



wwPDB EM Validation Summary Report ⓘ

Aug 1, 2024 – 04:14 PM JST

PDB ID : 8WGH
EMDB ID : EMD-37513
Title : Cryo-EM structure of the red-shifted *Fittonia albivenis* PSI-LHCI
Authors : Huang, G.Q.; Li, X.X.; Sui, S.F.; Qin, X.C.
Deposited on : 2023-09-21
Resolution : 2.40 Å(reported)

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

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

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	: FAILED
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.37.1

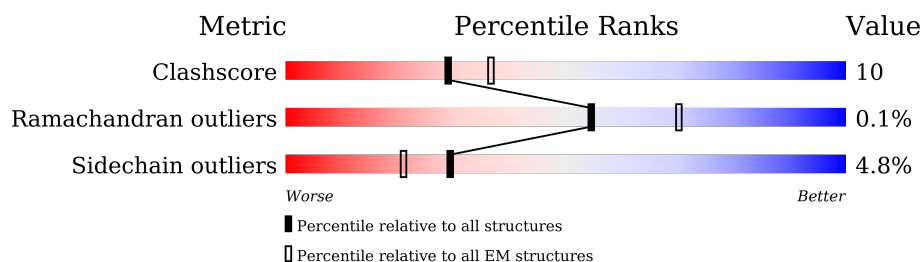
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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.








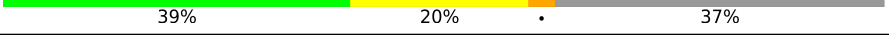


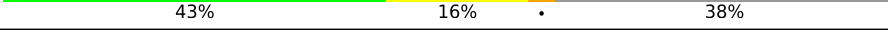
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	246	61% 18% • 19%
2	2	265	62% 16% • 21%
3	3	272	63% 17% • 19%
4	4	248	61% 18% 21%
5	A	750	81% 17% ..
6	B	734	86% 13% •
7	C	81	89% 9% ..
8	D	190	61% 12% • 26%
9	E	151	34% 7% 58%

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Mol	Chain	Length	Quality of chain
10	F	221	
11	G	145	
12	H	145	
13	I	36	
14	J	44	
15	K	132	
16	L	217	
17	N	173	
18	O	144	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CHL	1	301	X	-	-	-
19	CHL	1	306	X	-	-	-
19	CHL	2	301	X	-	-	-
19	CHL	2	305	X	-	-	-
19	CHL	2	306	X	-	-	-
19	CHL	2	307	X	-	-	-
19	CHL	2	314	X	-	-	-
19	CHL	3	306	X	-	-	-
19	CHL	4	305	X	-	-	-
19	CHL	4	306	X	-	-	-
19	CHL	4	307	X	-	-	-
19	CHL	4	315	X	-	-	-
20	CLA	1	302	X	-	-	-
20	CLA	1	303	X	-	-	-
20	CLA	1	304	X	-	-	-
20	CLA	1	305	X	-	-	-
20	CLA	1	307	X	-	-	-
20	CLA	1	308	X	-	-	-
20	CLA	1	309	X	-	-	-
20	CLA	1	310	X	-	-	-
20	CLA	1	311	X	-	-	-
20	CLA	1	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	1	313	X	-	-	-
20	CLA	1	314	X	-	-	-
20	CLA	1	321	X	-	-	-
20	CLA	2	302	X	-	-	-
20	CLA	2	303	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	308	X	-	-	-
20	CLA	2	309	X	-	-	-
20	CLA	2	310	X	-	-	-
20	CLA	2	311	X	-	-	-
20	CLA	2	312	X	-	-	-
20	CLA	2	313	X	-	-	-
20	CLA	3	301	X	-	-	-
20	CLA	3	302	X	-	-	-
20	CLA	3	303	X	-	-	-
20	CLA	3	304	X	-	-	-
20	CLA	3	305	X	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	310	X	-	-	-
20	CLA	3	311	X	-	-	-
20	CLA	3	312	X	-	-	-
20	CLA	3	313	X	-	-	-
20	CLA	3	314	X	-	-	-
20	CLA	4	301	X	-	-	-
20	CLA	4	302	X	-	-	-
20	CLA	4	303	X	-	-	-
20	CLA	4	304	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	-	-
20	CLA	4	311	X	-	-	-
20	CLA	4	312	X	-	-	-
20	CLA	4	313	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	819	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	853	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	F	802	X	-	-	-
20	CLA	F	804	X	-	-	-
20	CLA	F	805	X	-	-	-
20	CLA	G	603	X	-	-	-
20	CLA	G	604	X	-	-	-
20	CLA	G	605	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	J	101	X	-	-	-
20	CLA	J	103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	K	201	X	-	-	-
20	CLA	K	202	X	-	-	-
20	CLA	K	203	X	-	-	-
20	CLA	K	205	X	-	-	-
20	CLA	L	302	X	-	-	-
20	CLA	L	303	X	-	-	-
20	CLA	L	304	X	-	-	-
20	CLA	L	307	X	-	-	-
20	CLA	N	202	X	-	-	-
20	CLA	N	203	X	-	-	-
20	CLA	O	201	X	-	-	-
20	CLA	O	202	X	-	-	-
20	CLA	O	203	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 38187 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	199	Total	C	N	O	S	0	0
			1559	1016	261	278	4		

- Molecule 2 is a protein called Chlorophyll a-b binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	209	Total	C	N	O	S	0	0
			1626	1068	264	289	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total	C	N	O	S	0	0
			1727	1139	277	305	6		

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	197	Total	C	N	O	S	0	0
			1568	1027	253	283	5		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5831	3820	989	1003	19		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	SER	VAL	conflict	UNP A0A8A0WPY6

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5854	3843	996	1002	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	141	Total	C	N	O	S	0	0
			1116	714	193	206	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			511	324	92	95		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	153	Total	C	N	O	S	0	0
			1216	793	208	212	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	98	Total	C	N	O	0	0
			768	498	126	144		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	90	Total	C	N	O	0	0
			681	444	109	128		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	29	Total	C	N	O	S	0	0
			221	151	35	34	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	40	Total	C	N	O	S	0	0
			318	215	49	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	83	Total	C	N	O	S	0	0
			588	378	100	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	162	Total	C	N	O	S	0	0
			1225	812	195	217	1		

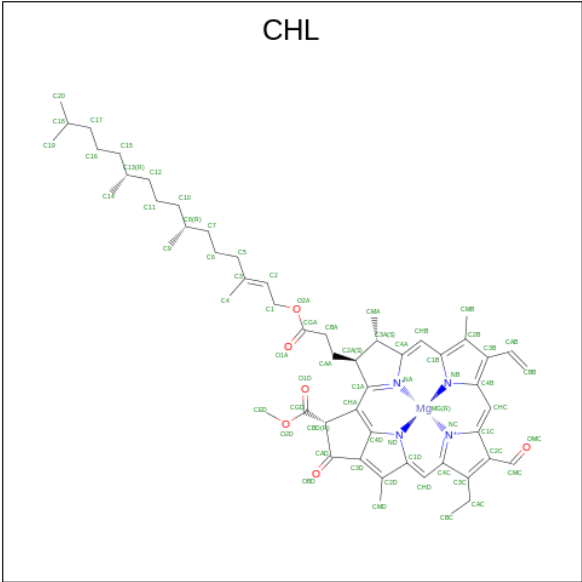
- Molecule 17 is a protein called Photosystem I reaction center subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	84	Total	C	N	O	S	0	0
			686	440	111	131	4		

- Molecule 18 is a protein called Photosystem I reaction center subunit O.

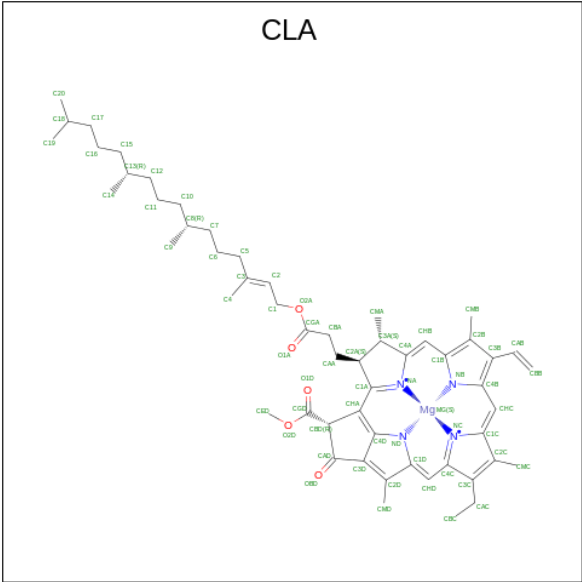
Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	89	Total	C	N	O	S	0	0
			705	475	112	117	1		

- Molecule 19 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
19	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
19	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
19	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
20	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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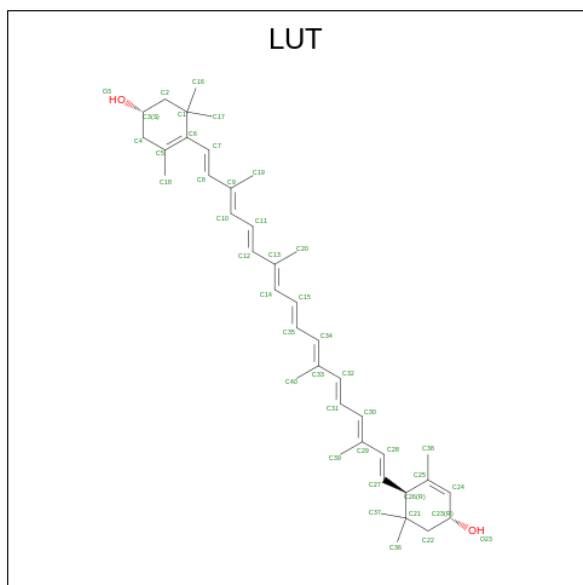
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	H	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	K	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



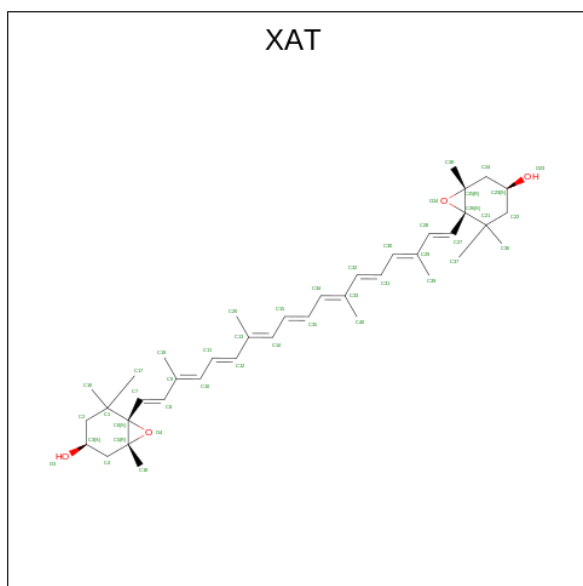
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	

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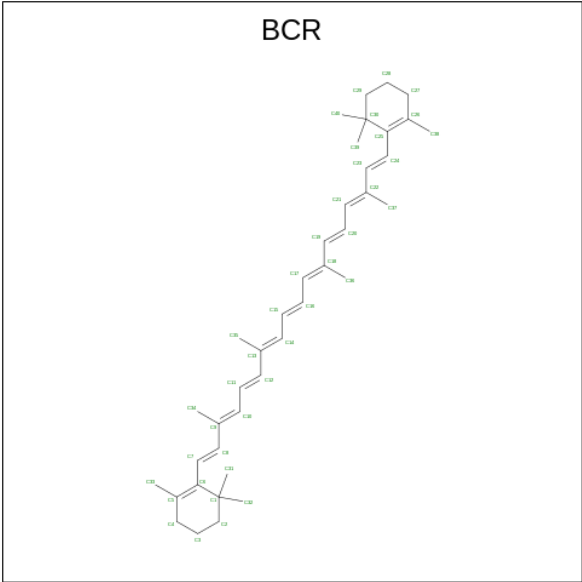
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	
21	O	1	Total	C	O	0
			42	40	2	
21	O	1	Total	C	O	0
			42	40	2	

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



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



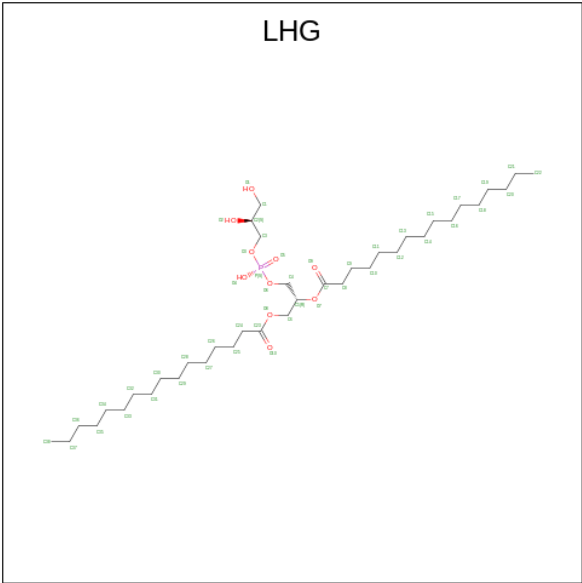
Mol	Chain	Residues	Atoms		AltConf
23	1	1	Total	C	0
			40	40	
23	2	1	Total	C	0
			40	40	
23	3	1	Total	C	0
			40	40	
23	4	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	

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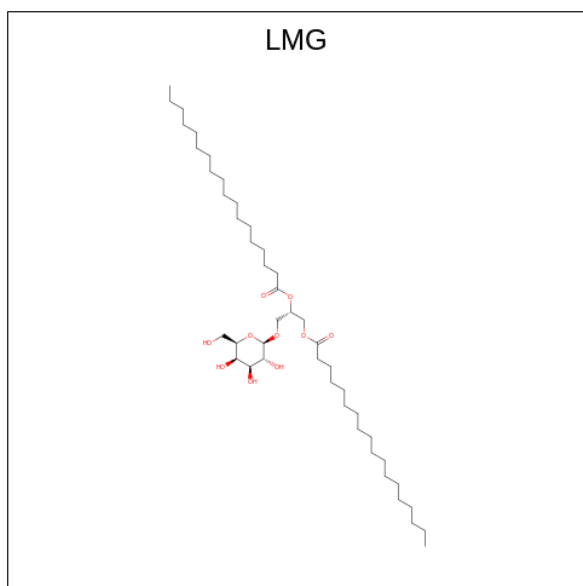
Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C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

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



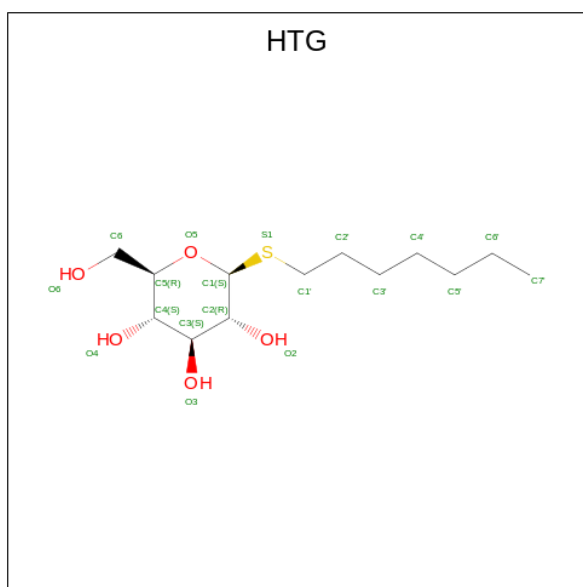
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	2	1	Total	C	O	P	0
			37	26	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			27	16	10	1	
24	B	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



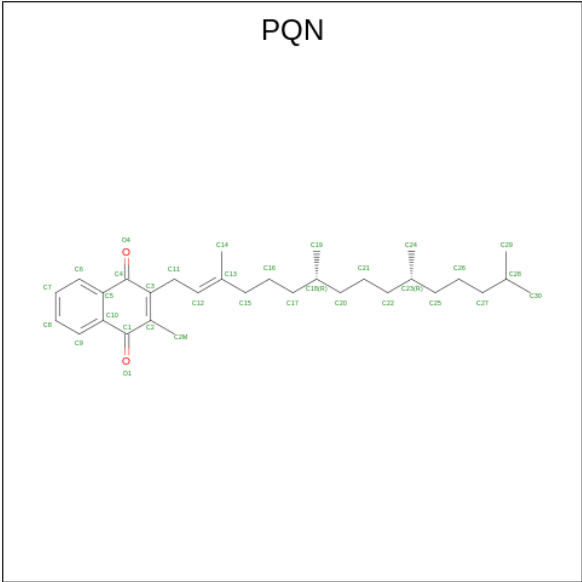
Mol	Chain	Residues	Atoms			AltConf
25	1	1	Total	C	O	0
			49	39	10	
25	1	1	Total	C	O	0
			44	34	10	
25	4	1	Total	C	O	0
			44	34	10	

- Molecule 26 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



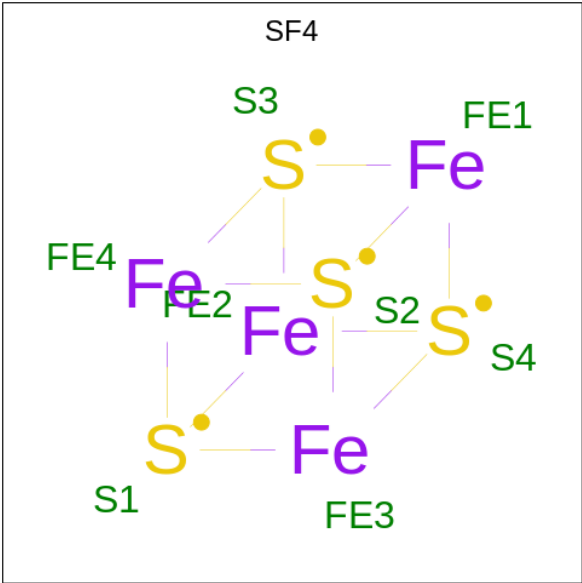
Mol	Chain	Residues	Atoms				AltConf
26	1	1	Total	C	O	S	0
			19	13	5	1	
26	4	1	Total	C	O	S	0
			19	13	5	1	
26	A	1	Total	C	O	S	0
			19	13	5	1	
26	B	1	Total	C	O	S	0
			19	13	5	1	
26	B	1	Total	C	O	S	0
			19	13	5	1	
26	F	1	Total	C	O	S	0
			19	13	5	1	
26	F	1	Total	C	O	S	0
			19	13	5	1	
26	G	1	Total	C	O	S	0
			19	13	5	1	
26	J	1	Total	C	O	S	0
			19	13	5	1	
26	N	1	Total	C	O	S	0
			19	13	5	1	

- Molecule 27 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



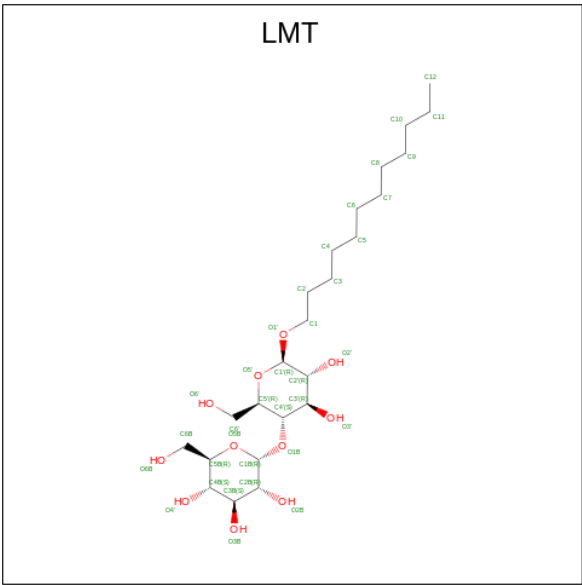
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	

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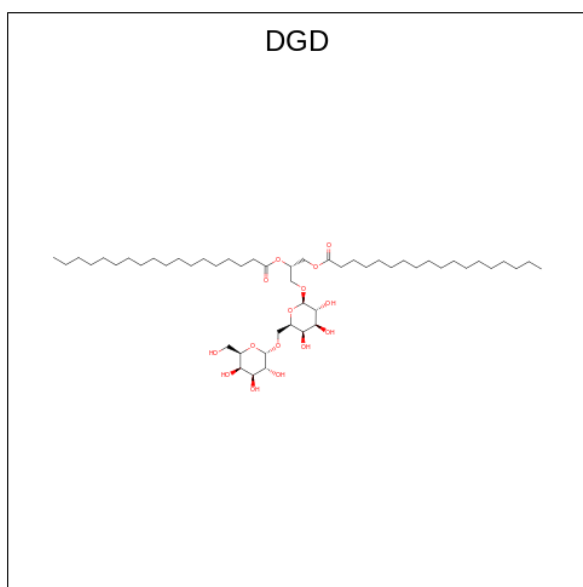
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
28	C	1	8	4	4	0

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	B	1	35	24	11	0
29	G	1	35	24	11	0

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

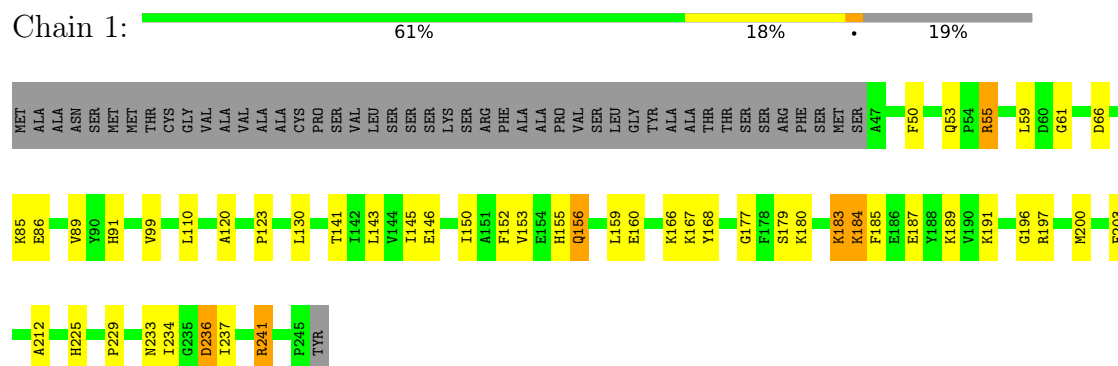


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	B	1	66	51	15	0

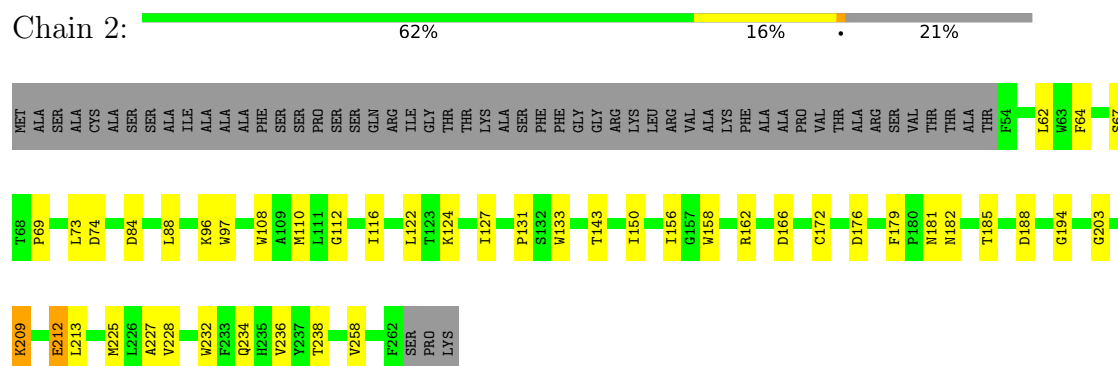
3 Residue-property plots [i](#)

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

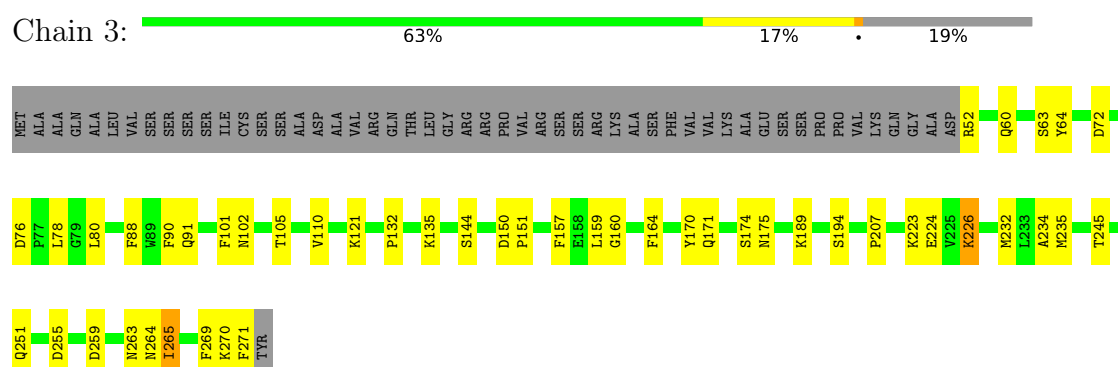
• Molecule 1: Chlorophyll a-b binding protein 1



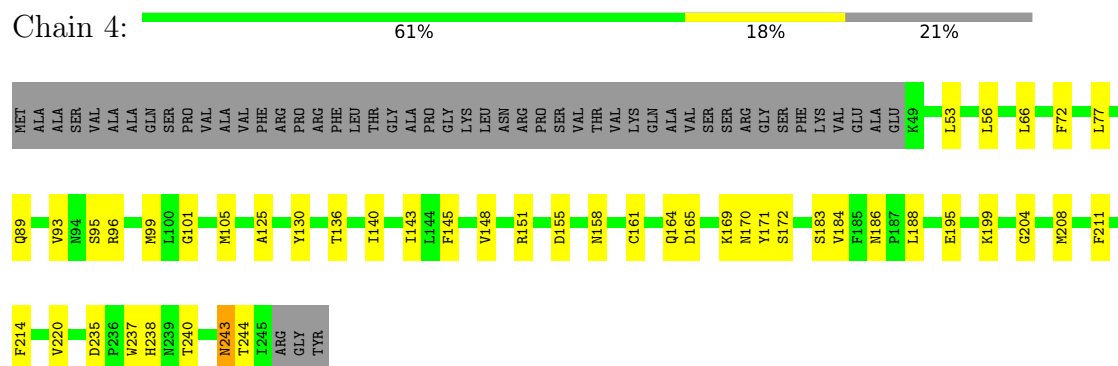
• Molecule 2: Chlorophyll a-b binding protein 2



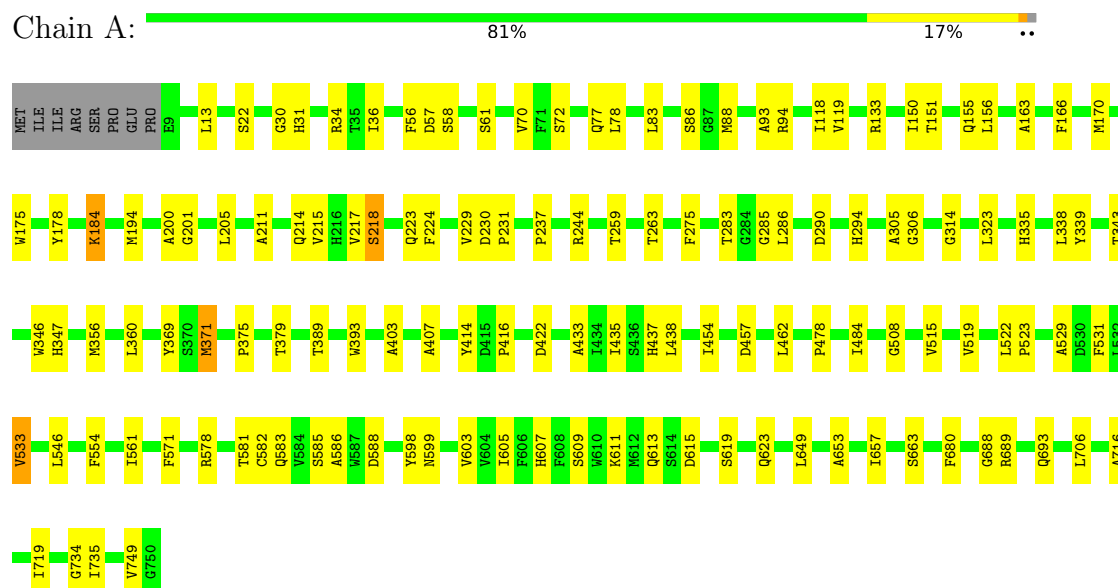
• Molecule 3: Chlorophyll a-b binding protein 3



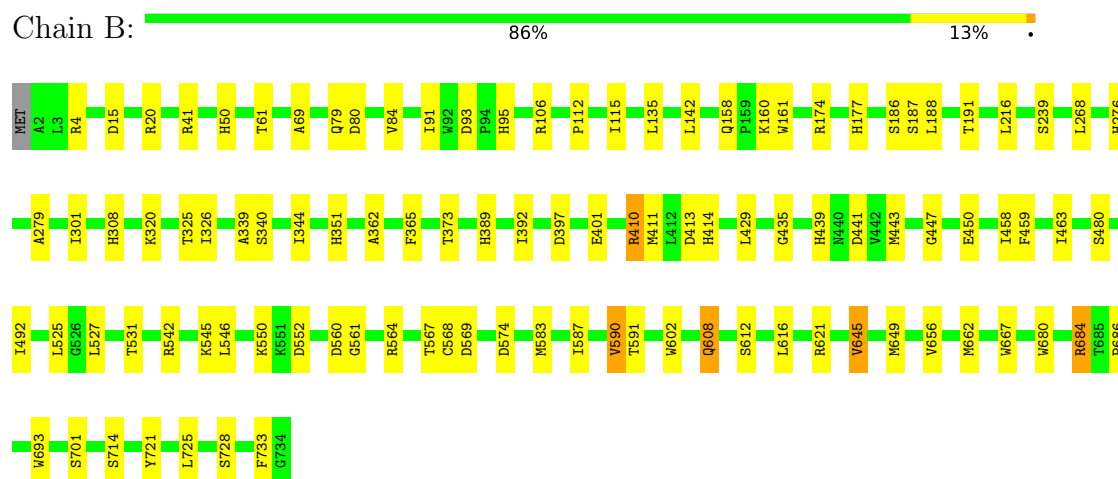
- Molecule 4: Chlorophyll a-b binding protein 4



- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 7: Photosystem I iron-sulfur center

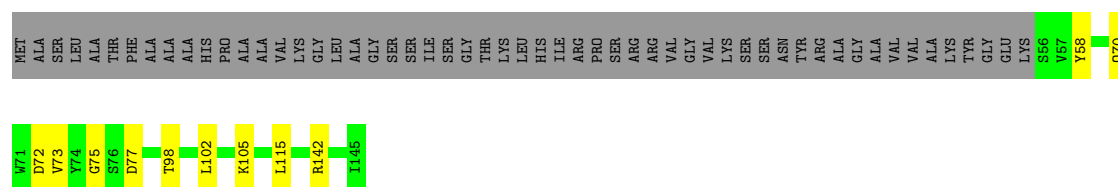
E89	ALA	MET
E93	SER	
M94	LEU	
	PHE	
M102	THR	
R103	LEU	
E104	SER	
G105	SER	
P106	PRO	
	TRP	
K110	LYS	
E115	GLN	
	SER	
L118	LEU	
	ALA	
T122	PRO	
R123	GLN	
L124	PHE	
R125	THR	
S126	ALA	
	ALA	
K129	LYS	
	ASN	
V137	PRO	
	LYS	
V143	PRO	
	LEU	
D150	PRO	
	ARG	
N176	ALA	
P177	VAL	
I178	ALA	
	ALA	
K181	MET	
	PRO	
V187	ILE	
	ARG	
	ALA	
	ALA	
L190	MET	
	ALA	
	PRO	
	GLU	
	GLU	
	SER	
	SER	
	ALA	
	ALA	
	GLY	
	PHE	
	T50	
	Q53	
	T68	
	Q75	
	E85	
	E92	

GLU	GLU	PRO	GLU	VAL	GLU	SER	ASP	THR	THR	PRO	ALA	ALA	ALA	CYS	THR	PHE	ALA	VAL	ALA	ALA	PRO	ASN	PHE	ALA	SER	SER	THR	ALA	THR	THR	LYS	PRO	PRO	ALA	VAL	PHE	GLY	MET		
V88	P91	S94	K95	V96	R101	S111	V112	V113	T114	M140	N141	Y142	V147	V150	ALA	ALA	ASP	GLU	PRO	GLU	ALA	ALA	ARG	VAL	ARG	ARG	ASN	LEU	LEU	PHE	VAL	MET	ARG	ALA	GLY	ASP	GLU	PRO	PRO	PRO

G200	F201	I202	W203	P204	V205	A206	Y207	Z208	R209	E210	F211	L212	M213	L216	I217	A218	K219	D220	VAL																																							
ALA	PRO	MET	PRO	ALA	VAL	ALA	D68	I69	S70	G71	L72	K76	K83	K84	E85	Q88	I89	E102	R119	F120	D121	G124	L128	S132	H137	M141	W147	F157	W163	V167	S170	P171	L172	S176	E185	L192	A193	S194	R195	I196	T197																	
MET	SER	LEU	THR	TLE	PRO	ALA	ASN	LEU	VAL	LEU	ASN	PRO	ARG	SER	ASN	LYS	SER	LEU	THR	GLN	SER	VAL	PRO	LYS	SER	SER	SER	ALA	ARG	PHE	VAL	CYS	SER	ASP	ASP	LYS	SER	SER	SER	SER	THR	PRO	GLN	SER	MET	LYS	ALA	PHE	SER	ALA	ALA	VAL	ALA	LEU	SER	ILE	LEU	LEU

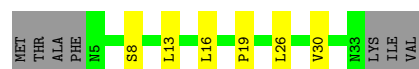
[illegible]

Chain H:  54% 8% 38%



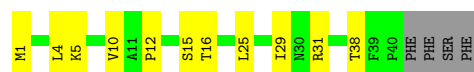
- Molecule 13: Photosystem I reaction center subunit VIII

Chain I:  64% 17% 19%



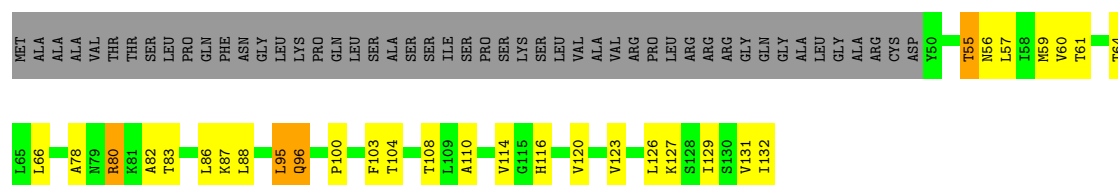
- Molecule 14: Photosystem I reaction center subunit IX

Chain J:  66% 25% 9%



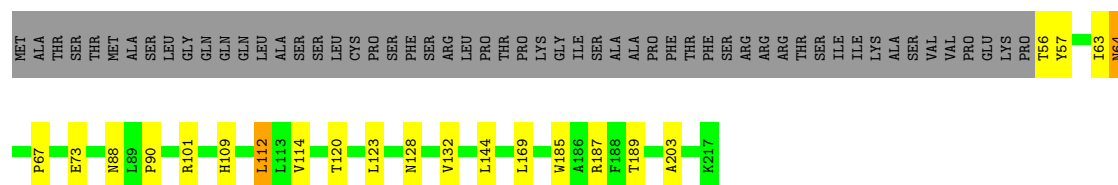
- Molecule 15: Photosystem I reaction center subunit psaK

Chain K:  39% 20% 37%




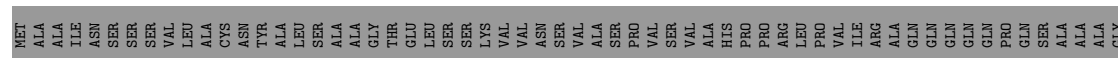
- Molecule 16: Photosystem I reaction center subunit XI

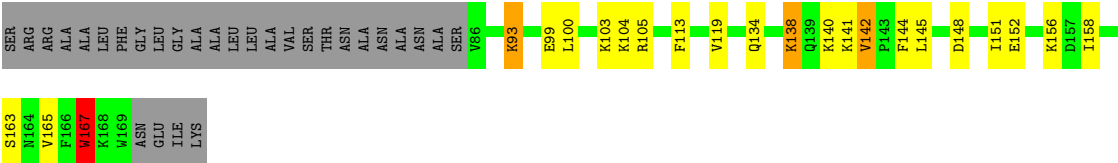
Chain L:  65% 9% 25%



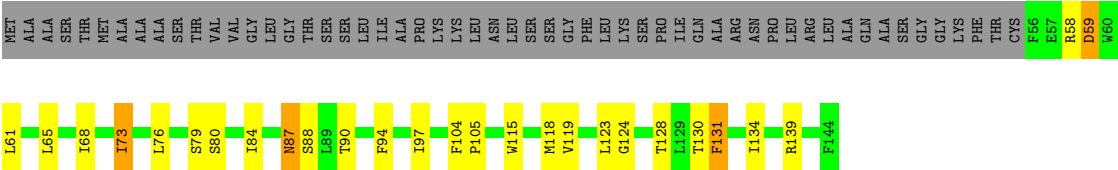
- Molecule 17: Photosystem I reaction center subunit N

Chain N:  35% 11% 51%





● Molecule 18: Photosystem I reaction center subunit O



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/1610	0.45	0/2195
2	2	0.34	0/1687	0.52	1/2313 (0.0%)
3	3	0.31	0/1791	0.47	1/2435 (0.0%)
4	4	0.27	0/1621	0.43	0/2215
5	A	0.26	0/6029	0.44	0/8223
6	B	0.26	0/6066	0.45	0/8285
7	C	0.25	0/628	0.50	0/852
8	D	0.27	0/1143	0.52	0/1546
9	E	0.27	0/522	0.51	0/710
10	F	0.27	0/1246	0.49	0/1681
11	G	0.52	0/788	0.49	0/1070
12	H	0.26	0/701	0.45	0/955
13	I	0.27	0/227	0.44	0/310
14	J	0.26	0/327	0.51	0/446
15	K	0.27	0/596	0.54	0/809
16	L	0.27	0/1263	0.45	0/1731
17	N	0.38	0/701	0.48	0/942
18	O	0.29	0/733	0.50	0/1001
All	All	0.28	0/27679	0.47	2/37719 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	226	LYS	CD-CE-NZ	-5.68	98.64	111.70
2	2	74	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1559	0	1536	38	0
2	2	1626	0	1570	37	0
3	3	1727	0	1651	36	0
4	4	1568	0	1517	36	0
5	A	5831	0	5683	94	0
6	B	5854	0	5635	69	0
7	C	615	0	600	3	0
8	D	1116	0	1122	13	0
9	E	511	0	510	6	0
10	F	1216	0	1245	37	0
11	G	768	0	740	7	0
12	H	681	0	671	7	0
13	I	221	0	237	3	0
14	J	318	0	331	9	0
15	K	588	0	619	21	0
16	L	1225	0	1240	15	0
17	N	686	0	664	18	0
18	O	705	0	686	19	0
19	1	100	0	72	6	0
19	2	238	0	169	23	0
19	3	47	0	30	3	0
19	4	198	0	143	12	0
20	1	744	0	720	32	0
20	2	485	0	445	21	0
20	3	633	0	499	24	0
20	4	593	0	524	35	0
20	A	2610	0	2708	132	0
20	B	2361	0	2424	96	0
20	F	156	0	138	7	0
20	G	141	0	105	0	0
20	H	56	0	51	3	0
20	J	107	0	103	2	0
20	K	197	0	158	8	0
20	L	206	0	177	8	0
20	N	95	0	69	2	0
20	O	157	0	135	16	0
21	1	84	0	112	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2	42	0	56	2	0
21	3	42	0	56	4	0
21	4	42	0	56	5	0
21	O	84	0	112	8	0
22	1	44	0	56	2	0
22	2	44	0	56	2	0
22	3	44	0	56	6	0
22	4	44	0	56	8	0
23	1	40	0	56	4	0
23	2	40	0	56	6	0
23	3	40	0	56	4	0
23	4	40	0	56	5	0
23	A	240	0	336	18	0
23	B	240	0	336	22	0
23	F	80	0	112	7	0
23	G	40	0	56	3	0
23	I	40	0	56	6	0
23	J	80	0	112	10	0
23	K	40	0	56	4	0
23	L	120	0	168	9	0
24	1	49	0	74	7	0
24	2	37	0	44	1	0
24	A	76	0	98	3	0
24	B	23	0	16	2	0
25	1	93	0	132	6	0
25	4	44	0	61	4	0
26	1	19	0	26	2	0
26	4	19	0	26	0	0
26	A	19	0	26	0	0
26	B	38	0	52	1	0
26	F	38	0	52	1	0
26	G	19	0	26	0	0
26	J	19	0	26	0	0
26	N	19	0	26	1	0
27	A	33	0	46	3	0
27	B	33	0	46	1	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	B	35	0	46	0	0
29	G	35	0	46	0	0
30	B	66	0	96	2	0
All	All	38187	0	37964	787	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 10.

The worst 5 of 787 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)
10:F:217:ILE:HG13	20:F:802:CLA:O1A	1.45	1.16
20:1:309:CLA:HAB	21:1:315:LUT:H32	1.42	0.98
19:2:306:CHL:HMB1	19:2:306:CHL:HBB1	1.49	0.93
20:3:309:CLA:HBC2	20:3:309:CLA:HHD	1.50	0.93
19:2:307:CHL:HBB1	19:2:307:CHL:HMB1	1.51	0.93

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	197/246 (80%)	194 (98%)	3 (2%)	0	100	100
2	2	207/265 (78%)	203 (98%)	3 (1%)	1 (0%)	29	41
3	3	218/272 (80%)	206 (94%)	12 (6%)	0	100	100
4	4	195/248 (79%)	189 (97%)	6 (3%)	0	100	100
5	A	740/750 (99%)	722 (98%)	18 (2%)	0	100	100
6	B	731/734 (100%)	716 (98%)	14 (2%)	1 (0%)	51	68
7	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
8	D	139/190 (73%)	135 (97%)	4 (3%)	0	100	100
9	E	61/151 (40%)	59 (97%)	2 (3%)	0	100	100
10	F	151/221 (68%)	150 (99%)	1 (1%)	0	100	100
11	G	96/145 (66%)	95 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	87 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	27/36 (75%)	27 (100%)	0	0	100	100
14	J	38/44 (86%)	38 (100%)	0	0	100	100
15	K	81/132 (61%)	75 (93%)	5 (6%)	1 (1%)	13	19
16	L	160/217 (74%)	157 (98%)	3 (2%)	0	100	100
17	N	82/173 (47%)	76 (93%)	5 (6%)	1 (1%)	13	19
18	O	87/144 (60%)	85 (98%)	2 (2%)	0	100	100
All	All	3376/4194 (80%)	3289 (97%)	83 (2%)	4 (0%)	54	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	172	CYS
6	B	362	ALA
17	N	167	TRP
15	K	96	GLN

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	162/198 (82%)	153 (94%)	9 (6%)	21	34
2	2	168/208 (81%)	164 (98%)	4 (2%)	49	68
3	3	175/217 (81%)	164 (94%)	11 (6%)	18	28
4	4	168/207 (81%)	163 (97%)	5 (3%)	41	61
5	A	600/608 (99%)	579 (96%)	21 (4%)	36	55
6	B	598/599 (100%)	577 (96%)	21 (4%)	36	55
7	C	70/71 (99%)	65 (93%)	5 (7%)	14	23
8	D	121/159 (76%)	110 (91%)	11 (9%)	9	14
9	E	57/124 (46%)	56 (98%)	1 (2%)	59	76
10	F	126/185 (68%)	112 (89%)	14 (11%)	6	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	G	84/125 (67%)	82 (98%)	2 (2%)	49	68
12	H	72/110 (66%)	69 (96%)	3 (4%)	30	47
13	I	25/31 (81%)	23 (92%)	2 (8%)	12	18
14	J	34/38 (90%)	33 (97%)	1 (3%)	42	62
15	K	61/99 (62%)	57 (93%)	4 (7%)	16	26
16	L	129/176 (73%)	125 (97%)	4 (3%)	40	60
17	N	74/139 (53%)	65 (88%)	9 (12%)	5	6
18	O	73/114 (64%)	65 (89%)	8 (11%)	6	8
All	All	2797/3408 (82%)	2662 (95%)	135 (5%)	29	41

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	L	67	PRO
17	N	138	LYS
18	O	65	LEU
5	A	663	SER
5	A	623	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	704	GLN
11	G	50	ASN
7	C	38	GLN
8	D	167	ASN
12	H	83	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

225 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	$\# Z > 2$
20	CLA	A	826	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
23	BCR	2	317	-	41,41,41	0.74	0	56,56,56	2.13	17 (30%)
20	CLA	3	301	3	60,68,73	1.54	7 (11%)	70,107,113	1.42	7 (10%)
28	SF4	C	101	-	0,12,12	-	-	-	-	-
20	CLA	A	814	-	50,58,73	1.67	5 (10%)	58,95,113	1.59	9 (15%)
20	CLA	1	305	-	52,60,73	1.66	6 (11%)	60,97,113	1.48	7 (11%)
20	CLA	1	321	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	9 (11%)
20	CLA	A	807	5	65,73,73	1.45	5 (7%)	76,113,113	1.42	9 (11%)
20	CLA	B	813	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
23	BCR	A	848	-	41,41,41	0.75	1 (2%)	56,56,56	1.88	15 (26%)
20	CLA	B	817	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	7 (9%)
20	CLA	K	203	-	46,54,73	1.72	7 (15%)	53,90,113	1.61	6 (11%)
20	CLA	A	810	20	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
20	CLA	B	820	-	50,58,73	1.68	5 (10%)	58,95,113	1.56	7 (12%)
20	CLA	B	812	-	55,63,73	1.61	5 (9%)	64,101,113	1.45	8 (12%)
20	CLA	B	822	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
20	CLA	B	823	-	60,68,73	1.54	7 (11%)	70,107,113	1.47	10 (14%)
20	CLA	3	309	-	46,54,73	2.15	11 (23%)	53,90,113	2.36	16 (30%)
26	HTG	F	807	-	19,19,19	1.06	2 (10%)	23,24,24	0.52	0
20	CLA	B	808	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
20	CLA	B	827	-	65,73,73	1.53	6 (9%)	76,113,113	1.33	9 (11%)
26	HTG	B	851	-	19,19,19	1.08	2 (10%)	23,24,24	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	A	847	-	41,41,41	0.68	0	56,56,56	2.00	16 (28%)
23	BCR	G	606	-	41,41,41	0.68	0	56,56,56	1.95	16 (28%)
23	BCR	F	801	-	41,41,41	0.68	0	56,56,56	1.79	14 (25%)
21	LUT	2	315	-	42,43,43	0.75	0	51,60,60	1.69	15 (29%)
26	HTG	B	850	-	19,19,19	1.06	2 (10%)	23,24,24	0.84	0
20	CLA	1	311	1	52,60,73	1.64	6 (11%)	60,97,113	1.57	7 (11%)
23	BCR	A	845	-	41,41,41	0.72	0	56,56,56	1.94	16 (28%)
20	CLA	B	837	-	47,55,73	1.73	6 (12%)	54,91,113	1.56	7 (12%)
24	LHG	B	849	-	22,22,48	1.19	2 (9%)	25,28,54	1.01	1 (4%)
20	CLA	4	313	-	45,53,73	1.79	5 (11%)	52,89,113	1.59	8 (15%)
20	CLA	A	828	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
25	LMG	1	323	-	44,44,55	0.99	2 (4%)	52,52,63	1.04	3 (5%)
20	CLA	3	313	-	45,53,73	1.80	5 (11%)	52,89,113	1.54	6 (11%)
20	CLA	A	812	-	65,73,73	1.47	5 (7%)	76,113,113	1.38	6 (7%)
20	CLA	4	311	4	52,60,73	1.64	6 (11%)	60,97,113	1.53	6 (10%)
20	CLA	B	829	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	6 (7%)
20	CLA	1	310	24	41,49,73	1.81	6 (14%)	47,84,113	1.69	8 (17%)
20	CLA	A	802	-	65,73,73	1.46	5 (7%)	76,113,113	1.39	7 (9%)
23	BCR	K	204	-	41,41,41	0.68	0	56,56,56	2.02	18 (32%)
20	CLA	A	801	-	65,73,73	1.48	5 (7%)	76,113,113	1.49	10 (13%)
23	BCR	L	305	-	41,41,41	0.70	0	56,56,56	2.09	13 (23%)
23	BCR	A	846	-	41,41,41	0.73	0	56,56,56	1.97	15 (26%)
20	CLA	A	829	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	7 (9%)
20	CLA	2	304	-	60,68,73	1.55	6 (10%)	70,107,113	1.40	7 (10%)
20	CLA	A	804	-	65,73,73	1.47	7 (10%)	76,113,113	1.42	6 (7%)
23	BCR	A	854	-	41,41,41	0.69	0	56,56,56	1.94	12 (21%)
20	CLA	2	309	2	60,68,73	1.53	6 (10%)	70,107,113	1.40	8 (11%)
20	CLA	A	819	-	45,53,73	1.77	6 (13%)	52,89,113	1.59	7 (13%)
20	CLA	1	313	-	55,63,73	1.61	5 (9%)	64,101,113	1.47	7 (10%)
20	CLA	3	308	3	50,58,73	1.66	6 (12%)	58,95,113	1.54	8 (13%)
20	CLA	K	202	-	60,68,73	1.55	6 (10%)	70,107,113	1.45	11 (15%)
20	CLA	L	304	-	50,58,73	1.67	6 (12%)	58,95,113	1.54	9 (15%)
20	CLA	A	818	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
23	BCR	L	301	-	41,41,41	0.72	0	56,56,56	1.96	13 (23%)
24	LHG	1	318	20	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CHL	2	306	-	48,56,74	2.32	16 (33%)	51,92,114	3.24	23 (45%)
20	CLA	1	304	-	52,60,73	1.65	6 (11%)	60,97,113	1.52	8 (13%)
20	CLA	F	804	-	45,53,73	1.79	6 (13%)	52,89,113	1.55	7 (13%)
20	CLA	A	809	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
20	CLA	1	309	1	60,68,73	1.50	5 (8%)	70,107,113	1.43	8 (11%)
20	CLA	2	310	24	41,49,73	1.81	5 (12%)	47,84,113	1.68	8 (17%)
19	CHL	2	307	-	51,59,74	2.33	21 (41%)	55,96,114	3.45	28 (50%)
20	CLA	A	841	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	9 (11%)
20	CLA	N	202	17	44,53,73	1.77	6 (13%)	50,89,113	1.58	7 (14%)
24	LHG	2	318	20	36,36,48	1.07	2 (5%)	39,42,54	1.13	3 (7%)
30	DGD	B	848	-	67,67,67	0.84	2 (2%)	81,81,81	0.94	4 (4%)
23	BCR	3	317	-	41,41,41	0.66	0	56,56,56	1.99	16 (28%)
21	LUT	O	205	-	42,43,43	0.85	1 (2%)	51,60,60	2.00	14 (27%)
20	CLA	B	804	-	45,53,73	1.76	5 (11%)	52,89,113	1.60	8 (15%)
20	CLA	1	314	1	46,54,73	1.73	6 (13%)	53,90,113	1.56	6 (11%)
26	HTG	A	852	-	19,19,19	1.27	2 (10%)	23,24,24	1.49	4 (17%)
20	CLA	1	302	1	65,73,73	1.48	7 (10%)	76,113,113	1.38	7 (9%)
20	CLA	O	201	24	52,60,73	1.66	6 (11%)	60,97,113	1.45	7 (11%)
19	CHL	2	305	-	43,51,74	2.42	19 (44%)	45,86,114	3.72	24 (53%)
27	PQN	A	842	-	34,34,34	1.62	2 (5%)	42,45,45	1.05	3 (7%)
20	CLA	B	821	-	56,64,73	1.61	6 (10%)	65,102,113	1.45	8 (12%)
20	CLA	J	103	14	42,50,73	1.83	6 (14%)	48,85,113	1.59	7 (14%)
20	CLA	A	827	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	8 (10%)
20	CLA	4	302	4	60,68,73	1.51	6 (10%)	70,107,113	1.46	7 (10%)
21	LUT	1	319	-	42,43,43	0.71	0	51,60,60	1.73	12 (23%)
20	CLA	B	835	-	51,59,73	1.64	6 (11%)	59,96,113	1.53	7 (11%)
20	CLA	B	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	8 (10%)
20	CLA	L	303	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	9 (11%)
20	CLA	O	202	-	45,53,73	2.01	8 (17%)	52,89,113	1.94	7 (13%)
23	BCR	B	845	-	41,41,41	0.69	0	56,56,56	1.99	17 (30%)
23	BCR	J	104	-	41,41,41	0.67	0	56,56,56	1.98	15 (26%)
20	CLA	B	838	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
22	XAT	3	316	-	39,47,47	0.88	0	54,74,74	2.72	21 (38%)
20	CLA	3	312	-	45,53,73	1.78	5 (11%)	52,89,113	1.58	7 (13%)
20	CLA	1	307	-	61,69,73	1.53	5 (8%)	71,108,113	1.40	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CHL	4	305	-	53,61,74	2.23	16 (30%)	57,98,114	3.06	26 (45%)
20	CLA	A	839	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	8 (10%)
20	CLA	B	805	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
20	CLA	B	811	-	54,62,73	1.67	7 (12%)	67,100,113	1.51	9 (13%)
20	CLA	B	815	-	60,68,73	1.51	5 (8%)	70,107,113	1.45	7 (10%)
20	CLA	B	828	-	65,73,73	1.50	5 (7%)	76,113,113	1.33	9 (11%)
20	CLA	N	203	-	50,58,73	1.70	5 (10%)	58,95,113	1.54	9 (15%)
21	LUT	O	204	-	42,43,43	0.76	0	51,60,60	1.73	12 (23%)
23	BCR	I	101	-	41,41,41	0.76	0	56,56,56	2.08	17 (30%)
26	HTG	1	322	-	19,19,19	1.06	2 (10%)	23,24,24	1.05	3 (13%)
20	CLA	B	807	-	55,63,73	1.59	6 (10%)	64,101,113	1.47	9 (14%)
20	CLA	3	314	-	46,54,73	1.78	5 (10%)	53,90,113	1.51	6 (11%)
22	XAT	4	317	-	39,47,47	0.88	0	54,74,74	2.65	19 (35%)
20	CLA	B	831	-	65,73,73	1.47	5 (7%)	76,113,113	1.34	7 (9%)
20	CLA	3	305	3	47,55,73	1.74	5 (10%)	54,91,113	1.52	7 (12%)
20	CLA	1	312	1	65,73,73	1.50	5 (7%)	76,113,113	1.34	7 (9%)
22	XAT	2	316	-	39,47,47	0.88	0	54,74,74	2.64	20 (37%)
20	CLA	A	815	-	45,53,73	1.78	6 (13%)	52,89,113	1.56	6 (11%)
20	CLA	A	833	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
21	LUT	4	316	-	42,43,43	0.76	0	51,60,60	1.61	13 (25%)
20	CLA	A	823	-	55,63,73	1.61	5 (9%)	64,101,113	1.43	9 (14%)
20	CLA	B	818	-	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
27	PQN	B	840	-	34,34,34	1.60	2 (5%)	42,45,45	1.12	3 (7%)
20	CLA	1	303	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	8 (10%)
20	CLA	A	824	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
20	CLA	A	813	-	45,53,73	1.77	5 (11%)	52,89,113	1.60	8 (15%)
20	CLA	A	817	-	65,73,73	1.49	7 (10%)	76,113,113	1.35	9 (11%)
20	CLA	A	835	5	45,53,73	1.80	5 (11%)	52,89,113	1.56	7 (13%)
24	LHG	A	844	20	26,26,48	1.25	2 (7%)	29,32,54	1.34	3 (10%)
20	CLA	2	313	-	43,51,73	1.78	6 (13%)	49,86,113	1.63	7 (14%)
20	CLA	A	822	-	51,59,73	1.67	6 (11%)	59,96,113	1.46	8 (13%)
21	LUT	3	315	-	42,43,43	0.75	0	51,60,60	1.59	12 (23%)
20	CLA	1	308	1	65,73,73	1.49	5 (7%)	76,113,113	1.36	7 (9%)
20	CLA	A	825	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	10 (13%)
29	LMT	B	847	-	36,36,36	0.40	0	47,47,47	0.68	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	2	311	2	52,60,73	1.63	6 (11%)	60,97,113	1.56	7 (11%)
20	CLA	A	808	5	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
20	CLA	4	303	-	60,68,73	1.53	7 (11%)	70,107,113	1.46	7 (10%)
20	CLA	B	832	-	58,66,73	1.56	6 (10%)	67,104,113	1.49	10 (14%)
23	BCR	F	806	-	41,41,41	0.71	0	56,56,56	2.03	17 (30%)
20	CLA	3	302	-	50,58,73	1.72	5 (10%)	58,95,113	1.50	8 (13%)
20	CLA	4	310	-	55,63,73	1.63	5 (9%)	64,101,113	1.41	8 (12%)
20	CLA	F	802	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
20	CLA	A	820	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
20	CLA	B	816	-	55,63,73	1.59	6 (10%)	64,101,113	1.45	8 (12%)
29	LMT	G	601	-	36,36,36	0.41	0	47,47,47	0.64	1 (2%)
21	LUT	1	315	-	42,43,43	0.76	0	51,60,60	1.64	14 (27%)
20	CLA	A	811	-	54,62,73	1.65	6 (11%)	62,99,113	1.44	8 (12%)
26	HTG	F	803	-	19,19,19	1.09	2 (10%)	23,24,24	0.55	0
20	CLA	A	806	-	65,73,73	1.45	5 (7%)	76,113,113	1.42	8 (10%)
20	CLA	B	810	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	8 (10%)
20	CLA	L	302	16	45,53,73	1.76	6 (13%)	52,89,113	1.66	7 (13%)
19	CHL	4	307	-	51,59,74	2.31	24 (47%)	55,96,114	3.13	24 (43%)
20	CLA	A	821	-	49,57,73	1.67	6 (12%)	55,93,113	1.58	7 (12%)
20	CLA	B	824	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	8 (10%)
20	CLA	O	203	-	60,68,73	1.53	6 (10%)	70,107,113	1.43	8 (11%)
23	BCR	1	317	-	41,41,41	0.68	0	56,56,56	1.91	18 (32%)
20	CLA	H	201	-	56,64,73	1.60	6 (10%)	65,102,113	1.45	7 (10%)
20	CLA	A	831	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	8 (10%)
20	CLA	B	834	-	45,53,73	1.75	5 (11%)	52,89,113	1.62	7 (13%)
20	CLA	3	310	-	52,60,73	1.67	6 (11%)	60,97,113	1.49	8 (13%)
23	BCR	A	849	-	41,41,41	0.72	0	56,56,56	1.97	15 (26%)
20	CLA	2	302	2	65,73,73	1.45	6 (9%)	76,113,113	1.39	8 (10%)
20	CLA	A	816	-	65,73,73	1.48	6 (9%)	76,113,113	1.33	8 (10%)
20	CLA	3	311	3	55,63,73	1.63	6 (10%)	64,101,113	1.45	8 (12%)
20	CLA	B	836	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
20	CLA	K	205	15	45,53,73	1.78	6 (13%)	52,89,113	1.56	6 (11%)
20	CLA	B	806	6	65,73,73	1.45	5 (7%)	76,113,113	1.38	8 (10%)
28	SF4	A	850	-	0,12,12	-	-	-	-	-
20	CLA	A	834	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CHL	4	315	-	43,51,74	2.35	18 (41%)	45,86,114	3.22	21 (46%)
20	CLA	G	605	11	46,54,73	1.76	5 (10%)	53,90,113	1.51	6 (11%)
19	CHL	3	306	-	47,55,74	2.40	21 (44%)	50,91,114	3.55	26 (52%)
26	HTG	G	602	-	19,19,19	1.08	2 (10%)	23,24,24	0.56	0
20	CLA	A	836	-	51,59,73	1.64	5 (9%)	59,96,113	1.57	9 (15%)
20	CLA	3	304	-	42,50,73	1.80	5 (11%)	48,85,113	1.67	6 (12%)
20	CLA	A	851	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	8 (10%)
28	SF4	C	102	-	0,12,12	-	-	-	-	-
20	CLA	F	805	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	6 (11%)
20	CLA	A	803	20	55,63,73	1.62	6 (10%)	64,101,113	1.49	9 (14%)
20	CLA	4	308	4	50,58,73	1.67	6 (12%)	58,95,113	1.52	9 (15%)
19	CHL	1	301	1	52,60,74	2.23	16 (30%)	56,97,114	2.70	23 (41%)
20	CLA	B	809	6	65,73,73	1.46	5 (7%)	76,113,113	1.41	8 (10%)
19	CHL	2	301	2	53,61,74	2.50	25 (47%)	57,98,114	3.86	30 (52%)
23	BCR	B	842	-	41,41,41	0.71	0	56,56,56	2.03	19 (33%)
19	CHL	1	306	1	48,56,74	2.33	19 (39%)	51,92,114	3.21	26 (50%)
20	CLA	L	307	-	45,53,73	1.80	6 (13%)	52,89,113	1.59	7 (13%)
20	CLA	3	303	-	45,53,73	1.77	5 (11%)	52,89,113	1.60	8 (15%)
20	CLA	3	307	3	50,58,73	1.65	6 (12%)	58,95,113	1.57	8 (13%)
20	CLA	B	819	-	65,73,73	1.48	7 (10%)	76,113,113	1.35	8 (10%)
20	CLA	4	301	4	46,54,73	1.76	5 (10%)	53,90,113	1.53	6 (11%)
24	LHG	A	843	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	3 (5%)
23	BCR	B	843	-	41,41,41	0.70	0	56,56,56	2.06	14 (25%)
26	HTG	4	320	-	19,19,19	1.12	2 (10%)	23,24,24	0.57	0
20	CLA	A	853	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
20	CLA	J	101	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	9 (11%)
20	CLA	B	802	-	65,73,73	1.48	6 (9%)	76,113,113	1.31	7 (9%)
25	LMG	1	320	-	49,49,55	0.94	2 (4%)	57,57,63	1.02	3 (5%)
20	CLA	B	839	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
20	CLA	G	604	-	50,58,73	1.69	5 (10%)	58,95,113	1.53	8 (13%)
20	CLA	B	825	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	9 (11%)
20	CLA	G	603	-	45,53,73	1.79	5 (11%)	52,89,113	1.58	7 (13%)
23	BCR	4	318	-	41,41,41	0.67	0	56,56,56	3.33	22 (39%)
19	CHL	4	306	-	51,59,74	2.42	23 (45%)	55,96,114	3.03	26 (47%)
20	CLA	B	830	-	50,58,73	1.67	6 (12%)	58,95,113	1.53	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	K	201	15	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
22	XAT	1	316	-	39,47,47	0.88	0	54,74,74	2.58	18 (33%)
20	CLA	B	833	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	9 (11%)
20	CLA	A	840	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	8 (10%)
23	BCR	B	841	-	41,41,41	0.71	0	56,56,56	1.89	16 (28%)
20	CLA	A	838	-	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
20	CLA	A	832	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	7 (9%)
23	BCR	J	102	-	41,41,41	0.68	0	56,56,56	1.97	17 (30%)
20	CLA	4	314	-	50,58,73	1.69	5 (10%)	58,95,113	1.51	9 (15%)
20	CLA	A	805	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
26	HTG	N	201	-	19,19,19	1.08	2 (10%)	23,24,24	0.61	0
25	LMG	4	319	-	44,44,55	0.98	2 (4%)	52,52,63	1.01	3 (5%)
20	CLA	2	308	2	50,58,73	1.65	6 (12%)	58,95,113	1.55	8 (13%)
23	BCR	B	844	-	41,41,41	0.71	0	56,56,56	1.85	15 (26%)
20	CLA	A	837	-	65,73,73	1.45	6 (9%)	76,113,113	1.43	8 (10%)
20	CLA	4	312	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	6 (7%)
23	BCR	L	306	-	41,41,41	0.72	0	56,56,56	2.09	13 (23%)
19	CHL	2	314	2	43,51,74	2.25	12 (27%)	45,86,114	2.96	18 (40%)
20	CLA	2	312	2	65,73,73	1.49	5 (7%)	76,113,113	1.36	9 (11%)
20	CLA	B	801	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	7 (9%)
20	CLA	A	830	-	50,58,73	1.66	6 (12%)	58,95,113	1.58	7 (12%)
20	CLA	4	304	-	50,58,73	2.02	13 (26%)	58,95,113	3.47	22 (37%)
23	BCR	B	846	-	41,41,41	0.71	0	56,56,56	1.76	14 (25%)
20	CLA	4	309	4	60,68,73	1.51	6 (10%)	70,107,113	1.42	9 (12%)
20	CLA	B	826	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
26	HTG	J	105	-	19,19,19	1.11	2 (10%)	23,24,24	0.56	0
20	CLA	B	814	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
20	CLA	2	303	-	49,57,73	1.70	6 (12%)	55,93,113	1.55	7 (12%)

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
20	CLA	A	826	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	2	317	-	-	2/29/63/63	0/2/2/2
20	CLA	3	301	3	1/1/14/20	6/31/109/115	-
28	SF4	C	101	-	-	-	0/6/5/5
20	CLA	A	814	-	1/1/12/20	7/19/97/115	-
20	CLA	1	305	-	1/1/12/20	3/22/100/115	-
20	CLA	1	321	-	1/1/15/20	7/37/115/115	-
20	CLA	A	807	5	1/1/15/20	10/37/115/115	-
20	CLA	B	813	-	1/1/15/20	14/37/115/115	-
23	BCR	A	848	-	-	0/29/63/63	0/2/2/2
20	CLA	B	817	-	1/1/15/20	13/37/115/115	-
20	CLA	K	203	-	1/1/11/20	6/15/93/115	-
20	CLA	A	810	20	1/1/15/20	16/37/115/115	-
20	CLA	B	820	-	1/1/12/20	1/19/97/115	-
20	CLA	B	812	-	1/1/13/20	6/25/103/115	-
20	CLA	B	822	-	1/1/15/20	12/37/115/115	-
20	CLA	B	823	-	1/1/14/20	12/31/109/115	-
20	CLA	3	309	-	-	4/15/93/115	-
26	HTG	F	807	-	-	2/10/30/30	0/1/1/1
20	CLA	B	808	-	1/1/15/20	5/37/115/115	-
20	CLA	B	827	-	1/1/15/20	14/37/115/115	-
26	HTG	B	851	-	-	2/10/30/30	0/1/1/1
23	BCR	A	847	-	-	2/29/63/63	0/2/2/2
23	BCR	G	606	-	-	0/29/63/63	0/2/2/2
23	BCR	F	801	-	-	3/29/63/63	0/2/2/2
21	LUT	2	315	-	-	2/29/67/67	0/2/2/2
26	HTG	B	850	-	-	8/10/30/30	0/1/1/1
20	CLA	1	311	1	1/1/12/20	7/22/100/115	-
23	BCR	A	845	-	-	6/29/63/63	0/2/2/2
20	CLA	B	837	-	1/1/11/20	2/16/94/115	-
24	LHG	B	849	-	-	7/26/26/53	-
20	CLA	4	313	-	1/1/11/20	1/13/91/115	-
20	CLA	A	828	-	1/1/15/20	11/37/115/115	-
25	LMG	1	323	-	-	10/39/59/70	0/1/1/1
20	CLA	3	313	-	1/1/11/20	3/13/91/115	-
20	CLA	A	812	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	311	4	1/1/12/20	5/22/100/115	-
20	CLA	B	829	-	1/1/15/20	6/37/115/115	-
20	CLA	1	310	24	1/1/10/20	2/8/86/115	-
20	CLA	A	802	-	1/1/15/20	15/37/115/115	-
23	BCR	K	204	-	-	6/29/63/63	0/2/2/2
20	CLA	A	801	-	1/1/15/20	11/37/115/115	-
23	BCR	L	305	-	-	4/29/63/63	0/2/2/2
23	BCR	A	846	-	-	0/29/63/63	0/2/2/2
20	CLA	A	829	-	1/1/15/20	9/37/115/115	-
20	CLA	2	304	-	1/1/14/20	10/31/109/115	-
20	CLA	A	804	-	1/1/15/20	10/37/115/115	-
23	BCR	A	854	-	-	0/29/63/63	0/2/2/2
20	CLA	2	309	2	1/1/14/20	6/31/109/115	-
20	CLA	A	819	-	1/1/11/20	2/13/91/115	-
20	CLA	1	313	-	1/1/13/20	11/25/103/115	-
20	CLA	3	308	3	1/1/12/20	1/19/97/115	-
20	CLA	K	202	-	1/1/14/20	7/31/109/115	-
20	CLA	L	304	-	1/1/12/20	2/19/97/115	-
20	CLA	A	818	-	1/1/15/20	9/37/115/115	-
23	BCR	L	301	-	-	4/29/63/63	0/2/2/2
24	LHG	1	318	20	-	13/53/53/53	-
19	CHL	2	306	-	3/3/16/26	10/18/116/137	-
20	CLA	1	304	-	1/1/12/20	5/22/100/115	-
20	CLA	F	804	-	1/1/11/20	3/13/91/115	-
20	CLA	A	809	-	1/1/15/20	14/37/115/115	-
20	CLA	1	309	1	1/1/14/20	4/31/109/115	-
20	CLA	2	310	24	1/1/10/20	4/8/86/115	-
19	CHL	2	307	-	3/3/17/26	9/21/119/137	-
20	CLA	A	841	-	1/1/15/20	23/37/115/115	-
20	CLA	N	202	17	1/1/11/20	4/13/91/115	-
24	LHG	2	318	20	-	12/41/41/53	-
30	DGD	B	848	-	-	10/55/95/95	0/2/2/2
23	BCR	3	317	-	-	4/29/63/63	0/2/2/2
21	LUT	O	205	-	-	6/29/67/67	0/2/2/2
20	CLA	B	804	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	314	1	1/1/11/20	3/15/93/115	-
26	HTG	A	852	-	-	2/10/30/30	0/1/1/1
20	CLA	1	302	1	1/1/15/20	10/37/115/115	-
20	CLA	O	201	24	1/1/12/20	9/22/100/115	-
19	CHL	2	305	-	3/3/15/26	3/12/110/137	-
27	PQN	A	842	-	-	7/23/43/43	0/2/2/2
20	CLA	B	821	-	1/1/13/20	9/27/105/115	-
20	CLA	J	103	14	1/1/10/20	4/10/88/115	-
20	CLA	A	827	-	1/1/15/20	16/37/115/115	-
20	CLA	4	302	4	1/1/14/20	8/31/109/115	-
21	LUT	1	319	-	-	2/29/67/67	0/2/2/2
20	CLA	B	835	-	1/1/12/20	3/21/99/115	-
20	CLA	B	803	-	1/1/15/20	10/37/115/115	-
20	CLA	L	303	-	1/1/15/20	12/37/115/115	-
20	CLA	O	202	-	1/1/11/20	7/13/91/115	-
23	BCR	B	845	-	-	2/29/63/63	0/2/2/2
23	BCR	J	104	-	-	2/29/63/63	0/2/2/2
20	CLA	B	838	-	1/1/15/20	5/37/115/115	-
22	XAT	3	316	-	-	0/31/93/93	0/4/4/4
20	CLA	3	312	-	1/1/11/20	3/13/91/115	-
20	CLA	1	307	-	1/1/14/20	12/33/111/115	-
19	CHL	4	305	-	3/3/17/26	5/24/122/137	-
20	CLA	A	839	-	1/1/15/20	16/37/115/115	-
20	CLA	B	805	-	1/1/15/20	15/37/115/115	-
20	CLA	B	811	-	1/1/13/20	8/25/101/115	-
20	CLA	B	815	-	1/1/14/20	9/31/109/115	-
20	CLA	B	828	-	1/1/15/20	15/37/115/115	-
20	CLA	N	203	-	1/1/12/20	8/19/97/115	-
21	LUT	O	204	-	-	1/29/67/67	0/2/2/2
23	BCR	I	101	-	-	8/29/63/63	0/2/2/2
26	HTG	1	322	-	-	0/10/30/30	0/1/1/1
20	CLA	B	807	-	1/1/13/20	8/25/103/115	-
20	CLA	3	314	-	1/1/11/20	4/15/93/115	-
22	XAT	4	317	-	-	0/31/93/93	0/4/4/4
20	CLA	B	831	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	305	3	1/1/11/20	7/16/94/115	-
20	CLA	1	312	1	1/1/15/20	15/37/115/115	-
22	XAT	2	316	-	-	0/31/93/93	0/4/4/4
20	CLA	A	815	-	1/1/11/20	0/13/91/115	-
20	CLA	A	833	-	1/1/15/20	10/37/115/115	-
21	LUT	4	316	-	-	2/29/67/67	0/2/2/2
20	CLA	A	823	-	1/1/13/20	4/25/103/115	-
20	CLA	B	818	-	1/1/14/20	11/31/109/115	-
27	PQN	B	840	-	-	1/23/43/43	0/2/2/2
20	CLA	1	303	-	1/1/15/20	10/37/115/115	-
20	CLA	A	824	-	1/1/15/20	11/37/115/115	-
20	CLA	A	813	-	1/1/11/20	2/13/91/115	-
20	CLA	A	817	-	1/1/15/20	14/37/115/115	-
20	CLA	A	835	5	1/1/11/20	9/13/91/115	-
24	LHG	A	844	20	-	12/31/31/53	-
20	CLA	2	313	-	1/1/10/20	4/11/89/115	-
20	CLA	A	822	-	1/1/12/20	7/21/99/115	-
21	LUT	3	315	-	-	2/29/67/67	0/2/2/2
20	CLA	1	308	1	1/1/15/20	12/37/115/115	-
20	CLA	A	825	-	1/1/15/20	3/37/115/115	-
29	LMT	B	847	-	-	6/21/61/61	0/2/2/2
20	CLA	2	311	2	1/1/12/20	8/22/100/115	-
20	CLA	A	808	5	1/1/15/20	16/37/115/115	-
20	CLA	4	303	-	1/1/14/20	9/31/109/115	-
20	CLA	B	832	-	1/1/13/20	2/29/107/115	-
23	BCR	F	806	-	-	2/29/63/63	0/2/2/2
20	CLA	3	302	-	1/1/12/20	4/19/97/115	-
20	CLA	4	310	-	1/1/13/20	7/25/103/115	-
20	CLA	F	802	-	1/1/15/20	9/37/115/115	-
20	CLA	A	820	-	1/1/15/20	8/37/115/115	-
20	CLA	B	816	-	1/1/13/20	6/25/103/115	-
29	LMT	G	601	-	-	4/21/61/61	0/2/2/2
21	LUT	1	315	-	-	2/29/67/67	0/2/2/2
20	CLA	A	811	-	1/1/12/20	5/24/102/115	-
26	HTG	F	803	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	806	-	1/1/15/20	10/37/115/115	-
20	CLA	B	810	-	1/1/15/20	11/37/115/115	-
20	CLA	L	302	16	1/1/11/20	6/13/91/115	-
19	CHL	4	307	-	3/3/17/26	3/21/119/137	-
20	CLA	A	821	-	1/1/11/20	9/18/96/115	-
20	CLA	B	824	-	1/1/15/20	14/37/115/115	-
20	CLA	O	203	-	1/1/14/20	7/31/109/115	-
23	BCR	1	317	-	-	2/29/63/63	0/2/2/2
20	CLA	H	201	-	1/1/13/20	11/27/105/115	-
20	CLA	A	831	-	1/1/15/20	15/37/115/115	-
20	CLA	B	834	-	1/1/11/20	1/13/91/115	-
20	CLA	3	310	-	1/1/12/20	0/22/100/115	-
23	BCR	A	849	-	-	4/29/63/63	0/2/2/2
20	CLA	2	302	2	1/1/15/20	7/37/115/115	-
20	CLA	A	816	-	1/1/15/20	10/37/115/115	-
20	CLA	3	311	3	1/1/13/20	1/25/103/115	-
20	CLA	B	836	-	1/1/15/20	6/37/115/115	-
20	CLA	K	205	15	1/1/11/20	0/13/91/115	-
20	CLA	B	806	6	1/1/15/20	13/37/115/115	-
28	SF4	A	850	-	-	-	0/6/5/5
20	CLA	A	834	-	1/1/15/20	11/37/115/115	-
19	CHL	4	315	-	3/3/15/26	4/12/110/137	-
20	CLA	G	605	11	1/1/11/20	6/15/93/115	-
19	CHL	3	306	-	3/3/16/26	5/17/115/137	-
26	HTG	G	602	-	-	0/10/30/30	0/1/1/1
20	CLA	A	836	-	1/1/12/20	6/21/99/115	-
20	CLA	3	304	-	1/1/10/20	0/10/88/115	-
20	CLA	A	851	-	1/1/15/20	15/37/115/115	-
28	SF4	C	102	-	-	-	0/6/5/5
20	CLA	F	805	-	1/1/11/20	6/15/93/115	-
20	CLA	A	803	20	1/1/13/20	6/25/103/115	-
20	CLA	4	308	4	1/1/12/20	4/19/97/115	-
19	CHL	1	301	1	3/3/17/26	10/23/121/137	-
20	CLA	B	809	6	1/1/15/20	4/37/115/115	-
19	CHL	2	301	2	3/3/17/26	8/24/122/137	-
23	BCR	B	842	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CHL	1	306	1	3/3/16/26	11/18/116/137	-
20	CLA	L	307	-	1/1/11/20	7/13/91/115	-
20	CLA	3	303	-	1/1/11/20	4/13/91/115	-
20	CLA	3	307	3	1/1/12/20	6/19/97/115	-
20	CLA	B	819	-	1/1/15/20	7/37/115/115	-
20	CLA	4	301	4	1/1/11/20	7/15/93/115	-
24	LHG	A	843	-	-	9/53/53/53	-
23	BCR	B	843	-	-	4/29/63/63	0/2/2/2
26	HTG	4	320	-	-	3/10/30/30	0/1/1/1
20	CLA	A	853	-	1/1/15/20	14/37/115/115	-
20	CLA	J	101	-	1/1/15/20	5/37/115/115	-
20	CLA	B	802	-	1/1/15/20	8/37/115/115	-
25	LMG	1	320	-	-	9/44/64/70	0/1/1/1
20	CLA	B	839	-	1/1/15/20	6/37/115/115	-
20	CLA	G	604	-	1/1/12/20	4/19/97/115	-
20	CLA	B	825	-	1/1/15/20	15/37/115/115	-
20	CLA	G	603	-	1/1/11/20	2/13/91/115	-
23	BCR	4	318	-	-	6/29/63/63	0/2/2/2
19	CHL	4	306	-	3/3/17/26	10/21/119/137	-
20	CLA	B	830	-	1/1/12/20	5/19/97/115	-
20	CLA	K	201	15	1/1/11/20	2/15/93/115	-
22	XAT	1	316	-	-	1/31/93/93	0/4/4/4
20	CLA	B	833	-	1/1/15/20	11/37/115/115	-
20	CLA	A	840	-	1/1/15/20	6/37/115/115	-
23	BCR	B	841	-	-	3/29/63/63	0/2/2/2
20	CLA	A	838	-	1/1/15/20	12/37/115/115	-
20	CLA	A	832	-	1/1/15/20	8/37/115/115	-
23	BCR	J	102	-	-	7/29/63/63	0/2/2/2
20	CLA	4	314	-	1/1/12/20	7/19/97/115	-
20	CLA	A	805	-	1/1/15/20	17/37/115/115	-
26	HTG	N	201	-	-	2/10/30/30	0/1/1/1
25	LMG	4	319	-	-	6/39/59/70	0/1/1/1
20	CLA	2	308	2	1/1/12/20	5/19/97/115	-
23	BCR	B	844	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	837	-	1/1/15/20	12/37/115/115	-
20	CLA	4	312	-	1/1/15/20	12/37/115/115	-
23	BCR	L	306	-	-	0/29/63/63	0/2/2/2
19	CHL	2	314	2	3/3/15/26	2/12/110/137	-
20	CLA	2	312	2	1/1/15/20	9/37/115/115	-
20	CLA	B	801	-	1/1/15/20	5/37/115/115	-
20	CLA	A	830	-	1/1/12/20	3/19/97/115	-
20	CLA	4	304	-	1/1/12/20	8/19/97/115	-
23	BCR	B	846	-	-	2/29/63/63	0/2/2/2
20	CLA	4	309	4	1/1/14/20	6/31/109/115	-
20	CLA	B	826	-	1/1/15/20	2/37/115/115	-
26	HTG	J	105	-	-	1/10/30/30	0/1/1/1
20	CLA	B	814	-	1/1/15/20	7/37/115/115	-
20	CLA	2	303	-	1/1/11/20	8/18/96/115	-

The worst 5 of 1148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	827	CLA	C4B-NB	8.01	1.42	1.35
20	1	303	CLA	C4B-NB	7.81	1.42	1.35
20	3	314	CLA	C4B-NB	7.77	1.42	1.35
20	3	309	CLA	C4B-NB	7.74	1.42	1.35
27	A	842	PQN	C3-C2	7.73	1.49	1.35

The worst 5 of 2091 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	318	BCR	C32-C1-C6	-15.04	85.90	110.30
20	4	304	CLA	O2D-CGD-CBD	14.88	137.72	111.27
19	2	301	CHL	O2D-CGD-CBD	14.22	136.54	111.27
19	2	305	CHL	O2D-CGD-CBD	12.66	133.77	111.27
20	4	304	CLA	O2D-CGD-O1D	-9.88	104.53	123.84

5 of 185 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	301	CHL	ND
19	1	301	CHL	NA
19	1	301	CHL	NC

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Mol	Chain	Res	Type	Atom
19	1	306	CHL	ND
19	1	306	CHL	NA

5 of 1463 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	301	CHL	C2-C3-C5-C6
19	1	301	CHL	C4-C3-C5-C6
19	1	306	CHL	C1A-C2A-CAA-CBA
19	1	306	CHL	C3A-C2A-CAA-CBA
19	1	306	CHL	C3C-C2C-CMC-OMC

There are no ring outliers.

