



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 05:29 PM JST

PDB ID : 6L35 / pdb_00006l35
EMDB ID : EMD-0821
Title : PSI-LHCI Supercomplex from *Physcometrella patens*
Authors : Zhao, L.; Yan, Q.J.; Qin, X.C.
Deposited on : 2019-10-09
Resolution : 3.23 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	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

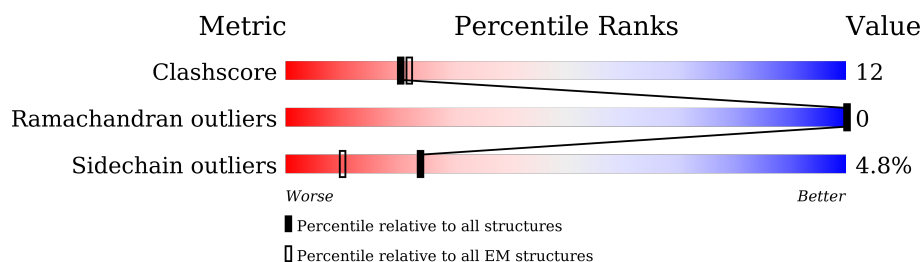
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.23 Å.

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





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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	742	77% 22% .
2	B	733	77% 22% .
3	C	80	70% 25% 5%
4	D	141	83% 16% .
5	E	62	71% 27% .
6	F	159	74% 24% .
7	G	98	68% 28% .
8	H	90	79% 20% .
9	I	34	68% 32%

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Mol	Chain	Length	Quality of chain
10	J	41	 78%22%
11	K	79	 65%30%5%
12	L	159	 73%26%.
13	M	29	 72%24%.
14	2	210	 77%20%..
15	6	192	 69%29%.
16	3	213	 71%28%.
17	5	205	 63%34%..

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
18	CLA	2	602	X	-	-	-
18	CLA	2	603	X	-	-	-
18	CLA	2	604	X	-	-	-
18	CLA	2	609	X	-	-	-
18	CLA	2	610	X	-	-	-
18	CLA	2	611	X	-	-	-
18	CLA	2	612	X	-	-	-
18	CLA	2	613	X	-	-	-
18	CLA	2	614	X	-	-	-
18	CLA	3	602	X	-	-	-
18	CLA	3	603	X	-	-	-
18	CLA	3	604	X	-	-	-
18	CLA	3	606	X	-	-	-
18	CLA	3	607	X	-	-	-
18	CLA	3	609	X	-	-	-
18	CLA	3	610	X	-	-	-
18	CLA	3	611	X	-	-	-
18	CLA	3	612	X	-	-	-
18	CLA	3	613	X	-	-	-
18	CLA	3	614	X	-	-	-
18	CLA	3	615	X	-	-	-
18	CLA	3	617	X	-	-	-
18	CLA	5	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	5	602	X	-	-	-
18	CLA	5	603	X	-	-	-
18	CLA	5	604	X	-	-	-
18	CLA	5	609	X	-	-	-
18	CLA	5	610	X	-	-	-
18	CLA	5	611	X	-	-	-
18	CLA	5	612	X	-	-	-
18	CLA	5	613	X	-	-	-
18	CLA	5	614	X	-	-	-
18	CLA	6	602	X	-	-	-
18	CLA	6	603	X	-	-	-
18	CLA	6	604	X	-	-	-
18	CLA	6	606	X	-	-	-
18	CLA	6	608	X	-	-	-
18	CLA	6	609	X	-	-	-
18	CLA	6	610	X	-	-	-
18	CLA	6	611	X	-	-	-
18	CLA	6	612	X	-	-	-
18	CLA	6	613	X	-	-	-
18	CLA	6	614	X	-	-	-
18	CLA	6	616	X	-	-	-
18	CLA	A	801	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	A	854	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	F	304	X	-	-	-
18	CLA	F	305	X	-	-	-
18	CLA	G	201	X	-	-	-
18	CLA	G	203	X	-	-	-
18	CLA	G	204	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	K	206	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-
22	SF4	C	101	-	-	X	-
22	SF4	C	102	-	-	X	-
25	CHL	2	601	X	-	-	-
25	CHL	2	606	X	-	-	-
25	CHL	2	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	2	608	X	-	-	-
25	CHL	2	616	X	-	-	-
25	CHL	3	608	X	-	-	-
25	CHL	5	606	X	-	-	-
25	CHL	5	607	X	-	-	-
25	CHL	5	608	X	-	-	-
25	CHL	5	615	X	-	-	-
25	CHL	6	601	X	-	-	-
25	CHL	6	607	X	-	-	-
27	XAT	2	620	-	-	X	-
27	XAT	5	620	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 34822 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5837	3827	993	998	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5849	3839	996	998	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			595	365	103	116	11		

- Molecule 4 is a protein called Predicted protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1104	707	196	198	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	62	Total	C	N	O	0	0
			487	309	87	91		

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	159	Total	C	N	O	S	0	0
			1226	793	209	221	3		

- Molecule 7 is a protein called Predicted protein PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	98	Total	C	N	O	0	0
			749	483	128	138		

- Molecule 8 is a protein called PsaH photosystem I reaction center subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	90	Total	C	N	O	S	0	0
			693	445	117	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			266	181	35	48	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			325	222	48	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	79	Total	C	N	O	S	0	0
			550	346	96	105	3		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1189	781	192	214	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	29	Total	C	N	O	0	0
			214	141	34	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	206	Total	C	N	O	S	0	0
			1595	1039	267	285	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	192	Total	C	N	O	S	0	0
			1473	961	247	264	1		

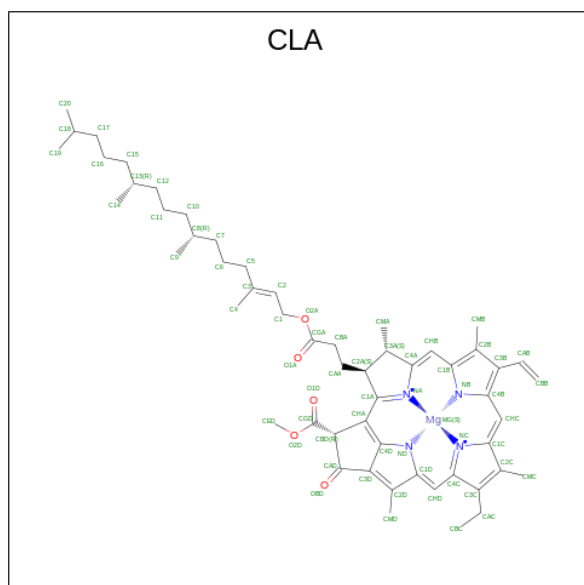
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	213	Total	C	N	O	S	0	0
			1644	1076	265	296	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	202	Total	C	N	O	S	0	0
			1566	1020	258	282	6		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	A	1	Total 43	C 33	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	G	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 42	C 34	Mg 1	N 4	O 3	0

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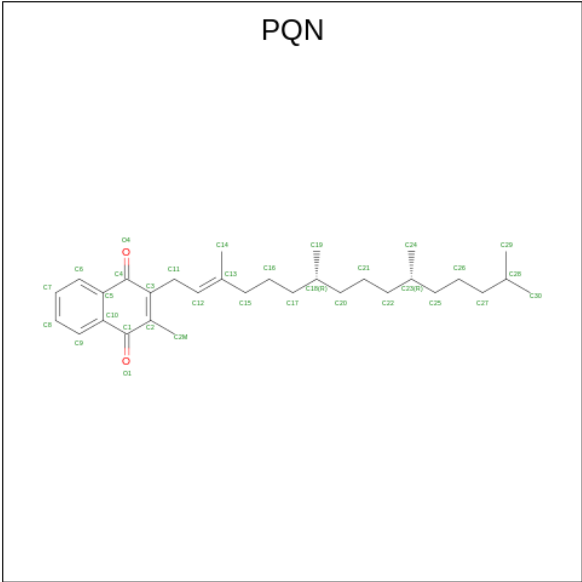
Mol	Chain	Residues	Atoms					AltConf
18	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	6	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	6	1	Total 43	C 33	Mg 1	N 4	O 5	0
18	6	1	Total 38	C 30	Mg 1	N 4	O 3	0
18	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6	1	Total 38	C 30	Mg 1	N 4	O 3	0
18	6	1	Total 43	C 33	Mg 1	N 4	O 5	0
18	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3	1	Total 42	C 32	Mg 1	N 4	O 5	0
18	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0

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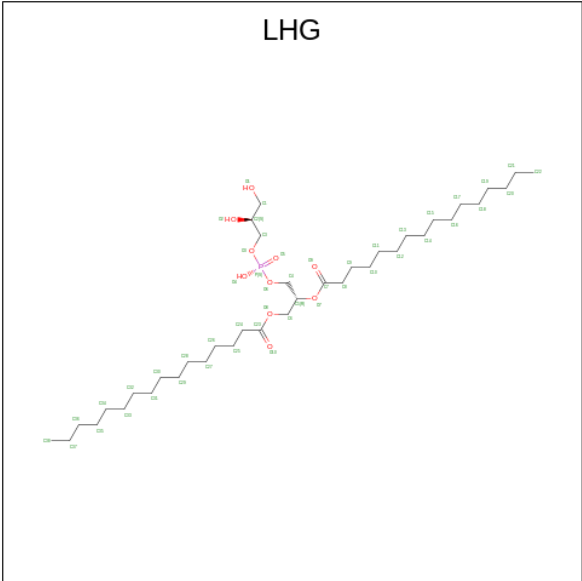
Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



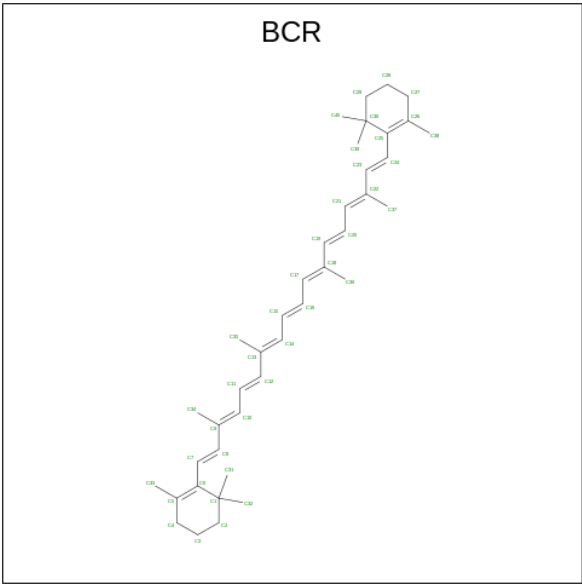
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			27	16	10	1	
20	B	1	Total	C	O	P	0
			23	12	10	1	
20	2	1	Total	C	O	P	0
			35	24	10	1	
20	6	1	Total	C	O	P	0
			28	17	10	1	
20	5	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



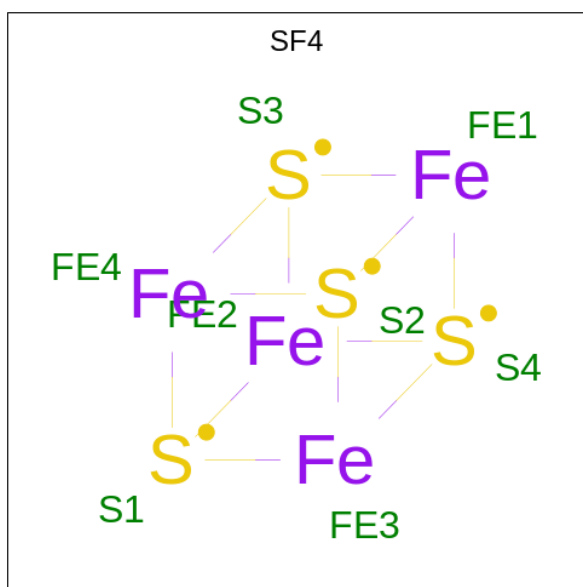
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

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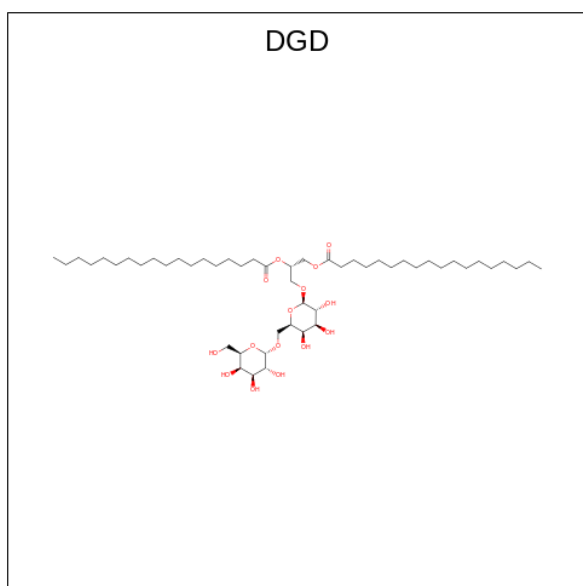
Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	2	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	5	1	Total C 40 40	0

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



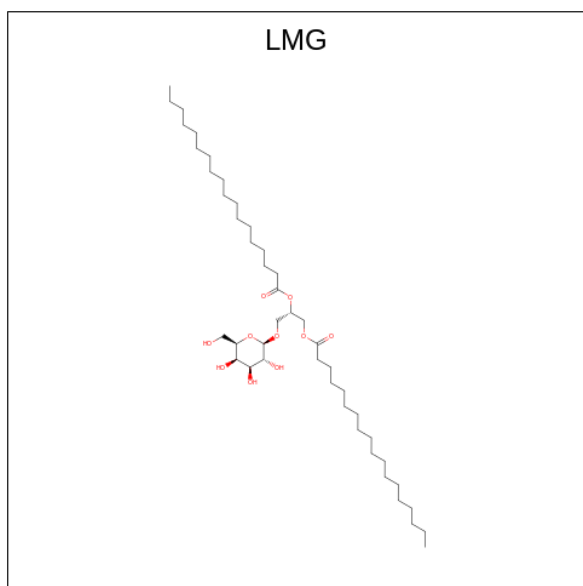
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



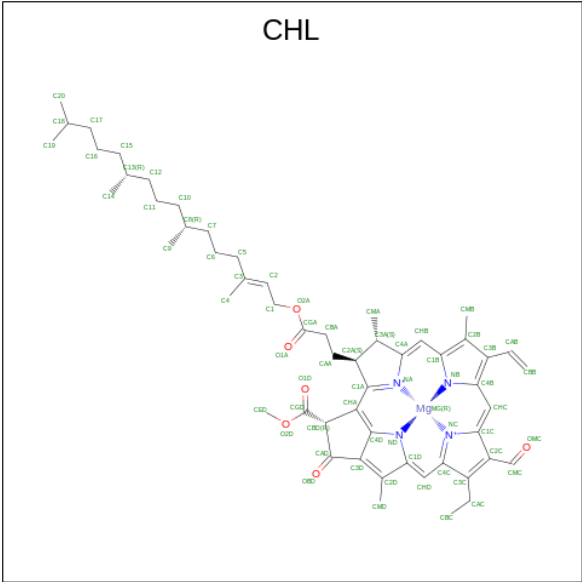
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			66	51	15	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



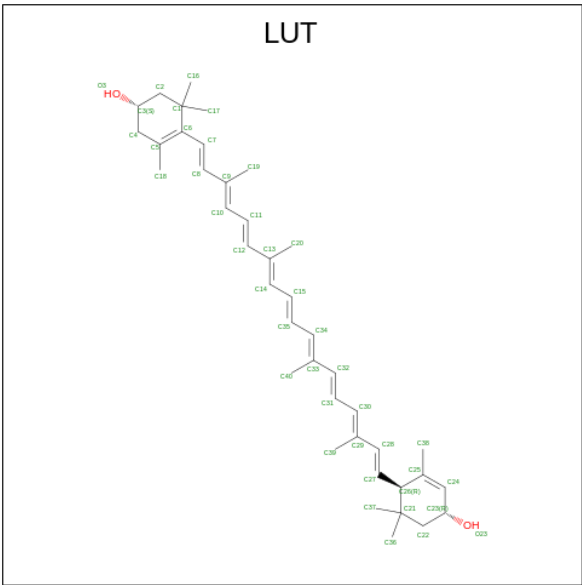
Mol	Chain	Residues	Atoms			AltConf
24	J	1	Total	C	O	0
			30	20	10	
24	2	1	Total	C	O	0
			13	7	6	
24	2	1	Total	C	O	0
			13	7	6	

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



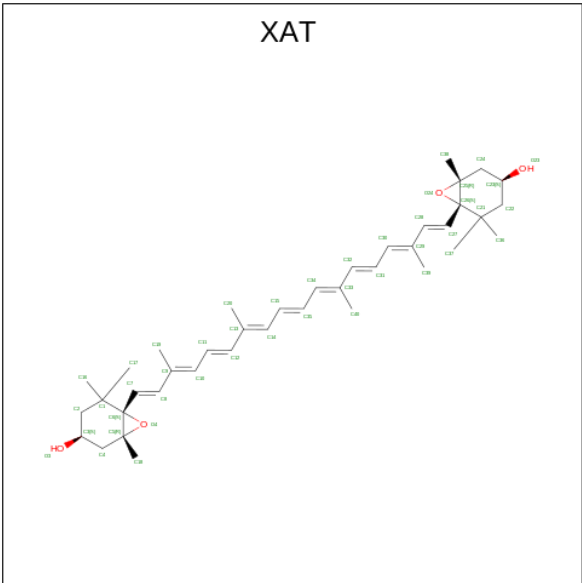
Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	2	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
26	2	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).




Mol	Chain	Residues	Atoms			AltConf
27	2	1	Total 44	C 40	O 4	0
27	6	1	Total 44	C 40	O 4	0
27	3	1	Total 44	C 40	O 4	0
27	5	1	Total 44	C 40	O 4	0

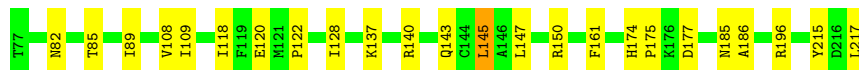
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  70% 25% 5%



- Molecule 4: Predicted protein PsaD

Chain D:  83% 16% .



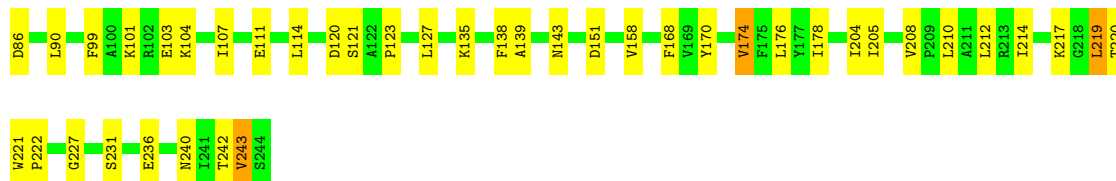
- Molecule 5: PsaE

Chain E:  71% 27% .



- Molecule 6: PSI-F

Chain F:  74% 24% .




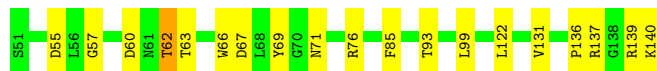
- Molecule 7: Predicted protein PsaG

Chain G:  68% 28% .



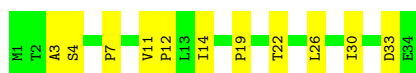
- Molecule 8: PsaH photosystem I reaction center subunit

Chain H:  79% 20% .

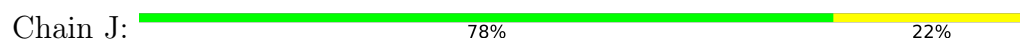


- Molecule 9: Photosystem I reaction center subunit VIII

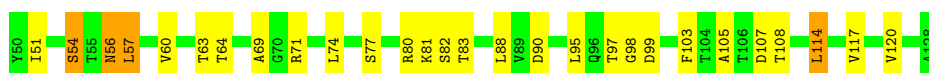
Chain I:  68% 32%



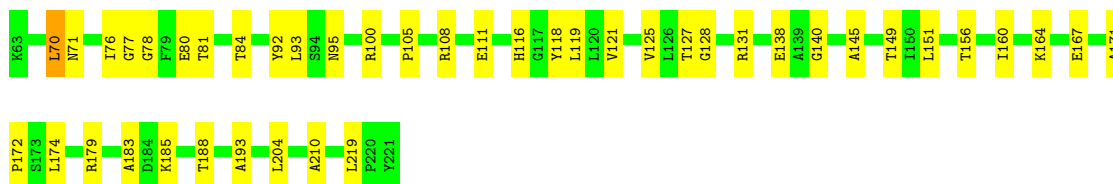
- Molecule 10: Photosystem I reaction center subunit IX



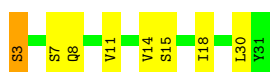
- Molecule 11: PsaK



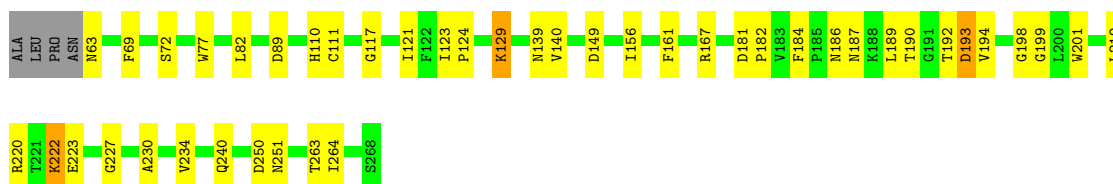
- Molecule 12: PSI subunit V



- Molecule 13: Photosystem I reaction center subunit XII

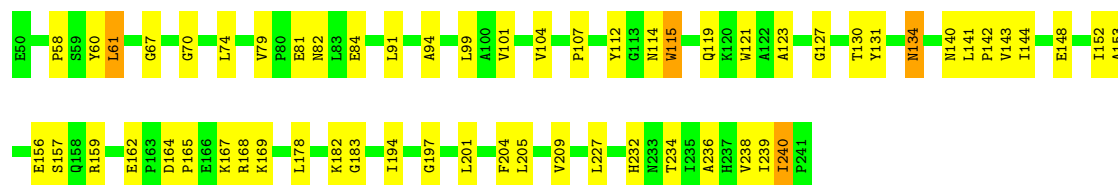


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



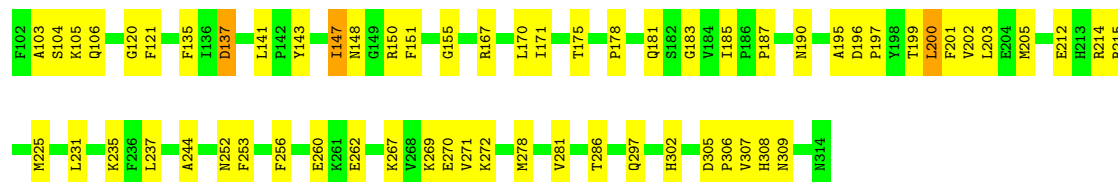
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic





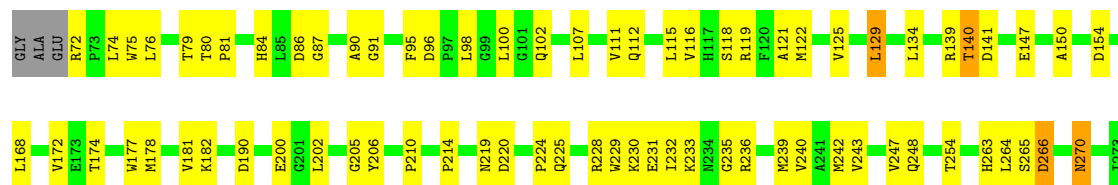
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 71% 28%



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

Chain 5: 63% 34%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/6032	0.40	0/8227
2	B	0.26	0/6063	0.41	0/8274
3	C	0.27	0/605	0.45	0/821
4	D	0.26	0/1132	0.45	0/1532
5	E	0.27	0/498	0.44	0/677
6	F	0.26	0/1251	0.43	0/1692
7	G	0.25	0/767	0.46	0/1046
8	H	0.25	0/710	0.42	0/961
9	I	0.27	0/273	0.45	0/373
10	J	0.26	0/334	0.39	0/457
11	K	0.26	0/556	0.51	0/752
12	L	0.26	0/1222	0.42	0/1671
13	M	0.24	0/215	0.37	0/290
14	2	0.26	0/1646	0.41	0/2252
15	6	0.26	0/1522	0.40	0/2081
16	3	0.27	0/1695	0.43	0/2302
17	5	0.26	0/1614	0.45	0/2201
All	All	0.26	0/26135	0.42	0/35609

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5837	0	5725	120	0
2	B	5849	0	5623	133	0
3	C	595	0	576	25	0
4	D	1104	0	1112	15	0
5	E	487	0	480	11	0
6	F	1226	0	1269	27	0
7	G	749	0	729	20	0
8	H	693	0	672	16	0
9	I	266	0	274	7	0
10	J	325	0	341	9	0
11	K	550	0	566	15	0
12	L	1189	0	1200	29	0
13	M	214	0	236	6	0
14	2	1595	0	1561	35	0
15	6	1473	0	1446	43	0
16	3	1644	0	1598	62	0
17	5	1566	0	1531	62	0
18	2	410	0	310	12	0
18	3	577	0	422	21	0
18	5	445	0	318	20	0
18	6	525	0	355	4	0
18	A	2421	0	2229	103	0
18	B	2093	0	1861	77	0
18	F	176	0	128	5	0
18	G	139	0	102	4	0
18	J	42	0	31	1	0
18	K	180	0	126	4	0
18	L	132	0	97	7	0
19	A	33	0	46	1	0
19	B	33	0	46	5	0
20	2	35	0	40	3	0
20	5	37	0	44	5	0
20	6	28	0	26	1	0
20	A	76	0	98	3	0
20	B	23	0	16	1	0
21	2	40	0	56	5	0
21	3	80	0	112	8	0
21	5	40	0	56	2	0
21	A	240	0	336	14	0
21	B	280	0	392	16	0
21	F	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	G	40	0	56	3	0
21	I	40	0	56	2	0
21	J	80	0	110	6	0
21	K	80	0	112	5	0
21	L	80	0	112	2	0
22	A	8	0	0	0	0
22	C	16	0	0	11	0
23	B	66	0	96	4	0
24	2	26	0	22	0	0
24	J	30	0	30	1	0
25	2	221	0	143	16	0
25	3	40	0	23	1	0
25	5	178	0	116	18	0
25	6	86	0	52	8	0
26	2	42	0	56	2	0
26	3	42	0	55	1	0
26	5	42	0	56	2	0
26	6	42	0	56	3	0
27	2	44	0	56	24	0
27	3	44	0	56	17	0
27	5	44	0	56	31	0
27	6	44	0	56	13	0
All	All	34822	0	33617	814	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 814 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)
14:2:121:ILE:HD11	27:2:620:XAT:C17	1.25	1.61
3:C:21:CYS:SG	22:C:101:SF4:FE2	1.20	1.34
3:C:14:CYS:SG	22:C:102:SF4:S4	2.29	1.29
14:2:121:ILE:CD1	27:2:620:XAT:H173	1.68	1.22
3:C:21:CYS:SG	22:C:101:SF4:S1	2.38	1.20

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/742 (100%)	700 (95%)	40 (5%)	0	100	100
2	B	731/733 (100%)	696 (95%)	35 (5%)	0	100	100
3	C	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
4	D	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
5	E	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
6	F	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
7	G	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
8	H	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	39/41 (95%)	39 (100%)	0	0	100	100
11	K	77/79 (98%)	66 (86%)	11 (14%)	0	100	100
12	L	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
13	M	27/29 (93%)	27 (100%)	0	0	100	100
14	2	204/210 (97%)	192 (94%)	12 (6%)	0	100	100
15	6	190/192 (99%)	170 (90%)	20 (10%)	0	100	100
16	3	211/213 (99%)	195 (92%)	16 (8%)	0	100	100
17	5	200/205 (98%)	173 (86%)	27 (14%)	0	100	100
All	All	3226/3267 (99%)	3013 (93%)	213 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/603 (100%)	580 (96%)	23 (4%)	28	58
2	B	595/595 (100%)	580 (98%)	15 (2%)	42	68
3	C	67/67 (100%)	63 (94%)	4 (6%)	16	45
4	D	115/115 (100%)	111 (96%)	4 (4%)	31	60
5	E	52/52 (100%)	49 (94%)	3 (6%)	17	46
6	F	128/129 (99%)	123 (96%)	5 (4%)	27	57
7	G	78/78 (100%)	68 (87%)	10 (13%)	3	16
8	H	72/73 (99%)	66 (92%)	6 (8%)	9	33
9	I	30/30 (100%)	29 (97%)	1 (3%)	33	61
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	56/57 (98%)	46 (82%)	10 (18%)	1	6
12	L	121/122 (99%)	114 (94%)	7 (6%)	17	46
13	M	24/24 (100%)	23 (96%)	1 (4%)	25	55
14	2	164/167 (98%)	153 (93%)	11 (7%)	13	41
15	6	148/148 (100%)	140 (95%)	8 (5%)	18	49
16	3	166/166 (100%)	158 (95%)	8 (5%)	21	52
17	5	162/164 (99%)	152 (94%)	10 (6%)	15	44
All	All	2616/2625 (100%)	2490 (95%)	126 (5%)	24	52

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	72	LEU
16	3	147	ILE
11	K	54	SER
16	3	137	ASP
17	5	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	130	GLN
14	2	261	HIS

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Mol	Chain	Res	Type
10	J	2	GLN
14	2	186	ASN
15	6	226	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

205 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	$\# Z > 2$
18	CLA	B	840	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	6 (7%)
18	CLA	B	832	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	9 (17%)
18	CLA	B	837	-	46,54,73	1.75	7 (15%)	53,90,113	1.57	8 (15%)
18	CLA	G	204	7	43,52,73	1.83	6 (13%)	49,88,113	1.56	7 (14%)
18	CLA	B	825	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
18	CLA	A	823	1	44,52,73	1.78	6 (13%)	51,88,113	1.66	6 (11%)
18	CLA	6	603	-	55,63,73	1.61	6 (10%)	64,101,113	1.49	8 (12%)
27	XAT	5	620	-	39,47,47	1.03	3 (7%)	54,74,74	2.76	21 (38%)
18	CLA	5	611	-	38,45,73	2.93	9 (23%)	41,76,113	1.45	8 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	810	-	46,54,73	1.74	6 (13%)	53,90,113	1.53	6 (11%)
19	PQN	A	844	-	34,34,34	0.39	0	42,45,45	0.47	0
18	CLA	A	804	-	65,73,73	1.46	7 (10%)	76,113,113	1.43	9 (11%)
18	CLA	A	819	-	45,53,73	1.77	7 (15%)	52,89,113	1.62	7 (13%)
18	CLA	2	612	-	41,49,73	1.87	6 (14%)	47,84,113	1.62	7 (14%)
18	CLA	6	602	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
18	CLA	6	613	15	45,53,73	1.79	6 (13%)	52,89,113	1.56	7 (13%)
18	CLA	A	820	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
18	CLA	3	602	16	60,68,73	1.54	5 (8%)	70,107,113	1.42	8 (11%)
25	CHL	5	606	-	41,49,74	2.24	13 (31%)	48,84,114	2.95	19 (39%)
21	BCR	B	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
21	BCR	I	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	4 (7%)
18	CLA	B	819	-	45,53,73	1.78	6 (13%)	52,89,113	1.61	8 (15%)
24	LMG	J	104	-	30,30,55	0.94	0	38,38,63	1.27	5 (13%)
18	CLA	B	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
20	LHG	A	847	18	26,26,48	0.83	1 (3%)	29,32,54	1.35	3 (10%)
18	CLA	A	839	-	65,73,73	1.45	5 (7%)	76,113,113	1.41	8 (10%)
24	LMG	2	618	-	13,13,55	1.07	0	18,18,63	1.54	4 (22%)
18	CLA	B	802	-	53,61,73	1.63	7 (13%)	61,98,113	1.42	8 (13%)
21	BCR	B	843	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	7 (12%)
18	CLA	A	830	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	6 (7%)
18	CLA	A	831	-	65,73,73	1.49	6 (9%)	76,113,113	1.44	7 (9%)
18	CLA	A	845	20	52,60,73	1.66	5 (9%)	60,97,113	1.52	8 (13%)
18	CLA	B	806	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
18	CLA	A	801	-	65,73,73	1.46	6 (9%)	76,113,113	1.33	7 (9%)
18	CLA	B	820	-	43,51,73	1.77	6 (13%)	49,86,113	1.64	6 (12%)
18	CLA	B	827	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	8 (15%)
18	CLA	2	609	14	55,63,73	1.60	6 (10%)	64,101,113	1.47	8 (12%)
18	CLA	3	614	-	39,48,73	1.89	6 (15%)	44,83,113	1.62	7 (15%)
25	CHL	6	607	15	40,49,74	2.53	16 (40%)	41,84,114	2.84	19 (46%)
18	CLA	3	615	-	37,44,73	1.95	6 (16%)	42,77,113	1.59	6 (14%)
18	CLA	A	828	-	46,54,73	1.73	7 (15%)	53,90,113	1.53	6 (11%)
18	CLA	3	609	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
18	CLA	5	602	-	45,53,73	1.82	6 (13%)	52,89,113	1.52	8 (15%)
18	CLA	5	610	-	55,63,73	1.61	6 (10%)	64,101,113	1.45	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	XAT	2	620	-	39,47,47	1.01	2 (5%)	54,74,74	3.14	22 (40%)
18	CLA	B	826	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	8 (10%)
18	CLA	6	610	15	42,51,73	1.83	6 (14%)	48,87,113	1.61	7 (14%)
18	CLA	5	613	17	45,53,73	1.78	6 (13%)	52,89,113	1.63	7 (13%)
18	CLA	A	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	7 (9%)
21	BCR	K	207	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	6 (10%)
18	CLA	B	814	-	43,52,73	1.81	6 (13%)	49,88,113	1.61	7 (14%)
18	CLA	A	825	-	55,63,73	1.62	6 (10%)	64,101,113	1.42	8 (12%)
18	CLA	A	821	-	44,52,73	1.81	6 (13%)	51,88,113	1.58	7 (13%)
20	LHG	5	622	-	36,36,48	0.72	1 (2%)	39,42,54	1.25	4 (10%)
18	CLA	A	805	-	55,63,73	1.56	7 (12%)	64,101,113	1.56	8 (12%)
21	BCR	A	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.26	9 (16%)
21	BCR	A	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	4 (7%)
18	CLA	A	824	-	51,59,73	1.68	6 (11%)	59,96,113	1.52	6 (10%)
18	CLA	A	836	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	7 (12%)
18	CLA	3	613	-	53,62,73	1.66	6 (11%)	61,100,113	1.46	8 (13%)
18	CLA	J	101	-	42,50,73	1.83	6 (14%)	48,85,113	1.57	6 (12%)
18	CLA	B	821	-	46,54,73	1.75	5 (10%)	53,90,113	1.54	7 (13%)
18	CLA	A	854	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	9 (11%)
18	CLA	5	614	-	43,51,73	1.81	6 (13%)	49,86,113	1.59	7 (14%)
18	CLA	2	613	14	45,53,73	1.79	5 (11%)	52,89,113	1.55	7 (13%)
18	CLA	A	811	-	45,53,73	1.77	6 (13%)	52,89,113	1.62	7 (13%)
22	SF4	C	101	3	0,12,12	-	-	-	-	-
18	CLA	B	811	-	54,62,73	1.68	7 (12%)	67,100,113	1.48	9 (13%)
21	BCR	A	850	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	6 (10%)
18	CLA	A	835	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	9 (11%)
18	CLA	2	610	14	45,53,73	1.72	7 (15%)	52,89,113	1.59	6 (11%)
25	CHL	5	607	-	43,51,74	2.44	15 (34%)	45,86,114	2.84	20 (44%)
18	CLA	B	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	9 (11%)
18	CLA	L	304	-	42,50,73	1.80	6 (14%)	48,85,113	1.67	7 (14%)
18	CLA	5	601	17	45,53,73	1.79	5 (11%)	52,89,113	1.56	7 (13%)
18	CLA	B	830	-	45,53,73	1.78	6 (13%)	52,89,113	1.62	7 (13%)
18	CLA	A	842	-	43,52,73	1.81	6 (13%)	49,88,113	1.56	7 (14%)
18	CLA	3	607	16	39,48,73	1.93	7 (17%)	48,83,113	1.67	9 (18%)
18	CLA	B	815	-	60,68,73	1.55	7 (11%)	70,107,113	1.39	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	611	20	41,50,73	1.85	6 (14%)	49,85,113	1.60	6 (12%)
18	CLA	A	827	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
21	BCR	3	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	6 (10%)
18	CLA	2	614	-	42,50,73	1.82	6 (14%)	48,85,113	1.59	7 (14%)
22	SF4	A	853	1,2	0,12,12	-	-	-	-	-
25	CHL	2	608	-	40,49,74	2.43	16 (40%)	41,84,114	2.87	18 (43%)
19	PQN	B	842	-	34,34,34	0.40	0	42,45,45	0.45	0
18	CLA	A	816	-	42,50,73	1.78	6 (14%)	48,85,113	1.69	7 (14%)
18	CLA	3	606	-	40,49,73	1.87	6 (15%)	45,84,113	1.61	6 (13%)
18	CLA	F	305	-	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
18	CLA	B	836	-	60,68,73	1.52	6 (10%)	70,107,113	1.44	7 (10%)
18	CLA	B	829	-	45,53,73	1.81	6 (13%)	52,89,113	1.64	7 (13%)
18	CLA	3	611	-	39,48,73	1.90	6 (15%)	44,83,113	1.68	8 (18%)
18	CLA	5	603	-	43,52,73	1.82	6 (13%)	49,88,113	1.57	6 (12%)
18	CLA	A	843	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	9 (11%)
25	CHL	6	601	15	44,53,74	2.38	16 (36%)	46,89,114	2.73	17 (36%)
18	CLA	A	802	-	45,53,73	1.75	6 (13%)	52,89,113	1.63	6 (11%)
21	BCR	B	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	5 (8%)
21	BCR	B	801	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	4 (7%)
18	CLA	A	832	-	41,49,73	1.81	6 (14%)	47,84,113	1.71	9 (19%)
18	CLA	B	841	20	65,73,73	1.49	6 (9%)	76,113,113	1.35	9 (11%)
18	CLA	A	818	-	65,73,73	1.47	7 (10%)	76,113,113	1.43	8 (10%)
18	CLA	K	201	11	46,54,73	1.84	7 (15%)	53,90,113	1.46	4 (7%)
21	BCR	2	621	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
25	CHL	3	608	-	39,48,74	2.42	15 (38%)	44,83,114	2.74	19 (43%)
20	LHG	B	851	18	22,22,48	0.83	0	25,28,54	1.20	1 (4%)
18	CLA	2	602	-	45,53,73	1.77	6 (13%)	52,89,113	1.59	7 (13%)
26	LUT	5	619	-	42,43,43	7.28	26 (61%)	51,60,60	3.85	19 (37%)
18	CLA	A	806	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
18	CLA	3	612	-	43,51,73	1.83	5 (11%)	49,86,113	1.56	6 (12%)
18	CLA	B	833	-	45,53,73	1.77	6 (13%)	52,89,113	1.65	9 (17%)
18	CLA	A	837	1	45,53,73	1.79	5 (11%)	52,89,113	1.59	9 (17%)
18	CLA	B	805	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	B	818	-	45,53,73	1.79	6 (13%)	52,89,113	1.55	7 (13%)
21	BCR	J	103	2	41,41,41	1.15	3 (7%)	56,56,56	1.30	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LHG	A	846	-	48,48,48	0.64	1 (2%)	51,54,54	1.27	6 (11%)
18	CLA	G	203	-	50,58,73	1.70	6 (12%)	58,95,113	1.51	8 (13%)
18	CLA	A	815	-	45,53,73	1.77	6 (13%)	52,89,113	1.57	8 (15%)
18	CLA	B	823	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	6 (11%)
25	CHL	2	601	14	45,53,74	2.33	15 (33%)	52,89,114	2.80	21 (40%)
18	CLA	5	604	-	43,51,73	1.78	5 (11%)	48,86,113	1.66	7 (14%)
18	CLA	A	814	-	65,73,73	1.45	7 (10%)	76,113,113	1.43	8 (10%)
18	CLA	A	838	-	51,59,73	1.68	5 (9%)	59,96,113	1.48	8 (13%)
21	BCR	B	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	7 (12%)
18	CLA	B	838	-	47,55,73	1.72	6 (12%)	54,91,113	1.57	8 (14%)
18	CLA	A	813	-	54,62,73	1.60	6 (11%)	62,99,113	1.48	6 (9%)
18	CLA	B	839	-	40,49,73	1.86	6 (15%)	45,84,113	1.61	6 (13%)
26	LUT	3	618	16	42,43,43	7.26	24 (57%)	51,60,60	3.85	22 (43%)
18	CLA	B	828	-	65,73,73	1.49	7 (10%)	76,113,113	1.31	8 (10%)
18	CLA	L	303	-	45,53,73	1.77	6 (13%)	52,89,113	1.58	7 (13%)
18	CLA	B	809	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
21	BCR	K	202	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
25	CHL	2	616	-	46,54,74	2.34	15 (32%)	49,90,114	2.78	18 (36%)
21	BCR	L	301	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
18	CLA	5	612	-	44,52,73	1.82	6 (13%)	51,88,113	1.59	7 (13%)
18	CLA	A	803	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
18	CLA	A	833	-	45,53,73	1.78	5 (11%)	52,89,113	1.63	7 (13%)
18	CLA	6	611	20	37,46,73	2.01	7 (18%)	46,81,113	1.70	9 (19%)
21	BCR	F	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	6 (10%)
18	CLA	A	829	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	9 (11%)
18	CLA	K	206	11	45,53,73	1.80	6 (13%)	52,89,113	1.54	7 (13%)
21	BCR	B	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
21	BCR	3	620	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	6 (10%)
21	BCR	A	856	-	41,41,41	1.15	2 (4%)	56,56,56	1.33	7 (12%)
18	CLA	3	610	-	41,49,73	1.82	7 (17%)	47,84,113	1.67	8 (17%)
18	CLA	B	831	-	49,57,73	1.69	6 (12%)	55,93,113	1.53	6 (10%)
18	CLA	F	303	-	45,53,73	1.78	5 (11%)	52,89,113	1.55	8 (15%)
22	SF4	C	102	3	0,12,12	-	-	-	-	-
18	CLA	B	834	-	45,53,73	1.80	6 (13%)	52,89,113	1.57	7 (13%)
25	CHL	2	607	-	43,51,74	2.37	15 (34%)	45,86,114	2.85	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	808	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	8 (15%)
18	CLA	6	606	-	39,48,73	1.87	6 (15%)	45,82,113	1.75	9 (20%)
25	CHL	5	608	-	51,59,74	2.16	16 (31%)	55,96,114	2.69	20 (36%)
18	CLA	6	612	-	45,53,73	1.79	6 (13%)	52,89,113	1.57	7 (13%)
18	CLA	B	816	-	53,62,73	1.64	6 (11%)	61,100,113	1.42	6 (9%)
18	CLA	6	604	-	49,57,73	1.70	6 (12%)	55,93,113	1.53	8 (14%)
20	LHG	2	622	14,18	34,34,48	0.72	0	37,40,54	1.27	4 (10%)
18	CLA	B	822	-	55,63,73	1.60	6 (10%)	64,101,113	1.49	8 (12%)
25	CHL	2	606	14	46,54,74	2.28	15 (32%)	49,90,114	2.87	18 (36%)
18	CLA	A	840	-	45,53,73	1.79	6 (13%)	52,89,113	1.55	6 (11%)
18	CLA	A	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
21	BCR	J	102	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	6 (10%)
18	CLA	5	609	17	43,51,73	1.79	6 (13%)	48,86,113	1.64	6 (12%)
18	CLA	K	203	-	45,53,73	1.79	6 (13%)	52,89,113	1.57	7 (13%)
18	CLA	A	841	-	65,73,73	1.48	7 (10%)	76,113,113	1.38	9 (11%)
18	CLA	6	608	-	43,52,73	1.83	6 (13%)	49,88,113	1.56	6 (12%)
24	LMG	2	617	-	13,13,55	1.01	0	18,18,63	1.55	4 (22%)
25	CHL	5	615	17	43,51,74	2.31	15 (34%)	45,86,114	2.89	20 (44%)
18	CLA	K	204	-	44,52,73	1.84	6 (13%)	55,88,113	1.65	8 (14%)
18	CLA	A	817	-	39,48,73	1.86	6 (15%)	44,83,113	1.68	8 (18%)
18	CLA	F	304	-	41,49,73	1.83	6 (14%)	47,84,113	1.67	7 (14%)
18	CLA	B	824	-	45,53,73	1.79	6 (13%)	52,89,113	1.59	8 (15%)
18	CLA	2	603	-	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
18	CLA	A	809	1	45,53,73	1.73	6 (13%)	52,89,113	1.65	8 (15%)
21	BCR	G	205	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	6 (10%)
21	BCR	A	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	6 (10%)
18	CLA	A	822	-	43,51,73	1.87	7 (16%)	54,87,113	1.65	8 (14%)
18	CLA	6	609	-	40,48,73	1.91	7 (17%)	50,83,113	1.70	10 (20%)
18	CLA	B	817	-	45,53,73	1.77	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	3	603	-	55,63,73	1.63	7 (12%)	64,101,113	1.43	6 (9%)
18	CLA	G	201	-	45,53,73	1.80	5 (11%)	52,89,113	1.56	7 (13%)
18	CLA	A	807	1	43,52,73	1.80	6 (13%)	49,88,113	1.57	6 (12%)
18	CLA	3	617	-	39,48,73	1.88	6 (15%)	44,83,113	1.69	8 (18%)
27	XAT	3	619	-	39,47,47	0.98	2 (5%)	54,74,74	2.74	20 (37%)
18	CLA	B	813	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	6	614	-	37,46,73	2.00	6 (16%)	46,81,113	1.69	11 (23%)
18	CLA	B	835	-	45,53,73	1.79	6 (13%)	52,89,113	1.57	7 (13%)
21	BCR	L	305	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	9 (16%)
27	XAT	6	619	-	39,47,47	0.98	2 (5%)	54,74,74	3.10	21 (38%)
18	CLA	2	604	-	50,58,73	1.65	6 (12%)	58,95,113	1.64	8 (13%)
18	CLA	B	804	-	45,53,73	1.76	6 (13%)	52,89,113	1.64	7 (13%)
18	CLA	B	812	-	45,53,73	1.77	5 (11%)	52,89,113	1.63	7 (13%)
18	CLA	L	302	-	45,53,73	1.78	6 (13%)	52,89,113	1.61	7 (13%)
21	BCR	B	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
18	CLA	A	810	1	45,53,73	1.79	6 (13%)	52,89,113	1.59	7 (13%)
18	CLA	3	604	-	41,50,73	1.92	7 (17%)	51,86,113	1.63	9 (17%)
18	CLA	6	616	15	43,51,73	1.91	6 (13%)	54,87,113	1.66	8 (14%)
21	BCR	A	852	-	41,41,41	1.16	2 (4%)	56,56,56	1.18	6 (10%)
23	DGD	B	850	-	67,67,67	0.86	2 (2%)	81,81,81	1.44	11 (13%)
18	CLA	B	808	-	50,58,73	1.67	7 (14%)	58,95,113	1.55	9 (15%)
18	CLA	F	301	-	45,53,73	1.77	6 (13%)	52,89,113	1.56	6 (11%)
20	LHG	6	620	18,15	27,27,48	0.80	1 (3%)	30,33,54	1.25	2 (6%)
26	LUT	6	617	-	42,43,43	7.20	25 (59%)	51,60,60	3.87	19 (37%)
21	BCR	5	621	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	5 (8%)
26	LUT	2	619	-	42,43,43	7.18	25 (59%)	51,60,60	4.12	21 (41%)
18	CLA	A	812	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)

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
18	CLA	B	840	-	1/1/15/20	12/37/115/115	-
18	CLA	B	832	-	1/1/11/20	6/13/91/115	-
18	CLA	B	837	-	1/1/11/20	4/15/93/115	-
18	CLA	G	204	7	1/1/11/20	4/11/89/115	-
18	CLA	B	825	-	1/1/15/20	11/37/115/115	-
18	CLA	A	823	1	1/1/11/20	5/11/89/115	-
18	CLA	6	603	-	1/1/13/20	13/25/103/115	-
27	XAT	5	620	-	-	3/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	5	611	-	1/1/7/20	5/10/70/115	-
18	CLA	B	810	-	1/1/11/20	9/15/93/115	-
19	PQN	A	844	-	-	8/23/43/43	0/2/2/2
18	CLA	A	804	-	1/1/15/20	9/37/115/115	-
18	CLA	A	819	-	1/1/11/20	6/13/91/115	-
18	CLA	2	612	-	1/1/10/20	0/8/86/115	-
18	CLA	6	602	-	1/1/11/20	7/13/91/115	-
18	CLA	6	613	15	1/1/11/20	7/13/91/115	-
18	CLA	A	820	-	1/1/11/20	4/13/91/115	-
18	CLA	3	602	16	1/1/14/20	9/31/109/115	-
25	CHL	5	606	-	3/3/15/26	2/10/106/137	-
21	BCR	B	846	-	-	17/29/63/63	0/2/2/2
21	BCR	I	101	-	-	5/29/63/63	0/2/2/2
18	CLA	B	819	-	1/1/11/20	3/13/91/115	-
24	LMG	J	104	-	-	12/25/45/70	0/1/1/1
18	CLA	B	803	-	1/1/15/20	10/37/115/115	-
20	LHG	A	847	18	-	19/31/31/53	-
18	CLA	A	839	-	1/1/15/20	15/37/115/115	-
24	LMG	2	618	-	-	2/4/24/70	0/1/1/1
18	CLA	B	802	-	1/1/12/20	3/23/101/115	-
21	BCR	B	843	-	-	9/29/63/63	0/2/2/2
18	CLA	A	830	-	1/1/15/20	5/37/115/115	-
18	CLA	A	831	-	1/1/15/20	14/37/115/115	-
18	CLA	A	845	20	1/1/12/20	10/22/100/115	-
18	CLA	B	806	2	1/1/15/20	19/37/115/115	-
18	CLA	A	801	-	1/1/15/20	7/37/115/115	-
18	CLA	B	820	-	1/1/10/20	1/11/89/115	-
18	CLA	B	827	-	1/1/11/20	5/13/91/115	-
18	CLA	2	609	14	1/1/13/20	11/25/103/115	-
18	CLA	3	614	-	1/1/10/20	1/6/84/115	-
25	CHL	6	607	15	3/3/15/26	2/8/106/137	-
18	CLA	3	615	-	1/1/8/20	0/0/74/115	-
18	CLA	A	828	-	1/1/11/20	7/15/93/115	-
18	CLA	3	609	-	1/1/11/20	1/13/91/115	-
18	CLA	5	602	-	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	5	610	-	1/1/13/20	3/25/103/115	-
27	XAT	2	620	-	-	3/31/93/93	0/4/4/4
18	CLA	B	826	-	1/1/15/20	12/37/115/115	-
18	CLA	6	610	15	1/1/11/20	1/9/87/115	-
18	CLA	5	613	17	1/1/11/20	5/13/91/115	-
18	CLA	A	826	-	1/1/15/20	12/37/115/115	-
21	BCR	K	207	-	-	11/29/63/63	0/2/2/2
18	CLA	B	814	-	1/1/11/20	1/11/89/115	-
18	CLA	A	825	-	1/1/13/20	9/25/103/115	-
18	CLA	A	821	-	1/1/11/20	6/11/89/115	-
20	LHG	5	622	-	-	19/41/41/53	-
18	CLA	A	805	-	1/1/13/20	10/25/103/115	-
21	BCR	A	851	-	-	9/29/63/63	0/2/2/2
21	BCR	A	848	-	-	6/29/63/63	0/2/2/2
18	CLA	A	824	-	1/1/12/20	9/21/99/115	-
18	CLA	A	836	-	1/1/12/20	0/19/97/115	-
18	CLA	3	613	-	1/1/13/20	7/23/101/115	-
18	CLA	J	101	-	1/1/10/20	5/10/88/115	-
18	CLA	B	821	-	1/1/11/20	7/15/93/115	-
18	CLA	A	854	-	1/1/15/20	15/37/115/115	-
18	CLA	5	614	-	1/1/10/20	7/11/89/115	-
18	CLA	2	613	14	1/1/11/20	6/13/91/115	-
18	CLA	A	811	-	1/1/11/20	2/13/91/115	-
22	SF4	C	101	3	-	-	0/6/5/5
18	CLA	B	811	-	1/1/13/20	9/25/101/115	-
21	BCR	A	850	-	-	3/29/63/63	0/2/2/2
18	CLA	A	835	-	1/1/15/20	7/37/115/115	-
18	CLA	2	610	14	1/1/11/20	4/13/91/115	-
25	CHL	5	607	-	3/3/15/26	4/12/110/137	-
18	CLA	B	807	-	1/1/15/20	12/37/115/115	-
18	CLA	L	304	-	1/1/10/20	2/10/88/115	-
18	CLA	5	601	17	1/1/11/20	2/13/91/115	-
18	CLA	B	830	-	1/1/11/20	1/13/91/115	-
18	CLA	A	842	-	1/1/11/20	3/11/89/115	-
18	CLA	3	607	16	1/1/10/20	1/8/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	815	-	1/1/14/20	11/31/109/115	-
18	CLA	2	611	20	1/1/10/20	0/7/85/115	-
18	CLA	A	827	-	1/1/15/20	12/37/115/115	-
21	BCR	3	622	-	-	10/29/63/63	0/2/2/2
18	CLA	2	614	-	1/1/10/20	2/10/88/115	-
22	SF4	A	853	1,2	-	-	0/6/5/5
25	CHL	2	608	-	3/3/15/26	1/8/106/137	-
19	PQN	B	842	-	-	9/23/43/43	0/2/2/2
18	CLA	A	816	-	1/1/10/20	4/10/88/115	-
18	CLA	3	606	-	1/1/10/20	0/8/86/115	-
18	CLA	F	305	-	1/1/11/20	5/13/91/115	-
18	CLA	B	836	-	1/1/14/20	7/31/109/115	-
18	CLA	B	829	-	1/1/11/20	0/13/91/115	-
18	CLA	3	611	-	1/1/10/20	2/6/84/115	-
18	CLA	5	603	-	1/1/11/20	4/11/89/115	-
18	CLA	A	843	-	1/1/15/20	10/37/115/115	-
25	CHL	6	601	15	3/3/16/26	3/13/111/137	-
18	CLA	A	802	-	1/1/11/20	7/13/91/115	-
21	BCR	B	845	-	-	19/29/63/63	0/2/2/2
21	BCR	B	801	-	-	7/29/63/63	0/2/2/2
18	CLA	A	832	-	1/1/10/20	6/8/86/115	-
18	CLA	B	841	20	1/1/15/20	14/37/115/115	-
18	CLA	A	818	-	1/1/15/20	18/37/115/115	-
18	CLA	K	201	11	1/1/11/20	7/15/93/115	-
25	CHL	3	608	-	3/3/15/26	2/6/104/137	-
21	BCR	2	621	-	-	8/29/63/63	0/2/2/2
20	LHG	B	851	18	-	10/26/26/53	-
18	CLA	2	602	-	1/1/11/20	6/13/91/115	-
26	LUT	5	619	-	-	8/29/67/67	0/2/2/2
18	CLA	A	806	-	1/1/15/20	14/37/115/115	-
18	CLA	3	612	-	1/1/10/20	2/11/89/115	-
18	CLA	B	833	-	1/1/11/20	8/13/91/115	-
18	CLA	A	837	1	1/1/11/20	2/13/91/115	-
18	CLA	B	805	-	1/1/15/20	11/37/115/115	-
18	CLA	B	818	-	1/1/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	J	103	2	-	23/29/63/63	0/2/2/2
20	LHG	A	846	-	-	24/53/53/53	-
18	CLA	G	203	-	1/1/12/20	7/19/97/115	-
18	CLA	A	815	-	1/1/11/20	5/13/91/115	-
18	CLA	B	823	-	1/1/11/20	5/13/91/115	-
25	CHL	2	601	14	3/3/16/26	8/15/111/137	-
18	CLA	5	604	-	1/1/10/20	5/9/88/115	-
18	CLA	A	814	-	1/1/15/20	16/37/115/115	-
18	CLA	A	838	-	1/1/12/20	3/21/99/115	-
21	BCR	B	848	-	-	13/29/63/63	0/2/2/2
18	CLA	B	838	-	1/1/11/20	2/16/94/115	-
18	CLA	A	813	-	1/1/12/20	3/24/102/115	-
18	CLA	B	839	-	1/1/10/20	0/8/86/115	-
26	LUT	3	618	16	-	7/29/67/67	0/2/2/2
18	CLA	B	828	-	1/1/15/20	10/37/115/115	-
18	CLA	L	303	-	1/1/11/20	0/13/91/115	-
18	CLA	B	809	-	1/1/15/20	9/37/115/115	-
25	CHL	2	616	-	3/3/16/26	6/15/113/137	-
21	BCR	K	202	-	-	8/29/63/63	0/2/2/2
21	BCR	L	301	-	-	10/29/63/63	0/2/2/2
18	CLA	5	612	-	1/1/11/20	5/11/89/115	-
18	CLA	A	803	-	1/1/15/20	7/37/115/115	-
18	CLA	A	833	-	1/1/11/20	7/13/91/115	-
18	CLA	6	611	20	1/1/10/20	1/4/80/115	-
21	BCR	F	302	-	-	14/29/63/63	0/2/2/2
18	CLA	A	829	-	1/1/15/20	20/37/115/115	-
18	CLA	K	206	11	1/1/11/20	5/13/91/115	-
21	BCR	B	847	-	-	2/29/63/63	0/2/2/2
21	BCR	3	620	-	-	9/29/63/63	0/2/2/2
21	BCR	A	856	-	-	7/29/63/63	0/2/2/2
18	CLA	3	610	-	1/1/10/20	3/8/86/115	-
18	CLA	B	831	-	1/1/11/20	7/18/96/115	-
18	CLA	F	303	-	1/1/11/20	4/13/91/115	-
22	SF4	C	102	3	-	-	0/6/5/5
18	CLA	B	834	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	2	607	-	3/3/15/26	3/12/110/137	-
18	CLA	A	808	-	1/1/11/20	3/13/91/115	-
18	CLA	6	606	-	1/1/9/20	3/8/82/115	-
25	CHL	5	608	-	3/3/17/26	8/21/119/137	-
18	CLA	6	612	-	1/1/11/20	2/13/91/115	-
18	CLA	B	816	-	1/1/13/20	3/23/101/115	-
18	CLA	6	604	-	1/1/11/20	8/18/96/115	-
20	LHG	2	622	14,18	-	23/39/39/53	-
18	CLA	B	822	-	1/1/13/20	8/25/103/115	-
25	CHL	2	606	14	3/3/16/26	5/15/113/137	-
18	CLA	A	840	-	1/1/11/20	4/13/91/115	-
18	CLA	A	834	-	1/1/15/20	12/37/115/115	-
21	BCR	J	102	-	-	9/29/63/63	0/2/2/2
18	CLA	5	609	17	1/1/10/20	6/9/87/115	-
18	CLA	K	203	-	1/1/11/20	4/13/91/115	-
18	CLA	A	841	-	1/1/15/20	13/37/115/115	-
18	CLA	6	608	-	1/1/11/20	3/11/89/115	-
25	CHL	5	615	17	3/3/15/26	3/12/110/137	-
24	LMG	2	617	-	-	4/4/24/70	0/1/1/1
18	CLA	K	204	-	1/1/11/20	5/13/89/115	-
18	CLA	A	817	-	1/1/10/20	0/6/84/115	-
18	CLA	F	304	-	1/1/10/20	2/8/86/115	-
18	CLA	B	824	-	1/1/11/20	2/13/91/115	-
18	CLA	2	603	-	1/1/11/20	5/13/91/115	-
18	CLA	A	809	1	1/1/11/20	5/13/91/115	-
21	BCR	G	205	-	-	5/29/63/63	0/2/2/2
21	BCR	A	849	-	-	8/29/63/63	0/2/2/2
18	CLA	A	822	-	1/1/11/20	2/11/87/115	-
18	CLA	6	609	-	1/1/10/20	3/8/84/115	-
18	CLA	B	817	-	1/1/11/20	2/13/91/115	-
18	CLA	3	603	-	1/1/13/20	6/25/103/115	-
18	CLA	G	201	-	1/1/11/20	5/13/91/115	-
18	CLA	A	807	1	1/1/11/20	4/11/89/115	-
18	CLA	3	617	-	1/1/10/20	2/6/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	XAT	3	619	-	-	0/31/93/93	0/4/4/4
18	CLA	B	813	-	1/1/15/20	16/37/115/115	-
18	CLA	6	614	-	1/1/10/20	2/4/80/115	-
18	CLA	B	835	-	1/1/11/20	8/13/91/115	-
21	BCR	L	305	-	-	10/29/63/63	0/2/2/2
27	XAT	6	619	-	-	1/31/93/93	0/4/4/4
18	CLA	2	604	-	1/1/12/20	7/19/97/115	-
18	CLA	B	804	-	1/1/11/20	5/13/91/115	-
18	CLA	B	812	-	1/1/11/20	3/13/91/115	-
18	CLA	L	302	-	1/1/11/20	2/13/91/115	-
21	BCR	B	844	-	-	6/29/63/63	0/2/2/2
18	CLA	A	810	1	1/1/11/20	4/13/91/115	-
18	CLA	3	604	-	1/1/11/20	0/9/85/115	-
18	CLA	6	616	15	1/1/11/20	4/11/87/115	-
21	BCR	A	852	-	-	11/29/63/63	0/2/2/2
23	DGD	B	850	-	-	29/55/95/95	0/2/2/2
18	CLA	B	808	-	1/1/12/20	2/19/97/115	-
18	CLA	F	301	-	1/1/11/20	3/13/91/115	-
20	LHG	6	620	18,15	-	17/32/32/53	-
26	LUT	6	617	-	-	12/29/67/67	0/2/2/2
21	BCR	5	621	-	-	9/29/63/63	0/2/2/2
26	LUT	2	619	-	-	7/29/67/67	0/2/2/2
18	CLA	A	812	-	1/1/15/20	11/37/115/115	-

The worst 5 of 1235 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	619	LUT	C34-C33	20.14	1.62	1.35
26	3	618	LUT	C34-C33	19.98	1.62	1.35
26	2	619	LUT	C34-C33	19.80	1.62	1.35
26	6	617	LUT	C34-C33	19.76	1.62	1.35
26	5	619	LUT	C14-C13	16.75	1.58	1.35

The worst 5 of 1658 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	619	LUT	C18-C5-C6	-14.02	108.78	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	619	LUT	C18-C5-C6	-12.36	110.65	124.53
26	6	617	LUT	C18-C5-C6	-12.10	110.94	124.53
26	2	619	LUT	C15-C14-C13	-11.96	110.24	127.31
26	3	618	LUT	C18-C5-C6	-11.81	111.26	124.53

5 of 180 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	801	CLA	ND
18	A	802	CLA	ND
18	A	803	CLA	ND
18	A	804	CLA	ND
18	A	805	CLA	ND

5 of 1358 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	801	CLA	CBD-CGD-O2D-CED
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

171 monomers are involved in 423 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	840	CLA	4	0
18	B	832	CLA	1	0
18	B	837	CLA	2	0
18	G	204	CLA	2	0
18	B	825	CLA	3	0
18	A	823	CLA	1	0
18	6	603	CLA	2	0
27	5	620	XAT	31	0
18	5	611	CLA	2	0
19	A	844	PQN	1	0
18	A	819	CLA	3	0
18	6	613	CLA	1	0
18	A	820	CLA	5	0
18	3	602	CLA	1	0
21	B	846	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	I	101	BCR	2	0
18	B	819	CLA	3	0
24	J	104	LMG	1	0
18	B	803	CLA	2	0
20	A	847	LHG	2	0
18	A	839	CLA	3	0
18	B	802	CLA	3	0
21	B	843	BCR	4	0
18	A	830	CLA	2	0
18	A	831	CLA	2	0
18	A	845	CLA	1	0
18	B	806	CLA	2	0
18	A	801	CLA	1	0
18	B	827	CLA	3	0
18	3	614	CLA	2	0
25	6	607	CHL	6	0
18	A	828	CLA	1	0
18	3	609	CLA	7	0
18	5	602	CLA	5	0
18	5	610	CLA	3	0
27	2	620	XAT	24	0
18	B	826	CLA	3	0
18	5	613	CLA	3	0
18	A	826	CLA	5	0
21	K	207	BCR	2	0
18	B	814	CLA	1	0
18	A	821	CLA	2	0
20	5	622	LHG	5	0
18	A	805	CLA	3	0
21	A	851	BCR	1	0
21	A	848	BCR	3	0
18	A	824	CLA	2	0
18	3	613	CLA	3	0
18	J	101	CLA	1	0
18	B	821	CLA	2	0
18	A	854	CLA	6	0
18	5	614	CLA	2	0
18	2	613	CLA	1	0
18	A	811	CLA	3	0
22	C	101	SF4	7	0
18	B	811	CLA	1	0
21	A	850	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	835	CLA	4	0
18	2	610	CLA	4	0
25	5	607	CHL	14	0
18	B	807	CLA	1	0
18	L	304	CLA	1	0
18	5	601	CLA	2	0
18	B	830	CLA	1	0
18	A	842	CLA	2	0
18	B	815	CLA	3	0
18	A	827	CLA	5	0
21	3	622	BCR	3	0
18	2	614	CLA	2	0
19	B	842	PQN	5	0
18	A	816	CLA	1	0
18	3	606	CLA	3	0
18	F	305	CLA	1	0
18	B	836	CLA	1	0
18	B	829	CLA	1	0
18	3	611	CLA	3	0
18	A	843	CLA	6	0
25	6	601	CHL	2	0
18	A	802	CLA	2	0
21	B	845	BCR	2	0
21	B	801	BCR	2	0
18	A	832	CLA	2	0
18	B	841	CLA	2	0
18	A	818	CLA	1	0
18	K	201	CLA	1	0
21	2	621	BCR	5	0
25	3	608	CHL	1	0
20	B	851	LHG	1	0
18	2	602	CLA	3	0
26	5	619	LUT	2	0
18	A	806	CLA	5	0
18	3	612	CLA	1	0
18	B	833	CLA	5	0
18	A	837	CLA	2	0
18	B	805	CLA	2	0
18	B	818	CLA	3	0
21	J	103	BCR	5	0
20	A	846	LHG	1	0
18	B	823	CLA	3	0

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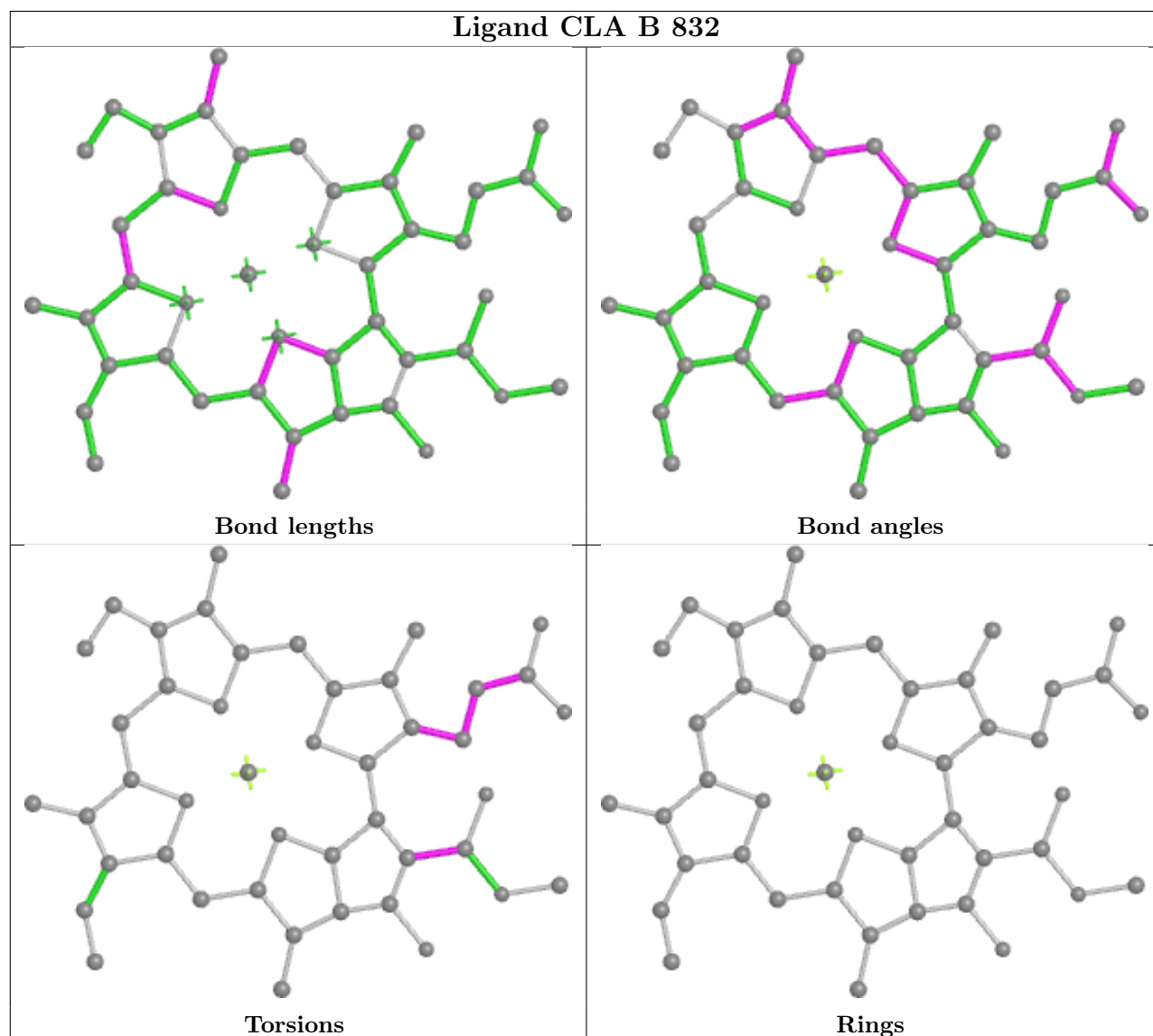
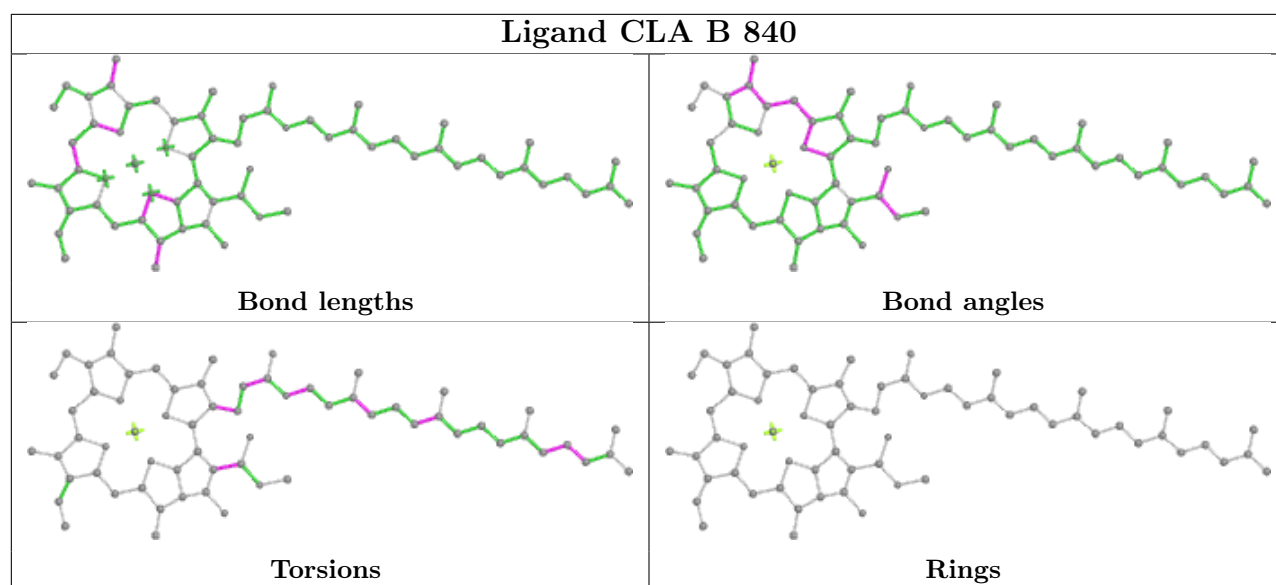
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18	5	604	CLA	1	0
18	A	814	CLA	6	0
18	A	838	CLA	2	0
21	B	848	BCR	4	0
18	B	838	CLA	2	0
18	A	813	CLA	1	0
18	B	839	CLA	3	0
26	3	618	LUT	1	0
18	B	828	CLA	5	0
18	L	303	CLA	2	0
18	B	809	CLA	4	0
21	K	202	BCR	3	0
25	2	616	CHL	1	0
21	L	301	BCR	1	0
18	5	612	CLA	1	0
18	A	803	CLA	2	0
18	A	833	CLA	3	0
21	F	302	BCR	4	0
18	A	829	CLA	9	0
21	B	847	BCR	2	0
21	3	620	BCR	5	0
21	A	856	BCR	4	0
18	B	831	CLA	2	0
22	C	102	SF4	4	0
18	B	834	CLA	1	0
25	2	607	CHL	5	0
18	A	808	CLA	2	0
25	5	608	CHL	4	0
18	B	816	CLA	2	0
20	2	622	LHG	3	0
18	B	822	CLA	1	0
25	2	606	CHL	9	0
18	A	840	CLA	1	0
18	A	834	CLA	2	0
21	J	102	BCR	1	0
18	5	609	CLA	1	0
18	K	203	CLA	1	0
18	A	841	CLA	2	0
18	K	204	CLA	2	0
18	A	817	CLA	1	0
18	F	304	CLA	2	0

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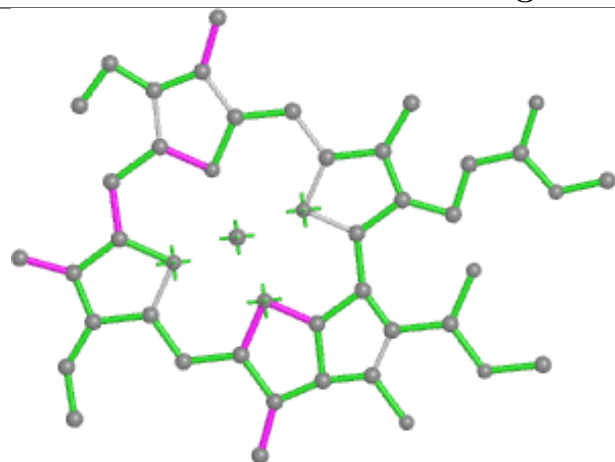
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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18	A	809	CLA	6	0
21	G	205	BCR	3	0
21	A	849	BCR	2	0
18	A	822	CLA	1	0
18	6	609	CLA	2	0
18	B	817	CLA	4	0
18	3	603	CLA	2	0
18	G	201	CLA	2	0
18	3	617	CLA	1	0
27	3	619	XAT	17	0
18	B	813	CLA	8	0
18	B	835	CLA	3	0
21	L	305	BCR	1	0
27	6	619	XAT	13	0
18	2	604	CLA	3	0
18	B	812	CLA	3	0
18	L	302	CLA	4	0
21	B	844	BCR	1	0
18	A	810	CLA	2	0
18	3	604	CLA	1	0
21	A	852	BCR	4	0
23	B	850	DGD	4	0
18	B	808	CLA	1	0
18	F	301	CLA	2	0
20	6	620	LHG	1	0
26	6	617	LUT	3	0
21	5	621	BCR	2	0
26	2	619	LUT	2	0
18	A	812	CLA	7	0

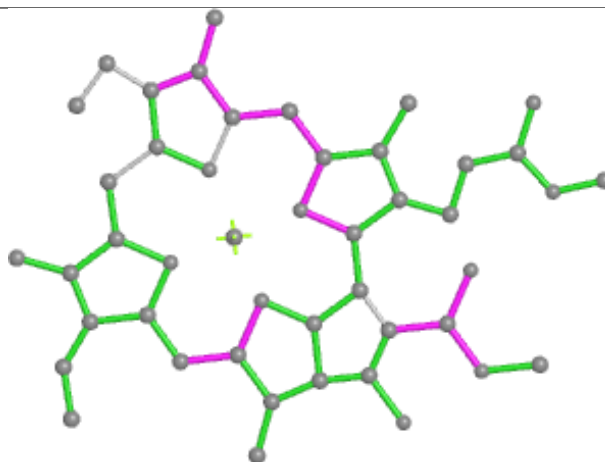
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



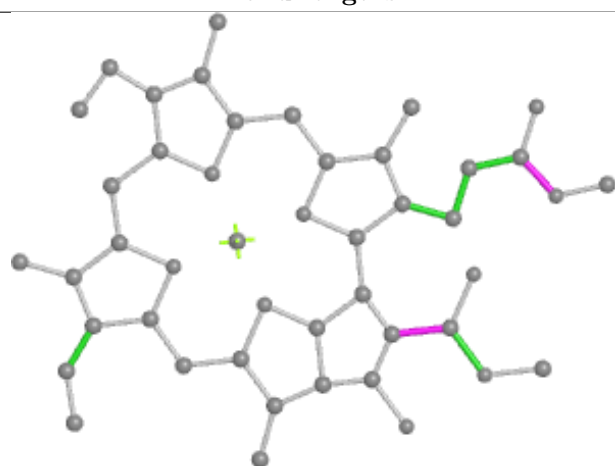
Ligand CLA B 837



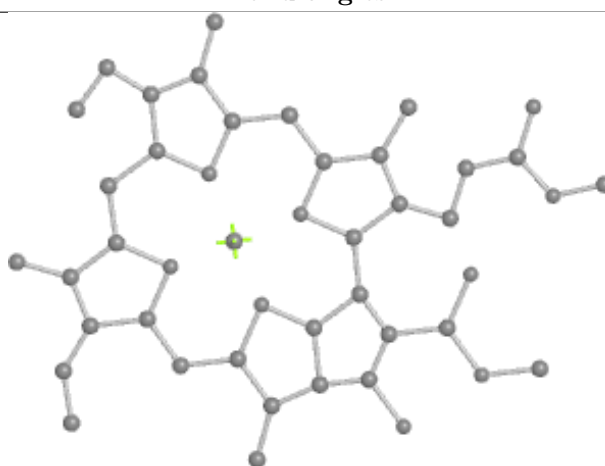
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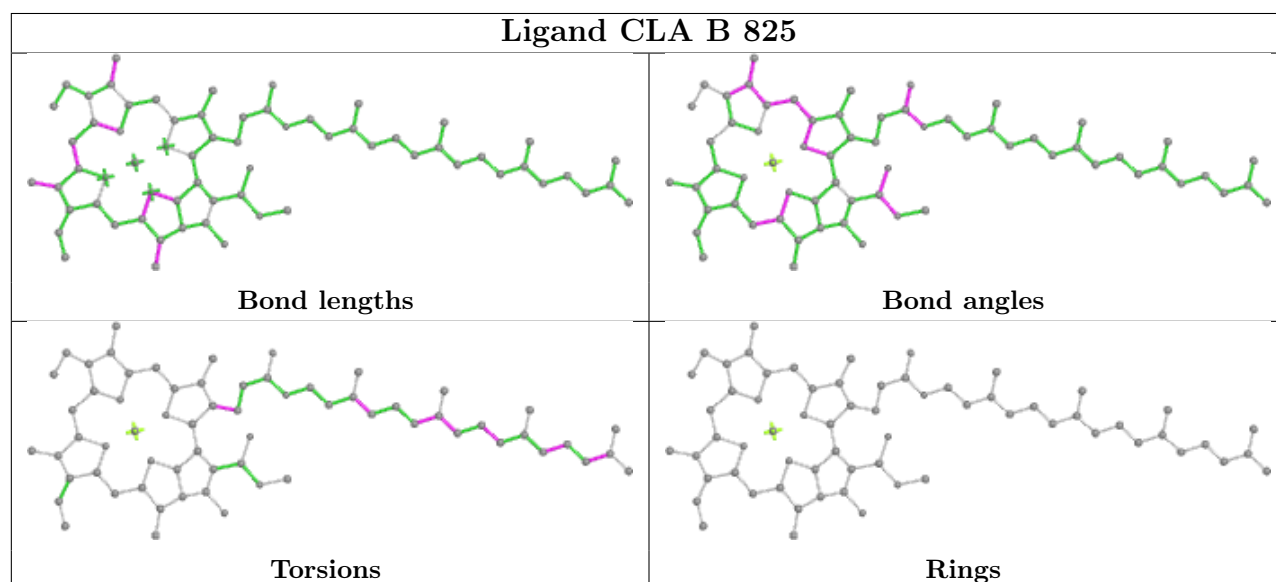
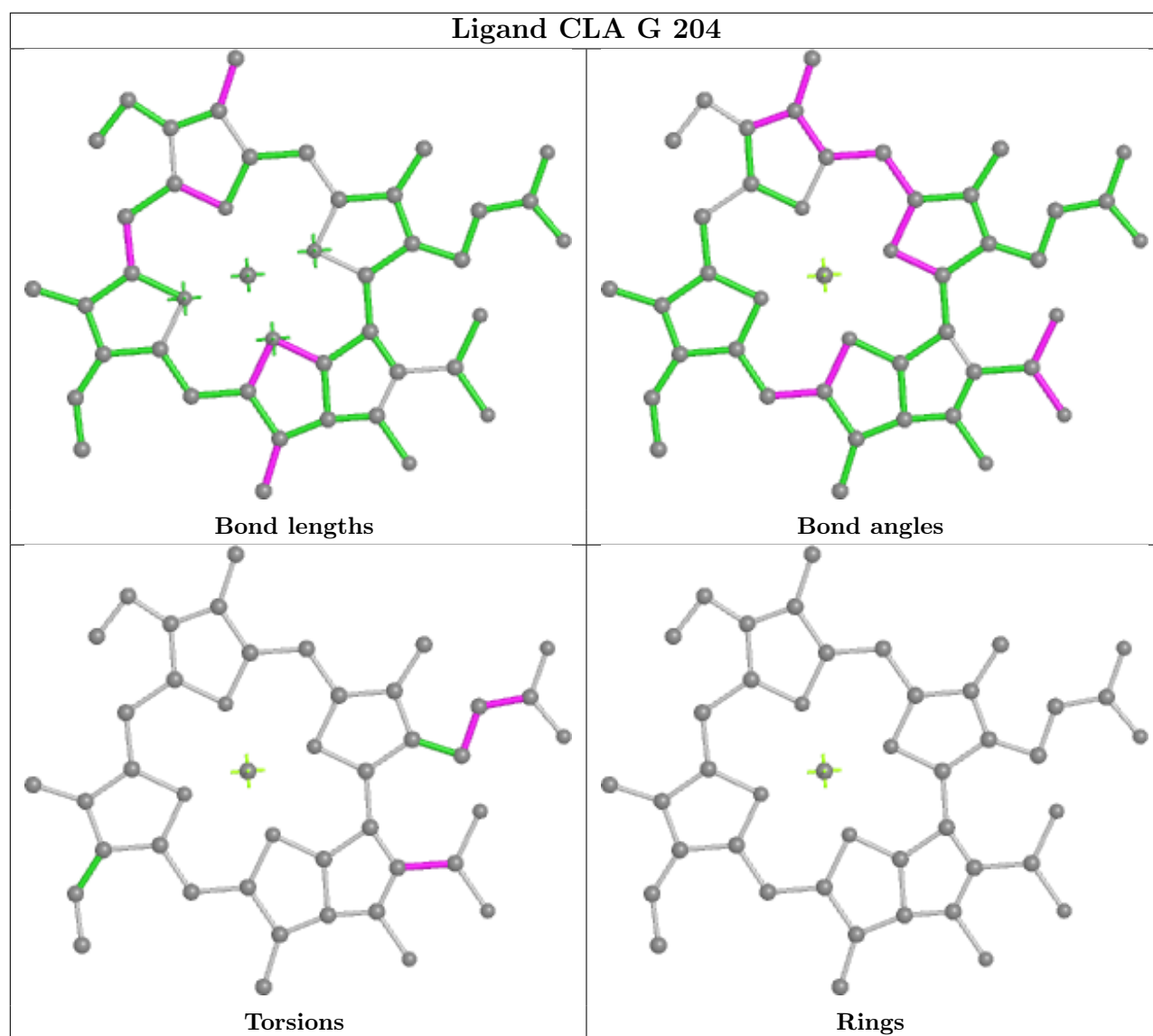
Bond angles



