



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 07:47 AM JST

PDB ID : 7WG5
EMDB ID : EMD-32477
Title : Cyclic electron transport supercomplex NDH-PSI from Arabidopsis
Authors : Pan, X.W.; Li, M.
Deposited on : 2021-12-28
Resolution : 3.89 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.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

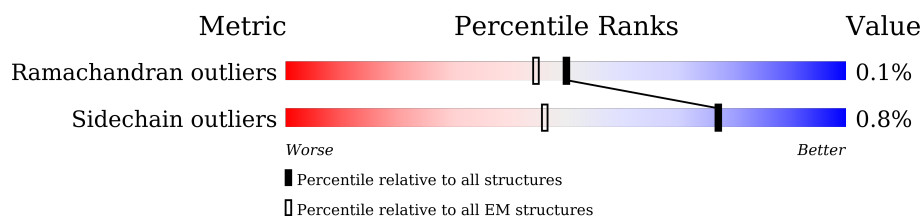
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.89 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	750	 98%
1	BA	750	 98%
2	AB	734	 99%
2	BB	734	 99%
3	AC	81	 99%
3	BC	81	 99%
4	AD	204	 69% 31%
4	BD	204	 68% 30%
5	AE	143	 47% 53%

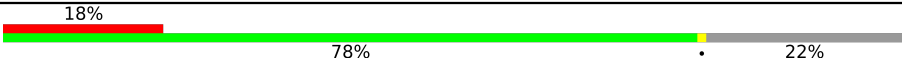
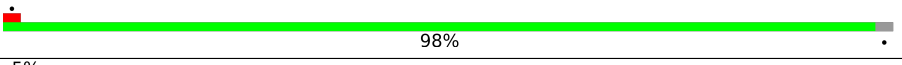

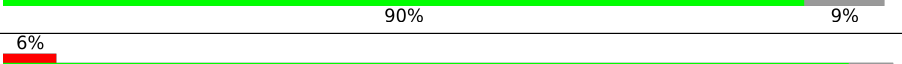
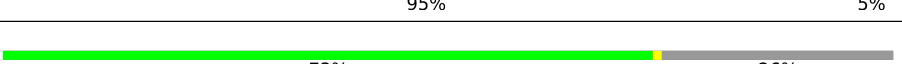
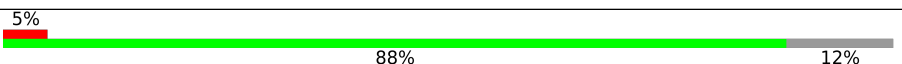

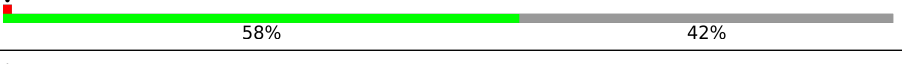
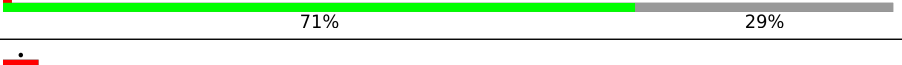

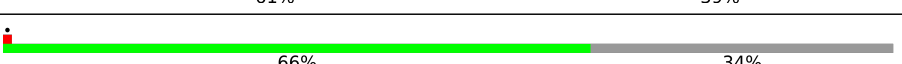
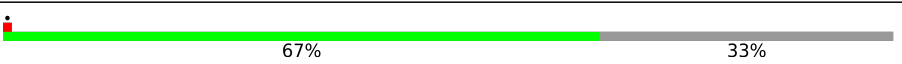

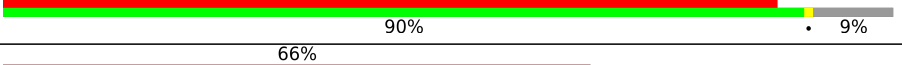
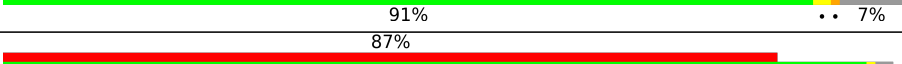
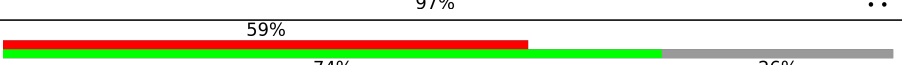
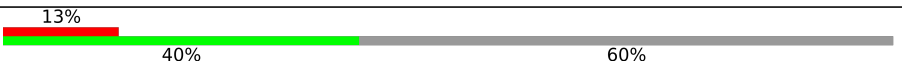
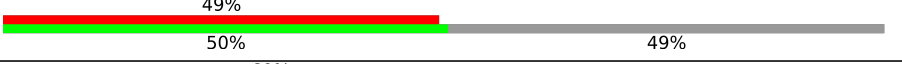


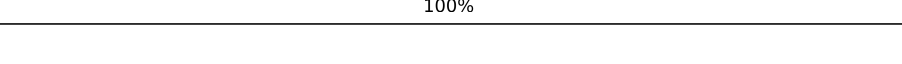
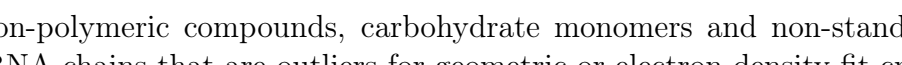


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Mol	Chain	Length	Quality of chain
5	BE	143	
6	AF	221	
6	BF	221	
7	AG	160	
7	BG	160	
8	AH	145	
8	BH	145	
9	AI	37	
9	BI	37	
10	AJ	44	
10	BJ	44	
11	AK	130	
11	BK	130	
12	AL	219	
12	BL	219	
13	A1	241	
13	B1	241	
14	A3	273	
14	B3	273	
15	A4	251	
16	A6	270	
17	B2	257	
18	B5	256	
19	A	360	
20	B	512	

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Mol	Chain	Length	Quality of chain
21	C	120	
22	D	506	
23	E	101	
24	F	746	
25	G	176	
26	a	461	
27	b	348	
28	c	204	
29	d	161	
30	e	212	
31	f	238	
32	g	190	
33	h	220	
34	i	217	
35	j	255	
36	H	393	
37	I	172	
38	J	158	
39	K	225	
40	L	191	
41	M	217	
42	N	209	
43	O	158	
44	T	122	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	A1	304	X	-	-	-
45	CLA	A1	305	X	-	-	-
45	CLA	A1	306	X	-	-	-
45	CLA	A1	307	X	-	-	-
45	CLA	A1	309	X	-	-	-
45	CLA	A1	310	X	-	-	-
45	CLA	A1	311	X	-	-	-
45	CLA	A1	312	X	-	-	-
45	CLA	A1	313	X	-	-	-
45	CLA	A1	314	X	-	-	-
45	CLA	A1	315	X	-	-	-
45	CLA	A1	316	X	-	-	-
45	CLA	A3	302	X	-	-	-
45	CLA	A3	303	X	-	-	-
45	CLA	A3	304	X	-	-	-
45	CLA	A3	305	X	-	-	-
45	CLA	A3	306	X	-	-	-
45	CLA	A3	308	X	-	-	-
45	CLA	A3	309	X	-	-	-
45	CLA	A3	310	X	-	-	-
45	CLA	A3	311	X	-	-	-
45	CLA	A3	312	X	-	-	-
45	CLA	A3	314	X	-	-	-
45	CLA	A3	315	X	-	-	-
45	CLA	A4	301	X	-	-	-
45	CLA	A4	302	X	-	-	-
45	CLA	A4	303	X	-	-	-
45	CLA	A4	307	X	-	-	-
45	CLA	A4	308	X	-	-	-
45	CLA	A4	309	X	-	-	-
45	CLA	A4	310	X	-	-	-
45	CLA	A4	311	X	-	-	-
45	CLA	A4	312	X	-	-	-
45	CLA	A4	313	X	-	-	-
45	CLA	A6	601	X	-	-	-
45	CLA	A6	603	X	-	-	-
45	CLA	A6	604	X	-	-	-
45	CLA	A6	605	X	-	-	-
45	CLA	A6	609	X	-	-	-
45	CLA	A6	610	X	-	-	-
45	CLA	A6	611	X	-	-	-
45	CLA	A6	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	A6	613	X	-	-	-
45	CLA	A6	614	X	-	-	-
45	CLA	AA	801	X	-	-	-
45	CLA	AA	802	X	-	-	-
45	CLA	AA	803	X	-	-	-
45	CLA	AA	805	X	-	-	-
45	CLA	AA	806	X	-	-	-
45	CLA	AA	807	X	-	-	-
45	CLA	AA	808	X	-	-	-
45	CLA	AA	809	X	-	-	-
45	CLA	AA	810	X	-	-	-
45	CLA	AA	811	X	-	-	-
45	CLA	AA	812	X	-	-	-
45	CLA	AA	813	X	-	-	-
45	CLA	AA	814	X	-	-	-
45	CLA	AA	816	X	-	-	-
45	CLA	AA	817	X	-	-	-
45	CLA	AA	819	X	-	-	-
45	CLA	AA	820	X	-	-	-
45	CLA	AA	821	X	-	-	-
45	CLA	AA	822	X	-	-	-
45	CLA	AA	823	X	-	-	-
45	CLA	AA	824	X	-	-	-
45	CLA	AA	825	X	-	-	-
45	CLA	AA	826	X	-	-	-
45	CLA	AA	827	X	-	-	-
45	CLA	AA	828	X	-	-	-
45	CLA	AA	829	X	-	-	-
45	CLA	AA	830	X	-	-	-
45	CLA	AA	831	X	-	-	-
45	CLA	AA	832	X	-	-	-
45	CLA	AA	833	X	-	-	-
45	CLA	AA	835	X	-	-	-
45	CLA	AA	837	X	-	-	-
45	CLA	AA	840	X	-	-	-
45	CLA	AA	842	X	-	-	-
45	CLA	AB	801	X	-	-	-
45	CLA	AB	802	X	-	-	-
45	CLA	AB	803	X	-	-	-
45	CLA	AB	804	X	-	-	-
45	CLA	AB	805	X	-	-	-
45	CLA	AB	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	AB	807	X	-	-	-
45	CLA	AB	809	X	-	-	-
45	CLA	AB	810	X	-	-	-
45	CLA	AB	811	X	-	-	-
45	CLA	AB	812	X	-	-	-
45	CLA	AB	813	X	-	-	-
45	CLA	AB	814	X	-	-	-
45	CLA	AB	815	X	-	-	-
45	CLA	AB	816	X	-	-	-
45	CLA	AB	817	X	-	-	-
45	CLA	AB	818	X	-	-	-
45	CLA	AB	819	X	-	-	-
45	CLA	AB	820	X	-	-	-
45	CLA	AB	821	X	-	-	-
45	CLA	AB	822	X	-	-	-
45	CLA	AB	824	X	-	-	-
45	CLA	AB	825	X	-	-	-
45	CLA	AB	826	X	-	-	-
45	CLA	AB	827	X	-	-	-
45	CLA	AB	828	X	-	-	-
45	CLA	AB	829	X	-	-	-
45	CLA	AB	830	X	-	-	-
45	CLA	AB	831	X	-	-	-
45	CLA	AB	833	X	-	-	-
45	CLA	AB	834	X	-	-	-
45	CLA	AB	837	X	-	-	-
45	CLA	AB	839	X	-	-	-
45	CLA	AB	840	X	-	-	-
45	CLA	AB	841	X	-	-	-
45	CLA	AB	842	X	-	-	-
45	CLA	AF	802	X	-	-	-
45	CLA	AF	803	X	-	-	-
45	CLA	AF	804	X	-	-	-
45	CLA	AG	201	X	-	-	-
45	CLA	AG	203	X	-	-	-
45	CLA	AG	204	X	-	-	-
45	CLA	AH	201	X	-	-	-
45	CLA	AJ	102	X	-	-	-
45	CLA	AK	201	X	-	-	-
45	CLA	AK	202	X	-	-	-
45	CLA	AK	203	X	-	-	-
45	CLA	AL	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	AL	305	X	-	-	-
45	CLA	B1	304	X	-	-	-
45	CLA	B1	305	X	-	-	-
45	CLA	B1	306	X	-	-	-
45	CLA	B1	307	X	-	-	-
45	CLA	B1	310	X	-	-	-
45	CLA	B1	311	X	-	-	-
45	CLA	B1	312	X	-	-	-
45	CLA	B1	313	X	-	-	-
45	CLA	B1	314	X	-	-	-
45	CLA	B1	315	X	-	-	-
45	CLA	B2	602	X	-	-	-
45	CLA	B2	603	X	-	-	-
45	CLA	B2	604	X	-	-	-
45	CLA	B2	608	X	-	-	-
45	CLA	B2	609	X	-	-	-
45	CLA	B2	610	X	-	-	-
45	CLA	B2	611	X	-	-	-
45	CLA	B2	612	X	-	-	-
45	CLA	B2	613	X	-	-	-
45	CLA	B3	301	X	-	-	-
45	CLA	B3	302	X	-	-	-
45	CLA	B3	303	X	-	-	-
45	CLA	B3	304	X	-	-	-
45	CLA	B3	305	X	-	-	-
45	CLA	B3	307	X	-	-	-
45	CLA	B3	308	X	-	-	-
45	CLA	B3	309	X	-	-	-
45	CLA	B3	310	X	-	-	-
45	CLA	B3	311	X	-	-	-
45	CLA	B3	312	X	-	-	-
45	CLA	B3	313	X	-	-	-
45	CLA	B3	314	X	-	-	-
45	CLA	B5	601	X	-	-	-
45	CLA	B5	603	X	-	-	-
45	CLA	B5	604	X	-	-	-
45	CLA	B5	608	X	-	-	-
45	CLA	B5	609	X	-	-	-
45	CLA	B5	611	X	-	-	-
45	CLA	B5	612	X	-	-	-
45	CLA	B5	613	X	-	-	-
45	CLA	BA	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	BA	802	X	-	-	-
45	CLA	BA	803	X	-	-	-
45	CLA	BA	805	X	-	-	-
45	CLA	BA	806	X	-	-	-
45	CLA	BA	807	X	-	-	-
45	CLA	BA	808	X	-	-	-
45	CLA	BA	810	X	-	-	-
45	CLA	BA	811	X	-	-	-
45	CLA	BA	812	X	-	-	-
45	CLA	BA	813	X	-	-	-
45	CLA	BA	814	X	-	-	-
45	CLA	BA	816	X	-	-	-
45	CLA	BA	819	X	-	-	-
45	CLA	BA	820	X	-	-	-
45	CLA	BA	822	X	-	-	-
45	CLA	BA	823	X	-	-	-
45	CLA	BA	824	X	-	-	-
45	CLA	BA	825	X	-	-	-
45	CLA	BA	827	X	-	-	-
45	CLA	BA	828	X	-	-	-
45	CLA	BA	829	X	-	-	-
45	CLA	BA	830	X	-	-	-
45	CLA	BA	831	X	-	-	-
45	CLA	BA	833	X	-	-	-
45	CLA	BA	835	X	-	-	-
45	CLA	BA	837	X	-	-	-
45	CLA	BA	838	X	-	-	-
45	CLA	BA	840	X	-	-	-
45	CLA	BA	841	X	-	-	-
45	CLA	BA	842	X	-	-	-
45	CLA	BA	844	X	-	-	-
45	CLA	BB	801	X	-	-	-
45	CLA	BB	802	X	-	-	-
45	CLA	BB	804	X	-	-	-
45	CLA	BB	805	X	-	-	-
45	CLA	BB	806	X	-	-	-
45	CLA	BB	807	X	-	-	-
45	CLA	BB	808	X	-	-	-
45	CLA	BB	810	X	-	-	-
45	CLA	BB	811	X	-	-	-
45	CLA	BB	812	X	-	-	-
45	CLA	BB	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	BB	814	X	-	-	-
45	CLA	BB	815	X	-	-	-
45	CLA	BB	816	X	-	-	-
45	CLA	BB	817	X	-	-	-
45	CLA	BB	818	X	-	-	-
45	CLA	BB	819	X	-	-	-
45	CLA	BB	820	X	-	-	-
45	CLA	BB	821	X	-	-	-
45	CLA	BB	822	X	-	-	-
45	CLA	BB	823	X	-	-	-
45	CLA	BB	825	X	-	-	-
45	CLA	BB	826	X	-	-	-
45	CLA	BB	828	X	-	-	-
45	CLA	BB	829	X	-	-	-
45	CLA	BB	830	X	-	-	-
45	CLA	BB	831	X	-	-	-
45	CLA	BB	832	X	-	-	-
45	CLA	BB	835	X	-	-	-
45	CLA	BB	837	X	-	-	-
45	CLA	BB	838	X	-	-	-
45	CLA	BB	841	X	-	-	-
45	CLA	BB	842	X	-	-	-
45	CLA	BB	843	X	-	-	-
45	CLA	BF	301	X	-	-	-
45	CLA	BF	302	X	-	-	-
45	CLA	BF	303	X	-	-	-
45	CLA	BG	201	X	-	-	-
45	CLA	BG	202	X	-	-	-
45	CLA	BH	201	X	-	-	-
45	CLA	BJ	102	X	-	-	-
45	CLA	BK	201	X	-	-	-
45	CLA	BK	202	X	-	-	-
45	CLA	BK	203	X	-	-	-
45	CLA	BL	304	X	-	-	-
54	CHL	A1	303	X	-	-	-
54	CHL	A1	308	X	-	-	-
54	CHL	A3	307	X	-	-	-
54	CHL	A4	304	X	-	-	-
54	CHL	A4	305	X	-	-	-
54	CHL	A4	306	X	-	-	-
54	CHL	A4	314	X	-	-	-
54	CHL	A6	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	CHL	A6	606	X	-	-	-
54	CHL	A6	607	X	-	-	-
54	CHL	A6	608	X	-	-	-
54	CHL	B1	303	X	-	-	-
54	CHL	B1	308	X	-	-	-
54	CHL	B2	601	X	-	-	-
54	CHL	B2	605	X	-	-	-
54	CHL	B2	606	X	-	-	-
54	CHL	B2	607	X	-	-	-
54	CHL	B2	614	X	-	-	-
54	CHL	B3	306	X	-	-	-
54	CHL	B5	605	X	-	-	-
54	CHL	B5	606	X	-	-	-
54	CHL	B5	607	X	-	-	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 112687 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	AA	742	Total	C	N	O	S	0	0
			5839	3826	992	1003	18		
1	BA	742	Total	C	N	O	S	0	0
			5841	3828	992	1003	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	734	Total	C	N	O	S	0	0
			5862	3847	999	1001	15		
2	BB	733	Total	C	N	O	S	0	0
			5854	3842	998	1000	14		

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

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

- Molecule 4 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	141	Total	C	N	O	S	0	0
			1112	712	193	203	4		
4	BD	143	Total	C	N	O	S	0	0
			1127	723	195	205	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AE	67	Total	C	N	O	0	0
			530	341	94	95		
5	BE	69	Total	C	N	O	0	0
			546	352	97	97		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	153	Total	C	N	O	S	0	0
			1213	792	208	210	3		
6	BF	154	Total	C	N	O	S	0	0
			1220	797	209	211	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AG	99	Total	C	N	O	0	0
			771	501	126	144		
7	BG	94	Total	C	N	O	0	0
			733	474	121	138		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AH	95	Total	C	N	O	0	0
			730	476	119	135		
8	BH	95	Total	C	N	O	0	0
			730	476	119	135		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	33	Total	C	N	O	S	0	0
			257	175	41	40	1		
9	BI	33	Total	C	N	O	S	0	0
			257	175	41	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	42	Total	C	N	O	S	0	0
			338	230	51	56	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	BJ	43	Total	C	N	O	S	0	0
			344	233	52	58	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psak, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	65	Total	C	N	O	S	0	0
			451	290	74	84	3		
11	BK	64	Total	C	N	O	S	0	0
			445	285	73	84	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	157	Total	C	N	O	S	0	0
			1173	775	187	209	2		
12	BL	159	Total	C	N	O	S	0	0
			1184	781	190	211	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	196	Total	C	N	O	S	0	0
			1511	984	251	271	5		
13	B1	172	Total	C	N	O	S	0	0
			1339	873	221	240	5		

- Molecule 14 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A3	219	Total	C	N	O	S	0	0
			1675	1096	272	302	5		
14	B3	221	Total	C	N	O	S	0	0
			1696	1111	276	304	5		

- Molecule 15 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A4	197	Total	C	N	O	S	0	0
			1562	1022	254	283	3		

- Molecule 16 is a protein called Photosystem I chlorophyll a/b-binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A6	212	Total	C	N	O	S	0	0
			1671	1088	272	299	12		

- Molecule 17 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B2	208	Total	C	N	O	S	0	0
			1607	1051	261	291	4		

- Molecule 18 is a protein called Photosystem I chlorophyll a/b-binding protein 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B5	206	Total	C	N	O	S	0	0
			1599	1045	263	285	6		

- Molecule 19 is a protein called NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	305	Total	C	N	O	S	0	0
			2372	1593	366	409	4		

- Molecule 20 is a protein called NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	486	Total	C	N	O	S	0	0
			3780	2495	577	679	29		

- Molecule 21 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	94	Total	C	N	O	S	0	0
			776	544	109	121	2		

- Molecule 22 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	497	Total	C	N	O	S	0	0
			3946	2656	599	666	25		

- Molecule 23 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	89	Total	C	N	O	S	0	0
			695	458	112	119	6		

- Molecule 24 is a protein called NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	677	Total	C	N	O	S	0	0
			5330	3558	829	915	28		

- Molecule 25 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	G	167	Total	C	N	O	S	0	0
			1281	858	194	224	5		

- Molecule 26 is a protein called Photosynthetic NDH subunit of subcomplex B 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	341	Total	C	N	O	S	0	0
			2655	1692	450	500	13		

- Molecule 27 is a protein called Photosynthetic NDH subunit of subcomplex B 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	307	Total	C	N	O	S	0	0
			2367	1508	392	452	15		

- Molecule 28 is a protein called Photosynthetic NDH subunit of subcomplex B 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	128	Total	C	N	O	S	0	0
			1005	636	180	183	6		

- Molecule 29 is a protein called NDH dependent flow 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	93	Total	C	N	O	S	0	0
			762	497	119	138	8		

- Molecule 30 is a protein called Photosynthetic NDH subunit of subcomplex B 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	150	Total	C	N	O	S	0	0
			1206	780	183	236	7		

- Molecule 31 is a protein called Photosynthetic NDH subunit of luminal location 1, chloro-
plastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	153	Total	C	N	O	S	0	0
			1277	823	219	233	2		

- Molecule 32 is a protein called Photosynthetic NDH subunit of luminal location 2, chloro-
plastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	115	Total	C	N	O	S	0	0
			965	620	159	180	6		

- Molecule 33 is a protein called Photosynthetic NDH subunit of luminal location 3, chloro-
plastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	145	Total	C	N	O	S	0	0
			1170	753	191	221	5		

- Molecule 34 is a protein called Photosynthetic NDH subunit of luminal location 4, chloro-
plastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	145	Total	C	N	O	S	0	0
			1098	698	190	204	6		

- Molecule 35 is a protein called Isoform 2 of Photosynthetic NDH subunit of luminal location
5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	173	Total	C	N	O	S	0	0
			1331	840	236	248	7		

- Molecule 36 is a protein called NAD(P)H-quinone oxidoreductase subunit H, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	H	356	Total	C	N	O	S	0	0
			2812	1830	465	499	18		

- Molecule 37 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	I	160	Total	C	N	O	S	0	0
			1236	776	214	233	13		

- Molecule 38 is a protein called NAD(P)H-quinone oxidoreductase subunit J, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	J	155	Total	C	N	O	S	0	0
			1116	722	189	202	3		

- Molecule 39 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	K	167	Total	C	N	O	S	0	0
			1199	765	203	221	10		

- Molecule 40 is a protein called NAD(P)H-quinone oxidoreductase subunit L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L	77	Total	C	N	O	S	0	0
			646	437	106	99	4		

- Molecule 41 is a protein called NAD(P)H-quinone oxidoreductase subunit M, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	M	110	Total	C	N	O	S	0	0
			771	494	132	143	2		

- Molecule 42 is a protein called NAD(P)H-quinone oxidoreductase subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N	146	Total	C	N	O	S	0	0
			908	584	156	166	2		

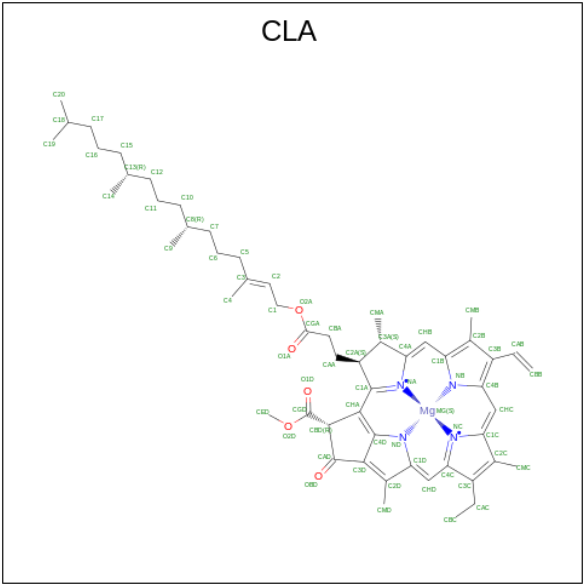
- Molecule 43 is a protein called NdhO.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	O	75	Total	C	N	O	0	0
			520	334	90	96		

- Molecule 44 is a protein called NdhT.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	T	122	Total	C	N	O	0	0
			610	366	122	122		

- Molecule 45 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	AA	1	Total 50	C 40	Mg 1	N 4	O 5	0
45	AA	1	Total 64	C 55	Mg 1	N 4	O 4	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 54	C 44	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	AA	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	AA	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	AA	1	Total 59	C 49	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	AA	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	AA	1	Total 54	C 44	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 59	C 49	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 47	C 37	Mg 1	N 4	O 5	0
45	AA	1	Total 56	C 46	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	AA	1	Total 51	C 41	Mg 1	N 4	O 5	0
45	AA	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	AA	1	Total 52	C 42	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 64	C 54	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 51	C 42	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 54	C 44	Mg 1	N 4	O 5	0
45	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	AB	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	AB	1	Total 59	C 49	Mg 1	N 4	O 5	0
45	AB	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	AB	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	AB	1	Total 50	C 40	Mg 1	N 4	O 5	0
45	AB	1	Total 47	C 37	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 62	C 52	Mg 1	N 4	O 5	0
45	AB	1	Total 62	C 52	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
45	AB	1	Total 56	C 46	Mg 1	N 4	O 5	0
45	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	AB	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	AB	1	Total 50	C 40	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 47	C 37	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AF	1	Total 57	C 47	Mg 1	N 4	O 5	0
45	AF	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	AF	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	AG	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	AG	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	AG	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	AH	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	AJ	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
45	AK	1	Total 35	C 29	Mg 1	N 4	O 1	0
45	AK	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	AK	1	Total 46	C 36	Mg 1	N 4	O 5	0
45	AL	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	AL	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	AL	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	A1	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	A1	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	A1	1	Total 49	C 39	Mg 1	N 4	O 5	0
45	A1	1	Total 40	C 32	Mg 1	N 4	O 3	0
45	A1	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	A1	1	Total 40	C 32	Mg 1	N 4	O 3	0
45	A1	1	Total 59	C 49	Mg 1	N 4	O 5	0
45	A1	1	Total 38	C 30	Mg 1	N 4	O 3	0
45	A1	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	A1	1	Total 64	C 54	Mg 1	N 4	O 5	0
45	A1	1	Total 38	C 30	Mg 1	N 4	O 3	0
45	A1	1	Total 43	C 33	Mg 1	N 4	O 5	0
45	A3	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	A3	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	A3	1	Total 42	C 32	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
45	A3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	A3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	A3	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	A3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	A3	1	Total 37	C 31	Mg 1	N 4	O 1	0
45	A3	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	A3	1	Total 54	C 44	Mg 1	N 4	O 5	0
45	A3	1	Total 40	C 32	Mg 1	N 4	O 3	0
45	A3	1	Total 36	C 30	Mg 1	N 4	O 1	0
45	A3	1	Total 40	C 32	Mg 1	N 4	O 3	0
45	A4	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	A4	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	A4	1	Total 43	C 33	Mg 1	N 4	O 5	0
45	A4	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	A4	1	Total 54	C 44	Mg 1	N 4	O 5	0
45	A4	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	A4	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	A4	1	Total 56	C 46	Mg 1	N 4	O 5	0
45	A4	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	A4	1	Total 50	C 40	Mg 1	N 4	O 5	0
45	A6	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
45	A6	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	A6	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	A6	1	Total 43	C 34	Mg 1	N 4	O 4	0
45	A6	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	A6	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	A6	1	Total 38	C 30	Mg 1	N 4	O 3	0
45	A6	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	A6	1	Total 64	C 55	Mg 1	N 4	O 4	0
45	A6	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 52	C 42	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 50	C 40	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 50	C 40	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	BA	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	BA	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	BA	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	BA	1	Total 56	C 46	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	BA	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	BA	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 53	C 43	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 47	C 37	Mg 1	N 4	O 5	0
45	BA	1	Total 56	C 46	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	BA	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	BA	1	Total 51	C 41	Mg 1	N 4	O 5	0
45	BA	1	Total 54	C 45	Mg 1	N 4	O 4	0
45	BA	1	Total 51	C 41	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BA	1	Total 42	C 33	Mg 1	N 4	O 4	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 52	C 42	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
45	BB	1	Total 54	C 44	Mg 1	N 4	O 5	0
45	BB	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 64	C 54	Mg 1	N 4	O 5	0
45	BB	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	BB	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	BB	1	Total 59	C 49	Mg 1	N 4	O 5	0
45	BB	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	BB	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	BB	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	BB	1	Total 46	C 36	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 62	C 52	Mg 1	N 4	O 5	0
45	BB	1	Total 62	C 52	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 56	C 46	Mg 1	N 4	O 5	0
45	BB	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	BB	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	BB	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	BB	1	Total 50	C 40	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 47	C 37	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	BF	1	Total 55	C 46	Mg 1	N 4	O 4	0
45	BF	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	BF	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	BG	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	BG	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	BH	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	BJ	1	Total 42	C 34	Mg 1	N 4	O 3	0
45	BK	1	Total 36	C 30	Mg 1	N 4	O 1	0
45	BK	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	BK	1	Total 46	C 36	Mg 1	N 4	O 5	0
45	BL	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
45	BL	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	BL	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	B1	1	Total 61	C 51	Mg 1	N 4	O 5	0
45	B1	1	Total 54	C 45	Mg 1	N 4	O 4	0
45	B1	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	B1	1	Total 40	C 32	Mg 1	N 4	O 3	0
45	B1	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	B1	1	Total 39	C 31	Mg 1	N 4	O 3	0
45	B1	1	Total 59	C 49	Mg 1	N 4	O 5	0
45	B1	1	Total 38	C 30	Mg 1	N 4	O 3	0
45	B1	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	B1	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	B1	1	Total 38	C 30	Mg 1	N 4	O 3	0
45	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	B2	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	B2	1	Total 43	C 34	Mg 1	N 4	O 4	0
45	B2	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	B2	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	B2	1	Total 38	C 30	Mg 1	N 4	O 3	0
45	B2	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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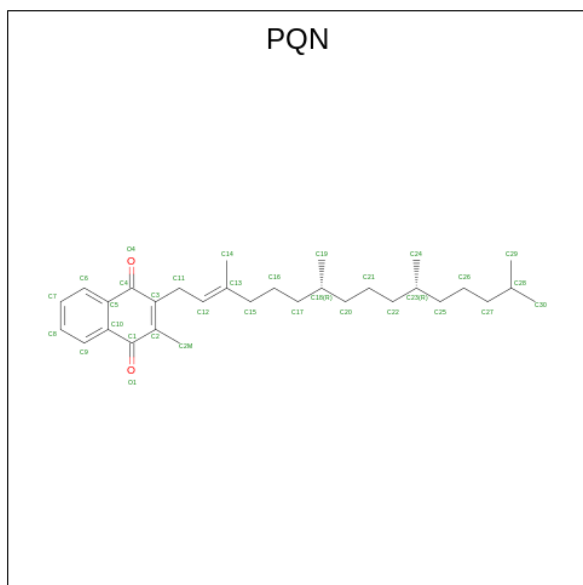
Mol	Chain	Residues	Atoms					AltConf
45	B2	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	B3	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	B3	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	B3	1	Total 42	C 32	Mg 1	N 4	O 5	0
45	B3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	B3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	B3	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	B3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	B3	1	Total 40	C 32	Mg 1	N 4	O 3	0
45	B3	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	B3	1	Total 54	C 44	Mg 1	N 4	O 5	0
45	B3	1	Total 40	C 32	Mg 1	N 4	O 3	0
45	B3	1	Total 36	C 30	Mg 1	N 4	O 1	0
45	B3	1	Total 40	C 32	Mg 1	N 4	O 3	0
45	B5	1	Total 46	C 36	Mg 1	N 4	O 5	0
45	B5	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	B5	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	B5	1	Total 43	C 33	Mg 1	N 4	O 5	0
45	B5	1	Total 44	C 34	Mg 1	N 4	O 5	0
45	B5	1	Total 54	C 44	Mg 1	N 4	O 5	0
45	B5	1	Total 42	C 34	Mg 1	N 4	O 3	0

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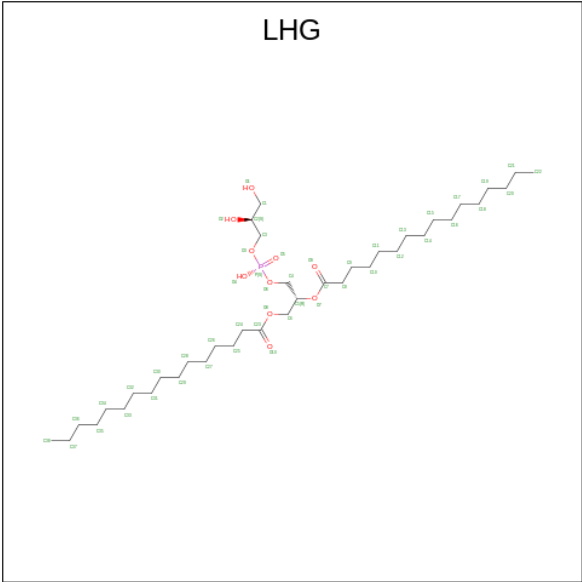
Mol	Chain	Residues	Atoms					AltConf
45	B5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 46 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
46	AA	1	Total	C	O	0
			33	31	2	
46	AB	1	Total	C	O	0
			33	31	2	
46	BA	1	Total	C	O	0
			33	31	2	
46	BB	1	Total	C	O	0
			33	31	2	

- Molecule 47 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



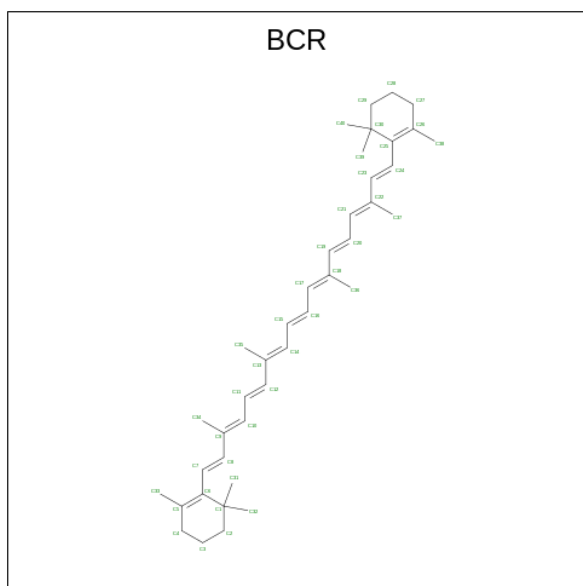
Mol	Chain	Residues	Atoms				AltConf
47	AA	1	Total	C	O	P	0
			49	38	10	1	
47	AJ	1	Total	C	O	P	0
			40	29	10	1	
47	A1	1	Total	C	O	P	0
			38	27	10	1	
47	A1	1	Total	C	O	P	0
			36	25	10	1	
47	A1	1	Total	C	O	P	0
			49	38	10	1	
47	A3	1	Total	C	O	P	0
			36	25	10	1	
47	A3	1	Total	C	O	P	0
			23	12	10	1	
47	A6	1	Total	C	O	P	0
			36	25	10	1	
47	BA	1	Total	C	O	P	0
			49	38	10	1	
47	BA	1	Total	C	O	P	0
			27	16	10	1	
47	BF	1	Total	C	O	P	0
			45	34	10	1	
47	B1	1	Total	C	O	P	0
			38	27	10	1	
47	B1	1	Total	C	O	P	0
			36	25	10	1	
47	B1	1	Total	C	O	P	0
			42	31	10	1	

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Mol	Chain	Residues	Atoms				AltConf
47	B2	1	Total	C	O	P	0
			35	24	10	1	
47	B3	1	Total	C	O	P	0
			23	12	10	1	
47	B5	1	Total	C	O	P	0
			30	19	10	1	
47	F	1	Total	C	O	P	0
			37	26	10	1	
47	a	1	Total	C	O	P	0
			29	18	10	1	

- Molecule 48 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AF	1	Total C 40 40	0
48	AF	1	Total C 40 40	0
48	AG	1	Total C 40 40	0
48	AI	1	Total C 40 40	0
48	AI	1	Total C 40 40	0
48	AJ	1	Total C 40 40	0
48	AJ	1	Total C 40 40	0
48	AK	1	Total C 40 40	0
48	AL	1	Total C 40 40	0
48	AL	1	Total C 40 40	0
48	A1	1	Total C 40 40	0
48	A3	1	Total C 40 40	0
48	A4	1	Total C 40 40	0
48	A6	1	Total C 40 40	0
48	BA	1	Total C 40 40	0

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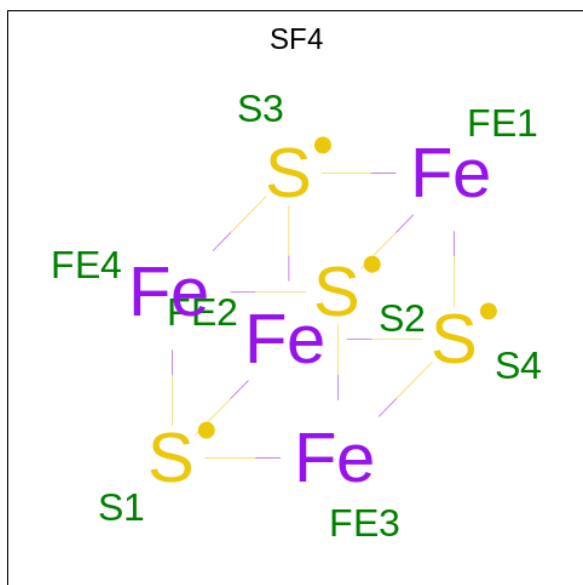
Mol	Chain	Residues	Atoms	AltConf
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BF	1	Total C 40 40	0
48	BG	1	Total C 40 40	0
48	BI	1	Total C 40 40	0
48	BJ	1	Total C 40 40	0
48	BJ	1	Total C 40 40	0
48	BK	1	Total C 40 40	0
48	BL	1	Total C 40 40	0
48	BL	1	Total C 40 40	0
48	BL	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
48	B2	1	Total	C	0
			40	40	
48	B3	1	Total	C	0
			40	40	
48	B5	1	Total	C	0
			40	40	

- Molecule 49 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



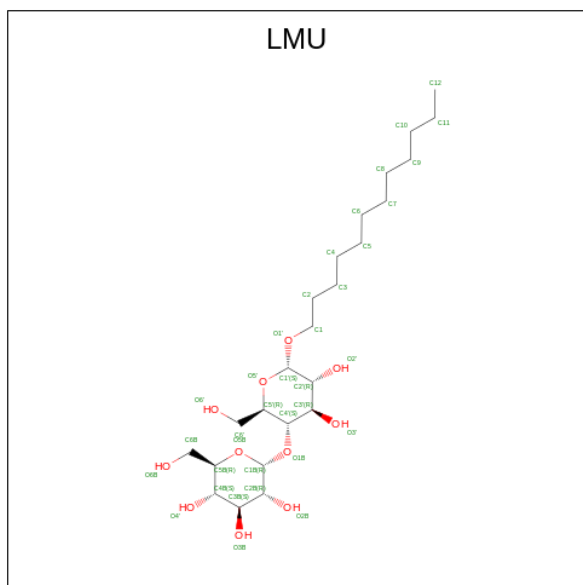
Mol	Chain	Residues	Atoms			AltConf
49	AA	1	Total	Fe	S	0
			8	4	4	
49	AC	1	Total	Fe	S	0
			8	4	4	
49	AC	1	Total	Fe	S	0
			8	4	4	
49	BA	1	Total	Fe	S	0
			8	4	4	
49	BC	1	Total	Fe	S	0
			8	4	4	
49	BC	1	Total	Fe	S	0
			8	4	4	
49	I	1	Total	Fe	S	0
			8	4	4	
49	I	1	Total	Fe	S	0
			8	4	4	

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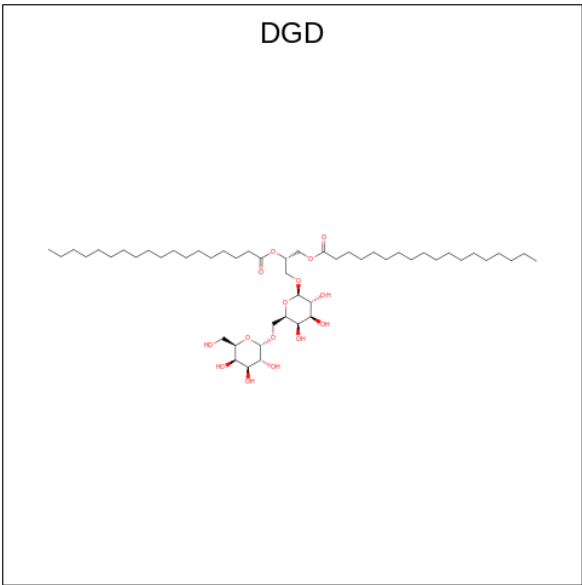
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
49	K	1	8	4	4	0

- Molecule 50 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



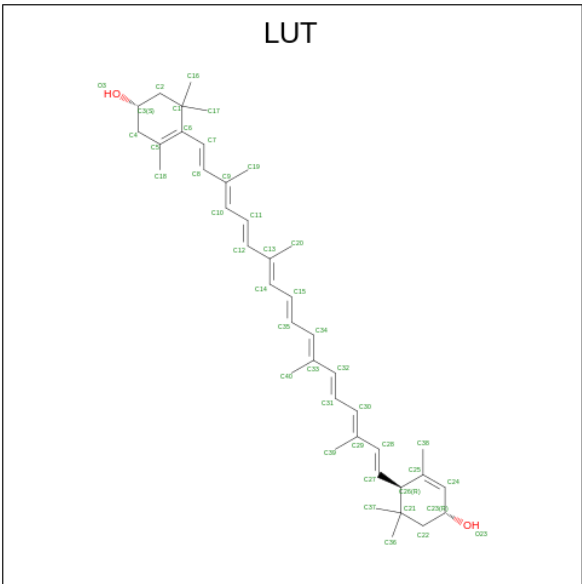
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	AA	1	35	24	11	0
50	AB	1	35	24	11	0
50	AB	1	35	24	11	0
50	AB	1	35	24	11	0
50	AL	1	34	23	11	0
50	BA	1	34	23	11	0
50	BA	1	33	22	11	0
50	BB	1	35	24	11	0

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



Mol	Chain	Residues	Atoms			AltConf
51	AB	1	Total	C	O	0
			66	51	15	
51	BB	1	Total	C	O	0
			66	51	15	

- Molecule 52 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



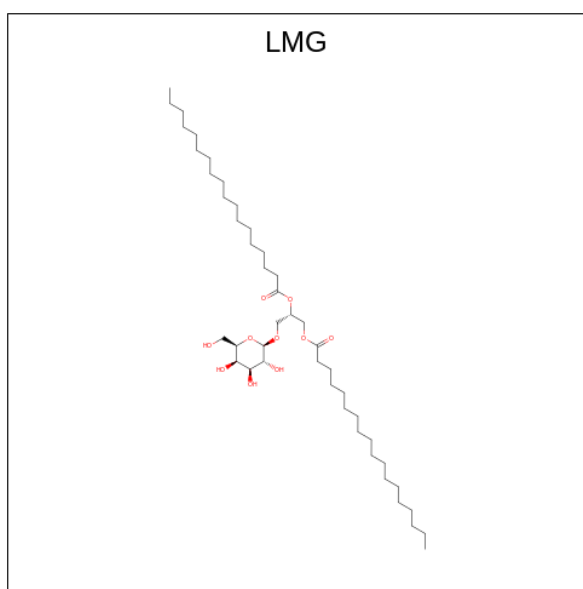
Mol	Chain	Residues	Atoms			AltConf
52	AF	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
52	A1	1	Total	C	O	0
			42	40	2	
52	A3	1	Total	C	O	0
			42	40	2	
52	A4	1	Total	C	O	0
			42	40	2	
52	A6	1	Total	C	O	0
			42	40	2	
52	B1	1	Total	C	O	0
			42	40	2	
52	B2	1	Total	C	O	0
			42	40	2	
52	B3	1	Total	C	O	0
			42	40	2	
52	B5	1	Total	C	O	0
			42	40	2	

- Molecule 53 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



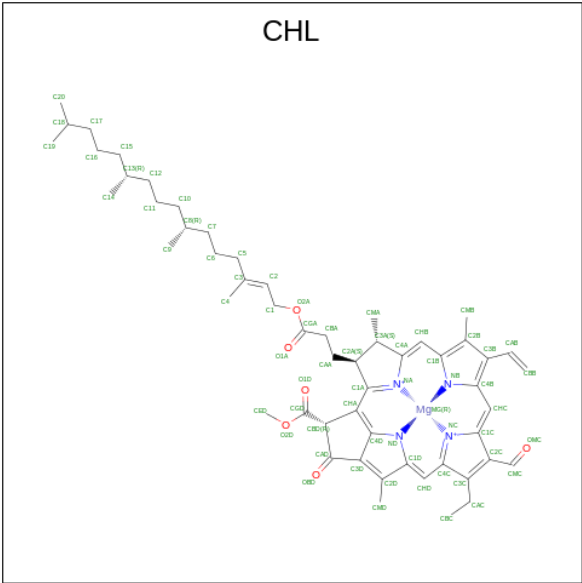
Mol	Chain	Residues	Atoms			AltConf
53	AG	1	Total	C	O	0
			38	28	10	
53	A1	1	Total	C	O	0
			44	34	10	
53	A4	1	Total	C	O	0
			39	29	10	

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Mol	Chain	Residues	Atoms			AltConf
53	B5	1	Total	C	O	0
			33	23	10	

- Molecule 54 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



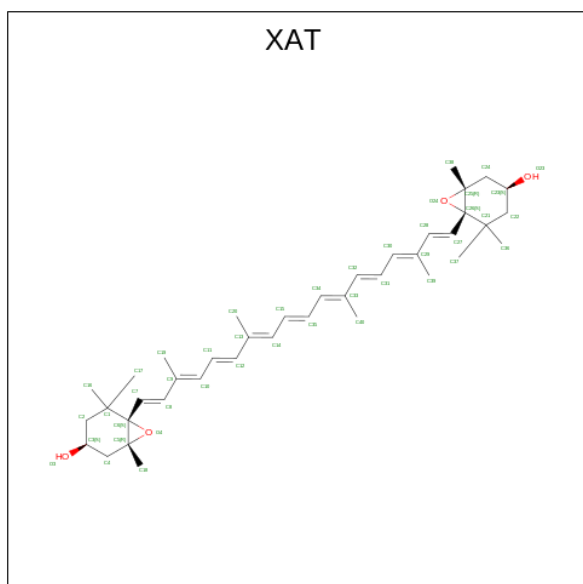
Mol	Chain	Residues	Atoms					AltConf
54	A1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
54	A1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
54	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
54	A4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
54	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A6	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
54	A6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
54	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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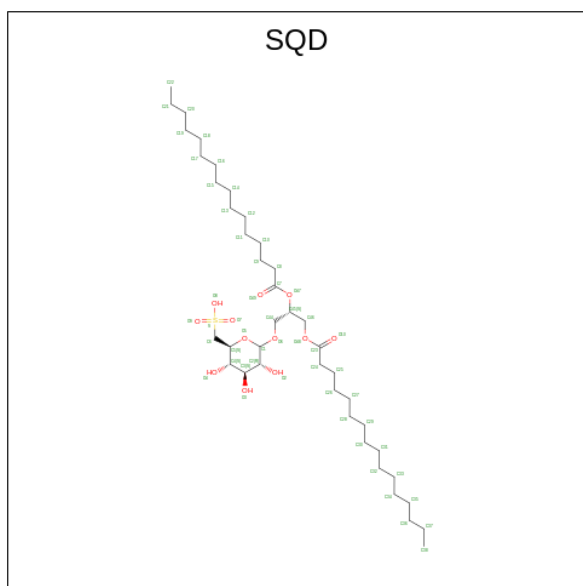
Mol	Chain	Residues	Atoms					AltConf
54	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
54	B1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
54	B1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
54	B2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
54	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
54	B5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	B5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
54	B5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

- Molecule 55 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



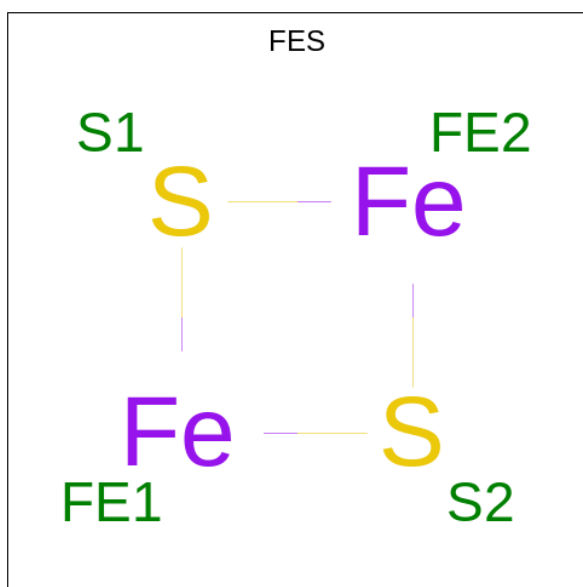
Mol	Chain	Residues	Atoms			AltConf
55	A1	1	Total	C	O	0
			44	40	4	
55	A3	1	Total	C	O	0
			44	40	4	
55	A4	1	Total	C	O	0
			44	40	4	
55	A6	1	Total	C	O	0
			44	40	4	
55	B1	1	Total	C	O	0
			44	40	4	
55	B2	1	Total	C	O	0
			44	40	4	
55	B3	1	Total	C	O	0
			44	40	4	
55	B5	1	Total	C	O	0
			44	40	4	

- Molecule 56 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
56	BJ	1	Total	C	O	S	0
			47	34	12	1	
56	e	1	Total	C	O	S	0
			34	21	12	1	

- Molecule 57 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
57	c	1	4	2	2	0

3 Residue-property plots [i](#)

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

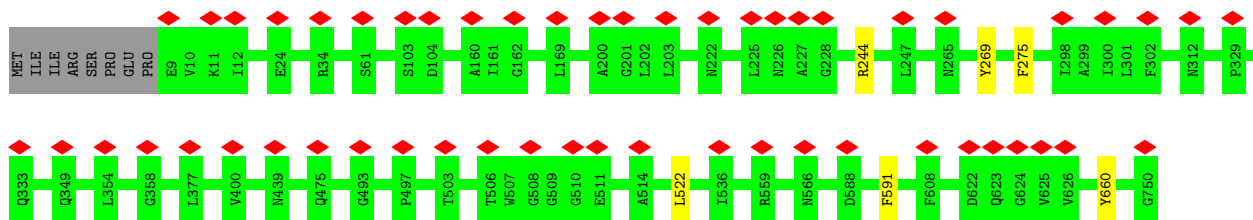
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain AA: 



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain BA: 



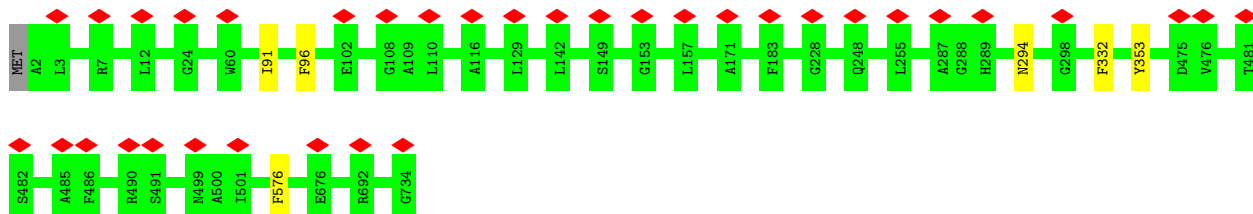
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain AB: 



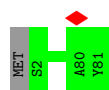
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain BB: 



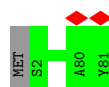
- Molecule 3: Photosystem I iron-sulfur center

Chain AC:  99%



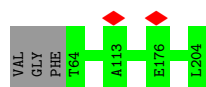
- Molecule 3: Photosystem I iron-sulfur center

Chain BC:  99%




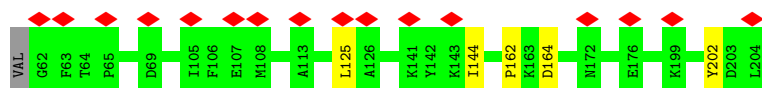
- Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain AD:  69% 31%



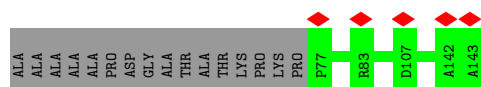
- Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain BD:  8% 68% 30%



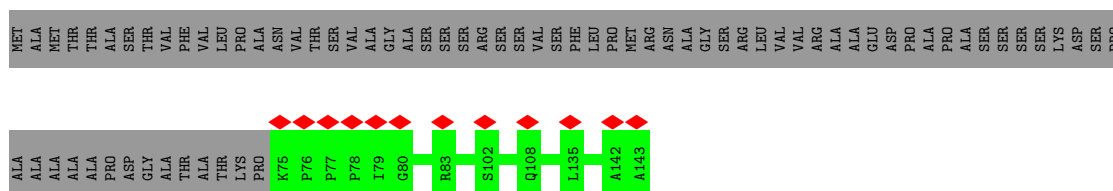
- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

Chain AE:  47% 53%

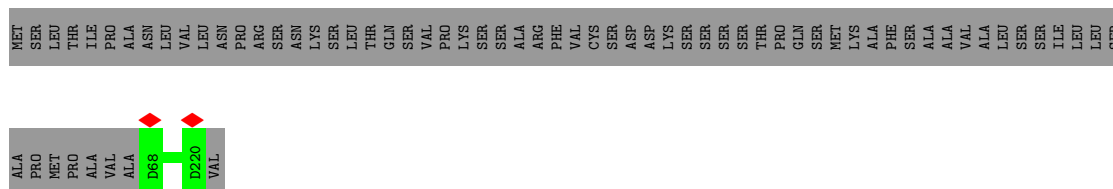


- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

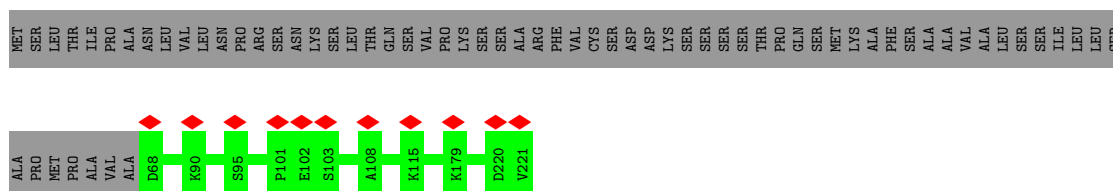
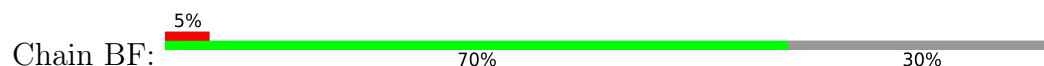
Chain BE:  8% 48% 52%



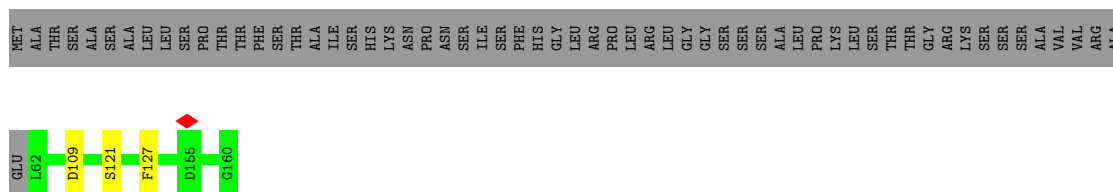
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



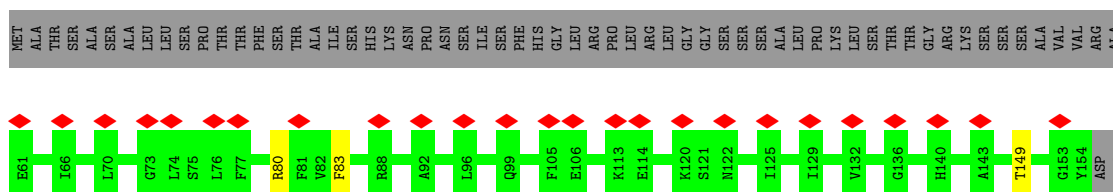
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



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

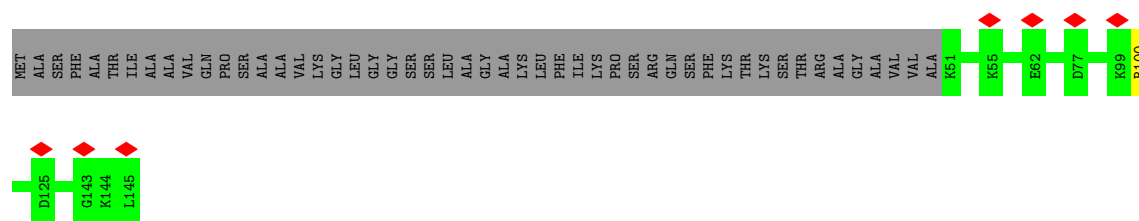


- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

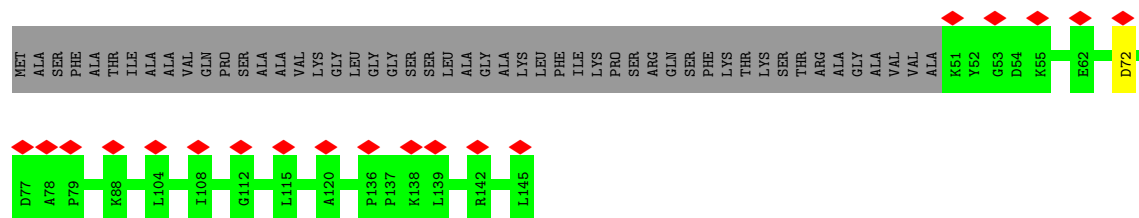


- Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic

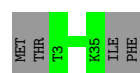
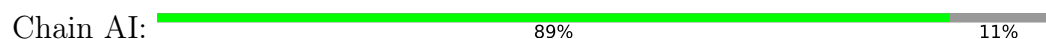




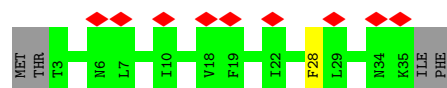
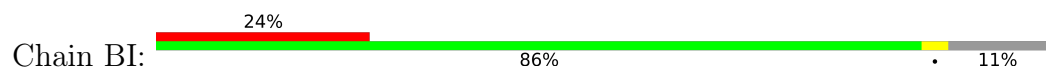
- Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic



- Molecule 9: Photosystem I reaction center subunit VIII



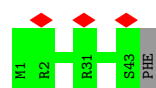
- Molecule 9: Photosystem I reaction center subunit VIII



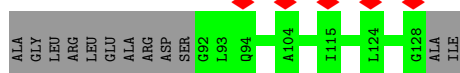
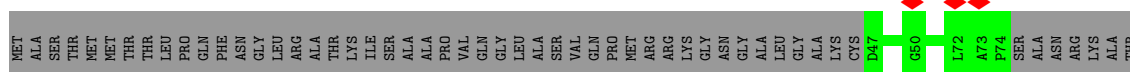
- Molecule 10: Photosystem I reaction center subunit IX



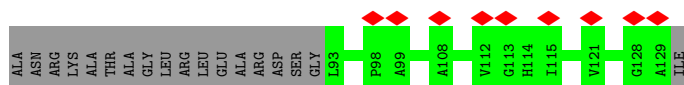
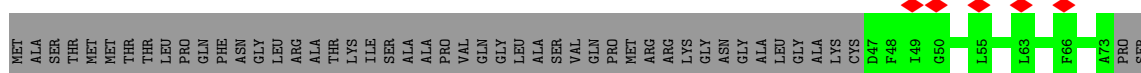
- Molecule 10: Photosystem I reaction center subunit IX



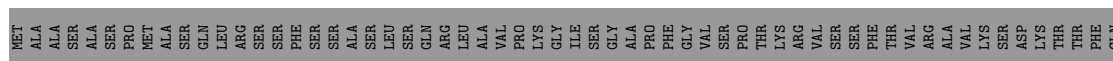
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



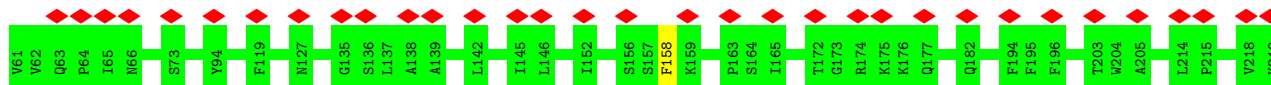
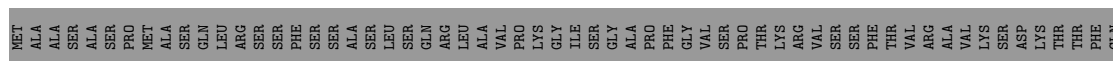
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



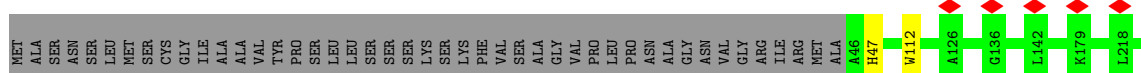
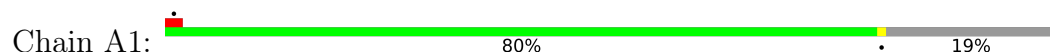
- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic



- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

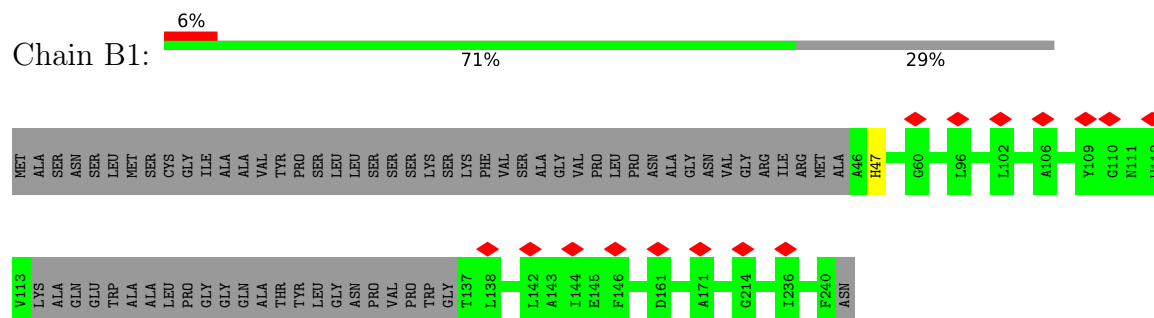


- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

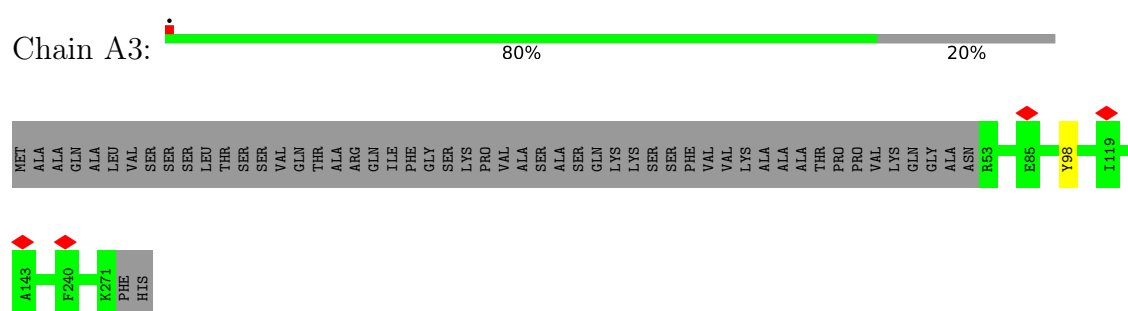




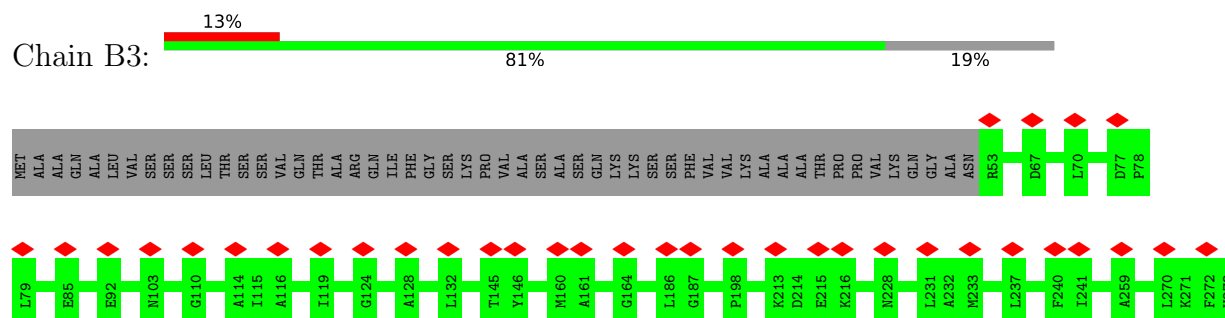
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



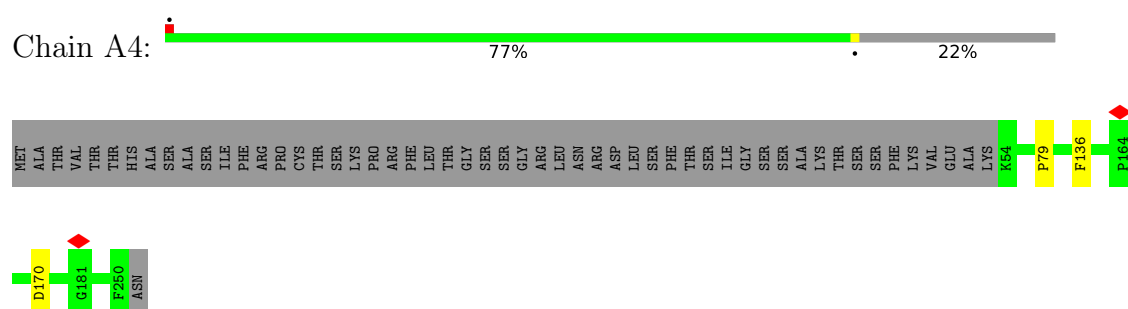
- Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic




- Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

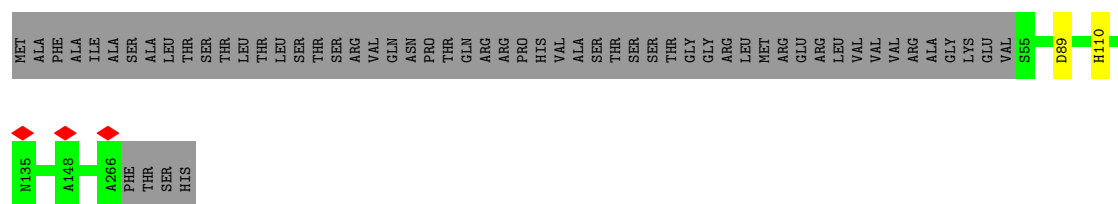


- Molecule 15: Chlorophyll a-b binding protein 4, chloroplastic




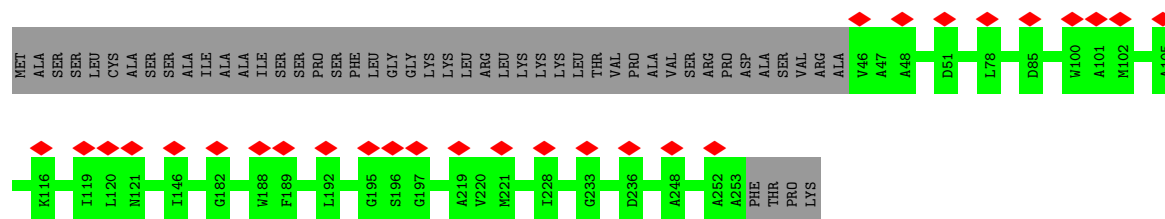
- Molecule 16: Photosystem I chlorophyll a/b-binding protein 6, chloroplastic

Chain A6:  78% 21%




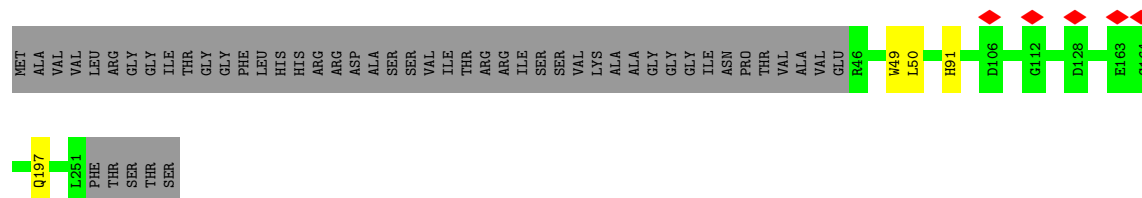
- Molecule 17: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

Chain B2:  11% 81% 19%




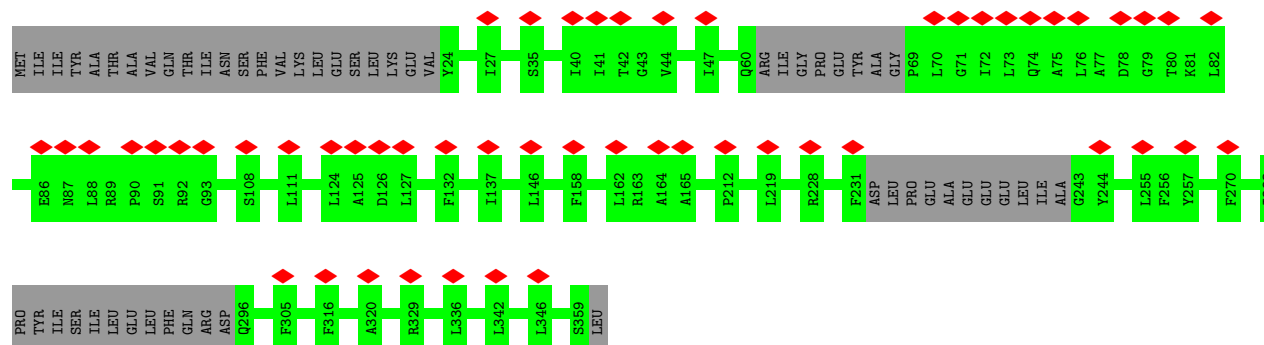
- Molecule 18: Photosystem I chlorophyll a/b-binding protein 5, chloroplastic

Chain B5:  79% 20%



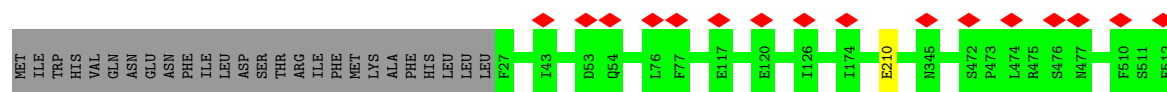
- Molecule 19: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic

Chain A:  15% 85% 15%

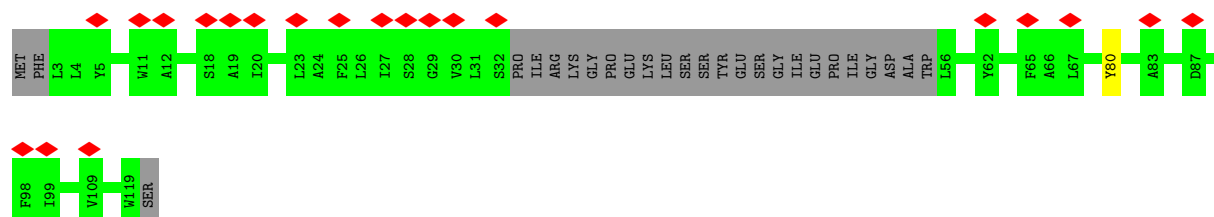
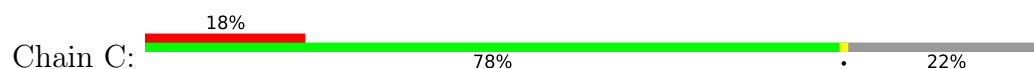


- Molecule 20: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic

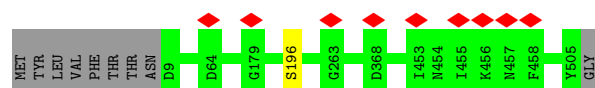
Chain B:  95% 5%



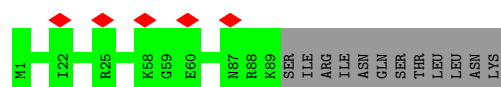
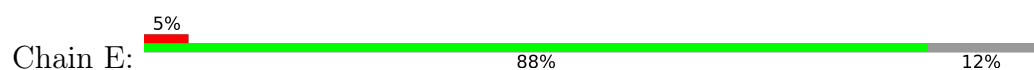
- Molecule 21: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic



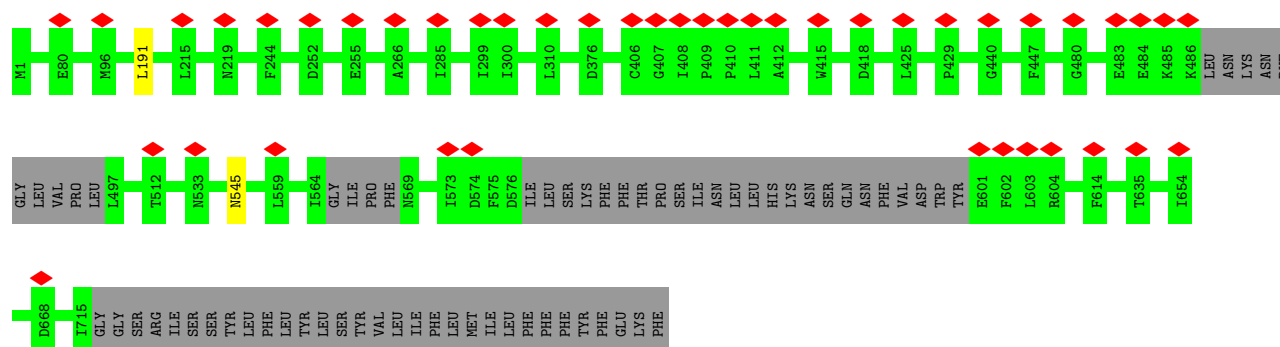
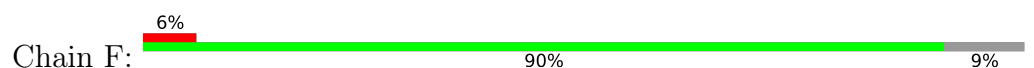
- Molecule 22: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic



- Molecule 23: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic

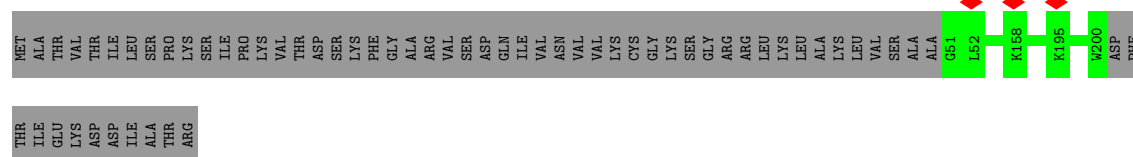


- Molecule 24: NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic

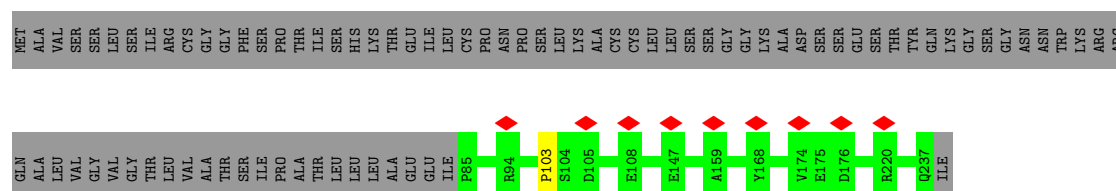


- Molecule 25: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic

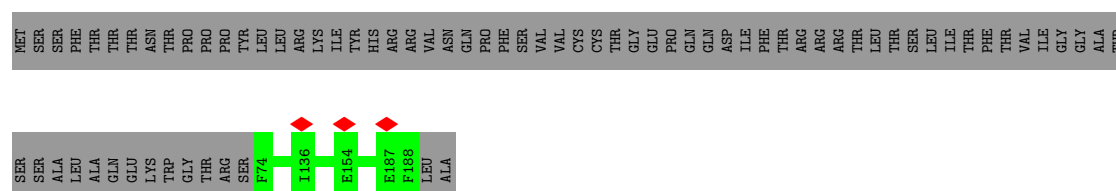




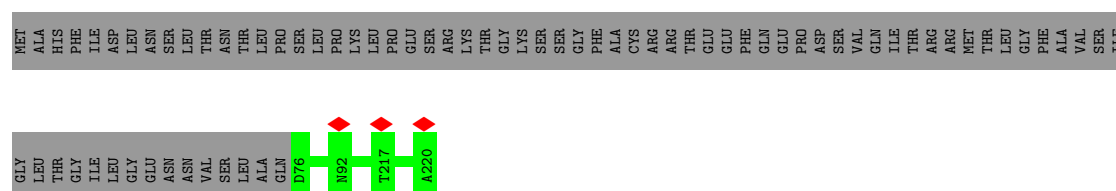
- Molecule 31: Photosynthetic NDH subunit of luminal location 1, chloroplastic



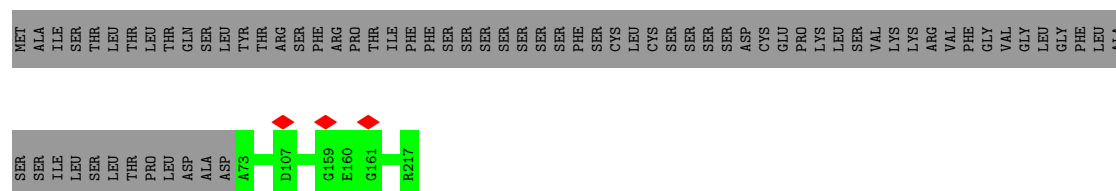
- Molecule 32: Photosynthetic NDH subunit of luminal location 2, chloroplastic



- Molecule 33: Photosynthetic NDH subunit of luminal location 3, chloroplastic

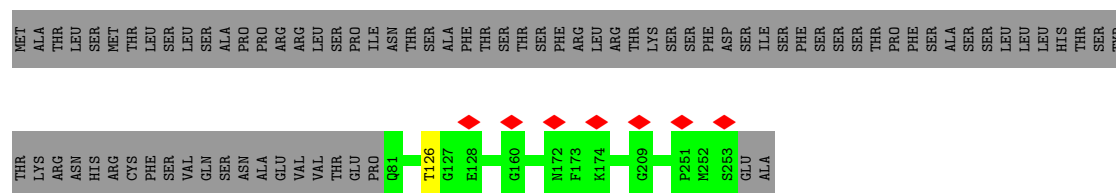


- Molecule 34: Photosynthetic NDH subunit of luminal location 4, chloroplastic

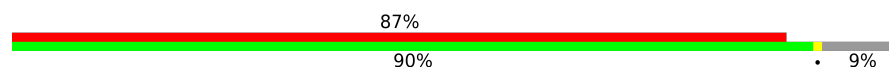


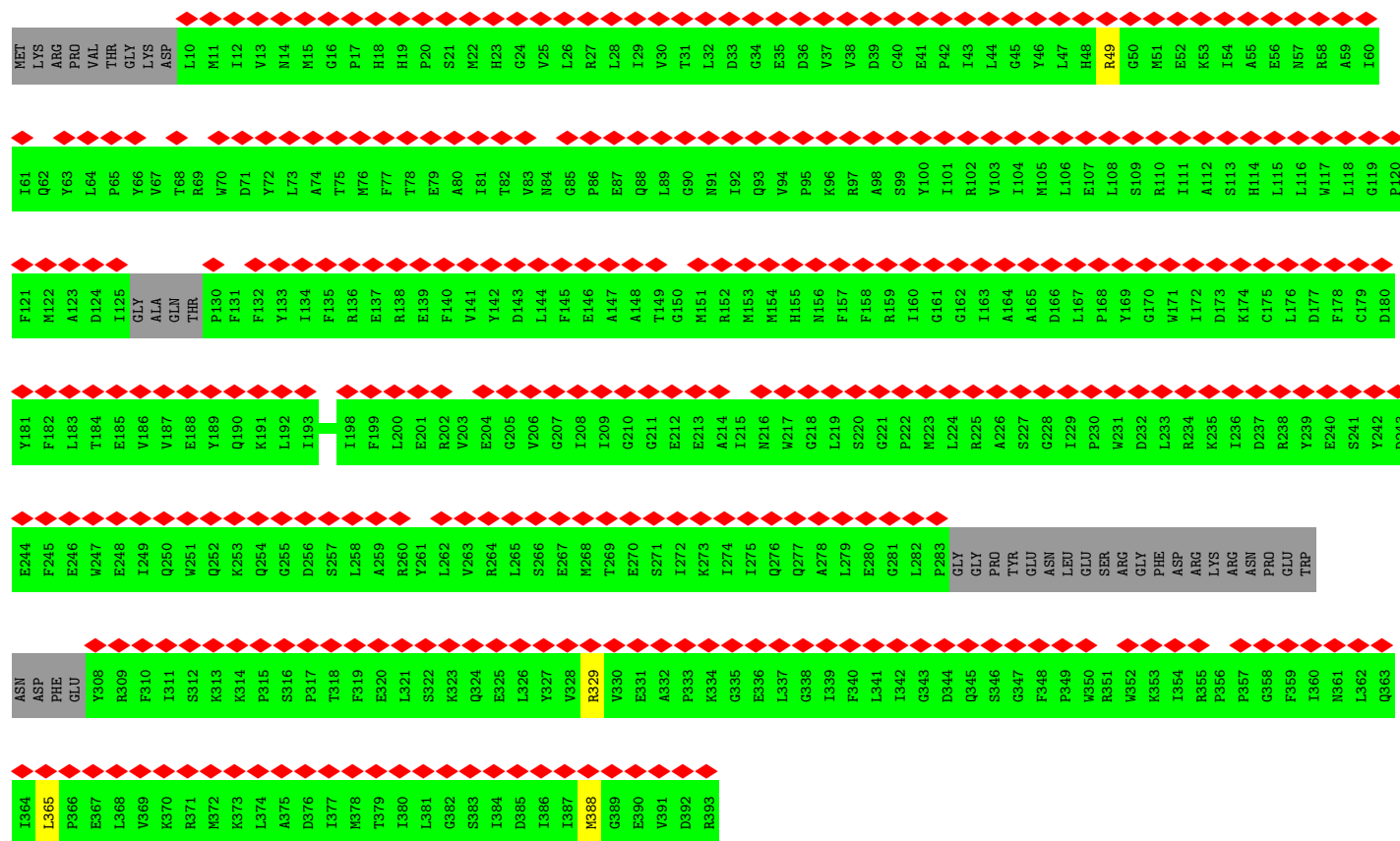
- Molecule 35: Isoform 2 of Photosynthetic NDH subunit of luminal location 5, chloroplastic

Chain j:  67% 32%

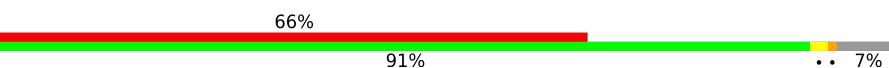


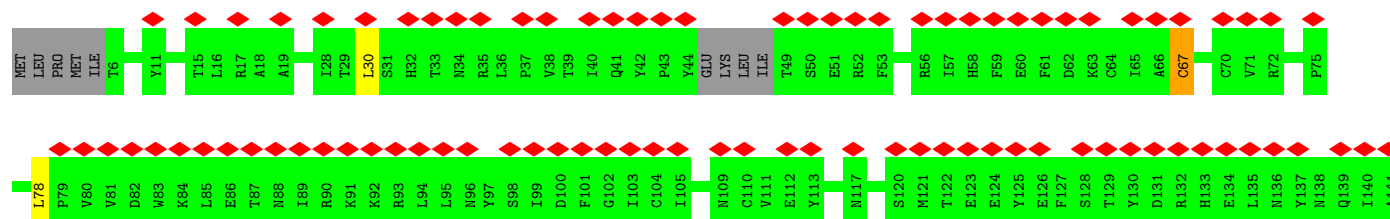
• Molecule 36: NAD(P)H-quinone oxidoreductase subunit H, chloroplastic

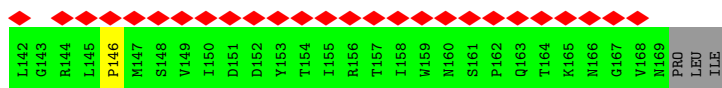
Chain H:  87% 90% 9%



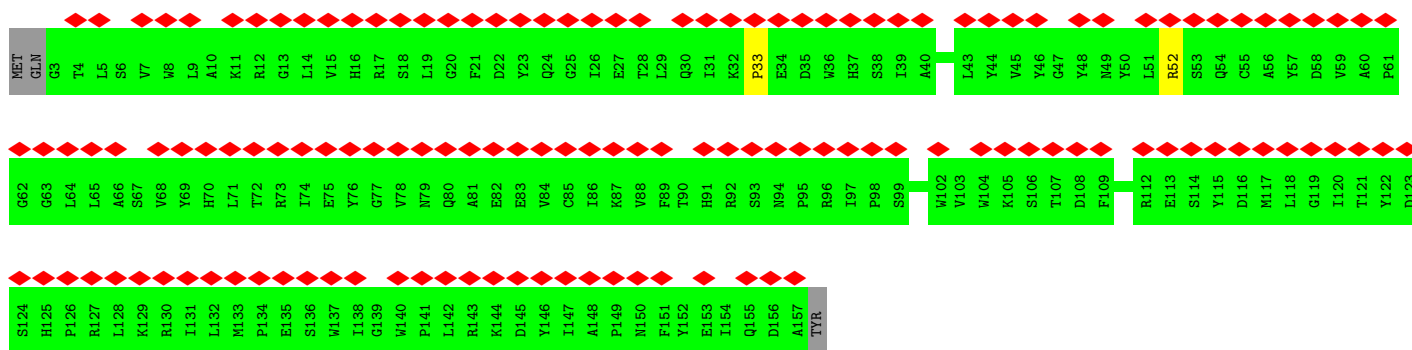
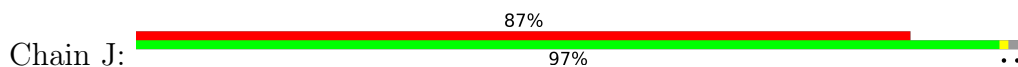
• Molecule 37: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic

Chain I:  66% 91% 7%

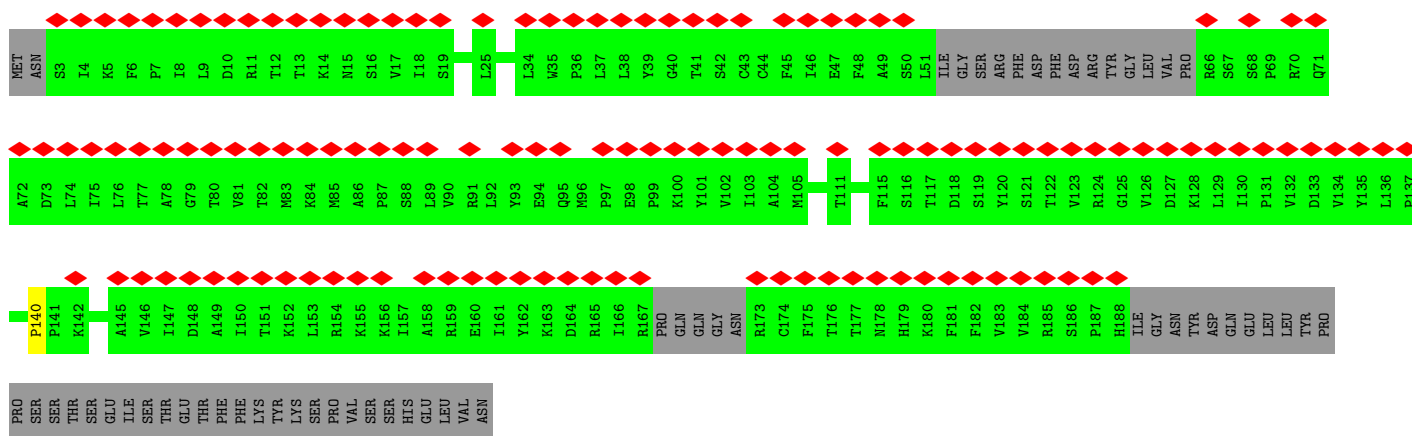
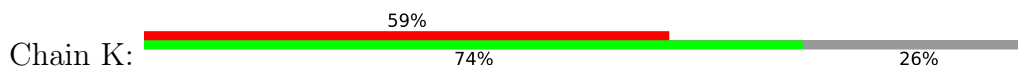




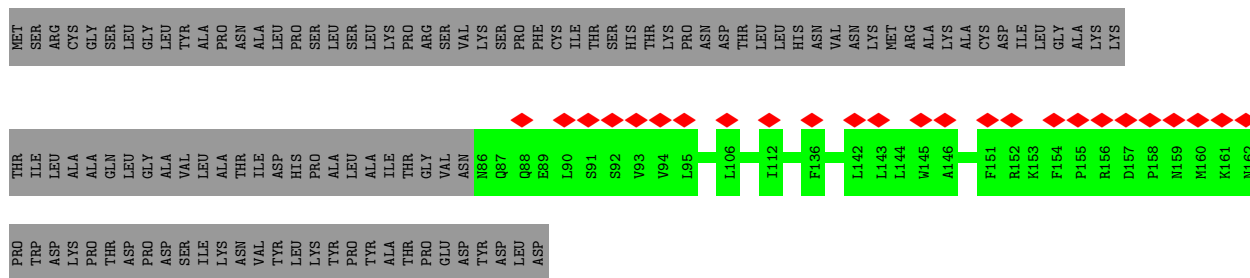
- Molecule 38: NAD(P)H-quinone oxidoreductase subunit J, chloroplastic



- Molecule 39: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic



- Molecule 40: NAD(P)H-quinone oxidoreductase subunit L, chloroplastic



- Molecule 41: NAD(P)H-quinone oxidoreductase subunit M, chloroplastic

X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	X21	X22	X23	X24	X25	X26	X27	X28	X29	X30	X31	X32	X33	X34	X35	X36	X37	X38	X39	X40	X41	X42	X43	X44	X45	X46	X47	X48	X49	X50	X51	X52	X53	X54	X55	X56	X57	X58	X59	X60
X61	X62	X63	X64	X65	X66	X67	X68	X69	X70	X71	X72	X73	X74	X75	X76	X77	X78	X79	X80	X81	X82	X83	X84	X85	X86	X87	X88	X89	X90	X91	X92	X93	X94	X95	X96	X97	X103	X110	X111	X112	X113	X114	X120	X121	X122														

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.37	0/6037	0.53	0/8236
1	BA	0.36	0/6039	0.54	0/8239
2	AB	0.36	0/6073	0.53	0/8291
2	BB	0.37	0/6065	0.54	0/8281
3	AC	0.37	0/628	0.61	0/852
3	BC	0.38	0/628	0.60	0/852
4	AD	0.31	0/1140	0.58	0/1542
4	BD	0.34	0/1156	0.61	0/1563
5	AE	0.32	0/542	0.50	0/736
5	BE	0.30	0/559	0.50	0/760
6	AF	0.31	0/1243	0.53	0/1677
6	BF	0.31	0/1250	0.55	0/1687
7	AG	0.37	0/791	0.51	0/1072
7	BG	0.32	0/750	0.50	0/1016
8	AH	0.30	0/751	0.52	0/1018
8	BH	0.31	0/751	0.52	0/1018
9	AI	0.30	0/264	0.45	0/359
9	BI	0.37	0/264	0.56	0/359
10	AJ	0.37	0/348	0.58	0/474
10	BJ	0.33	0/354	0.67	0/482
11	AK	0.31	0/456	0.53	0/617
11	BK	0.35	0/449	0.60	0/607
12	AL	0.31	0/1208	0.52	0/1650
12	BL	0.33	0/1218	0.53	0/1663
13	A1	0.31	0/1562	0.51	0/2131
13	B1	0.29	0/1381	0.51	0/1879
14	A3	0.31	0/1726	0.51	0/2347
14	B3	0.31	0/1749	0.51	0/2378
15	A4	0.33	0/1611	0.52	0/2194
16	A6	0.32	0/1732	0.55	0/2363
17	B2	0.29	0/1663	0.53	0/2277
18	B5	0.30	0/1646	0.54	0/2239

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	A	0.31	0/2430	0.60	0/3312
20	B	0.37	0/3872	0.62	0/5263
21	C	0.38	0/802	0.56	0/1094
22	D	0.41	0/4058	0.63	0/5509
23	E	0.33	0/705	0.56	0/952
24	F	0.36	0/5478	0.58	0/7446
25	G	0.31	0/1307	0.62	0/1785
26	a	0.37	0/2708	0.62	0/3668
27	b	0.31	0/2417	0.57	0/3265
28	c	0.33	0/1030	0.62	0/1401
29	d	0.41	0/784	0.59	0/1057
30	e	0.34	0/1241	0.59	0/1685
31	f	0.30	0/1312	0.57	0/1777
32	g	0.28	0/986	0.51	0/1329
33	h	0.32	0/1193	0.59	0/1610
34	i	0.32	0/1124	0.56	0/1523
35	j	0.32	0/1357	0.57	0/1823
36	H	0.28	0/2877	0.55	0/3894
37	I	0.32	0/1256	0.57	0/1701
38	J	0.26	0/1142	0.50	0/1545
39	K	0.32	0/1222	0.57	0/1656
40	L	0.32	0/669	0.58	0/911
41	M	0.34	0/783	0.56	0/1062
42	N	0.41	0/921	0.53	0/1252
43	O	0.35	0/525	0.51	0/705
All	All	0.34	0/94233	0.56	0/128084

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	AA	740/750 (99%)	686 (93%)	53 (7%)	1 (0%)	48	80
1	BA	740/750 (99%)	692 (94%)	48 (6%)	0	100	100
2	AB	732/734 (100%)	695 (95%)	37 (5%)	0	100	100
2	BB	731/734 (100%)	696 (95%)	35 (5%)	0	100	100
3	AC	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
3	BC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	AD	139/204 (68%)	126 (91%)	13 (9%)	0	100	100
4	BD	141/204 (69%)	121 (86%)	18 (13%)	2 (1%)	9	39
5	AE	65/143 (46%)	58 (89%)	7 (11%)	0	100	100
5	BE	67/143 (47%)	61 (91%)	6 (9%)	0	100	100
6	AF	151/221 (68%)	144 (95%)	7 (5%)	0	100	100
6	BF	152/221 (69%)	149 (98%)	3 (2%)	0	100	100
7	AG	97/160 (61%)	90 (93%)	7 (7%)	0	100	100
7	BG	92/160 (58%)	84 (91%)	8 (9%)	0	100	100
8	AH	93/145 (64%)	89 (96%)	4 (4%)	0	100	100
8	BH	93/145 (64%)	87 (94%)	6 (6%)	0	100	100
9	AI	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
9	BI	31/37 (84%)	29 (94%)	2 (6%)	0	100	100
10	AJ	40/44 (91%)	38 (95%)	2 (5%)	0	100	100
10	BJ	41/44 (93%)	38 (93%)	3 (7%)	0	100	100
11	AK	61/130 (47%)	57 (93%)	4 (7%)	0	100	100
11	BK	60/130 (46%)	53 (88%)	7 (12%)	0	100	100
12	AL	155/219 (71%)	145 (94%)	10 (6%)	0	100	100
12	BL	157/219 (72%)	149 (95%)	8 (5%)	0	100	100
13	A1	194/241 (80%)	178 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	B1	168/241 (70%)	160 (95%)	8 (5%)	0	100	100
14	A3	217/273 (80%)	192 (88%)	25 (12%)	0	100	100
14	B3	219/273 (80%)	206 (94%)	13 (6%)	0	100	100
15	A4	195/251 (78%)	185 (95%)	10 (5%)	0	100	100
16	A6	210/270 (78%)	197 (94%)	13 (6%)	0	100	100
17	B2	206/257 (80%)	191 (93%)	15 (7%)	0	100	100
18	B5	204/256 (80%)	188 (92%)	15 (7%)	1 (0%)	25	60
19	A	297/360 (82%)	279 (94%)	18 (6%)	0	100	100
20	B	484/512 (94%)	443 (92%)	40 (8%)	1 (0%)	44	75
21	C	90/120 (75%)	87 (97%)	3 (3%)	0	100	100
22	D	495/506 (98%)	453 (92%)	42 (8%)	0	100	100
23	E	87/101 (86%)	79 (91%)	8 (9%)	0	100	100
24	F	669/746 (90%)	614 (92%)	55 (8%)	0	100	100
25	G	163/176 (93%)	151 (93%)	12 (7%)	0	100	100
26	a	339/461 (74%)	277 (82%)	61 (18%)	1 (0%)	37	70
27	b	301/348 (86%)	267 (89%)	34 (11%)	0	100	100
28	c	126/204 (62%)	109 (86%)	17 (14%)	0	100	100
29	d	91/161 (56%)	78 (86%)	13 (14%)	0	100	100
30	e	148/212 (70%)	122 (82%)	26 (18%)	0	100	100
31	f	151/238 (63%)	132 (87%)	18 (12%)	1 (1%)	19	54
32	g	113/190 (60%)	113 (100%)	0	0	100	100
33	h	143/220 (65%)	130 (91%)	13 (9%)	0	100	100
34	i	143/217 (66%)	125 (87%)	18 (13%)	0	100	100
35	j	171/255 (67%)	150 (88%)	21 (12%)	0	100	100
36	H	350/393 (89%)	315 (90%)	35 (10%)	0	100	100
37	I	156/172 (91%)	132 (85%)	22 (14%)	2 (1%)	10	41
38	J	153/158 (97%)	134 (88%)	19 (12%)	0	100	100
39	K	161/225 (72%)	137 (85%)	23 (14%)	1 (1%)	22	57
40	L	75/191 (39%)	67 (89%)	8 (11%)	0	100	100
41	M	106/217 (49%)	94 (89%)	12 (11%)	0	100	100
42	N	144/209 (69%)	128 (89%)	15 (10%)	1 (1%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	O	69/158 (44%)	62 (90%)	7 (10%)	0	100	100
All	All	11603/14548 (80%)	10637 (92%)	955 (8%)	11 (0%)	50	80

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	BD	164	ASP
39	K	140	PRO
26	a	230	ASN
42	N	166	LYS
18	B5	49	TRP

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	AA	600/610 (98%)	591 (98%)	9 (2%)	60	74
1	BA	601/610 (98%)	595 (99%)	6 (1%)	73	81
2	AB	598/600 (100%)	591 (99%)	7 (1%)	67	78
2	BB	597/600 (100%)	591 (99%)	6 (1%)	73	81
3	AC	70/71 (99%)	70 (100%)	0	100	100
3	BC	70/71 (99%)	70 (100%)	0	100	100
4	AD	120/170 (71%)	120 (100%)	0	100	100
4	BD	121/170 (71%)	118 (98%)	3 (2%)	42	62
5	AE	56/114 (49%)	56 (100%)	0	100	100
5	BE	58/114 (51%)	58 (100%)	0	100	100
6	AF	125/185 (68%)	125 (100%)	0	100	100
6	BF	126/185 (68%)	126 (100%)	0	100	100
7	AG	83/133 (62%)	80 (96%)	3 (4%)	30	54
7	BG	79/133 (59%)	76 (96%)	3 (4%)	28	52
8	AH	77/113 (68%)	76 (99%)	1 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BH	77/113 (68%)	76 (99%)	1 (1%)	65	76
9	AI	29/33 (88%)	29 (100%)	0	100	100
9	BI	29/33 (88%)	28 (97%)	1 (3%)	32	55
10	AJ	37/39 (95%)	37 (100%)	0	100	100
10	BJ	38/39 (97%)	38 (100%)	0	100	100
11	AK	47/95 (50%)	47 (100%)	0	100	100
11	BK	46/95 (48%)	46 (100%)	0	100	100
12	AL	119/174 (68%)	116 (98%)	3 (2%)	42	62
12	BL	120/174 (69%)	119 (99%)	1 (1%)	79	84
13	A1	151/190 (80%)	149 (99%)	2 (1%)	65	76
13	B1	138/190 (73%)	137 (99%)	1 (1%)	81	86
14	A3	168/211 (80%)	167 (99%)	1 (1%)	84	88
14	B3	170/211 (81%)	170 (100%)	0	100	100
15	A4	164/210 (78%)	161 (98%)	3 (2%)	54	71
16	A6	177/226 (78%)	175 (99%)	2 (1%)	70	79
17	B2	165/205 (80%)	165 (100%)	0	100	100
18	B5	166/205 (81%)	163 (98%)	3 (2%)	54	71
19	A	258/312 (83%)	258 (100%)	0	100	100
20	B	420/446 (94%)	420 (100%)	0	100	100
21	C	78/103 (76%)	77 (99%)	1 (1%)	65	76
22	D	430/439 (98%)	429 (100%)	1 (0%)	92	94
23	E	75/87 (86%)	75 (100%)	0	100	100
24	F	561/661 (85%)	559 (100%)	2 (0%)	89	91
25	G	145/154 (94%)	145 (100%)	0	100	100
26	a	288/397 (72%)	286 (99%)	2 (1%)	81	86
27	b	263/297 (89%)	262 (100%)	1 (0%)	89	91
28	c	112/177 (63%)	112 (100%)	0	100	100
29	d	81/143 (57%)	81 (100%)	0	100	100
30	e	125/178 (70%)	125 (100%)	0	100	100
31	f	134/207 (65%)	134 (100%)	0	100	100
32	g	104/172 (60%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	h	127/192 (66%)	127 (100%)	0	100	100
34	i	114/180 (63%)	114 (100%)	0	100	100
35	j	143/219 (65%)	142 (99%)	1 (1%)	81	86
36	H	291/342 (85%)	287 (99%)	4 (1%)	62	75
37	I	132/159 (83%)	129 (98%)	3 (2%)	45	64
38	J	87/140 (62%)	85 (98%)	2 (2%)	45	64
39	K	114/205 (56%)	114 (100%)	0	100	100
40	L	66/171 (39%)	66 (100%)	0	100	100
41	M	58/195 (30%)	57 (98%)	1 (2%)	56	72
42	N	49/174 (28%)	48 (98%)	1 (2%)	50	68
43	O	36/138 (26%)	36 (100%)	0	100	100
All	All	9513/12210 (78%)	9438 (99%)	75 (1%)	77	84

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	D	196	SER
38	J	33	PRO
24	F	545	ASN
36	H	329	ARG
13	A1	112	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
30	e	193	ASN
31	f	179	ASN
34	i	198	ASN
13	B1	208	GLN
11	BK	94	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

423 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	$\# Z > 2$
45	CLA	AA	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	9 (11%)
45	CLA	BA	844	47	41,49,73	1.90	5 (12%)	47,84,113	1.43	8 (17%)
45	CLA	B1	313	13	45,53,73	1.78	7 (15%)	52,89,113	1.51	6 (11%)
54	CHL	A3	307	-	45,53,74	2.29	16 (35%)	52,89,114	2.69	21 (40%)
45	CLA	AB	801	-	65,73,73	1.47	9 (13%)	76,113,113	1.59	14 (18%)
48	BCR	AJ	101	-	41,41,41	0.89	1 (2%)	56,56,56	1.98	16 (28%)
45	CLA	AB	833	-	65,73,73	1.49	9 (13%)	76,113,113	1.18	7 (9%)
54	CHL	A4	305	-	41,49,74	2.25	13 (31%)	51,84,114	2.78	20 (39%)
48	BCR	BA	856	-	41,41,41	0.93	1 (2%)	56,56,56	2.15	17 (30%)
45	CLA	A1	307	-	39,48,73	1.89	9 (23%)	45,82,113	1.74	11 (24%)
45	CLA	A1	312	47	37,46,73	2.01	7 (18%)	46,81,113	1.43	10 (21%)
45	CLA	AA	834	-	65,73,73	1.47	10 (15%)	76,113,113	1.48	14 (18%)
45	CLA	BA	827	-	65,73,73	1.47	6 (9%)	76,113,113	1.23	7 (9%)
45	CLA	AL	303	12	41,49,73	1.91	7 (17%)	47,84,113	1.46	8 (17%)
48	BCR	BB	848	-	41,41,41	0.81	0	56,56,56	2.15	19 (33%)
45	CLA	A3	304	-	41,50,73	1.94	7 (17%)	51,86,113	1.50	9 (17%)
45	CLA	BB	836	-	60,68,73	1.56	8 (13%)	70,107,113	1.38	7 (10%)
52	LUT	A3	316	-	42,43,43	0.84	0	51,60,60	1.78	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	LHG	A1	320	45	48,48,48	0.93	2 (4%)	51,54,54	0.84	2 (3%)
48	BCR	BA	855	-	41,41,41	0.77	0	56,56,56	2.19	24 (42%)
47	LHG	AJ	104	-	39,39,48	1.06	2 (5%)	42,45,54	0.92	2 (4%)
57	FES	c	301	28	0,4,4	-	-	-	-	-
54	CHL	A6	602	16	51,60,74	2.24	18 (35%)	54,97,114	2.65	26 (48%)
48	BCR	AJ	103	-	41,41,41	0.74	0	56,56,56	2.38	22 (39%)
45	CLA	A4	308	15	54,62,73	1.67	8 (14%)	62,99,113	1.29	9 (14%)
45	CLA	BB	804	-	65,73,73	1.49	9 (13%)	76,113,113	1.27	8 (10%)
45	CLA	AB	832	-	65,73,73	1.50	10 (15%)	76,113,113	1.30	9 (11%)
45	CLA	BA	837	-	51,59,73	1.63	8 (15%)	59,96,113	1.47	7 (11%)
55	XAT	B5	615	-	39,47,47	0.99	2 (5%)	54,74,74	2.41	18 (33%)
45	CLA	BB	816	-	64,72,73	1.51	9 (14%)	75,112,113	1.35	8 (10%)
52	LUT	B2	615	-	42,43,43	0.81	0	51,60,60	1.98	15 (29%)
45	CLA	BB	812	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	10 (13%)
45	CLA	BA	835	-	45,53,73	1.81	7 (15%)	52,89,113	1.43	6 (11%)
45	CLA	AB	805	-	41,49,73	1.81	6 (14%)	47,84,113	1.55	8 (17%)
45	CLA	AA	824	-	53,62,73	1.68	8 (15%)	61,100,113	1.50	11 (18%)
45	CLA	BA	817	-	60,68,73	1.52	6 (10%)	70,107,113	1.37	11 (15%)
48	BCR	AL	302	-	41,41,41	0.78	0	56,56,56	2.22	22 (39%)
45	CLA	B5	613	-	45,53,73	1.80	7 (15%)	52,89,113	1.37	7 (13%)
45	CLA	AB	836	-	42,50,73	1.86	7 (16%)	48,85,113	1.52	7 (14%)
45	CLA	AJ	102	10	42,50,73	1.84	5 (11%)	48,85,113	1.48	7 (14%)
47	LHG	B1	318	45	41,41,48	1.01	2 (4%)	44,47,54	0.95	2 (4%)
45	CLA	A1	314	-	63,72,73	1.52	8 (12%)	73,112,113	1.30	9 (12%)
45	CLA	BA	832	-	56,64,73	1.59	8 (14%)	65,102,113	1.31	8 (12%)
47	LHG	B1	301	45	37,37,48	1.08	2 (5%)	40,43,54	1.01	3 (7%)
45	CLA	A6	610	16	55,63,73	1.67	9 (16%)	64,101,113	1.33	10 (15%)
49	SF4	K	301	39	0,12,12	-	-	-	-	-
48	BCR	BB	847	-	41,41,41	0.87	1 (2%)	56,56,56	1.93	11 (19%)
45	CLA	A3	309	14	41,49,73	1.88	8 (19%)	47,84,113	1.49	10 (21%)
45	CLA	B5	609	18	54,62,73	1.67	9 (16%)	62,99,113	1.26	8 (12%)
45	CLA	BB	838	-	50,58,73	1.67	7 (14%)	58,95,113	1.50	9 (15%)
45	CLA	BB	839	-	65,73,73	1.49	8 (12%)	76,113,113	1.28	6 (7%)
45	CLA	BA	830	-	65,73,73	1.53	9 (13%)	76,113,113	1.23	8 (10%)
48	BCR	AF	801	-	41,41,41	0.86	1 (2%)	56,56,56	1.56	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	AA	816	-	45,53,73	1.82	9 (20%)	52,89,113	1.58	9 (17%)
45	CLA	BA	838	-	55,62,73	1.69	8 (14%)	59,99,113	1.45	11 (18%)
45	CLA	AA	804	-	52,60,73	1.65	8 (15%)	60,97,113	1.54	7 (11%)
45	CLA	A3	305	-	40,49,73	1.90	7 (17%)	45,84,113	1.45	7 (15%)
45	CLA	B3	304	-	40,49,73	1.91	7 (17%)	45,84,113	1.44	7 (15%)
47	LHG	A1	302	-	35,35,48	1.10	2 (5%)	38,41,54	1.04	2 (5%)
45	CLA	B2	609	17	55,63,73	1.66	8 (14%)	64,101,113	1.34	10 (15%)
48	BCR	B5	616	-	41,41,41	0.79	0	56,56,56	2.31	23 (41%)
45	CLA	AB	828	-	65,73,73	1.46	8 (12%)	76,113,113	1.43	8 (10%)
45	CLA	B3	308	14	41,49,73	1.85	8 (19%)	47,84,113	1.45	7 (14%)
45	CLA	AA	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.40	12 (15%)
45	CLA	BB	821	-	55,63,73	1.64	8 (14%)	64,101,113	1.14	5 (7%)
48	BCR	BA	850	-	41,41,41	0.78	0	56,56,56	2.09	11 (19%)
45	CLA	AB	817	-	55,63,73	1.63	8 (14%)	64,101,113	1.34	7 (10%)
45	CLA	A3	311	14	43,51,73	1.82	5 (11%)	49,86,113	1.48	7 (14%)
48	BCR	AB	846	-	41,41,41	0.86	0	56,56,56	2.07	16 (28%)
45	CLA	AA	814	-	45,53,73	1.81	9 (20%)	52,89,113	1.45	8 (15%)
45	CLA	BB	819	-	59,67,73	1.57	9 (15%)	68,105,113	1.40	9 (13%)
45	CLA	B5	612	18	57,65,73	1.62	8 (14%)	66,103,113	1.28	7 (10%)
54	CHL	B5	606	-	40,48,74	2.31	13 (32%)	50,83,114	2.83	21 (42%)
45	CLA	BB	828	-	62,70,73	1.51	7 (11%)	72,109,113	1.48	11 (15%)
45	CLA	AA	821	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	9 (11%)
52	LUT	B3	315	-	42,43,43	0.97	1 (2%)	51,60,60	2.10	17 (33%)
45	CLA	BF	303	-	41,49,73	1.86	6 (14%)	47,84,113	1.47	8 (17%)
53	LMG	AG	202	-	38,38,55	1.14	3 (7%)	46,46,63	1.07	2 (4%)
45	CLA	AA	819	-	65,73,73	1.48	10 (15%)	76,113,113	1.43	9 (11%)
45	CLA	BK	203	-	46,54,73	1.73	6 (13%)	53,90,113	1.54	6 (11%)
45	CLA	AA	838	-	55,63,73	1.61	9 (16%)	64,101,113	1.29	10 (15%)
45	CLA	BA	813	-	65,73,73	1.46	7 (10%)	76,113,113	1.33	8 (10%)
54	CHL	A4	306	-	46,54,74	2.32	17 (36%)	49,90,114	2.85	21 (42%)
45	CLA	BA	804	-	52,60,73	1.66	7 (13%)	60,97,113	1.56	11 (18%)
45	CLA	B5	610	47	42,50,73	1.86	7 (16%)	48,85,113	1.47	7 (14%)
47	LHG	BA	846	45	26,26,48	1.06	2 (7%)	29,32,54	1.00	1 (3%)
45	CLA	BL	304	-	43,51,73	1.78	6 (13%)	49,86,113	1.47	7 (14%)
45	CLA	BA	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	AB	821	-	50,58,73	1.70	8 (16%)	58,95,113	1.49	8 (13%)
54	CHL	B1	308	-	40,49,74	2.55	18 (45%)	41,84,114	2.79	17 (41%)
45	CLA	A6	613	16	64,72,73	1.53	8 (12%)	74,111,113	1.28	7 (9%)
45	CLA	AA	839	-	52,60,73	1.66	8 (15%)	60,97,113	1.37	7 (11%)
45	CLA	BA	812	-	54,62,73	1.59	9 (16%)	62,99,113	1.46	8 (12%)
48	BCR	AK	204	-	41,41,41	1.02	3 (7%)	56,56,56	2.06	14 (25%)
45	CLA	AB	814	-	65,73,73	1.49	10 (15%)	76,113,113	1.30	7 (9%)
45	CLA	AB	823	-	65,73,73	1.50	9 (13%)	76,113,113	1.31	9 (11%)
48	BCR	AG	205	-	41,41,41	0.93	0	56,56,56	2.00	18 (32%)
45	CLA	A4	301	15	60,68,73	1.55	9 (15%)	70,107,113	1.33	10 (14%)
45	CLA	AF	802	-	57,65,73	1.58	11 (19%)	66,103,113	1.43	9 (13%)
55	XAT	A3	317	-	39,47,47	0.97	1 (2%)	54,74,74	2.31	19 (35%)
45	CLA	AA	820	-	45,53,73	1.78	8 (17%)	52,89,113	1.46	7 (13%)
48	BCR	BB	849	-	41,41,41	0.90	1 (2%)	56,56,56	1.86	16 (28%)
45	CLA	A6	609	16	45,53,73	1.80	7 (15%)	52,89,113	1.42	7 (13%)
45	CLA	AB	819	-	60,68,73	1.53	9 (15%)	70,107,113	1.64	12 (17%)
45	CLA	BA	826	-	53,61,73	1.62	7 (13%)	61,98,113	1.40	10 (16%)
47	LHG	F	801	-	36,36,48	0.73	1 (2%)	39,42,54	1.22	3 (7%)
48	BCR	AA	845	-	41,41,41	1.03	2 (4%)	56,56,56	1.91	13 (23%)
45	CLA	AF	804	-	41,49,73	1.87	7 (17%)	47,84,113	1.59	8 (17%)
45	CLA	B3	310	14	43,51,73	1.82	5 (11%)	49,86,113	1.44	8 (16%)
51	DGD	AB	851	-	67,67,67	0.80	2 (2%)	81,81,81	0.99	4 (4%)
45	CLA	AA	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.56	9 (11%)
45	CLA	AG	201	-	43,52,73	1.87	7 (16%)	49,88,113	1.48	7 (14%)
55	XAT	A6	616	-	39,47,47	0.98	2 (5%)	54,74,74	2.49	21 (38%)
45	CLA	B2	602	17	65,73,73	1.51	9 (13%)	76,113,113	1.26	10 (13%)
50	LMU	AB	850	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
54	CHL	A1	308	13	40,49,74	2.48	18 (45%)	41,84,114	2.86	17 (41%)
45	CLA	B3	313	-	37,44,73	1.95	9 (24%)	42,77,113	1.35	7 (16%)
46	PQN	AB	843	-	34,34,34	3.39	11 (32%)	42,45,45	1.83	6 (14%)
46	PQN	BA	843	-	34,34,34	3.47	12 (35%)	42,45,45	1.62	5 (11%)
45	CLA	AB	807	2	65,73,73	1.45	10 (15%)	76,113,113	1.35	8 (10%)
45	CLA	AK	202	-	45,53,73	1.82	6 (13%)	52,89,113	1.41	7 (13%)
45	CLA	AB	831	-	43,51,73	1.84	9 (20%)	49,86,113	1.33	8 (16%)
45	CLA	A3	308	14	45,53,73	1.80	8 (17%)	52,89,113	1.43	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	A3	303	14	55,63,73	1.67	9 (16%)	64,101,113	1.46	9 (14%)
54	CHL	B2	607	-	46,54,74	2.33	17 (36%)	49,90,114	2.82	20 (40%)
45	CLA	AA	812	-	54,62,73	1.61	9 (16%)	62,99,113	1.51	8 (12%)
51	DGD	BB	850	-	67,67,67	0.81	2 (2%)	81,81,81	0.98	4 (4%)
56	SQD	e	301	-	33,34,54	1.20	6 (18%)	42,45,65	1.77	10 (23%)
45	CLA	B1	304	13	61,69,73	1.52	7 (11%)	71,108,113	1.39	8 (11%)
45	CLA	A1	316	13	43,51,73	1.89	7 (16%)	54,87,113	1.63	9 (16%)
45	CLA	AB	804	-	65,73,73	1.45	10 (15%)	76,113,113	1.69	15 (19%)
45	CLA	A3	306	14	41,49,73	1.90	7 (17%)	51,84,113	1.67	9 (17%)
45	CLA	BK	202	-	45,53,73	1.81	6 (13%)	52,89,113	1.47	7 (13%)
45	CLA	BB	830	-	65,73,73	1.50	9 (13%)	76,113,113	1.26	8 (10%)
45	CLA	BA	815	-	42,50,73	1.79	8 (19%)	48,85,113	1.51	6 (12%)
48	BCR	BB	803	-	41,41,41	0.85	0	56,56,56	1.99	19 (33%)
45	CLA	A1	311	13	59,67,73	1.57	7 (11%)	69,106,113	1.27	8 (11%)
45	CLA	BB	806	-	41,49,73	1.80	7 (17%)	47,84,113	1.58	9 (19%)
48	BCR	AA	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.12	20 (35%)
45	CLA	BB	810	-	65,73,73	1.50	8 (12%)	76,113,113	1.33	12 (15%)
49	SF4	AA	850	1,2	0,12,12	-	-	-	-	-
45	CLA	B1	306	-	41,49,73	1.86	5 (12%)	47,84,113	1.45	7 (14%)
45	CLA	B2	604	-	43,51,73	1.84	6 (13%)	48,86,113	1.43	7 (14%)
48	BCR	BA	848	-	41,41,41	0.80	0	56,56,56	2.03	17 (30%)
48	BCR	BB	846	-	41,41,41	0.85	1 (2%)	56,56,56	2.14	19 (33%)
45	CLA	A1	305	-	55,63,73	1.63	7 (12%)	64,101,113	1.60	10 (15%)
56	SQD	BJ	104	-	46,47,54	1.28	5 (10%)	55,58,65	4.16	12 (21%)
45	CLA	AA	836	1	45,53,73	1.85	7 (15%)	52,89,113	1.47	8 (15%)
45	CLA	A4	302	15	44,52,73	1.85	8 (18%)	55,88,113	1.61	9 (16%)
47	LHG	BA	845	-	48,48,48	0.88	2 (4%)	51,54,54	0.97	3 (5%)
45	CLA	AH	201	-	60,68,73	1.60	7 (11%)	70,107,113	1.36	10 (14%)
52	LUT	B5	614	-	42,43,43	0.83	1 (2%)	51,60,60	1.85	15 (29%)
45	CLA	BB	801	-	65,73,73	1.47	9 (13%)	76,113,113	1.47	13 (17%)
54	CHL	A4	304	-	40,49,74	2.45	16 (40%)	42,84,114	2.82	20 (47%)
45	CLA	BG	201	-	42,50,73	1.85	7 (16%)	48,85,113	1.28	7 (14%)
48	BCR	B2	617	-	41,41,41	0.89	1 (2%)	56,56,56	2.47	23 (41%)
47	LHG	A1	301	45	37,37,48	1.07	2 (5%)	40,43,54	0.97	3 (7%)
45	CLA	AA	815	-	40,49,73	1.79	5 (12%)	44,83,113	1.62	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	LMU	BB	851	-	36,36,36	1.10	2 (5%)	47,47,47	0.89	0
45	CLA	BB	805	-	65,73,73	1.43	10 (15%)	76,113,113	1.56	12 (15%)
47	LHG	a	501	-	28,28,48	0.89	1 (3%)	31,34,54	1.24	2 (6%)
48	BCR	AB	849	-	41,41,41	0.83	0	56,56,56	2.41	24 (42%)
45	CLA	BA	841	-	65,73,73	1.47	8 (12%)	76,113,113	1.55	11 (14%)
45	CLA	AB	838	-	65,73,73	1.46	7 (10%)	76,113,113	1.34	8 (10%)
54	CHL	B5	607	-	45,53,74	2.37	17 (37%)	49,89,114	2.81	19 (38%)
48	BCR	AA	848	-	41,41,41	0.77	1 (2%)	56,56,56	1.97	16 (28%)
45	CLA	A3	313	-	39,48,73	1.91	7 (17%)	44,83,113	1.46	8 (18%)
45	CLA	AB	816	-	43,51,73	1.80	7 (16%)	49,86,113	1.42	6 (12%)
45	CLA	BB	811	2	65,73,73	1.48	10 (15%)	76,113,113	1.37	9 (11%)
45	CLA	AA	803	-	65,73,73	1.47	10 (15%)	76,113,113	1.36	11 (14%)
45	CLA	A1	304	13	60,68,73	1.52	9 (15%)	69,106,113	1.33	8 (11%)
50	LMU	AB	852	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
45	CLA	AA	810	-	65,72,73	1.55	9 (13%)	71,111,113	1.29	7 (9%)
48	BCR	A3	318	-	41,41,41	0.98	1 (2%)	56,56,56	2.77	20 (35%)
45	CLA	BA	802	-	65,73,73	1.54	9 (13%)	76,113,113	1.38	6 (7%)
49	SF4	BA	852	1,2	0,12,12	-	-	-	-	-
45	CLA	AB	809	-	65,73,73	1.52	8 (12%)	76,113,113	1.36	10 (13%)
45	CLA	B5	601	18	46,54,73	1.75	8 (17%)	53,90,113	1.37	7 (13%)
48	BCR	BL	305	-	41,41,41	0.78	0	56,56,56	2.22	20 (35%)
48	BCR	BG	203	-	41,41,41	0.91	2 (4%)	56,56,56	6.99	26 (46%)
45	CLA	BA	834	-	65,73,73	1.49	9 (13%)	76,113,113	1.47	10 (13%)
45	CLA	BA	801	-	65,73,73	1.50	7 (10%)	76,113,113	1.20	6 (7%)
45	CLA	BB	808	2	65,73,73	1.47	9 (13%)	76,113,113	1.33	7 (9%)
45	CLA	AA	801	-	65,73,73	1.50	7 (10%)	76,113,113	1.27	8 (10%)
45	CLA	AB	811	-	65,73,73	1.46	8 (12%)	76,113,113	1.48	10 (13%)
45	CLA	BA	811	-	65,73,73	1.50	8 (12%)	76,113,113	1.28	8 (10%)
45	CLA	BA	821	-	65,73,73	1.50	9 (13%)	76,113,113	1.39	10 (13%)
46	PQN	BB	844	-	34,34,34	3.42	10 (29%)	42,45,45	1.66	8 (19%)
45	CLA	AB	837	-	50,58,73	1.69	9 (18%)	58,95,113	1.51	8 (13%)
53	LMG	B5	617	-	33,33,55	1.18	2 (6%)	41,41,63	1.20	4 (9%)
45	CLA	B3	311	-	53,62,73	1.69	7 (13%)	61,100,113	1.25	6 (9%)
45	CLA	A3	312	-	53,62,73	1.67	7 (13%)	61,100,113	1.39	8 (13%)
45	CLA	A6	603	16	65,73,73	1.51	9 (13%)	76,113,113	1.29	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	BCR	A4	317	-	41,41,41	0.82	0	56,56,56	2.37	23 (41%)
45	CLA	AB	841	-	65,73,73	1.54	9 (13%)	76,113,113	1.22	6 (7%)
55	XAT	B2	616	-	39,47,47	1.01	1 (2%)	54,74,74	2.30	20 (37%)
52	LUT	A6	615	-	42,43,43	0.90	1 (2%)	51,60,60	1.59	12 (23%)
54	CHL	B2	606	-	43,51,74	2.40	16 (37%)	45,86,114	2.78	17 (37%)
48	BCR	BA	851	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	20 (35%)
45	CLA	BL	302	12	45,53,73	1.85	8 (17%)	52,89,113	1.60	11 (21%)
45	CLA	A6	611	47	38,45,73	2.88	9 (23%)	41,76,113	1.68	9 (21%)
45	CLA	AA	830	-	65,73,73	1.52	9 (13%)	76,113,113	1.31	8 (10%)
45	CLA	BL	303	-	60,68,73	1.58	8 (13%)	70,107,113	1.37	10 (14%)
45	CLA	AB	803	-	65,73,73	1.49	8 (12%)	76,113,113	1.23	7 (9%)
45	CLA	B1	314	-	60,68,73	1.60	7 (11%)	70,107,113	1.24	10 (14%)
50	LMU	AA	851	-	36,36,36	1.16	2 (5%)	47,47,47	1.04	2 (4%)
45	CLA	AA	806	1	65,73,73	1.49	9 (13%)	76,113,113	1.38	8 (10%)
48	BCR	AI	102	-	41,41,41	0.86	0	56,56,56	2.54	18 (32%)
47	LHG	BF	305	-	44,44,48	0.97	2 (4%)	47,50,54	1.09	3 (6%)
45	CLA	AA	826	-	59,67,73	1.56	9 (15%)	68,105,113	1.28	8 (11%)
48	BCR	A6	617	-	41,41,41	0.99	2 (4%)	56,56,56	2.01	16 (28%)
45	CLA	BB	827	-	62,70,73	1.52	8 (12%)	72,109,113	1.27	8 (11%)
55	XAT	A4	316	-	39,47,47	0.95	2 (5%)	54,74,74	2.29	16 (29%)
45	CLA	BA	824	-	55,63,73	1.63	9 (16%)	64,101,113	1.39	8 (12%)
45	CLA	A6	614	-	43,51,73	1.89	6 (13%)	49,86,113	1.47	7 (14%)
45	CLA	A1	313	13	45,53,73	1.78	7 (15%)	52,89,113	1.57	7 (13%)
45	CLA	A6	605	-	43,51,73	1.83	8 (18%)	48,86,113	1.40	7 (14%)
48	BCR	B3	317	-	41,41,41	0.84	0	56,56,56	3.61	28 (50%)
45	CLA	AB	808	-	51,59,73	1.67	9 (17%)	58,95,113	1.45	7 (12%)
45	CLA	A4	312	-	45,53,73	1.81	7 (15%)	52,89,113	1.40	7 (13%)
48	BCR	BL	301	-	41,41,41	0.87	1 (2%)	56,56,56	2.36	14 (25%)
47	LHG	A3	319	45	22,22,48	1.44	2 (9%)	25,28,54	1.27	2 (8%)
45	CLA	BA	820	-	45,53,73	1.73	7 (15%)	52,89,113	1.50	6 (11%)
45	CLA	A6	612	16	44,52,73	1.84	7 (15%)	51,88,113	1.37	6 (11%)
48	BCR	AF	805	-	41,41,41	0.81	0	56,56,56	1.86	14 (25%)
52	LUT	B1	316	-	42,43,43	1.60	8 (19%)	51,60,60	1.51	10 (19%)
52	LUT	AF	806	-	42,43,43	1.03	3 (7%)	51,60,60	1.72	12 (23%)
45	CLA	B3	307	14	45,53,73	1.79	6 (13%)	52,89,113	1.50	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	A3	310	47	36,45,73	1.97	6 (16%)	43,79,113	1.48	8 (18%)
45	CLA	AB	802	-	64,72,73	1.60	8 (12%)	79,112,113	1.34	9 (11%)
45	CLA	B3	309	47	39,48,73	1.93	5 (12%)	44,83,113	1.40	7 (15%)
45	CLA	A1	306	-	49,57,73	1.71	7 (14%)	55,93,113	1.45	8 (14%)
48	BCR	BF	304	-	41,41,41	0.87	1 (2%)	56,56,56	1.94	19 (33%)
45	CLA	BA	810	-	65,73,73	1.50	9 (13%)	76,113,113	1.22	7 (9%)
45	CLA	BA	842	-	65,73,73	1.50	7 (10%)	76,113,113	1.31	7 (9%)
45	CLA	BB	817	-	41,50,73	1.80	7 (17%)	46,85,113	1.48	7 (15%)
49	SF4	BC	102	3	0,12,12	-	-	-	-	-
45	CLA	AA	807	-	50,58,73	1.69	8 (16%)	58,95,113	1.43	6 (10%)
45	CLA	AA	802	-	65,73,73	1.53	10 (15%)	76,113,113	1.42	6 (7%)
45	CLA	AA	813	-	65,73,73	1.47	9 (13%)	76,113,113	1.38	8 (10%)
45	CLA	BF	302	-	42,50,73	1.85	8 (19%)	48,85,113	1.57	8 (16%)
45	CLA	BA	816	-	45,53,73	1.81	7 (15%)	52,89,113	1.45	8 (15%)
45	CLA	BB	802	-	65,73,73	1.55	9 (13%)	76,113,113	1.42	8 (10%)
45	CLA	AA	831	-	47,55,73	1.78	9 (19%)	54,91,113	1.43	7 (12%)
45	CLA	AB	815	-	65,73,73	1.46	8 (12%)	76,113,113	1.39	9 (11%)
45	CLA	BB	823	-	45,54,73	1.75	6 (13%)	51,90,113	1.31	8 (15%)
45	CLA	BB	841	-	65,73,73	1.48	9 (13%)	76,113,113	1.30	7 (9%)
45	CLA	A6	601	15	46,54,73	1.73	8 (17%)	53,90,113	1.46	8 (15%)
45	CLA	B3	302	14	55,63,73	1.61	7 (12%)	64,101,113	1.34	8 (12%)
45	CLA	B3	303	-	41,50,73	1.94	7 (17%)	51,86,113	1.55	9 (17%)
45	CLA	BB	832	-	43,51,73	1.83	8 (18%)	49,86,113	1.30	6 (12%)
45	CLA	B5	611	18	40,49,73	1.87	8 (20%)	45,84,113	1.47	7 (15%)
45	CLA	BH	201	-	60,68,73	1.60	7 (11%)	70,107,113	1.29	8 (11%)
48	BCR	BI	101	-	41,41,41	0.92	2 (4%)	56,56,56	2.15	21 (37%)
45	CLA	A4	303	-	43,51,73	1.86	7 (16%)	54,87,113	1.59	9 (16%)
45	CLA	BB	814	-	43,51,73	1.78	6 (13%)	49,86,113	1.48	8 (16%)
45	CLA	AB	829	-	65,73,73	1.50	9 (13%)	76,113,113	1.33	9 (11%)
45	CLA	AA	808	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	9 (11%)
54	CHL	A6	607	-	43,51,74	2.34	16 (37%)	45,86,114	2.83	19 (42%)
45	CLA	AB	810	2	65,73,73	1.48	11 (16%)	76,113,113	1.38	6 (7%)
45	CLA	A3	302	14	60,68,73	1.57	8 (13%)	70,107,113	1.22	9 (12%)
45	CLA	BB	842	-	65,73,73	1.50	9 (13%)	76,113,113	1.30	7 (9%)
45	CLA	AA	823	-	41,49,73	1.93	7 (17%)	47,84,113	1.46	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	AA	841	-	65,73,73	1.50	9 (13%)	76,113,113	1.34	8 (10%)
45	CLA	AL	305	-	42,50,73	1.85	8 (19%)	48,85,113	1.57	8 (16%)
45	CLA	AA	832	-	56,64,73	1.60	6 (10%)	65,102,113	1.36	10 (15%)
45	CLA	AG	204	7	45,53,73	1.84	7 (15%)	52,89,113	1.46	7 (13%)
45	CLA	B5	604	-	43,51,73	1.91	7 (16%)	54,87,113	1.53	10 (18%)
45	CLA	AA	817	-	60,68,73	1.55	6 (10%)	70,107,113	1.36	9 (12%)
45	CLA	B2	611	17	44,52,73	1.85	7 (15%)	51,88,113	1.42	7 (13%)
45	CLA	BB	815	-	65,73,73	1.47	9 (13%)	76,113,113	1.49	11 (14%)
45	CLA	BA	819	-	65,73,73	1.48	9 (13%)	76,113,113	1.34	9 (11%)
45	CLA	AA	842	-	65,73,73	1.48	8 (12%)	76,113,113	1.41	11 (14%)
48	BCR	BL	306	-	41,41,41	0.88	1 (2%)	56,56,56	11.27	26 (46%)
52	LUT	A4	315	-	42,43,43	0.95	2 (4%)	51,60,60	1.84	15 (29%)
45	CLA	AB	840	-	65,73,73	1.54	9 (13%)	76,113,113	1.25	7 (9%)
45	CLA	BB	807	-	65,73,73	1.49	7 (10%)	76,113,113	1.33	10 (13%)
48	BCR	BA	847	-	41,41,41	0.99	1 (2%)	56,56,56	1.63	11 (19%)
45	CLA	BB	831	-	56,64,73	1.63	9 (16%)	65,102,113	1.38	6 (9%)
45	CLA	AK	203	-	46,54,73	1.78	9 (19%)	53,90,113	1.47	7 (13%)
48	BCR	AB	844	-	41,41,41	0.86	0	56,56,56	2.28	23 (41%)
45	CLA	BA	839	-	51,59,73	1.69	8 (15%)	59,96,113	1.41	8 (13%)
45	CLA	BB	835	-	65,73,73	1.53	9 (13%)	76,113,113	1.14	5 (6%)
45	CLA	B5	608	18	44,52,73	1.86	9 (20%)	51,88,113	1.44	7 (13%)
54	CHL	B1	303	13	49,58,74	2.23	17 (34%)	52,95,114	2.63	22 (42%)
48	BCR	A1	319	-	41,41,41	0.90	1 (2%)	56,56,56	3.13	20 (35%)
45	CLA	AB	842	47	65,73,73	1.46	8 (12%)	76,113,113	1.37	10 (13%)
45	CLA	BB	822	-	41,49,73	1.83	8 (19%)	47,84,113	1.56	7 (14%)
45	CLA	A1	309	-	43,52,73	1.87	6 (13%)	49,88,113	1.42	9 (18%)
52	LUT	A1	317	-	42,43,43	0.94	1 (2%)	51,60,60	1.88	13 (25%)
45	CLA	A4	313	-	50,58,73	1.72	8 (16%)	58,95,113	1.47	10 (17%)
45	CLA	AB	834	-	65,73,73	1.49	9 (13%)	76,113,113	1.23	9 (11%)
45	CLA	AB	827	-	62,70,73	1.50	7 (11%)	72,109,113	1.50	9 (12%)
54	CHL	A4	314	15	40,49,74	2.26	13 (32%)	45,84,114	2.77	17 (37%)
48	BCR	AA	846	-	41,41,41	0.82	0	56,56,56	2.12	21 (37%)
48	BCR	AL	306	-	41,41,41	0.94	1 (2%)	56,56,56	2.01	21 (37%)
45	CLA	BA	829	-	65,73,73	1.49	9 (13%)	76,113,113	1.31	9 (11%)
45	CLA	B3	305	-	41,49,73	1.89	7 (17%)	51,84,113	1.73	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	AA	835	-	43,52,73	1.85	8 (18%)	49,88,113	1.47	7 (14%)
54	CHL	B2	601	17	53,61,74	2.20	16 (30%)	57,98,114	2.66	25 (43%)
48	BCR	AB	847	-	41,41,41	0.87	0	56,56,56	2.02	14 (25%)
47	LHG	B3	318	45	22,22,48	1.49	2 (9%)	25,28,54	1.38	2 (8%)
45	CLA	BB	820	-	60,68,73	1.51	7 (11%)	70,107,113	1.62	11 (15%)
45	CLA	BB	840	-	47,55,73	1.71	7 (14%)	54,91,113	1.43	8 (14%)
45	CLA	AB	839	-	47,55,73	1.74	8 (17%)	54,91,113	1.56	7 (12%)
47	LHG	AA	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.89	2 (3%)
45	CLA	B1	311	13	59,67,73	1.59	6 (10%)	69,106,113	1.22	8 (11%)
49	SF4	BC	101	3	0,12,12	-	-	-	-	-
48	BCR	BJ	103	-	41,41,41	0.75	0	56,56,56	2.37	21 (37%)
45	CLA	B2	613	-	43,51,73	1.81	6 (13%)	49,86,113	1.44	8 (16%)
45	CLA	AB	835	-	60,68,73	1.55	8 (13%)	70,107,113	1.37	8 (11%)
48	BCR	BA	849	-	41,41,41	0.84	0	56,56,56	2.01	18 (32%)
49	SF4	I	202	37	0,12,12	-	-	-	-	-
45	CLA	BA	840	-	65,73,73	1.44	8 (12%)	76,113,113	1.33	8 (10%)
55	XAT	B3	316	-	39,47,47	0.97	1 (2%)	54,74,74	2.48	21 (38%)
45	CLA	BA	825	-	65,73,73	1.47	7 (10%)	76,113,113	1.31	6 (7%)
45	CLA	BA	818	-	56,64,73	1.64	8 (14%)	65,102,113	1.32	8 (12%)
45	CLA	AA	840	-	65,73,73	1.51	8 (12%)	76,113,113	1.31	10 (13%)
45	CLA	B1	315	-	37,46,73	2.00	7 (18%)	46,81,113	1.61	9 (19%)
45	CLA	B3	312	-	39,48,73	1.93	6 (15%)	44,83,113	1.40	7 (15%)
49	SF4	AC	101	3	0,12,12	-	-	-	-	-
47	LHG	B5	618	45	29,29,48	1.17	2 (6%)	32,35,54	1.20	3 (9%)
45	CLA	AB	822	-	47,55,73	1.77	7 (14%)	54,91,113	1.35	7 (12%)
45	CLA	BB	826	-	65,73,73	1.51	10 (15%)	76,113,113	1.30	7 (9%)
50	LMU	AL	301	-	35,35,36	1.23	2 (5%)	46,46,47	1.05	5 (10%)
45	CLA	B2	610	47	38,45,73	2.83	10 (26%)	41,76,113	1.61	9 (21%)
53	LMG	A1	321	-	44,44,55	1.03	2 (4%)	52,52,63	1.19	5 (9%)
45	CLA	AK	201	11	37,43,73	2.45	10 (27%)	45,75,113	1.48	8 (17%)
45	CLA	AB	813	-	43,51,73	1.78	6 (13%)	49,86,113	1.44	8 (16%)
45	CLA	BA	814	-	45,53,73	1.81	9 (20%)	52,89,113	1.51	8 (15%)
45	CLA	B3	314	-	39,48,73	1.87	6 (15%)	44,83,113	1.46	7 (15%)
45	CLA	AA	827	-	65,73,73	1.48	7 (10%)	76,113,113	1.34	8 (10%)
45	CLA	BA	803	-	65,73,73	1.41	7 (10%)	76,113,113	1.37	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	AA	822	-	42,50,73	1.86	6 (14%)	48,85,113	1.50	8 (16%)
54	CHL	B2	614	17	43,51,74	2.35	15 (34%)	45,86,114	2.87	19 (42%)
45	CLA	AB	806	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	9 (11%)
47	LHG	A3	301	-	35,35,48	1.09	2 (5%)	38,41,54	1.01	2 (5%)
54	CHL	A6	606	-	42,50,74	2.35	15 (35%)	45,85,114	2.88	20 (44%)
48	BCR	AA	847	-	41,41,41	1.00	2 (4%)	56,56,56	2.28	24 (42%)
45	CLA	B1	307	-	39,48,73	1.94	5 (12%)	45,82,113	1.55	7 (15%)
45	CLA	B1	312	47	37,46,73	1.97	7 (18%)	46,81,113	1.60	9 (19%)
54	CHL	A1	303	13	50,59,74	2.22	15 (30%)	53,96,114	2.68	24 (45%)
45	CLA	A3	314	-	37,44,73	1.97	8 (21%)	42,77,113	1.42	7 (16%)
45	CLA	B1	305	-	54,62,73	1.64	8 (14%)	62,99,113	1.53	10 (16%)
45	CLA	B1	309	-	43,52,73	1.85	7 (16%)	49,88,113	1.44	7 (14%)
45	CLA	BA	808	1	65,73,73	1.49	8 (12%)	76,113,113	1.23	8 (10%)
46	PQN	AA	843	-	34,34,34	3.42	10 (29%)	42,45,45	1.74	8 (19%)
45	CLA	AA	825	-	65,73,73	1.48	6 (9%)	76,113,113	1.33	6 (7%)
45	CLA	A4	307	15	45,53,73	1.85	7 (15%)	52,89,113	1.36	7 (13%)
48	BCR	BJ	101	-	41,41,41	0.89	0	56,56,56	1.70	14 (25%)
45	CLA	BB	809	-	52,60,73	1.69	8 (15%)	60,97,113	1.33	7 (11%)
45	CLA	AF	803	-	42,50,73	1.88	8 (19%)	48,85,113	1.57	8 (16%)
45	CLA	BA	823	-	41,49,73	1.86	6 (14%)	47,84,113	1.49	9 (19%)
45	CLA	B1	310	13	38,47,73	1.99	7 (18%)	47,82,113	1.54	10 (21%)
50	LMU	BA	854	-	34,34,36	1.18	2 (5%)	45,45,47	0.91	2 (4%)
45	CLA	BK	201	11	37,44,73	2.00	7 (18%)	46,77,113	1.73	9 (19%)
49	SF4	AC	102	3	0,12,12	-	-	-	-	-
45	CLA	BA	807	-	50,58,73	1.70	7 (14%)	58,95,113	1.34	7 (12%)
45	CLA	BA	831	-	47,55,73	1.79	8 (17%)	54,91,113	1.49	10 (18%)
45	CLA	BB	813	-	54,62,73	1.66	8 (14%)	67,100,113	1.50	11 (16%)
54	CHL	B2	605	-	42,50,74	2.37	16 (38%)	45,85,114	2.84	18 (40%)
54	CHL	A6	608	-	50,58,74	2.26	16 (32%)	58,95,114	2.64	21 (36%)
48	BCR	AB	845	-	41,41,41	0.85	1 (2%)	56,56,56	1.93	17 (30%)
45	CLA	AB	818	-	59,67,73	1.58	8 (13%)	68,105,113	1.34	10 (14%)
45	CLA	BG	202	7	45,53,73	1.81	6 (13%)	52,89,113	1.56	7 (13%)
45	CLA	AB	830	-	56,64,73	1.62	9 (16%)	65,102,113	1.39	7 (10%)
45	CLA	BB	829	-	65,73,73	1.46	9 (13%)	76,113,113	1.32	7 (9%)
45	CLA	BA	809	1	50,58,73	1.73	8 (16%)	58,95,113	1.44	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	A3	315	-	39,48,73	1.86	6 (15%)	44,83,113	1.42	7 (15%)
45	CLA	BB	843	47	65,73,73	1.52	9 (13%)	76,113,113	1.27	7 (9%)
45	CLA	AB	825	-	65,73,73	1.49	10 (15%)	76,113,113	1.34	9 (11%)
45	CLA	BB	837	-	42,50,73	1.86	5 (11%)	48,85,113	1.45	7 (14%)
45	CLA	BF	301	-	55,63,73	1.58	7 (12%)	62,100,113	1.37	7 (11%)
47	LHG	B2	618	45	34,34,48	1.04	2 (5%)	37,40,54	0.96	2 (5%)
48	BCR	BK	204	-	41,41,41	0.88	1 (2%)	56,56,56	2.14	21 (37%)
50	LMU	AB	853	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	2 (4%)
55	XAT	A1	318	-	39,47,47	0.91	2 (5%)	54,74,74	2.42	24 (44%)
45	CLA	A4	311	-	55,64,73	1.64	7 (12%)	63,102,113	1.31	7 (11%)
45	CLA	B3	301	14	60,68,73	1.58	9 (15%)	70,107,113	1.22	8 (11%)
45	CLA	BB	833	-	43,51,73	1.80	7 (16%)	49,86,113	1.65	8 (16%)
45	CLA	BB	818	-	55,63,73	1.61	8 (14%)	64,101,113	1.33	8 (12%)
45	CLA	AA	829	-	65,73,73	1.46	9 (13%)	76,113,113	1.49	11 (14%)
45	CLA	A1	310	13	40,48,73	1.92	7 (17%)	50,83,113	1.65	10 (20%)
45	CLA	AA	837	-	51,59,73	1.62	7 (13%)	59,96,113	1.59	9 (15%)
45	CLA	B2	608	17	45,53,73	1.80	7 (15%)	52,89,113	1.39	8 (15%)
45	CLA	BA	822	-	42,50,73	1.83	6 (14%)	48,85,113	1.56	7 (14%)
54	CHL	B3	306	-	45,53,74	2.28	16 (35%)	52,89,114	2.69	20 (38%)
47	LHG	B1	302	-	35,35,48	1.09	2 (5%)	38,41,54	0.99	2 (5%)
45	CLA	A4	309	-	42,50,73	1.79	5 (11%)	48,85,113	1.53	7 (14%)
45	CLA	AB	812	-	54,62,73	1.66	8 (14%)	67,100,113	1.52	12 (17%)
45	CLA	B5	603	-	44,52,73	1.87	7 (15%)	55,88,113	1.58	8 (14%)
45	CLA	AA	809	1	50,58,73	1.77	9 (18%)	58,95,113	1.48	11 (18%)
45	CLA	BJ	102	10	42,50,73	1.84	5 (11%)	48,85,113	1.48	7 (14%)
48	BCR	BB	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.19	18 (32%)
45	CLA	BA	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.30	8 (10%)
49	SF4	I	201	37	0,12,12	-	-	-	-	-
48	BCR	AA	852	-	41,41,41	0.94	2 (4%)	56,56,56	2.19	17 (30%)
48	BCR	AI	101	-	41,41,41	0.92	1 (2%)	56,56,56	2.05	20 (35%)
45	CLA	AA	818	-	59,67,73	1.58	9 (15%)	68,105,113	1.33	8 (11%)
47	LHG	A6	618	45	35,35,48	1.05	2 (5%)	38,41,54	0.97	2 (5%)
45	CLA	AA	811	-	65,73,73	1.49	7 (10%)	76,113,113	1.31	8 (10%)
48	BCR	AB	848	-	41,41,41	0.89	1 (2%)	56,56,56	1.97	18 (32%)
45	CLA	A6	604	-	41,50,73	1.90	6 (14%)	46,85,113	1.60	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	AL	304	-	60,68,73	1.57	9 (15%)	70,107,113	1.41	10 (14%)
45	CLA	BA	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.36	9 (11%)
45	CLA	A4	310	15	40,49,73	1.90	8 (20%)	45,84,113	1.47	7 (15%)
53	LMG	A4	318	-	39,39,55	1.00	2 (5%)	47,47,63	1.40	7 (14%)
55	XAT	B1	317	-	39,47,47	0.93	2 (5%)	54,74,74	2.43	18 (33%)
45	CLA	B2	603	-	43,52,73	1.85	7 (16%)	49,88,113	1.58	8 (16%)
45	CLA	B2	612	17	65,73,73	1.52	7 (10%)	76,113,113	1.29	8 (10%)
45	CLA	BB	825	-	45,53,73	1.79	8 (17%)	52,89,113	1.37	6 (11%)
45	CLA	BA	806	1	65,73,73	1.50	8 (12%)	76,113,113	1.33	7 (9%)
45	CLA	AB	826	-	62,70,73	1.52	9 (14%)	72,109,113	1.32	7 (9%)
45	CLA	AB	824	-	43,51,73	1.77	10 (23%)	49,86,113	1.57	8 (16%)
45	CLA	AG	203	-	42,50,73	1.85	6 (14%)	48,85,113	1.44	7 (14%)
45	CLA	BB	834	-	65,73,73	1.51	10 (15%)	76,113,113	1.31	8 (10%)
45	CLA	BA	836	1	45,53,73	1.81	6 (13%)	52,89,113	1.53	8 (15%)
45	CLA	AB	820	-	55,63,73	1.70	8 (14%)	64,101,113	1.28	6 (9%)
45	CLA	BB	824	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	10 (13%)
45	CLA	B5	602	18	60,68,73	1.62	9 (15%)	70,107,113	1.29	6 (8%)
50	LMU	BA	853	-	35,35,36	1.15	2 (5%)	46,46,47	0.93	0
54	CHL	B5	605	-	40,49,74	2.42	17 (42%)	42,84,114	2.80	18 (42%)
45	CLA	A1	315	-	37,46,73	1.99	7 (18%)	46,81,113	1.69	11 (23%)

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
45	CLA	AA	833	-	1/1/15/20	19/37/115/115	-
45	CLA	BA	844	47	1/1/10/20	4/8/86/115	-
45	CLA	B1	313	13	1/1/11/20	5/13/91/115	-
54	CHL	A3	307	-	3/3/16/26	4/13/111/137	-
45	CLA	AB	801	-	1/1/15/20	17/37/115/115	-
48	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
45	CLA	AB	833	-	1/1/15/20	10/37/115/115	-
54	CHL	A4	305	-	3/3/15/26	0/10/106/137	-
48	BCR	BA	856	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	A1	307	-	1/1/9/20	4/8/82/115	-
45	CLA	A1	312	47	1/1/10/20	0/4/80/115	-
45	CLA	AA	834	-	-	15/37/115/115	-
45	CLA	BA	827	-	1/1/15/20	14/37/115/115	-
45	CLA	AL	303	12	1/1/10/20	5/8/86/115	-
48	BCR	BB	848	-	-	2/29/63/63	0/2/2/2
45	CLA	A3	304	-	1/1/11/20	0/9/85/115	-
45	CLA	BB	836	-	-	11/31/109/115	-
52	LUT	A3	316	-	-	0/29/67/67	0/2/2/2
47	LHG	A1	320	45	-	16/53/53/53	-
48	BCR	BA	855	-	-	4/29/63/63	0/2/2/2
47	LHG	AJ	104	-	-	16/44/44/53	-
57	FES	c	301	28	-	-	0/1/1/1
54	CHL	A6	602	16	3/3/17/26	6/22/120/137	-
48	BCR	AJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	A4	308	15	1/1/12/20	4/24/102/115	-
45	CLA	BB	804	-	1/1/15/20	15/37/115/115	-
45	CLA	AB	832	-	-	7/37/115/115	-
45	CLA	BA	837	-	1/1/12/20	3/21/99/115	-
55	XAT	B5	615	-	-	0/31/93/93	0/4/4/4
45	CLA	BB	816	-	1/1/15/20	15/35/113/115	-
52	LUT	B2	615	-	-	0/29/67/67	0/2/2/2
45	CLA	BB	812	-	1/1/15/20	13/37/115/115	-
45	CLA	BA	835	-	1/1/11/20	6/13/91/115	-
45	CLA	AB	805	-	1/1/10/20	2/8/86/115	-
45	CLA	AA	824	-	1/1/13/20	7/23/101/115	-
45	CLA	BA	817	-	-	9/31/109/115	-
48	BCR	AL	302	-	-	5/29/63/63	0/2/2/2
45	CLA	B5	613	-	1/1/11/20	5/13/91/115	-
45	CLA	AJ	102	10	1/1/10/20	3/10/88/115	-
45	CLA	AB	836	-	-	2/10/88/115	-
47	LHG	B1	318	45	-	12/46/46/53	-
45	CLA	A1	314	-	1/1/15/20	12/35/113/115	-
45	CLA	BA	832	-	-	7/27/105/115	-
47	LHG	B1	301	45	-	7/42/42/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	A6	610	16	1/1/13/20	4/25/103/115	-
49	SF4	K	301	39	-	-	0/6/5/5
48	BCR	BB	847	-	-	6/29/63/63	0/2/2/2
45	CLA	A3	309	14	1/1/10/20	3/8/86/115	-
45	CLA	B5	609	18	1/1/12/20	3/24/102/115	-
45	CLA	BB	838	-	1/1/12/20	5/19/97/115	-
45	CLA	BB	839	-	-	8/37/115/115	-
45	CLA	BA	830	-	1/1/15/20	13/37/115/115	-
48	BCR	AF	801	-	-	2/29/63/63	0/2/2/2
45	CLA	AA	816	-	1/1/11/20	6/13/91/115	-
45	CLA	BA	838	-	1/1/12/20	11/25/99/115	-
45	CLA	AA	804	-	-	7/22/100/115	-
45	CLA	A3	305	-	1/1/10/20	4/8/86/115	-
45	CLA	B3	304	-	1/1/10/20	4/8/86/115	-
47	LHG	A1	302	-	-	15/40/40/53	-
45	CLA	B2	609	17	1/1/13/20	6/25/103/115	-
48	BCR	B5	616	-	-	2/29/63/63	0/2/2/2
45	CLA	AB	828	-	1/1/15/20	13/37/115/115	-
45	CLA	B3	308	14	1/1/10/20	3/8/86/115	-
45	CLA	AA	805	-	1/1/15/20	17/37/115/115	-
45	CLA	BB	821	-	1/1/13/20	6/25/103/115	-
48	BCR	BA	850	-	-	3/29/63/63	0/2/2/2
45	CLA	AB	817	-	1/1/13/20	8/25/103/115	-
45	CLA	A3	311	14	1/1/10/20	0/11/89/115	-
48	BCR	AB	846	-	-	6/29/63/63	0/2/2/2
45	CLA	AA	814	-	1/1/11/20	5/13/91/115	-
45	CLA	BB	819	-	1/1/13/20	12/30/108/115	-
45	CLA	B5	612	18	1/1/13/20	8/28/106/115	-
45	CLA	BB	828	-	1/1/14/20	9/34/112/115	-
45	CLA	AA	821	-	1/1/15/20	15/37/115/115	-
52	LUT	B3	315	-	-	4/29/67/67	0/2/2/2
45	CLA	BF	303	-	1/1/10/20	2/8/86/115	-
53	LMG	AG	202	-	-	5/33/53/70	0/1/1/1
45	CLA	AA	819	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BK	203	-	1/1/11/20	5/15/93/115	-
45	CLA	AA	838	-	-	6/25/103/115	-
45	CLA	BA	813	-	1/1/15/20	17/37/115/115	-
54	CHL	A4	306	-	3/3/16/26	2/15/113/137	-
45	CLA	BA	804	-	-	5/22/100/115	-
45	CLA	B5	610	47	-	4/10/88/115	-
47	LHG	BA	846	45	-	7/30/30/53	-
45	CLA	BL	304	-	1/1/10/20	5/11/89/115	-
45	CLA	BA	828	-	1/1/15/20	14/37/115/115	-
45	CLA	AB	821	-	1/1/12/20	7/19/97/115	-
54	CHL	B1	308	-	3/3/15/26	0/8/106/137	-
45	CLA	A6	613	16	1/1/14/20	7/35/113/115	-
45	CLA	AA	839	-	-	6/22/100/115	-
45	CLA	BA	812	-	1/1/12/20	5/24/102/115	-
48	BCR	AK	204	-	-	6/29/63/63	0/2/2/2
45	CLA	AB	814	-	1/1/15/20	14/37/115/115	-
45	CLA	AB	823	-	-	19/37/115/115	-
48	BCR	AG	205	-	-	2/29/63/63	0/2/2/2
45	CLA	A4	301	15	1/1/14/20	8/31/109/115	-
45	CLA	AF	802	-	1/1/13/20	10/28/106/115	-
55	XAT	A3	317	-	-	0/31/93/93	0/4/4/4
45	CLA	AA	820	-	1/1/11/20	3/13/91/115	-
48	BCR	BB	849	-	-	2/29/63/63	0/2/2/2
45	CLA	A6	609	16	1/1/11/20	3/13/91/115	-
45	CLA	AB	819	-	1/1/14/20	14/31/109/115	-
45	CLA	BA	826	-	-	6/23/101/115	-
47	LHG	F	801	-	-	21/41/41/53	-
48	BCR	AA	845	-	-	2/29/63/63	0/2/2/2
45	CLA	AF	804	-	1/1/10/20	2/8/86/115	-
45	CLA	B3	310	14	1/1/10/20	2/11/89/115	-
51	DGD	AB	851	-	-	21/55/95/95	0/2/2/2
45	CLA	AA	828	-	1/1/15/20	15/37/115/115	-
45	CLA	AG	201	-	1/1/11/20	3/11/89/115	-
55	XAT	A6	616	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	B2	602	17	1/1/15/20	9/37/115/115	-
50	LMU	AB	850	-	-	9/21/61/61	0/2/2/2
54	CHL	A1	308	13	3/3/15/26	2/8/106/137	-
45	CLA	B3	313	-	1/1/8/20	0/0/74/115	-
46	PQN	AB	843	-	-	8/23/43/43	0/2/2/2
46	PQN	BA	843	-	-	8/23/43/43	0/2/2/2
45	CLA	AB	807	2	1/1/15/20	11/37/115/115	-
45	CLA	AK	202	-	1/1/11/20	5/13/91/115	-
45	CLA	AB	831	-	1/1/10/20	3/11/89/115	-
45	CLA	A3	308	14	1/1/11/20	5/13/91/115	-
45	CLA	A3	303	14	1/1/13/20	8/25/103/115	-
54	CHL	B2	607	-	3/3/16/26	4/15/113/137	-
45	CLA	AA	812	-	1/1/12/20	9/24/102/115	-
51	DGD	BB	850	-	-	13/55/95/95	0/2/2/2
56	SQD	e	301	-	-	10/29/49/69	0/1/1/1
45	CLA	B1	304	13	1/1/14/20	7/33/111/115	-
45	CLA	A1	316	13	1/1/11/20	9/11/87/115	-
45	CLA	AB	804	-	1/1/15/20	16/37/115/115	-
45	CLA	A3	306	14	1/1/10/20	0/10/86/115	-
45	CLA	BK	202	-	1/1/11/20	6/13/91/115	-
45	CLA	BB	830	-	1/1/15/20	11/37/115/115	-
45	CLA	BA	815	-	-	4/10/88/115	-
48	BCR	BB	803	-	-	4/29/63/63	0/2/2/2
45	CLA	A1	311	13	1/1/14/20	3/29/107/115	-
45	CLA	BB	806	-	1/1/10/20	2/8/86/115	-
48	BCR	AA	849	-	-	8/29/63/63	0/2/2/2
45	CLA	BB	810	-	1/1/15/20	15/37/115/115	-
49	SF4	AA	850	1,2	-	-	0/6/5/5
45	CLA	B1	306	-	1/1/10/20	3/8/86/115	-
45	CLA	B2	604	-	1/1/10/20	4/9/88/115	-
48	BCR	BA	848	-	-	4/29/63/63	0/2/2/2
48	BCR	BB	846	-	-	6/29/63/63	0/2/2/2
45	CLA	A1	305	-	1/1/13/20	7/25/103/115	-
56	SQD	BJ	104	-	-	21/42/62/69	0/1/1/1
45	CLA	AA	836	1	-	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	A4	302	15	1/1/11/20	5/13/89/115	-
47	LHG	BA	845	-	-	29/53/53/53	-
45	CLA	AH	201	-	1/1/14/20	10/31/109/115	-
52	LUT	B5	614	-	-	1/29/67/67	0/2/2/2
45	CLA	BB	801	-	1/1/15/20	17/37/115/115	-
54	CHL	A4	304	-	3/3/15/26	1/8/106/137	-
45	CLA	BG	201	-	1/1/10/20	7/10/88/115	-
48	BCR	B2	617	-	-	0/29/63/63	0/2/2/2
47	LHG	A1	301	45	-	11/42/42/53	-
45	CLA	AA	815	-	-	3/10/88/115	-
50	LMU	BB	851	-	-	10/21/61/61	0/2/2/2
45	CLA	BB	805	-	1/1/15/20	14/37/115/115	-
47	LHG	a	501	-	-	17/33/33/53	-
48	BCR	AB	849	-	-	5/29/63/63	0/2/2/2
45	CLA	BA	841	-	1/1/15/20	15/37/115/115	-
45	CLA	AB	838	-	-	7/37/115/115	-
54	CHL	B5	607	-	3/3/16/26	5/13/111/137	-
48	BCR	AA	848	-	-	4/29/63/63	0/2/2/2
45	CLA	A3	313	-	-	1/6/84/115	-
45	CLA	AB	816	-	1/1/10/20	4/11/89/115	-
45	CLA	BB	811	2	1/1/15/20	15/37/115/115	-
45	CLA	AA	803	-	1/1/15/20	15/37/115/115	-
45	CLA	A1	304	13	1/1/13/20	11/31/109/115	-
50	LMU	AB	852	-	-	9/21/61/61	0/2/2/2
45	CLA	AA	810	-	1/1/14/20	10/37/111/115	-
48	BCR	A3	318	-	-	4/29/63/63	0/2/2/2
45	CLA	BA	802	-	1/1/15/20	4/37/115/115	-
49	SF4	BA	852	1,2	-	-	0/6/5/5
45	CLA	AB	809	-	1/1/15/20	16/37/115/115	-
45	CLA	B5	601	18	1/1/11/20	8/15/93/115	-
48	BCR	BL	305	-	-	2/29/63/63	0/2/2/2
48	BCR	BG	203	-	-	6/29/63/63	0/2/2/2
45	CLA	BB	808	2	1/1/15/20	10/37/115/115	-
45	CLA	BA	801	-	1/1/15/20	9/37/115/115	-
45	CLA	BA	834	-	-	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AA	801	-	1/1/15/20	13/37/115/115	-
45	CLA	AB	811	-	1/1/15/20	15/37/115/115	-
45	CLA	BA	811	-	1/1/15/20	14/37/115/115	-
45	CLA	BA	821	-	-	12/37/115/115	-
46	PQN	BB	844	-	-	9/23/43/43	0/2/2/2
45	CLA	AB	837	-	1/1/12/20	7/19/97/115	-
53	LMG	B5	617	-	-	14/28/48/70	0/1/1/1
45	CLA	B3	311	-	1/1/13/20	7/23/101/115	-
45	CLA	A3	312	-	1/1/13/20	11/23/101/115	-
45	CLA	A6	603	16	1/1/15/20	9/37/115/115	-
48	BCR	A4	317	-	-	2/29/63/63	0/2/2/2
45	CLA	AB	841	-	1/1/15/20	7/37/115/115	-
55	XAT	B2	616	-	-	0/31/93/93	0/4/4/4
54	CHL	B2	606	-	3/3/15/26	2/12/110/137	-
52	LUT	A6	615	-	-	0/29/67/67	0/2/2/2
48	BCR	BA	851	-	-	8/29/63/63	0/2/2/2
45	CLA	BL	302	12	-	4/13/91/115	-
45	CLA	A6	611	47	1/1/7/20	6/10/70/115	-
45	CLA	AA	830	-	1/1/15/20	14/37/115/115	-
45	CLA	B1	314	-	1/1/14/20	9/31/109/115	-
45	CLA	AB	803	-	1/1/15/20	17/37/115/115	-
45	CLA	BL	303	-	-	7/31/109/115	-
50	LMU	AA	851	-	-	10/21/61/61	0/2/2/2
45	CLA	AA	806	1	1/1/15/20	13/37/115/115	-
48	BCR	AI	102	-	-	3/29/63/63	0/2/2/2
47	LHG	BF	305	-	-	18/49/49/53	-
45	CLA	AA	826	-	1/1/13/20	11/30/108/115	-
48	BCR	A6	617	-	-	2/29/63/63	0/2/2/2
45	CLA	BB	827	-	-	8/34/112/115	-
55	XAT	A4	316	-	-	0/31/93/93	0/4/4/4
45	CLA	BA	824	-	1/1/13/20	8/25/103/115	-
45	CLA	A6	614	-	1/1/10/20	2/11/89/115	-
45	CLA	A1	313	13	1/1/11/20	4/13/91/115	-
45	CLA	A6	605	-	1/1/10/20	1/9/88/115	-
48	BCR	B3	317	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AB	808	-	-	5/20/98/115	-
45	CLA	A4	312	-	1/1/11/20	4/13/91/115	-
48	BCR	BL	301	-	-	6/29/63/63	0/2/2/2
47	LHG	A3	319	45	-	14/26/26/53	-
45	CLA	BA	820	-	1/1/11/20	4/13/91/115	-
45	CLA	A6	612	16	1/1/11/20	6/11/89/115	-
48	BCR	AF	805	-	-	6/29/63/63	0/2/2/2
52	LUT	B1	316	-	-	14/29/67/67	0/2/2/2
52	LUT	AF	806	-	-	0/29/67/67	0/2/2/2
45	CLA	B3	307	14	1/1/11/20	3/13/91/115	-
45	CLA	A3	310	47	1/1/9/20	0/0/78/115	-
45	CLA	AB	802	-	1/1/15/20	16/37/113/115	-
45	CLA	B3	309	47	1/1/10/20	0/6/84/115	-
45	CLA	A1	306	-	1/1/11/20	9/18/96/115	-
48	BCR	BF	304	-	-	7/29/63/63	0/2/2/2
45	CLA	BA	810	-	1/1/15/20	12/37/115/115	-
45	CLA	BA	842	-	1/1/15/20	13/37/115/115	-
45	CLA	BB	817	-	1/1/10/20	4/9/87/115	-
49	SF4	BC	102	3	-	-	0/6/5/5
45	CLA	AA	807	-	1/1/12/20	4/19/97/115	-
45	CLA	AA	802	-	1/1/15/20	8/37/115/115	-
45	CLA	AA	813	-	1/1/15/20	17/37/115/115	-
45	CLA	BF	302	-	1/1/10/20	3/10/88/115	-
45	CLA	BA	816	-	1/1/11/20	2/13/91/115	-
45	CLA	BB	802	-	1/1/15/20	16/37/115/115	-
45	CLA	AA	831	-	1/1/11/20	7/16/94/115	-
45	CLA	AB	815	-	1/1/15/20	17/37/115/115	-
45	CLA	BB	823	-	1/1/11/20	4/14/92/115	-
45	CLA	BB	841	-	1/1/15/20	7/37/115/115	-
45	CLA	A6	601	15	1/1/11/20	2/15/93/115	-
45	CLA	B3	302	14	1/1/13/20	6/25/103/115	-
45	CLA	B3	303	-	1/1/11/20	2/9/85/115	-
45	CLA	BB	832	-	1/1/10/20	4/11/89/115	-
45	CLA	B5	611	18	1/1/10/20	4/8/86/115	-
45	CLA	BH	201	-	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	BCR	BI	101	-	-	6/29/63/63	0/2/2/2
45	CLA	A4	303	-	1/1/11/20	4/11/87/115	-
45	CLA	BB	814	-	1/1/10/20	1/11/89/115	-
45	CLA	AB	829	-	1/1/15/20	15/37/115/115	-
45	CLA	AA	808	1	1/1/15/20	10/37/115/115	-
54	CHL	A6	607	-	3/3/15/26	2/12/110/137	-
45	CLA	AB	810	2	1/1/15/20	16/37/115/115	-
45	CLA	A3	302	14	1/1/14/20	6/31/109/115	-
45	CLA	BB	842	-	1/1/15/20	9/37/115/115	-
45	CLA	AA	823	-	1/1/10/20	4/8/86/115	-
45	CLA	AA	841	-	-	10/37/115/115	-
45	CLA	AL	305	-	1/1/10/20	5/10/88/115	-
45	CLA	AA	832	-	1/1/13/20	7/27/105/115	-
45	CLA	AG	204	7	1/1/11/20	4/13/91/115	-
45	CLA	B5	604	-	1/1/11/20	3/11/87/115	-
45	CLA	AA	817	-	1/1/14/20	6/31/109/115	-
45	CLA	B2	611	17	1/1/11/20	7/11/89/115	-
45	CLA	BB	815	-	1/1/15/20	20/37/115/115	-
45	CLA	BA	819	-	1/1/15/20	13/37/115/115	-
45	CLA	AA	842	-	1/1/15/20	18/37/115/115	-
48	BCR	BL	306	-	-	15/29/63/63	0/2/2/2
52	LUT	A4	315	-	-	1/29/67/67	0/2/2/2
45	CLA	AB	840	-	1/1/15/20	7/37/115/115	-
45	CLA	BB	807	-	1/1/15/20	13/37/115/115	-
48	BCR	BA	847	-	-	5/29/63/63	0/2/2/2
45	CLA	BB	831	-	1/1/13/20	8/27/105/115	-
45	CLA	AK	203	-	1/1/11/20	7/15/93/115	-
48	BCR	AB	844	-	-	5/29/63/63	0/2/2/2
45	CLA	BA	839	-	-	6/21/99/115	-
45	CLA	BB	835	-	1/1/15/20	16/37/115/115	-
45	CLA	B5	608	18	1/1/11/20	4/11/89/115	-
54	CHL	B1	303	13	3/3/17/26	3/19/117/137	-
48	BCR	A1	319	-	-	4/29/63/63	0/2/2/2
45	CLA	AB	842	47	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BB	822	-	1/1/10/20	2/8/86/115	-
45	CLA	A1	309	-	1/1/11/20	5/11/89/115	-
52	LUT	A1	317	-	-	0/29/67/67	0/2/2/2
45	CLA	A4	313	-	1/1/12/20	9/19/97/115	-
45	CLA	AB	834	-	1/1/15/20	16/37/115/115	-
45	CLA	AB	827	-	1/1/14/20	14/34/112/115	-
54	CHL	A4	314	15	3/3/15/26	0/10/106/137	-
48	BCR	AA	846	-	-	6/29/63/63	0/2/2/2
48	BCR	AL	306	-	-	5/29/63/63	0/2/2/2
45	CLA	BA	829	-	1/1/15/20	11/37/115/115	-
45	CLA	B3	305	-	1/1/10/20	2/10/86/115	-
45	CLA	AA	835	-	1/1/11/20	0/11/89/115	-
54	CHL	B2	601	17	3/3/17/26	9/24/122/137	-
48	BCR	AB	847	-	-	0/29/63/63	0/2/2/2
47	LHG	B3	318	45	-	11/26/26/53	-
45	CLA	BB	820	-	1/1/14/20	12/31/109/115	-
45	CLA	BB	840	-	-	4/16/94/115	-
45	CLA	AB	839	-	1/1/11/20	3/16/94/115	-
47	LHG	AA	844	-	-	18/53/53/53	-
45	CLA	B1	311	13	1/1/14/20	3/29/107/115	-
49	SF4	BC	101	3	-	-	0/6/5/5
48	BCR	BJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	B2	613	-	1/1/10/20	1/11/89/115	-
45	CLA	AB	835	-	-	7/31/109/115	-
48	BCR	BA	849	-	-	4/29/63/63	0/2/2/2
49	SF4	I	202	37	-	-	0/6/5/5
45	CLA	BA	840	-	1/1/15/20	13/37/115/115	-
55	XAT	B3	316	-	-	0/31/93/93	0/4/4/4
45	CLA	BA	825	-	1/1/15/20	15/37/115/115	-
45	CLA	BA	818	-	-	6/27/105/115	-
45	CLA	AA	840	-	1/1/15/20	14/37/115/115	-
45	CLA	B1	315	-	1/1/10/20	0/4/80/115	-
45	CLA	B3	312	-	1/1/10/20	0/6/84/115	-
49	SF4	AC	101	3	-	-	0/6/5/5
47	LHG	B5	618	45	-	13/34/34/53	-
45	CLA	AB	822	-	1/1/11/20	5/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BB	826	-	1/1/15/20	10/37/115/115	-
50	LMU	AL	301	-	-	11/20/60/61	0/2/2/2
45	CLA	B2	610	47	1/1/7/20	7/10/70/115	-
53	LMG	A1	321	-	-	17/39/59/70	0/1/1/1
45	CLA	AK	201	11	1/1/8/20	0/2/74/115	-
45	CLA	AB	813	-	1/1/10/20	3/11/89/115	-
45	CLA	BA	814	-	1/1/11/20	6/13/91/115	-
45	CLA	B3	314	-	1/1/10/20	0/6/84/115	-
45	CLA	AA	827	-	1/1/15/20	18/37/115/115	-
45	CLA	BA	803	-	1/1/15/20	18/37/115/115	-
45	CLA	AA	822	-	1/1/10/20	3/10/88/115	-
54	CHL	B2	614	17	3/3/15/26	0/12/110/137	-
45	CLA	AB	806	-	1/1/15/20	15/37/115/115	-
54	CHL	A6	606	-	3/3/15/26	2/10/108/137	-
47	LHG	A3	301	-	-	11/40/40/53	-
48	BCR	AA	847	-	-	13/29/63/63	0/2/2/2
45	CLA	B1	307	-	1/1/9/20	4/8/82/115	-
45	CLA	B1	312	47	1/1/10/20	0/4/80/115	-
54	CHL	A1	303	13	3/3/17/26	4/21/119/137	-
45	CLA	A3	314	-	1/1/8/20	0/0/74/115	-
45	CLA	B1	305	-	1/1/12/20	6/23/101/115	-
45	CLA	B1	309	-	-	2/11/89/115	-
45	CLA	BA	808	1	1/1/15/20	10/37/115/115	-
46	PQN	AA	843	-	-	6/23/43/43	0/2/2/2
45	CLA	AA	825	-	1/1/15/20	10/37/115/115	-
45	CLA	A4	307	15	1/1/11/20	1/13/91/115	-
48	BCR	BJ	101	-	-	0/29/63/63	0/2/2/2
45	CLA	BB	809	-	-	5/22/100/115	-
45	CLA	AF	803	-	1/1/10/20	2/10/88/115	-
45	CLA	BA	823	-	1/1/10/20	4/8/86/115	-
45	CLA	B1	310	13	1/1/10/20	3/6/82/115	-
50	LMU	BA	854	-	-	8/19/59/61	0/2/2/2
45	CLA	BK	201	11	1/1/8/20	0/2/74/115	-
49	SF4	AC	102	3	-	-	0/6/5/5
45	CLA	BA	807	-	1/1/12/20	4/19/97/115	-
45	CLA	BA	831	-	1/1/11/20	7/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BB	813	-	1/1/13/20	4/25/101/115	-
54	CHL	B2	605	-	3/3/15/26	3/10/108/137	-
54	CHL	A6	608	-	3/3/17/26	8/19/117/137	-
48	BCR	AB	845	-	-	6/29/63/63	0/2/2/2
45	CLA	AB	818	-	1/1/13/20	10/30/108/115	-
45	CLA	BG	202	7	1/1/11/20	6/13/91/115	-
45	CLA	AB	830	-	1/1/13/20	10/27/105/115	-
45	CLA	BB	829	-	1/1/15/20	17/37/115/115	-
45	CLA	BA	809	1	-	9/19/97/115	-
45	CLA	A3	315	-	1/1/10/20	0/6/84/115	-
45	CLA	BB	843	47	1/1/15/20	11/37/115/115	-
45	CLA	AB	825	-	1/1/15/20	14/37/115/115	-
45	CLA	BB	837	-	1/1/10/20	4/10/88/115	-
45	CLA	BF	301	-	1/1/12/20	8/24/102/115	-
47	LHG	B2	618	45	-	22/39/39/53	-
48	BCR	BK	204	-	-	1/29/63/63	0/2/2/2
50	LMU	AB	853	-	-	13/21/61/61	0/2/2/2
55	XAT	A1	318	-	-	0/31/93/93	0/4/4/4
45	CLA	A4	311	-	1/1/13/20	7/26/104/115	-
45	CLA	B3	301	14	1/1/14/20	5/31/109/115	-
45	CLA	BB	833	-	-	4/11/89/115	-
45	CLA	BB	818	-	1/1/13/20	8/25/103/115	-
45	CLA	AA	829	-	1/1/15/20	18/37/115/115	-
45	CLA	A1	310	13	1/1/10/20	2/8/84/115	-
45	CLA	AA	837	-	1/1/12/20	6/21/99/115	-
45	CLA	B2	608	17	1/1/11/20	3/13/91/115	-
45	CLA	BA	822	-	1/1/10/20	8/10/88/115	-
54	CHL	B3	306	-	3/3/16/26	5/13/111/137	-
47	LHG	B1	302	-	-	14/40/40/53	-
45	CLA	A4	309	-	1/1/10/20	3/10/88/115	-
45	CLA	AB	812	-	1/1/13/20	8/25/101/115	-
45	CLA	B5	603	-	1/1/11/20	4/13/89/115	-
45	CLA	AA	809	1	1/1/12/20	5/19/97/115	-
45	CLA	BJ	102	10	1/1/10/20	4/10/88/115	-
48	BCR	BB	845	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BA	833	-	1/1/15/20	15/37/115/115	-
54	CHL	B5	605	-	3/3/15/26	2/8/106/137	-
49	SF4	I	201	37	-	-	0/6/5/5
48	BCR	AA	852	-	-	5/29/63/63	0/2/2/2
48	BCR	AI	101	-	-	7/29/63/63	0/2/2/2
45	CLA	AA	818	-	-	7/30/108/115	-
47	LHG	A6	618	45	-	17/40/40/53	-
45	CLA	AA	811	-	1/1/15/20	11/37/115/115	-
48	BCR	AB	848	-	-	2/29/63/63	0/2/2/2
45	CLA	A6	604	-	1/1/10/20	2/9/87/115	-
45	CLA	AL	304	-	-	9/31/109/115	-
45	CLA	BA	805	-	1/1/15/20	22/37/115/115	-
45	CLA	A4	310	15	1/1/10/20	5/8/86/115	-
53	LMG	A4	318	-	-	15/34/54/70	0/1/1/1
55	XAT	B1	317	-	-	0/31/93/93	0/4/4/4
45	CLA	B2	603	-	1/1/11/20	4/11/89/115	-
45	CLA	B2	612	17	1/1/15/20	13/37/115/115	-
45	CLA	BB	825	-	1/1/11/20	6/13/91/115	-
45	CLA	BA	806	1	1/1/15/20	18/37/115/115	-
45	CLA	AB	826	-	1/1/14/20	6/34/112/115	-
45	CLA	AB	824	-	1/1/10/20	4/11/89/115	-
45	CLA	AG	203	-	1/1/10/20	3/10/88/115	-
45	CLA	BB	834	-	-	9/37/115/115	-
45	CLA	BA	836	1	-	6/13/91/115	-
45	CLA	AB	820	-	1/1/13/20	8/25/103/115	-
45	CLA	BB	824	-	-	18/37/115/115	-
45	CLA	B5	602	18	-	9/31/109/115	-
50	LMU	BA	853	-	-	9/20/60/61	0/2/2/2
54	CHL	B5	606	-	3/3/15/26	2/8/104/137	-
45	CLA	A1	315	-	1/1/10/20	0/4/80/115	-

The worst 5 of 2732 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	611	CLA	C1A-NA	12.32	1.40	1.29
45	B2	610	CLA	C1A-NA	11.85	1.40	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BB	844	PQN	C12-C13	9.75	1.56	1.33
46	AA	843	PQN	C12-C13	9.56	1.55	1.33
46	BA	843	PQN	C12-C13	9.52	1.55	1.33

The worst 5 of 4157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BL	306	BCR	C37-C22-C21	-32.50	77.40	122.92
48	BL	306	BCR	C35-C13-C14	-31.52	78.78	122.92
48	BL	306	BCR	C34-C9-C10	-29.92	81.01	122.92
48	BG	203	BCR	C35-C13-C14	-29.72	81.29	122.92
48	BL	306	BCR	C37-C22-C23	-27.87	74.16	118.08

5 of 310 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
45	AA	801	CLA	ND
45	AA	802	CLA	ND
45	AA	803	CLA	ND
45	AA	805	CLA	ND
45	AA	806	CLA	ND

5 of 3005 torsion outliers are listed below:

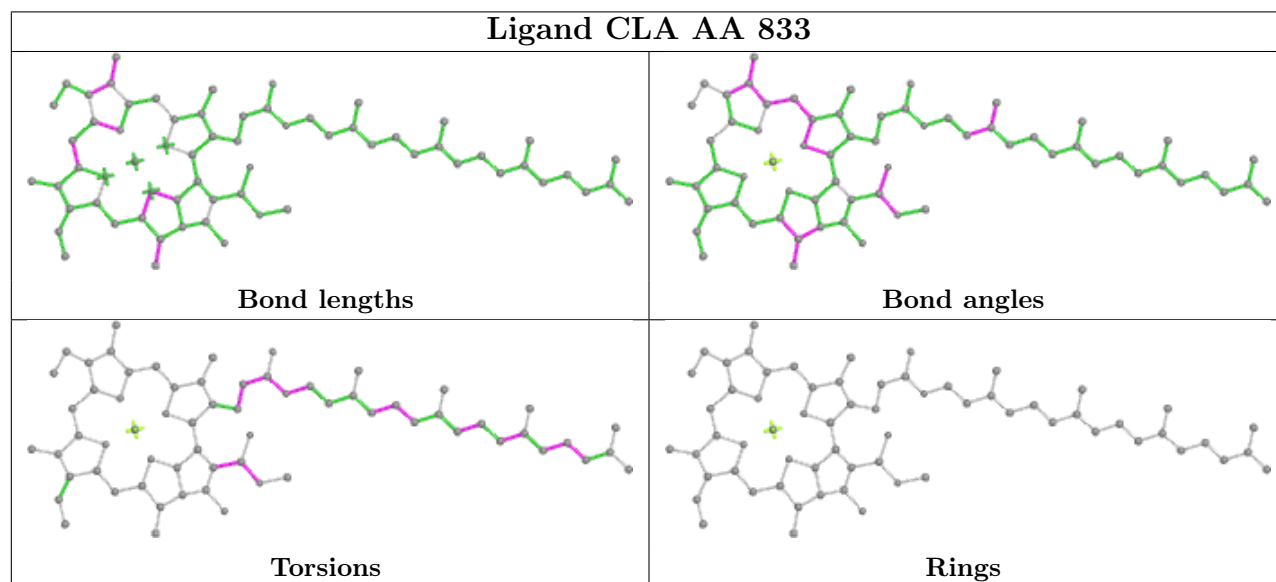
Mol	Chain	Res	Type	Atoms
45	AA	801	CLA	CBD-CGD-O2D-CED
45	AA	802	CLA	CBD-CGD-O2D-CED
45	AA	804	CLA	C1A-C2A-CAA-CBA
45	AA	804	CLA	C3A-C2A-CAA-CBA
45	AA	805	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

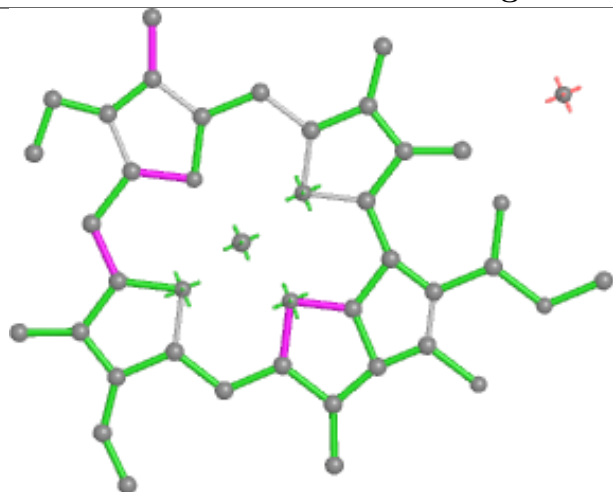
No monomer is involved in short contacts.