193 monomers are involved in 527 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	826	CLA	5	0
23	2	317	BCR	6	0
20	3	301	CLA	1	0
20	A	814	CLA	1	0
20	1	321	CLA	5	0
20	A	807	CLA	4	0
20	B	813	CLA	7	0
23	A	848	BCR	4	0
20	B	817	CLA	5	0
20	K	203	CLA	1	0
20	A	810	CLA	7	0
20	B	812	CLA	3	0
20	B	822	CLA	2	0
20	B	823	CLA	4	0
20	3	309	CLA	7	0
26	F	807	HTG	1	0
20	B	808	CLA	4	0
20	B	827	CLA	4	0
23	A	847	BCR	2	0
23	G	606	BCR	3	0
23	F	801	BCR	4	0
21	2	315	LUT	2	0
26	B	850	HTG	1	0
20	1	311	CLA	2	0
23	A	845	BCR	2	0
20	B	837	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	849	LHG	2	0
20	4	313	CLA	2	0
20	A	828	CLA	2	0
25	1	323	LMG	3	0
20	3	313	CLA	1	0
20	A	812	CLA	6	0
20	4	311	CLA	2	0
20	B	829	CLA	3	0
20	1	310	CLA	1	0
20	A	802	CLA	3	0
23	K	204	BCR	4	0
20	A	801	CLA	7	0
23	L	305	BCR	4	0
23	A	846	BCR	1	0
20	A	829	CLA	1	0
20	2	304	CLA	2	0
20	A	804	CLA	6	0
23	A	854	BCR	6	0
20	2	309	CLA	2	0
20	1	313	CLA	3	0
20	3	308	CLA	2	0
20	K	202	CLA	2	0
20	A	818	CLA	4	0
23	L	301	BCR	2	0
24	1	318	LHG	7	0
19	2	306	CHL	8	0
20	1	304	CLA	2	0
20	A	809	CLA	3	0
20	1	309	CLA	2	0
20	2	310	CLA	4	0
19	2	307	CHL	3	0
20	A	841	CLA	3	0
24	2	318	LHG	1	0
30	B	848	DGD	2	0
23	3	317	BCR	4	0
21	O	205	LUT	5	0
20	B	804	CLA	1	0
20	1	302	CLA	3	0
20	O	201	CLA	4	0
19	2	305	CHL	5	0
27	A	842	PQN	3	0
20	B	821	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	J	103	CLA	1	0
20	A	827	CLA	6	0
20	4	302	CLA	5	0
21	1	319	LUT	4	0
20	B	835	CLA	3	0
20	B	803	CLA	4	0
20	L	303	CLA	5	0
20	O	202	CLA	6	0
23	B	845	BCR	5	0
23	J	104	BCR	2	0
20	B	838	CLA	3	0
22	3	316	XAT	6	0
20	1	307	CLA	3	0
19	4	305	CHL	4	0
20	A	839	CLA	1	0
20	B	805	CLA	6	0
20	B	815	CLA	1	0
20	B	828	CLA	5	0
20	N	203	CLA	2	0
21	O	204	LUT	3	0
23	I	101	BCR	6	0
26	1	322	HTG	2	0
20	B	807	CLA	2	0
20	3	314	CLA	2	0
22	4	317	XAT	8	0
20	B	831	CLA	5	0
20	1	312	CLA	4	0
22	2	316	XAT	2	0
20	A	833	CLA	4	0
21	4	316	LUT	5	0
20	A	823	CLA	7	0
20	B	818	CLA	3	0
27	B	840	PQN	1	0
20	1	303	CLA	6	0
20	A	824	CLA	4	0
20	A	817	CLA	5	0
20	A	835	CLA	1	0
24	A	844	LHG	1	0
20	2	313	CLA	1	0
20	A	822	CLA	3	0
21	3	315	LUT	4	0
20	1	308	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	825	CLA	6	0
20	2	311	CLA	3	0
20	A	808	CLA	5	0
20	4	303	CLA	8	0
20	B	832	CLA	4	0
23	F	806	BCR	3	0
20	F	802	CLA	4	0
20	A	820	CLA	4	0
20	B	816	CLA	2	0
21	1	315	LUT	4	0
20	A	811	CLA	5	0
20	A	806	CLA	4	0
20	B	810	CLA	3	0
20	L	302	CLA	3	0
19	4	307	CHL	1	0
20	A	821	CLA	3	0
20	B	824	CLA	9	0
20	O	203	CLA	6	0
23	1	317	BCR	4	0
20	H	201	CLA	3	0
20	A	831	CLA	5	0
20	B	834	CLA	3	0
20	3	310	CLA	1	0
23	A	849	BCR	4	0
20	2	302	CLA	2	0
20	A	816	CLA	2	0
20	3	311	CLA	4	0
20	B	836	CLA	2	0
20	K	205	CLA	3	0
20	B	806	CLA	2	0
20	A	834	CLA	3	0
19	4	315	CHL	5	0
19	3	306	CHL	3	0
20	A	836	CLA	3	0
20	3	304	CLA	1	0
20	A	851	CLA	5	0
20	F	805	CLA	3	0
20	A	803	CLA	3	0
20	4	308	CLA	7	0
19	1	301	CHL	3	0
20	B	809	CLA	4	0
19	2	301	CHL	10	0

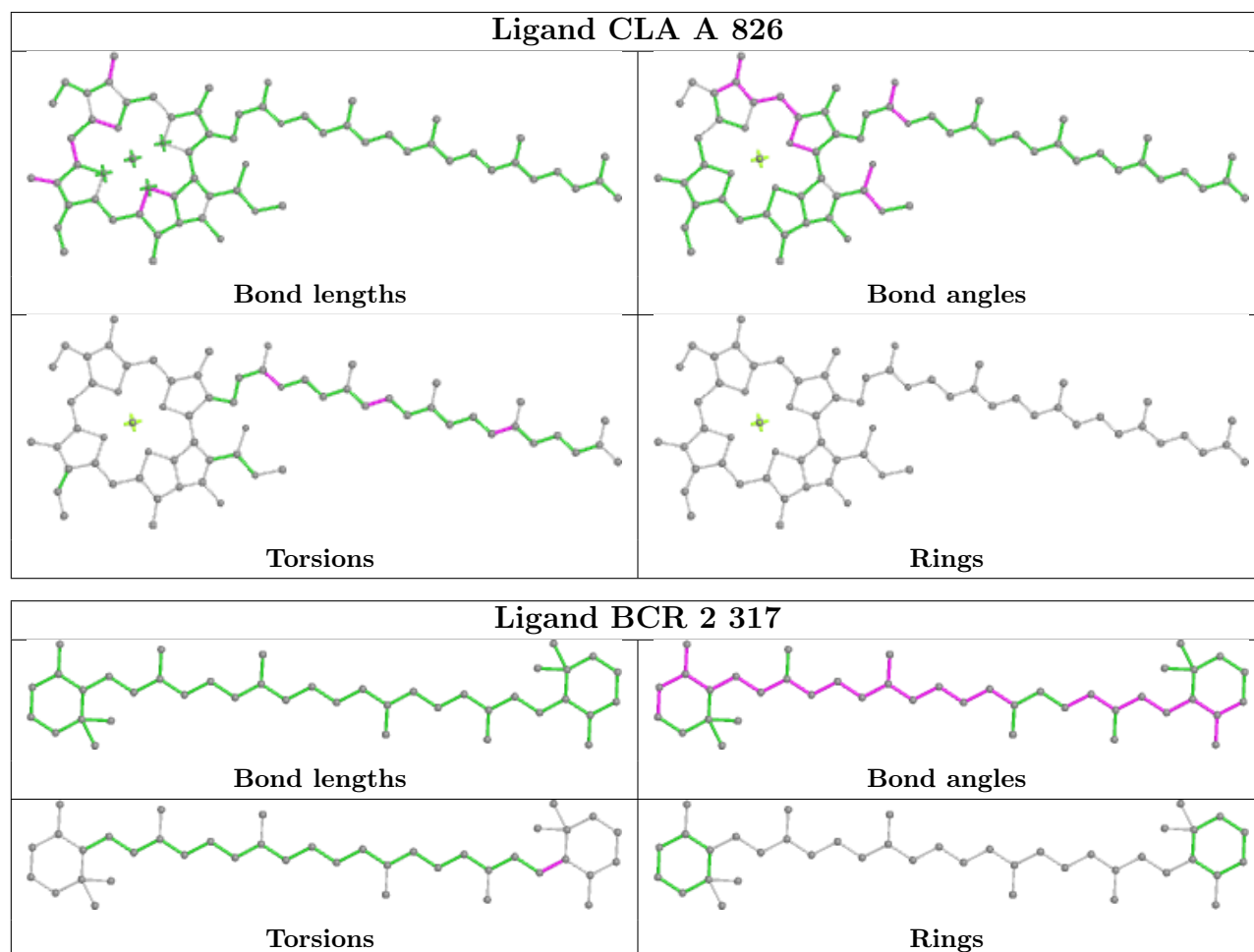
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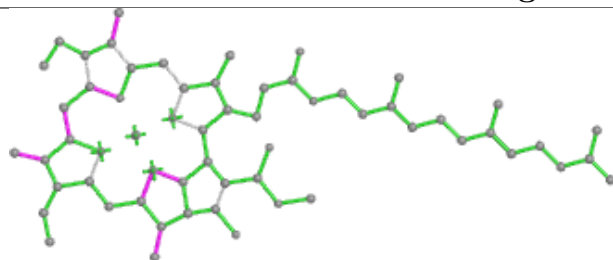
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	842	BCR	1	0
19	1	306	CHL	3	0
20	3	307	CLA	7	0
20	B	819	CLA	2	0
20	4	301	CLA	6	0
24	A	843	LHG	2	0
23	B	843	BCR	2	0
20	A	853	CLA	5	0
20	J	101	CLA	1	0
20	B	802	CLA	5	0
25	1	320	LMG	3	0
20	B	839	CLA	3	0
20	B	825	CLA	4	0
23	4	318	BCR	5	0
19	4	306	CHL	3	0
20	B	830	CLA	2	0
20	K	201	CLA	2	0
22	1	316	XAT	2	0
20	B	833	CLA	2	0
20	A	840	CLA	1	0
23	B	841	BCR	8	0
20	A	838	CLA	4	0
20	A	832	CLA	1	0
23	J	102	BCR	8	0
20	4	314	CLA	2	0
20	A	805	CLA	5	0
26	N	201	HTG	1	0
25	4	319	LMG	4	0
20	2	308	CLA	6	0
23	B	844	BCR	3	0
20	A	837	CLA	3	0
20	4	312	CLA	5	0
23	L	306	BCR	3	0
19	2	314	CHL	1	0
20	2	312	CLA	4	0
20	B	801	CLA	4	0
20	4	304	CLA	3	0
23	B	846	BCR	3	0
20	4	309	CLA	3	0
20	B	826	CLA	1	0
20	2	303	CLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

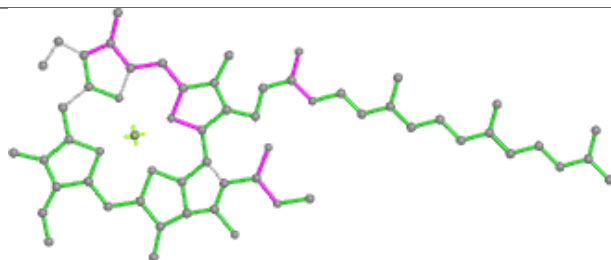
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



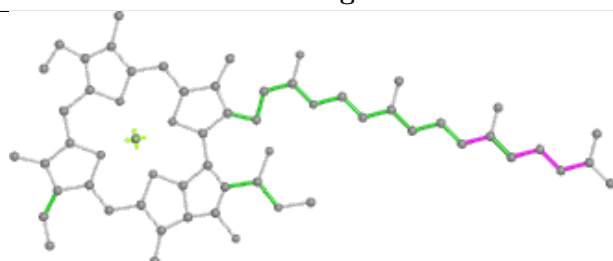
Ligand CLA 3 301



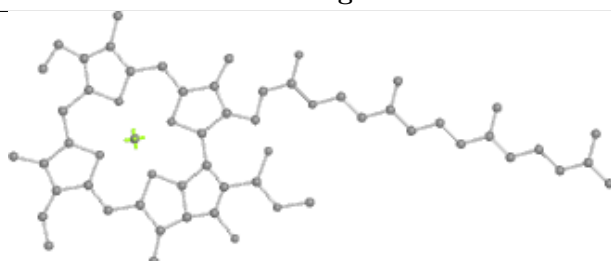
Bond lengths



Bond angles

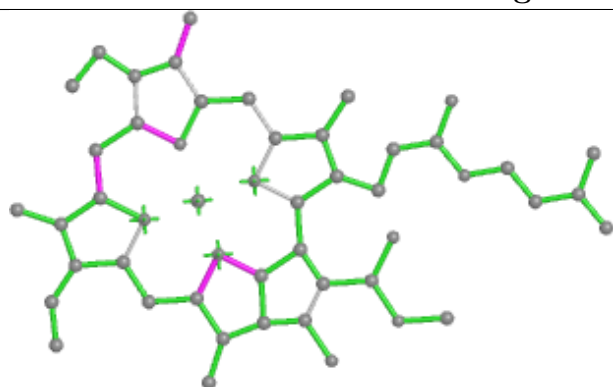


Torsions

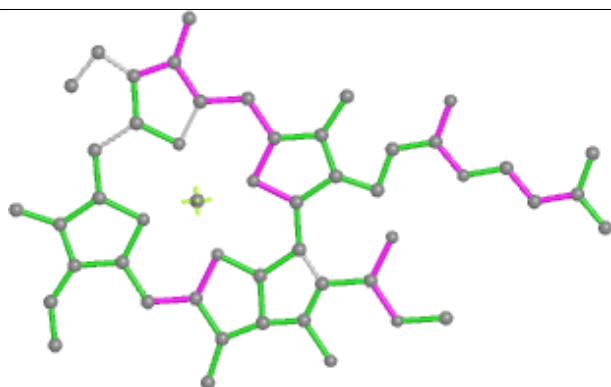


Rings

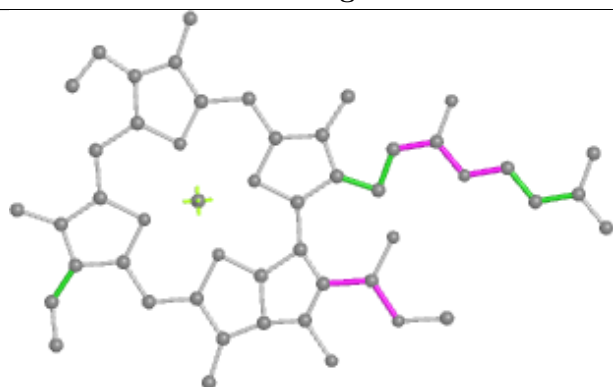
Ligand CLA A 814



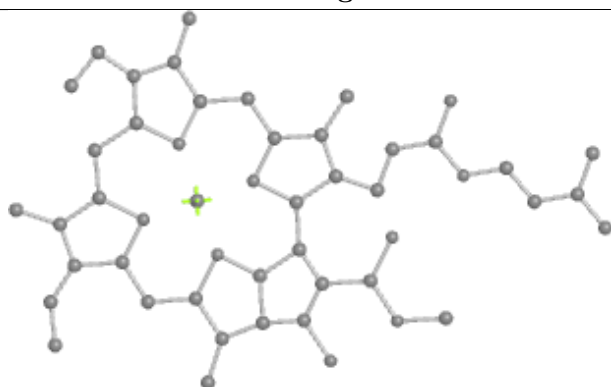
Bond lengths



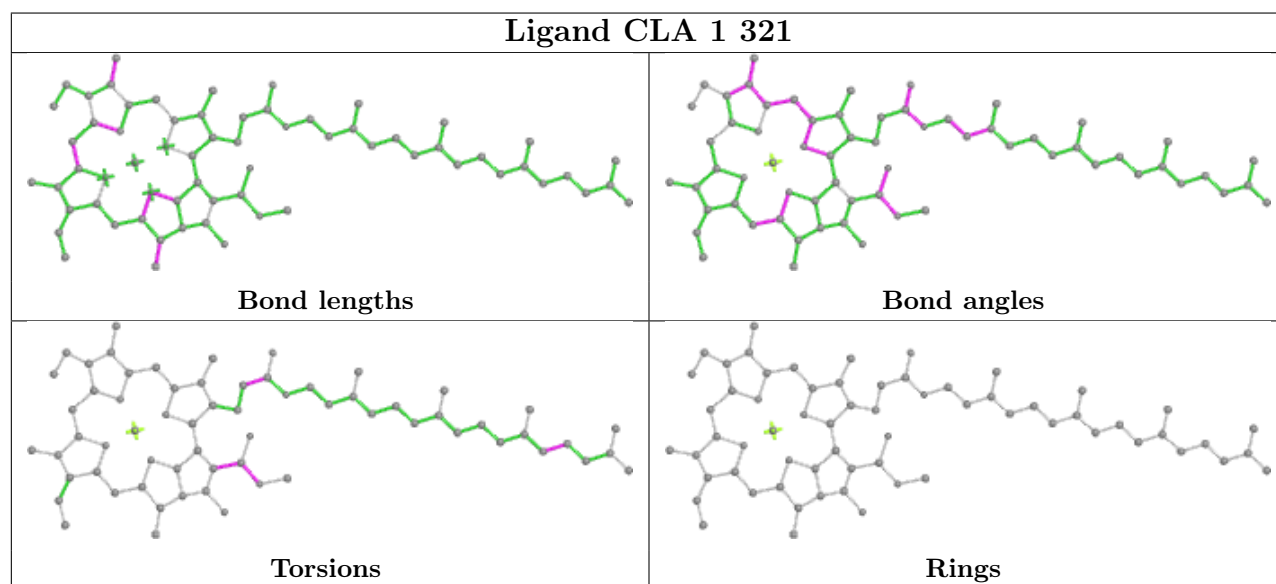
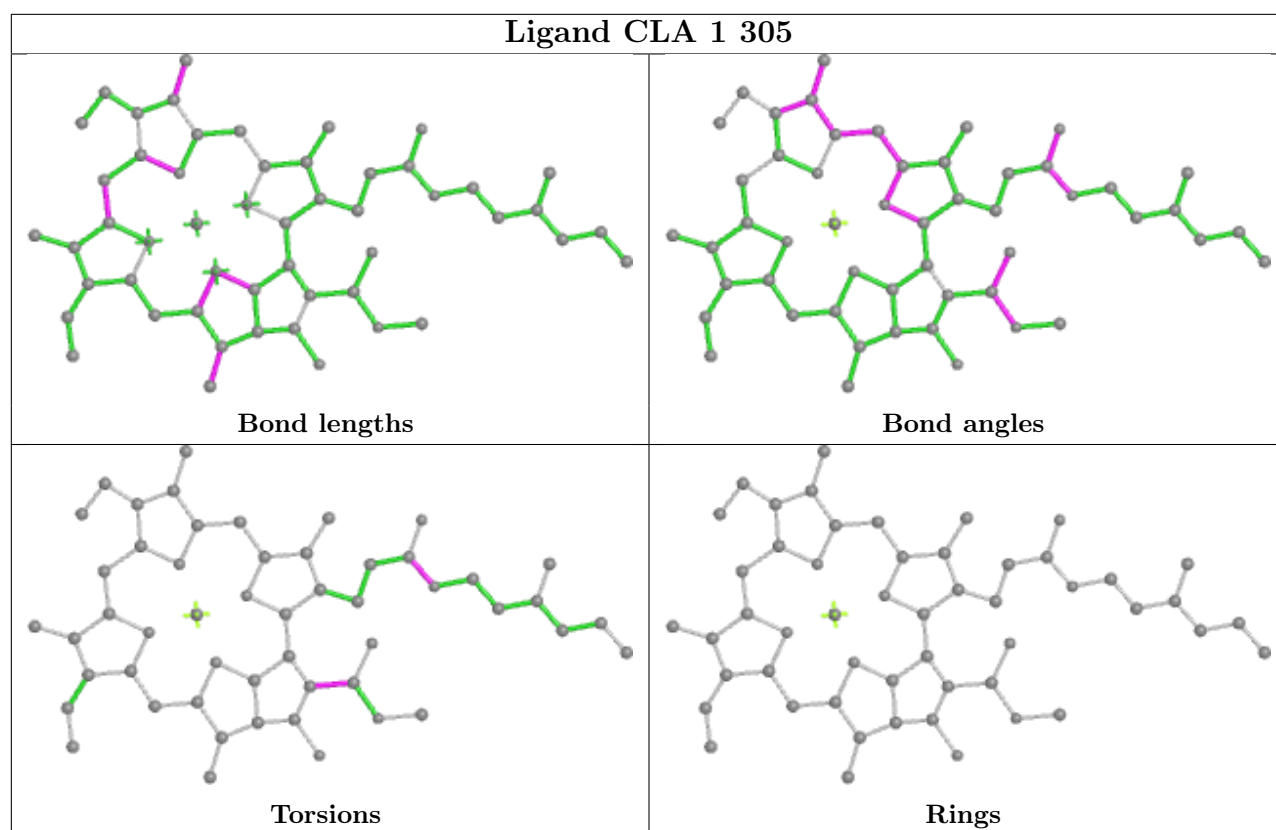
Bond angles

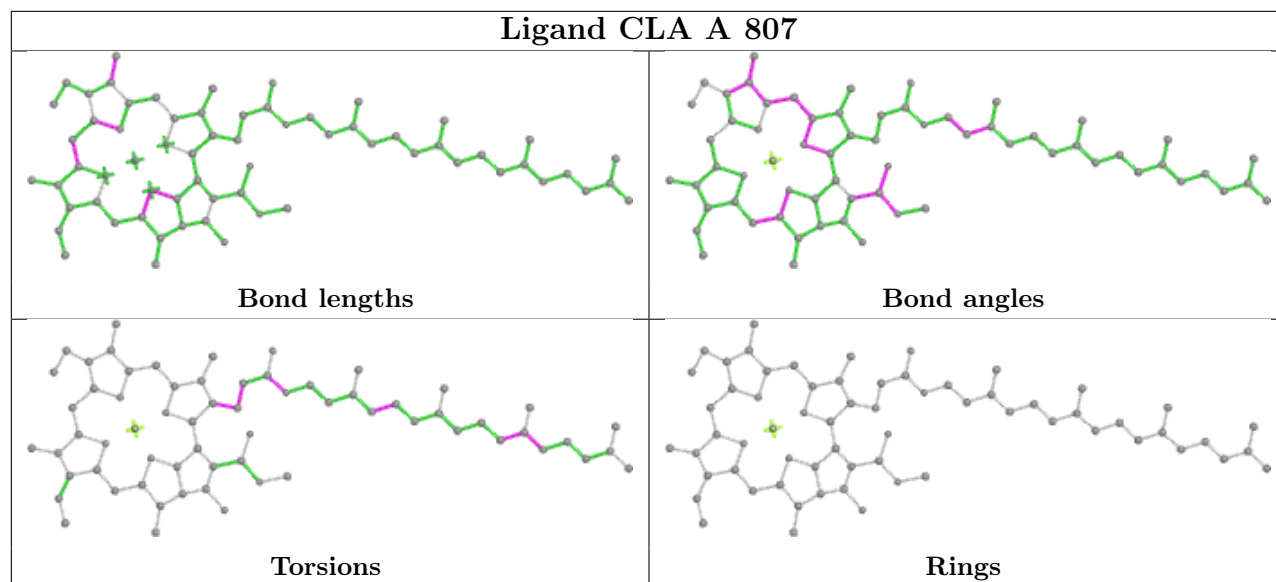
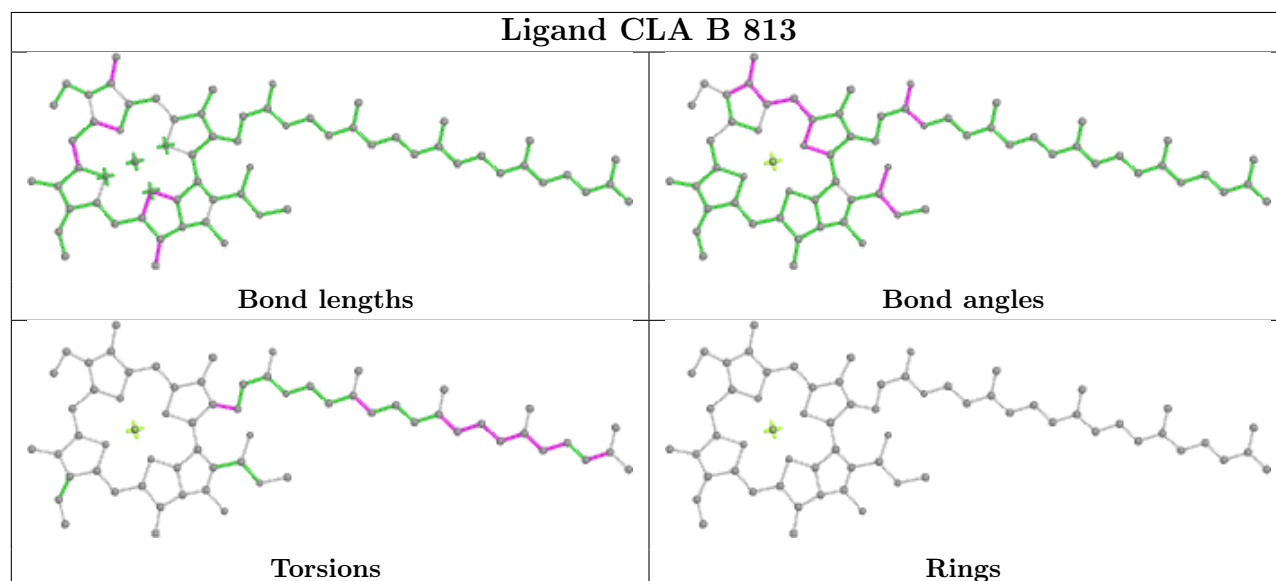
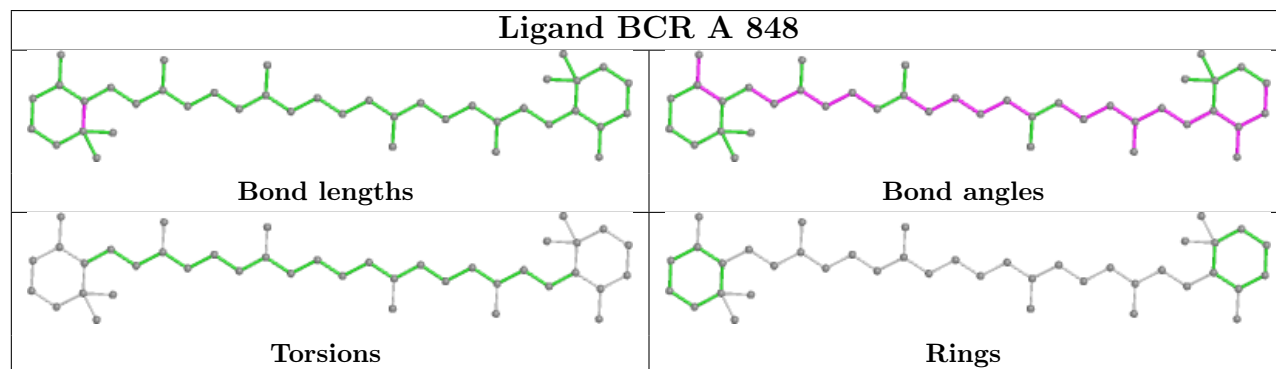


Torsions

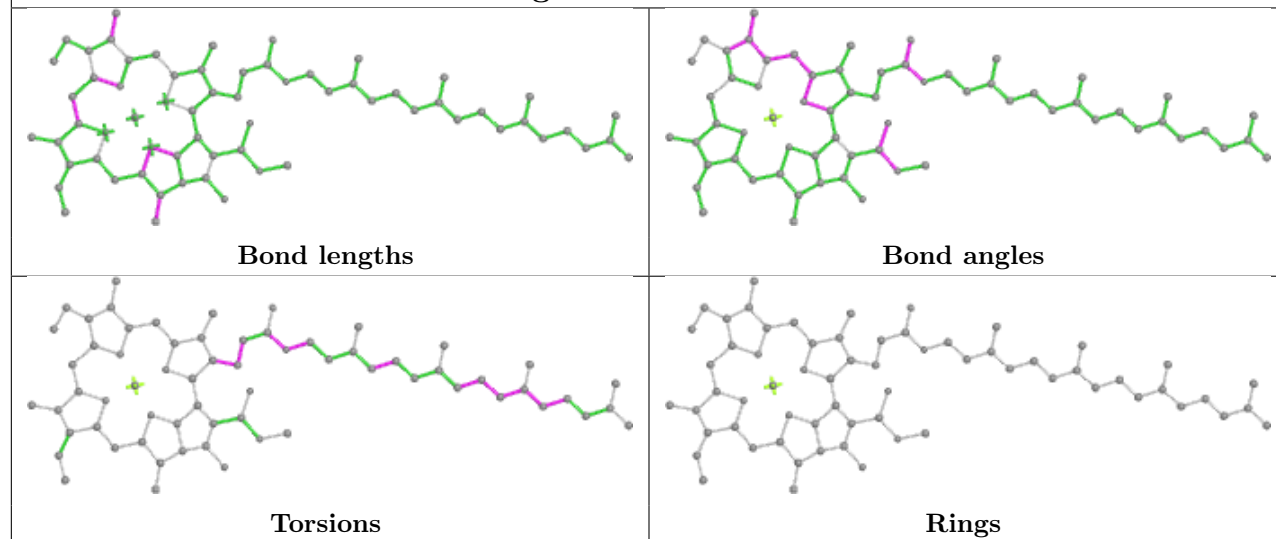


Rings

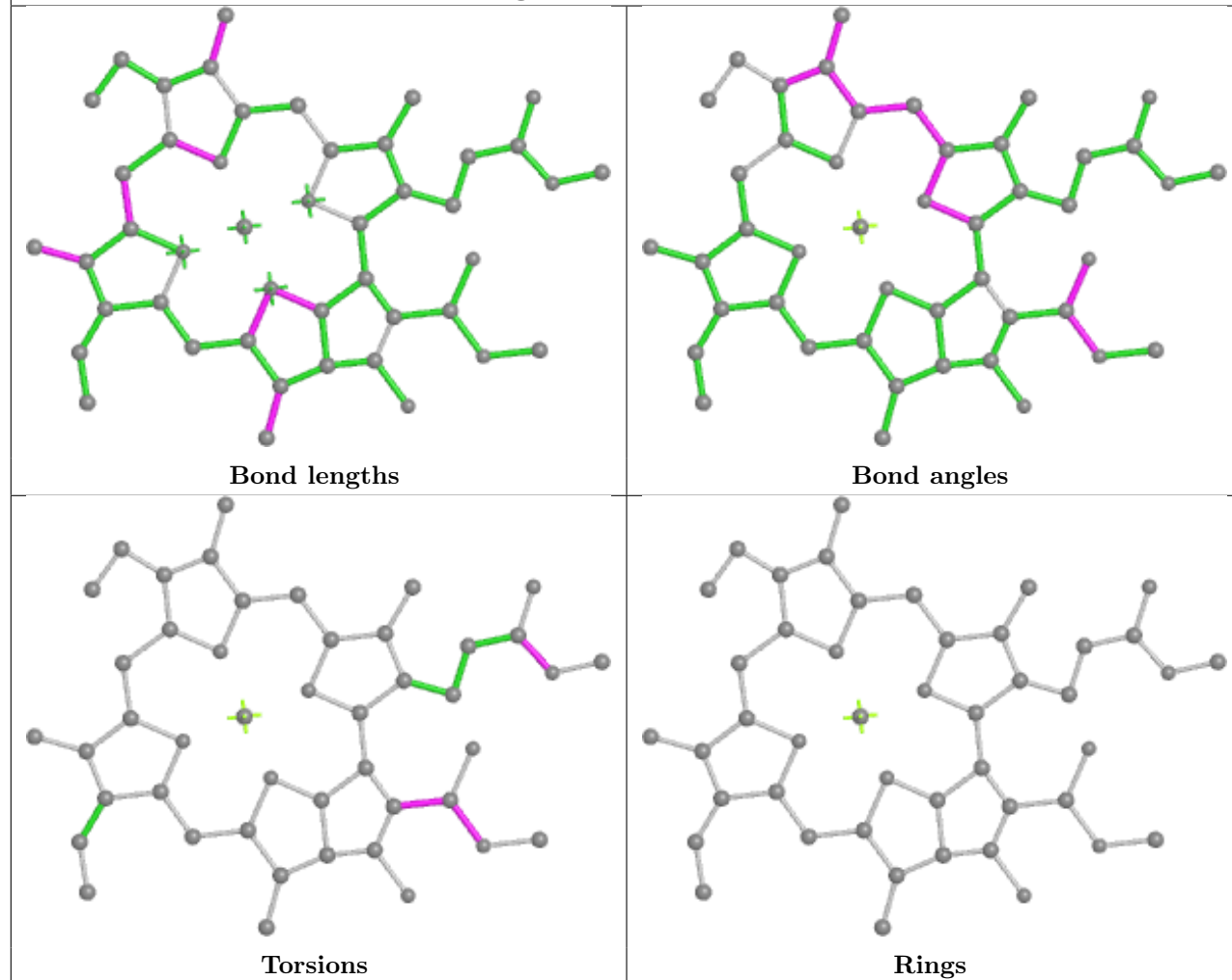


Ligand CLA A 807**Ligand CLA B 813****Ligand BCR A 848**

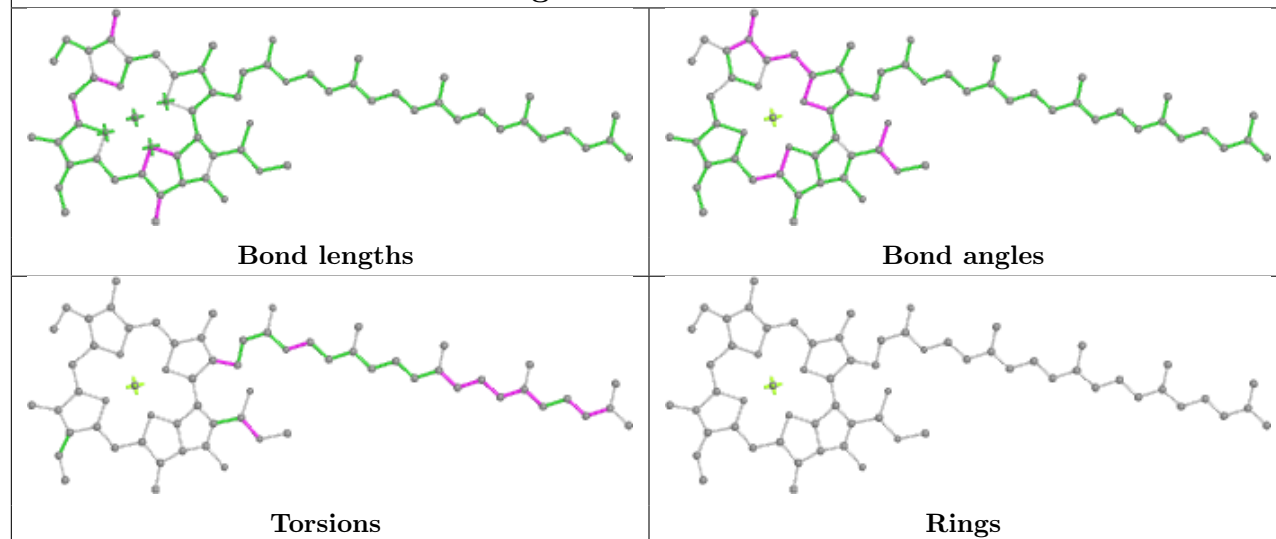
Ligand CLA B 817



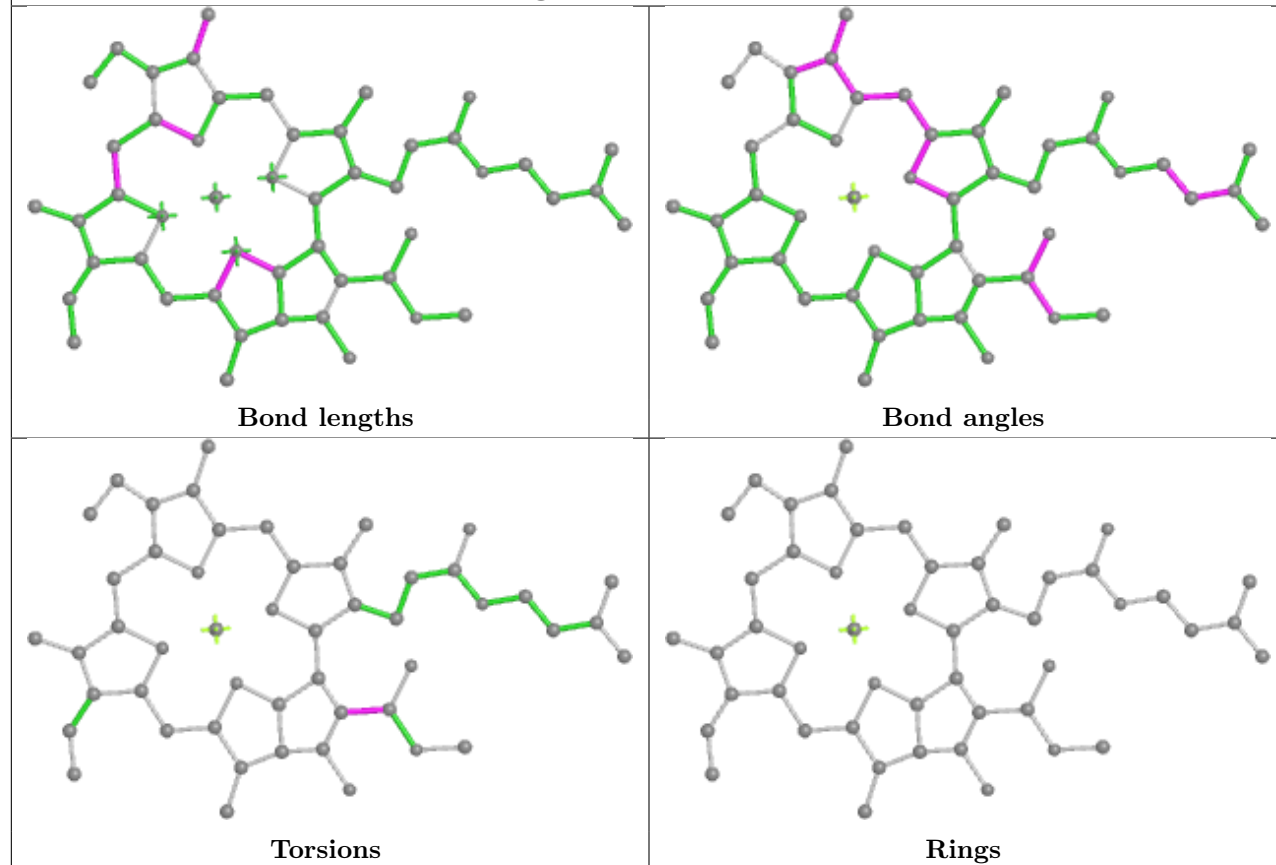
Ligand CLA K 203



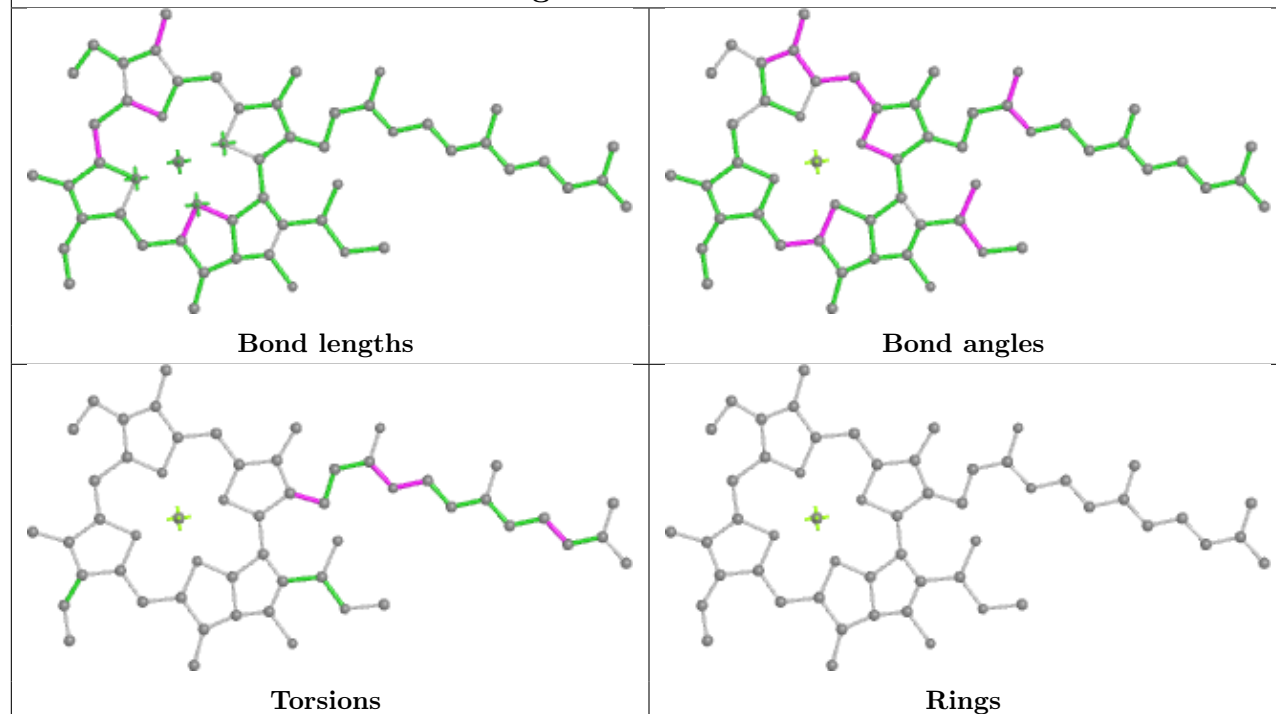
Ligand CLA A 810



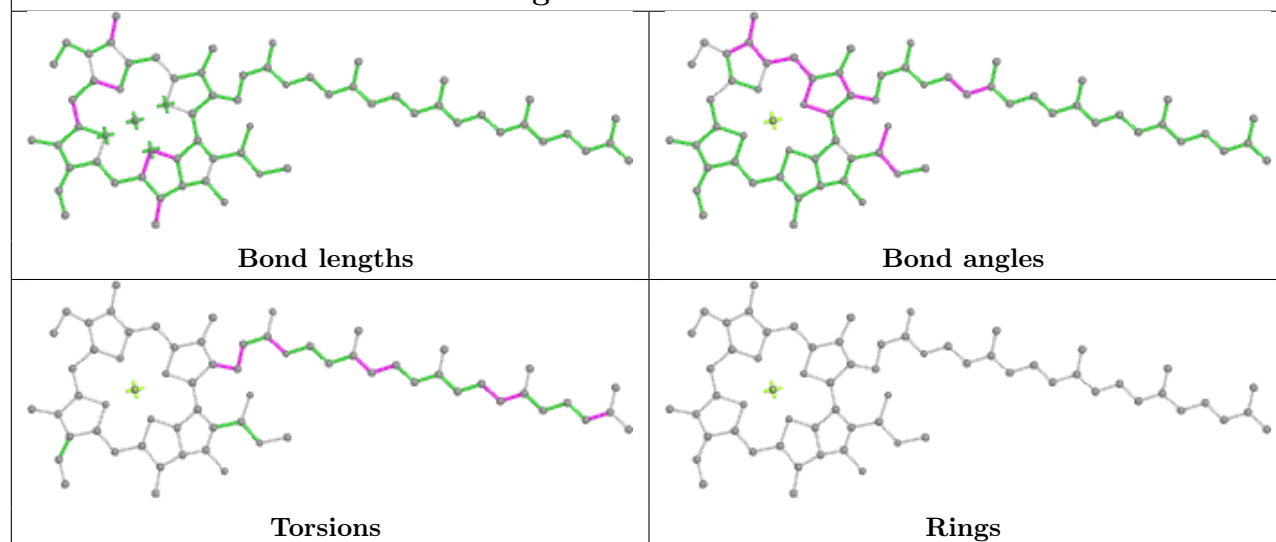
Ligand CLA B 820

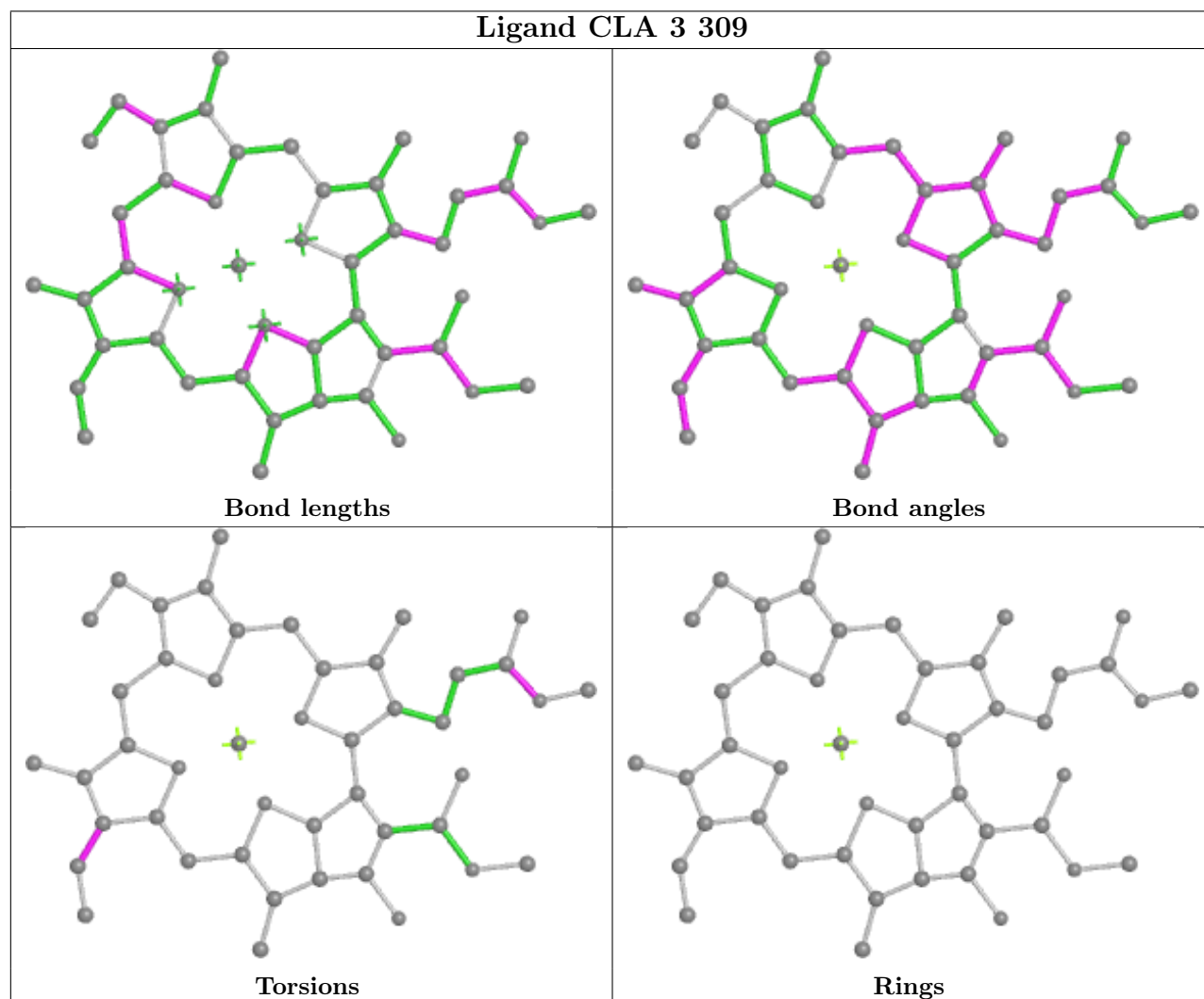
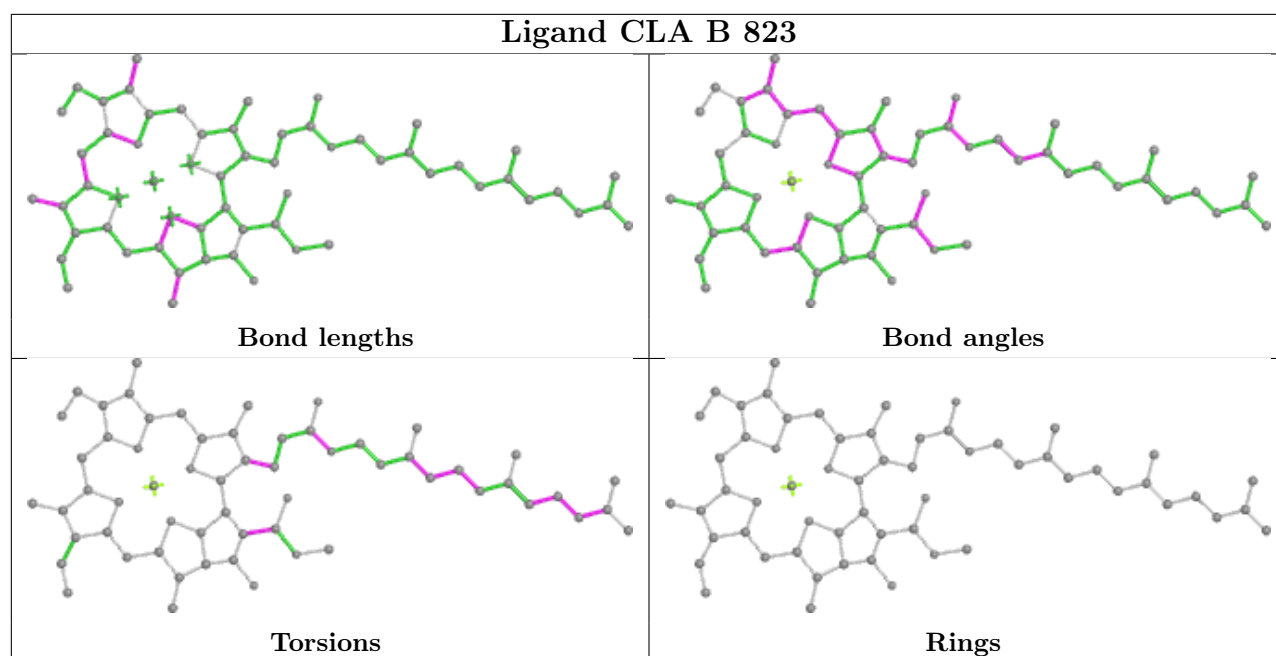


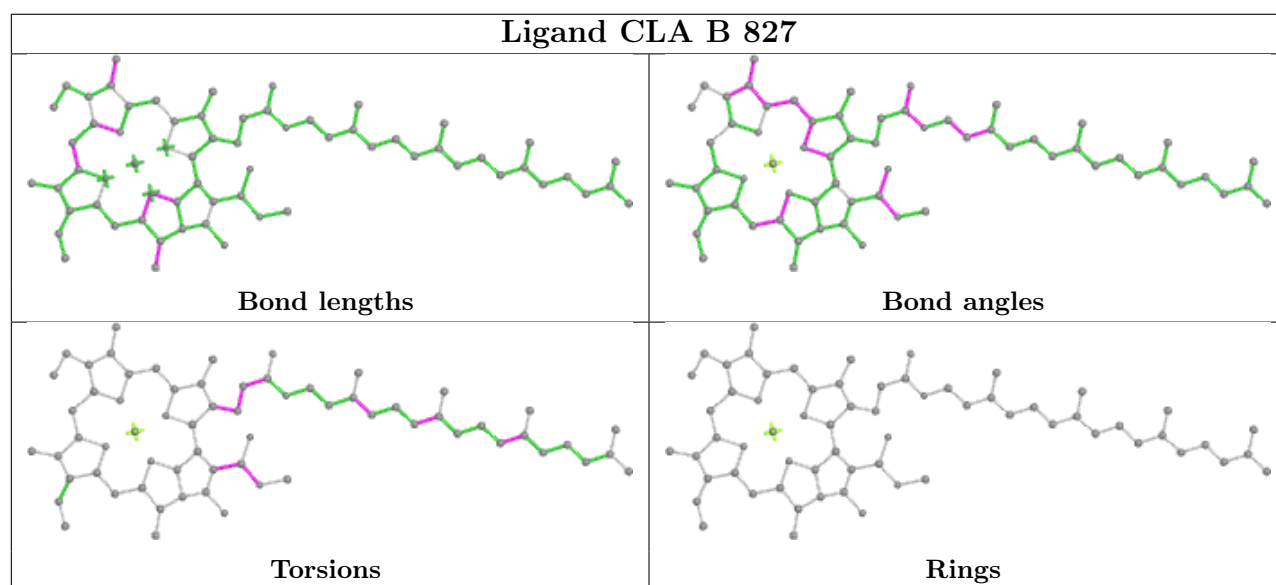
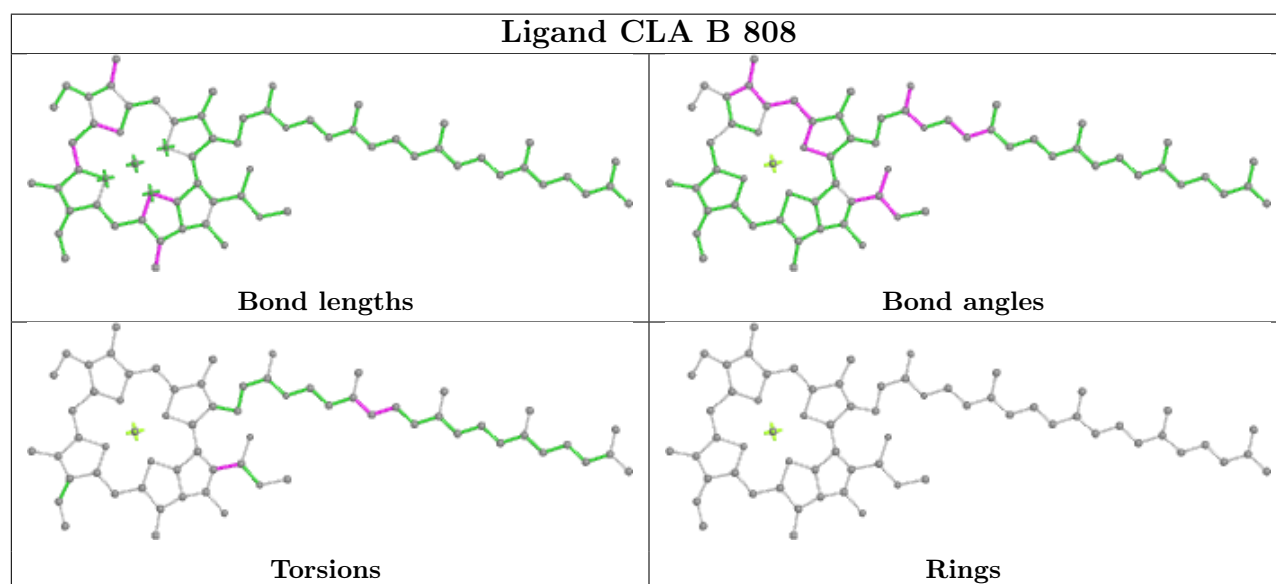
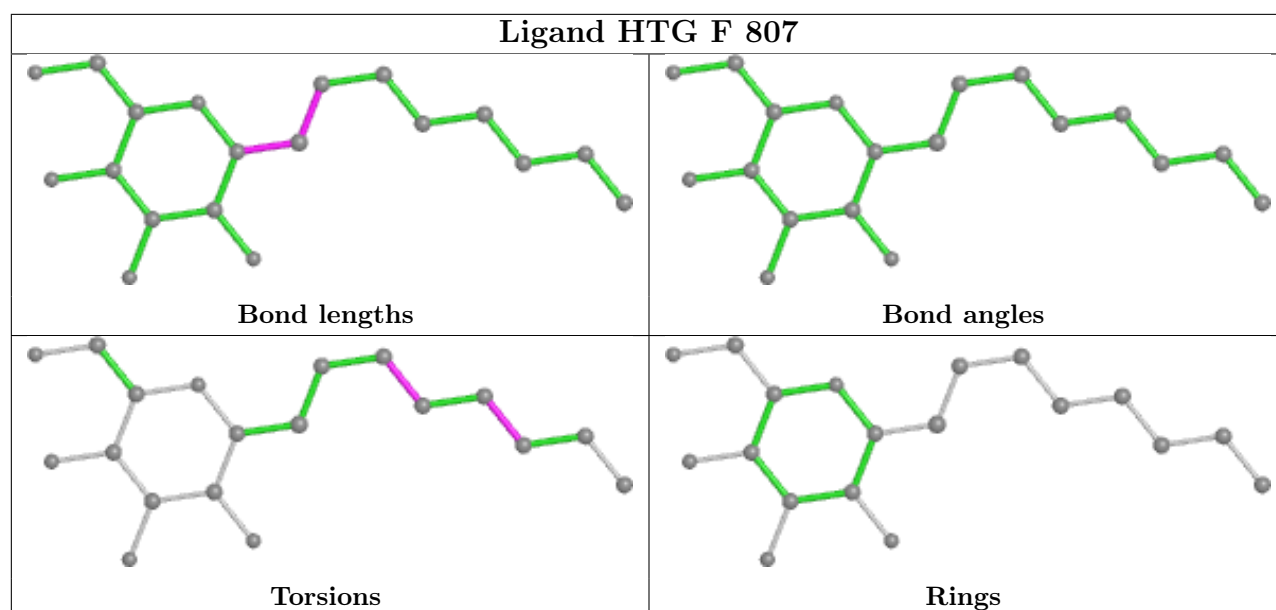
Ligand CLA B 812

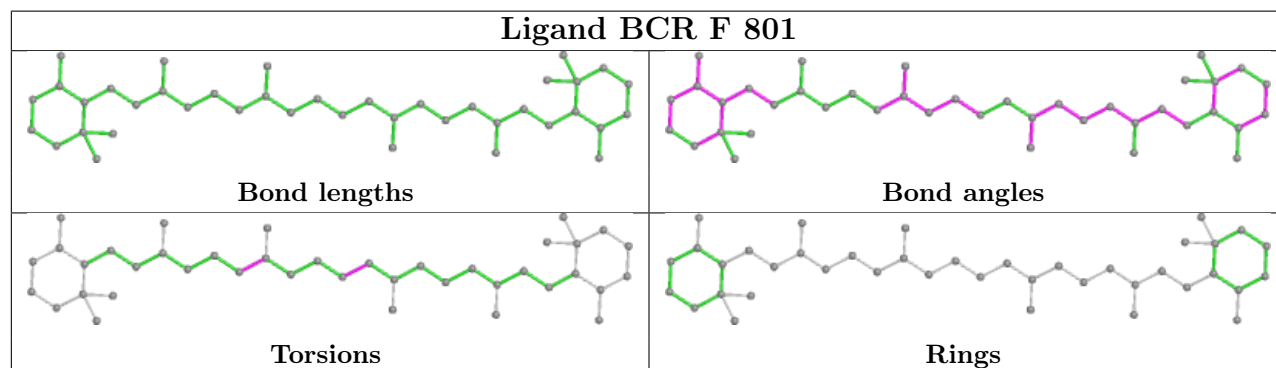
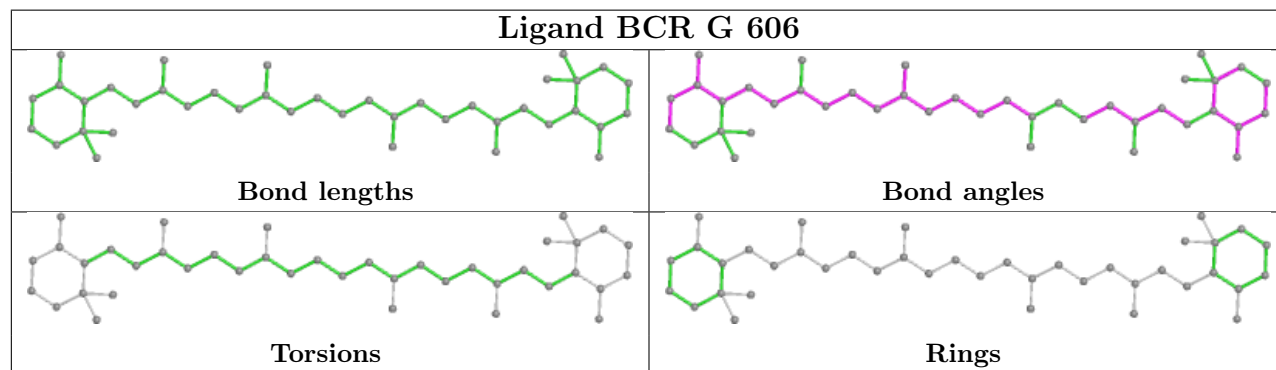
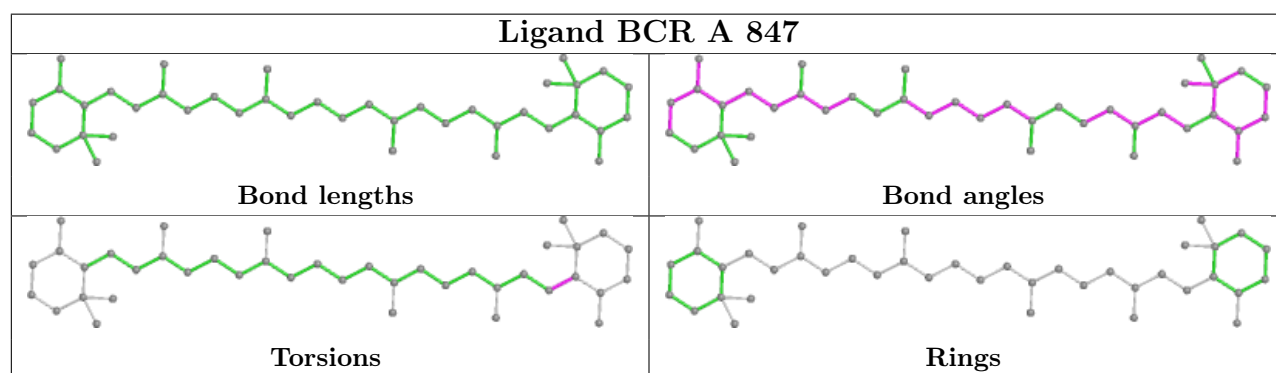
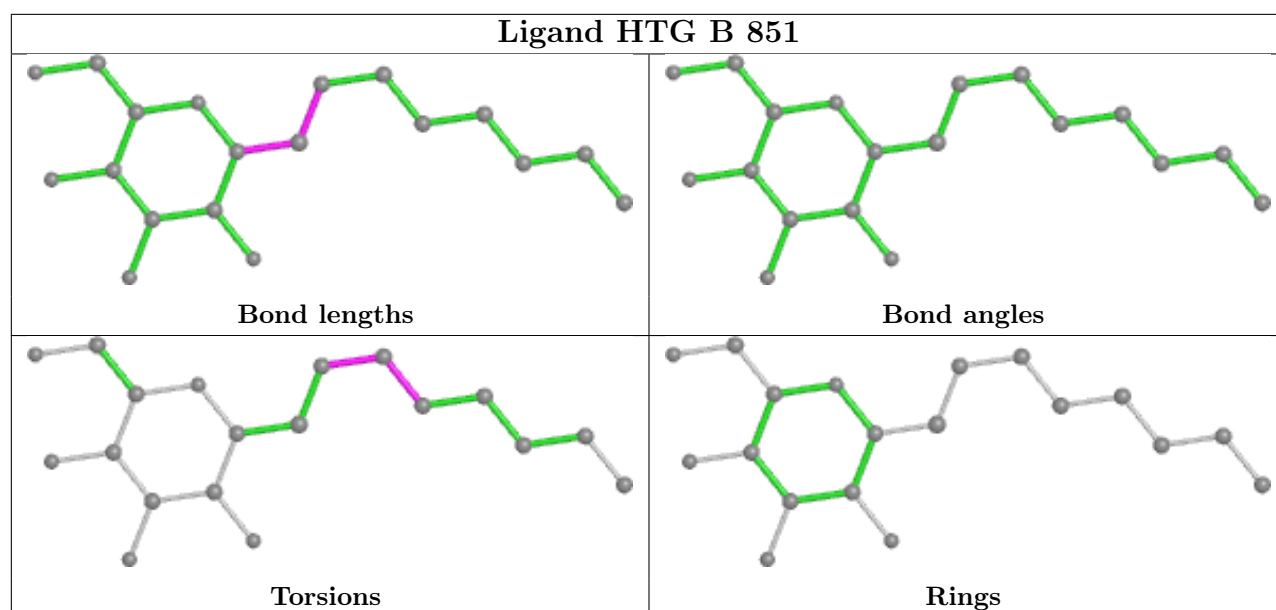


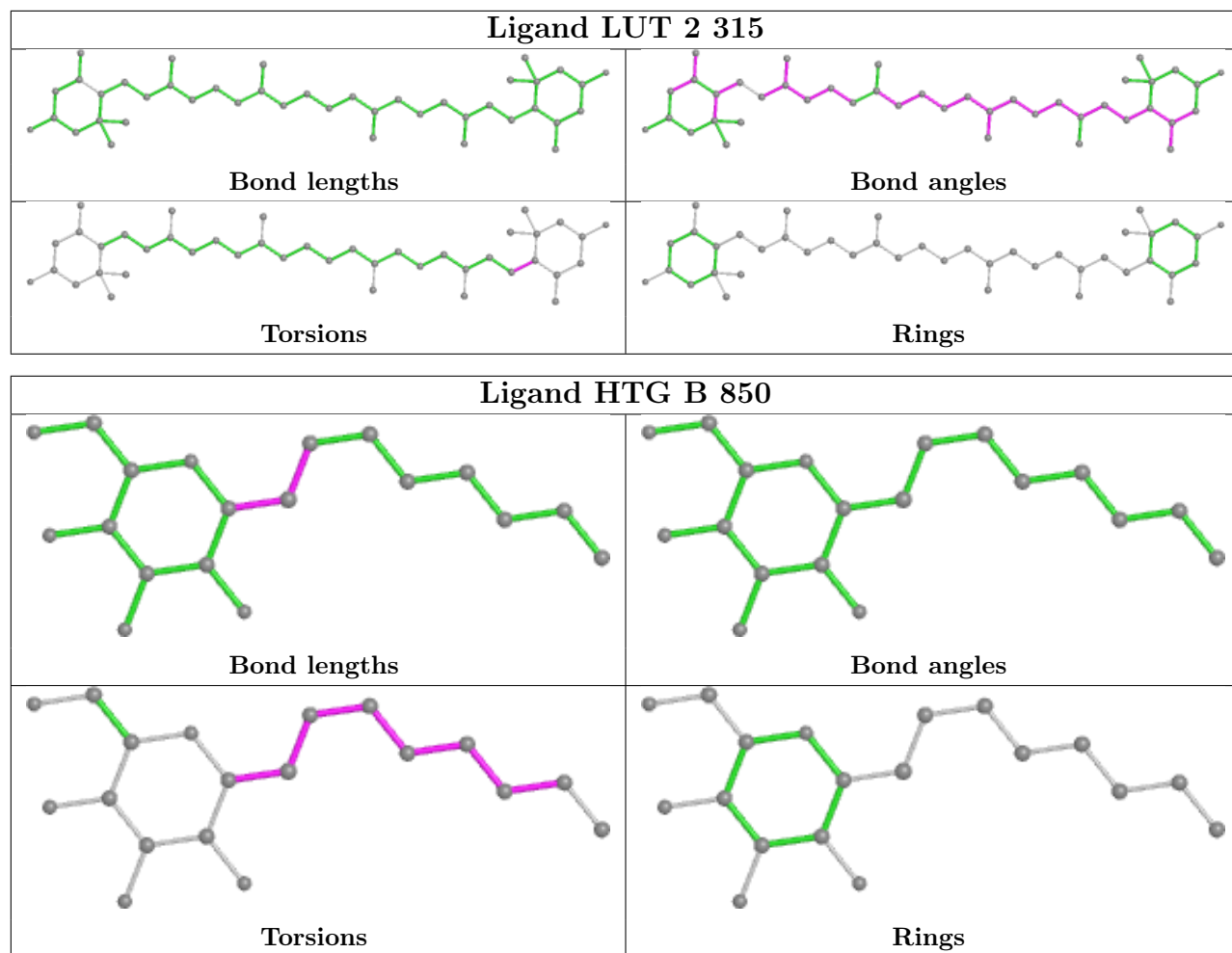
Ligand CLA B 822

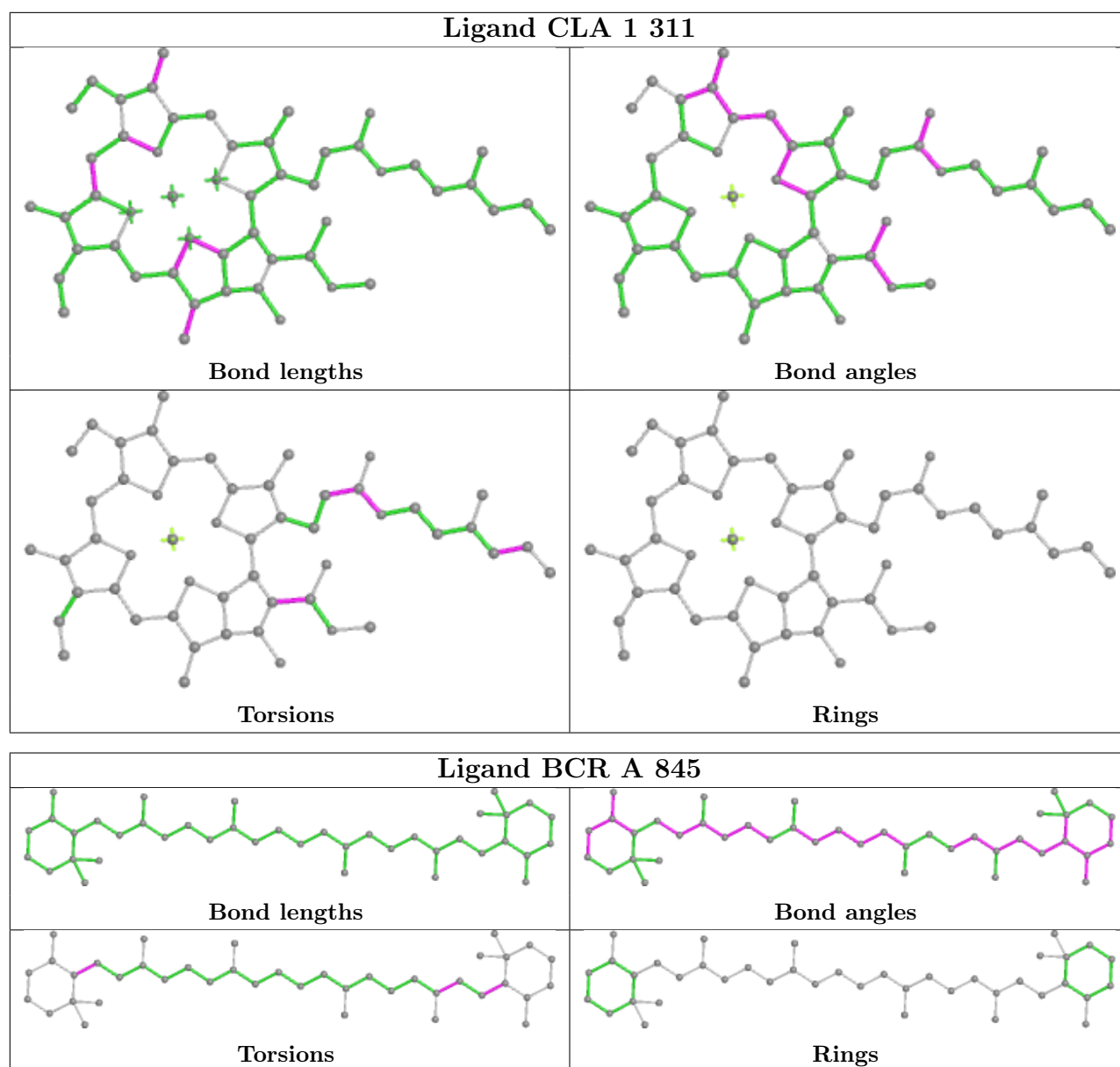




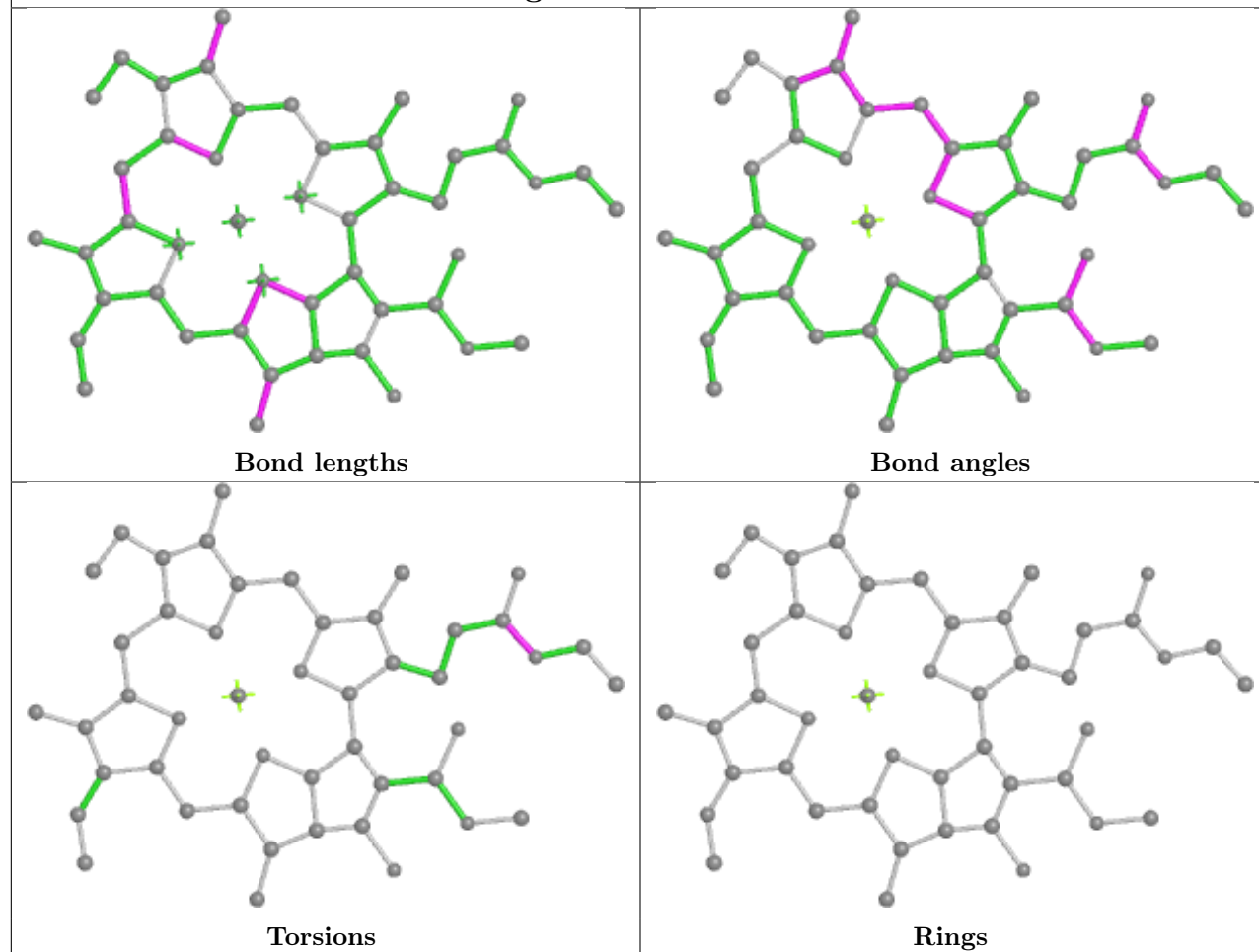




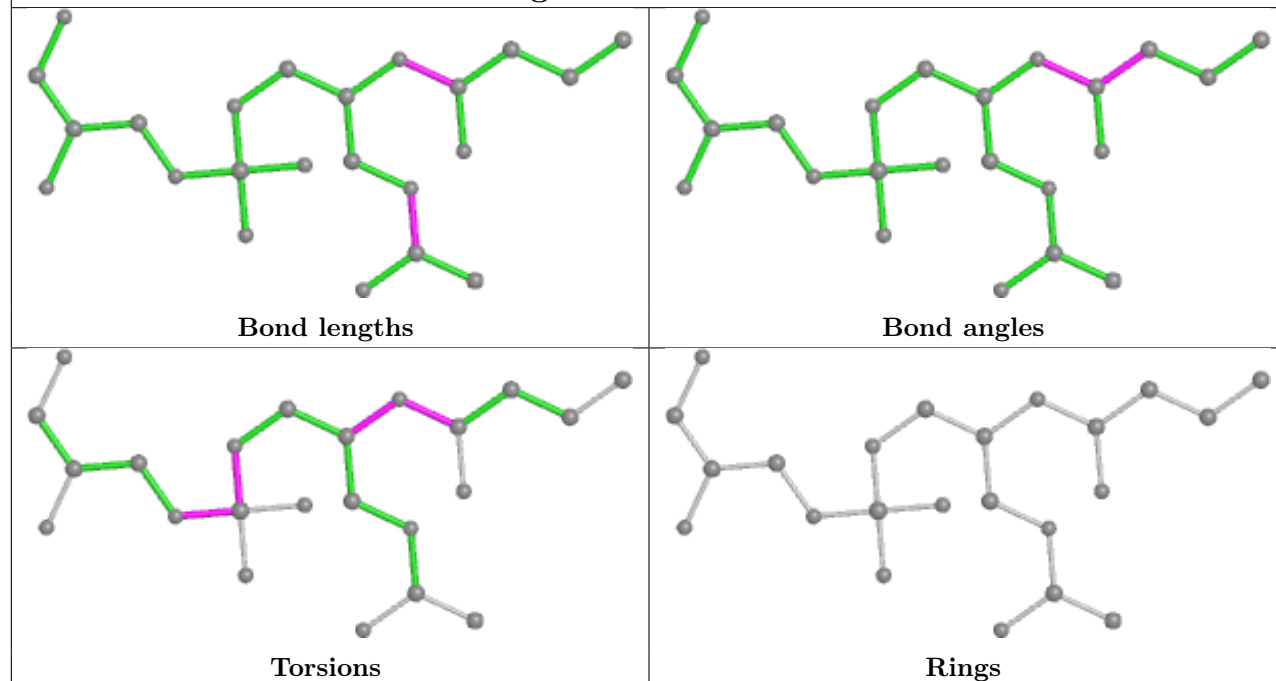




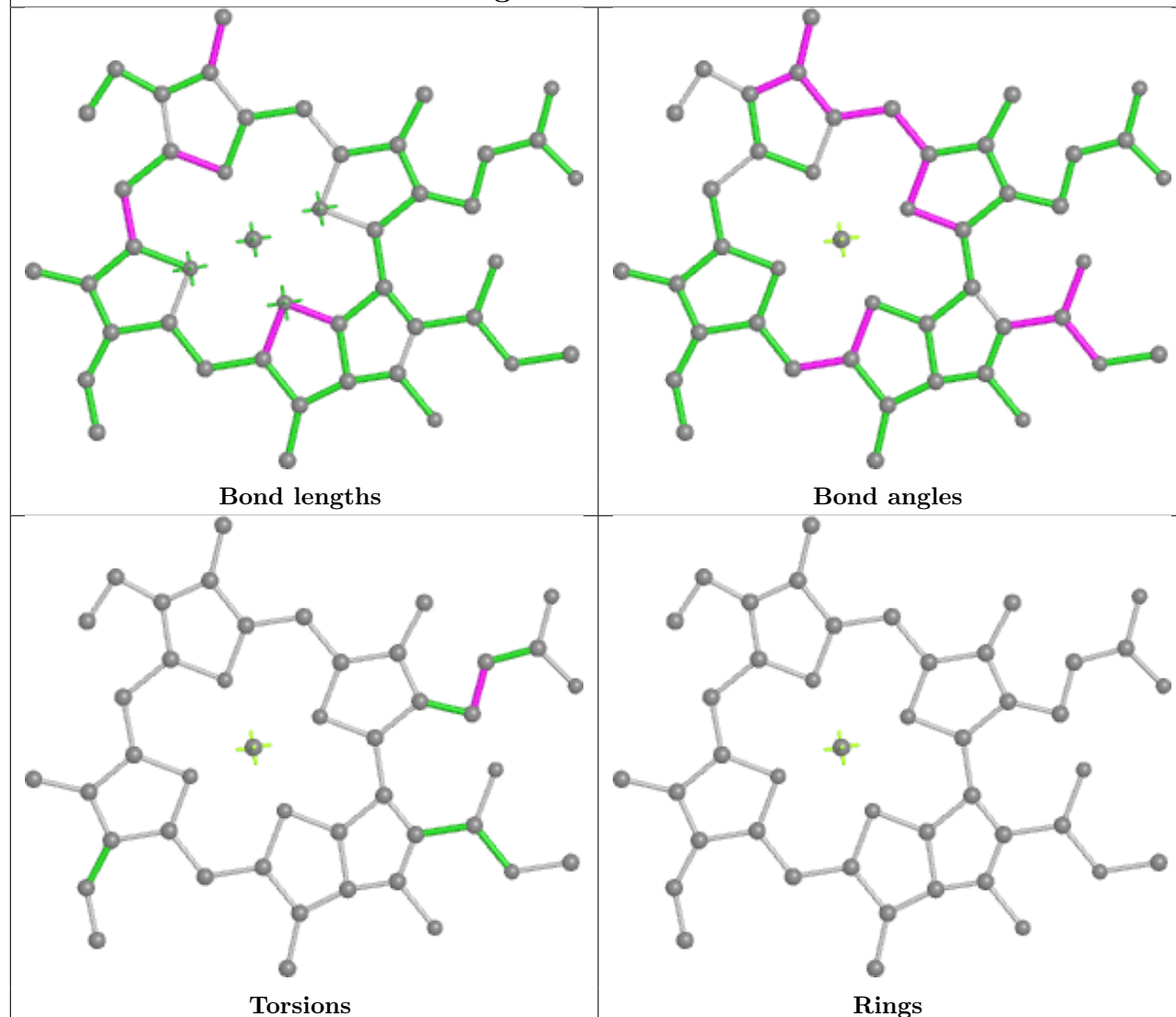
Ligand CLA B 837



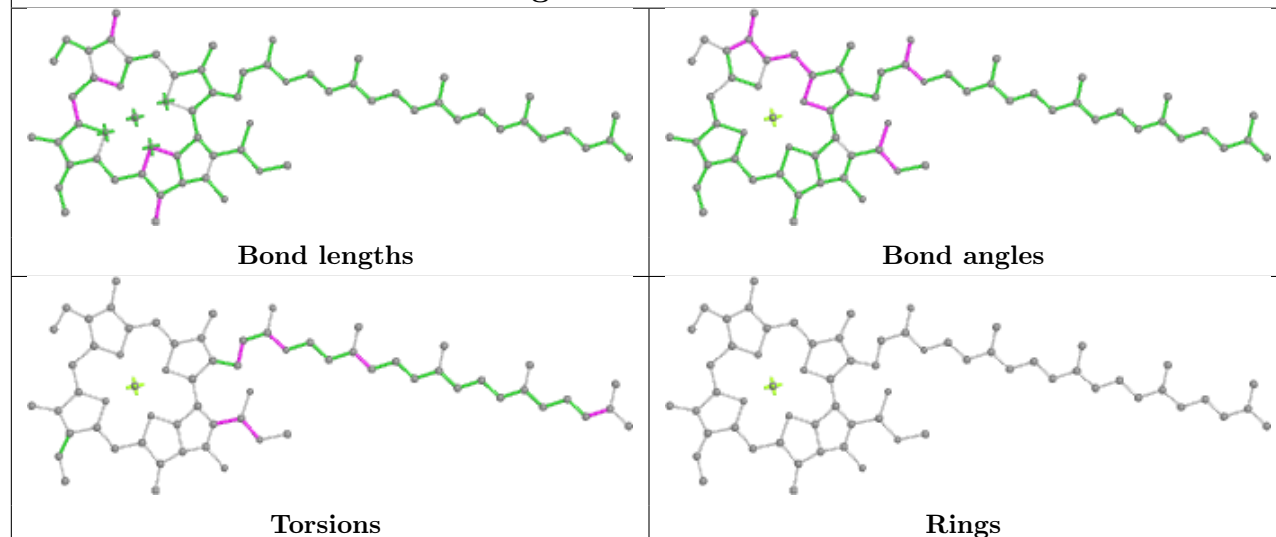
Ligand LHG B 849

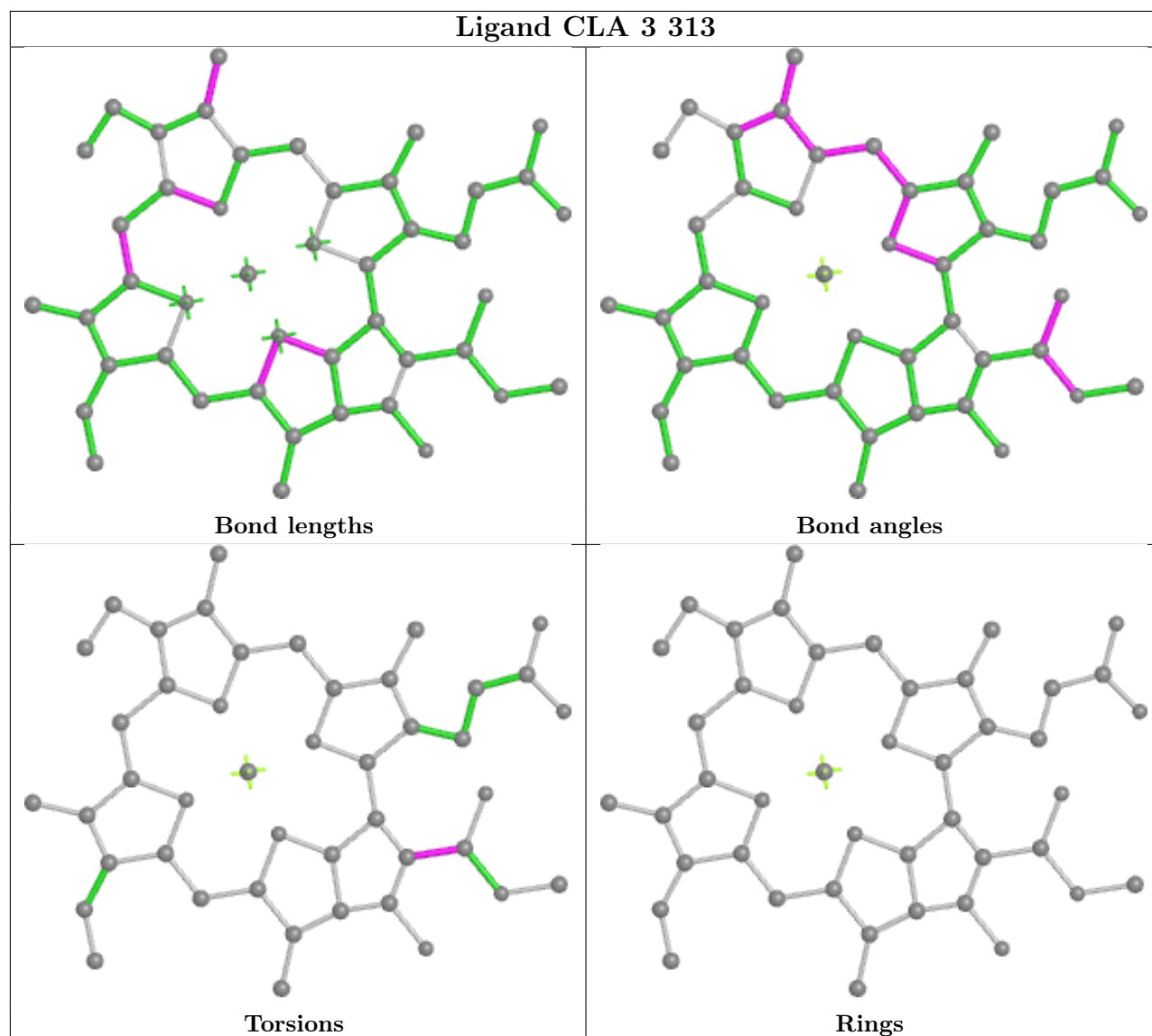
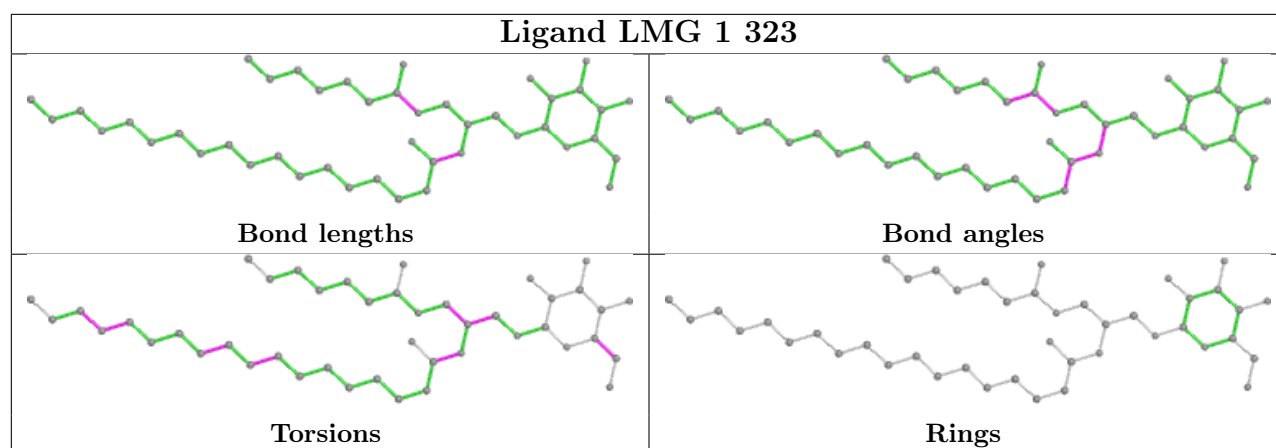