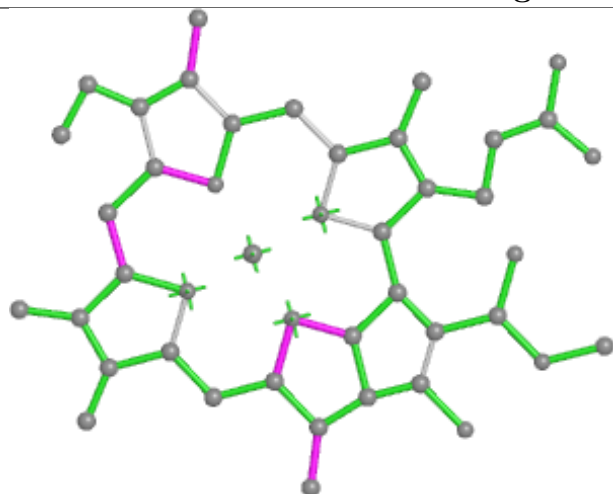
Torsions



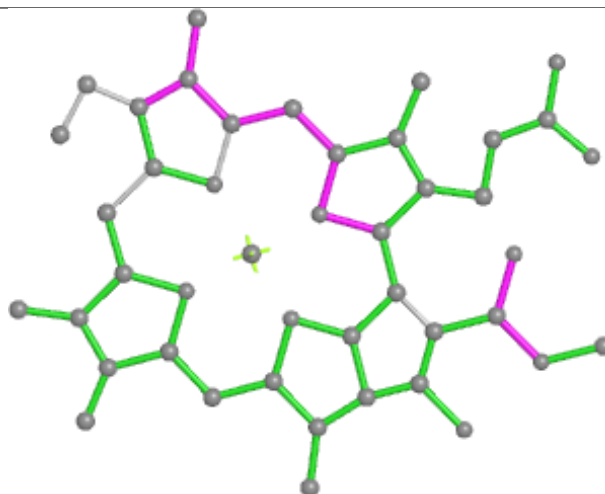
Rings



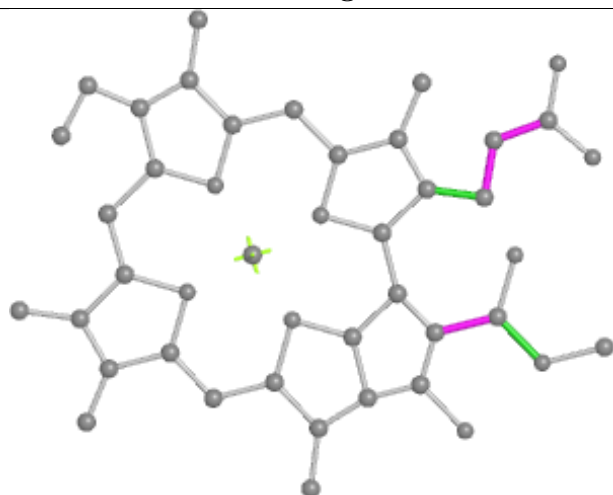
Ligand CLA A 823



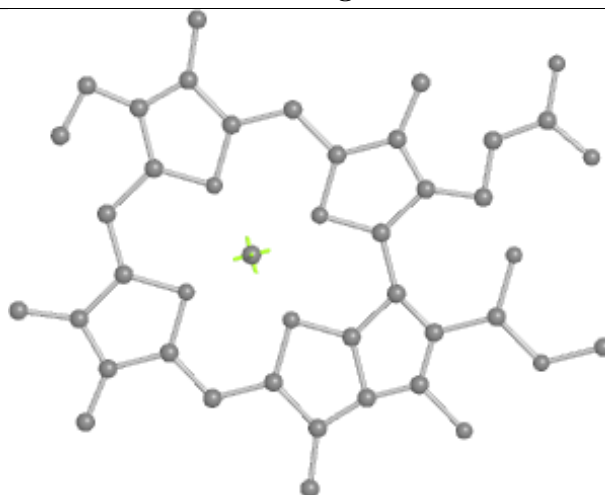
Bond lengths



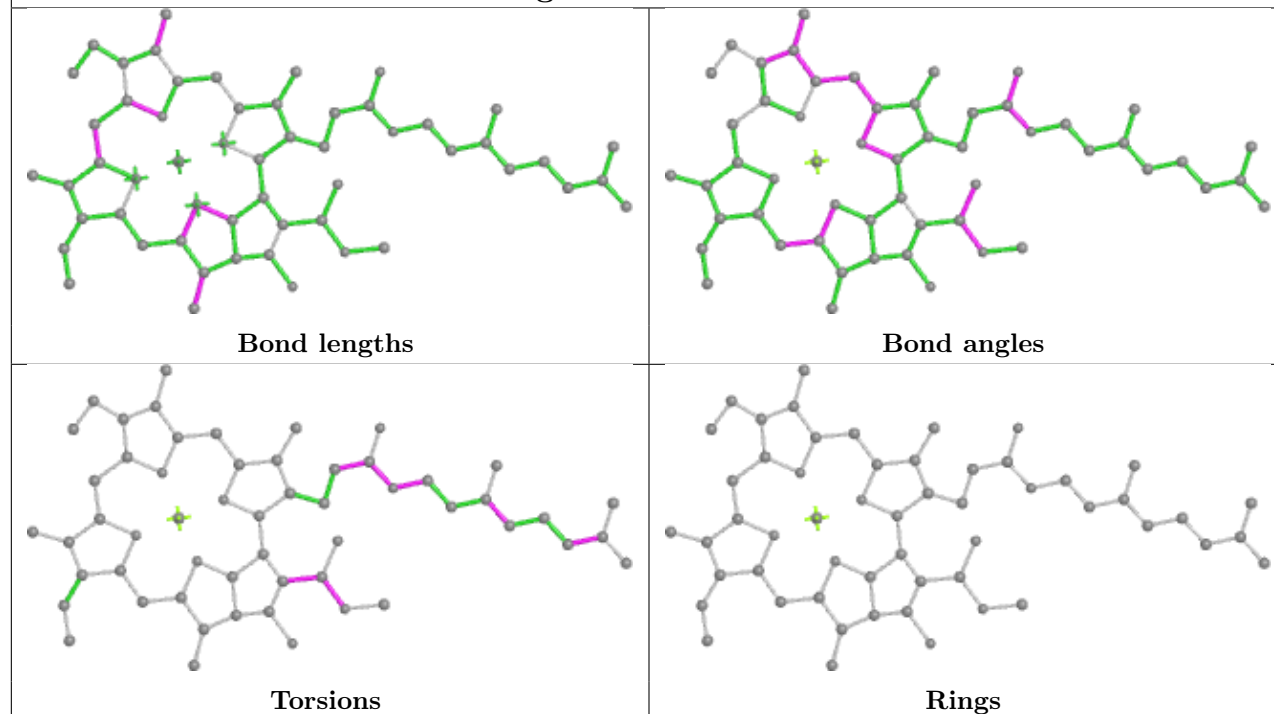
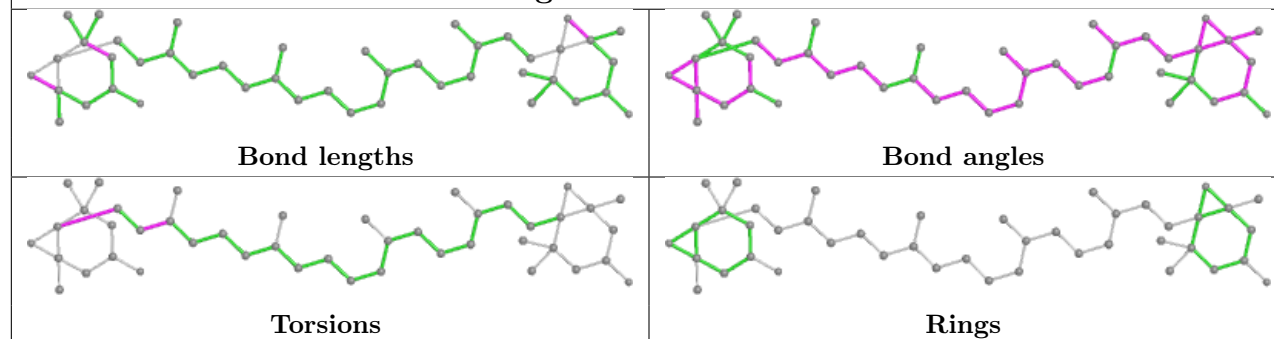
Bond angles



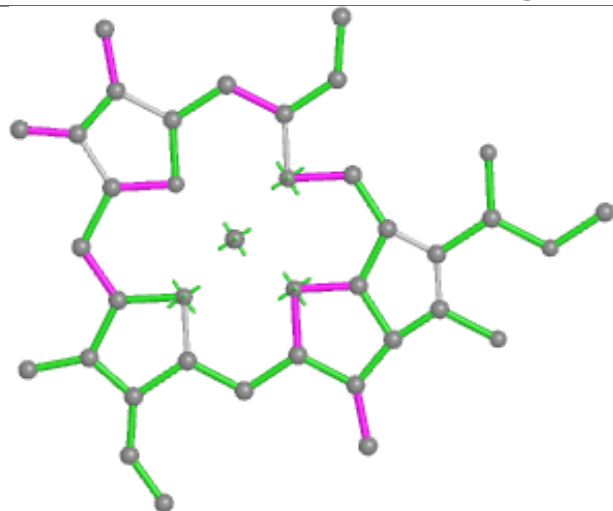
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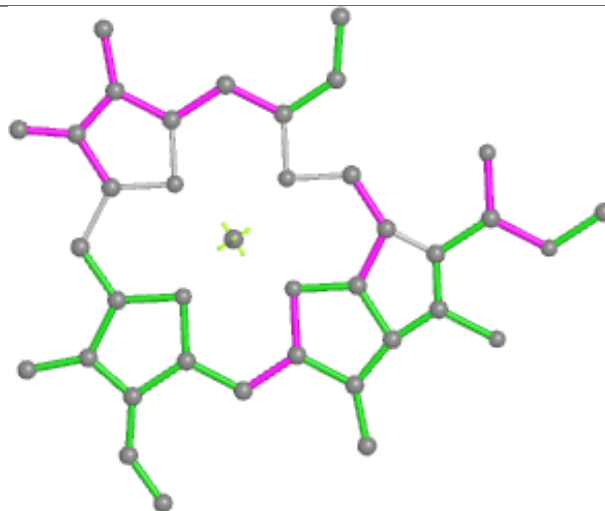
Rings

Ligand CLA 6 603**Ligand XAT 5 620**

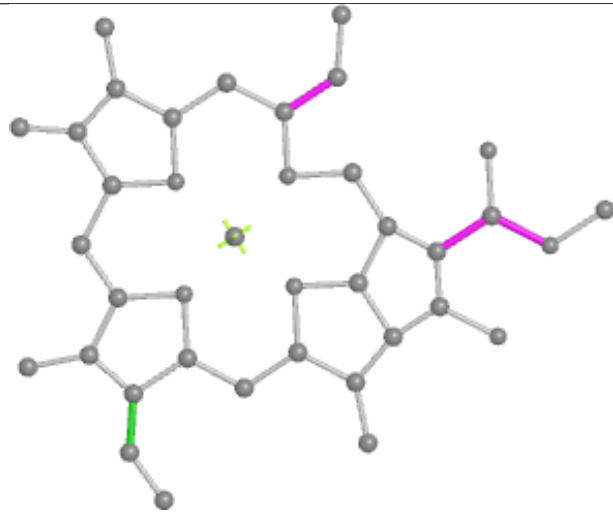
Ligand CLA 5 611



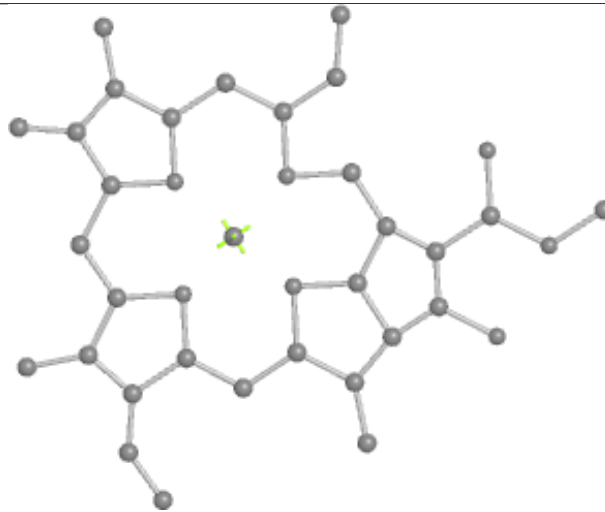
Bond lengths



Bond angles

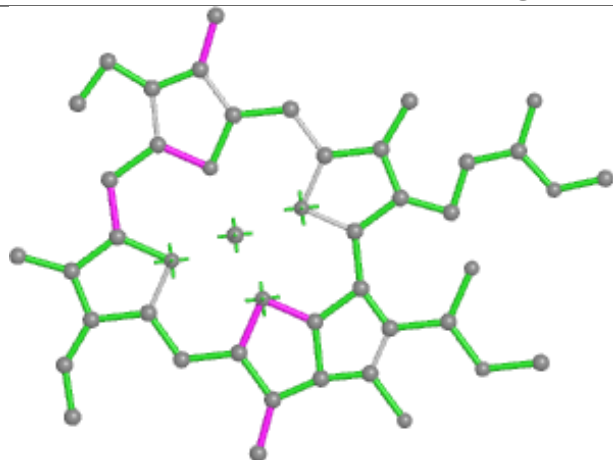


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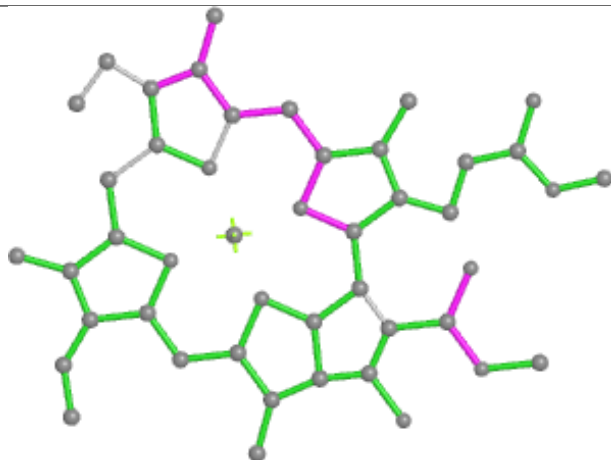


Rings

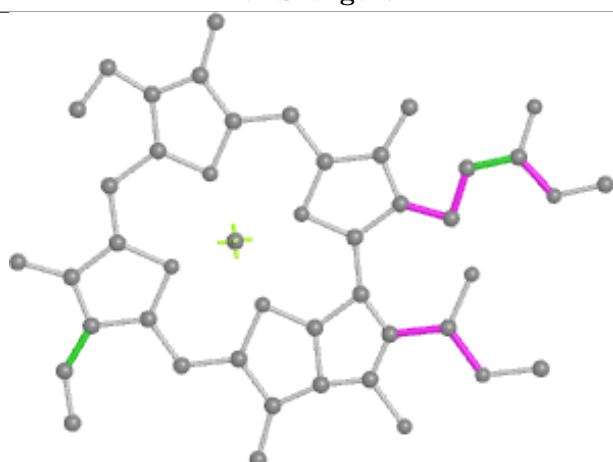
Ligand CLA B 810



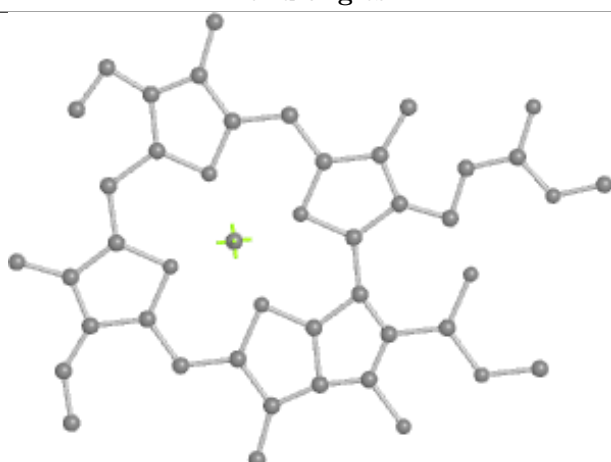
Bond lengths



Bond angles

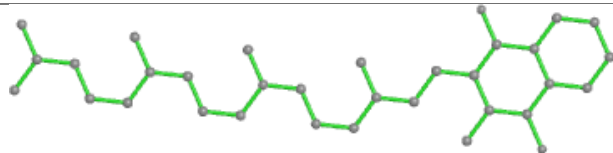


Torsions

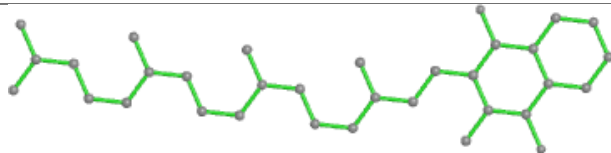


Rings

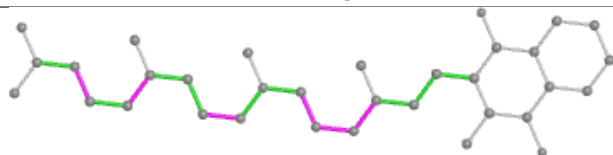
Ligand PQN A 844



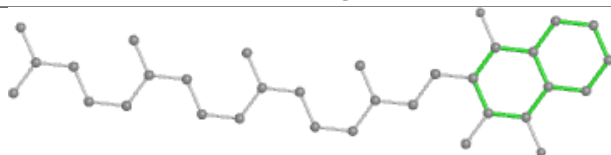
Bond lengths



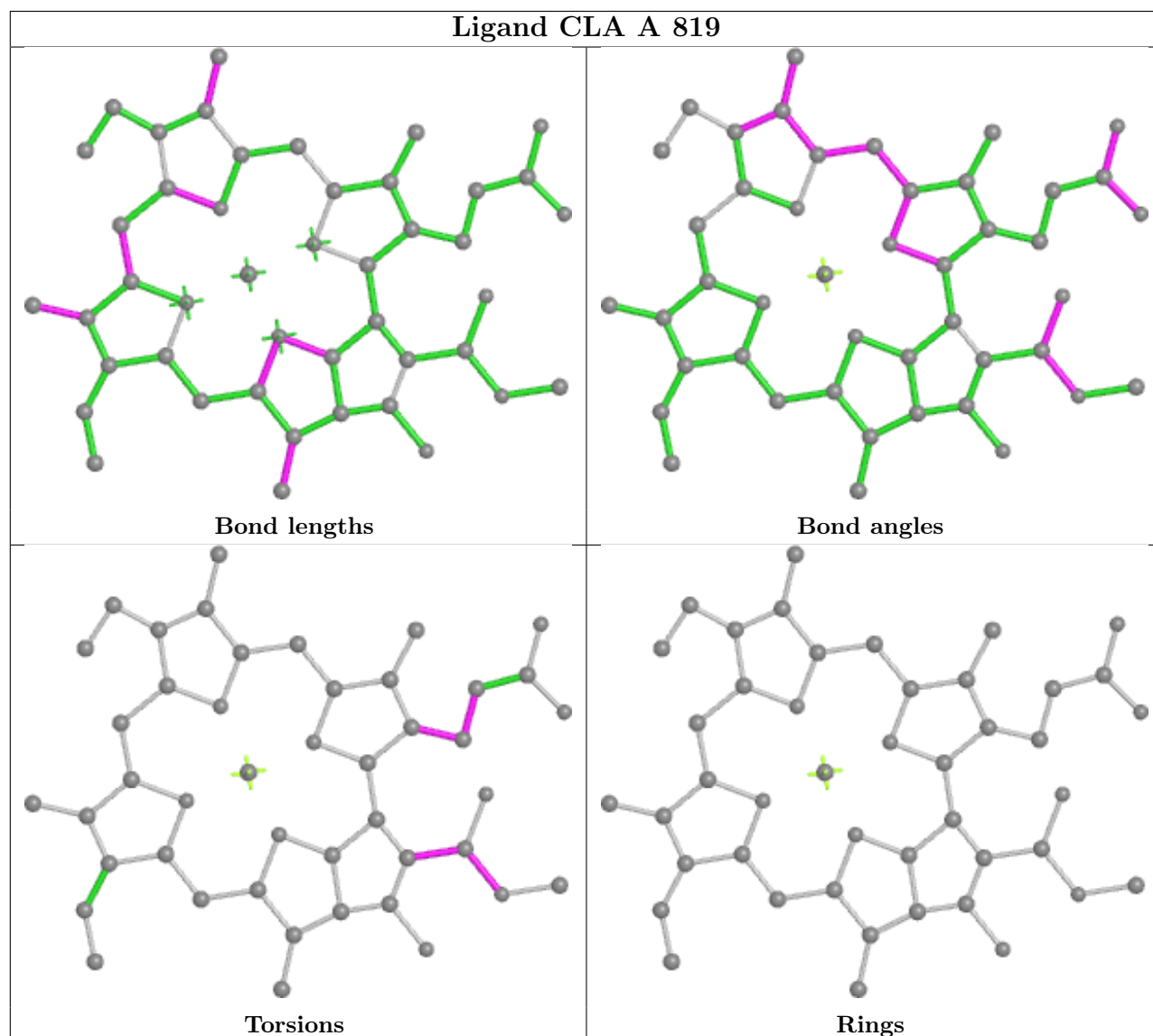
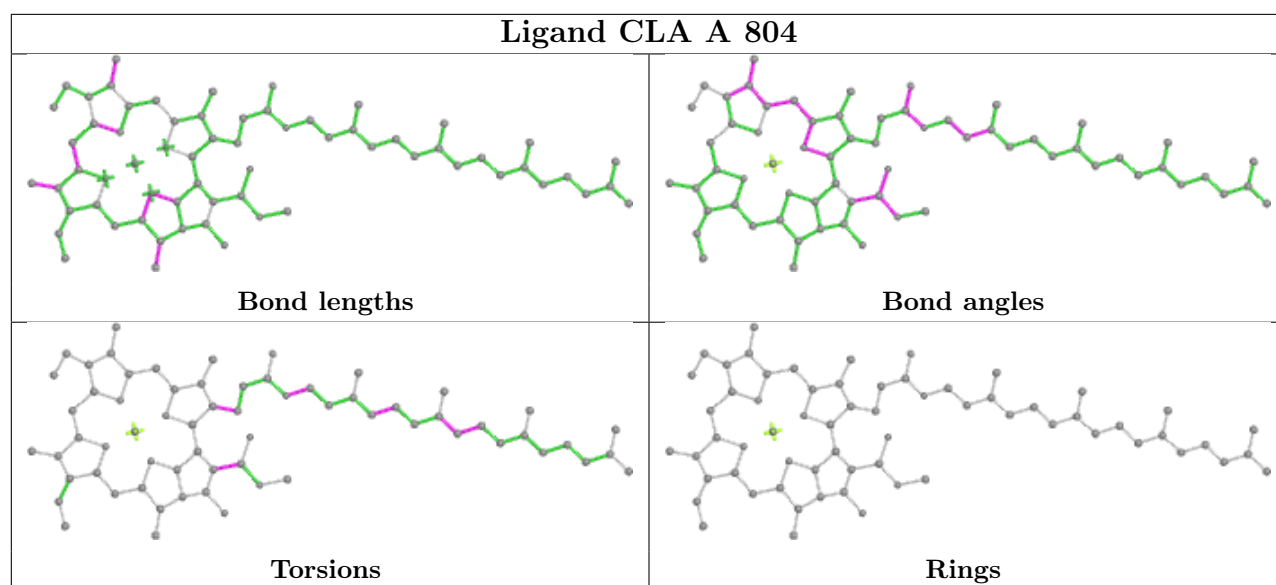
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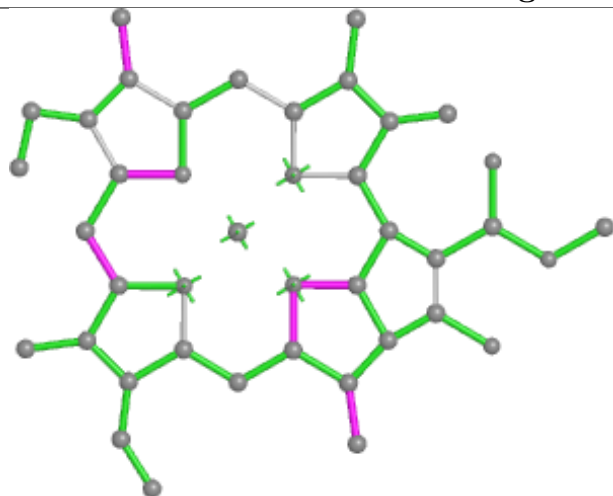
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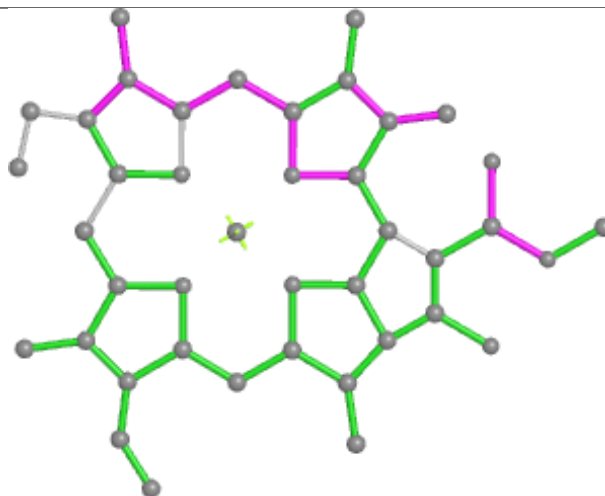
Rings



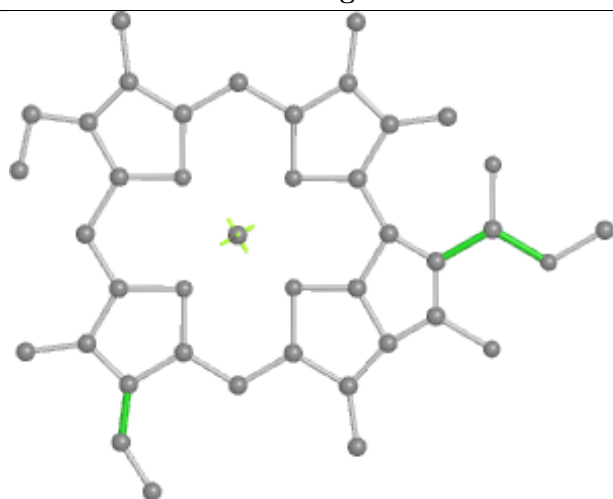
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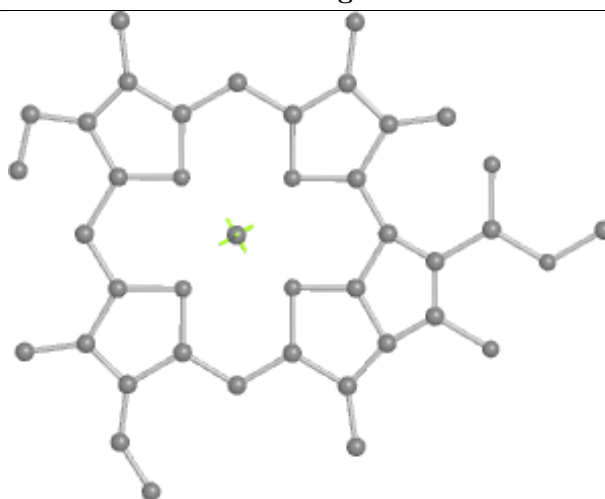
Bond lengths



Bond angles

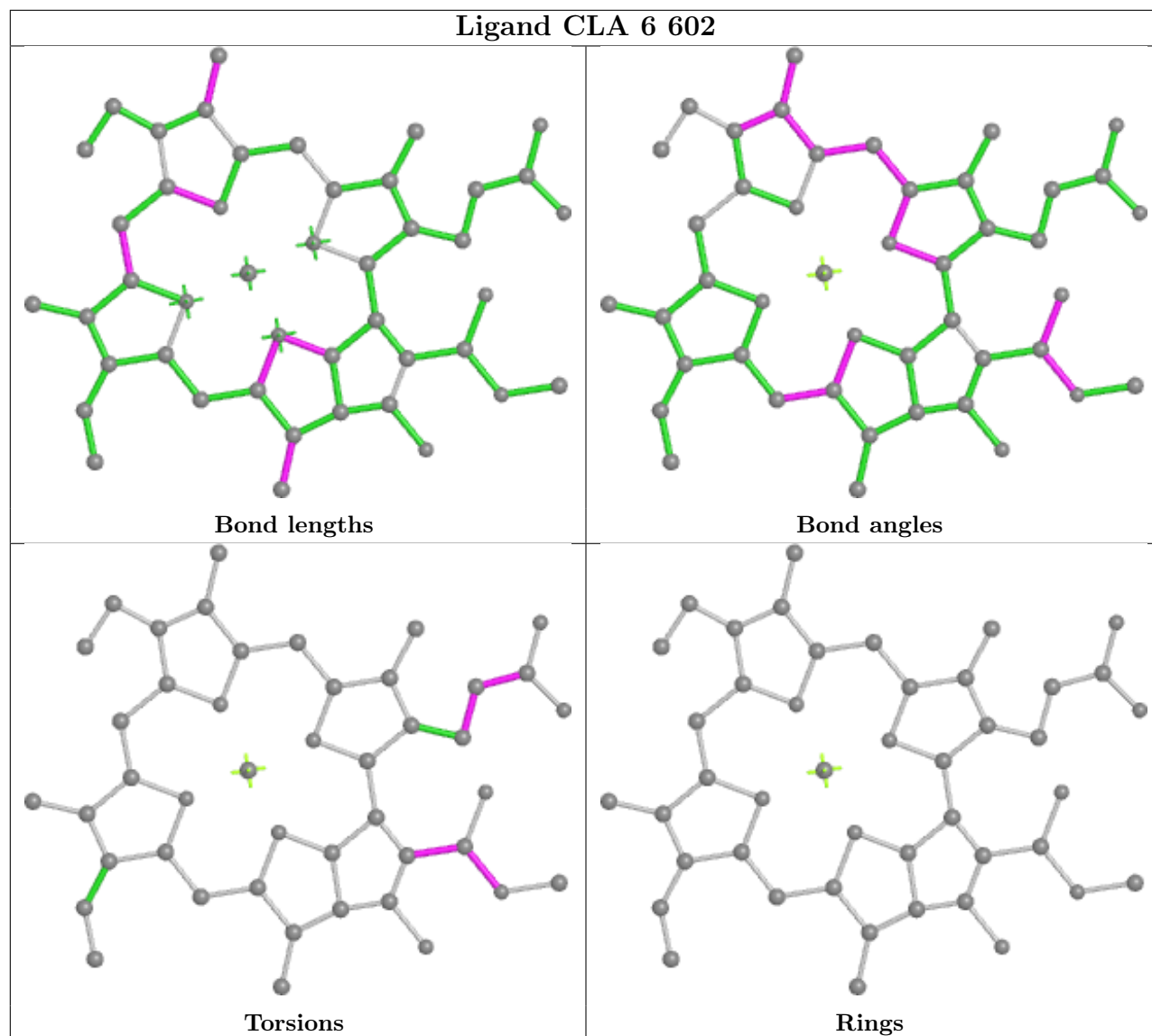


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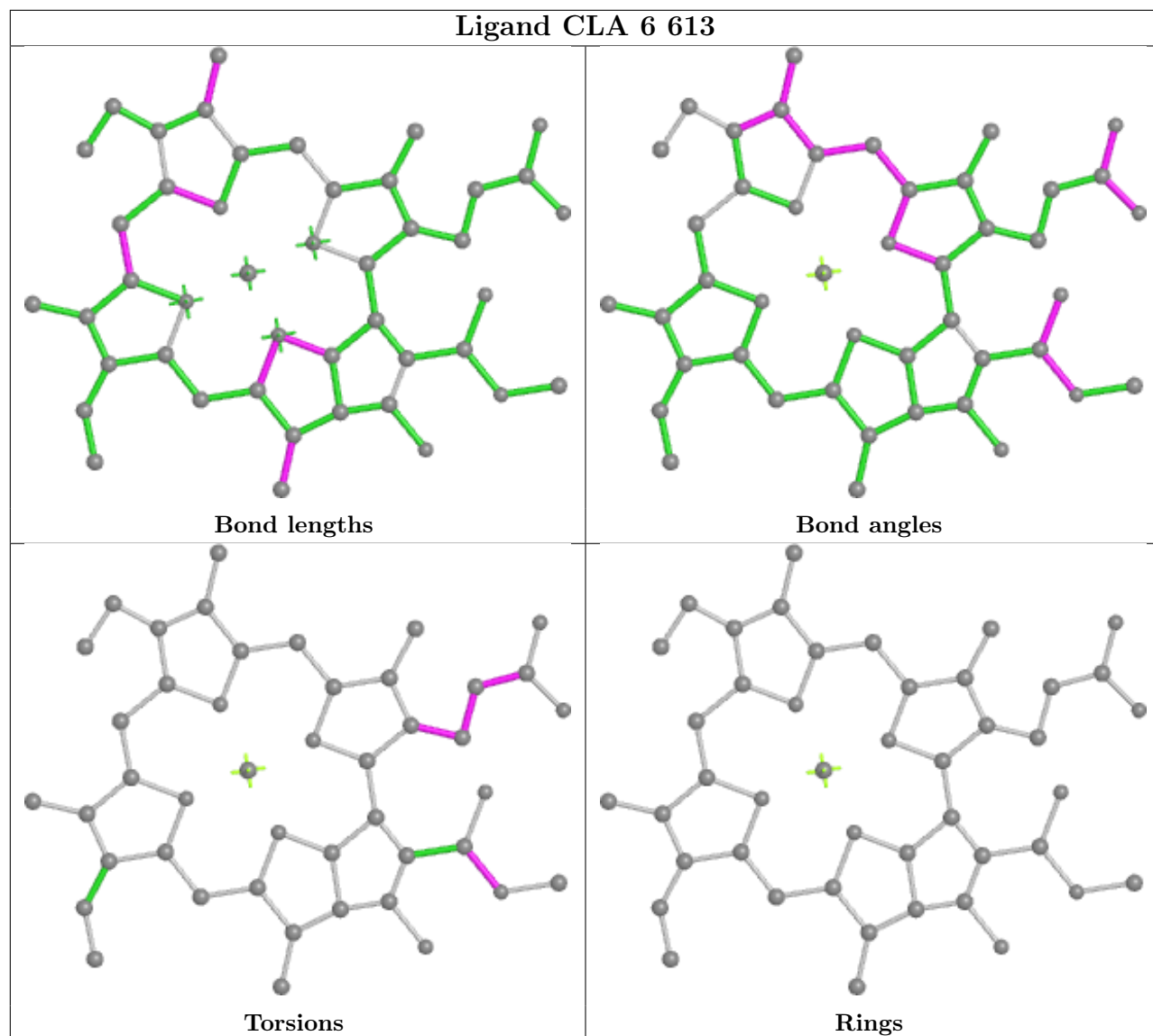


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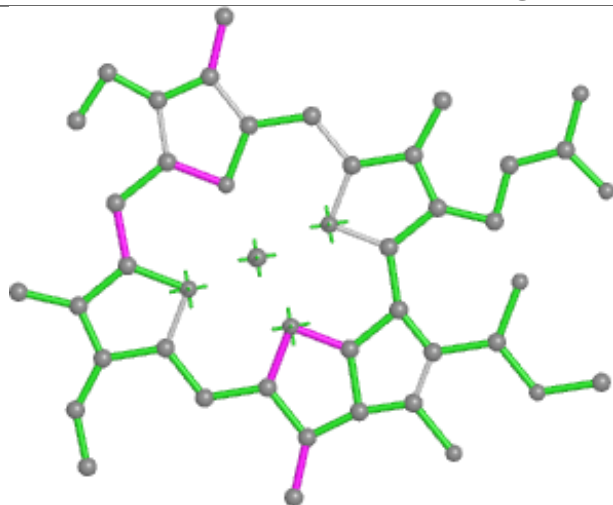
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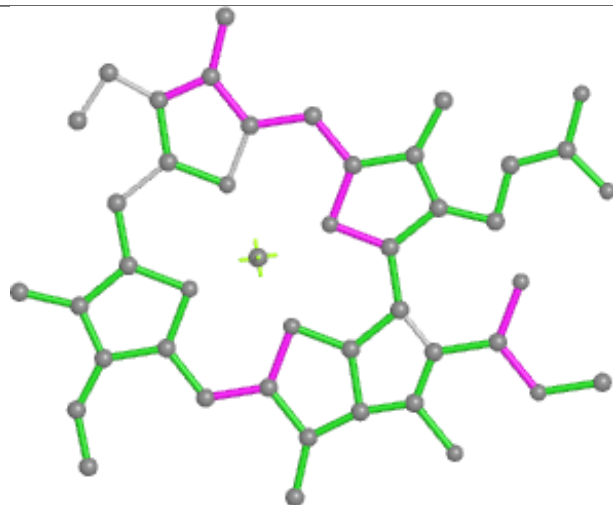
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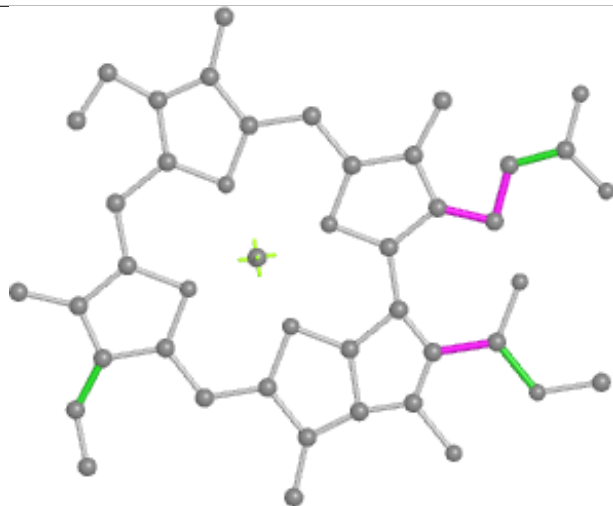
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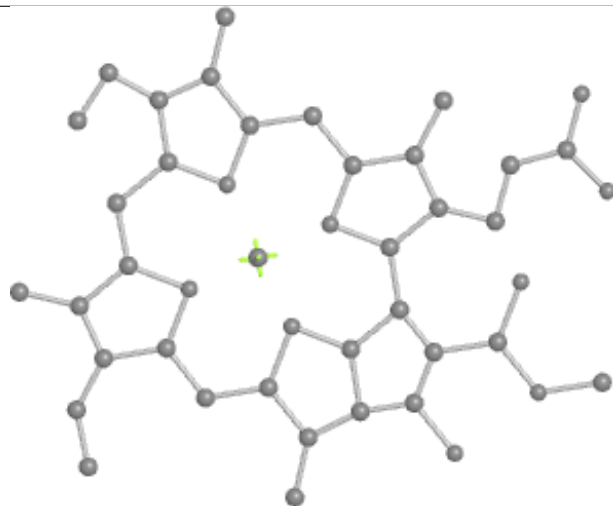
Bond lengths



Bond angles

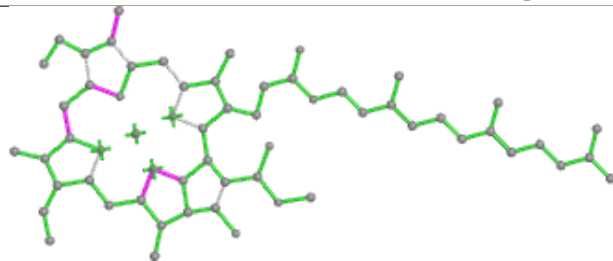


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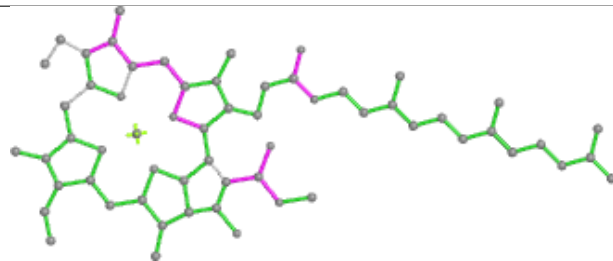


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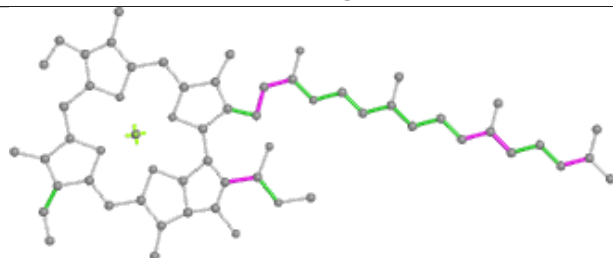
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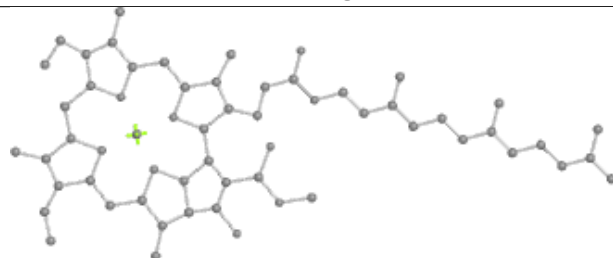
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Bond angles

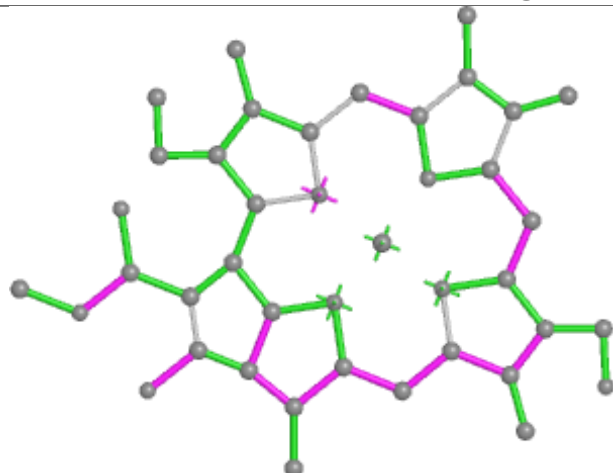


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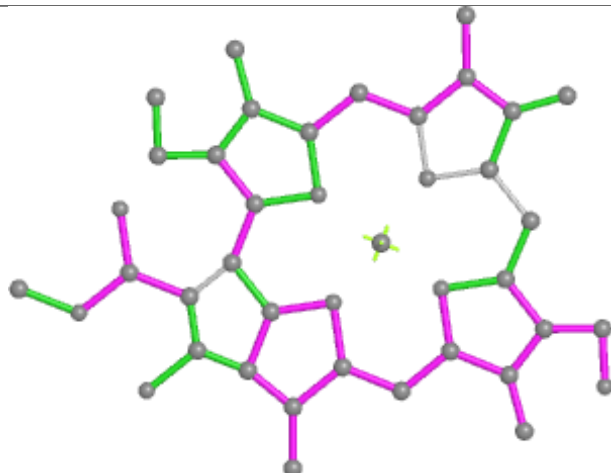


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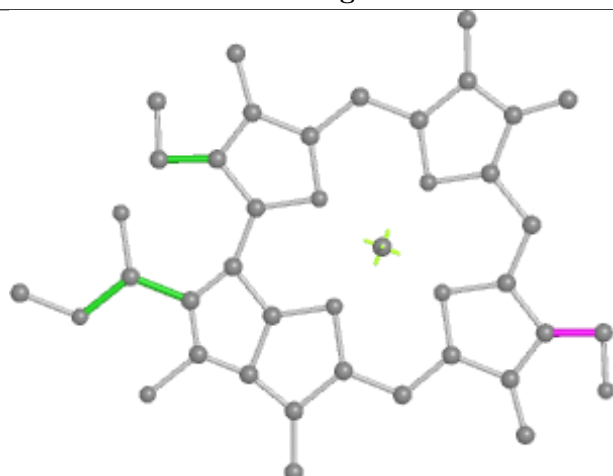
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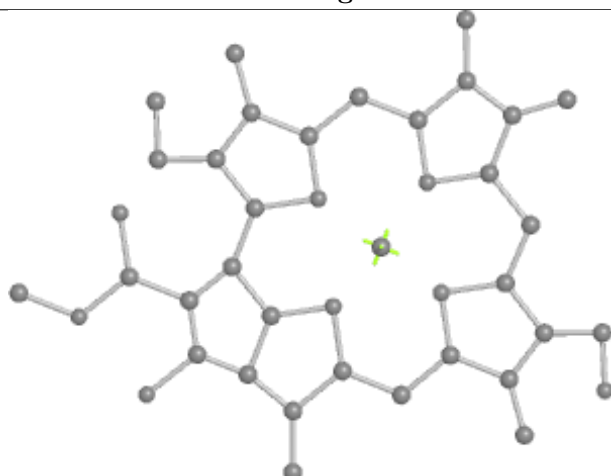
Bond lengths



Bond angles

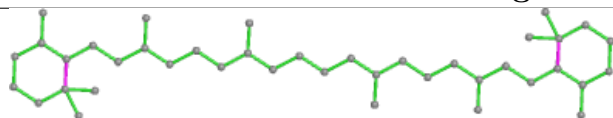


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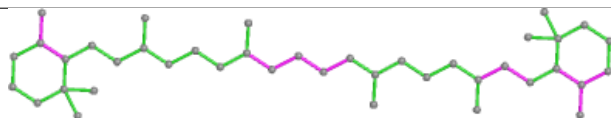


Rings

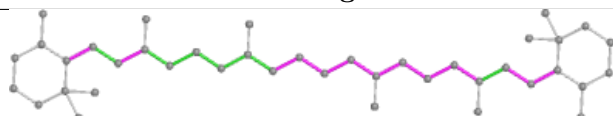
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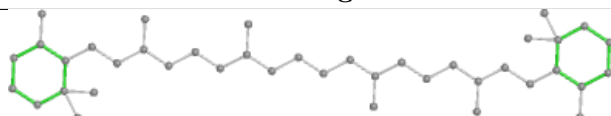
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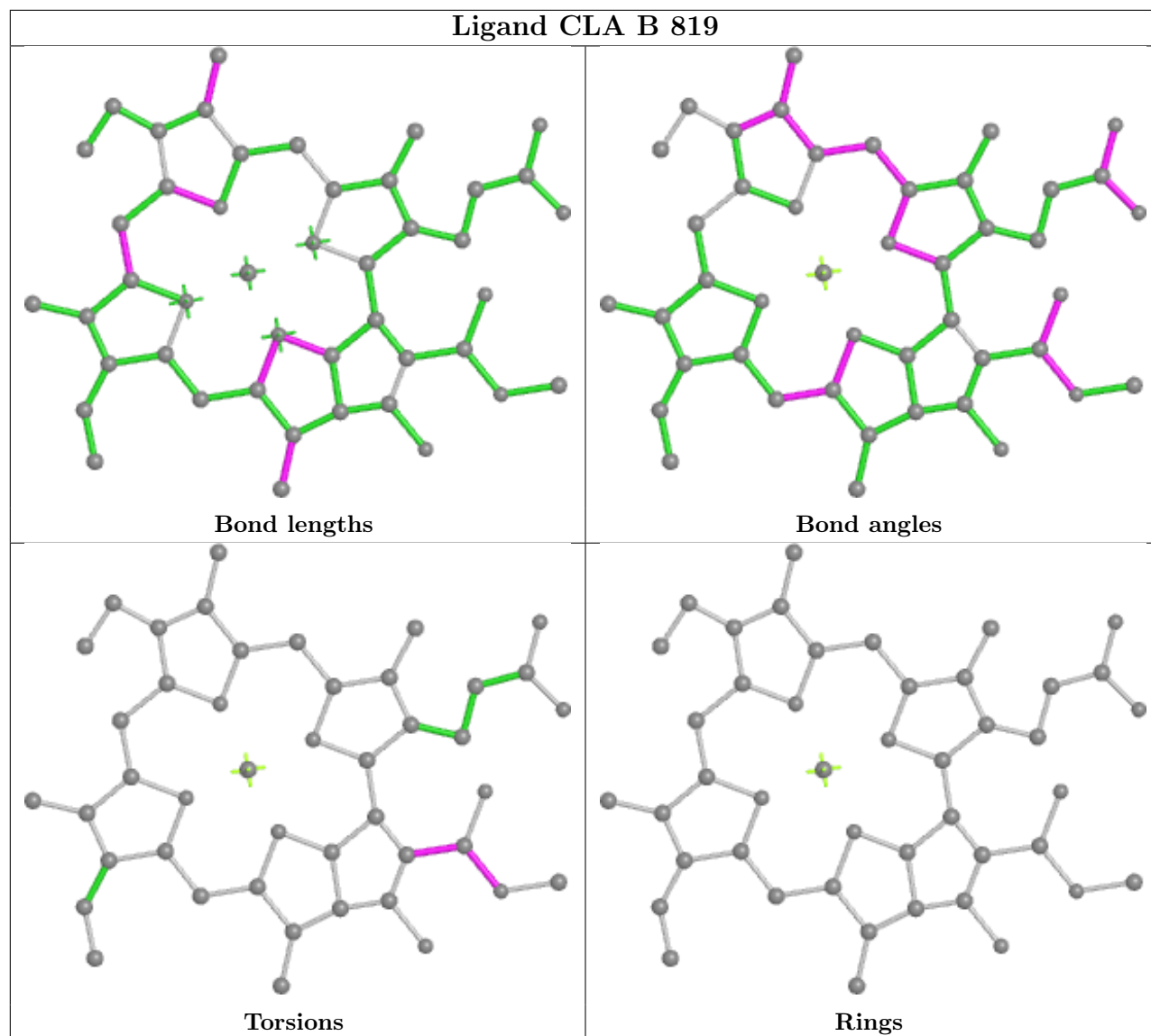
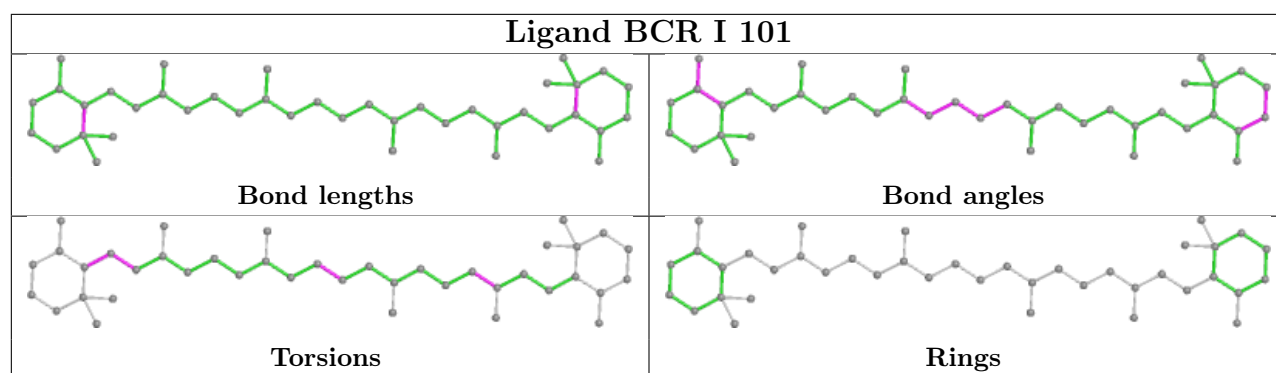
Bond angles

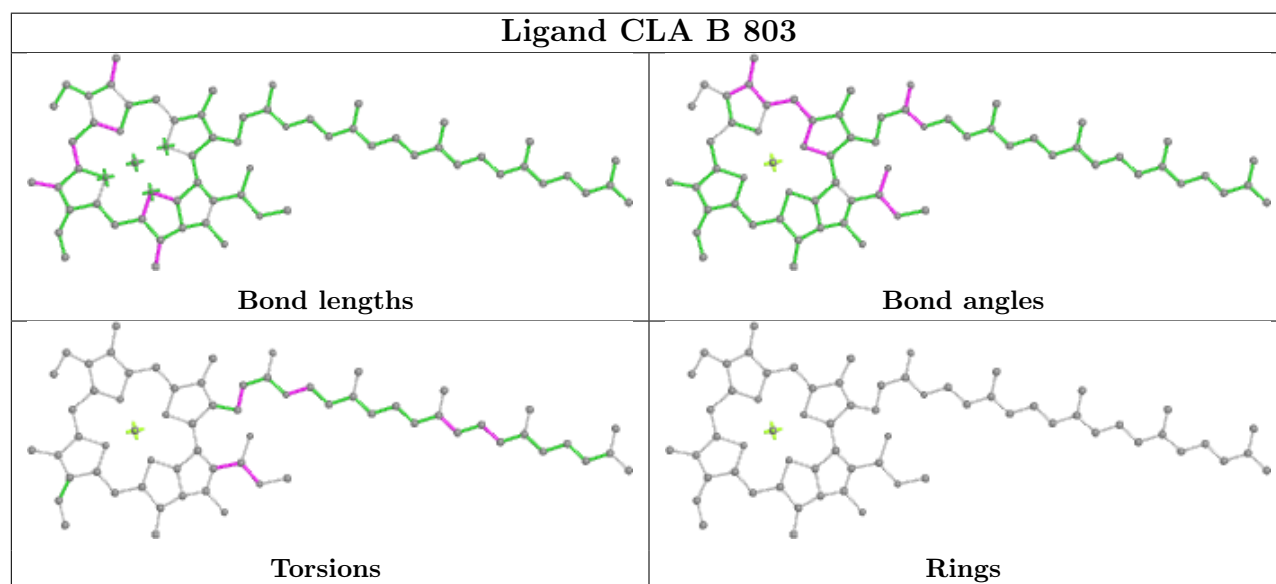
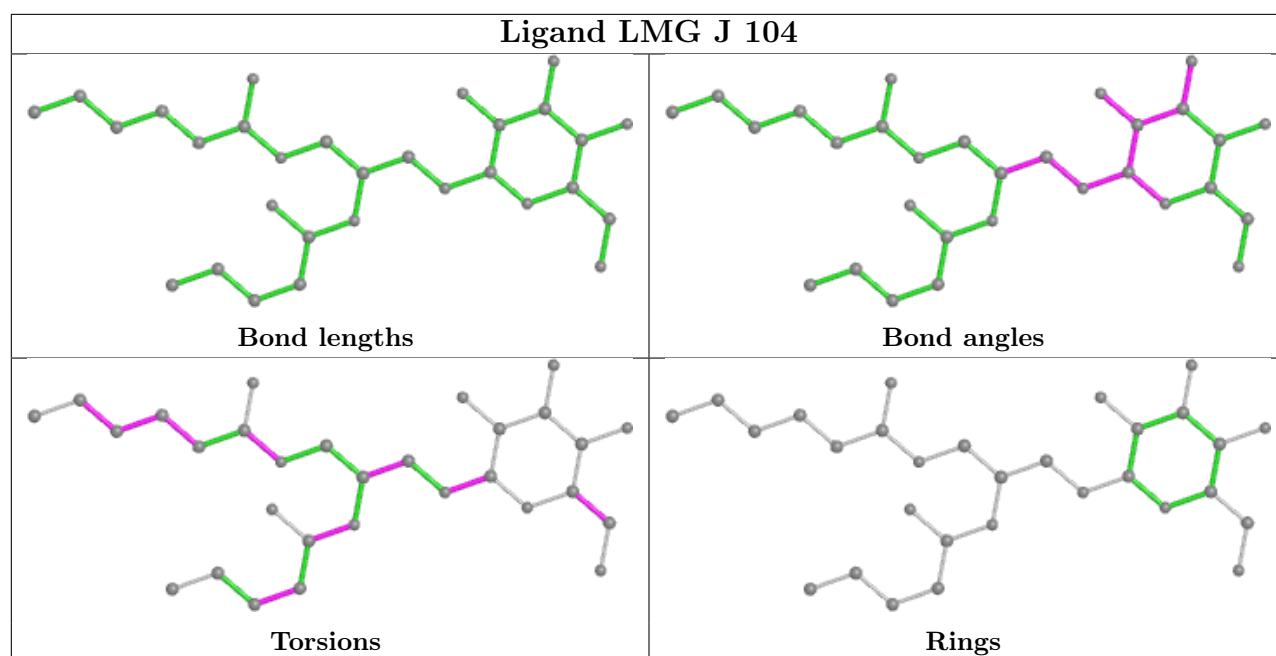


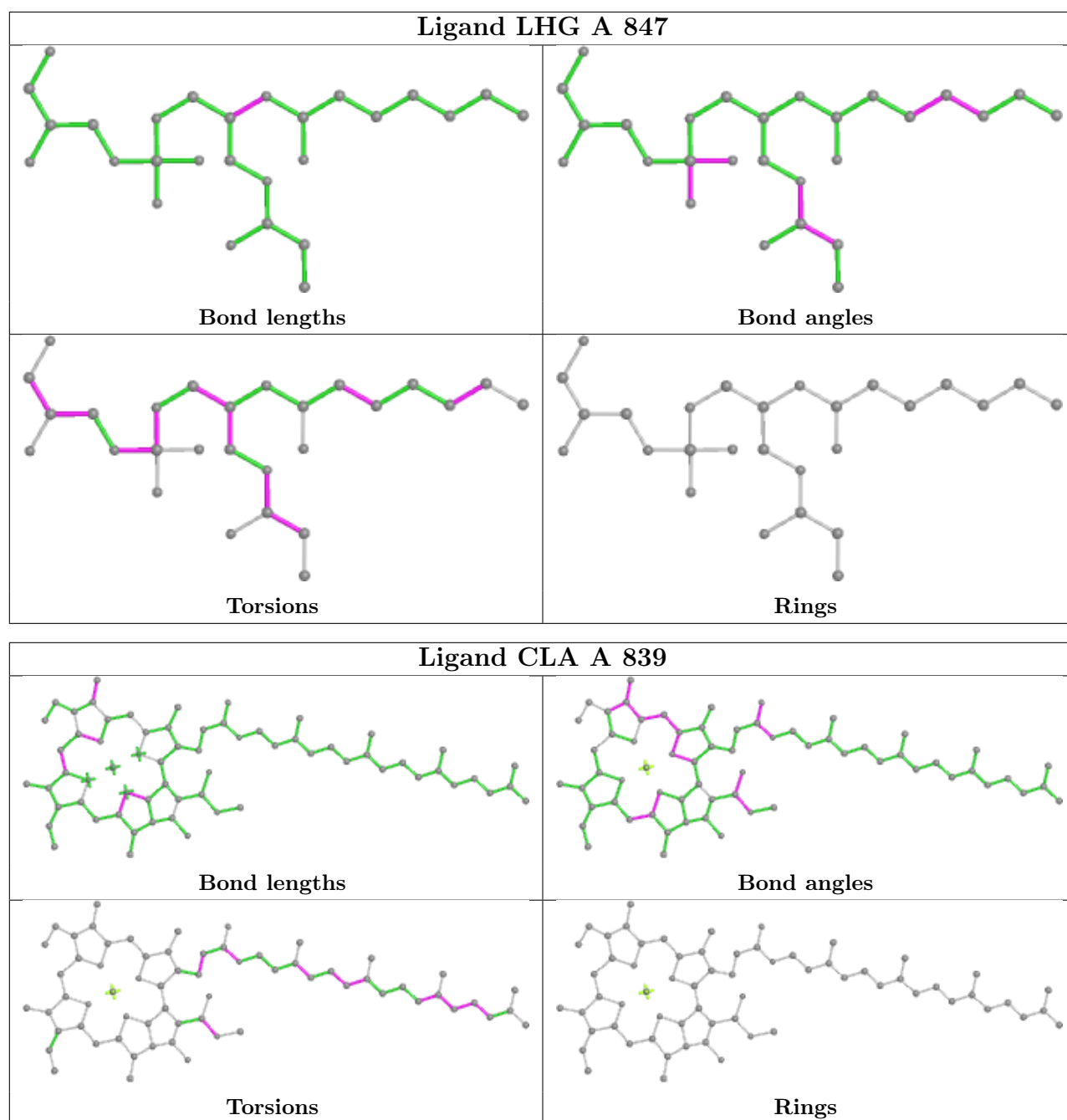
Torsions

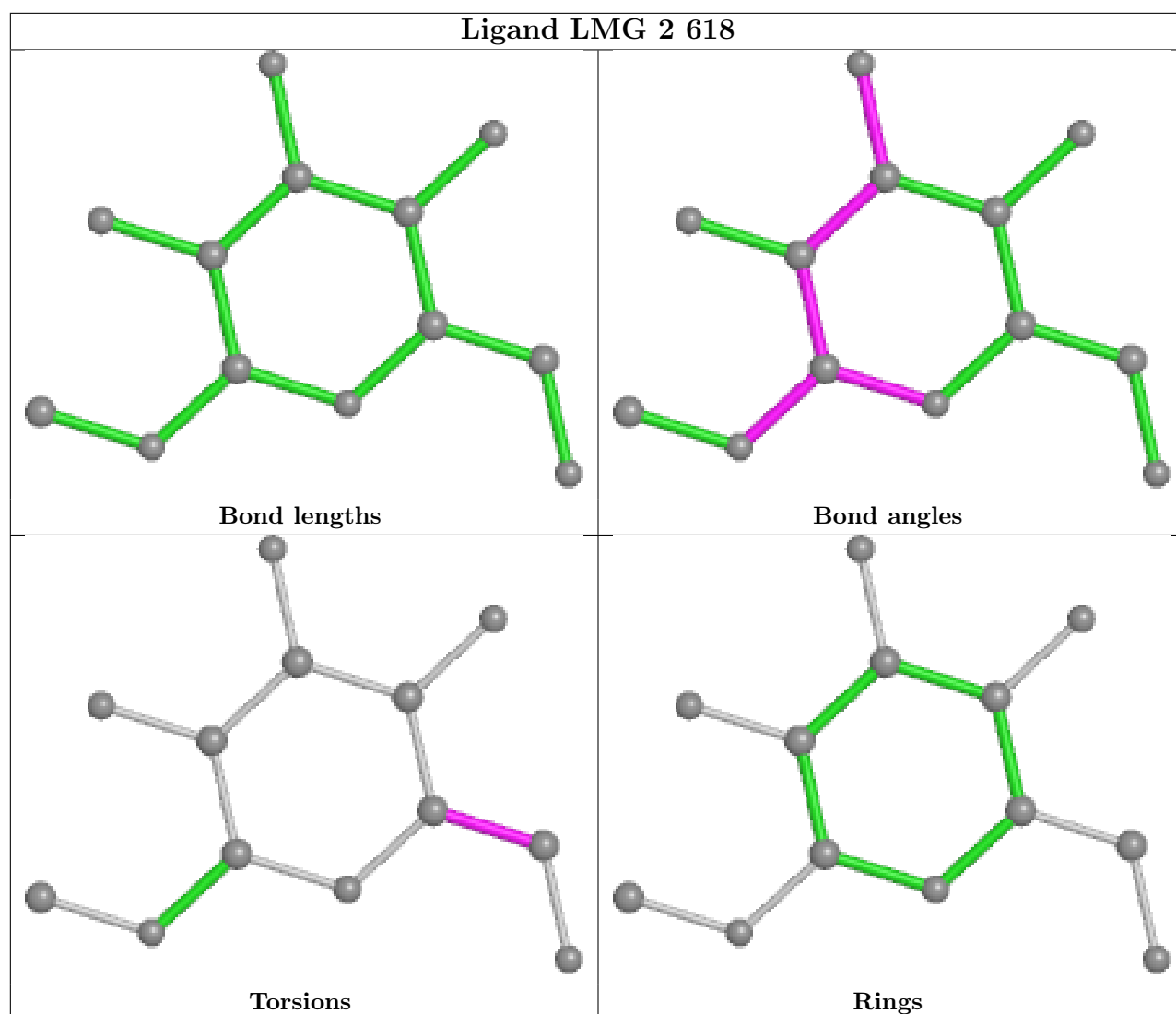


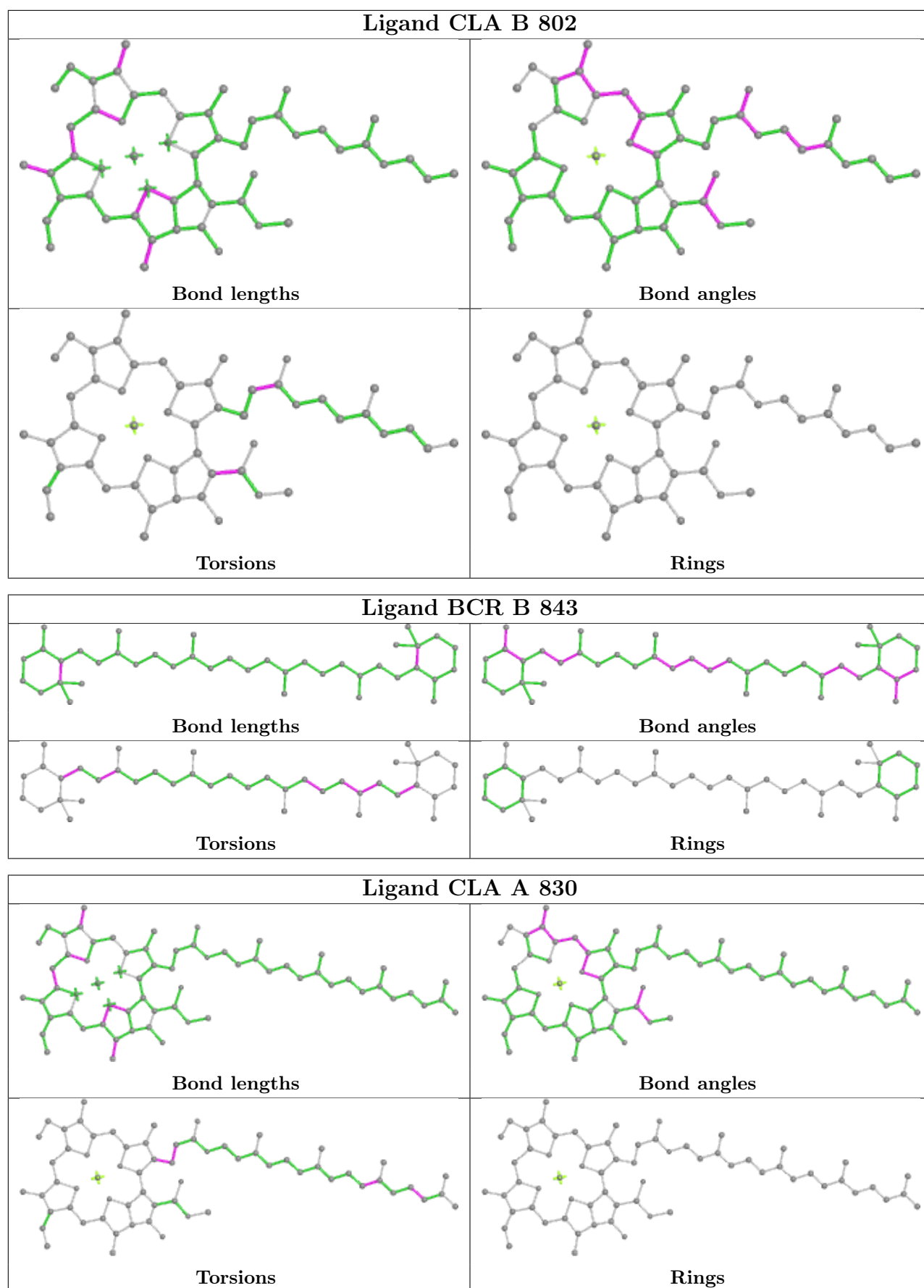
Rings



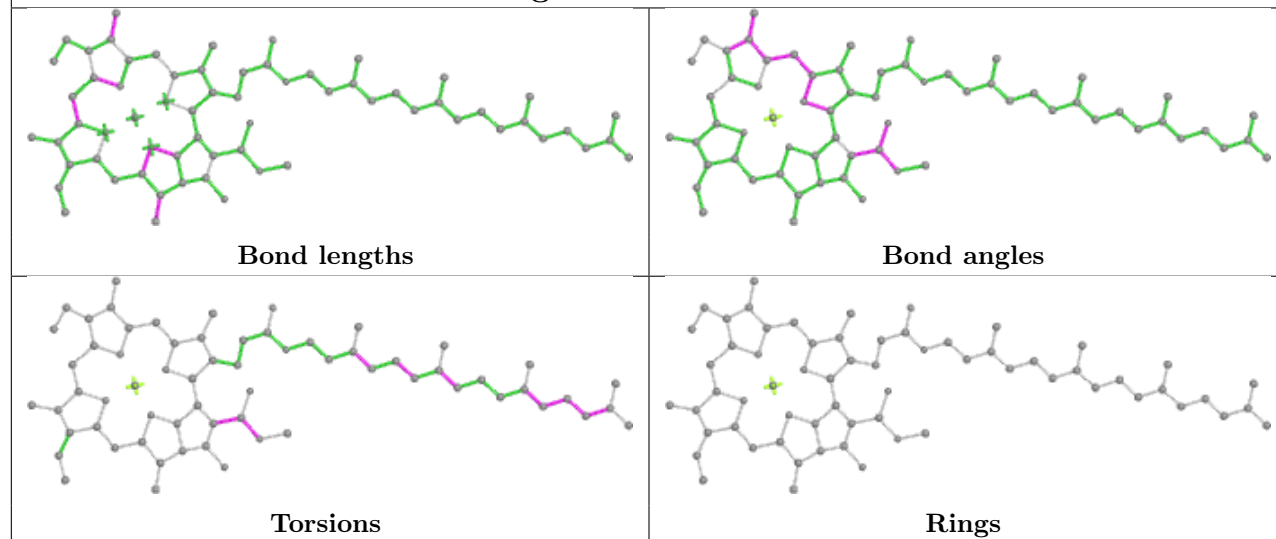




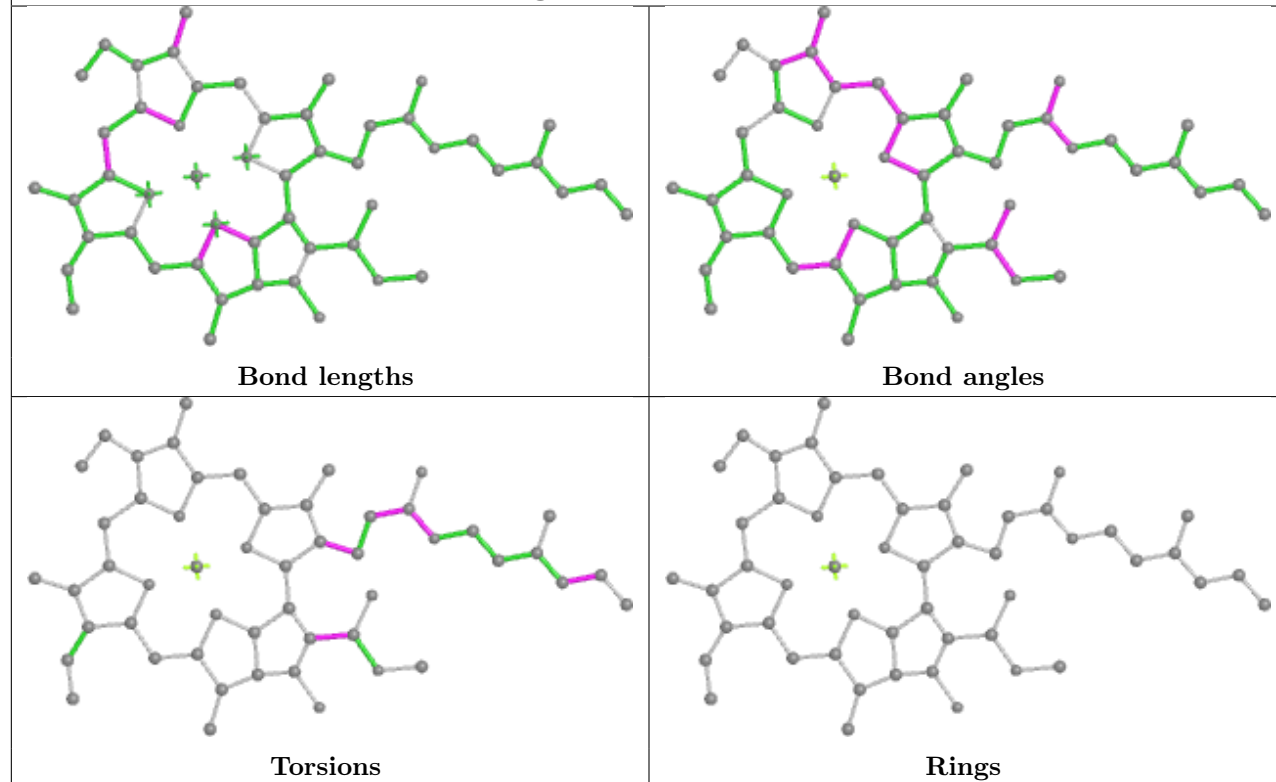


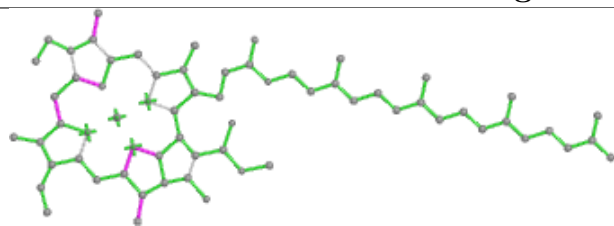
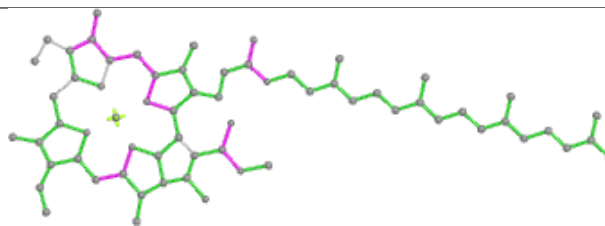
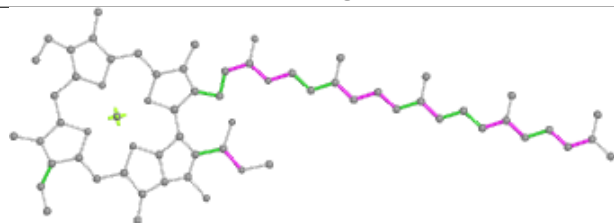
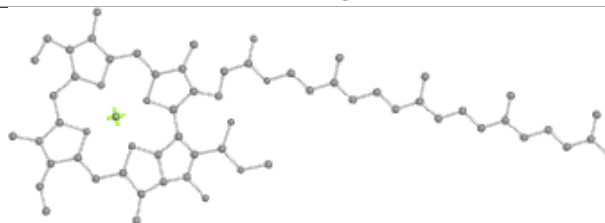
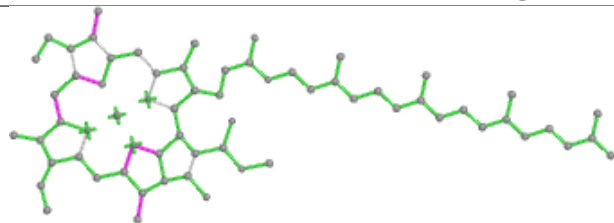
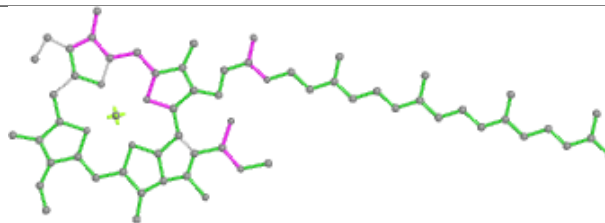
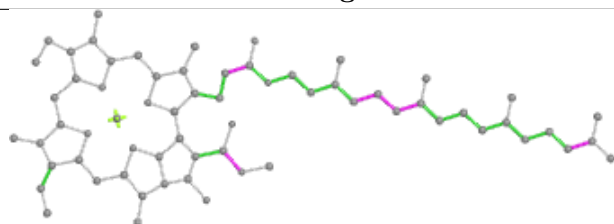
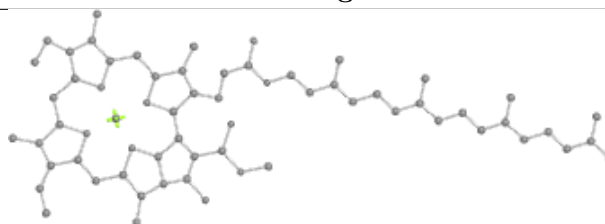