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

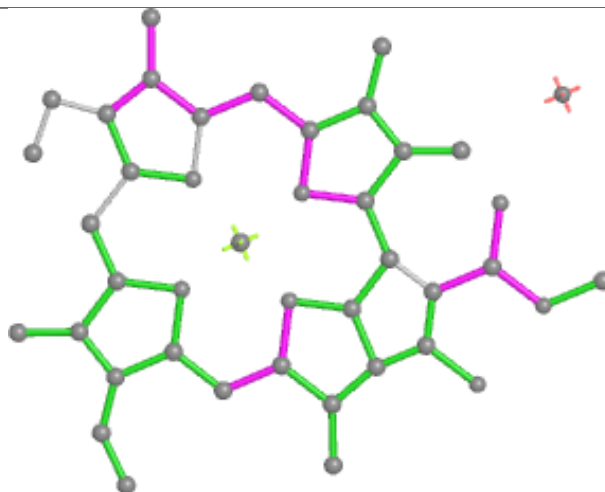
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



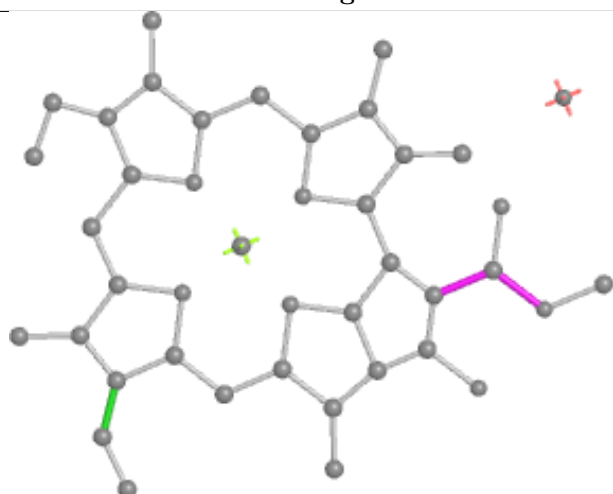
Ligand CLA BA 844



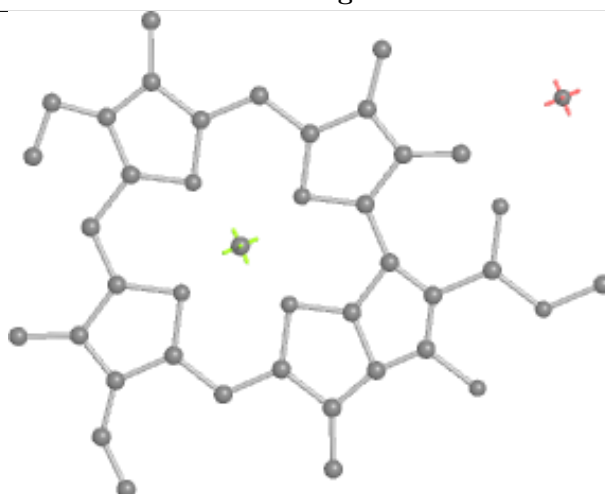
Bond lengths



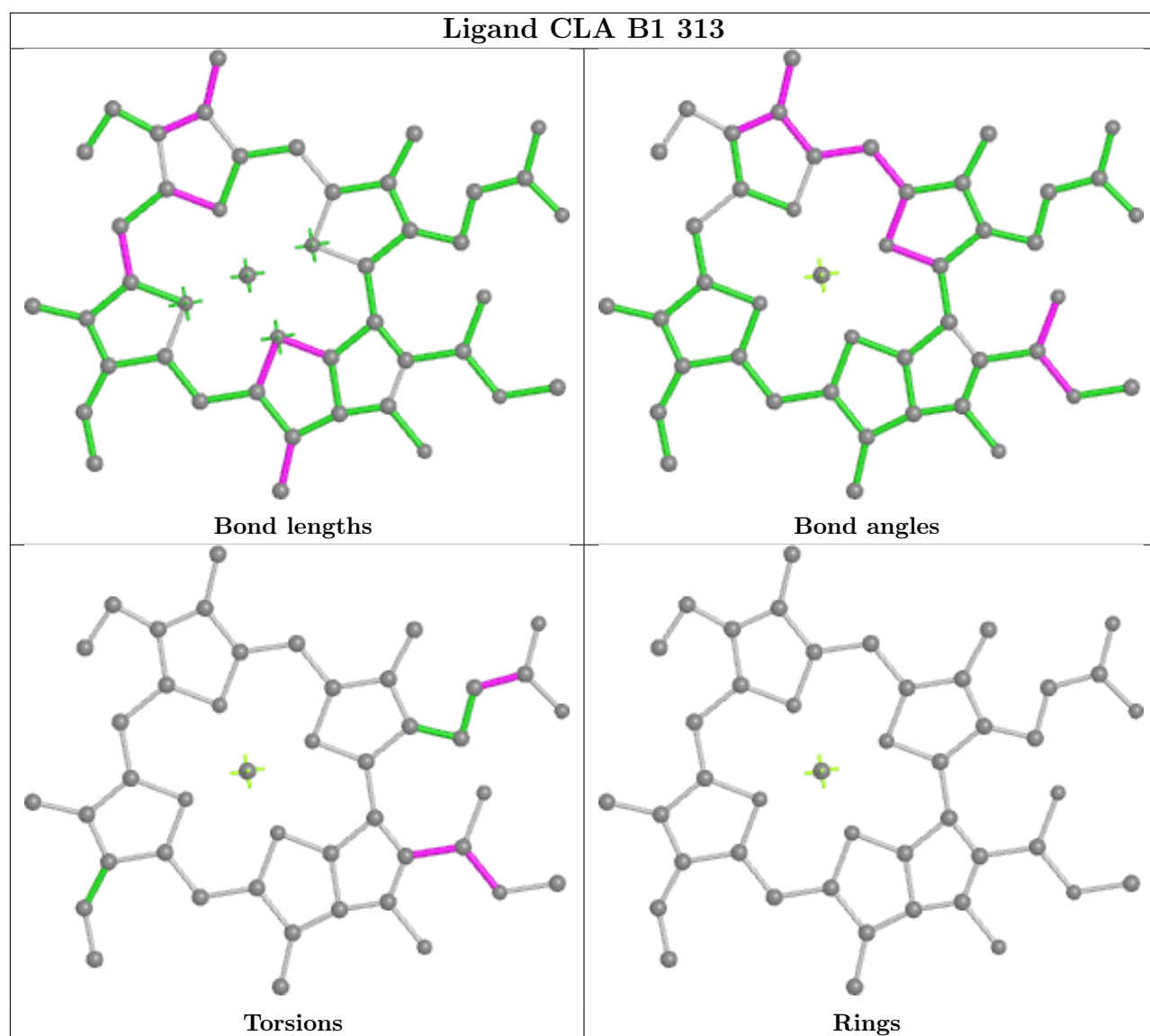
Bond angles



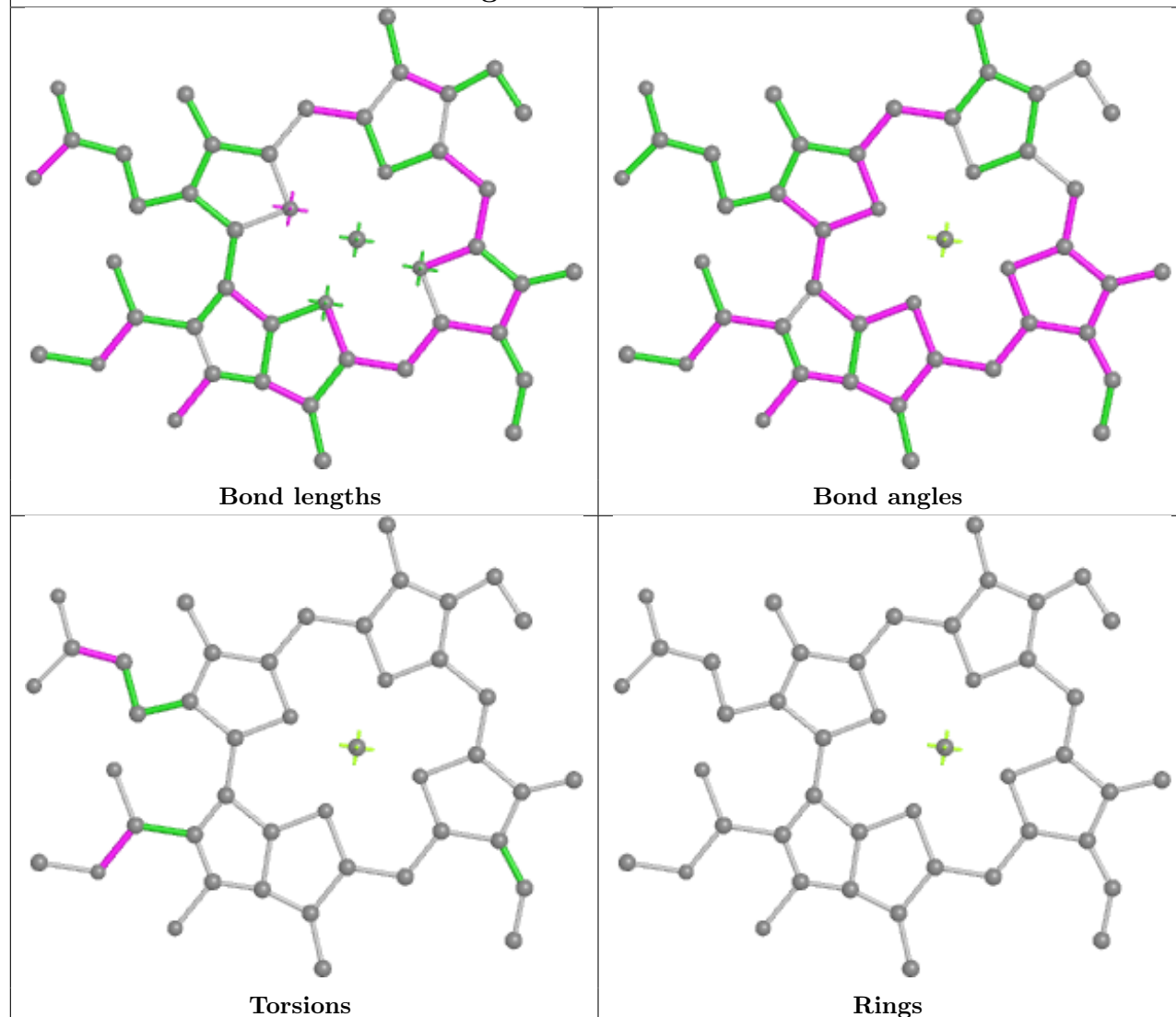
Torsions



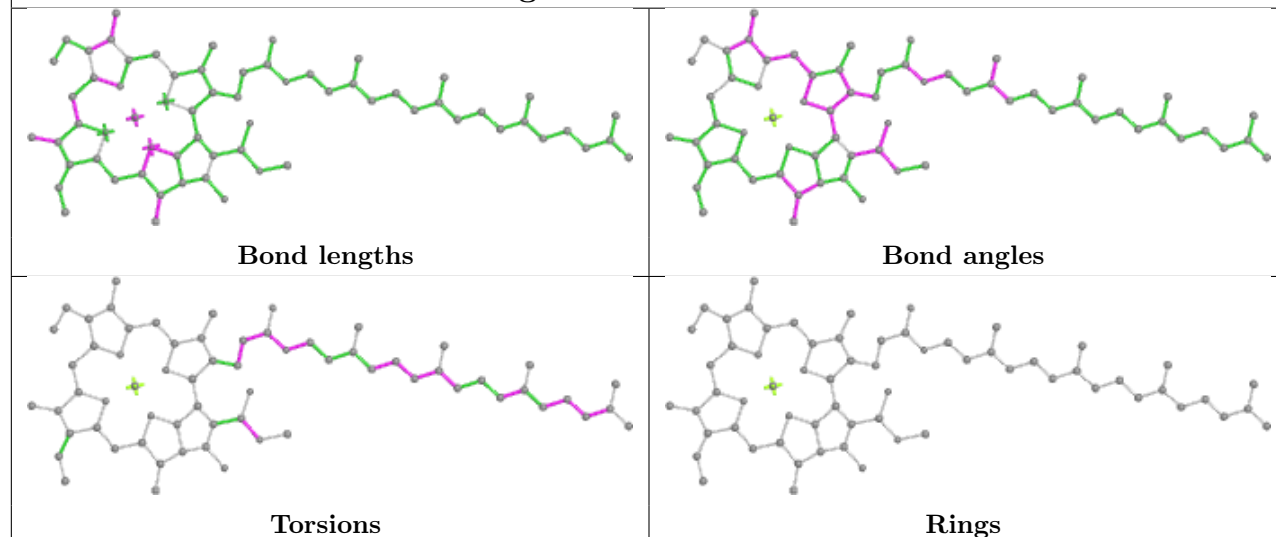
Rings

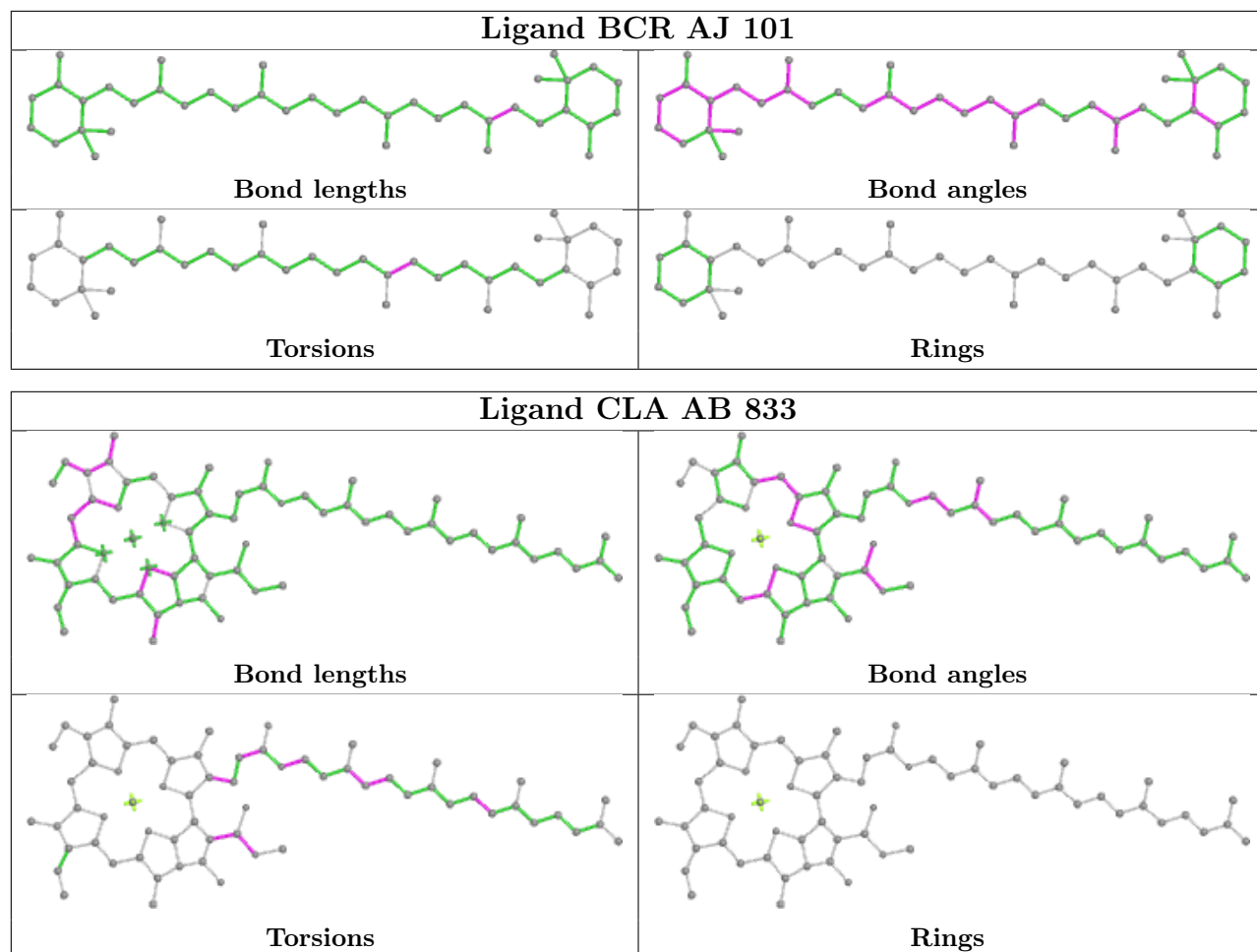


Ligand CHL A3 307

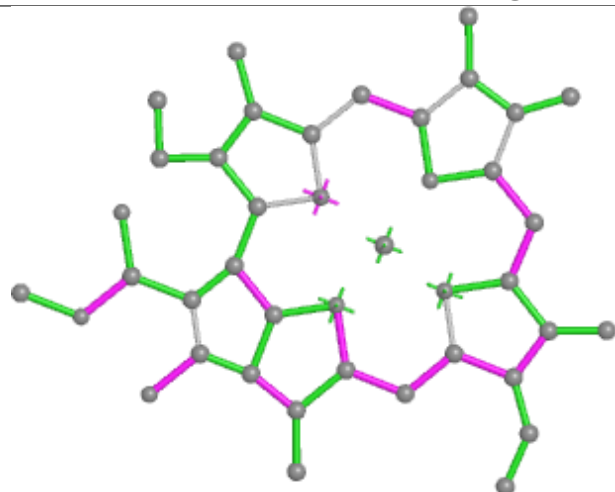


Ligand CLA AB 801

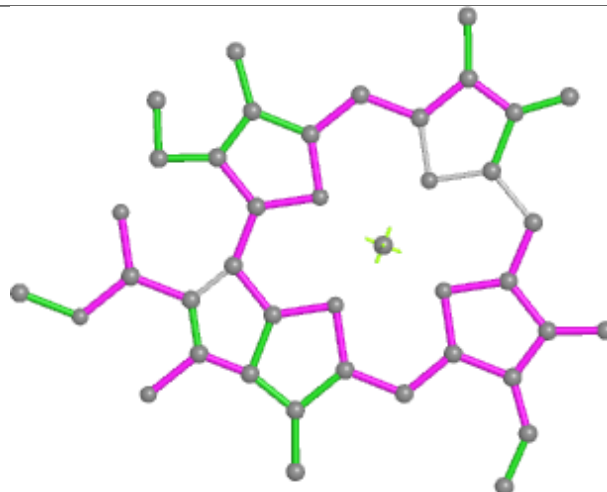




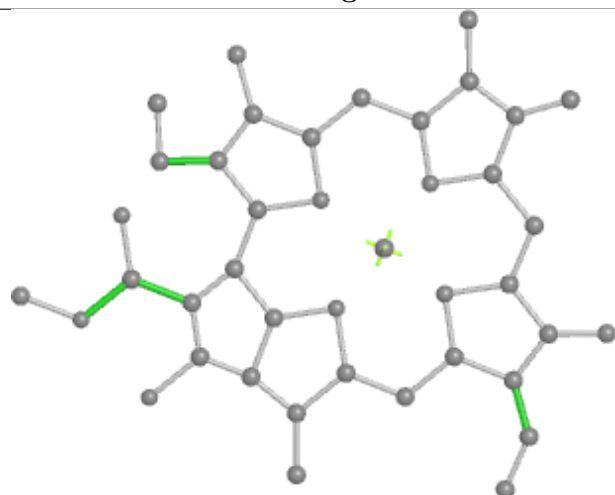
Ligand CHL A4 305



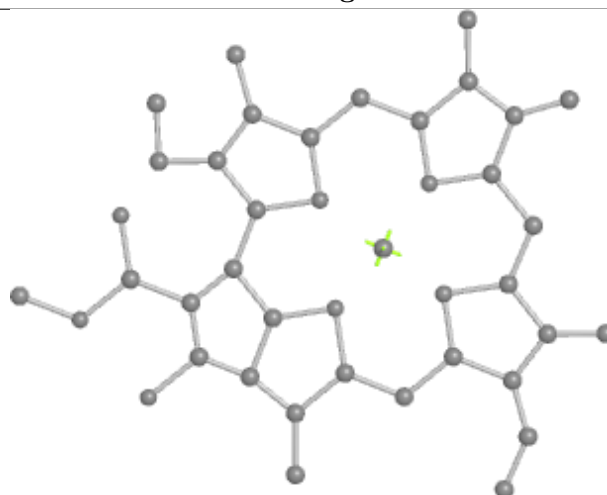
Bond lengths



Bond angles

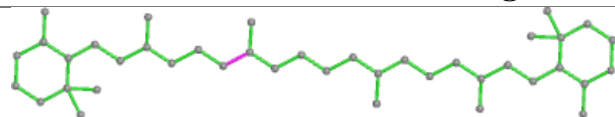


Torsions

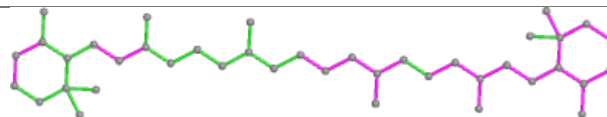


Rings

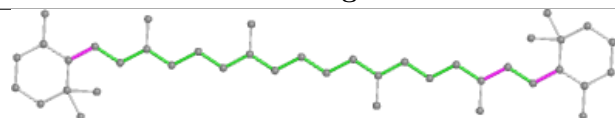
Ligand BCR BA 856



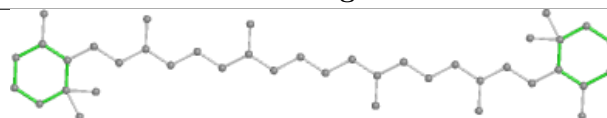
Bond lengths



Bond angles

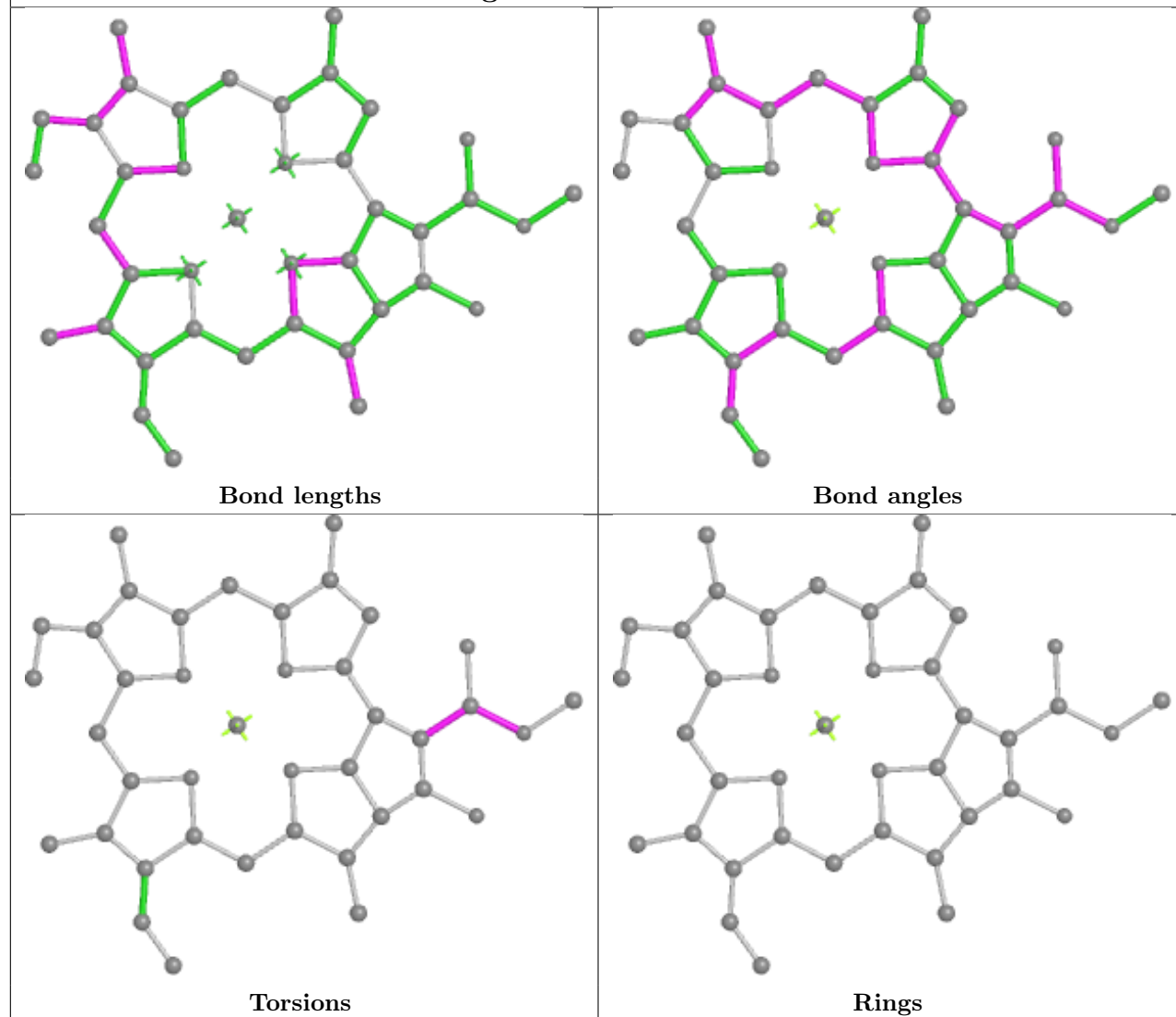


Torsions

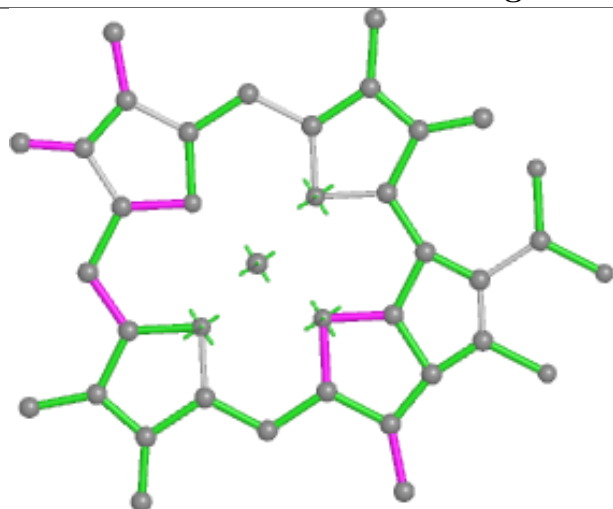


Rings

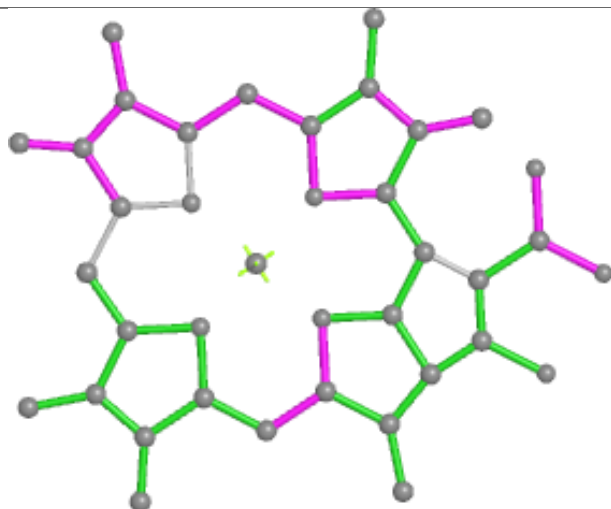
Ligand CLA A1 307



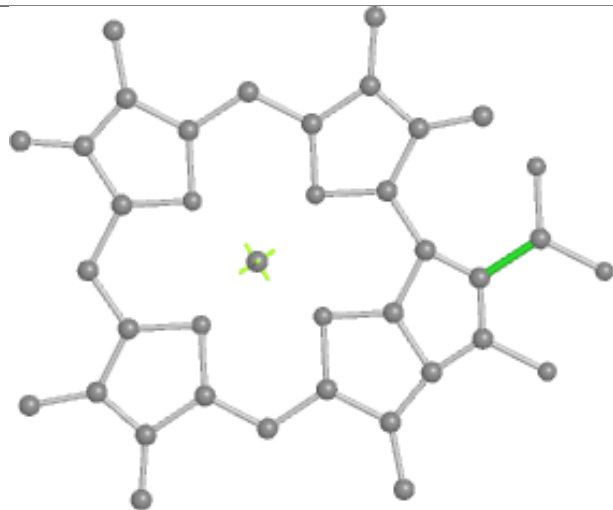
Ligand CLA A1 312



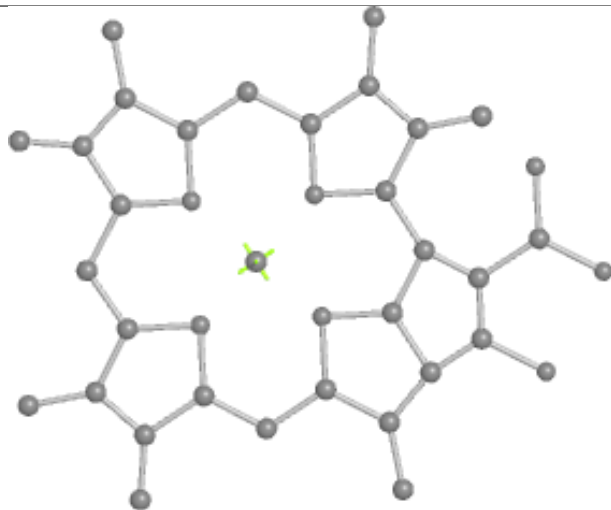
Bond lengths



Bond angles

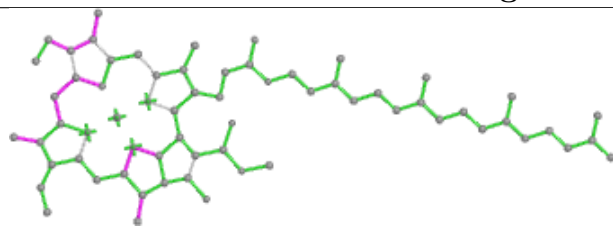


Torsions

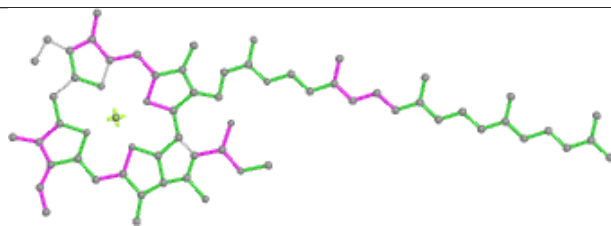


Rings

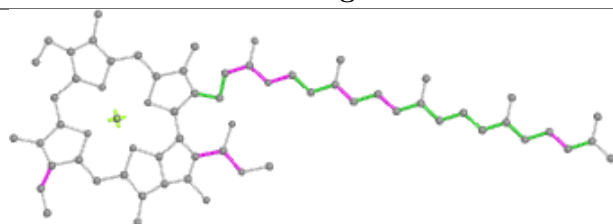
Ligand CLA AA 834



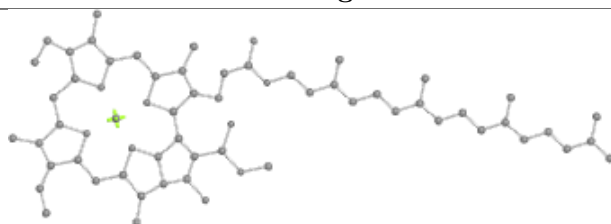
Bond lengths



Bond angles

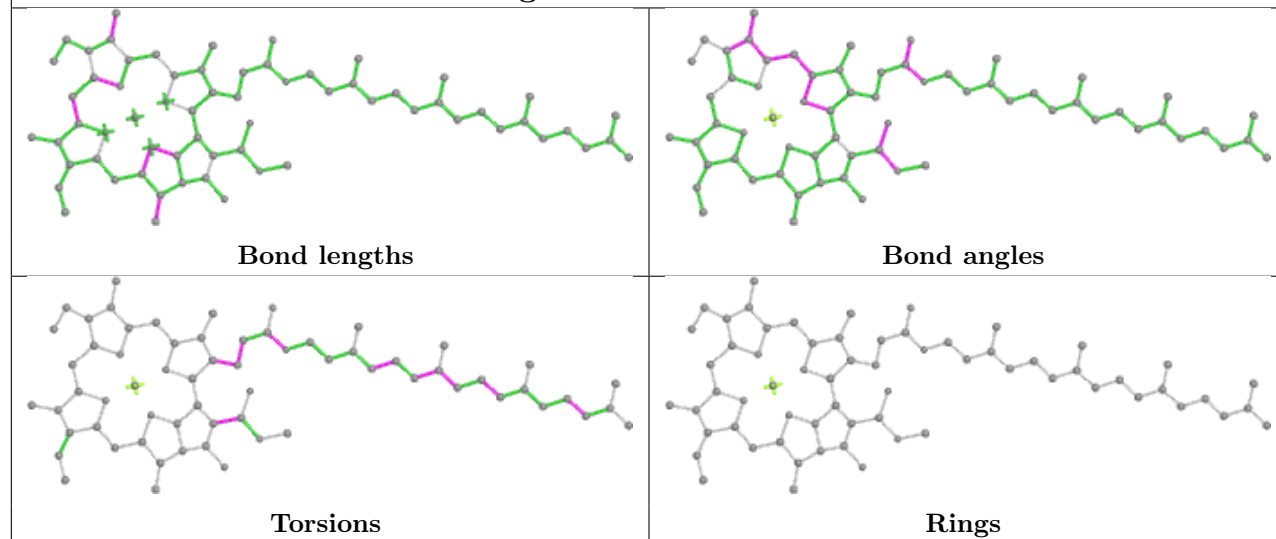


Torsions

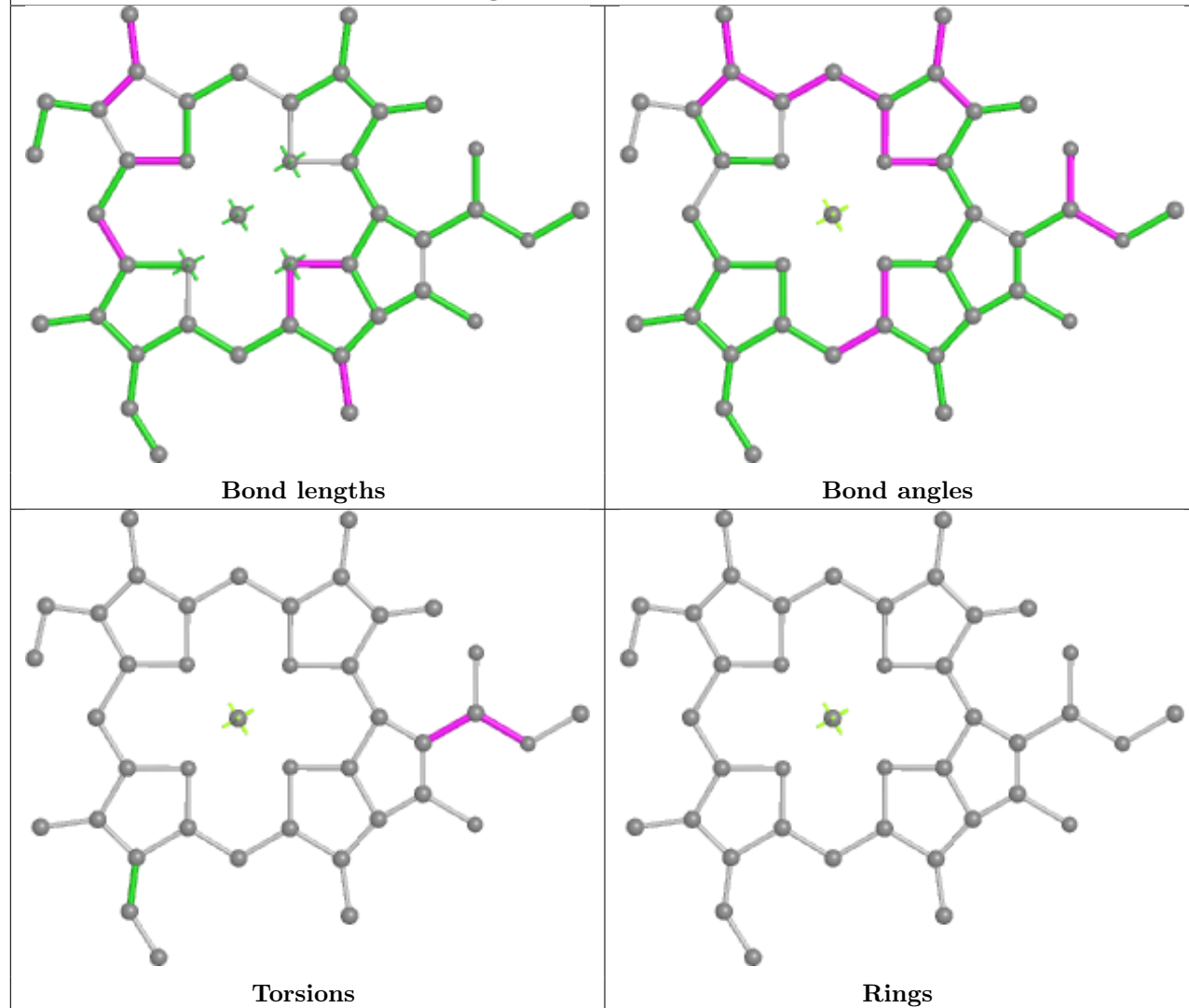


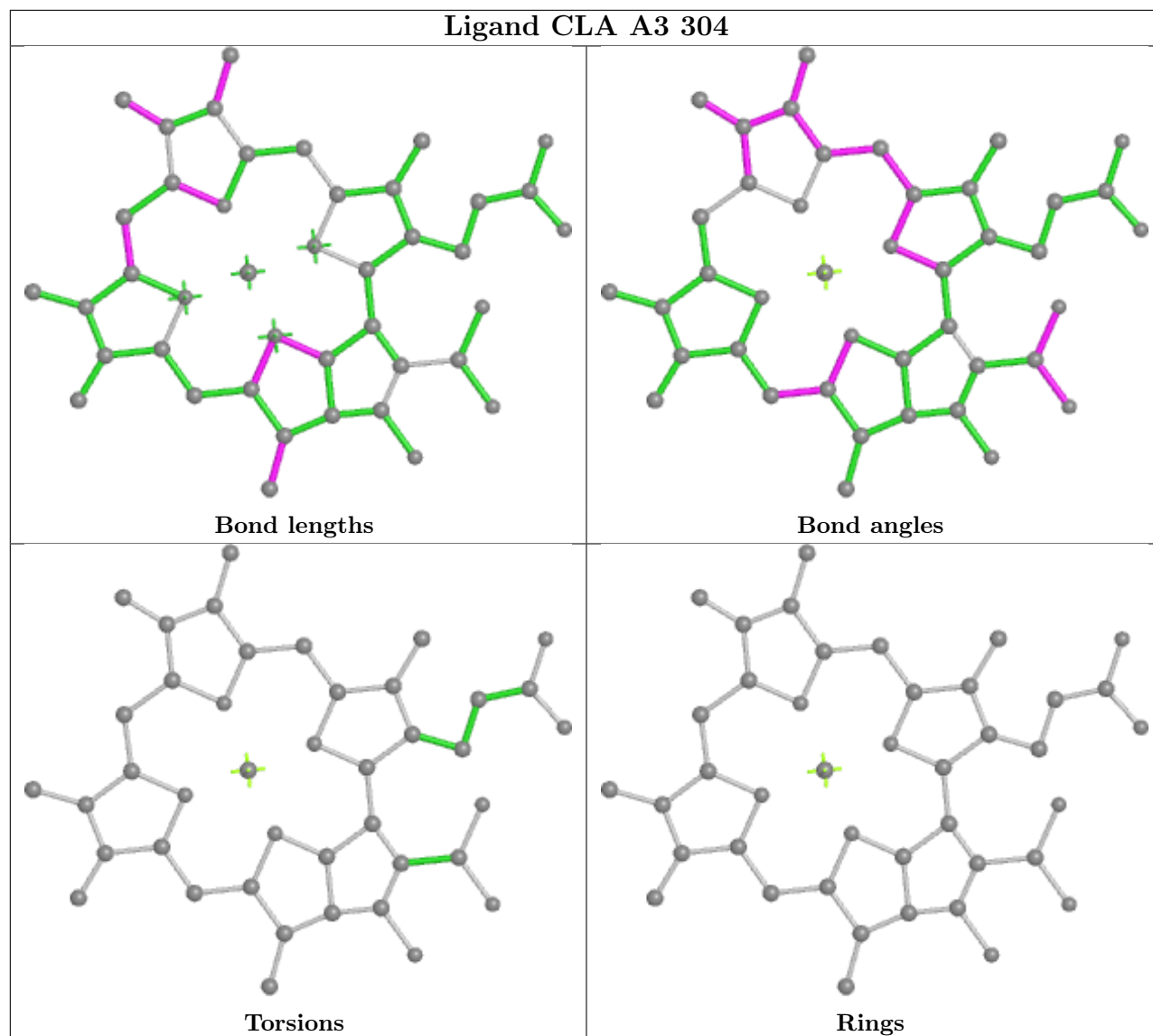
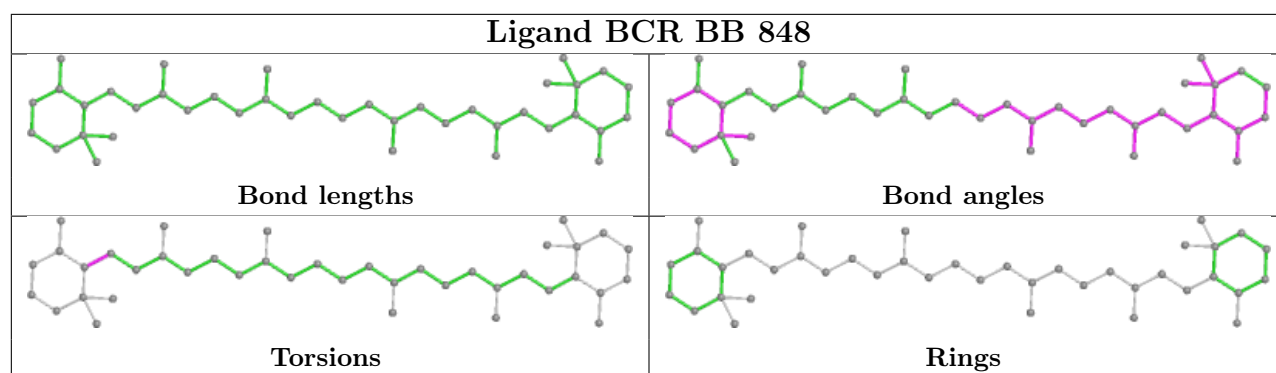
Rings

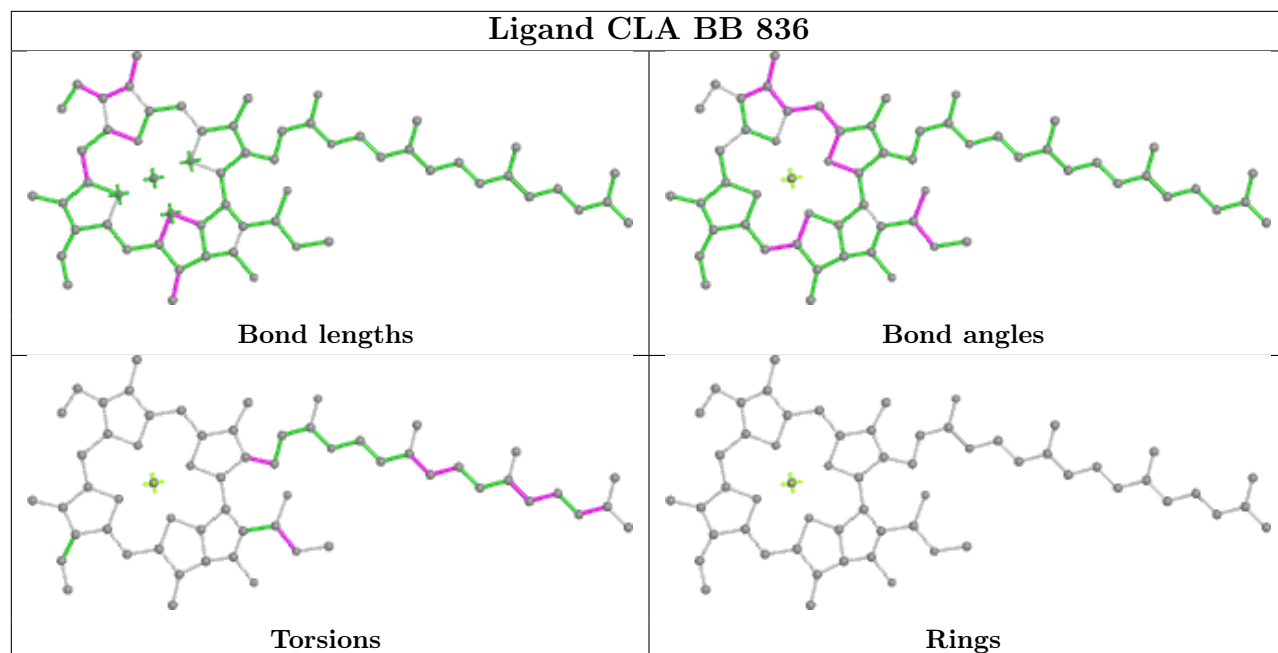
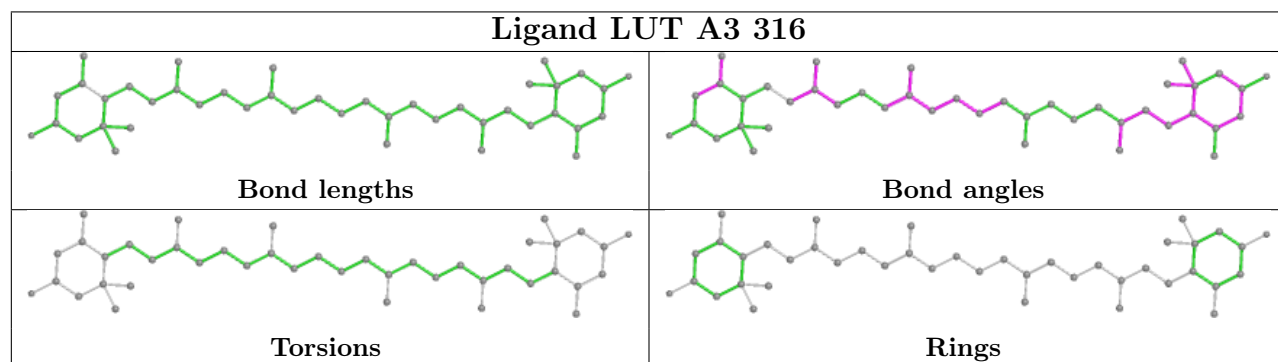
Ligand CLA BA 827

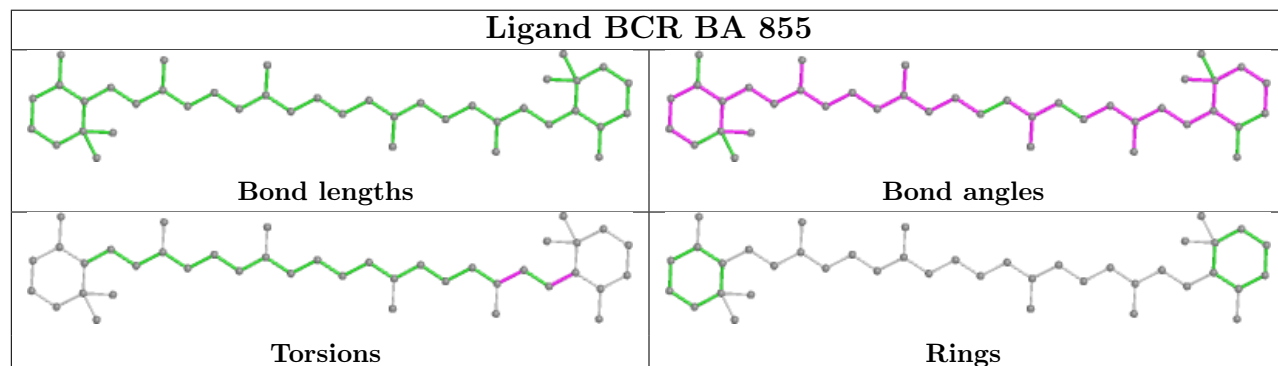
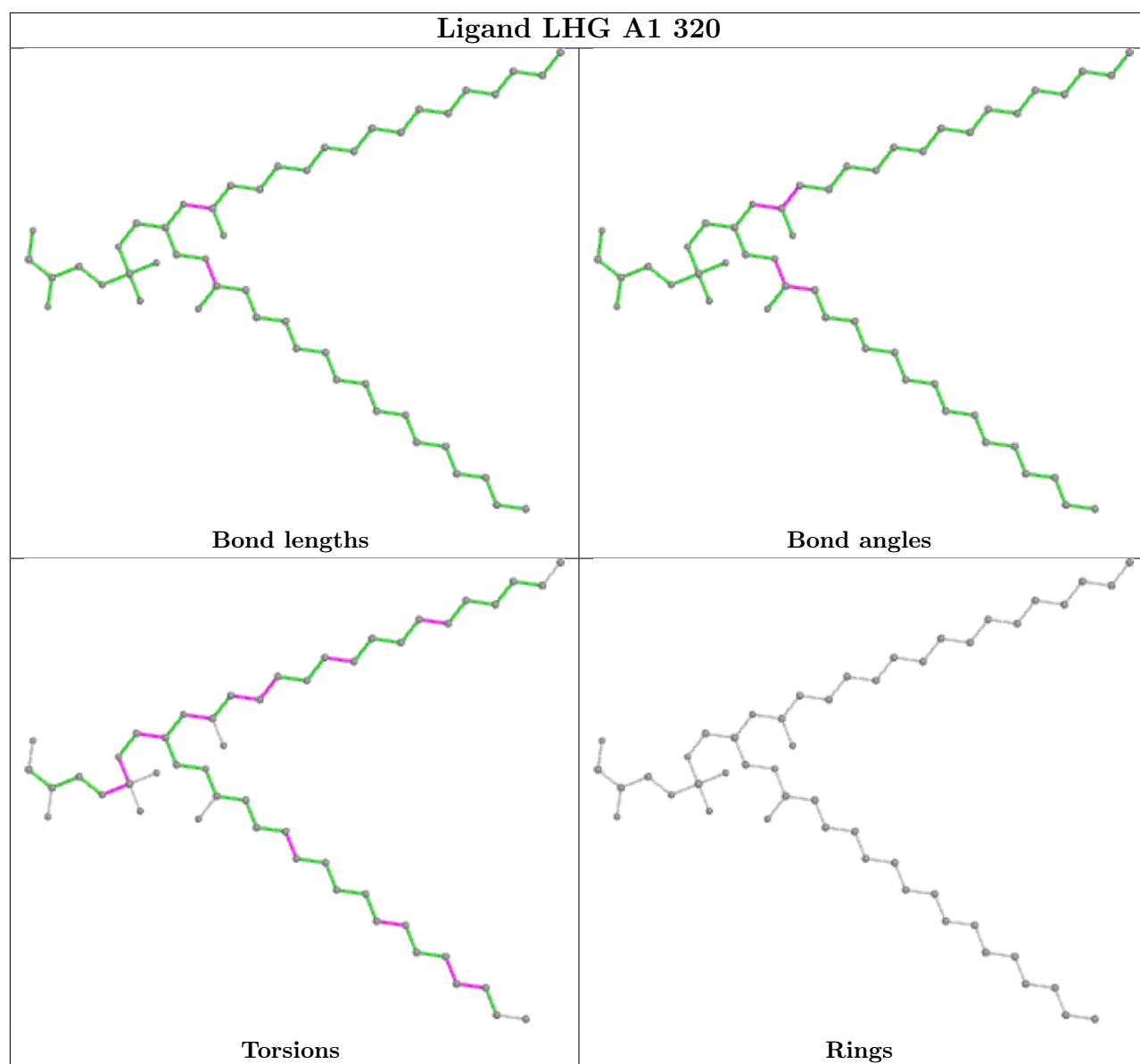


Ligand CLA AL 303

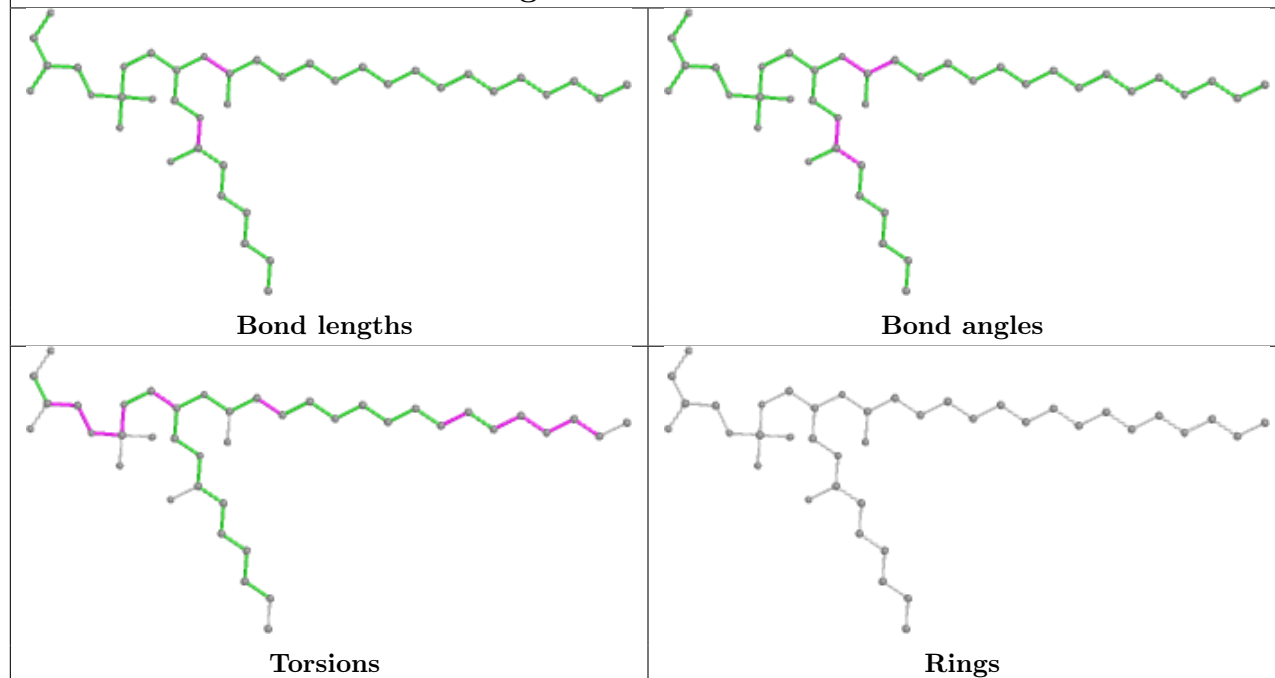




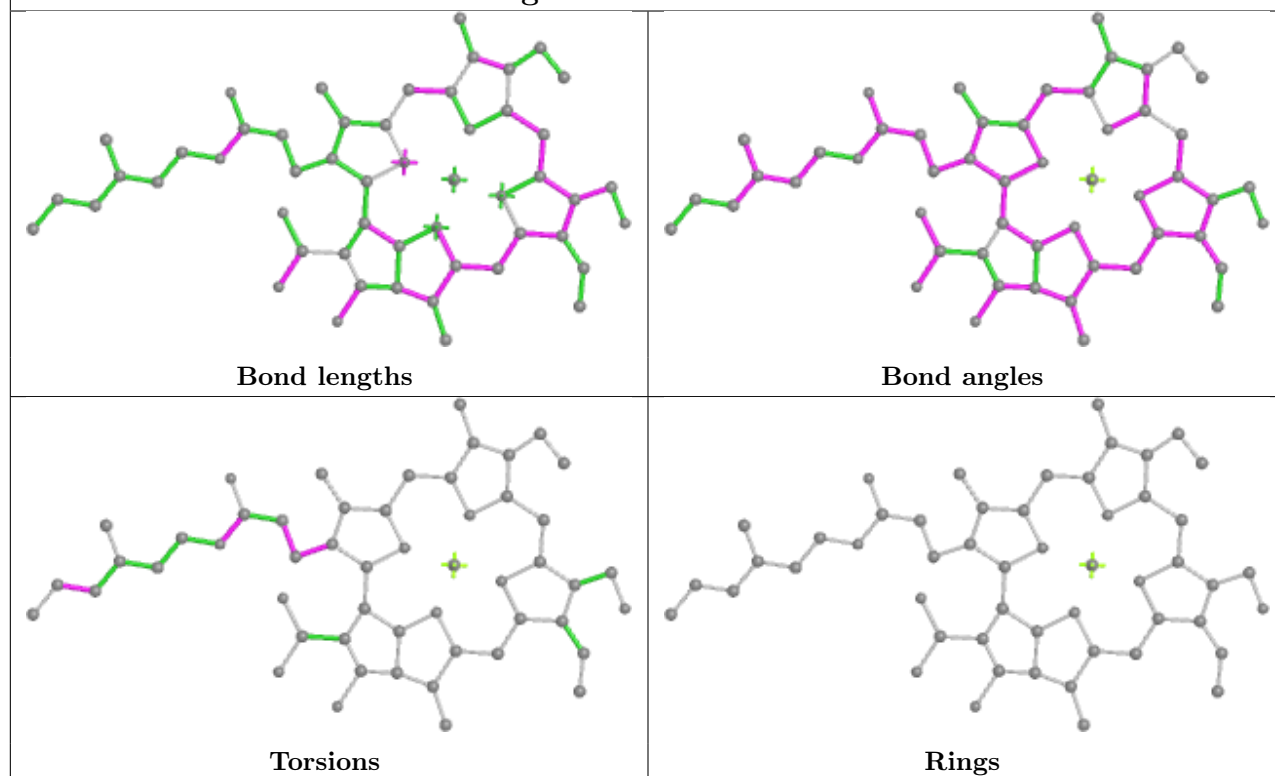
Ligand CLA BB 836**Ligand LUT A3 316**

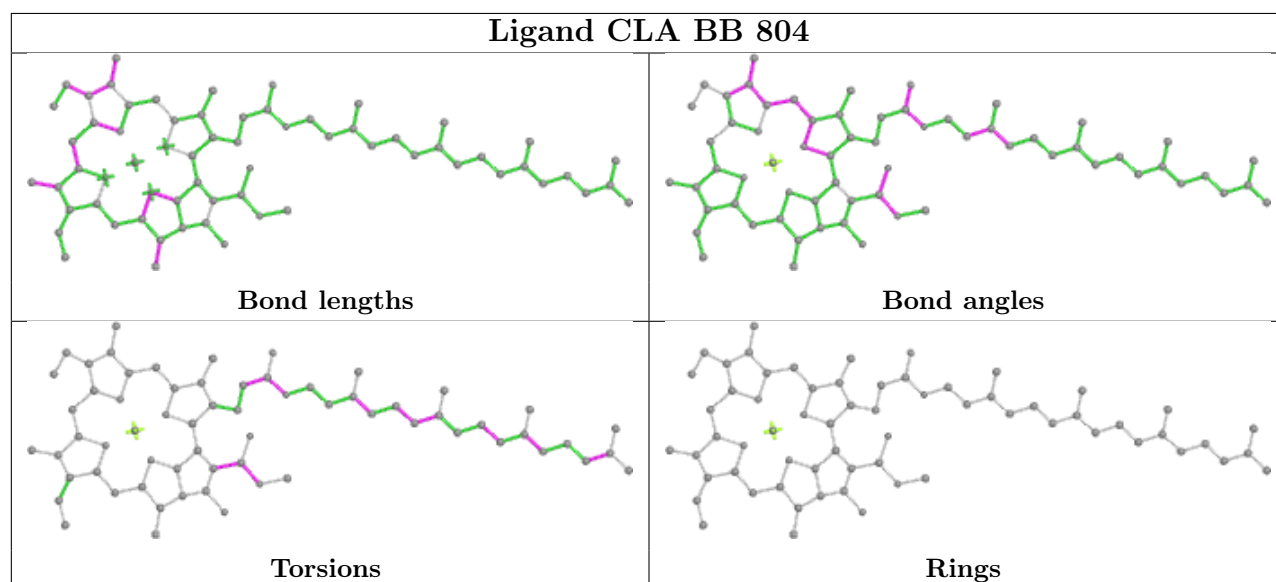
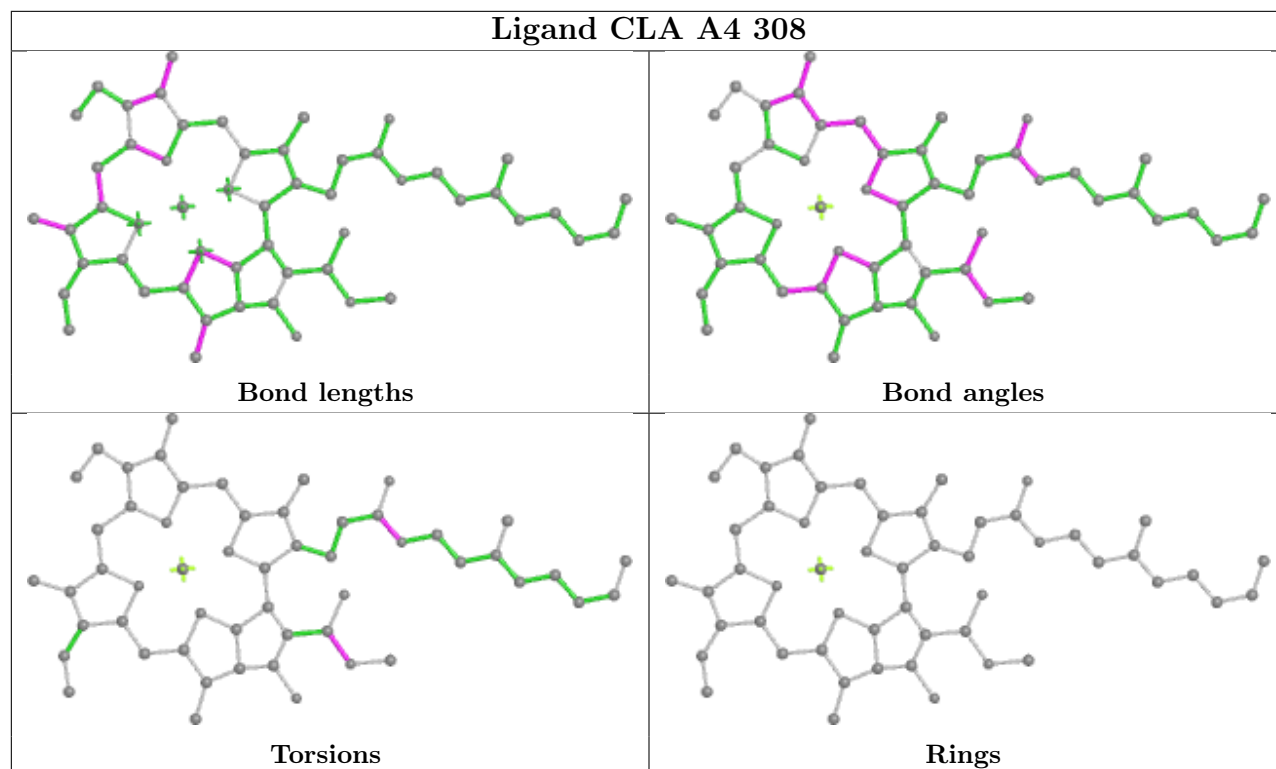
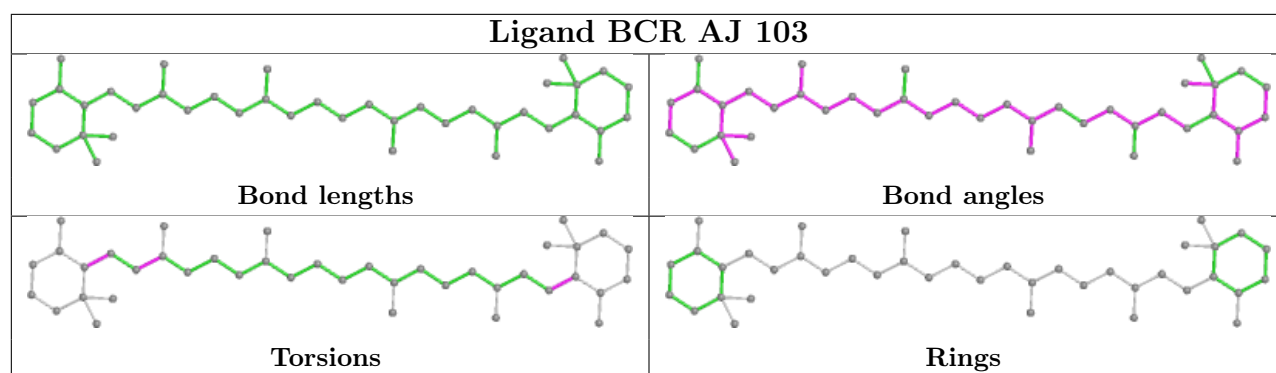


Ligand LHG AJ 104

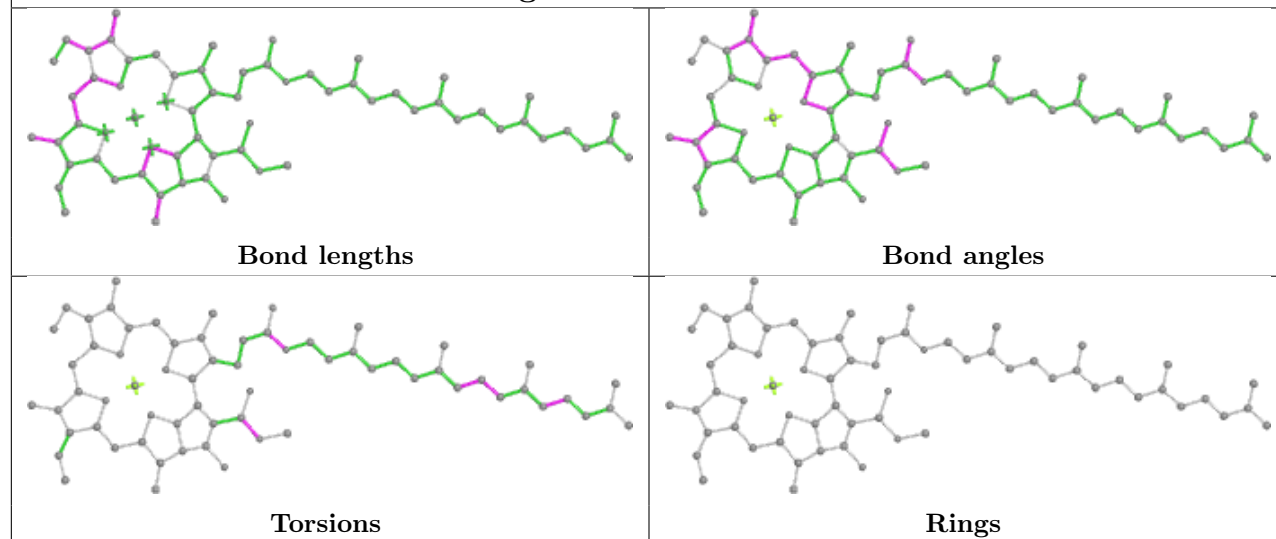


Ligand CHL A6 602

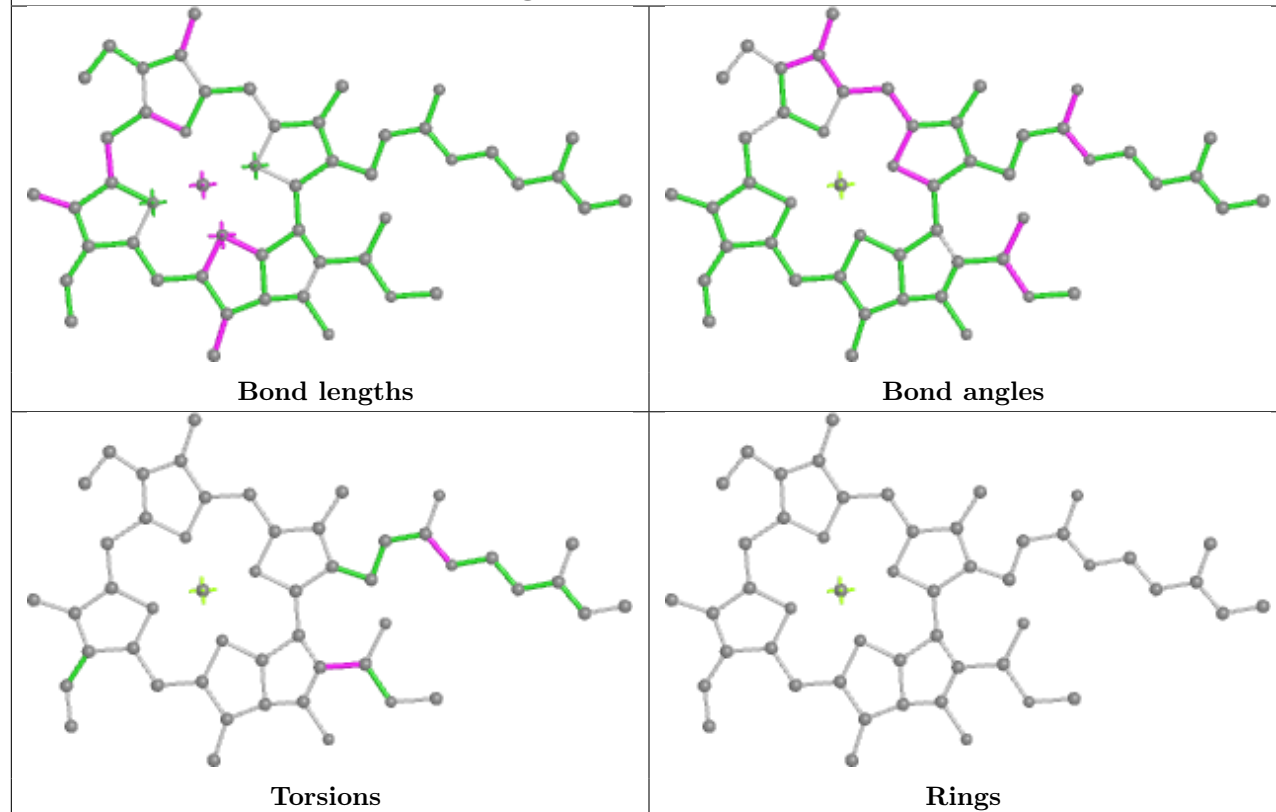


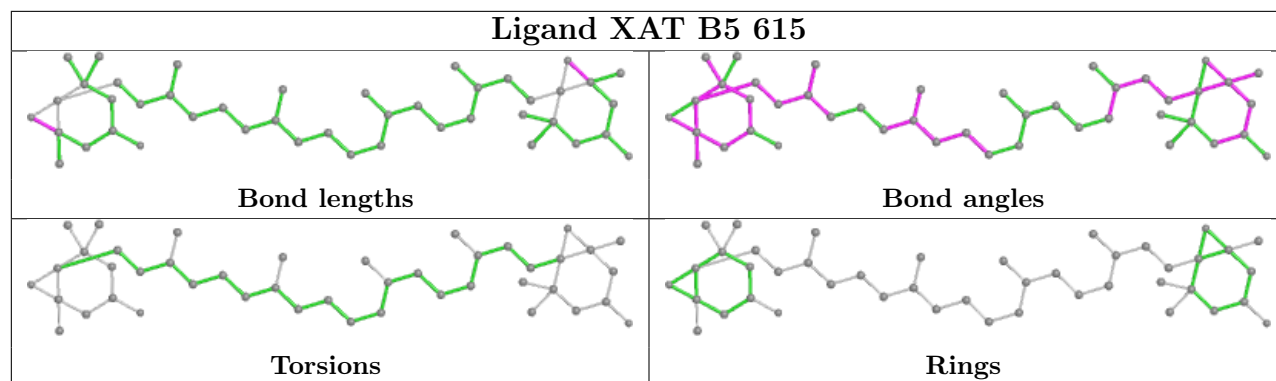
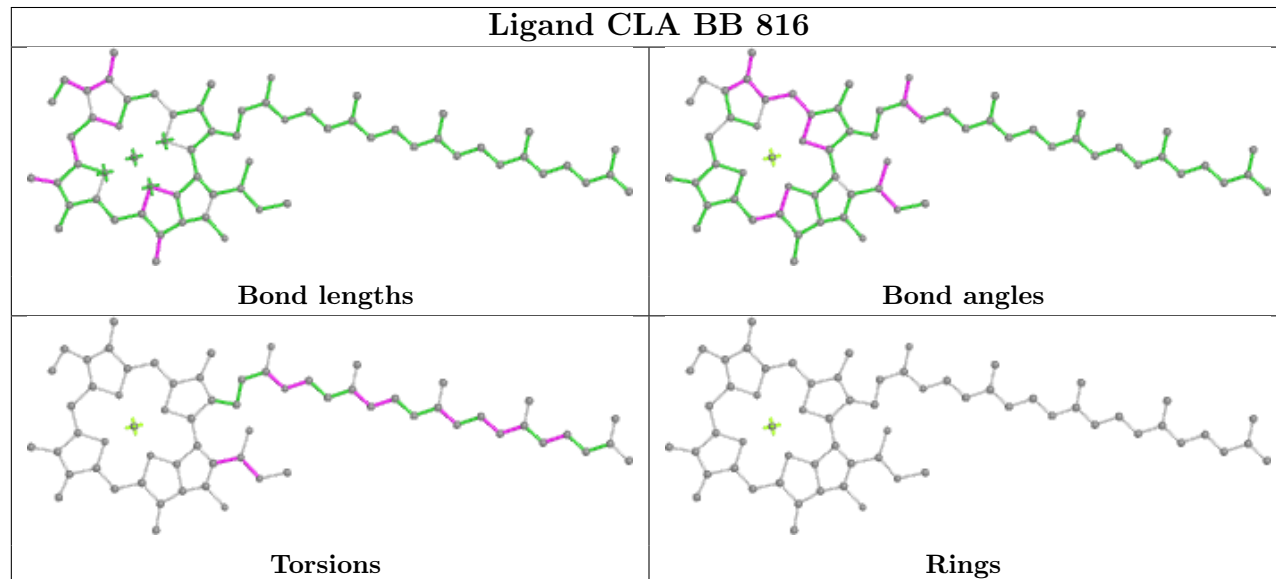
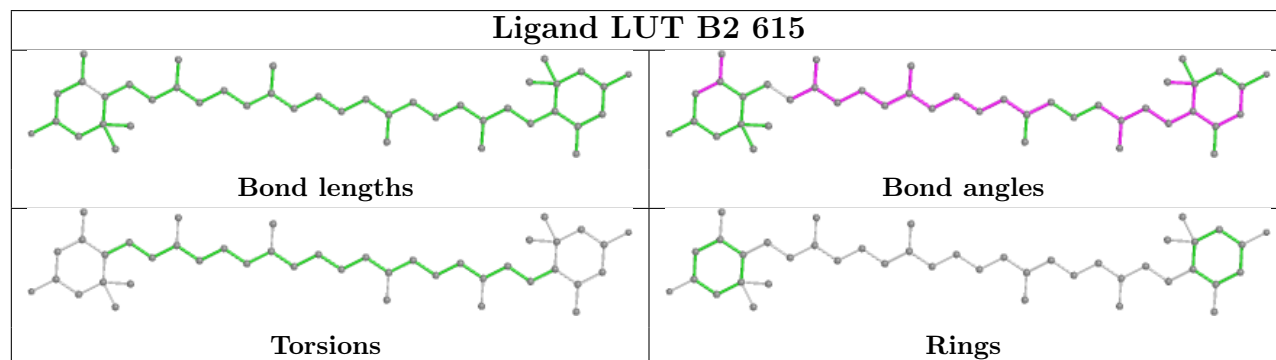


Ligand CLA AB 832

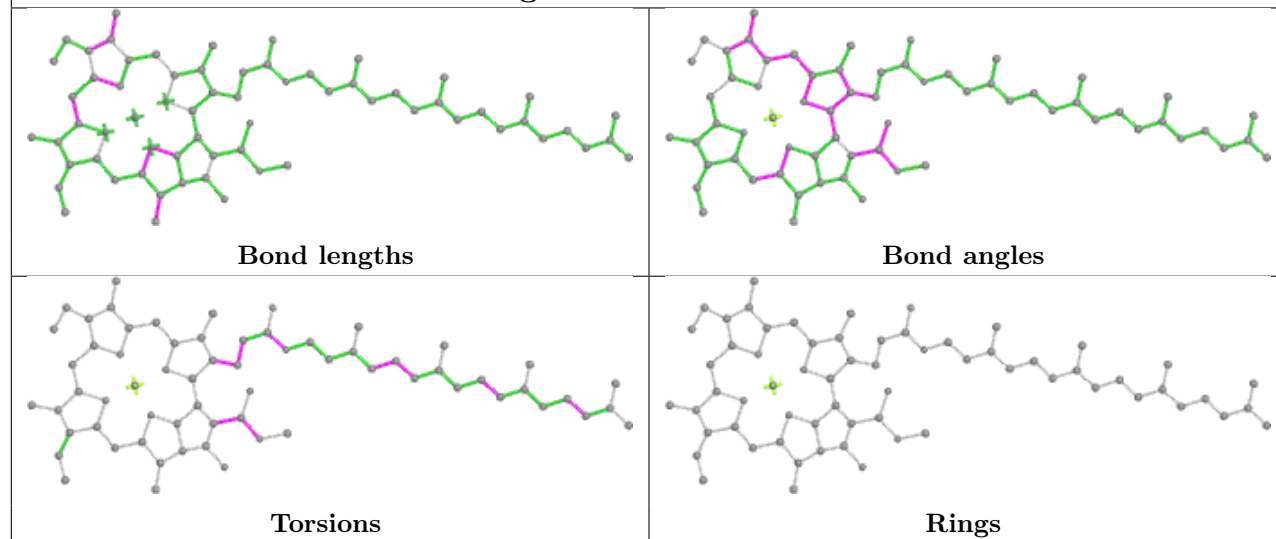


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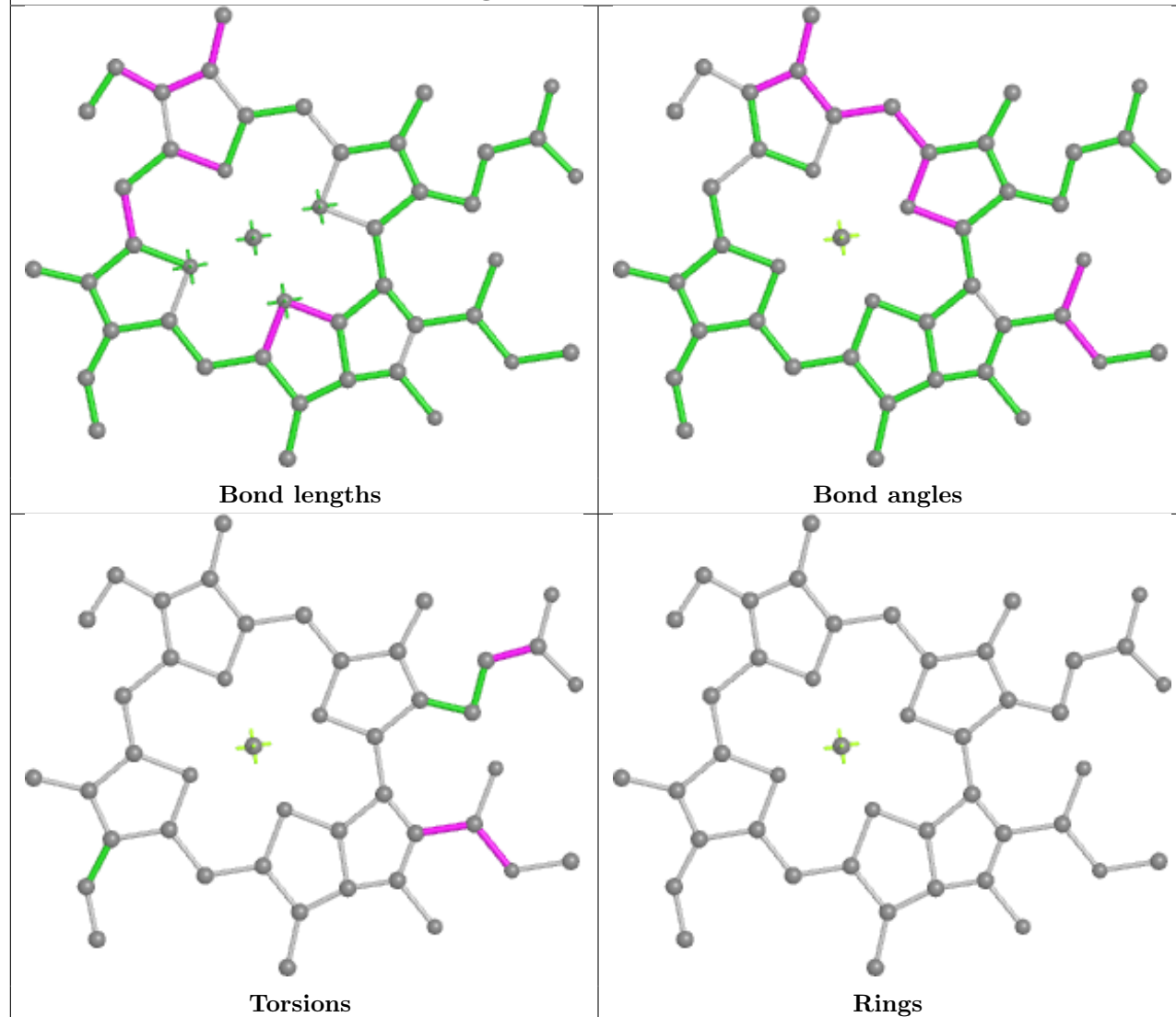


Ligand XAT B5 615**Ligand CLA BB 816****Ligand LUT B2 615**

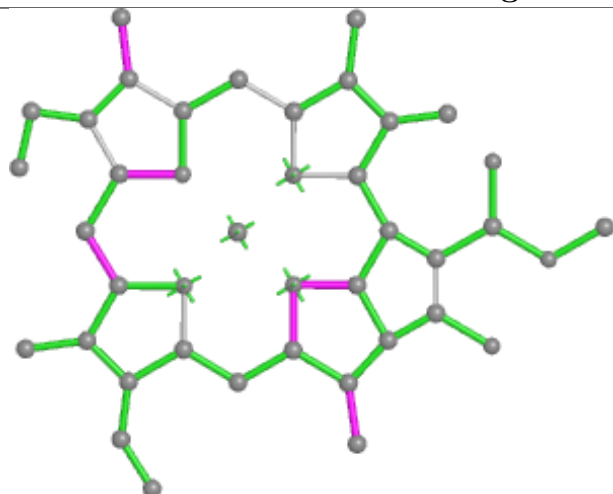
Ligand CLA BB 812



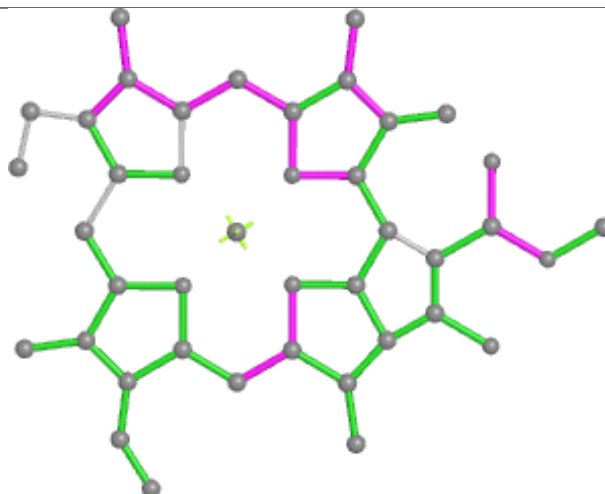
Ligand CLA BA 835



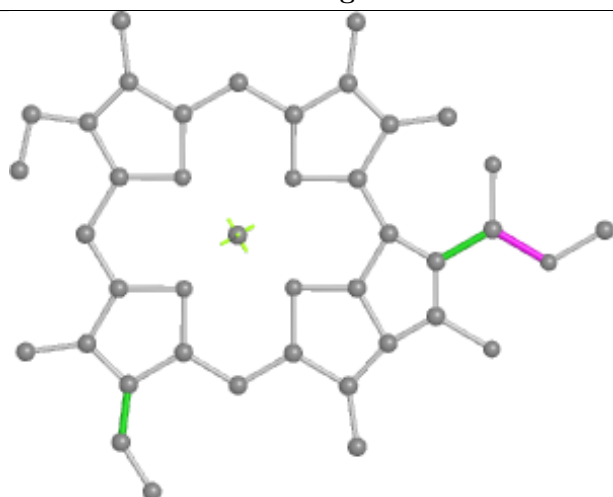
Ligand CLA AB 805



Bond lengths



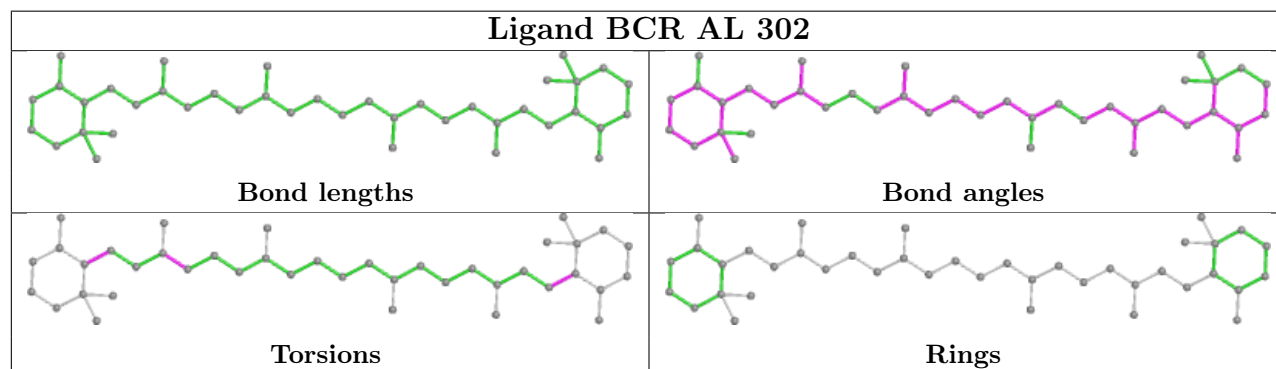
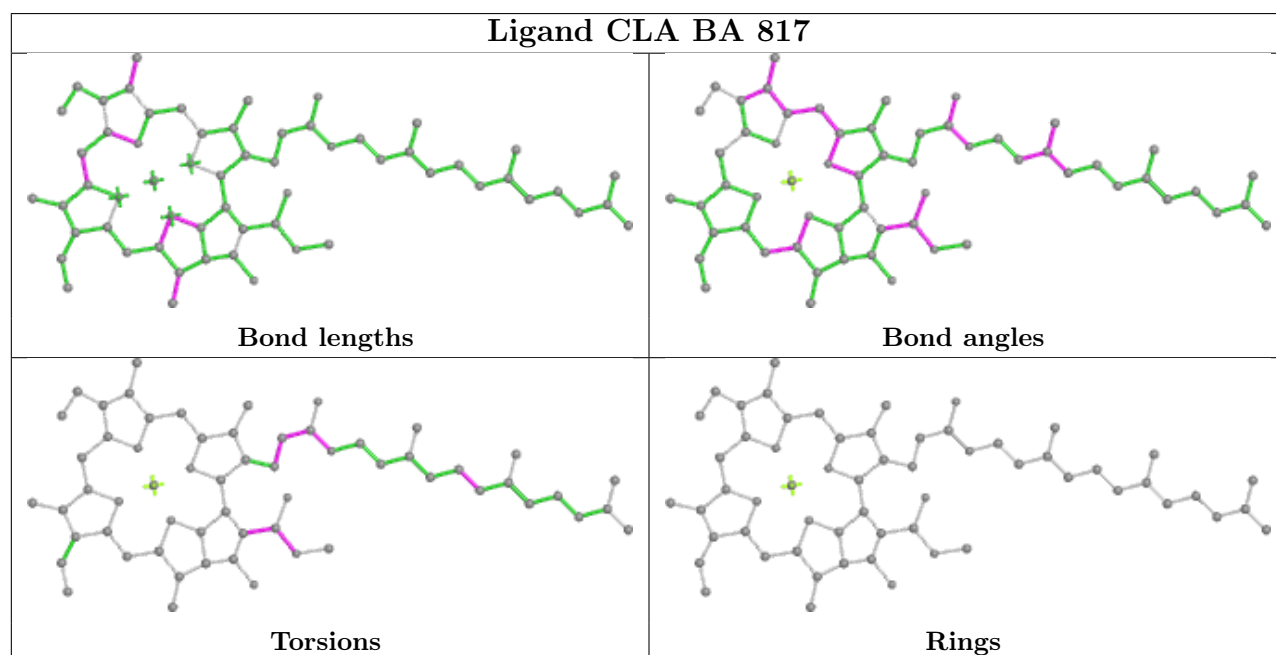
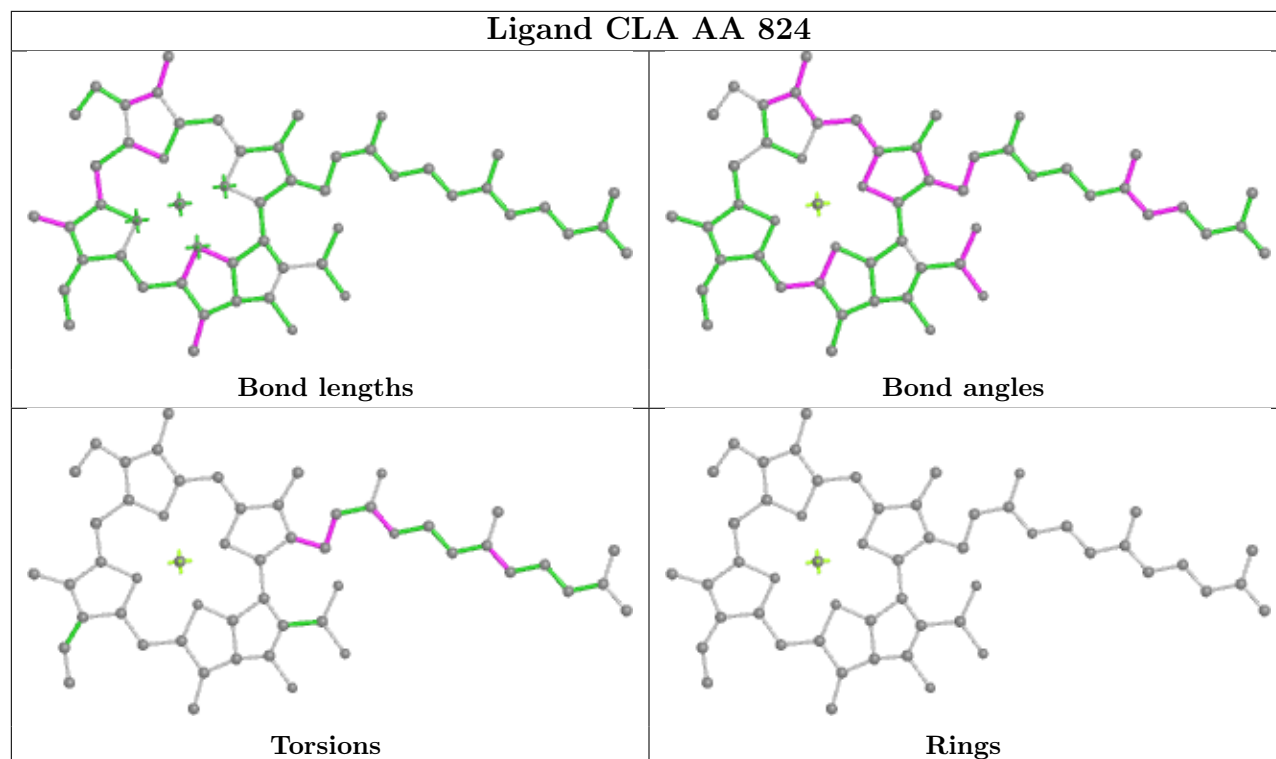
Bond angles



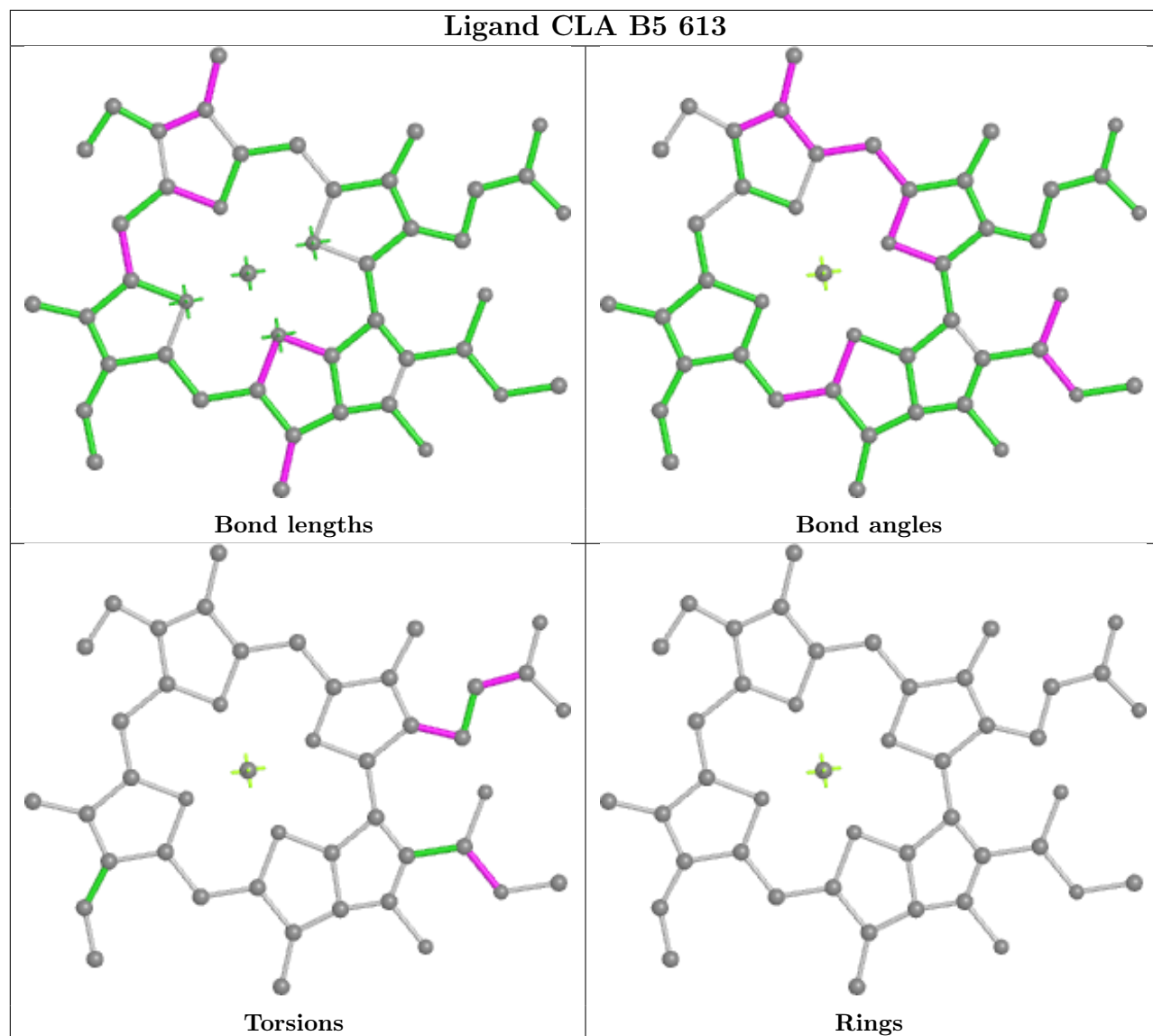
Torsions



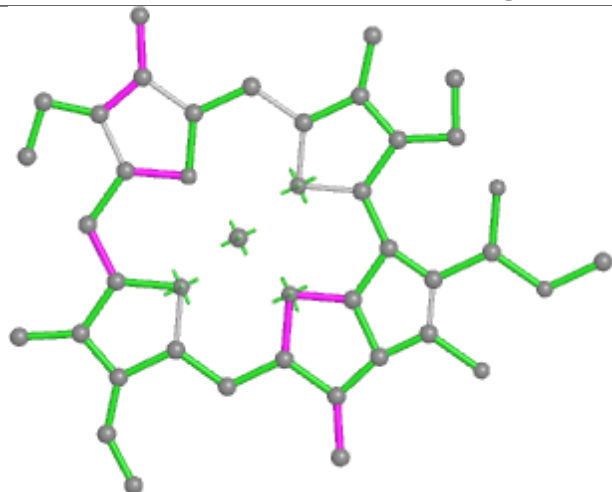
Rings



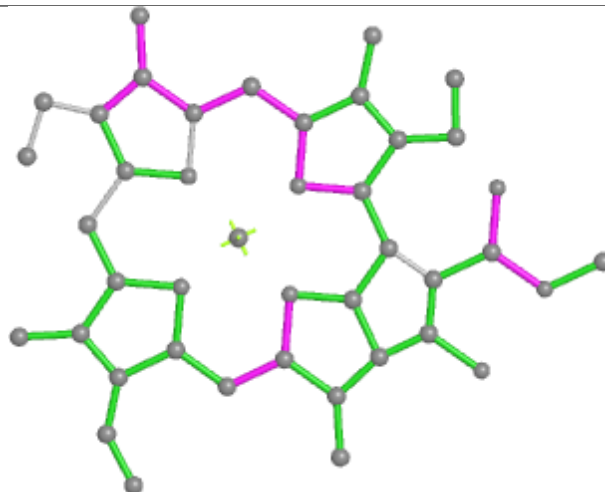
Ligand CLA B5 613



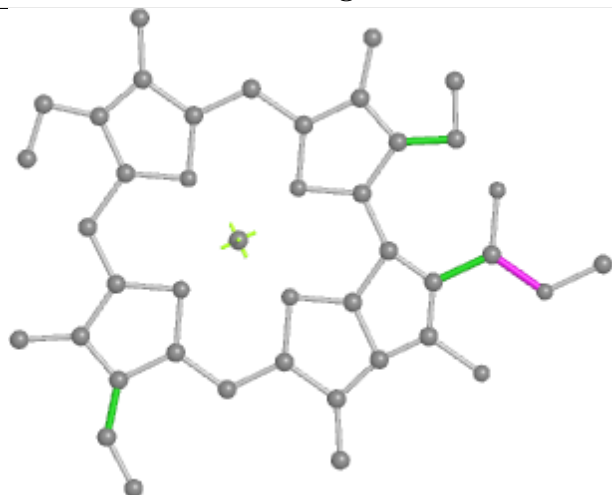
Ligand CLA AB 836



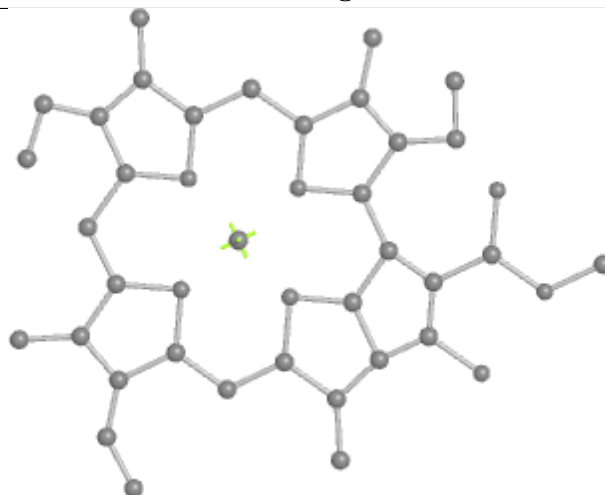
Bond lengths



Bond angles

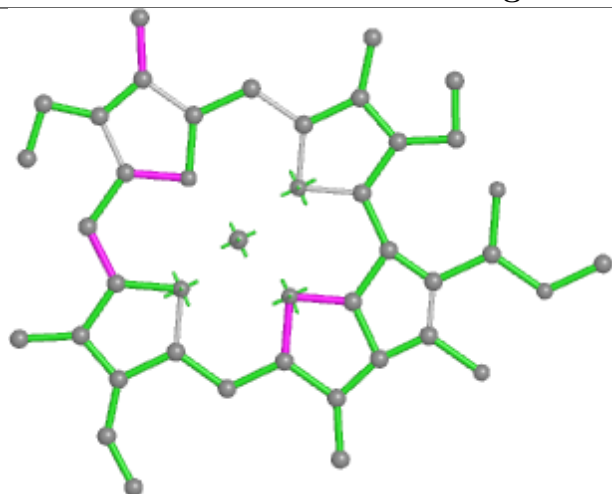


Torsions

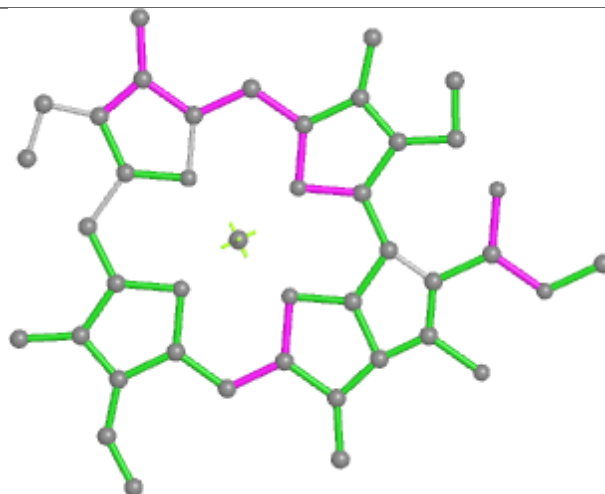


Rings

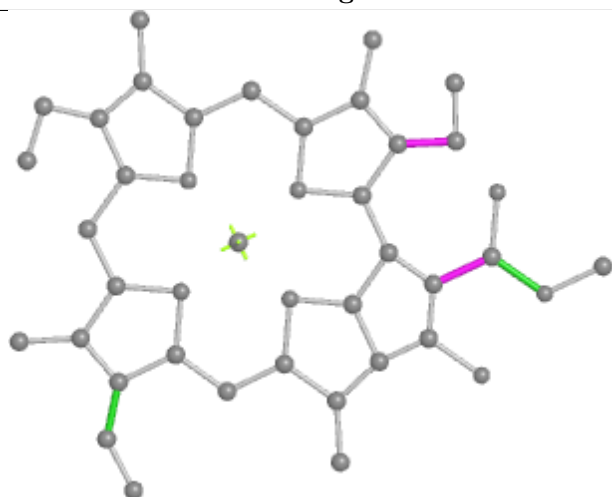
Ligand CLA AJ 102



Bond lengths



Bond angles

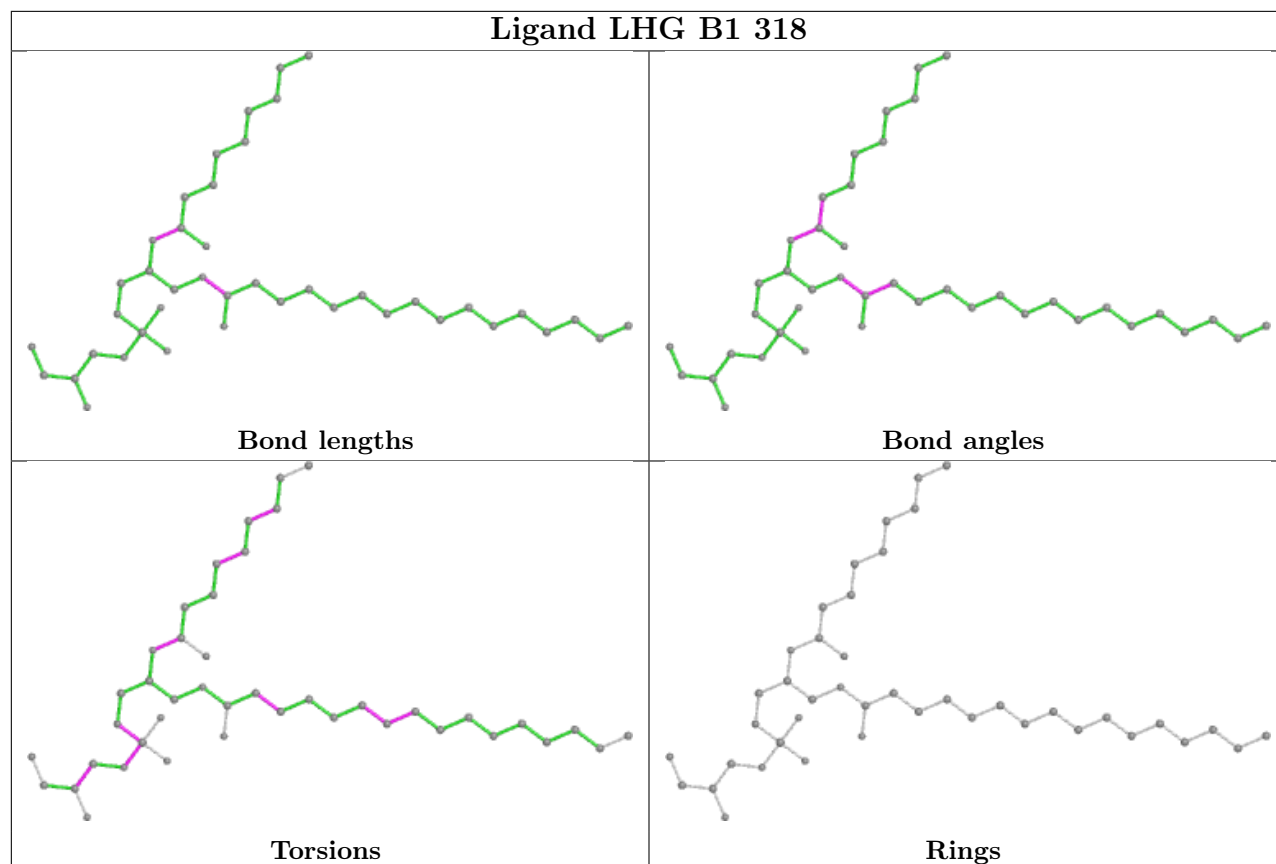


Torsions

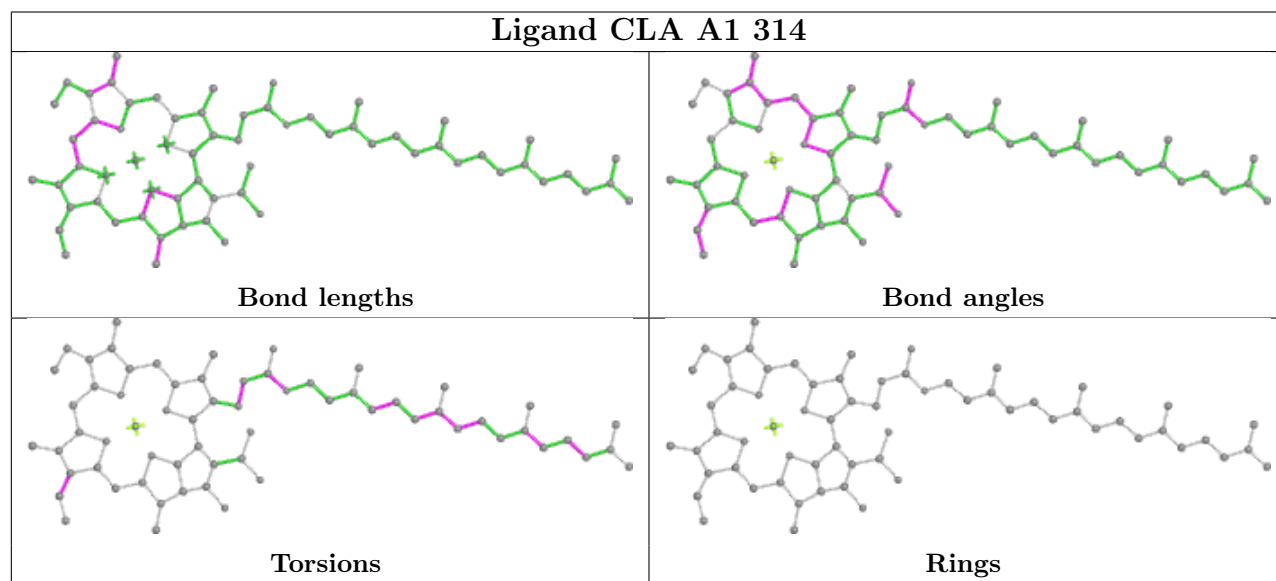


Rings

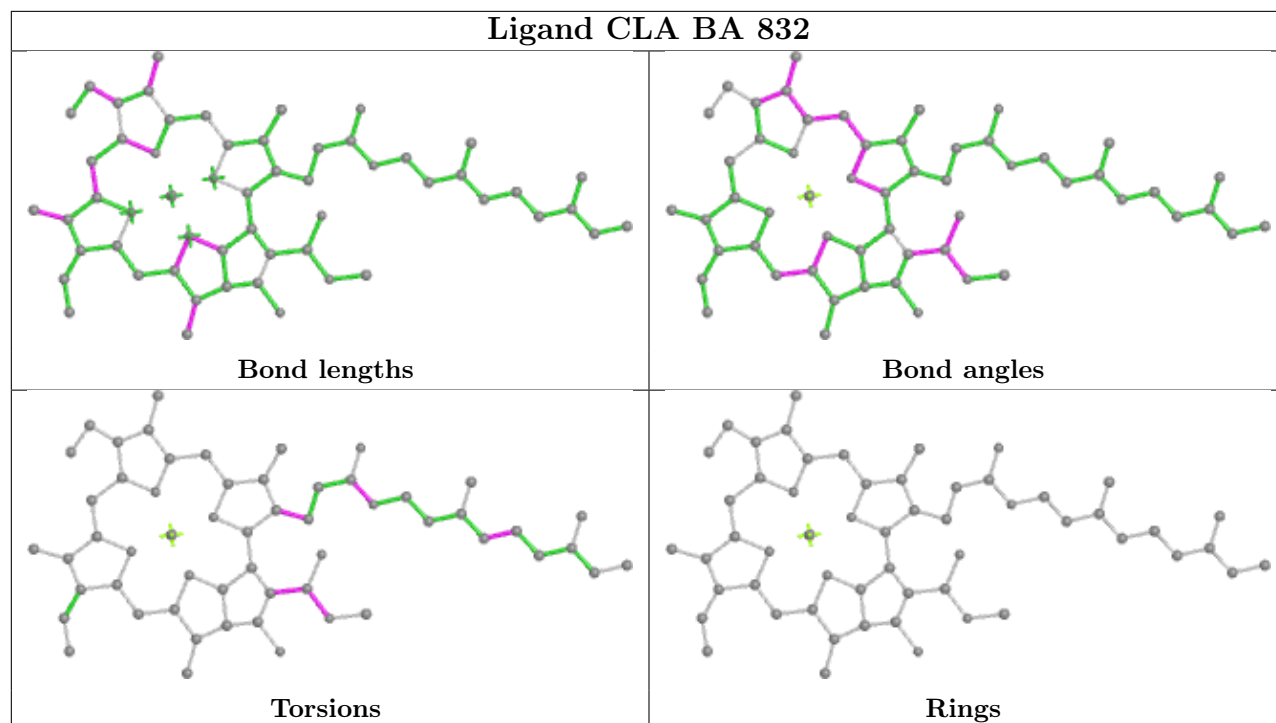
Ligand LHG B1 318



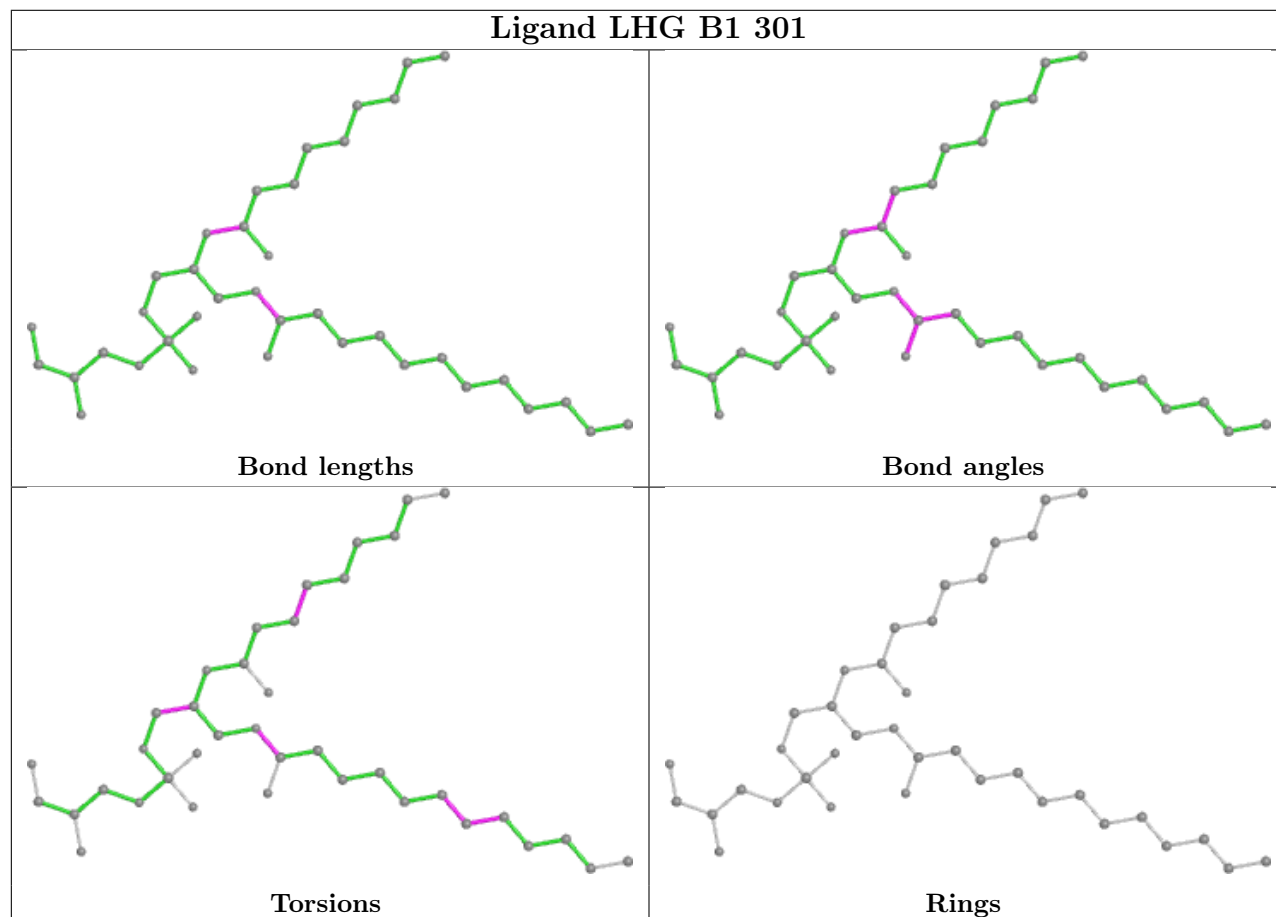
Ligand CLA A1 314

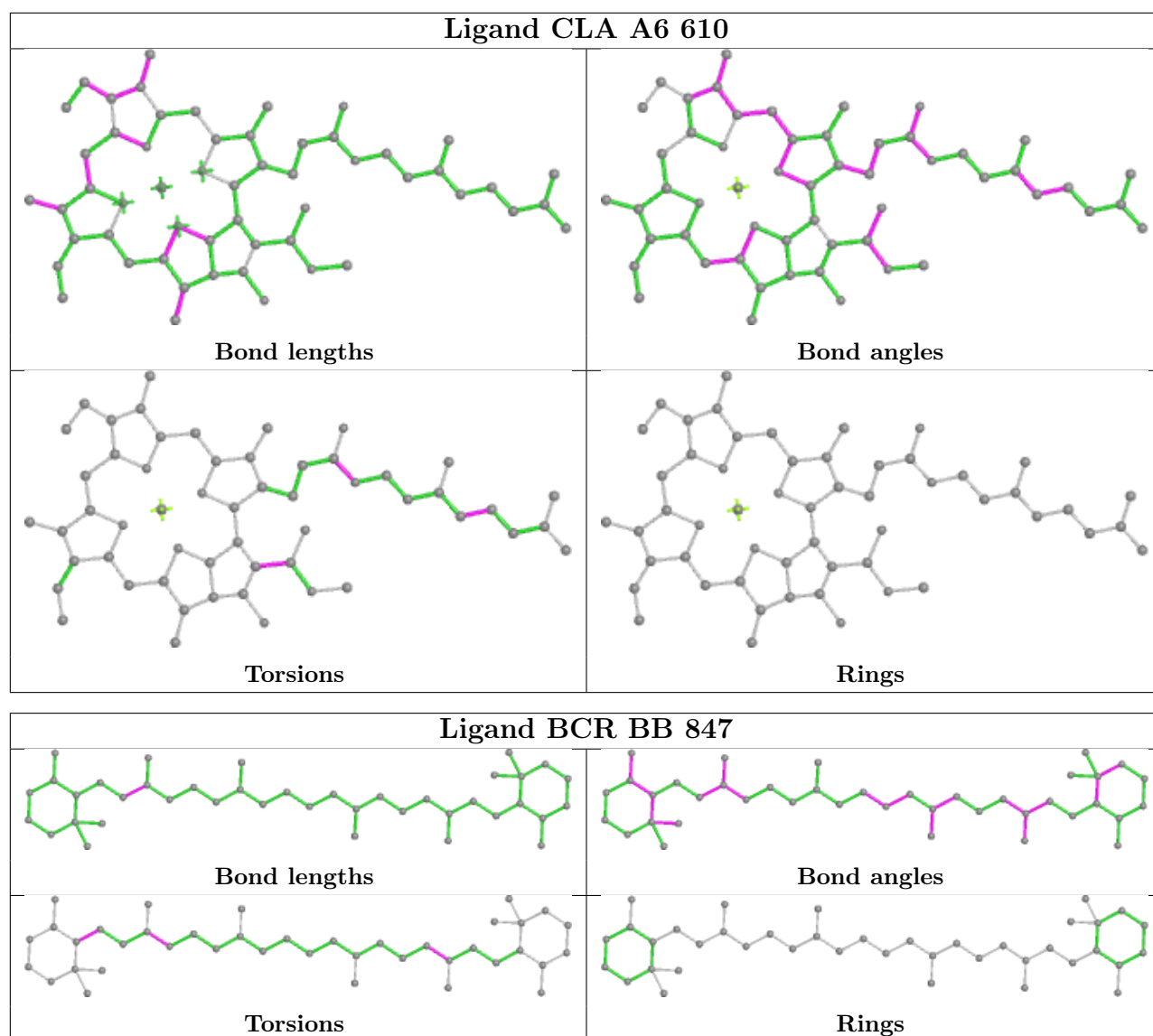


Ligand CLA BA 832

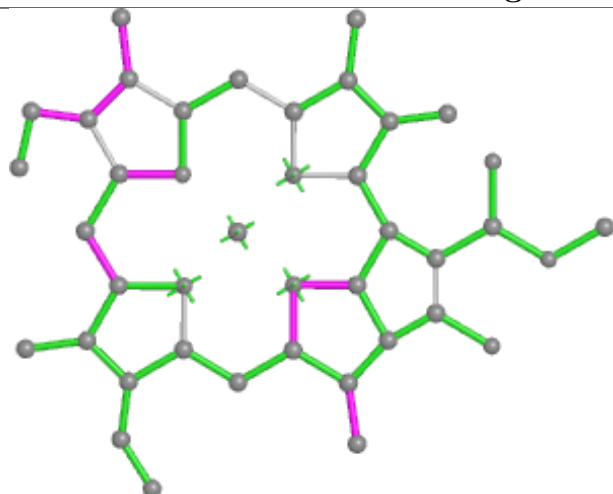


Ligand LHG B1 301

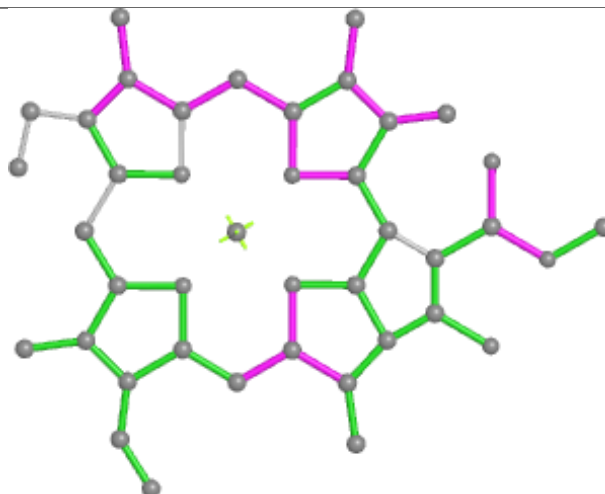




Ligand CLA A3 309



Bond lengths



Bond angles

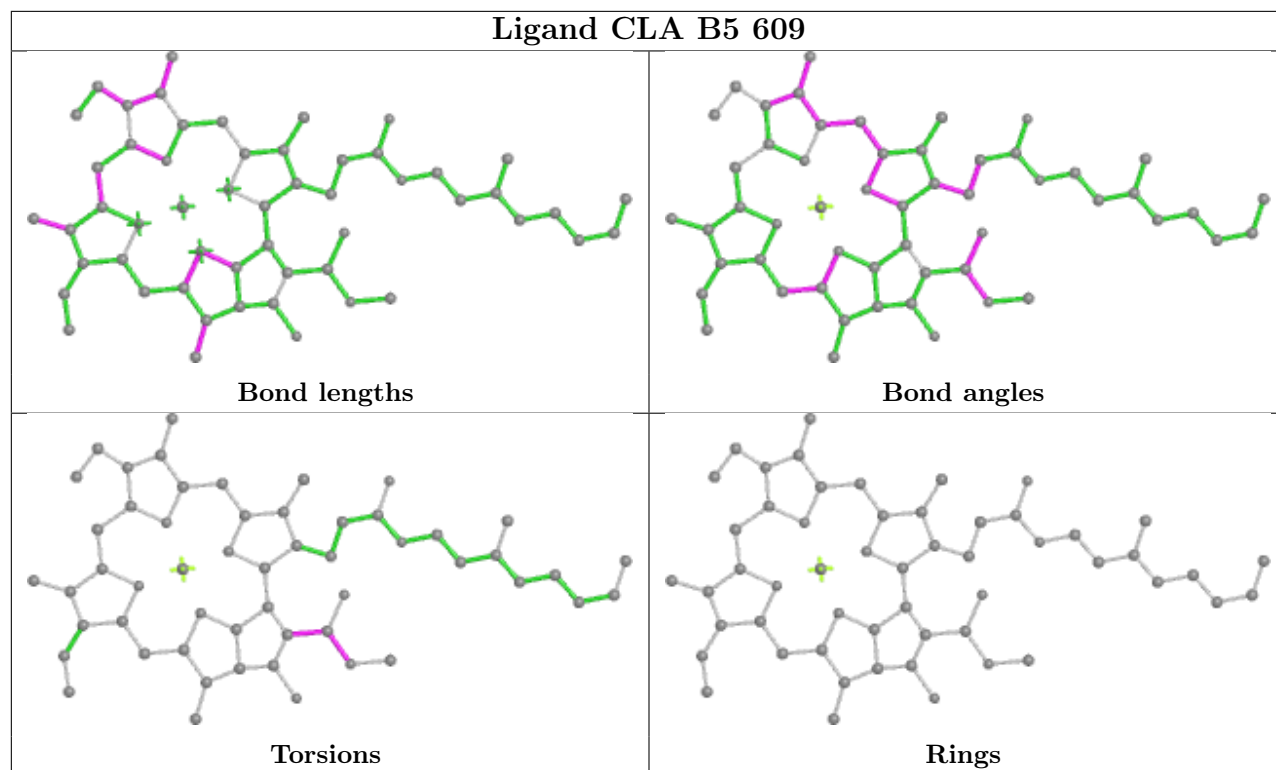


Torsions

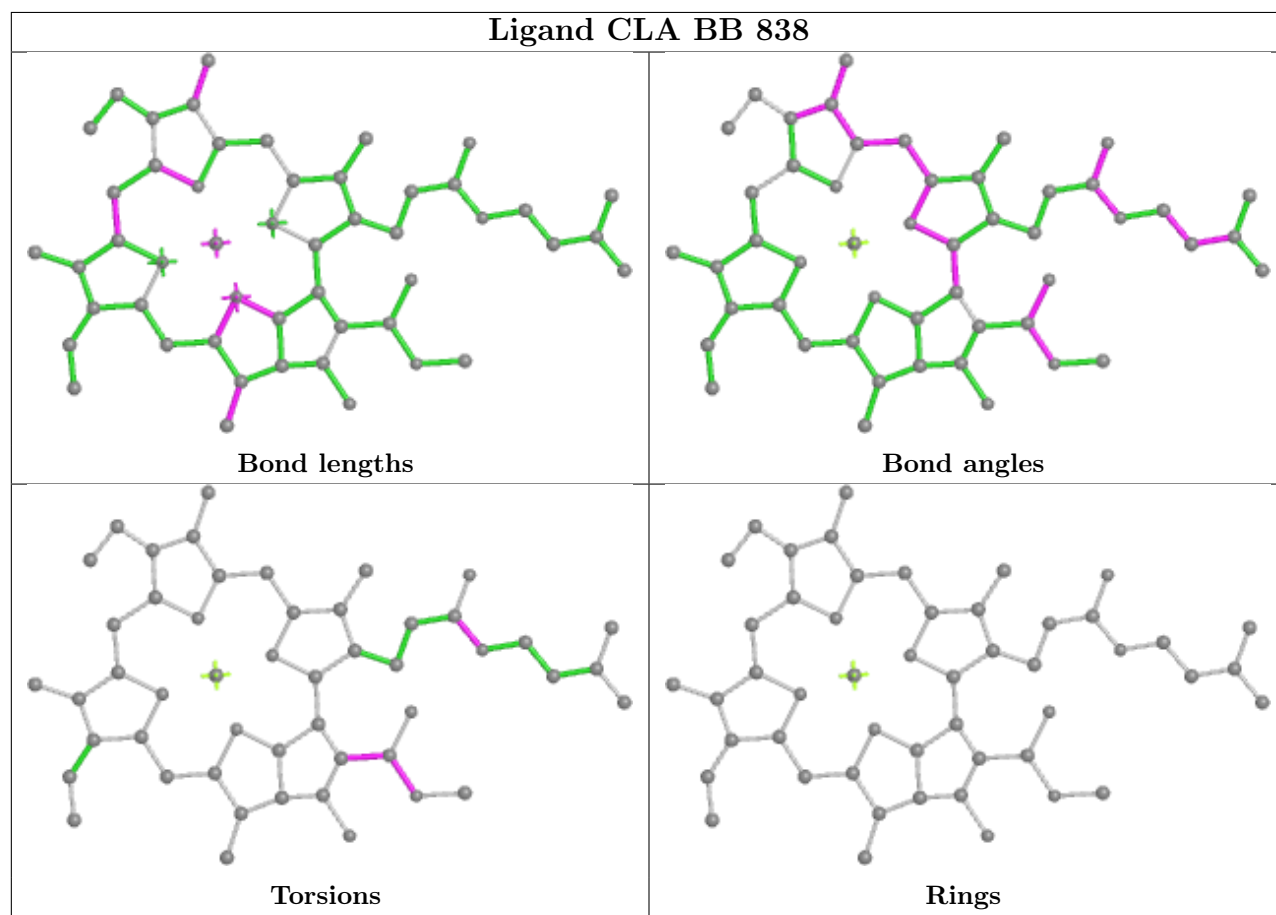


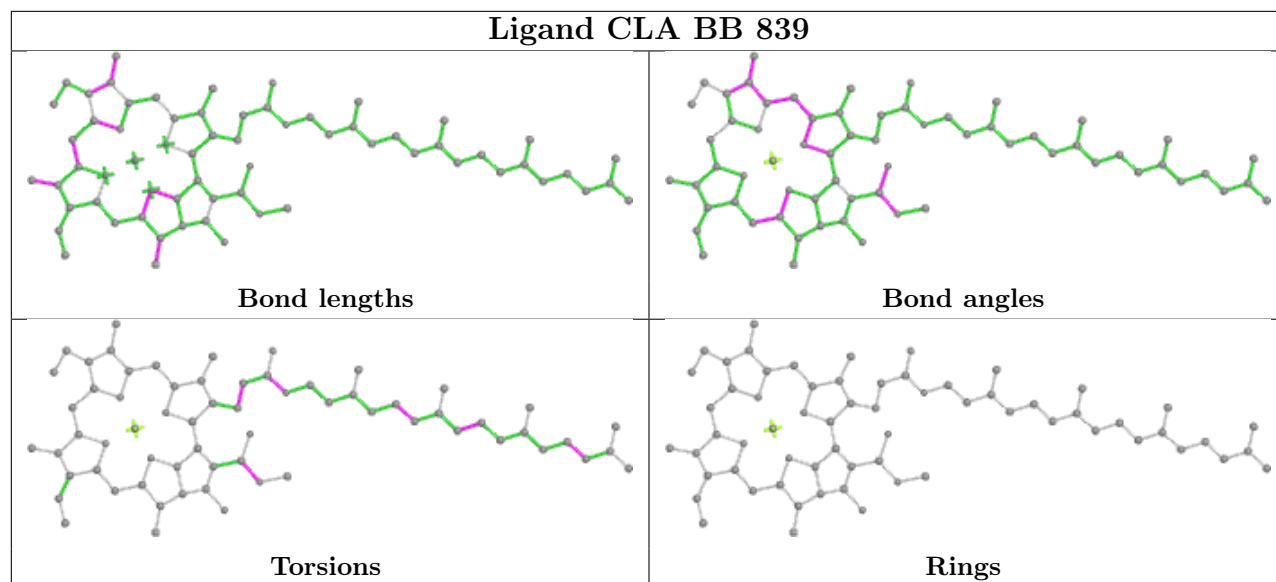
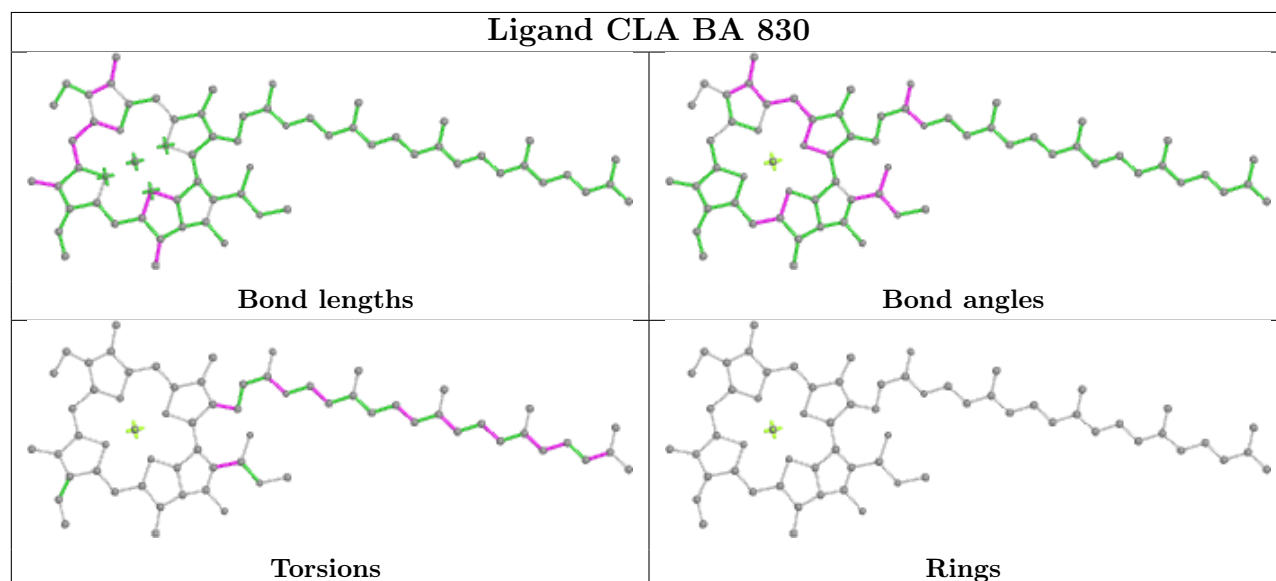
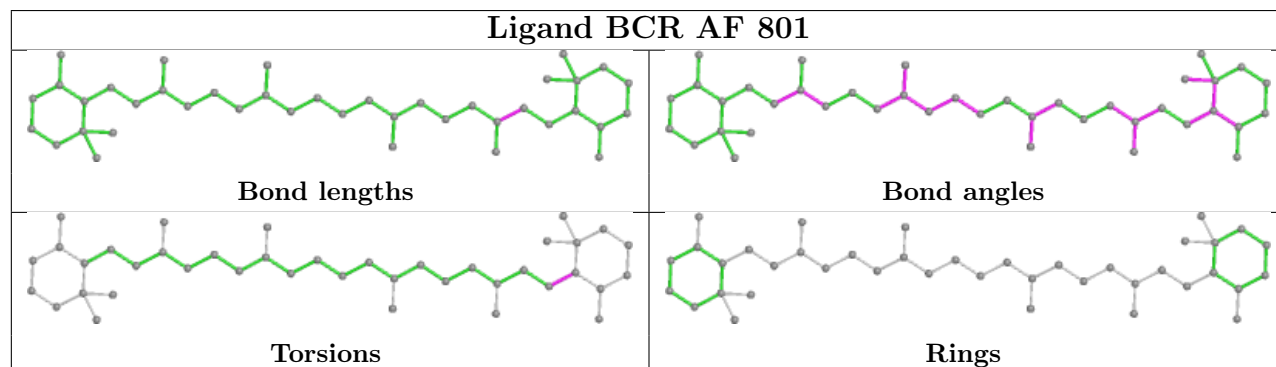
Rings

