



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 12:14 PM JST

PDB ID : 7WG5 / pdb_00007wg5
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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

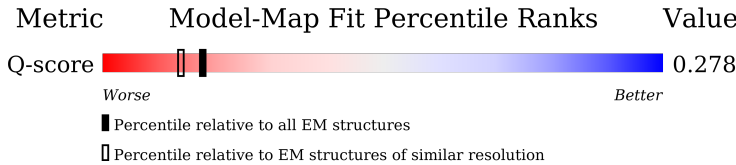
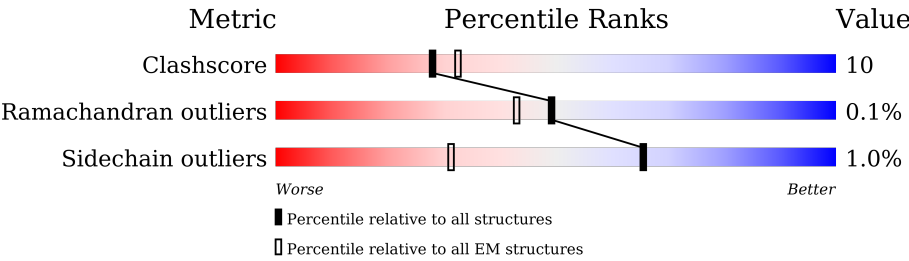
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8712 (3.39 - 4.39)

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	
1	BA	750	
2	AB	734	
2	BB	734	

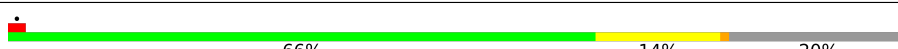
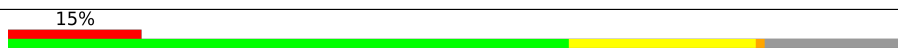
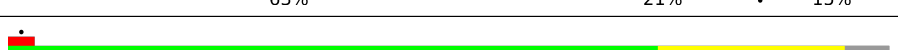
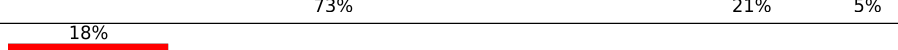
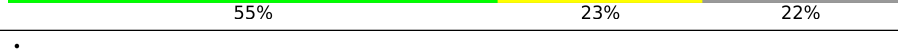
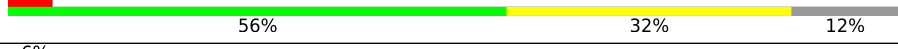
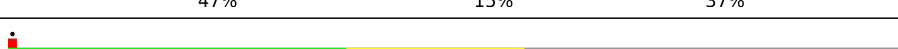
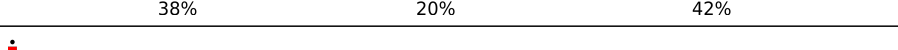
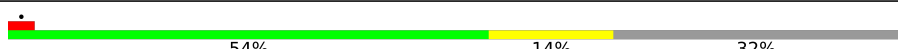
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Mol	Chain	Length	Quality of chain
3	AC	81	
3	BC	81	
4	AD	204	
4	BD	204	
5	AE	143	
5	BE	143	
6	AF	221	
6	BF	221	
7	AG	160	
7	BG	160	
8	AH	145	
8	BH	145	
9	AI	37	
9	BI	37	
10	AJ	44	
10	BJ	44	
11	AK	130	
11	BK	130	
12	AL	219	
12	BL	219	
13	A1	241	
13	B1	241	
14	A3	273	
14	B3	273	
15	A4	251	

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Mol	Chain	Length	Quality of chain
16	A6	270	
17	B2	257	
18	B5	256	
19	A	360	
20	B	512	
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	

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Mol	Chain	Length	Quality of chain
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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	BG	202	-	-	X	-
49	SF4	AC	102	-	-	X	-
49	SF4	BC	102	-	-	X	-
49	SF4	I	202	-	-	X	-
57	FES	c	301	-	-	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		

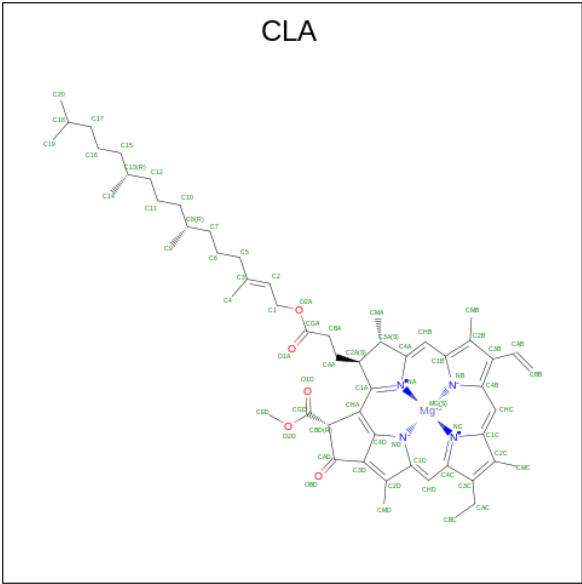
- Molecule 43 is a protein called NdhO.

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 (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				AltConf
45	AA	1	Total	C	Mg	N	O
			65	55	1	4	5
45	AA	1	Total	C	Mg	N	O
			65	55	1	4	5
45	AA	1	Total	C	Mg	N	O
			65	55	1	4	5
45	AA	1	Total	C	Mg	N	O
			52	42	1	4	5
45	AA	1	Total	C	Mg	N	O
			65	55	1	4	5
45	AA	1	Total	C	Mg	N	O
			65	55	1	4	5
45	AA	1	Total	C	Mg	N	O
			50	40	1	4	5
45	AA	1	Total	C	Mg	N	O
			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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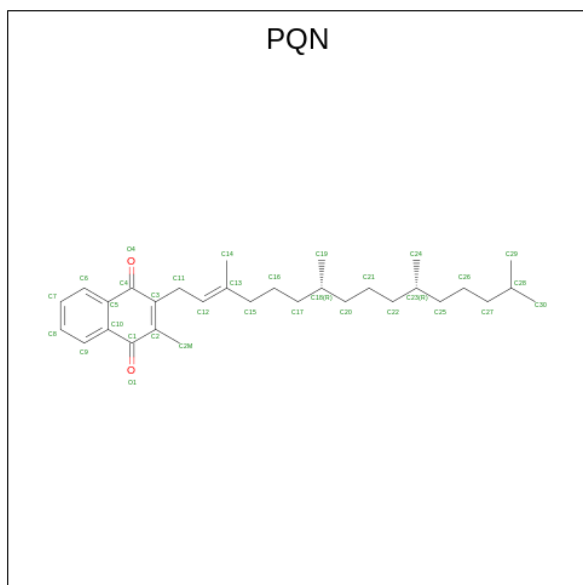
Mol	Chain	Residues	Atoms					AltConf
45	B2	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	B3	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	B3	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	B3	1	Total 42	C 32	Mg 1	N 4	O 5	0
45	B3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	B3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	B3	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	B3	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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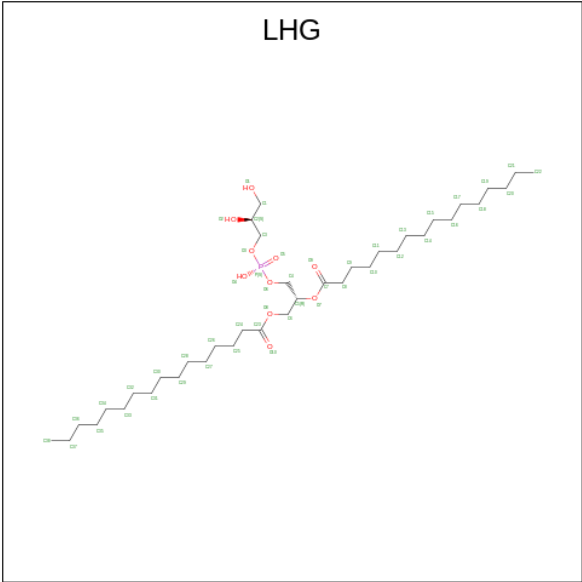
Mol	Chain	Residues	Atoms					AltConf
45	B5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 46 is PHYLLOQUINONE (CCD ID: 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 (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



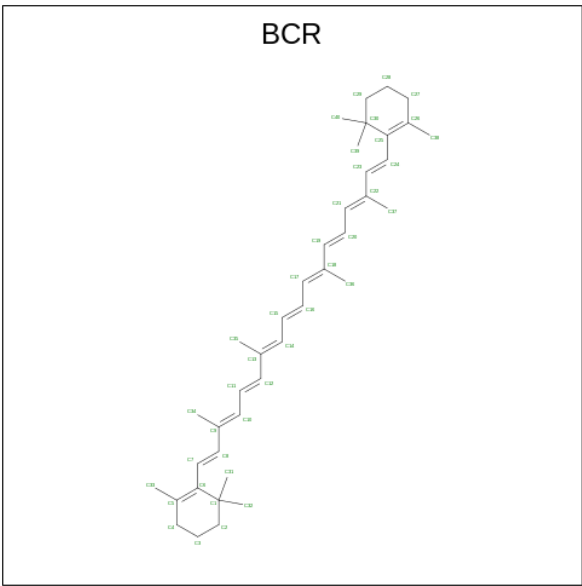
Mol	Chain	Residues	Atoms				AltConf
47	AA	1	Total	C	O	P	0
			49	38	10	1	
47	AJ	1	Total	C	O	P	0
			40	29	10	1	
47	A1	1	Total	C	O	P	0
			38	27	10	1	
47	A1	1	Total	C	O	P	0
			36	25	10	1	
47	A1	1	Total	C	O	P	0
			49	38	10	1	
47	A3	1	Total	C	O	P	0
			36	25	10	1	
47	A3	1	Total	C	O	P	0
			23	12	10	1	
47	A6	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 (CCD ID: BCR) (formula: C₄₀H₅₆).



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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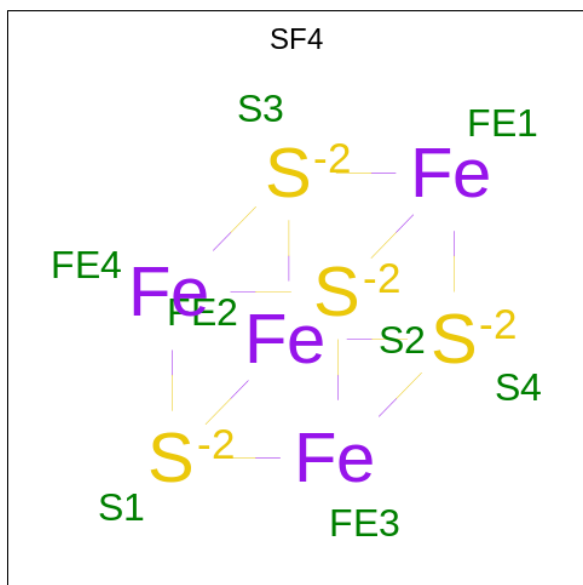
Mol	Chain	Residues	Atoms	AltConf
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	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 (CCD ID: SF4) (formula: Fe_4S_4).



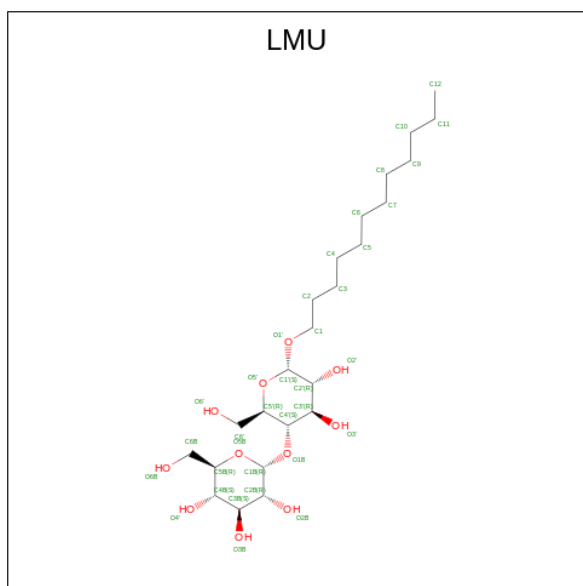
Mol	Chain	Residues	Atoms			AltConf
49	AA	1	Total	Fe	S	0
			8	4	4	
49	AC	1	Total	Fe	S	0
			8	4	4	
49	AC	1	Total	Fe	S	0
			8	4	4	
49	BA	1	Total	Fe	S	0
			8	4	4	
49	BC	1	Total	Fe	S	0
			8	4	4	
49	BC	1	Total	Fe	S	0
			8	4	4	
49	I	1	Total	Fe	S	0
			8	4	4	
49	I	1	Total	Fe	S	0
			8	4	4	

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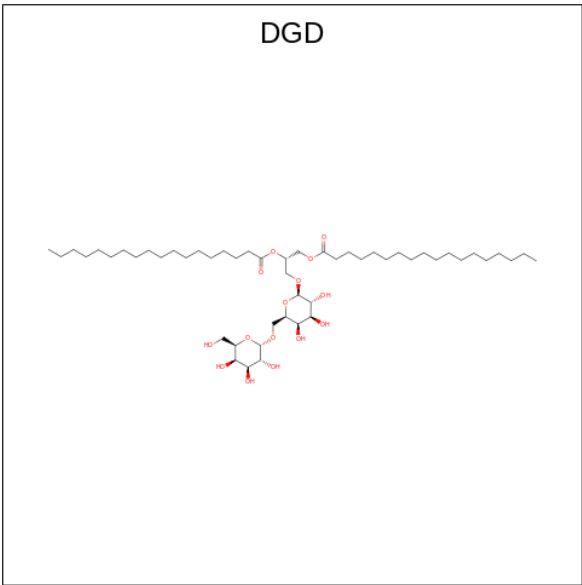
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
49	K	1	8	4	4	0

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



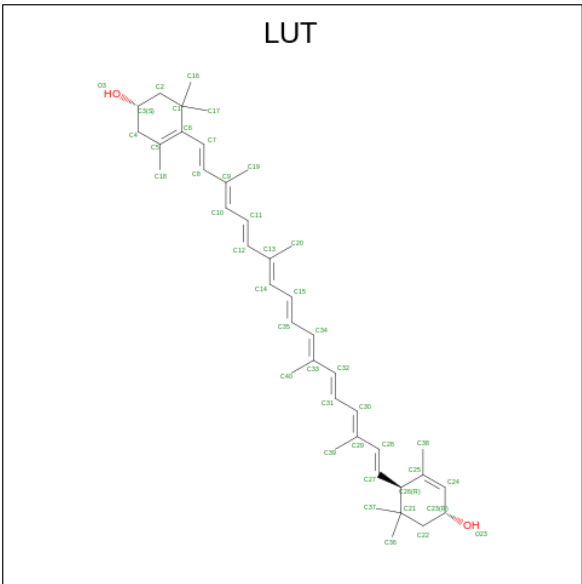
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	AA	1	35	24	11	0
50	AB	1	35	24	11	0
50	AB	1	35	24	11	0
50	AB	1	35	24	11	0
50	AL	1	34	23	11	0
50	BA	1	34	23	11	0
50	BA	1	33	22	11	0
50	BB	1	35	24	11	0

- Molecule 51 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: 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 (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



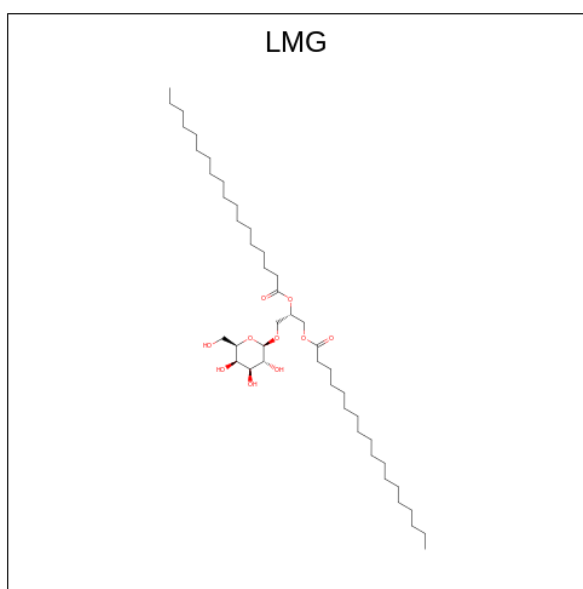
Mol	Chain	Residues	Atoms			AltConf
52	AF	1	Total	C	O	0
			42	40	2	

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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 (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



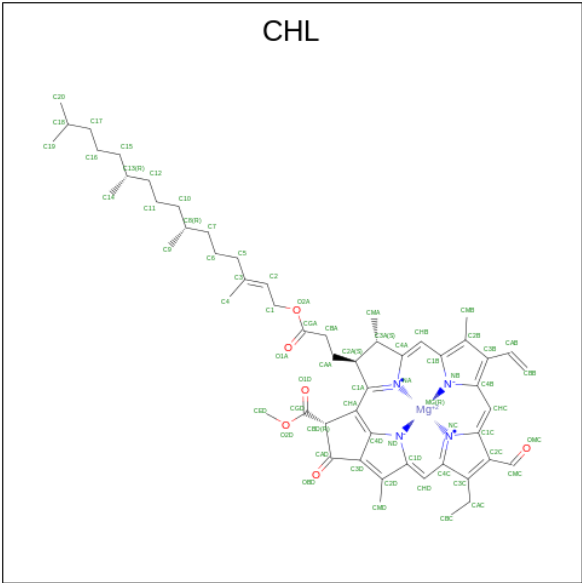
Mol	Chain	Residues	Atoms			AltConf
53	AG	1	Total	C	O	0
			38	28	10	
53	A1	1	Total	C	O	0
			44	34	10	
53	A4	1	Total	C	O	0
			39	29	10	

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

- Molecule 54 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



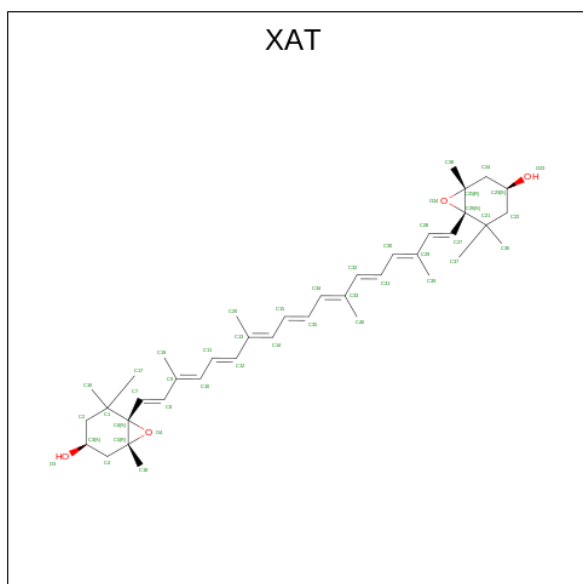
Mol	Chain	Residues	Atoms					AltConf
54	A1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
54	A1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
54	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
54	A4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
54	A4	1	Total	C	Mg	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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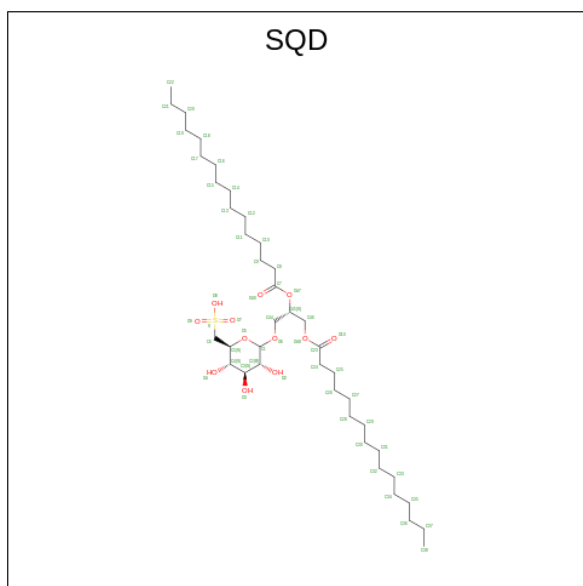
Mol	Chain	Residues	Atoms					AltConf
54	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
54	B1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
54	B1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
54	B2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	B2	1	Total	C	Mg	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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



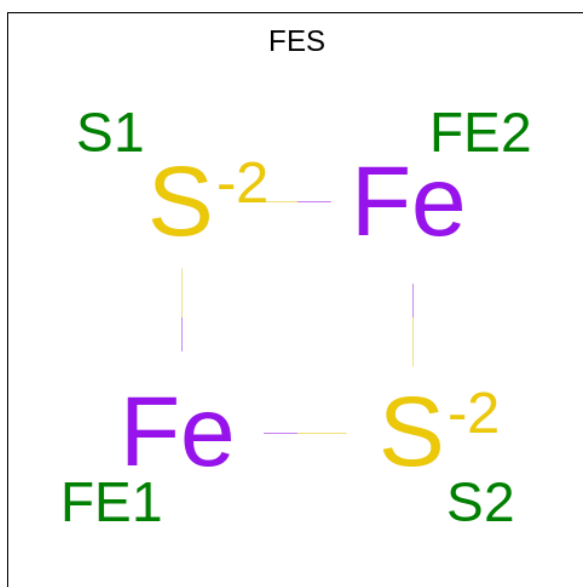
Mol	Chain	Residues	Atoms			AltConf
55	A1	1	Total	C	O	0
			44	40	4	
55	A3	1	Total	C	O	0
			44	40	4	
55	A4	1	Total	C	O	0
			44	40	4	
55	A6	1	Total	C	O	0
			44	40	4	
55	B1	1	Total	C	O	0
			44	40	4	
55	B2	1	Total	C	O	0
			44	40	4	
55	B3	1	Total	C	O	0
			44	40	4	
55	B5	1	Total	C	O	0
			44	40	4	

- Molecule 56 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: 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 (CCD ID: FES) (formula: Fe_2S_2).

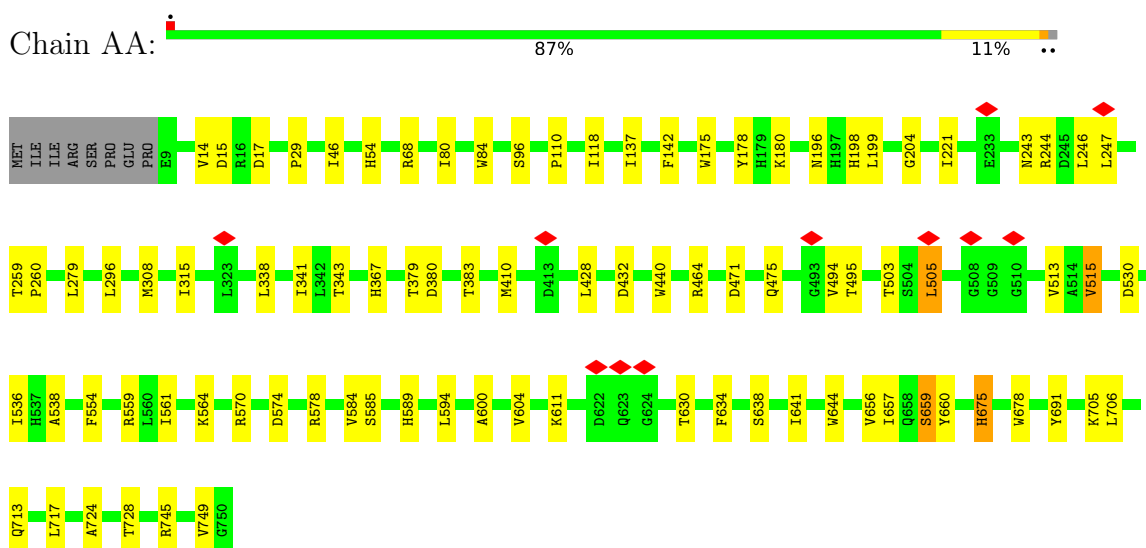


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
57	c	1	4	2	2	0

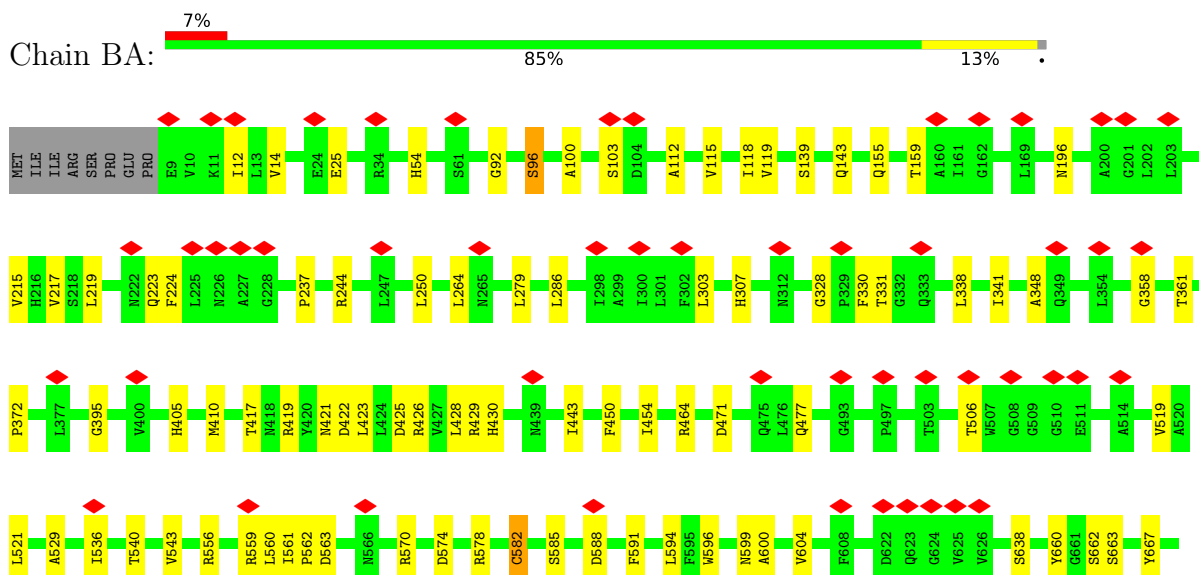
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

