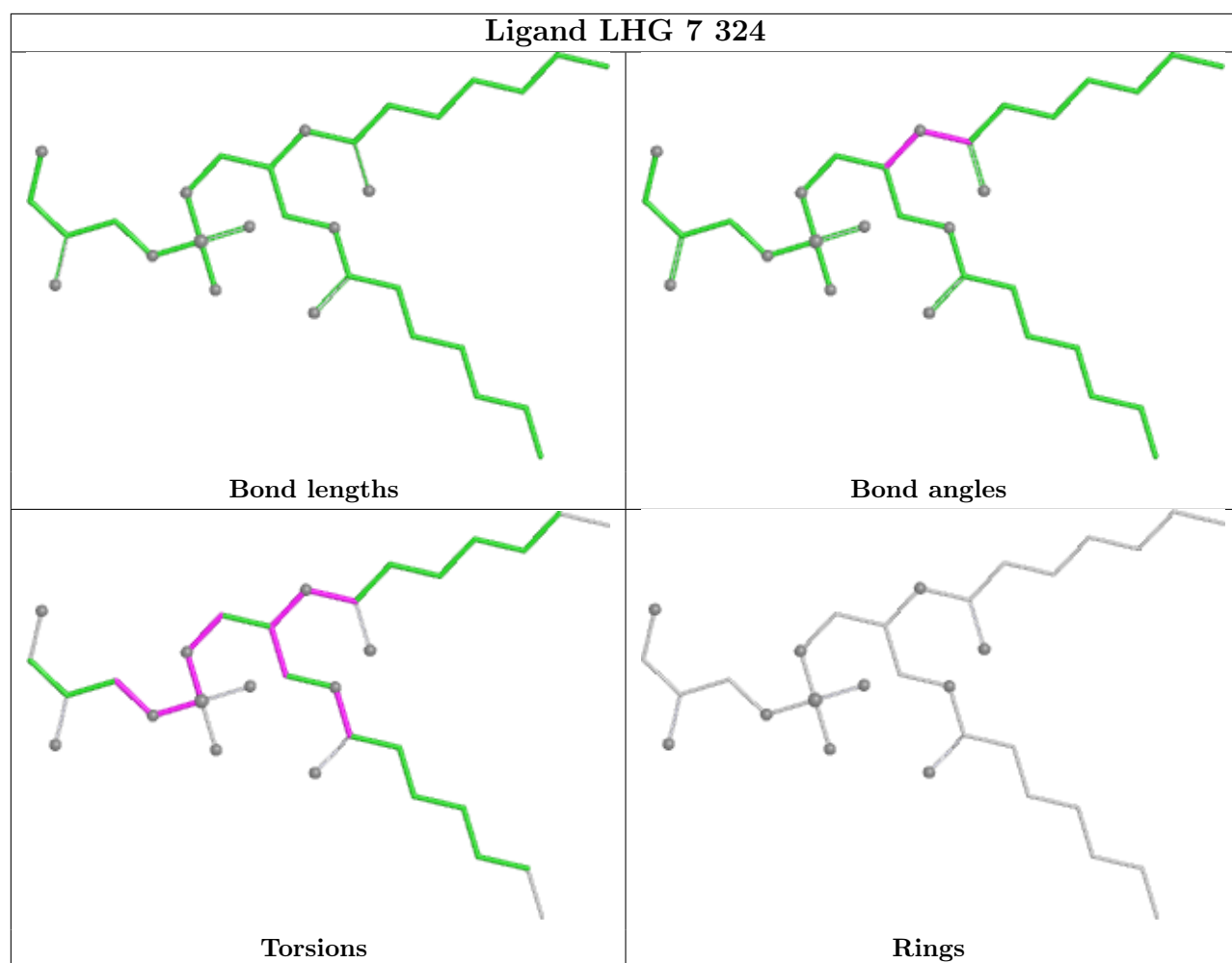


Ligand CLA G 203

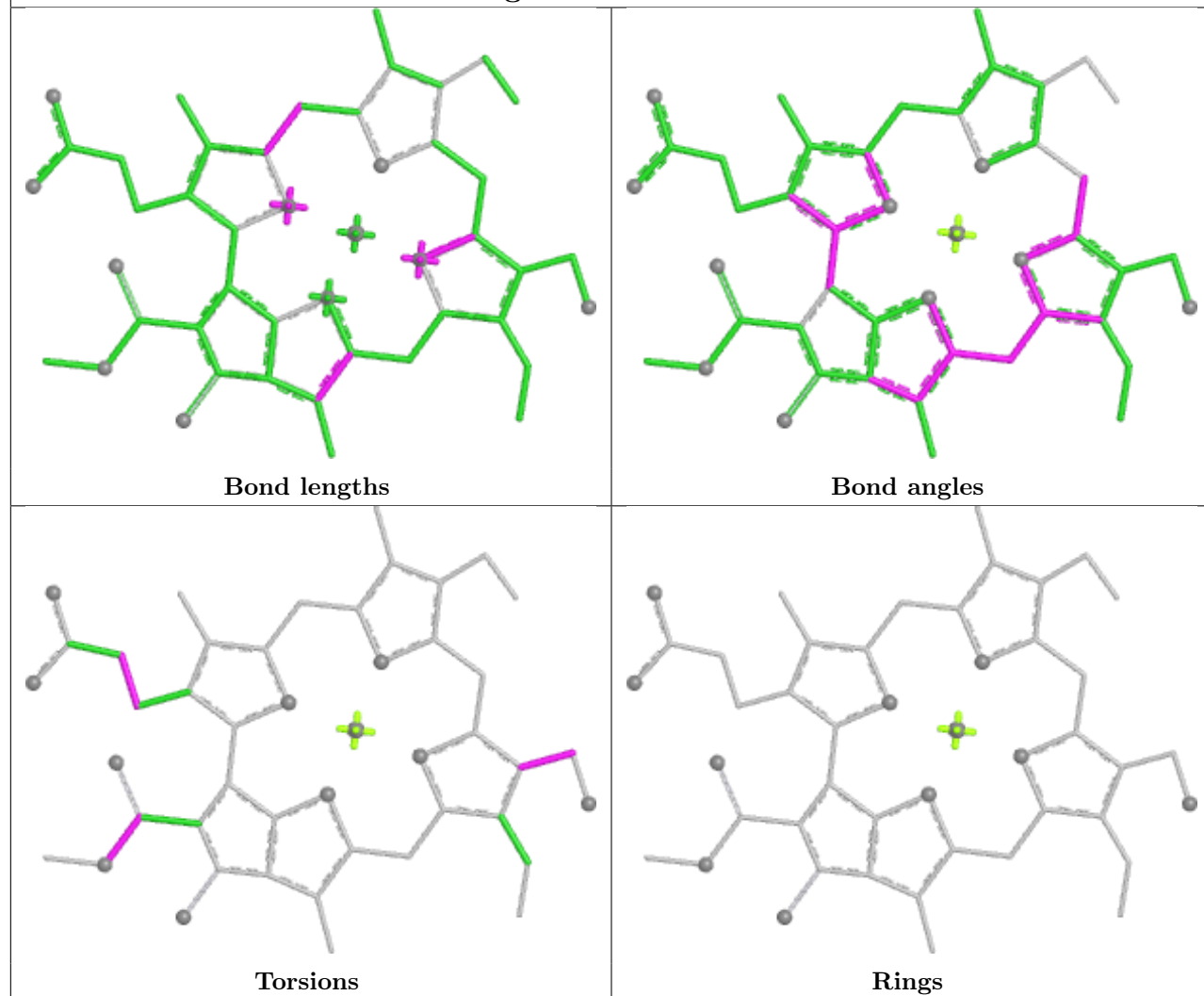


Ligand LMU A 855

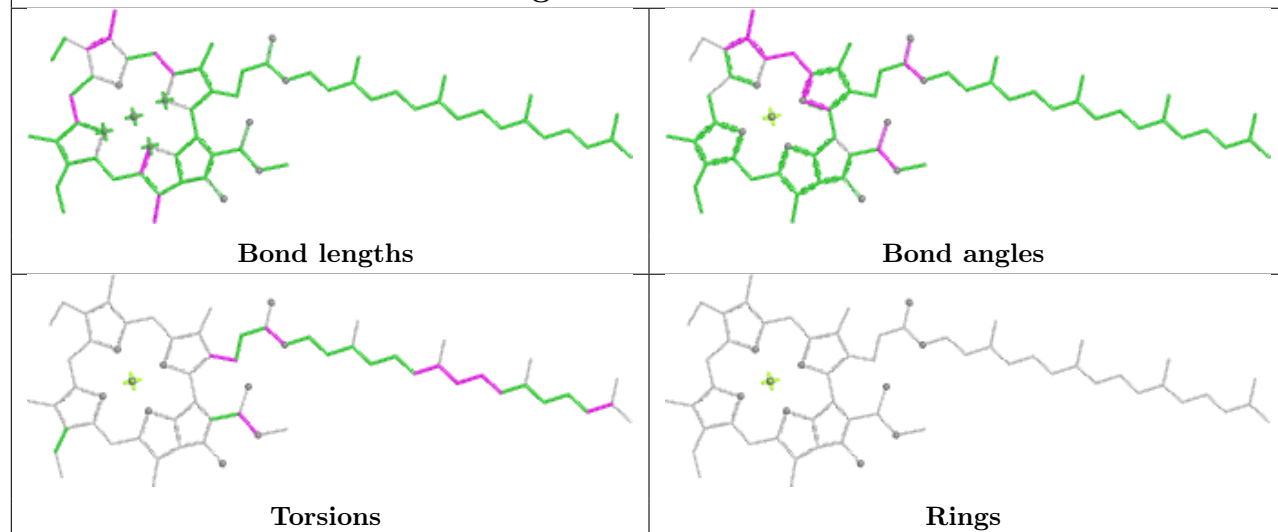




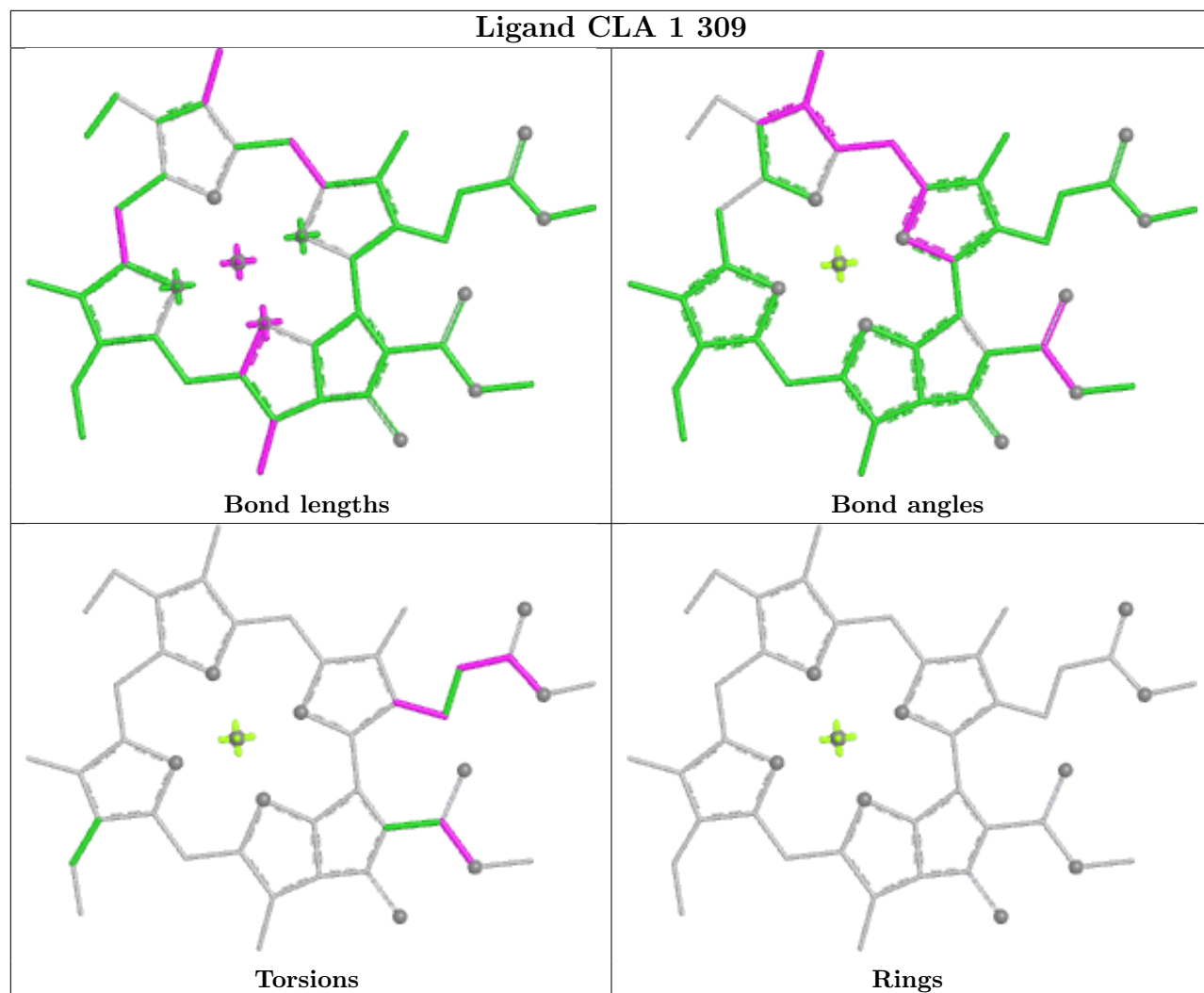
Ligand CHL 7 307



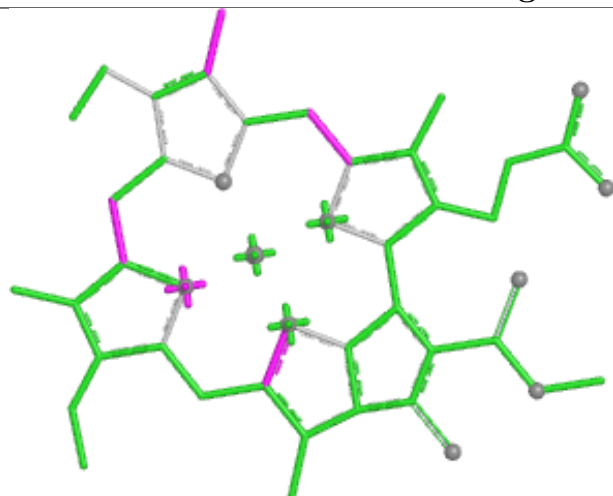
Ligand CLA B 804



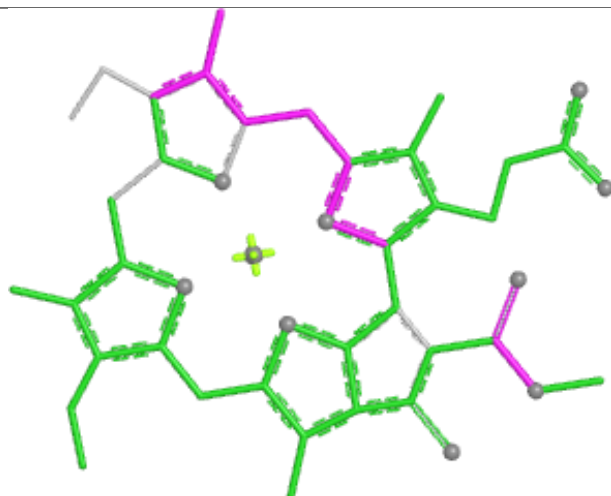
Ligand CLA 1 309



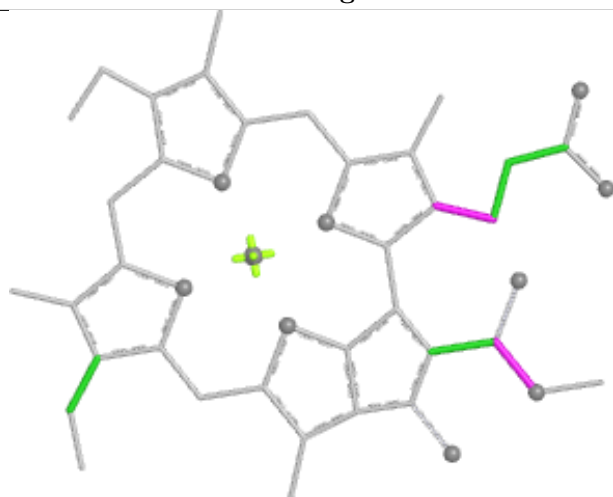
Ligand CLA a 307



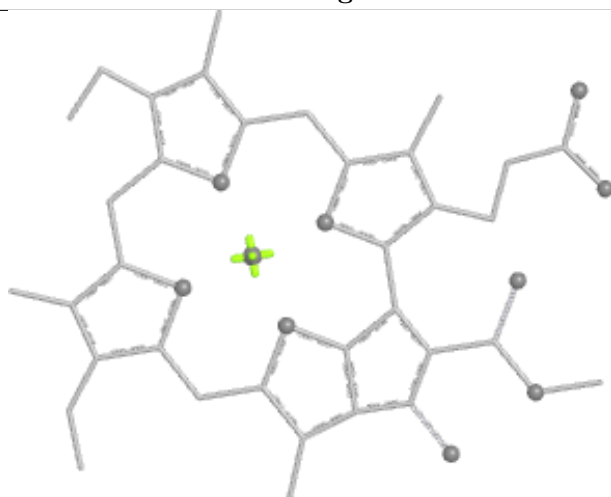
Bond lengths



Bond angles

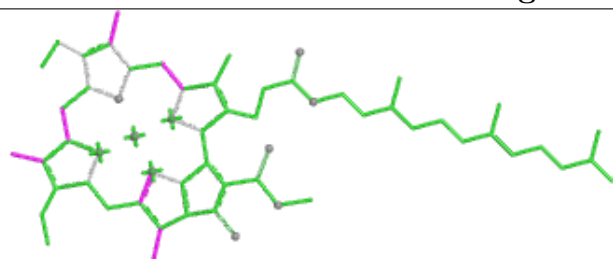


Torsions

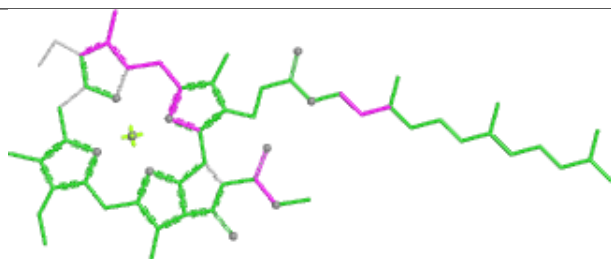


Rings

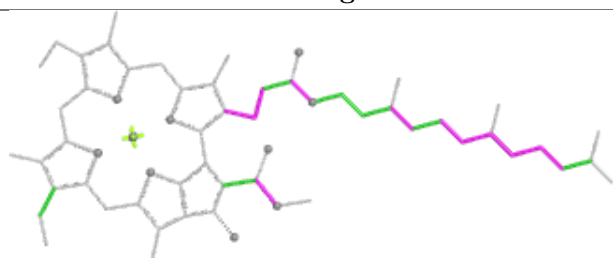
Ligand CLA a 309



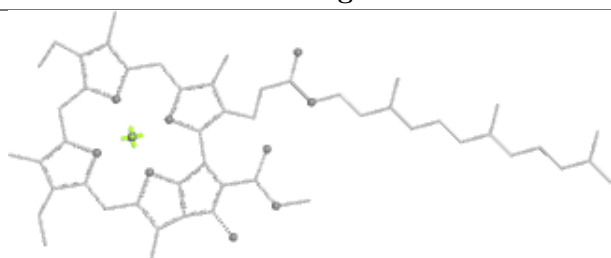
Bond lengths



Bond angles

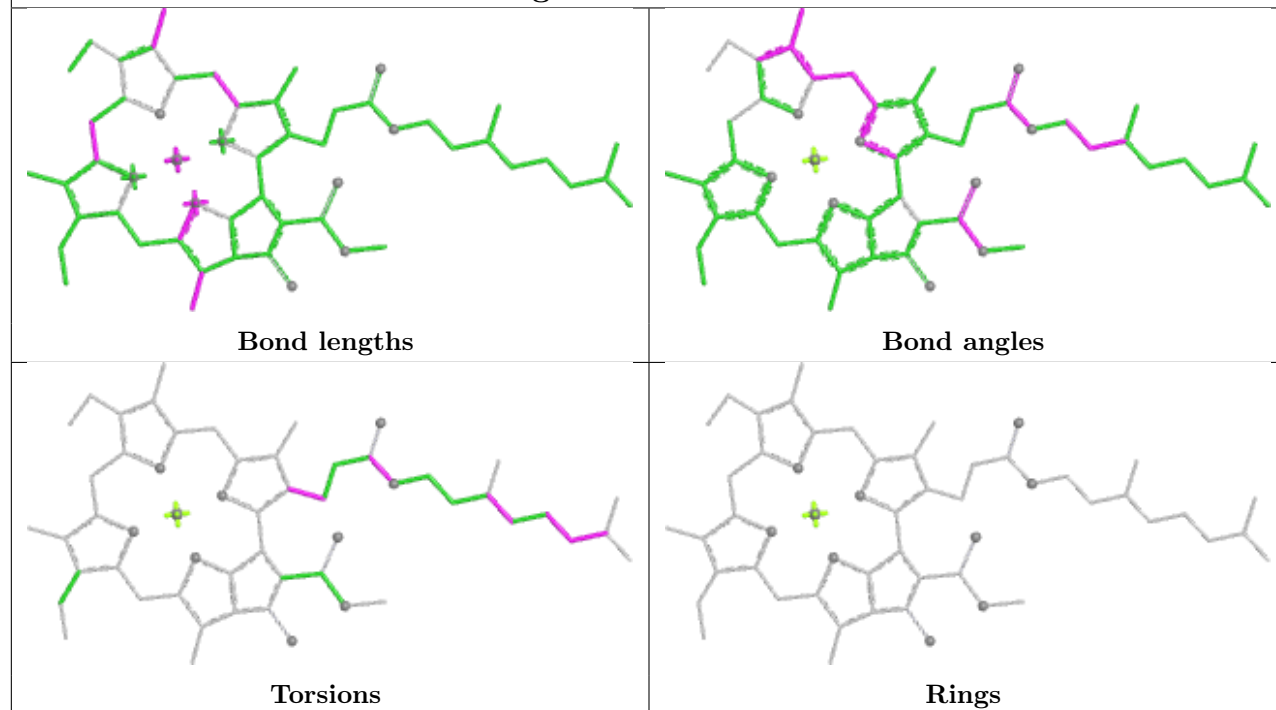


Torsions

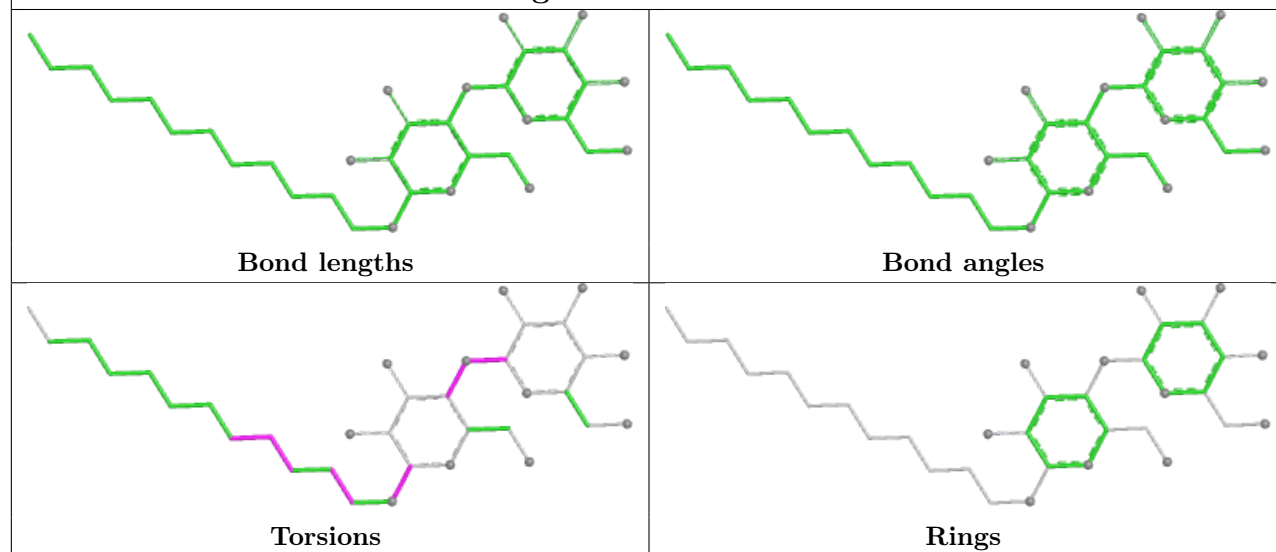


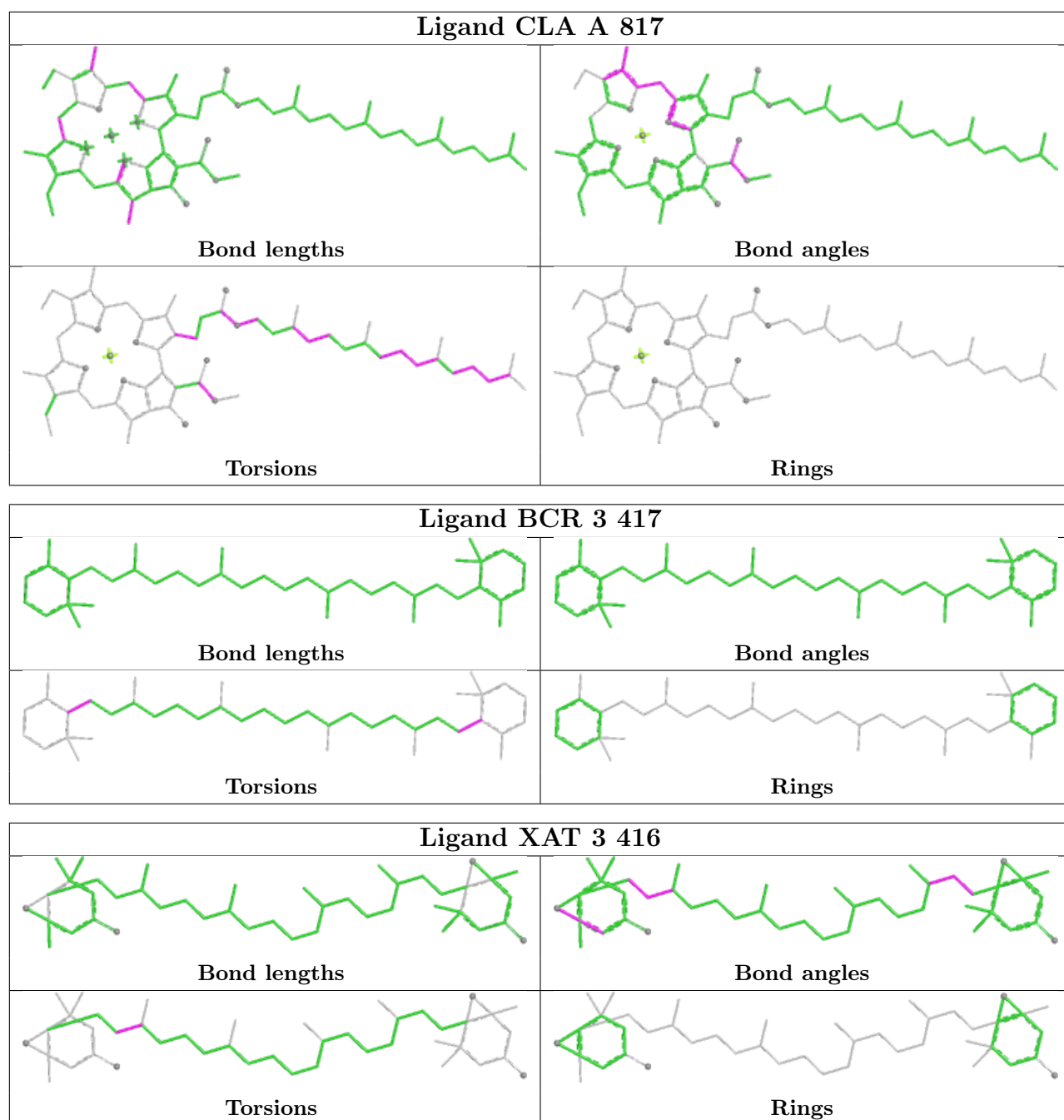
Rings

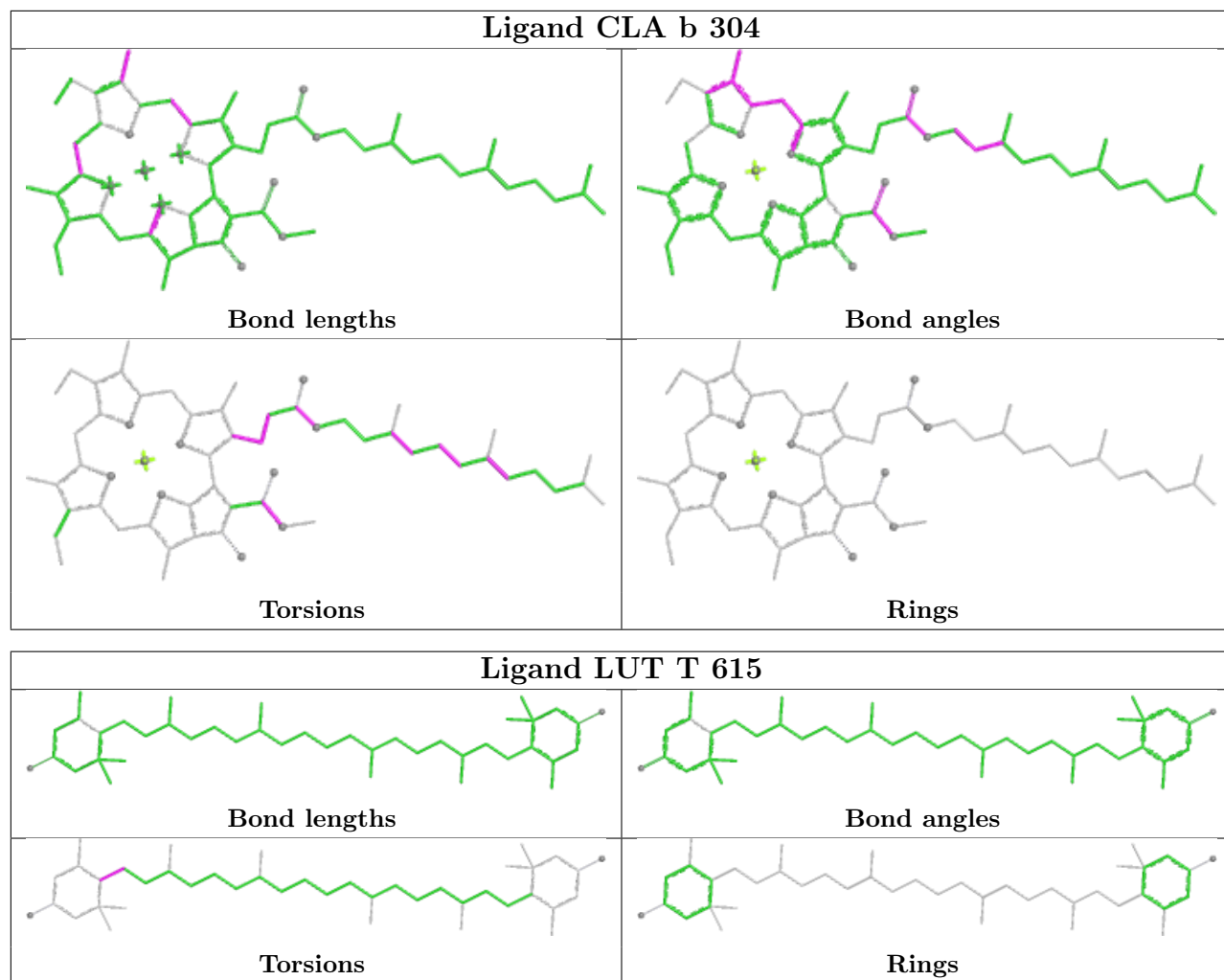
Ligand CLA B 824



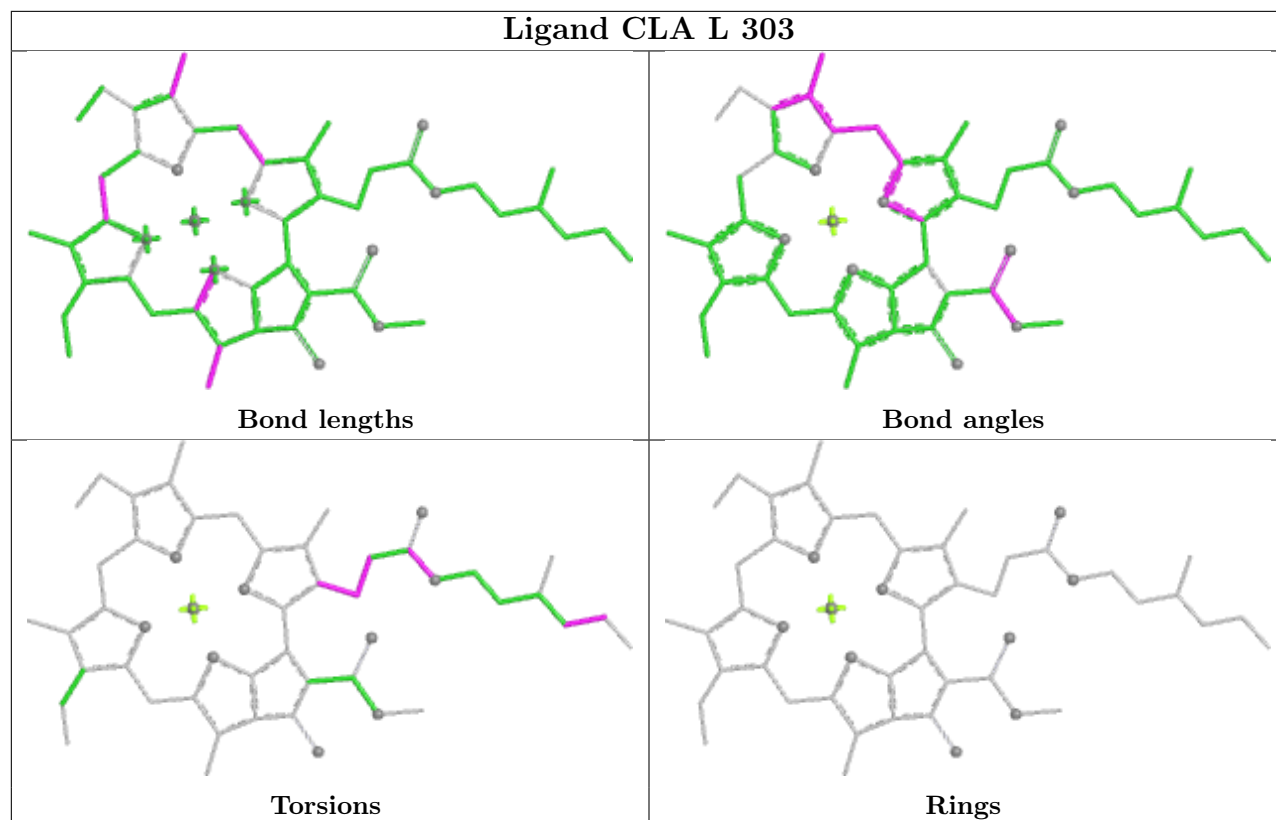
Ligand LMU 1 318



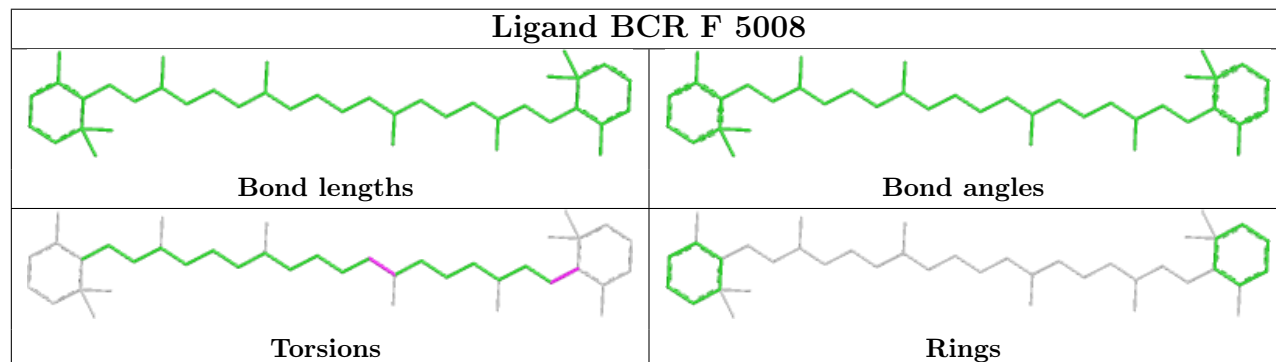


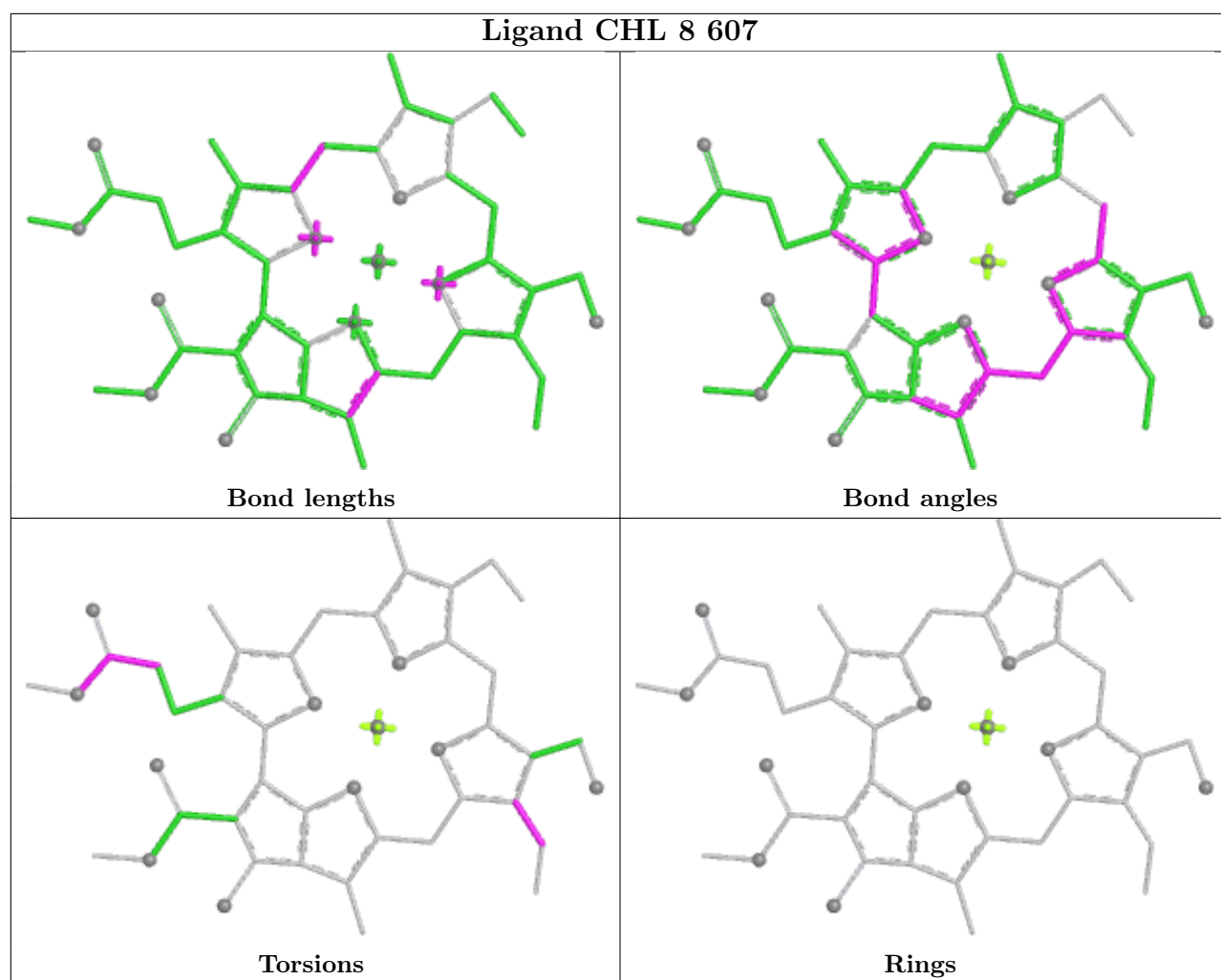


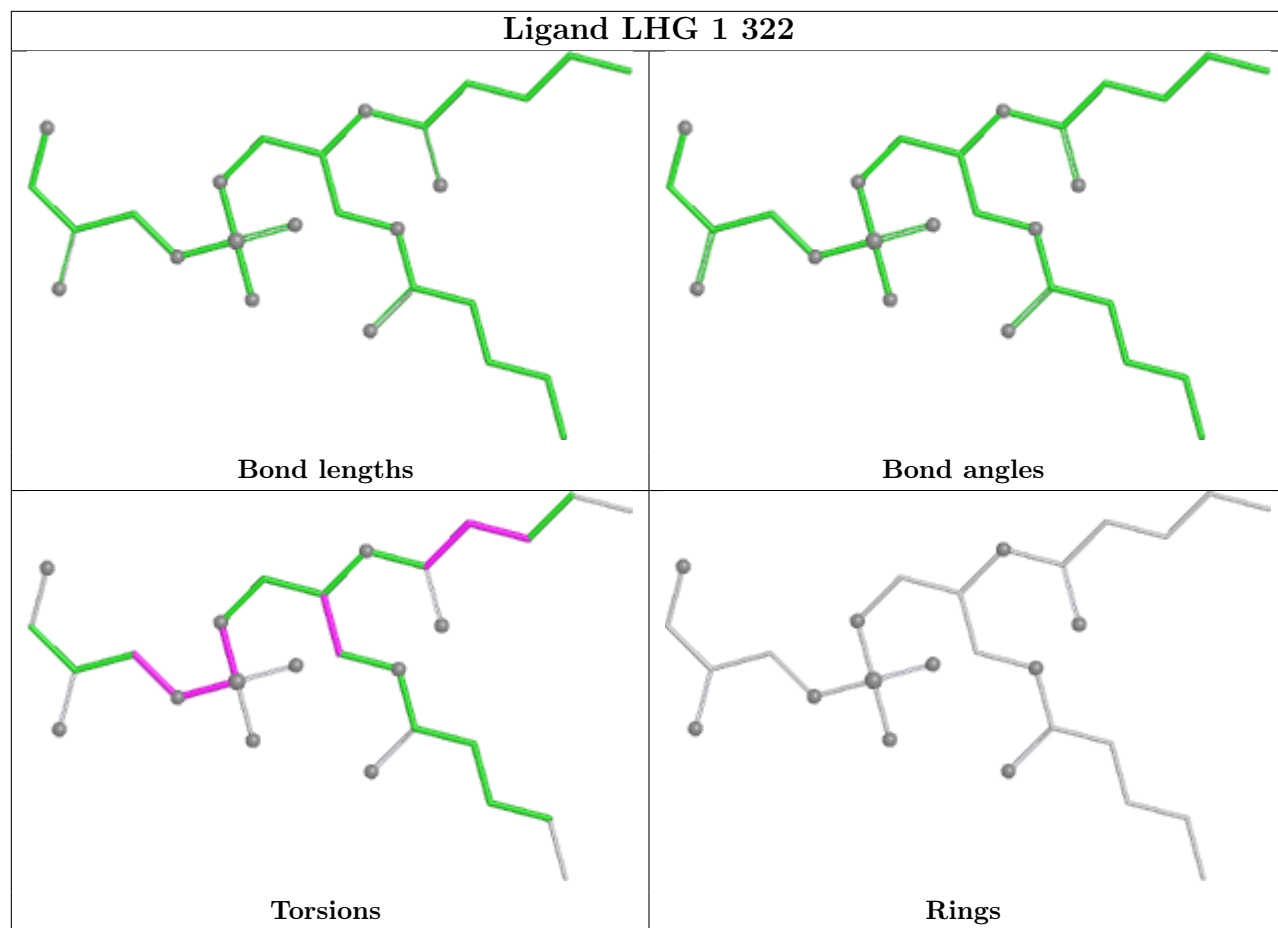
Ligand CLA L 303



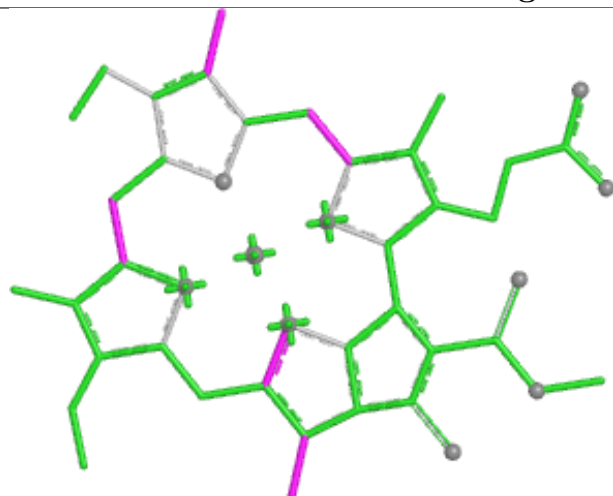
Ligand BCR F 5008



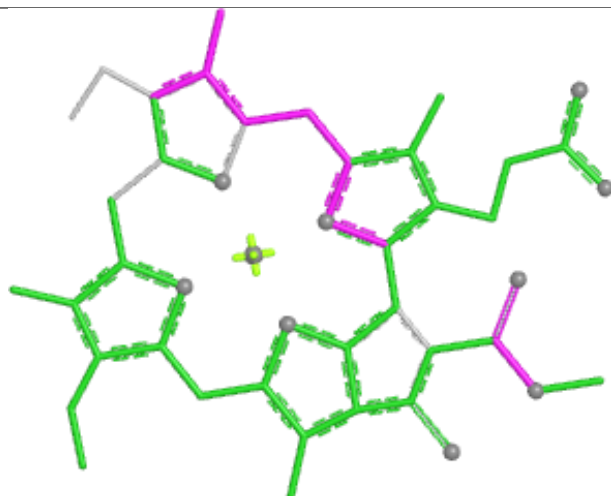




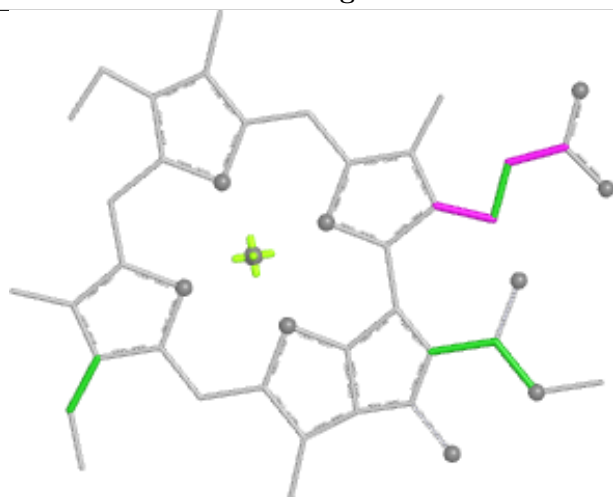
Ligand CLA 7 310



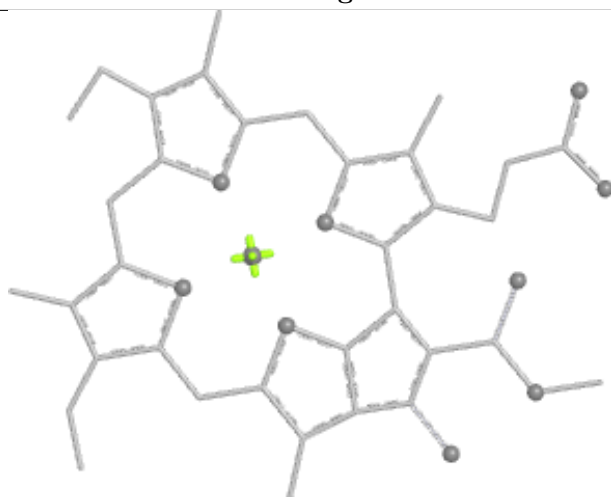
Bond lengths



Bond angles

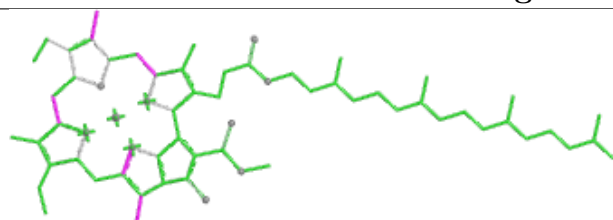


Torsions

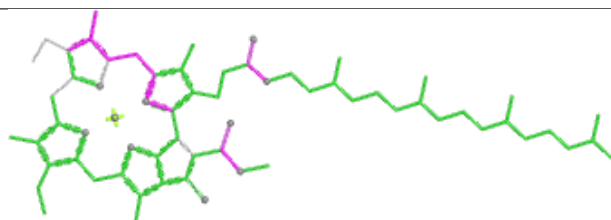


Rings

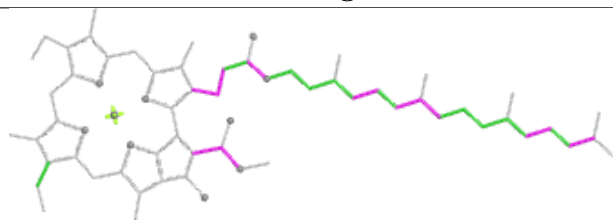
Ligand CLA T 612



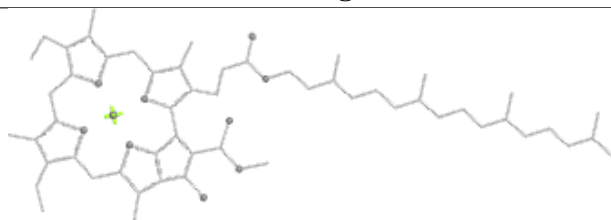
Bond lengths



Bond angles

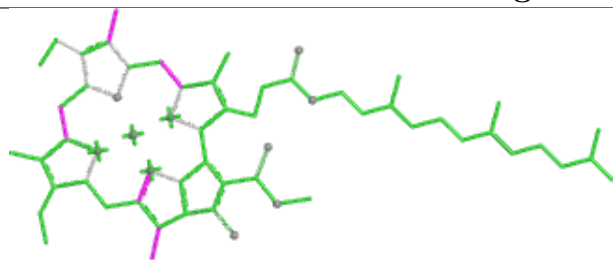


Torsions

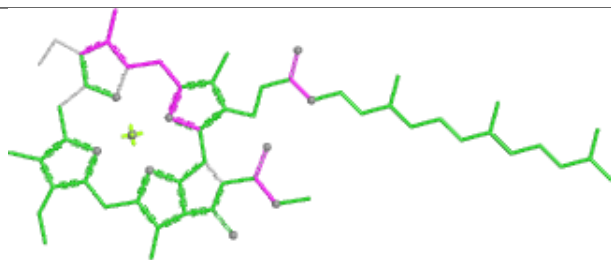


Rings

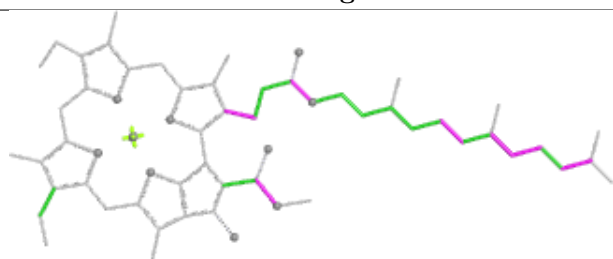
Ligand CLA A 825



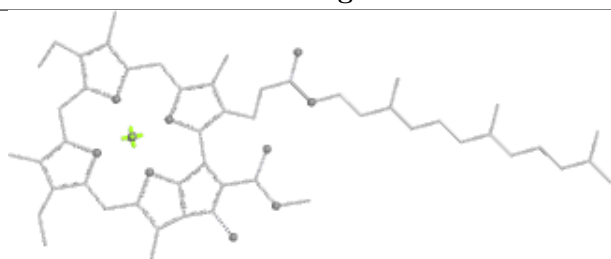
Bond lengths



Bond angles

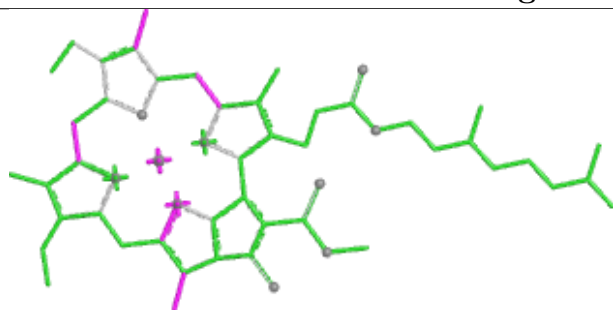


Torsions

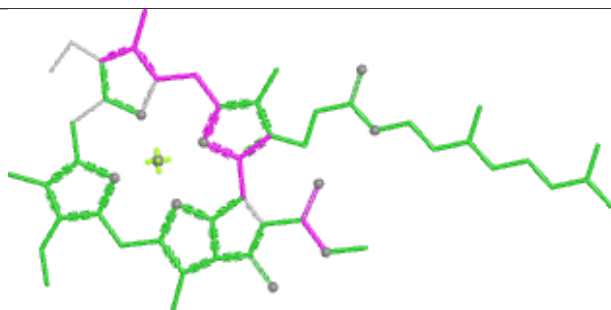


Rings

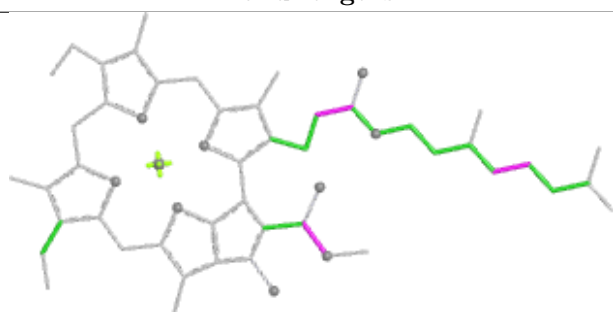
Ligand CLA 9 603



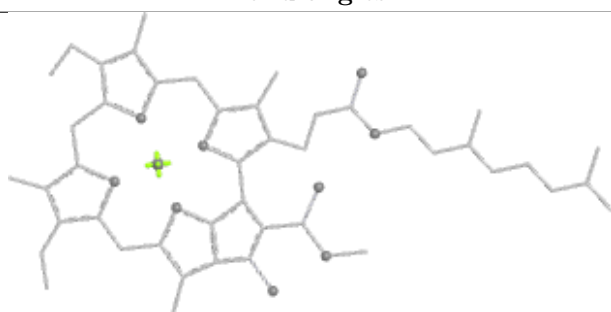
Bond lengths



Bond angles

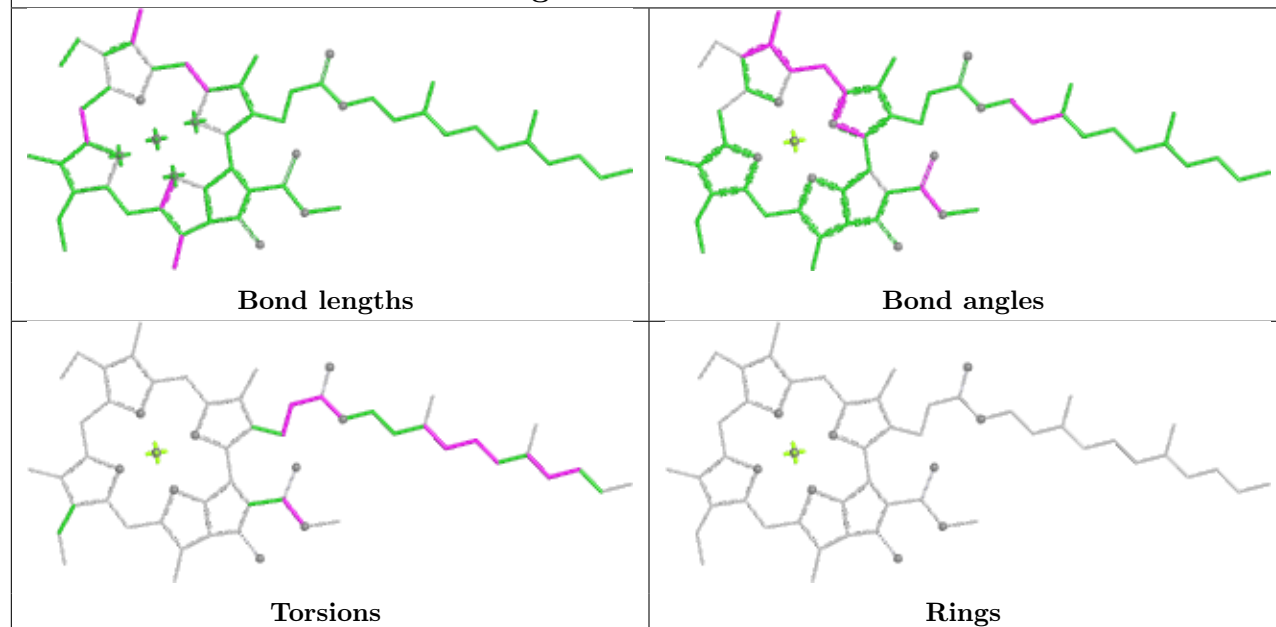


Torsions

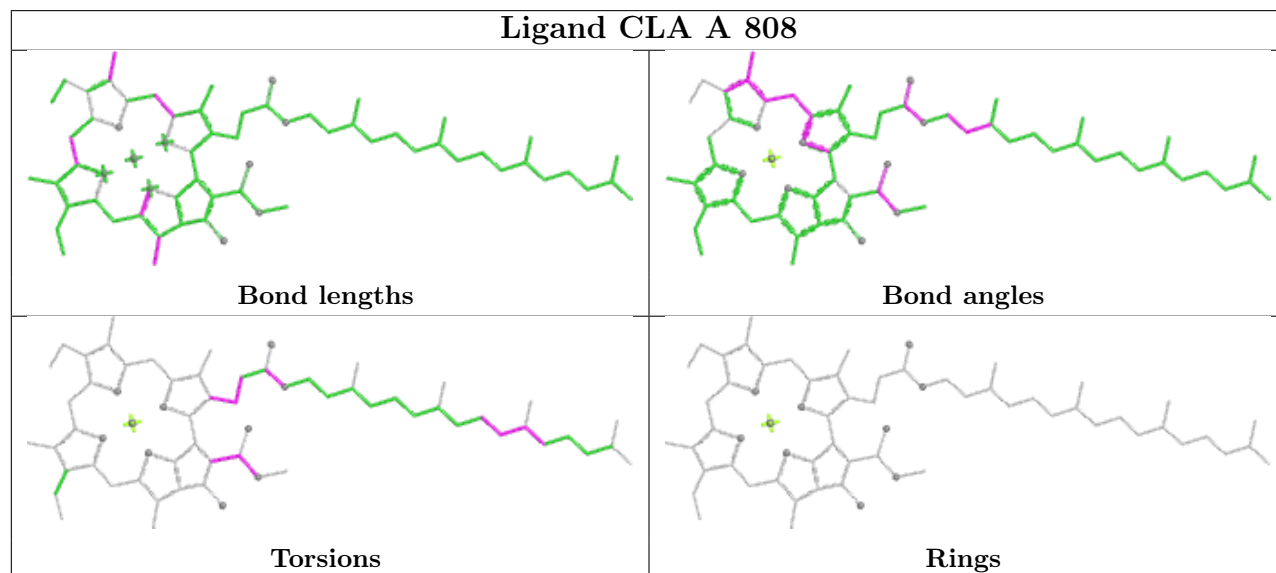


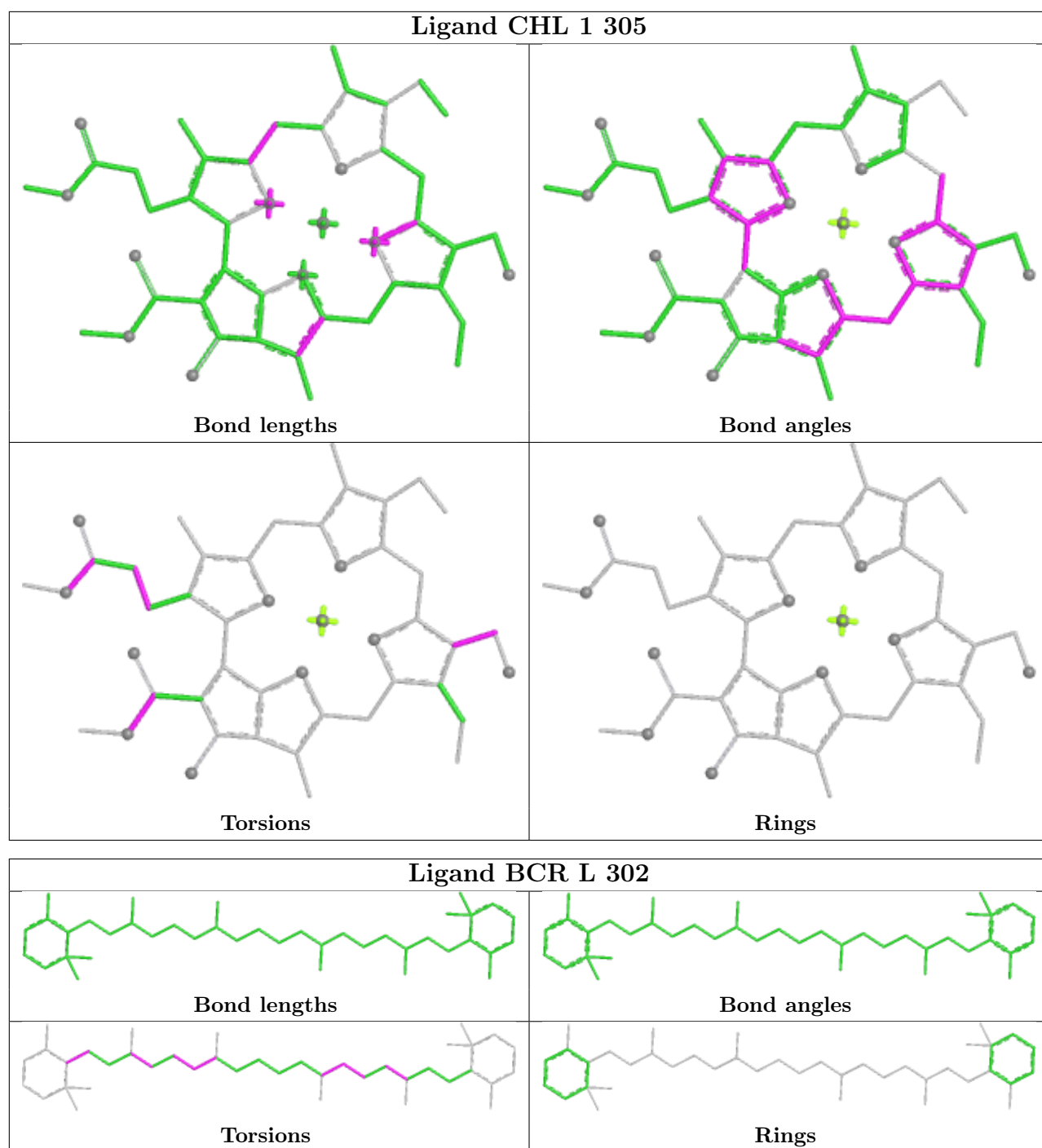
Rings

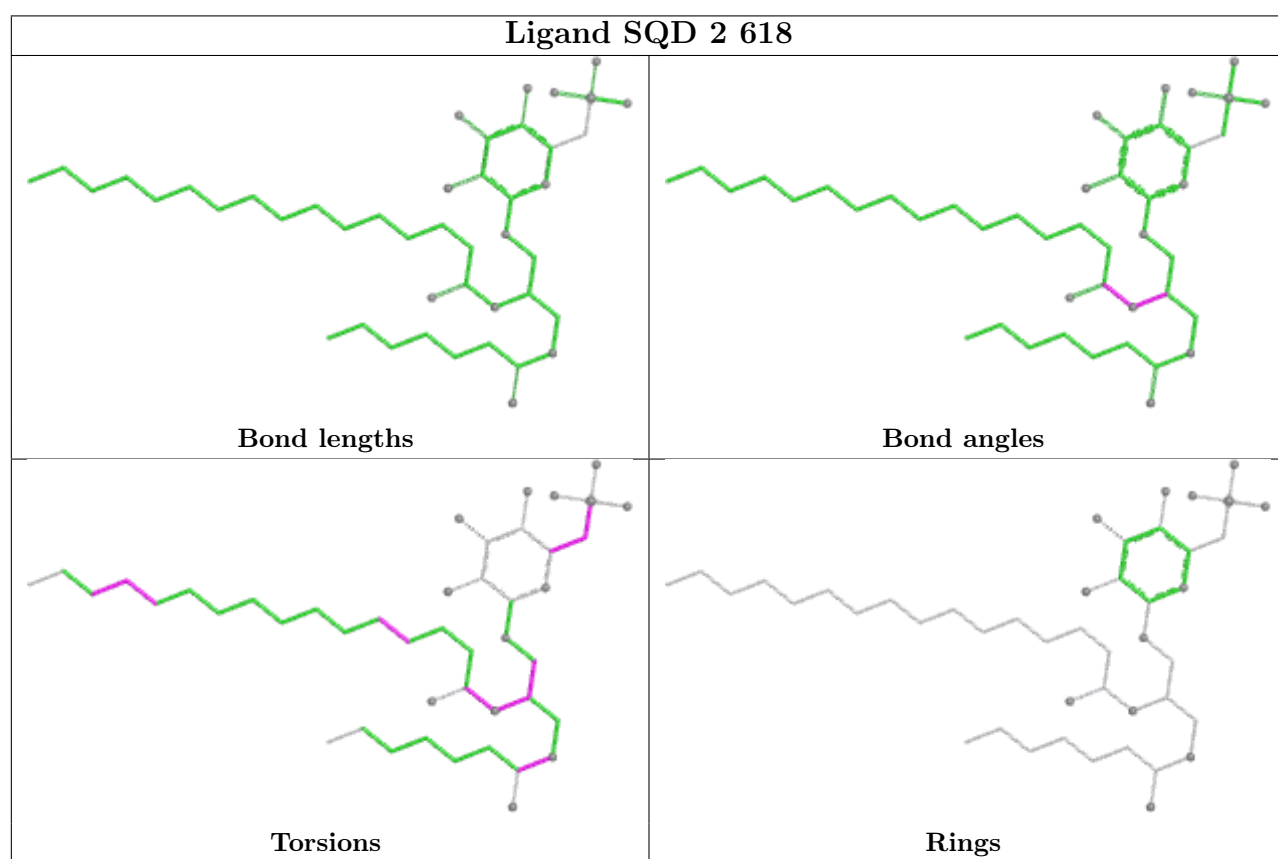
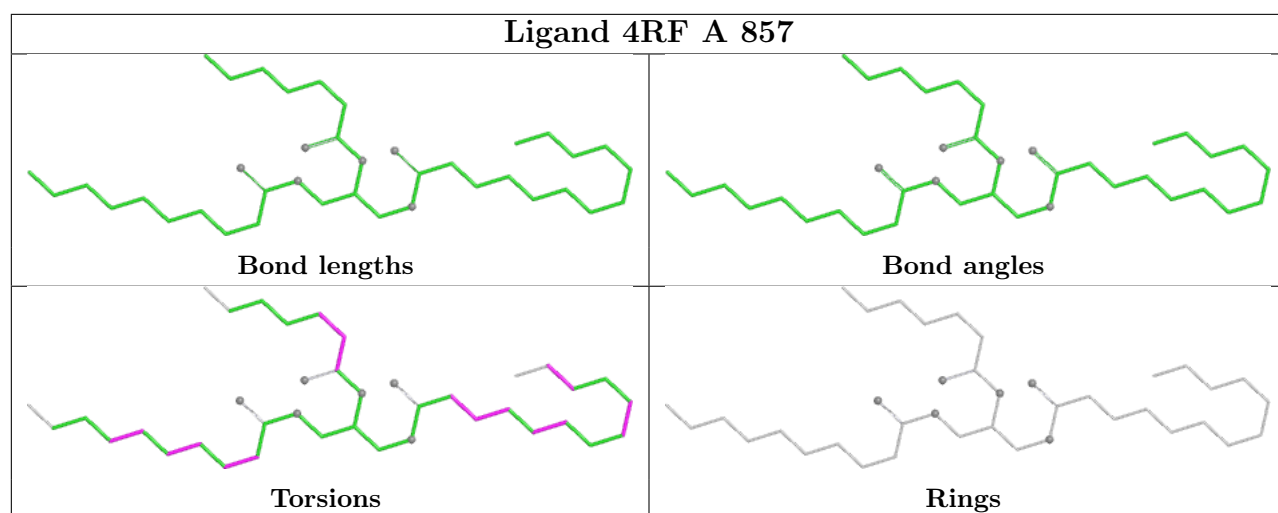
Ligand CLA A 822



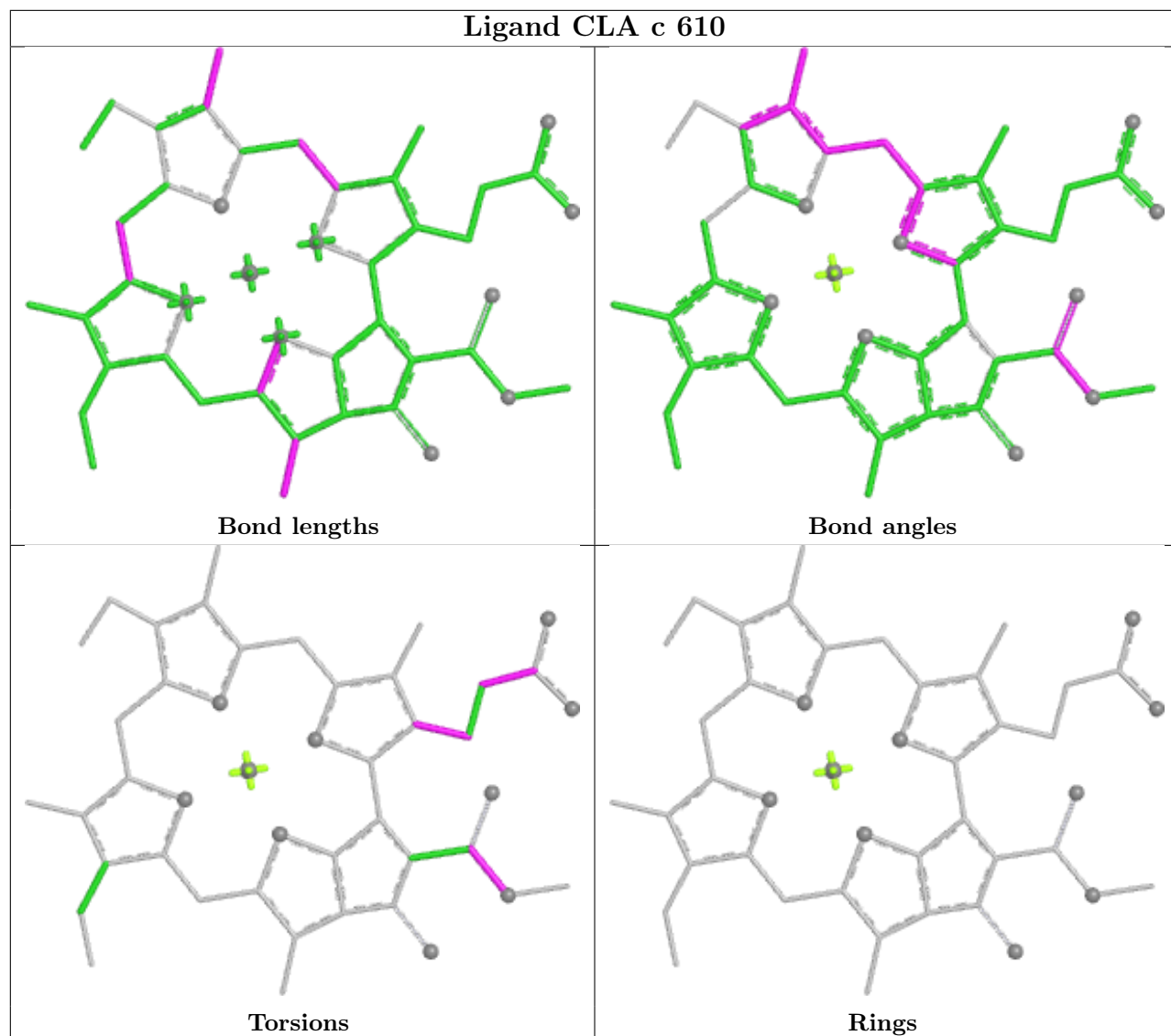
Ligand CLA A 808



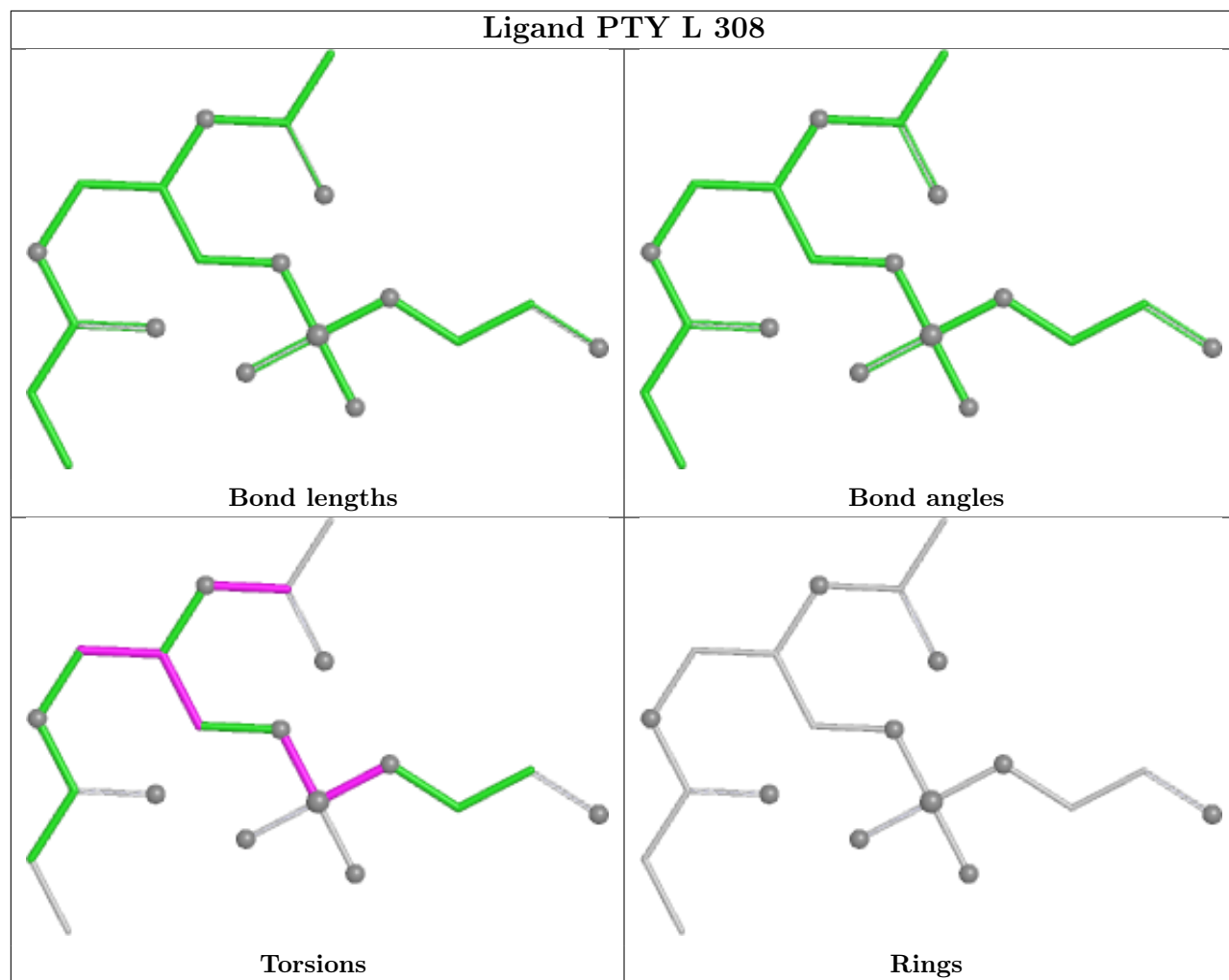




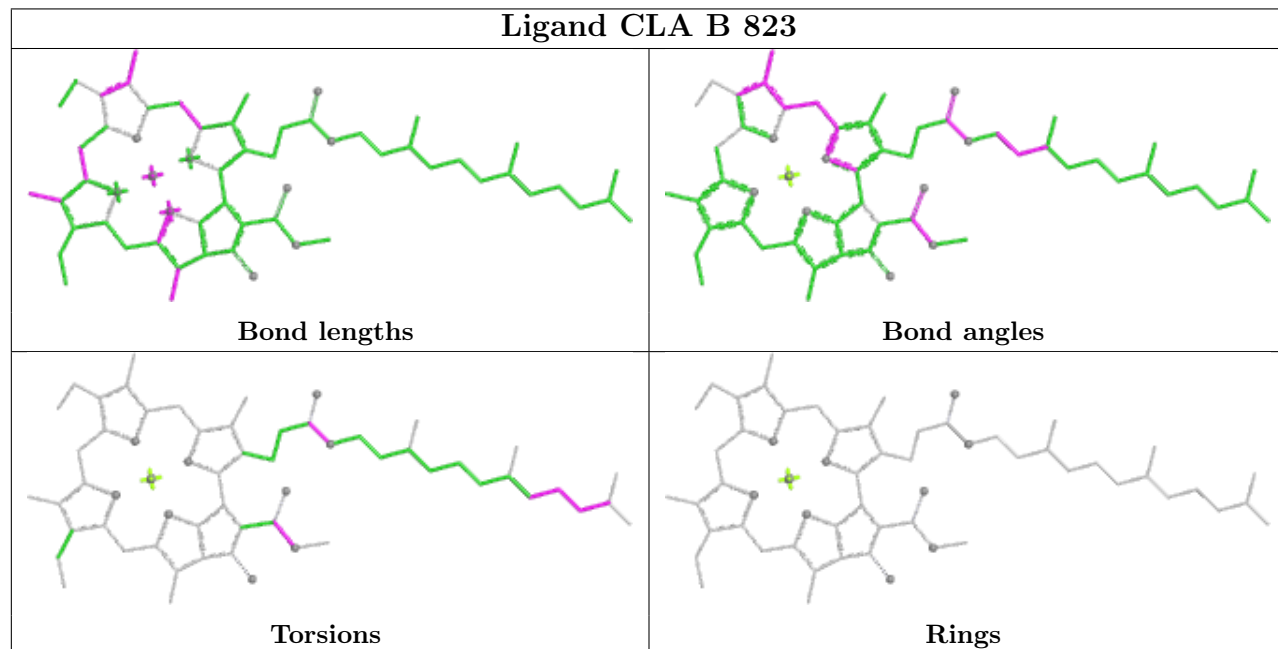
Ligand CLA c 610

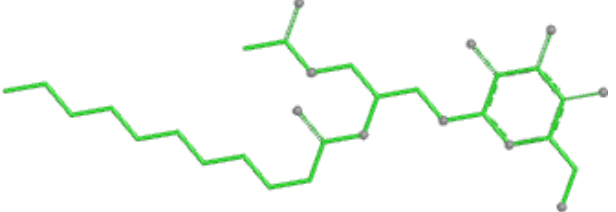
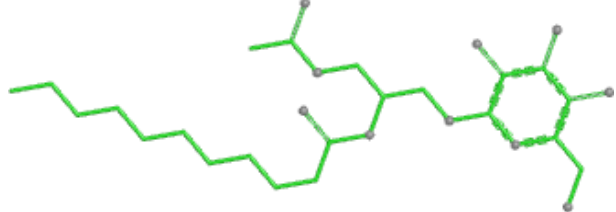
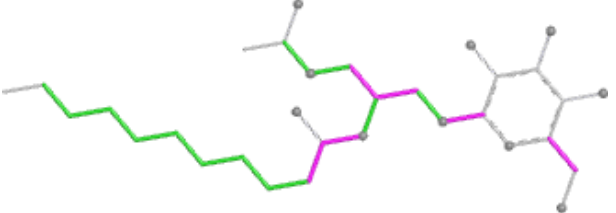
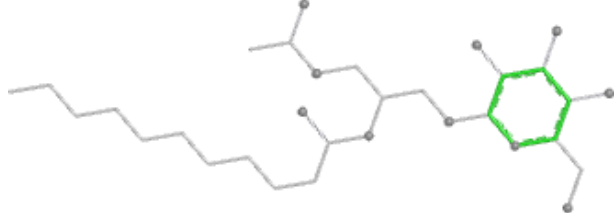


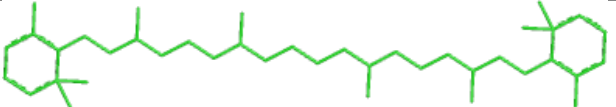
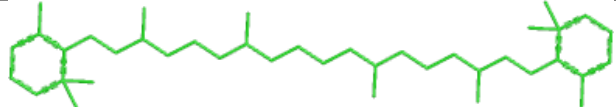
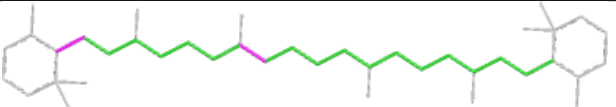
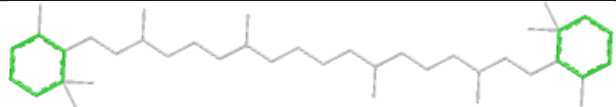
Ligand PTY L 308