Ligand CLA B5 609

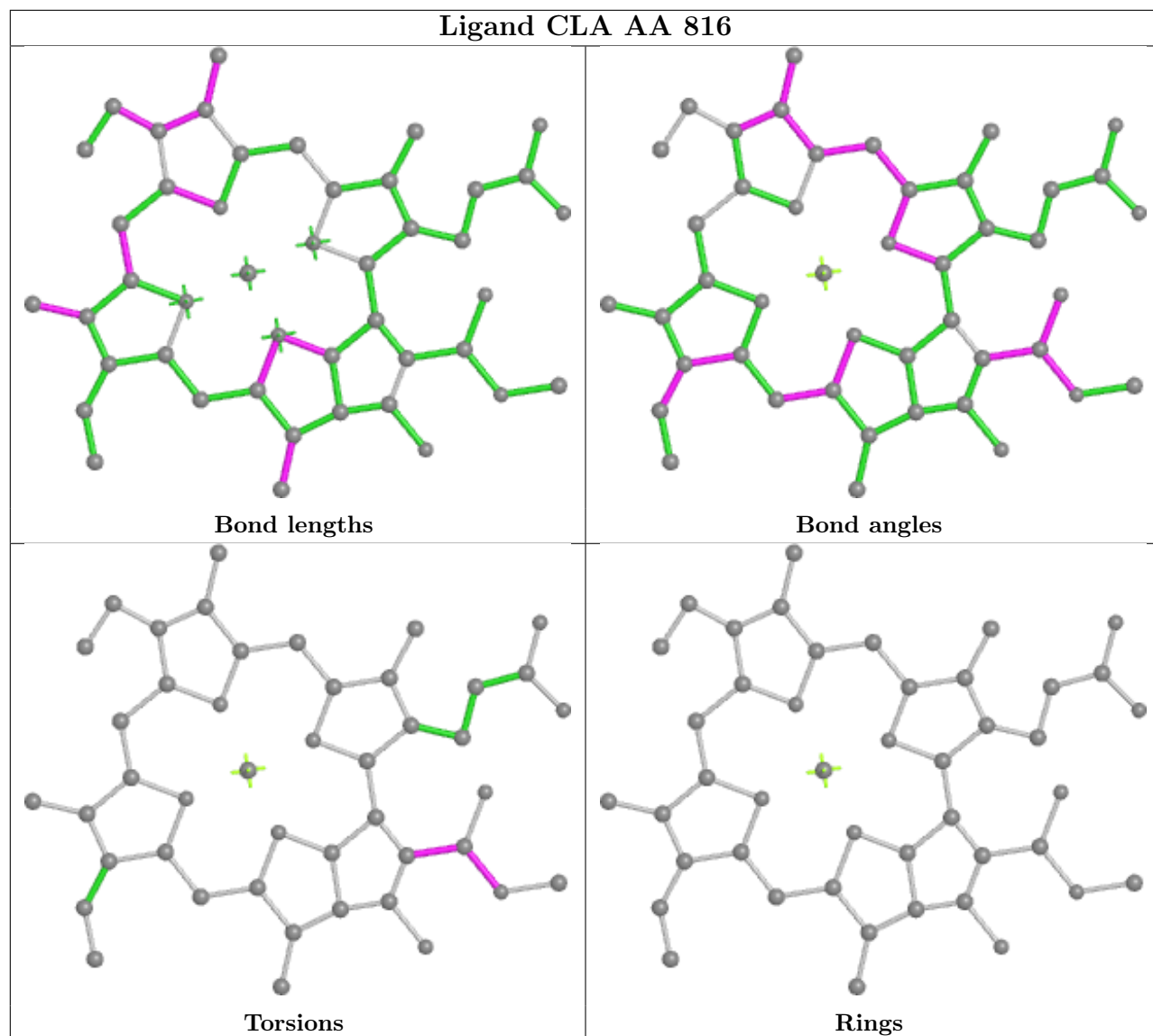


Ligand CLA BB 838

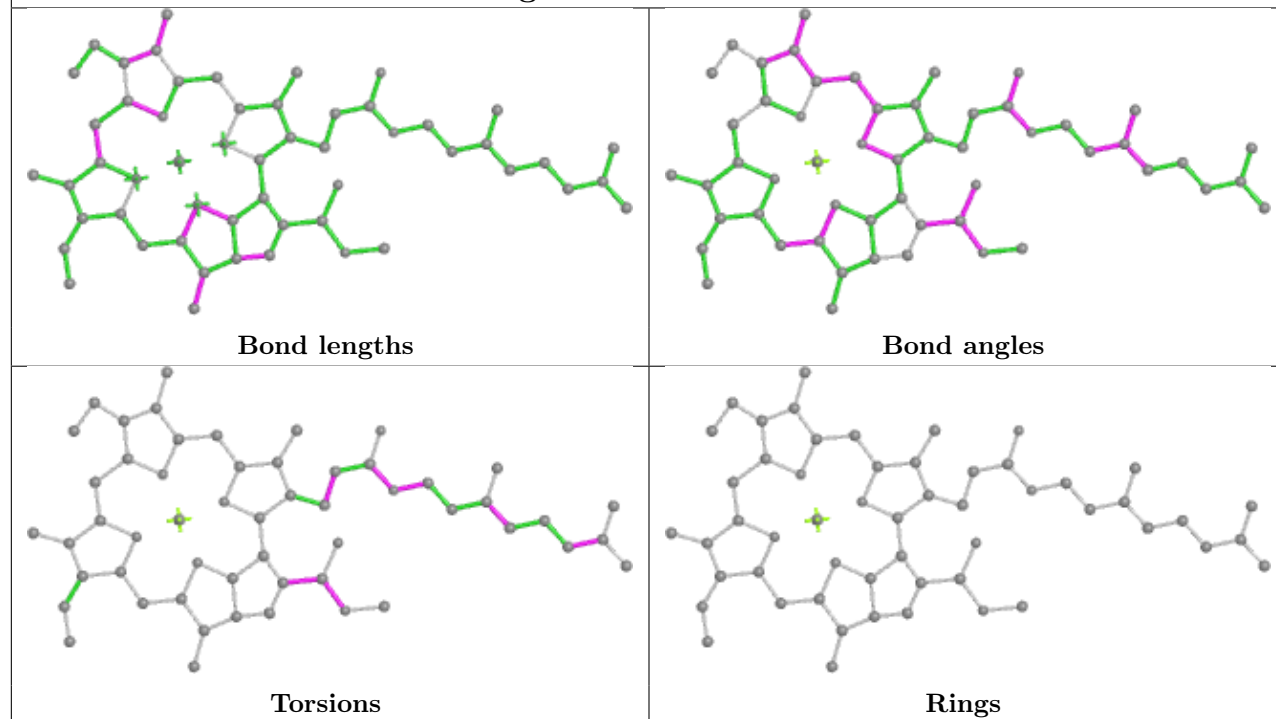


Ligand CLA BB 839**Ligand CLA BA 830****Ligand BCR AF 801**

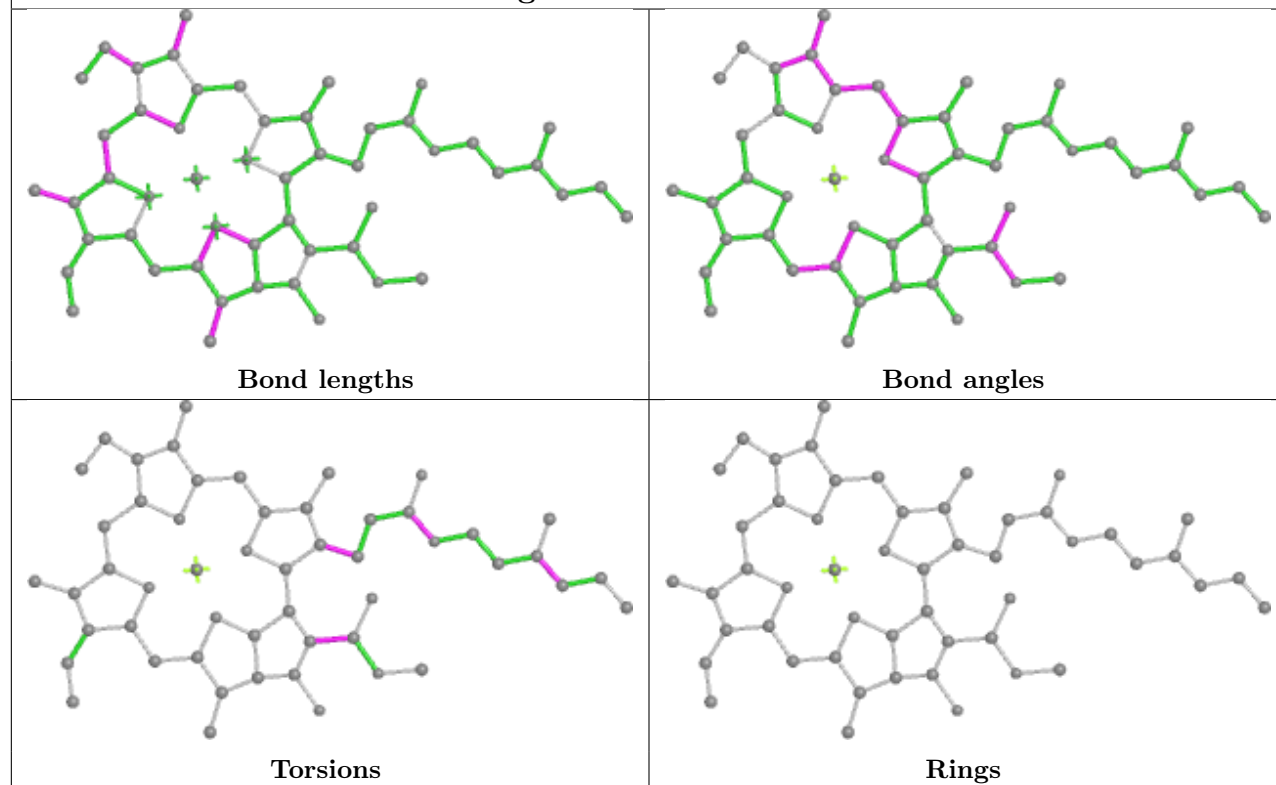
Ligand CLA AA 816



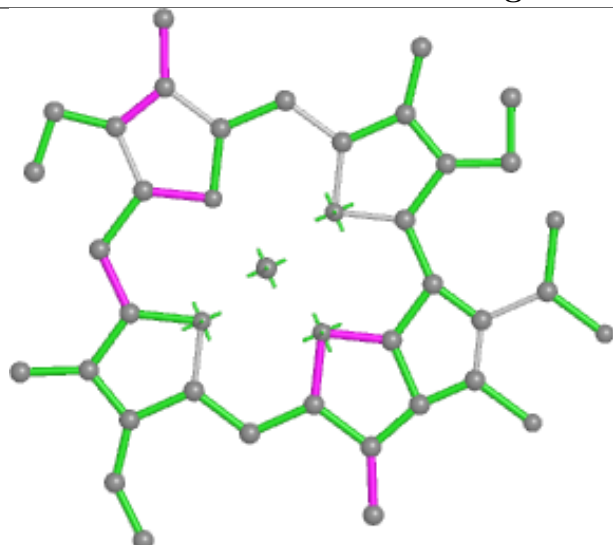
Ligand CLA BA 838



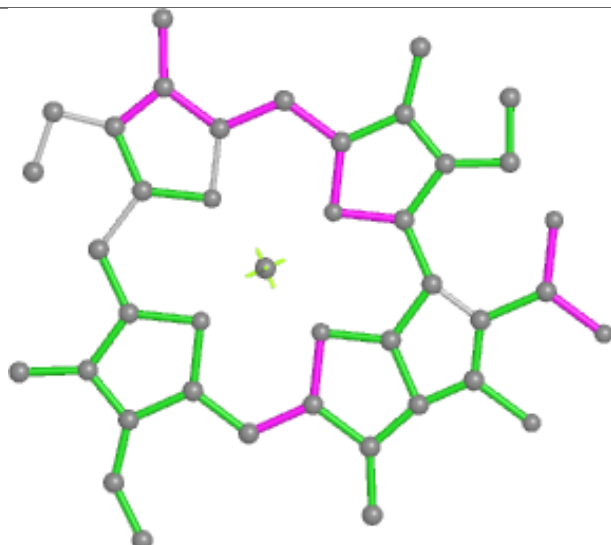
Ligand CLA AA 804



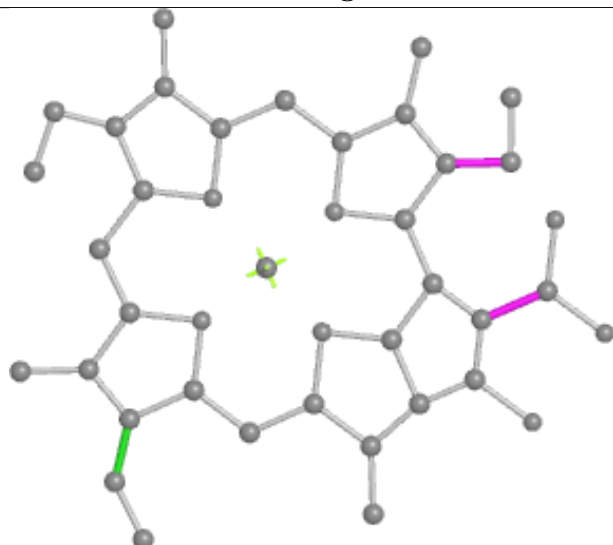
Ligand CLA A3 305



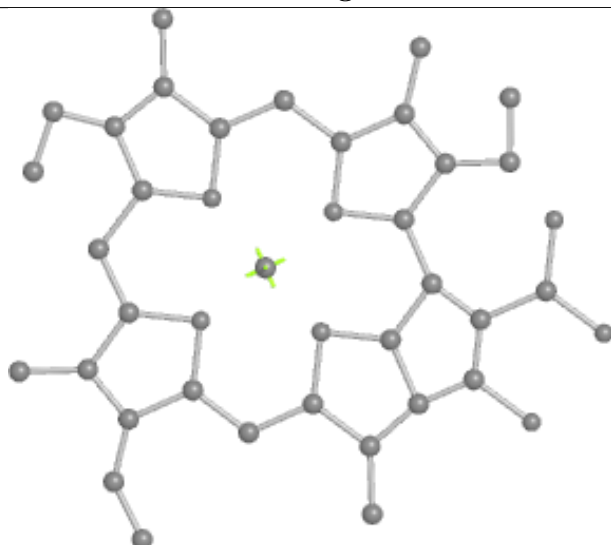
Bond lengths



Bond angles

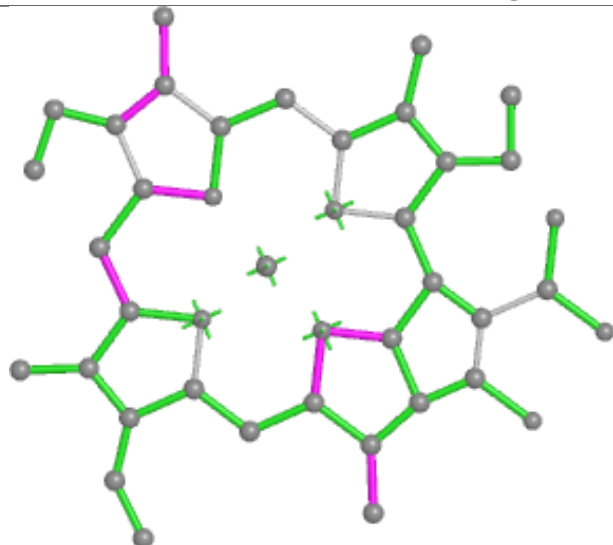


Torsions

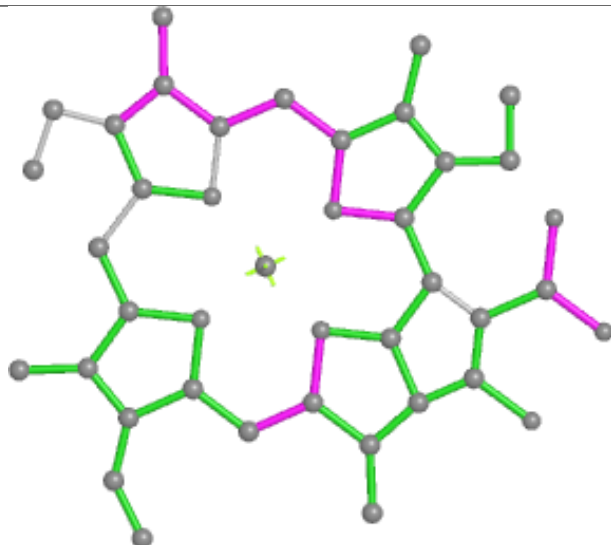


Rings

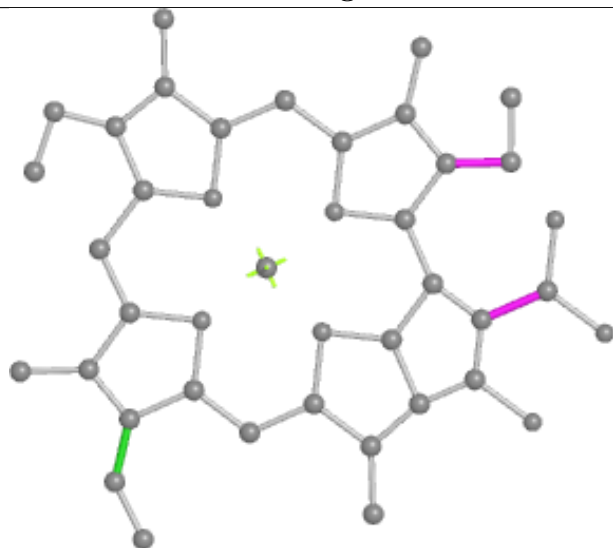
Ligand CLA B3 304



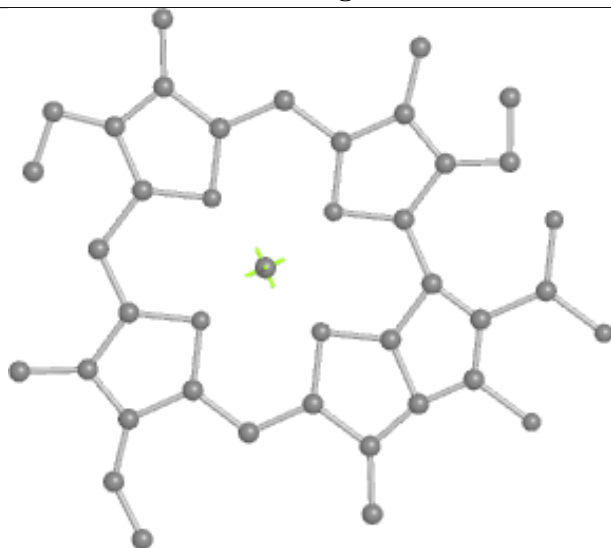
Bond lengths



Bond angles

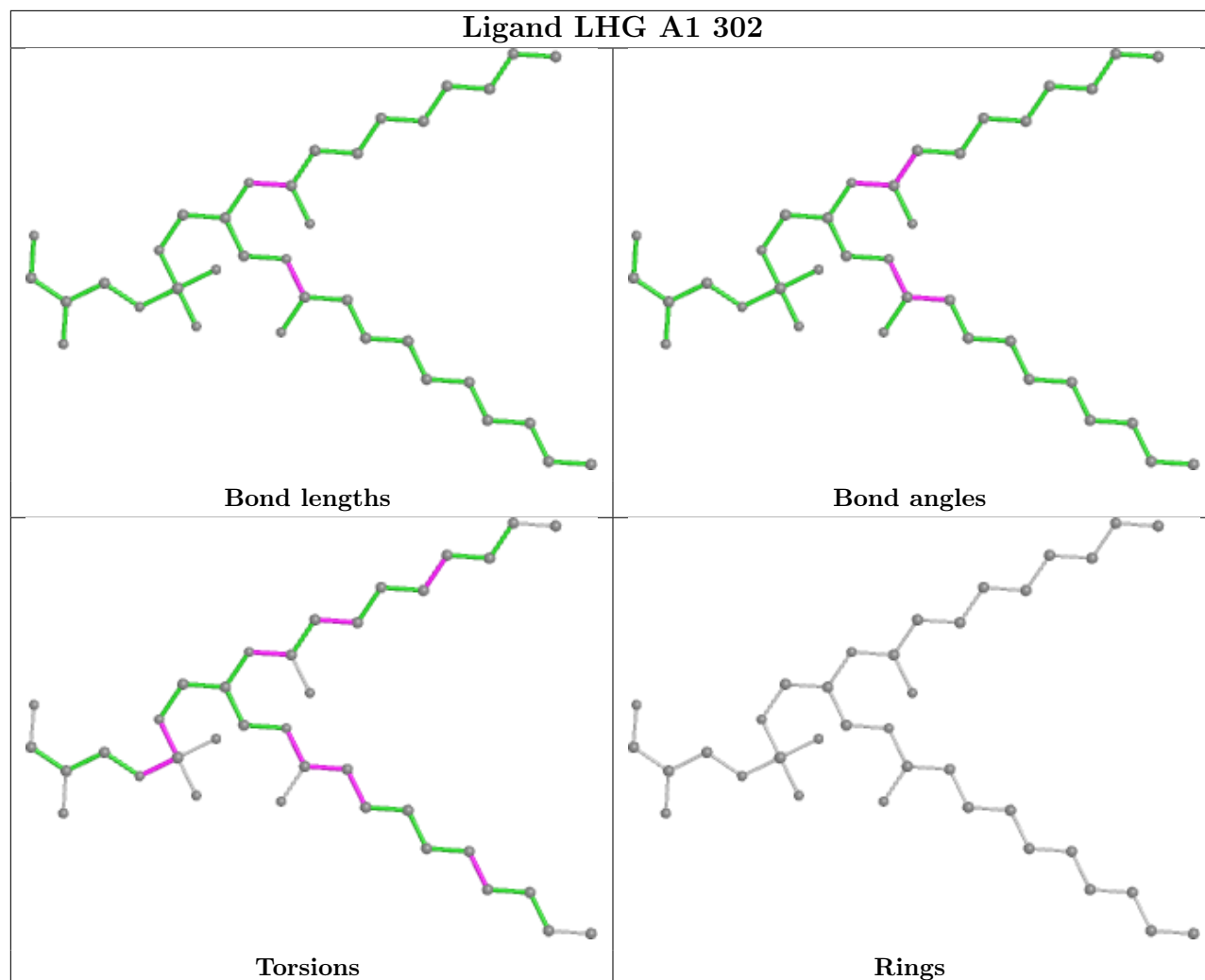


Torsions

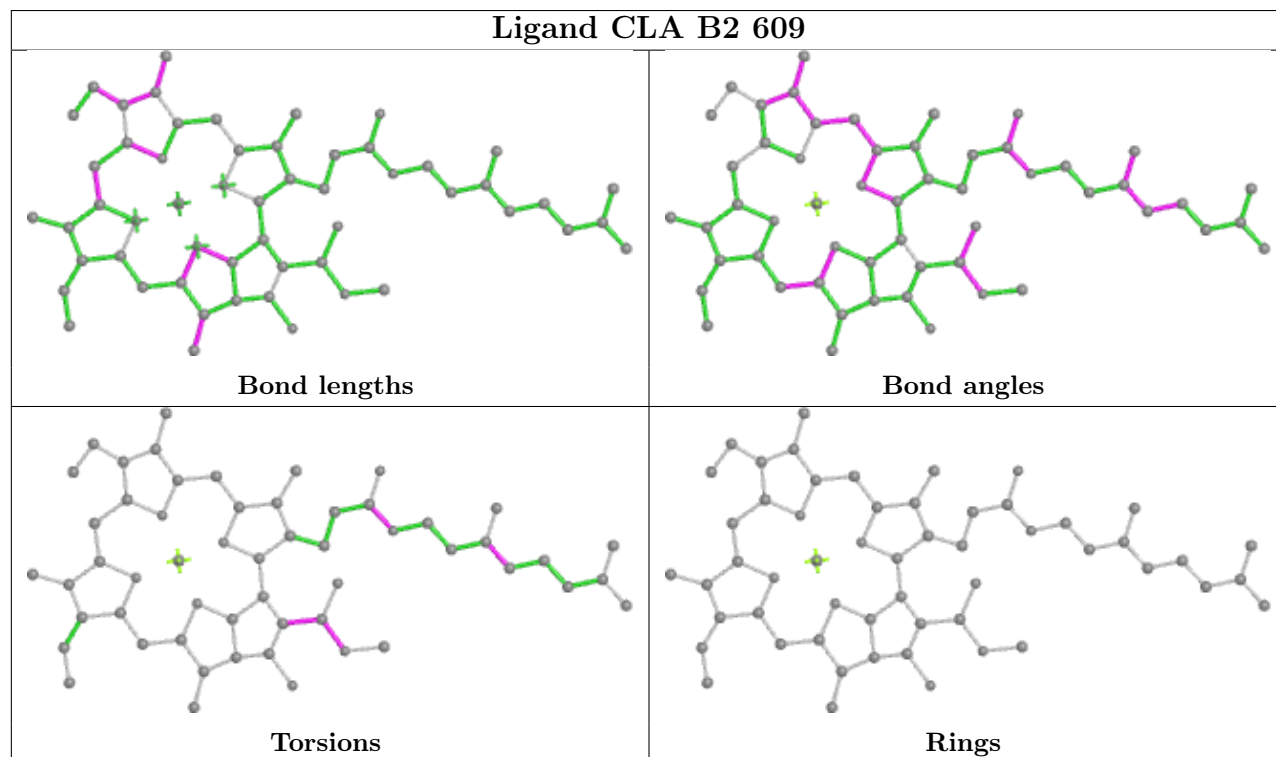


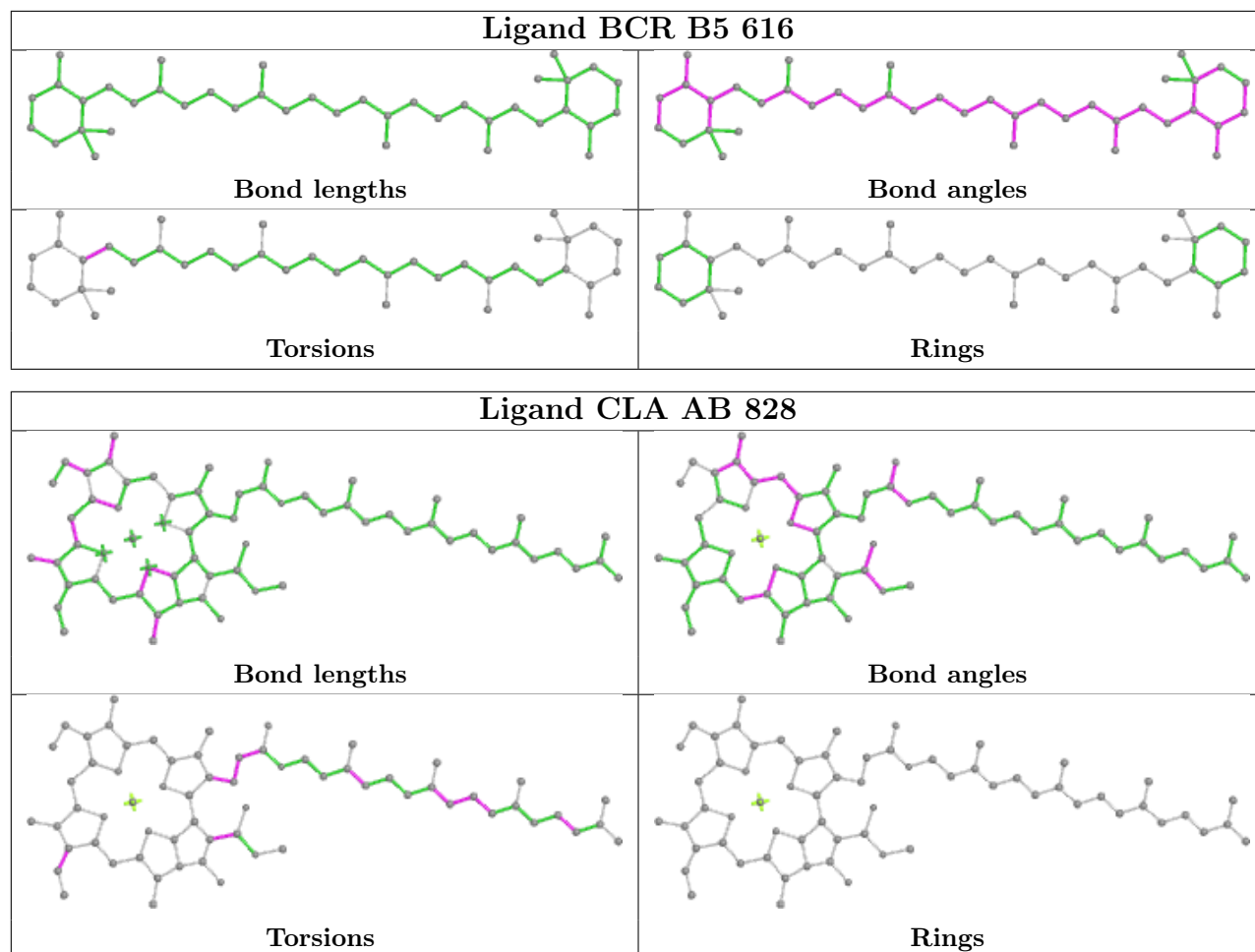
Rings

Ligand LHG A1 302

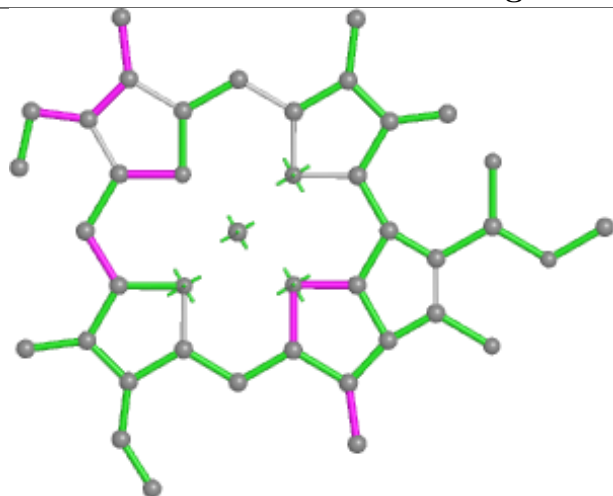


Ligand CLA B2 609

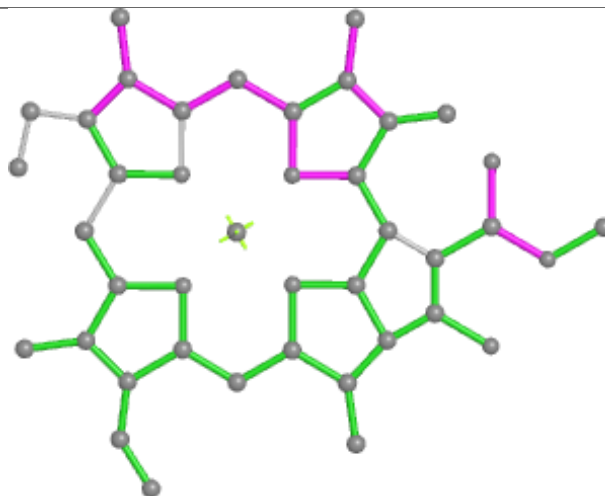




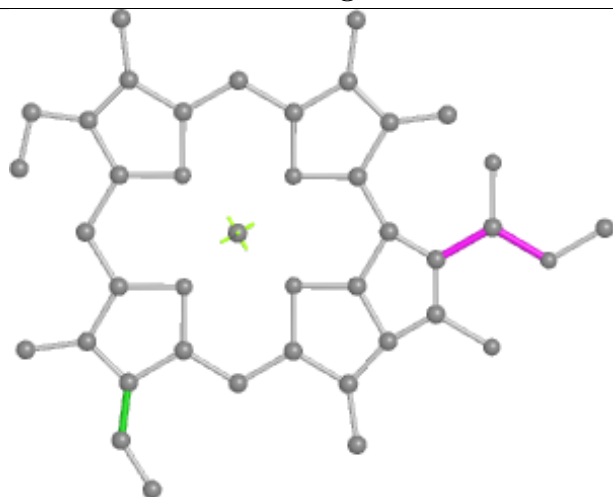
Ligand CLA B3 308



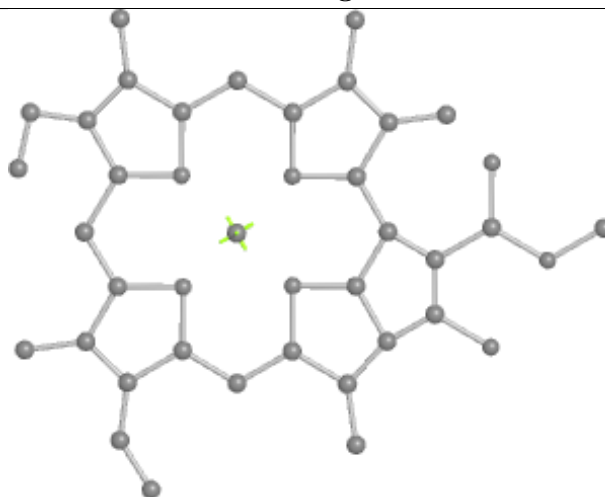
Bond lengths



Bond angles

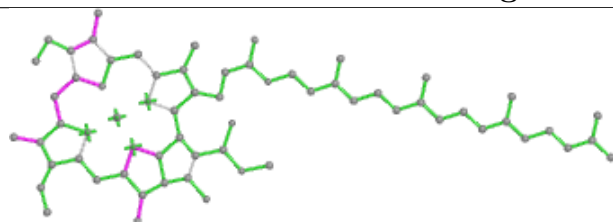


Torsions

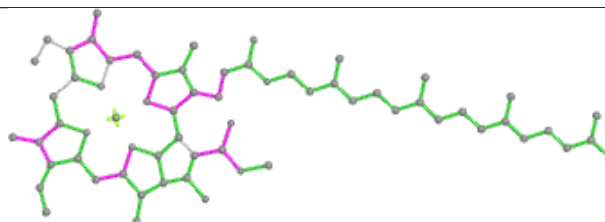


Rings

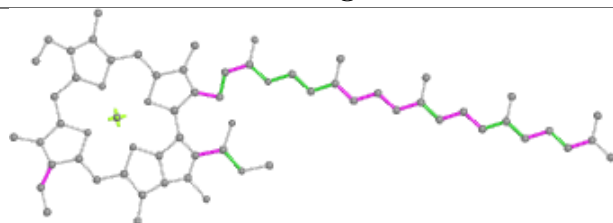
Ligand CLA AA 805



Bond lengths



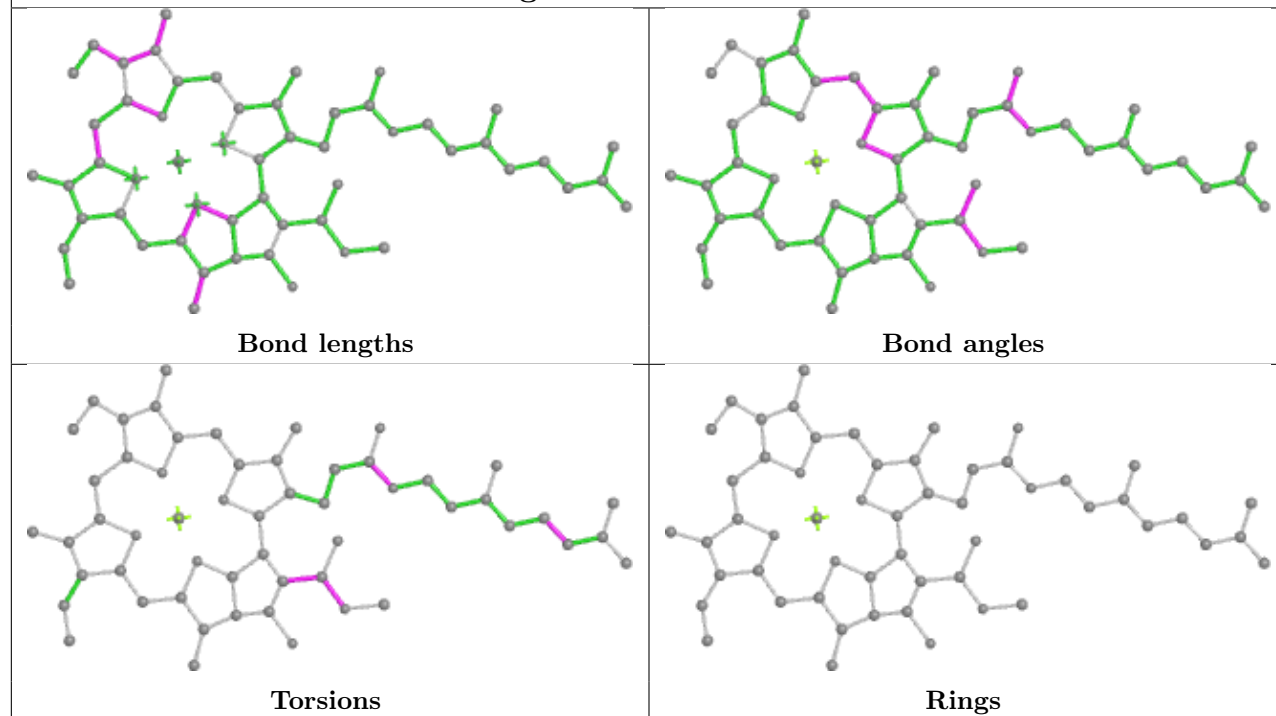
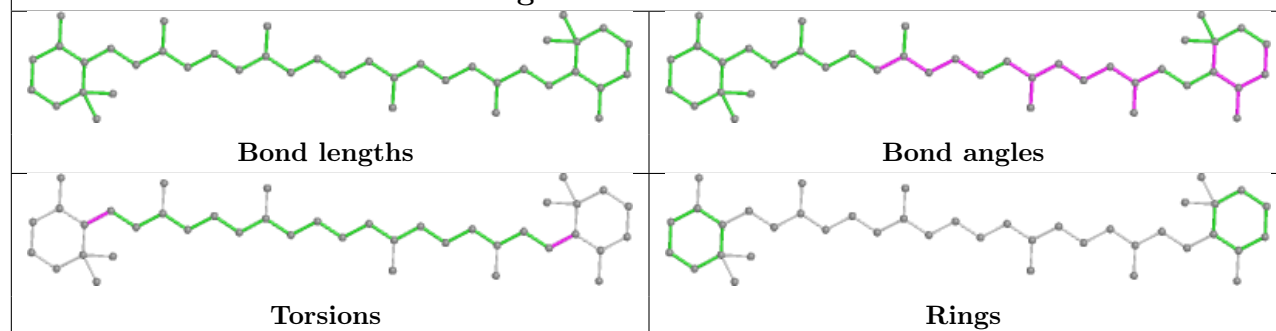
Bond angles

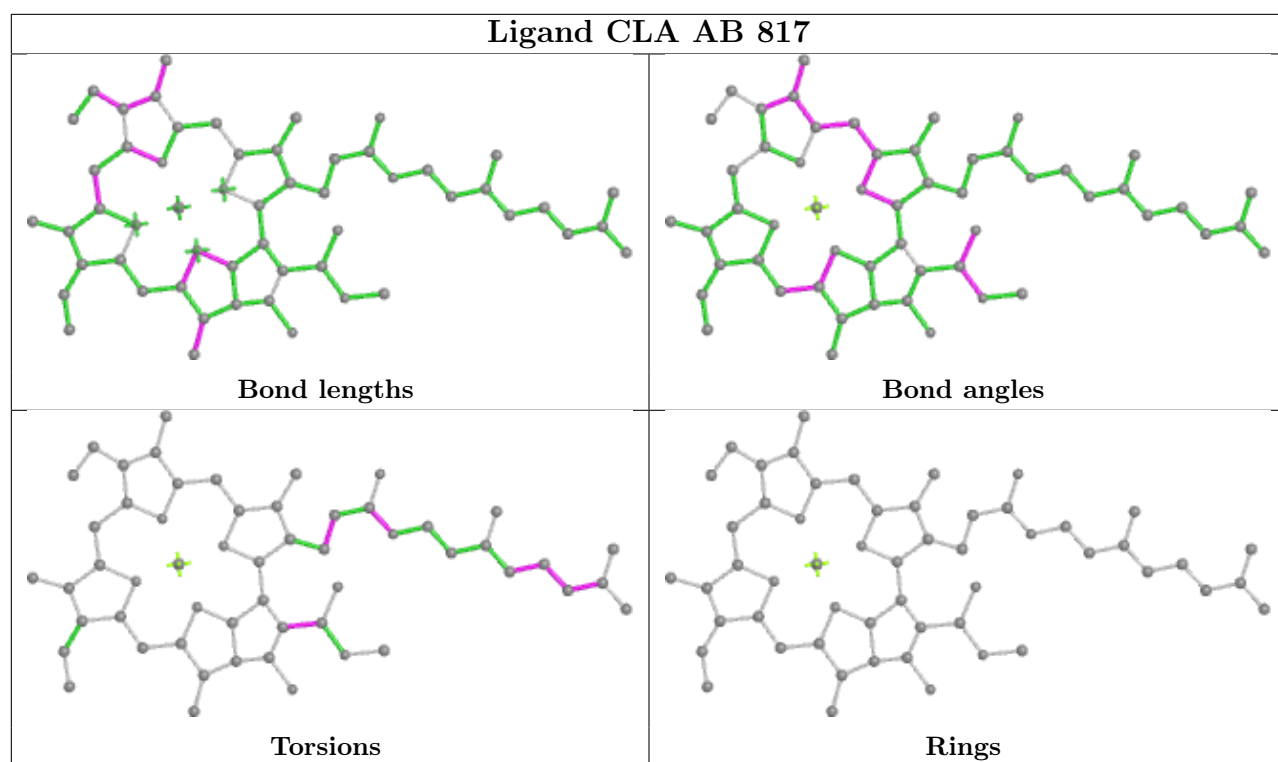


Torsions

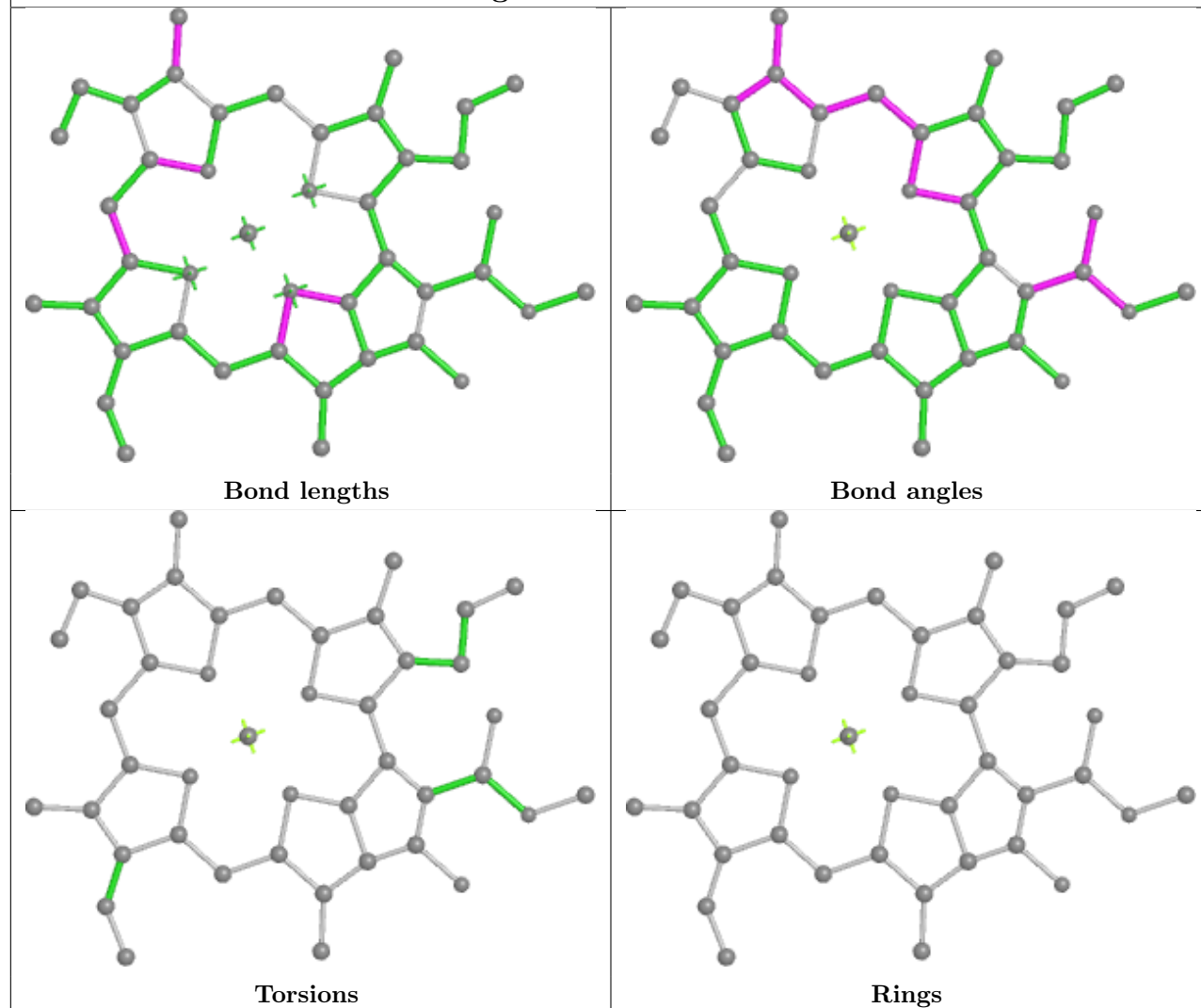


Rings

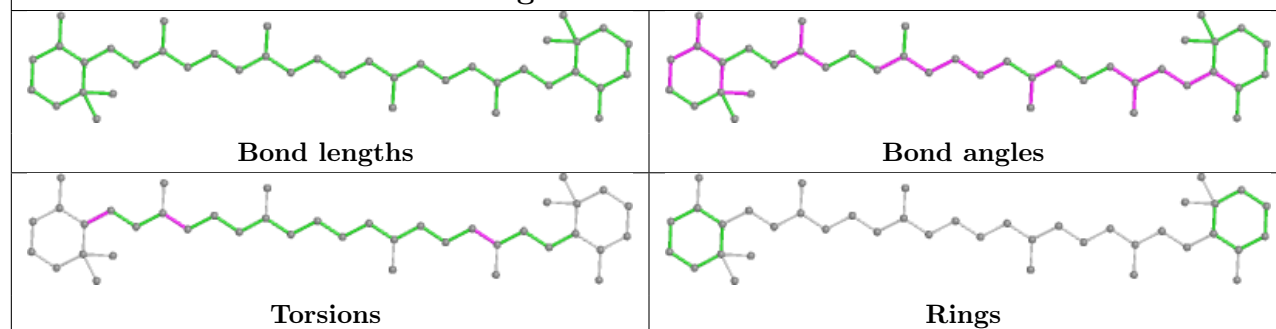
Ligand CLA BB 821**Ligand BCR BA 850**



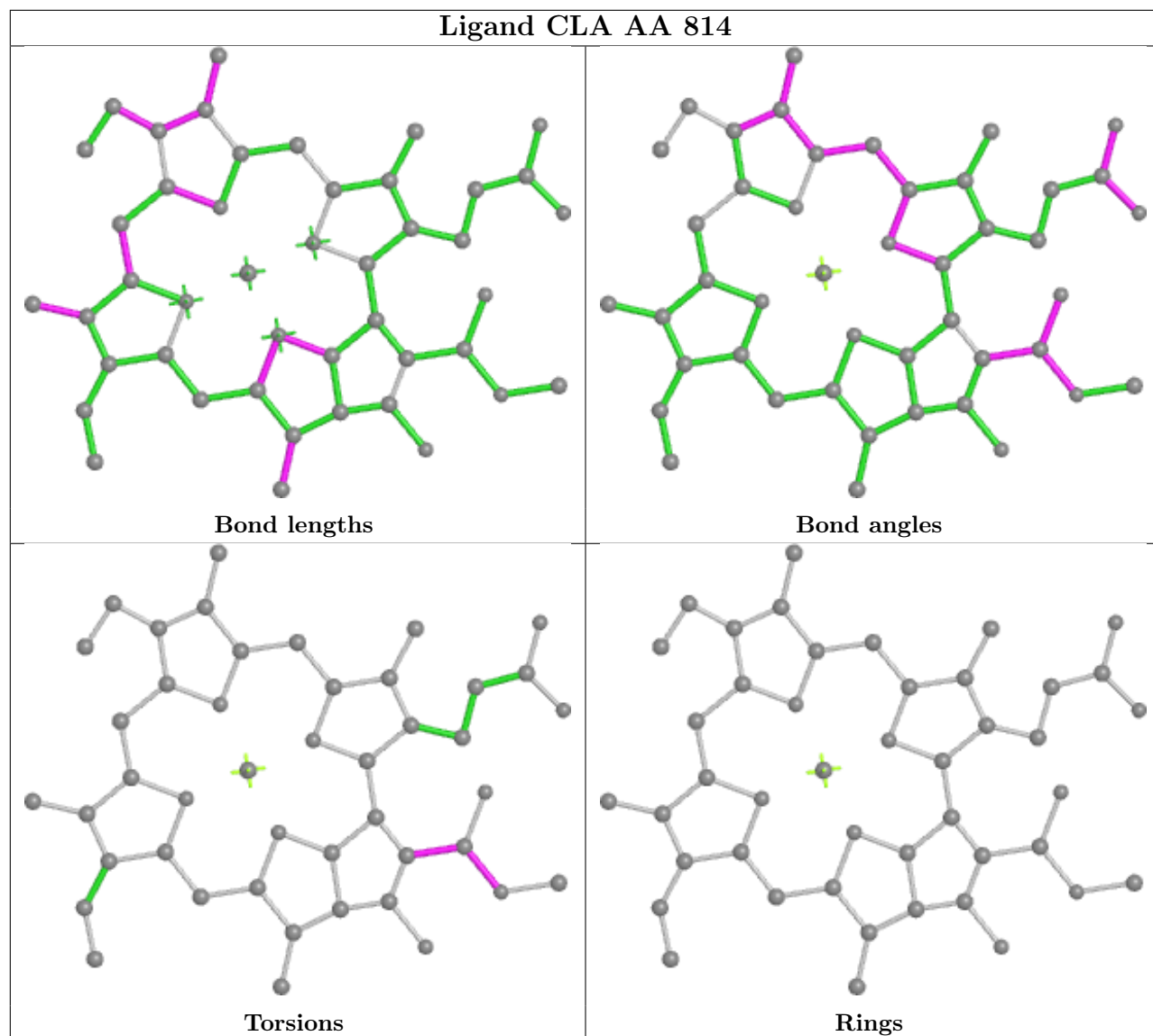
Ligand CLA A3 311



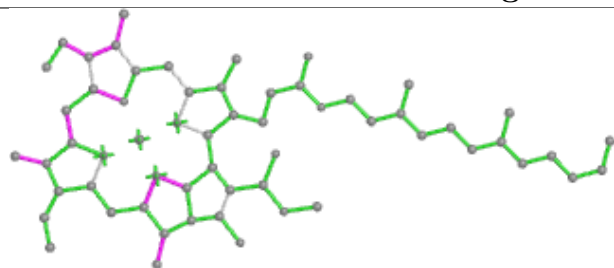
Ligand BCR AB 846



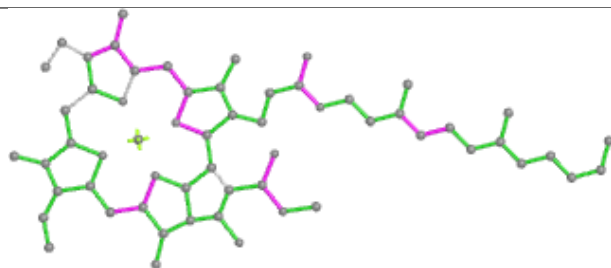
Ligand CLA AA 814



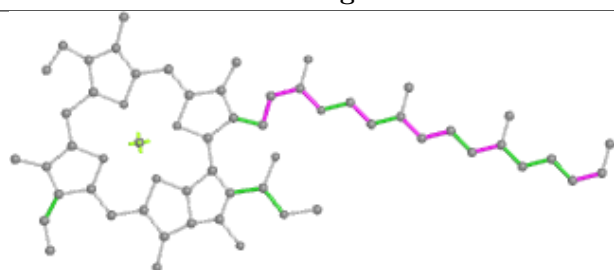
Ligand CLA BB 819



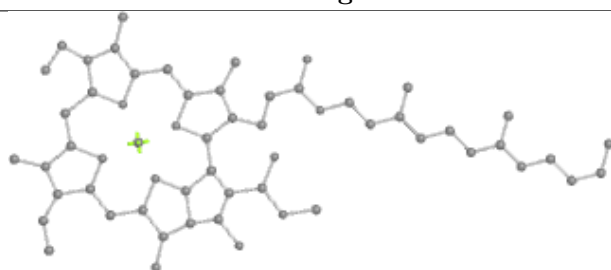
Bond lengths



Bond angles

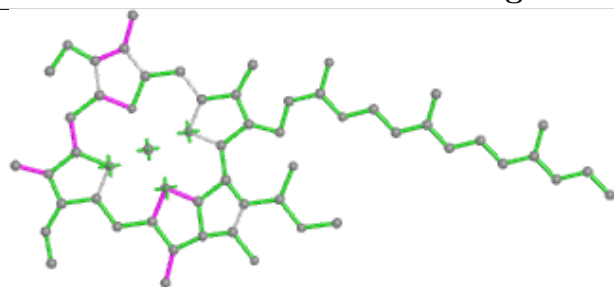


Torsions

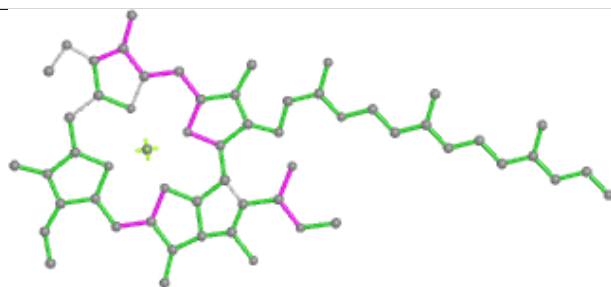


Rings

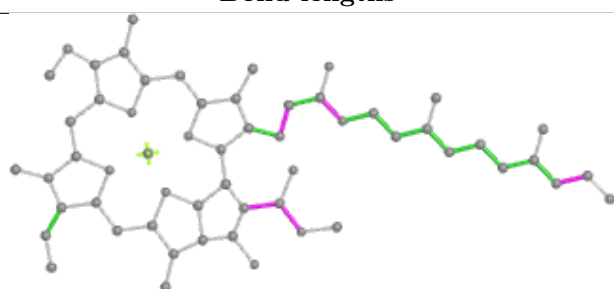
Ligand CLA B5 612



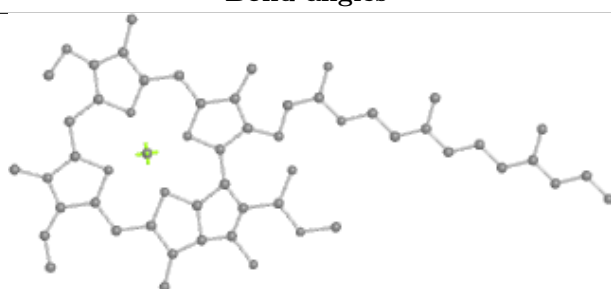
Bond lengths



Bond angles

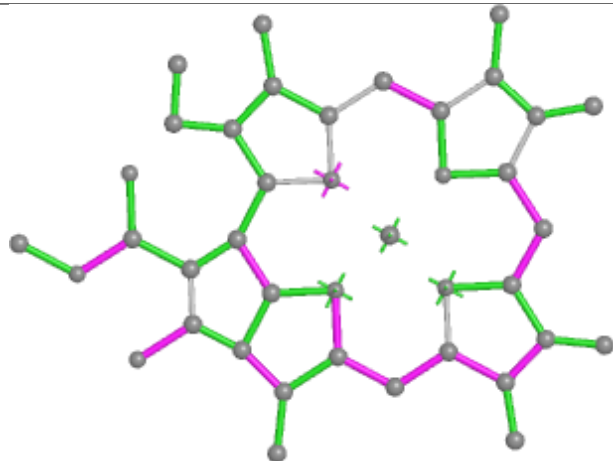


Torsions

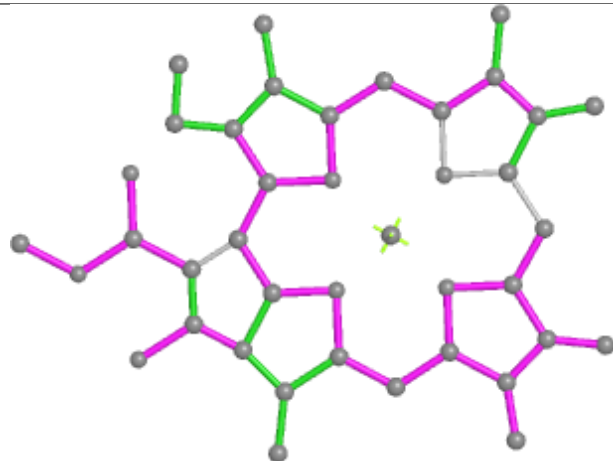


Rings

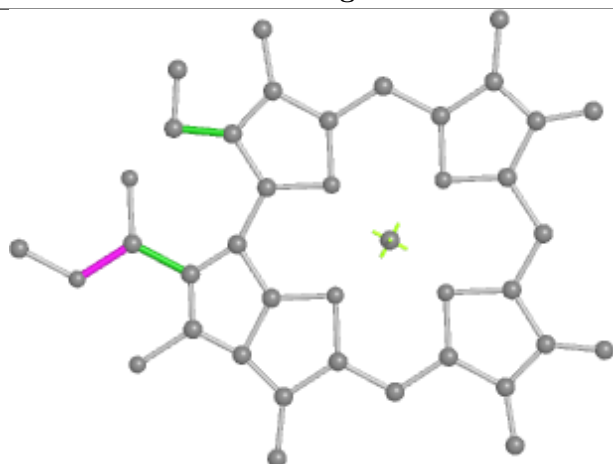
Ligand CHL B5 606



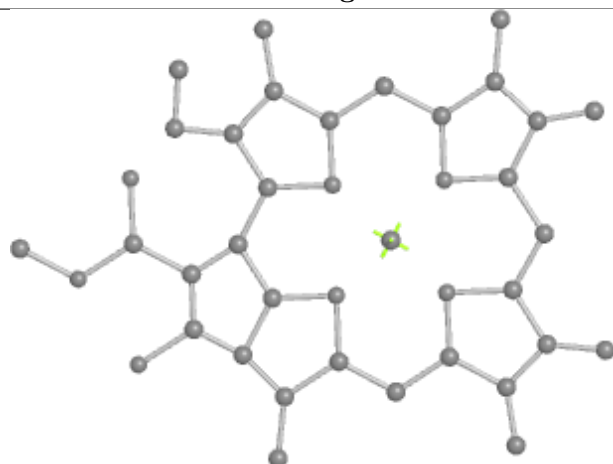
Bond lengths



Bond angles

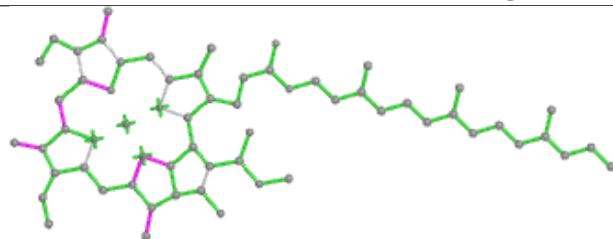


Torsions

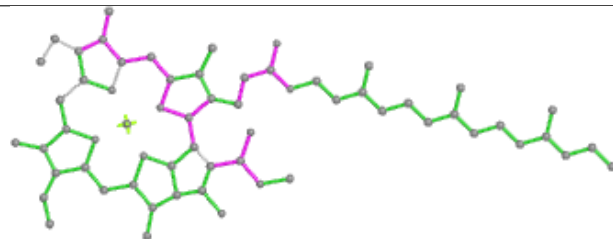


Rings

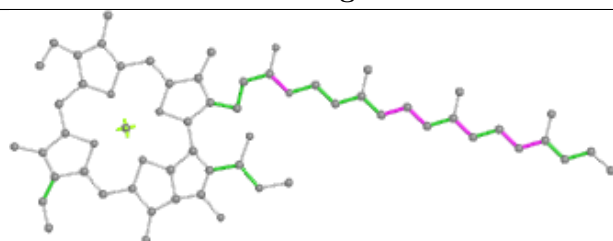
Ligand CLA BB 828



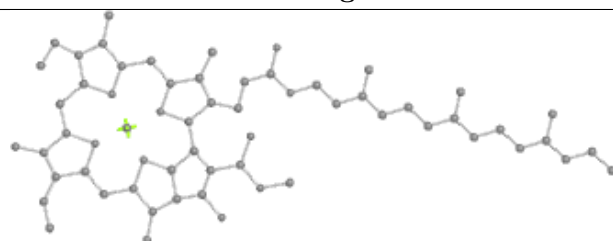
Bond lengths



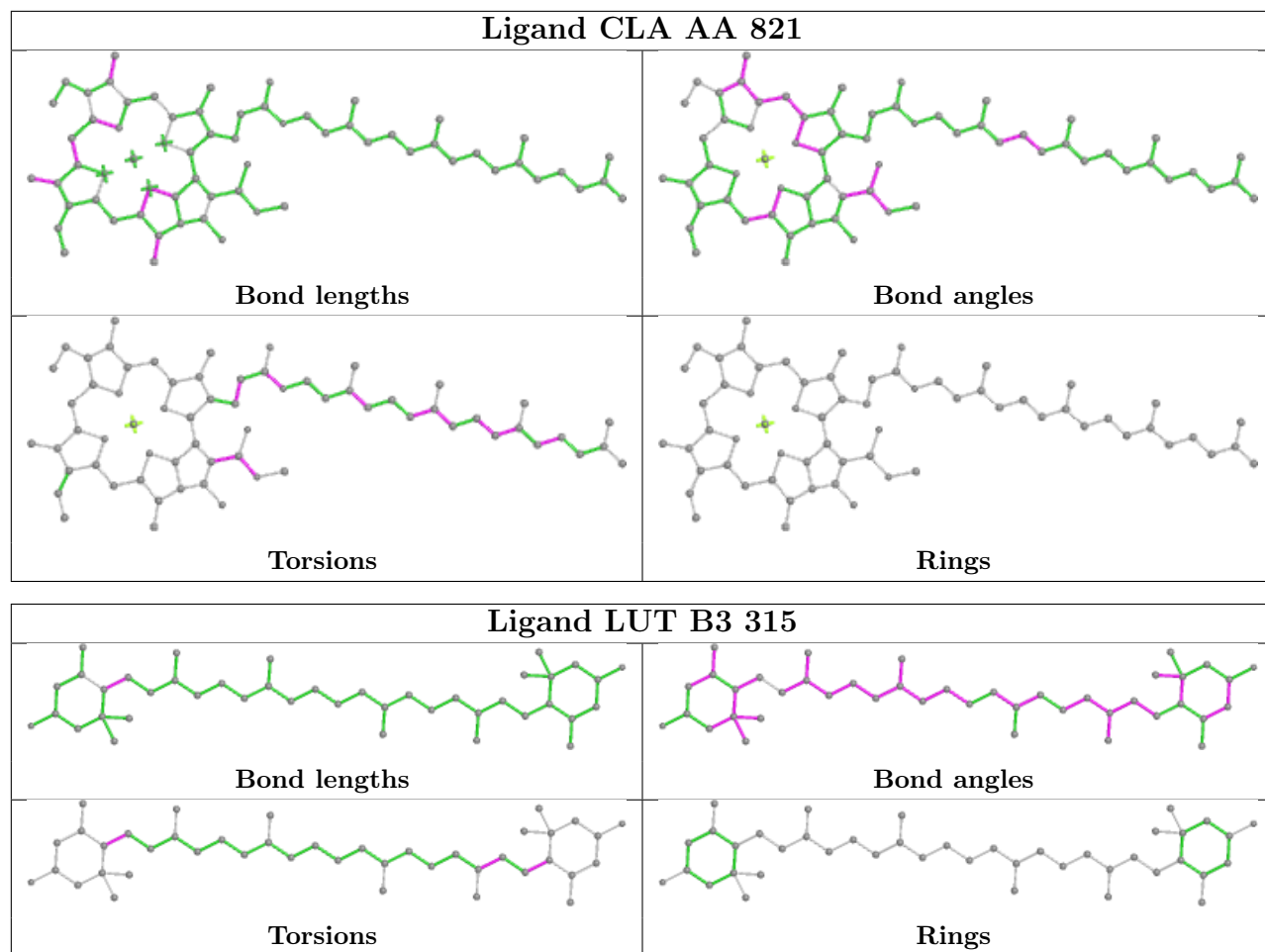
Bond angles



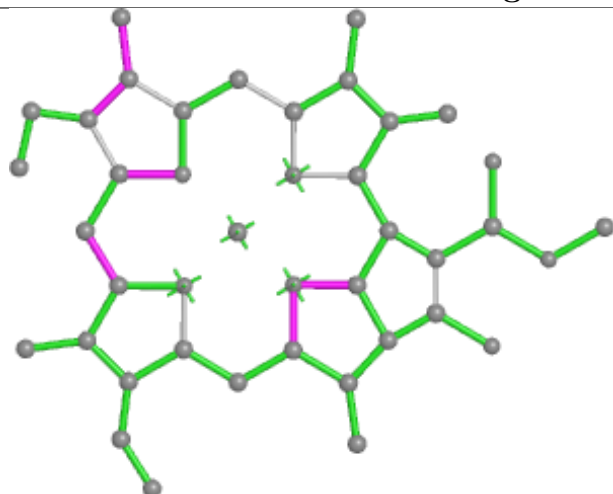
Torsions



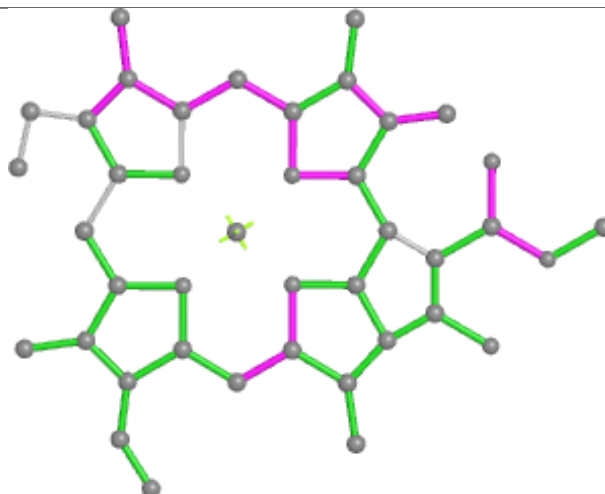
Rings



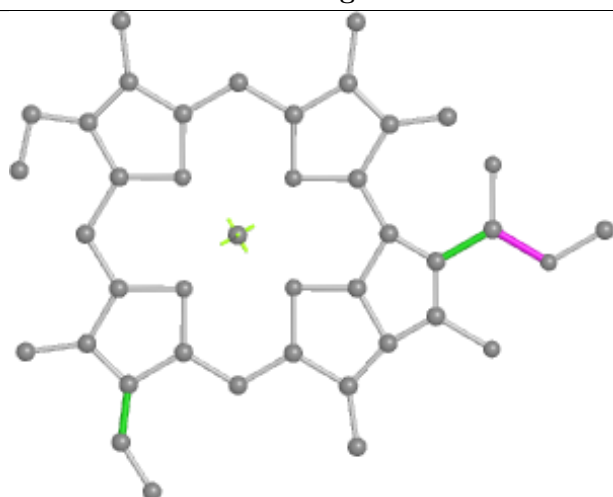
Ligand CLA BF 303



Bond lengths



Bond angles

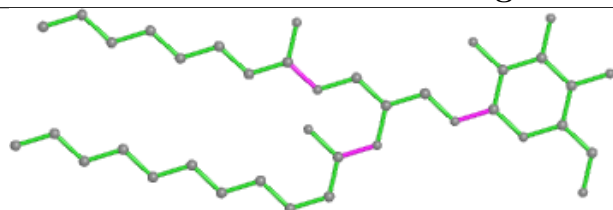


Torsions

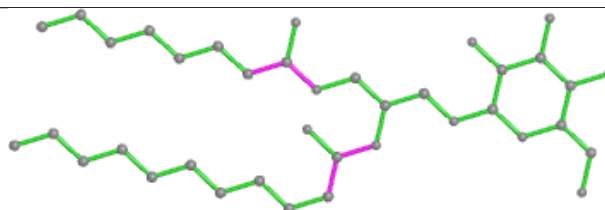


Rings

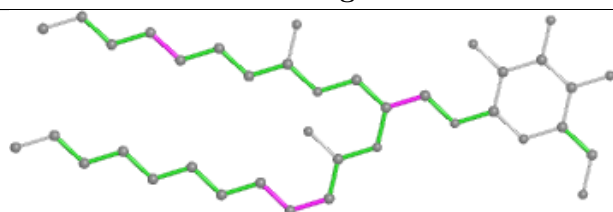
Ligand LMG AG 202



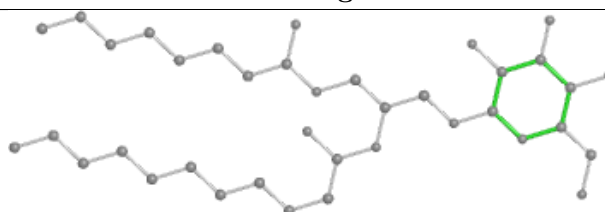
Bond lengths



Bond angles

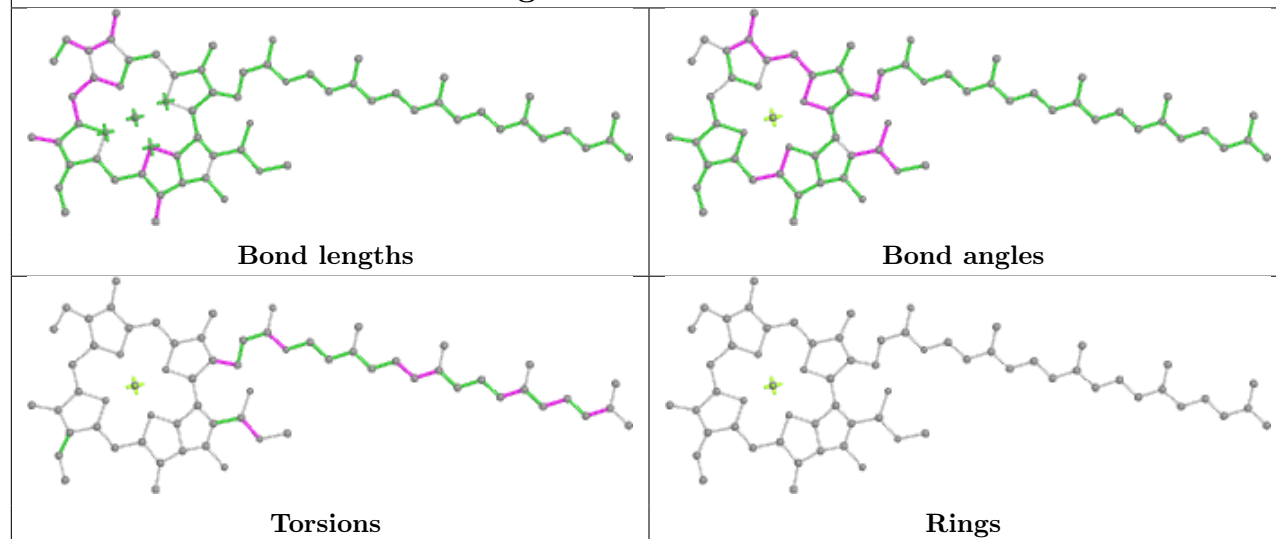


Torsions

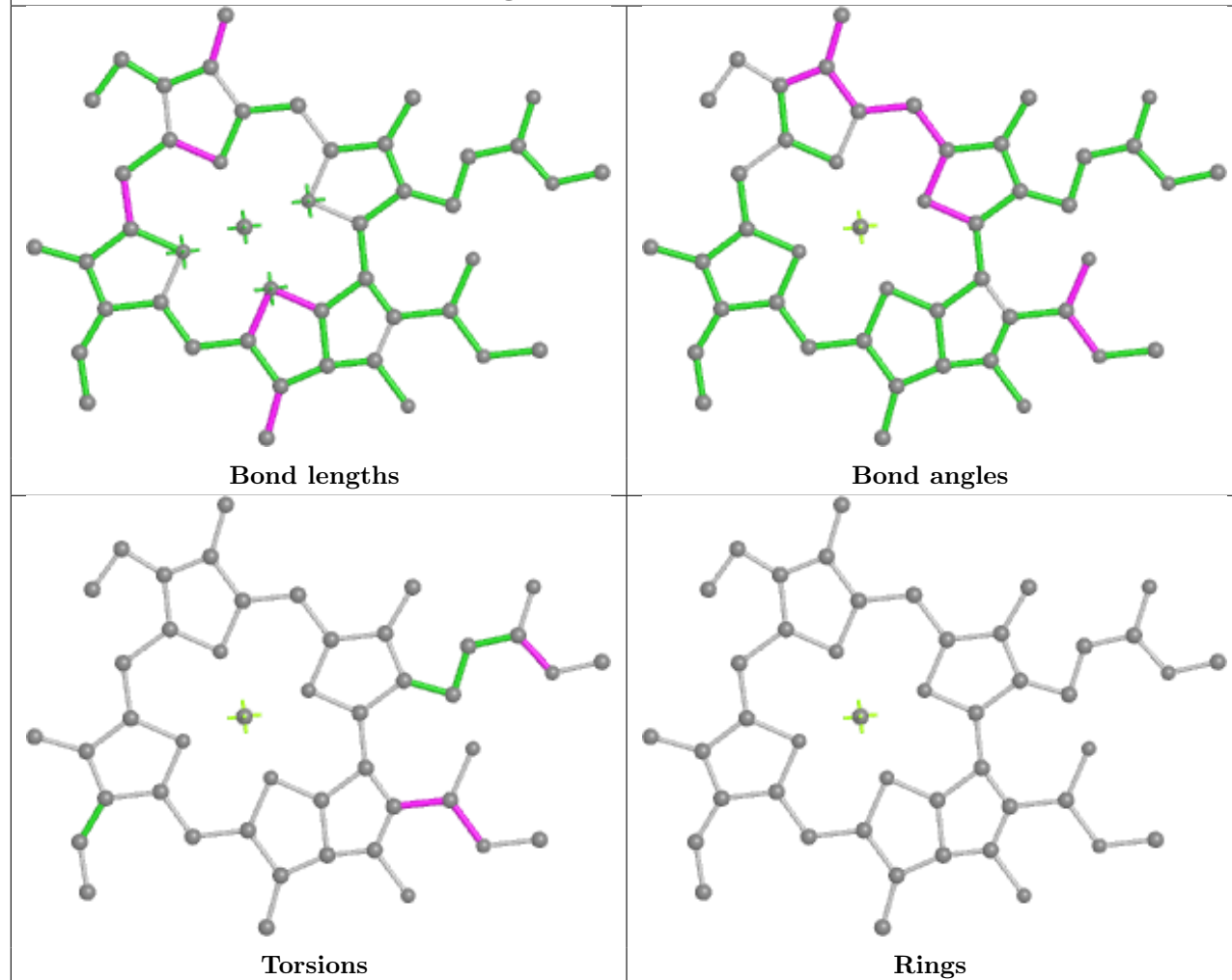


Rings

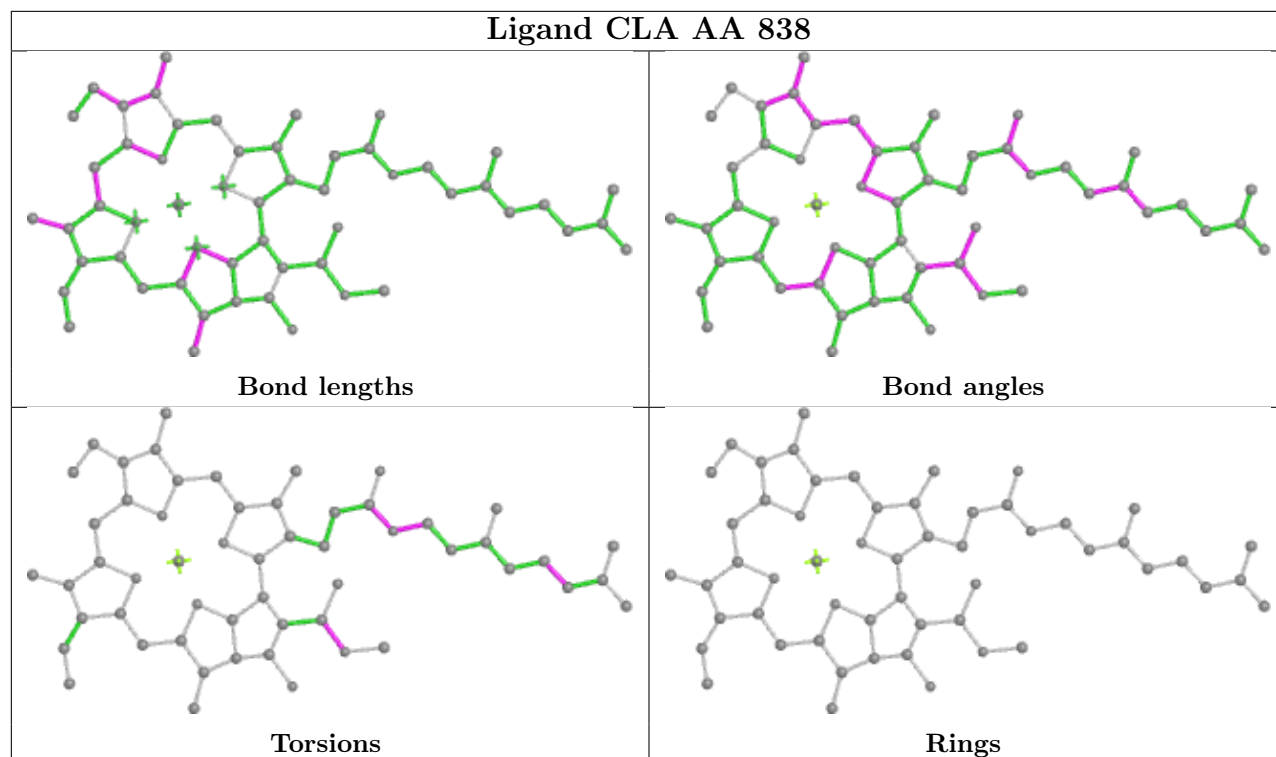
Ligand CLA AA 819



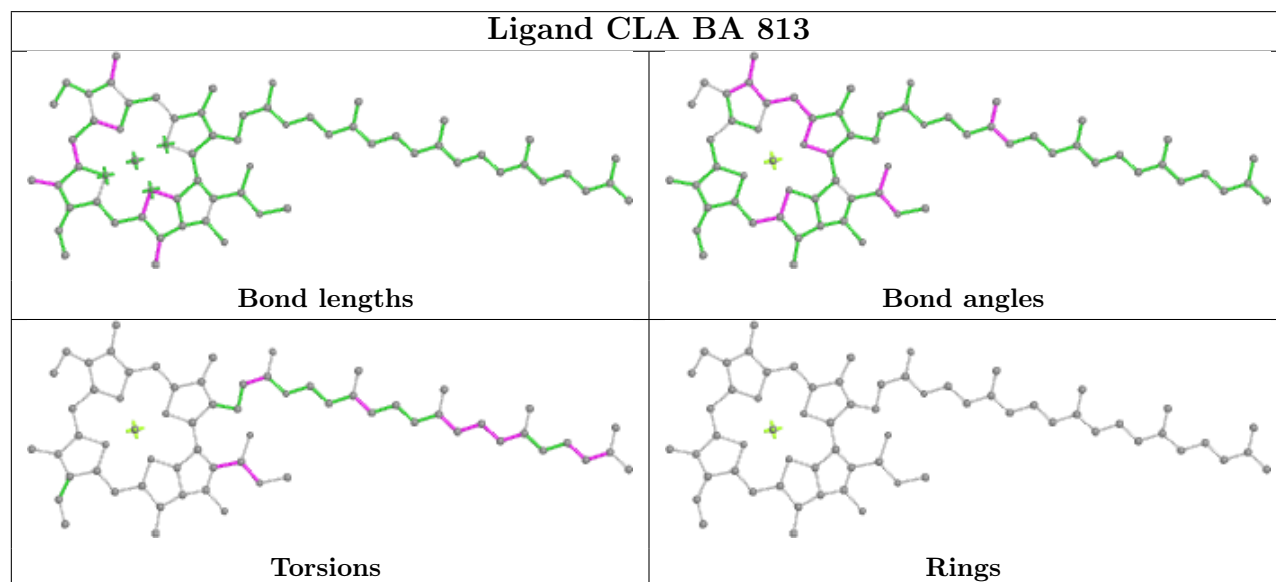
Ligand CLA BK 203



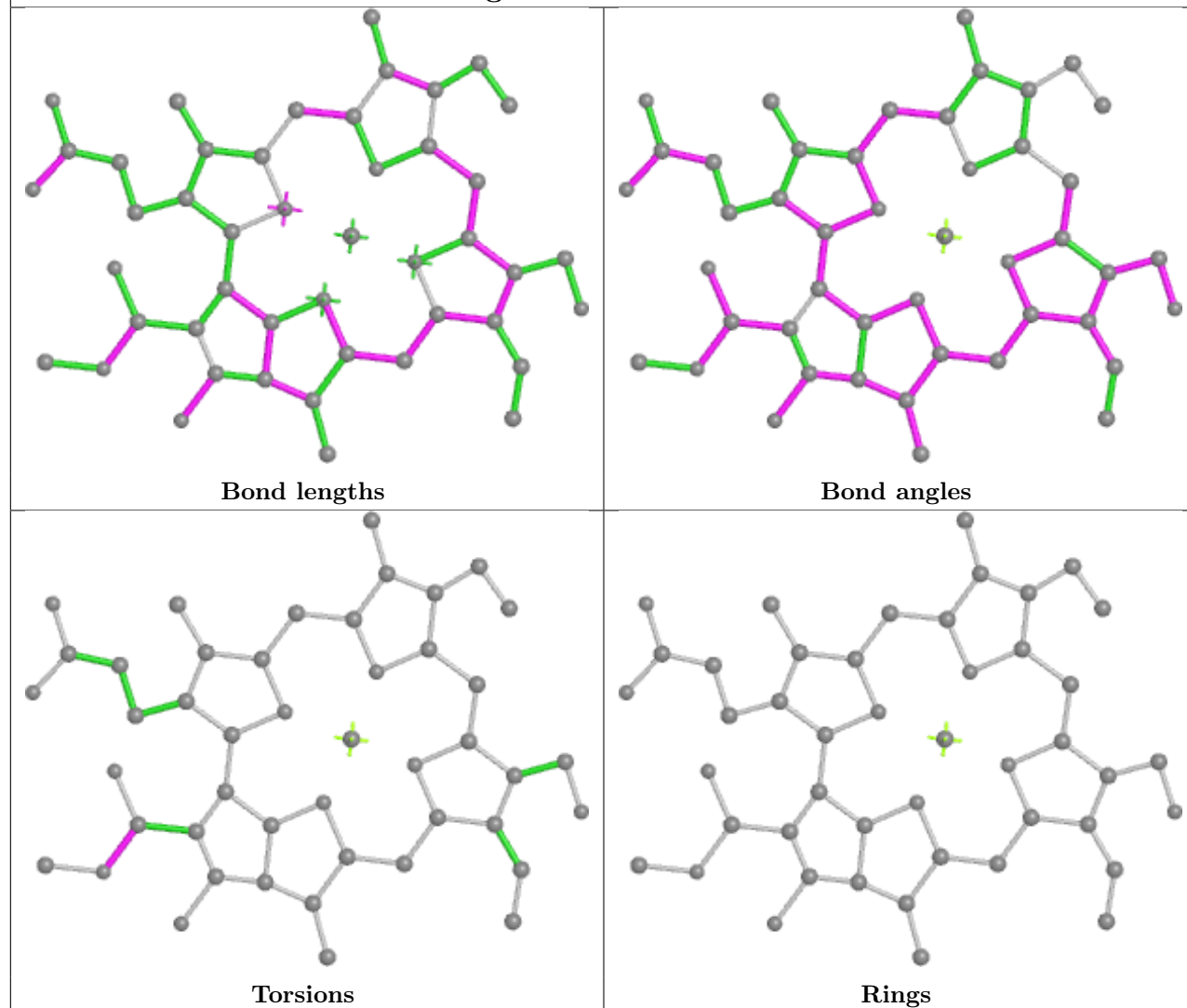
Ligand CLA AA 838

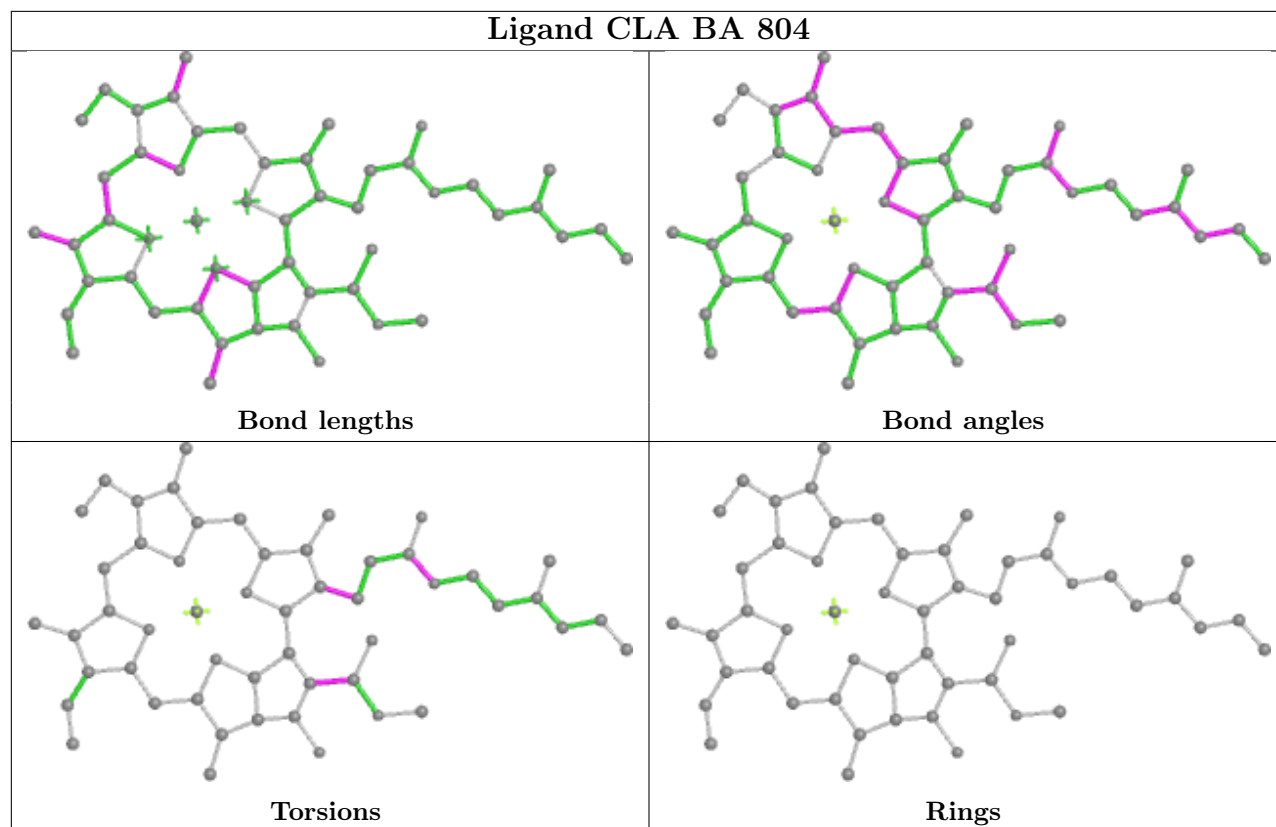


Ligand CLA BA 813

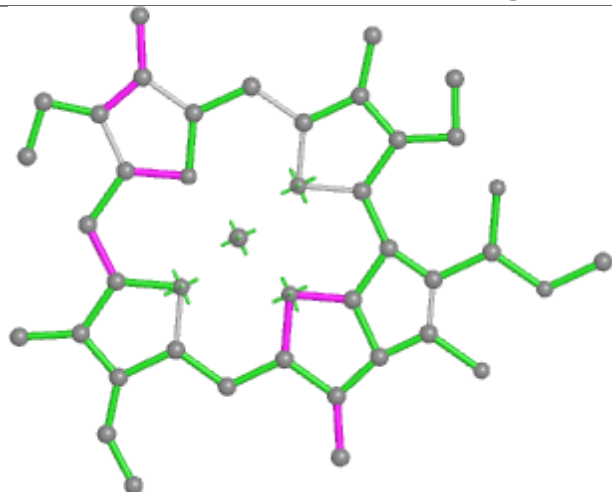


Ligand CHL A4 306

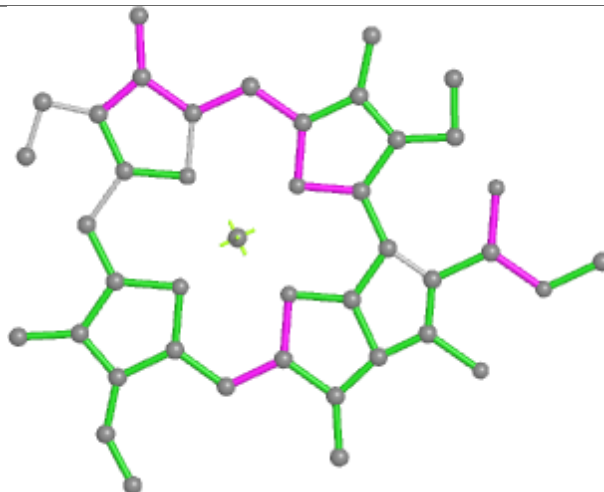




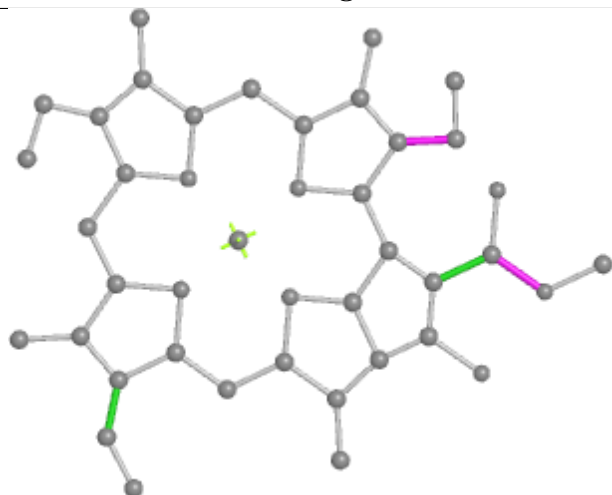
Ligand CLA B5 610



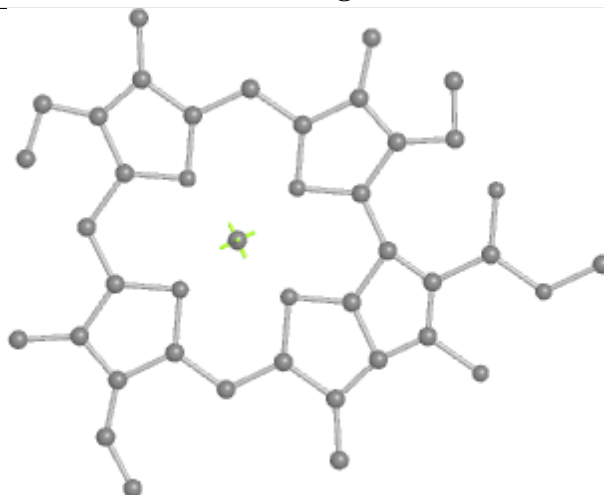
Bond lengths



Bond angles

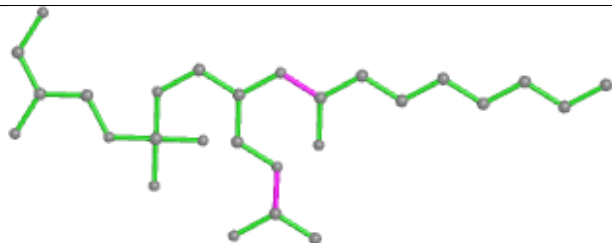


Torsions

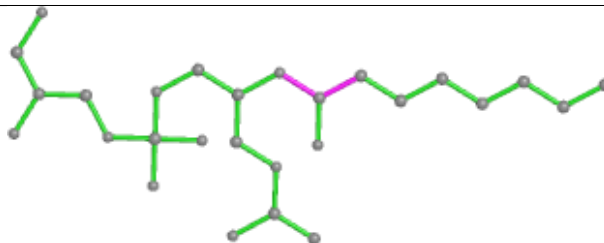


Rings

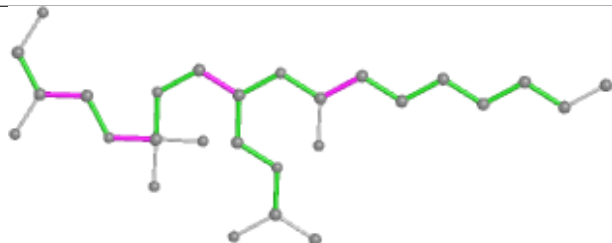
Ligand LHG BA 846



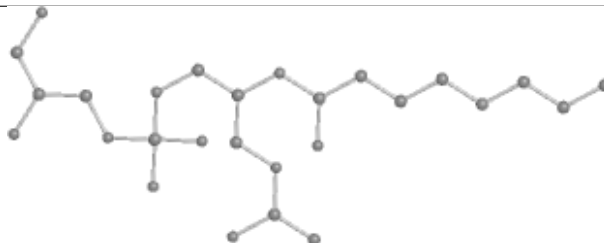
Bond lengths



Bond angles

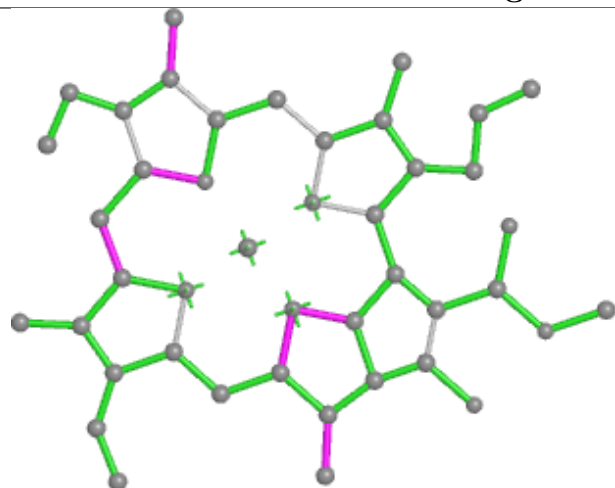


Torsions

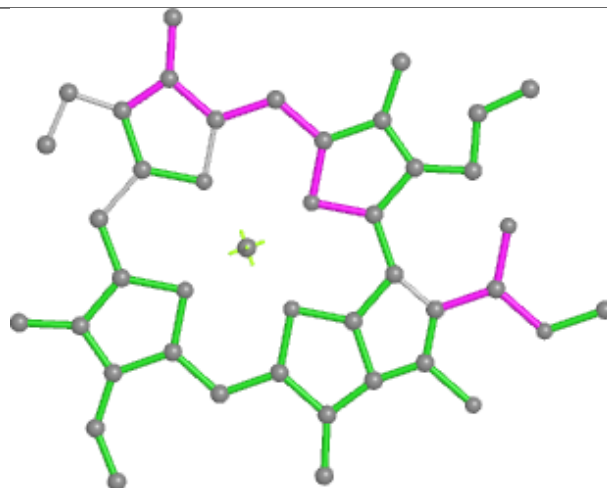


Rings

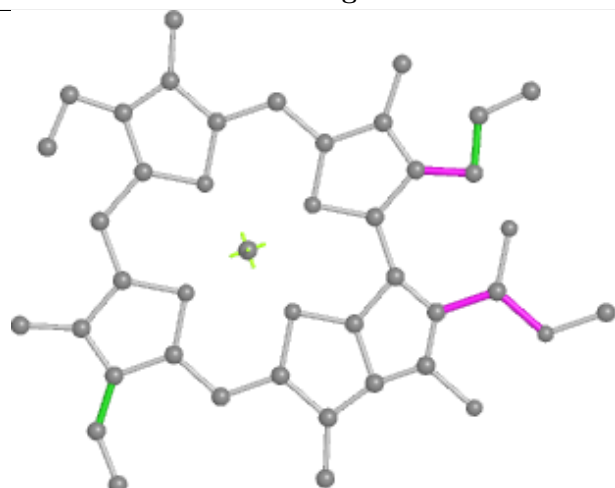
Ligand CLA BL 304



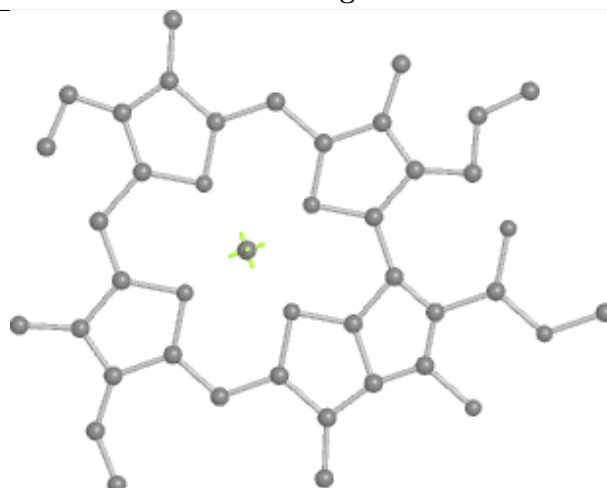
Bond lengths



Bond angles

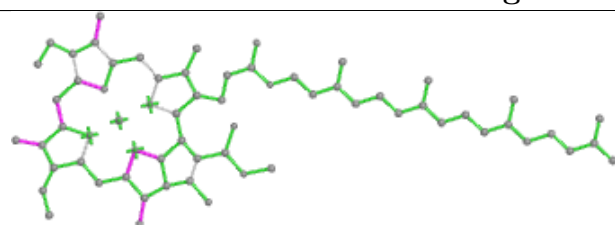


Torsions

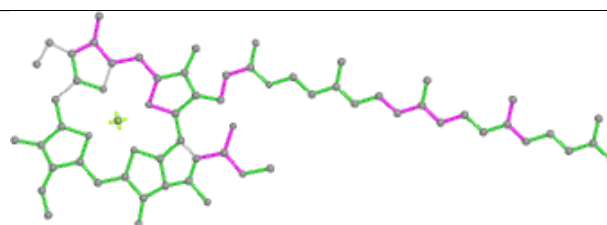


Rings

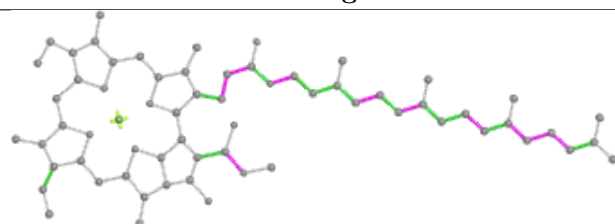
Ligand CLA BA 828



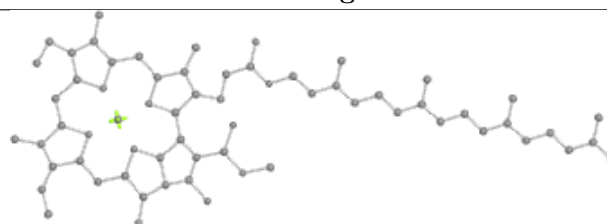
Bond lengths



Bond angles

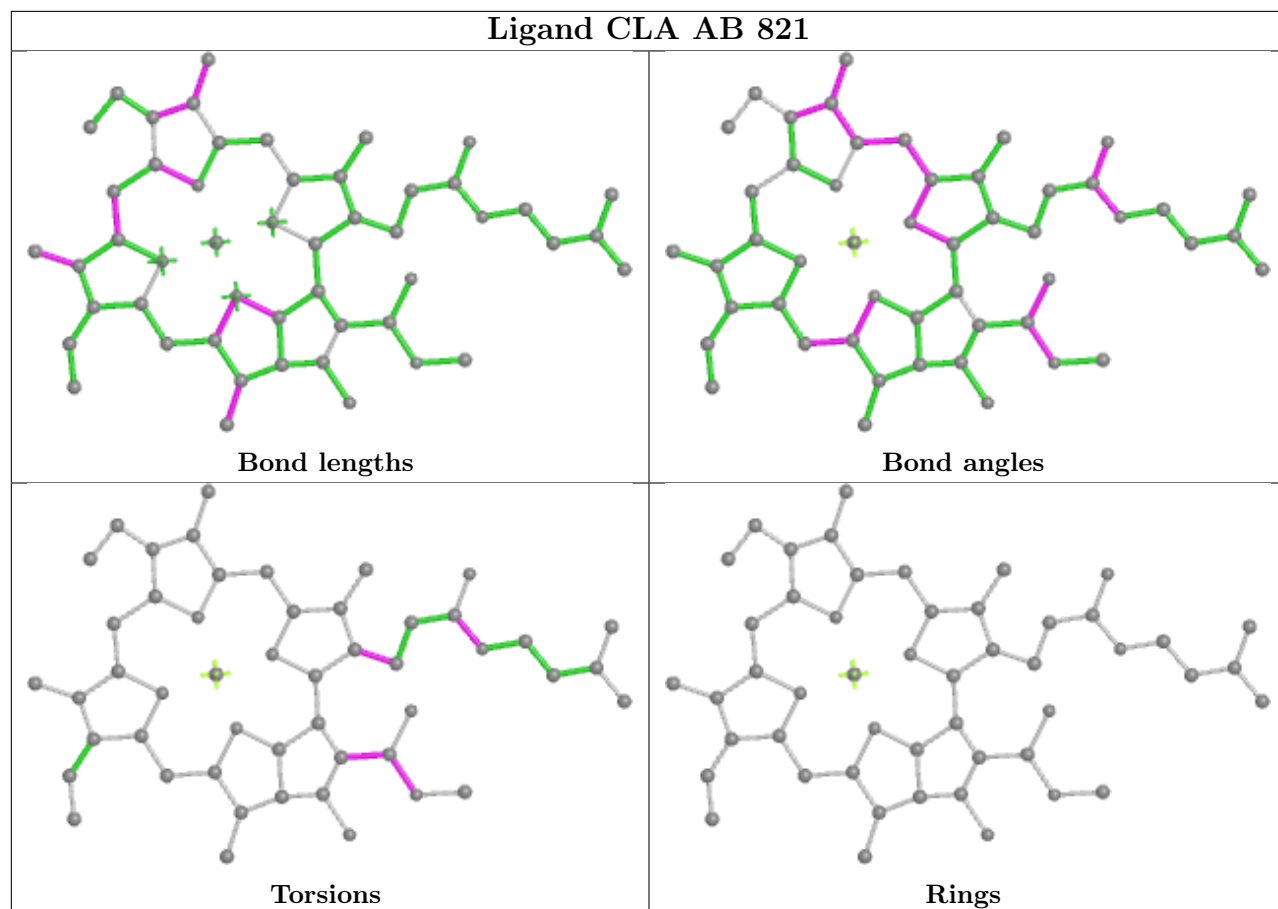


Torsions

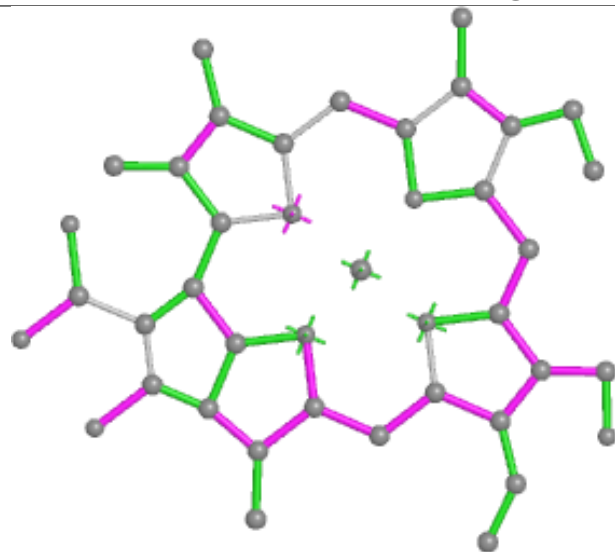


Rings

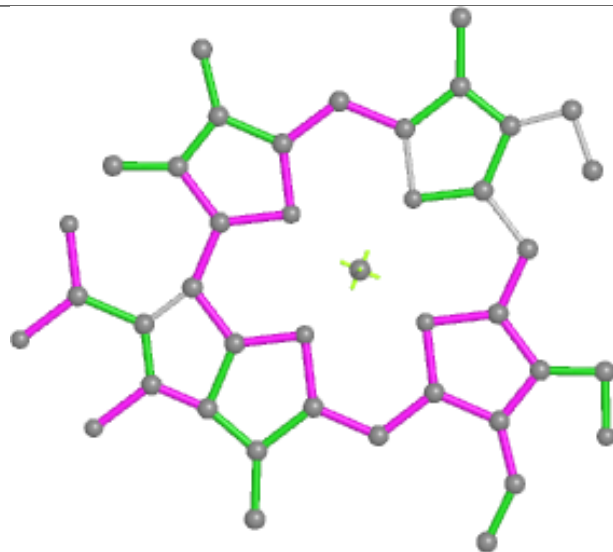
Ligand CLA AB 821



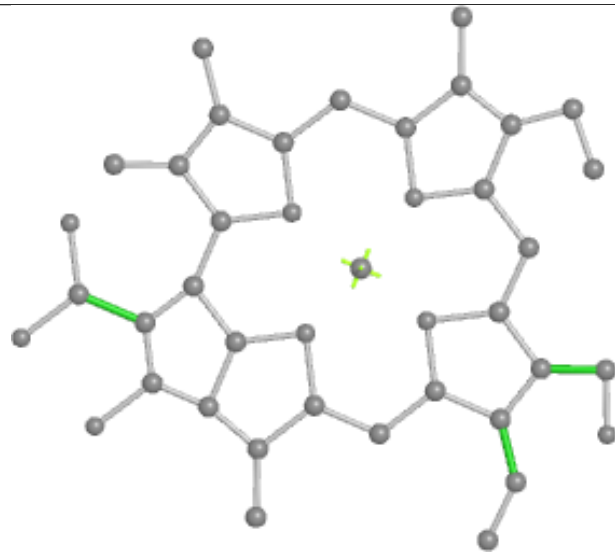
Ligand CHL B1 308



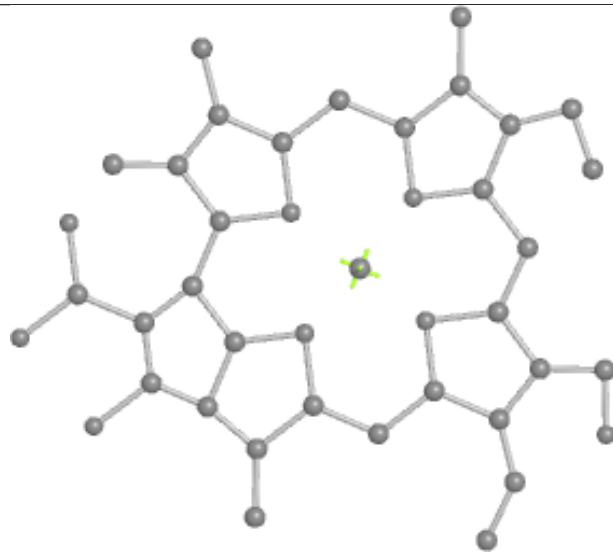
Bond lengths



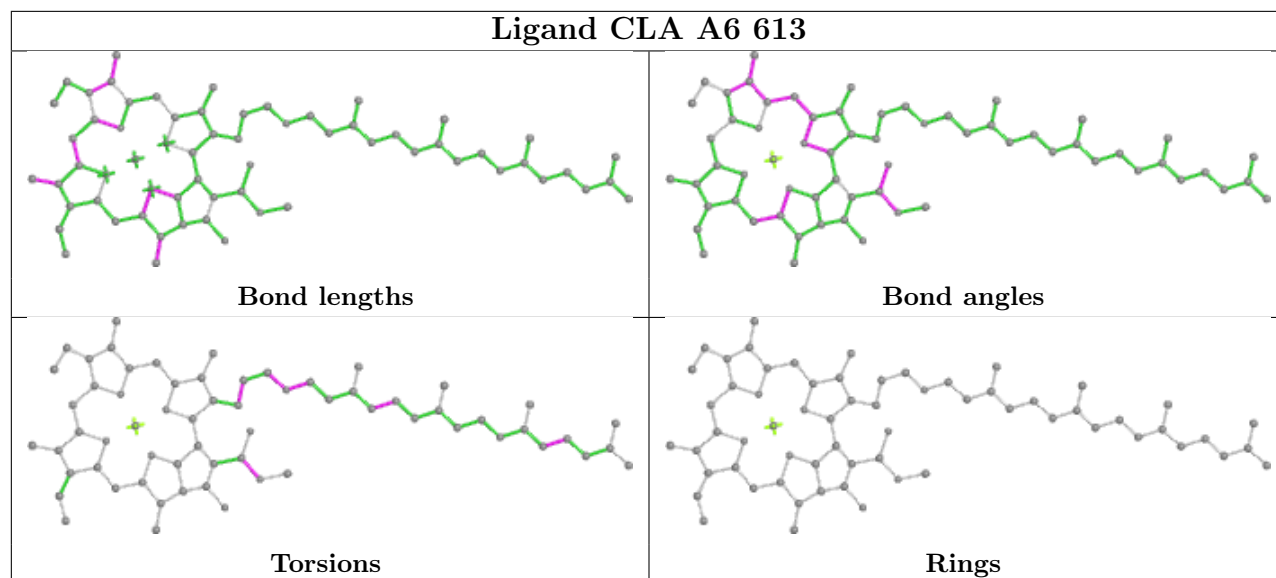
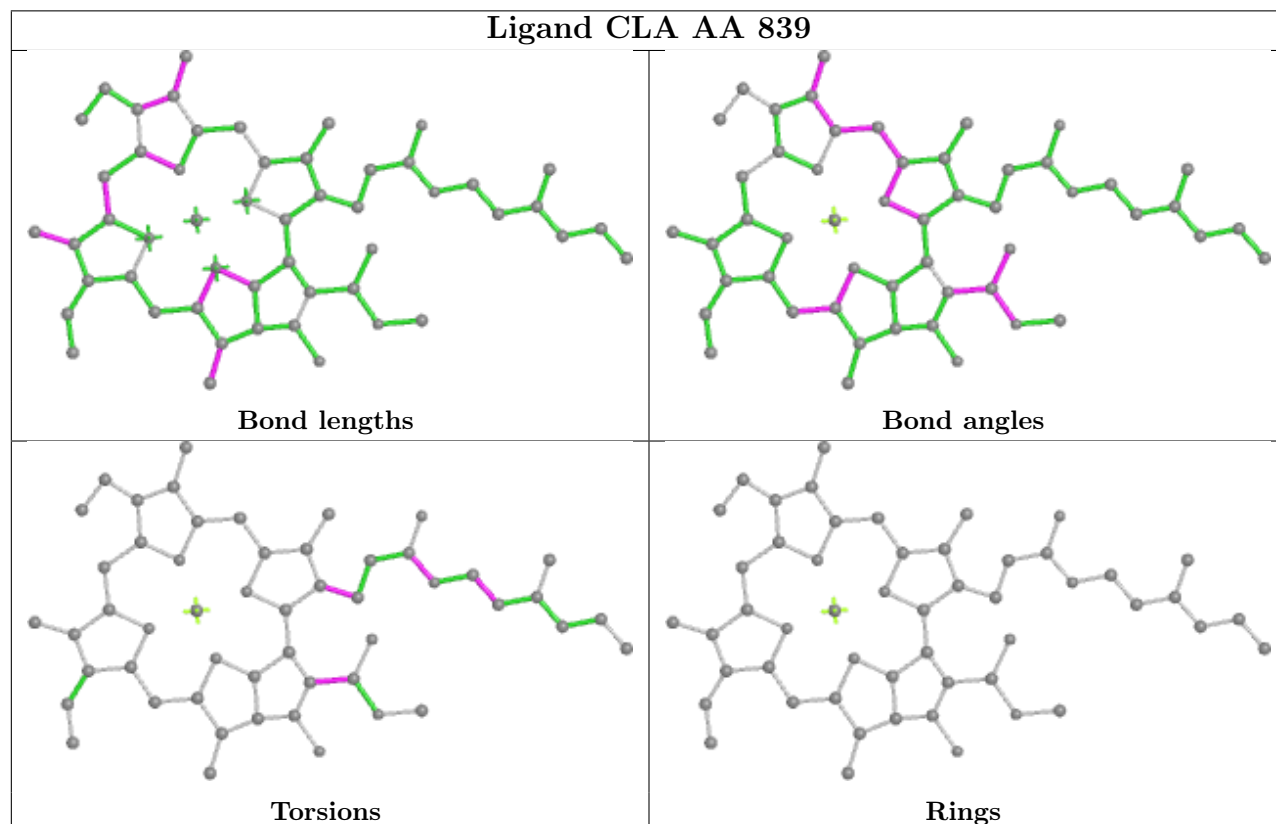
Bond angles

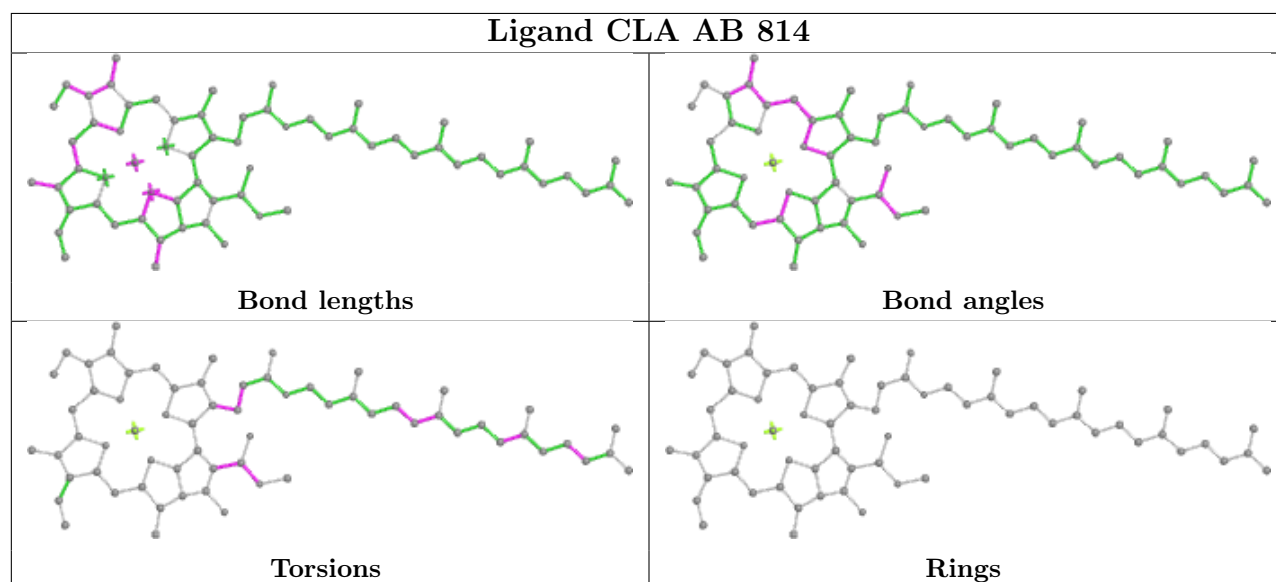
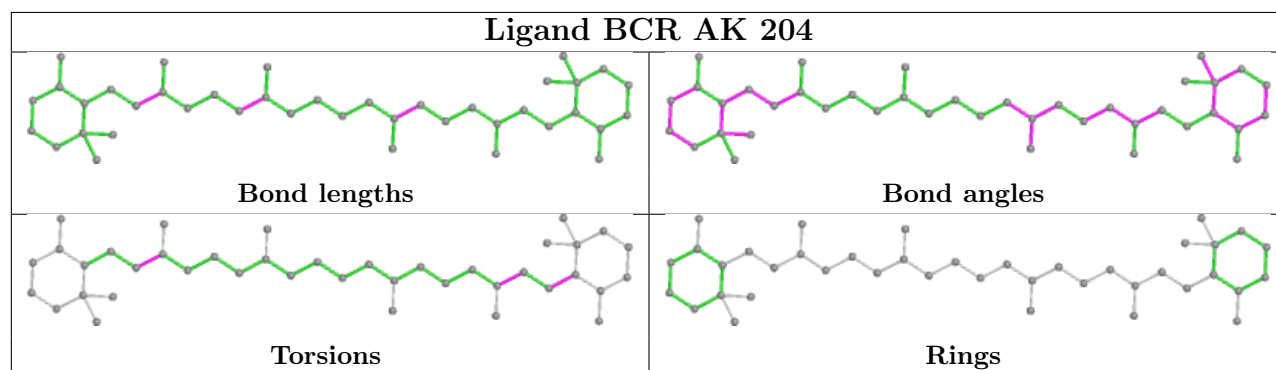
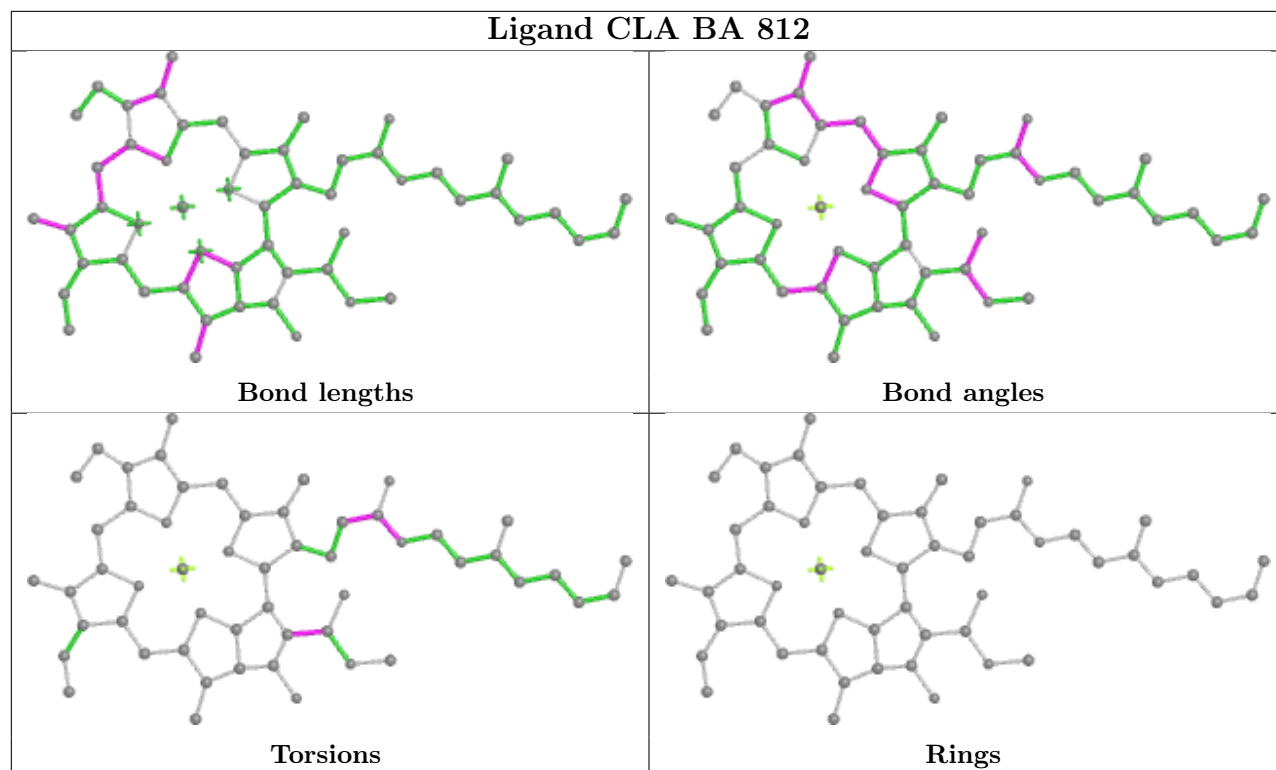


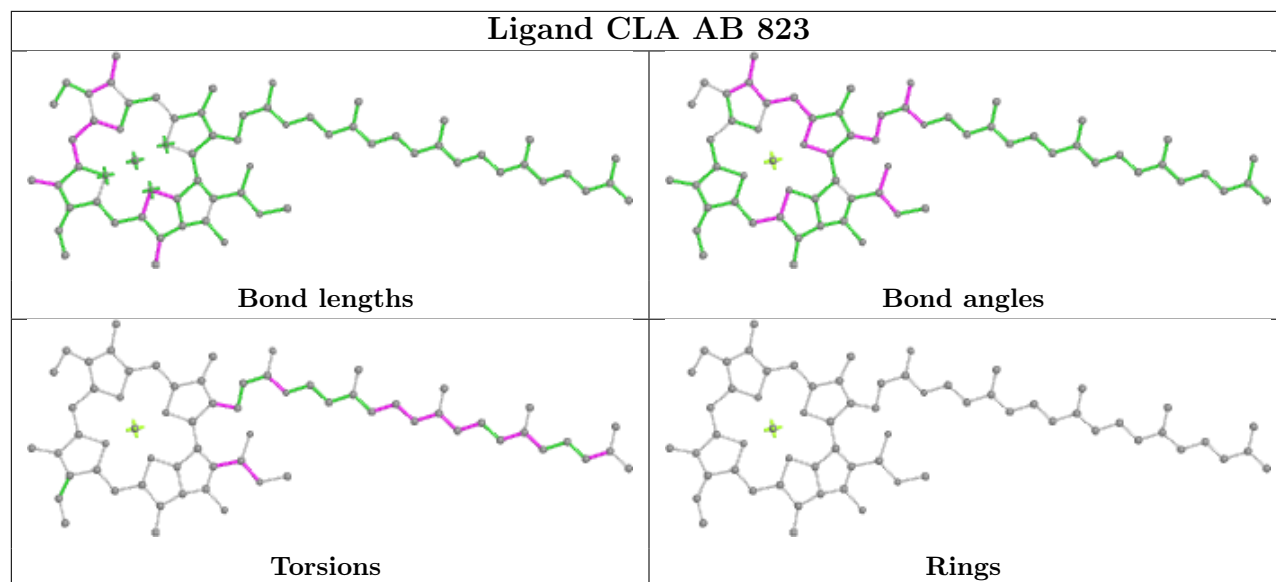
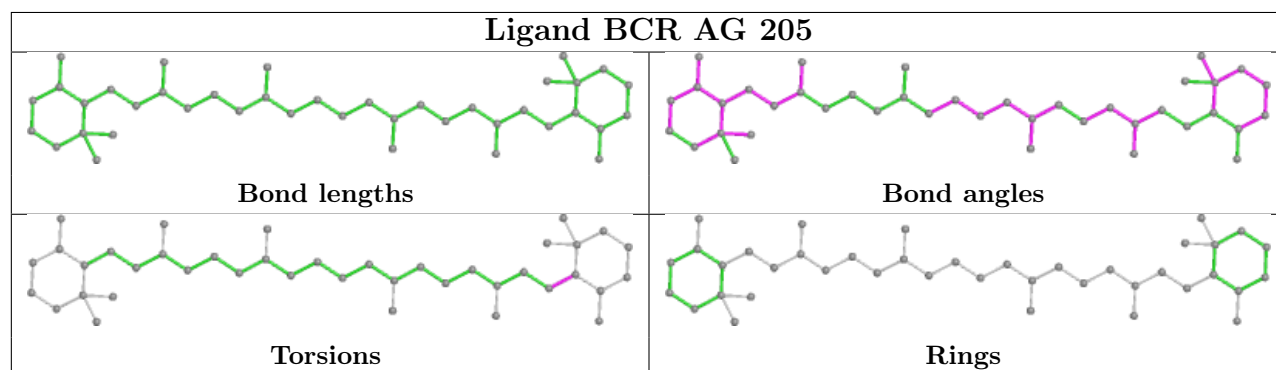
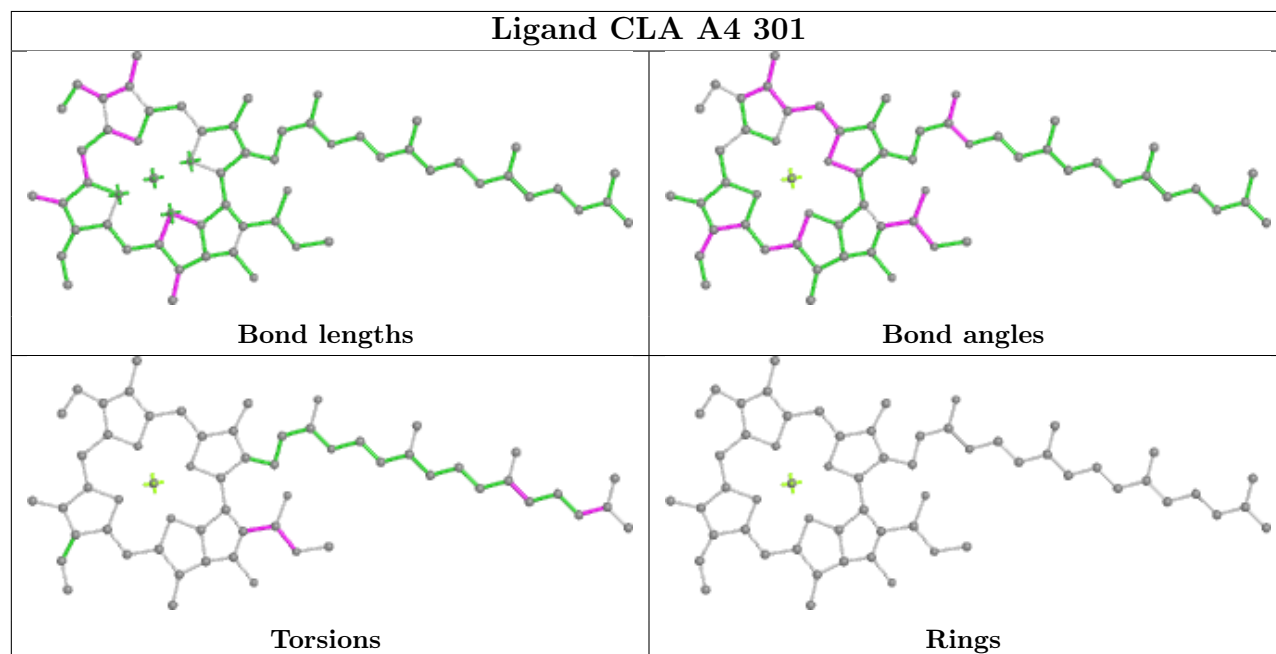
Torsions

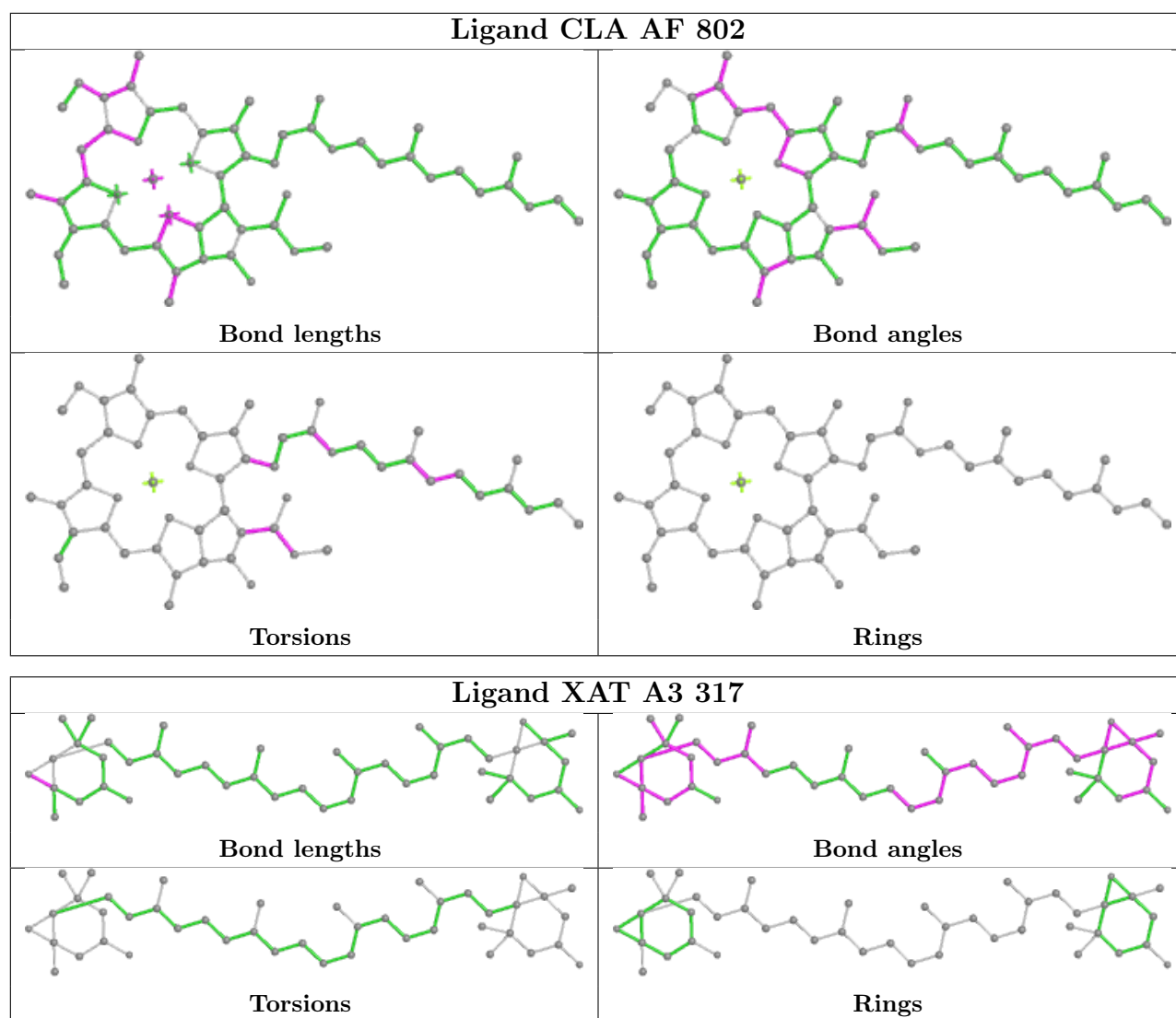


Rings

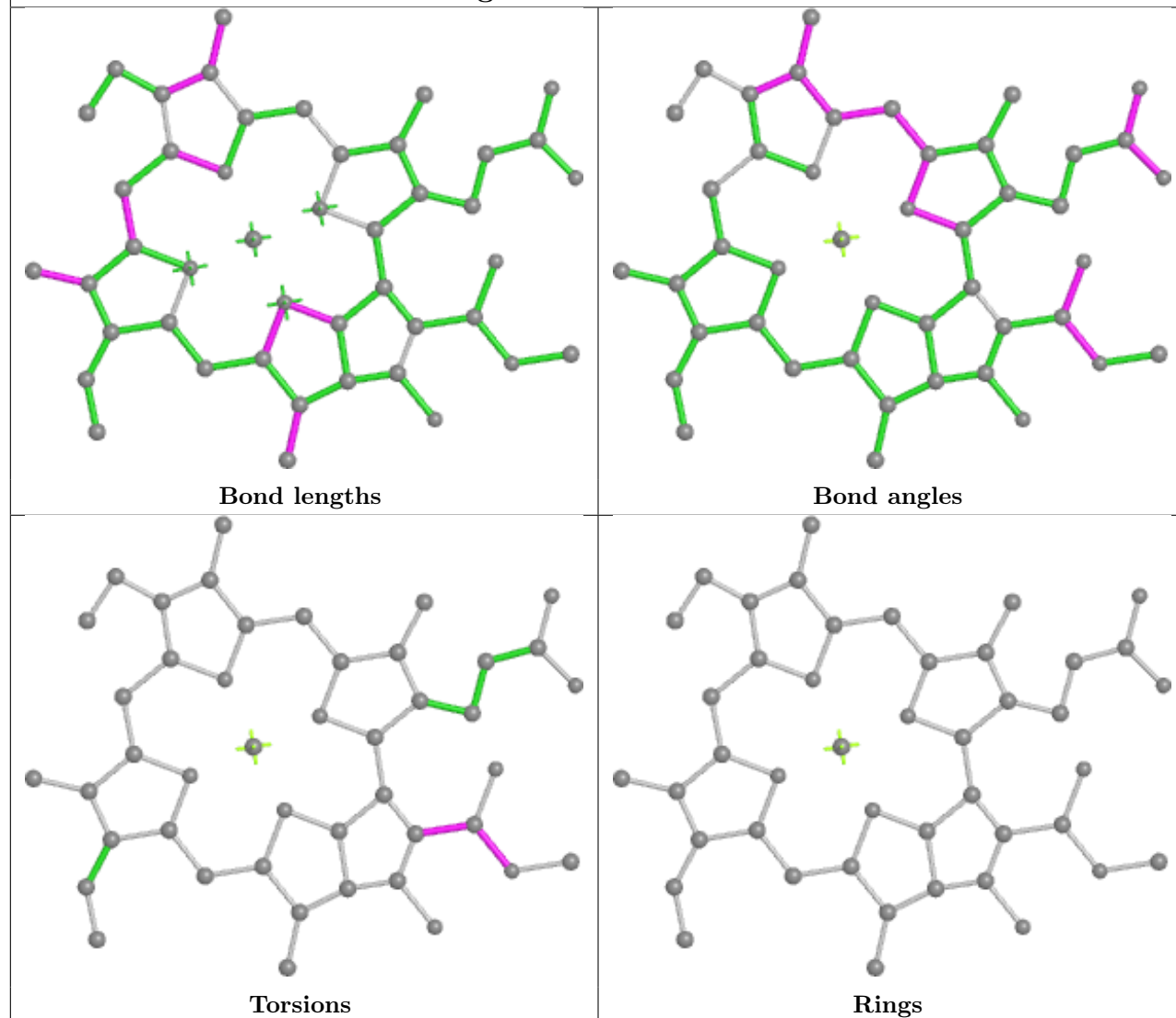
Ligand CLA A6 613**Ligand CLA AA 839**



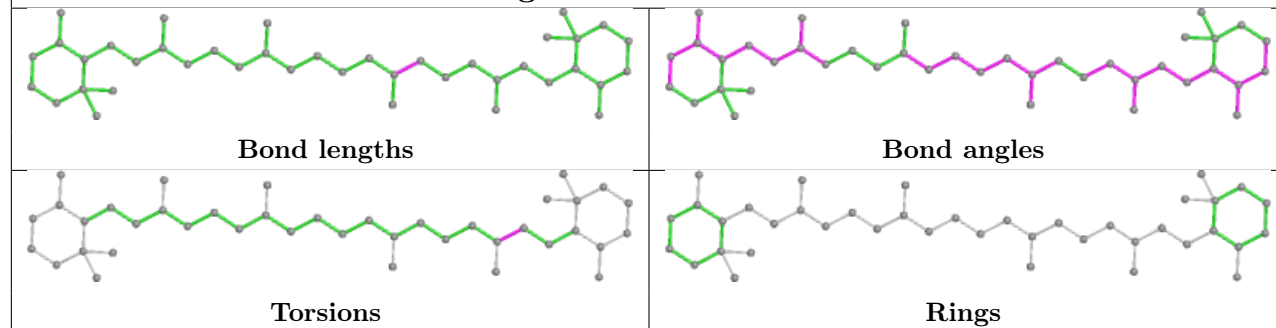
Ligand CLA AB 823**Ligand BCR AG 205****Ligand CLA A4 301**



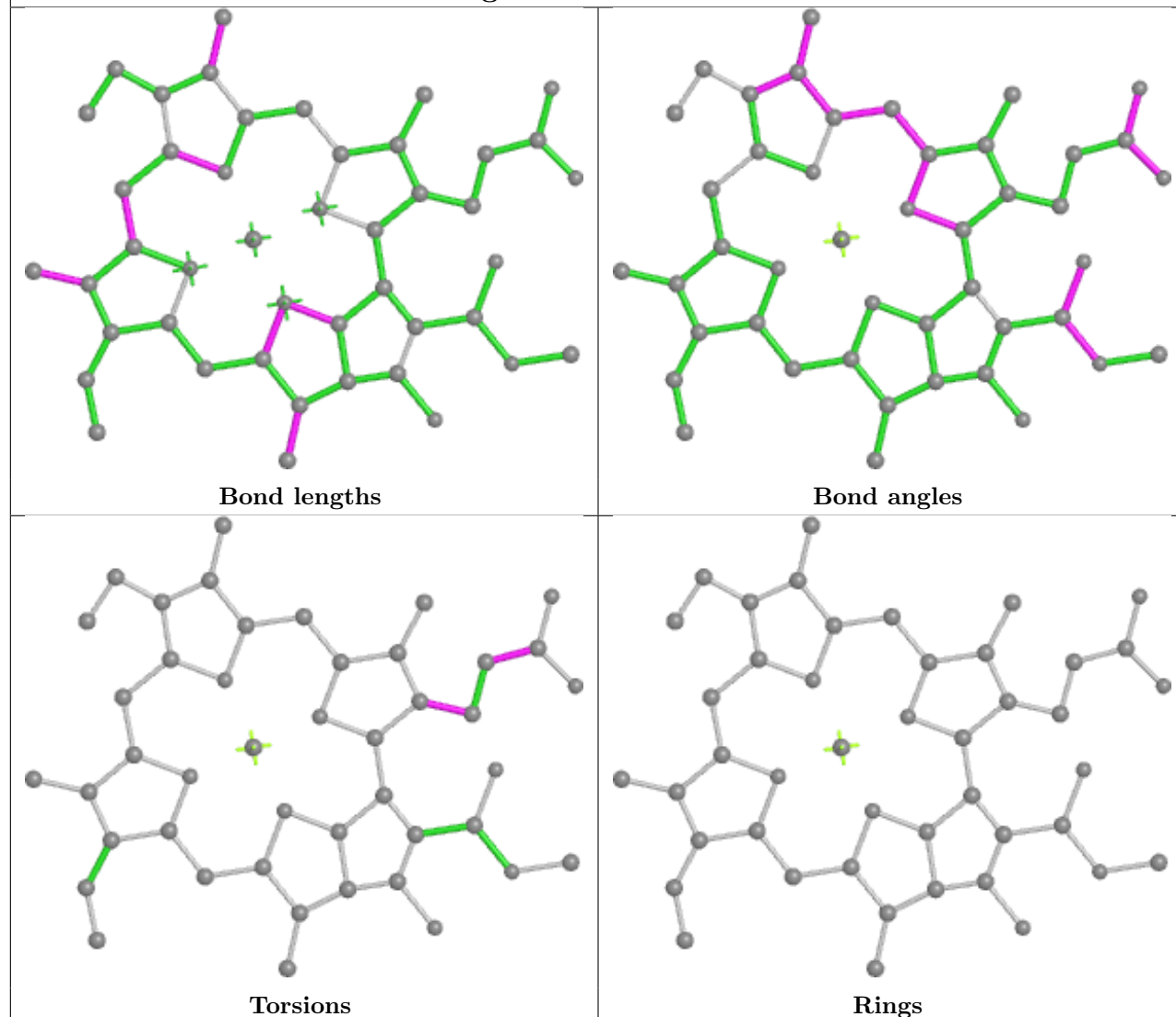
Ligand CLA AA 820



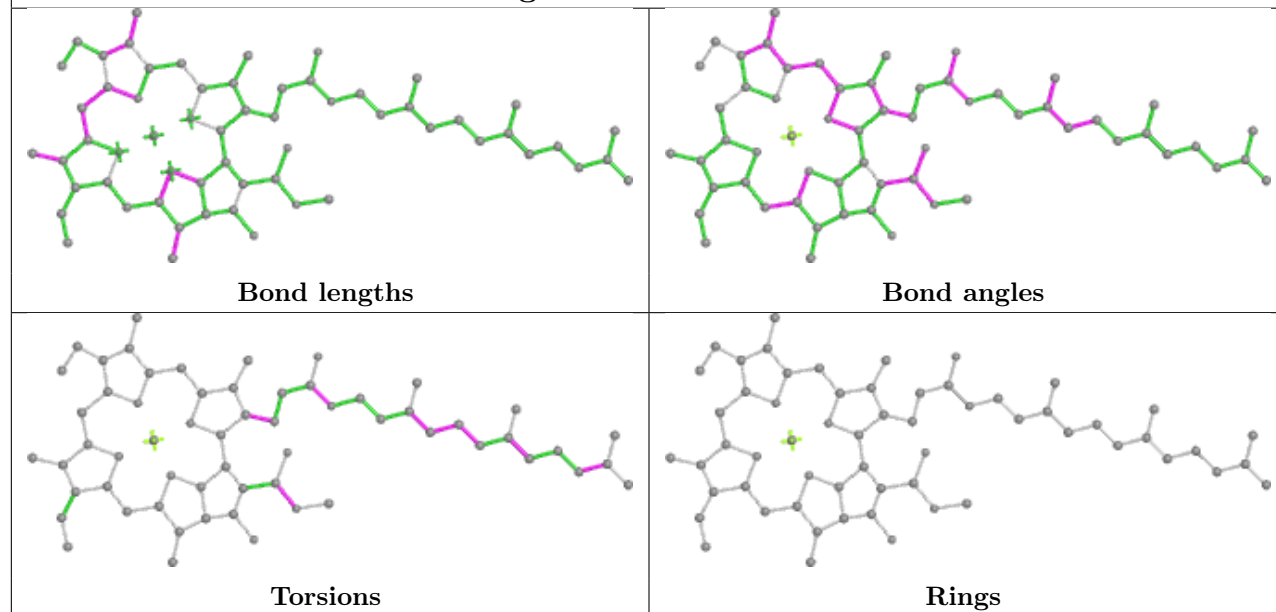
Ligand BCR BB 849



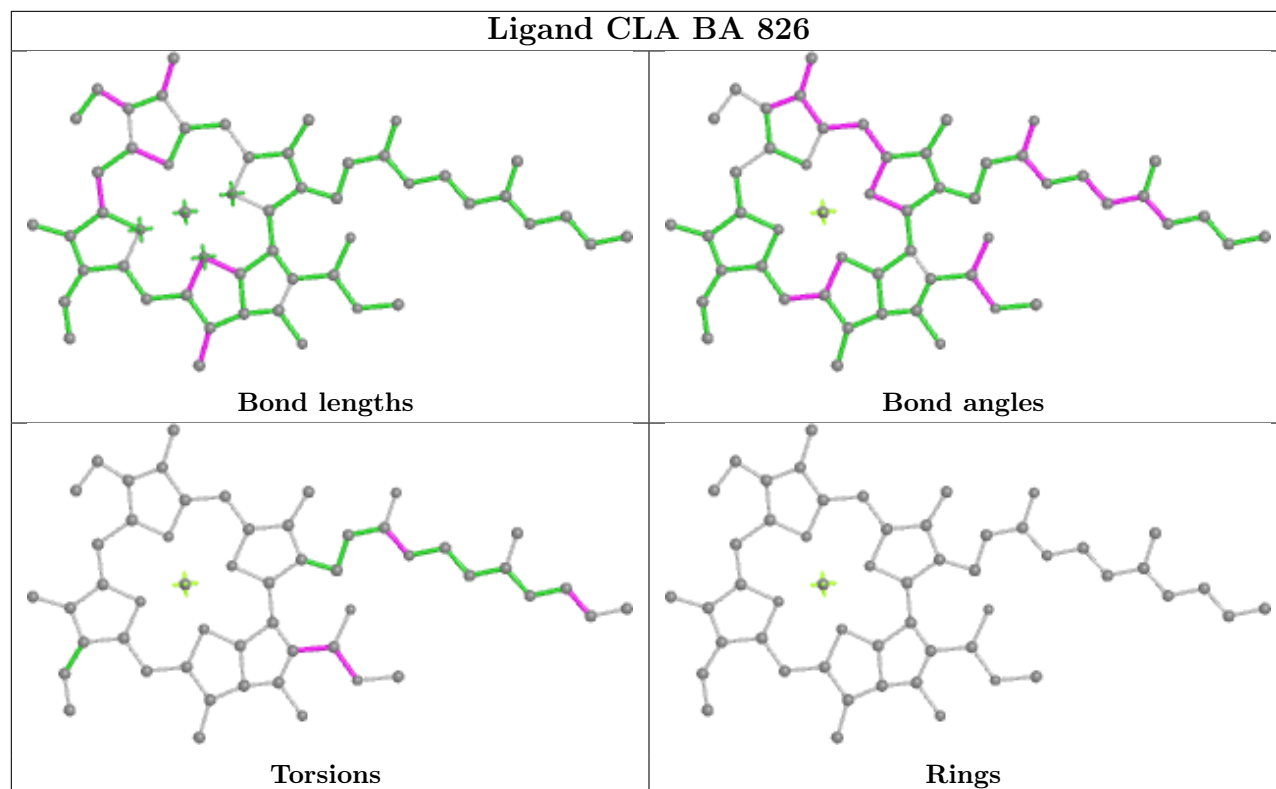
Ligand CLA A6 609



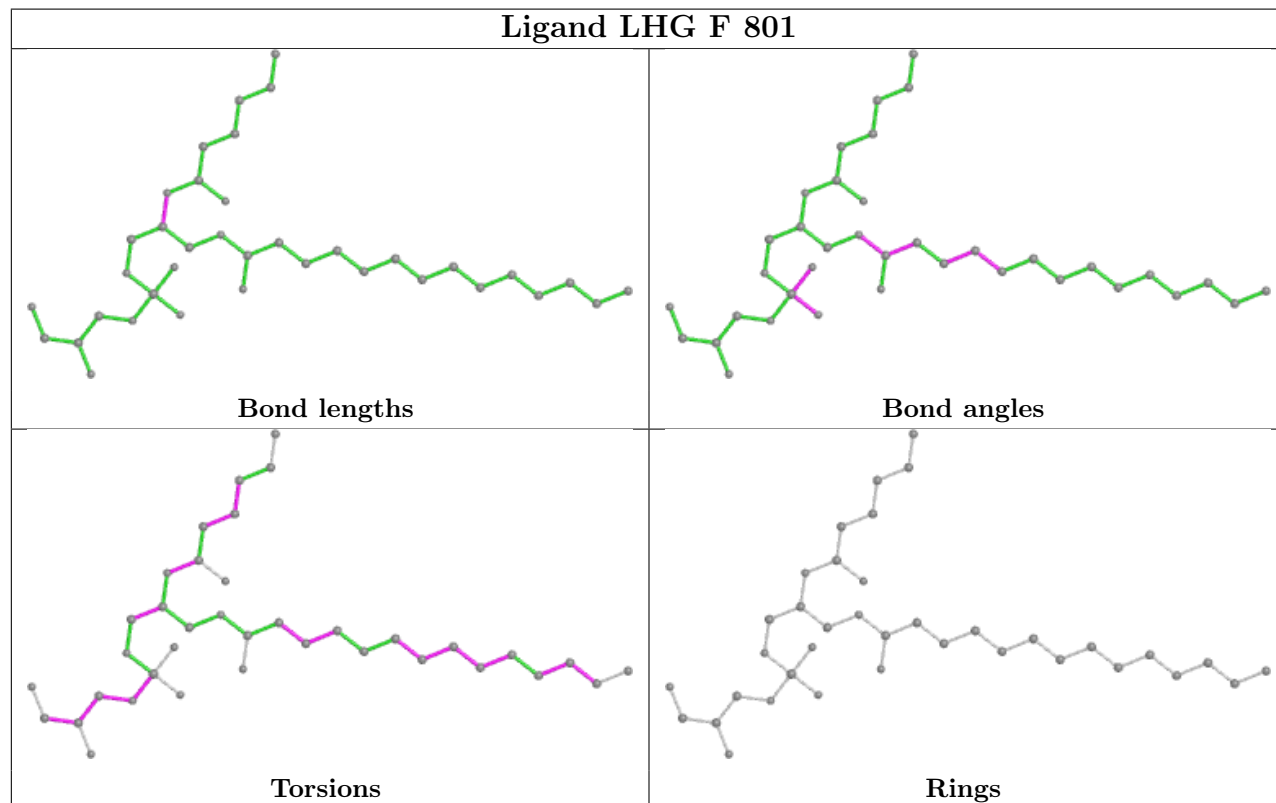
Ligand CLA AB 819



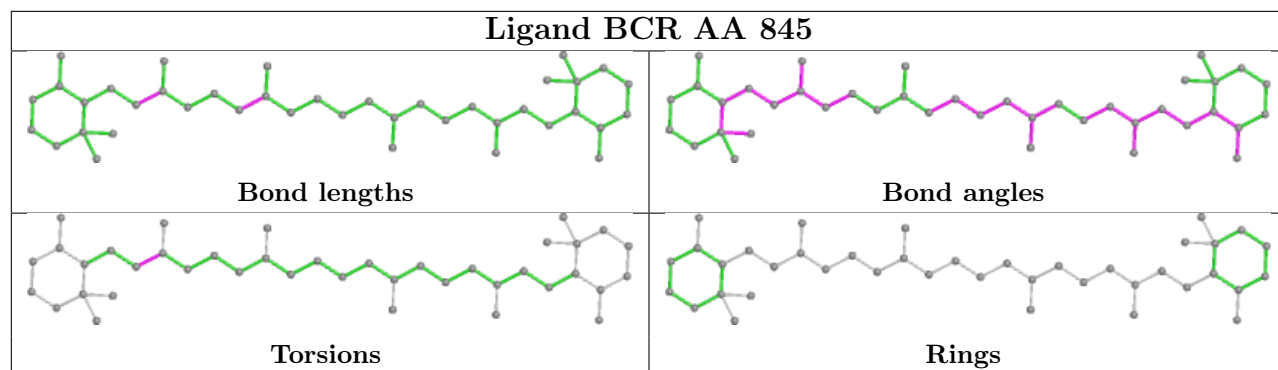
Ligand CLA BA 826



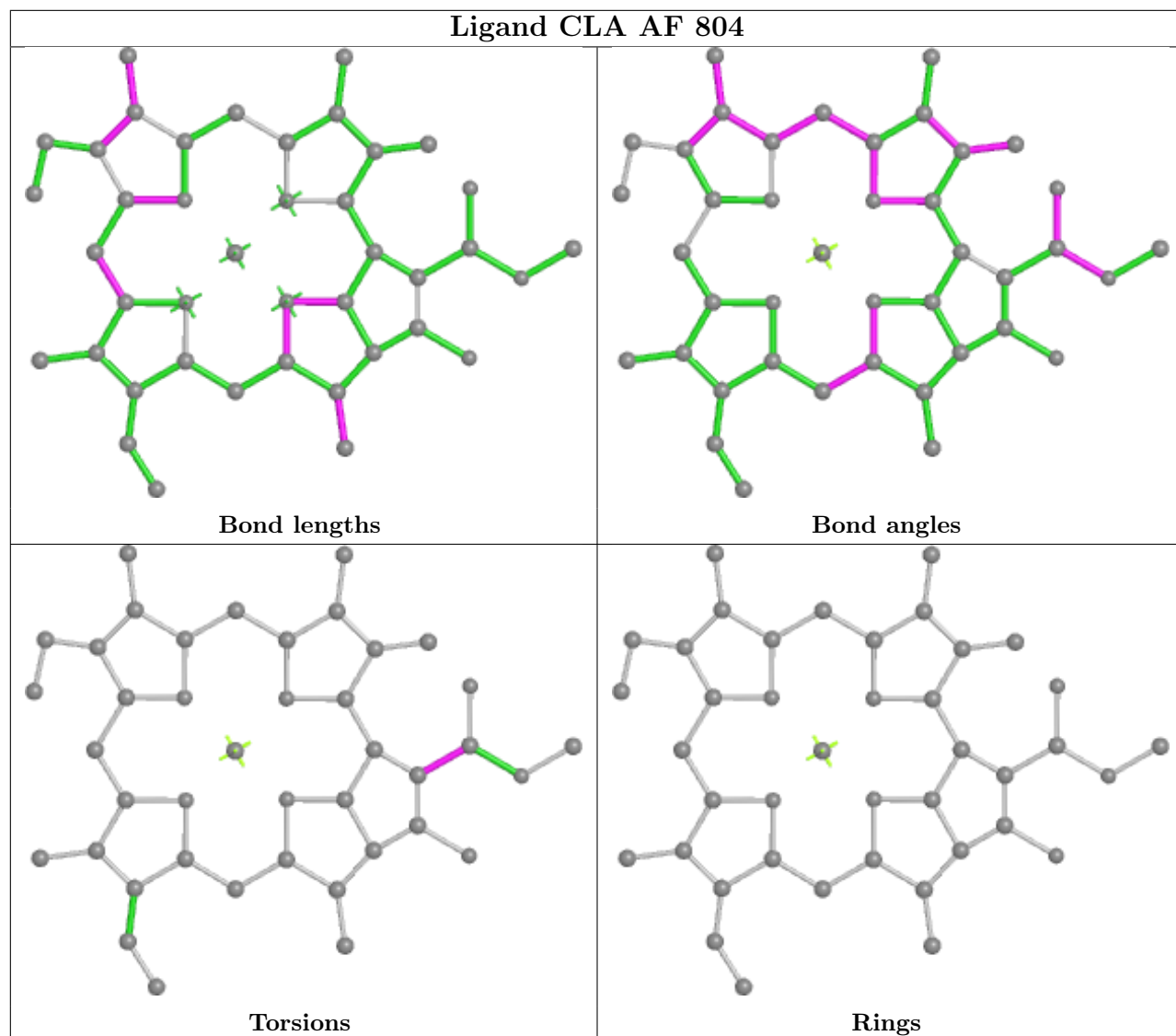
Ligand LHG F 801



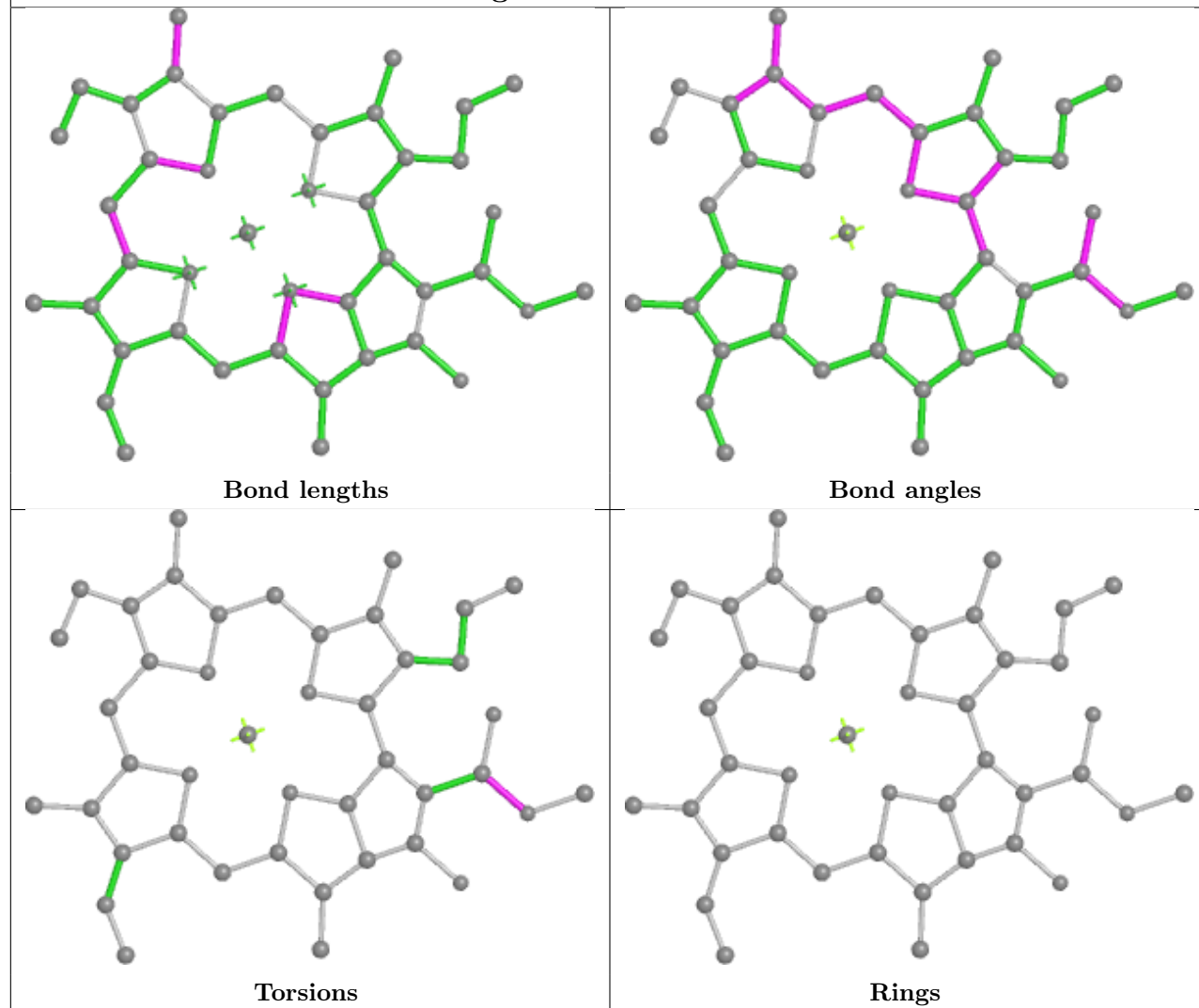
Ligand BCR AA 845



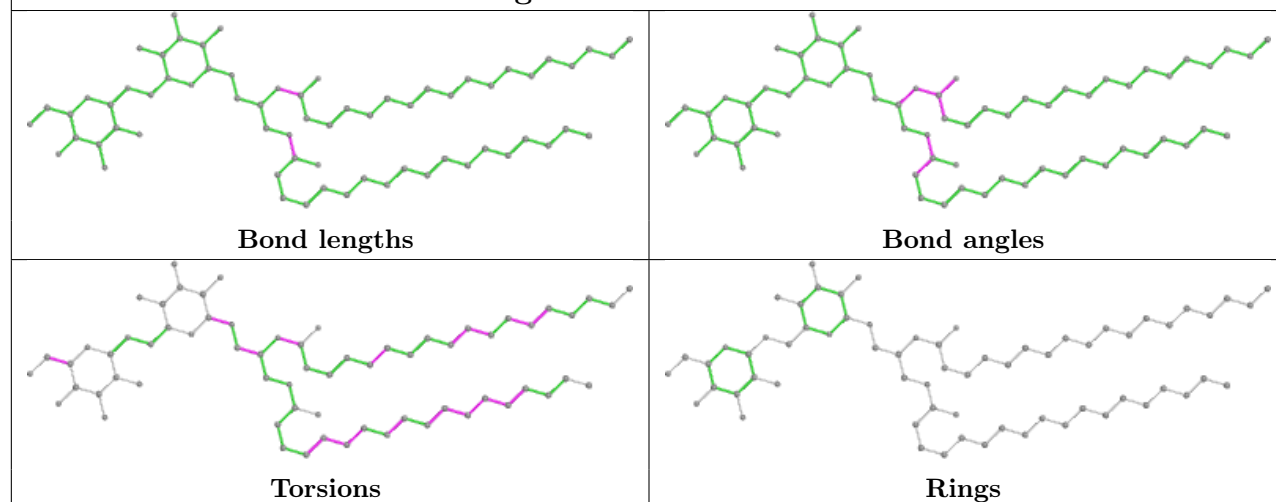
Ligand CLA AF 804



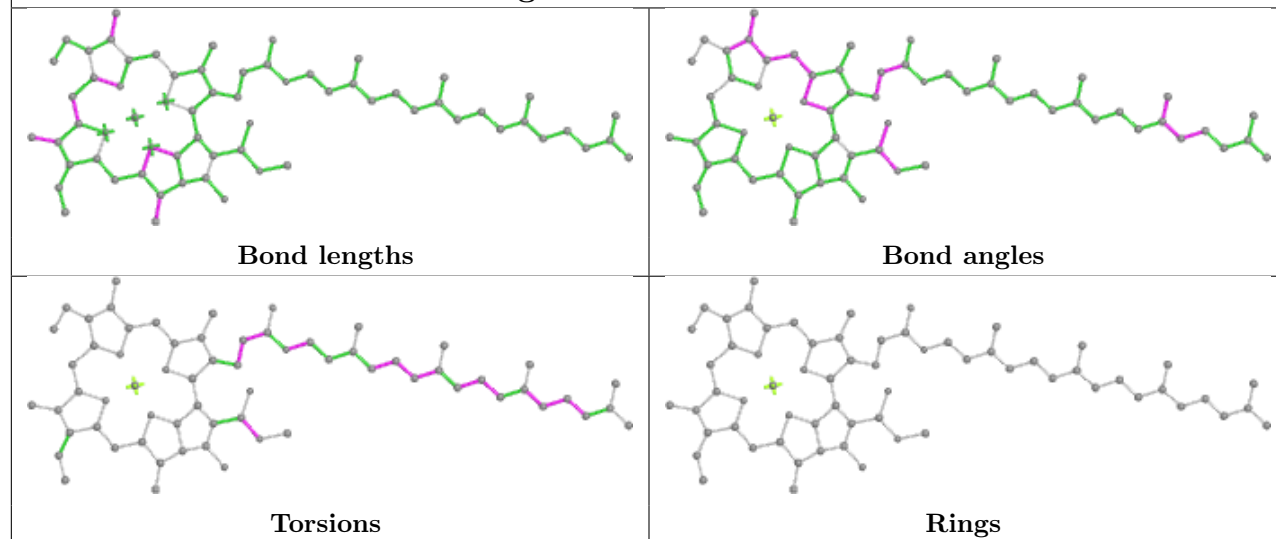
Ligand CLA B3 310



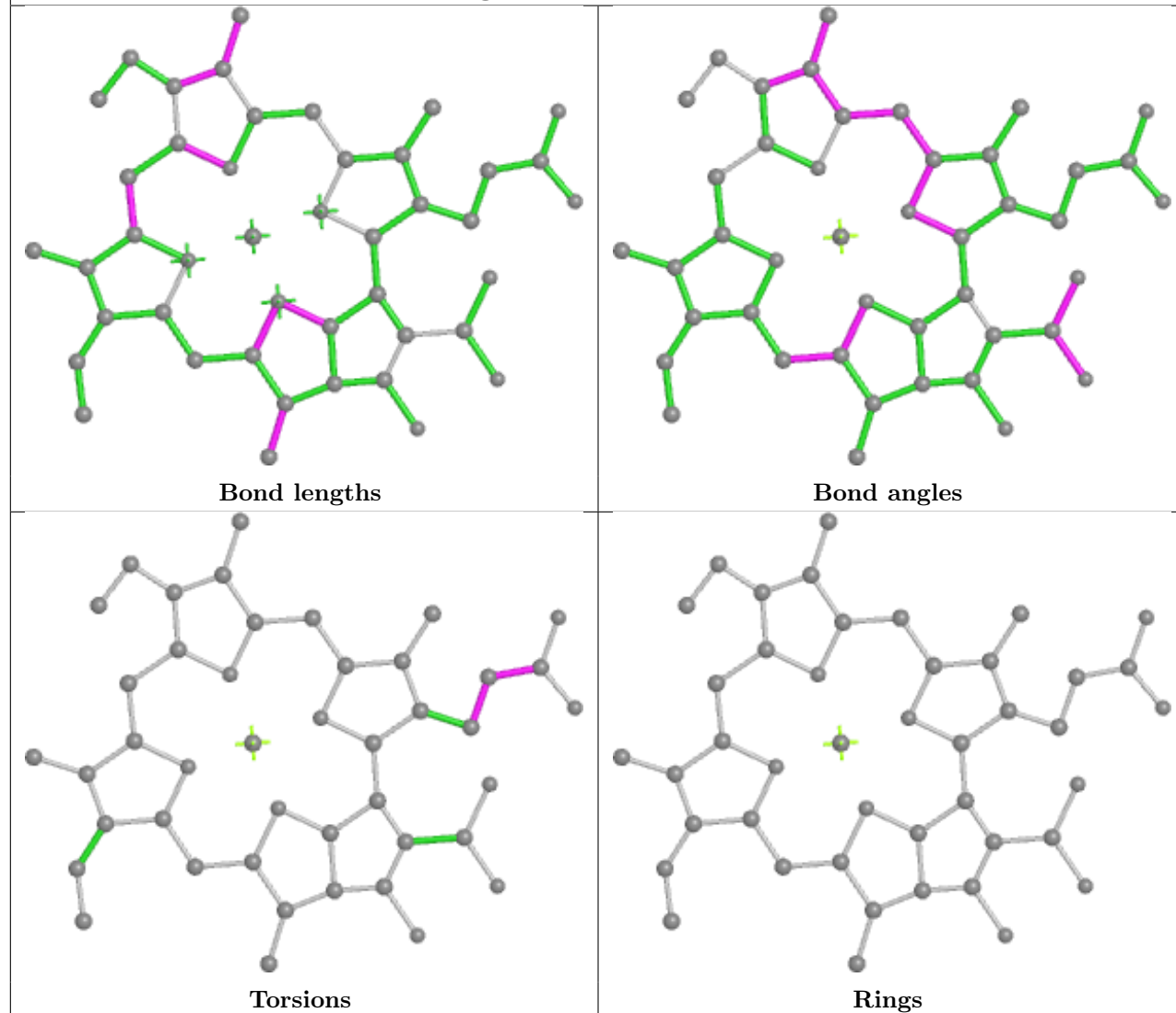
Ligand DGD AB 851

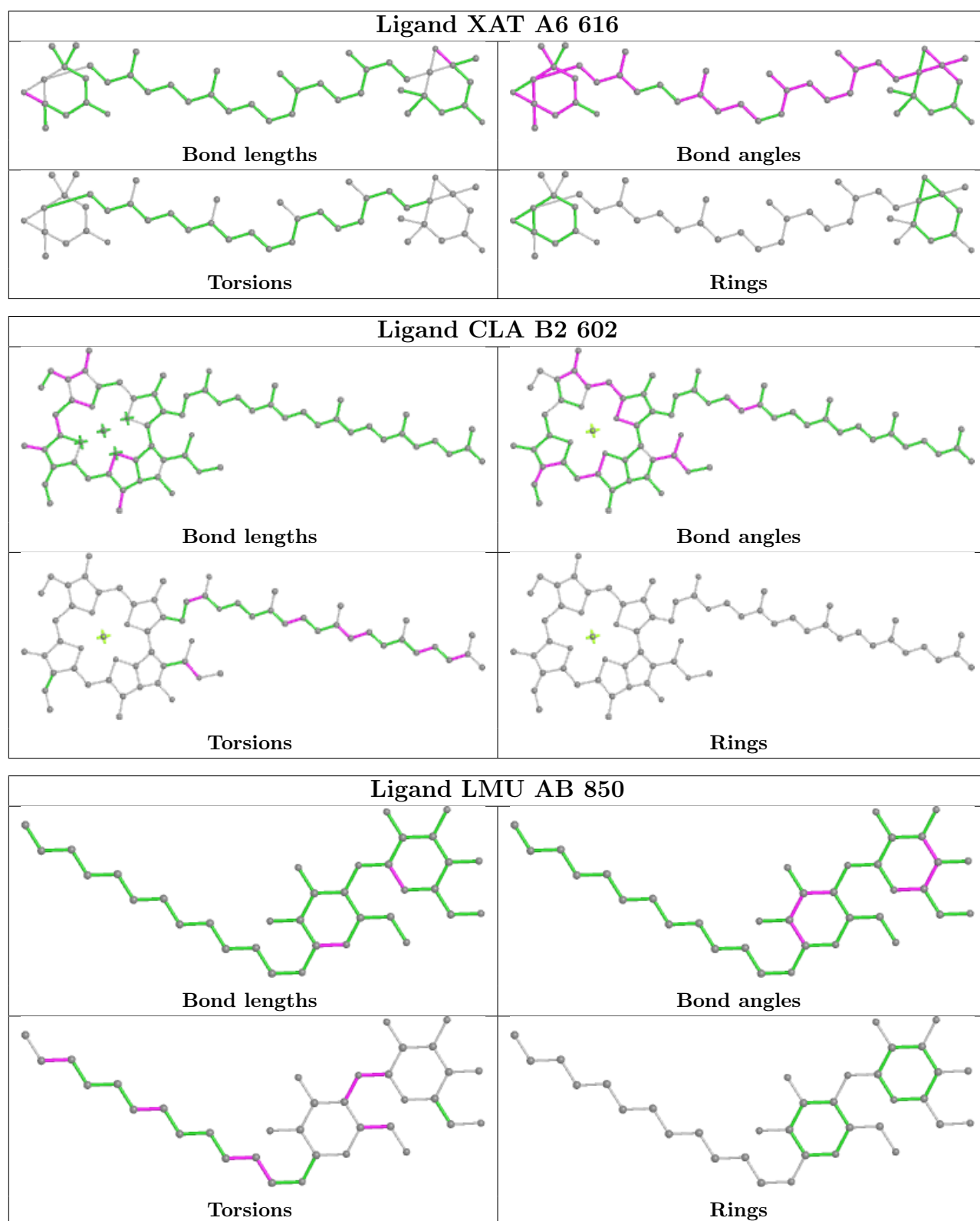


Ligand CLA AA 828

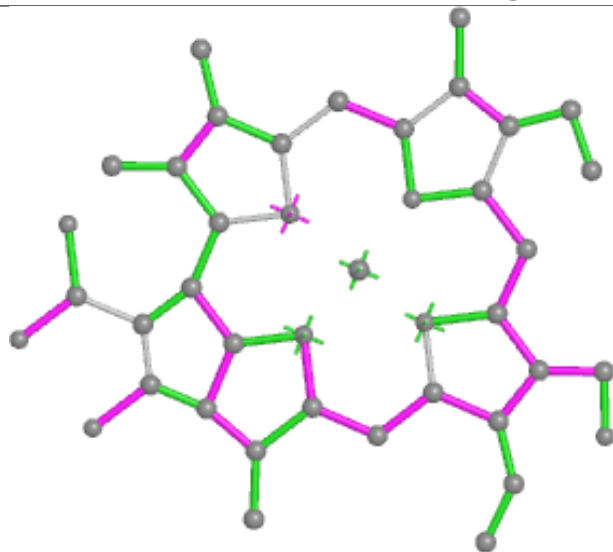


Ligand CLA AG 201

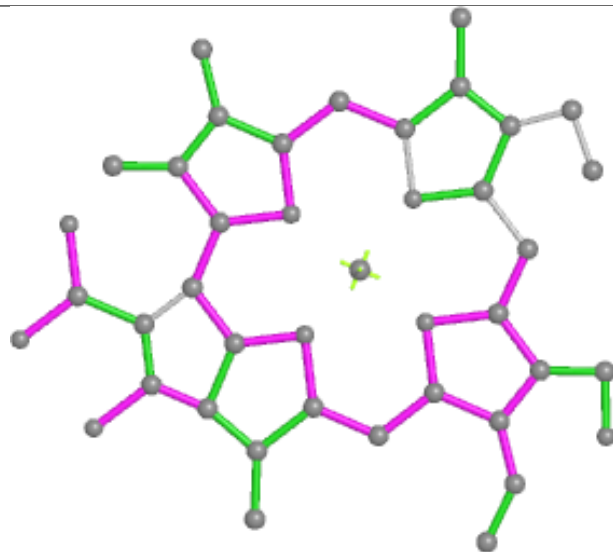




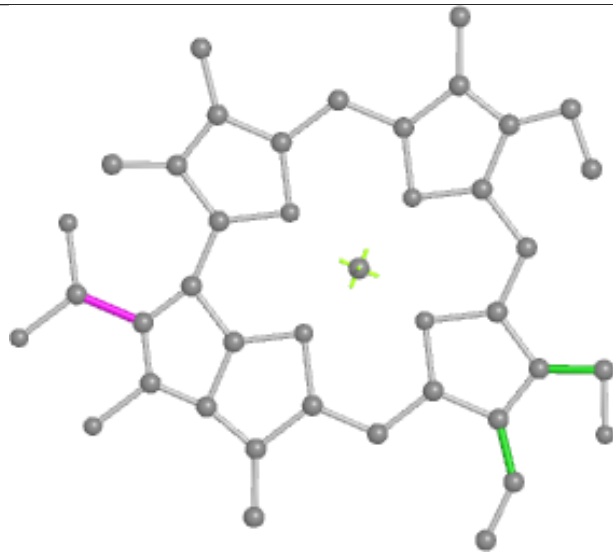
Ligand CHL A1 308



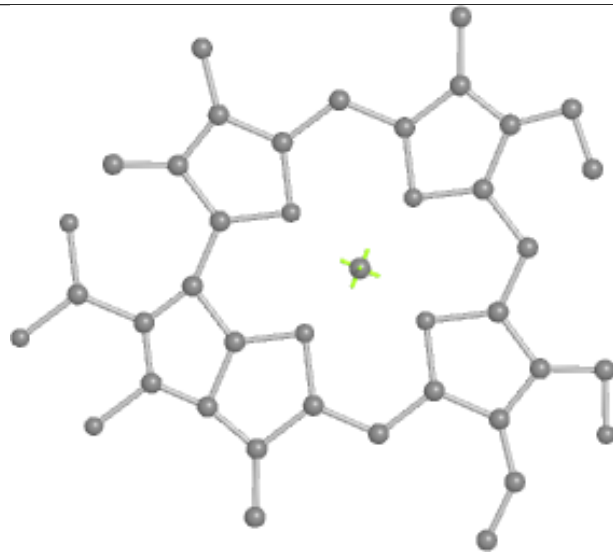
Bond lengths



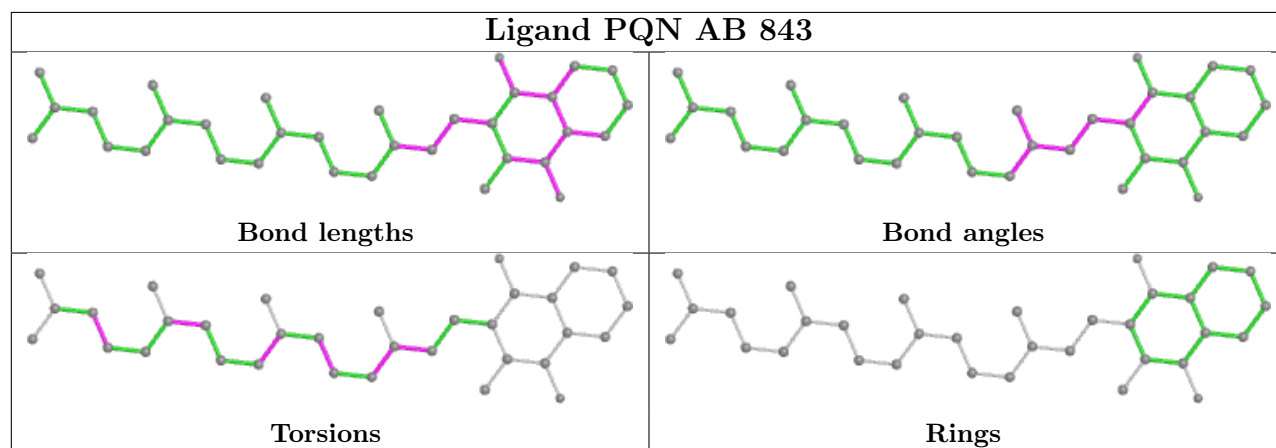
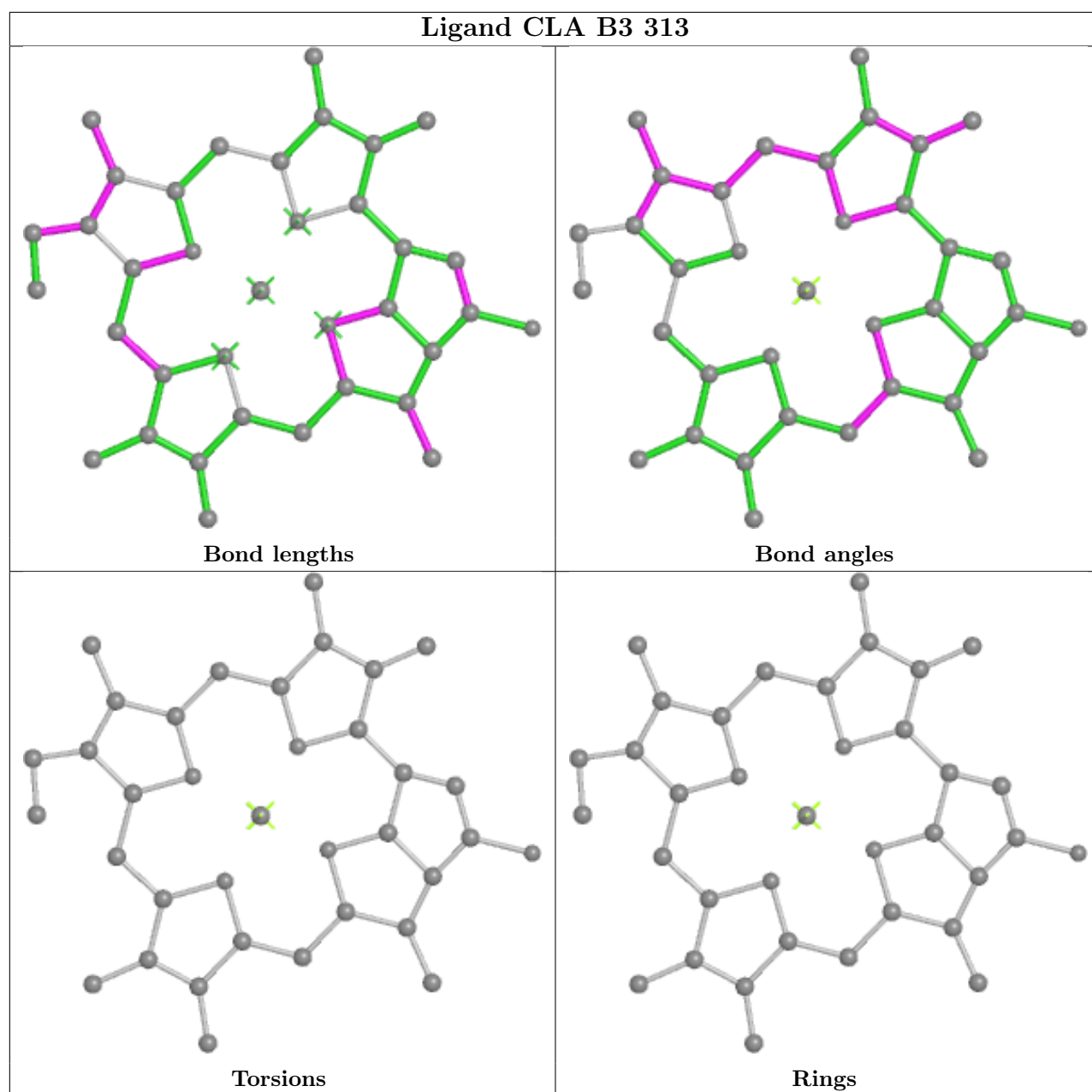
Bond angles