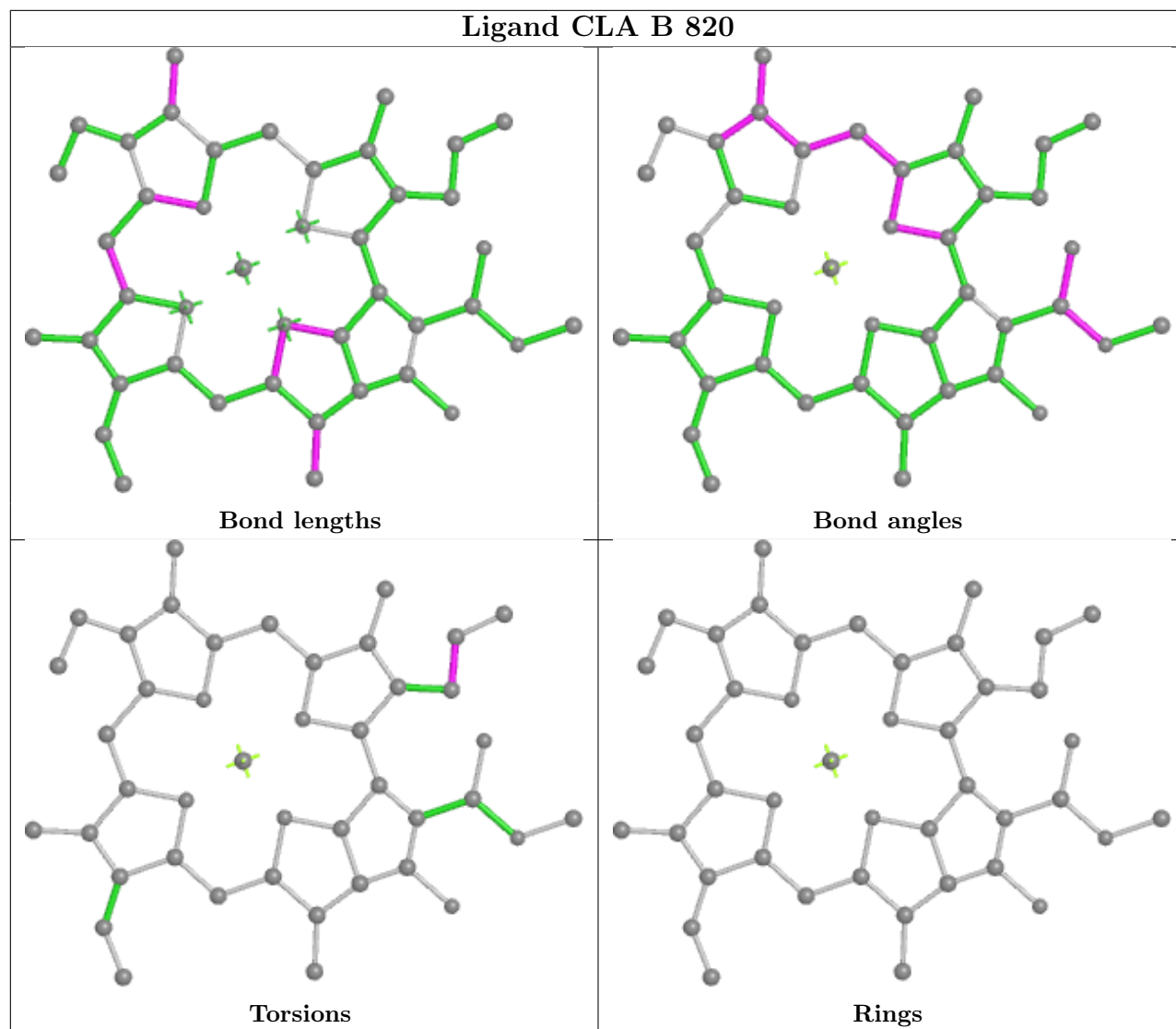
Ligand CLA A 831



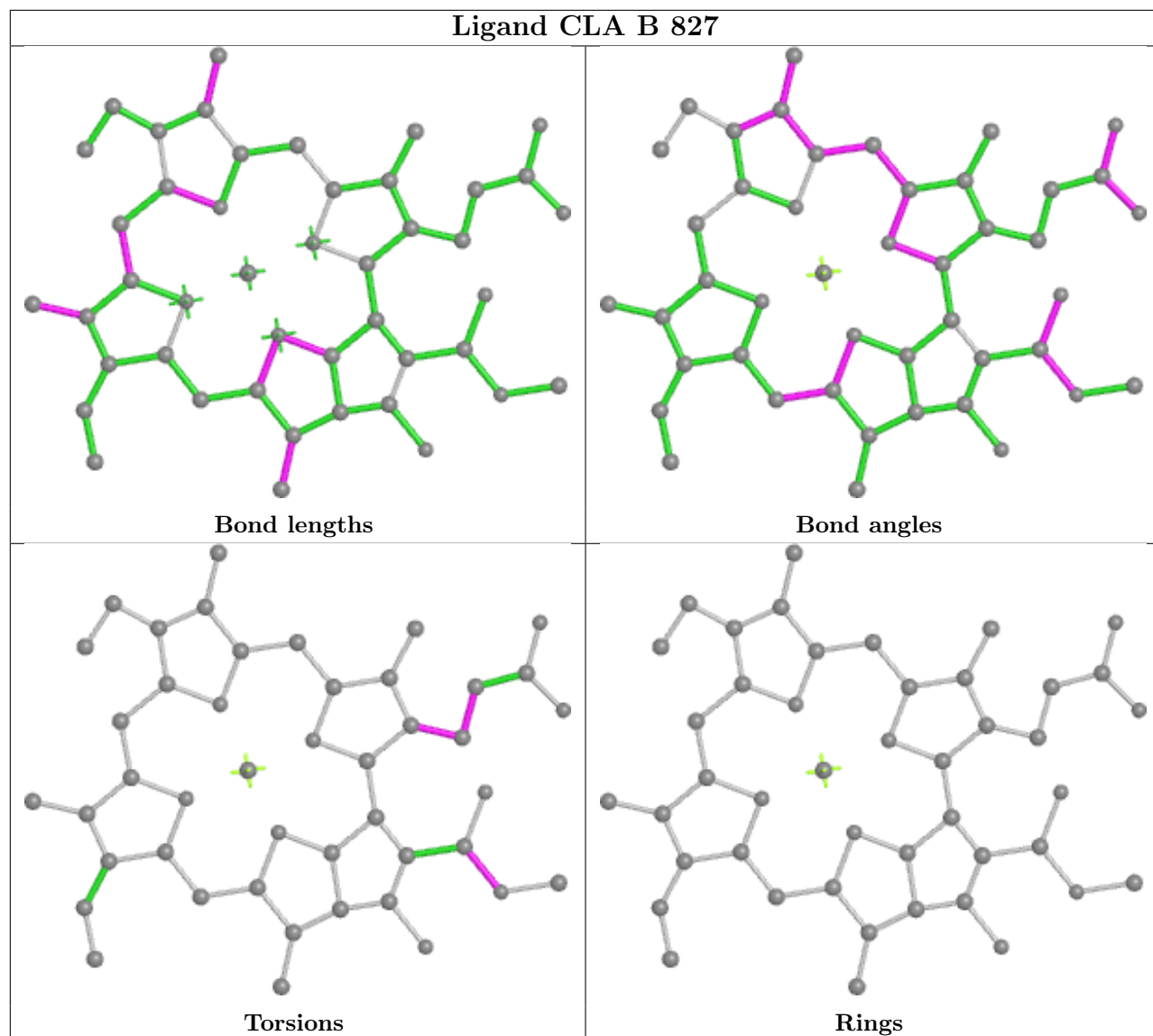
Ligand CLA A 845

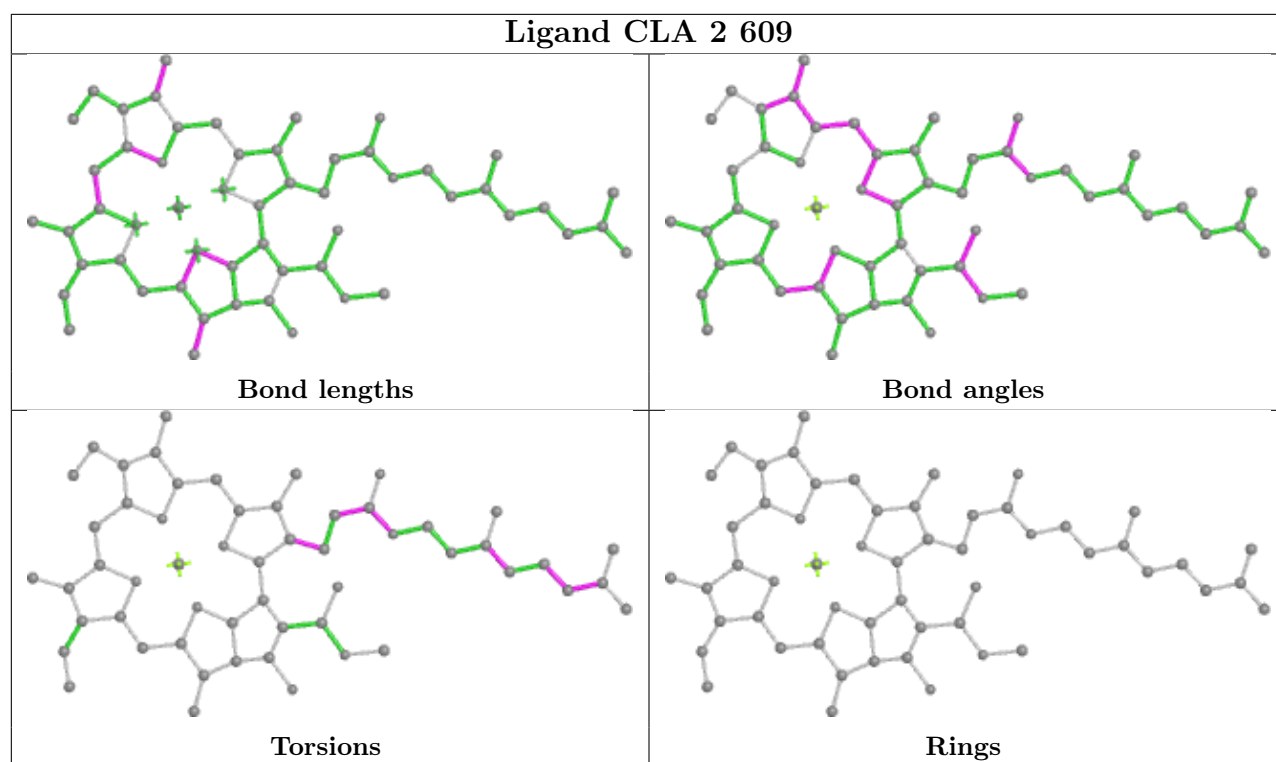


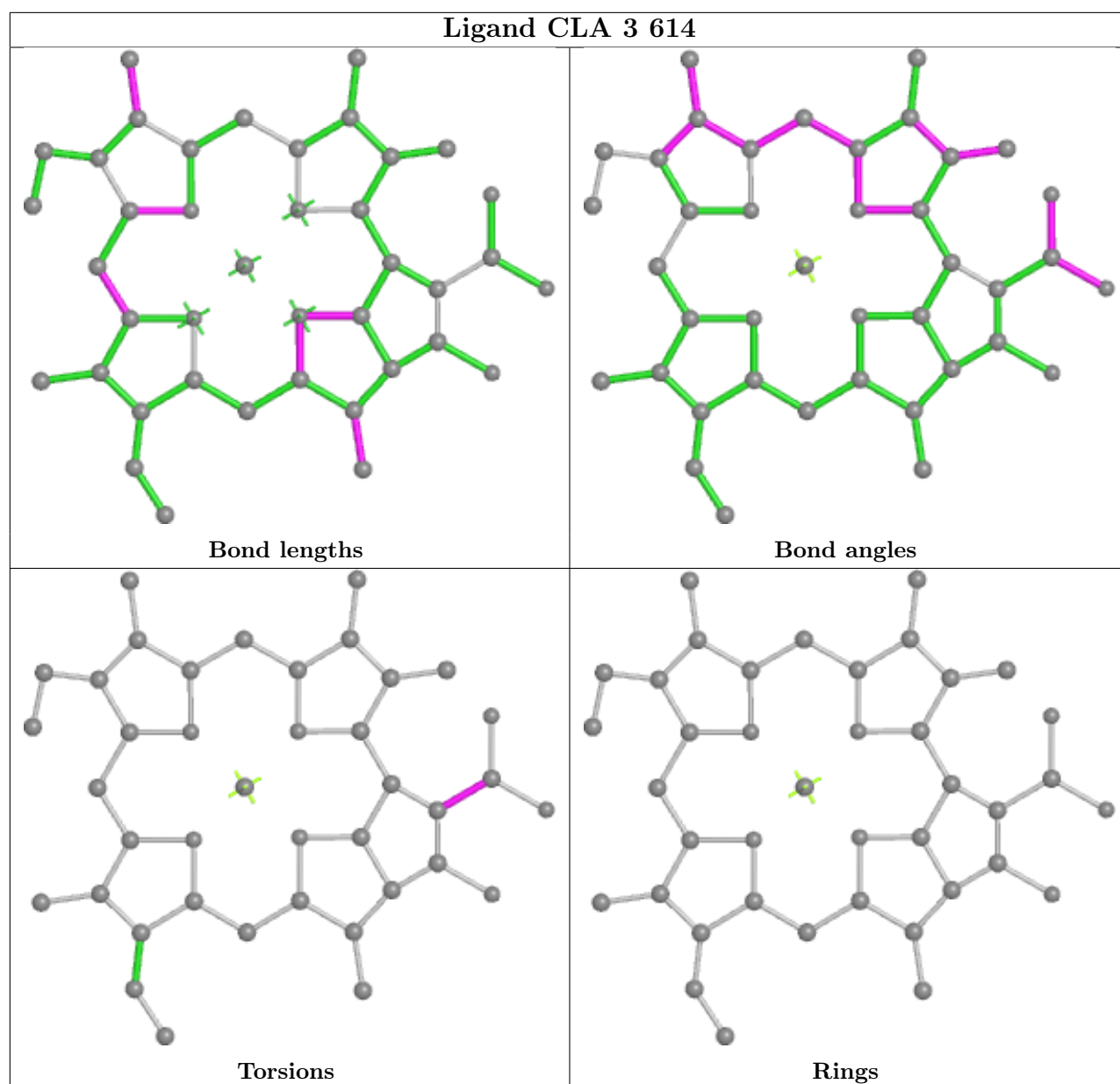
Ligand CLA B 806**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 801****Bond lengths****Bond angles****Torsions****Rings**



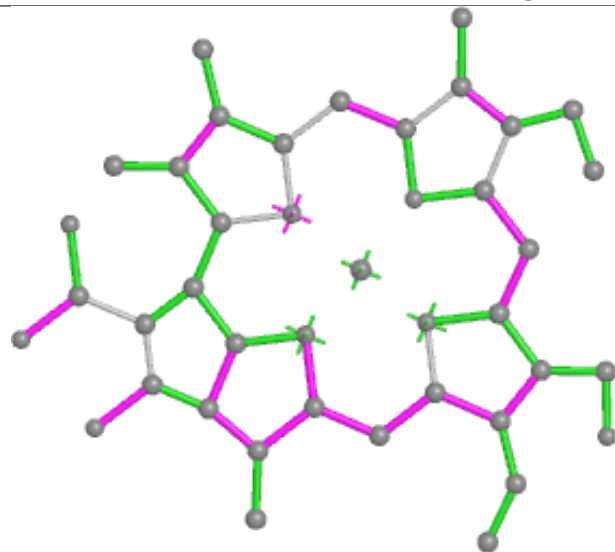
Ligand CLA B 827



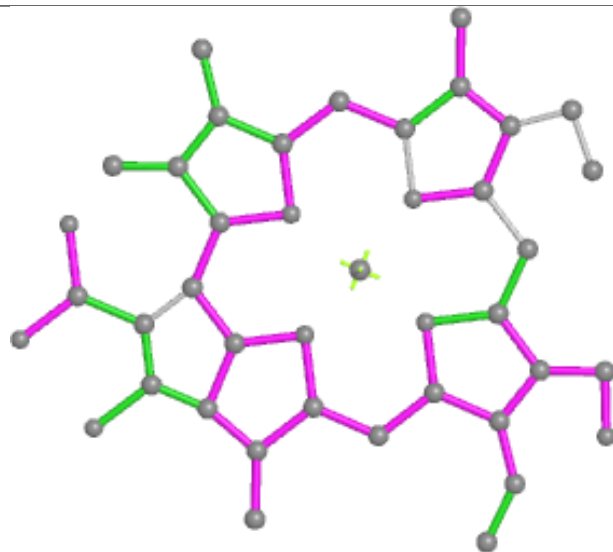




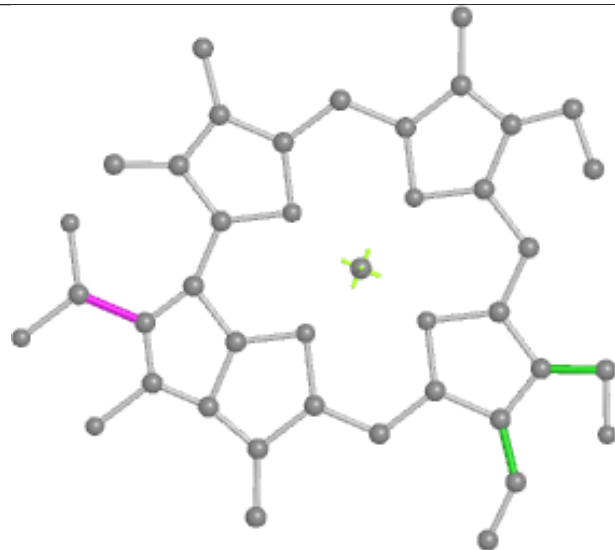
Ligand CHL 6 607



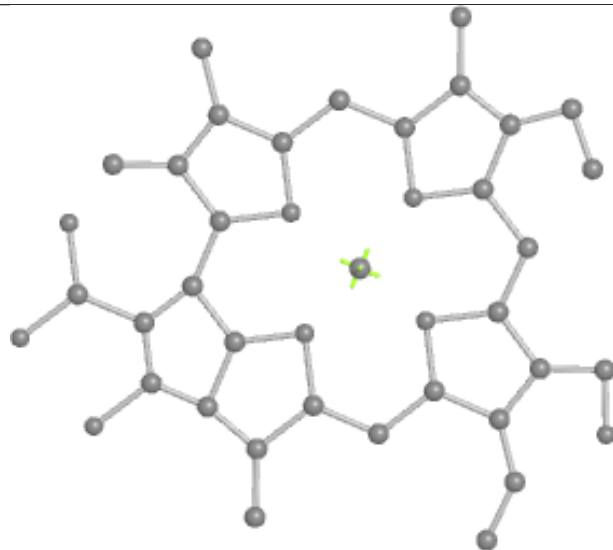
Bond lengths



Bond angles

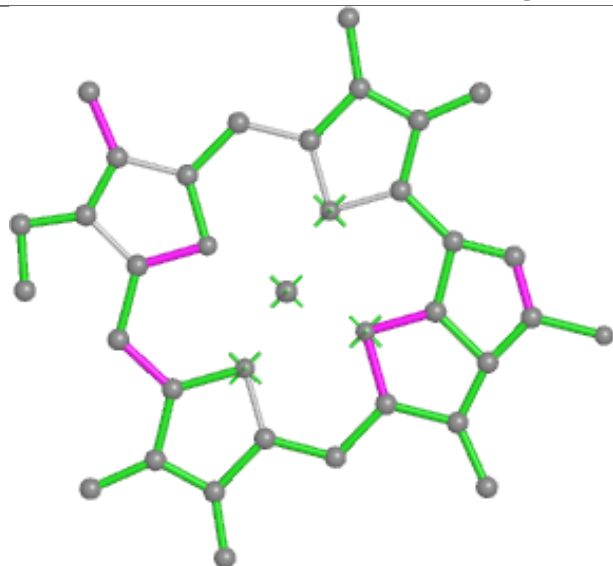


Torsions

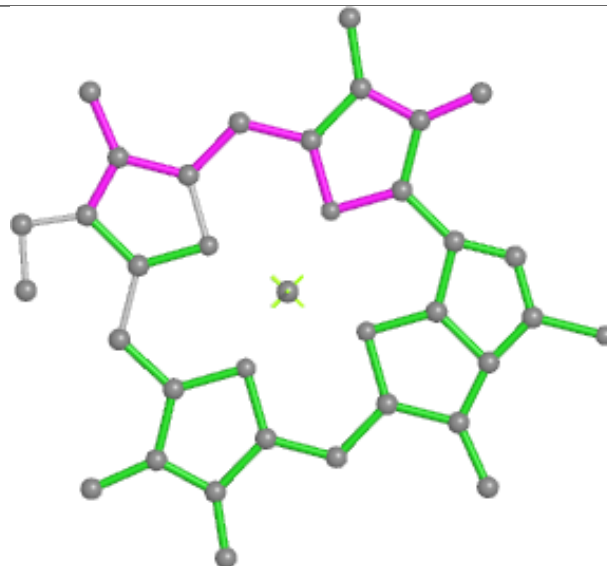


Rings

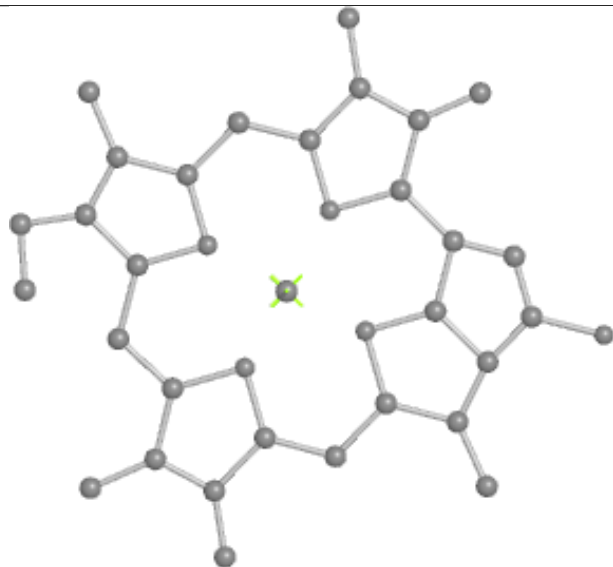
Ligand CLA 3 615



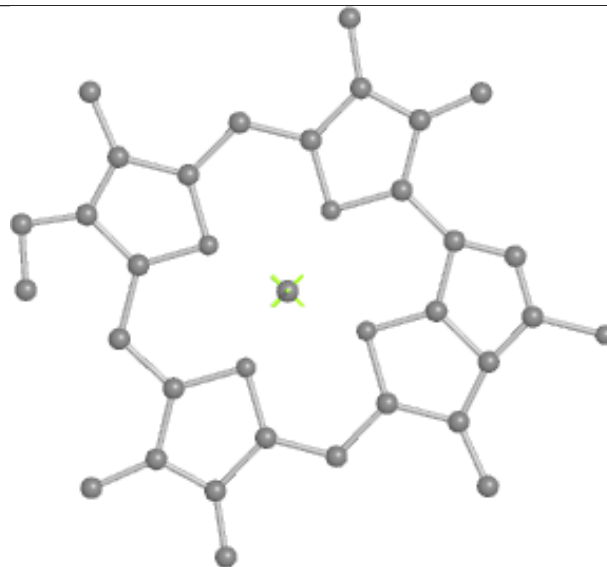
Bond lengths



Bond angles

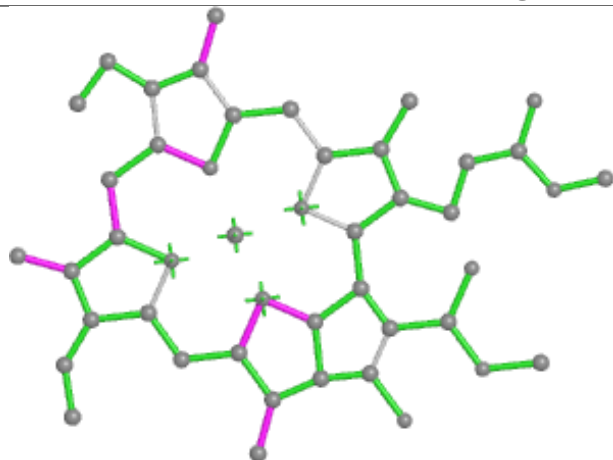


Torsions

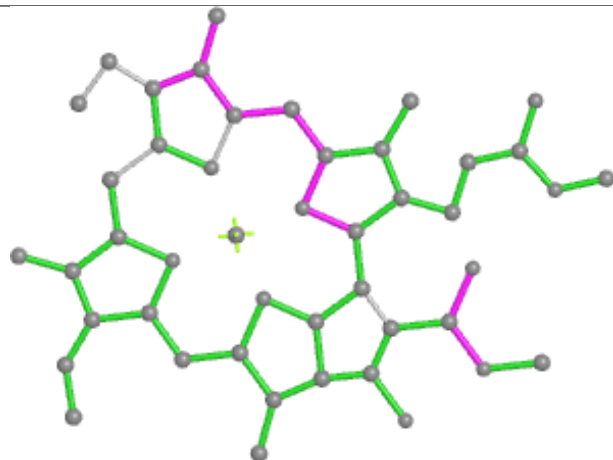


Rings

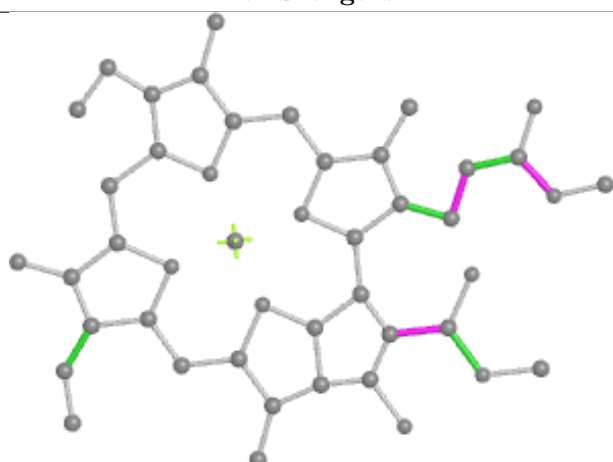
Ligand CLA A 828



Bond lengths



Bond angles

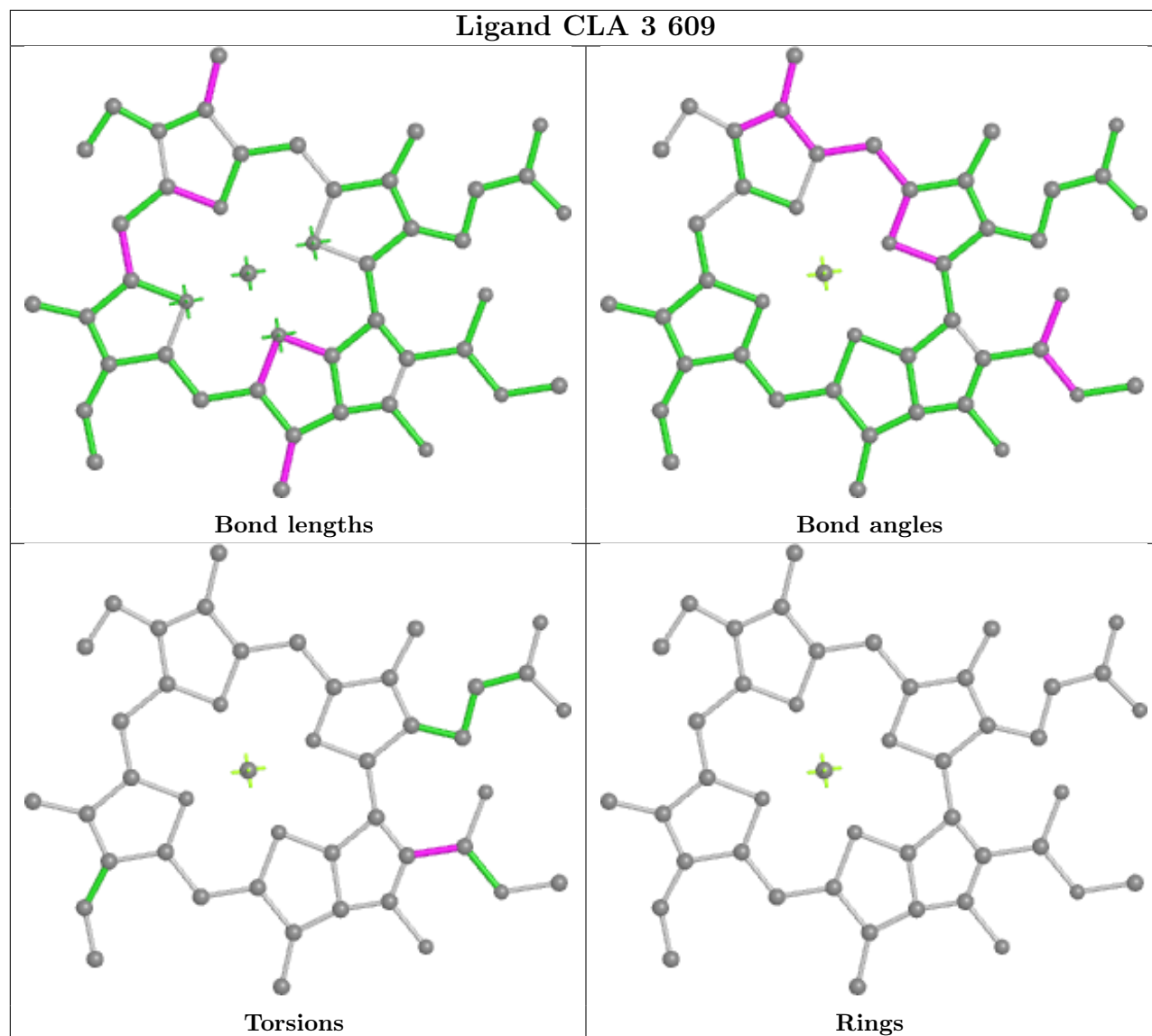


Torsions

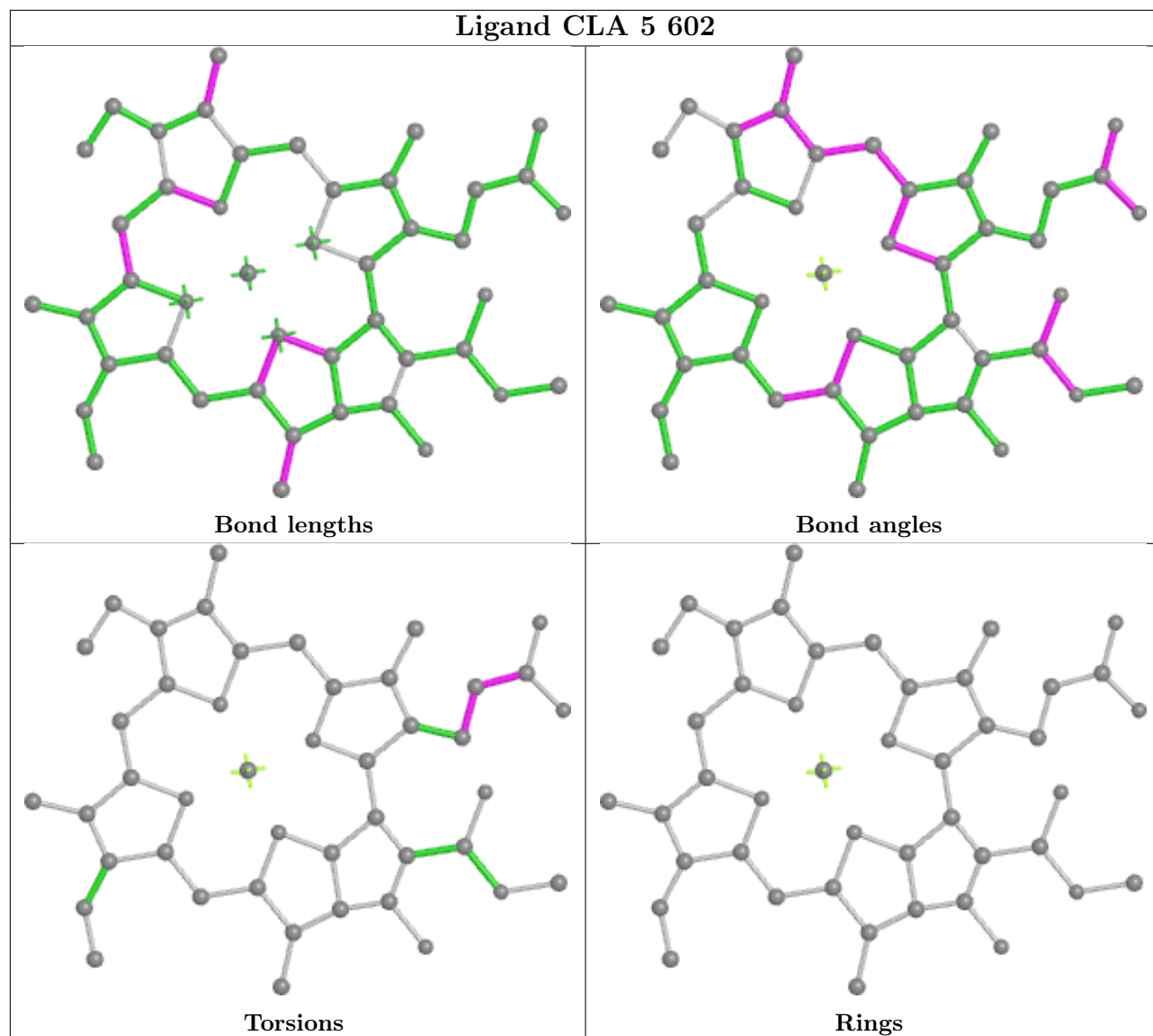


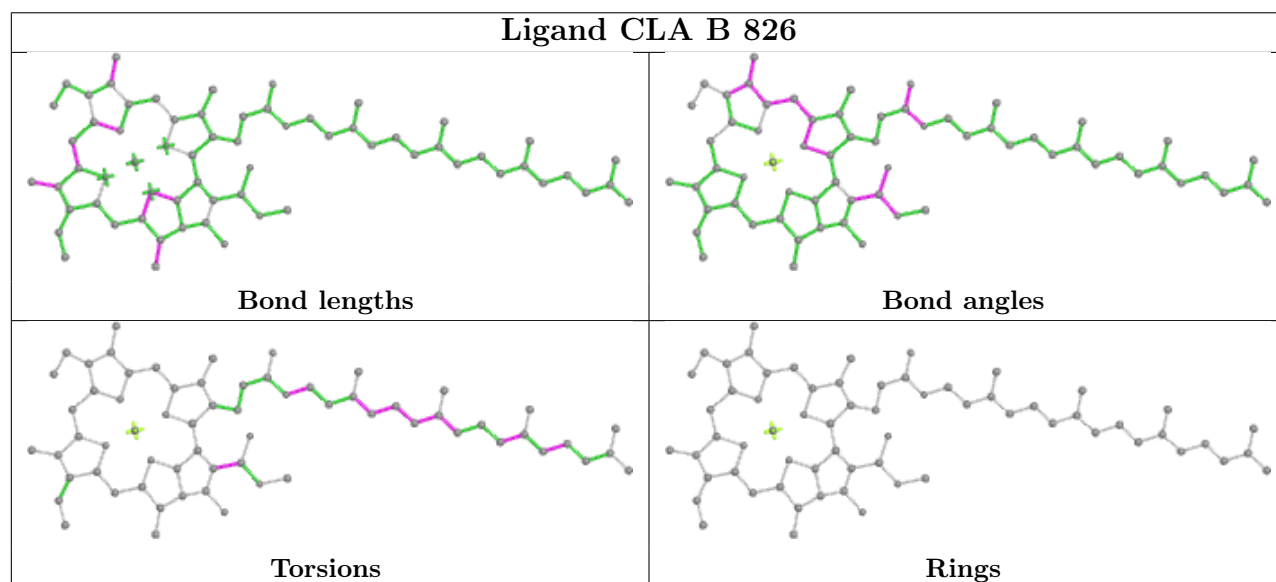
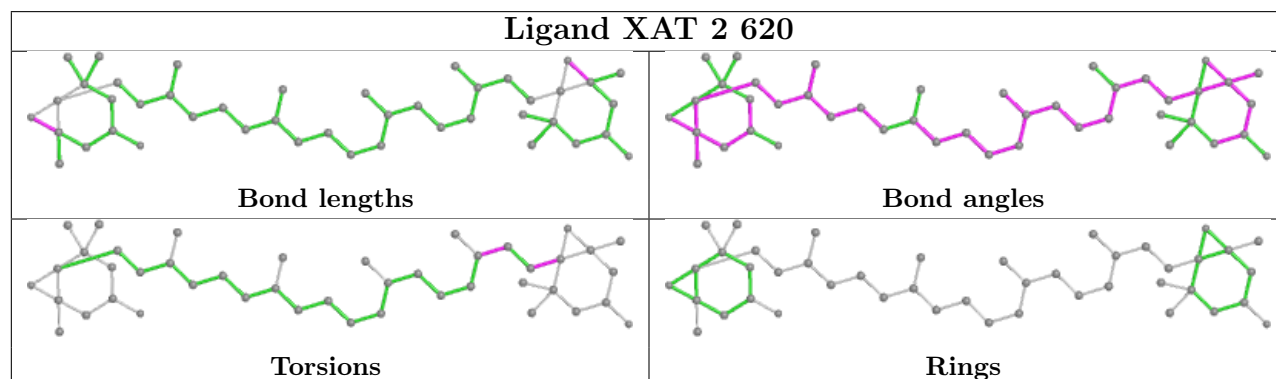
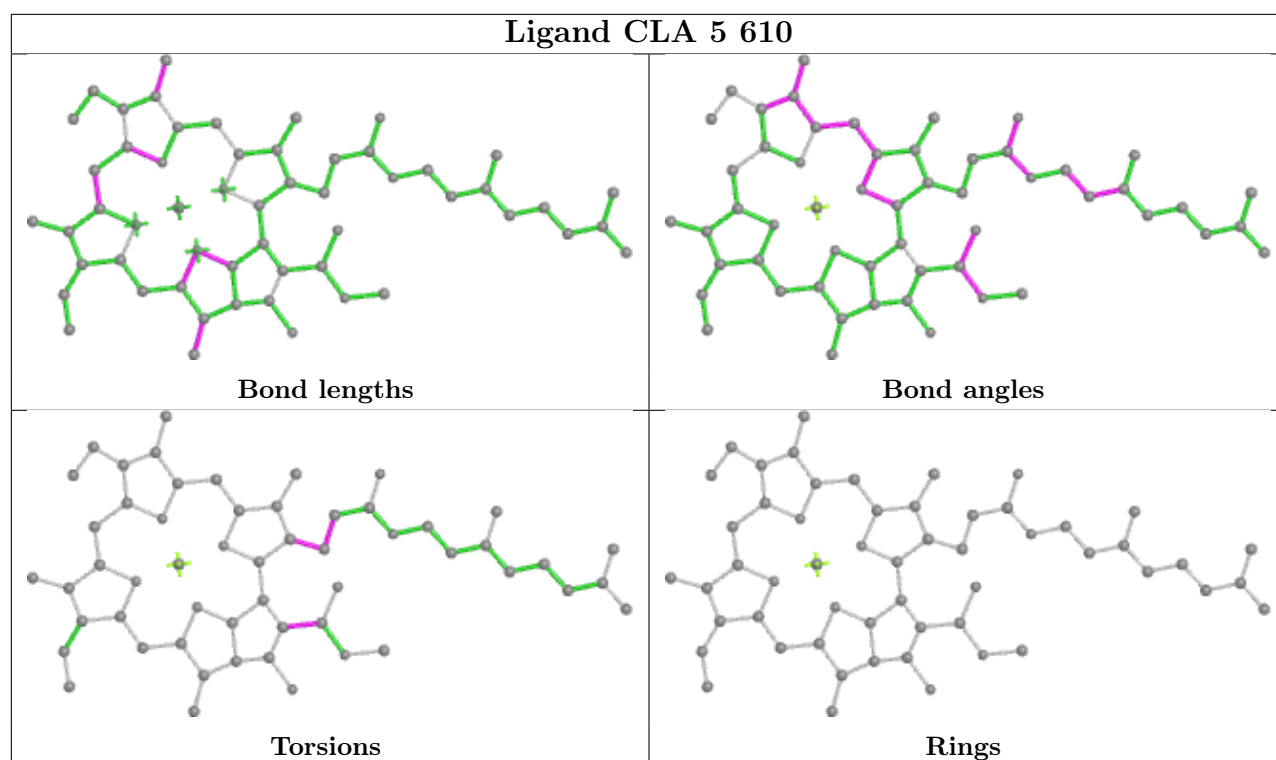
Rings

Ligand CLA 3 609

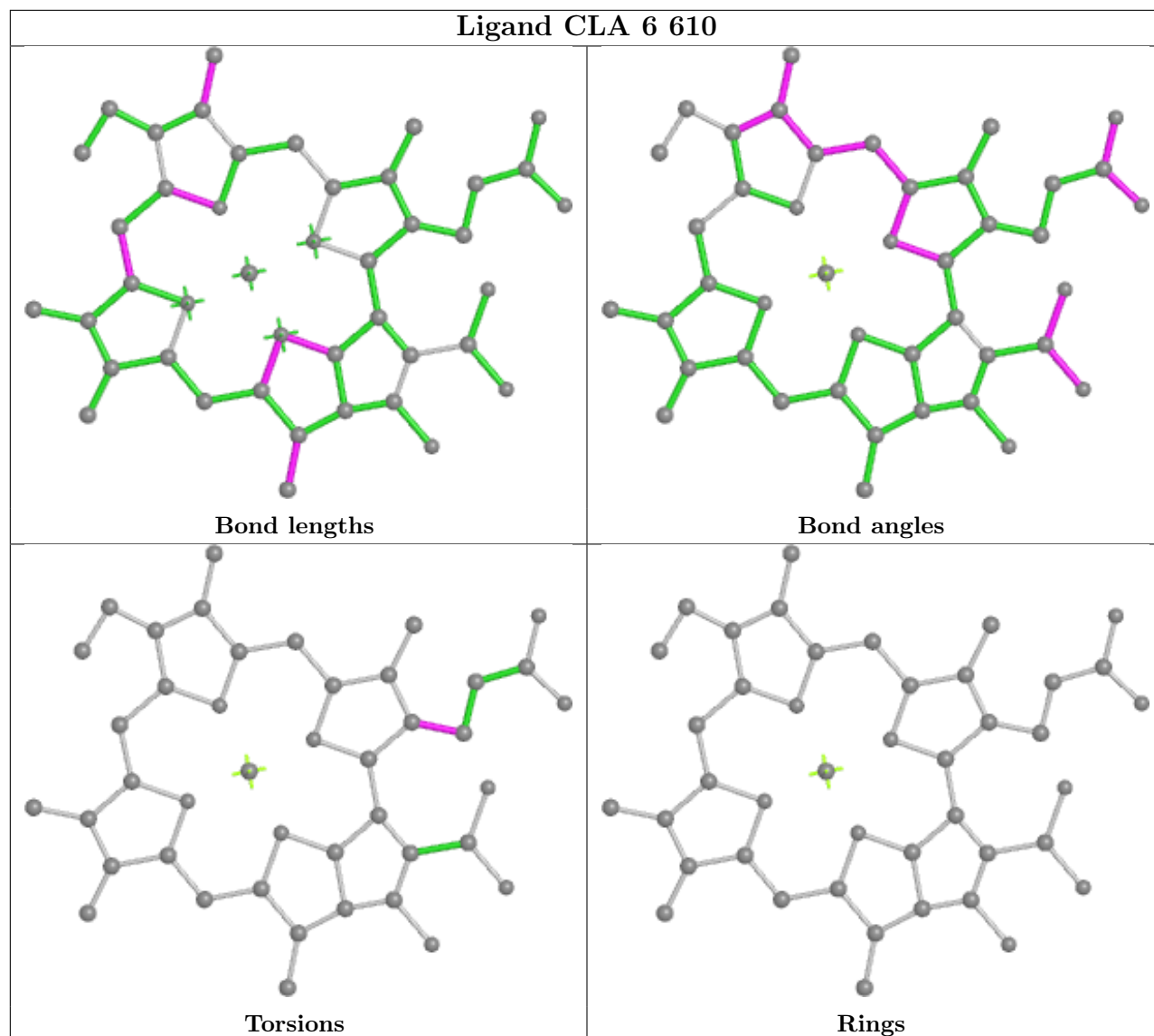


Ligand CLA 5 602

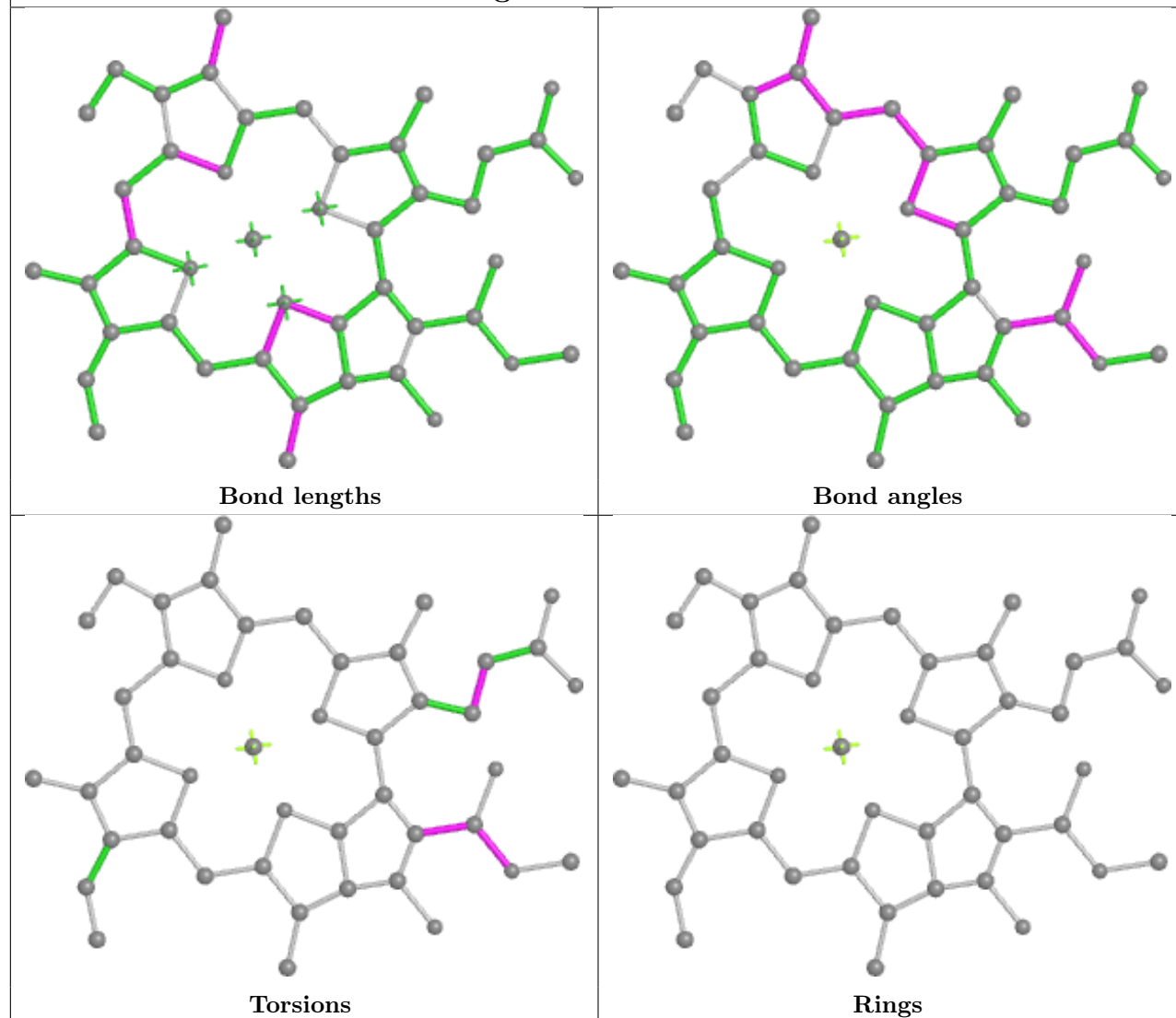




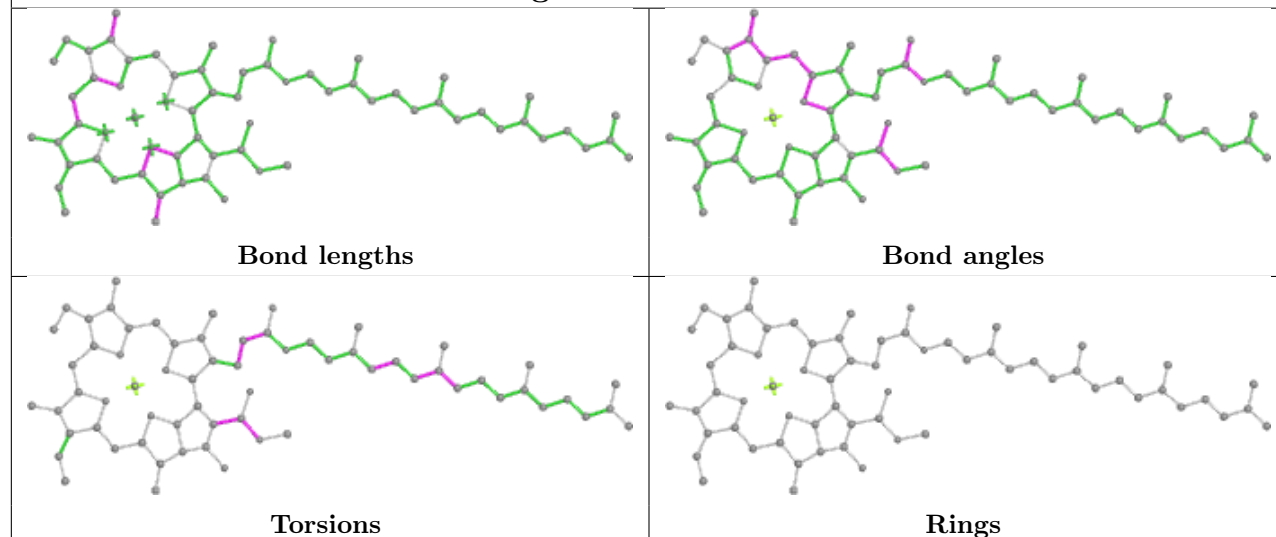
Ligand CLA 6 610

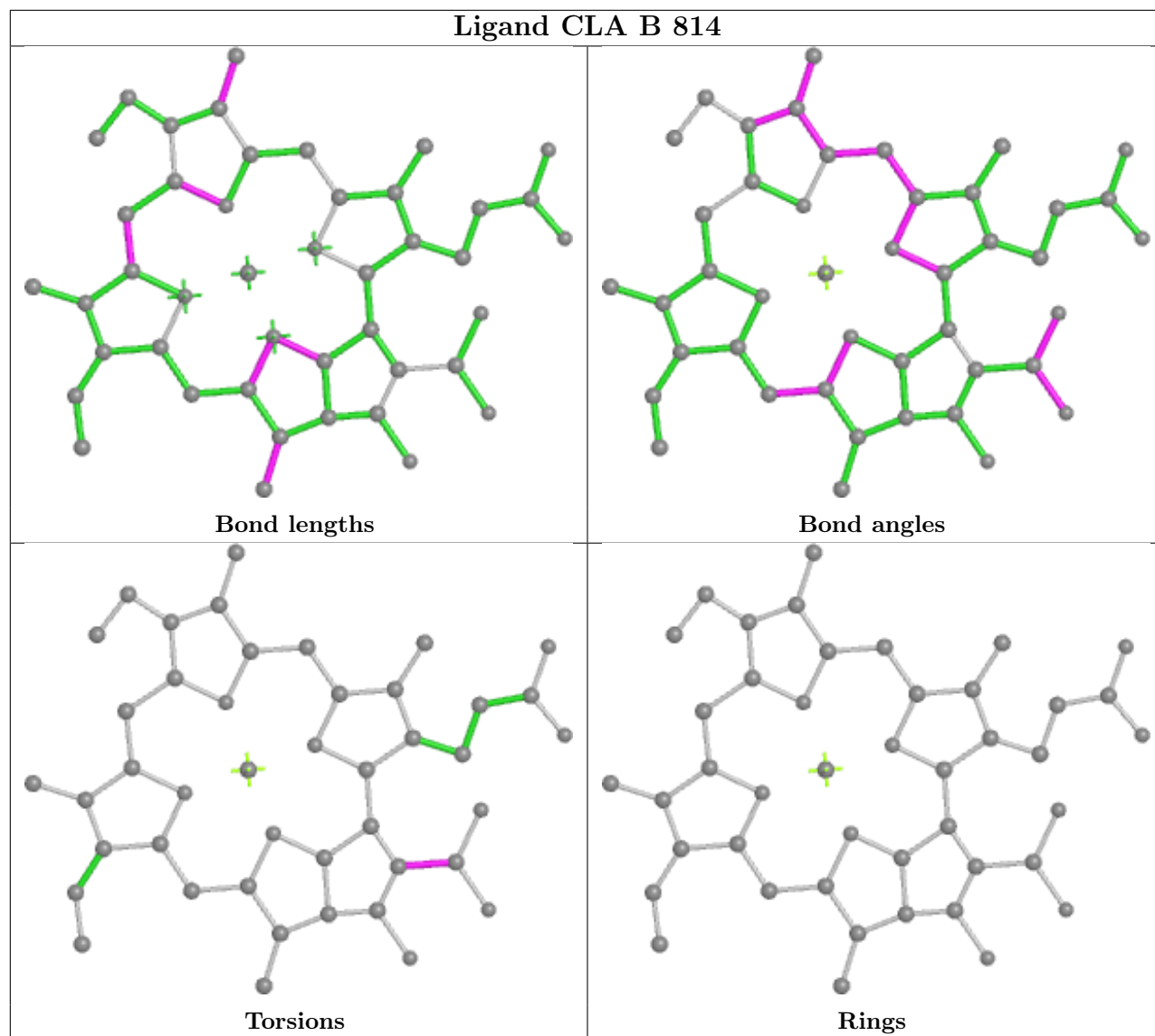
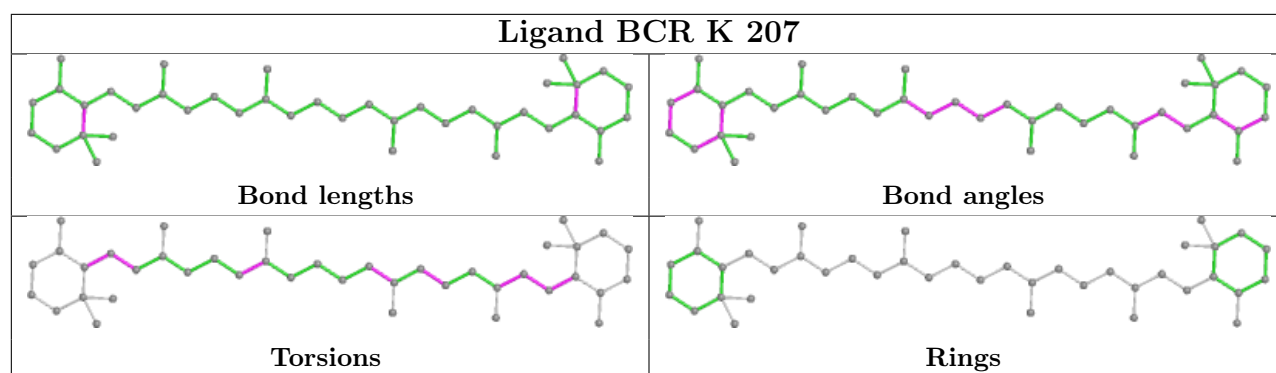


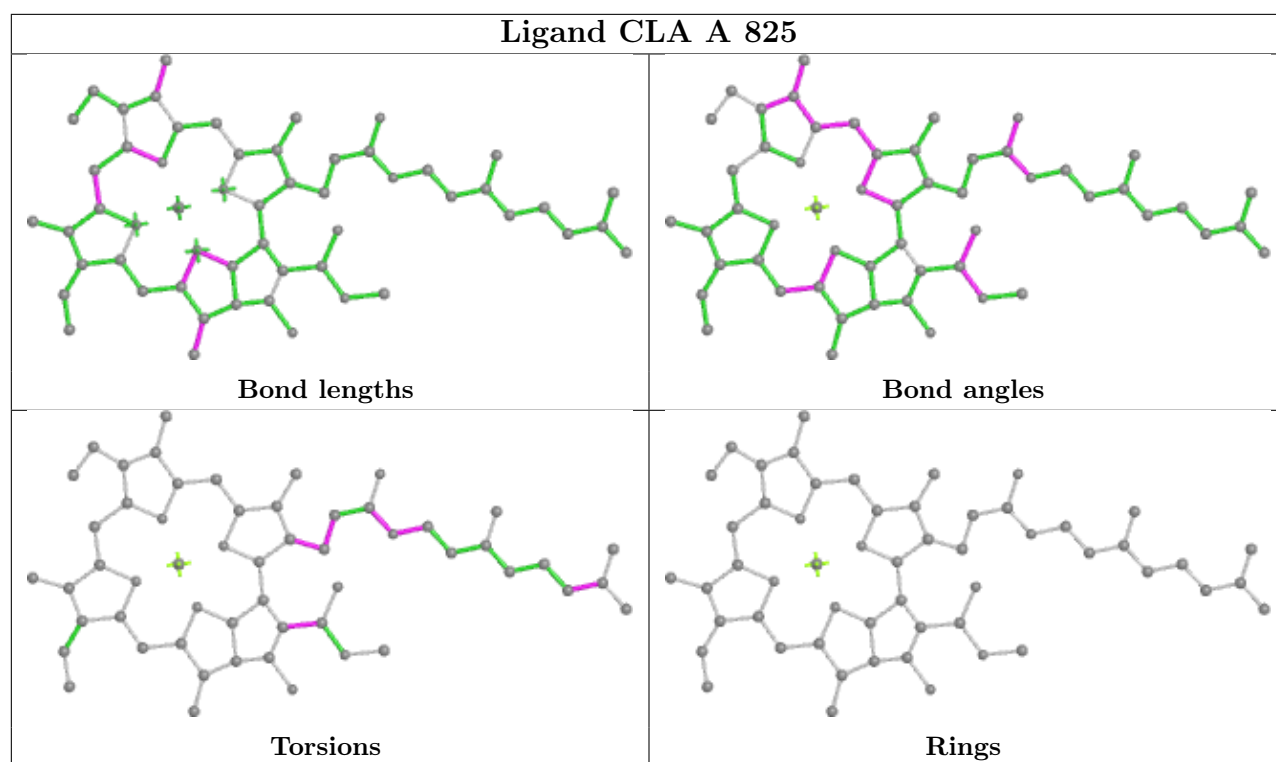
Ligand CLA 5 613



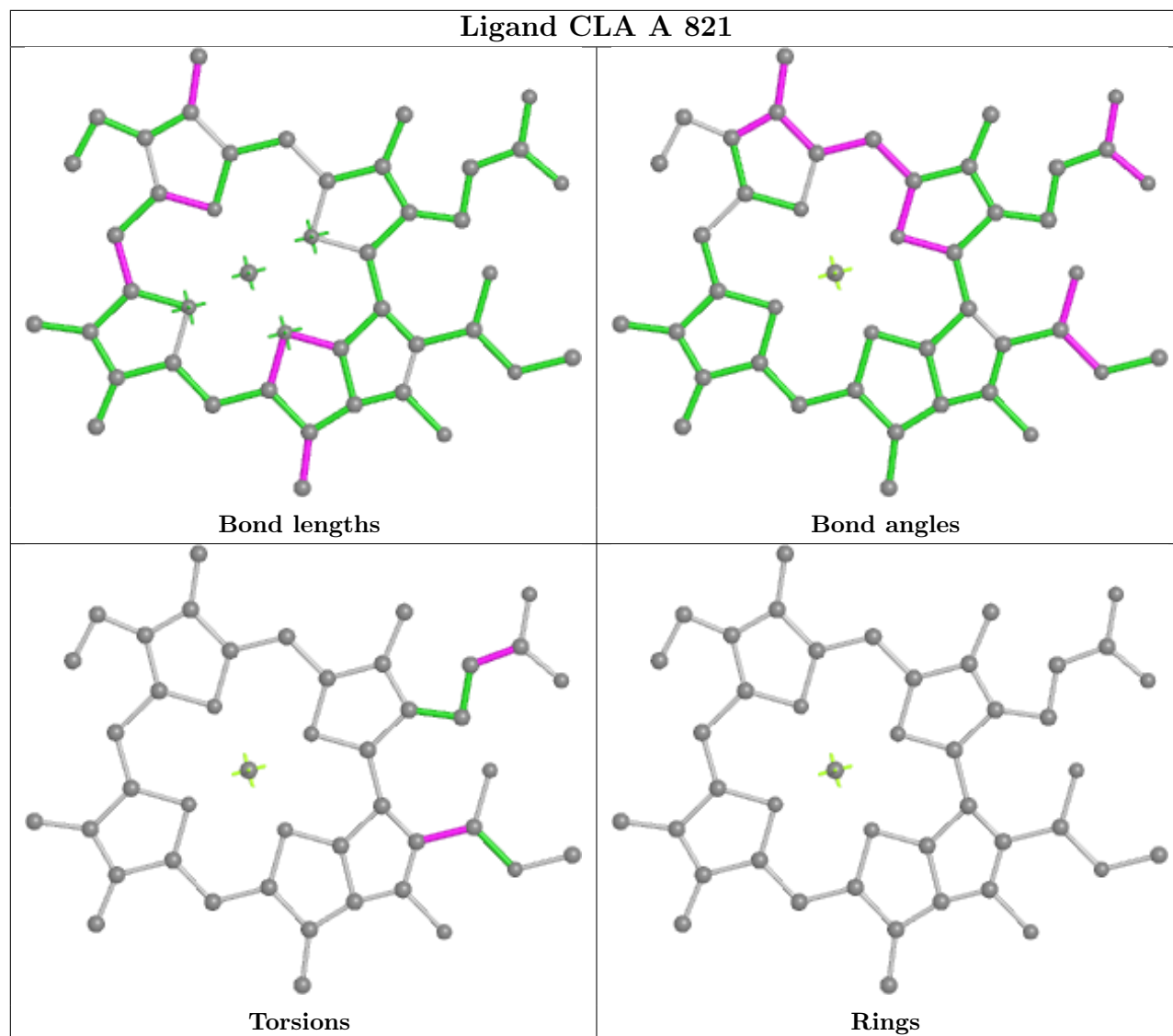
Ligand CLA A 826



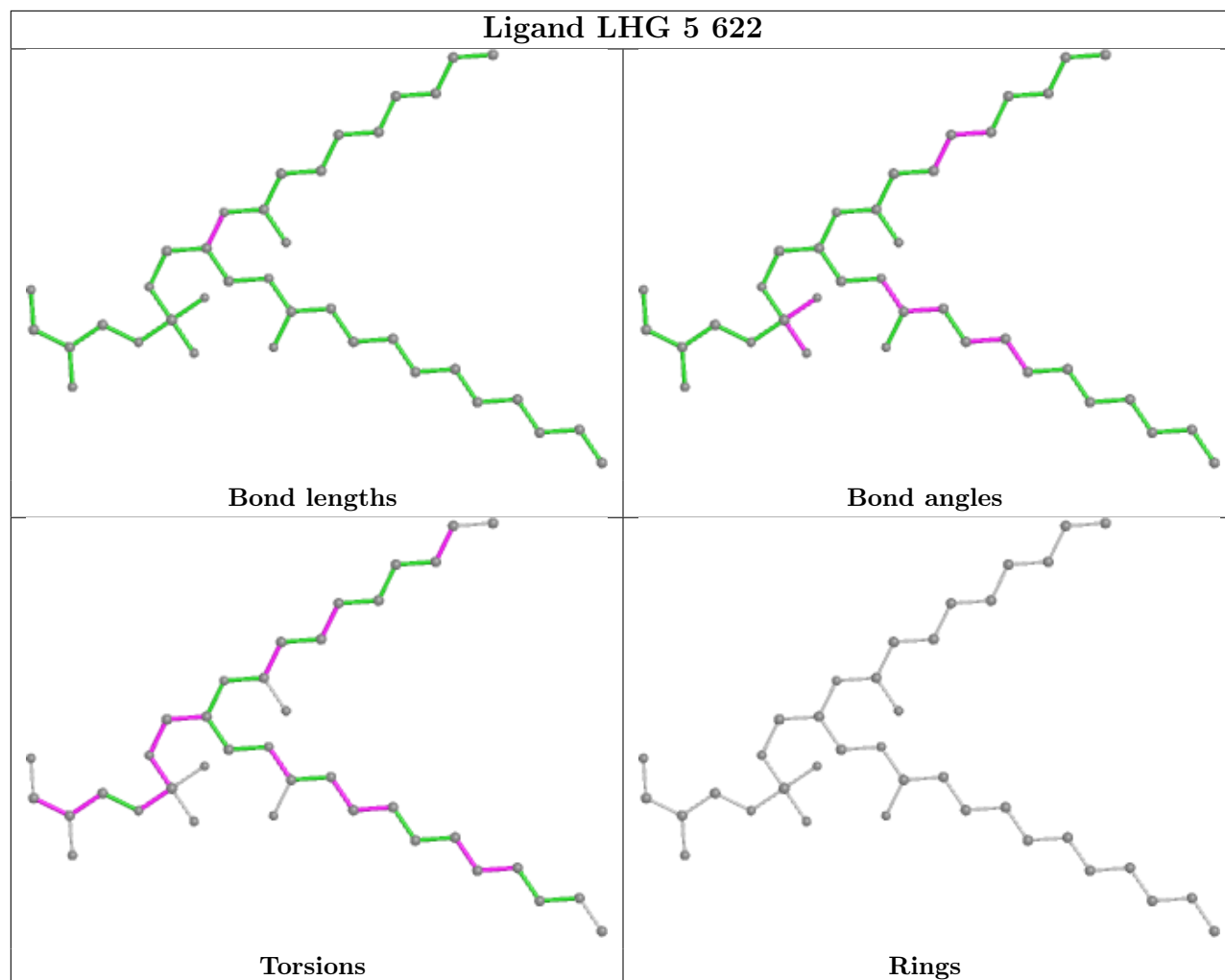




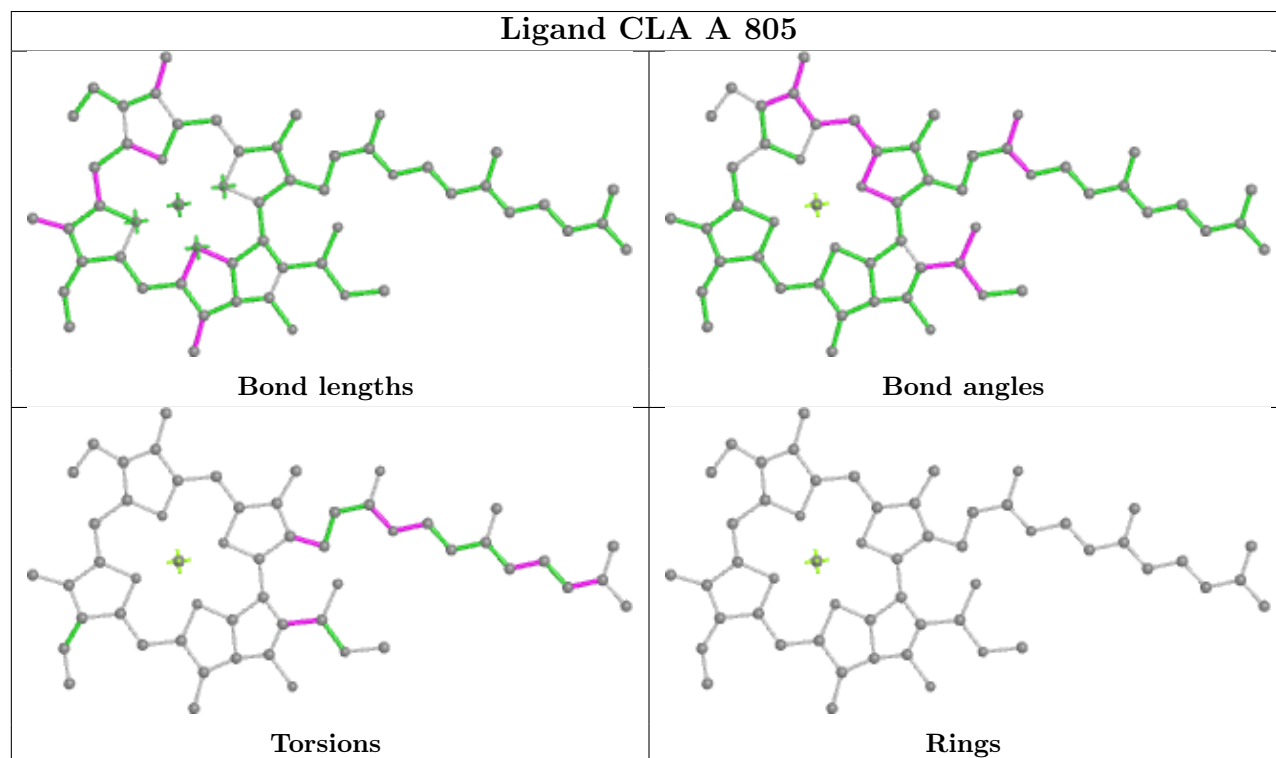
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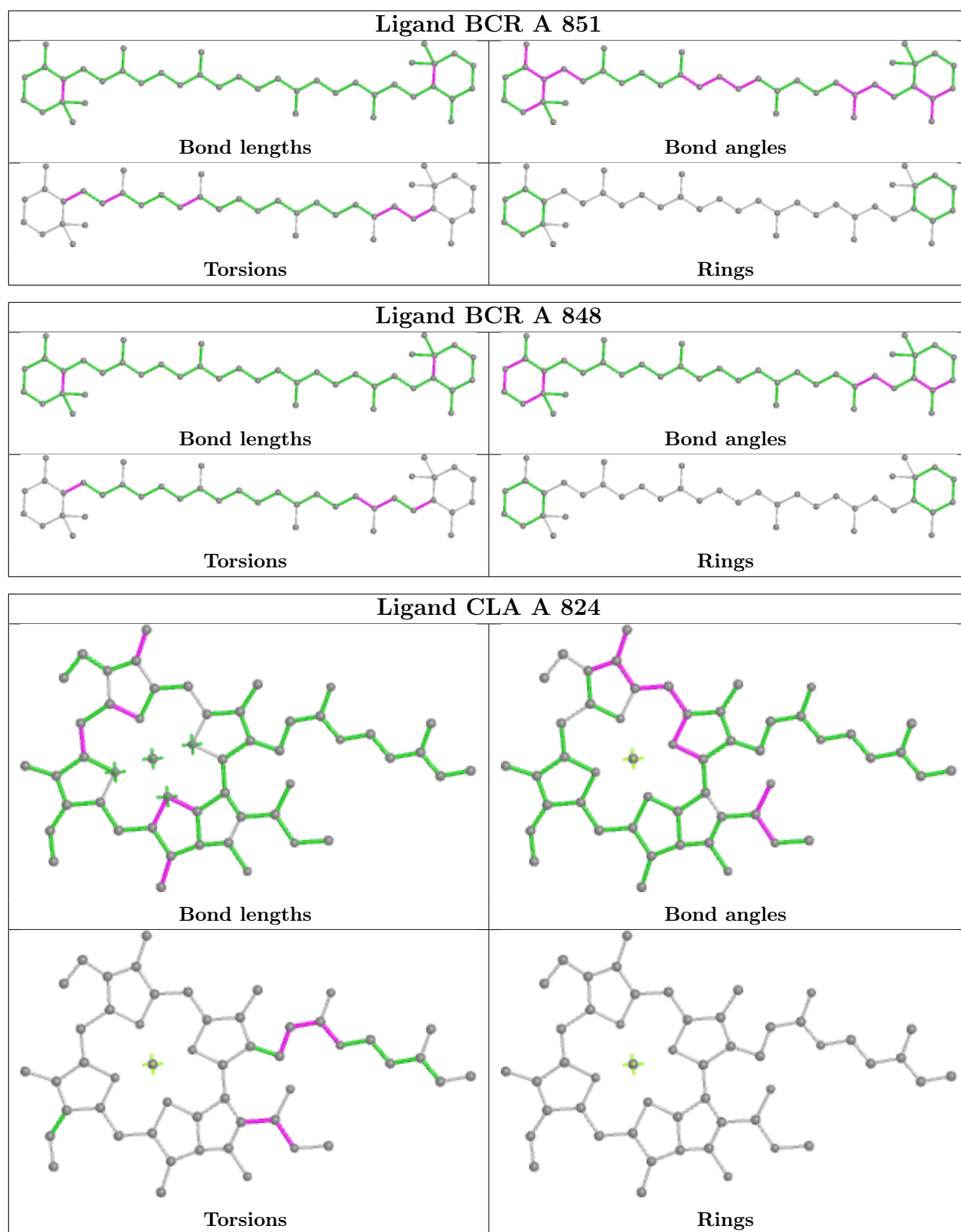