Ligand CLA 4 313

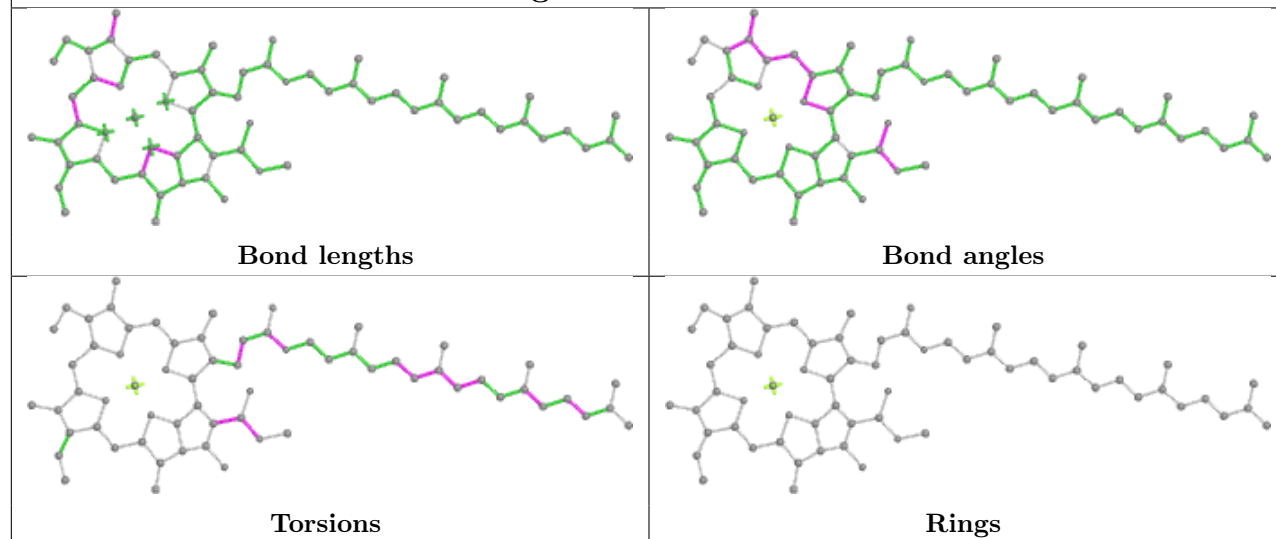


Ligand CLA A 828

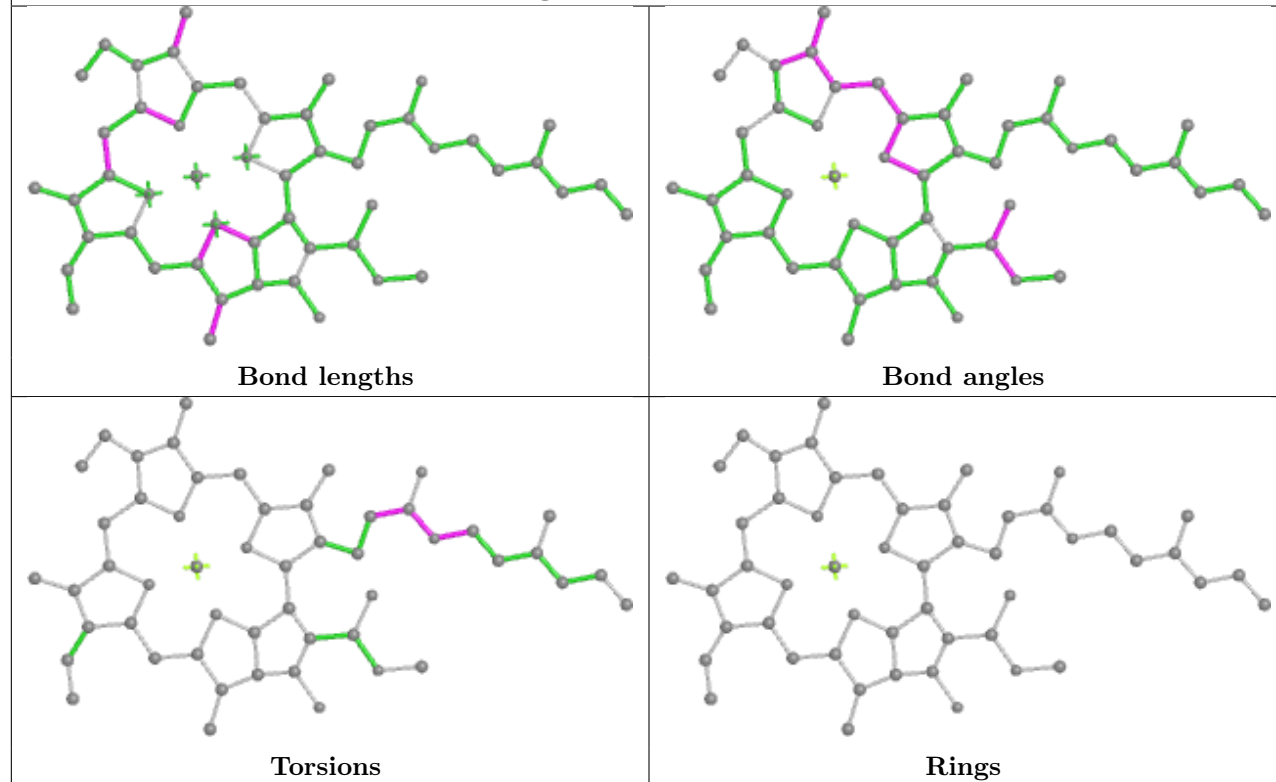




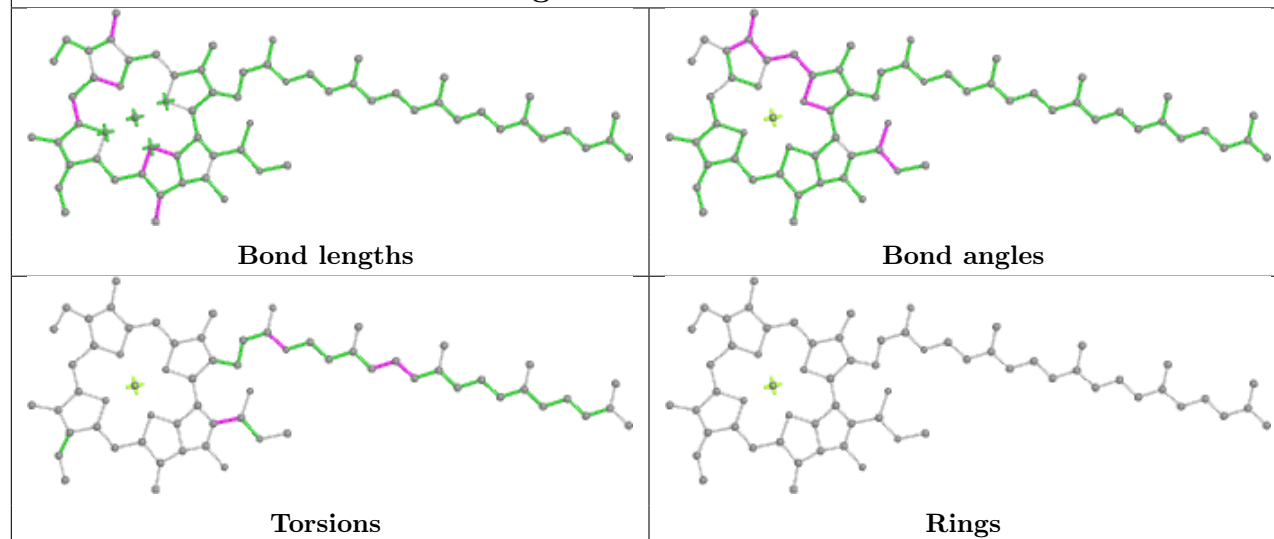
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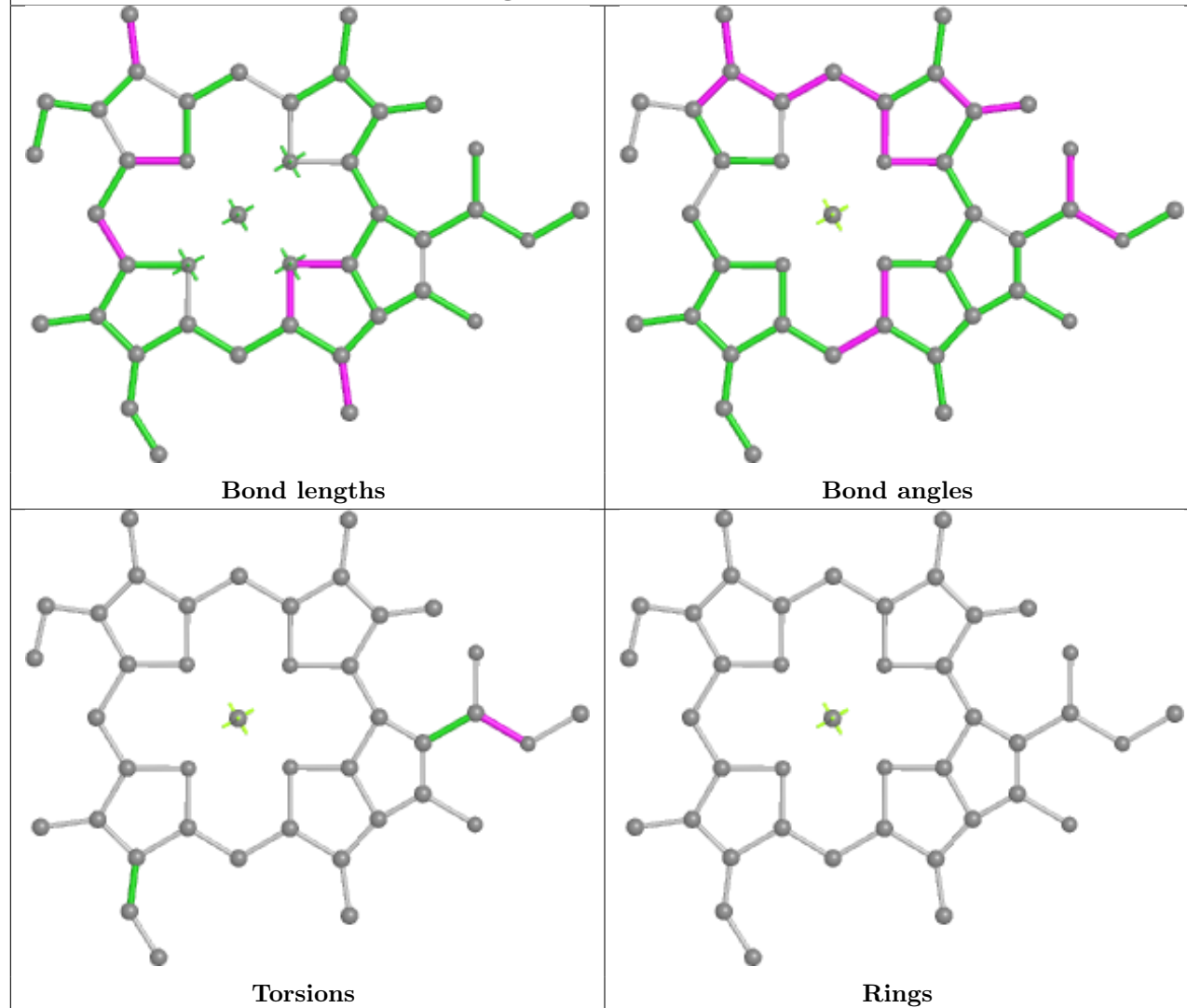
Ligand CLA 4 311

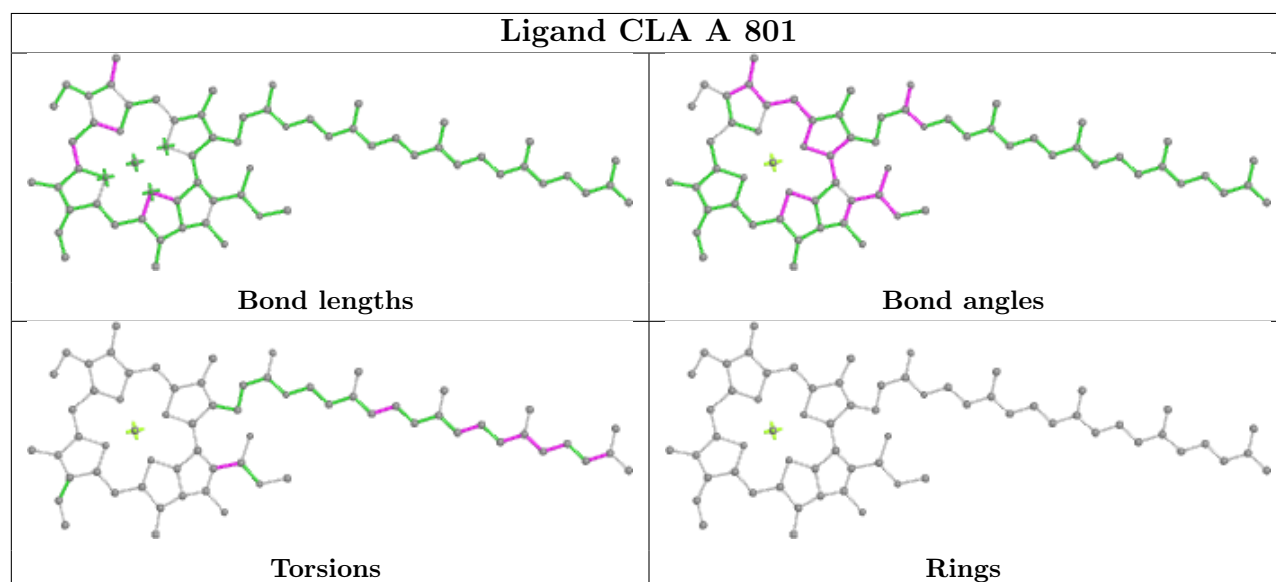
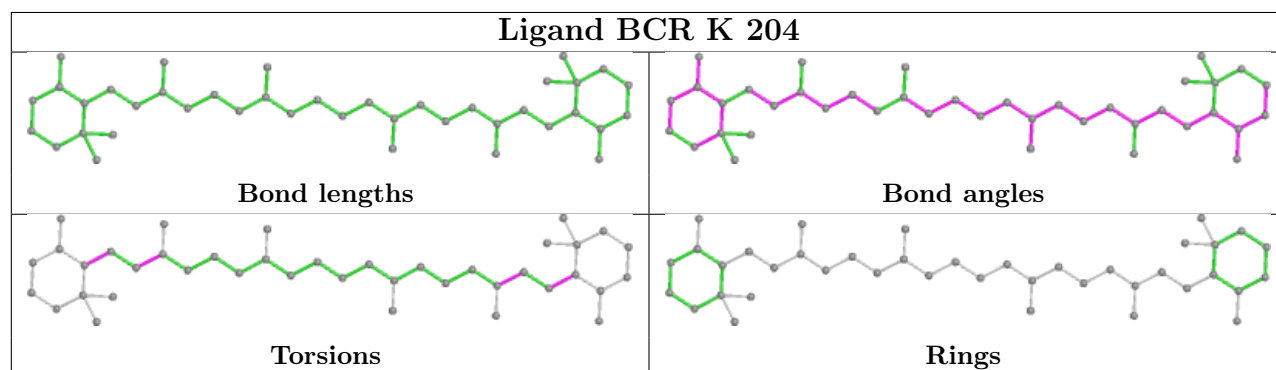
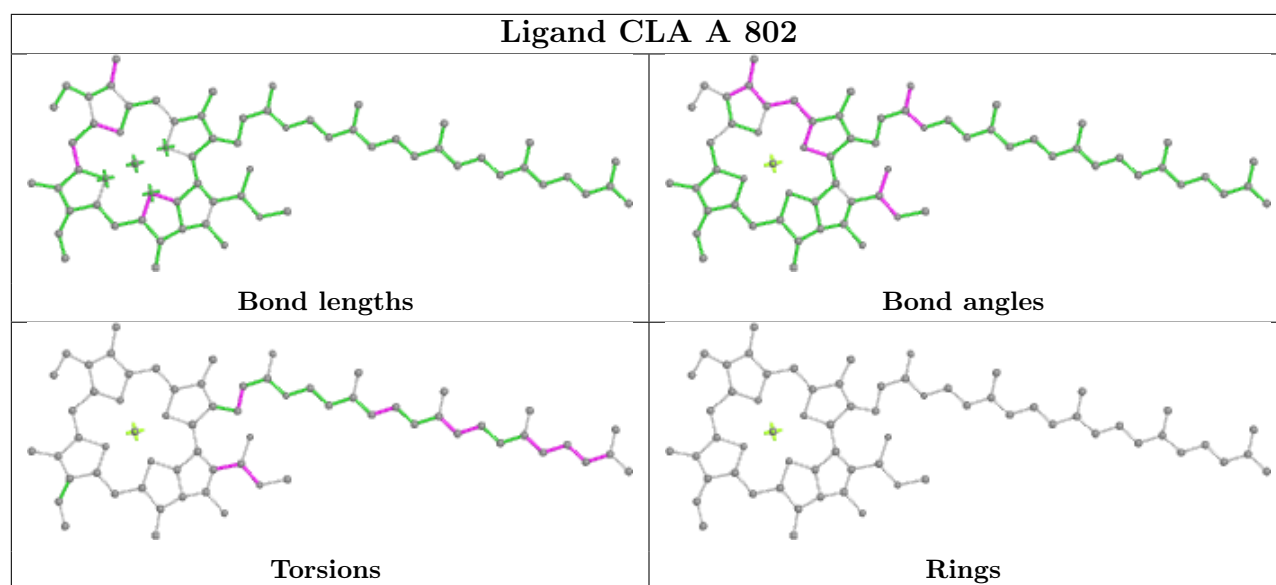


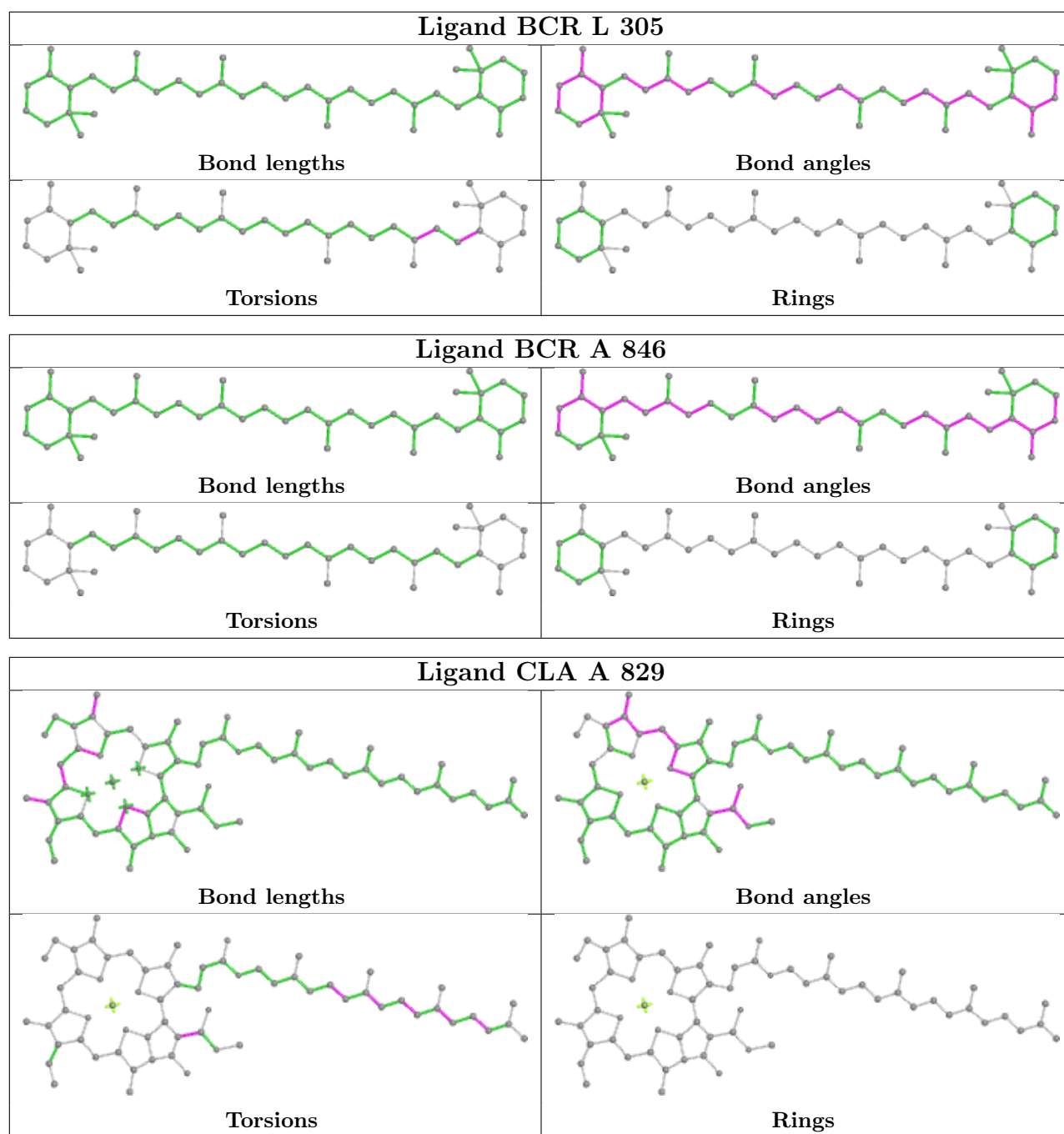
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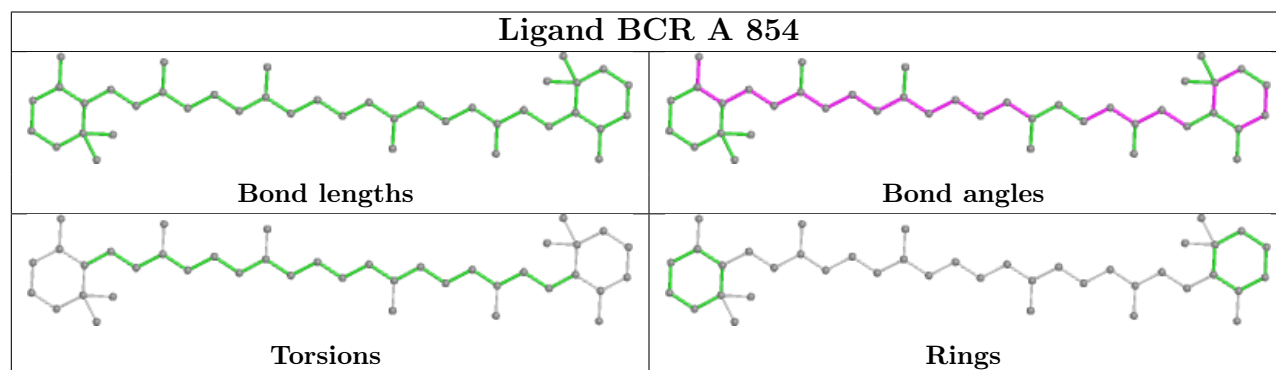
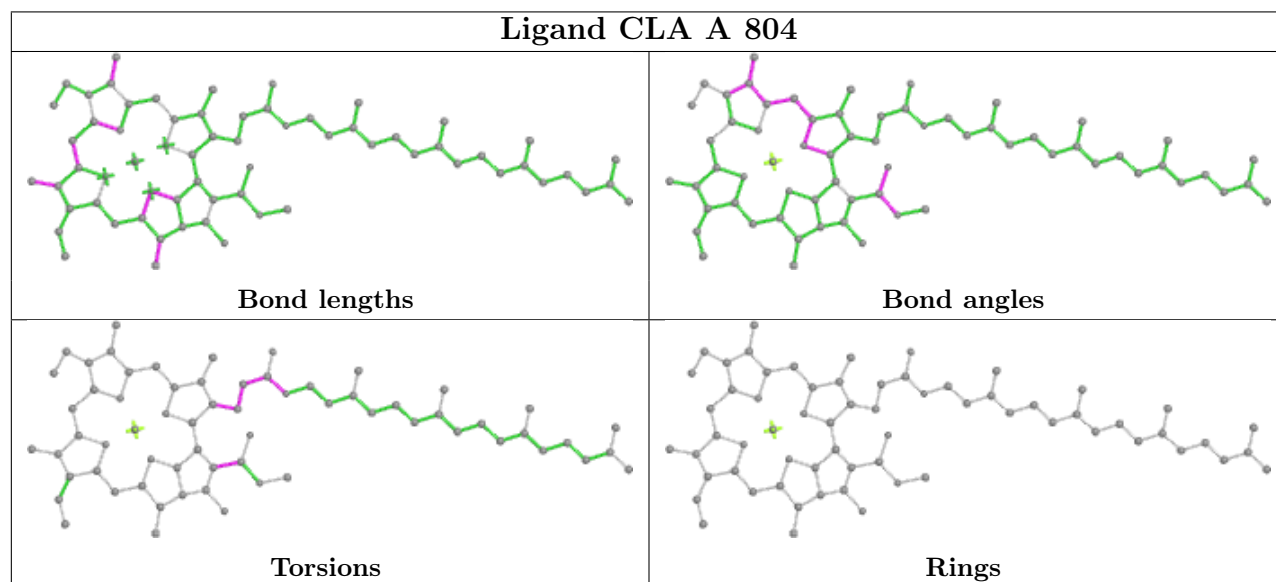
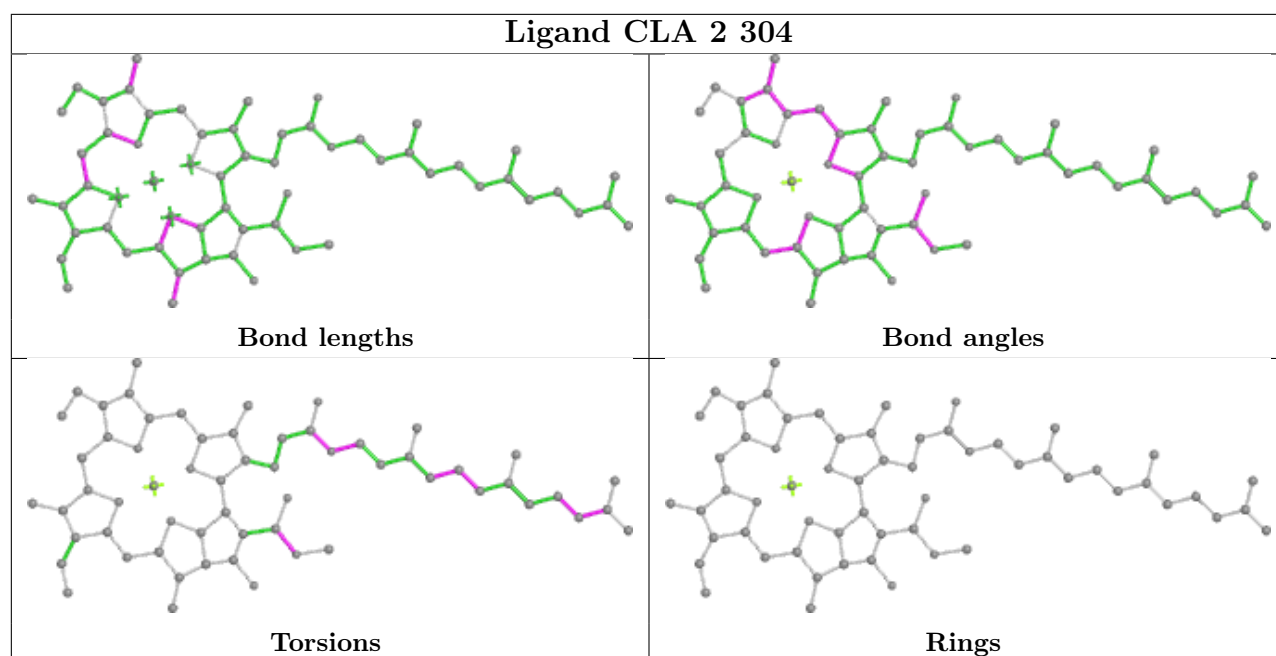


Ligand CLA 1 310

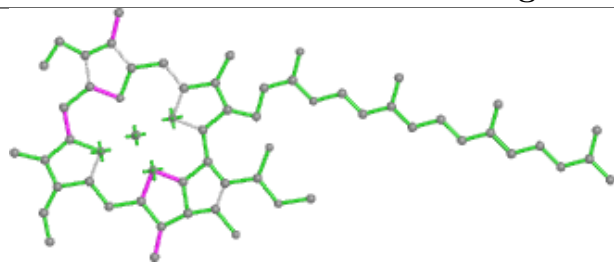




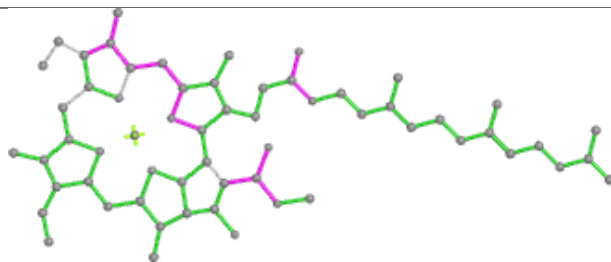




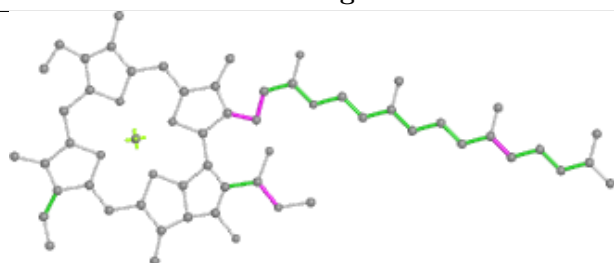
Ligand CLA 2 309



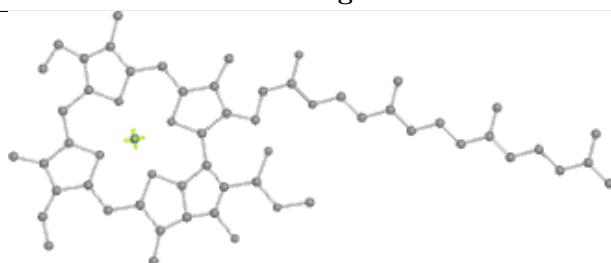
Bond lengths



Bond angles

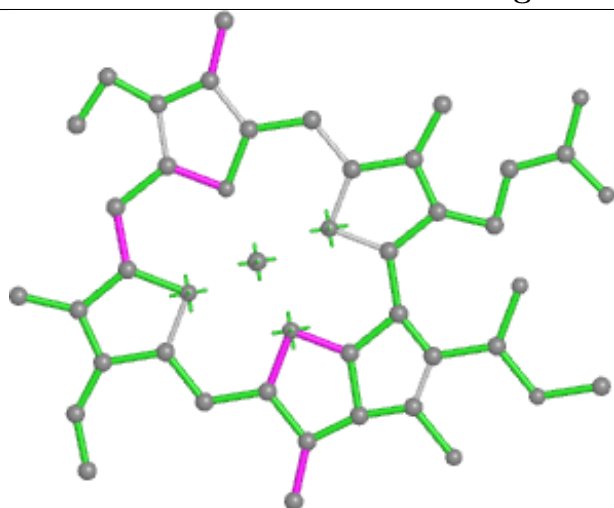


Torsions

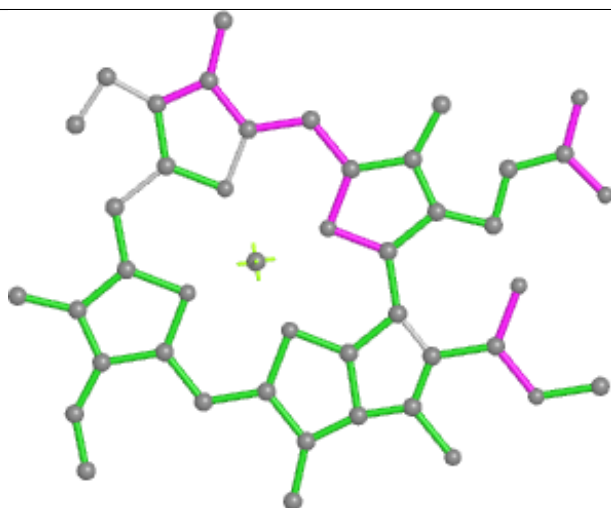


Rings

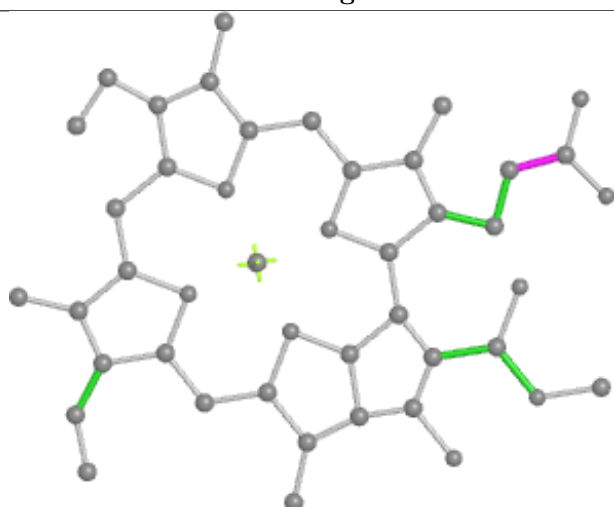
Ligand CLA A 819



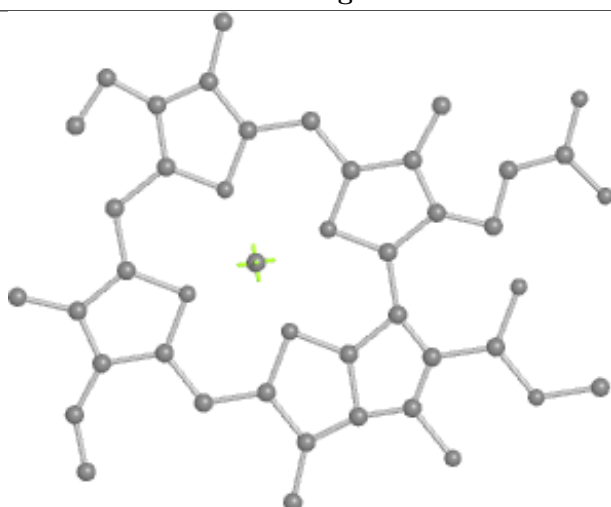
Bond lengths



Bond angles

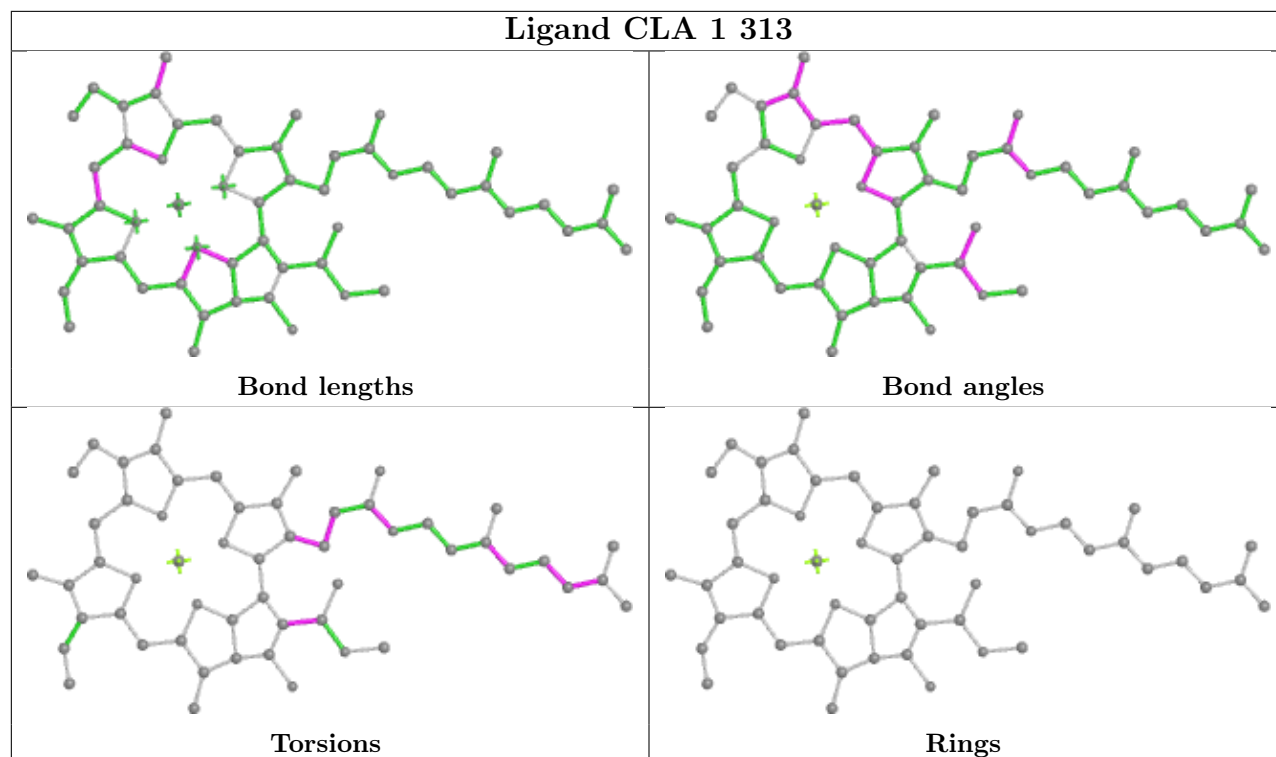


Torsions

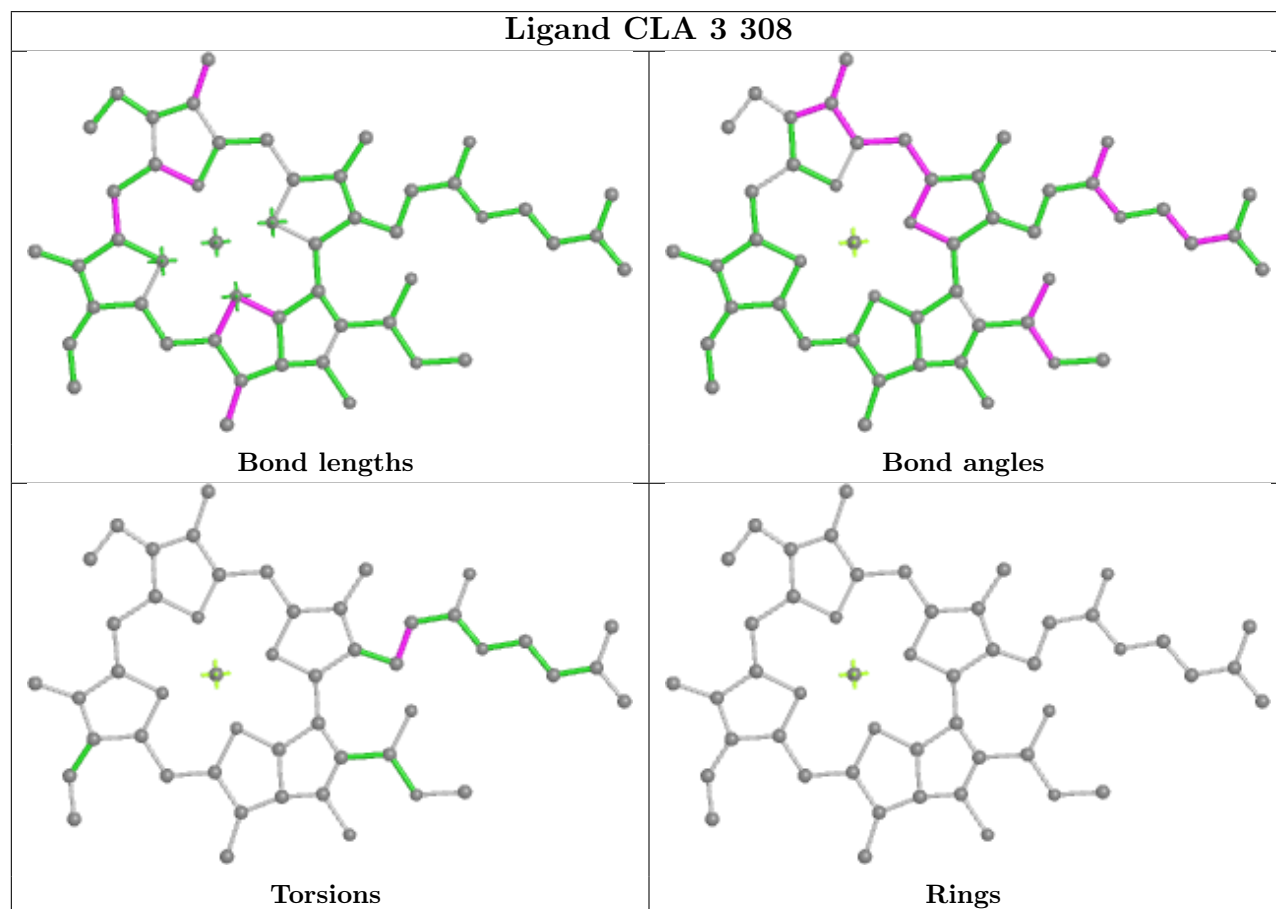


Rings

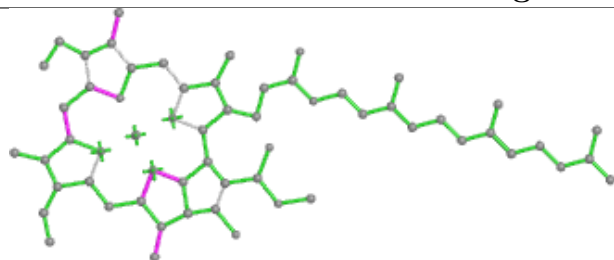
Ligand CLA 1 313



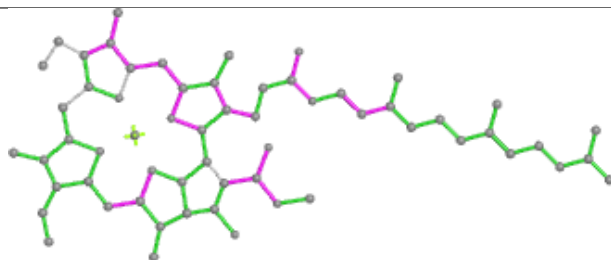
Ligand CLA 3 308



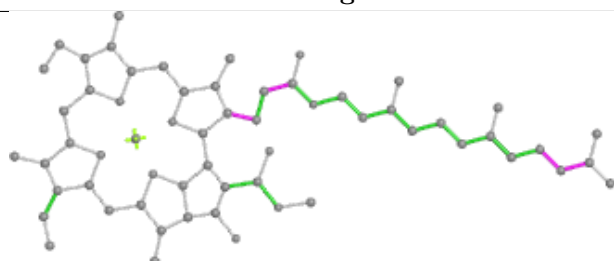
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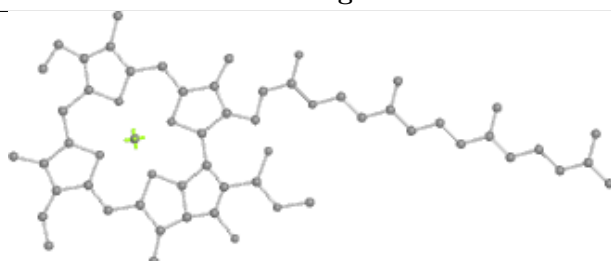
Bond lengths



Bond angles

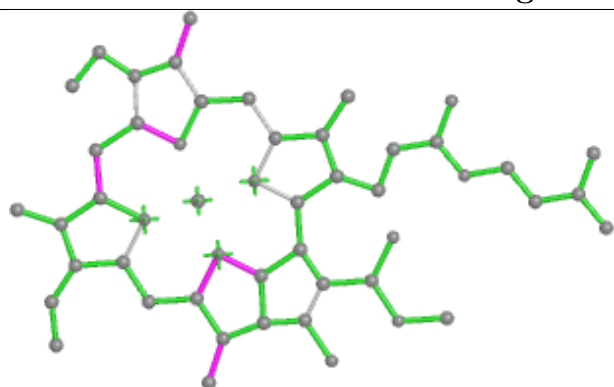


Torsions

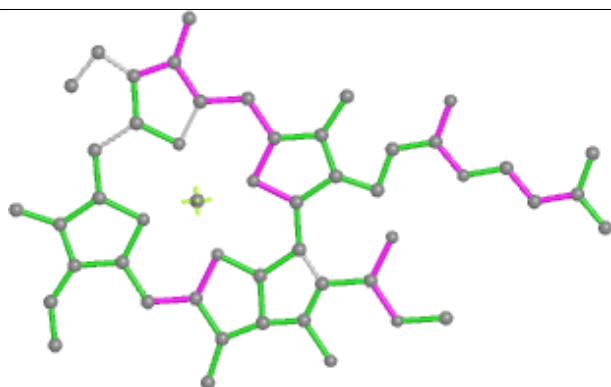


Rings

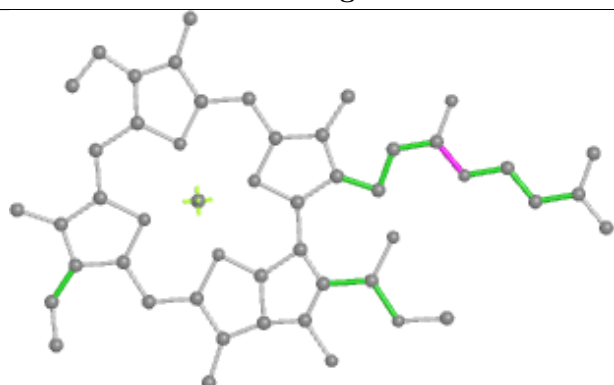
Ligand CLA L 304



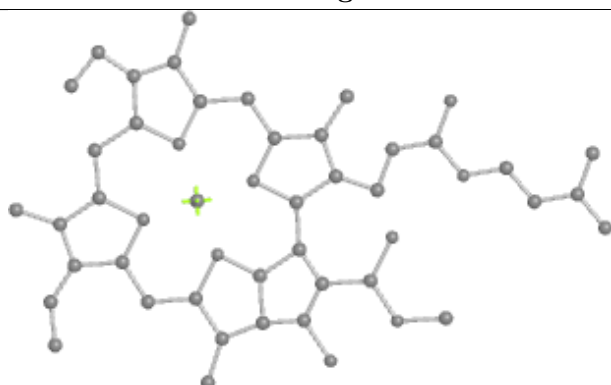
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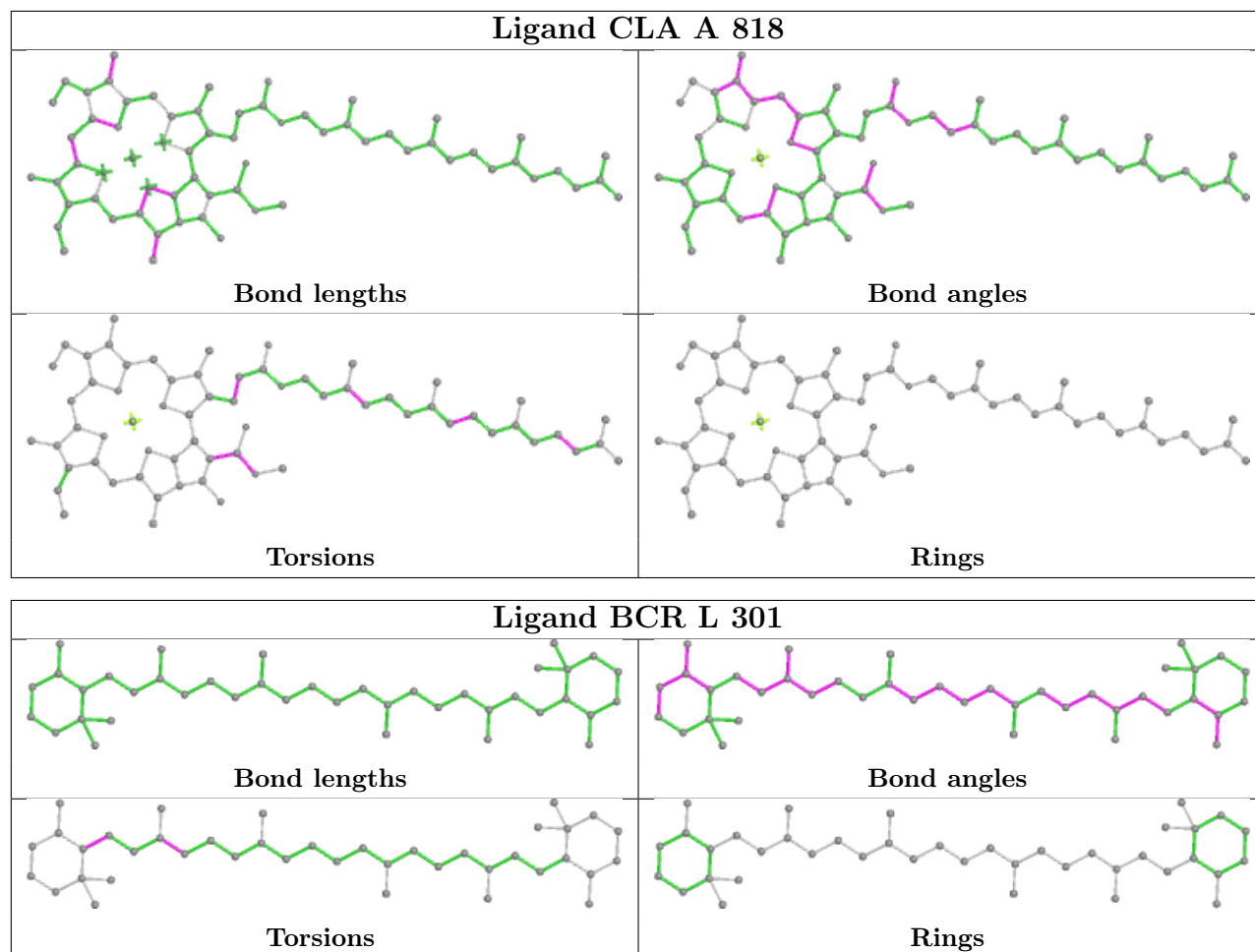
Bond angles

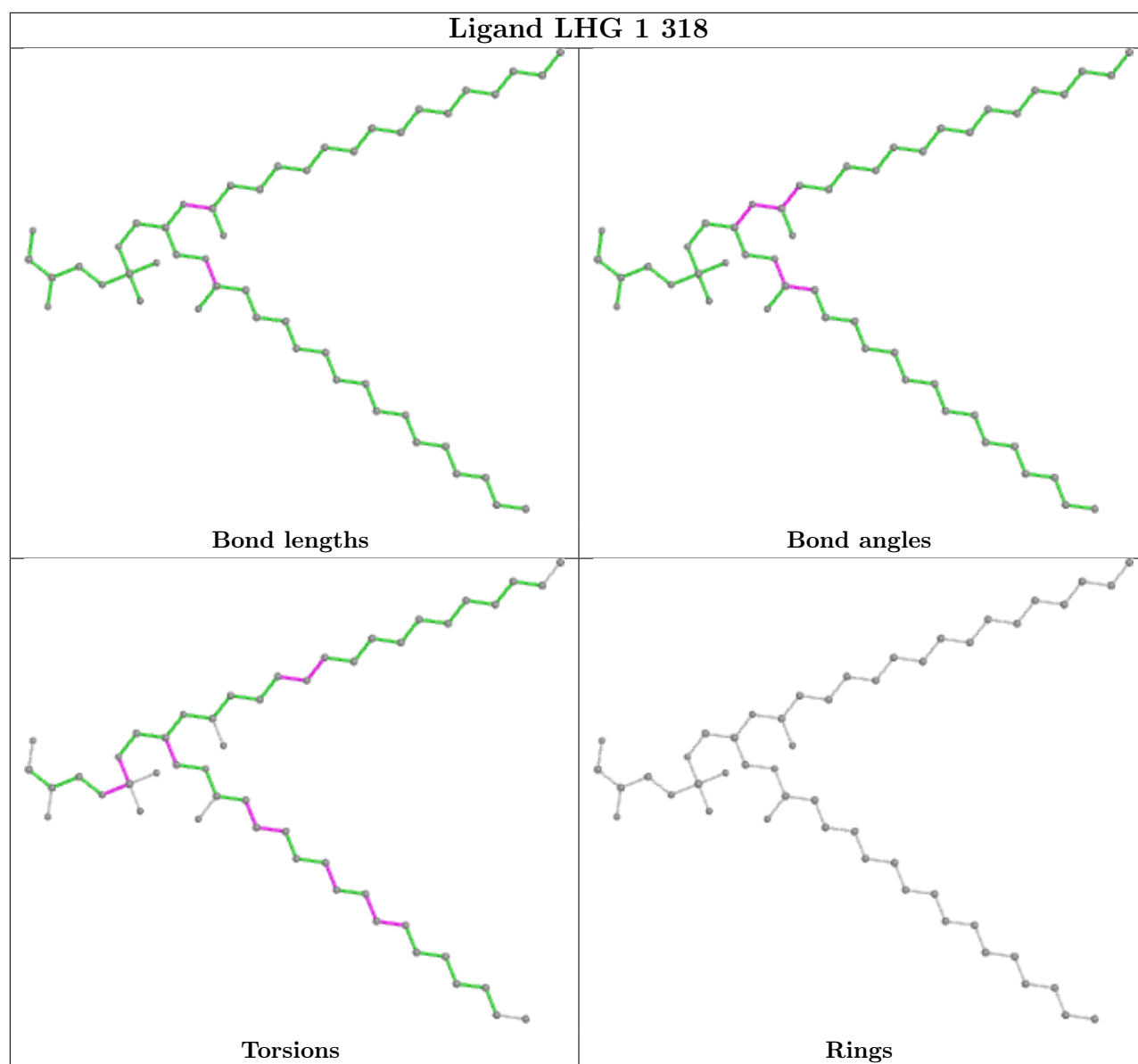


Torsions

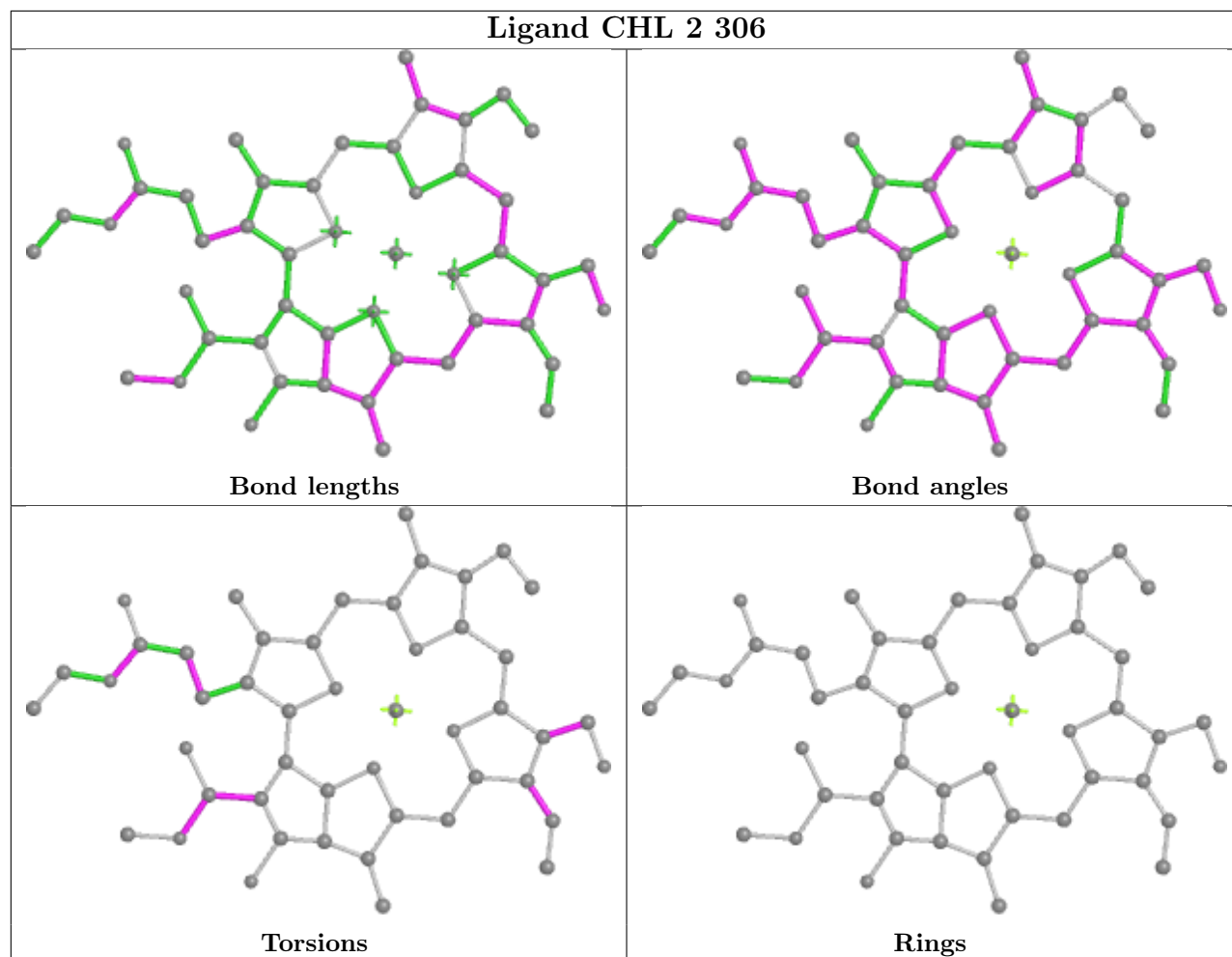


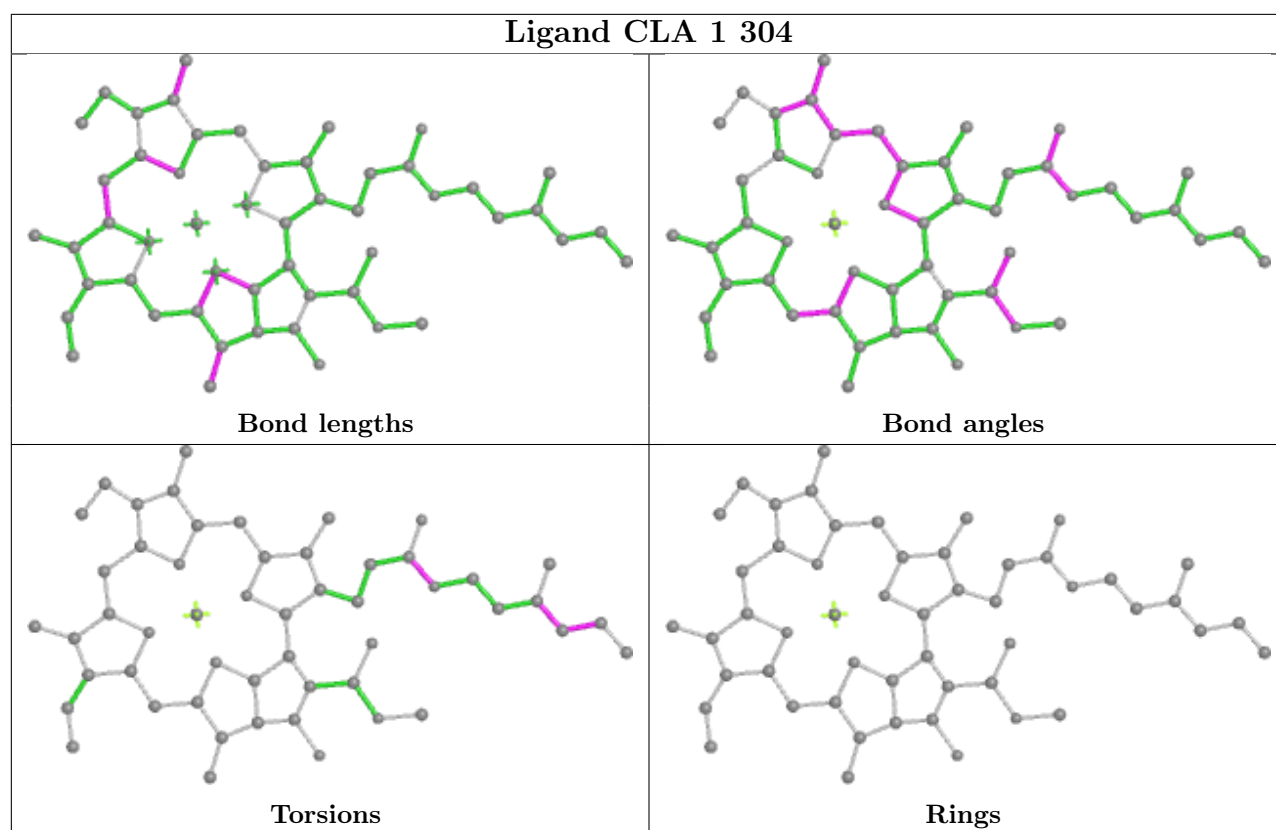
Rings



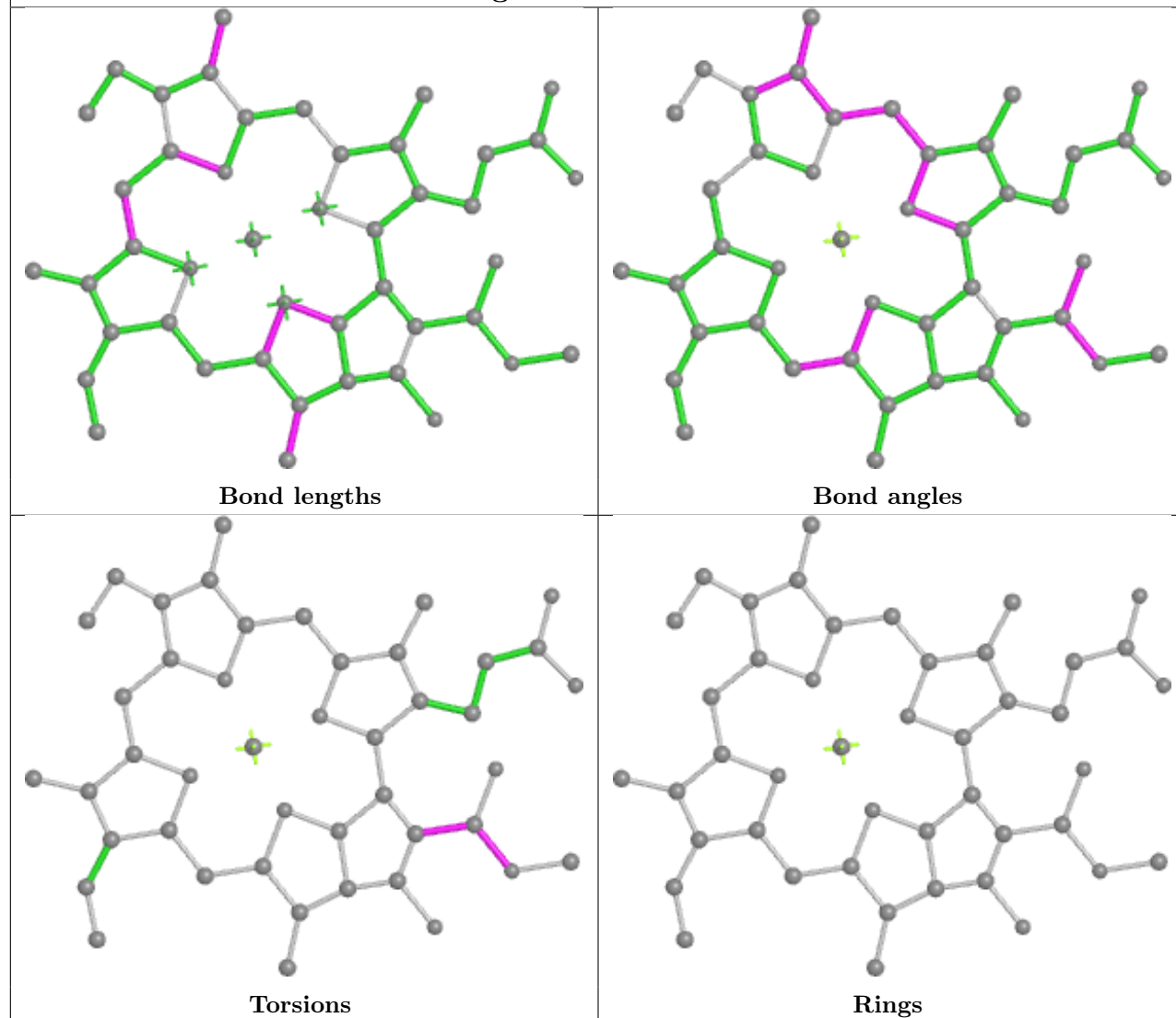


Ligand CHL 2 306

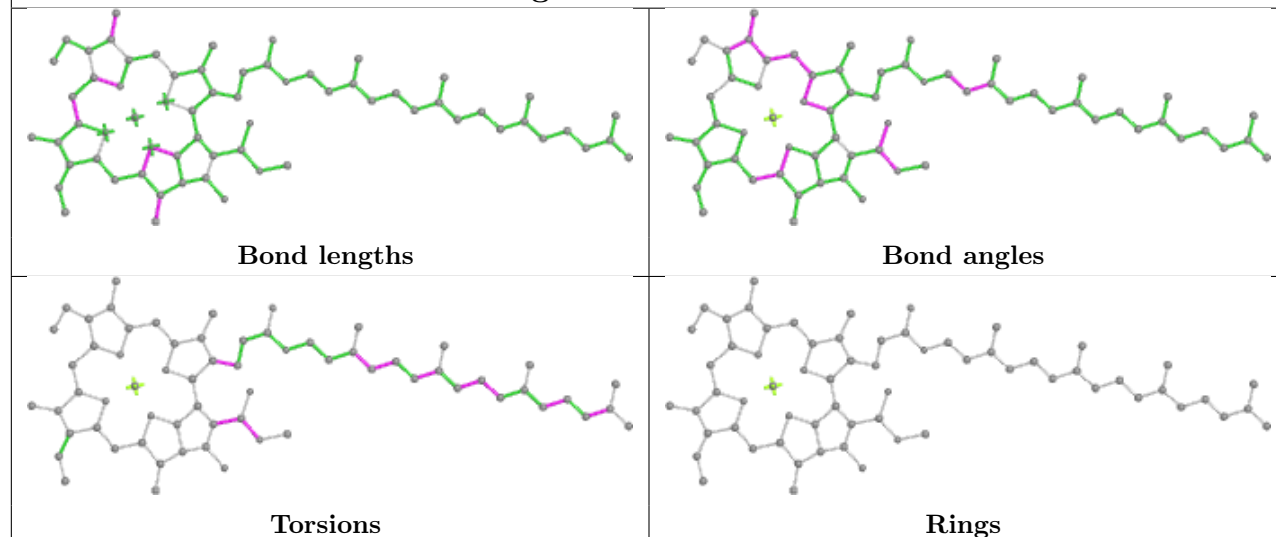




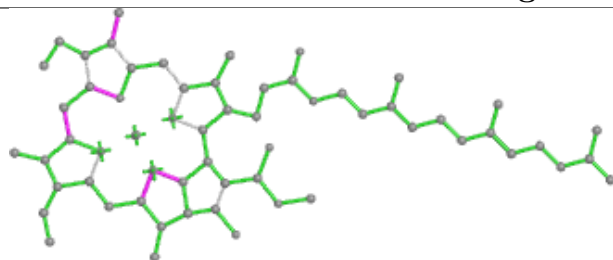
Ligand CLA F 804



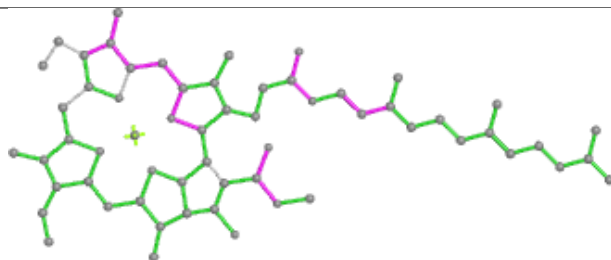
Ligand CLA A 809



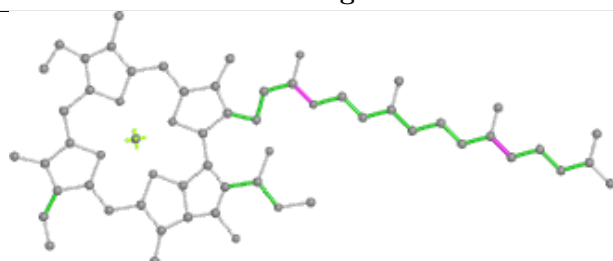
Ligand CLA 1 309



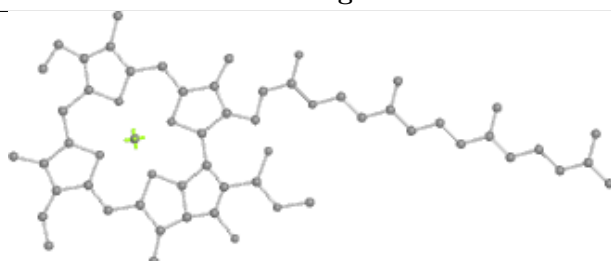
Bond lengths



Bond angles

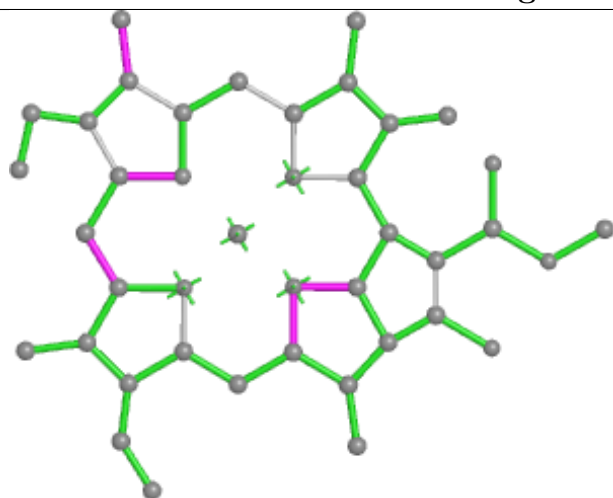


Torsions

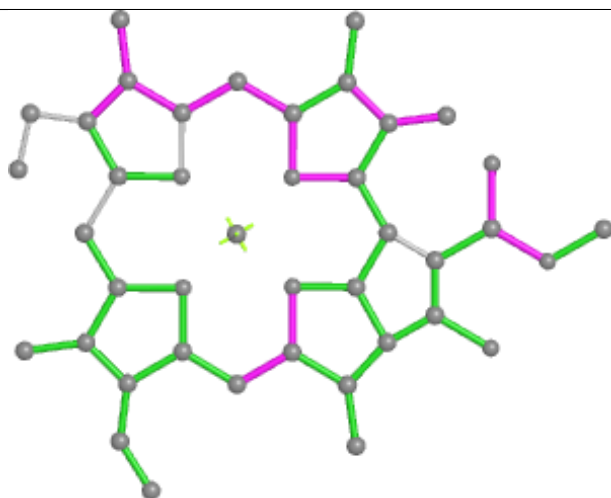


Rings

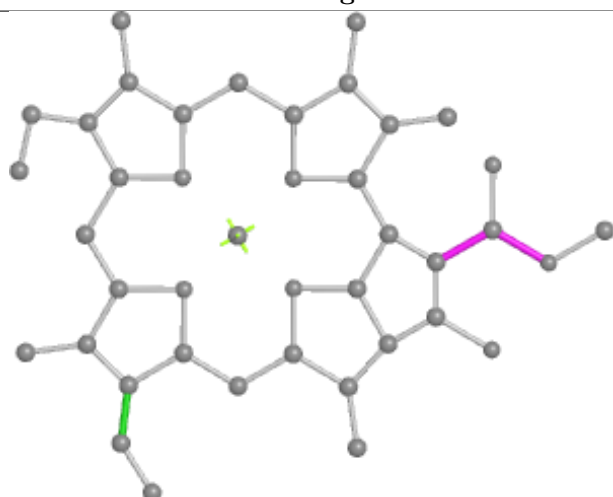
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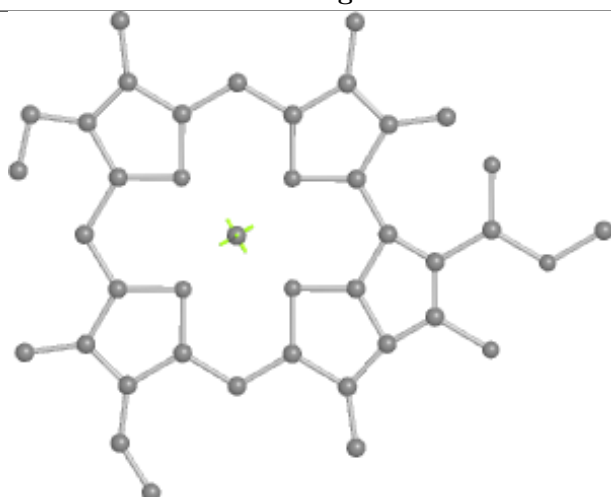
Bond lengths