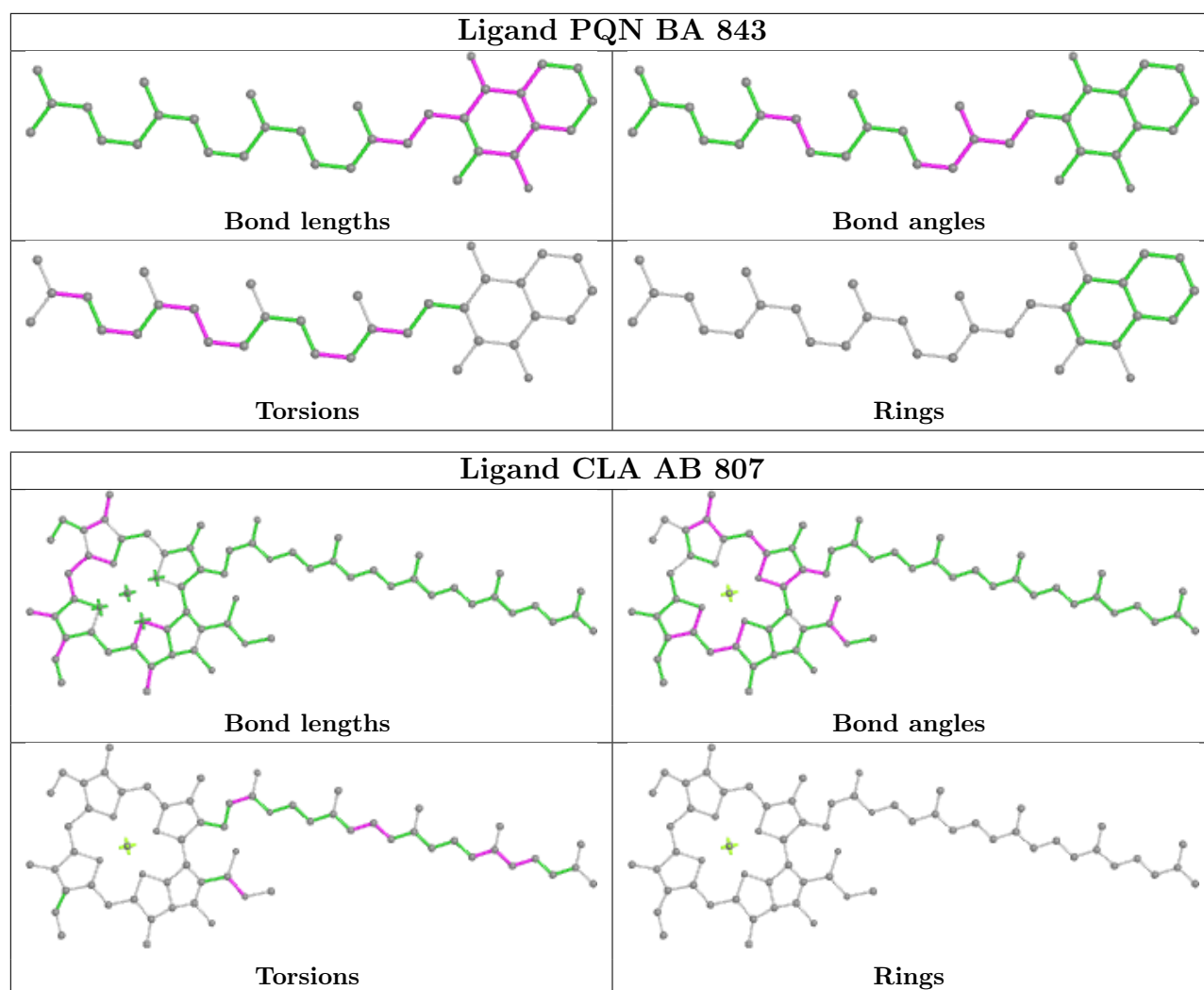


Torsions

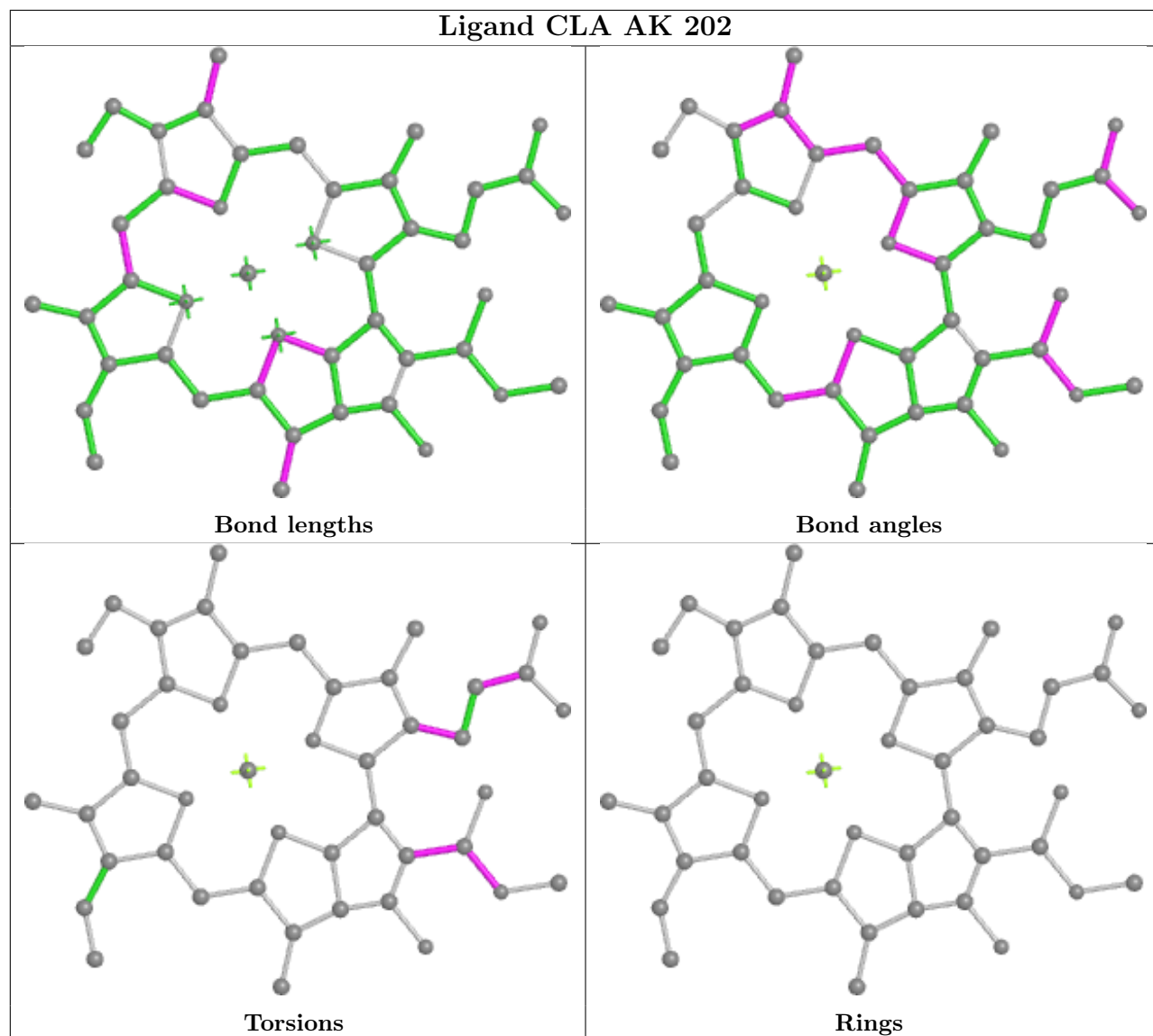


Rings

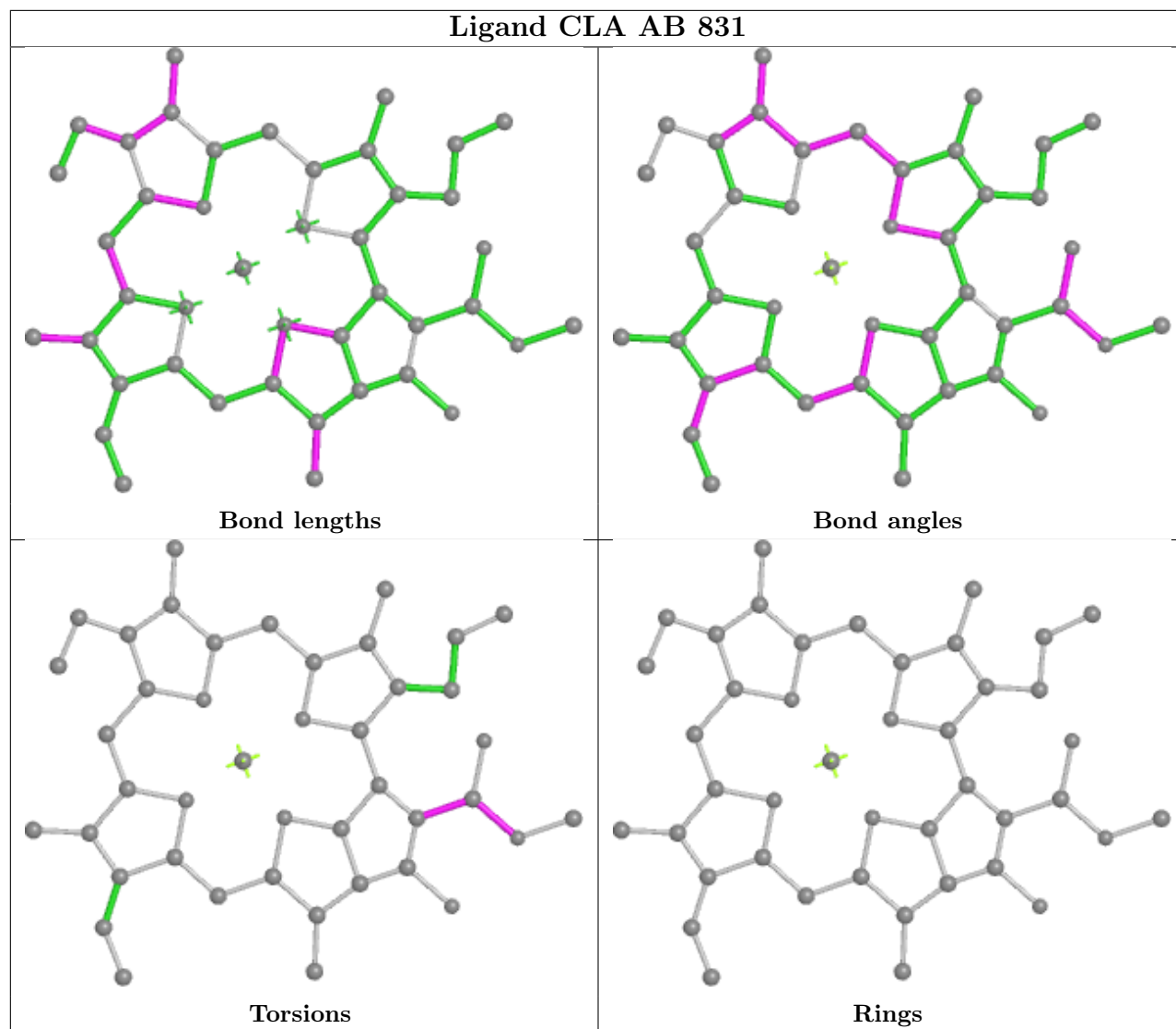




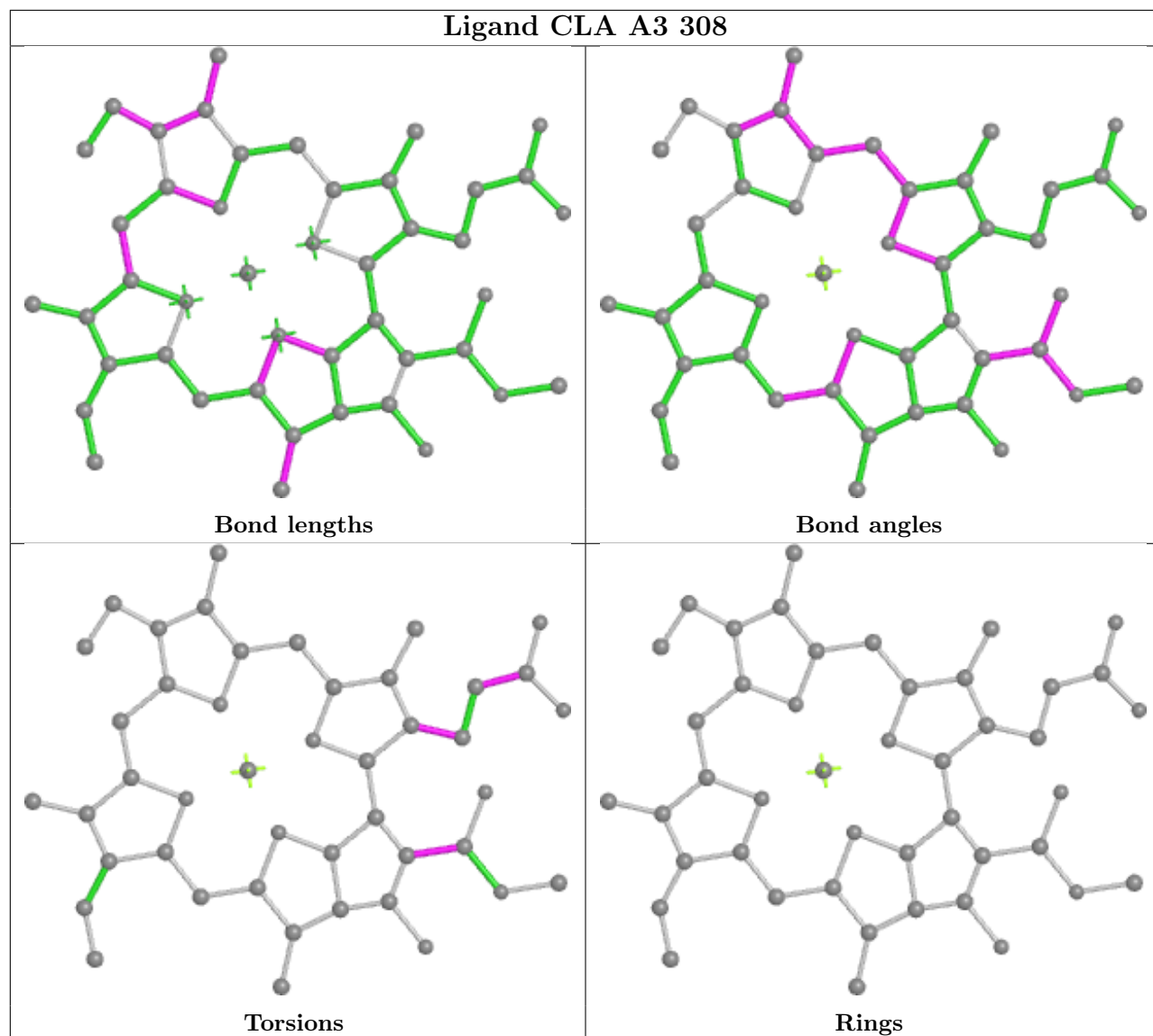
Ligand CLA AK 202

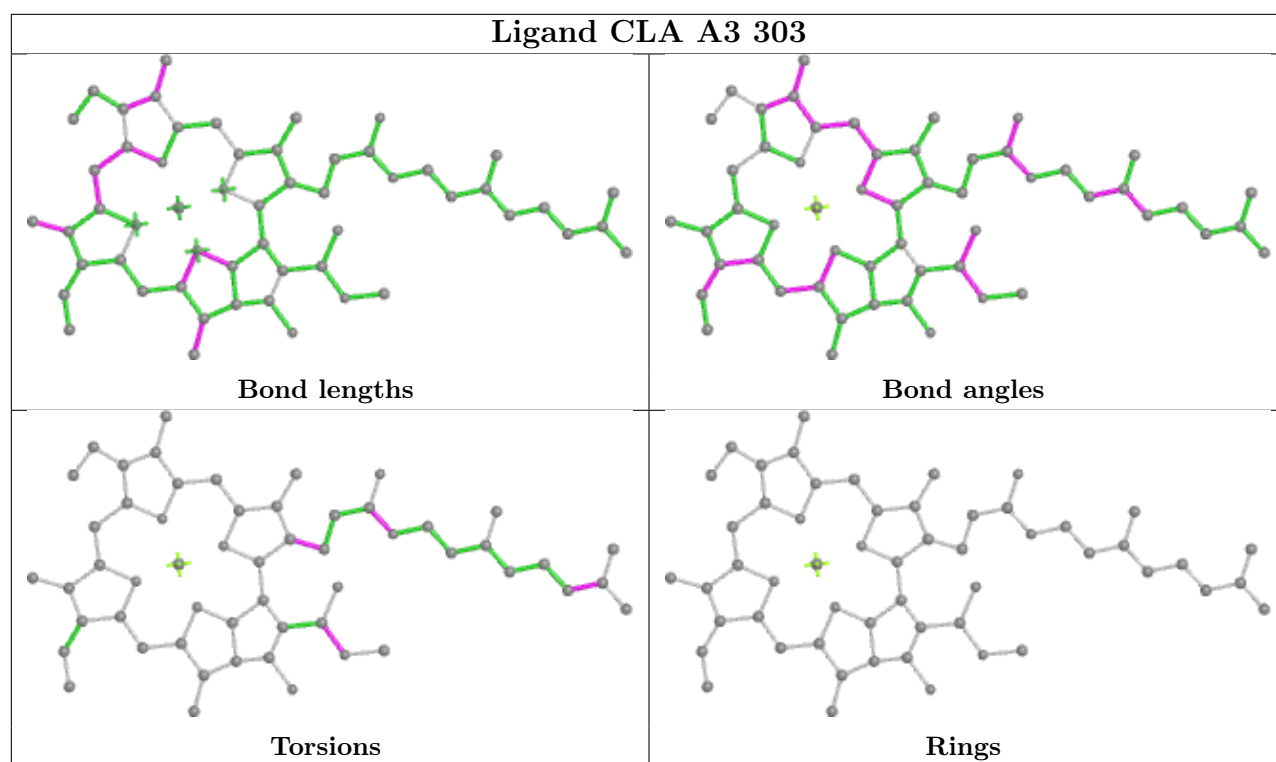


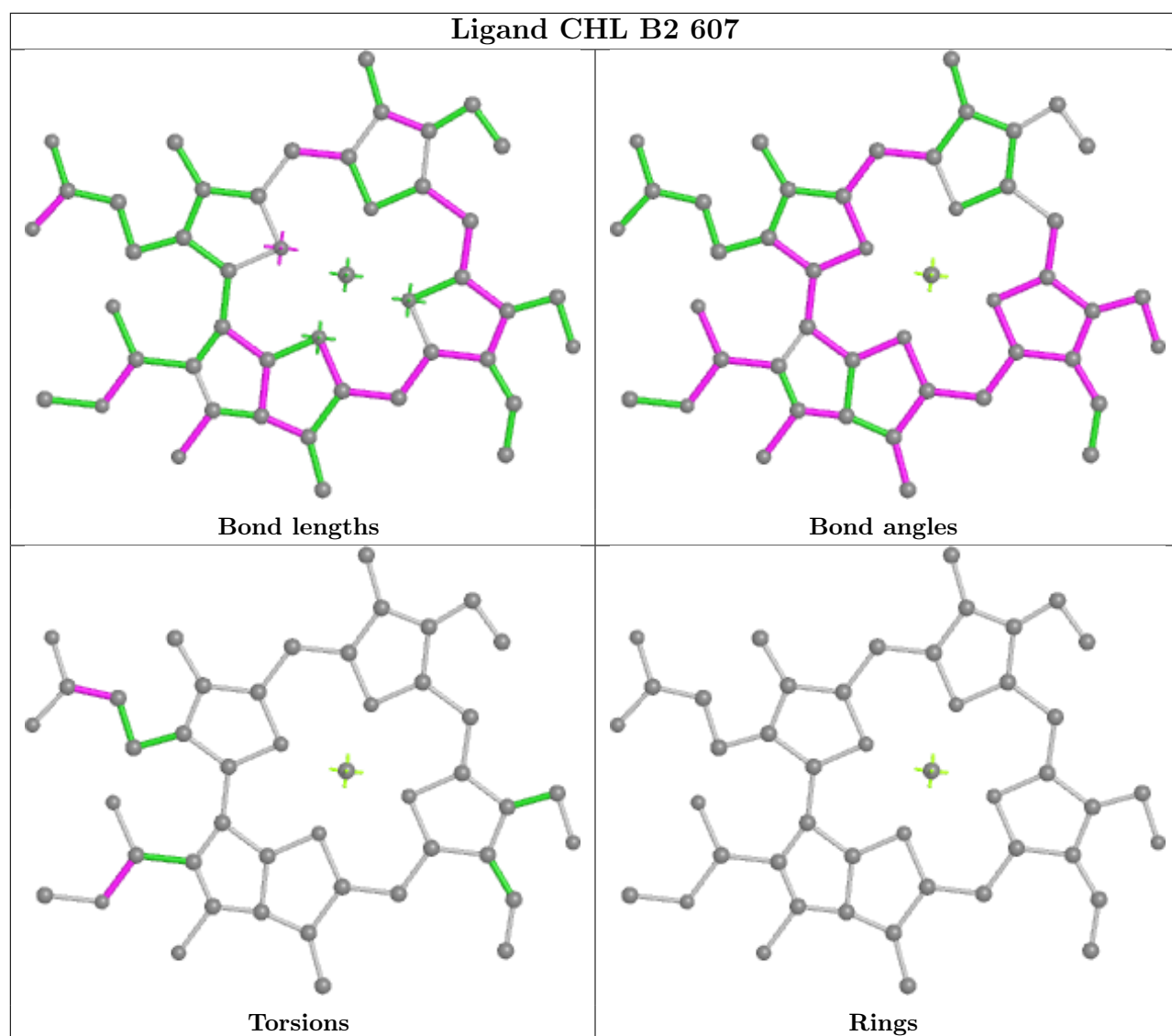
Ligand CLA AB 831



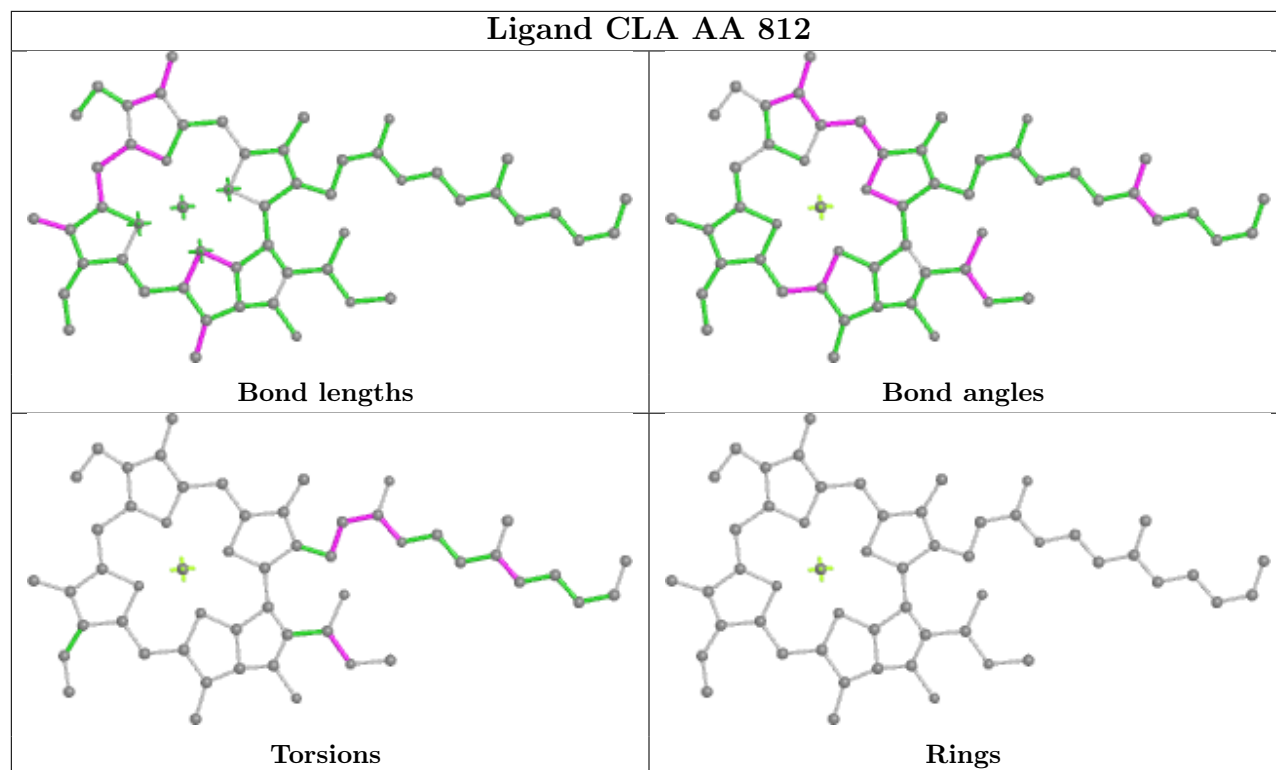
Ligand CLA A3 308



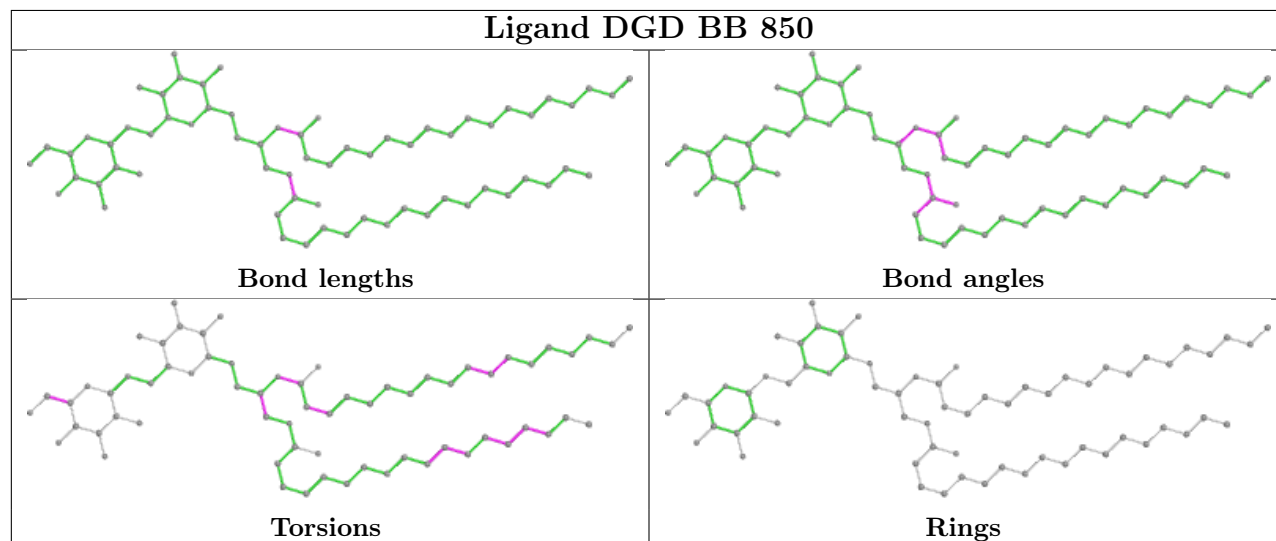


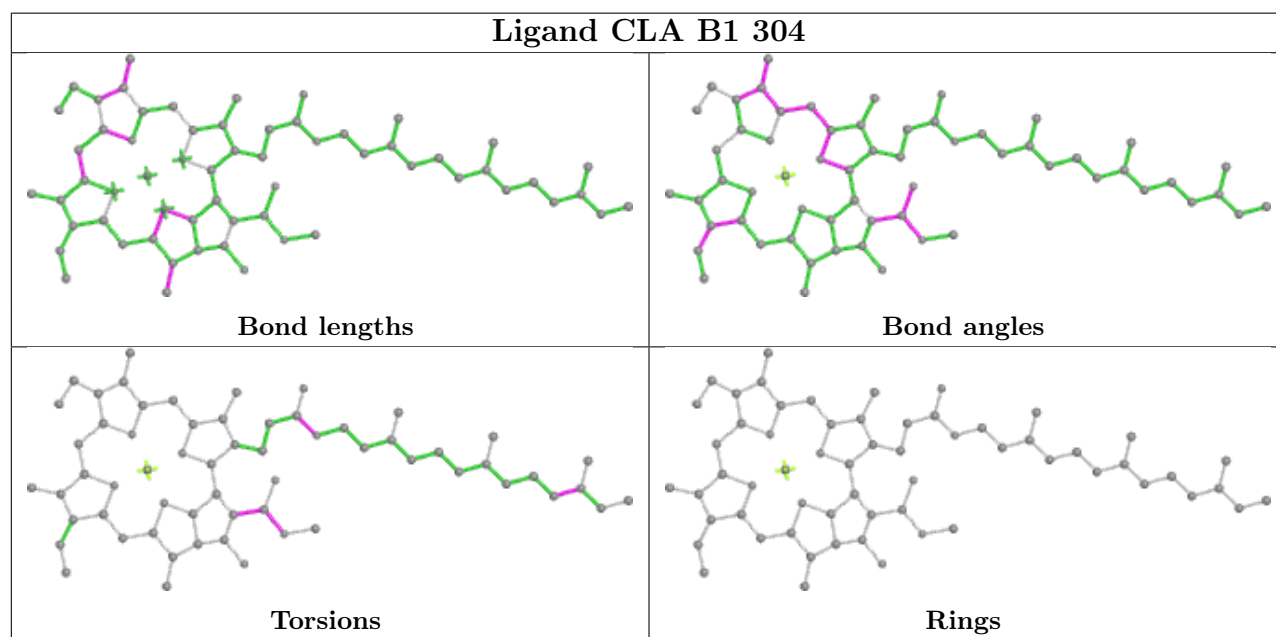
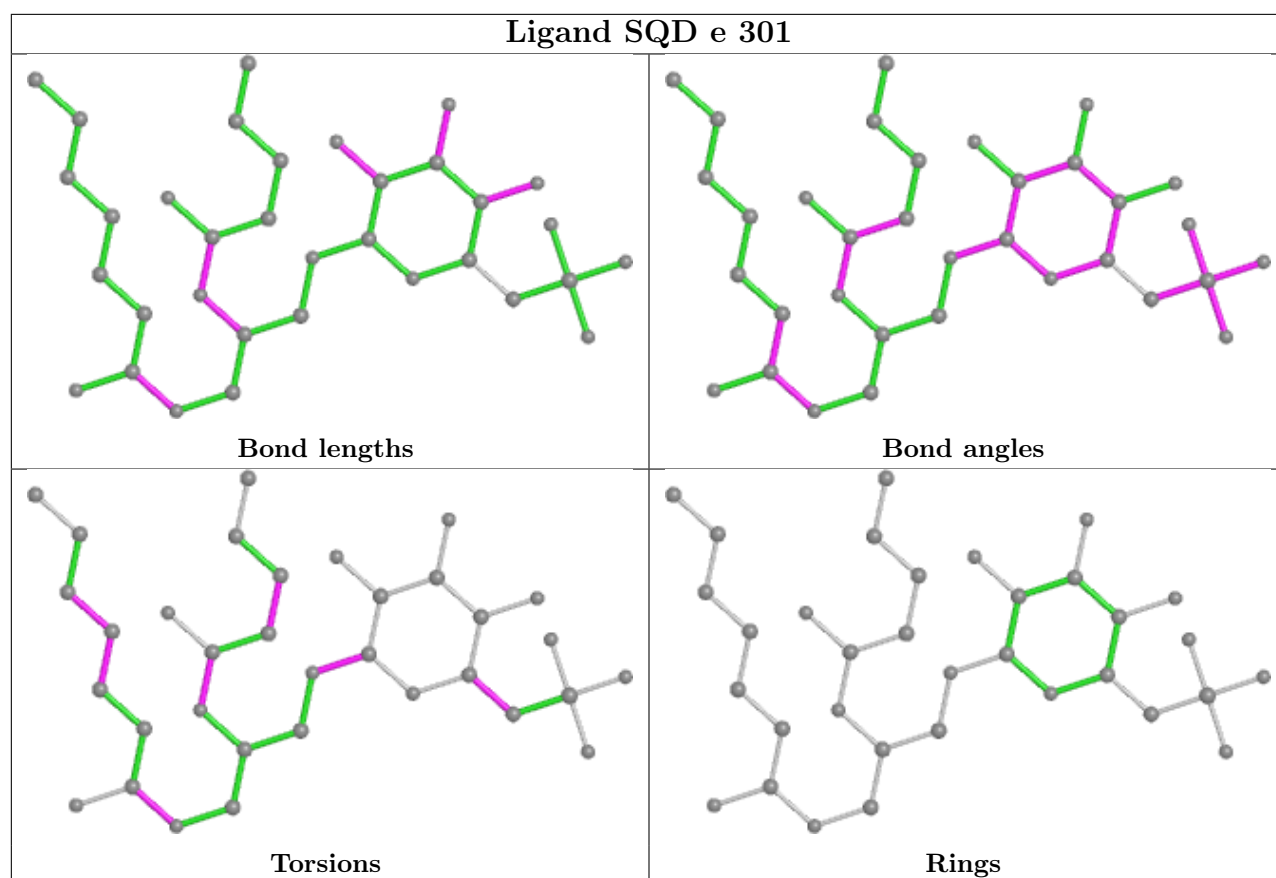


Ligand CLA AA 812

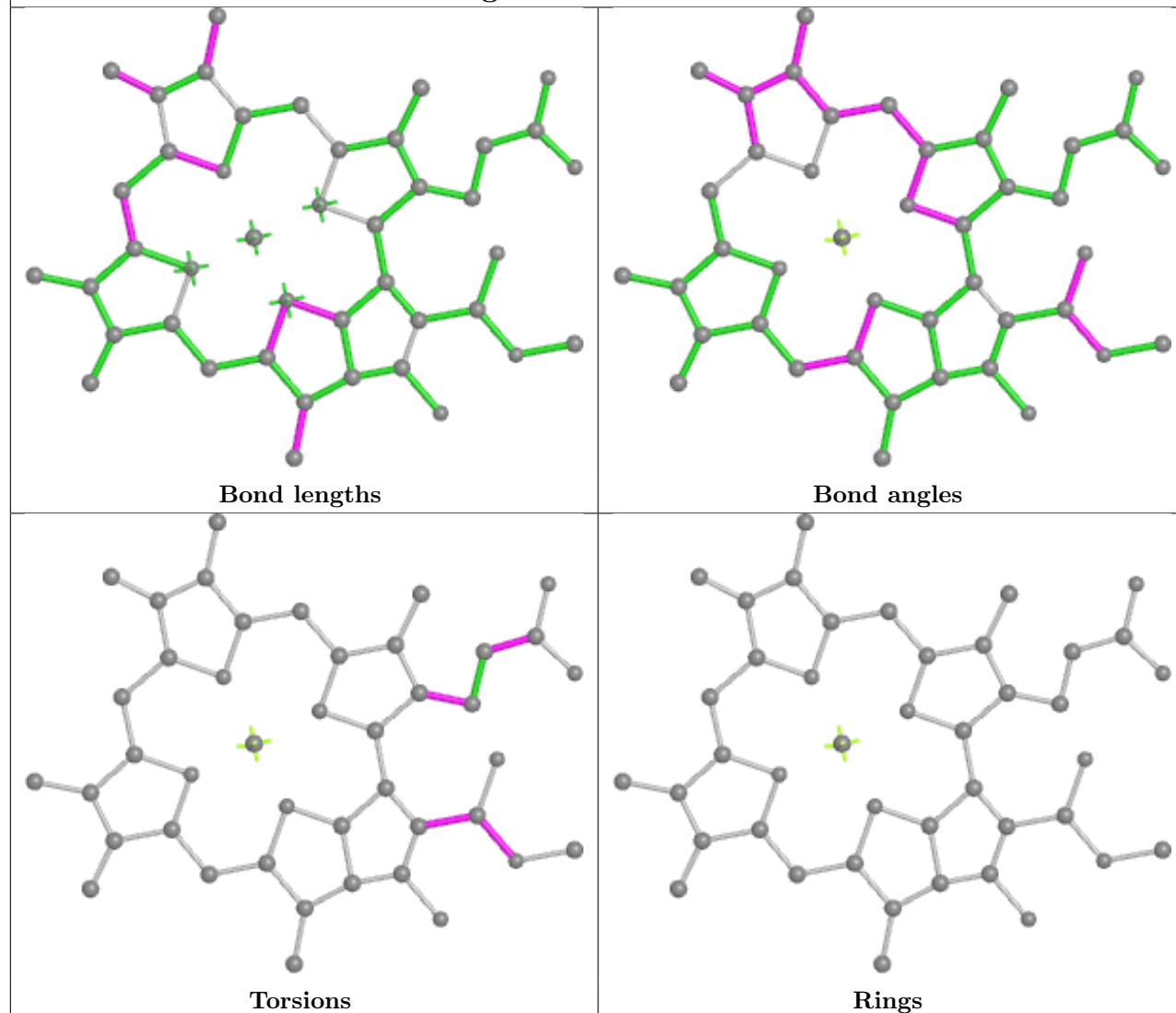


Ligand DGD BB 850

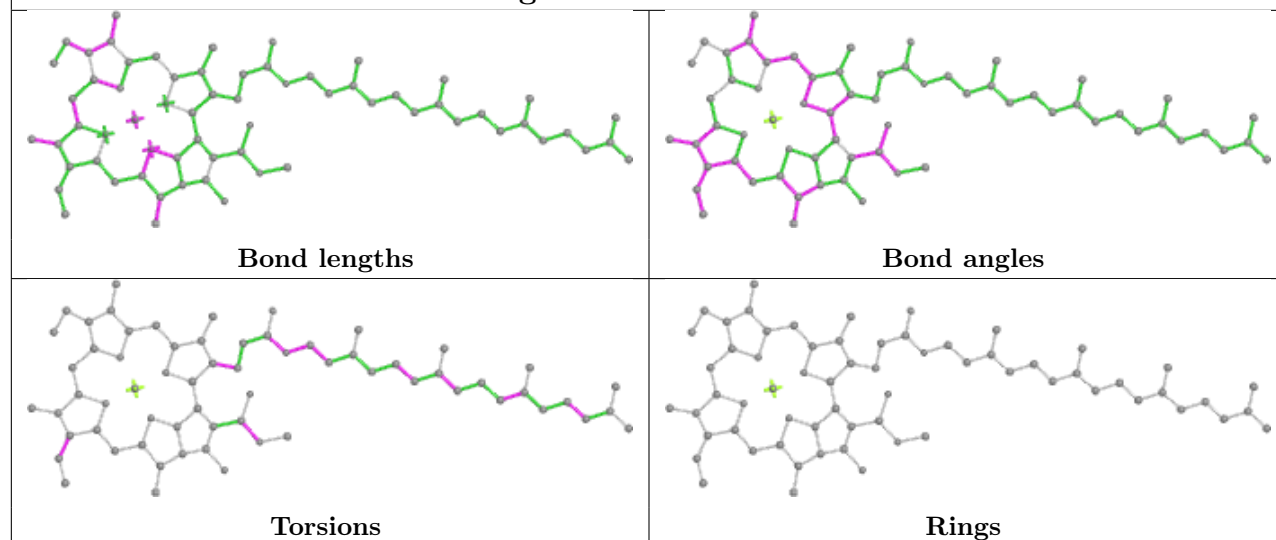




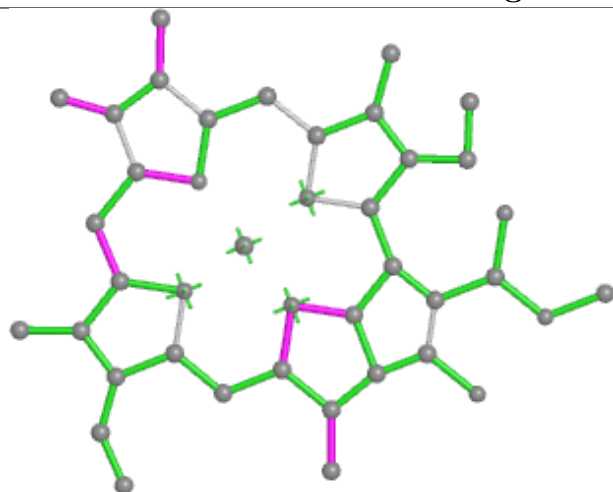
Ligand CLA A1 316



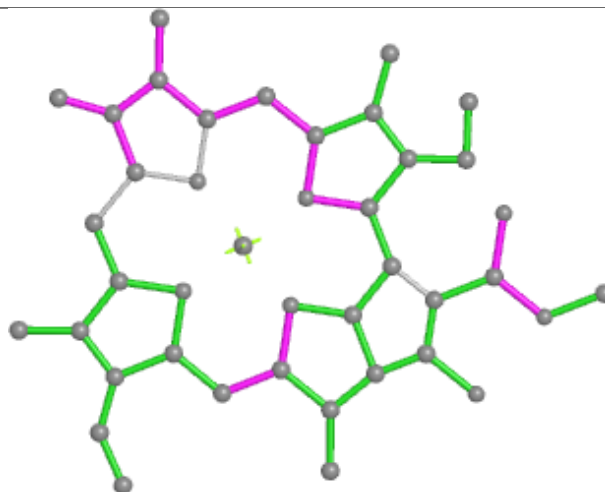
Ligand CLA AB 804



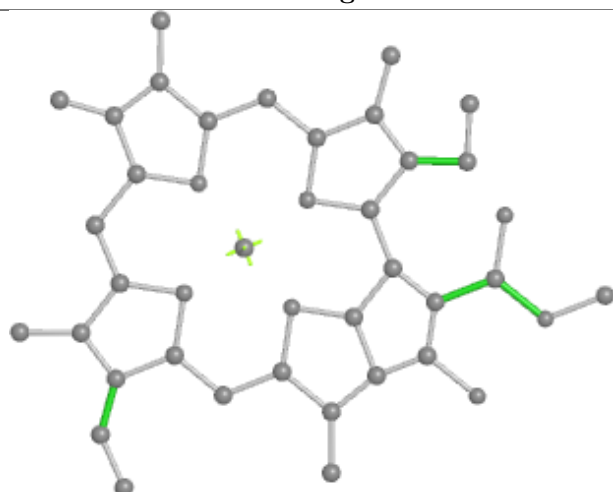
Ligand CLA A3 306



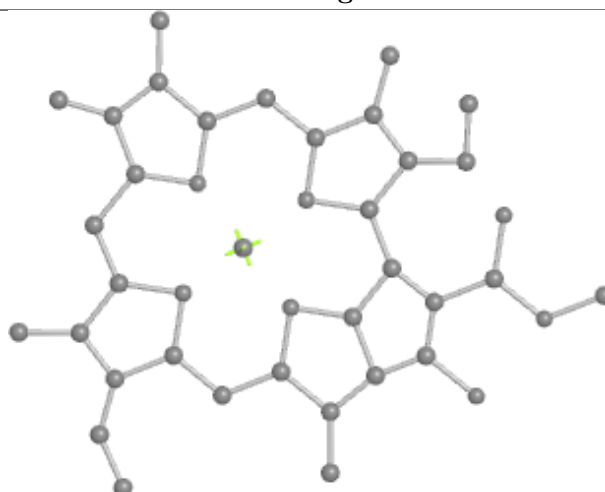
Bond lengths



Bond angles

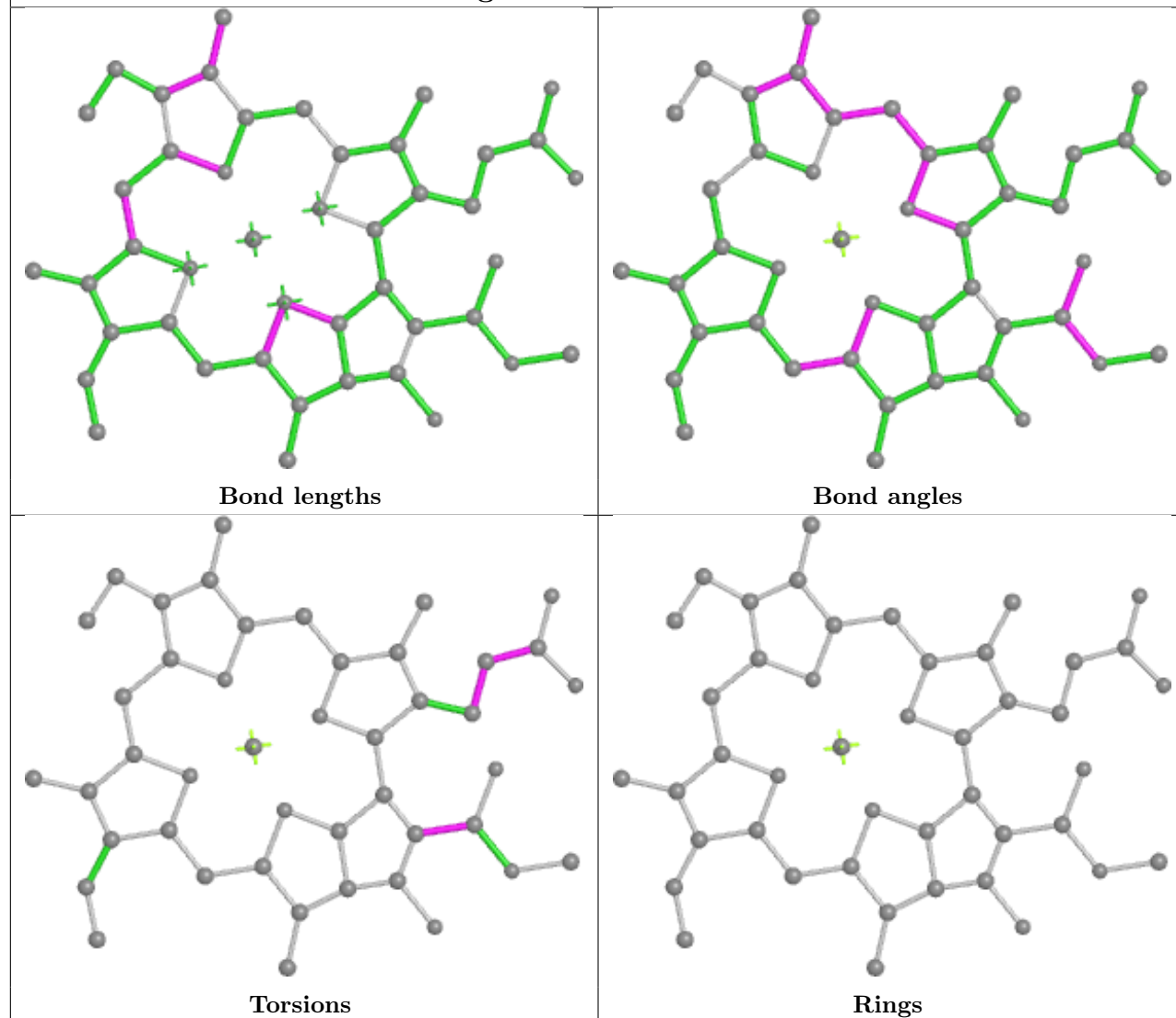


Torsions

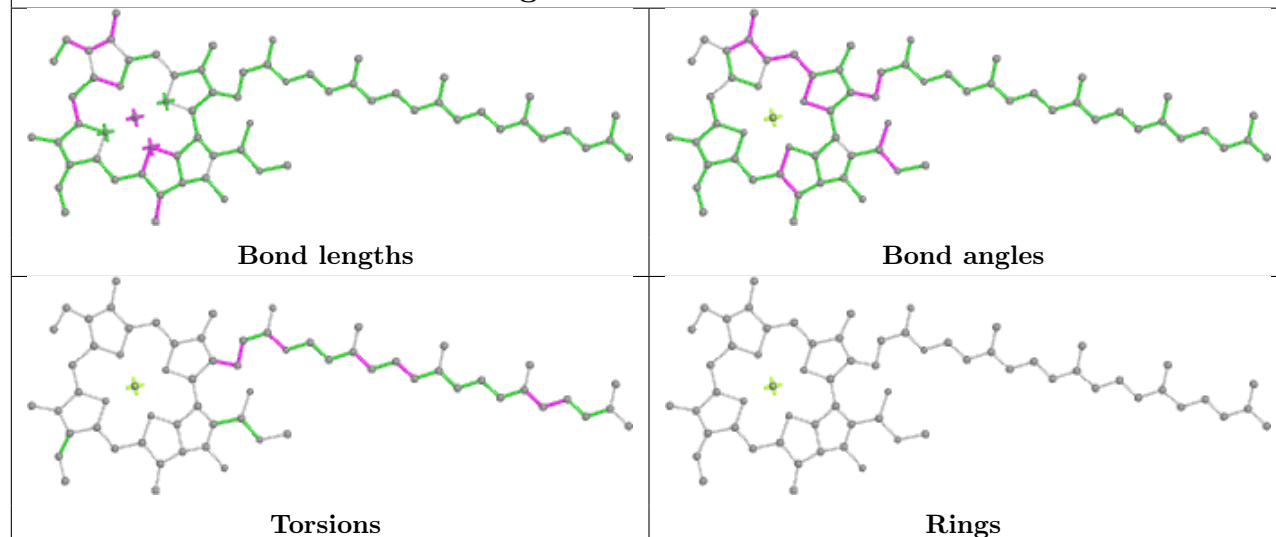


Rings

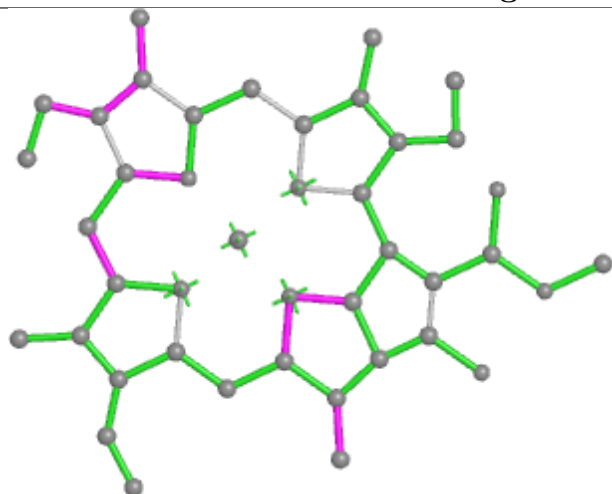
Ligand CLA BK 202



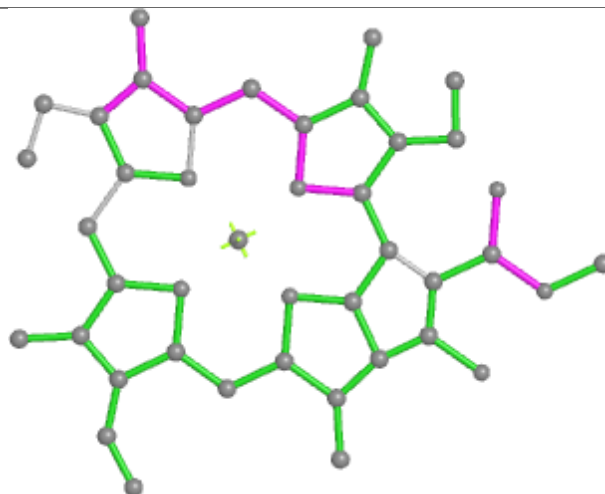
Ligand CLA BB 830



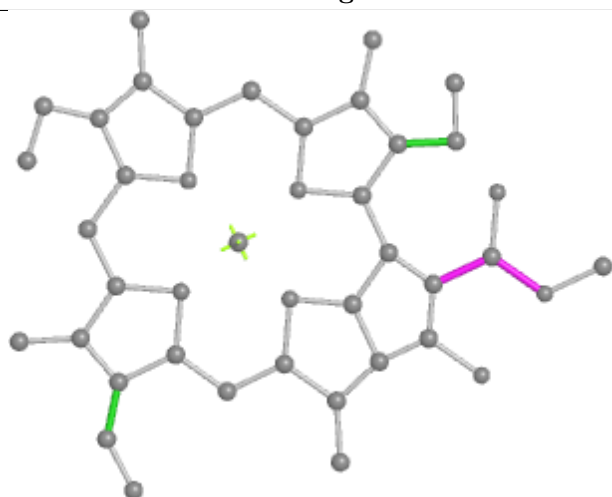
Ligand CLA BA 815



Bond lengths



Bond angles

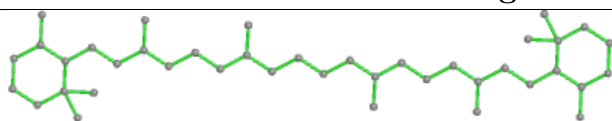


Torsions

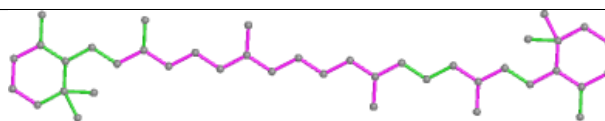


Rings

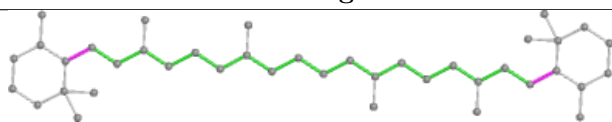
Ligand BCR BB 803



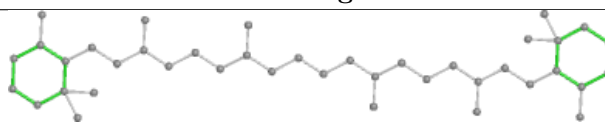
Bond lengths



Bond angles

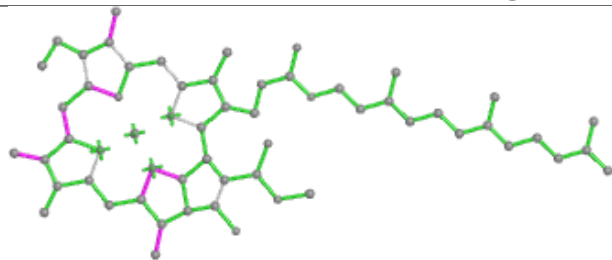


Torsions

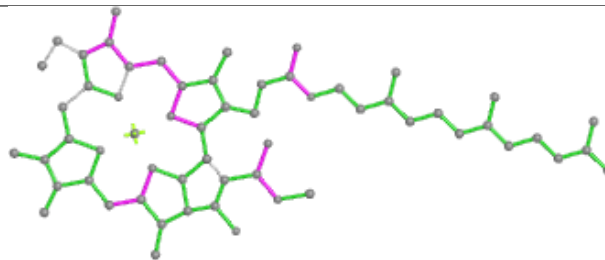


Rings

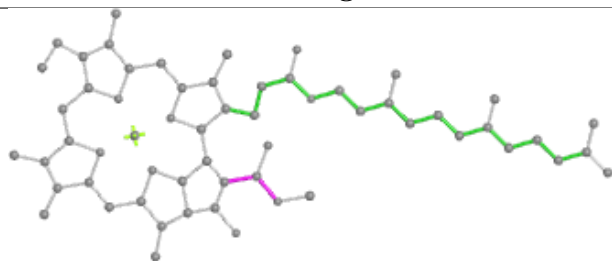
Ligand CLA A1 311



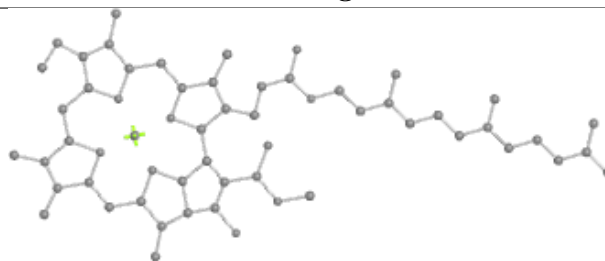
Bond lengths



Bond angles

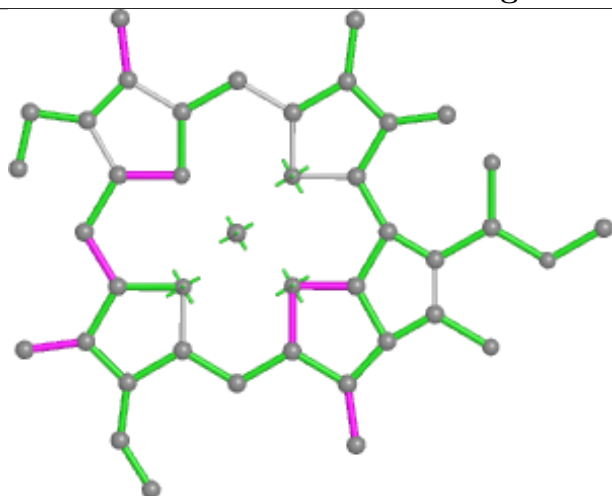


Torsions

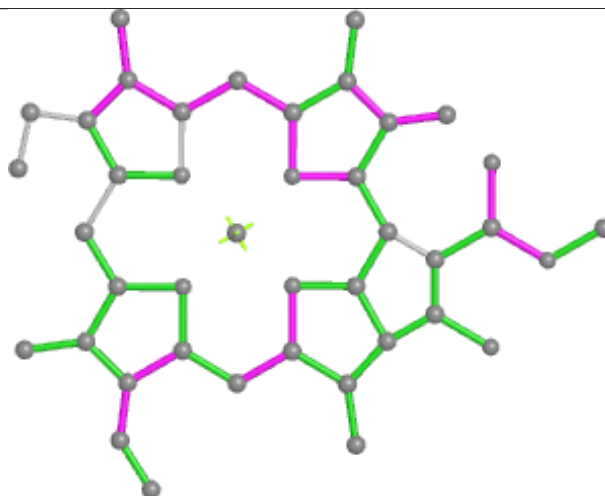


Rings

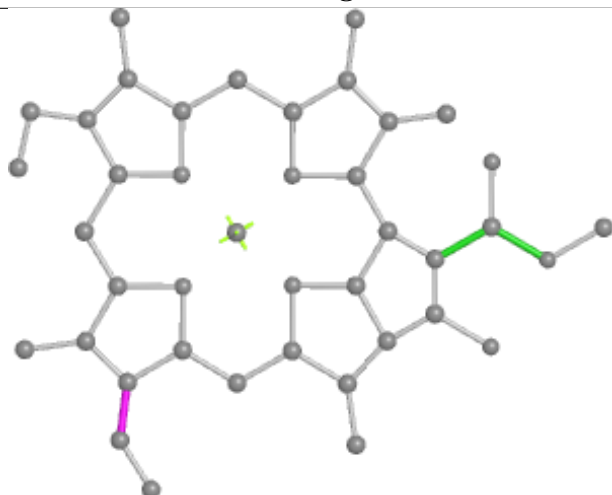
Ligand CLA BB 806



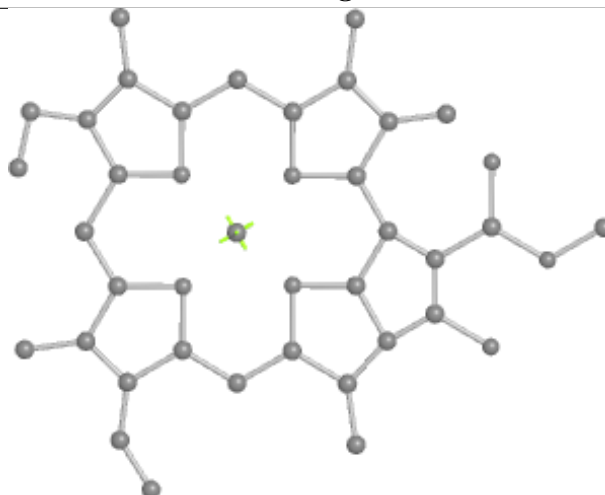
Bond lengths



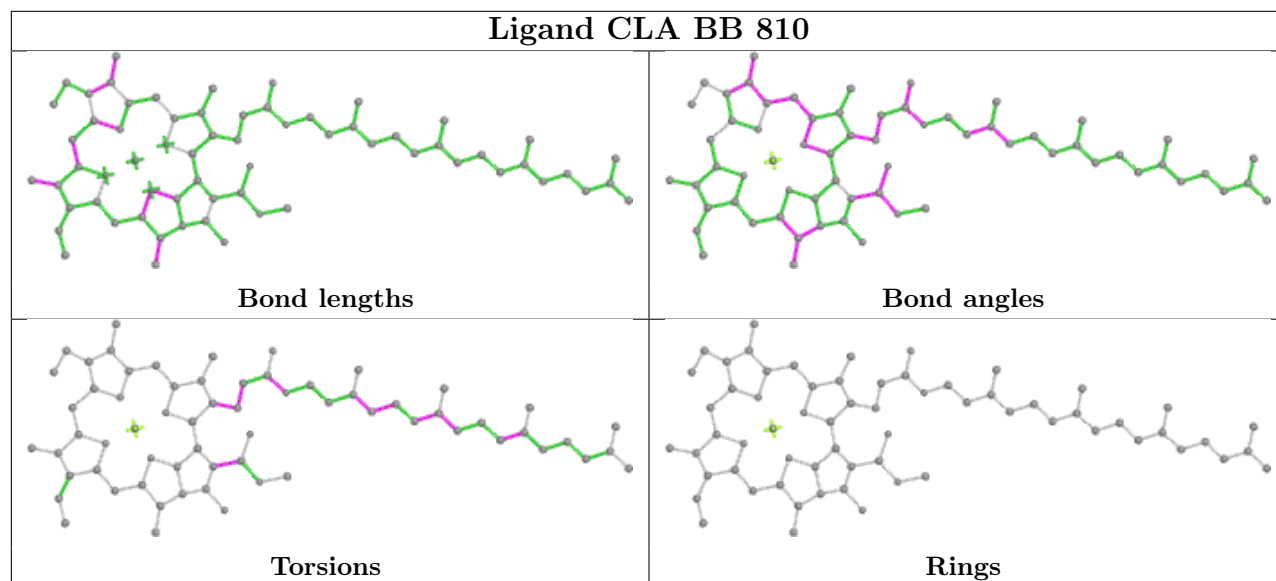
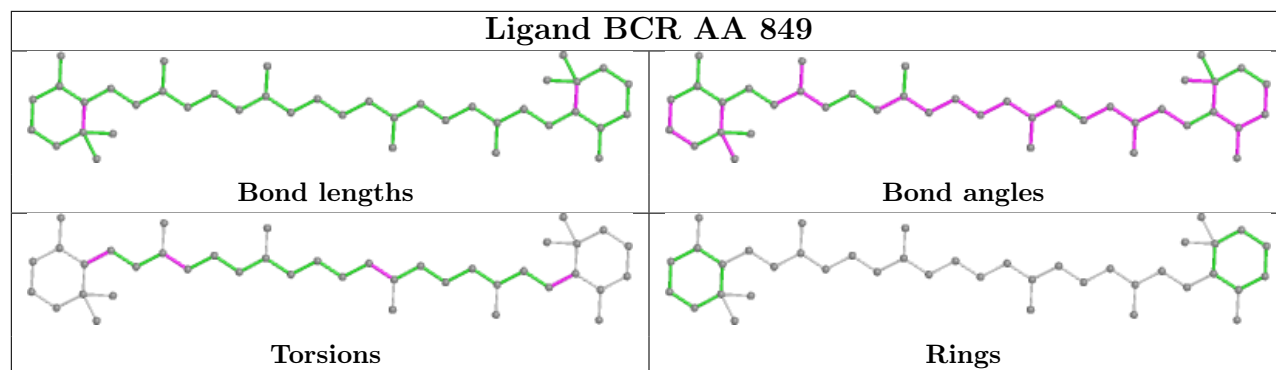
Bond angles



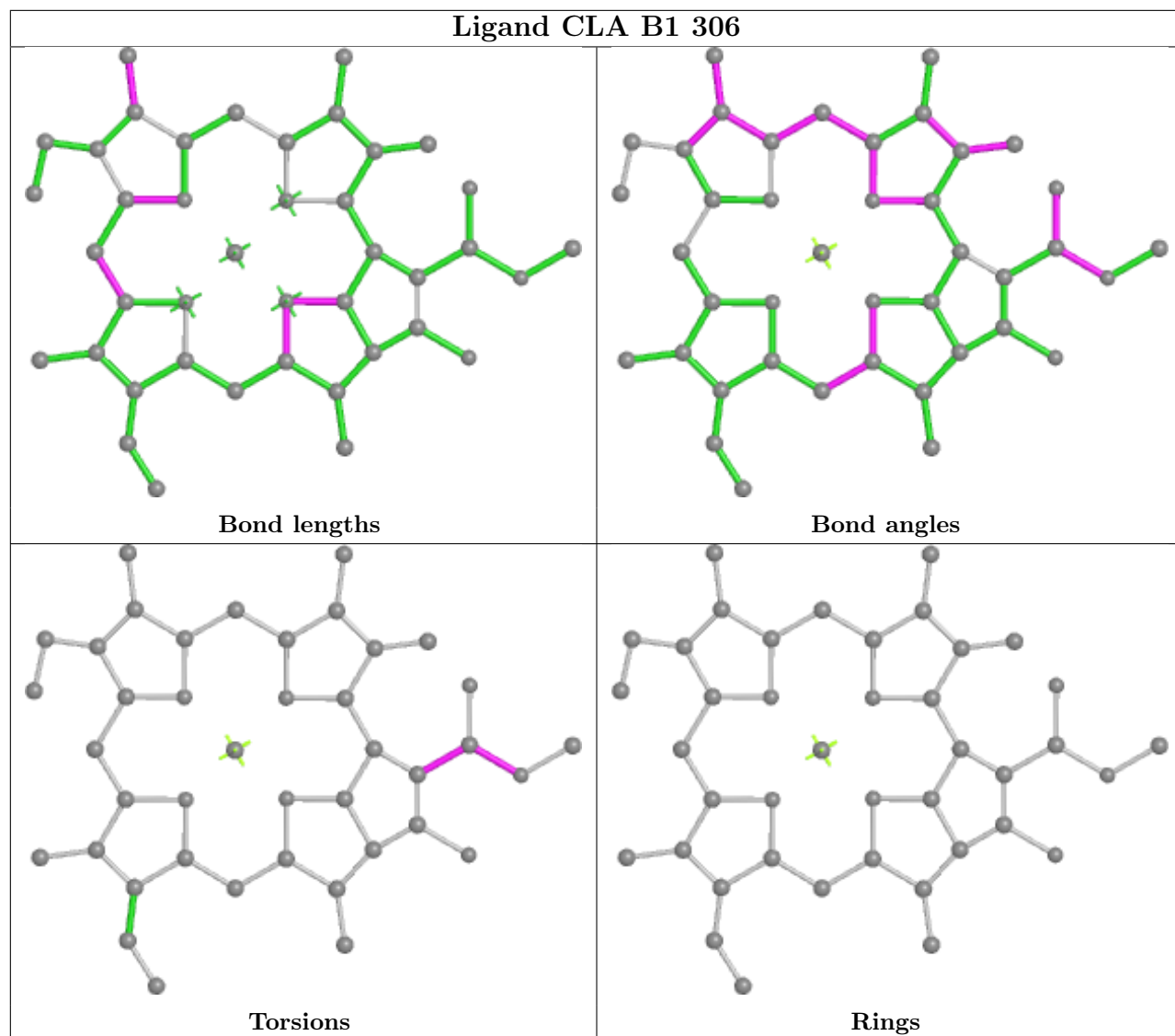
Torsions



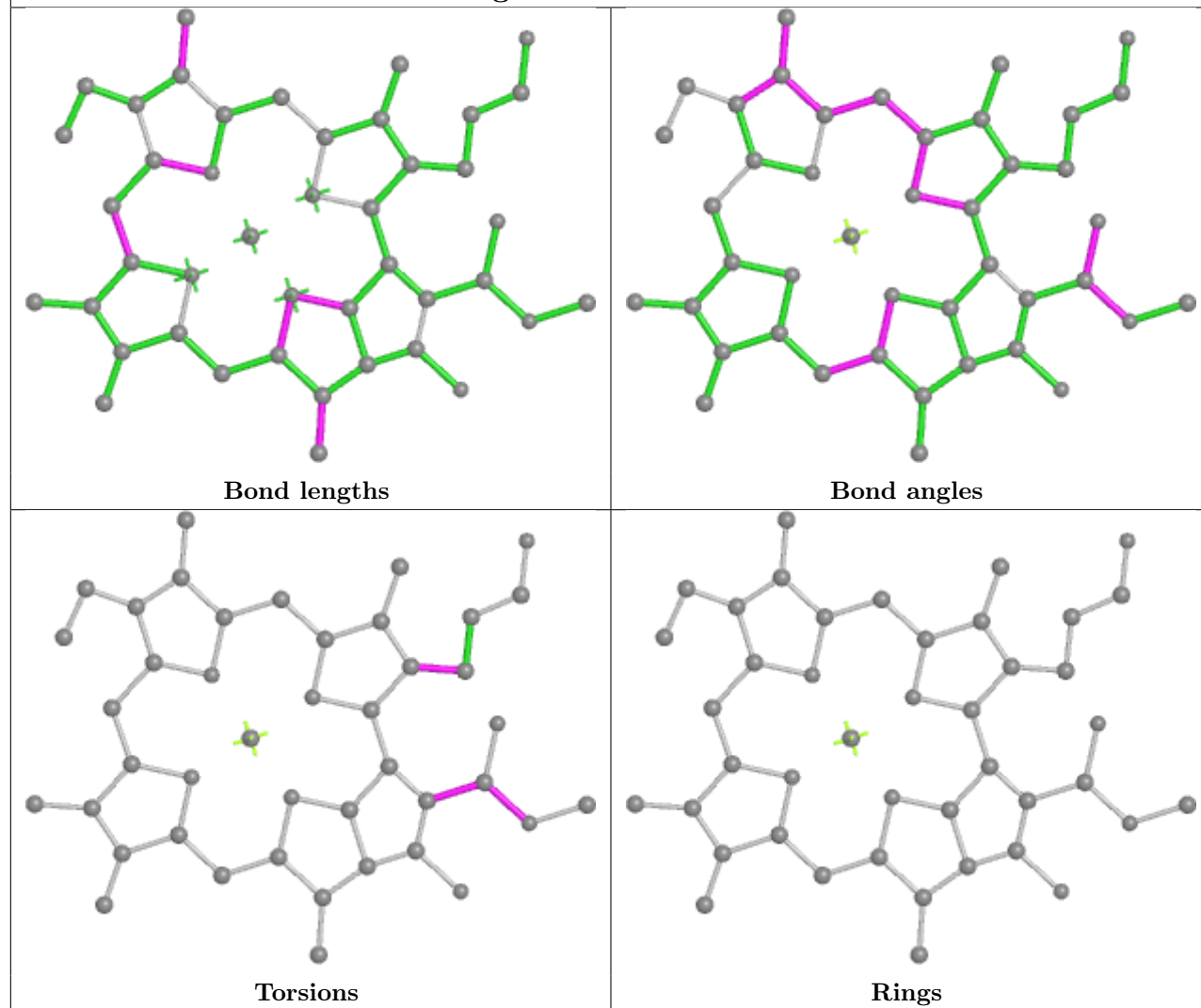
Rings



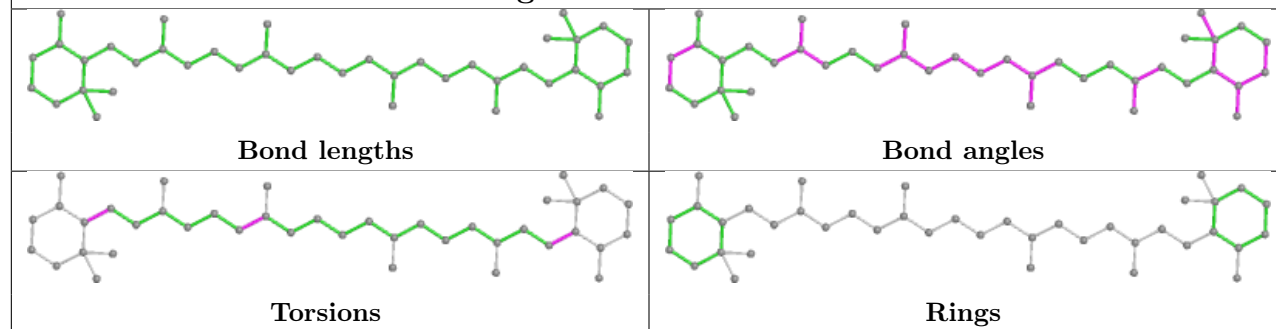
Ligand CLA B1 306

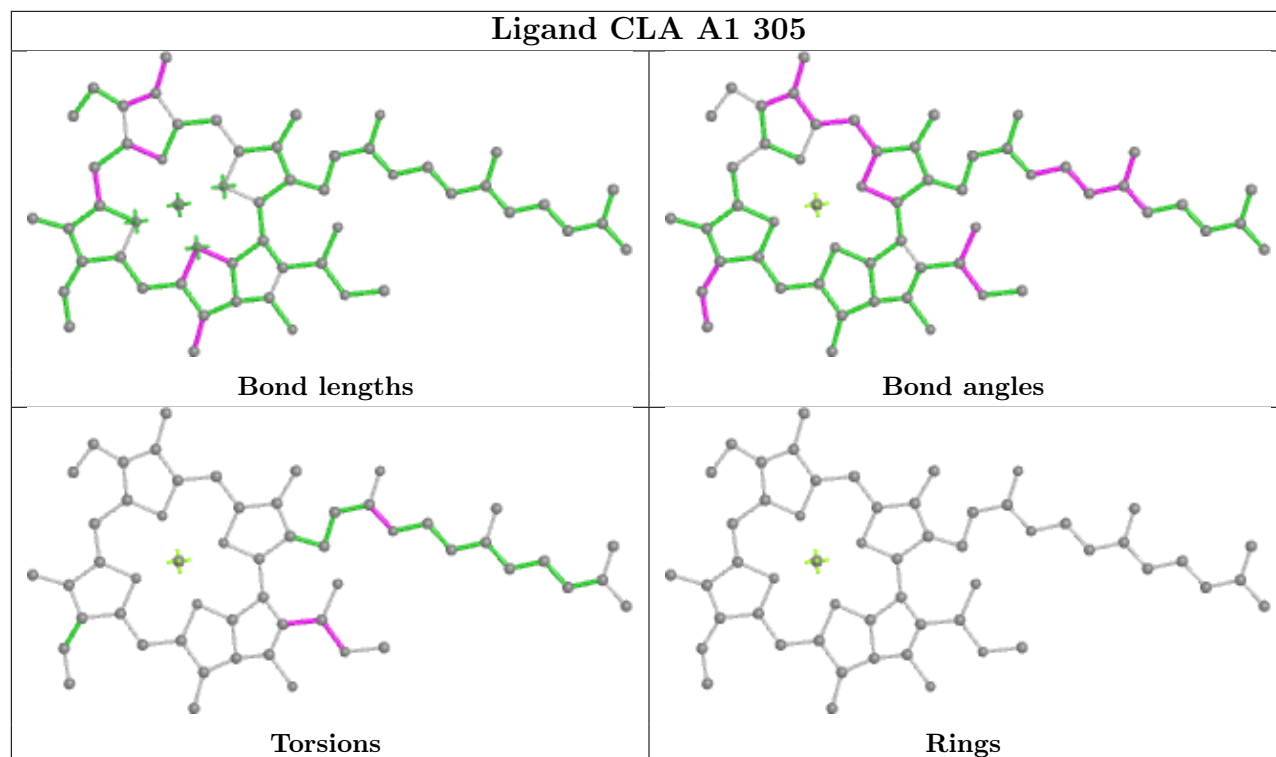
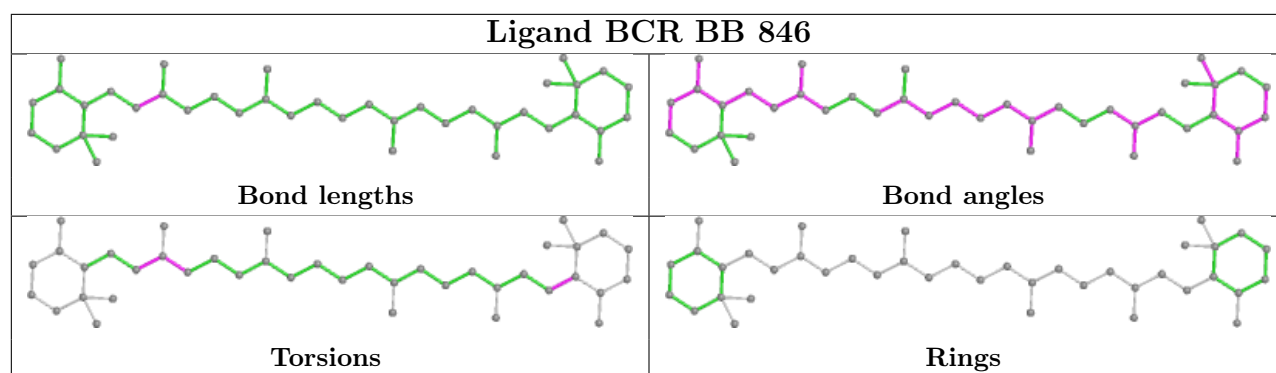


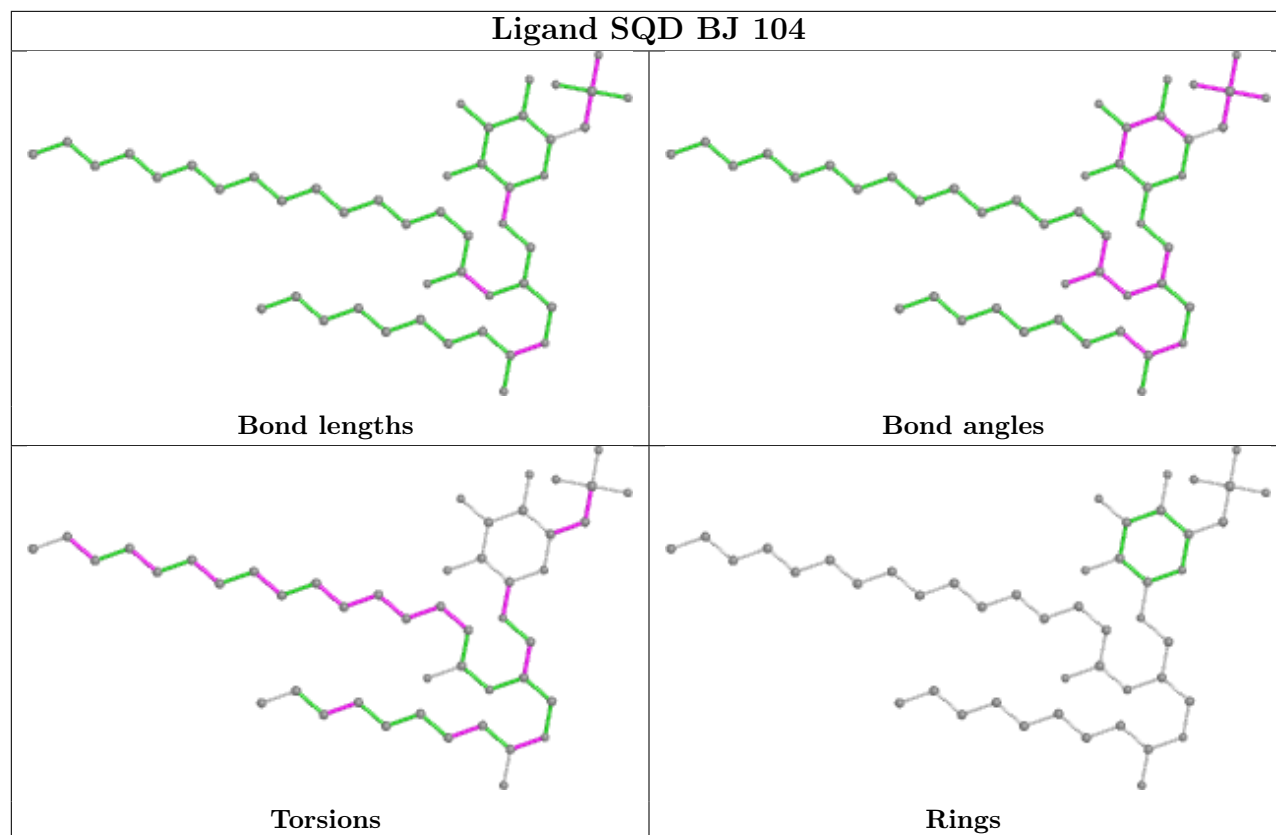
Ligand CLA B2 604



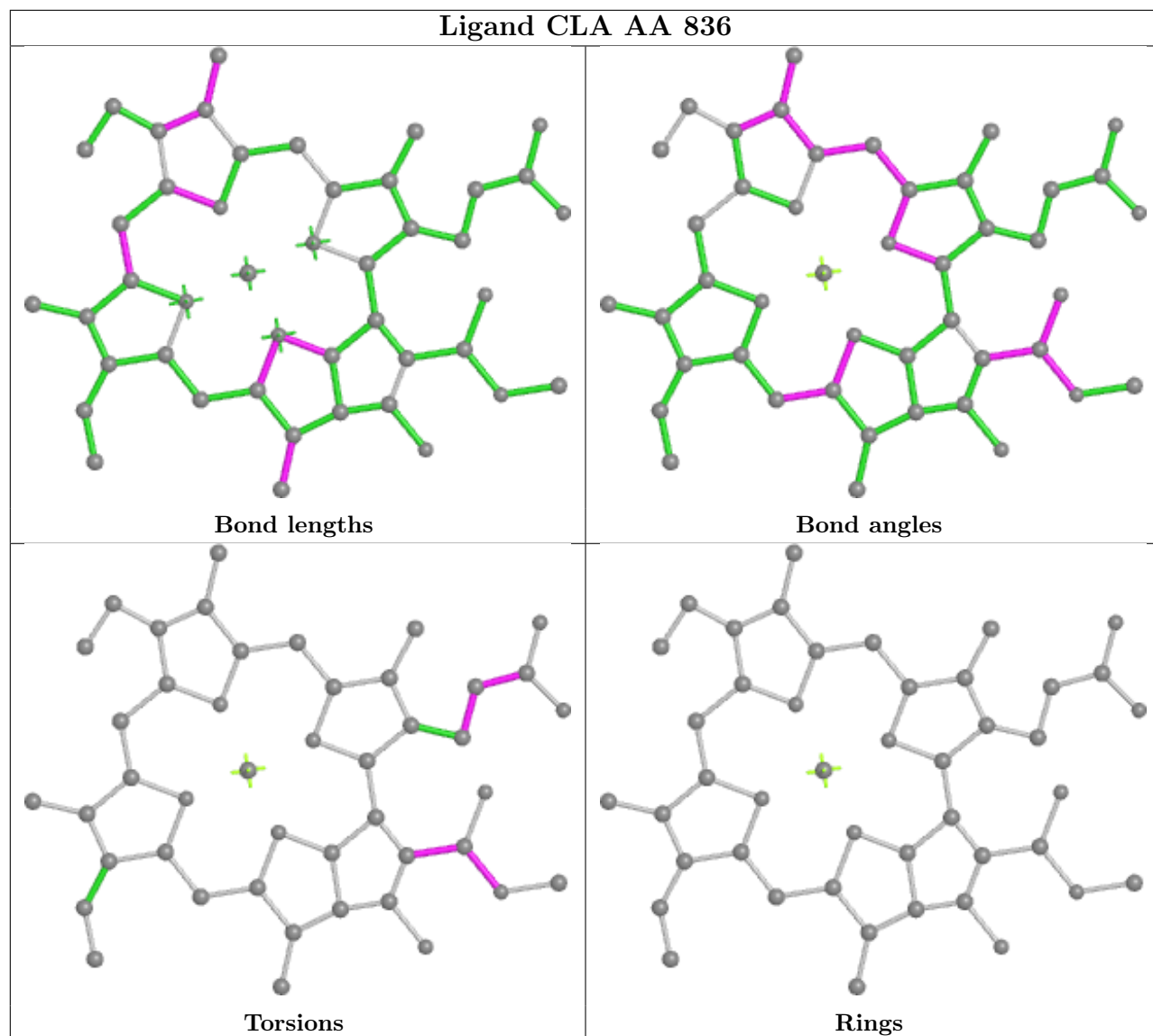
Ligand BCR BA 848



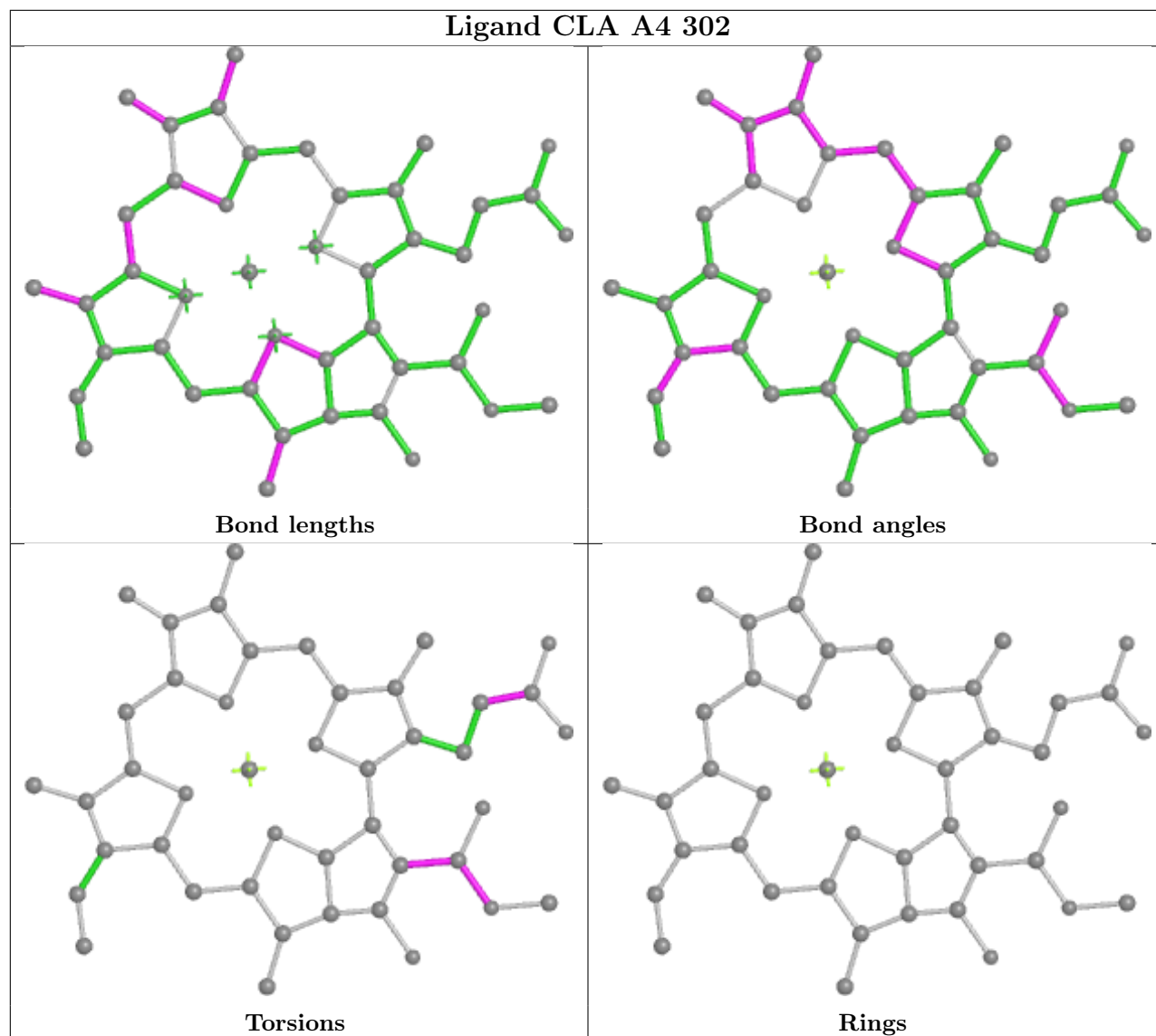


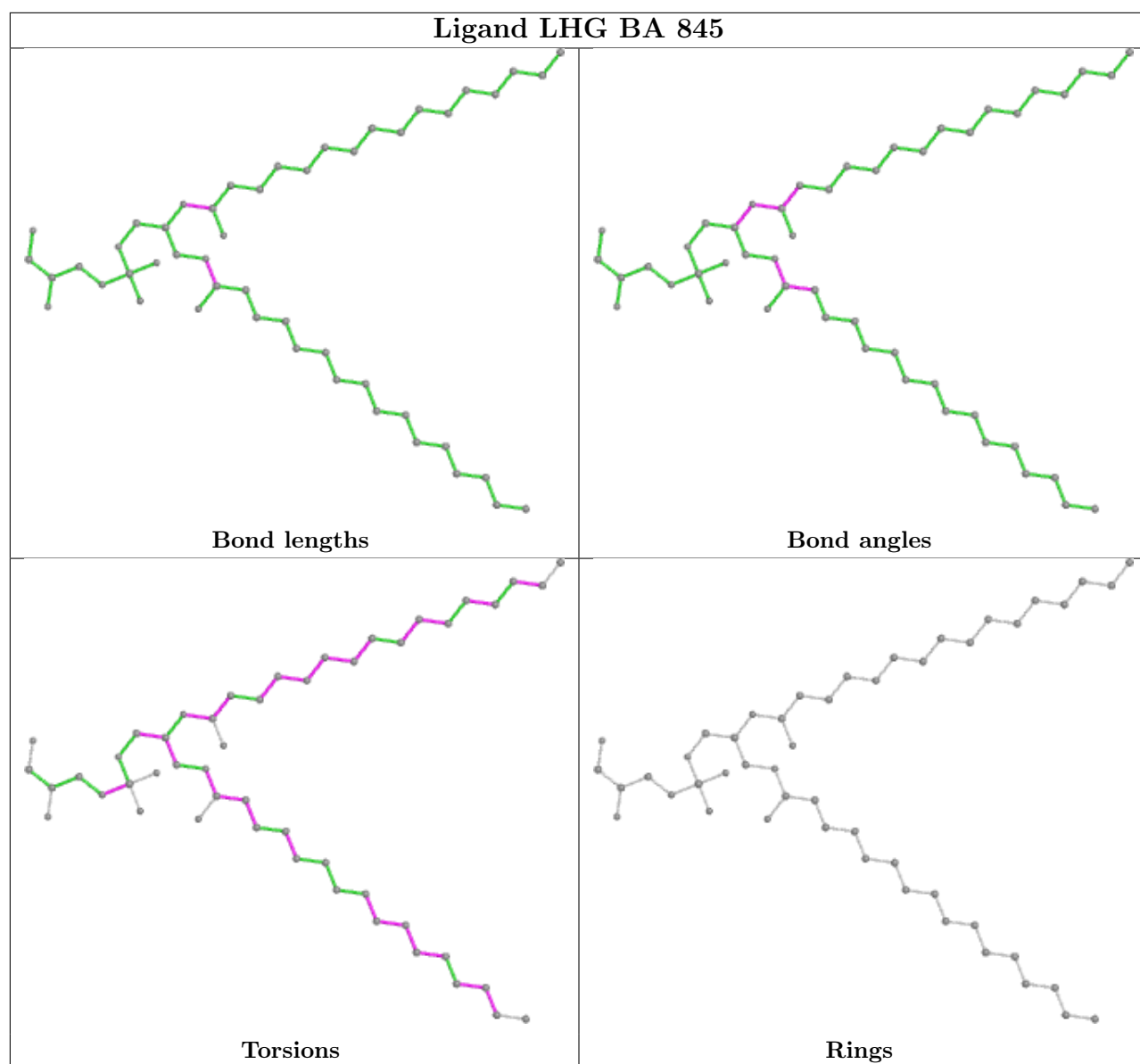


Ligand CLA AA 836

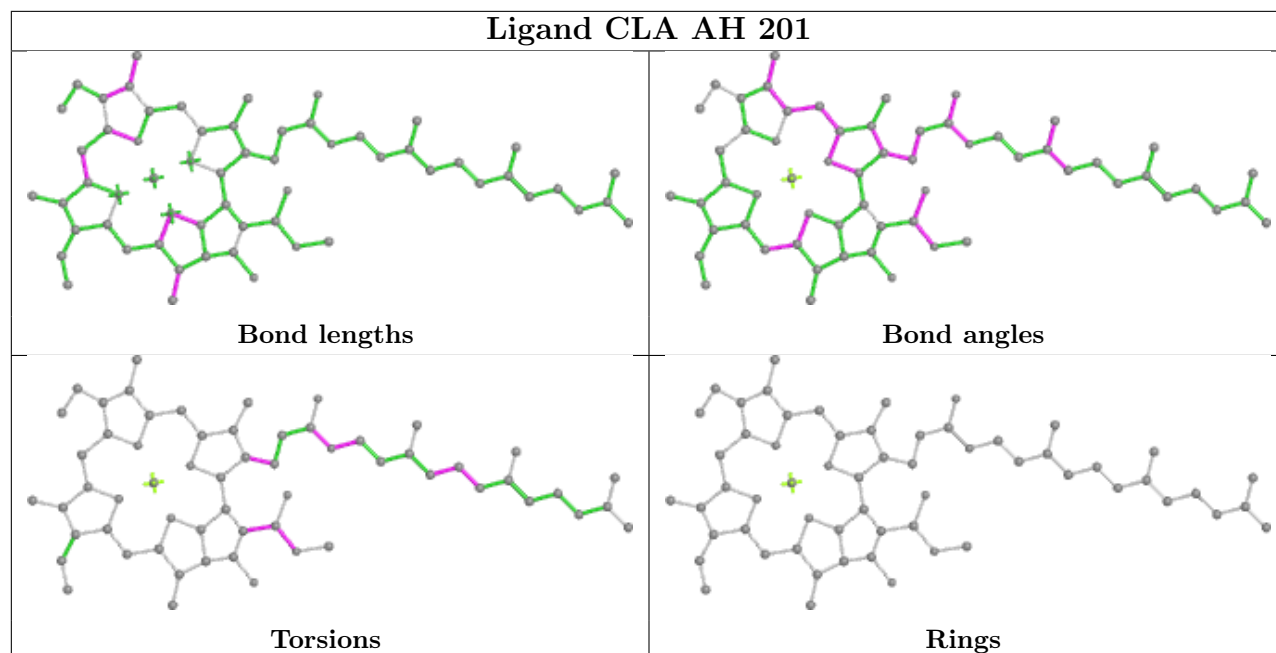


Ligand CLA A4 302

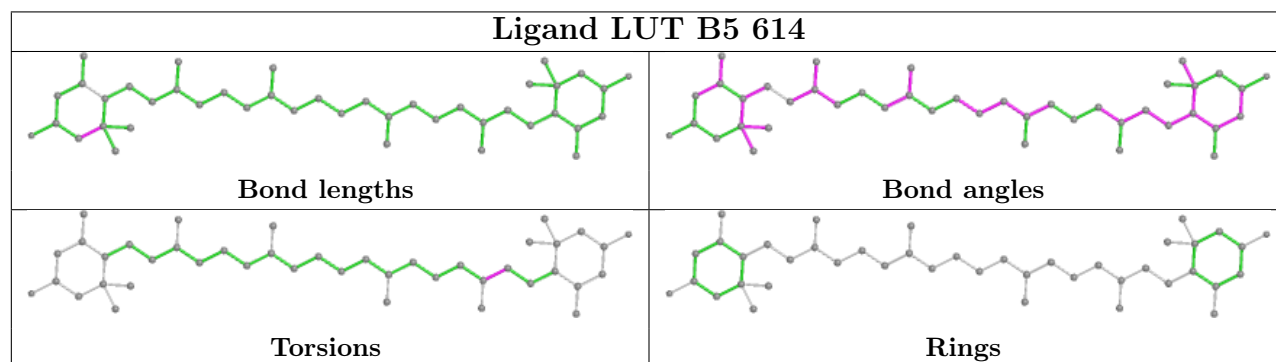




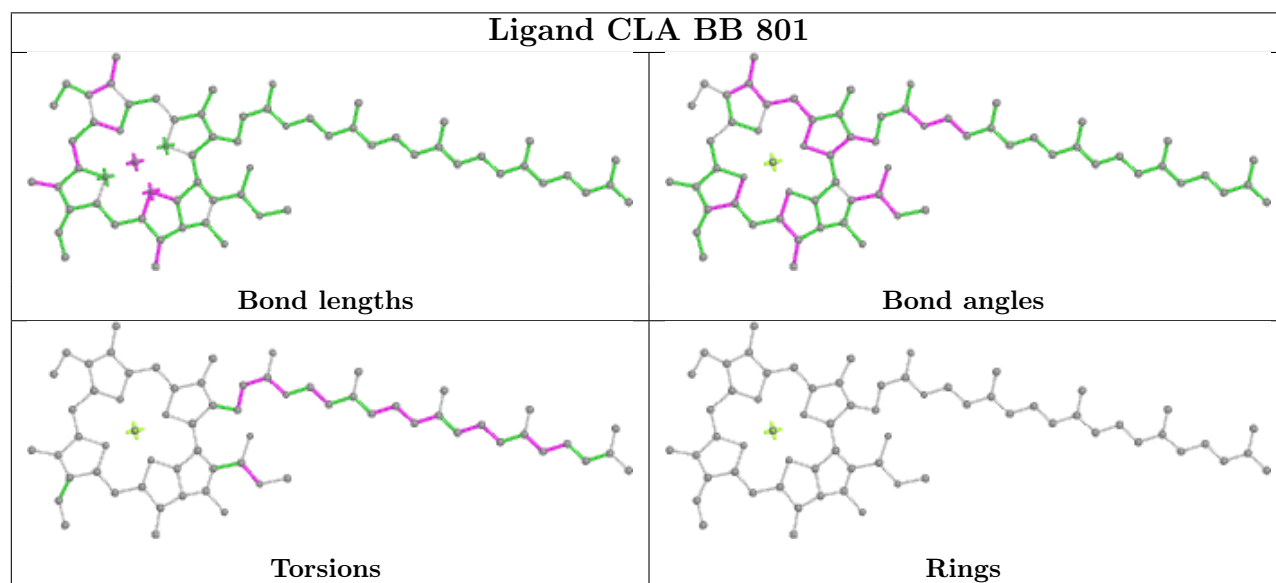
Ligand CLA AH 201

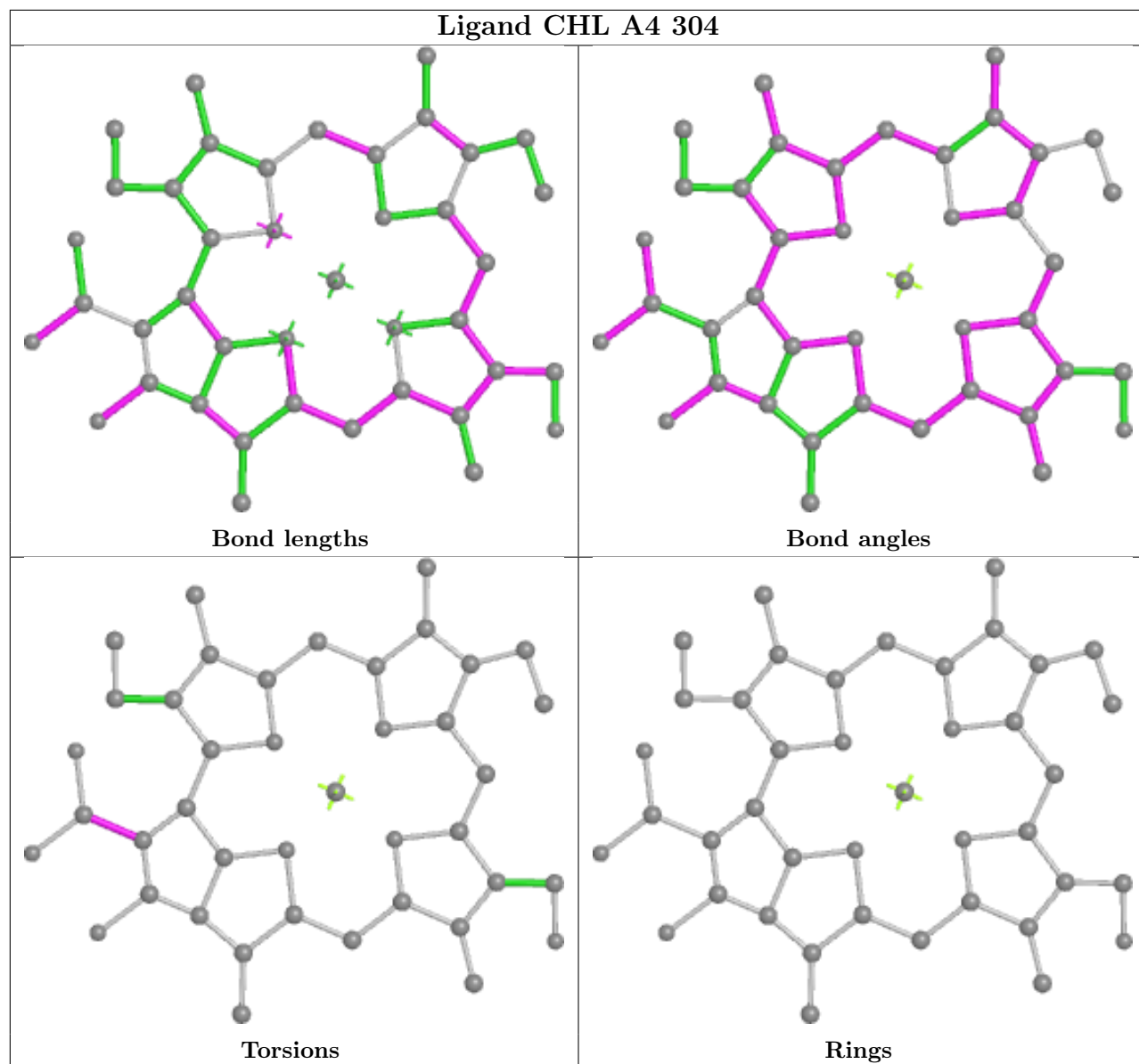


Ligand LUT B5 614

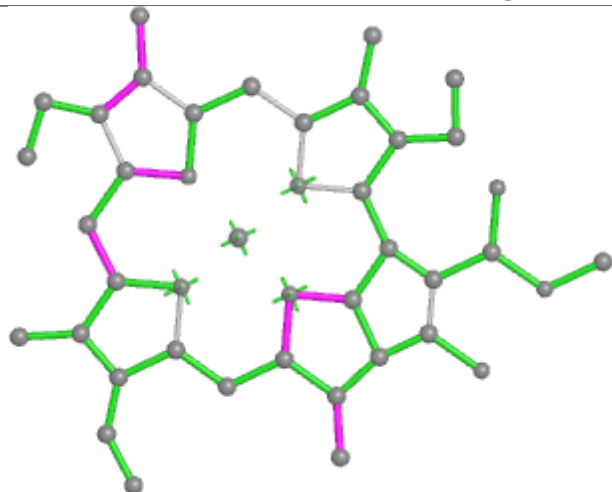


Ligand CLA BB 801

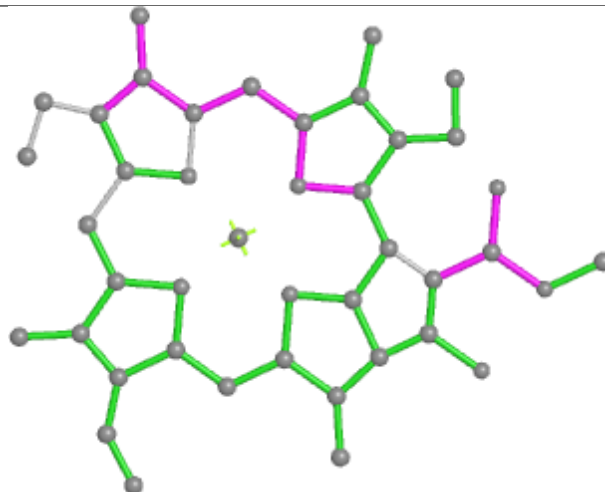




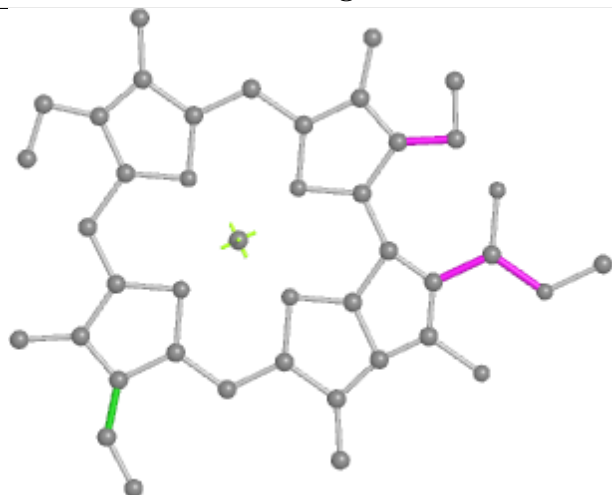
Ligand CLA BG 201



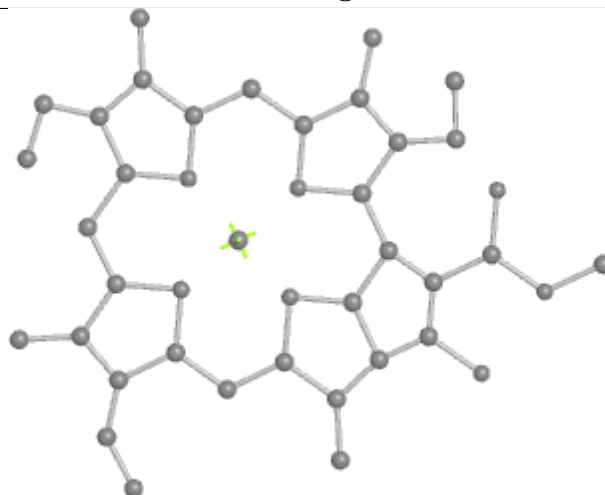
Bond lengths



Bond angles

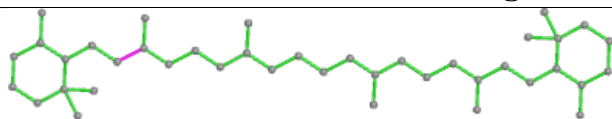


Torsions

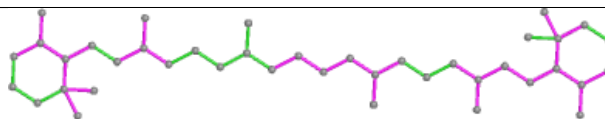


Rings

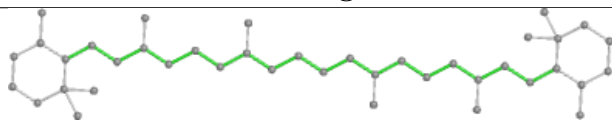
Ligand BCR B2 617



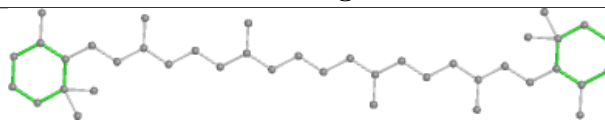
Bond lengths



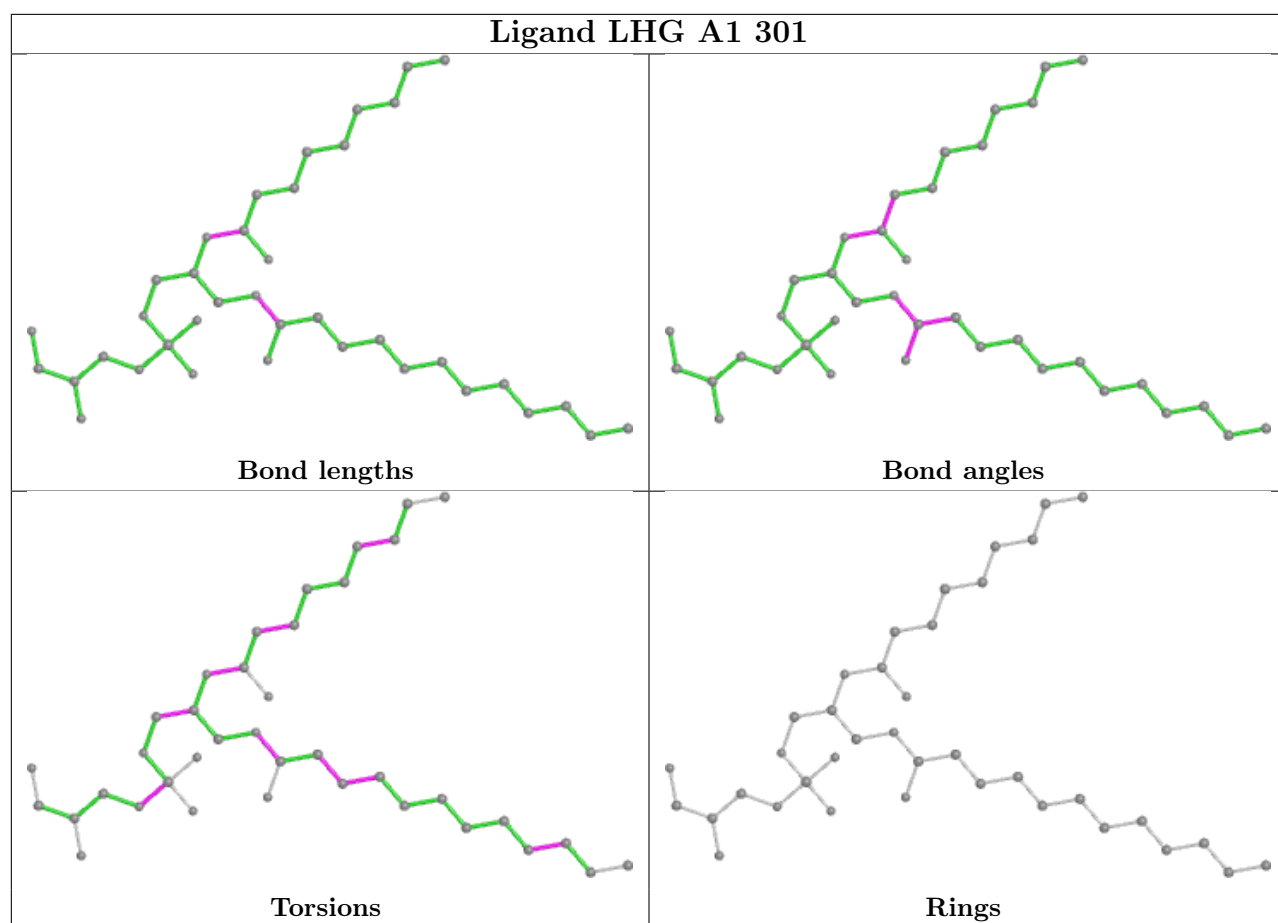
Bond angles



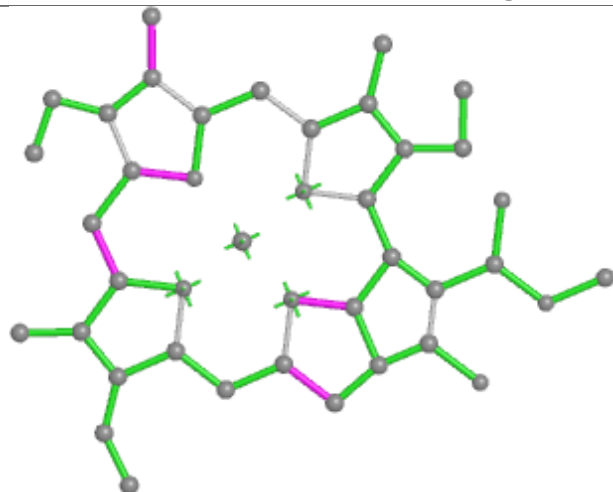
Torsions



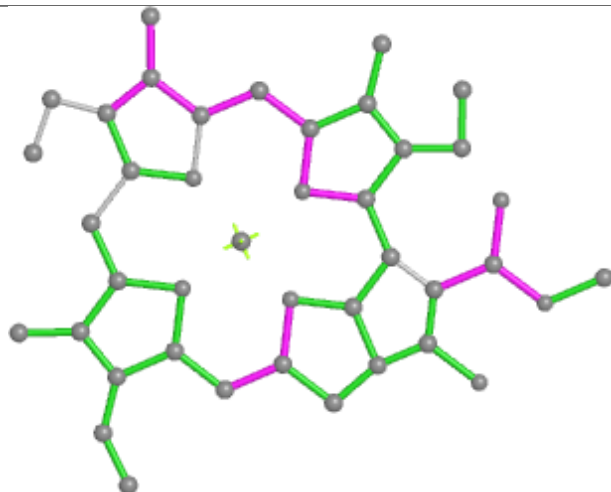
Rings



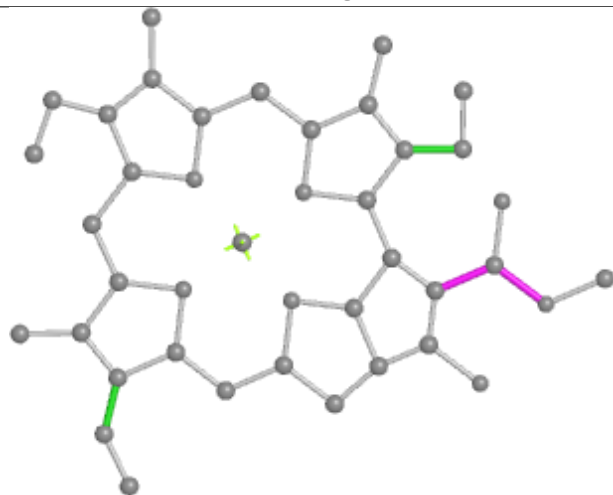
Ligand CLA AA 815



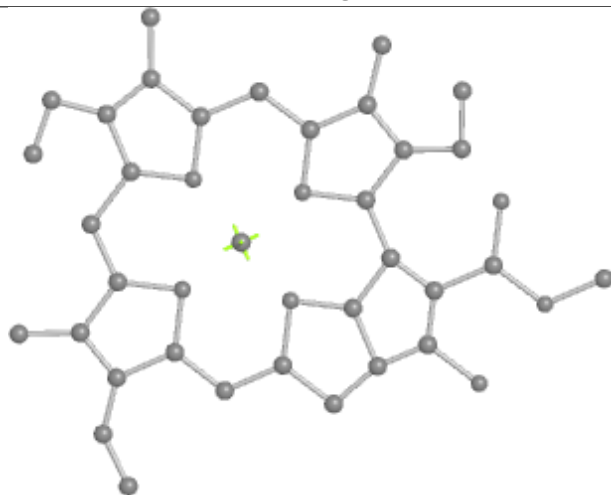
Bond lengths



Bond angles

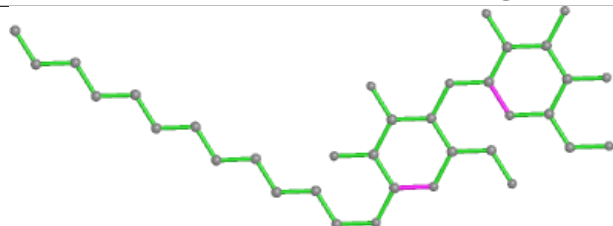


Torsions

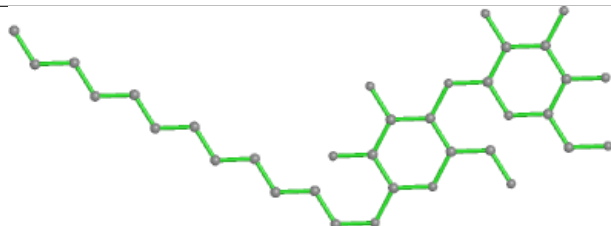


Rings

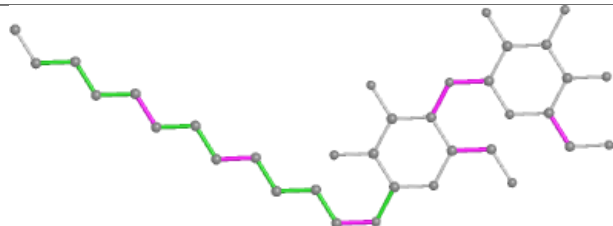
Ligand LMU BB 851



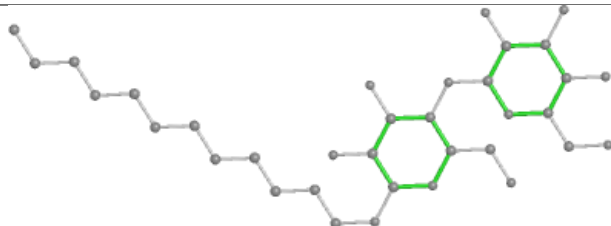
Bond lengths



Bond angles

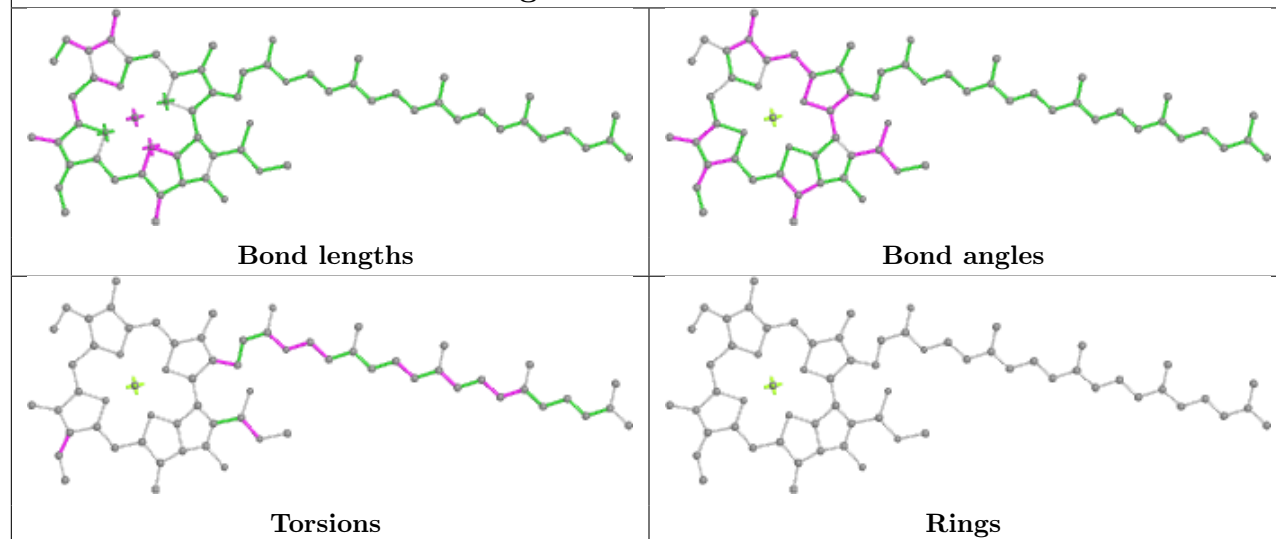


Torsions

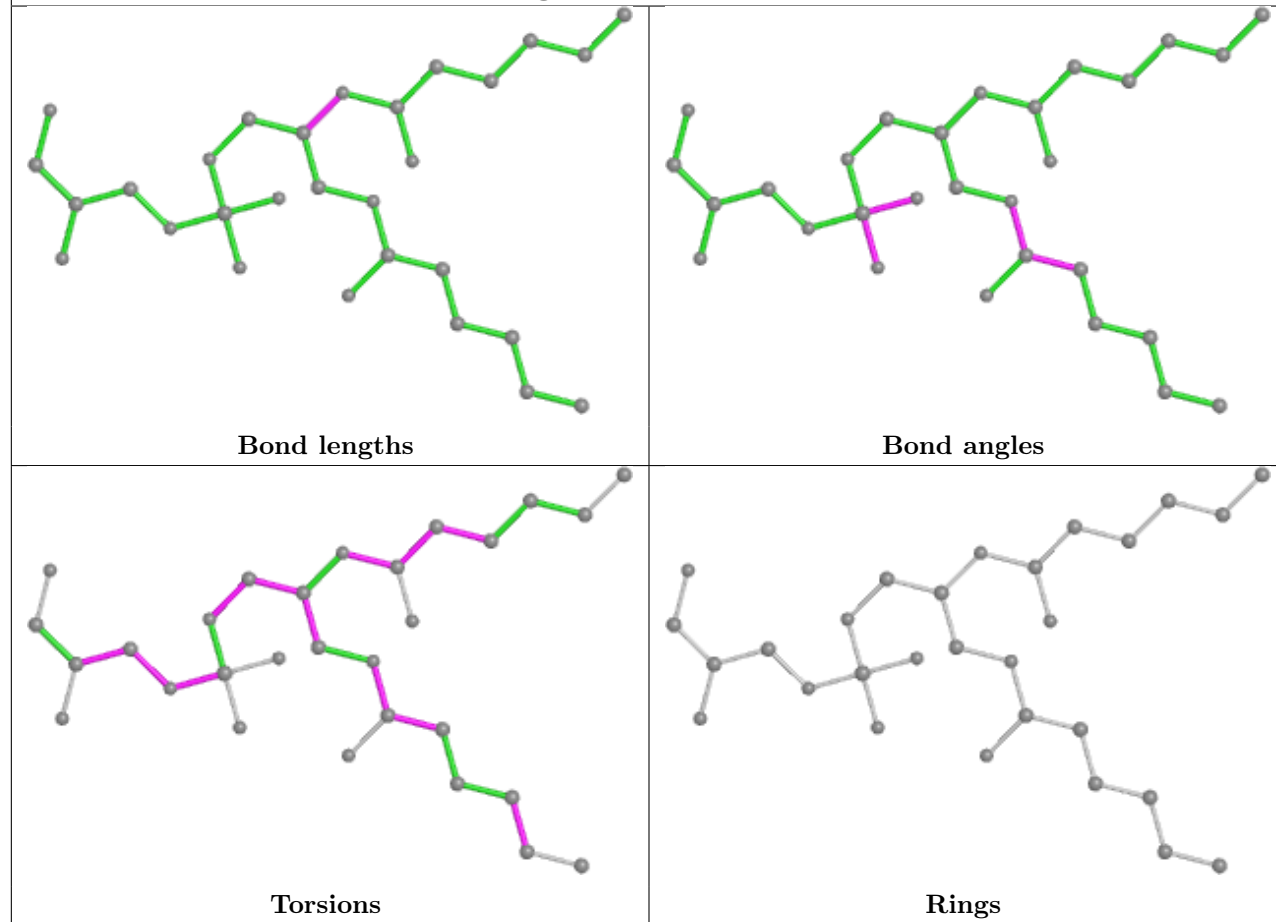


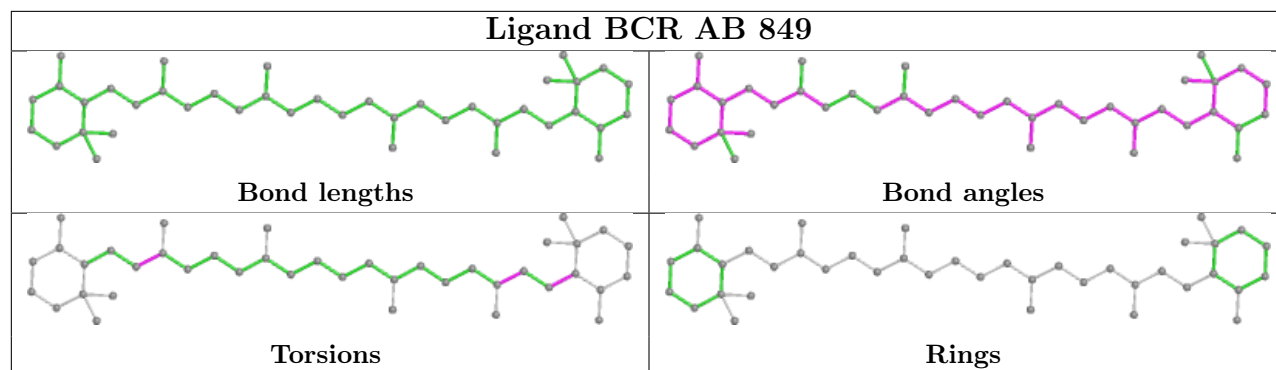
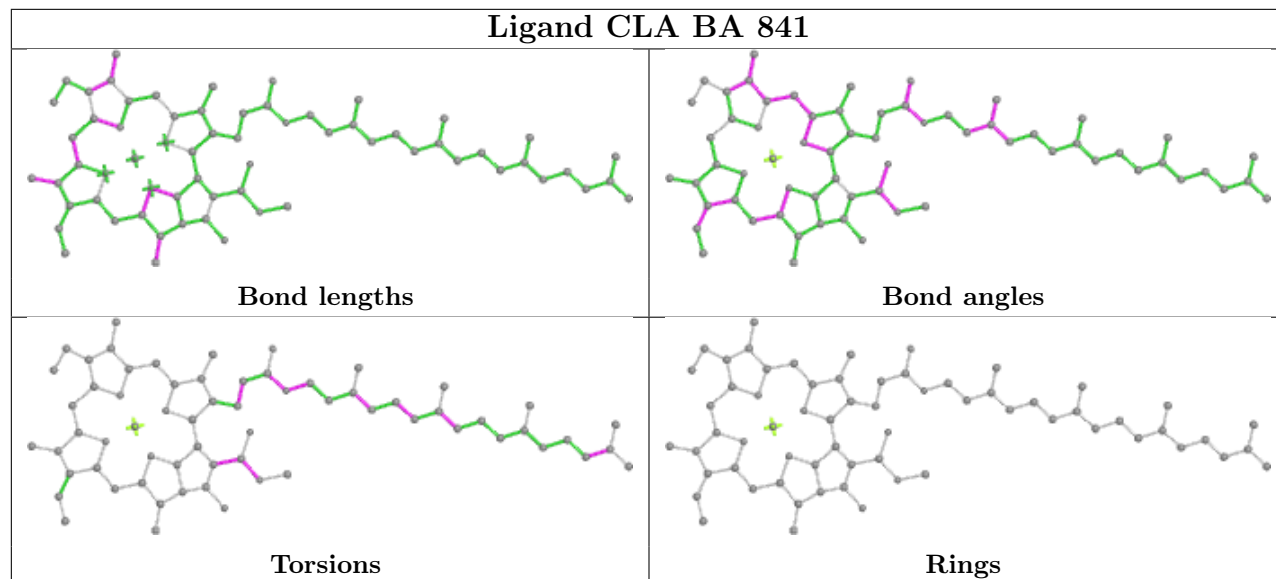
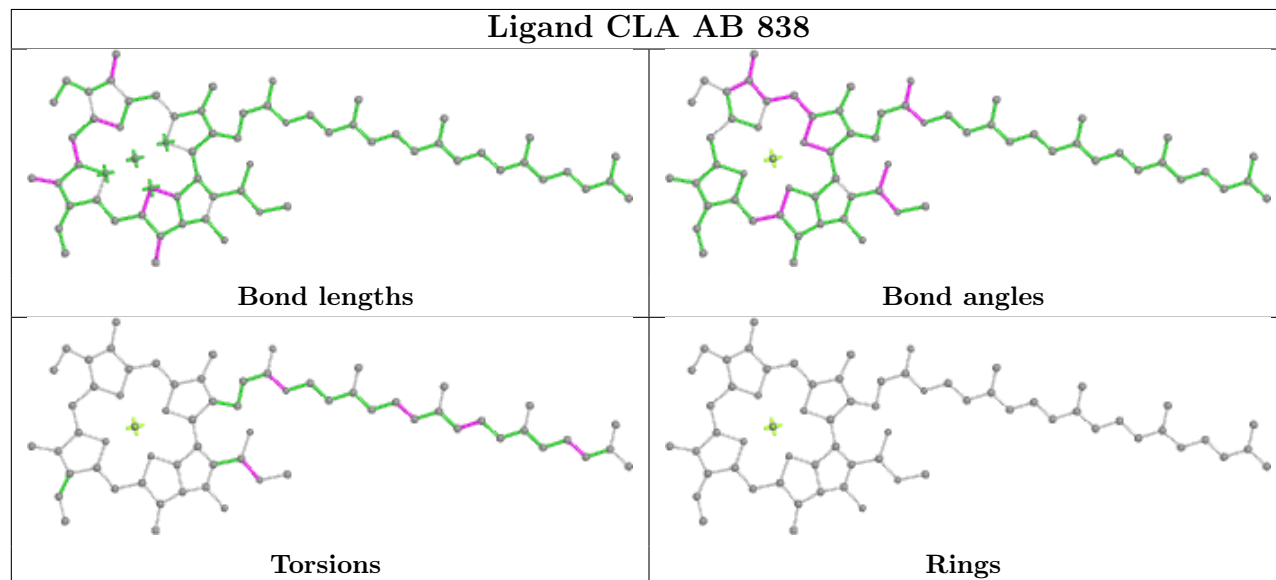
Rings

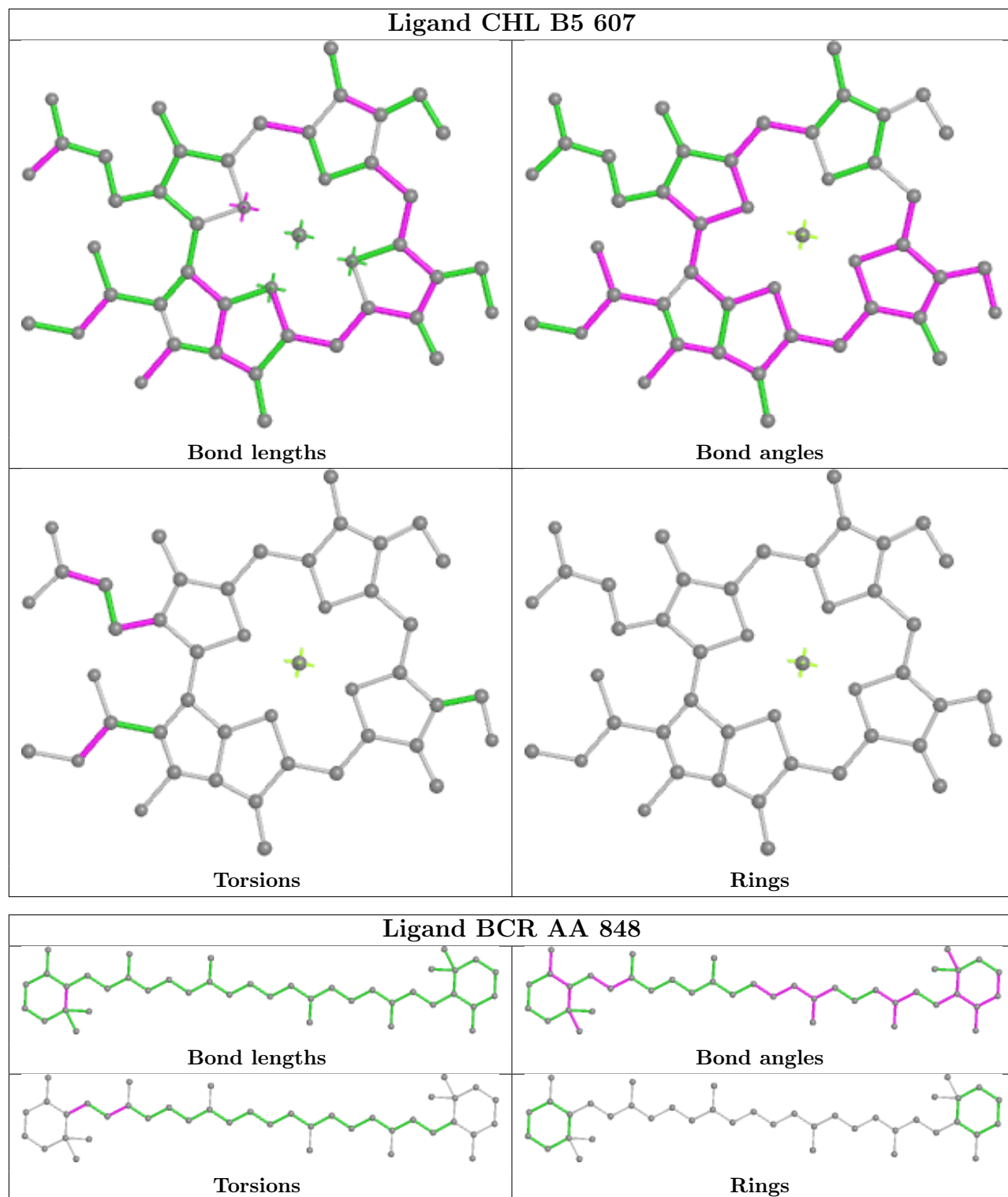
Ligand CLA BB 805

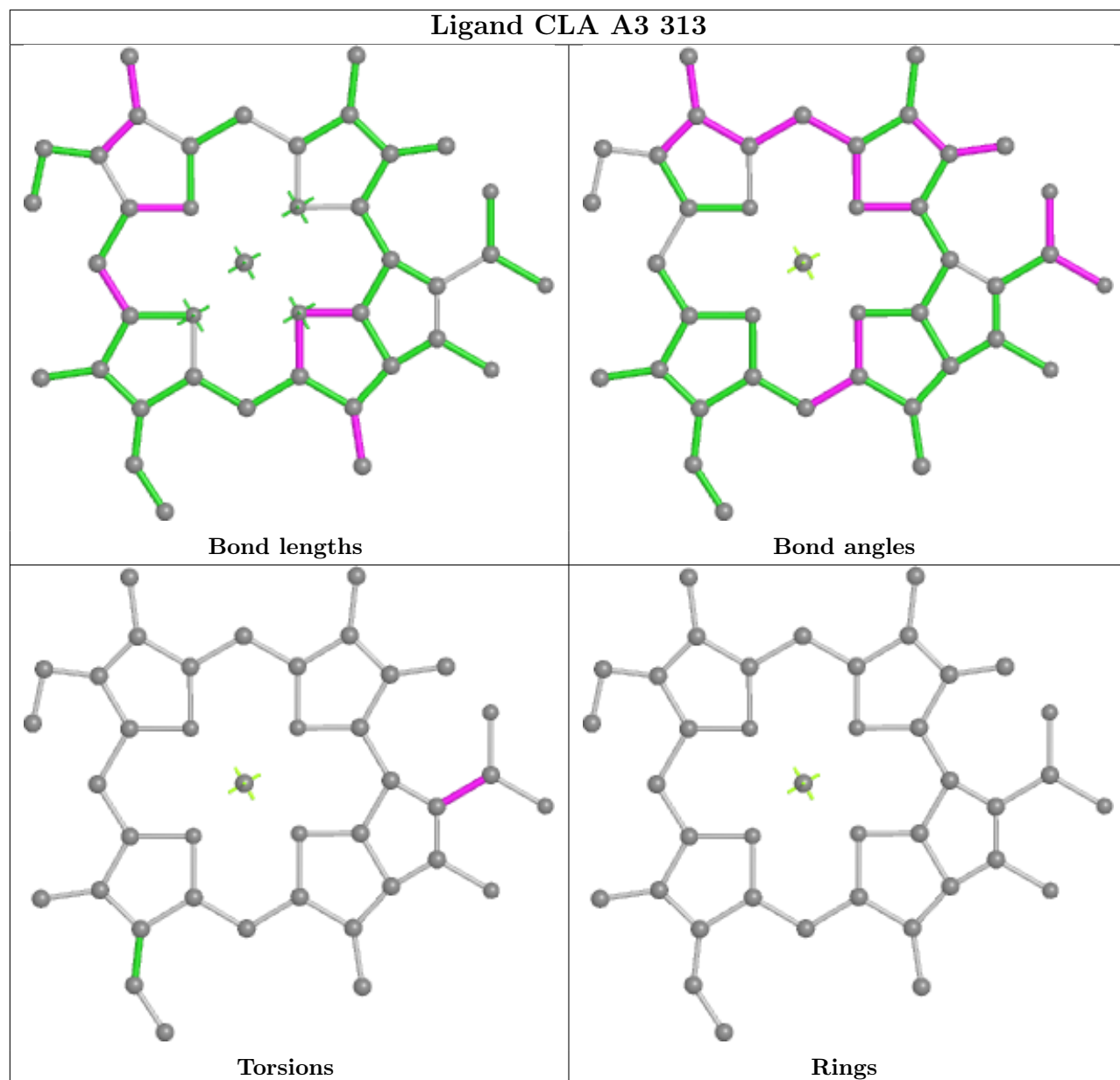


Ligand LHG a 501

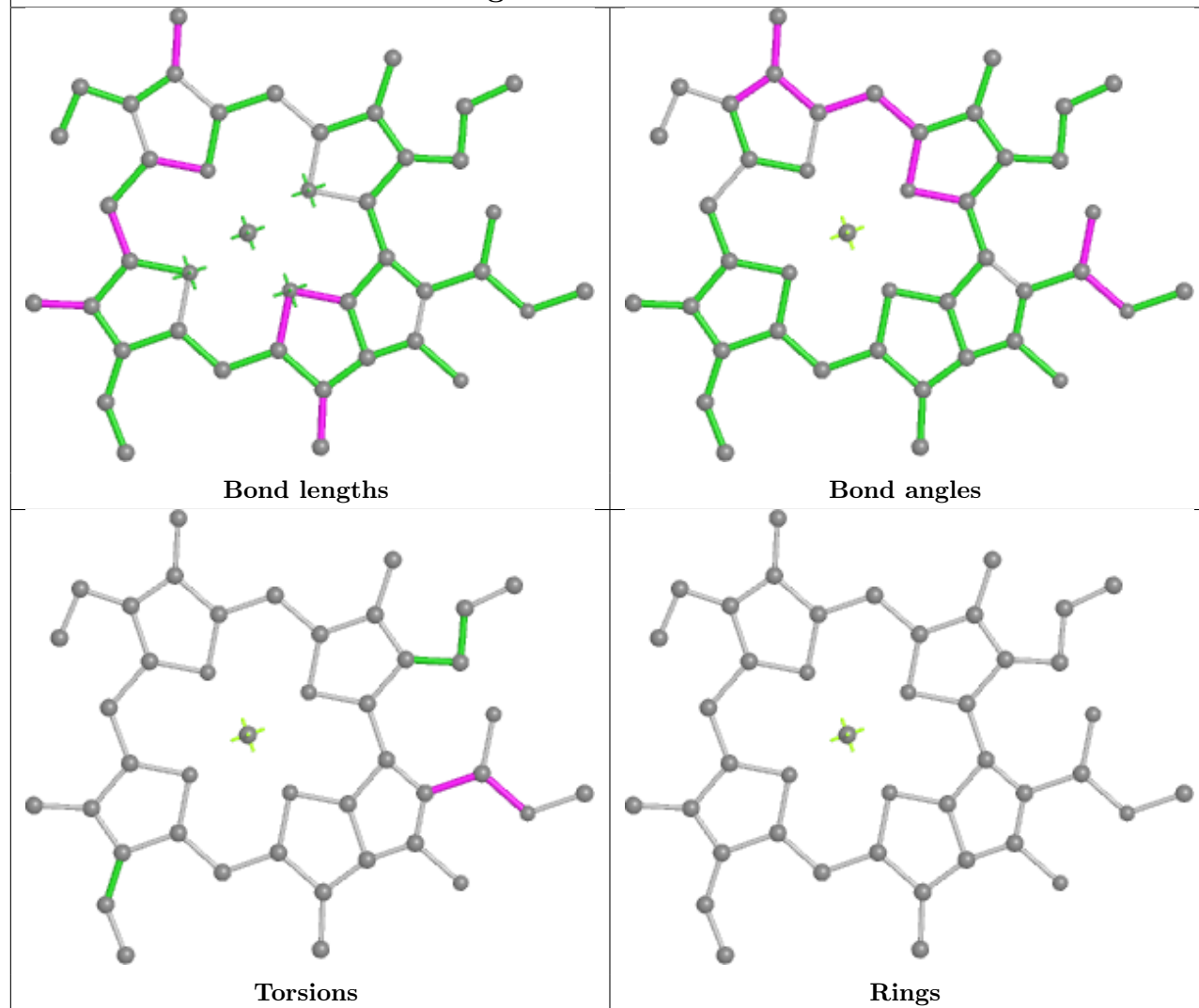


Ligand BCR AB 849**Ligand CLA BA 841****Ligand CLA AB 838**

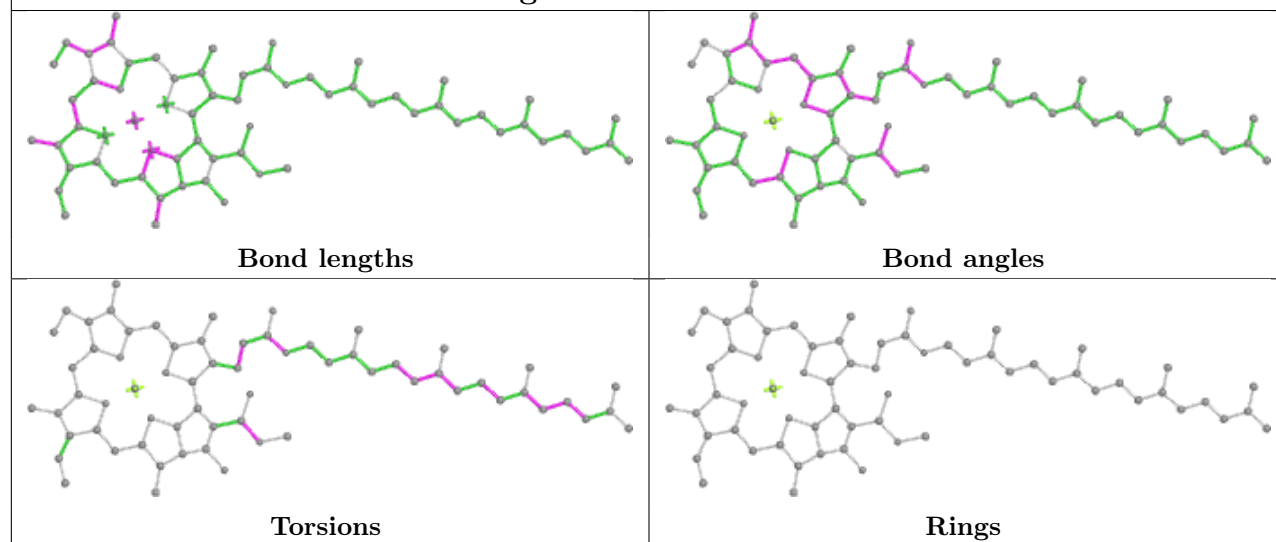


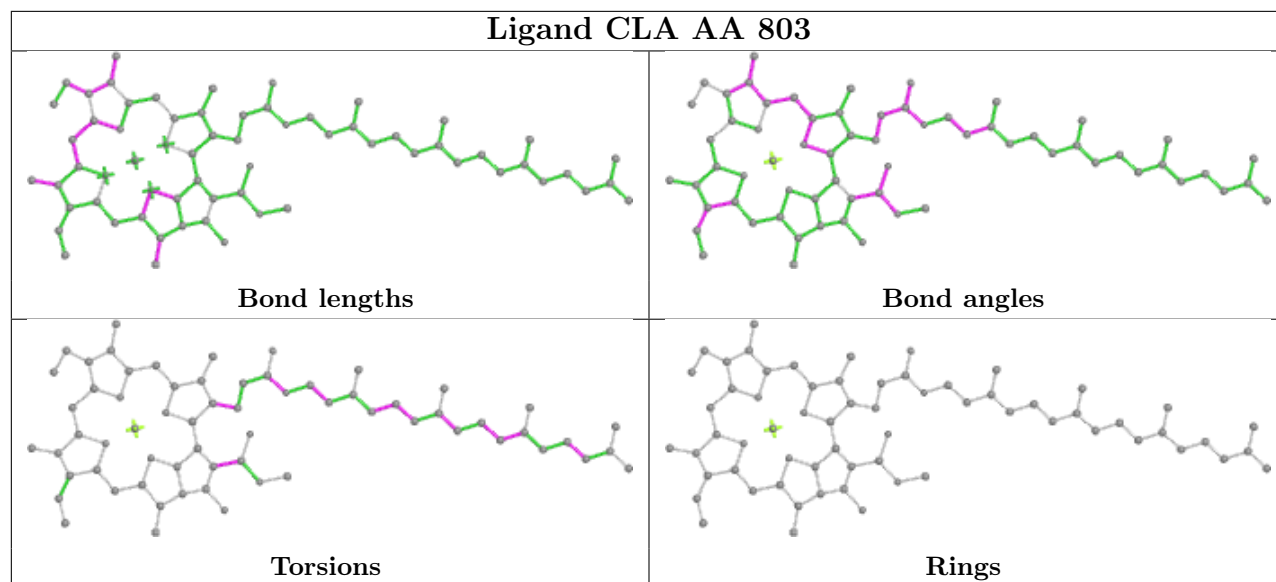
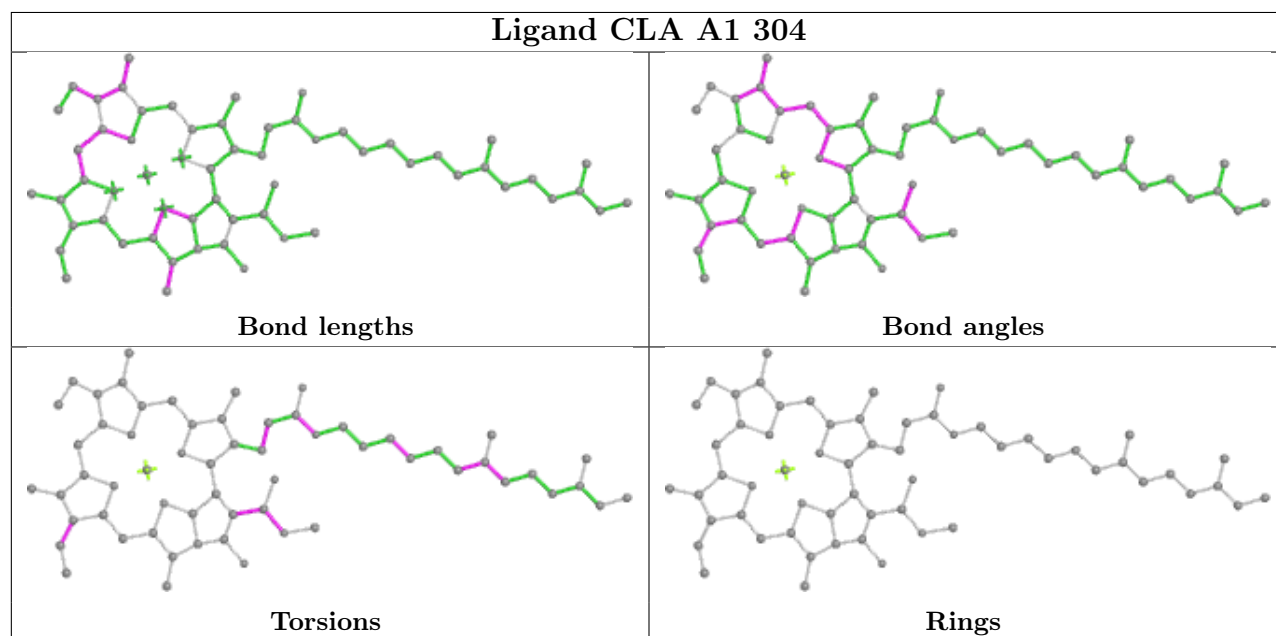


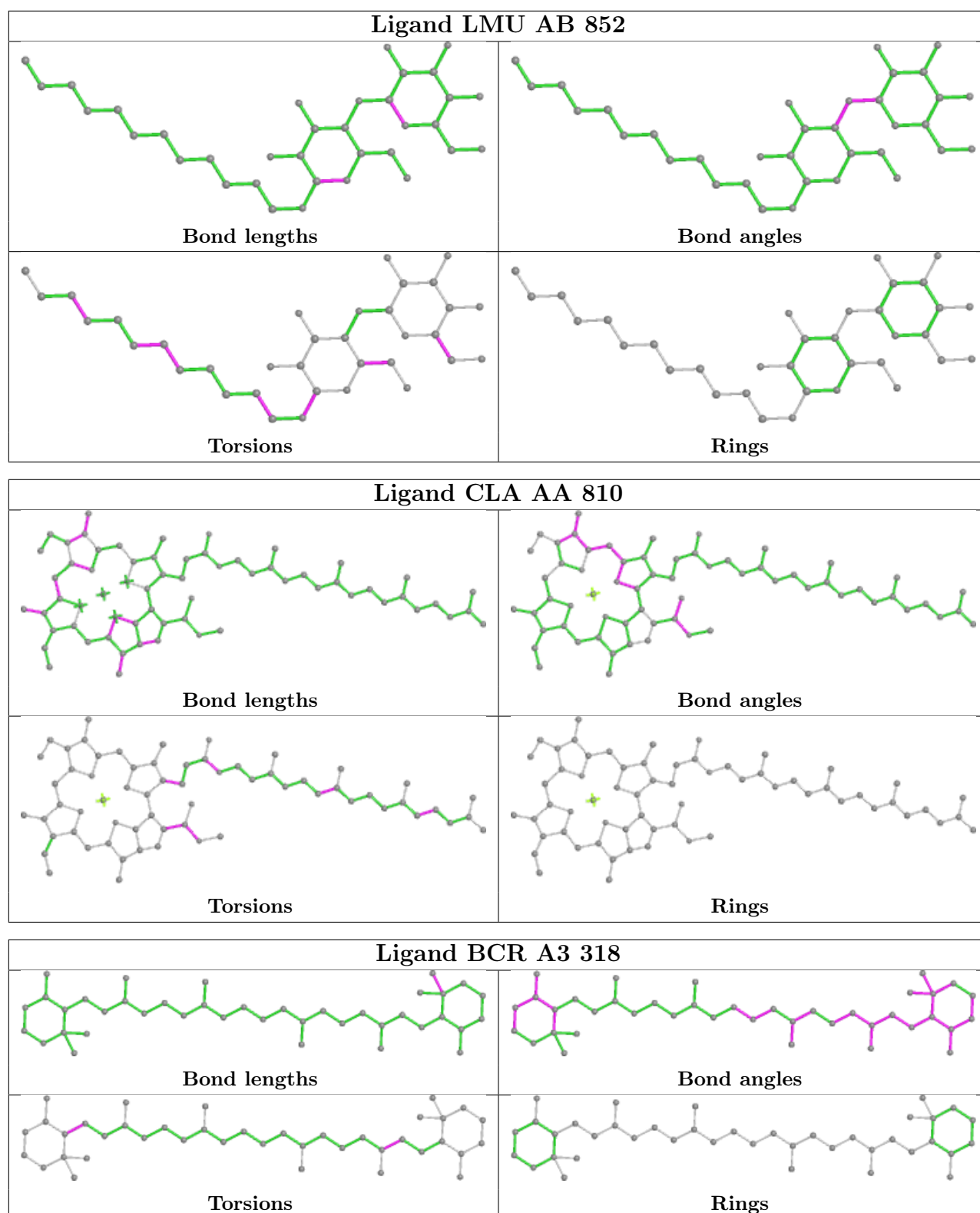
Ligand CLA AB 816

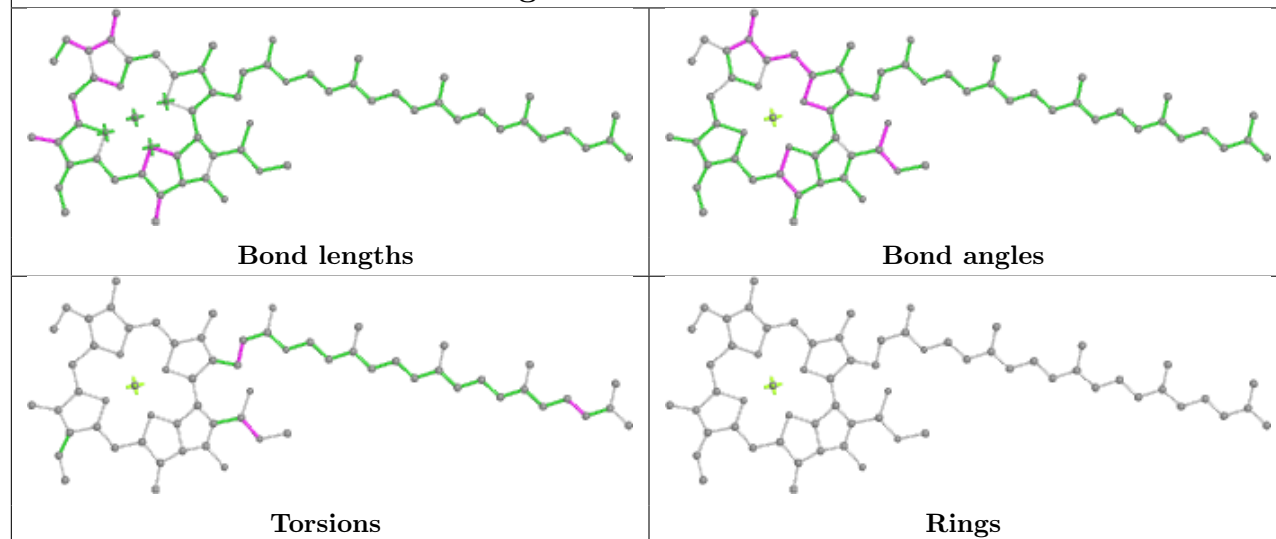
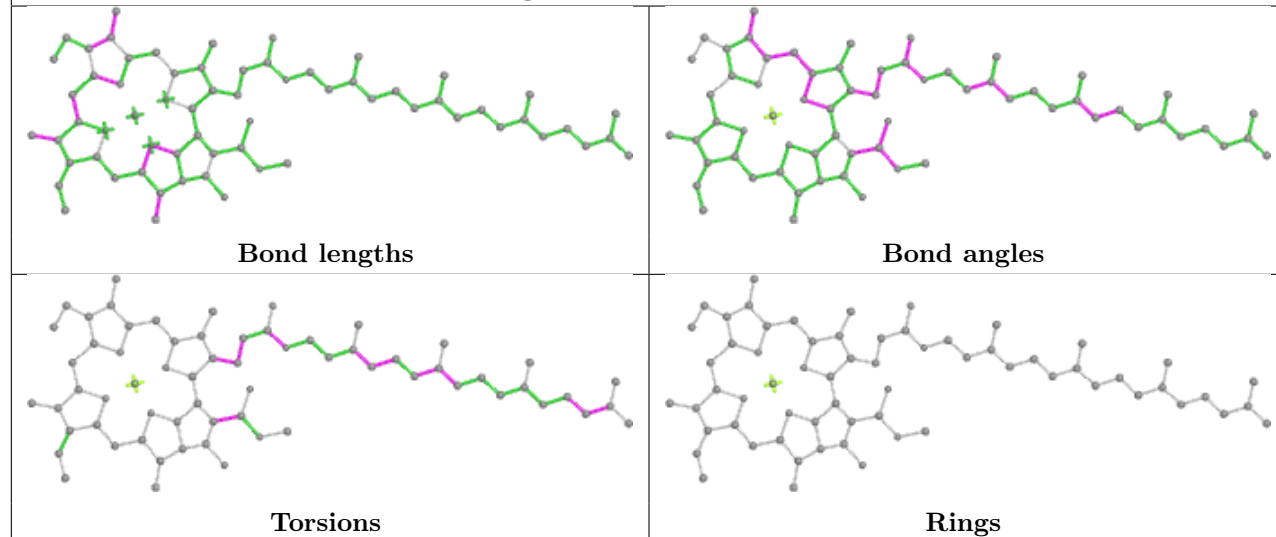


Ligand CLA BB 811

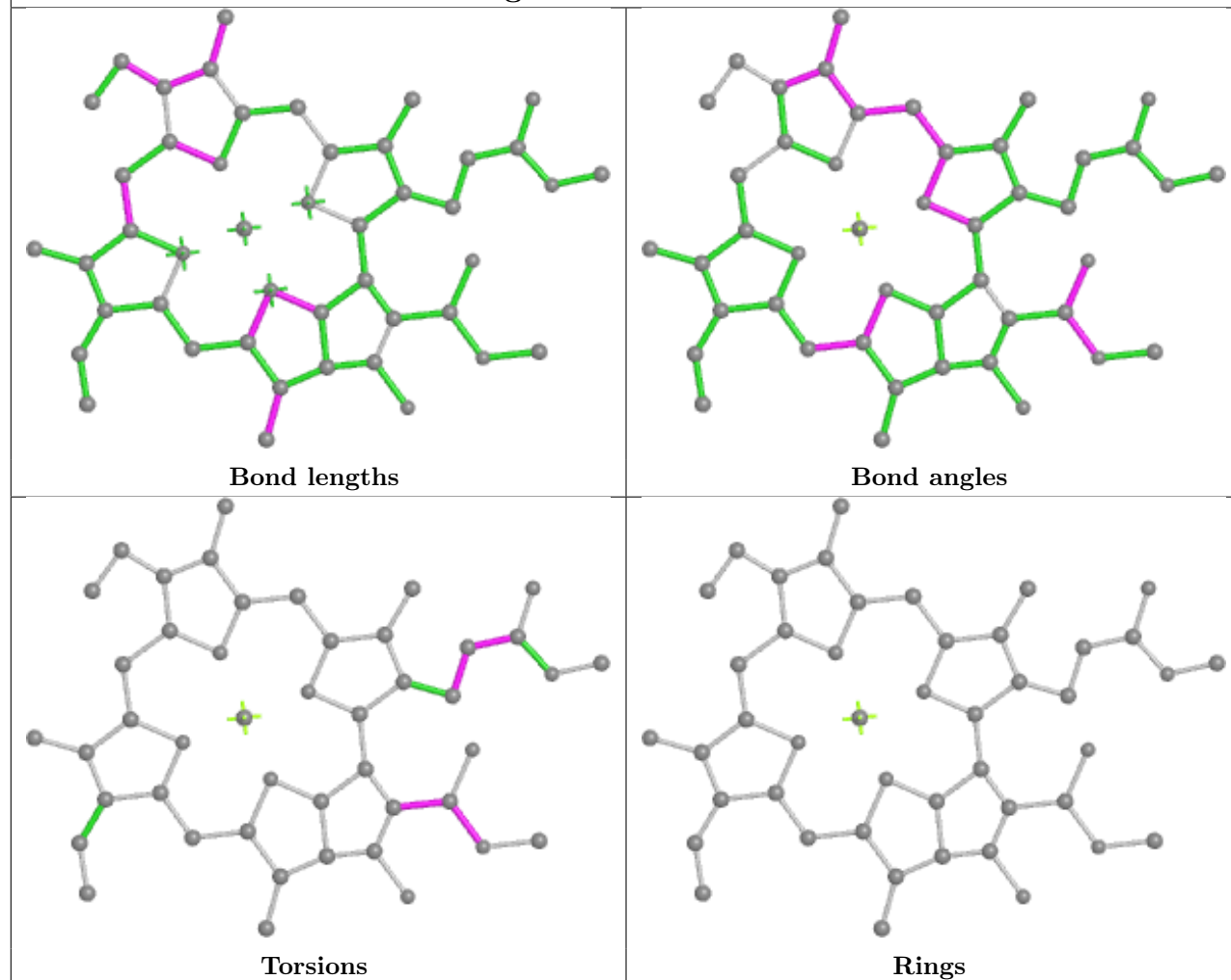


Ligand CLA AA 803**Ligand CLA A1 304**

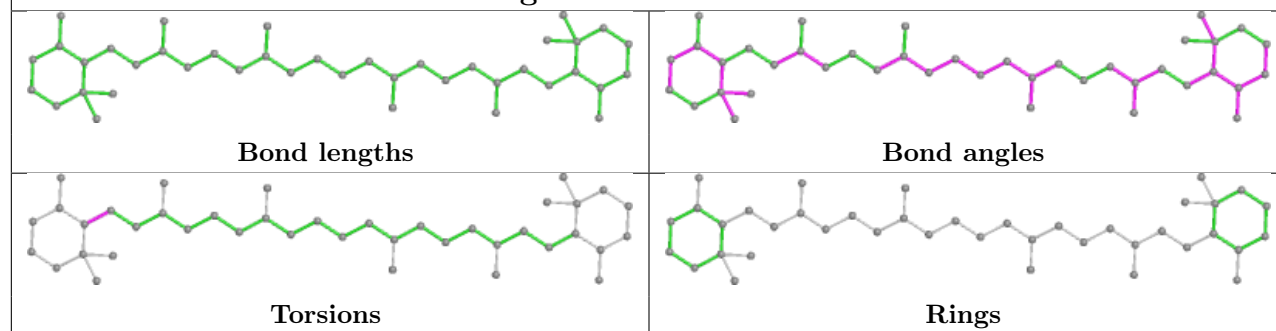


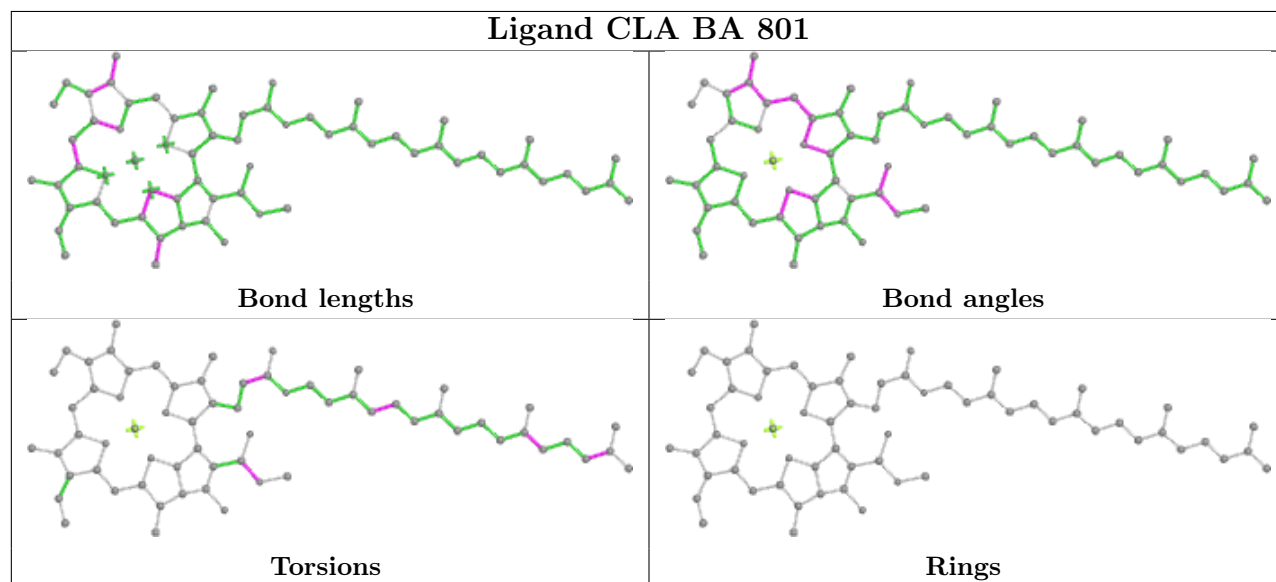
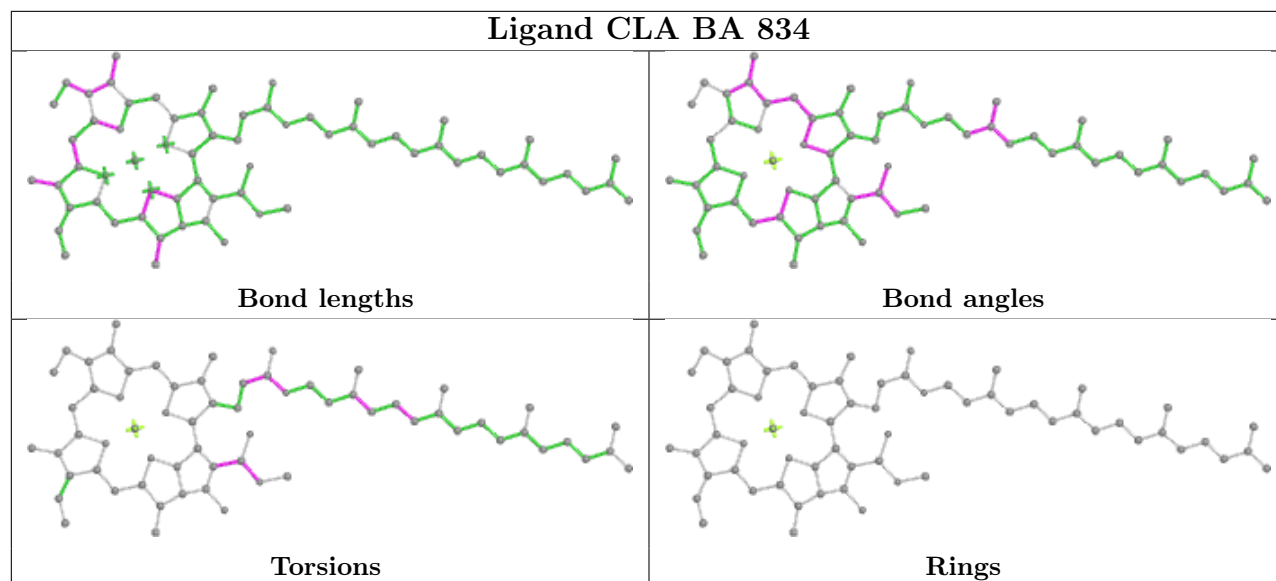
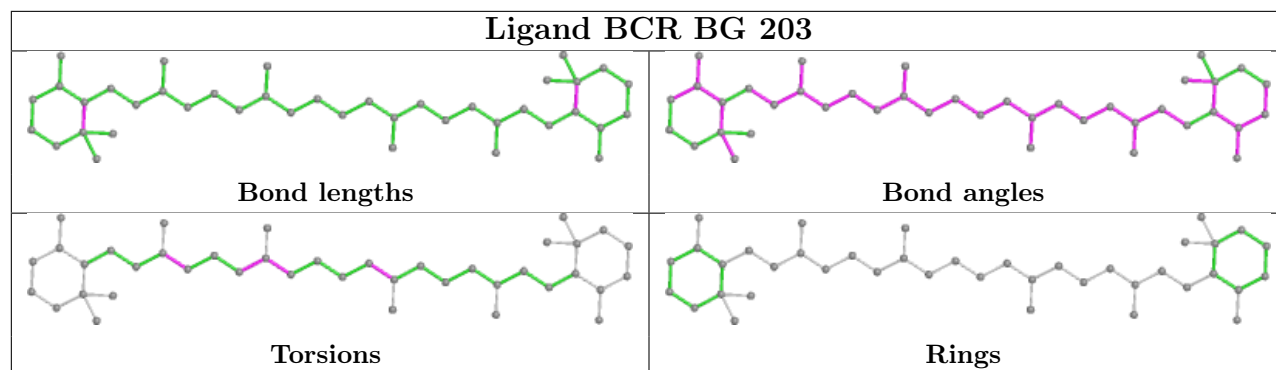
Ligand CLA BA 802**Ligand CLA AB 809**

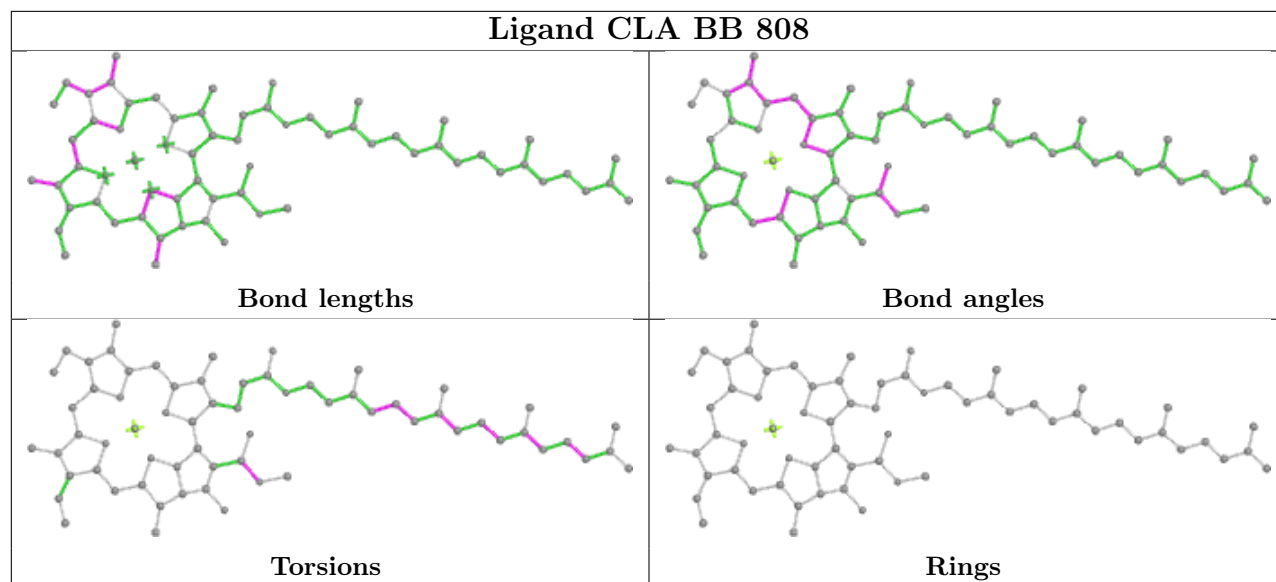
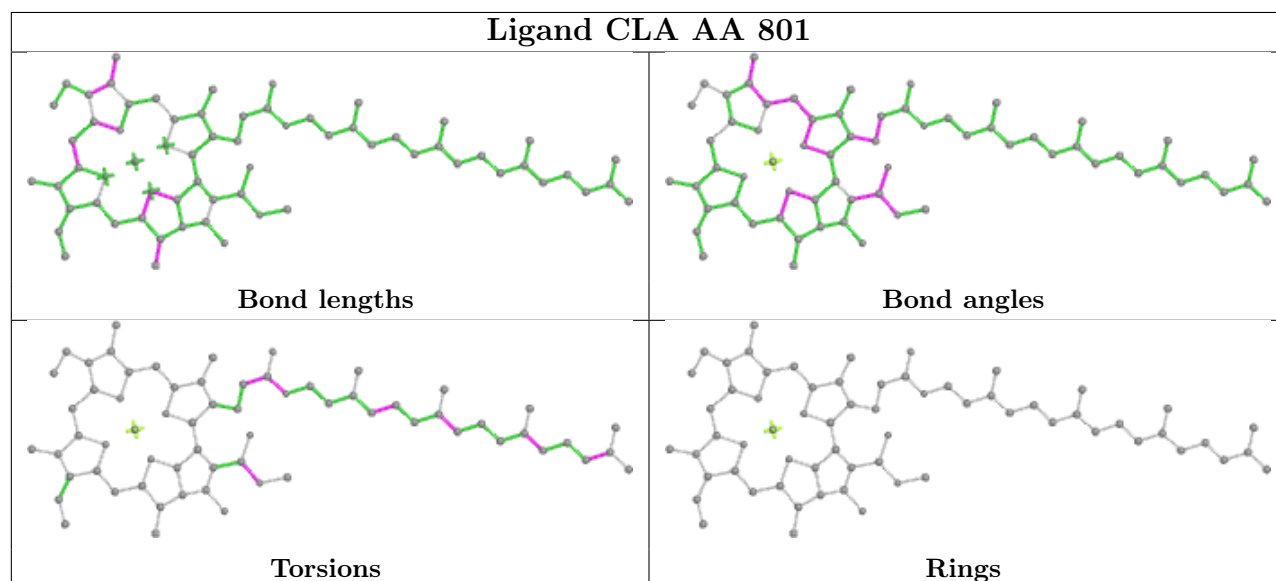
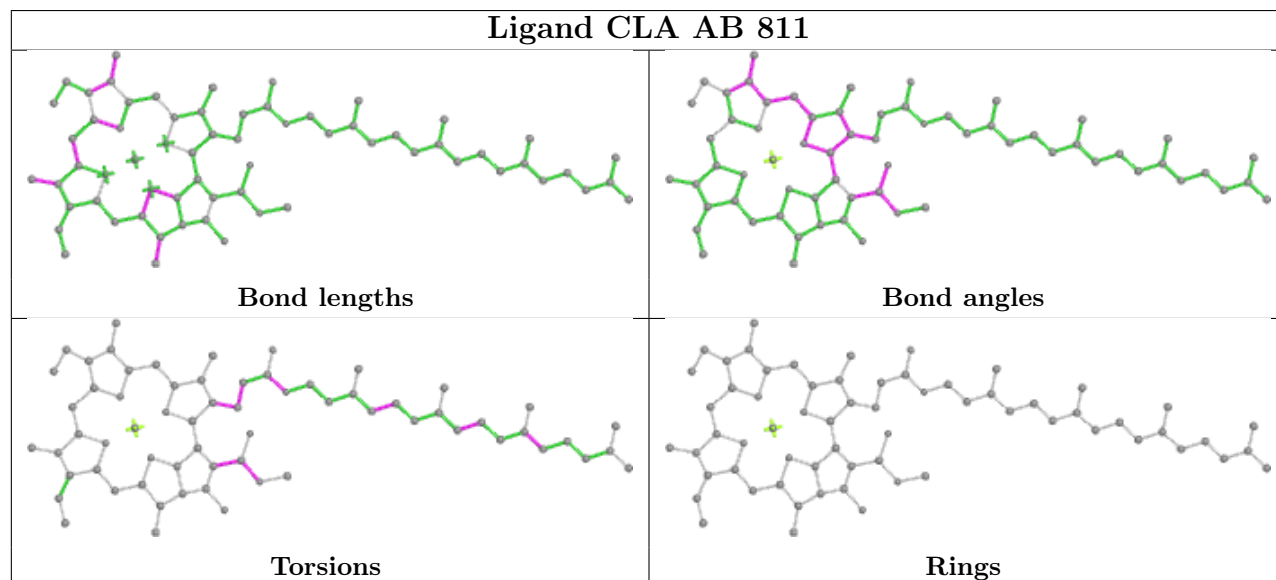
Ligand CLA B5 601