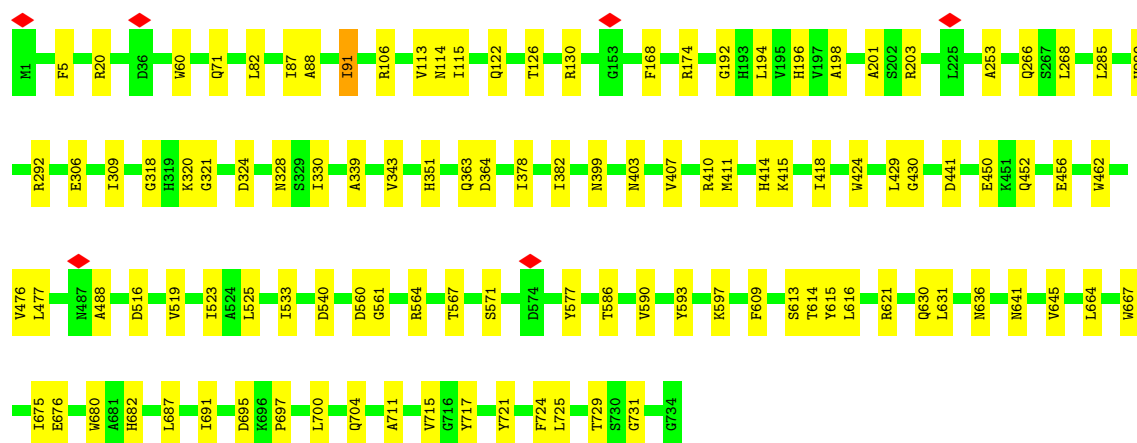


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

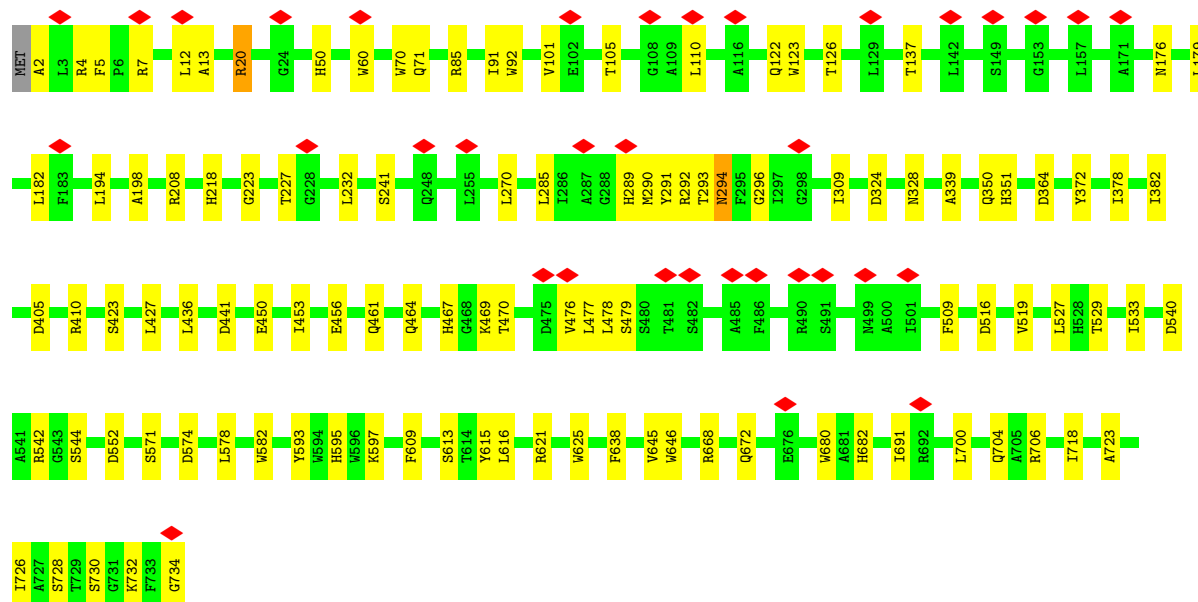
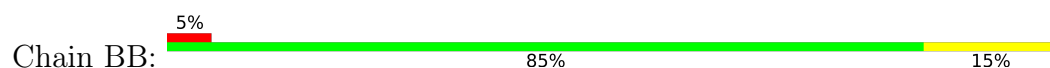




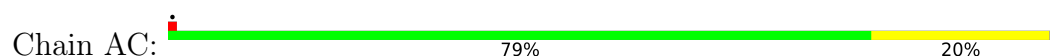
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



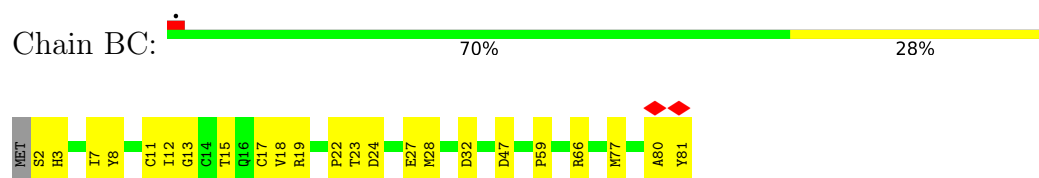
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



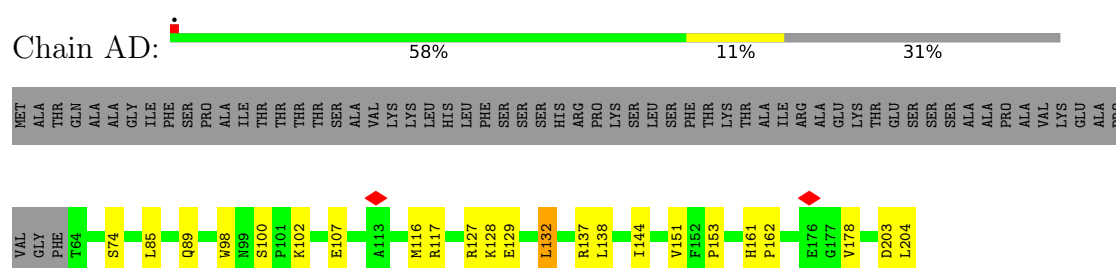
- Molecule 3: Photosystem I iron-sulfur center



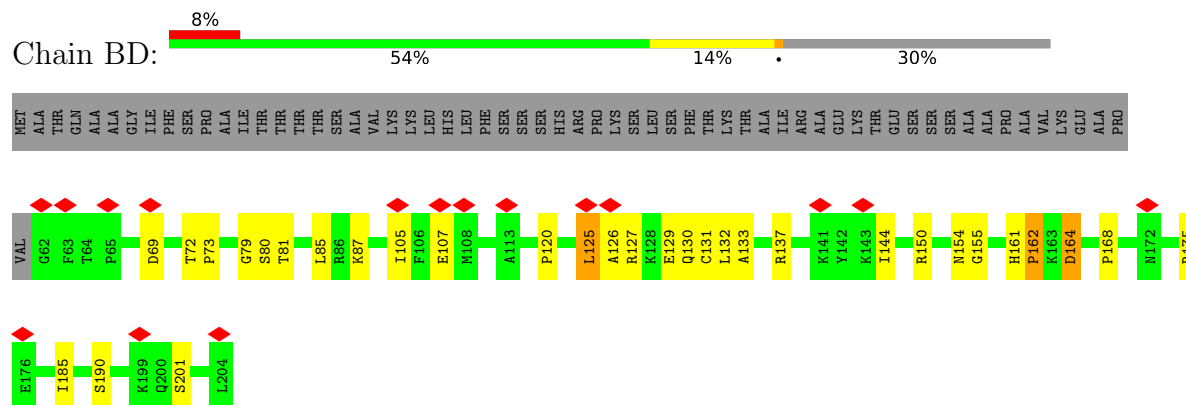
- Molecule 3: Photosystem I iron-sulfur center



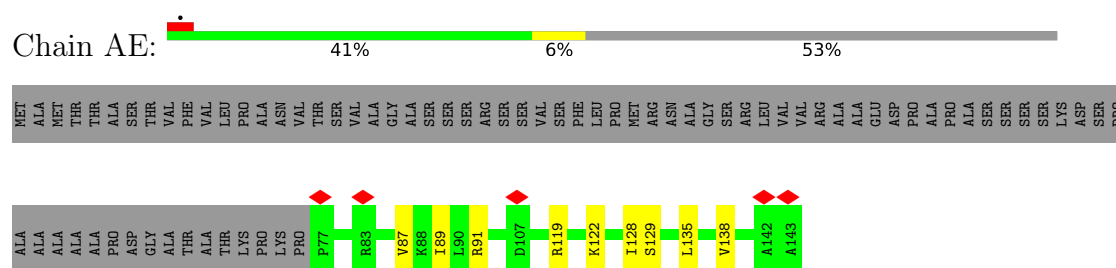
- Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic



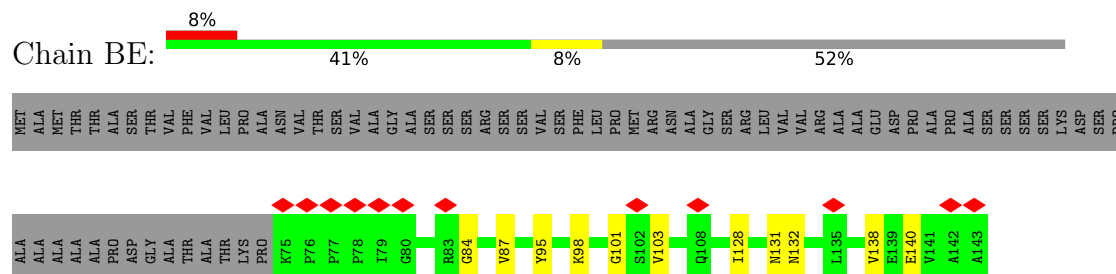
- Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic



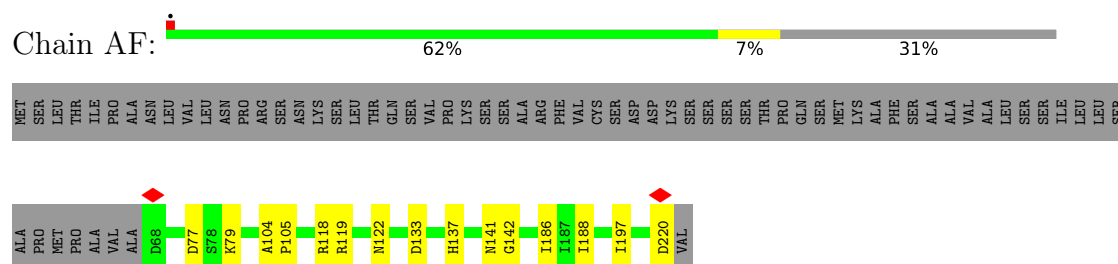
- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic



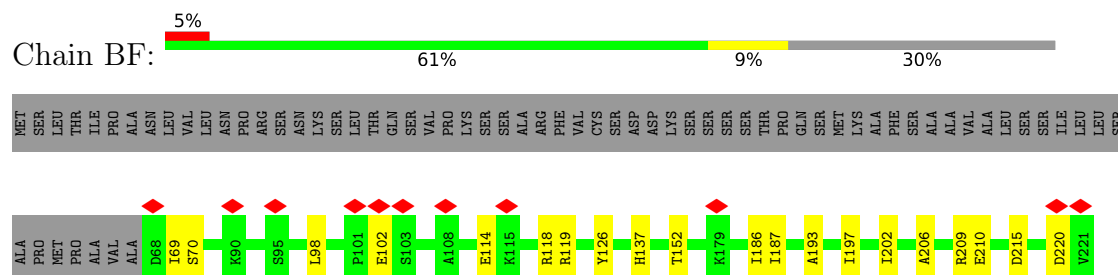
- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic



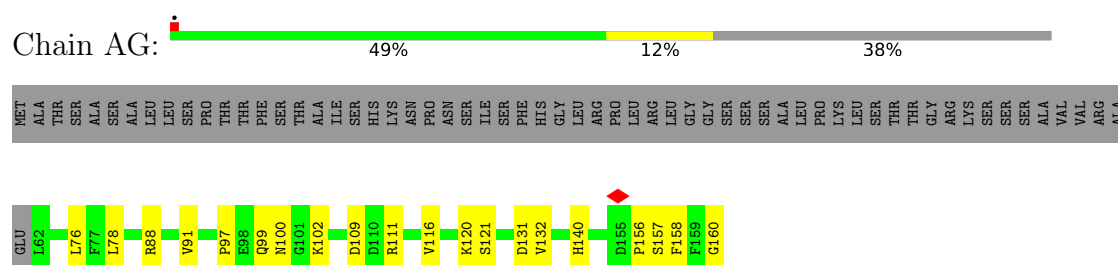
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



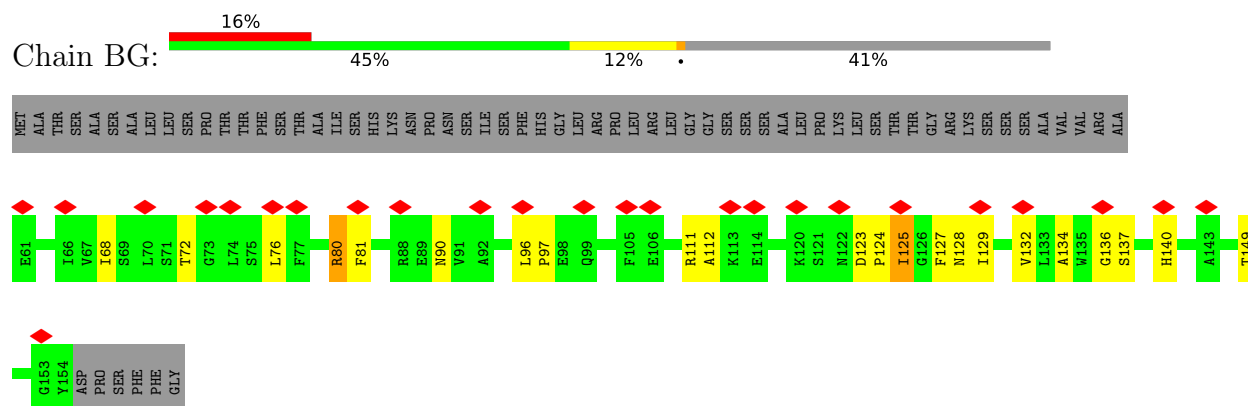
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



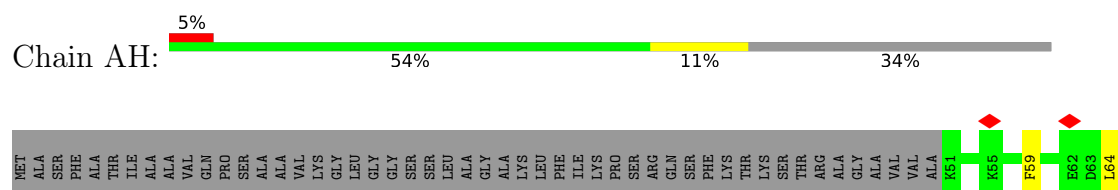
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

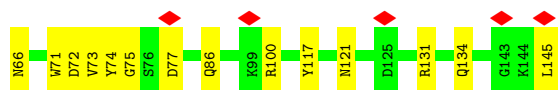


- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

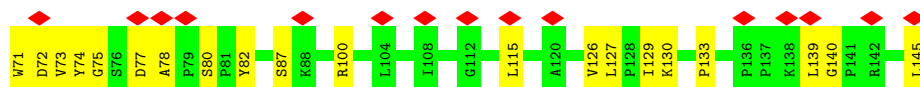
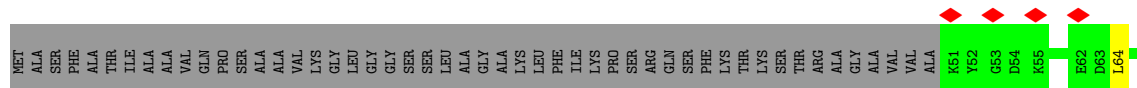


- Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic

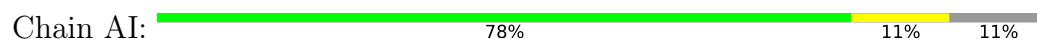




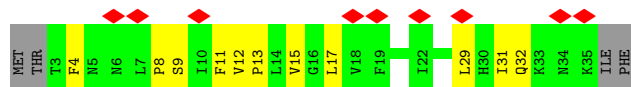
- Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic



- Molecule 9: Photosystem I reaction center subunit VIII



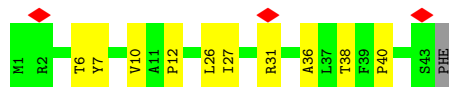
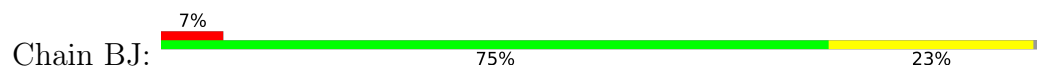
- Molecule 9: Photosystem I reaction center subunit VIII



- Molecule 10: Photosystem I reaction center subunit IX

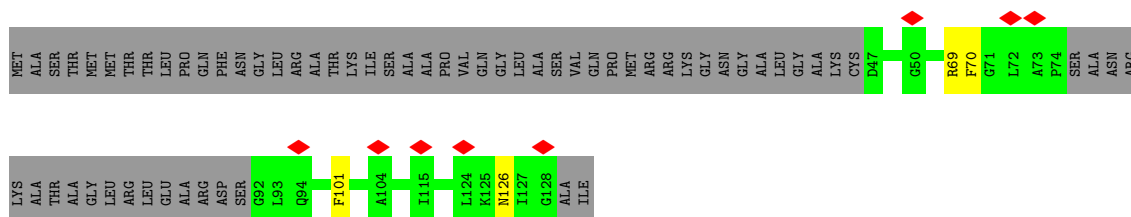


- Molecule 10: Photosystem I reaction center subunit IX

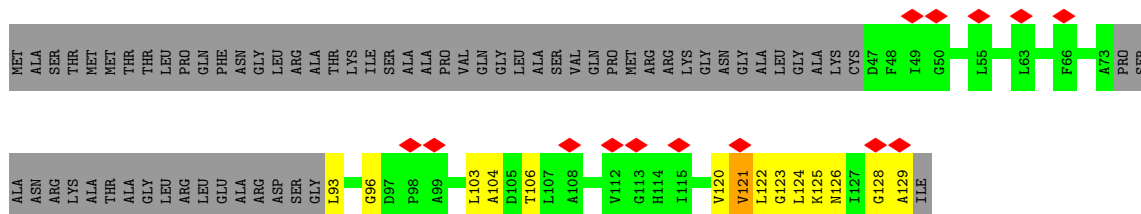
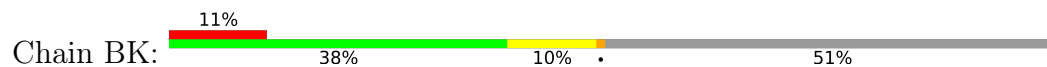


- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

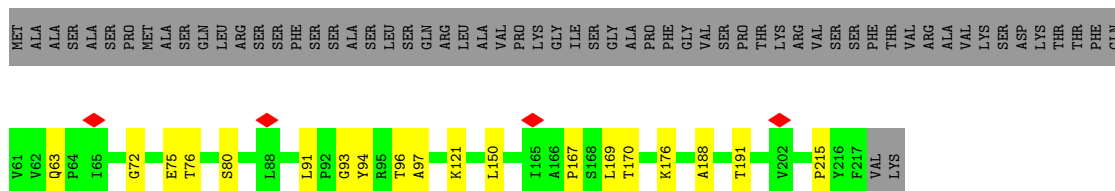




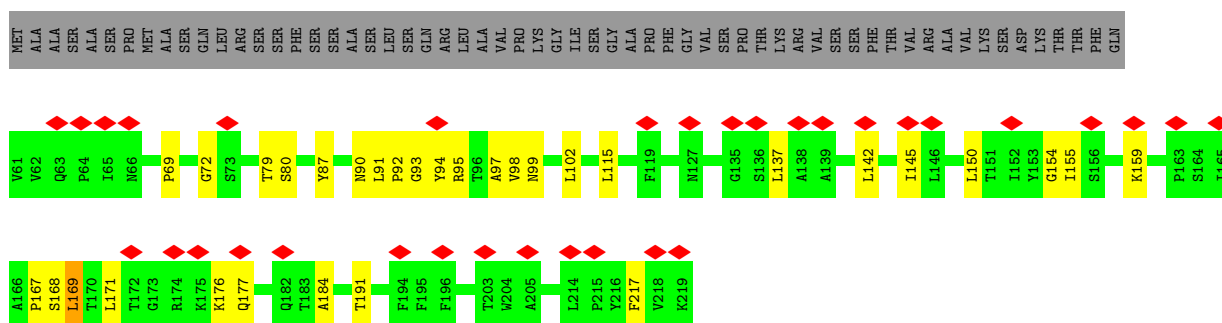
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



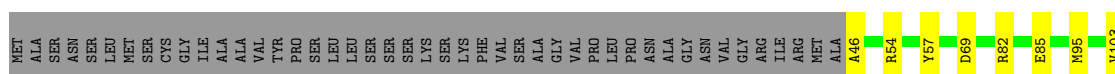
- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

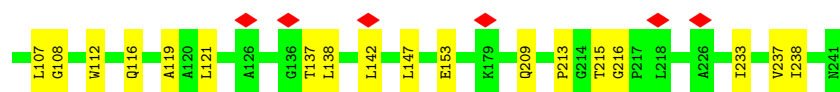


- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

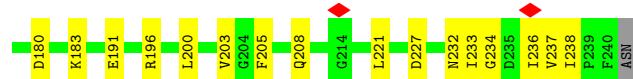
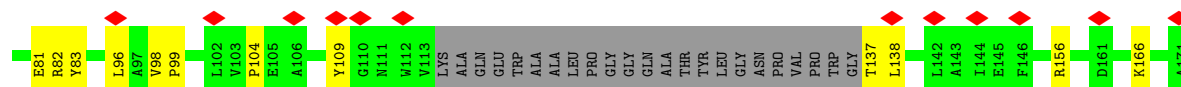
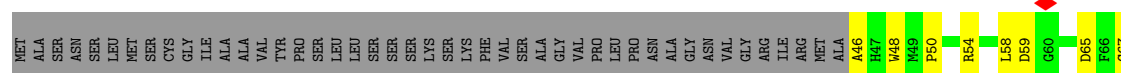


- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

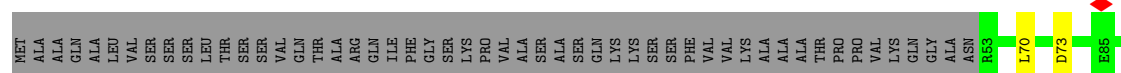
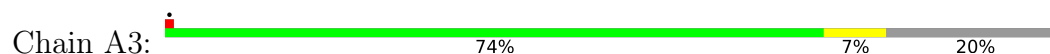




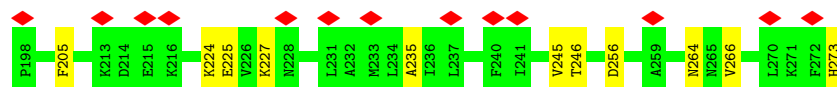
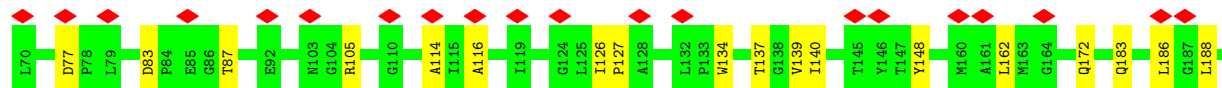
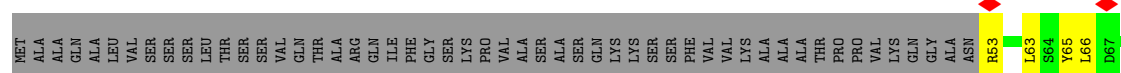
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