Ligand LHG 5 622

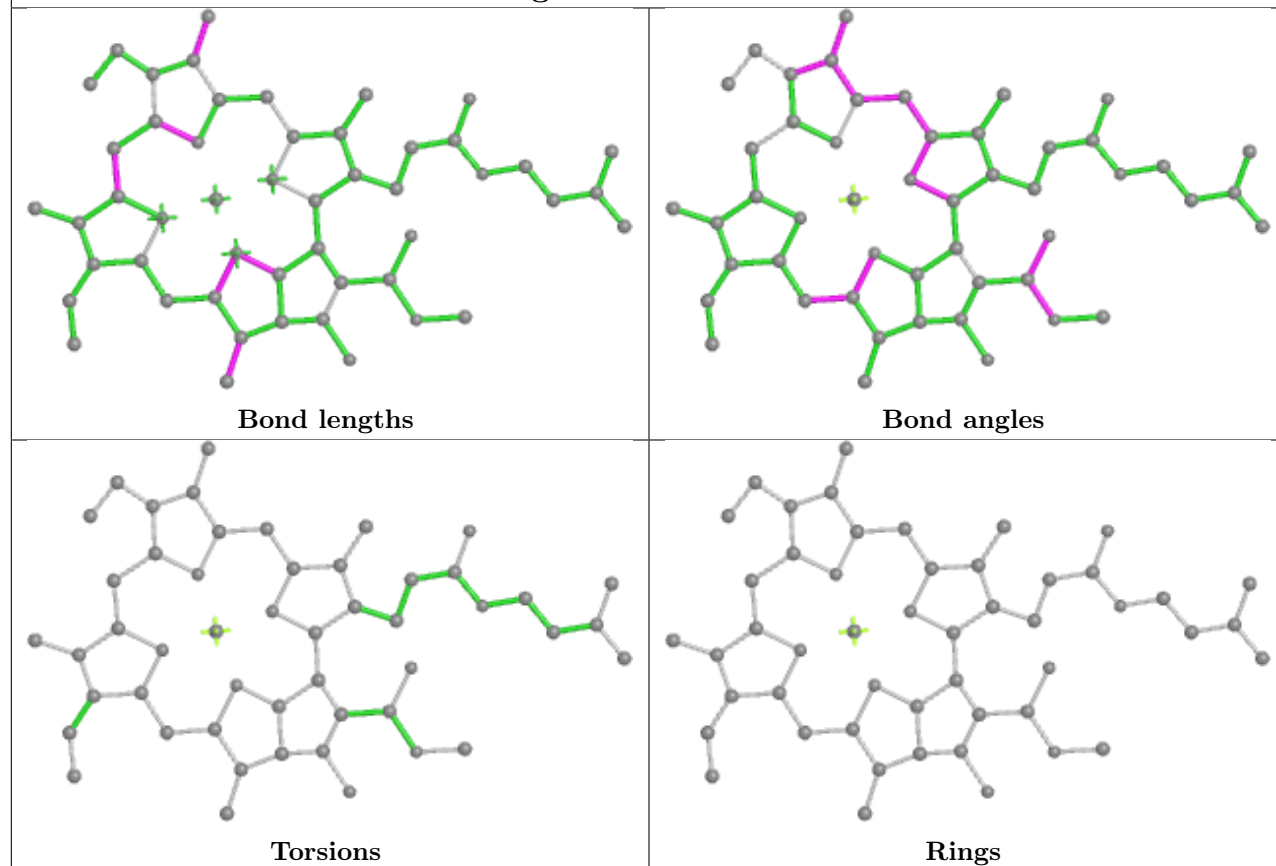


Ligand CLA A 805

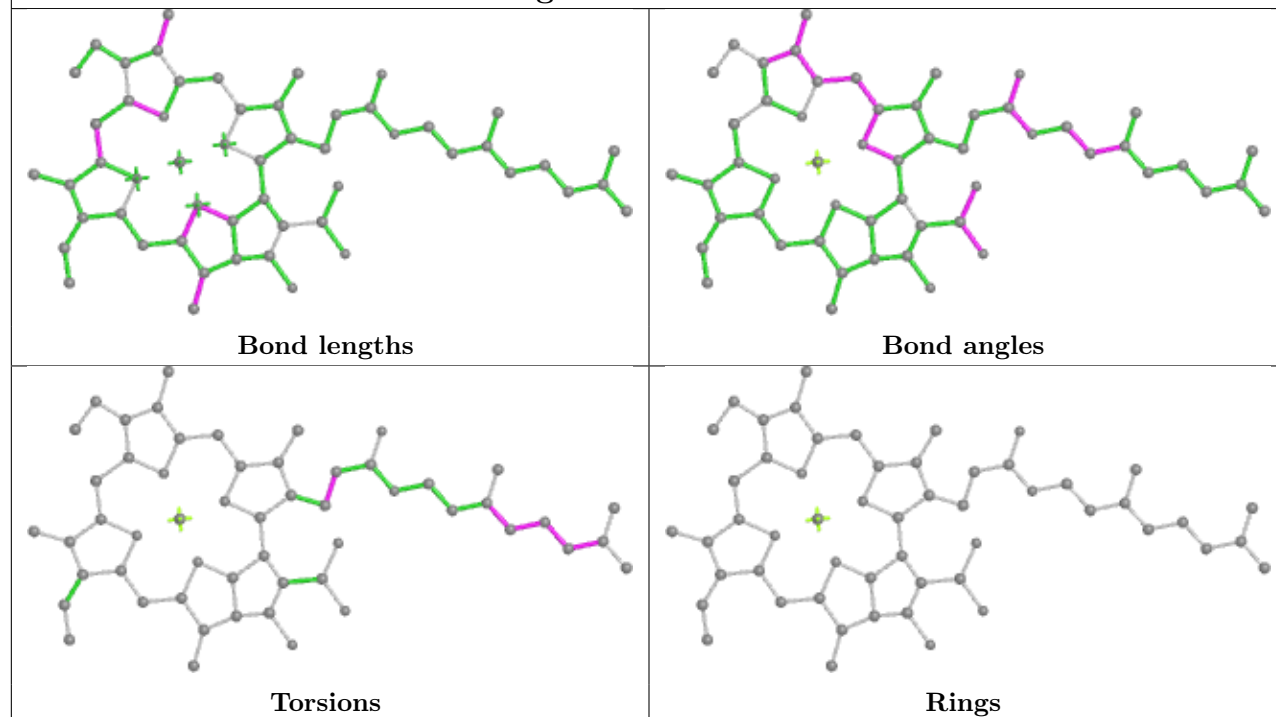




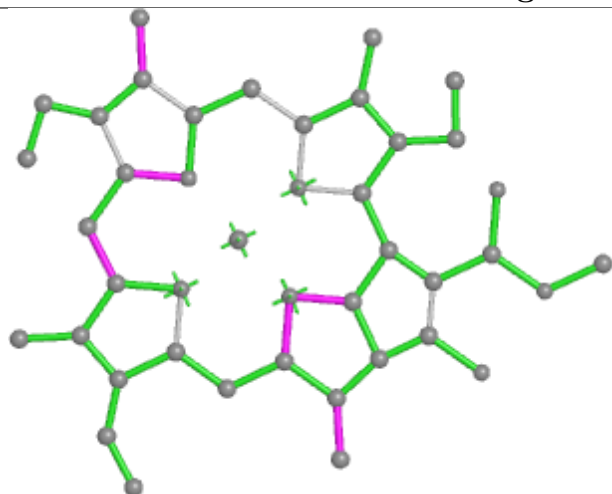
Ligand CLA A 836



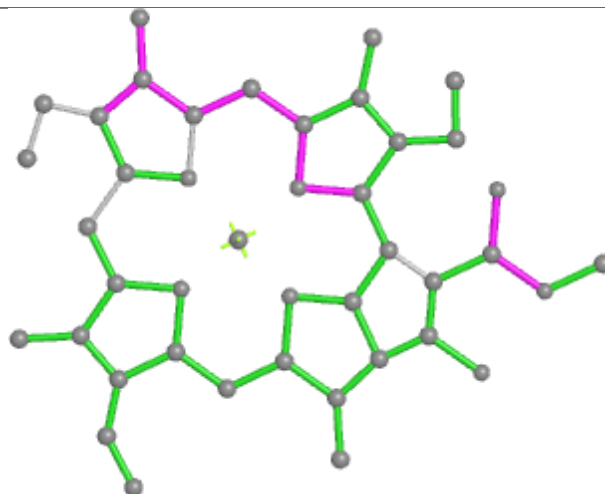
Ligand CLA 3 613



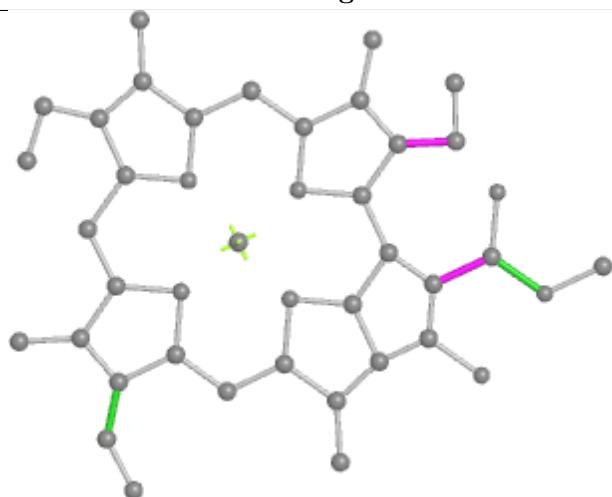
Ligand CLA J 101



Bond lengths



Bond angles

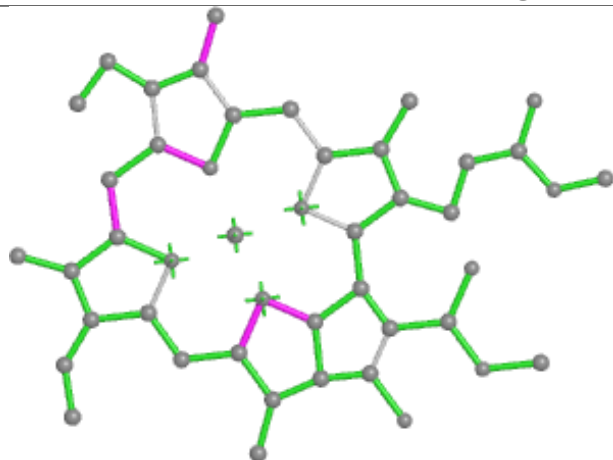


Torsions

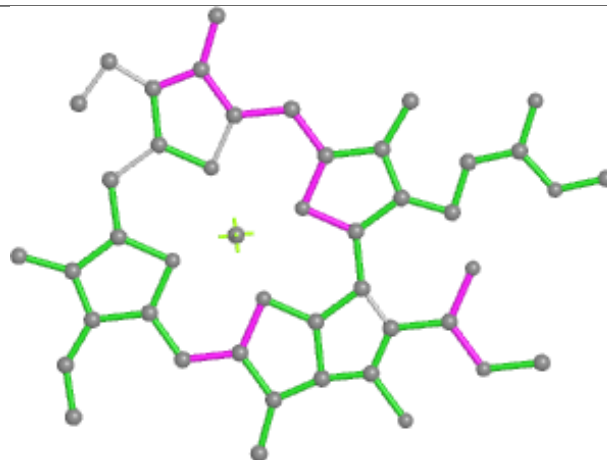


Rings

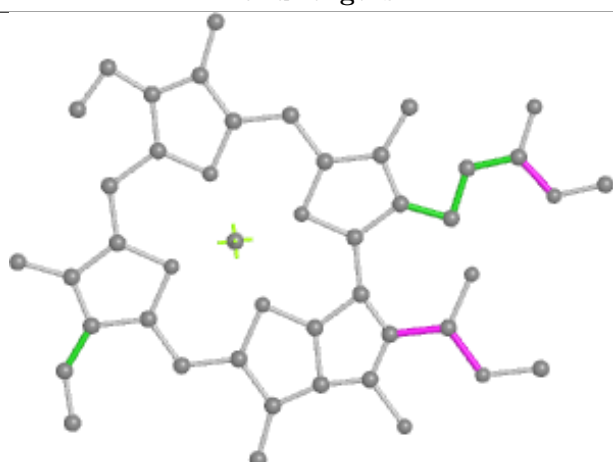
Ligand CLA B 821



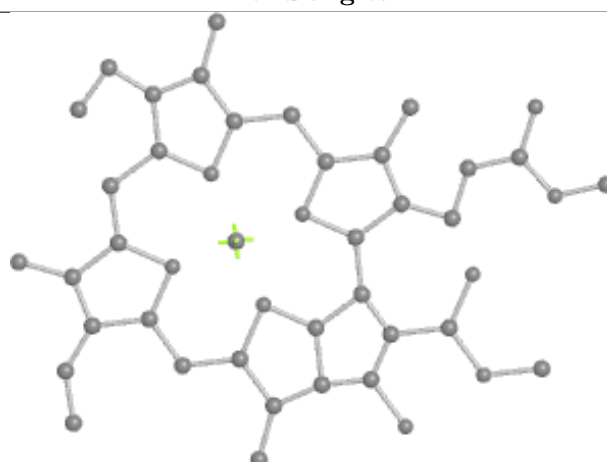
Bond lengths



Bond angles

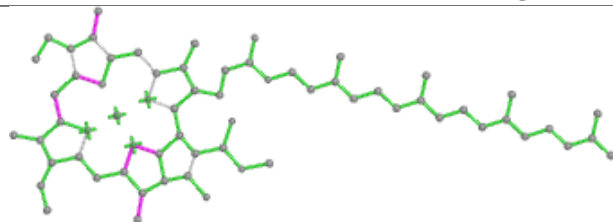


Torsions

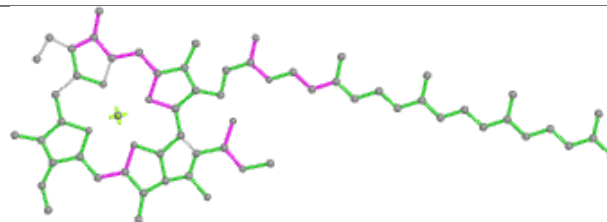


Rings

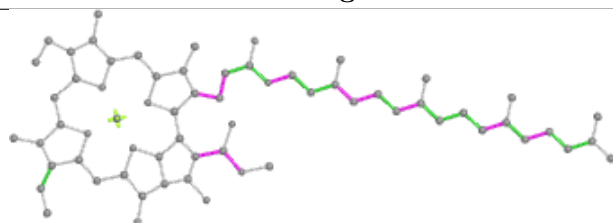
Ligand CLA A 854



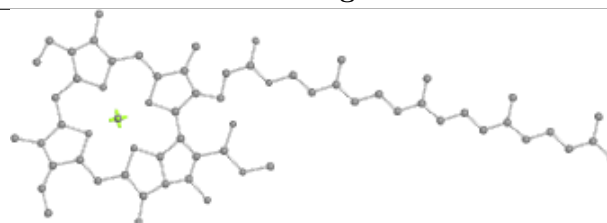
Bond lengths



Bond angles

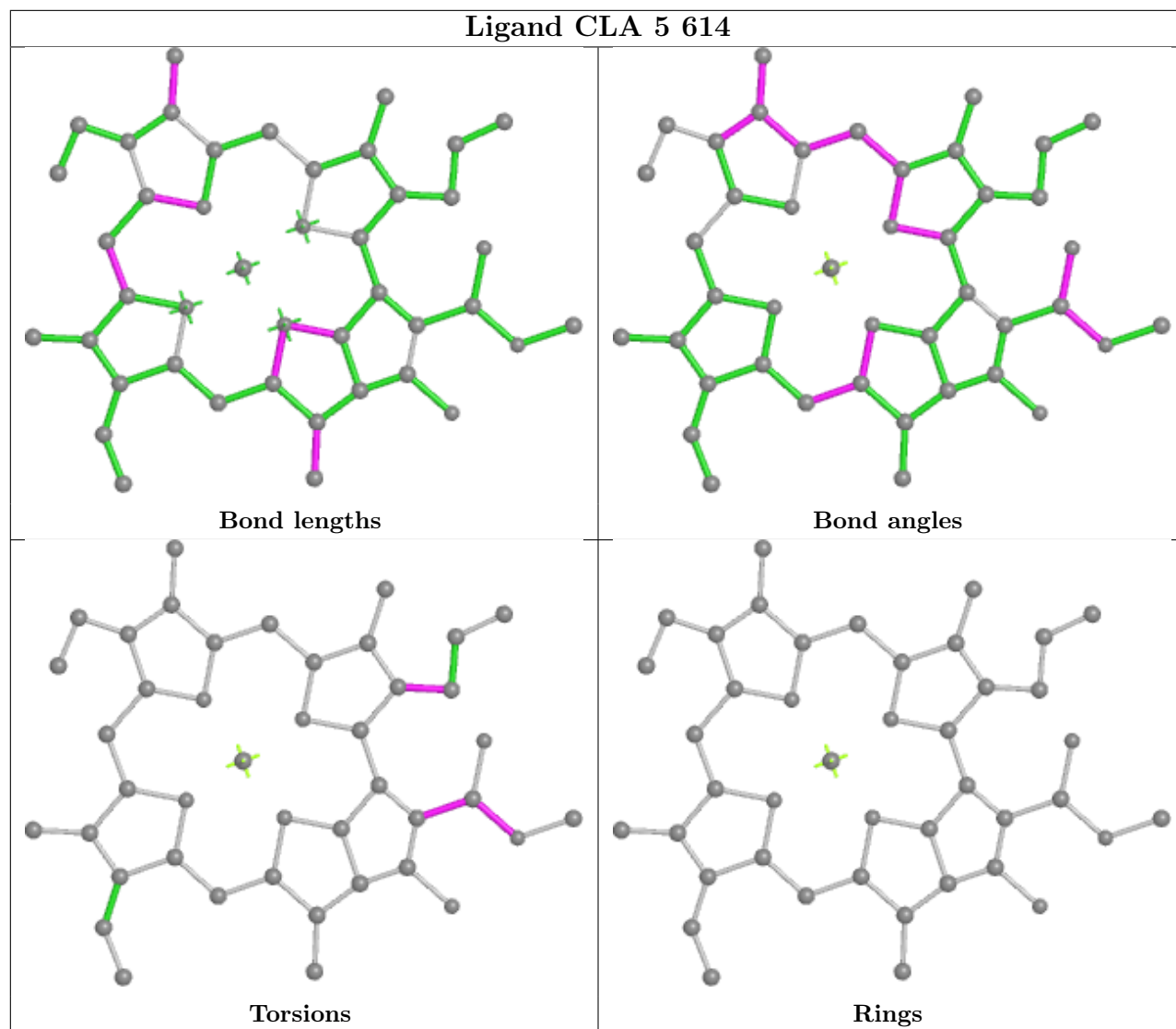


Torsions

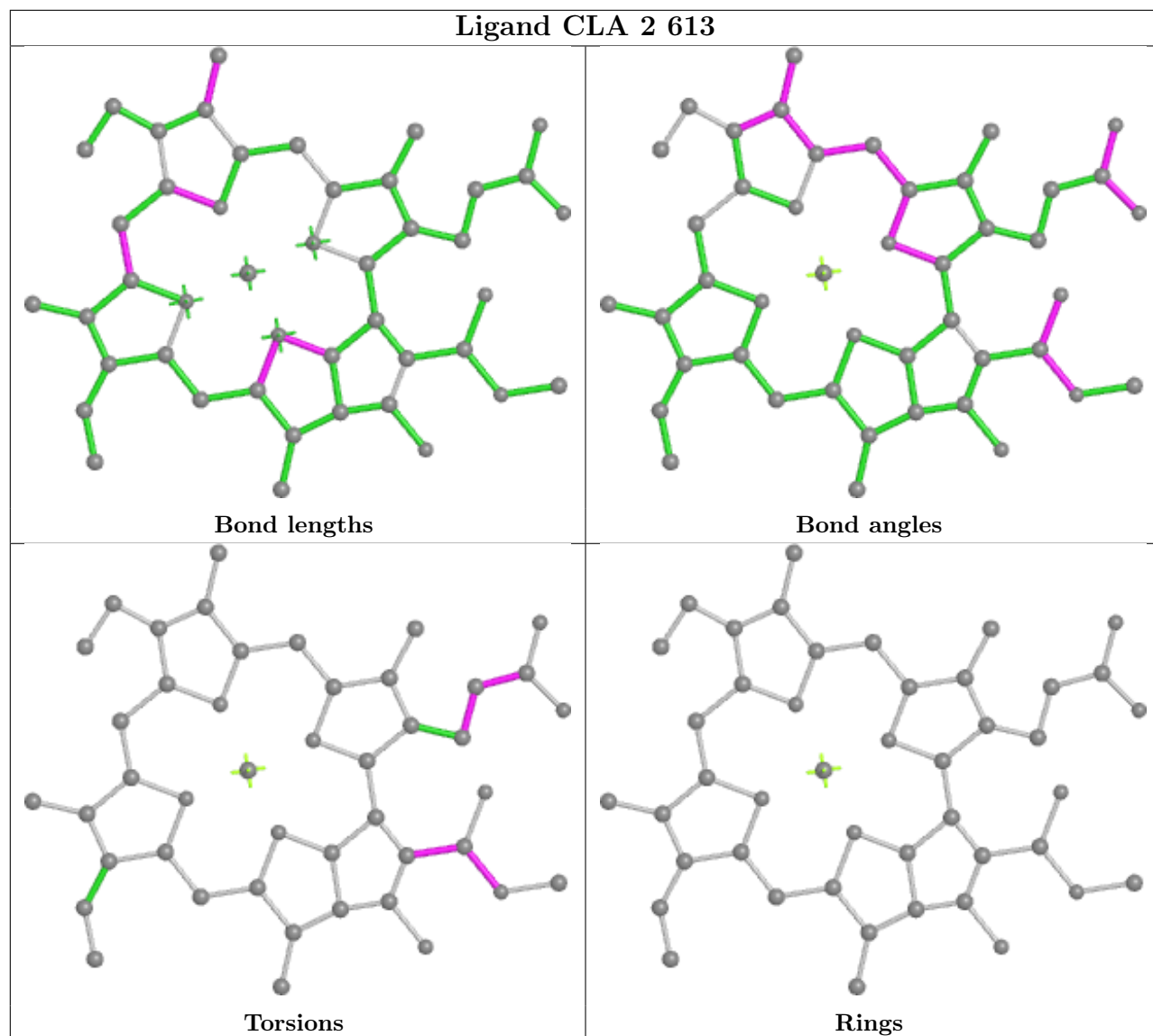


Rings

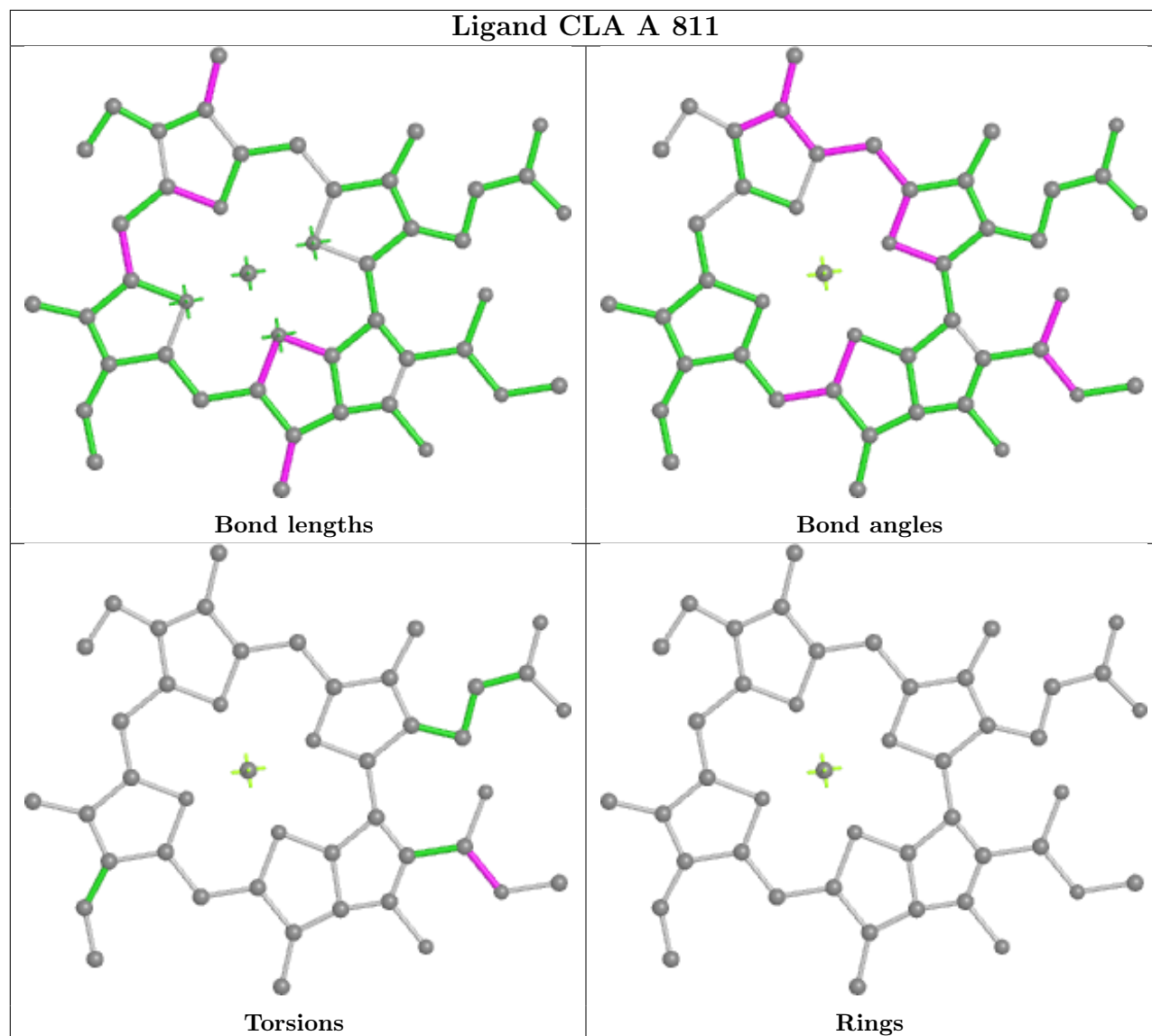
Ligand CLA 5 614

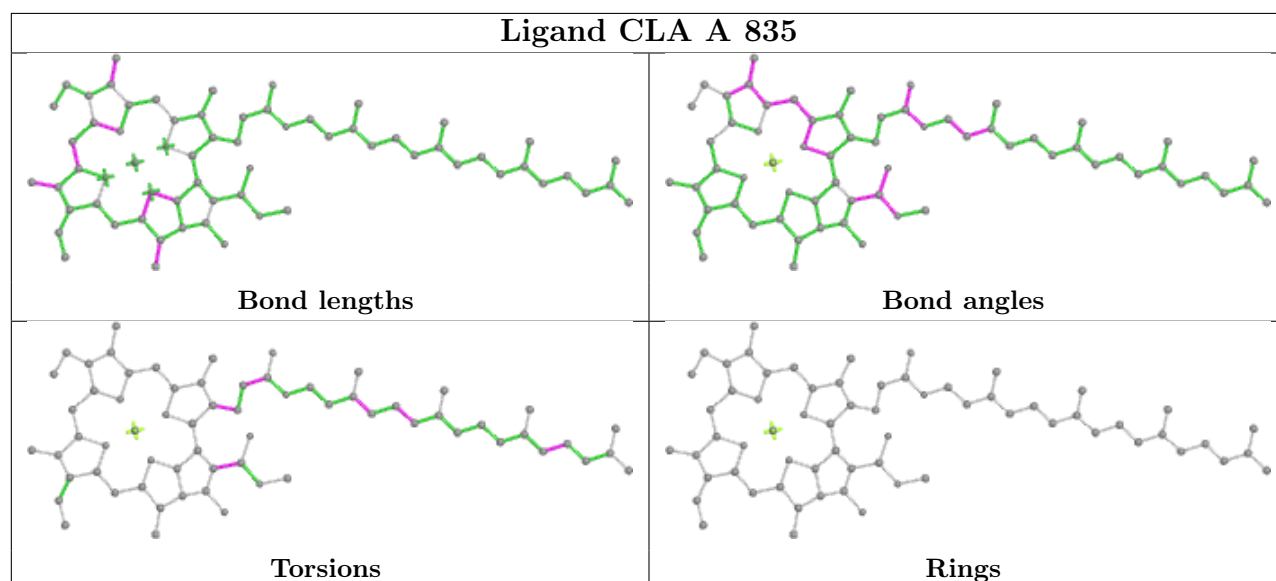
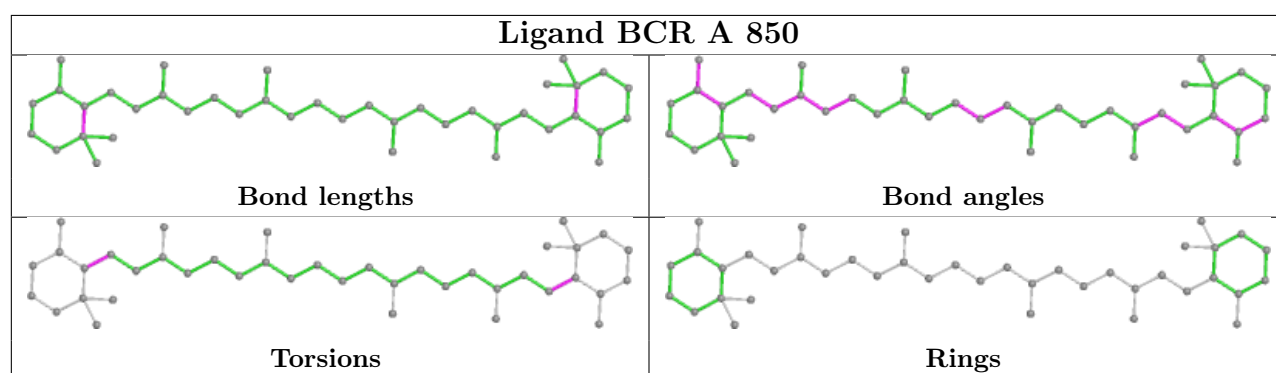
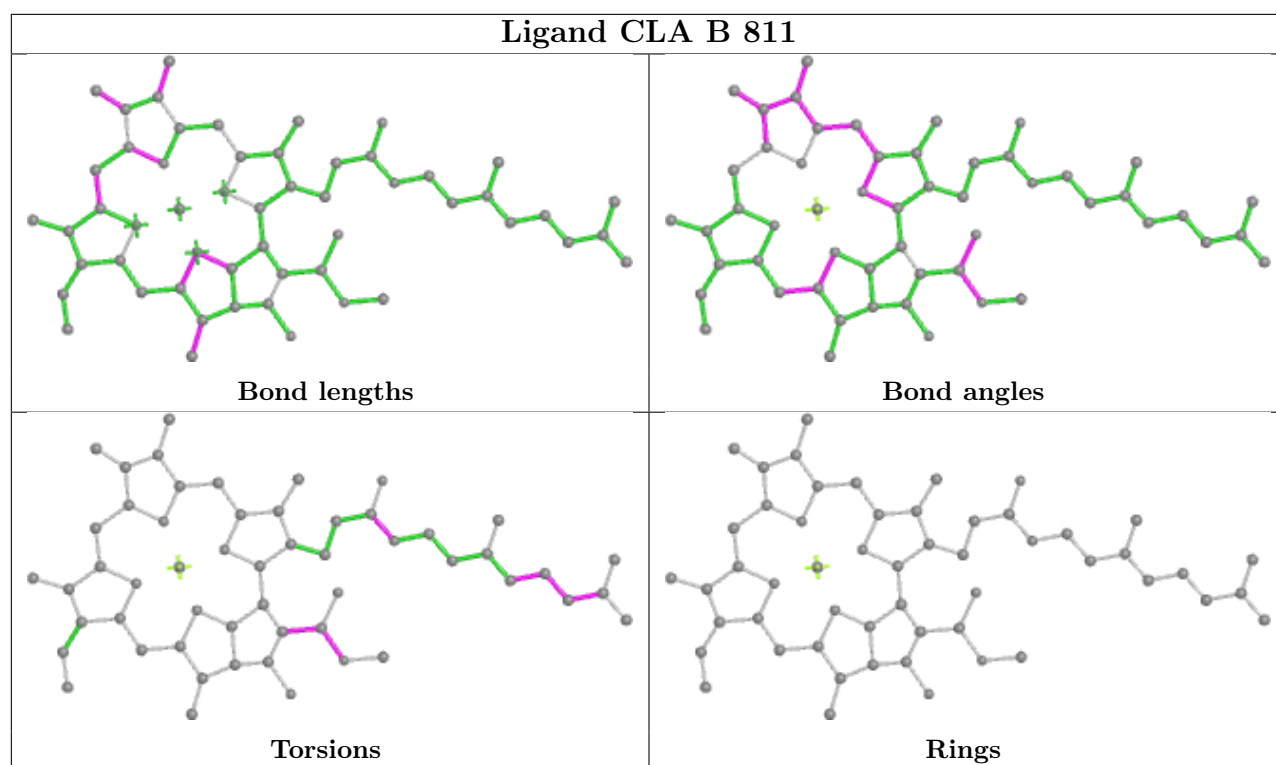


Ligand CLA 2 613

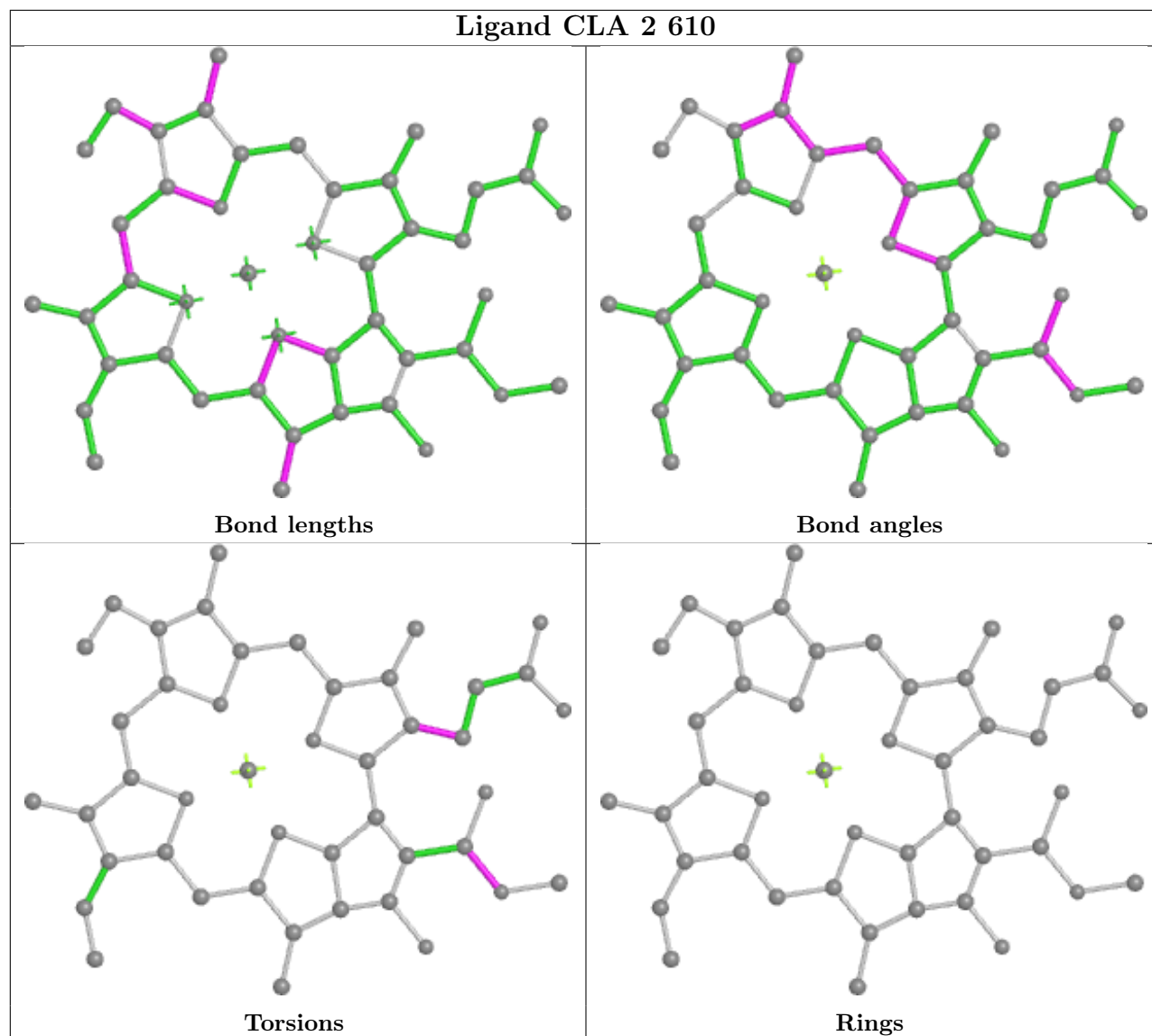


Ligand CLA A 811

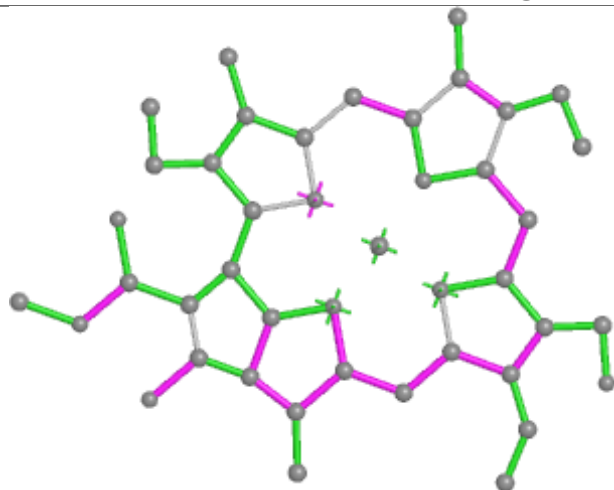




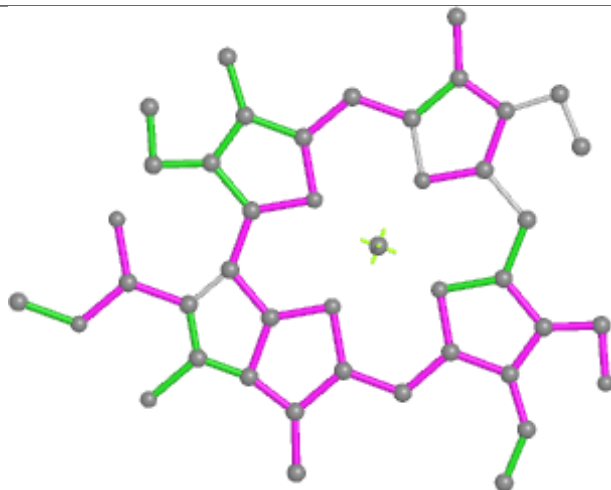
Ligand CLA 2 610



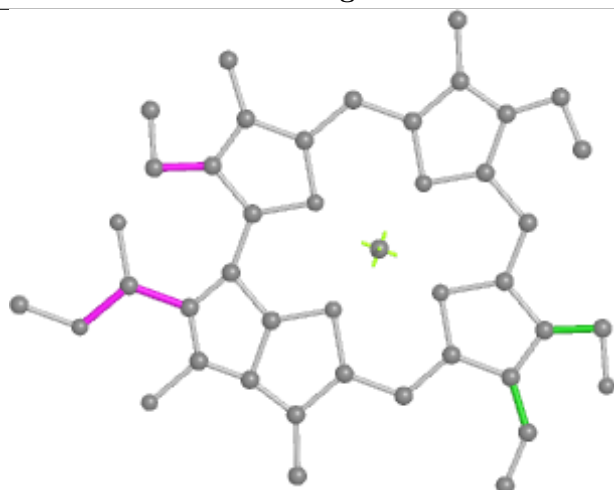
Ligand CHL 5 607



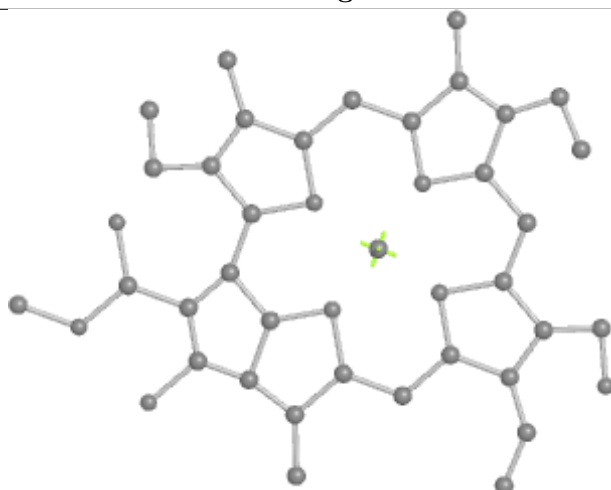
Bond lengths



Bond angles

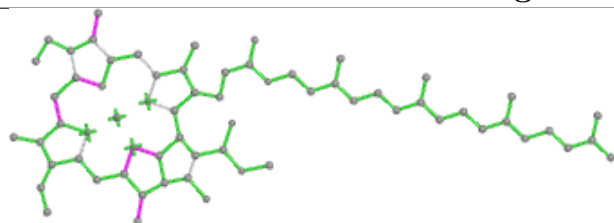


Torsions

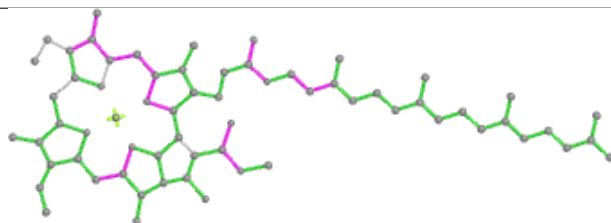


Rings

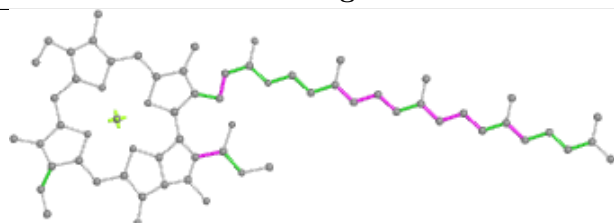
Ligand CLA B 807



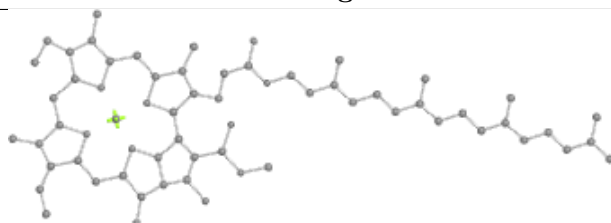
Bond lengths



Bond angles

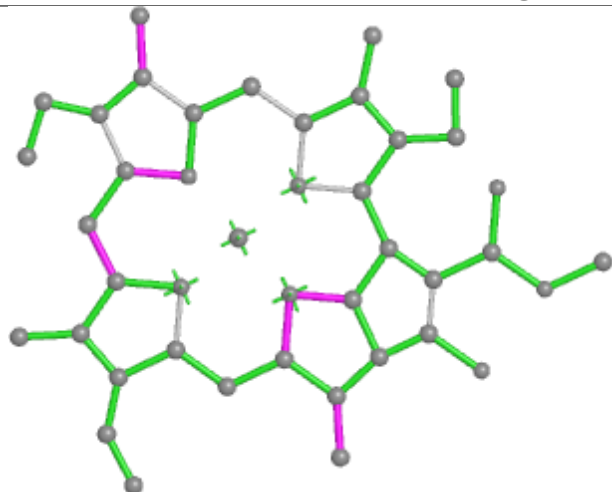


Torsions

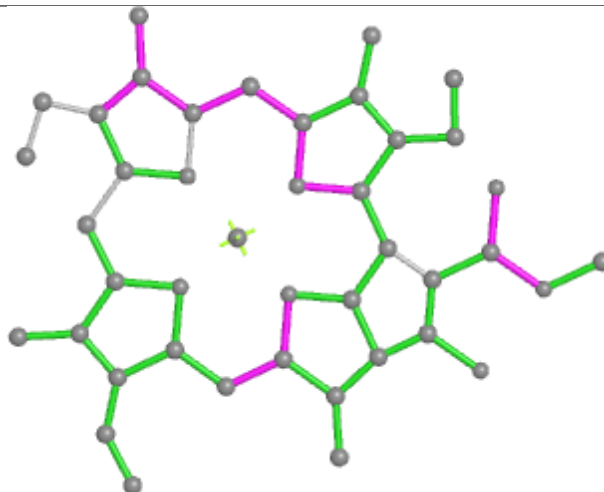


Rings

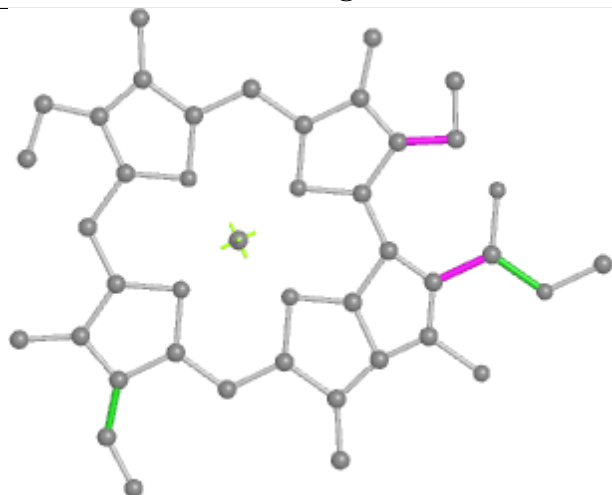
Ligand CLA L 304



Bond lengths



Bond angles

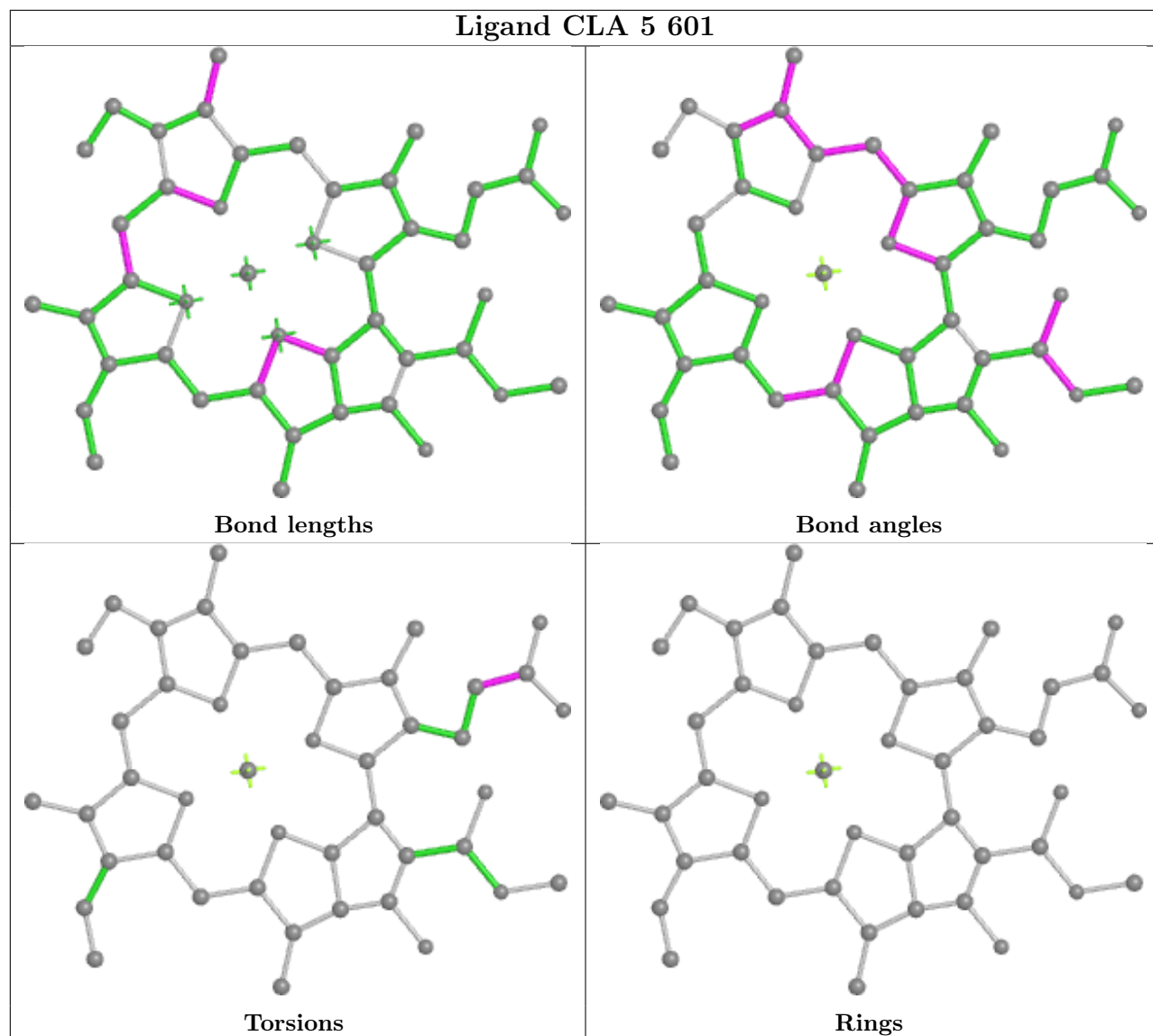


Torsions

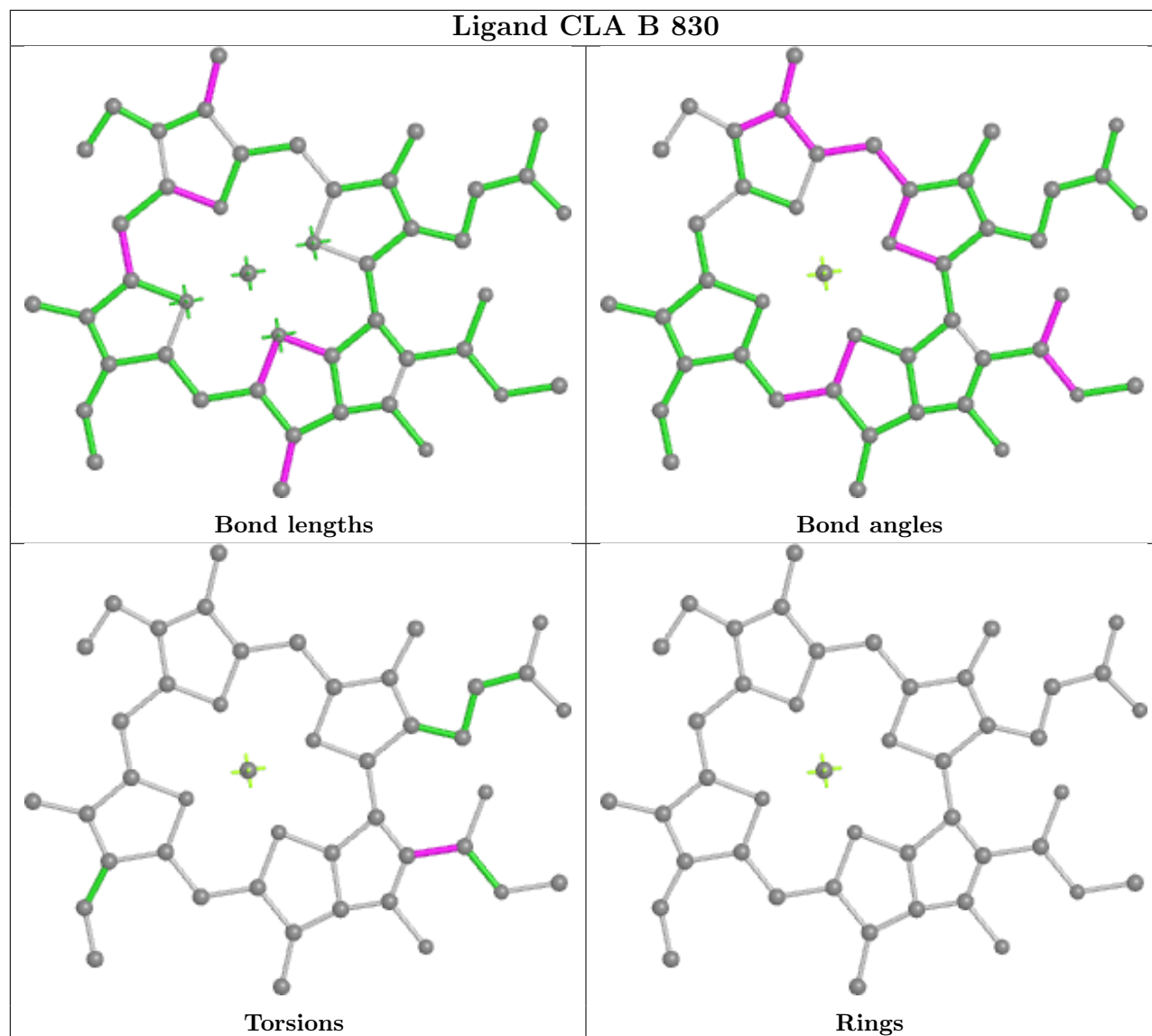


Rings

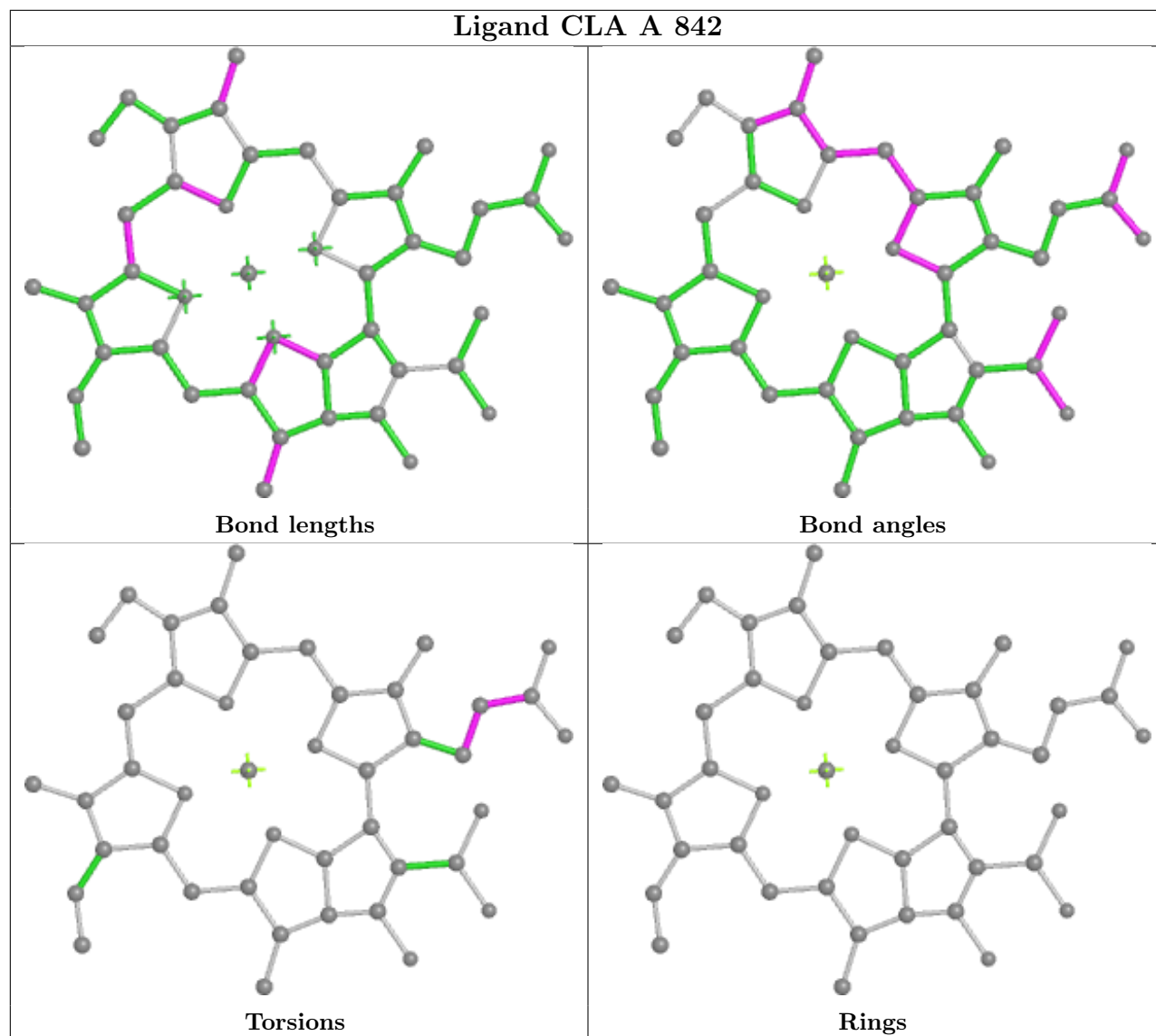
Ligand CLA 5 601



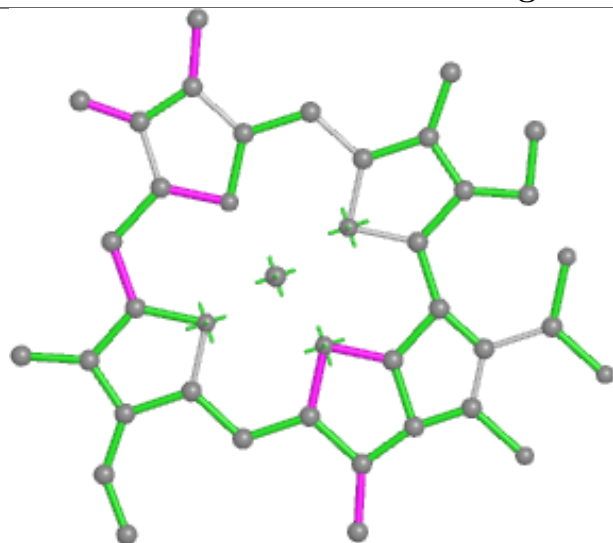
Ligand CLA B 830



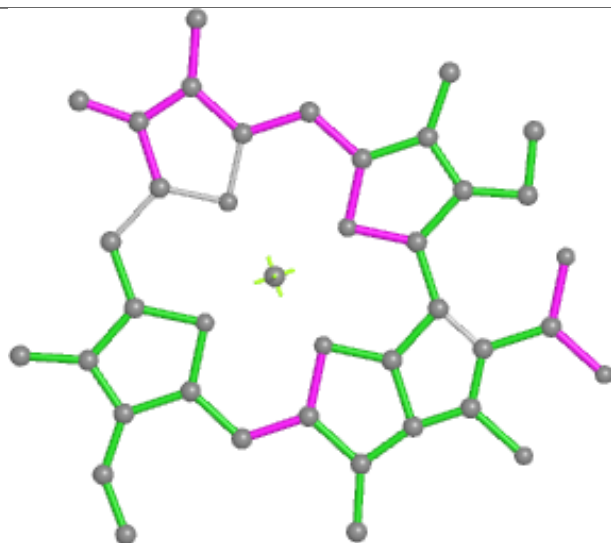
Ligand CLA A 842



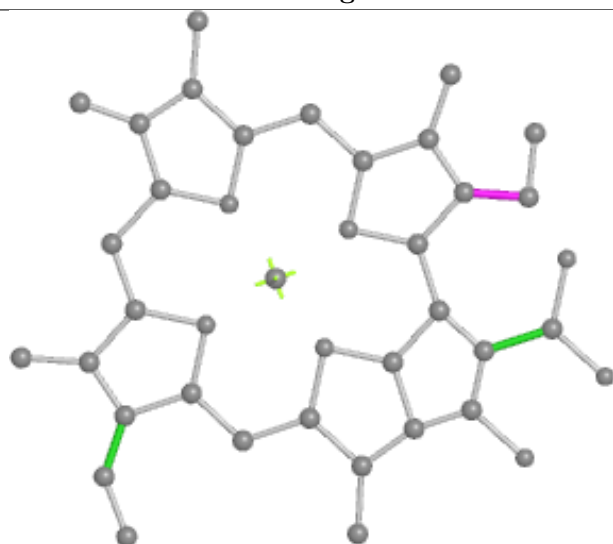
Ligand CLA 3 607



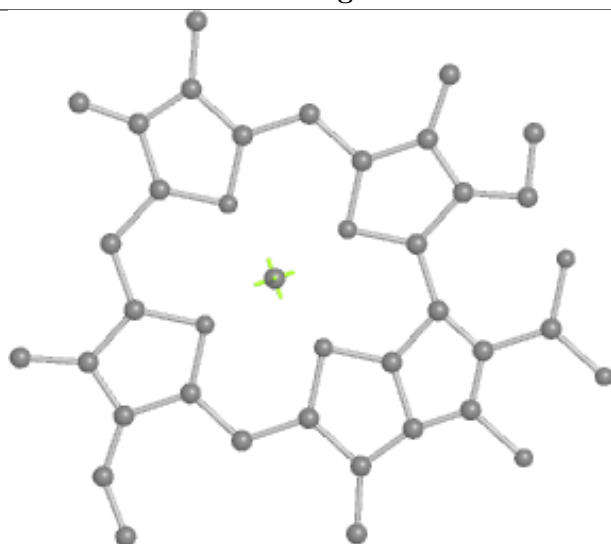
Bond lengths



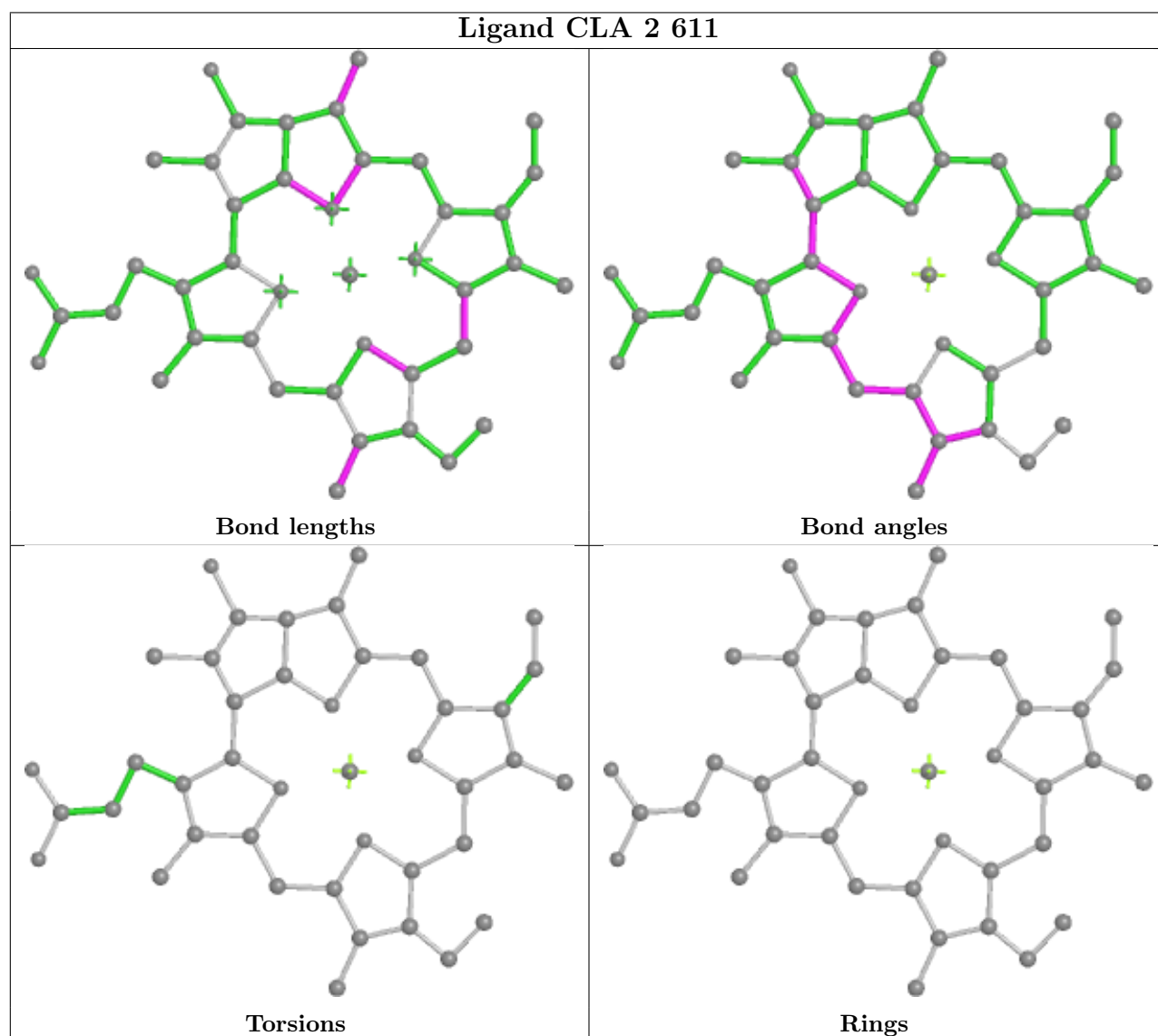
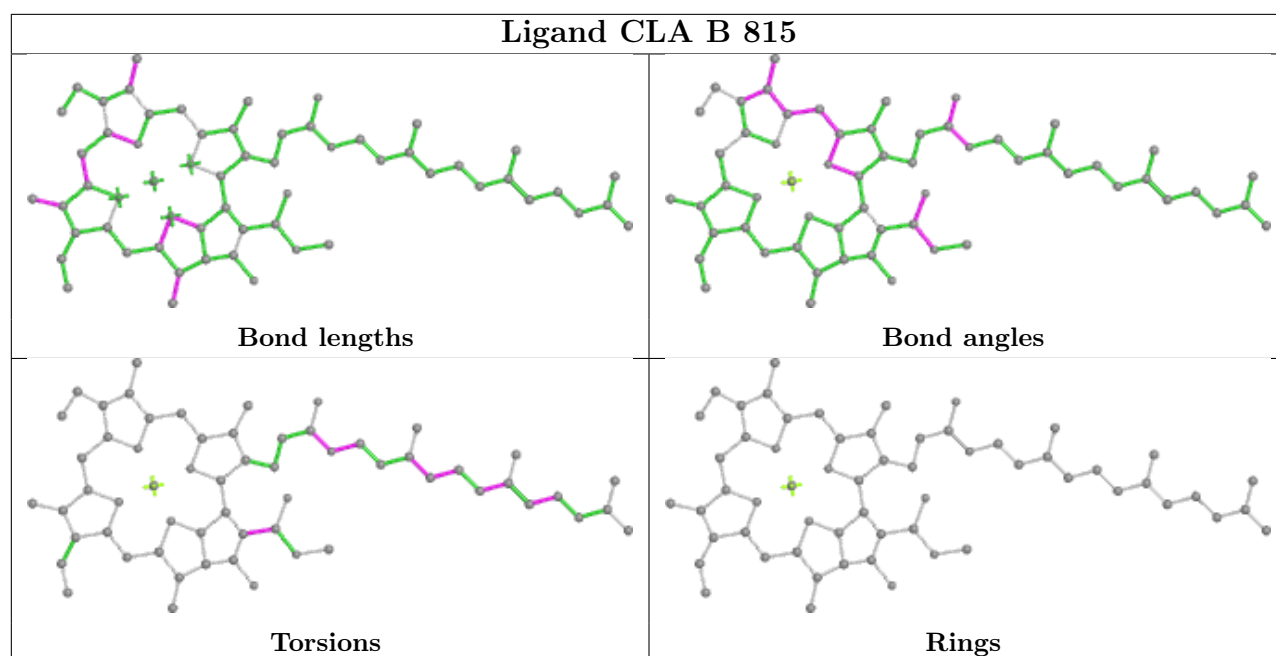
Bond angles

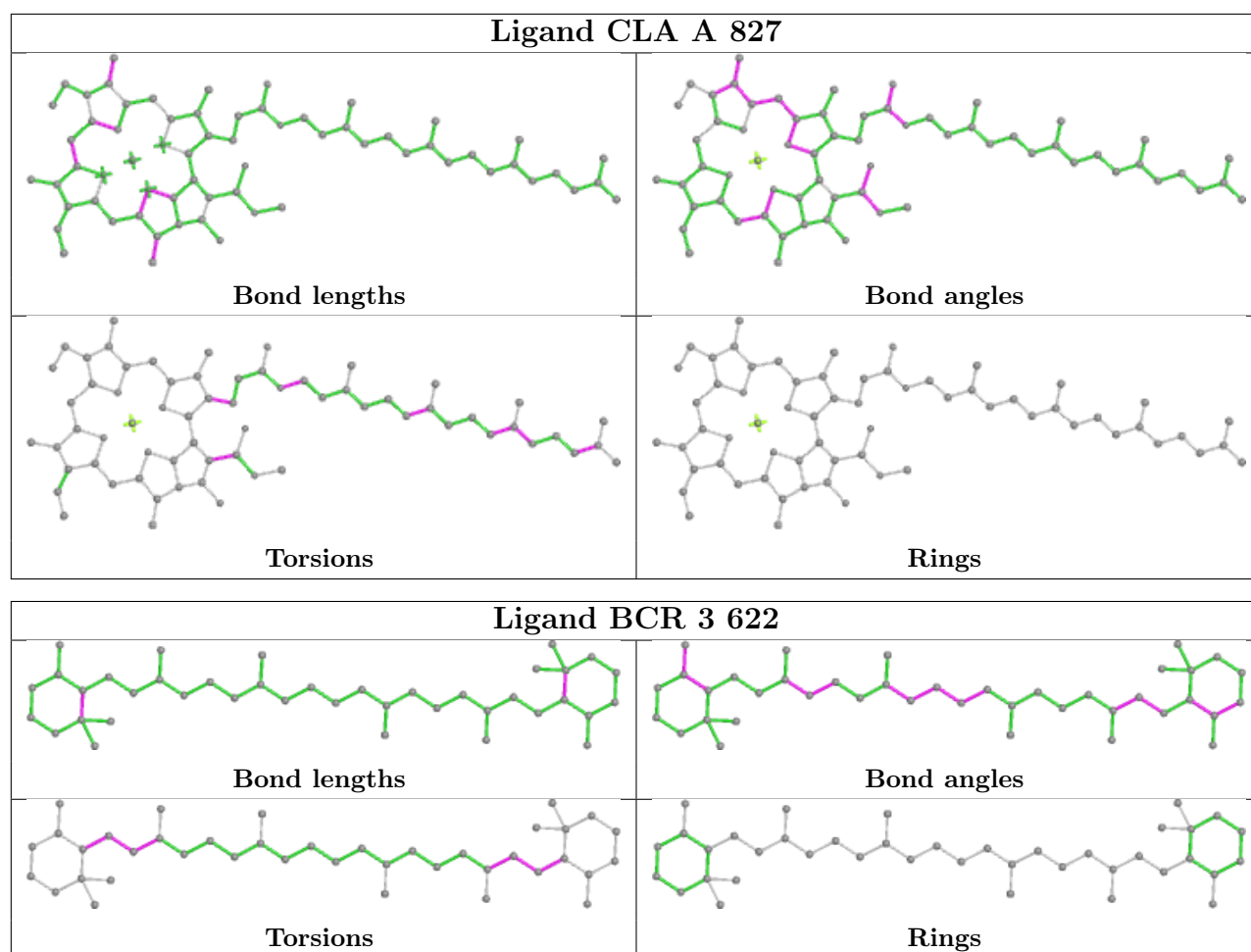


Torsions

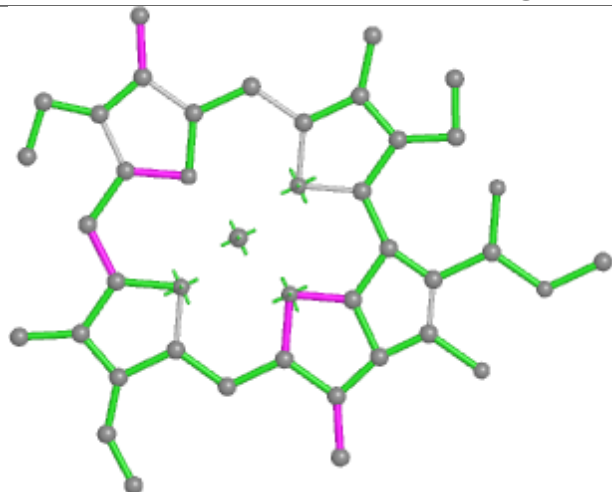


Rings

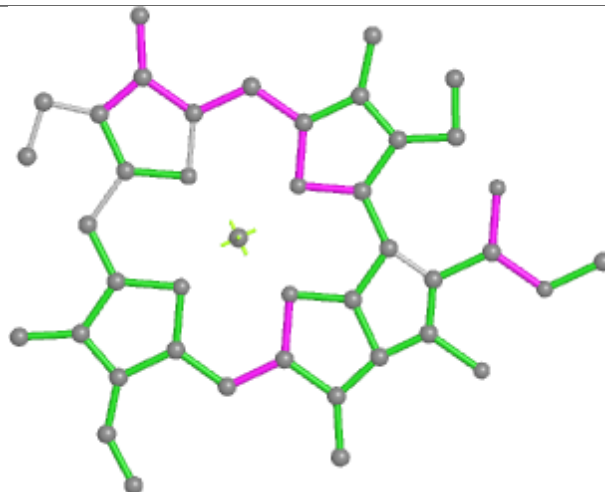




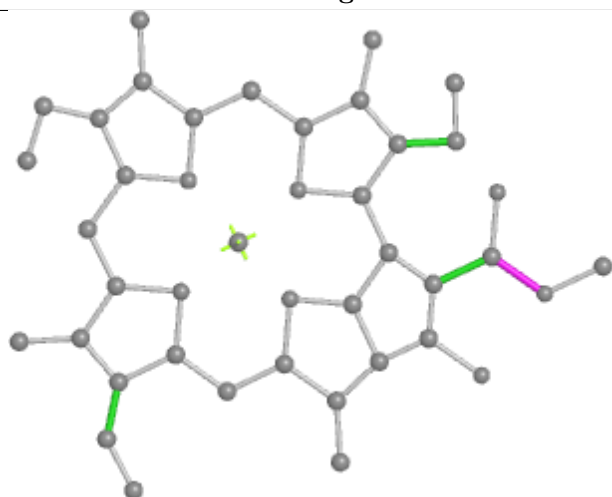
Ligand CLA 2 614



Bond lengths



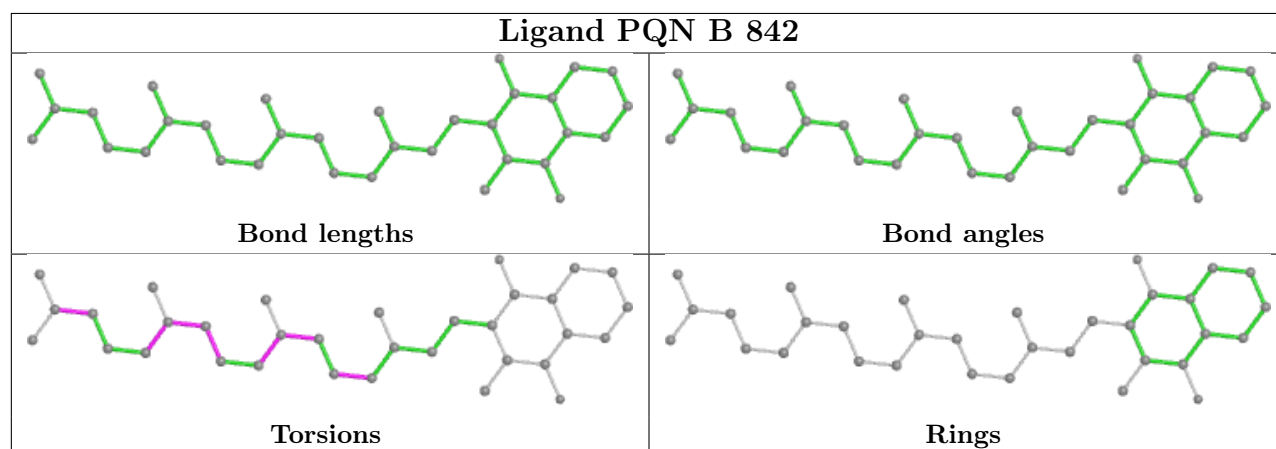
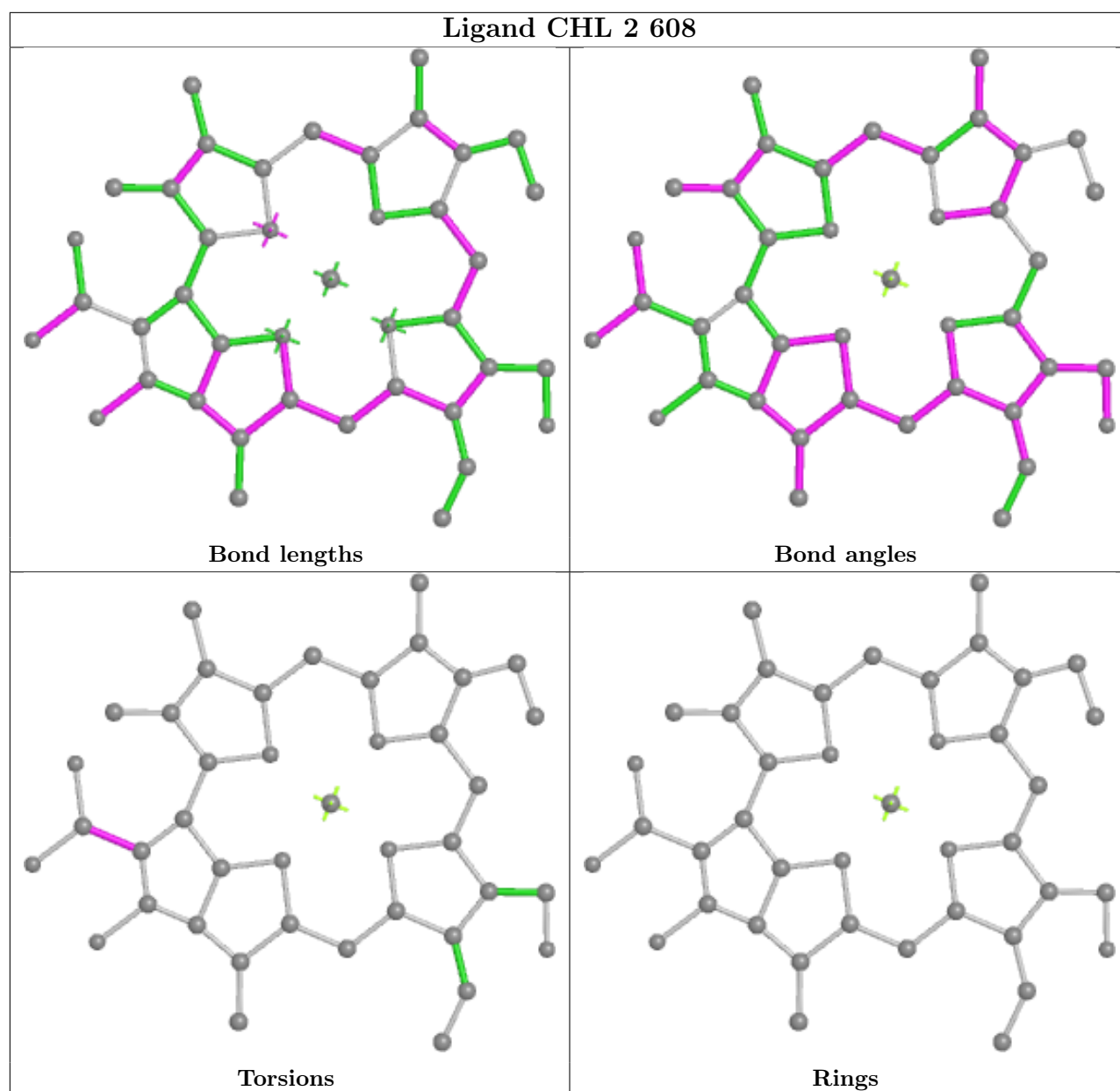
Bond angles