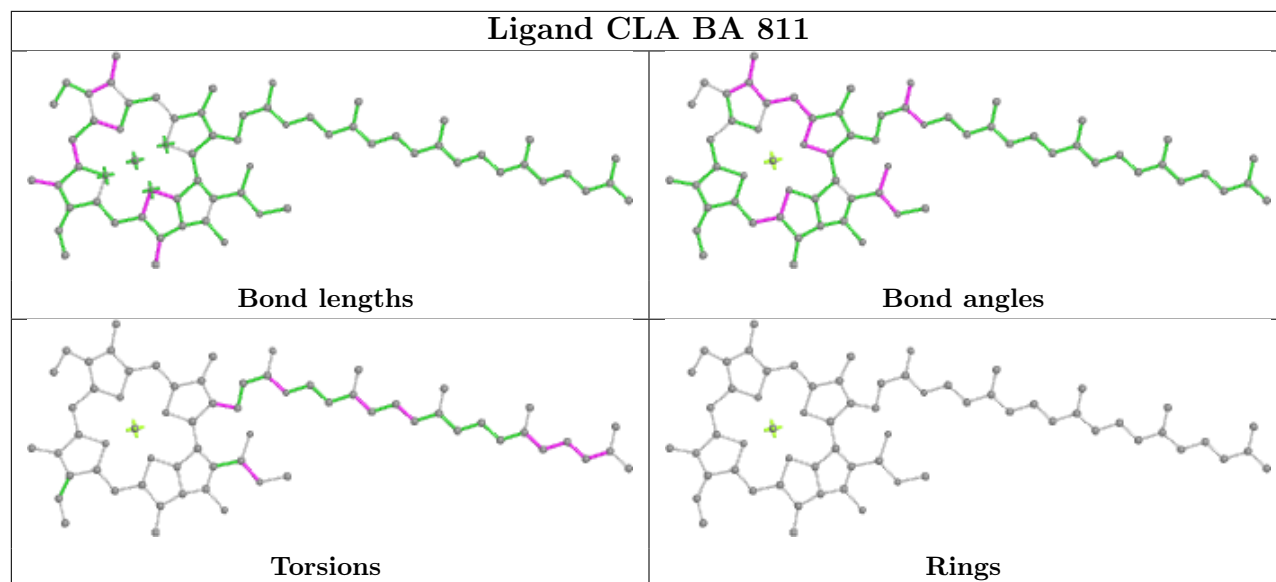
Ligand BCR BL 305



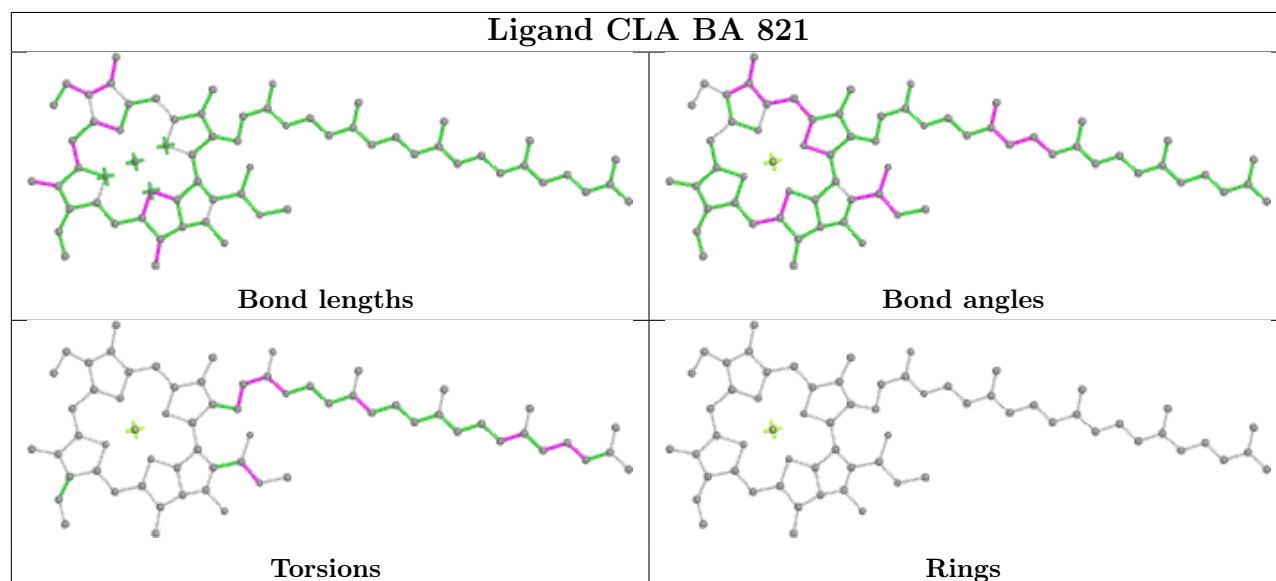


Ligand CLA BB 808**Ligand CLA AA 801****Ligand CLA AB 811**

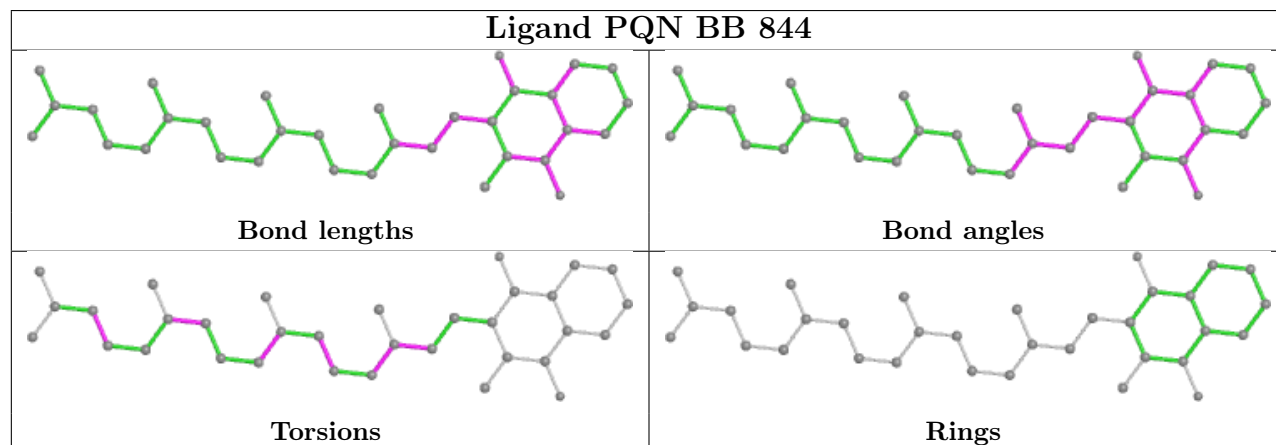
Ligand CLA BA 811



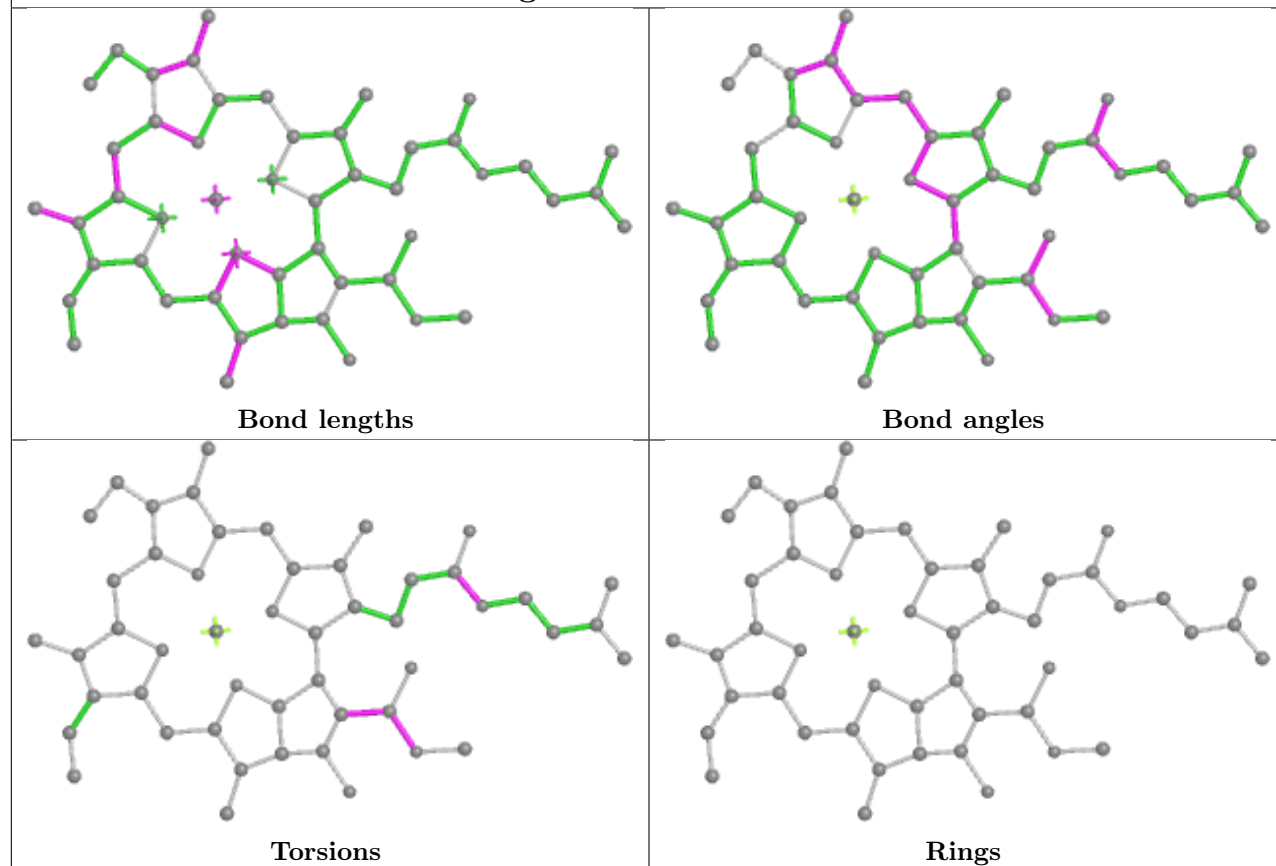
Ligand CLA BA 821



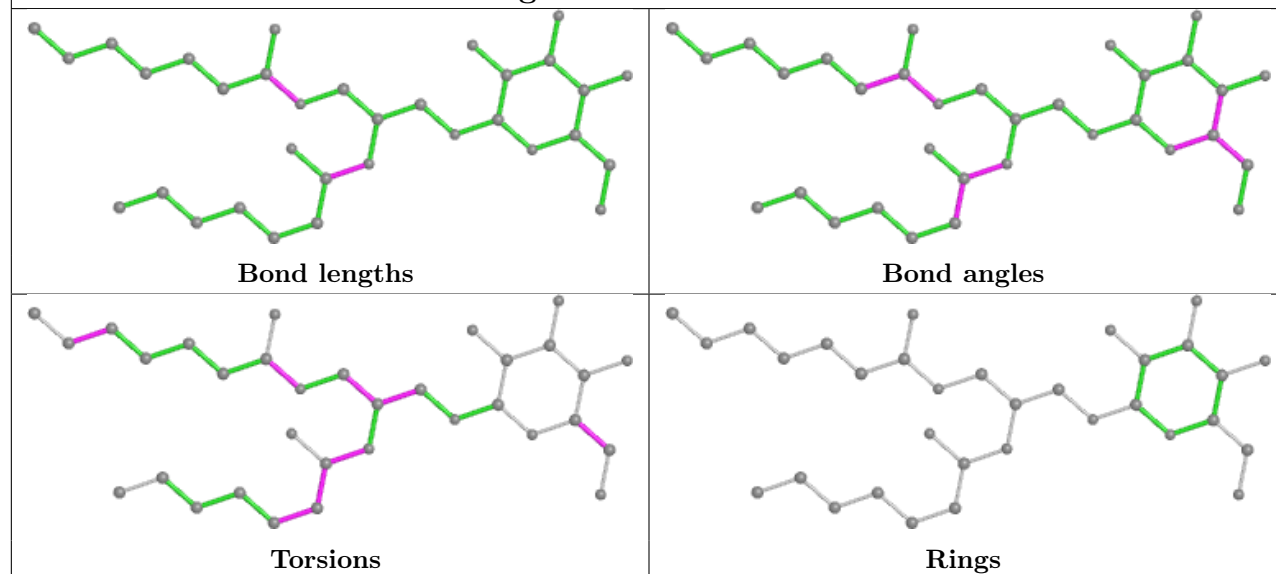
Ligand PQN BB 844



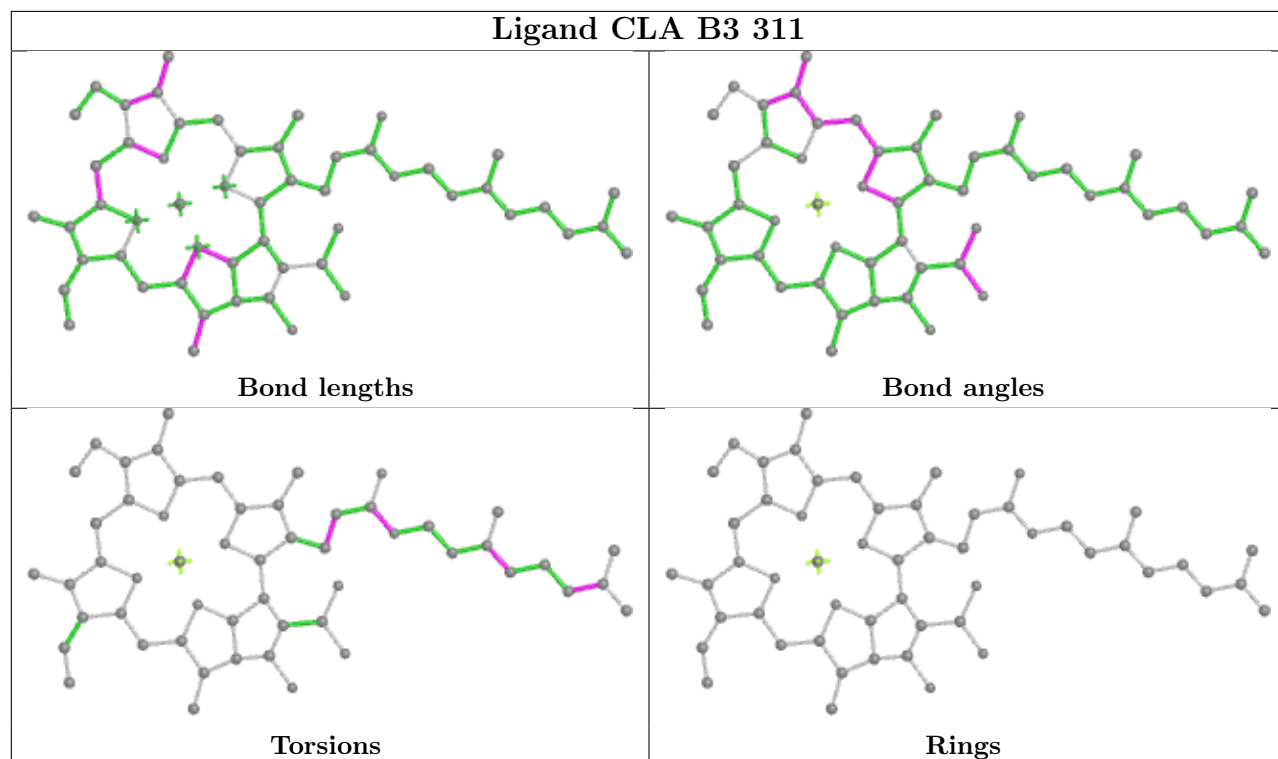
Ligand CLA AB 837



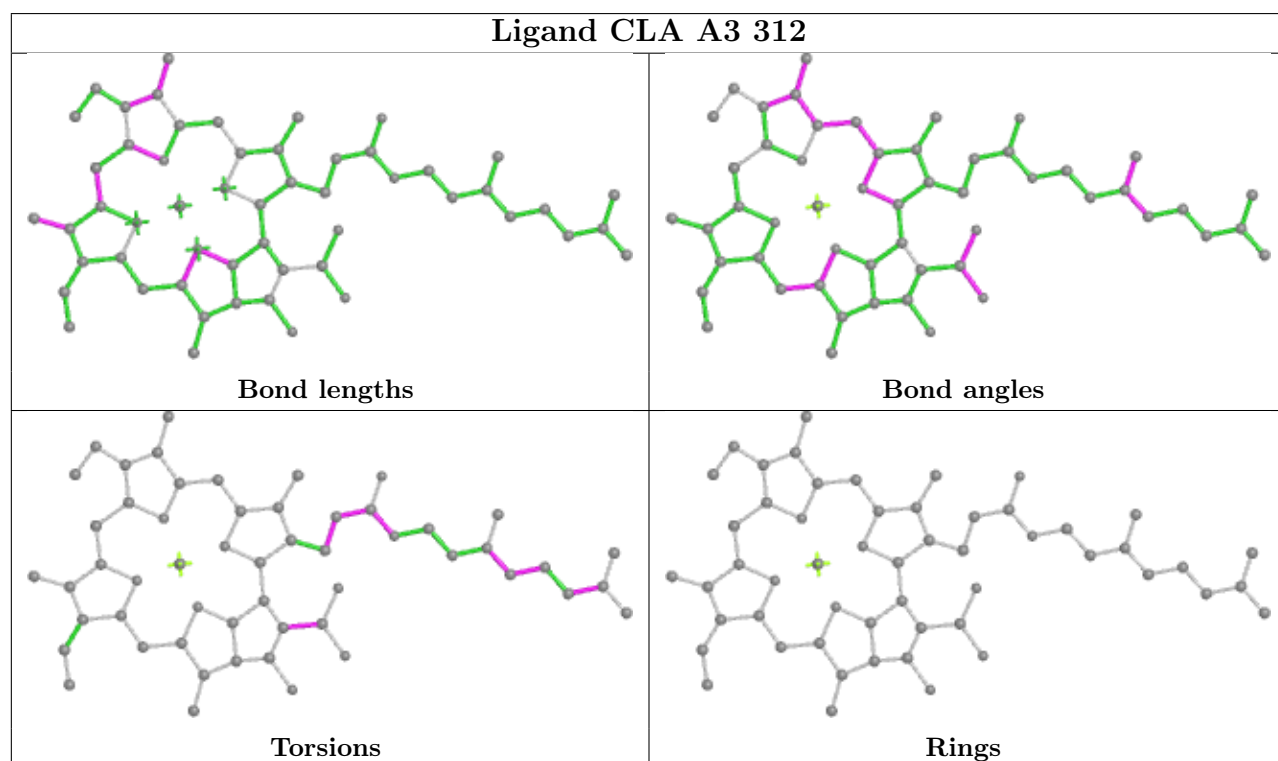
Ligand LMG B5 617

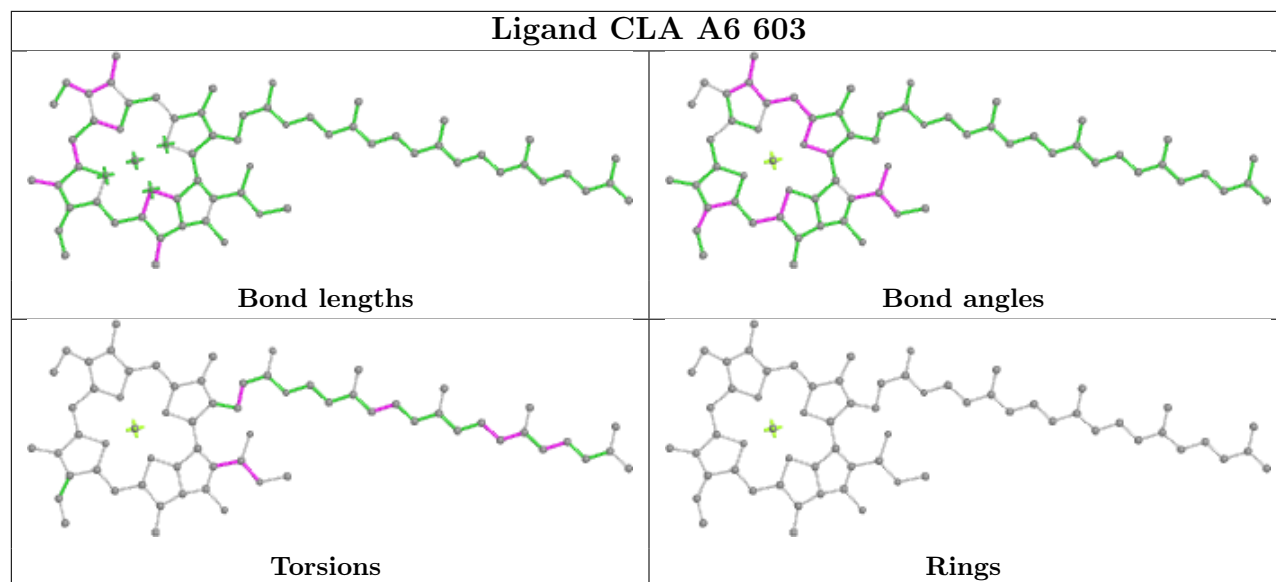
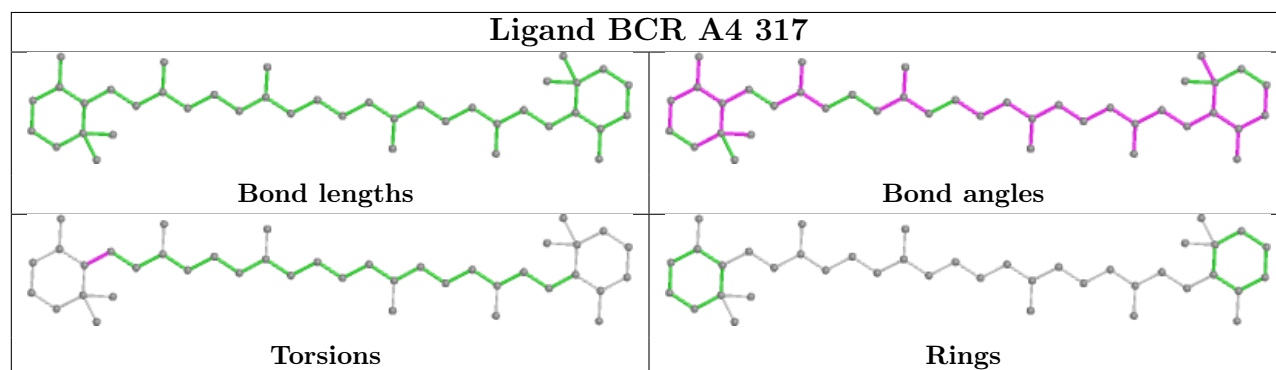
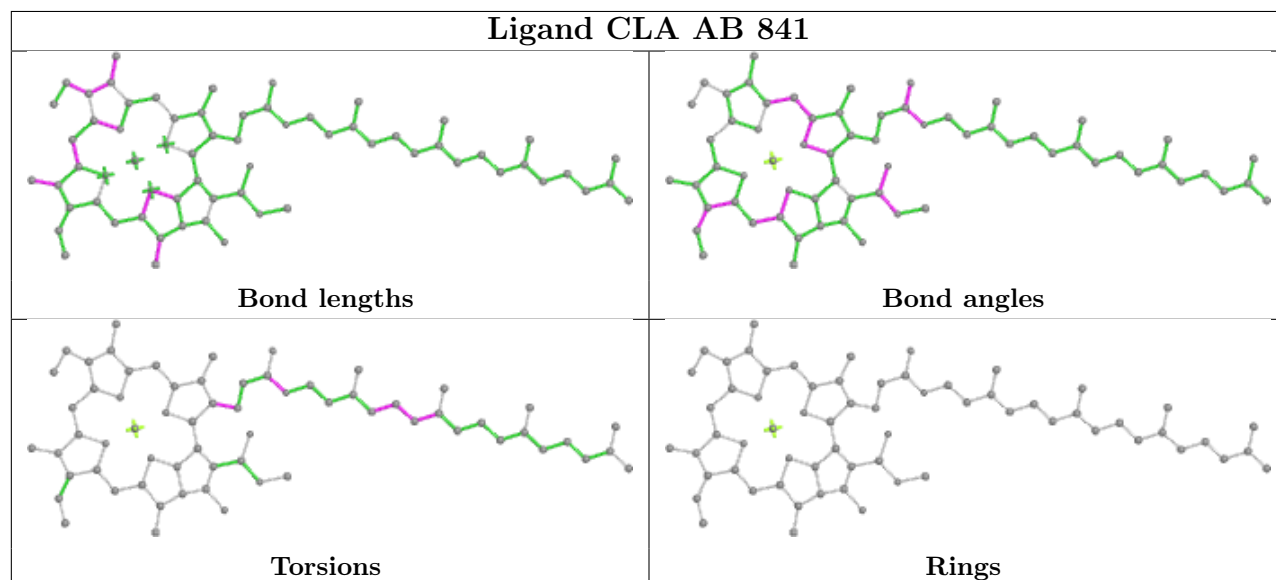


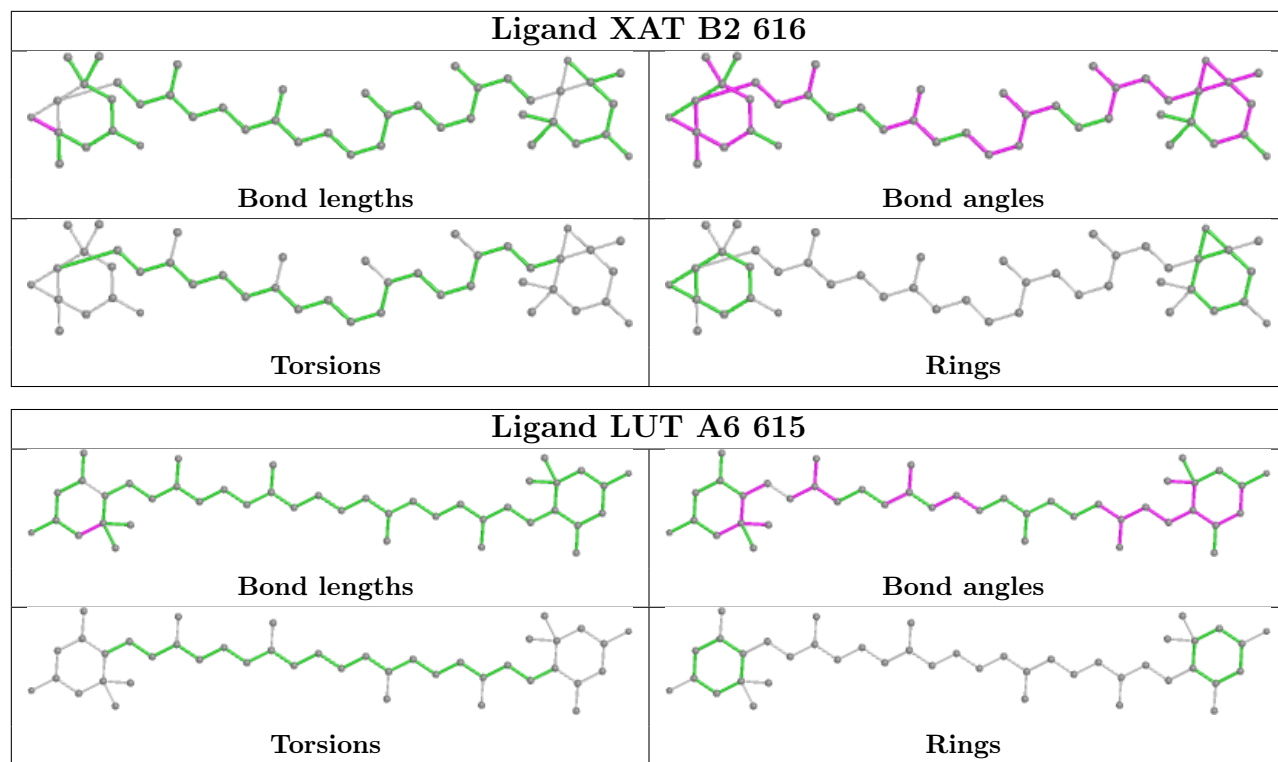
Ligand CLA B3 311



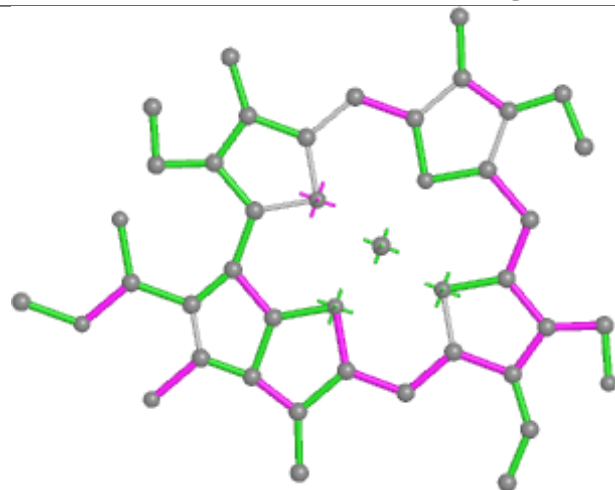
Ligand CLA A3 312



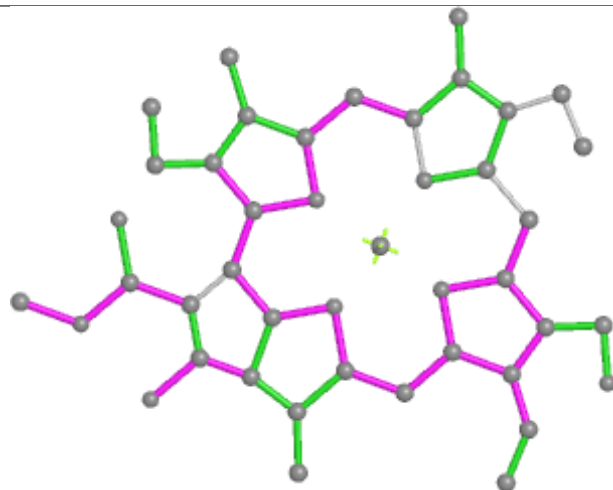
Ligand CLA A6 603**Ligand BCR A4 317****Ligand CLA AB 841**



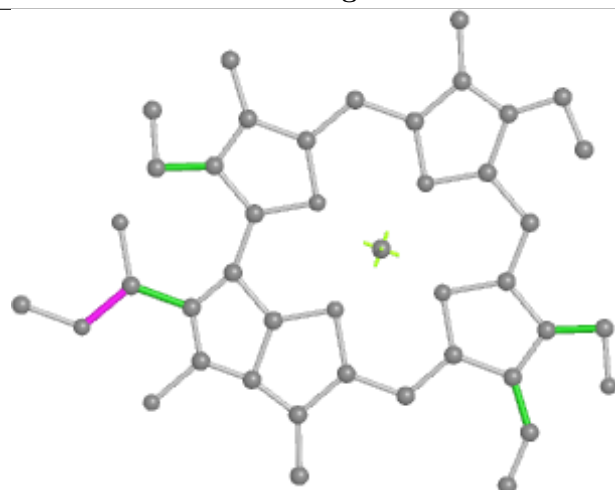
Ligand CHL B2 606



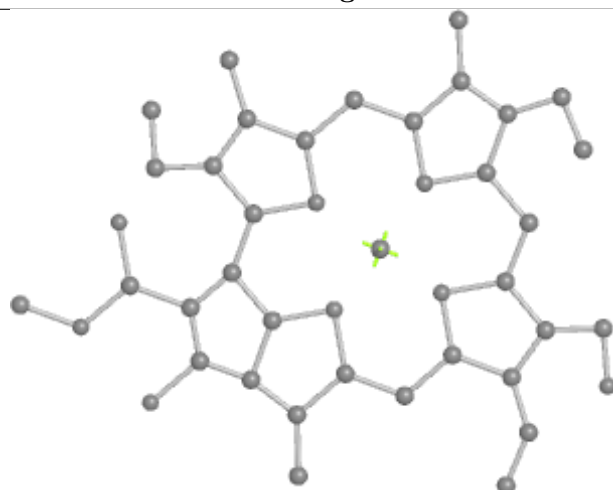
Bond lengths



Bond angles

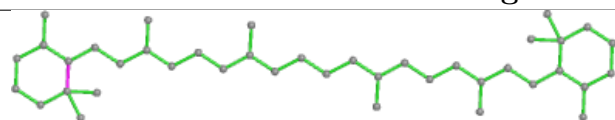


Torsions

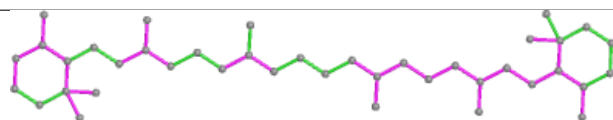


Rings

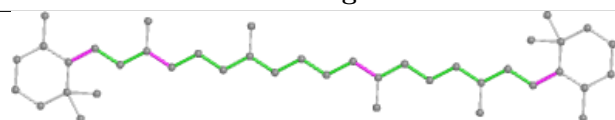
Ligand BCR BA 851



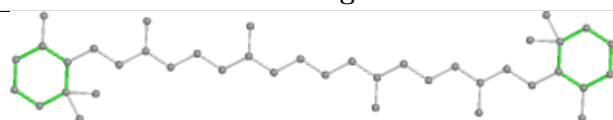
Bond lengths



Bond angles

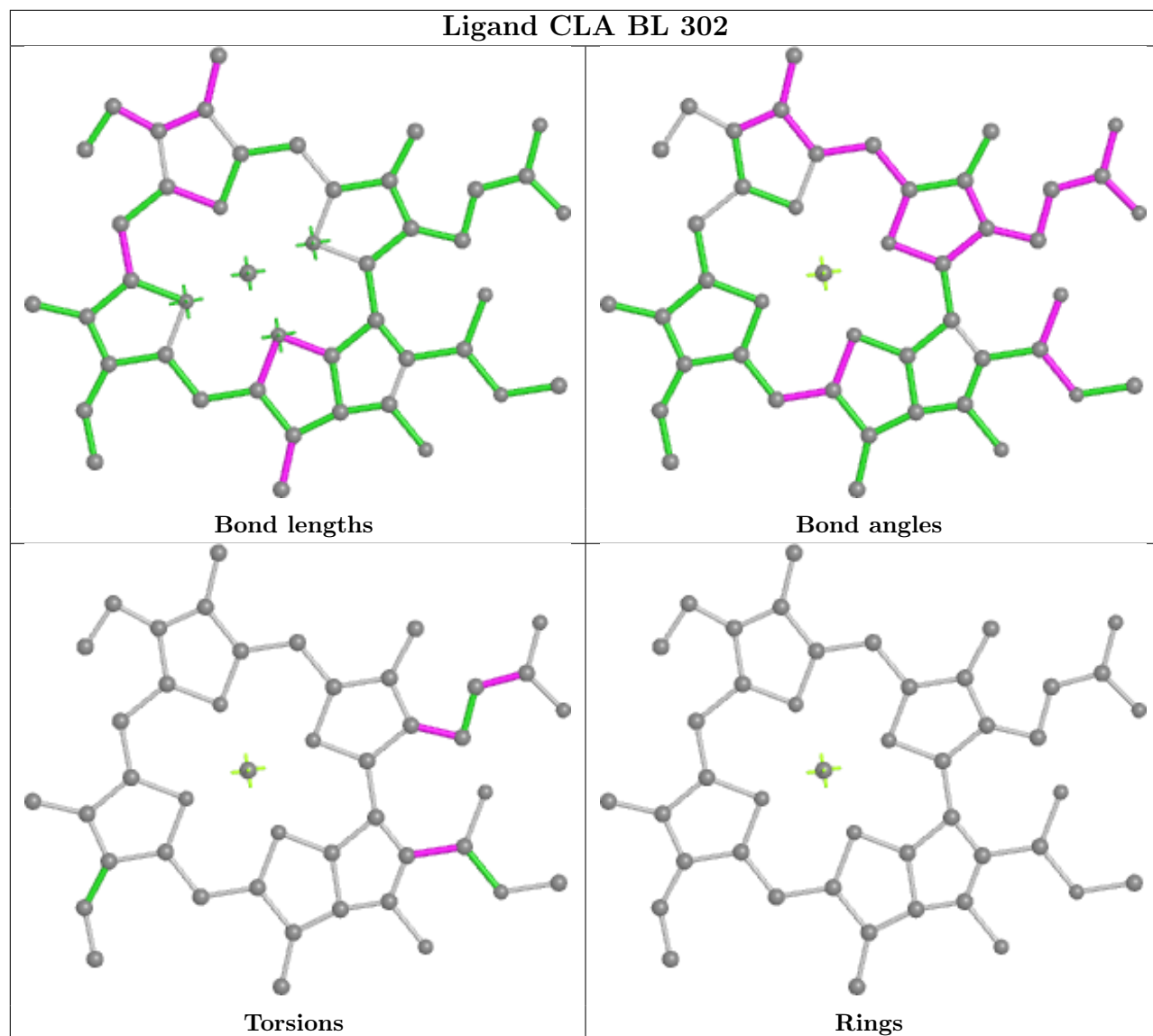


Torsions

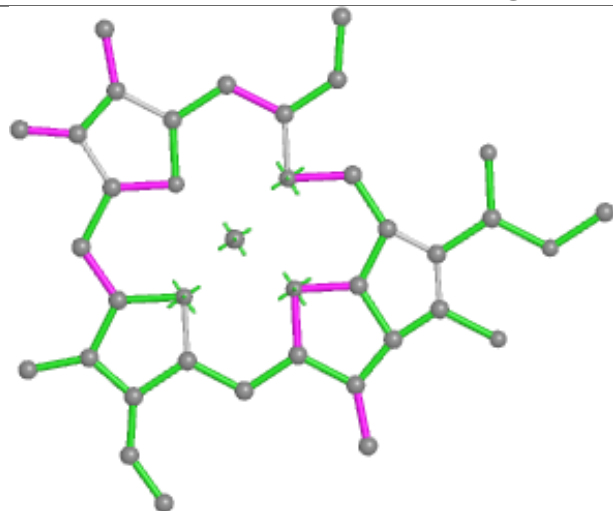


Rings

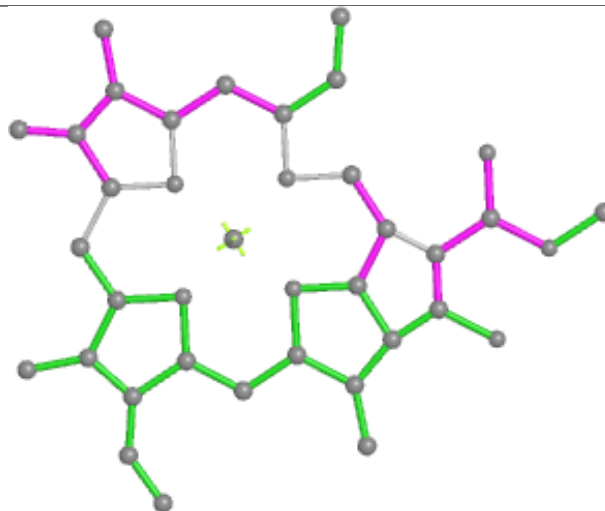
Ligand CLA BL 302



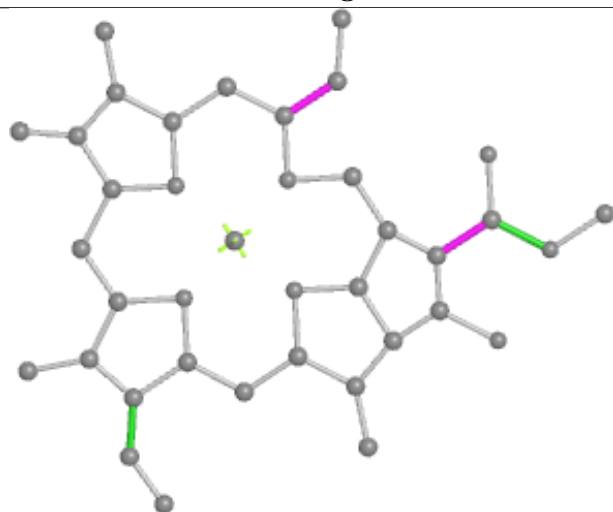
Ligand CLA A6 611



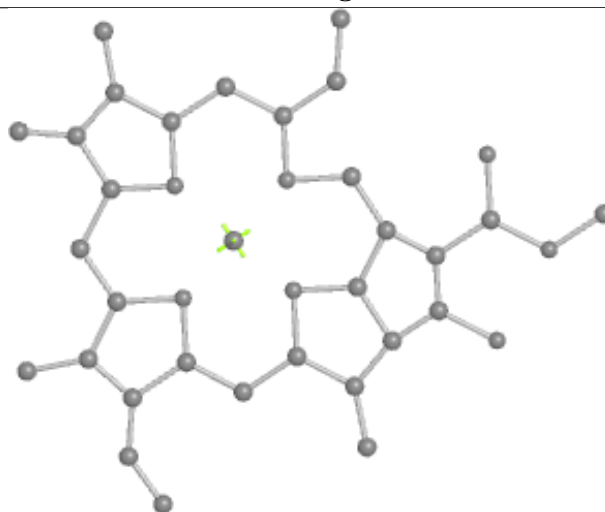
Bond lengths



Bond angles

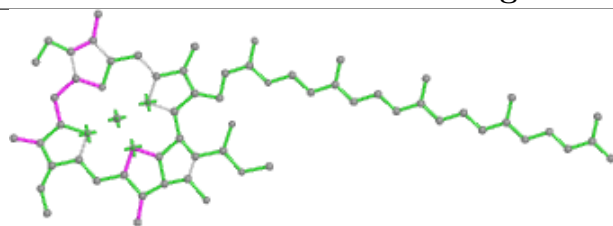


Torsions

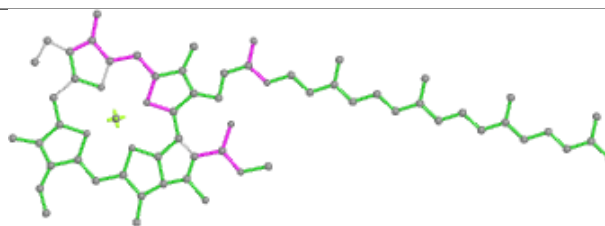


Rings

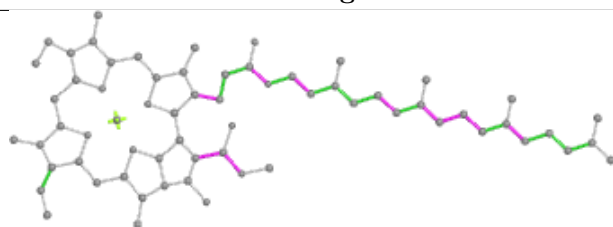
Ligand CLA AA 830



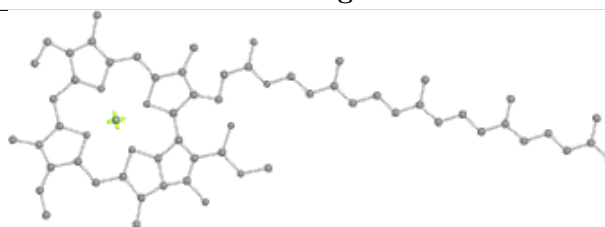
Bond lengths



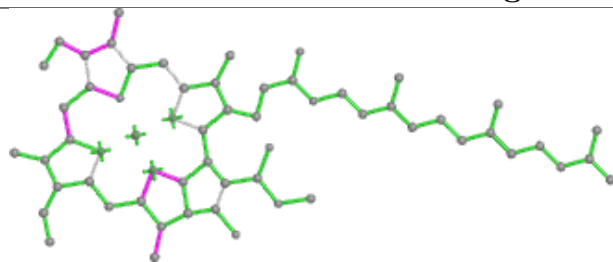
Bond angles



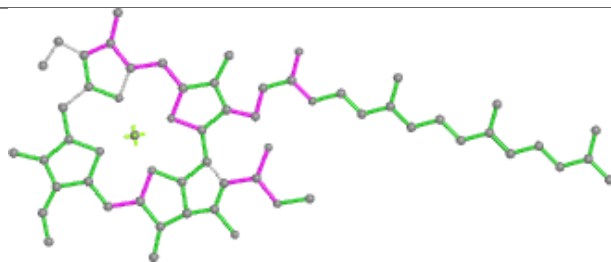
Torsions



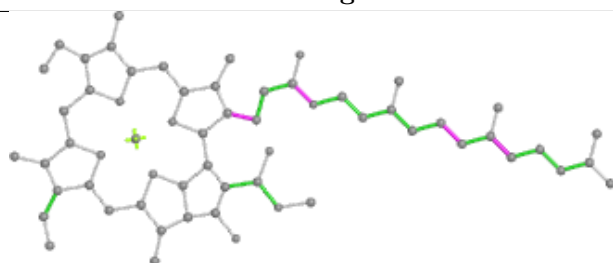
Rings

Ligand CLA BL 303

Bond lengths



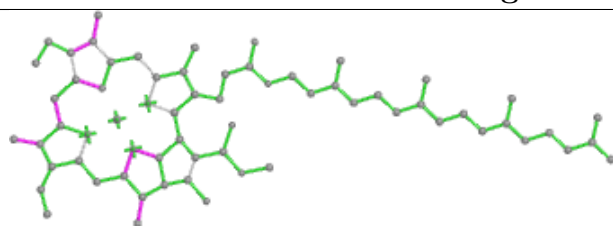
Bond angles



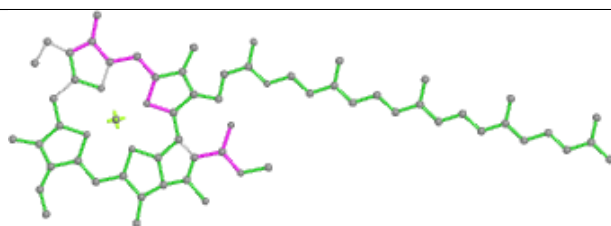
Torsions



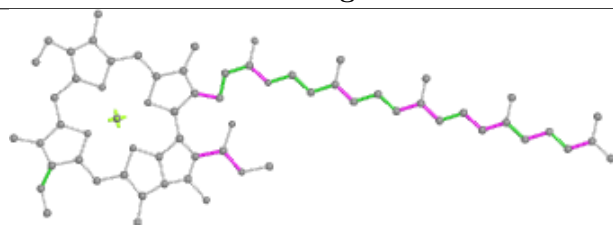
Rings

Ligand CLA AB 803

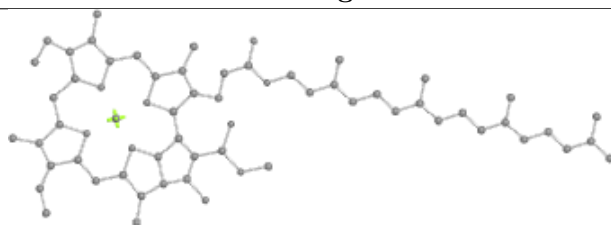
Bond lengths



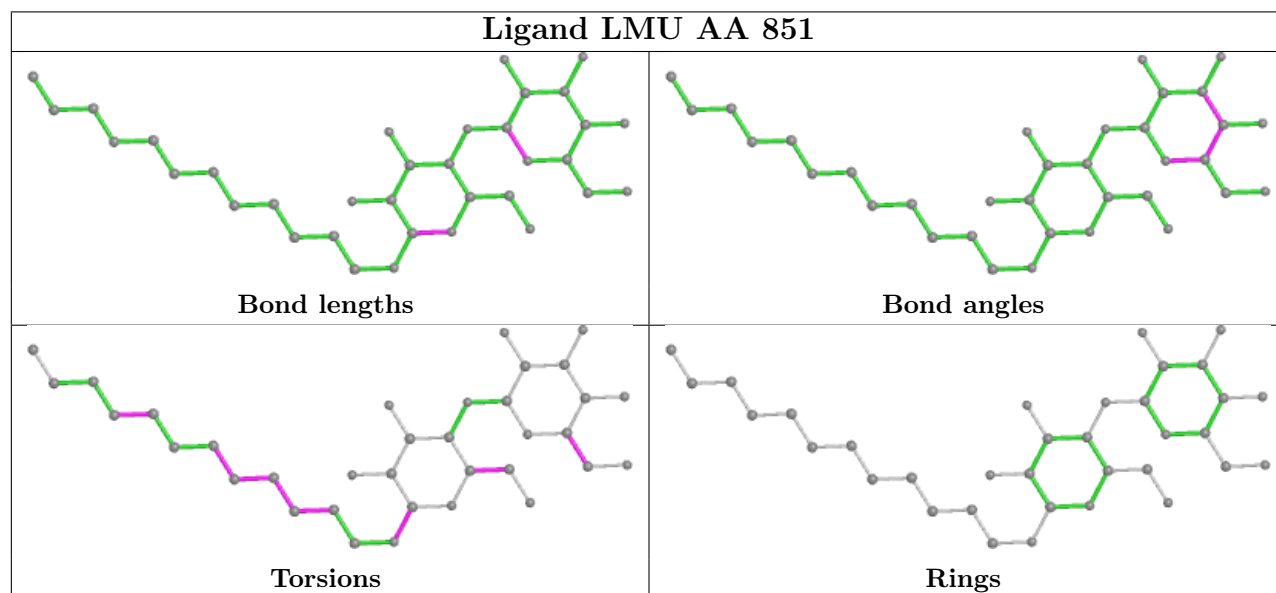
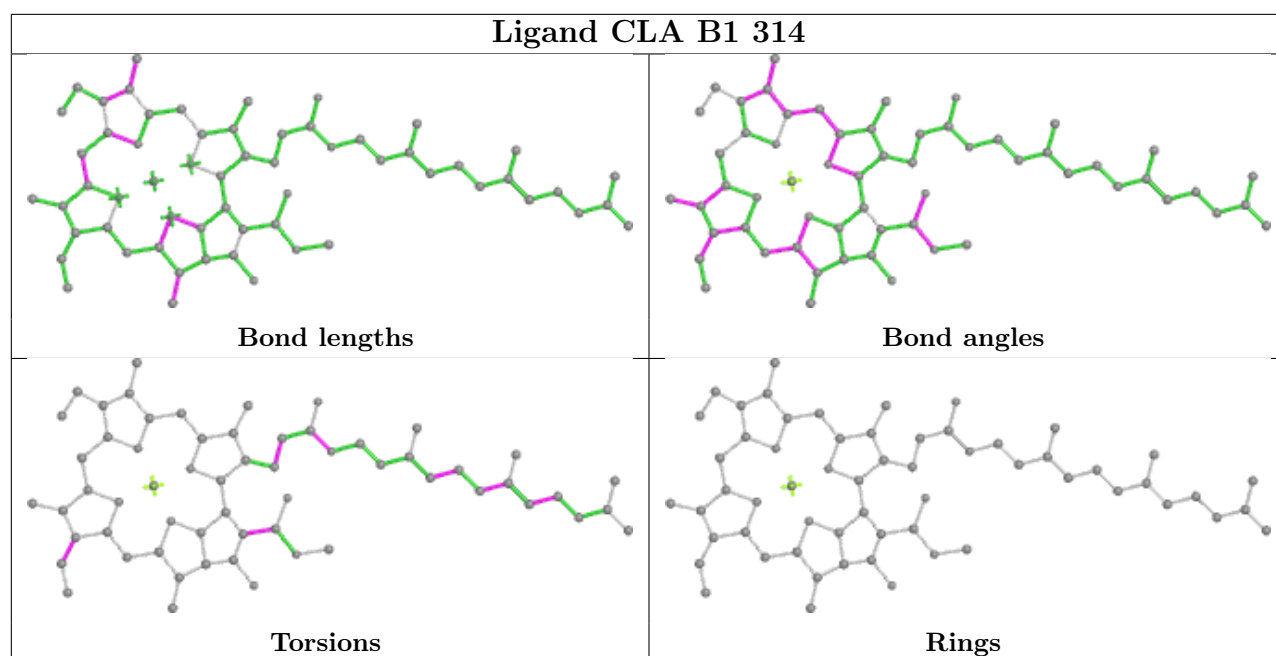
Bond angles

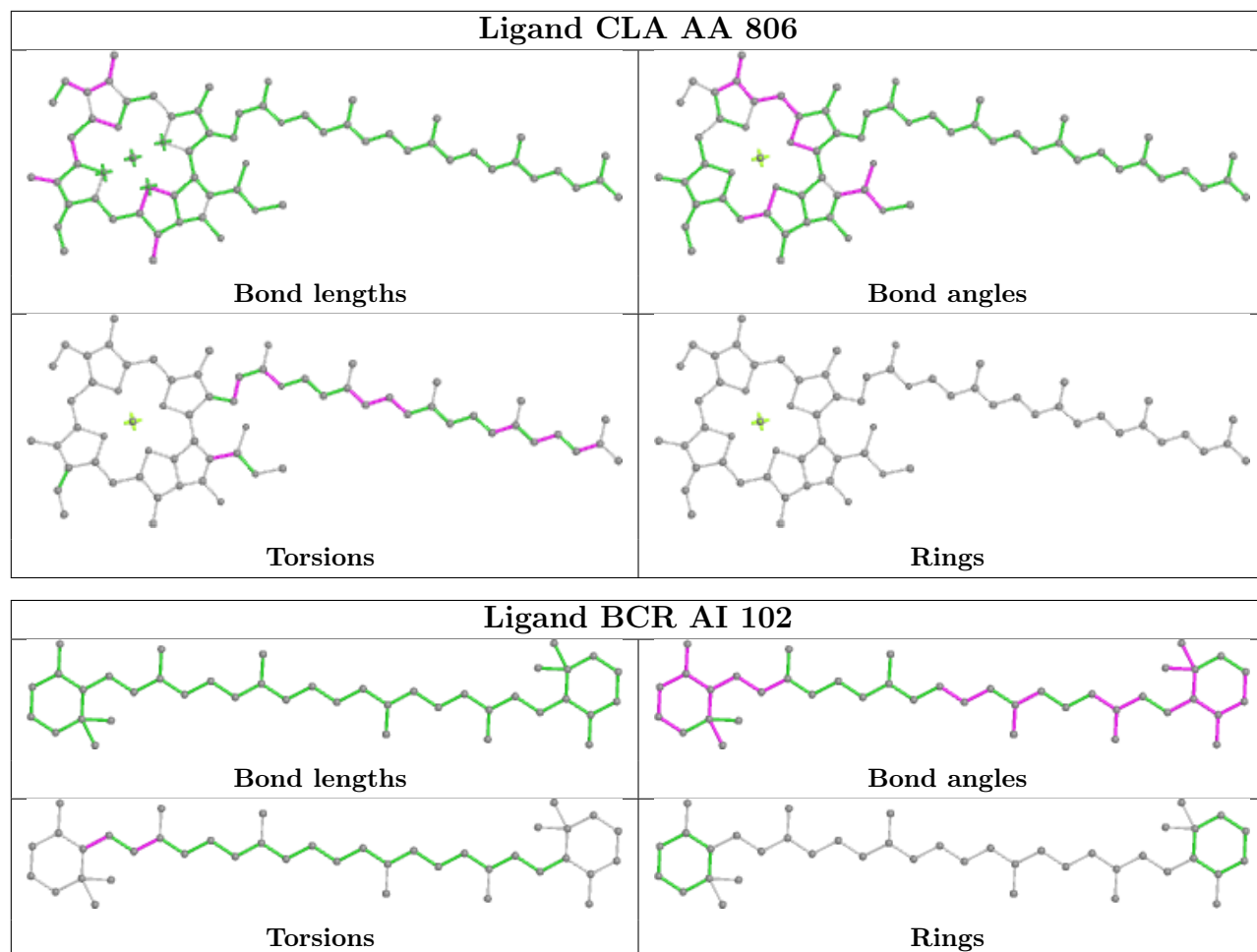


Torsions

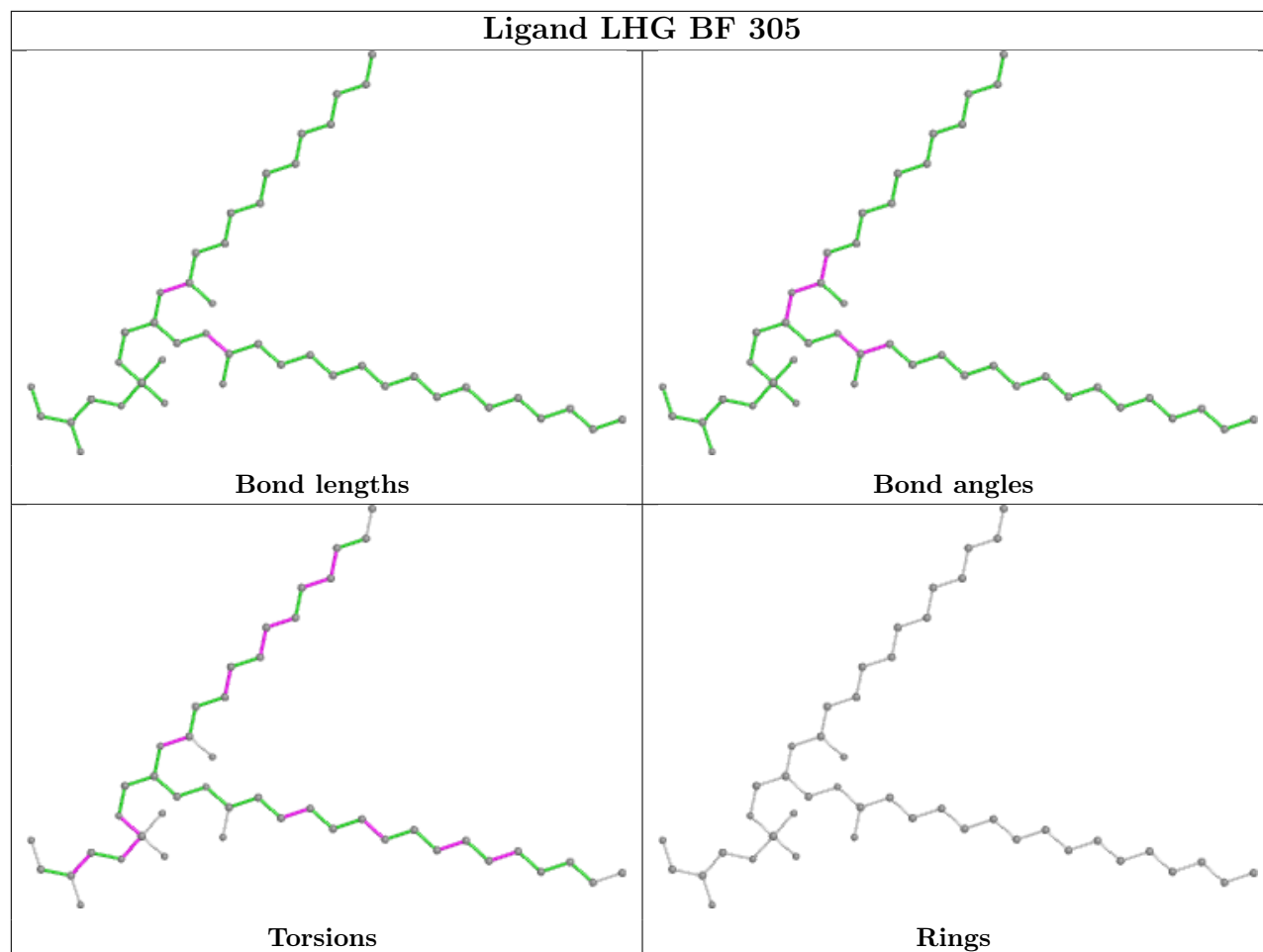


Rings

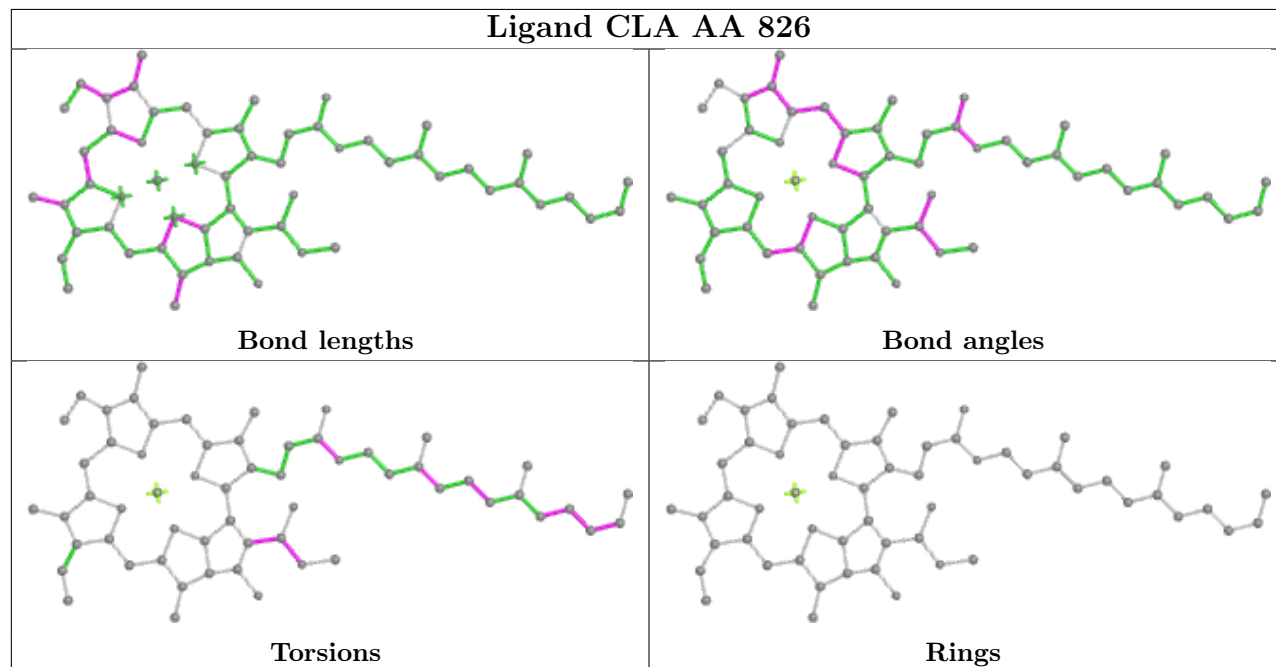


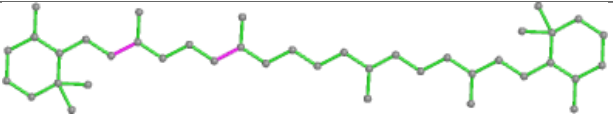
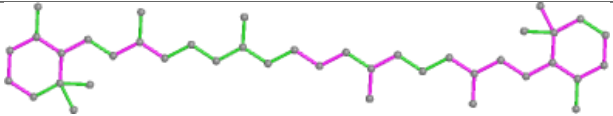
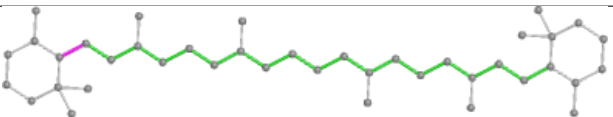
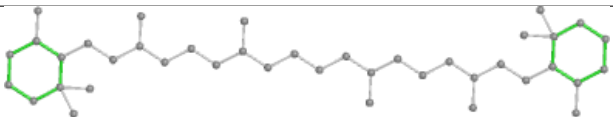
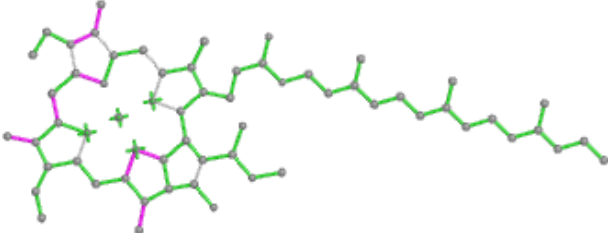
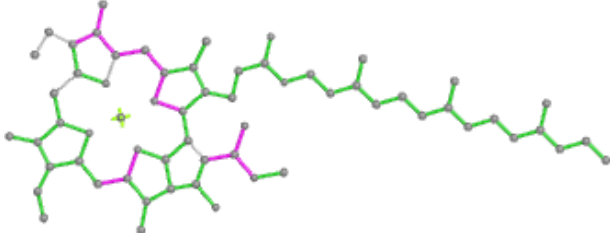
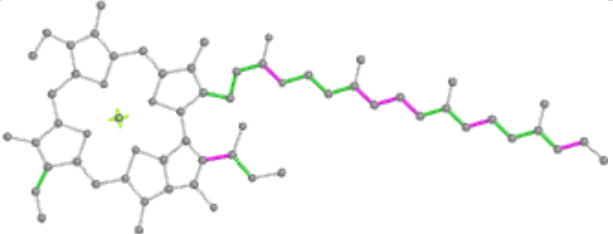
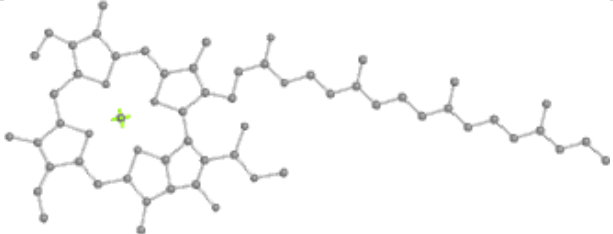
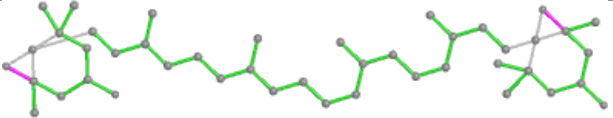
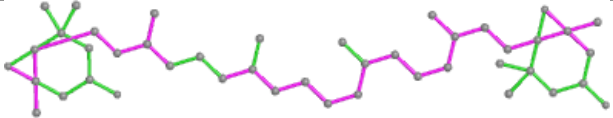
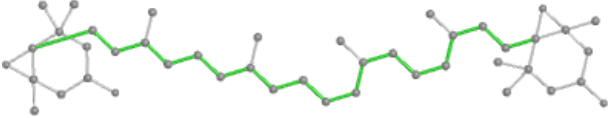
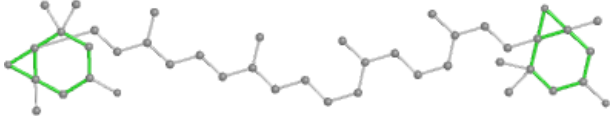


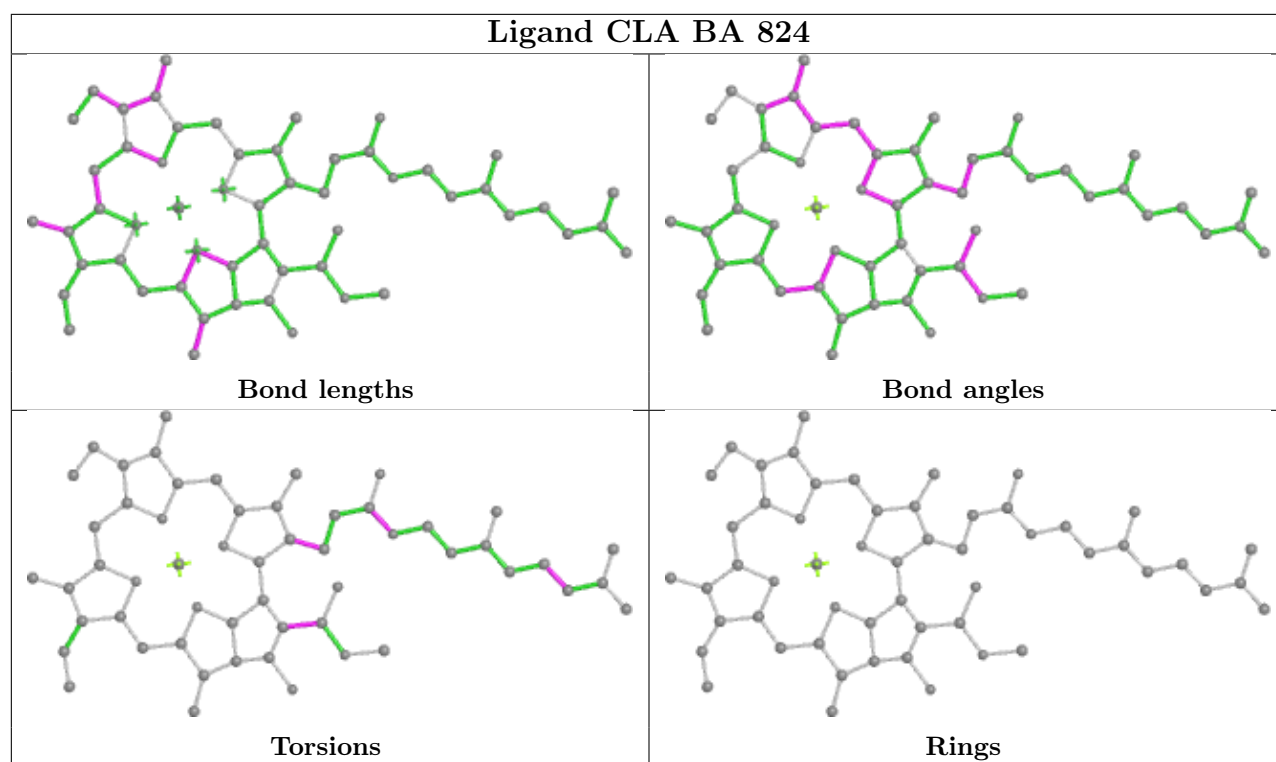
Ligand LHG BF 305



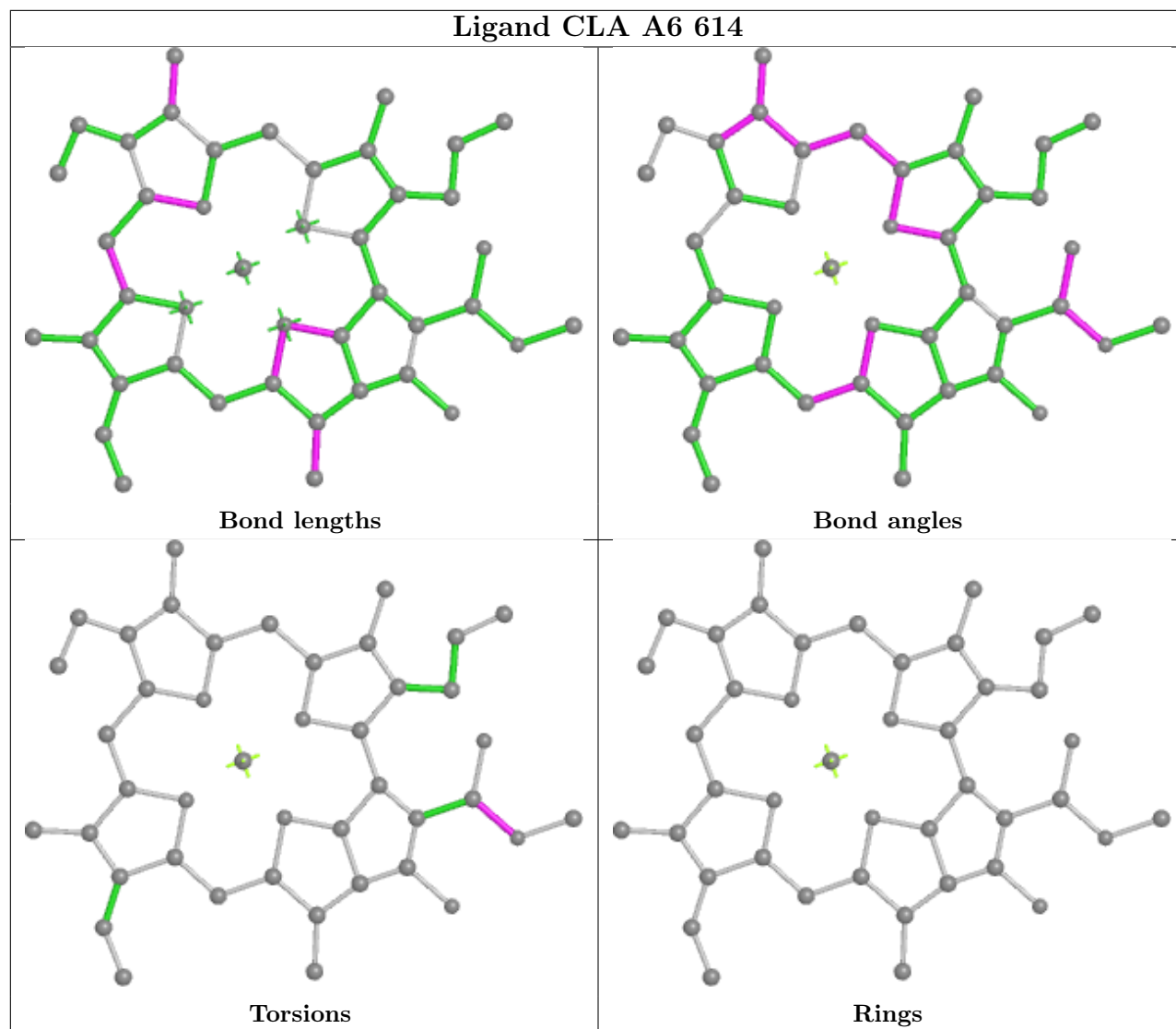
Ligand CLA AA 826



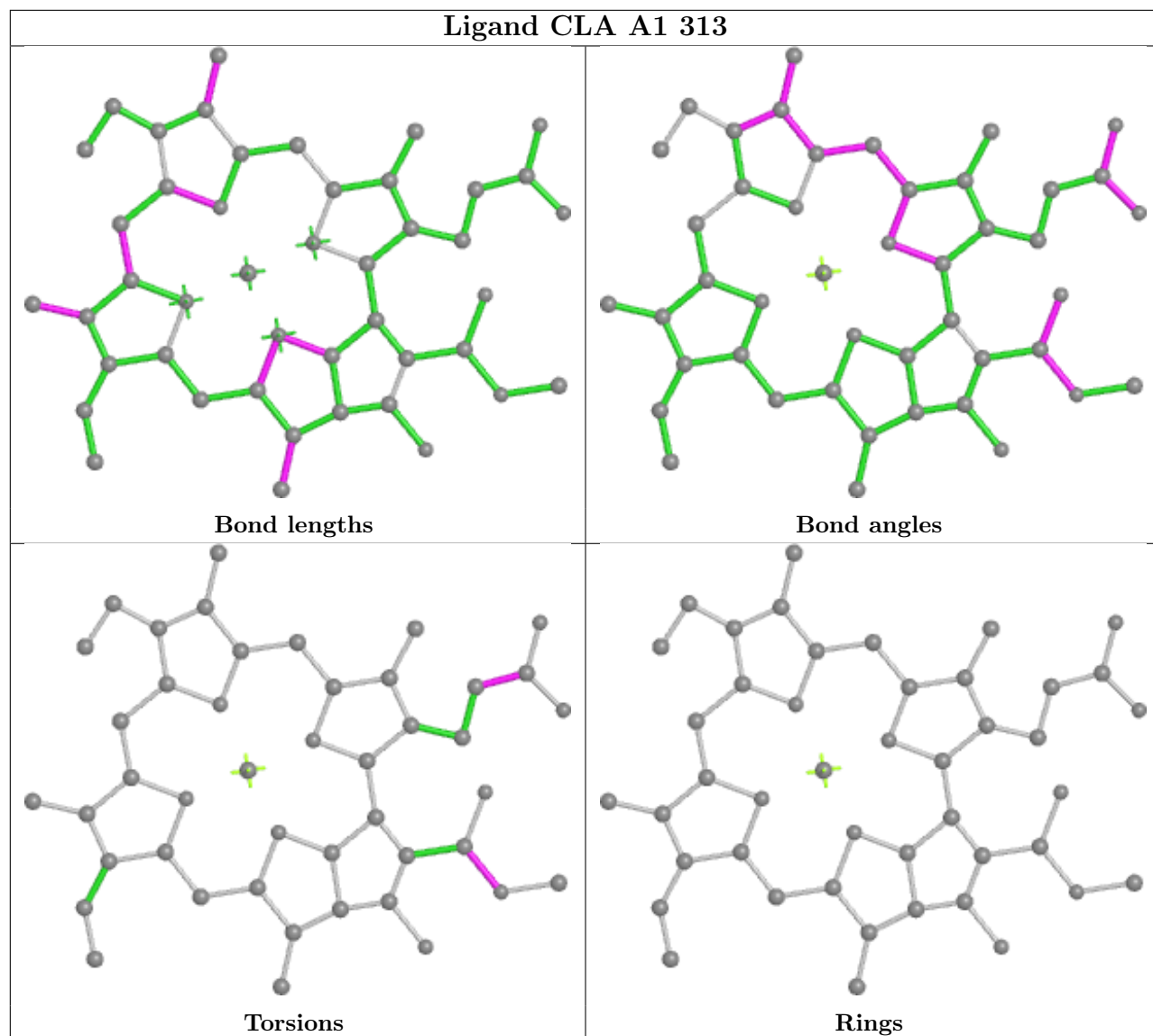
Ligand BCR A6 617	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA BB 827	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand XAT A4 316	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

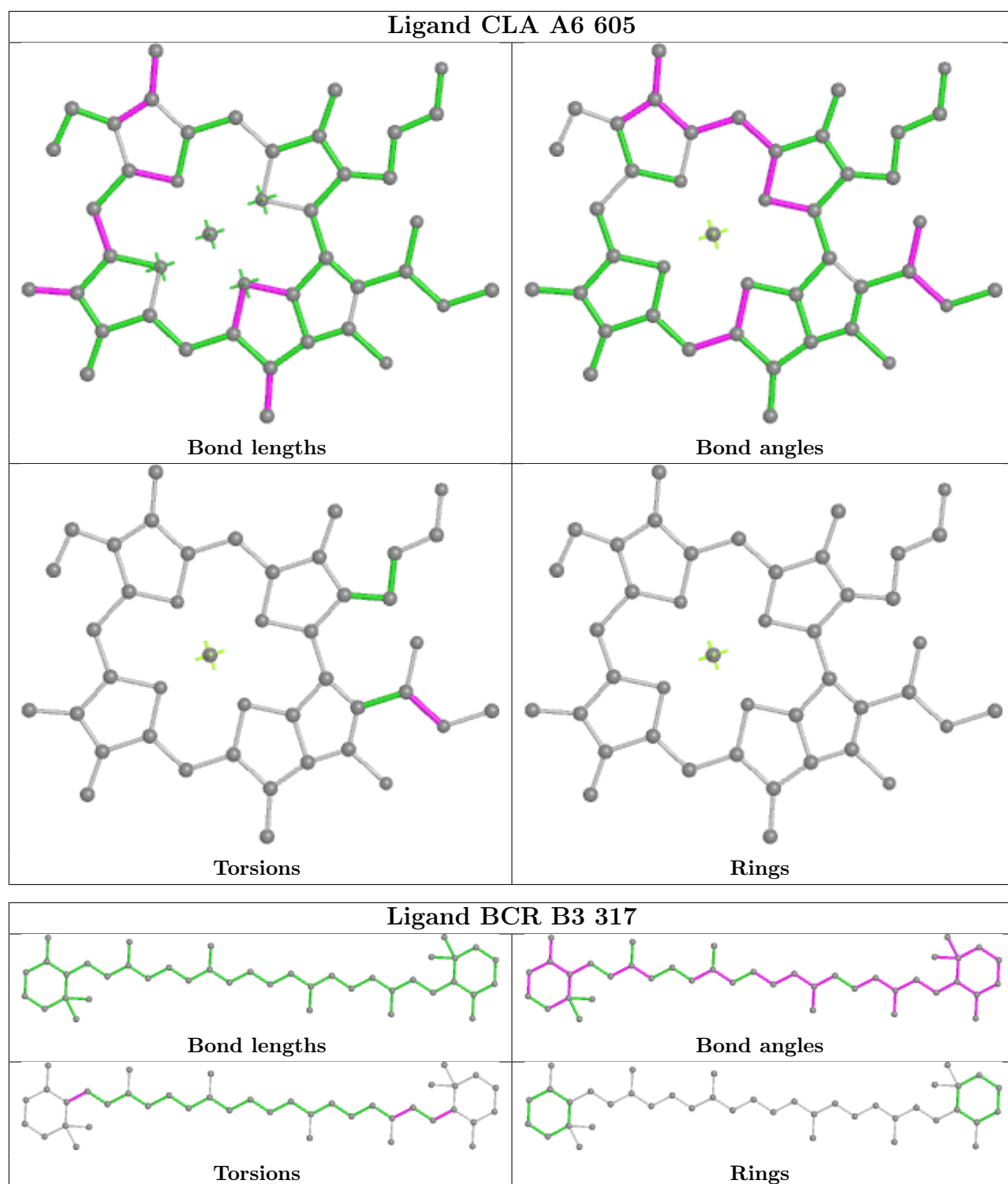


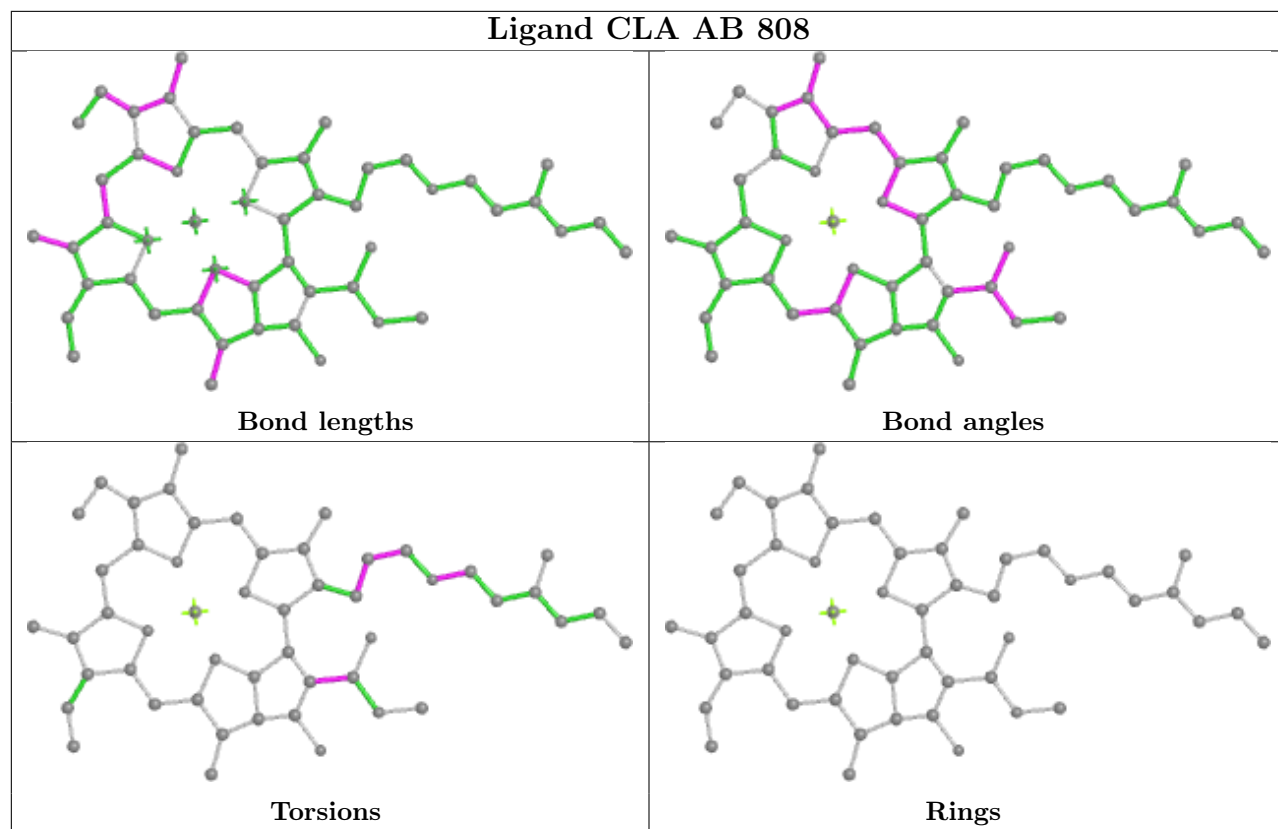
Ligand CLA A6 614



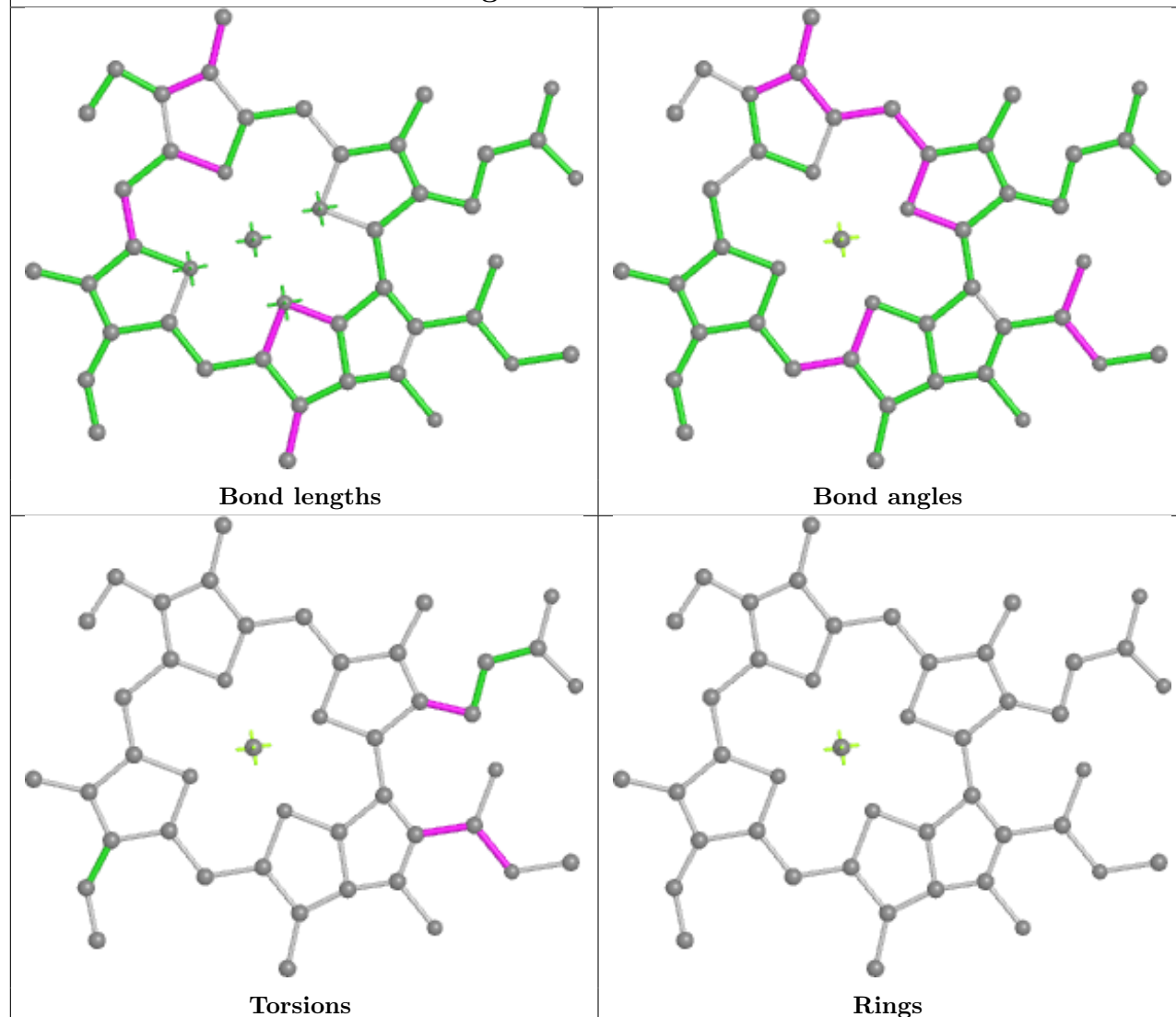
Ligand CLA A1 313



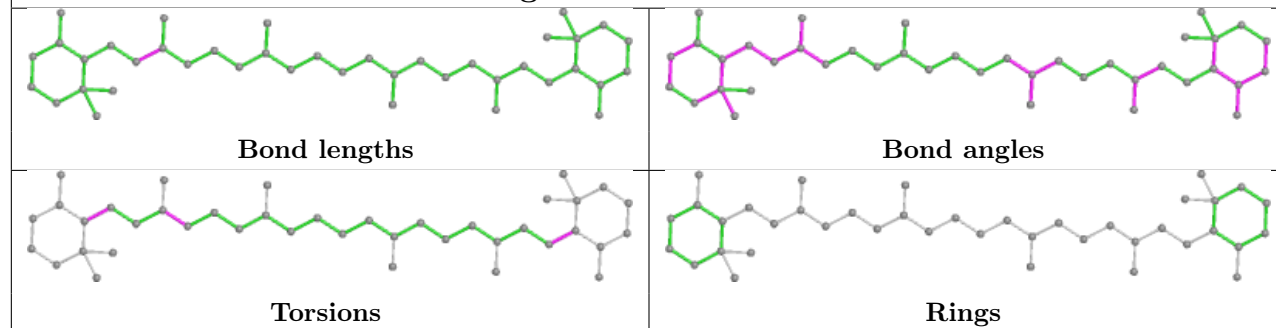


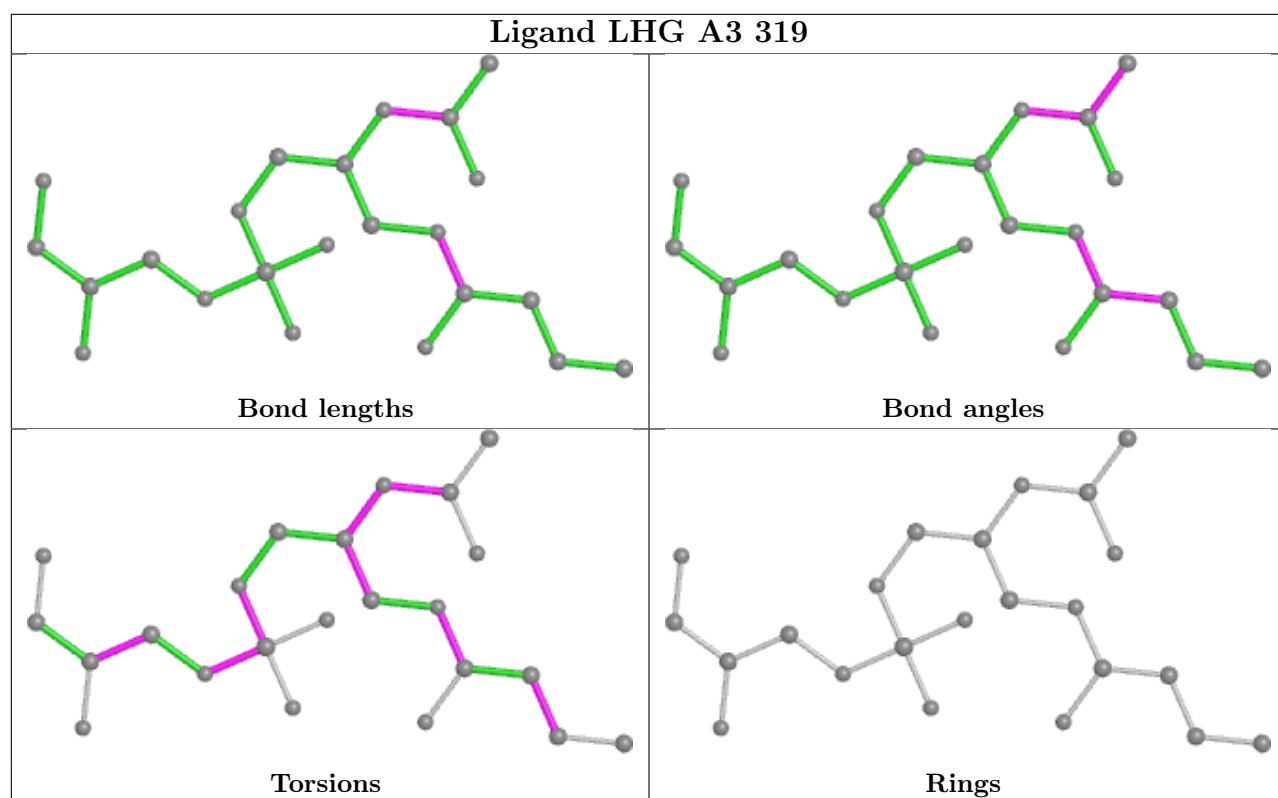


Ligand CLA A4 312

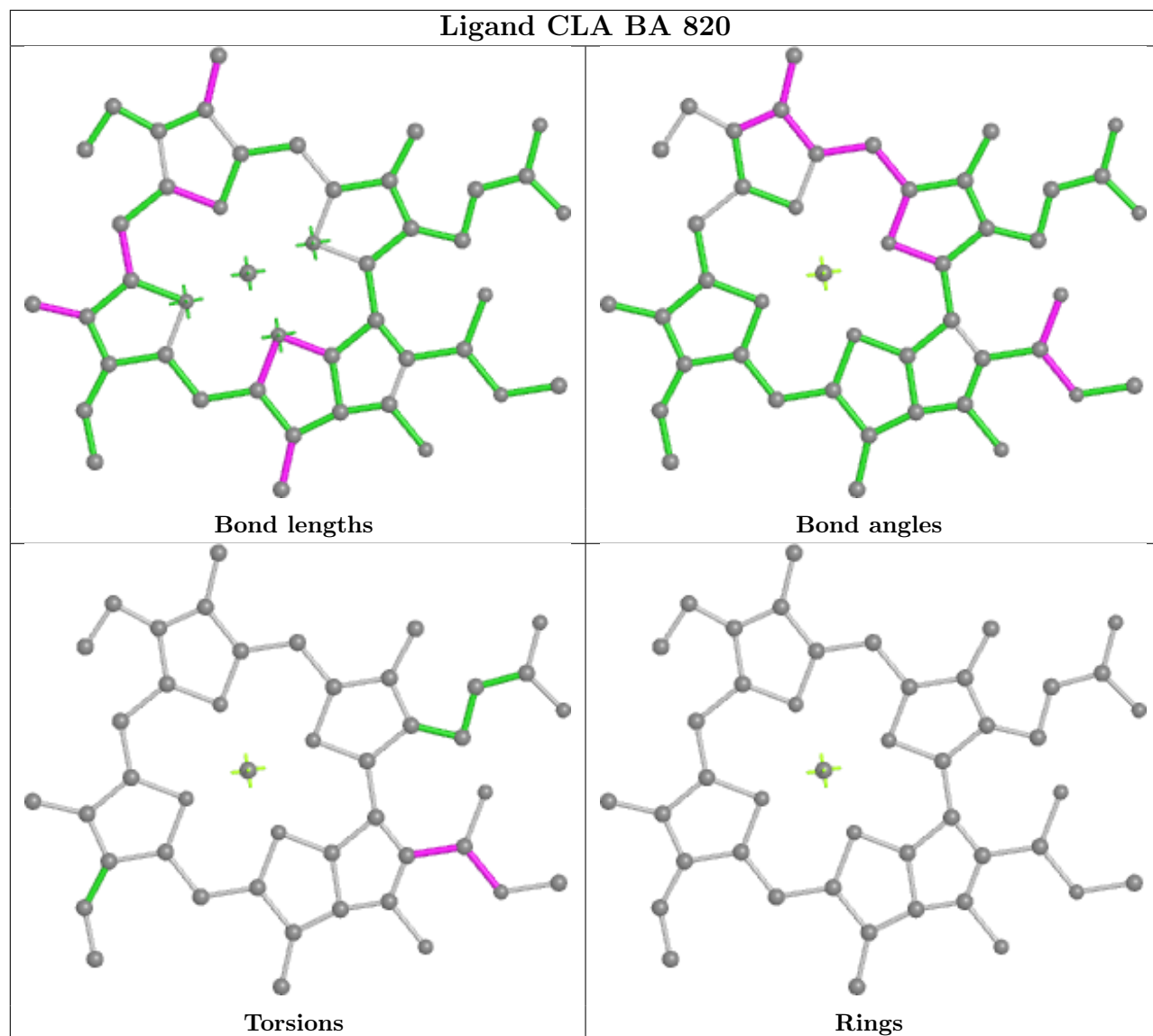


Ligand BCR BL 301

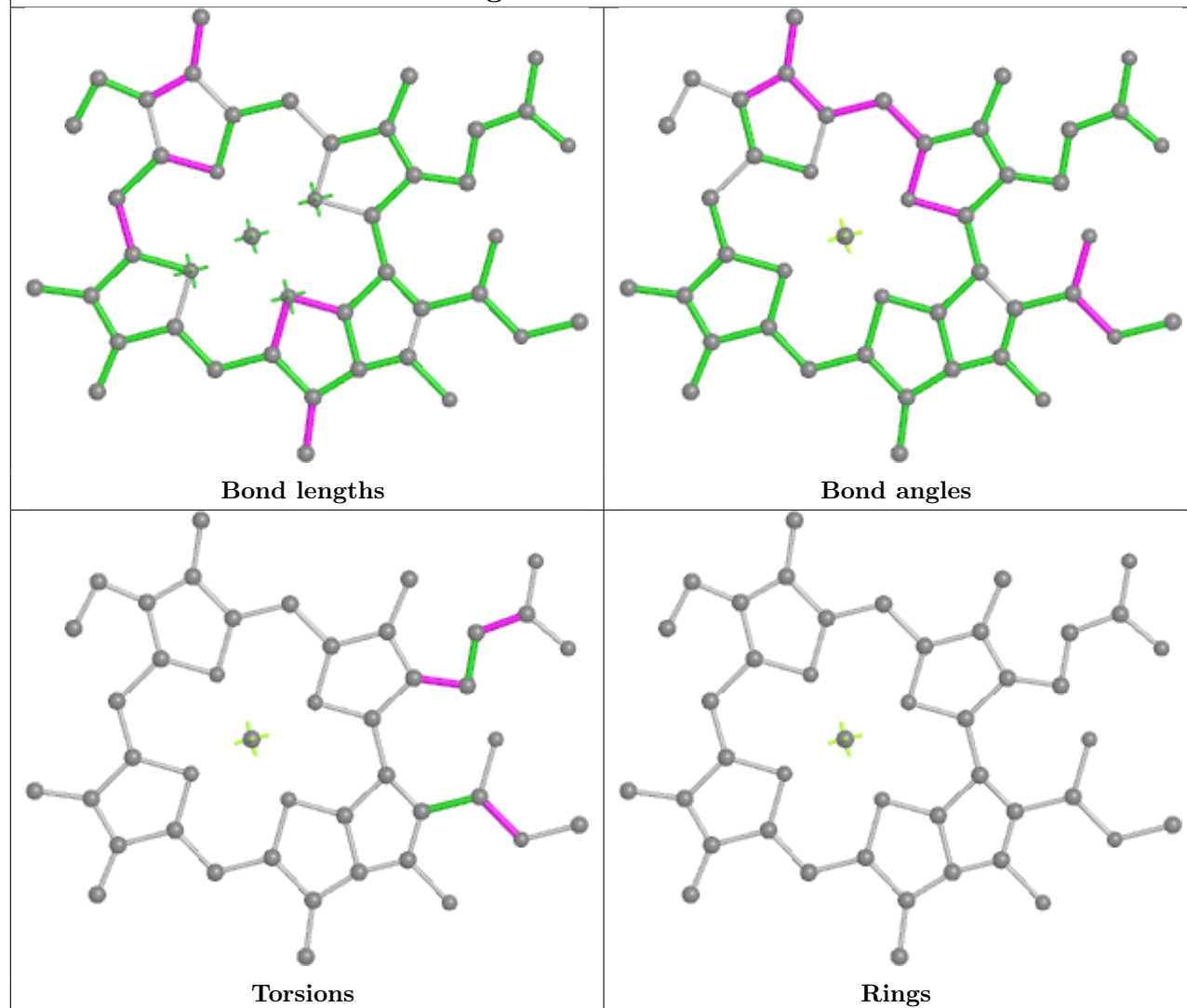




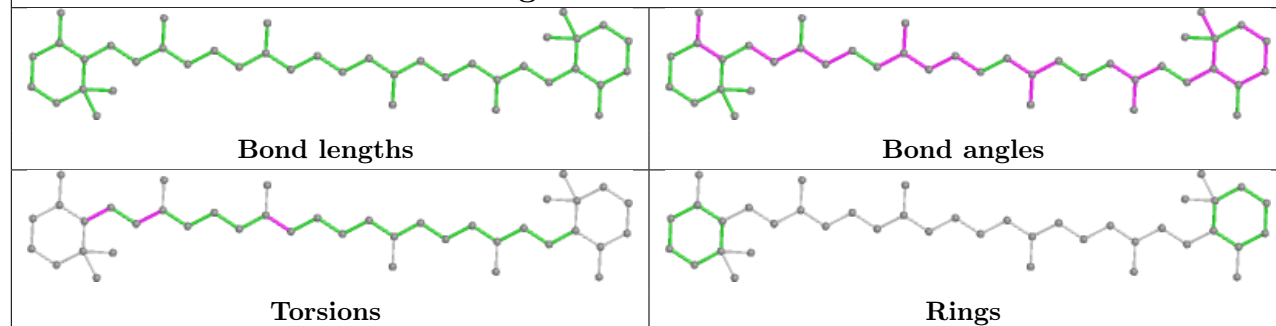
Ligand CLA BA 820

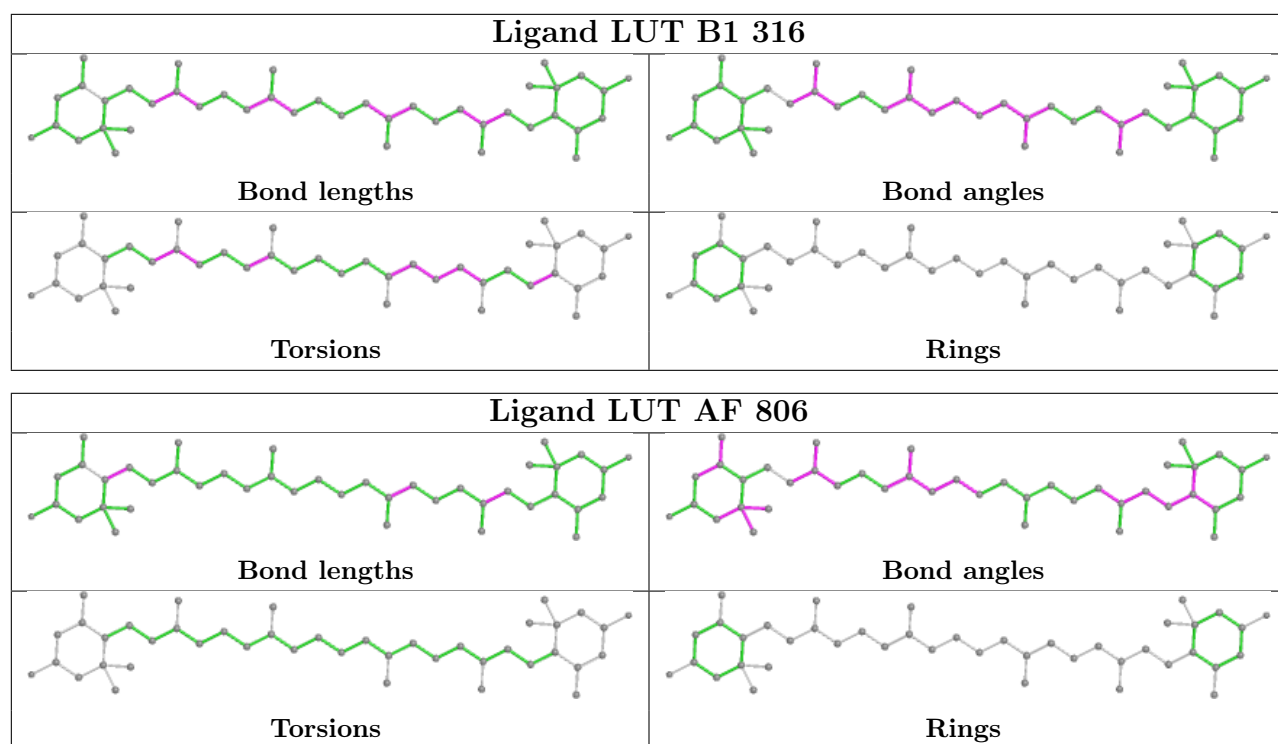


Ligand CLA A6 612

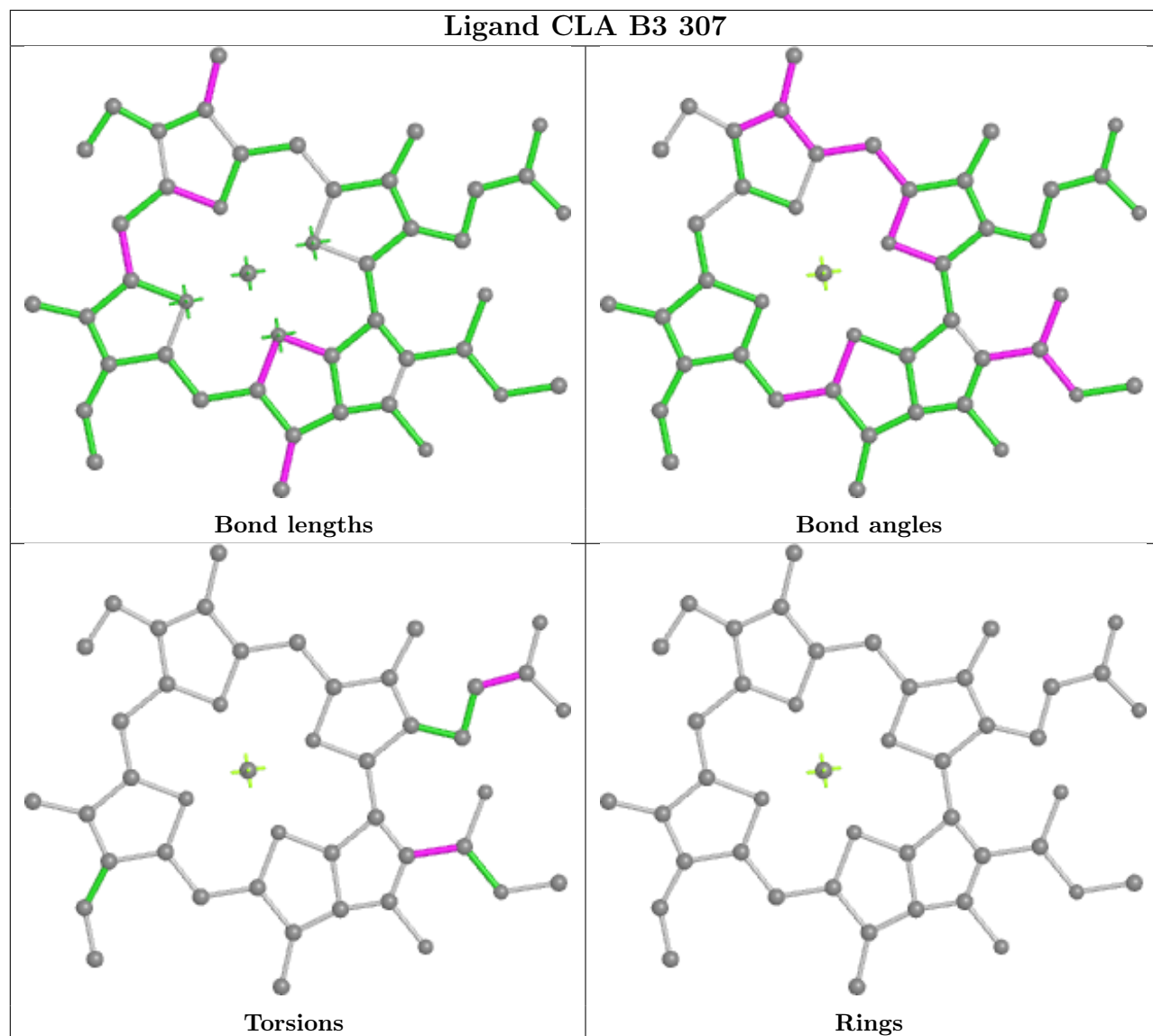


Ligand BCR AF 805

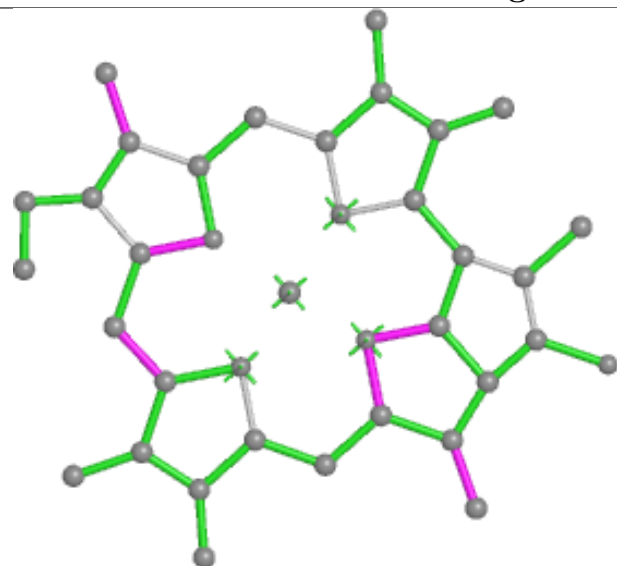




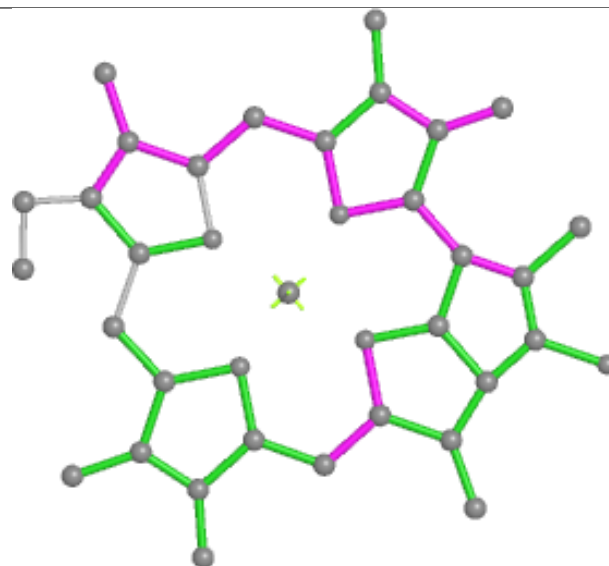
Ligand CLA B3 307



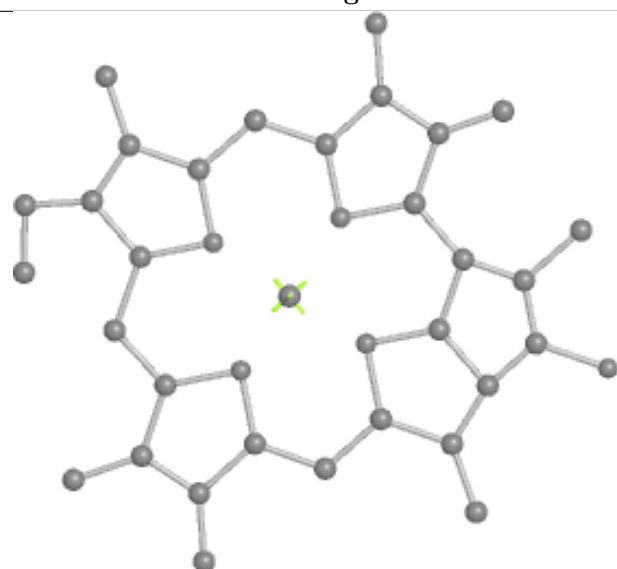
Ligand CLA A3 310



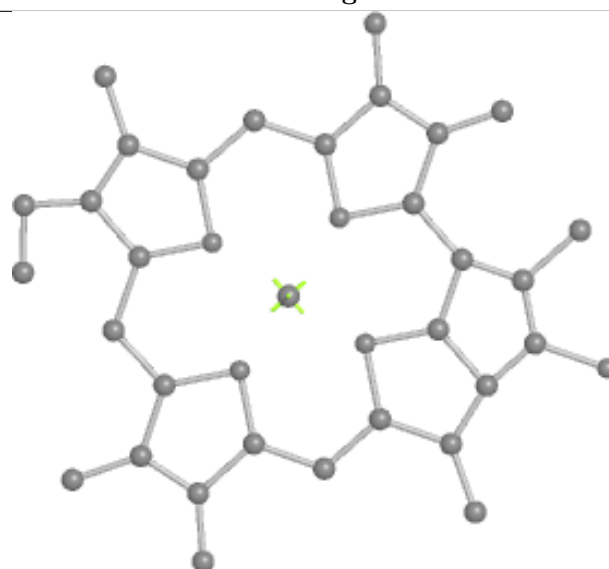
Bond lengths



Bond angles

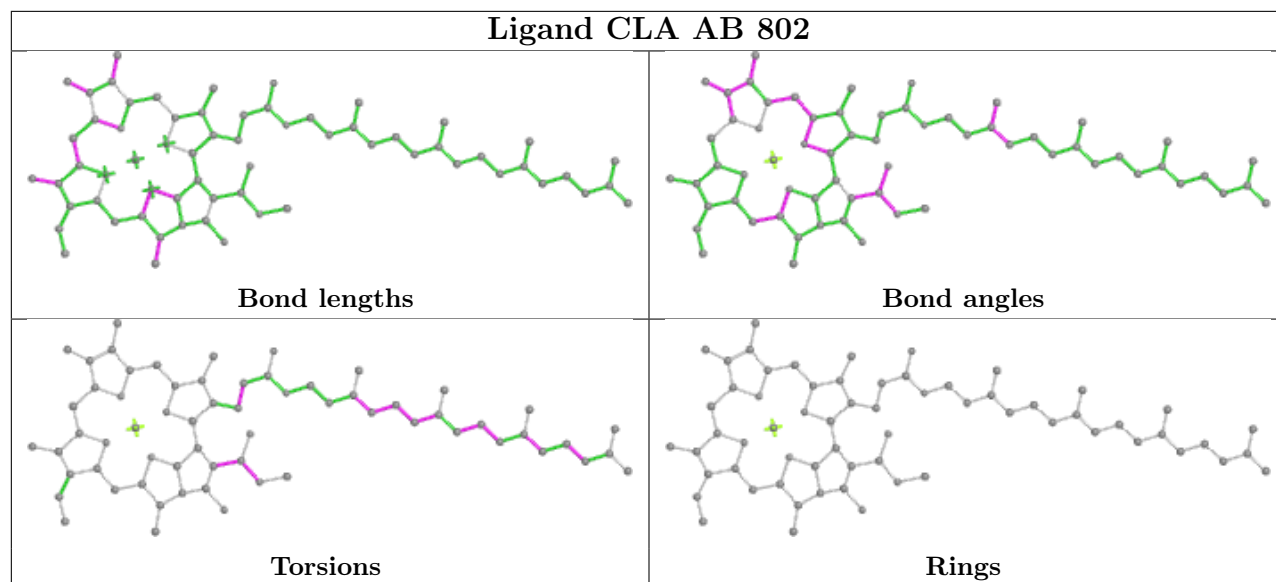


Torsions

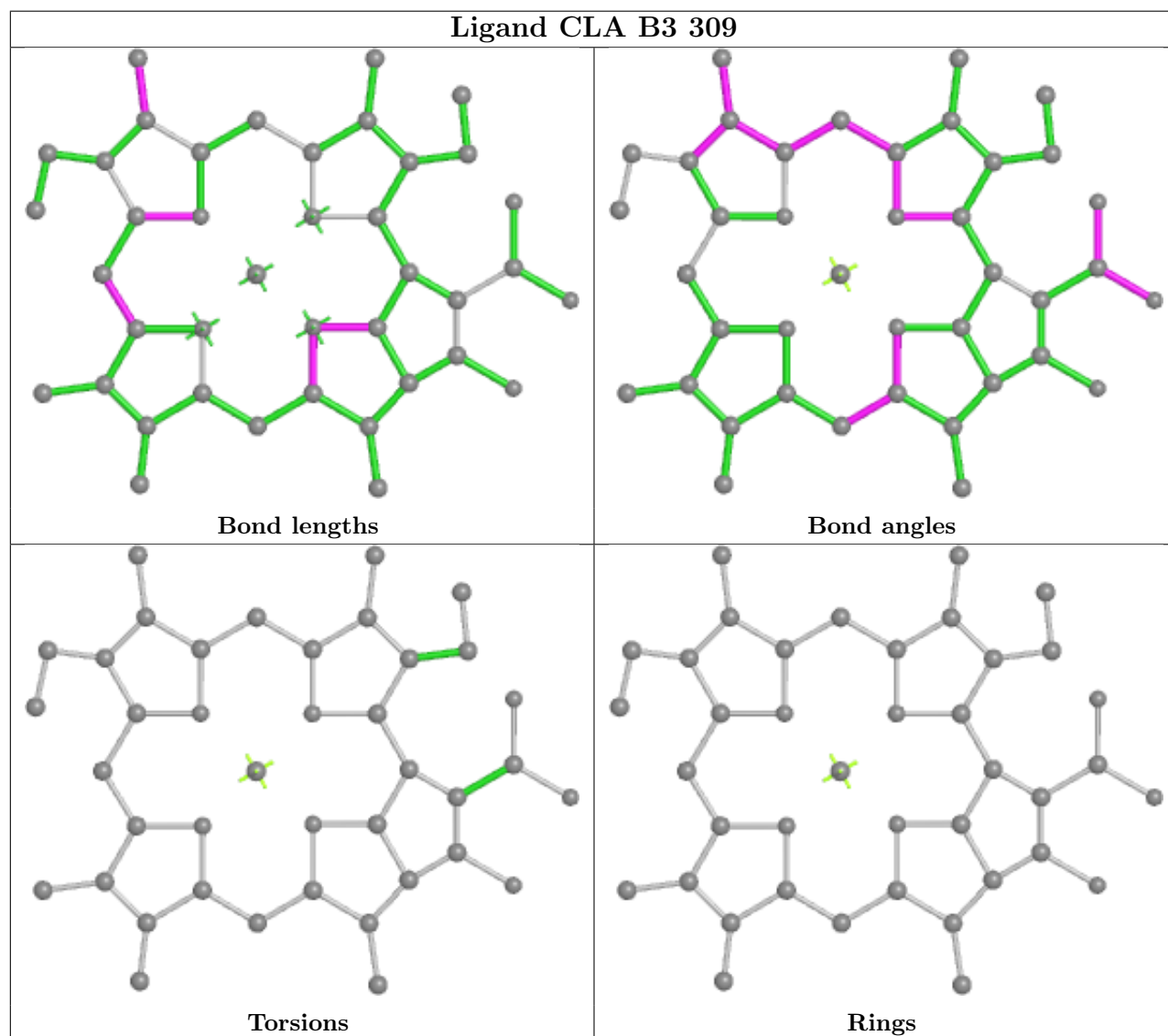


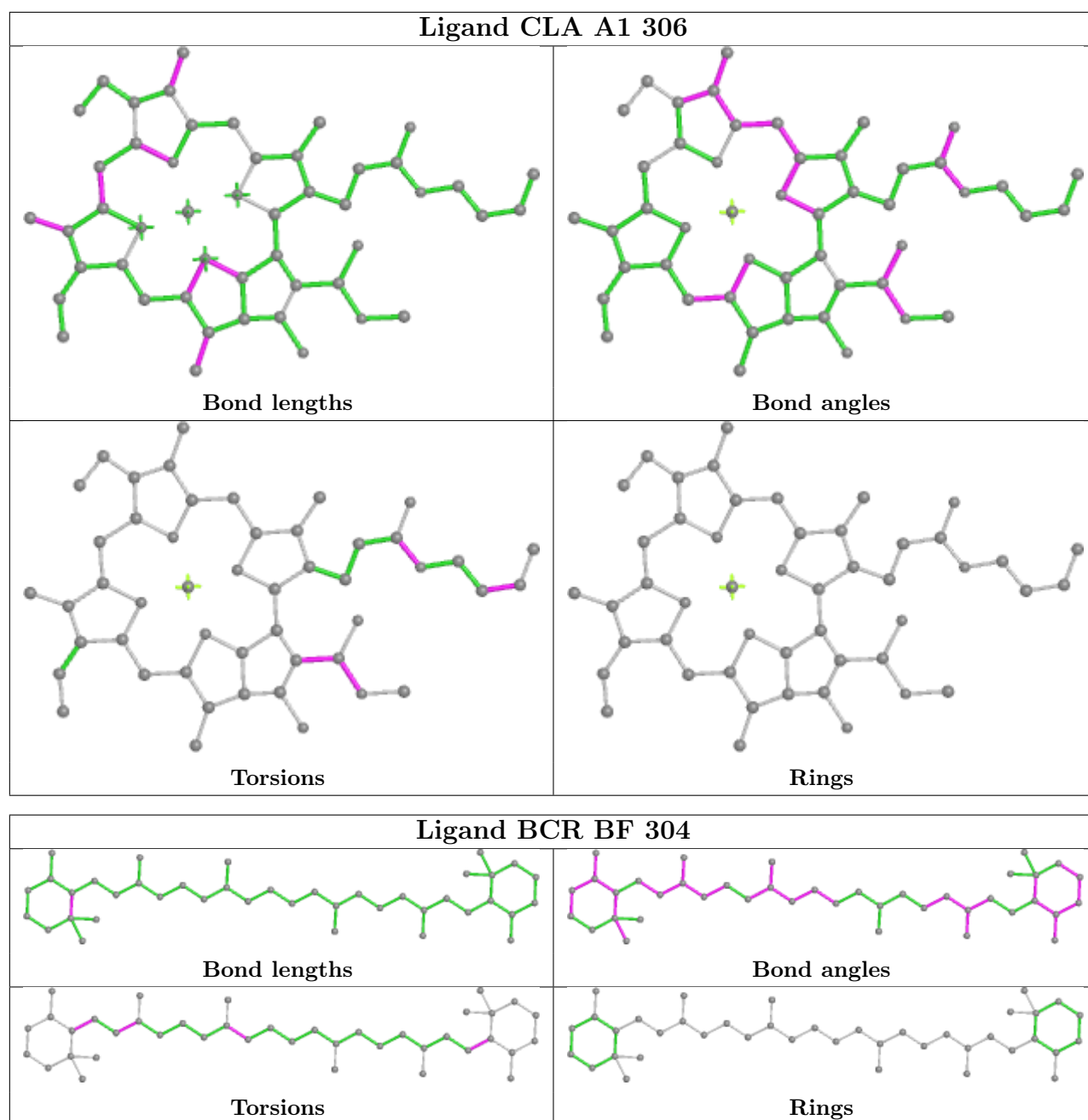
Rings

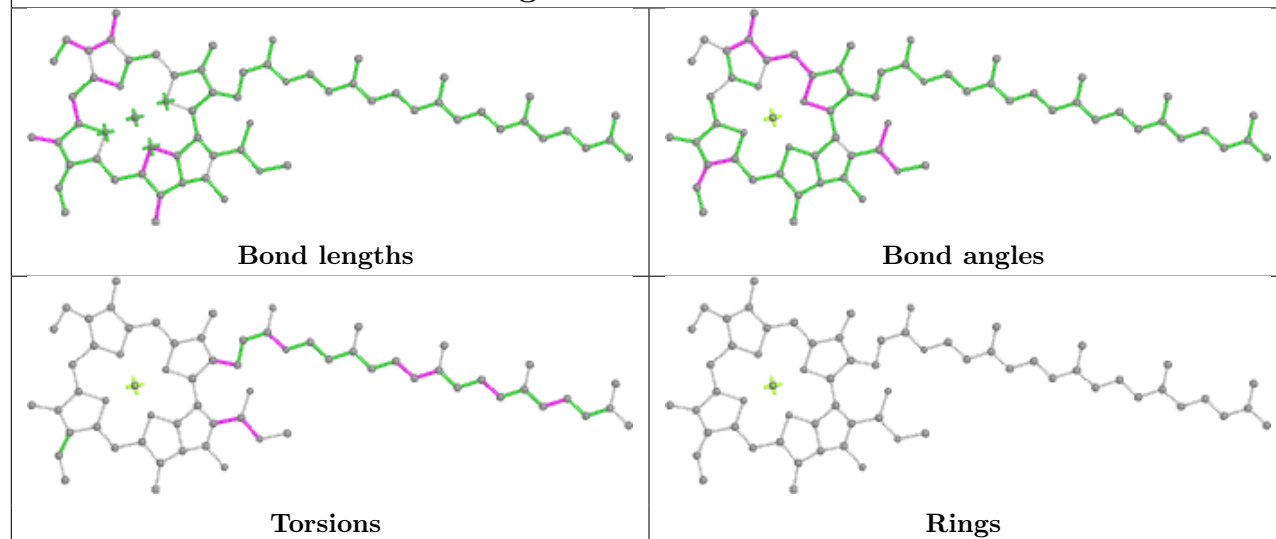
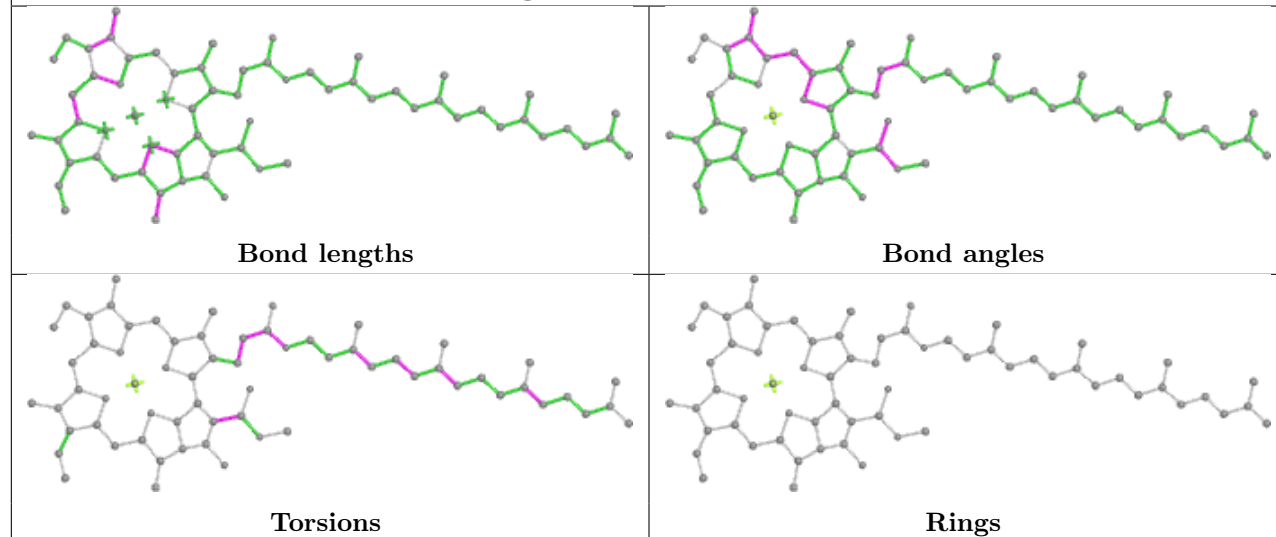
Ligand CLA AB 802