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

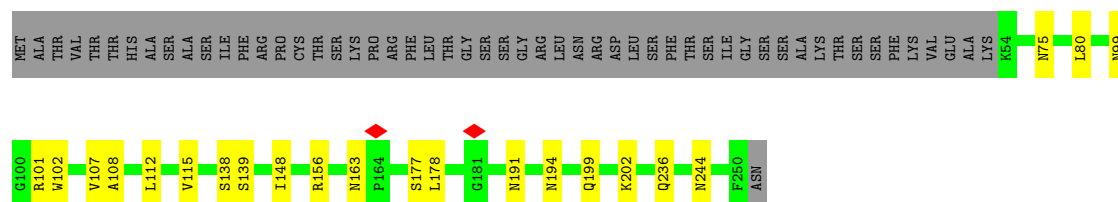


- Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

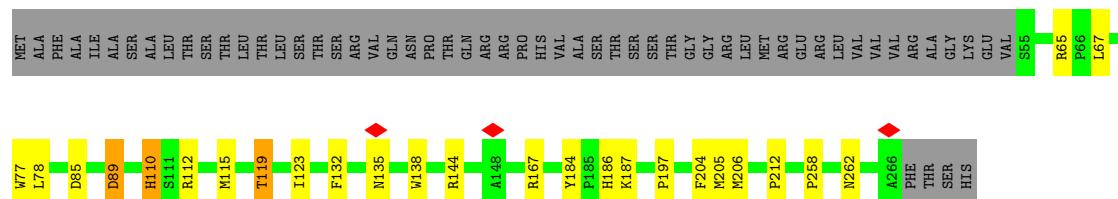


- Molecule 15: Chlorophyll a-b binding protein 4, chloroplastic

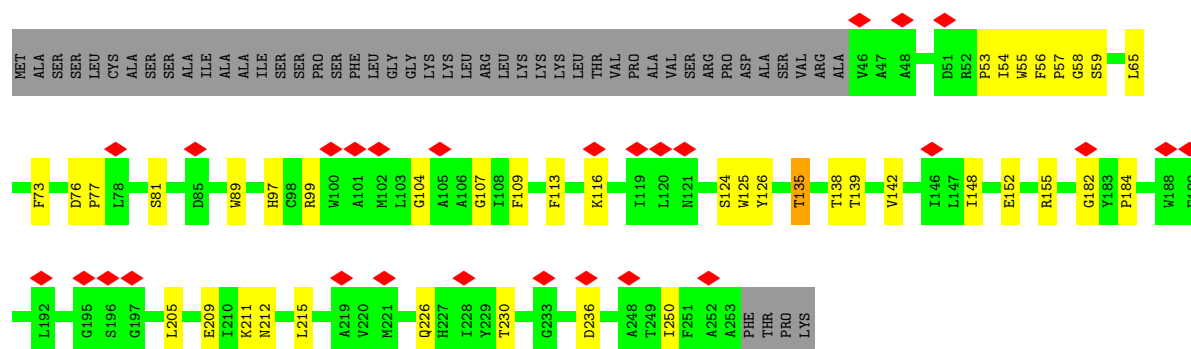




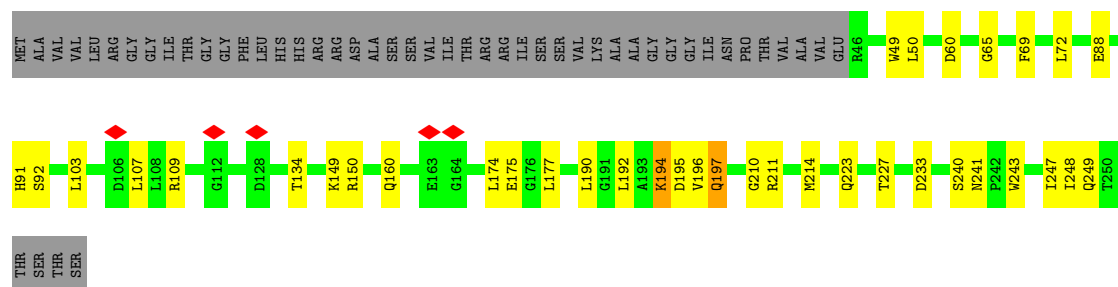
- Molecule 16: Photosystem I chlorophyll a/b-binding protein 6, chloroplastic



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

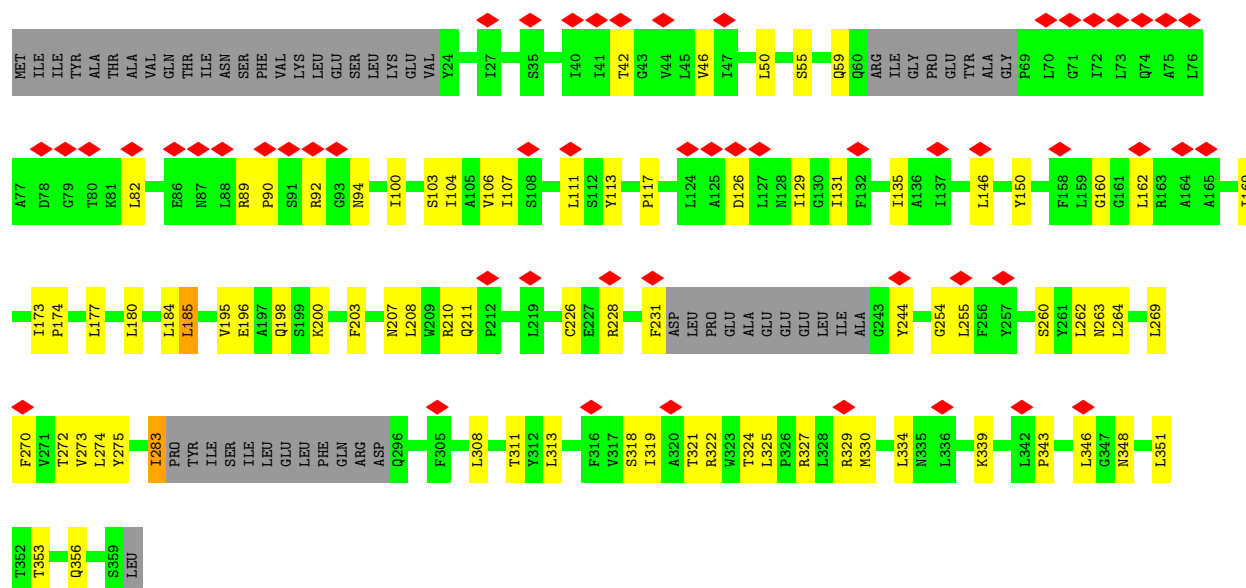


- Molecule 18: Photosystem I chlorophyll a/b-binding protein 5, chloroplastic



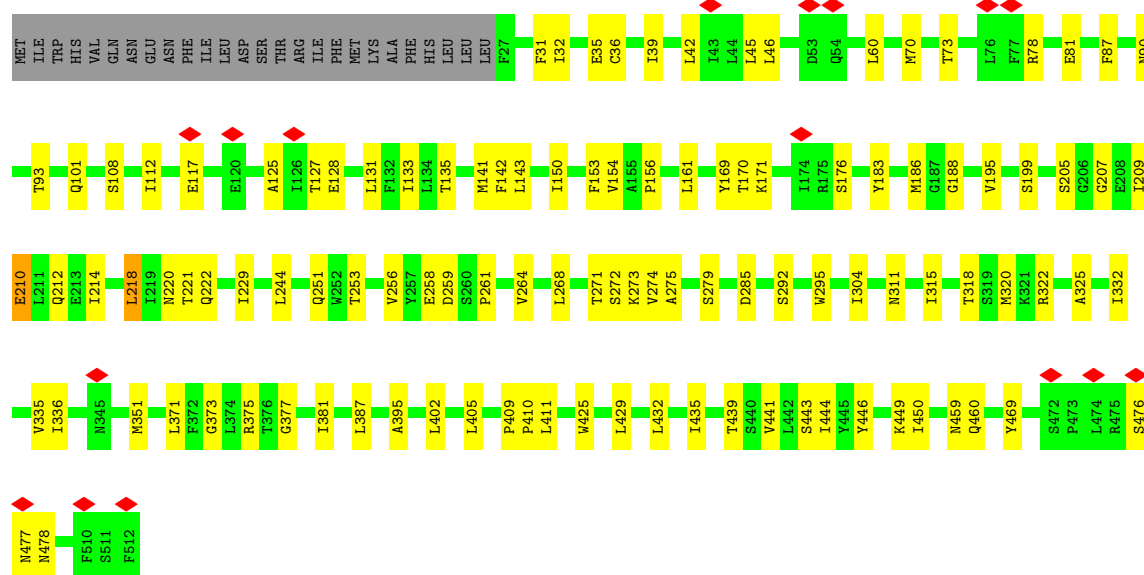
- Molecule 19: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic





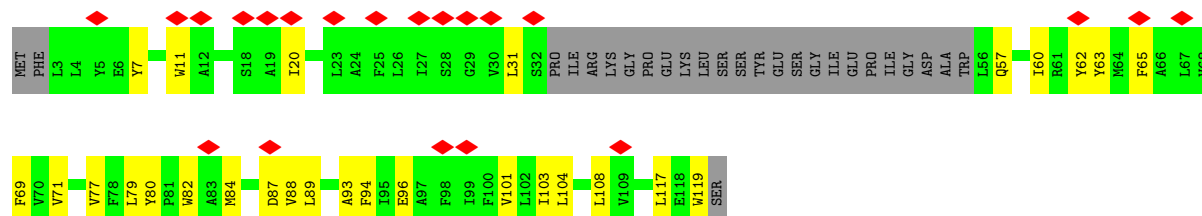
- Molecule 20: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic

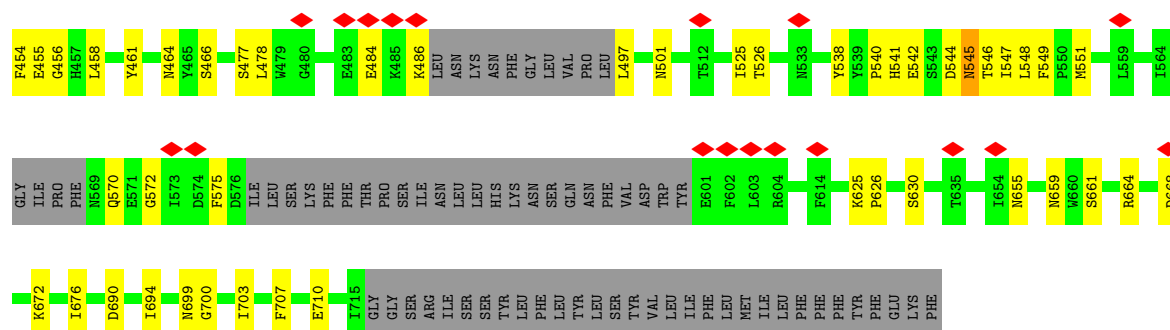
Chain B: 73% 21% 5%



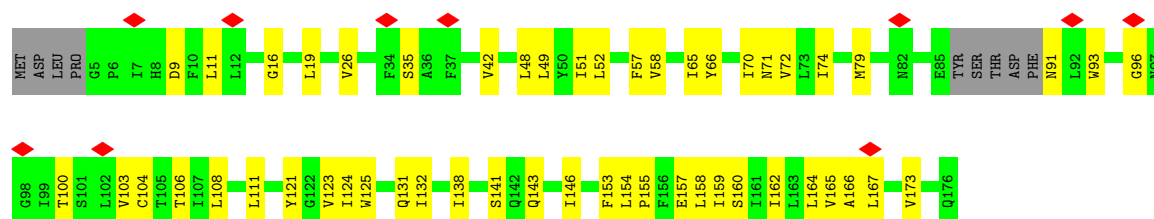
- Molecule 21: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic

Chain C: 18% 55% 23% 22%

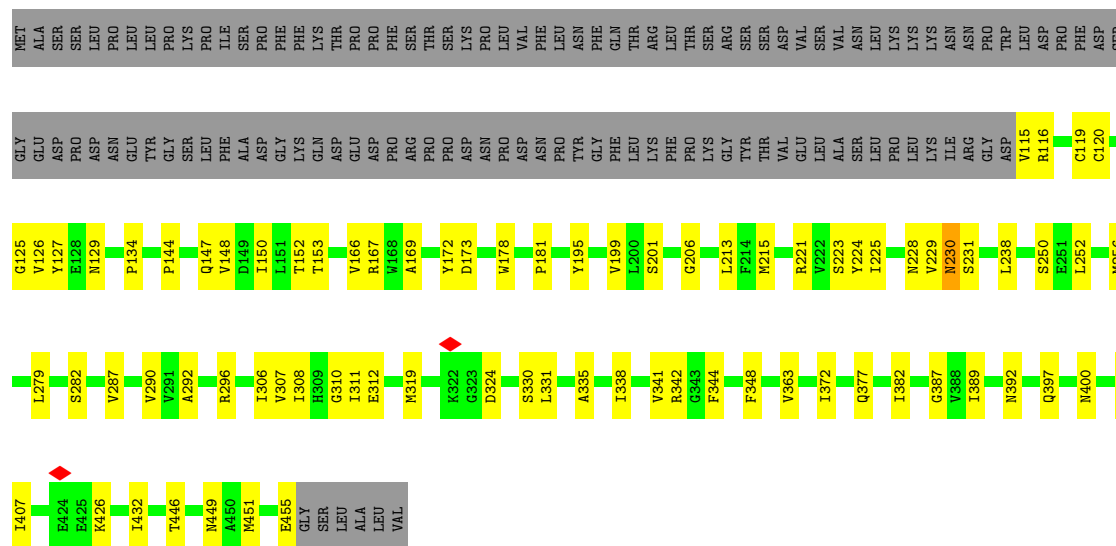




- Molecule 25: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic



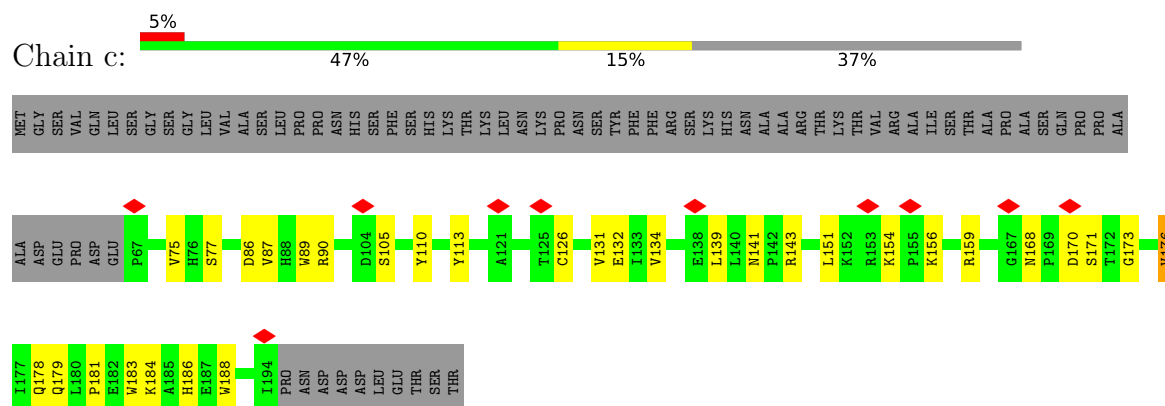
- Molecule 26: Photosynthetic NDH subunit of subcomplex B 1, chloroplastic



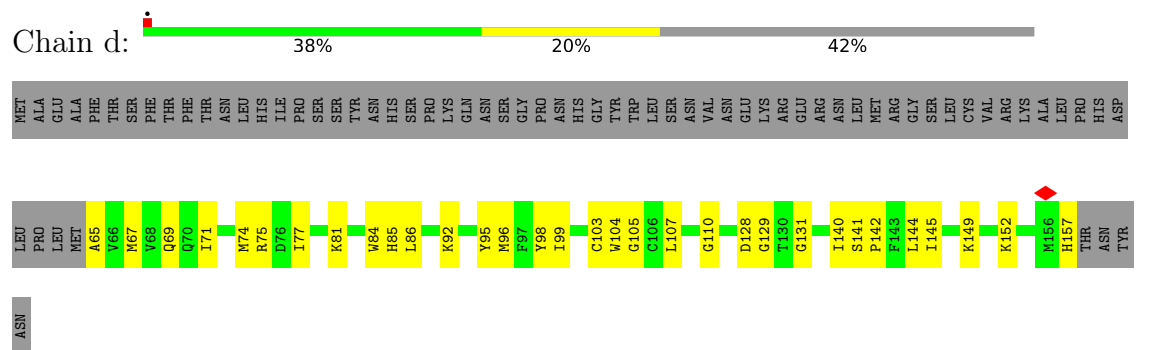
- Molecule 27: Photosynthetic NDH subunit of subcomplex B 2, chloroplastic



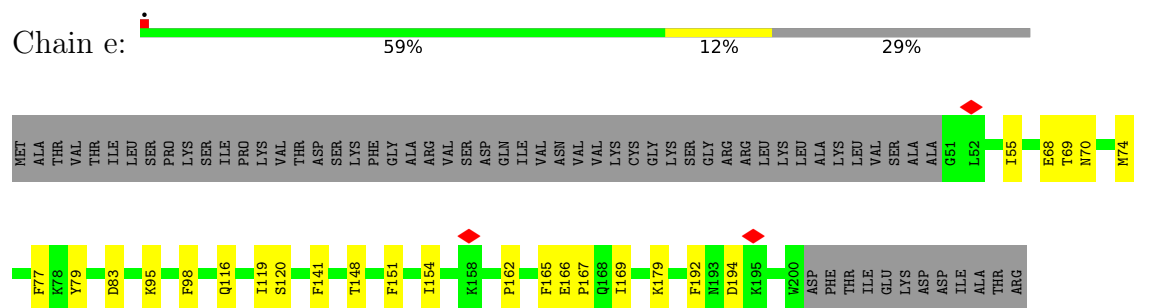
- Molecule 28: Photosynthetic NDH subunit of subcomplex B 3, chloroplastic



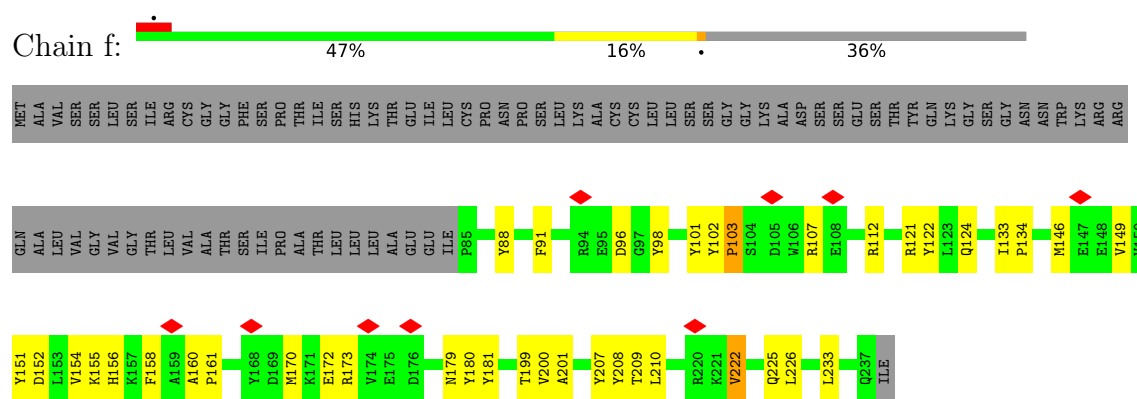
- Molecule 29: NDH dependent flow 6



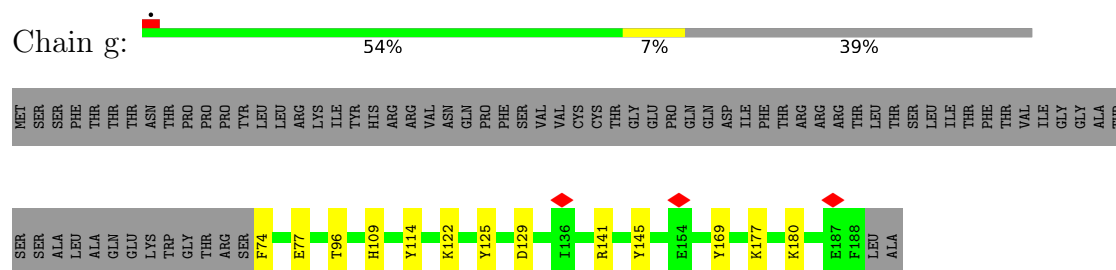
- Molecule 30: Photosynthetic NDH subunit of subcomplex B 5, chloroplastic



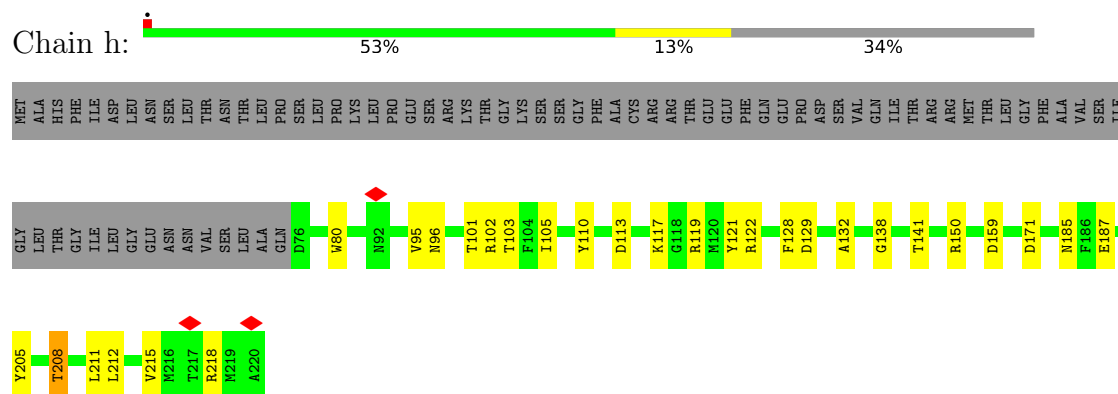
- Molecule 31: Photosynthetic NDH subunit of lumenal location 1, chloroplastic



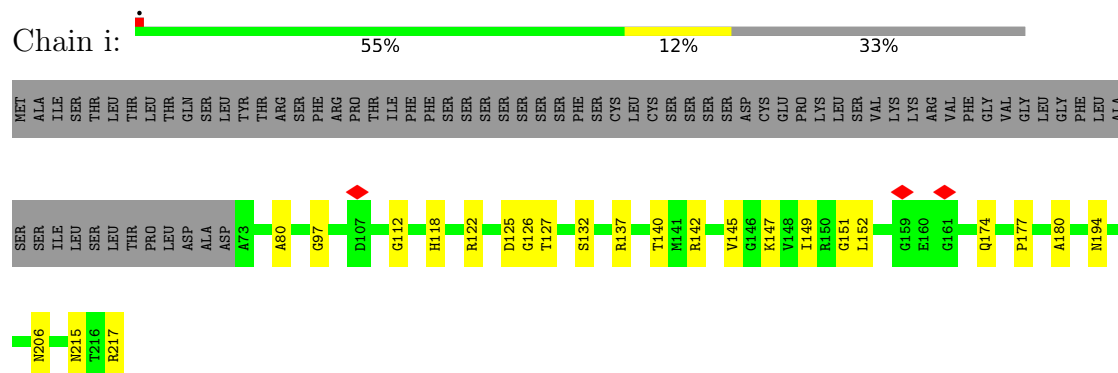
- Molecule 32: Photosynthetic NDH subunit of luminal location 2, chloroplastic



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

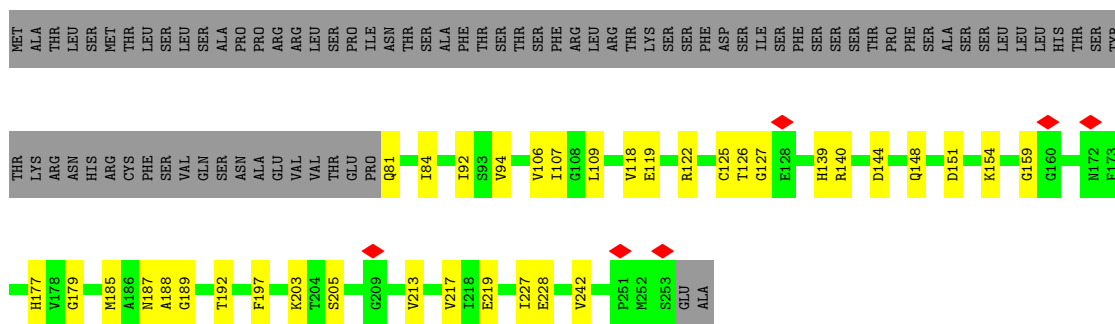


- Molecule 34: Photosynthetic NDH subunit of luminal location 4, chloroplastic

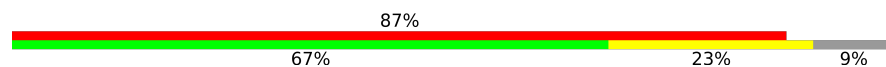


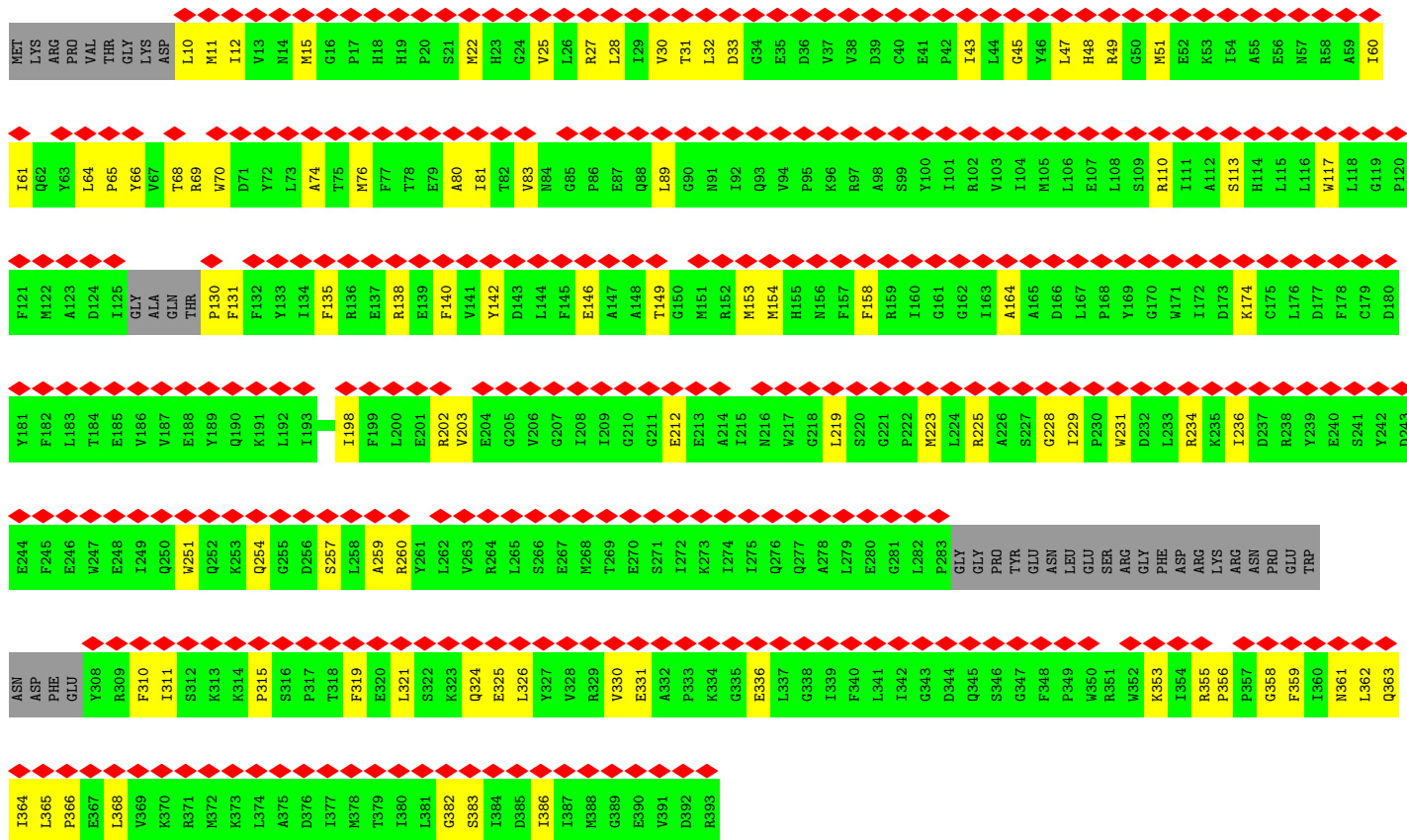
- Molecule 35: Isoform 2 of Photosynthetic NDH subunit of luminal location 5, chloroplastic