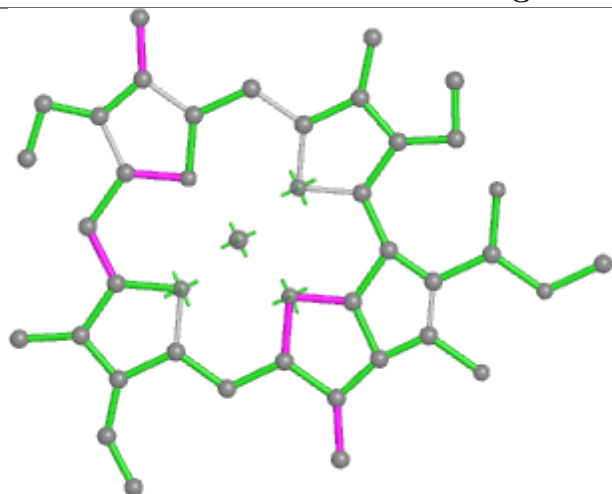
Torsions



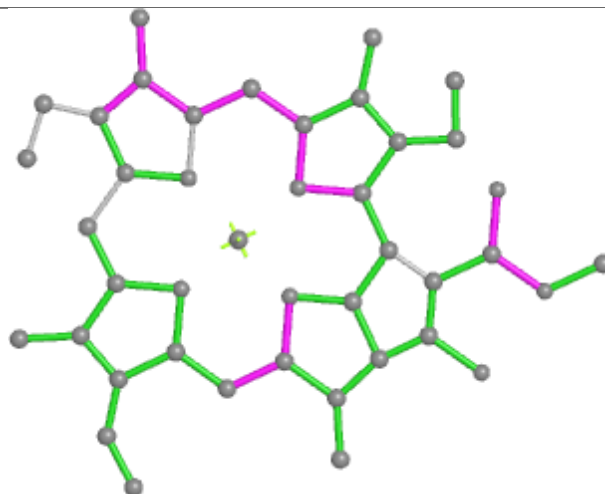
Rings



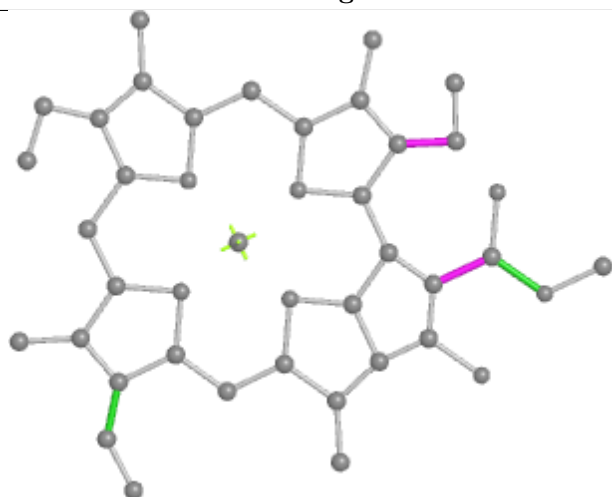
Ligand CLA A 816



Bond lengths



Bond angles

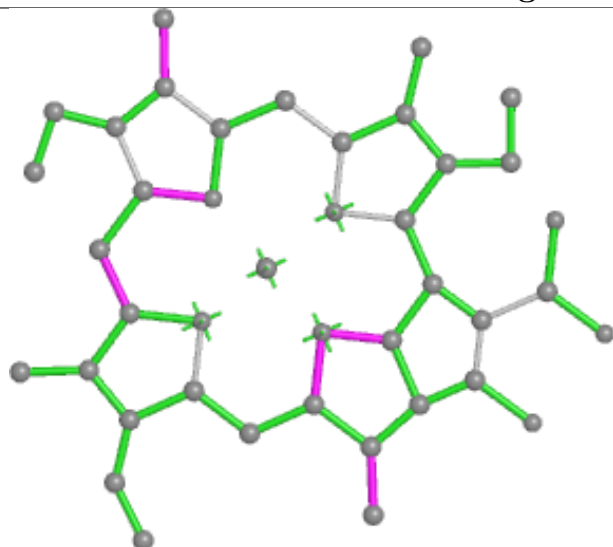


Torsions

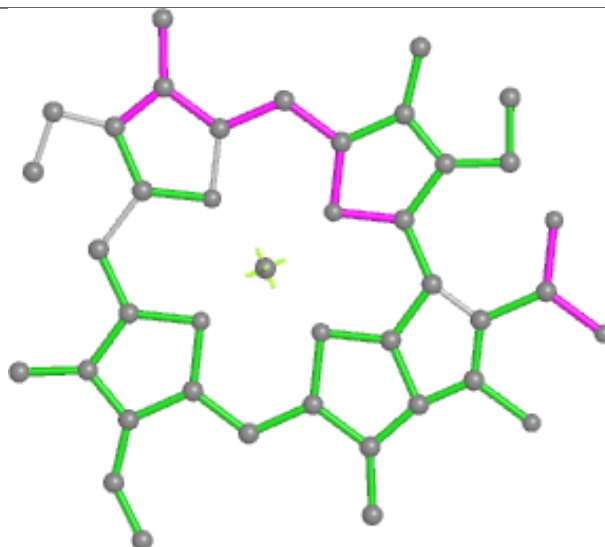


Rings

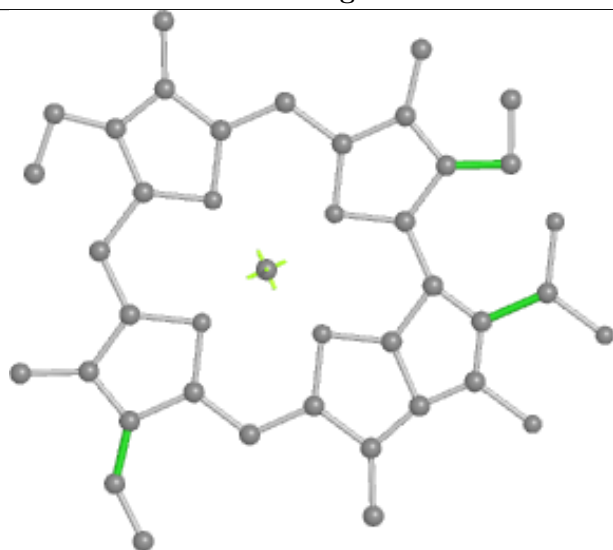
Ligand CLA 3 606



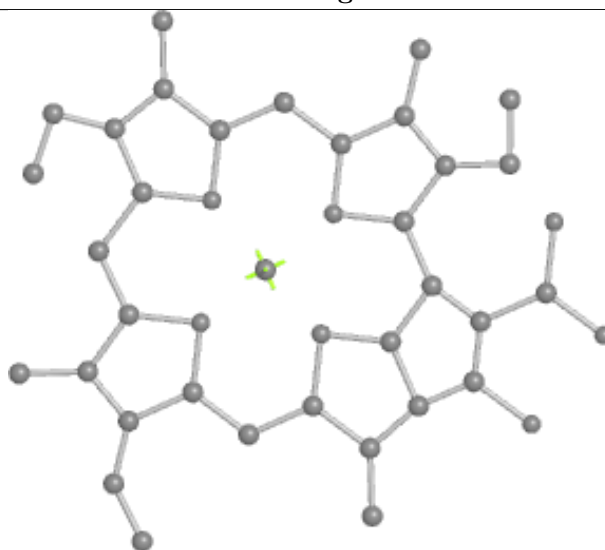
Bond lengths



Bond angles

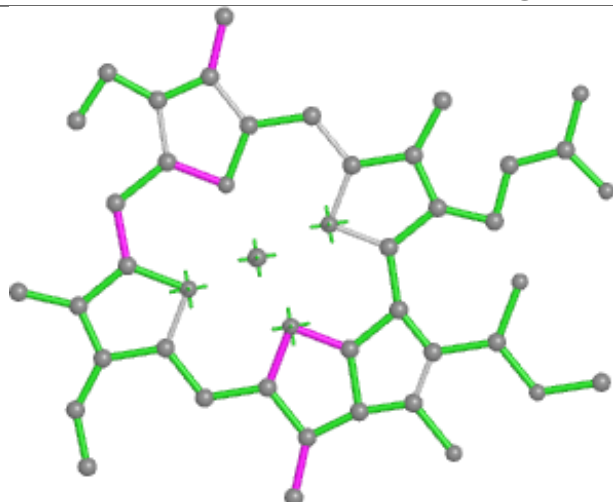


Torsions

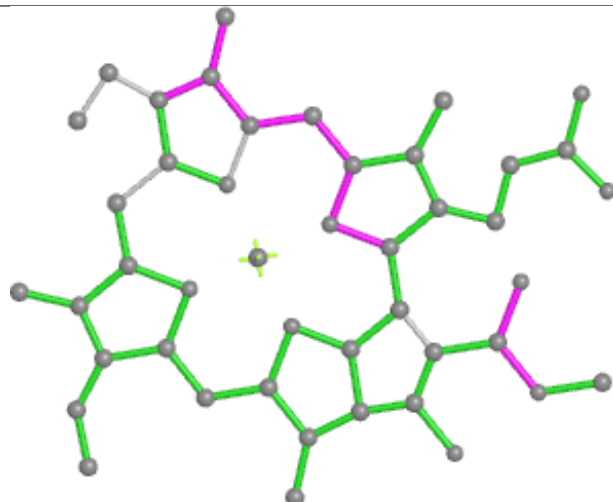


Rings

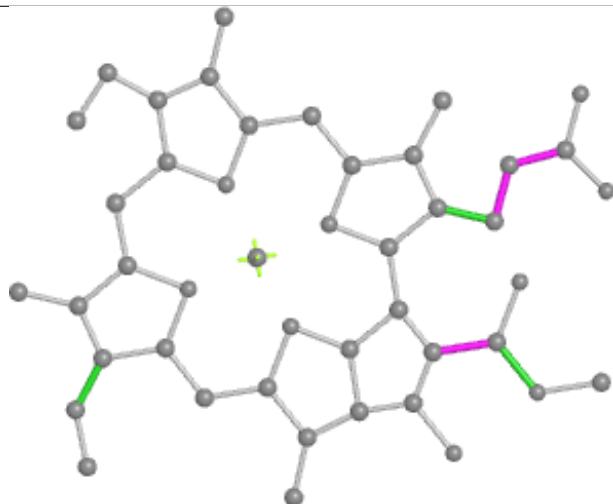
Ligand CLA F 305



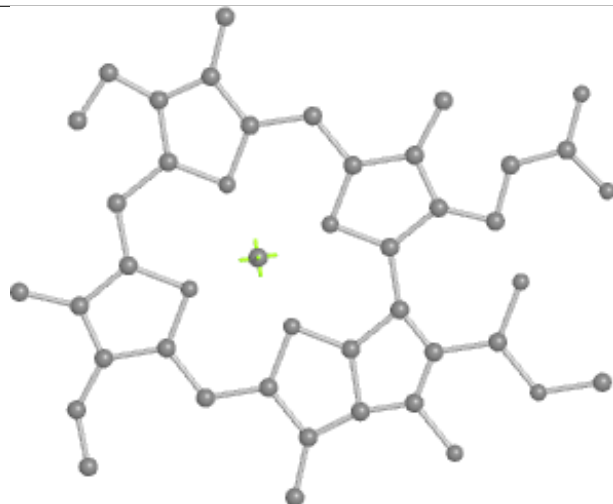
Bond lengths



Bond angles

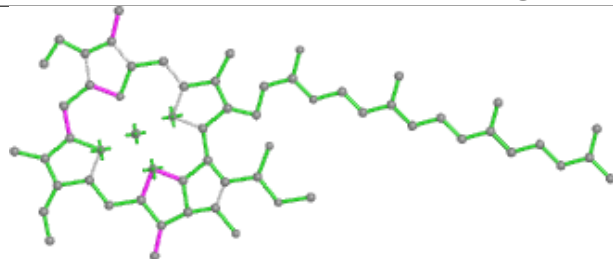


Torsions

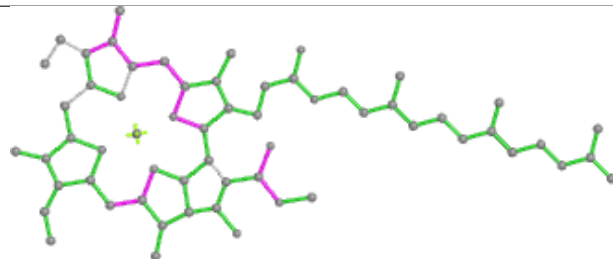


Rings

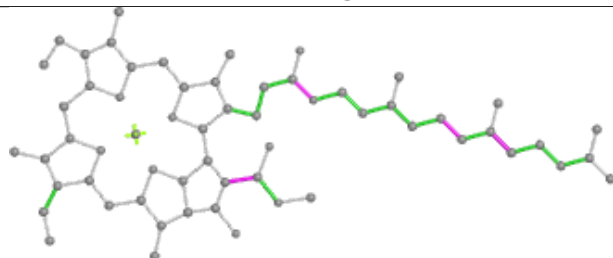
Ligand CLA B 836



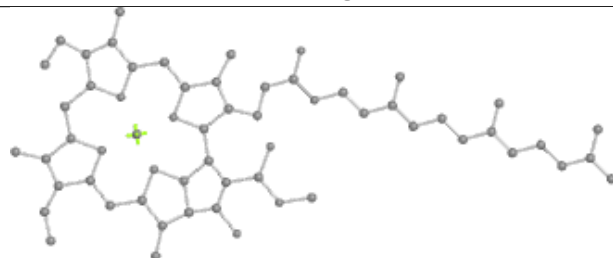
Bond lengths



Bond angles

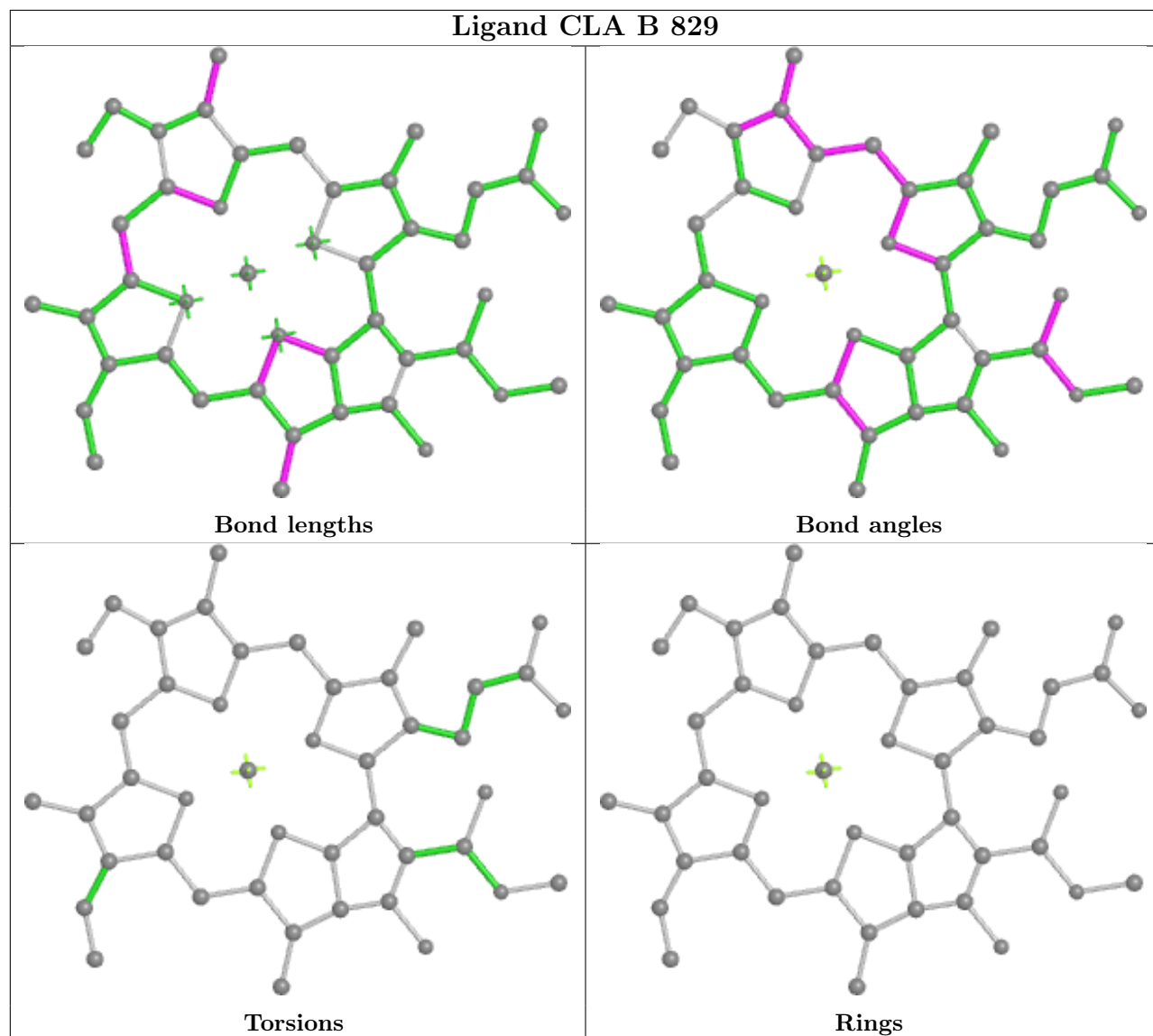


Torsions

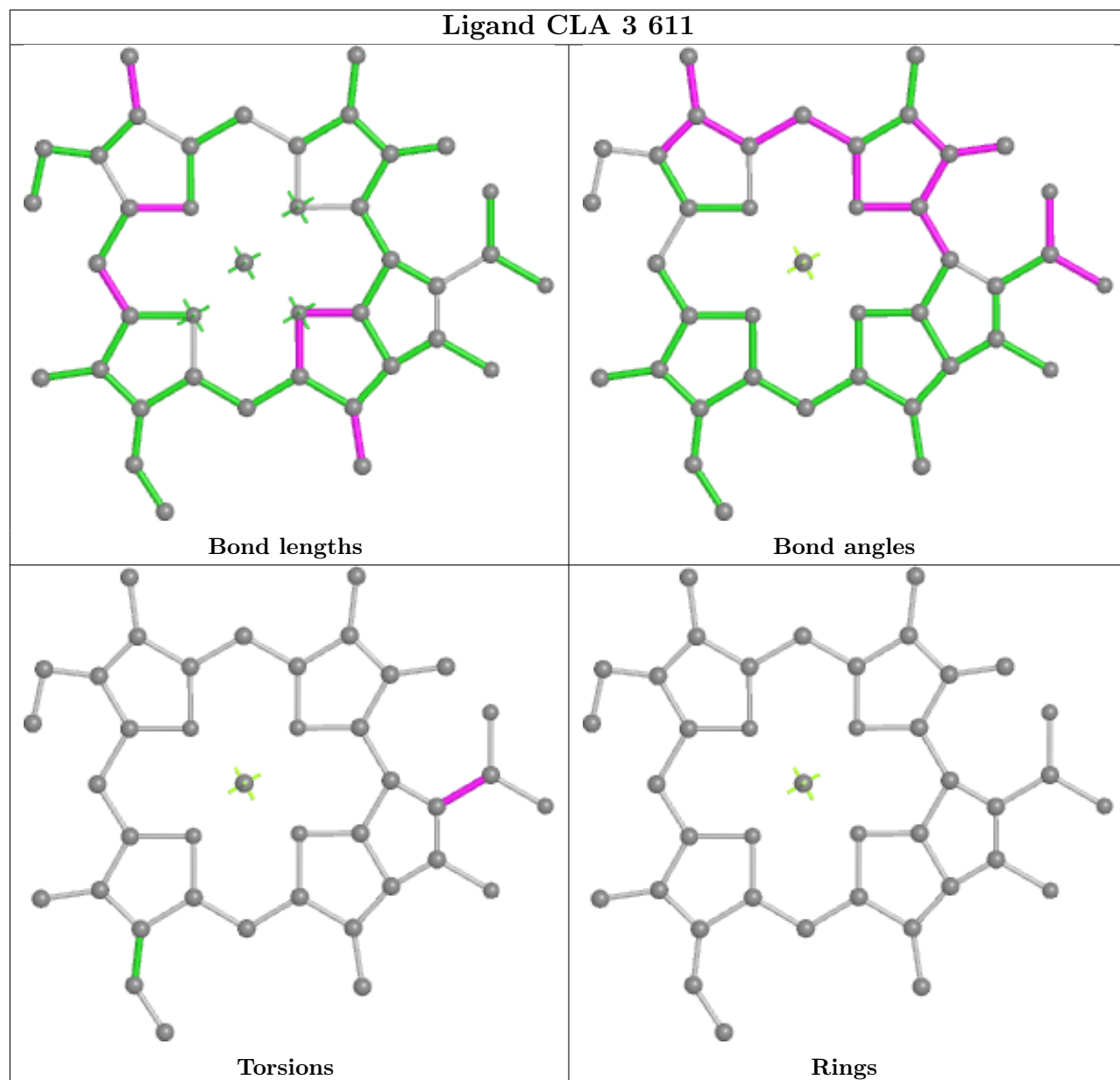


Rings

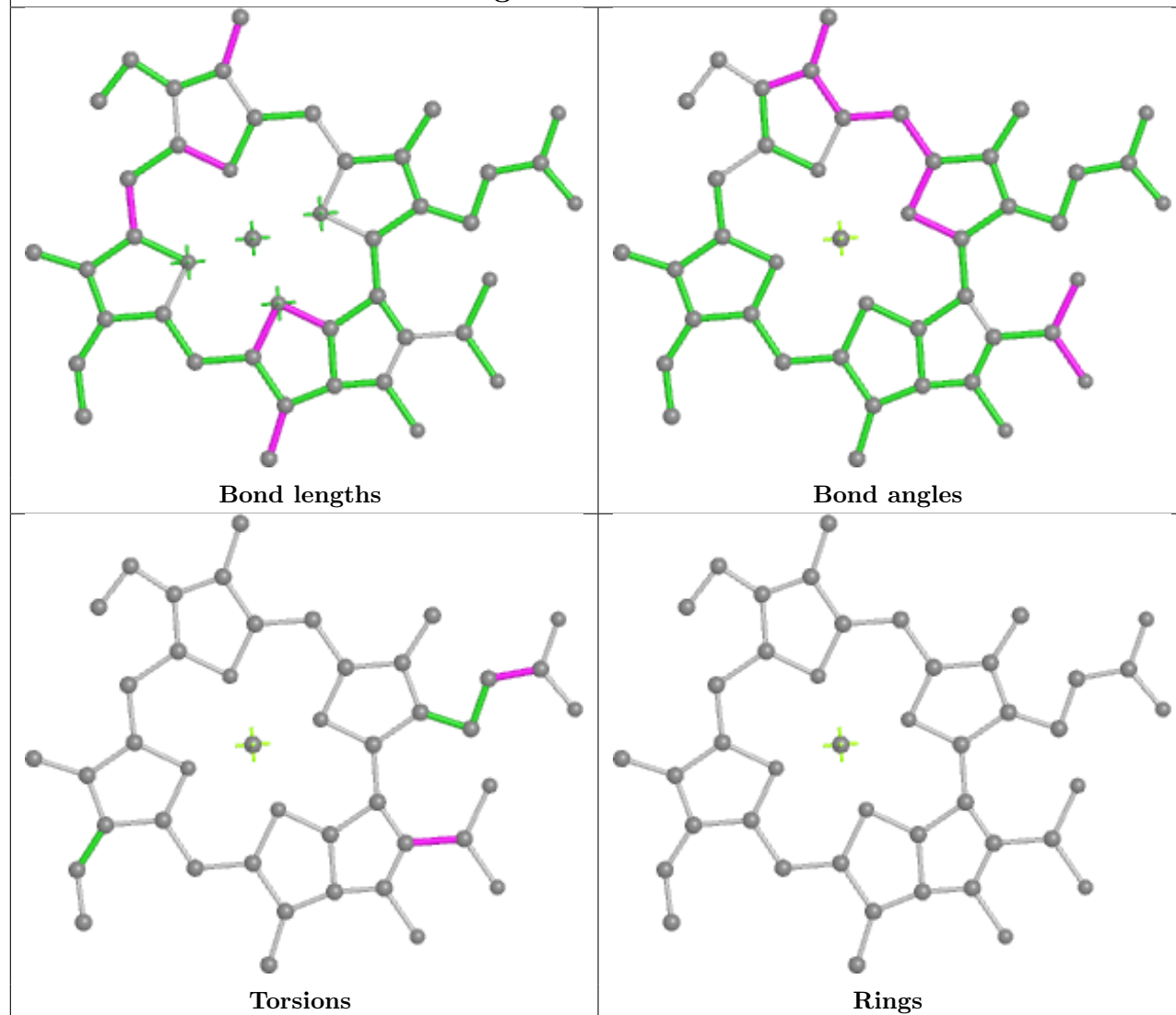
Ligand CLA B 829



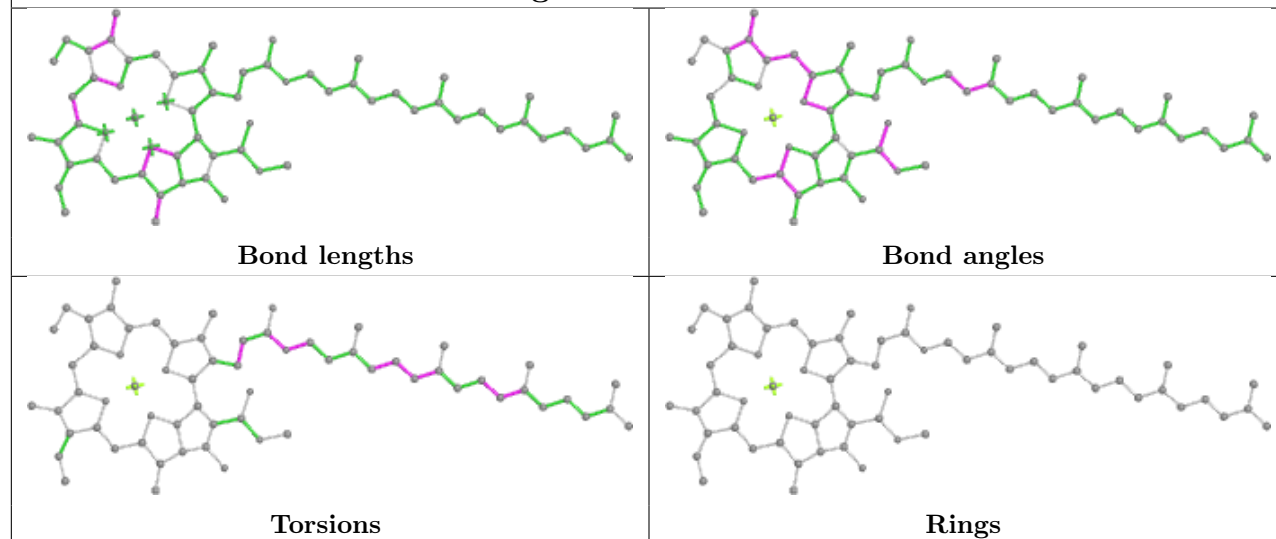
Ligand CLA 3 611



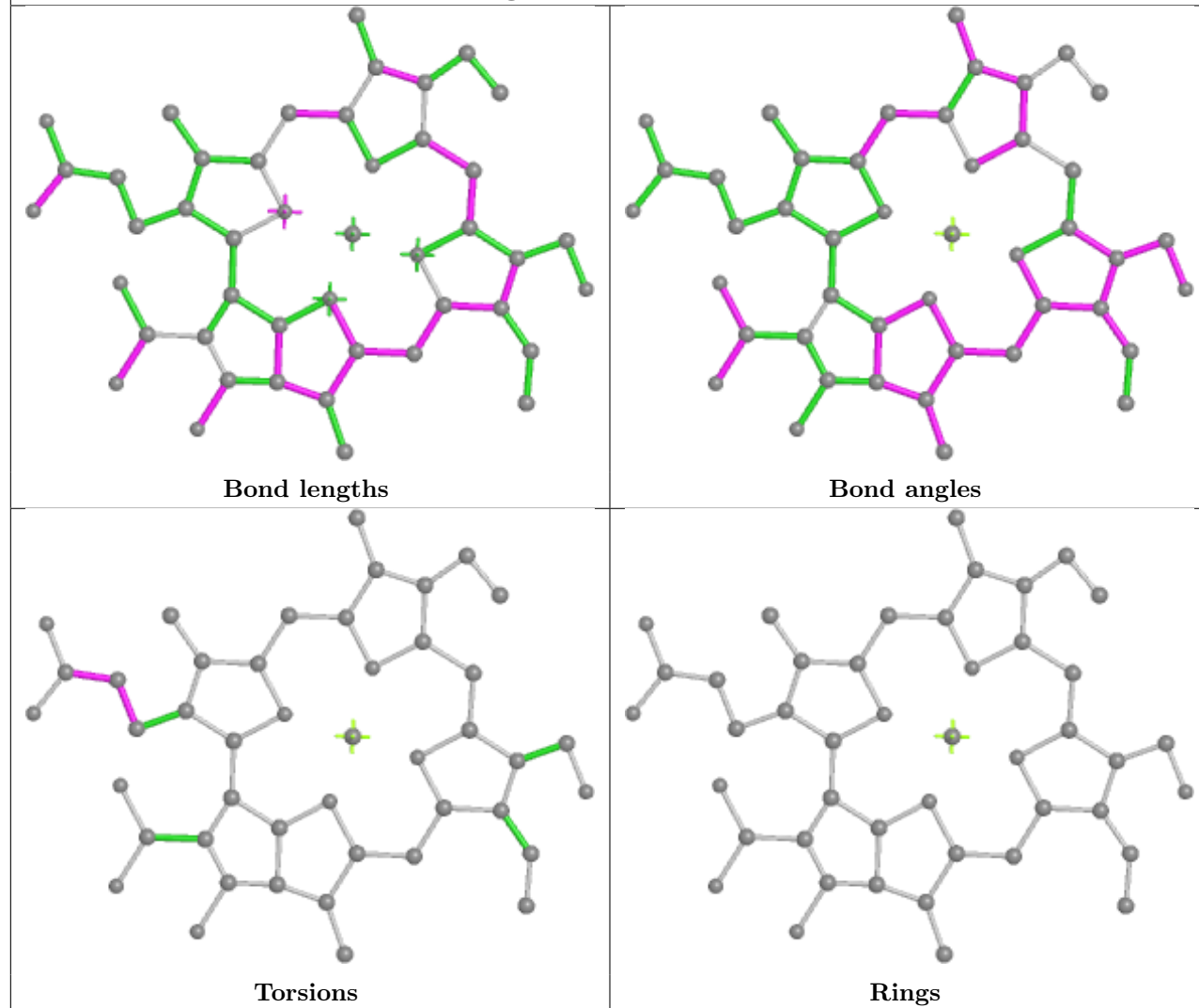
Ligand CLA 5 603



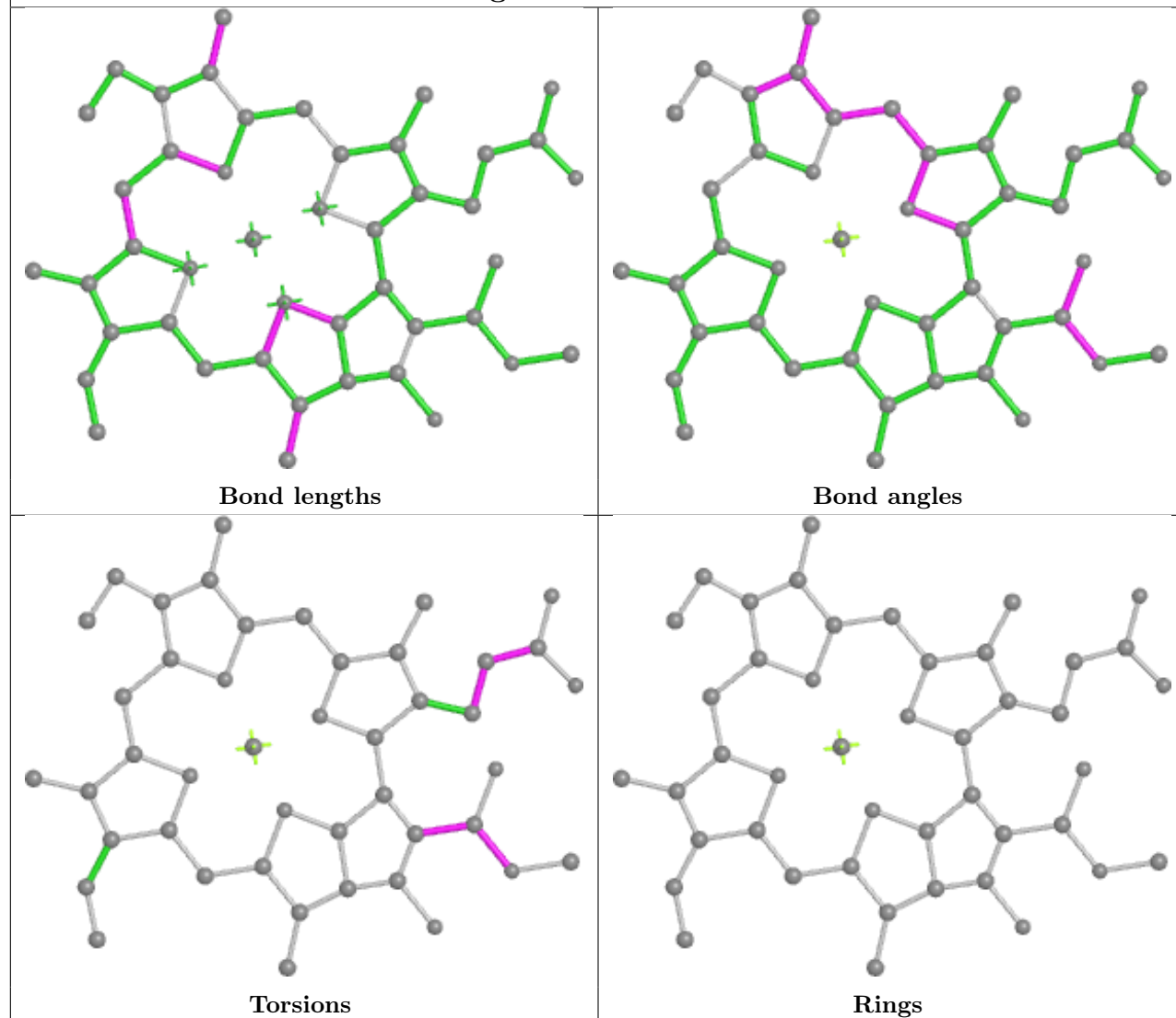
Ligand CLA A 843



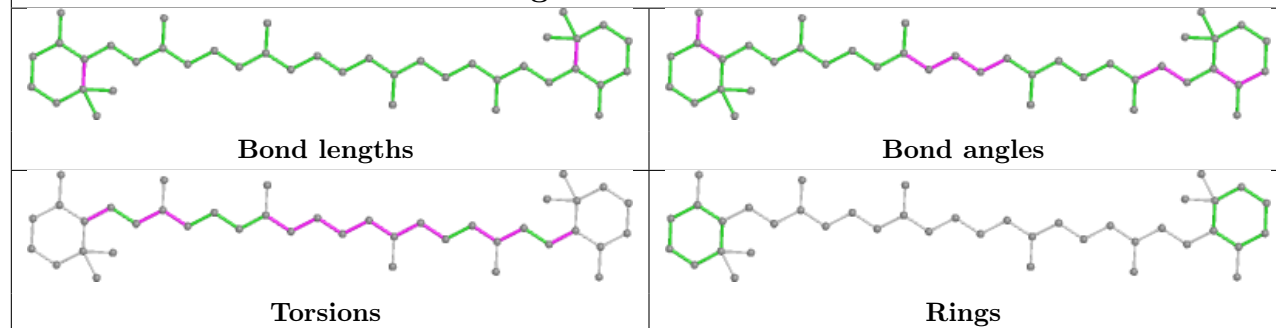
Ligand CHL 6 601

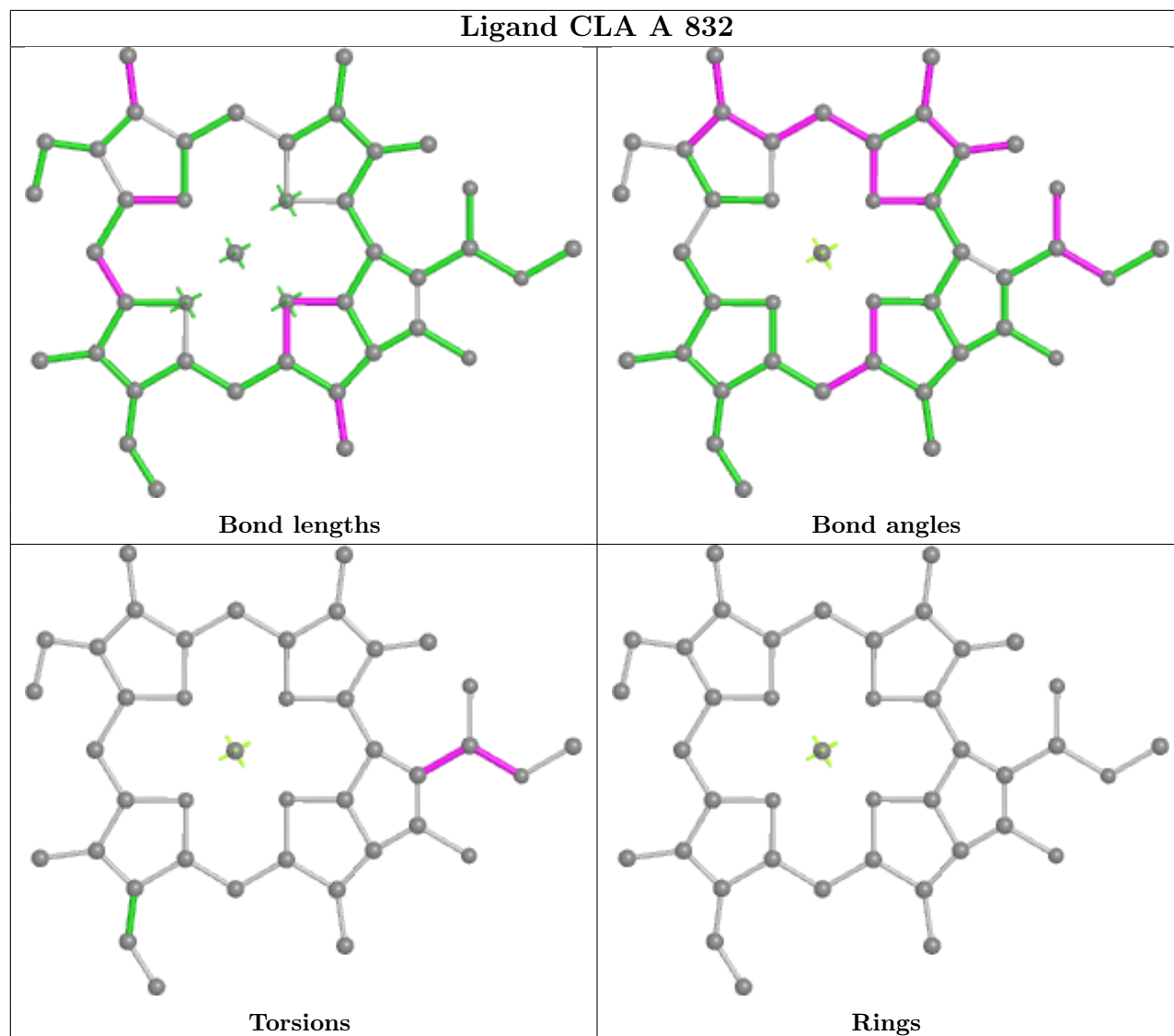
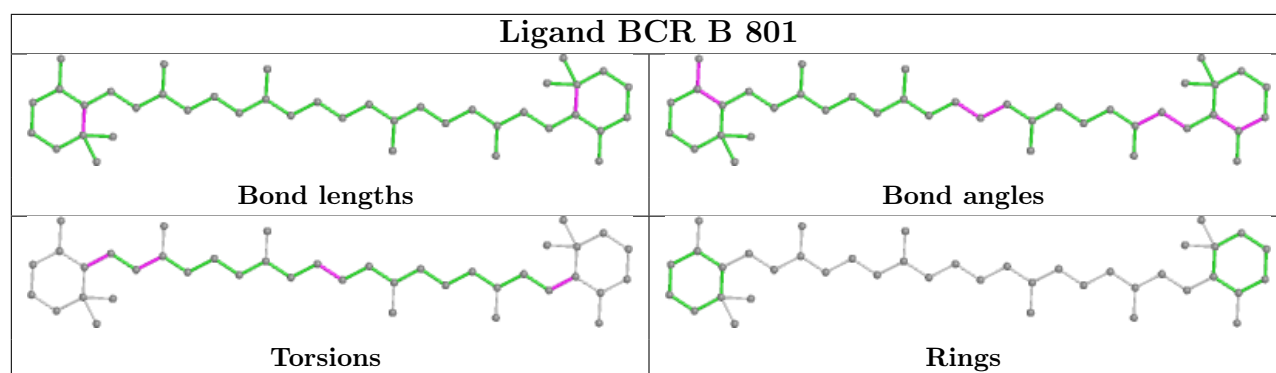


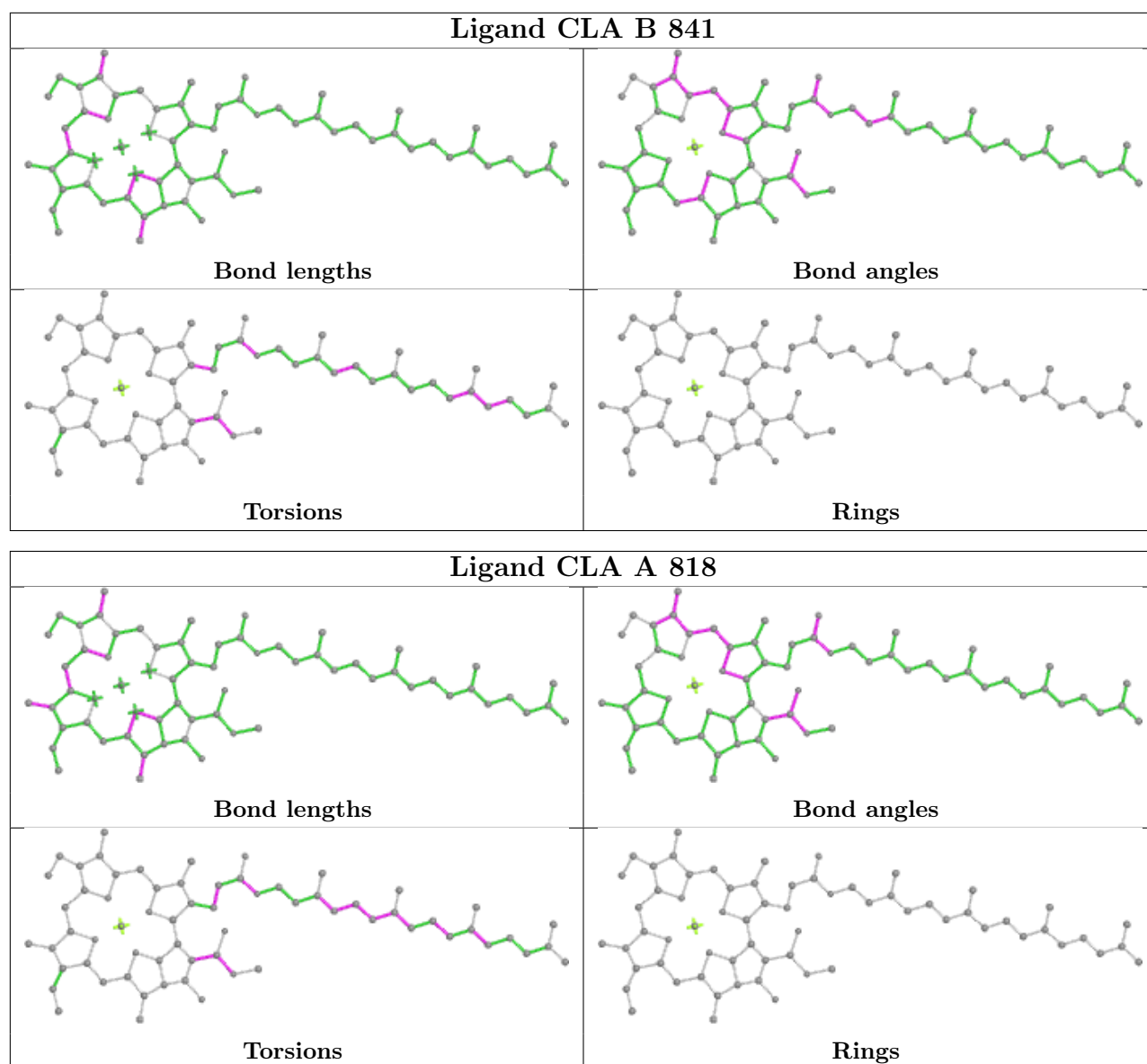
Ligand CLA A 802



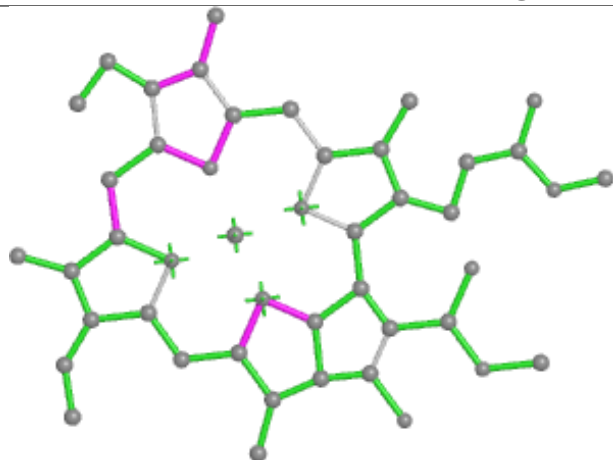
Ligand BCR B 845



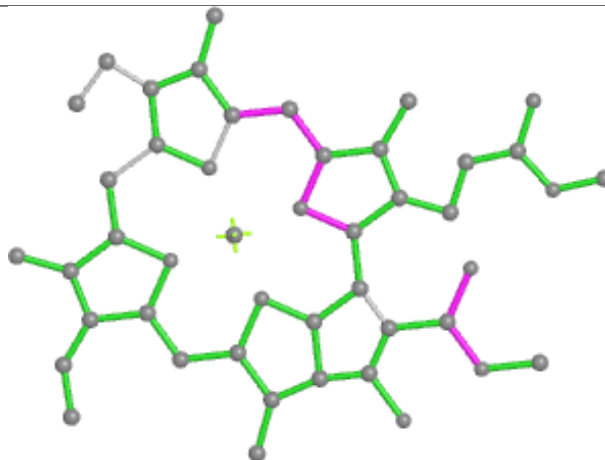




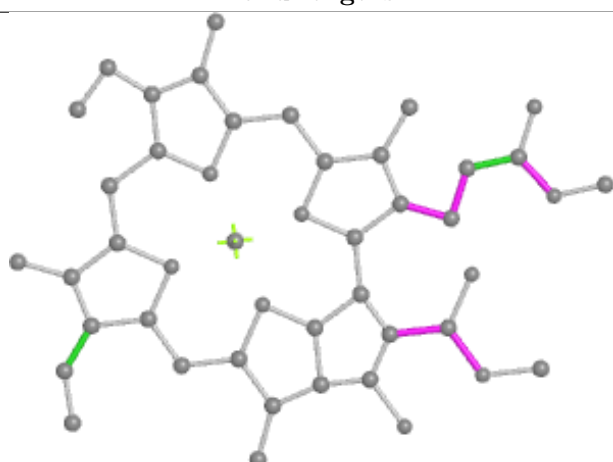
Ligand CLA K 201



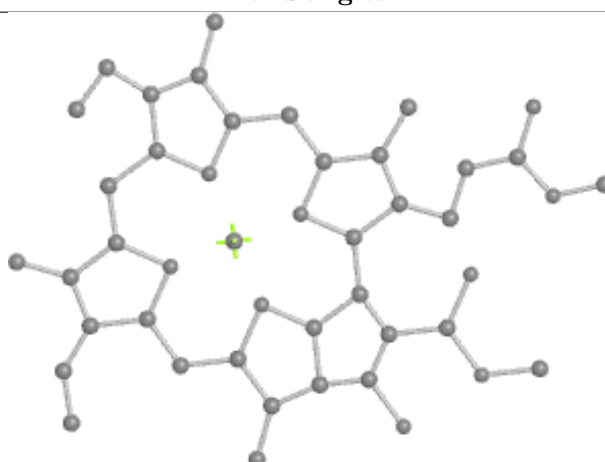
Bond lengths



Bond angles

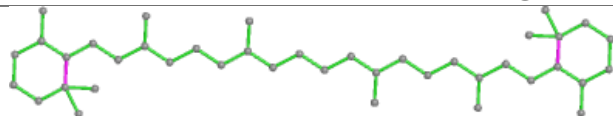


Torsions

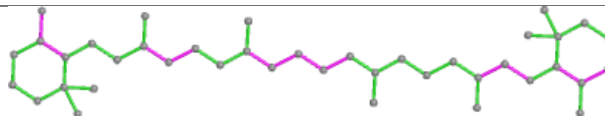


Rings

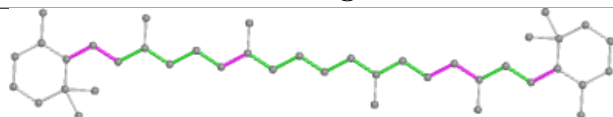
Ligand BCR 2 621



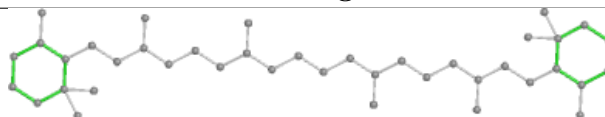
Bond lengths



Bond angles

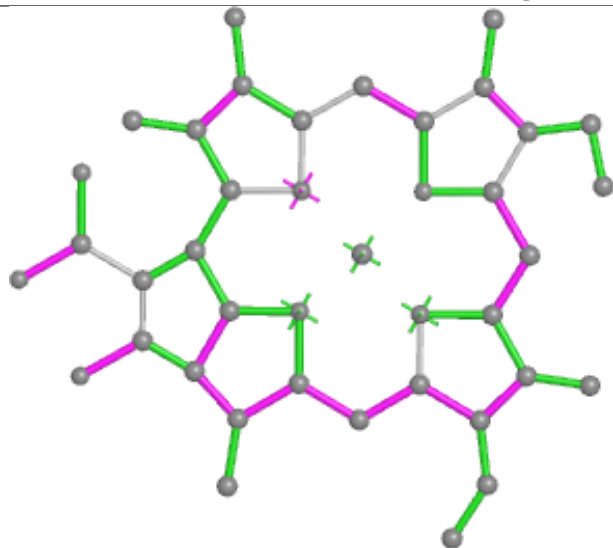


Torsions

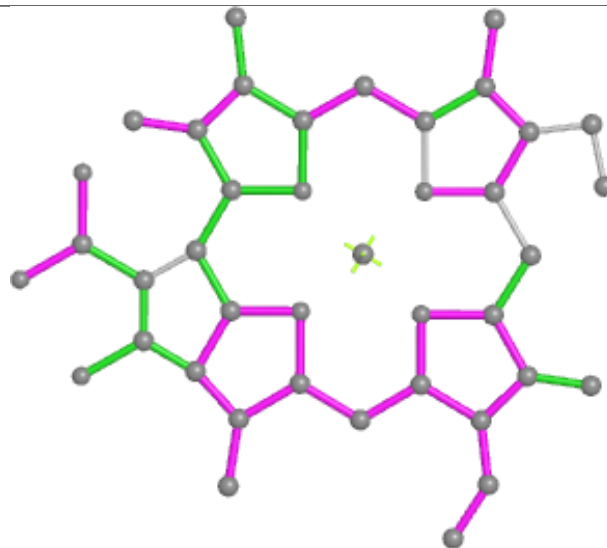


Rings

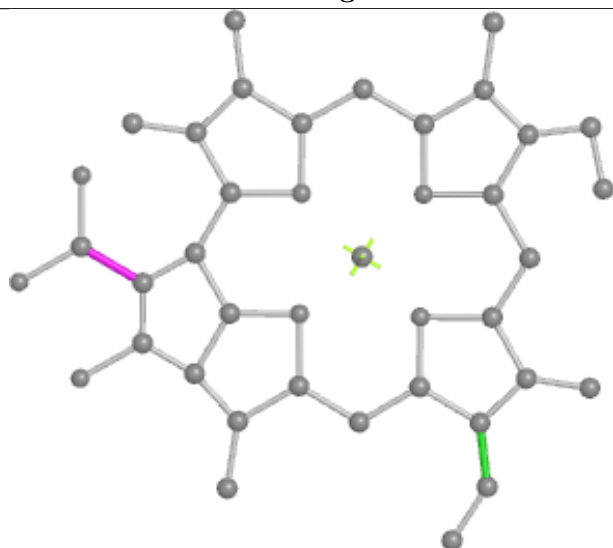
Ligand CHL 3 608



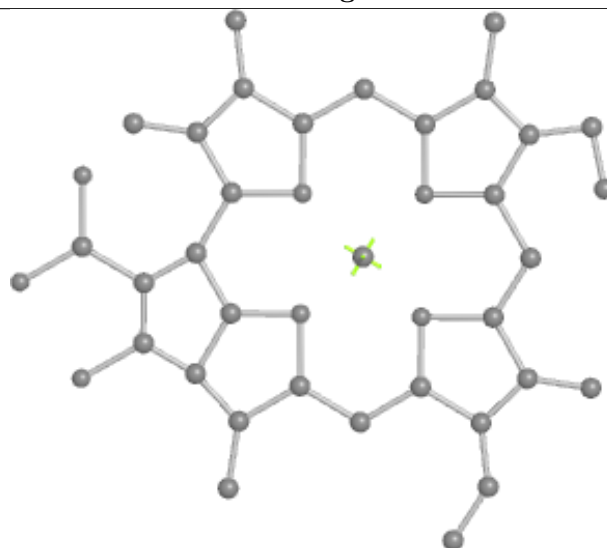
Bond lengths



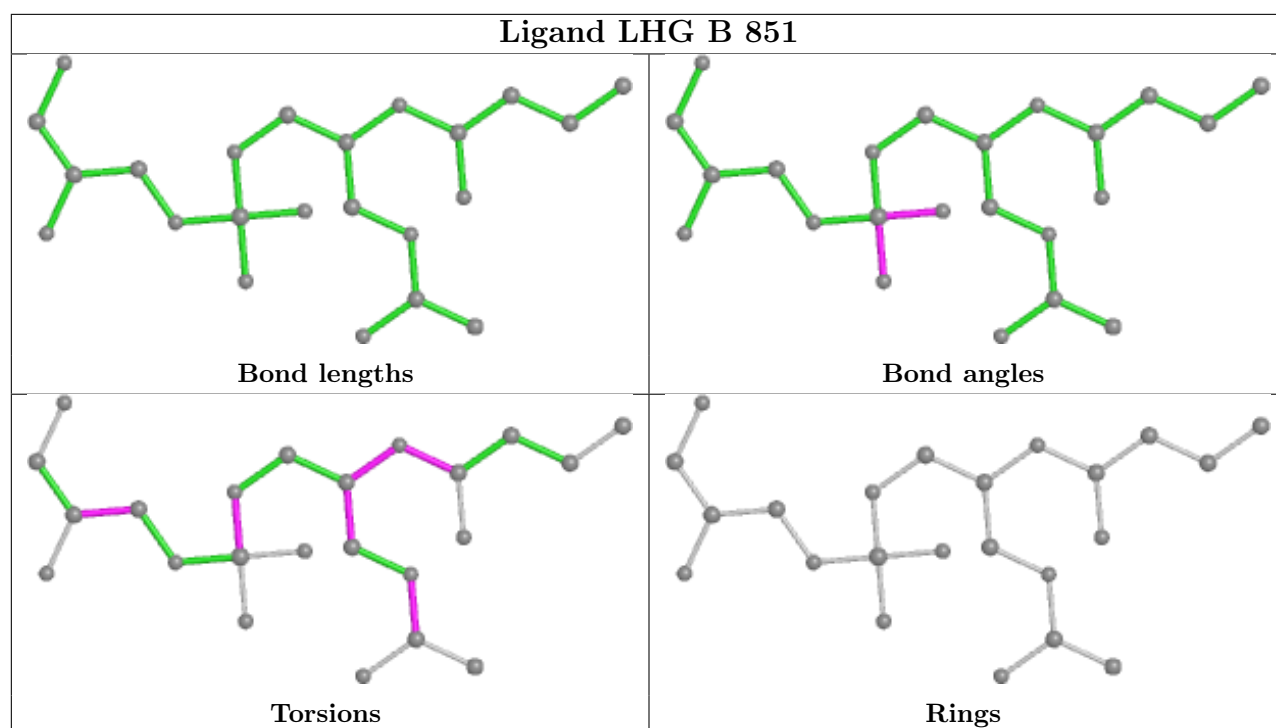
Bond angles



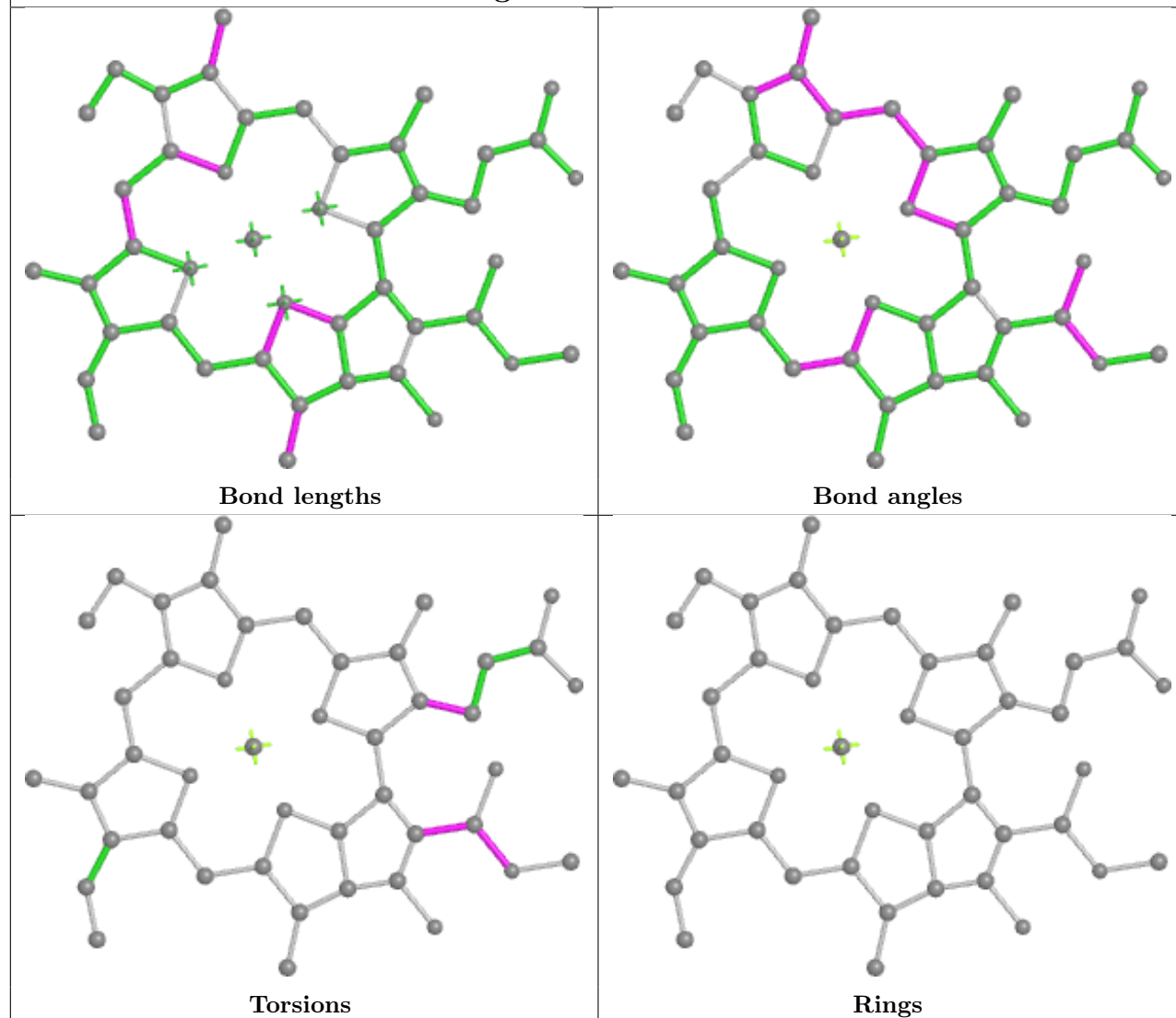
Torsions



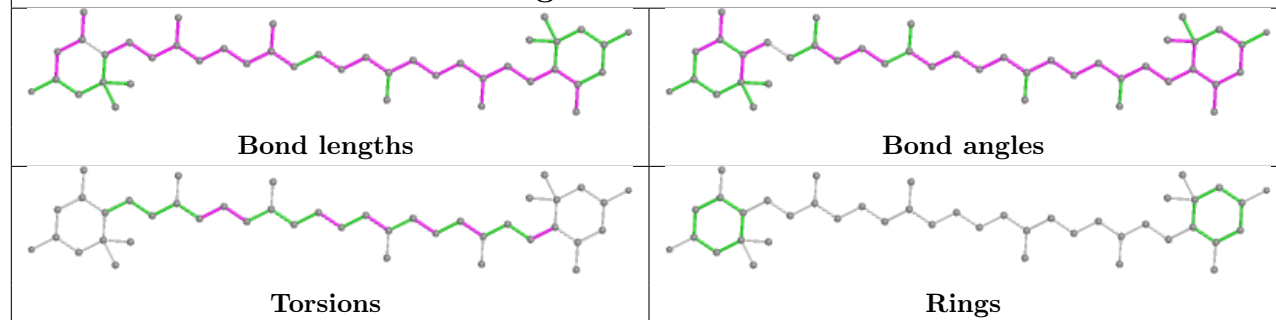
Rings



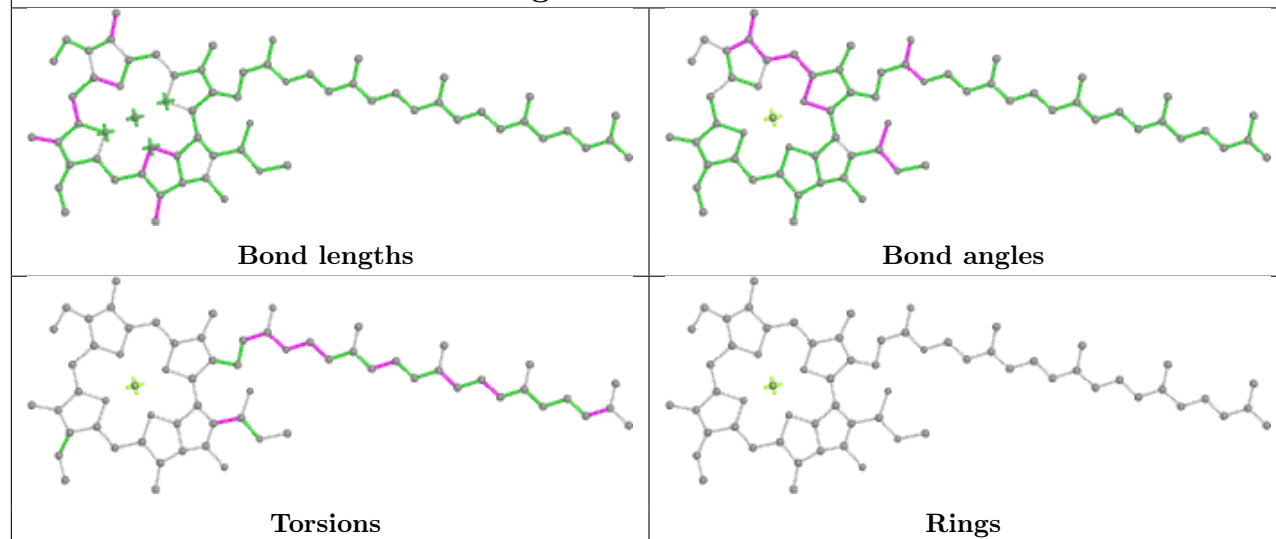
Ligand CLA 2 602



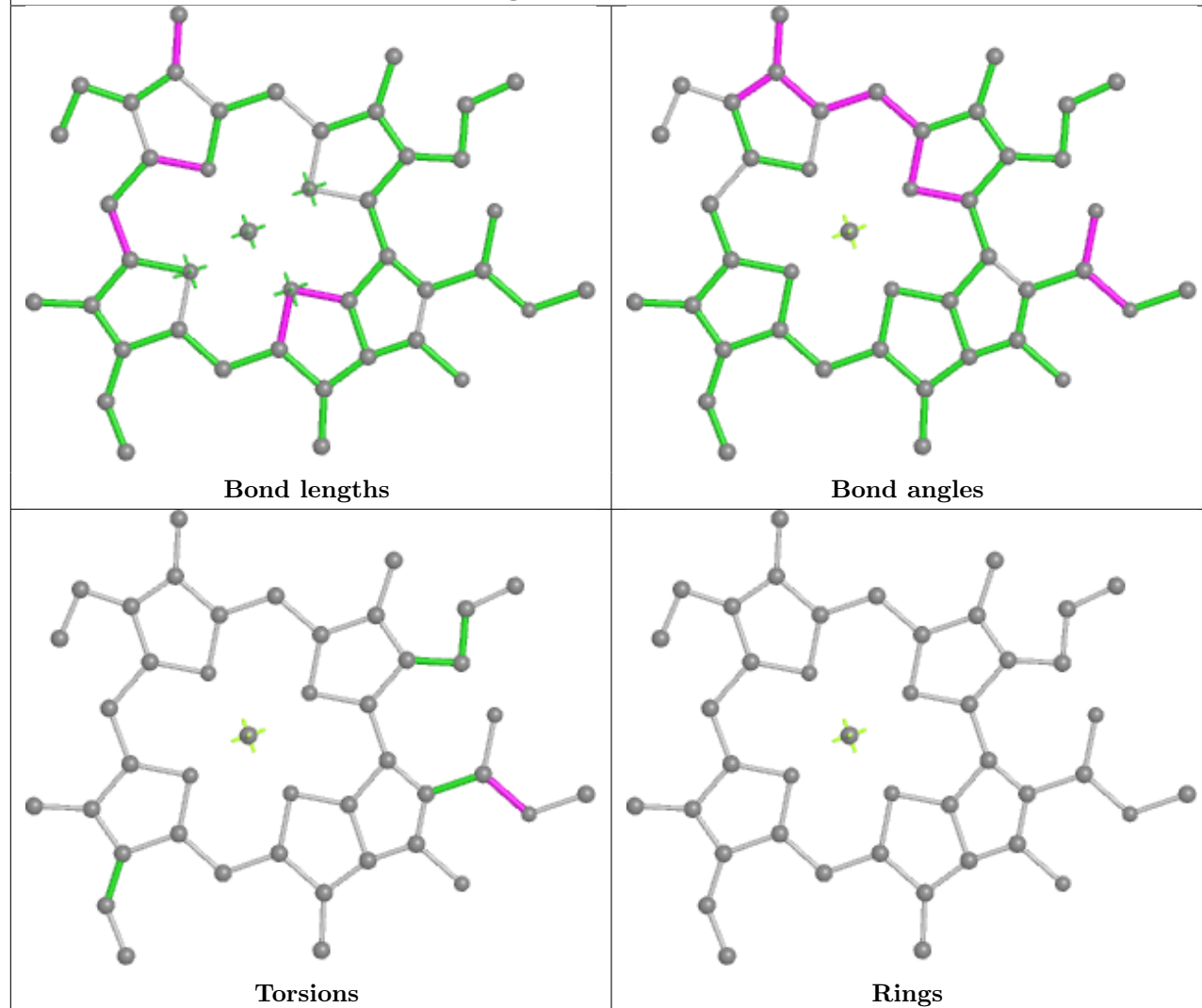
Ligand LUT 5 619



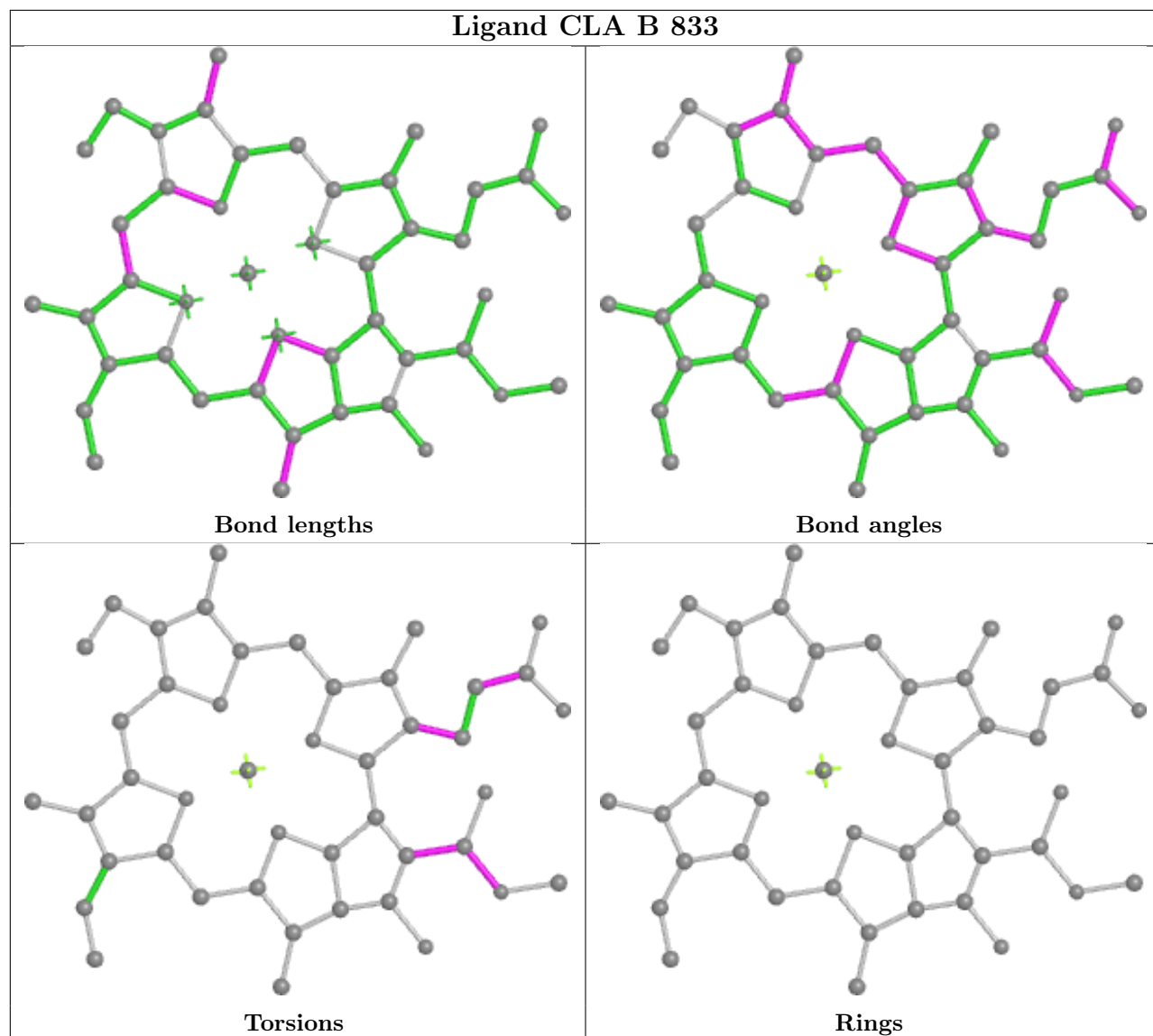
Ligand CLA A 806



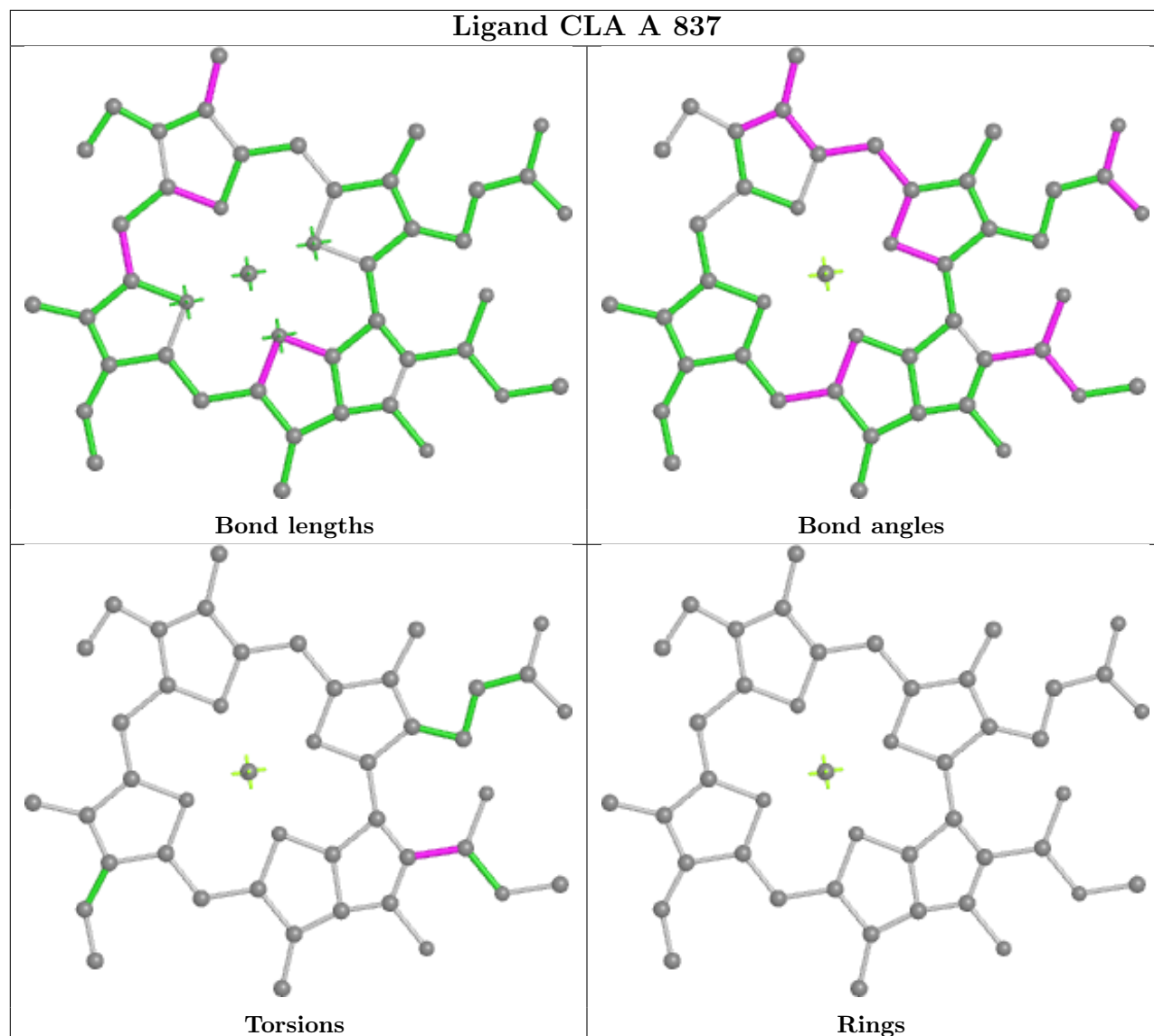
Ligand CLA 3 612



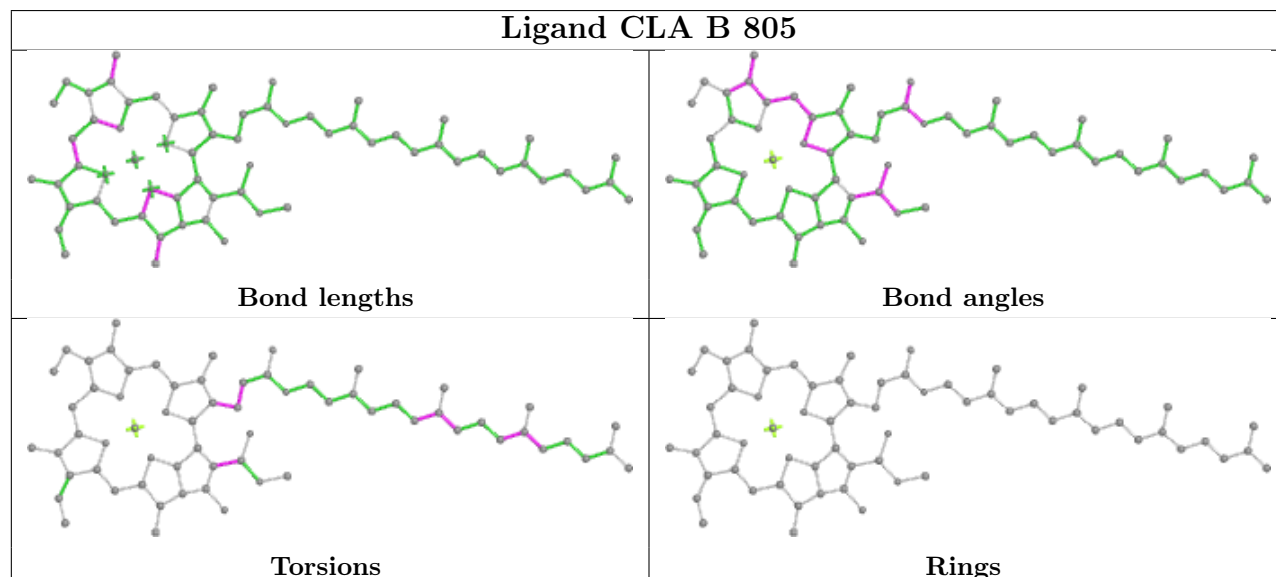
Ligand CLA B 833



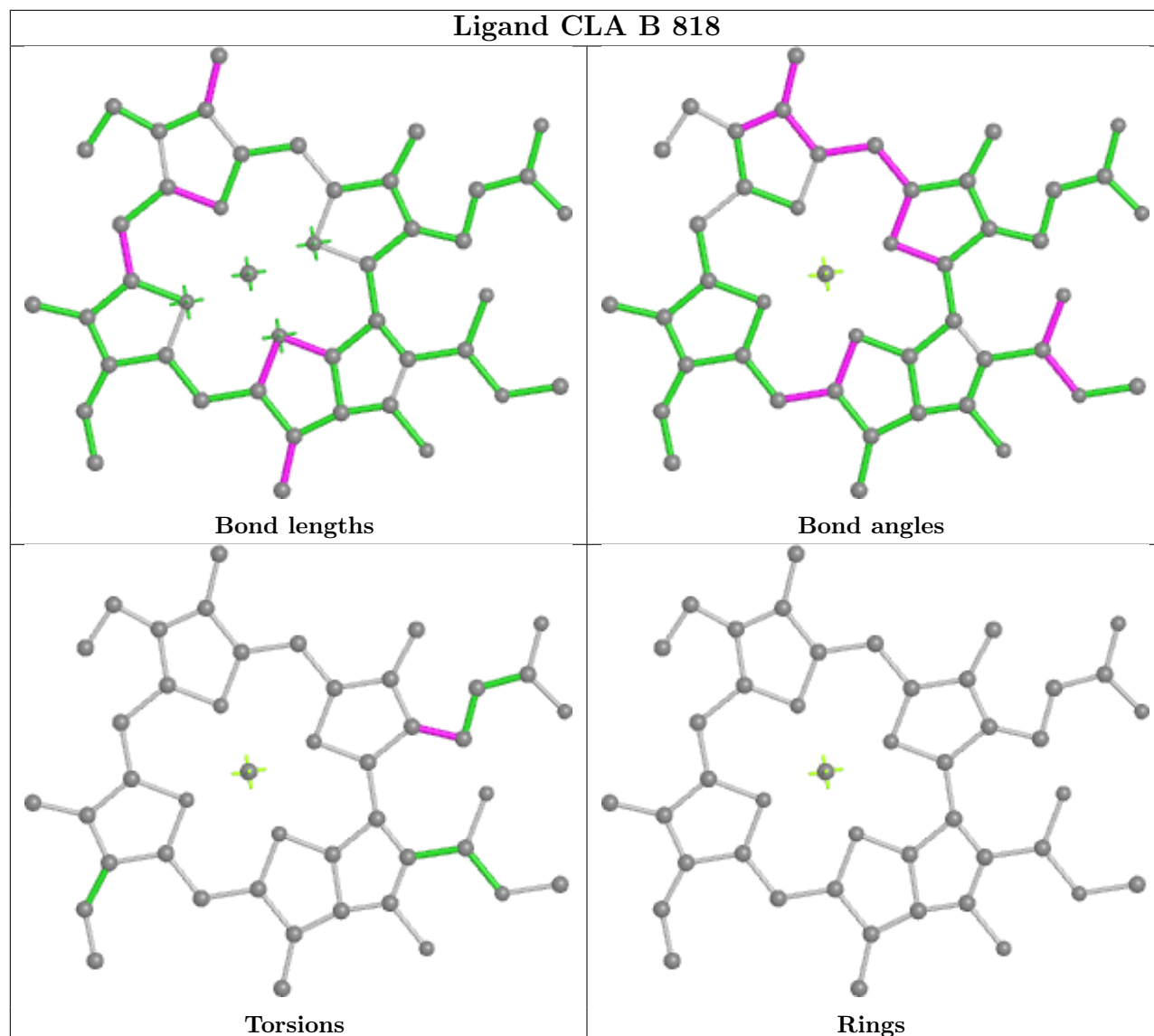
Ligand CLA A 837



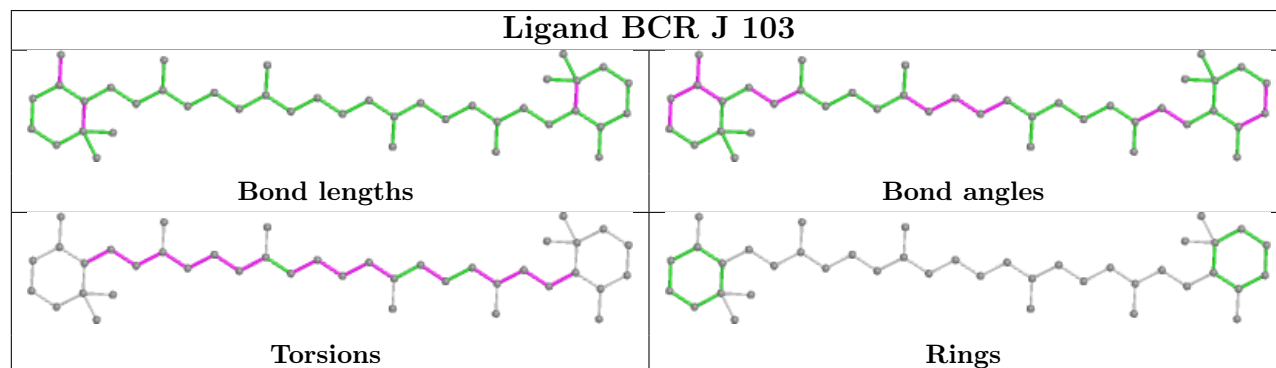
Ligand CLA B 805

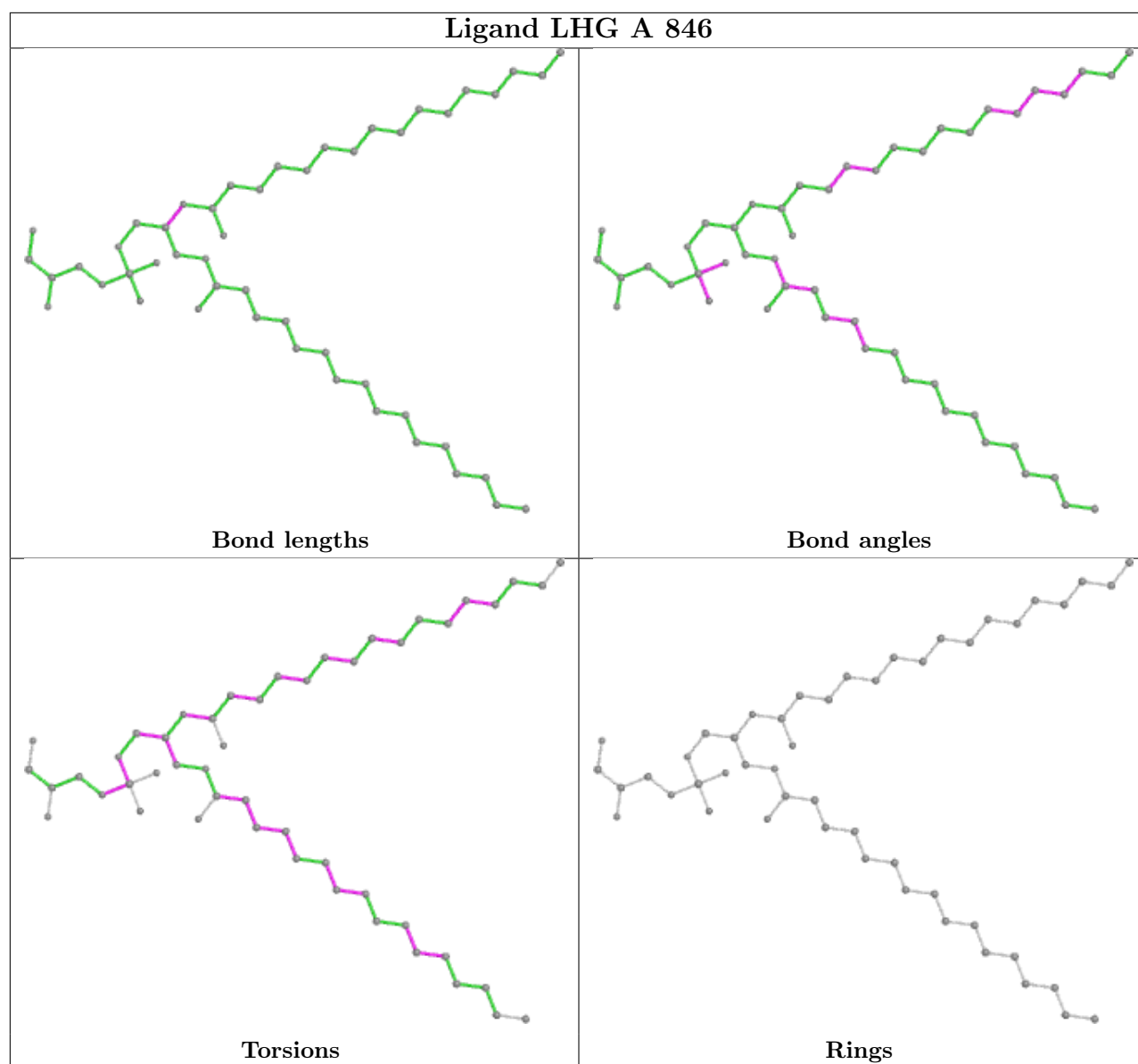


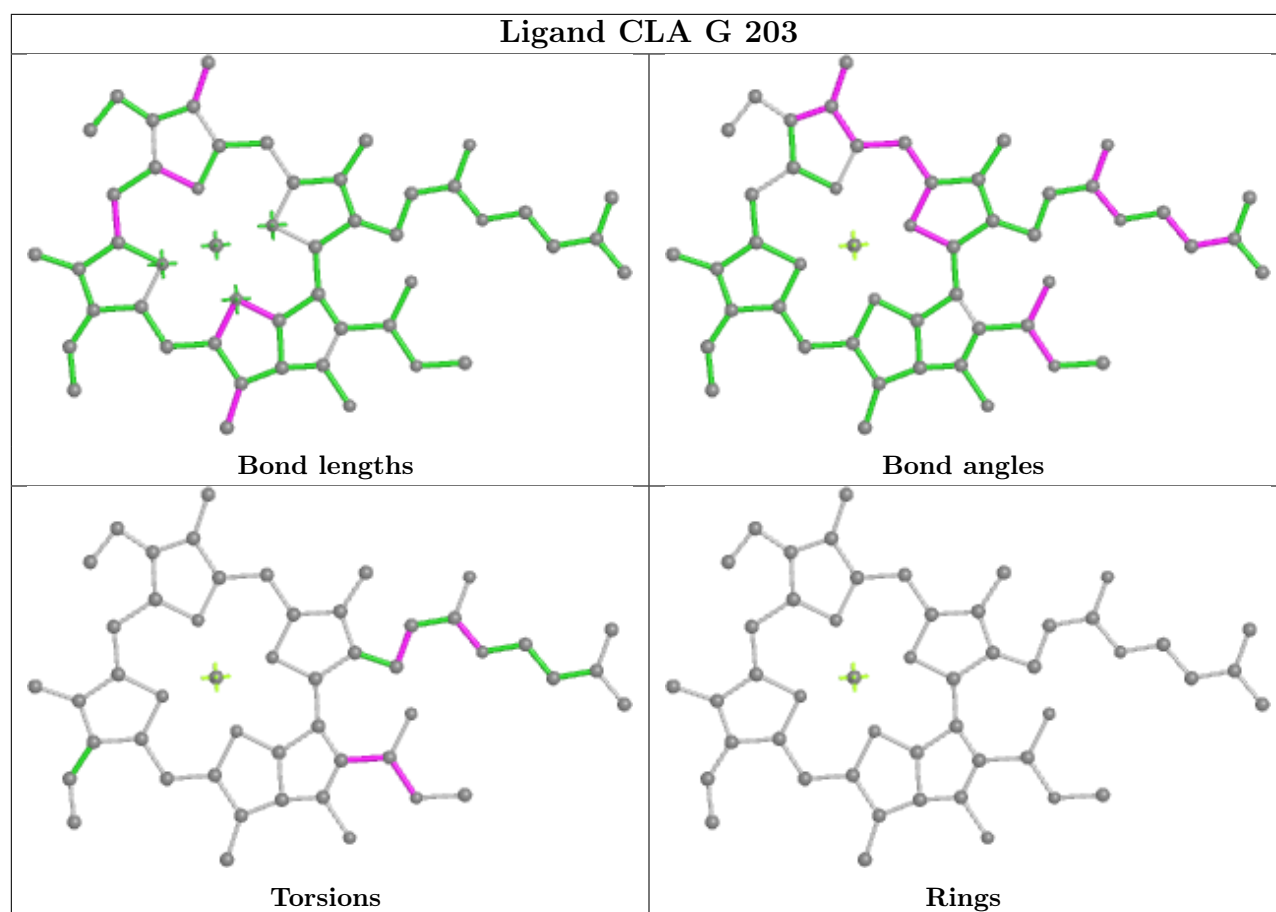
Ligand CLA B 818



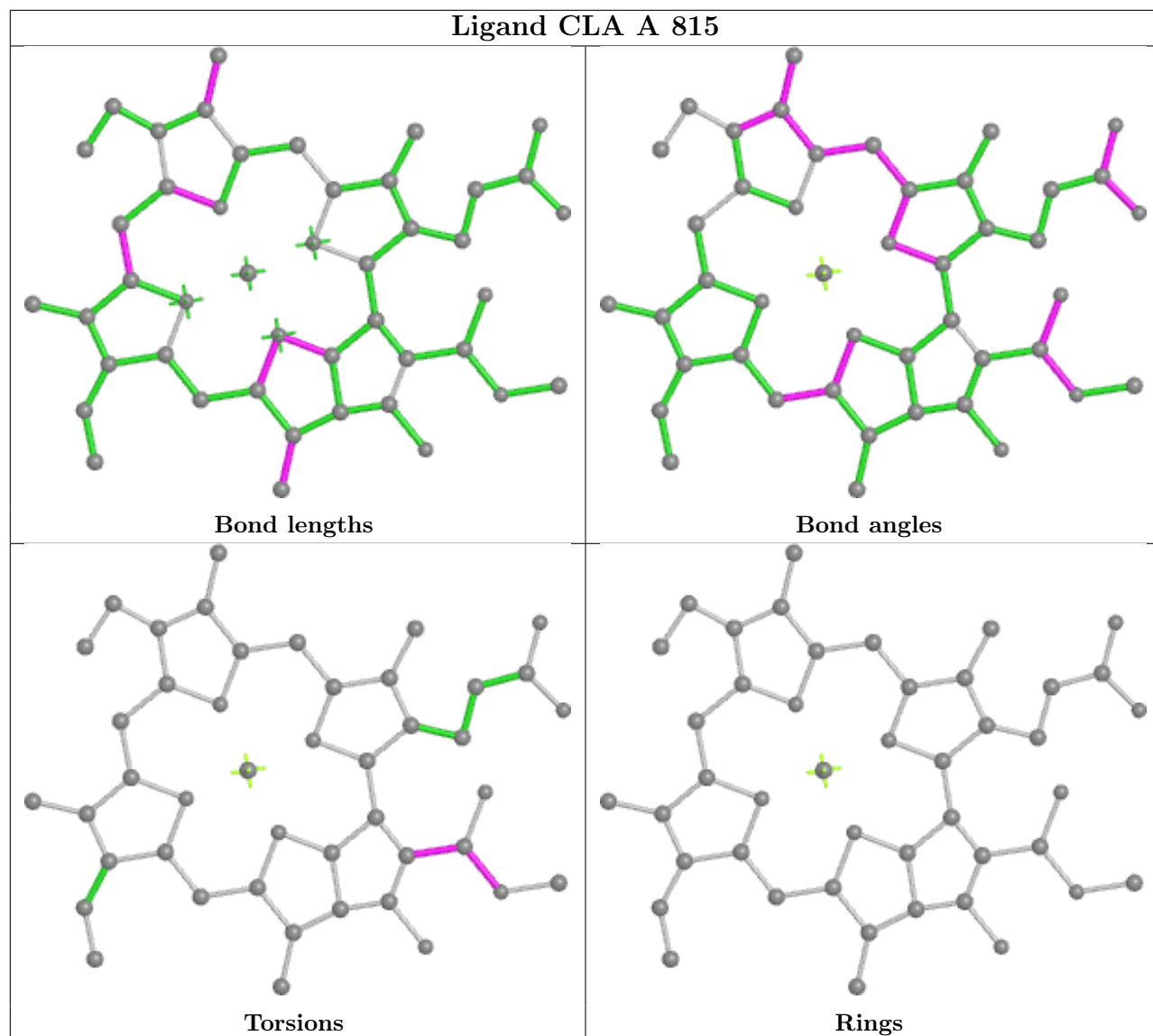
Ligand BCR J 103



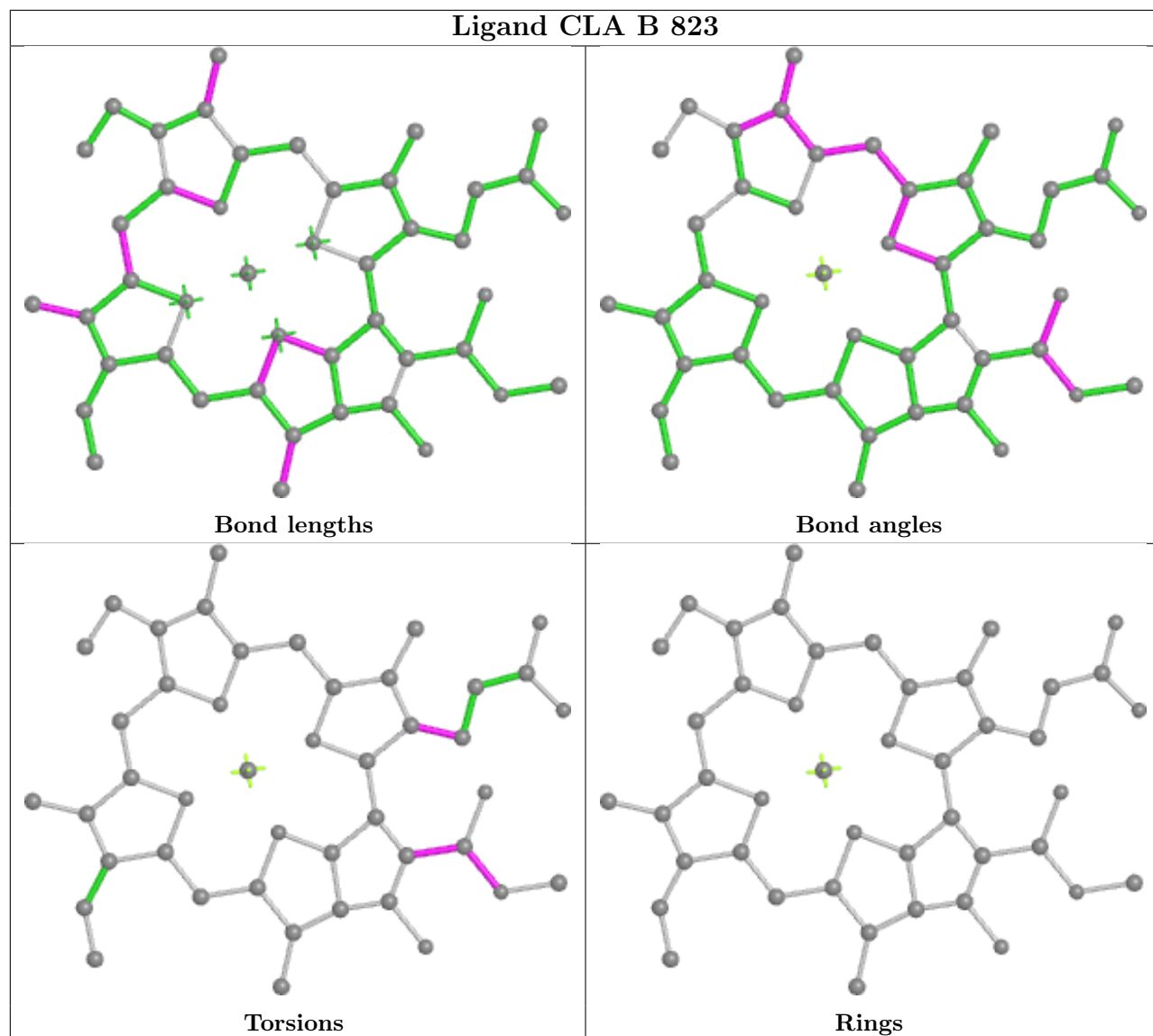


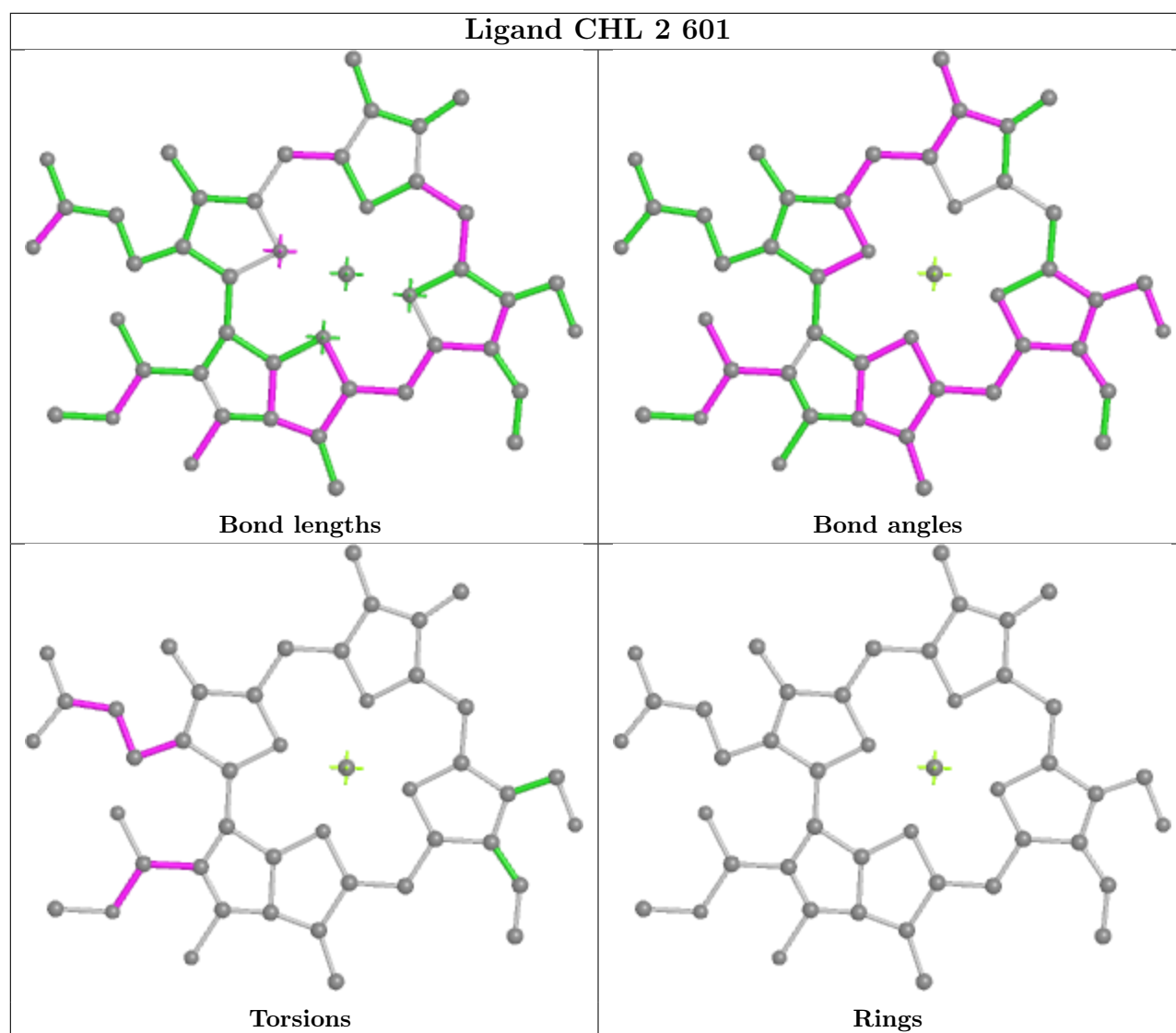


Ligand CLA A 815

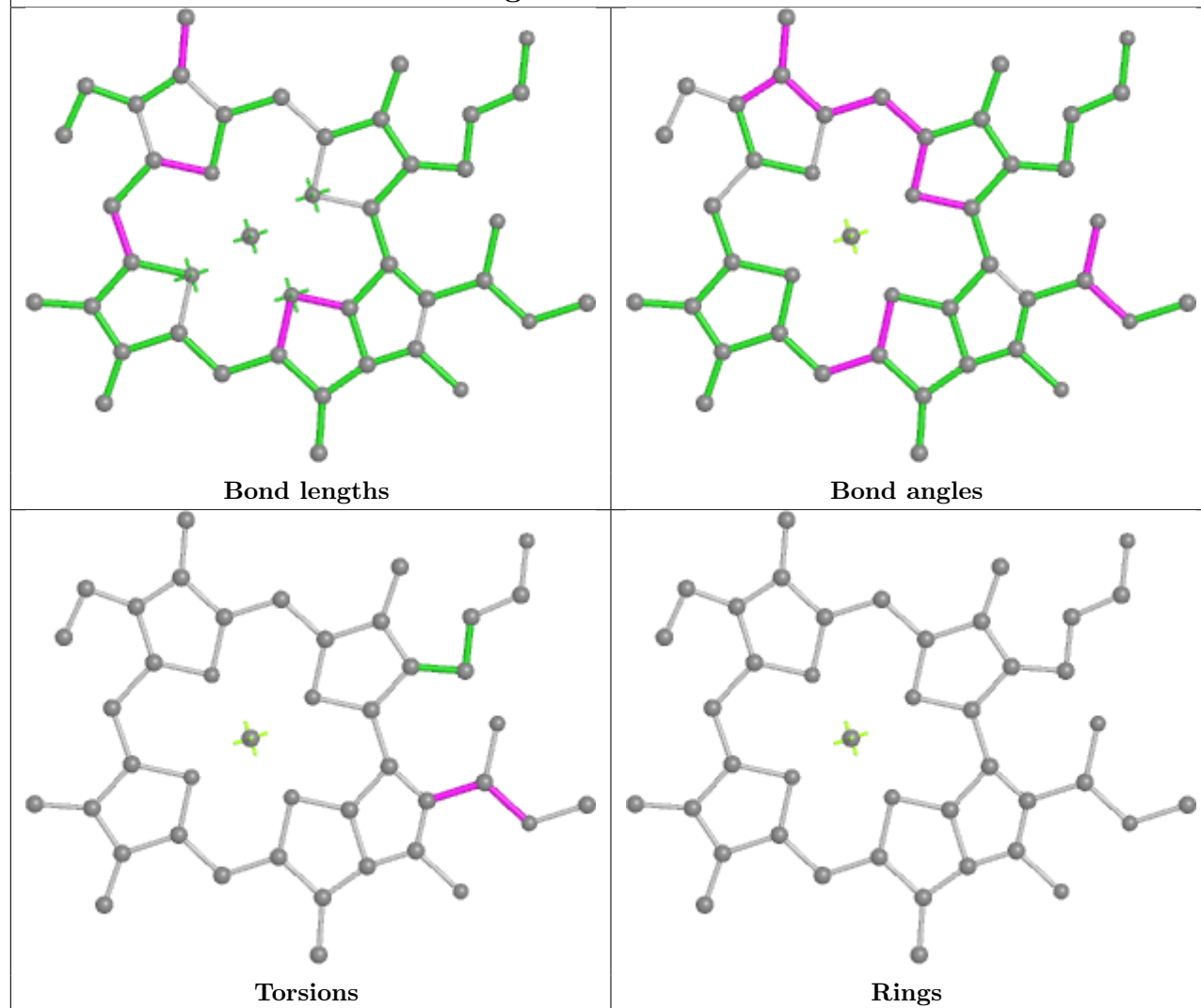


Ligand CLA B 823

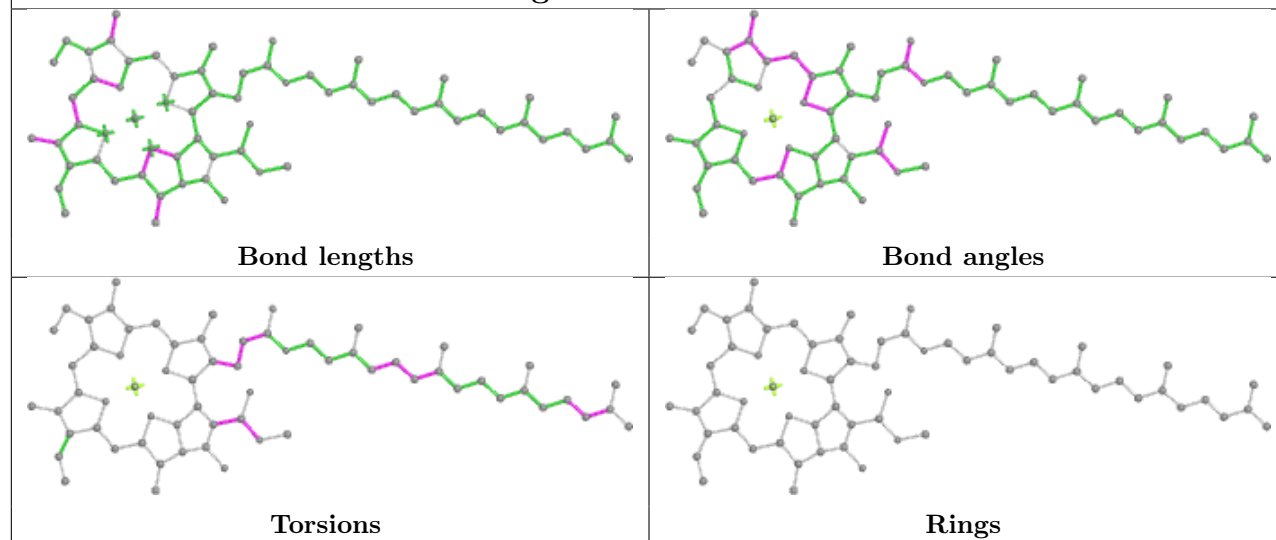


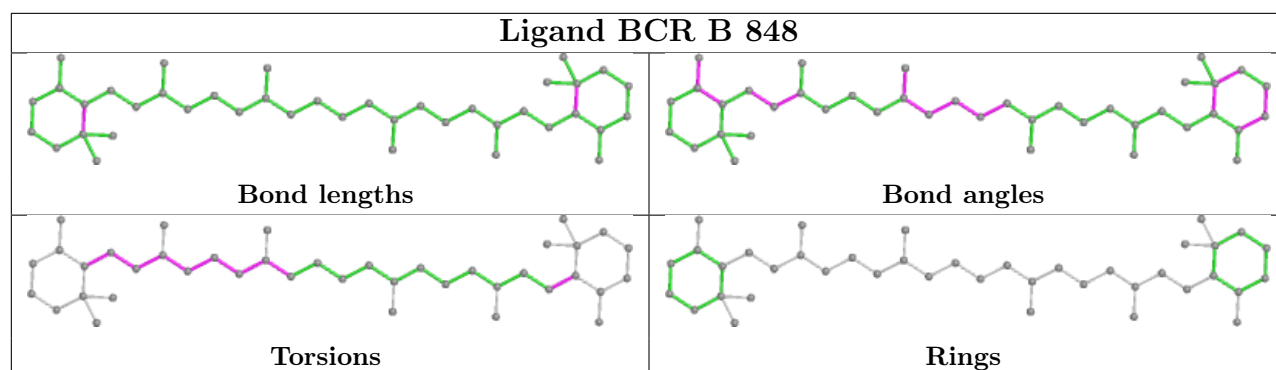
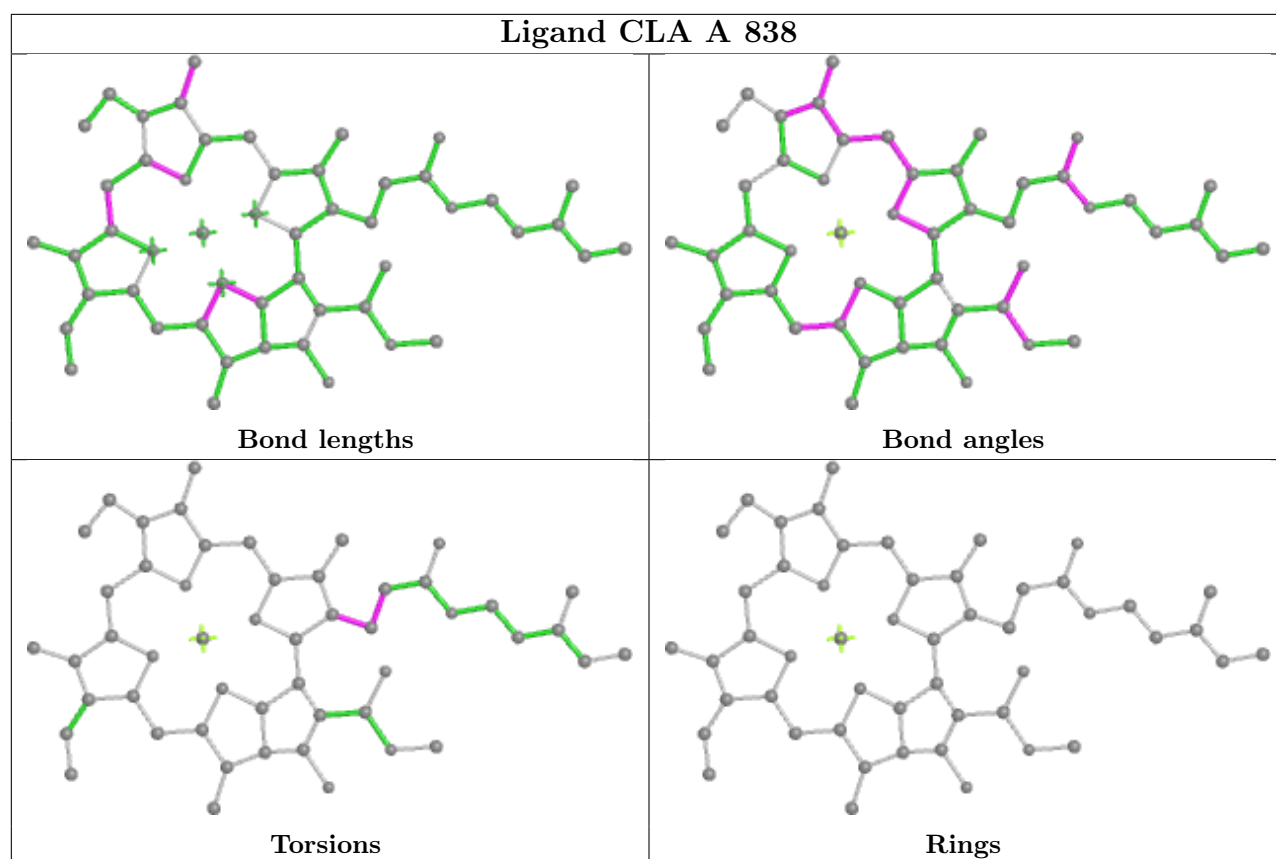