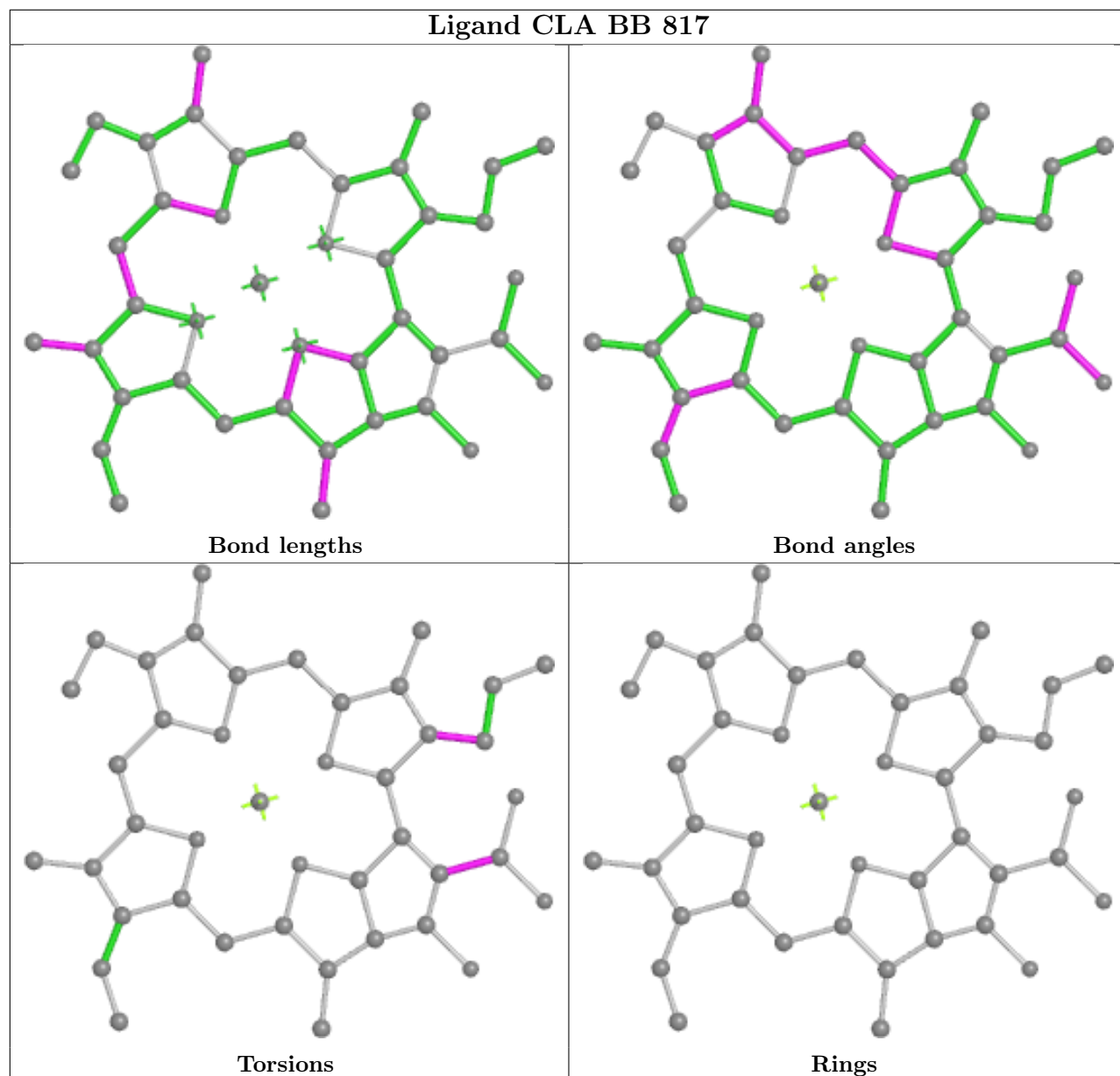
Ligand CLA B3 309



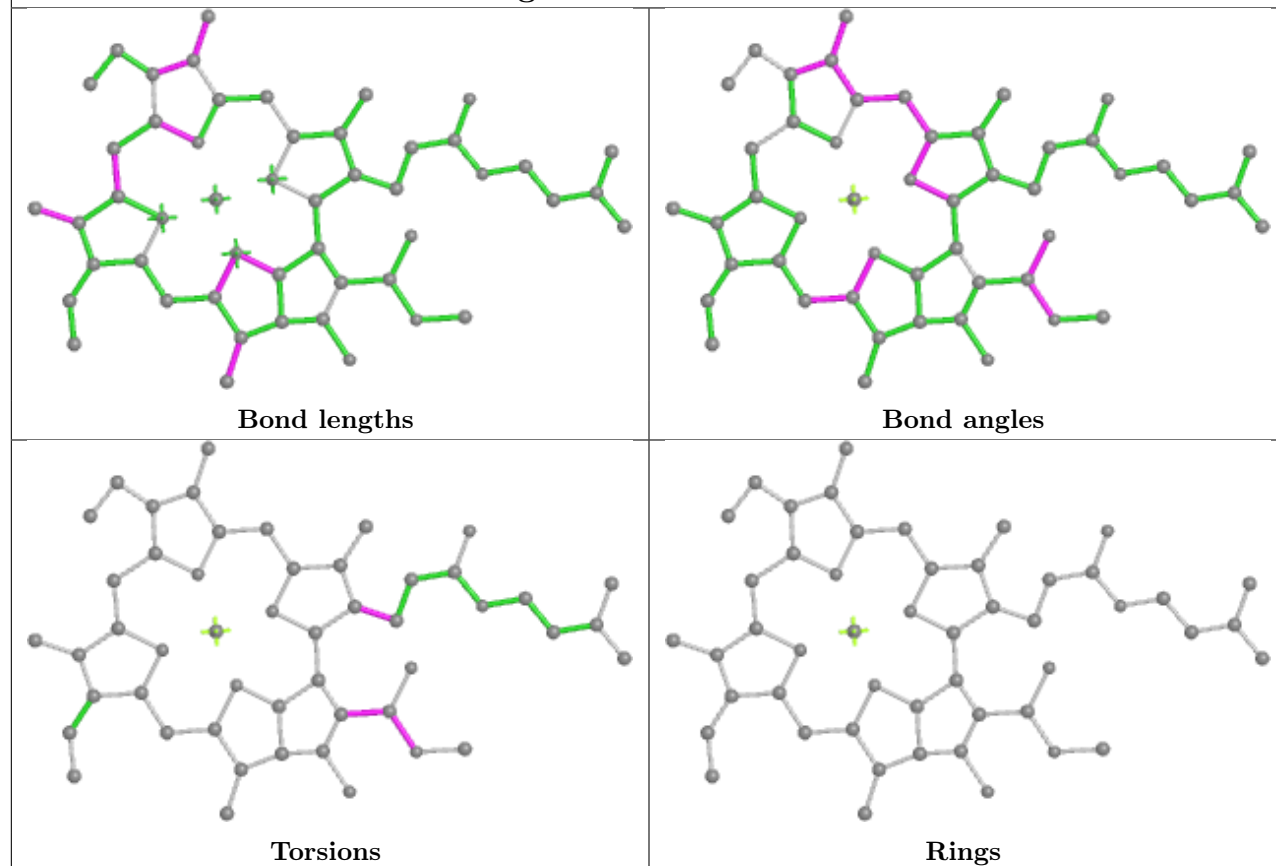


Ligand CLA BA 810**Ligand CLA BA 842**

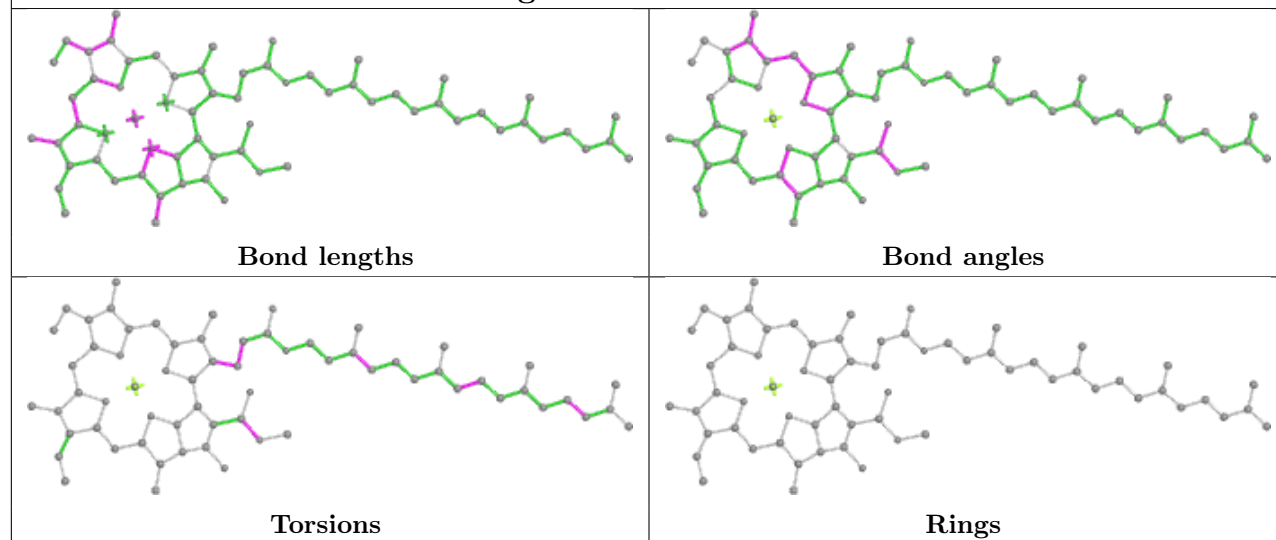
Ligand CLA BB 817



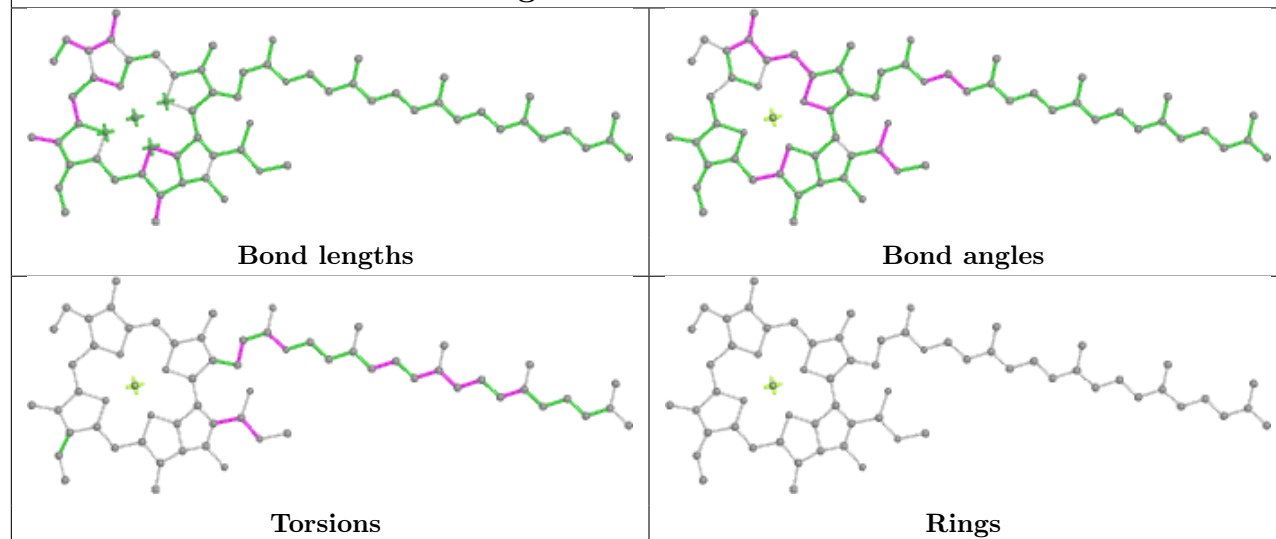
Ligand CLA AA 807



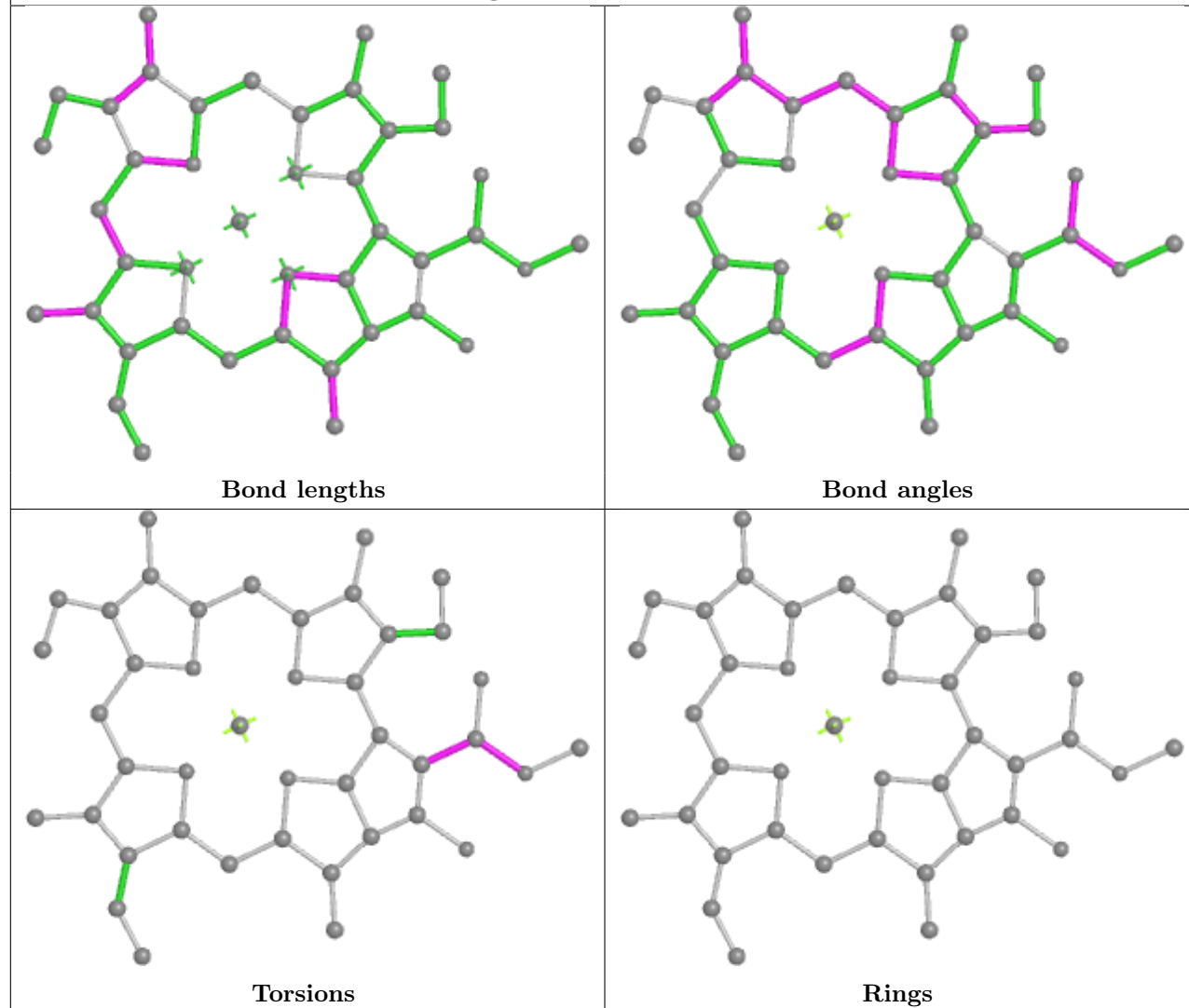
Ligand CLA AA 802



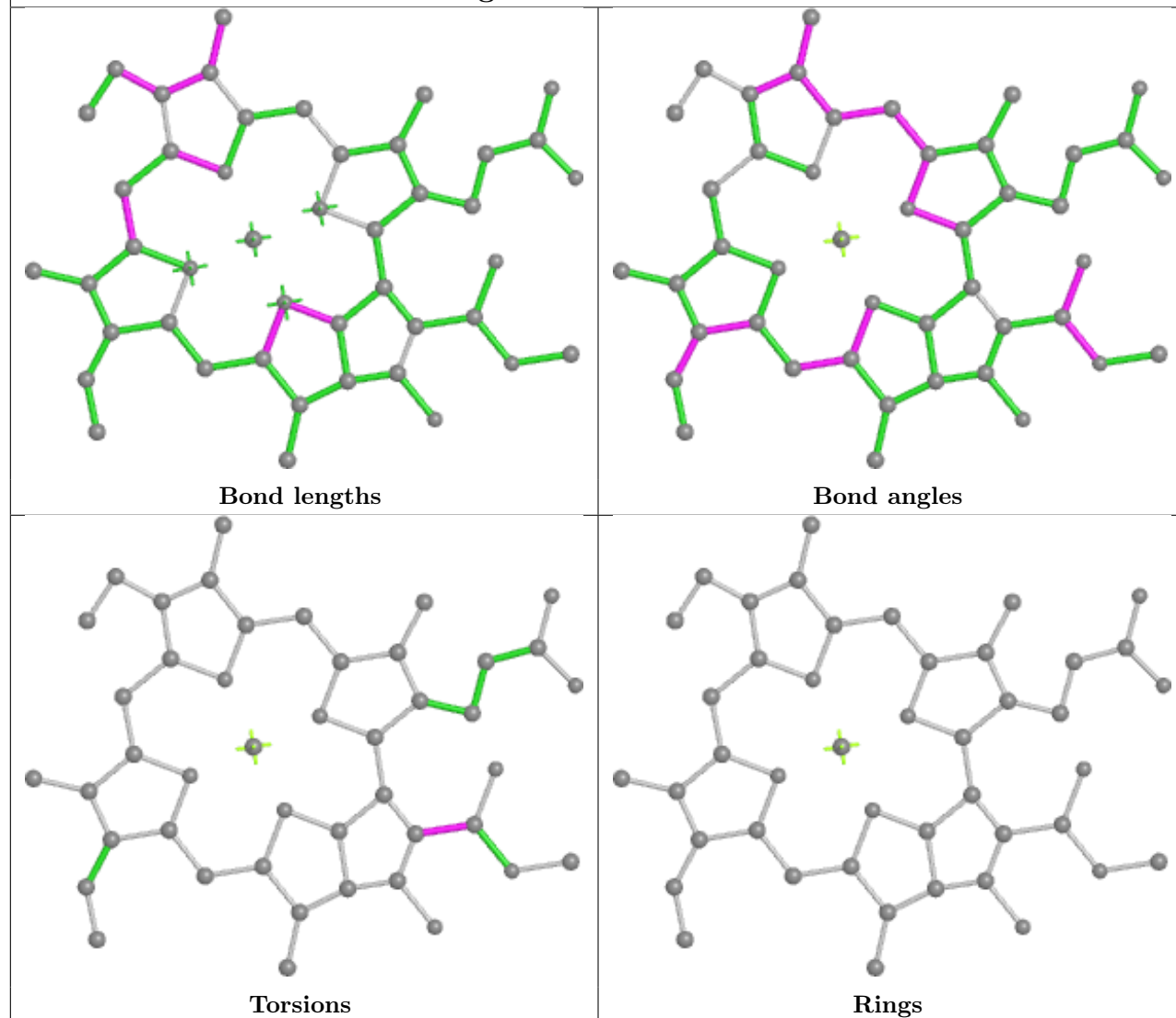
Ligand CLA AA 813



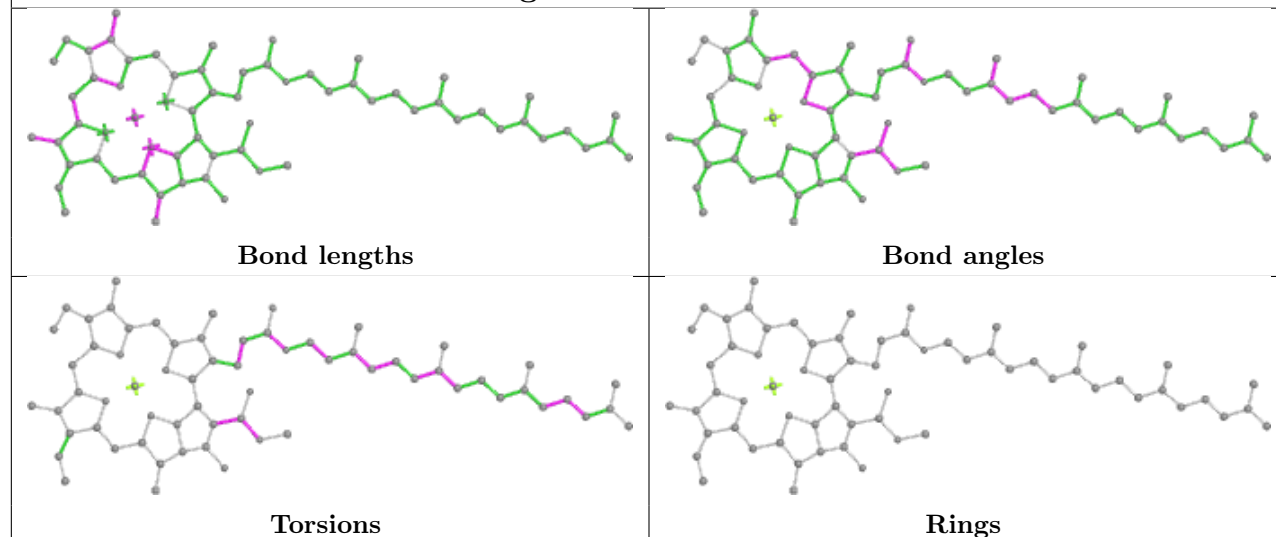
Ligand CLA BF 302



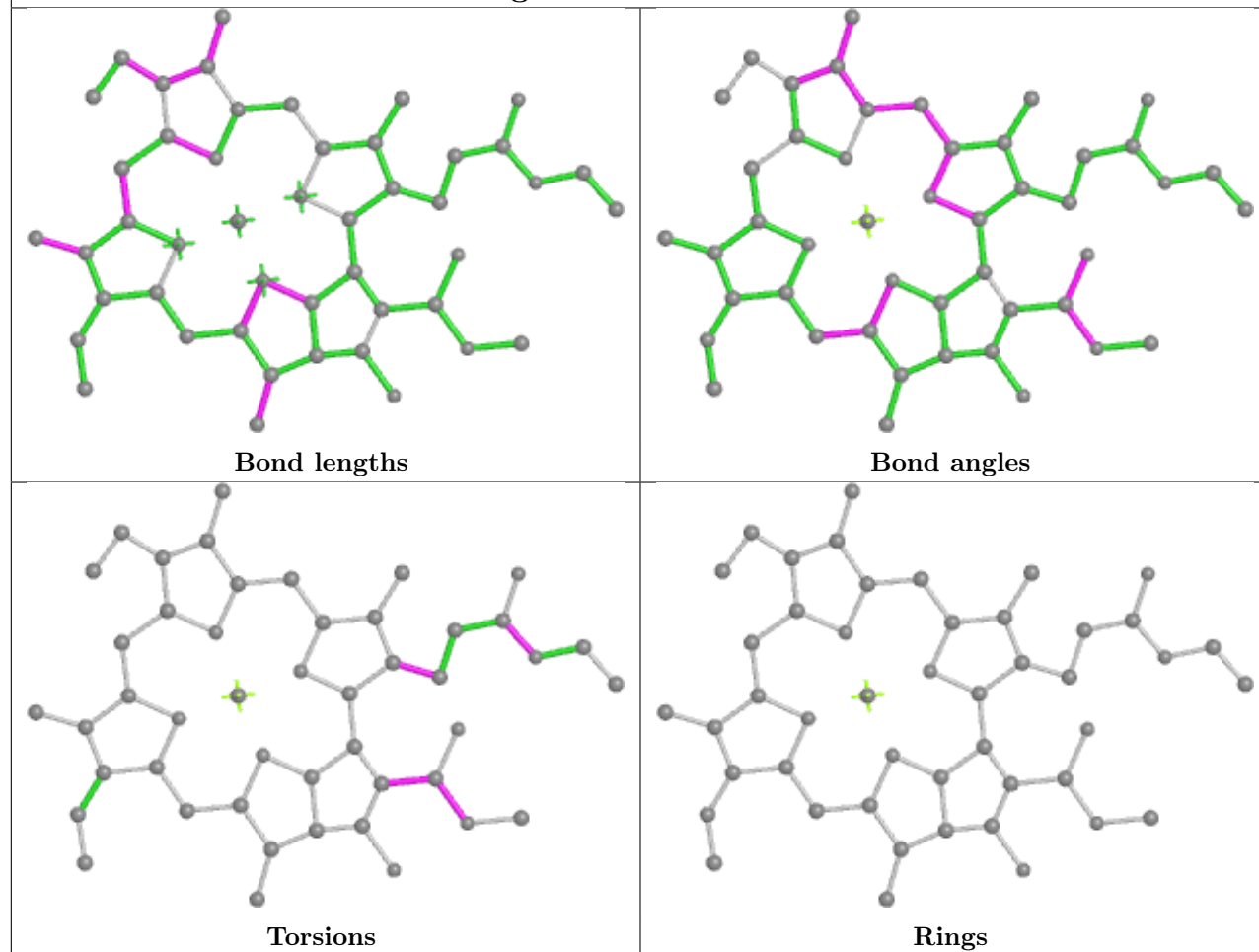
Ligand CLA BA 816



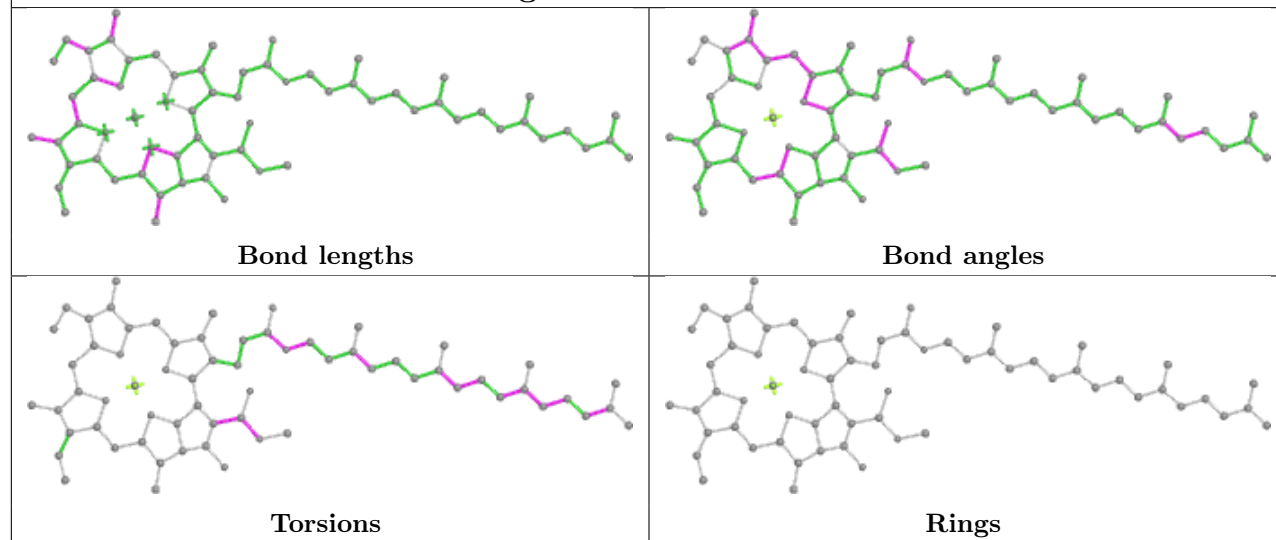
Ligand CLA BB 802



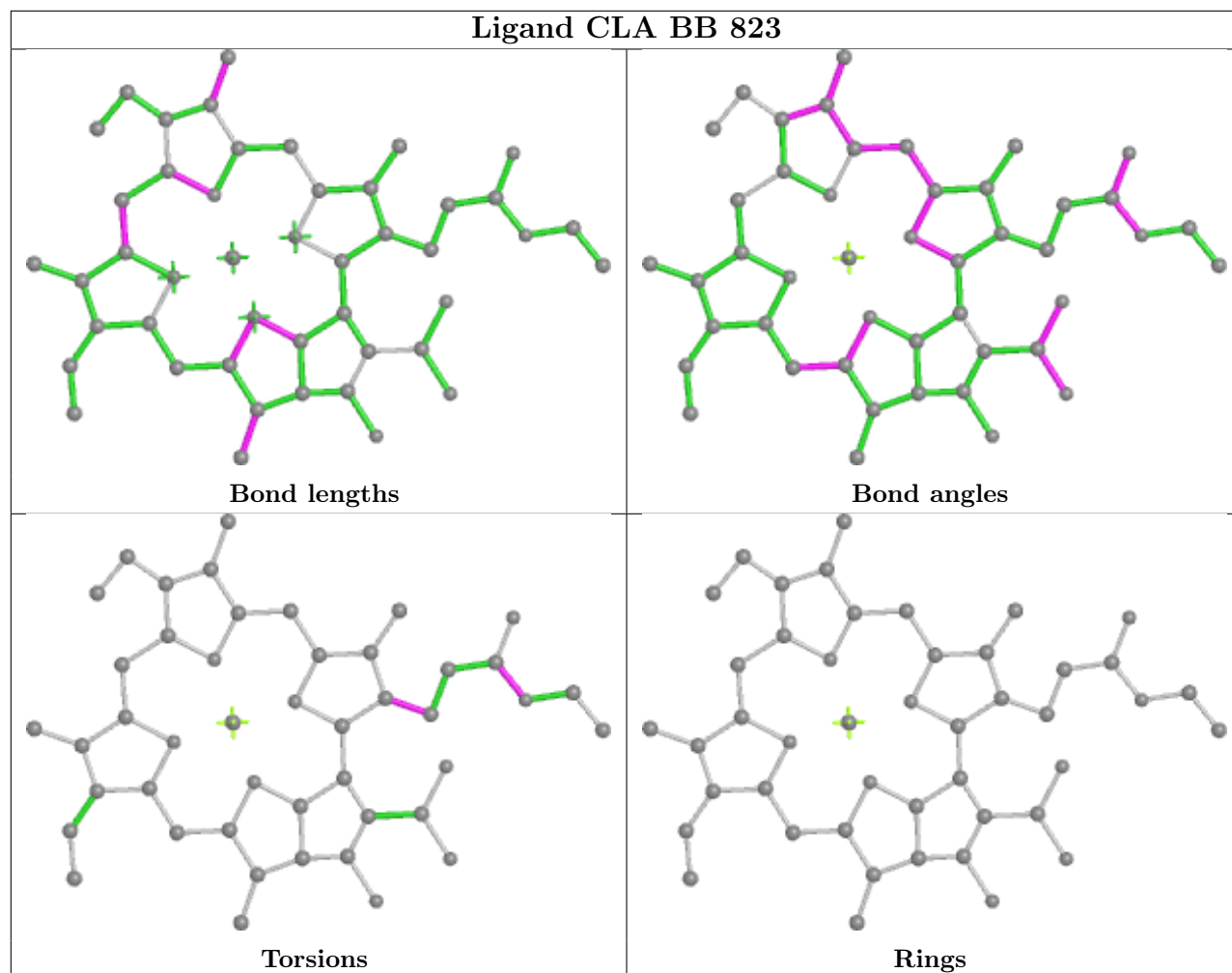
Ligand CLA AA 831



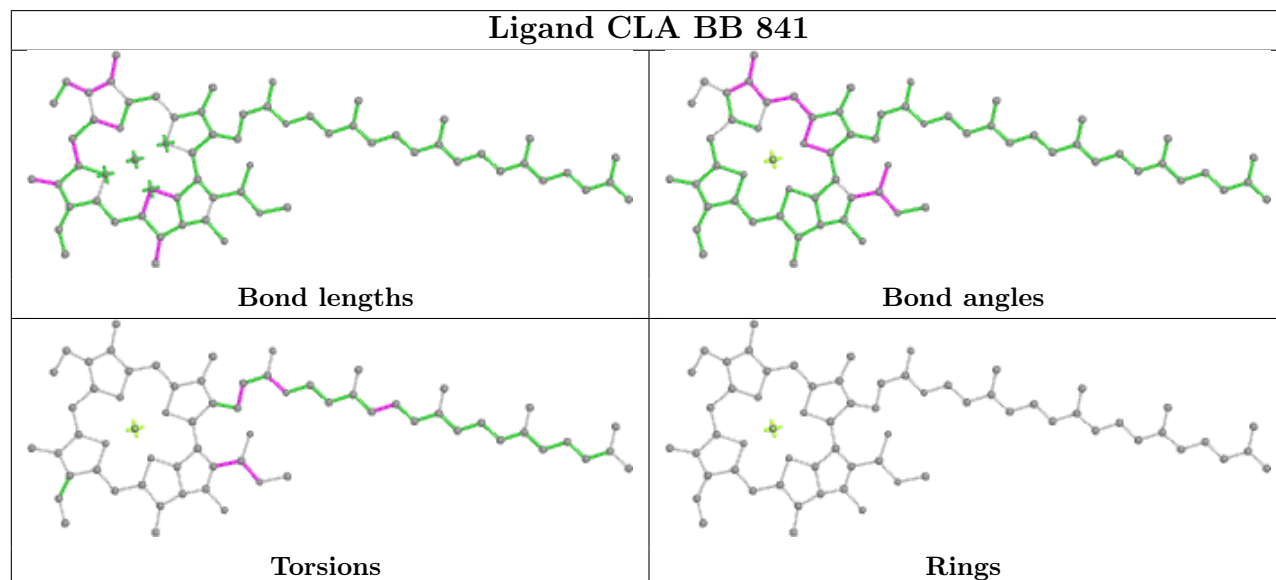
Ligand CLA AB 815



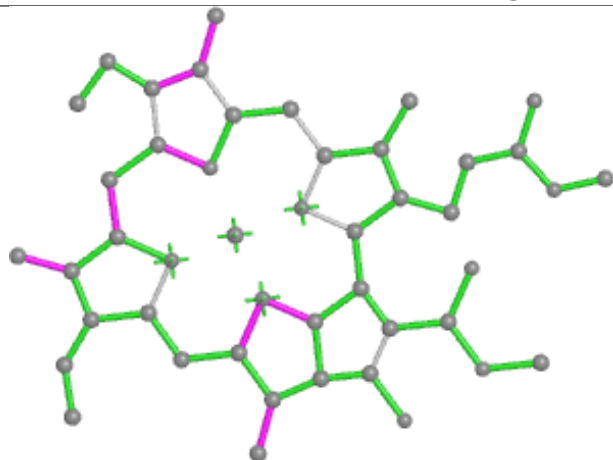
Ligand CLA BB 823



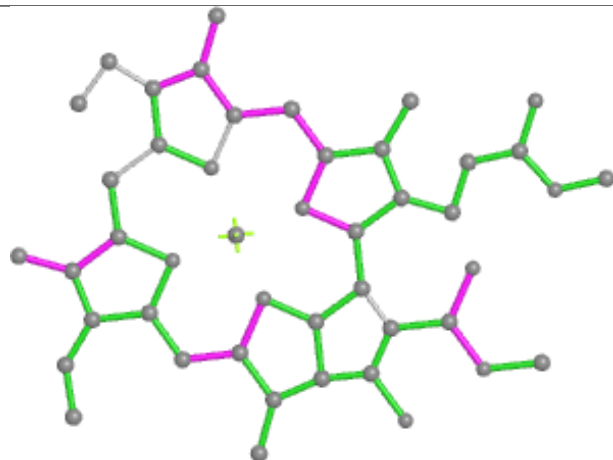
Ligand CLA BB 841



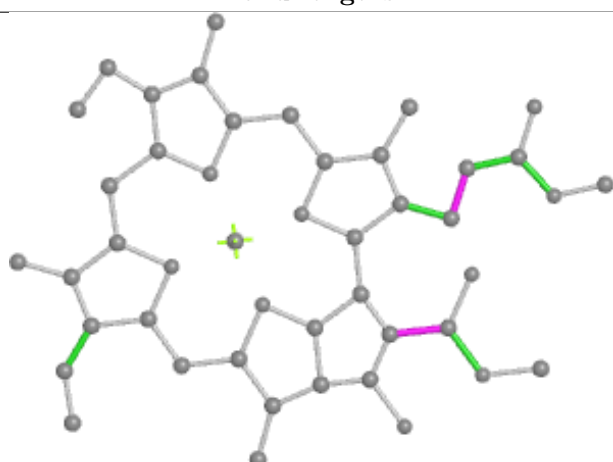
Ligand CLA A6 601



Bond lengths



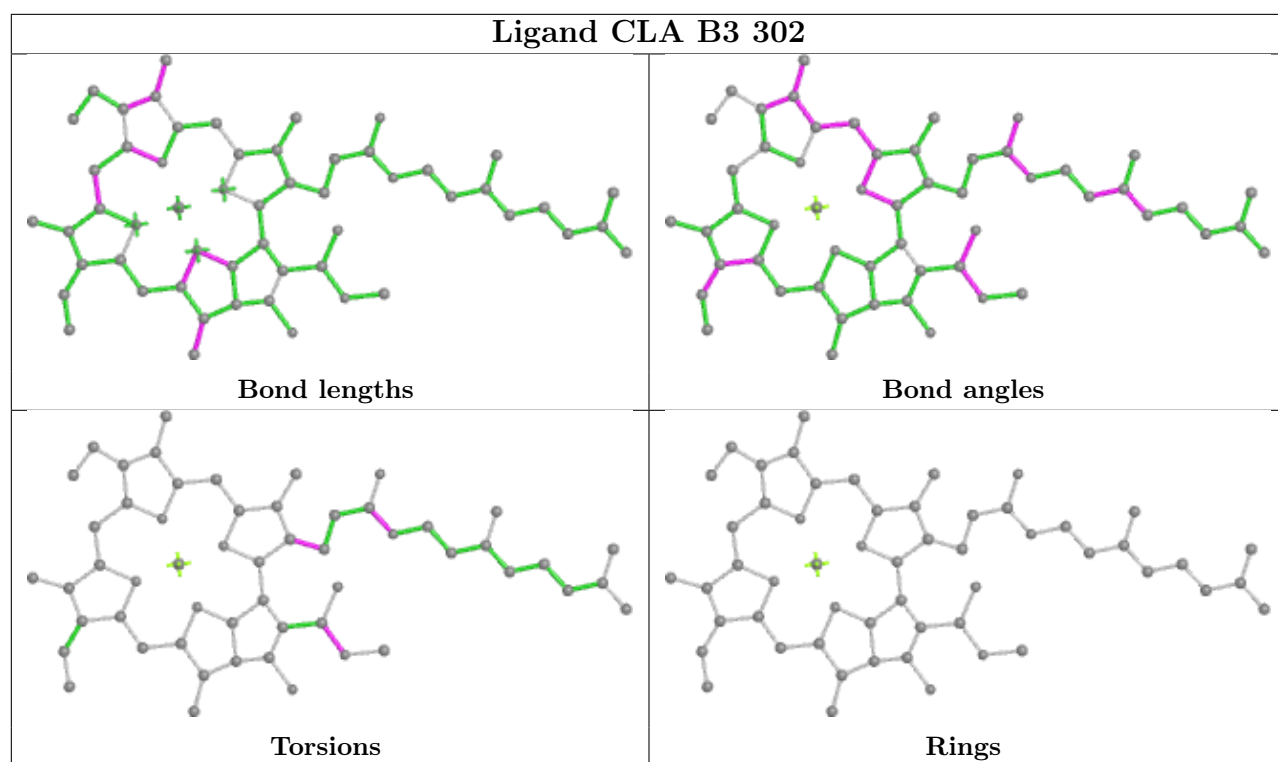
Bond angles



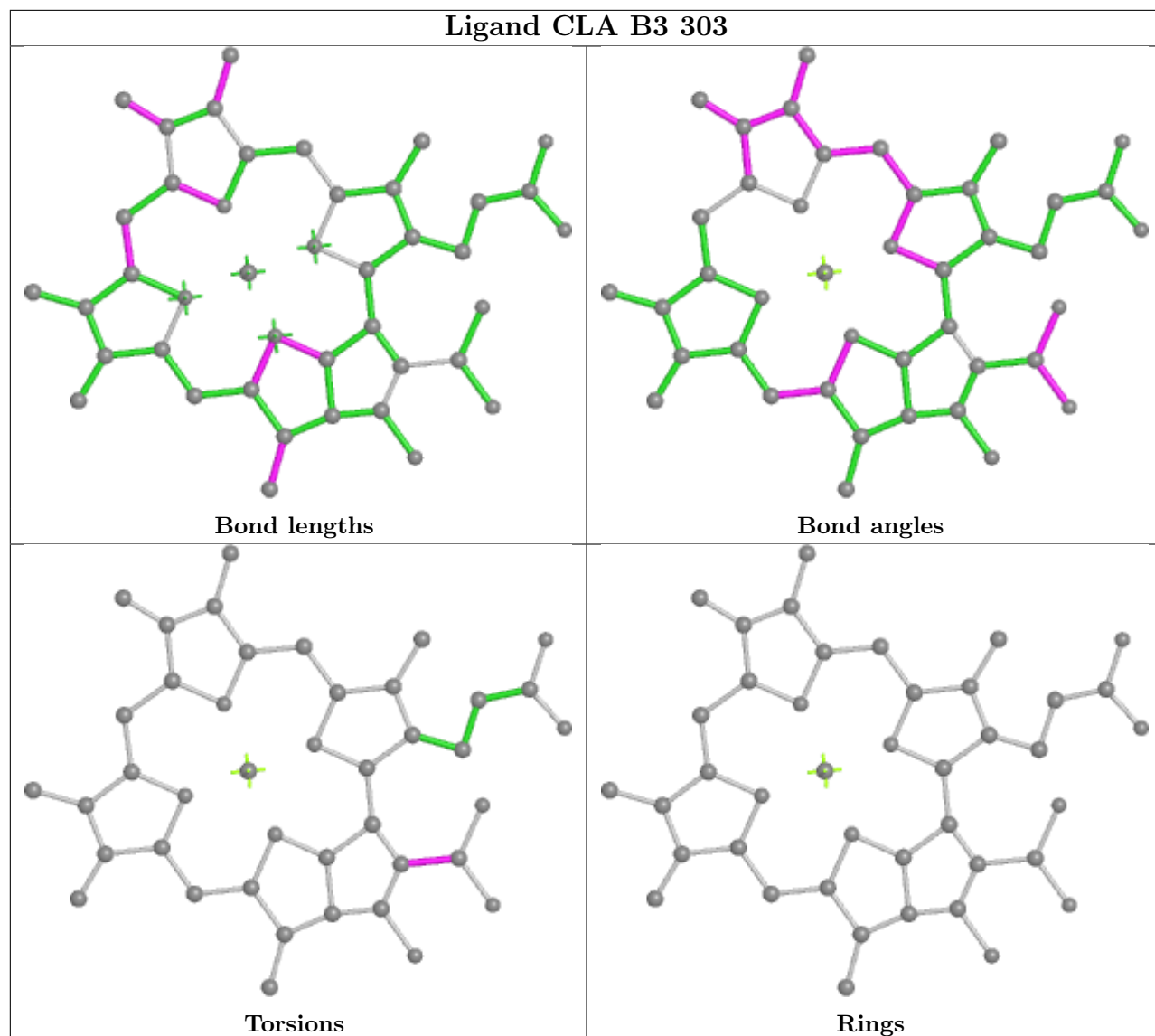
Torsions



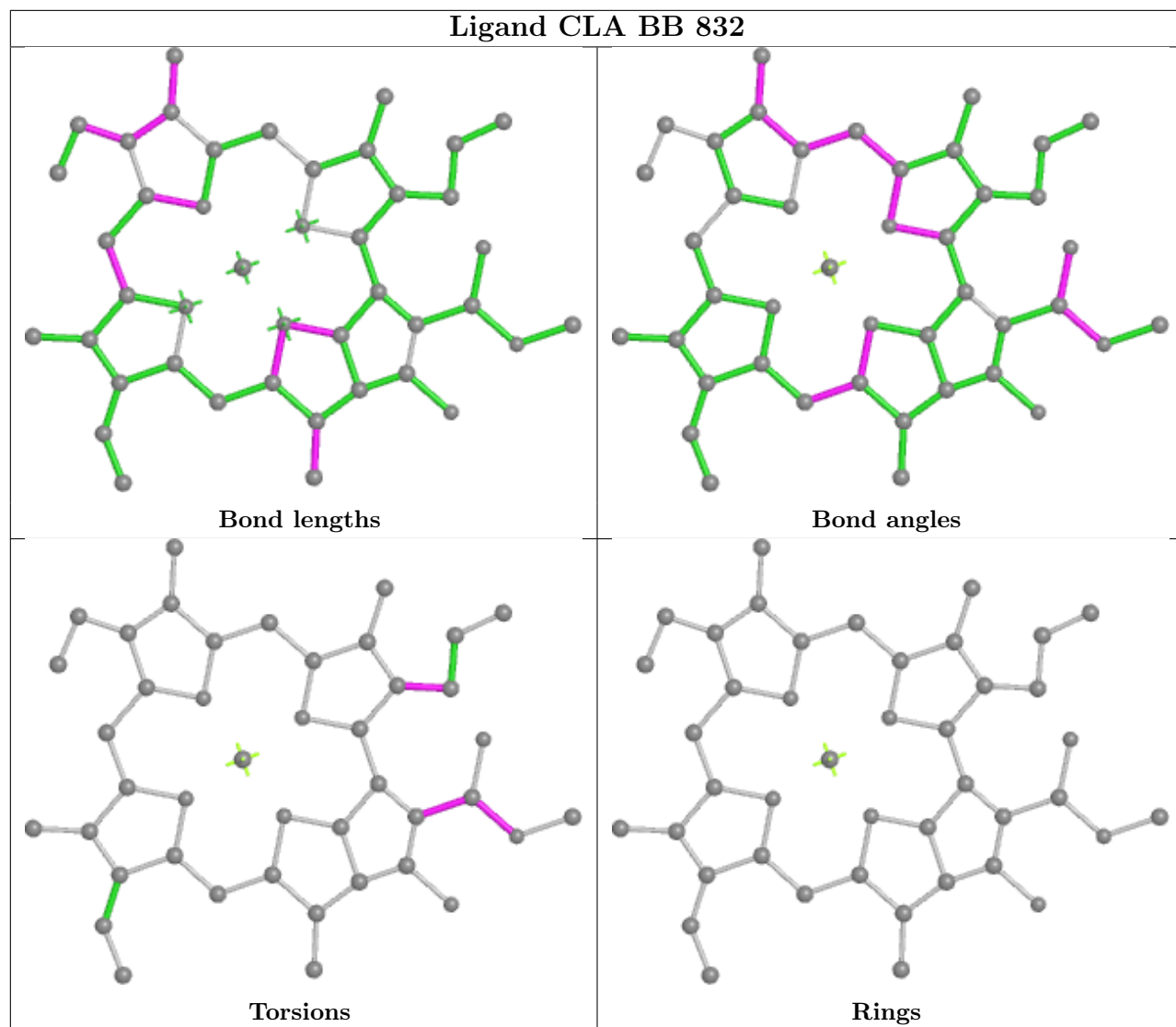
Rings



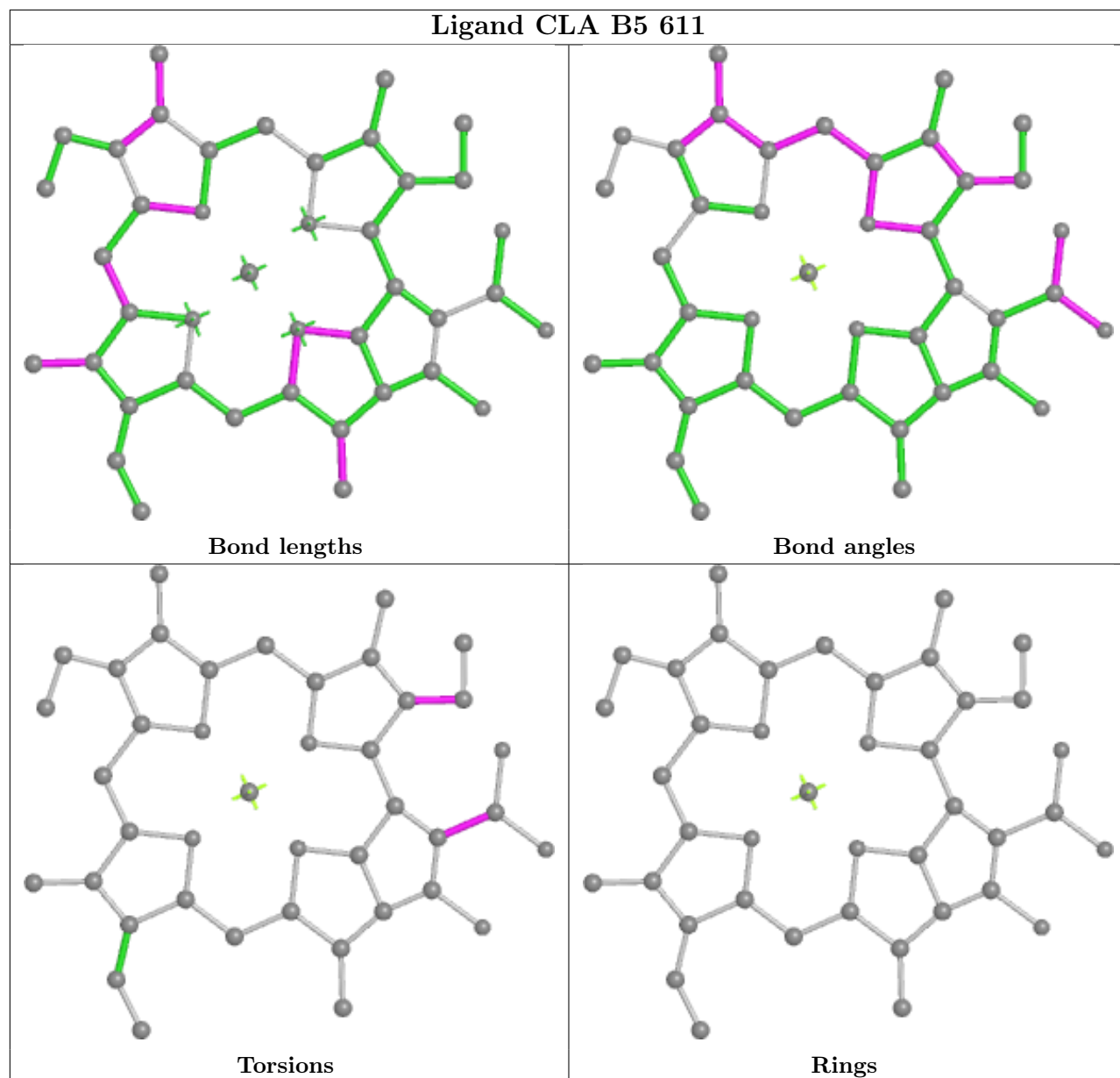
Ligand CLA B3 303

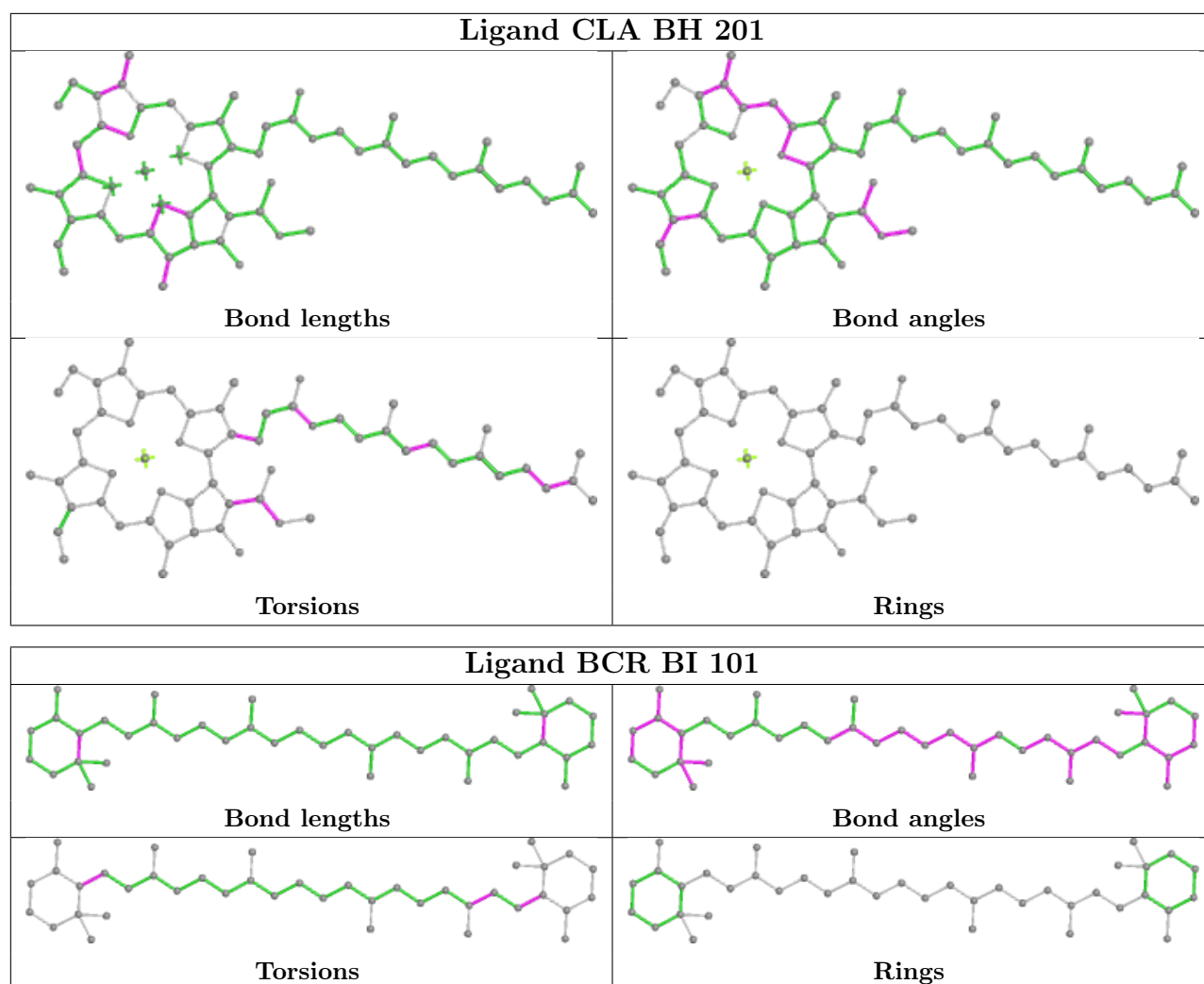


Ligand CLA BB 832

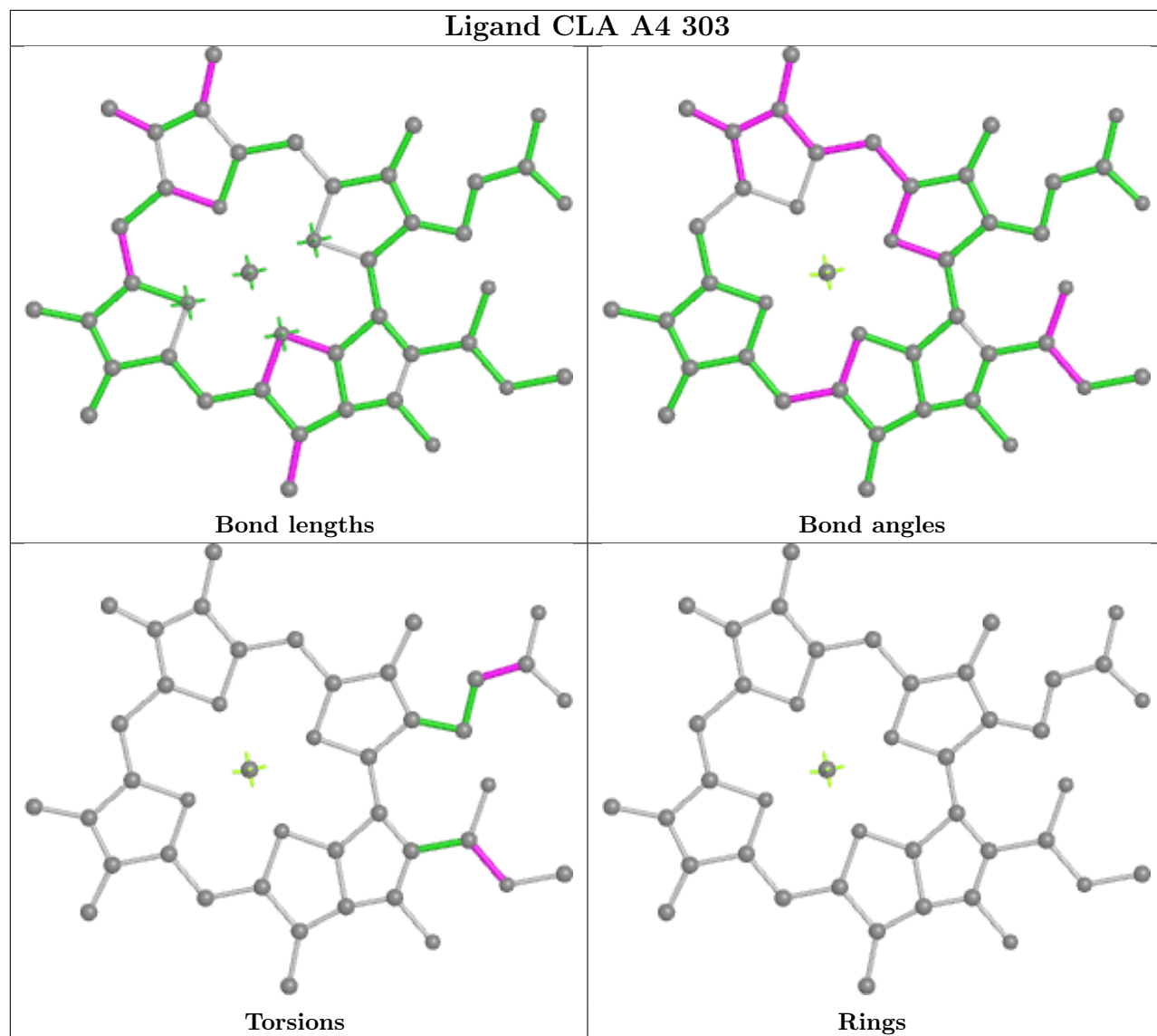


Ligand CLA B5 611

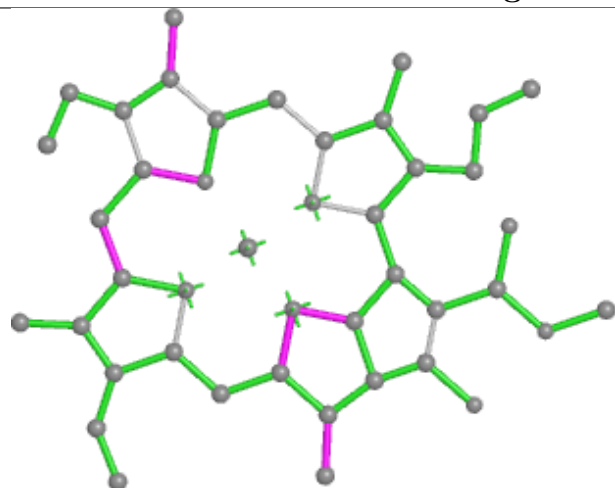




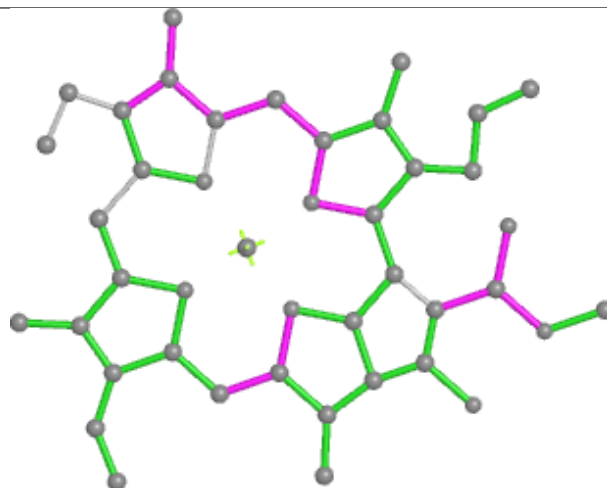
Ligand CLA A4 303



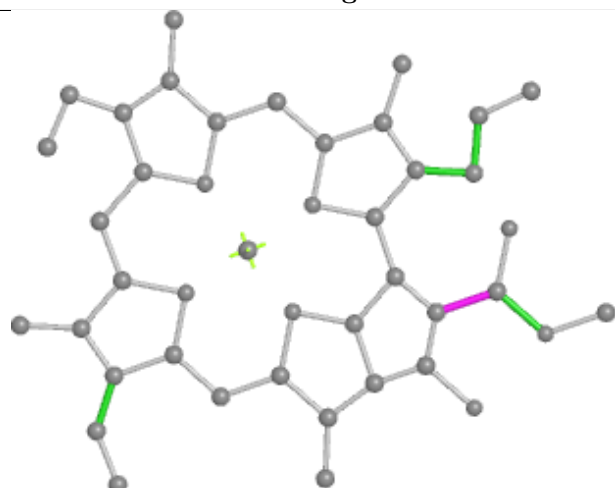
Ligand CLA BB 814



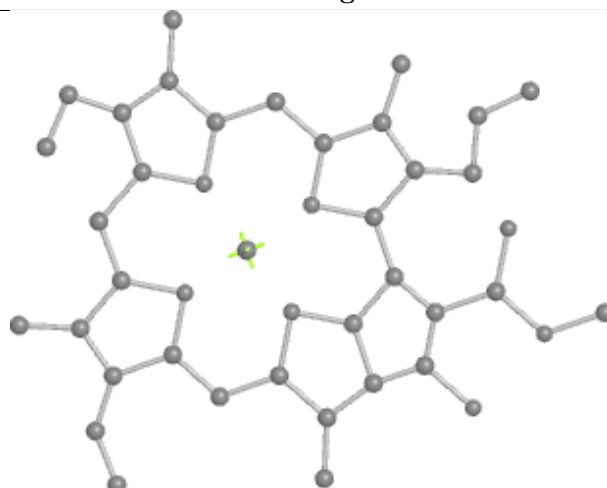
Bond lengths



Bond angles

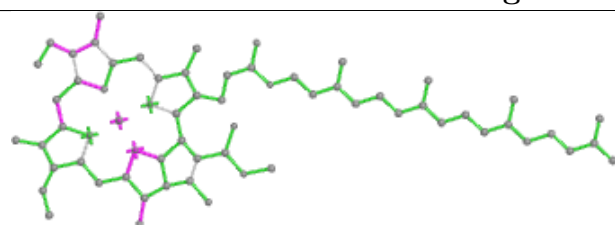


Torsions

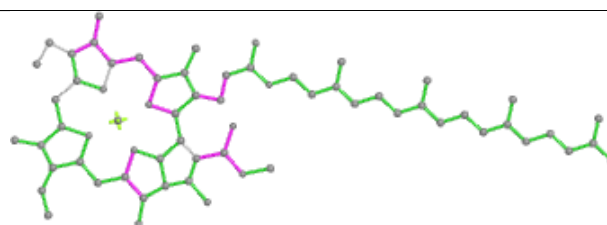


Rings

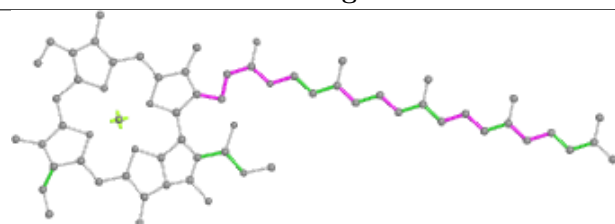
Ligand CLA AB 829



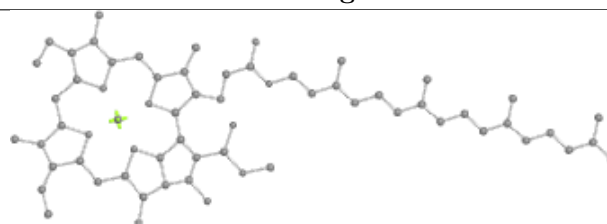
Bond lengths



Bond angles

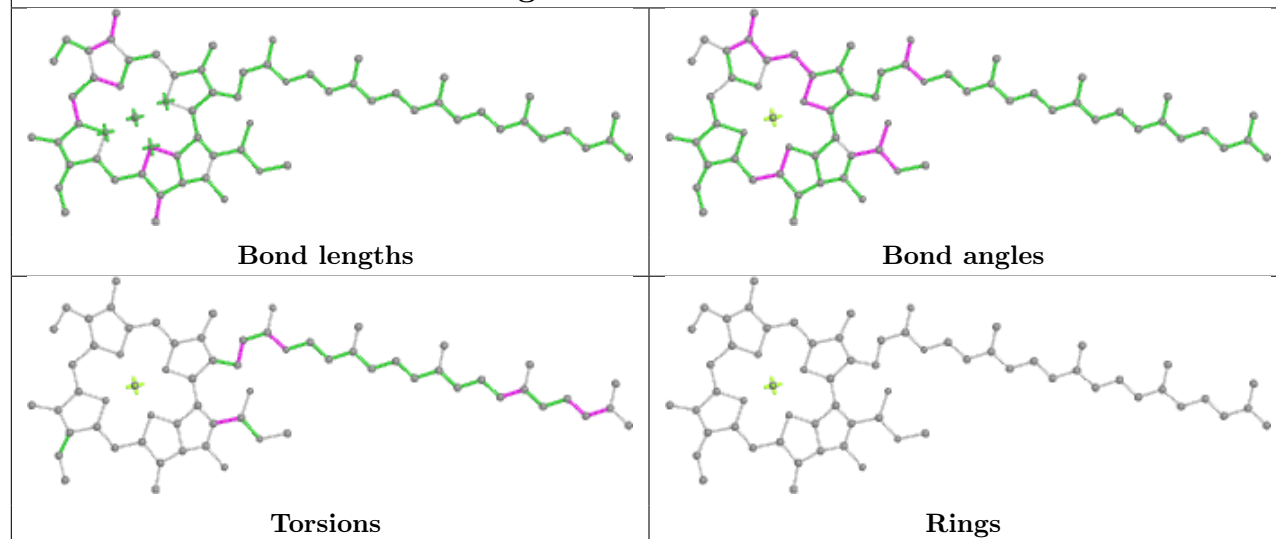


Torsions

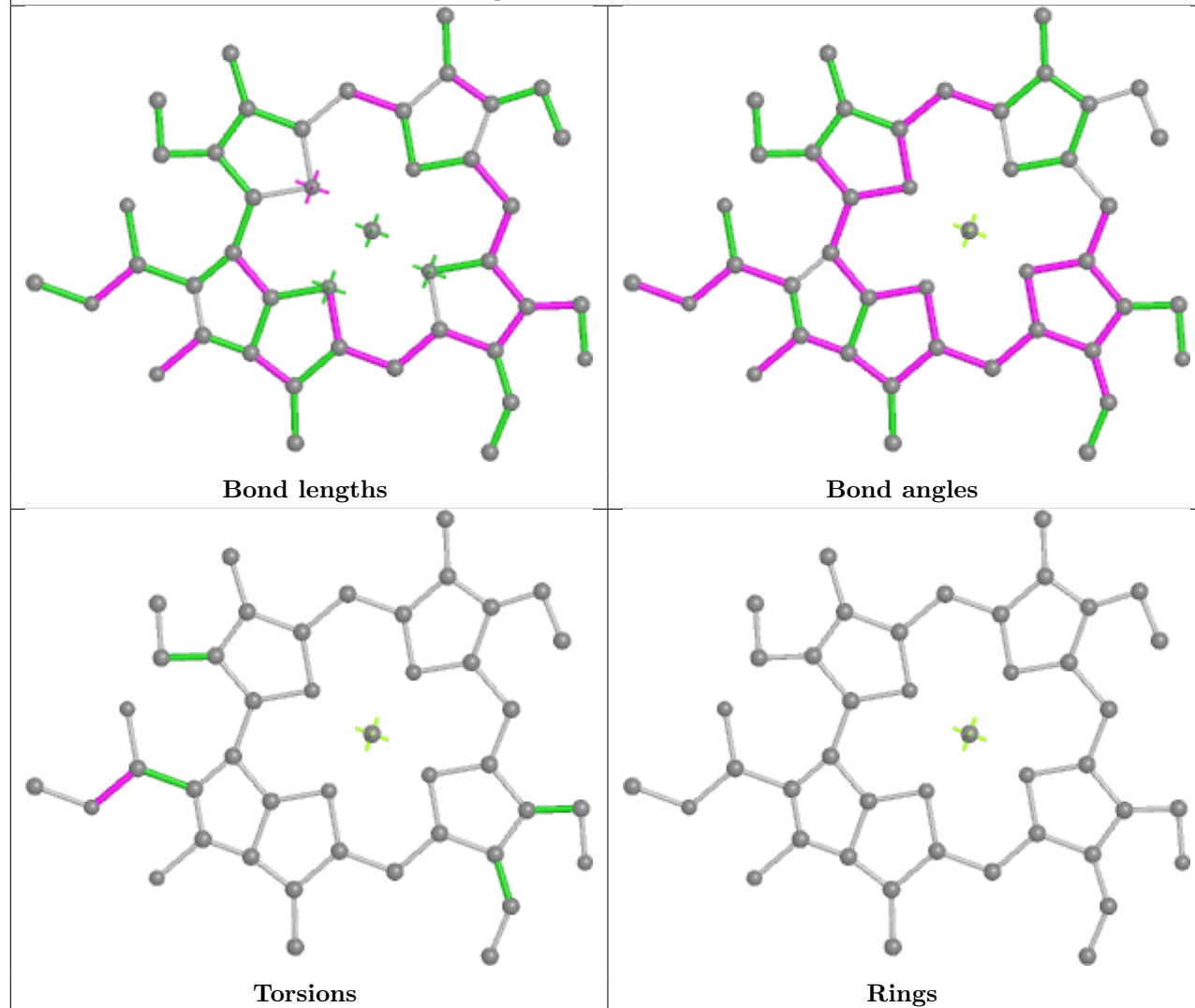


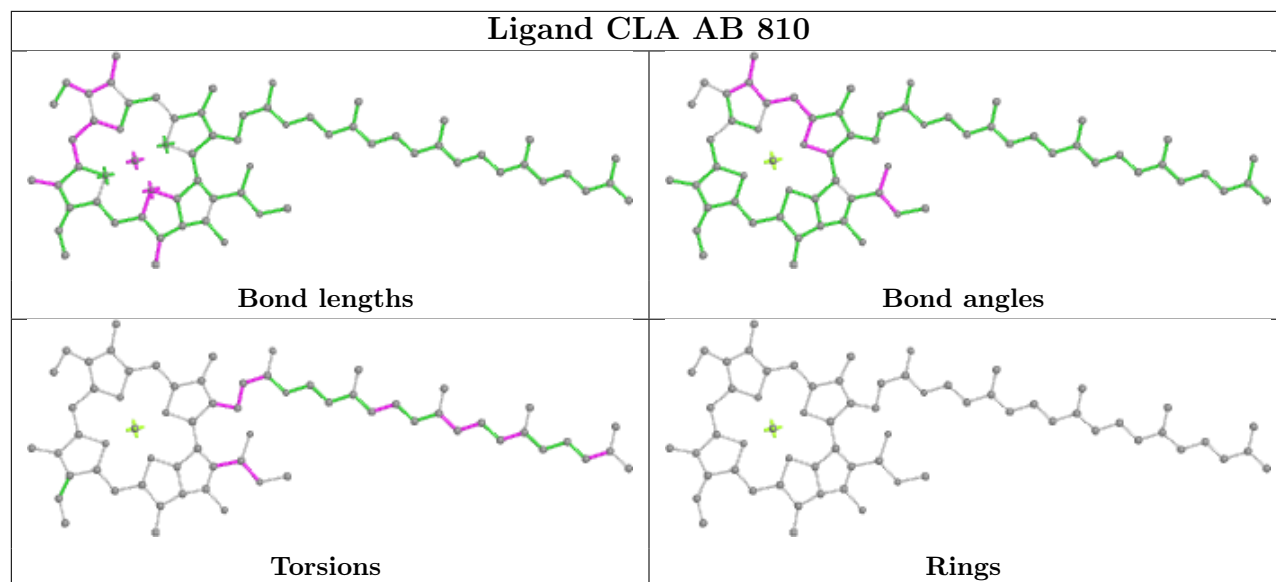
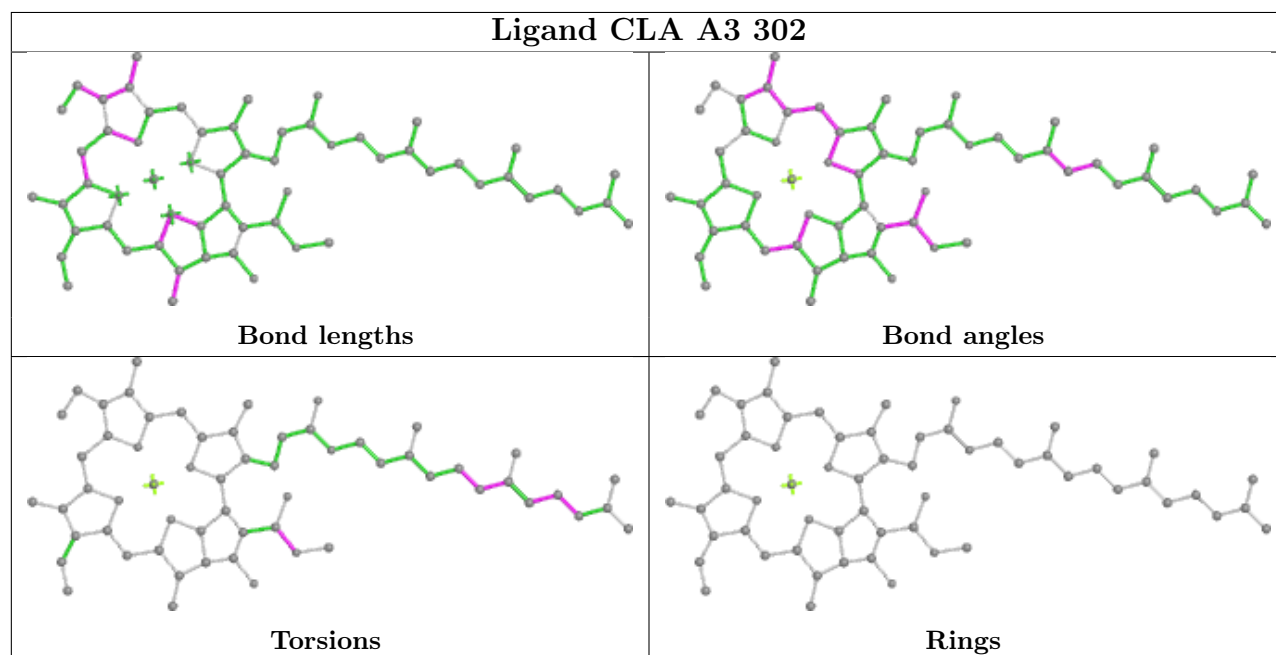
Rings

Ligand CLA AA 808

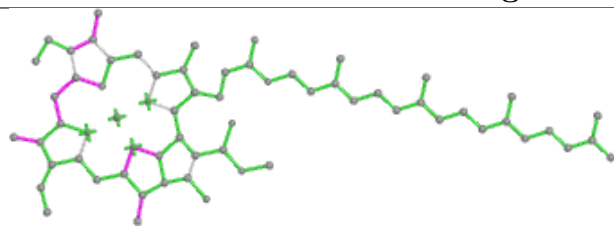


Ligand CHL A6 607

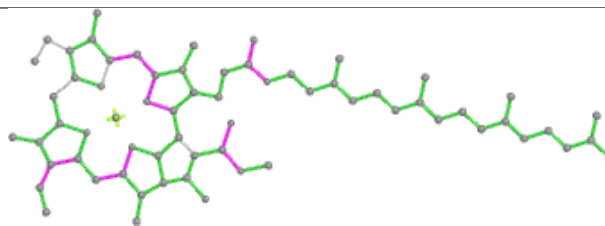


Ligand CLA AB 810**Ligand CLA A3 302**

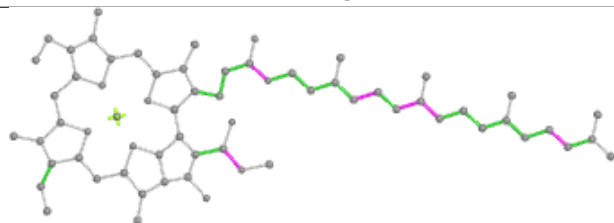
Ligand CLA BB 842



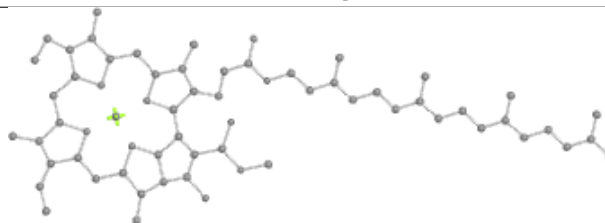
Bond lengths



Bond angles

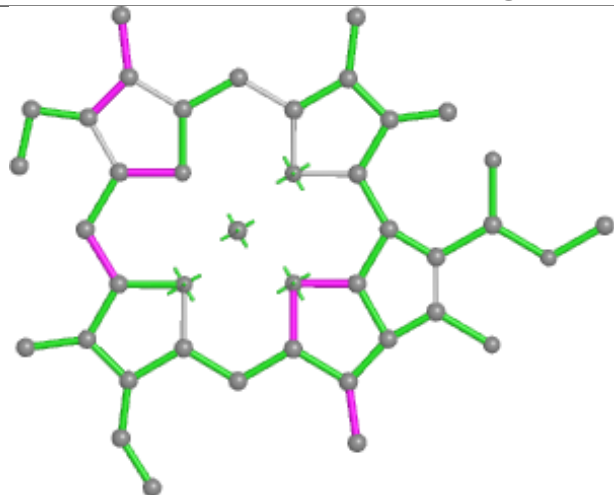


Torsions

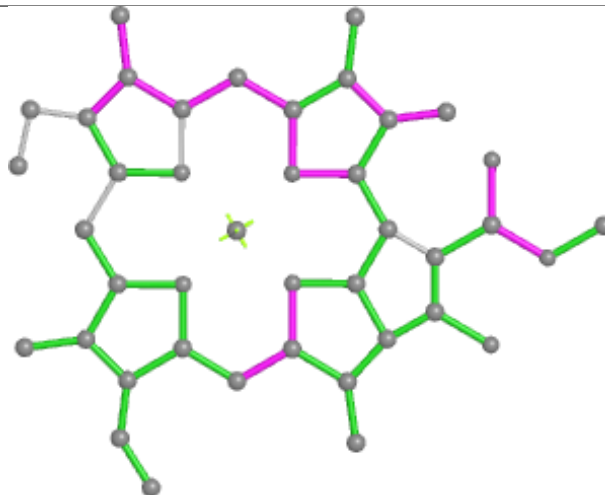


Rings

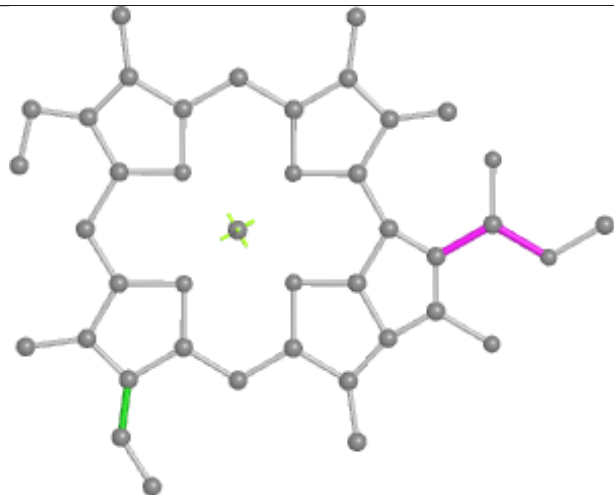
Ligand CLA AA 823



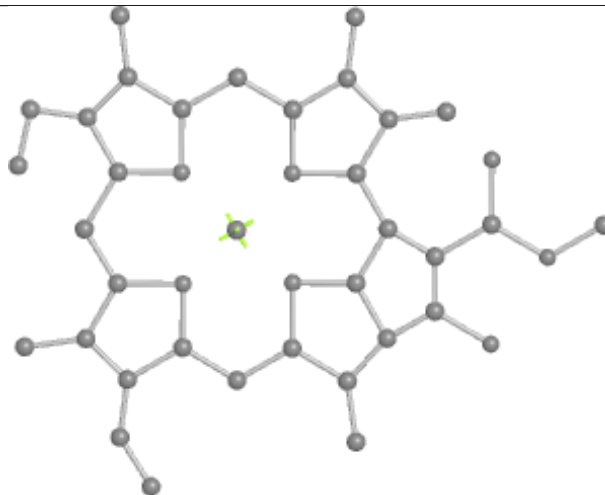
Bond lengths



Bond angles

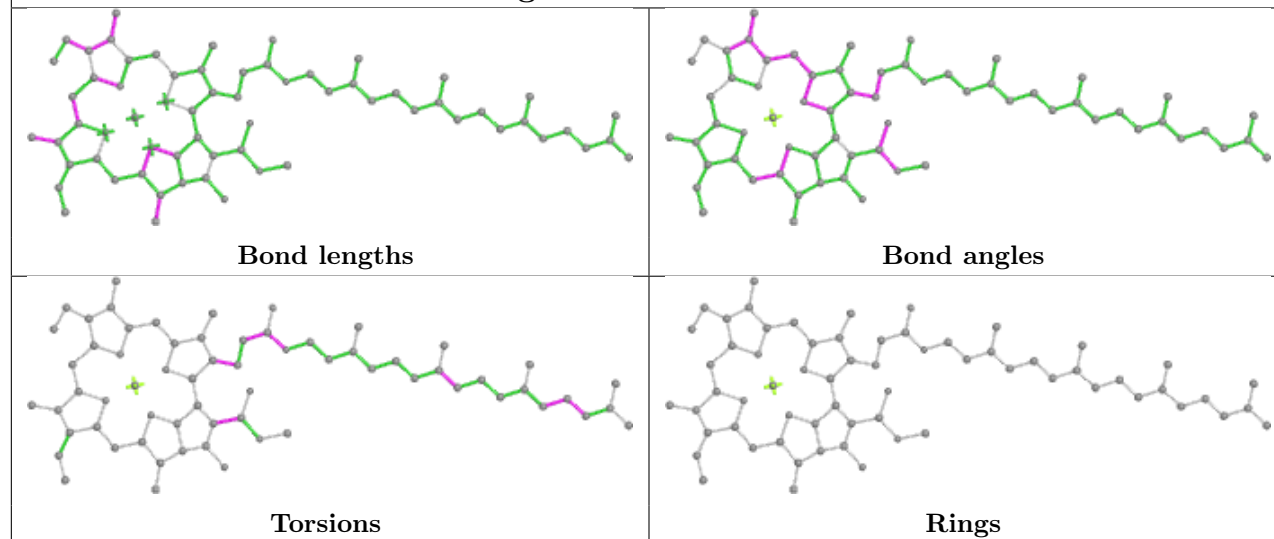


Torsions

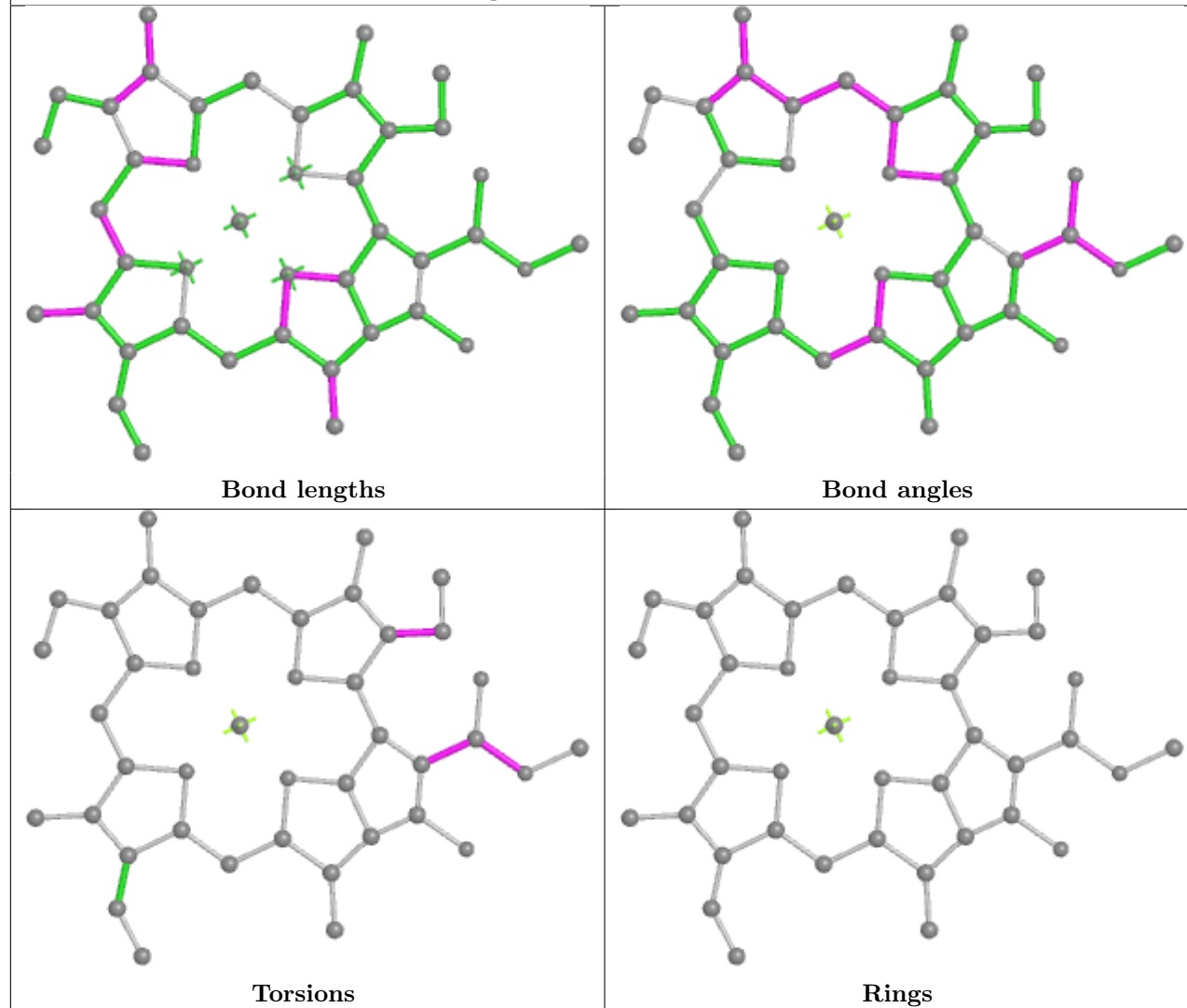


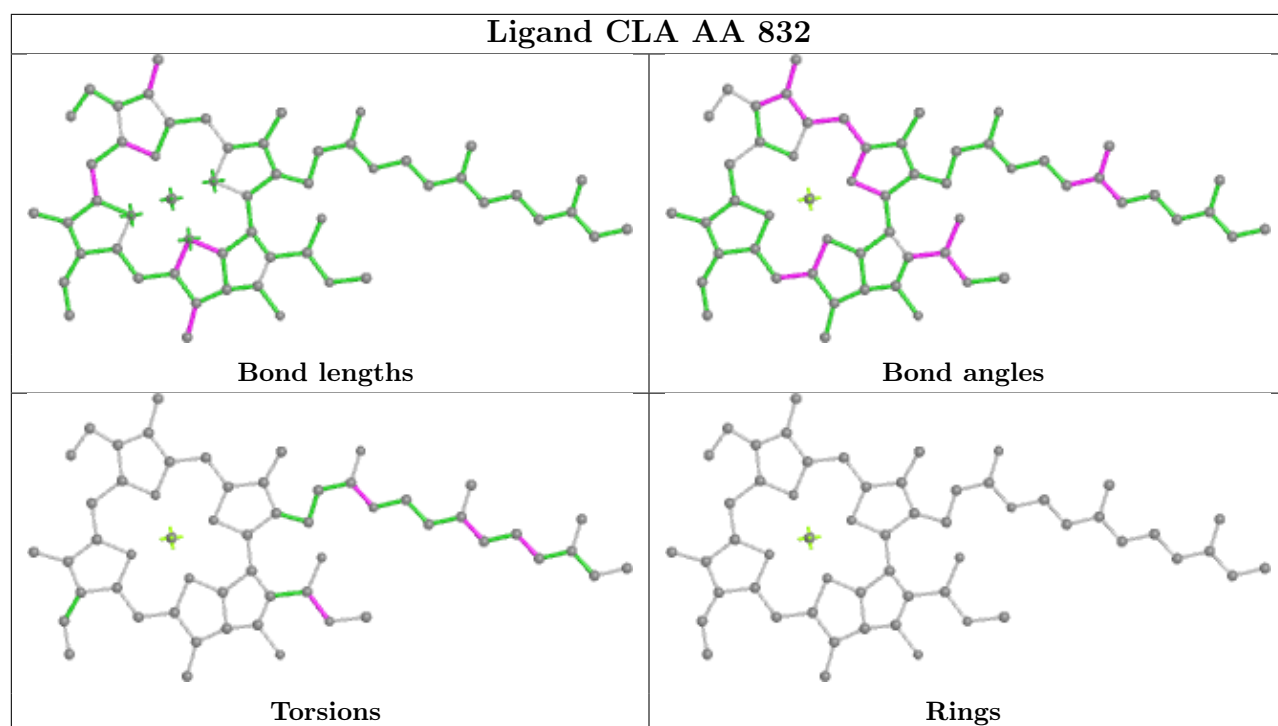
Rings

Ligand CLA AA 841

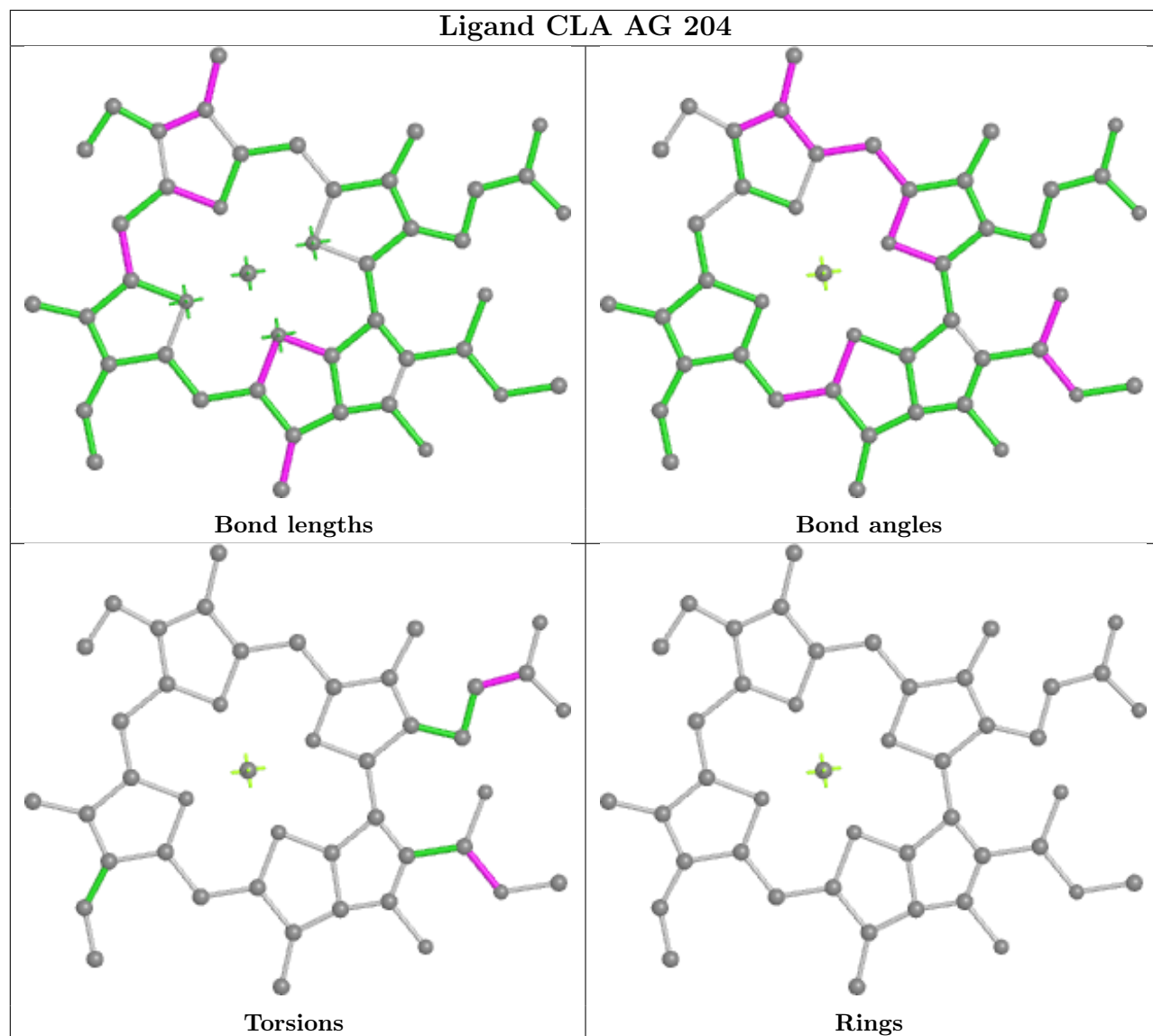


Ligand CLA AL 305

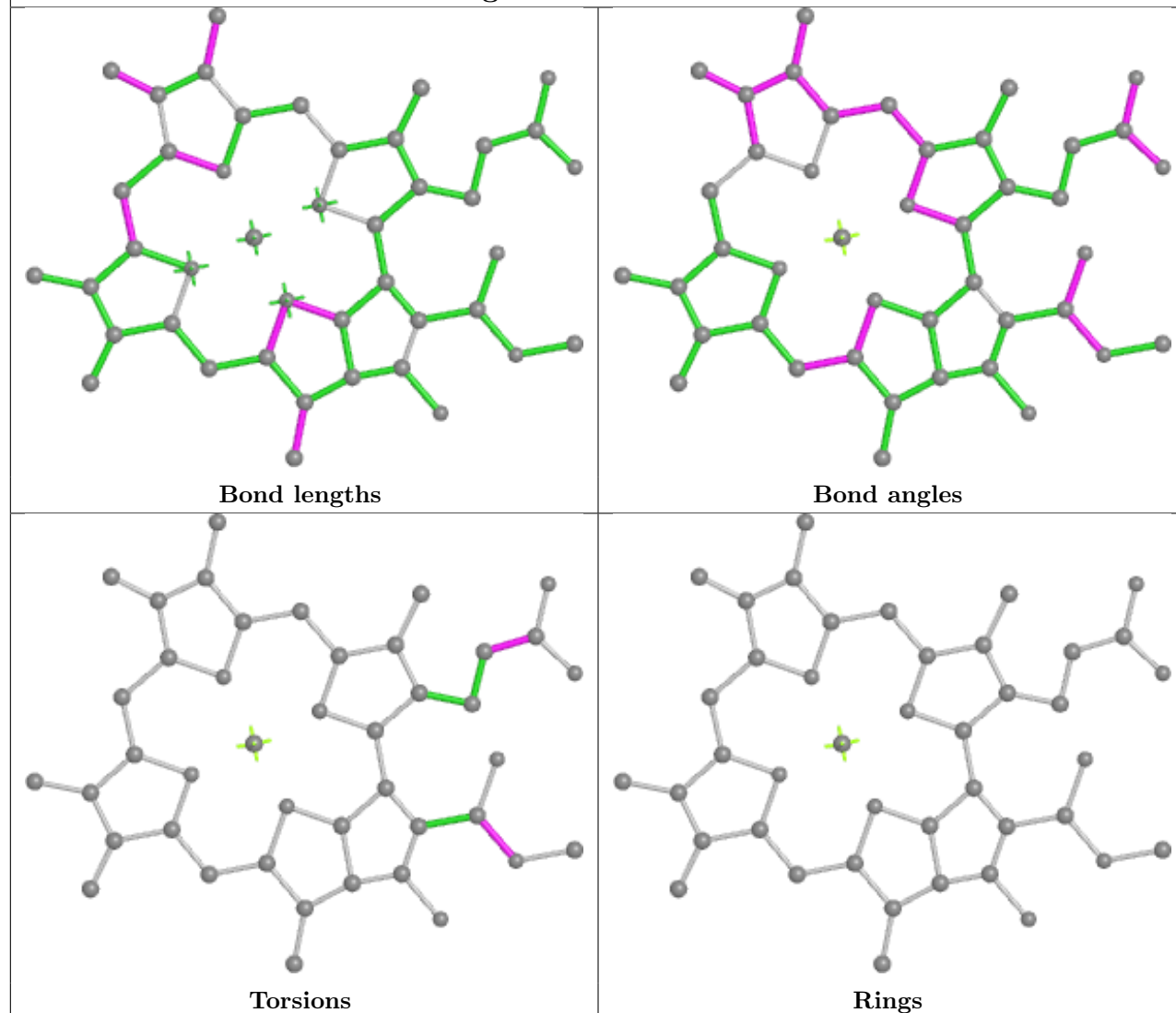




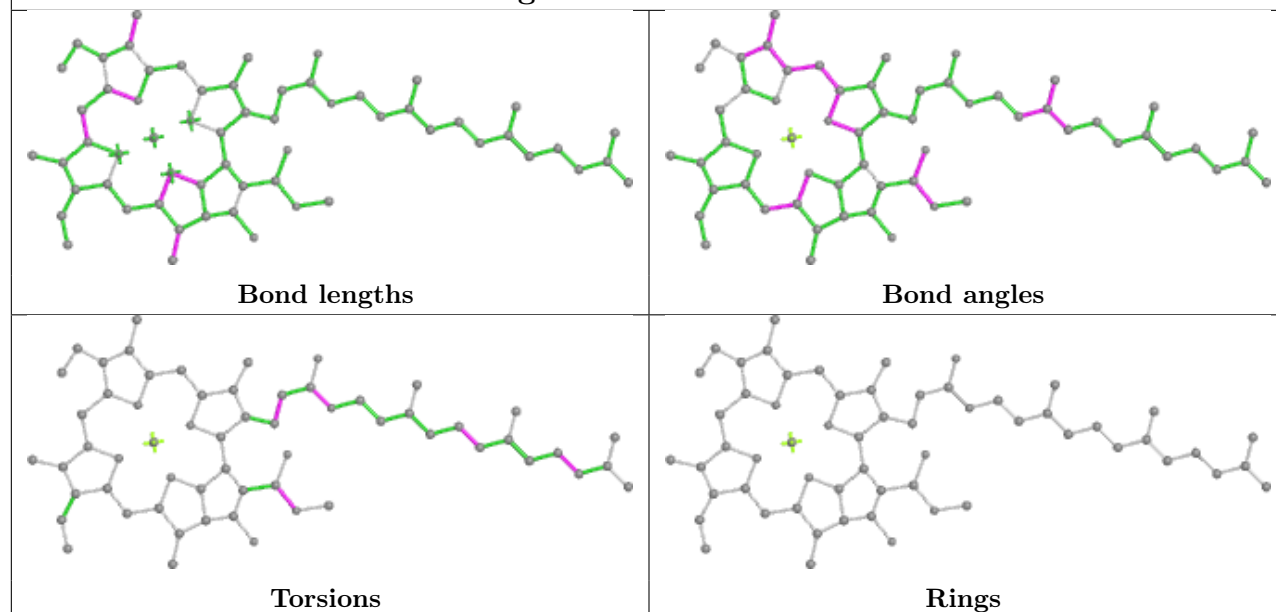
Ligand CLA AG 204



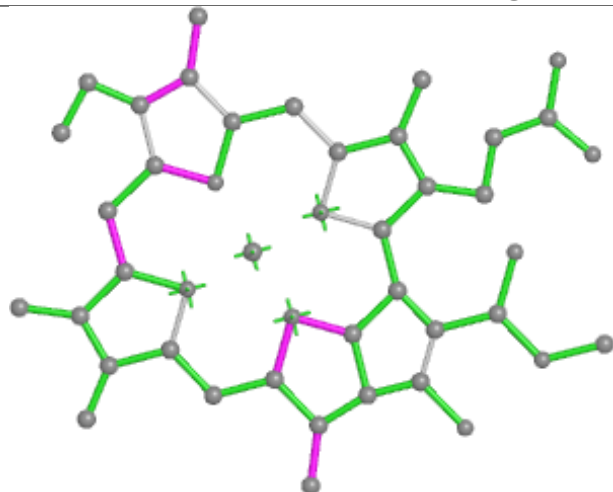
Ligand CLA B5 604



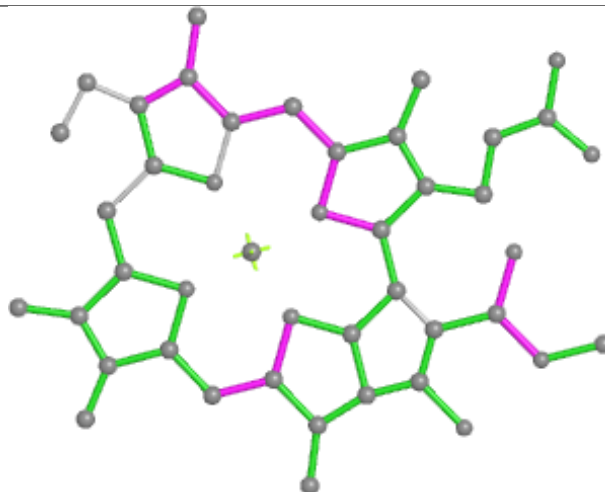
Ligand CLA AA 817



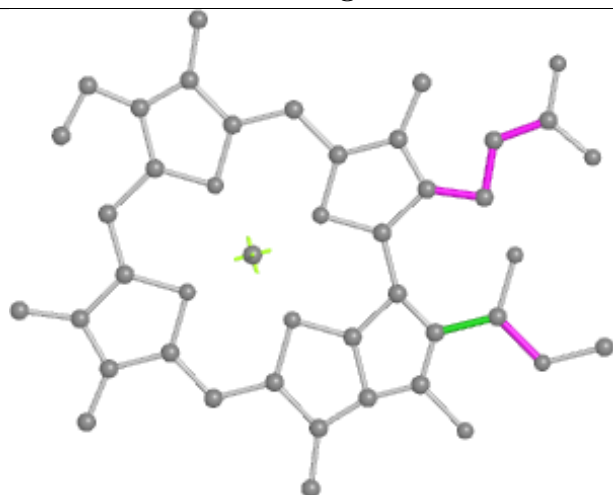
Ligand CLA B2 611



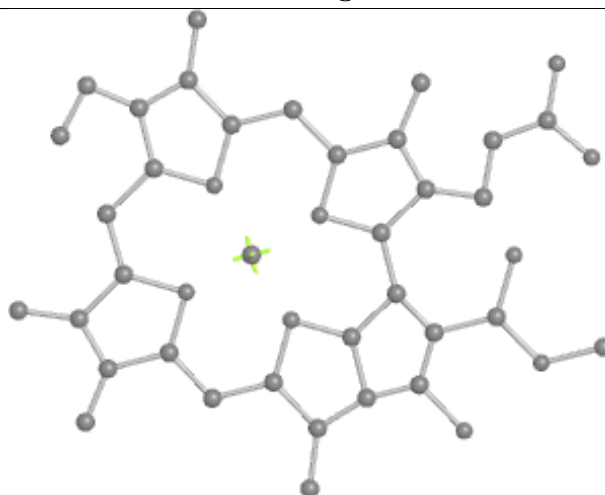
Bond lengths



Bond angles

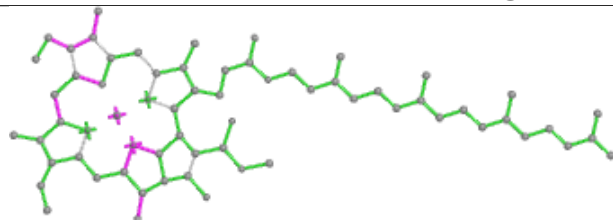


Torsions

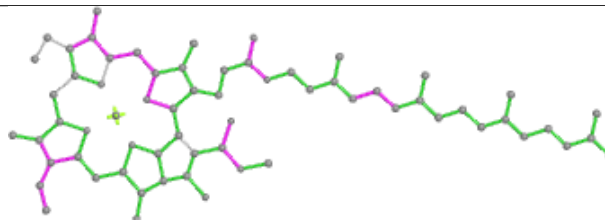


Rings

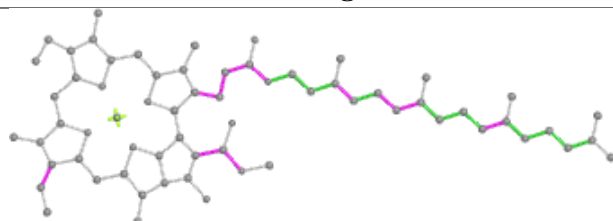
Ligand CLA BB 815



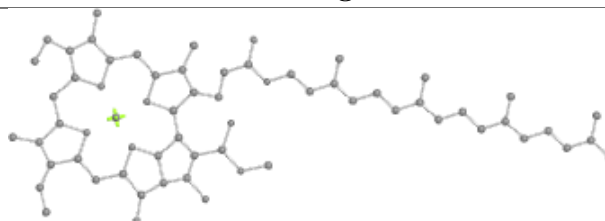
Bond lengths



Bond angles

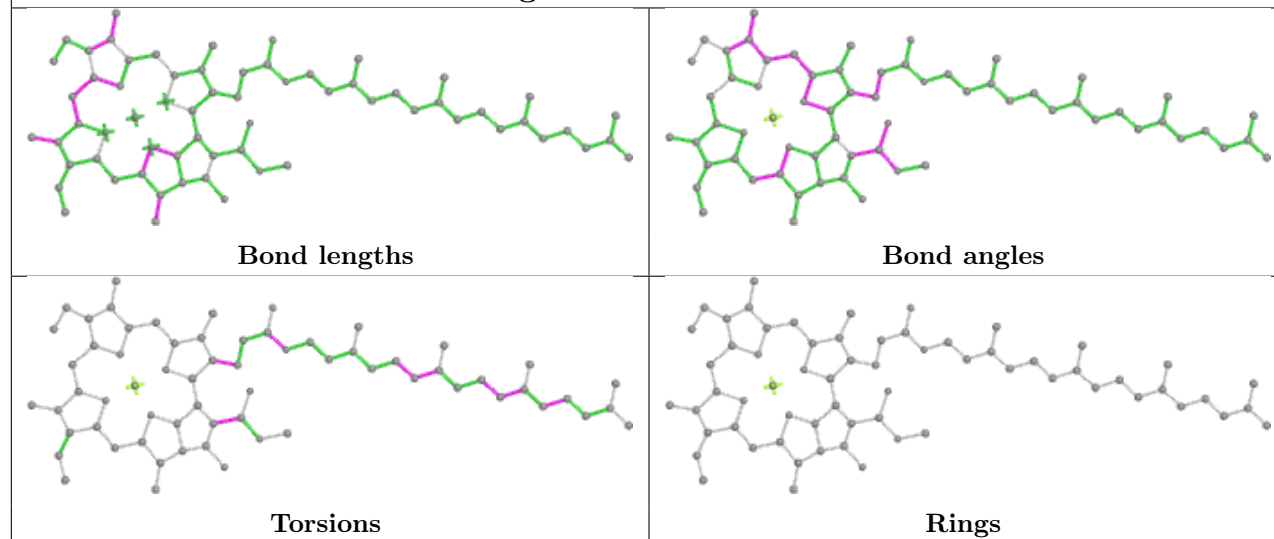


Torsions

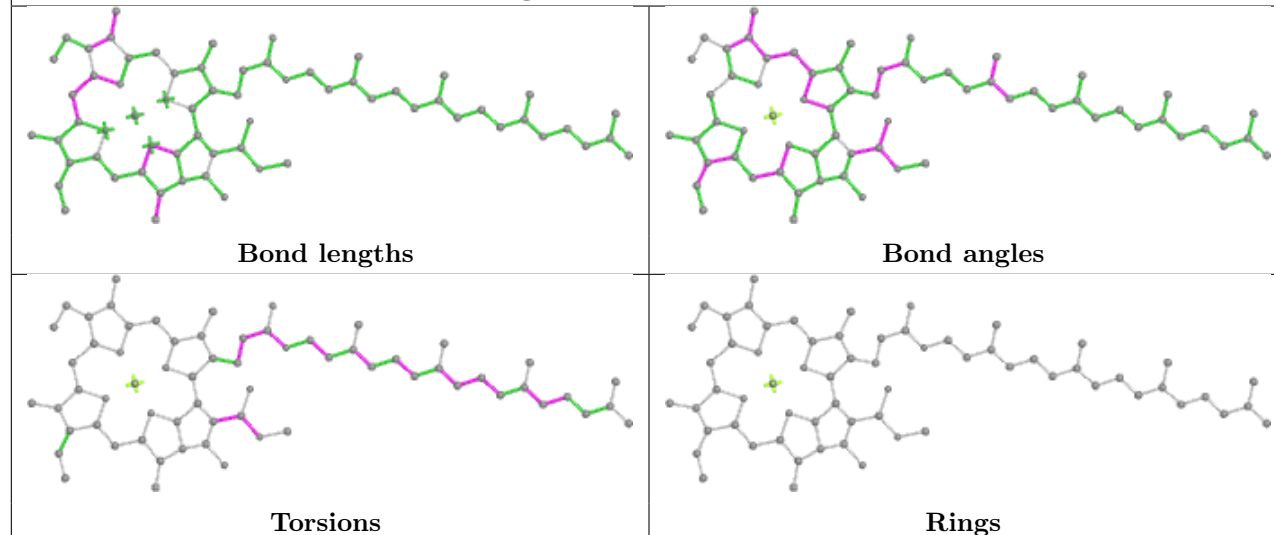


Rings

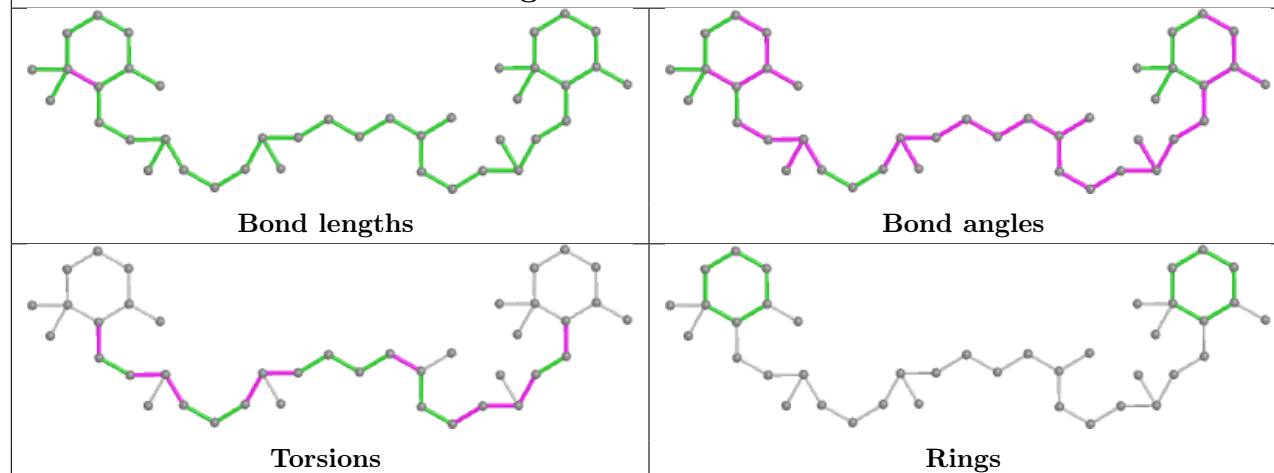
Ligand CLA BA 819

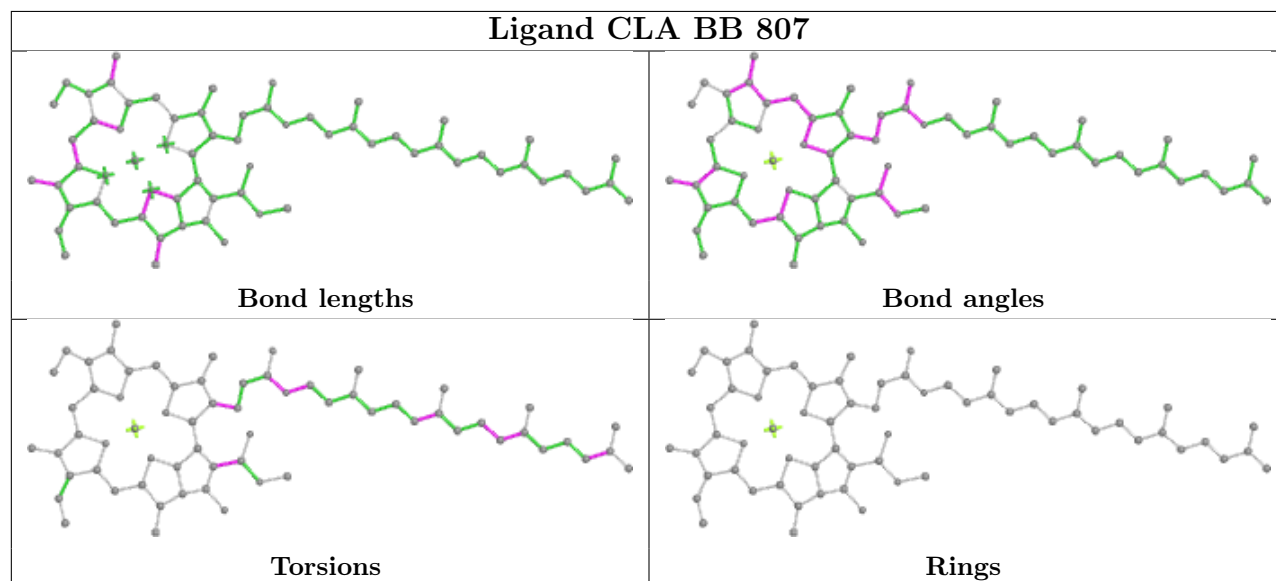
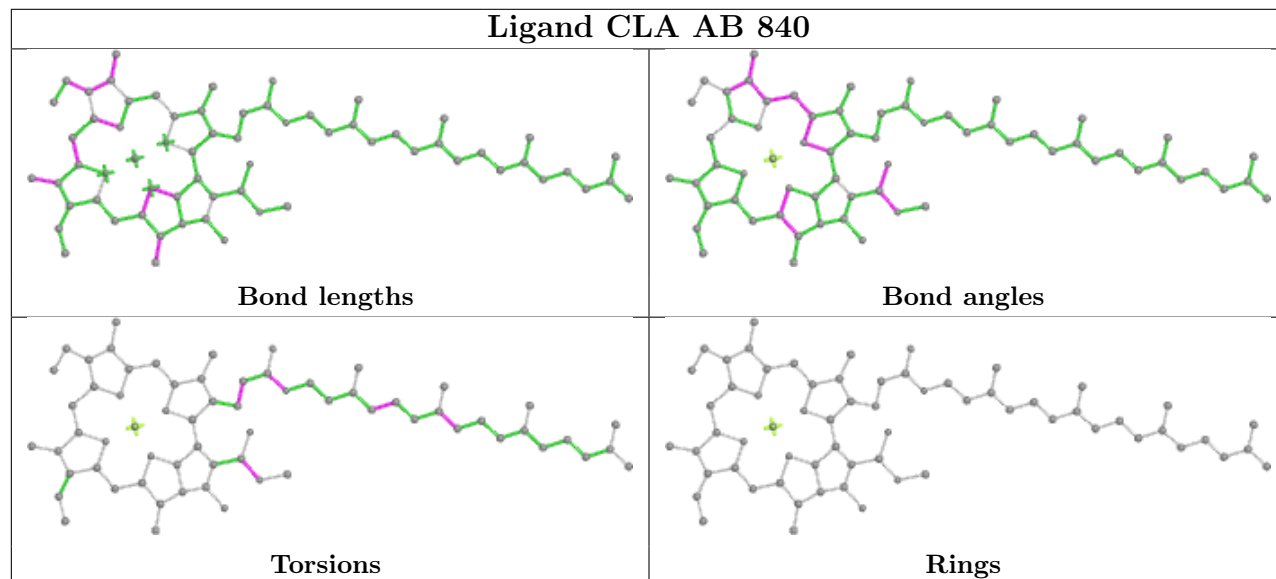
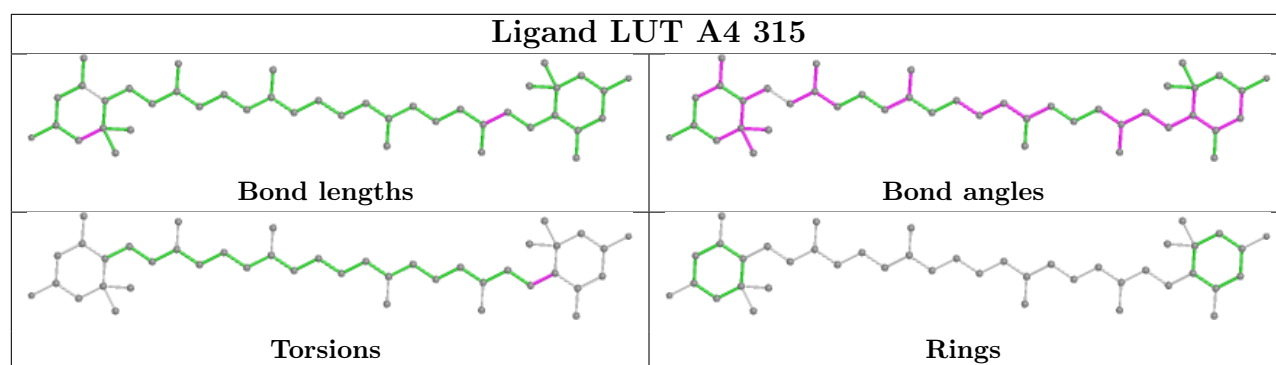


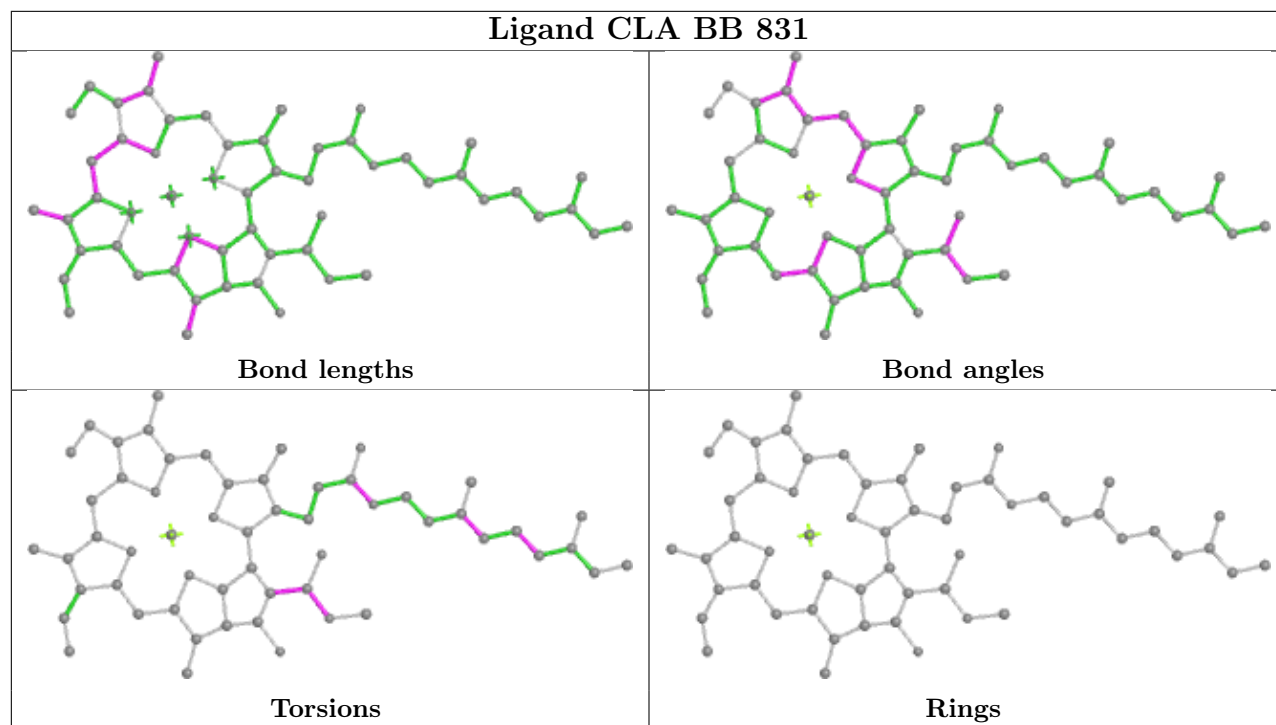
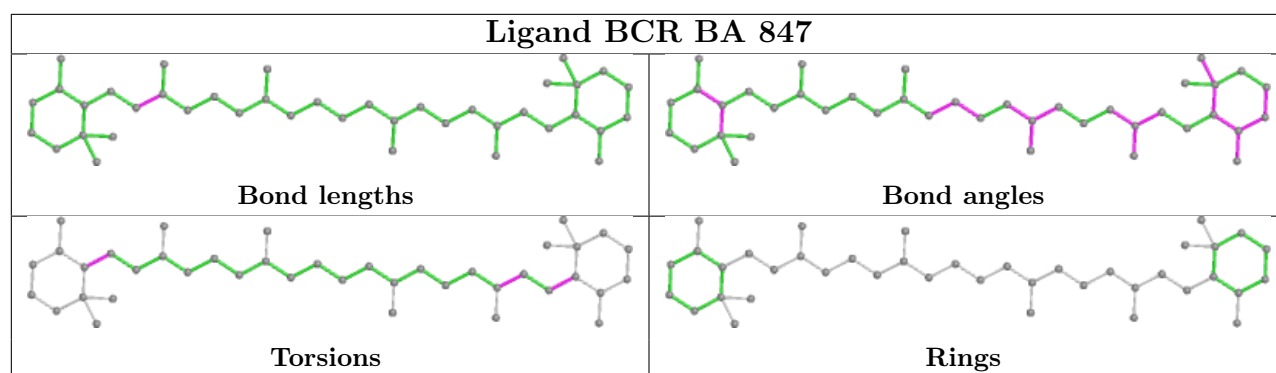
Ligand CLA AA 842



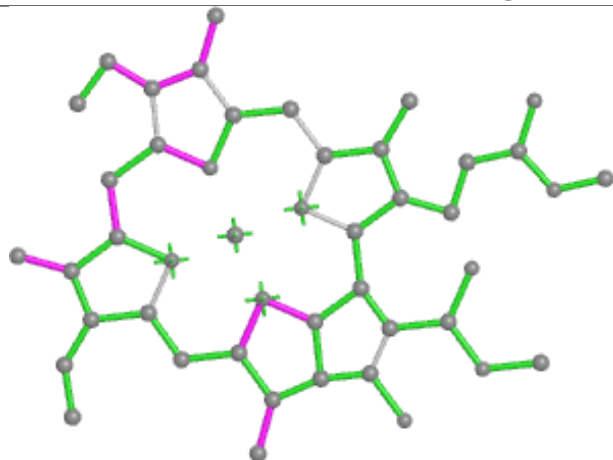
Ligand BCR BL 306



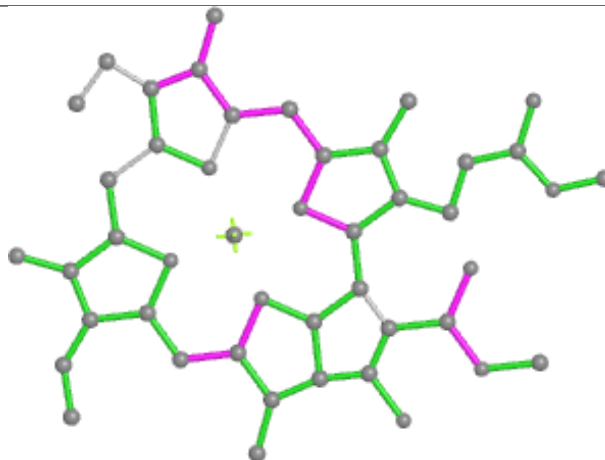




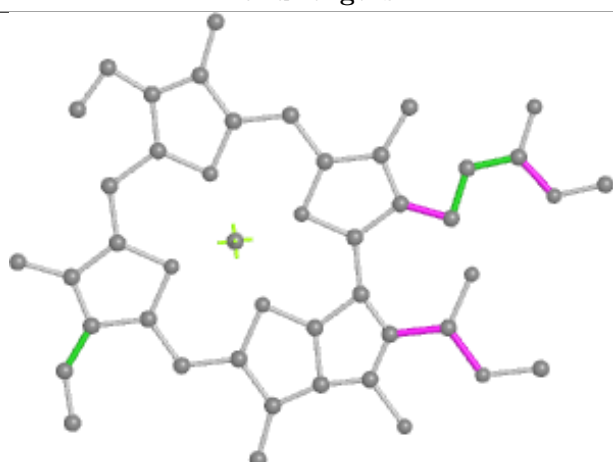
Ligand CLA AK 203



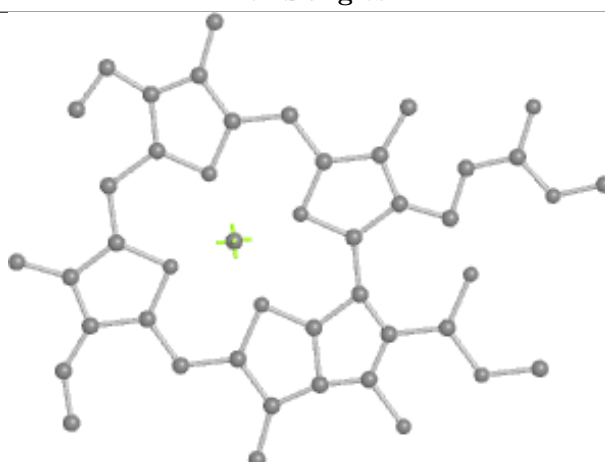
Bond lengths



Bond angles

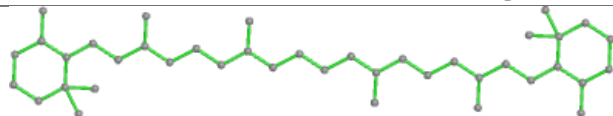


Torsions

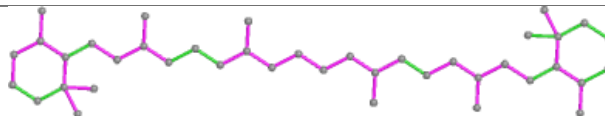


Rings

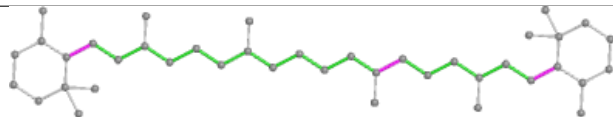
Ligand BCR AB 844



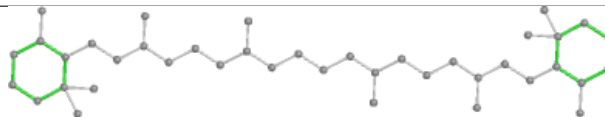
Bond lengths



Bond angles

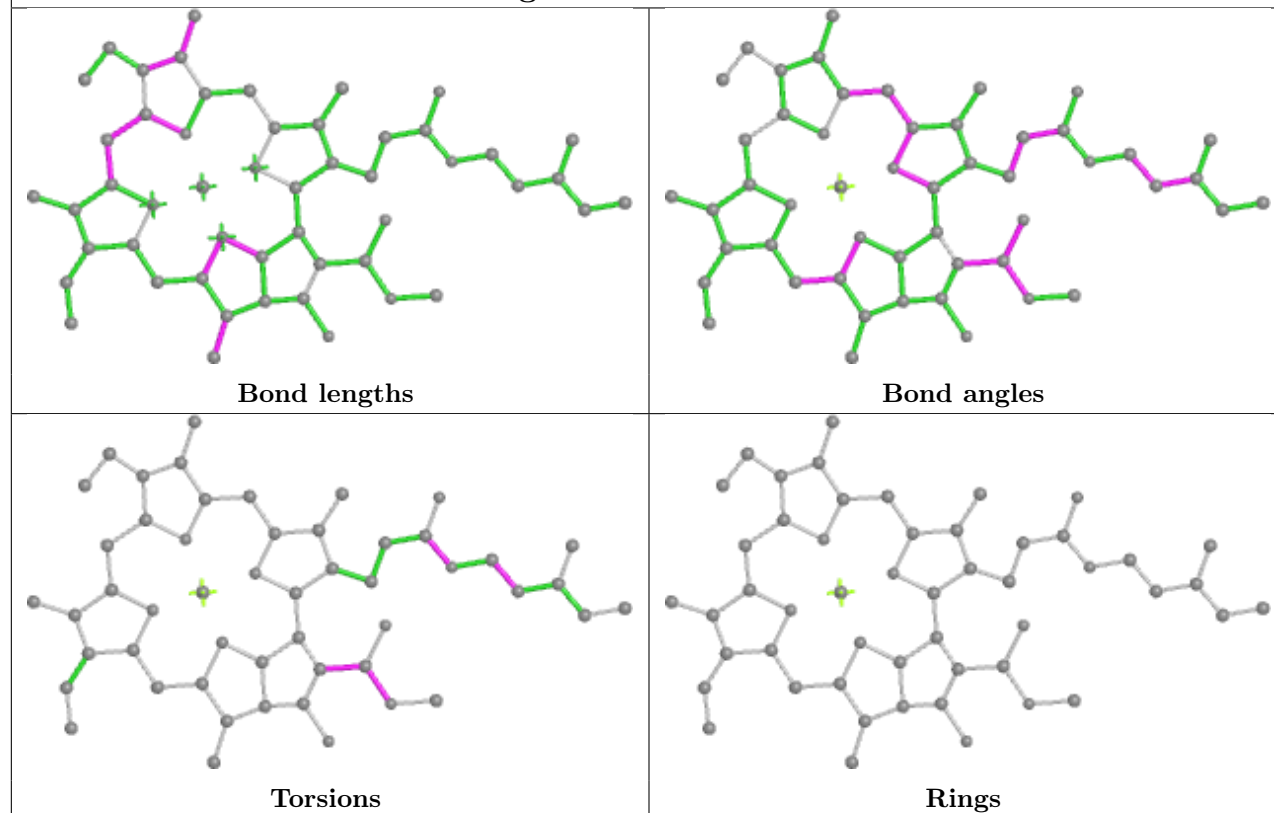


Torsions

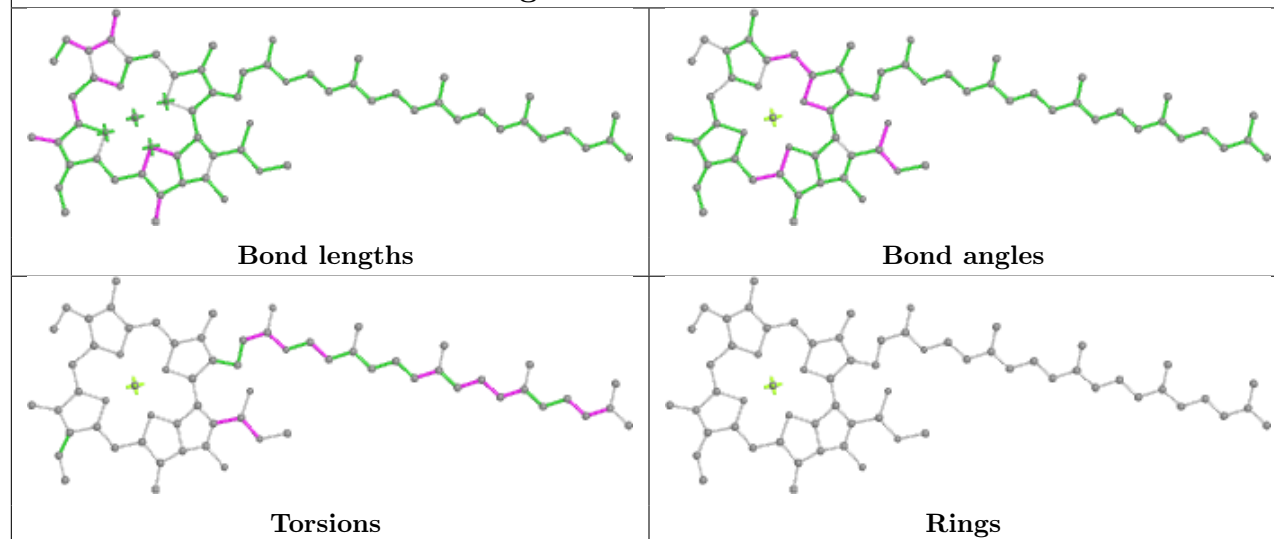


Rings

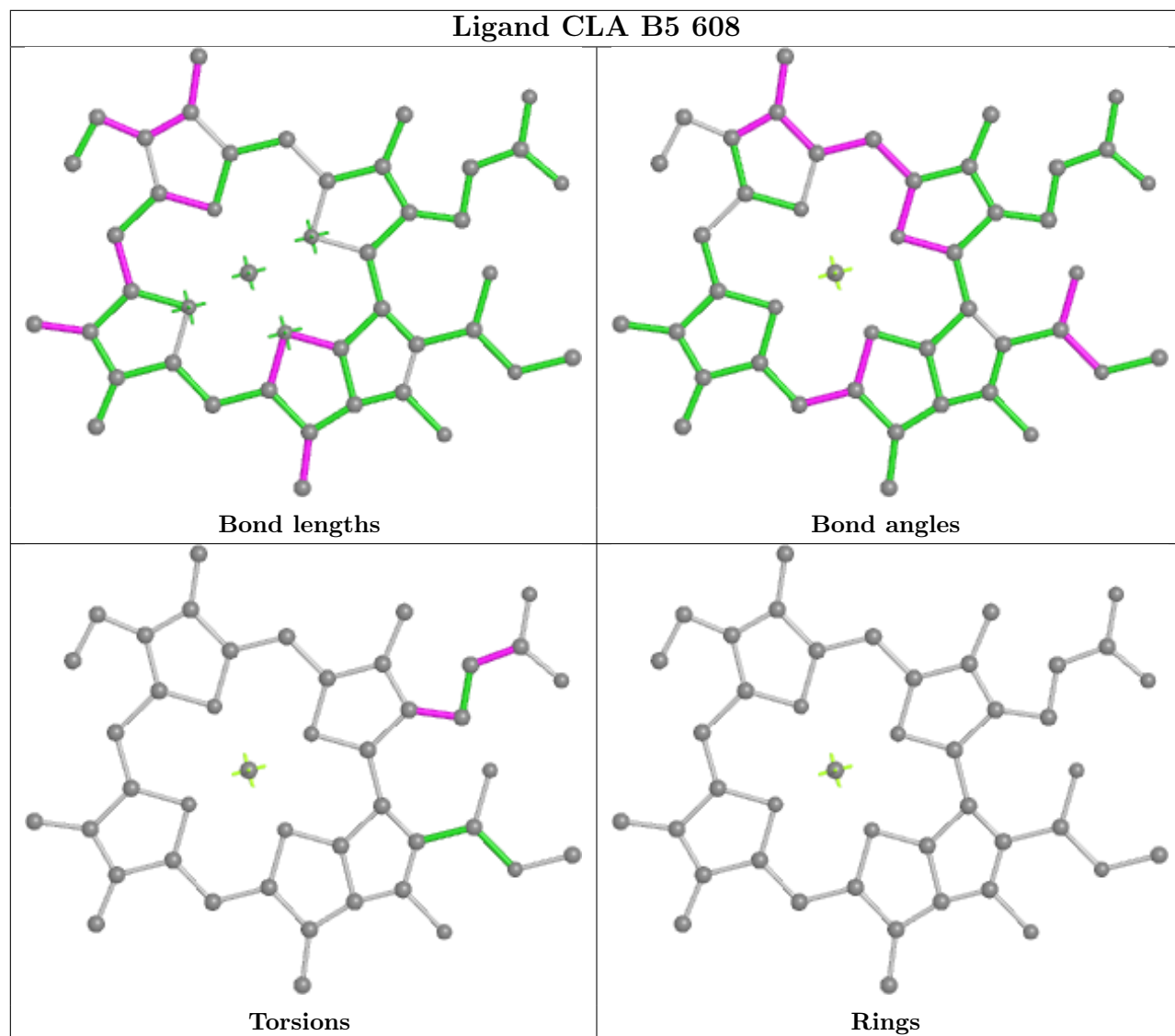
Ligand CLA BA 839

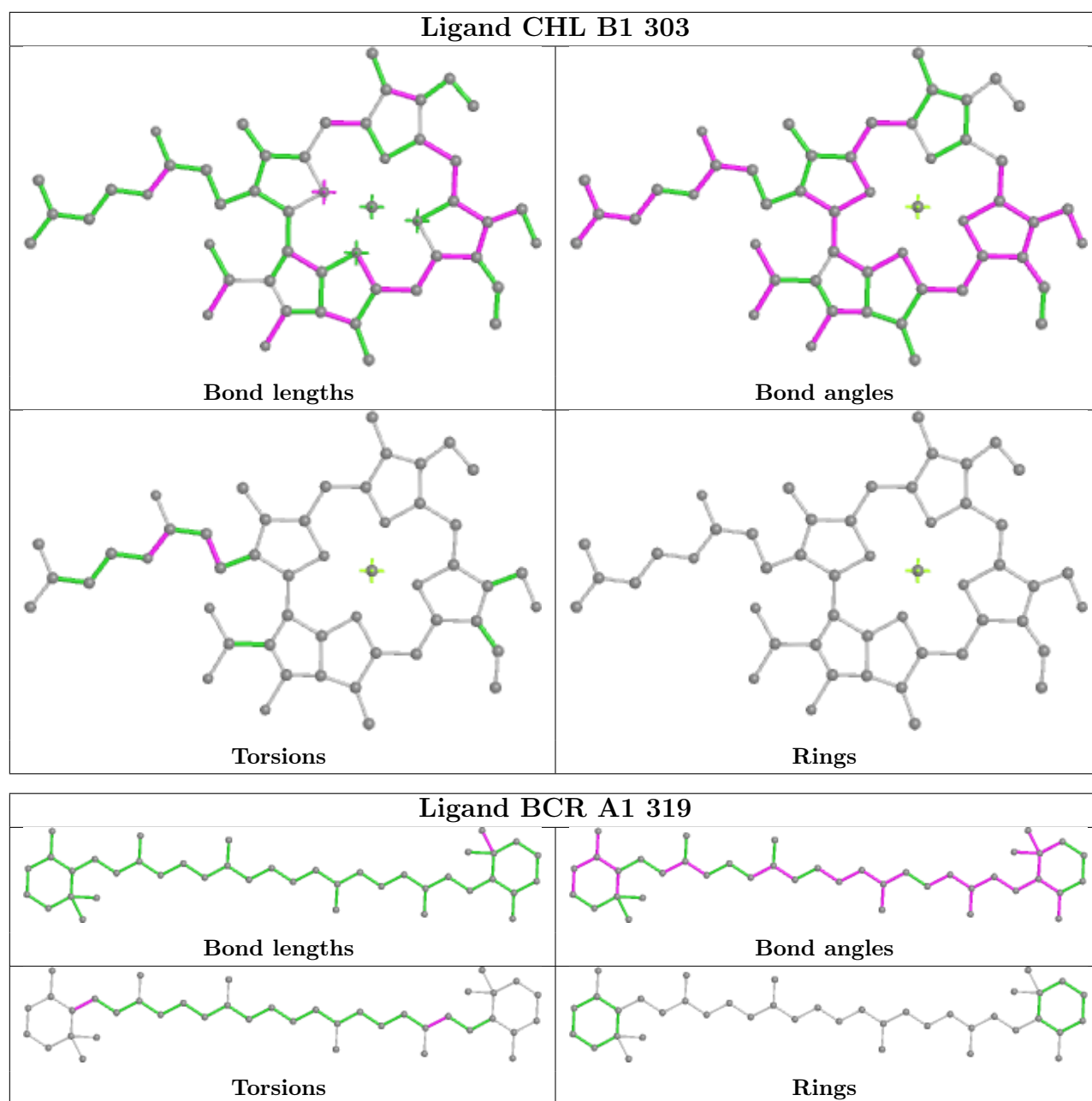


Ligand CLA BB 835

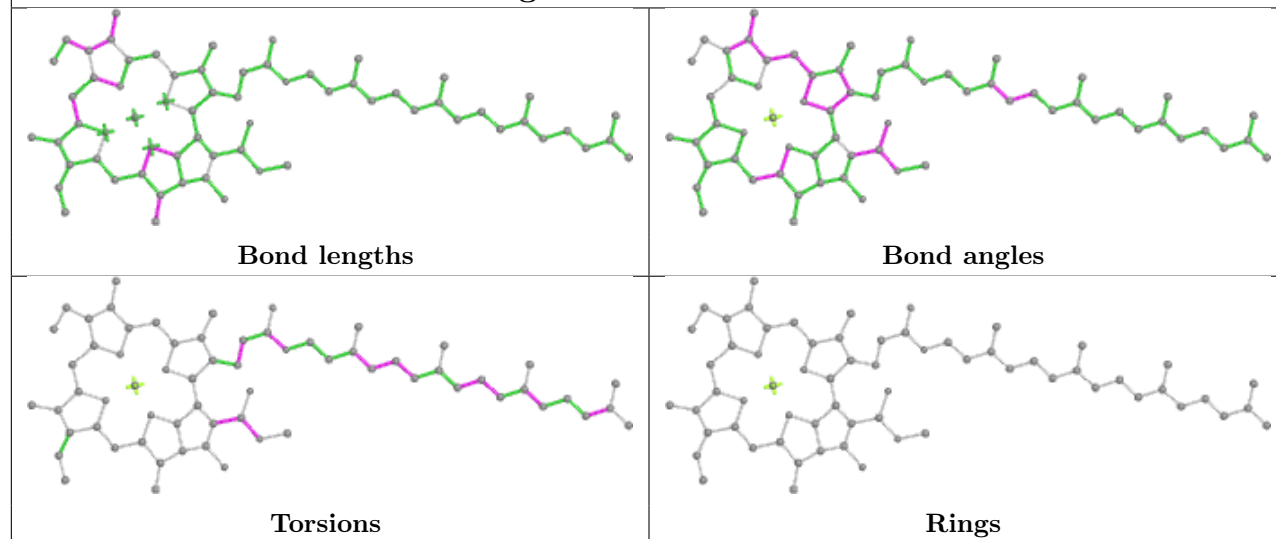


Ligand CLA B5 608

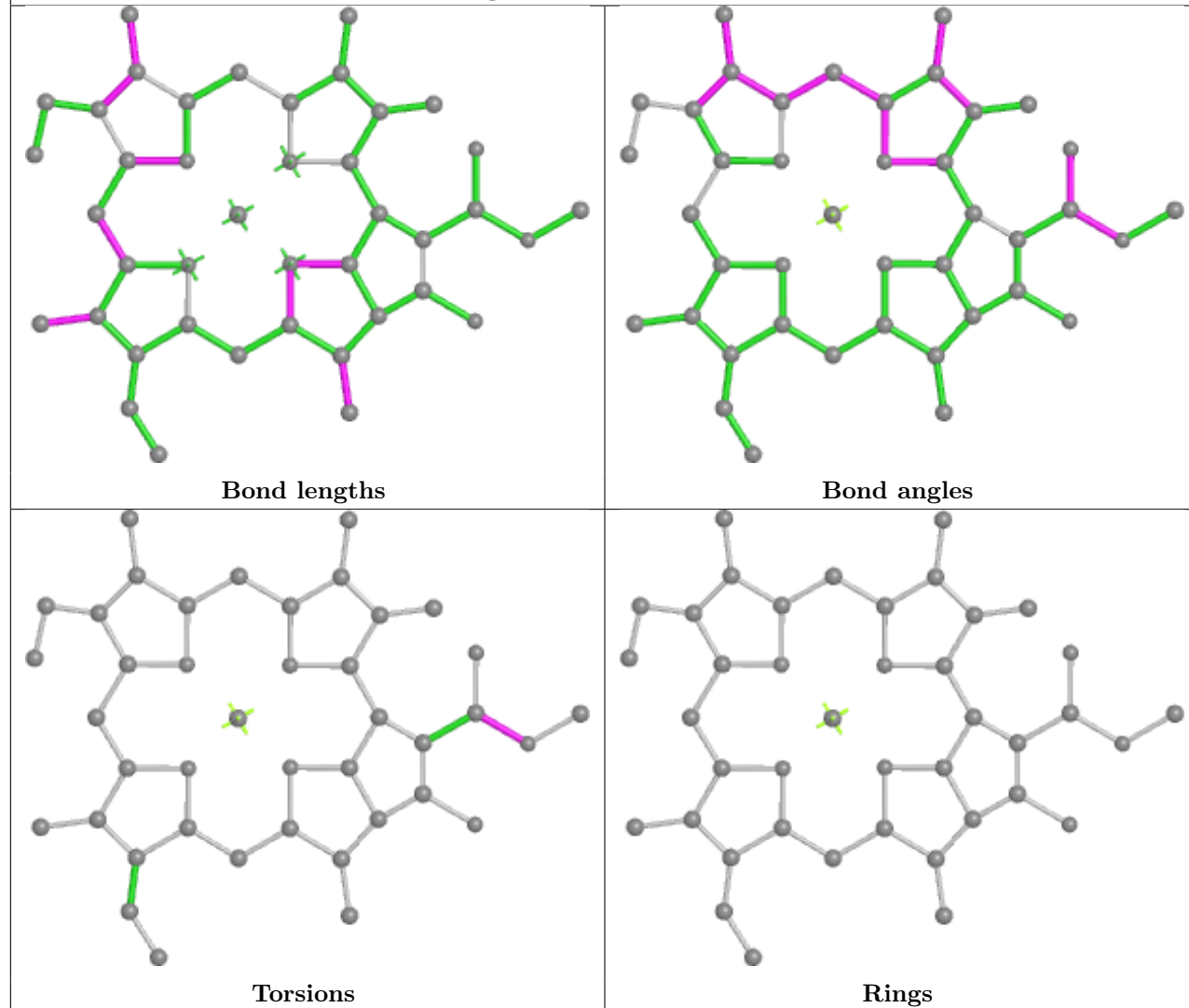




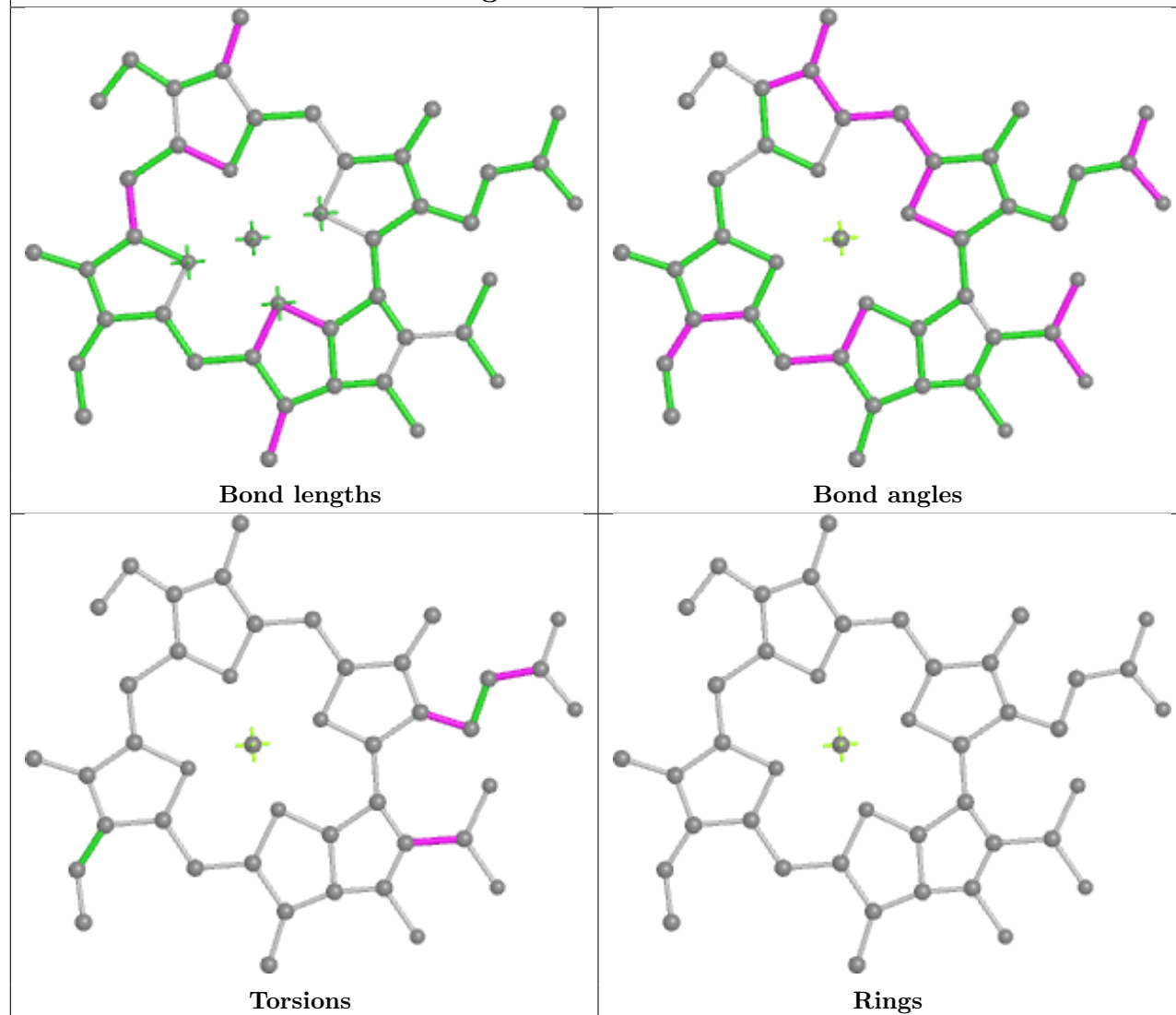
Ligand CLA AB 842



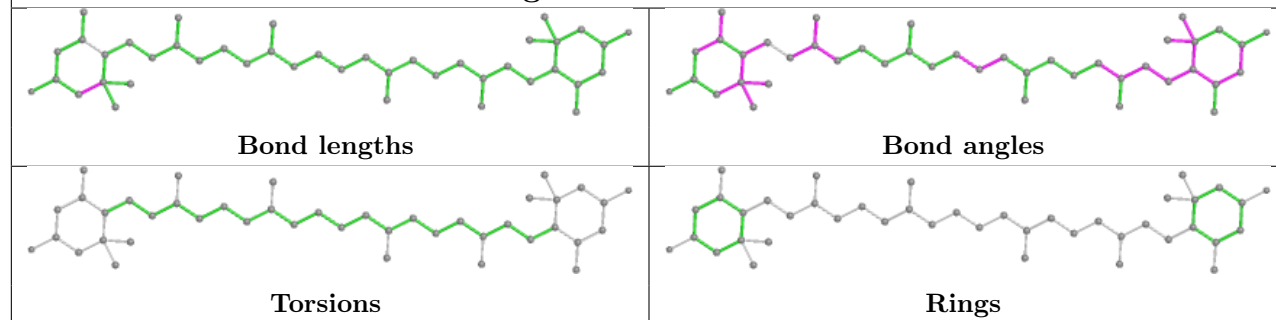
Ligand CLA BB 822



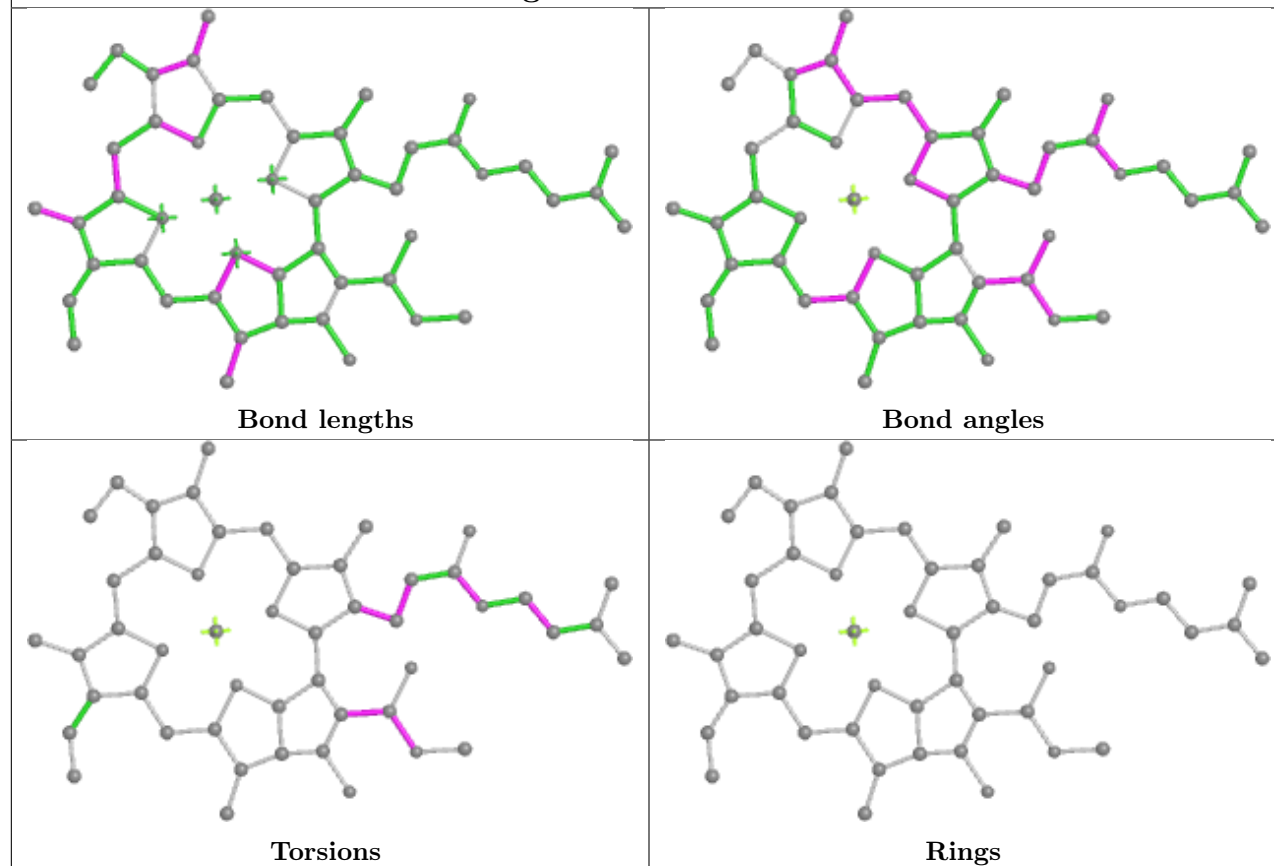
Ligand CLA A1 309



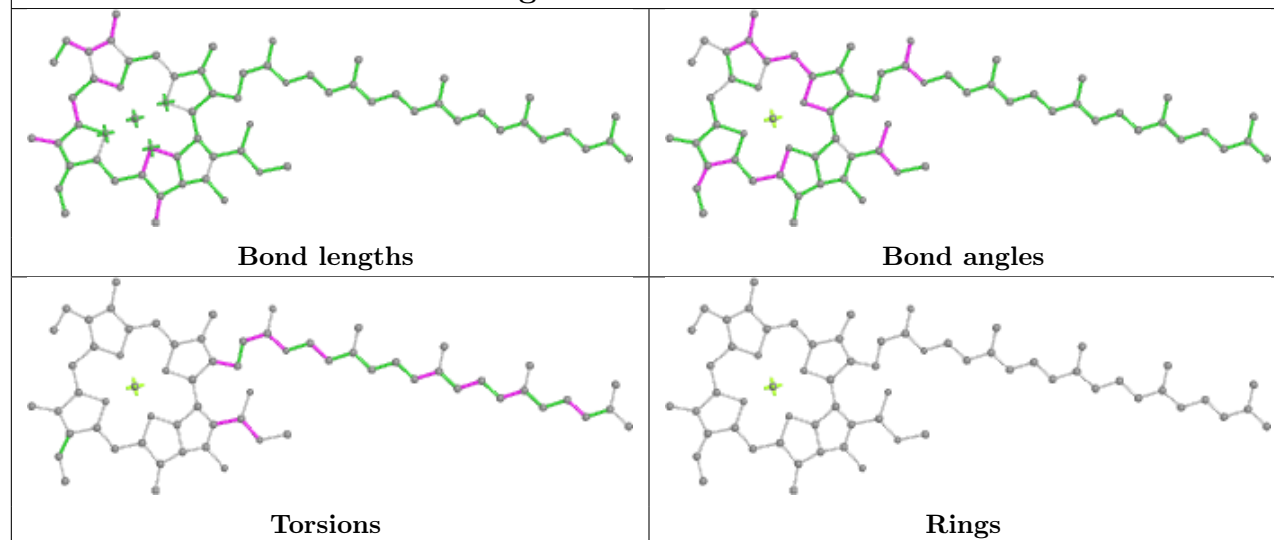
Ligand LUT A1 317

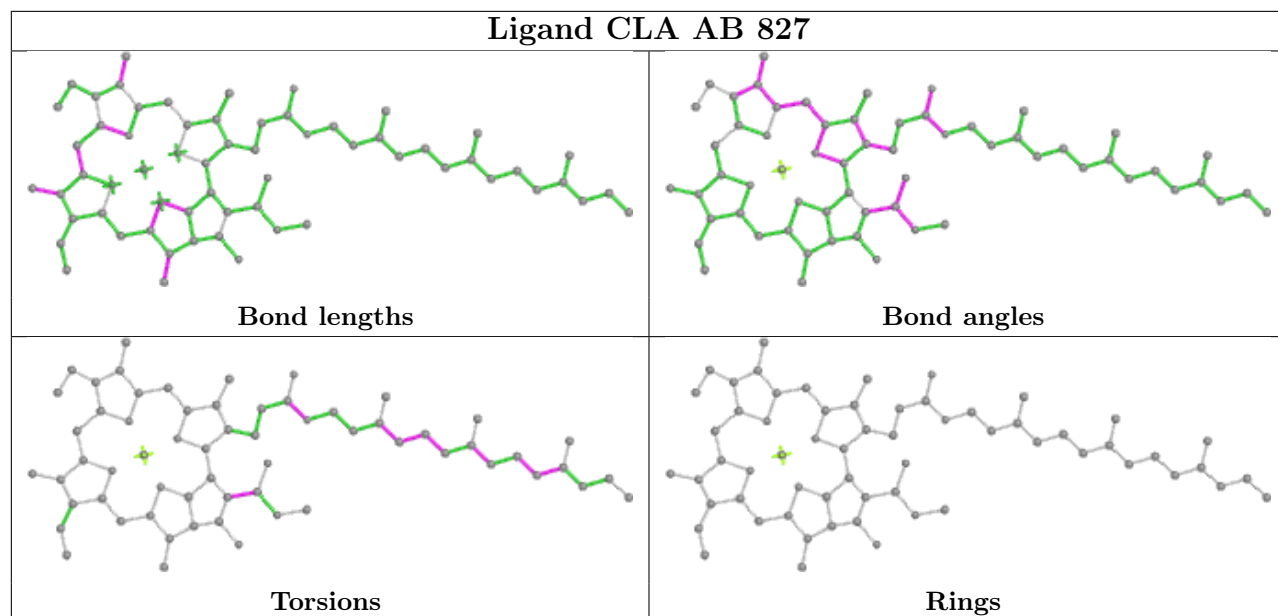


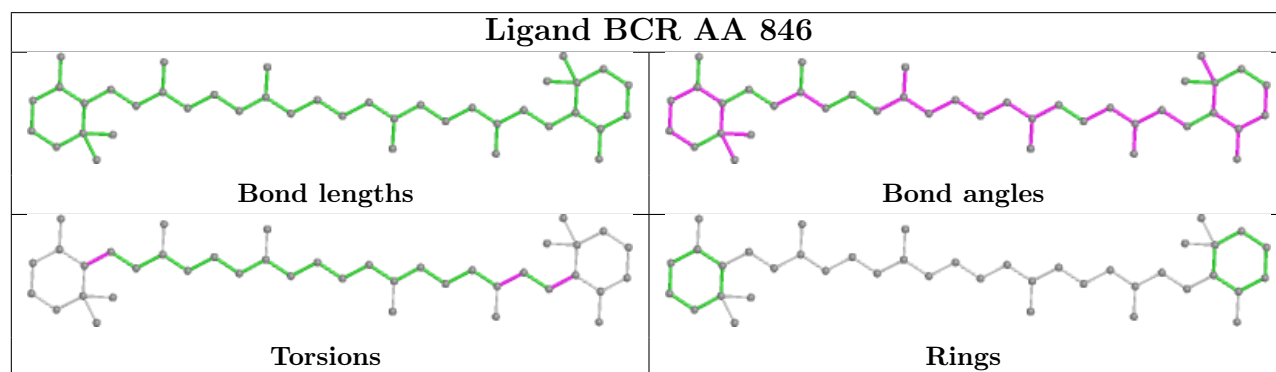
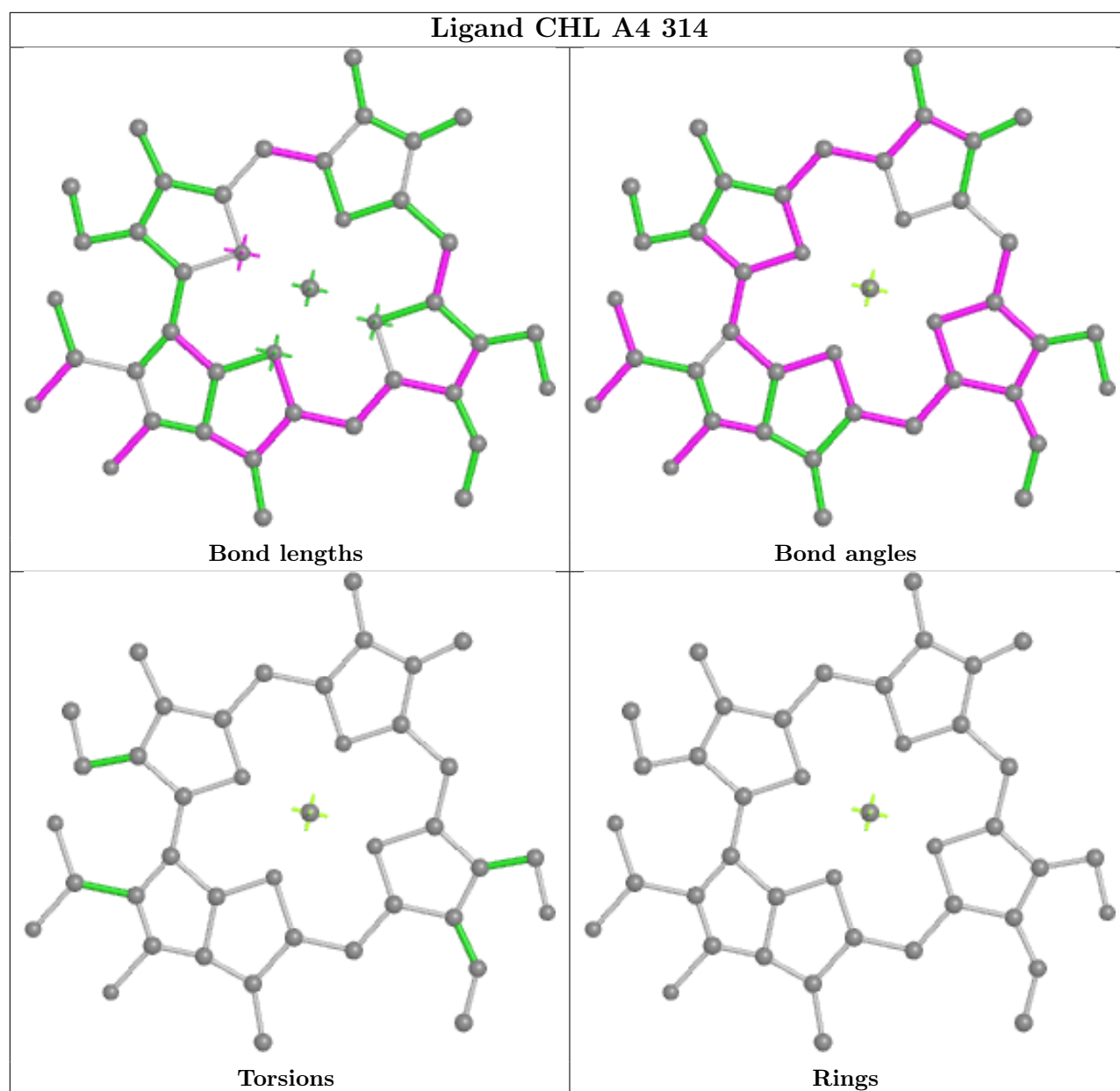
Ligand CLA A4 313

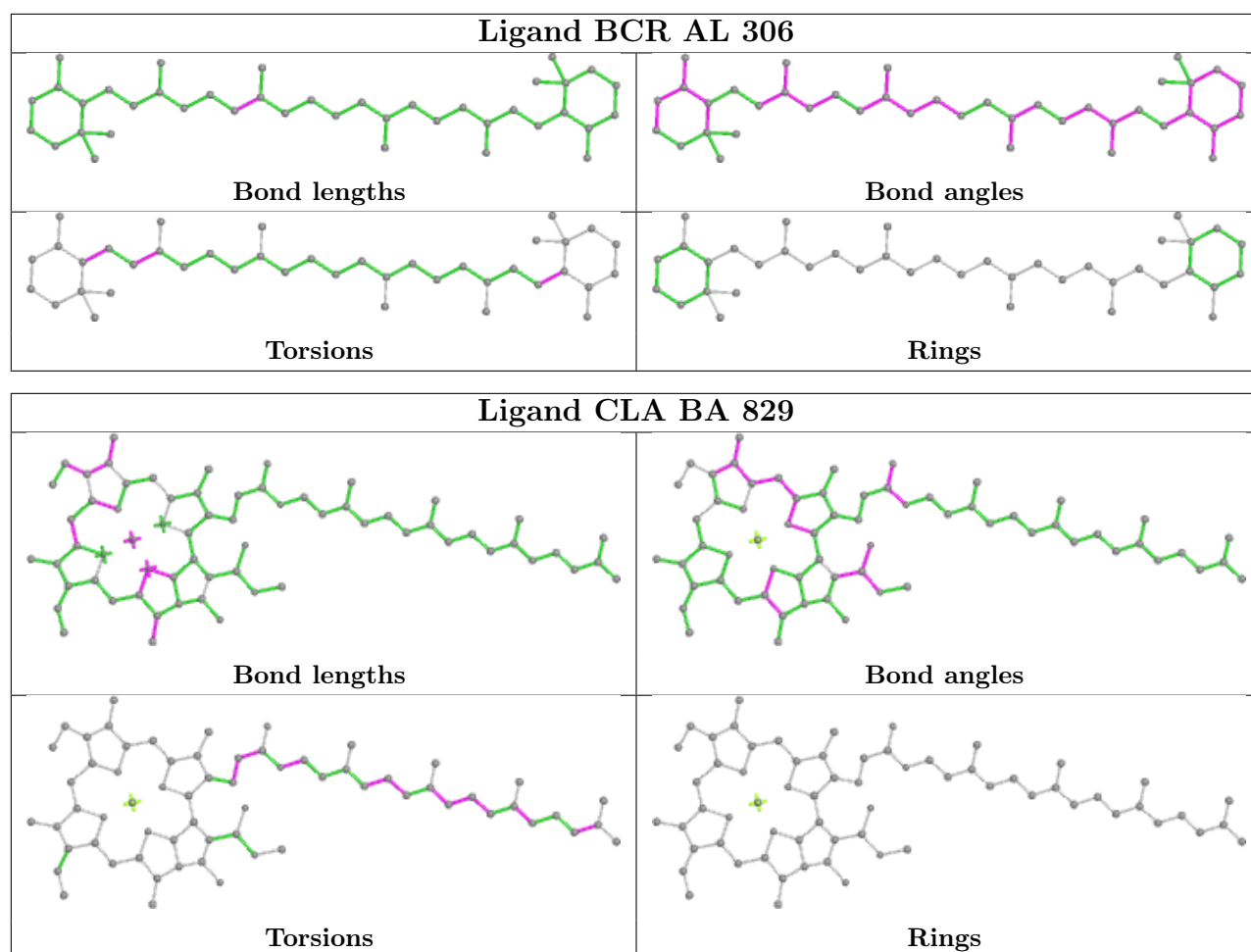


Ligand CLA AB 834

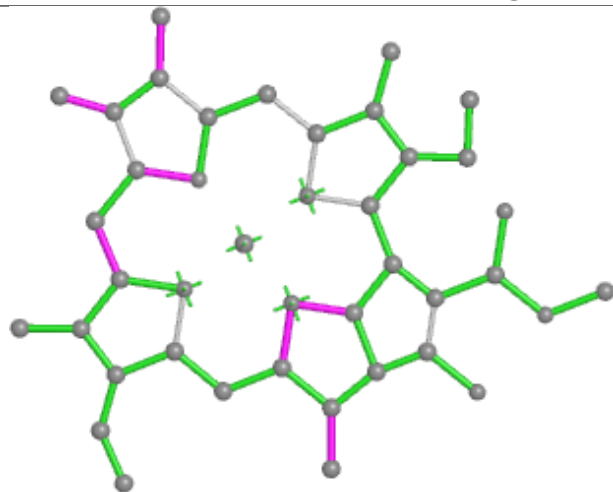




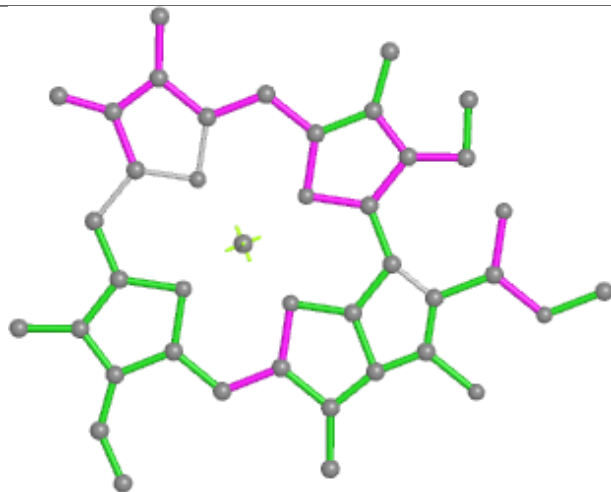




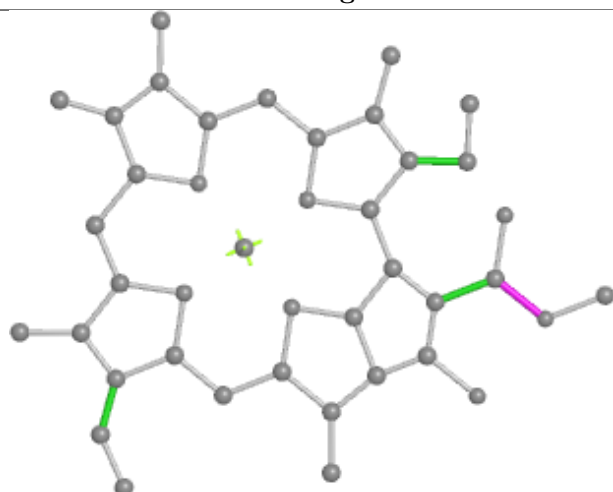
Ligand CLA B3 305



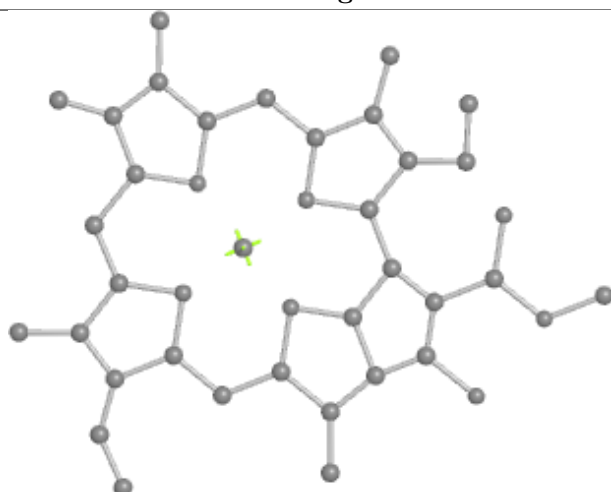
Bond lengths



Bond angles

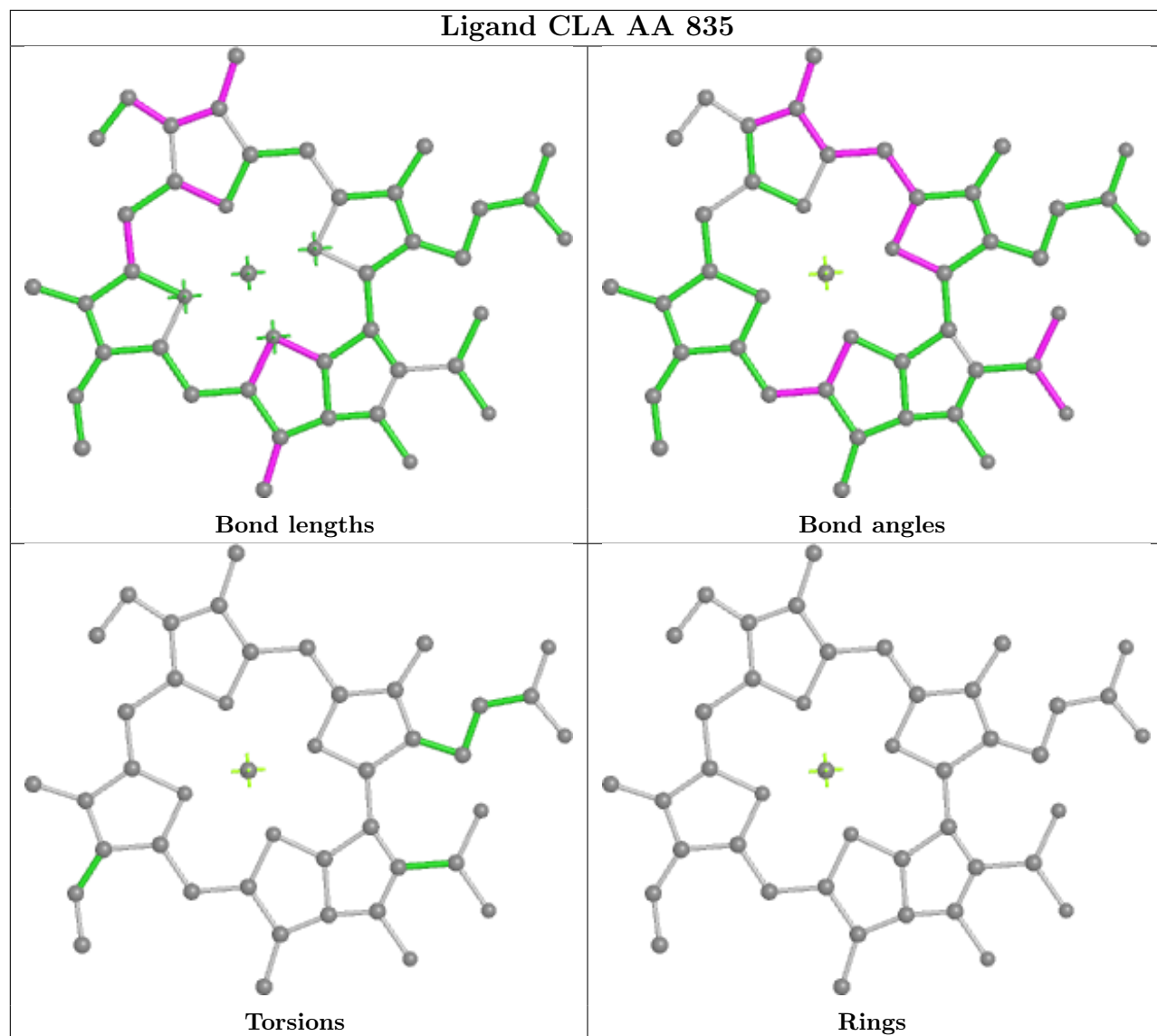


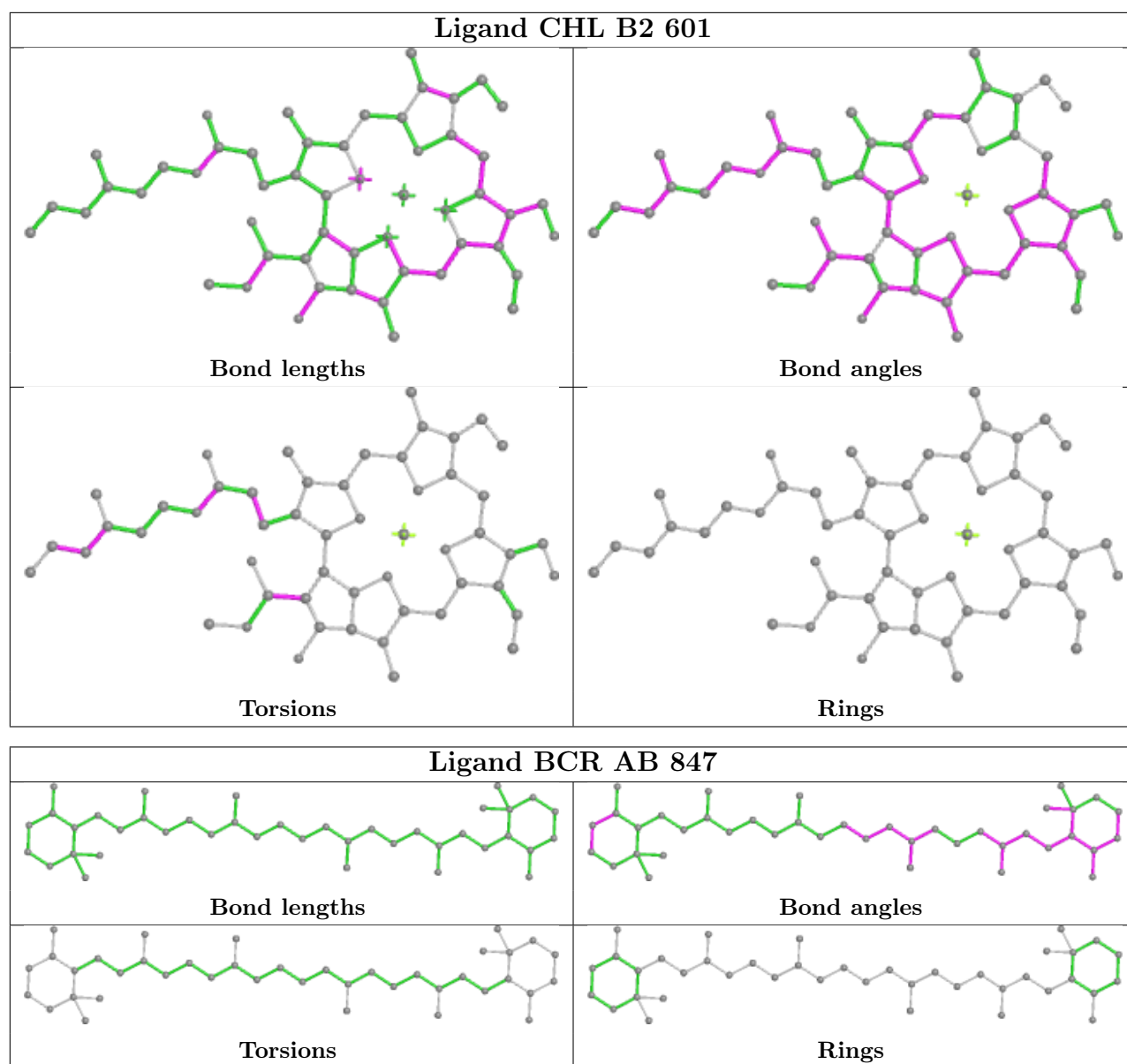
Torsions

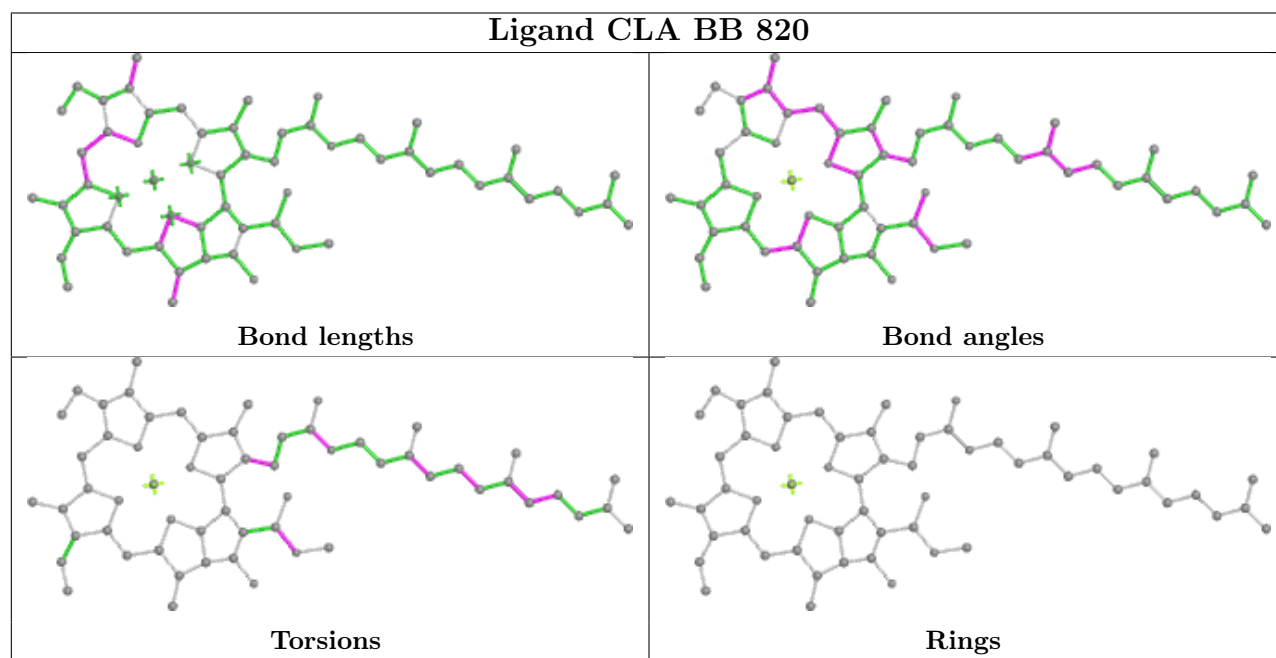
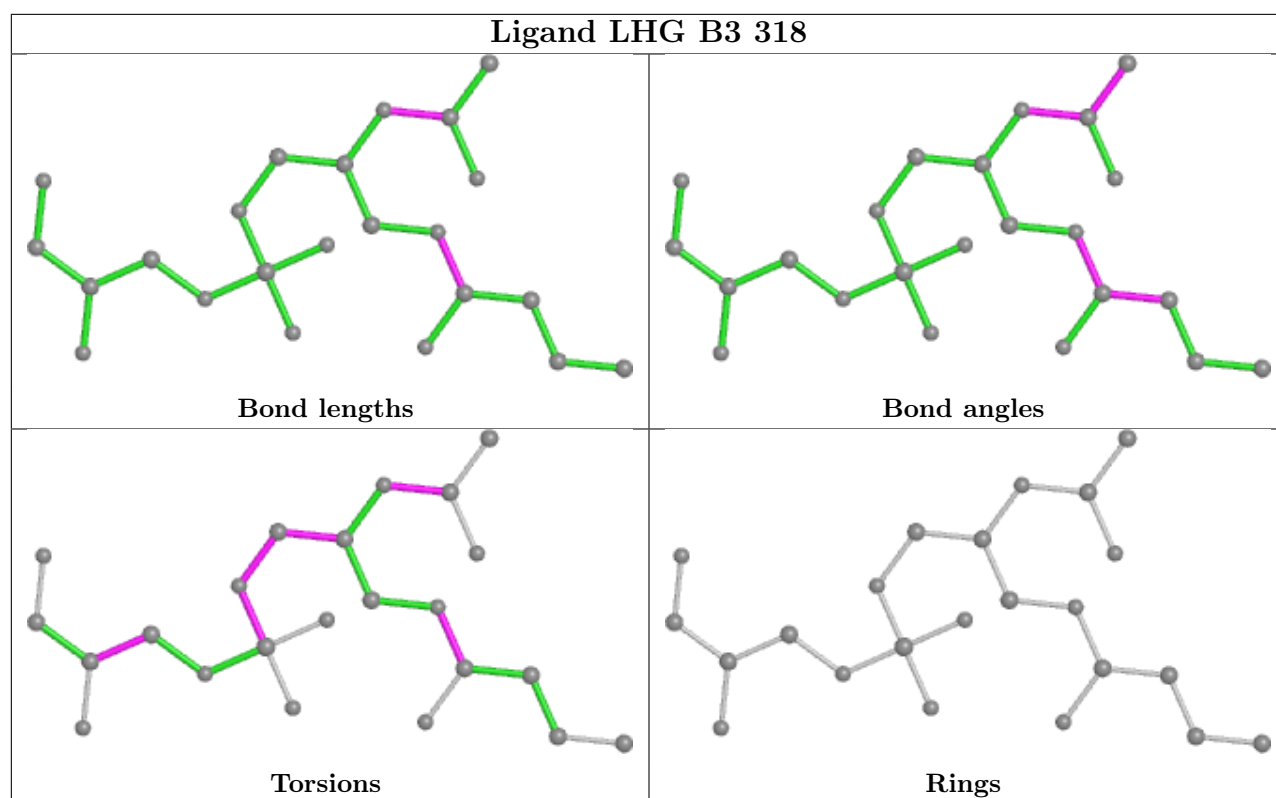


Rings

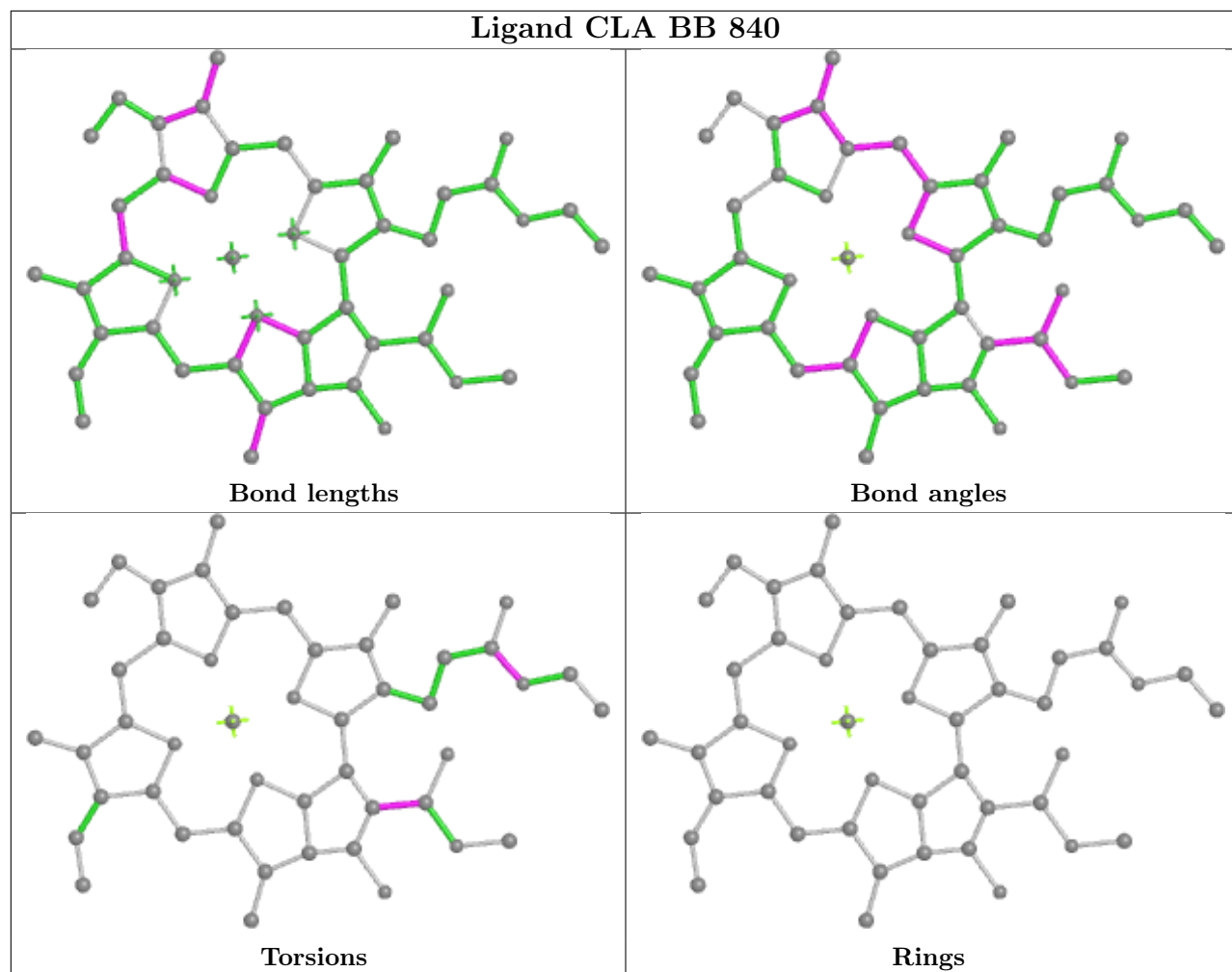
Ligand CLA AA 835



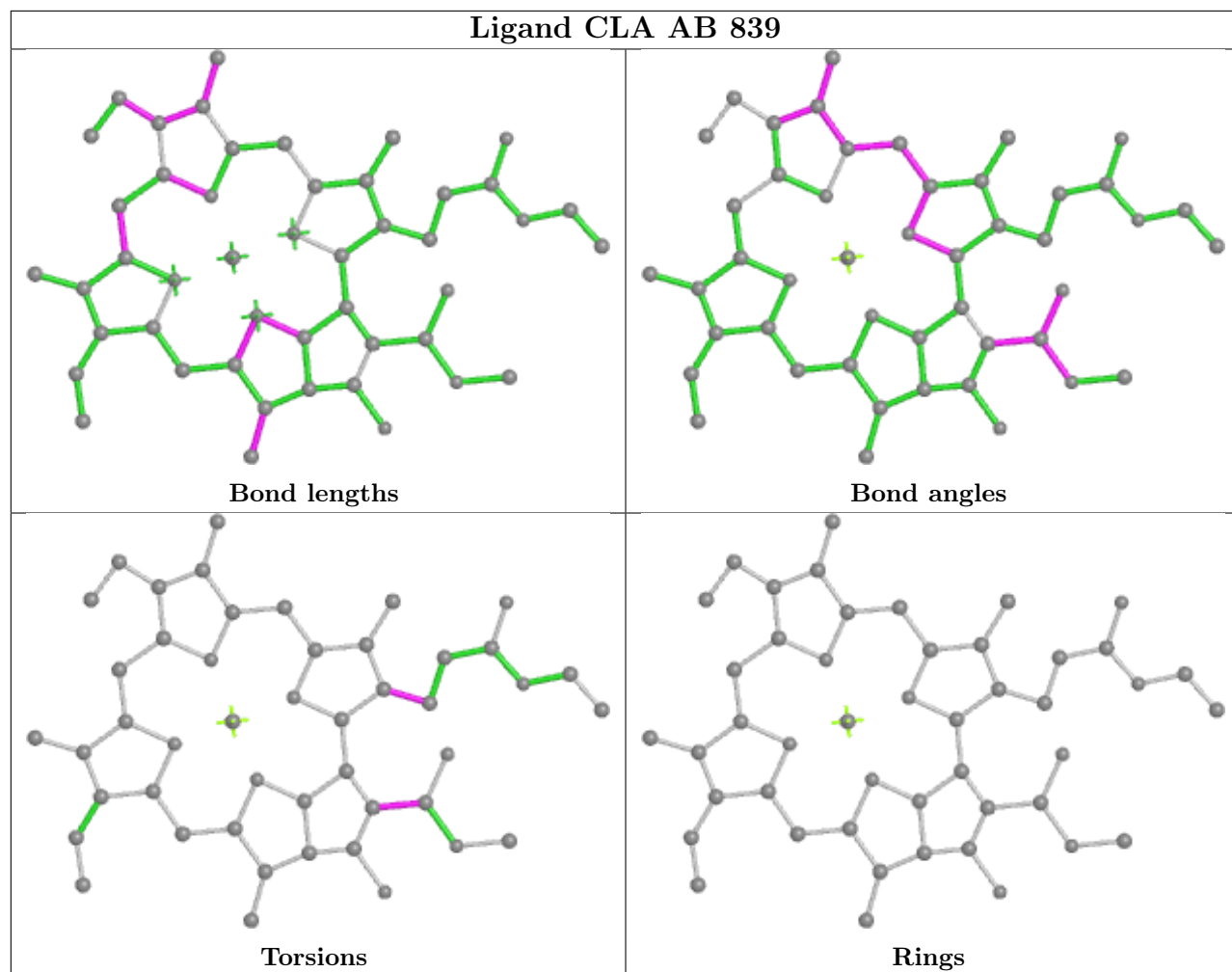


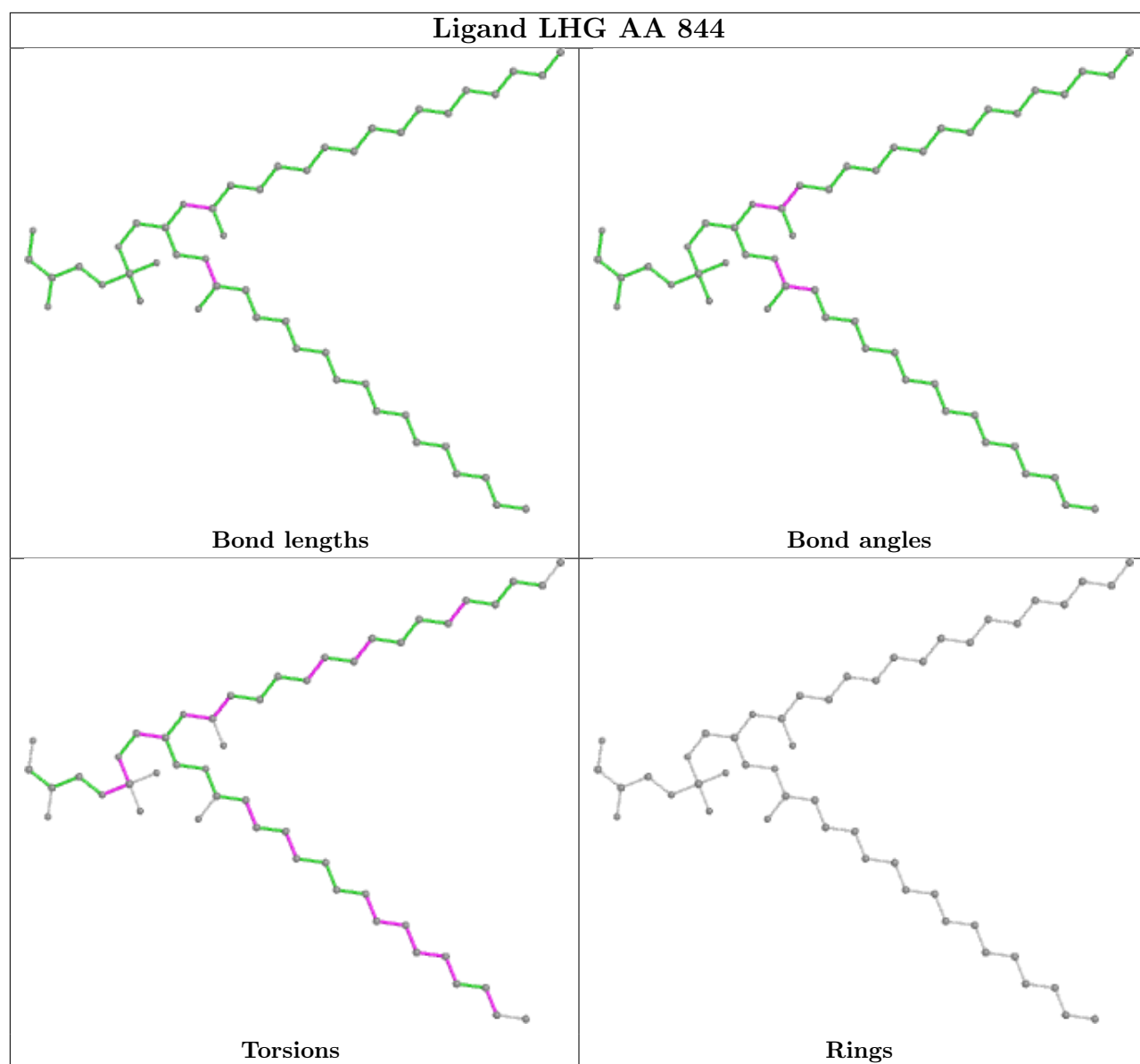


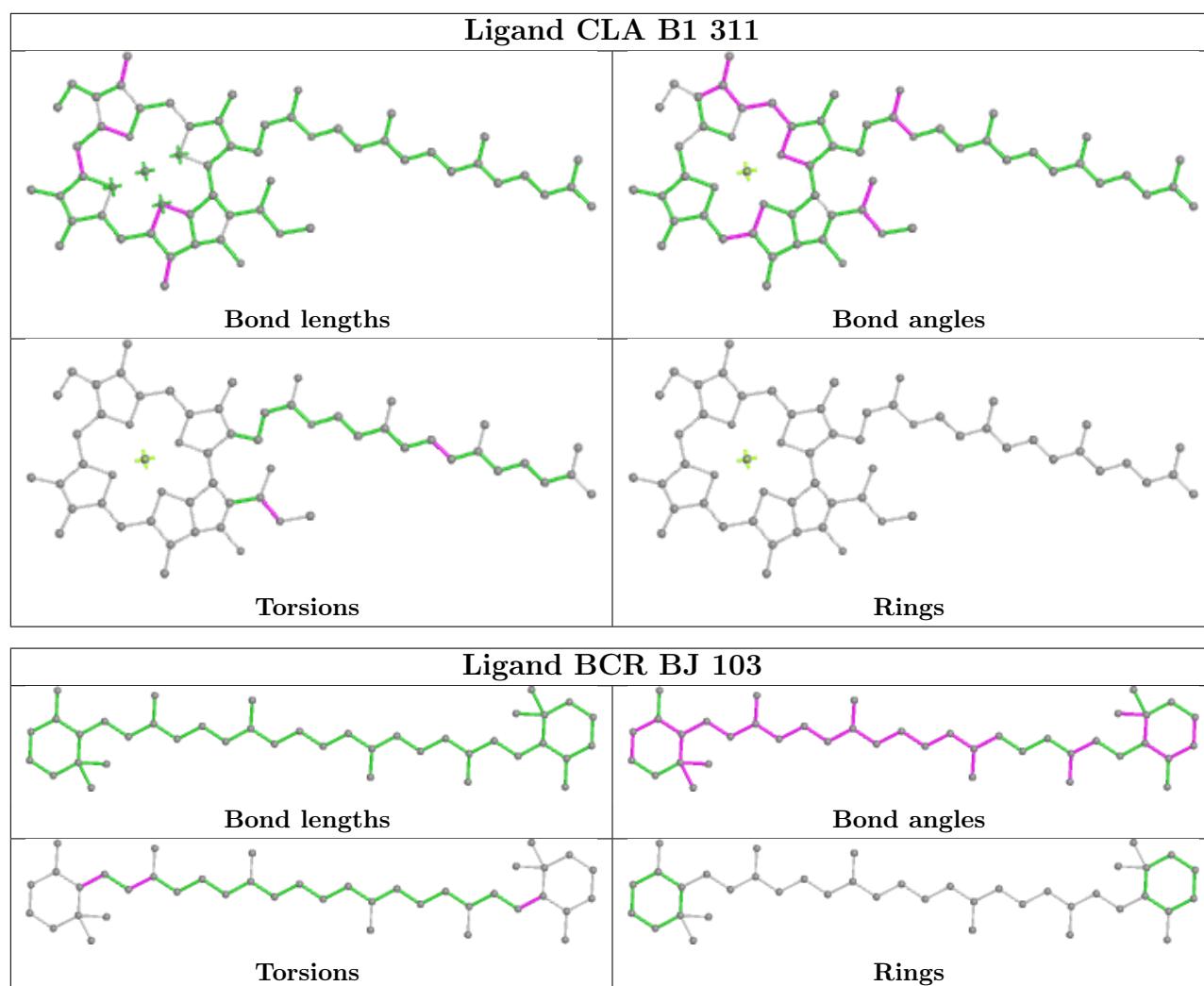
Ligand CLA BB 840



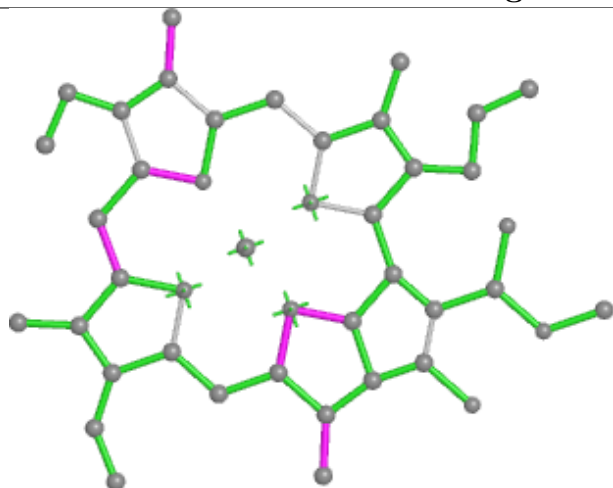
Ligand CLA AB 839



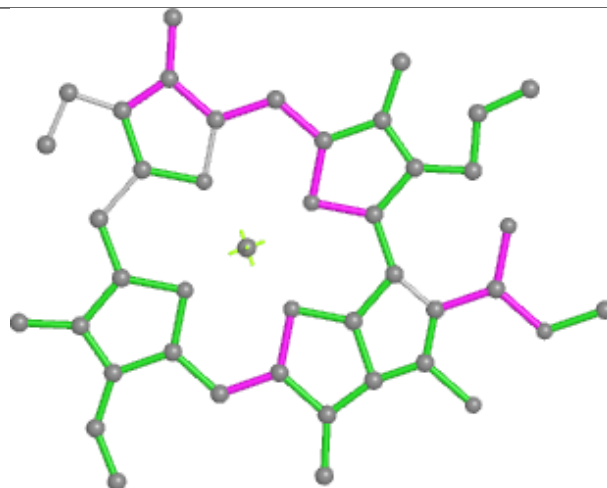




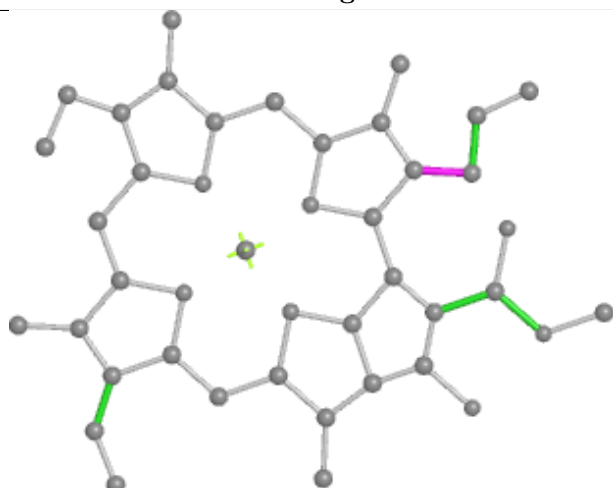
Ligand CLA B2 613



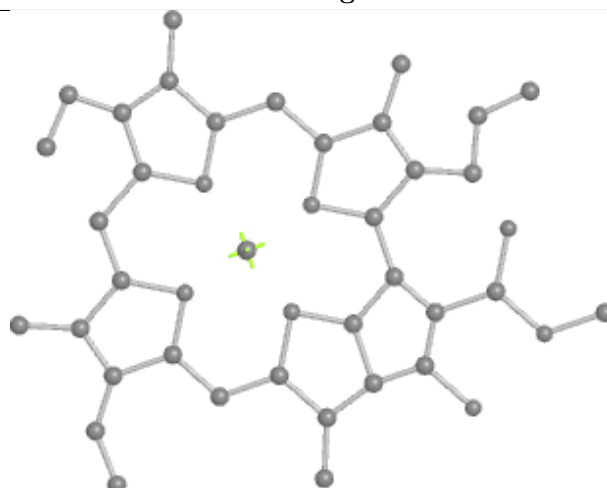
Bond lengths



Bond angles

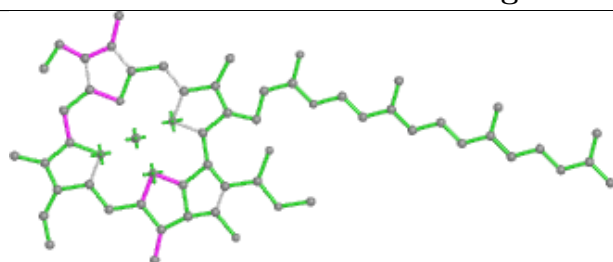


Torsions

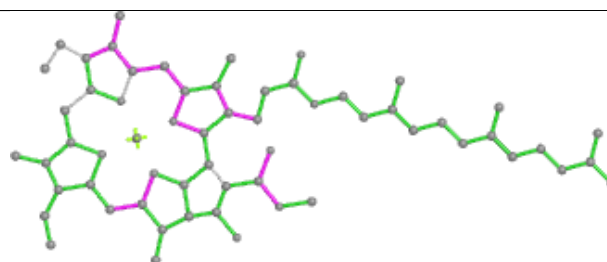


Rings

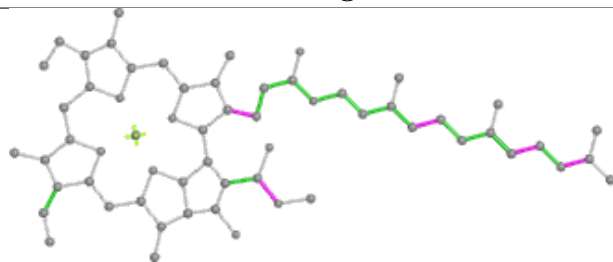
Ligand CLA AB 835



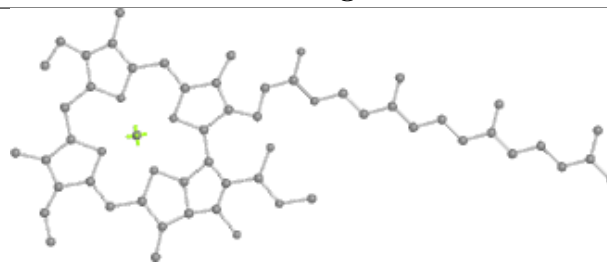
Bond lengths



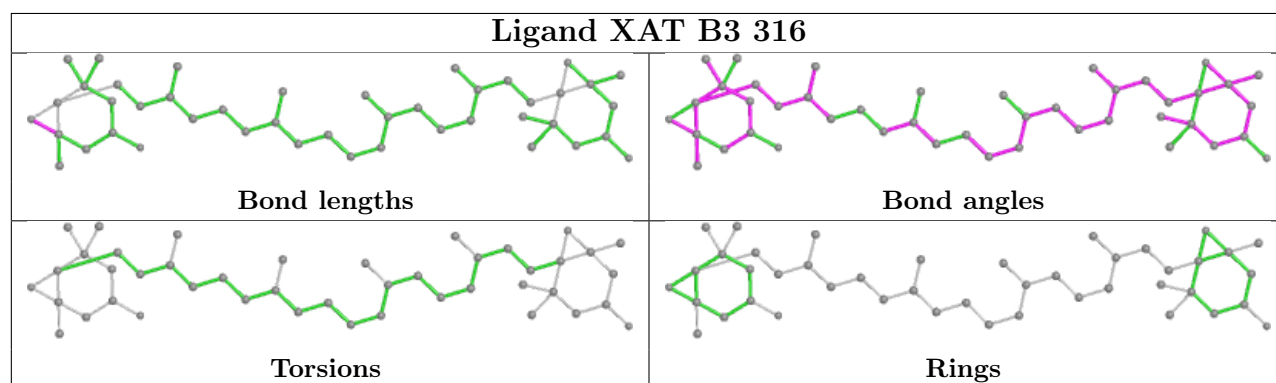
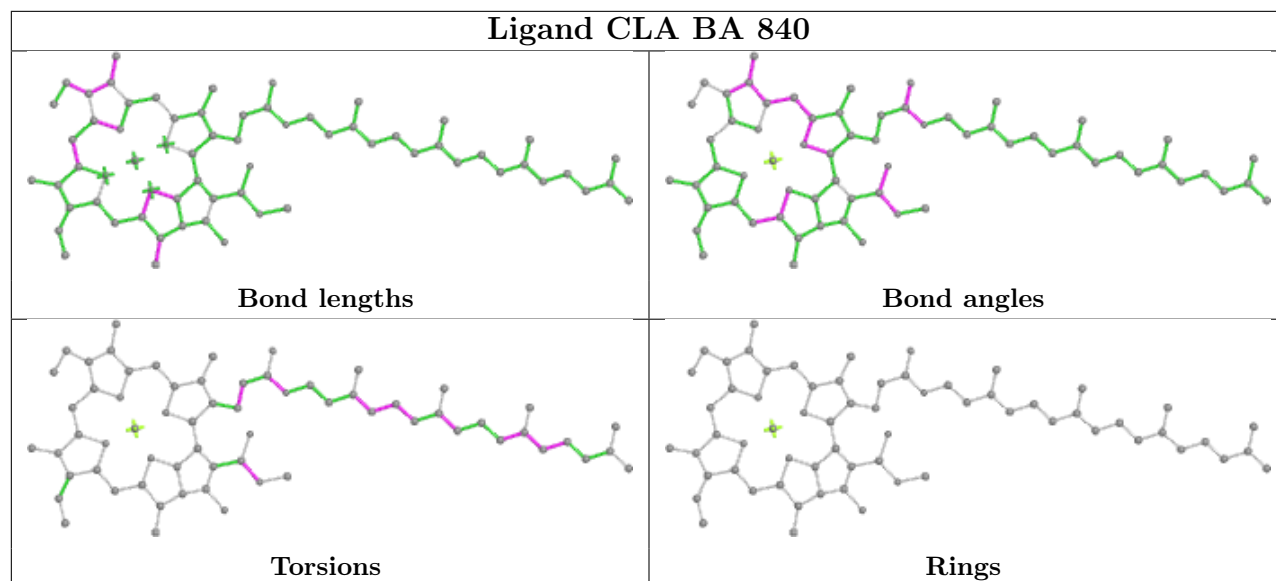
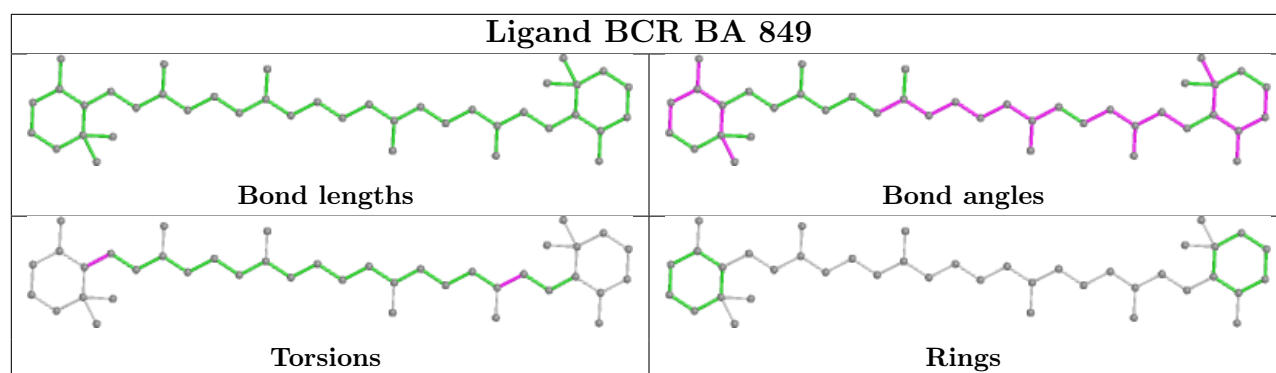
Bond angles