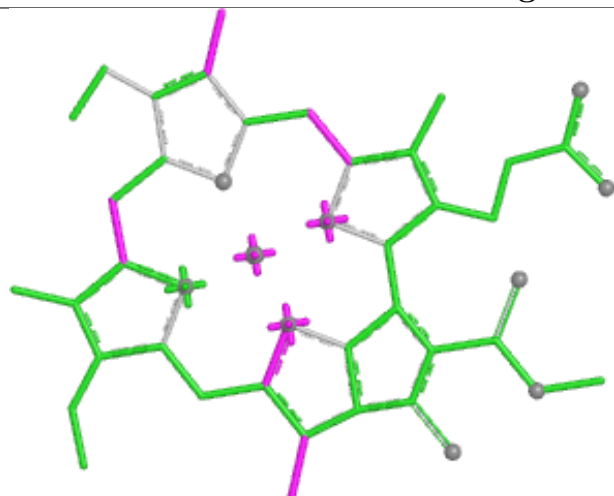
Ligand CLA B 823



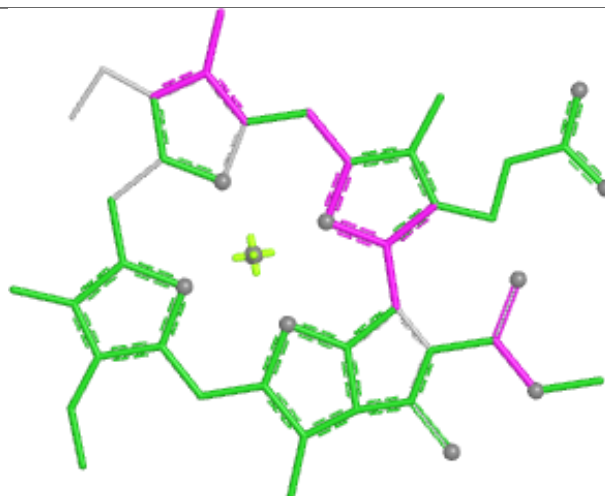
Ligand LMG A 801			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR I 203			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

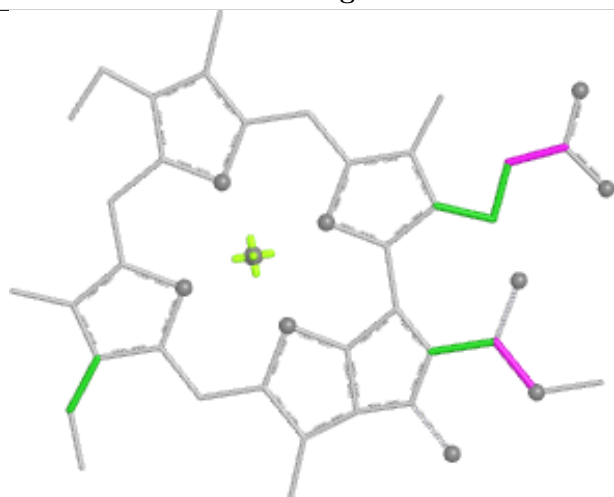
Ligand CLA 9 605



Bond lengths



Bond angles

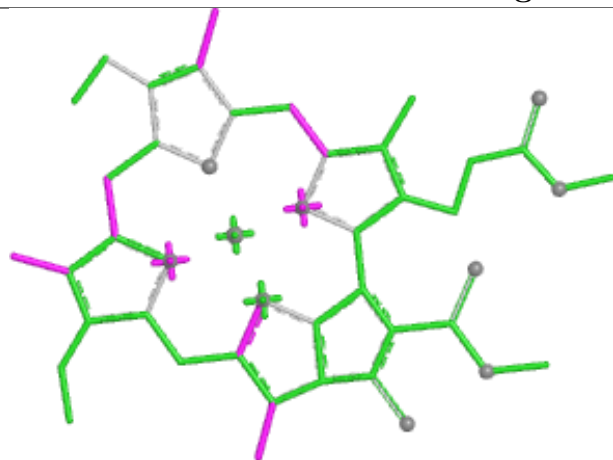


Torsions

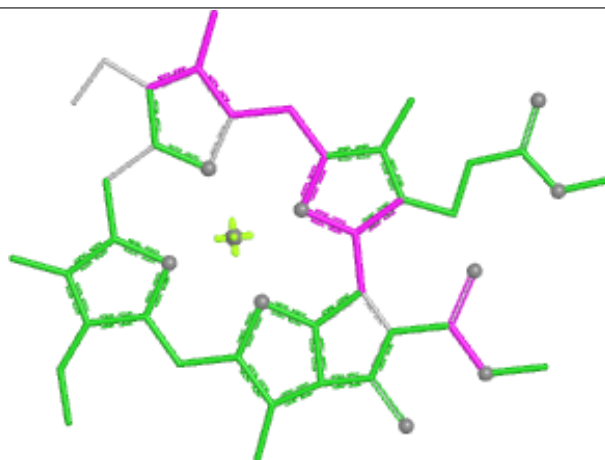


Rings

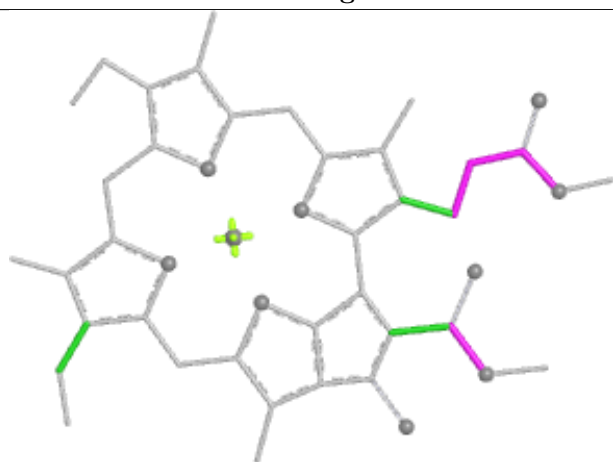
Ligand CLA T 606



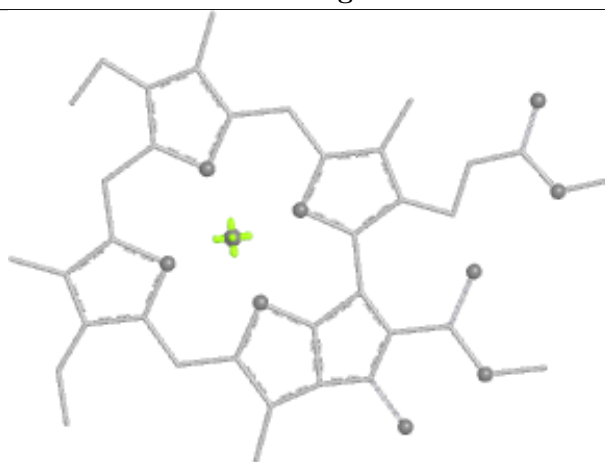
Bond lengths



Bond angles

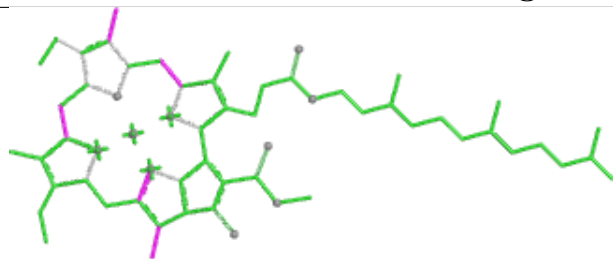


Torsions

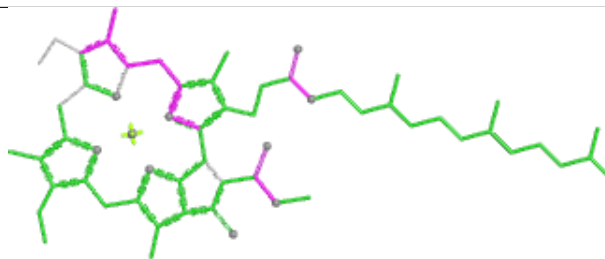


Rings

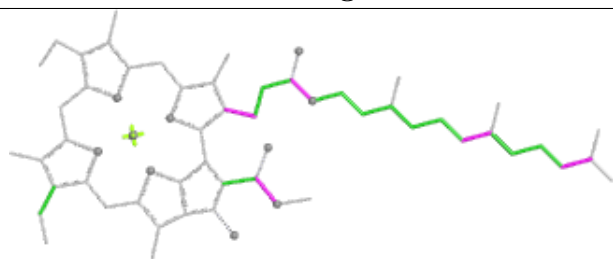
Ligand CLA 1 311



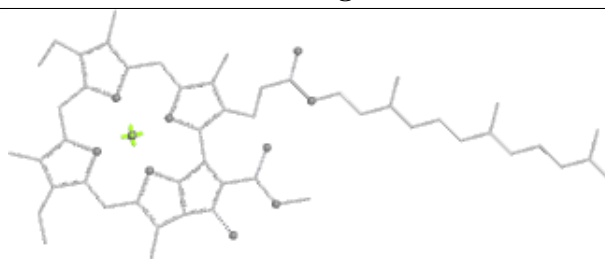
Bond lengths



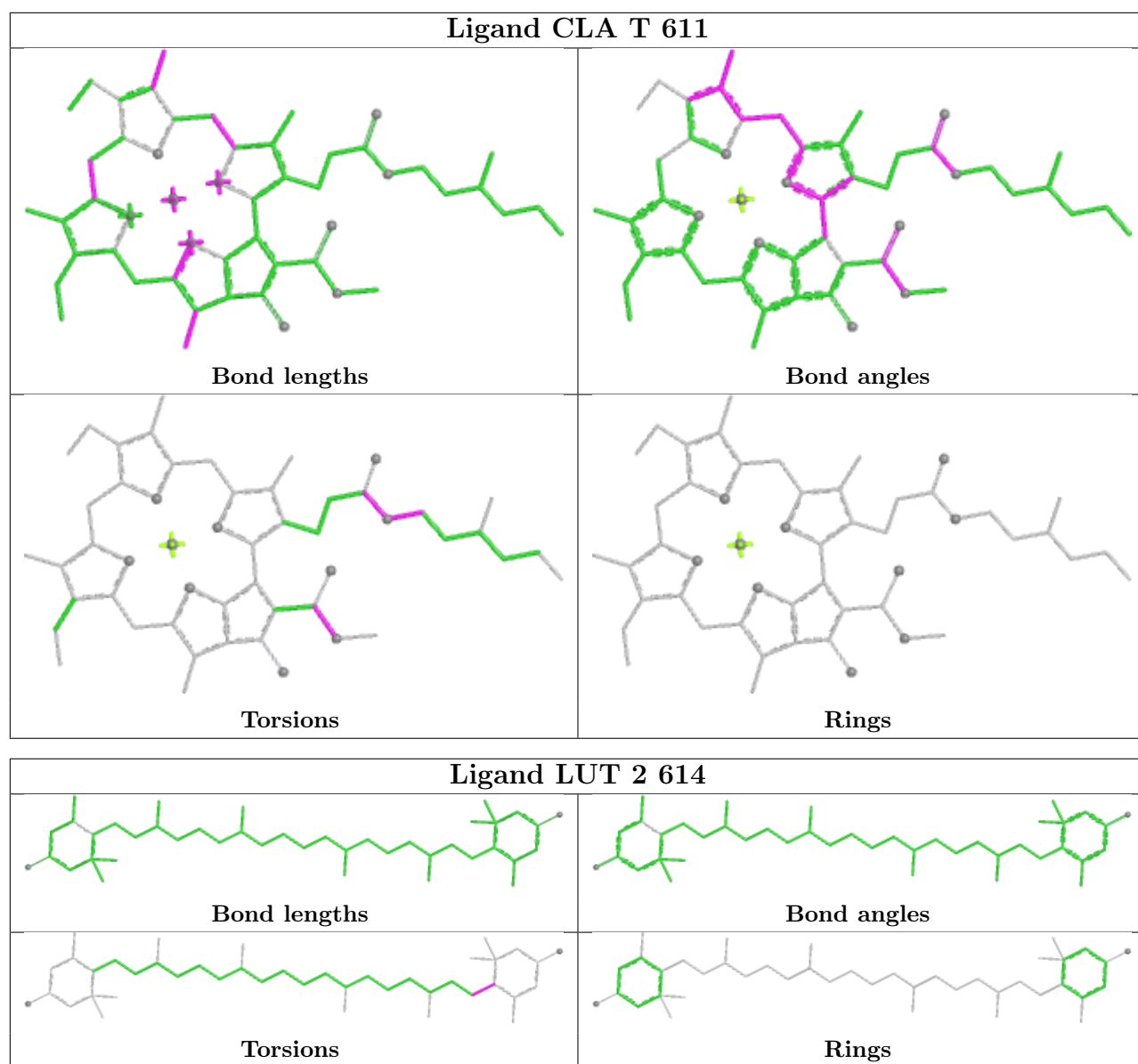
Bond angles

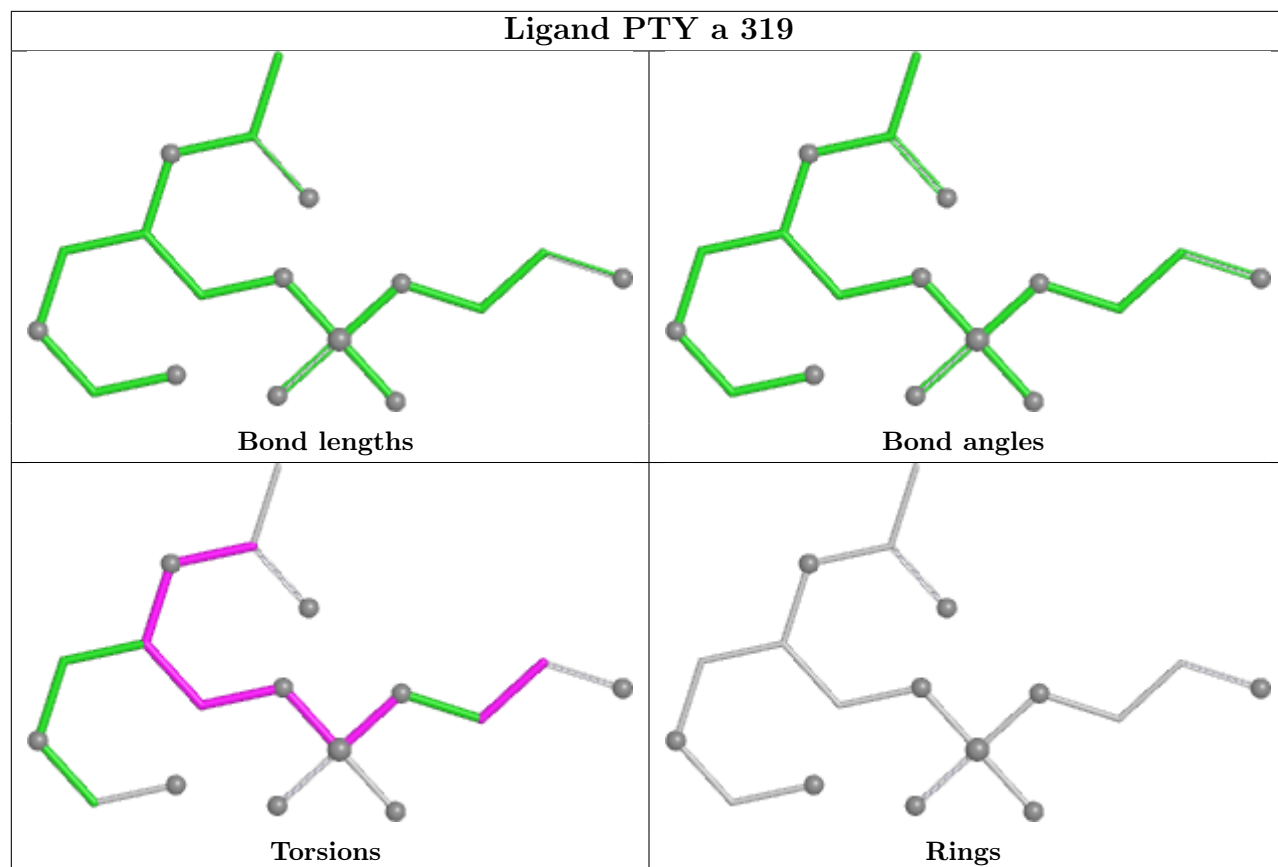


Torsions

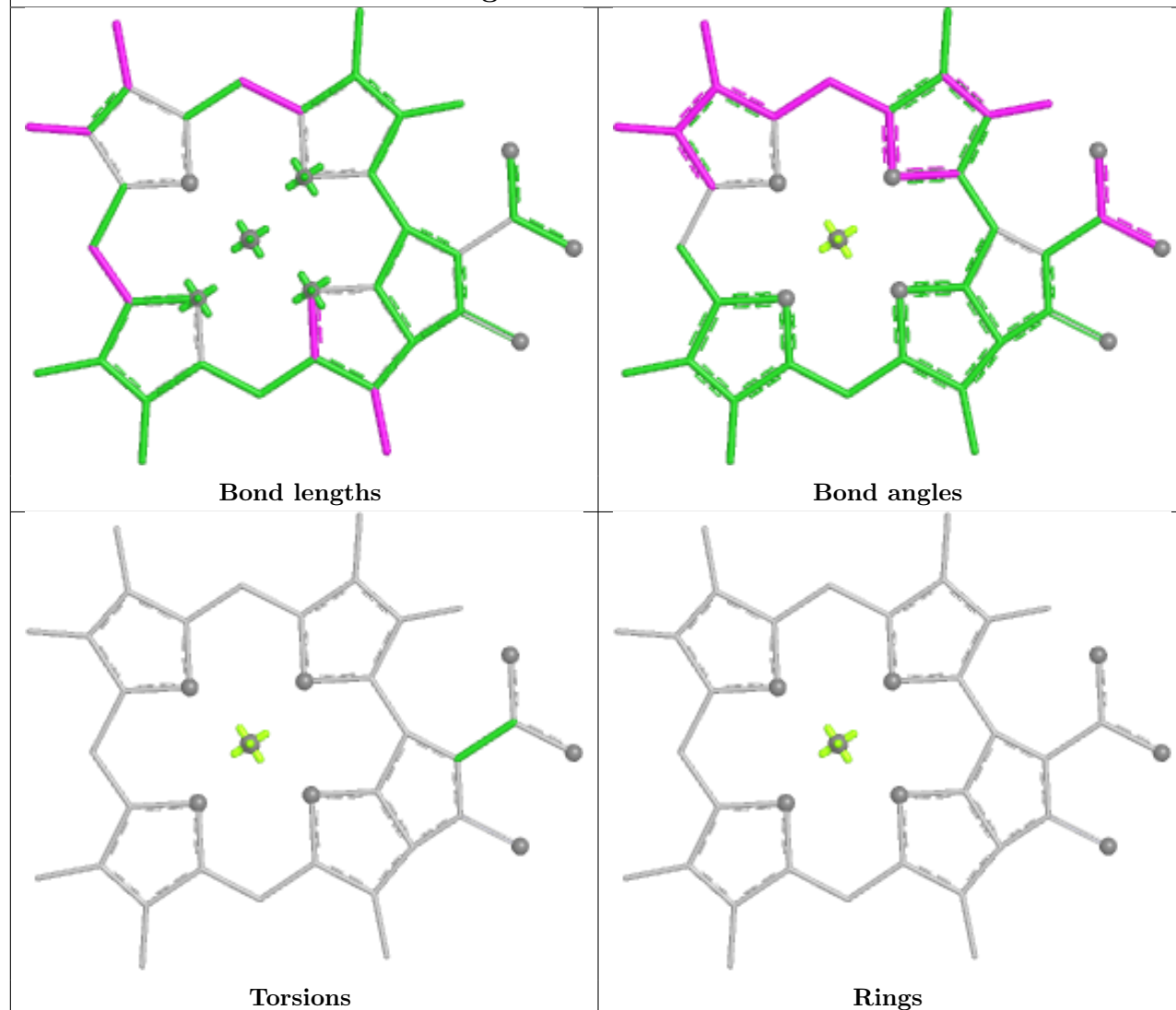


Rings

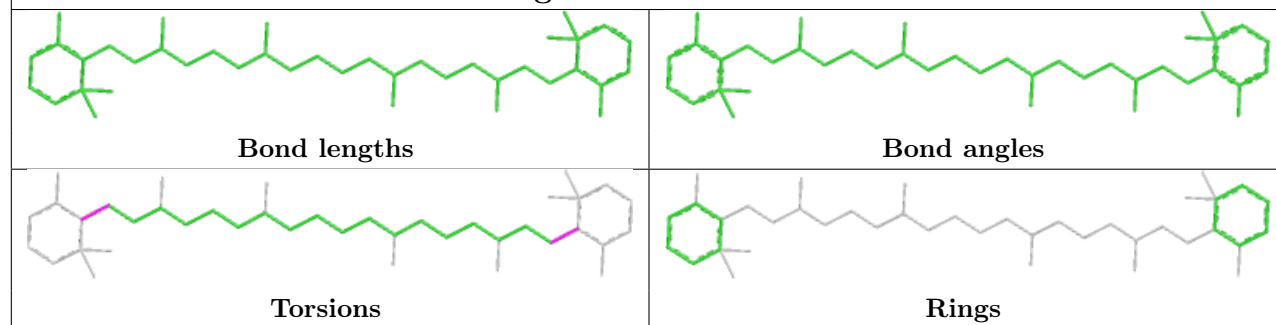


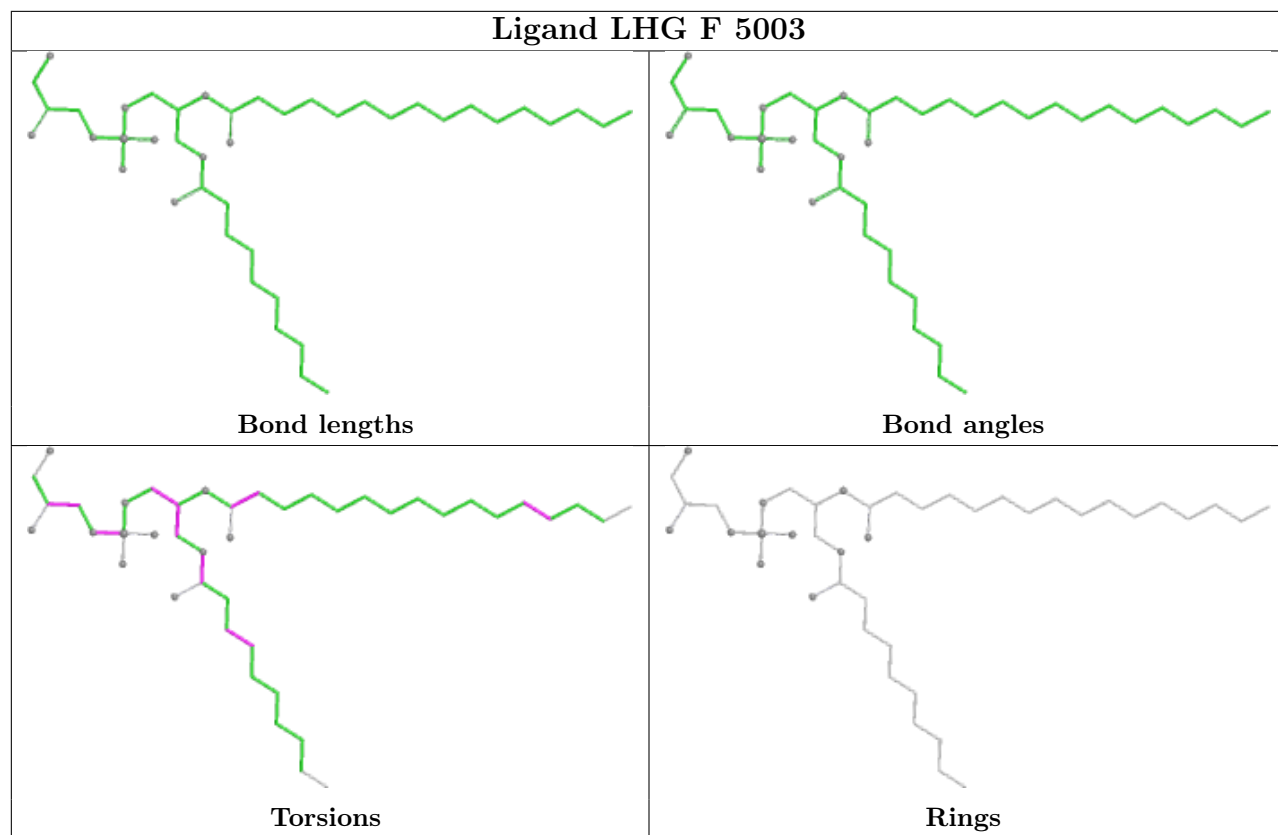


Ligand CLA O 2002

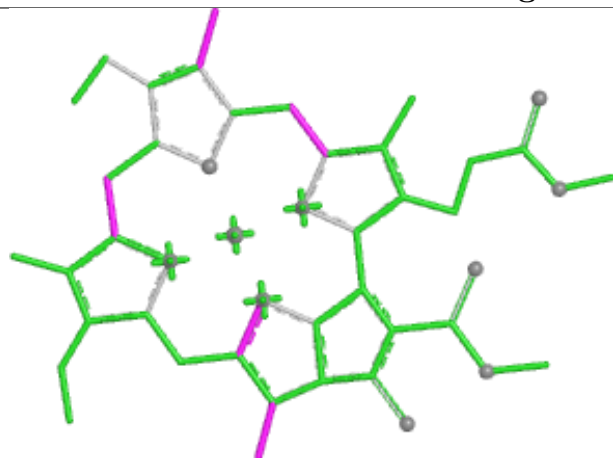


Ligand BCR 8 618

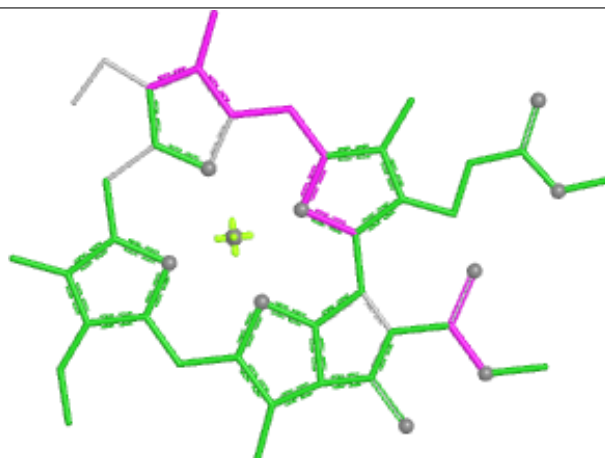




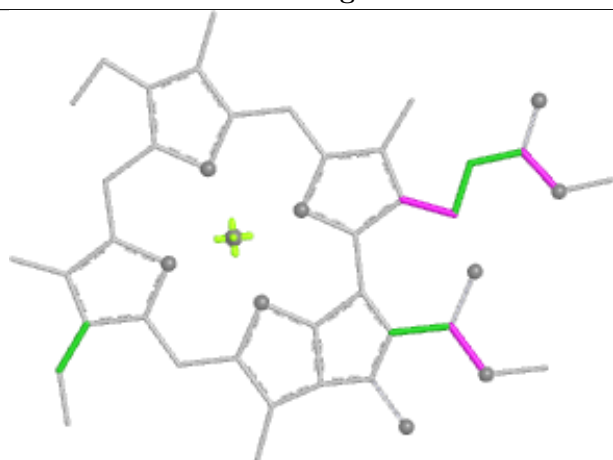
Ligand CLA 8 614



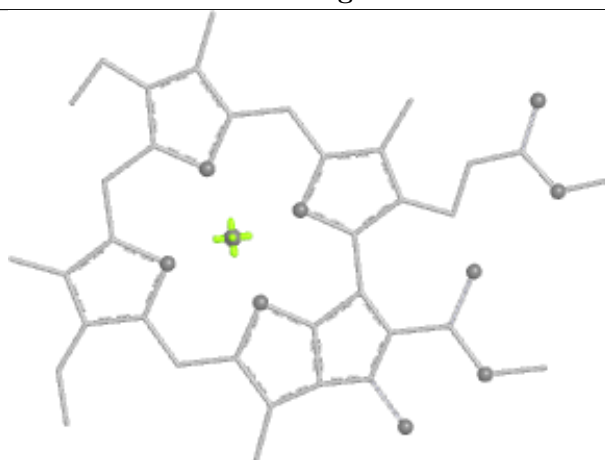
Bond lengths



Bond angles

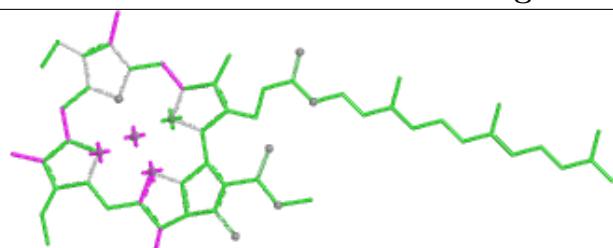


Torsions

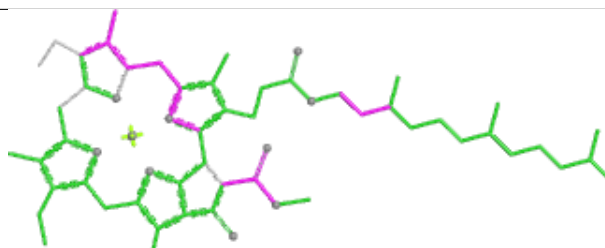


Rings

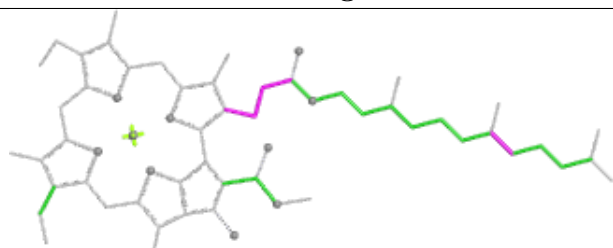
Ligand CLA B 820



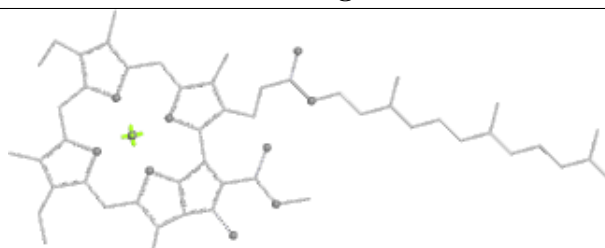
Bond lengths



Bond angles

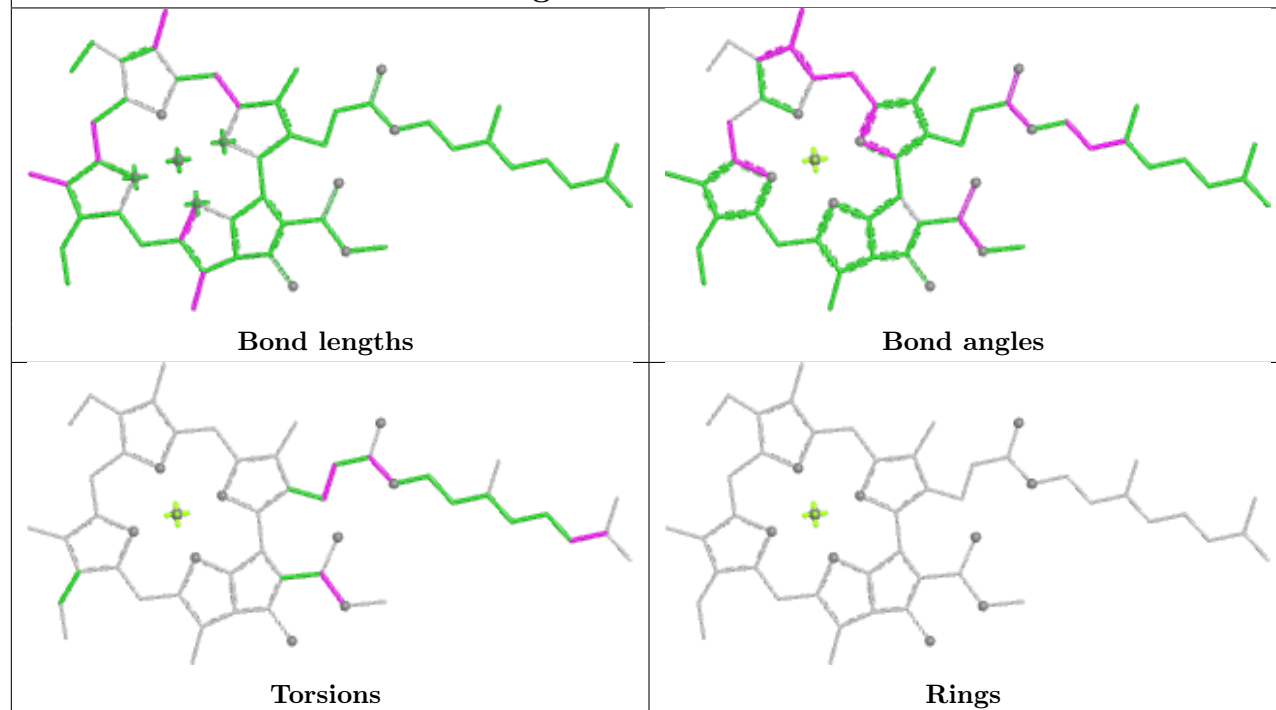


Torsions

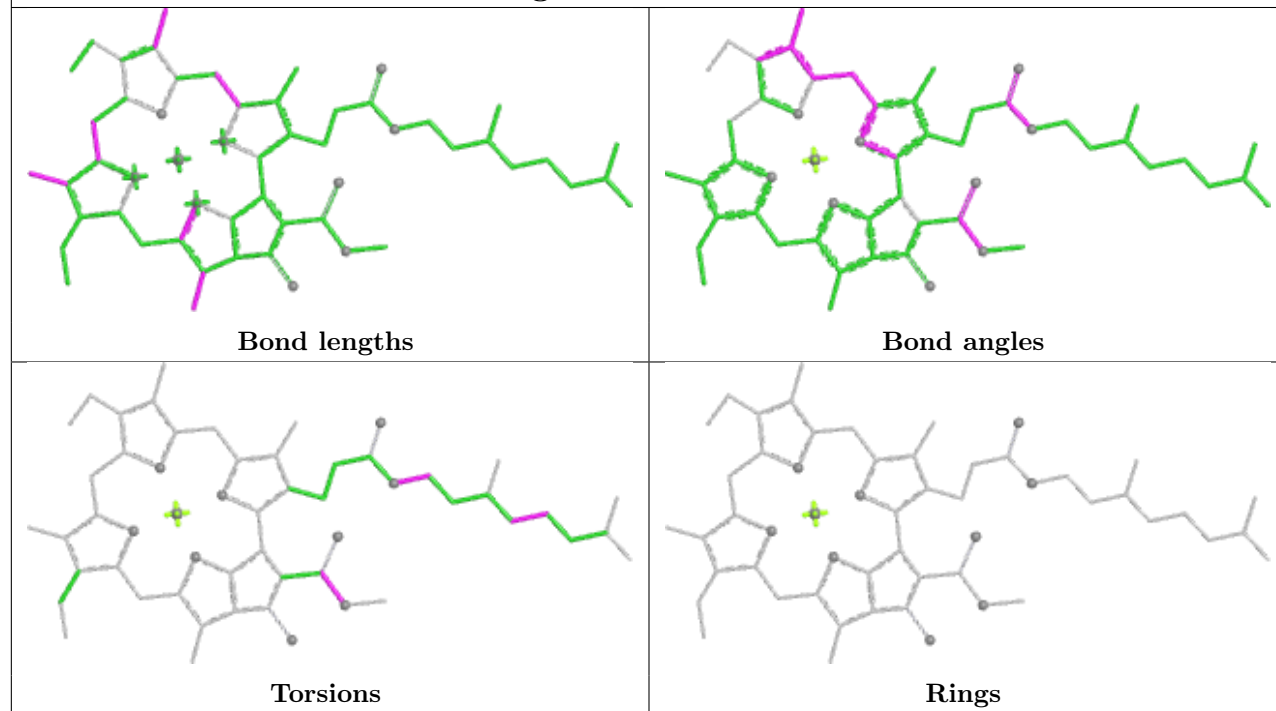


Rings

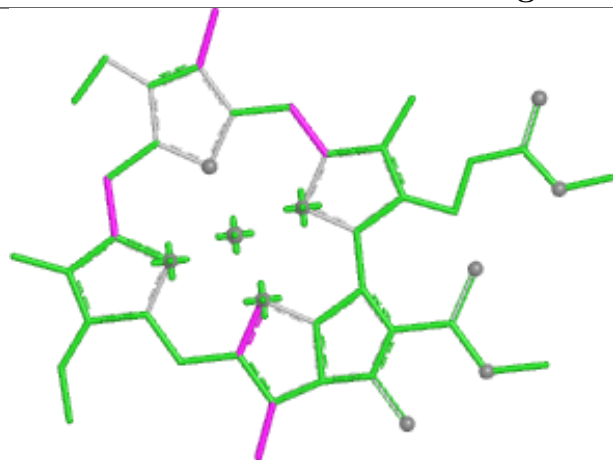
Ligand CLA T 609



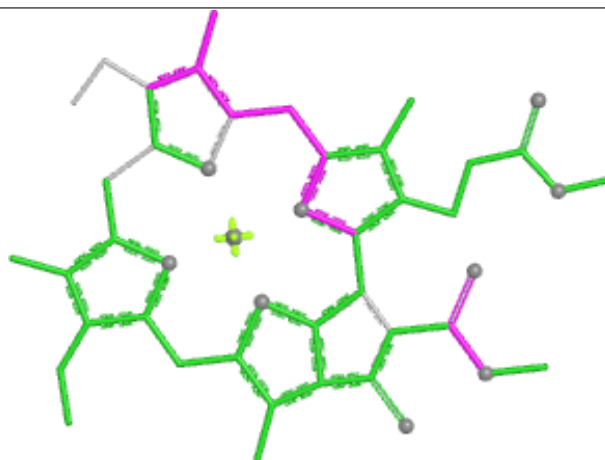
Ligand CLA A 833



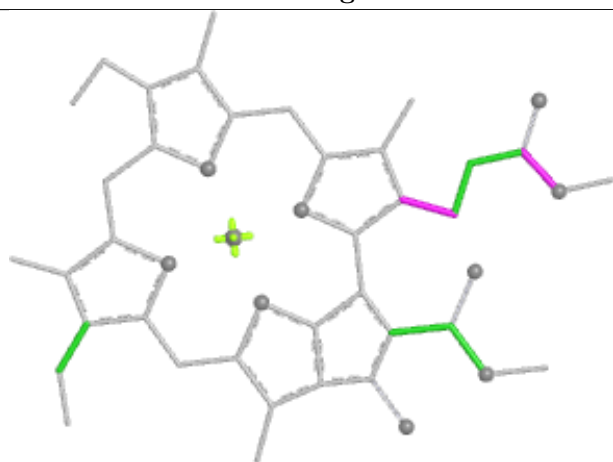
Ligand CLA b 310



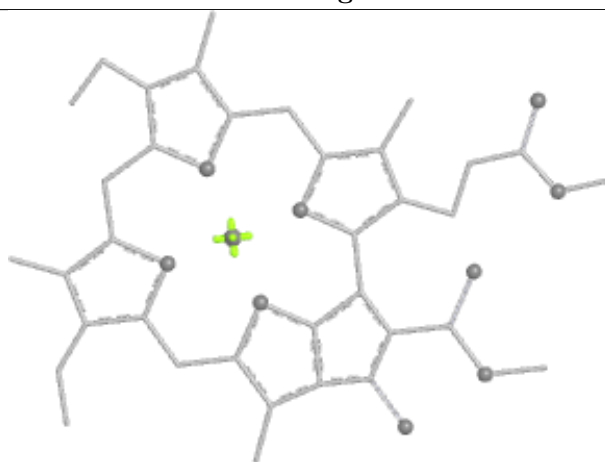
Bond lengths



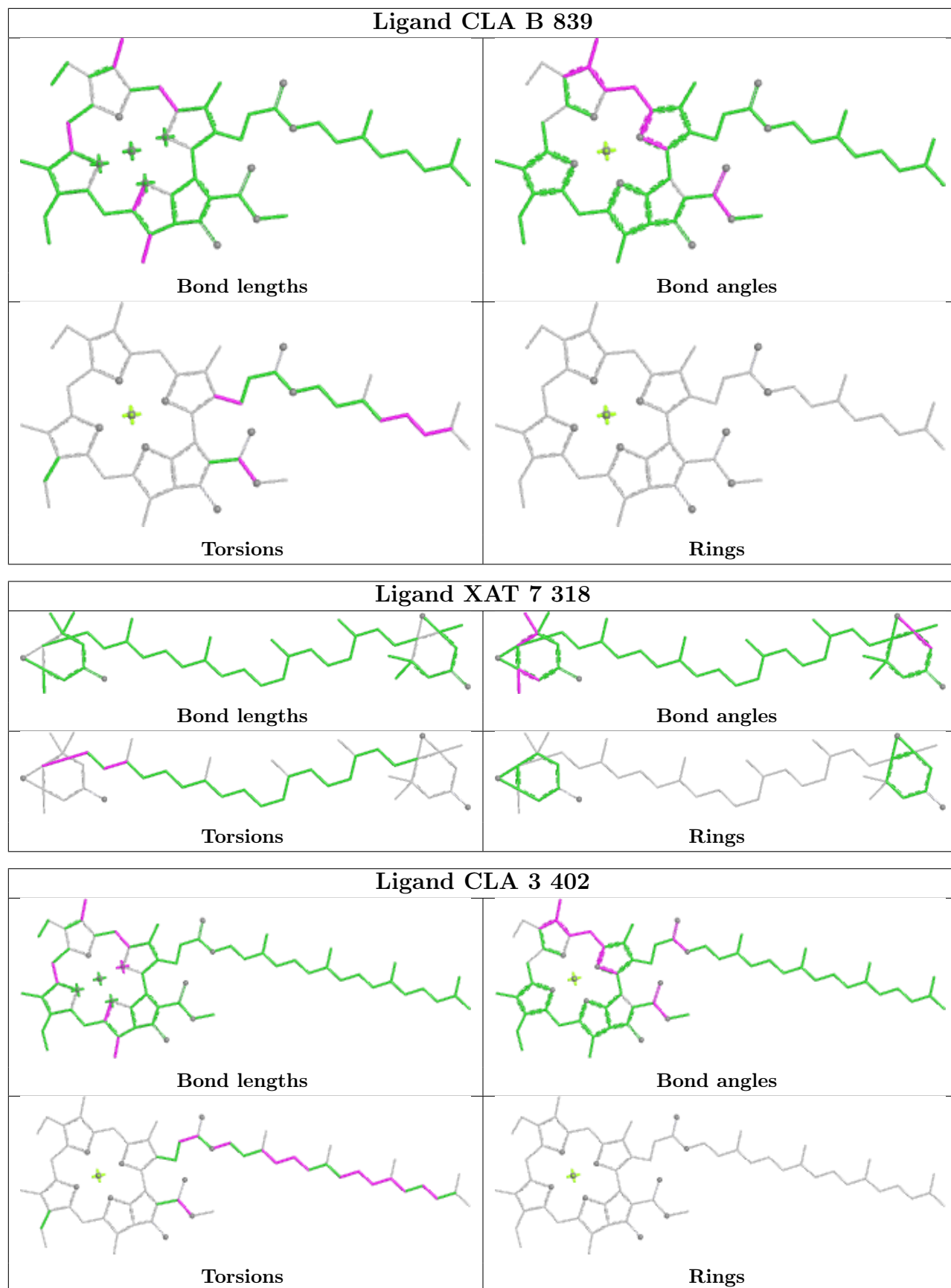
Bond angles



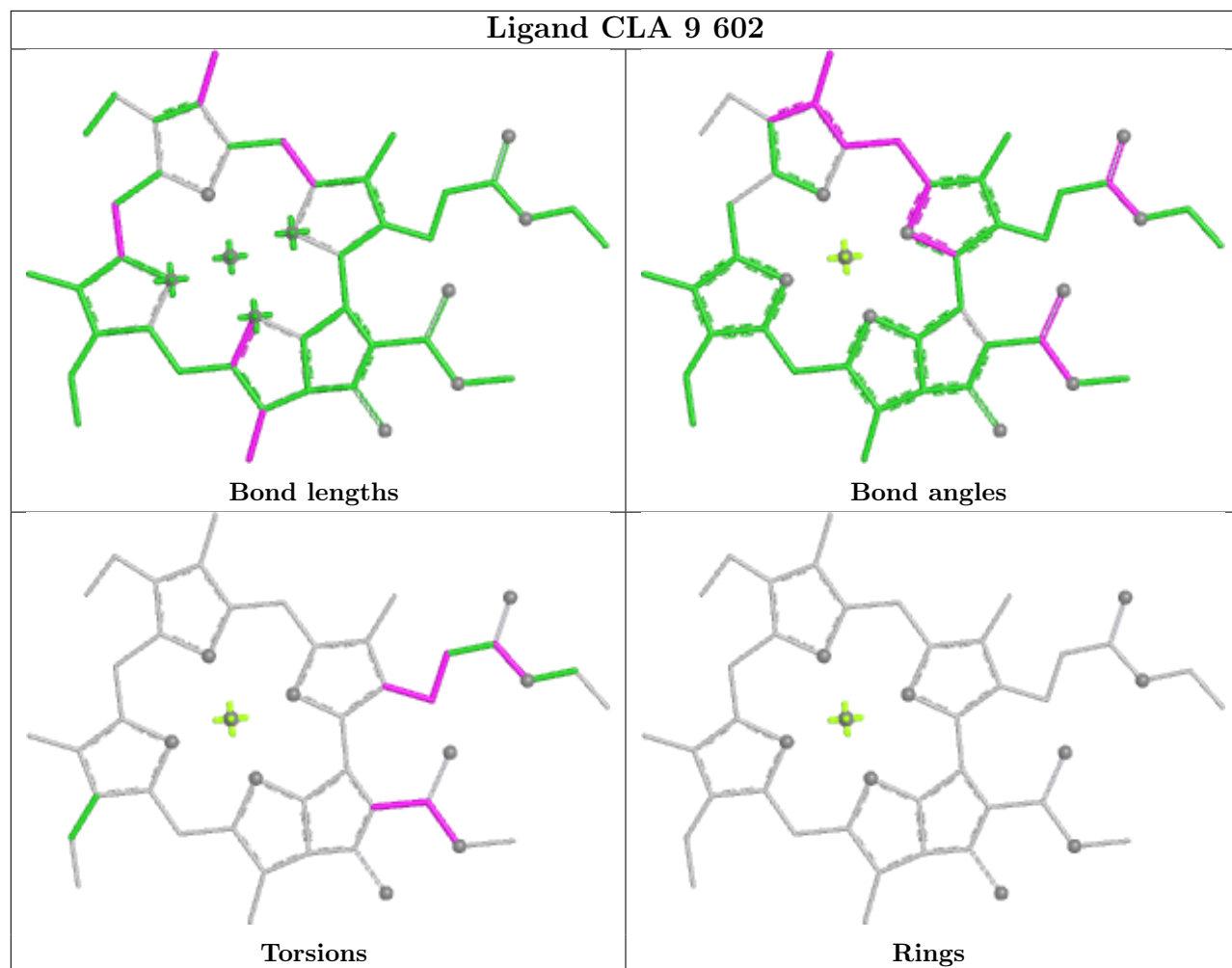
Torsions



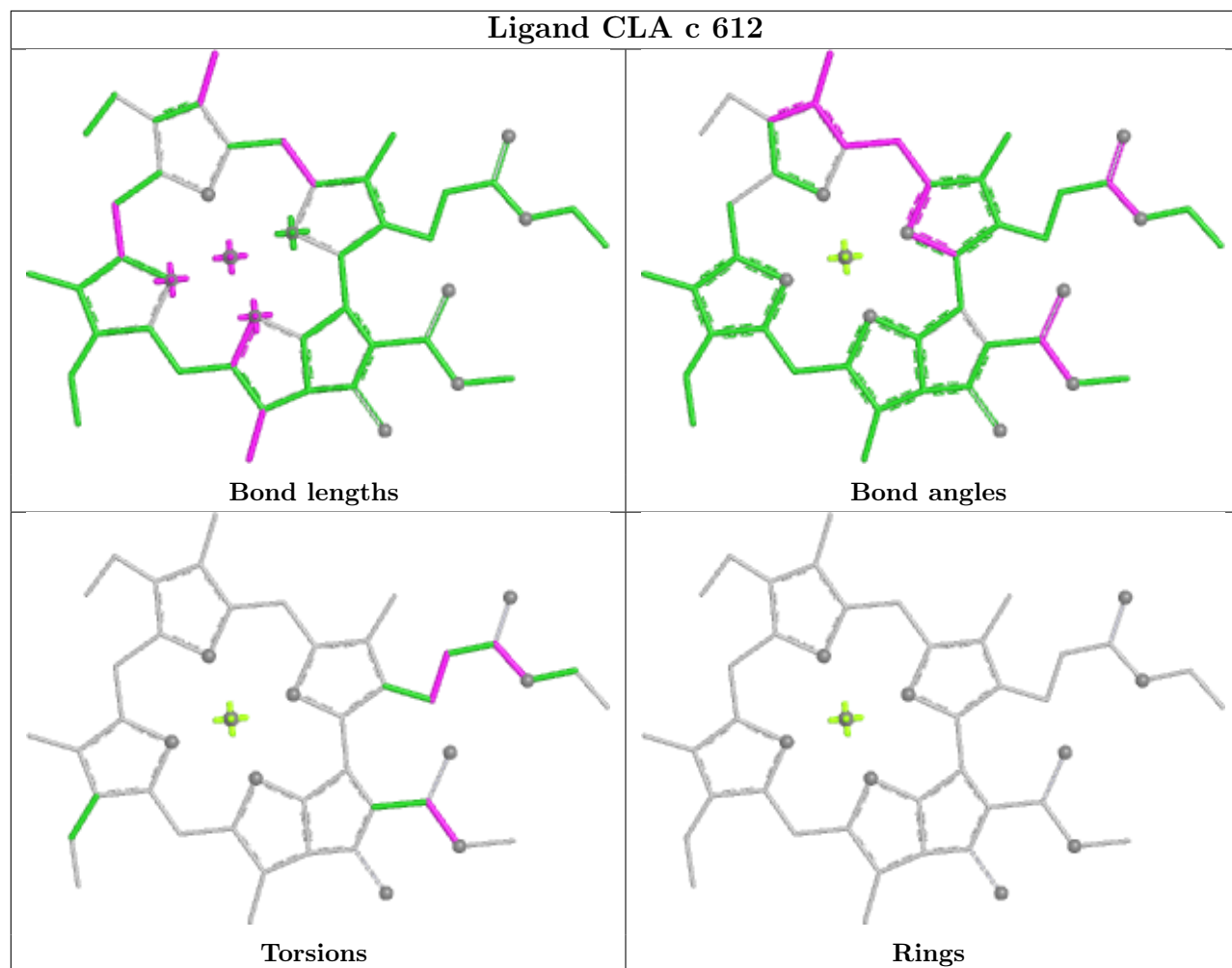
Rings



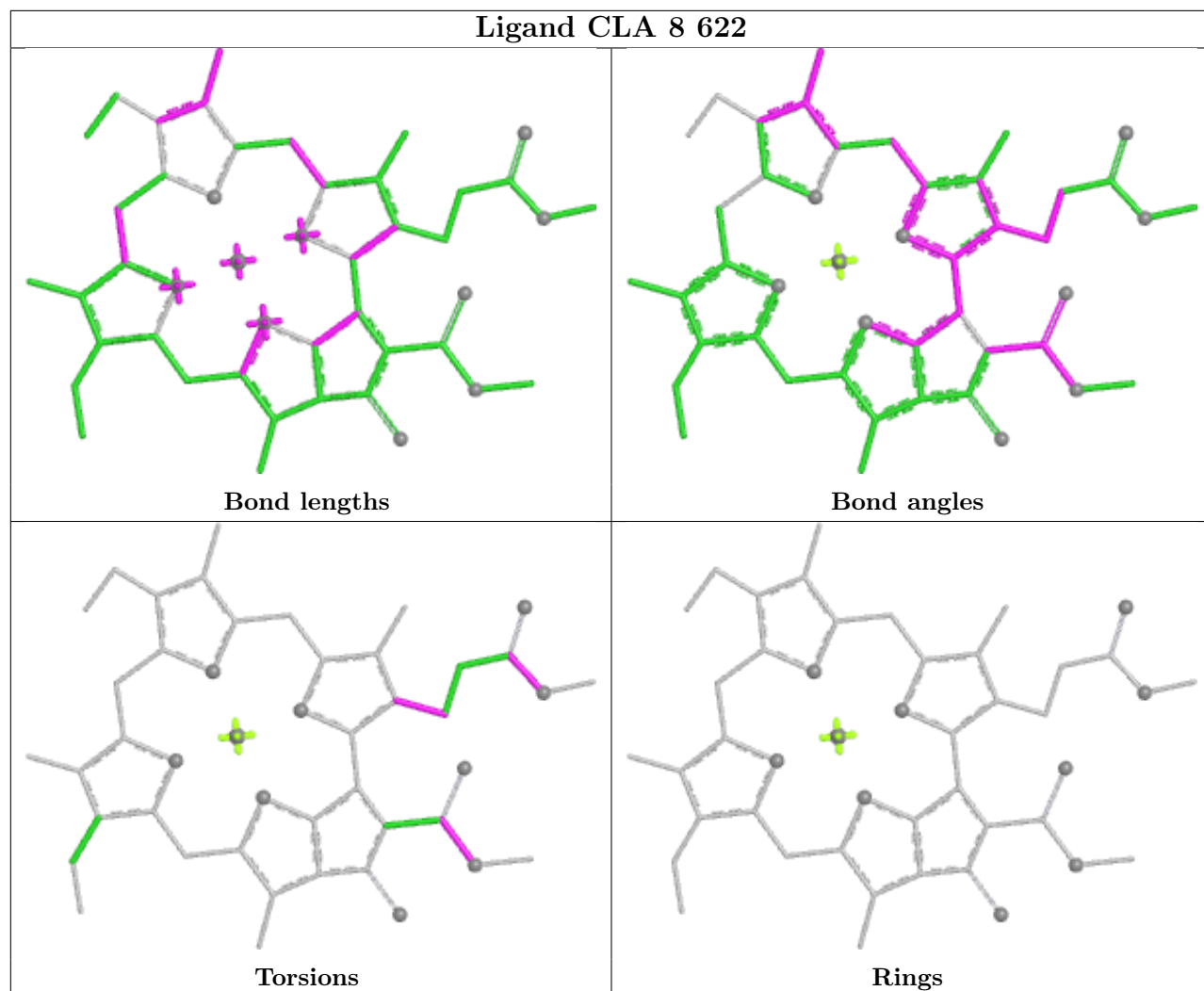
Ligand CLA 9 602



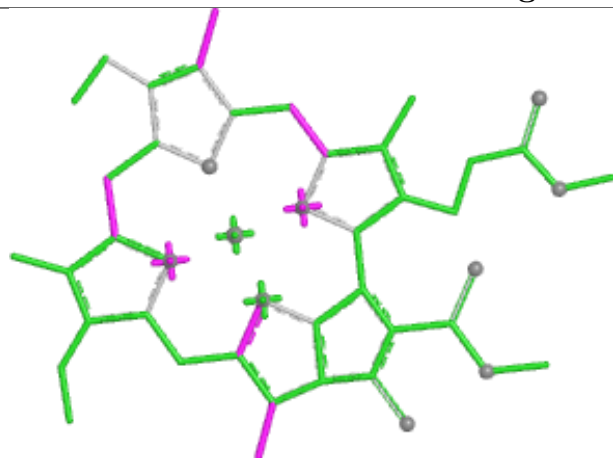
Ligand CLA c 612



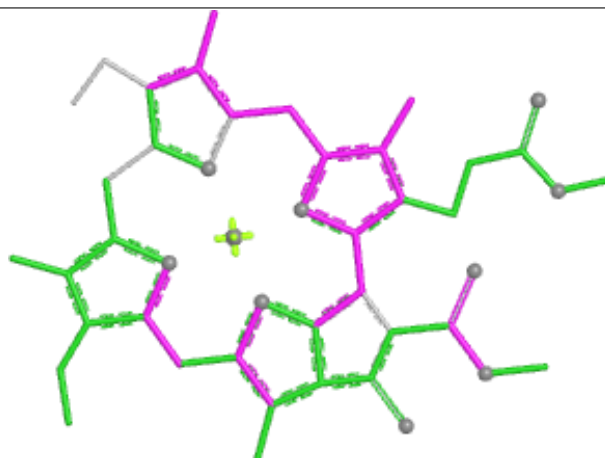
Ligand CLA 8 622



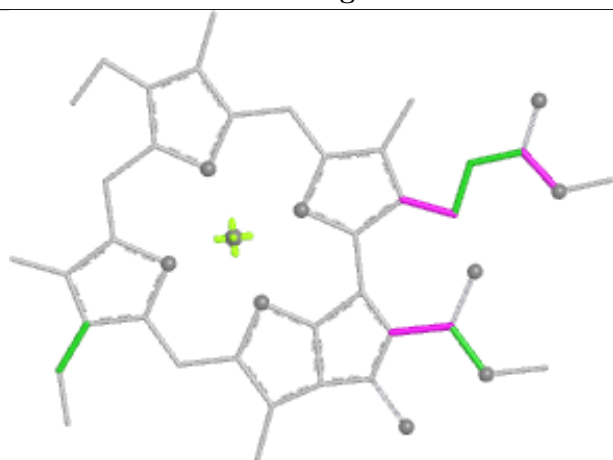
Ligand CLA 9 601



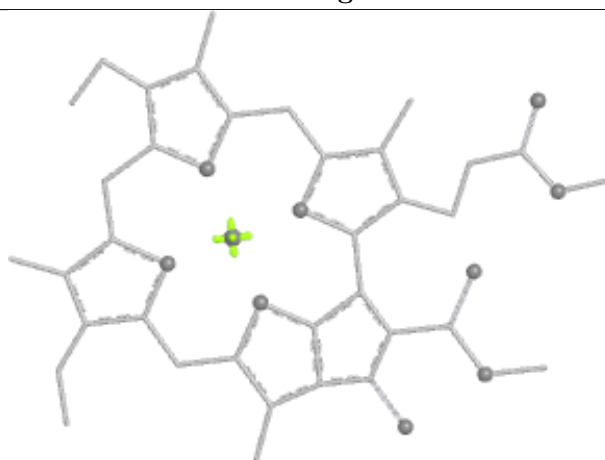
Bond lengths



Bond angles

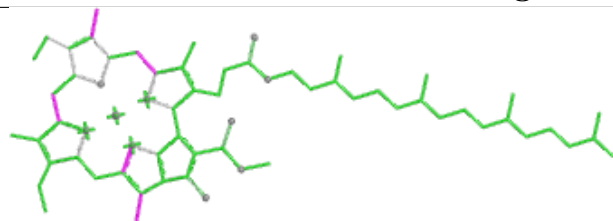


Torsions

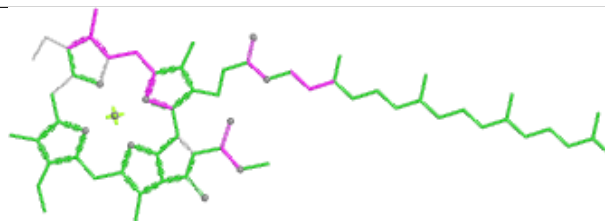


Rings

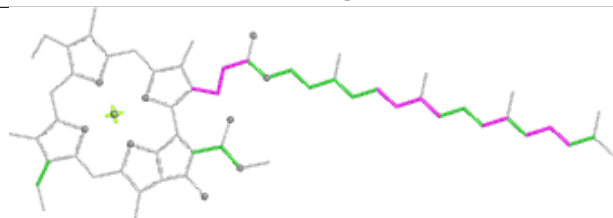
Ligand CLA A 841



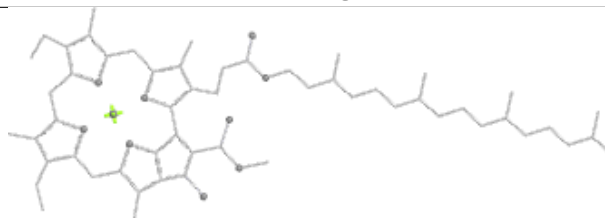
Bond lengths



Bond angles

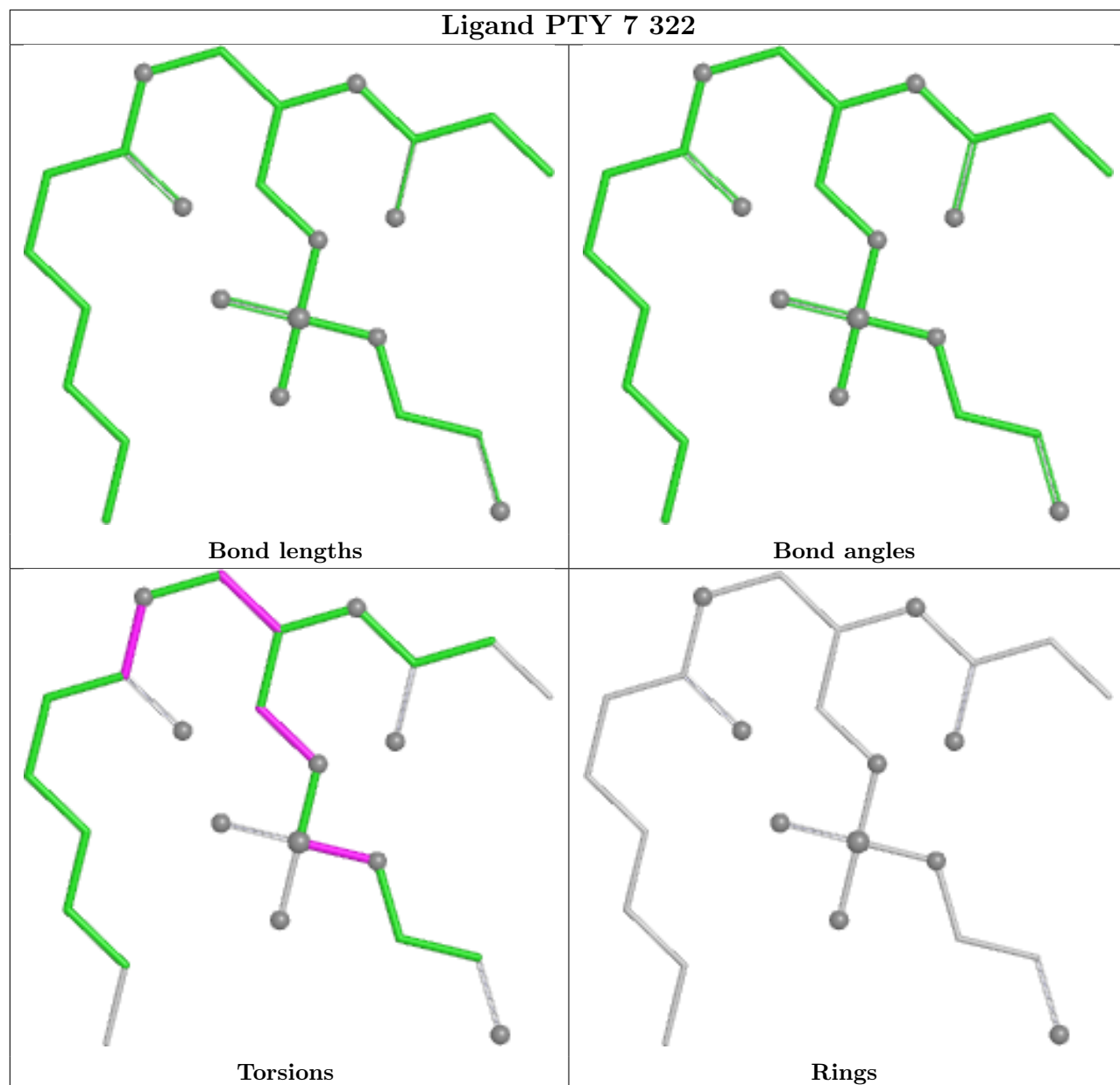


Torsions

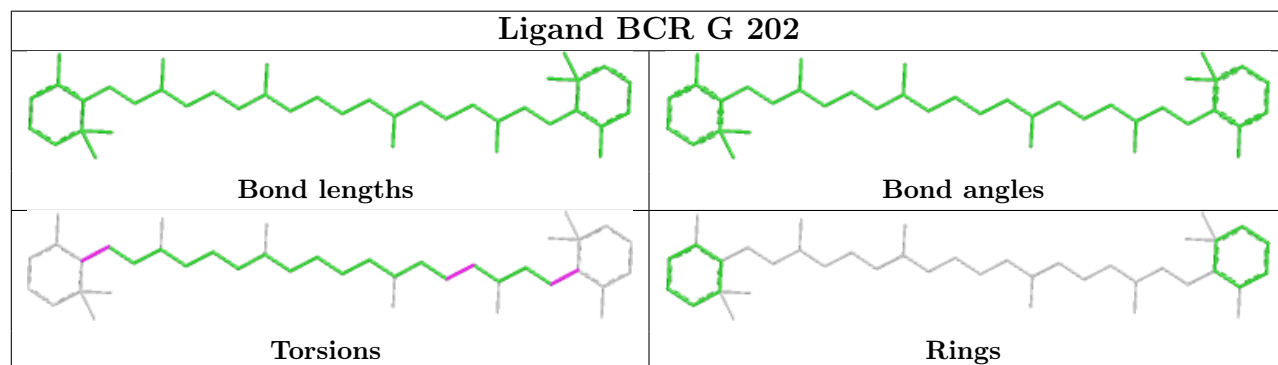


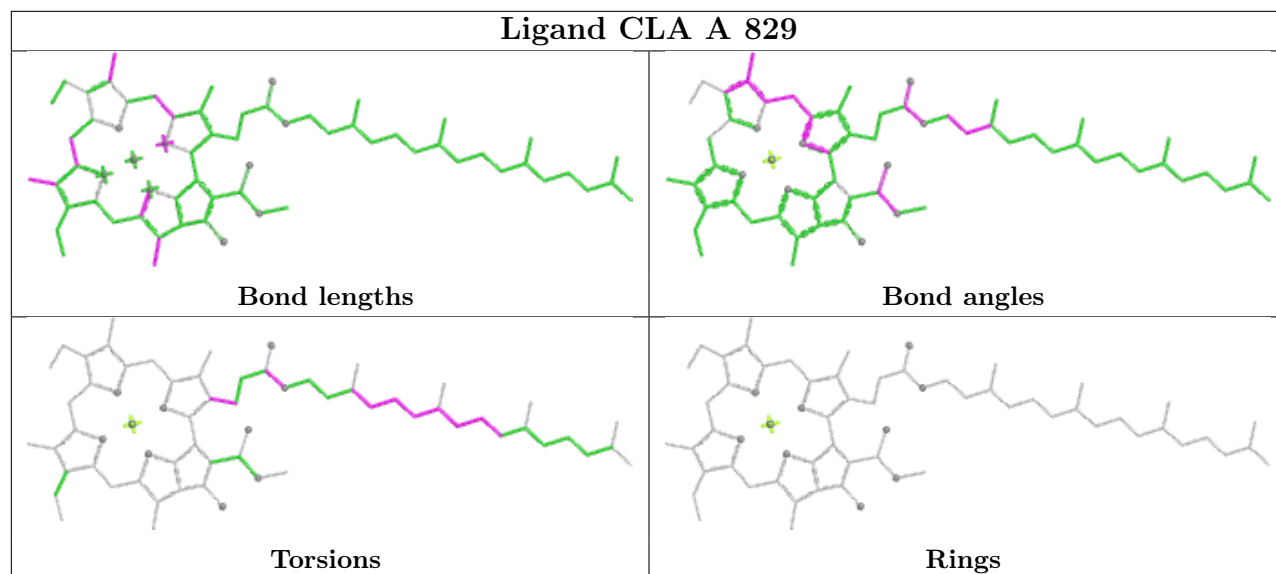
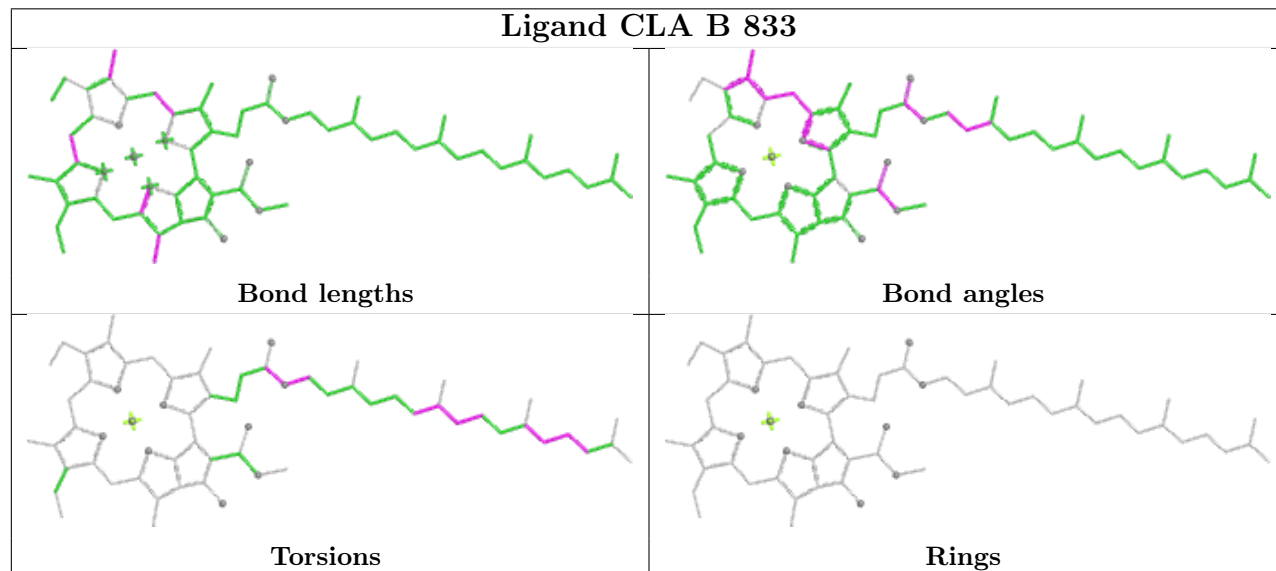
Rings

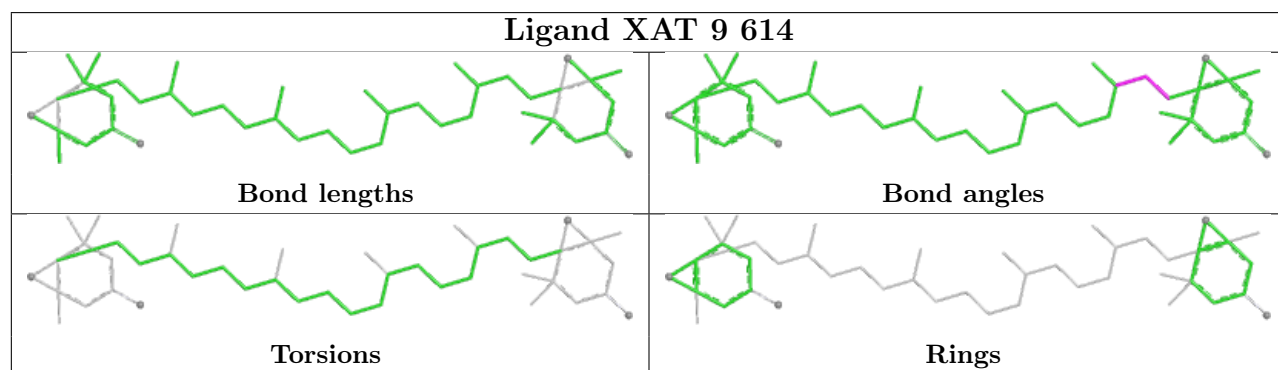
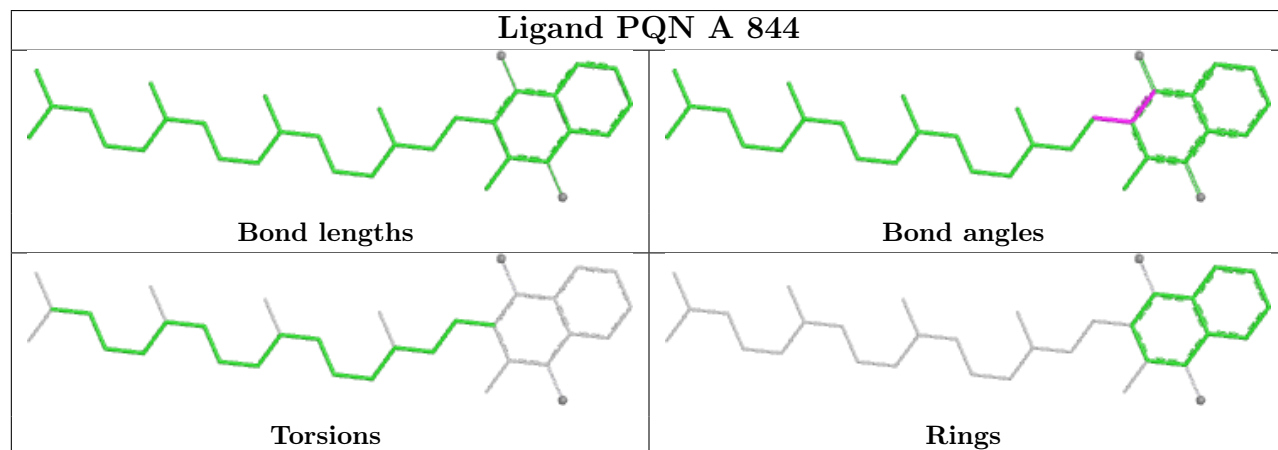
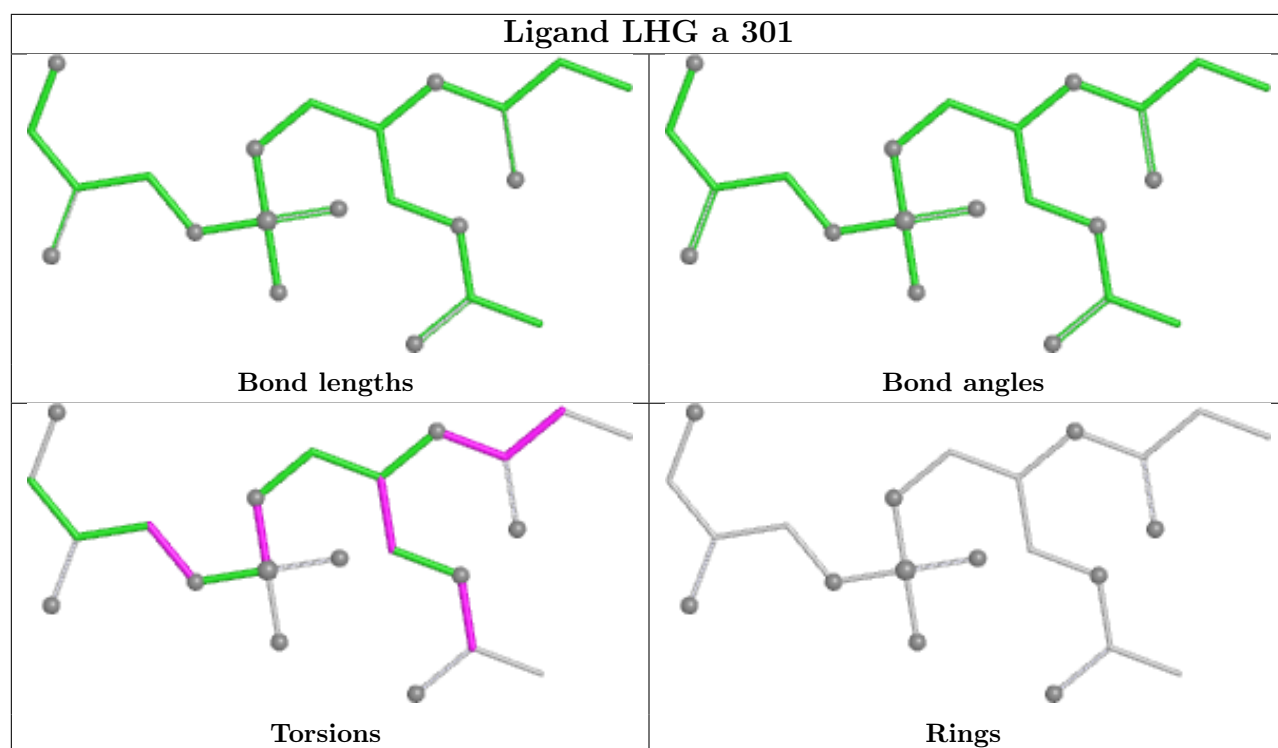
Ligand PTY 7 322

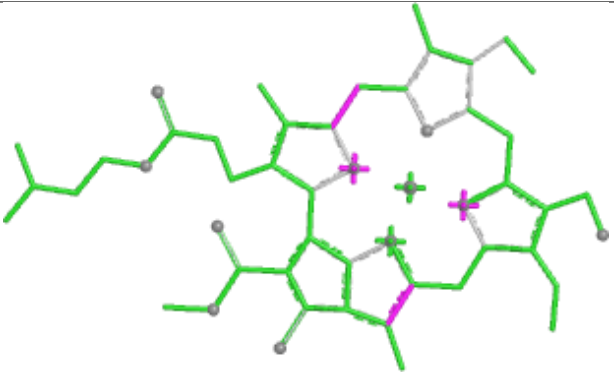
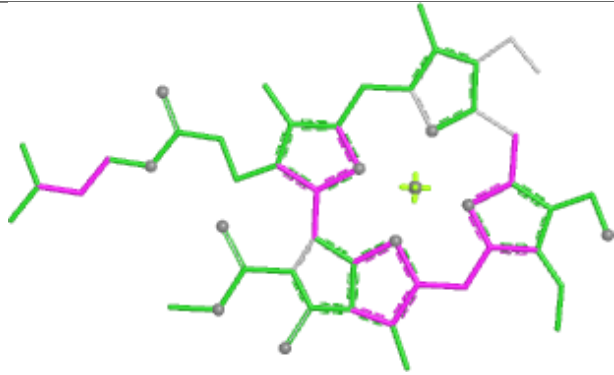
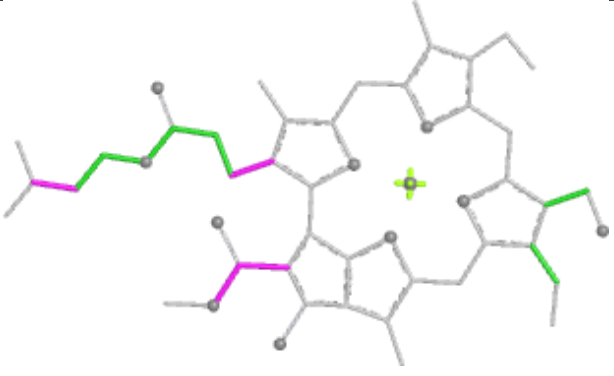
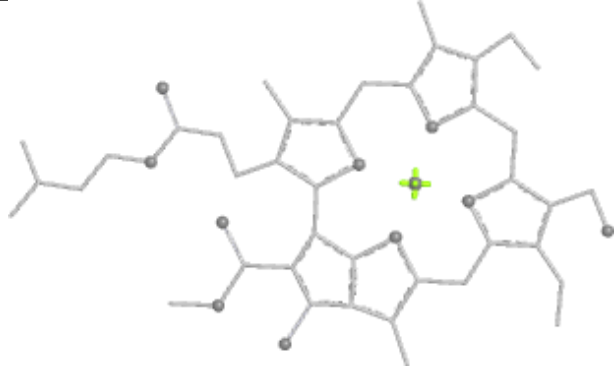
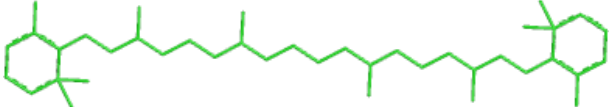
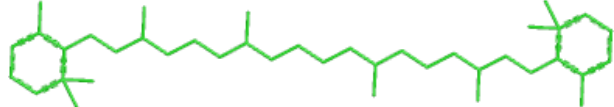
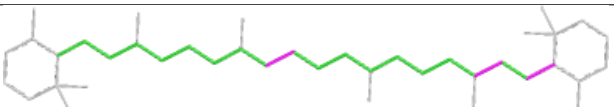
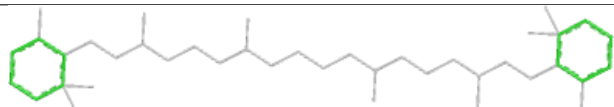