Ligand CLA 5 604

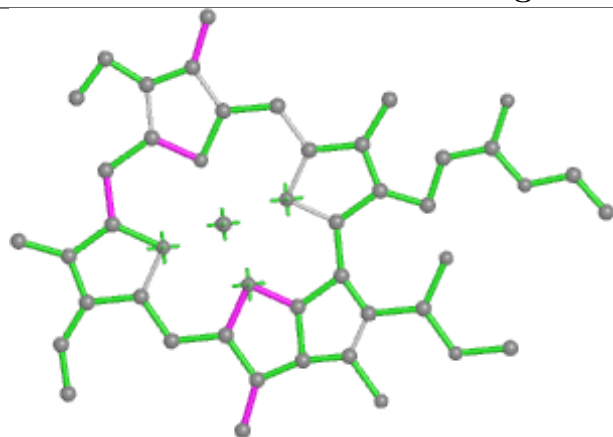


Ligand CLA A 814

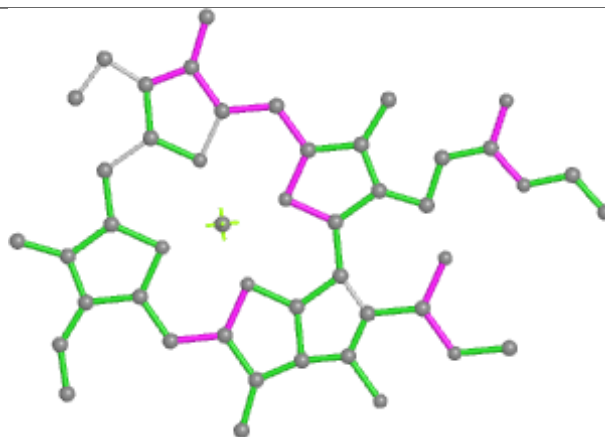




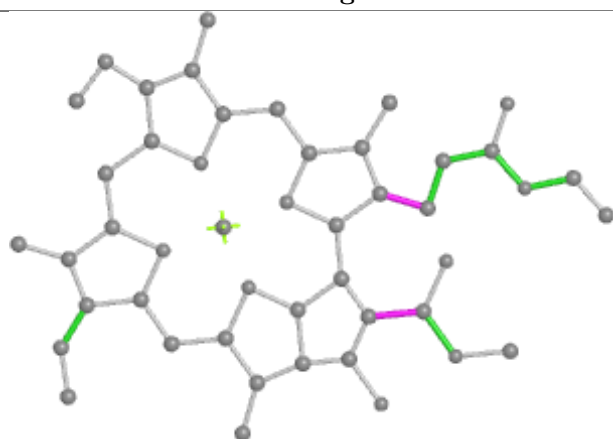
Ligand CLA B 838



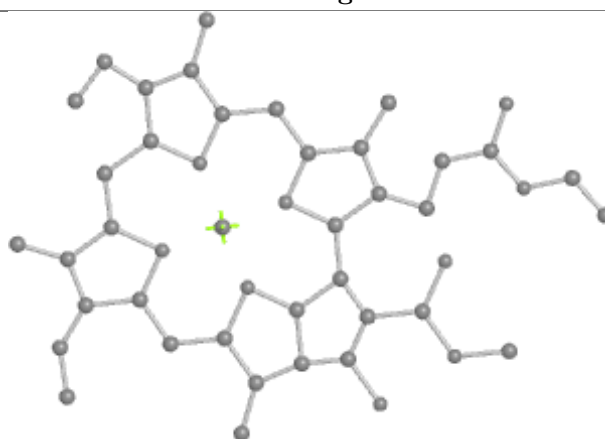
Bond lengths



Bond angles

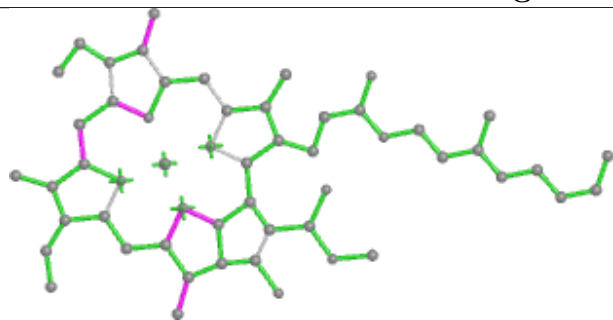


Torsions

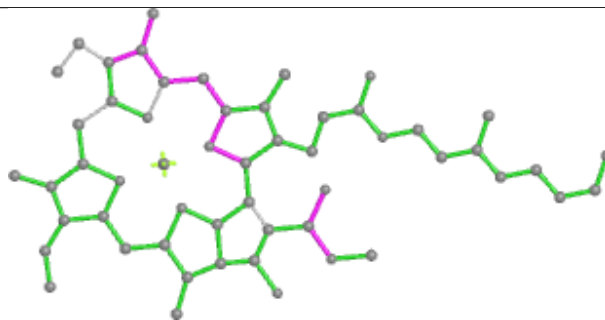


Rings

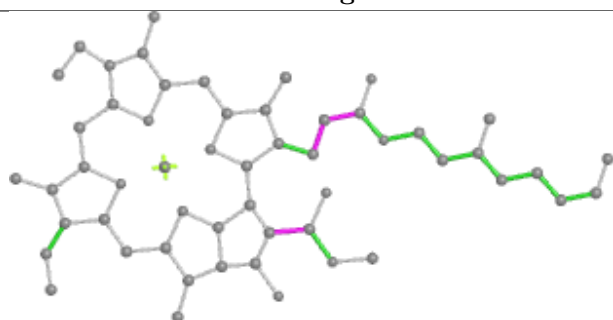
Ligand CLA A 813



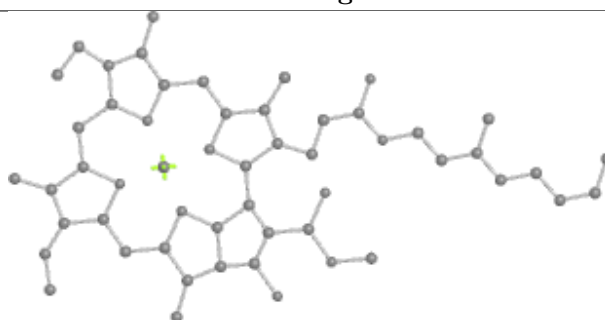
Bond lengths



Bond angles

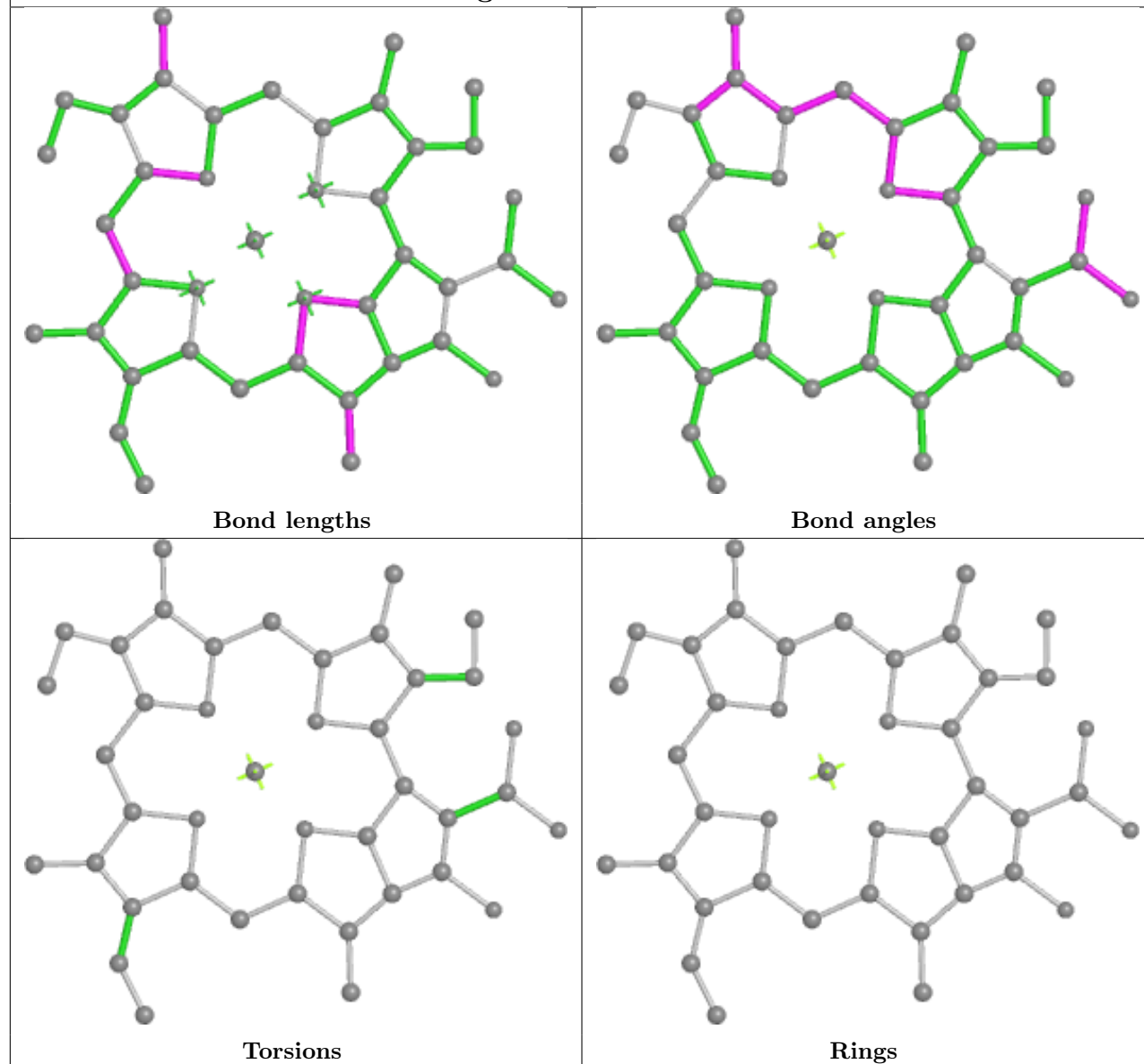


Torsions

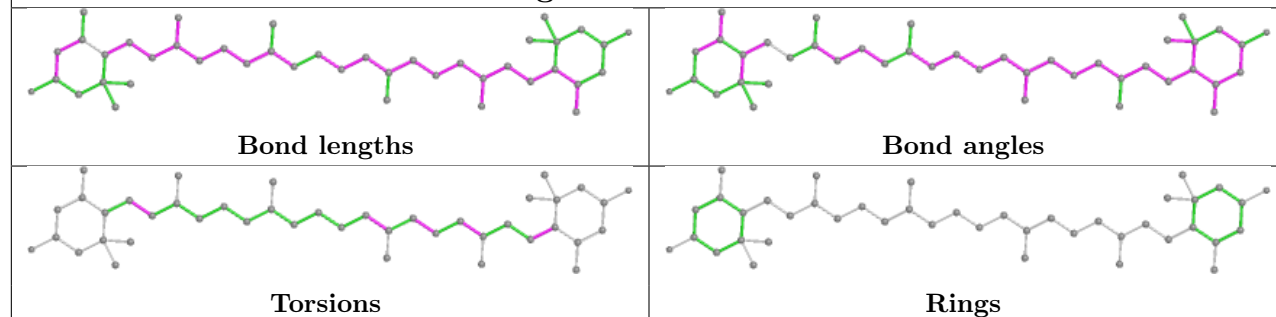


Rings

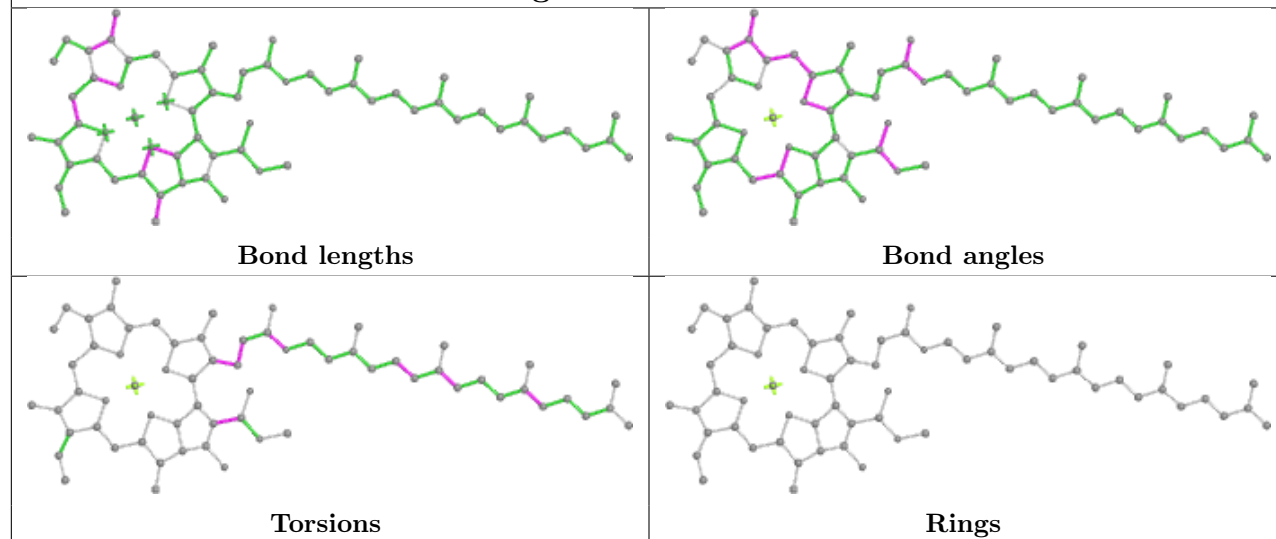
Ligand CLA B 839



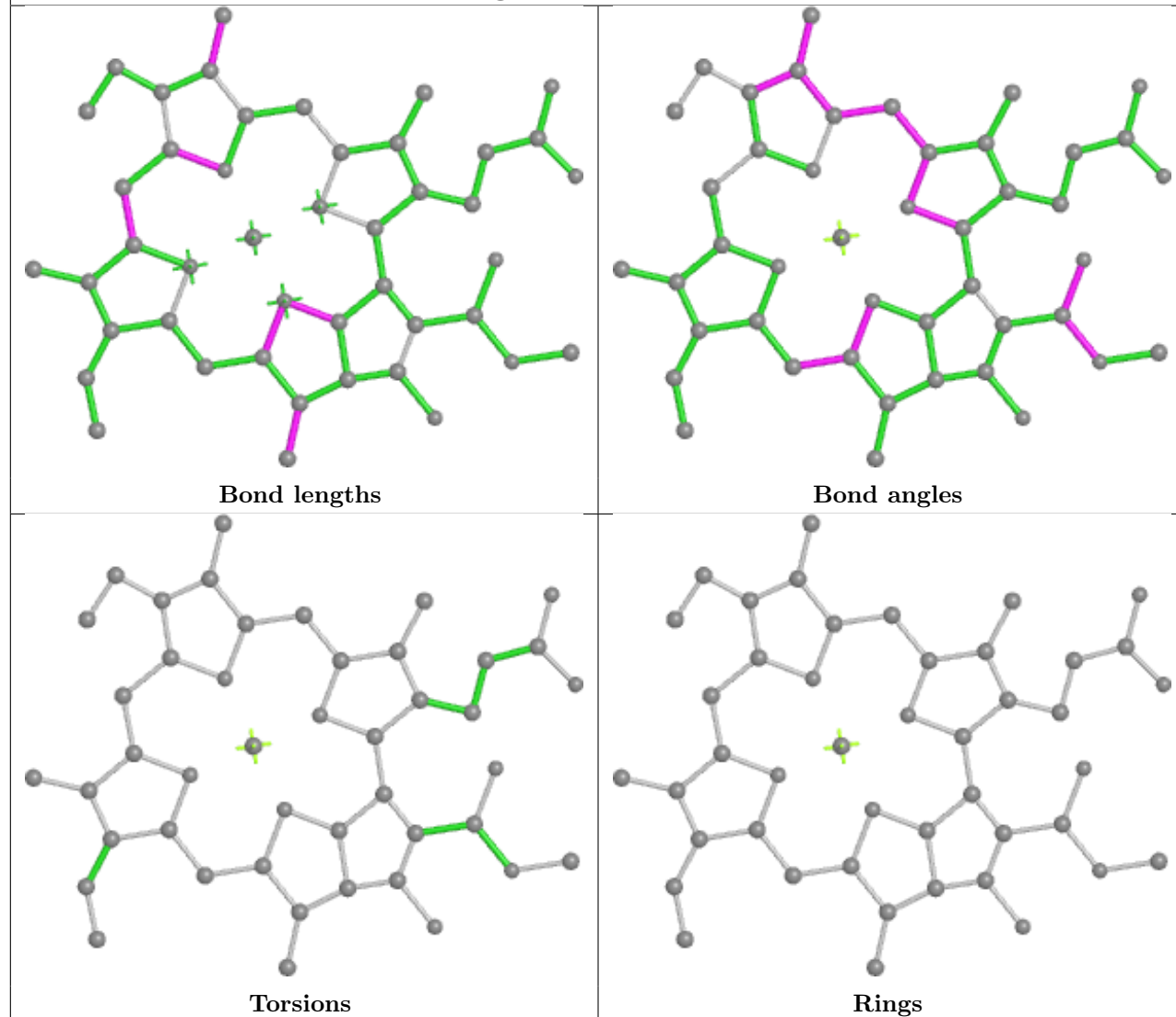
Ligand LUT 3 618

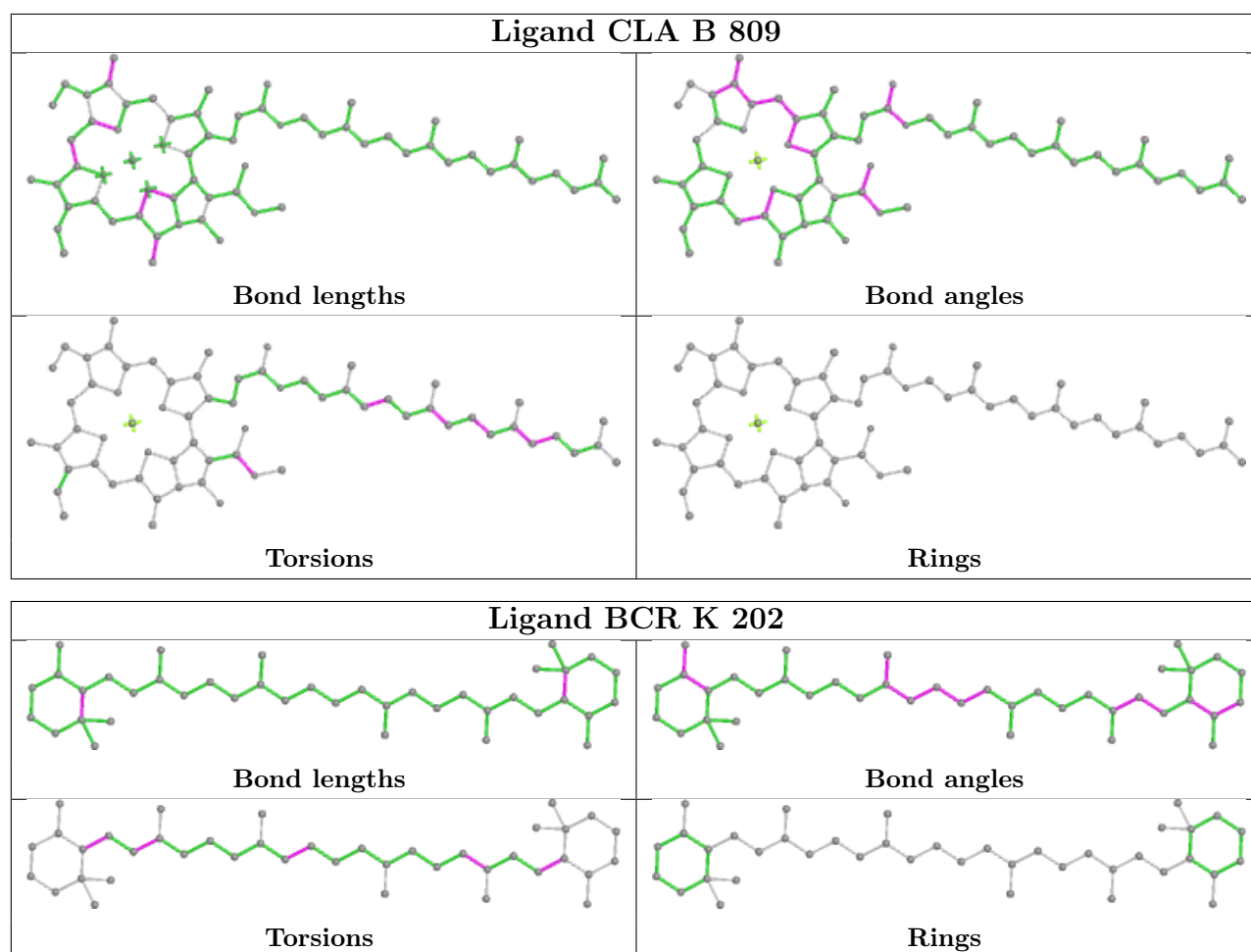


Ligand CLA B 828

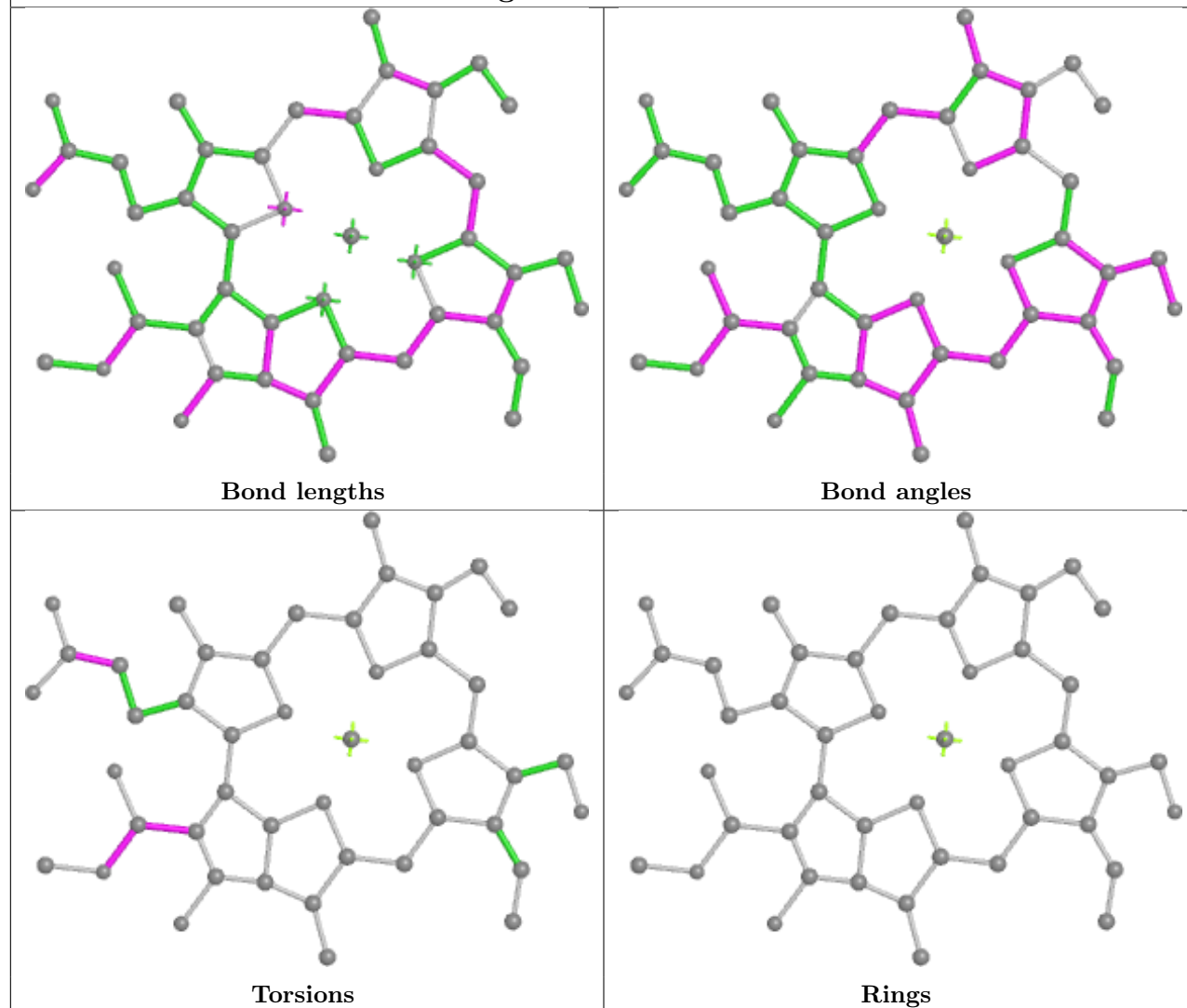


Ligand CLA L 303

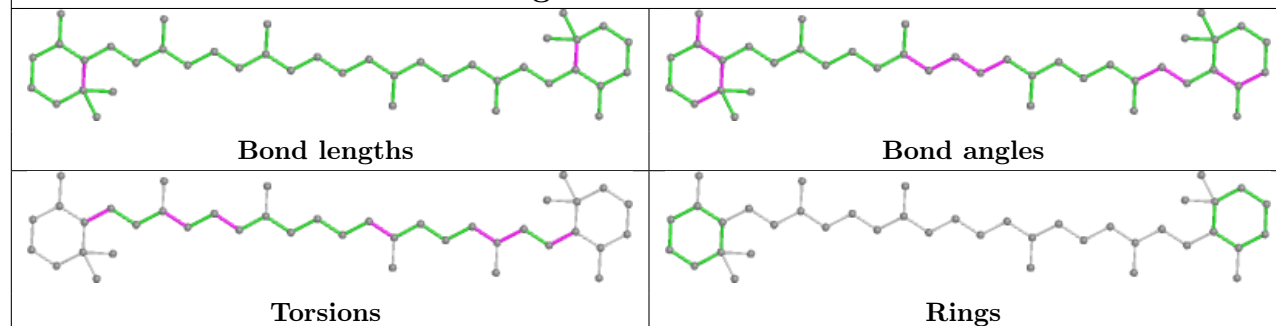




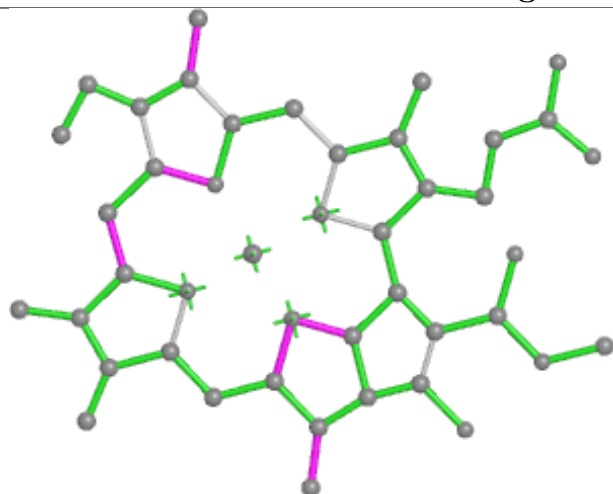
Ligand CHL 2 616



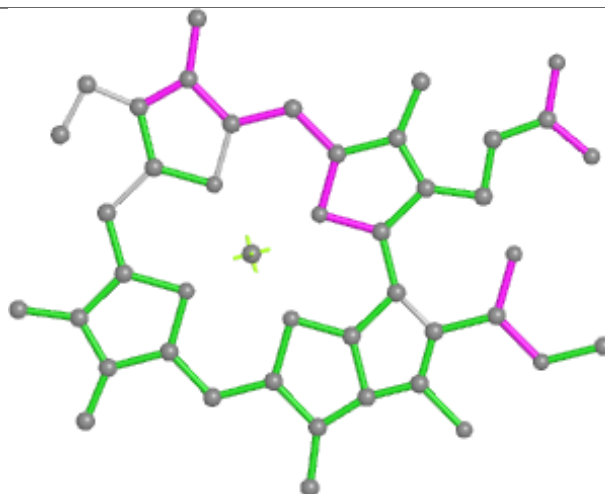
Ligand BCR L 301



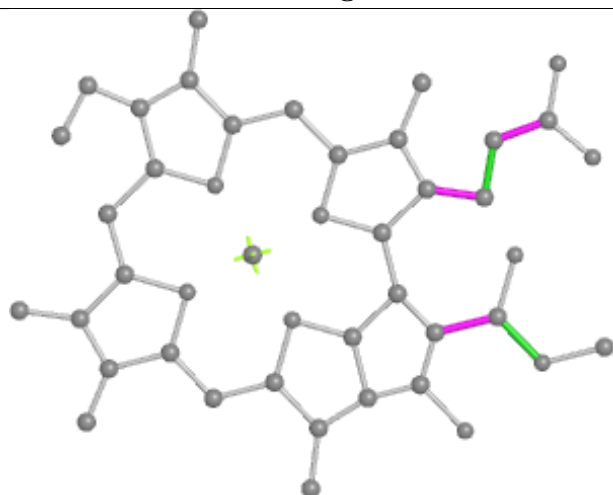
Ligand CLA 5 612



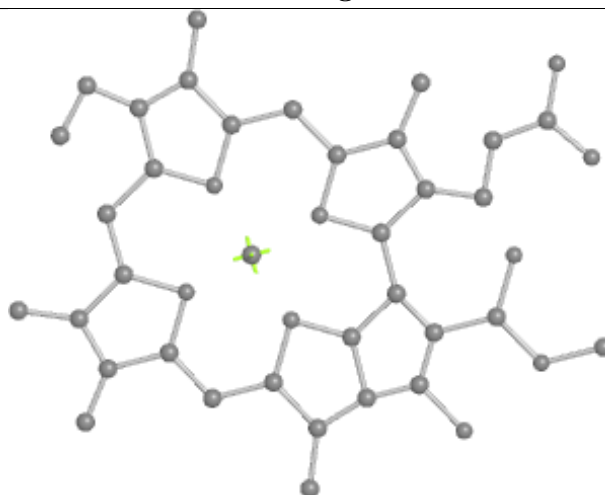
Bond lengths



Bond angles

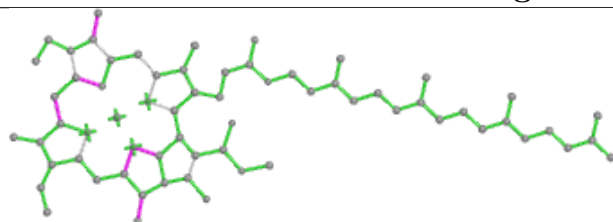


Torsions

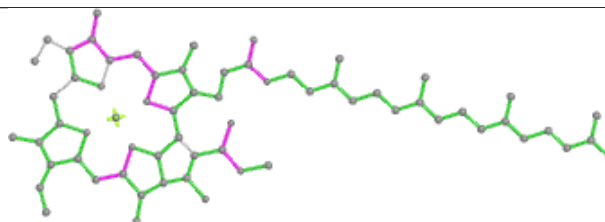


Rings

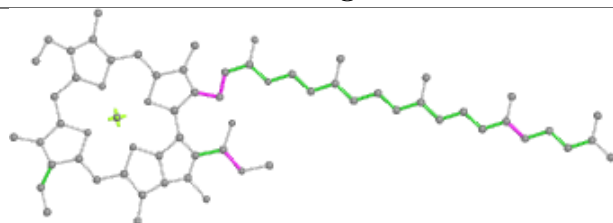
Ligand CLA A 803



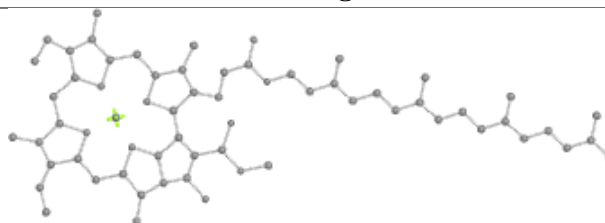
Bond lengths



Bond angles

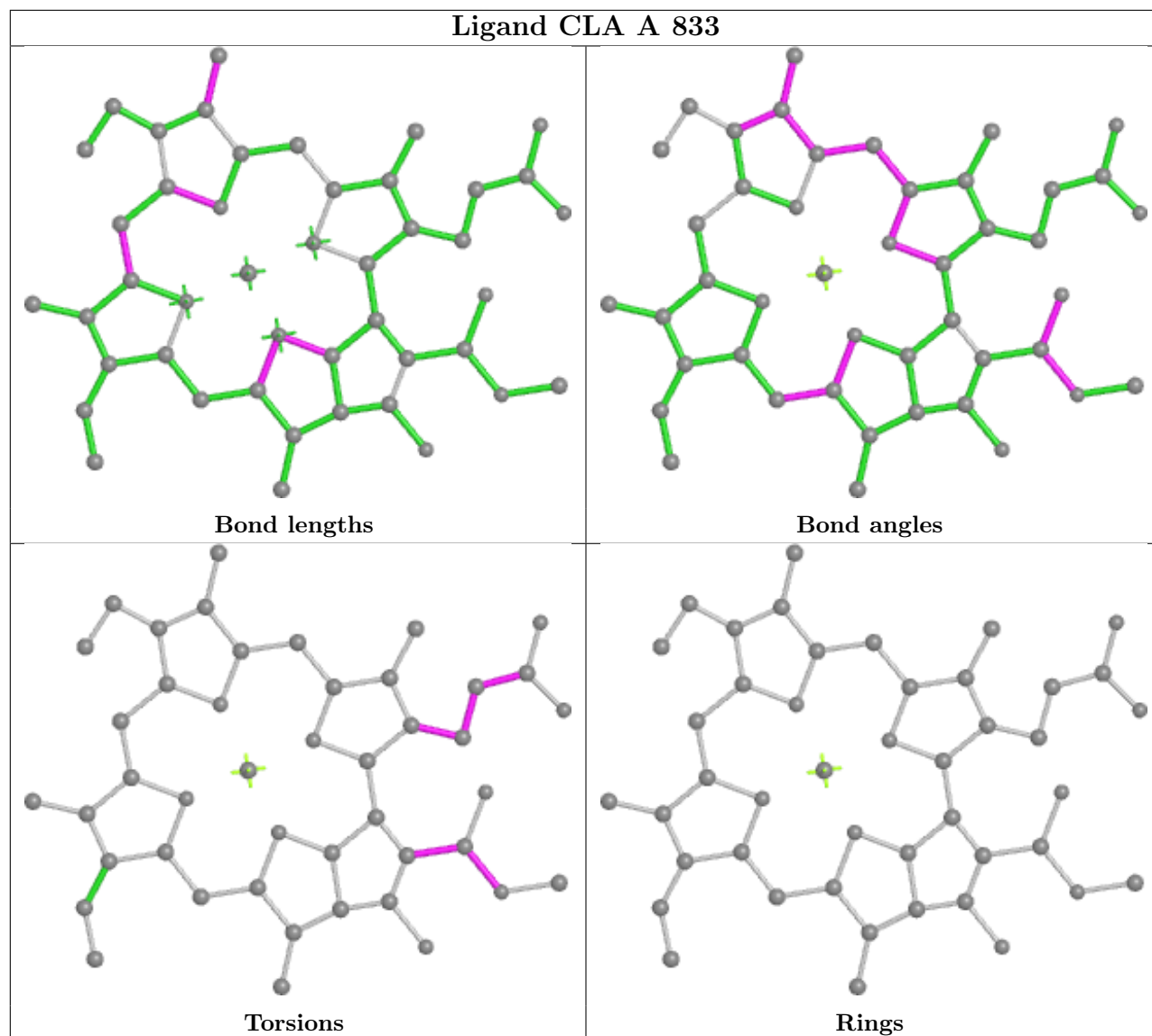


Torsions

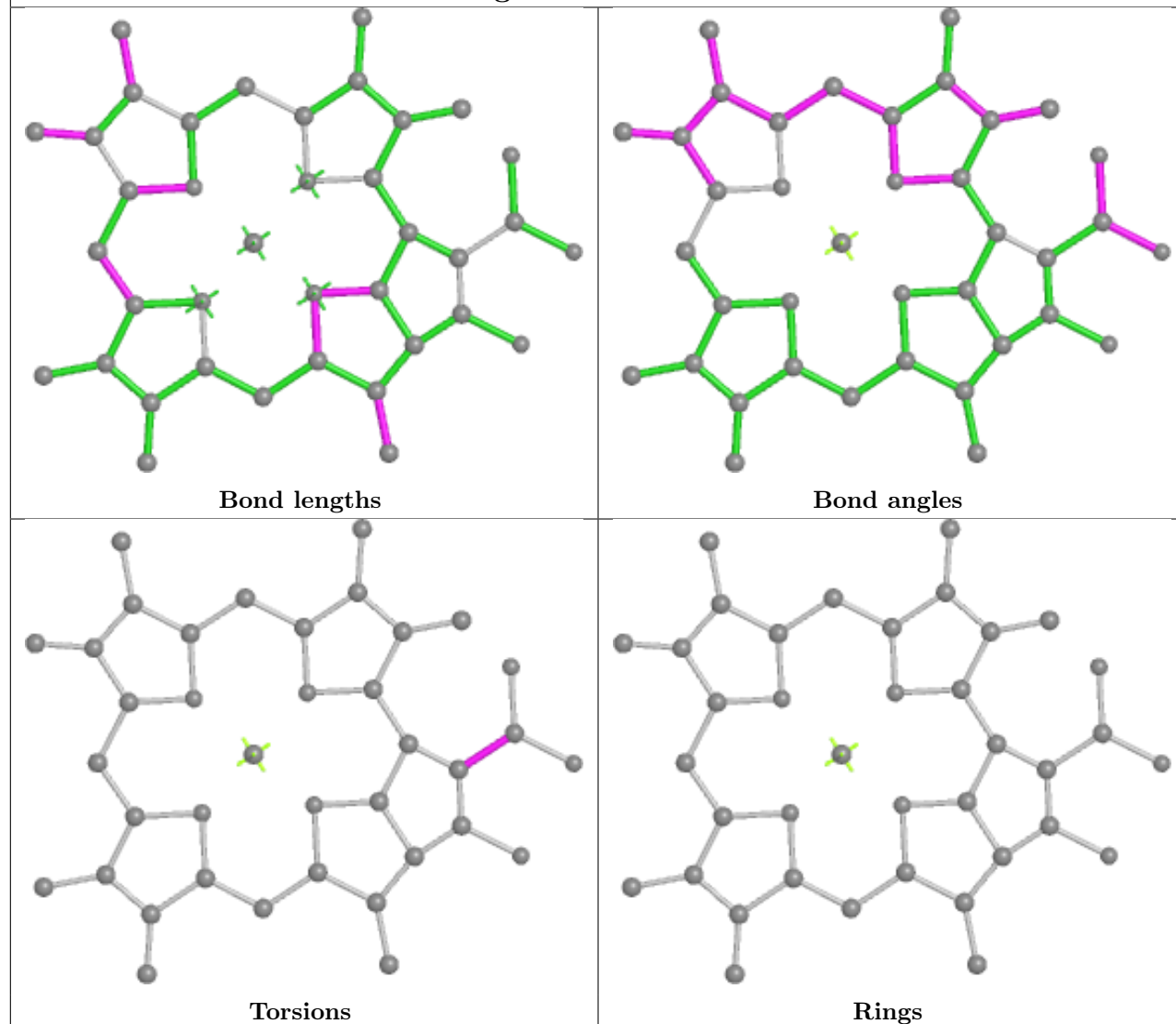


Rings

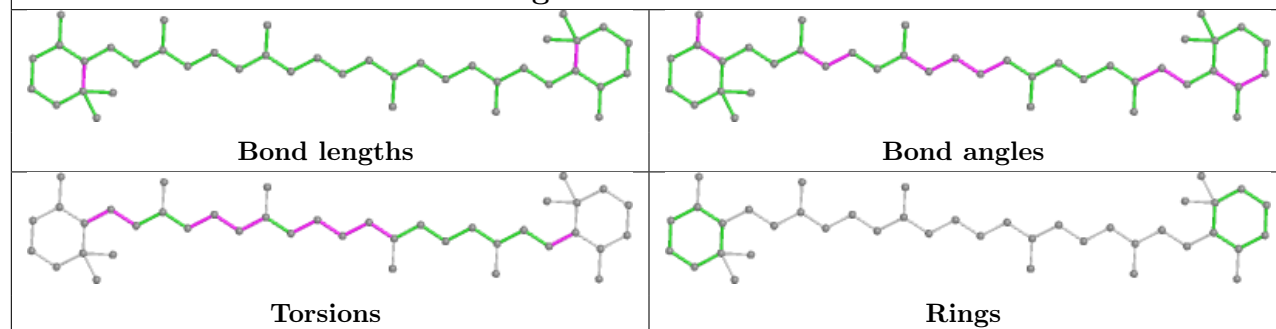
Ligand CLA A 833



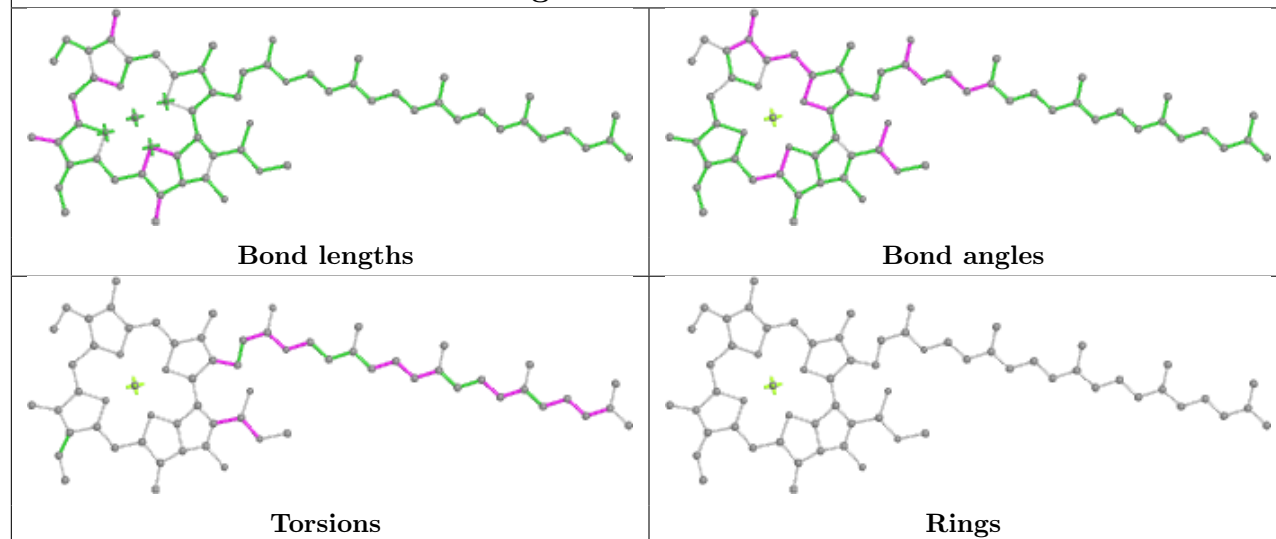
Ligand CLA 6 611



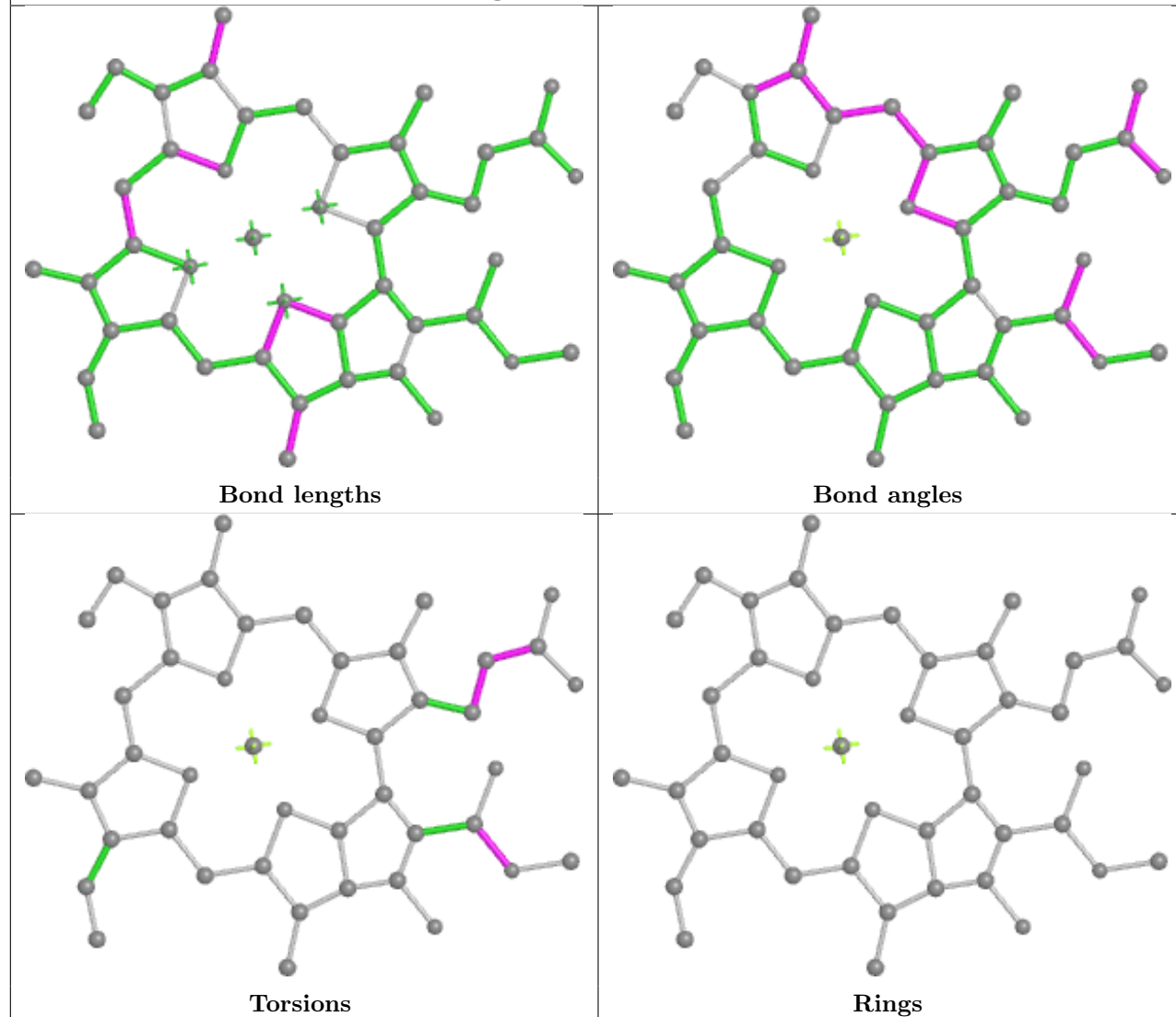
Ligand BCR F 302

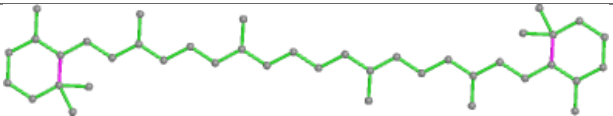
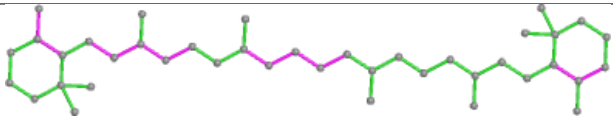
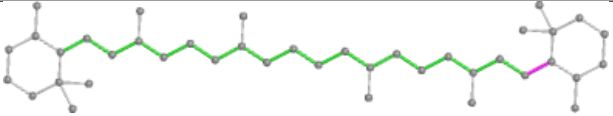
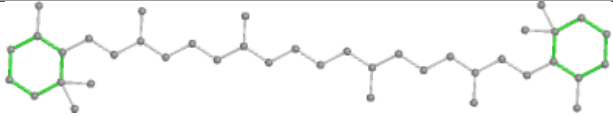


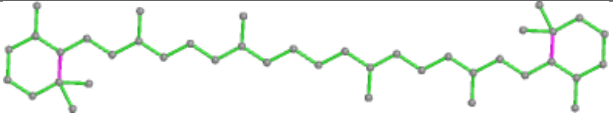
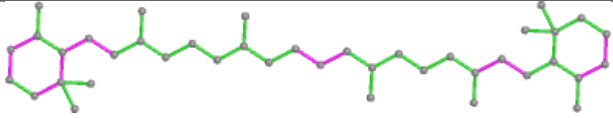
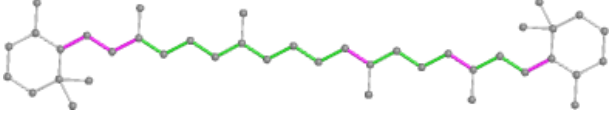
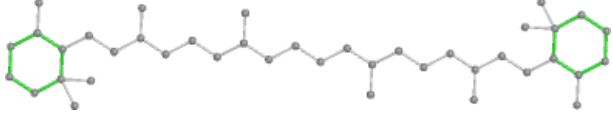
Ligand CLA A 829

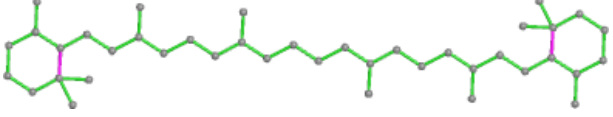
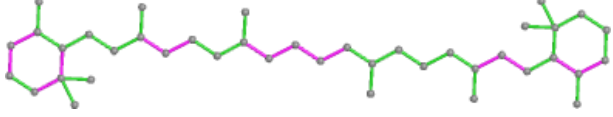
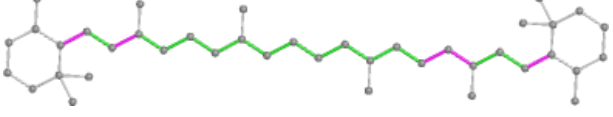
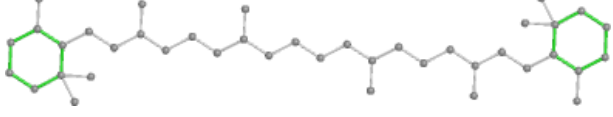


Ligand CLA K 206

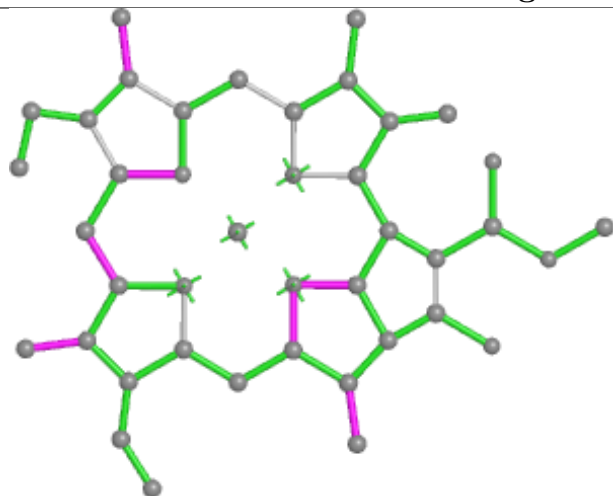


Ligand BCR B 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

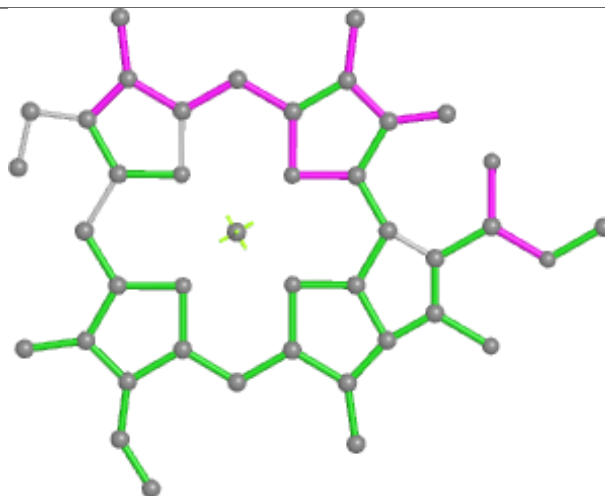
Ligand BCR 3 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 856	
	