Bond angles

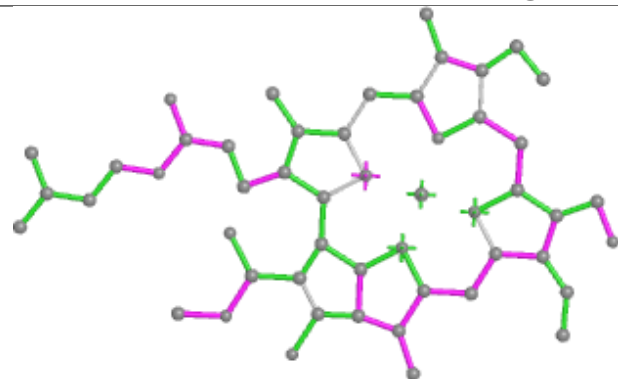


Torsions

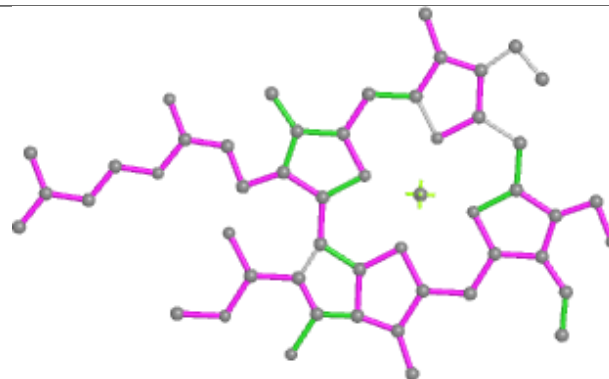


Rings

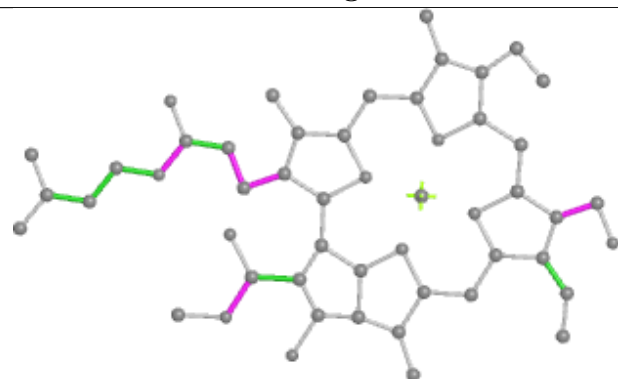
Ligand CHL 2 307



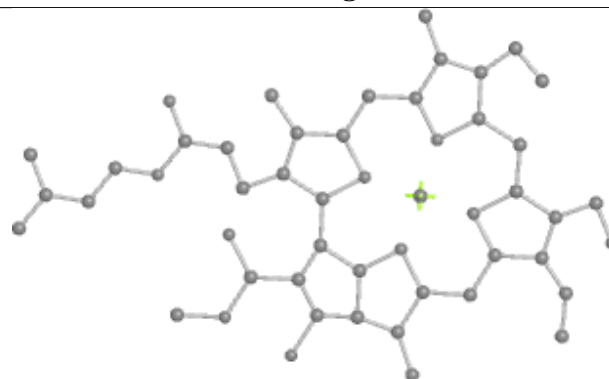
Bond lengths



Bond angles

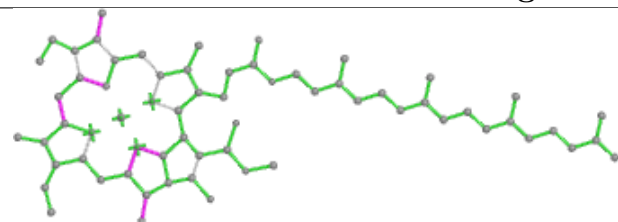


Torsions

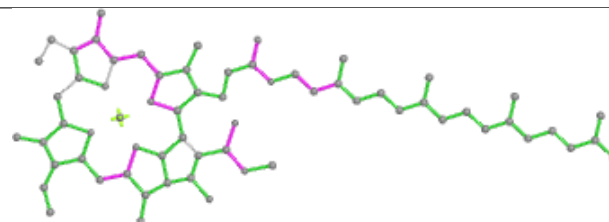


Rings

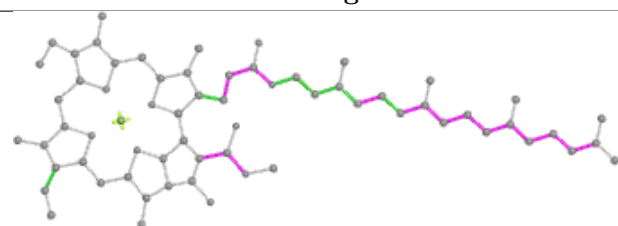
Ligand CLA A 841



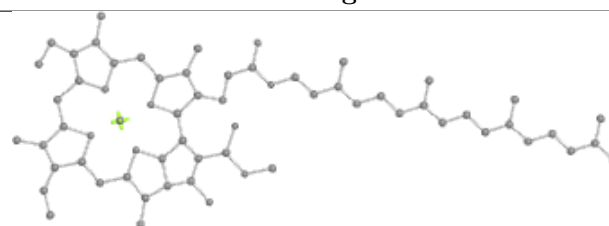
Bond lengths



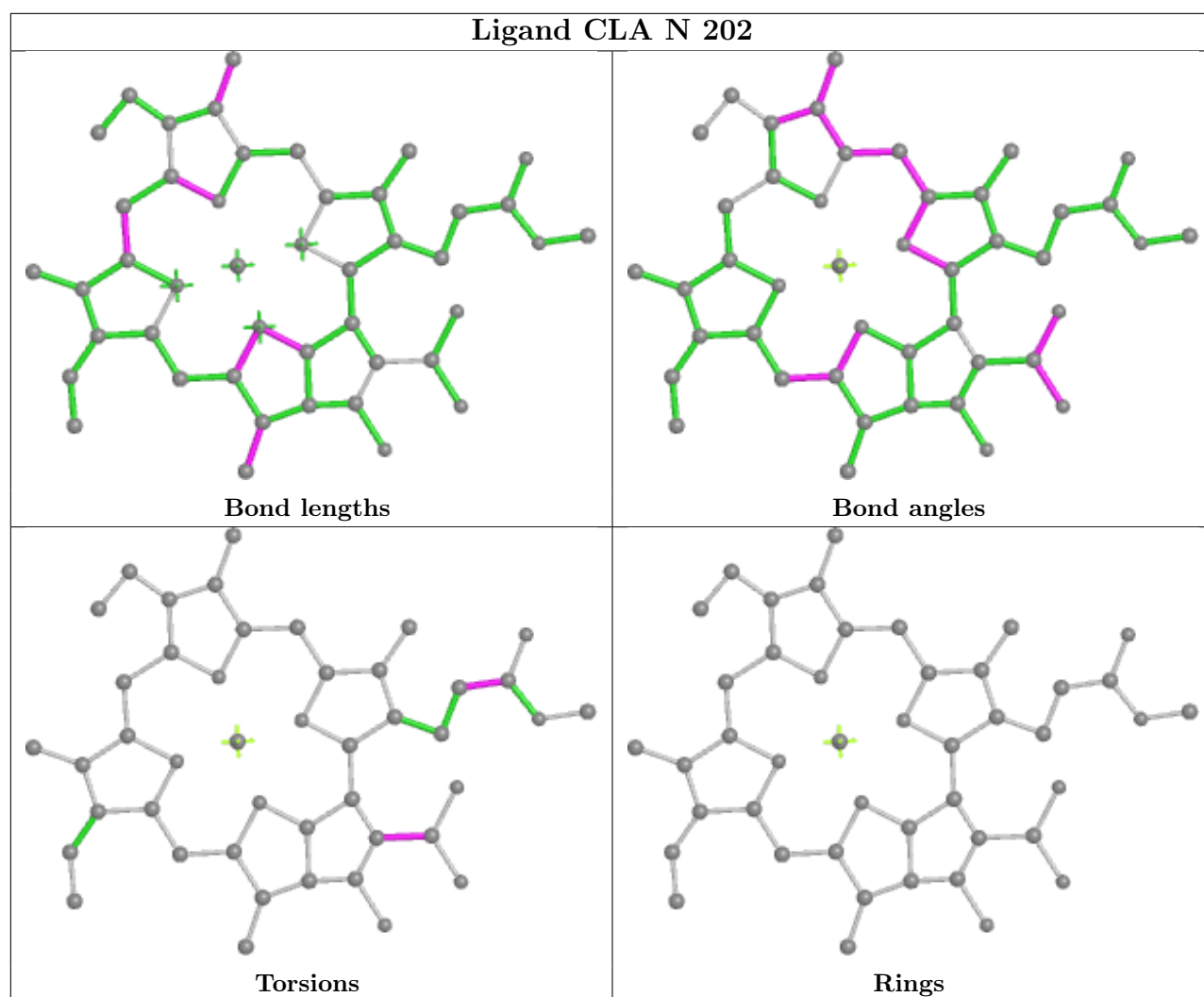
Bond angles



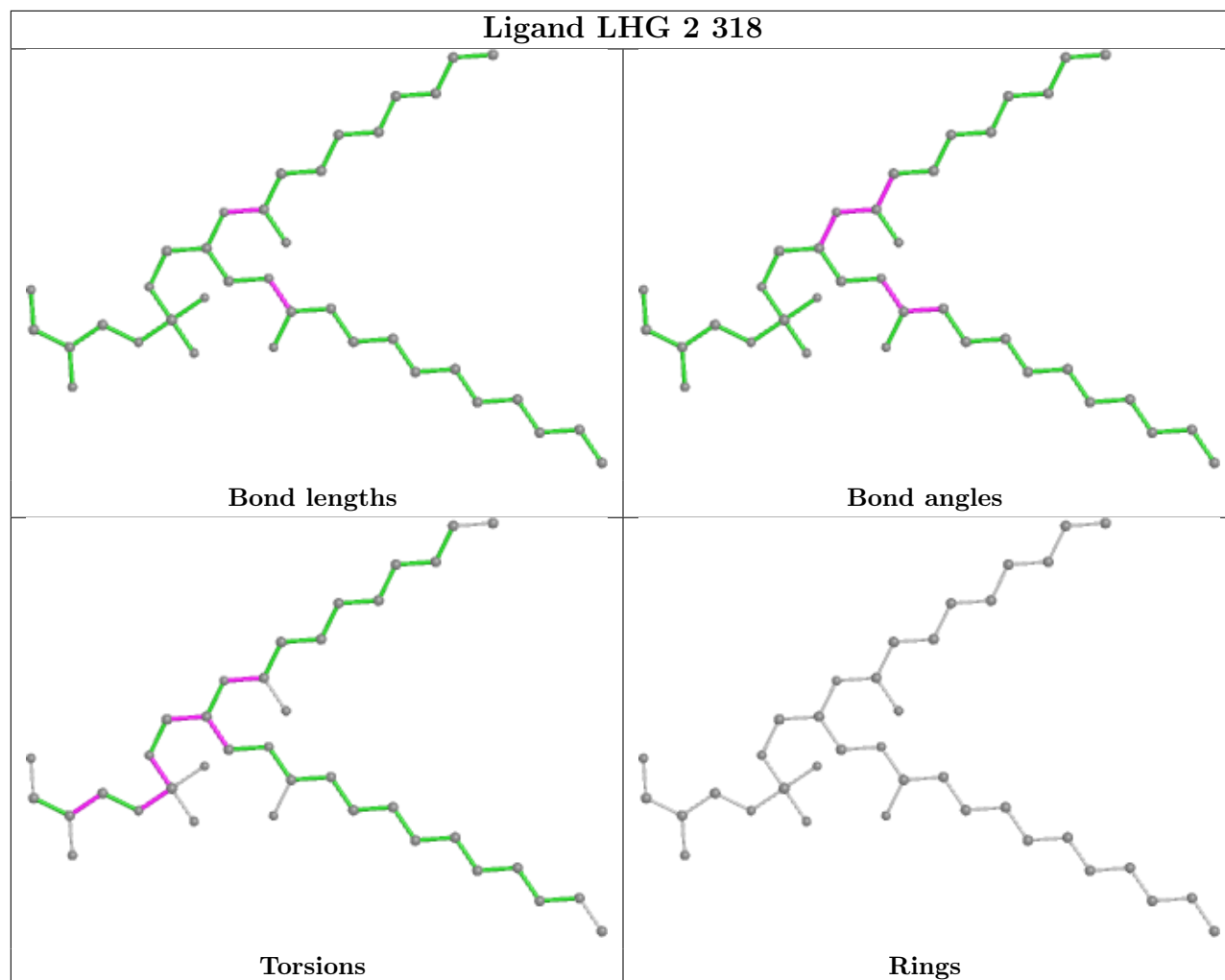
Torsions



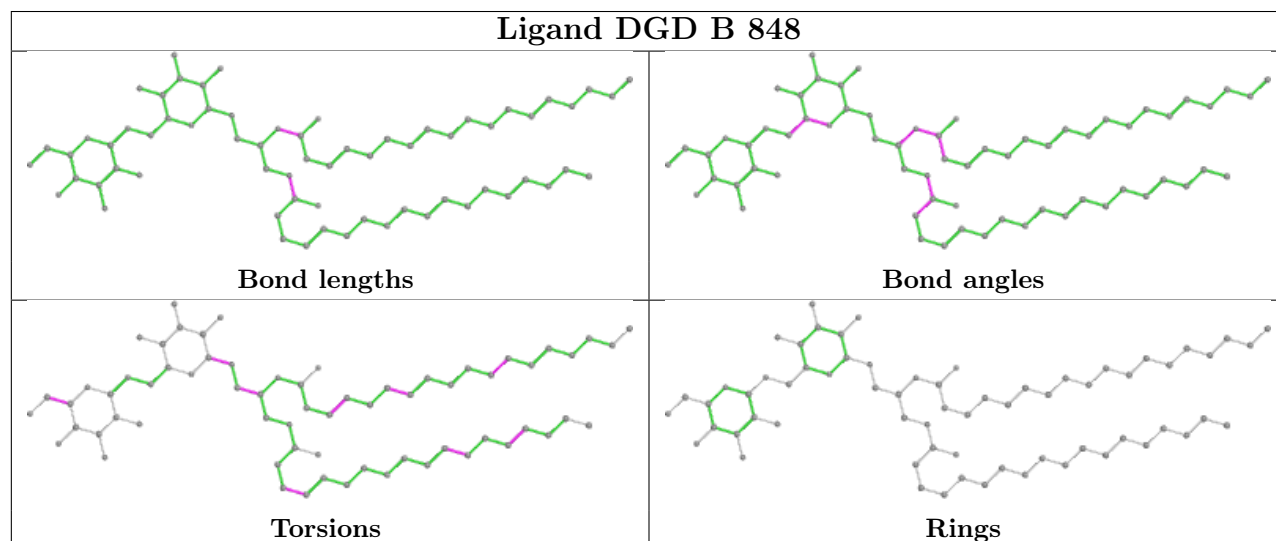
Rings

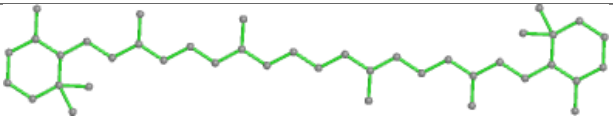
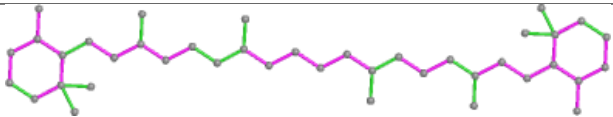
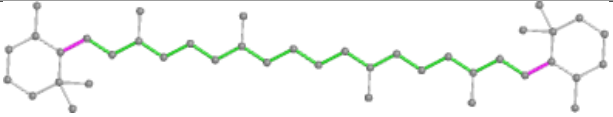
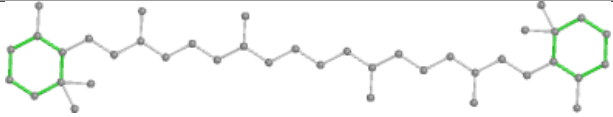


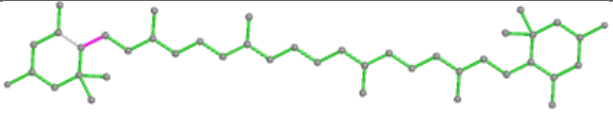
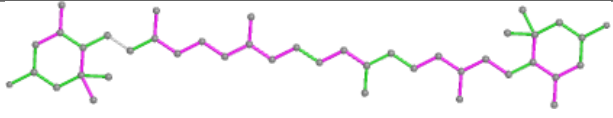
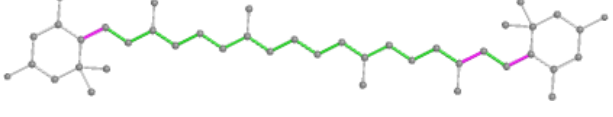
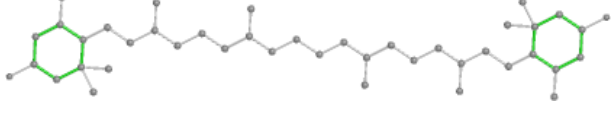
Ligand LHG 2 318



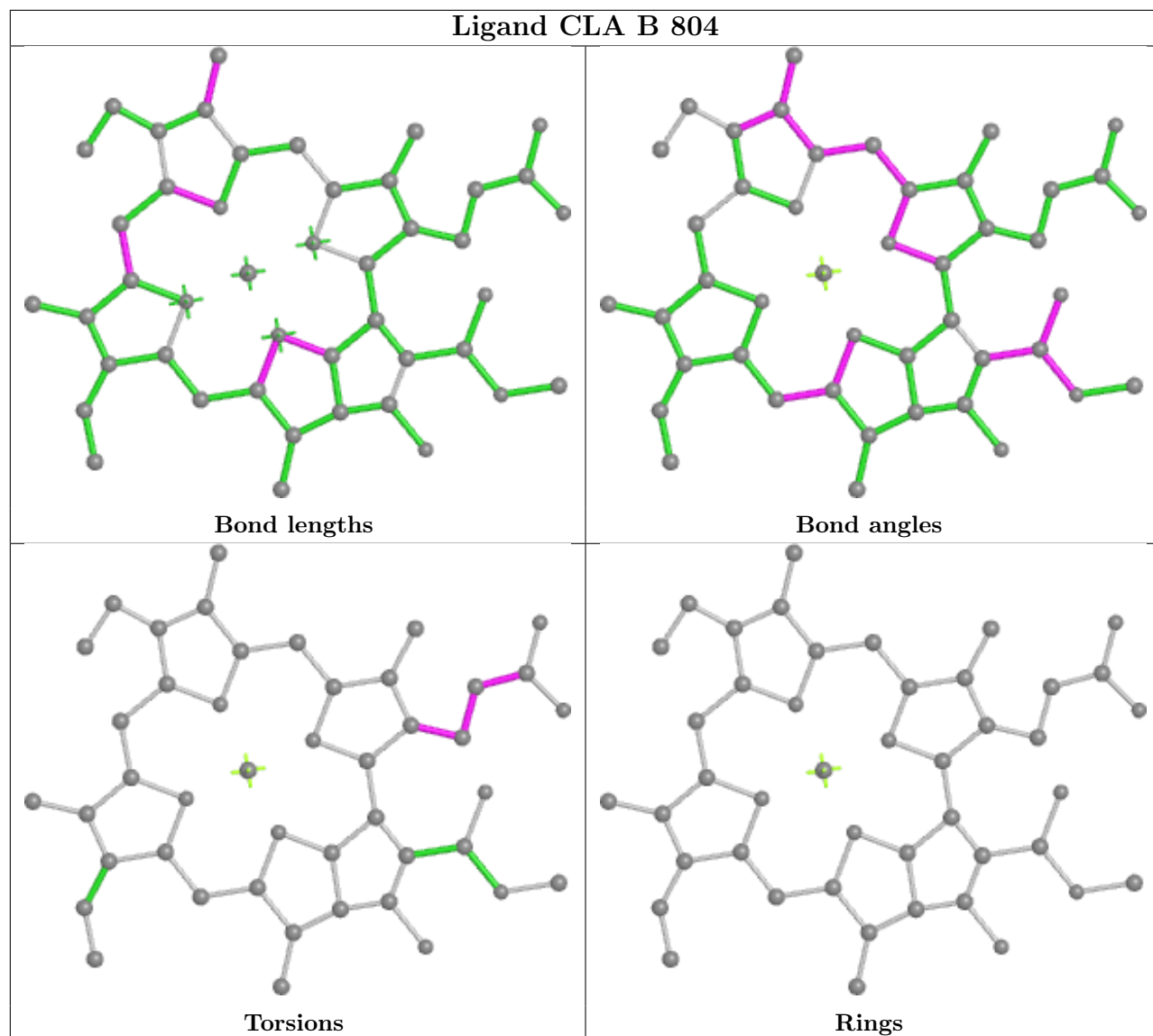
Ligand DGD B 848



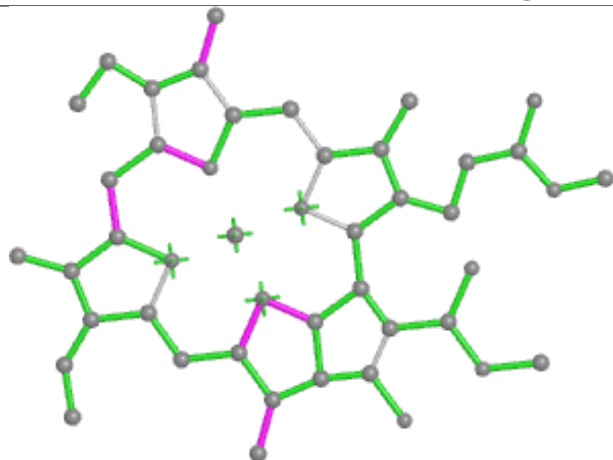
Ligand BCR 3 317	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand LUT O 205	
	Bond lengths
	Bond angles
	Torsions
	Rings

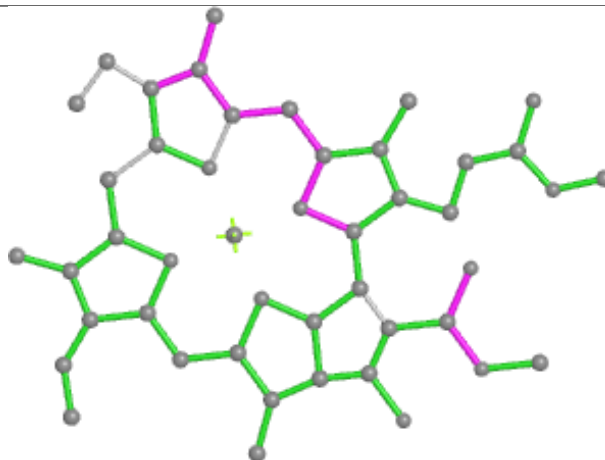
Ligand CLA B 804



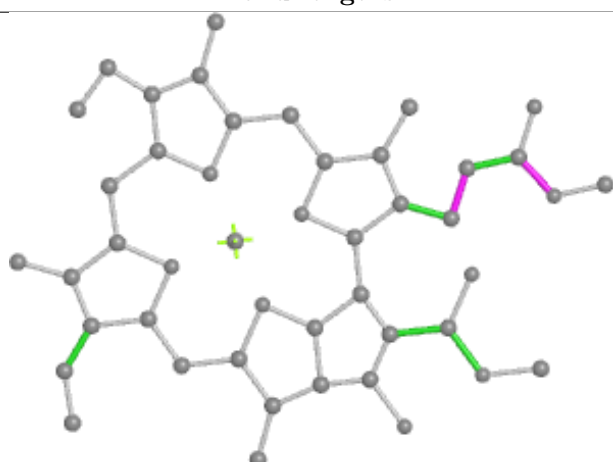
Ligand CLA 1 314



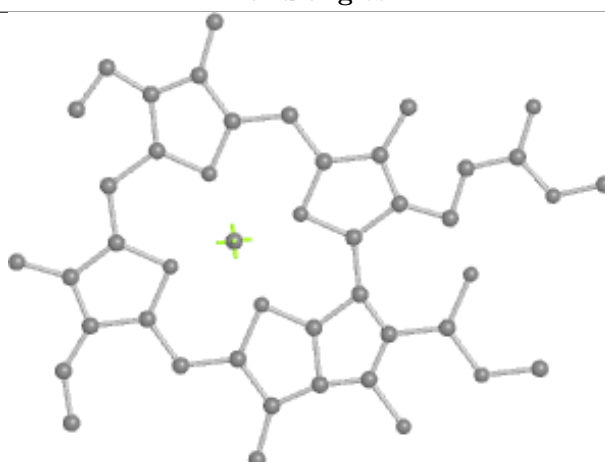
Bond lengths



Bond angles

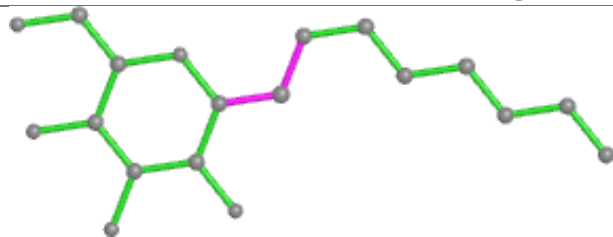


Torsions

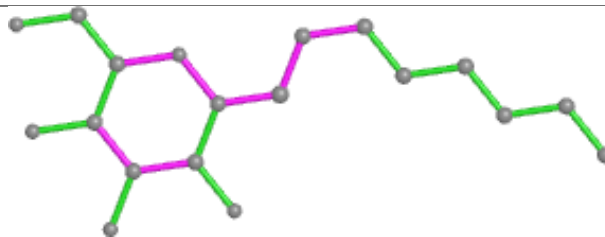


Rings

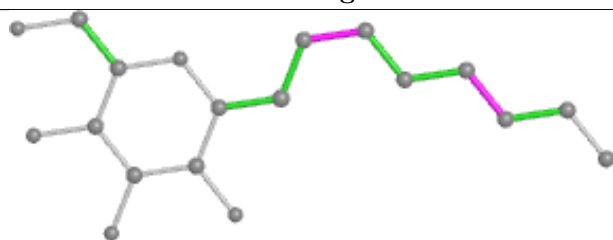
Ligand HTG A 852



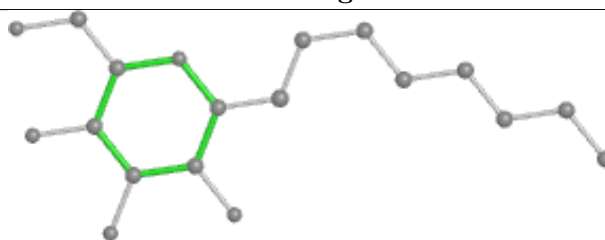
Bond lengths



Bond angles

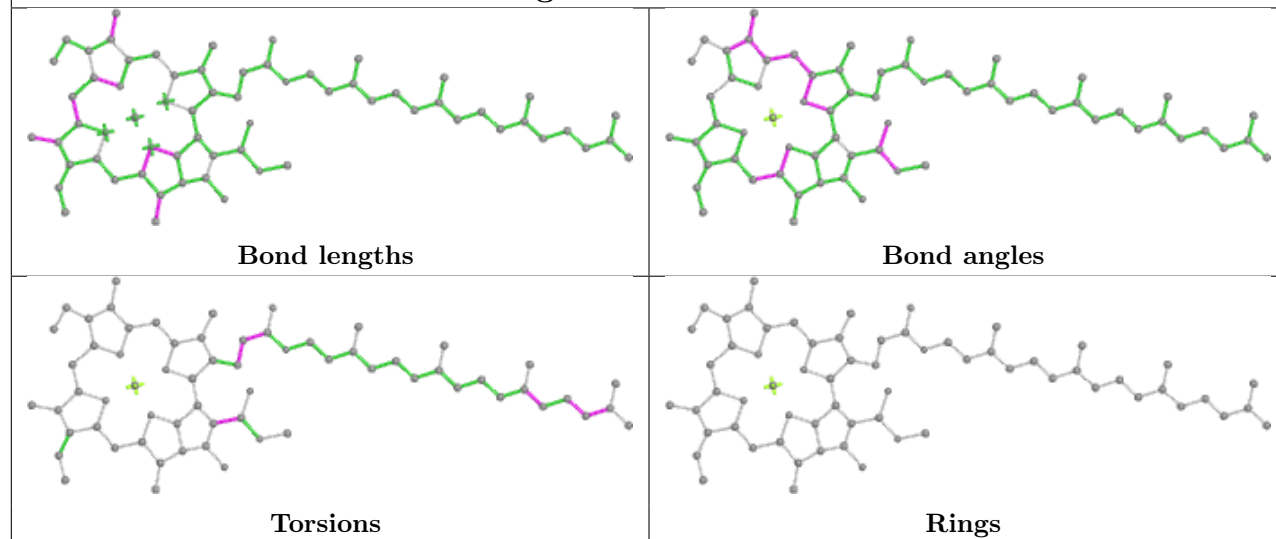


Torsions

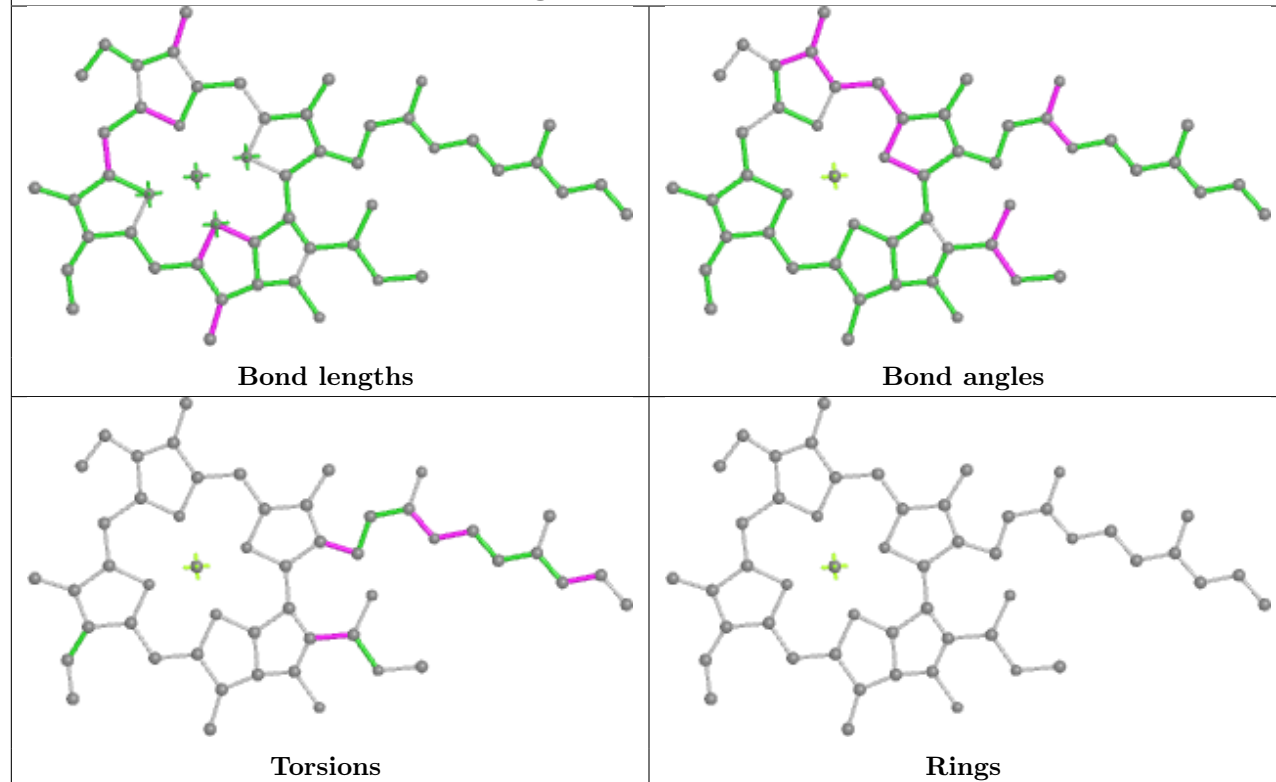


Rings

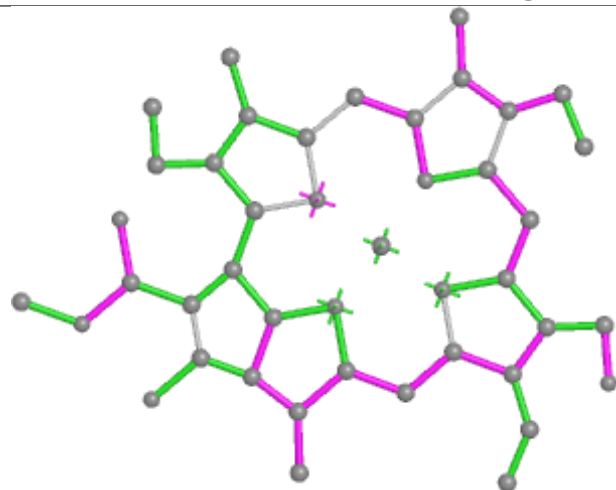
Ligand CLA 1 302



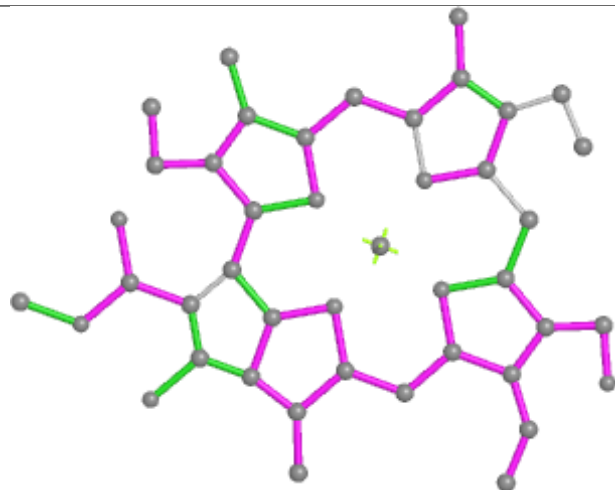
Ligand CLA O 201



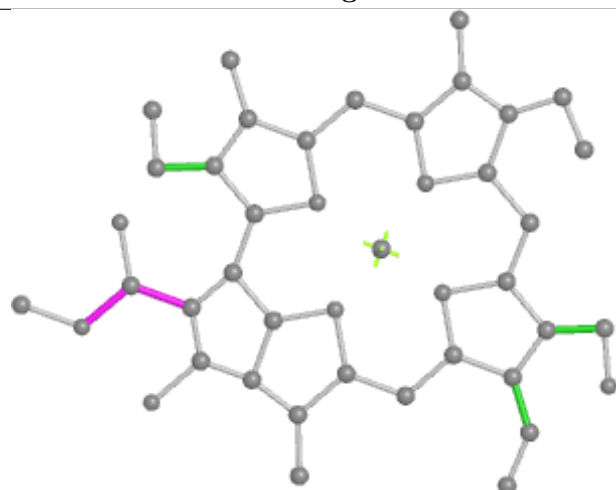
Ligand CHL 2 305



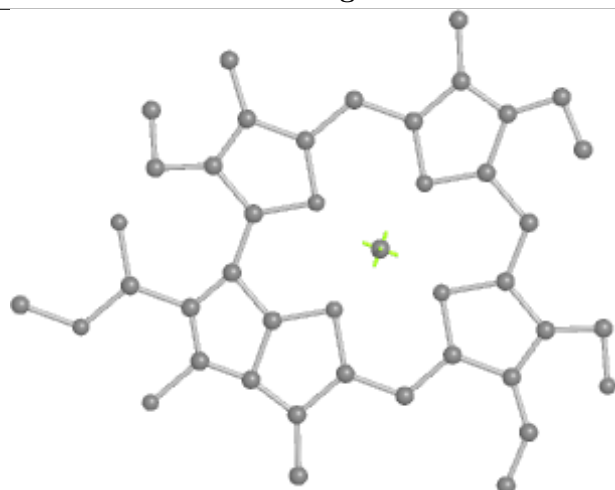
Bond lengths



Bond angles

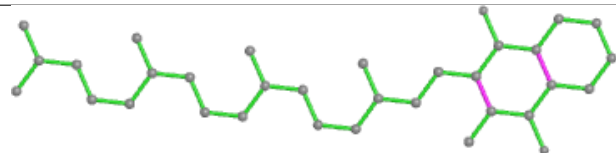


Torsions

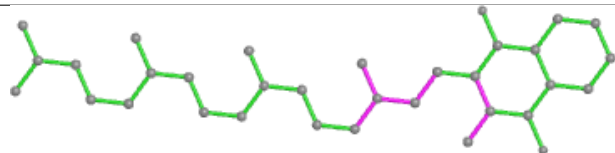


Rings

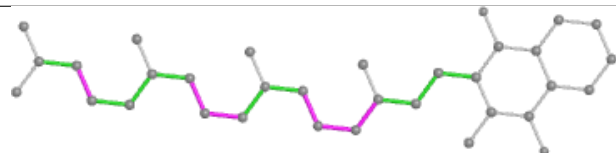
Ligand PQN A 842



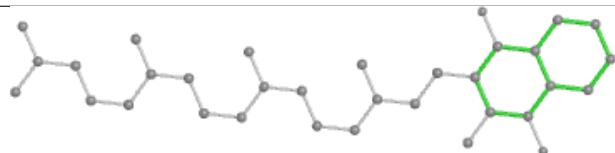
Bond lengths



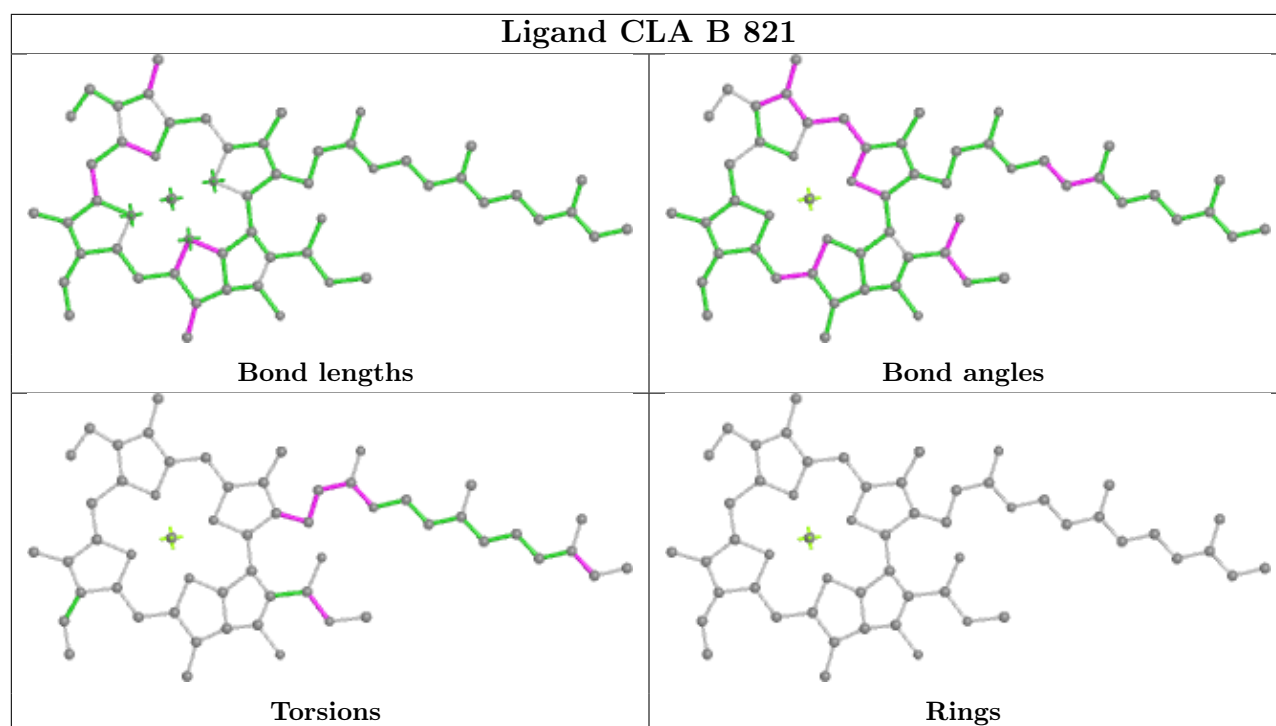
Bond angles



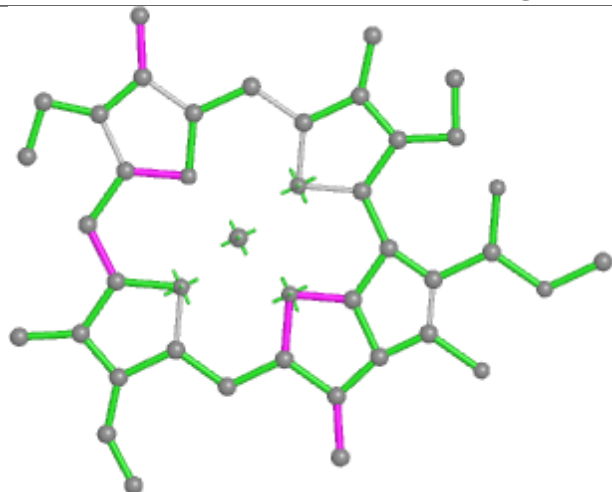
Torsions



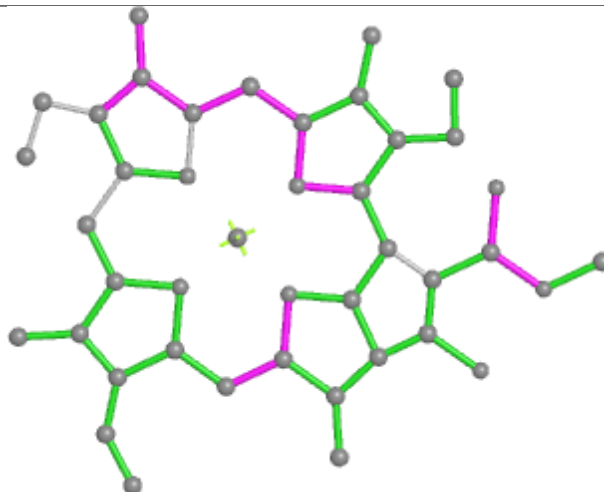
Rings



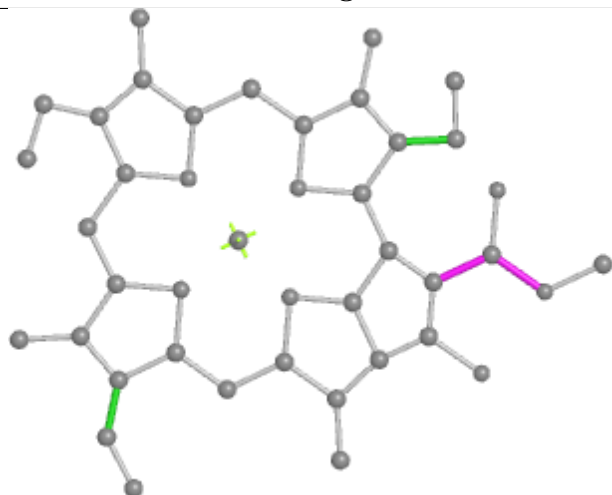
Ligand CLA J 103



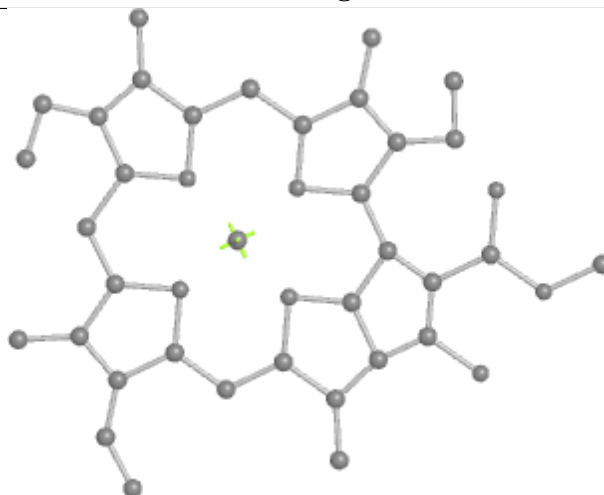
Bond lengths



Bond angles

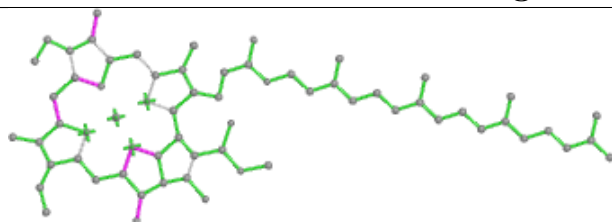


Torsions

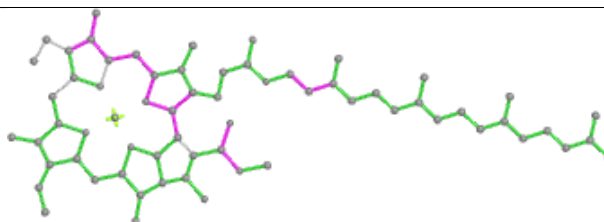


Rings

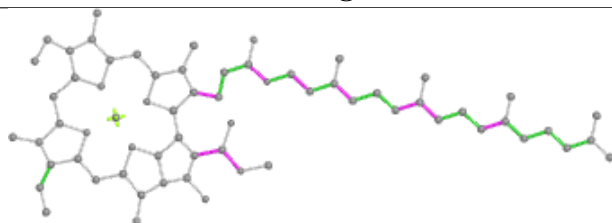
Ligand CLA A 827



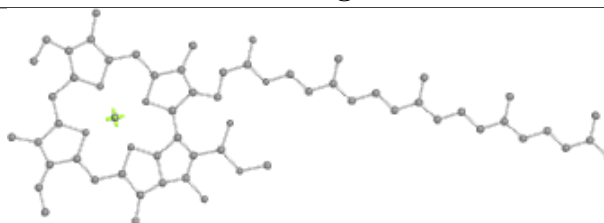
Bond lengths



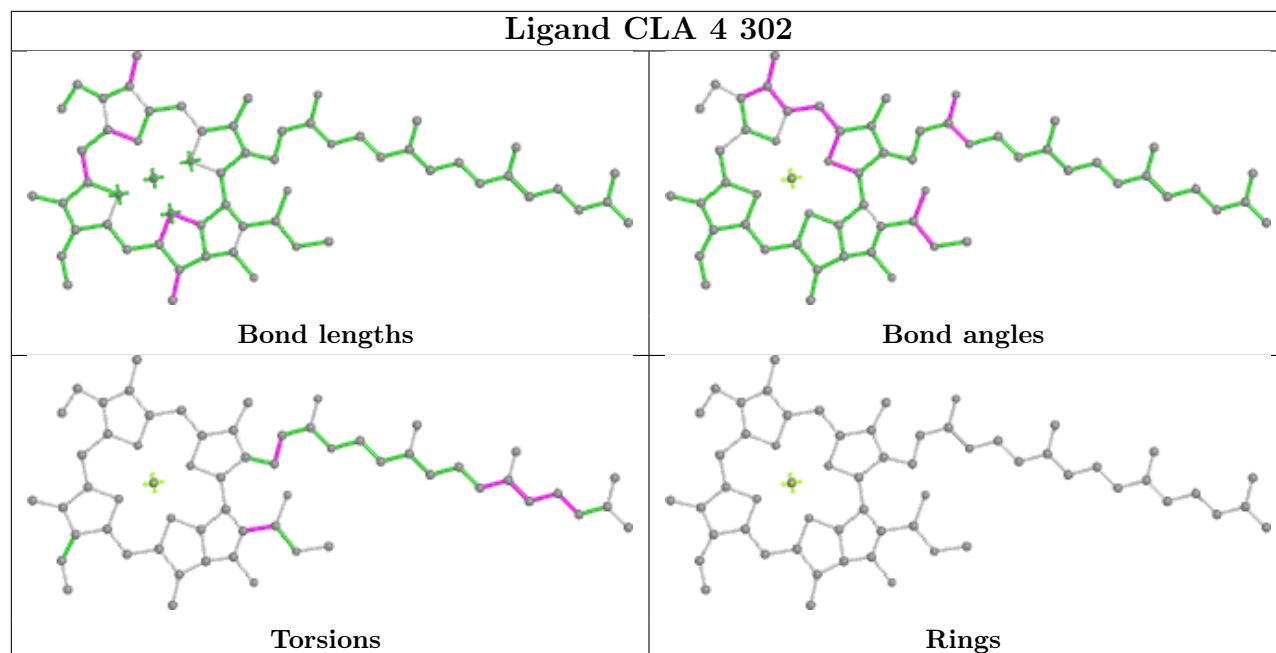
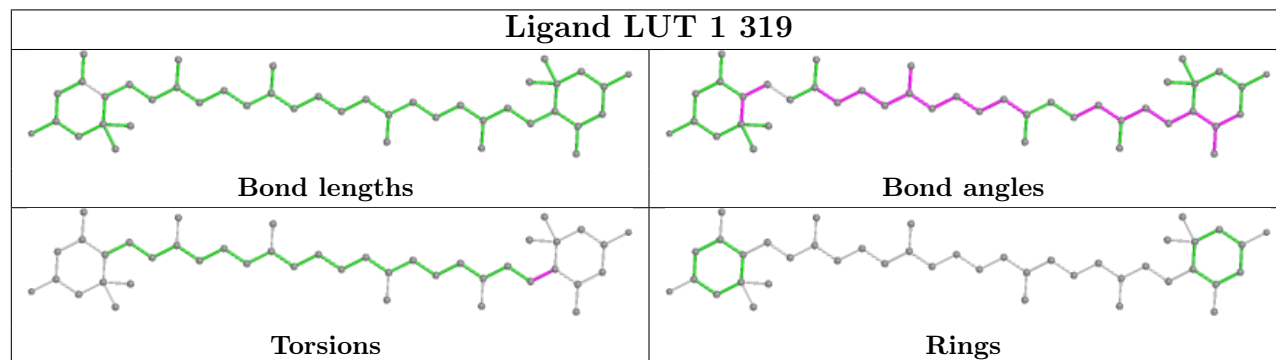
Bond angles



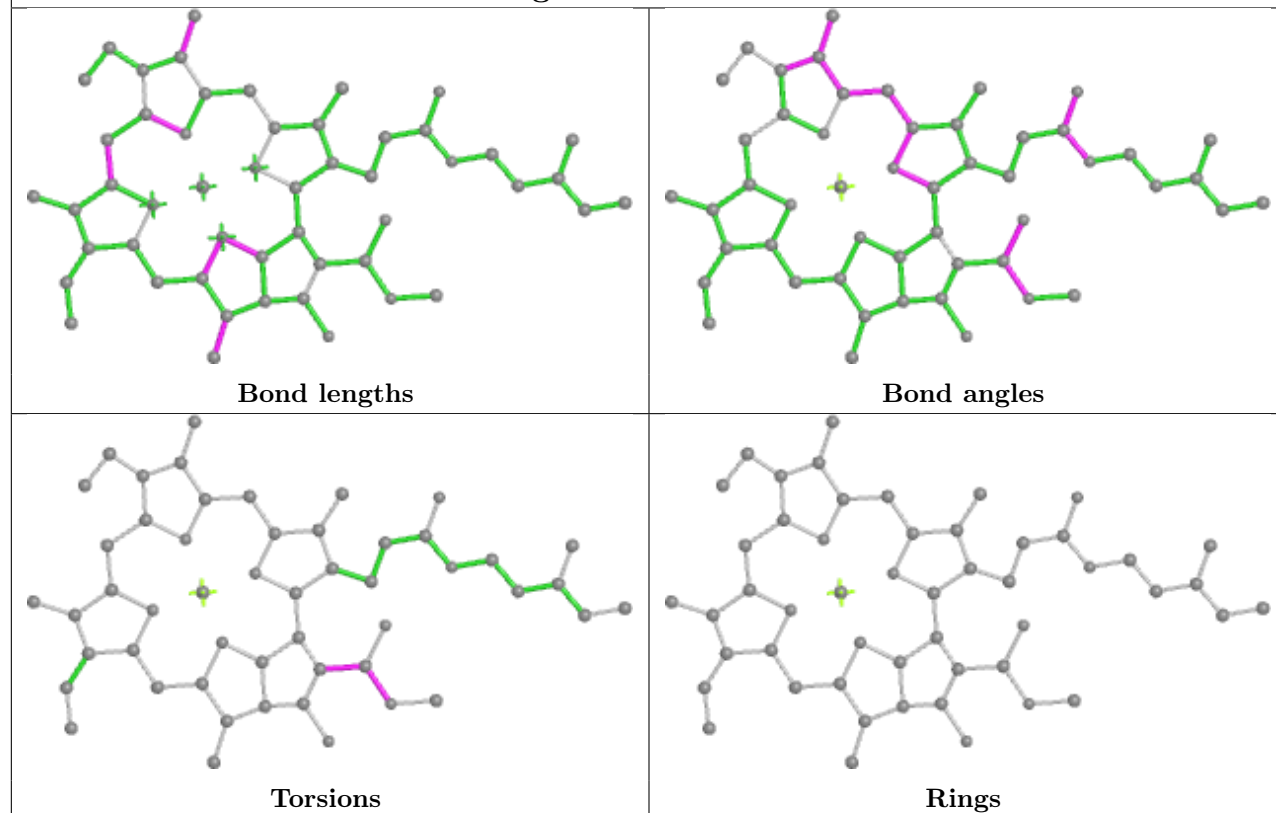
Torsions



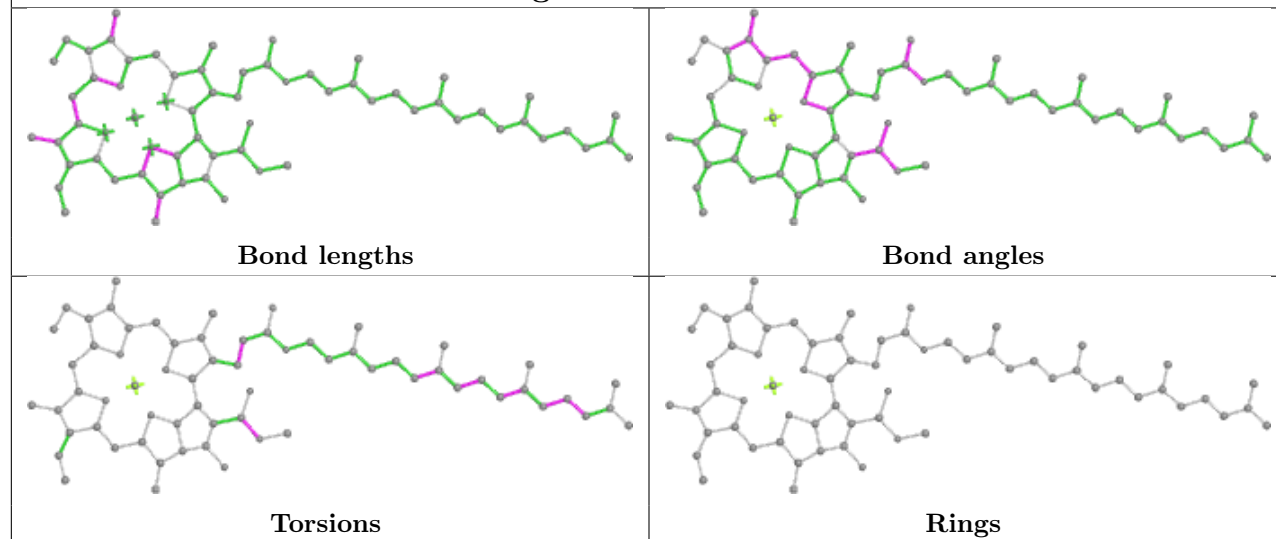
Rings

Ligand CLA 4 302**Ligand LUT 1 319**

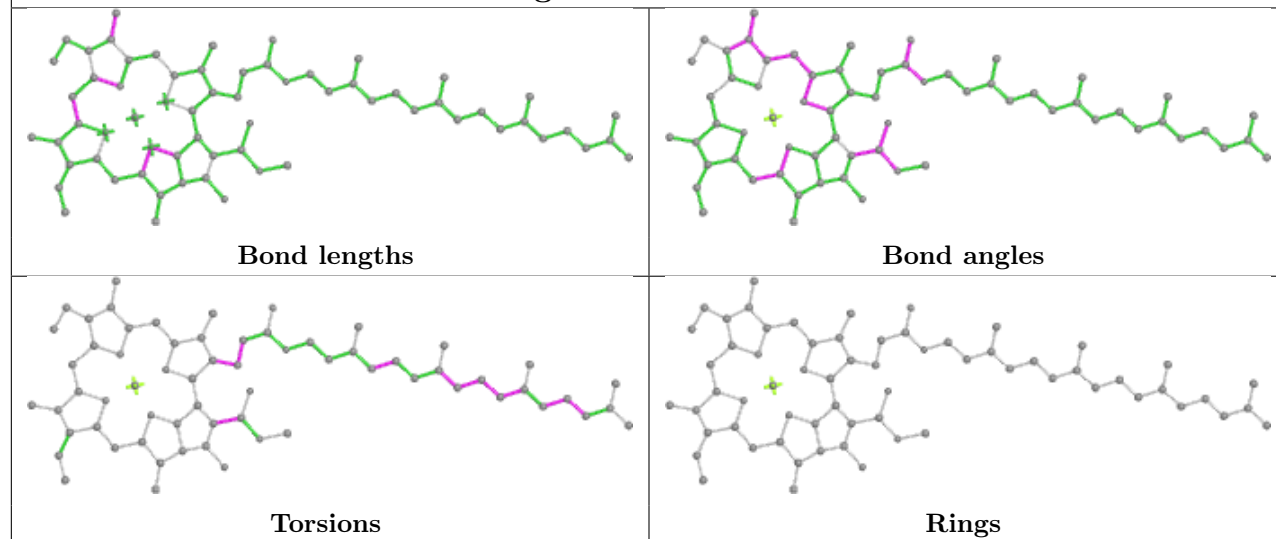
Ligand CLA B 835



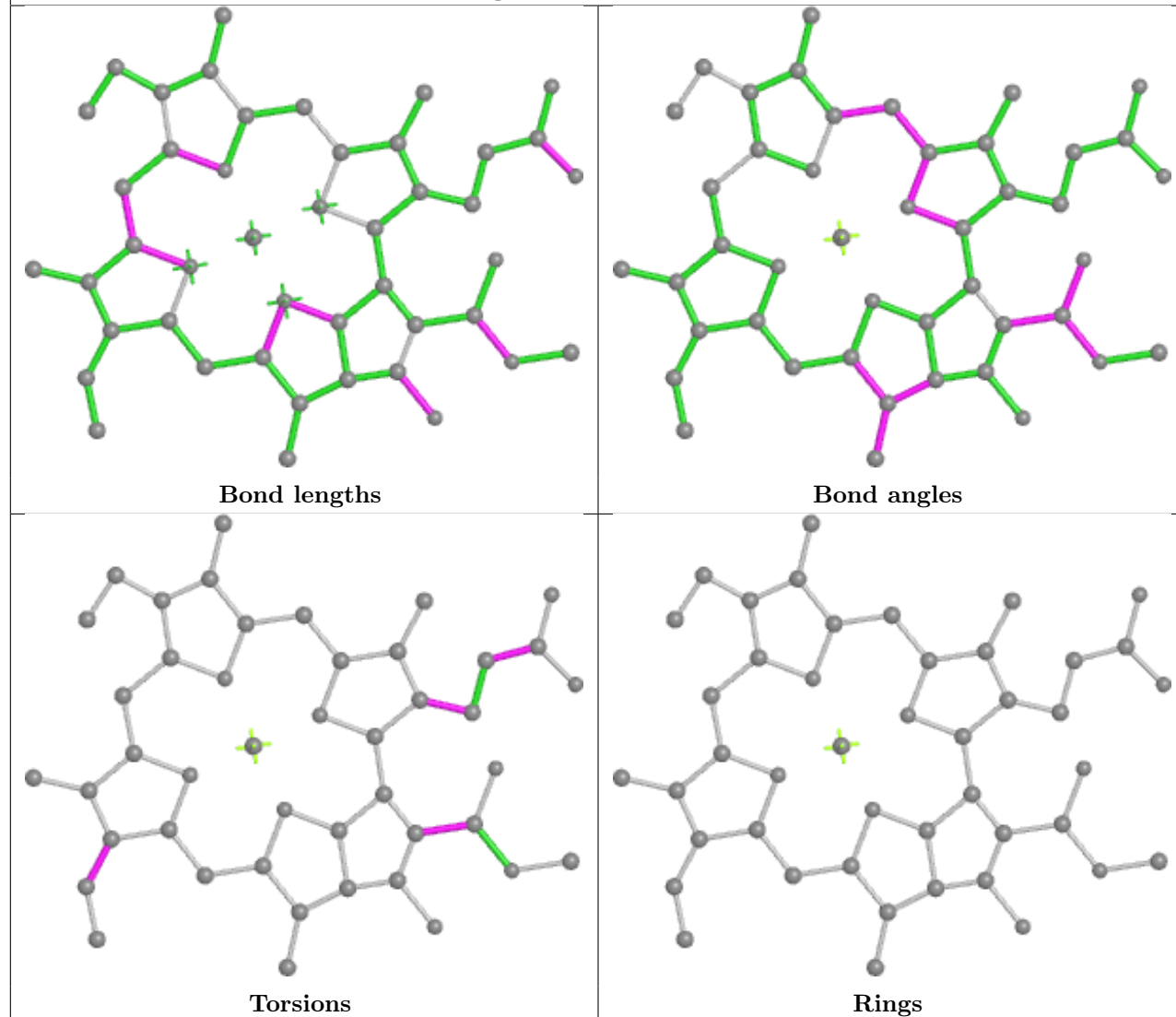
Ligand CLA B 803

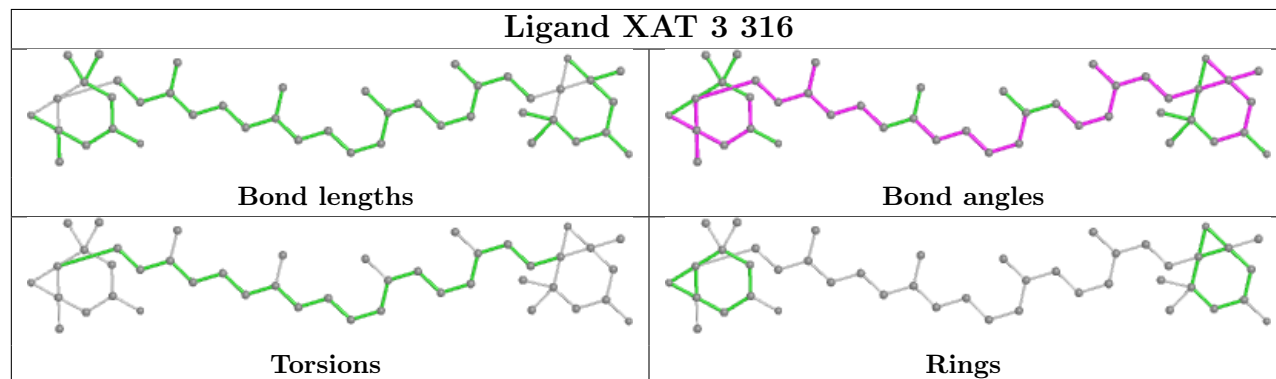
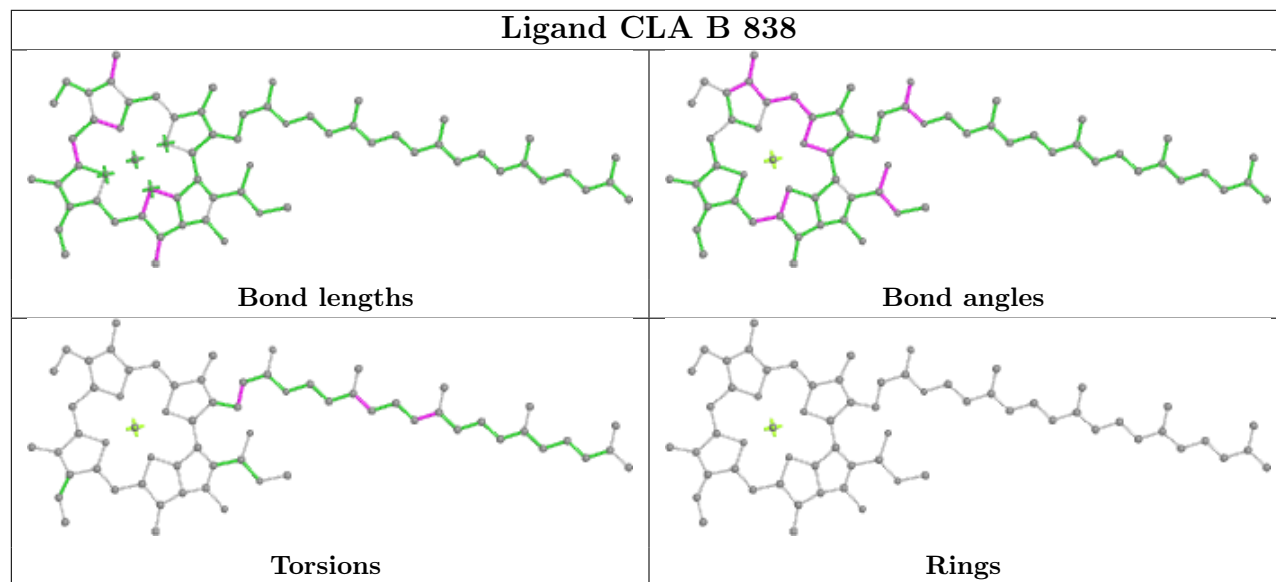
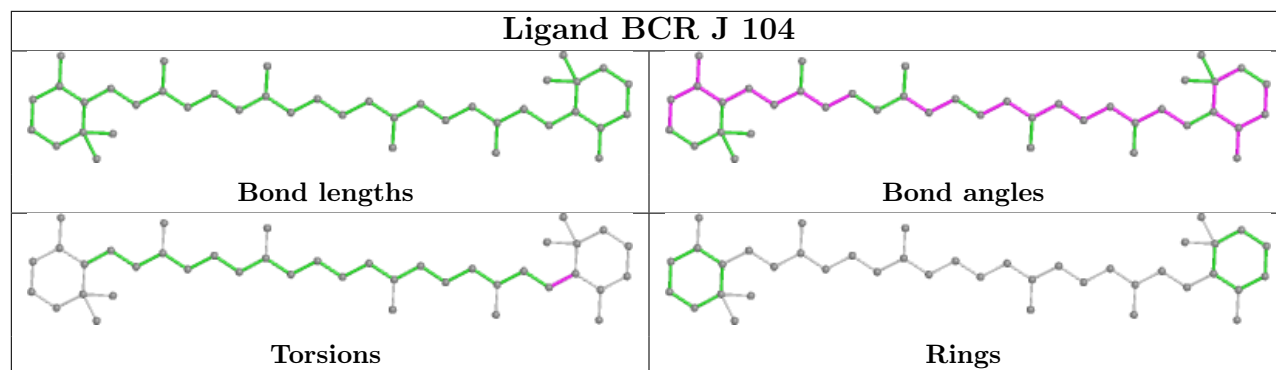
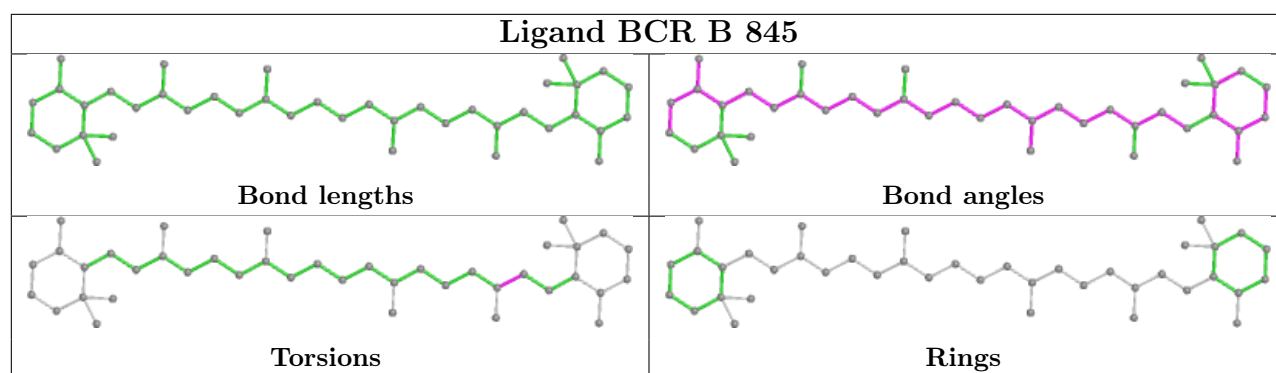


Ligand CLA L 303

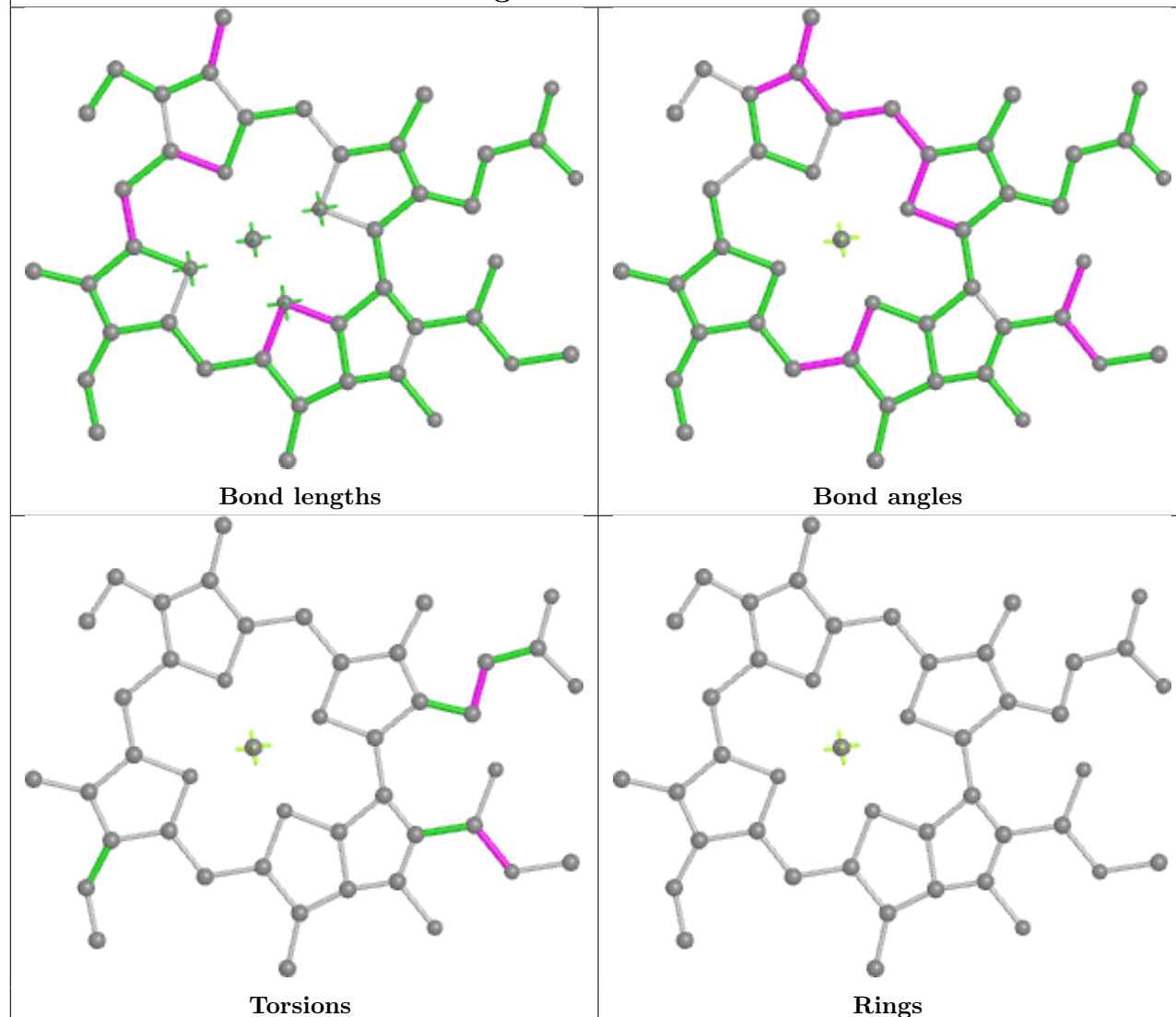


Ligand CLA O 202

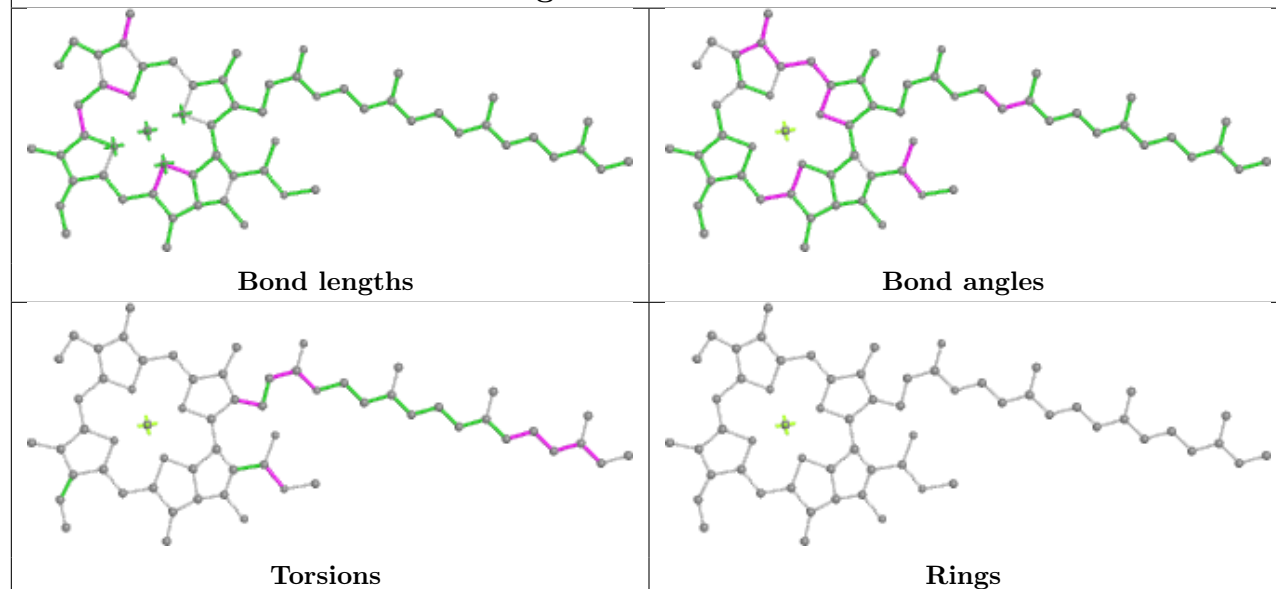


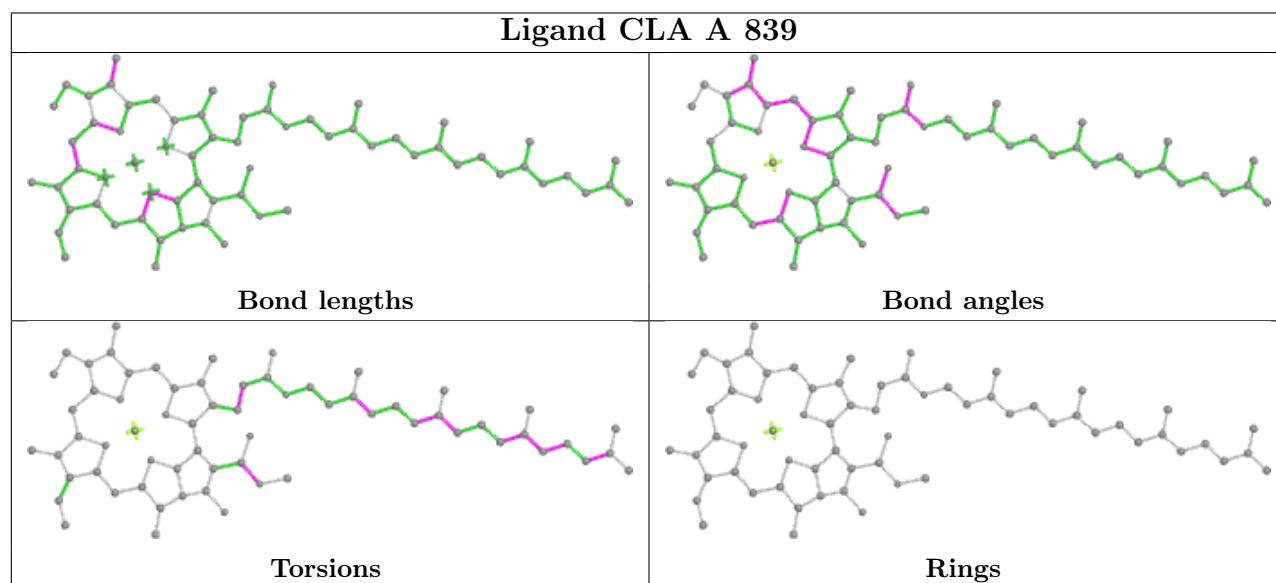
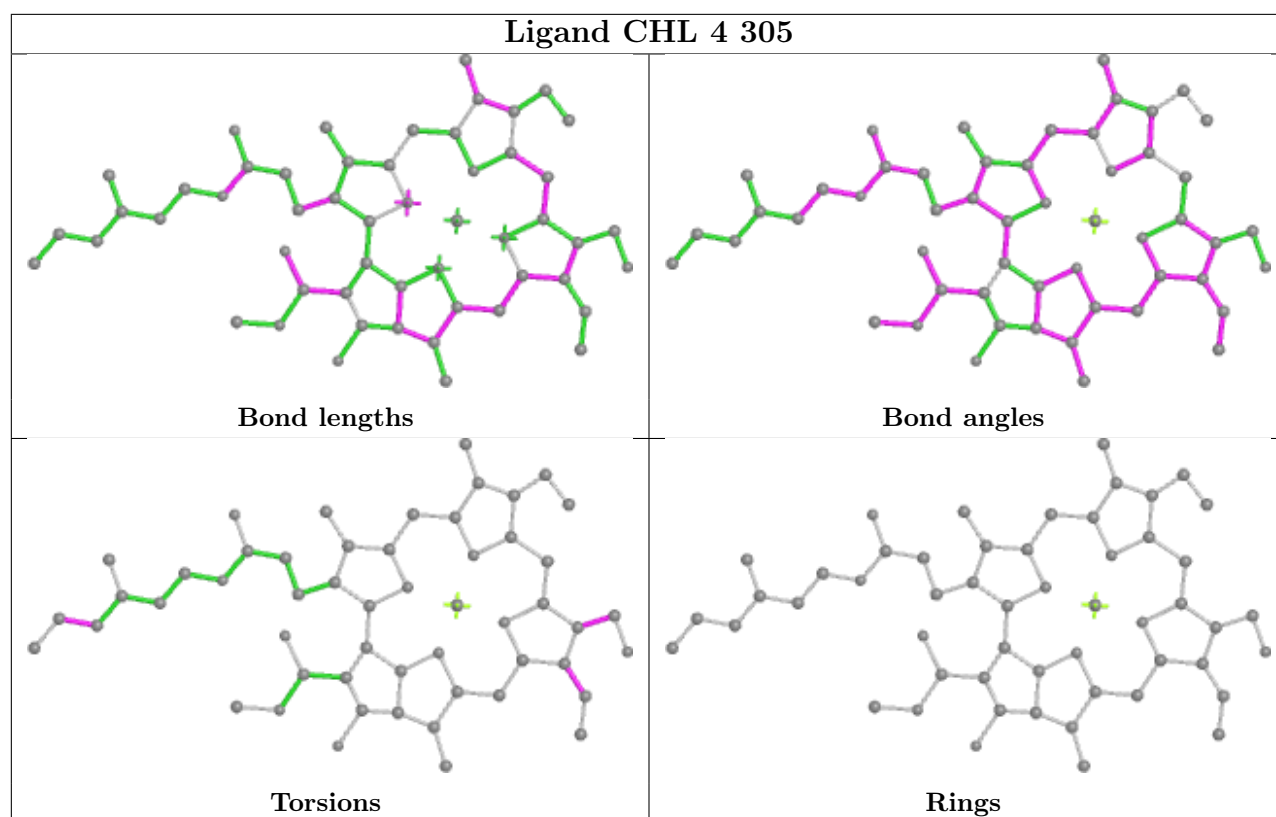