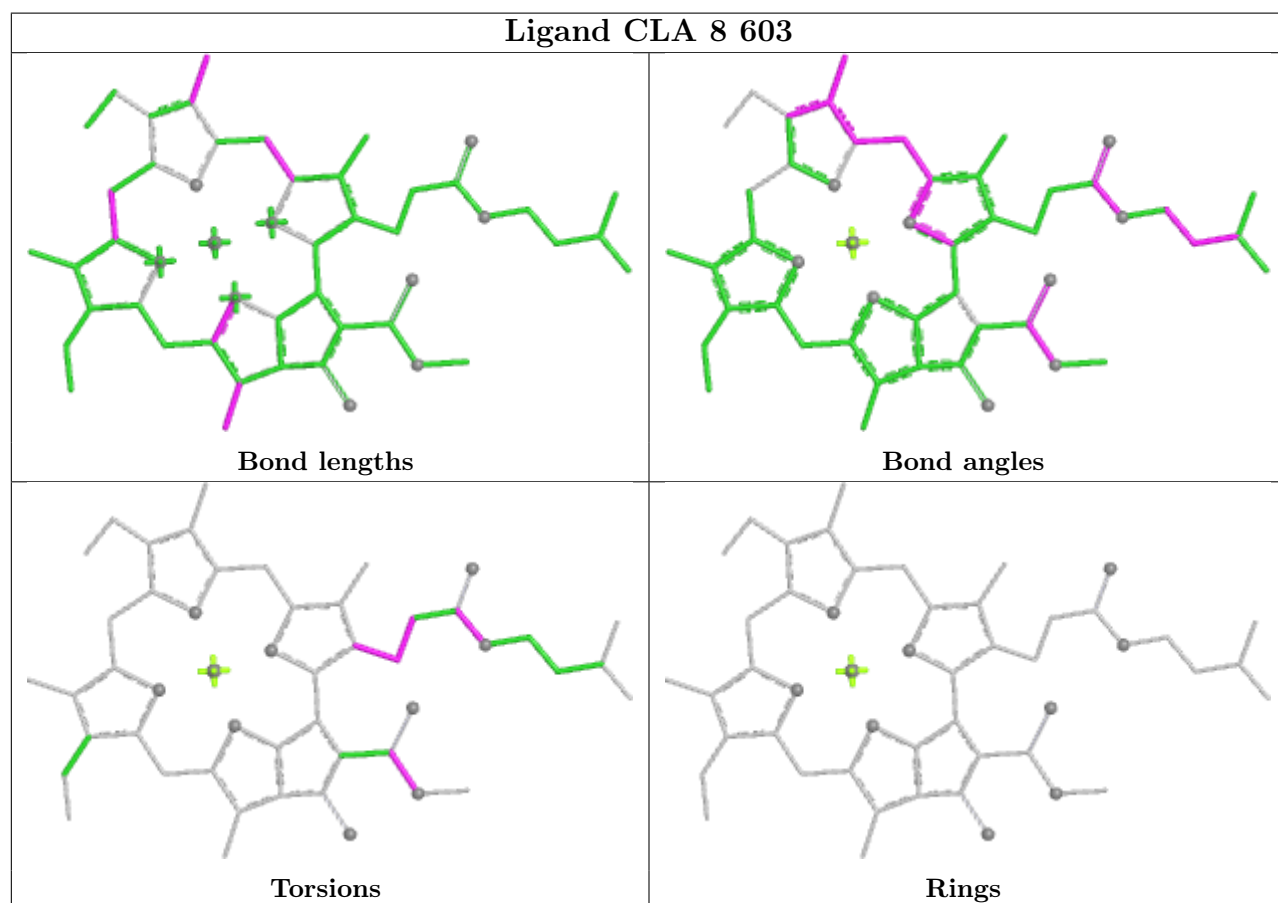
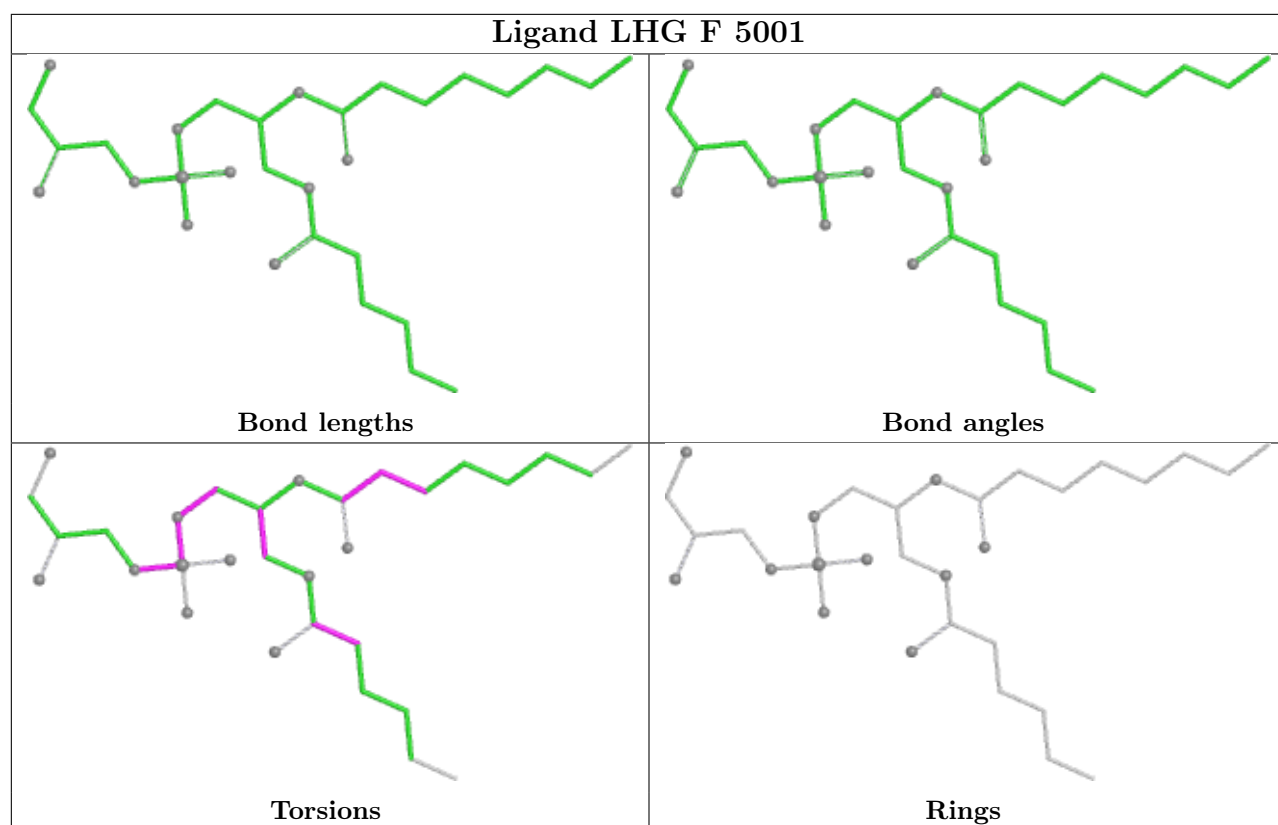
Ligand BCR G 202



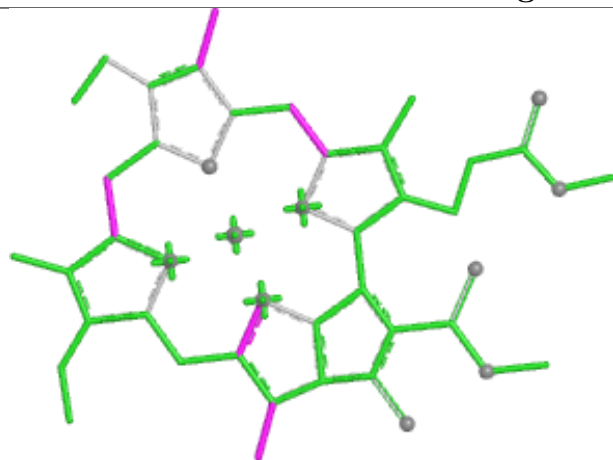
Ligand CLA A 829**Ligand CLA B 833**



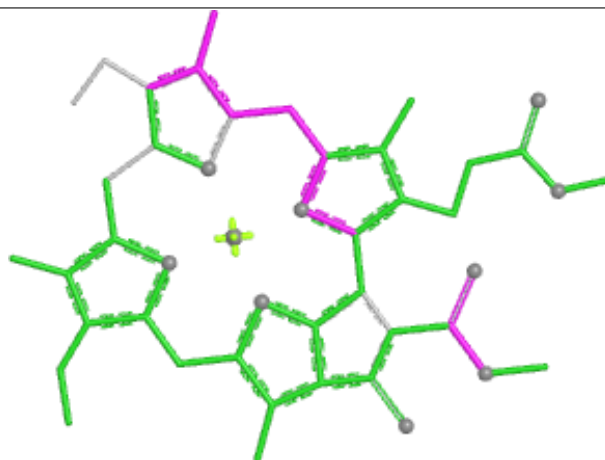
Ligand CHL 8 601	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR a 317	
	
Bond lengths	Bond angles
	
Torsions	Rings



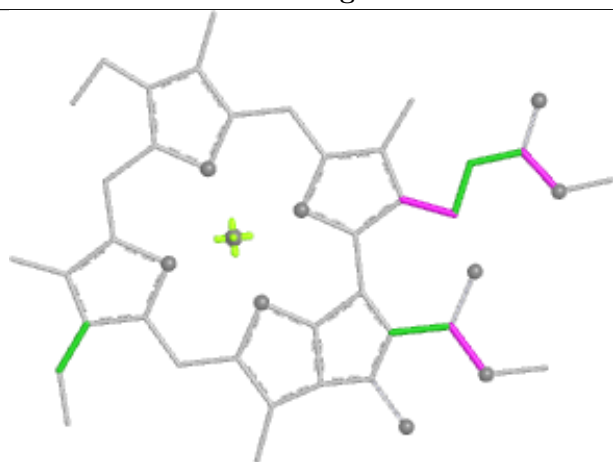
Ligand CLA b 315



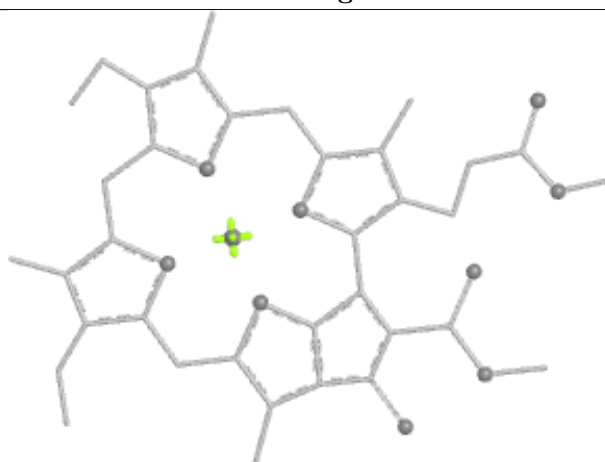
Bond lengths



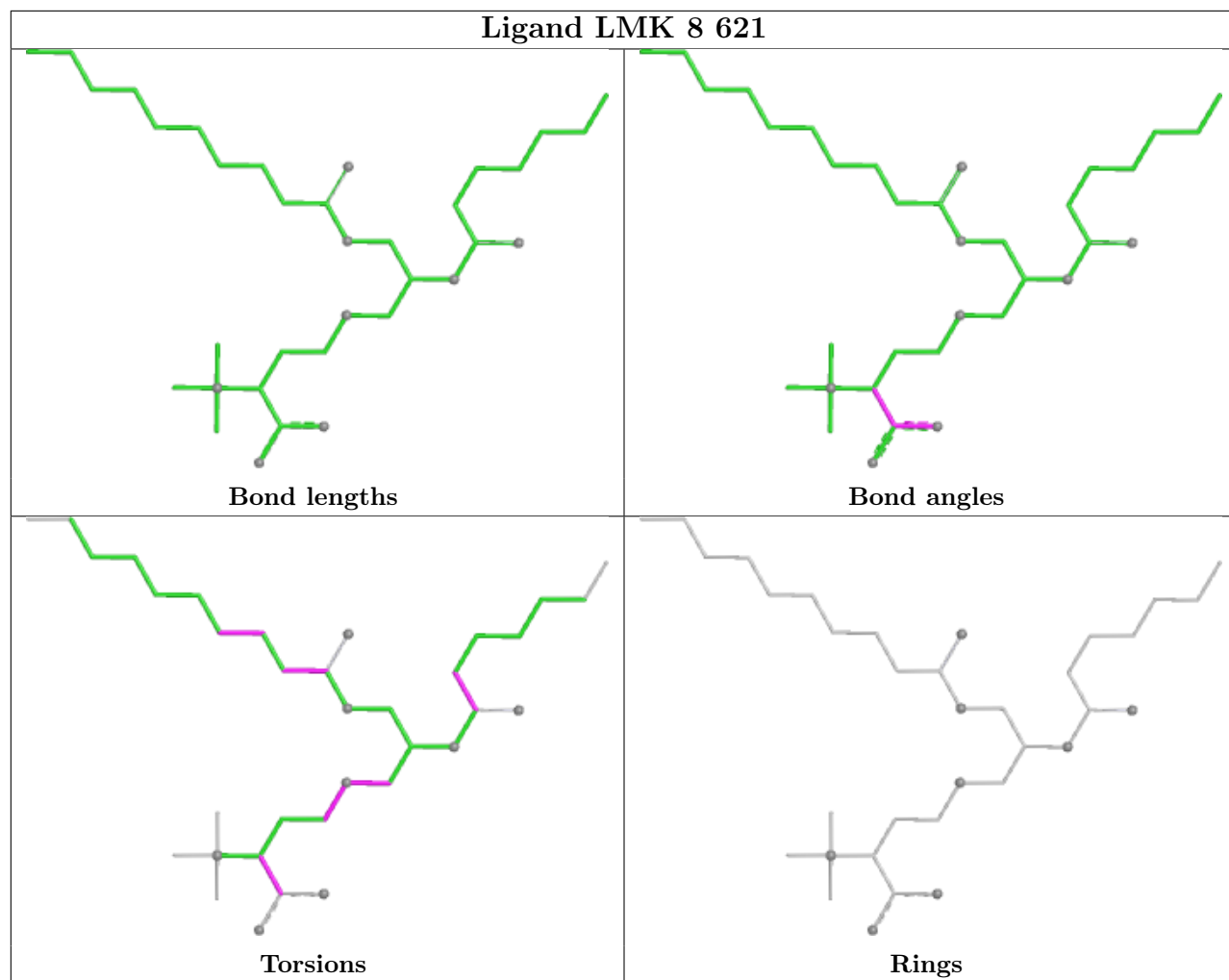
Bond angles



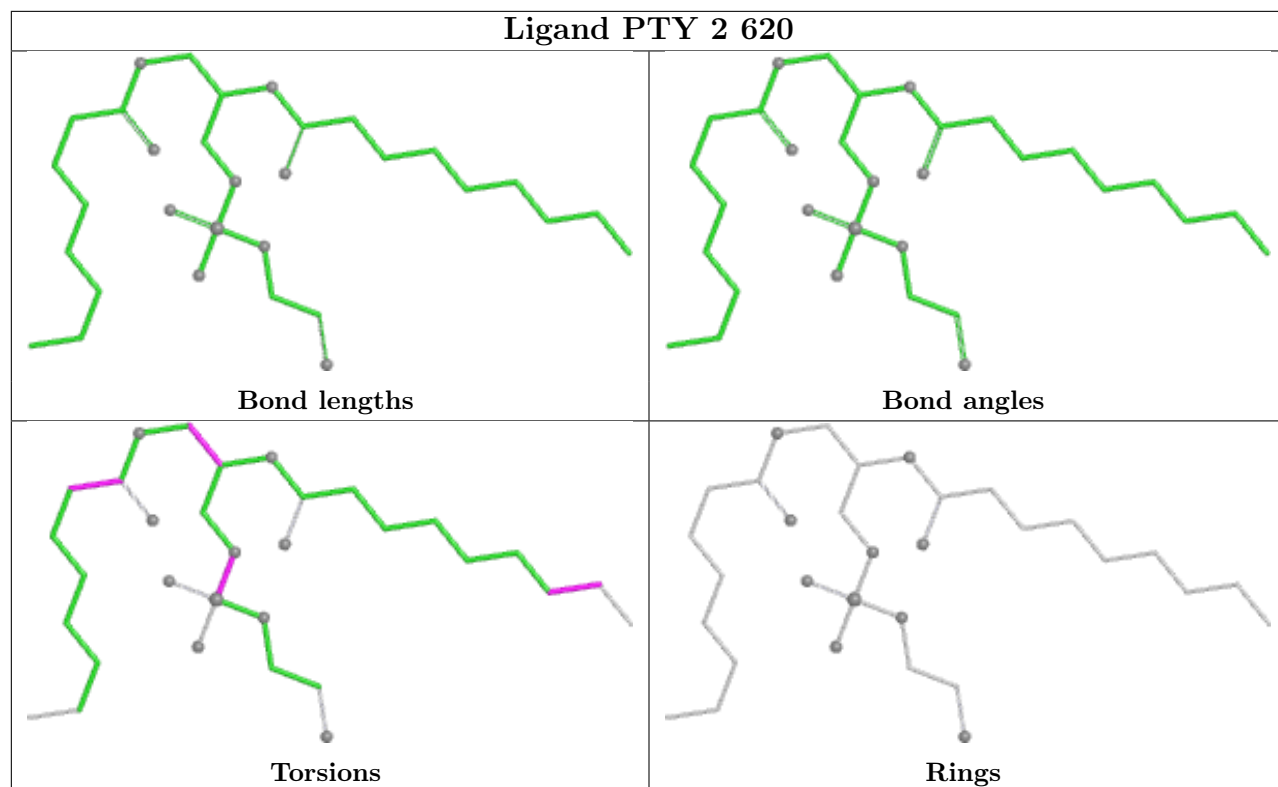
Torsions



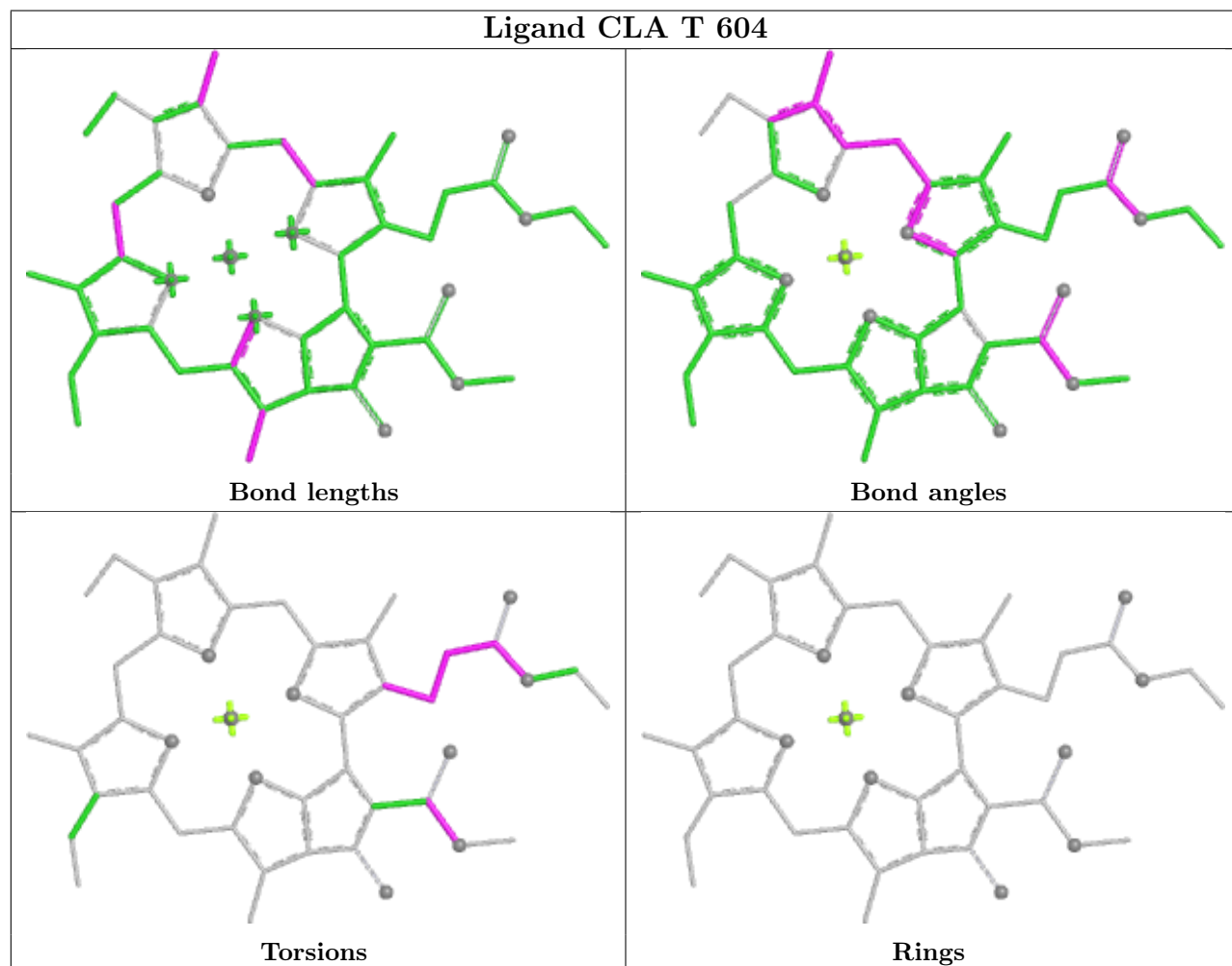
Rings

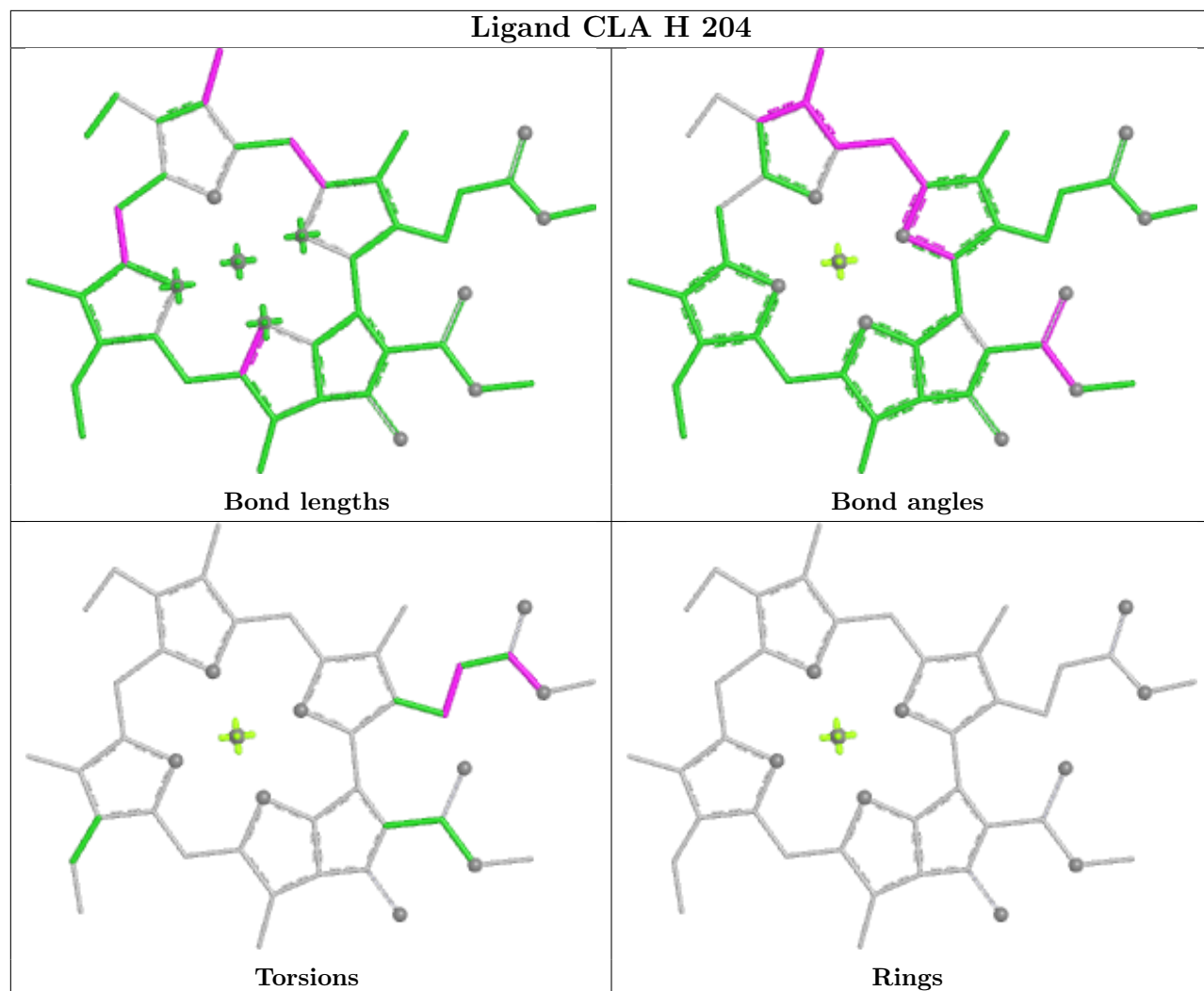


Ligand PTY 2 620

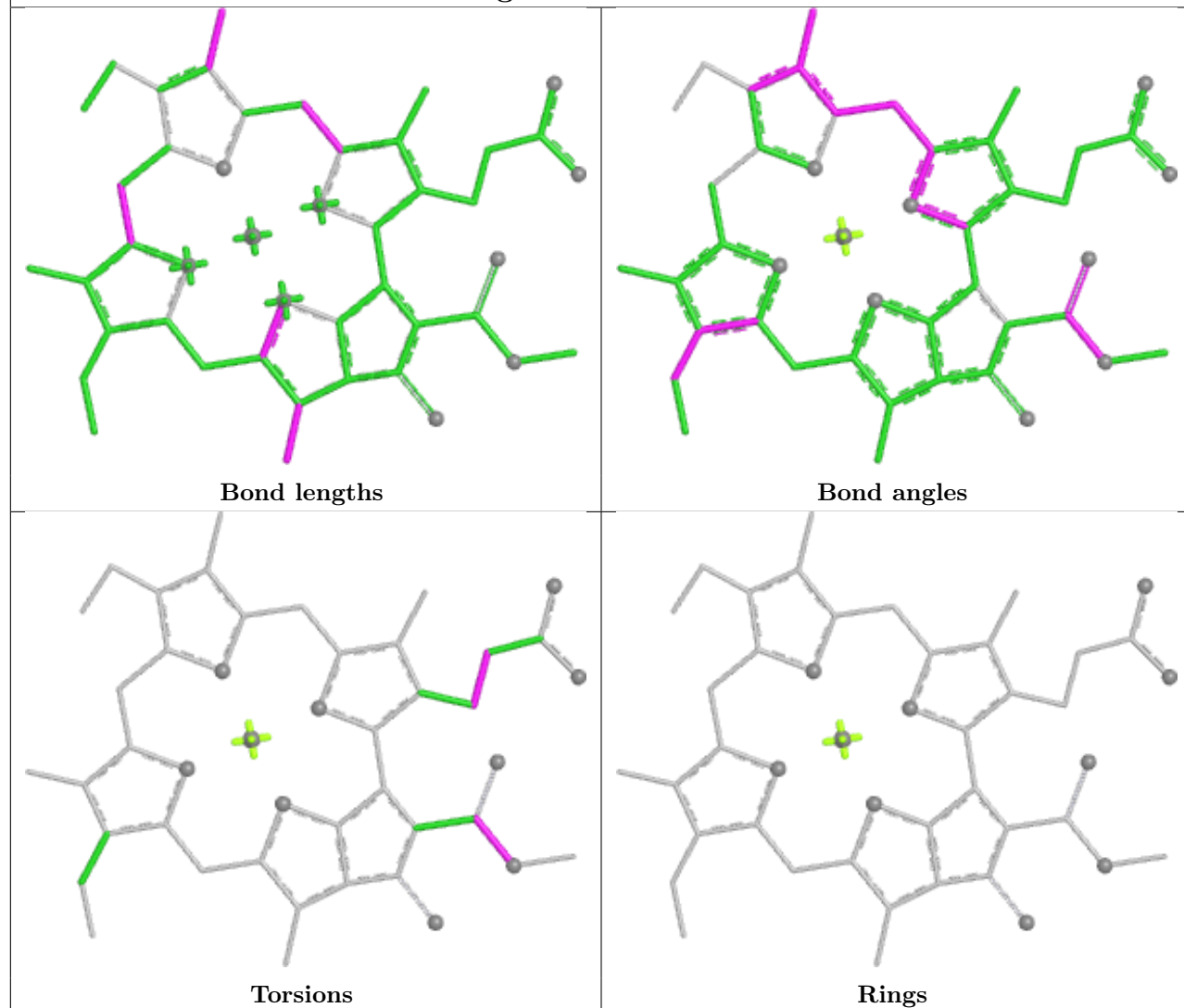


Ligand CLA T 604

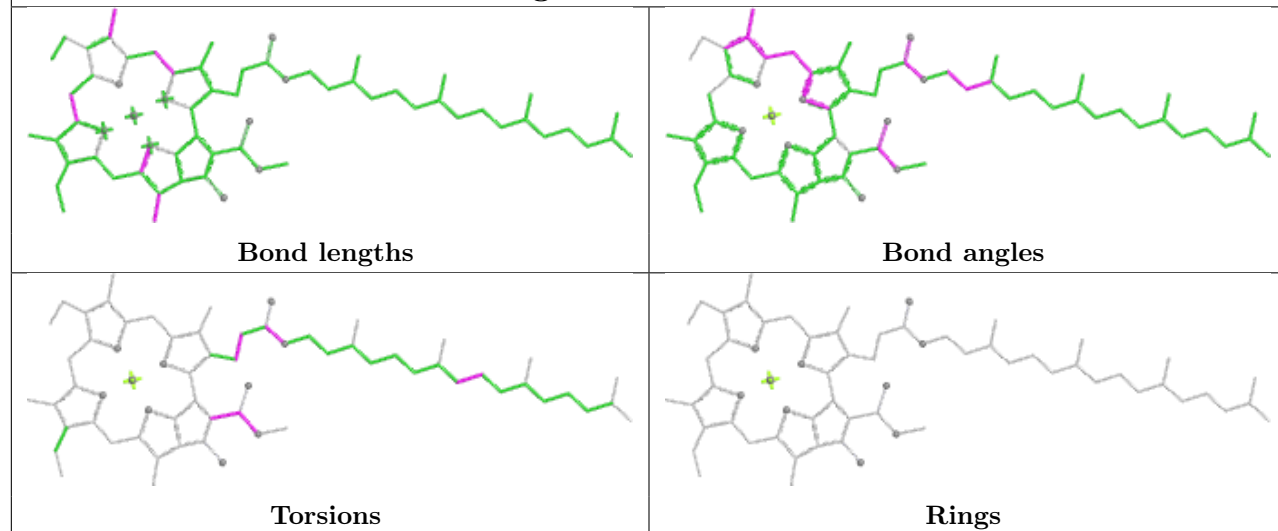




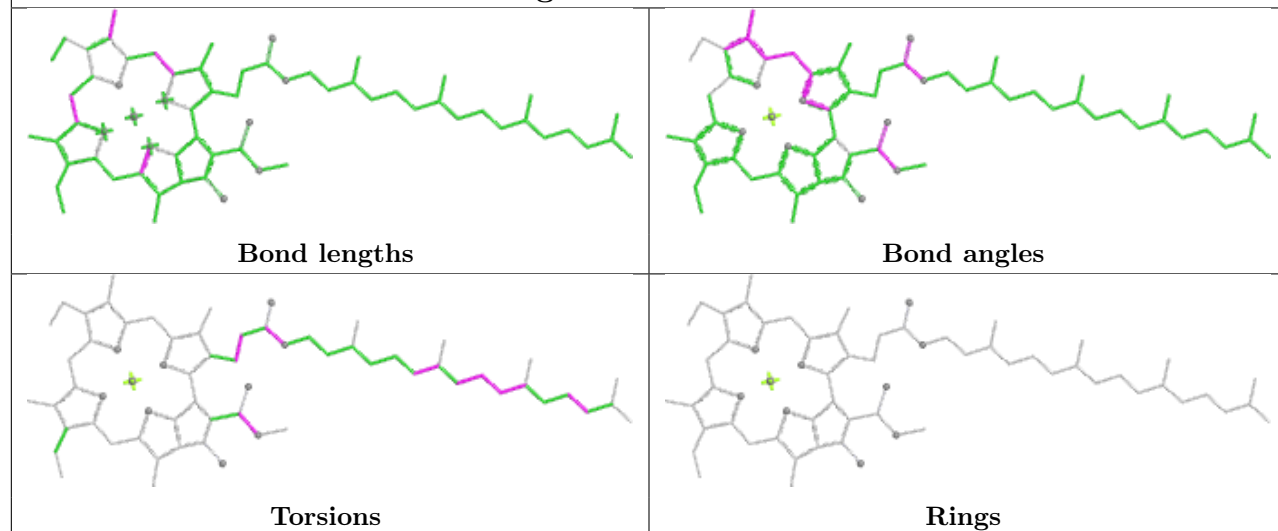
Ligand CLA a 305



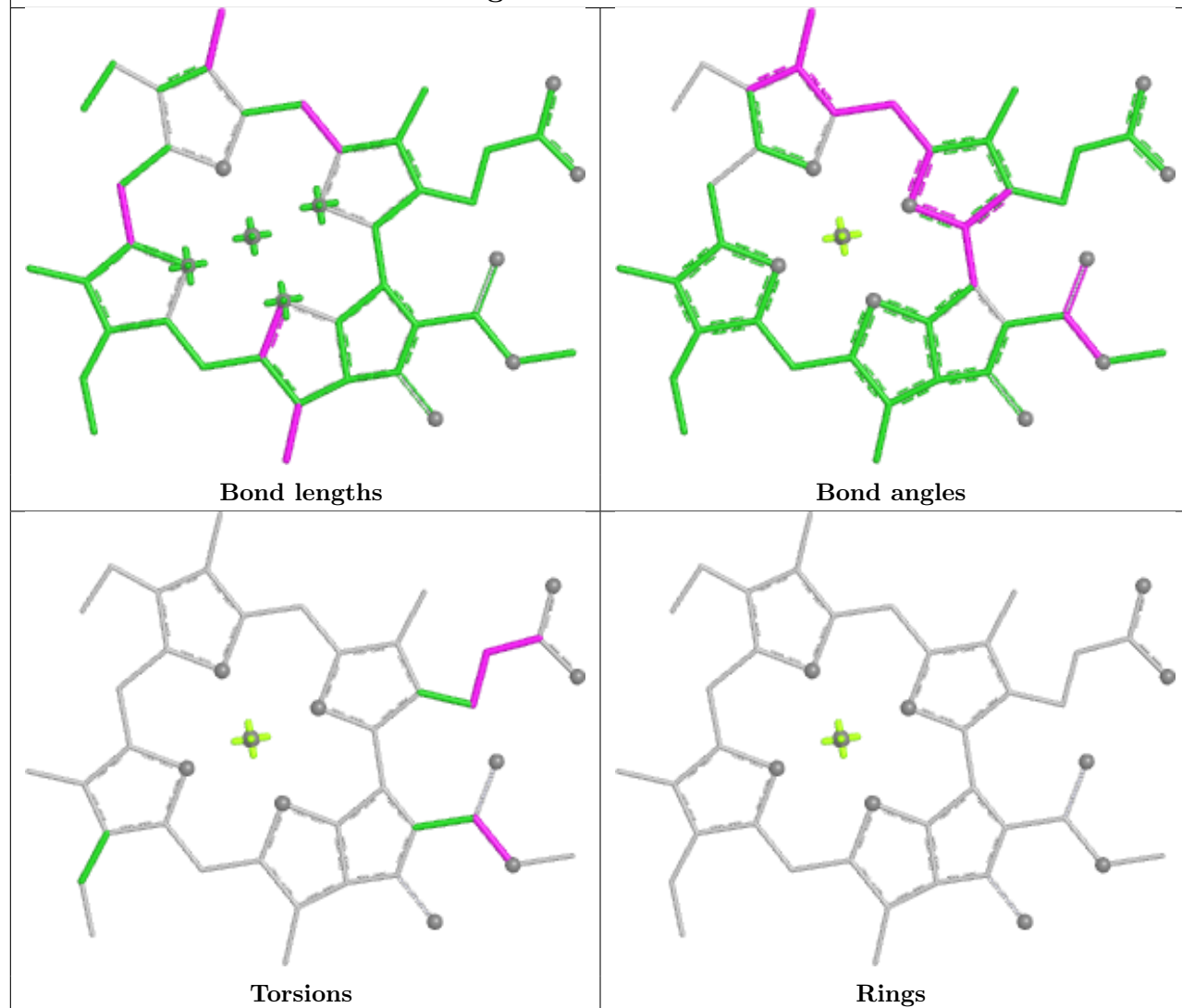
Ligand CLA B 828

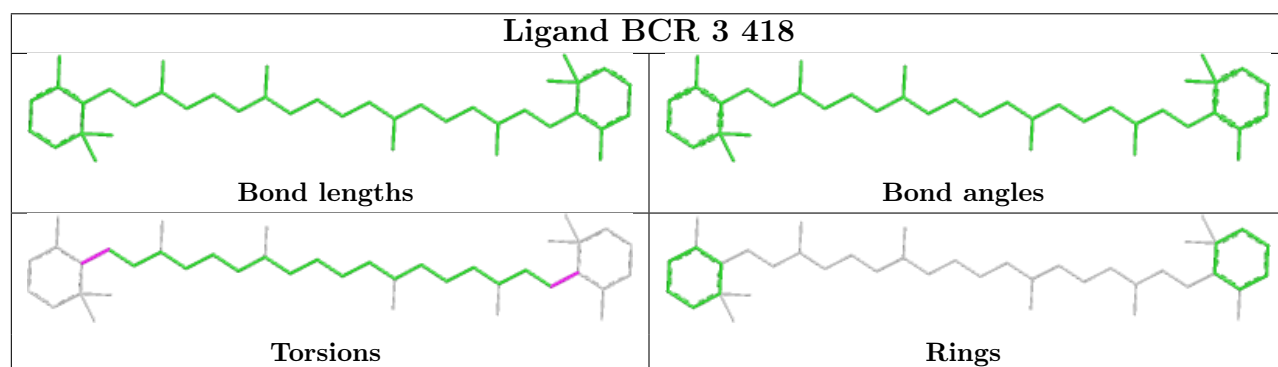
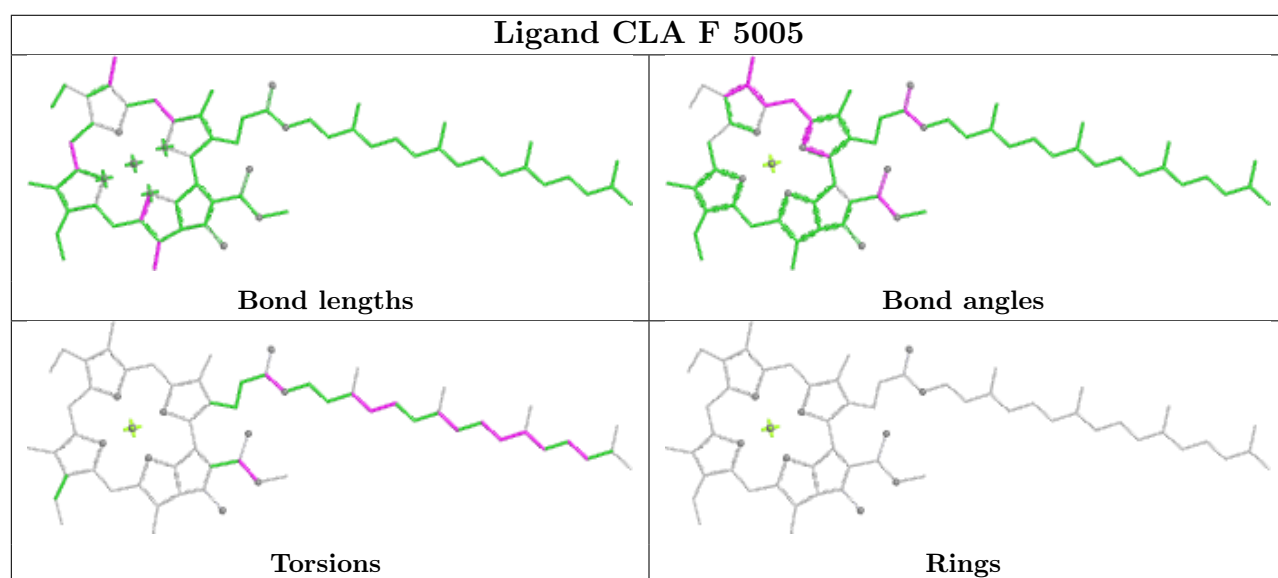
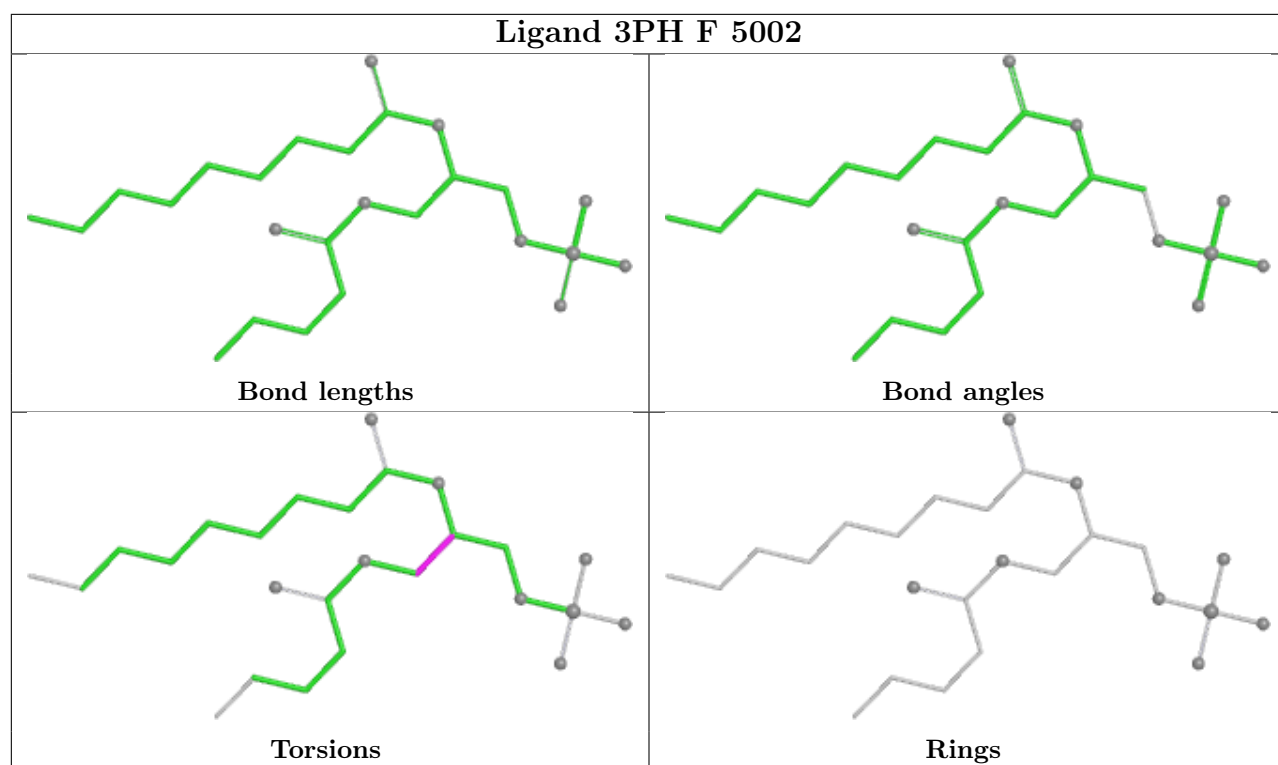


Ligand CLA a 302

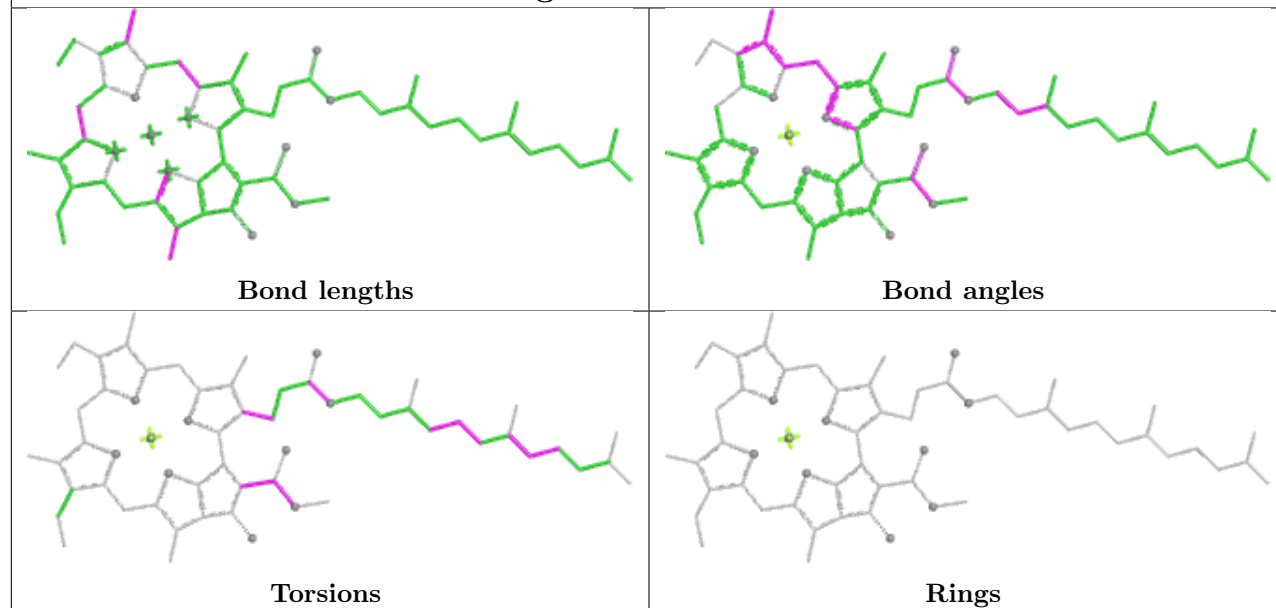


Ligand CLA J 5002

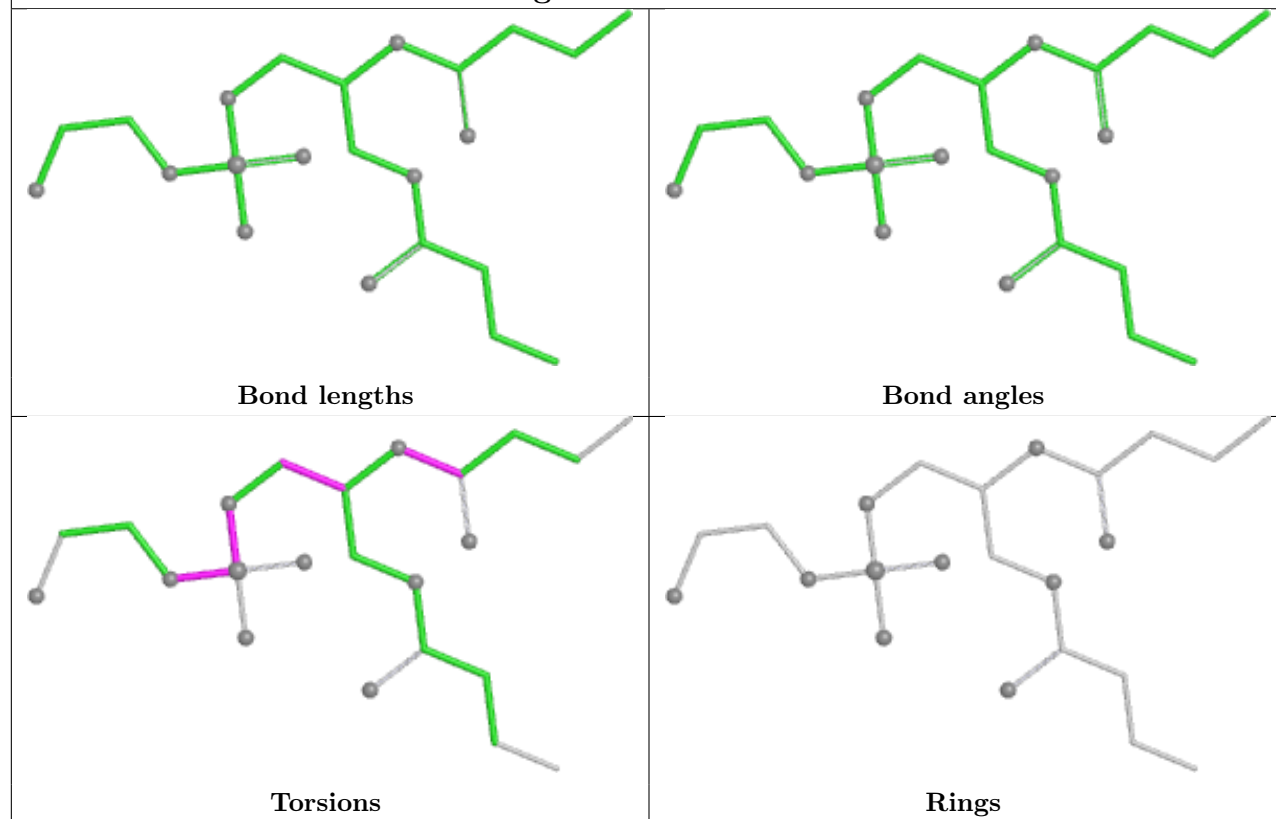




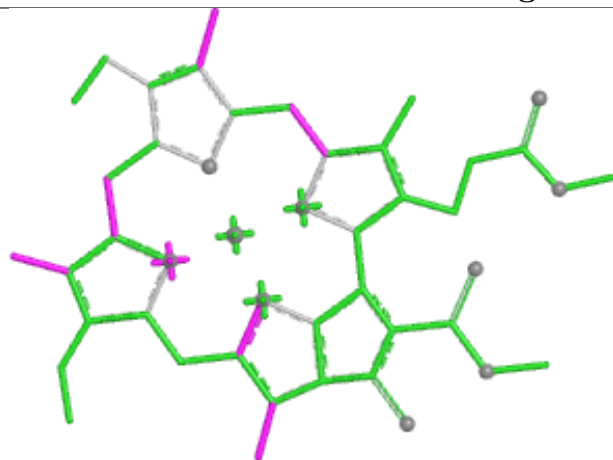
Ligand CLA 3 409



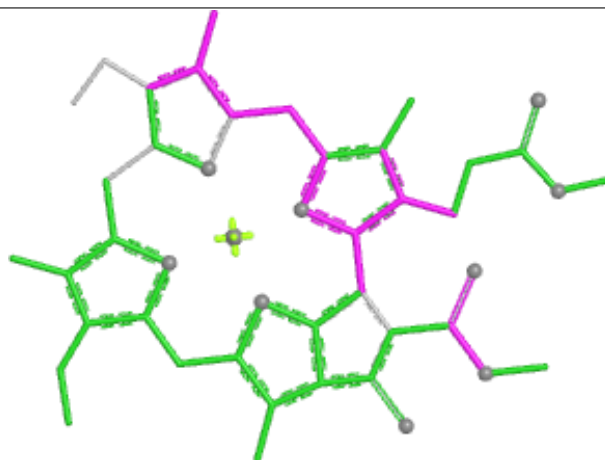
Ligand LHG b 303



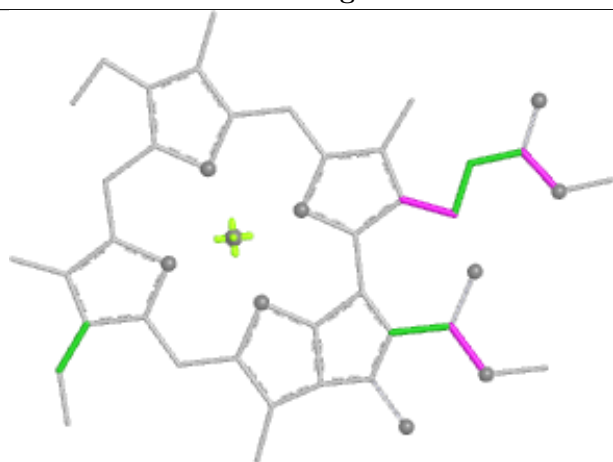
Ligand CLA 1 310



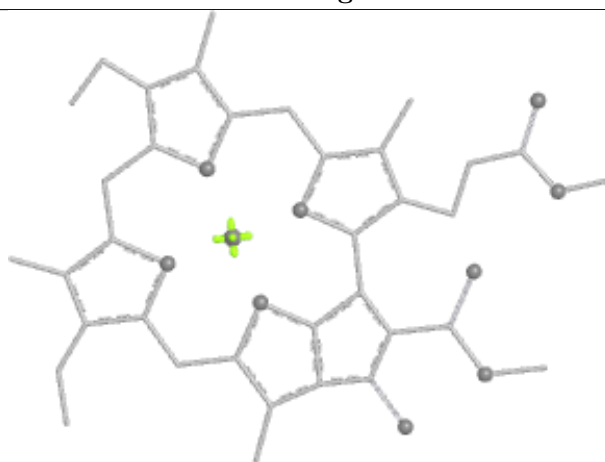
Bond lengths



Bond angles

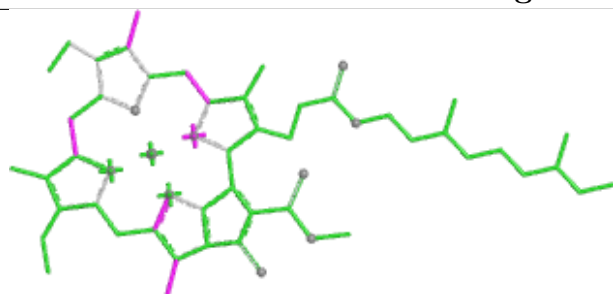


Torsions

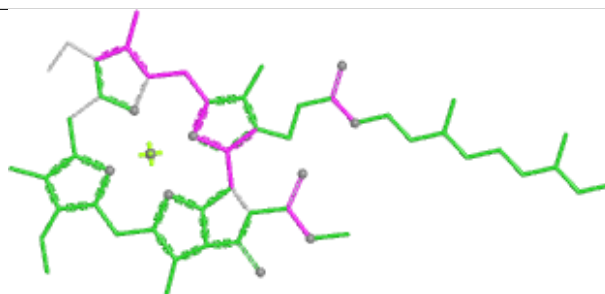


Rings

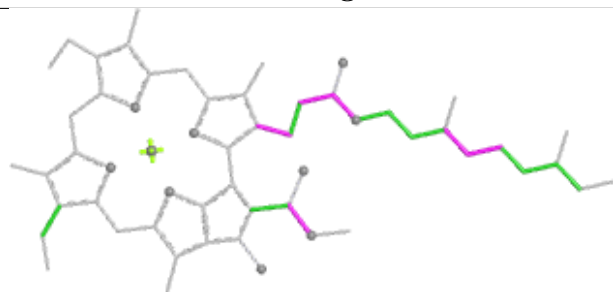
Ligand CLA T 603



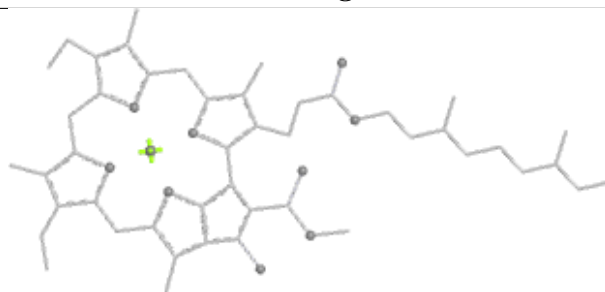
Bond lengths



Bond angles

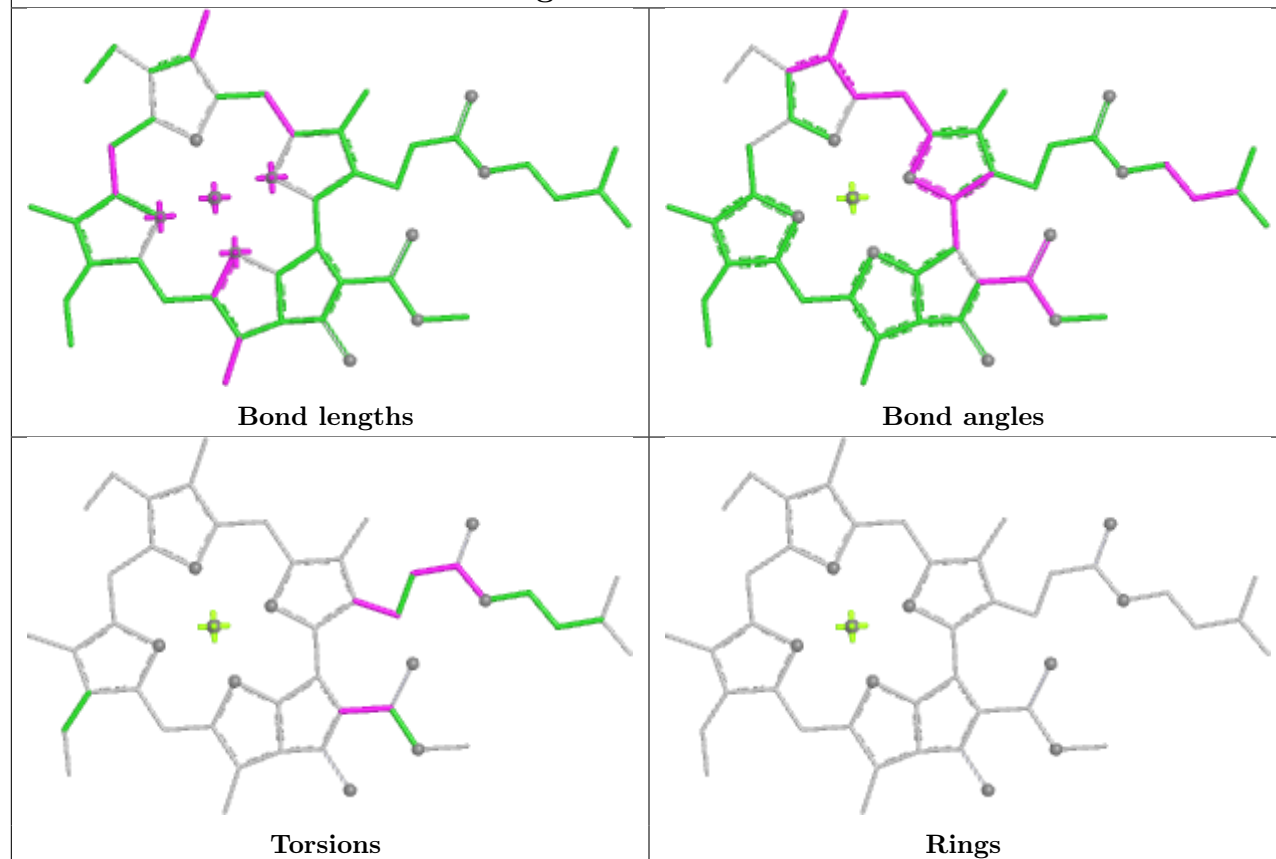


Torsions

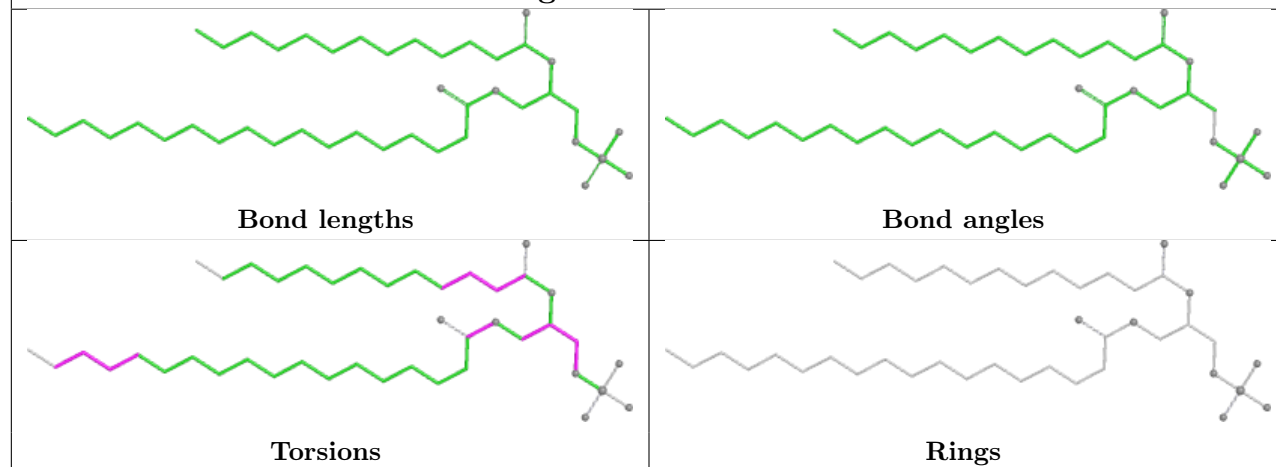


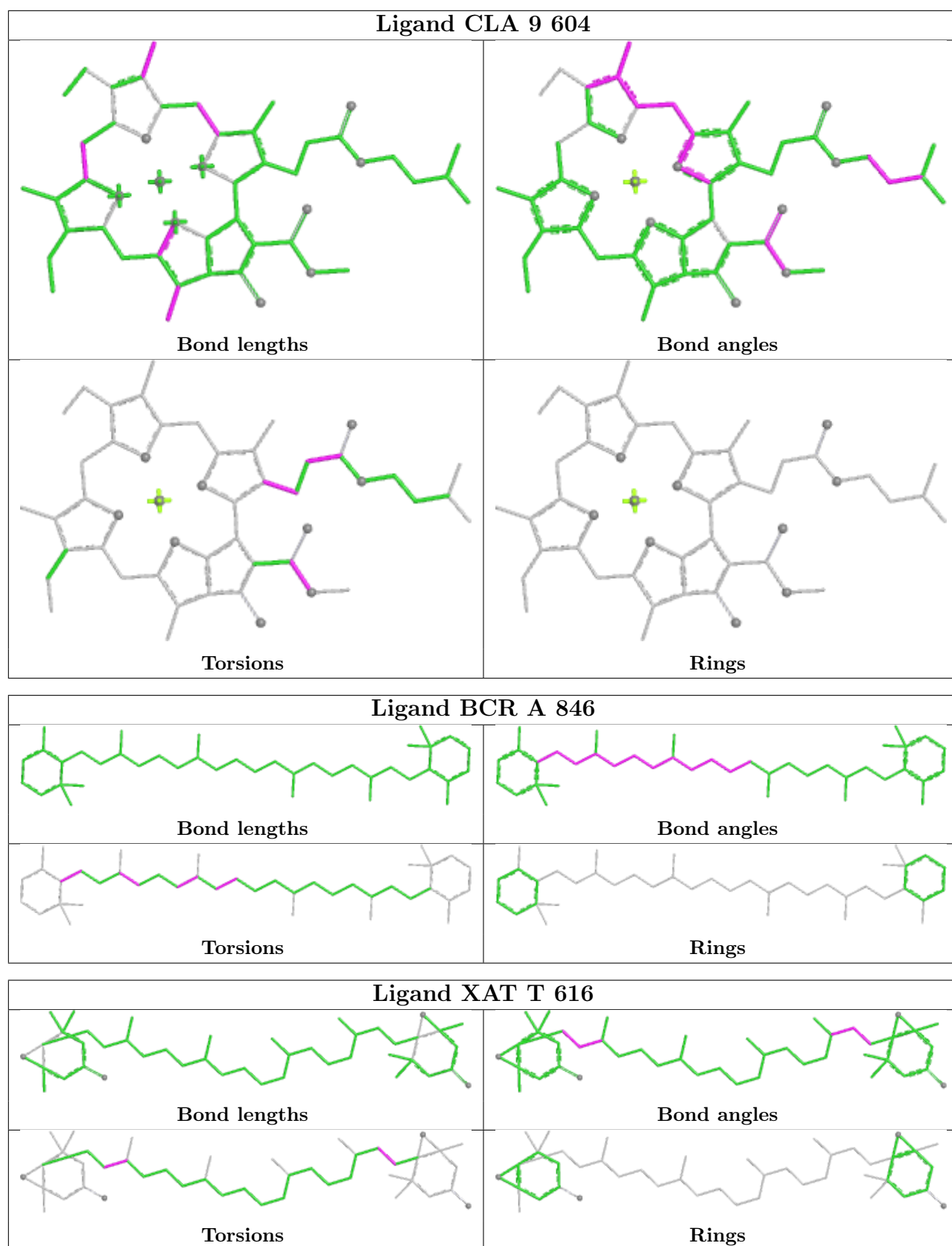
Rings

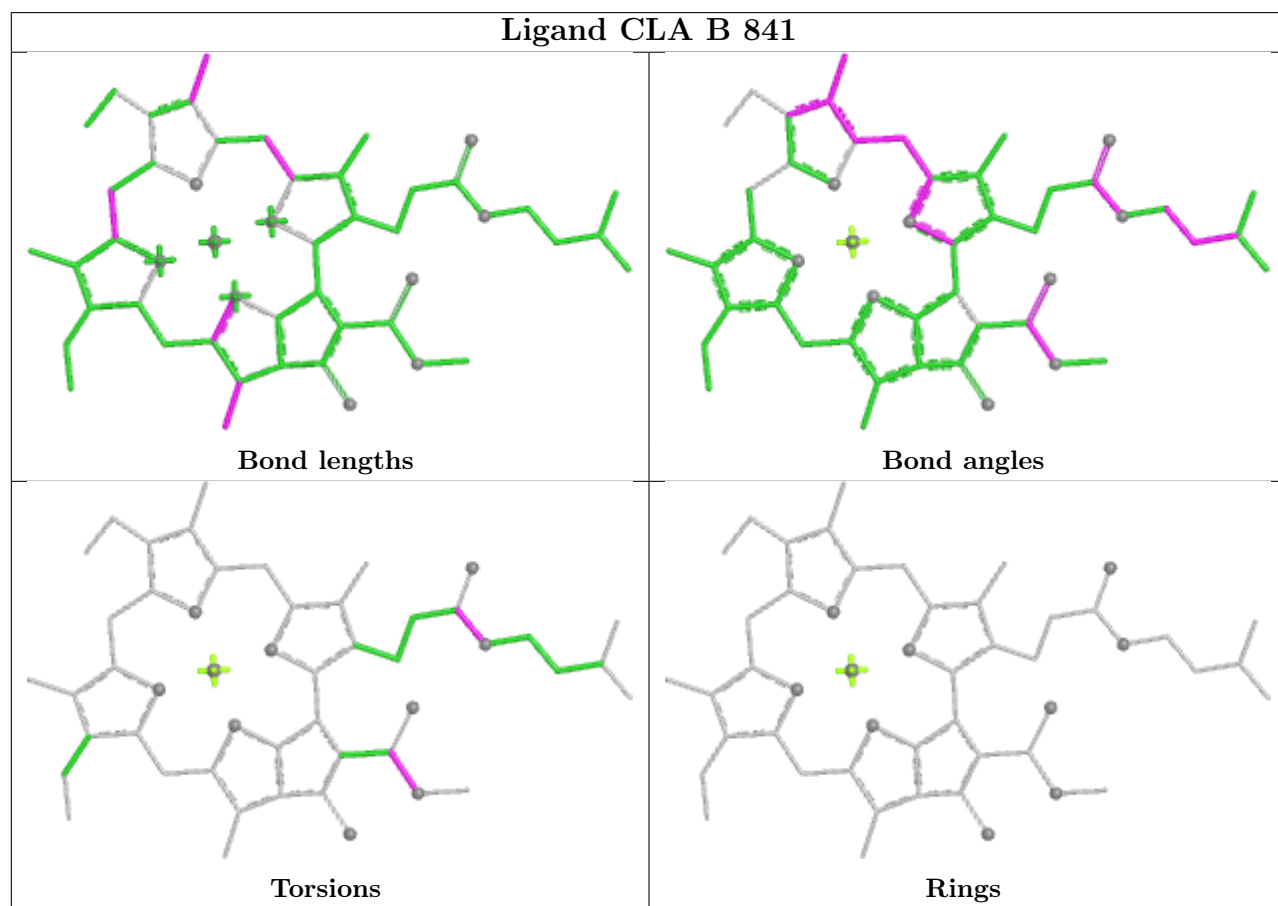
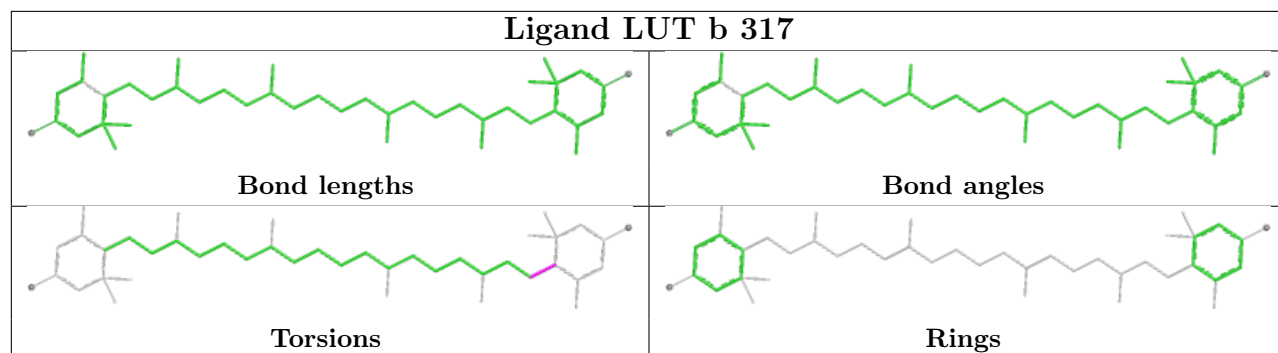
Ligand CLA 8 612

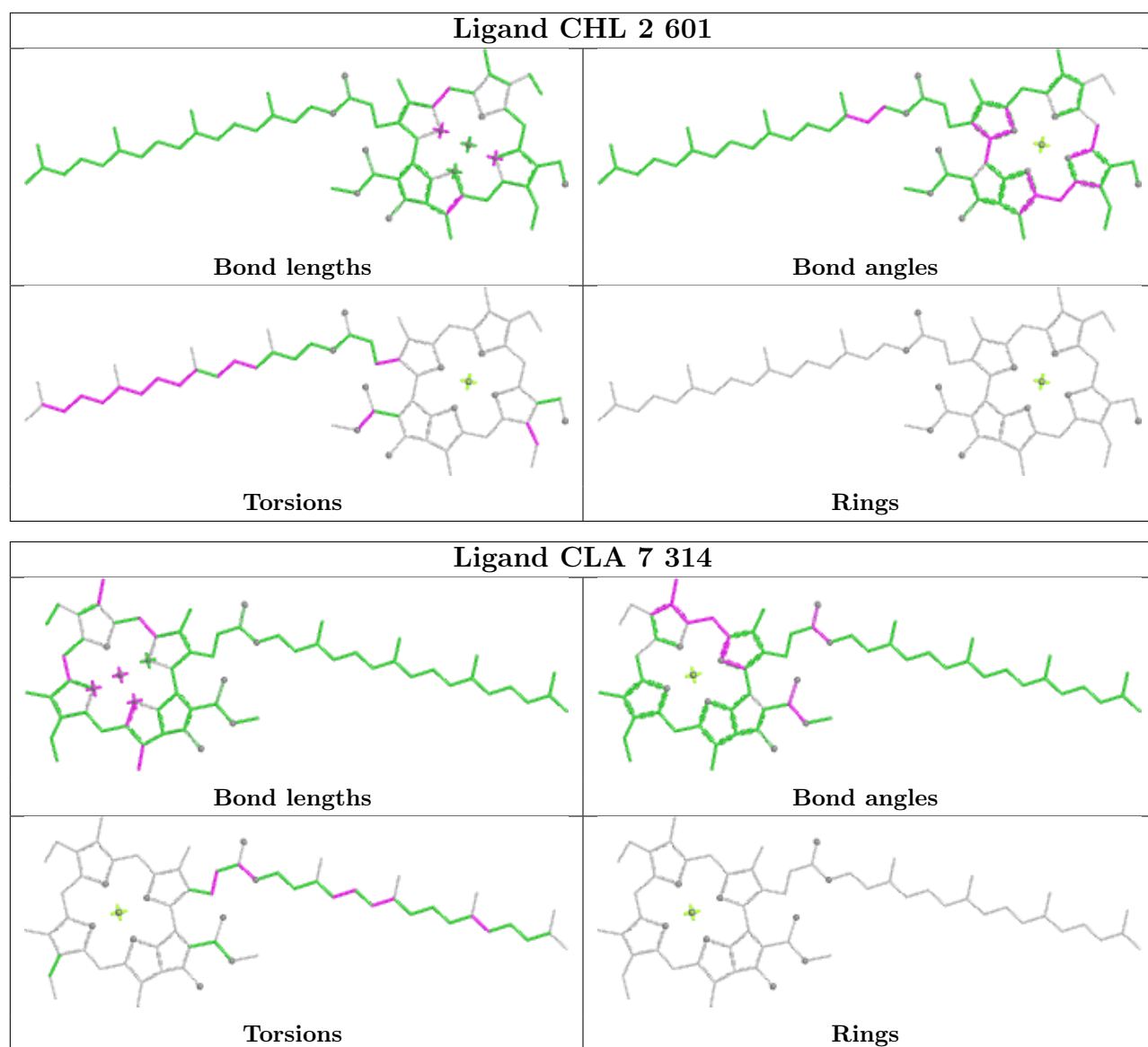


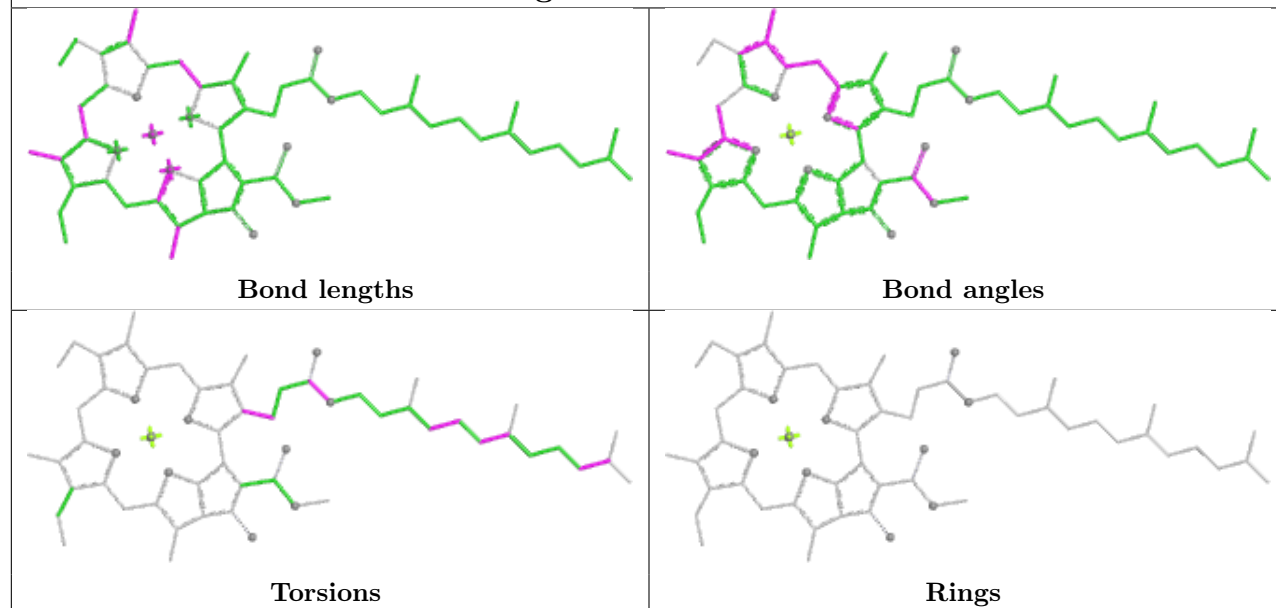
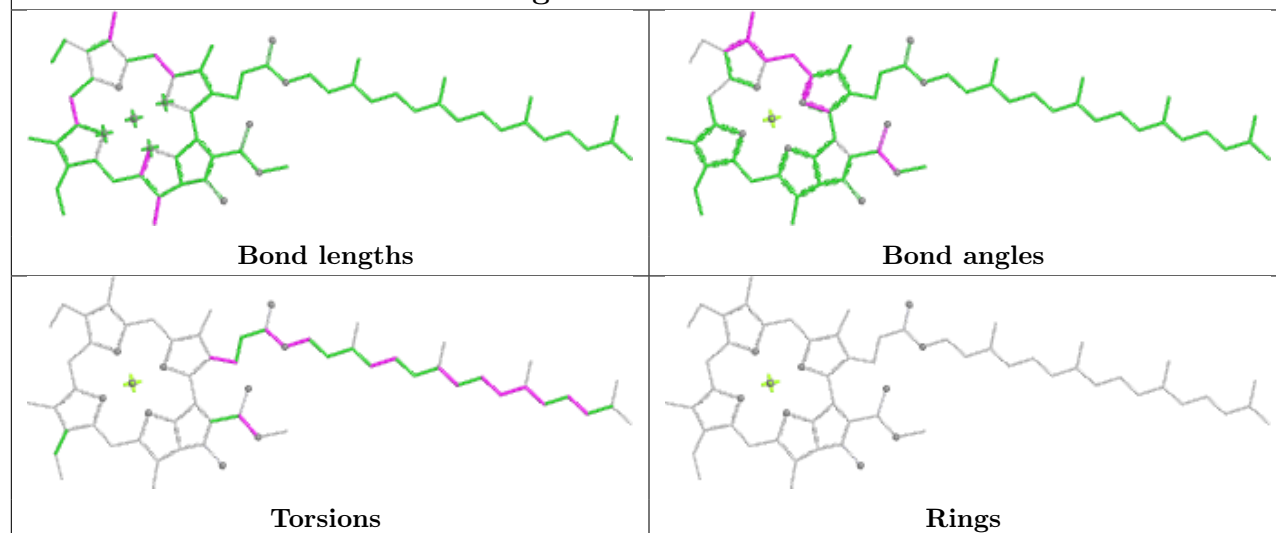
Ligand 3PH 2 619