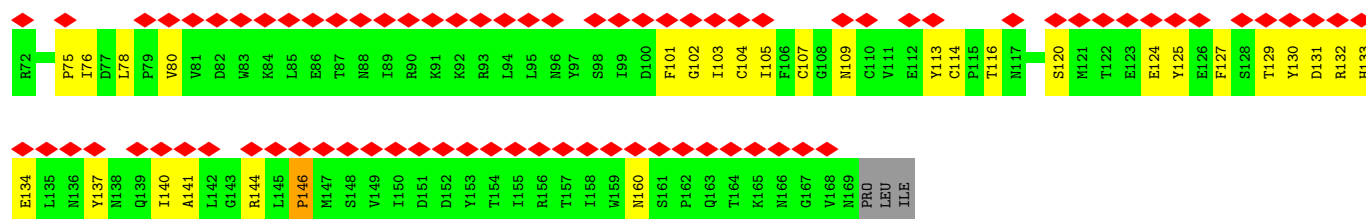
Chain j: 



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

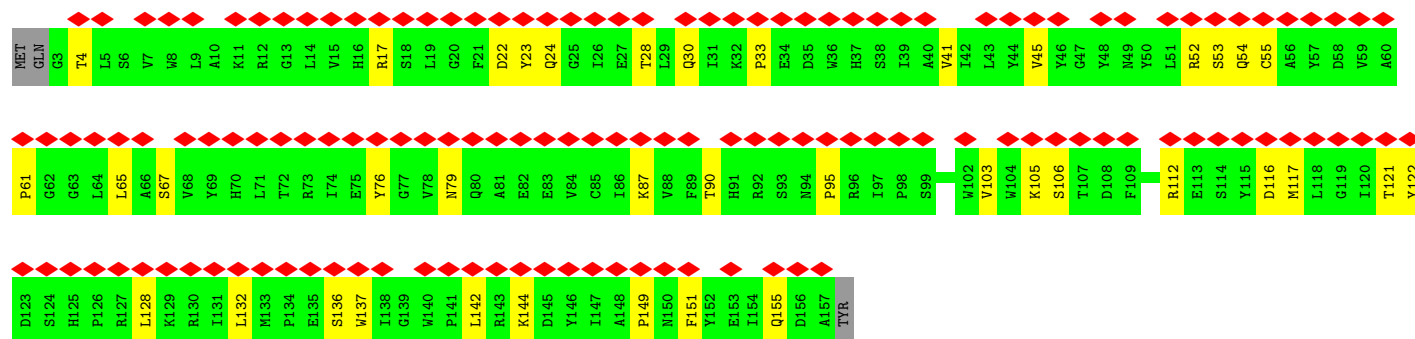
Chain H: 





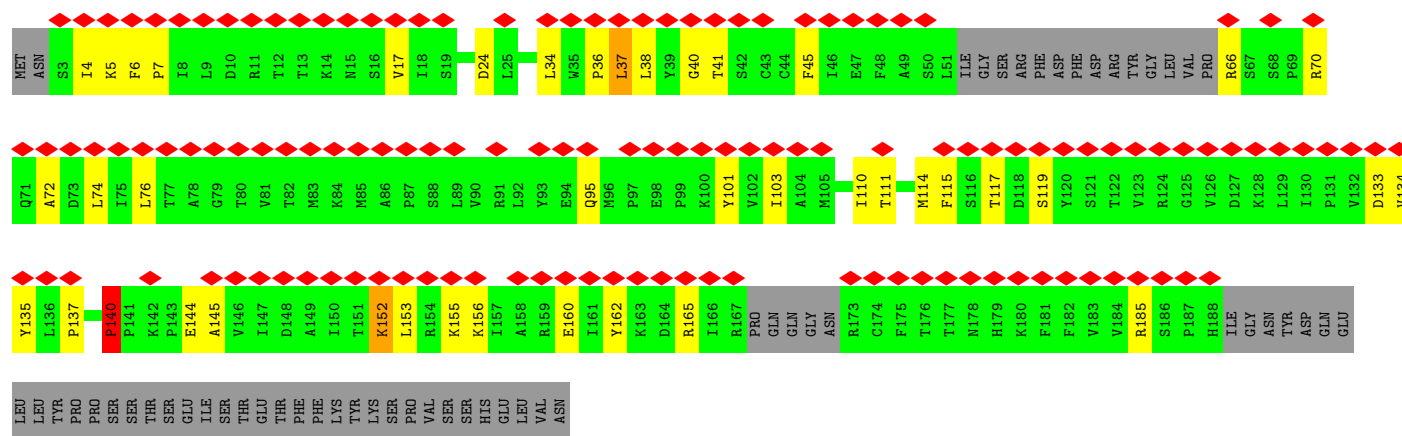
• Molecule 38: NAD(P)H-quinone oxidoreductase subunit J, chloroplastic

Chain J: .



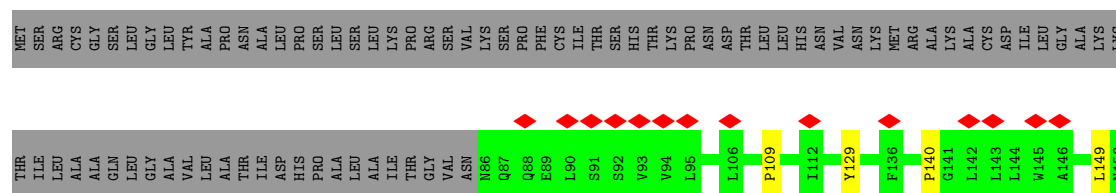
• Molecule 39: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic

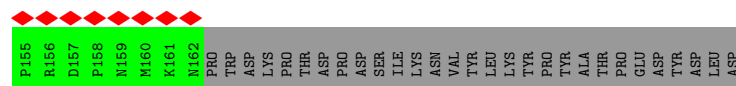
Chain K: .



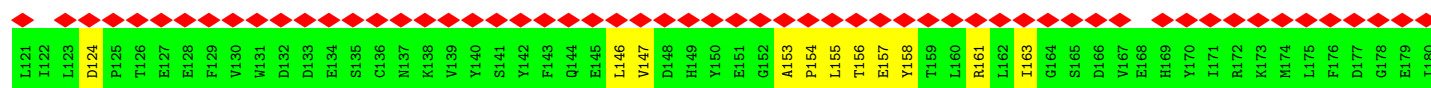
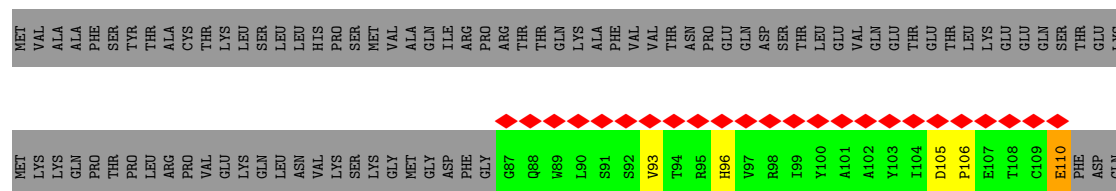
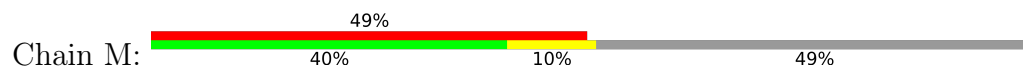
• Molecule 40: NAD(P)H-quinone oxidoreductase subunit L, chloroplastic

Chain L: .

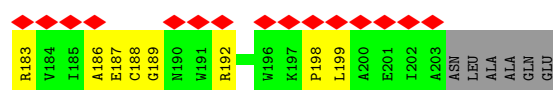
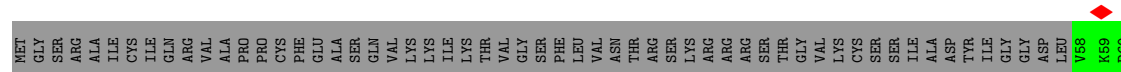




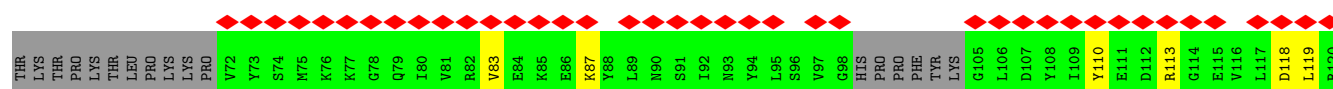
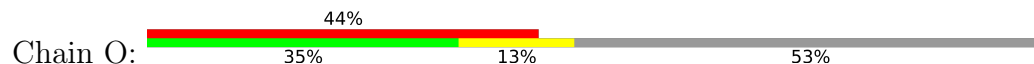
- Molecule 41: NAD(P)H-quinone oxidoreductase subunit M, chloroplastic

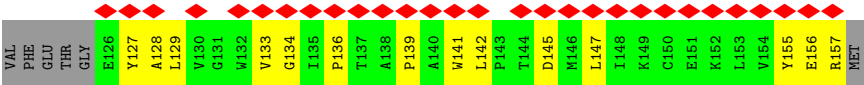


- Molecule 42: NAD(P)H-quinone oxidoreductase subunit N, chloroplastic

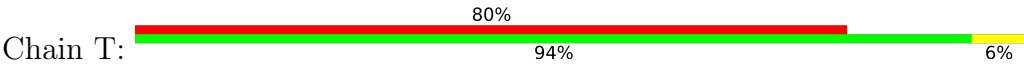


- Molecule 43: NdhO





• Molecule 44: NdhT



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: CLA, SF4, CHL, BCR, LHG, SQD, XAT, LUT, DGD, LMG, LMU, PQN, FES

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	0.32	1/6037 (0.0%)	0.47	0/8236
1	BA	0.31	0/6039	0.48	1/8239 (0.0%)
2	AB	0.30	0/6073	0.44	0/8291
2	BB	0.31	0/6065	0.48	1/8281 (0.0%)
3	AC	0.37	0/628	0.57	0/852
3	BC	0.39	0/628	0.63	0/852
4	AD	0.22	0/1140	0.45	0/1542
4	BD	0.32	0/1156	0.55	0/1563
5	AE	0.20	0/542	0.36	0/736
5	BE	0.20	0/559	0.37	0/760
6	AF	0.23	0/1243	0.44	0/1677
6	BF	0.25	0/1250	0.46	0/1687
7	AG	0.41	1/791 (0.1%)	0.49	0/1072
7	BG	0.31	0/750	0.54	0/1016
8	AH	0.19	0/751	0.41	0/1018
8	BH	0.25	0/751	0.48	0/1018
9	AI	0.22	0/264	0.39	0/359
9	BI	0.39	0/264	0.84	2/359 (0.6%)
10	AJ	0.31	0/348	0.54	0/474
10	BJ	0.29	0/354	0.52	0/482
11	AK	0.28	0/456	0.45	0/617
11	BK	0.40	0/449	0.68	1/607 (0.2%)
12	AL	0.26	0/1208	0.47	1/1650 (0.1%)
12	BL	0.28	0/1218	0.50	0/1663
13	A1	0.32	1/1562 (0.1%)	0.47	0/2131
13	B1	0.22	0/1381	0.43	0/1879
14	A3	0.22	0/1726	0.41	0/2347
14	B3	0.21	0/1749	0.39	0/2378
15	A4	0.27	0/1611	0.45	0/2194
16	A6	0.28	0/1732	0.49	0/2363
17	B2	0.23	0/1663	0.47	0/2277
18	B5	0.25	0/1646	0.48	1/2239 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	A	0.26	0/2430	0.60	0/3312
20	B	0.31	0/3872	0.64	2/5263 (0.0%)
21	C	0.35	1/802 (0.1%)	0.59	0/1094
22	D	0.37	0/4058	0.63	1/5509 (0.0%)
23	E	0.28	0/705	0.56	0/952
24	F	0.30	0/5478	0.63	6/7446 (0.1%)
25	G	0.27	0/1307	0.63	2/1785 (0.1%)
26	a	0.33	0/2708	0.70	0/3668
27	b	0.22	0/2417	0.60	0/3265
28	c	0.33	0/1030	0.70	0/1401
29	d	0.38	0/784	0.68	0/1057
30	e	0.26	0/1241	0.62	0/1685
31	f	0.24	0/1312	0.60	0/1777
32	g	0.22	0/986	0.51	0/1329
33	h	0.25	0/1193	0.64	0/1610
34	i	0.24	0/1124	0.53	0/1523
35	j	0.26	0/1357	0.60	0/1823
36	H	0.25	0/2877	0.53	0/3894
37	I	0.37	0/1256	0.66	1/1701 (0.1%)
38	J	0.22	0/1142	0.48	0/1545
39	K	0.34	0/1222	0.69	2/1656 (0.1%)
40	L	0.28	0/669	0.61	1/911 (0.1%)
41	M	0.31	0/783	0.54	0/1062
42	N	0.43	0/921	0.60	0/1252
43	O	0.29	0/525	0.40	0/705
All	All	0.30	4/94233 (0.0%)	0.54	22/128084 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A1	103	VAL	CA-CB	8.58	1.58	1.54
7	AG	156	PRO	C-O	-6.81	1.15	1.24
21	C	20	ILE	C-N	5.55	1.40	1.34
1	AA	17	ASP	C-O	-5.00	1.21	1.23

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	140	PRO	N-CA-C	8.24	120.75	110.70
9	BI	9	SER	CA-C-N	-7.60	114.79	122.77
9	BI	9	SER	C-N-CA	-7.60	114.79	122.77
12	AL	215	PRO	N-CA-C	-6.45	106.29	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	37	LEU	N-CA-C	-6.34	105.91	113.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	5839	0	5683	76	0
1	BA	5841	0	5690	110	0
2	AB	5862	0	5649	97	0
2	BB	5854	0	5637	114	0
3	AC	615	0	593	16	0
3	BC	615	0	595	38	0
4	AD	1112	0	1122	14	0
4	BD	1127	0	1134	52	0
5	AE	530	0	536	14	0
5	BE	546	0	555	13	0
6	AF	1213	0	1243	10	0
6	BF	1220	0	1252	14	0
7	AG	771	0	749	16	0
7	BG	733	0	718	82	0
8	AH	730	0	720	25	0
8	BH	730	0	720	71	0
9	AI	257	0	274	7	0
9	BI	257	0	274	34	0
10	AJ	338	0	351	14	0
10	BJ	344	0	356	13	0
11	AK	451	0	462	11	0
11	BK	445	0	453	36	0
12	AL	1173	0	1162	27	0
12	BL	1184	0	1179	73	0
13	A1	1511	0	1464	16	0
13	B1	1339	0	1316	39	0
14	A3	1675	0	1647	11	0
14	B3	1696	0	1663	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A4	1562	0	1516	22	0
16	A6	1671	0	1599	56	0
17	B2	1607	0	1555	56	0
18	B5	1599	0	1581	37	0
19	A	2372	0	2454	64	0
20	B	3780	0	3840	87	0
21	C	776	0	777	30	0
22	D	3946	0	4068	107	0
23	E	695	0	732	34	0
24	F	5330	0	5289	175	0
25	G	1281	0	1340	59	0
26	a	2655	0	2673	67	0
27	b	2367	0	2371	60	0
28	c	1005	0	1006	22	0
29	d	762	0	730	49	0
30	e	1206	0	1110	27	0
31	f	1277	0	1235	31	0
32	g	965	0	945	12	0
33	h	1170	0	1176	26	0
34	i	1098	0	1082	21	0
35	j	1331	0	1320	22	0
36	H	2812	0	2795	93	0
37	I	1236	0	1180	70	0
38	J	1116	0	938	65	0
39	K	1199	0	1106	82	0
40	L	646	0	630	12	0
41	M	771	0	652	43	0
42	N	908	0	717	59	0
43	O	520	0	438	20	0
44	T	610	0	133	12	0
45	A1	575	0	447	8	0
45	A3	575	0	420	2	0
45	A4	480	0	376	5	0
45	A6	485	0	399	14	0
45	AA	2411	0	2371	32	0
45	AB	2452	0	2461	37	0
45	AF	140	0	113	1	0
45	AG	131	0	94	5	0
45	AH	60	0	59	1	0
45	AJ	42	0	31	1	0
45	AK	126	0	88	12	0
45	AL	143	0	119	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B1	519	0	402	8	0
45	B2	442	0	366	15	0
45	B3	578	0	422	6	0
45	B5	476	0	368	4	0
45	BA	2446	0	2387	39	0
45	BB	2422	0	2404	50	0
45	BF	138	0	110	1	0
45	BG	87	0	64	48	0
45	BH	60	0	59	0	0
45	BJ	42	0	31	0	0
45	BK	127	0	88	7	0
45	BL	148	0	125	11	0
46	AA	33	0	46	3	0
46	AB	33	0	46	2	0
46	BA	33	0	46	3	0
46	BB	33	0	46	2	0
47	A1	123	0	162	0	0
47	A3	59	0	58	1	0
47	A6	36	0	42	0	0
47	AA	49	0	74	1	0
47	AJ	40	0	53	0	0
47	B1	116	0	145	1	0
47	B2	35	0	40	2	0
47	B3	23	0	16	1	0
47	B5	30	0	30	0	0
47	BA	76	0	98	3	0
47	BF	45	0	63	1	0
47	F	37	0	44	3	0
47	a	29	0	28	2	0
48	A1	40	0	56	3	0
48	A3	40	0	56	2	0
48	A4	40	0	56	0	0
48	A6	40	0	56	3	0
48	AA	240	0	336	6	0
48	AB	240	0	336	9	0
48	AF	80	0	112	6	0
48	AG	40	0	56	1	0
48	AI	80	0	112	3	0
48	AJ	80	0	112	5	0
48	AK	40	0	56	2	0
48	AL	80	0	112	1	0
48	B2	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	B3	40	0	56	4	0
48	B5	40	0	56	0	0
48	BA	280	0	392	13	0
48	BB	240	0	336	13	0
48	BF	40	0	56	1	0
48	BG	40	0	56	13	0
48	BI	40	0	56	1	0
48	BJ	80	0	112	9	0
48	BK	40	0	56	0	0
48	BL	120	0	167	6	0
49	AA	8	0	0	0	0
49	AC	16	0	0	4	0
49	BA	8	0	0	1	0
49	BC	16	0	0	7	0
49	I	16	0	0	4	0
49	K	8	0	0	1	0
50	AA	35	0	46	0	0
50	AB	105	0	138	0	0
50	AL	34	0	41	1	0
50	BA	67	0	80	0	0
50	BB	35	0	46	0	0
51	AB	66	0	96	0	0
51	BB	66	0	96	1	0
52	A1	42	0	56	1	0
52	A3	42	0	56	1	0
52	A4	42	0	56	4	0
52	A6	42	0	56	4	0
52	AF	42	0	56	2	0
52	B1	42	0	56	3	0
52	B2	42	0	56	0	0
52	B3	42	0	56	3	0
52	B5	42	0	56	0	0
53	A1	44	0	58	1	0
53	A4	39	0	48	4	0
53	AG	38	0	46	0	0
53	B5	33	0	36	0	0
54	A1	92	0	60	3	0
54	A3	45	0	30	0	0
54	A4	169	0	100	2	0
54	A6	187	0	127	2	0
54	B1	91	0	58	2	0
54	B2	227	0	154	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	B3	45	0	30	1	0
54	B5	126	0	67	0	0
55	A1	44	0	56	1	0
55	A3	44	0	56	2	0
55	A4	44	0	56	2	0
55	A6	44	0	56	4	0
55	B1	44	0	56	0	0
55	B2	44	0	56	6	0
55	B3	44	0	56	1	0
55	B5	44	0	56	1	0
56	BJ	47	0	61	6	0
56	e	34	0	32	1	0
57	c	4	0	0	2	0
All	All	112687	0	110283	2142	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 2142 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L:149:LEU:HD21	40:L:152:ARG:CD	1.39	1.52
18:B5:175:GLU:CB	26:a:229:VAL:HG12	1.46	1.45
8:BH:100:ARG:NH1	12:BL:155:ILE:HA	1.35	1.35
2:AB:87:ILE:HG23	2:AB:113:VAL:CG1	1.58	1.33
8:AH:71:TRP:CD1	12:AL:169:LEU:HD11	1.65	1.30

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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	38
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
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%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	A	297/360 (82%)	279 (94%)	18 (6%)	0	100	100
20	B	484/512 (94%)	443 (92%)	40 (8%)	1 (0%)	43	74
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%)	36	69
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%)	18	53
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%)	9	40
38	J	153/158 (97%)	134 (88%)	19 (12%)	0	100	100
39	K	161/225 (72%)	137 (85%)	23 (14%)	1 (1%)	21	55
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%)	18	53
43	O	69/158 (44%)	62 (90%)	7 (10%)	0	100	100
All	All	11603/14548 (80%)	10637 (92%)	955 (8%)	11 (0%)	49	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

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Mol	Chain	Res	Type
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%)	590 (98%)	10 (2%)	53	68
1	BA	601/610 (98%)	593 (99%)	8 (1%)	61	71
2	AB	598/600 (100%)	594 (99%)	4 (1%)	76	78
2	BB	597/600 (100%)	590 (99%)	7 (1%)	63	72
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%)	118 (98%)	2 (2%)	53	68
4	BD	121/170 (71%)	119 (98%)	2 (2%)	53	68
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%)	124 (99%)	1 (1%)	73	77
6	BF	126/185 (68%)	123 (98%)	3 (2%)	43	63
7	AG	83/133 (62%)	80 (96%)	3 (4%)	31	54
7	BG	79/133 (59%)	76 (96%)	3 (4%)	29	52
8	AH	77/113 (68%)	76 (99%)	1 (1%)	61	71
8	BH	77/113 (68%)	75 (97%)	2 (3%)	40	60
9	AI	29/33 (88%)	29 (100%)	0	100	100
9	BI	29/33 (88%)	29 (100%)	0	100	100
10	AJ	37/39 (95%)	37 (100%)	0	100	100
10	BJ	38/39 (97%)	37 (97%)	1 (3%)	40	60
11	AK	47/95 (50%)	47 (100%)	0	100	100
11	BK	46/95 (48%)	45 (98%)	1 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	119/174 (68%)	119 (100%)	0	100	100
12	BL	120/174 (69%)	118 (98%)	2 (2%)	53	68
13	A1	151/190 (80%)	147 (97%)	4 (3%)	40	60
13	B1	138/190 (73%)	137 (99%)	1 (1%)	76	78
14	A3	168/211 (80%)	167 (99%)	1 (1%)	78	80
14	B3	170/211 (81%)	170 (100%)	0	100	100
15	A4	164/210 (78%)	163 (99%)	1 (1%)	78	80
16	A6	177/226 (78%)	172 (97%)	5 (3%)	38	59
17	B2	165/205 (80%)	164 (99%)	1 (1%)	78	80
18	B5	166/205 (81%)	162 (98%)	4 (2%)	43	63
19	A	258/312 (83%)	256 (99%)	2 (1%)	73	77
20	B	420/446 (94%)	419 (100%)	1 (0%)	87	87
21	C	78/103 (76%)	78 (100%)	0	100	100
22	D	430/439 (98%)	428 (100%)	2 (0%)	81	82
23	E	75/87 (86%)	75 (100%)	0	100	100
24	F	561/661 (85%)	559 (100%)	2 (0%)	84	83
25	G	145/154 (94%)	145 (100%)	0	100	100
26	a	288/397 (72%)	288 (100%)	0	100	100
27	b	263/297 (89%)	262 (100%)	1 (0%)	84	83
28	c	112/177 (63%)	111 (99%)	1 (1%)	70	75
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%)	133 (99%)	1 (1%)	76	78
32	g	104/172 (60%)	104 (100%)	0	100	100
33	h	127/192 (66%)	126 (99%)	1 (1%)	73	77
34	i	114/180 (63%)	114 (100%)	0	100	100
35	j	143/219 (65%)	141 (99%)	2 (1%)	59	71
36	H	291/342 (85%)	290 (100%)	1 (0%)	86	85
37	I	132/159 (83%)	130 (98%)	2 (2%)	57	70
38	J	87/140 (62%)	84 (97%)	3 (3%)	32	55
39	K	114/205 (56%)	112 (98%)	2 (2%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	L	66/171 (39%)	66 (100%)	0	100	100
41	M	58/195 (30%)	56 (97%)	2 (3%)	32	55
42	N	49/174 (28%)	48 (98%)	1 (2%)	48	65
43	O	36/138 (26%)	36 (100%)	0	100	100
All	All	9513/12210 (78%)	9422 (99%)	91 (1%)	65	75