Ligand CLA 3 312

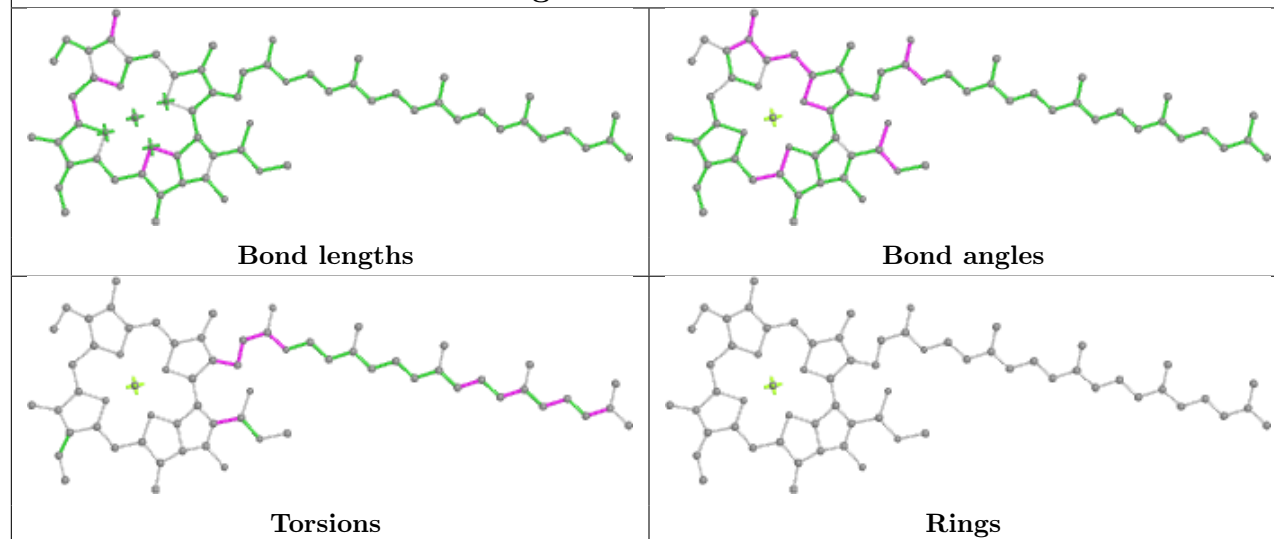


Ligand CLA 1 307

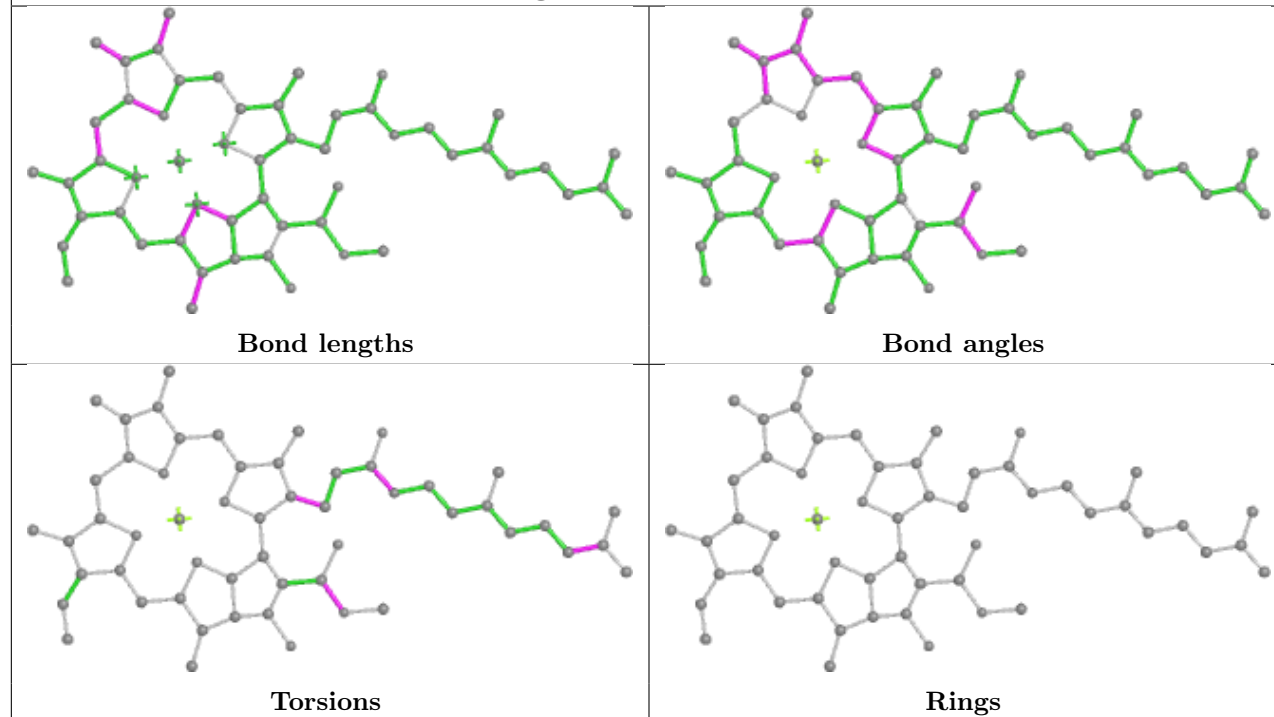


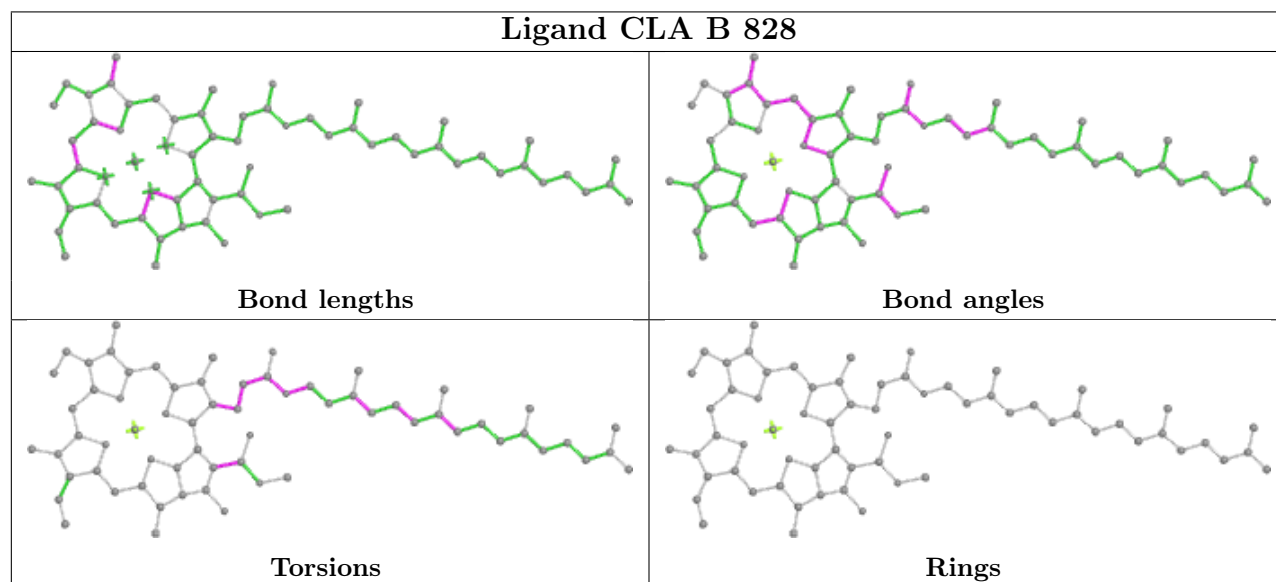
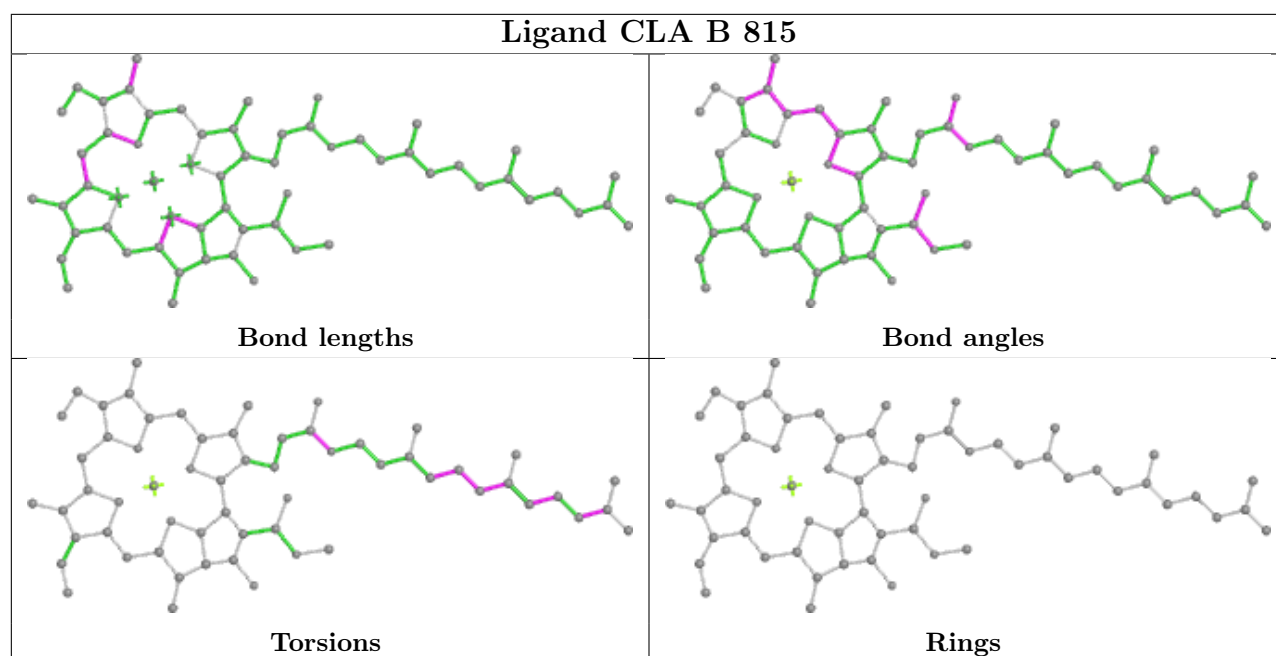


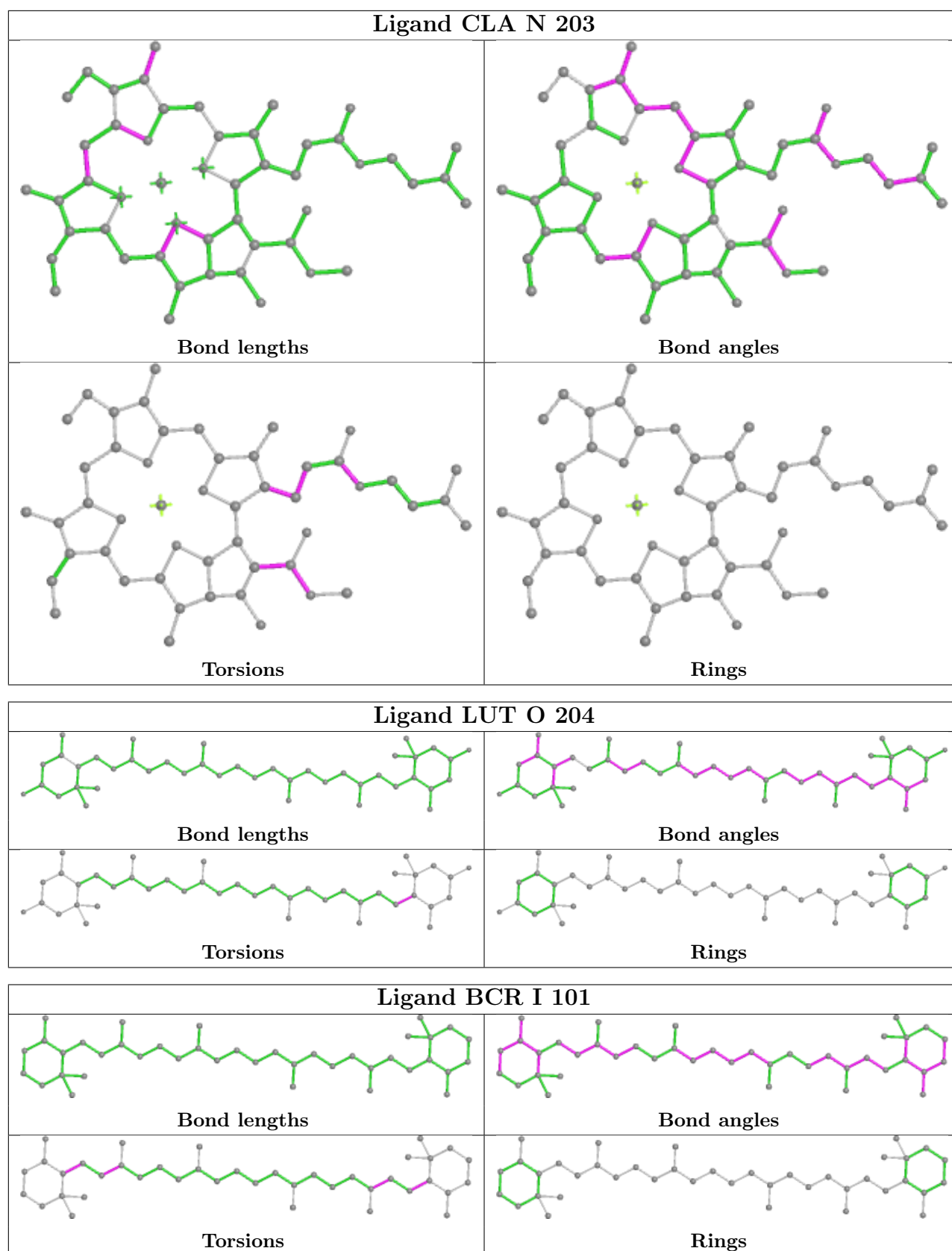
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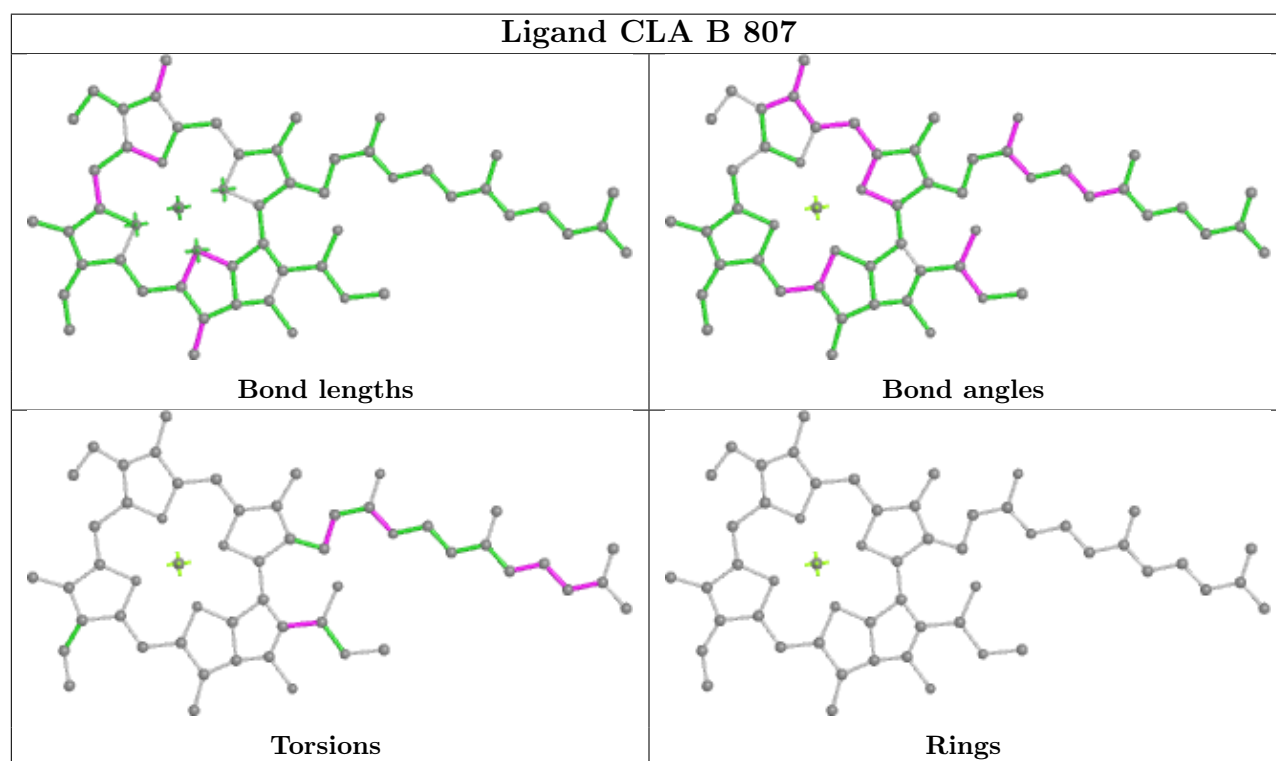
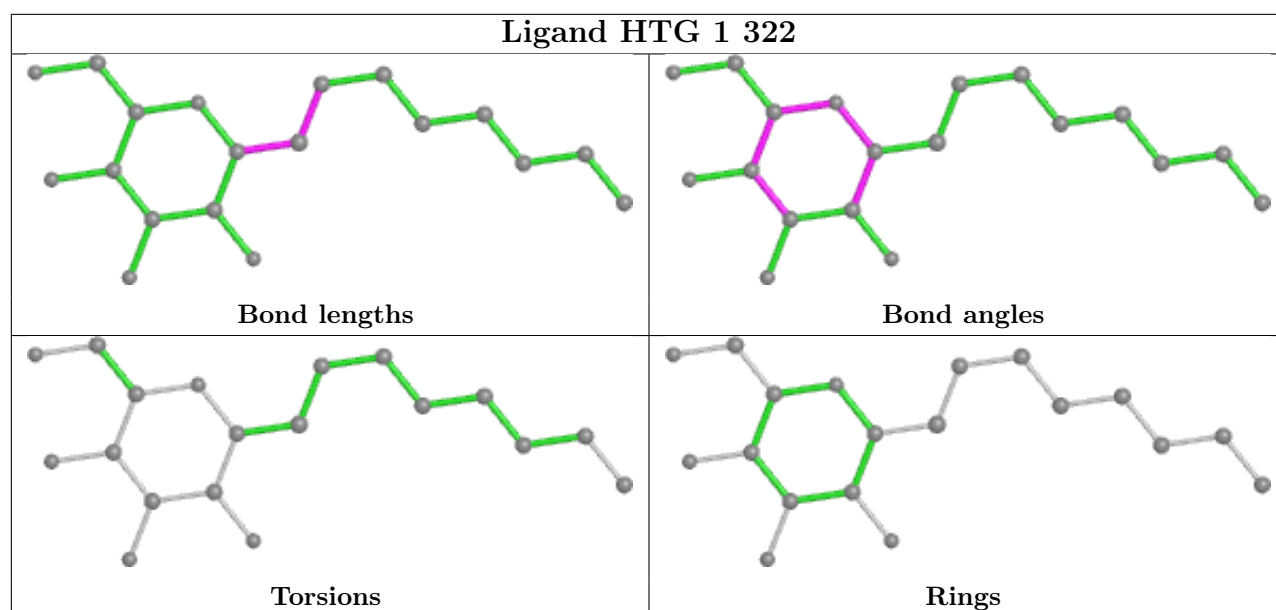


Ligand CLA B 811

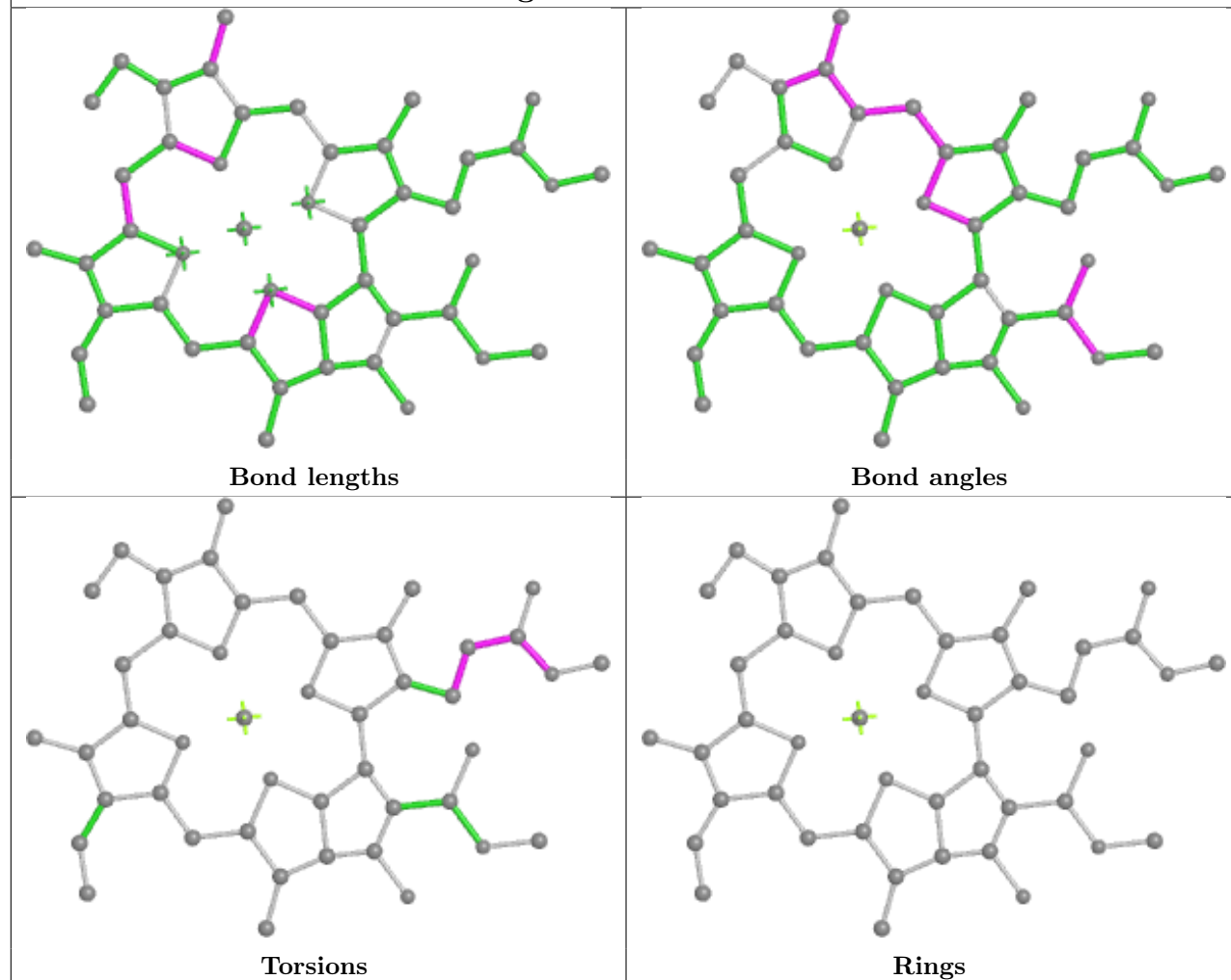




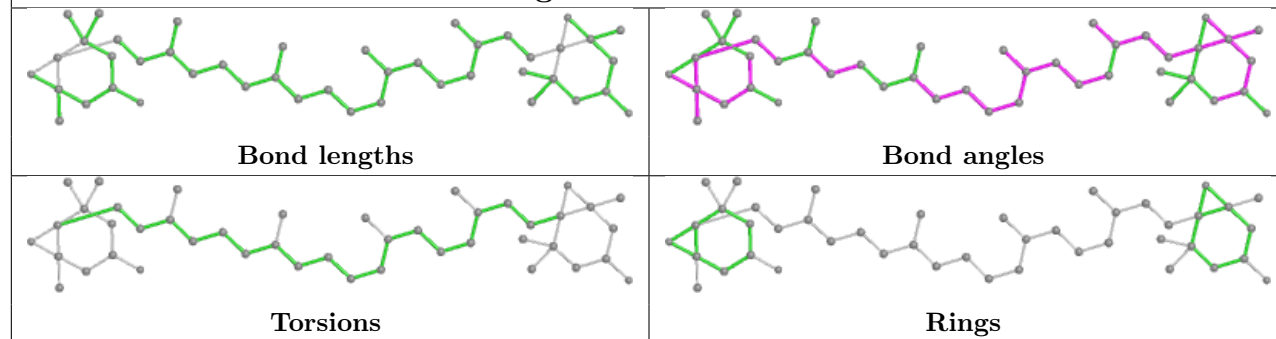




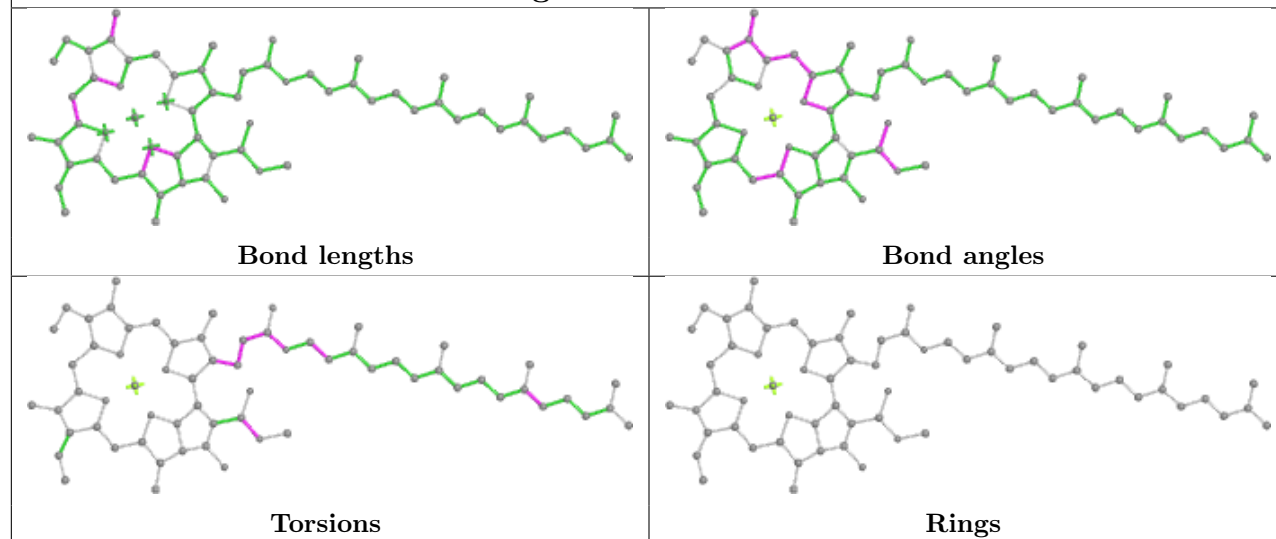
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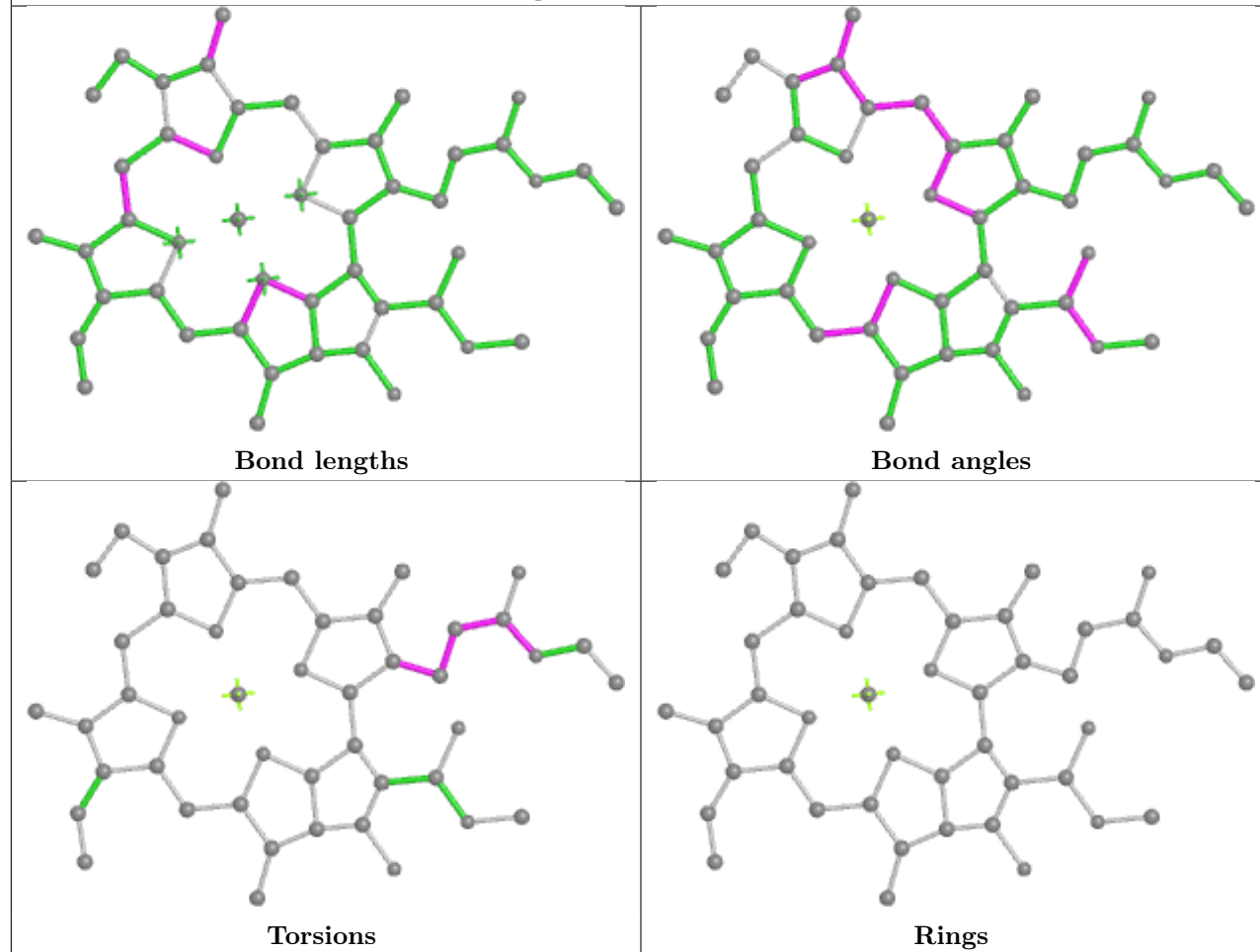
Ligand XAT 4 317

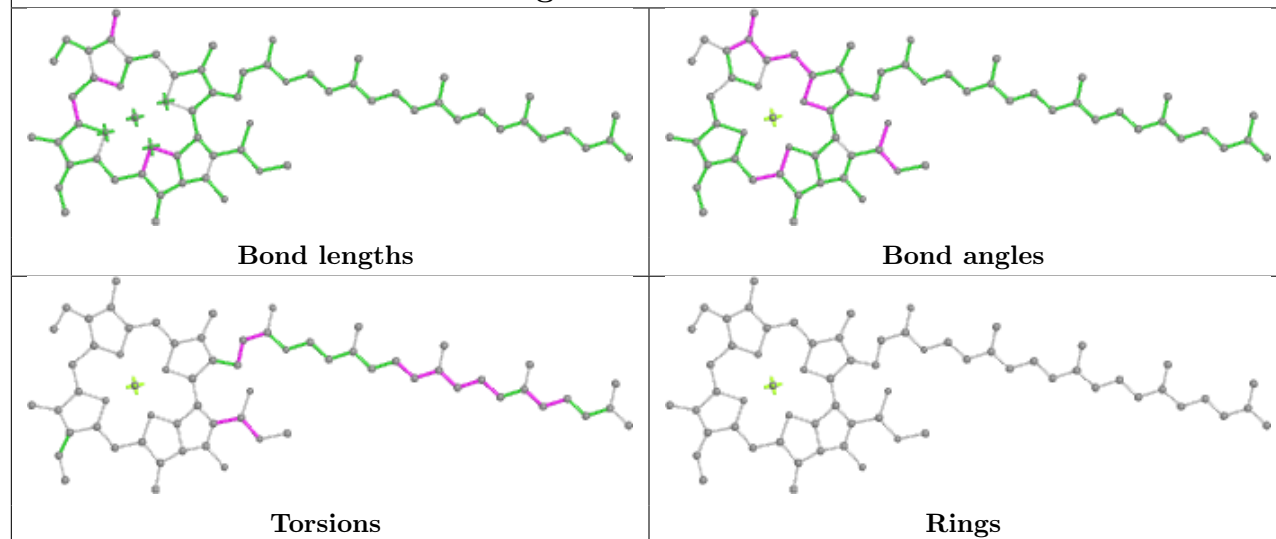
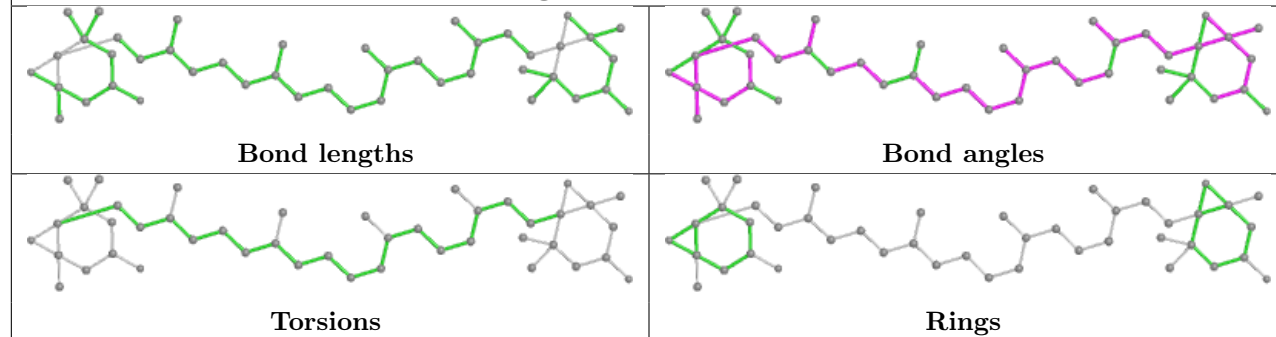


Ligand CLA B 831

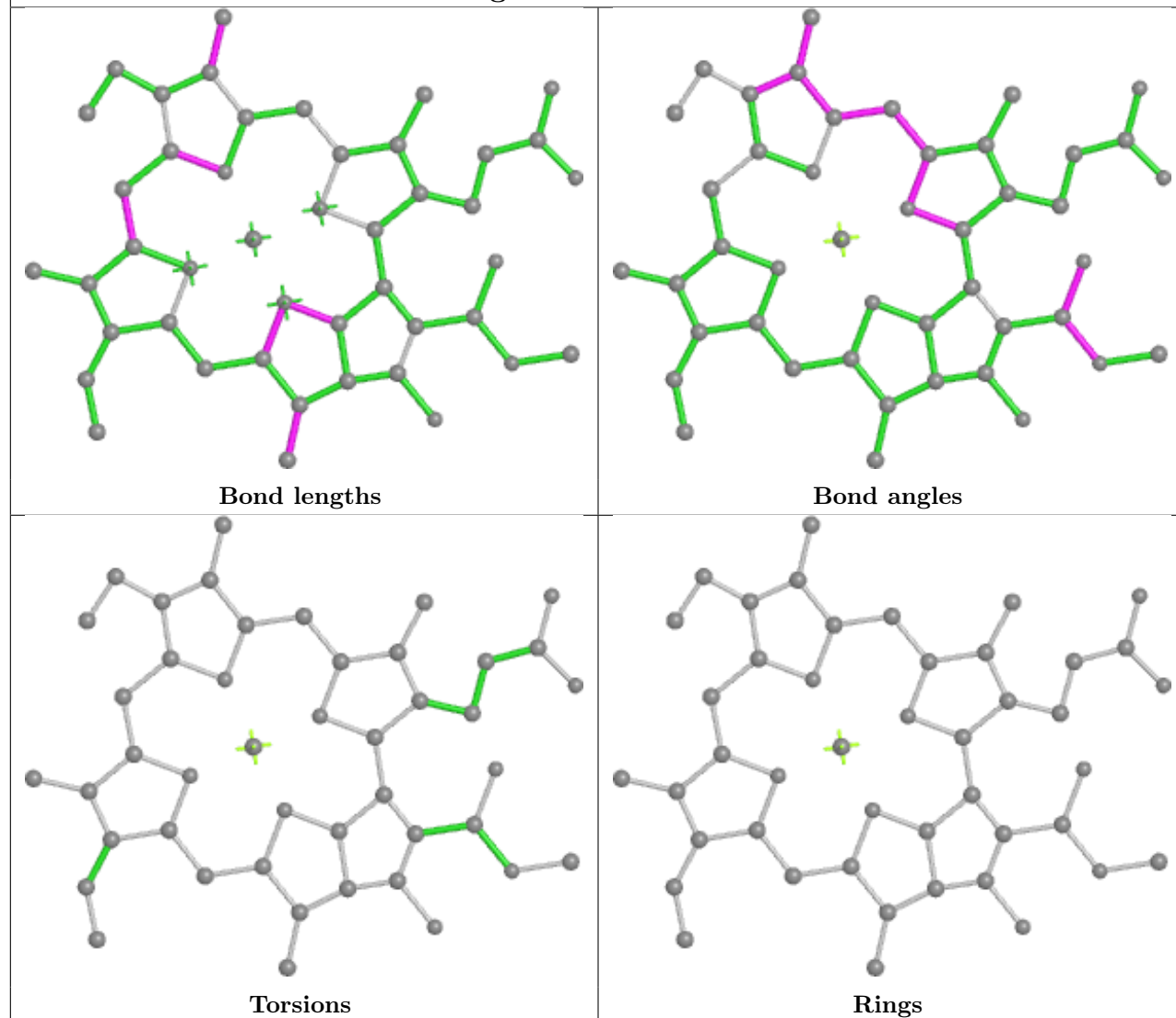


Ligand CLA 3 305

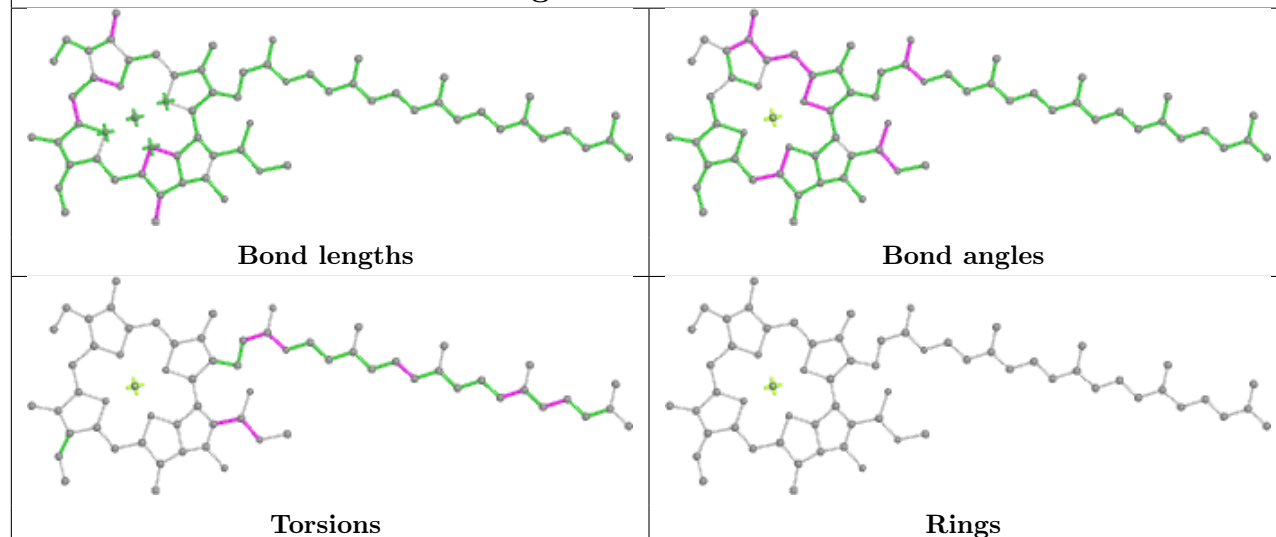


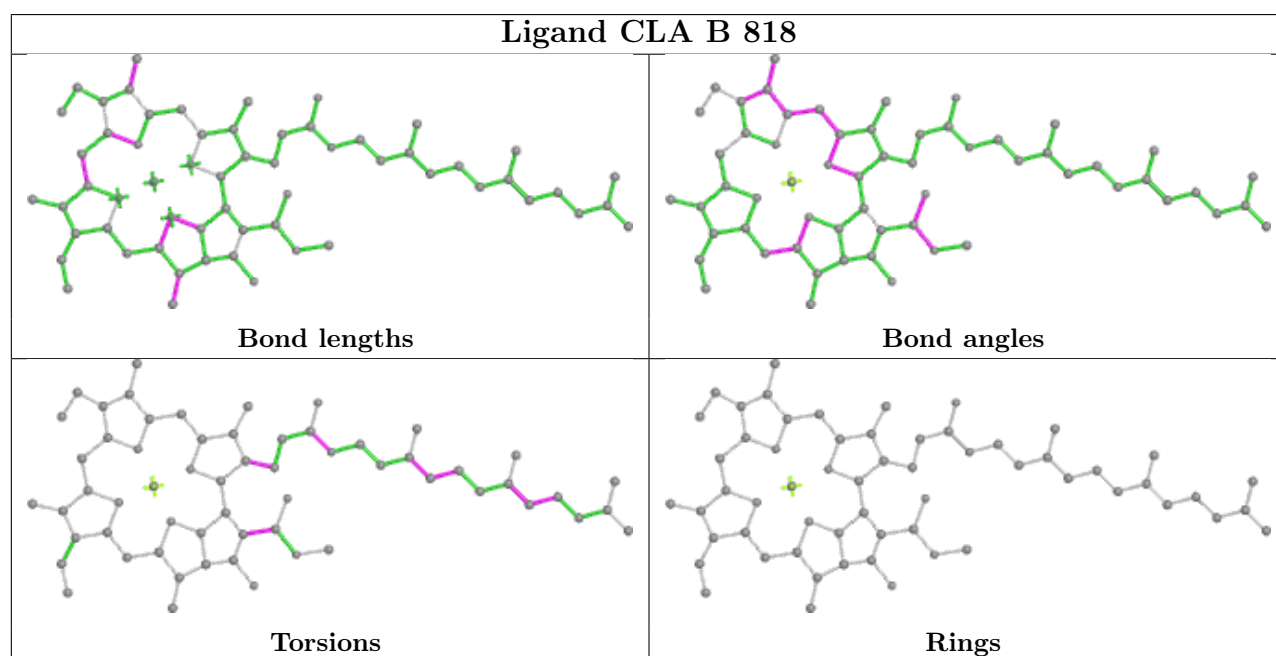
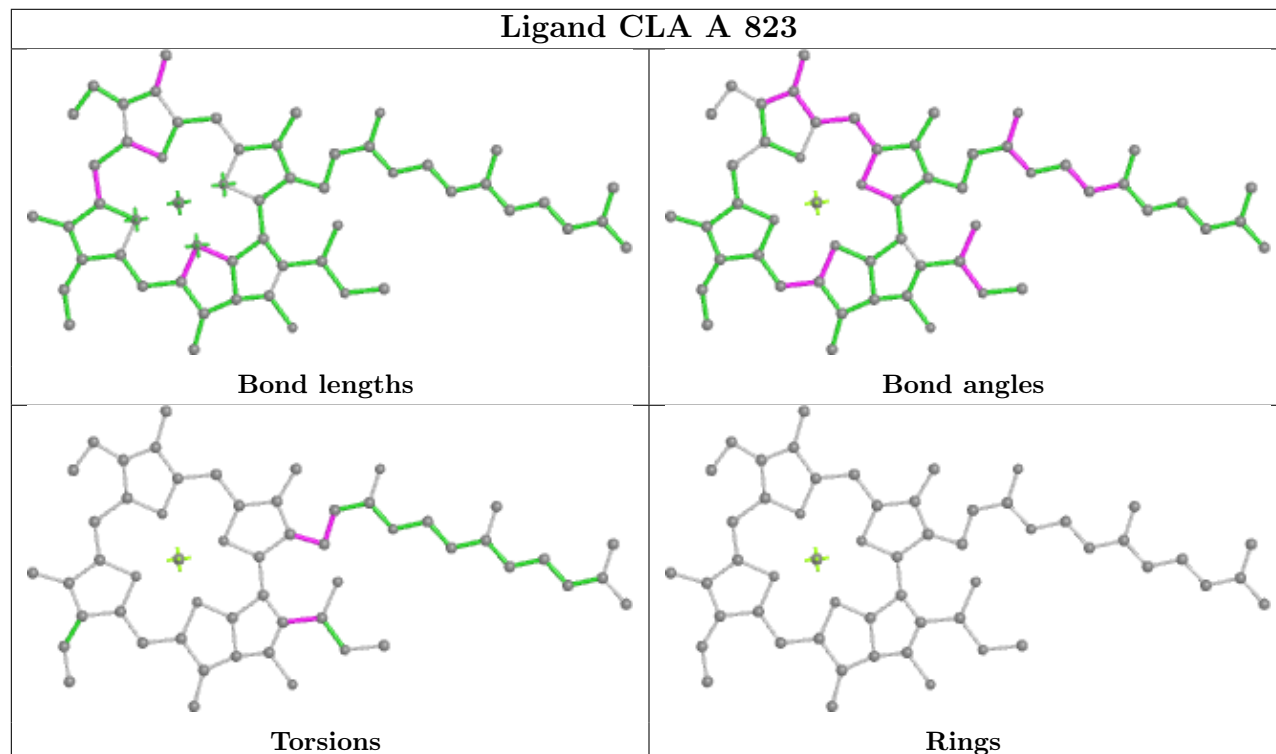
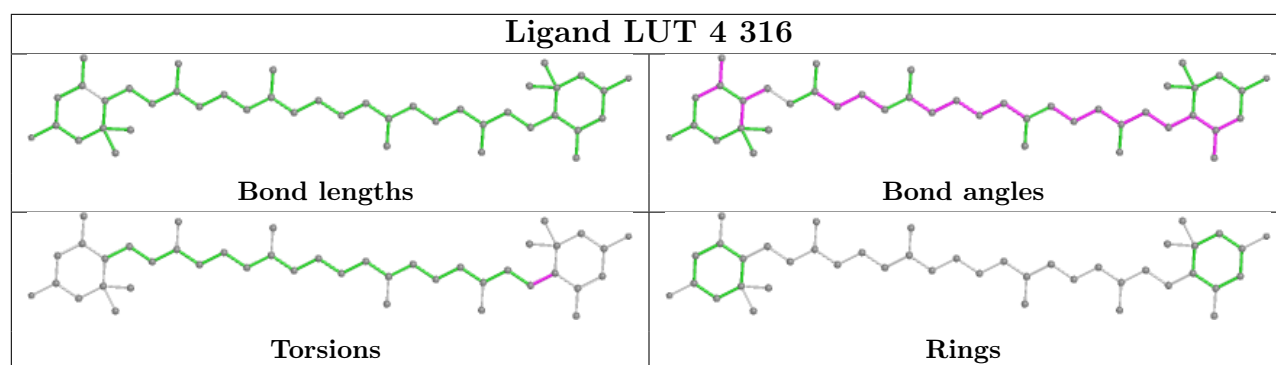
Ligand CLA 1 312**Ligand XAT 2 316**

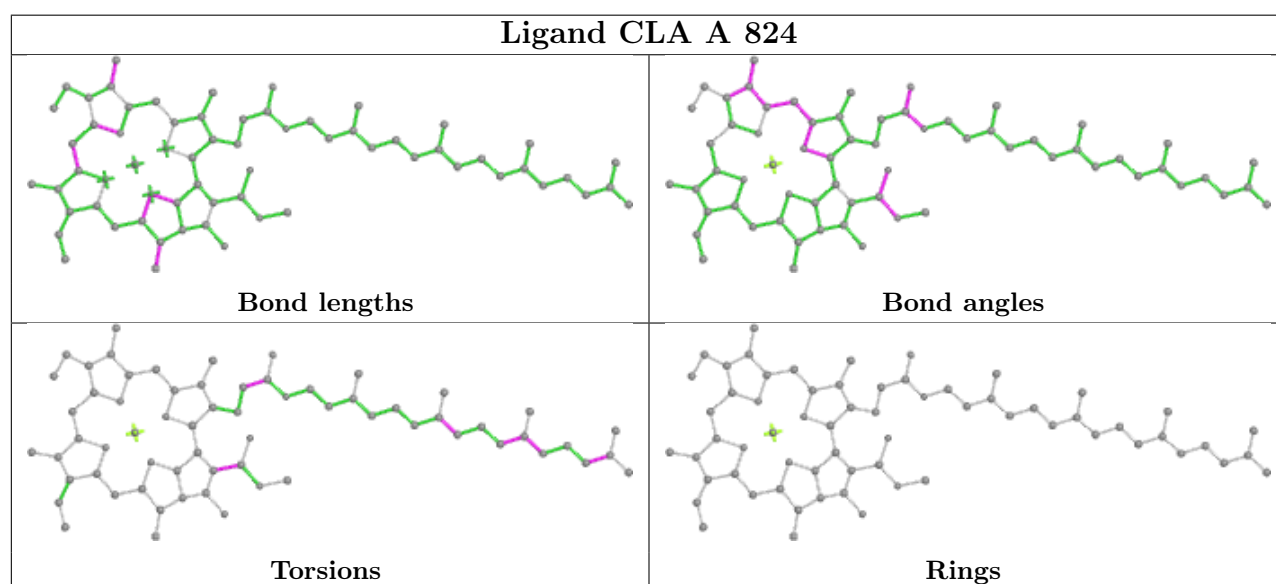
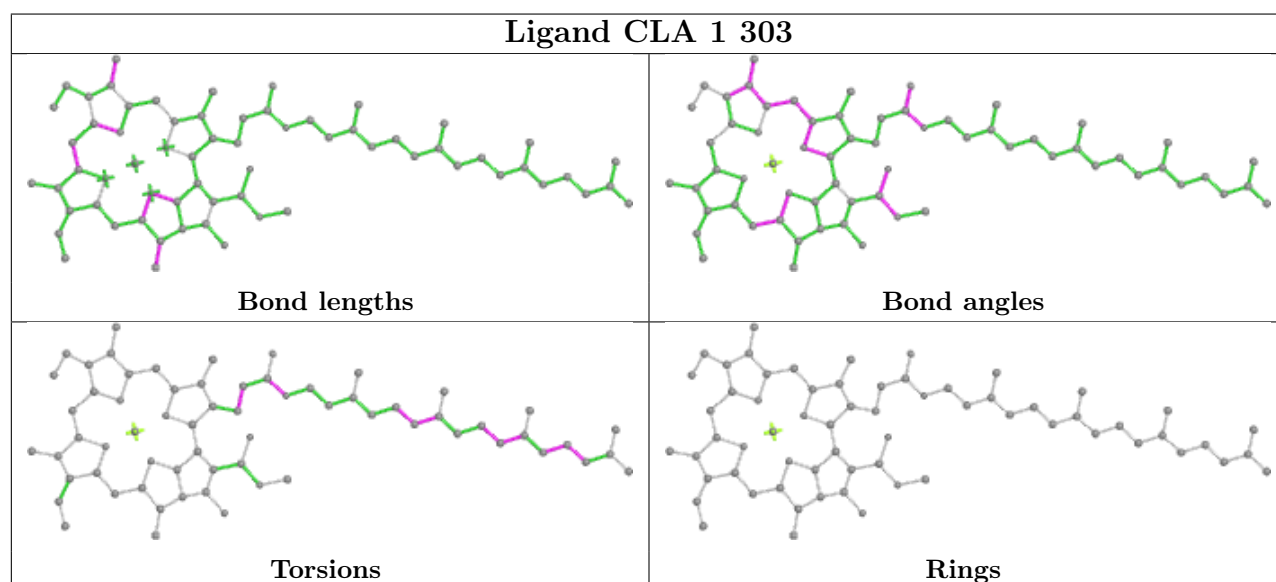
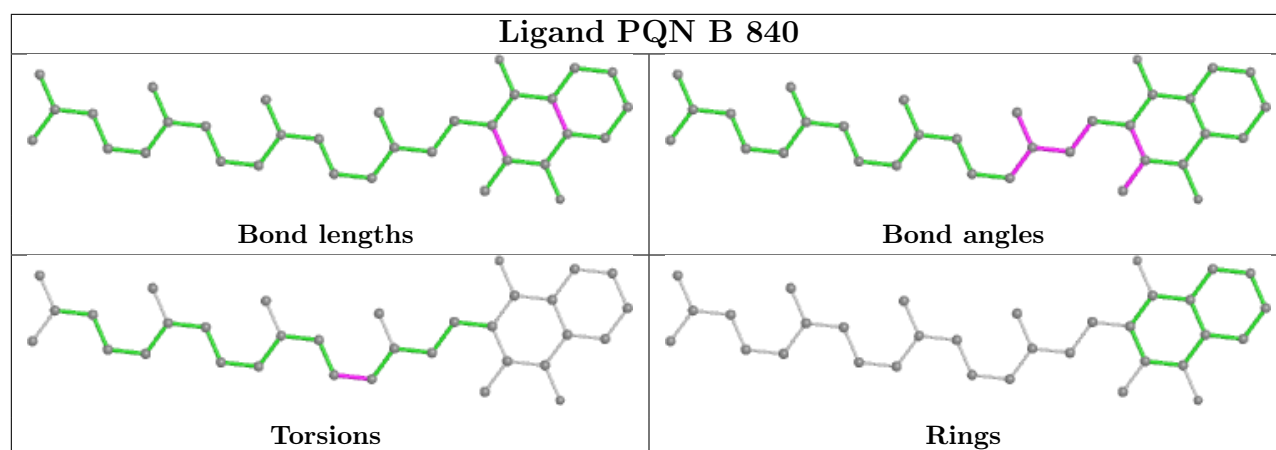
Ligand CLA A 815



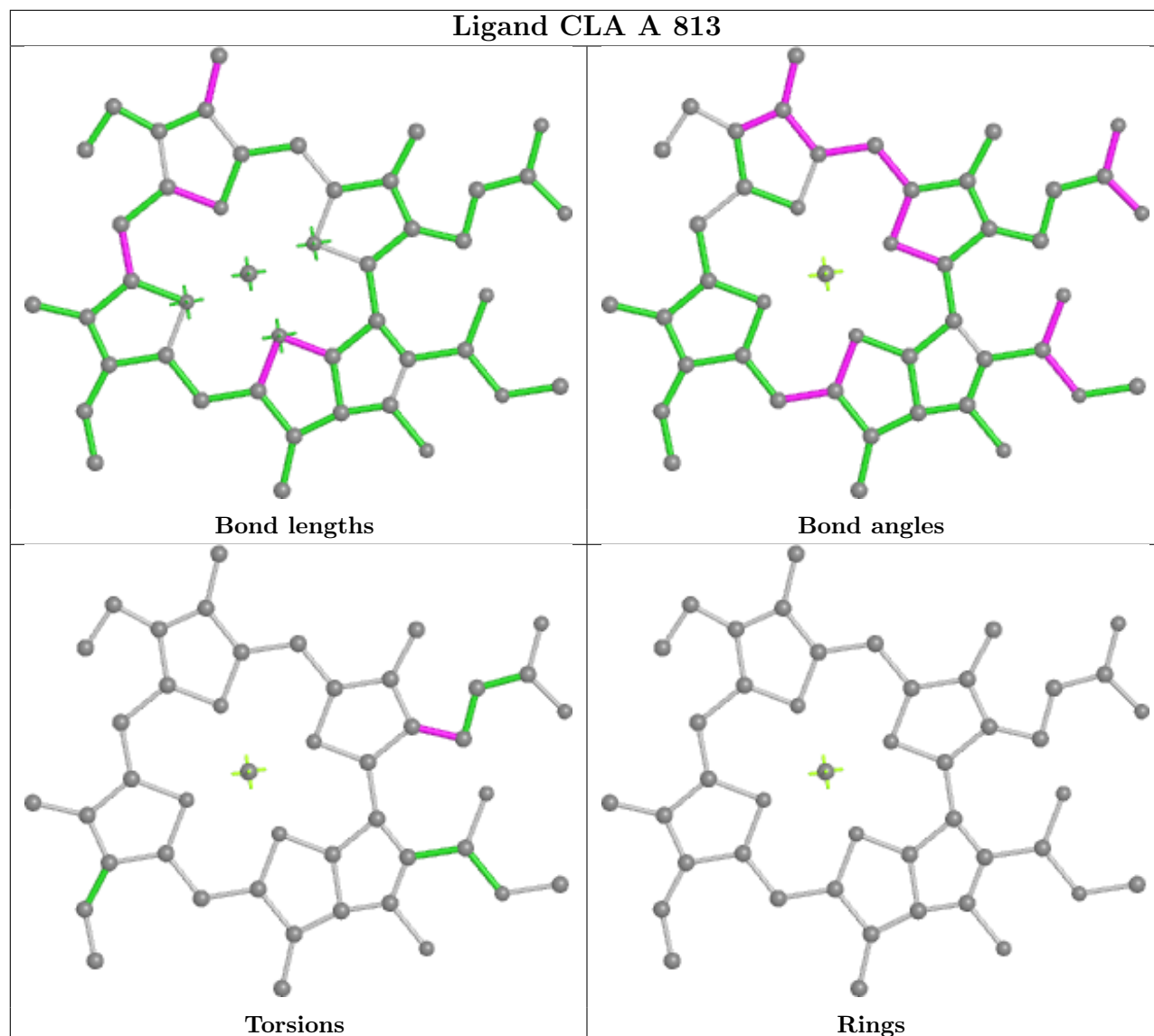
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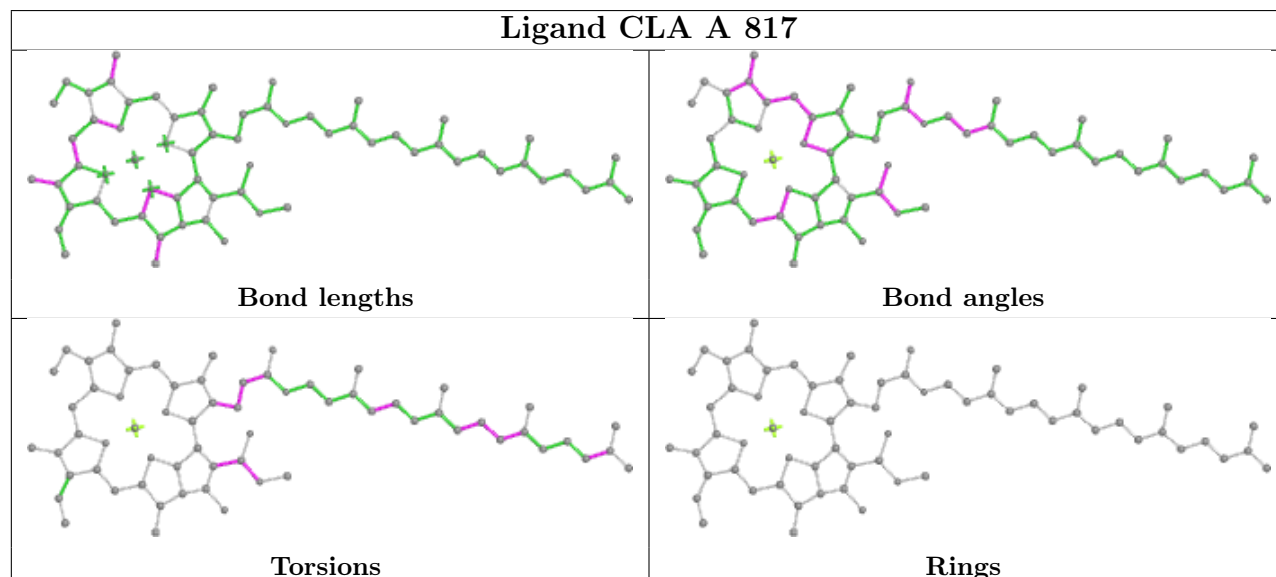




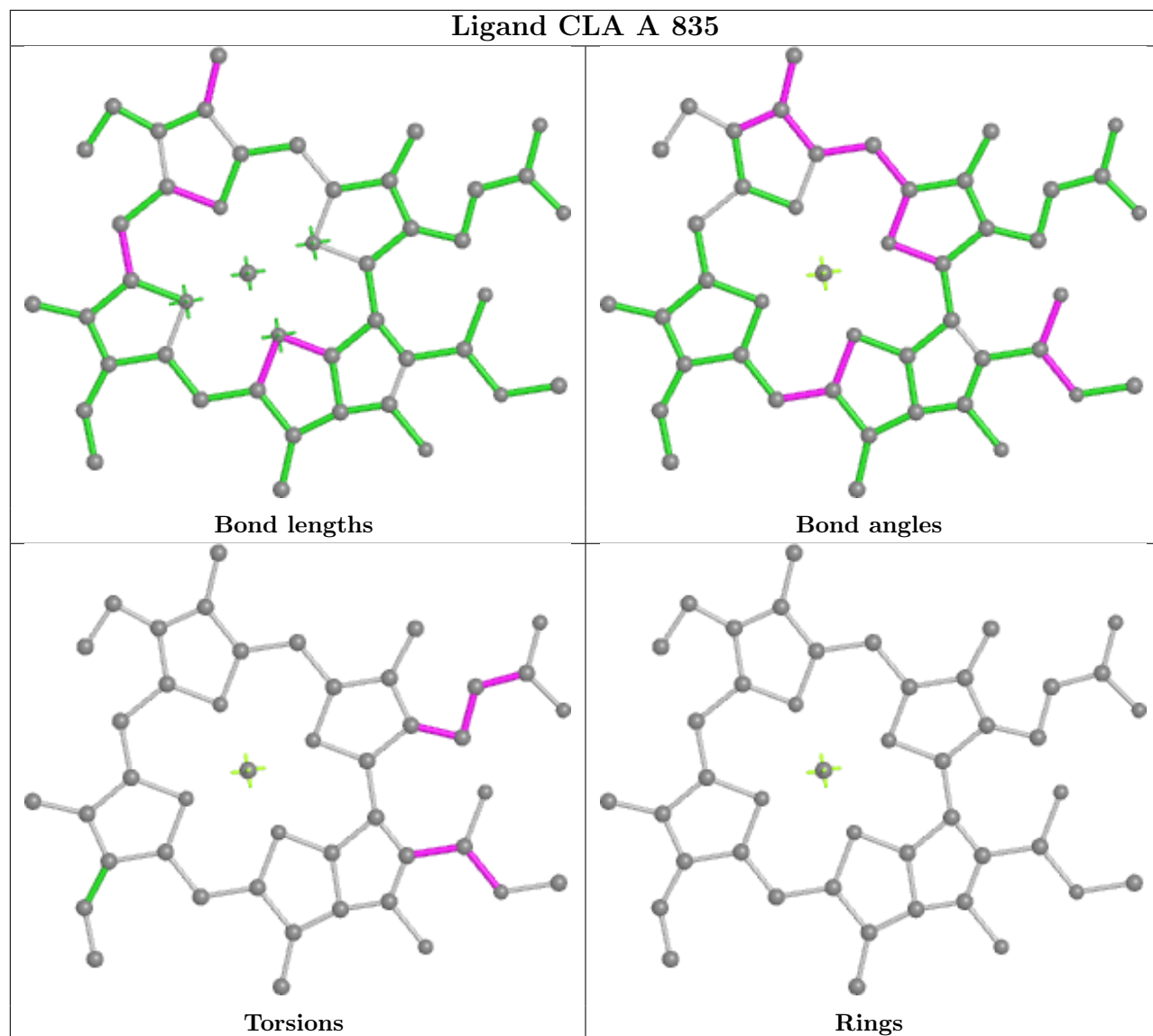
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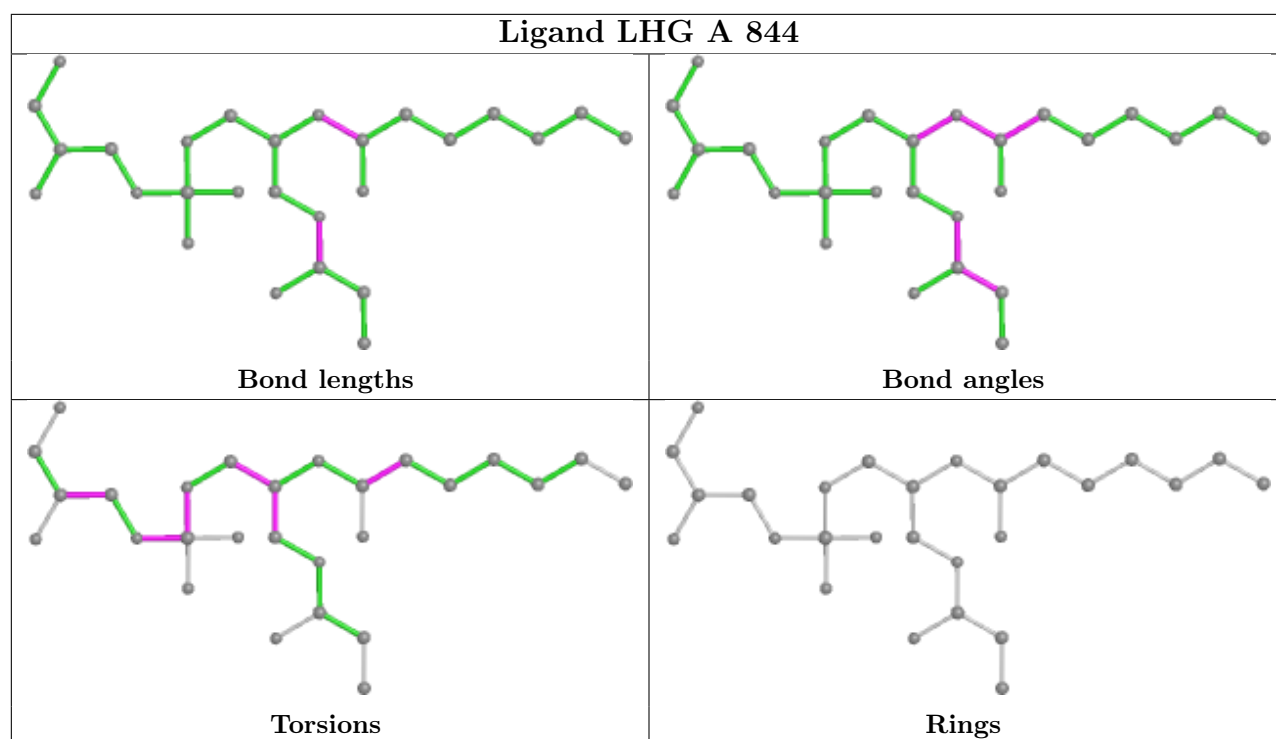


Ligand CLA A 817

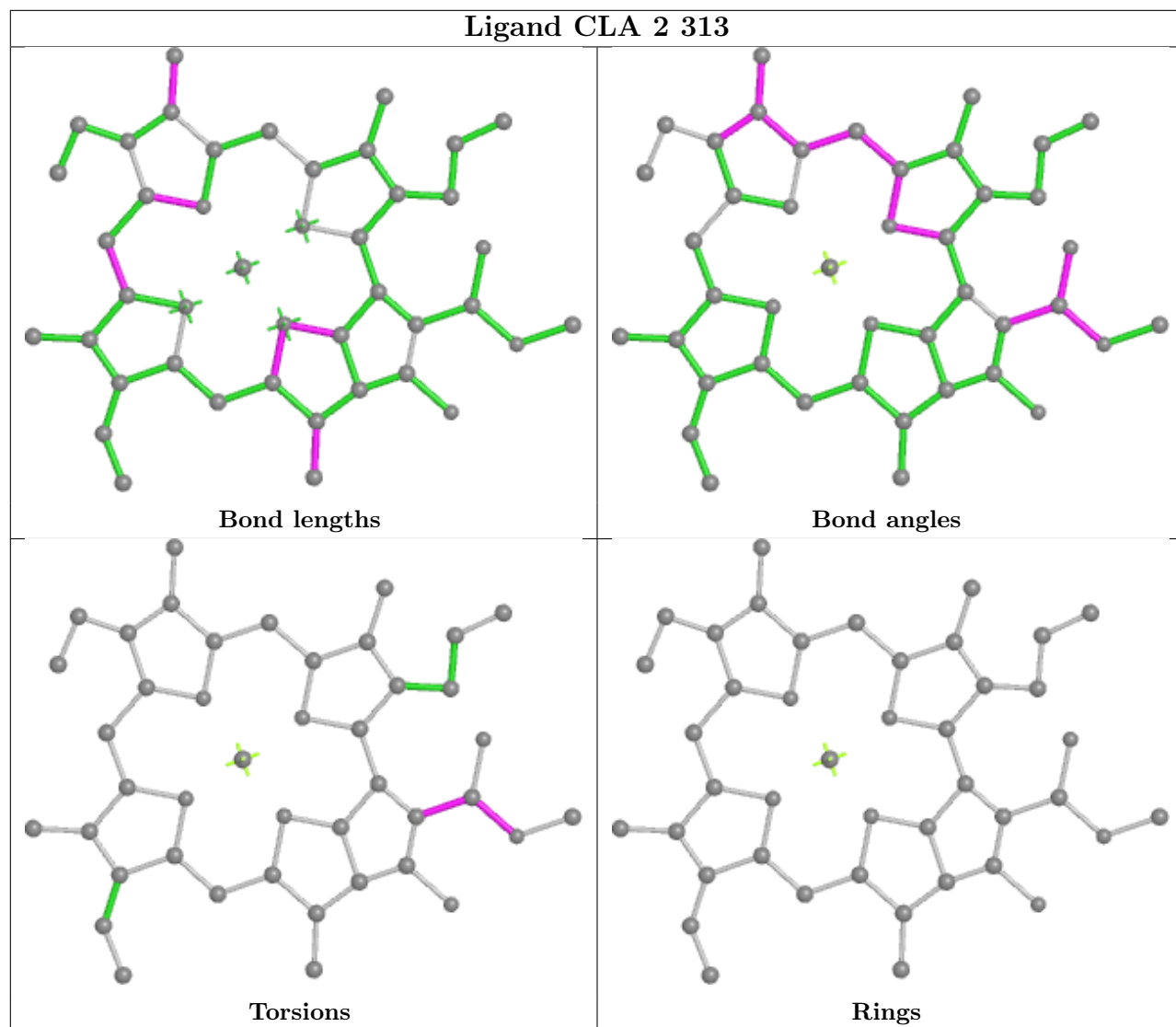


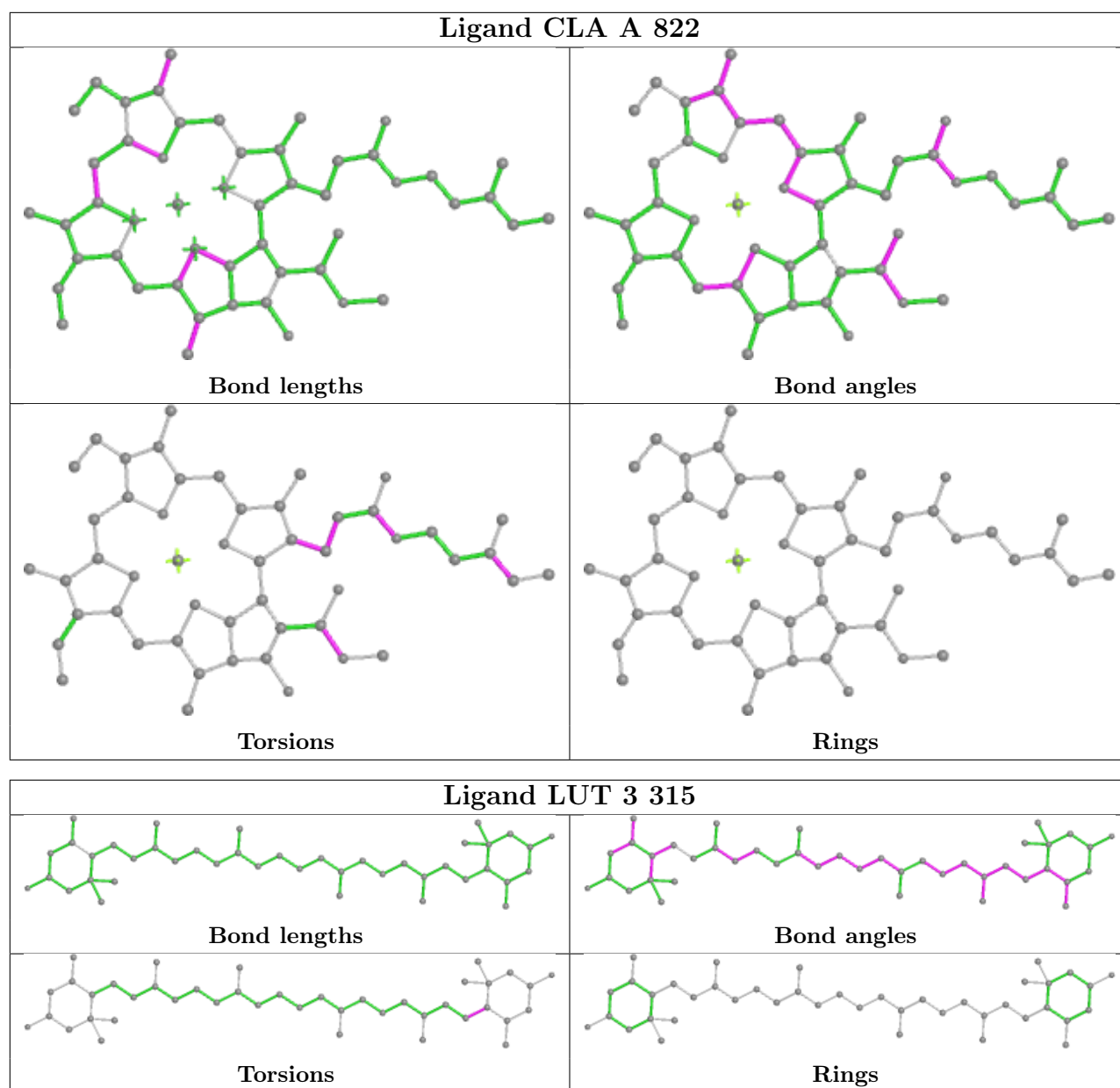
Ligand CLA A 835



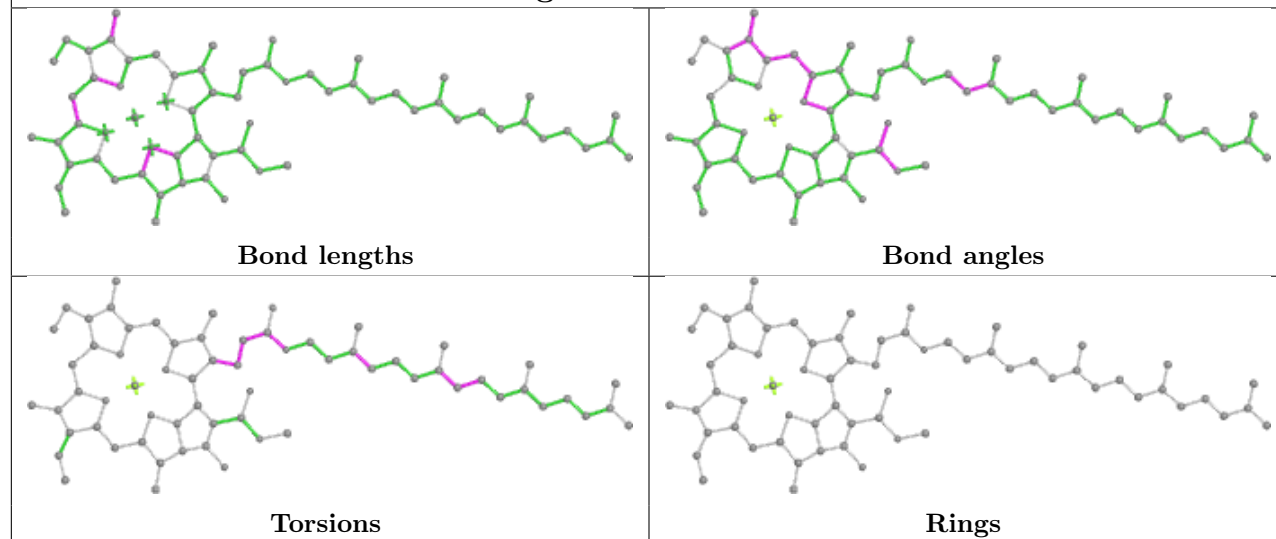


Ligand CLA 2 313

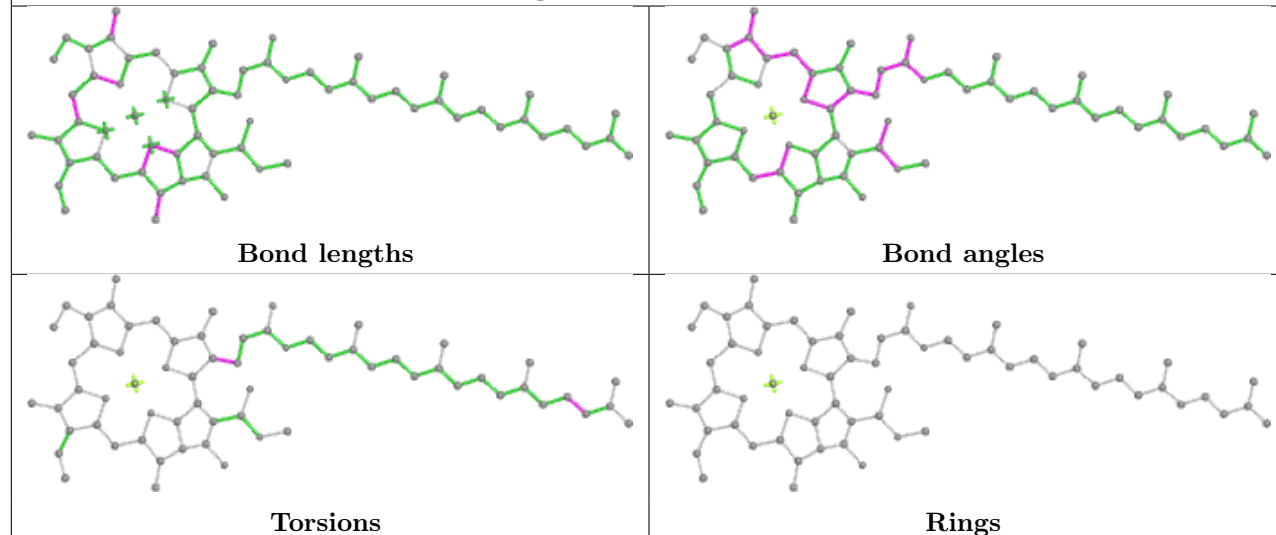




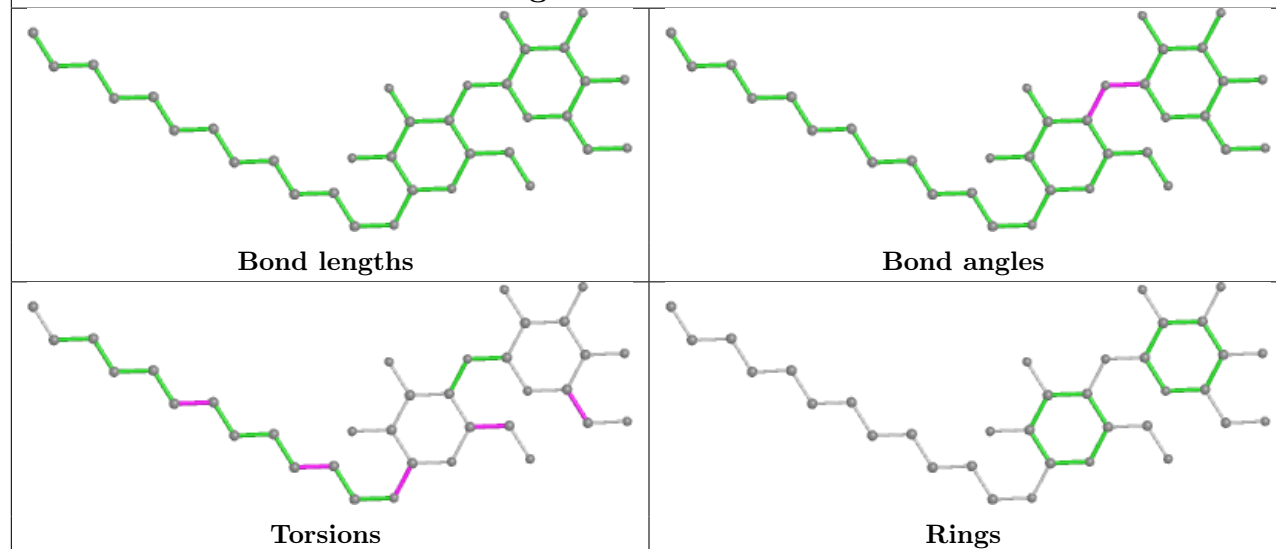
Ligand CLA 1 308

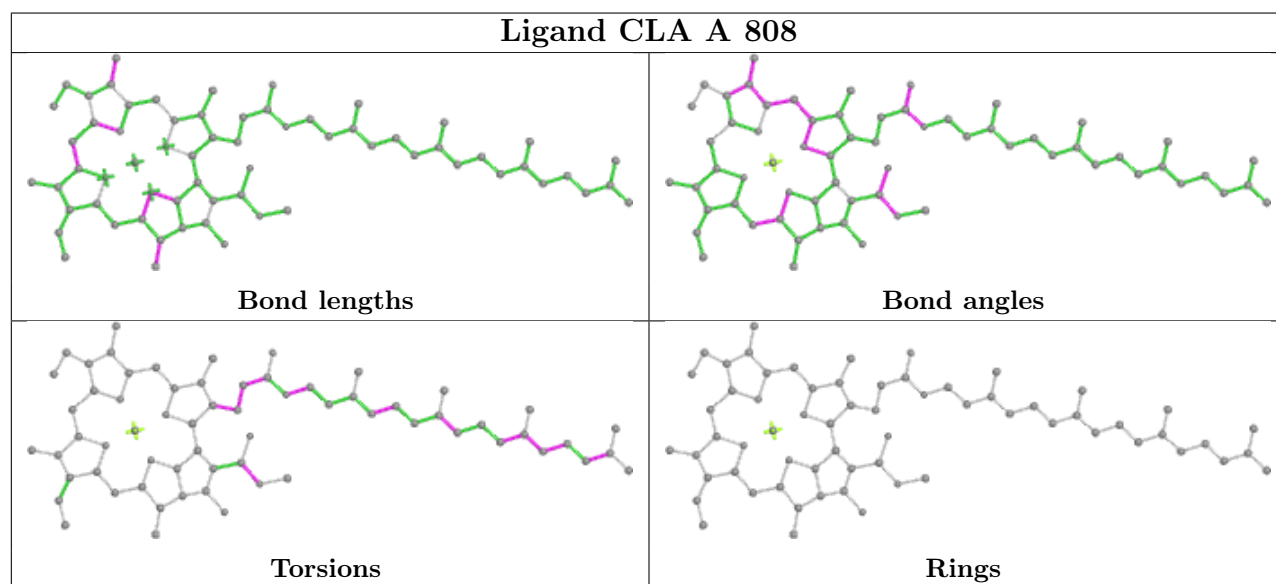
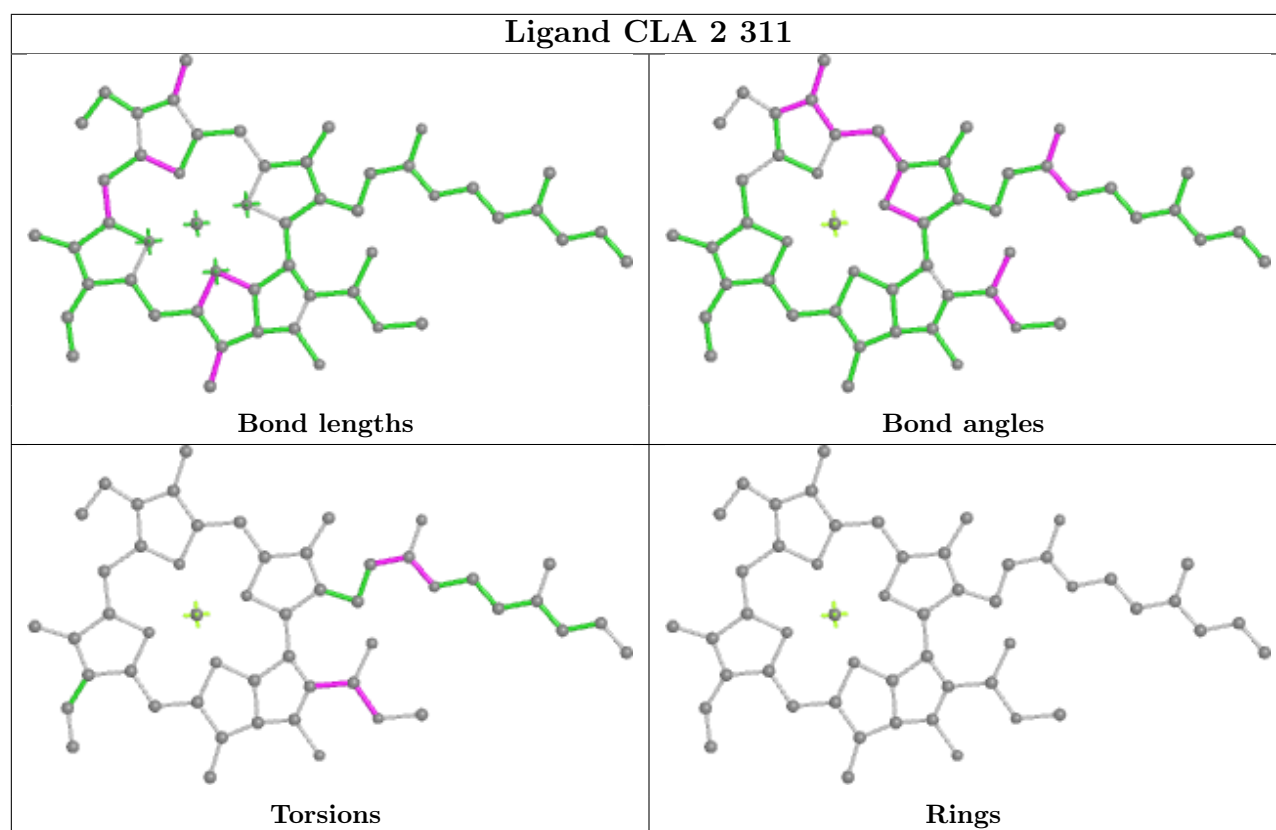