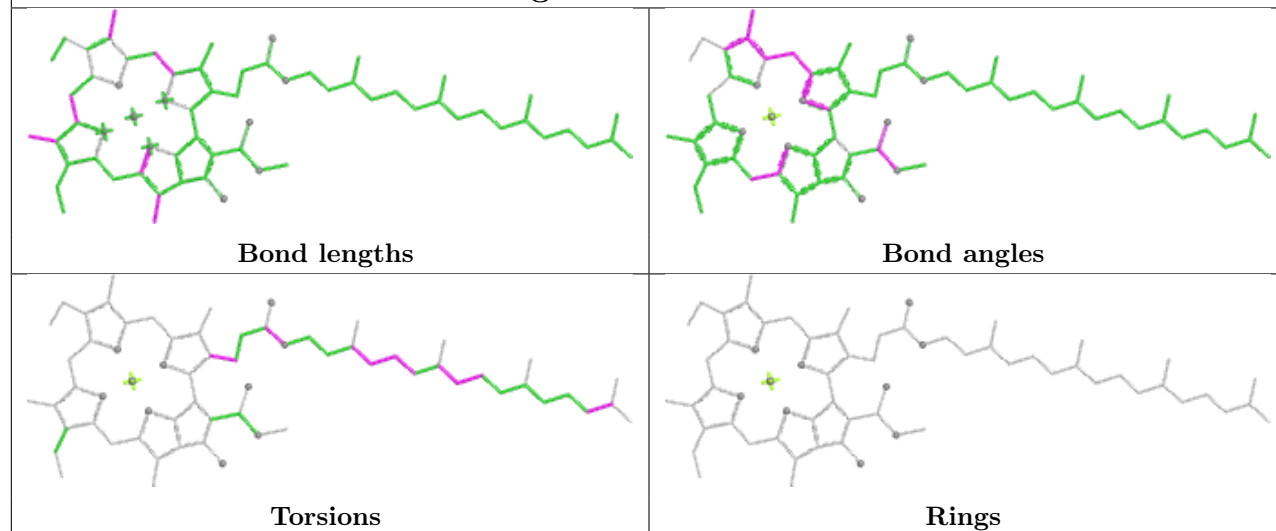




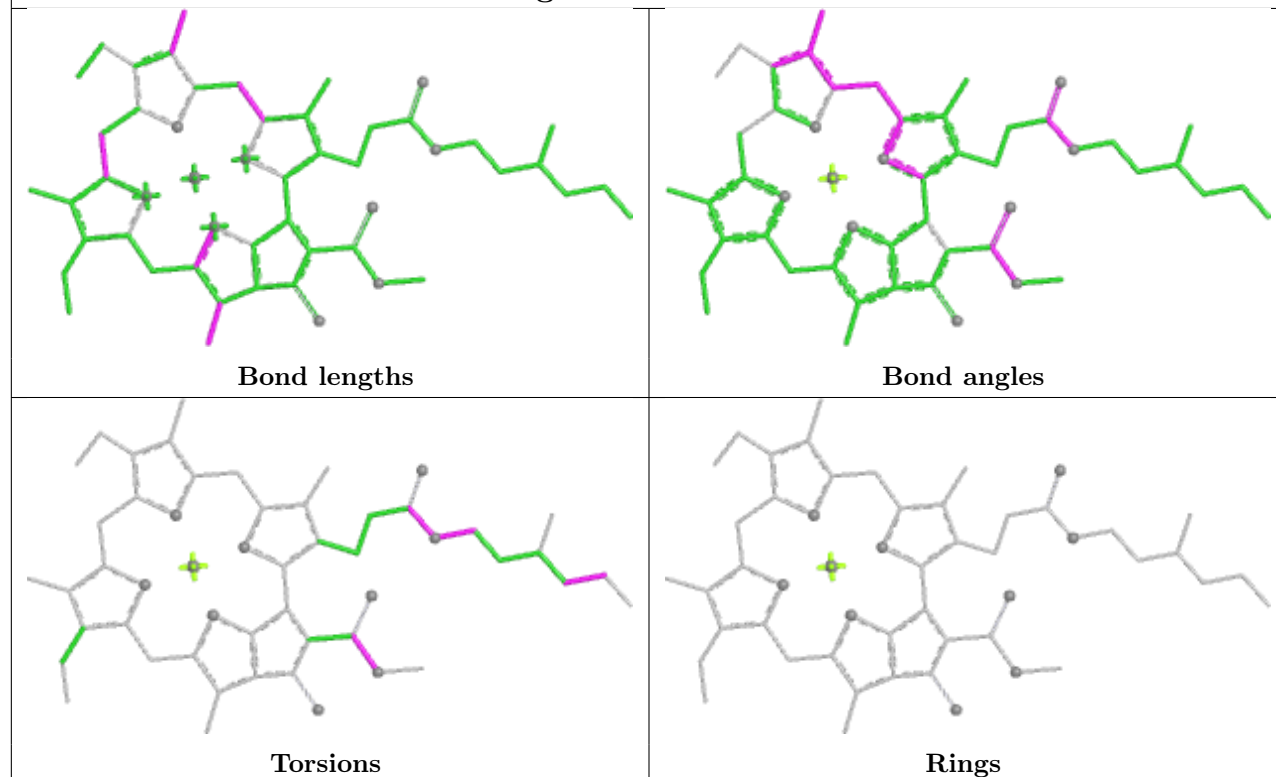


Ligand CLA b 311**Ligand CLA B 821**

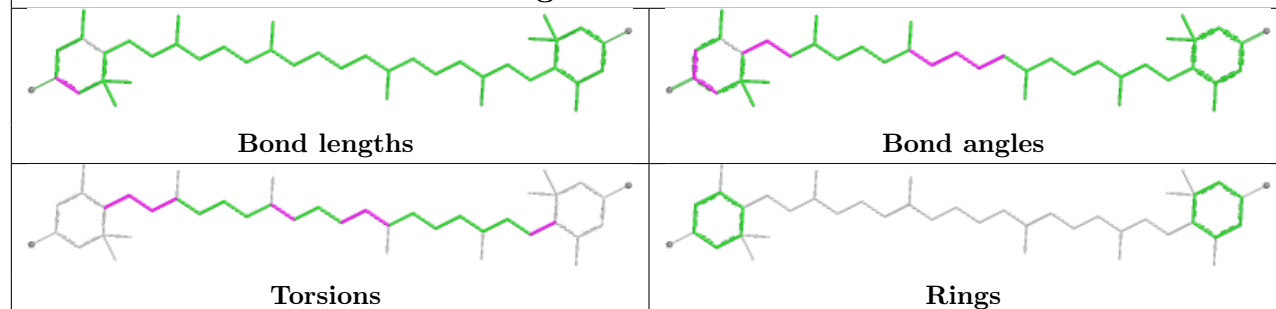
Ligand CLA A 807

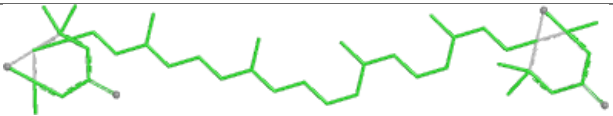
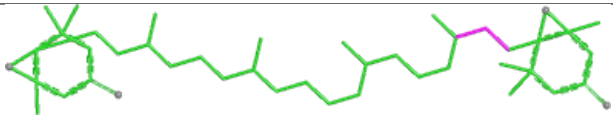
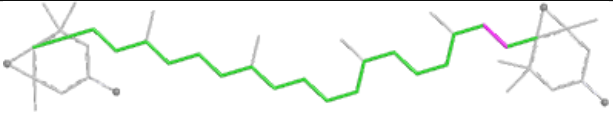
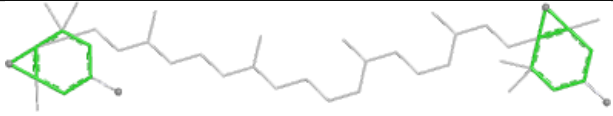


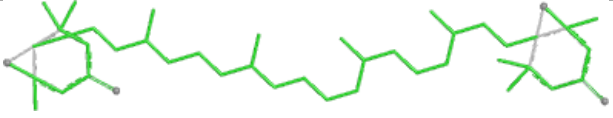
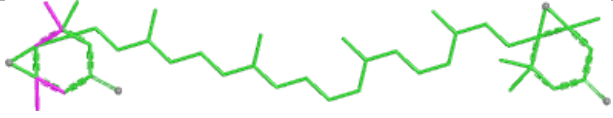
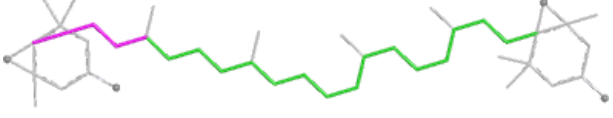
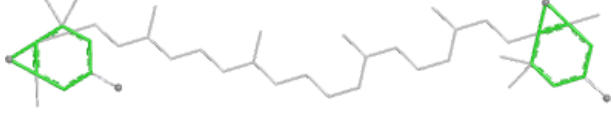
Ligand CLA 7 313

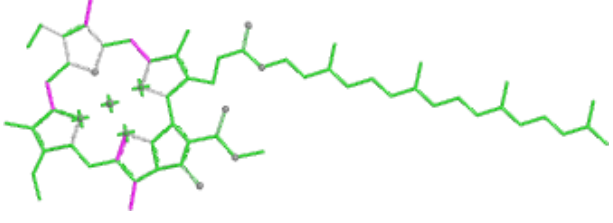
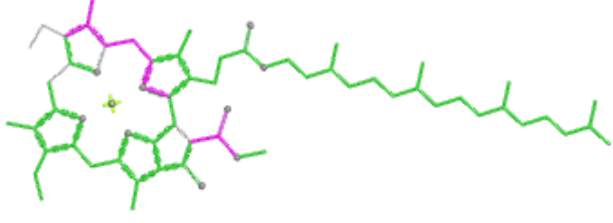
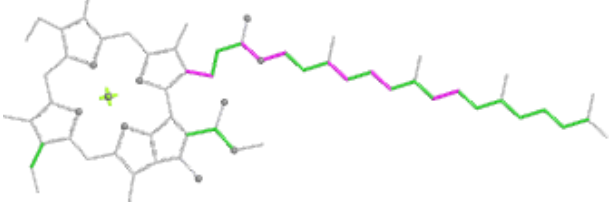
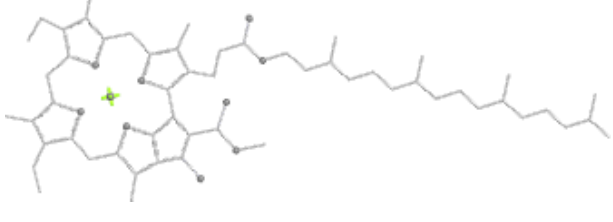


Ligand LUT 1 314

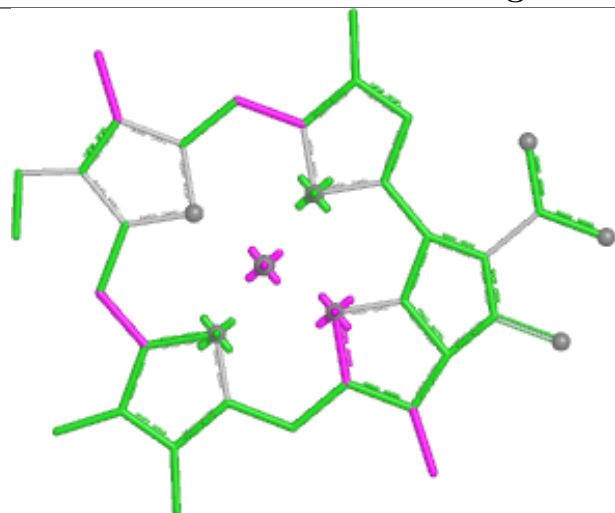


Ligand XAT b 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

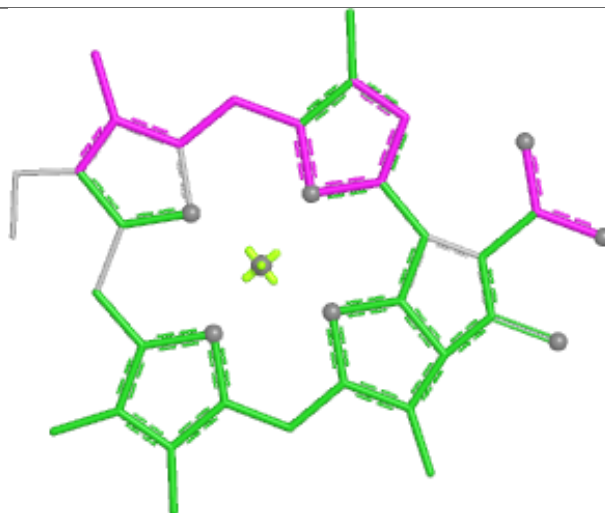
Ligand XAT c 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

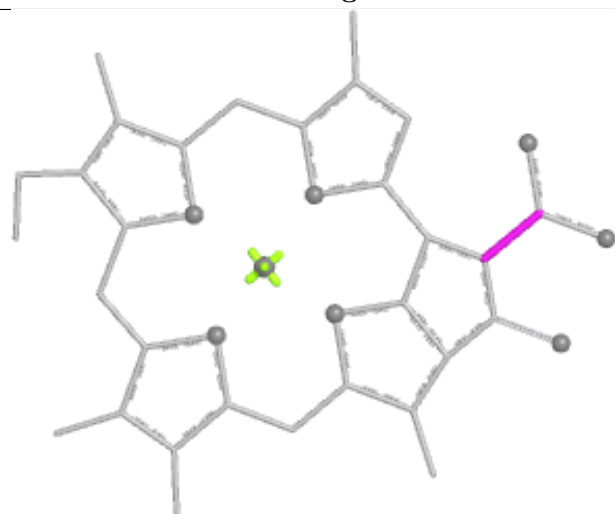
Ligand CLA O 2001



Bond lengths



Bond angles

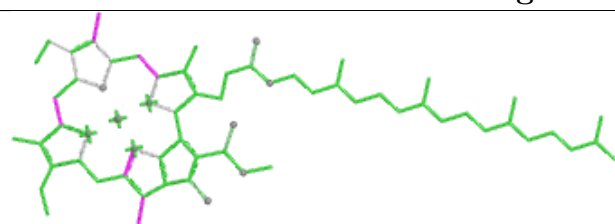


Torsions

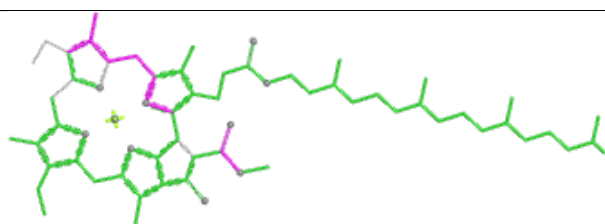


Rings

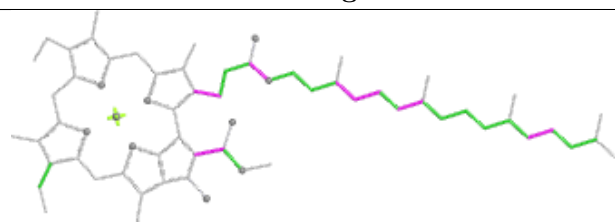
Ligand CLA B 816



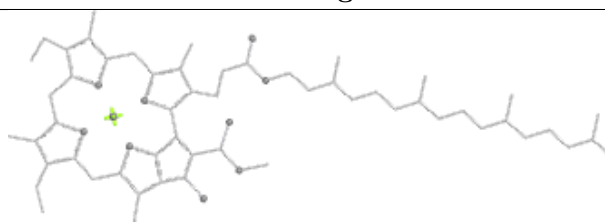
Bond lengths



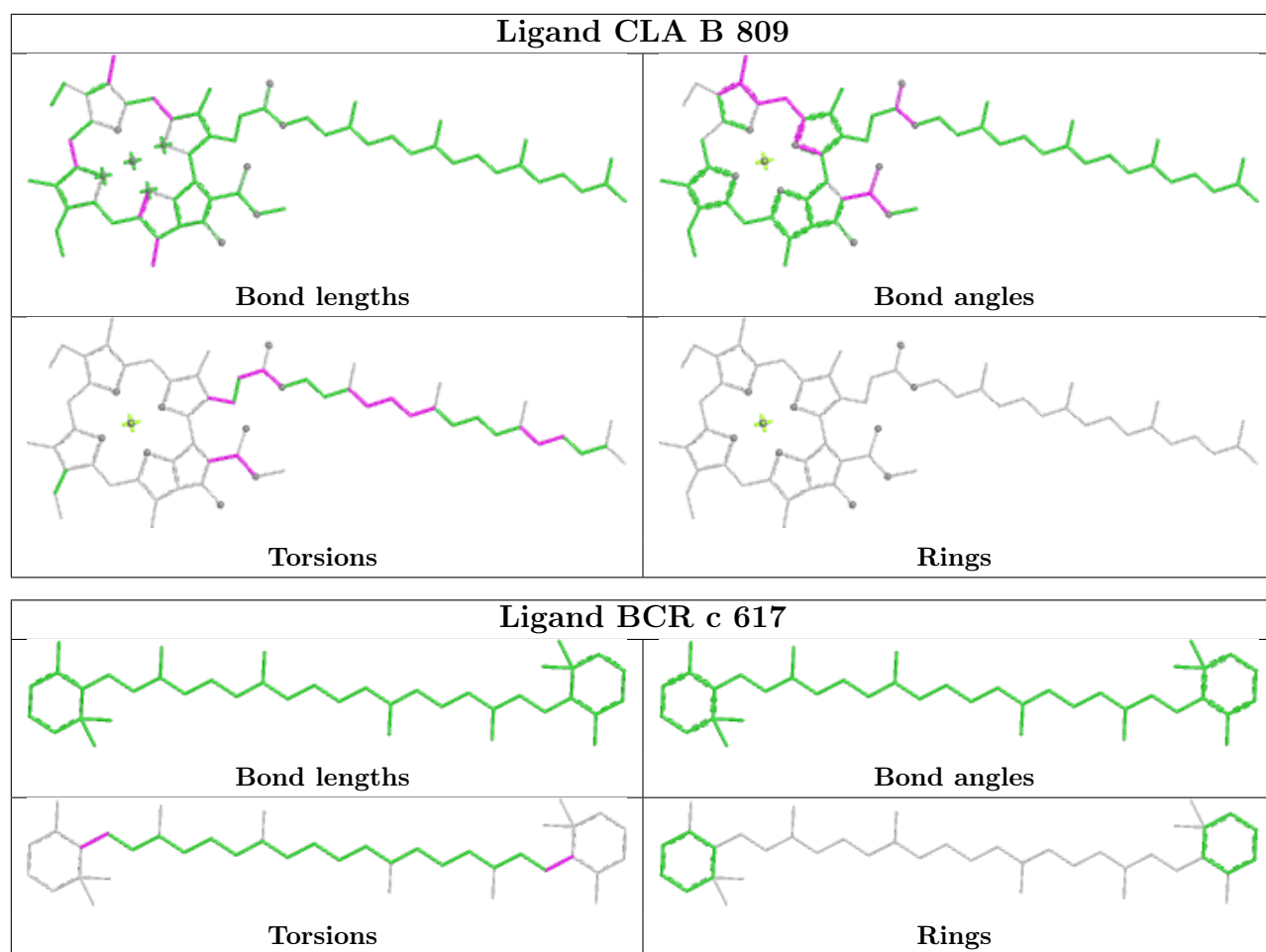
Bond angles



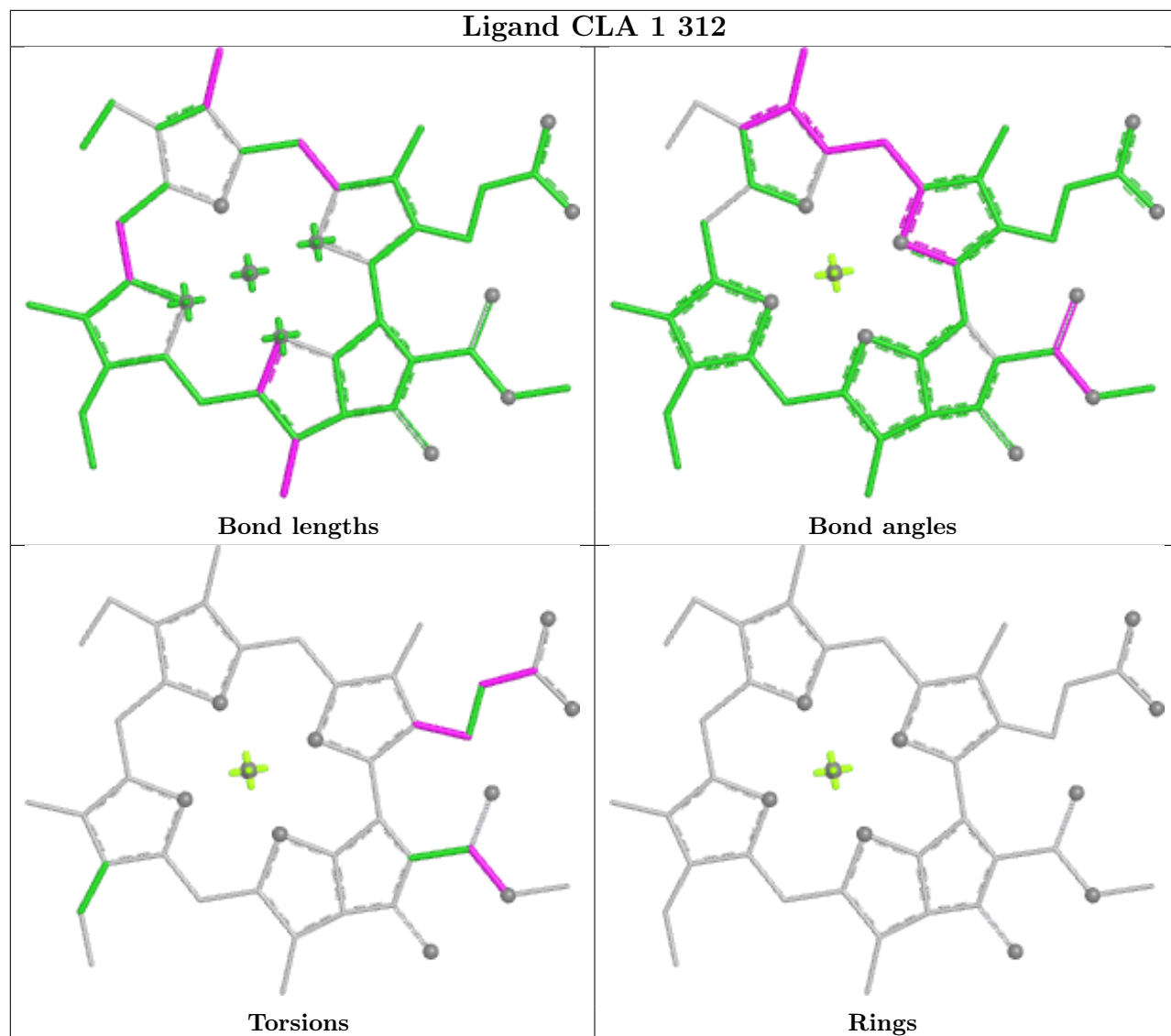
Torsions

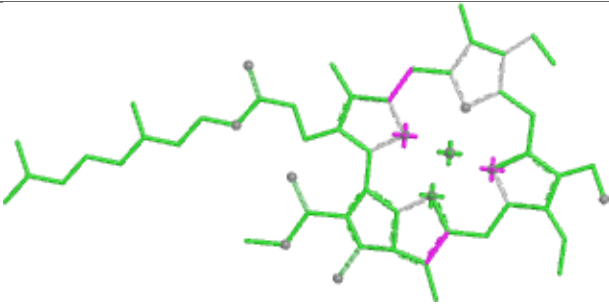
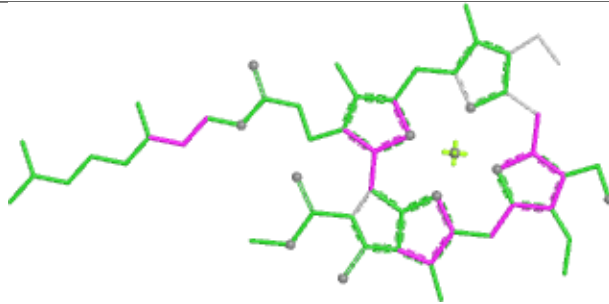
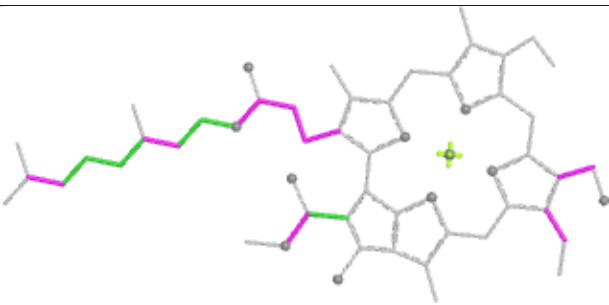
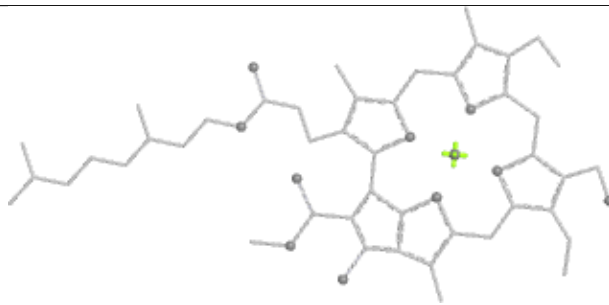


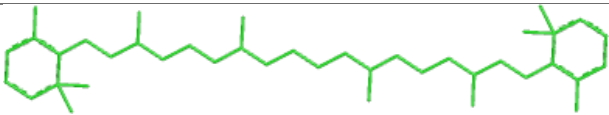
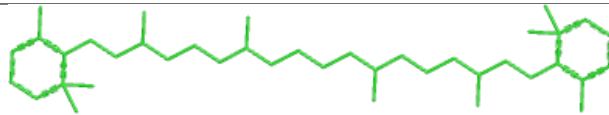
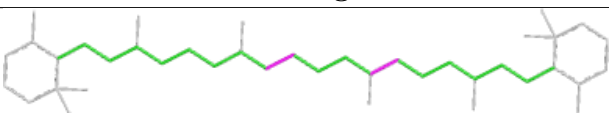
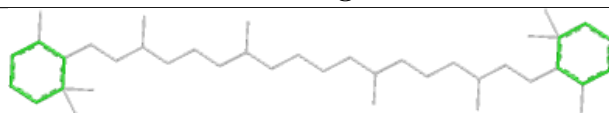
Rings

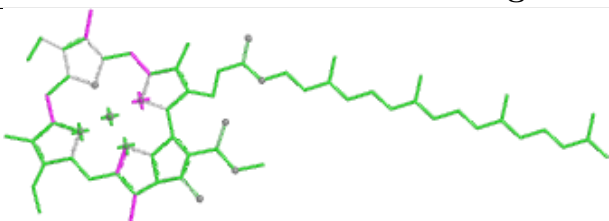
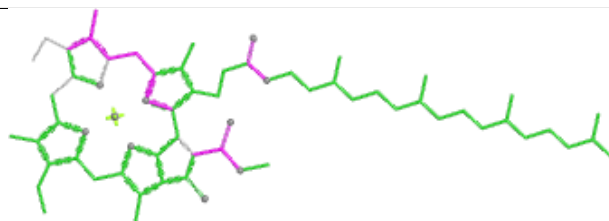
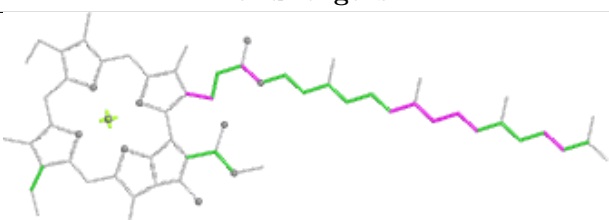
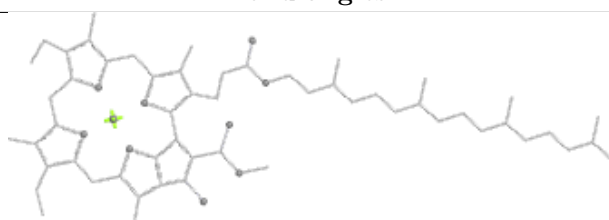


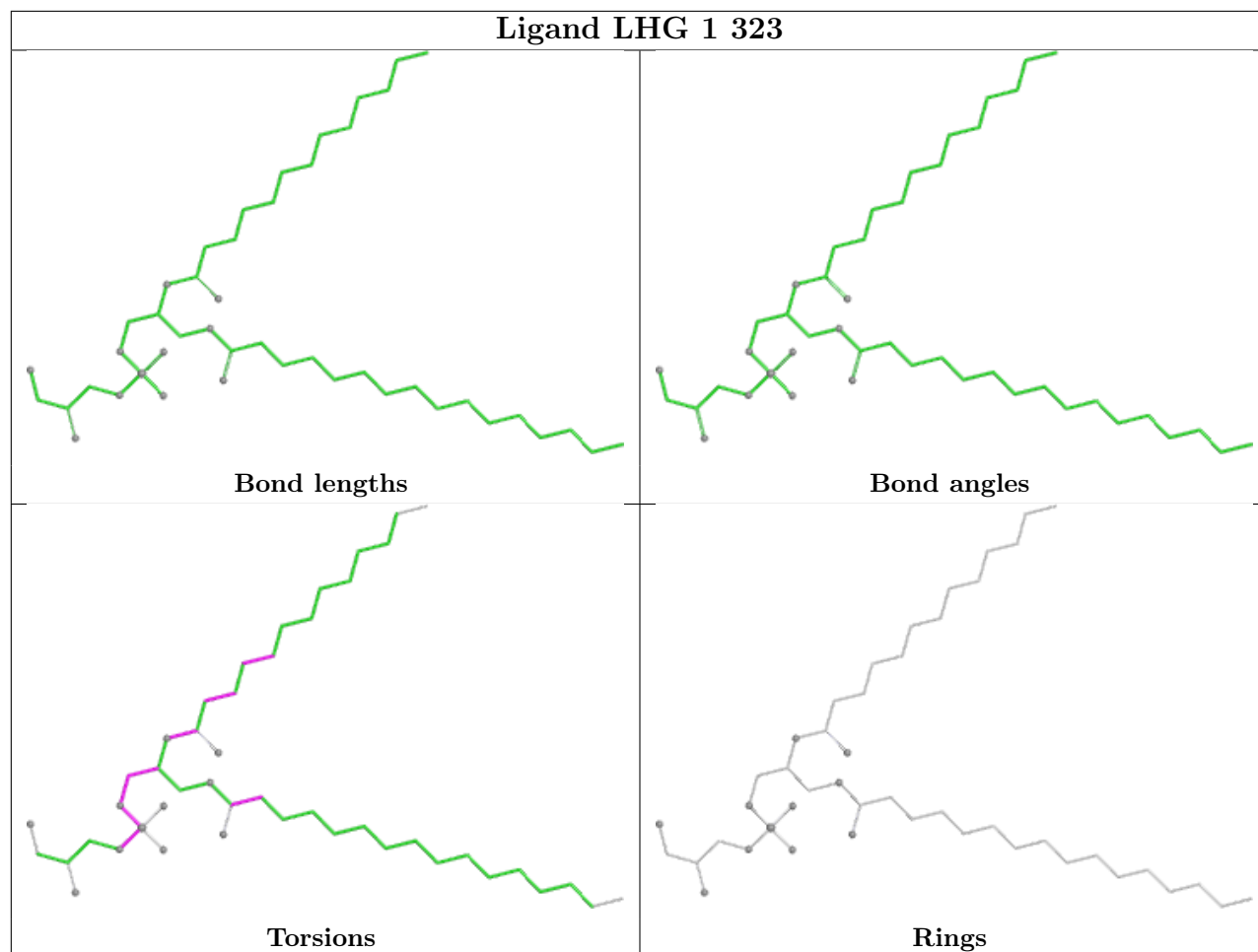
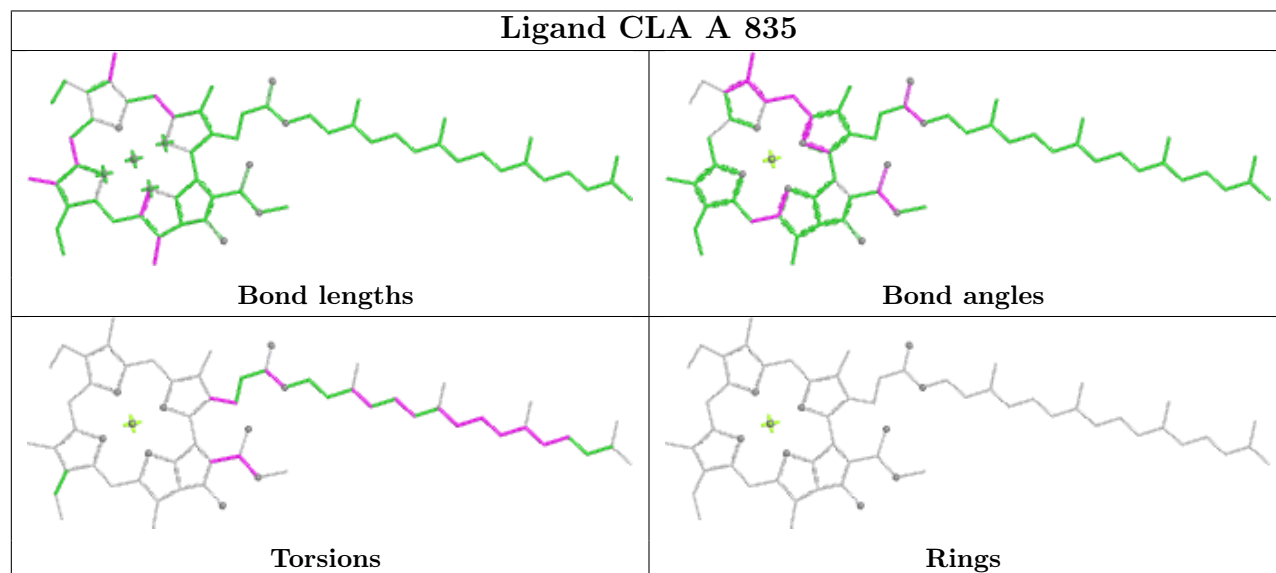
Ligand CLA 1 312



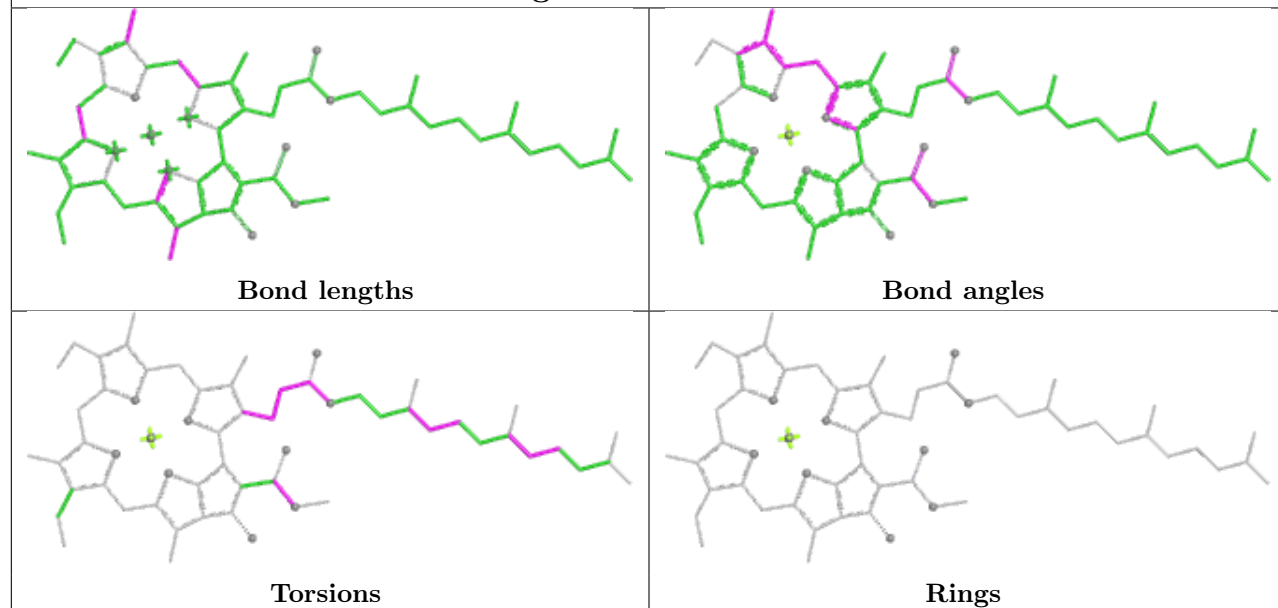
Ligand CHL T 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

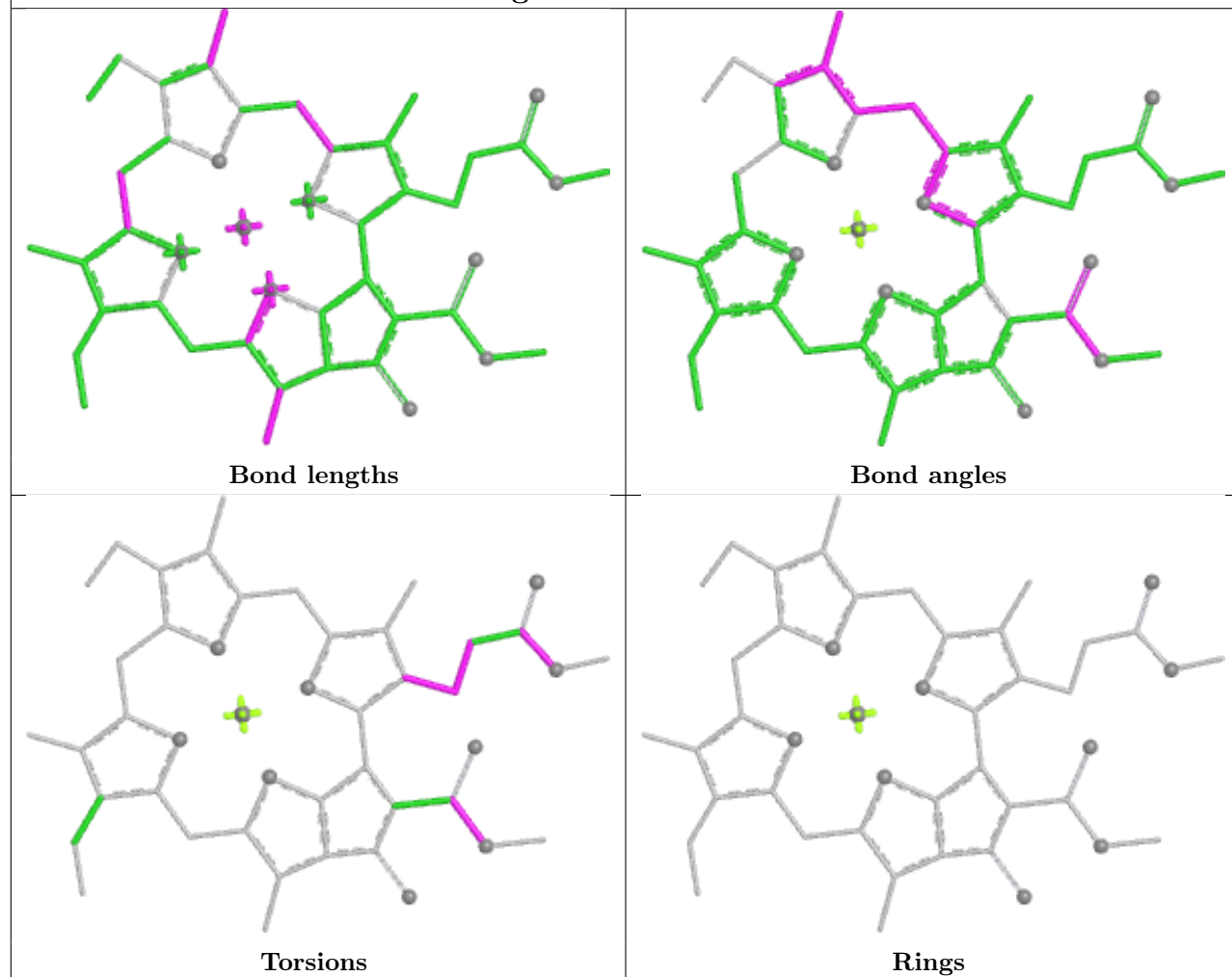
Ligand CLA A 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG 1 323**Ligand CLA A 835**

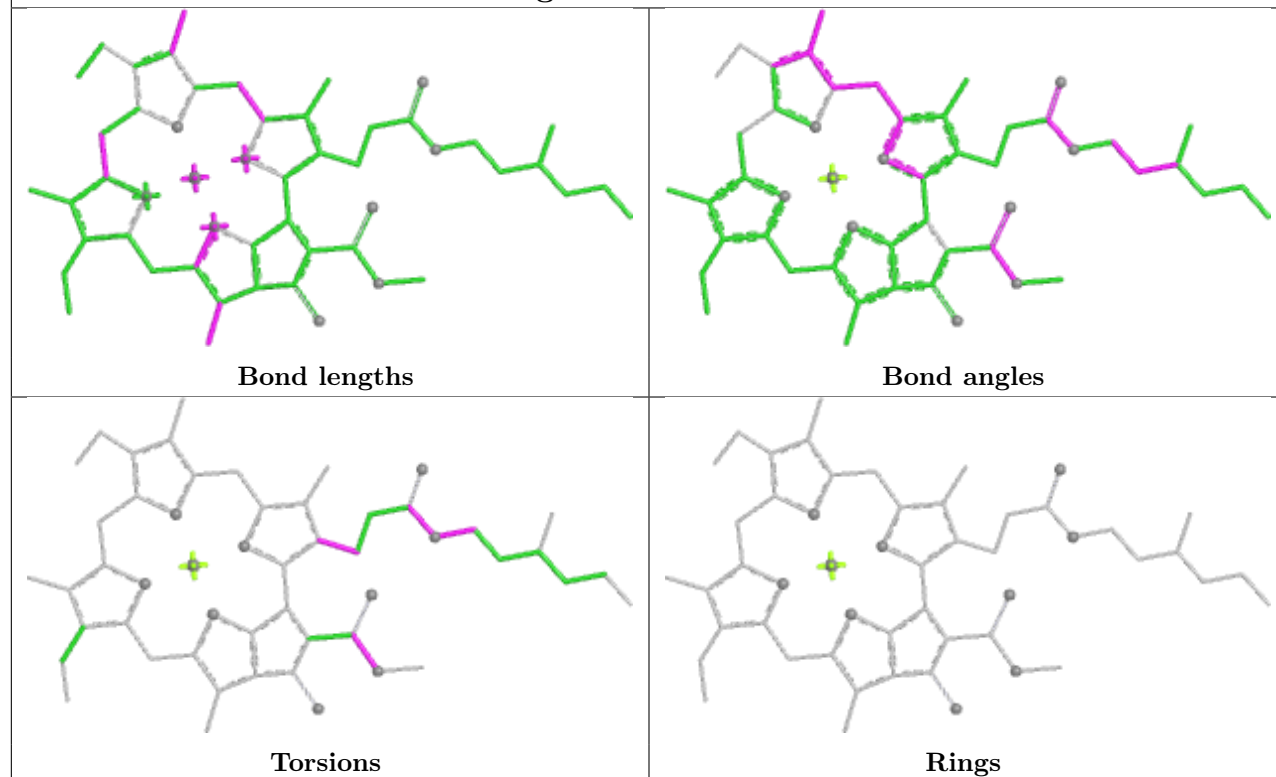
Ligand CLA B 830



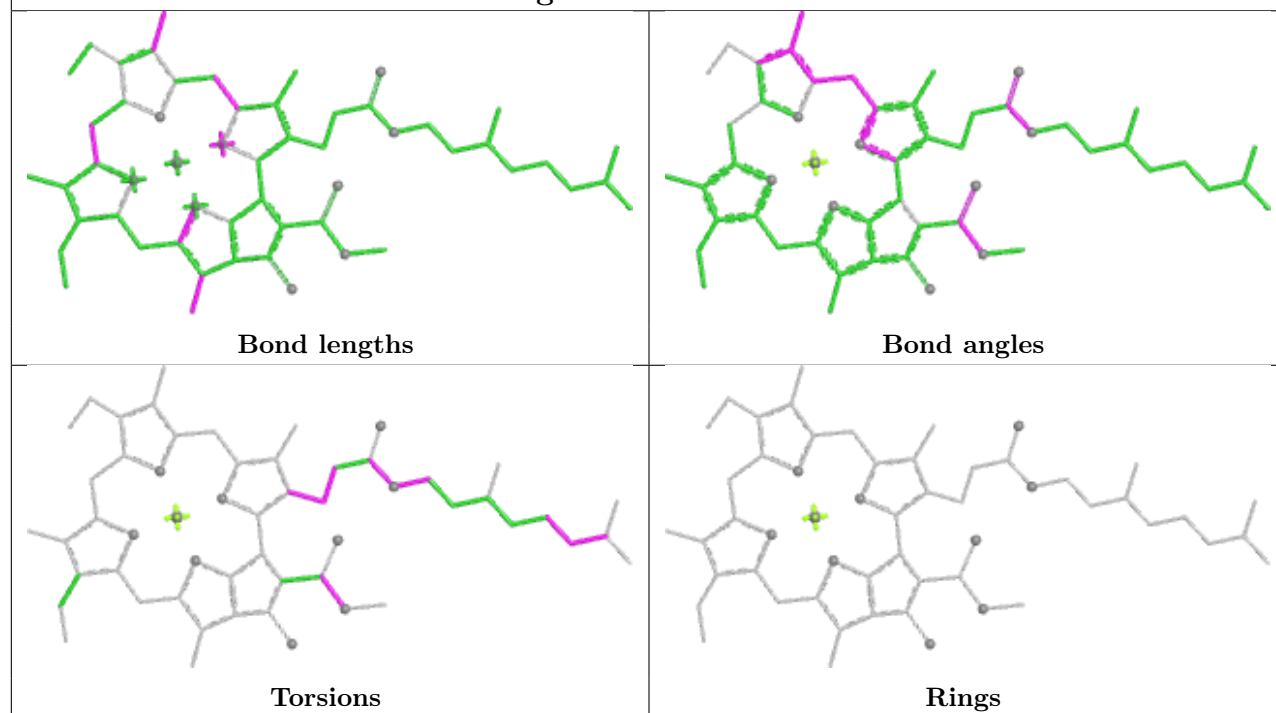
Ligand CLA G 204

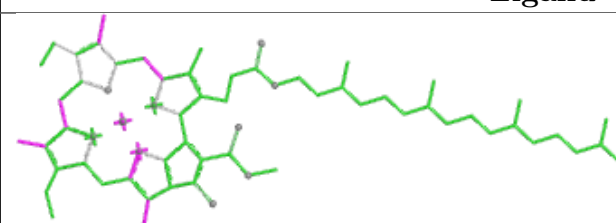
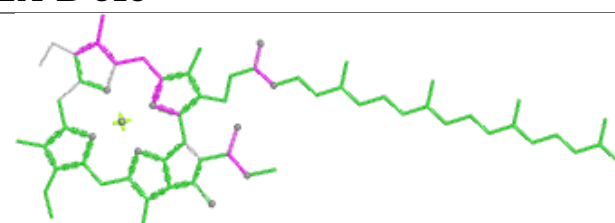
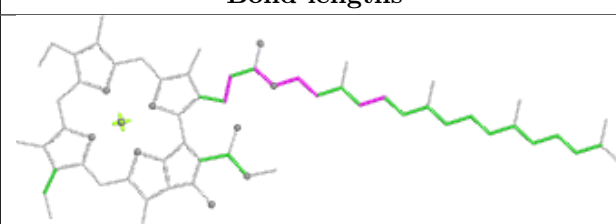
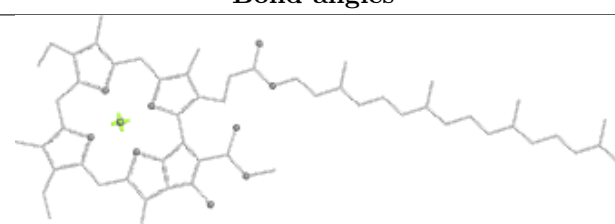




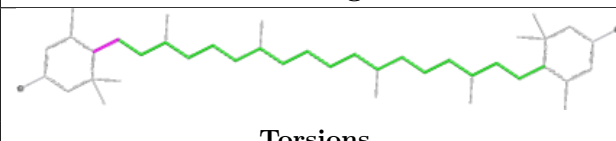
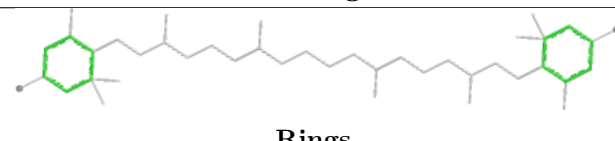
Ligand CLA 3 410


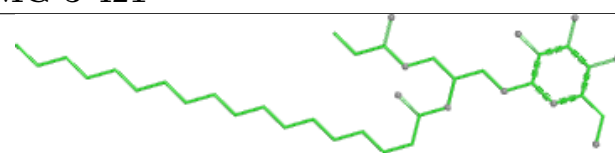
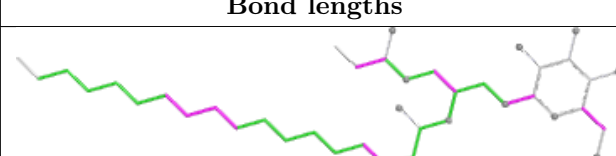
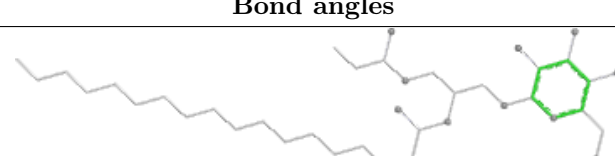


Ligand CLA 7 305

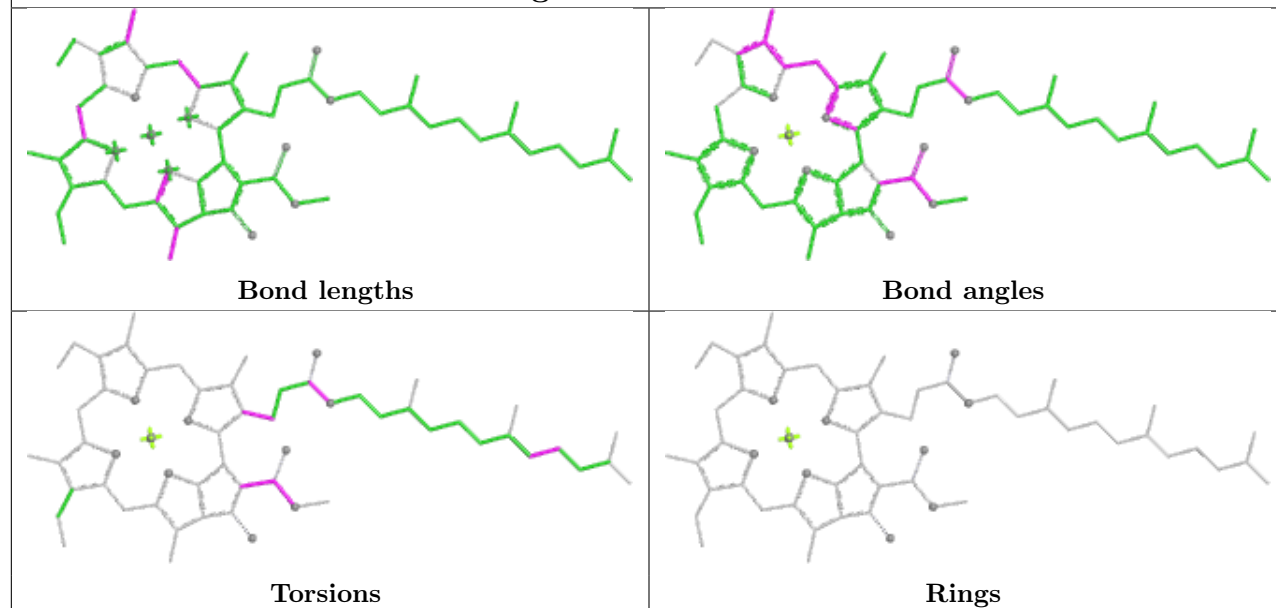


Ligand CLA B 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

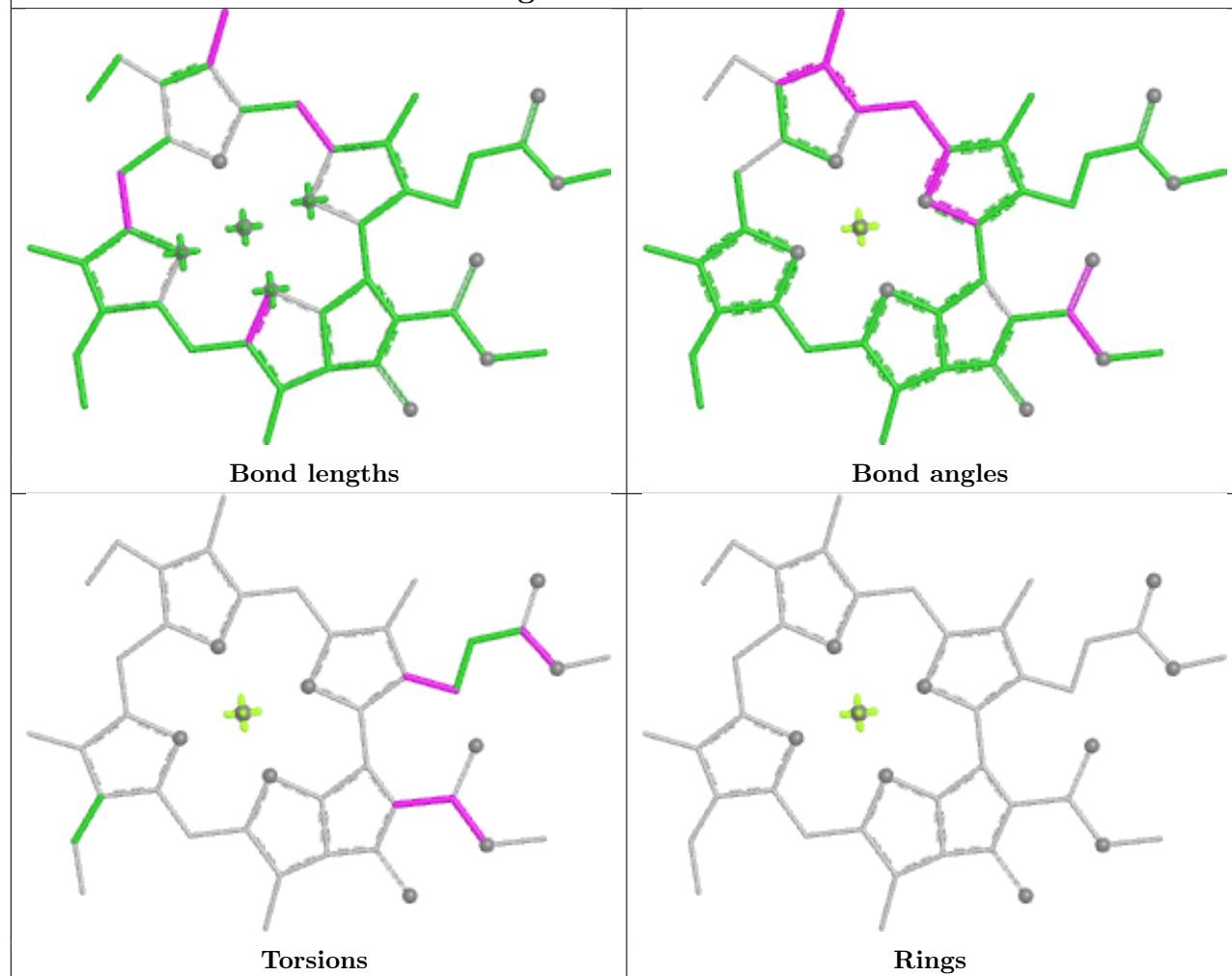
Ligand LUT 7 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

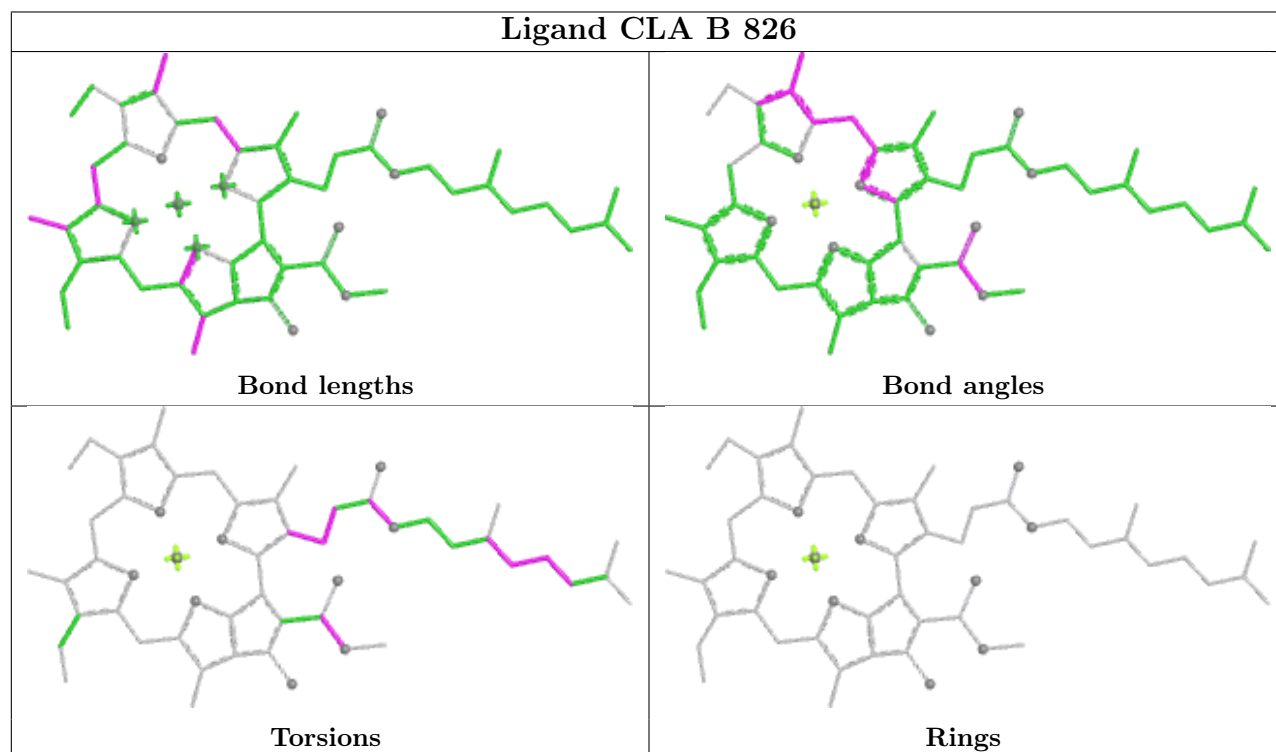
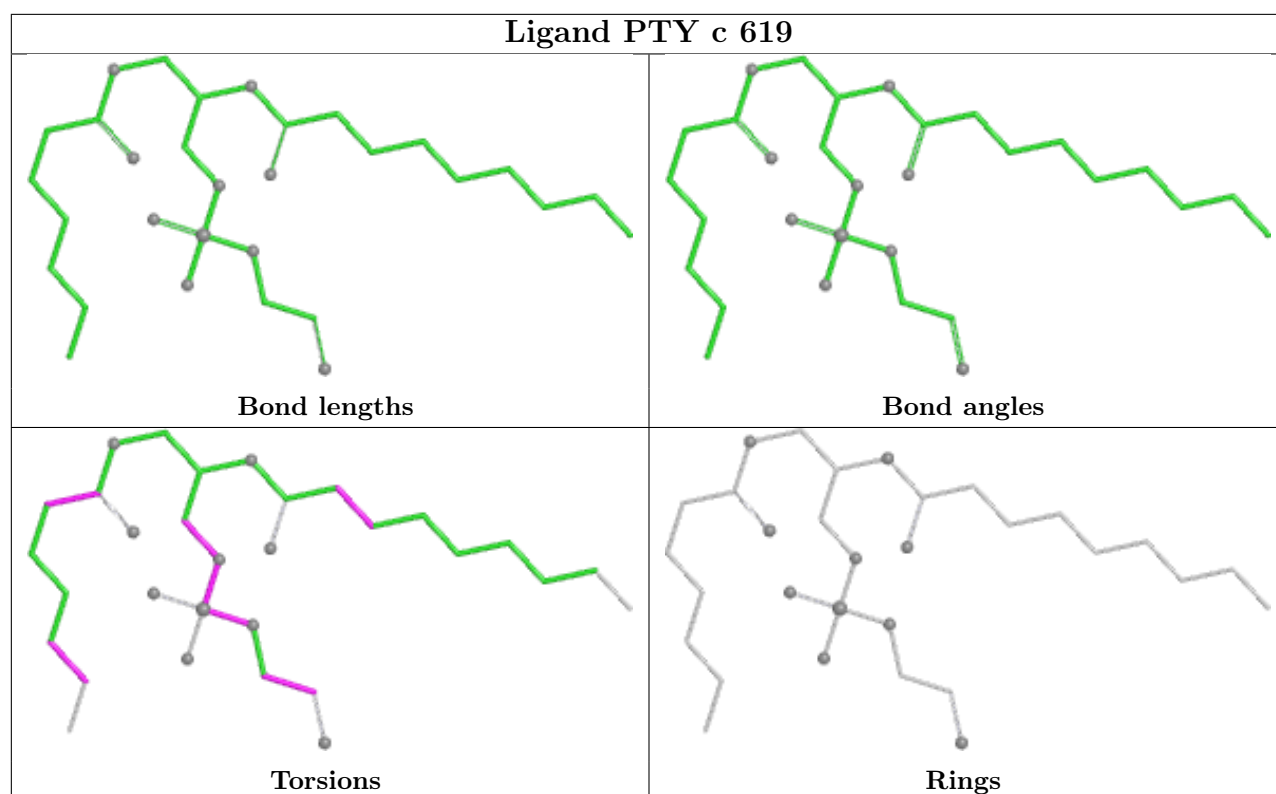
Ligand LMG 3 421	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 806

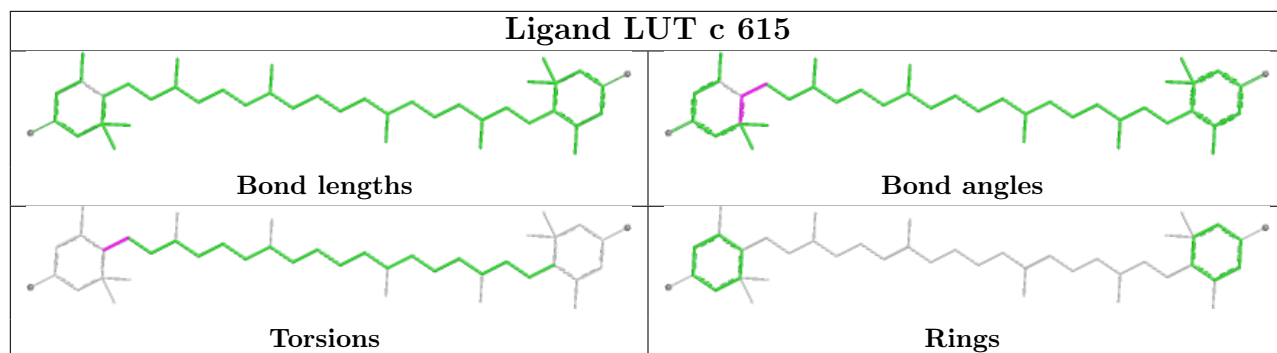


Ligand CLA 9 609

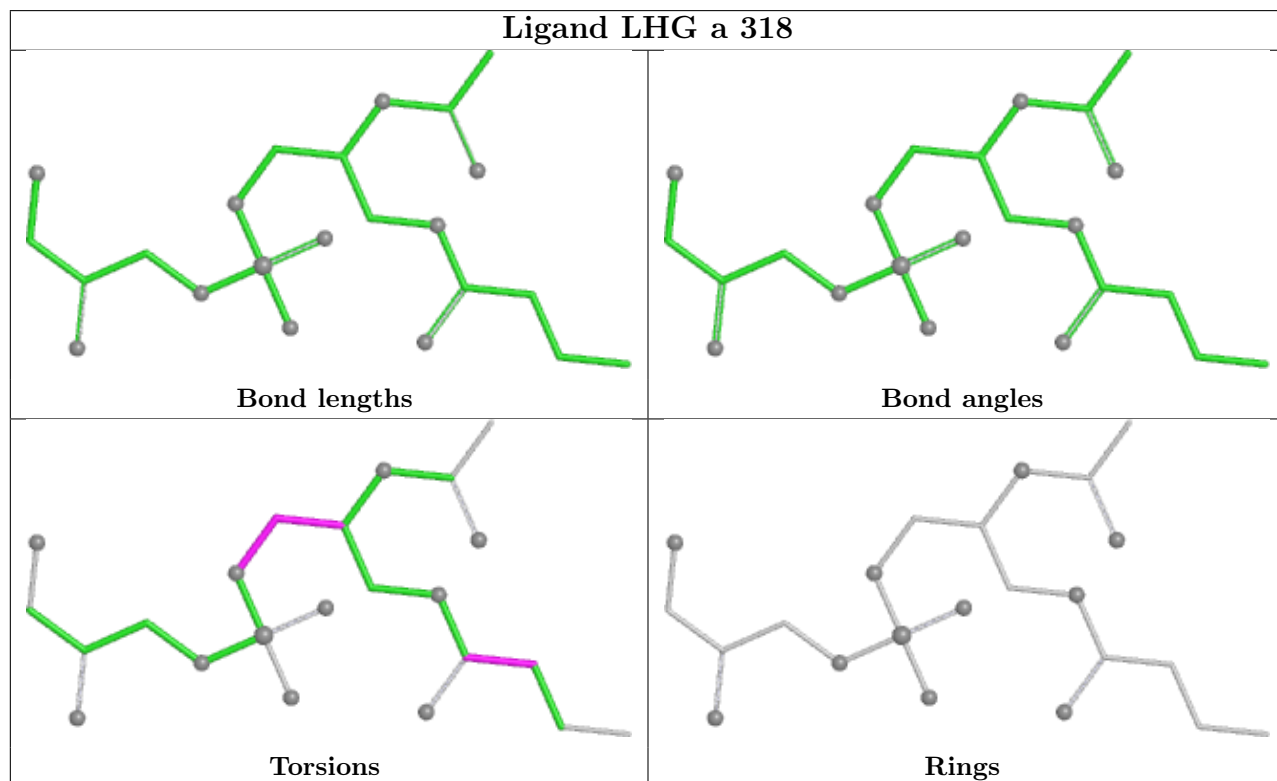




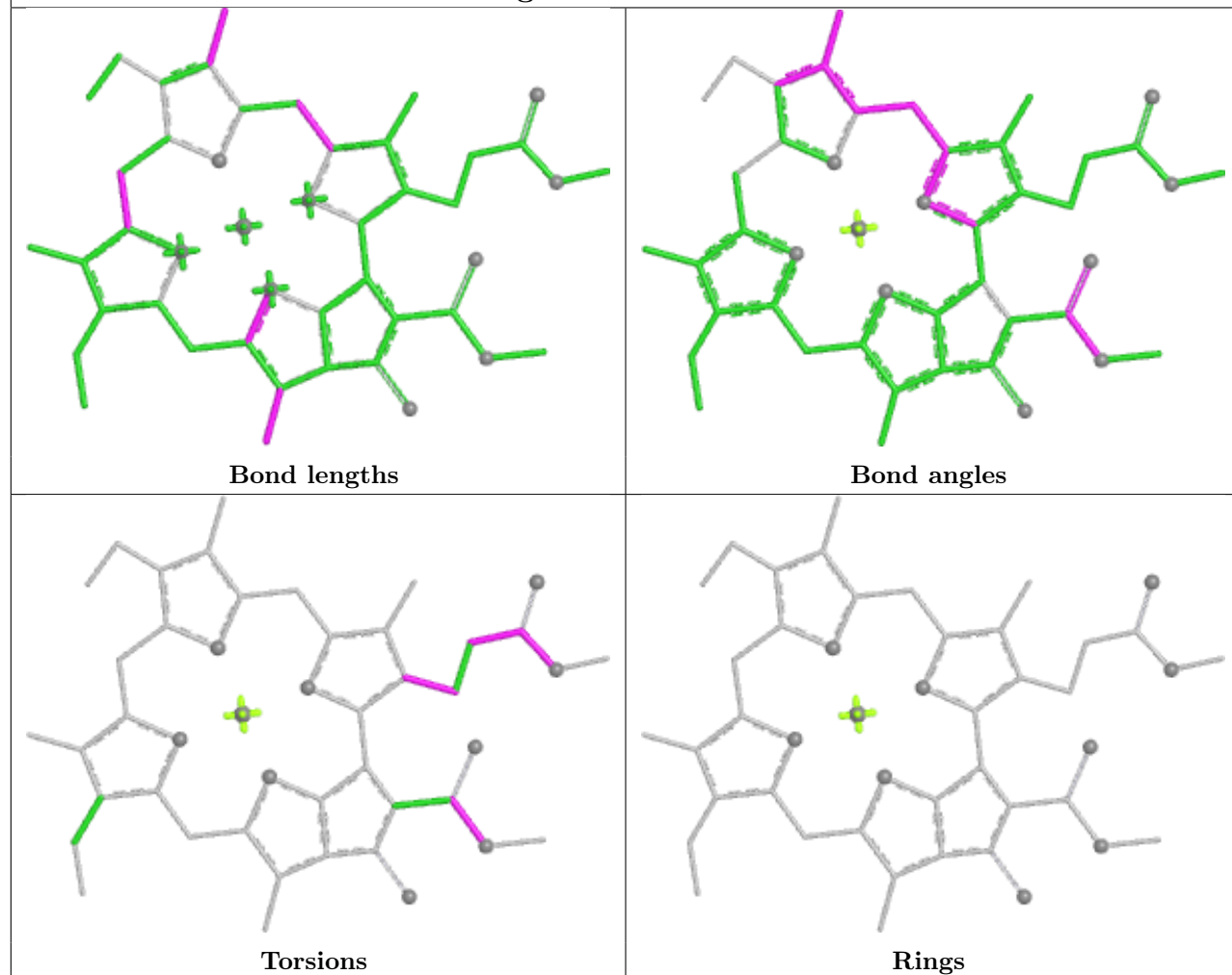
Ligand LUT c 615



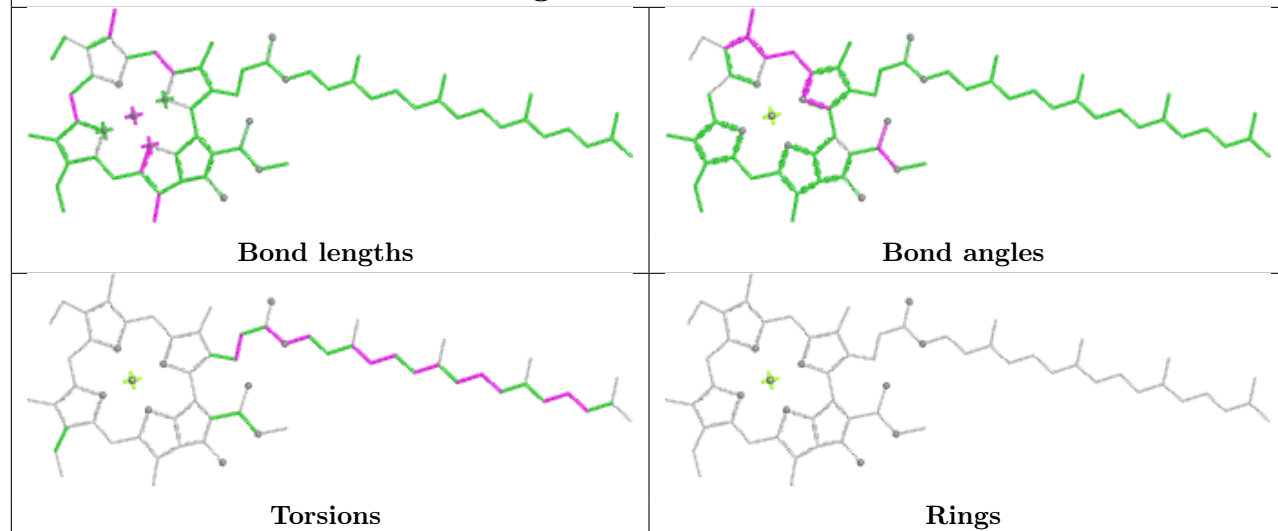
Ligand LHG a 318

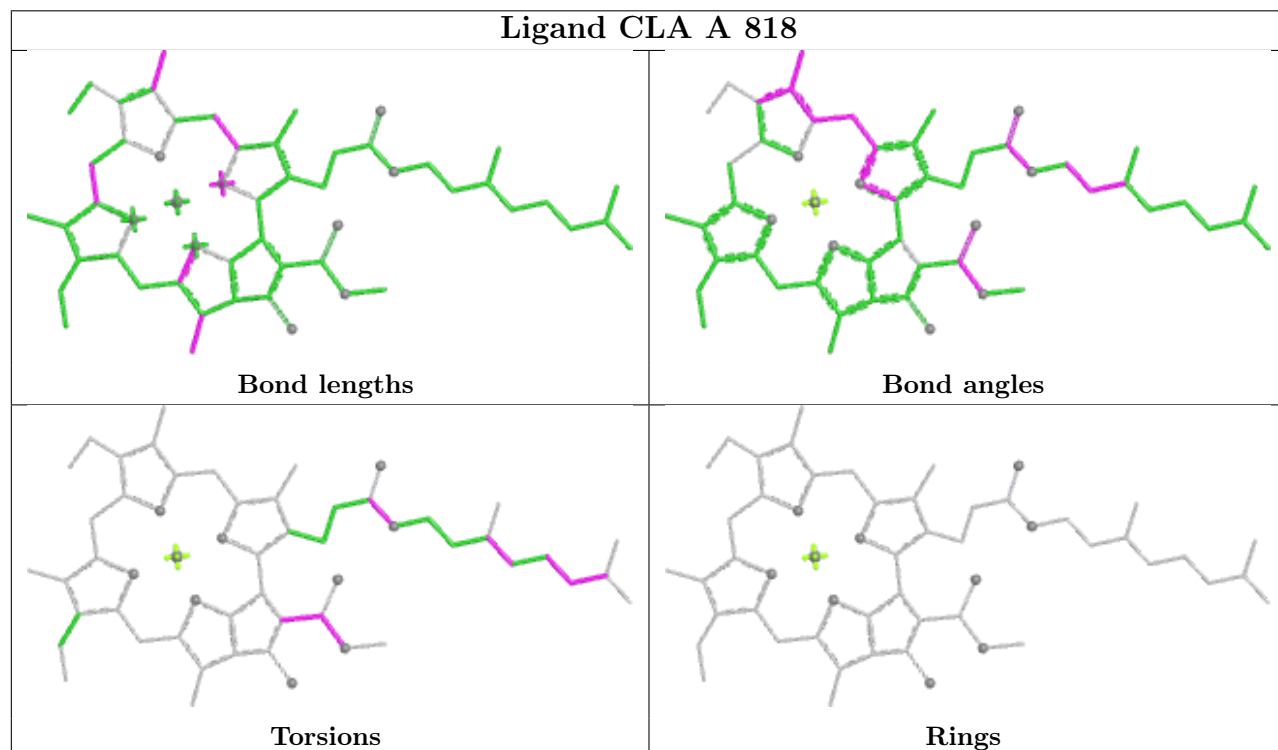
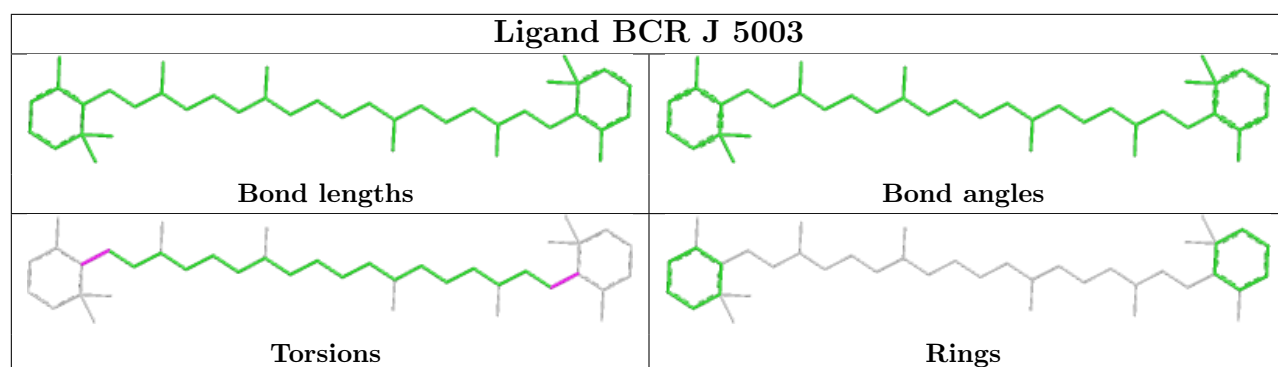