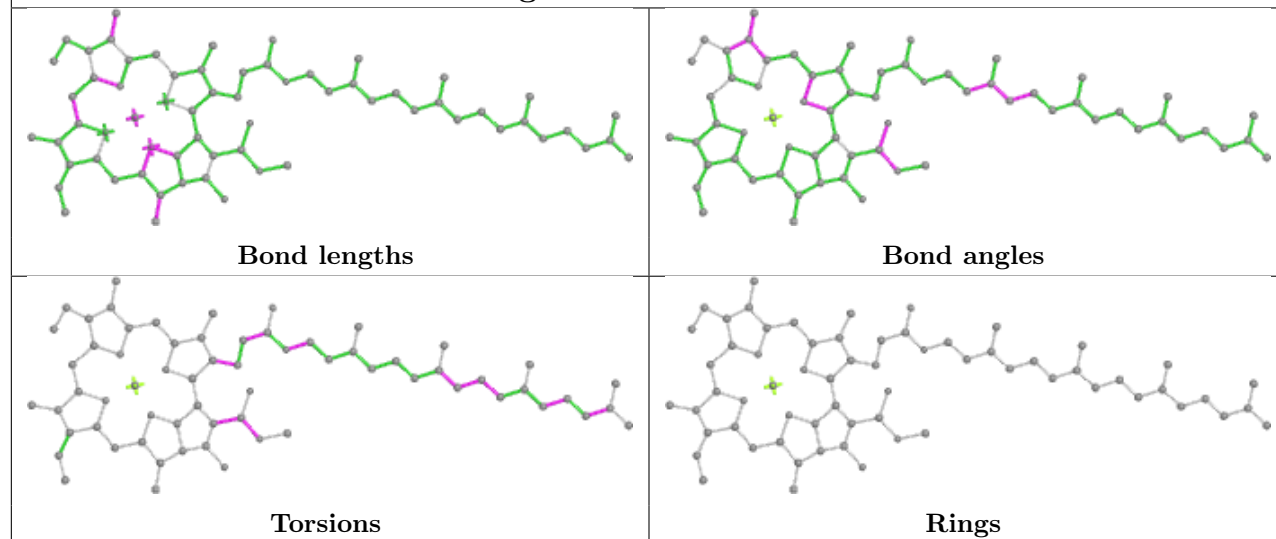
Torsions



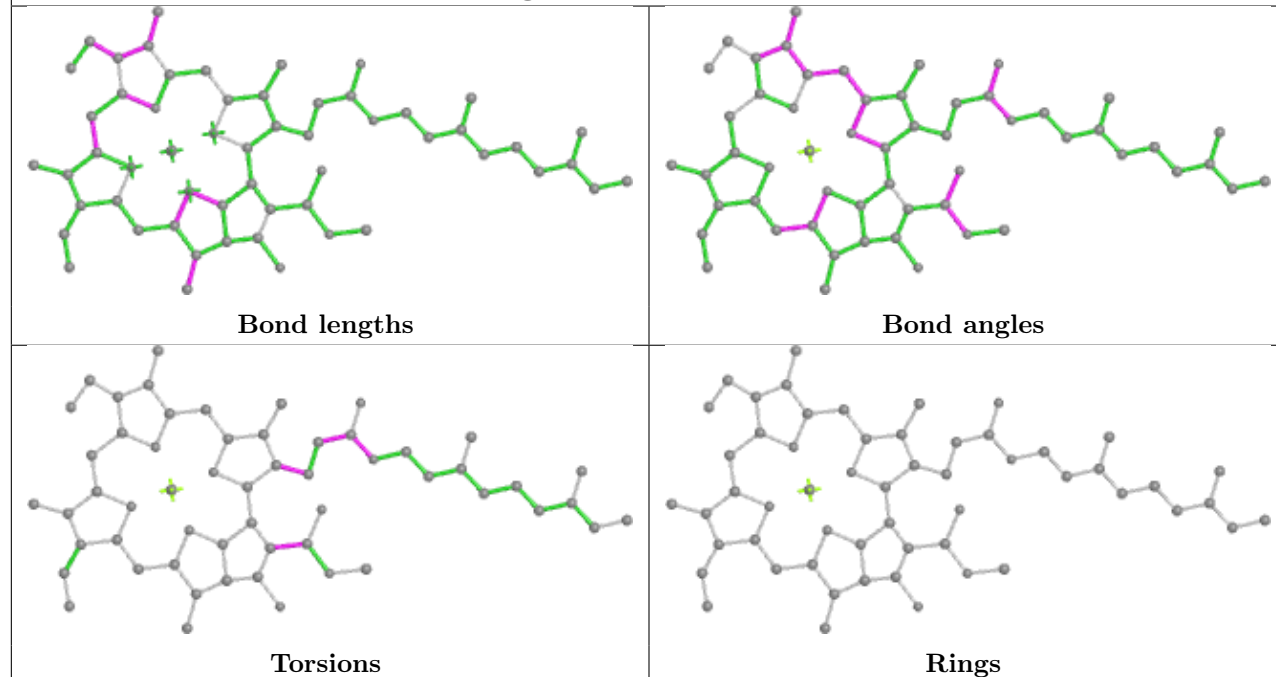
Rings



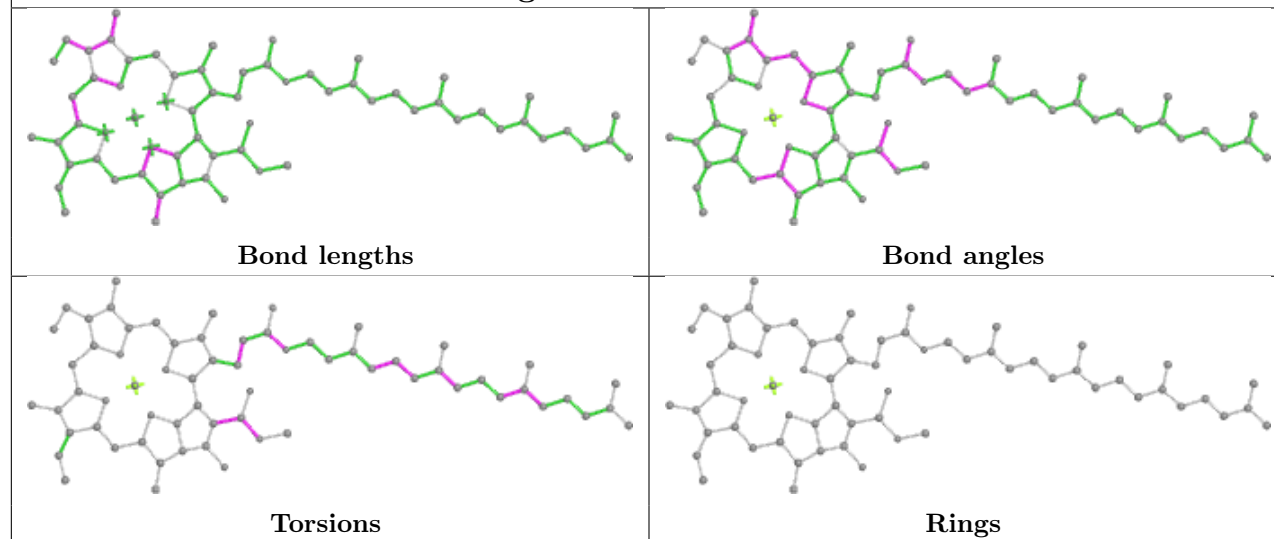
Ligand CLA BA 825



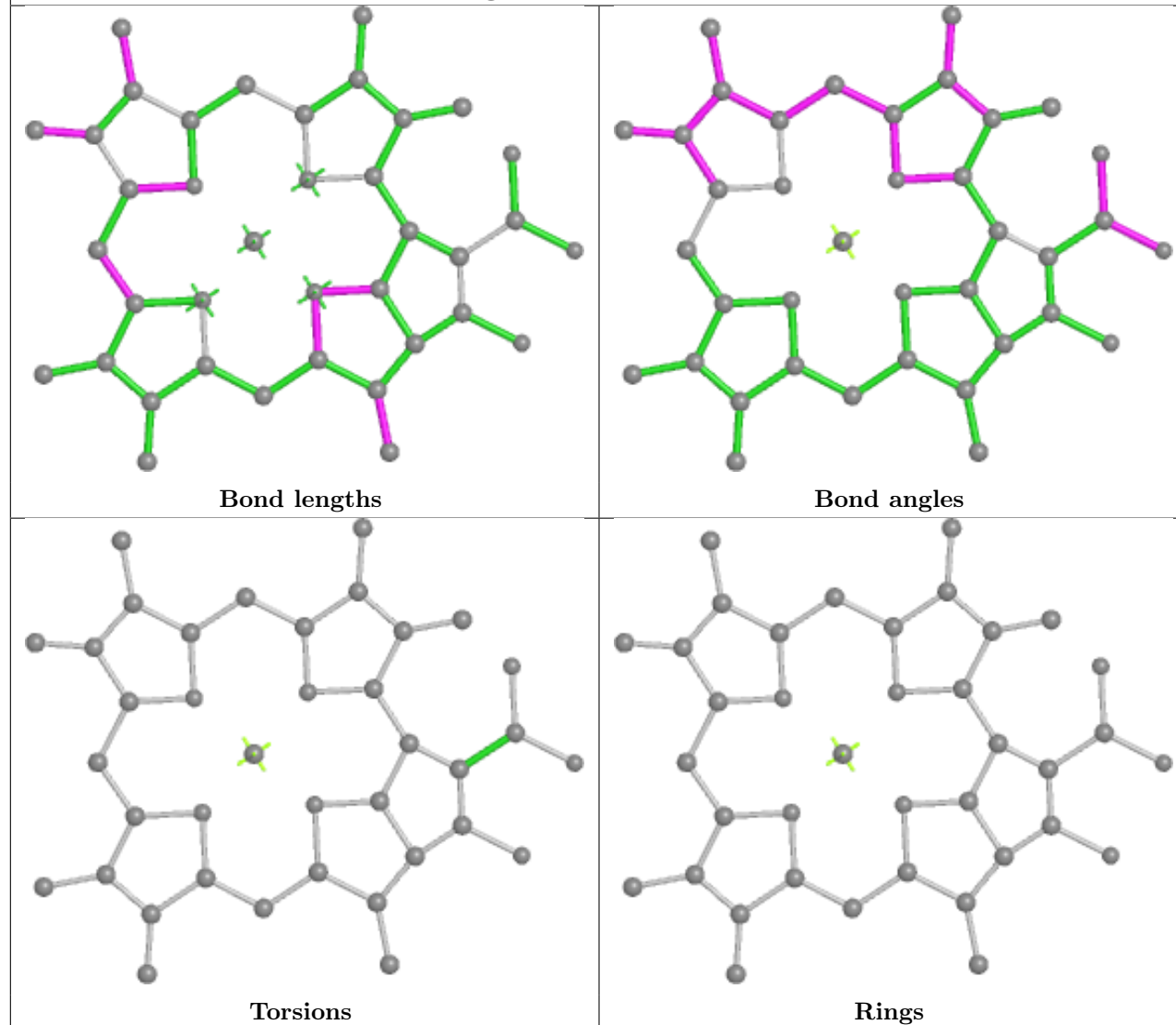
Ligand CLA BA 818

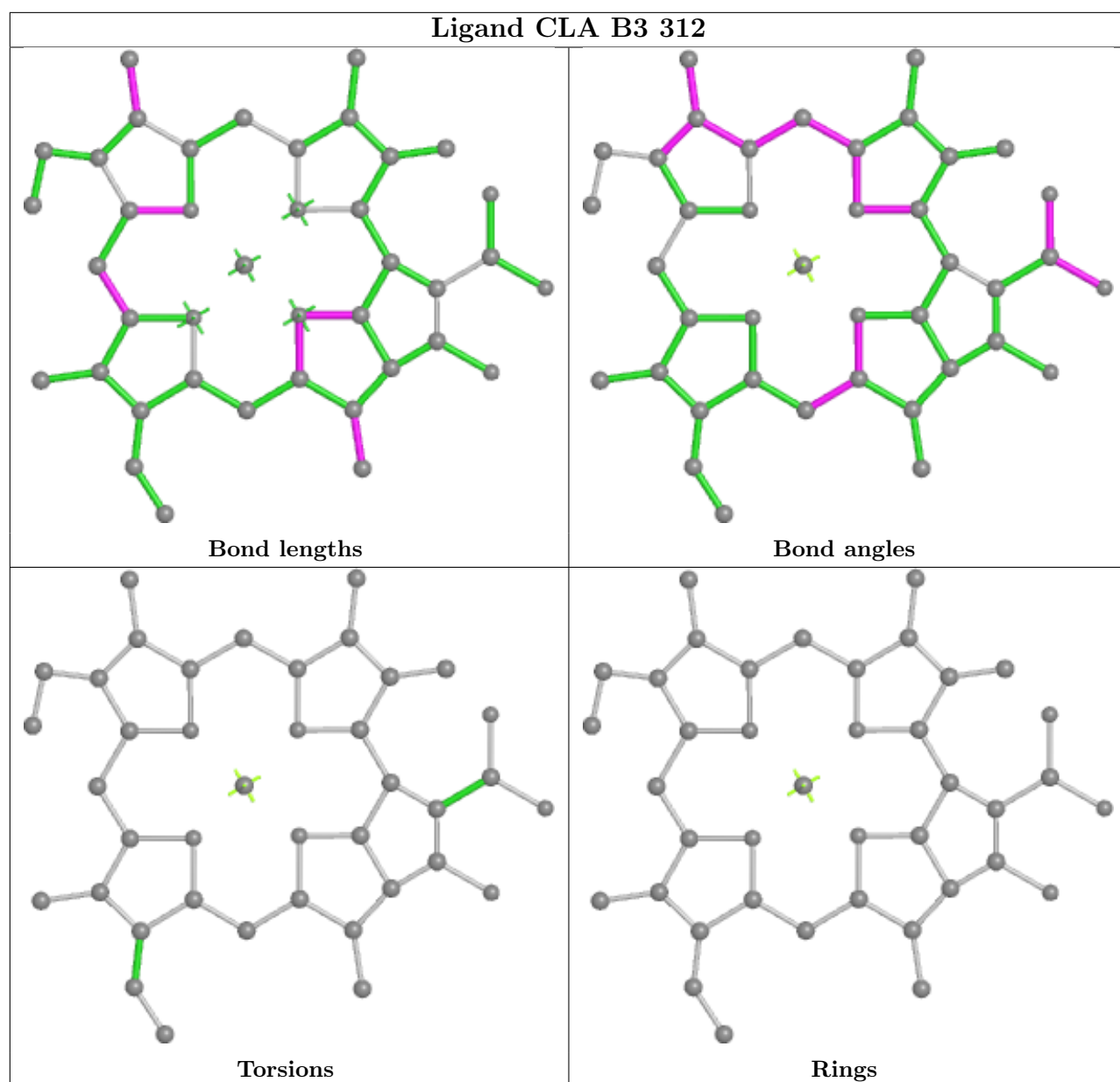


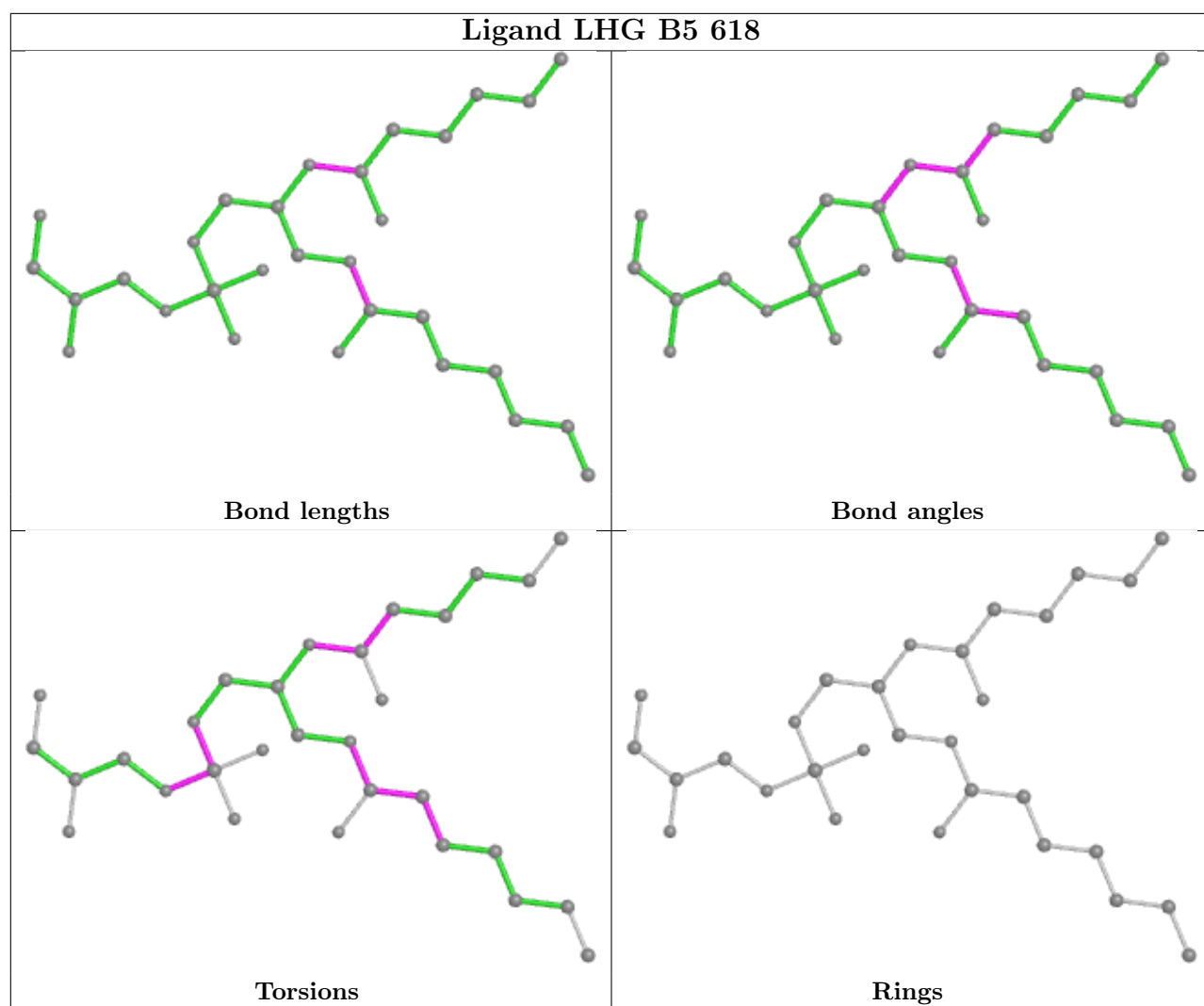
Ligand CLA AA 840



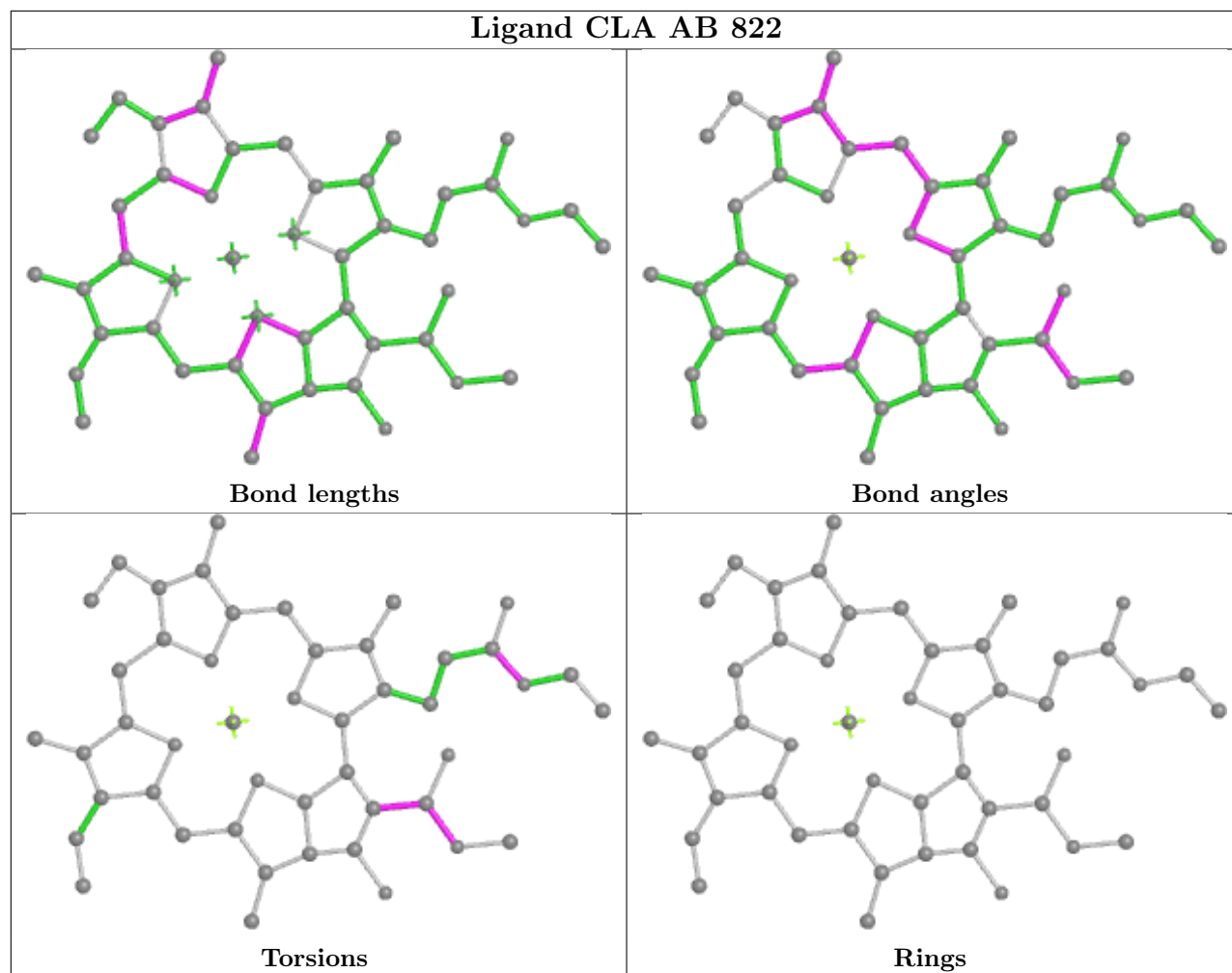
Ligand CLA B1 315



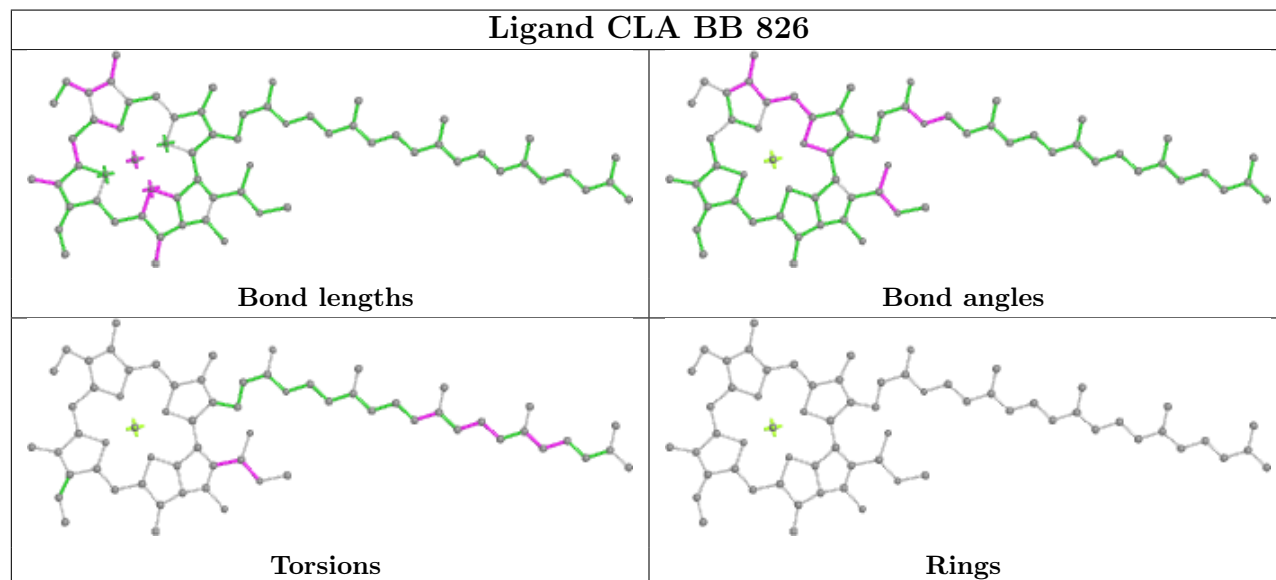


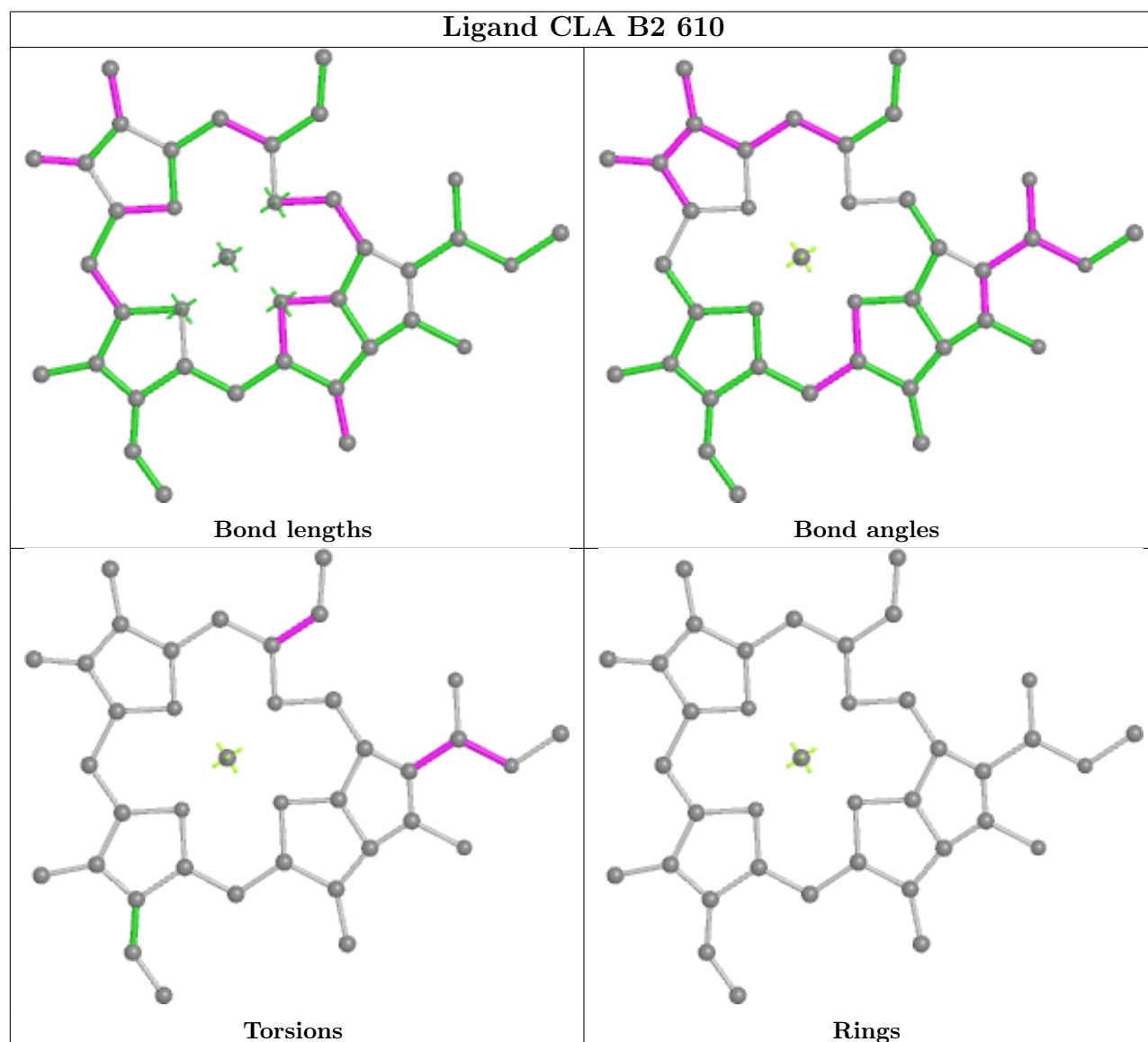
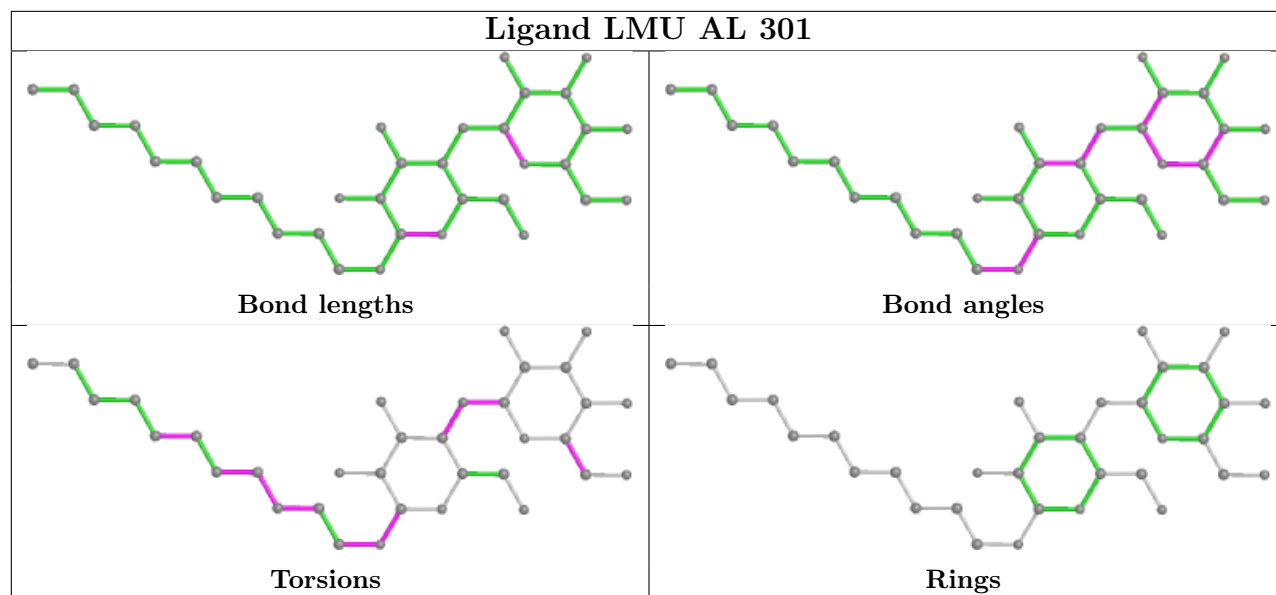


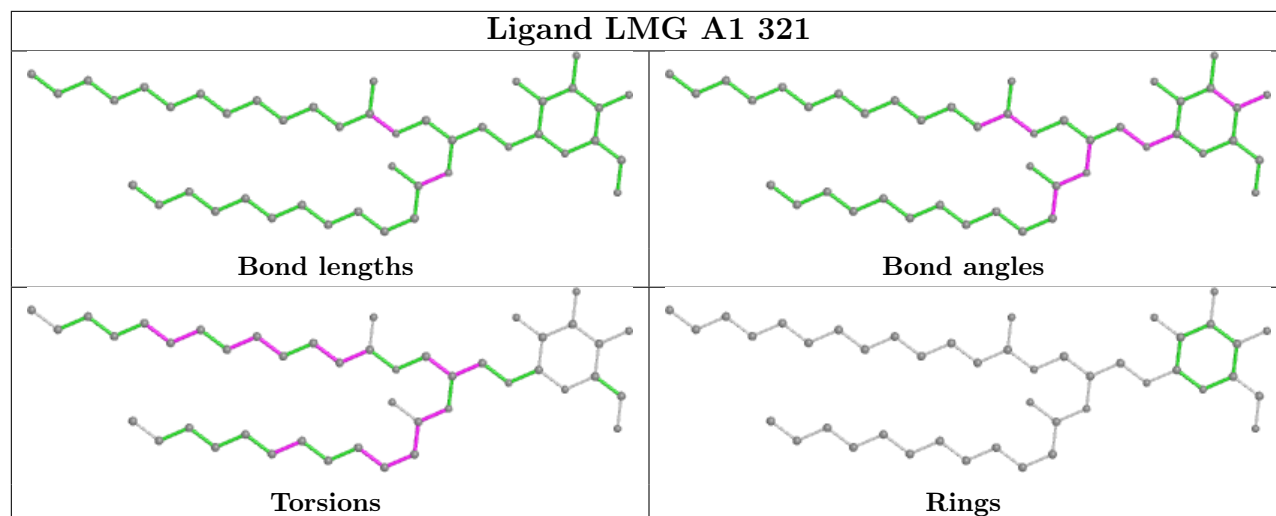
Ligand CLA AB 822



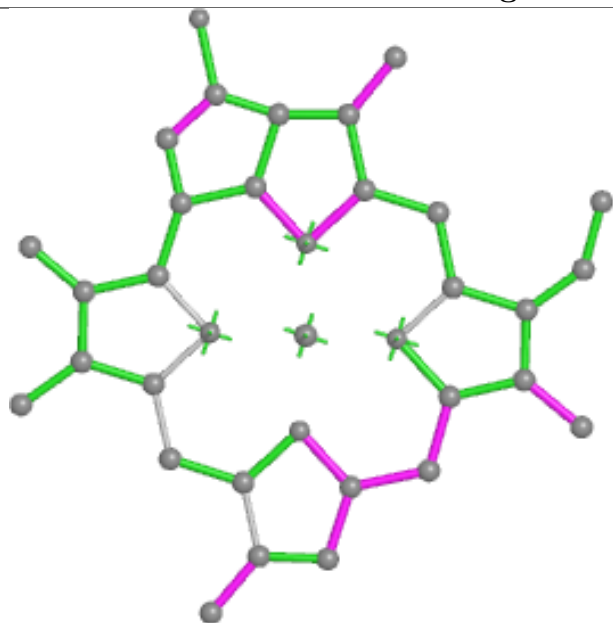
Ligand CLA BB 826



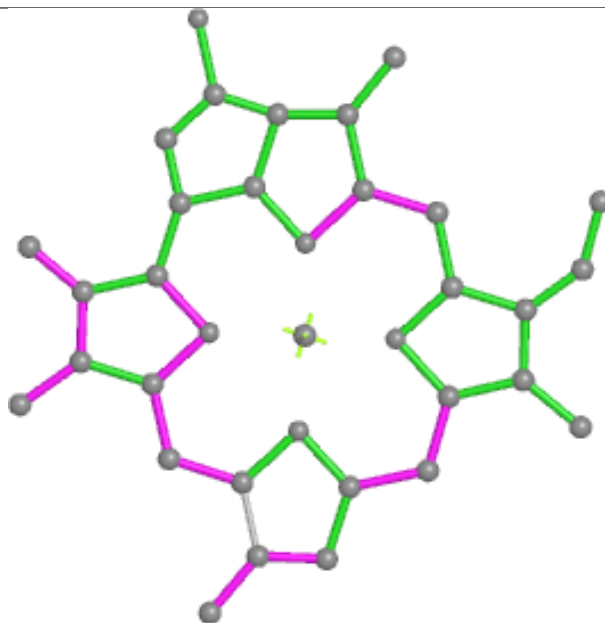




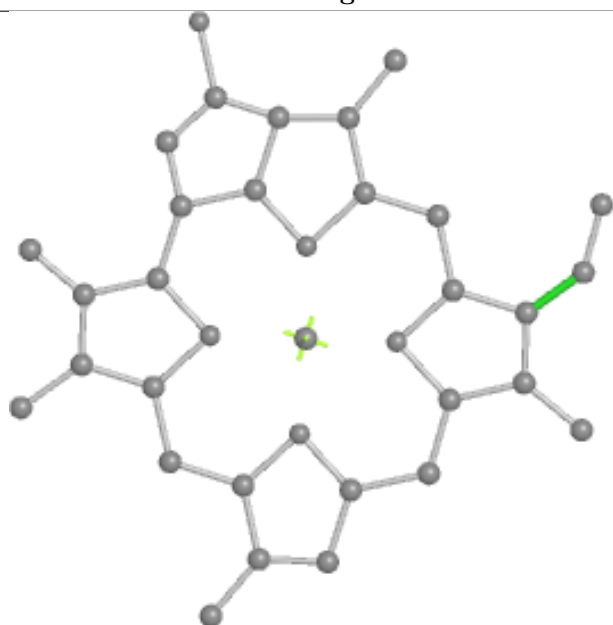
Ligand CLA AK 201



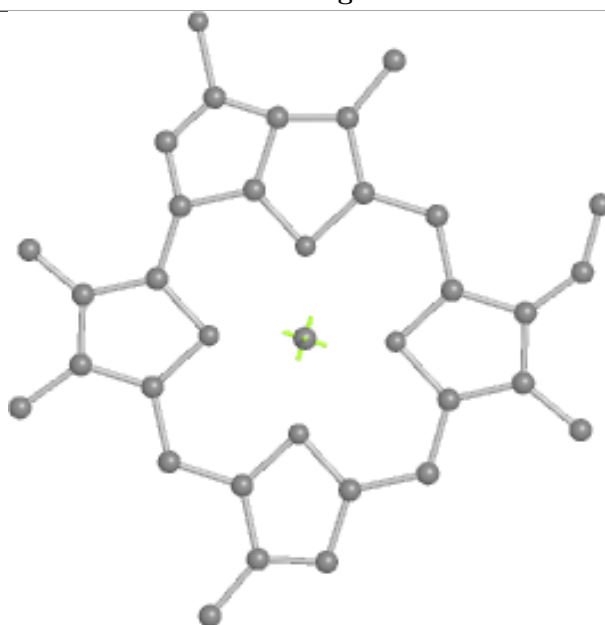
Bond lengths



Bond angles

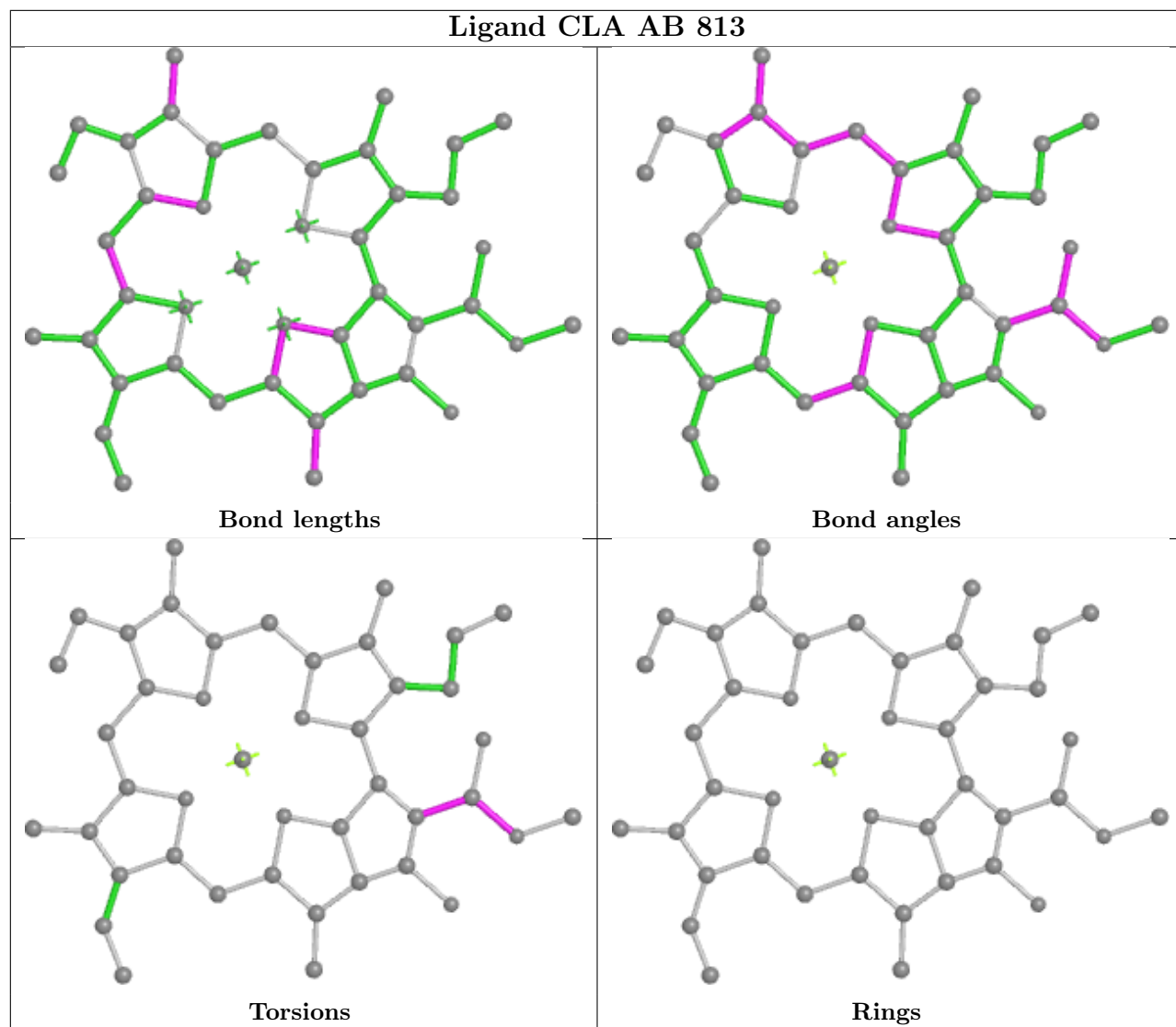


Torsions

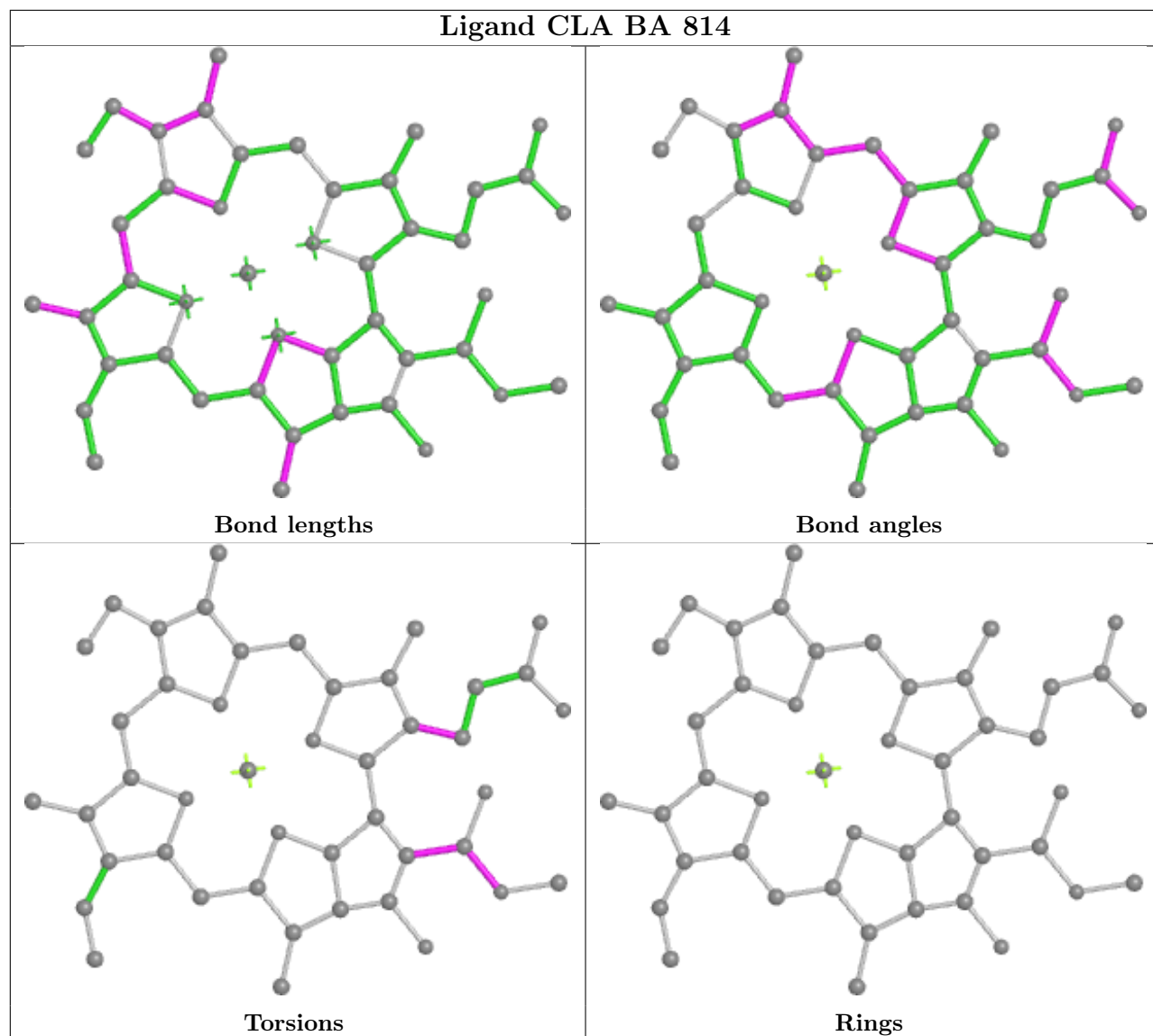


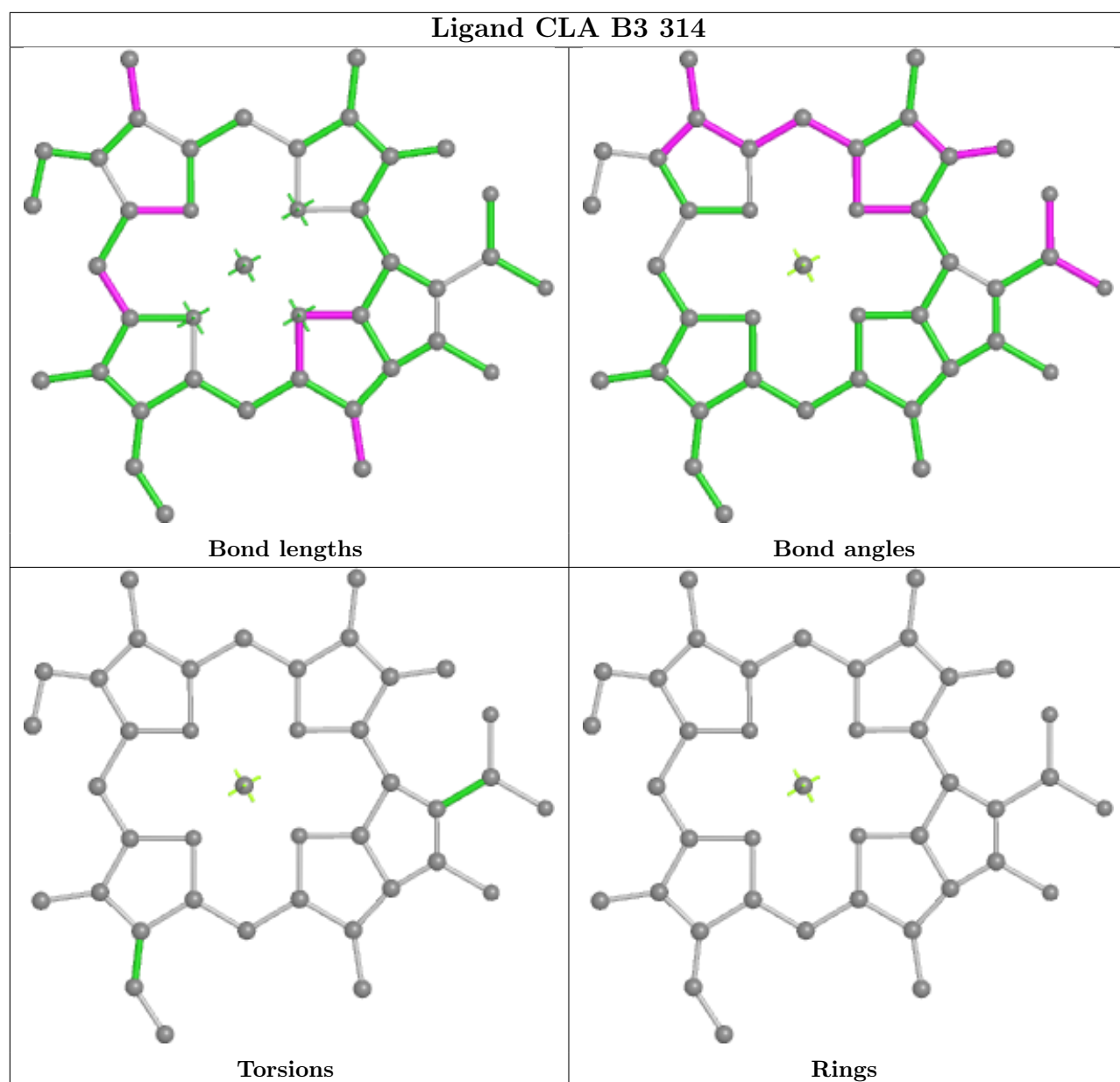
Rings

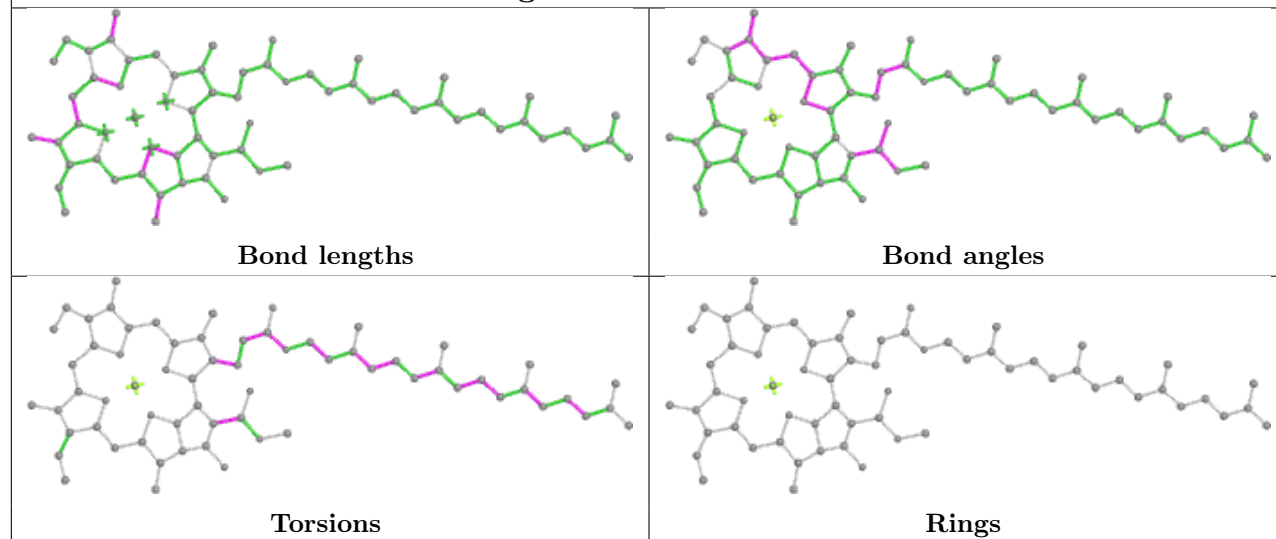
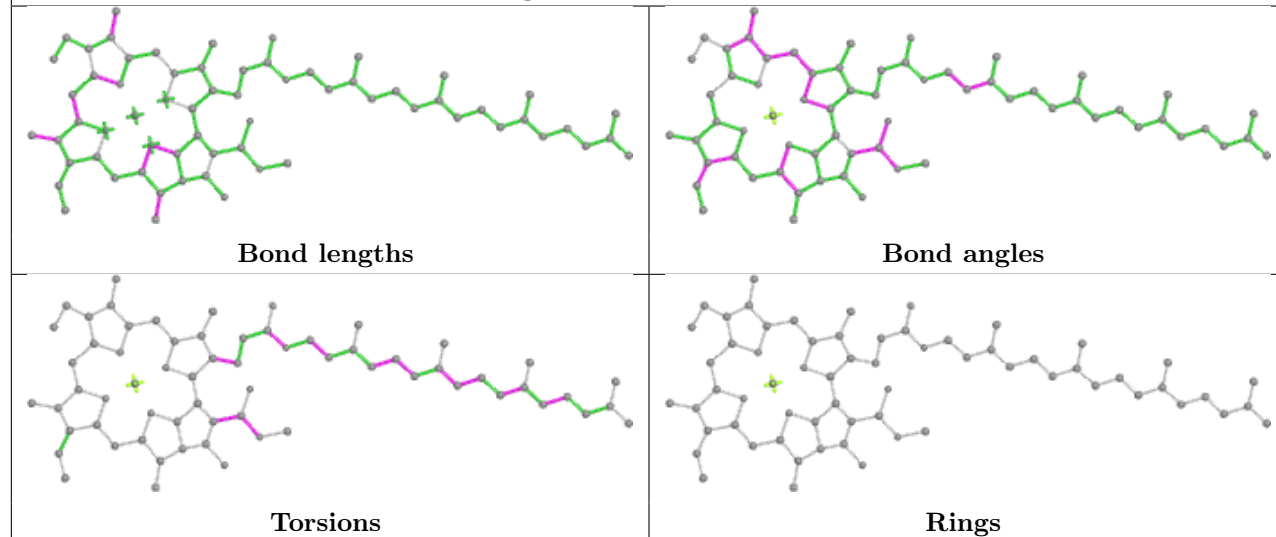
Ligand CLA AB 813



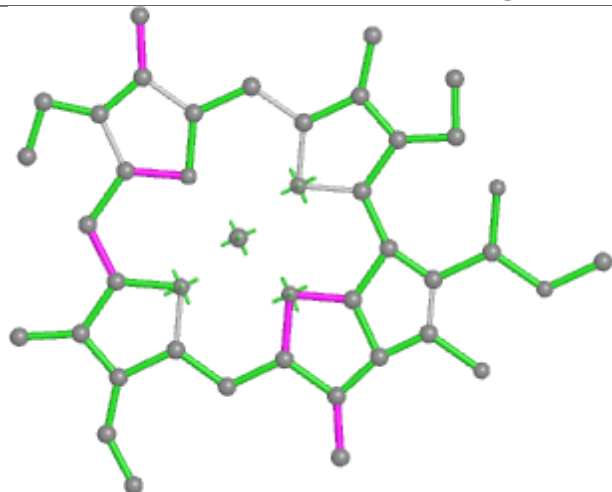
Ligand CLA BA 814



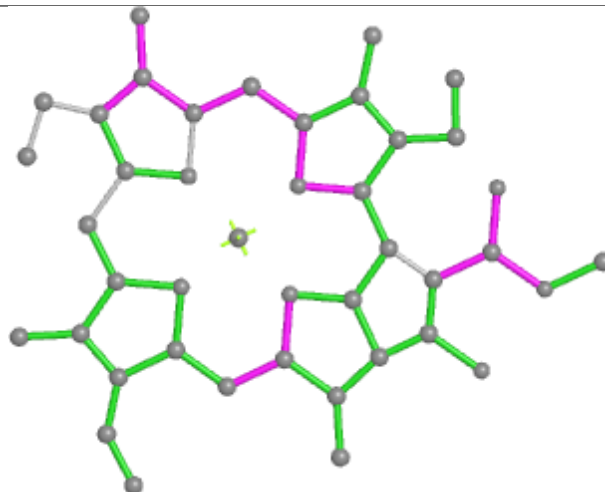


Ligand CLA AA 827**Ligand CLA BA 803**

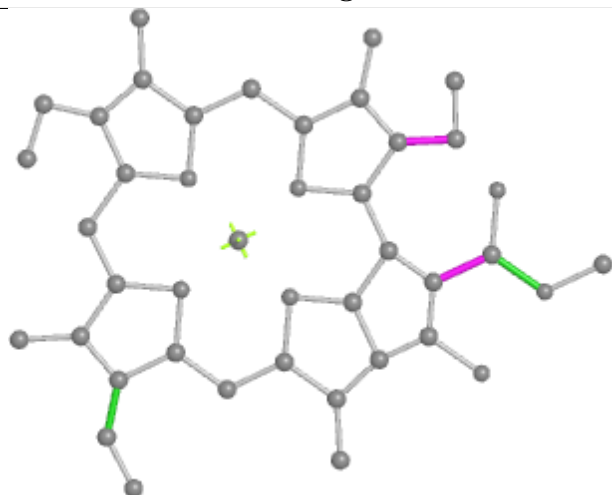
Ligand CLA AA 822



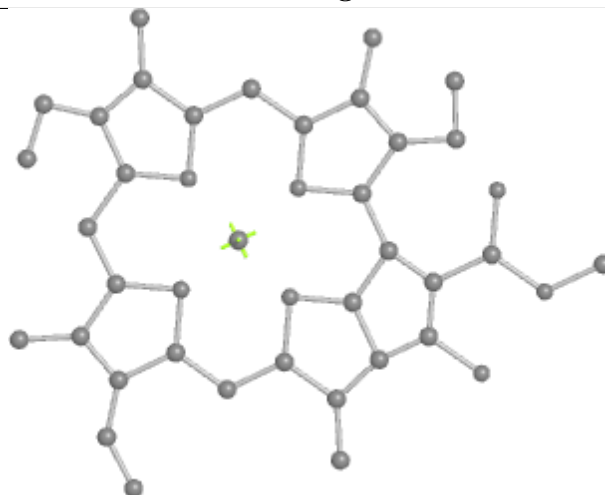
Bond lengths



Bond angles

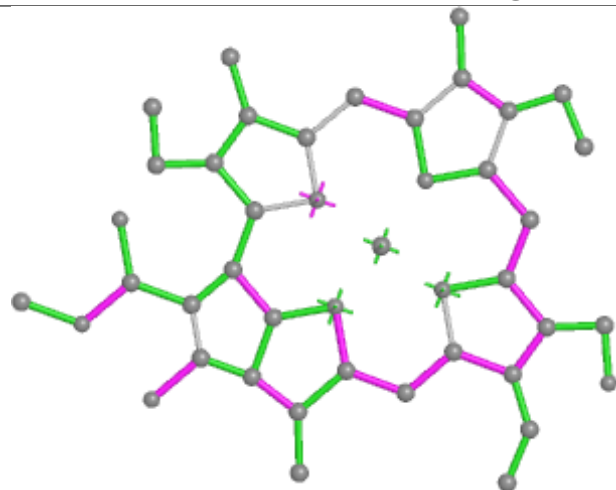


Torsions

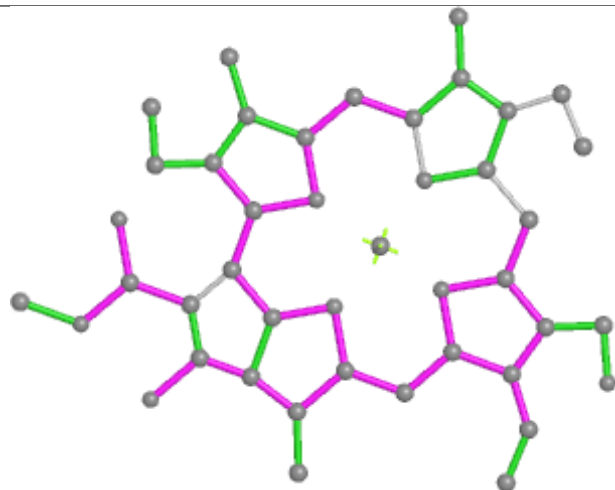


Rings

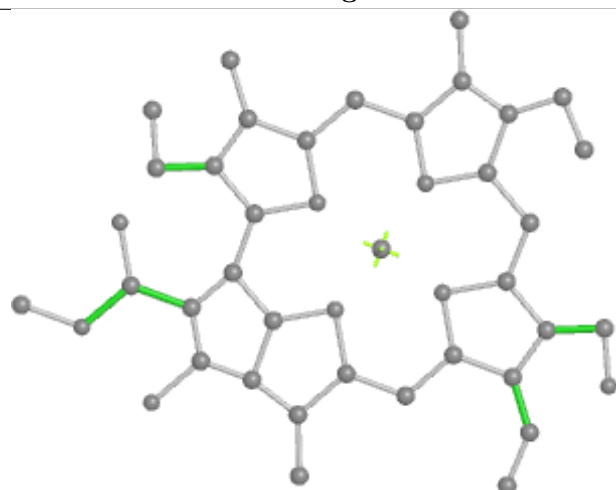
Ligand CHL B2 614



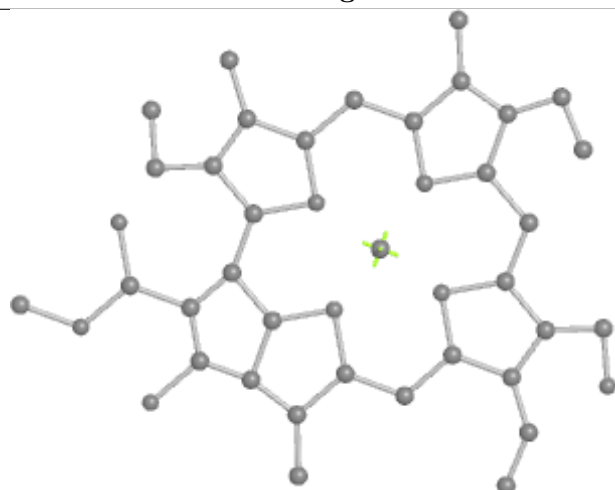
Bond lengths



Bond angles

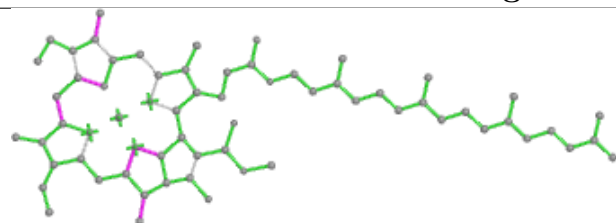


Torsions

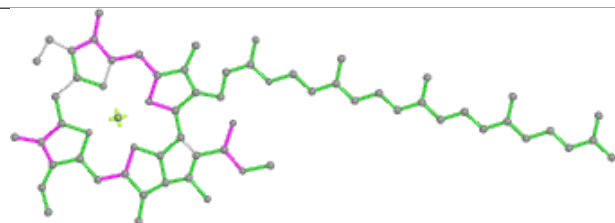


Rings

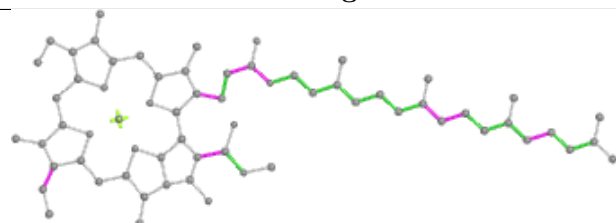
Ligand CLA AB 806



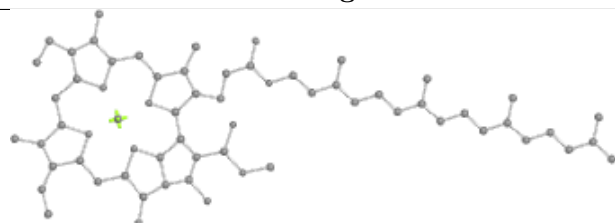
Bond lengths



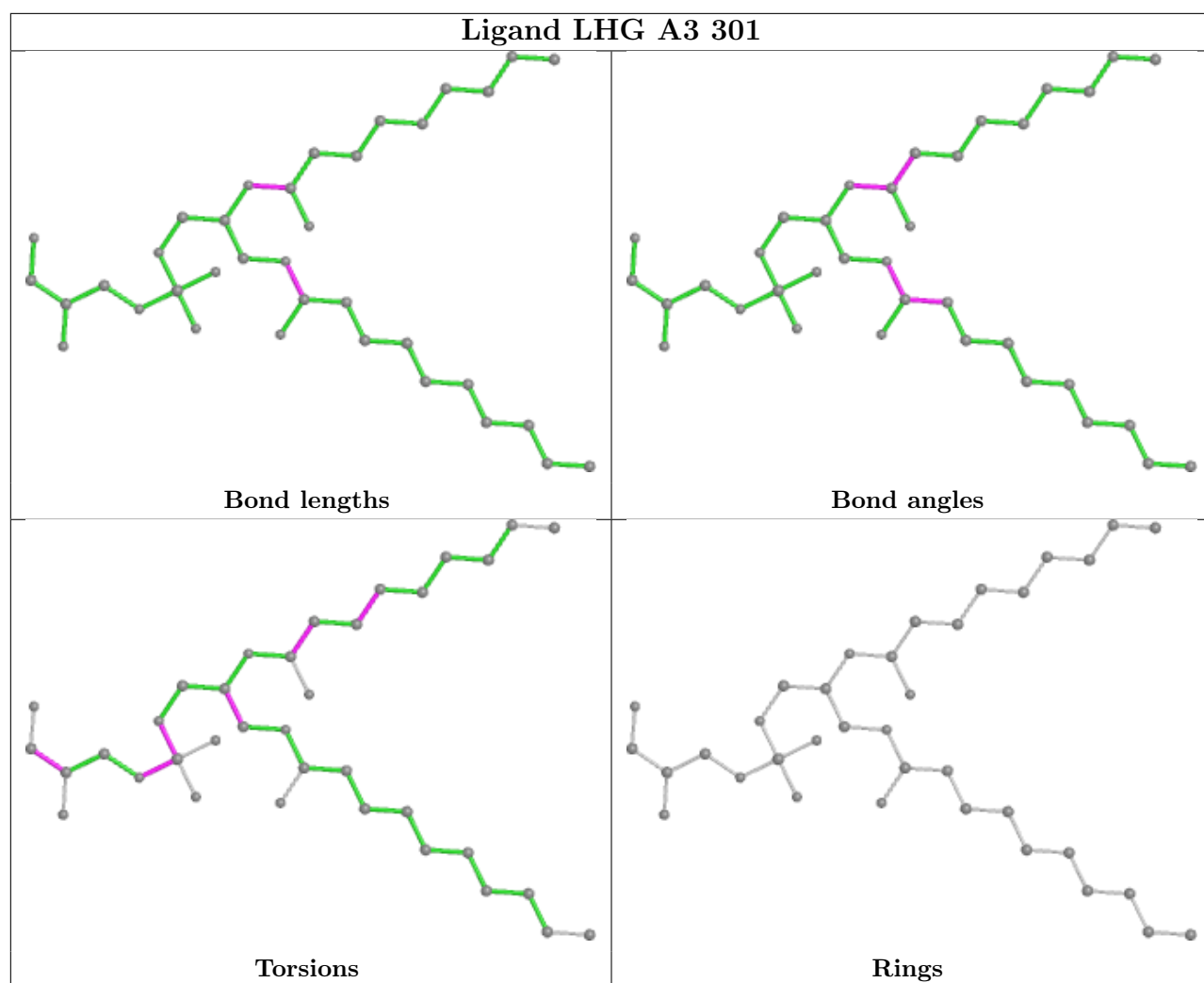
Bond angles



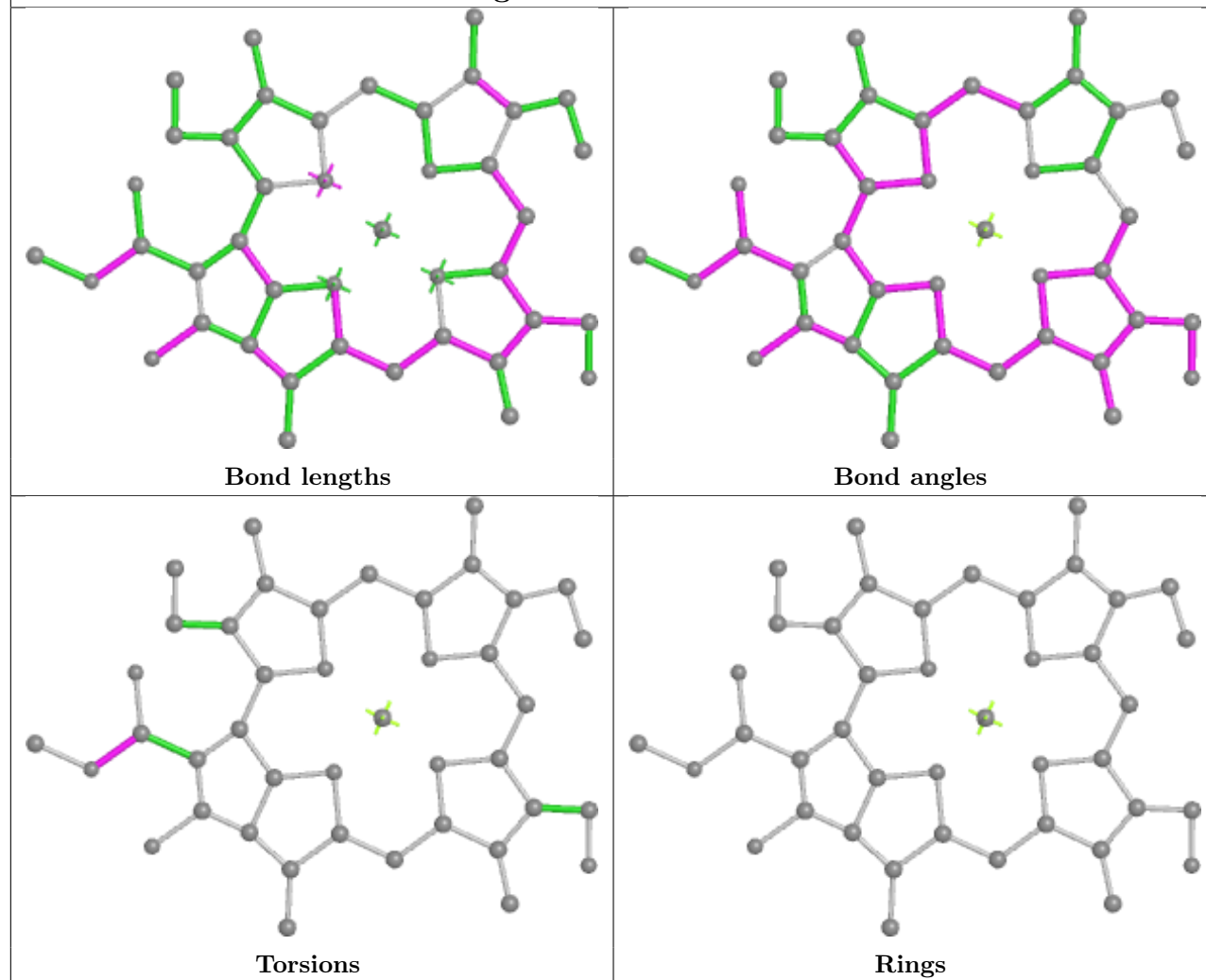
Torsions



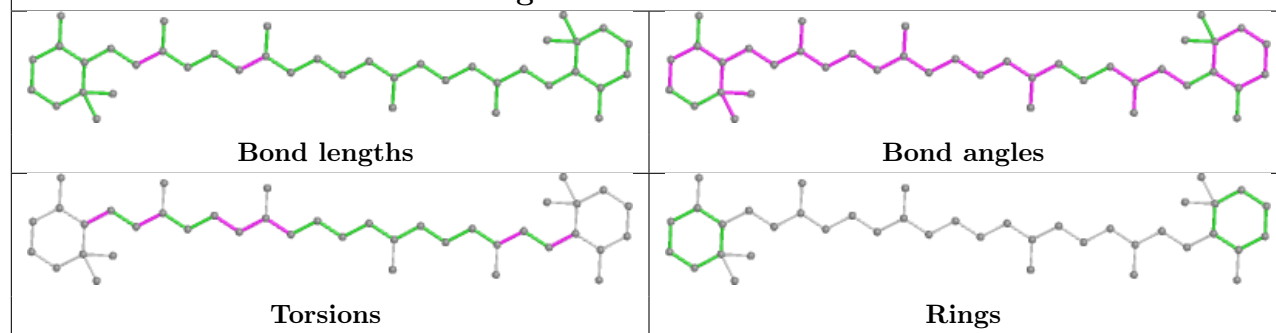
Rings



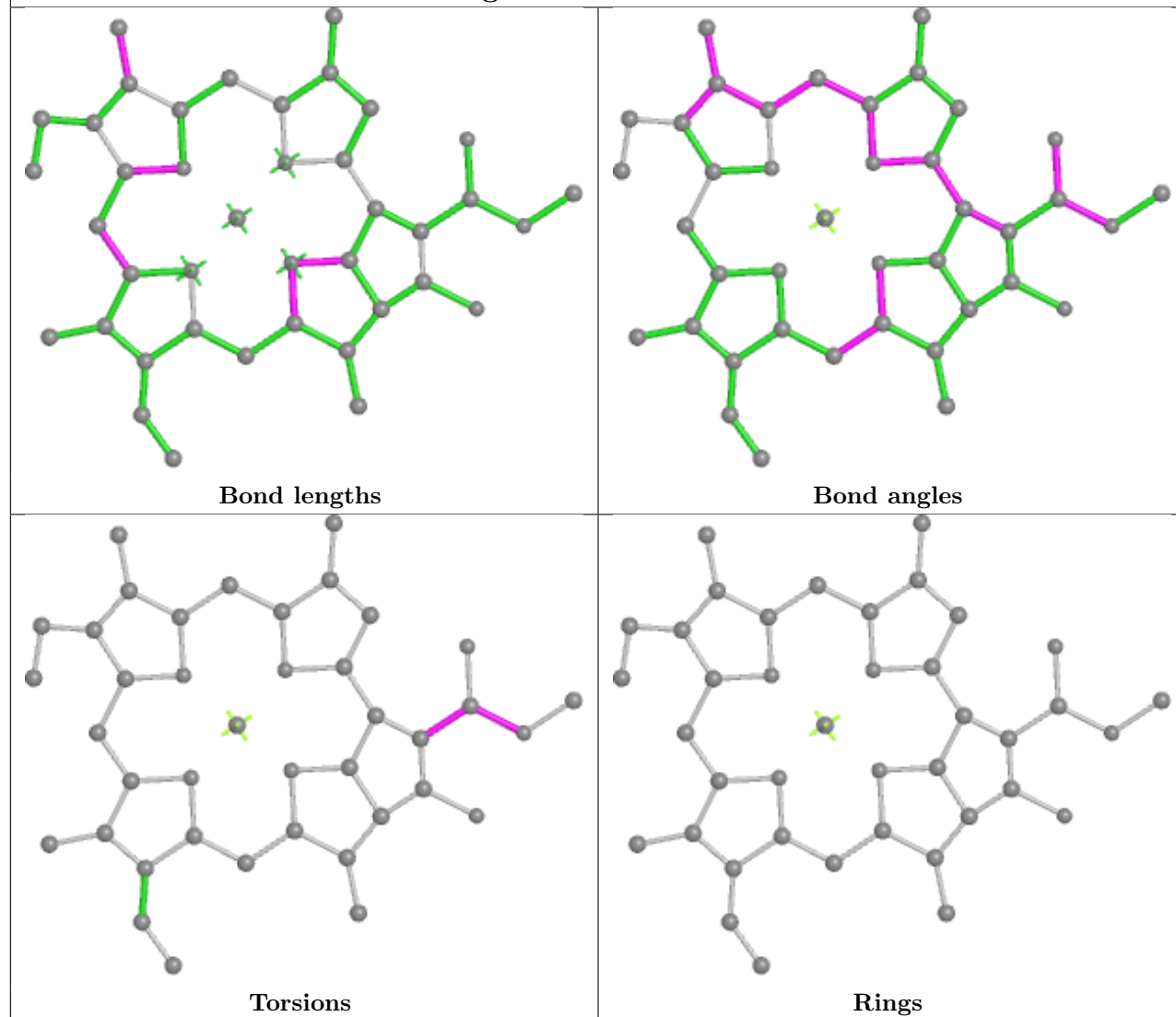
Ligand CHL A6 606



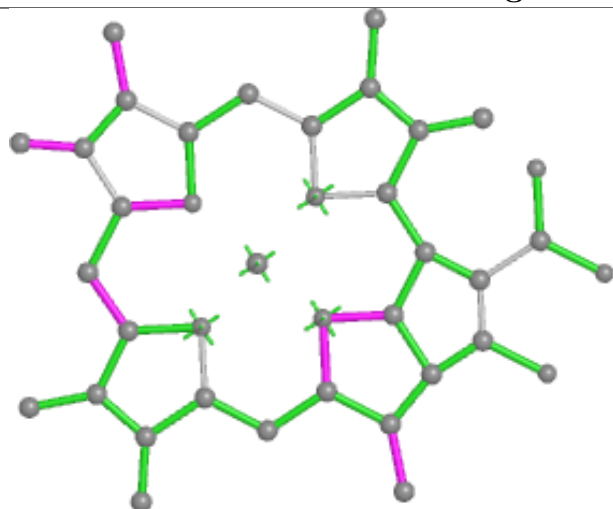
Ligand BCR AA 847



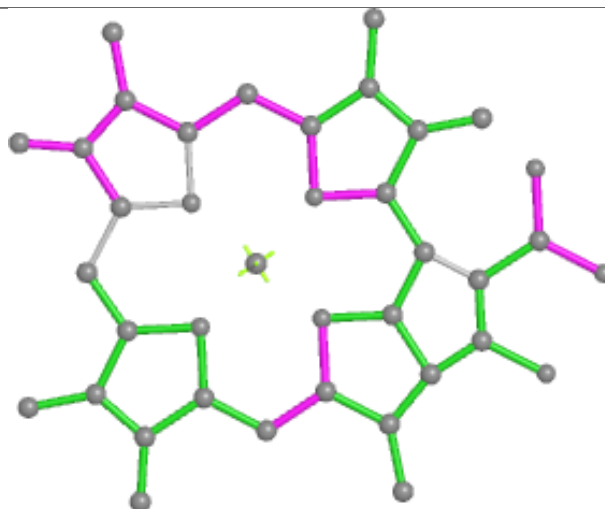
Ligand CLA B1 307



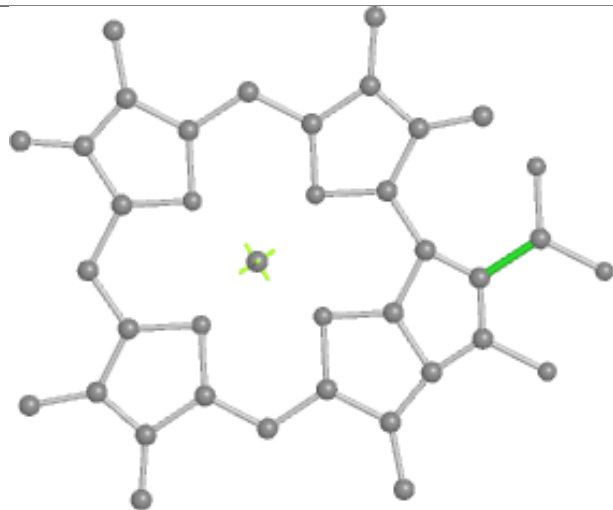
Ligand CLA B1 312



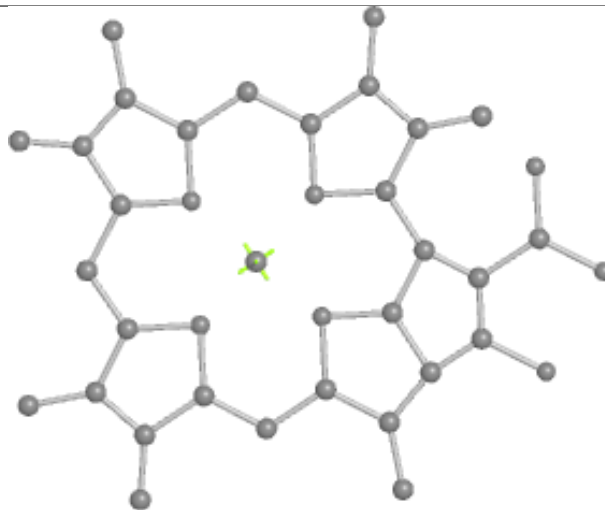
Bond lengths



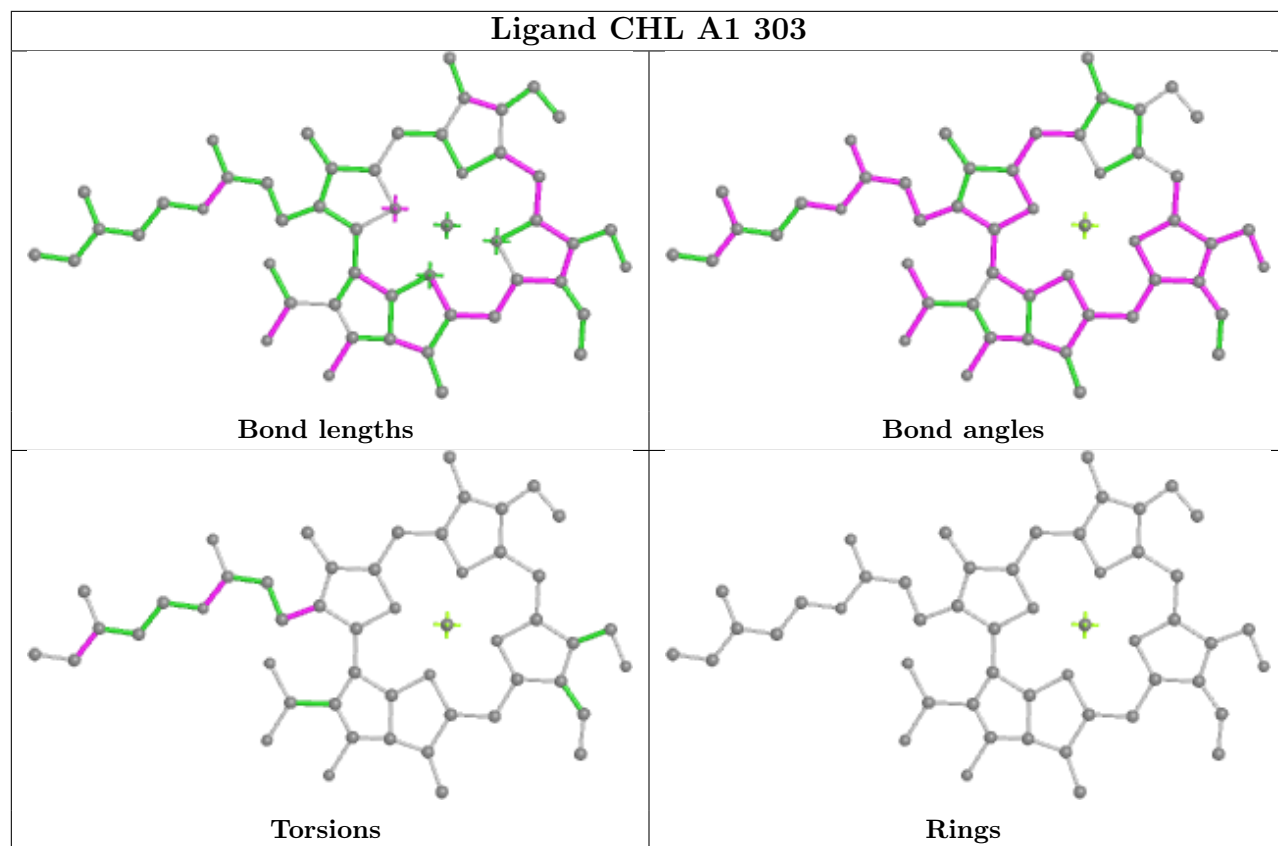
Bond angles



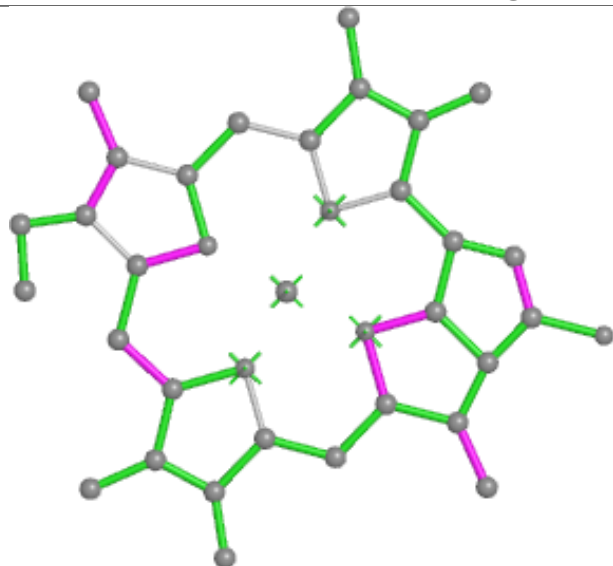
Torsions



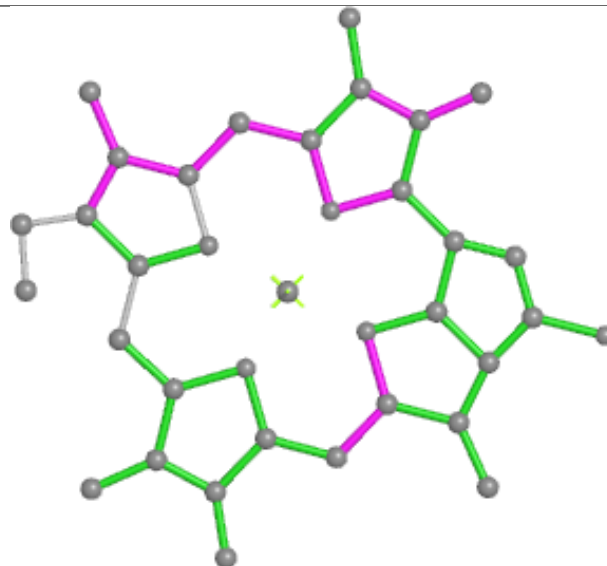
Rings



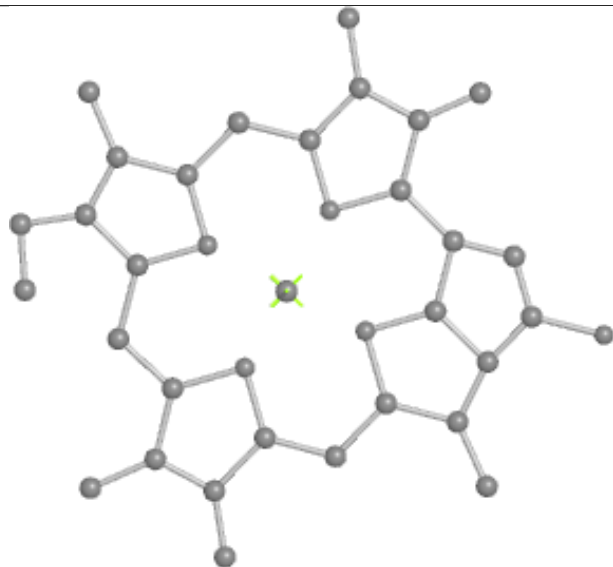
Ligand CLA A3 314



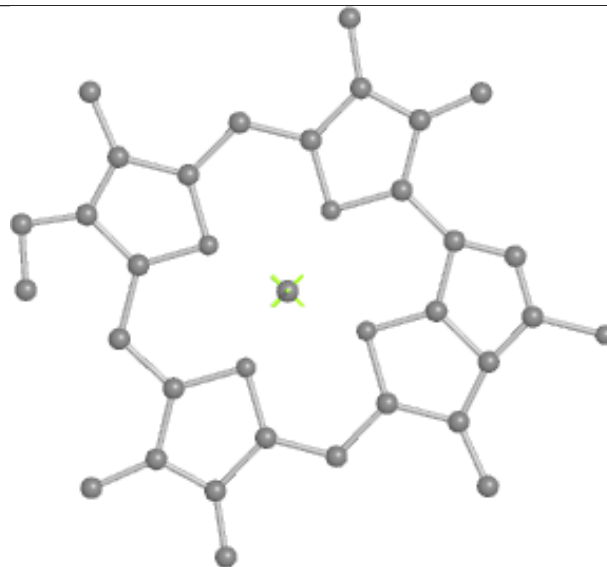
Bond lengths



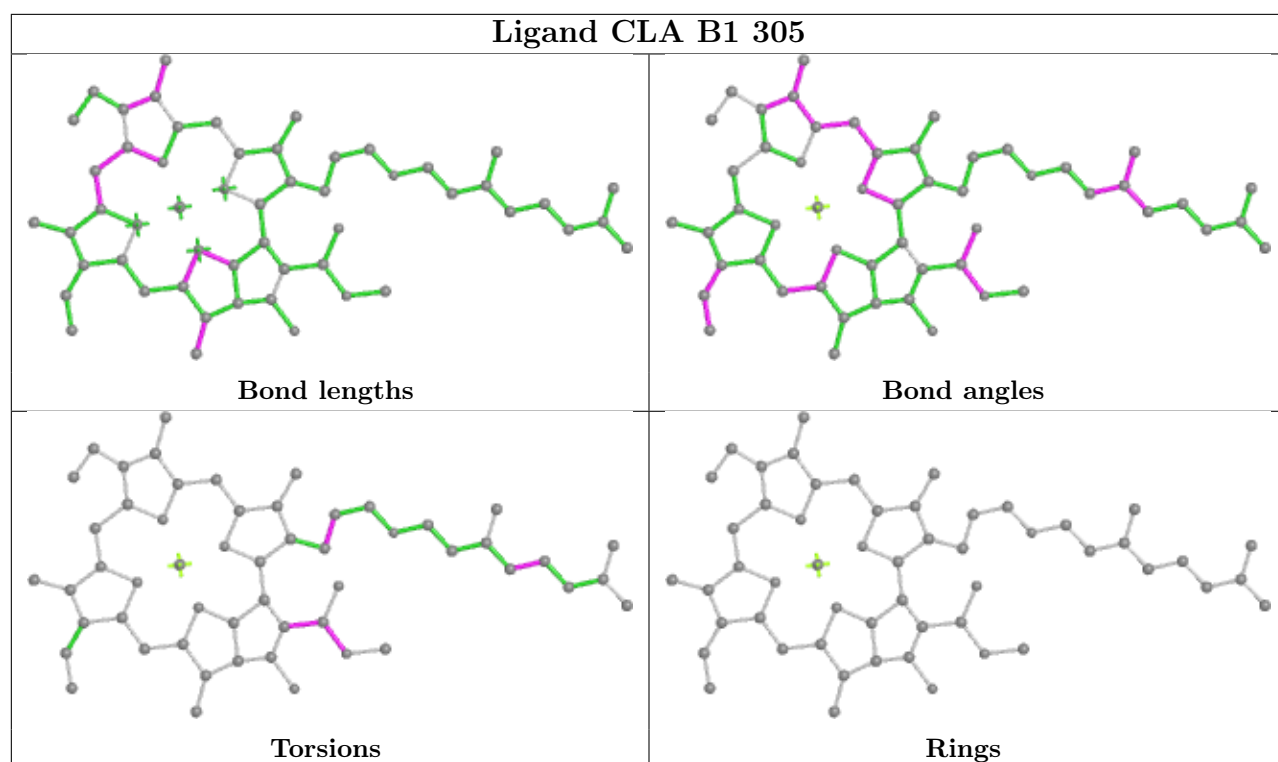
Bond angles



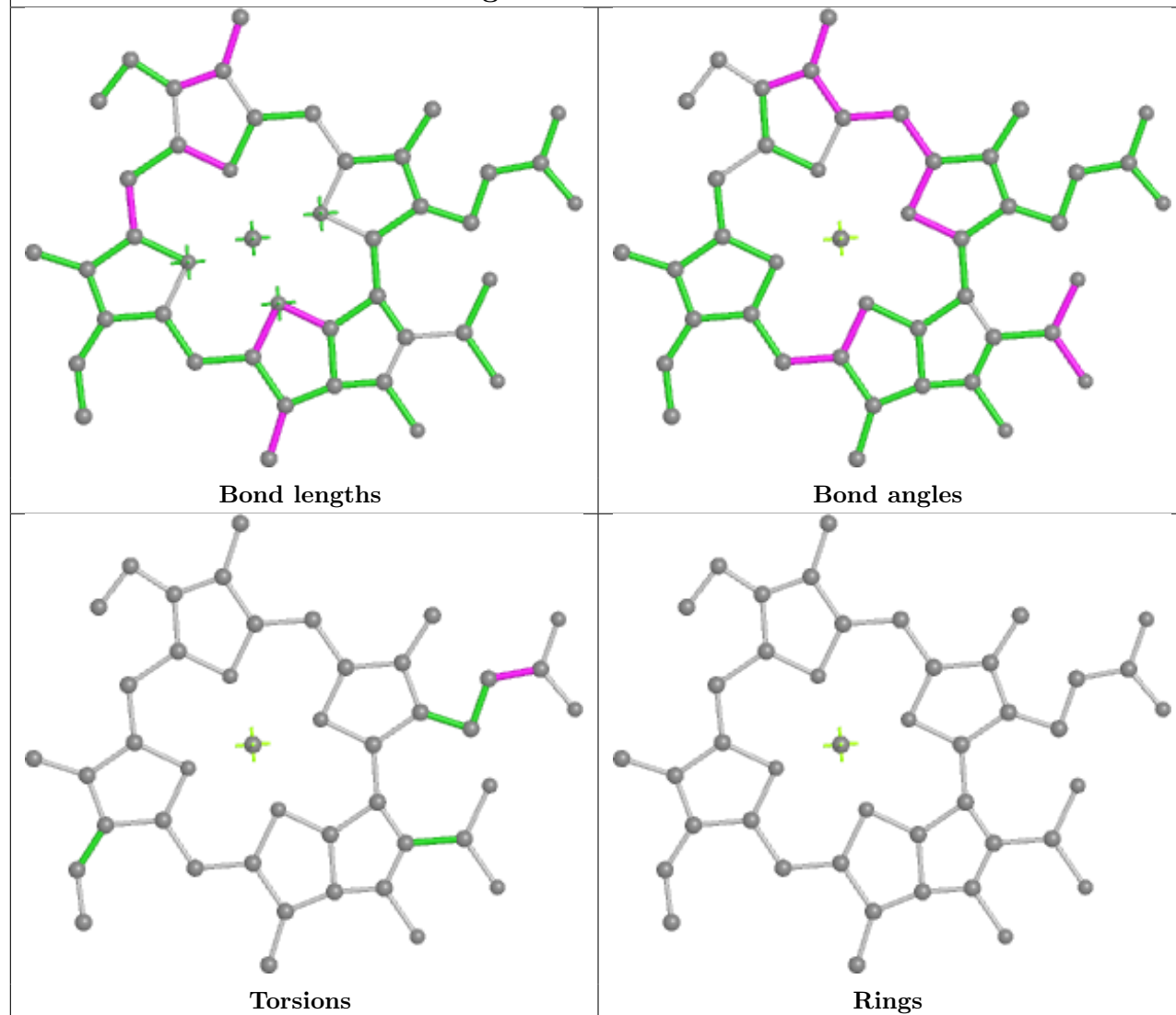
Torsions



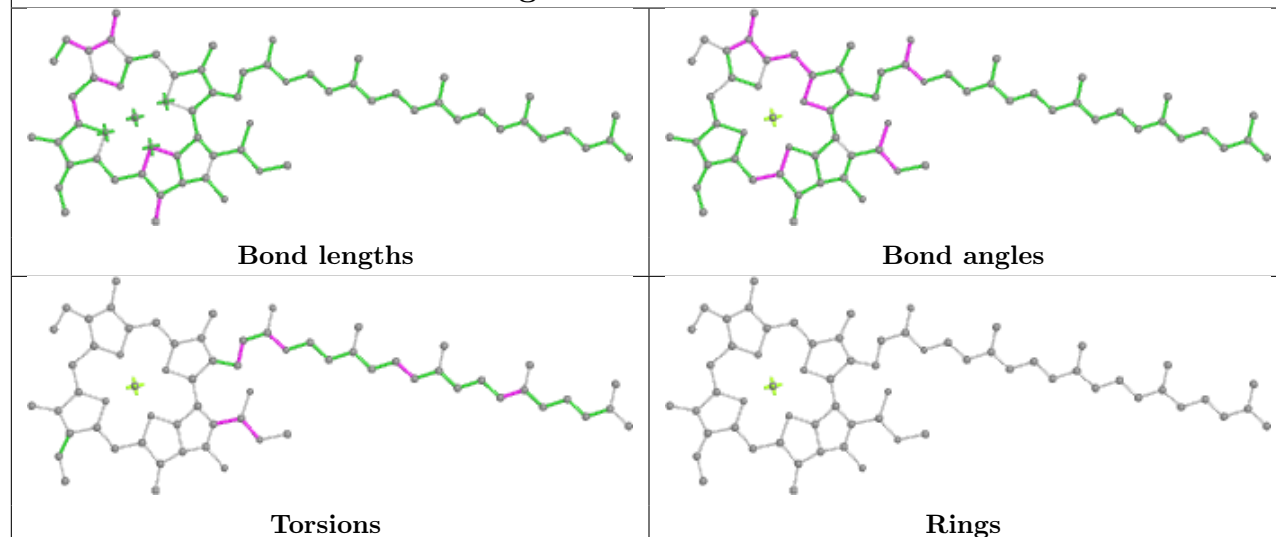
Rings

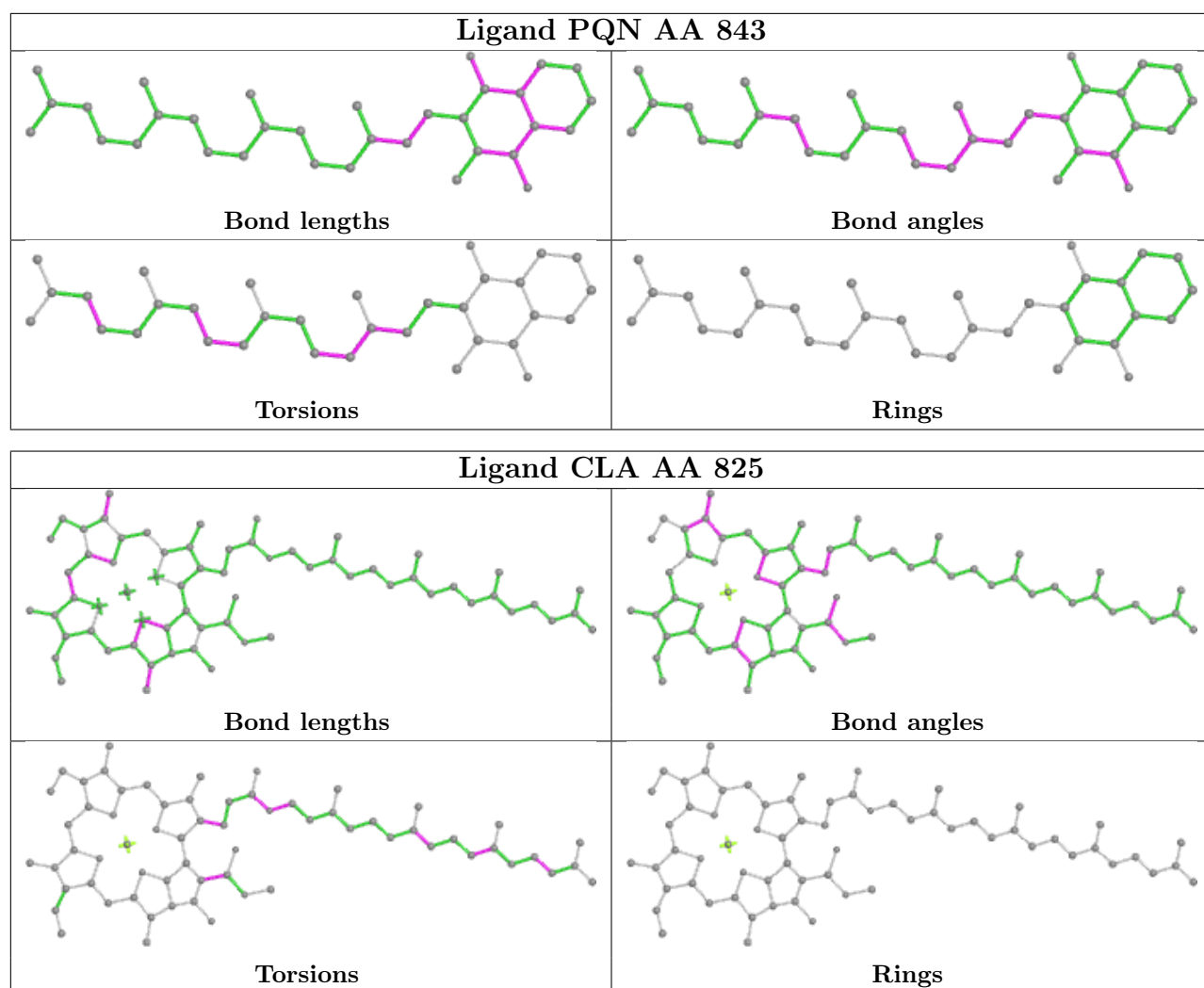


Ligand CLA B1 309

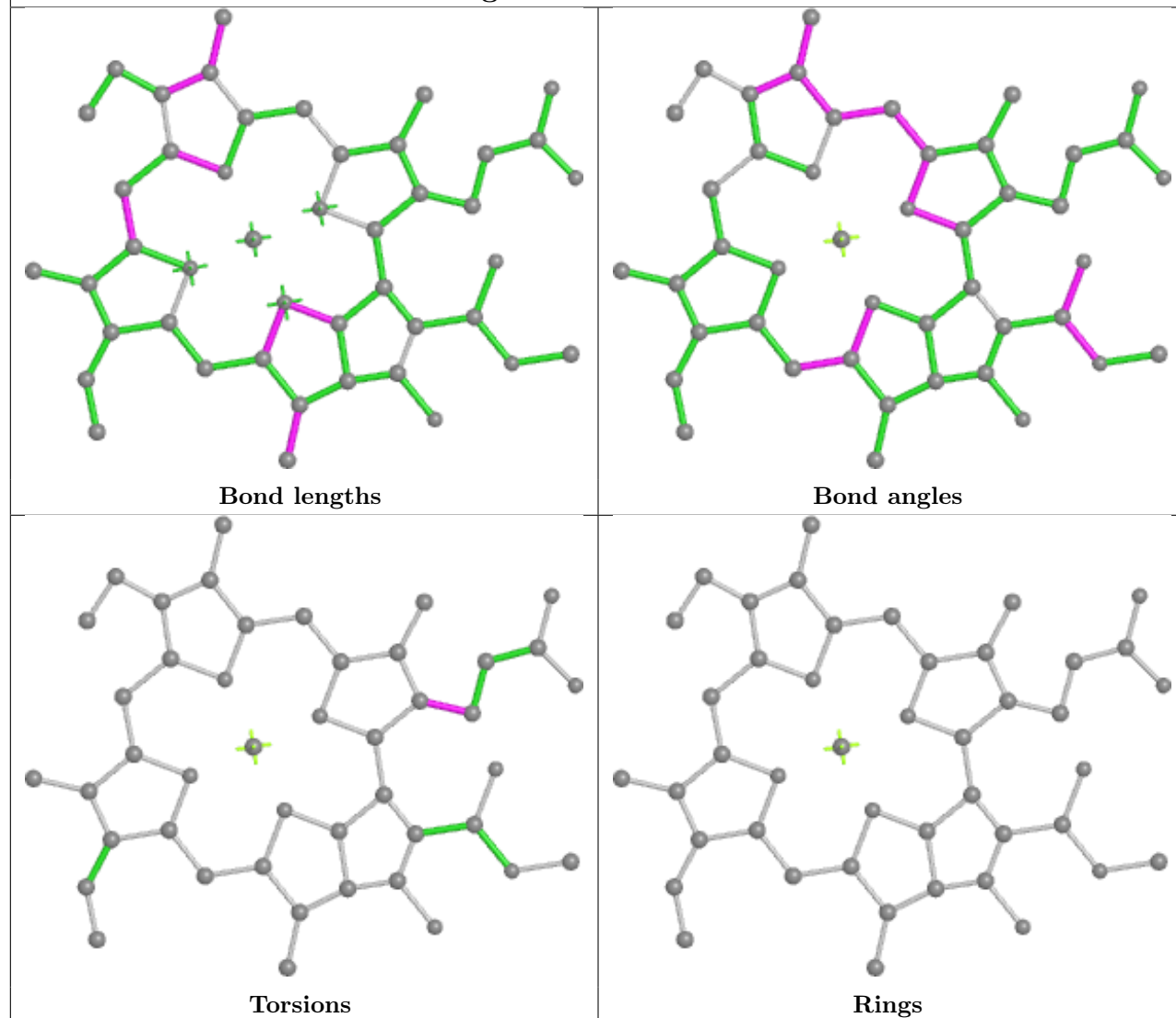


Ligand CLA BA 808

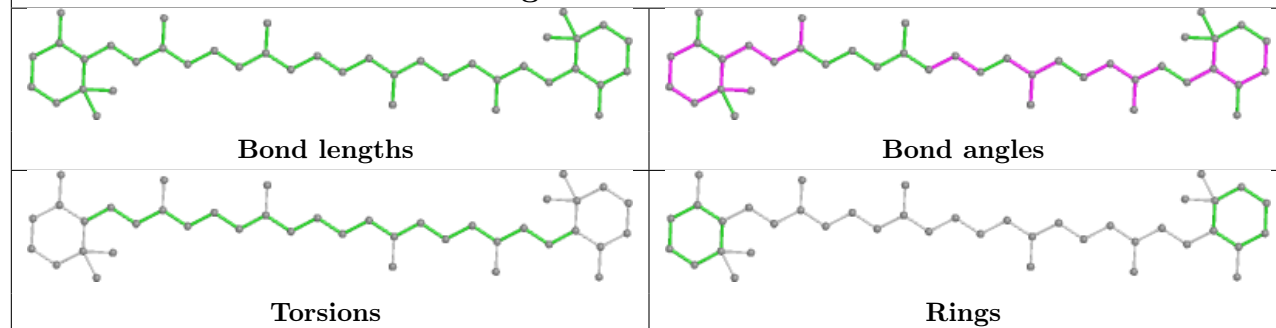


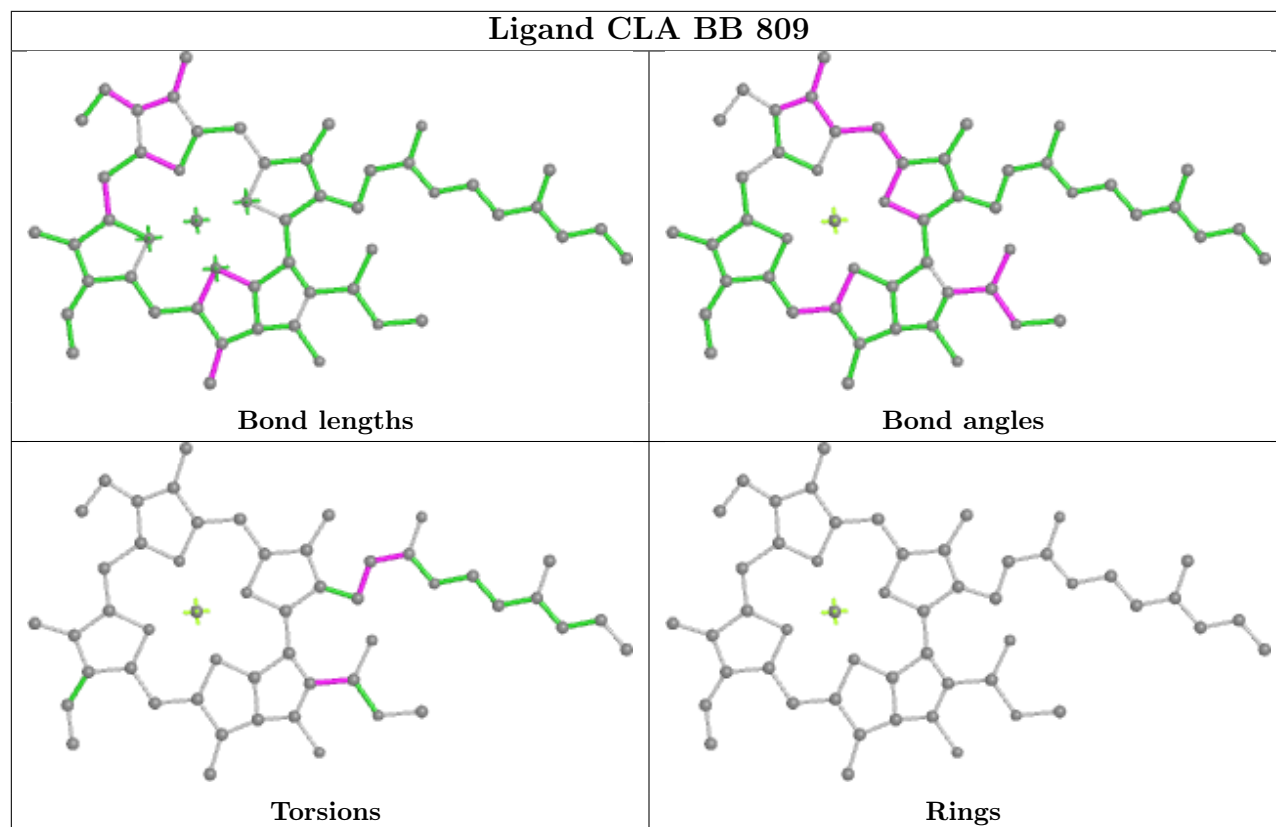


Ligand CLA A4 307

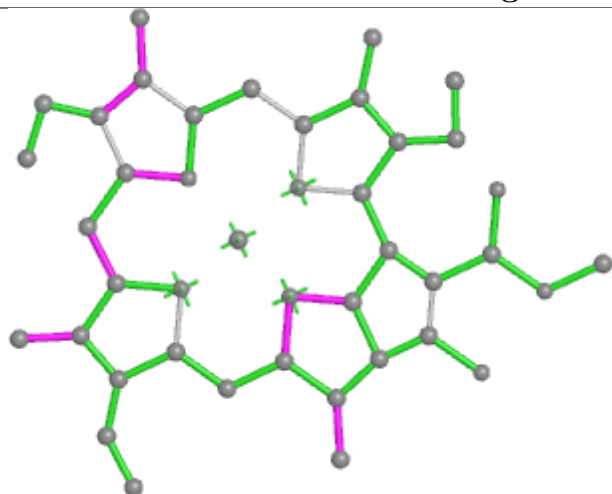


Ligand BCR BJ 101

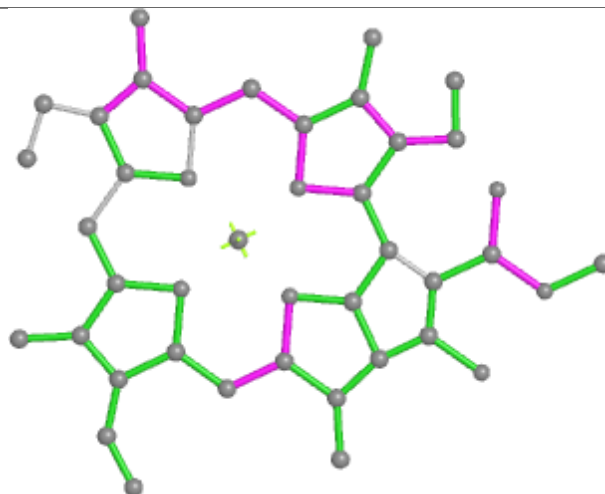




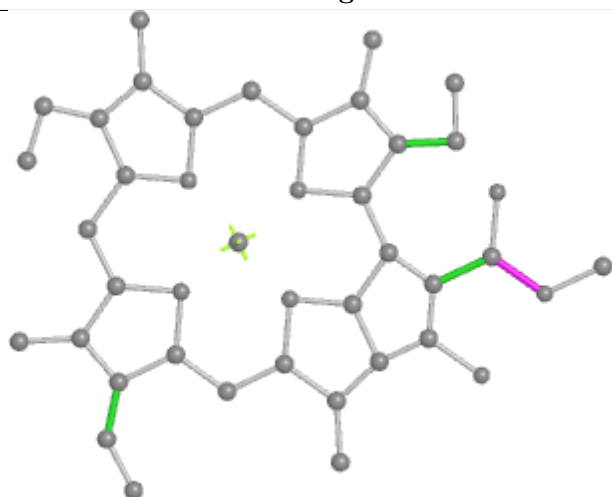
Ligand CLA AF 803



Bond lengths



Bond angles

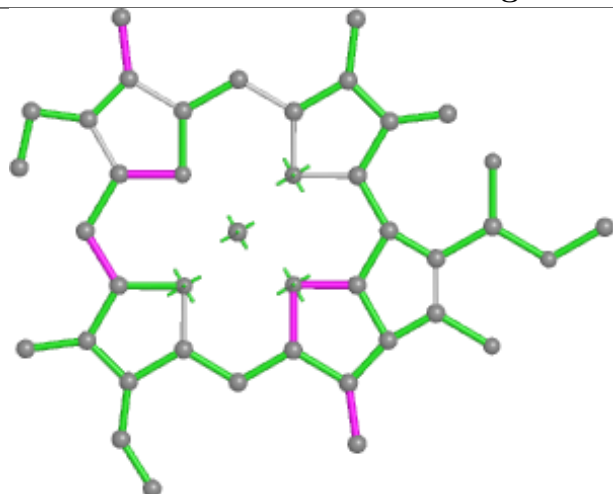


Torsions

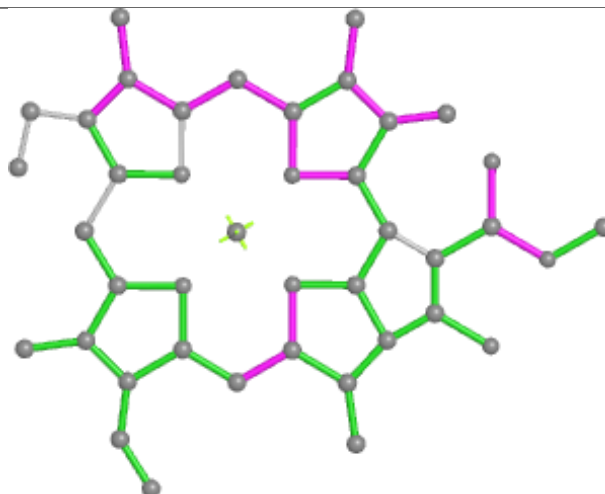


Rings

Ligand CLA BA 823



Bond lengths



Bond angles

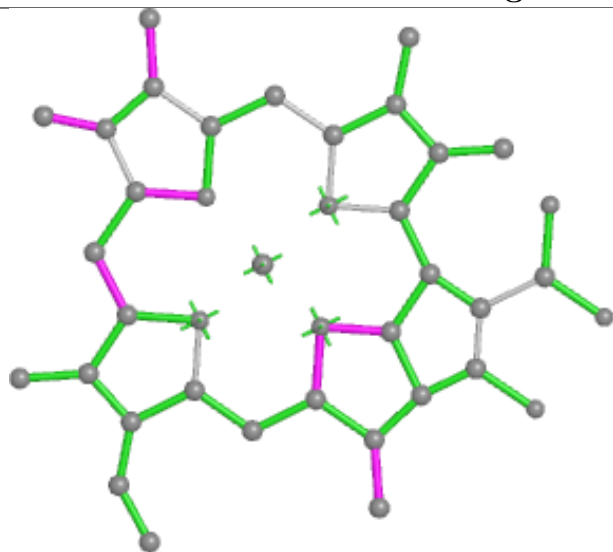


Torsions

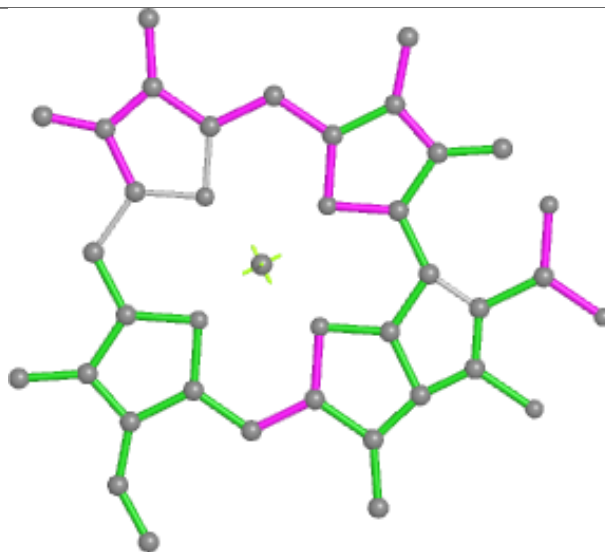


Rings

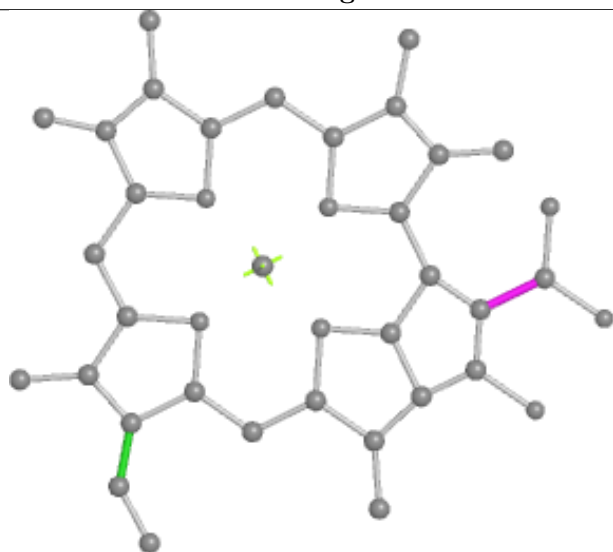
Ligand CLA B1 310



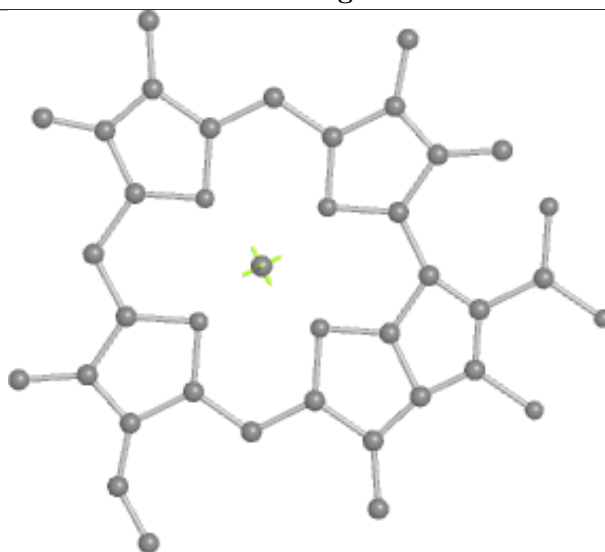
Bond lengths



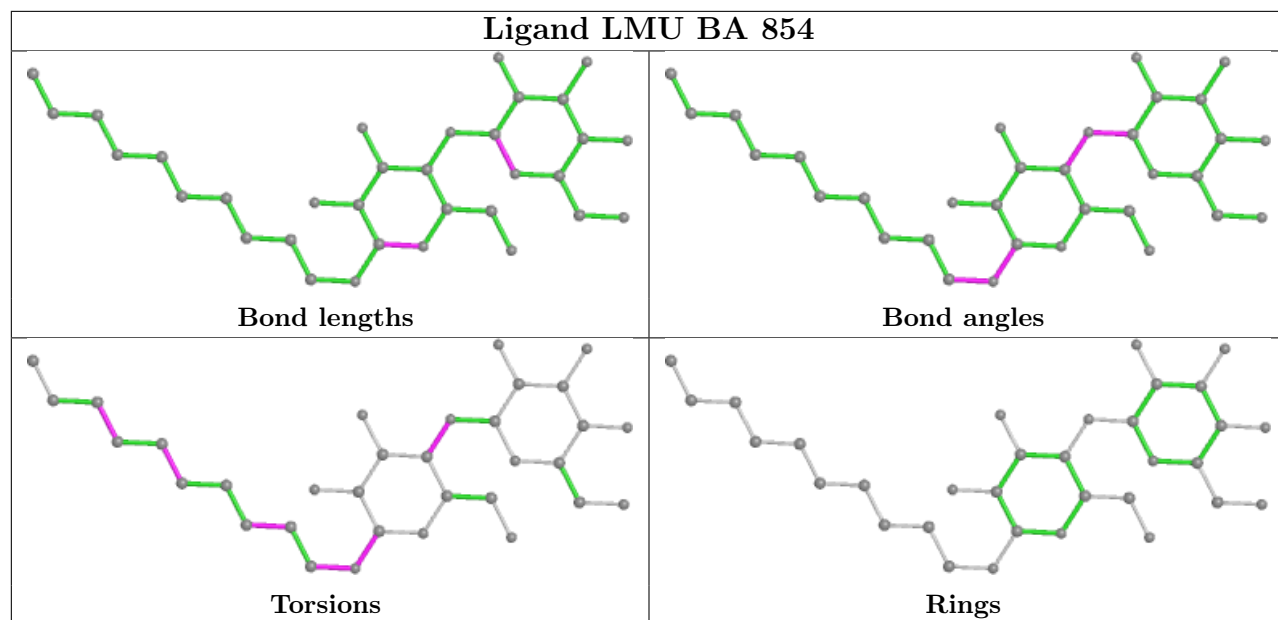
Bond angles



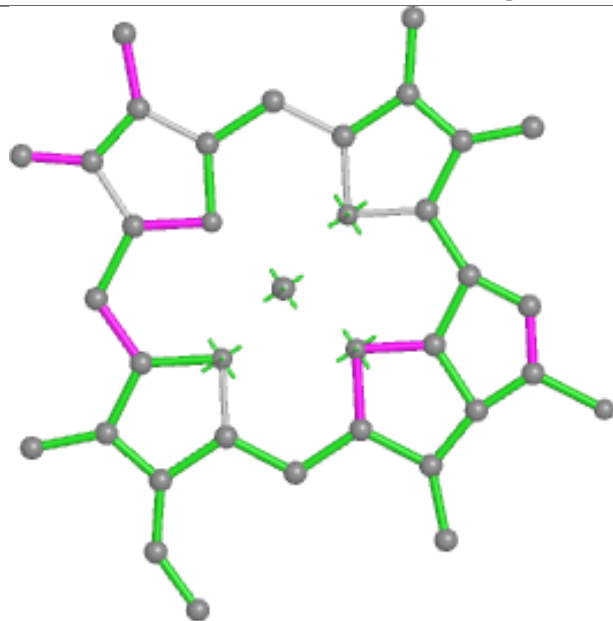
Torsions



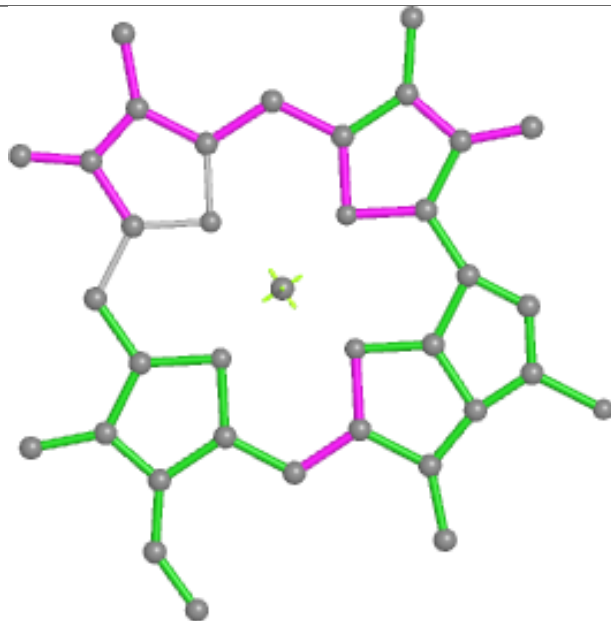
Rings



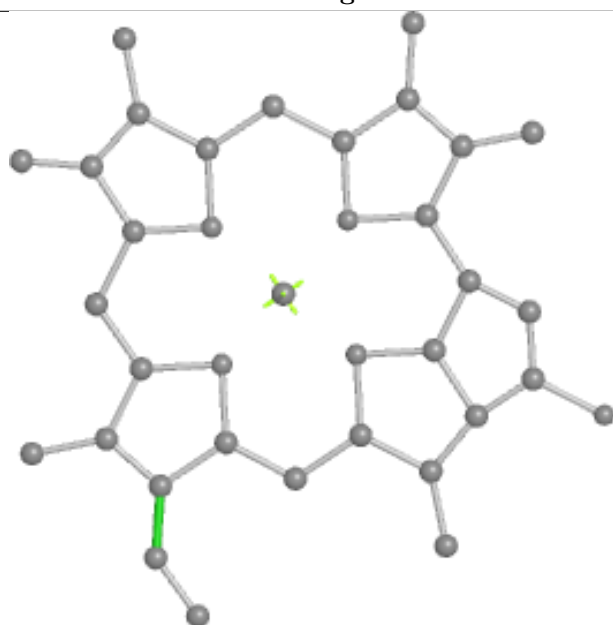
Ligand CLA BK 201



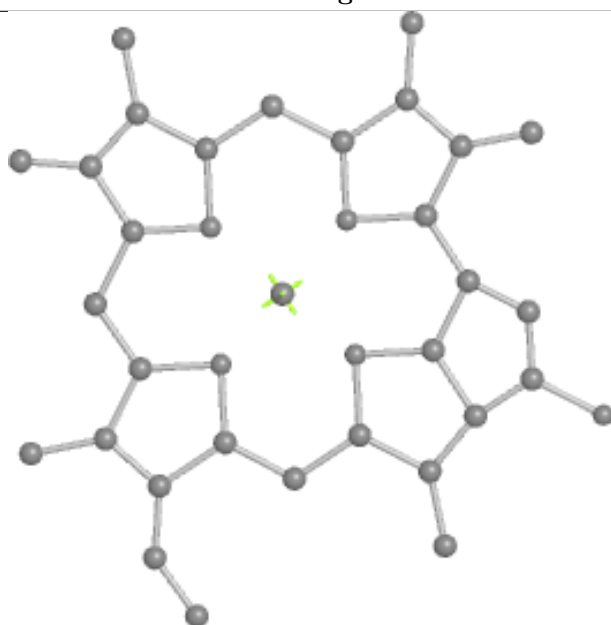
Bond lengths



Bond angles

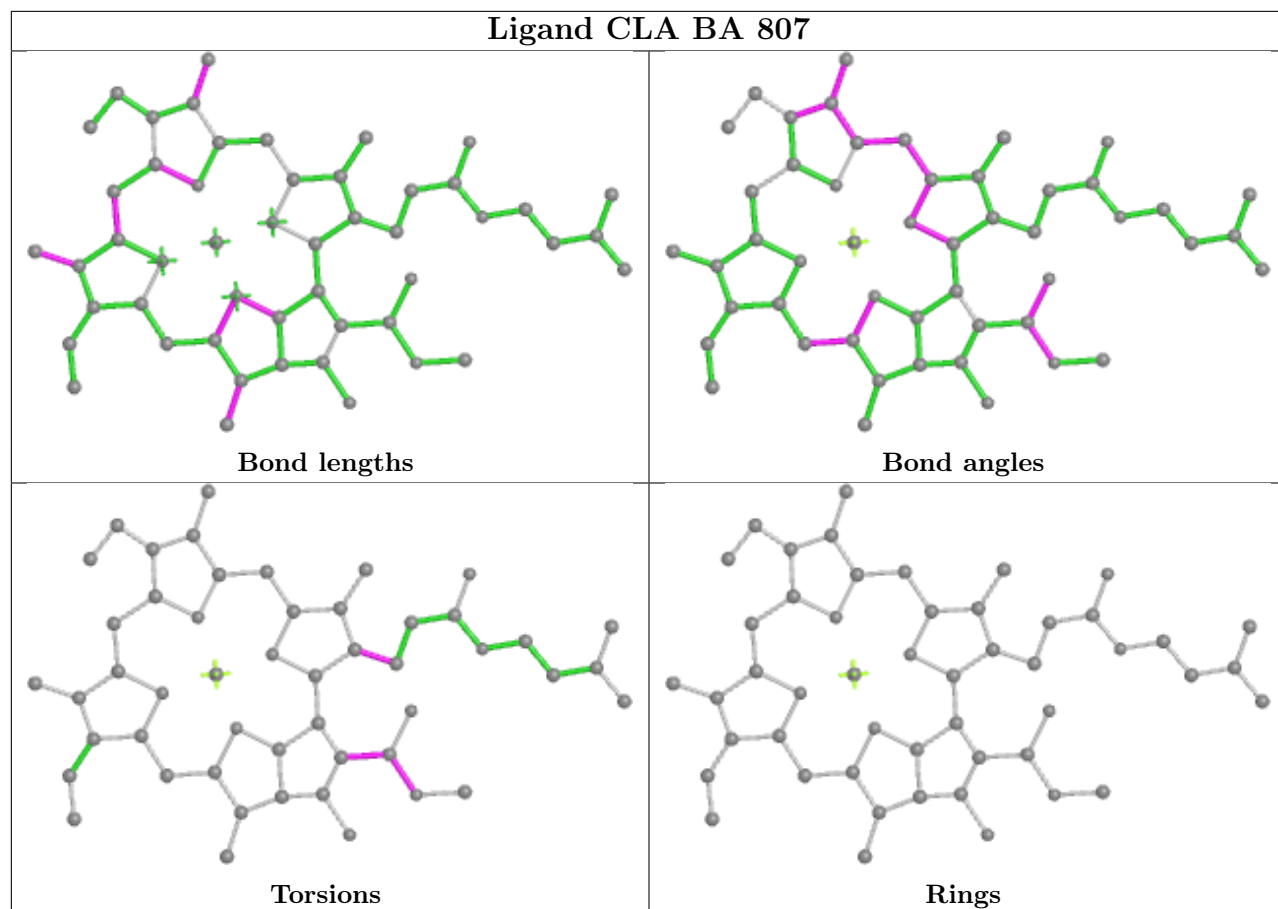


Torsions

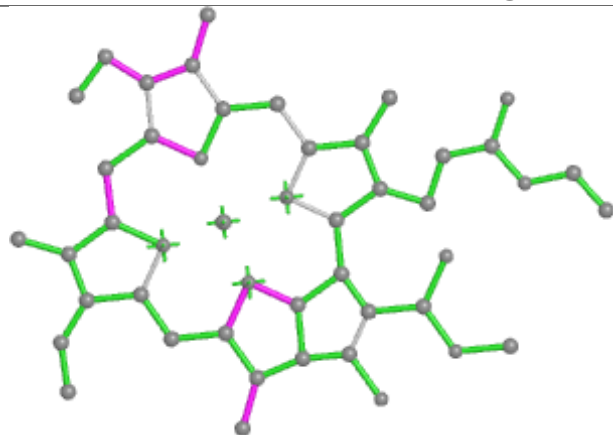


Rings

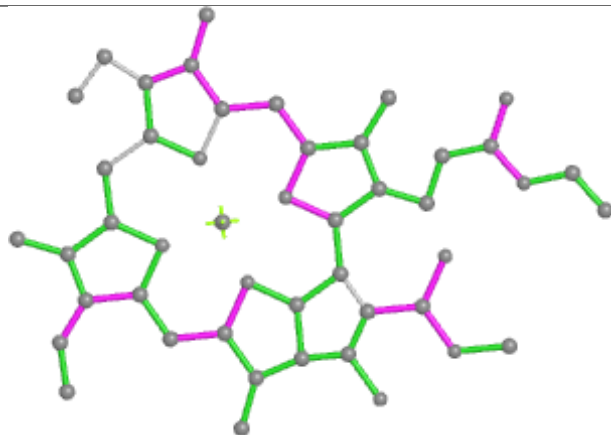
Ligand CLA BA 807



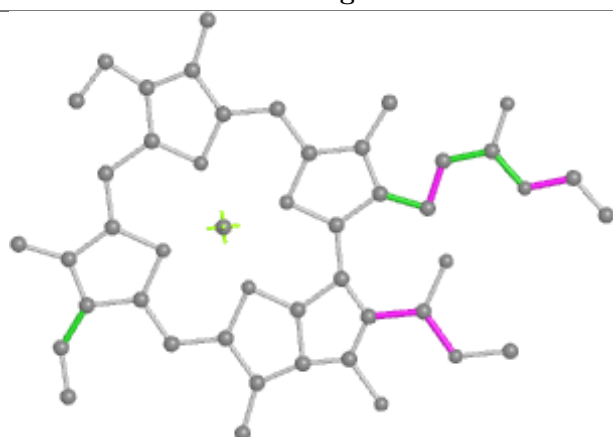
Ligand CLA BA 831



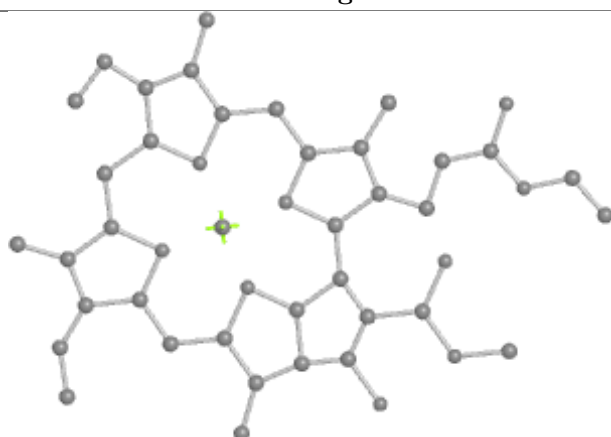
Bond lengths



Bond angles

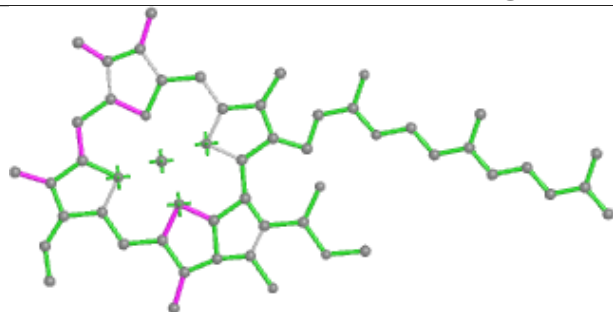


Torsions

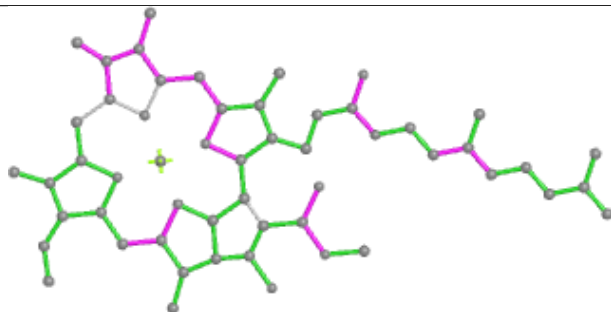


Rings

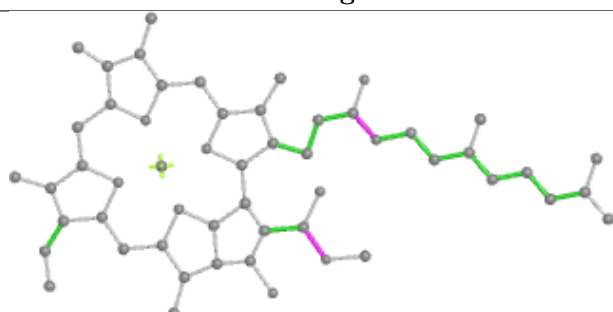
Ligand CLA BB 813



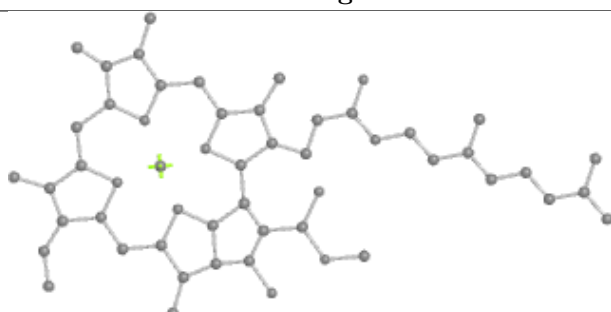
Bond lengths



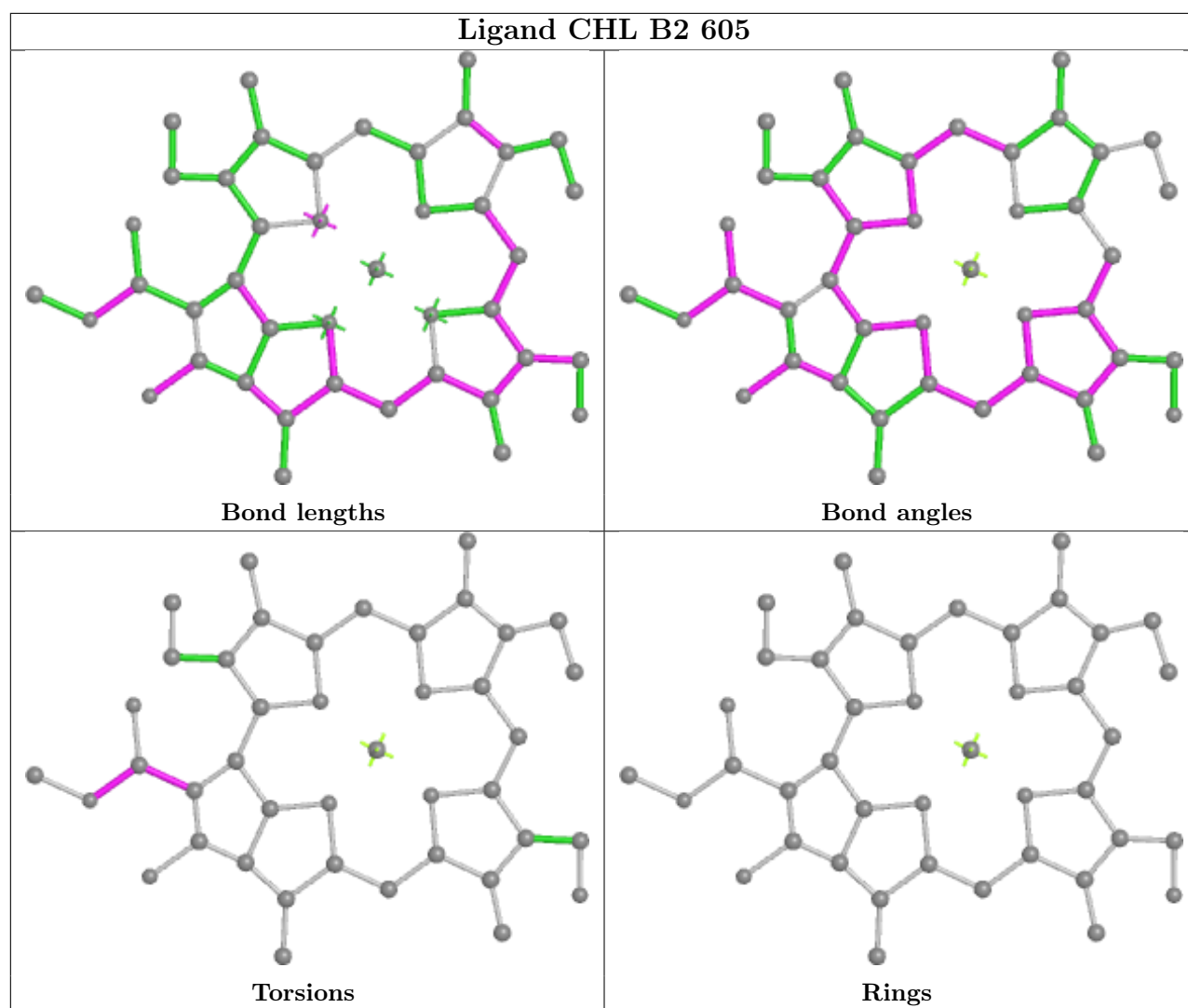
Bond angles

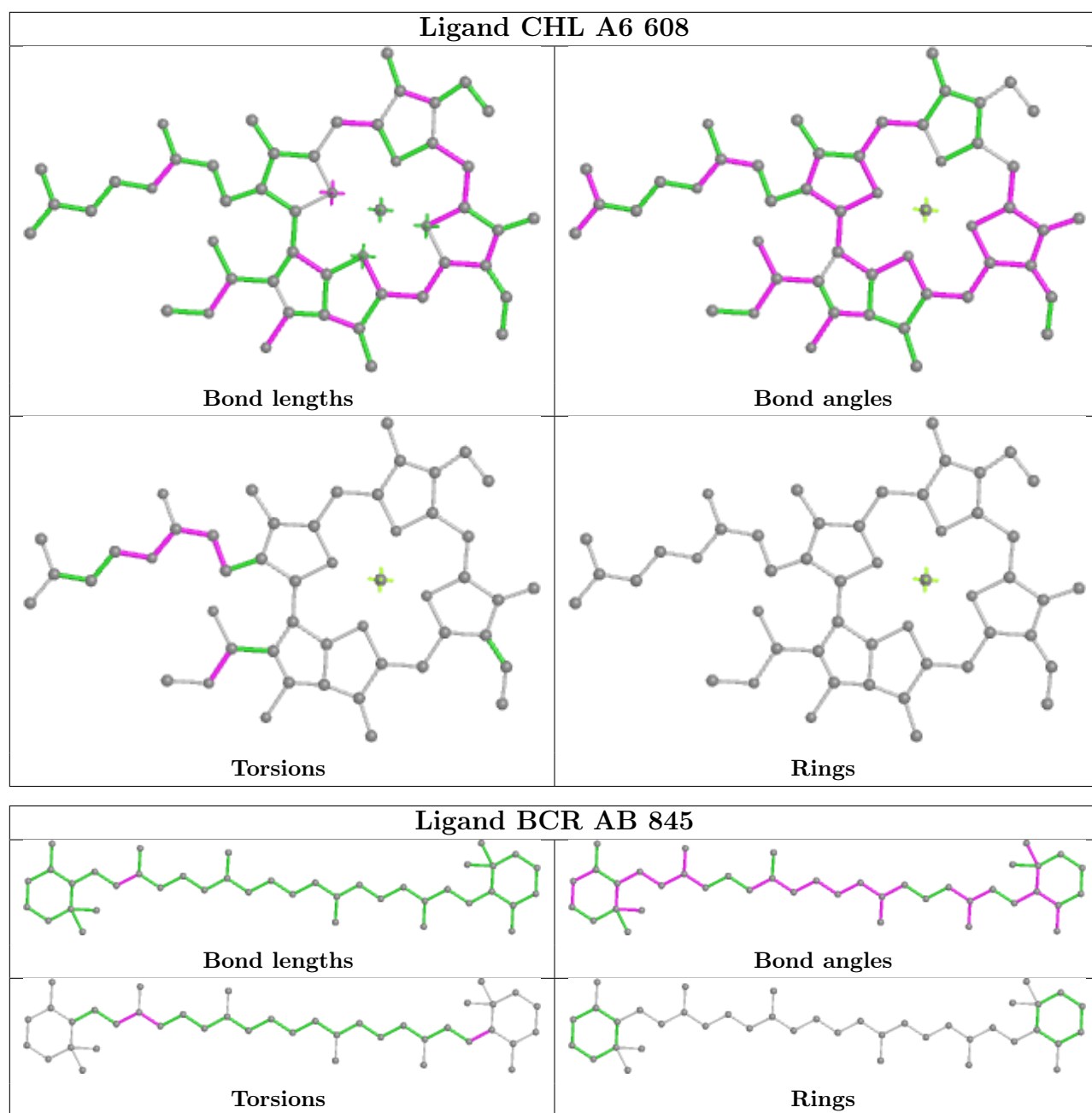


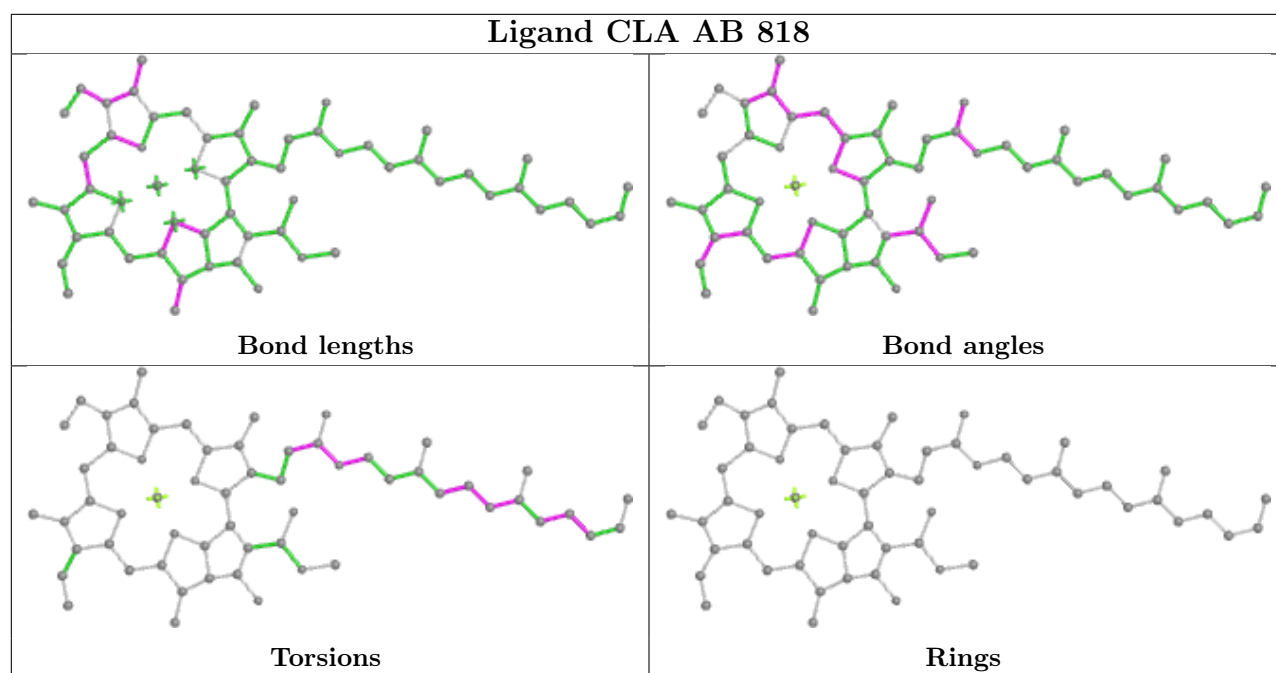
Torsions



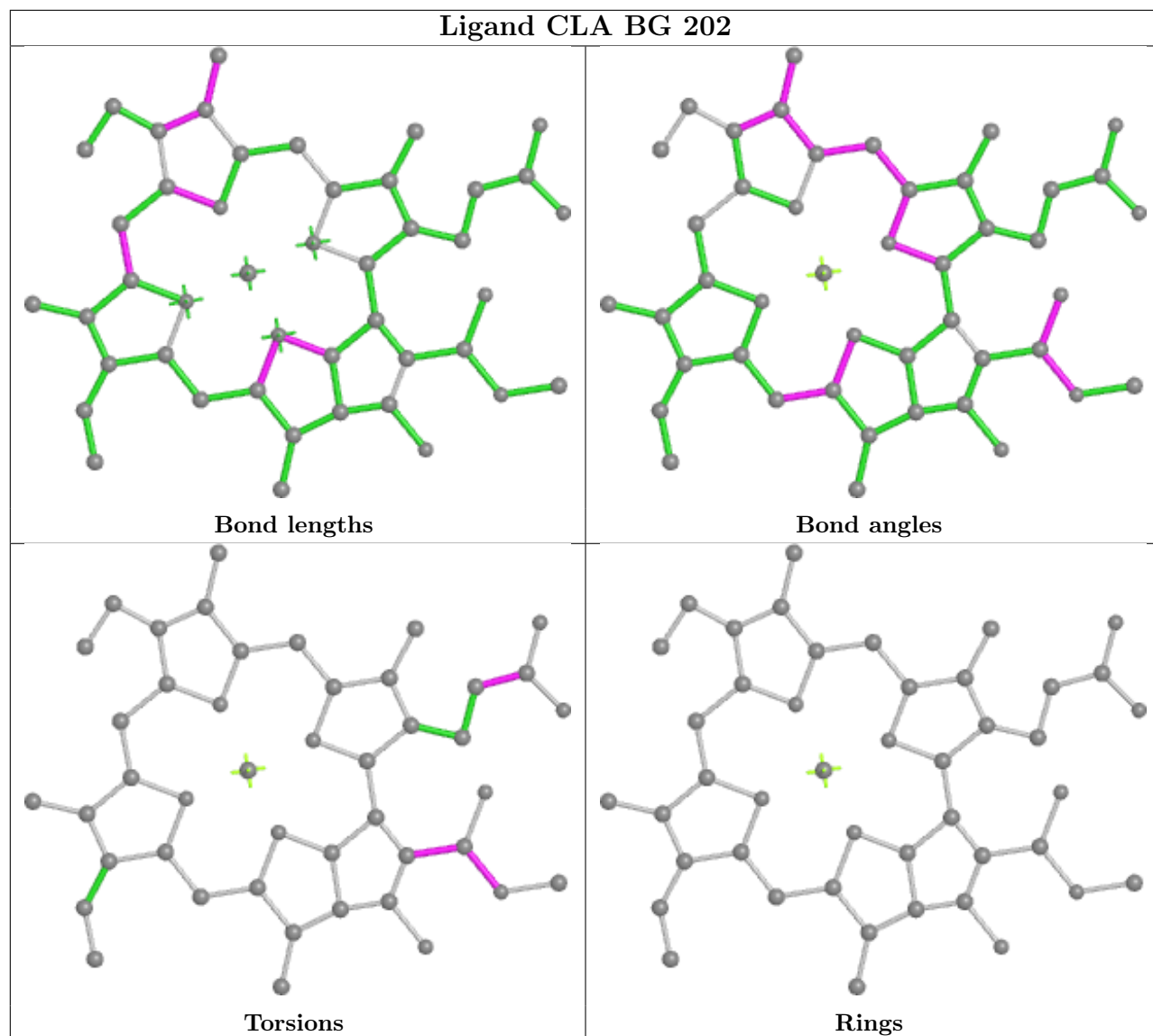
Rings



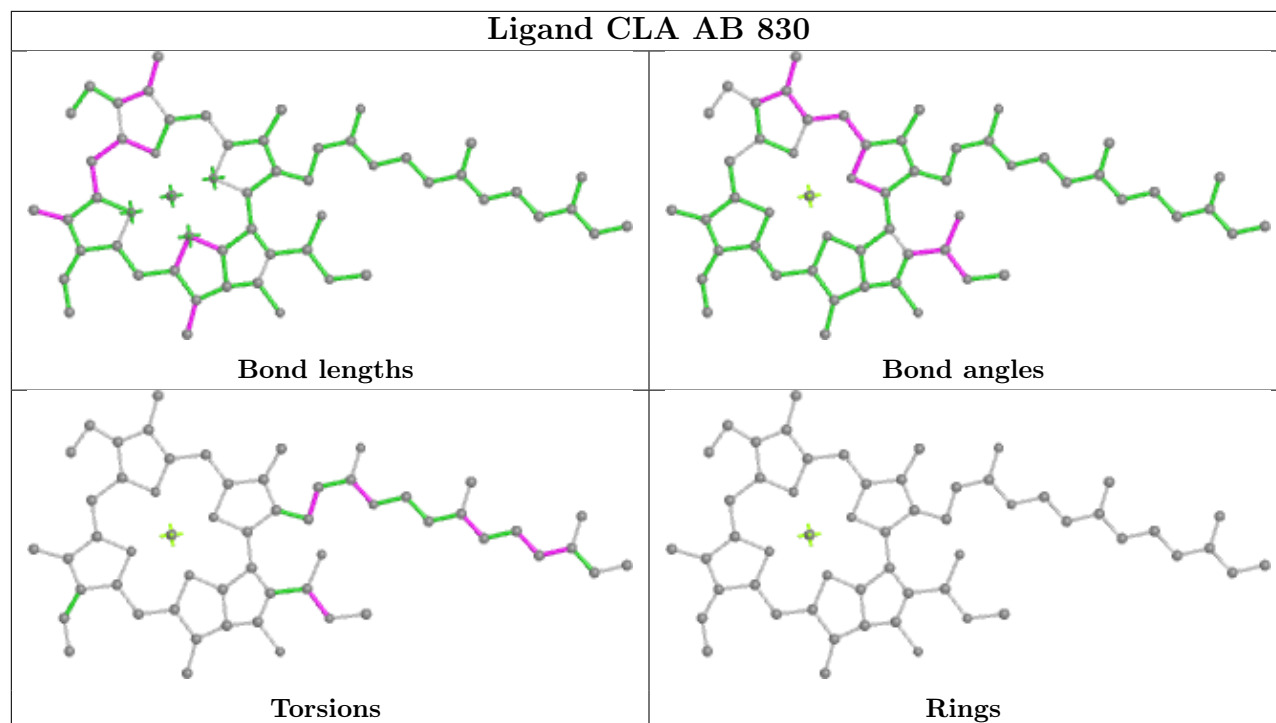




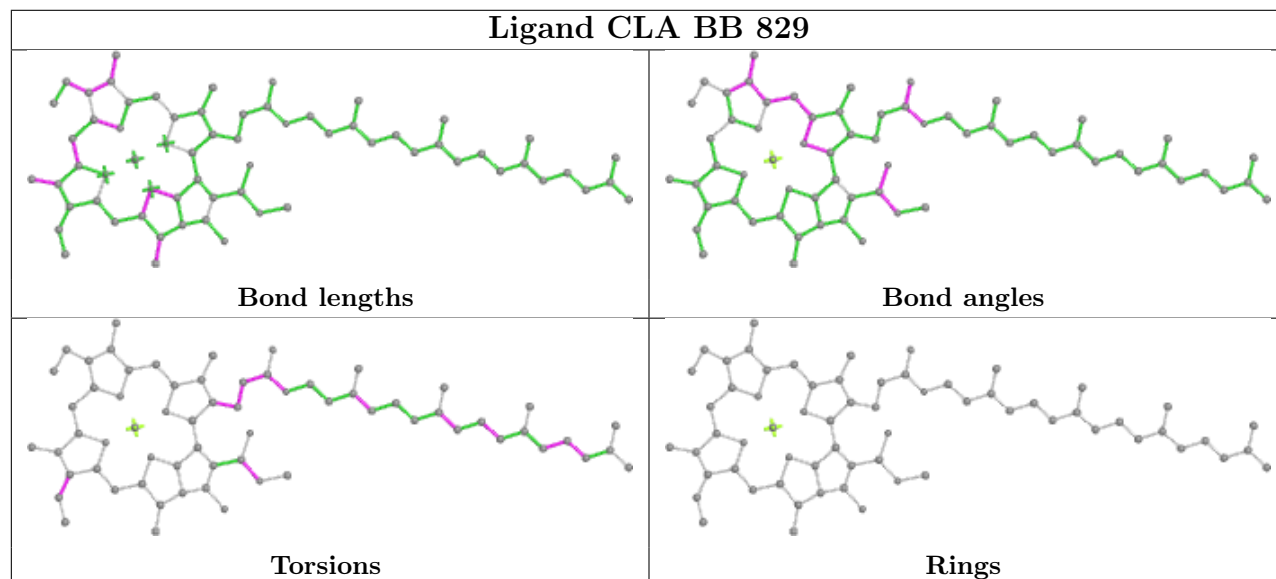
Ligand CLA BG 202



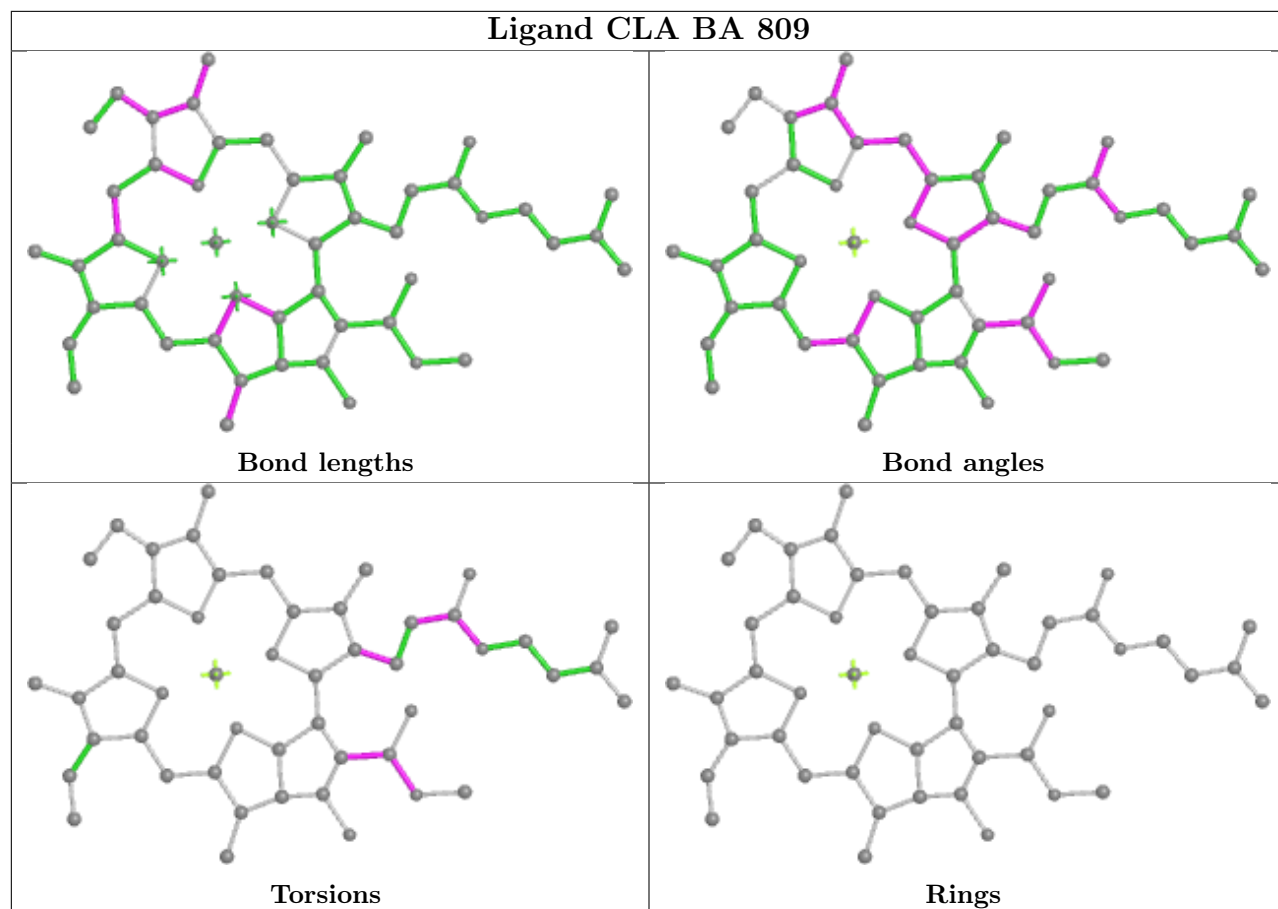
Ligand CLA AB 830

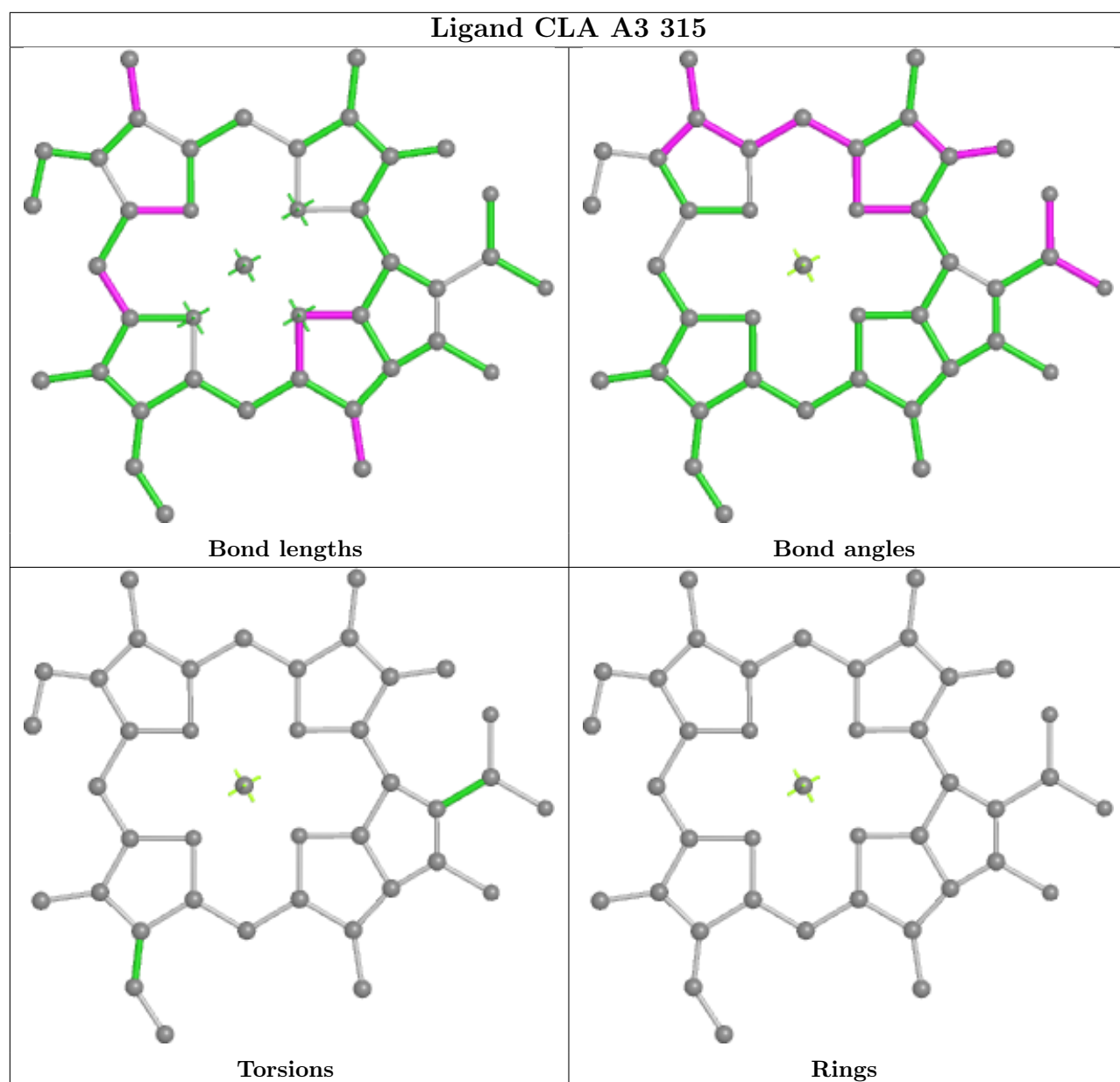


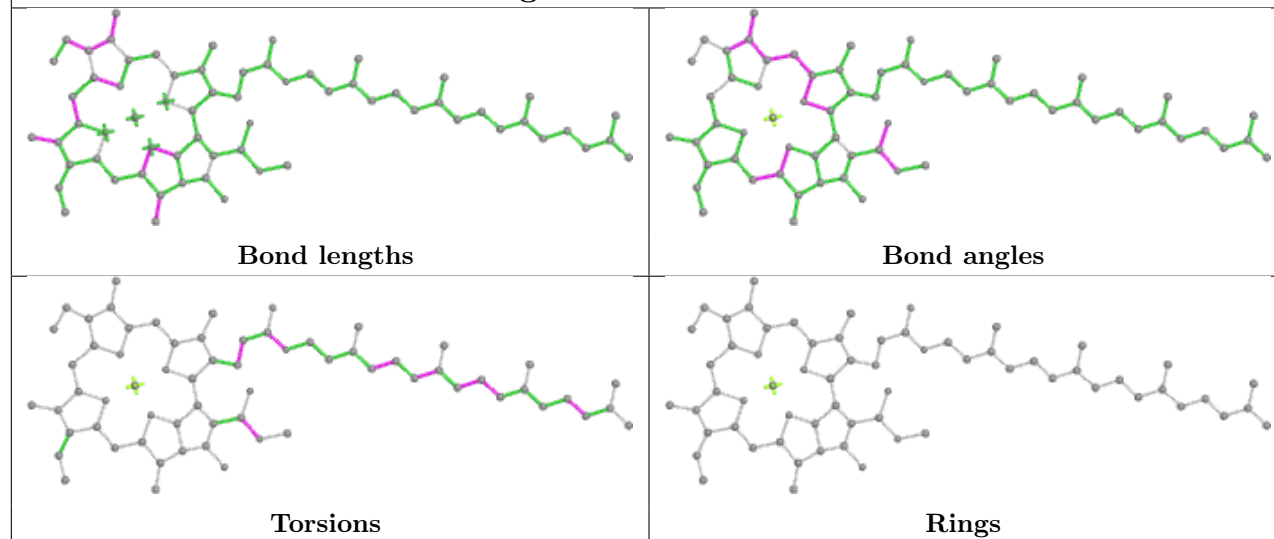
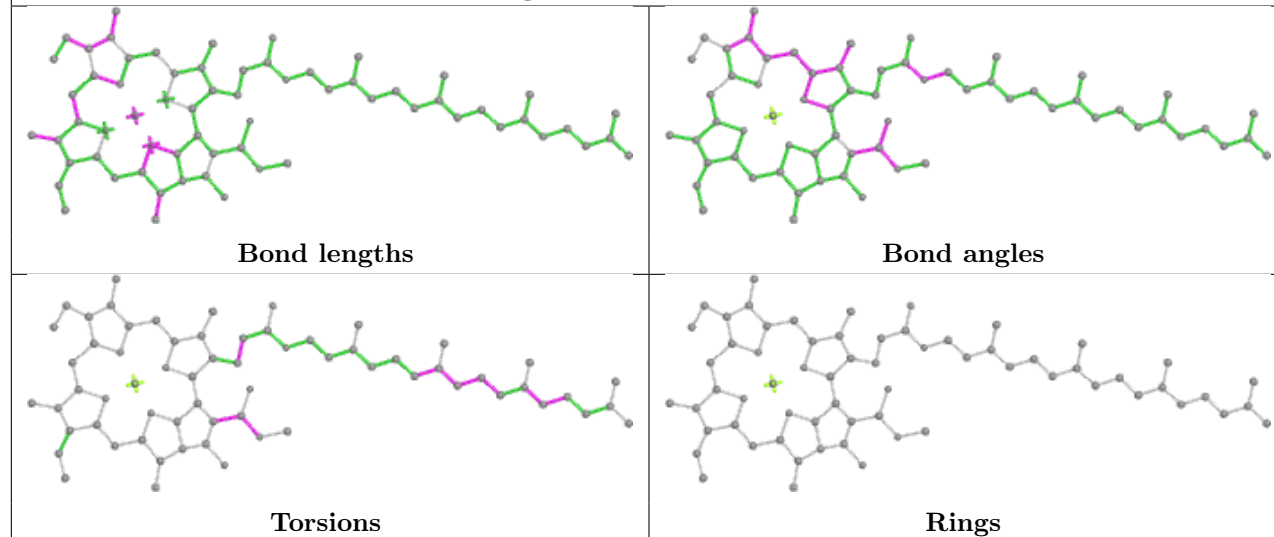
Ligand CLA BB 829