Bond lengths	Bond angles
	
Torsions	Rings

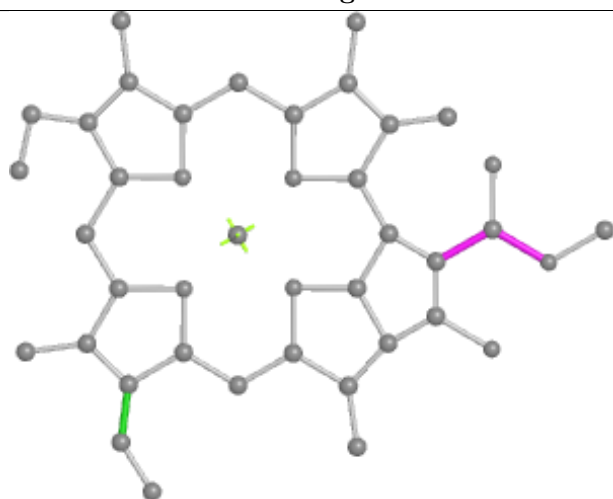
Ligand CLA 3 610



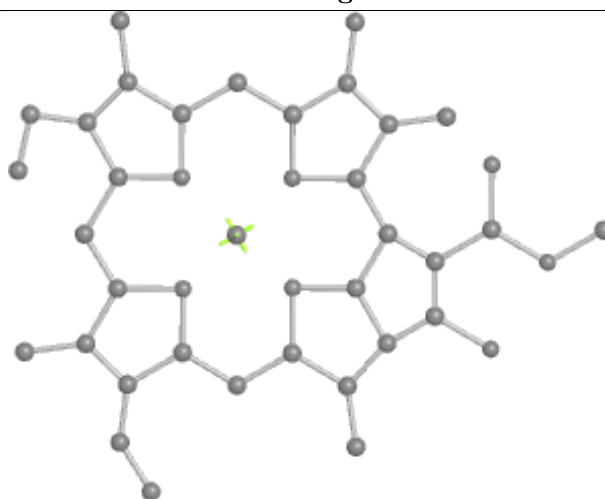
Bond lengths



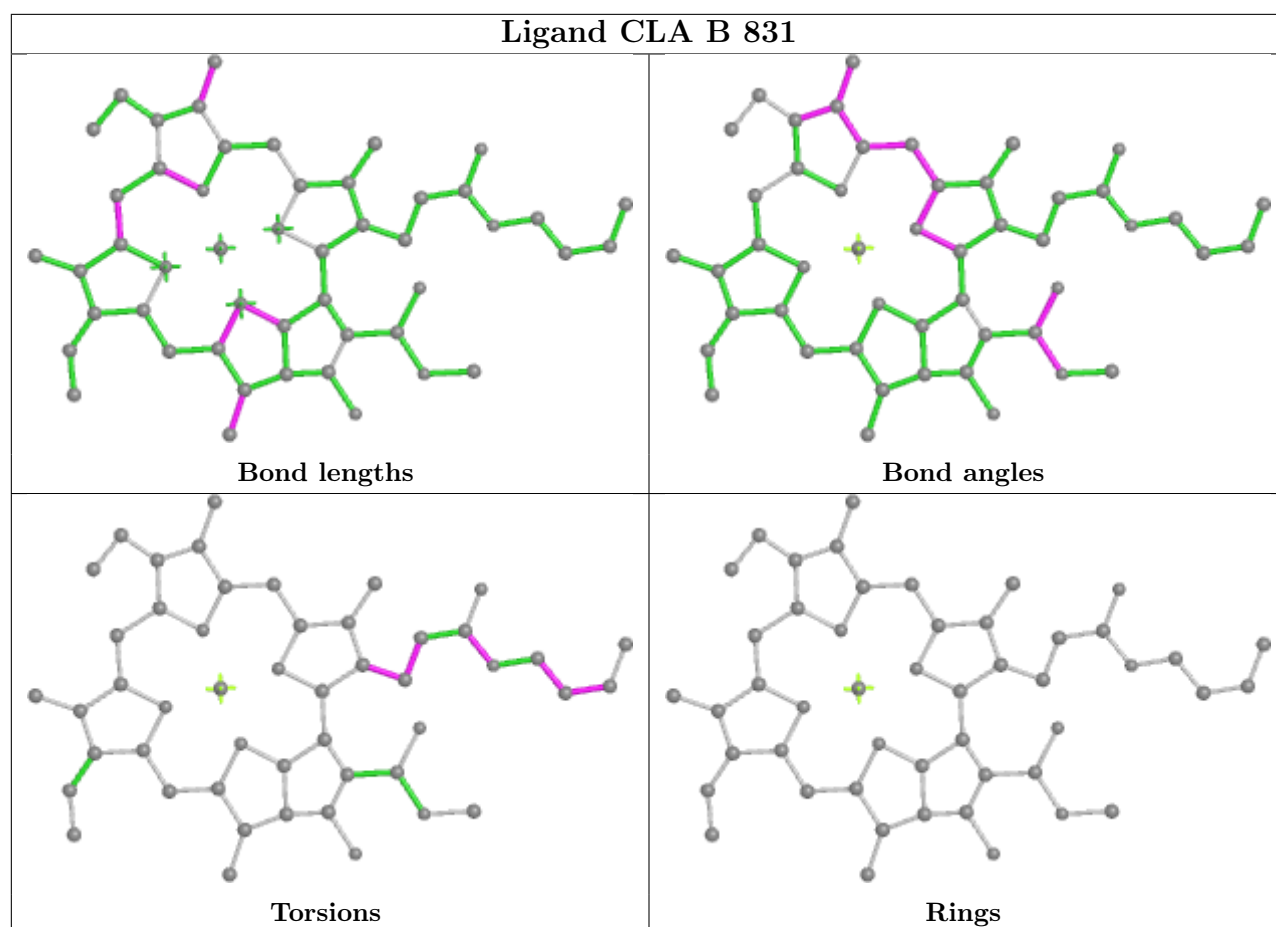
Bond angles



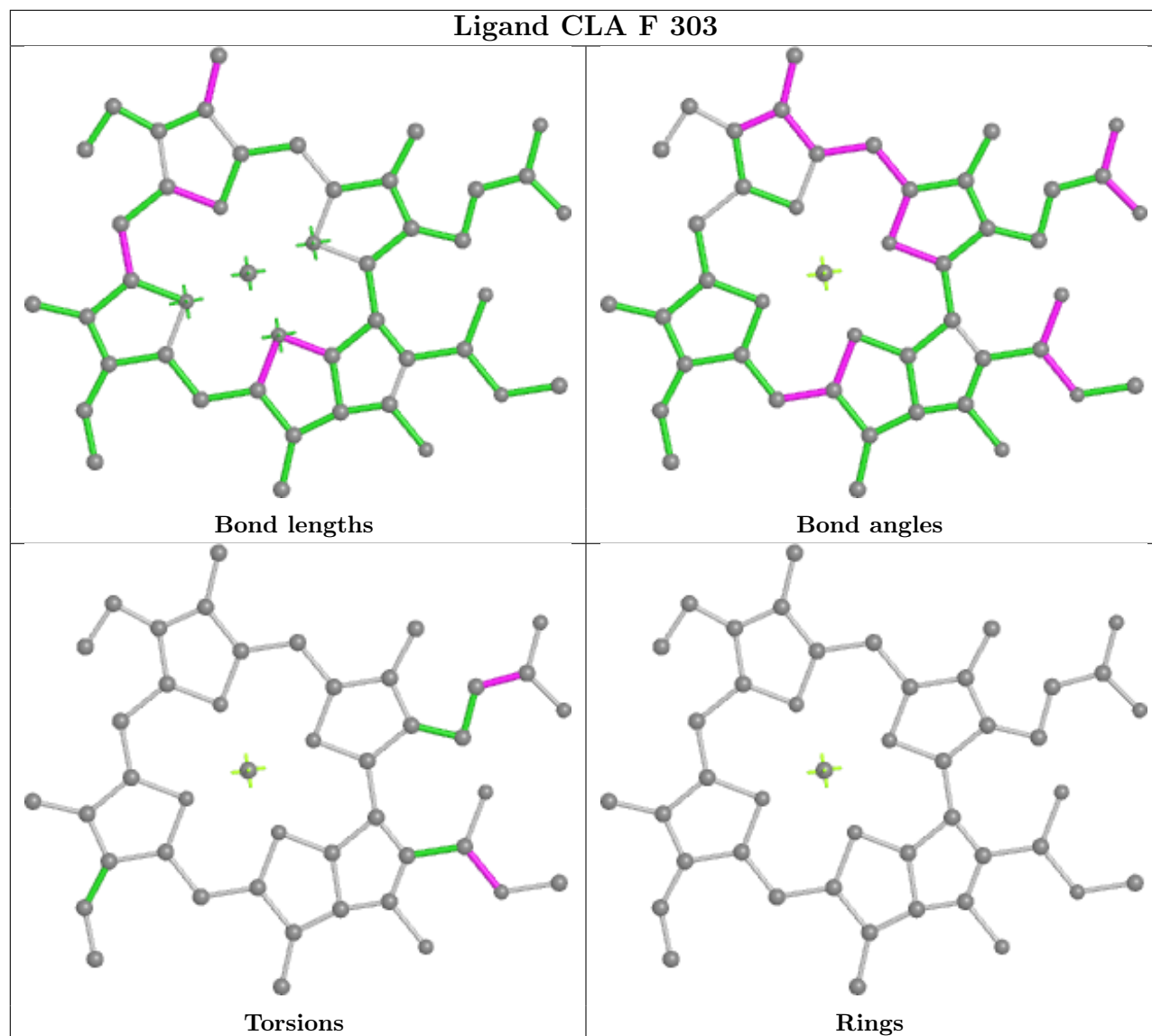
Torsions



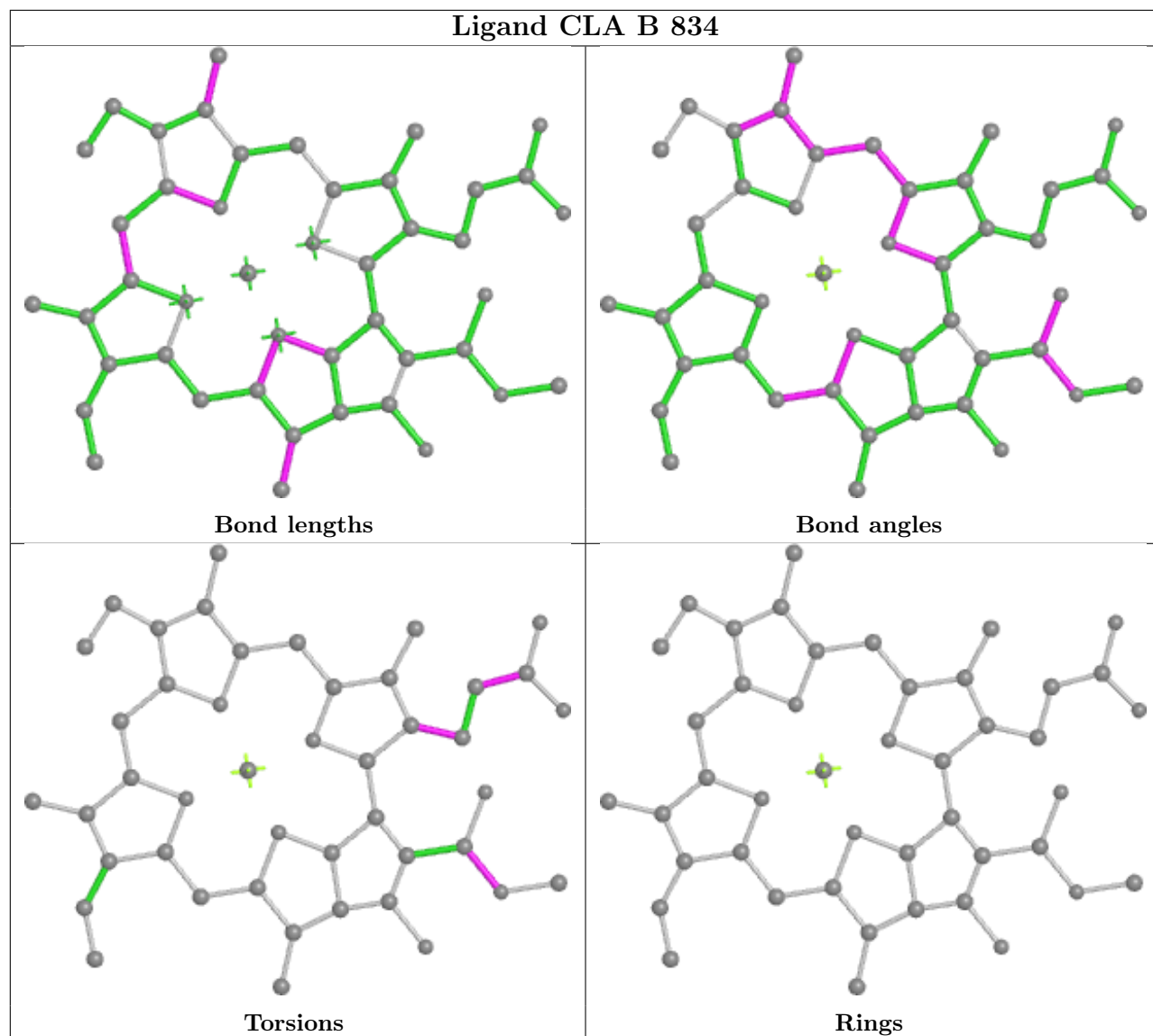
Rings



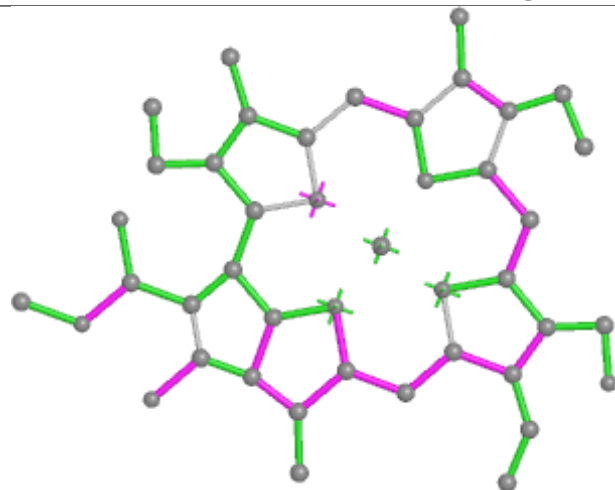
Ligand CLA F 303



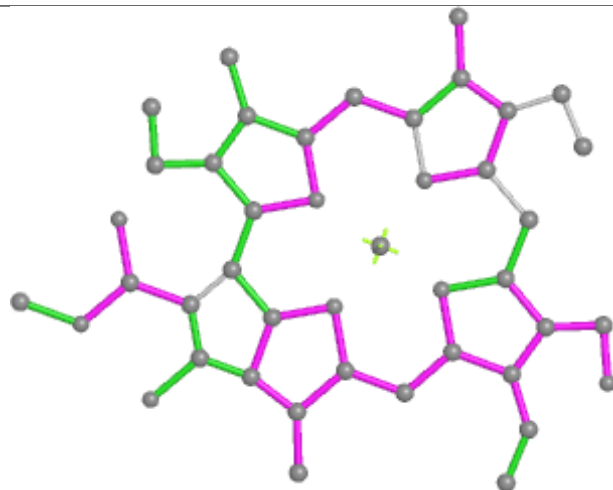
Ligand CLA B 834



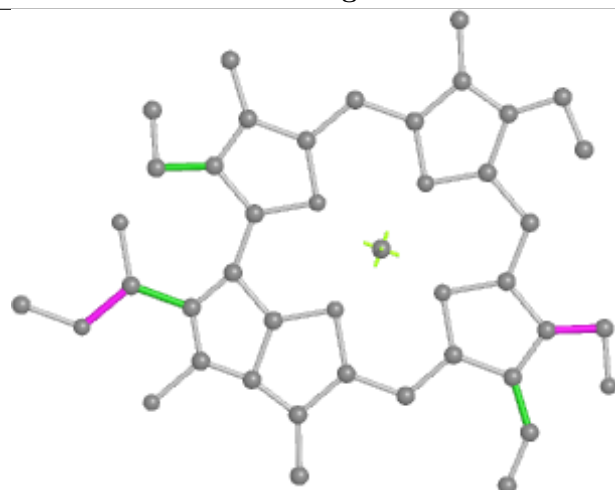
Ligand CHL 2 607



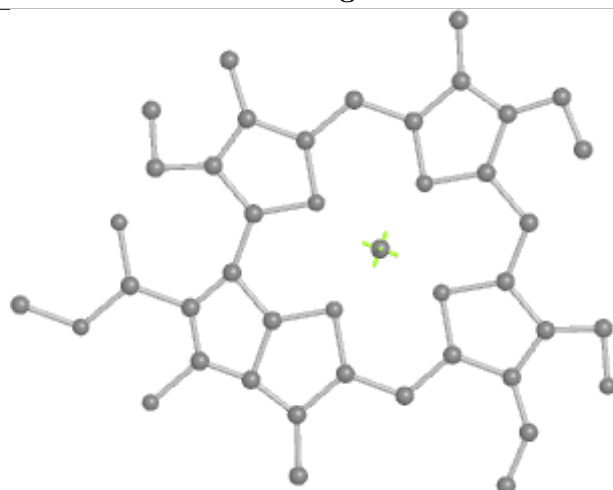
Bond lengths



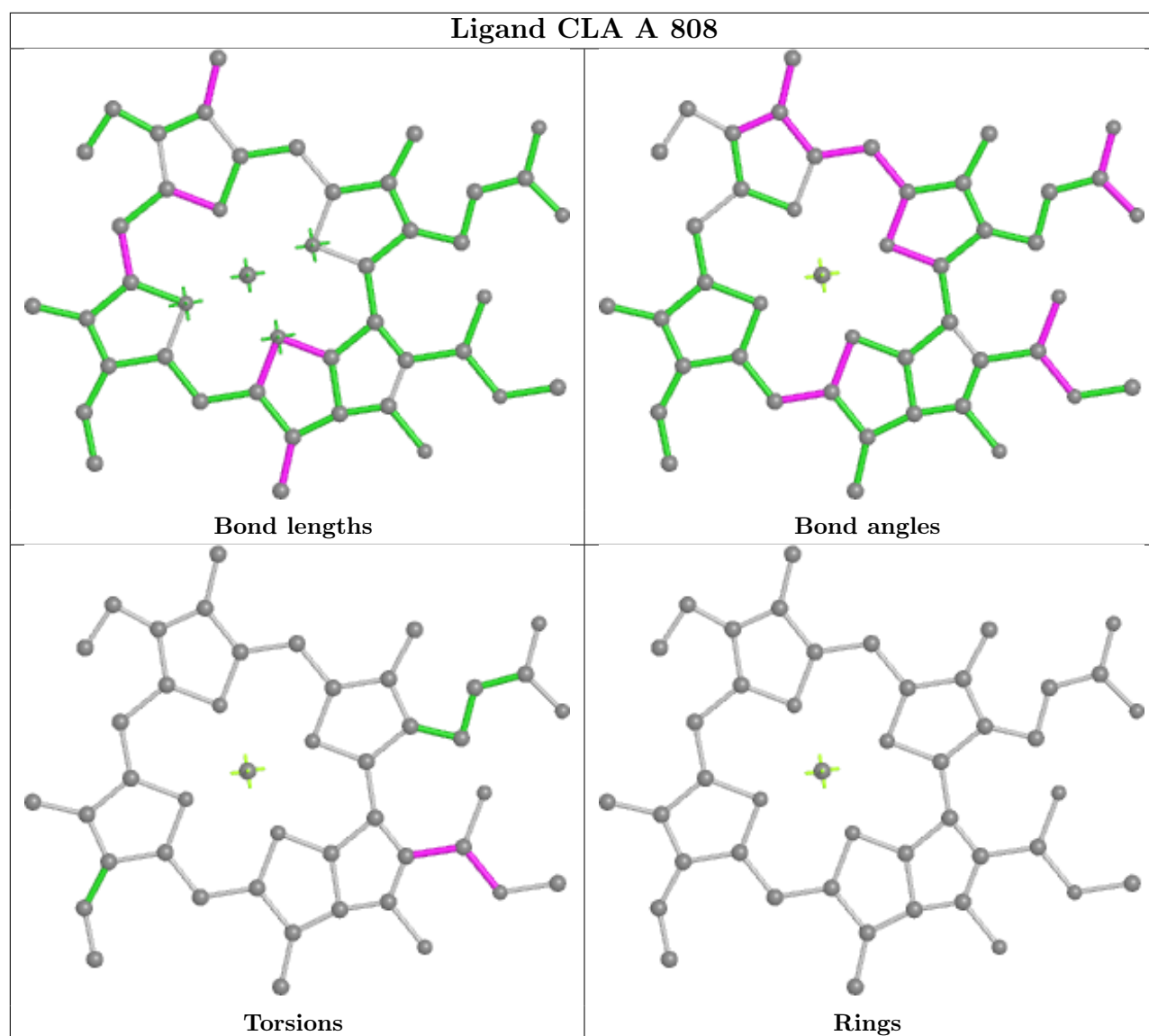
Bond angles



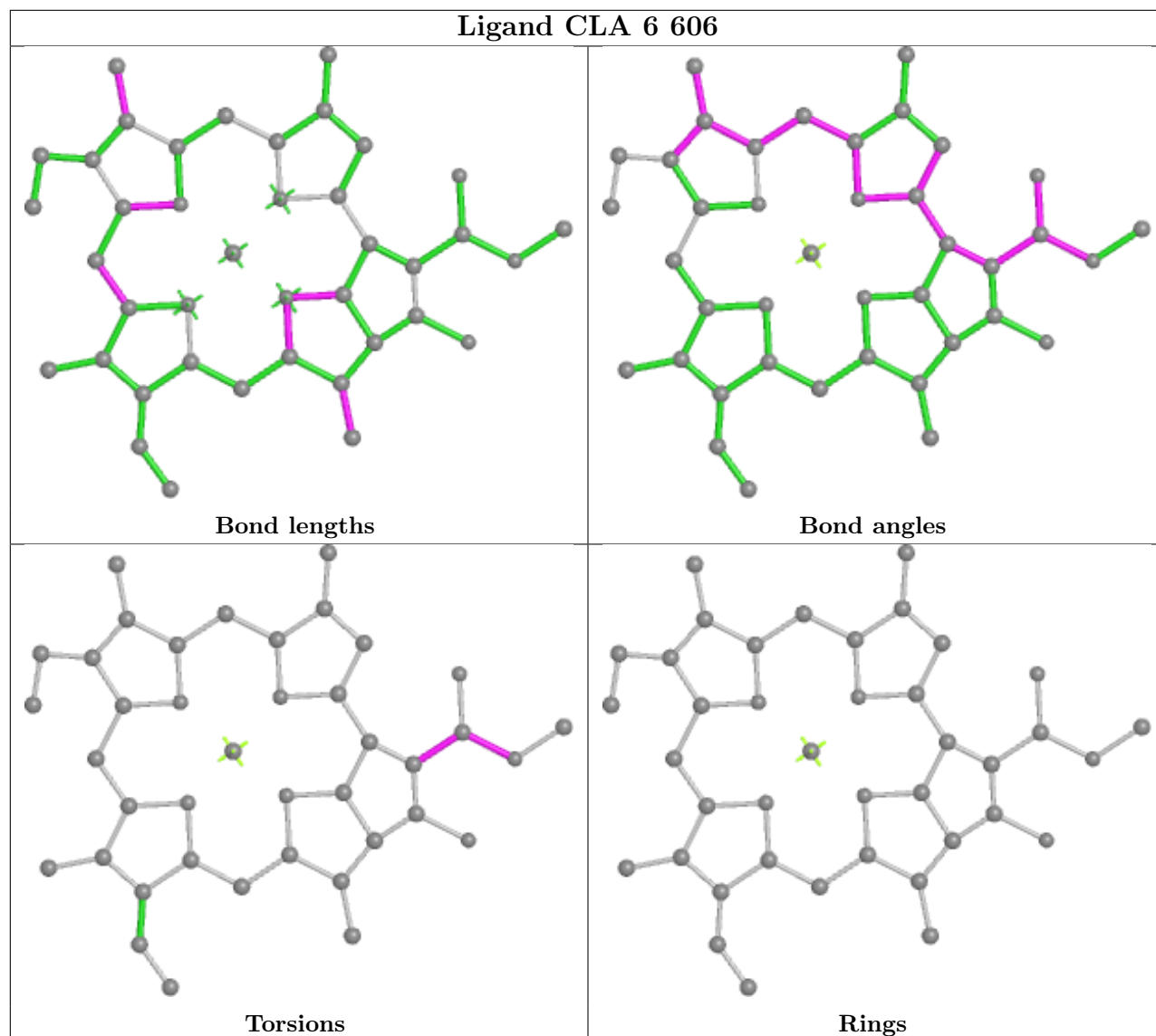
Torsions



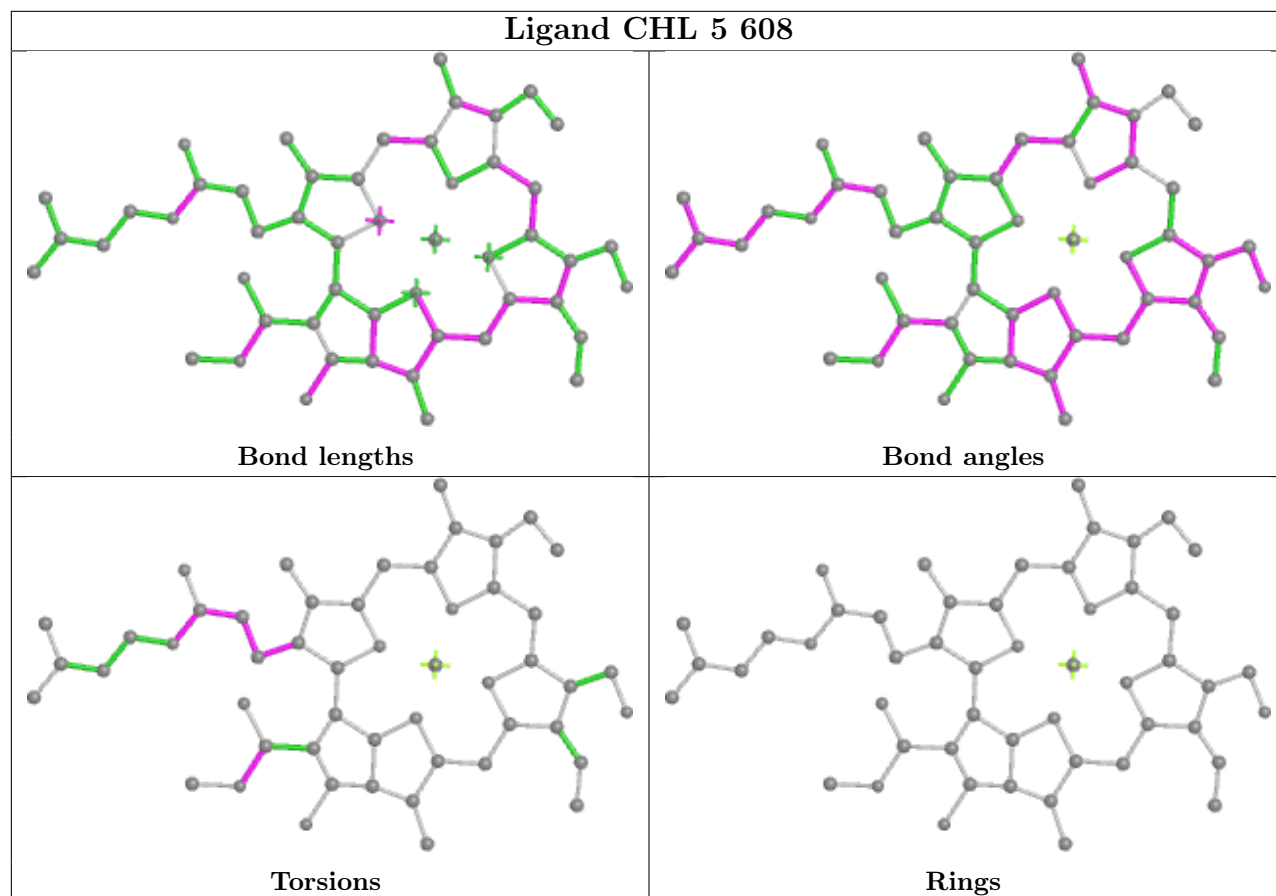
Rings



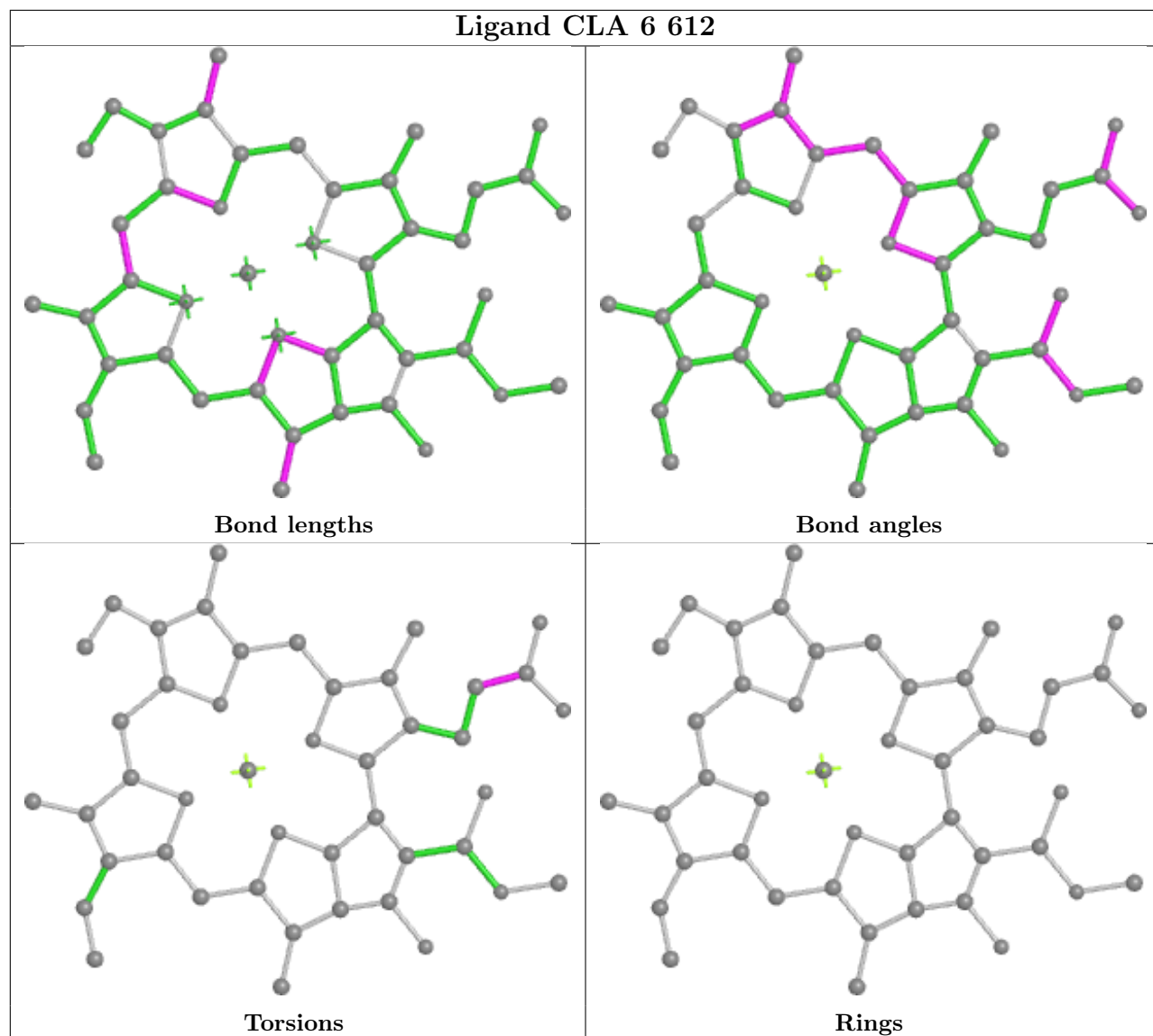
Ligand CLA 6 606



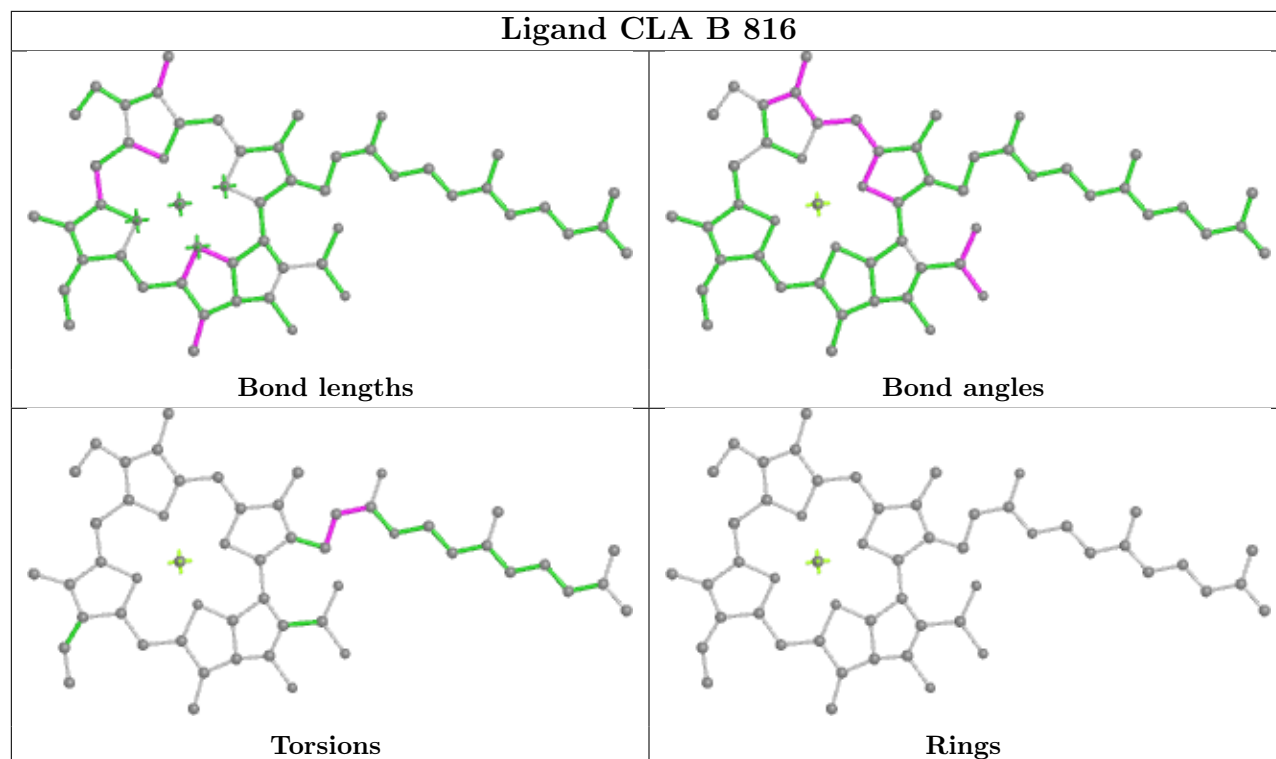
Ligand CHL 5 608



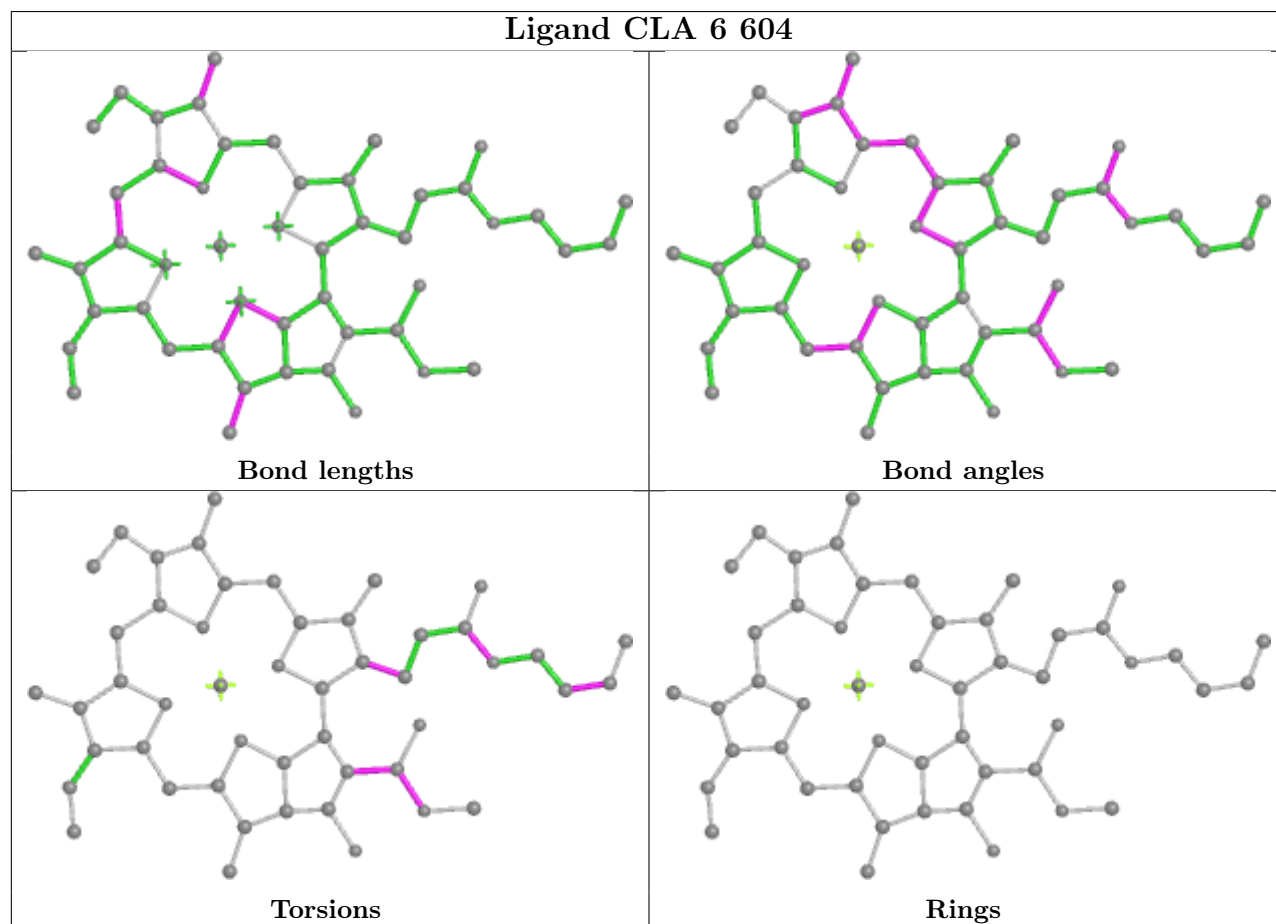
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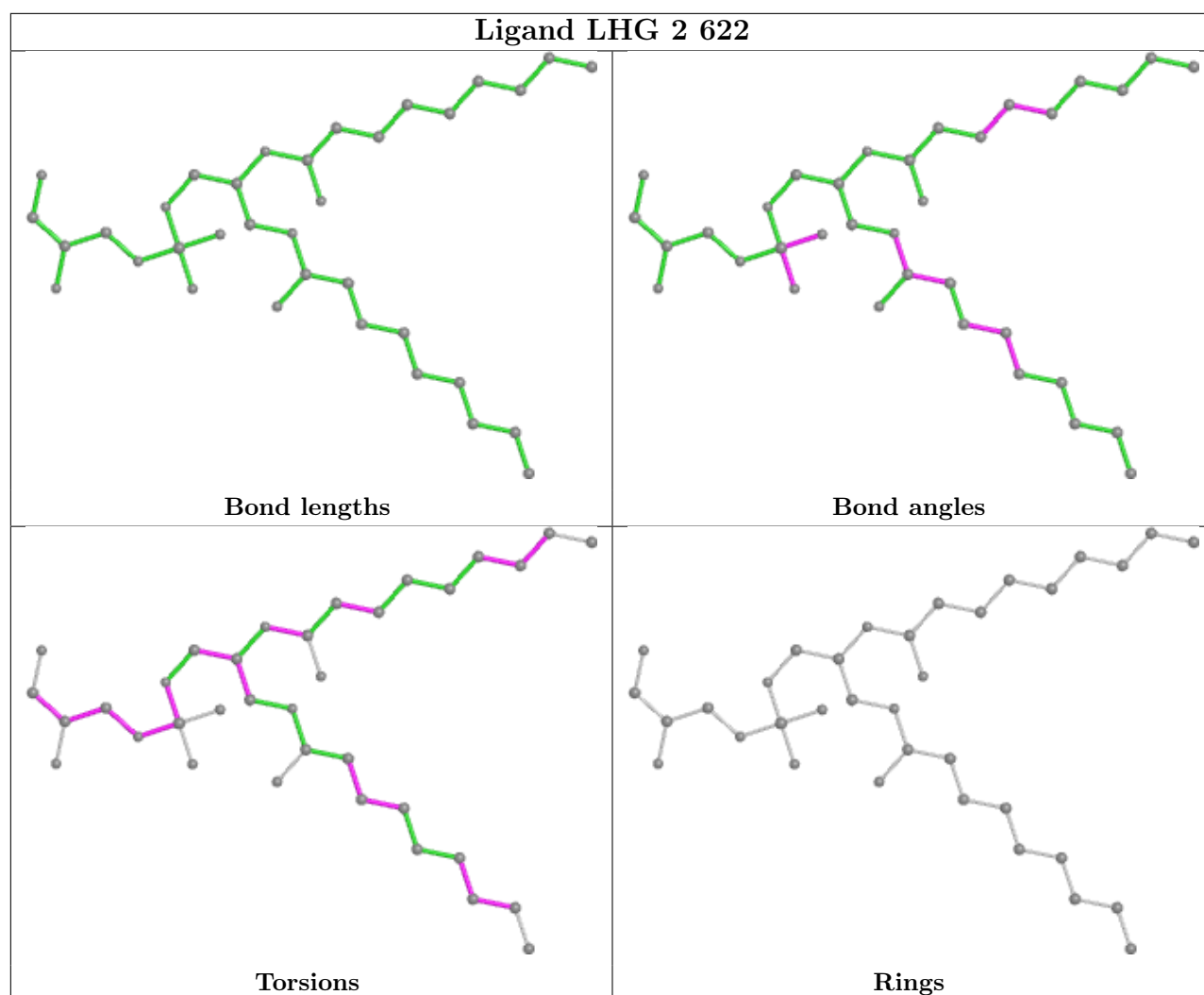


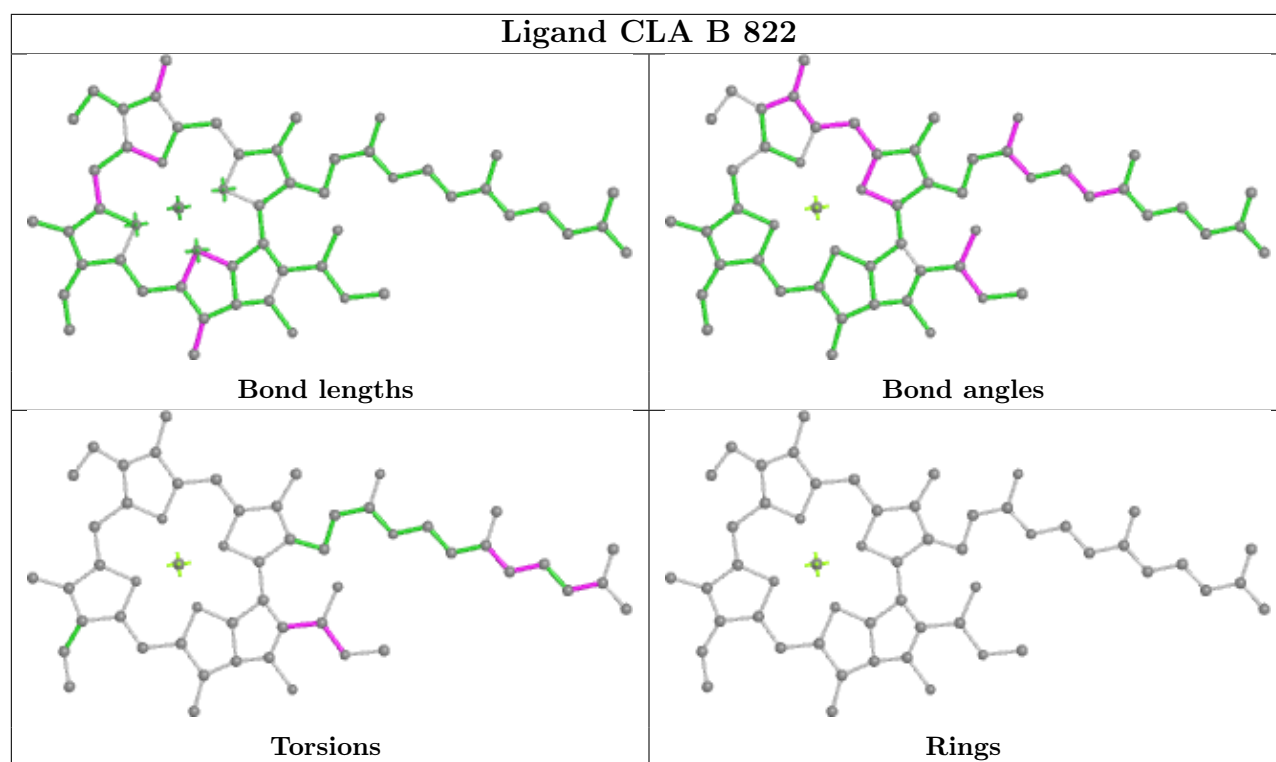
Ligand CLA B 816



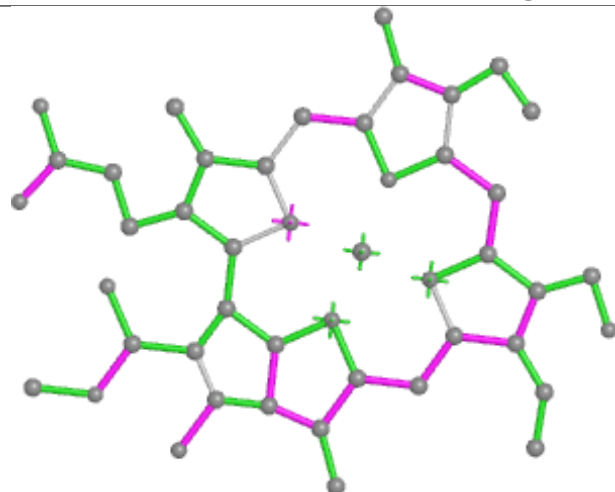
Ligand CLA 6 604



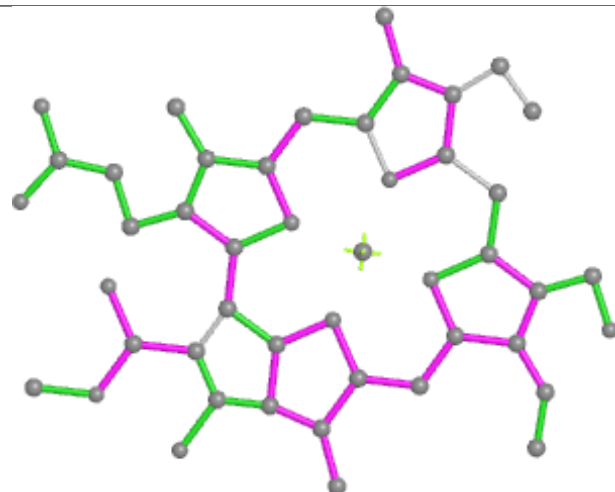




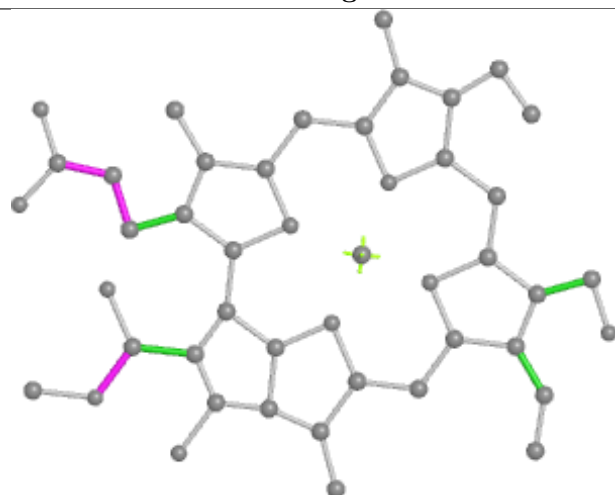
Ligand CHL 2 606



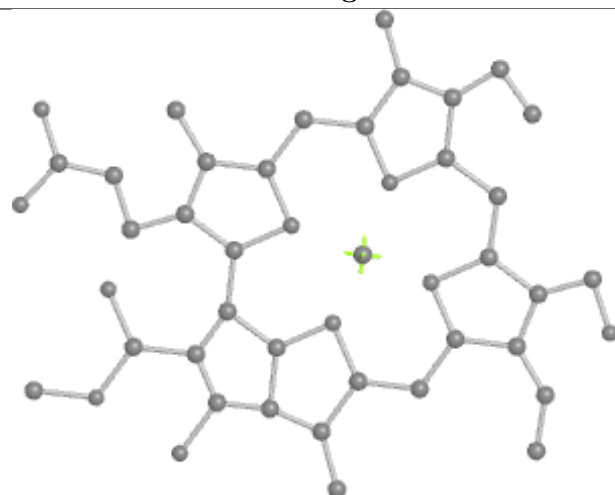
Bond lengths



Bond angles

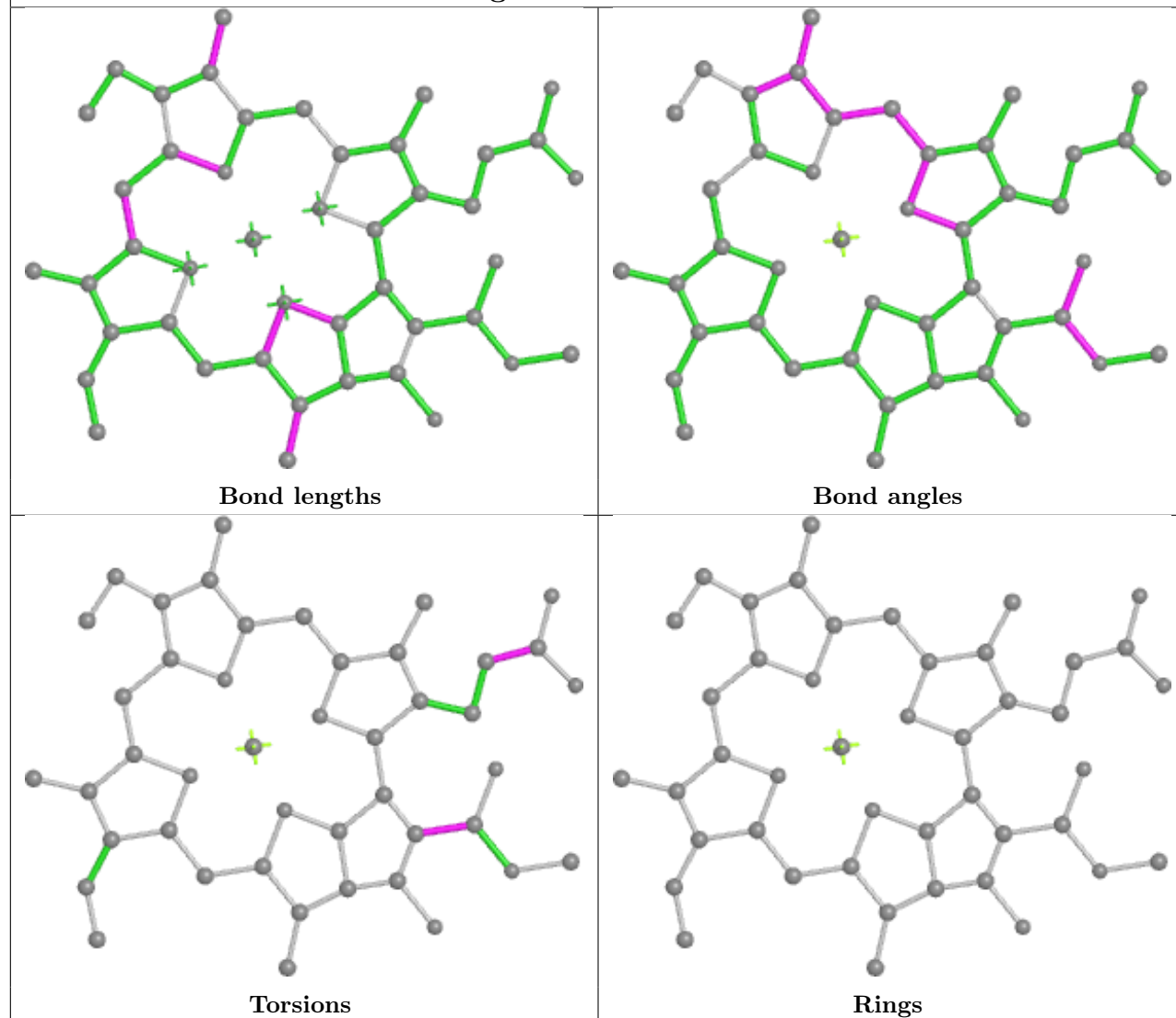


Torsions

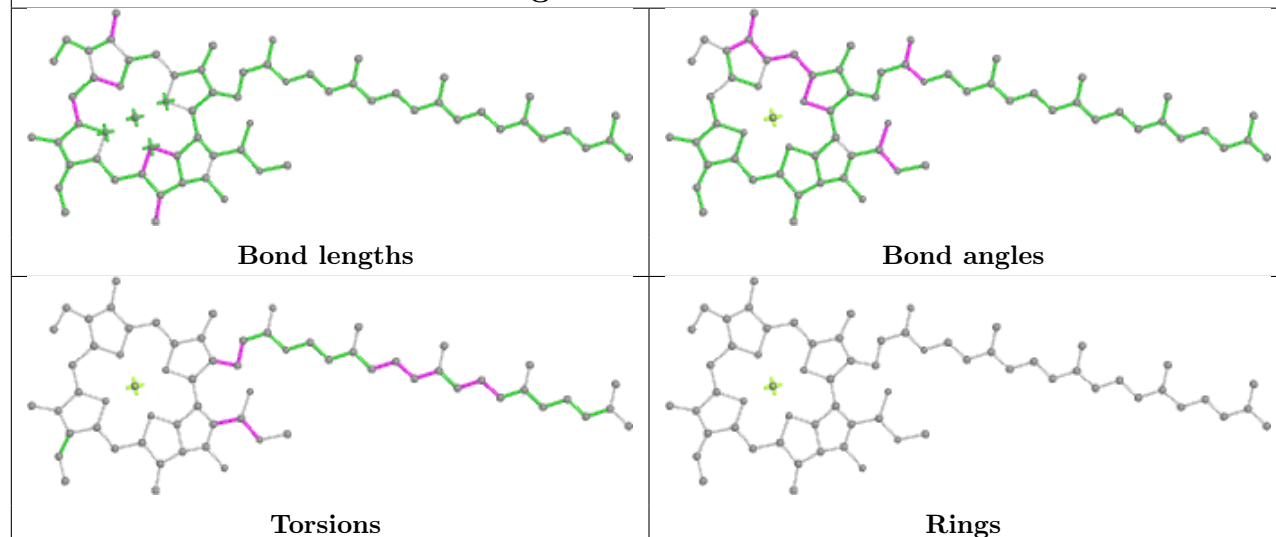


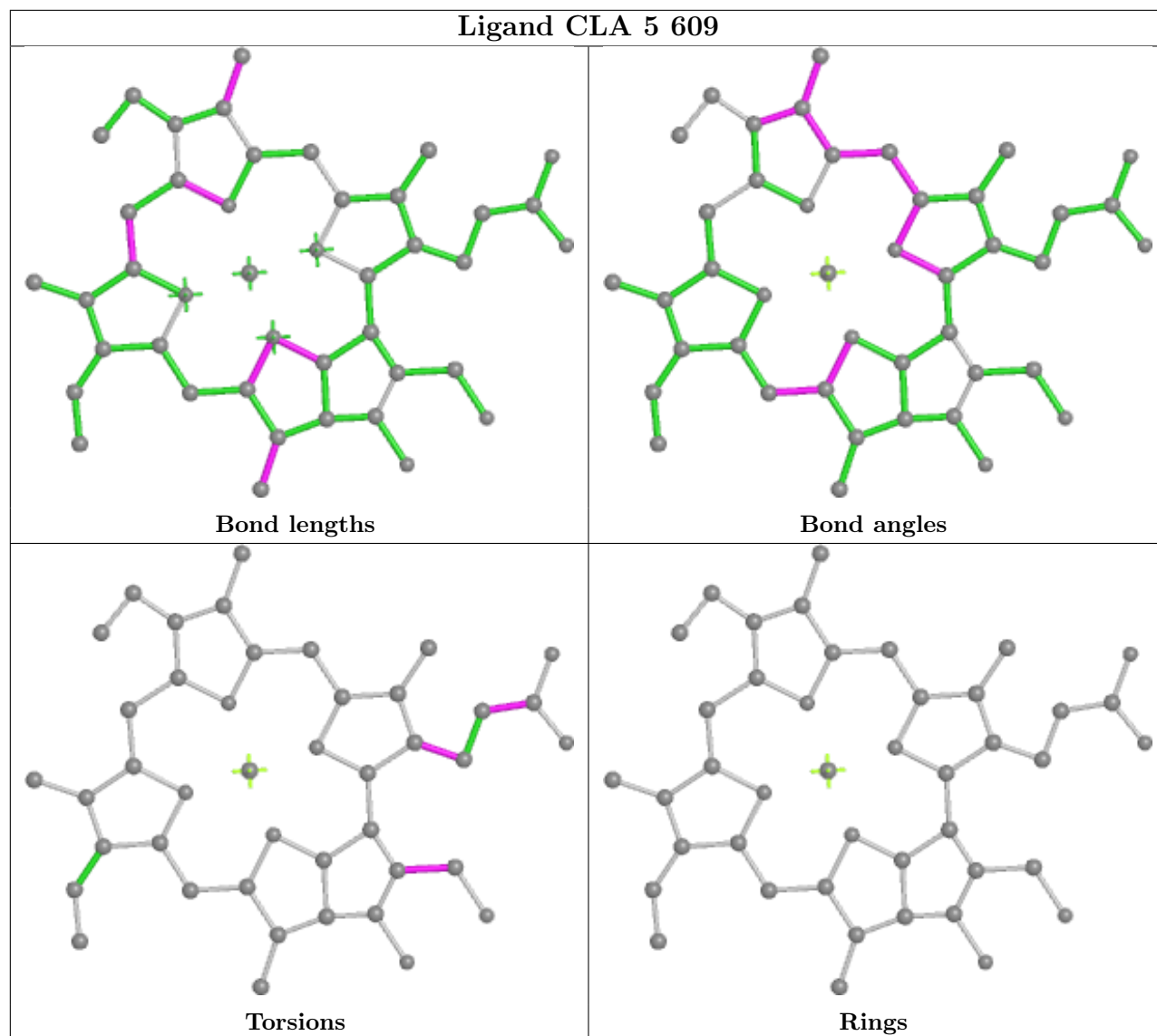
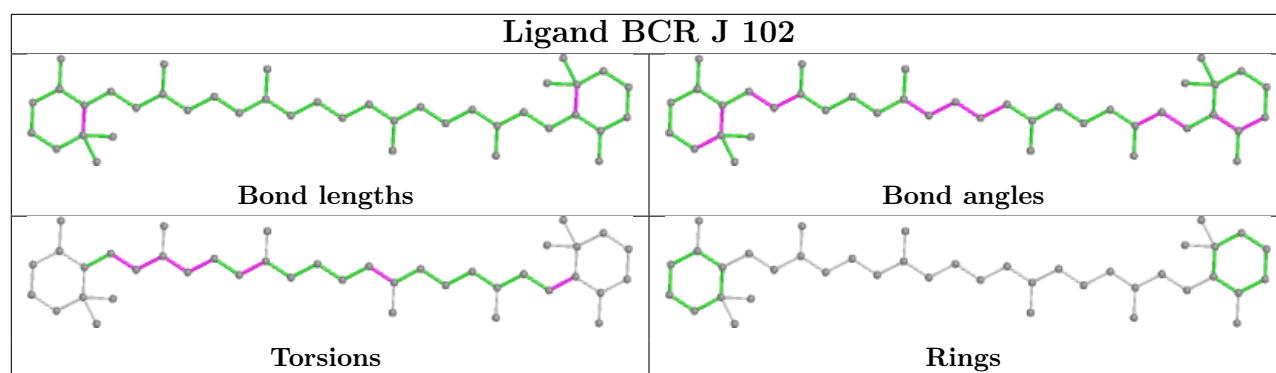
Rings

Ligand CLA A 840

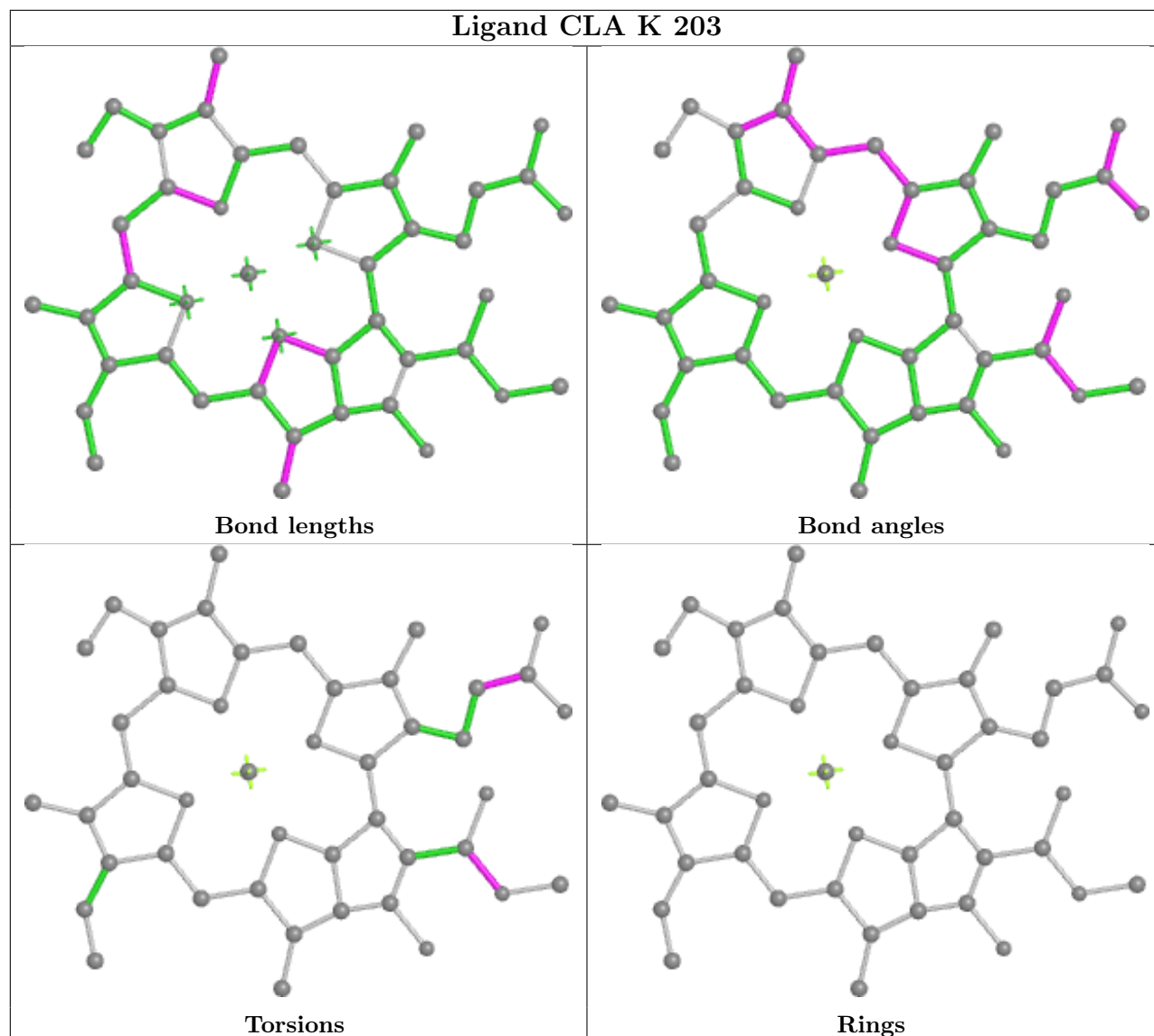


Ligand CLA A 834

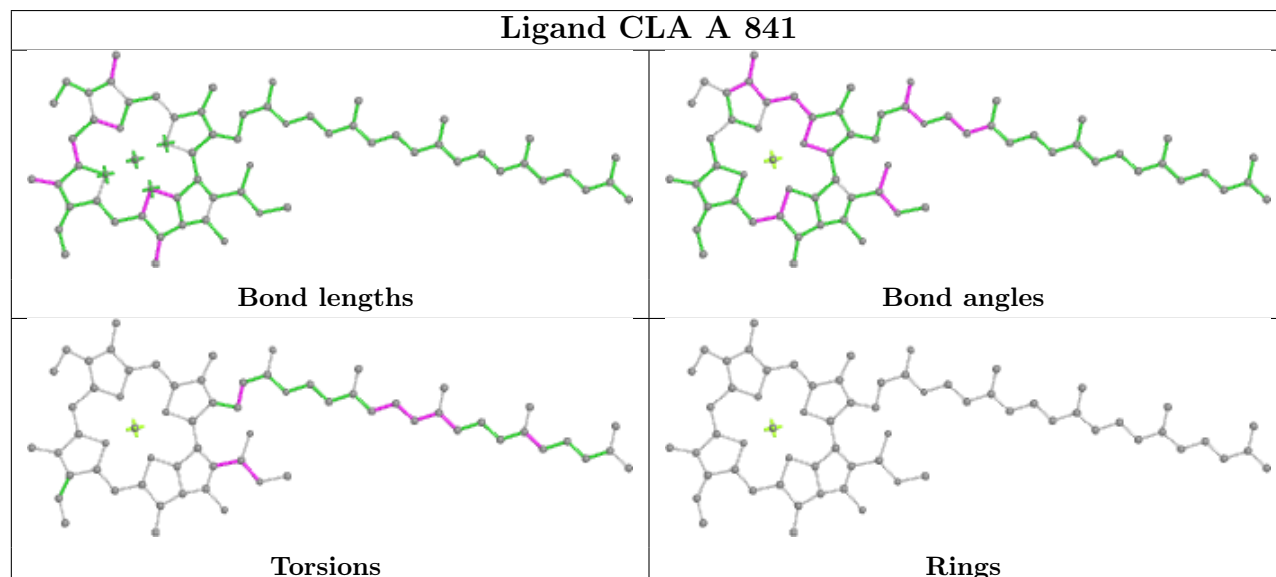




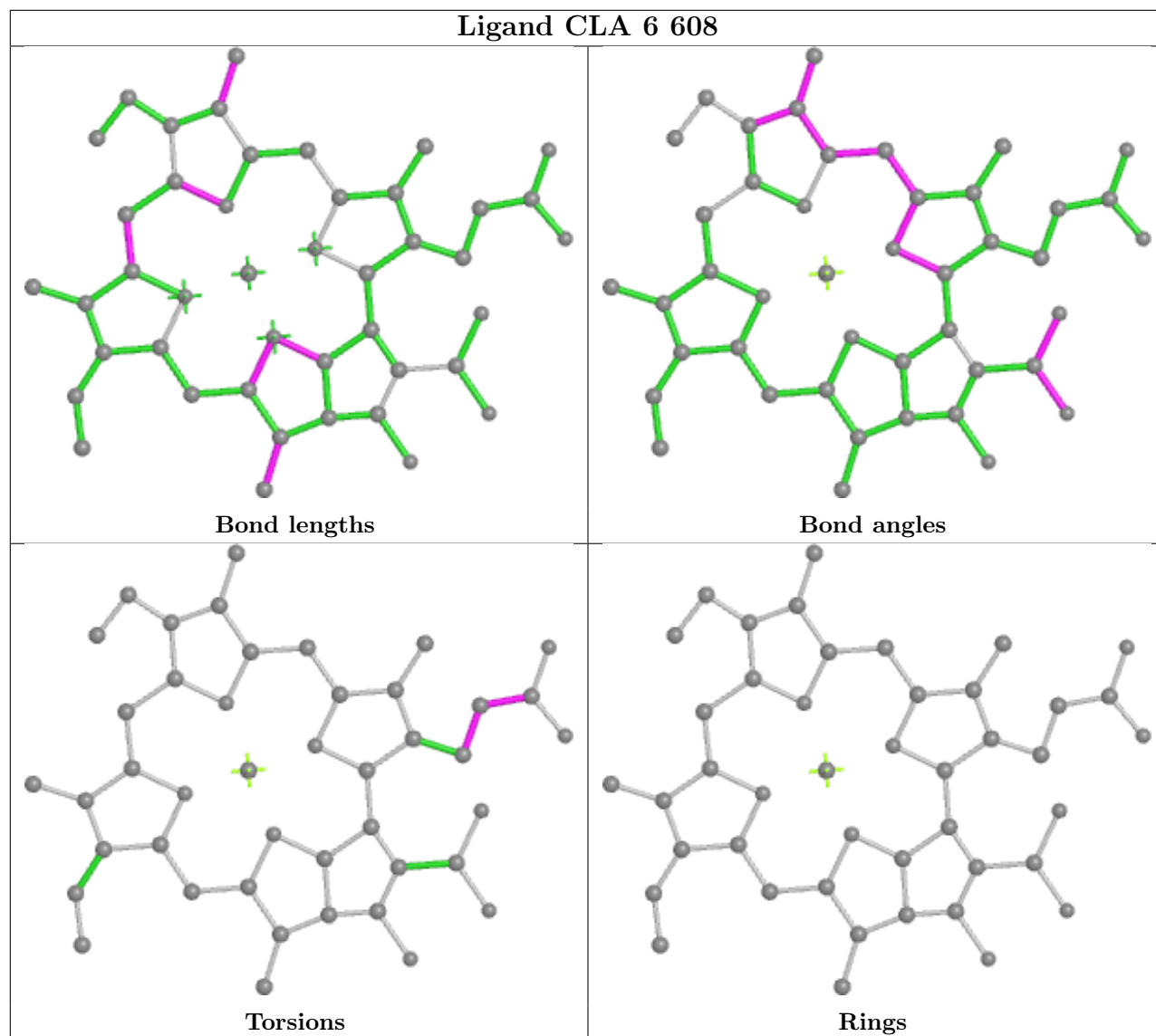
Ligand CLA K 203

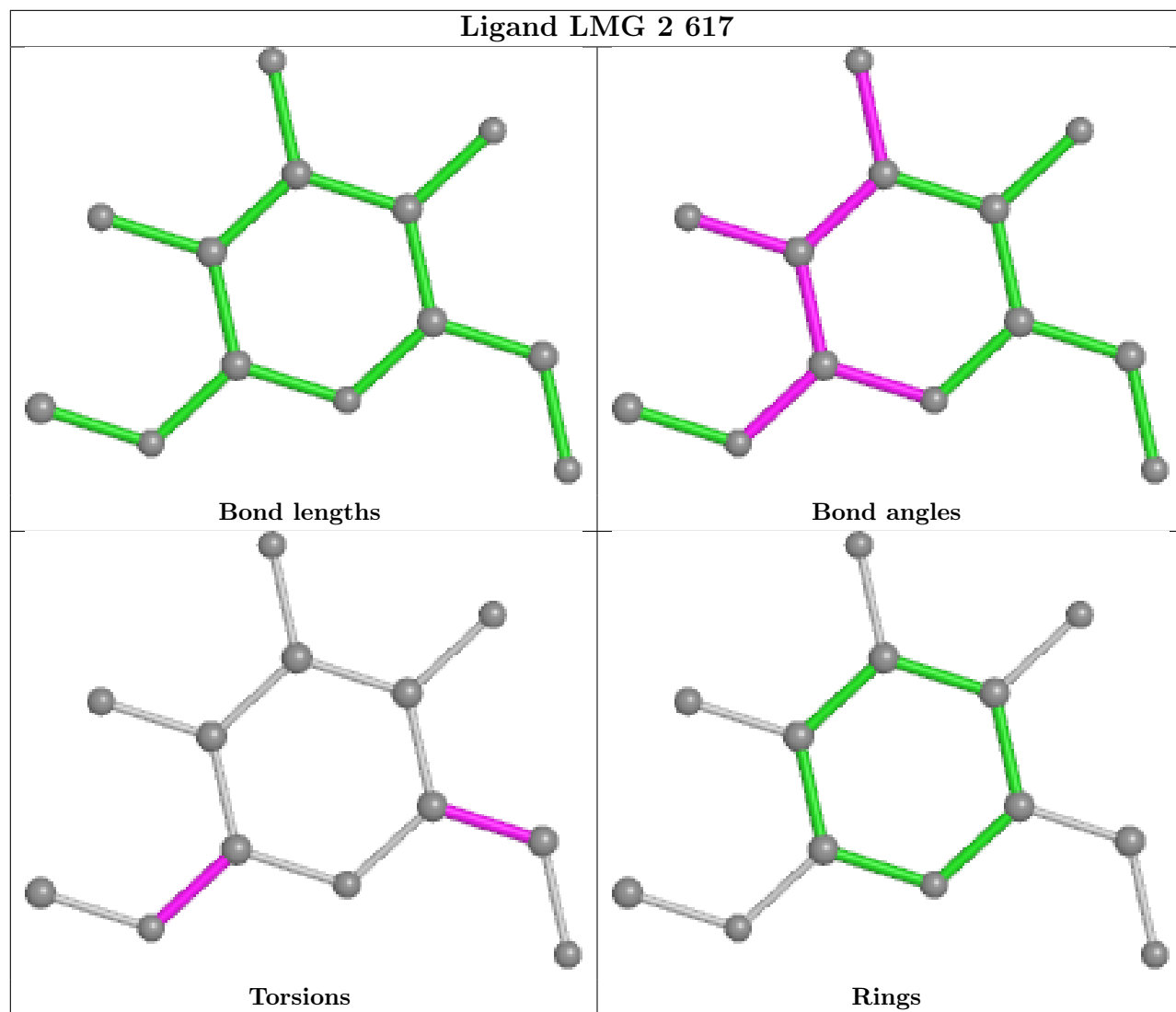


Ligand CLA A 841

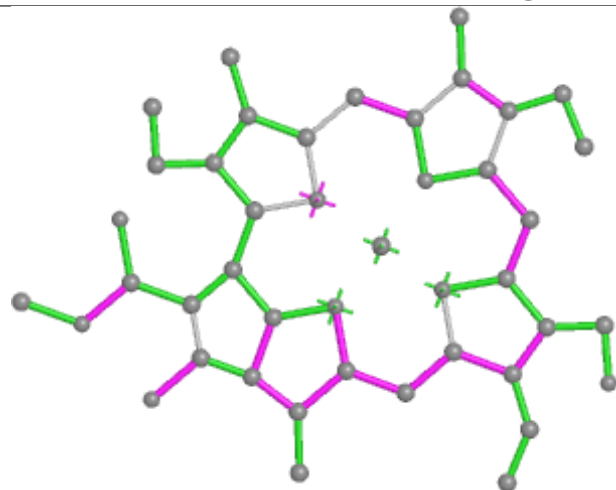


Ligand CLA 6 608

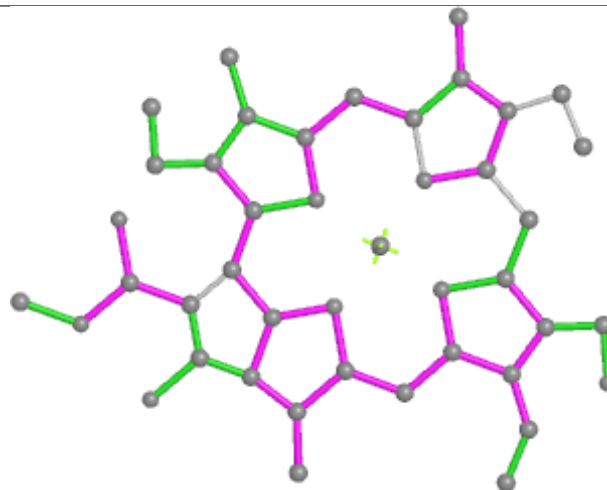




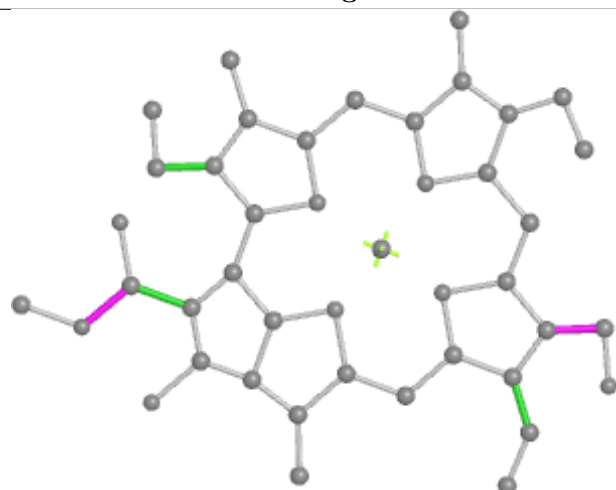
Ligand CHL 5 615



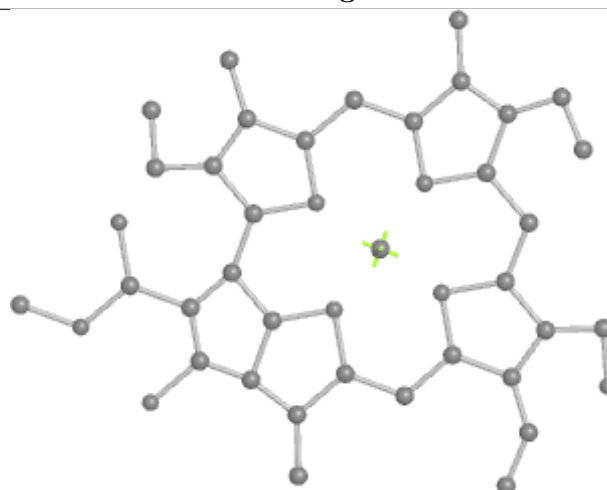
Bond lengths



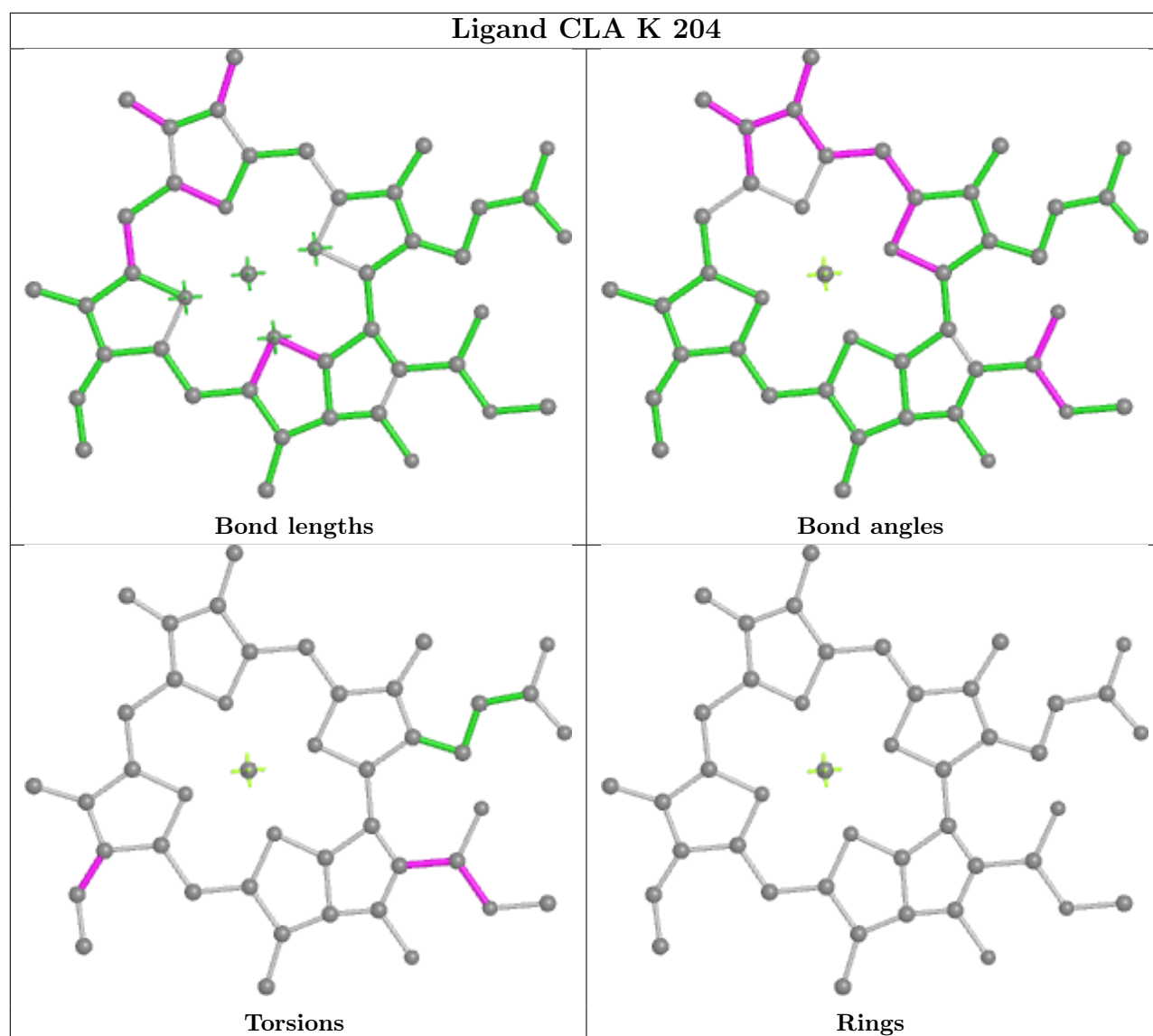
Bond angles

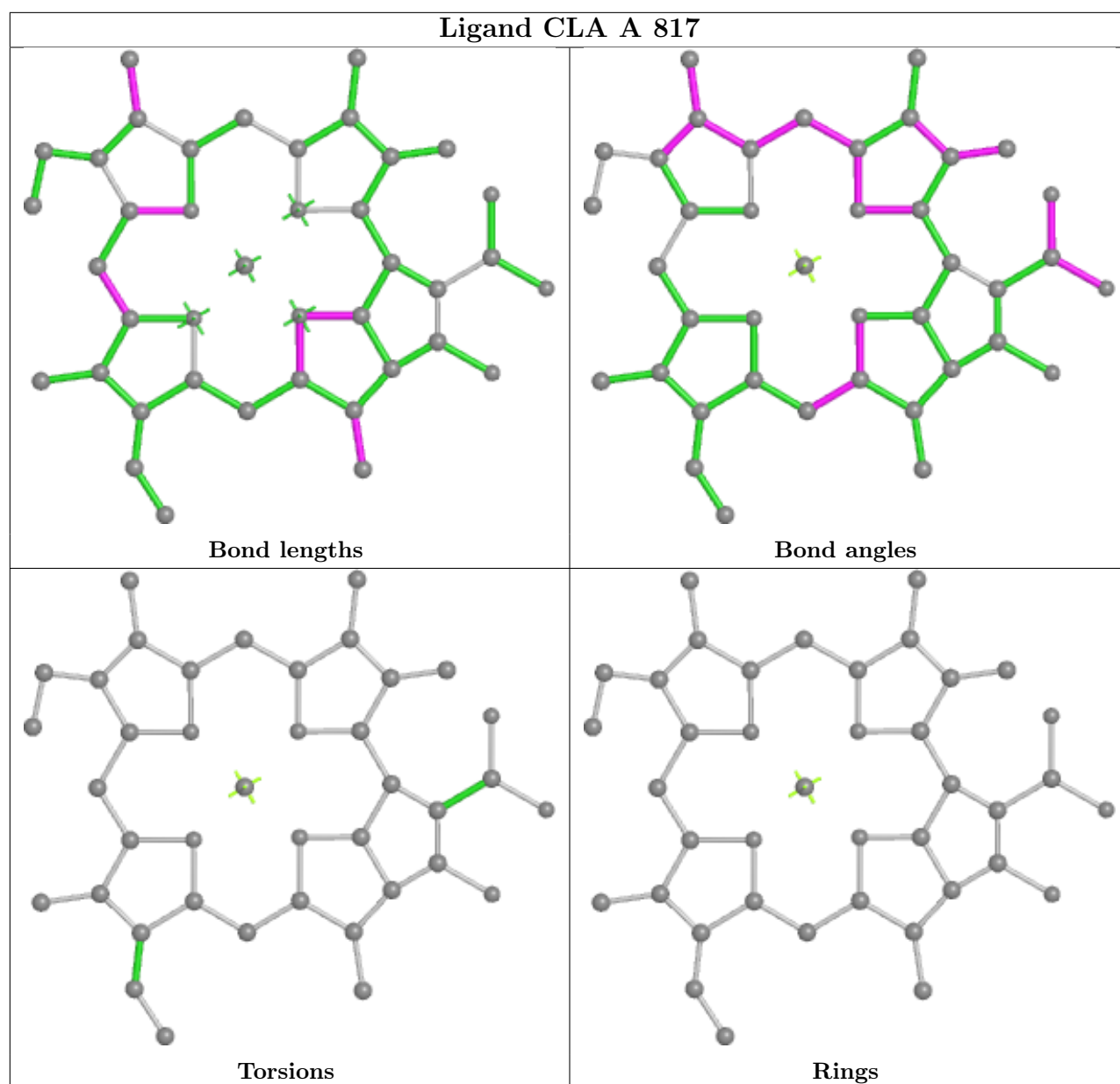


Torsions

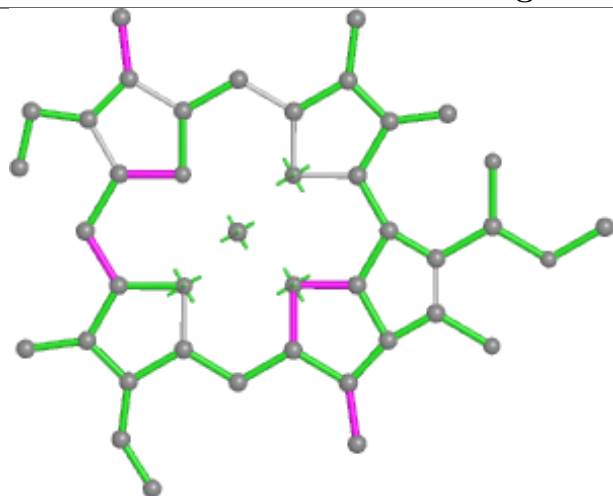


Rings

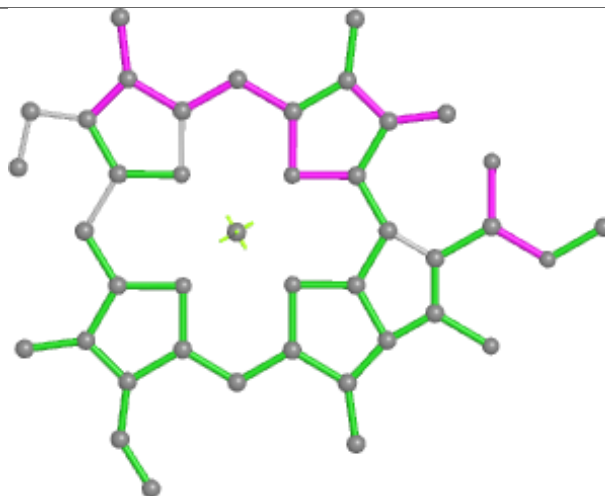




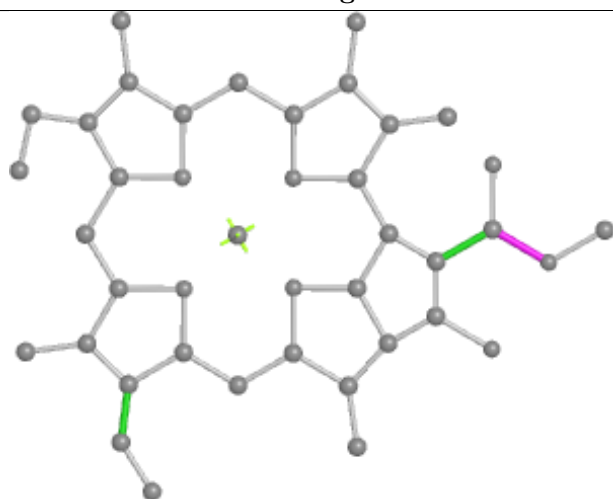
Ligand CLA F 304



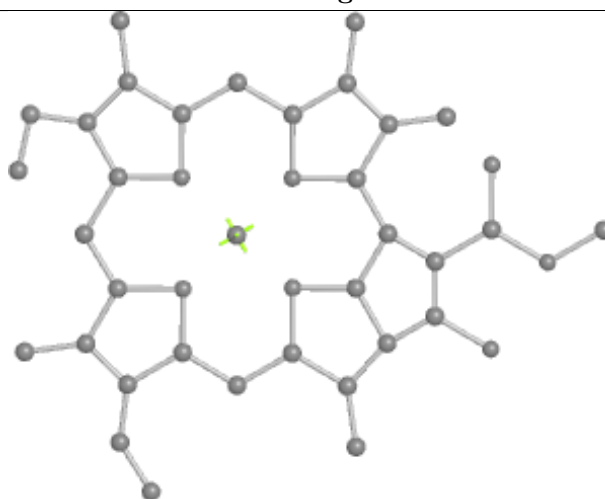
Bond lengths



Bond angles

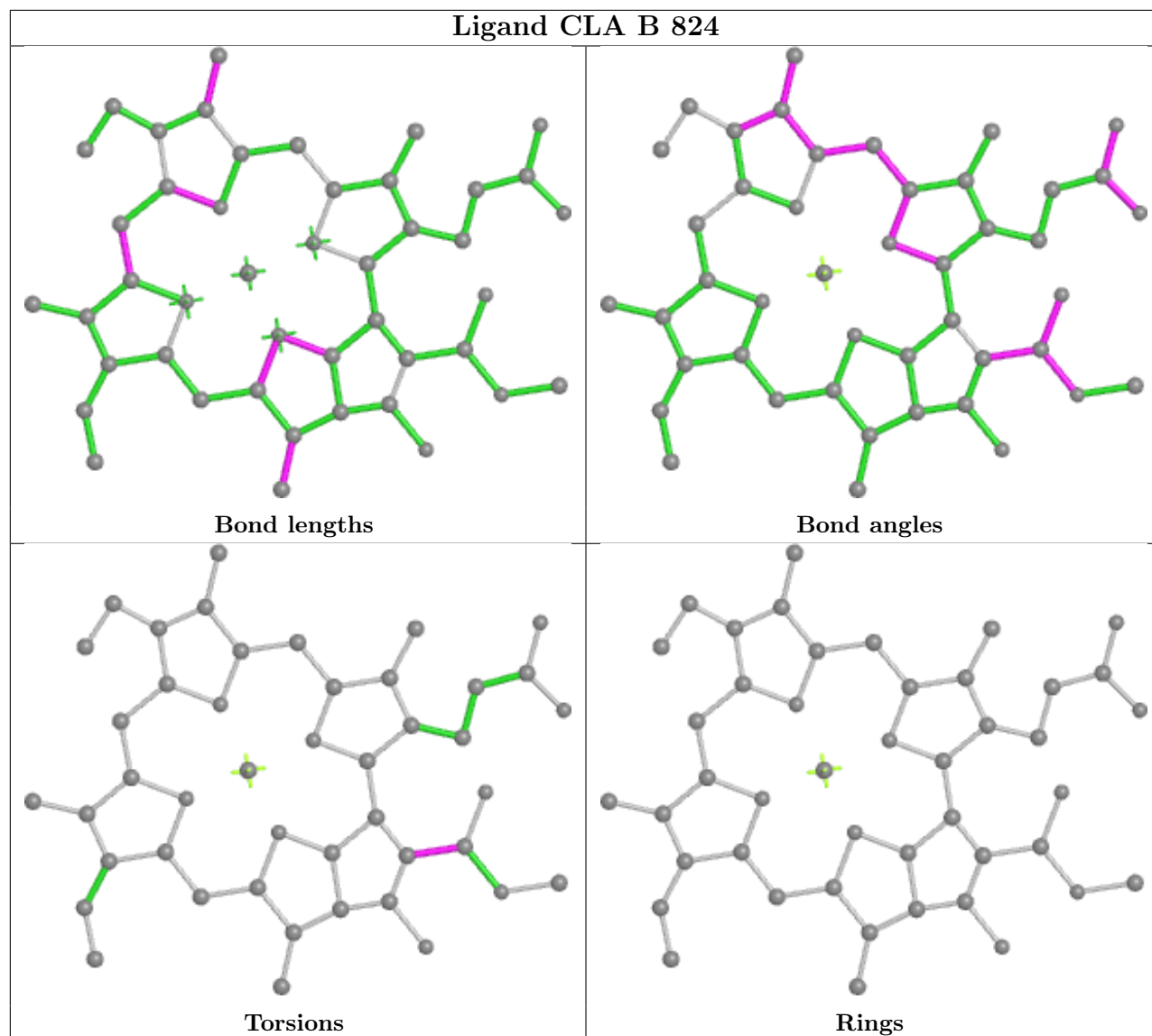


Torsions

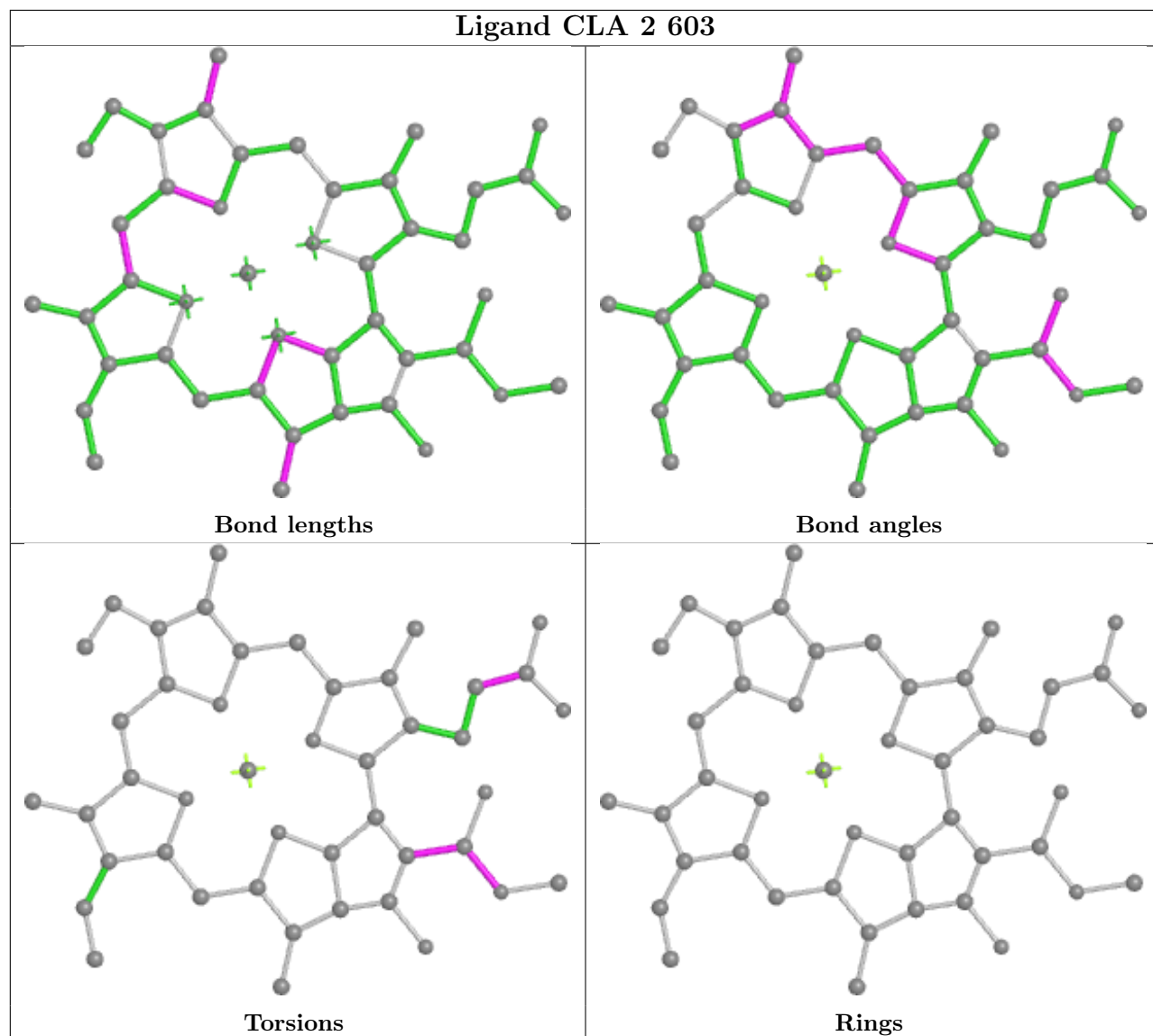


Rings

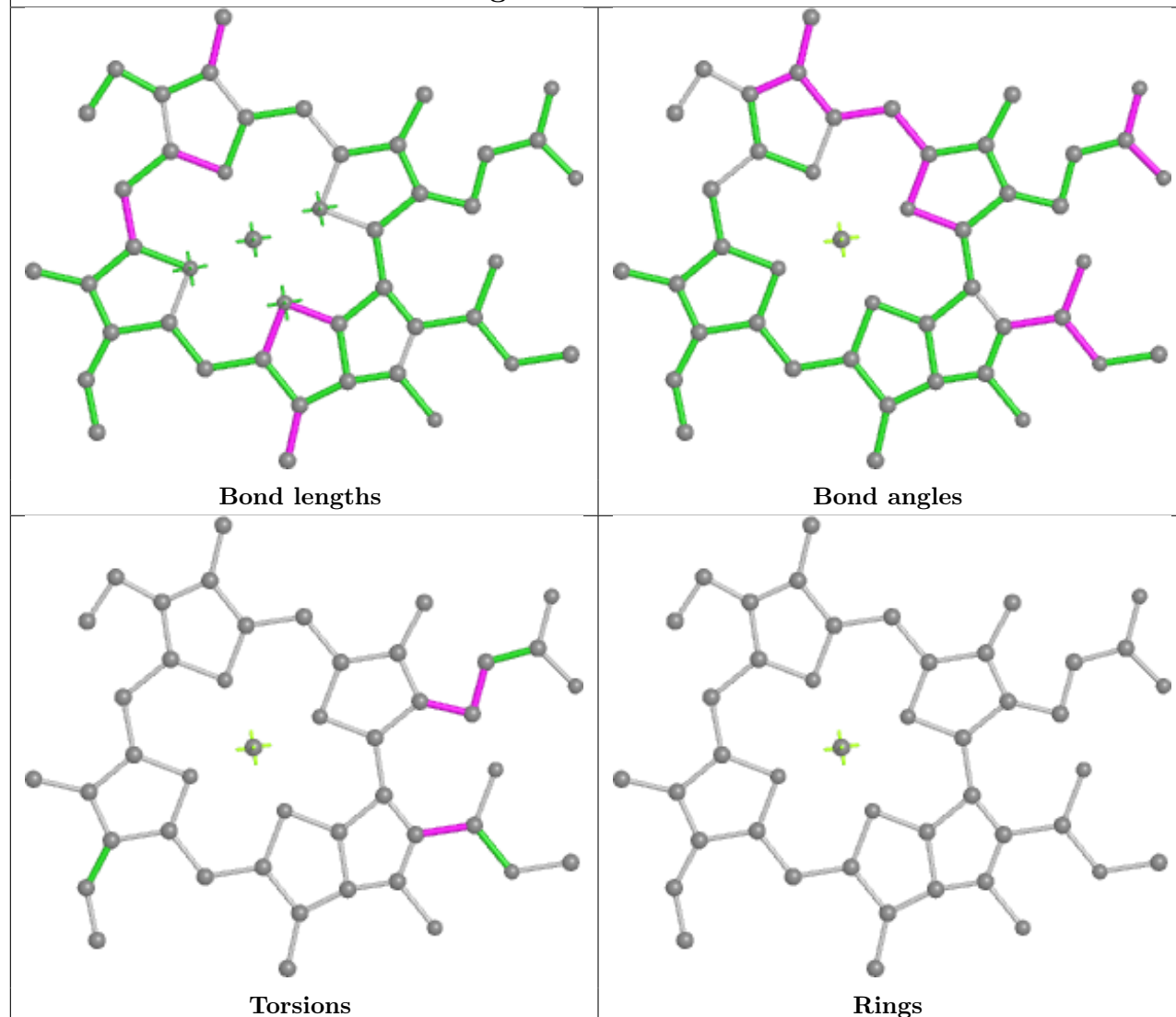
Ligand CLA B 824



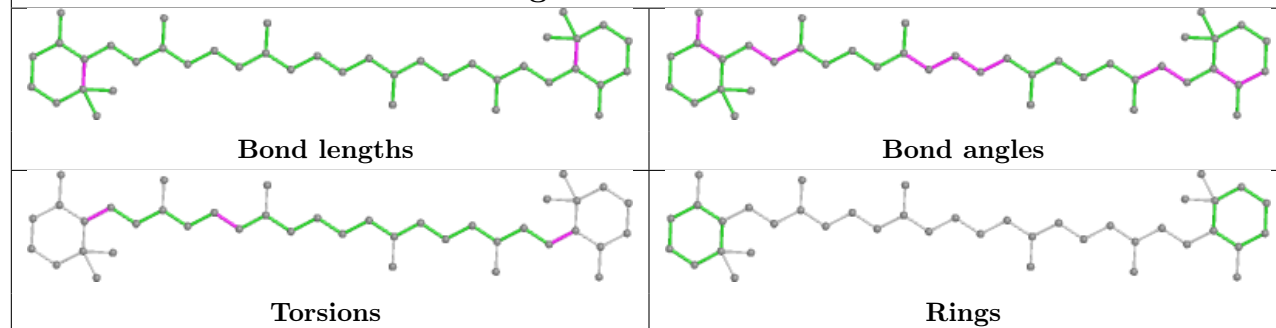
Ligand CLA 2 603

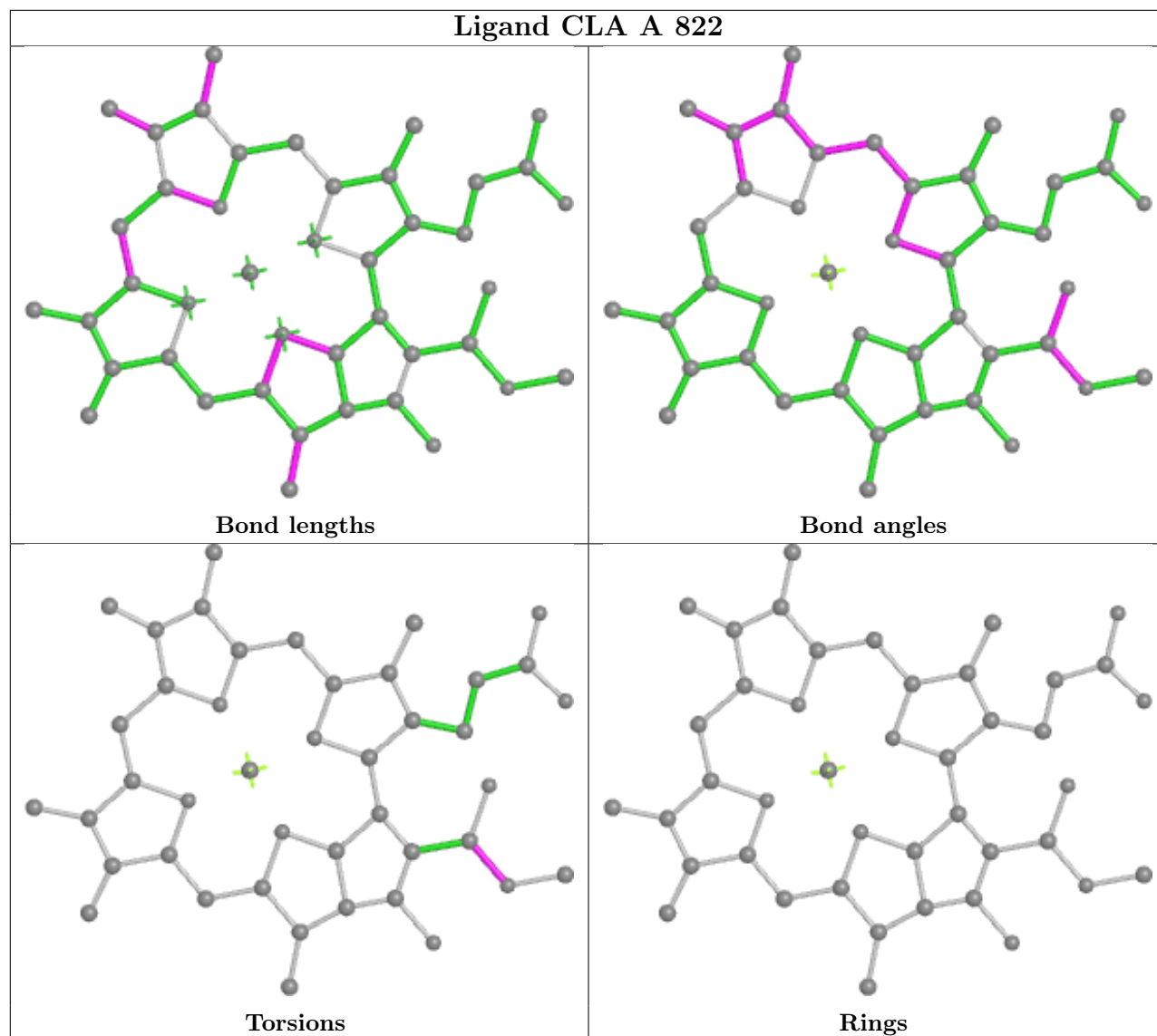
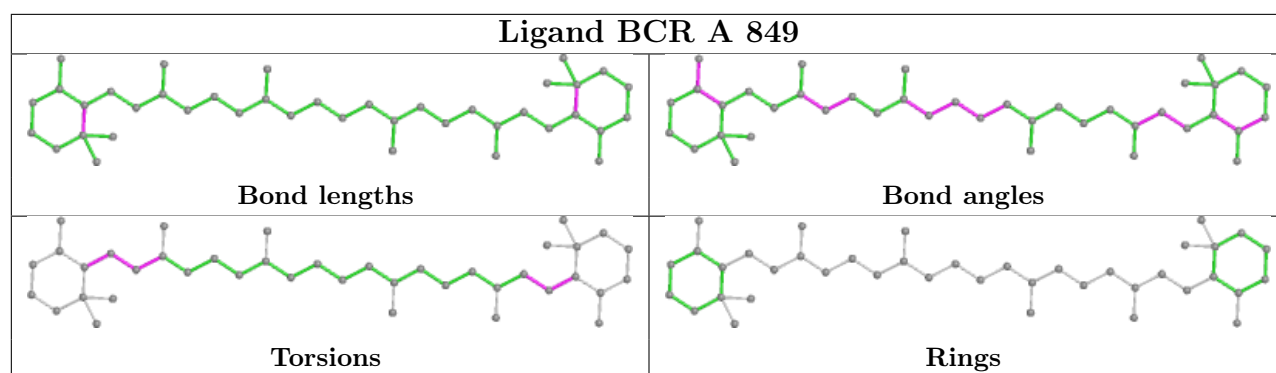