Ligand CLA a 313

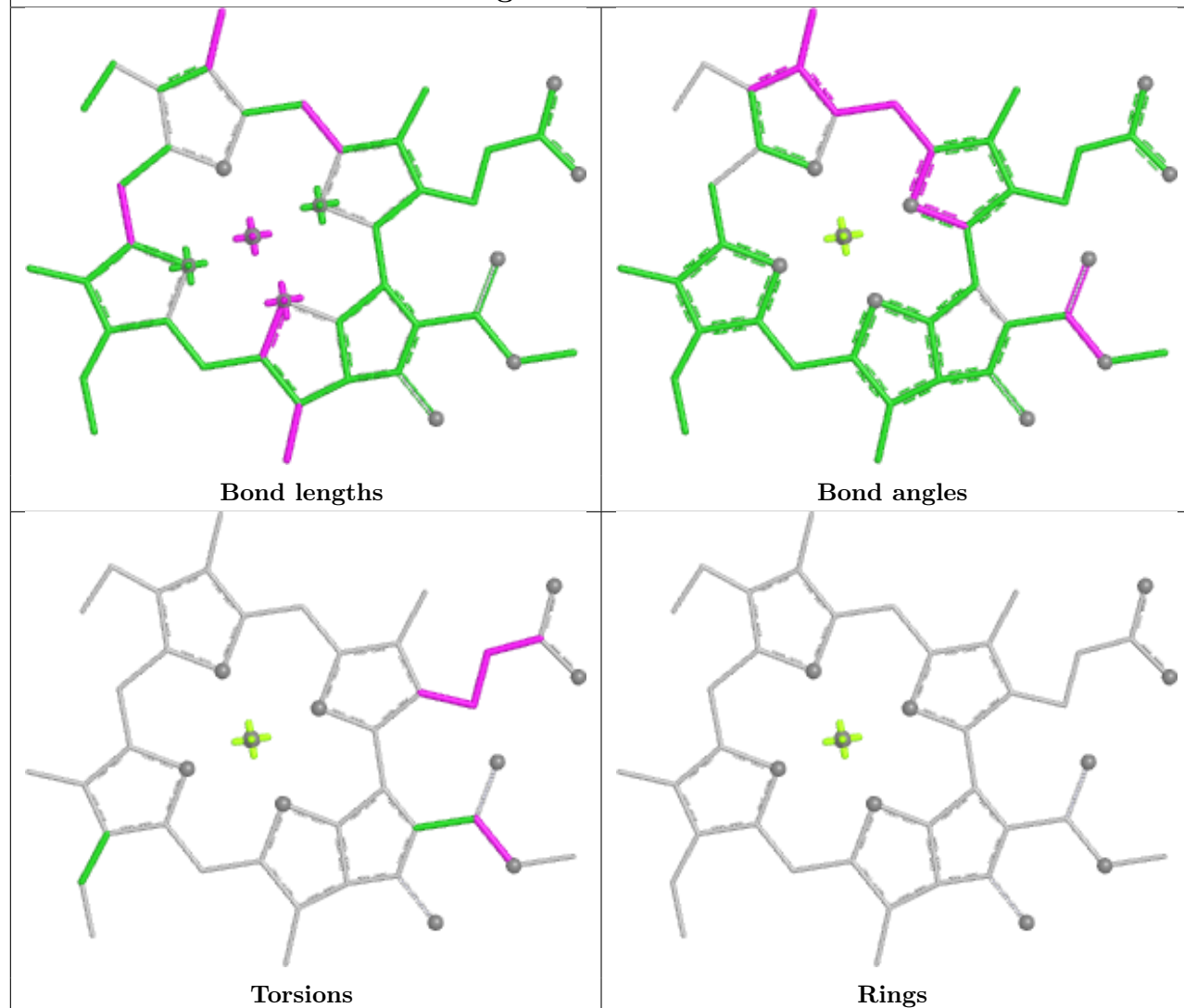


Ligand CLA B 844

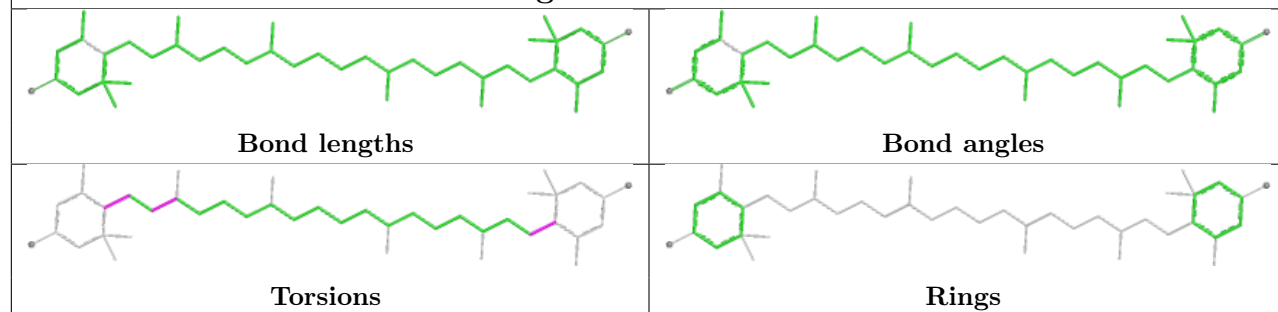




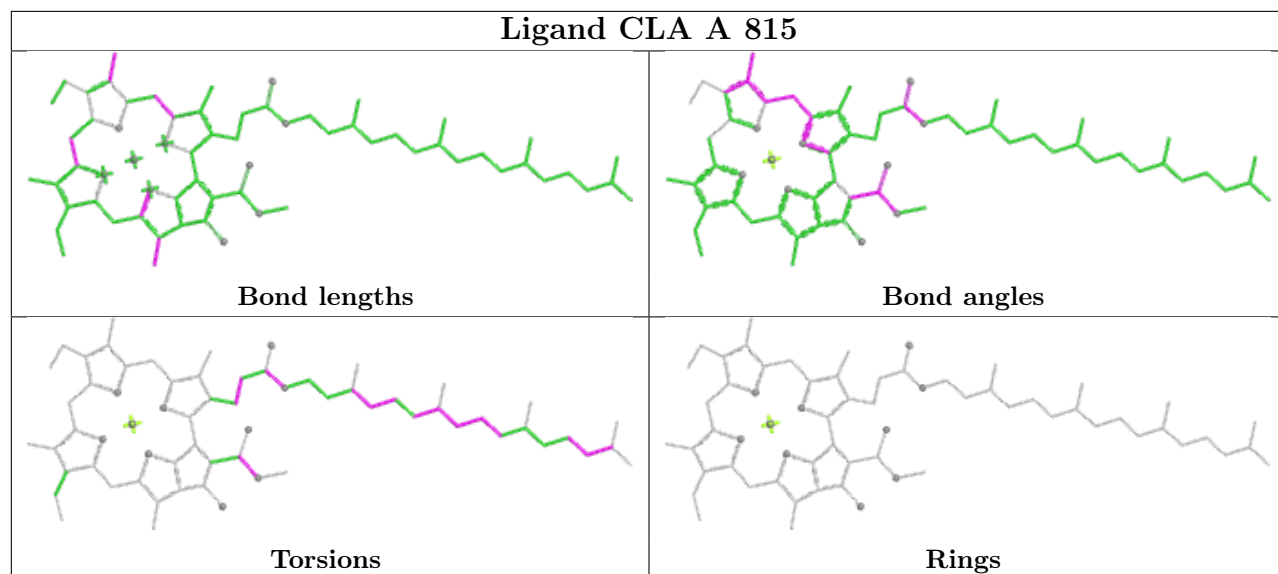
Ligand CLA 1 313



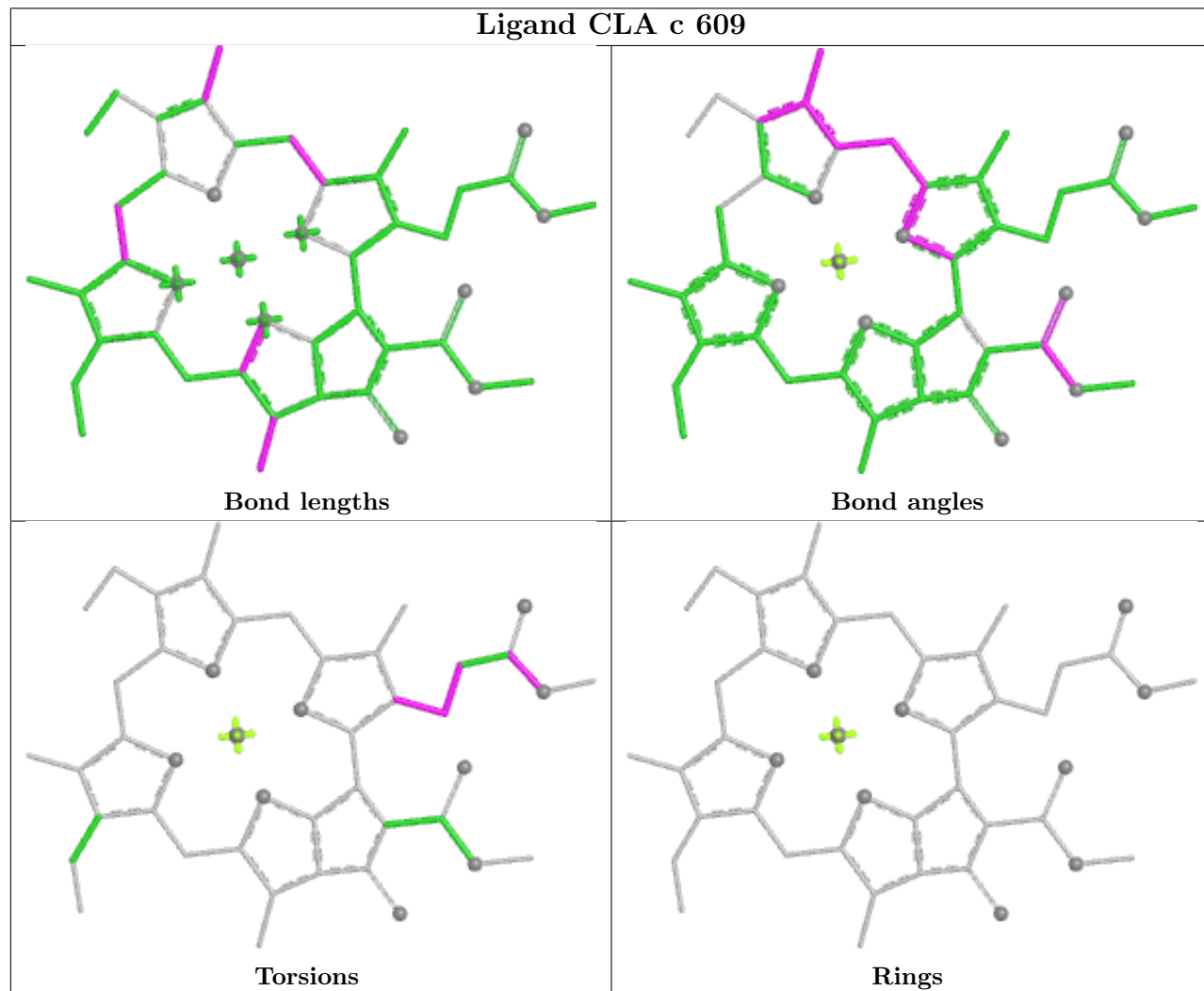
Ligand LUT 3 415

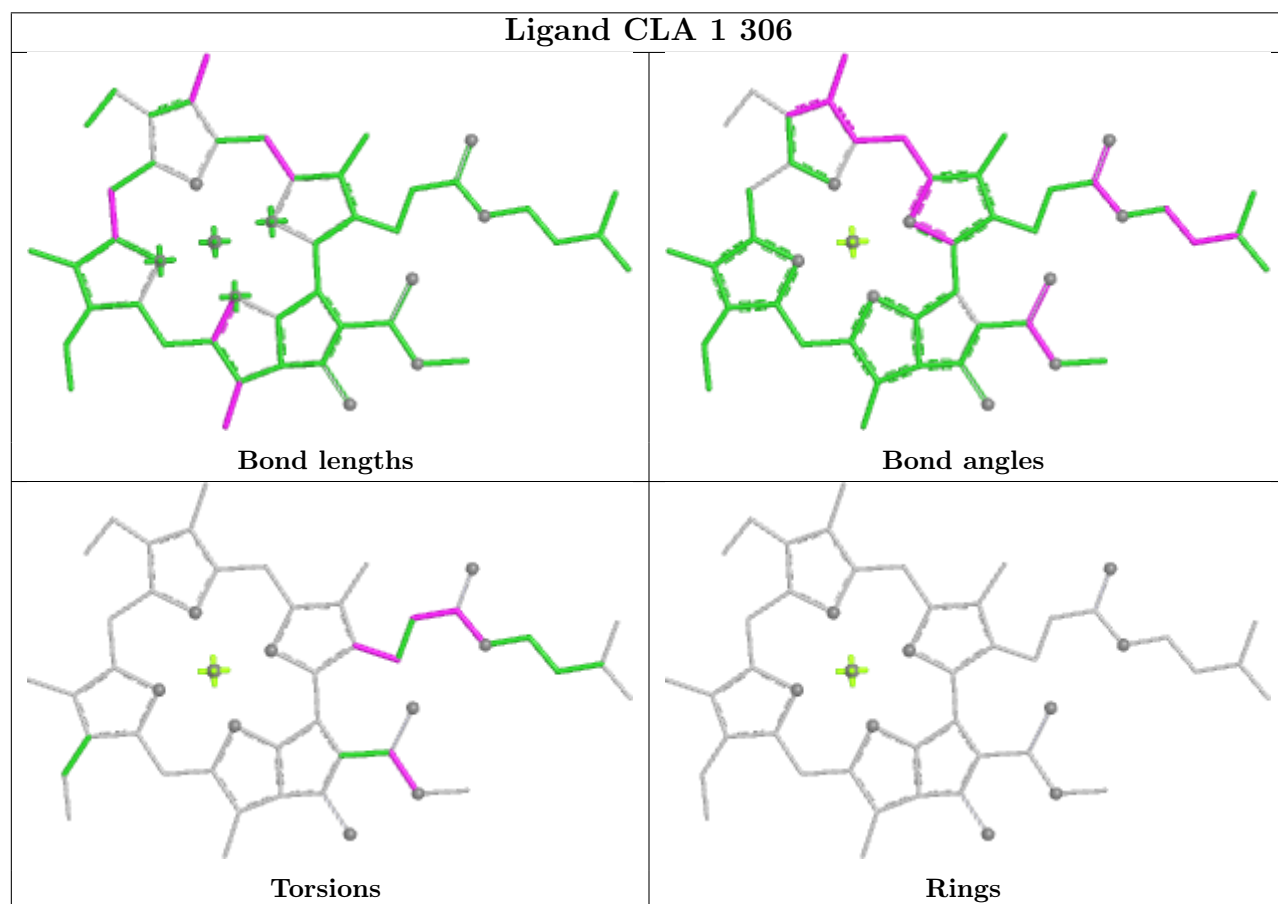
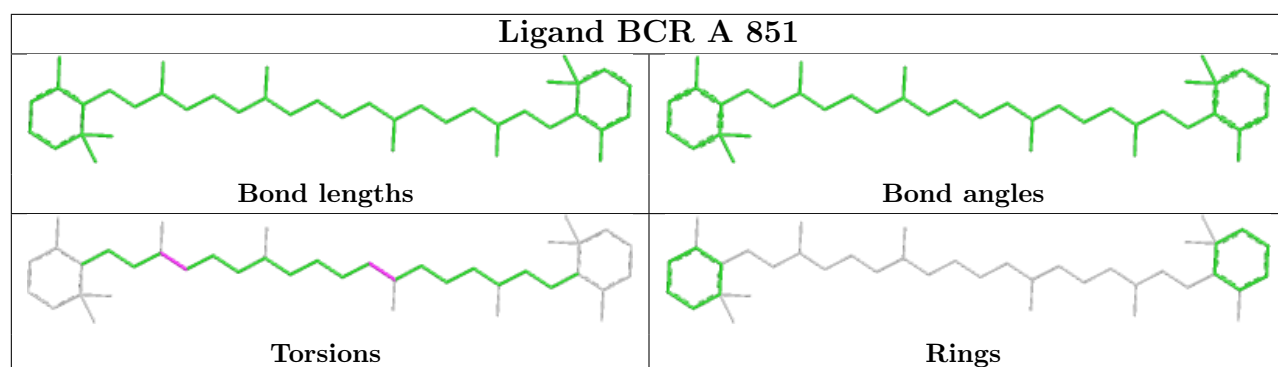


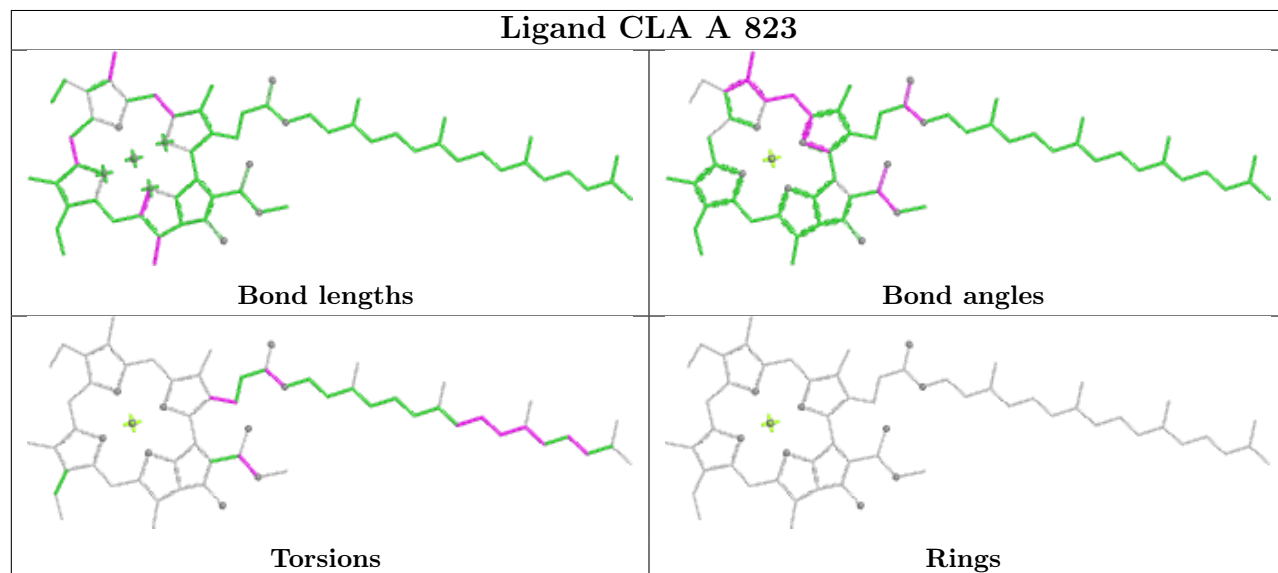
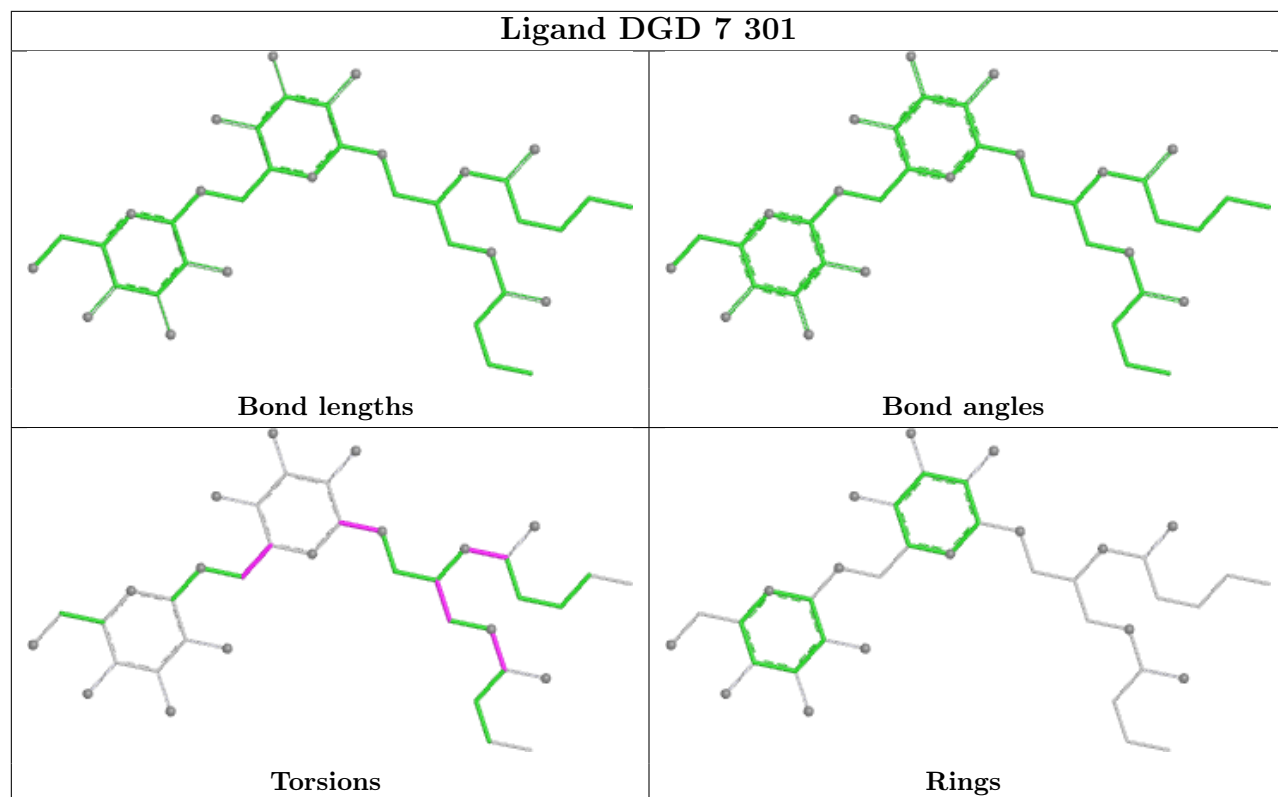
Ligand CLA A 815

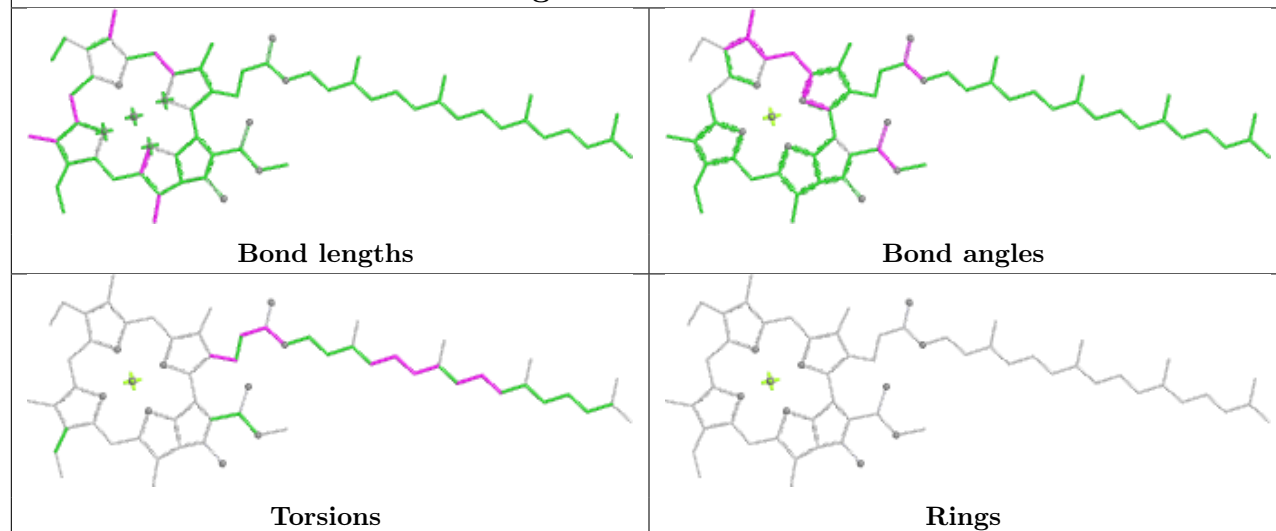
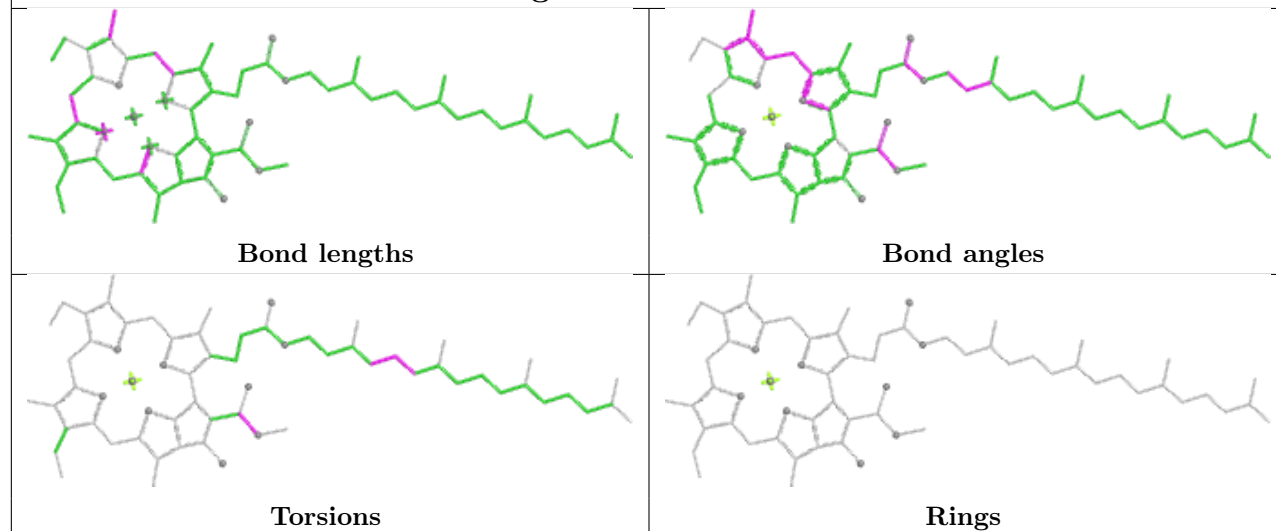


Ligand CLA c 609

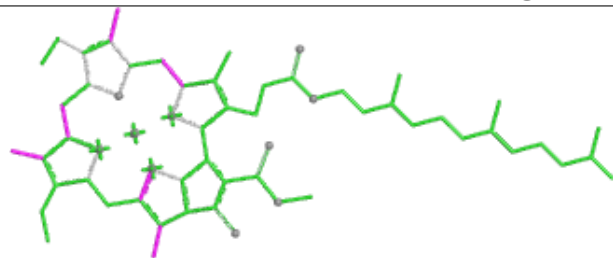




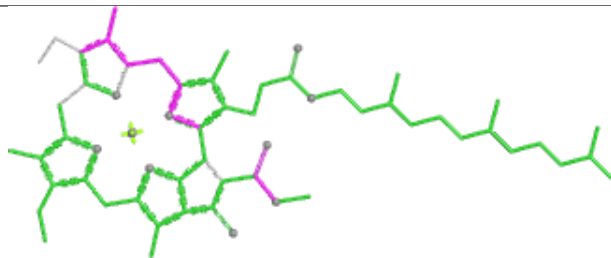


Ligand CLA B 819**Ligand CLA A 834**

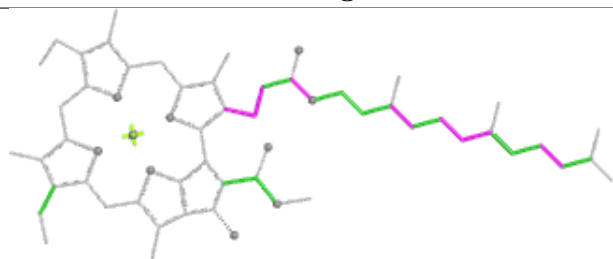
Ligand CLA 1 308



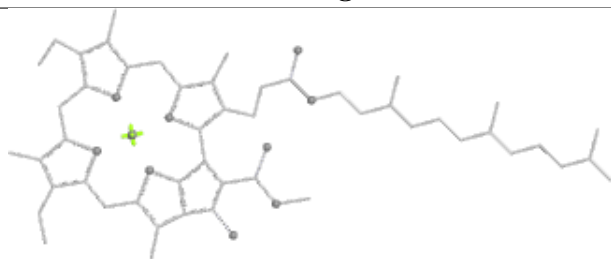
Bond lengths



Bond angles

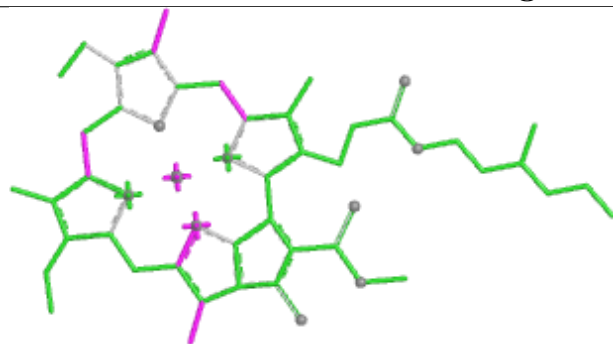


Torsions

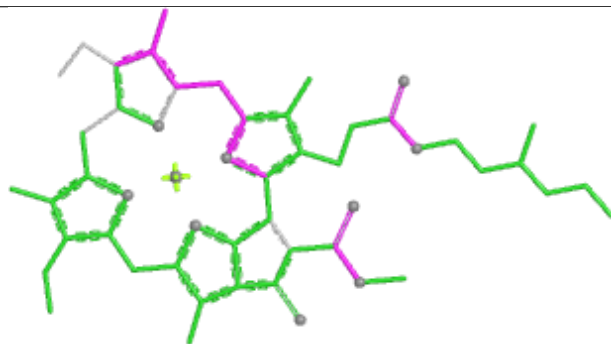


Rings

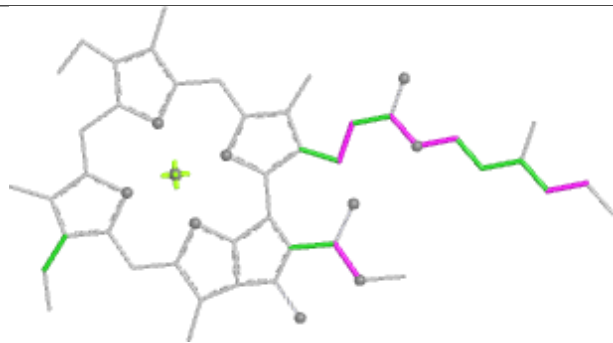
Ligand CLA 8 613



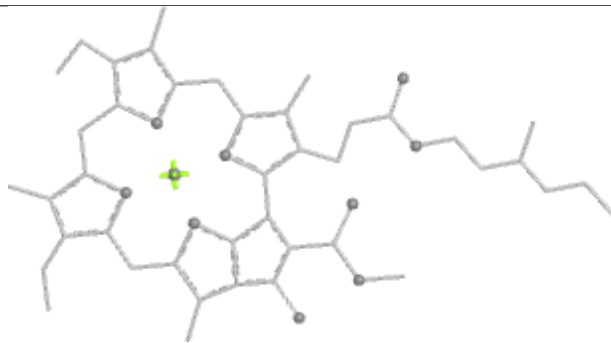
Bond lengths



Bond angles

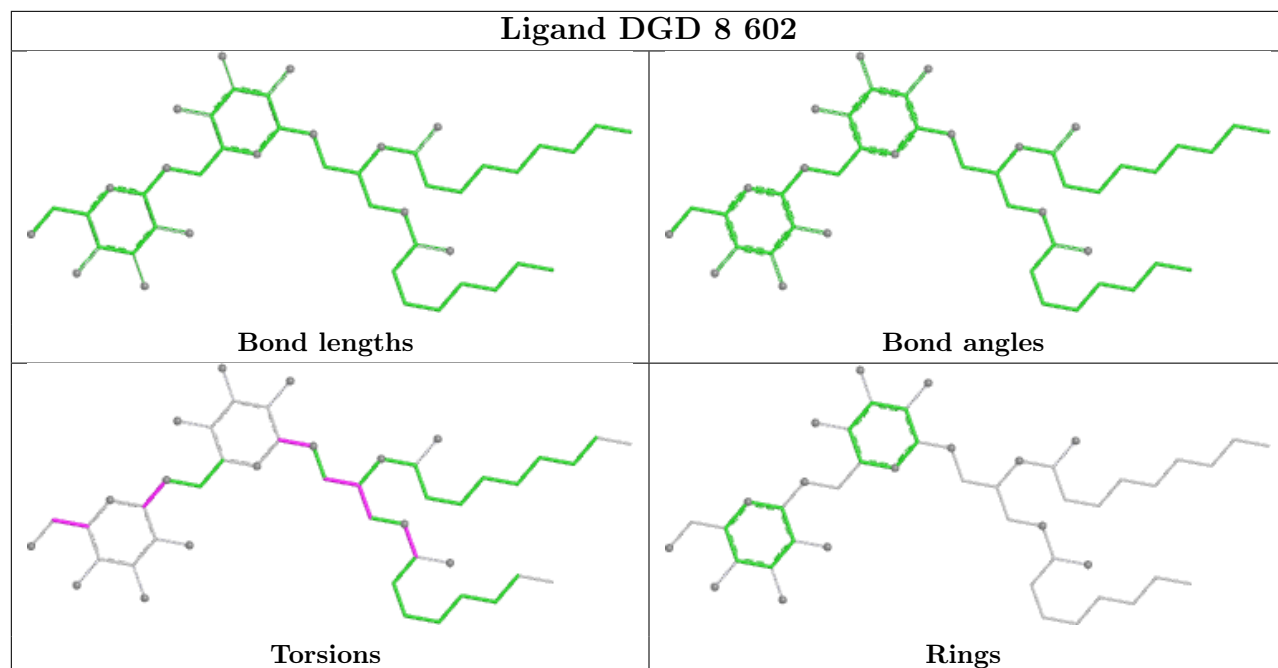


Torsions

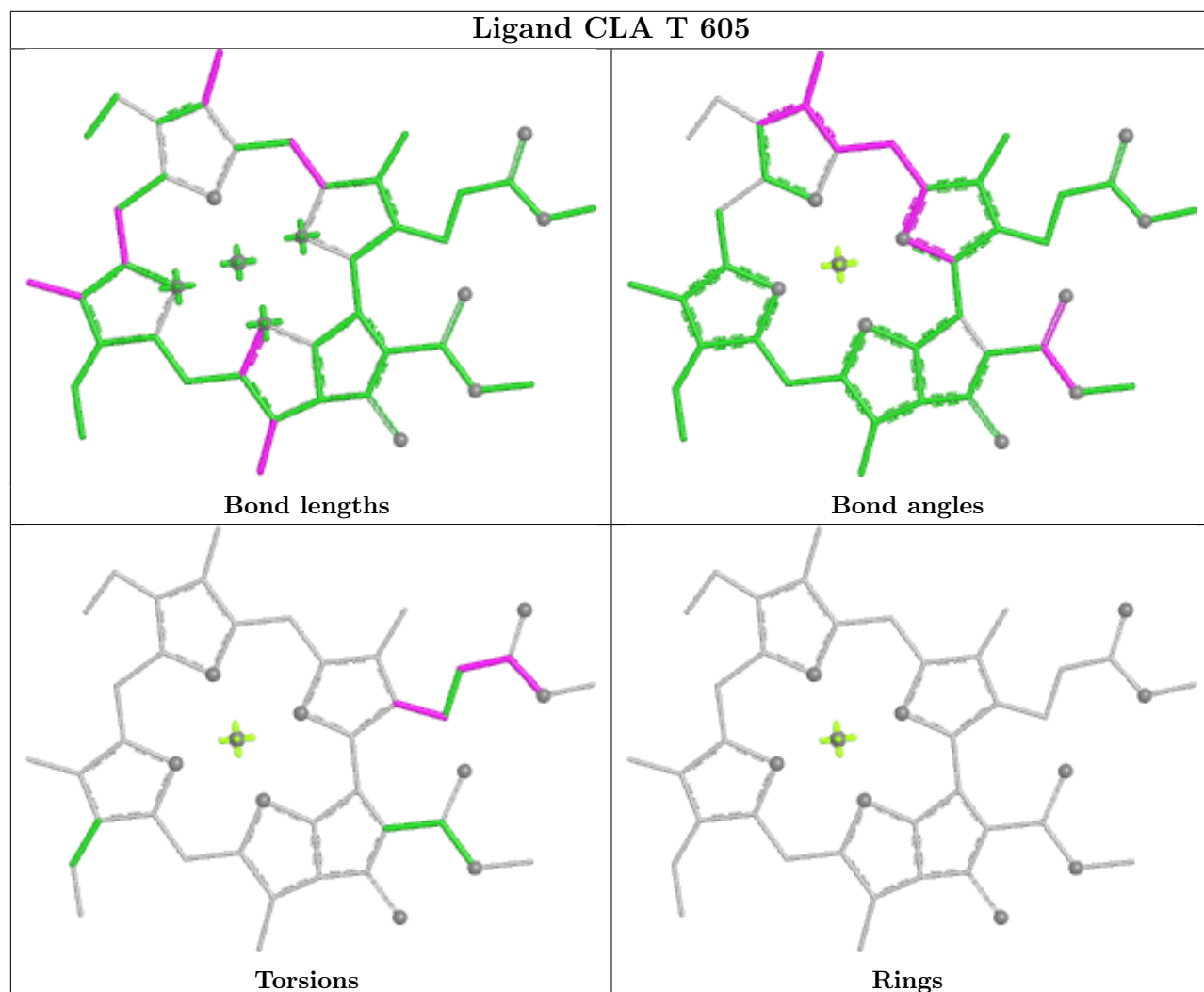


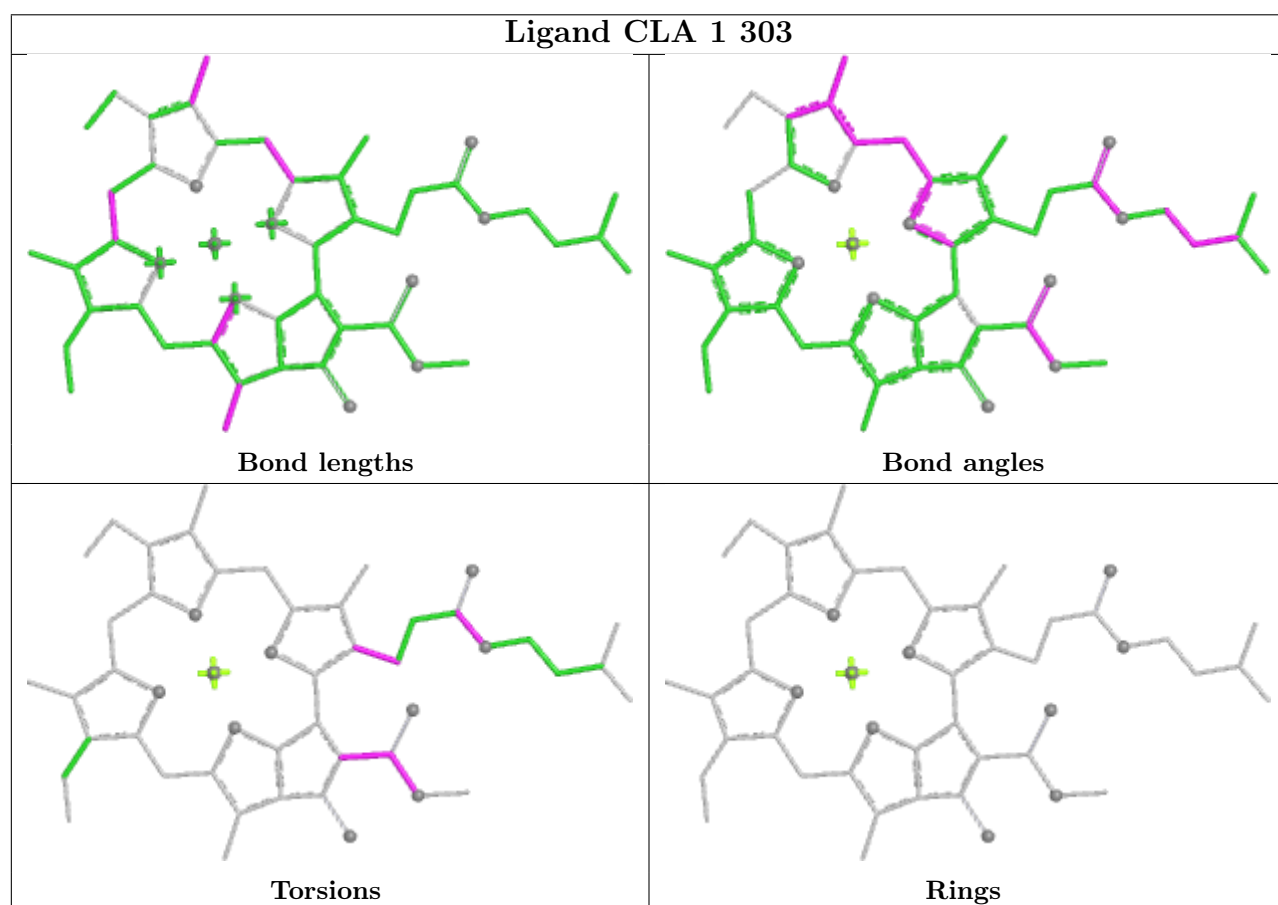
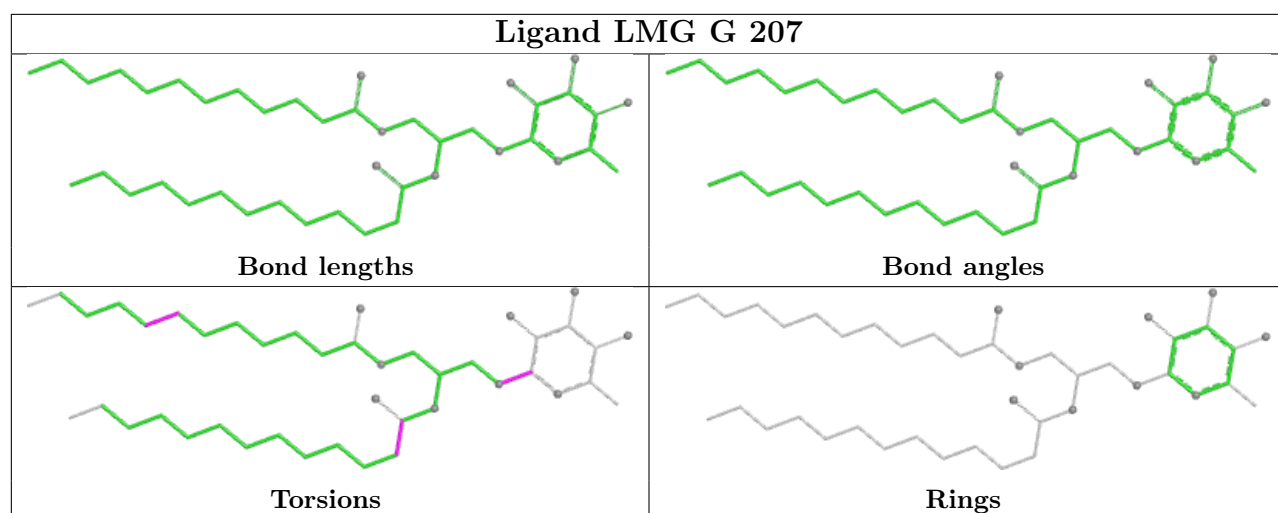
Rings

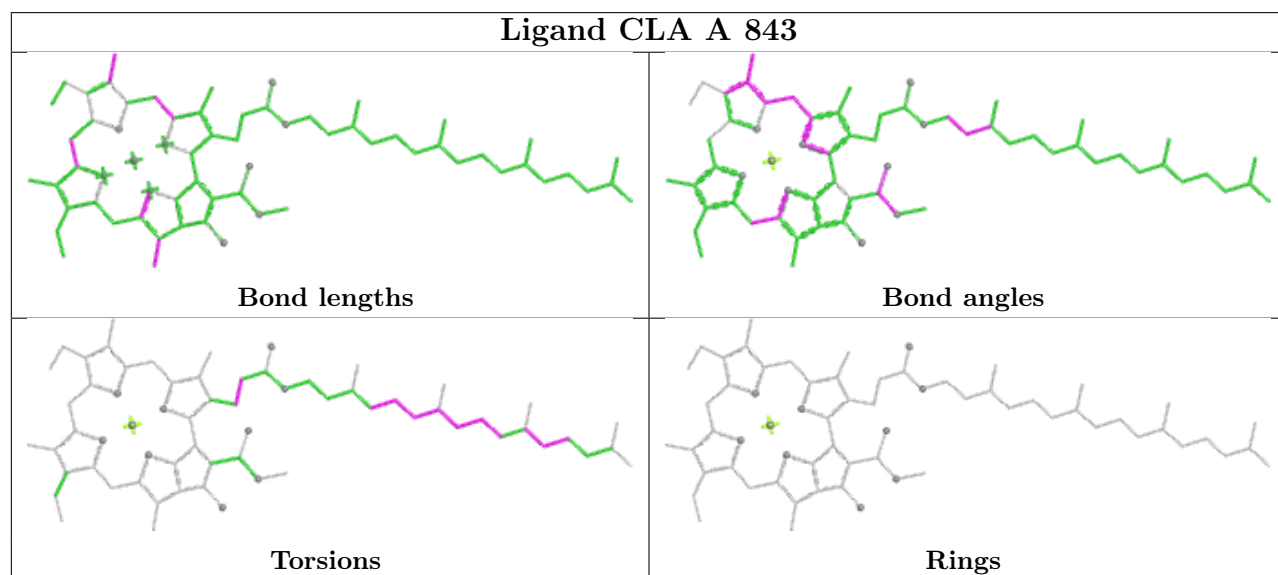
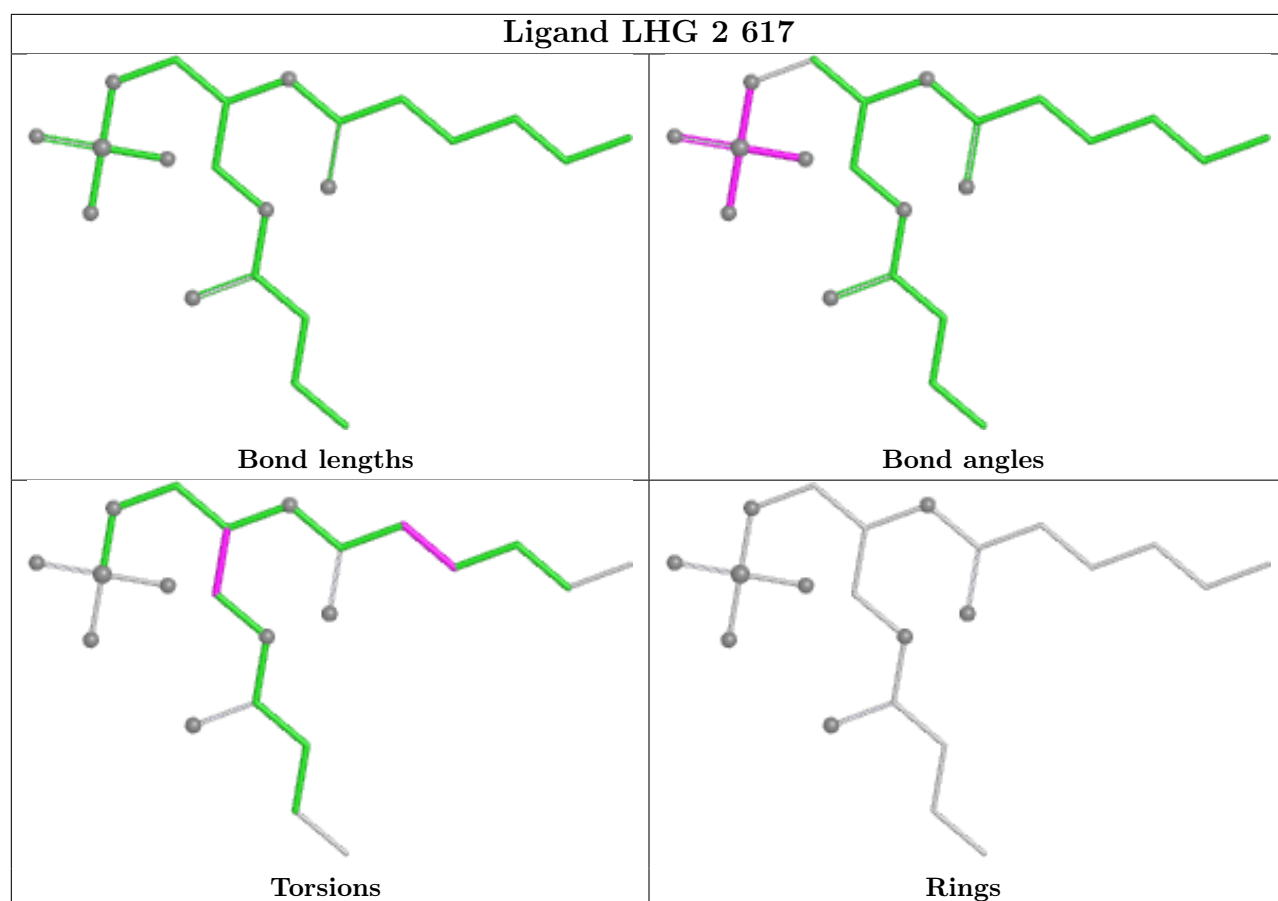
Ligand DGD 8 602

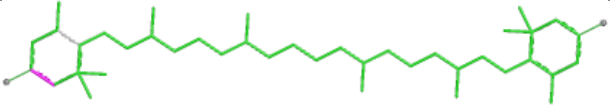
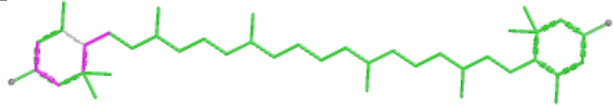
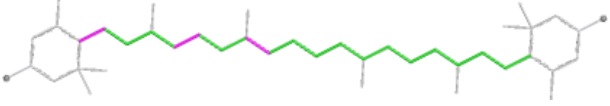
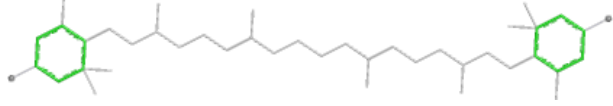


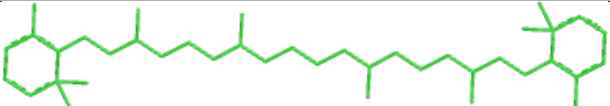
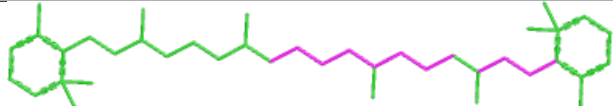
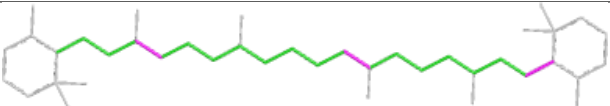
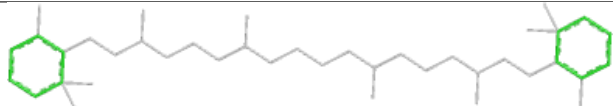
Ligand CLA T 605

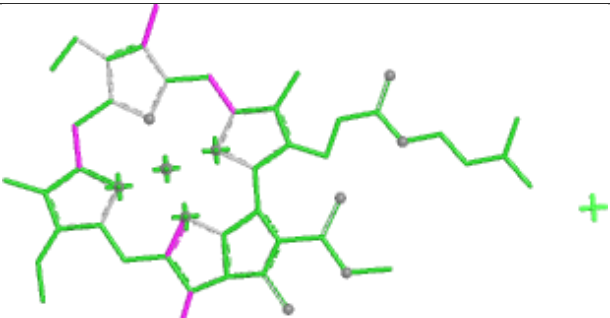
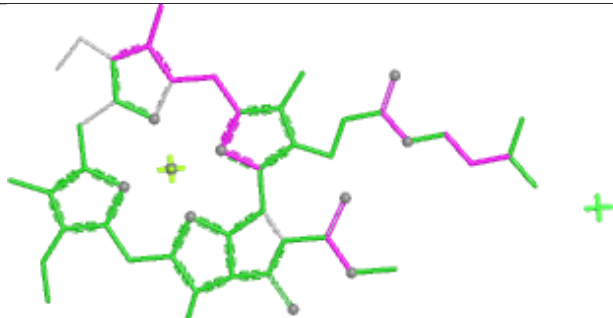
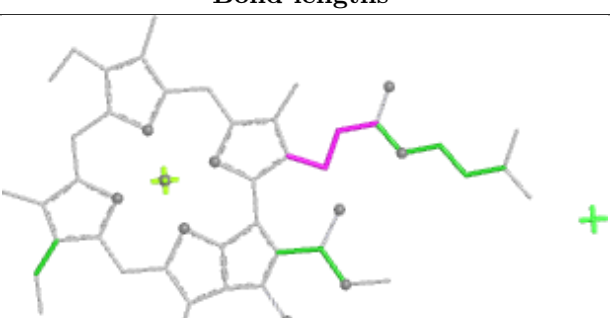
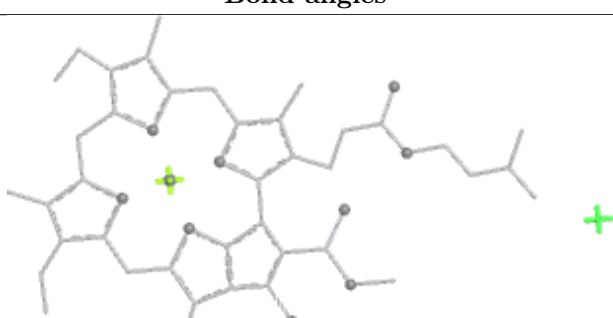


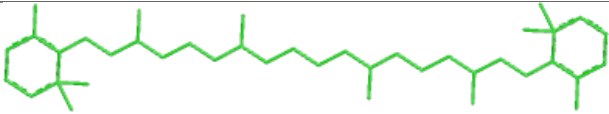
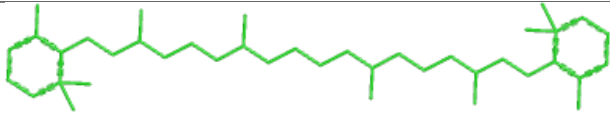
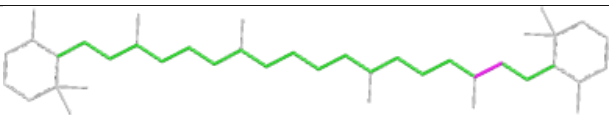
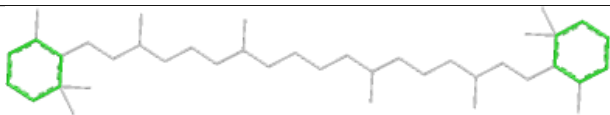


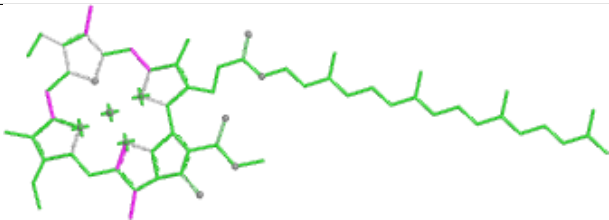
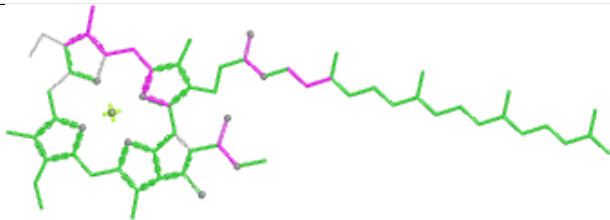
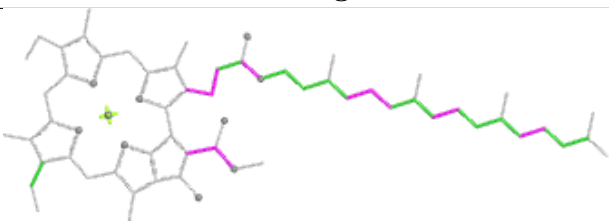
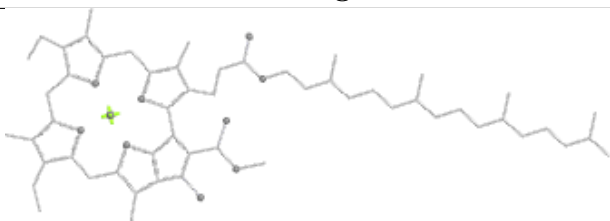


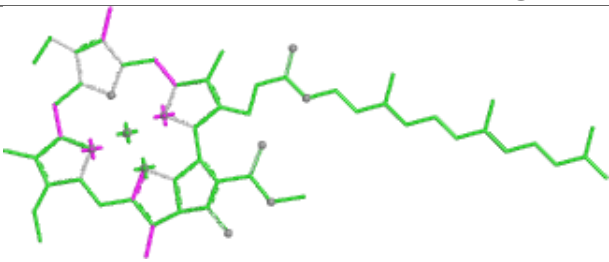
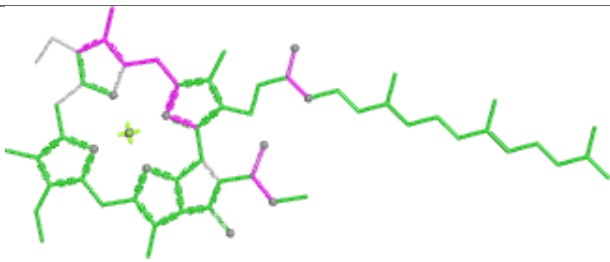
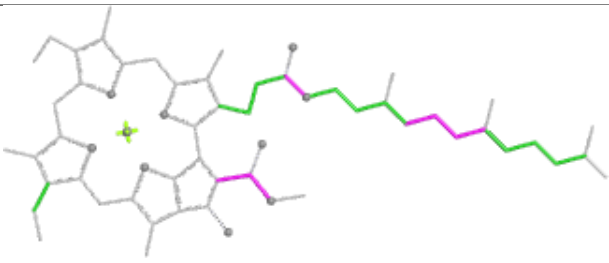
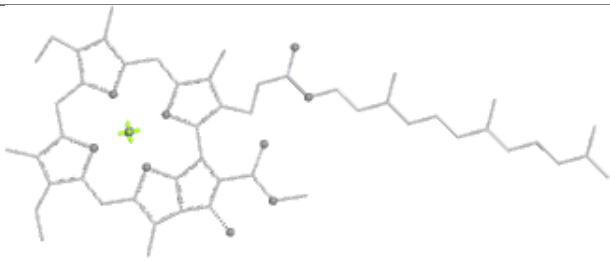
Ligand LUT B 801			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

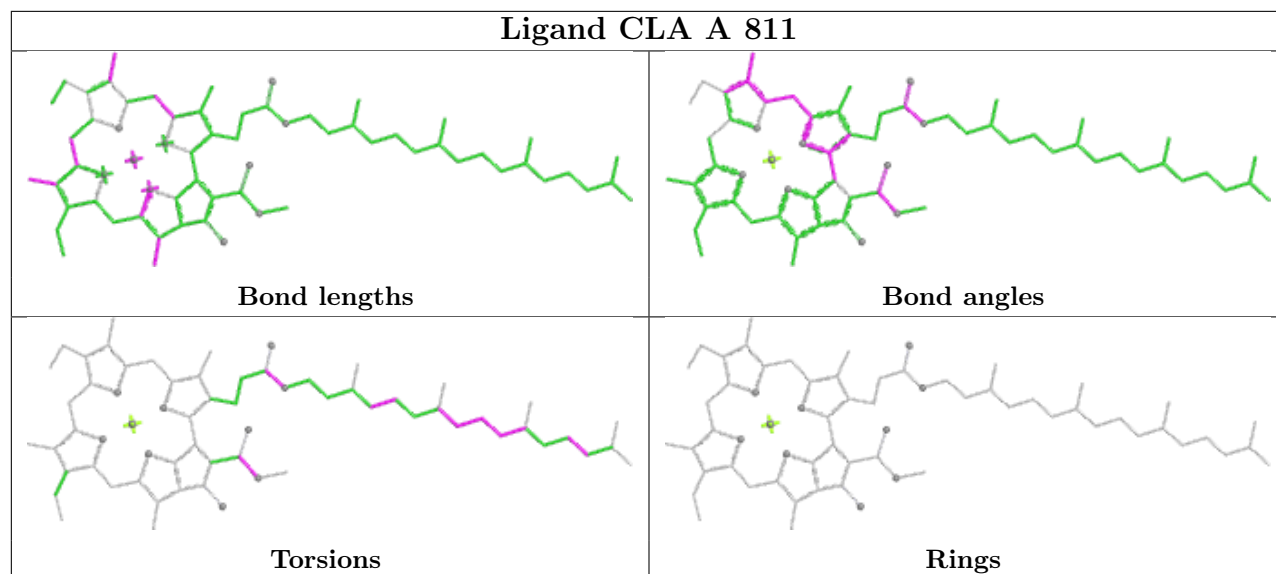
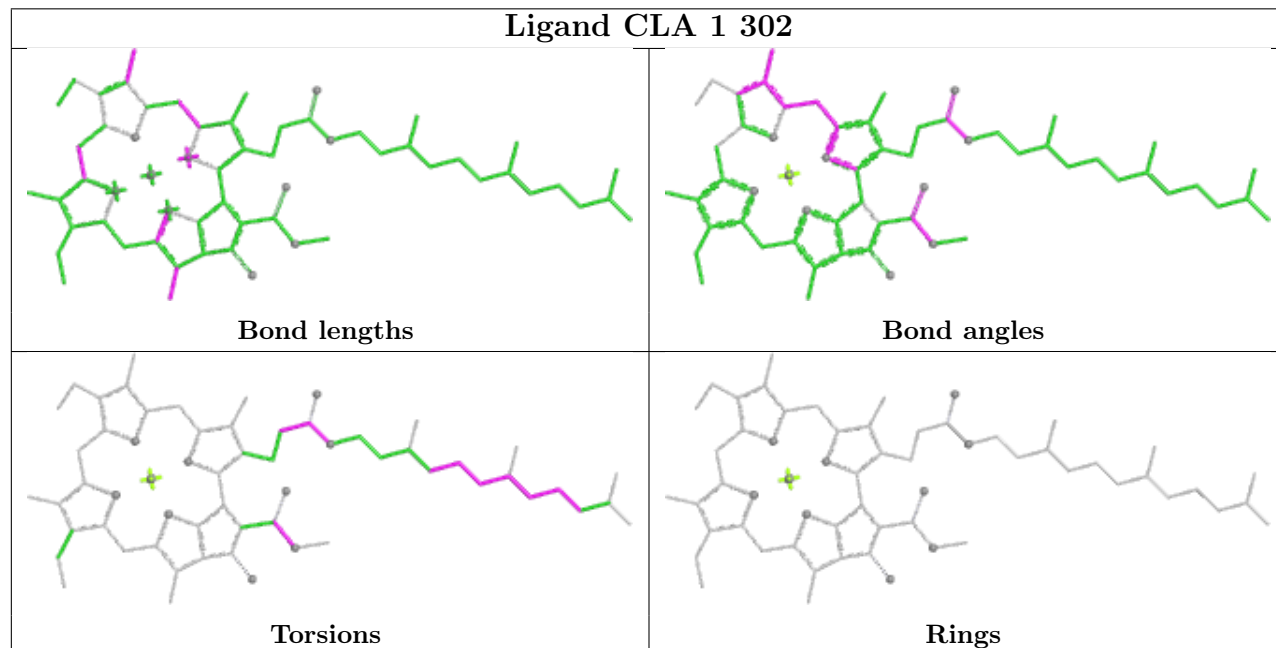
Ligand BCR B 805			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

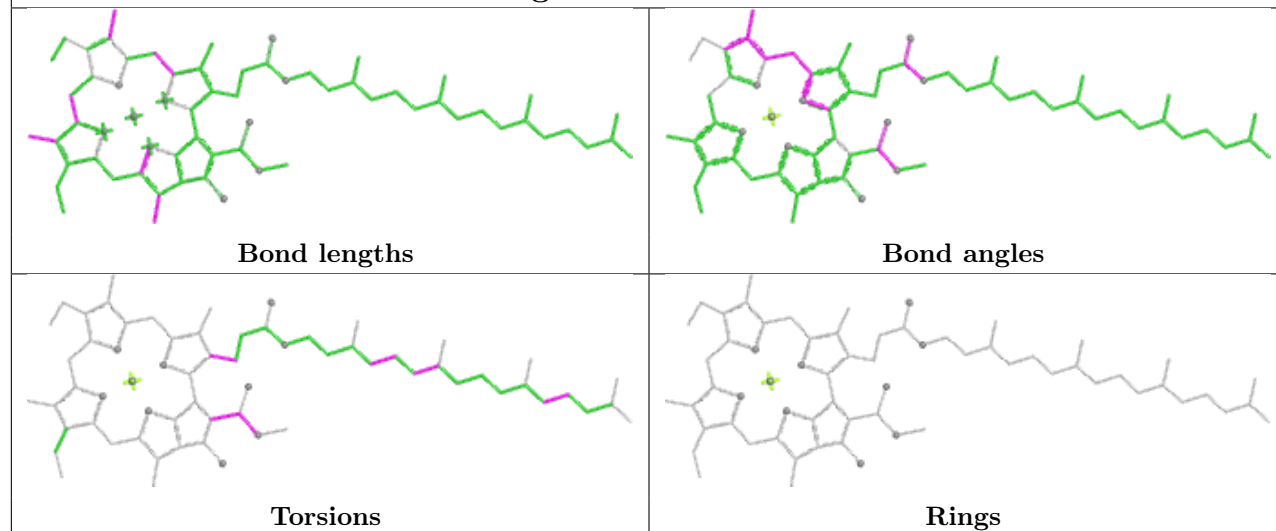
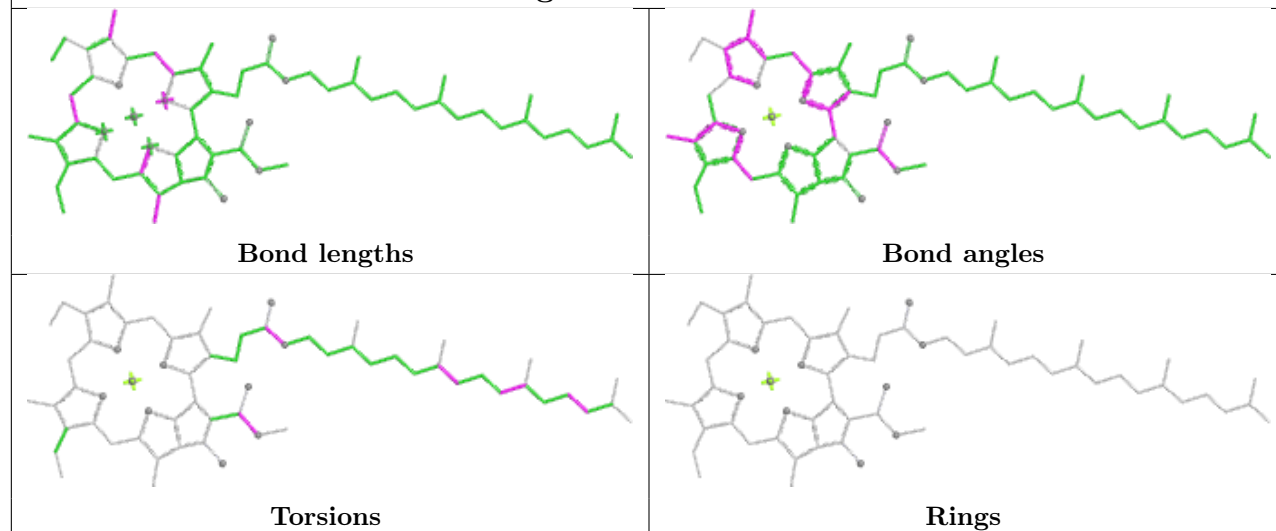
Ligand CLA a 314			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

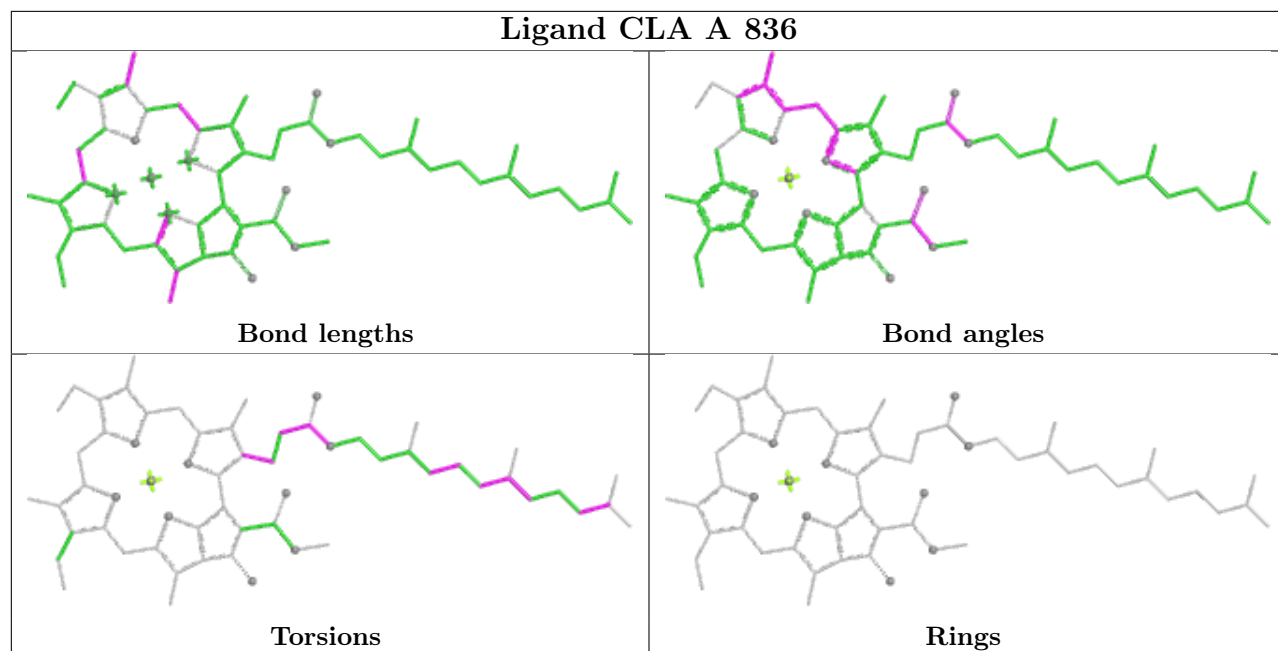
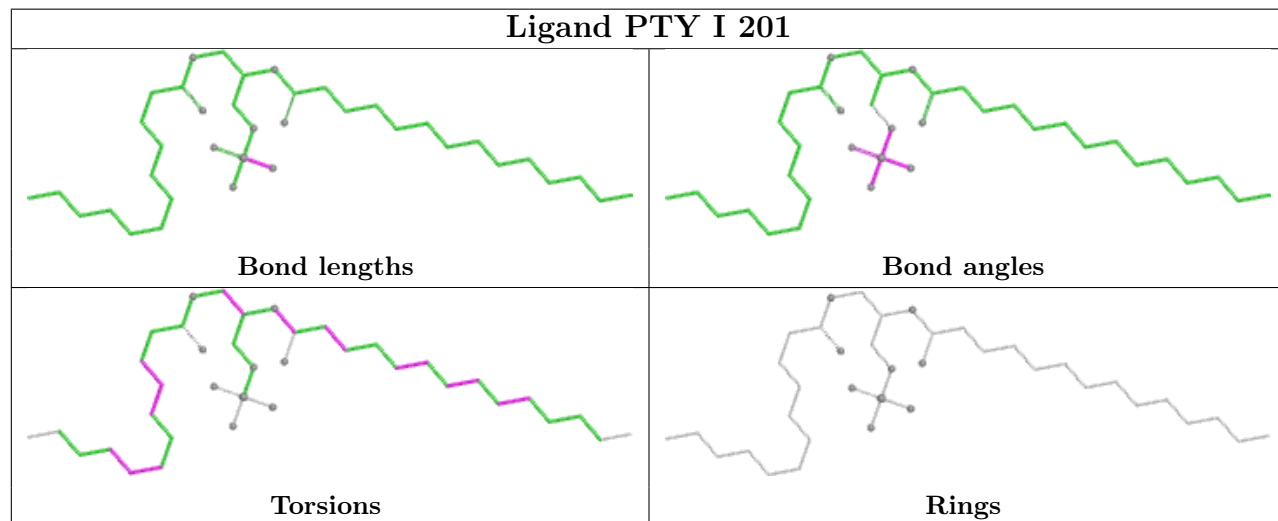
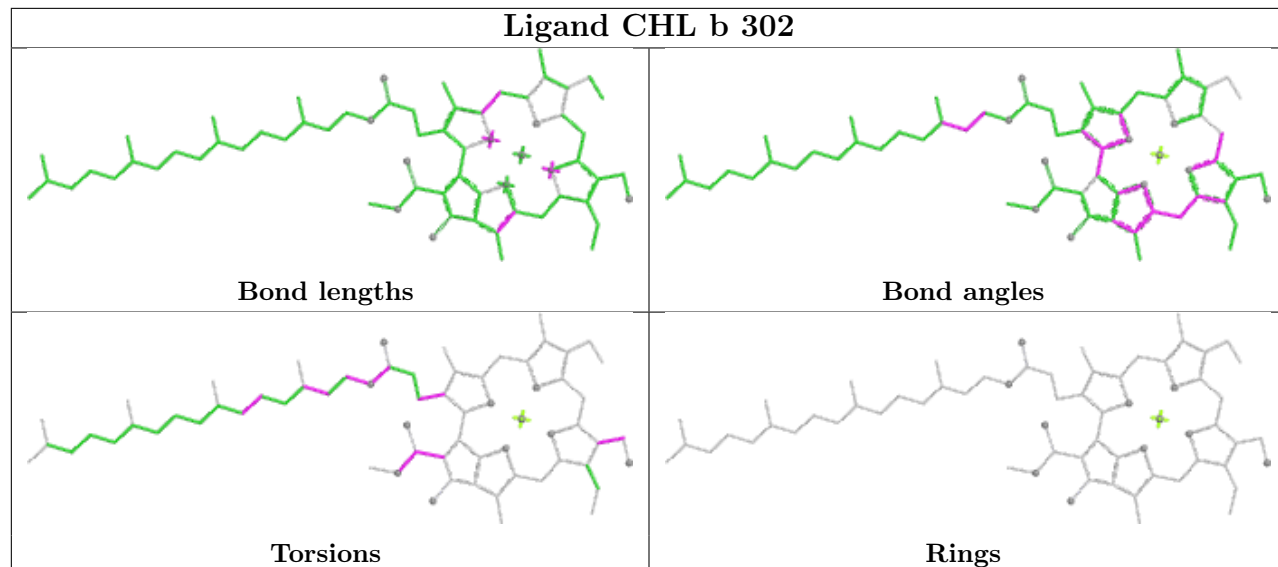
Ligand BCR B 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

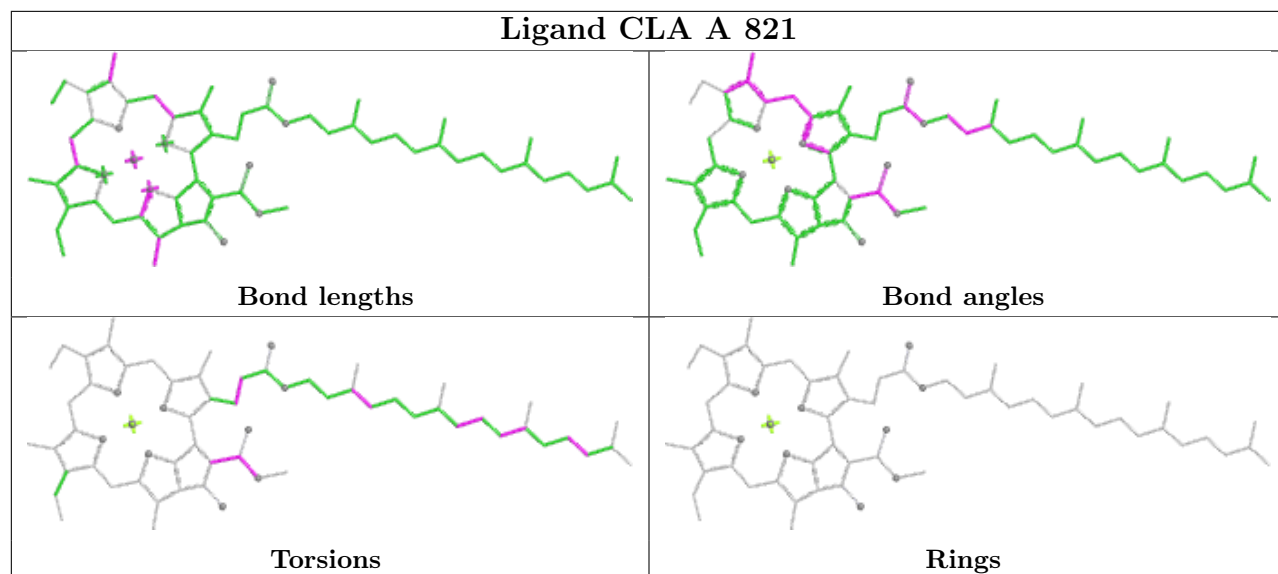
Ligand CLA 2 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 811**Ligand CLA 1 302**

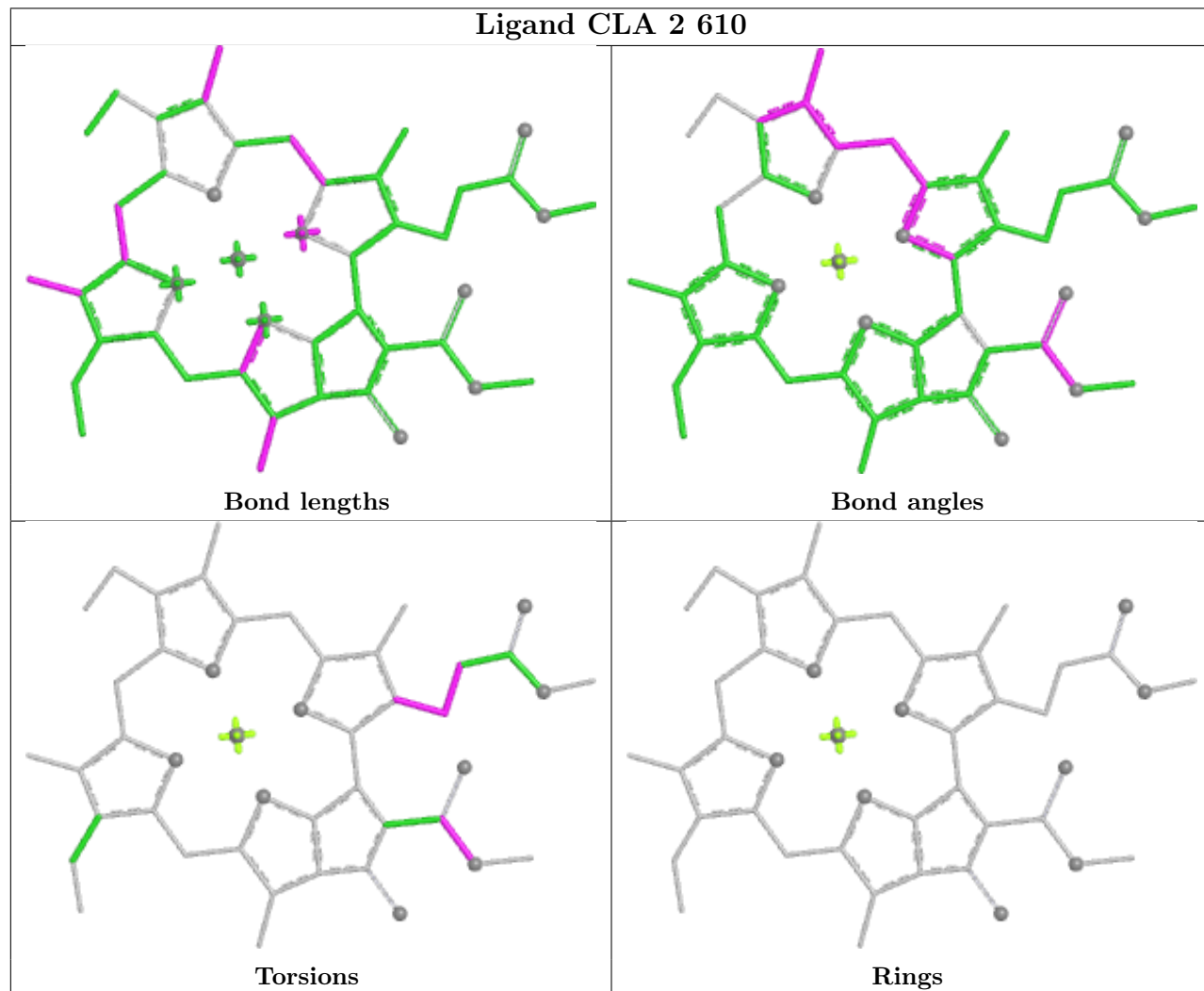
Ligand CLA A 832**Ligand CLA 1 321**

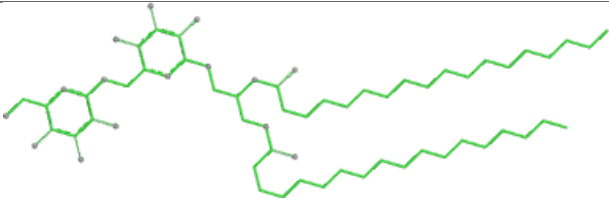
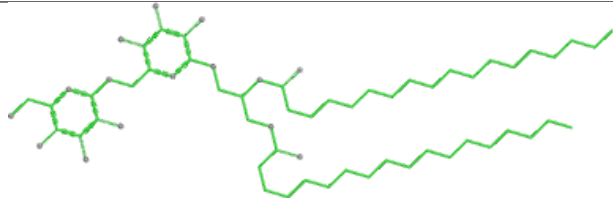
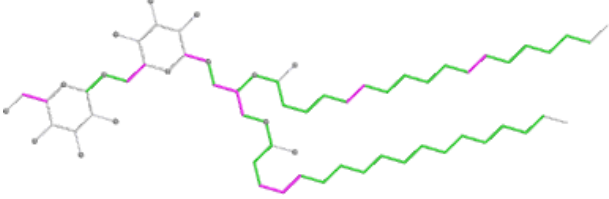
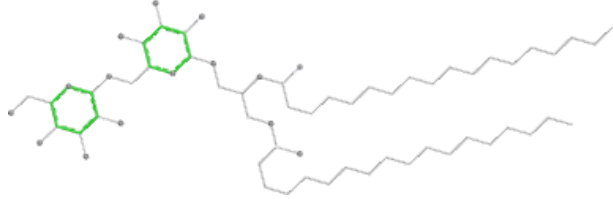
Ligand CLA A 836**Ligand PTY I 201****Ligand CHL b 302**

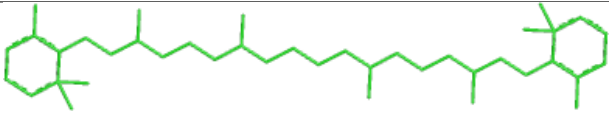
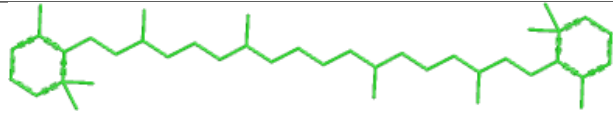
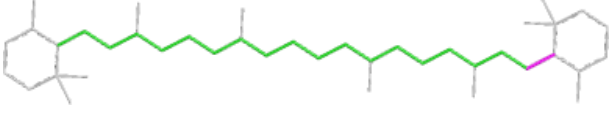
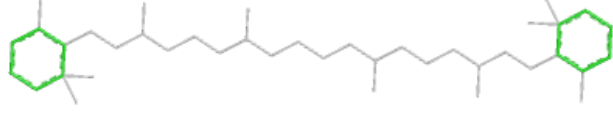
Ligand CLA A 821

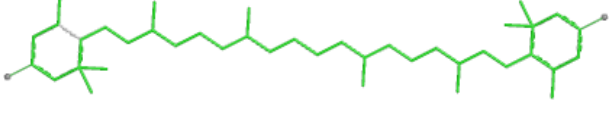
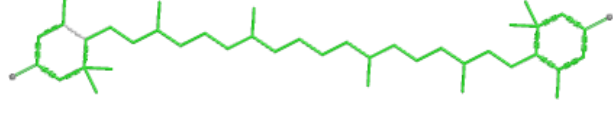

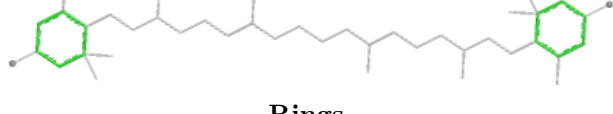


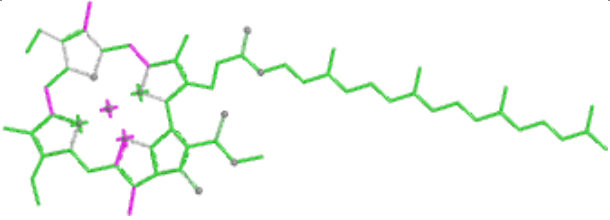
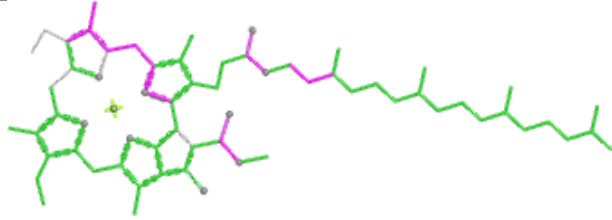
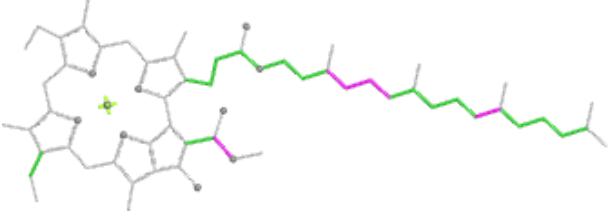
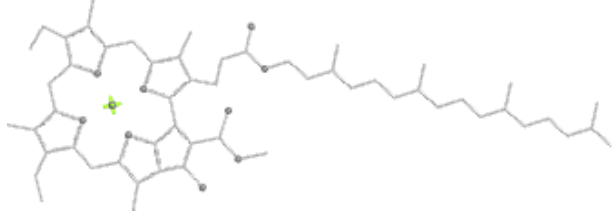
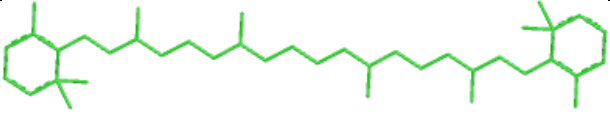
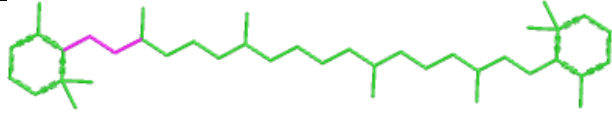
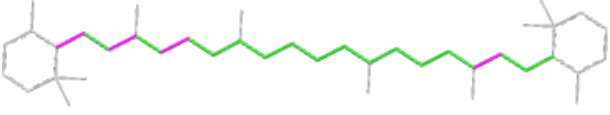
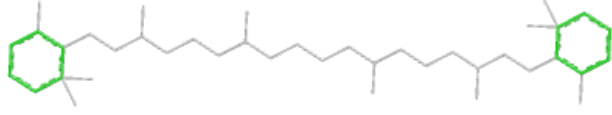
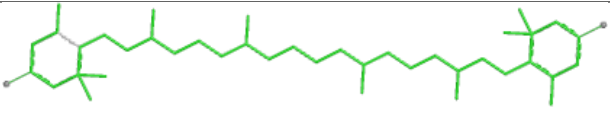
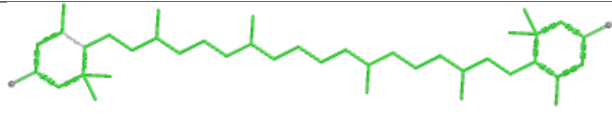
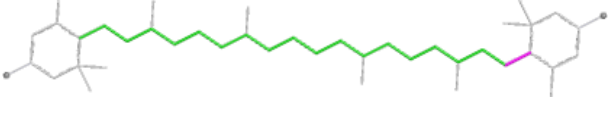
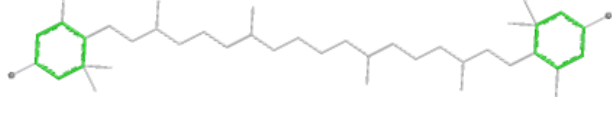
Ligand CLA 2 610