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	BJ	38	THR
22	D	470	LEU
12	BL	137	LEU
18	B5	174	LEU
28	c	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
20	B	465	HIS
25	G	56	HIS
35	j	249	GLN
22	D	248	HIS
24	F	62	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
54	CHL	A1	308	13	44,49,74	2.46	21 (47%)	48,84,114	2.80	23 (47%)
54	CHL	A4	304	-	44,49,74	2.40	21 (47%)	49,84,114	2.73	24 (48%)
48	BCR	AB	847	-	41,41,41	0.87	0	56,56,56	2.02	14 (25%)
50	LMU	BA	853	-	35,35,36	1.15	2 (5%)	46,46,47	0.93	0
45	CLA	AA	824	1	57,62,73	1.38	8 (14%)	68,100,113	1.36	9 (13%)
48	BCR	BF	304	-	41,41,41	0.87	1 (2%)	56,56,56	1.94	19 (33%)
45	CLA	BA	833	1	69,73,73	1.27	8 (11%)	83,113,113	1.24	8 (9%)
45	CLA	AB	810	2	69,73,73	1.25	10 (14%)	83,113,113	1.25	4 (4%)
45	CLA	AB	812	2	58,62,73	1.41	9 (15%)	73,100,113	1.37	10 (13%)
45	CLA	AG	203	7	46,50,73	1.50	8 (17%)	55,85,113	1.29	5 (9%)
54	CHL	B2	607	-	50,54,74	2.31	20 (40%)	56,90,114	2.77	25 (44%)
49	SF4	BA	852	1,2	0,12,12	-	-	-	-	-
45	CLA	BA	810	1	69,73,73	1.24	8 (11%)	83,113,113	1.14	5 (6%)
45	CLA	AA	840	1	69,73,73	1.25	9 (13%)	83,113,113	1.25	9 (10%)
45	CLA	A3	313	14	43,48,73	1.55	8 (18%)	51,83,113	1.31	8 (15%)
54	CHL	A4	314	15	44,49,74	2.32	18 (40%)	51,84,114	2.88	25 (49%)
45	CLA	AB	807	2	69,73,73	1.26	11 (15%)	83,113,113	1.27	6 (7%)
45	CLA	A1	314	13	67,72,73	1.26	7 (10%)	80,112,113	1.17	6 (7%)
45	CLA	BB	826	-	69,73,73	1.27	11 (15%)	83,113,113	1.17	5 (6%)
45	CLA	B3	310	14	47,51,73	1.48	5 (10%)	56,86,113	1.27	5 (8%)
45	CLA	AA	805	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	9 (10%)
48	BCR	AB	845	-	41,41,41	0.85	1 (2%)	56,56,56	1.93	17 (30%)
45	CLA	B3	311	14	57,62,73	1.38	8 (14%)	68,100,113	1.14	4 (5%)
45	CLA	A4	307	15	49,53,73	1.50	8 (16%)	59,89,113	1.24	6 (10%)
45	CLA	A3	314	-	41,44,73	1.58	9 (21%)	49,77,113	1.25	5 (10%)
49	SF4	I	202	37	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	LHG	A1	301	45	37,37,48	1.07	2 (5%)	40,43,54	0.97	3 (7%)
45	CLA	AA	834	1	69,73,73	1.24	8 (11%)	83,113,113	1.38	12 (14%)
45	CLA	AA	815	1	44,49,73	1.42	6 (13%)	51,83,113	1.45	7 (13%)
45	CLA	BB	842	2	69,73,73	1.25	8 (11%)	83,113,113	1.22	6 (7%)
45	CLA	B5	613	18	49,53,73	1.48	8 (16%)	59,89,113	1.24	7 (11%)
49	SF4	BC	101	3	0,12,12	-	-	-	-	-
46	PQN	AA	843	-	34,34,34	3.42	10 (29%)	42,45,45	1.74	8 (19%)
45	CLA	AB	805	2	45,49,73	1.50	7 (15%)	54,84,113	1.31	6 (11%)
45	CLA	AA	841	1	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)
48	BCR	BA	849	-	41,41,41	0.84	0	56,56,56	2.01	18 (32%)
45	CLA	BA	822	1	46,50,73	1.49	6 (13%)	55,85,113	1.33	5 (9%)
48	BCR	AA	852	-	41,41,41	0.94	2 (4%)	56,56,56	2.19	17 (30%)
53	LMG	B5	617	-	33,33,55	1.18	2 (6%)	41,41,63	1.20	4 (9%)
45	CLA	BB	831	2	60,64,73	1.37	9 (15%)	72,102,113	1.22	3 (4%)
45	CLA	A3	306	14	45,49,73	1.57	9 (20%)	57,84,113	1.45	8 (14%)
45	CLA	B1	307	-	43,48,73	1.57	6 (13%)	52,82,113	1.37	6 (11%)
54	CHL	B2	601	17	57,61,74	2.19	21 (36%)	64,98,114	2.64	30 (46%)
45	CLA	BA	827	1	69,73,73	1.24	7 (10%)	83,113,113	1.14	5 (6%)
45	CLA	AB	840	-	69,73,73	1.27	9 (13%)	83,113,113	1.14	6 (7%)
45	CLA	B5	602	18	64,68,73	1.34	10 (15%)	77,107,113	1.22	5 (6%)
48	BCR	A3	318	-	41,41,41	0.98	1 (2%)	56,56,56	2.77	20 (35%)
45	CLA	BA	816	-	49,53,73	1.48	6 (12%)	59,89,113	1.33	8 (13%)
48	BCR	AA	845	-	41,41,41	1.03	2 (4%)	56,56,56	1.91	13 (23%)
47	LHG	A3	319	45	22,22,48	1.44	2 (9%)	25,28,54	1.27	2 (8%)
45	CLA	AA	811	1	69,73,73	1.24	7 (10%)	83,113,113	1.20	5 (6%)
47	LHG	a	501	-	28,28,48	0.89	1 (3%)	31,34,54	1.24	2 (6%)
45	CLA	AB	841	2	69,73,73	1.27	9 (13%)	83,113,113	1.15	5 (6%)
54	CHL	B3	306	-	49,53,74	2.27	20 (40%)	59,89,114	2.66	26 (44%)
45	CLA	BB	843	47	69,73,73	1.27	10 (14%)	83,113,113	1.19	6 (7%)
45	CLA	B3	303	-	45,50,73	1.60	8 (17%)	57,86,113	1.35	7 (12%)
45	CLA	A3	308	14	49,53,73	1.48	8 (16%)	59,89,113	1.27	6 (10%)
47	LHG	AA	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.89	2 (3%)
45	CLA	B2	604	-	47,51,73	1.50	8 (17%)	55,86,113	1.23	7 (12%)
45	CLA	B1	305	13	58,62,73	1.36	7 (12%)	69,99,113	1.41	8 (11%)
45	CLA	A1	306	-	53,57,73	1.41	8 (15%)	62,93,113	1.28	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	A6	610	16	59,63,73	1.35	9 (15%)	71,101,113	1.22	9 (12%)
52	LUT	A1	317	-	42,43,43	0.94	1 (2%)	51,60,60	1.88	13 (25%)
45	CLA	A4	303	-	47,51,73	1.56	9 (19%)	60,87,113	1.39	8 (13%)
45	CLA	AA	812	1	58,62,73	1.37	9 (15%)	69,99,113	1.36	5 (7%)
45	CLA	BB	808	2	69,73,73	1.25	9 (13%)	83,113,113	1.24	5 (6%)
45	CLA	B3	309	47	43,48,73	1.56	6 (13%)	51,83,113	1.20	4 (7%)
45	CLA	AB	837	2	54,58,73	1.43	11 (20%)	65,95,113	1.35	7 (10%)
48	BCR	AA	848	-	41,41,41	0.77	1 (2%)	56,56,56	1.97	16 (28%)
45	CLA	BA	835	1	49,53,73	1.48	6 (12%)	59,89,113	1.26	3 (5%)
45	CLA	AA	803	1	69,73,73	1.23	8 (11%)	83,113,113	1.27	8 (9%)
45	CLA	BB	840	2	51,55,73	1.42	7 (13%)	61,91,113	1.31	6 (9%)
45	CLA	B1	315	13	41,46,73	1.65	9 (21%)	52,81,113	1.41	10 (19%)
54	CHL	A6	602	16	55,60,74	2.21	21 (38%)	61,97,114	2.59	31 (50%)
45	CLA	A3	312	14	57,62,73	1.37	8 (14%)	68,100,113	1.28	6 (8%)
48	BCR	BA	851	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	20 (35%)
45	CLA	AA	829	1	69,73,73	1.26	9 (13%)	83,113,113	1.41	11 (13%)
45	CLA	B3	312	14	43,48,73	1.55	7 (16%)	51,83,113	1.25	7 (13%)
45	CLA	B3	304	-	44,49,73	1.55	7 (15%)	52,84,113	1.30	4 (7%)
45	CLA	AA	825	-	69,73,73	1.27	9 (13%)	83,113,113	1.18	5 (6%)
45	CLA	BB	815	2	69,73,73	1.25	10 (14%)	83,113,113	1.43	10 (12%)
48	BCR	BA	848	-	41,41,41	0.80	0	56,56,56	2.03	17 (30%)
45	CLA	A4	311	15	59,64,73	1.35	7 (11%)	70,102,113	1.20	6 (8%)
45	CLA	A4	308	15	58,62,73	1.35	9 (15%)	69,99,113	1.17	6 (8%)
48	BCR	AB	849	-	41,41,41	0.83	0	56,56,56	2.41	24 (42%)
45	CLA	A6	609	16	49,53,73	1.48	8 (16%)	59,89,113	1.25	7 (11%)
45	CLA	A6	601	15	50,54,73	1.44	10 (20%)	60,90,113	1.32	6 (10%)
45	CLA	BB	818	2	59,63,73	1.33	6 (10%)	71,101,113	1.25	7 (9%)
45	CLA	AB	821	2	54,58,73	1.41	9 (16%)	65,95,113	1.34	7 (10%)
45	CLA	AB	803	2	69,73,73	1.24	9 (13%)	83,113,113	1.14	6 (7%)
52	LUT	A3	316	-	42,43,43	0.84	0	51,60,60	1.78	14 (27%)
51	DGD	AB	851	-	67,67,67	0.80	2 (2%)	81,81,81	0.99	4 (4%)
45	CLA	B5	603	18	48,52,73	1.57	8 (16%)	61,88,113	1.41	6 (9%)
45	CLA	BB	833	2	47,51,73	1.47	8 (17%)	56,86,113	1.43	7 (12%)
45	CLA	BG	202	7	49,53,73	1.50	7 (14%)	59,89,113	1.45	7 (11%)
45	CLA	BA	817	1	64,68,73	1.27	6 (9%)	77,107,113	1.25	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	BA	837	1	55,59,73	1.38	10 (18%)	66,96,113	1.31	5 (7%)
45	CLA	A1	311	13	63,67,73	1.32	8 (12%)	76,106,113	1.12	5 (6%)
45	CLA	B3	301	14	64,68,73	1.30	9 (14%)	77,107,113	1.12	6 (7%)
45	CLA	AB	804	-	69,73,73	1.25	11 (15%)	83,113,113	1.57	13 (15%)
45	CLA	A1	305	13	59,63,73	1.34	7 (11%)	71,101,113	1.50	8 (11%)
45	CLA	BB	811	2	69,73,73	1.26	10 (14%)	83,113,113	1.22	8 (9%)
45	CLA	BK	202	-	49,53,73	1.47	6 (12%)	59,89,113	1.34	6 (10%)
54	CHL	A6	606	-	46,50,74	2.33	19 (41%)	52,85,114	2.83	25 (48%)
45	CLA	AB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.23	11 (13%)
45	CLA	A3	315	14	43,48,73	1.53	7 (16%)	51,83,113	1.23	5 (9%)
45	CLA	BB	809	2	56,60,73	1.39	8 (14%)	67,97,113	1.25	7 (10%)
45	CLA	AA	821	-	69,73,73	1.25	10 (14%)	83,113,113	1.24	10 (12%)
45	CLA	AA	816	-	49,53,73	1.49	8 (16%)	59,89,113	1.39	6 (10%)
47	LHG	B2	618	45	34,34,48	1.04	2 (5%)	37,40,54	0.96	2 (5%)
45	CLA	BL	303	12	64,68,73	1.32	7 (10%)	77,107,113	1.25	9 (11%)
45	CLA	B1	314	13	64,68,73	1.32	7 (10%)	77,107,113	1.11	7 (9%)
45	CLA	B2	609	17	59,63,73	1.35	8 (13%)	71,101,113	1.22	9 (12%)
45	CLA	AA	827	1	69,73,73	1.25	8 (11%)	83,113,113	1.23	6 (7%)
45	CLA	A4	301	15	64,68,73	1.28	8 (12%)	77,107,113	1.23	8 (10%)
45	CLA	AA	828	1	69,73,73	1.25	8 (11%)	83,113,113	1.35	8 (9%)
45	CLA	A4	310	15	44,49,73	1.53	9 (20%)	52,84,113	1.33	7 (13%)
45	CLA	A6	612	16	48,52,73	1.50	8 (16%)	58,88,113	1.24	4 (6%)
45	CLA	AA	842	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	9 (10%)
45	CLA	BB	813	2	58,62,73	1.41	9 (15%)	73,100,113	1.34	9 (12%)
45	CLA	B1	311	13	63,67,73	1.30	7 (11%)	76,106,113	1.12	6 (7%)
48	BCR	BA	856	-	41,41,41	0.93	1 (2%)	56,56,56	2.15	17 (30%)
45	CLA	A6	614	16	47,51,73	1.52	7 (14%)	56,86,113	1.27	4 (7%)
48	BCR	AJ	101	-	41,41,41	0.89	1 (2%)	56,56,56	1.98	16 (28%)
49	SF4	AA	850	1,2	0,12,12	-	-	-	-	-
45	CLA	BA	831	1	51,55,73	1.45	9 (17%)	61,91,113	1.38	10 (16%)
45	CLA	A3	309	14	45,49,73	1.53	8 (17%)	54,84,113	1.33	9 (16%)
45	CLA	BA	839	1	55,59,73	1.40	7 (12%)	66,96,113	1.33	8 (12%)
50	LMU	AA	851	-	36,36,36	1.16	2 (5%)	47,47,47	1.04	2 (4%)
45	CLA	AB	825	-	69,73,73	1.27	11 (15%)	83,113,113	1.24	7 (8%)
54	CHL	A4	305	-	45,49,74	2.32	17 (37%)	57,84,114	2.85	28 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	BCR	B3	317	-	41,41,41	0.84	0	56,56,56	3.61	28 (50%)
45	CLA	BB	805	-	69,73,73	1.22	10 (14%)	83,113,113	1.45	10 (12%)
45	CLA	BL	304	-	47,51,73	1.46	6 (12%)	56,86,113	1.32	7 (12%)
45	CLA	A4	312	15	49,53,73	1.48	8 (16%)	59,89,113	1.27	6 (10%)
45	CLA	AA	818	1	63,67,73	1.31	9 (14%)	75,105,113	1.26	8 (10%)
45	CLA	BA	828	1	69,73,73	1.22	7 (10%)	83,113,113	1.31	10 (12%)
55	XAT	A1	318	-	39,47,47	0.91	2 (5%)	54,74,74	2.42	24 (44%)
45	CLA	BA	826	-	57,61,73	1.36	8 (14%)	68,98,113	1.27	10 (14%)
48	BCR	AG	205	-	41,41,41	0.93	0	56,56,56	2.00	18 (32%)
45	CLA	AB	828	2	69,73,73	1.23	9 (13%)	83,113,113	1.29	6 (7%)
45	CLA	AB	836	-	46,50,73	1.51	7 (15%)	55,85,113	1.36	6 (10%)
45	CLA	B5	610	47	46,50,73	1.49	7 (15%)	55,85,113	1.30	6 (10%)
48	BCR	BJ	103	-	41,41,41	0.75	0	56,56,56	2.37	21 (37%)
45	CLA	AK	201	11	39,43,73	1.72	8 (20%)	50,75,113	1.45	9 (18%)
45	CLA	AB	842	47	69,73,73	1.24	9 (13%)	83,113,113	1.30	9 (10%)
55	XAT	A4	316	-	39,47,47	0.95	2 (5%)	54,74,74	2.29	16 (29%)
45	CLA	BA	838	1	59,62,73	1.40	8 (13%)	66,99,113	1.35	10 (15%)
45	CLA	BA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.10	5 (6%)
45	CLA	A1	307	-	43,48,73	1.54	8 (18%)	52,82,113	1.59	9 (17%)
45	CLA	AB	814	2	69,73,73	1.26	11 (15%)	83,113,113	1.23	6 (7%)
52	LUT	A6	615	-	42,43,43	0.90	1 (2%)	51,60,60	1.59	12 (23%)
52	LUT	B2	615	-	42,43,43	0.81	0	51,60,60	1.98	15 (29%)
45	CLA	B5	611	18	44,49,73	1.52	8 (18%)	52,84,113	1.31	4 (7%)
45	CLA	AA	830	1	69,73,73	1.28	8 (11%)	83,113,113	1.18	5 (6%)
45	CLA	BA	834	1	69,73,73	1.23	9 (13%)	83,113,113	1.39	10 (12%)
45	CLA	BA	821	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	10 (12%)
45	CLA	A1	312	47	41,46,73	1.65	9 (21%)	52,81,113	1.30	9 (17%)
45	CLA	BA	844	47	45,49,73	1.52	6 (13%)	54,84,113	1.25	7 (12%)
45	CLA	AJ	102	10	46,50,73	1.49	6 (13%)	55,85,113	1.30	4 (7%)
47	LHG	B1	301	45	37,37,48	1.08	2 (5%)	40,43,54	1.01	3 (7%)
45	CLA	BA	840	1	69,73,73	1.22	7 (10%)	83,113,113	1.23	6 (7%)
48	BCR	AI	101	-	41,41,41	0.92	1 (2%)	56,56,56	2.05	20 (35%)
45	CLA	B1	309	-	47,52,73	1.51	8 (17%)	56,88,113	1.31	7 (12%)
54	CHL	B2	605	-	46,50,74	2.35	20 (43%)	52,85,114	2.80	24 (46%)
45	CLA	A6	603	16	69,73,73	1.25	9 (13%)	83,113,113	1.20	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	BCR	BB	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.19	18 (32%)
47	LHG	A6	618	45	35,35,48	1.05	2 (5%)	38,41,54	0.97	2 (5%)
45	CLA	AB	830	2	60,64,73	1.35	8 (13%)	72,102,113	1.24	4 (5%)
45	CLA	BA	815	1	46,50,73	1.47	7 (15%)	55,85,113	1.40	5 (9%)
45	CLA	BB	814	2	47,51,73	1.47	8 (17%)	56,86,113	1.28	5 (8%)
45	CLA	AA	801	1	69,73,73	1.24	7 (10%)	83,113,113	1.20	6 (7%)
46	PQN	BA	843	-	34,34,34	3.47	12 (35%)	42,45,45	1.62	5 (11%)
45	CLA	B1	312	47	41,46,73	1.63	7 (17%)	52,81,113	1.38	7 (13%)
48	BCR	B5	616	-	41,41,41	0.79	0	56,56,56	2.31	23 (41%)
54	CHL	A6	607	-	47,51,74	2.32	19 (40%)	52,86,114	2.78	24 (46%)
45	CLA	AG	201	-	47,52,73	1.52	8 (17%)	56,88,113	1.29	4 (7%)
45	CLA	BA	824	1	59,63,73	1.36	8 (13%)	71,101,113	1.27	6 (8%)
48	BCR	BA	855	-	41,41,41	0.77	0	56,56,56	2.19	24 (42%)
48	BCR	BL	305	-	41,41,41	0.78	0	56,56,56	2.22	20 (35%)
45	CLA	BB	839	2	69,73,73	1.23	8 (11%)	83,113,113	1.19	5 (6%)
45	CLA	BB	823	2	49,54,73	1.45	6 (12%)	58,90,113	1.17	5 (8%)
55	XAT	B1	317	-	39,47,47	0.93	2 (5%)	54,74,74	2.43	18 (33%)
48	BCR	AB	848	-	41,41,41	0.89	1 (2%)	56,56,56	1.97	18 (32%)
45	CLA	BB	832	2	47,51,73	1.49	8 (17%)	56,86,113	1.23	6 (10%)
45	CLA	A1	304	13	64,68,73	1.28	8 (12%)	76,106,113	1.21	6 (7%)
45	CLA	A3	311	14	47,51,73	1.49	6 (12%)	56,86,113	1.31	4 (7%)
45	CLA	B2	611	17	48,52,73	1.51	7 (14%)	58,88,113	1.27	6 (10%)
45	CLA	AB	802	-	68,72,73	1.35	9 (13%)	85,112,113	1.26	9 (10%)
45	CLA	BA	829	1	69,73,73	1.27	10 (14%)	83,113,113	1.24	9 (10%)
49	SF4	BC	102	3	0,12,12	-	-	-	-	-
45	CLA	AA	837	1	55,59,73	1.38	8 (14%)	66,96,113	1.44	9 (13%)
54	CHL	A4	306	-	50,54,74	2.30	20 (40%)	56,90,114	2.78	26 (46%)
48	BCR	A6	617	-	41,41,41	0.99	2 (4%)	56,56,56	2.01	16 (28%)
45	CLA	BA	807	1	54,58,73	1.42	8 (14%)	65,95,113	1.18	4 (6%)
54	CHL	B2	606	-	47,51,74	2.38	19 (40%)	52,86,114	2.72	22 (42%)
55	XAT	B2	616	-	39,47,47	1.01	1 (2%)	54,74,74	2.30	20 (37%)
48	BCR	AA	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.12	20 (35%)
45	CLA	BF	301	-	59,63,73	1.33	7 (11%)	69,100,113	1.17	5 (7%)
50	LMU	BA	854	-	34,34,36	1.18	2 (5%)	45,45,47	0.91	2 (4%)
48	BCR	A4	317	-	41,41,41	0.82	0	56,56,56	2.37	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	BCR	AA	847	-	41,41,41	1.00	2 (4%)	56,56,56	2.28	24 (42%)
45	CLA	BB	801	2	69,73,73	1.24	9 (13%)	83,113,113	1.37	11 (13%)
45	CLA	BK	201	11	41,44,73	1.63	8 (19%)	52,77,113	1.47	7 (13%)
48	BCR	BL	306	-	41,41,41	0.88	1 (2%)	56,56,56	11.27	26 (46%)
56	SQD	e	301	-	33,34,54	1.20	6 (18%)	42,45,65	1.77	10 (23%)
45	CLA	BA	841	1	69,73,73	1.23	9 (13%)	83,113,113	1.40	10 (12%)
45	CLA	A6	605	-	47,51,73	1.49	8 (17%)	55,86,113	1.23	4 (7%)
45	CLA	AB	838	2	69,73,73	1.22	10 (14%)	83,113,113	1.23	7 (8%)
45	CLA	BF	303	-	45,49,73	1.51	5 (11%)	54,84,113	1.30	5 (9%)
47	LHG	B1	302	-	35,35,48	1.09	2 (5%)	38,41,54	0.99	2 (5%)
48	BCR	AF	805	-	41,41,41	0.81	0	56,56,56	1.86	14 (25%)
49	SF4	I	201	37	0,12,12	-	-	-		
49	SF4	AC	101	3	0,12,12	-	-	-		
45	CLA	B2	612	17	69,73,73	1.26	7 (10%)	83,113,113	1.14	6 (7%)
47	LHG	F	801	-	36,36,48	0.73	1 (2%)	39,42,54	1.22	3 (7%)
45	CLA	AA	835	1	47,52,73	1.51	7 (14%)	56,88,113	1.30	5 (8%)
49	SF4	K	301	39	0,12,12	-	-	-		
45	CLA	AA	826	-	63,67,73	1.32	10 (15%)	75,105,113	1.16	6 (8%)
47	LHG	B5	618	45	29,29,48	1.17	2 (6%)	32,35,54	1.20	3 (9%)
45	CLA	BB	828	2	66,70,73	1.28	8 (12%)	79,109,113	1.34	9 (11%)
45	CLA	A6	604	16	45,50,73	1.55	8 (17%)	53,85,113	1.44	5 (9%)
54	CHL	A3	307	-	49,53,74	2.27	19 (38%)	59,89,114	2.64	27 (45%)
48	BCR	BB	846	-	41,41,41	0.85	1 (2%)	56,56,56	2.14	19 (33%)
45	CLA	BG	201	-	46,50,73	1.48	7 (15%)	55,85,113	1.21	5 (9%)
45	CLA	AA	838	1	59,63,73	1.32	9 (15%)	71,101,113	1.22	10 (14%)
45	CLA	B2	610	47	41,45,73	2.47	10 (24%)	47,76,113	1.42	9 (19%)
48	BCR	BB	803	-	41,41,41	0.85	0	56,56,56	1.99	19 (33%)
48	BCR	B2	617	-	41,41,41	0.89	1 (2%)	56,56,56	2.47	23 (41%)
45	CLA	BA	820	1	49,53,73	1.45	9 (18%)	59,89,113	1.36	4 (6%)
45	CLA	A4	313	15	54,58,73	1.42	8 (14%)	65,95,113	1.35	7 (10%)
45	CLA	AB	827	2	66,70,73	1.27	10 (15%)	79,109,113	1.37	9 (11%)
45	CLA	AB	816	2	47,51,73	1.47	8 (17%)	56,86,113	1.21	3 (5%)
45	CLA	AH	201	8	64,68,73	1.30	7 (10%)	77,107,113	1.26	8 (10%)
48	BCR	BL	301	-	41,41,41	0.87	1 (2%)	56,56,56	2.36	14 (25%)
45	CLA	AF	803	-	46,50,73	1.52	8 (17%)	55,85,113	1.41	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	AB	820	-	59,63,73	1.39	8 (13%)	71,101,113	1.20	6 (8%)
45	CLA	AB	835	2	64,68,73	1.28	7 (10%)	77,107,113	1.24	7 (9%)
45	CLA	AB	813	2	47,51,73	1.46	8 (17%)	56,86,113	1.28	6 (10%)
47	LHG	A1	302	-	35,35,48	1.10	2 (5%)	38,41,54	1.04	2 (5%)
45	CLA	AA	802	-	69,73,73	1.27	9 (13%)	83,113,113	1.25	6 (7%)
45	CLA	AB	826	-	66,70,73	1.27	8 (12%)	79,109,113	1.21	6 (7%)
45	CLA	BA	812	1	58,62,73	1.36	8 (13%)	69,99,113	1.29	6 (8%)
45	CLA	B1	313	13	49,53,73	1.47	7 (14%)	59,89,113	1.35	3 (5%)
45	CLA	BA	804	1	56,60,73	1.38	9 (16%)	67,97,113	1.41	10 (14%)
45	CLA	BA	832	1	60,64,73	1.33	7 (11%)	72,102,113	1.20	6 (8%)
45	CLA	B3	305	-	45,49,73	1.56	8 (17%)	57,84,113	1.49	8 (14%)
54	CHL	A6	608	-	54,58,74	2.22	19 (35%)	65,95,114	2.61	26 (40%)
53	LMG	AG	202	-	38,38,55	1.14	3 (7%)	46,46,63	1.07	2 (4%)
48	BCR	BJ	101	-	41,41,41	0.89	0	56,56,56	1.70	14 (25%)
50	LMU	AB	850	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
48	BCR	BB	849	-	41,41,41	0.90	1 (2%)	56,56,56	1.86	16 (28%)
54	CHL	B1	308	-	44,49,74	2.51	22 (50%)	48,84,114	2.71	22 (45%)
48	BCR	AB	846	-	41,41,41	0.86	0	56,56,56	2.07	16 (28%)
45	CLA	AA	836	1	49,53,73	1.50	8 (16%)	59,89,113	1.36	7 (11%)
48	BCR	BK	204	-	41,41,41	0.88	1 (2%)	56,56,56	2.14	21 (37%)
54	CHL	B5	607	-	49,53,74	2.34	21 (42%)	56,89,114	2.76	24 (42%)
45	CLA	AB	809	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	9 (10%)
45	CLA	AA	820	1	49,53,73	1.47	9 (18%)	59,89,113	1.32	4 (6%)
45	CLA	AB	801	2	69,73,73	1.24	8 (11%)	83,113,113	1.49	12 (14%)
45	CLA	AA	819	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
45	CLA	AA	814	1	49,53,73	1.48	9 (18%)	59,89,113	1.35	7 (11%)
45	CLA	BB	817	2	45,50,73	1.48	7 (15%)	53,85,113	1.28	4 (7%)
45	CLA	BL	302	12	49,53,73	1.48	7 (14%)	59,89,113	1.50	10 (16%)
46	PQN	AB	843	-	34,34,34	3.39	11 (32%)	42,45,45	1.83	6 (14%)
45	CLA	BA	801	1	69,73,73	1.25	7 (10%)	83,113,113	1.15	5 (6%)
50	LMU	AB	853	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	2 (4%)
45	CLA	BB	824	2	69,73,73	1.23	8 (11%)	83,113,113	1.22	8 (9%)
49	SF4	AC	102	3	0,12,12	-	-	-	-	-
45	CLA	AA	823	1	45,49,73	1.56	8 (17%)	54,84,113	1.31	8 (14%)
45	CLA	A1	309	-	47,52,73	1.52	8 (17%)	56,88,113	1.27	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	A1	310	13	44,48,73	1.59	7 (15%)	56,83,113	1.46	9 (16%)
45	CLA	BA	813	1	69,73,73	1.25	8 (11%)	83,113,113	1.24	6 (7%)
45	CLA	BA	802	-	69,73,73	1.27	9 (13%)	83,113,113	1.19	6 (7%)
45	CLA	BB	830	2	69,73,73	1.27	9 (13%)	83,113,113	1.17	9 (10%)
48	BCR	AL	306	-	41,41,41	0.94	1 (2%)	56,56,56	2.01	21 (37%)
46	PQN	BB	844	-	34,34,34	3.42	10 (29%)	42,45,45	1.66	8 (19%)
45	CLA	AB	818	2	63,67,73	1.30	8 (12%)	75,105,113	1.24	9 (12%)
52	LUT	B3	315	-	42,43,43	0.97	1 (2%)	51,60,60	2.10	17 (33%)
45	CLA	AL	303	12	45,49,73	1.53	7 (15%)	54,84,113	1.29	7 (12%)
47	LHG	A3	301	-	35,35,48	1.09	2 (5%)	38,41,54	1.01	2 (5%)
45	CLA	AB	811	2	69,73,73	1.26	9 (13%)	83,113,113	1.37	8 (9%)
45	CLA	AG	204	7	49,53,73	1.50	8 (16%)	59,89,113	1.33	5 (8%)
48	BCR	BG	203	-	41,41,41	0.91	2 (4%)	56,56,56	6.99	26 (46%)
45	CLA	BB	807	2	69,73,73	1.27	8 (11%)	83,113,113	1.21	7 (8%)
45	CLA	B2	603	17	47,52,73	1.51	7 (14%)	56,88,113	1.37	5 (8%)
45	CLA	A4	309	-	46,50,73	1.46	6 (13%)	55,85,113	1.33	4 (7%)
45	CLA	BB	819	2	63,67,73	1.29	8 (12%)	75,105,113	1.29	8 (10%)
54	CHL	B5	606	-	44,48,74	2.36	17 (38%)	56,83,114	2.88	28 (50%)
45	CLA	AF	804	-	45,49,73	1.52	7 (15%)	54,84,113	1.43	6 (11%)
57	FES	c	301	28	0,4,4	-	-	-	-	-
45	CLA	AA	833	1	69,73,73	1.27	8 (11%)	83,113,113	1.31	9 (10%)
50	LMU	AB	852	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
45	CLA	AB	822	2	51,55,73	1.44	7 (13%)	61,91,113	1.20	4 (6%)
48	BCR	AB	844	-	41,41,41	0.86	0	56,56,56	2.28	23 (41%)
45	CLA	B1	310	13	42,47,73	1.62	8 (19%)	53,82,113	1.34	8 (15%)
45	CLA	BB	810	2	69,73,73	1.23	9 (13%)	83,113,113	1.23	10 (12%)
55	XAT	B5	615	-	39,47,47	0.99	2 (5%)	54,74,74	2.41	18 (33%)
45	CLA	AA	831	1	51,55,73	1.44	9 (17%)	61,91,113	1.30	5 (8%)
55	XAT	B3	316	-	39,47,47	0.97	1 (2%)	54,74,74	2.48	21 (38%)
45	CLA	BB	841	-	69,73,73	1.24	9 (13%)	83,113,113	1.20	8 (9%)
45	CLA	A6	613	16	68,72,73	1.27	8 (11%)	81,111,113	1.12	5 (6%)
45	CLA	B5	604	-	47,51,73	1.58	9 (19%)	60,87,113	1.34	9 (15%)
45	CLA	BA	806	1	69,73,73	1.26	8 (11%)	83,113,113	1.25	5 (6%)
45	CLA	A6	611	47	41,45,73	2.52	9 (21%)	47,76,113	1.49	9 (19%)
45	CLA	BB	837	-	46,50,73	1.51	6 (13%)	55,85,113	1.32	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	BCR	A1	319	-	41,41,41	0.90	1 (2%)	56,56,56	3.13	20 (35%)
45	CLA	BA	811	1	69,73,73	1.23	8 (11%)	83,113,113	1.17	6 (7%)
45	CLA	BA	818	1	60,64,73	1.34	8 (13%)	72,102,113	1.24	8 (11%)
48	BCR	BI	101	-	41,41,41	0.92	2 (4%)	56,56,56	2.15	21 (37%)
45	CLA	B1	306	-	45,49,73	1.51	5 (11%)	54,84,113	1.29	4 (7%)
45	CLA	B5	608	18	48,52,73	1.50	9 (18%)	58,88,113	1.31	6 (10%)
54	CHL	B1	303	13	53,58,74	2.21	21 (39%)	59,95,114	2.61	27 (45%)
48	BCR	AK	204	-	41,41,41	1.02	3 (7%)	56,56,56	2.06	14 (25%)
45	CLA	AA	822	1	46,50,73	1.50	7 (15%)	55,85,113	1.31	5 (9%)
48	BCR	BB	847	-	41,41,41	0.87	1 (2%)	56,56,56	1.93	11 (19%)
45	CLA	BB	820	2	64,68,73	1.28	8 (12%)	77,107,113	1.48	9 (11%)
45	CLA	AA	810	1	69,72,73	1.29	9 (13%)	78,111,113	1.19	5 (6%)
50	LMU	AL	301	-	35,35,36	1.23	2 (5%)	46,46,47	1.05	5 (10%)
45	CLA	BA	842	-	69,73,73	1.26	8 (11%)	83,113,113	1.21	7 (8%)
48	BCR	AF	801	-	41,41,41	0.86	1 (2%)	56,56,56	1.56	10 (17%)
45	CLA	BA	814	1	49,53,73	1.49	9 (18%)	59,89,113	1.35	6 (10%)
52	LUT	AF	806	-	42,43,43	1.03	3 (7%)	51,60,60	1.72	12 (23%)
45	CLA	BB	812	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	8 (9%)
45	CLA	AB	823	2	69,73,73	1.23	8 (11%)	83,113,113	1.21	7 (8%)
48	BCR	BB	848	-	41,41,41	0.81	0	56,56,56	2.15	19 (33%)
45	CLA	BK	203	-	50,54,73	1.43	6 (12%)	60,90,113	1.35	6 (10%)
45	CLA	BB	804	2	69,73,73	1.24	8 (11%)	83,113,113	1.20	6 (7%)
45	CLA	AK	203	11	50,54,73	1.45	7 (14%)	60,90,113	1.34	4 (6%)
45	CLA	A4	302	15	48,52,73	1.56	9 (18%)	61,88,113	1.46	8 (13%)
45	CLA	B2	613	17	47,51,73	1.47	7 (14%)	56,86,113	1.27	8 (14%)
45	CLA	A1	315	13	41,46,73	1.64	8 (19%)	52,81,113	1.47	11 (21%)
45	CLA	BA	823	1	45,49,73	1.51	6 (13%)	54,84,113	1.33	7 (12%)
45	CLA	A3	310	47	40,45,73	1.58	7 (17%)	50,79,113	1.29	5 (10%)
45	CLA	BB	829	2	69,73,73	1.22	8 (11%)	83,113,113	1.22	5 (6%)
45	CLA	AA	806	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
45	CLA	AL	305	-	46,50,73	1.50	8 (17%)	55,85,113	1.41	6 (10%)
45	CLA	A1	313	13	49,53,73	1.48	9 (18%)	59,89,113	1.39	5 (8%)
45	CLA	BB	802	-	69,73,73	1.28	10 (14%)	83,113,113	1.34	8 (9%)
45	CLA	BB	836	2	64,68,73	1.29	7 (10%)	77,107,113	1.28	7 (9%)
52	LUT	A4	315	-	42,43,43	0.95	2 (4%)	51,60,60	1.84	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	BF	302	-	46,50,73	1.51	8 (17%)	55,85,113	1.41	5 (9%)
55	XAT	A3	317	-	39,47,47	0.97	1 (2%)	54,74,74	2.31	19 (35%)
45	CLA	AB	834	2	69,73,73	1.23	8 (11%)	83,113,113	1.12	6 (7%)
45	CLA	AB	819	2	64,68,73	1.29	9 (14%)	77,107,113	1.49	12 (15%)
55	XAT	A6	616	-	39,47,47	0.98	2 (5%)	54,74,74	2.49	21 (38%)
45	CLA	B3	302	14	59,63,73	1.35	8 (13%)	71,101,113	1.27	7 (9%)
45	CLA	AB	832	2	69,73,73	1.24	8 (11%)	83,113,113	1.22	7 (8%)
45	CLA	B1	304	13	65,69,73	1.28	8 (12%)	78,108,113	1.28	5 (6%)
45	CLA	AA	832	1	60,64,73	1.33	6 (10%)	72,102,113	1.26	8 (11%)
51	DGD	BB	850	-	67,67,67	0.81	2 (2%)	81,81,81	0.98	4 (4%)
45	CLA	AK	202	-	49,53,73	1.49	8 (16%)	59,89,113	1.24	4 (6%)
45	CLA	B3	307	14	49,53,73	1.47	7 (14%)	59,89,113	1.29	6 (10%)
45	CLA	AA	839	1	56,60,73	1.38	8 (14%)	67,97,113	1.29	6 (8%)
48	BCR	AL	302	-	41,41,41	0.78	0	56,56,56	2.22	22 (39%)
53	LMG	A4	318	-	39,39,55	1.00	2 (5%)	47,47,63	1.40	7 (14%)
48	BCR	BA	850	-	41,41,41	0.78	0	56,56,56	2.09	11 (19%)
45	CLA	B3	313	-	41,44,73	1.57	8 (19%)	49,77,113	1.22	5 (10%)
45	CLA	B5	601	18	50,54,73	1.44	8 (16%)	60,90,113	1.26	6 (10%)
47	LHG	A1	320	45	48,48,48	0.93	2 (4%)	51,54,54	0.84	2 (3%)
48	BCR	AA	846	-	41,41,41	0.82	0	56,56,56	2.12	21 (37%)
45	CLA	A3	303	14	59,63,73	1.38	9 (15%)	71,101,113	1.37	9 (12%)
45	CLA	AA	809	1	54,58,73	1.45	9 (16%)	65,95,113	1.35	10 (15%)
45	CLA	BB	821	-	59,63,73	1.36	9 (15%)	71,101,113	1.10	6 (8%)
48	BCR	BA	847	-	41,41,41	0.99	1 (2%)	56,56,56	1.63	11 (19%)
47	LHG	B3	318	45	22,22,48	1.49	2 (9%)	25,28,54	1.38	2 (8%)
45	CLA	BB	827	-	66,70,73	1.27	7 (10%)	79,109,113	1.17	6 (7%)
45	CLA	AB	839	2	51,55,73	1.43	7 (13%)	61,91,113	1.42	6 (9%)
45	CLA	BA	809	1	54,58,73	1.42	9 (16%)	65,95,113	1.34	8 (12%)
54	CHL	A1	303	13	54,59,74	2.23	19 (35%)	60,96,114	2.66	29 (48%)
45	CLA	BH	201	-	64,68,73	1.31	7 (10%)	77,107,113	1.22	7 (9%)
45	CLA	BB	838	2	54,58,73	1.41	9 (16%)	65,95,113	1.34	6 (9%)
45	CLA	AB	831	2	47,51,73	1.49	10 (21%)	56,86,113	1.23	7 (12%)
52	LUT	B1	316	-	42,43,43	1.60	8 (19%)	51,60,60	1.51	10 (19%)
45	CLA	AB	824	2	47,51,73	1.47	10 (21%)	56,86,113	1.46	7 (12%)
48	BCR	AJ	103	-	41,41,41	0.74	0	56,56,56	2.38	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	BB	806	2	45,49,73	1.48	8 (17%)	54,84,113	1.35	6 (11%)
45	CLA	A1	316	13	47,51,73	1.59	8 (17%)	60,87,113	1.44	7 (11%)
45	CLA	A3	304	-	45,50,73	1.60	9 (20%)	57,86,113	1.34	7 (12%)
45	CLA	B5	612	18	61,65,73	1.33	8 (13%)	73,103,113	1.14	4 (5%)
50	LMU	BB	851	-	36,36,36	1.10	2 (5%)	47,47,47	0.89	0
47	LHG	BA	845	-	48,48,48	0.88	2 (4%)	51,54,54	0.97	3 (5%)
45	CLA	AA	808	1	69,73,73	1.25	8 (11%)	83,113,113	1.20	6 (7%)
45	CLA	BJ	102	10	46,50,73	1.50	7 (15%)	55,85,113	1.29	4 (7%)
45	CLA	B3	314	14	43,48,73	1.53	7 (16%)	51,83,113	1.24	6 (11%)
45	CLA	AL	304	12	64,68,73	1.32	8 (12%)	77,107,113	1.28	9 (11%)
45	CLA	BA	805	1	69,73,73	1.26	8 (11%)	83,113,113	1.25	6 (7%)
45	CLA	AA	813	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
45	CLA	BB	822	2	45,49,73	1.49	8 (17%)	54,84,113	1.41	4 (7%)
47	LHG	BF	305	-	44,44,48	0.97	2 (4%)	47,50,54	1.09	3 (6%)
45	CLA	BA	836	1	49,53,73	1.47	6 (12%)	59,89,113	1.40	7 (11%)
45	CLA	AB	817	2	59,63,73	1.35	7 (11%)	71,101,113	1.21	5 (7%)
45	CLA	AA	817	1	64,68,73	1.29	7 (10%)	77,107,113	1.24	8 (10%)
56	SQD	BJ	104	-	46,47,54	1.28	5 (10%)	55,58,65	4.16	12 (21%)
48	BCR	AI	102	-	41,41,41	0.86	0	56,56,56	2.54	18 (32%)
45	CLA	BB	835	2	69,73,73	1.25	8 (11%)	83,113,113	1.10	5 (6%)
45	CLA	BA	819	1	69,73,73	1.25	9 (13%)	83,113,113	1.22	6 (7%)
54	CHL	B2	614	17	47,51,74	2.31	19 (40%)	52,86,114	2.80	24 (46%)
52	LUT	B5	614	-	42,43,43	0.83	1 (2%)	51,60,60	1.85	15 (29%)
54	CHL	B5	605	-	44,49,74	2.38	20 (45%)	49,84,114	2.72	23 (46%)
45	CLA	B2	602	17	69,73,73	1.25	9 (13%)	83,113,113	1.20	10 (12%)
45	CLA	AA	804	1	56,60,73	1.37	9 (16%)	67,97,113	1.37	7 (10%)
45	CLA	AB	833	2	69,73,73	1.24	7 (10%)	83,113,113	1.18	8 (9%)
45	CLA	AF	802	-	61,65,73	1.33	10 (16%)	73,103,113	1.30	7 (9%)
45	CLA	BA	808	1	69,73,73	1.23	7 (10%)	83,113,113	1.15	6 (7%)
45	CLA	A3	302	14	64,68,73	1.30	8 (12%)	77,107,113	1.16	8 (10%)
45	CLA	BB	816	2	68,72,73	1.25	9 (13%)	82,112,113	1.23	9 (10%)
45	CLA	BB	825	2	49,53,73	1.47	7 (14%)	59,89,113	1.29	7 (11%)
45	CLA	AB	808	2	55,59,73	1.39	8 (14%)	65,95,113	1.33	7 (10%)
45	CLA	B2	608	17	49,53,73	1.47	7 (14%)	59,89,113	1.24	7 (11%)
45	CLA	BA	803	1	69,73,73	1.21	8 (11%)	83,113,113	1.25	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	AB	806	2	69,73,73	1.25	8 (11%)	83,113,113	1.22	6 (7%)
45	CLA	B5	609	18	58,62,73	1.36	9 (15%)	69,99,113	1.17	7 (10%)
45	CLA	A3	305	-	44,49,73	1.54	8 (18%)	52,84,113	1.30	5 (9%)
45	CLA	BB	834	2	69,73,73	1.24	7 (10%)	83,113,113	1.28	9 (10%)
53	LMG	A1	321	-	44,44,55	1.03	2 (4%)	52,52,63	1.19	5 (9%)
45	CLA	B3	308	14	45,49,73	1.50	7 (15%)	54,84,113	1.29	4 (7%)
47	LHG	AJ	104	-	39,39,48	1.06	2 (5%)	42,45,54	0.92	2 (4%)
47	LHG	B1	318	45	41,41,48	1.01	2 (4%)	44,47,54	0.95	2 (4%)
45	CLA	BA	825	-	69,73,73	1.25	9 (13%)	83,113,113	1.21	5 (6%)
45	CLA	AA	807	1	54,58,73	1.42	9 (16%)	65,95,113	1.27	4 (6%)
45	CLA	AB	815	2	69,73,73	1.22	10 (14%)	83,113,113	1.27	10 (12%)
47	LHG	BA	846	45	26,26,48	1.06	2 (7%)	29,32,54	1.00	1 (3%)