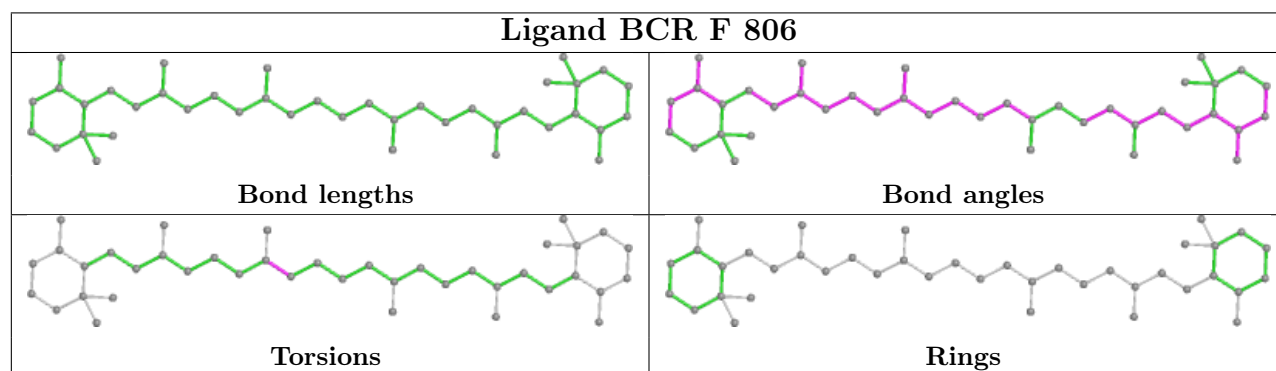
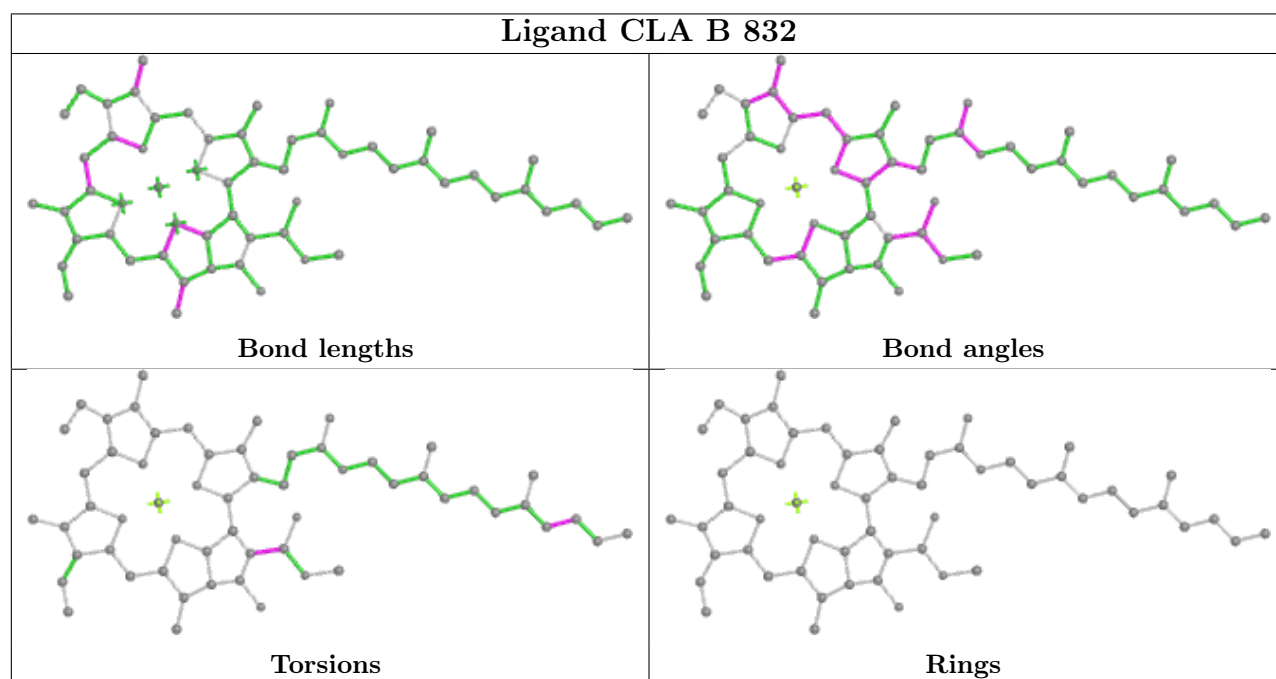
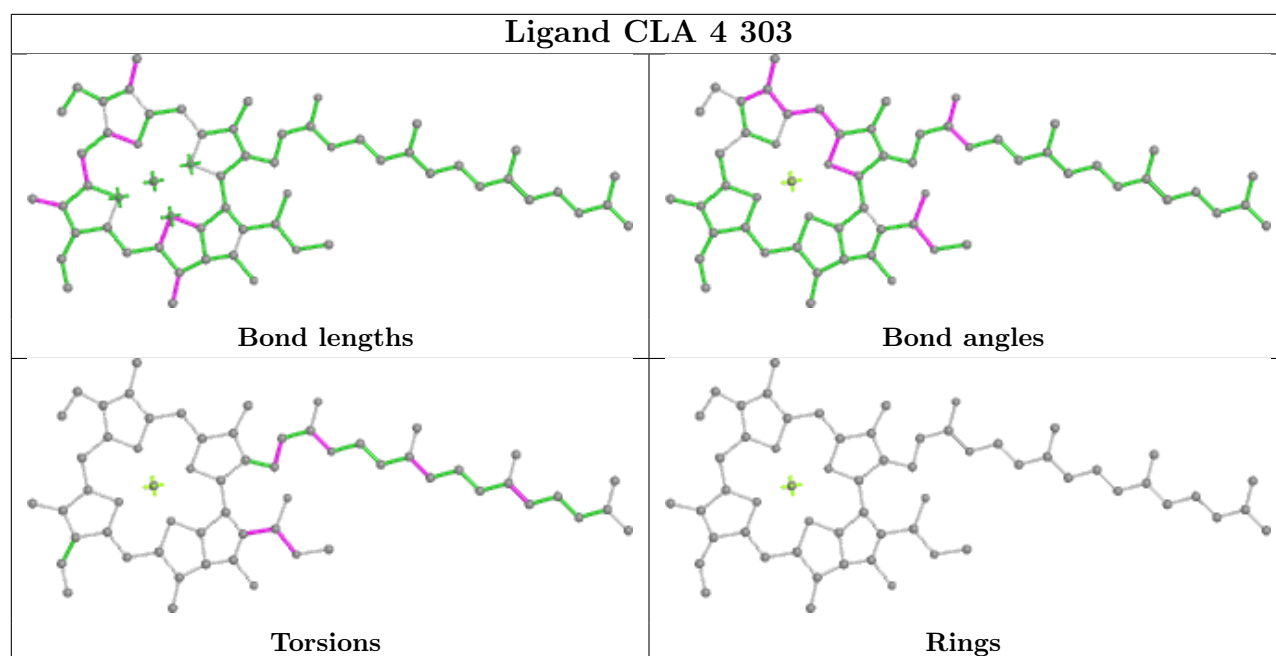
Ligand CLA A 825



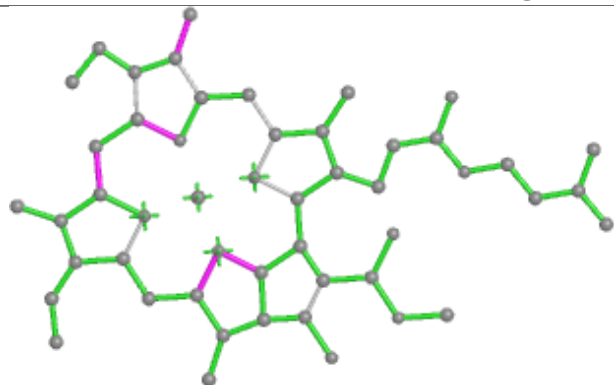
Ligand LMT B 847



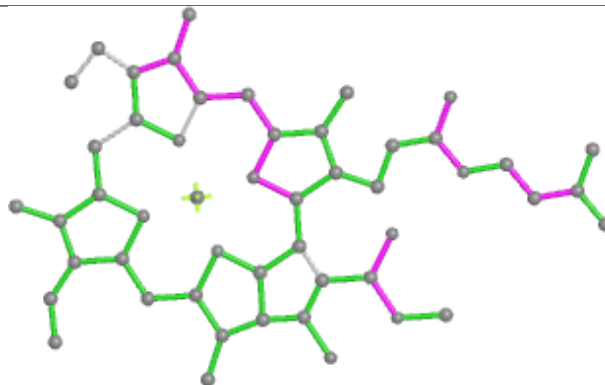




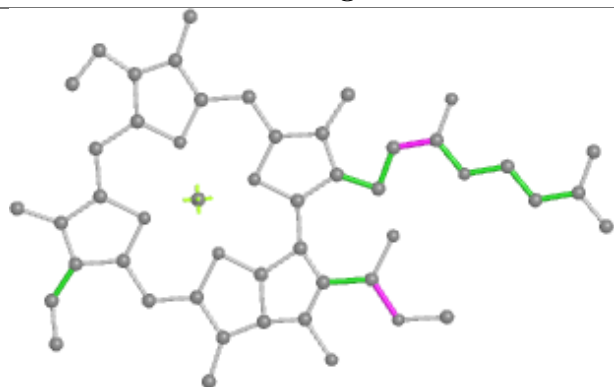
Ligand CLA 3 302



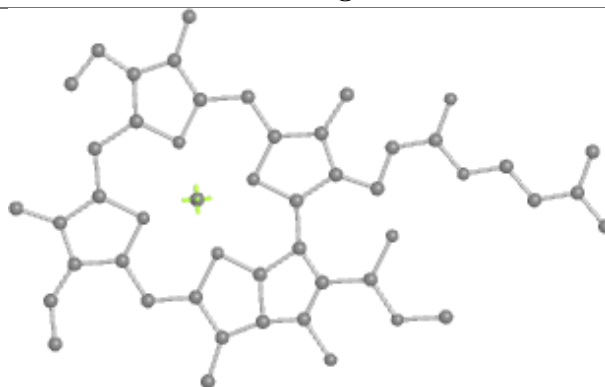
Bond lengths



Bond angles

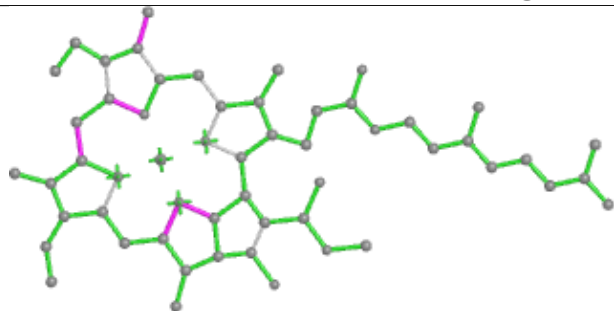


Torsions

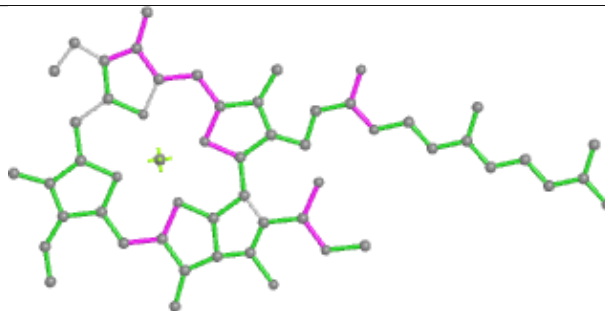


Rings

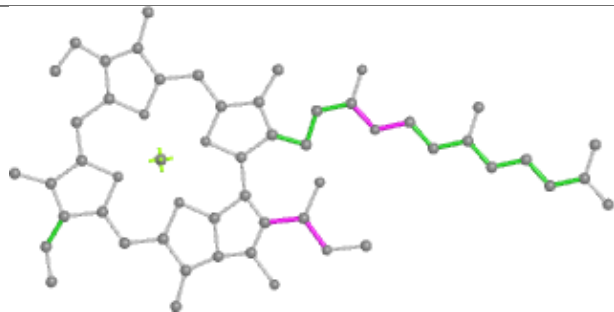
Ligand CLA 4 310



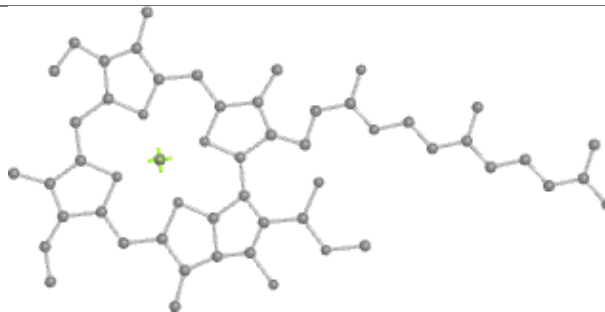
Bond lengths



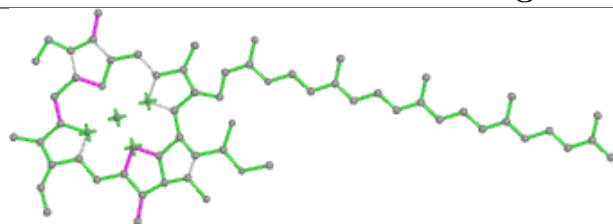
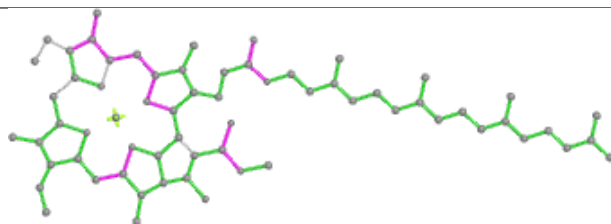
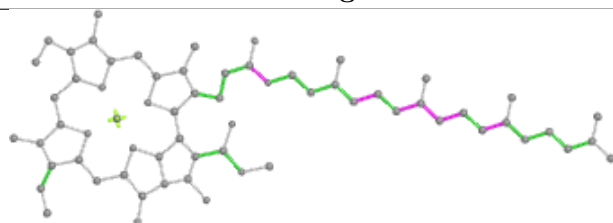
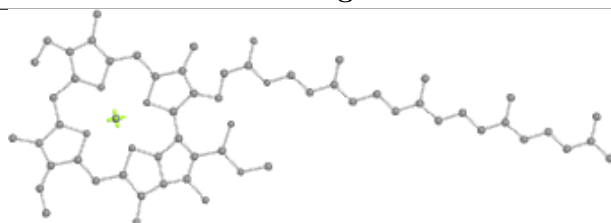
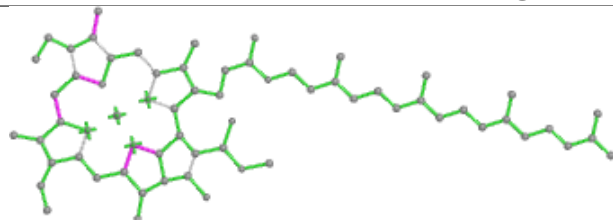
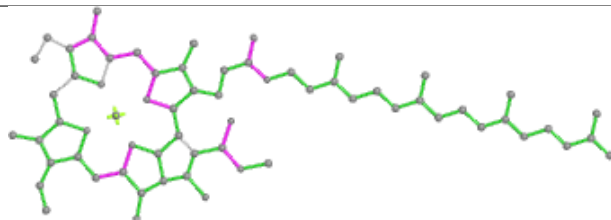
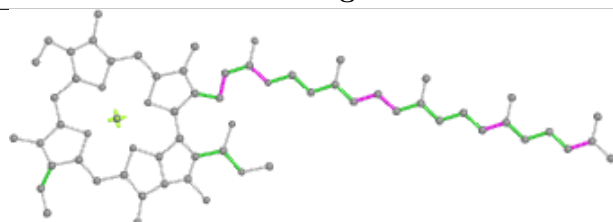
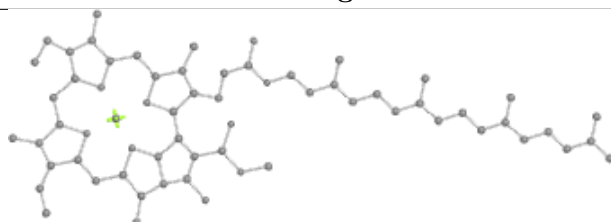
Bond angles

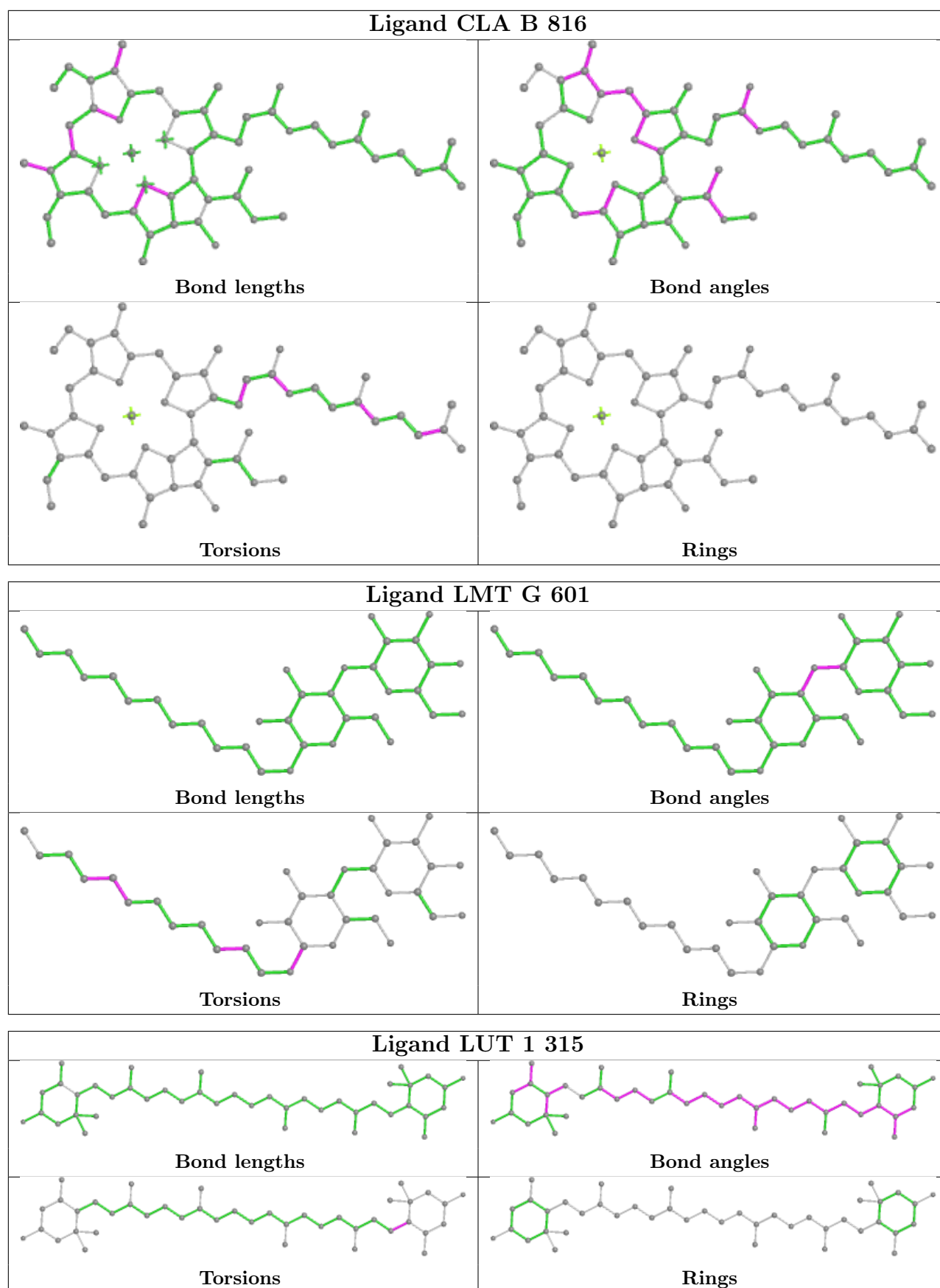


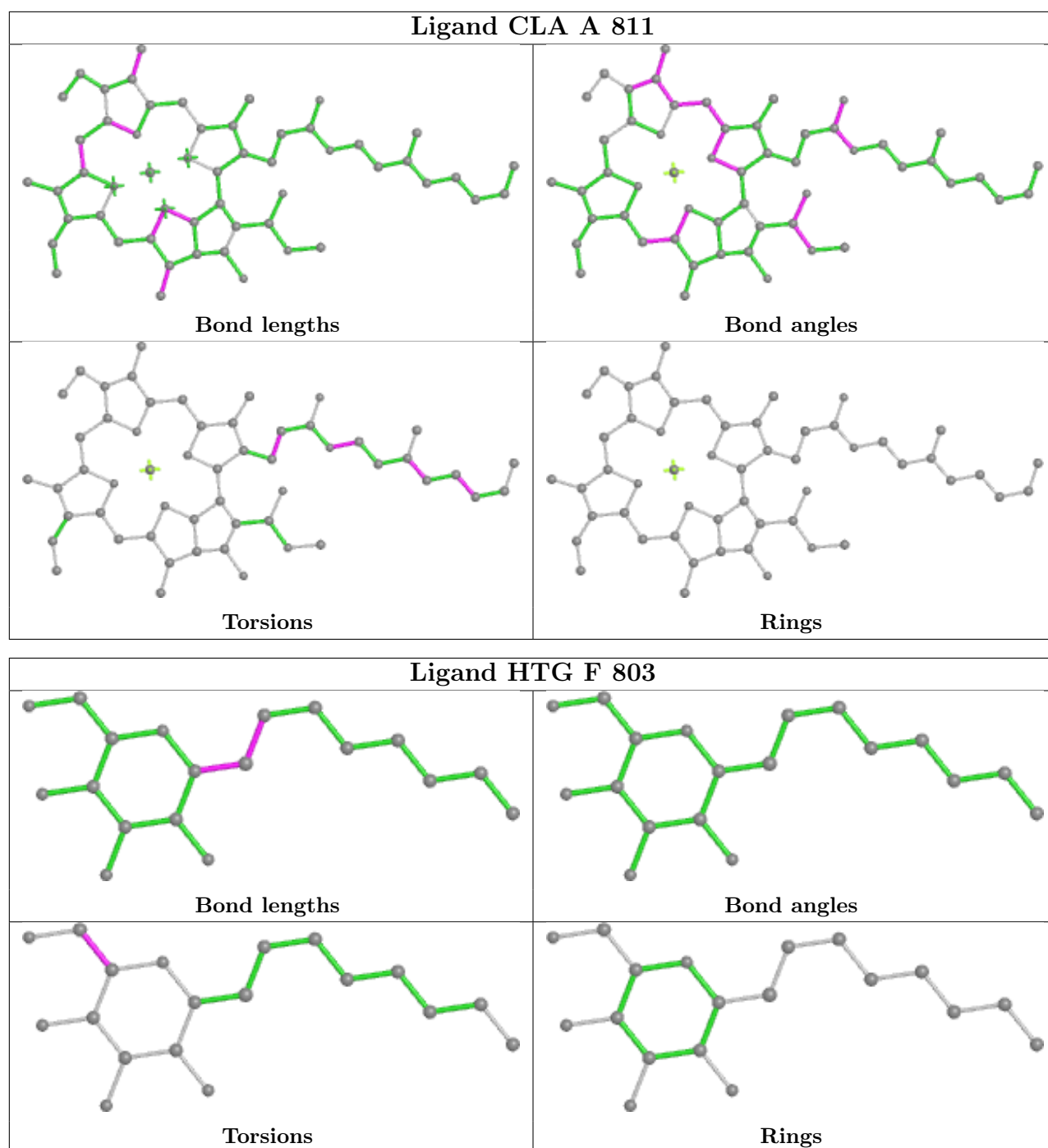
Torsions

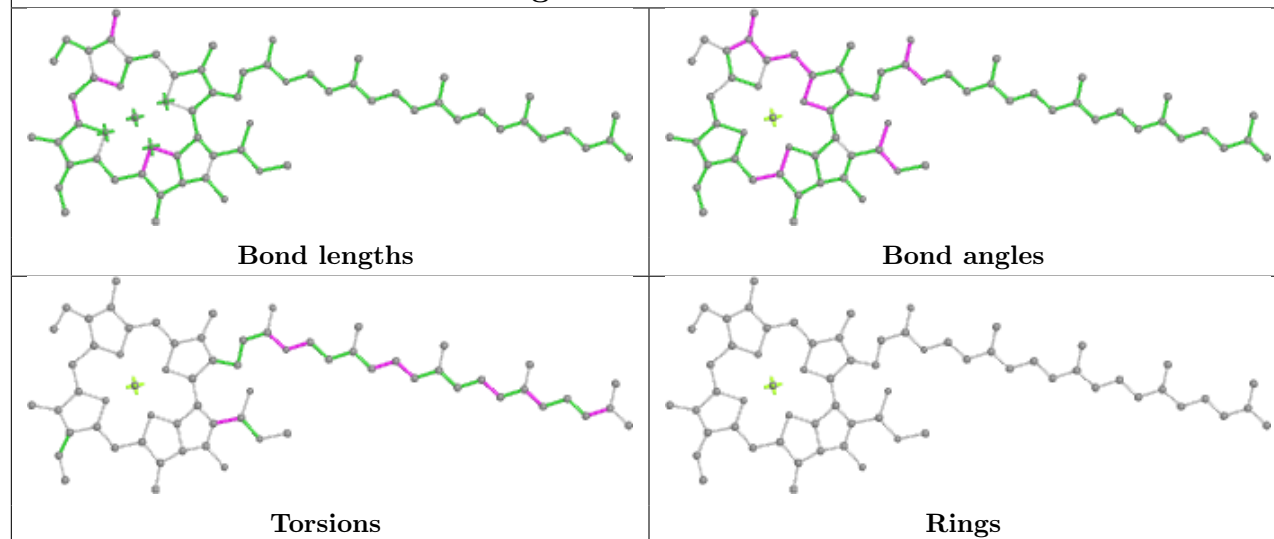
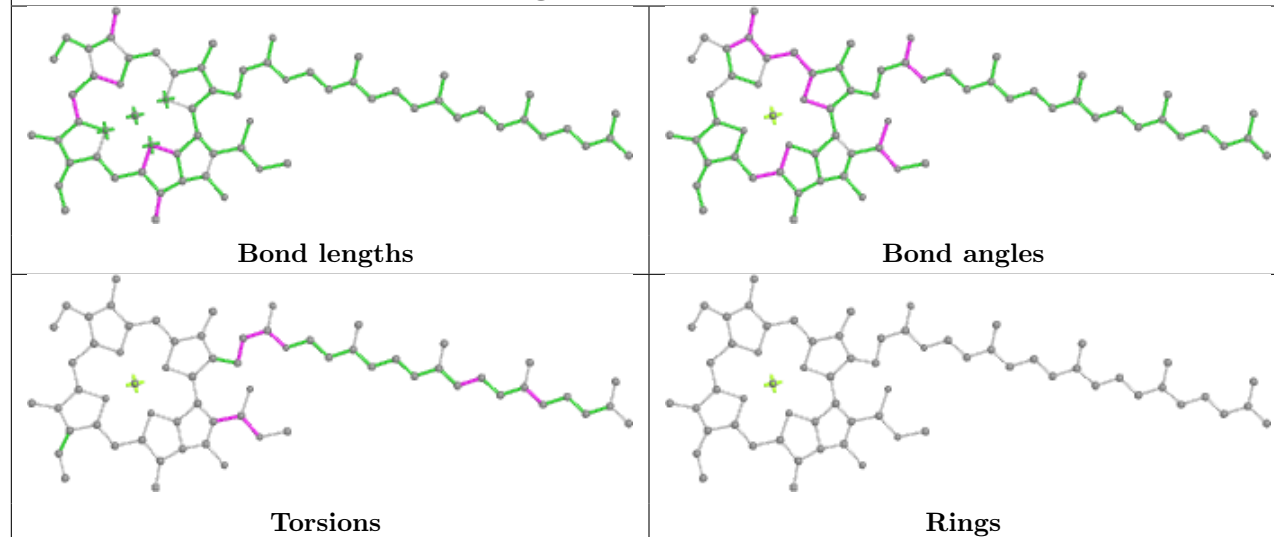


Rings

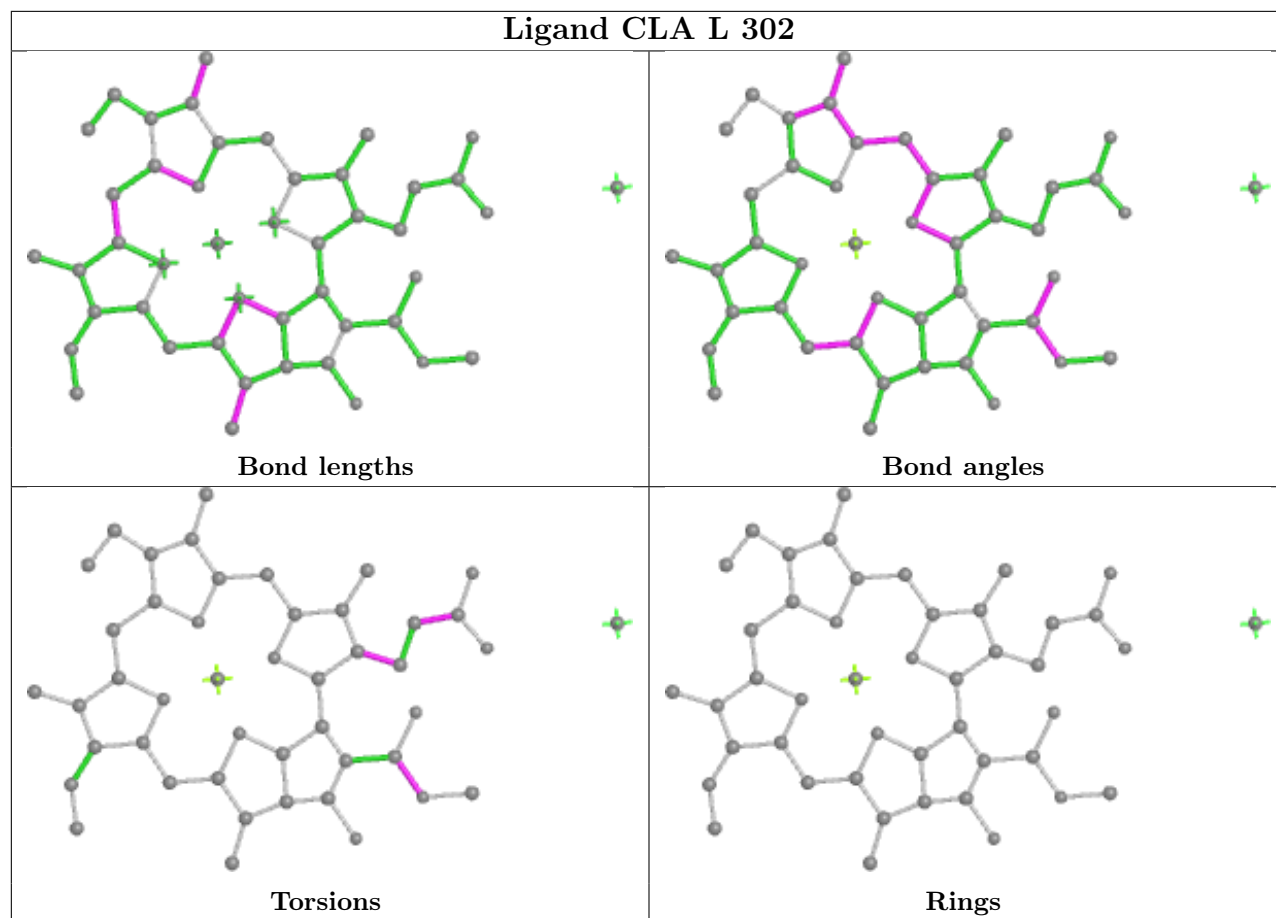
Ligand CLA F 802**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 820****Bond lengths****Bond angles****Torsions****Rings**



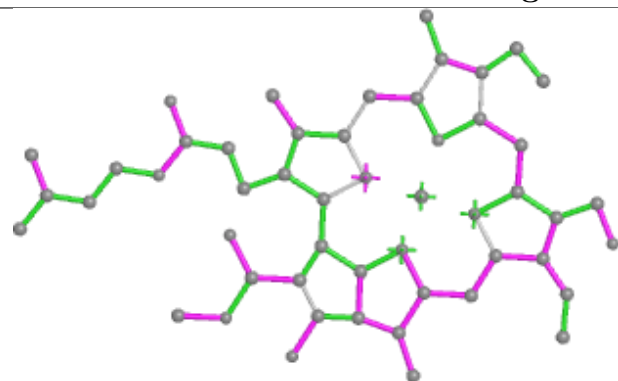


Ligand CLA A 806**Ligand CLA B 810**

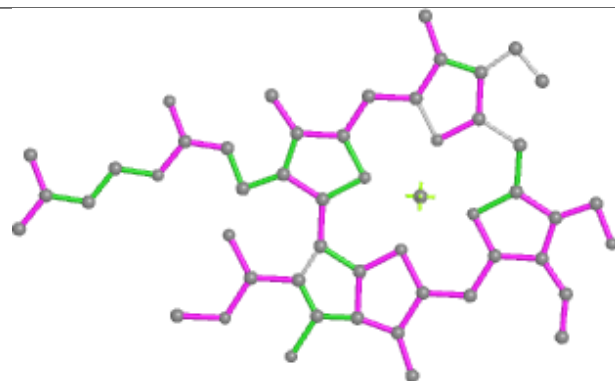
Ligand CLA L 302



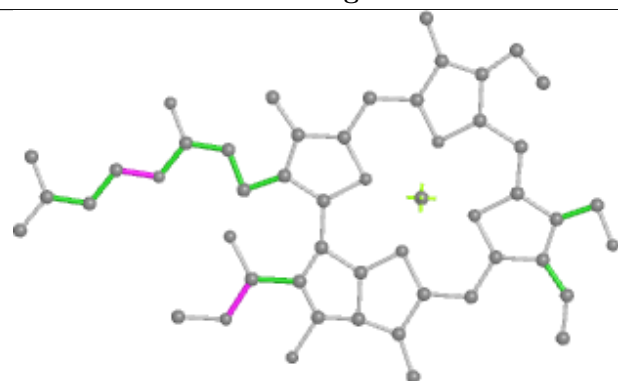
Ligand CHL 4 307



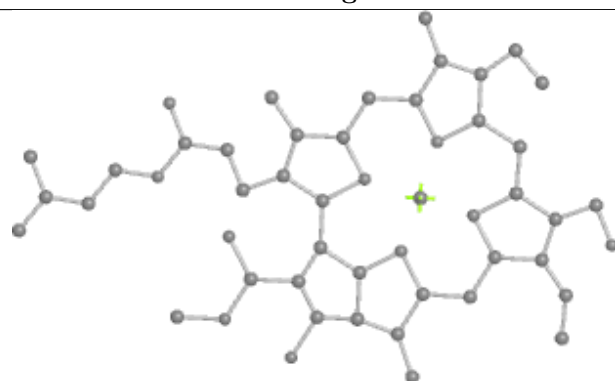
Bond lengths



Bond angles

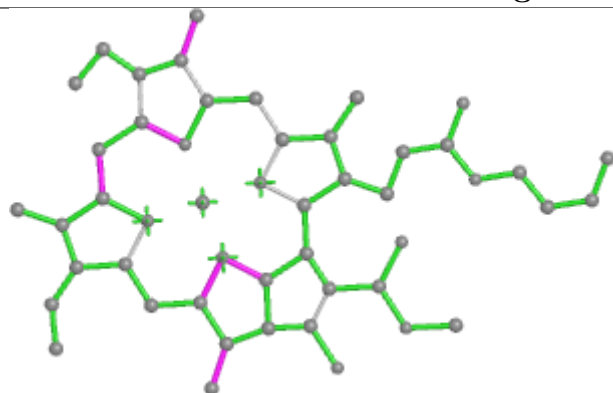


Torsions

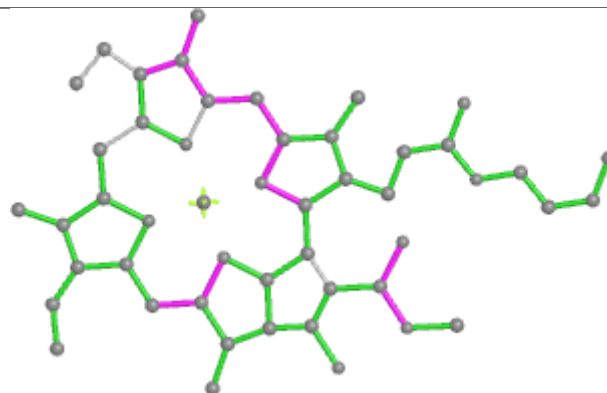


Rings

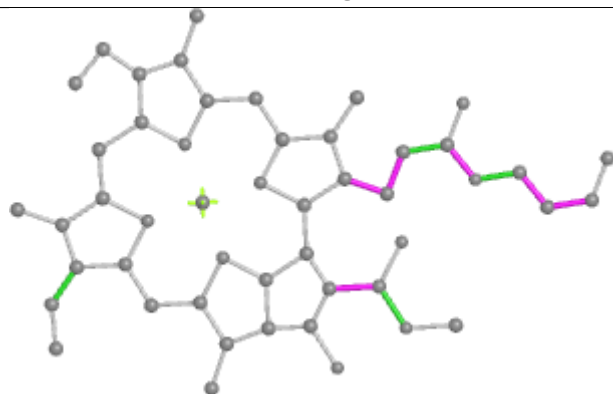
Ligand CLA A 821



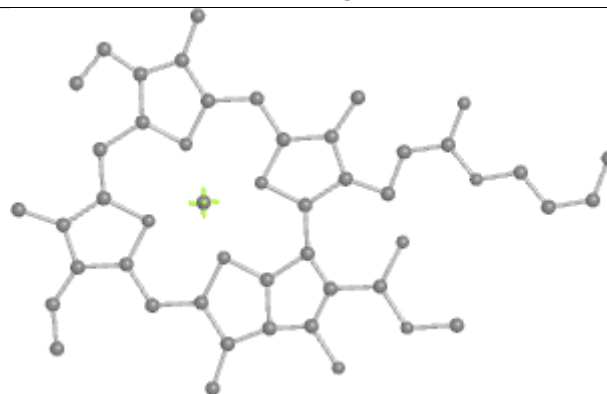
Bond lengths



Bond angles

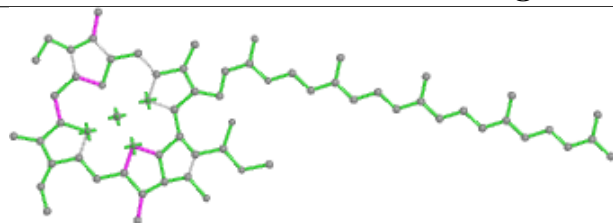


Torsions

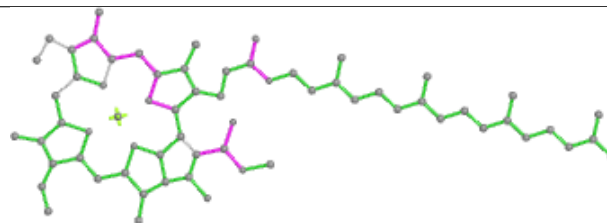


Rings

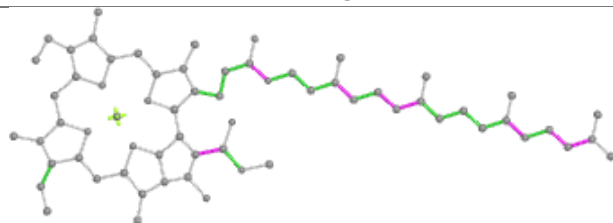
Ligand CLA B 824



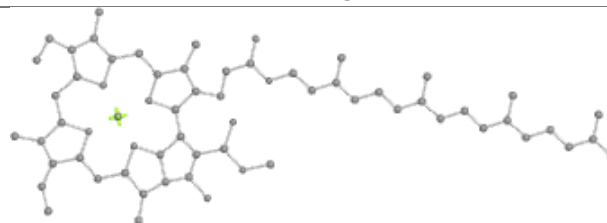
Bond lengths



Bond angles

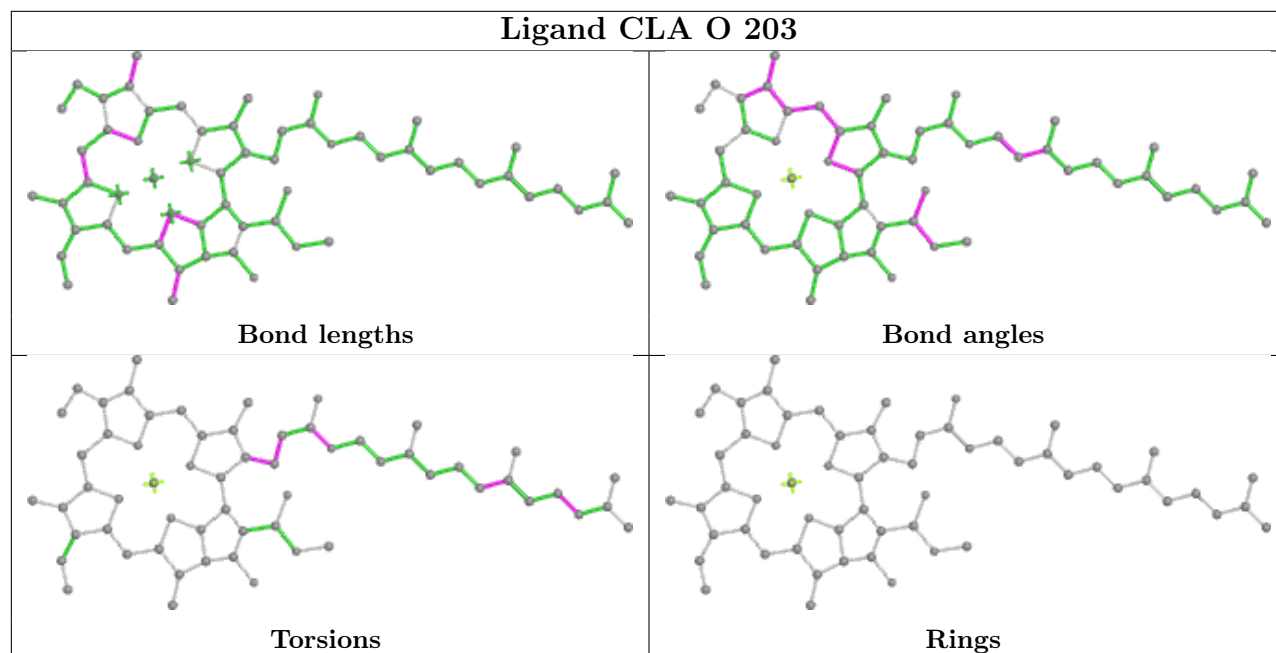


Torsions

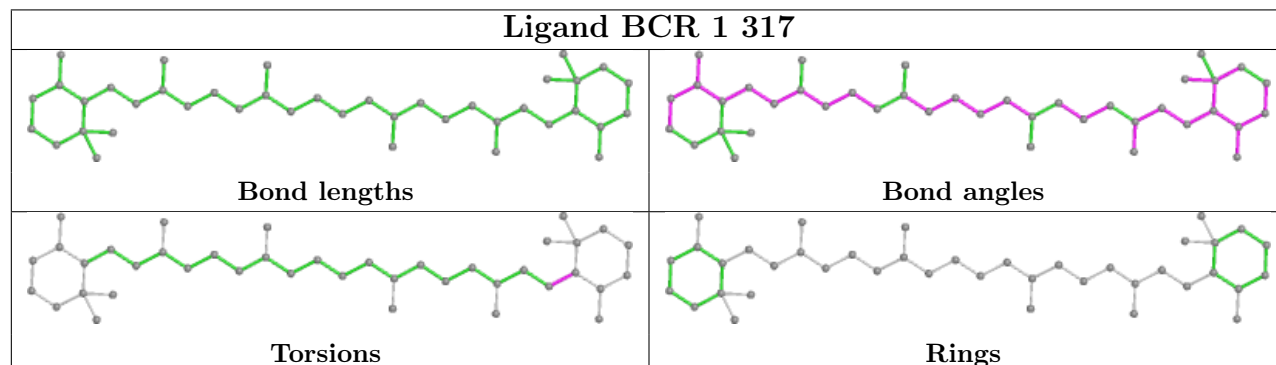


Rings

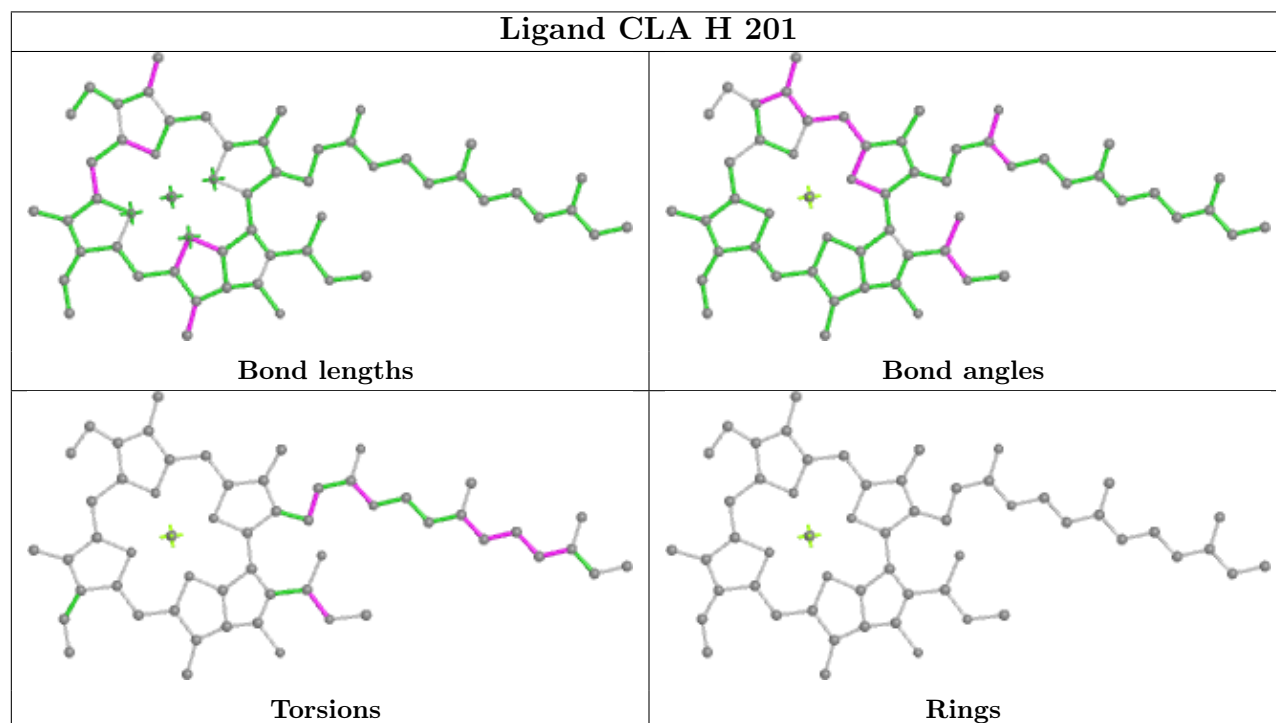
Ligand CLA O 203



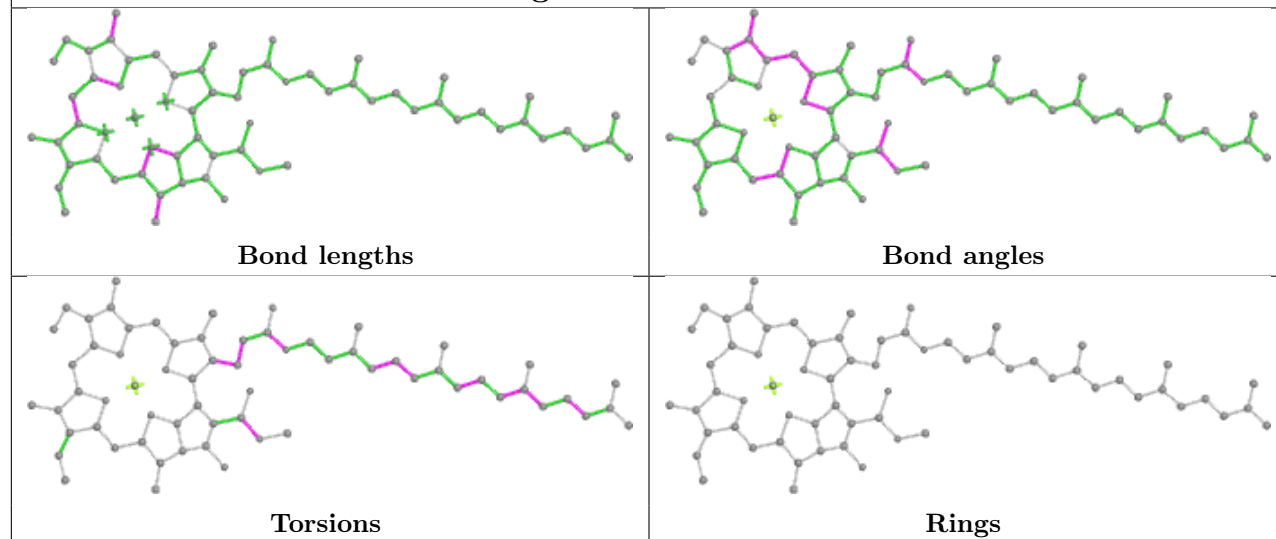
Ligand BCR 1 317



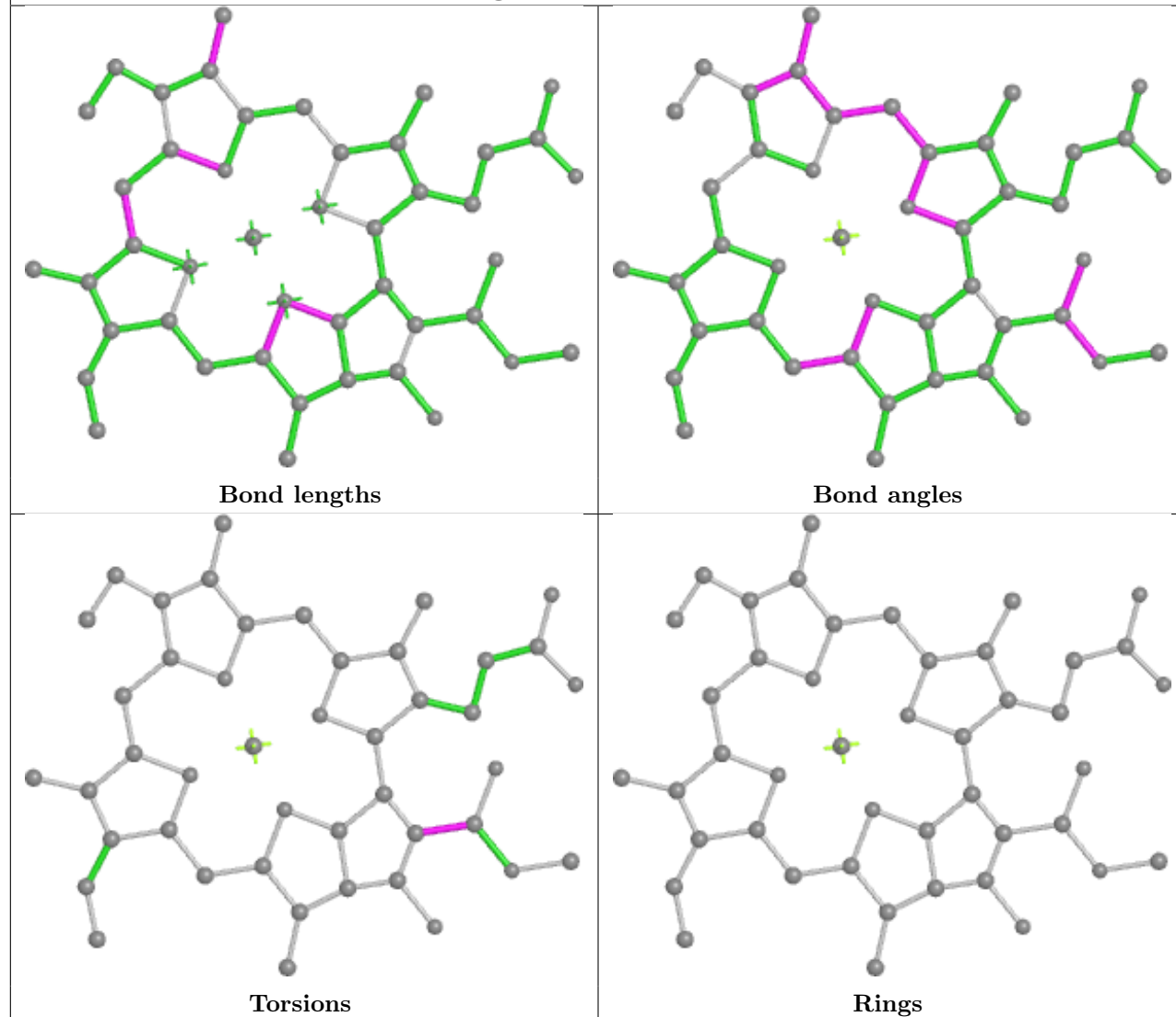
Ligand CLA H 201

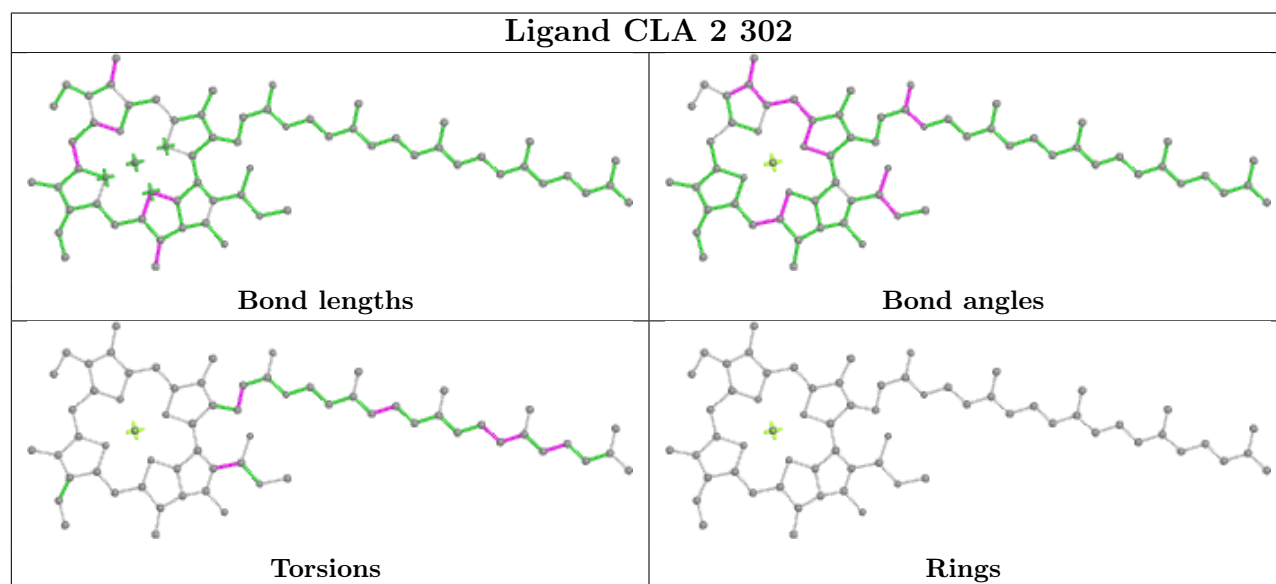
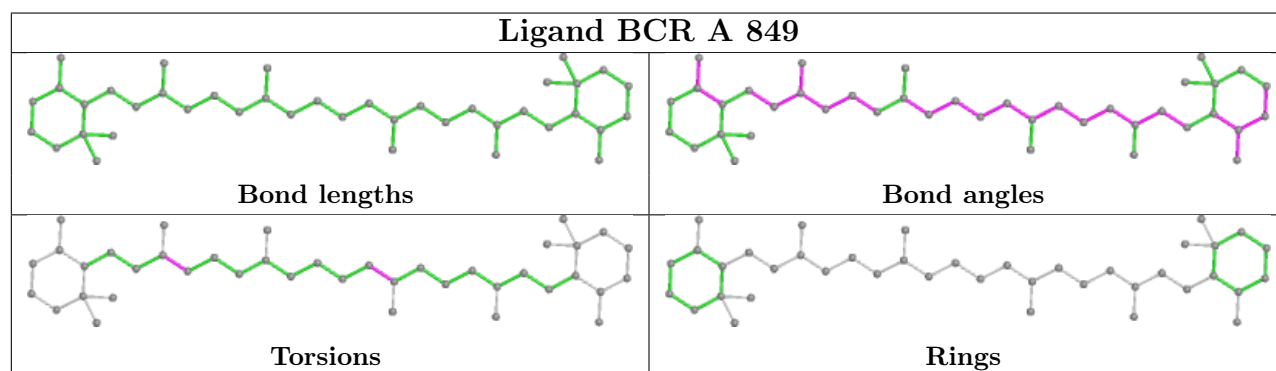
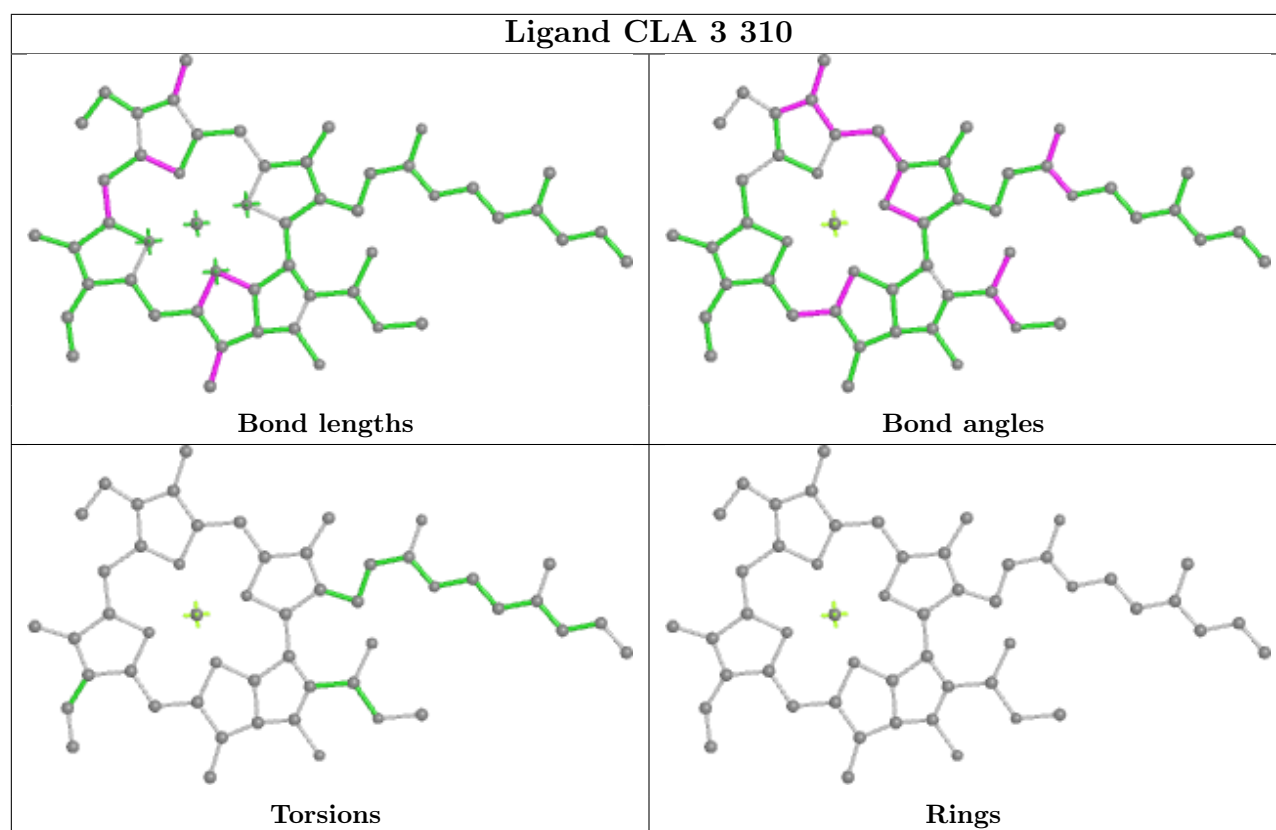


Ligand CLA A 831

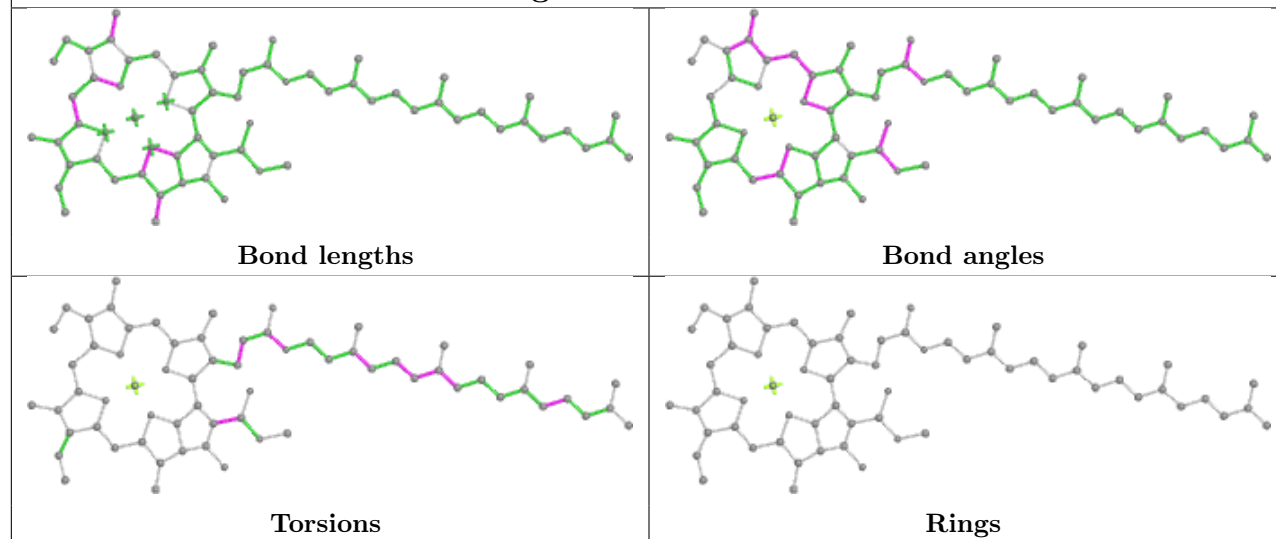


Ligand CLA B 834

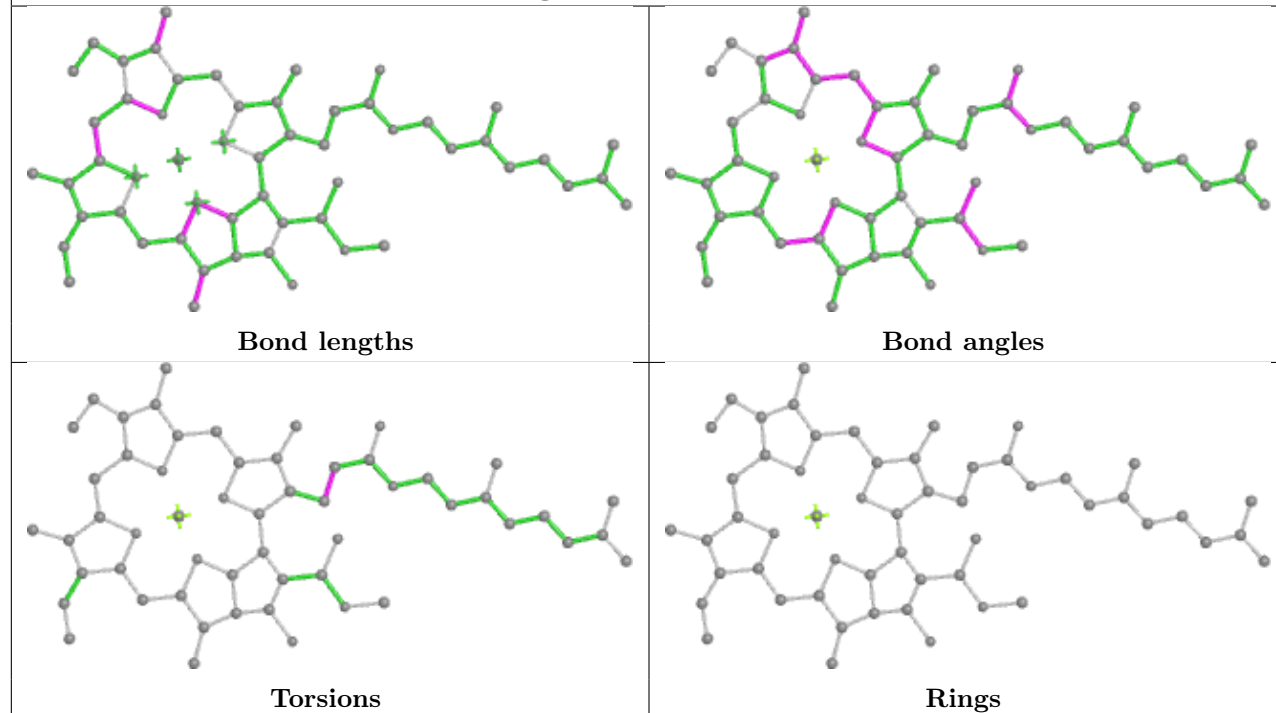




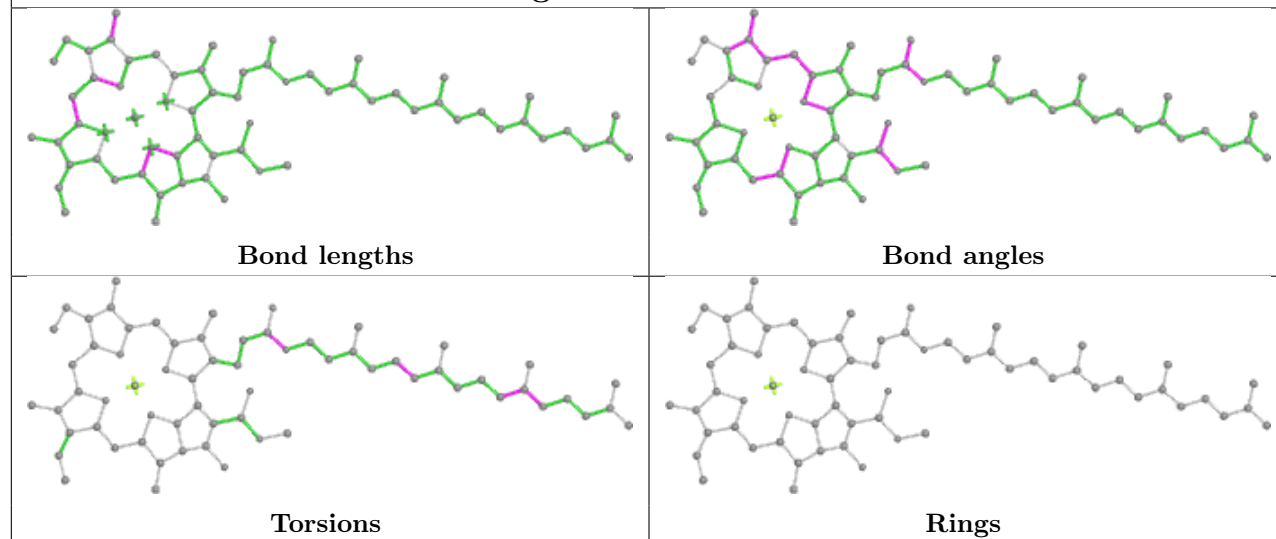
Ligand CLA A 816



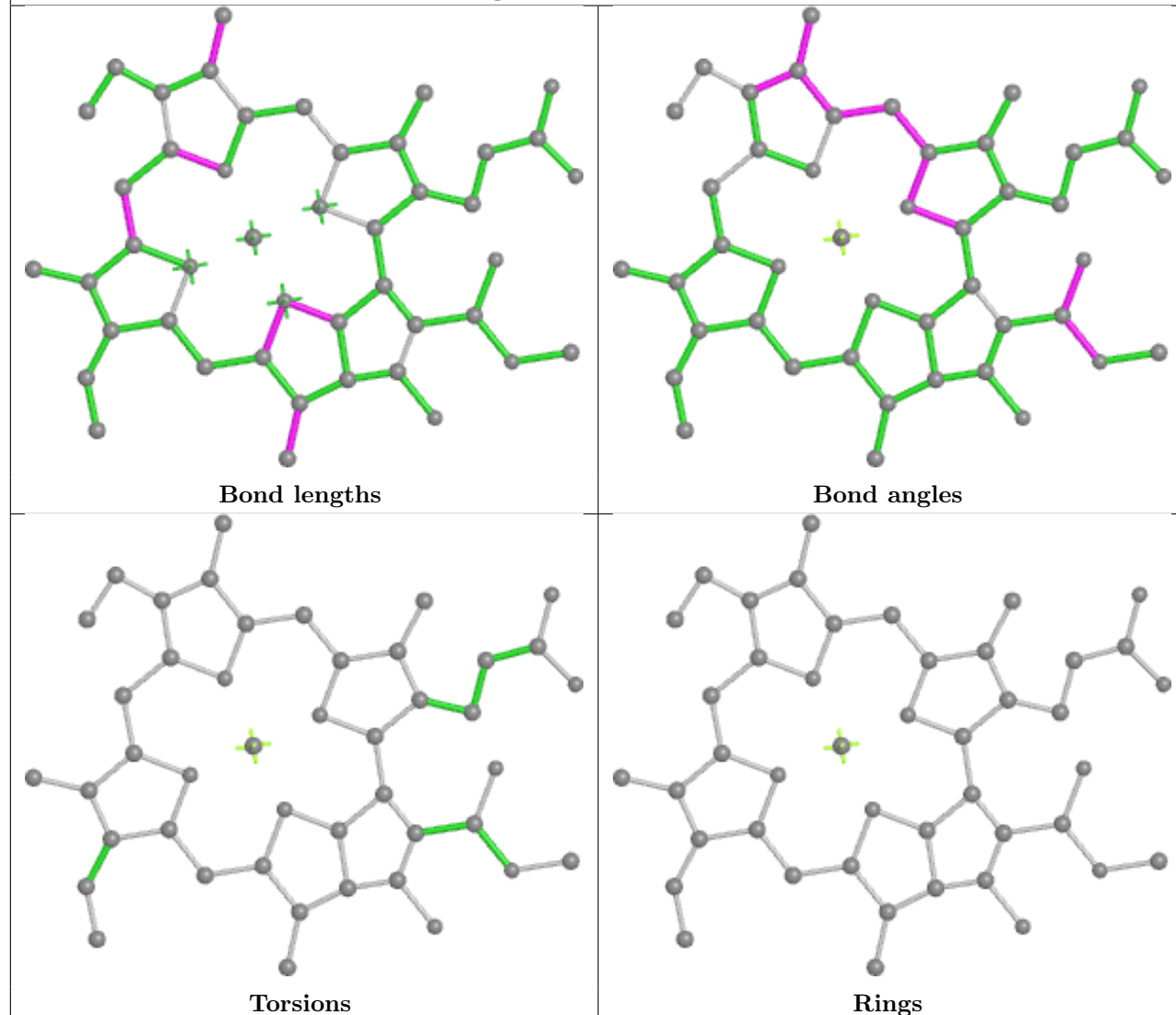
Ligand CLA 3 311

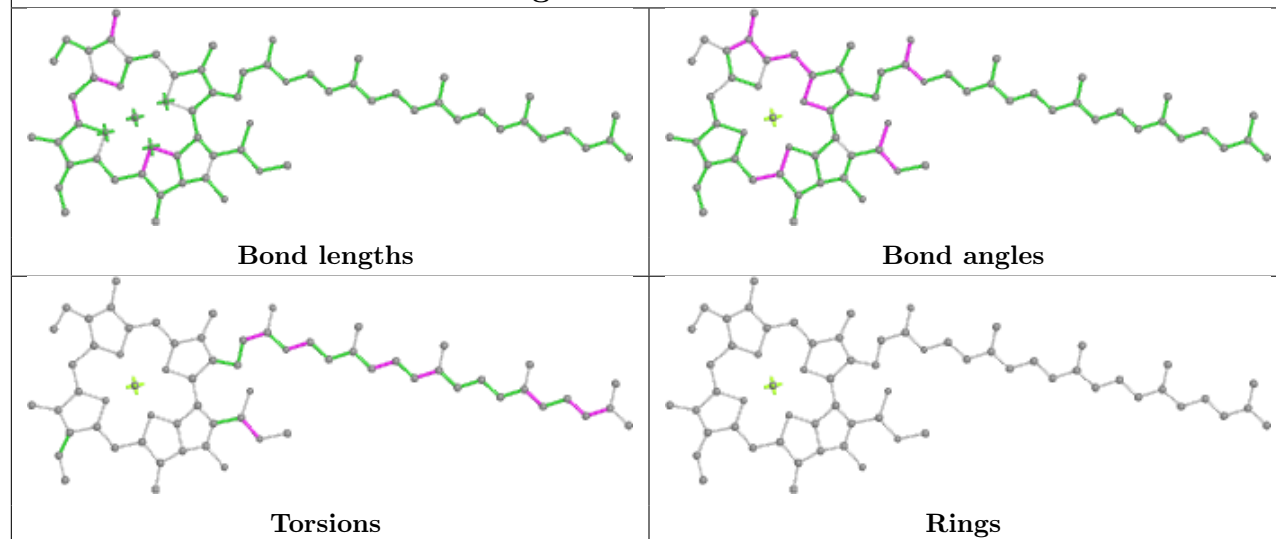
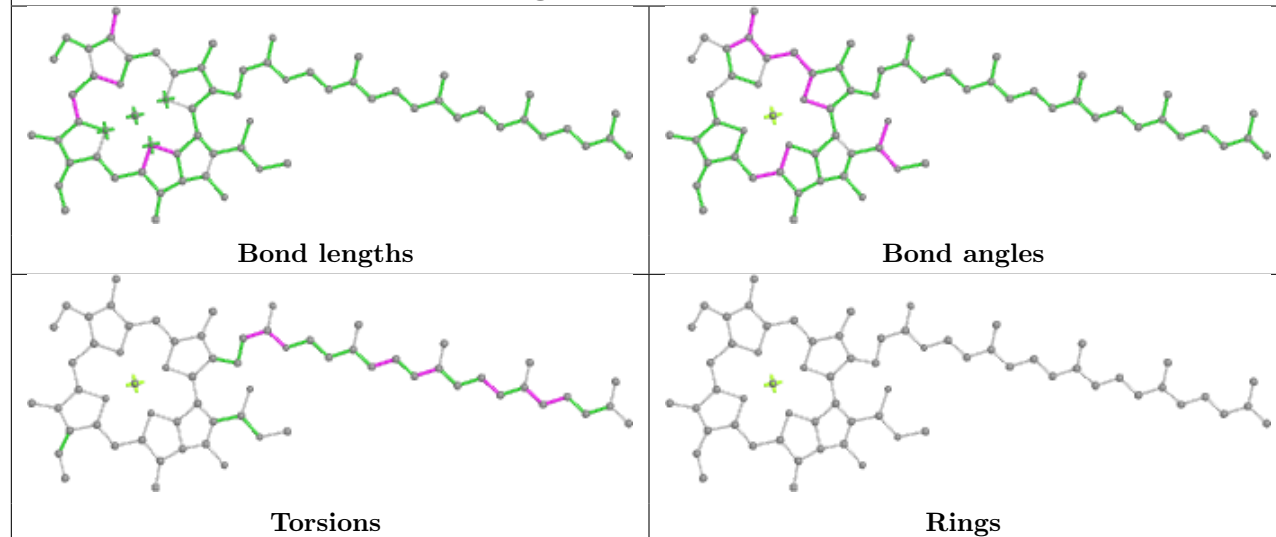