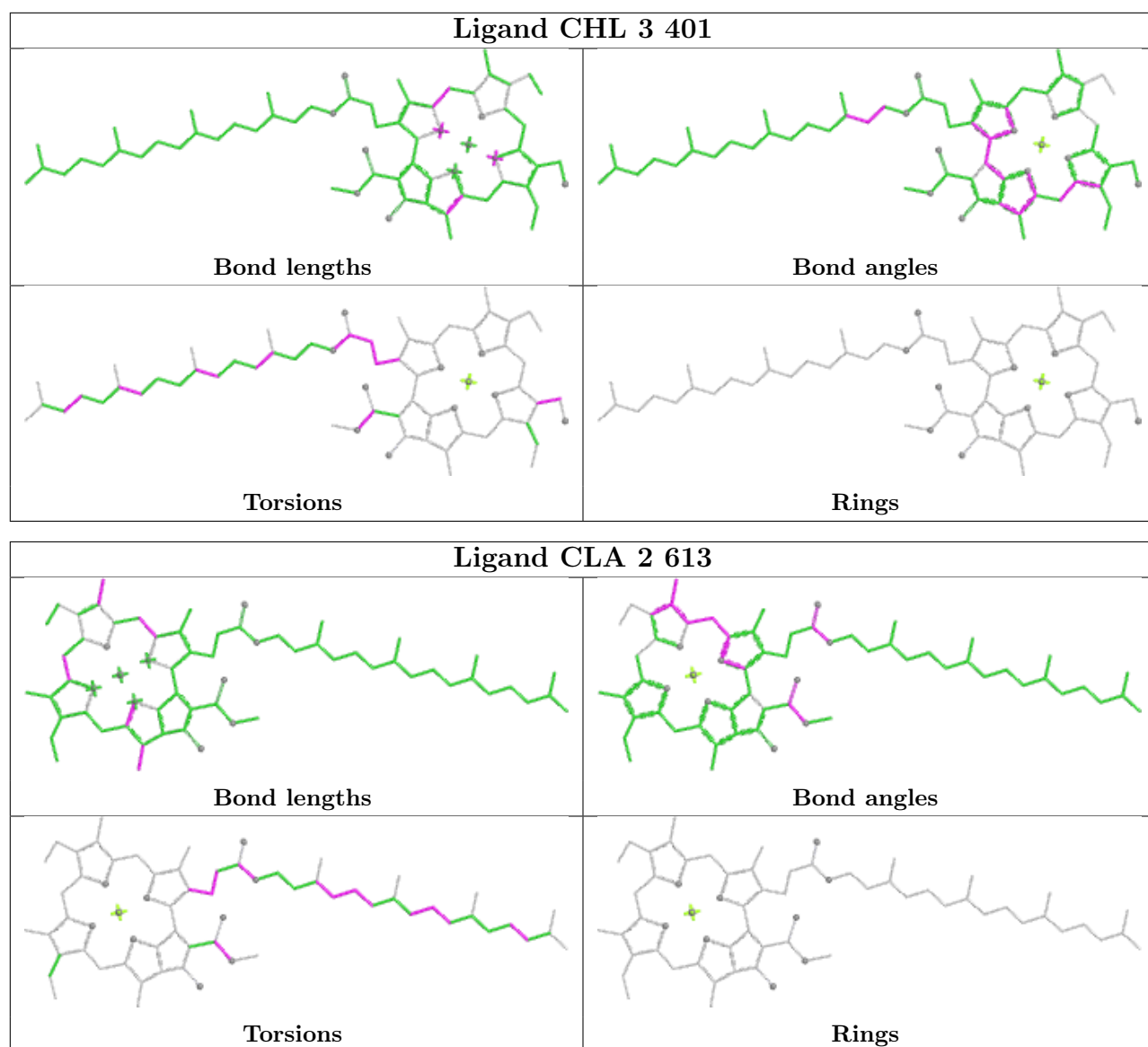


Ligand DGD A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

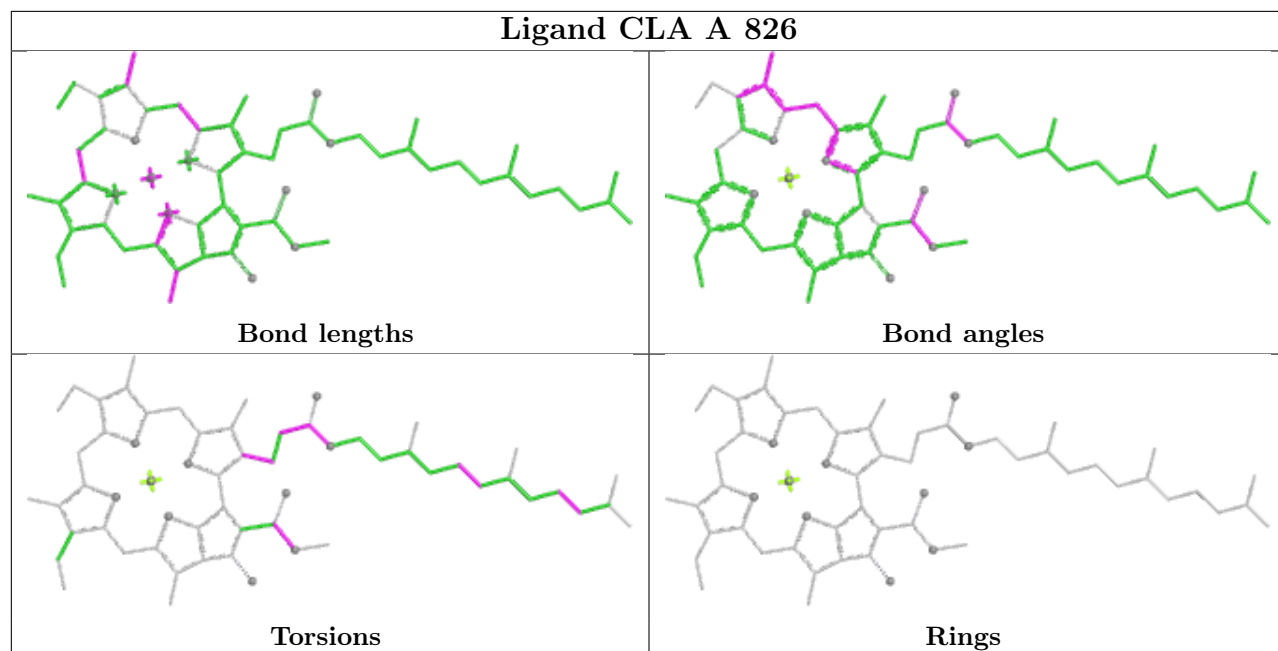
Ligand BCR b 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 2 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

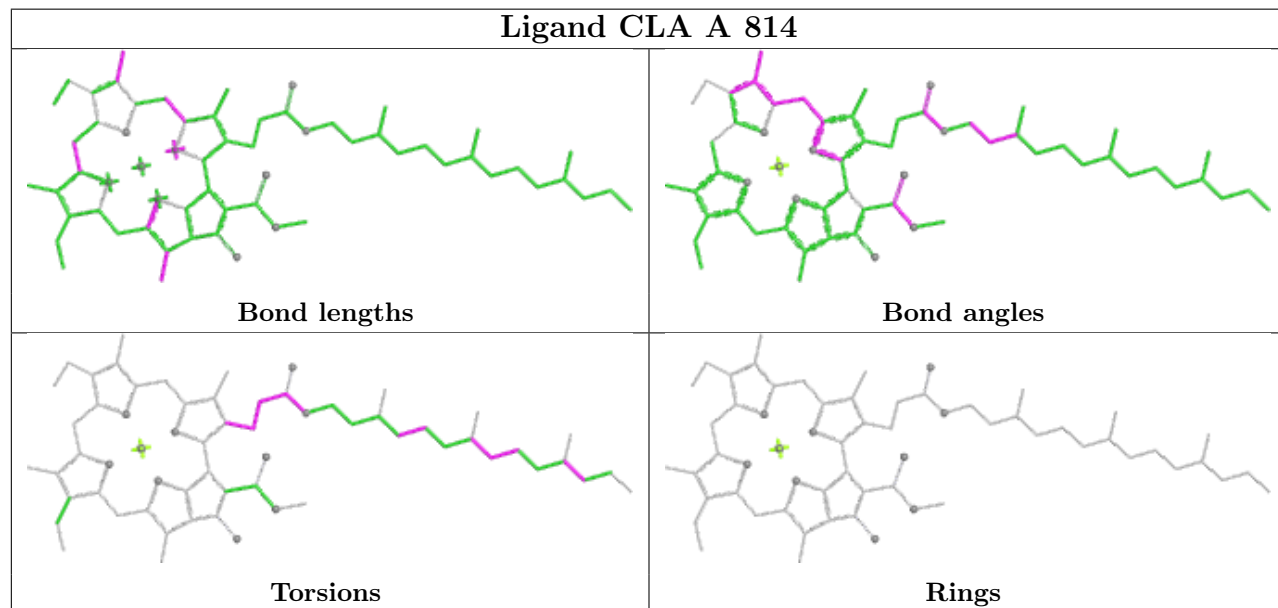
Ligand CLA B 812	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 847	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT 8 616	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



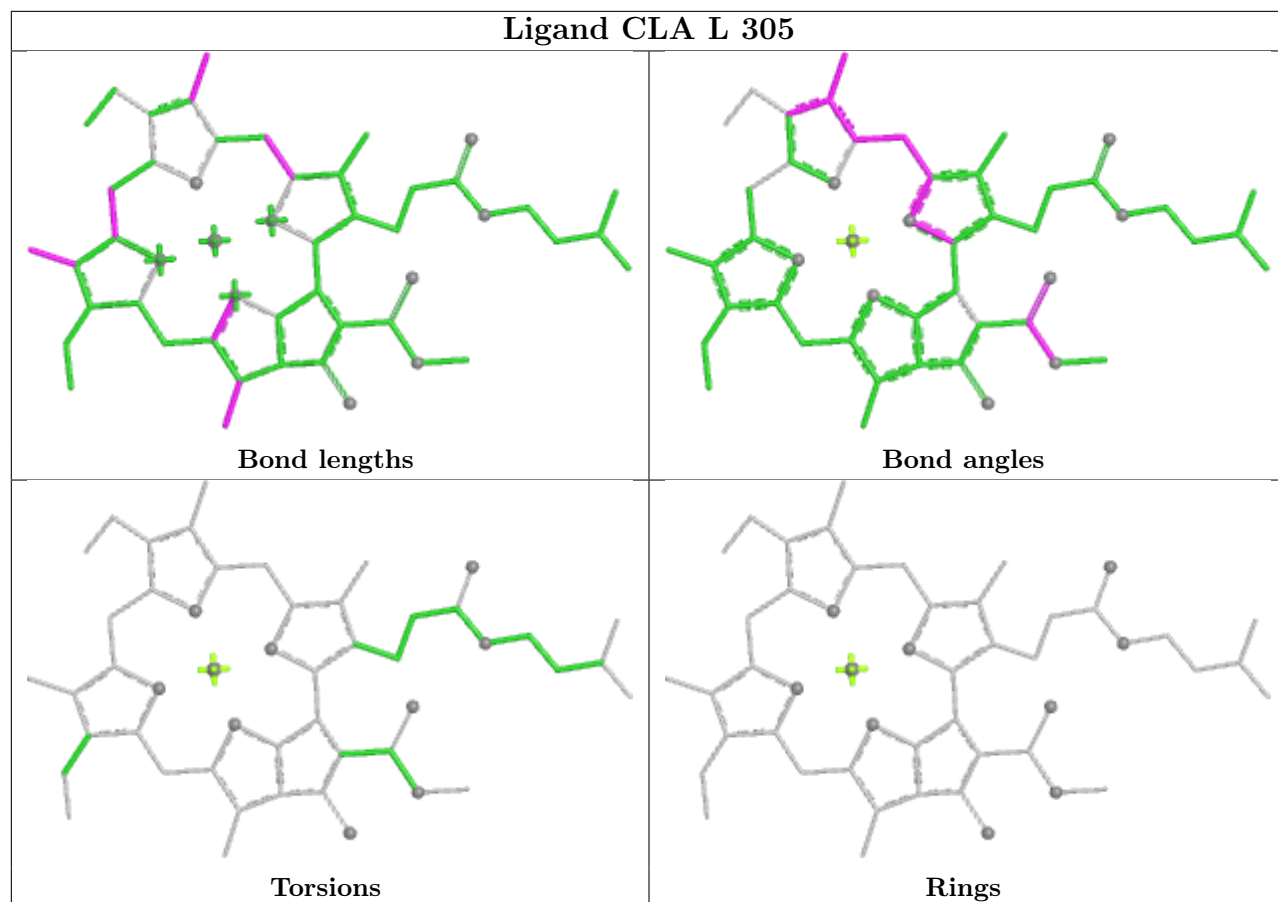
Ligand CLA A 826



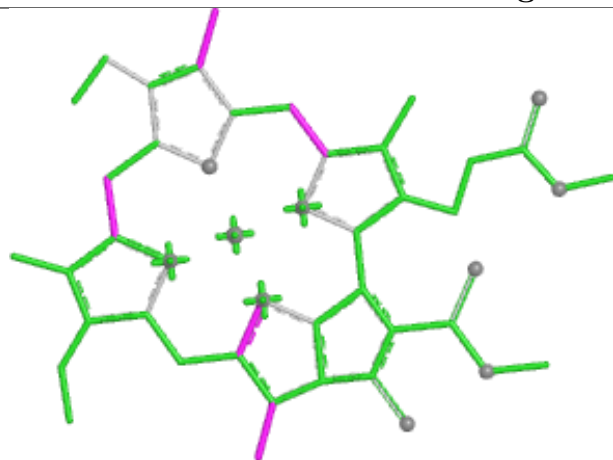
Ligand CLA A 814



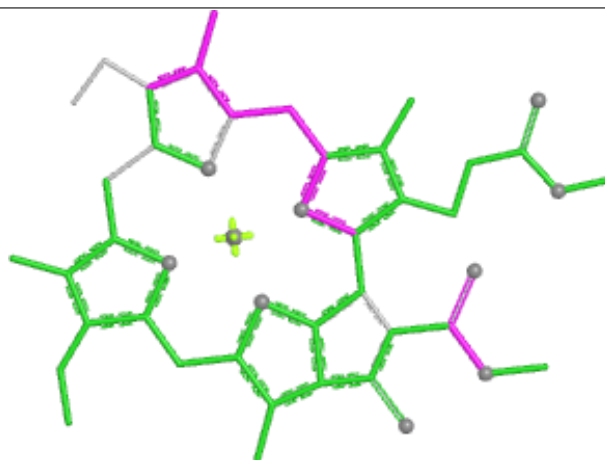
Ligand CLA L 305



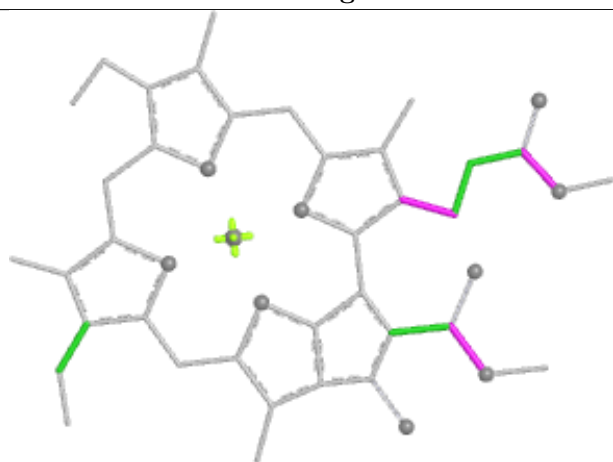
Ligand CLA b 312



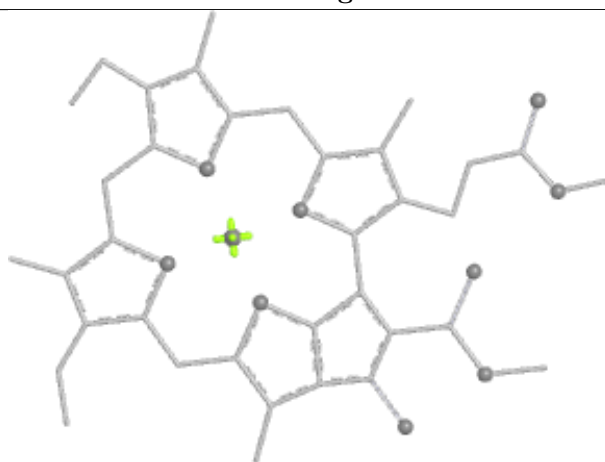
Bond lengths



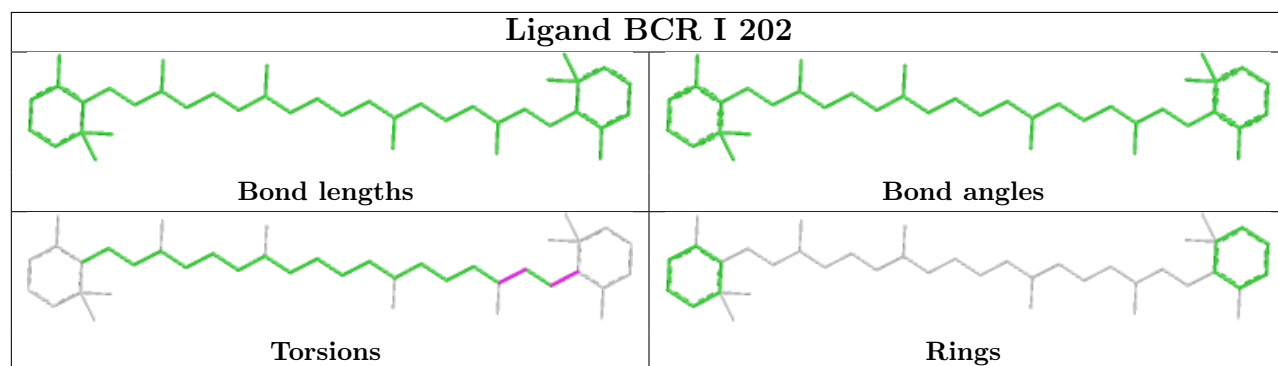
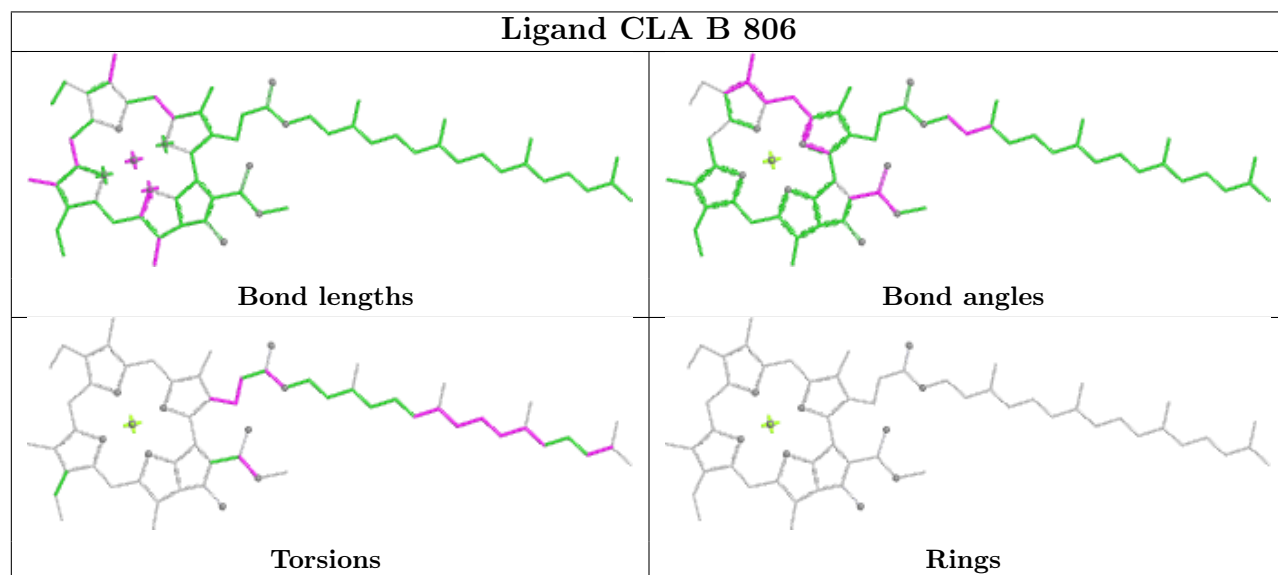
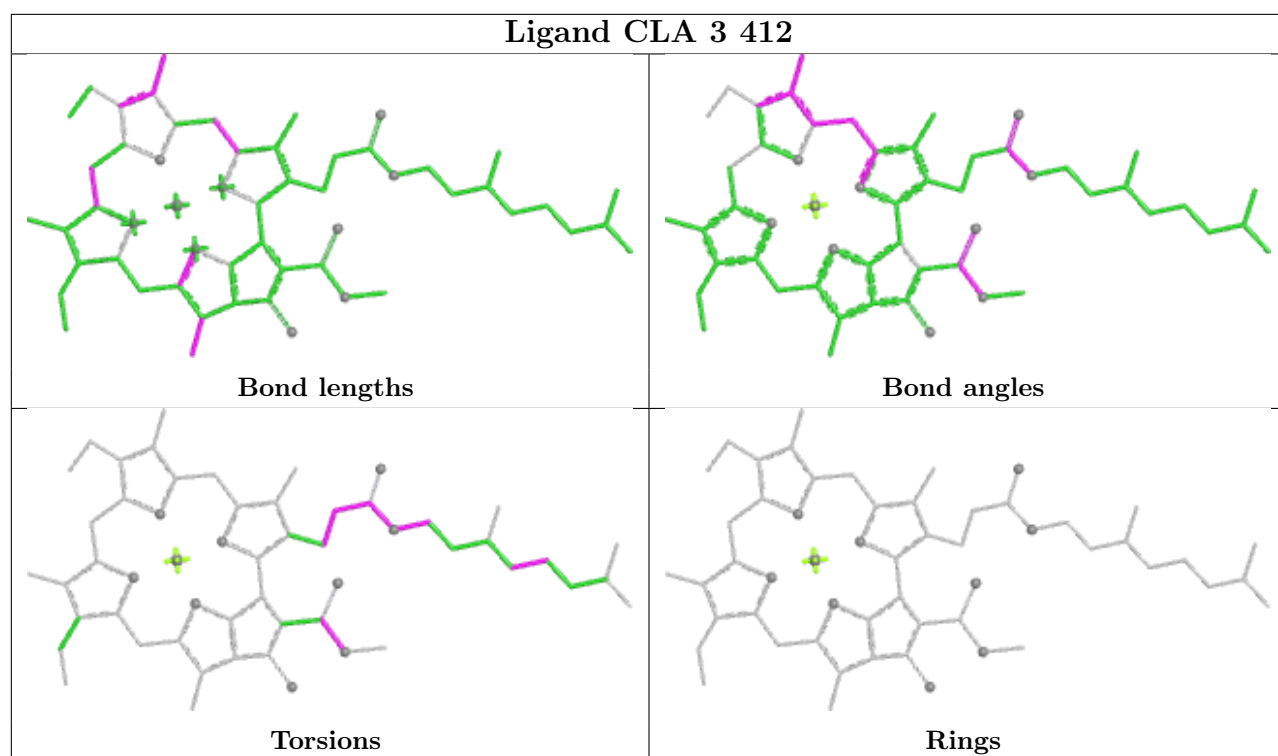
Bond angles



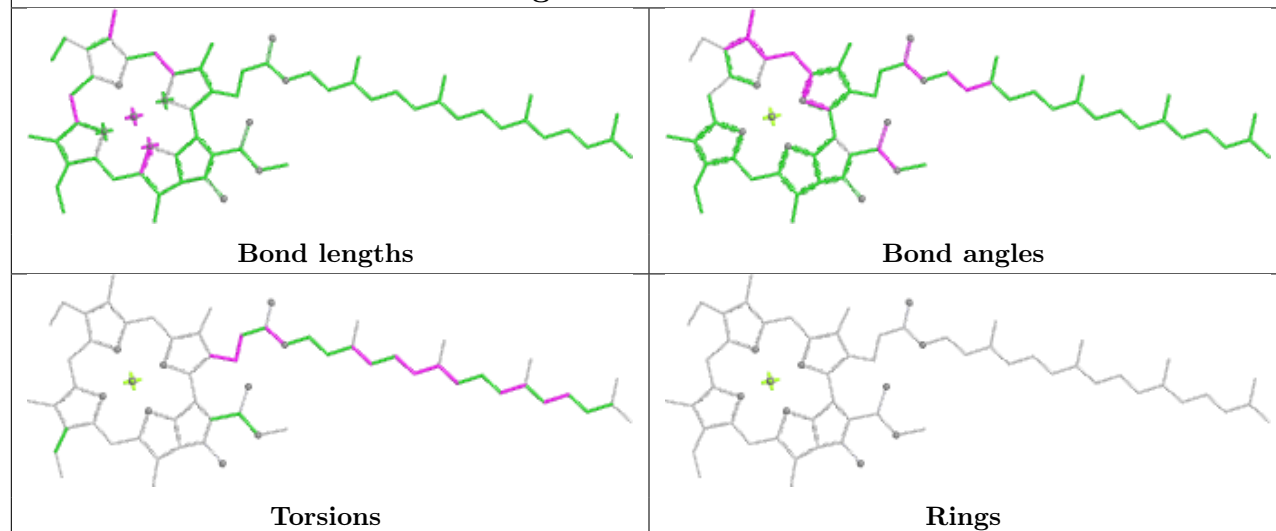
Torsions



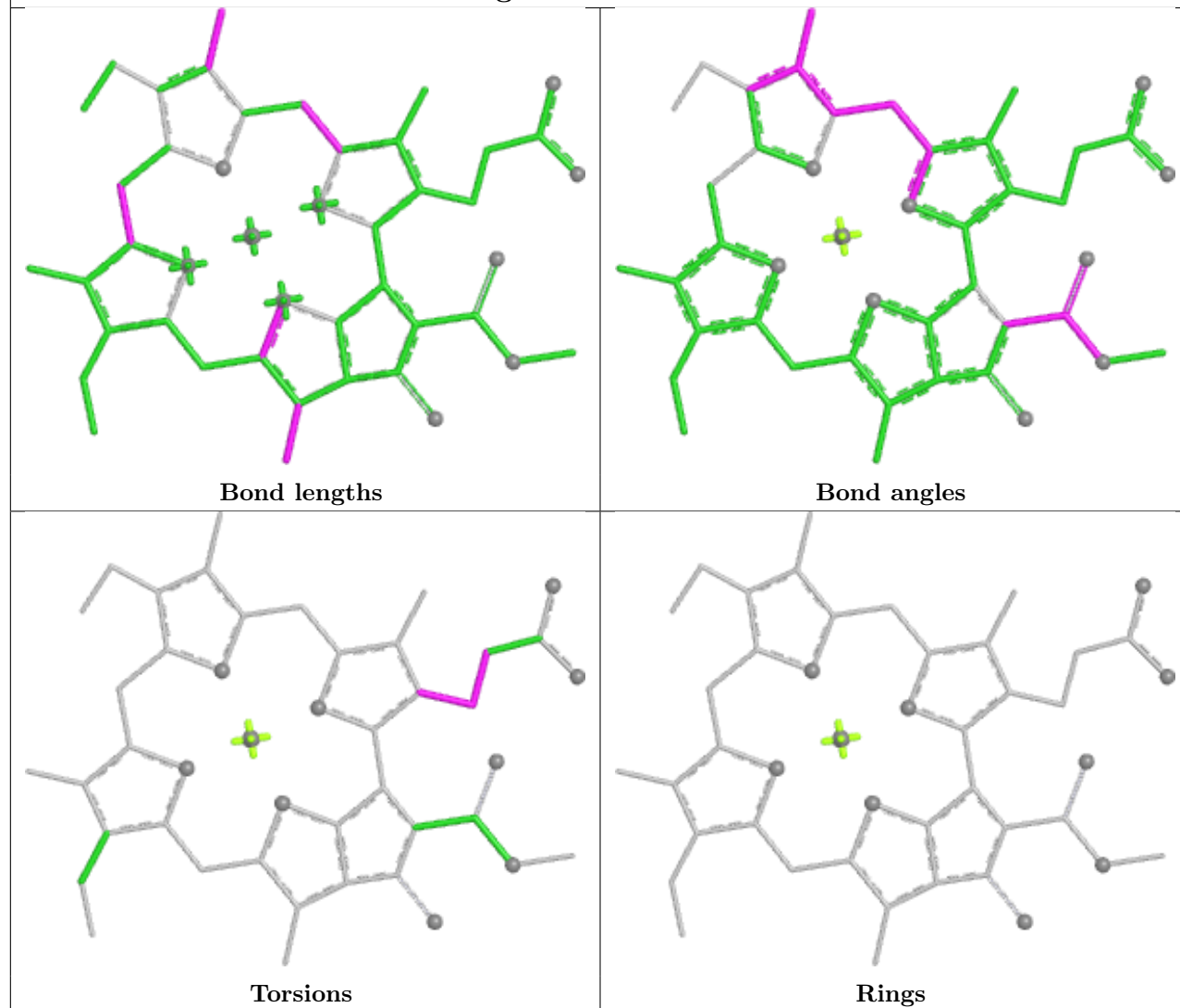
Rings



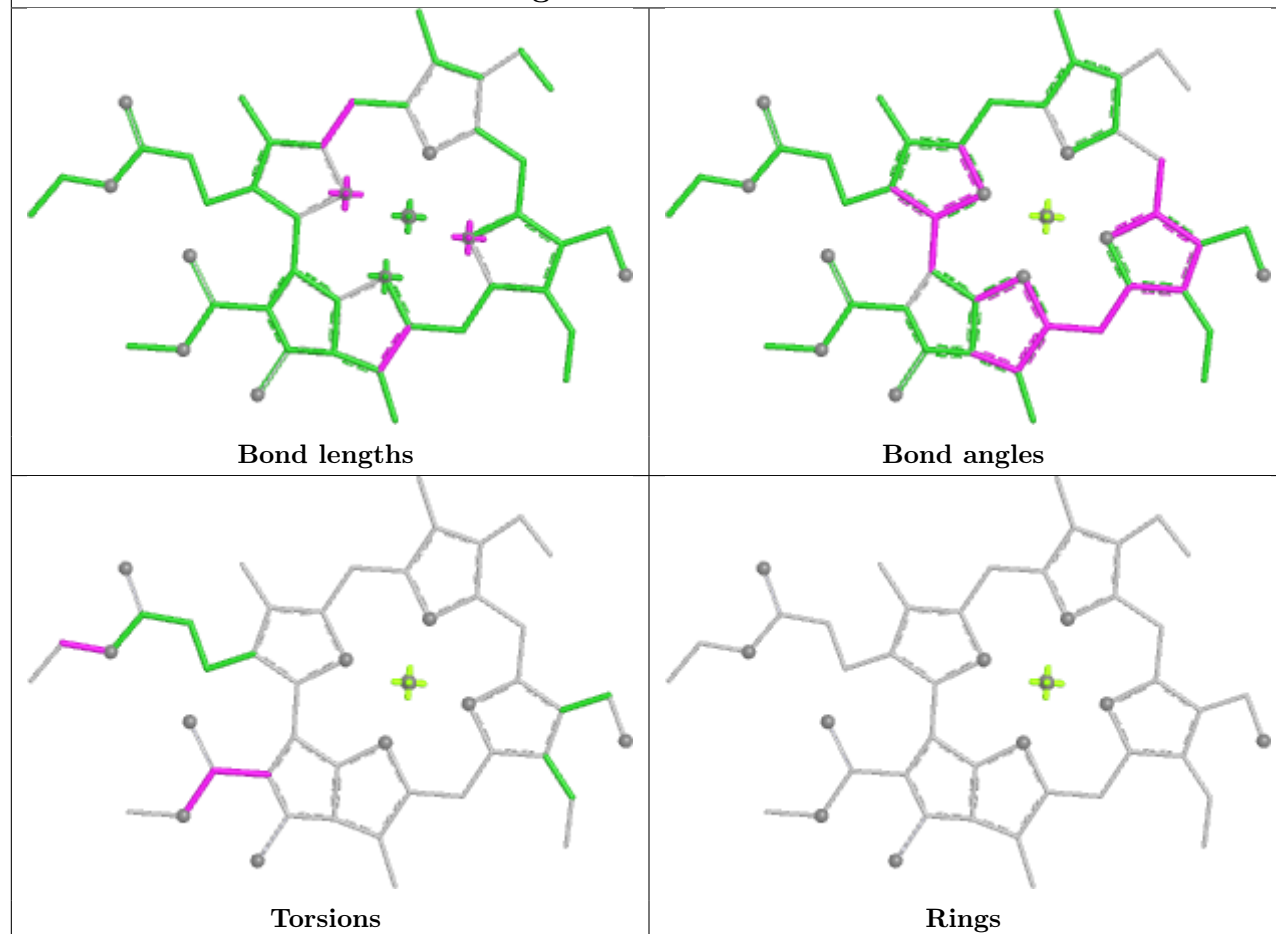
Ligand CLA B 822



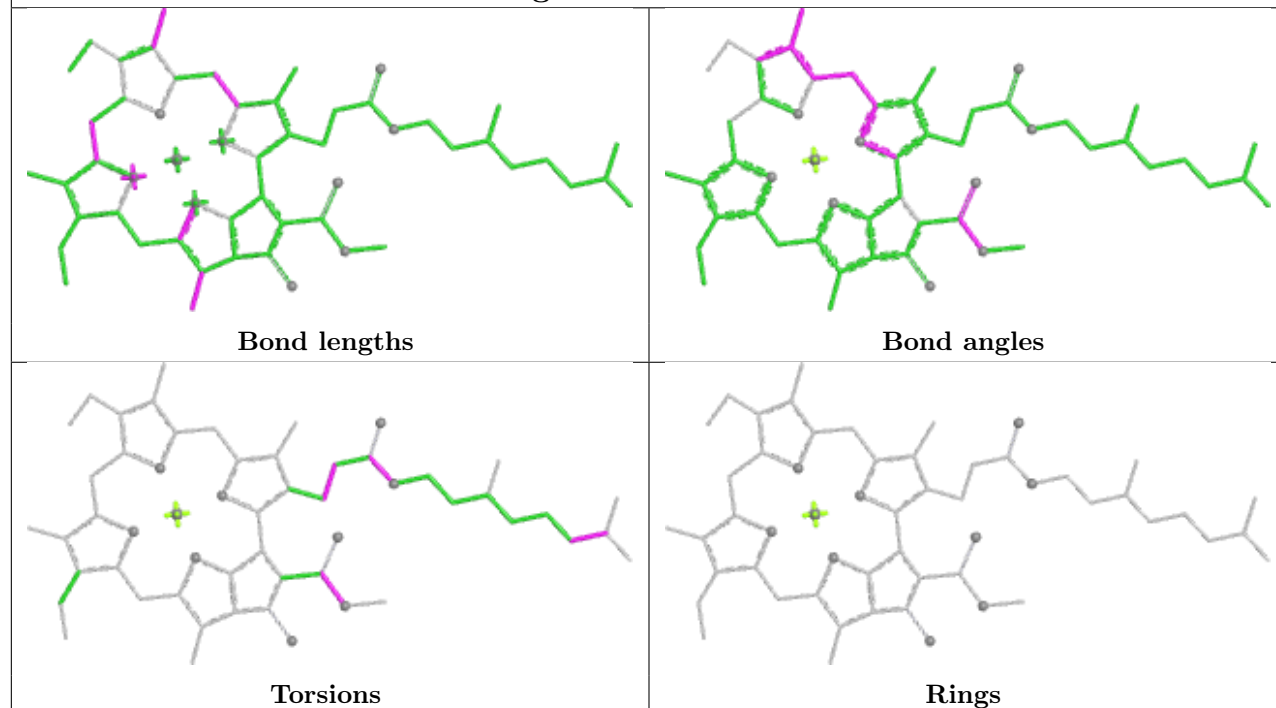
Ligand CLA 2 608



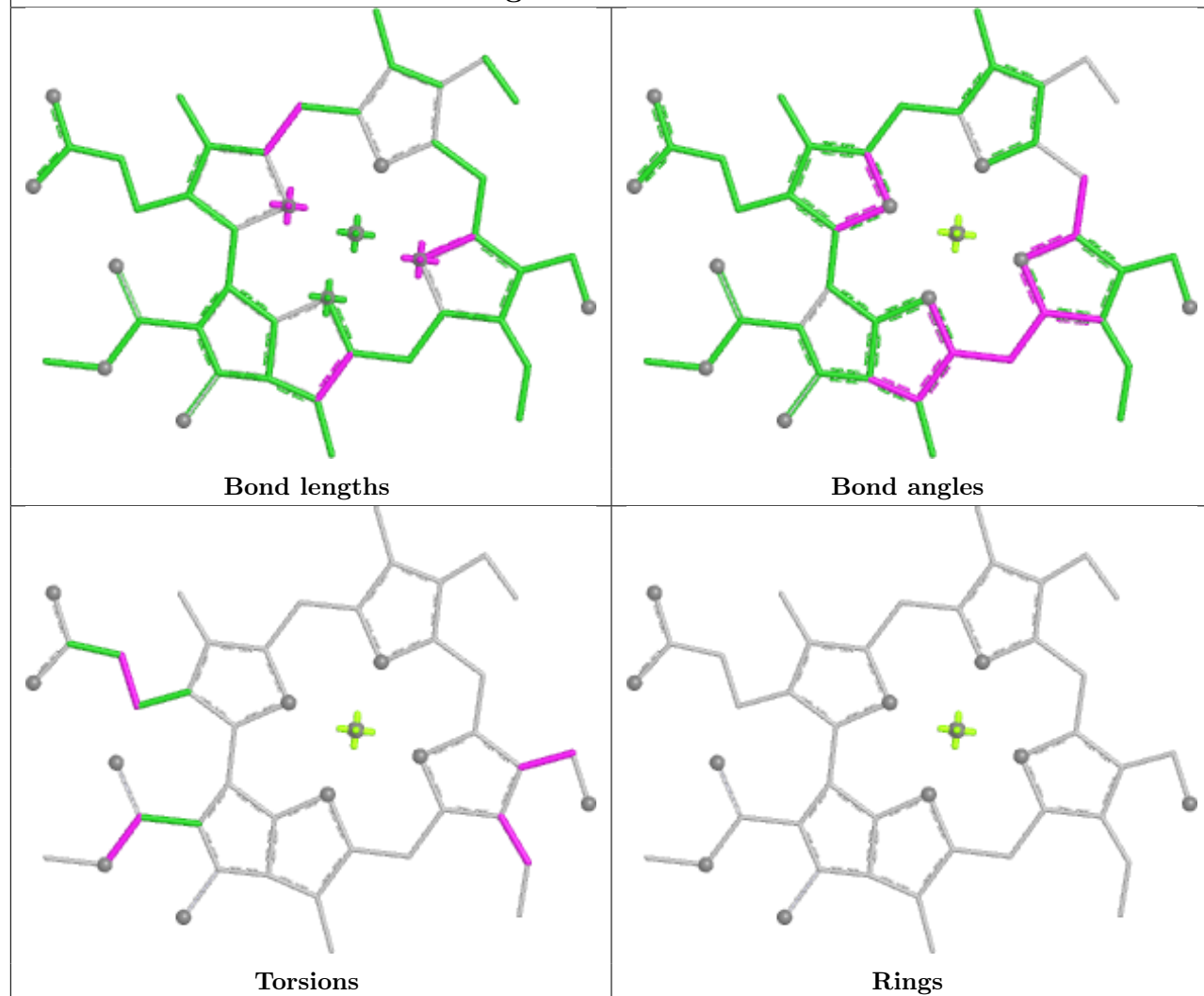
Ligand CHL T 601



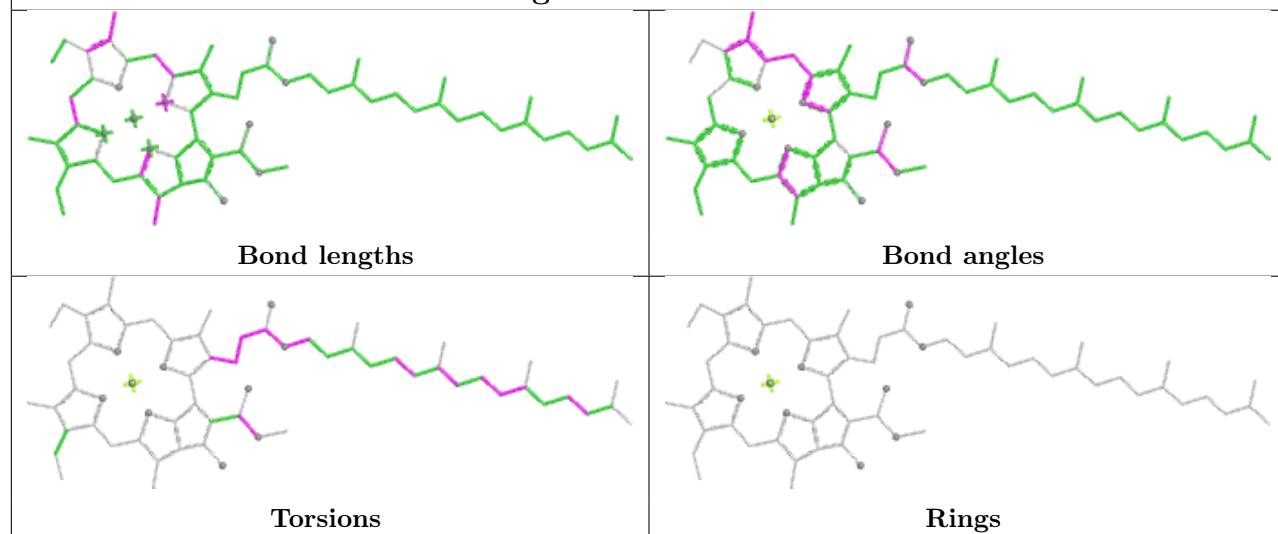
Ligand CLA B 811

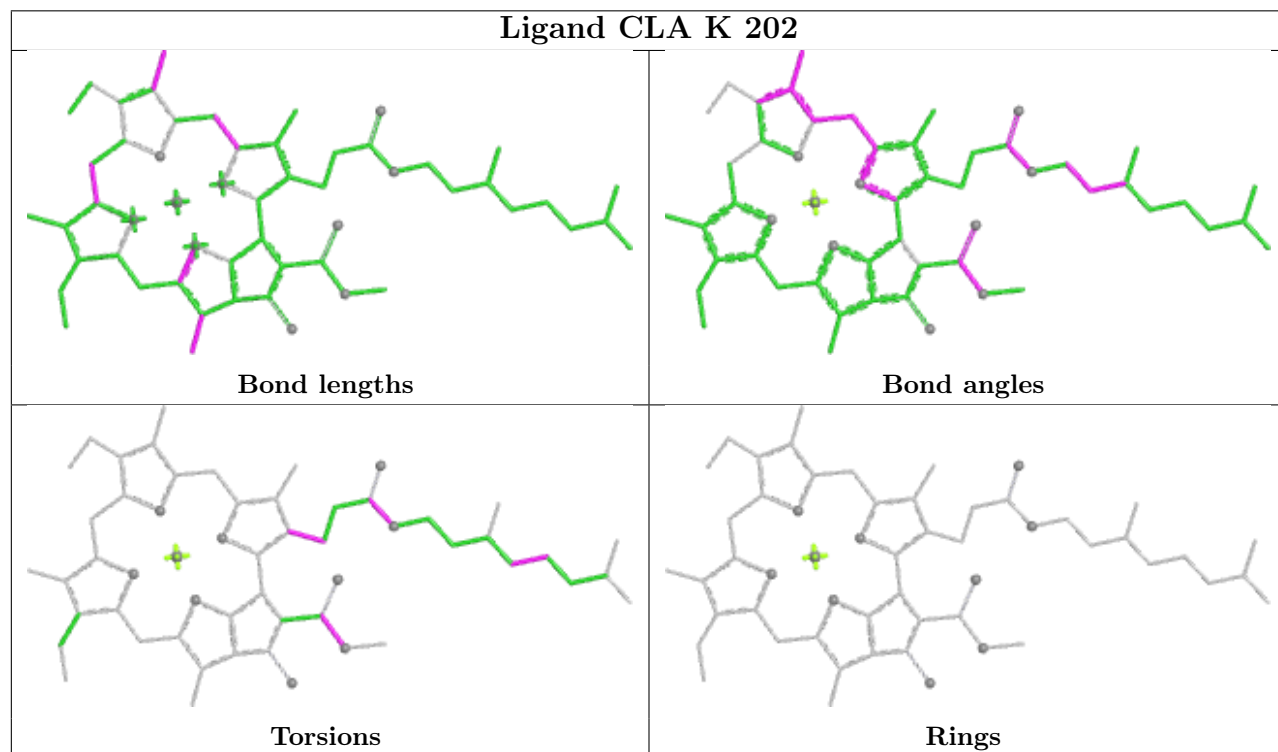
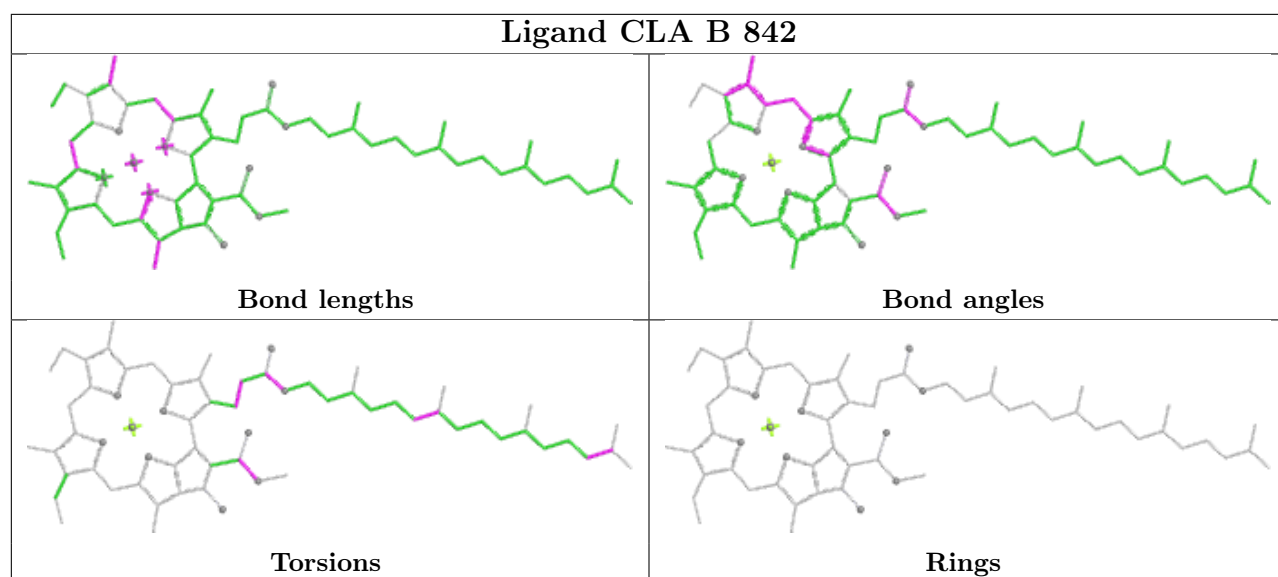


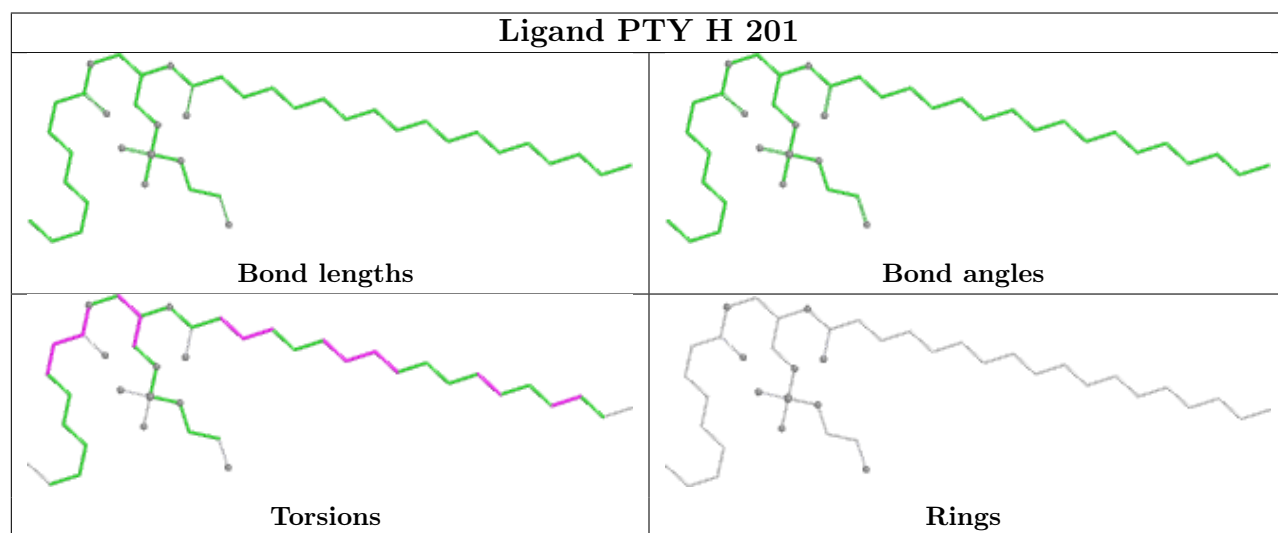
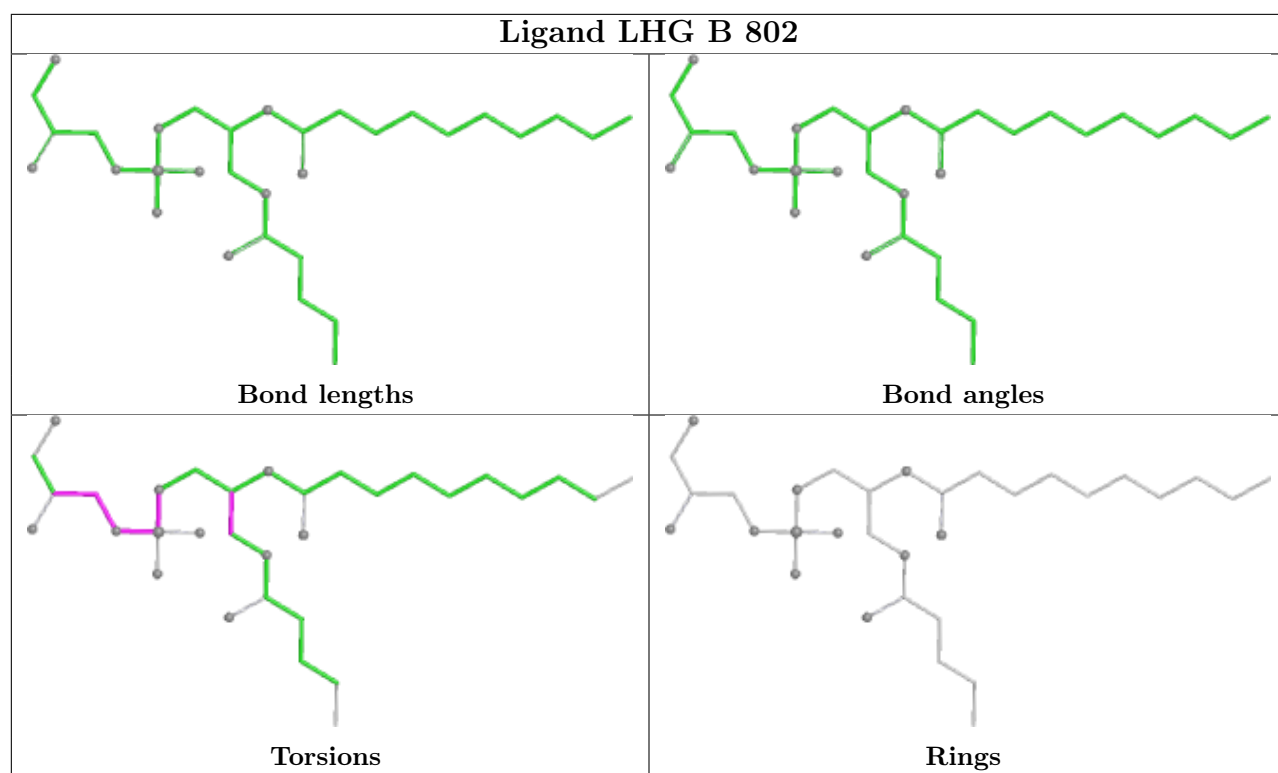
Ligand CHL c 605

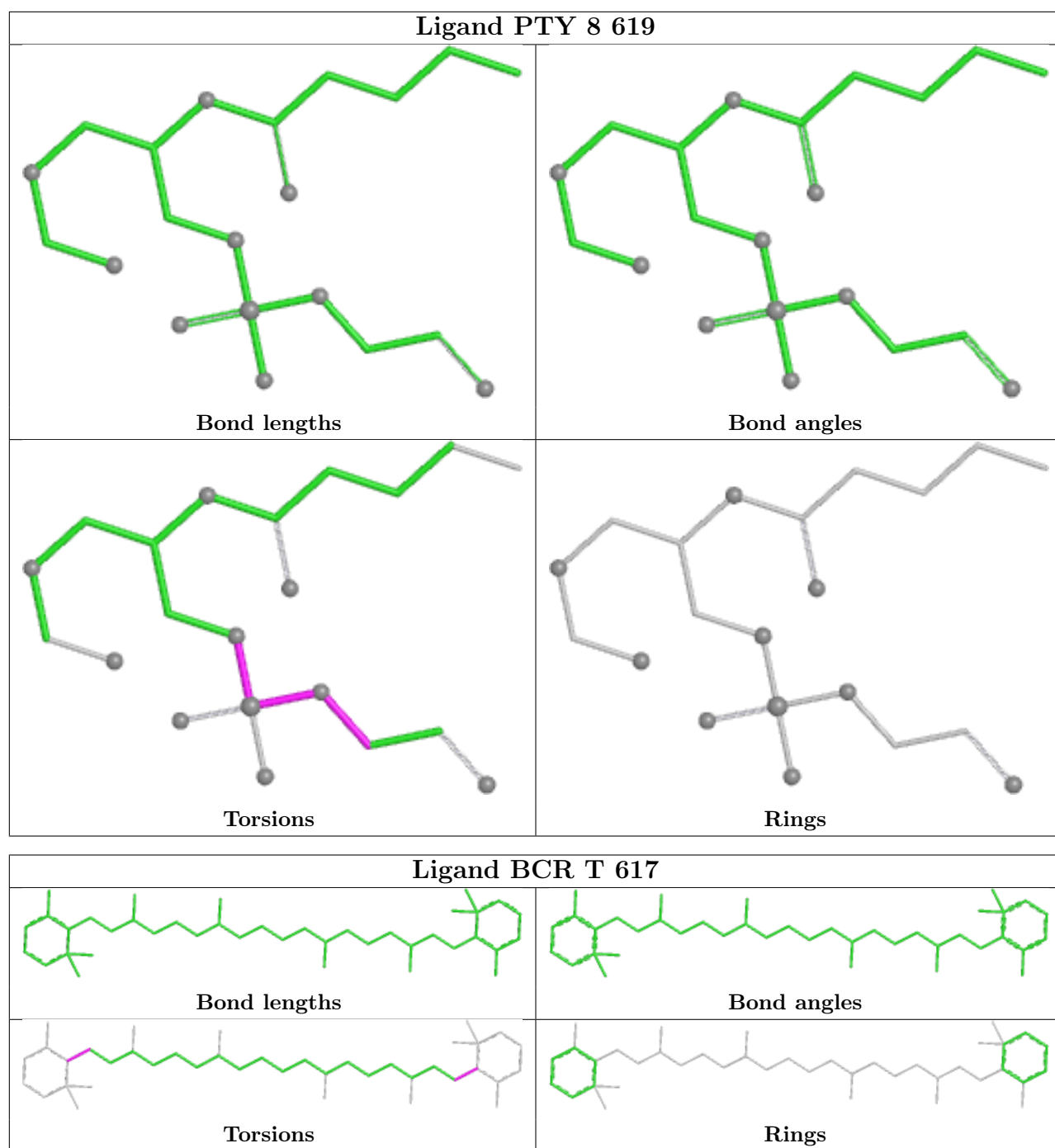


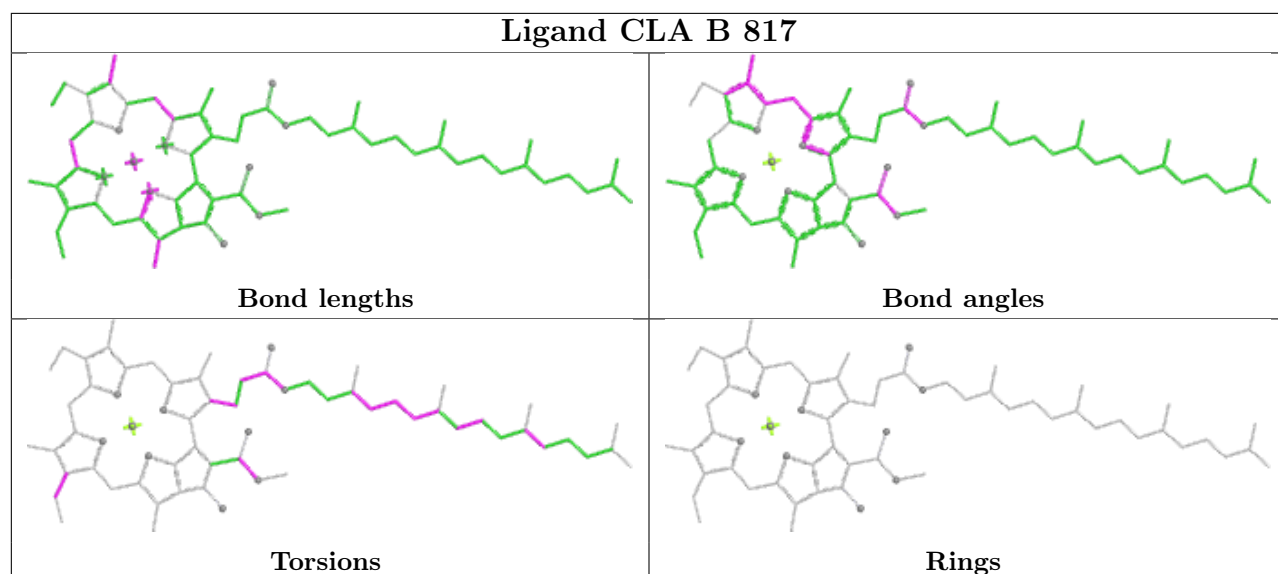
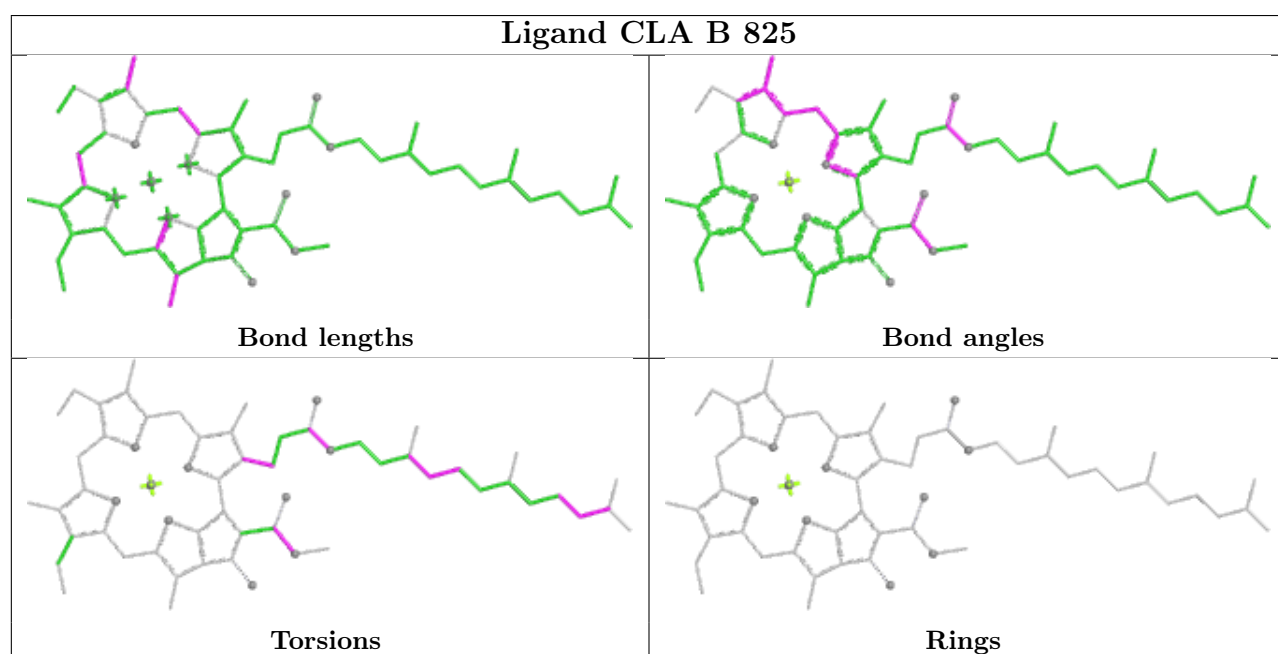
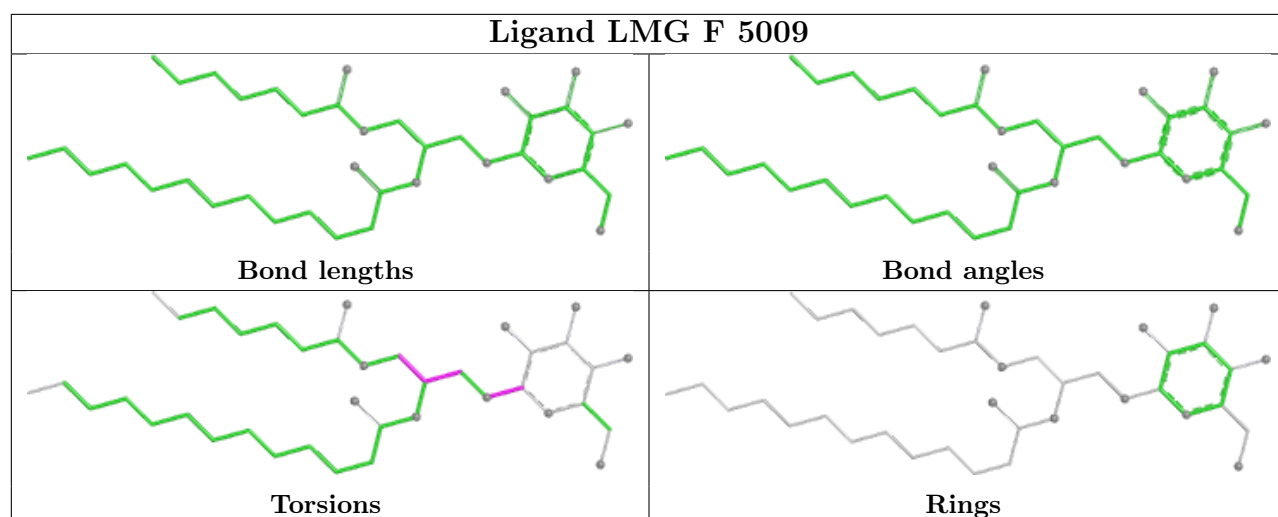
Ligand CLA B 832



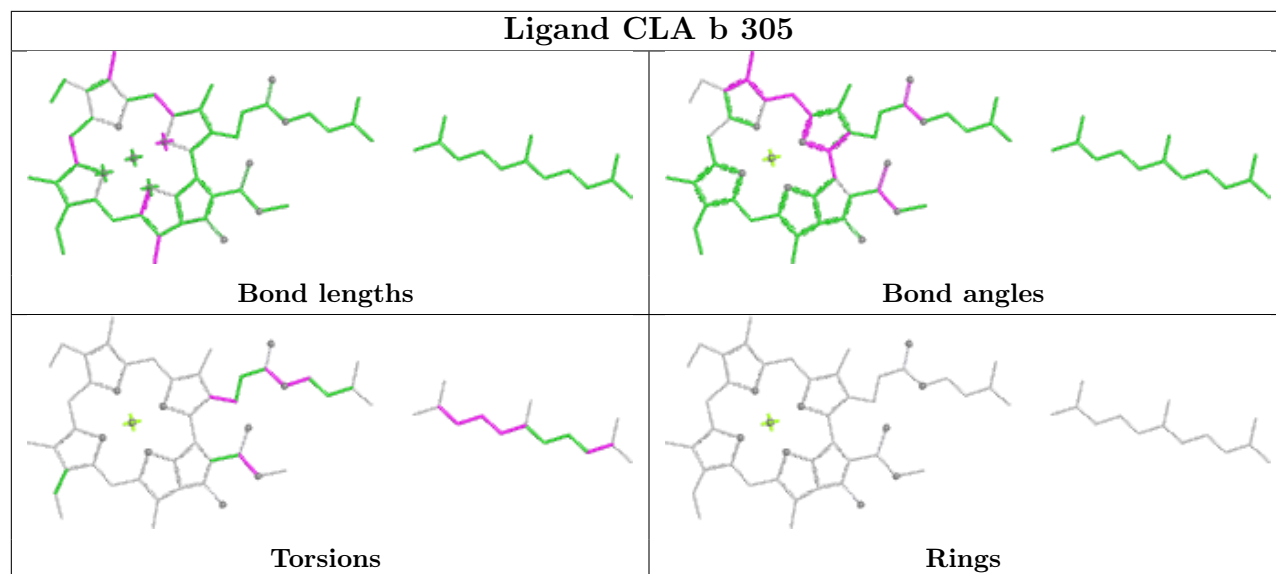




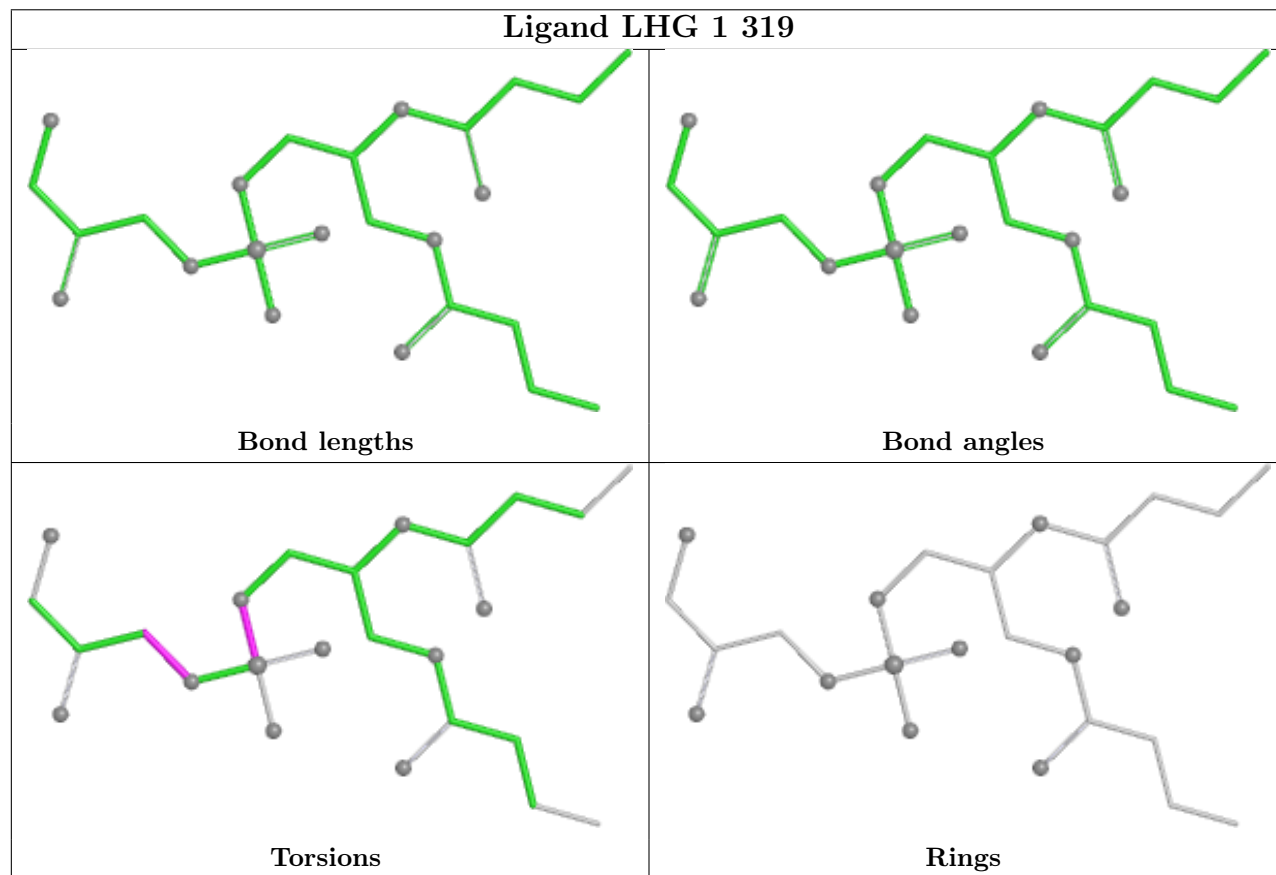




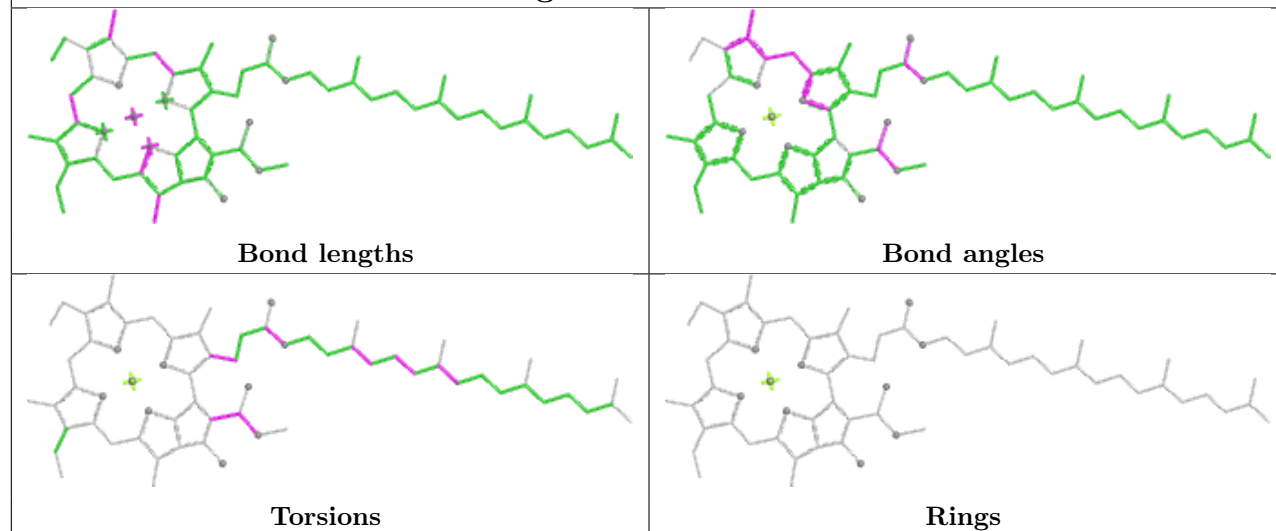
Ligand CLA b 305



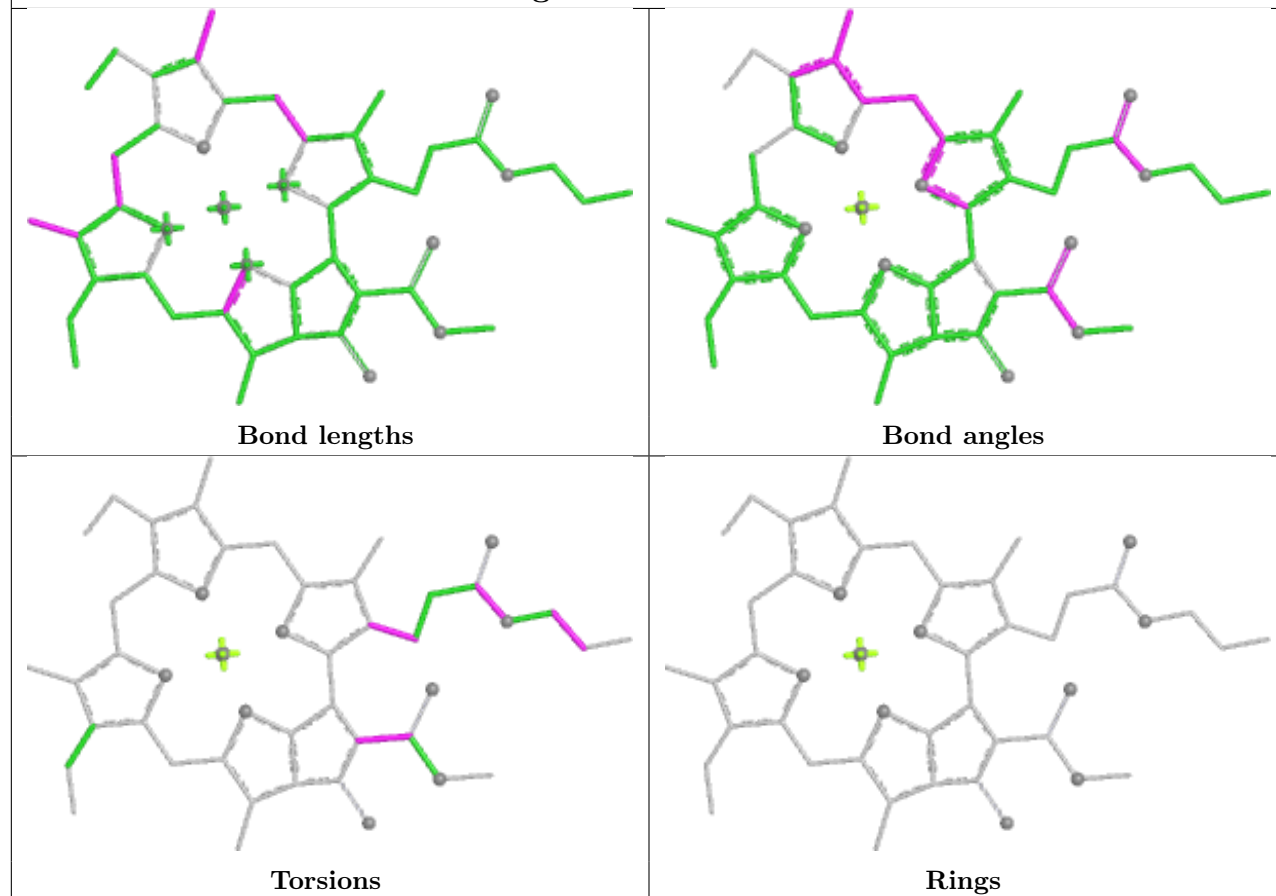
Ligand LHG 1 319

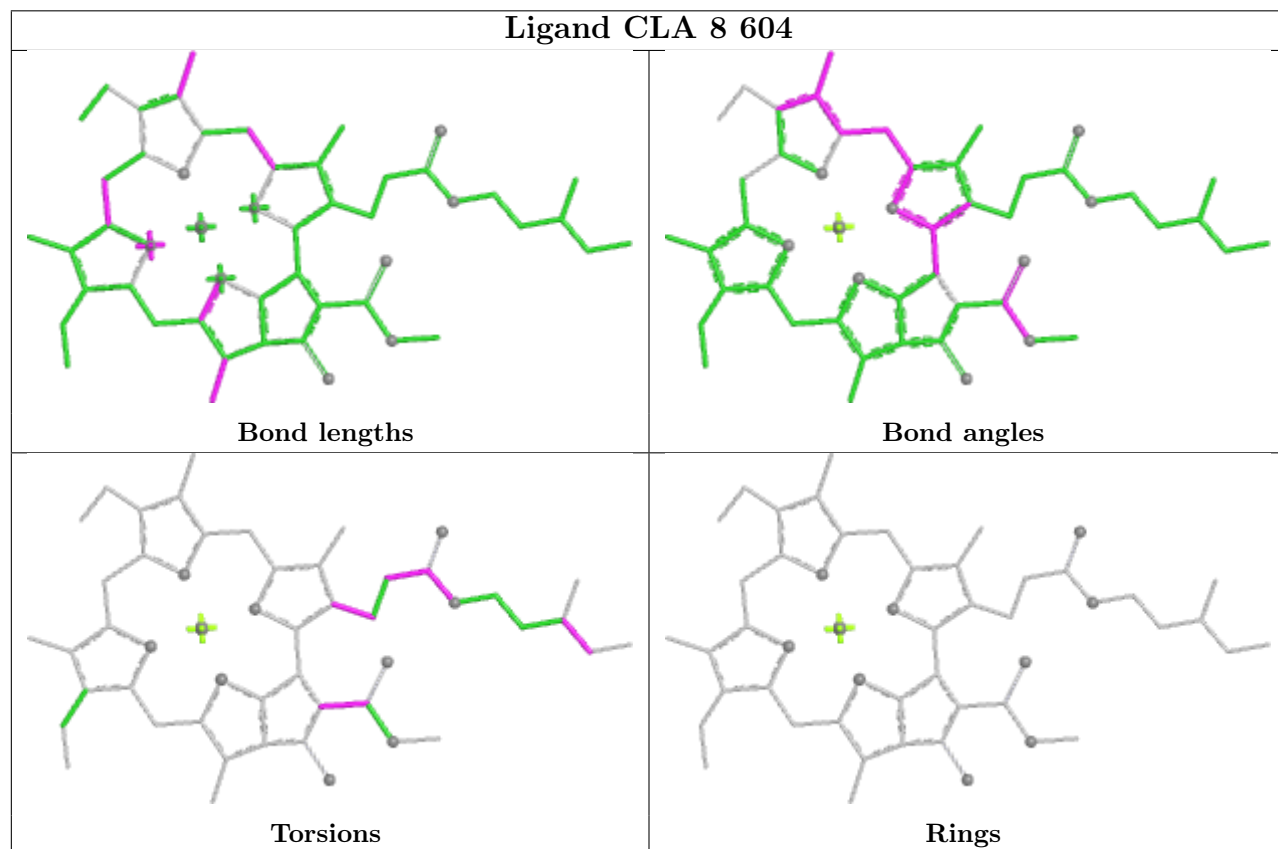
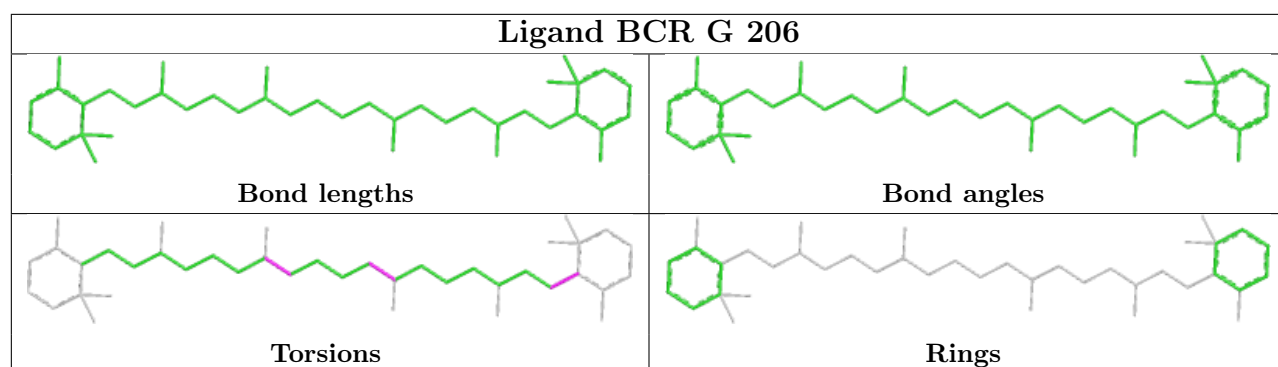