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
54	CHL	A1	308	13	-	2/10/86/117	-
54	CHL	A4	304	-	-	1/10/86/117	-
48	BCR	AB	847	-	-	0/29/63/63	0/2/2/2
50	LMU	BA	853	-	-	9/20/60/61	0/2/2/2
45	CLA	AA	824	1	-	9/25/101/115	-
48	BCR	BF	304	-	-	7/29/63/63	0/2/2/2
45	CLA	BA	833	1	-	17/39/115/115	-
45	CLA	AB	810	2	-	17/39/115/115	-
45	CLA	AB	812	2	-	8/25/101/115	-
45	CLA	AG	203	7	-	4/12/88/115	-
54	CHL	B2	607	-	-	4/17/93/117	-
49	SF4	BA	852	1,2	-	-	0/6/5/5
45	CLA	BA	810	1	-	12/39/115/115	-
45	CLA	AA	840	1	-	16/39/115/115	-
45	CLA	A3	313	14	-	3/8/84/115	-
54	CHL	A4	314	15	-	0/10/86/117	-
45	CLA	AB	807	2	-	11/39/115/115	-
45	CLA	A1	314	13	-	14/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BB	826	-	-	10/39/115/115	-
45	CLA	B3	310	14	-	2/13/89/115	-
45	CLA	AA	805	1	-	17/39/115/115	-
48	BCR	AB	845	-	-	6/29/63/63	0/2/2/2
45	CLA	B3	311	14	-	8/25/101/115	-
45	CLA	A4	307	15	-	3/15/91/115	-
45	CLA	A3	314	-	-	2/2/74/115	-
49	SF4	I	202	37	-	-	0/6/5/5
47	LHG	A1	301	45	-	11/42/42/53	-
45	CLA	AA	834	1	-	17/39/115/115	-
45	CLA	AA	815	1	-	3/12/88/115	-
45	CLA	BB	842	2	-	11/39/115/115	-
45	CLA	B5	613	18	-	7/15/91/115	-
49	SF4	BC	101	3	-	-	0/6/5/5
46	PQN	AA	843	-	-	6/23/43/43	0/2/2/2
45	CLA	AB	805	2	-	2/10/86/115	-
45	CLA	AA	841	1	-	12/39/115/115	-
48	BCR	BA	849	-	-	4/29/63/63	0/2/2/2
45	CLA	BA	822	1	-	8/12/88/115	-
48	BCR	AA	852	-	-	5/29/63/63	0/2/2/2
53	LMG	B5	617	-	-	14/28/48/70	0/1/1/1
45	CLA	BB	831	2	-	8/29/105/115	-
45	CLA	A3	306	14	-	0/10/86/115	-
45	CLA	B1	307	-	-	4/10/82/115	-
54	CHL	B2	601	17	-	9/26/102/117	-
45	CLA	BA	827	1	-	14/39/115/115	-
45	CLA	AB	840	-	-	7/39/115/115	-
45	CLA	B5	602	18	-	11/33/109/115	-
48	BCR	A3	318	-	-	4/29/63/63	0/2/2/2
45	CLA	BA	816	-	-	4/15/91/115	-
48	BCR	AA	845	-	-	2/29/63/63	0/2/2/2
47	LHG	A3	319	45	-	14/26/26/53	-
45	CLA	AA	811	1	-	13/39/115/115	-
47	LHG	a	501	-	-	17/33/33/53	-
45	CLA	AB	841	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CHL	B3	306	-	-	5/15/91/117	-
45	CLA	BB	843	47	-	13/39/115/115	-
45	CLA	B3	303	-	-	2/9/85/115	-
45	CLA	A3	308	14	-	7/15/91/115	-
47	LHG	AA	844	-	-	18/53/53/53	-
45	CLA	B2	604	-	-	4/11/88/115	-
45	CLA	B1	305	13	-	6/25/101/115	-
45	CLA	A1	306	-	-	9/20/96/115	-
45	CLA	A6	610	16	-	6/27/103/115	-
52	LUT	A1	317	-	-	0/29/67/67	0/2/2/2
45	CLA	A4	303	-	-	4/11/87/115	-
45	CLA	AA	812	1	-	9/26/102/115	-
45	CLA	BB	808	2	-	10/39/115/115	-
45	CLA	B3	309	47	-	2/8/84/115	-
45	CLA	AB	837	2	-	7/21/97/115	-
48	BCR	AA	848	-	-	4/29/63/63	0/2/2/2
45	CLA	BA	835	1	-	6/15/91/115	-
45	CLA	AA	803	1	-	15/39/115/115	-
45	CLA	BB	840	2	-	4/18/94/115	-
45	CLA	B1	315	13	-	0/4/80/115	-
54	CHL	A6	602	16	-	6/24/100/117	-
45	CLA	A3	312	14	-	13/25/101/115	-
48	BCR	BA	851	-	-	8/29/63/63	0/2/2/2
45	CLA	AA	829	1	-	18/39/115/115	-
45	CLA	B3	312	14	-	2/8/84/115	-
45	CLA	B3	304	-	-	6/10/86/115	-
45	CLA	AA	825	-	-	10/39/115/115	-
45	CLA	BB	815	2	-	21/39/115/115	-
48	BCR	BA	848	-	-	4/29/63/63	0/2/2/2
45	CLA	A4	311	15	-	8/28/104/115	-
45	CLA	A4	308	15	-	6/26/102/115	-
48	BCR	AB	849	-	-	5/29/63/63	0/2/2/2
45	CLA	A6	609	16	-	3/15/91/115	-
45	CLA	A6	601	15	-	2/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BB	818	2	-	9/27/103/115	-
45	CLA	AB	821	2	-	9/21/97/115	-
45	CLA	AB	803	2	-	19/39/115/115	-
52	LUT	A3	316	-	-	0/29/67/67	0/2/2/2
51	DGD	AB	851	-	-	21/55/95/95	0/2/2/2
45	CLA	B5	603	18	-	4/13/89/115	-
45	CLA	BB	833	2	-	4/13/89/115	-
45	CLA	BG	202	7	-	6/15/91/115	-
45	CLA	BA	817	1	-	9/33/109/115	-
45	CLA	BA	837	1	-	3/23/99/115	-
45	CLA	A1	311	13	-	3/31/107/115	-
45	CLA	B3	301	14	-	7/33/109/115	-
45	CLA	AB	804	-	-	16/39/115/115	-
45	CLA	A1	305	13	-	8/27/103/115	-
45	CLA	BB	811	2	-	15/39/115/115	-
45	CLA	BK	202	-	-	8/15/91/115	-
54	CHL	A6	606	-	-	2/12/88/117	-
45	CLA	AB	829	2	-	15/39/115/115	-
45	CLA	A3	315	14	-	0/8/84/115	-
45	CLA	BB	809	2	-	6/24/100/115	-
45	CLA	AA	821	-	-	15/39/115/115	-
45	CLA	AA	816	-	-	8/15/91/115	-
47	LHG	B2	618	45	-	22/39/39/53	-
45	CLA	BL	303	12	-	9/33/109/115	-
45	CLA	B1	314	13	-	9/33/109/115	-
45	CLA	B2	609	17	-	8/27/103/115	-
45	CLA	AA	827	1	-	18/39/115/115	-
45	CLA	A4	301	15	-	10/33/109/115	-
45	CLA	AA	828	1	-	15/39/115/115	-
45	CLA	A4	310	15	-	7/10/86/115	-
45	CLA	A6	612	16	-	8/13/89/115	-
45	CLA	AA	842	-	-	20/39/115/115	-
45	CLA	BB	813	2	-	4/25/101/115	-
45	CLA	B1	311	13	-	3/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	BCR	BA	856	-	-	5/29/63/63	0/2/2/2
45	CLA	A6	614	16	-	4/13/89/115	-
48	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
49	SF4	AA	850	1,2	-	-	0/6/5/5
45	CLA	BA	831	1	-	9/18/94/115	-
45	CLA	A3	309	14	-	5/10/86/115	-
45	CLA	BA	839	1	-	7/23/99/115	-
50	LMU	AA	851	-	-	10/21/61/61	0/2/2/2
45	CLA	AB	825	-	-	14/39/115/115	-
54	CHL	A4	305	-	-	0/10/86/117	-
48	BCR	B3	317	-	-	6/29/63/63	0/2/2/2
45	CLA	BB	805	-	-	14/39/115/115	-
45	CLA	BL	304	-	-	5/13/89/115	-
45	CLA	A4	312	15	-	6/15/91/115	-
45	CLA	AA	818	1	-	9/32/108/115	-
45	CLA	BA	828	1	-	14/39/115/115	-
55	XAT	A1	318	-	-	0/31/93/93	0/4/4/4
45	CLA	BA	826	-	-	6/25/101/115	-
48	BCR	AG	205	-	-	2/29/63/63	0/2/2/2
45	CLA	AB	828	2	-	13/39/115/115	-
45	CLA	AB	836	-	-	3/12/88/115	-
45	CLA	B5	610	47	-	6/12/88/115	-
48	BCR	BJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	AK	201	11	-	0/2/74/115	-
45	CLA	AB	842	47	-	20/39/115/115	-
55	XAT	A4	316	-	-	0/31/93/93	0/4/4/4
45	CLA	BA	838	1	-	11/27/99/115	-
45	CLA	BA	830	1	-	13/39/115/115	-
45	CLA	A1	307	-	-	6/10/82/115	-
45	CLA	AB	814	2	-	16/39/115/115	-
52	LUT	A6	615	-	-	0/29/67/67	0/2/2/2
52	LUT	B2	615	-	-	0/29/67/67	0/2/2/2
45	CLA	B5	611	18	-	4/10/86/115	-
45	CLA	AA	830	1	-	14/39/115/115	-
45	CLA	BA	834	1	-	13/39/115/115	-
45	CLA	BA	821	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	A1	312	47	-	0/4/80/115	-
45	CLA	BA	844	47	-	4/10/86/115	-
45	CLA	AJ	102	10	-	5/12/88/115	-
47	LHG	B1	301	45	-	7/42/42/53	-
45	CLA	BA	840	1	-	13/39/115/115	-
48	BCR	AI	101	-	-	7/29/63/63	0/2/2/2
45	CLA	B1	309	-	-	4/13/89/115	-
54	CHL	B2	605	-	-	3/12/88/117	-
45	CLA	A6	603	16	-	11/39/115/115	-
48	BCR	BB	845	-	-	4/29/63/63	0/2/2/2
47	LHG	A6	618	45	-	17/40/40/53	-
45	CLA	AB	830	2	-	10/29/105/115	-
45	CLA	BA	815	1	-	4/12/88/115	-
45	CLA	BB	814	2	-	1/13/89/115	-
45	CLA	AA	801	1	-	13/39/115/115	-
46	PQN	BA	843	-	-	8/23/43/43	0/2/2/2
45	CLA	B1	312	47	-	0/4/80/115	-
48	BCR	B5	616	-	-	2/29/63/63	0/2/2/2
54	CHL	A6	607	-	-	2/14/90/117	-
45	CLA	AG	201	-	-	5/13/89/115	-
45	CLA	BA	824	1	-	10/27/103/115	-
48	BCR	BA	855	-	-	4/29/63/63	0/2/2/2
48	BCR	BL	305	-	-	2/29/63/63	0/2/2/2
45	CLA	BB	839	2	-	8/39/115/115	-
45	CLA	BB	823	2	-	4/16/92/115	-
55	XAT	B1	317	-	-	0/31/93/93	0/4/4/4
48	BCR	AB	848	-	-	2/29/63/63	0/2/2/2
45	CLA	BB	832	2	-	6/13/89/115	-
45	CLA	A1	304	13	-	11/33/109/115	-
45	CLA	A3	311	14	-	1/13/89/115	-
45	CLA	B2	611	17	-	7/13/89/115	-
45	CLA	AB	802	-	-	16/37/113/115	-
45	CLA	BA	829	1	-	11/39/115/115	-
49	SF4	BC	102	3	-	-	0/6/5/5
45	CLA	AA	837	1	-	6/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CHL	A4	306	-	-	2/17/93/117	-
48	BCR	A6	617	-	-	2/29/63/63	0/2/2/2
45	CLA	BA	807	1	-	4/21/97/115	-
54	CHL	B2	606	-	-	2/14/90/117	-
55	XAT	B2	616	-	-	0/31/93/93	0/4/4/4
48	BCR	AA	849	-	-	8/29/63/63	0/2/2/2
45	CLA	BF	301	-	-	8/26/102/115	-
50	LMU	BA	854	-	-	8/19/59/61	0/2/2/2
48	BCR	A4	317	-	-	2/29/63/63	0/2/2/2
48	BCR	AA	847	-	-	13/29/63/63	0/2/2/2
45	CLA	BB	801	2	-	17/39/115/115	-
45	CLA	BK	201	11	-	0/2/74/115	-
48	BCR	BL	306	-	-	15/29/63/63	0/2/2/2
56	SQD	e	301	-	-	10/29/49/69	0/1/1/1
45	CLA	BA	841	1	-	17/39/115/115	-
45	CLA	A6	605	-	-	3/11/88/115	-
45	CLA	AB	838	2	-	7/39/115/115	-
45	CLA	BF	303	-	-	2/10/86/115	-
47	LHG	B1	302	-	-	14/40/40/53	-
48	BCR	AF	805	-	-	6/29/63/63	0/2/2/2
49	SF4	I	201	37	-	-	0/6/5/5
49	SF4	AC	101	3	-	-	0/6/5/5
45	CLA	B2	612	17	-	13/39/115/115	-
47	LHG	F	801	-	-	21/41/41/53	-
45	CLA	AA	835	1	-	2/13/89/115	-
49	SF4	K	301	39	-	-	0/6/5/5
45	CLA	AA	826	-	-	12/32/108/115	-
47	LHG	B5	618	45	-	13/34/34/53	-
45	CLA	BB	828	2	-	9/36/112/115	-
45	CLA	A6	604	16	-	2/11/87/115	-
54	CHL	A3	307	-	-	4/15/91/117	-
48	BCR	BB	846	-	-	6/29/63/63	0/2/2/2
45	CLA	BG	201	-	-	7/12/88/115	-
45	CLA	AA	838	1	-	8/27/103/115	-
45	CLA	B2	610	47	-	7/10/70/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	BCR	BB	803	-	-	4/29/63/63	0/2/2/2
48	BCR	B2	617	-	-	0/29/63/63	0/2/2/2
45	CLA	BA	820	1	-	6/15/91/115	-
45	CLA	A4	313	15	-	11/21/97/115	-
45	CLA	AB	827	2	-	14/36/112/115	-
45	CLA	AB	816	2	-	4/13/89/115	-
45	CLA	AH	201	8	-	12/33/109/115	-
48	BCR	BL	301	-	-	6/29/63/63	0/2/2/2
45	CLA	AF	803	-	-	3/12/88/115	-
45	CLA	AB	820	-	-	10/27/103/115	-
45	CLA	AB	835	2	-	7/33/109/115	-
45	CLA	AB	813	2	-	5/13/89/115	-
47	LHG	A1	302	-	-	15/40/40/53	-
45	CLA	AA	802	-	-	8/39/115/115	-
45	CLA	AB	826	-	-	6/36/112/115	-
45	CLA	BA	812	1	-	5/26/102/115	-
45	CLA	B1	313	13	-	5/15/91/115	-
45	CLA	BA	804	1	-	5/24/100/115	-
45	CLA	BA	832	1	-	7/29/105/115	-
45	CLA	B3	305	-	-	2/10/86/115	-
54	CHL	A6	608	-	-	8/21/97/117	-
53	LMG	AG	202	-	-	5/33/53/70	0/1/1/1
48	BCR	BJ	101	-	-	0/29/63/63	0/2/2/2
50	LMU	AB	850	-	-	9/21/61/61	0/2/2/2
48	BCR	BB	849	-	-	2/29/63/63	0/2/2/2
54	CHL	B1	308	-	-	0/10/86/117	-
48	BCR	AB	846	-	-	6/29/63/63	0/2/2/2
45	CLA	AA	836	1	-	9/15/91/115	-
48	BCR	BK	204	-	-	1/29/63/63	0/2/2/2
54	CHL	B5	607	-	-	5/15/91/117	-
45	CLA	AB	809	2	-	16/39/115/115	-
45	CLA	AA	820	1	-	5/15/91/115	-
45	CLA	AB	801	2	-	17/39/115/115	-
45	CLA	AA	819	1	-	14/39/115/115	-
45	CLA	AA	814	1	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BB	817	2	-	4/11/87/115	-
45	CLA	BL	302	12	-	6/15/91/115	-
46	PQN	AB	843	-	-	8/23/43/43	0/2/2/2
45	CLA	BA	801	1	-	9/39/115/115	-
50	LMU	AB	853	-	-	13/21/61/61	0/2/2/2
45	CLA	BB	824	2	-	18/39/115/115	-
49	SF4	AC	102	3	-	-	0/6/5/5
45	CLA	AA	823	1	-	6/10/86/115	-
45	CLA	A1	309	-	-	7/13/89/115	-
45	CLA	A1	310	13	-	2/8/84/115	-
45	CLA	BA	813	1	-	17/39/115/115	-
45	CLA	BA	802	-	-	4/39/115/115	-
45	CLA	BB	830	2	-	11/39/115/115	-
48	BCR	AL	306	-	-	5/29/63/63	0/2/2/2
46	PQN	BB	844	-	-	9/23/43/43	0/2/2/2
45	CLA	AB	818	2	-	12/32/108/115	-
52	LUT	B3	315	-	-	4/29/67/67	0/2/2/2
45	CLA	AL	303	12	-	7/10/86/115	-
47	LHG	A3	301	-	-	11/40/40/53	-
45	CLA	AB	811	2	-	15/39/115/115	-
45	CLA	AG	204	7	-	6/15/91/115	-
48	BCR	BG	203	-	-	6/29/63/63	0/2/2/2
45	CLA	BB	807	2	-	13/39/115/115	-
45	CLA	B2	603	17	-	4/13/89/115	-
45	CLA	A4	309	-	-	5/12/88/115	-
45	CLA	BB	819	2	-	14/32/108/115	-
54	CHL	B5	606	-	-	2/8/84/117	-
45	CLA	AF	804	-	-	4/10/86/115	-
57	FES	c	301	28	-	-	0/1/1/1
45	CLA	AA	833	1	-	21/39/115/115	-
50	LMU	AB	852	-	-	9/21/61/61	0/2/2/2
45	CLA	AB	822	2	-	7/18/94/115	-
48	BCR	AB	844	-	-	5/29/63/63	0/2/2/2
45	CLA	B1	310	13	-	3/6/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BB	810	2	-	15/39/115/115	-
55	XAT	B5	615	-	-	0/31/93/93	0/4/4/4
45	CLA	AA	831	1	-	9/18/94/115	-
55	XAT	B3	316	-	-	0/31/93/93	0/4/4/4
45	CLA	BB	841	-	-	7/39/115/115	-
45	CLA	A6	613	16	-	7/37/113/115	-
45	CLA	B5	604	-	-	3/11/87/115	-
45	CLA	BA	806	1	-	18/39/115/115	-
45	CLA	A6	611	47	-	6/10/70/115	-
45	CLA	BB	837	-	-	6/12/88/115	-
48	BCR	A1	319	-	-	4/29/63/63	0/2/2/2
45	CLA	BA	811	1	-	16/39/115/115	-
45	CLA	BA	818	1	-	8/29/105/115	-
48	BCR	BI	101	-	-	6/29/63/63	0/2/2/2
45	CLA	B1	306	-	-	3/10/86/115	-
45	CLA	B5	608	18	-	5/13/89/115	-
54	CHL	B1	303	13	-	3/21/97/117	-
48	BCR	AK	204	-	-	6/29/63/63	0/2/2/2
45	CLA	AA	822	1	-	5/12/88/115	-
48	BCR	BB	847	-	-	6/29/63/63	0/2/2/2
45	CLA	BB	820	2	-	12/33/109/115	-
45	CLA	AA	810	1	-	10/39/111/115	-
50	LMU	AL	301	-	-	11/20/60/61	0/2/2/2
45	CLA	BA	842	-	-	15/39/115/115	-
48	BCR	AF	801	-	-	2/29/63/63	0/2/2/2
45	CLA	BA	814	1	-	8/15/91/115	-
52	LUT	AF	806	-	-	0/29/67/67	0/2/2/2
45	CLA	BB	812	2	-	13/39/115/115	-
45	CLA	AB	823	2	-	19/39/115/115	-
48	BCR	BB	848	-	-	2/29/63/63	0/2/2/2
45	CLA	BK	203	-	-	5/17/93/115	-
45	CLA	BB	804	2	-	16/39/115/115	-
45	CLA	AK	203	11	-	9/17/93/115	-
45	CLA	A4	302	15	-	5/13/89/115	-
45	CLA	B2	613	17	-	1/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	A1	315	13	-	0/4/80/115	-
45	CLA	BA	823	1	-	6/10/86/115	-
45	CLA	A3	310	47	-	2/2/78/115	-
45	CLA	BB	829	2	-	17/39/115/115	-
45	CLA	AA	806	1	-	13/39/115/115	-
45	CLA	AL	305	-	-	5/12/88/115	-
45	CLA	A1	313	13	-	4/15/91/115	-
45	CLA	BB	802	-	-	16/39/115/115	-
45	CLA	BB	836	2	-	11/33/109/115	-
52	LUT	A4	315	-	-	1/29/67/67	0/2/2/2
45	CLA	BF	302	-	-	3/12/88/115	-
55	XAT	A3	317	-	-	0/31/93/93	0/4/4/4
45	CLA	AB	834	2	-	18/39/115/115	-
45	CLA	AB	819	2	-	14/33/109/115	-
55	XAT	A6	616	-	-	0/31/93/93	0/4/4/4
45	CLA	B3	302	14	-	6/27/103/115	-
45	CLA	AB	832	2	-	9/39/115/115	-
45	CLA	B1	304	13	-	7/35/111/115	-
45	CLA	AA	832	1	-	7/29/105/115	-
51	DGD	BB	850	-	-	13/55/95/95	0/2/2/2
45	CLA	AK	202	-	-	7/15/91/115	-
45	CLA	B3	307	14	-	3/15/91/115	-
45	CLA	AA	839	1	-	6/24/100/115	-
48	BCR	AL	302	-	-	5/29/63/63	0/2/2/2
53	LMG	A4	318	-	-	15/34/54/70	0/1/1/1
48	BCR	BA	850	-	-	3/29/63/63	0/2/2/2
45	CLA	B3	313	-	-	2/2/74/115	-
45	CLA	B5	601	18	-	10/17/93/115	-
47	LHG	A1	320	45	-	16/53/53/53	-
48	BCR	AA	846	-	-	6/29/63/63	0/2/2/2
45	CLA	A3	303	14	-	10/27/103/115	-
45	CLA	AA	809	1	-	7/21/97/115	-
45	CLA	BB	821	-	-	8/27/103/115	-
48	BCR	BA	847	-	-	5/29/63/63	0/2/2/2
47	LHG	B3	318	45	-	11/26/26/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BB	827	-	-	8/36/112/115	-
45	CLA	AB	839	2	-	3/18/94/115	-
45	CLA	BA	809	1	-	11/21/97/115	-
54	CHL	A1	303	13	-	4/23/99/117	-
45	CLA	BH	201	-	-	13/33/109/115	-
45	CLA	BB	838	2	-	5/21/97/115	-
45	CLA	AB	831	2	-	5/13/89/115	-
52	LUT	B1	316	-	-	14/29/67/67	0/2/2/2
45	CLA	AB	824	2	-	5/13/89/115	-
48	BCR	AJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	BB	806	2	-	2/10/86/115	-
45	CLA	A1	316	13	-	9/11/87/115	-
45	CLA	A3	304	-	-	0/9/85/115	-
45	CLA	B5	612	18	-	8/30/106/115	-
50	LMU	BB	851	-	-	10/21/61/61	0/2/2/2
47	LHG	BA	845	-	-	29/53/53/53	-
45	CLA	AA	808	1	-	10/39/115/115	-
45	CLA	BJ	102	10	-	4/12/88/115	-
45	CLA	B3	314	14	-	0/8/84/115	-
45	CLA	AL	304	12	-	9/33/109/115	-
45	CLA	BA	805	1	-	22/39/115/115	-
45	CLA	AA	813	1	-	19/39/115/115	-
45	CLA	BB	822	2	-	2/10/86/115	-
47	LHG	BF	305	-	-	18/49/49/53	-
45	CLA	BA	836	1	-	8/15/91/115	-
45	CLA	AB	817	2	-	8/27/103/115	-
45	CLA	AA	817	1	-	6/33/109/115	-
56	SQD	BJ	104	-	-	21/42/62/69	0/1/1/1
48	BCR	AI	102	-	-	3/29/63/63	0/2/2/2
45	CLA	BB	835	2	-	18/39/115/115	-
45	CLA	BA	819	1	-	13/39/115/115	-
54	CHL	B2	614	17	-	0/14/90/117	-
52	LUT	B5	614	-	-	1/29/67/67	0/2/2/2
54	CHL	B5	605	-	-	2/10/86/117	-
45	CLA	B2	602	17	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AA	804	1	-	7/24/100/115	-
45	CLA	AB	833	2	-	10/39/115/115	-
45	CLA	AF	802	-	-	10/30/106/115	-
45	CLA	BA	808	1	-	12/39/115/115	-
45	CLA	A3	302	14	-	8/33/109/115	-
45	CLA	BB	816	2	-	15/37/113/115	-
45	CLA	BB	825	2	-	8/15/91/115	-
45	CLA	AB	808	2	-	6/22/98/115	-
45	CLA	B2	608	17	-	4/15/91/115	-
45	CLA	BA	803	1	-	19/39/115/115	-
45	CLA	AB	806	2	-	15/39/115/115	-
45	CLA	B5	609	18	-	5/26/102/115	-
45	CLA	A3	305	-	-	6/10/86/115	-
45	CLA	BB	834	2	-	11/39/115/115	-
53	LMG	A1	321	-	-	17/39/59/70	0/1/1/1
45	CLA	B3	308	14	-	5/10/86/115	-
47	LHG	AJ	104	-	-	16/44/44/53	-
47	LHG	B1	318	45	-	12/46/46/53	-
45	CLA	BA	825	-	-	15/39/115/115	-
45	CLA	AA	807	1	-	4/21/97/115	-
45	CLA	AB	815	2	-	17/39/115/115	-
47	LHG	BA	846	45	-	7/30/30/53	-