Ligand CLA B 836

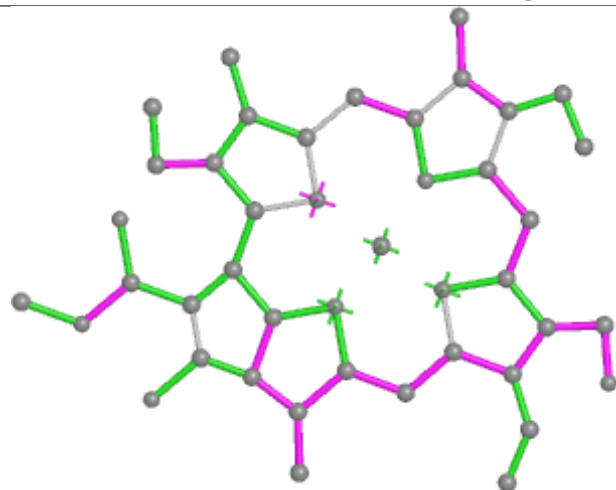


Ligand CLA K 205

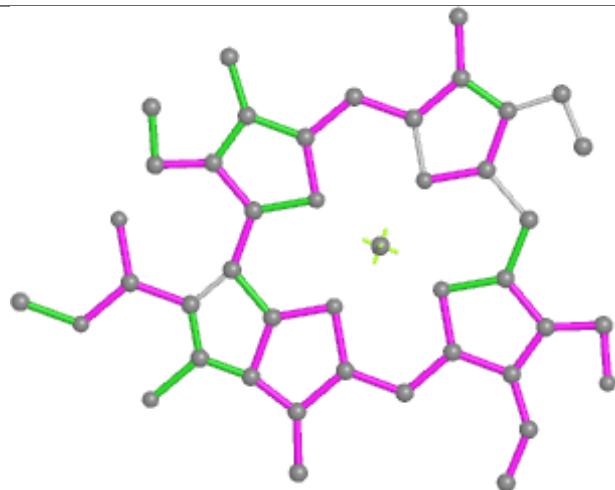


Ligand CLA B 806**Ligand CLA A 834**

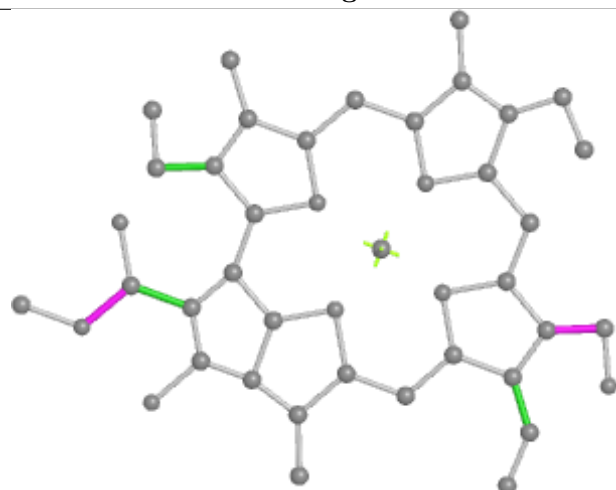
Ligand CHL 4 315



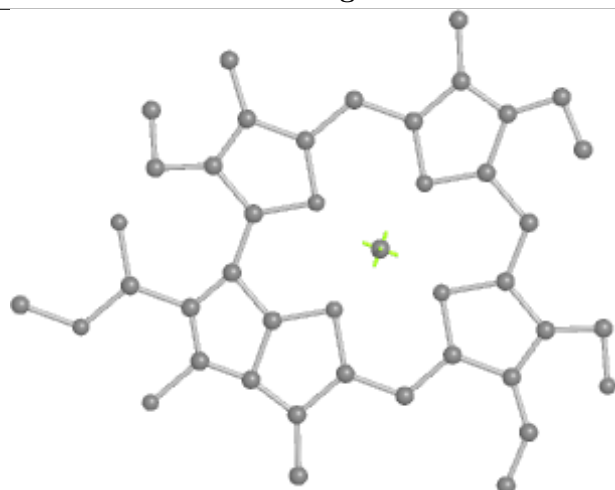
Bond lengths



Bond angles

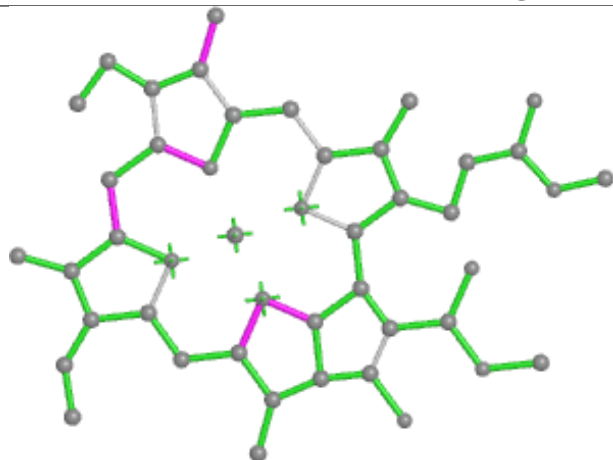


Torsions

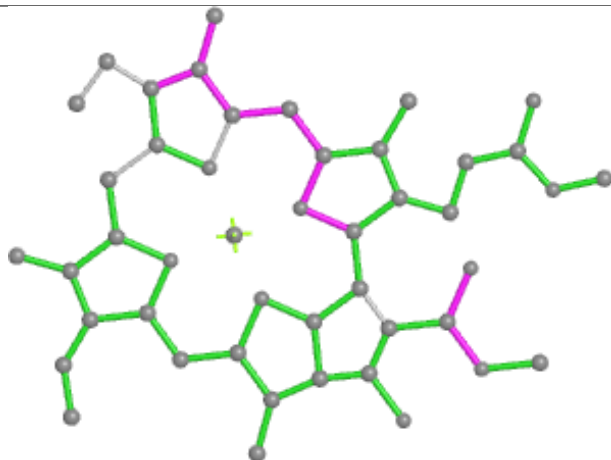


Rings

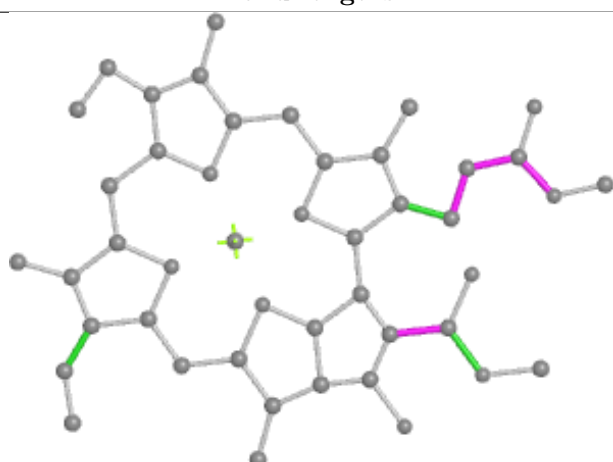
Ligand CLA G 605



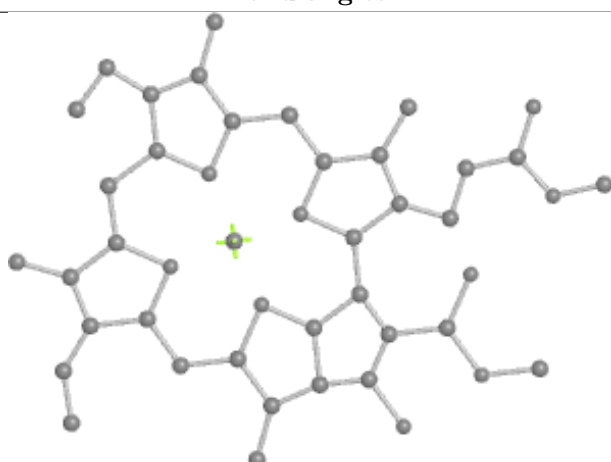
Bond lengths



Bond angles

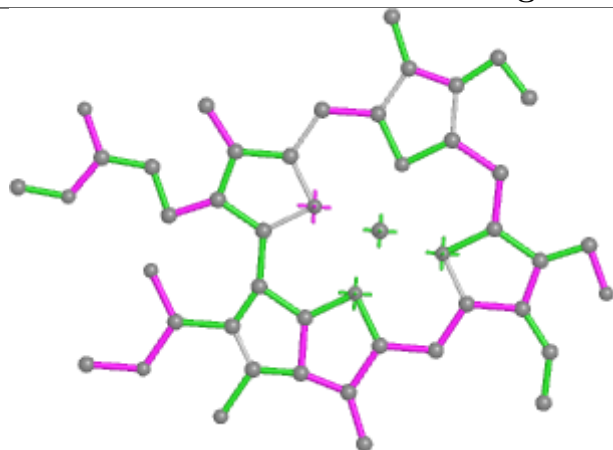


Torsions

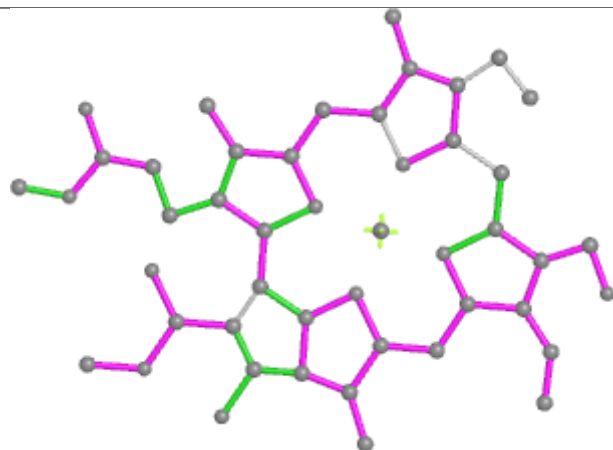


Rings

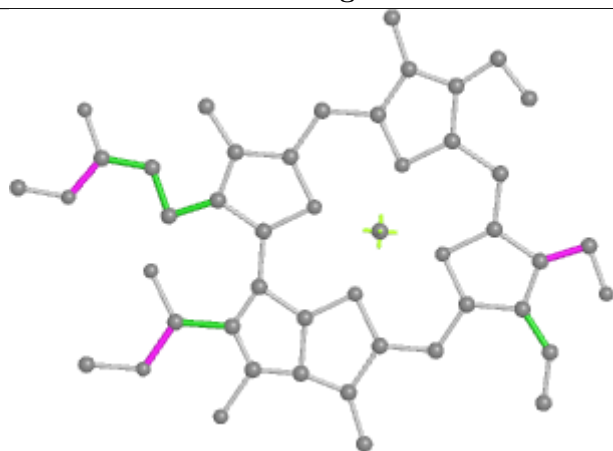
Ligand CHL 3 306



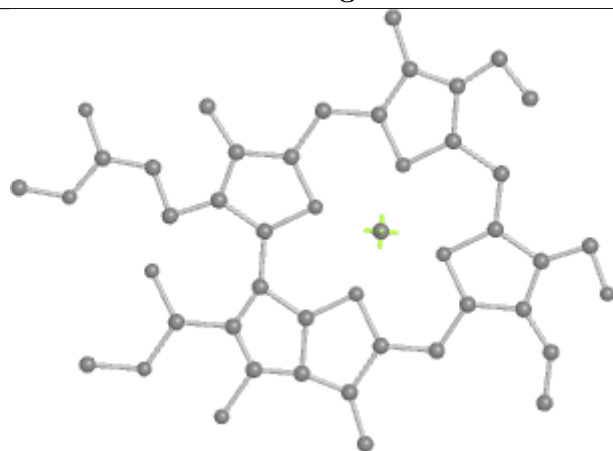
Bond lengths



Bond angles

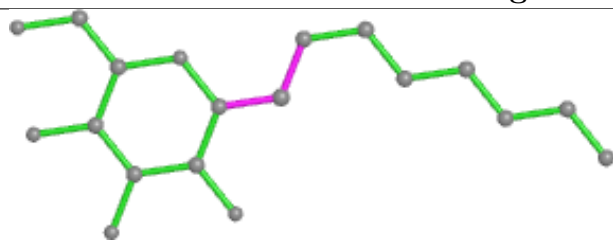


Torsions

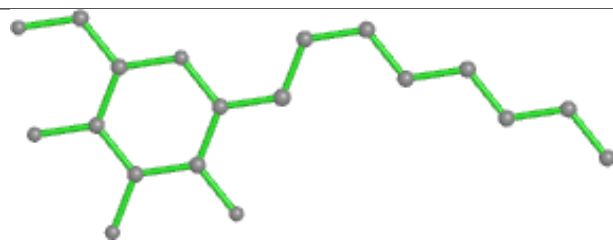


Rings

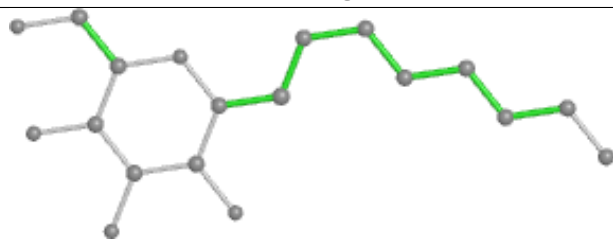
Ligand HTG G 602



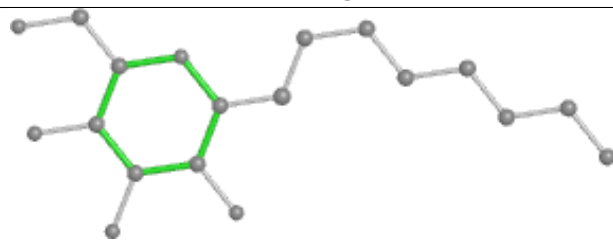
Bond lengths



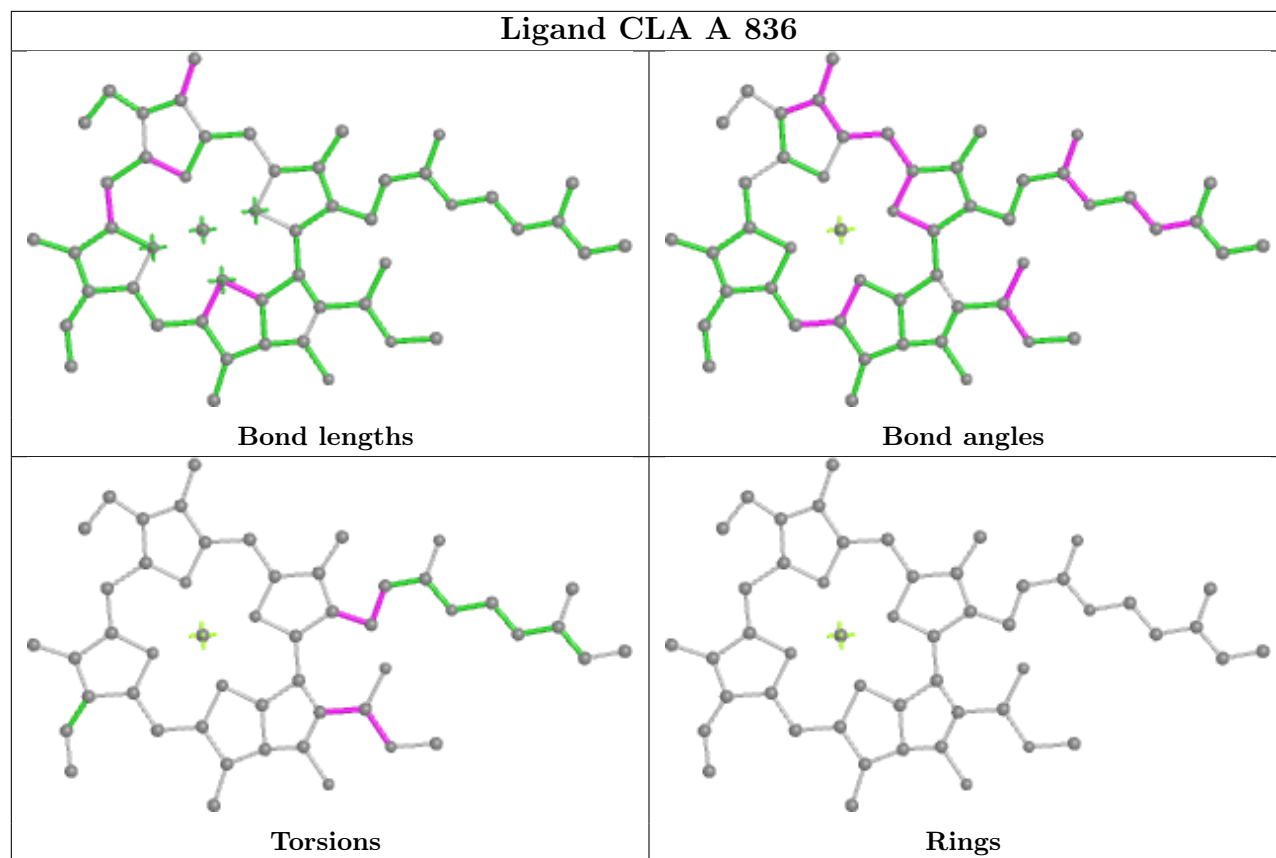
Bond angles



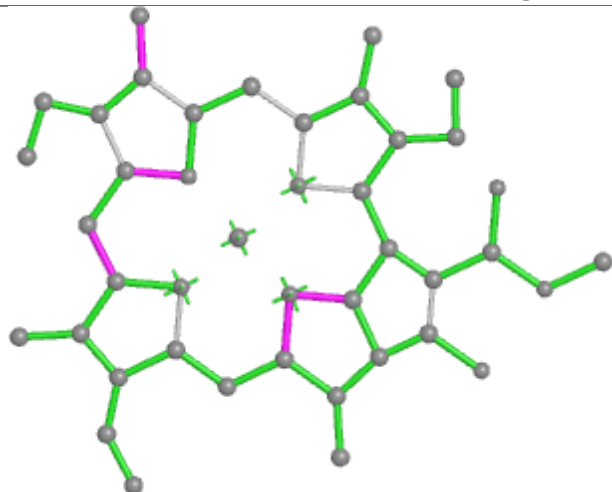
Torsions



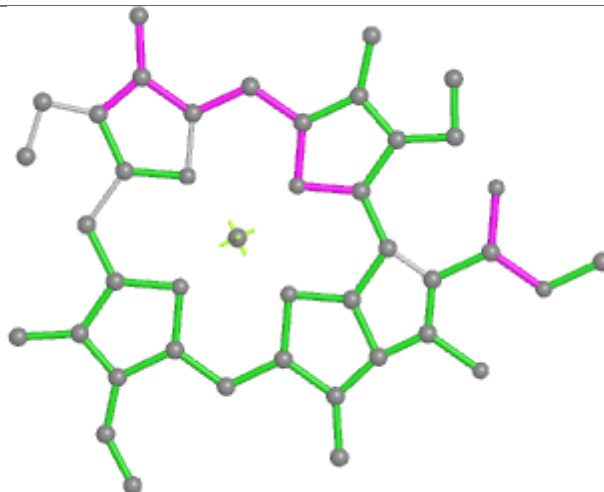
Rings



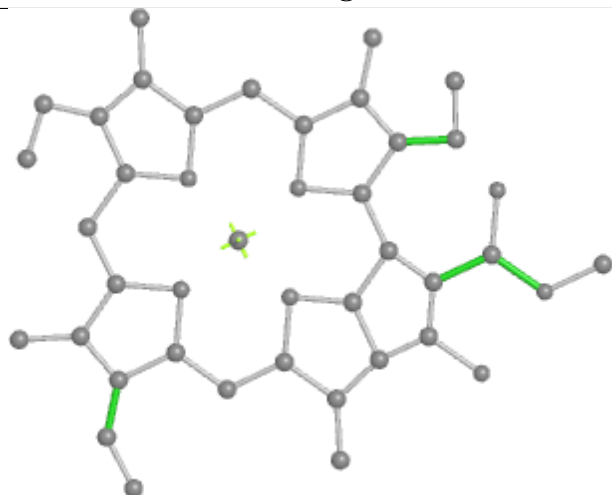
Ligand CLA 3 304



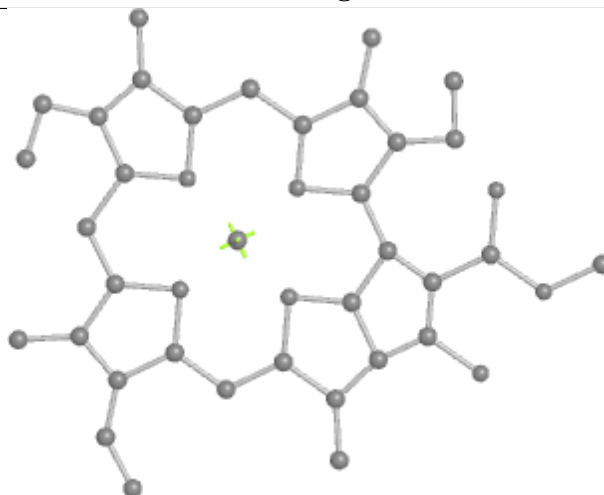
Bond lengths



Bond angles

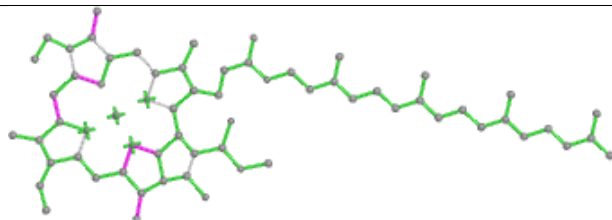


Torsions

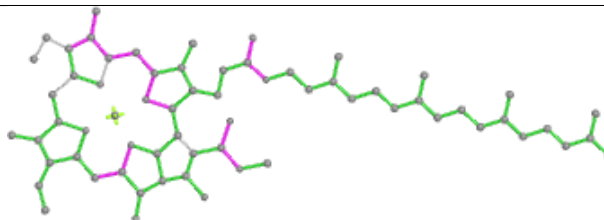


Rings

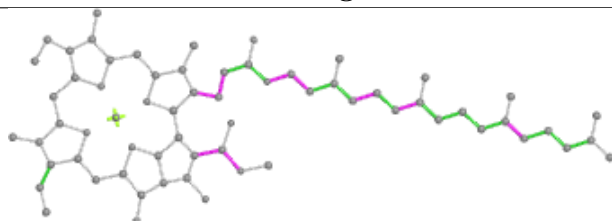
Ligand CLA A 851



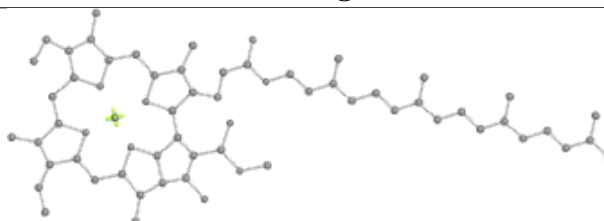
Bond lengths



Bond angles

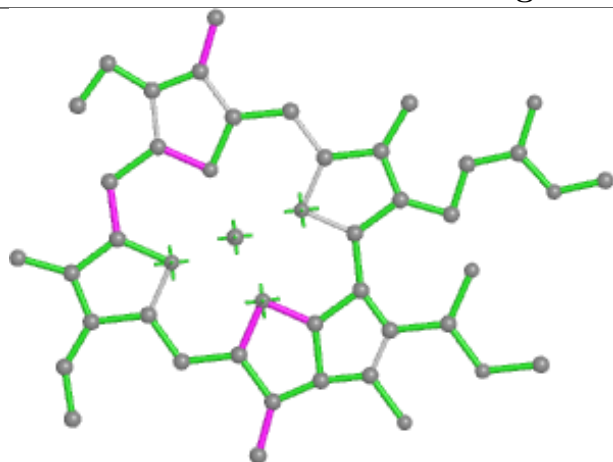


Torsions

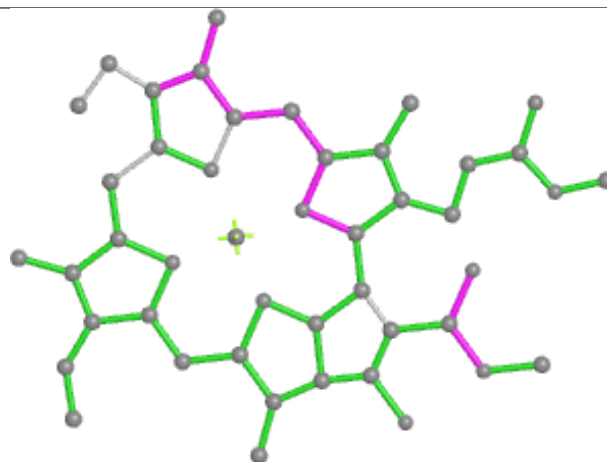


Rings

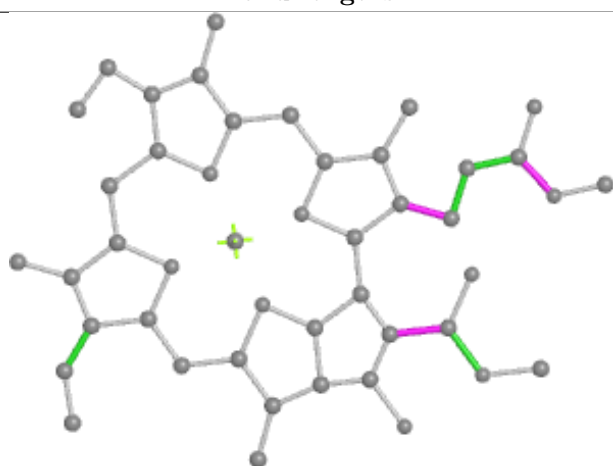
Ligand CLA F 805



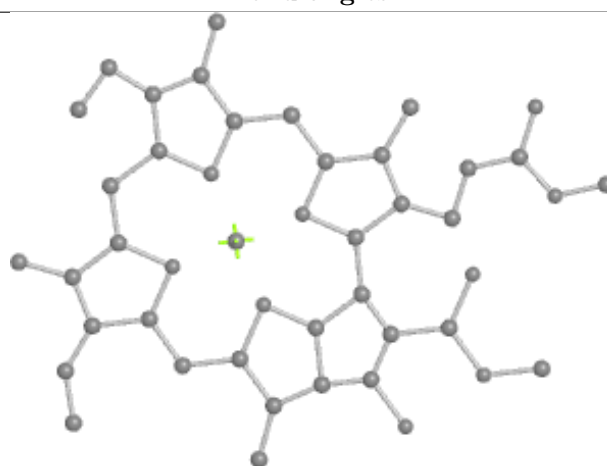
Bond lengths



Bond angles

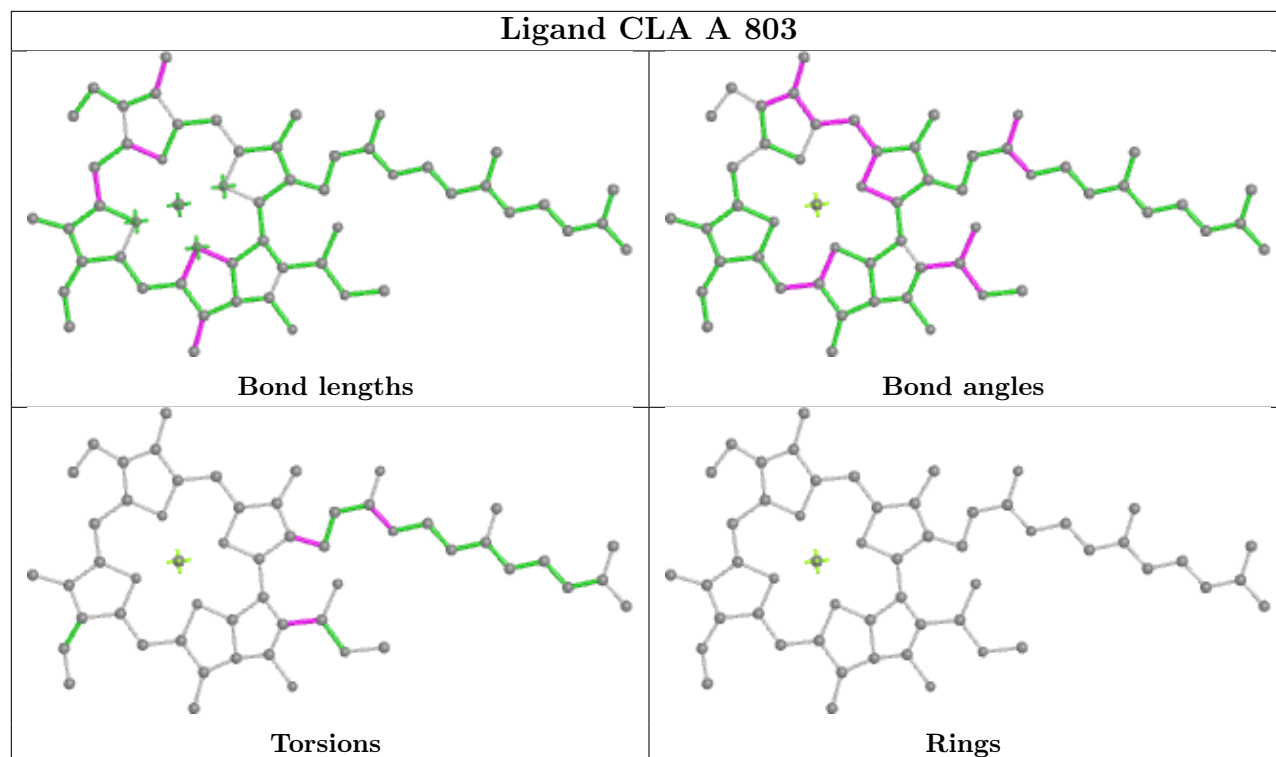


Torsions

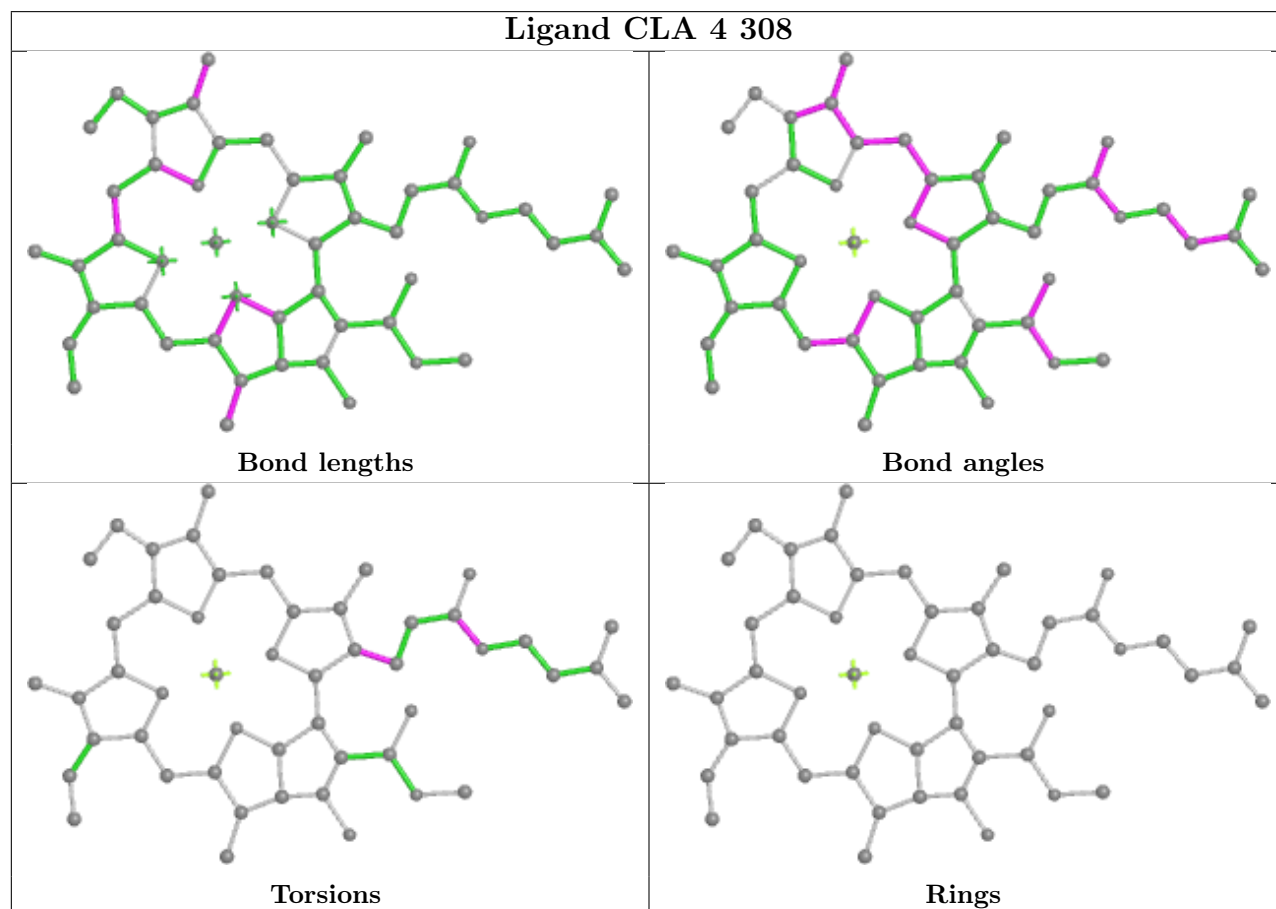


Rings

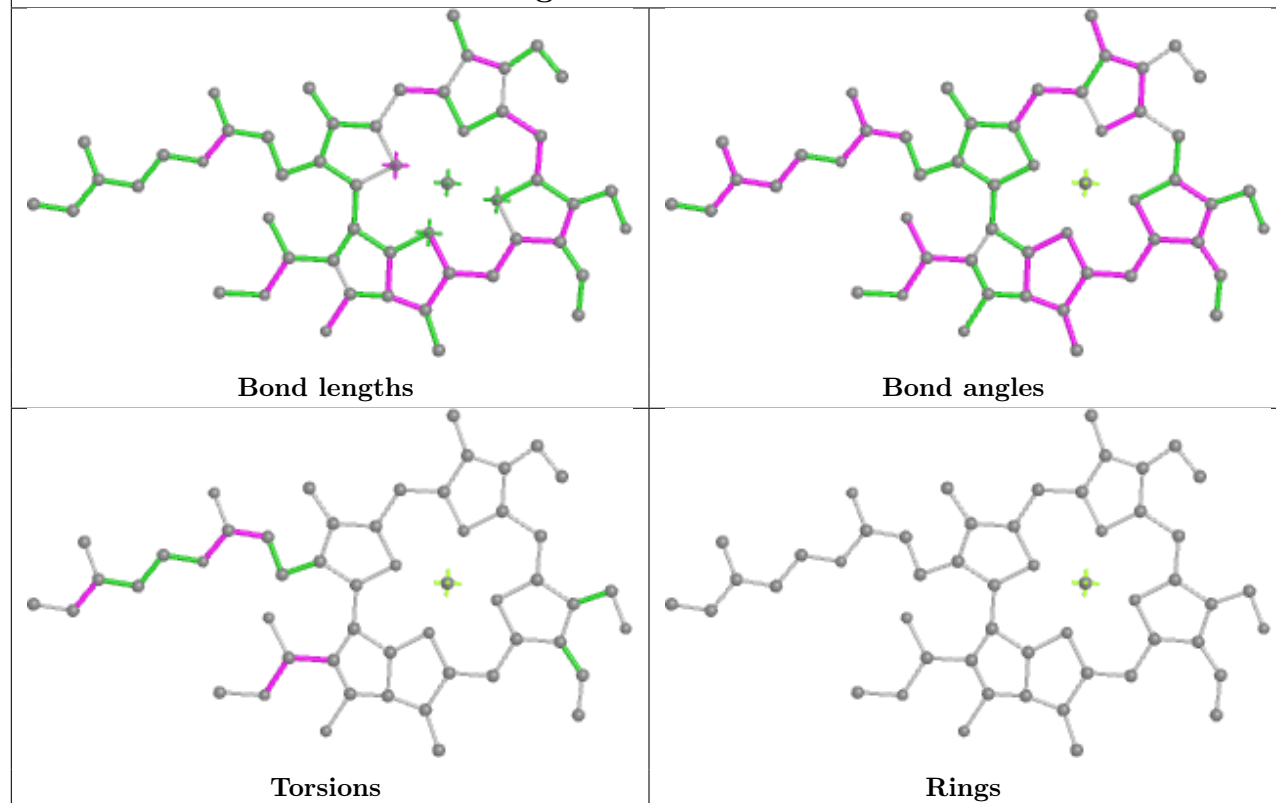
Ligand CLA A 803



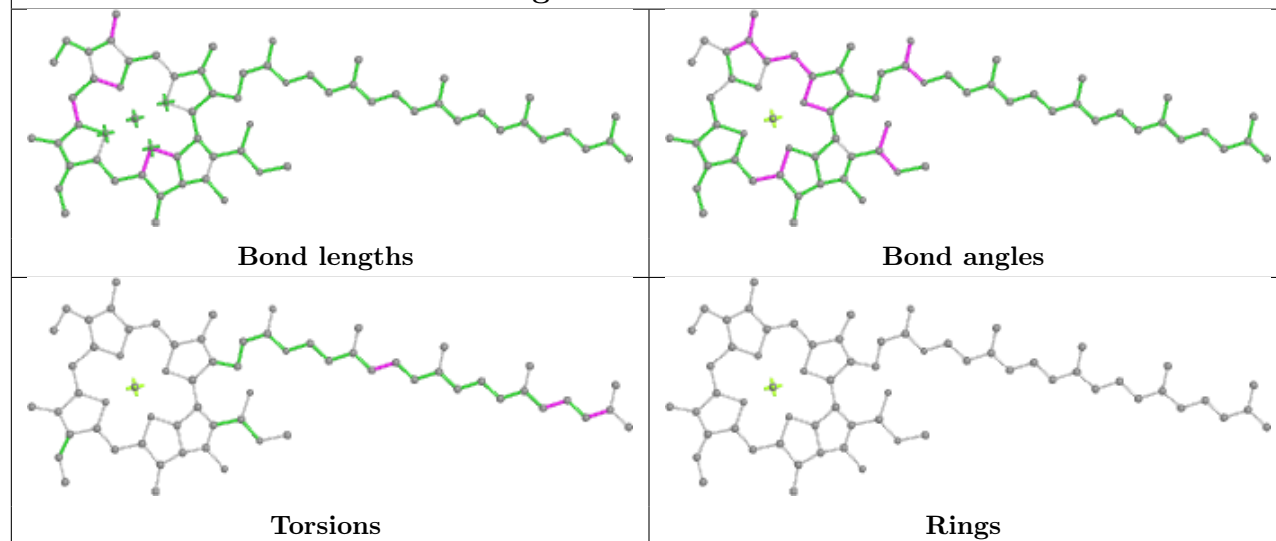
Ligand CLA 4 308

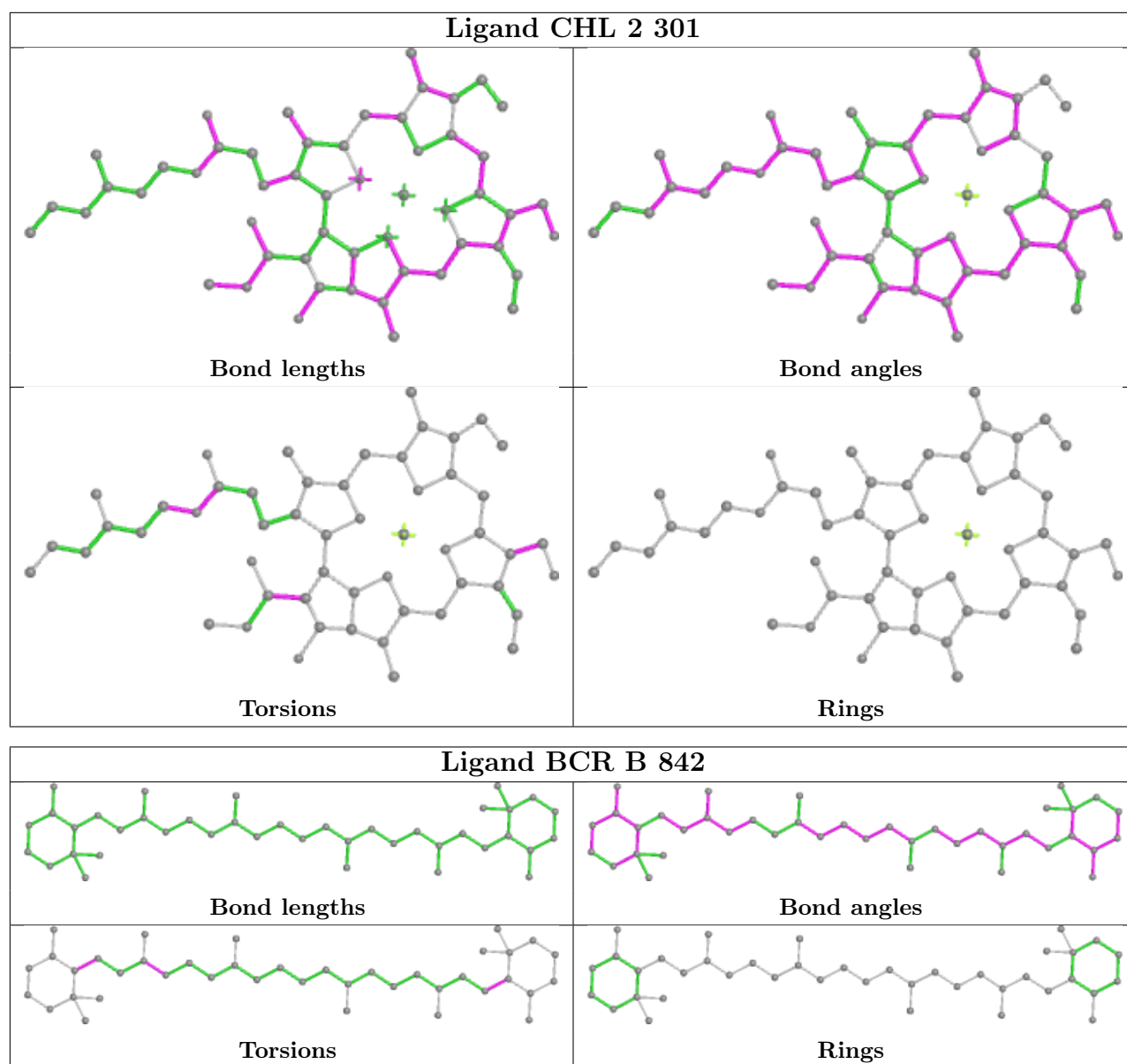


Ligand CHL 1 301

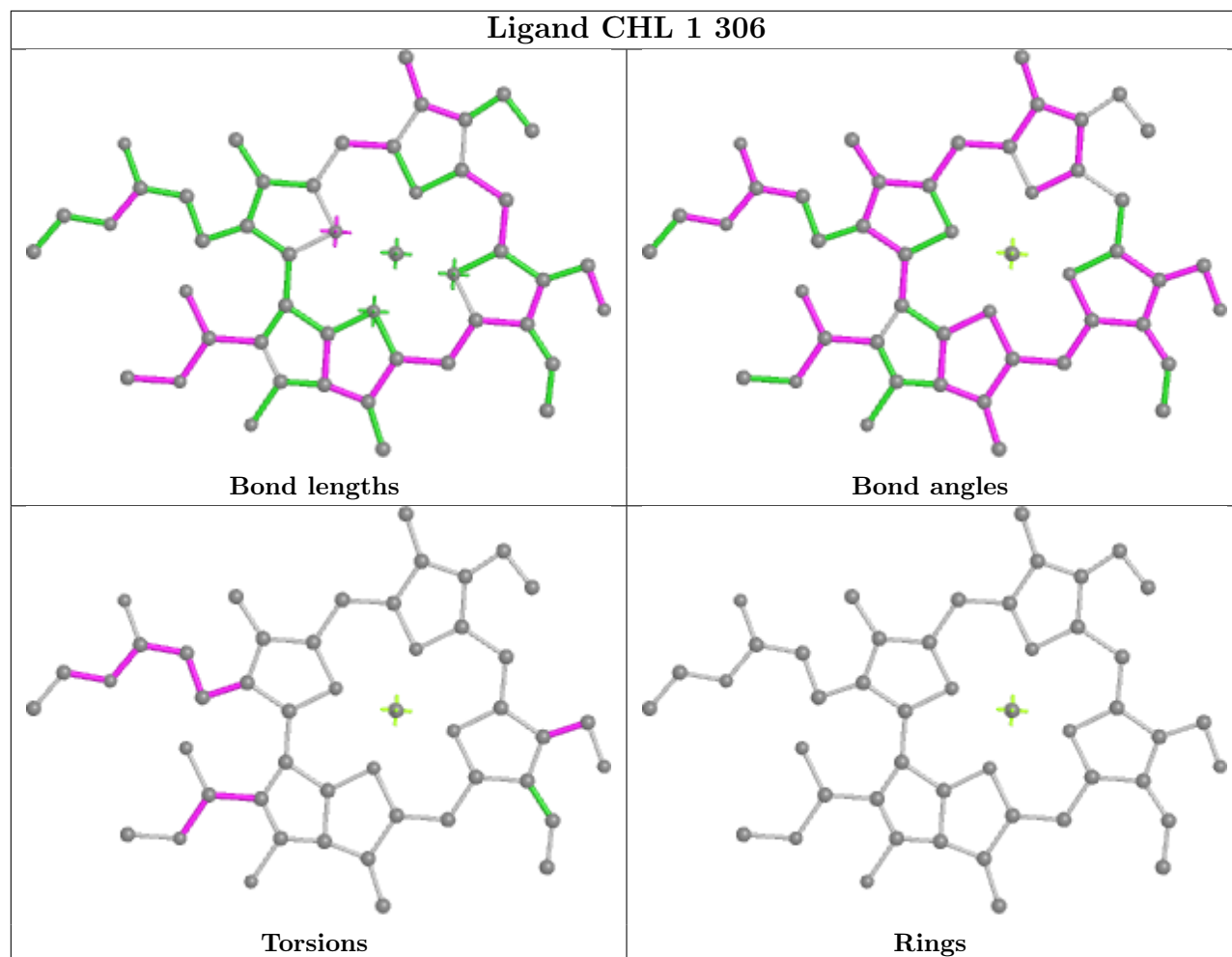


Ligand CLA B 809

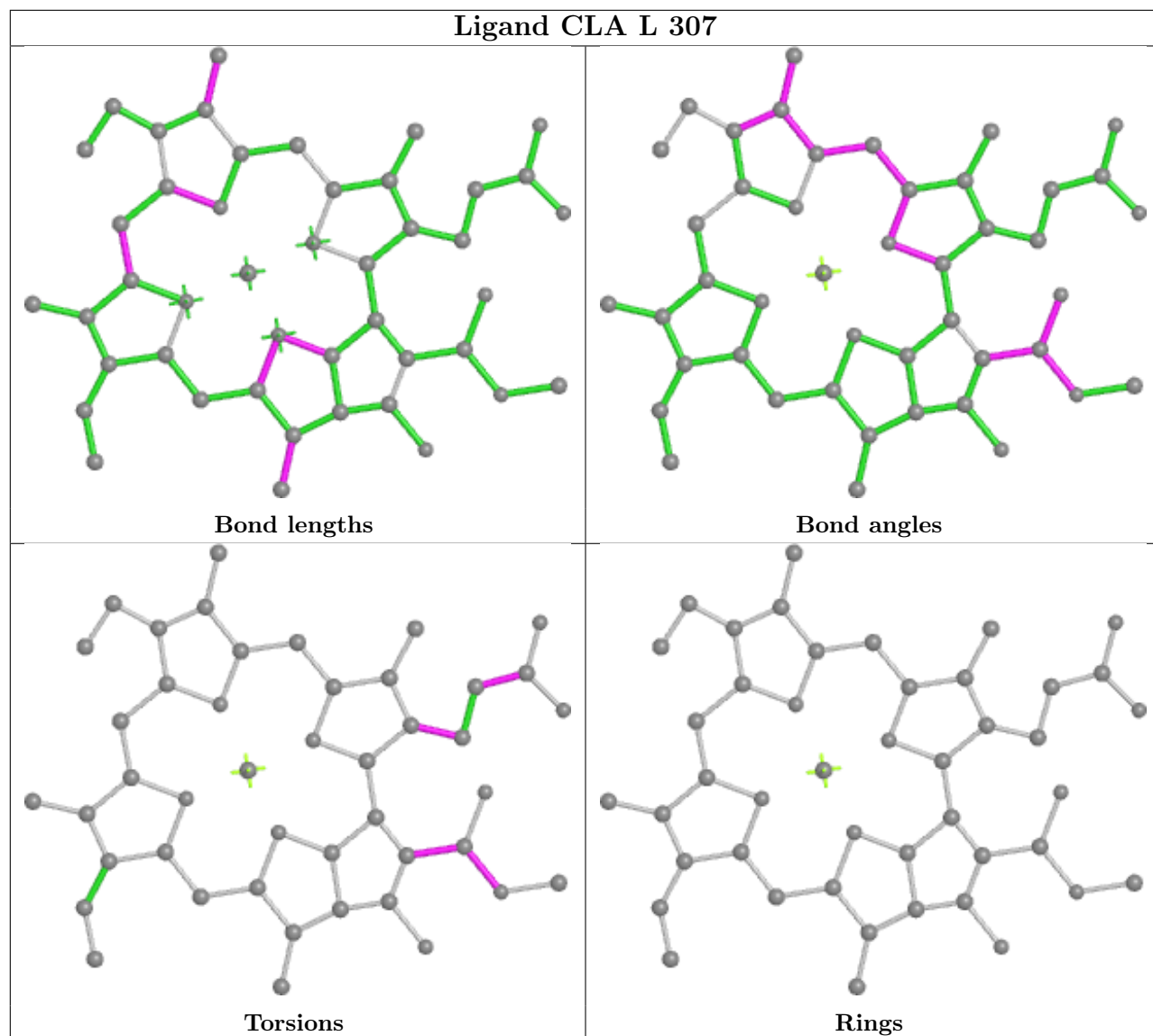




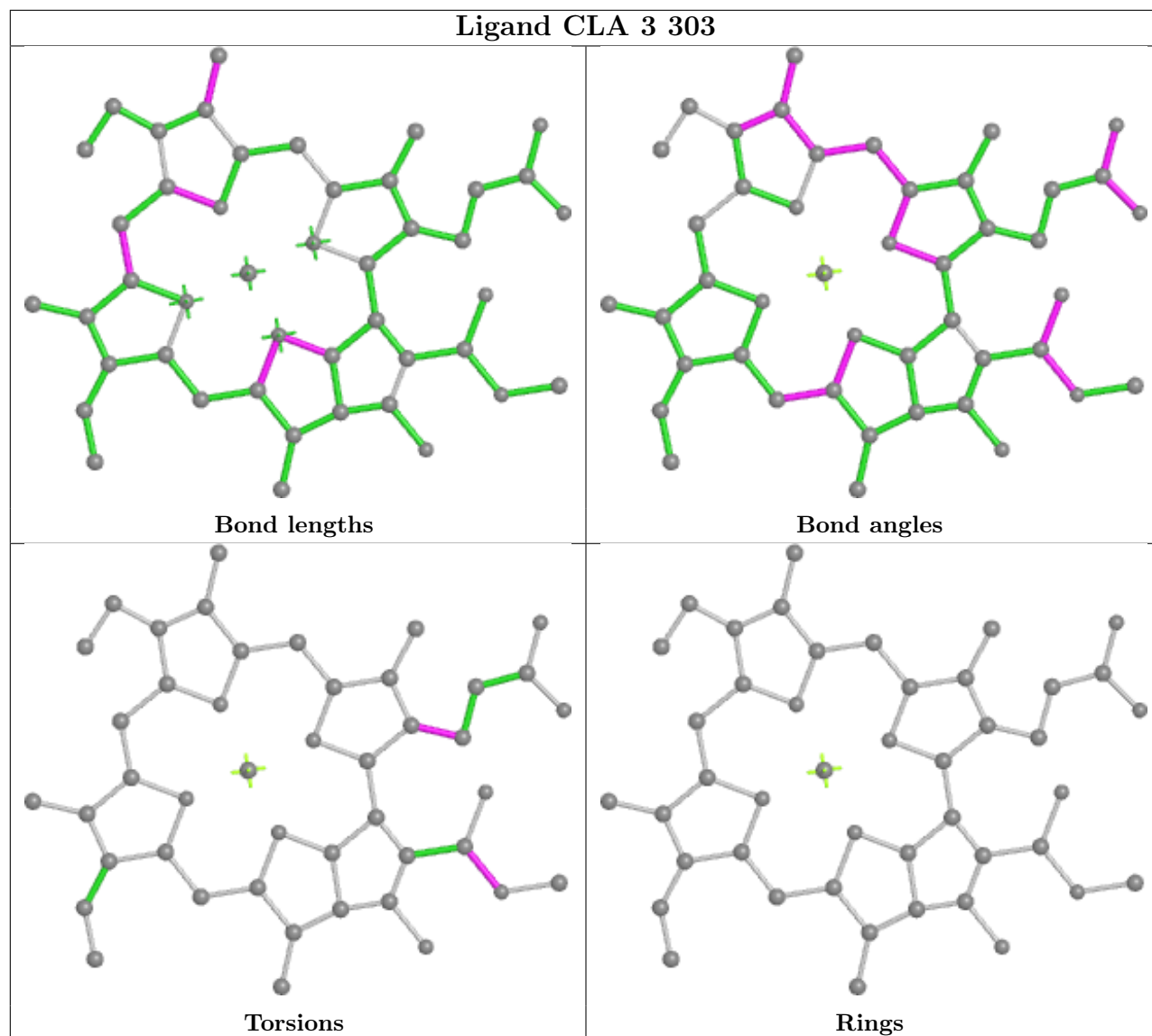
Ligand CHL 1 306



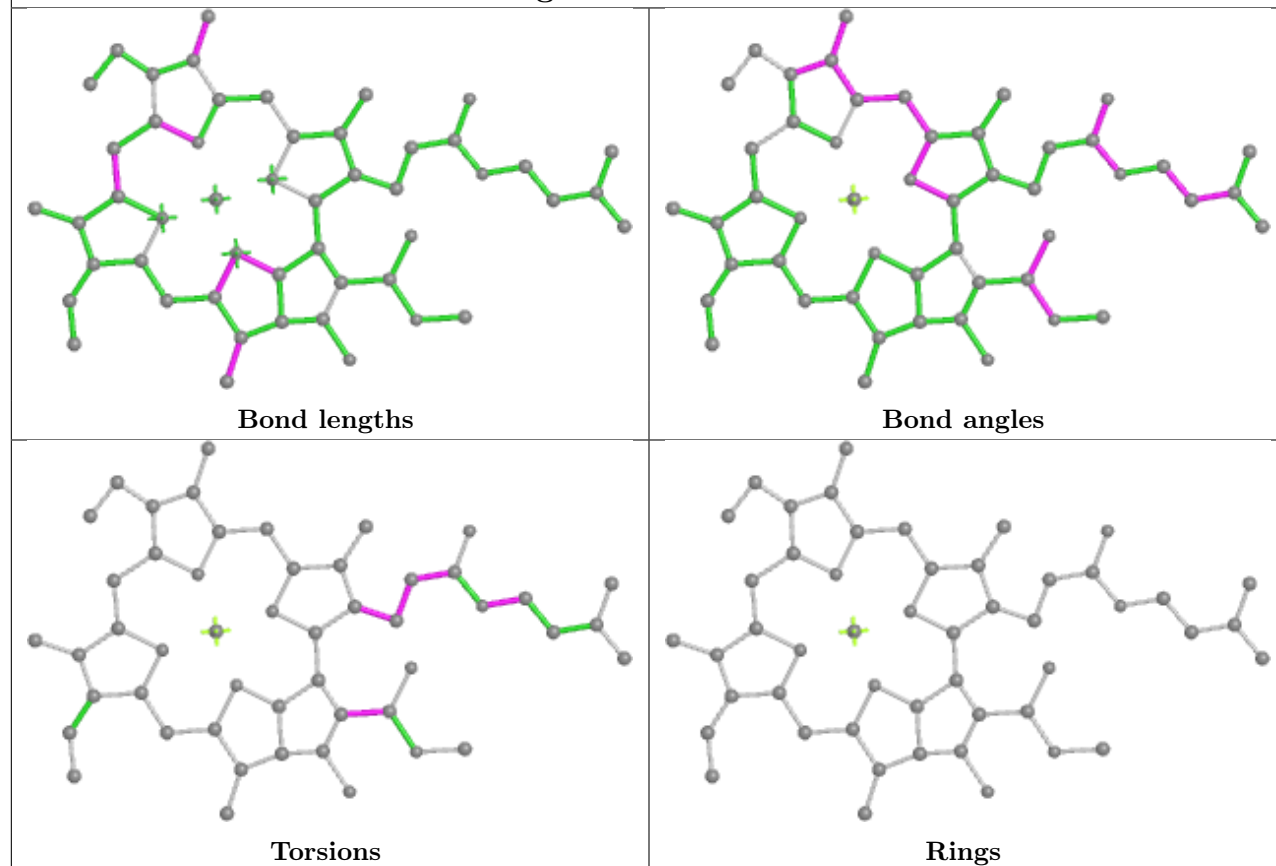
Ligand CLA L 307



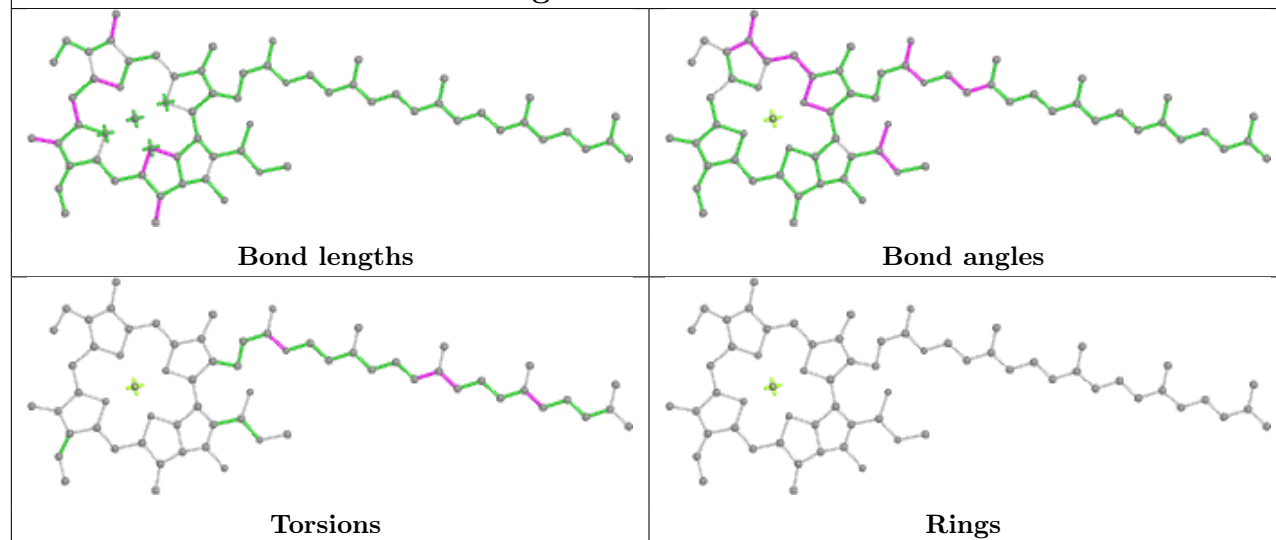
Ligand CLA 3 303



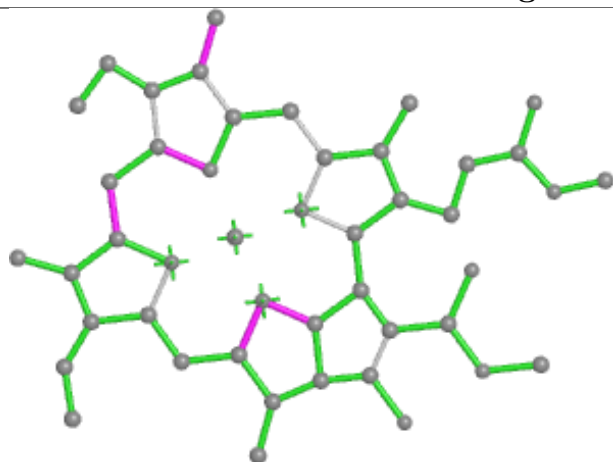
Ligand CLA 3 307



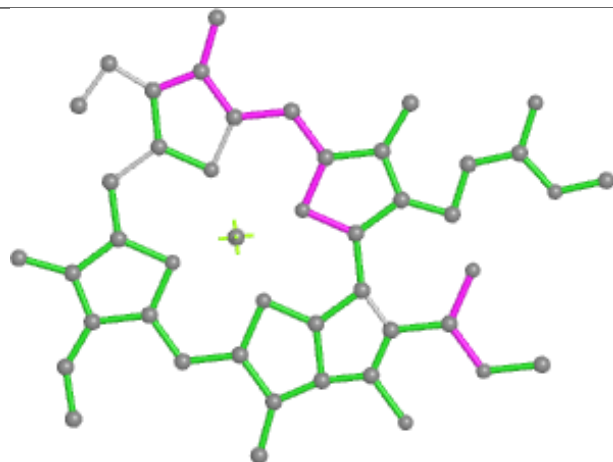
Ligand CLA B 819



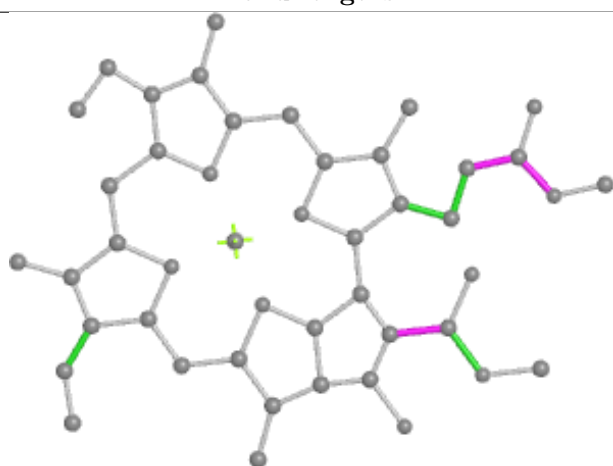
Ligand CLA 4 301



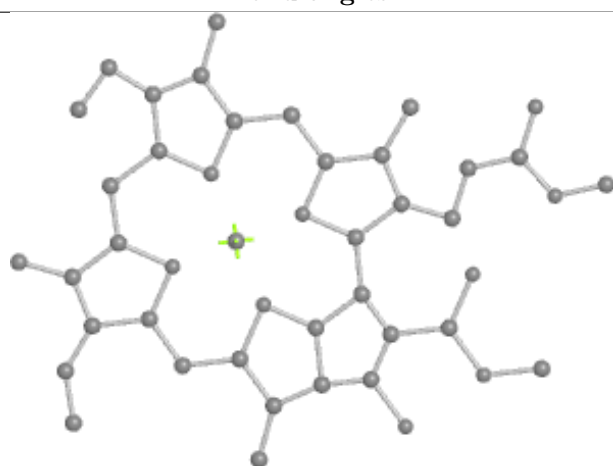
Bond lengths



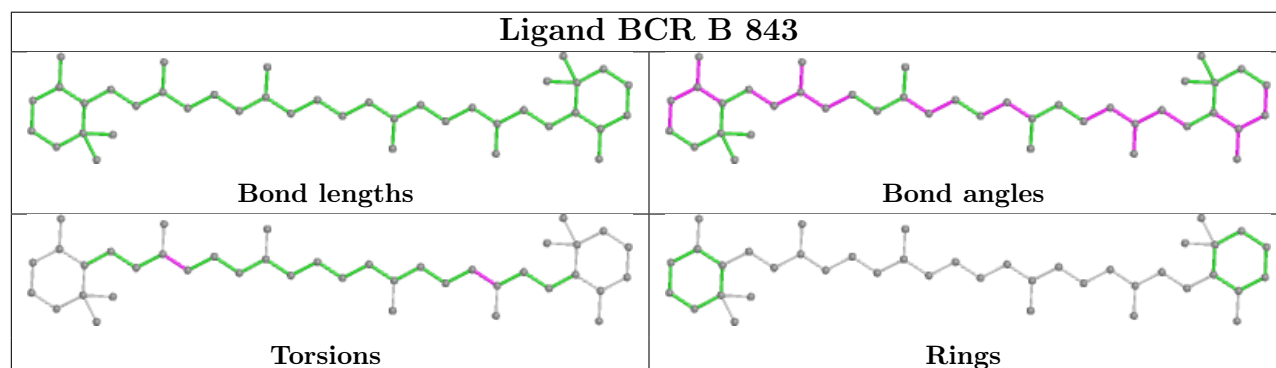
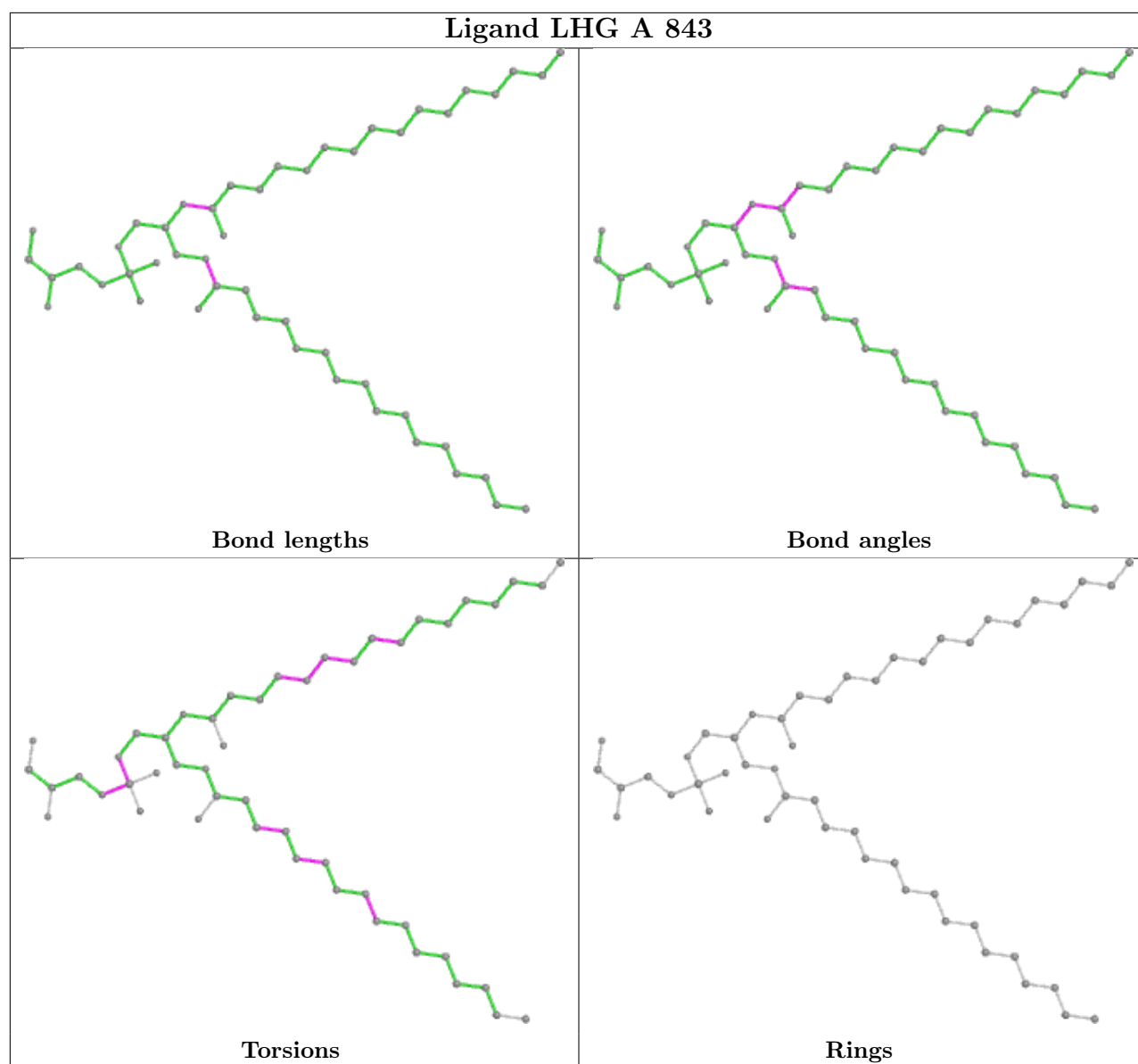
Bond angles

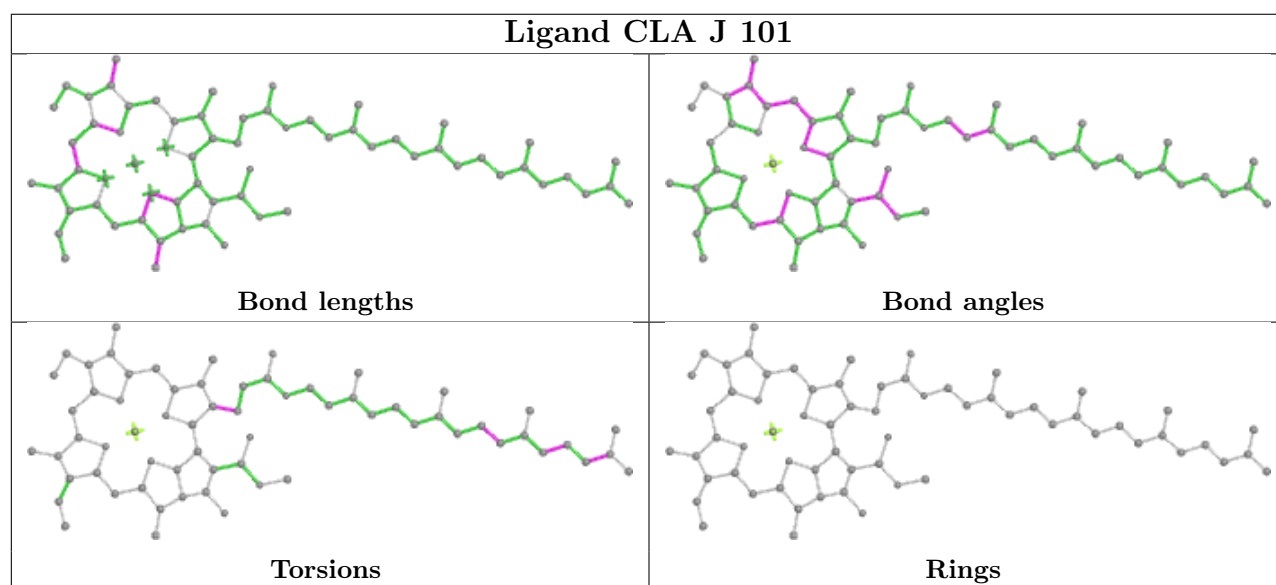
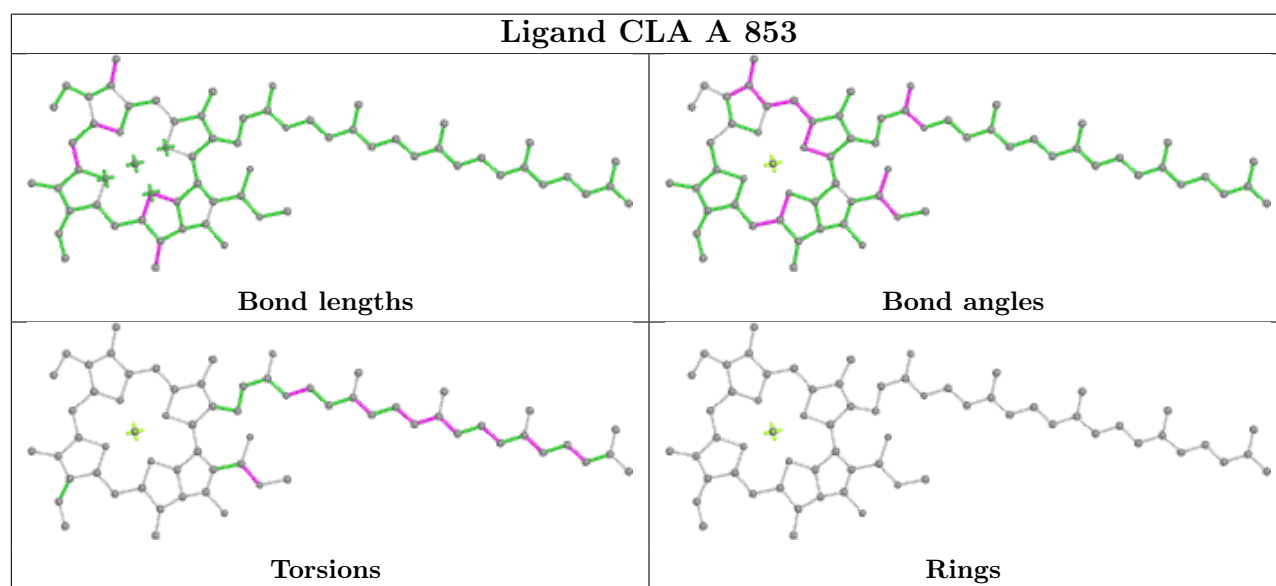
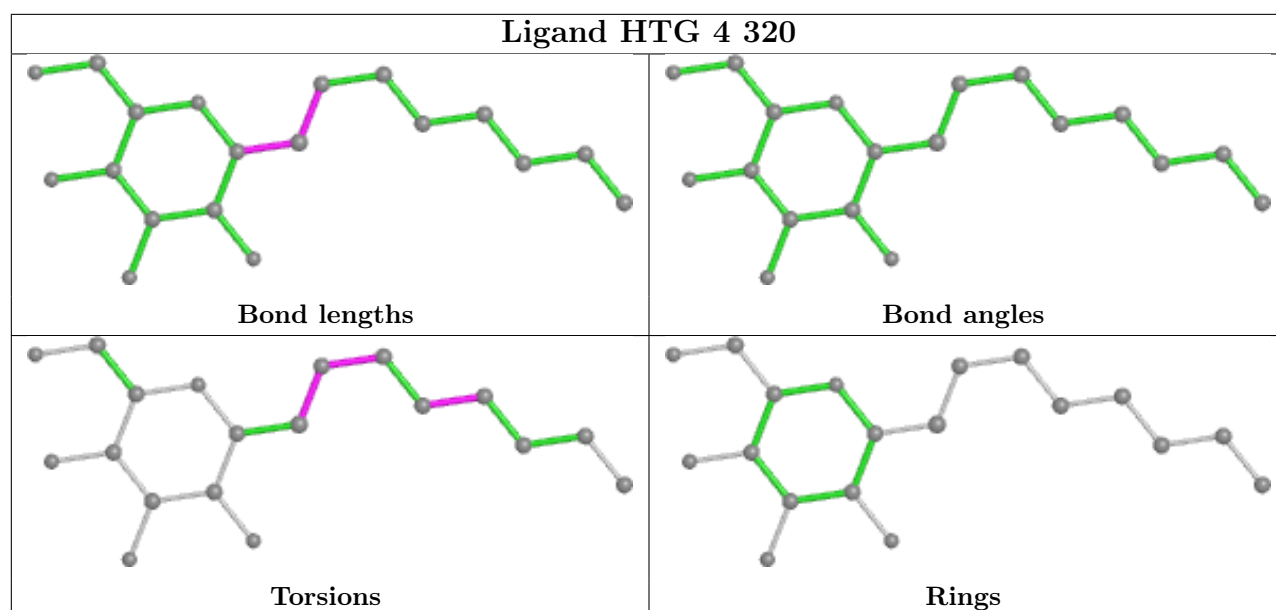


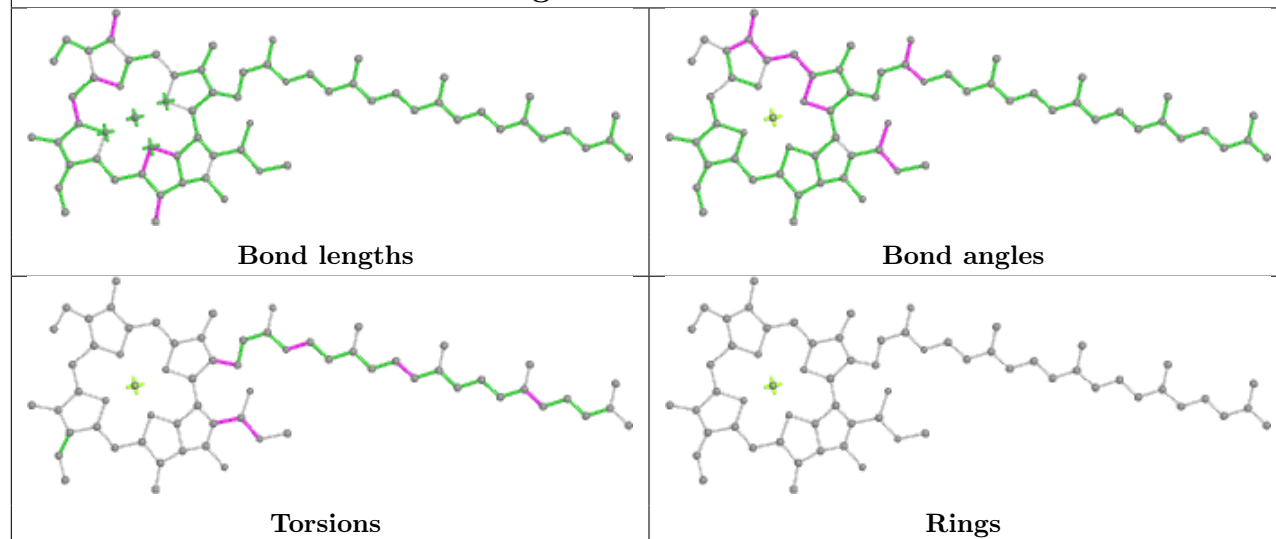
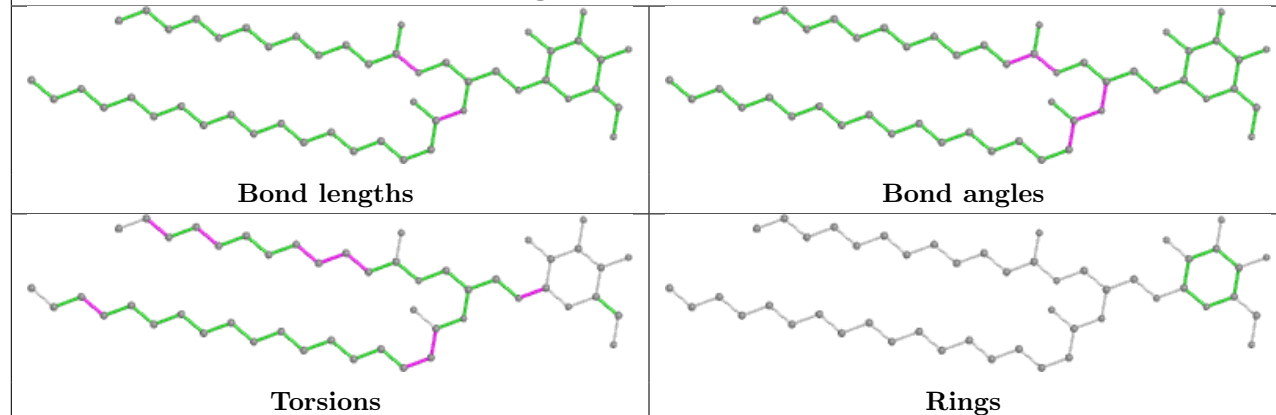
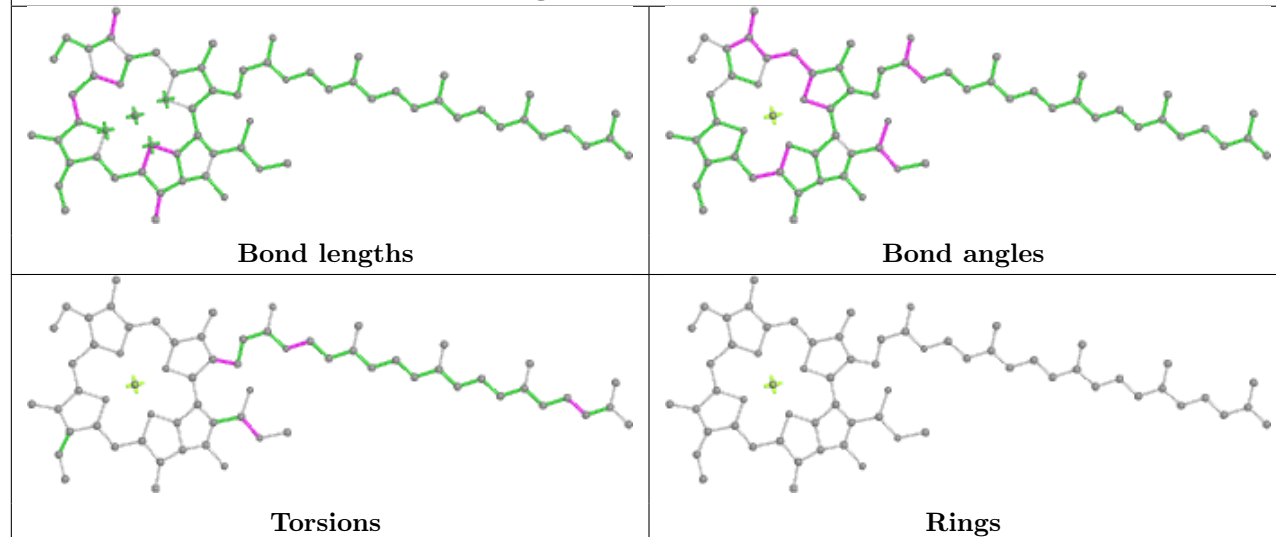
Torsions