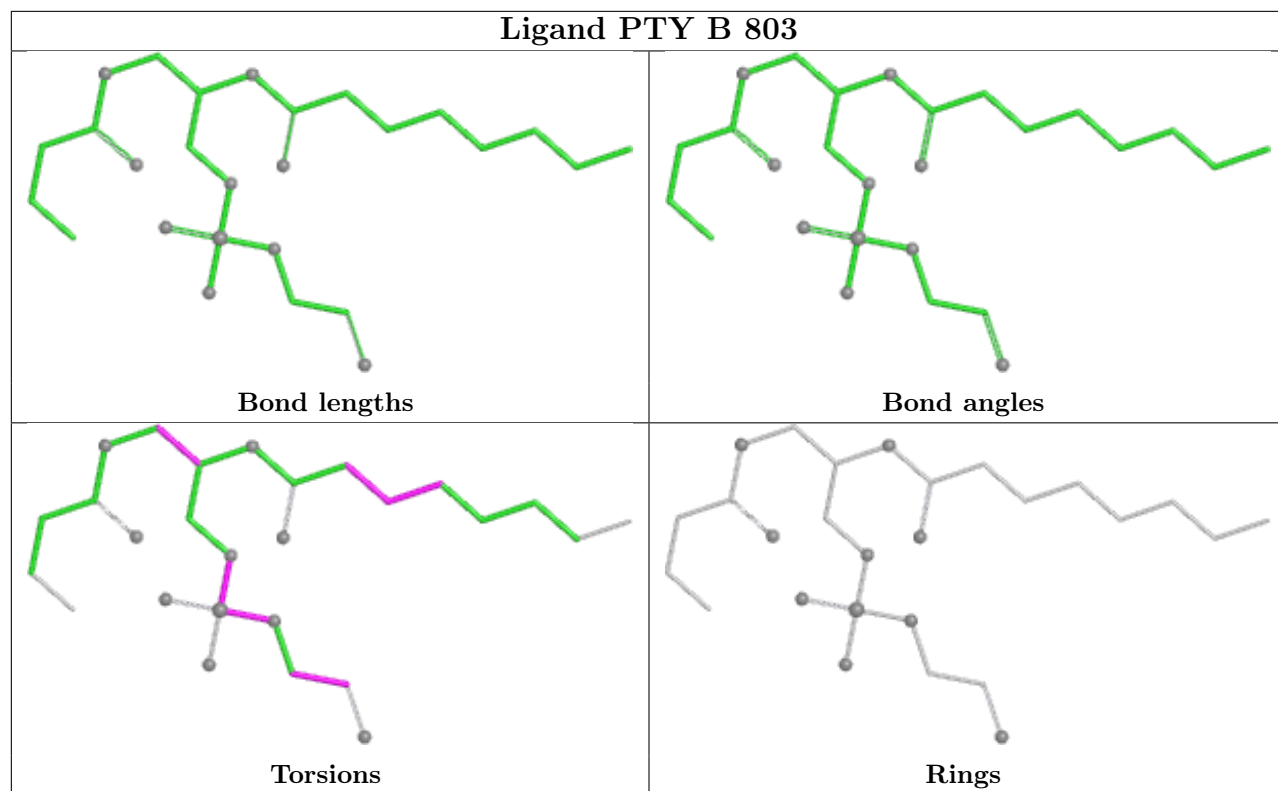
Ligand CLA 3 407



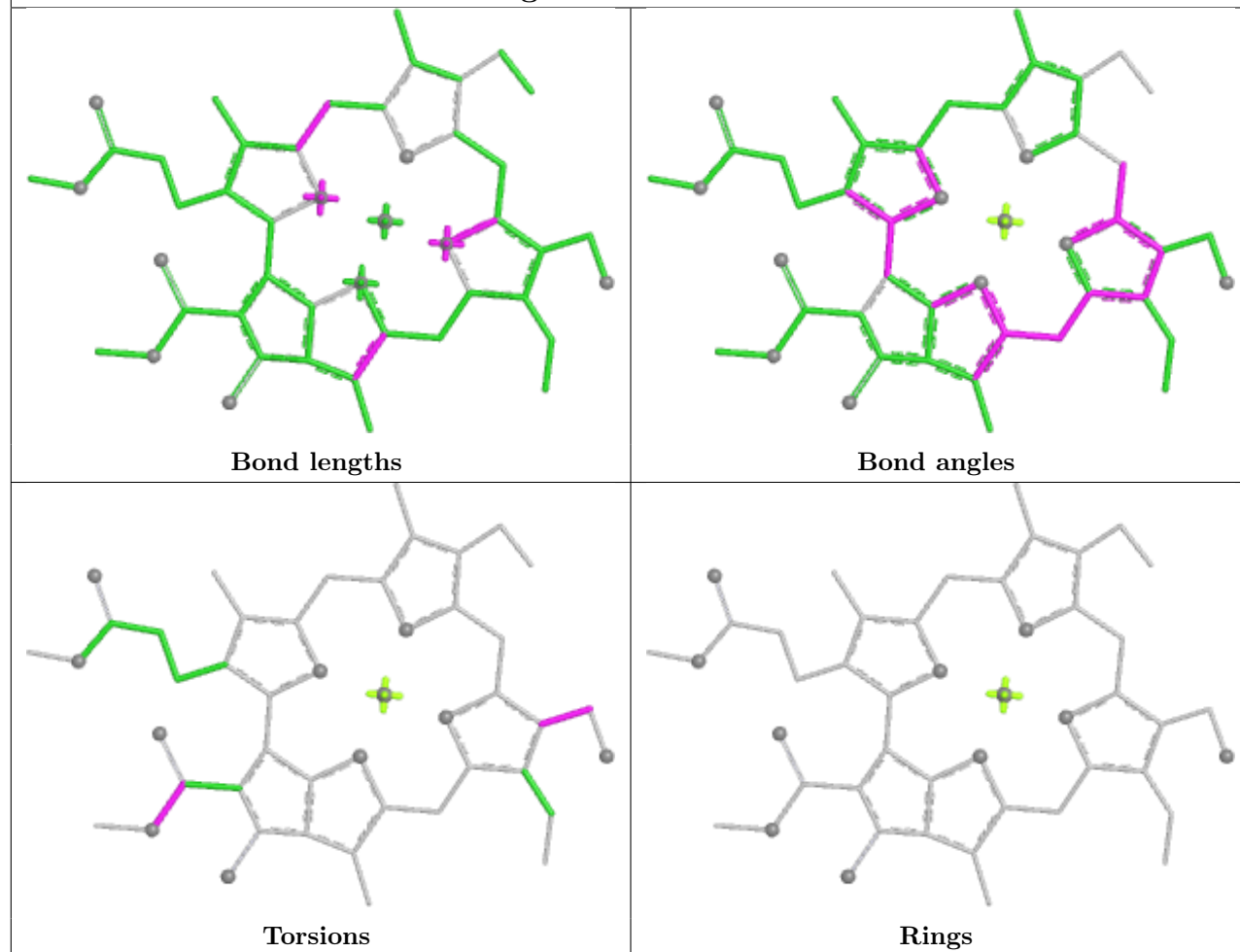
Ligand CLA B 808



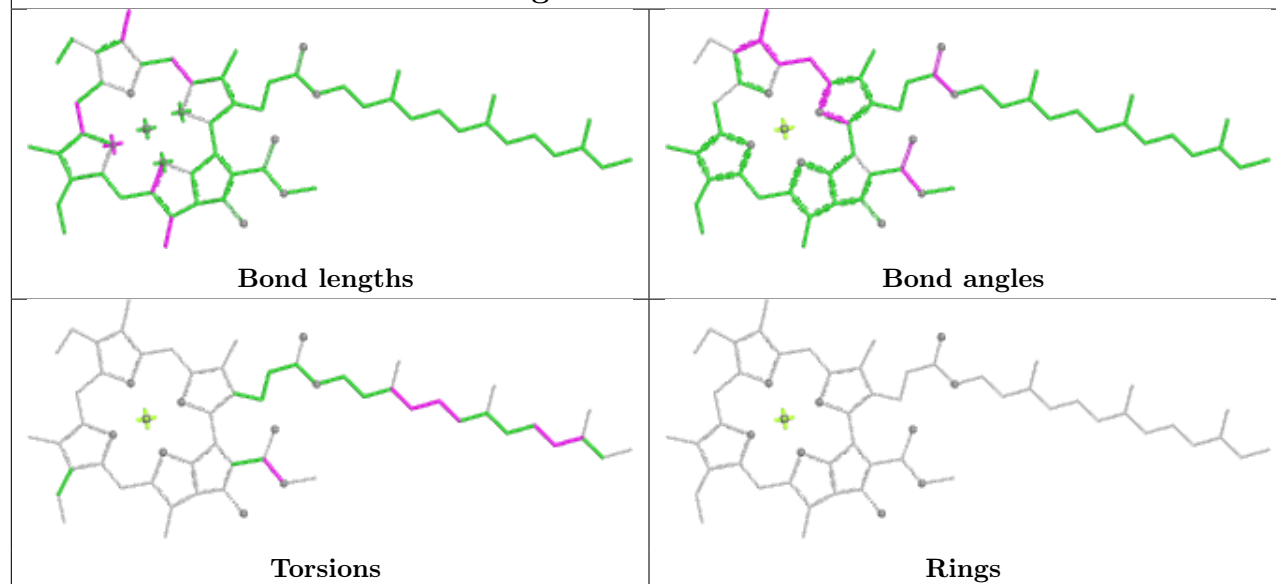


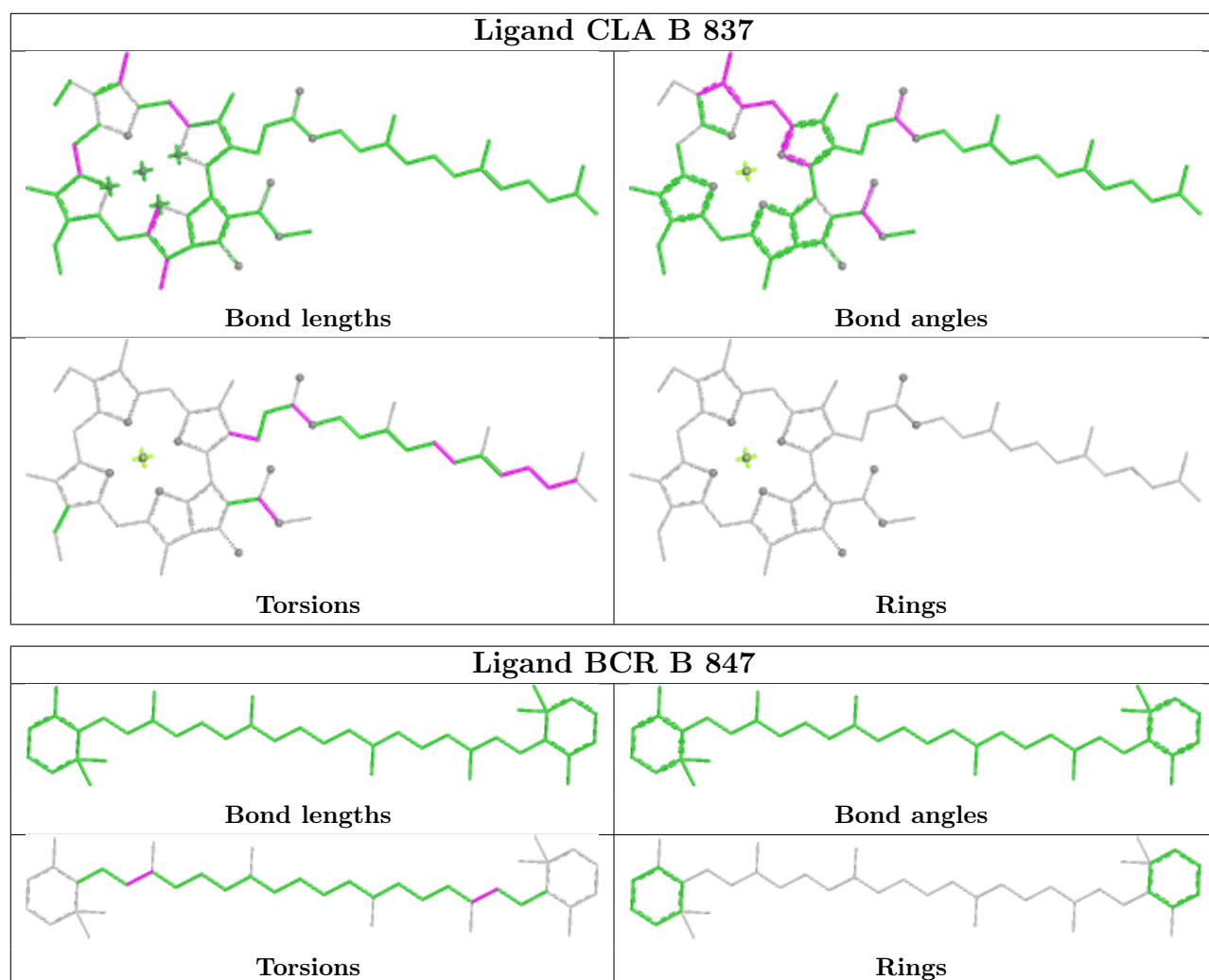


Ligand CHL a 306

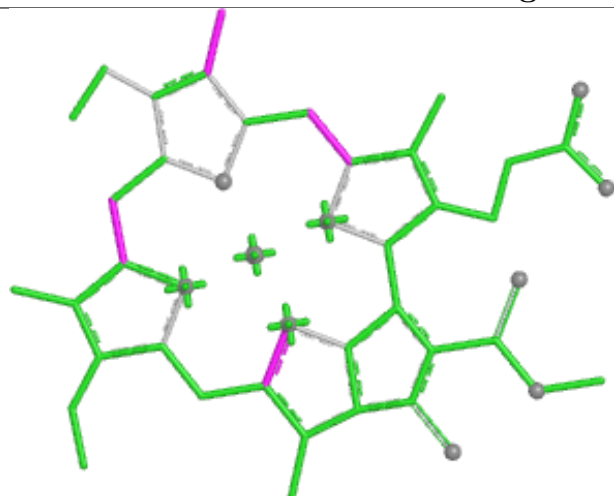


Ligand CLA A 856

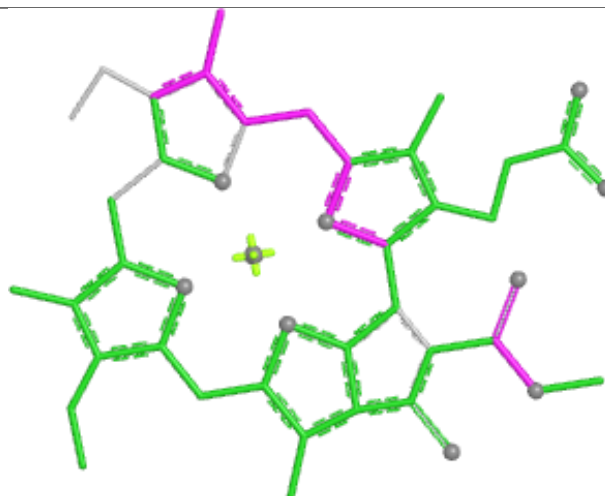




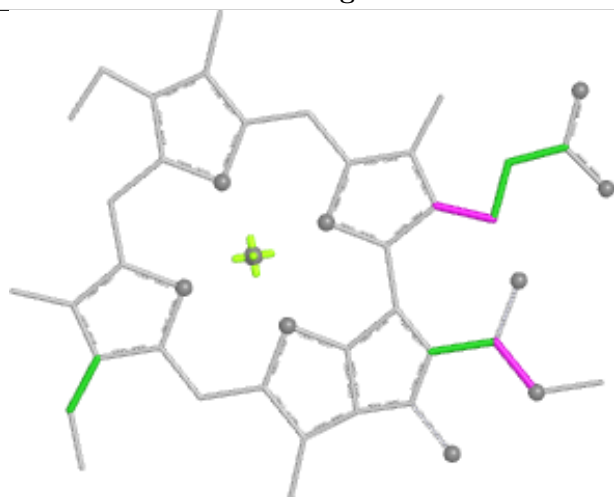
Ligand CLA c 614



Bond lengths



Bond angles

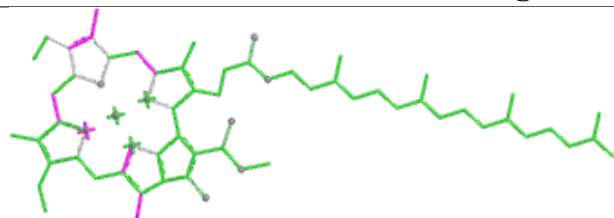


Torsions

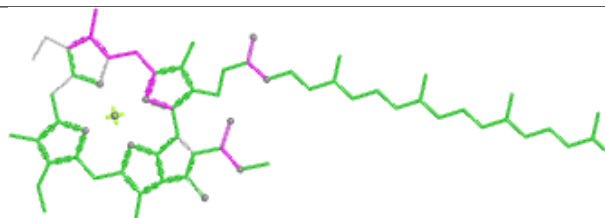


Rings

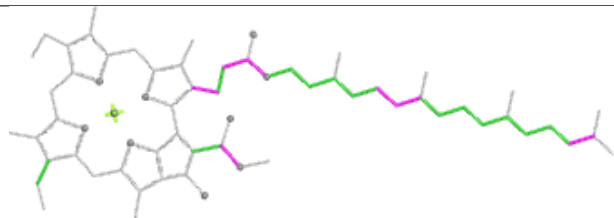
Ligand CLA B 843



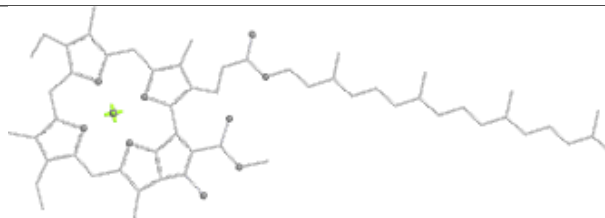
Bond lengths



Bond angles

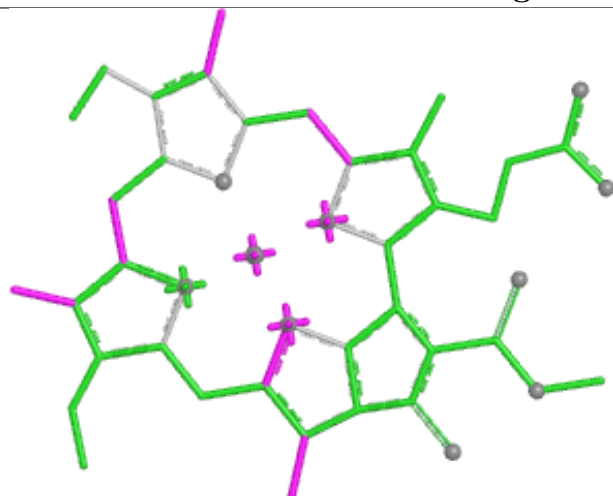


Torsions

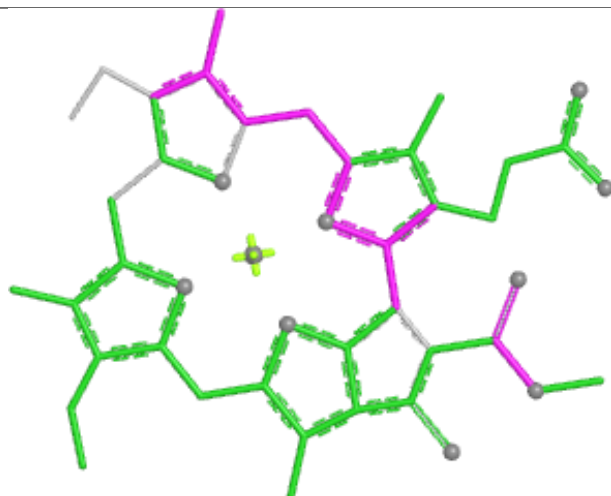


Rings

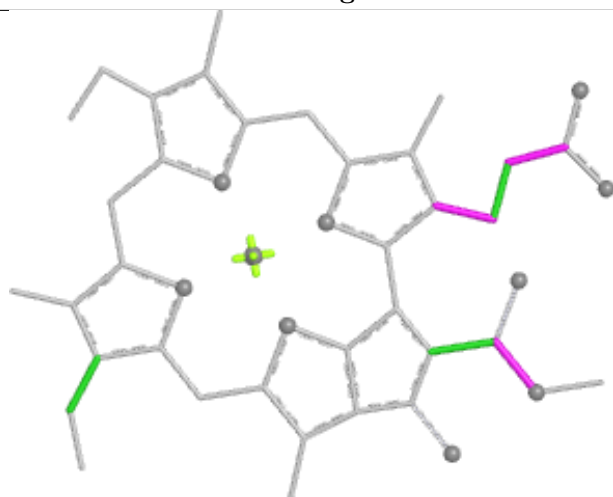
Ligand CLA K 203



Bond lengths



Bond angles

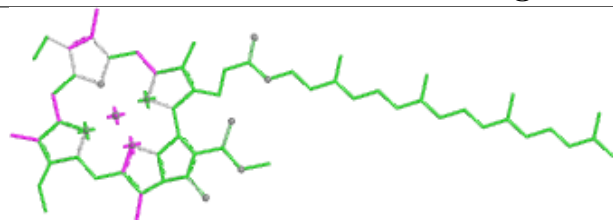


Torsions

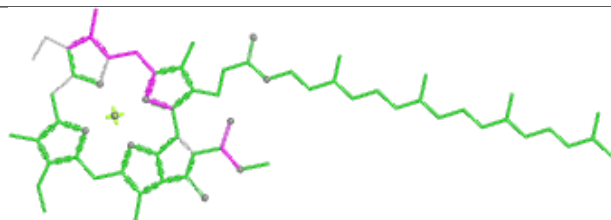


Rings

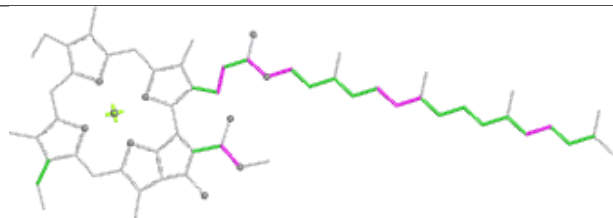
Ligand CLA A 804



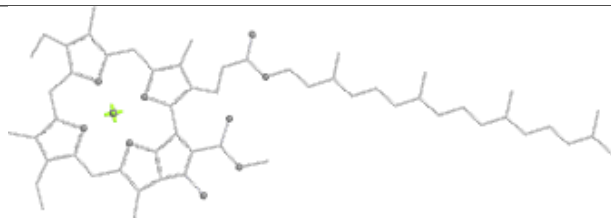
Bond lengths



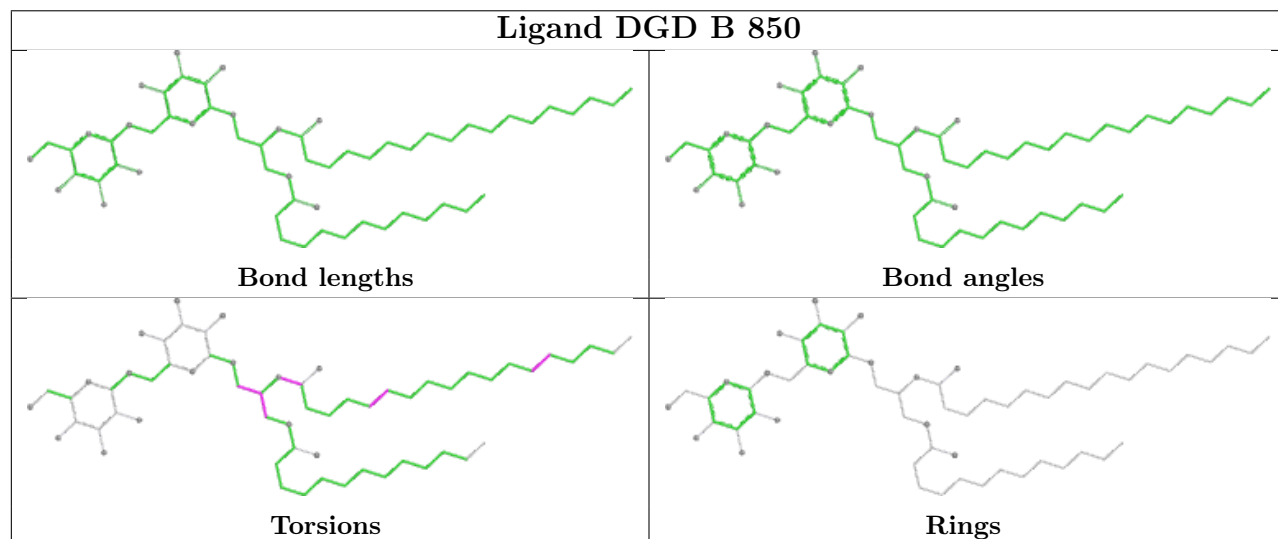
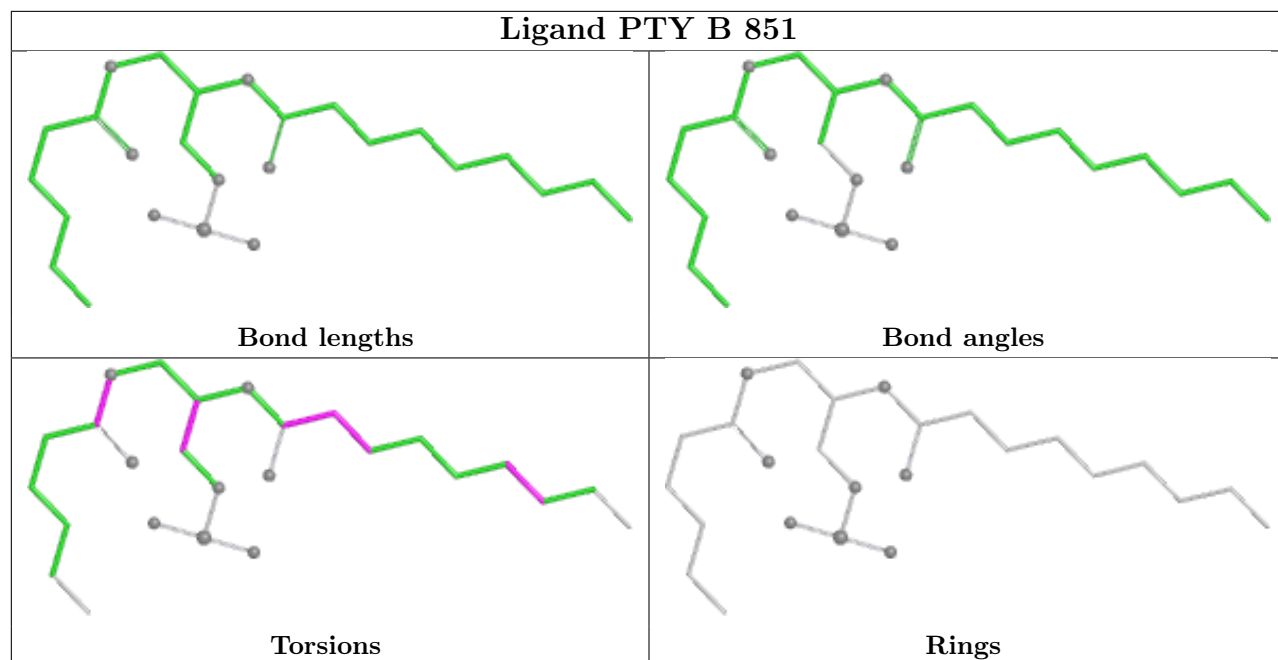
Bond angles



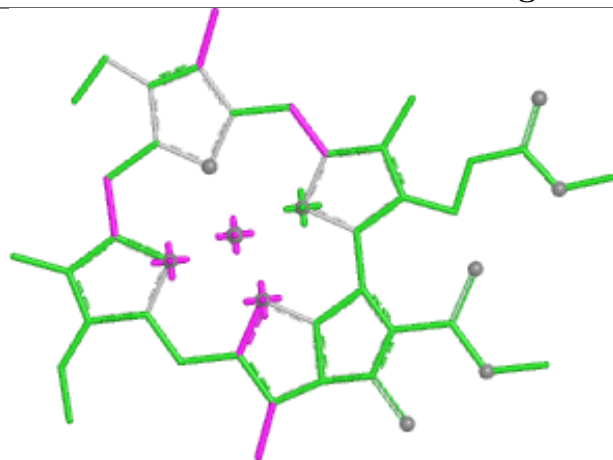
Torsions



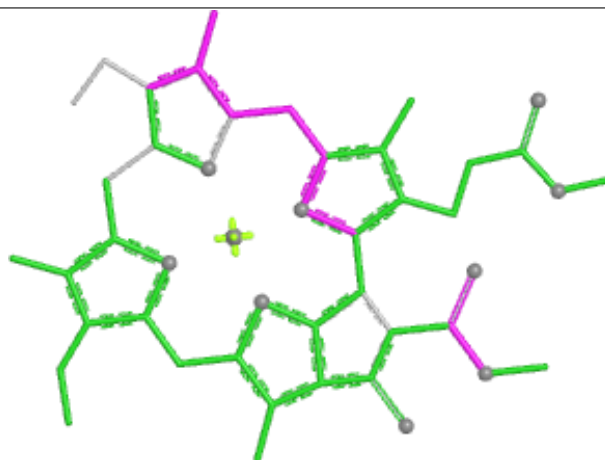
Rings



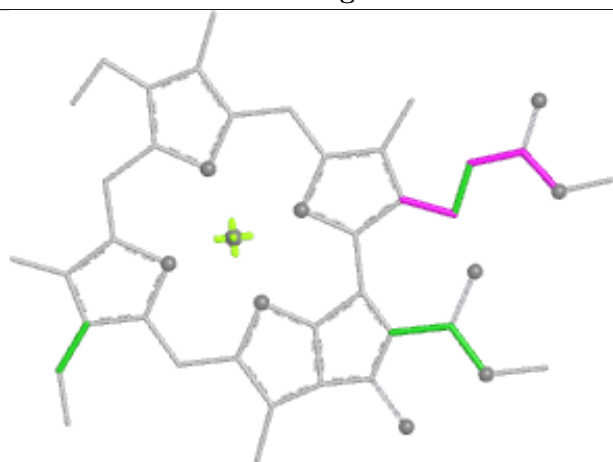
Ligand CLA 8 609



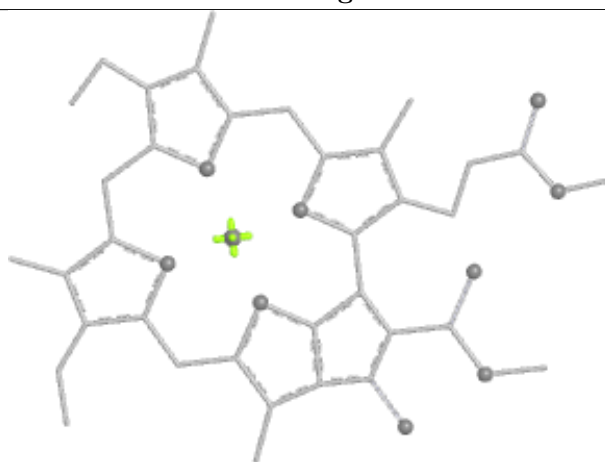
Bond lengths



Bond angles

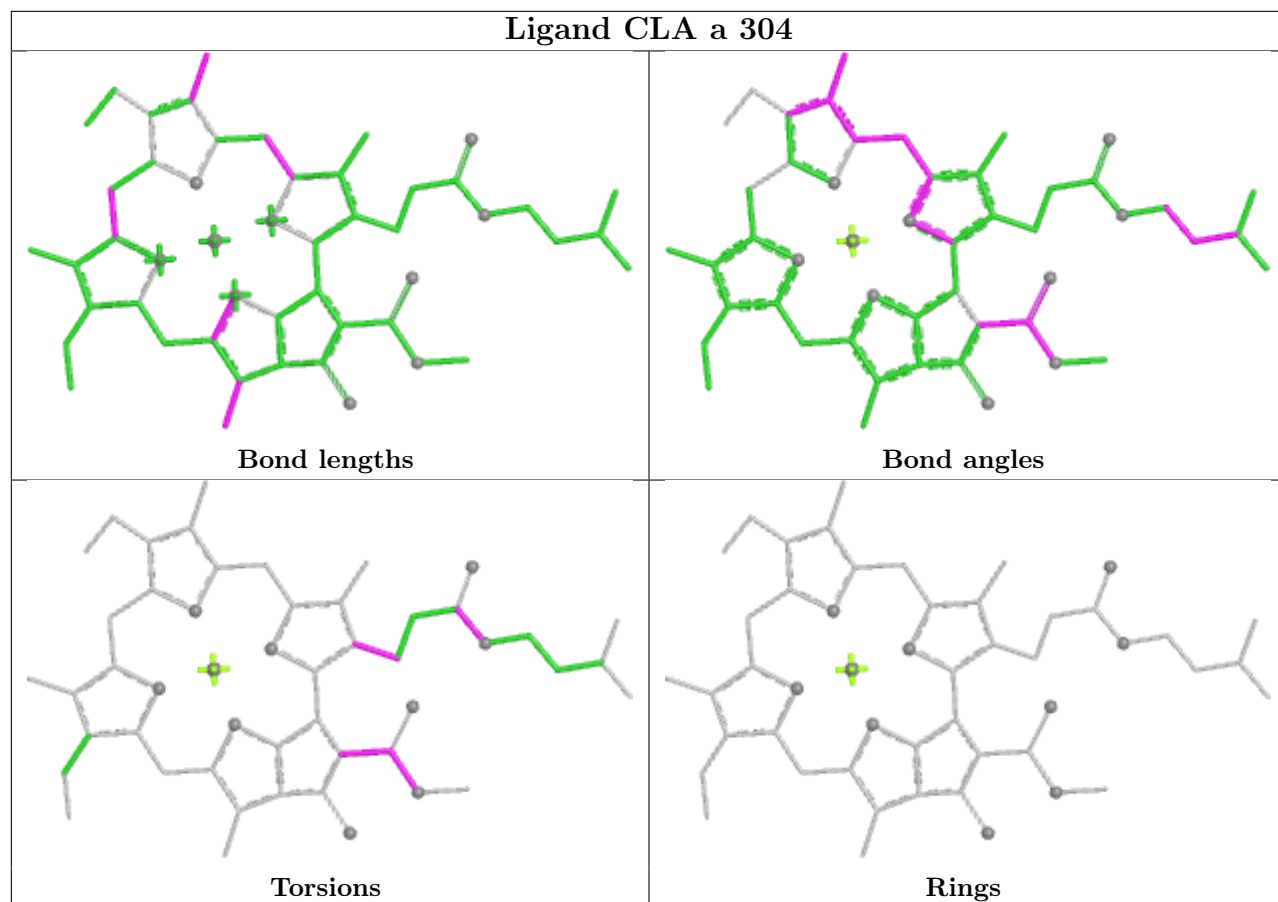


Torsions

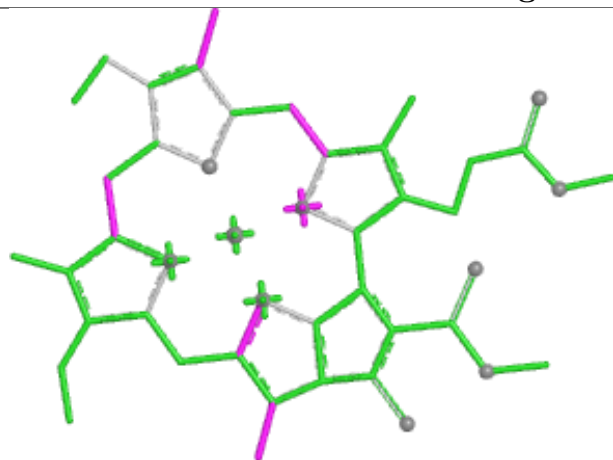


Rings

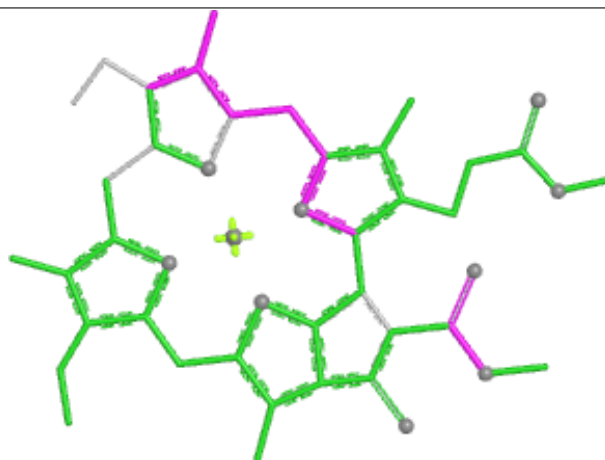
Ligand CLA a 304



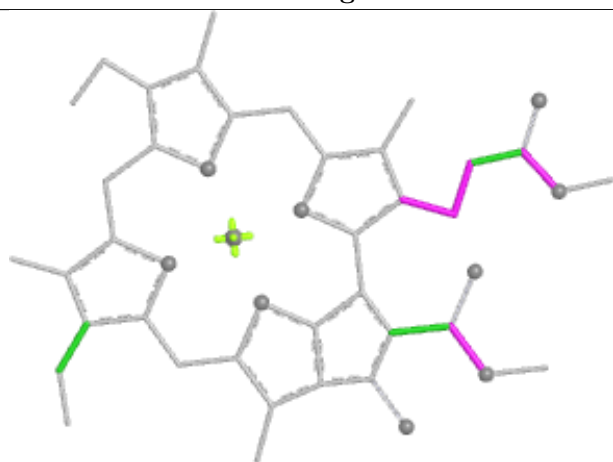
Ligand CLA 8 605



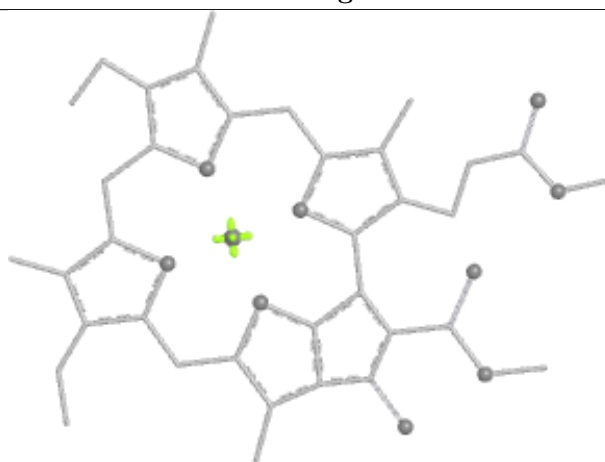
Bond lengths



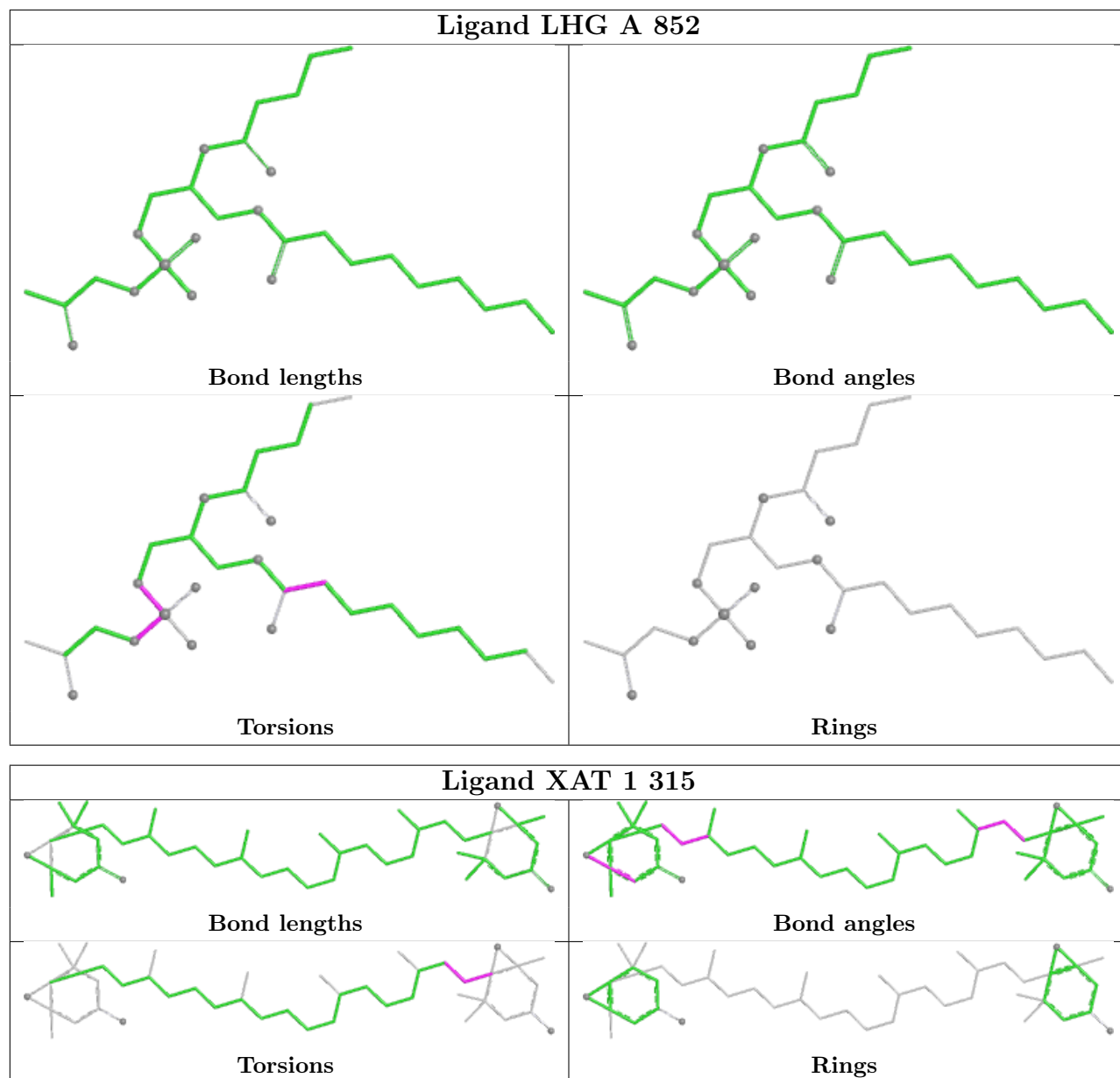
Bond angles



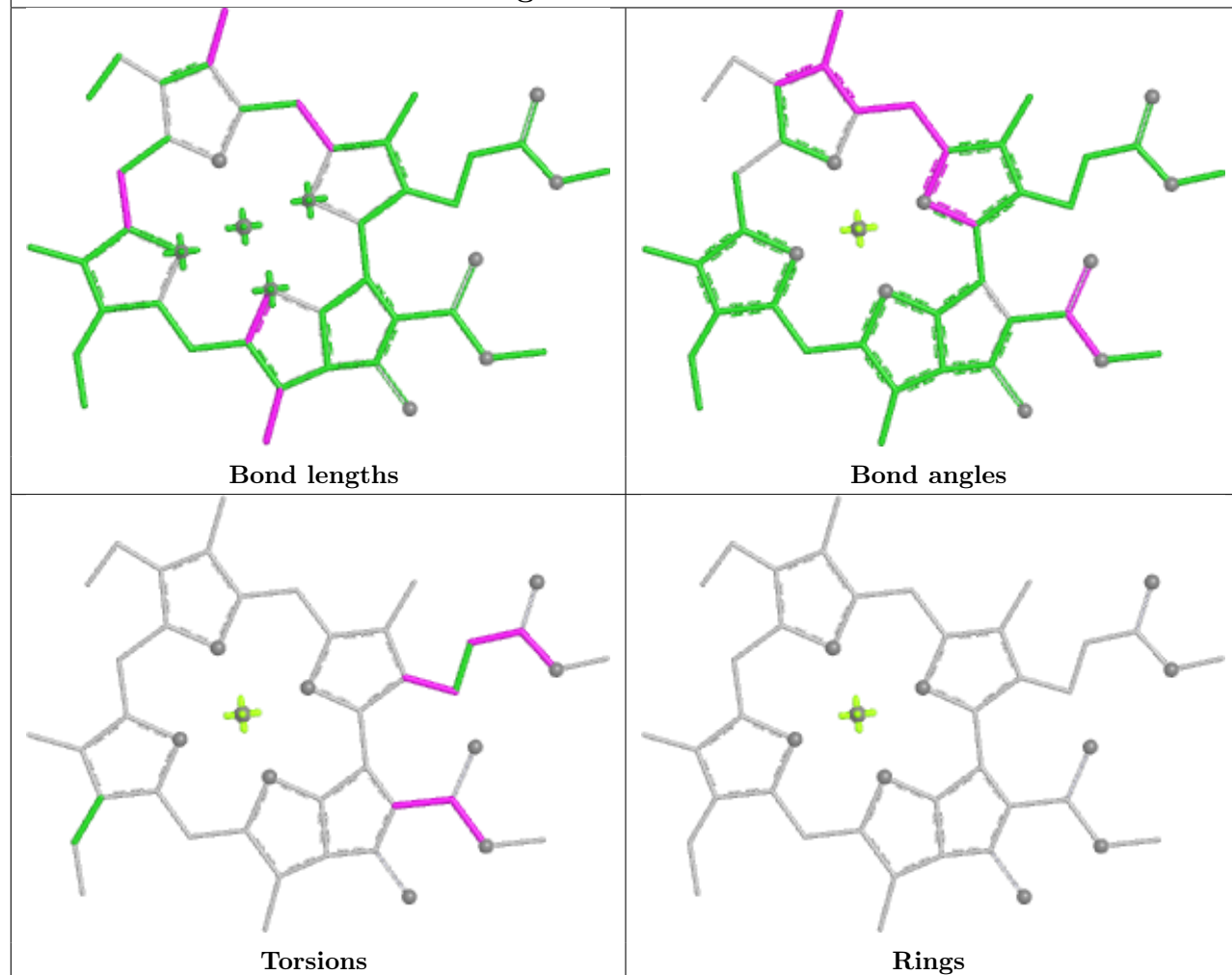
Torsions



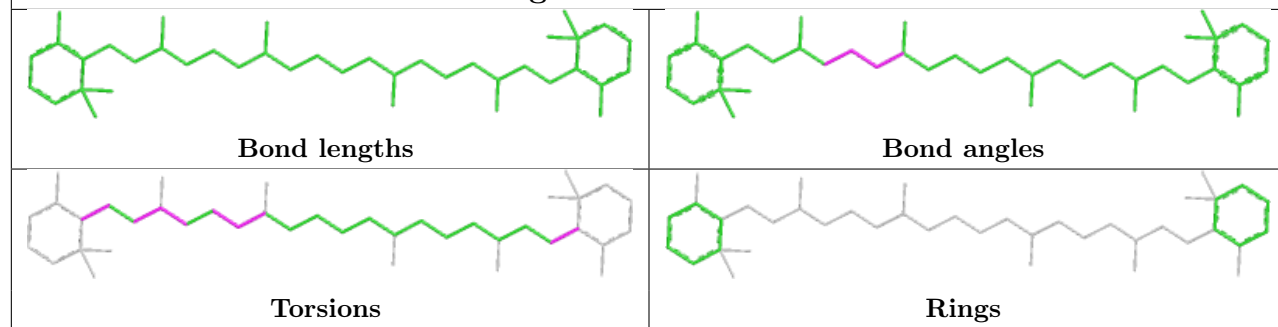
Rings

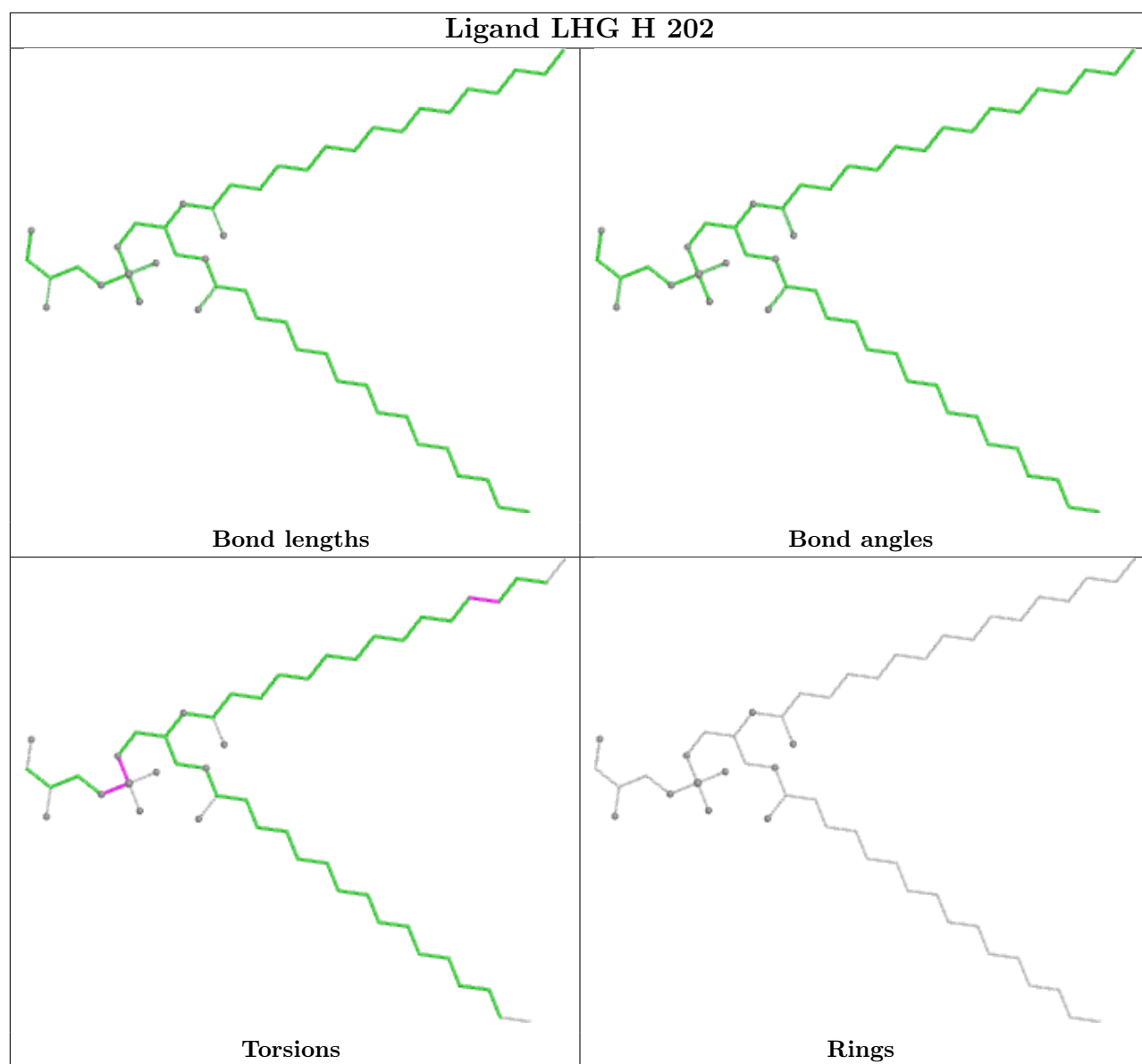


Ligand CLA 2 607

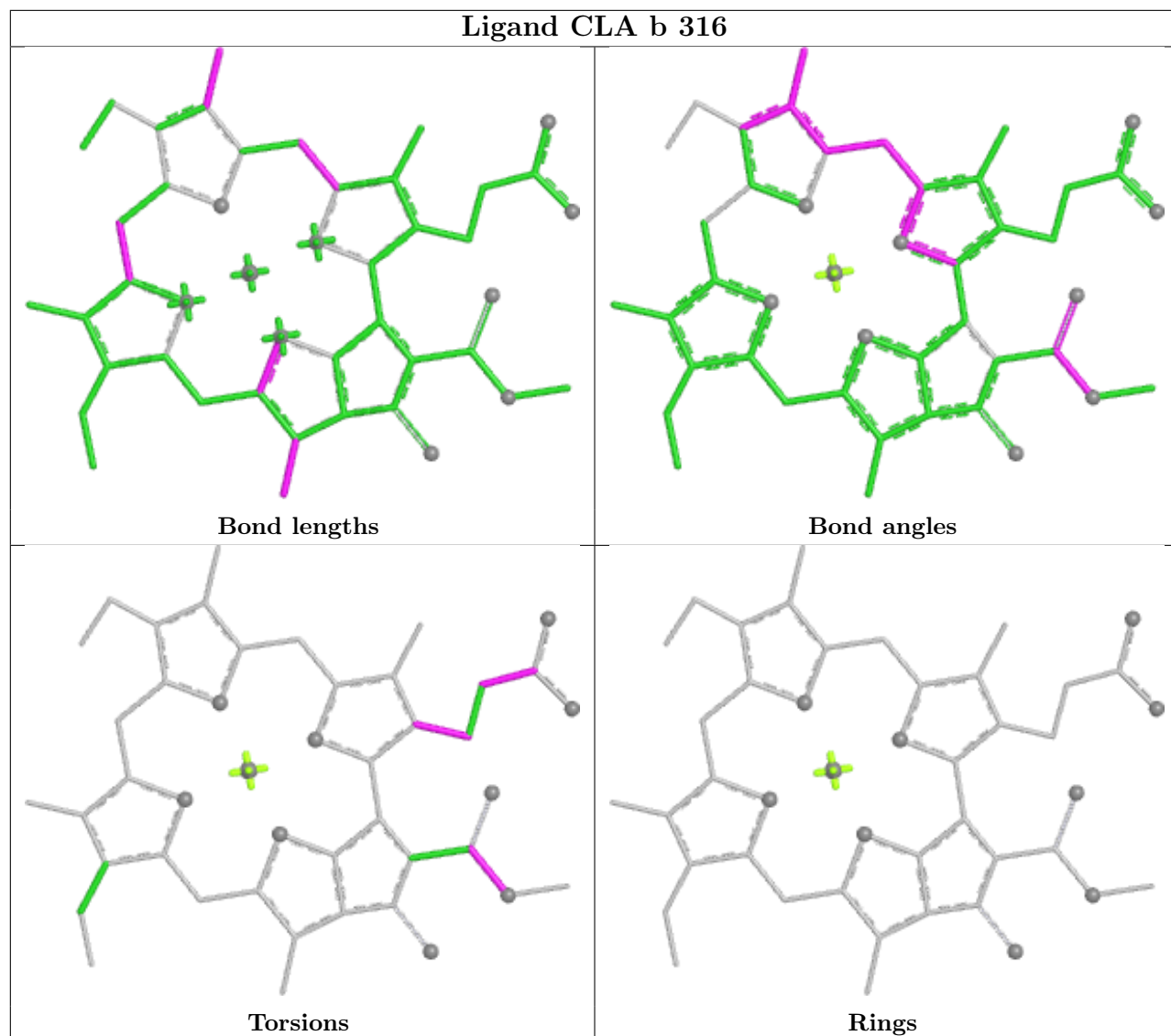


Ligand BCR K 205

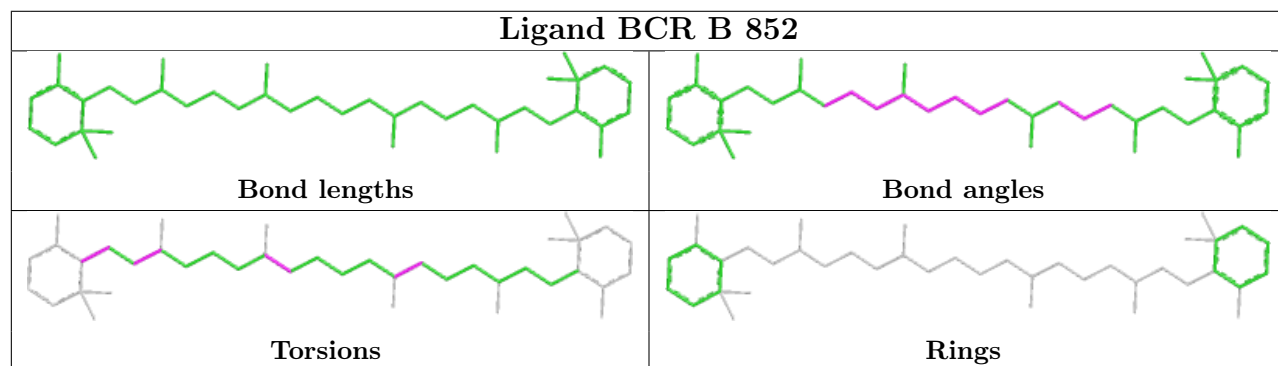


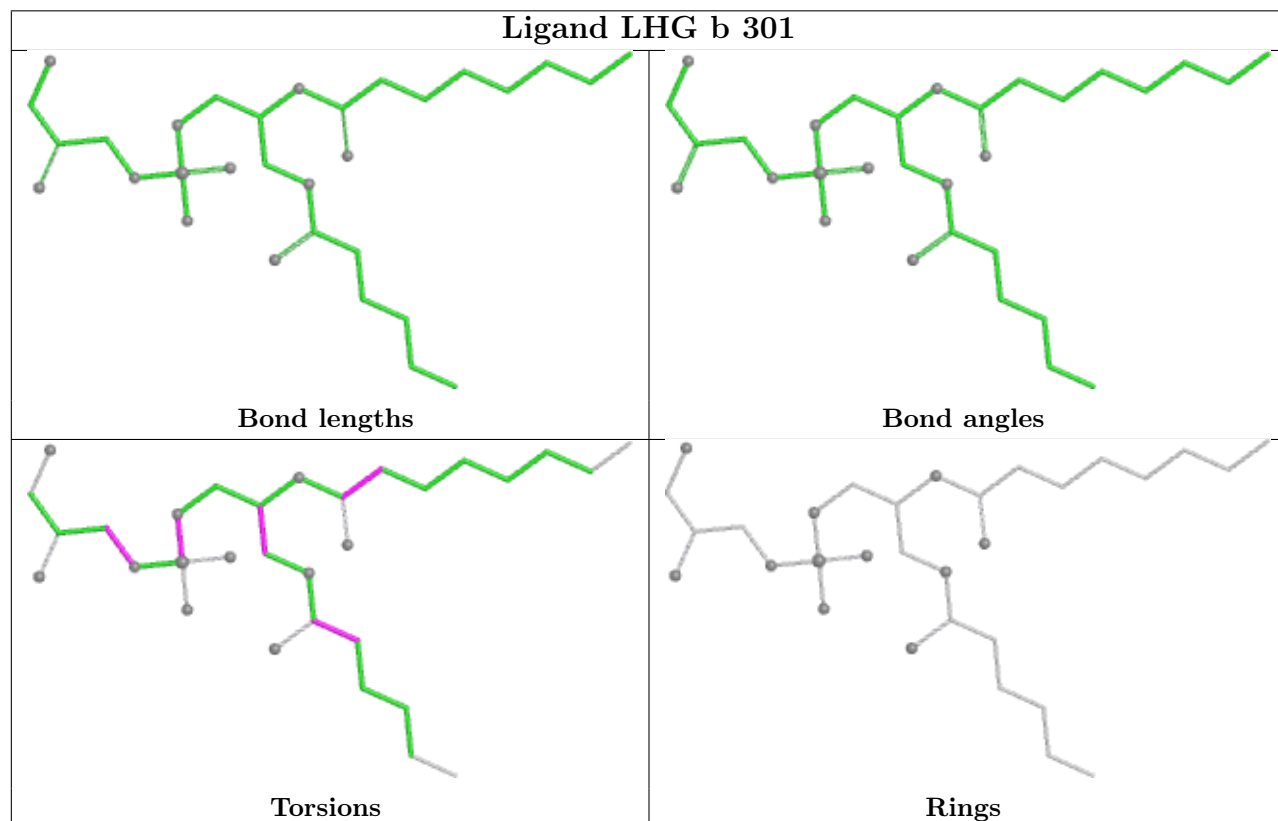
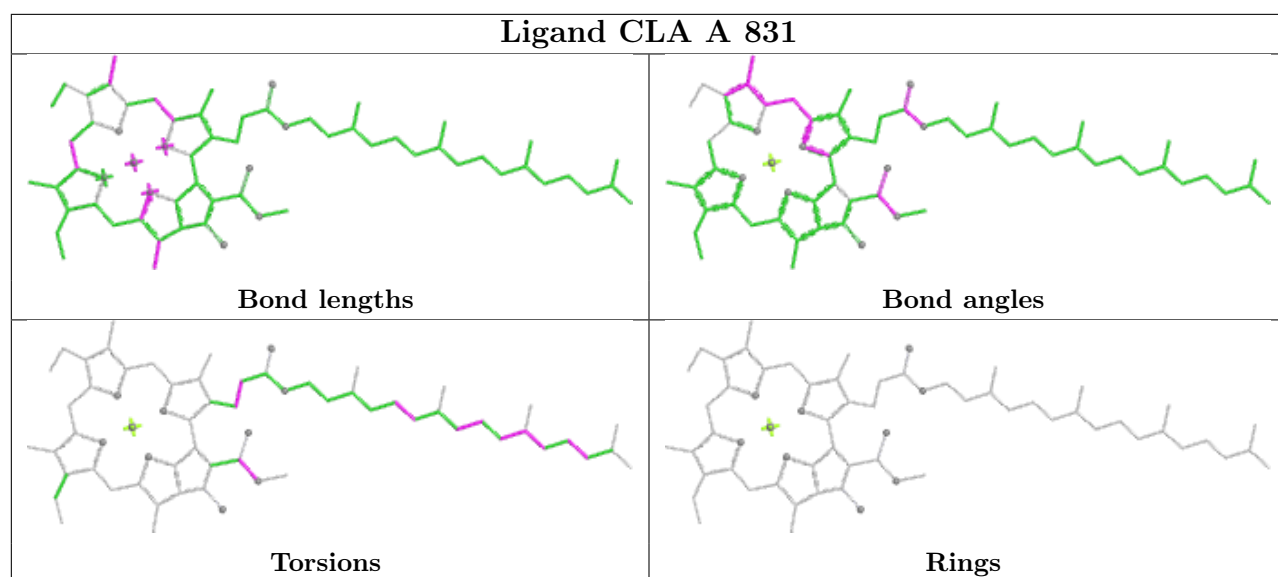


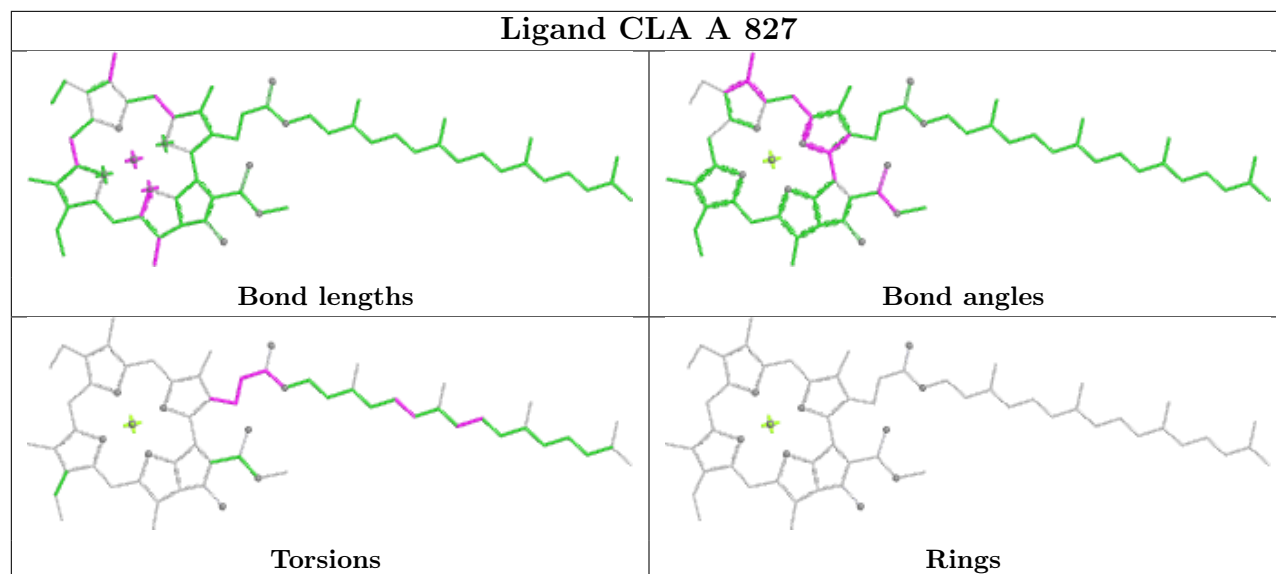
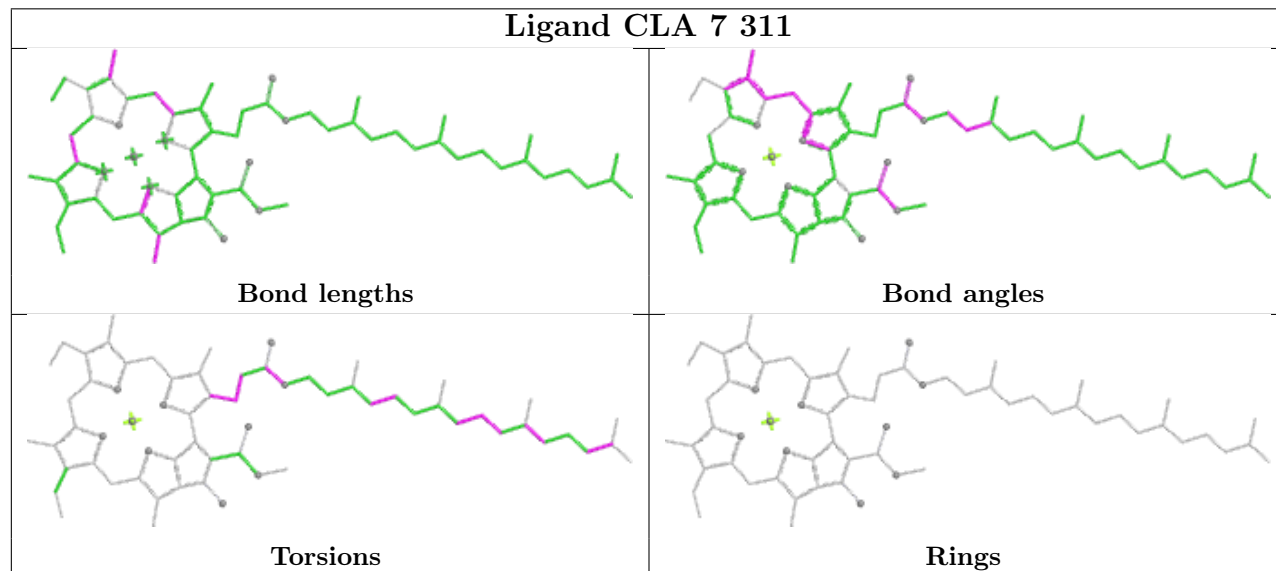
Ligand CLA b 316



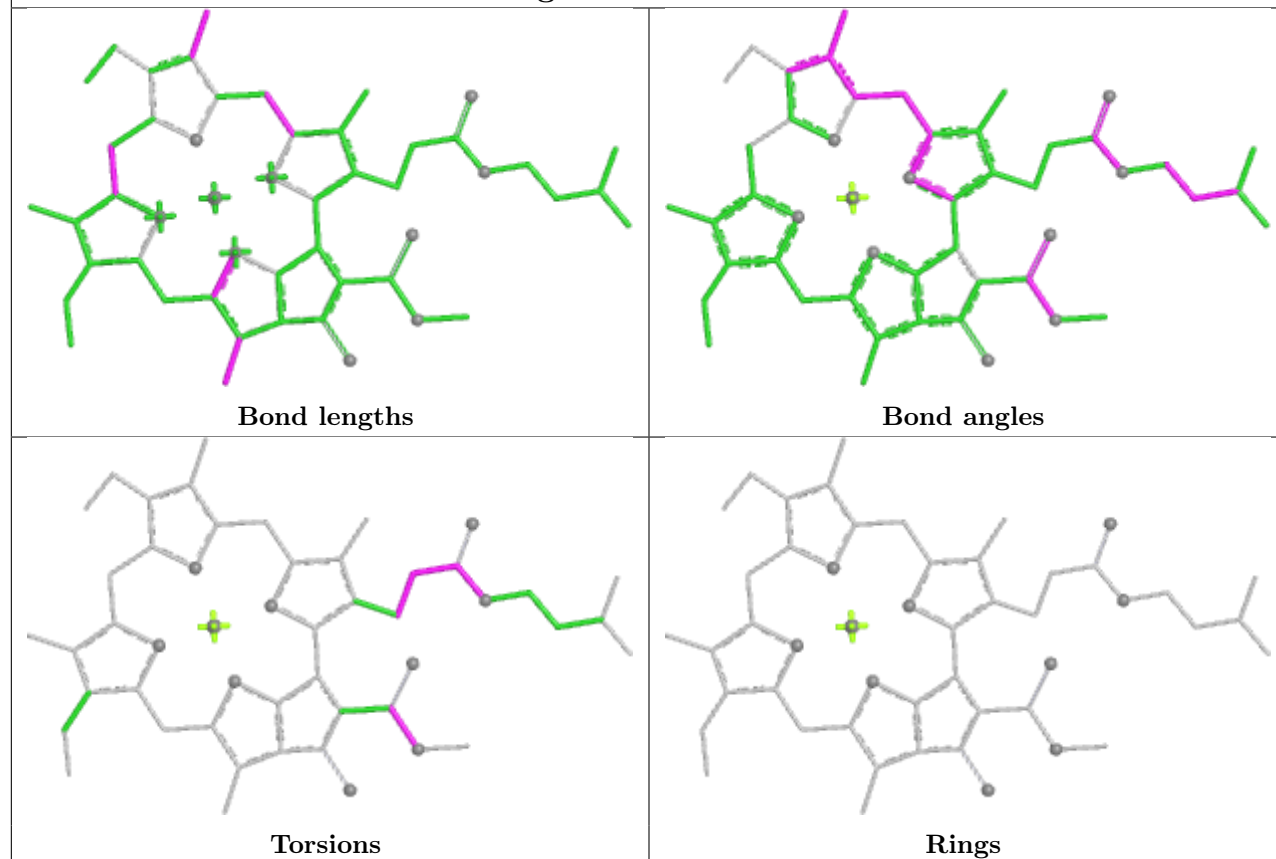
Ligand BCR B 852



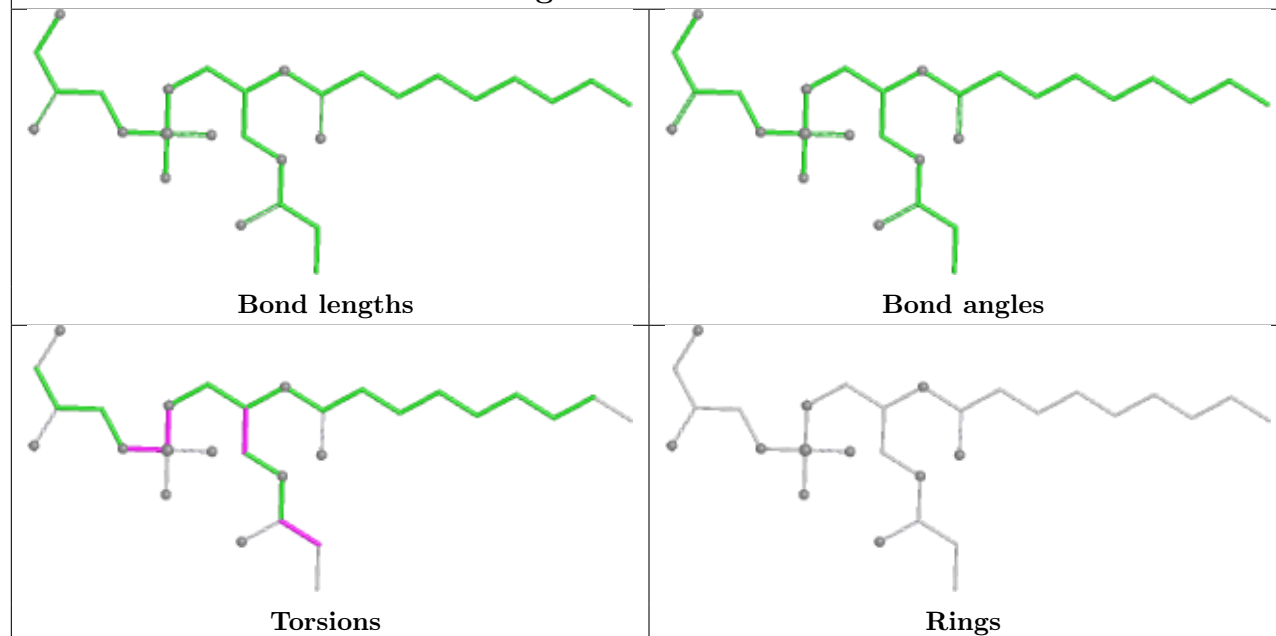


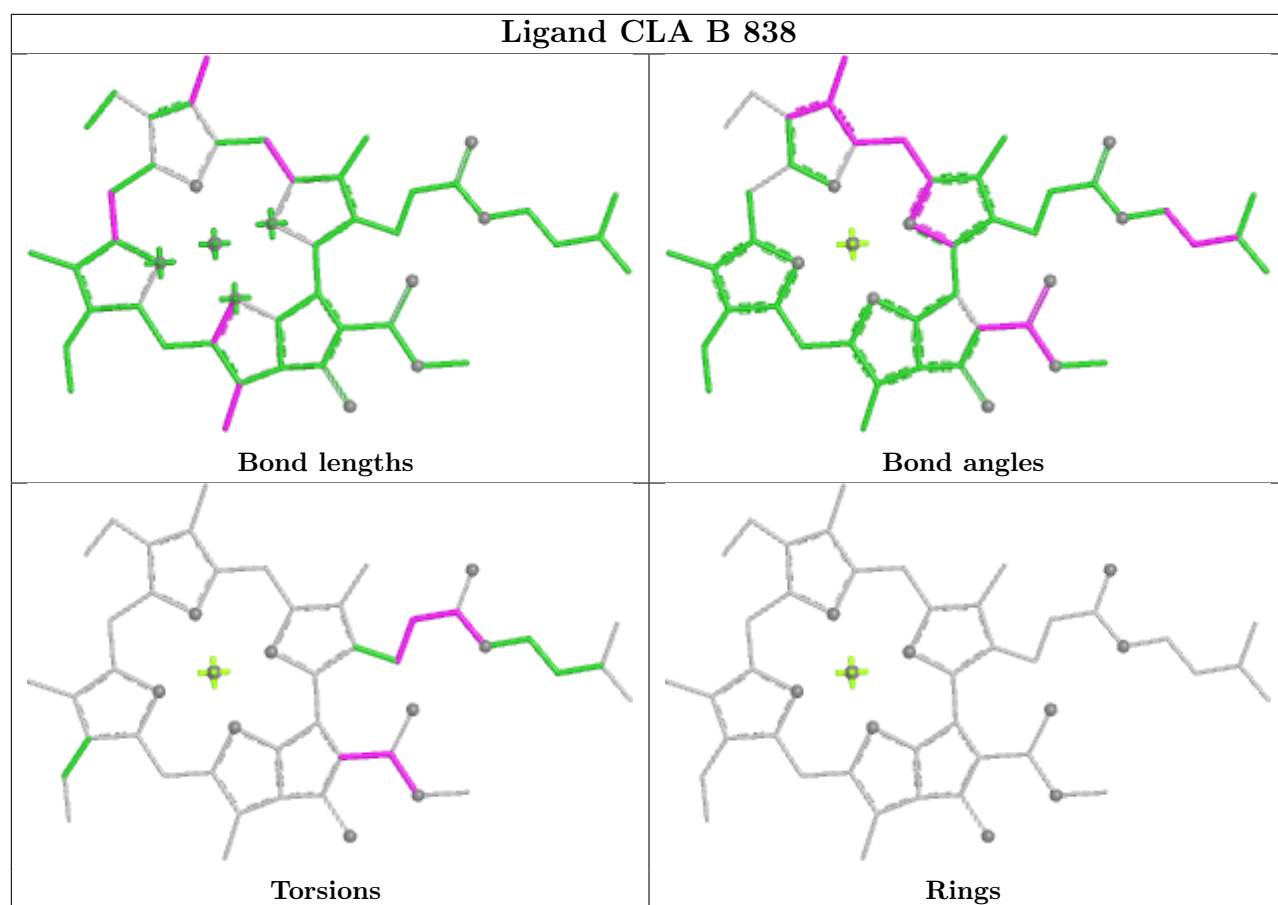
Ligand CLA A 827**Ligand CLA 7 311**

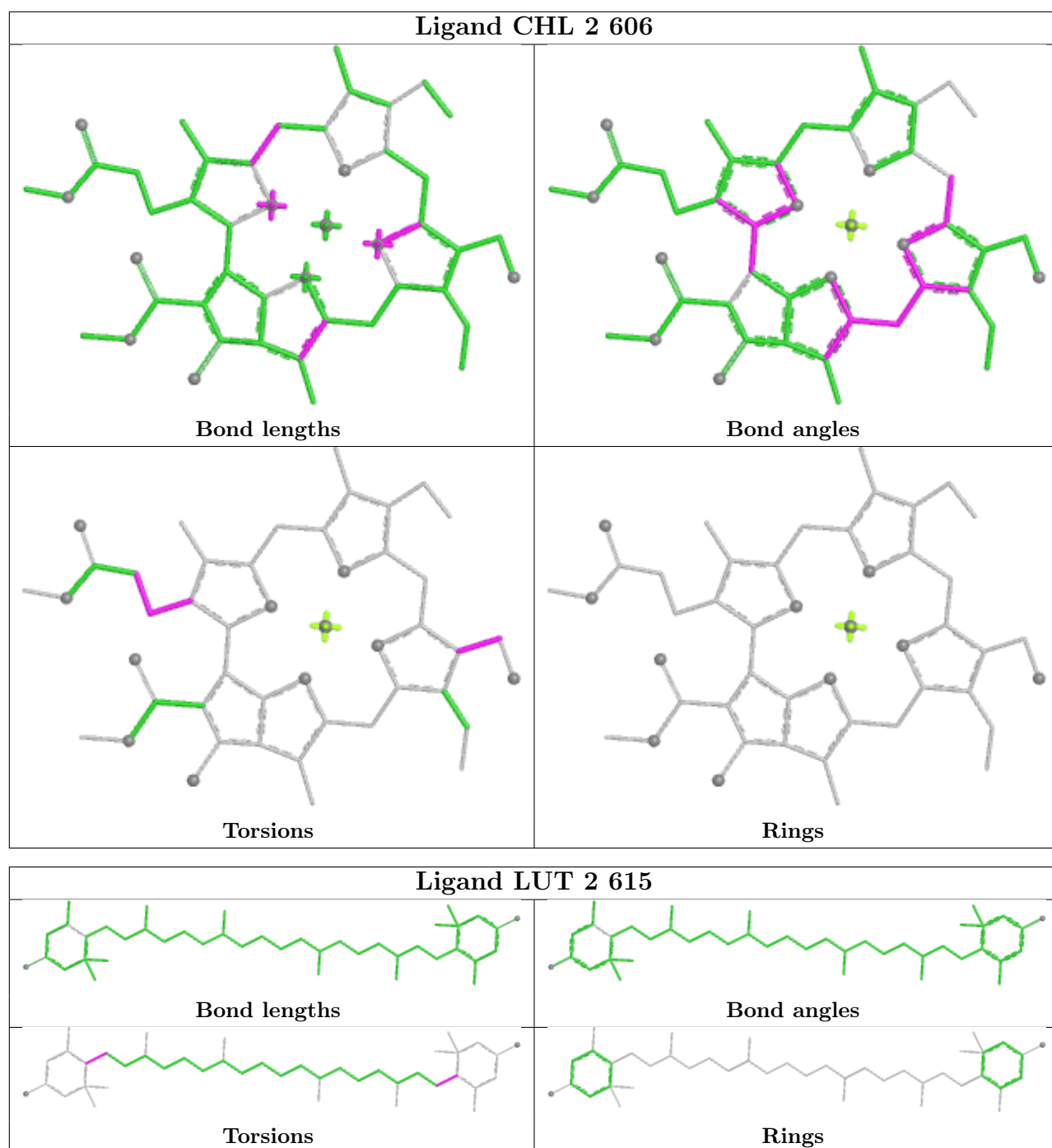
Ligand CLA c 613



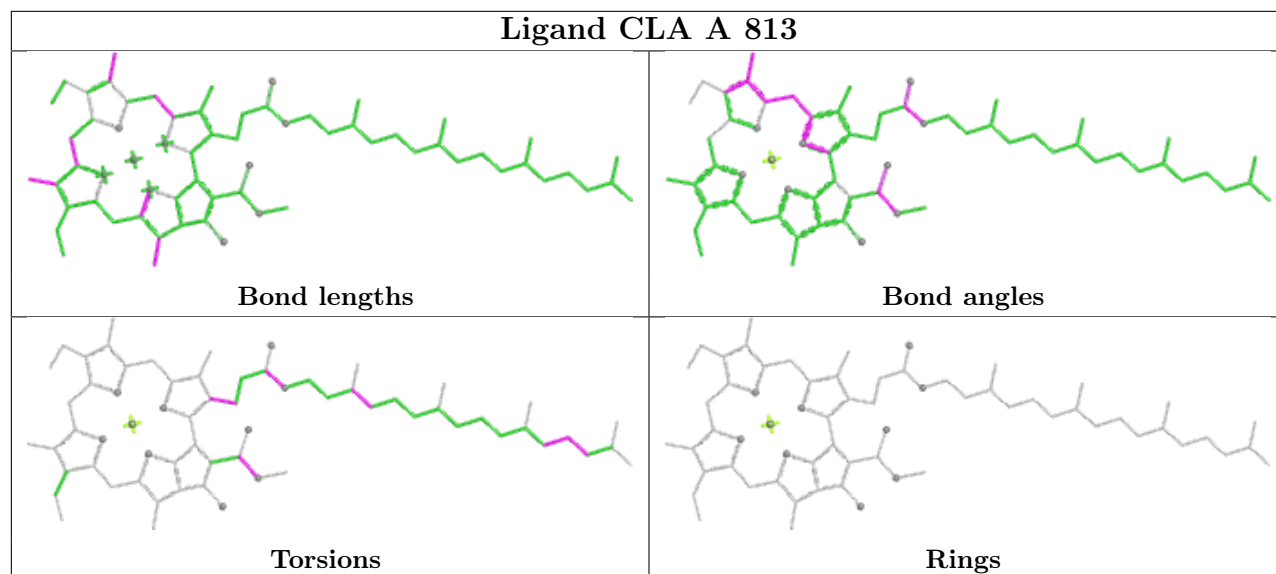
Ligand LHG c 618



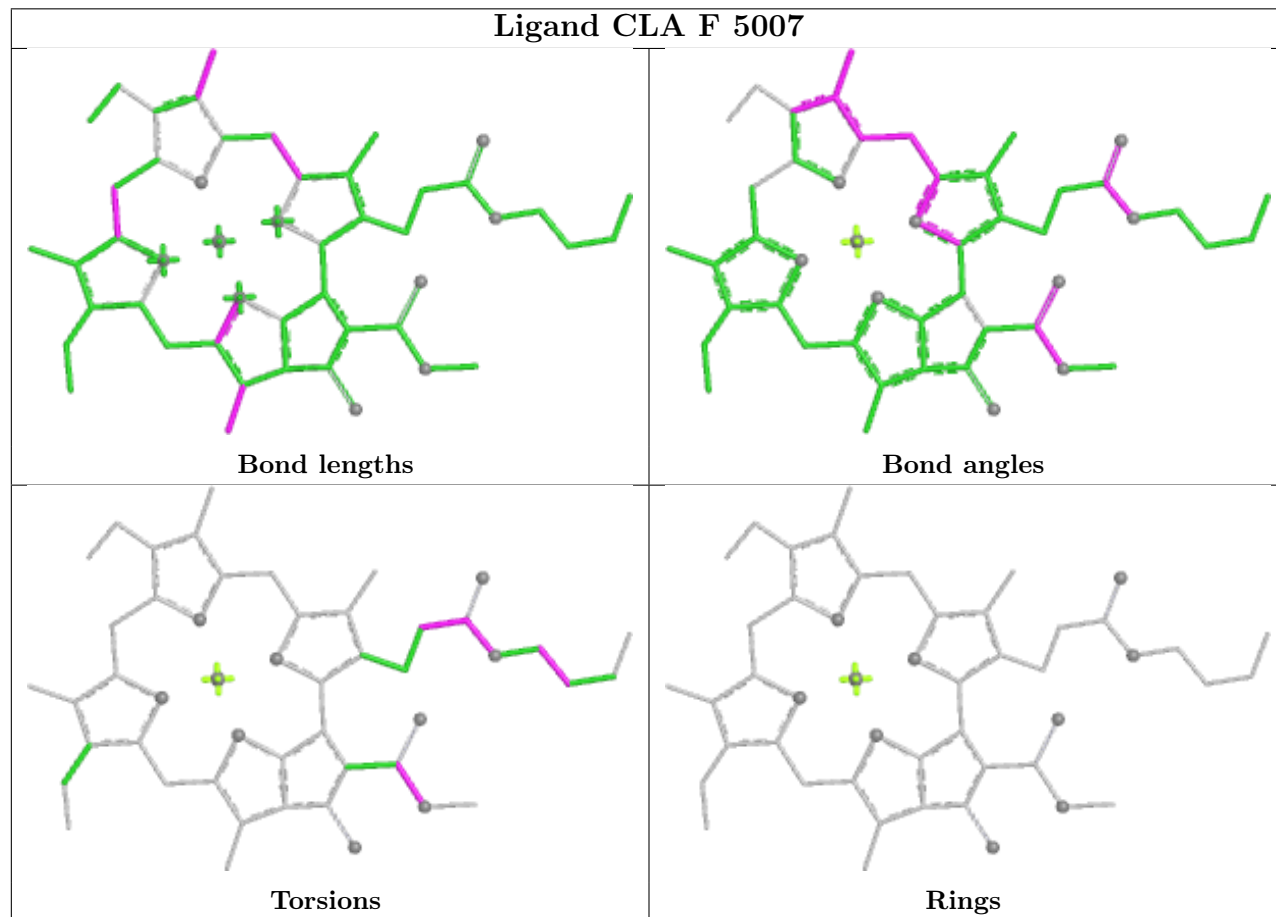


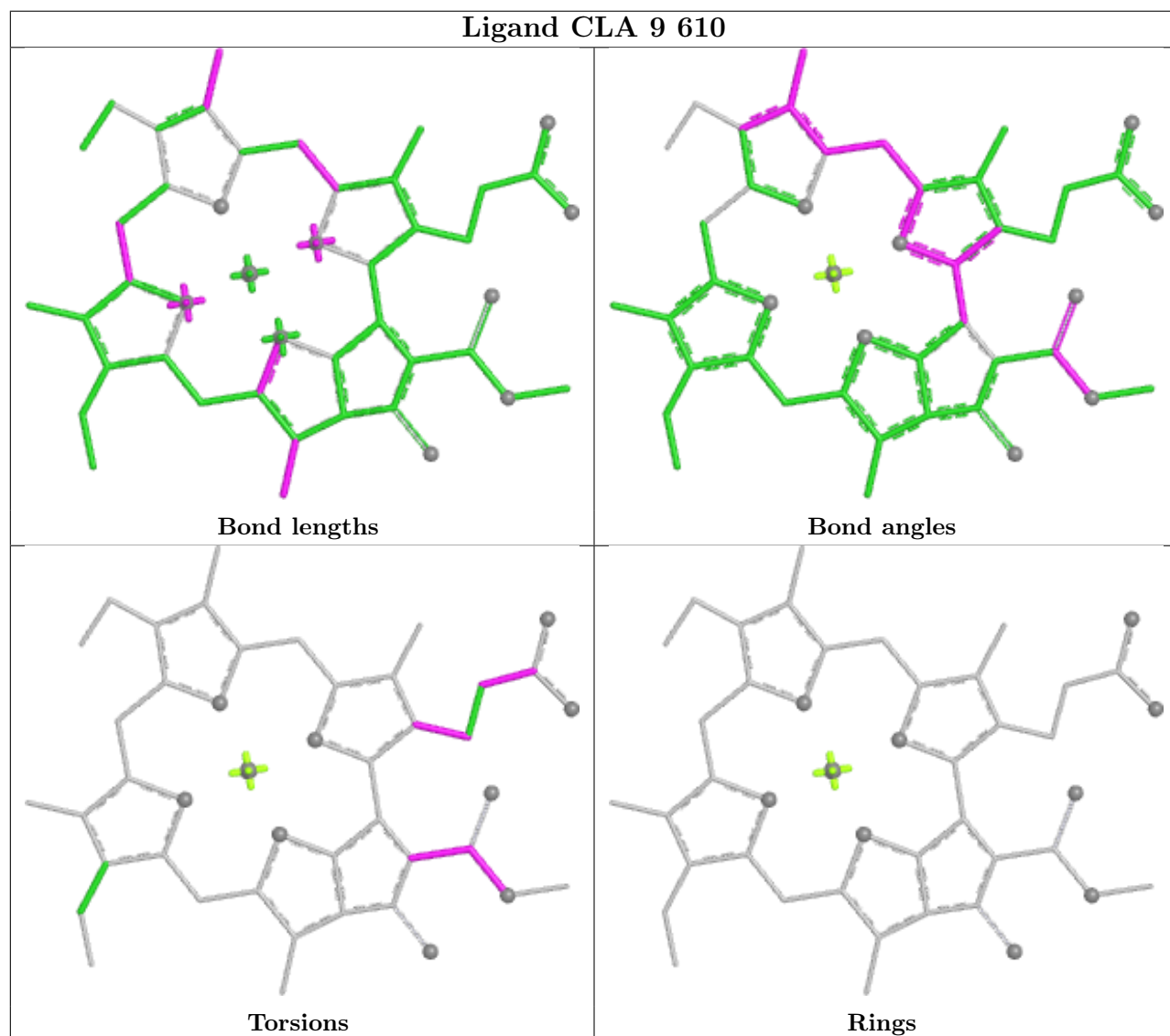
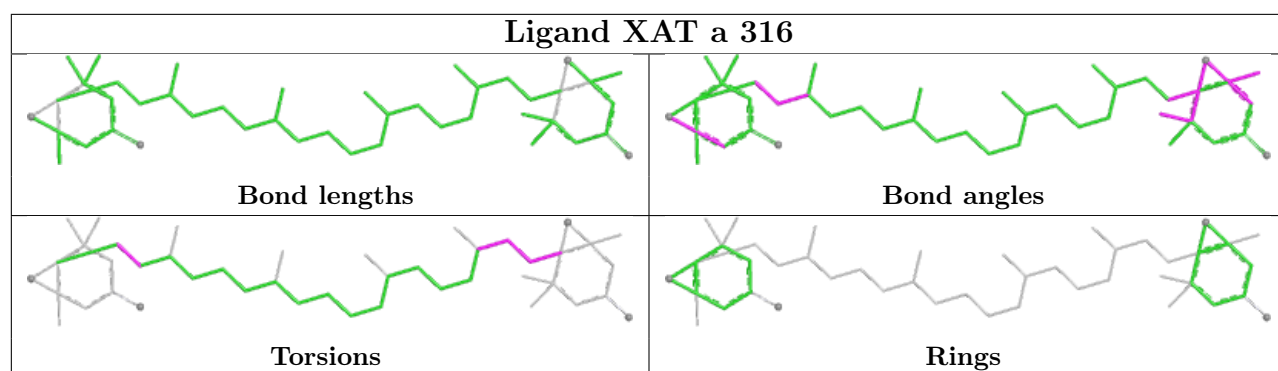