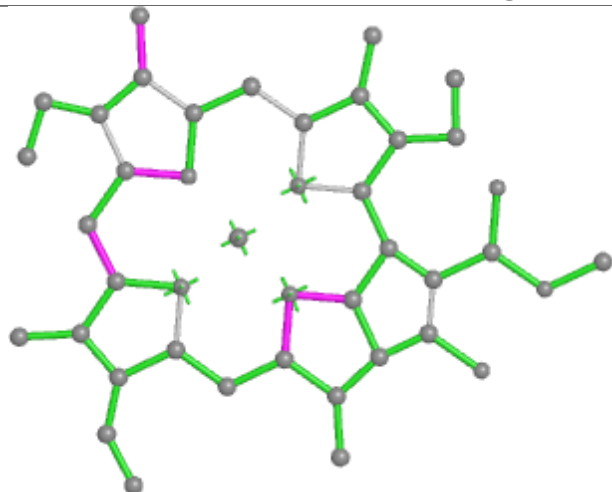
Ligand CLA BA 809



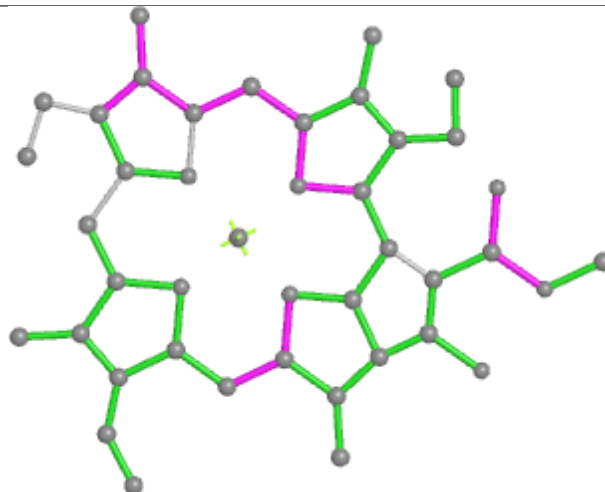


Ligand CLA BB 843**Ligand CLA AB 825**

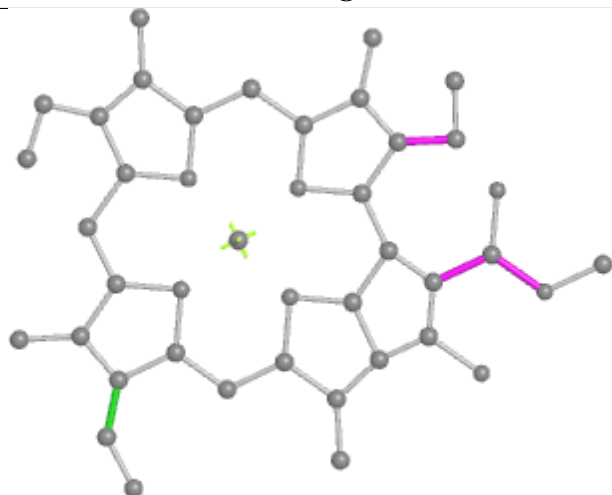
Ligand CLA BB 837



Bond lengths



Bond angles

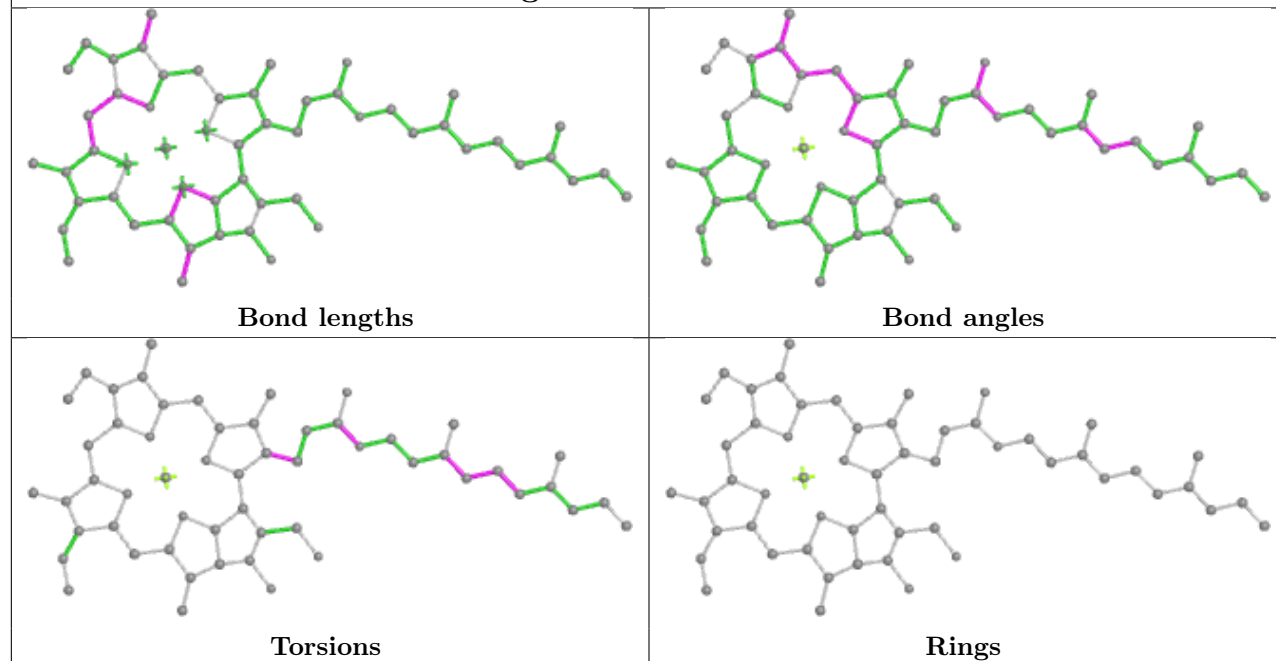


Torsions

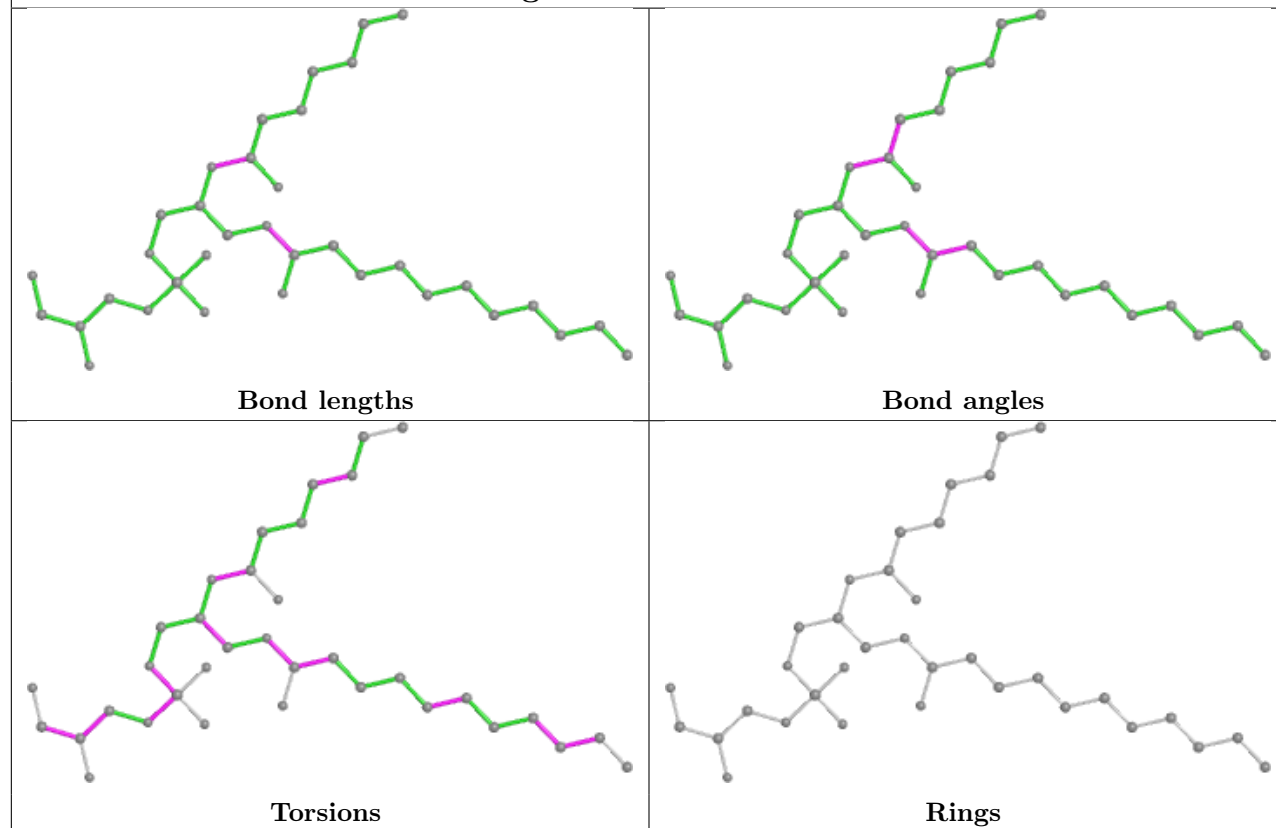


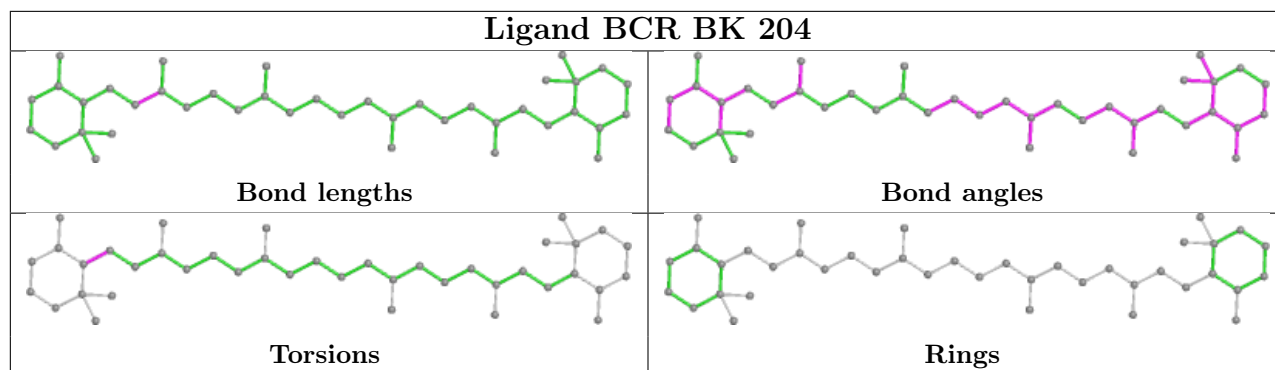
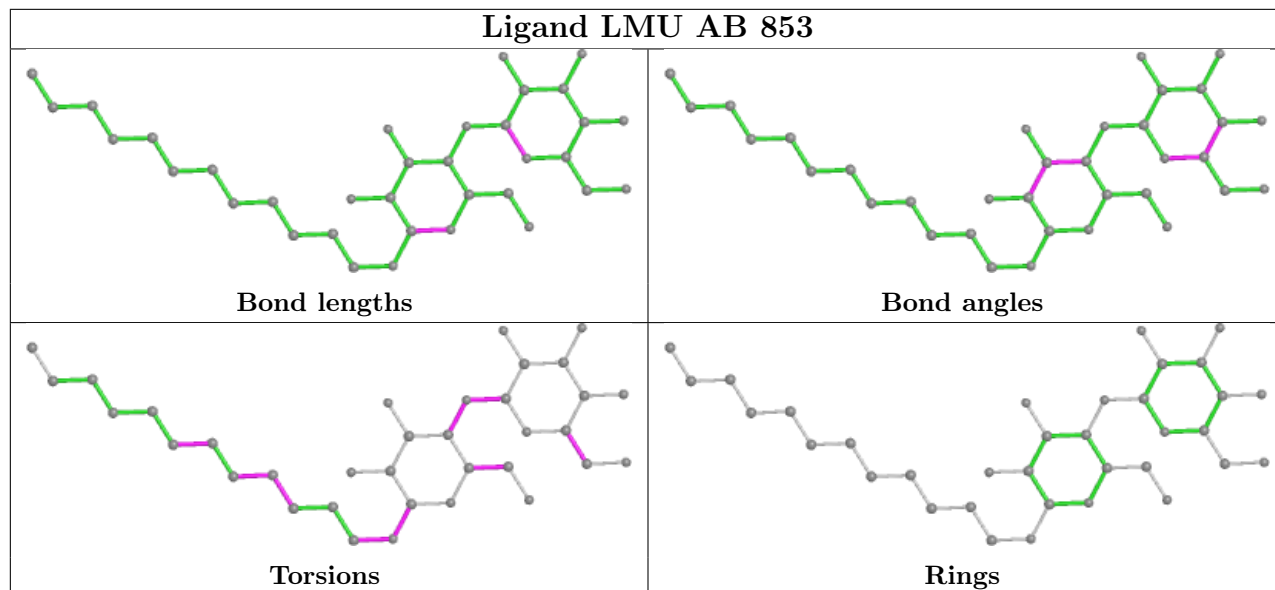
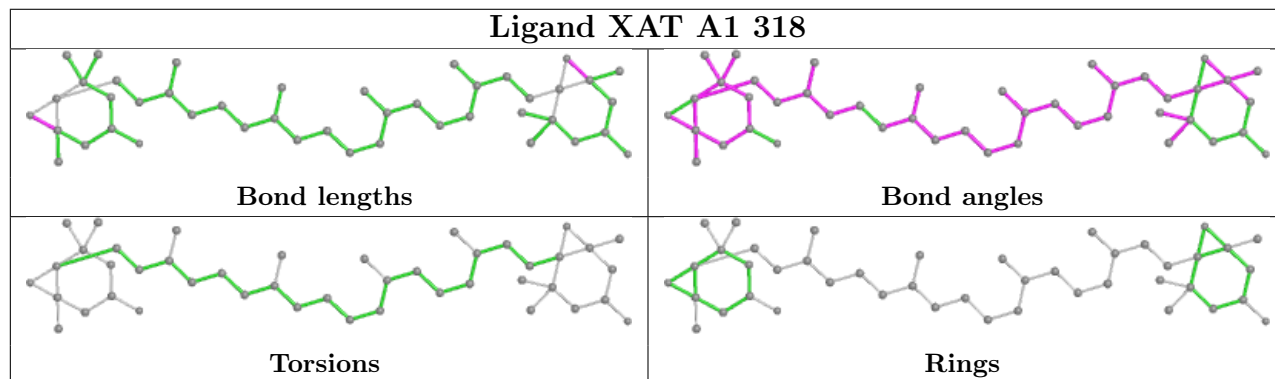
Rings

Ligand CLA BF 301

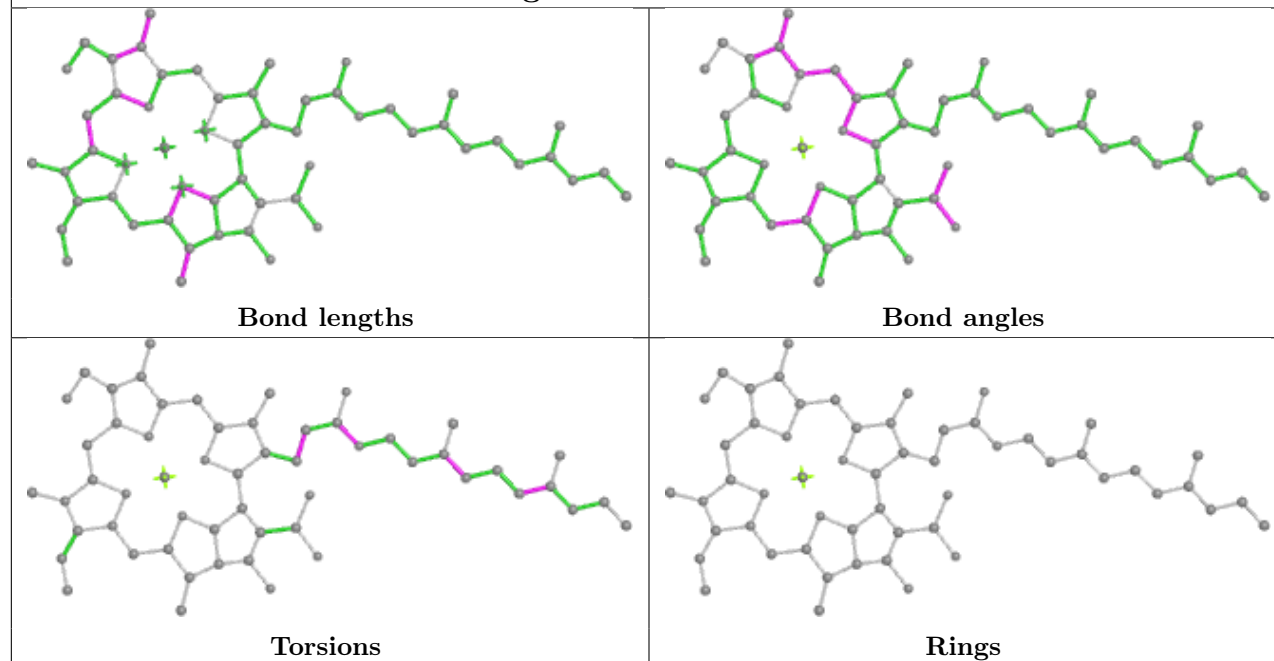


Ligand LHG B2 618

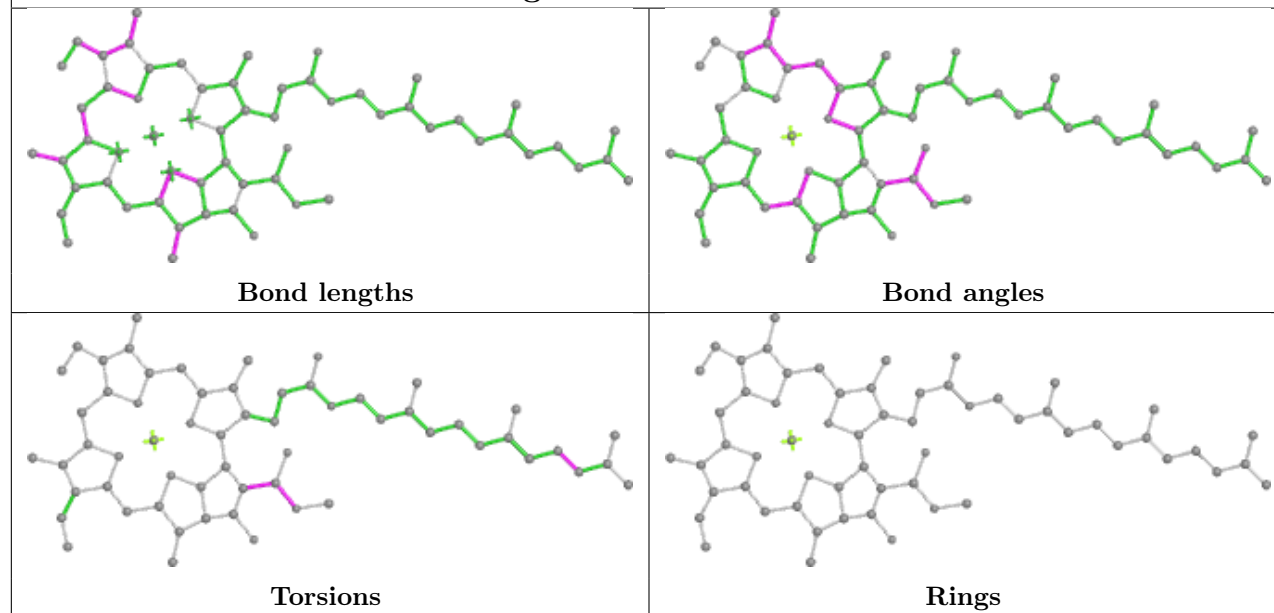


Ligand BCR BK 204**Ligand LMU AB 853****Ligand XAT A1 318**

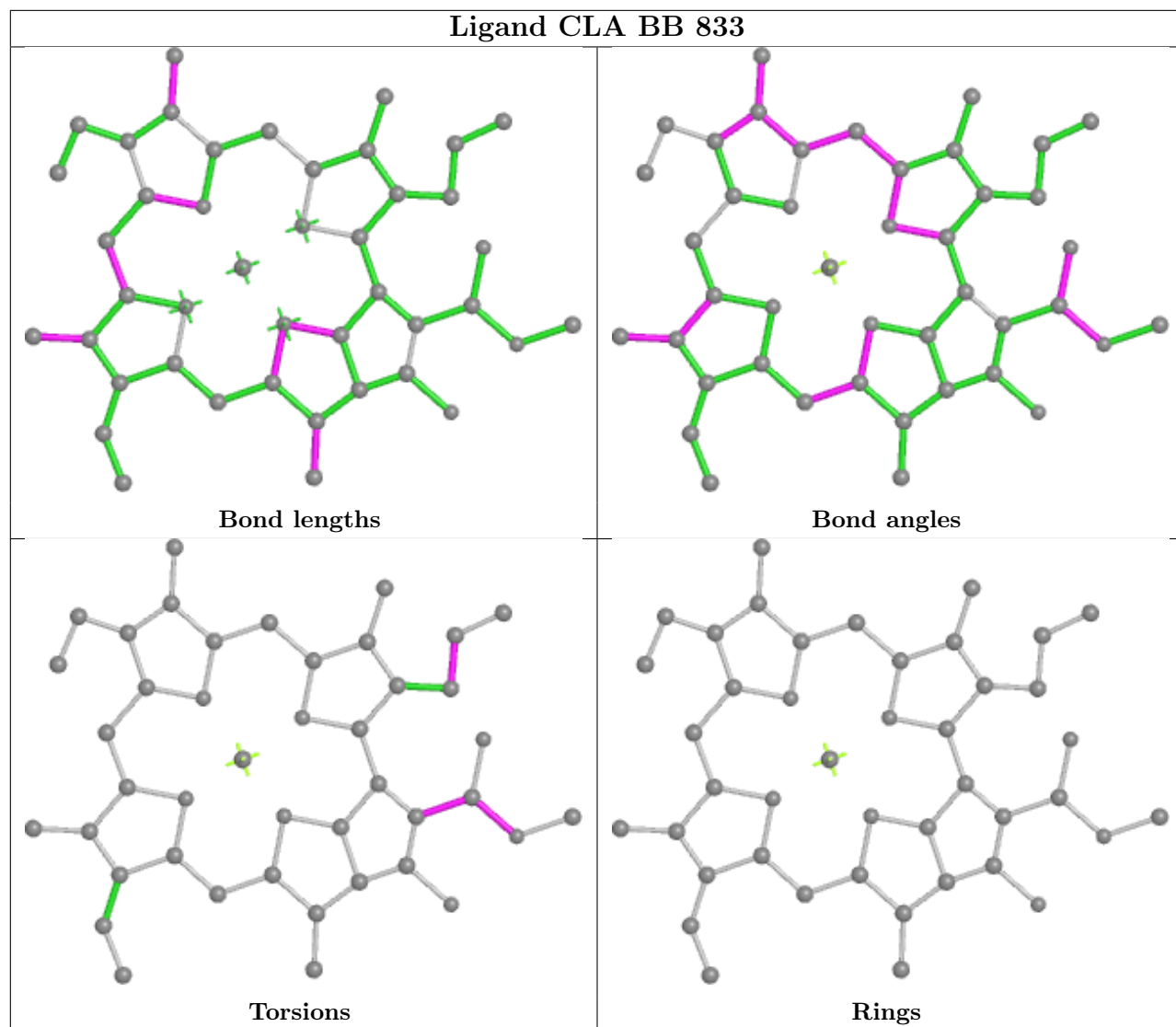
Ligand CLA A4 311



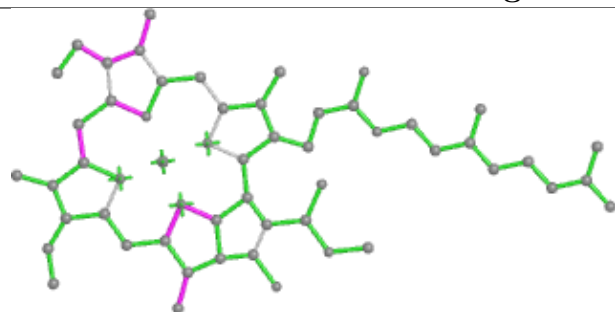
Ligand CLA B3 301



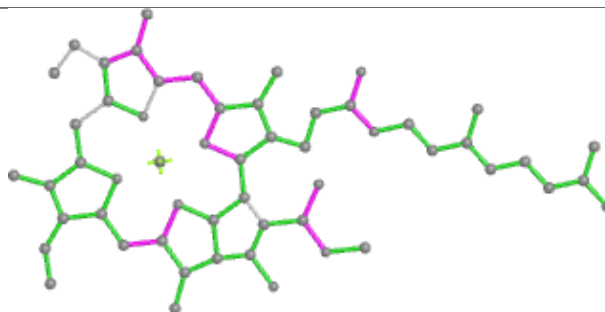
Ligand CLA BB 833



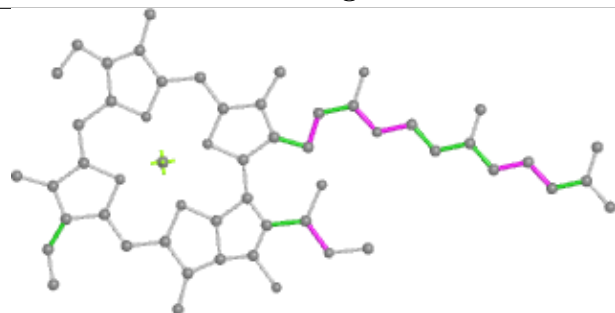
Ligand CLA BB 818



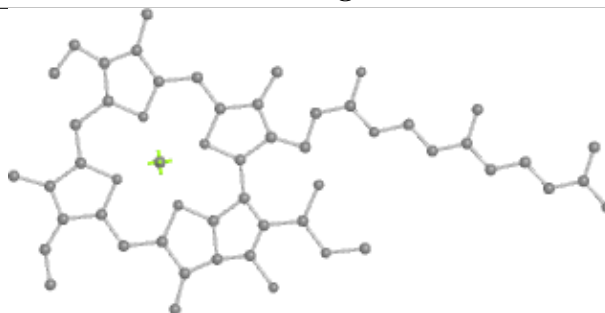
Bond lengths



Bond angles

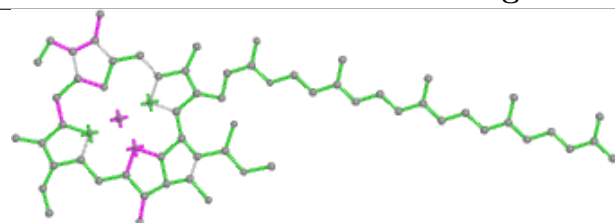


Torsions

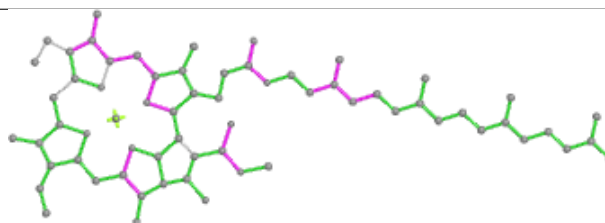


Rings

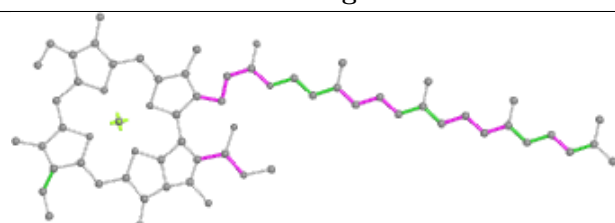
Ligand CLA AA 829



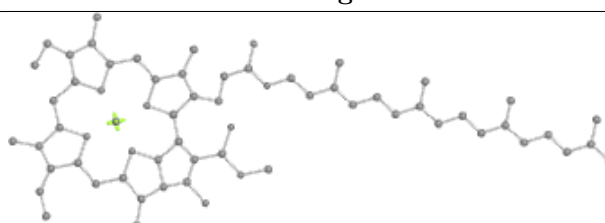
Bond lengths



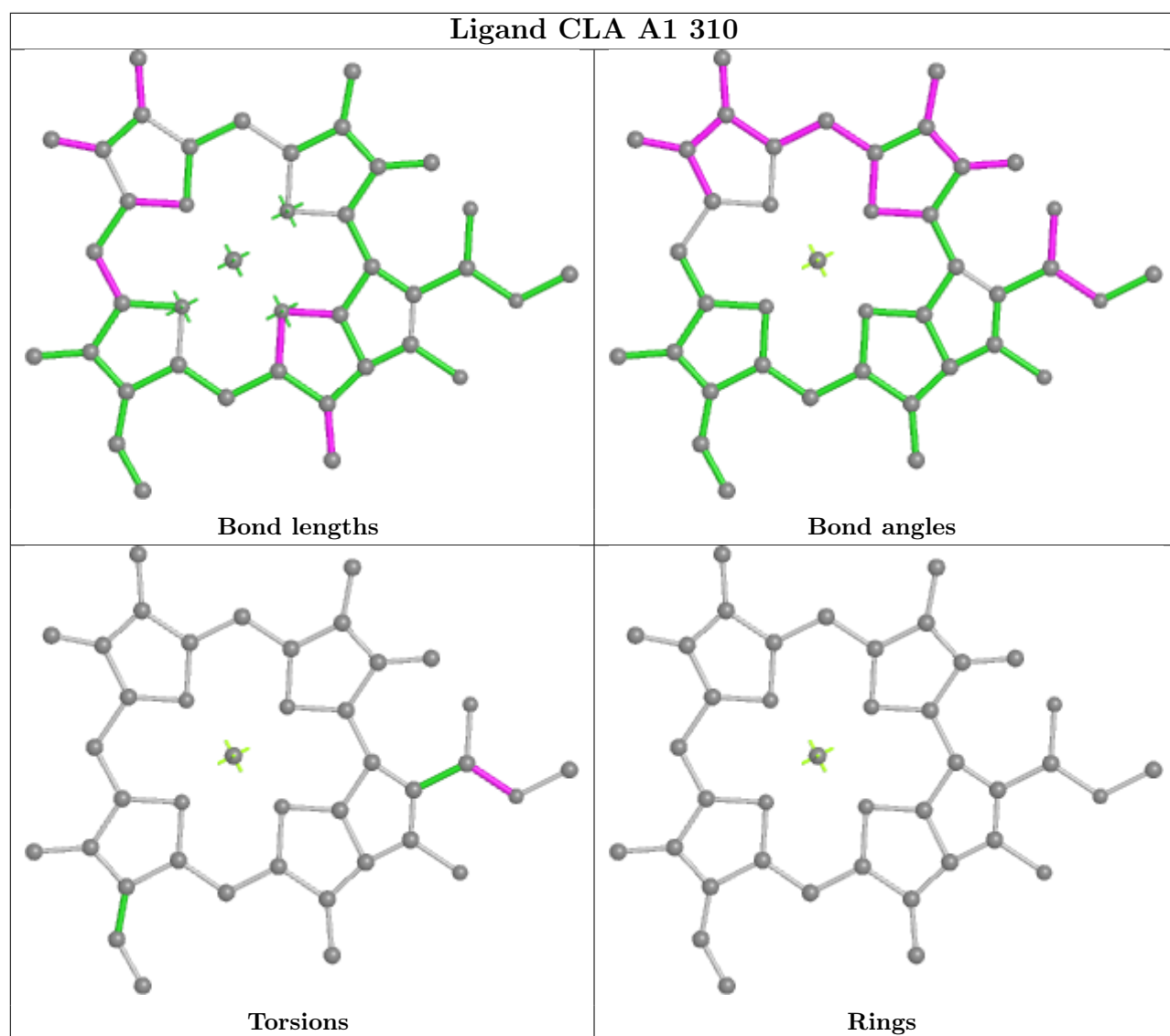
Bond angles

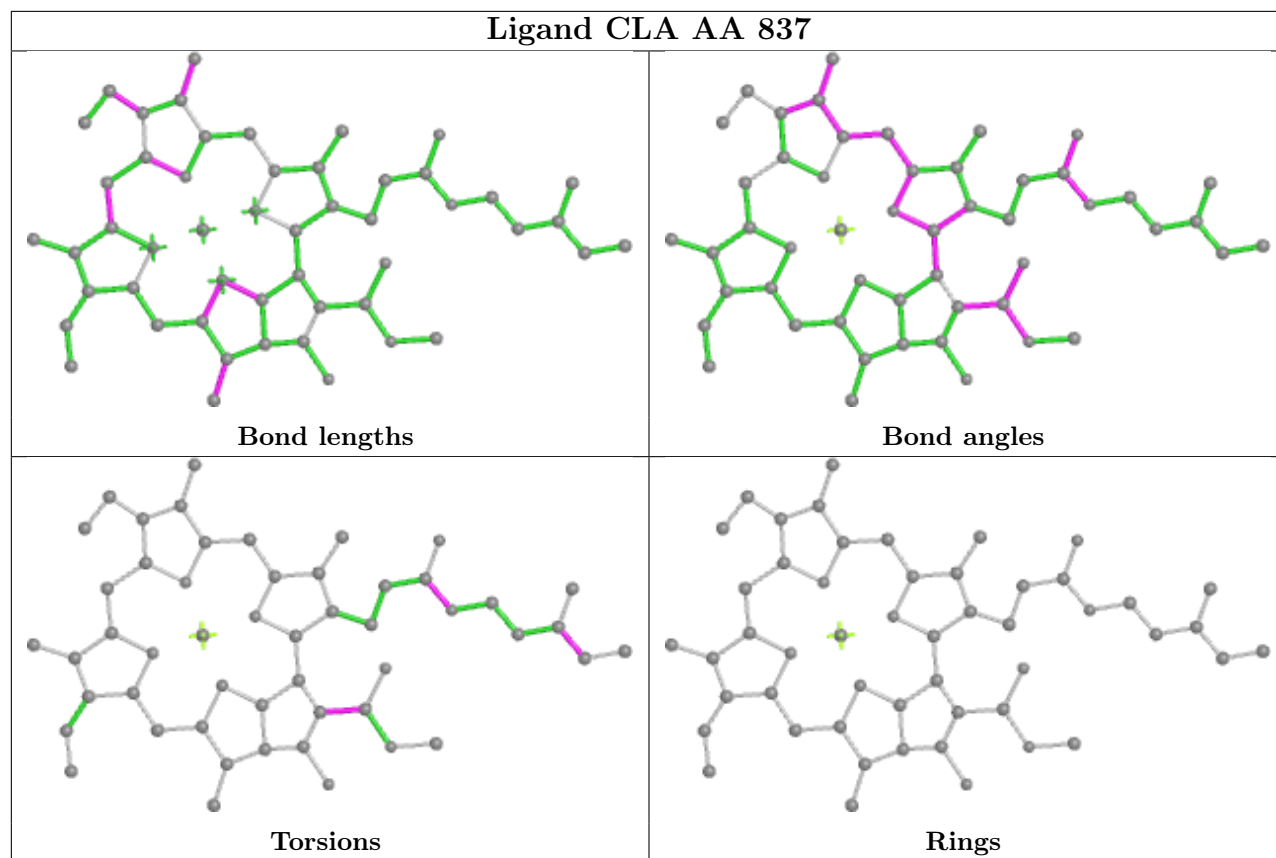


Torsions

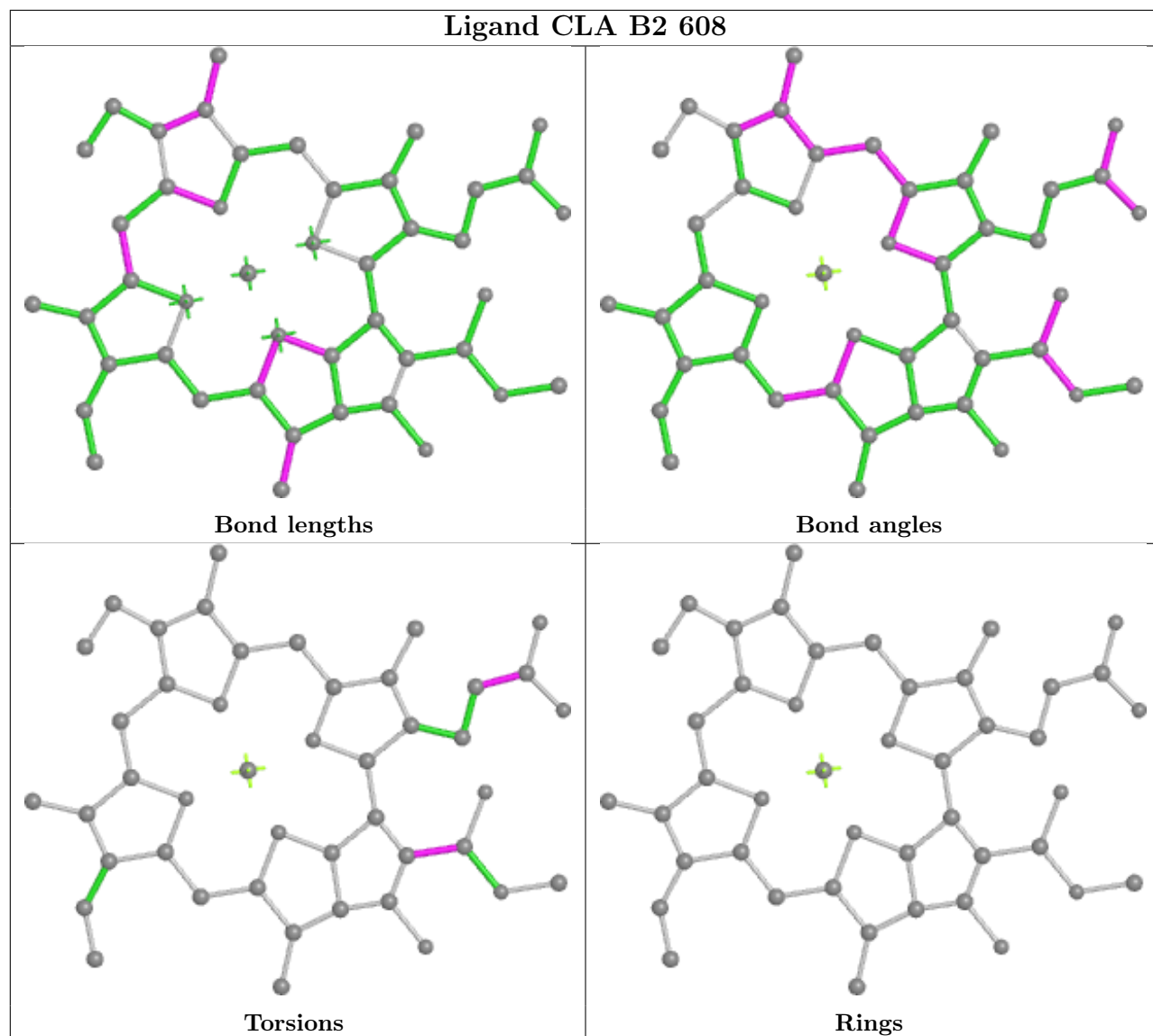


Rings

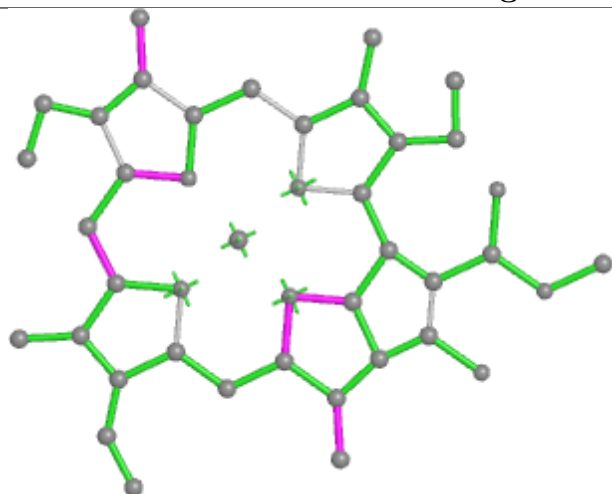




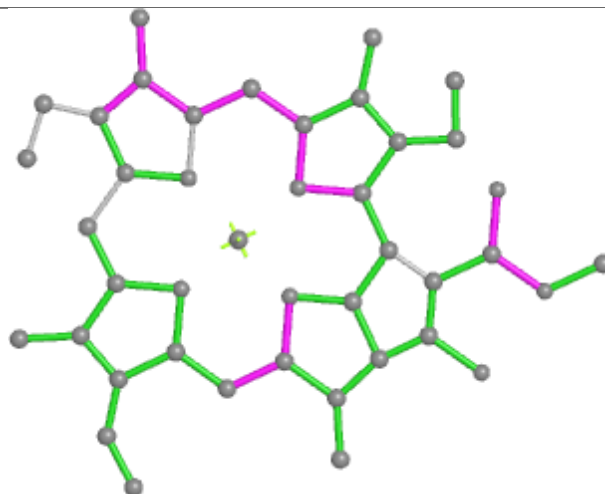
Ligand CLA B2 608



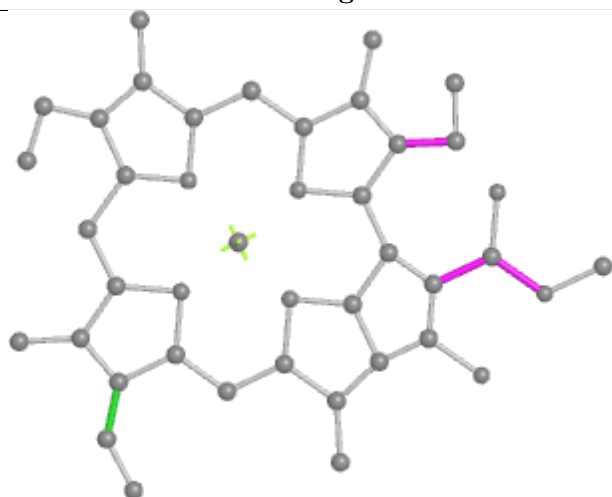
Ligand CLA BA 822



Bond lengths



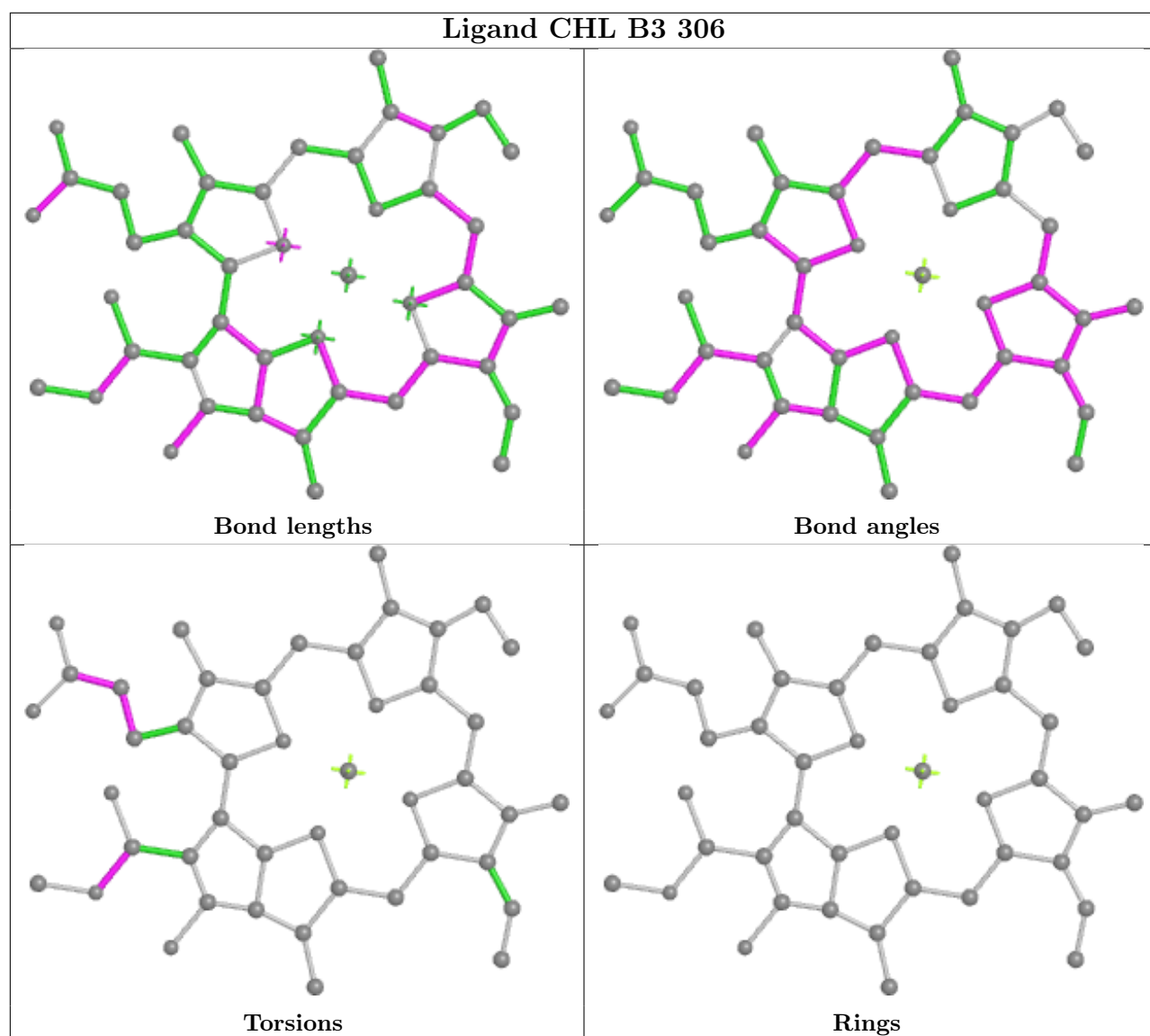
Bond angles

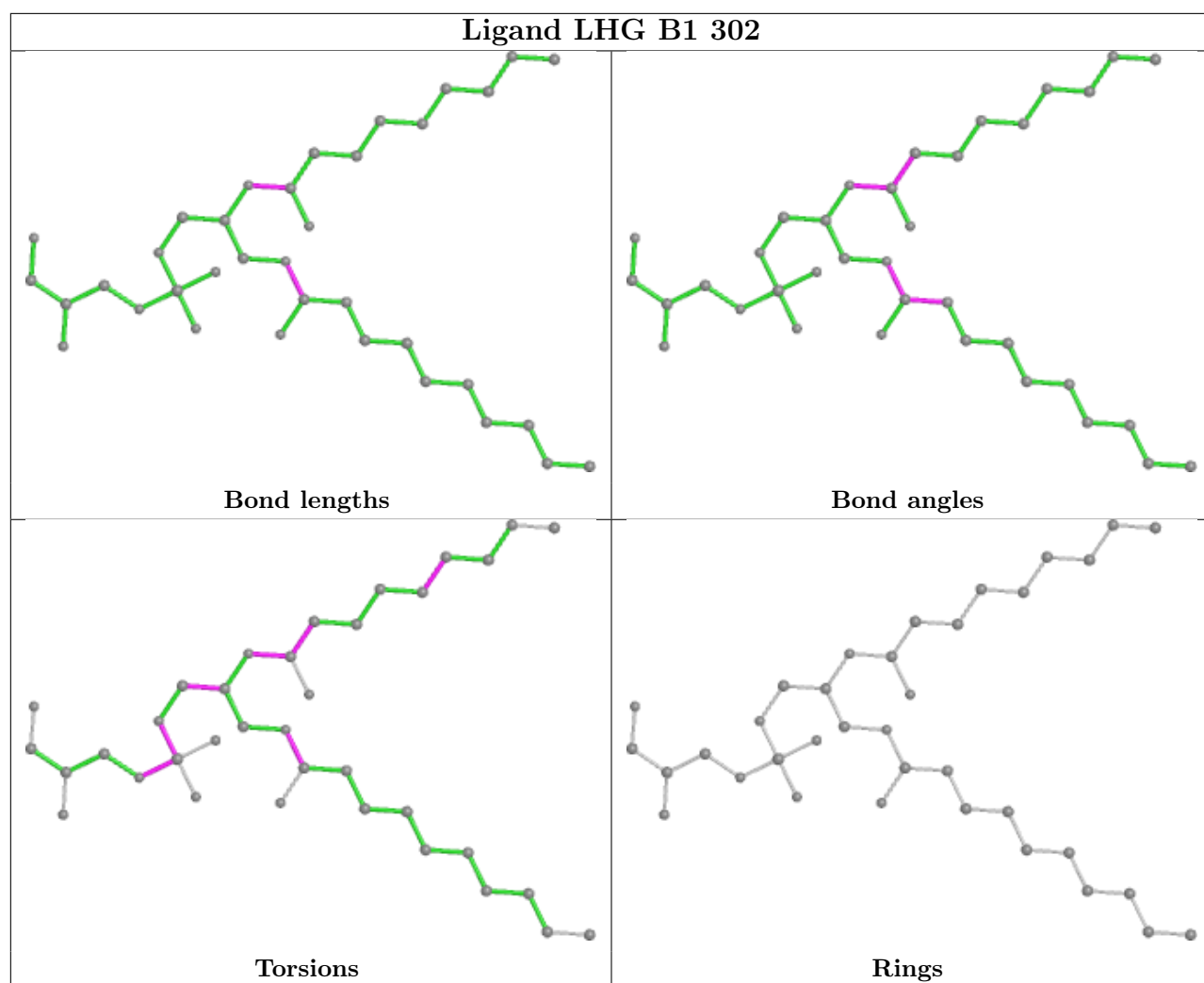


Torsions

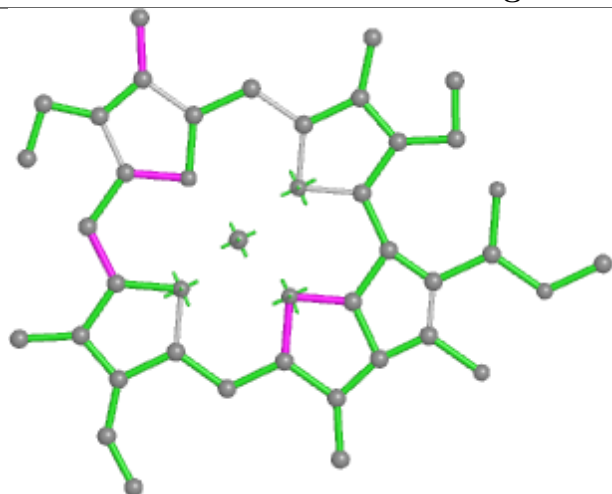


Rings

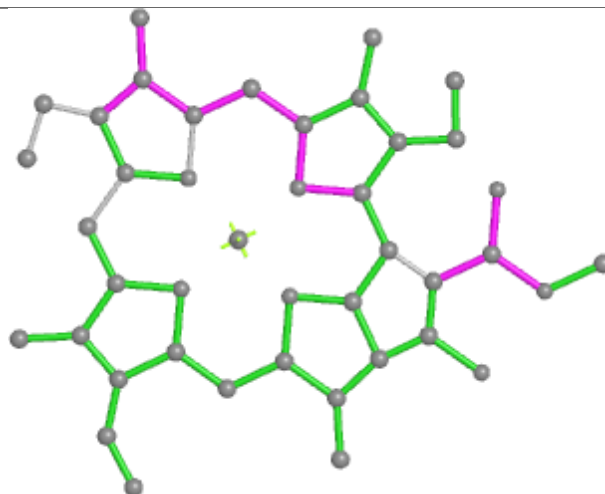




Ligand CLA A4 309



Bond lengths



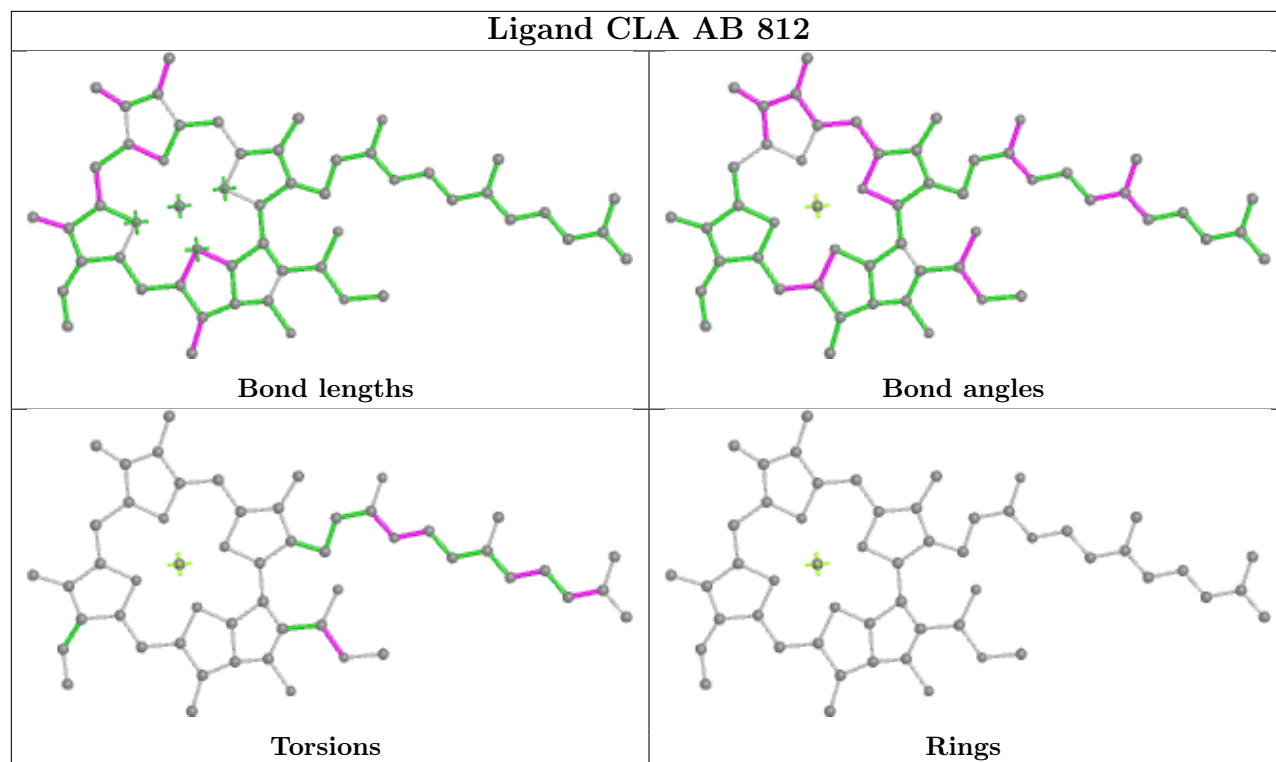
Bond angles



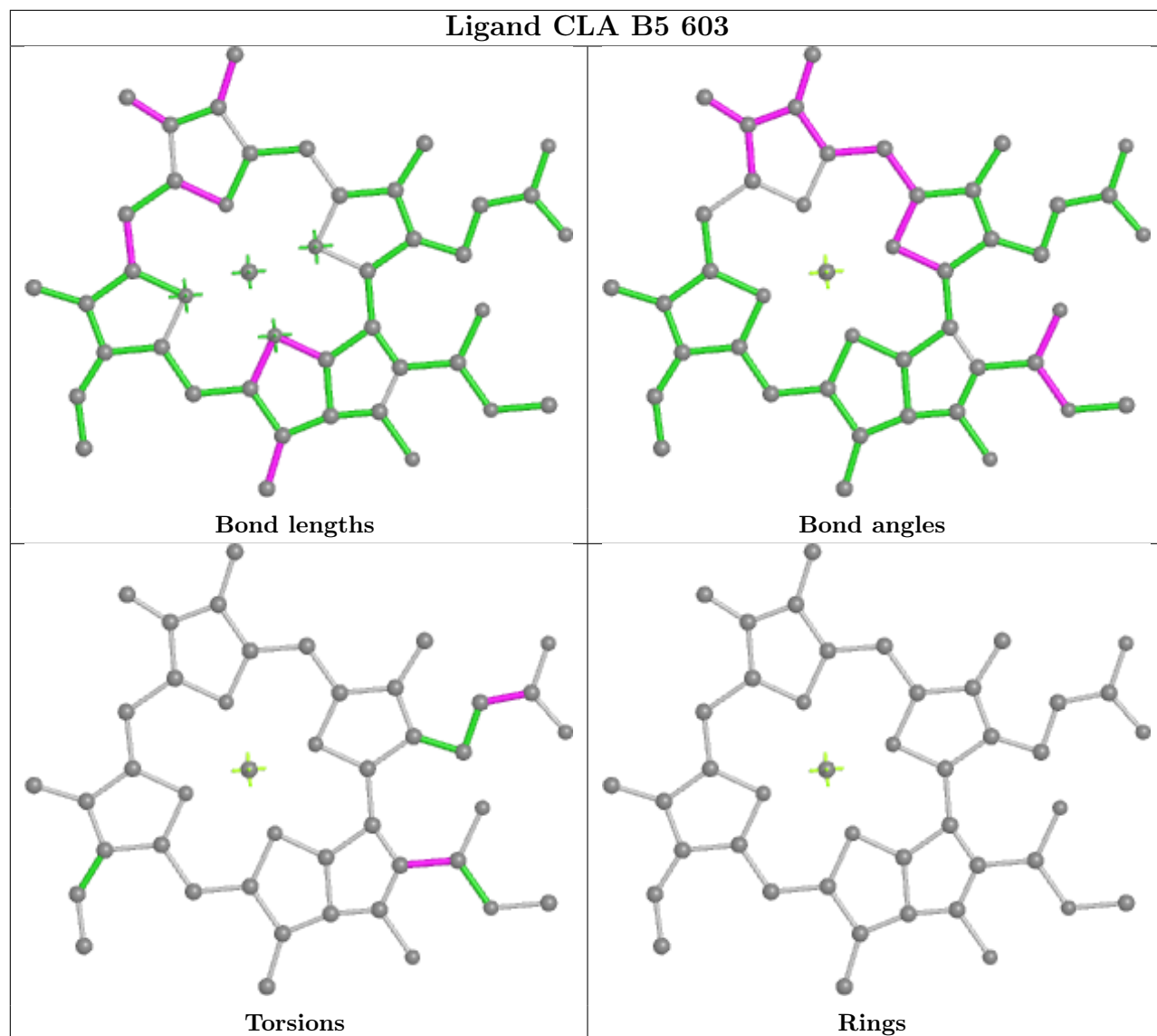
Torsions



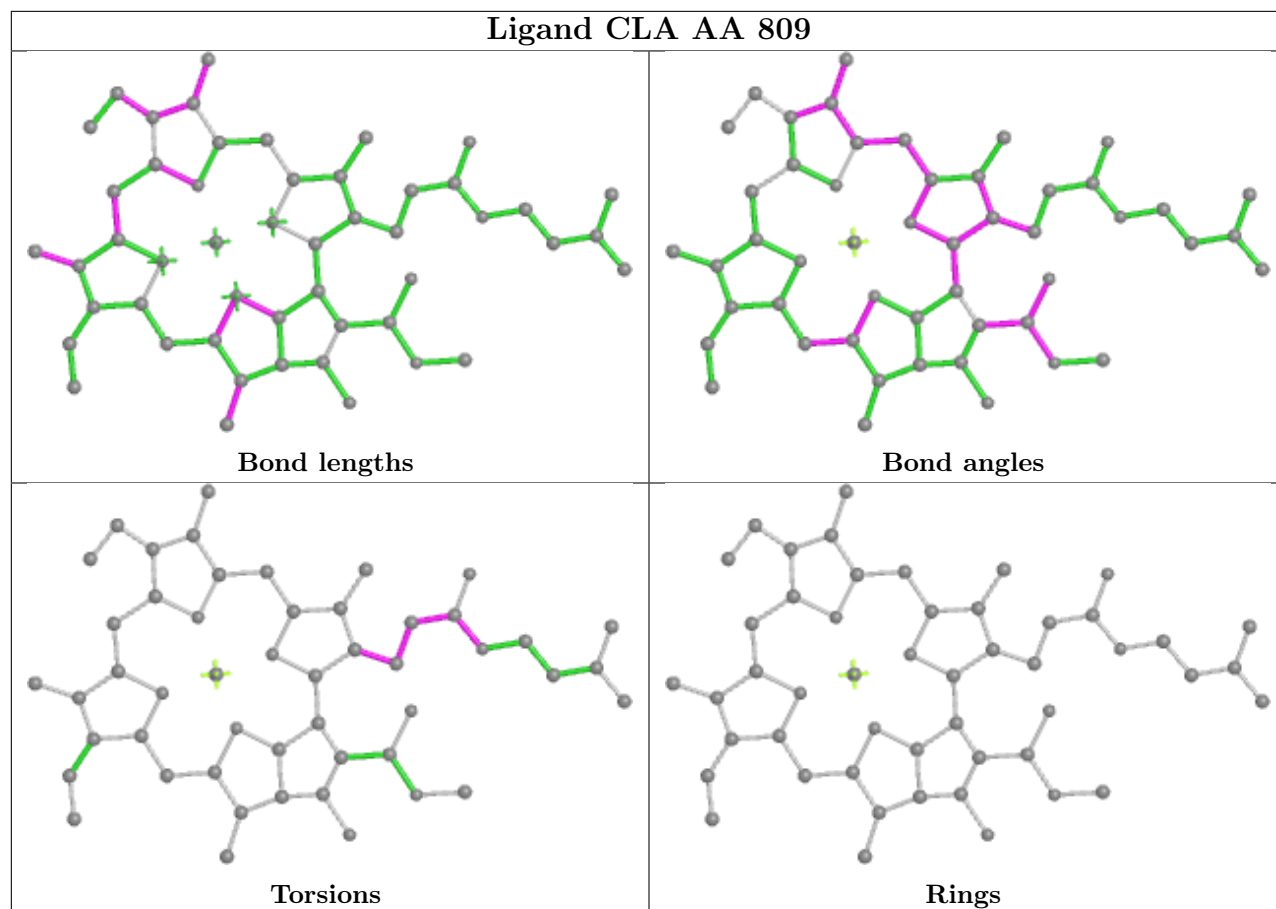
Rings



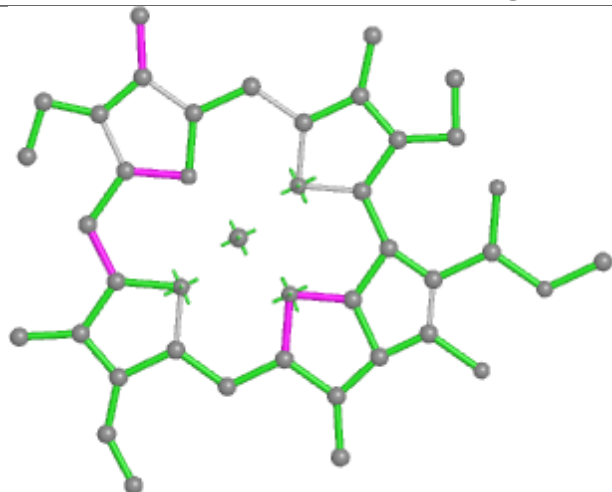
Ligand CLA B5 603



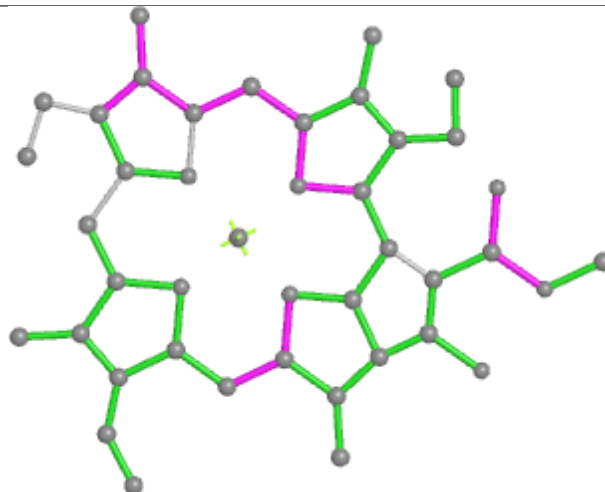
Ligand CLA AA 809



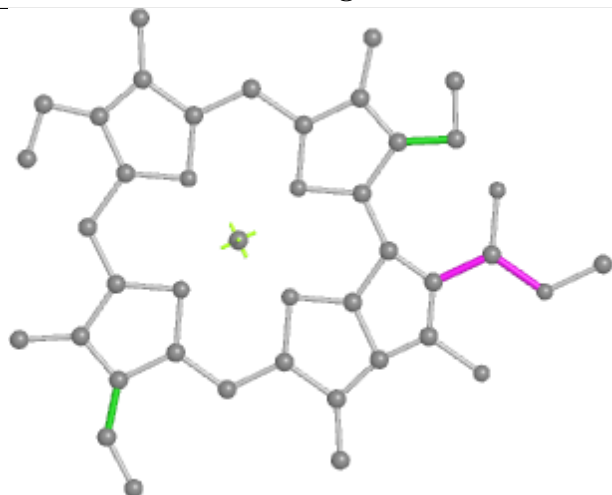
Ligand CLA BJ 102



Bond lengths



Bond angles

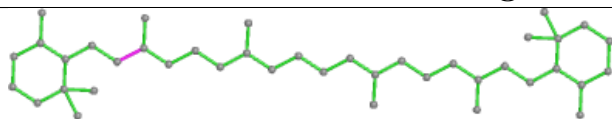


Torsions

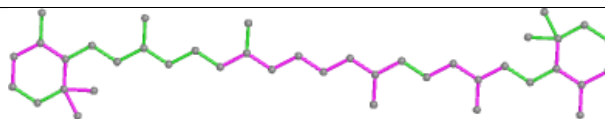


Rings

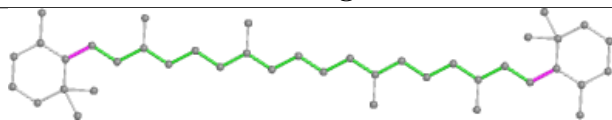
Ligand BCR BB 845



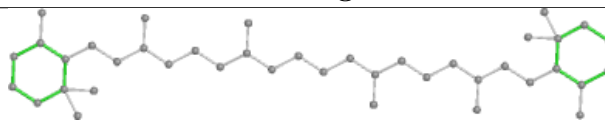
Bond lengths



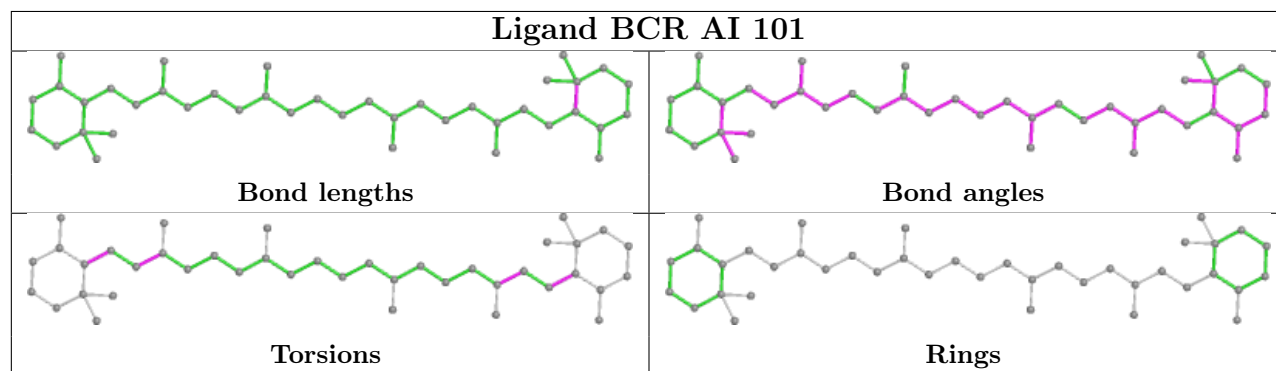
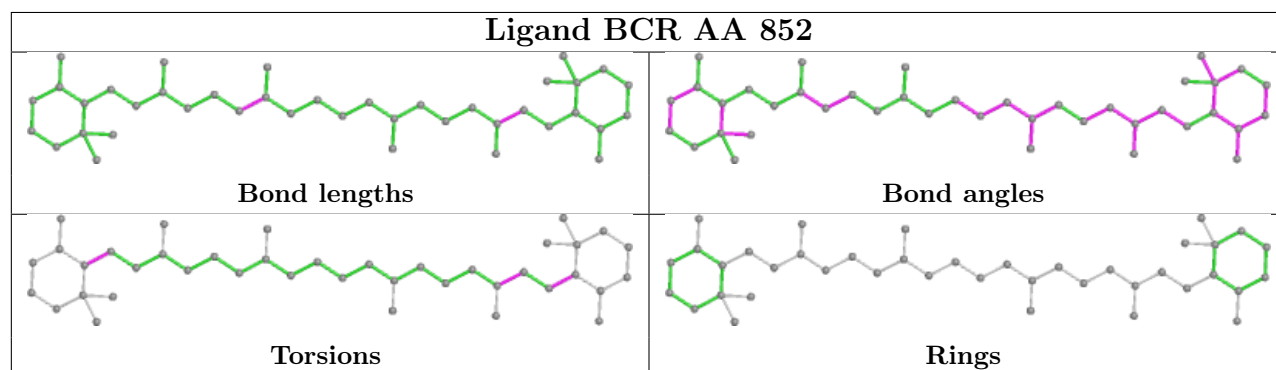
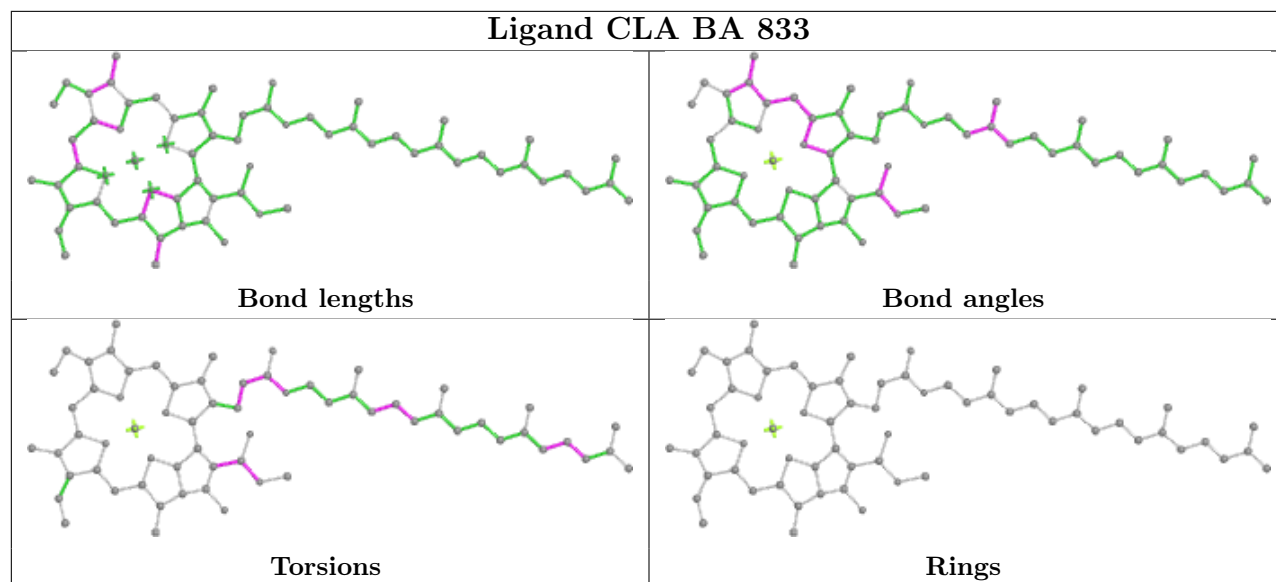
Bond angles



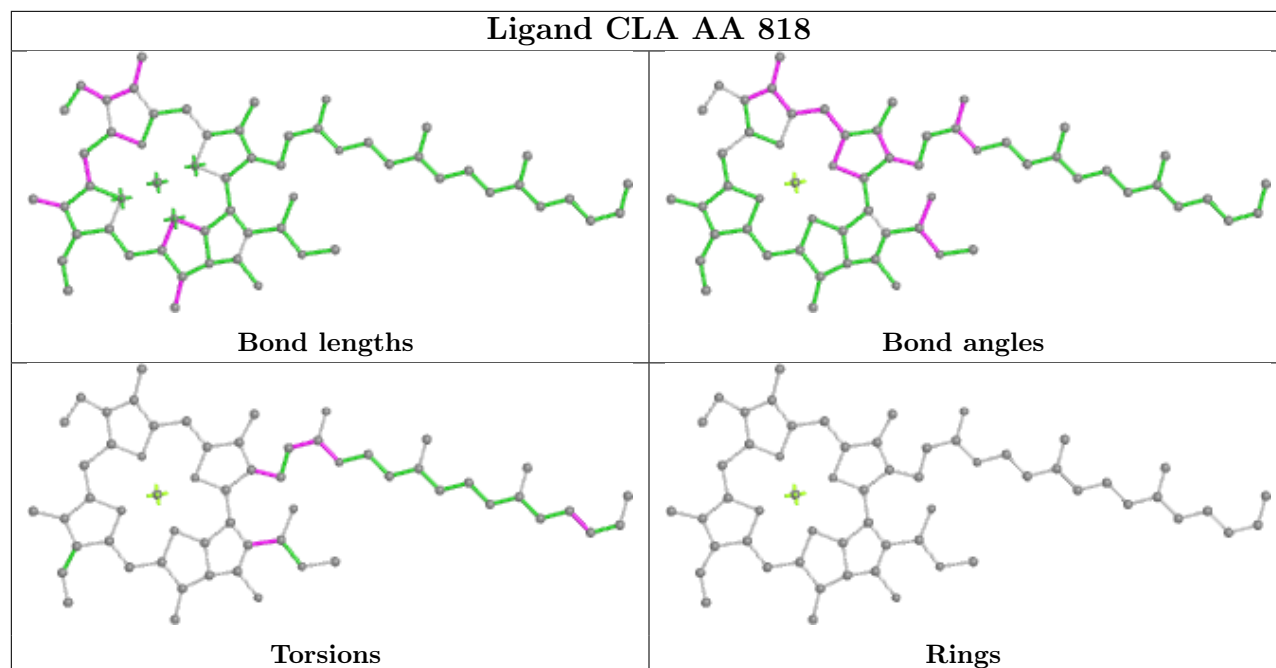
Torsions



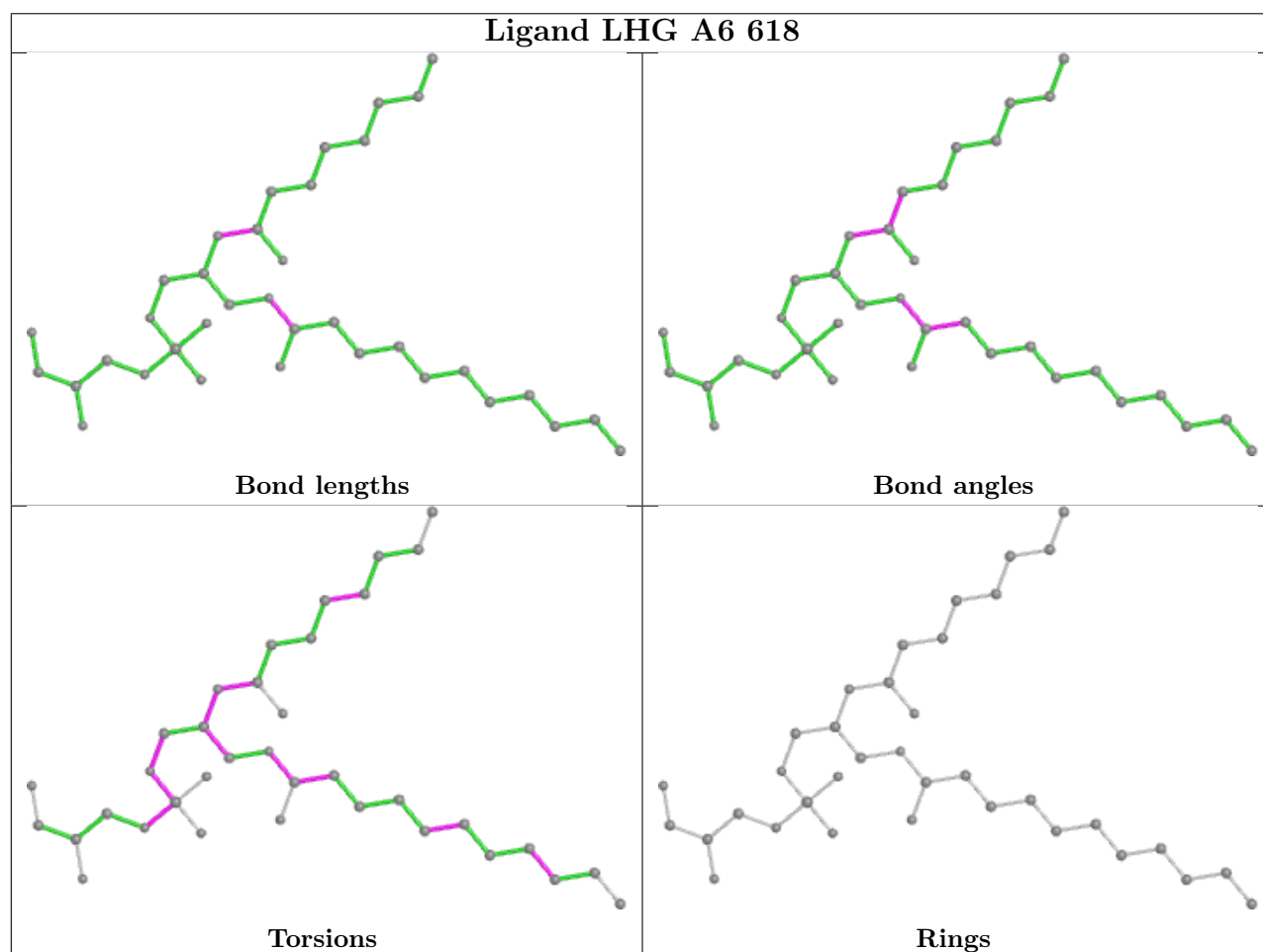
Rings

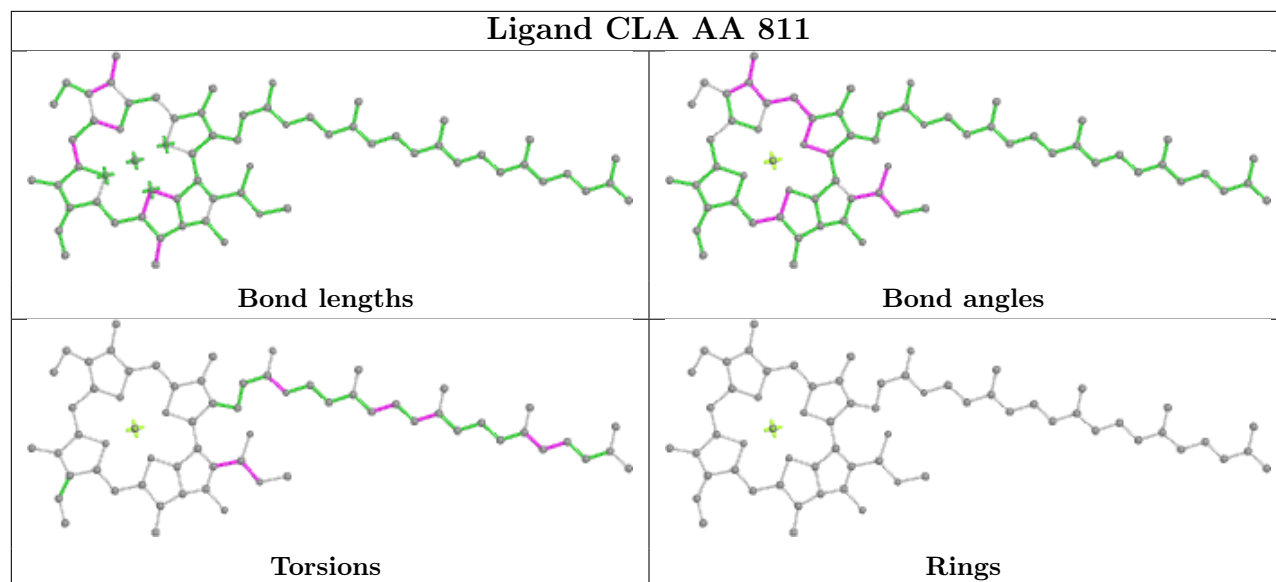
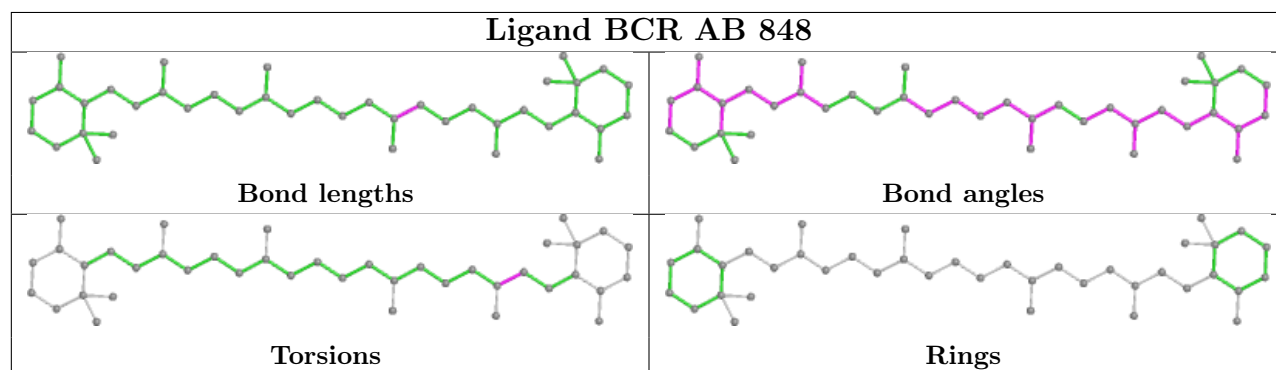


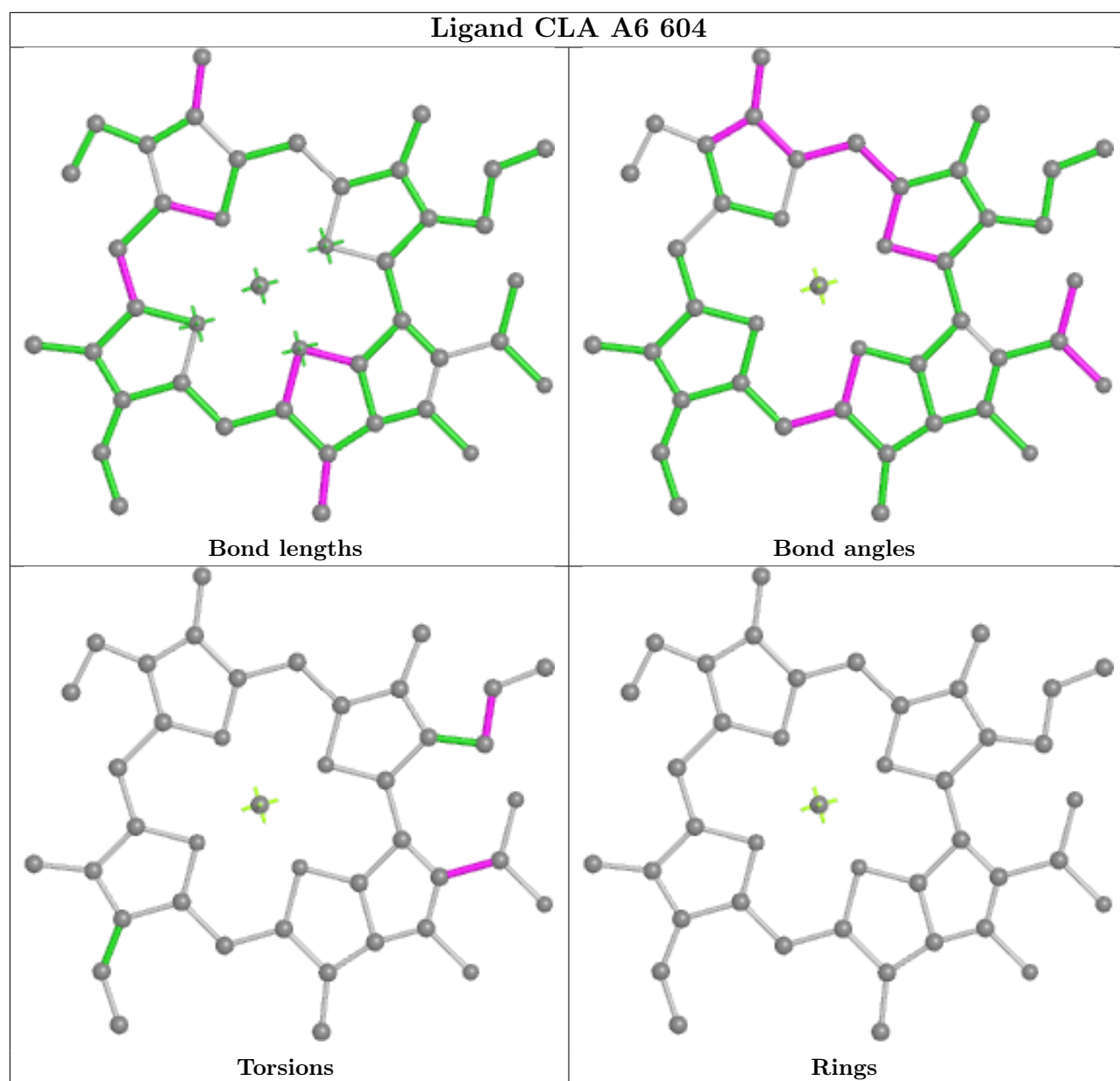
Ligand CLA AA 818

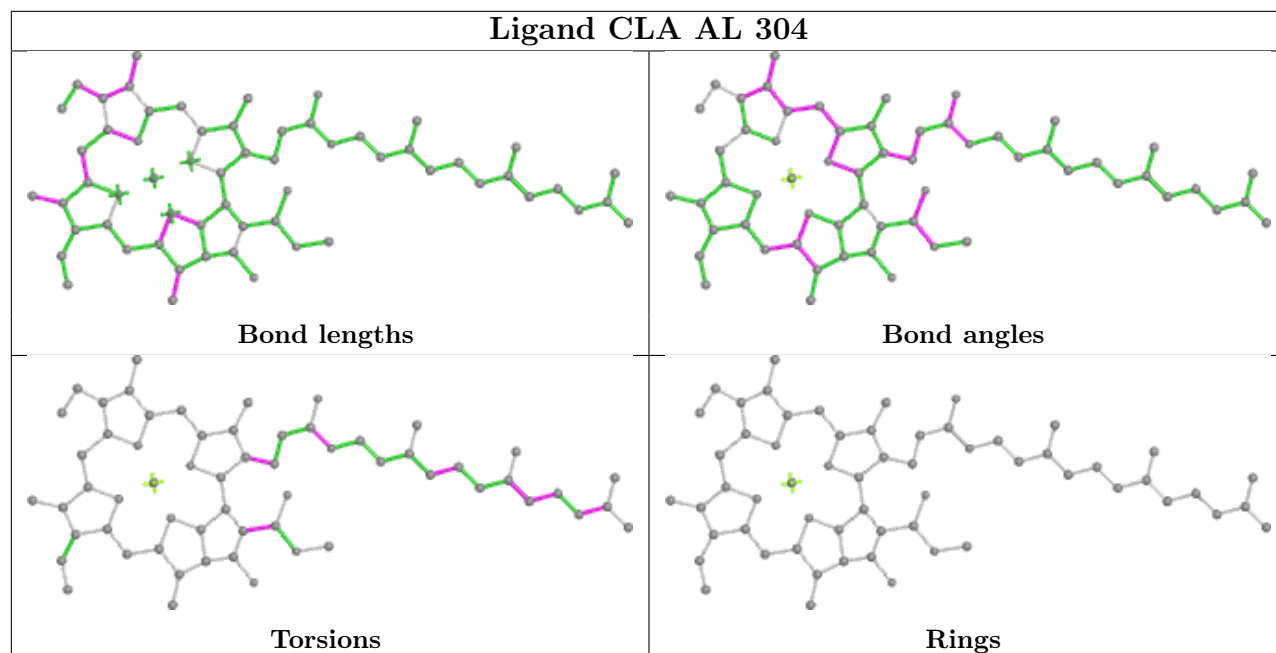
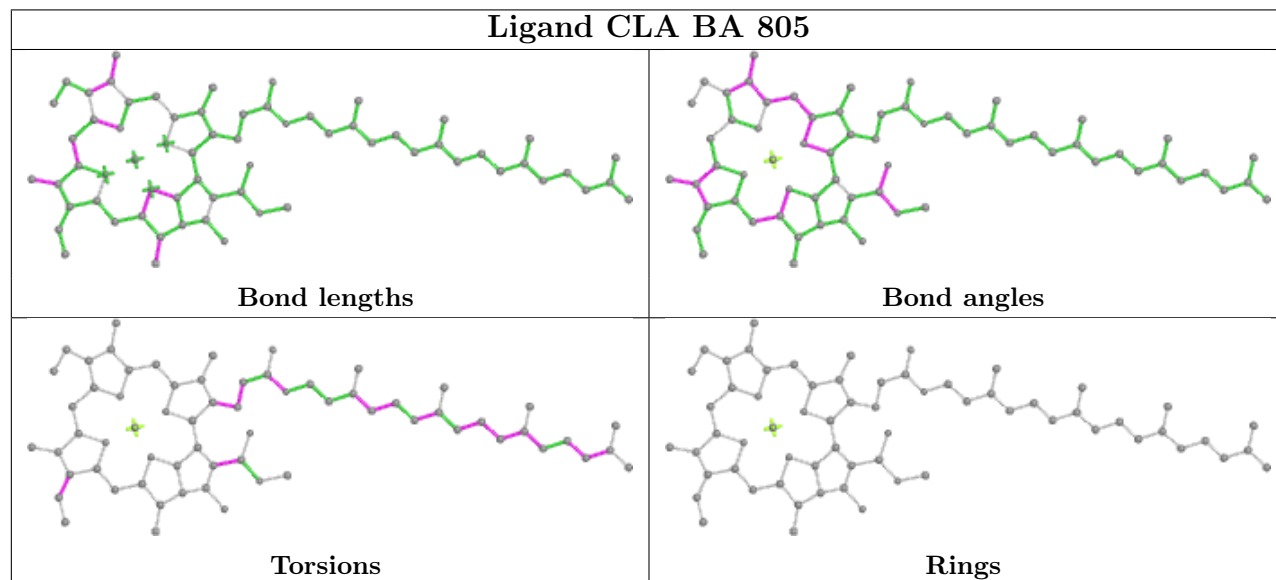


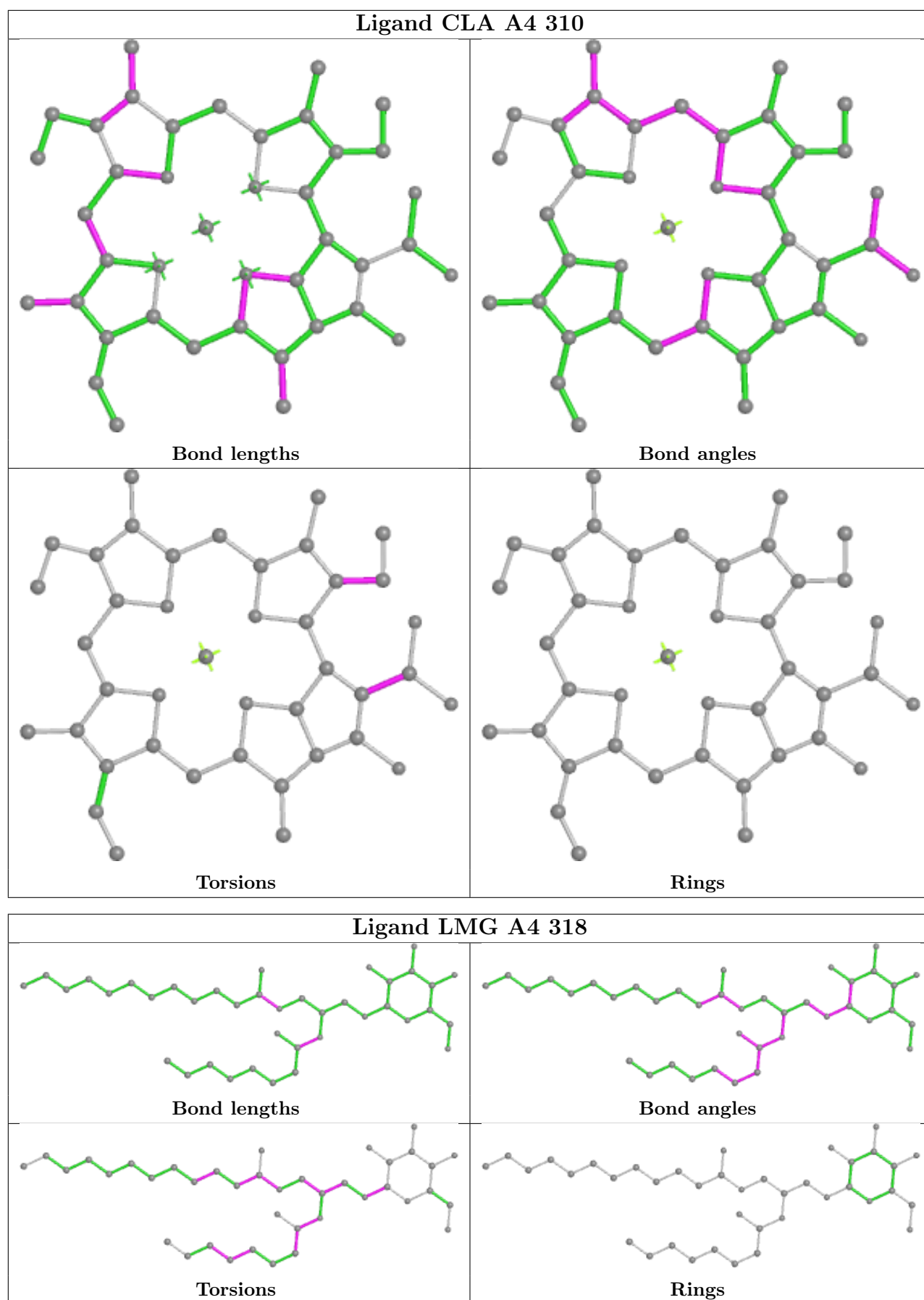
Ligand LHG A6 618



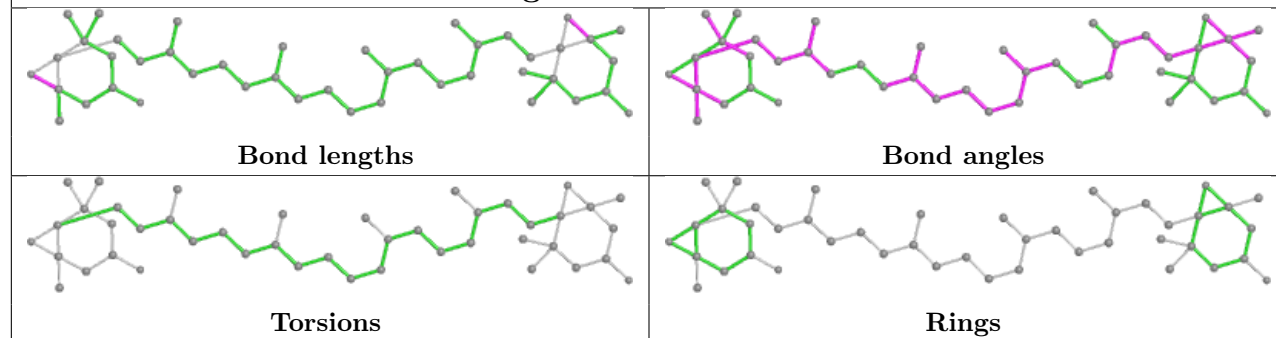
Ligand CLA AA 811**Ligand BCR AB 848**



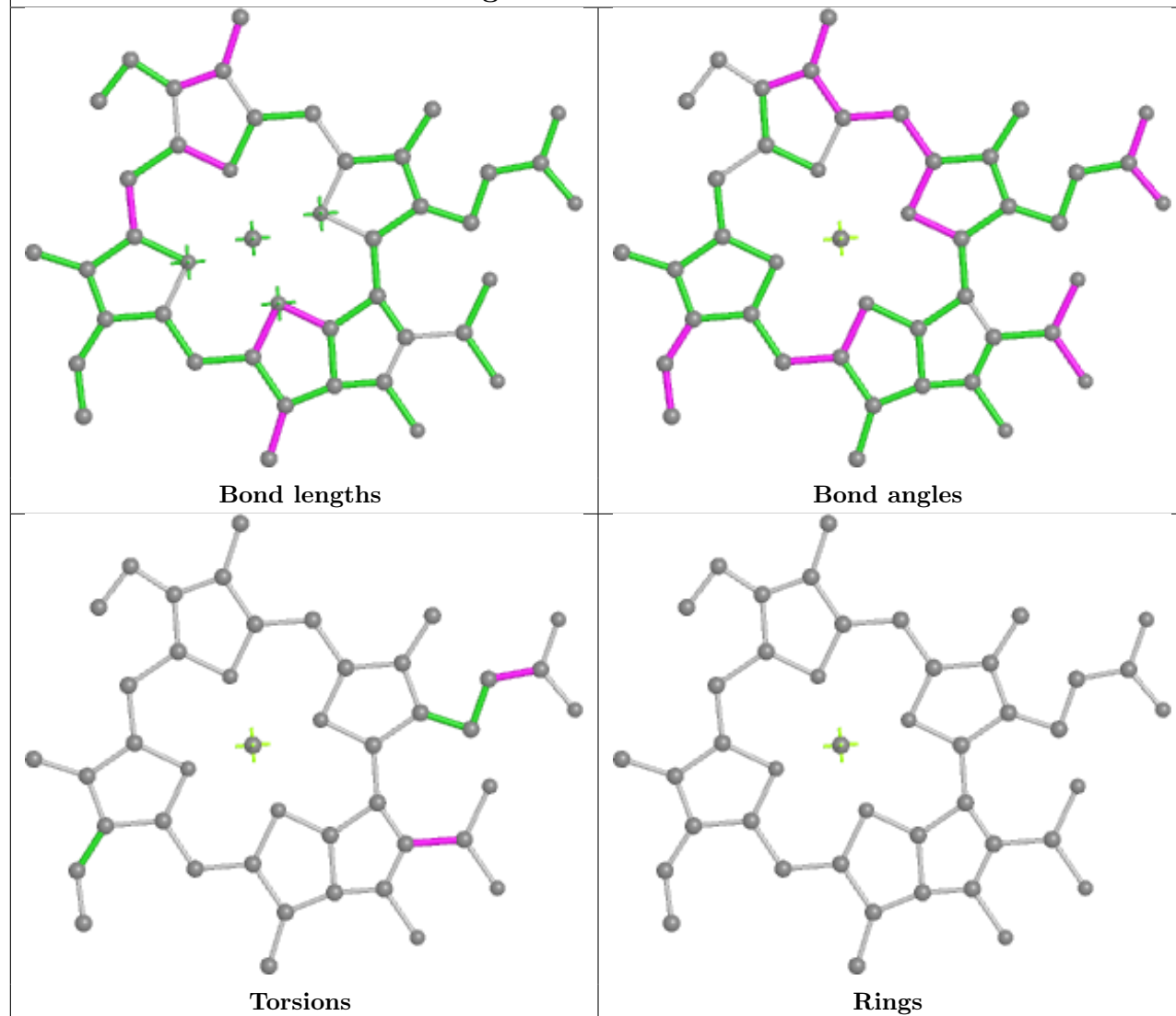
Ligand CLA AL 304**Ligand CLA BA 805**



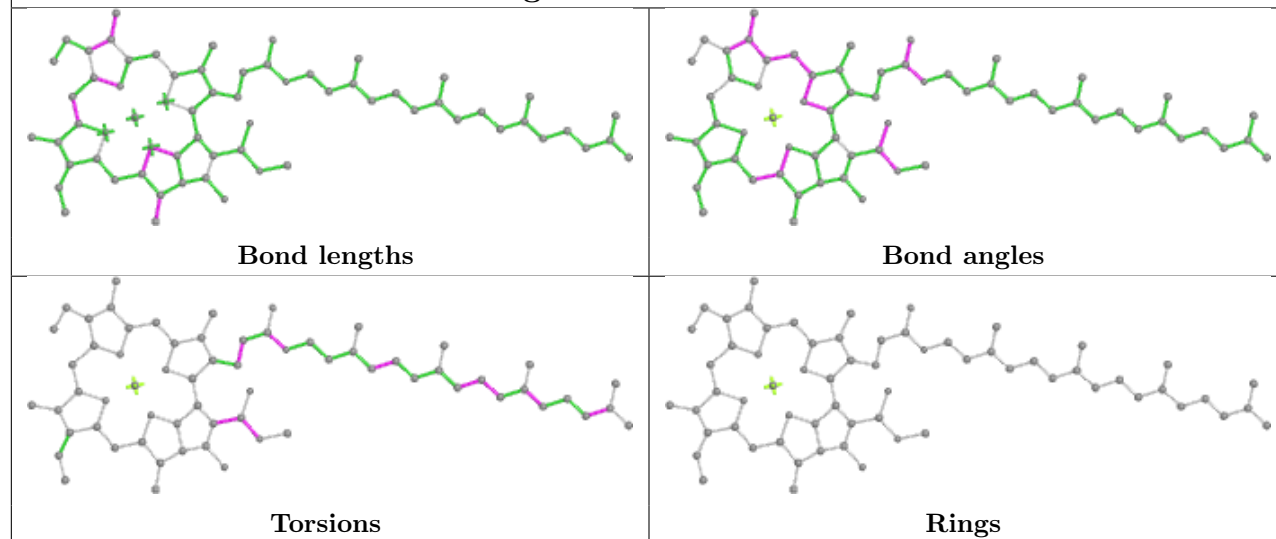
Ligand XAT B1 317



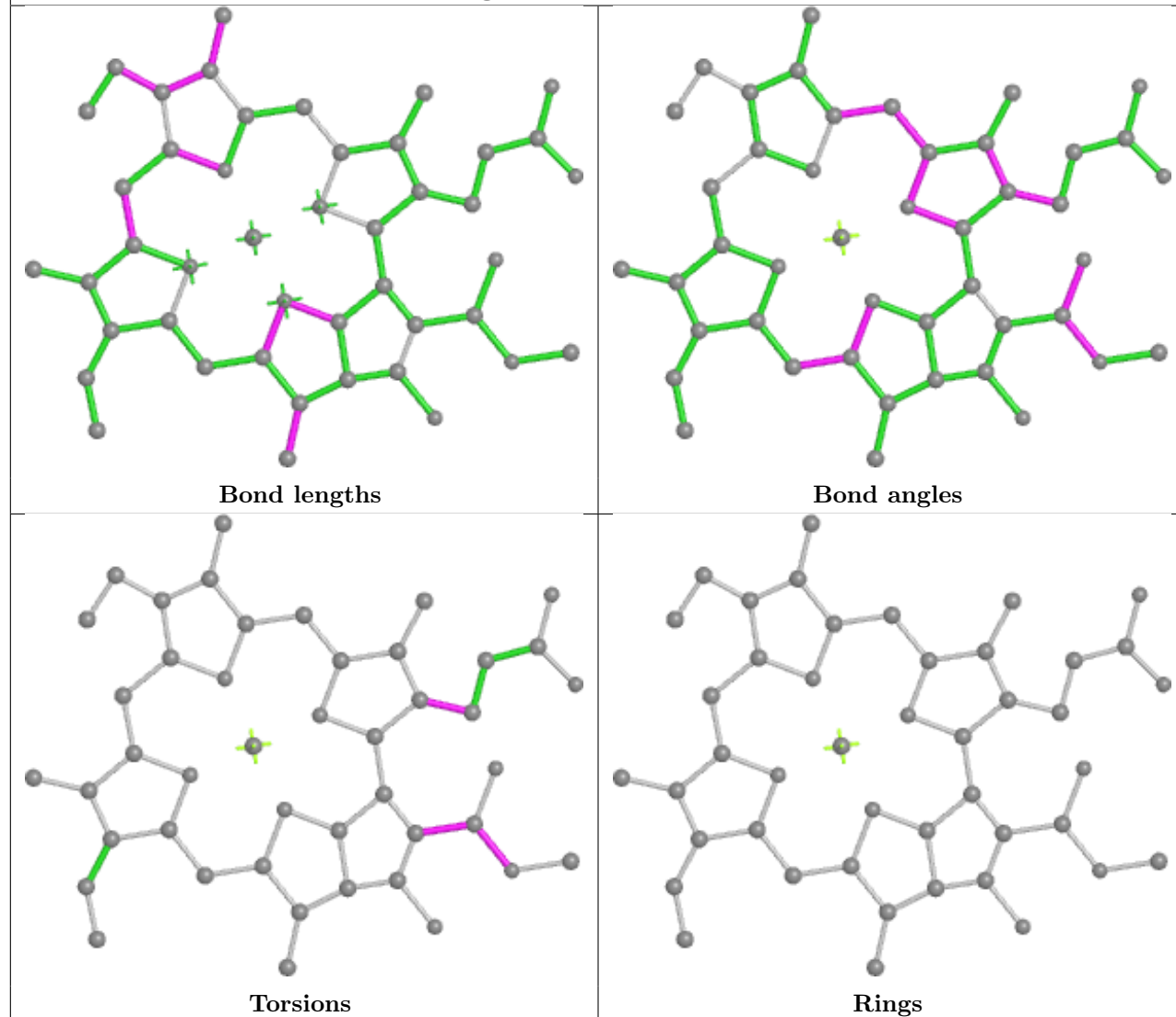
Ligand CLA B2 603



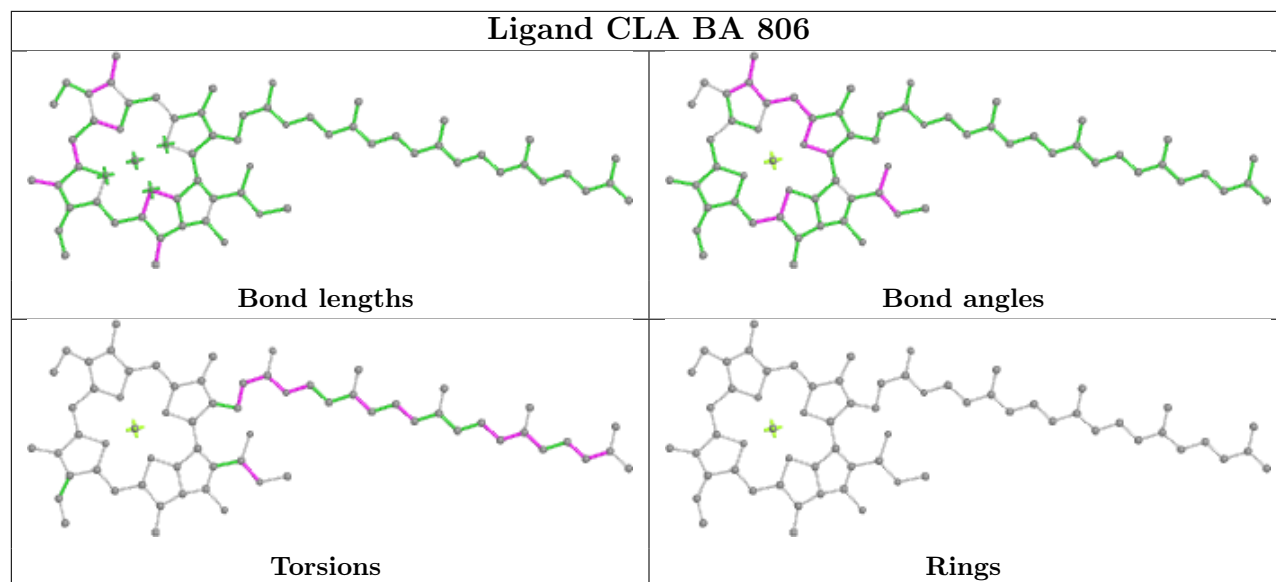
Ligand CLA B2 612



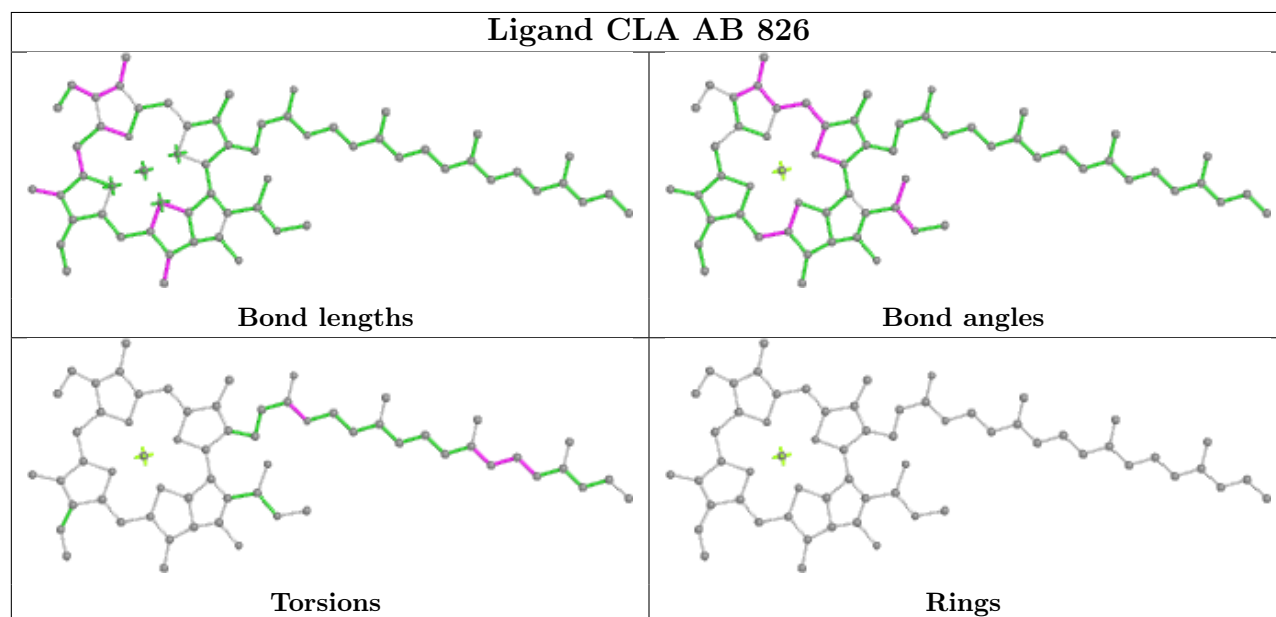
Ligand CLA BB 825



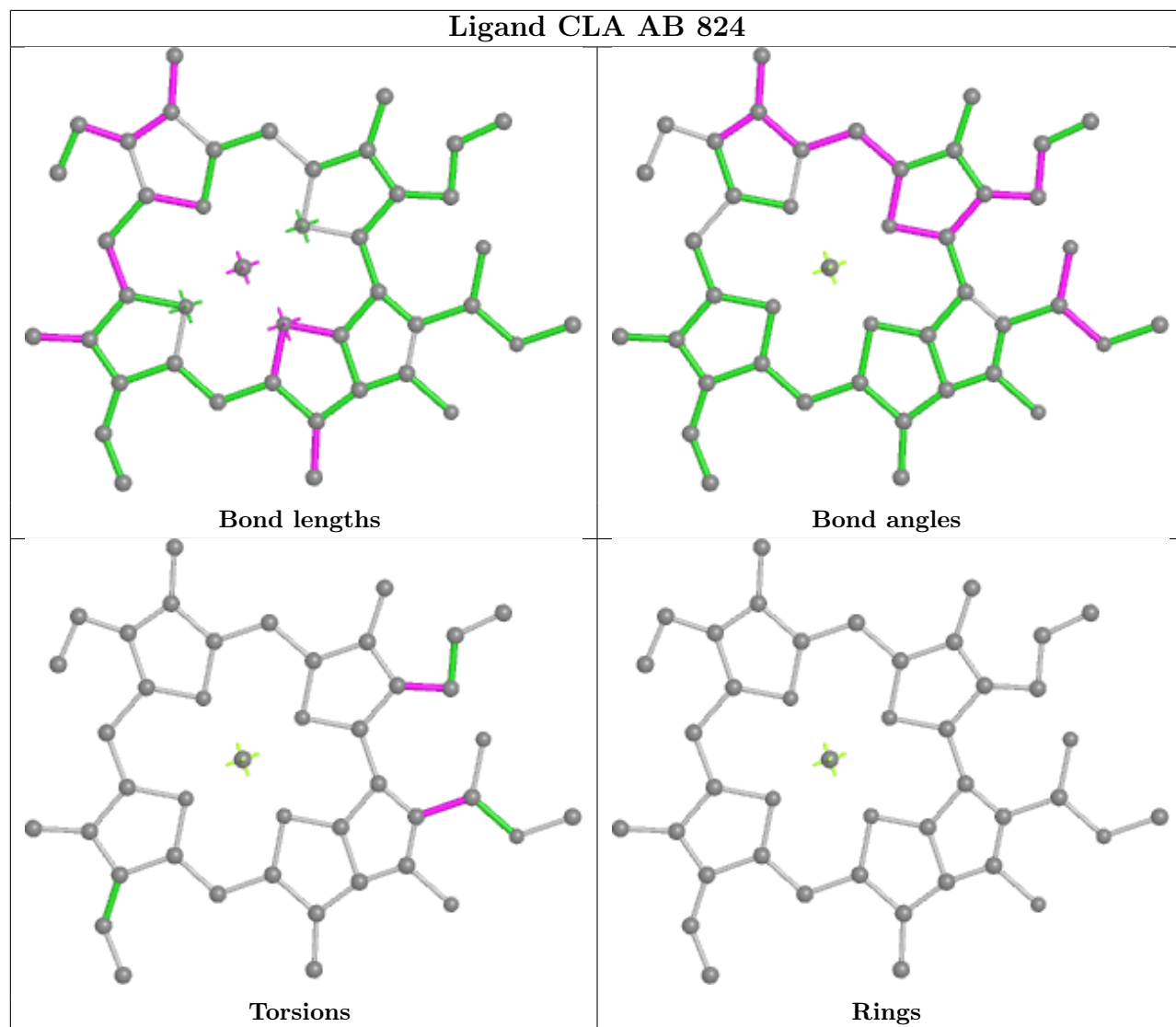
Ligand CLA BA 806



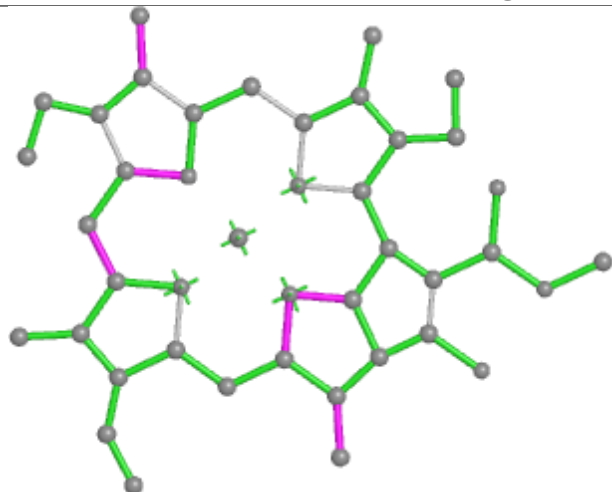
Ligand CLA AB 826



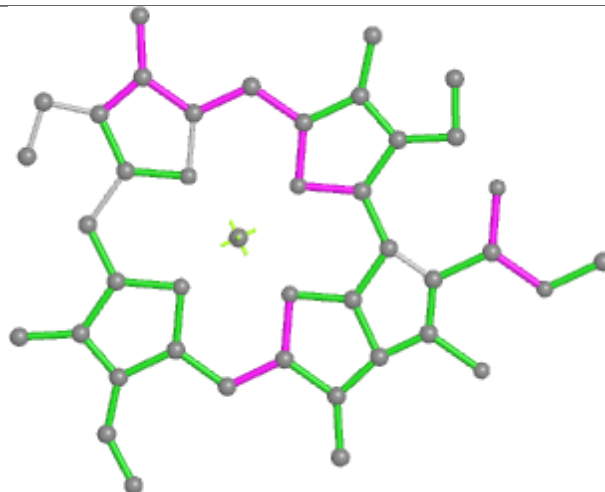
Ligand CLA AB 824



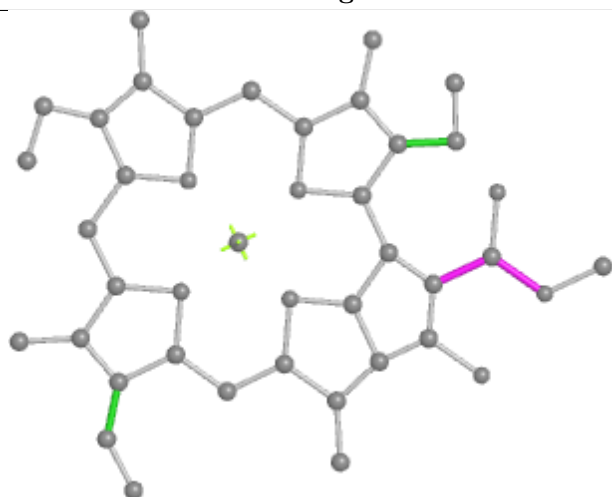
Ligand CLA AG 203



Bond lengths



Bond angles

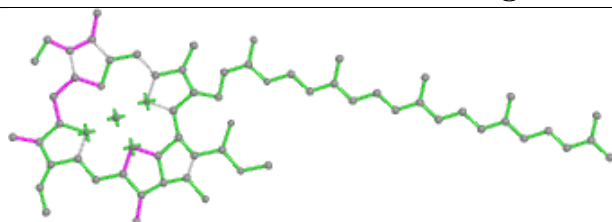


Torsions

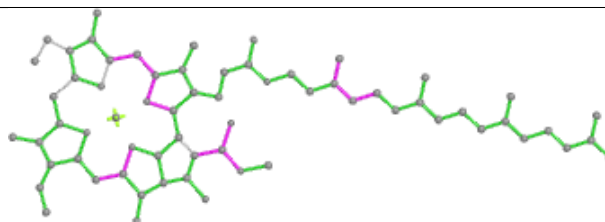


Rings

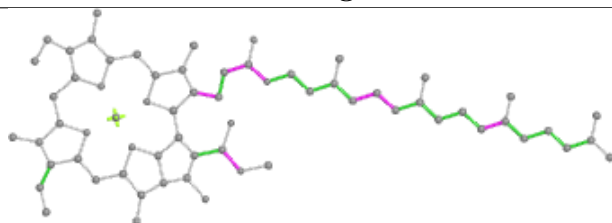
Ligand CLA BB 834



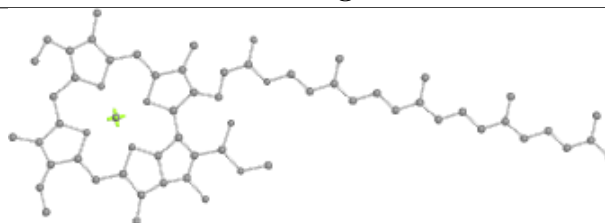
Bond lengths



Bond angles

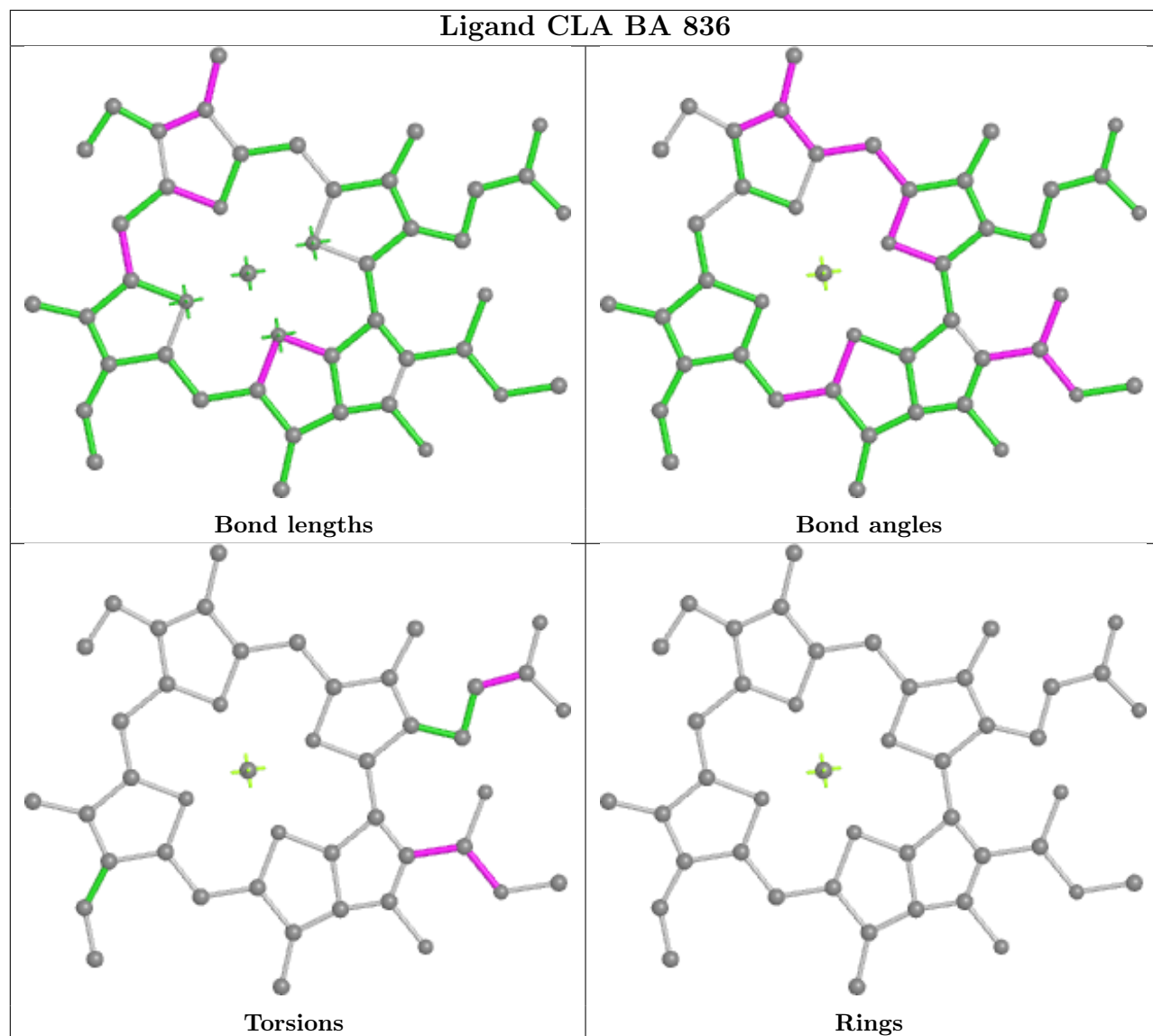


Torsions

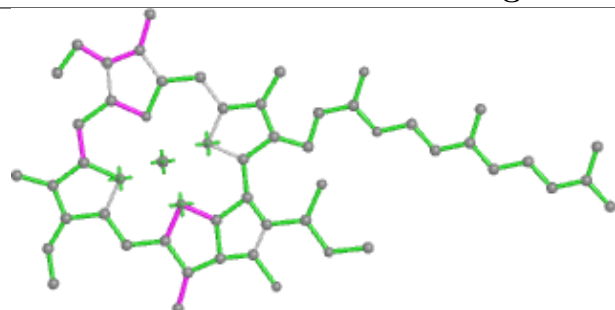


Rings

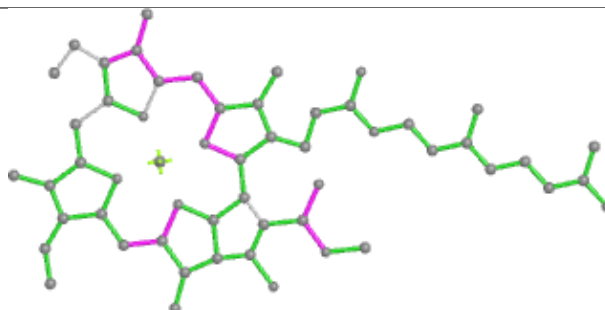
Ligand CLA BA 836



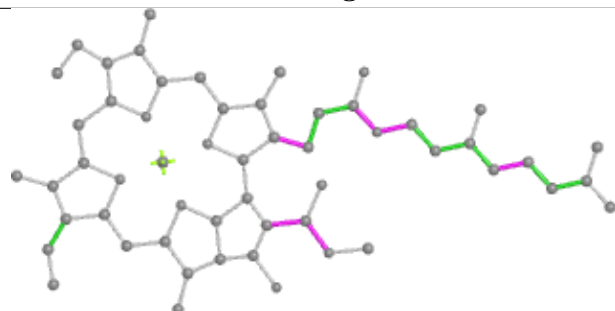
Ligand CLA AB 820



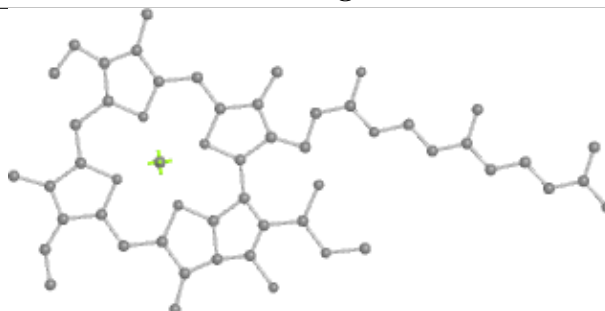
Bond lengths



Bond angles

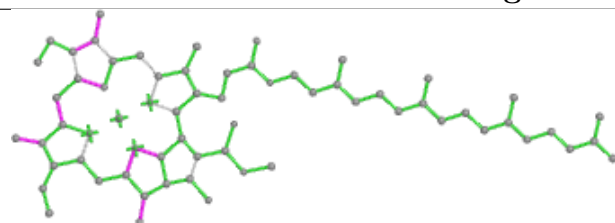


Torsions

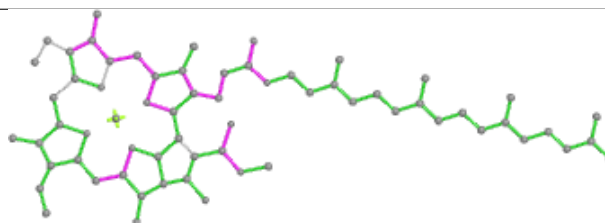


Rings

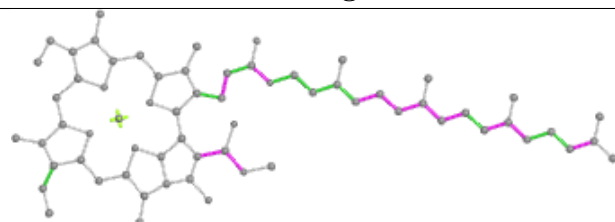
Ligand CLA BB 824



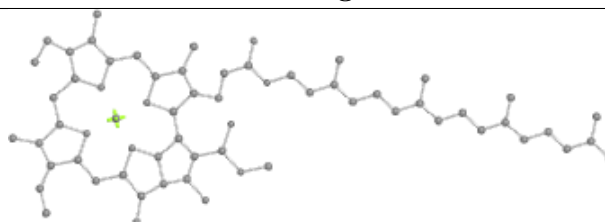
Bond lengths



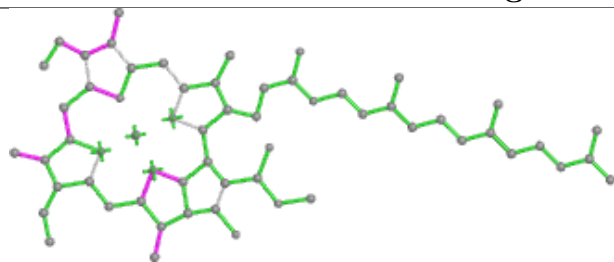
Bond angles



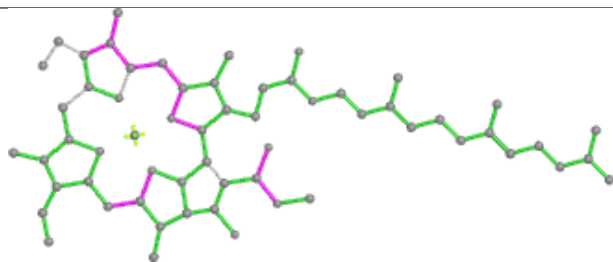
Torsions



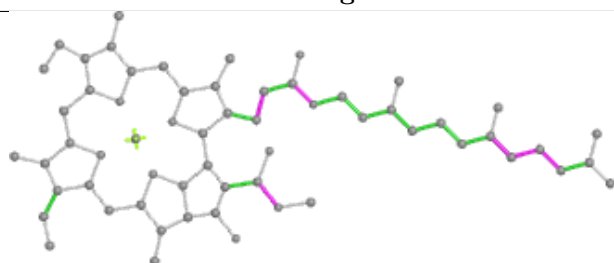
Rings

Ligand CLA B5 602

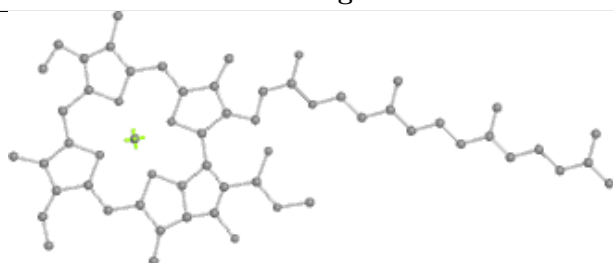
Bond lengths



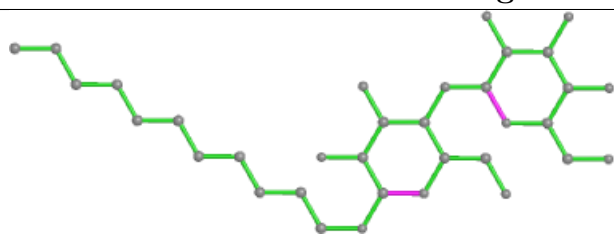
Bond angles



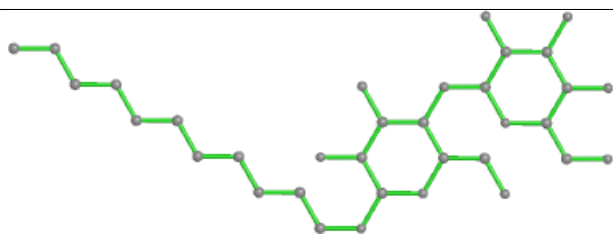
Torsions



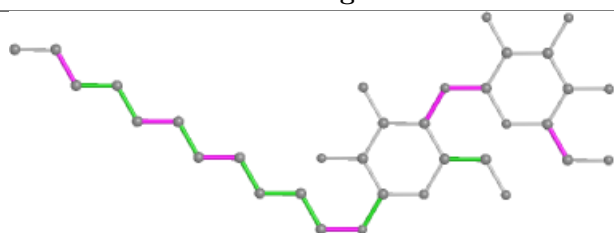
Rings

Ligand LMU BA 853

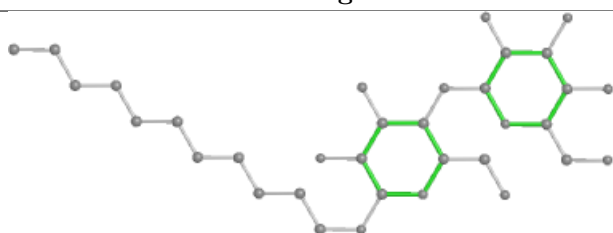
Bond lengths



Bond angles

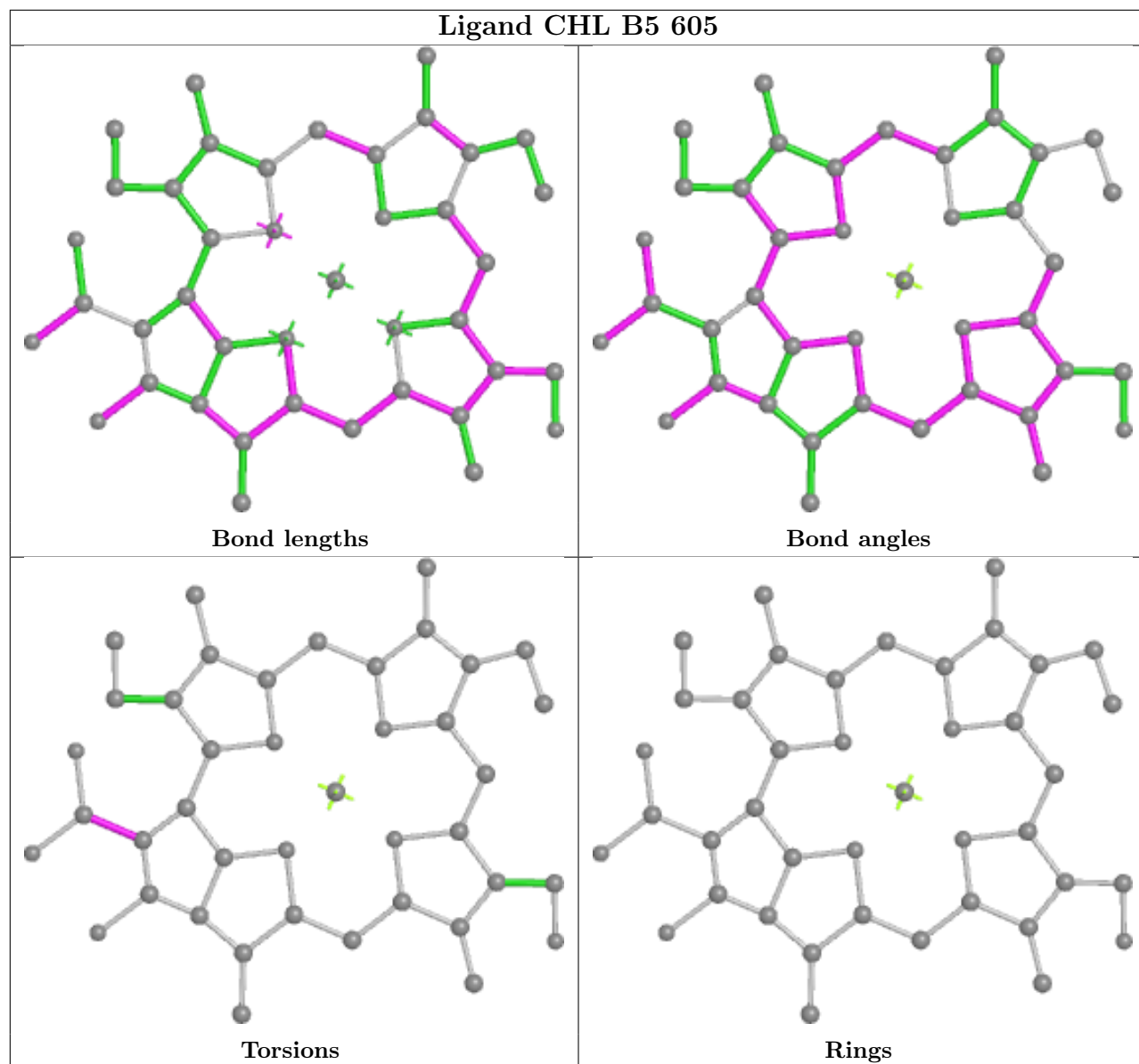


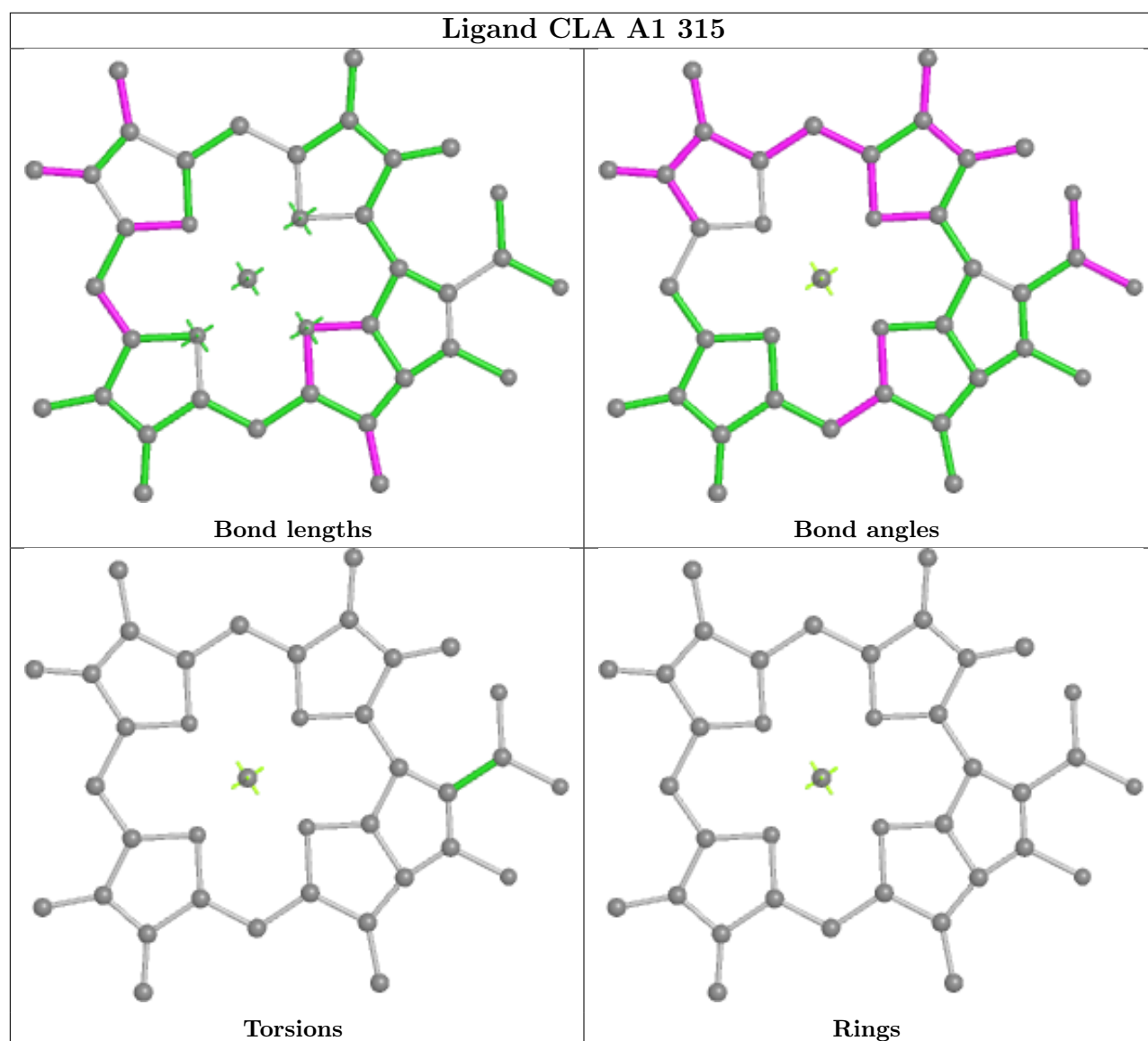
Torsions



Rings

Ligand CHL B5 605





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

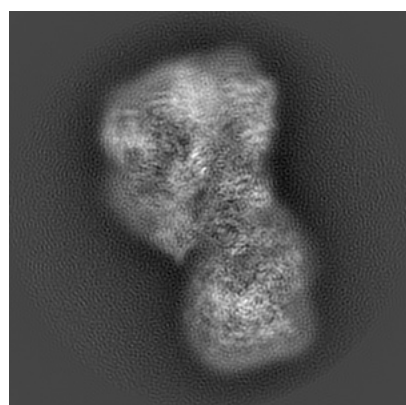
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32477. These allow visual inspection of the internal detail of the map and identification of artifacts.

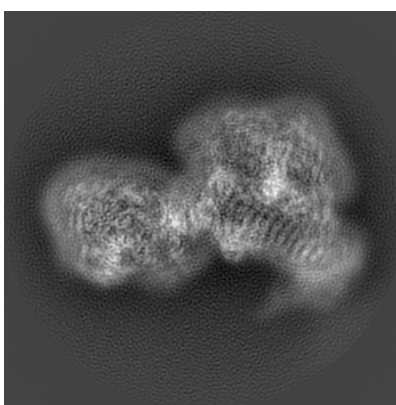
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

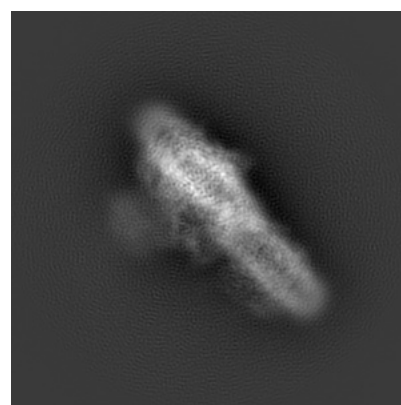
6.1.1 Primary map



X



Y

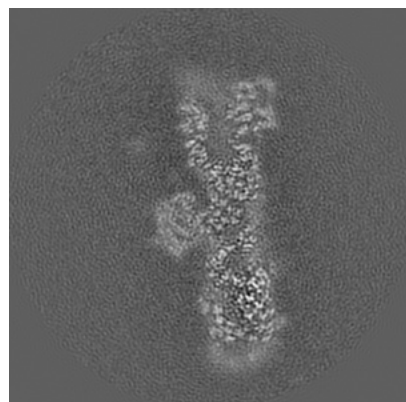


Z

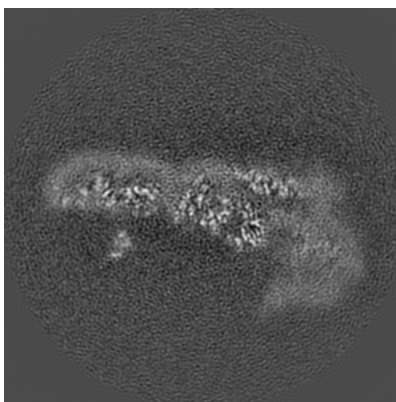
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

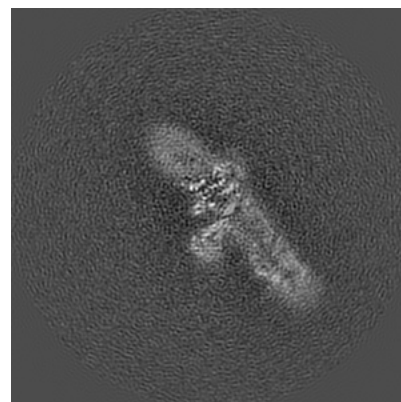
6.2.1 Primary map



X Index: 200



Y Index: 200

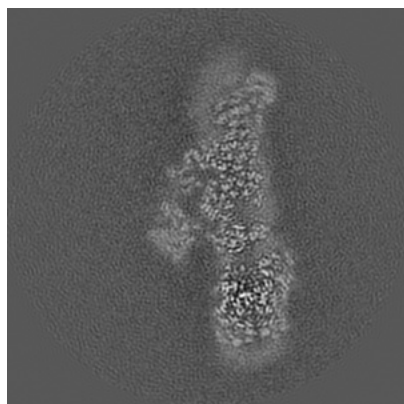


Z Index: 200

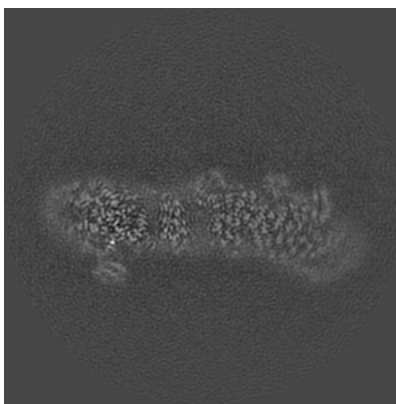
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

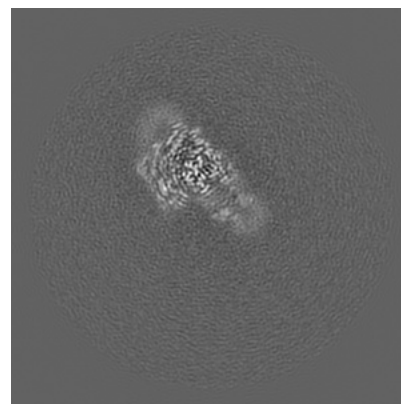
6.3.1 Primary map



X Index: 185



Y Index: 235

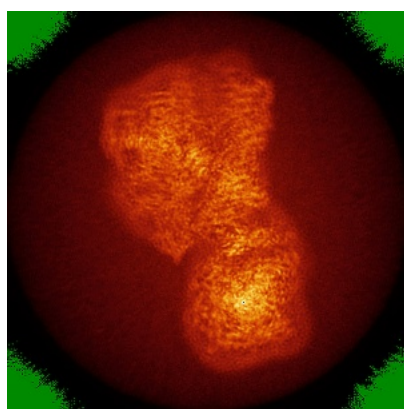


Z Index: 112

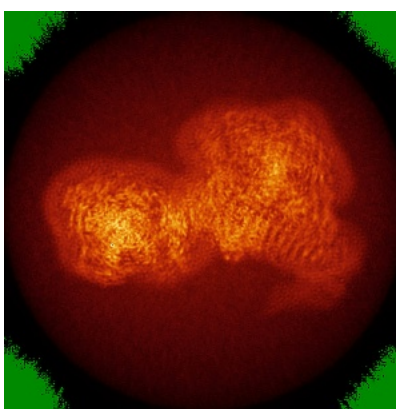
The images above show the largest variance slices of the map in three orthogonal directions.

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

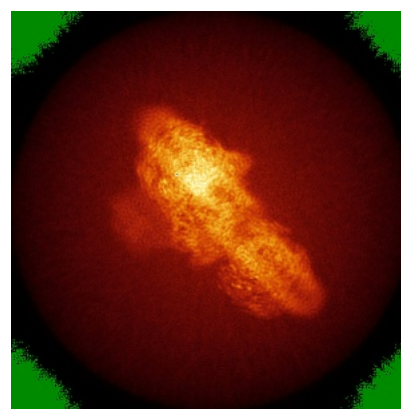
6.4.1 Primary map



X



Y



Z

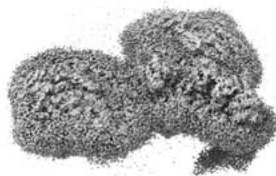
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

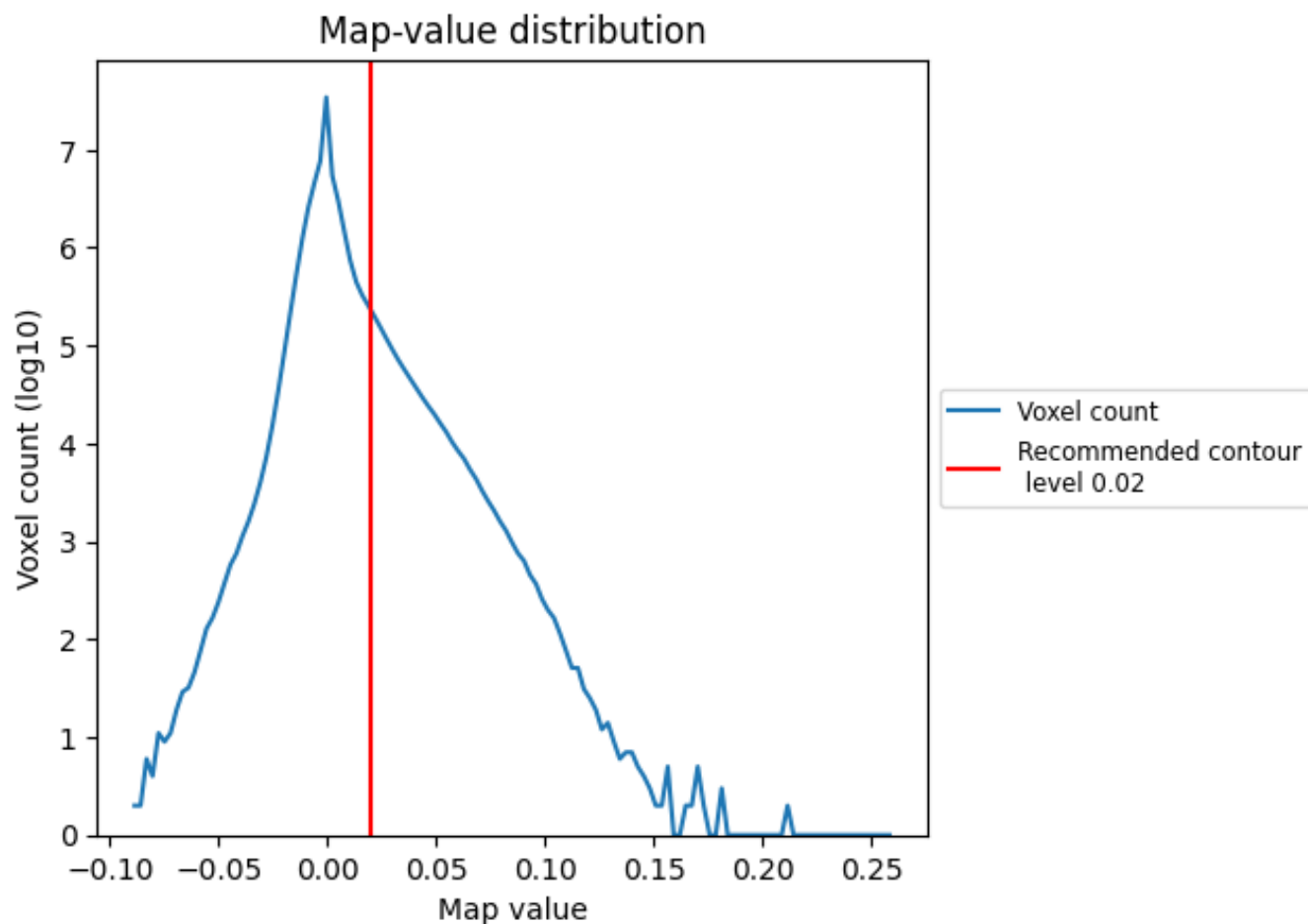
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

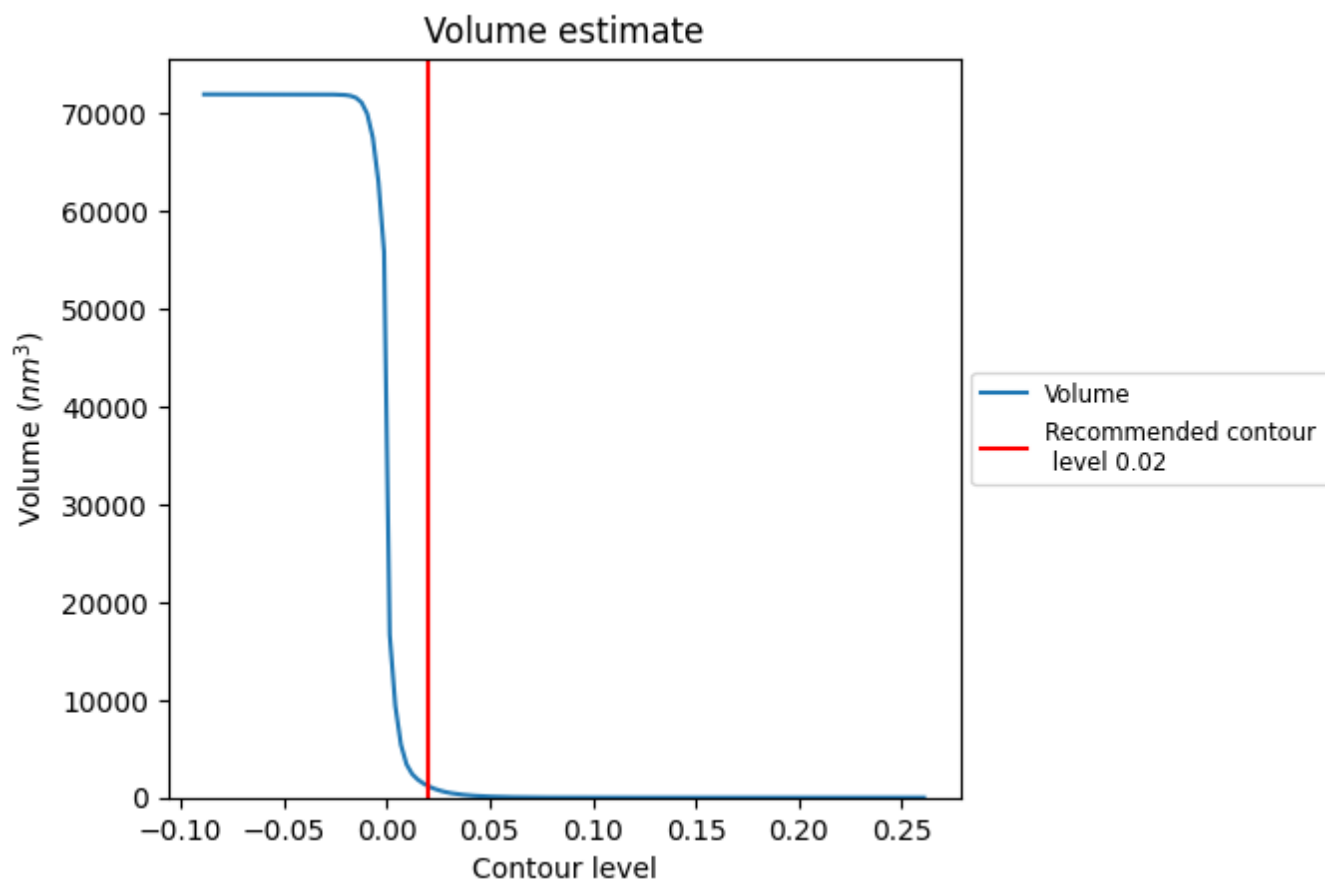
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

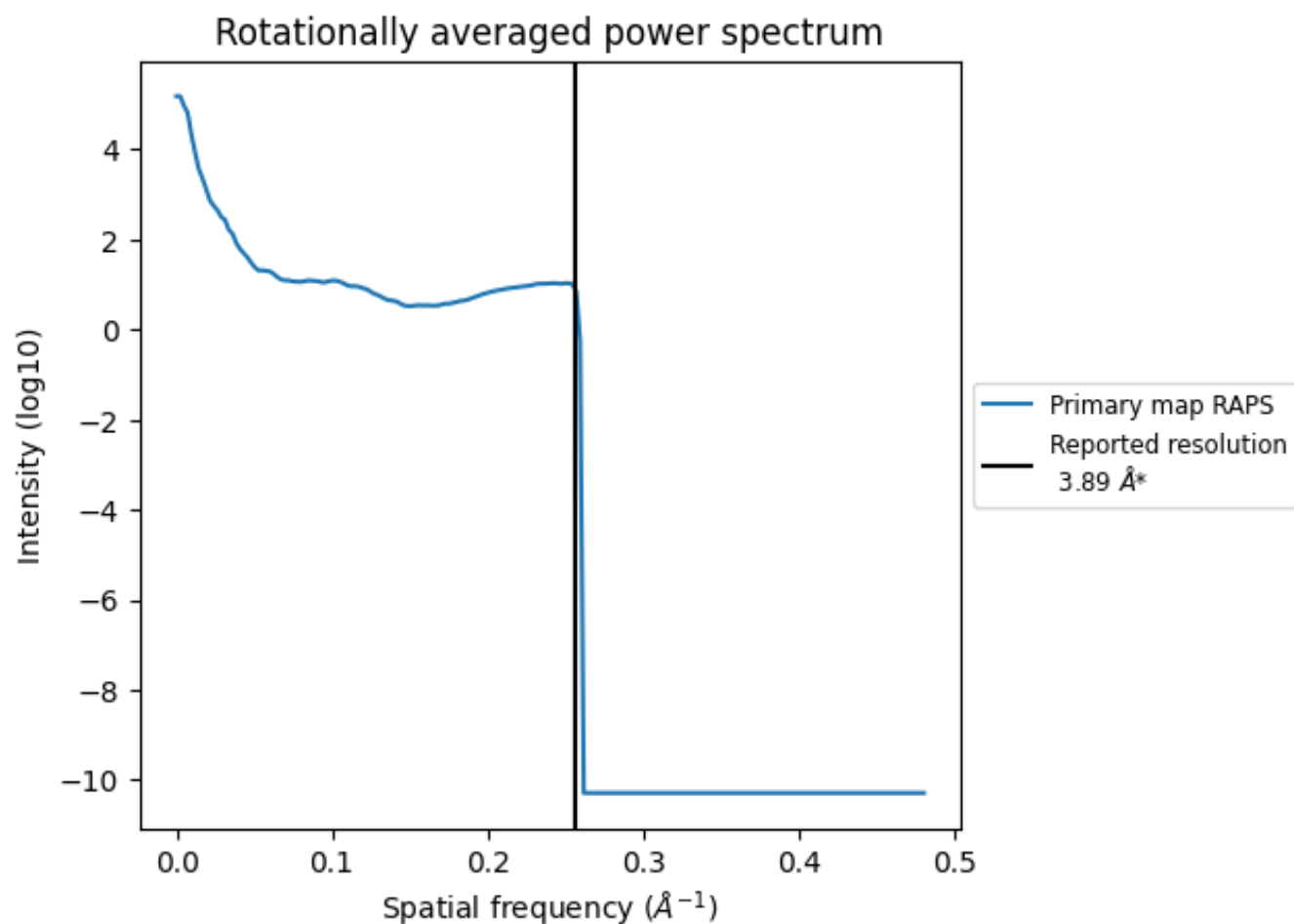
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1193 nm^3 ; this corresponds to an approximate mass of 1078 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.257 Å⁻¹

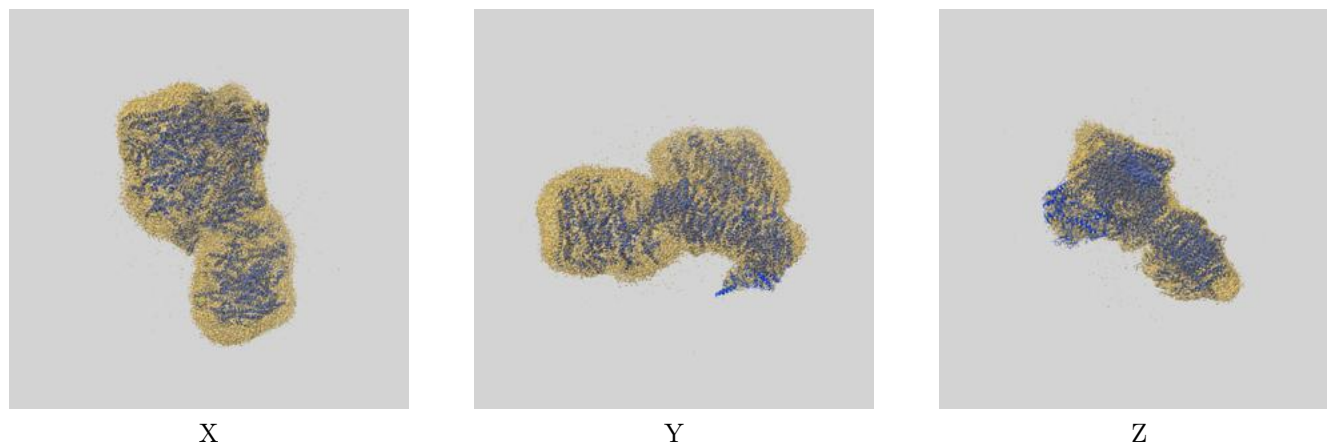
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

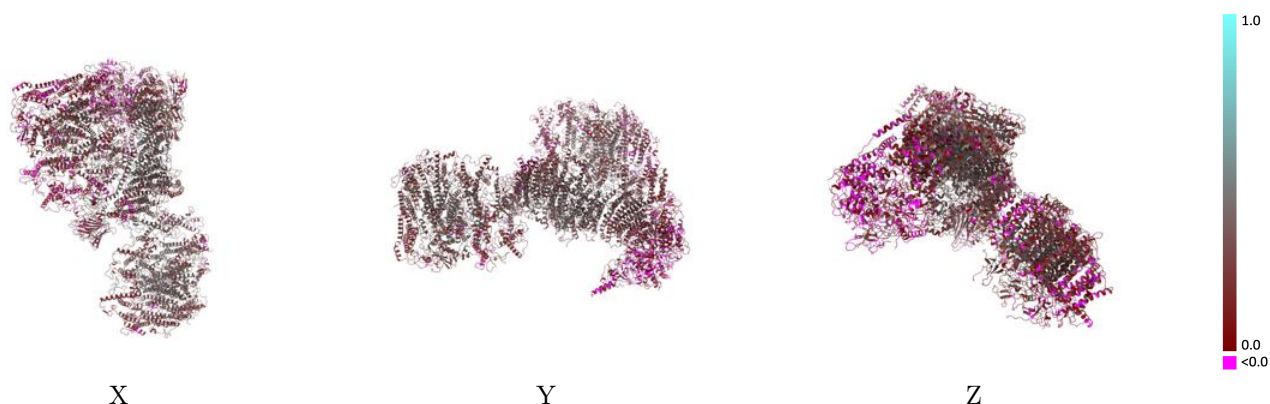
This section contains information regarding the fit between EMDB map EMD-32477 and PDB model 7WG5. Per-residue inclusion information can be found in [section 3](#) on [page 46](#).

9.1 Map-model overlay [i](#)



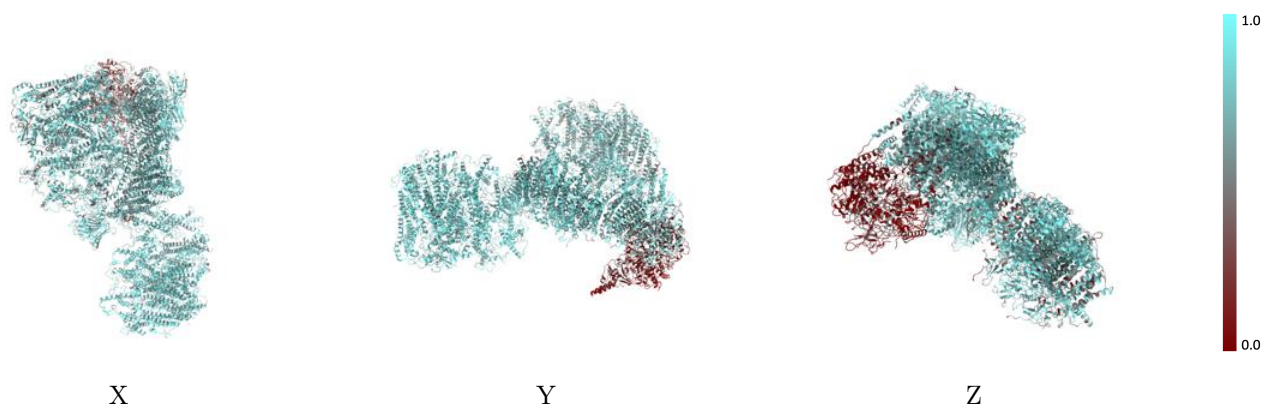
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



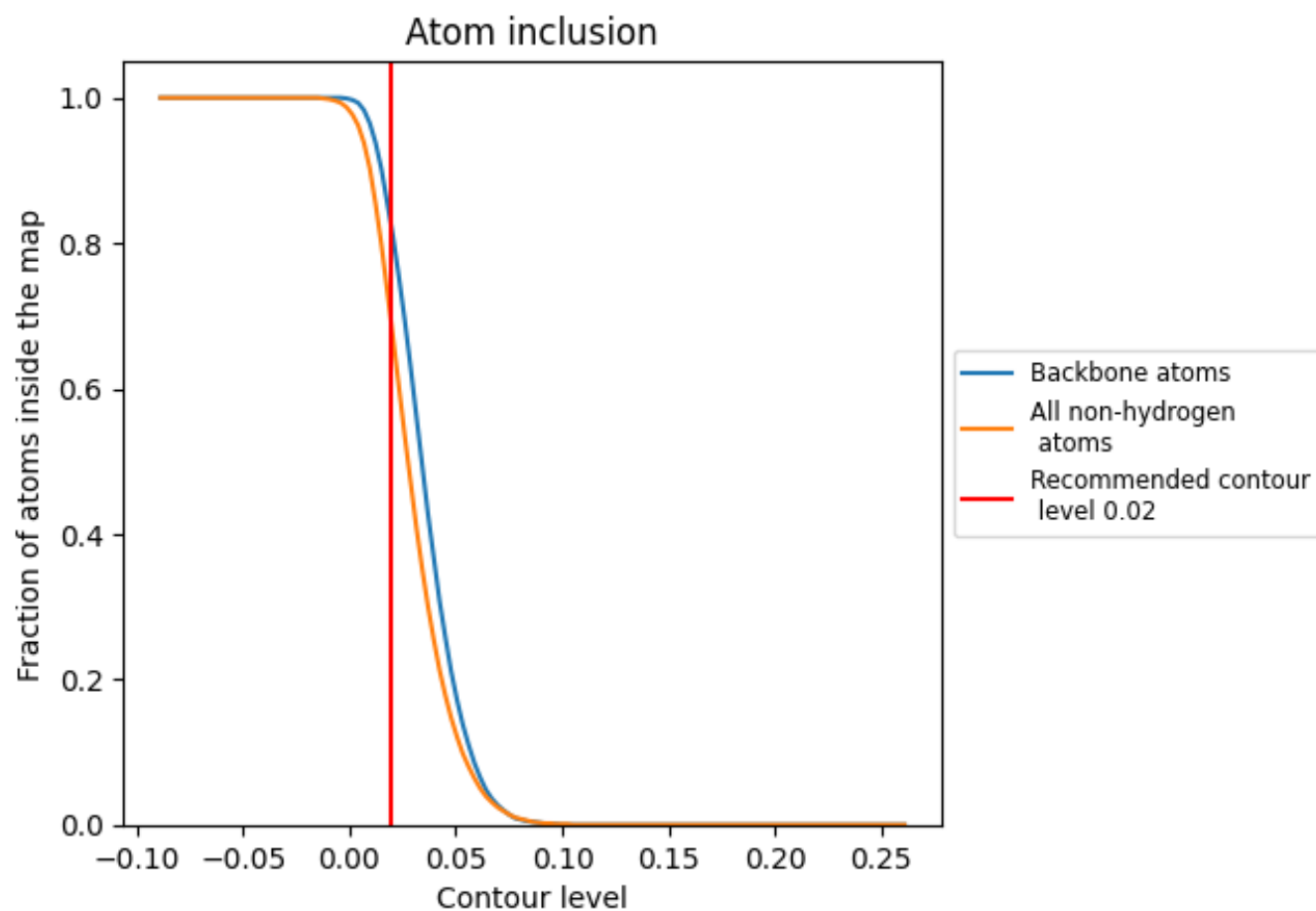
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

















































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.2780
A	 0.6080	 0.1850
A1	 0.7370	 0.2670
A3	 0.7700	 0.2850
A4	 0.7720	 0.3150
A6	 0.7980	 0.3780
AA	 0.7720	 0.3600
AB	 0.7770	 0.3740
AC	 0.8600	 0.3480
AD	 0.7990	 0.3020
AE	 0.7820	 0.3420
AF	 0.8030	 0.3850
AG	 0.7630	 0.2510
AH	 0.7180	 0.1970
AI	 0.6970	 0.2870
AJ	 0.7650	 0.3900
AK	 0.6720	 0.1590
AL	 0.7300	 0.2350
B	 0.7500	 0.3510
B1	 0.6830	 0.2740
B2	 0.6620	 0.1940
B3	 0.6670	 0.1720
B5	 0.7600	 0.3430
BA	 0.6660	 0.2590
BB	 0.6890	 0.2790
BC	 0.7820	 0.2570
BD	 0.6810	 0.1900
BE	 0.6530	 0.2750
BF	 0.7310	 0.3310
BG	 0.5700	 0.1030
BH	 0.6430	 0.1250
BI	 0.5080	 0.1090
BJ	 0.6880	 0.3150
BK	 0.5580	 0.0830
BL	 0.5590	 0.1090



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Chain	Atom inclusion	Q-score
C	 0.5990	 0.2350
D	 0.7970	 0.4030
E	 0.7000	 0.3040
F	 0.7410	 0.3140
G	 0.6920	 0.2930
H	 0.0960	 0.0450
I	 0.2630	 0.0770
J	 0.1660	 0.0950
K	 0.2170	 0.1070
L	 0.5280	 0.1300
M	 0.1140	 0.0580
N	 0.1750	 0.1100
O	 0.1100	 0.1230
T	 0.2430	 0.0880
a	 0.7990	 0.3570
b	 0.7730	 0.2460
c	 0.7430	 0.3020
d	 0.8280	 0.3790
e	 0.7900	 0.3720
f	 0.7530	 0.2040
g	 0.7560	 0.2360
h	 0.8010	 0.3240
i	 0.7870	 0.3360
j	 0.7610	 0.3130