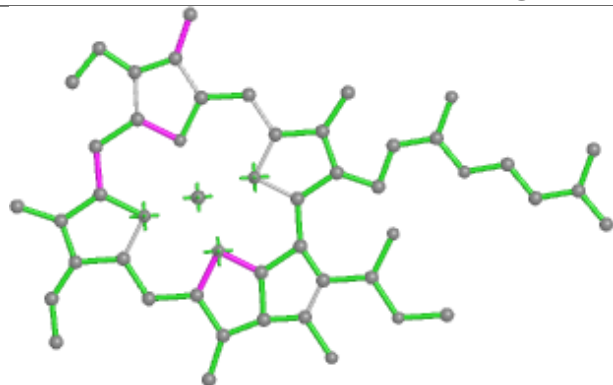
Rings



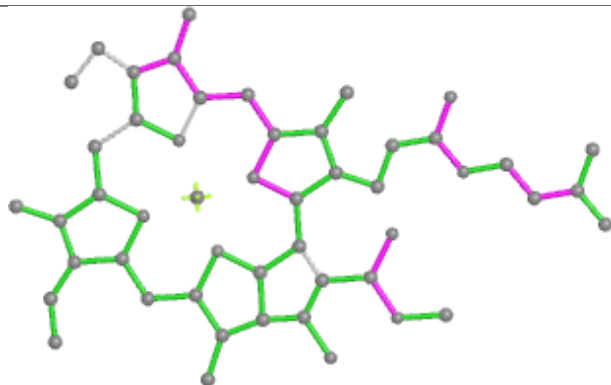


Ligand CLA B 802**Ligand LMG 1 320****Ligand CLA B 839**

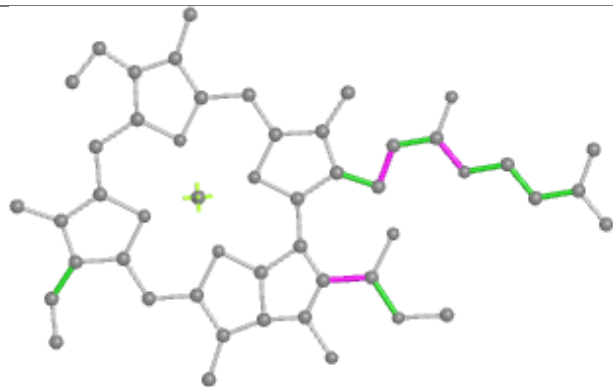
Ligand CLA G 604



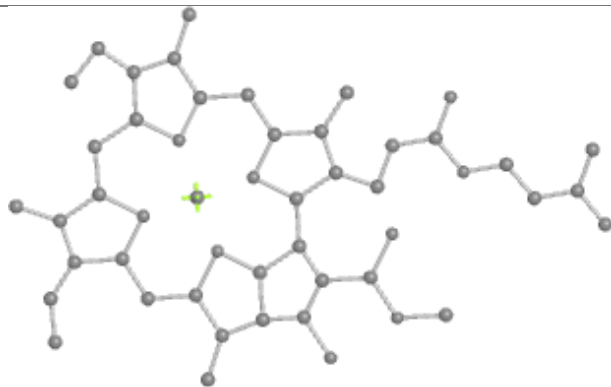
Bond lengths



Bond angles

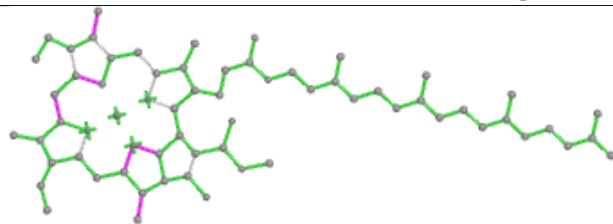


Torsions

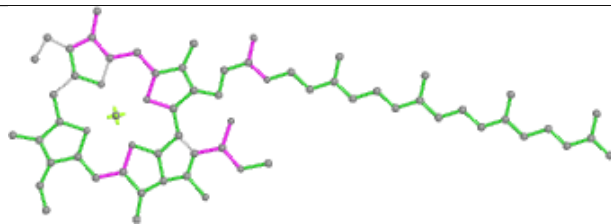


Rings

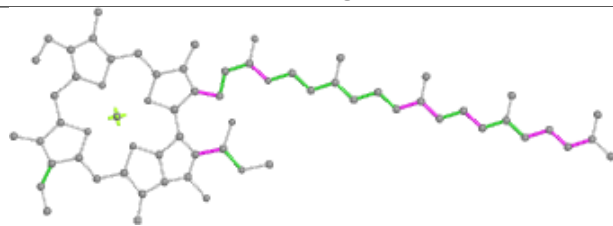
Ligand CLA B 825



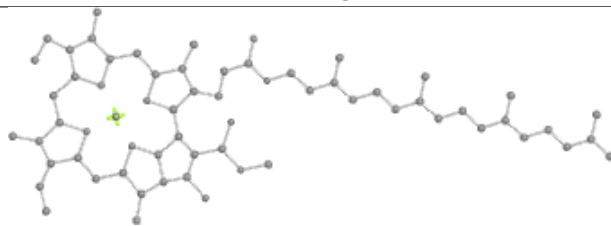
Bond lengths



Bond angles

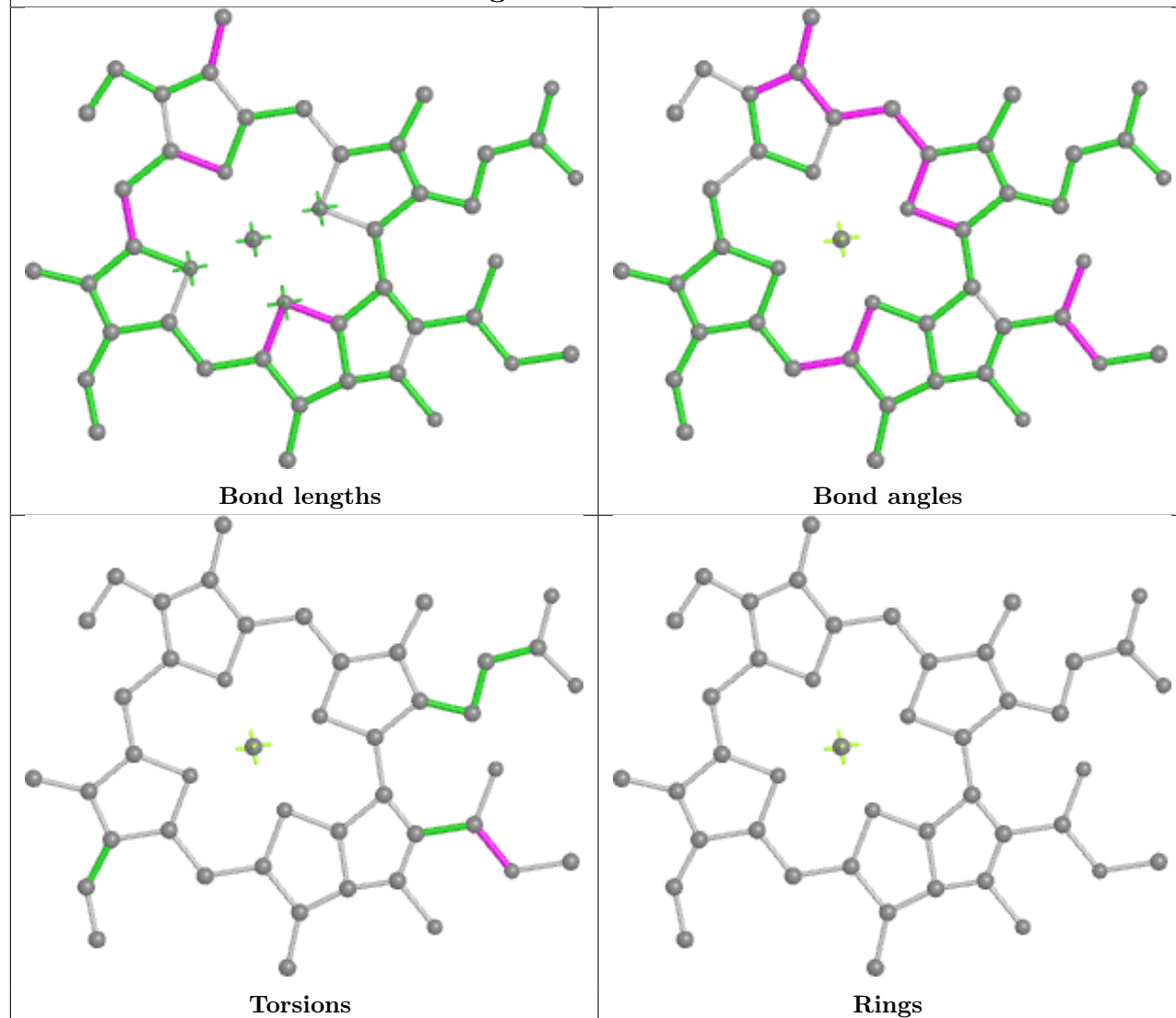


Torsions

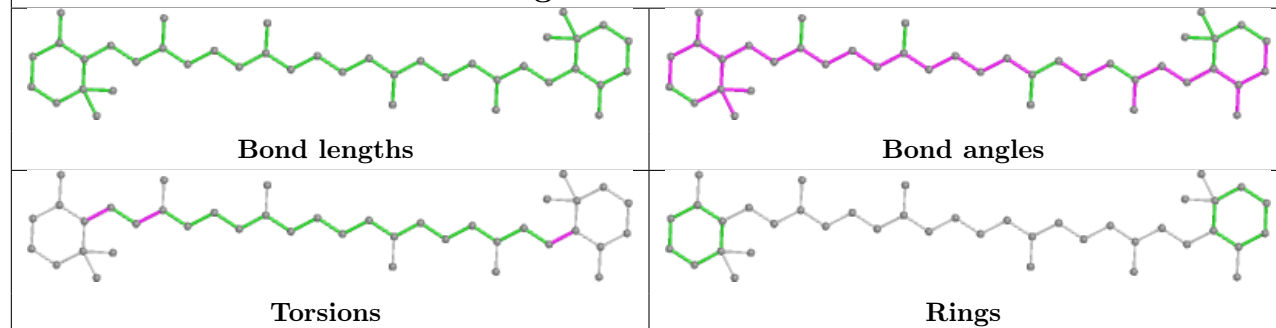


Rings

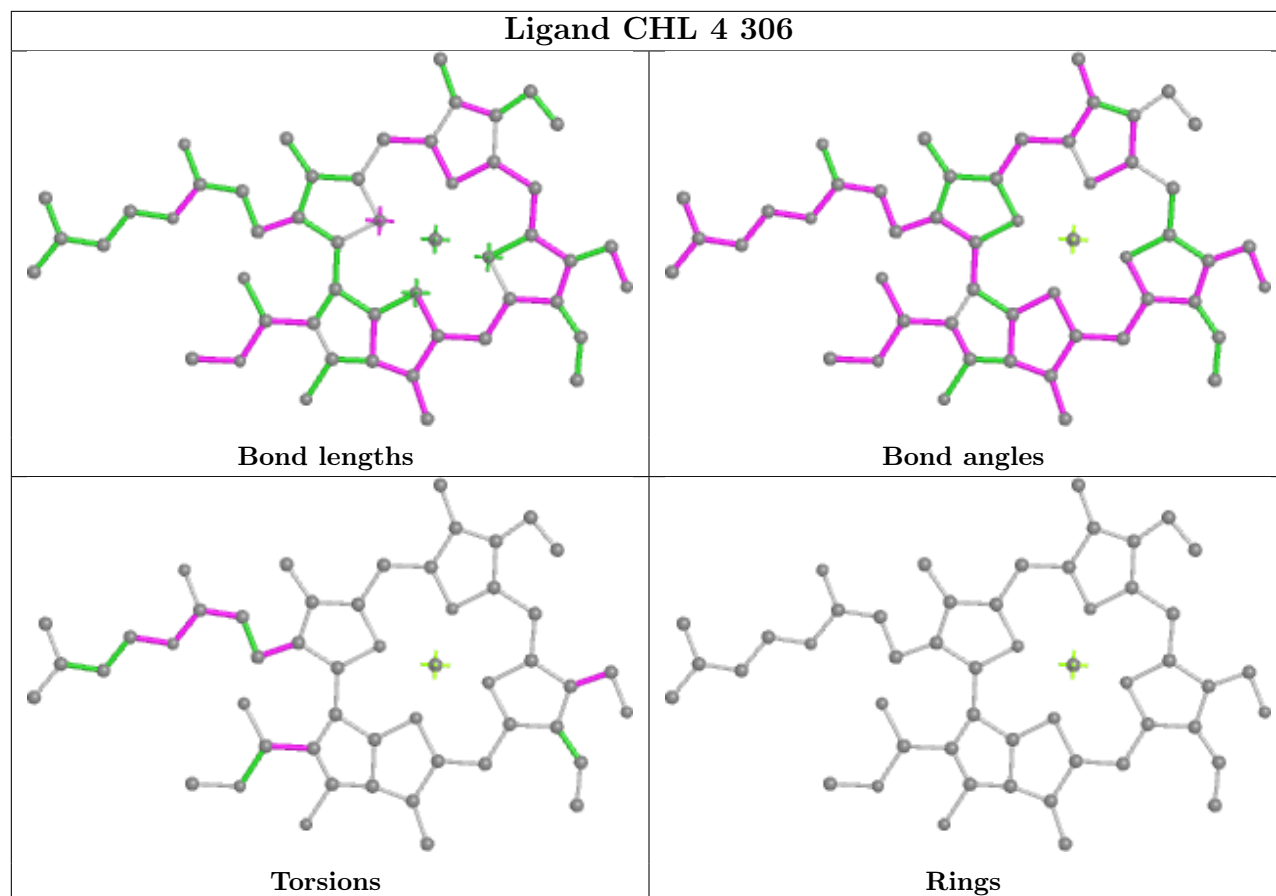
Ligand CLA G 603

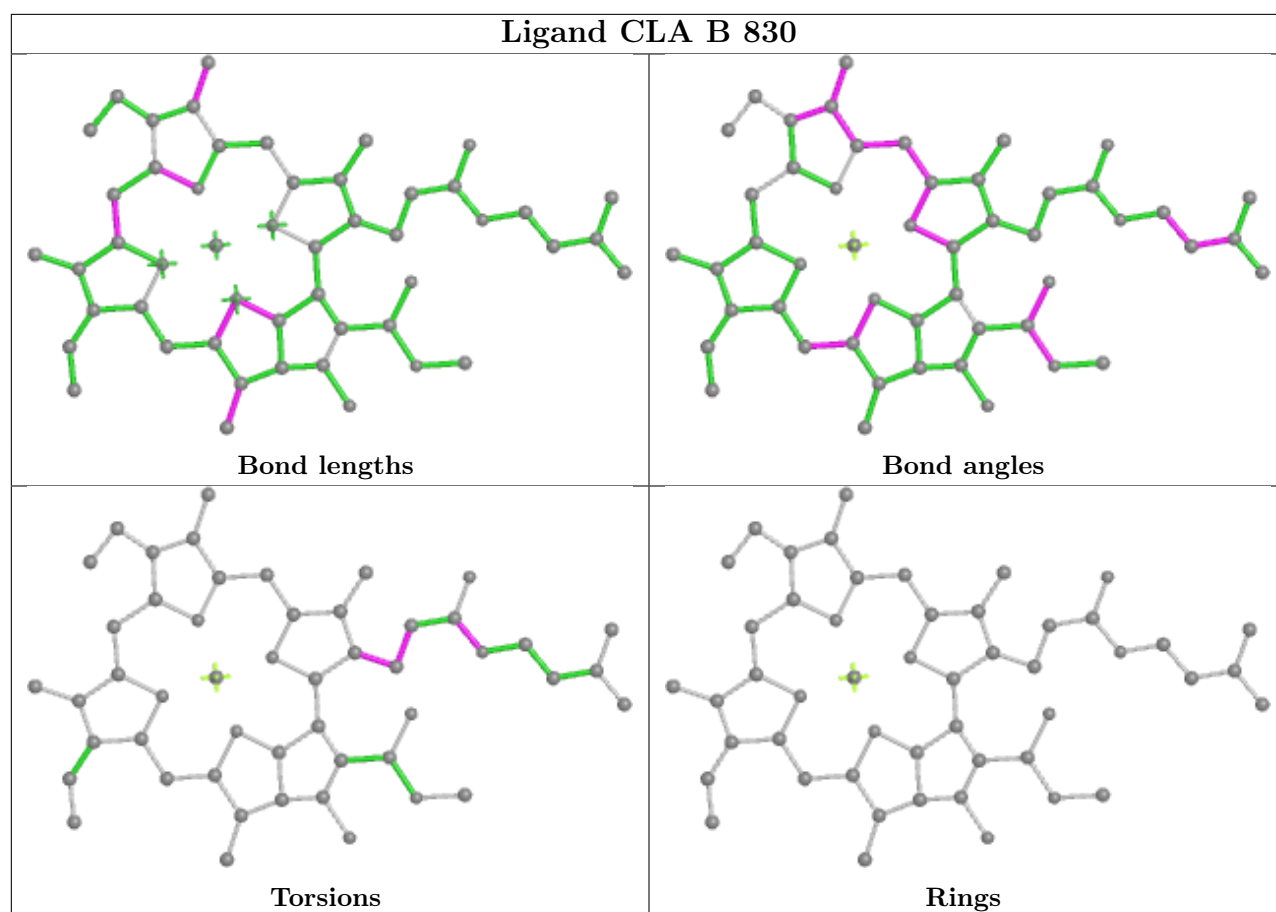


Ligand BCR 4 318

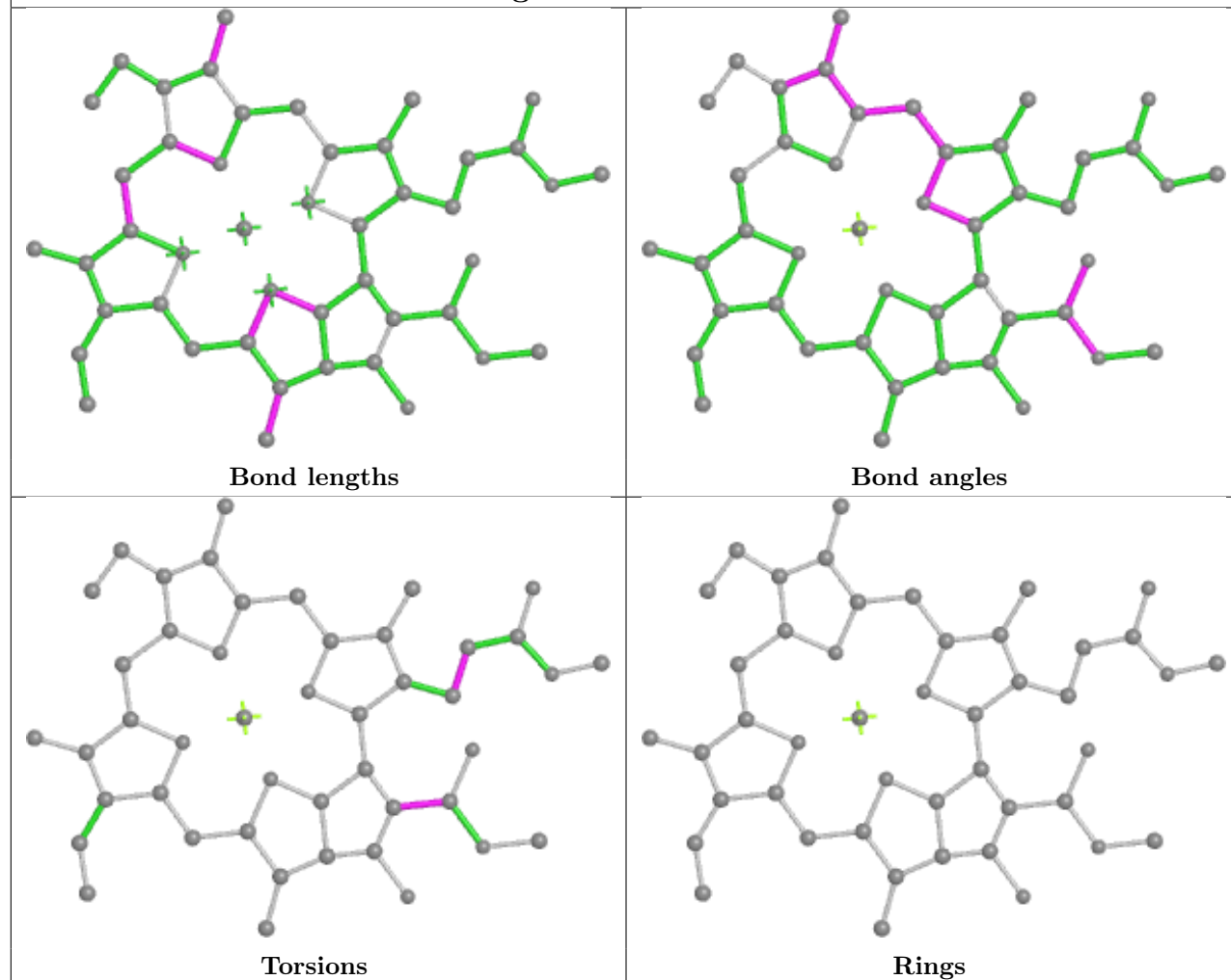


Ligand CHL 4 306

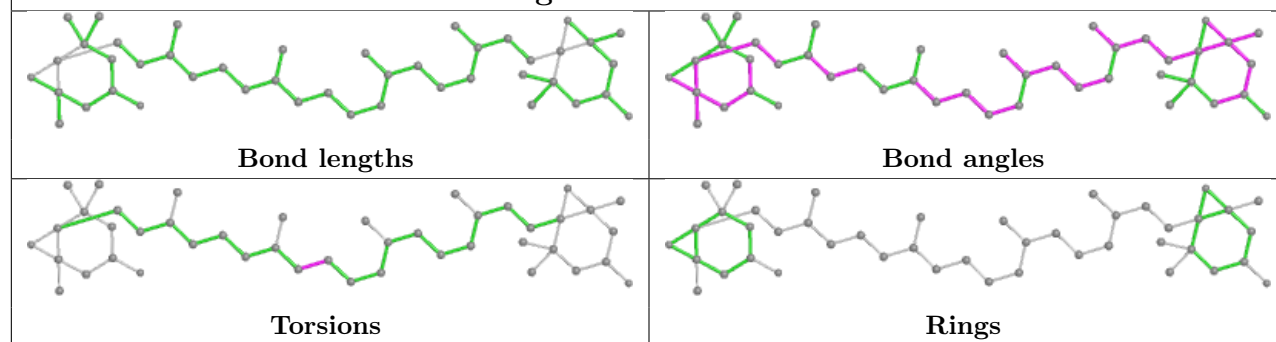


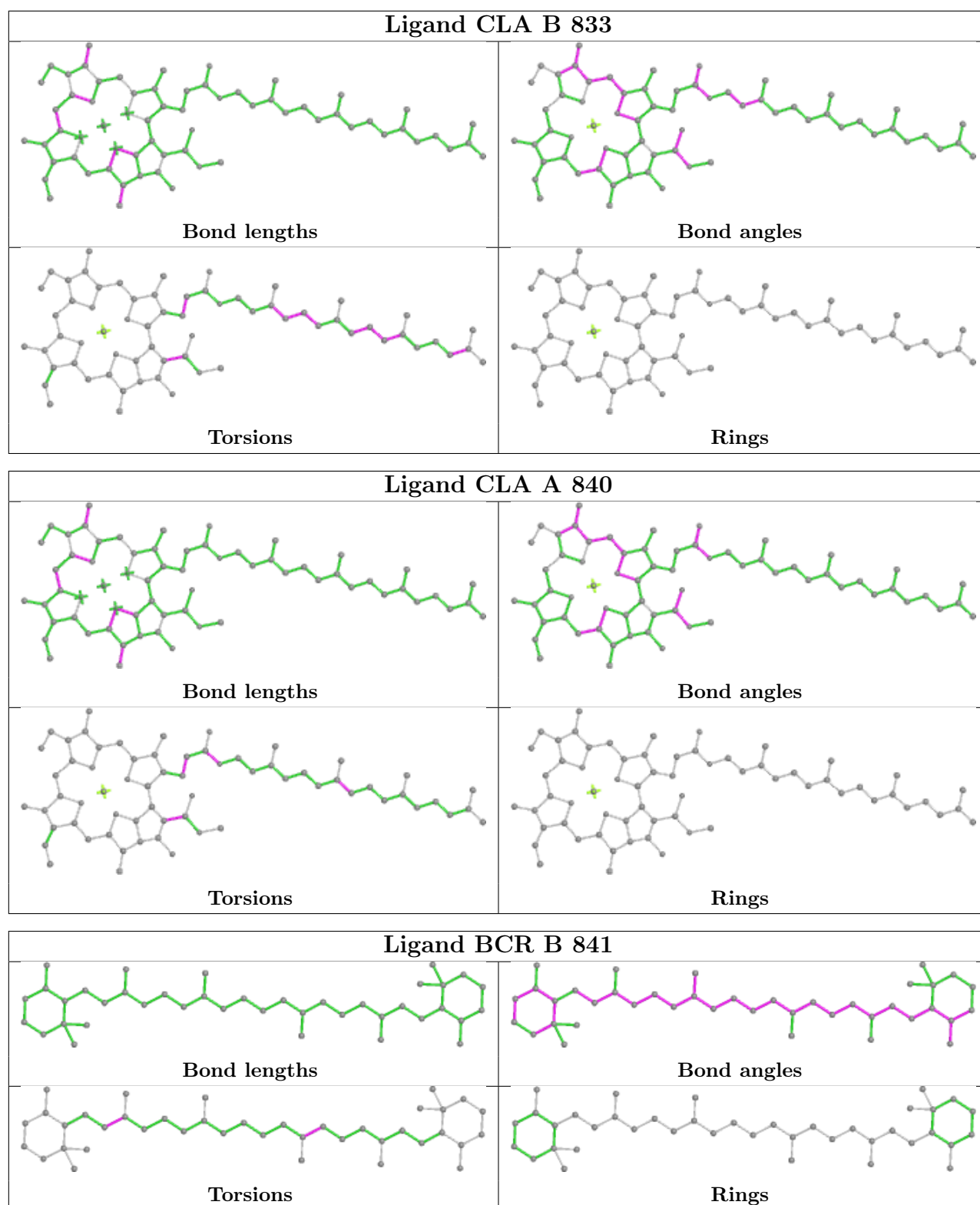


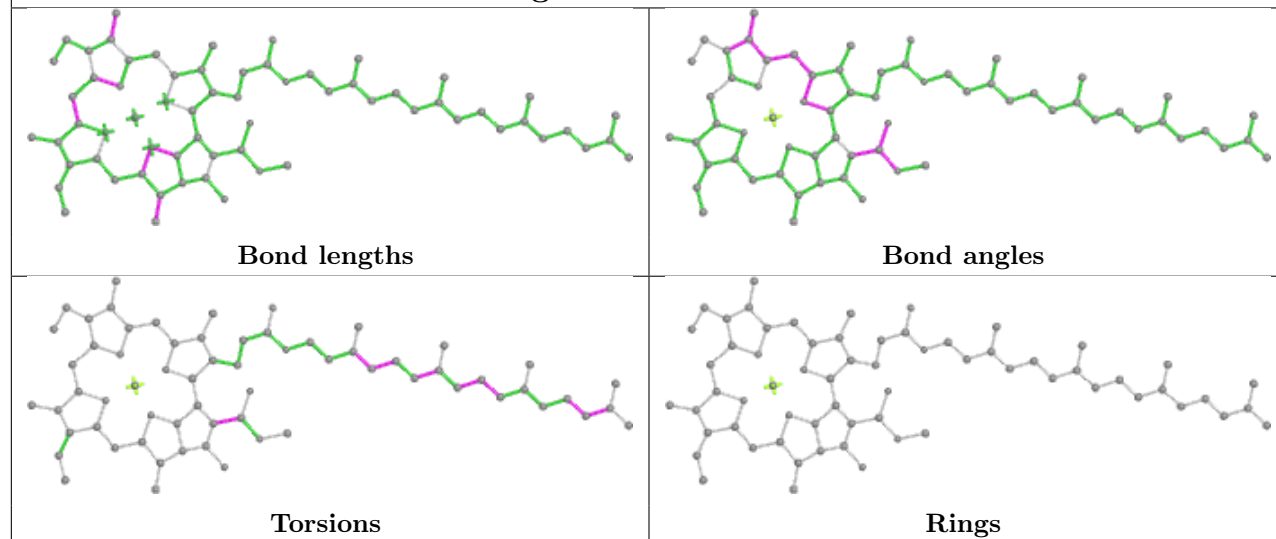
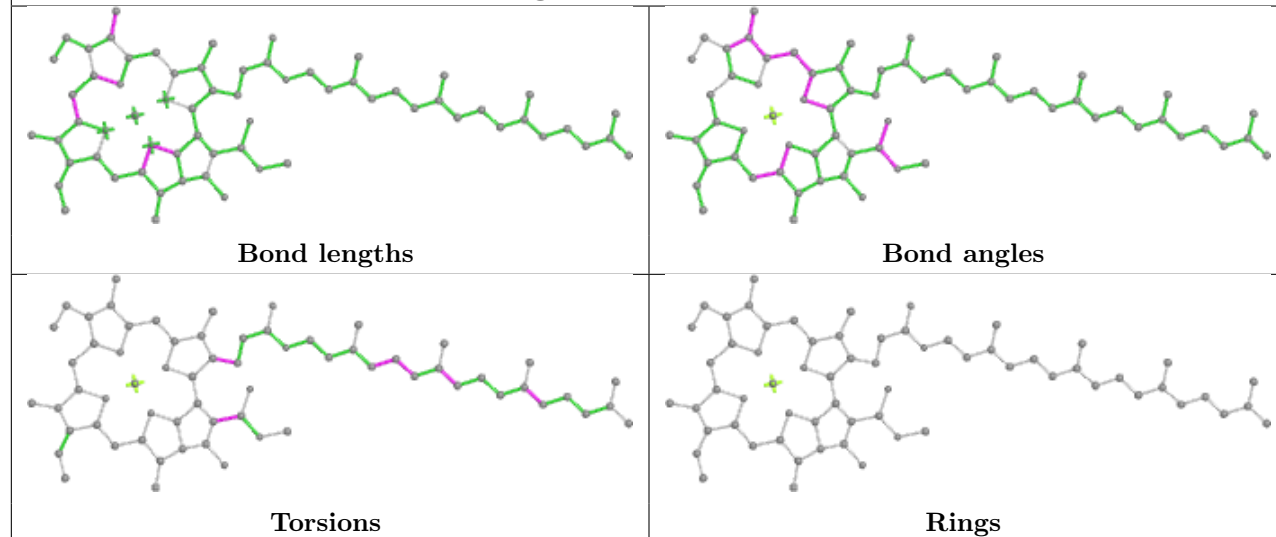
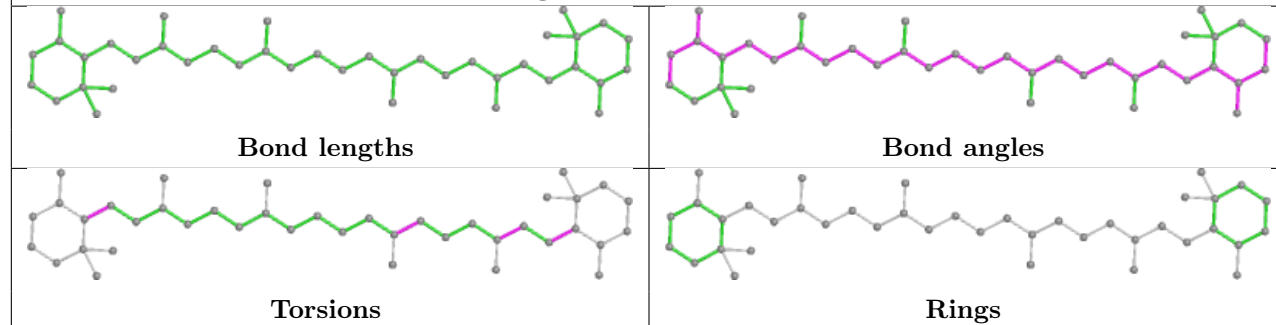
Ligand CLA K 201



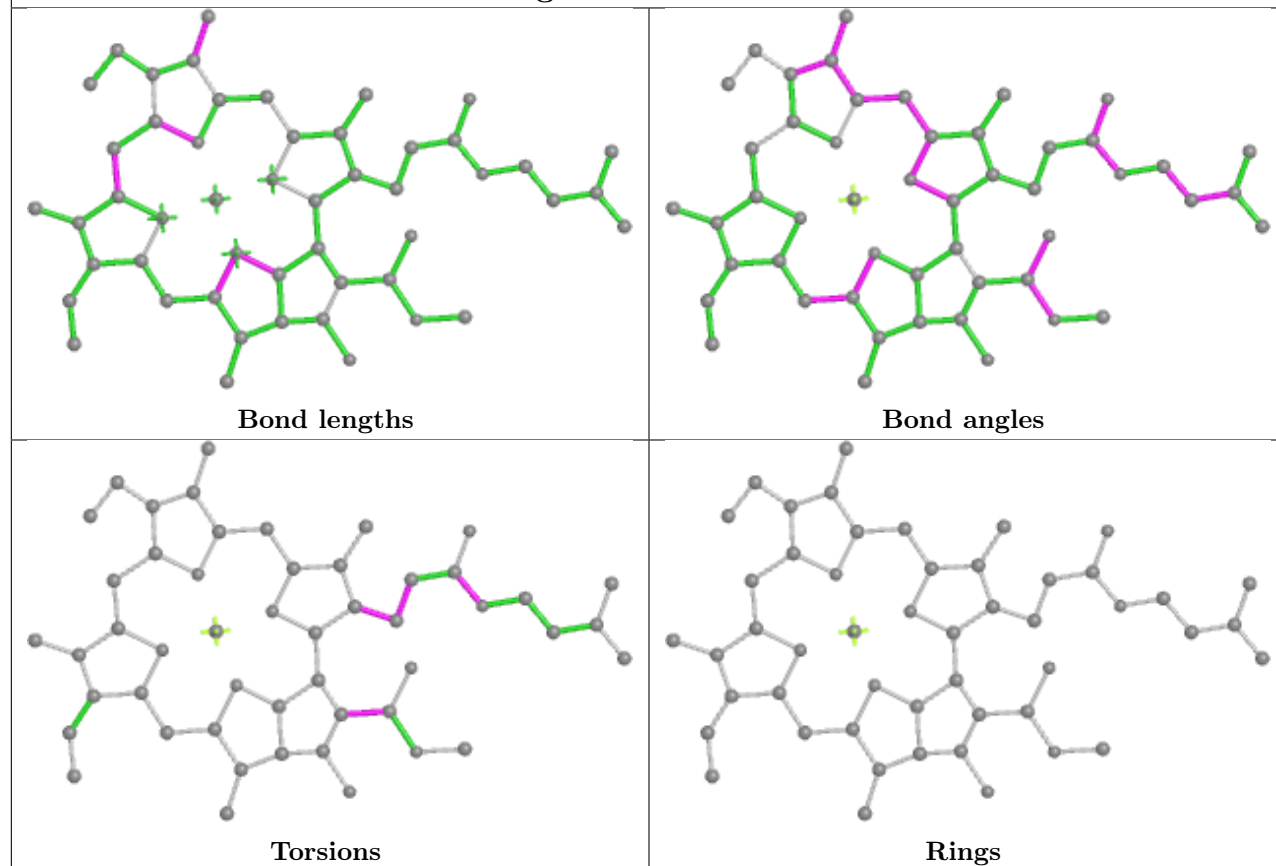
Ligand XAT 1 316



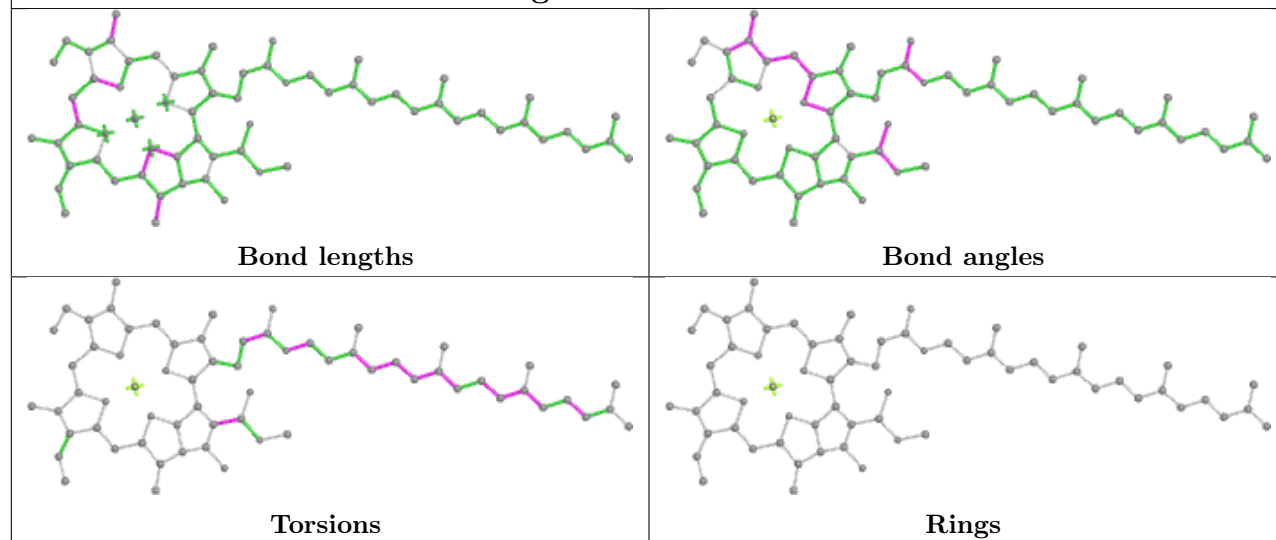


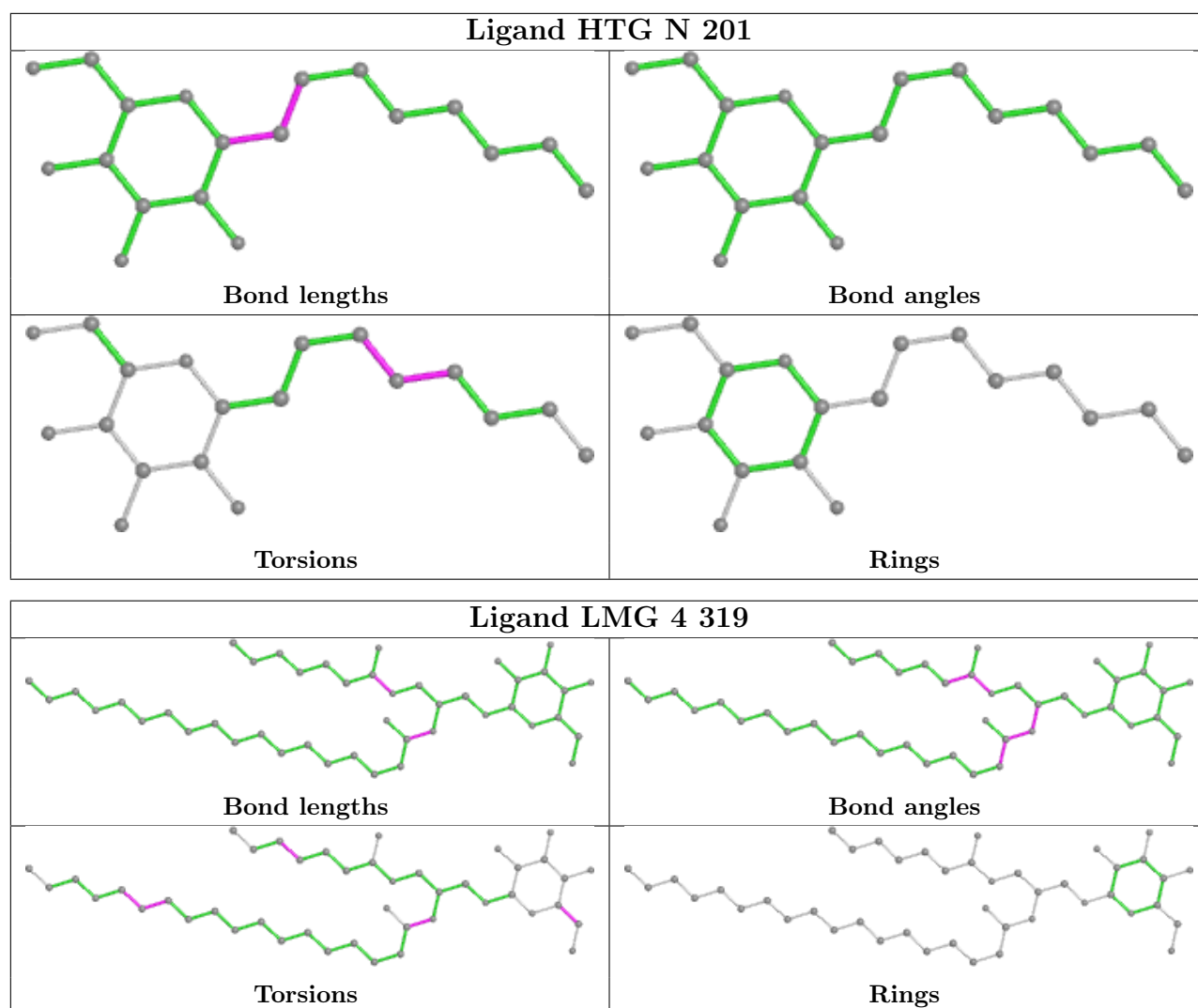
Ligand CLA A 838**Ligand CLA A 832****Ligand BCR J 102**

Ligand CLA 4 314

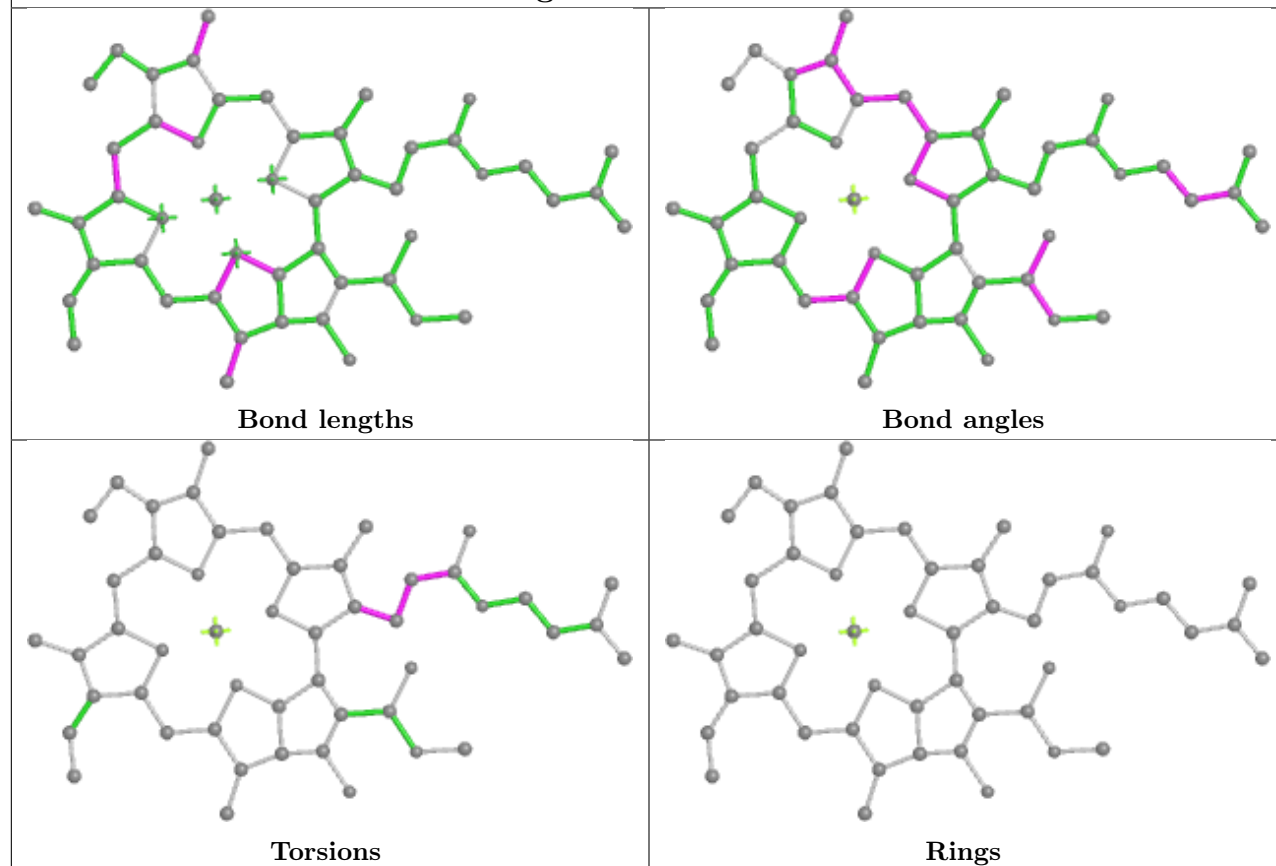


Ligand CLA A 805

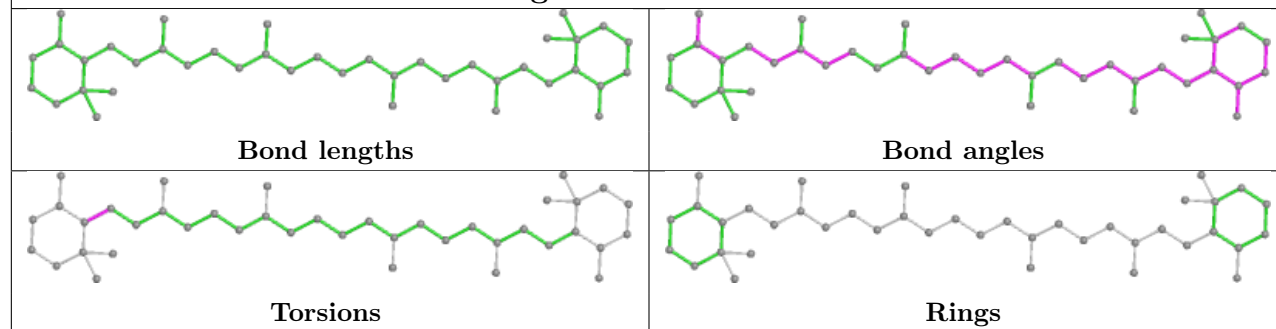


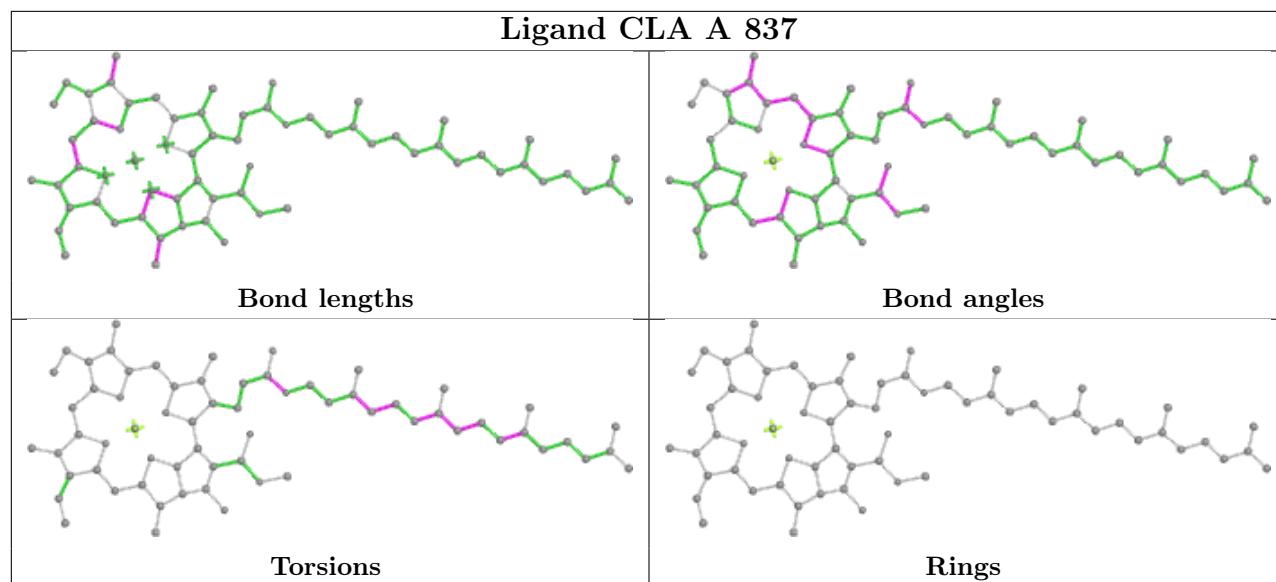
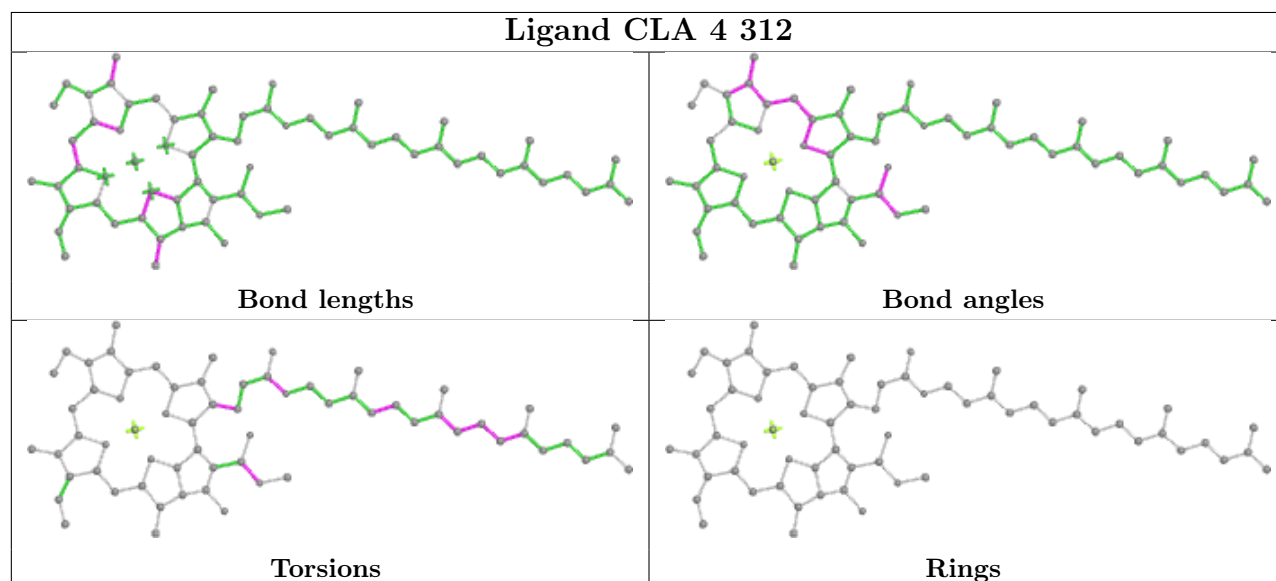
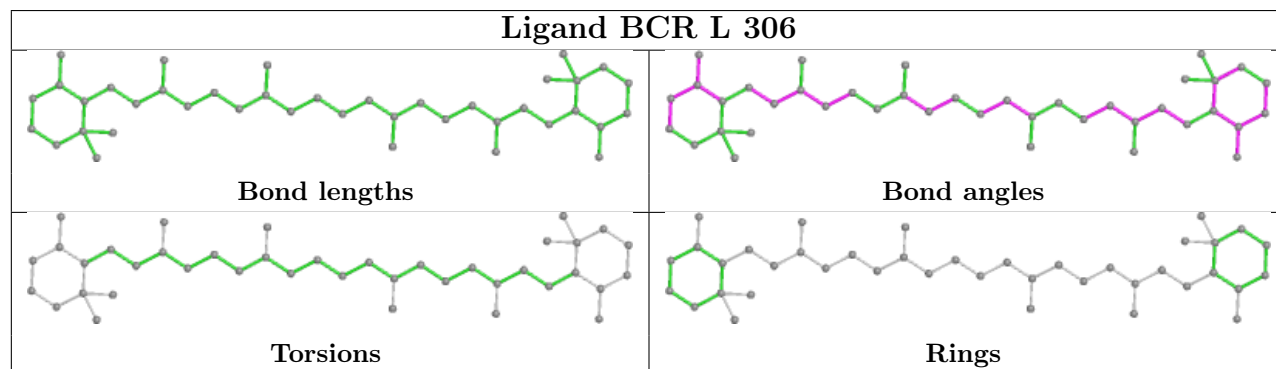


Ligand CLA 2 308

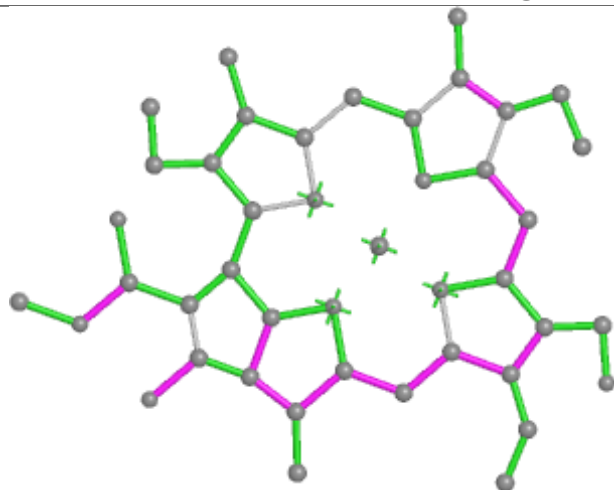


Ligand BCR B 844

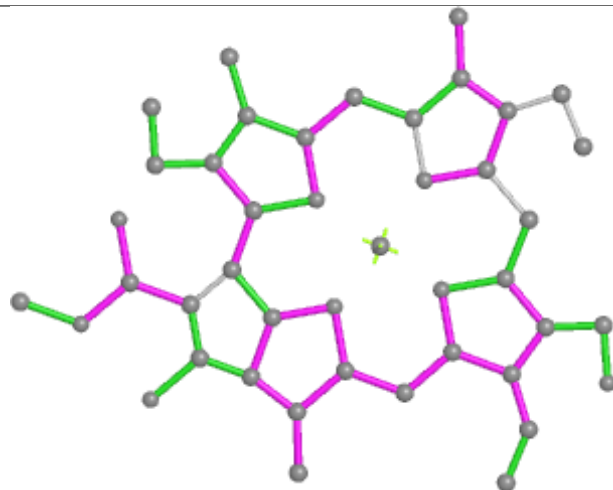


Ligand CLA A 837**Ligand CLA 4 312****Ligand BCR L 306**

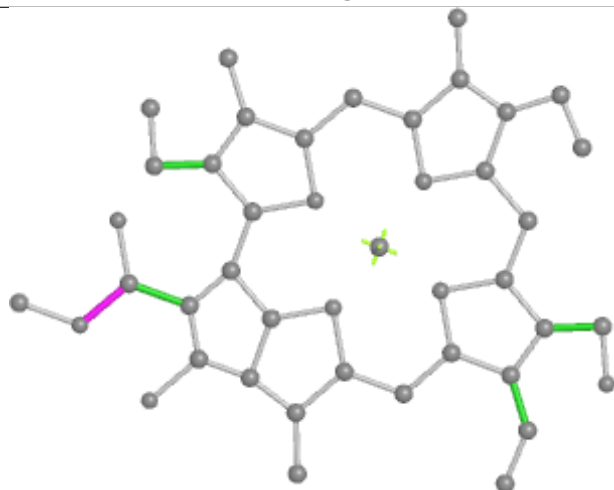
Ligand CHL 2 314



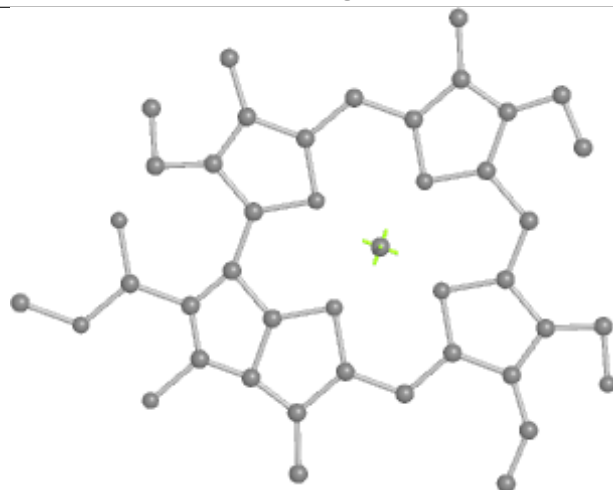
Bond lengths



Bond angles

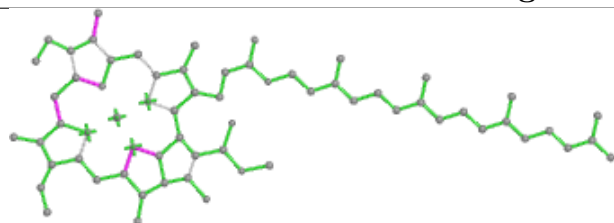


Torsions

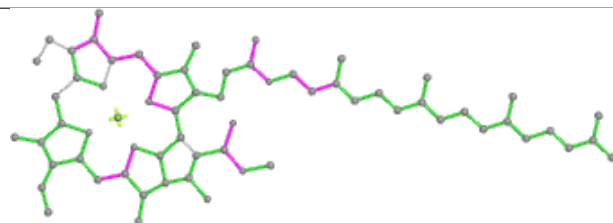


Rings

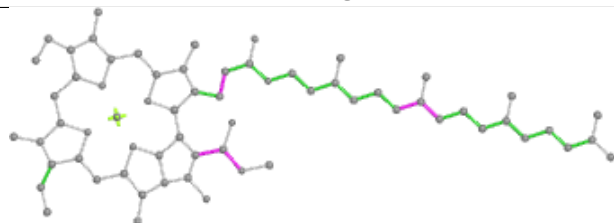
Ligand CLA 2 312



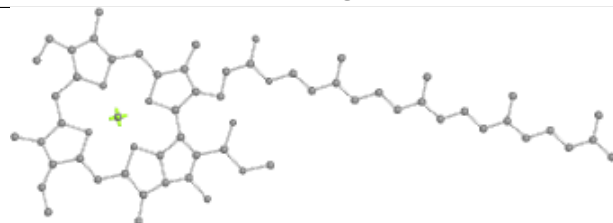
Bond lengths



Bond angles

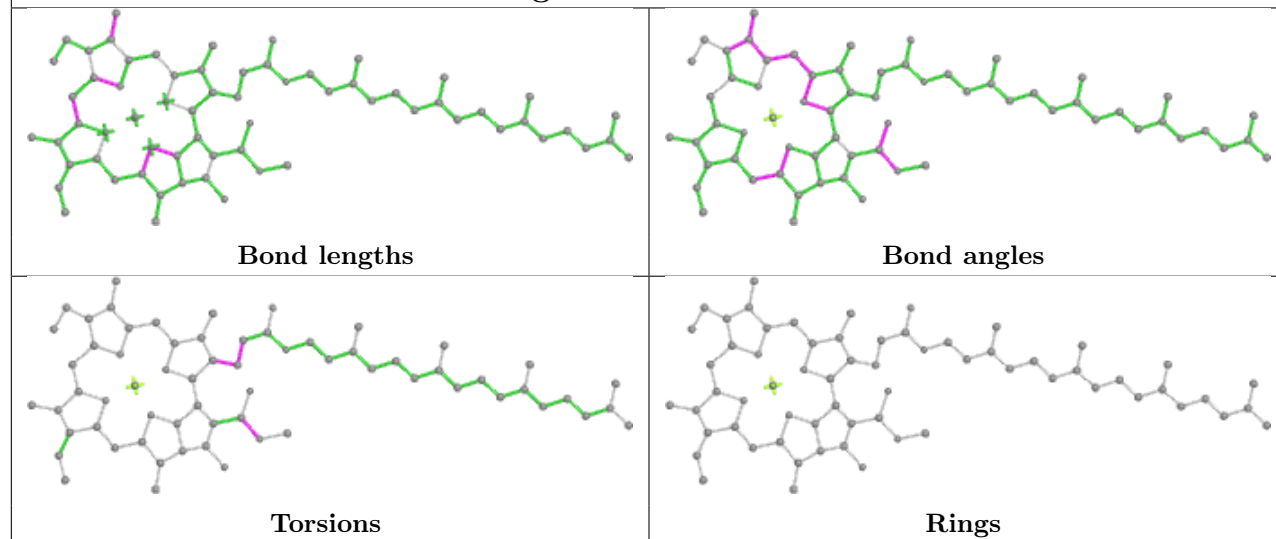


Torsions

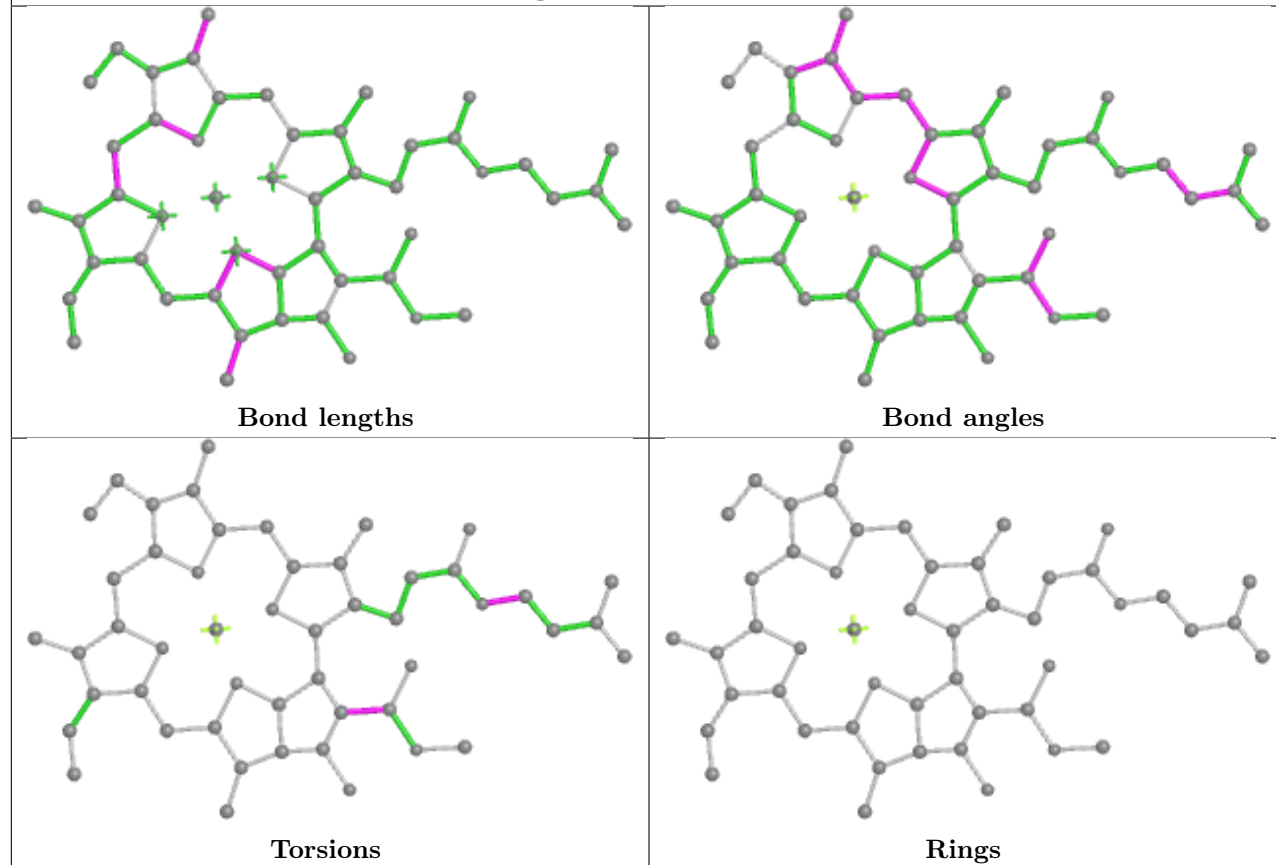


Rings

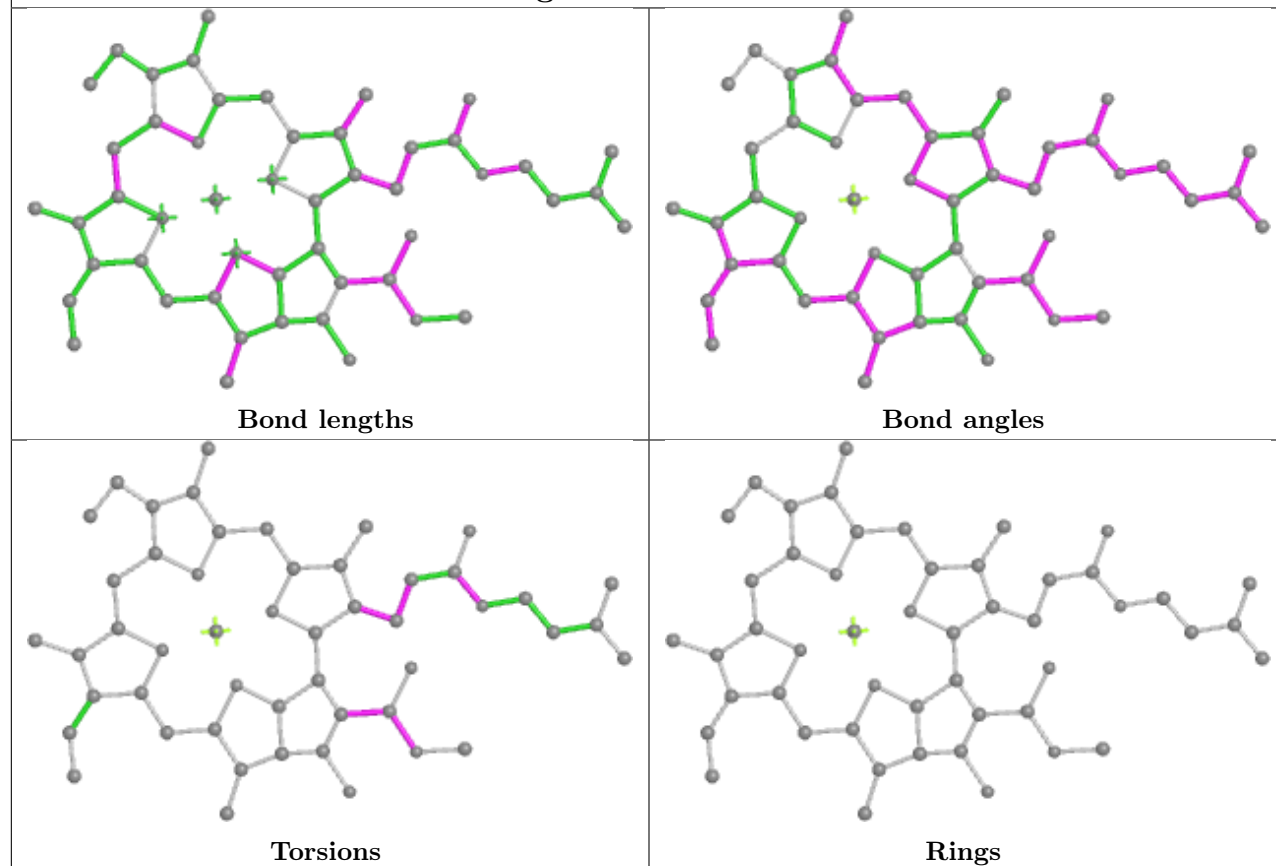
Ligand CLA B 801



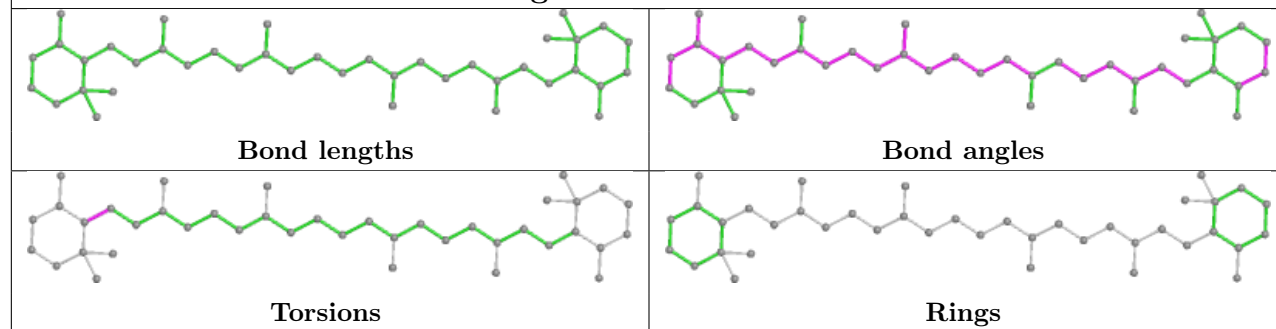
Ligand CLA A 830

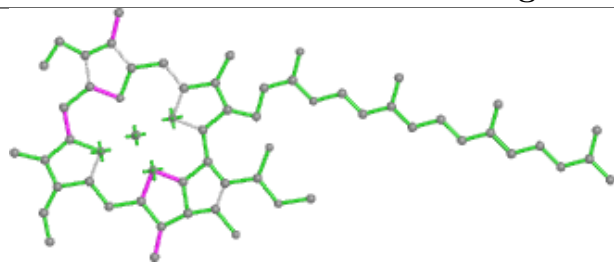
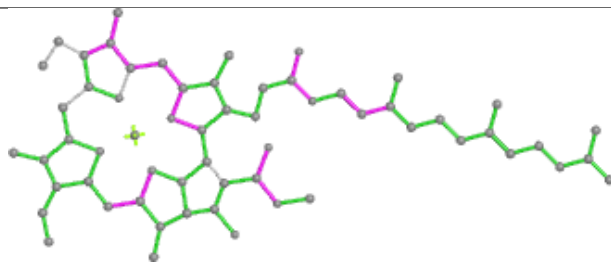
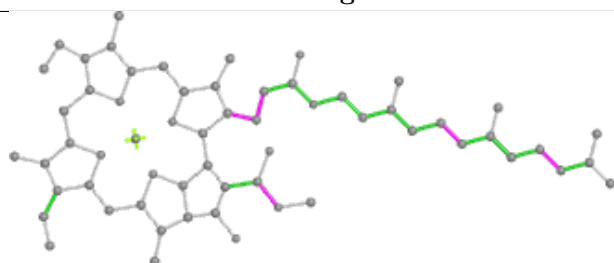
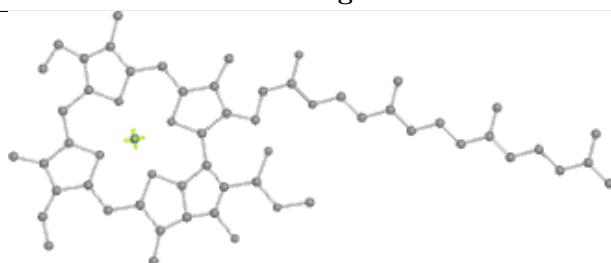
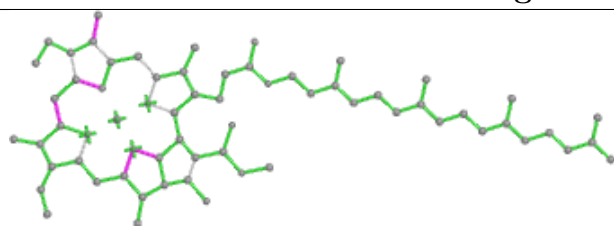
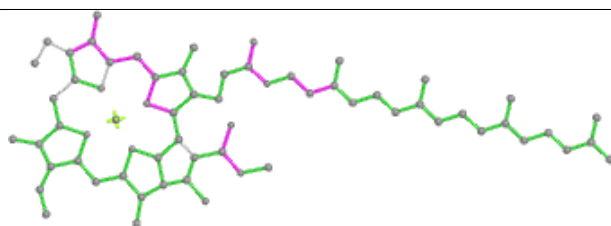
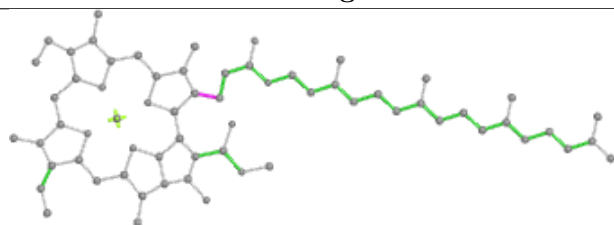
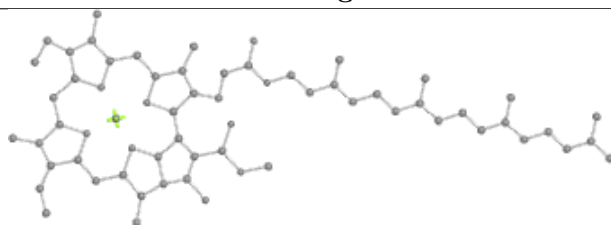


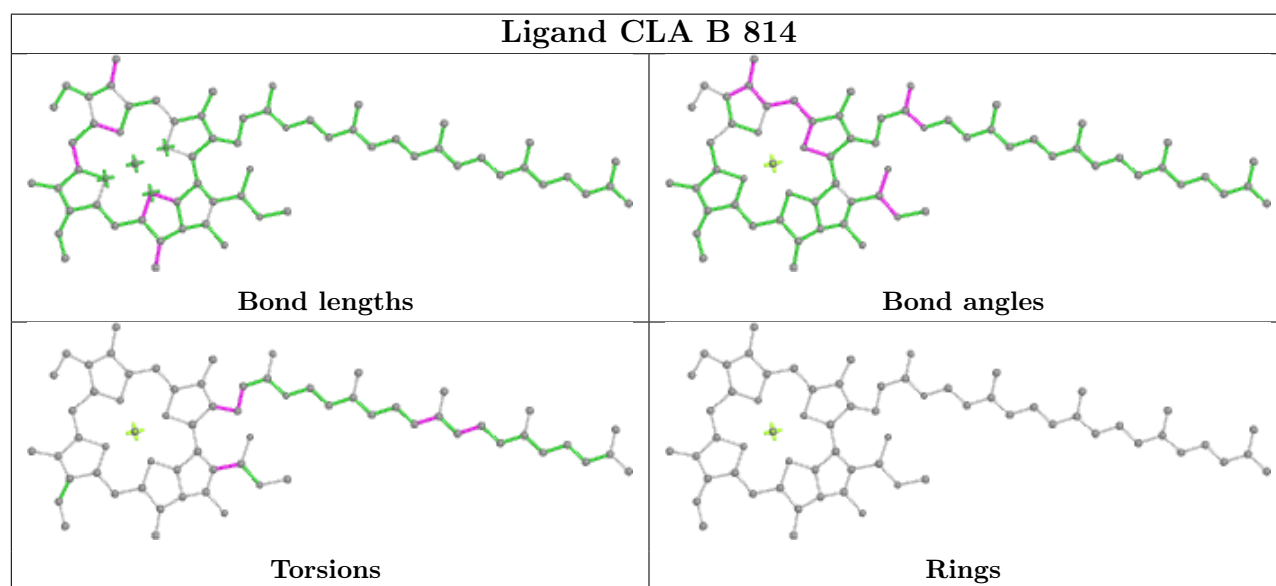
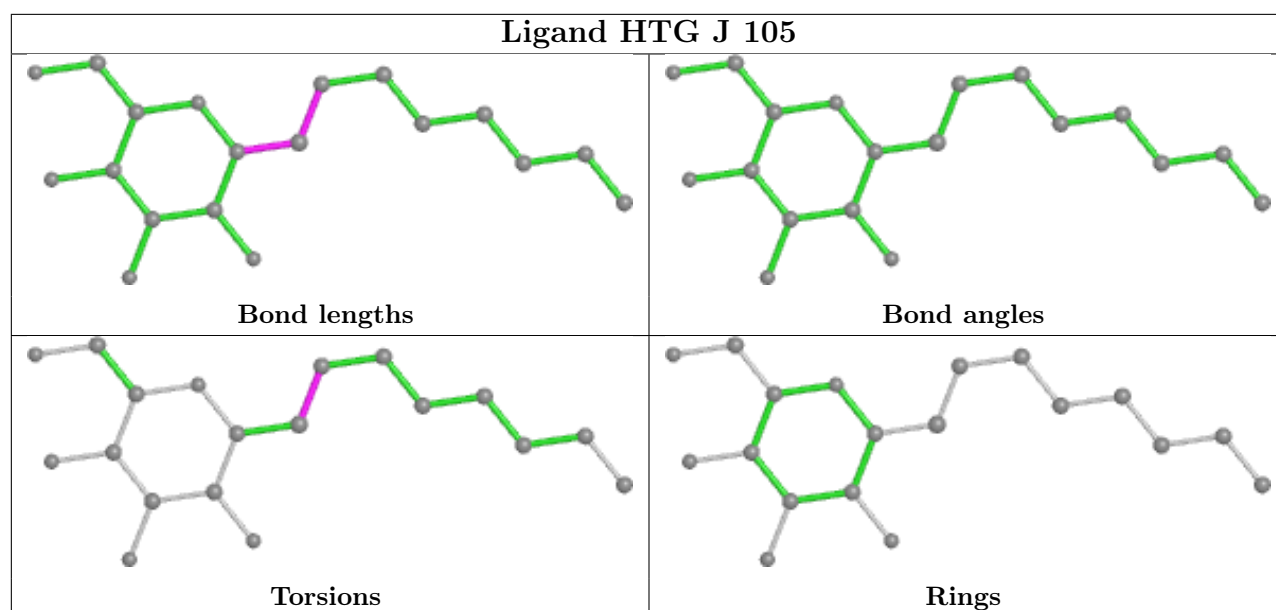
Ligand CLA 4 304

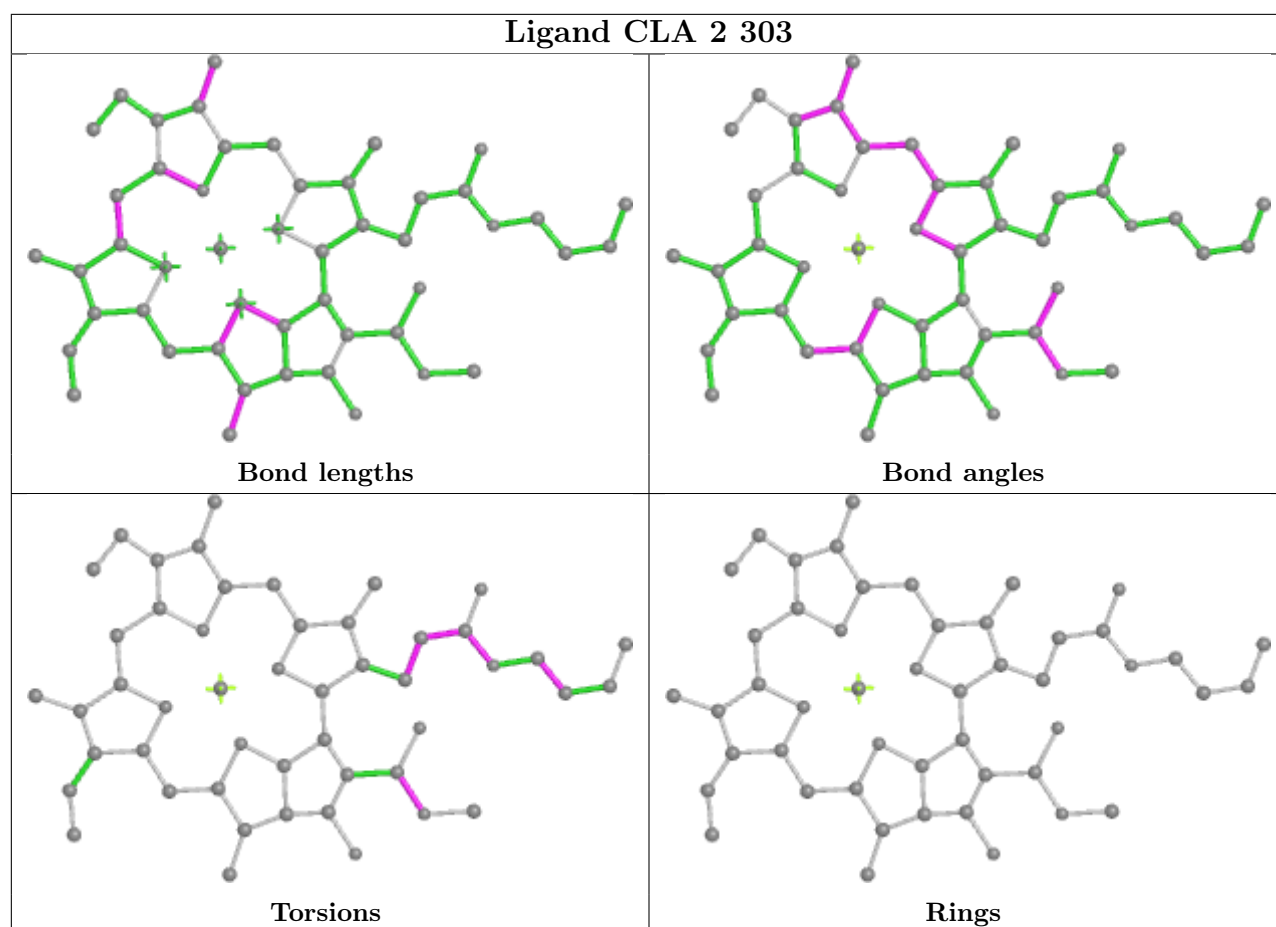


Ligand BCR B 846



Ligand CLA 4 309**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 826****Bond lengths****Bond angles****Torsions****Rings**





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.