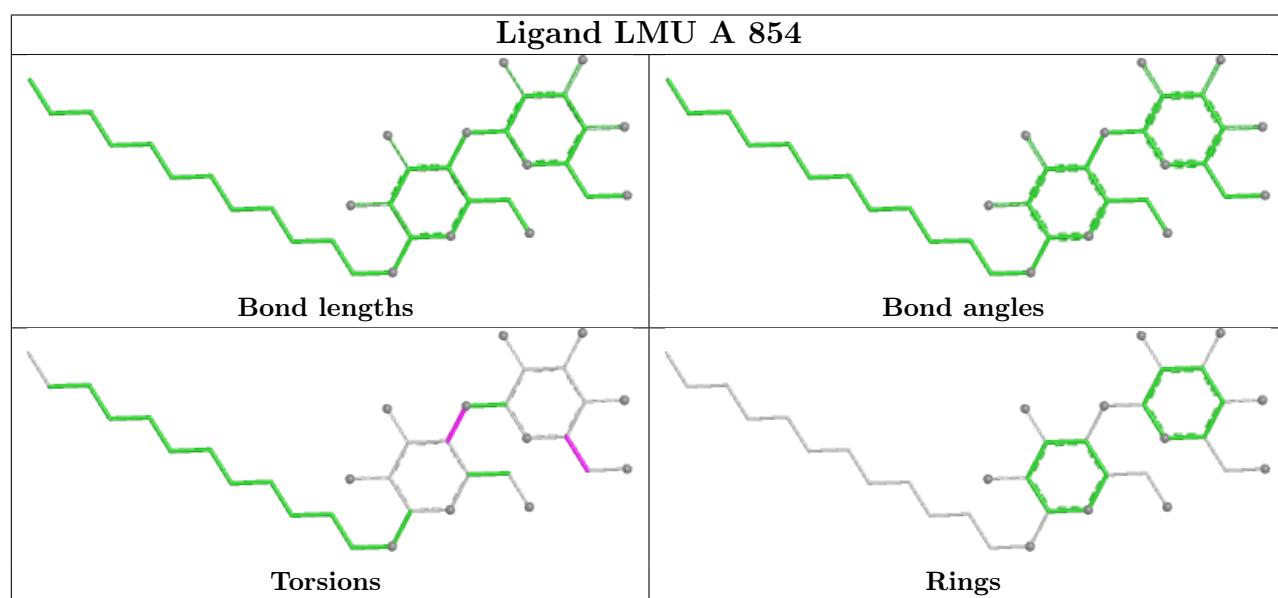
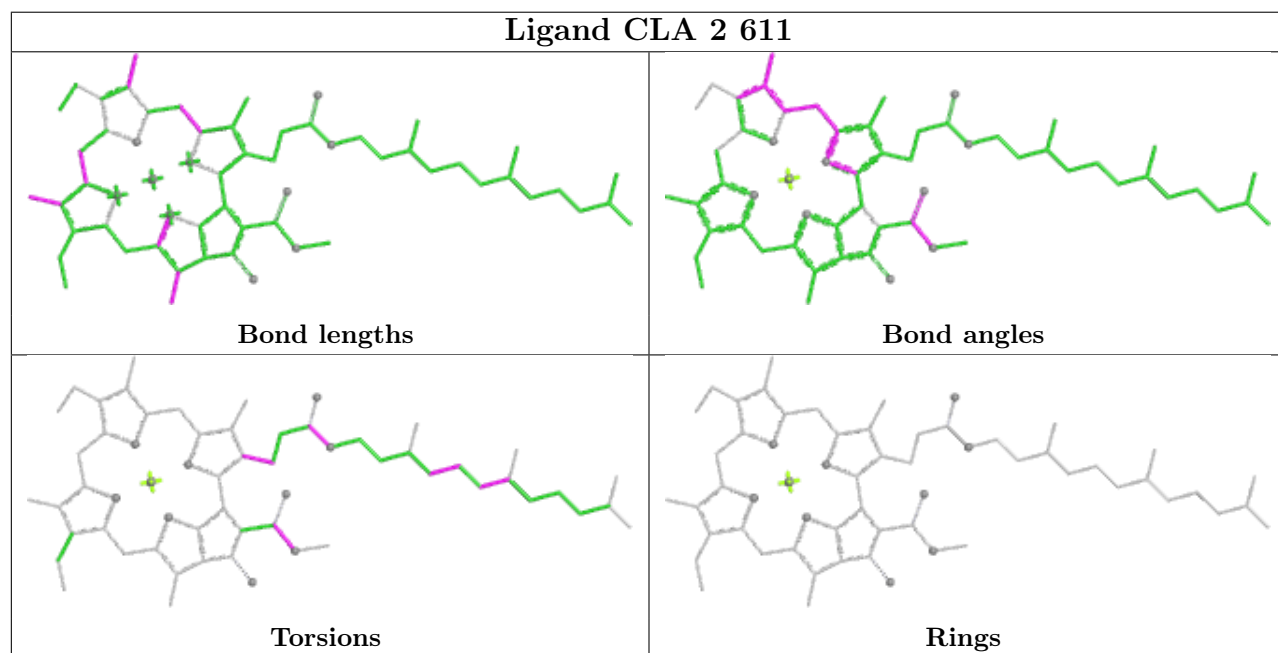
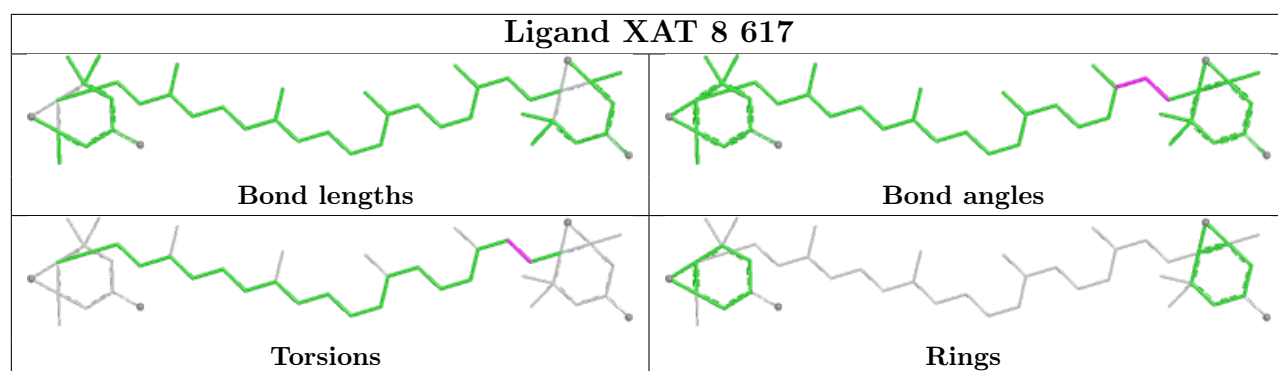
Ligand CLA A 813



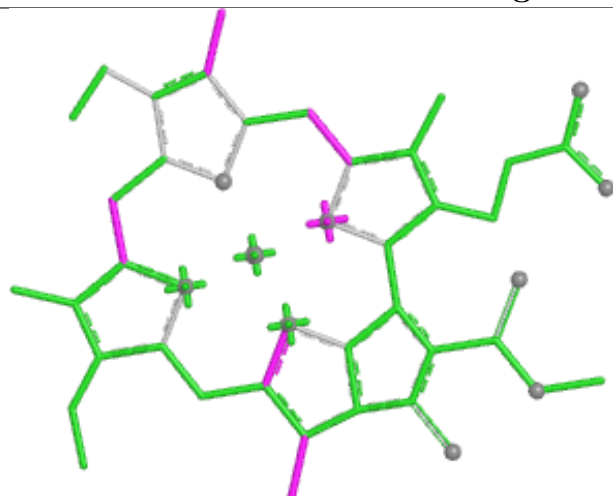
Ligand CLA F 5007



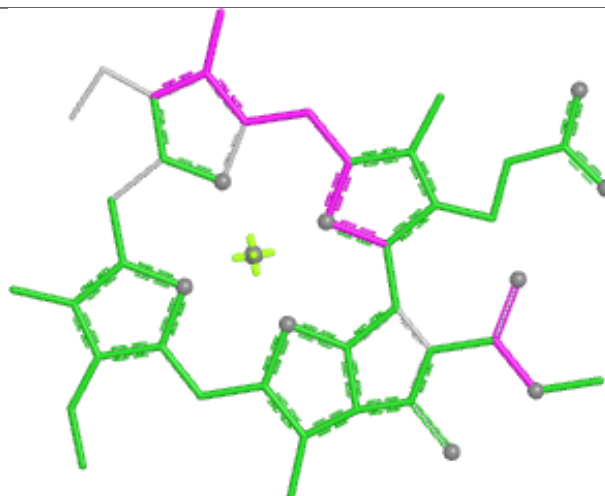




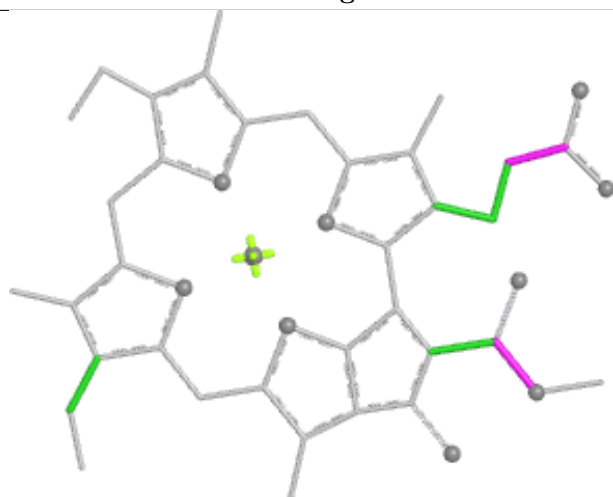
Ligand CLA K 201



Bond lengths



Bond angles

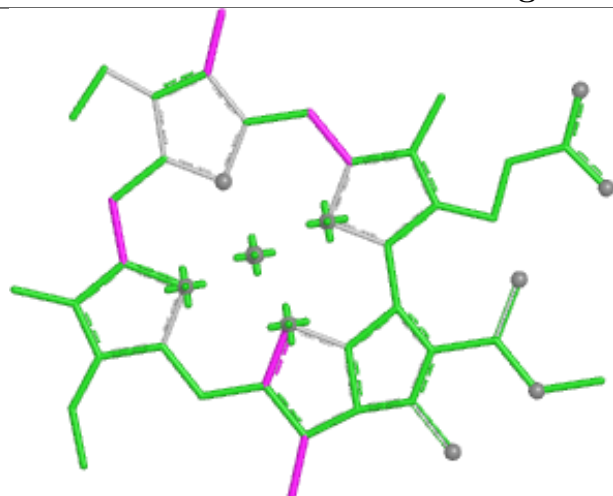


Torsions

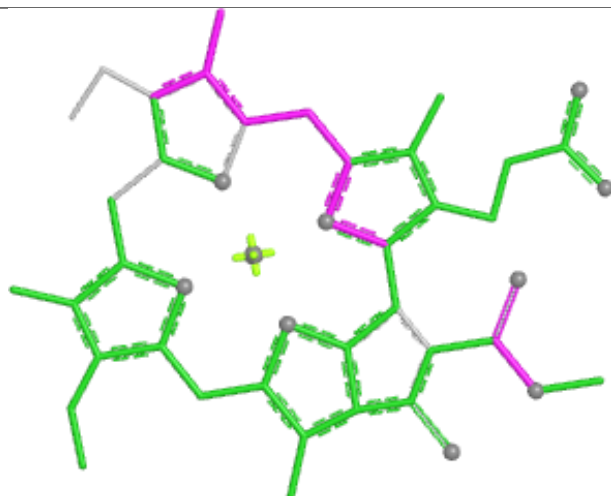


Rings

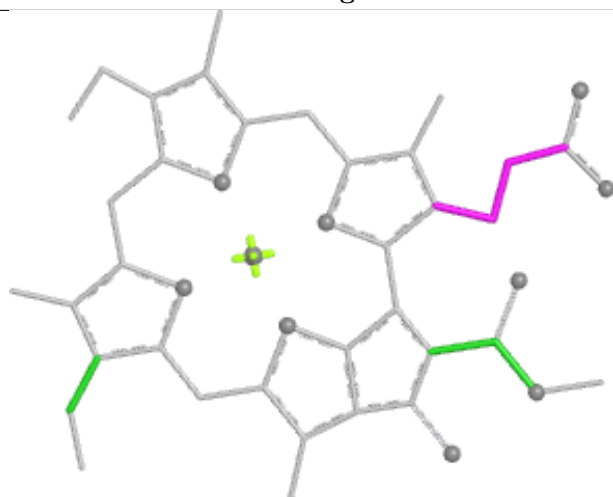
Ligand CLA 8 615



Bond lengths



Bond angles

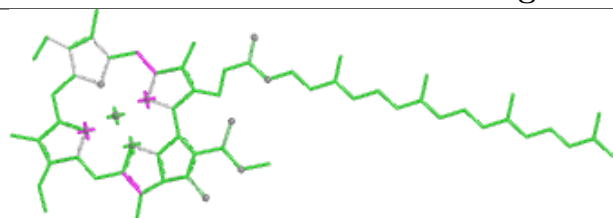


Torsions

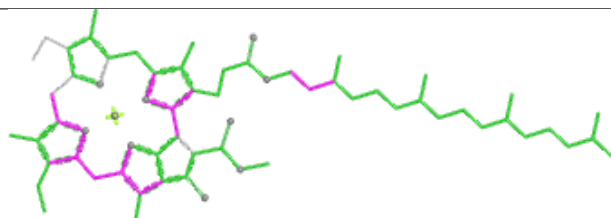


Rings

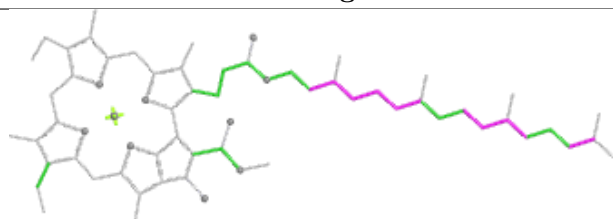
Ligand CL0 A 803



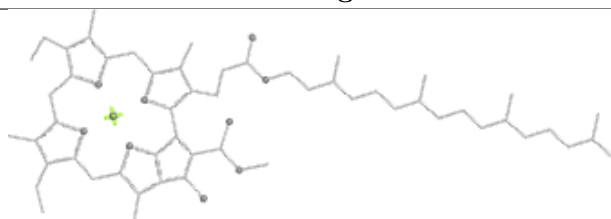
Bond lengths



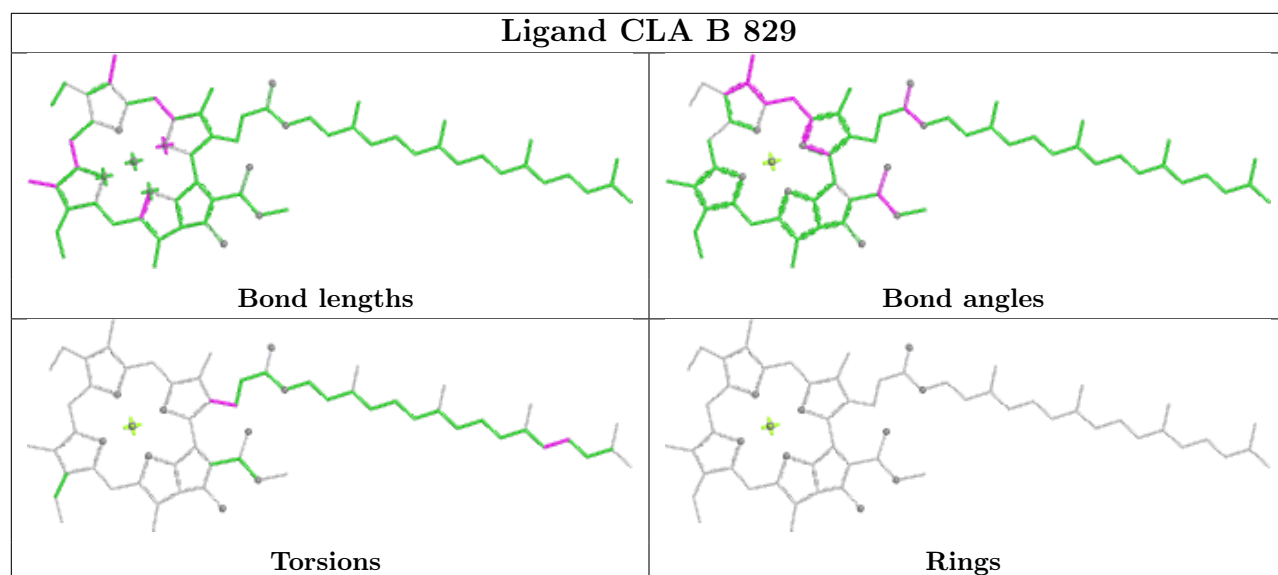
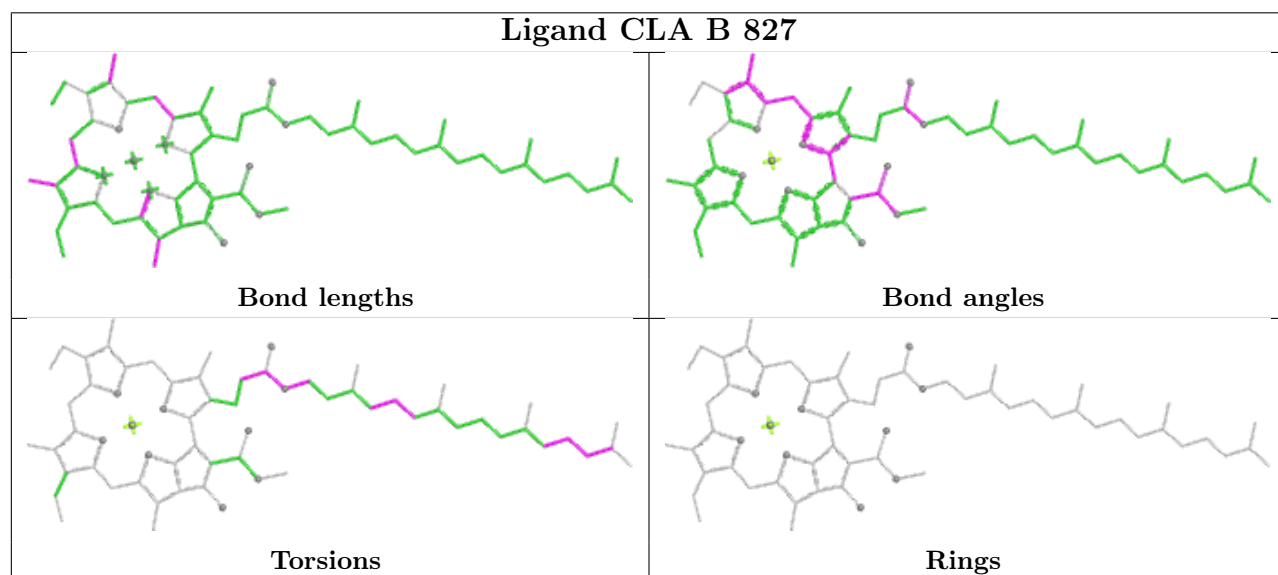
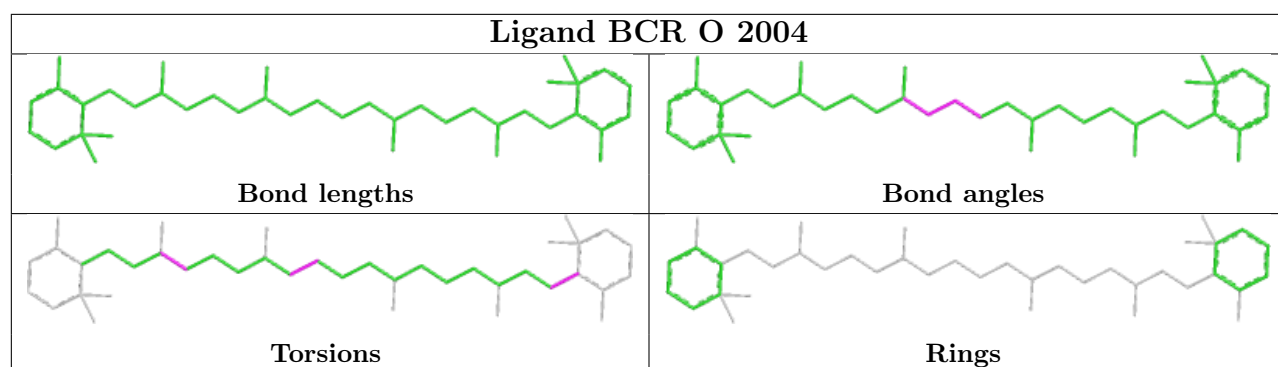
Bond angles

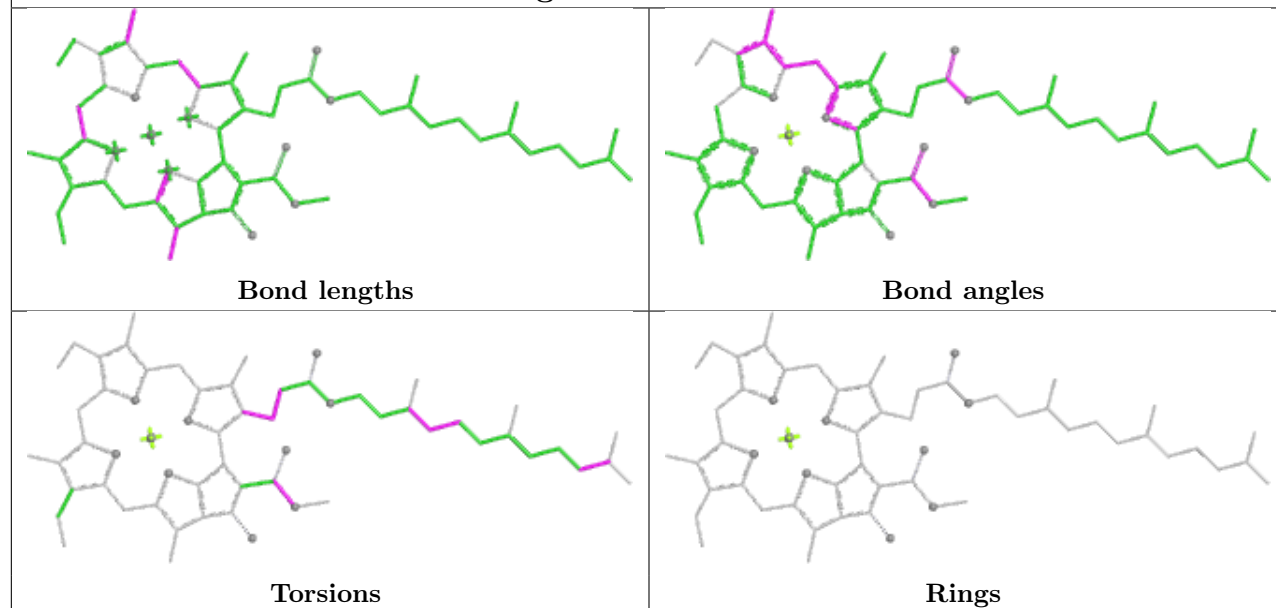
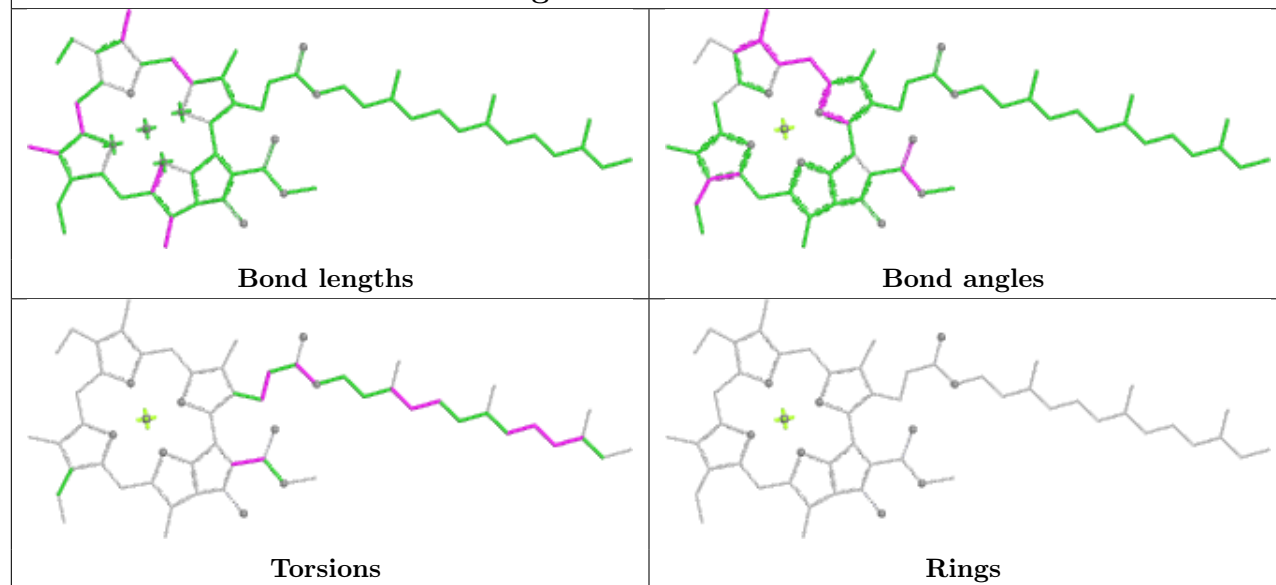


Torsions

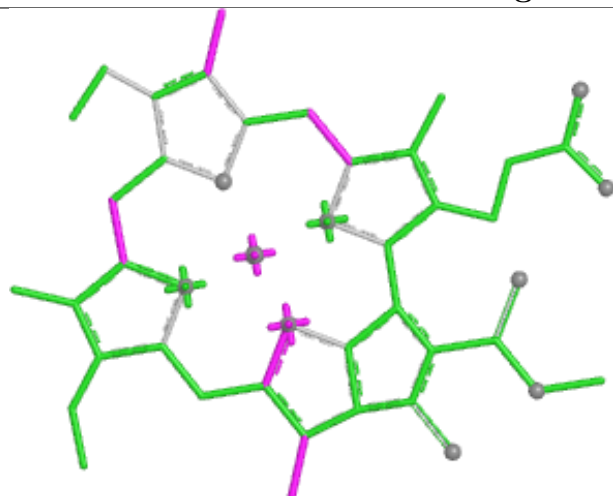


Rings

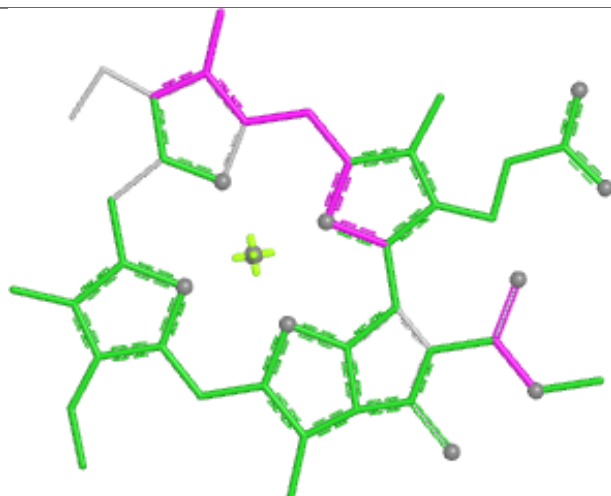


Ligand CLA 9 608**Ligand CLA A 820**

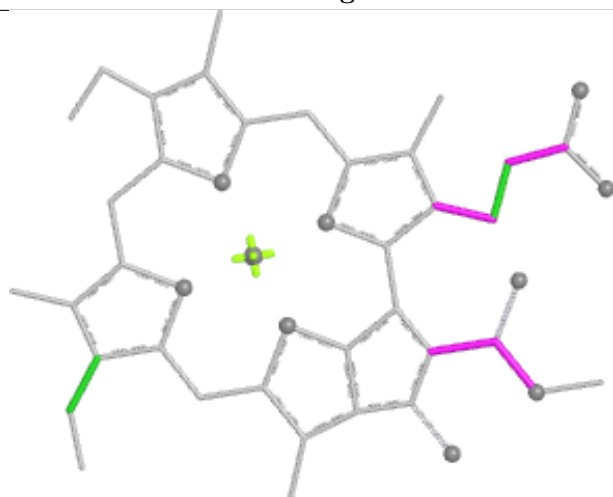
Ligand CLA T 608



Bond lengths



Bond angles

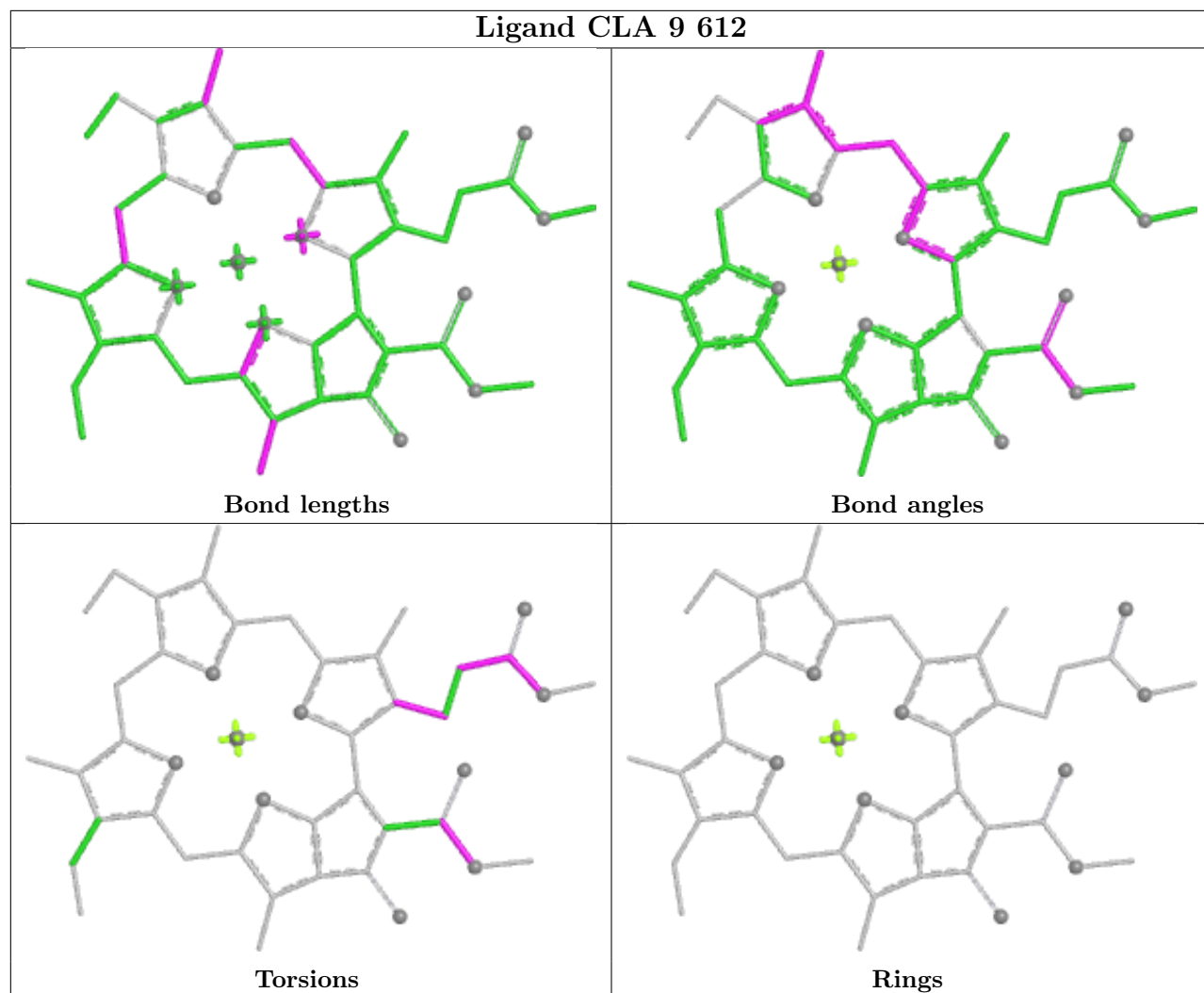


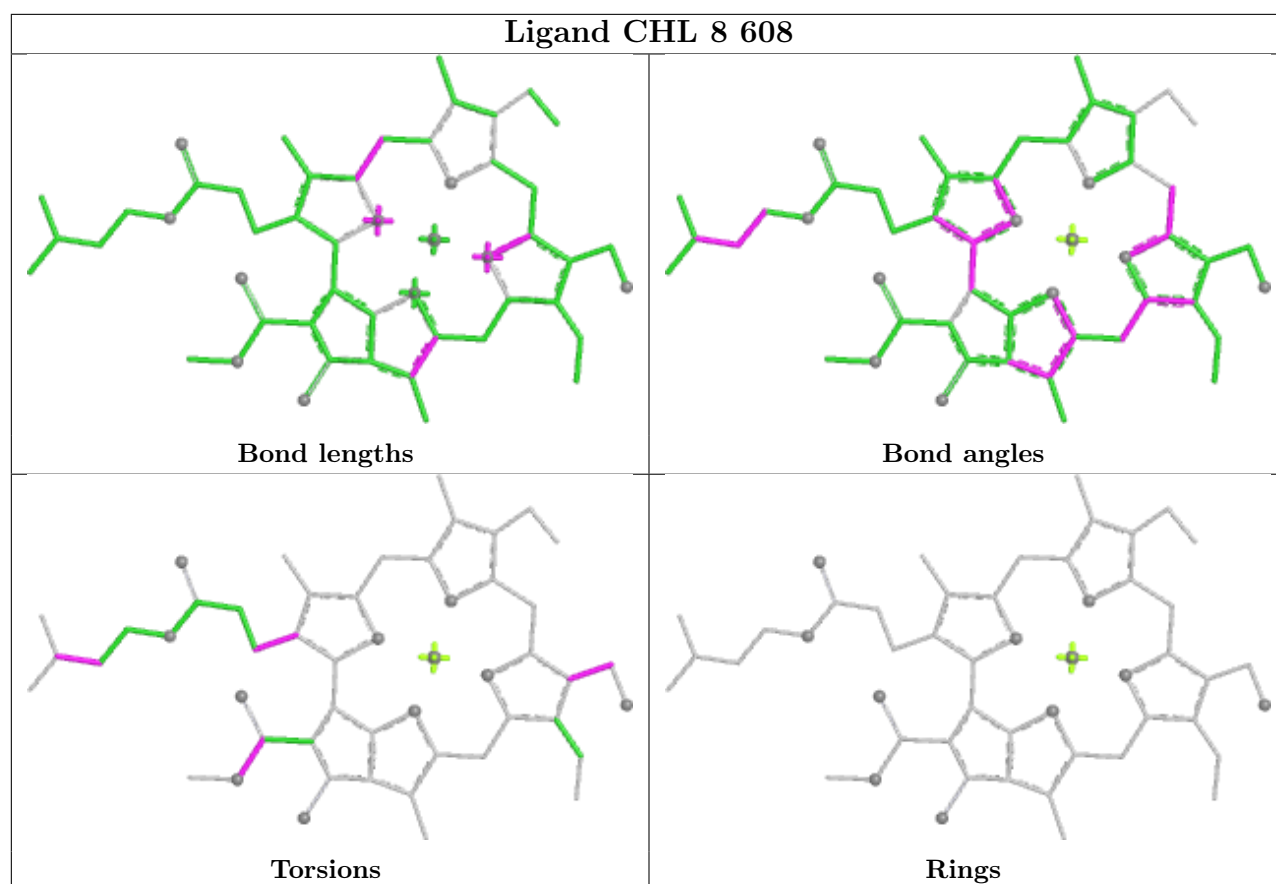
Torsions



Rings

Ligand CLA 9 612





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.

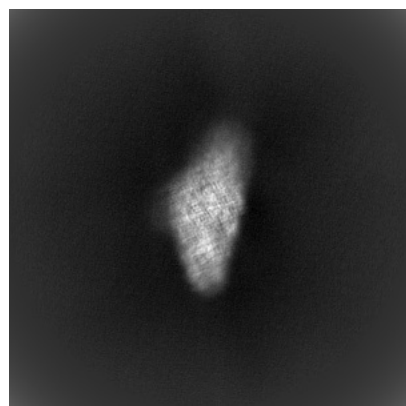
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48262. These allow visual inspection of the internal detail of the map and identification of artifacts.

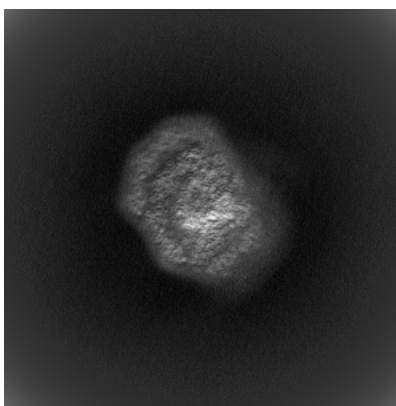
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

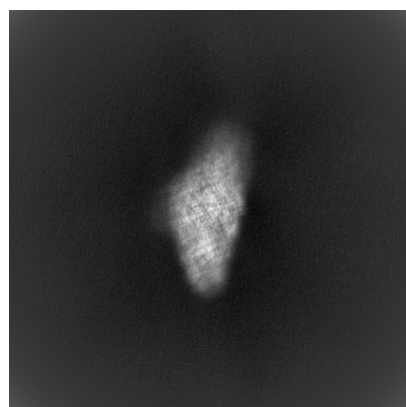


Y

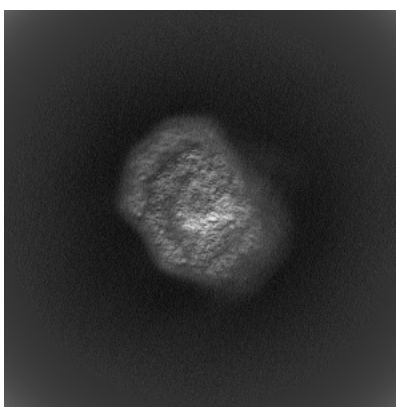


Z

6.1.2 Raw map



X



Y

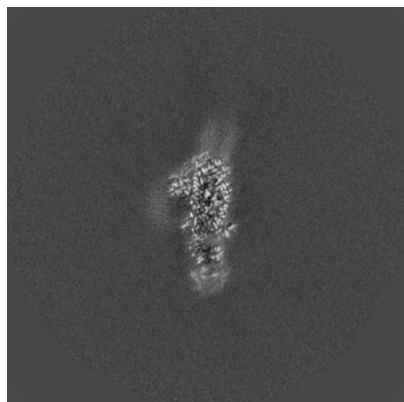


Z

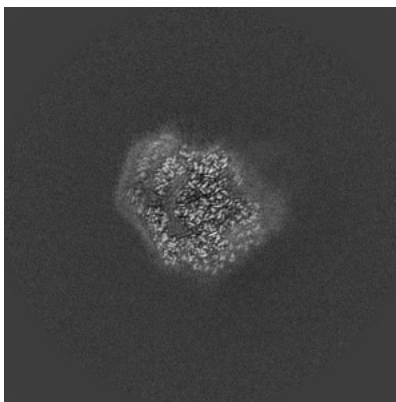
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

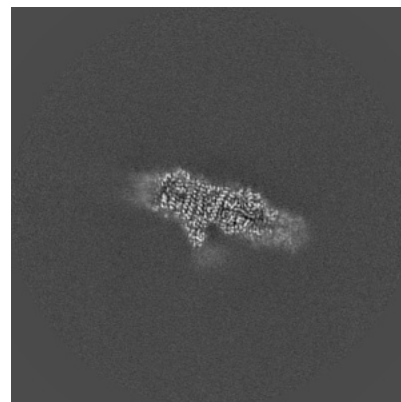
6.2.1 Primary map



X Index: 240

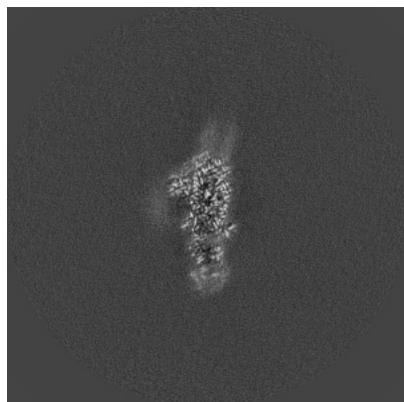


Y Index: 240

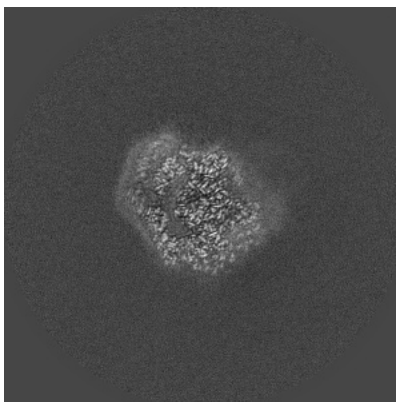


Z Index: 240

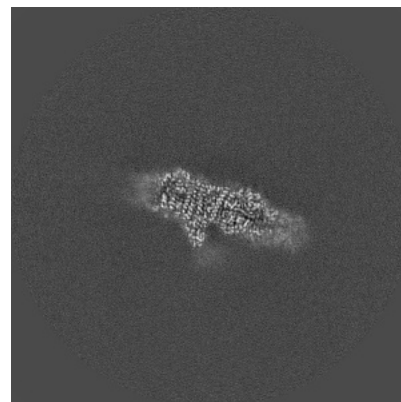
6.2.2 Raw map



X Index: 240



Y Index: 240

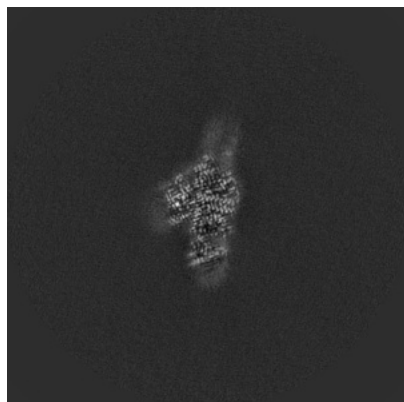


Z Index: 240

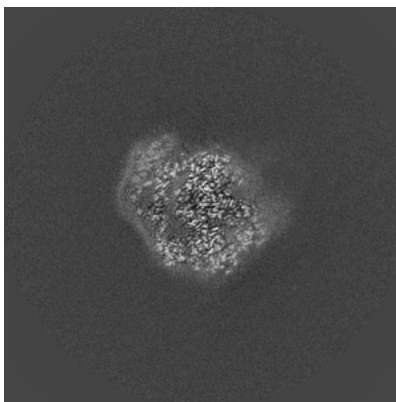
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

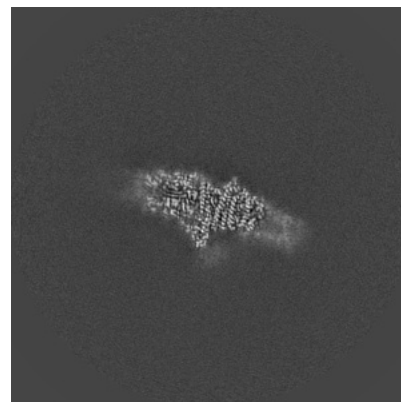
6.3.1 Primary map



X Index: 228

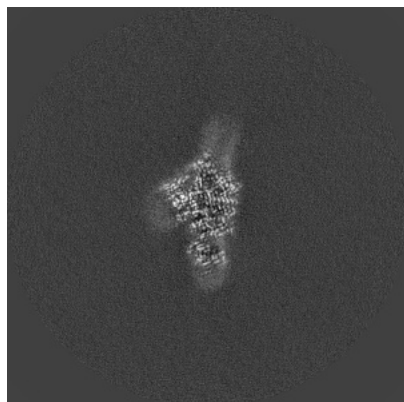


Y Index: 243

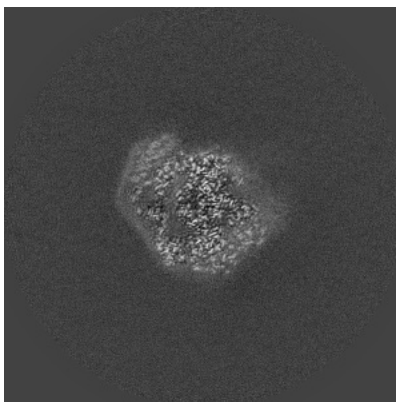


Z Index: 249

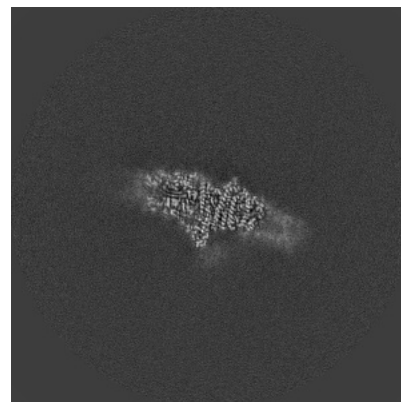
6.3.2 Raw map



X Index: 231



Y Index: 242



Z Index: 249

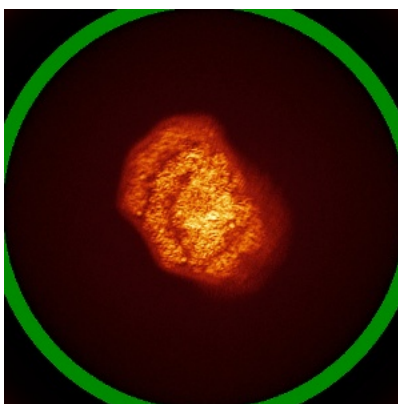
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

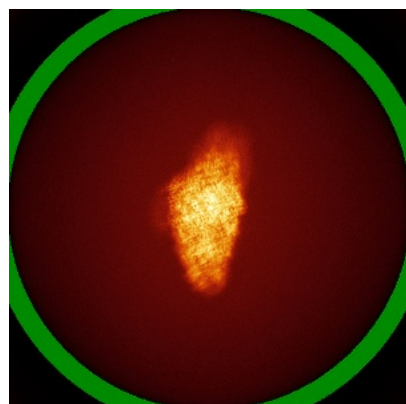


Y

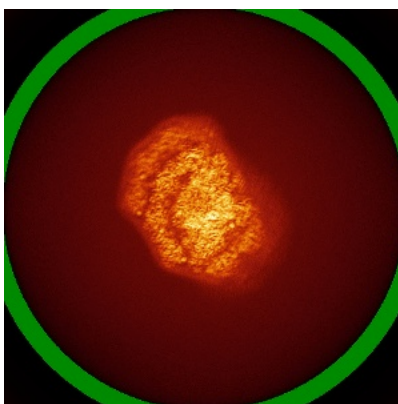


Z

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 0.0128. 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.

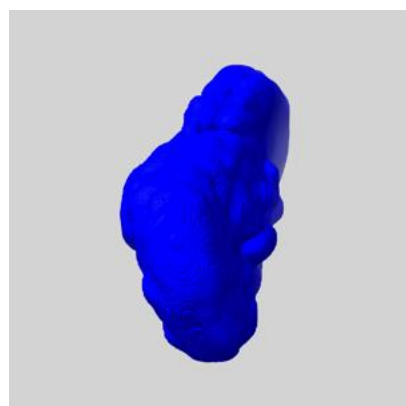
6.6 Mask visualisation [i](#)

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

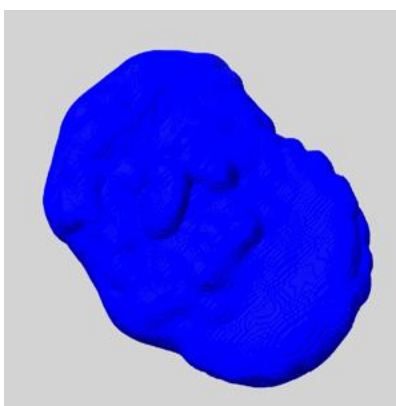
A mask typically either:

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

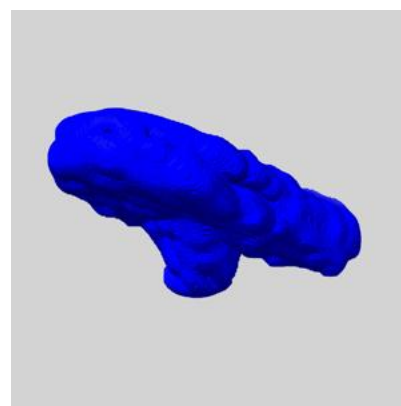
6.6.1 emd_48262_msk_1.map [i](#)



X



Y

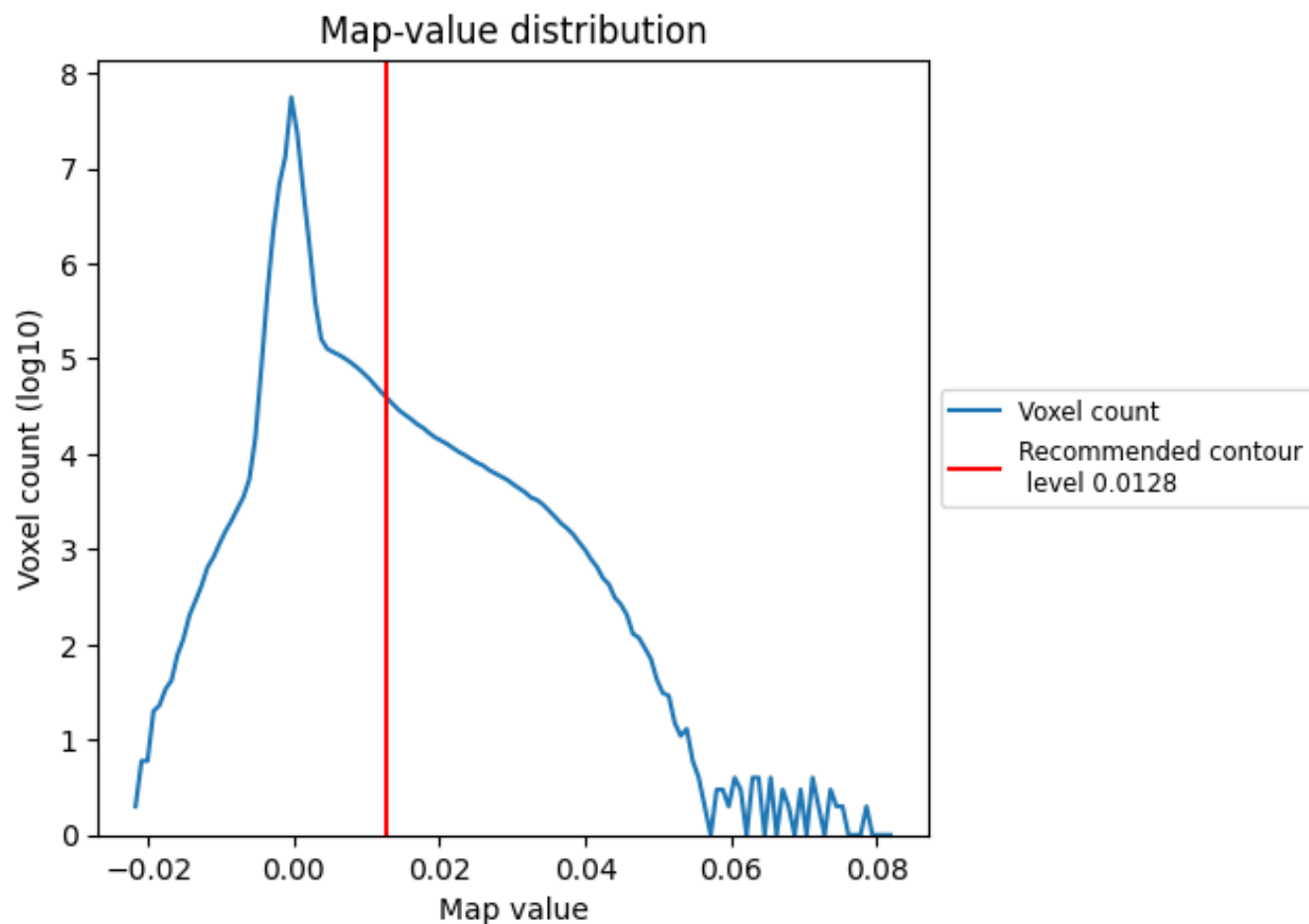


Z

7 Map analysis [i](#)

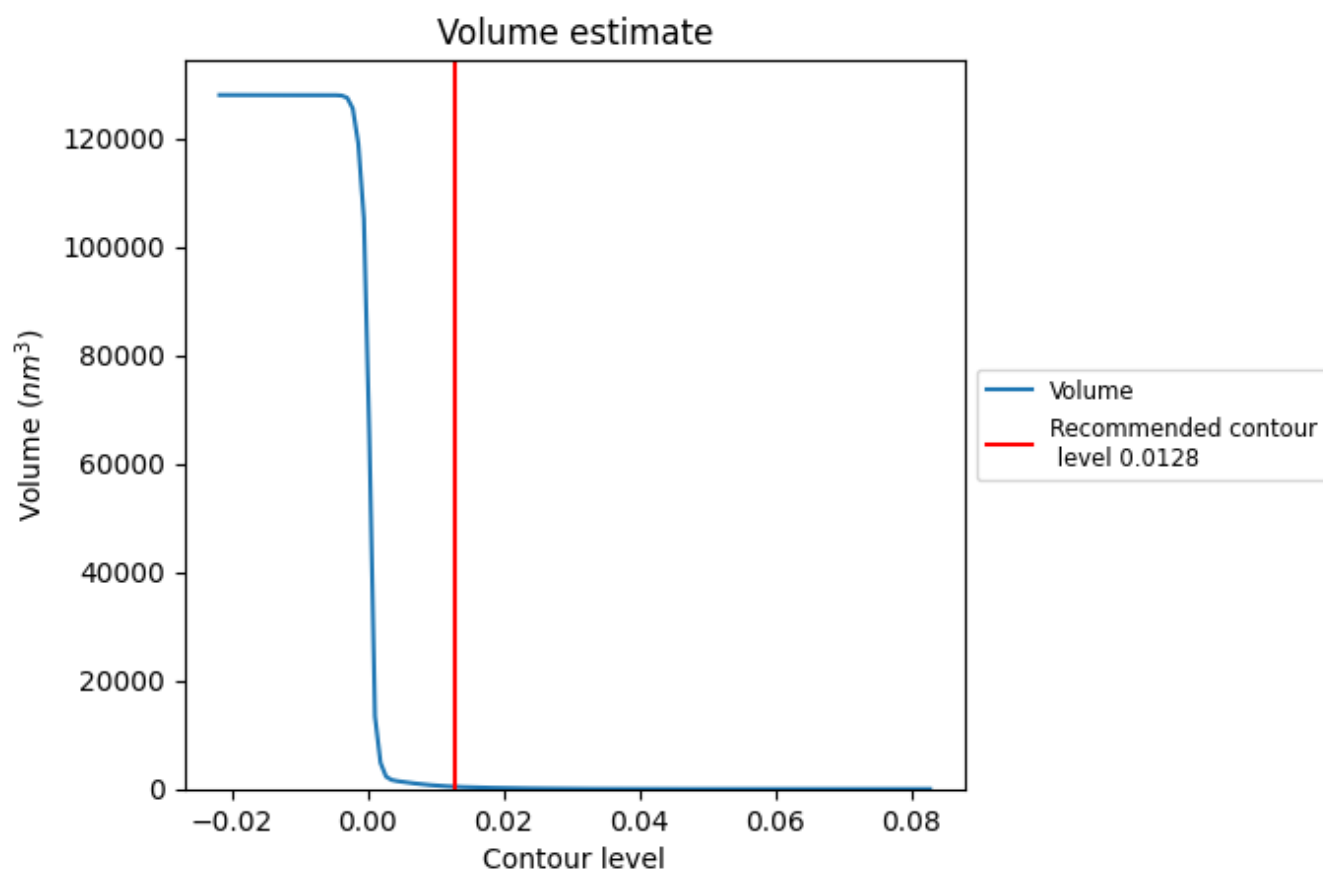
This section contains the results of statistical analysis of the map.

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.

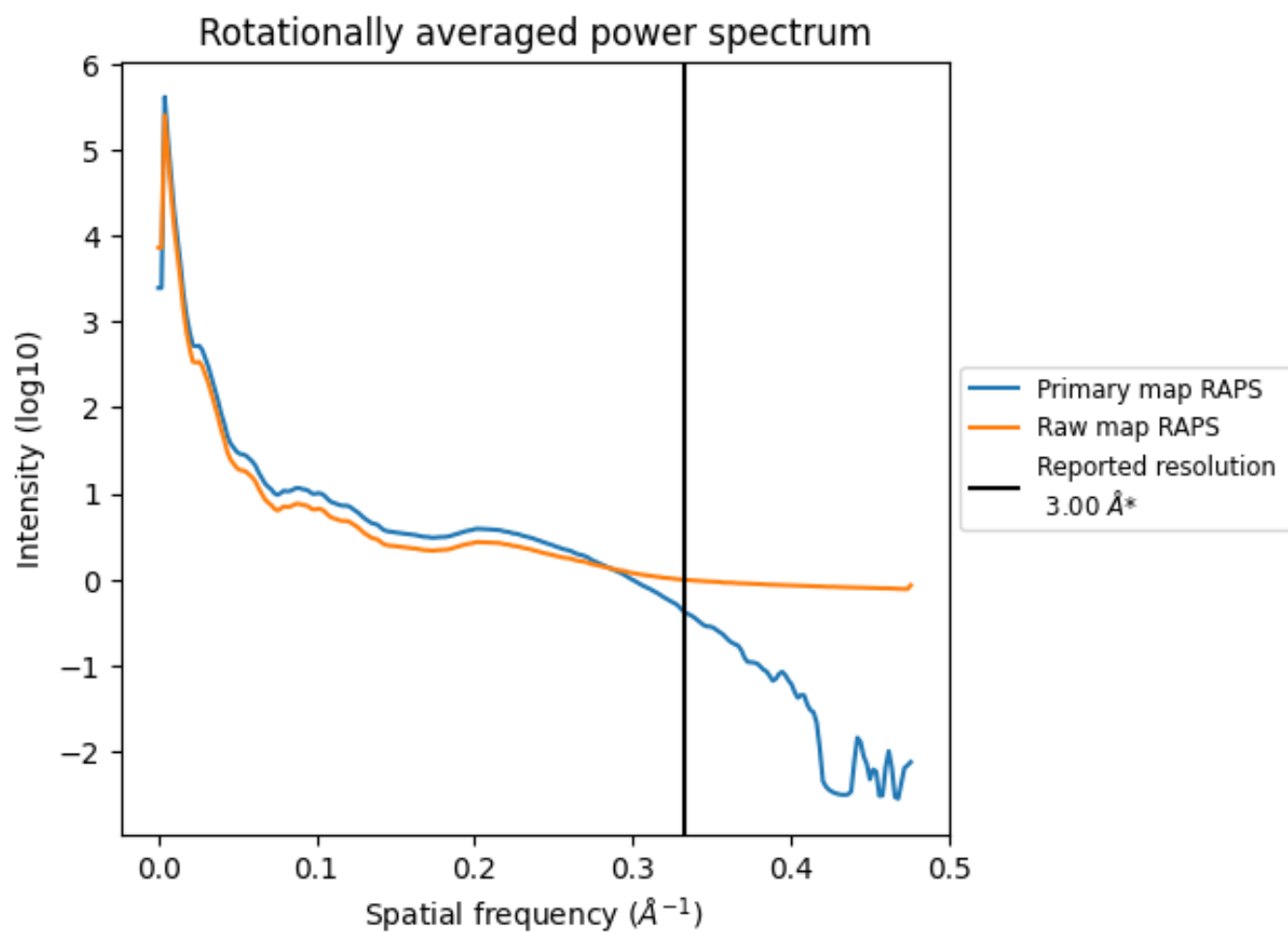
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 425 nm^3 ; this corresponds to an approximate mass of 384 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 ⓘ

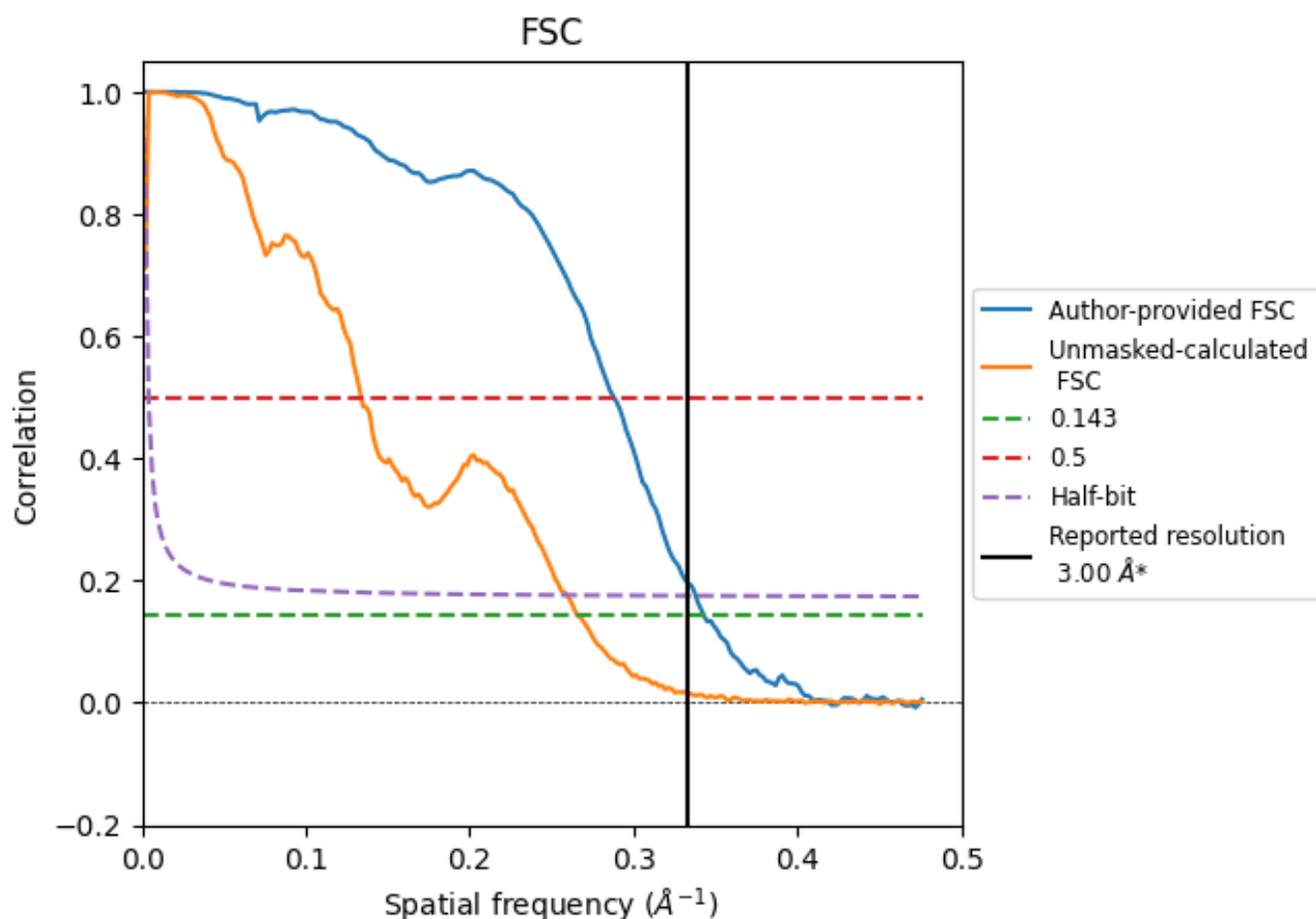


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

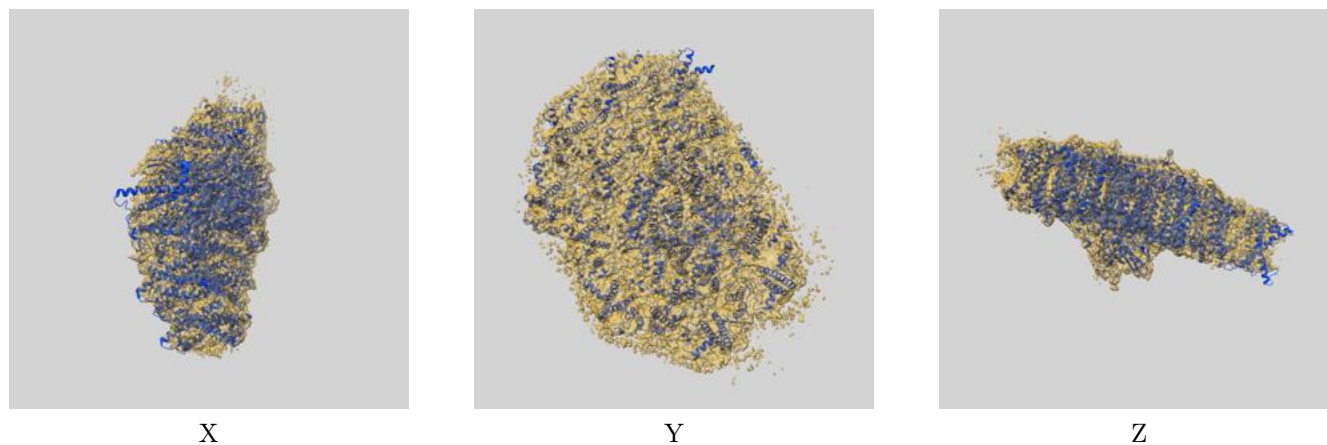
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.92	3.47	2.96
Unmasked-calculated*	3.76	7.47	416.67

*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 3.76 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

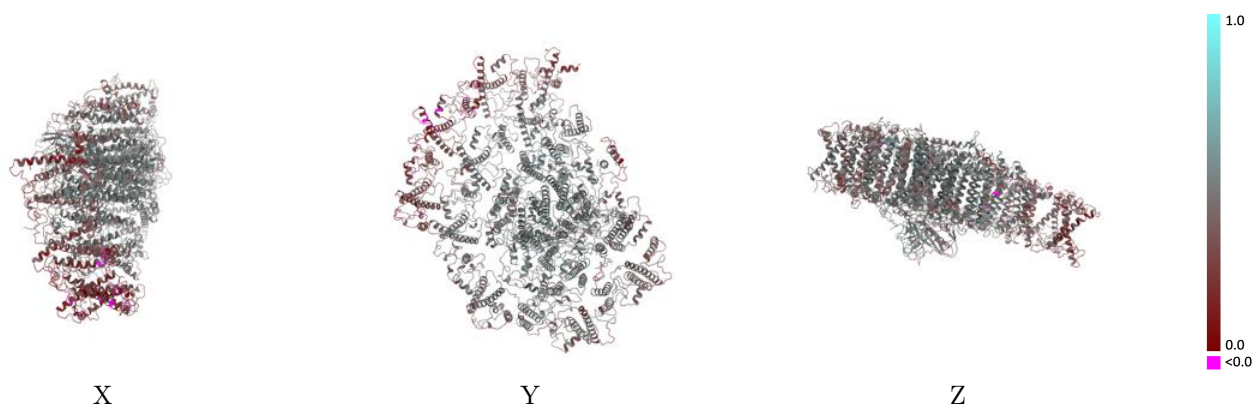
This section contains information regarding the fit between EMDB map EMD-48262 and PDB model 9MGW. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

9.1 Map-model overlay [i](#)



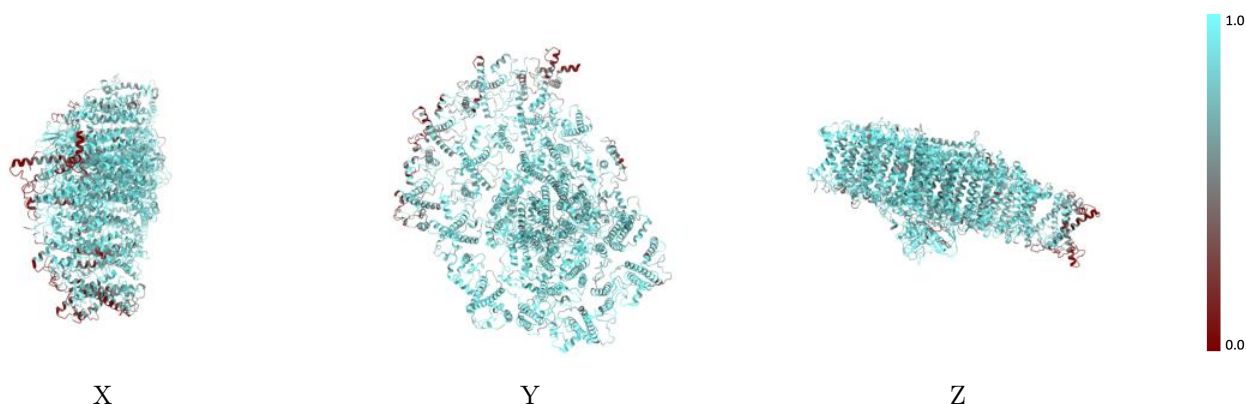
The images above show the 3D surface view of the map at the recommended contour level 0.0128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



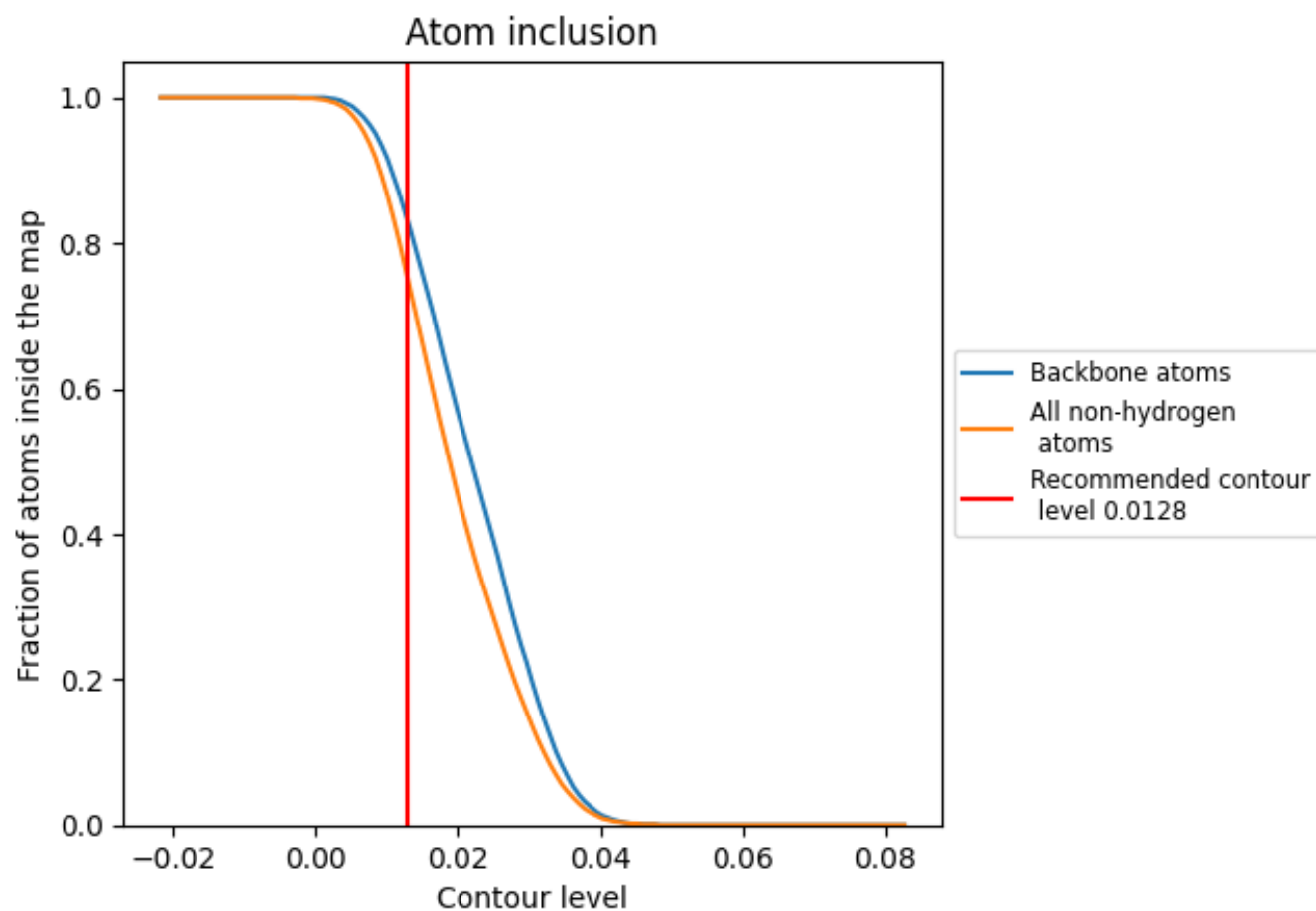
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0128).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.0128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.4180
1	 0.8060	 0.4130
2	 0.7430	 0.3890
3	 0.8160	 0.4590
7	 0.7990	 0.4530
8	 0.7930	 0.4380
9	 0.8030	 0.4050
A	 0.8370	 0.5050
B	 0.8470	 0.4970
C	 0.9190	 0.4990
D	 0.8770	 0.4690
E	 0.8490	 0.4990
F	 0.7890	 0.4480
G	 0.7660	 0.4190
H	 0.6470	 0.3730
I	 0.7740	 0.4220
J	 0.8350	 0.4460
K	 0.7720	 0.3550
L	 0.7530	 0.4130
O	 0.6530	 0.3420
T	 0.3940	 0.2670
a	 0.5860	 0.2630
b	 0.5470	 0.2100
c	 0.6510	 0.2690