The worst 5 of 2908 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
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 3852 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 3232 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.

224 monomers are involved in 480 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	A1	308	CHL	1	0
48	AB	847	BCR	3	0
48	BF	304	BCR	1	0
45	AB	810	CLA	2	0
45	AB	812	CLA	1	0
45	AG	203	CLA	1	0
54	B2	607	CHL	3	0
49	BA	852	SF4	1	0
45	BA	810	CLA	1	0
45	A1	314	CLA	2	0
45	B3	310	CLA	1	0
48	AB	845	BCR	1	0
45	B3	311	CLA	1	0
45	A4	307	CLA	1	0
49	I	202	SF4	3	0
45	AA	834	CLA	1	0
45	AA	815	CLA	1	0
45	B5	613	CLA	1	0
46	AA	843	PQN	3	0
45	AA	841	CLA	1	0
48	BA	849	BCR	2	0
54	B2	601	CHL	12	0
45	AB	840	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	B5	602	CLA	1	0
48	A3	318	BCR	2	0
45	AA	811	CLA	1	0
47	a	501	LHG	2	0
54	B3	306	CHL	1	0
45	B3	303	CLA	1	0
45	A3	308	CLA	1	0
47	AA	844	LHG	1	0
45	B1	305	CLA	1	0
45	A1	306	CLA	2	0
45	A6	610	CLA	10	0
52	A1	317	LUT	1	0
48	AA	848	BCR	2	0
45	AA	803	CLA	1	0
45	BB	840	CLA	1	0
48	BA	851	BCR	6	0
45	AA	825	CLA	2	0
45	BB	815	CLA	7	0
48	BA	848	BCR	1	0
45	A4	311	CLA	1	0
45	A6	601	CLA	1	0
45	AB	803	CLA	3	0
52	A3	316	LUT	1	0
45	BG	202	CLA	39	0
45	A1	311	CLA	2	0
45	A1	305	CLA	1	0
45	BK	202	CLA	4	0
45	BB	809	CLA	6	0
47	B2	618	LHG	2	0
45	BL	303	CLA	1	0
45	B1	314	CLA	1	0
45	B2	609	CLA	2	0
45	AA	827	CLA	4	0
45	A4	301	CLA	1	0
45	AA	828	CLA	1	0
45	BB	813	CLA	1	0
45	B1	311	CLA	1	0
48	BA	856	BCR	1	0
48	AJ	101	BCR	4	0
45	AB	825	CLA	1	0
48	B3	317	BCR	4	0
45	BB	805	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BL	304	CLA	2	0
45	AA	818	CLA	2	0
55	A1	318	XAT	1	0
48	AG	205	BCR	1	0
45	AB	828	CLA	1	0
48	BJ	103	BCR	3	0
45	AK	201	CLA	7	0
45	AB	842	CLA	1	0
55	A4	316	XAT	2	0
45	BA	830	CLA	4	0
45	AB	814	CLA	1	0
52	A6	615	LUT	4	0
45	AA	830	CLA	1	0
45	BA	834	CLA	1	0
45	AJ	102	CLA	1	0
47	B1	301	LHG	1	0
45	BA	840	CLA	4	0
45	B1	309	CLA	1	0
48	BB	845	BCR	2	0
45	AA	801	CLA	11	0
46	BA	843	PQN	3	0
48	BA	855	BCR	2	0
48	BL	305	BCR	2	0
45	BB	823	CLA	2	0
48	AB	848	BCR	2	0
45	B2	611	CLA	1	0
45	AB	802	CLA	4	0
45	BA	829	CLA	1	0
49	BC	102	SF4	7	0
54	A4	306	CHL	2	0
48	A6	617	BCR	3	0
54	B2	606	CHL	1	0
55	B2	616	XAT	6	0
48	AA	849	BCR	2	0
48	AA	847	BCR	1	0
45	BB	801	CLA	3	0
45	BK	201	CLA	3	0
48	BL	306	BCR	1	0
56	e	301	SQD	1	0
45	BA	841	CLA	1	0
45	AB	838	CLA	1	0
48	AF	805	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	I	201	SF4	1	0
49	AC	101	SF4	1	0
45	B2	612	CLA	3	0
47	F	801	LHG	3	0
49	K	301	SF4	1	0
45	BB	828	CLA	2	0
45	A6	604	CLA	2	0
48	BB	846	BCR	1	0
45	BG	201	CLA	9	0
45	AA	838	CLA	1	0
45	B2	610	CLA	1	0
48	BB	803	BCR	5	0
48	B2	617	BCR	2	0
45	BA	820	CLA	1	0
45	A4	313	CLA	1	0
45	AB	827	CLA	4	0
45	AH	201	CLA	1	0
48	BL	301	BCR	3	0
45	AF	803	CLA	1	0
45	AA	802	CLA	1	0
45	BA	812	CLA	1	0
45	BA	832	CLA	1	0
54	A6	608	CHL	2	0
48	BJ	101	BCR	6	0
48	BB	849	BCR	2	0
48	AB	846	BCR	1	0
45	AB	809	CLA	2	0
45	AA	820	CLA	1	0
45	AB	801	CLA	1	0
45	BL	302	CLA	8	0
46	AB	843	PQN	2	0
45	BA	801	CLA	14	0
49	AC	102	SF4	3	0
45	BA	802	CLA	3	0
45	BB	830	CLA	1	0
46	BB	844	PQN	2	0
45	AB	818	CLA	2	0
52	B3	315	LUT	3	0
47	A3	301	LHG	1	0
45	AG	204	CLA	4	0
48	BG	203	BCR	13	0
45	B2	603	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A4	309	CLA	1	0
45	BB	819	CLA	1	0
57	c	301	FES	2	0
45	AA	833	CLA	1	0
45	AB	822	CLA	1	0
48	AB	844	BCR	2	0
45	BB	810	CLA	1	0
55	B5	615	XAT	1	0
55	B3	316	XAT	1	0
45	BB	841	CLA	5	0
45	A6	613	CLA	1	0
45	BA	806	CLA	2	0
48	A1	319	BCR	3	0
45	BA	811	CLA	1	0
48	BI	101	BCR	1	0
45	B1	306	CLA	2	0
45	B5	608	CLA	1	0
54	B1	303	CHL	2	0
48	AK	204	BCR	2	0
48	BB	847	BCR	1	0
45	BB	820	CLA	1	0
45	AA	810	CLA	1	0
50	AL	301	LMU	1	0
45	BA	842	CLA	1	0
48	AF	801	BCR	4	0
52	AF	806	LUT	2	0
45	BB	812	CLA	5	0
48	BB	848	BCR	2	0
45	BB	804	CLA	2	0
45	AK	203	CLA	1	0
45	BB	829	CLA	1	0
45	AA	806	CLA	1	0
45	BB	802	CLA	4	0
52	A4	315	LUT	4	0
45	BF	302	CLA	1	0
55	A3	317	XAT	2	0
45	AB	834	CLA	3	0
55	A6	616	XAT	4	0
45	B1	304	CLA	2	0
51	BB	850	DGD	1	0
45	AK	202	CLA	4	0
48	AL	302	BCR	1	0