Ligand CLA A 809

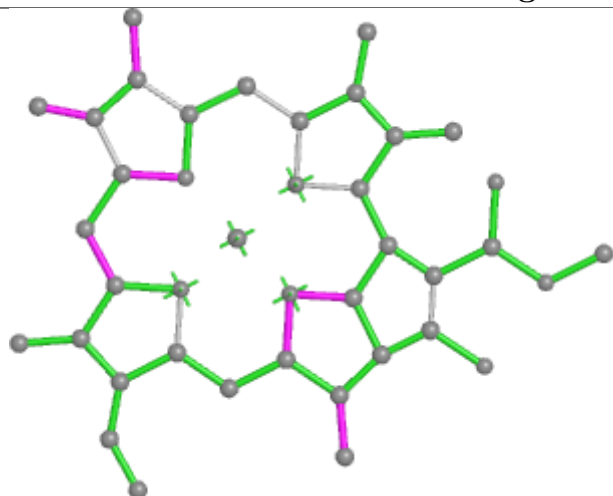


Ligand BCR G 205

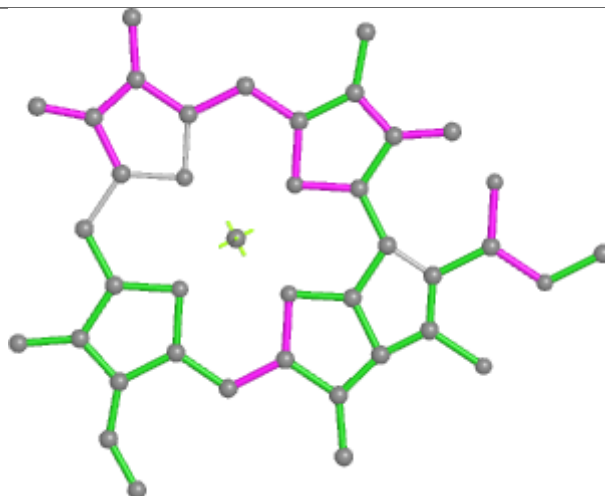




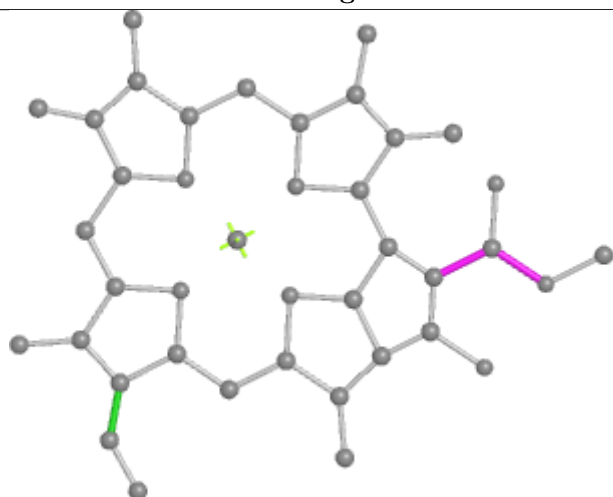
Ligand CLA 6 609



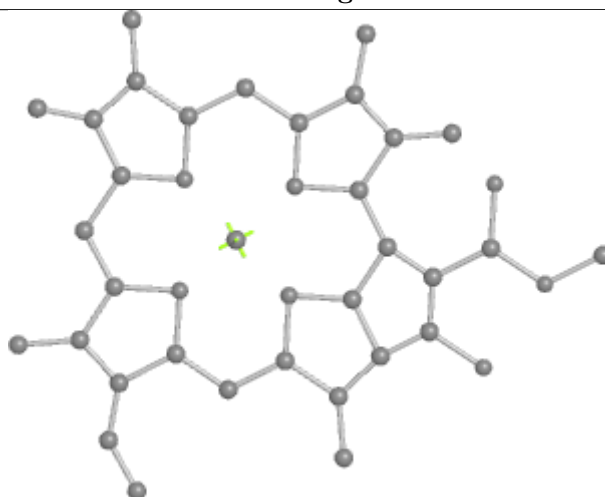
Bond lengths



Bond angles

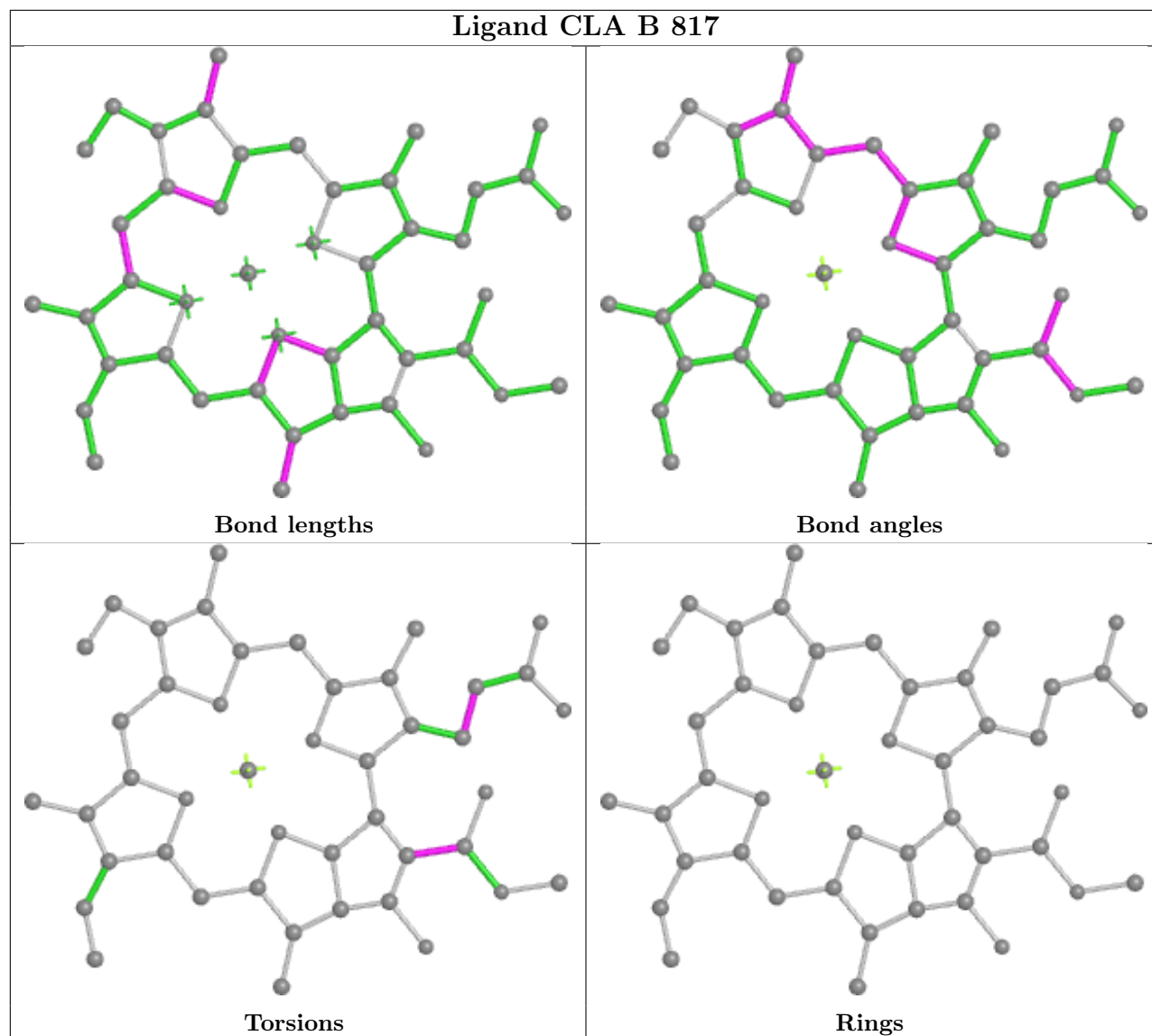


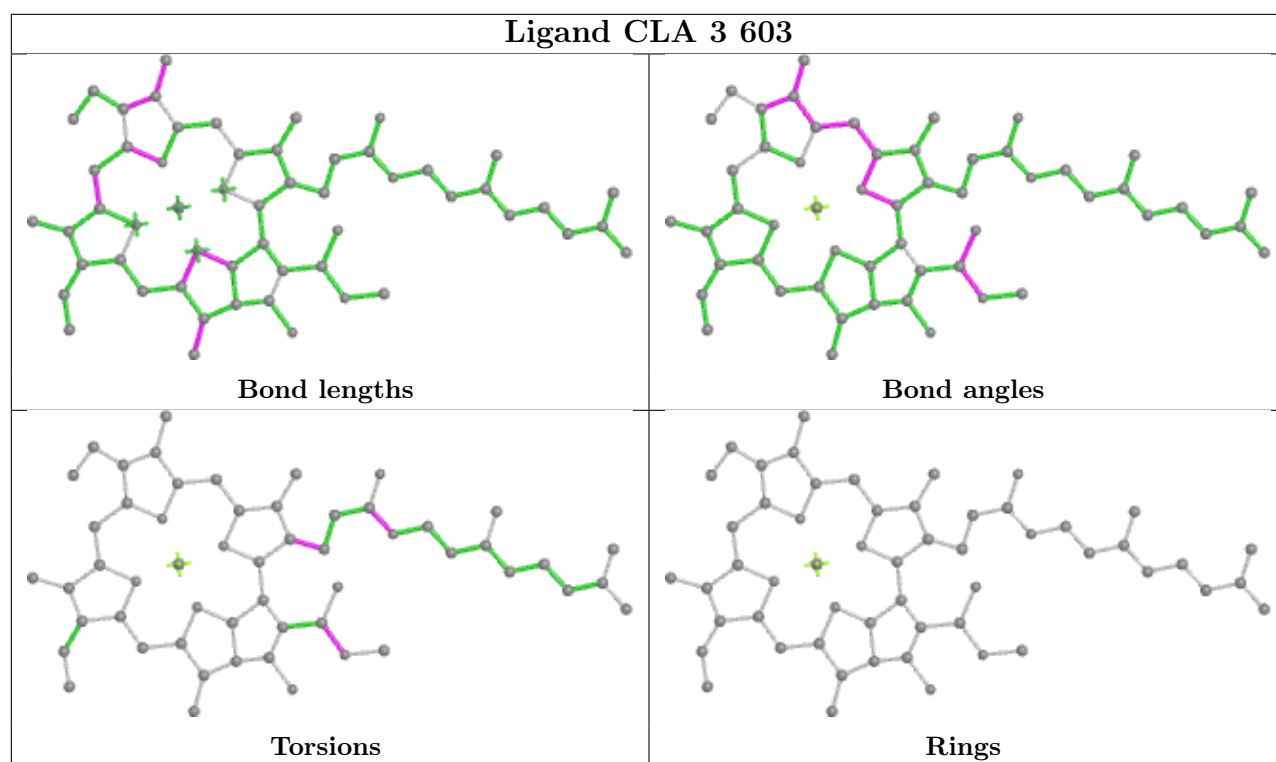
Torsions



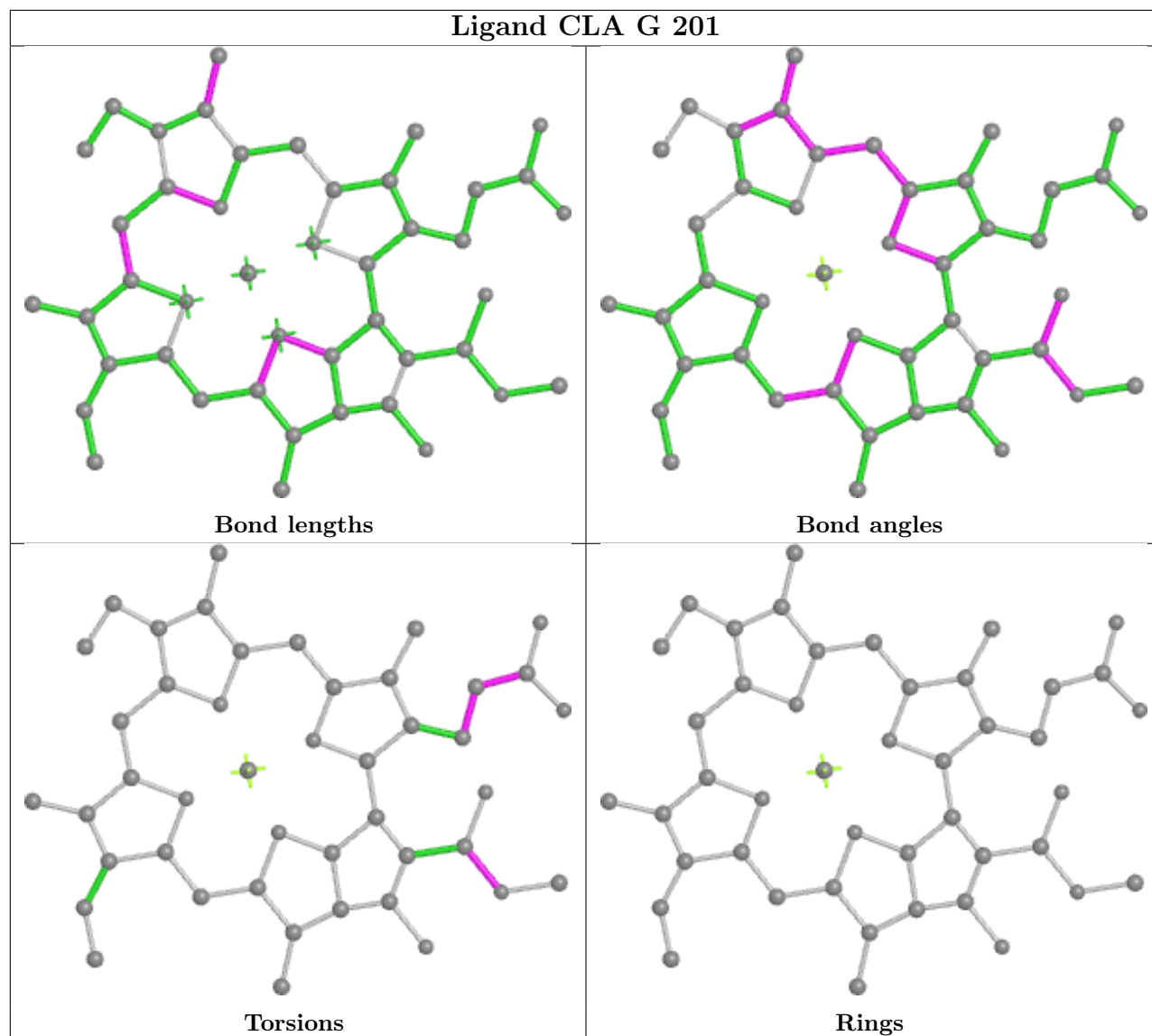
Rings

Ligand CLA B 817

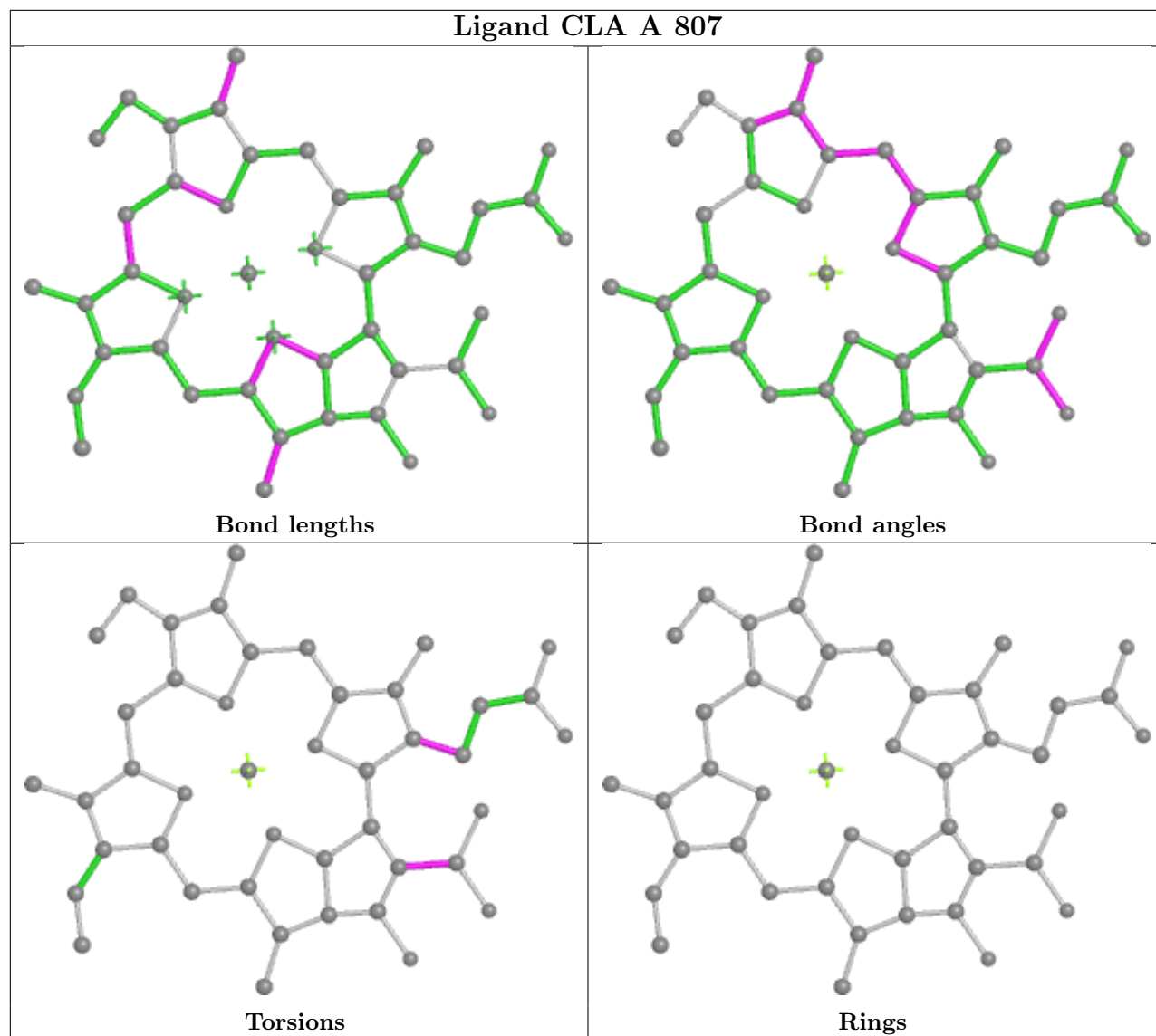




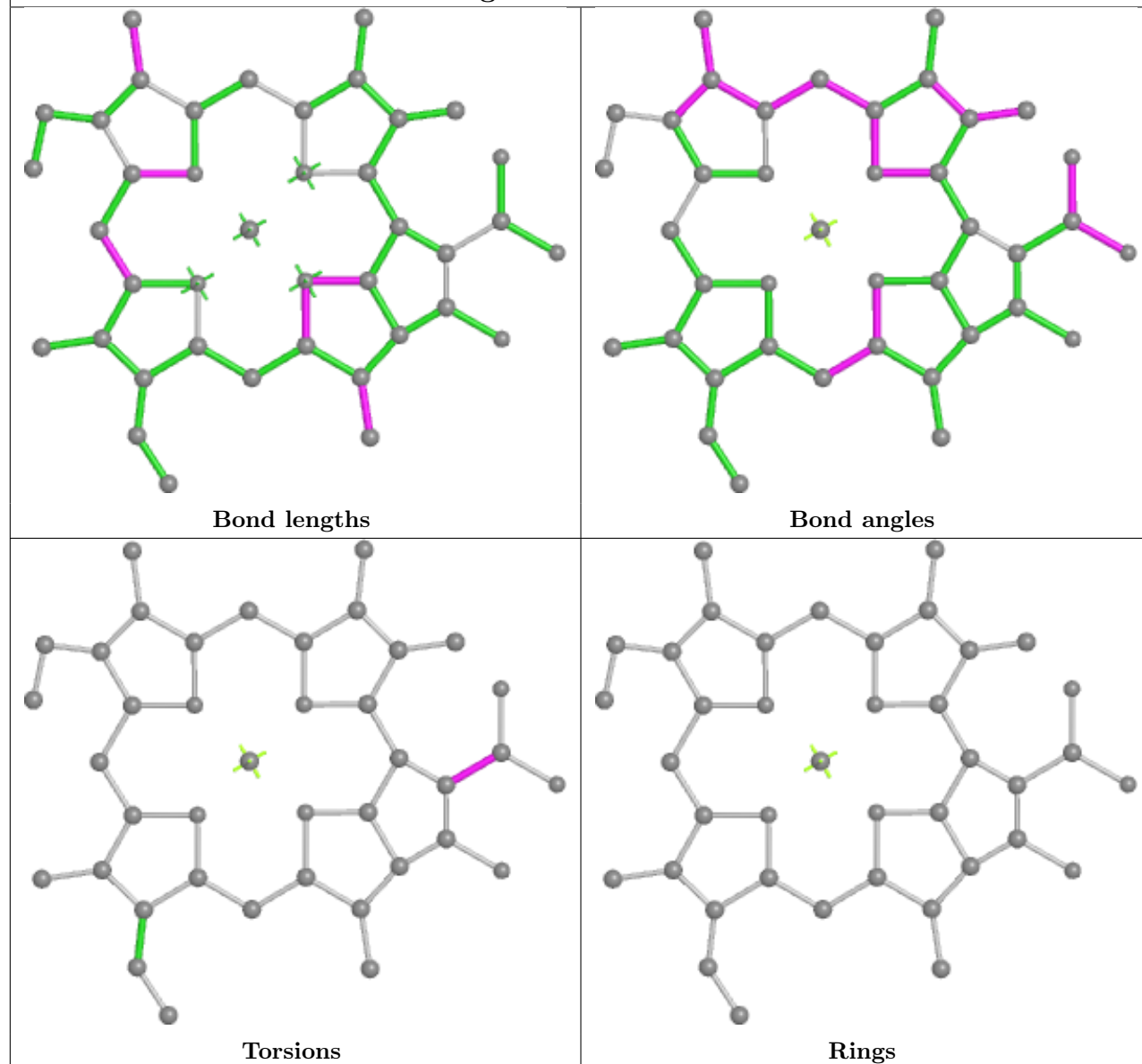
Ligand CLA G 201



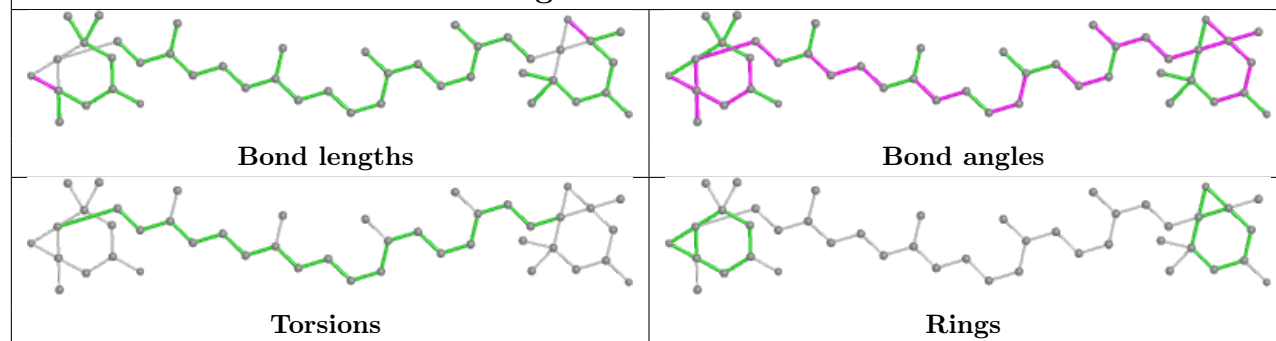
Ligand CLA A 807



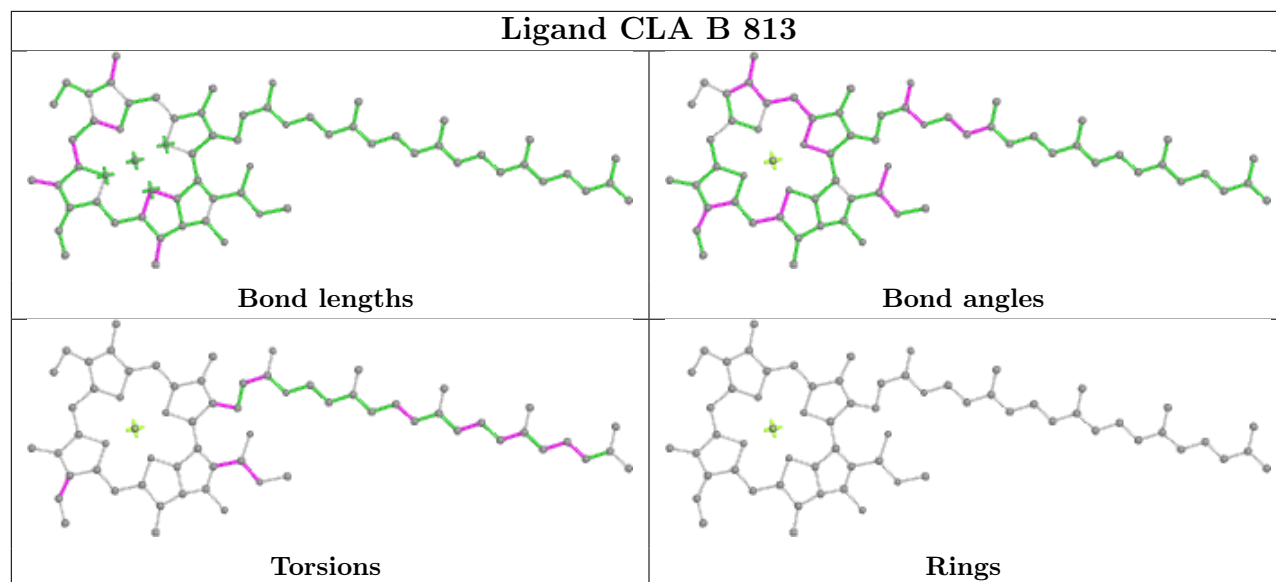
Ligand CLA 3 617



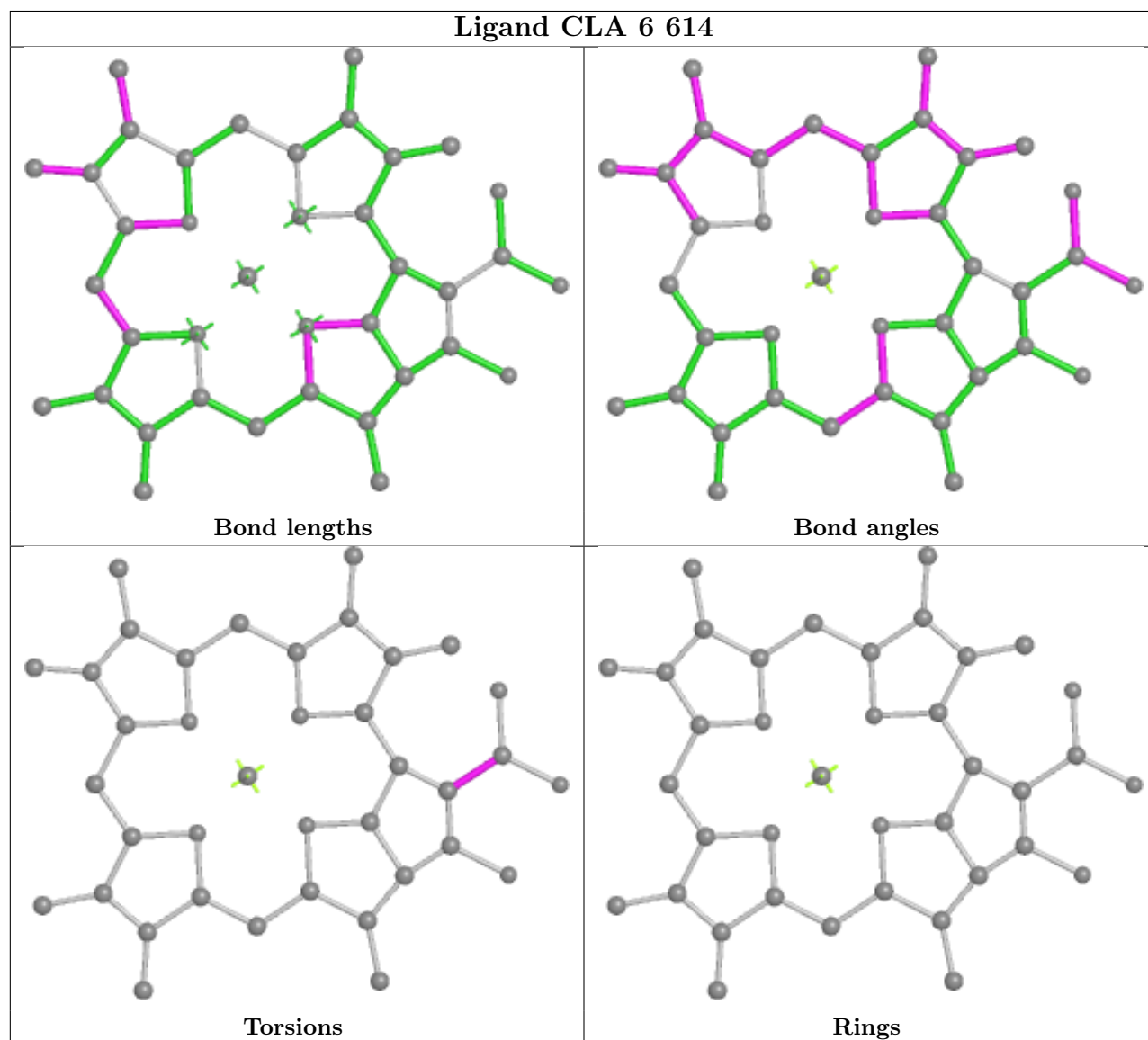
Ligand XAT 3 619



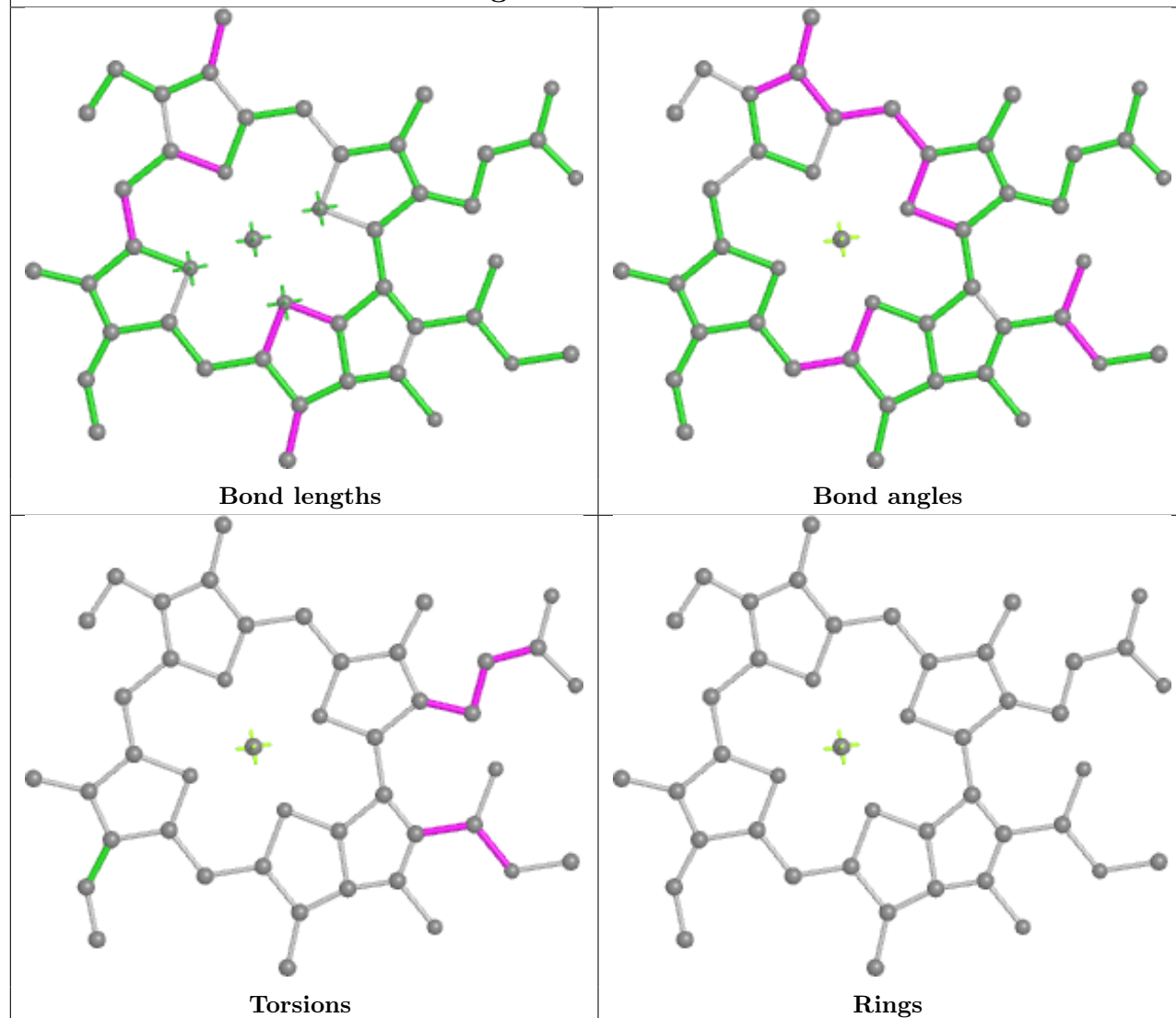
Ligand CLA B 813



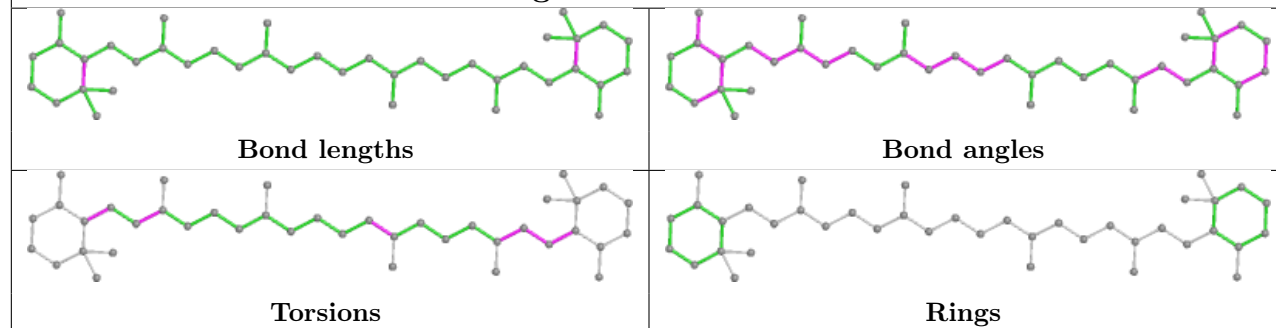
Ligand CLA 6 614

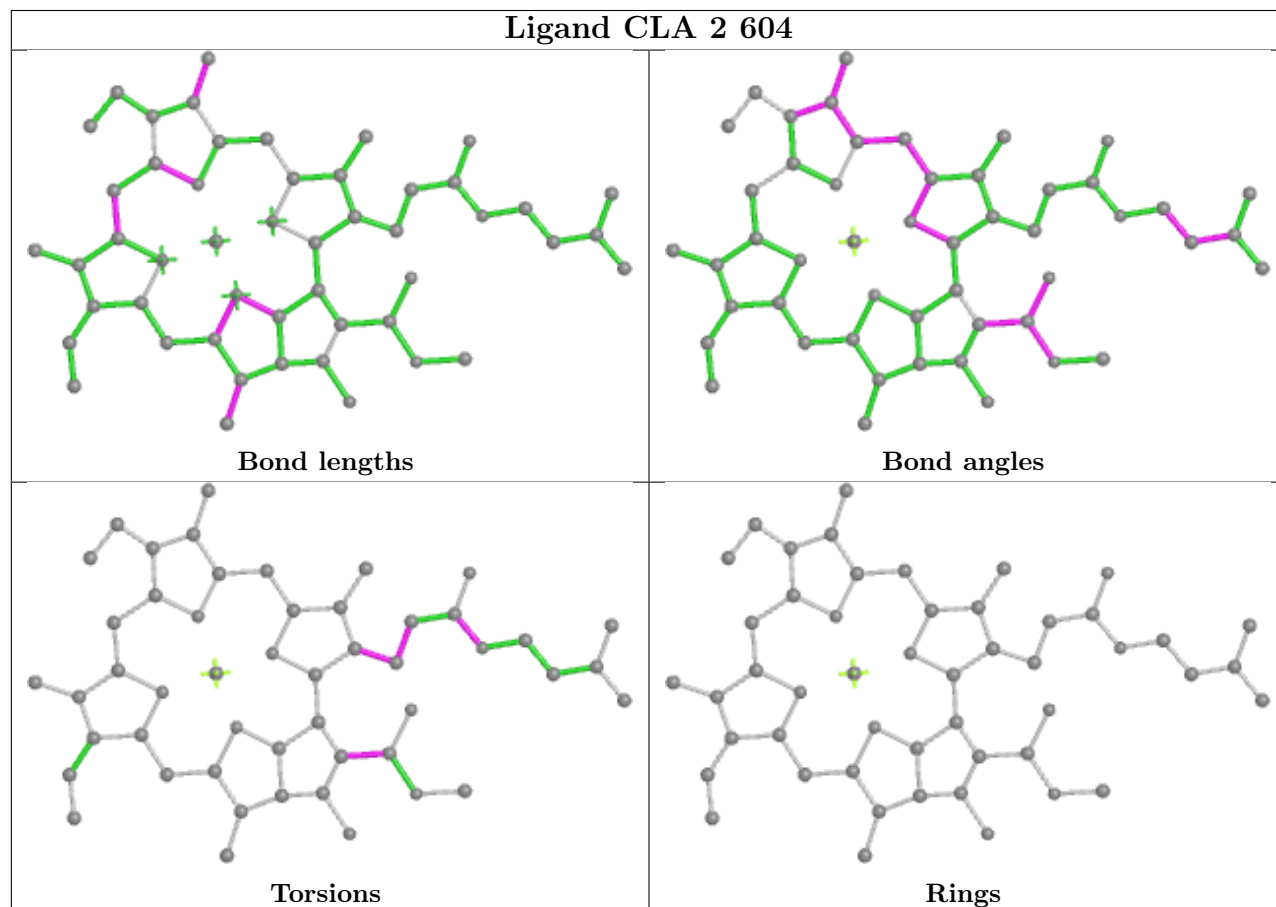
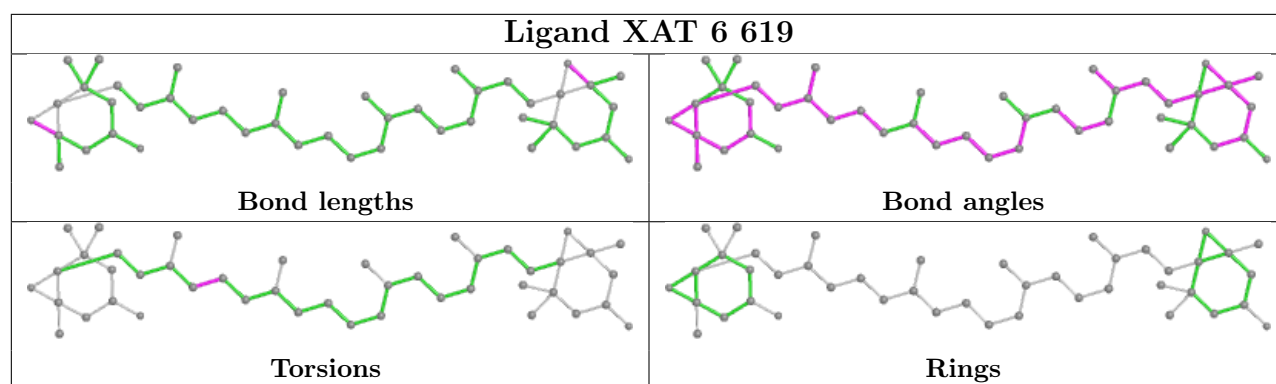


Ligand CLA B 835

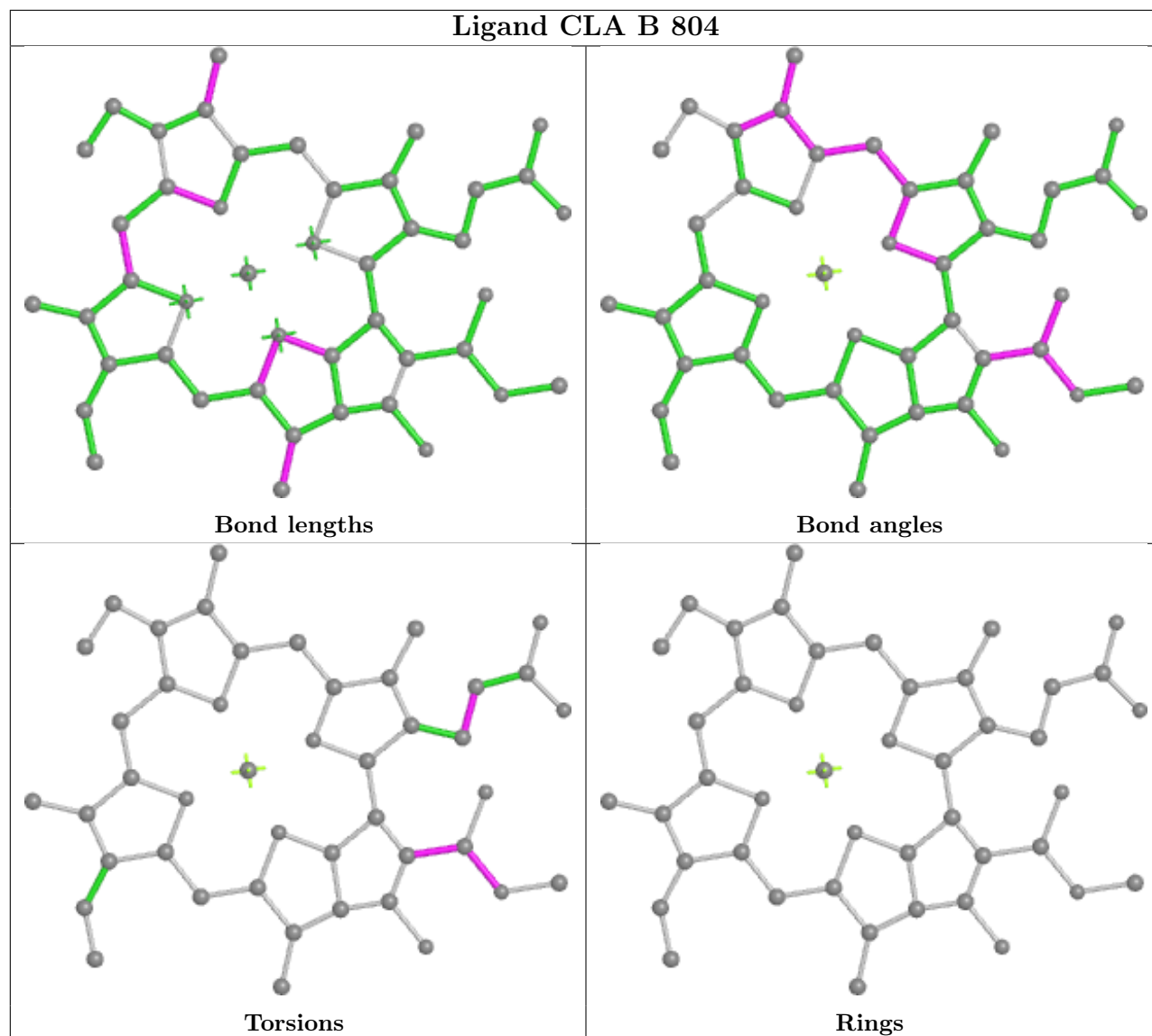


Ligand BCR L 305

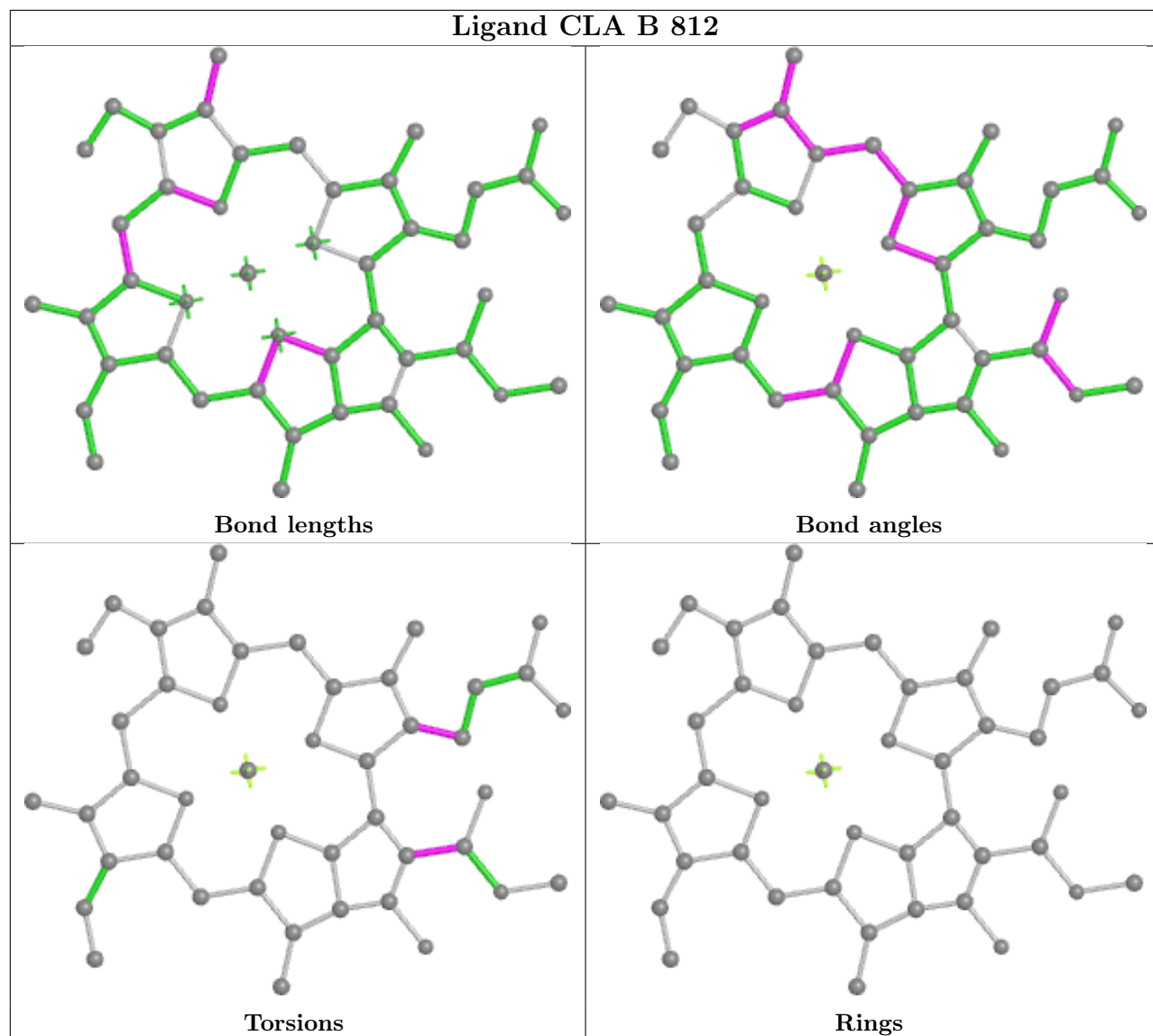




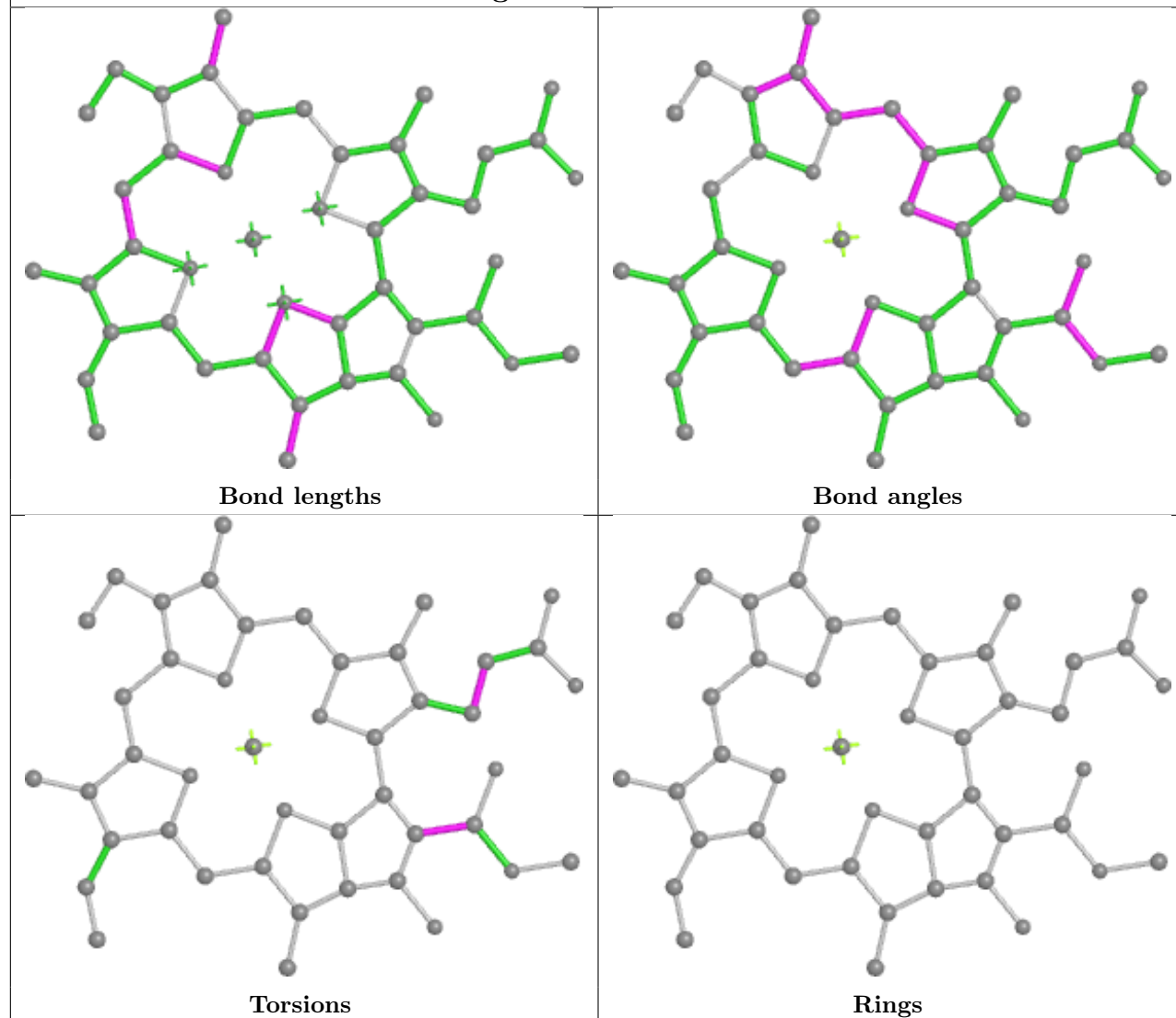
Ligand CLA B 804



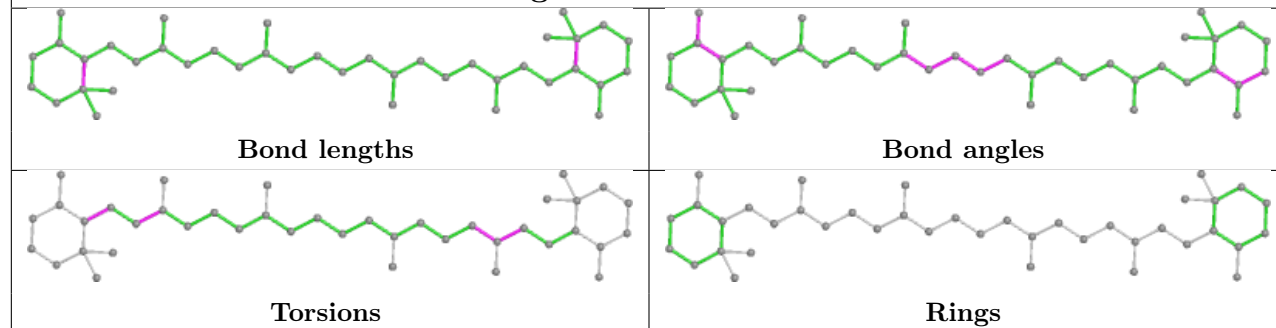
Ligand CLA B 812



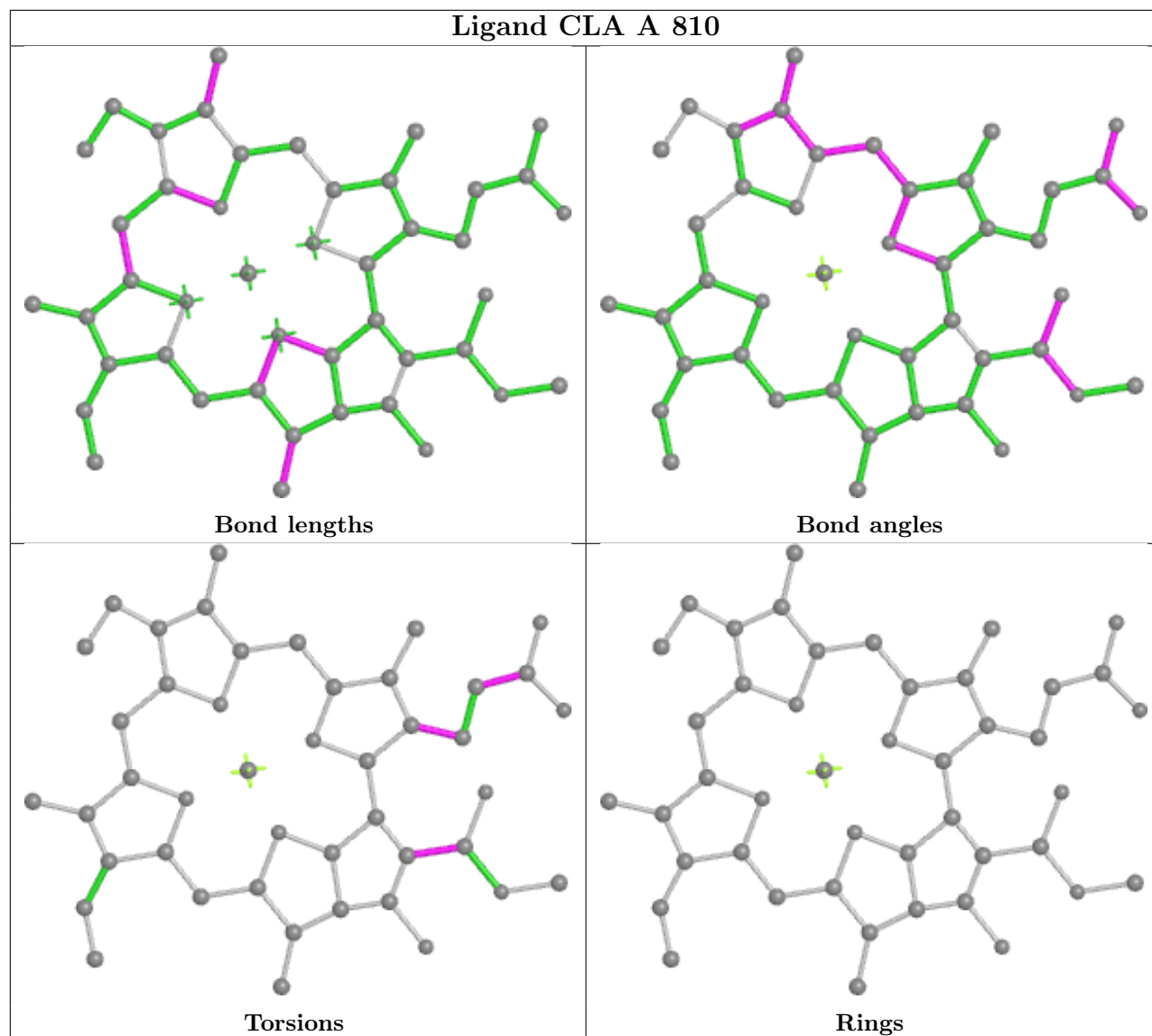
Ligand CLA L 302



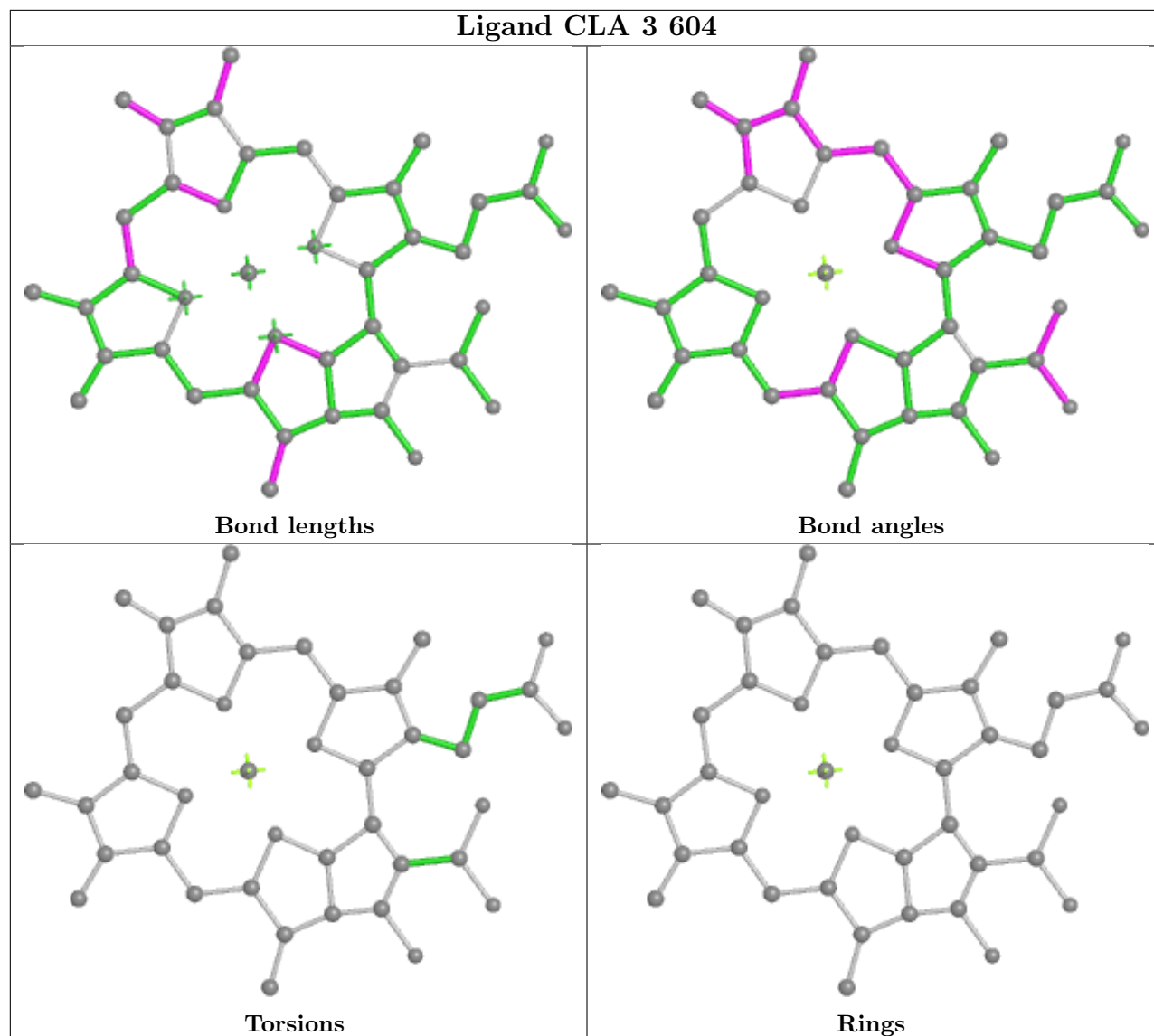
Ligand BCR B 844



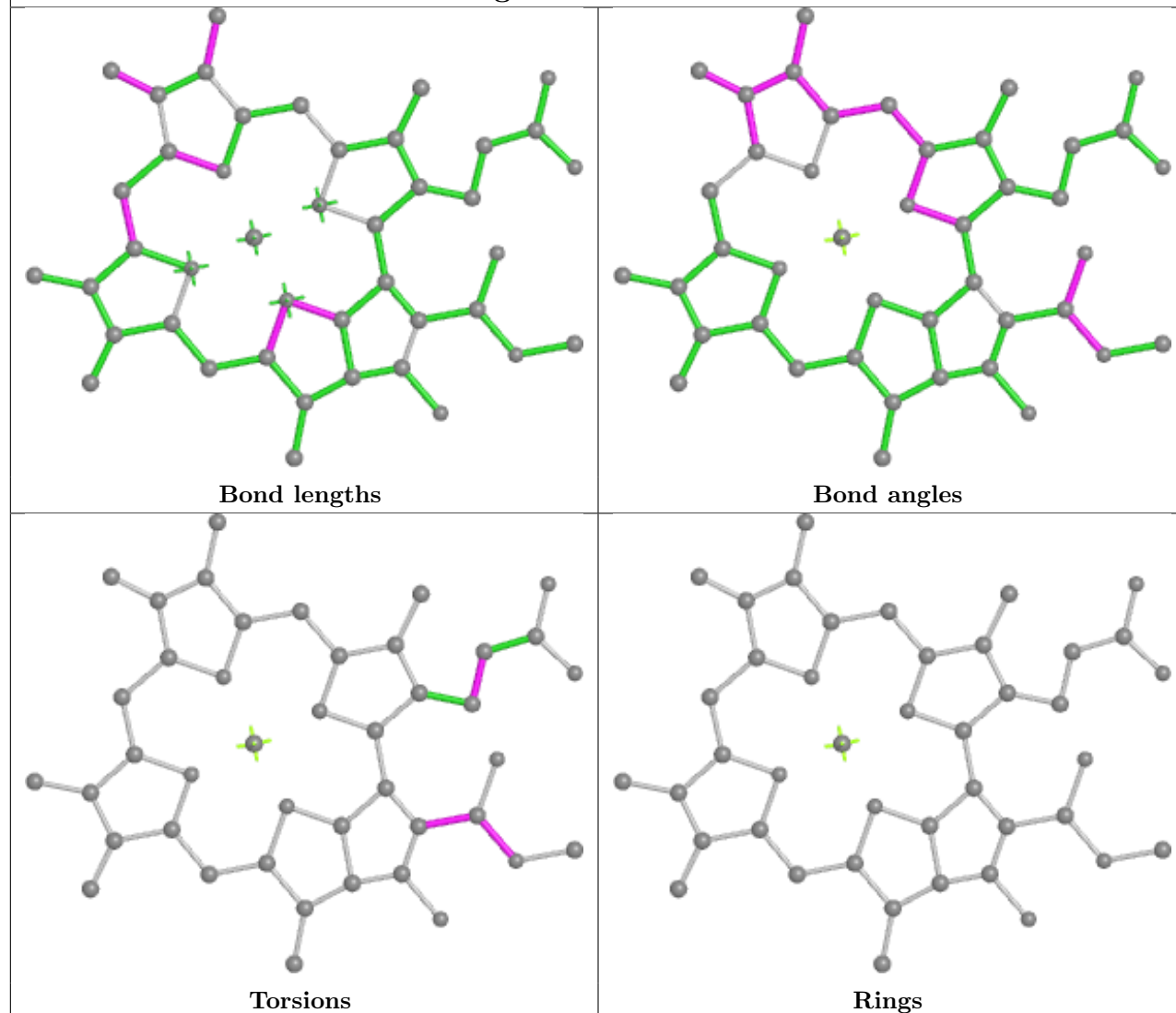
Ligand CLA A 810



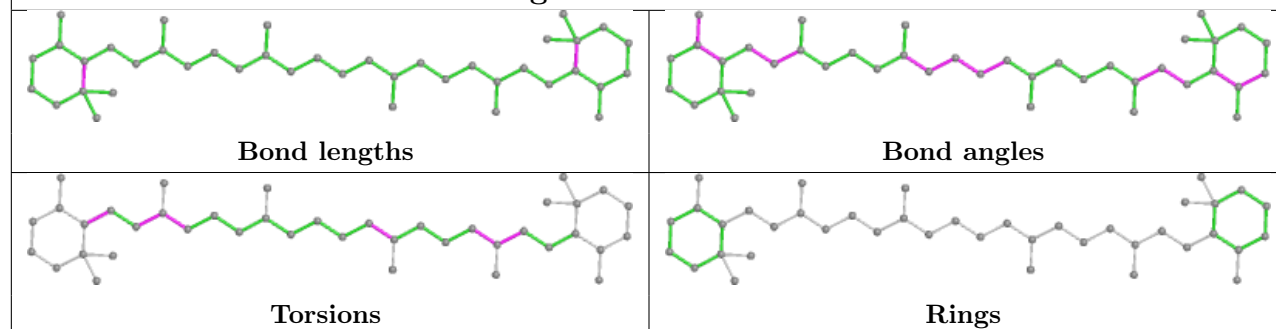
Ligand CLA 3 604

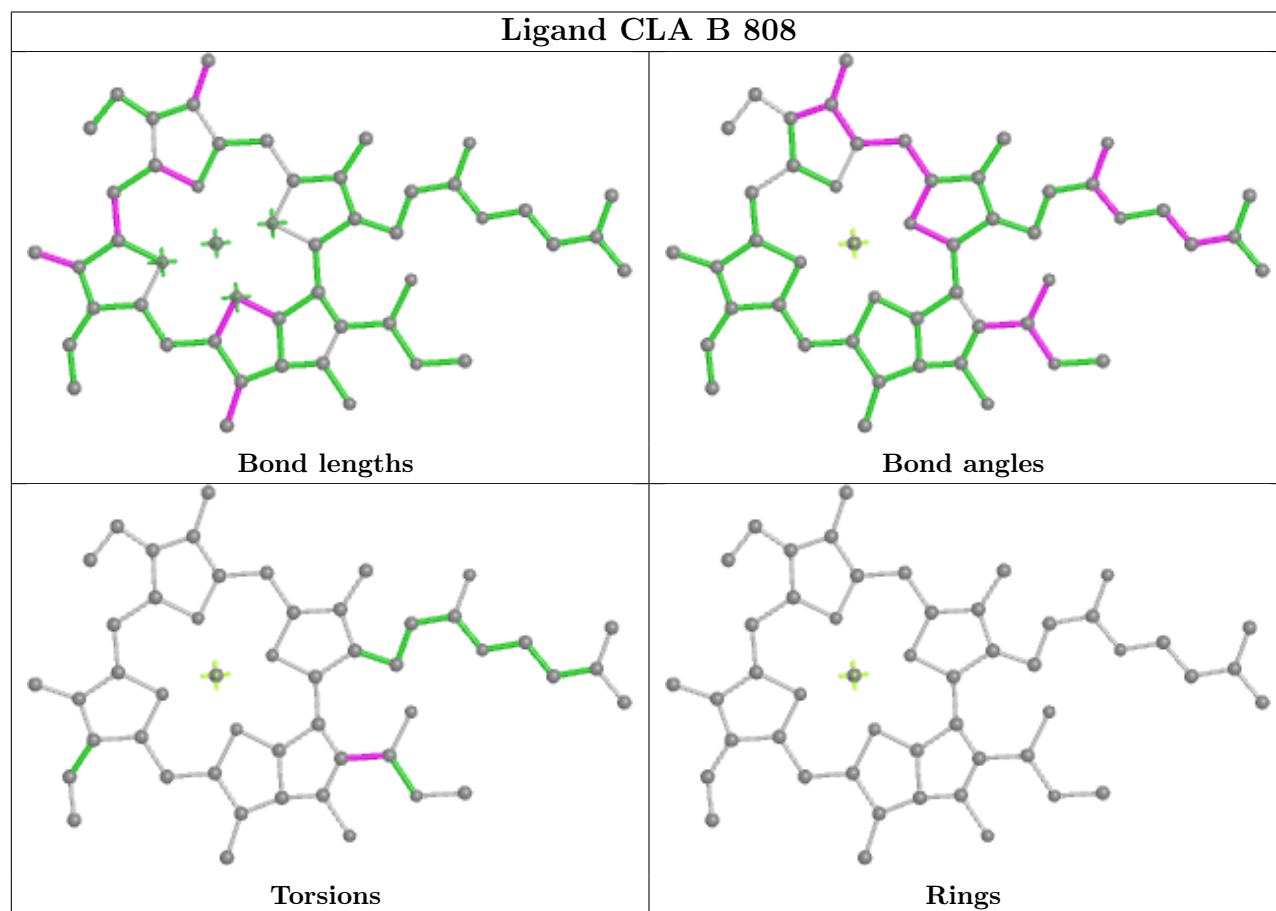
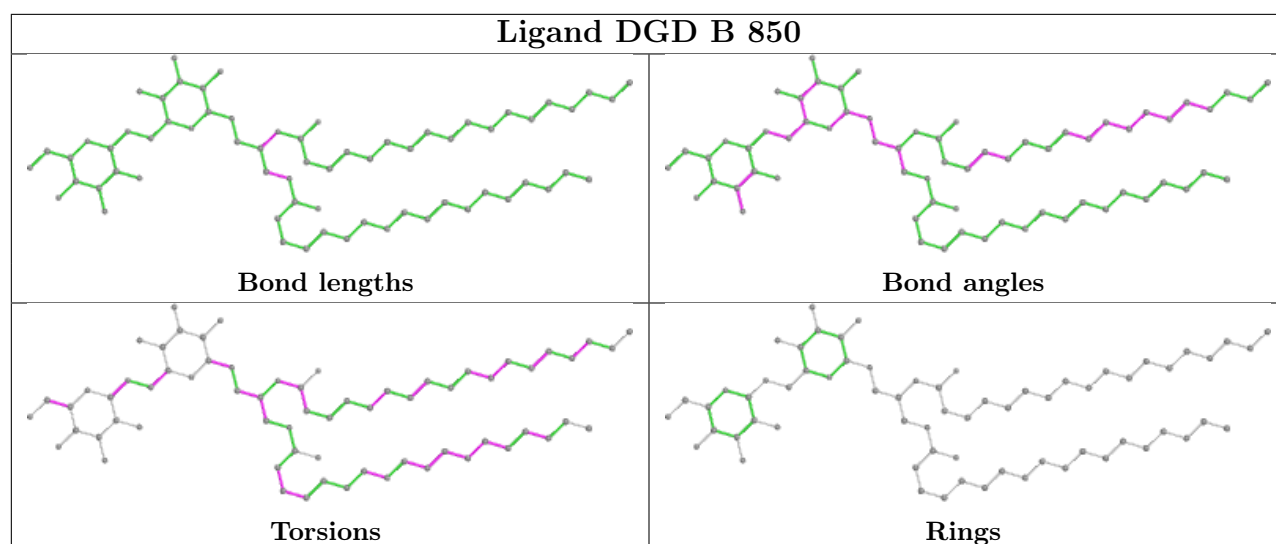


Ligand CLA 6 616

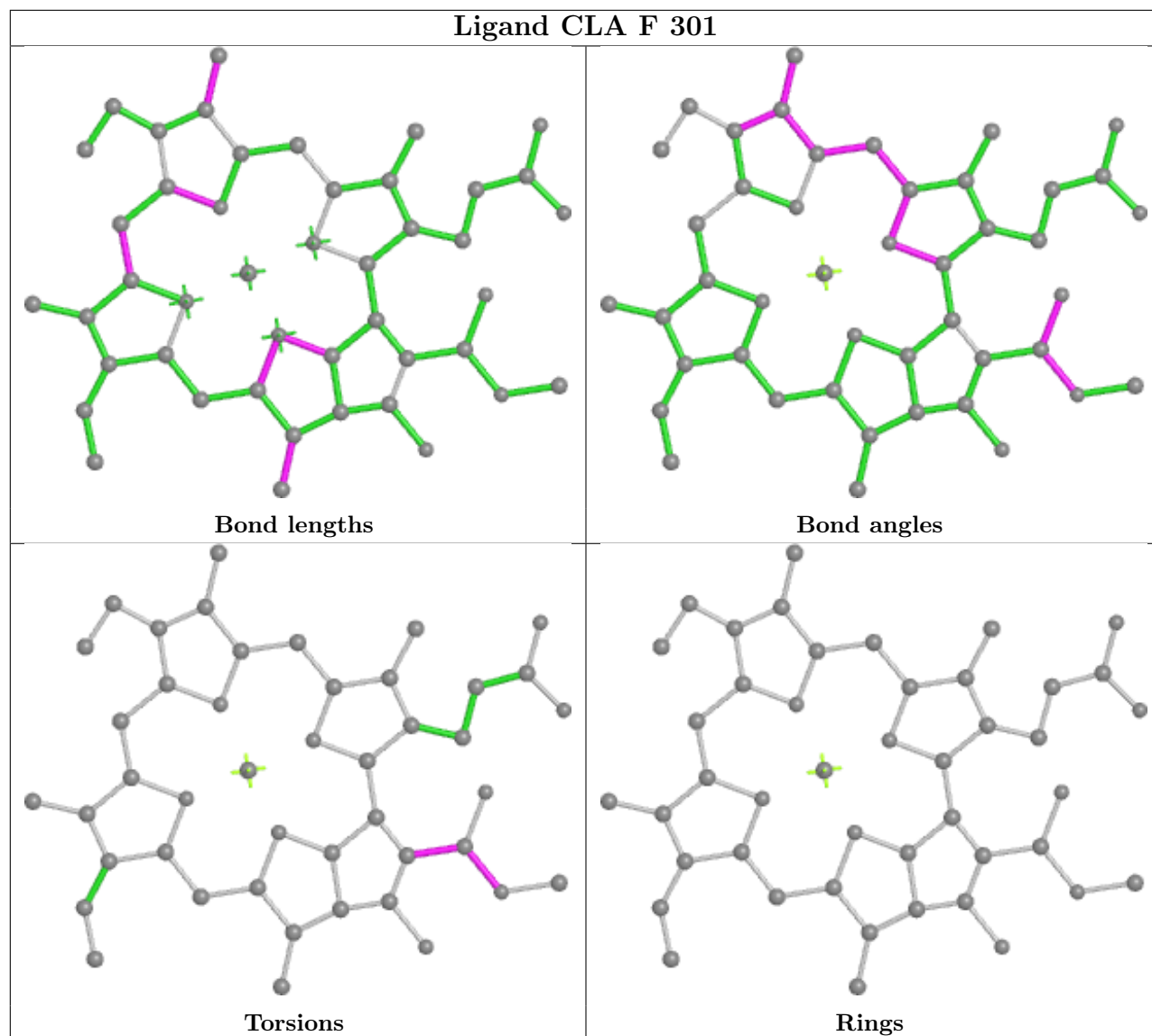


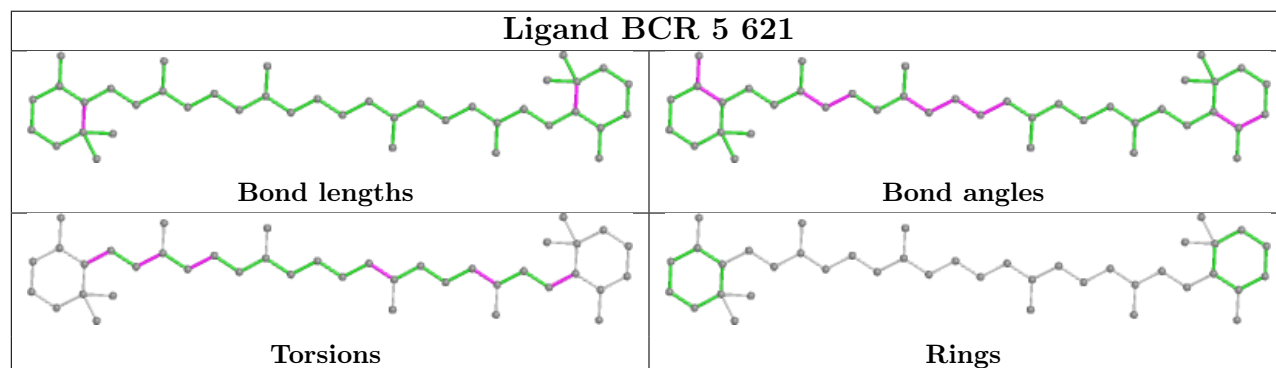
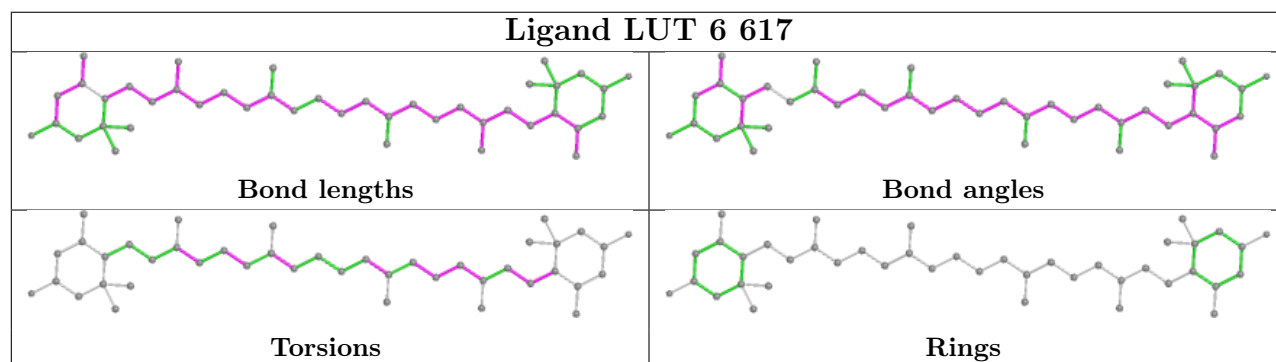
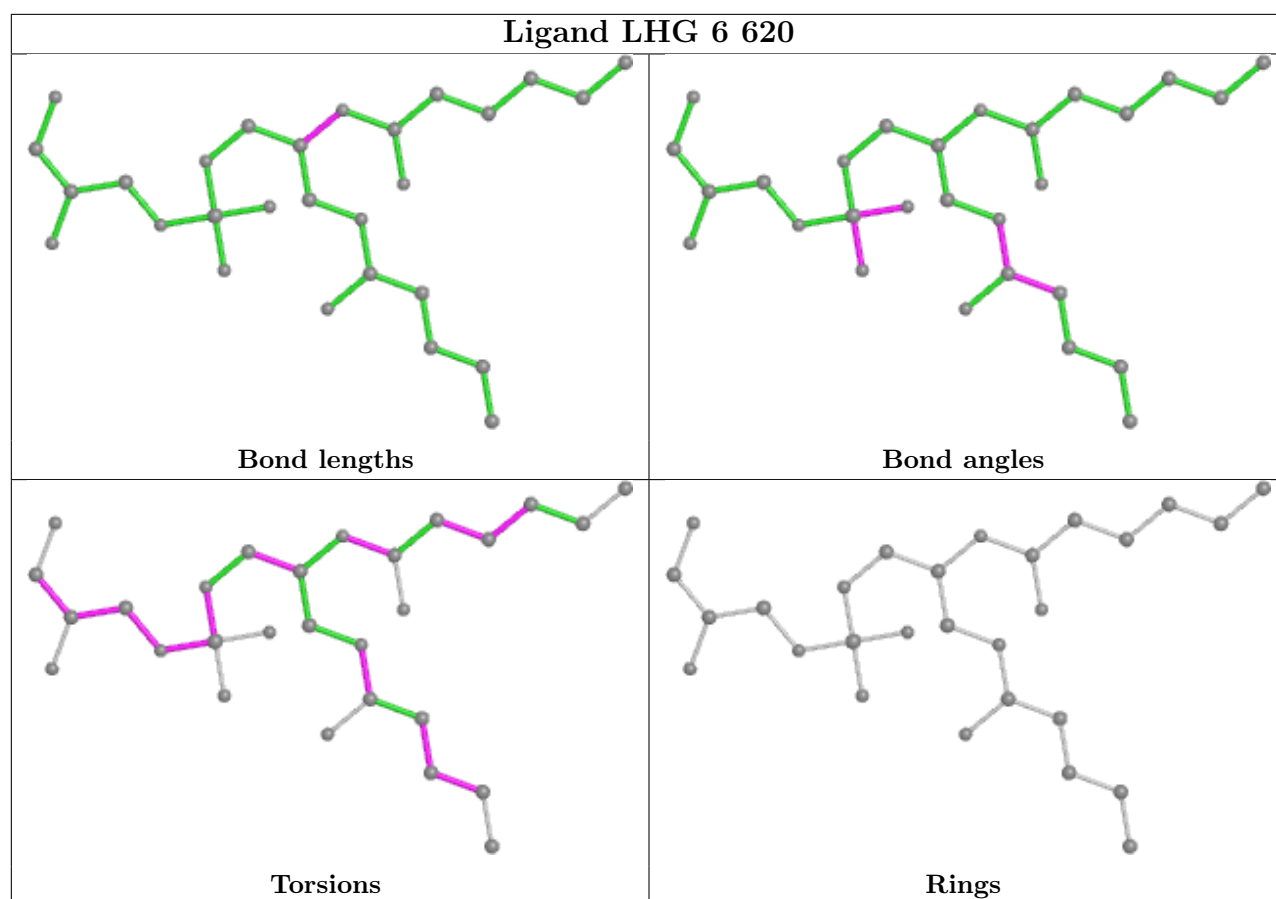
Ligand BCR A 852

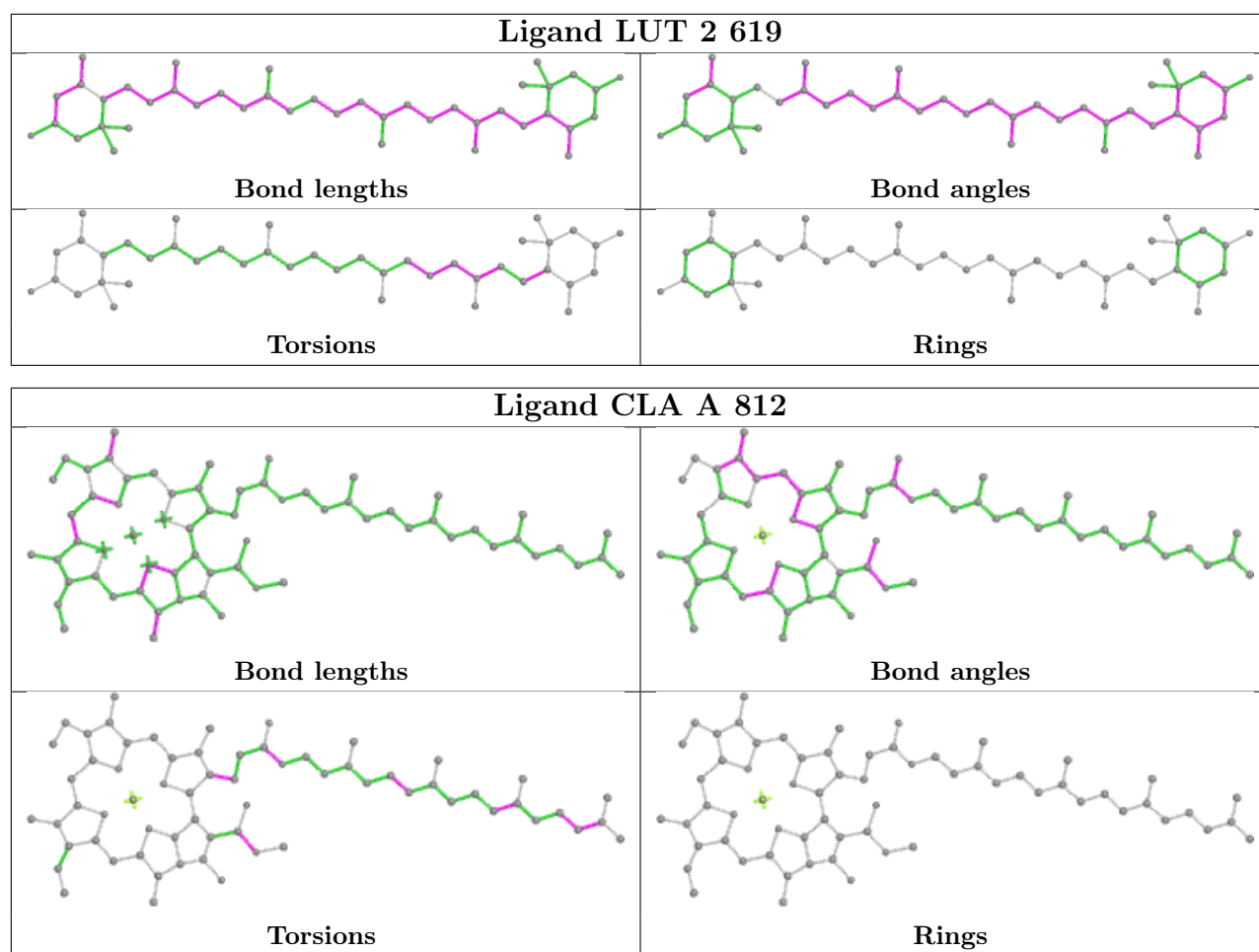




Ligand CLA F 301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-0821. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

6.5 Orthogonal surface views ⓘ

This section was not generated.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.