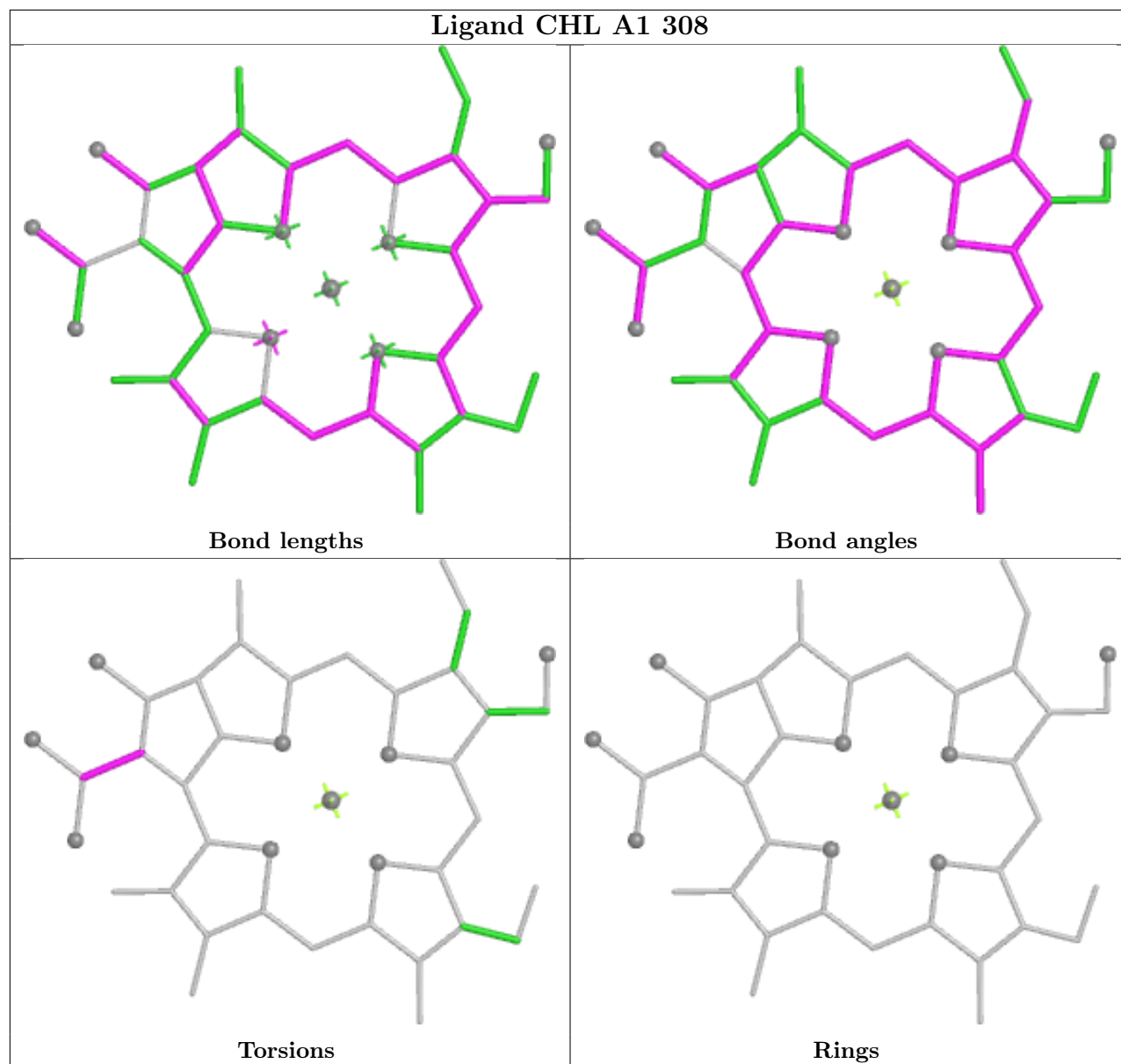
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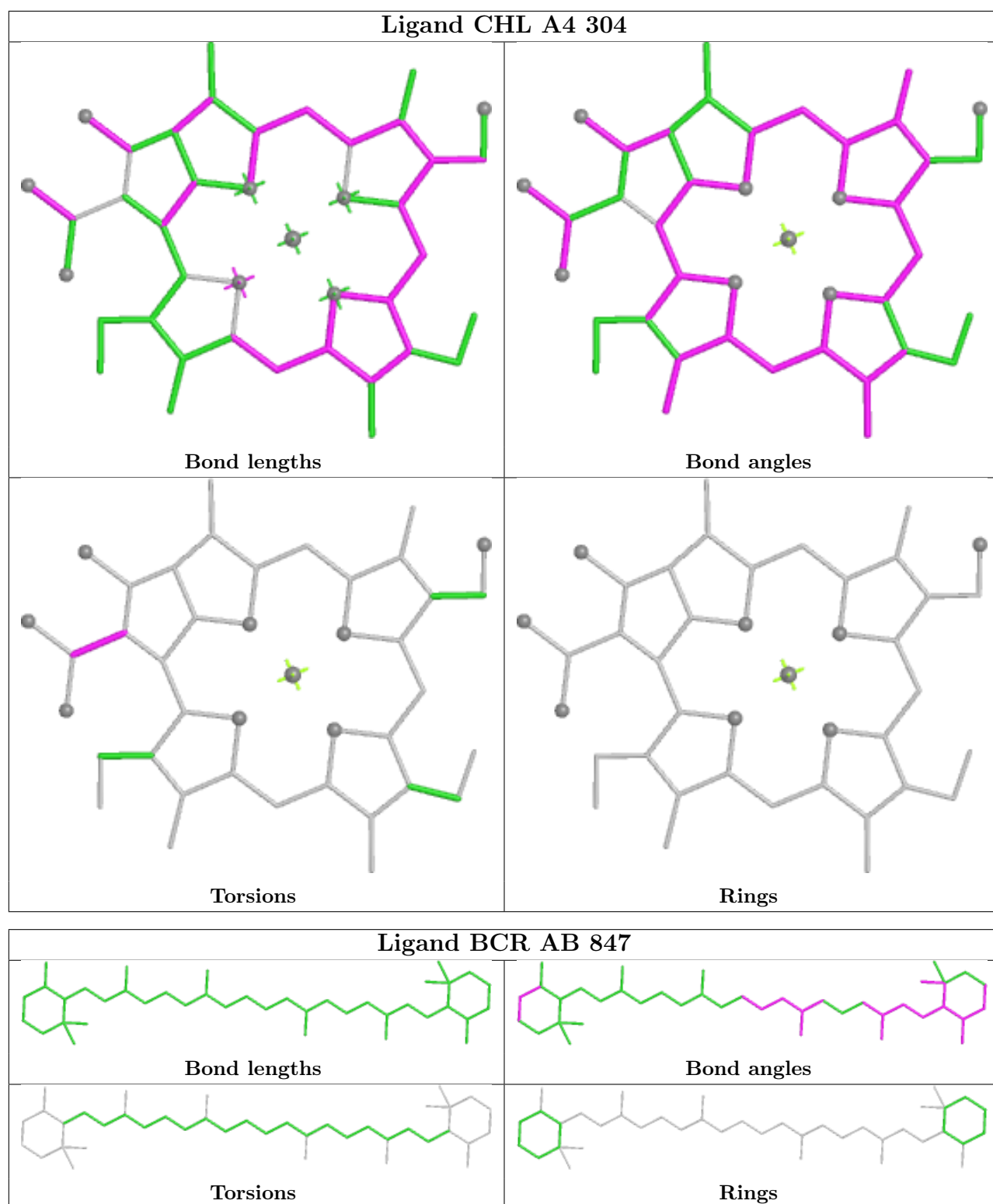
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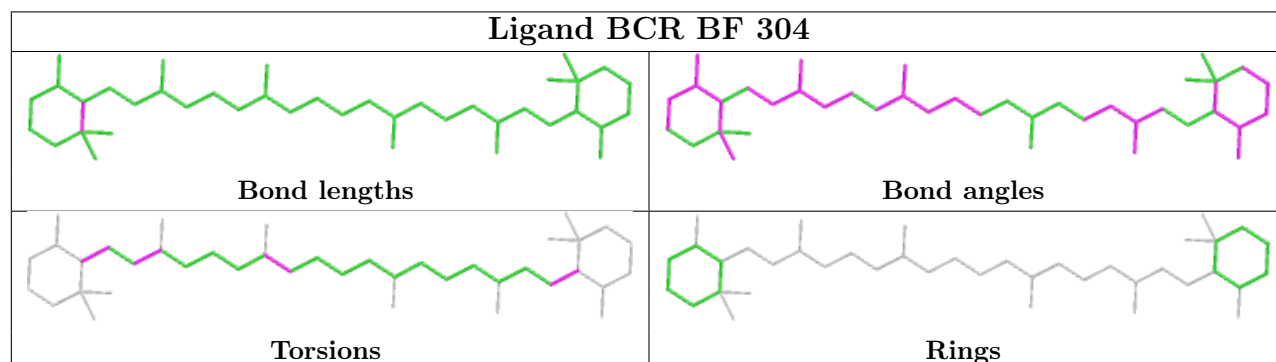
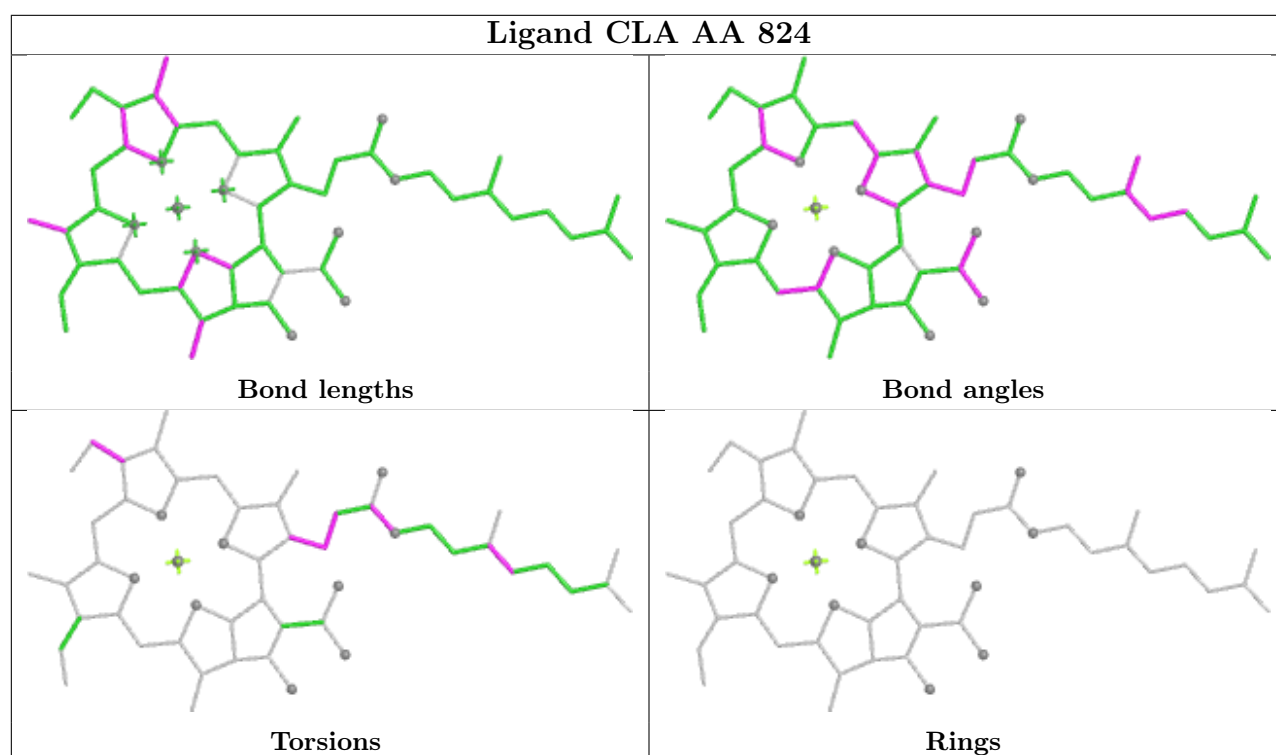
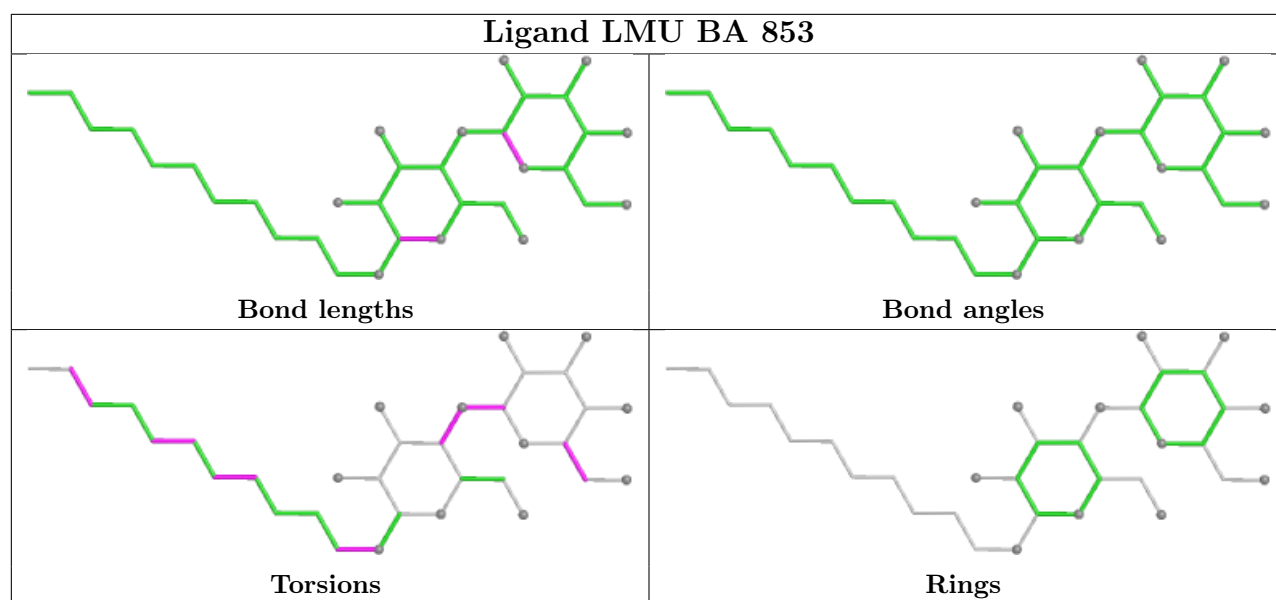
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	A4	318	LMG	4	0
45	B3	313	CLA	3	0
48	AA	846	BCR	1	0
45	BB	821	CLA	1	0
48	BA	847	BCR	1	0
47	B3	318	LHG	1	0
45	BB	827	CLA	1	0
45	AB	839	CLA	2	0
54	A1	303	CHL	2	0
45	BB	838	CLA	1	0
45	AB	831	CLA	1	0
52	B1	316	LUT	3	0
45	AB	824	CLA	1	0
48	AJ	103	BCR	1	0
45	A1	316	CLA	1	0
45	A3	304	CLA	1	0
45	B5	612	CLA	1	0
47	BA	845	LHG	2	0
45	AL	304	CLA	1	0
45	BA	805	CLA	1	0
47	BF	305	LHG	1	0
45	AA	817	CLA	1	0
56	BJ	104	SQD	6	0
48	AI	102	BCR	3	0
45	B2	602	CLA	5	0
45	AB	833	CLA	2	0
45	BA	808	CLA	4	0
45	BB	816	CLA	1	0
45	AB	808	CLA	4	0
45	BA	803	CLA	3	0
45	BB	834	CLA	2	0
53	A1	321	LMG	1	0
47	BA	846	LHG	1	0

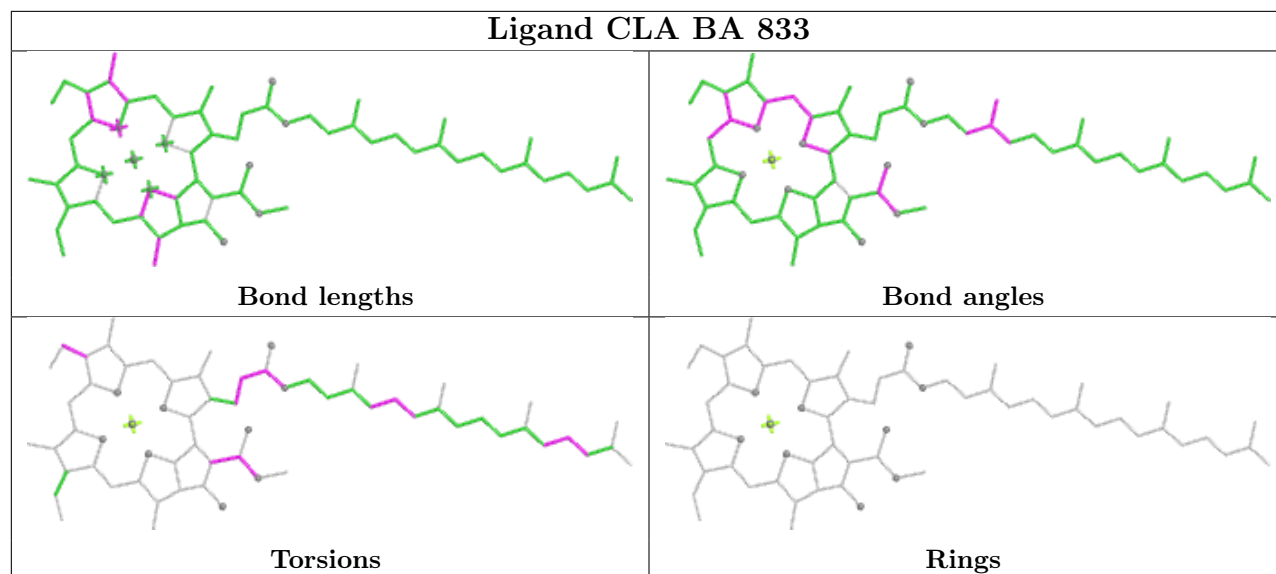
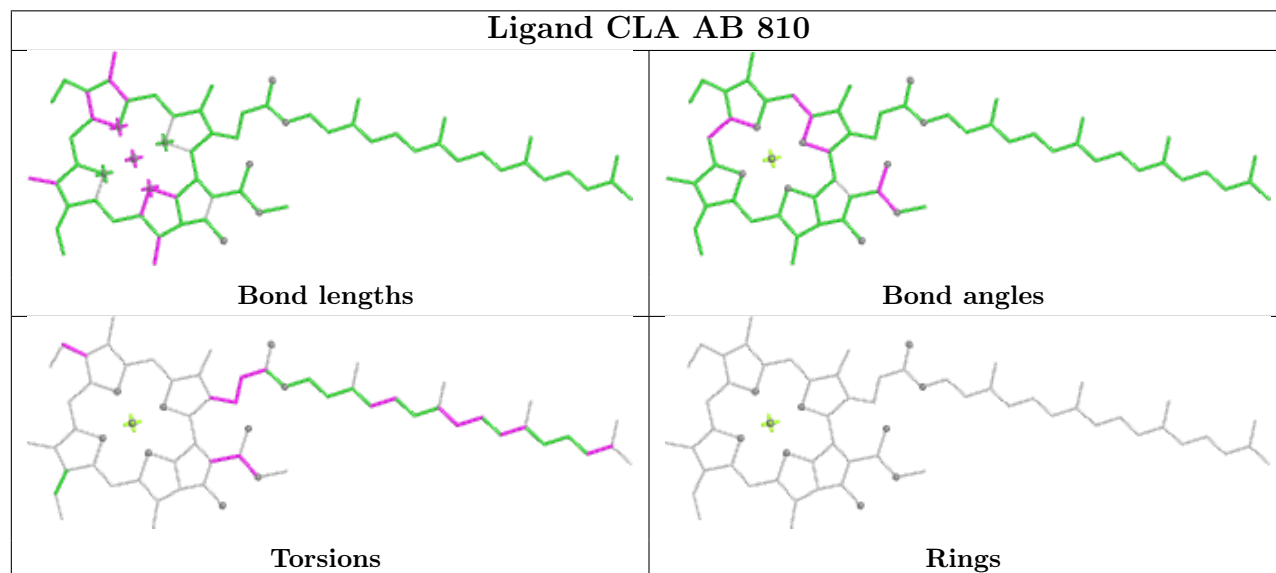
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

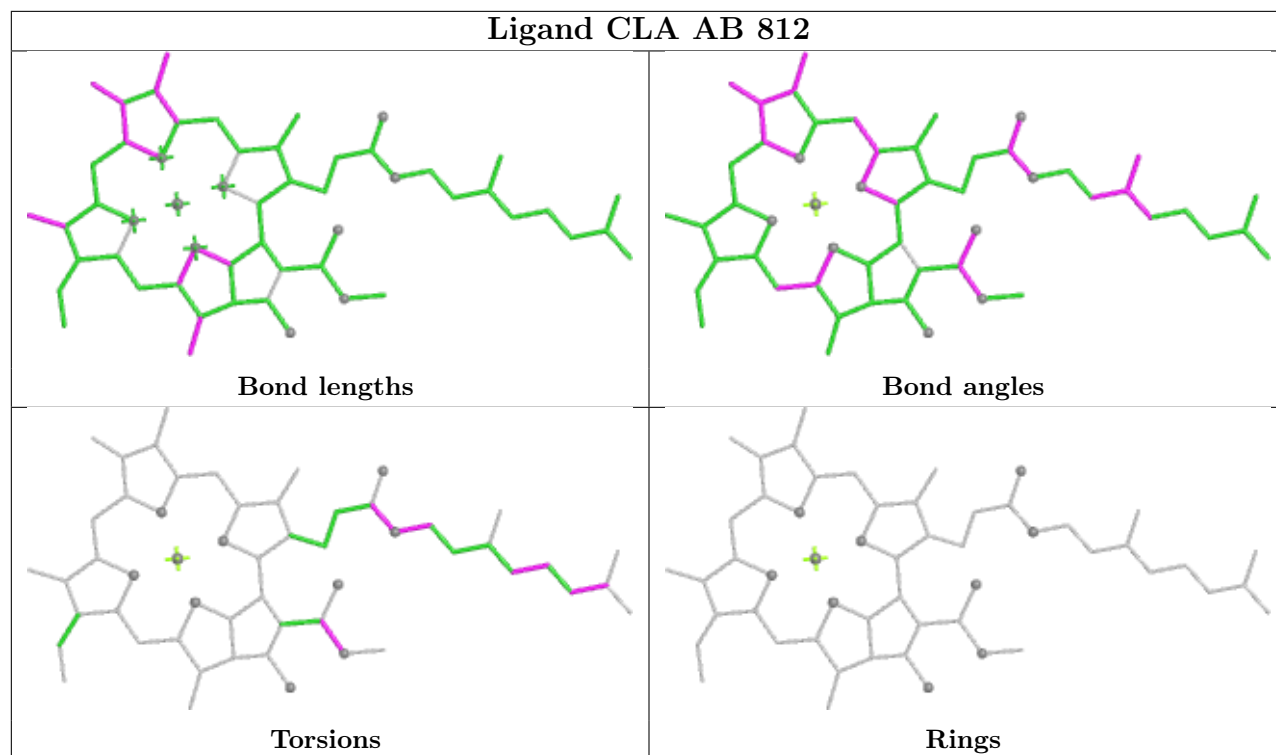
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



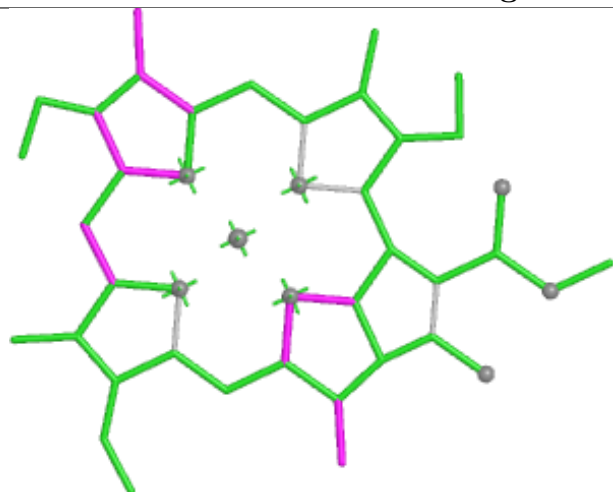




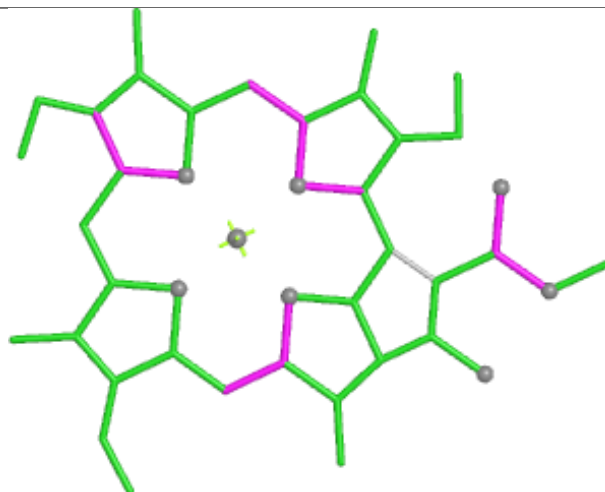
Ligand CLA BA 833**Ligand CLA AB 810**



Ligand CLA AG 203



Bond lengths



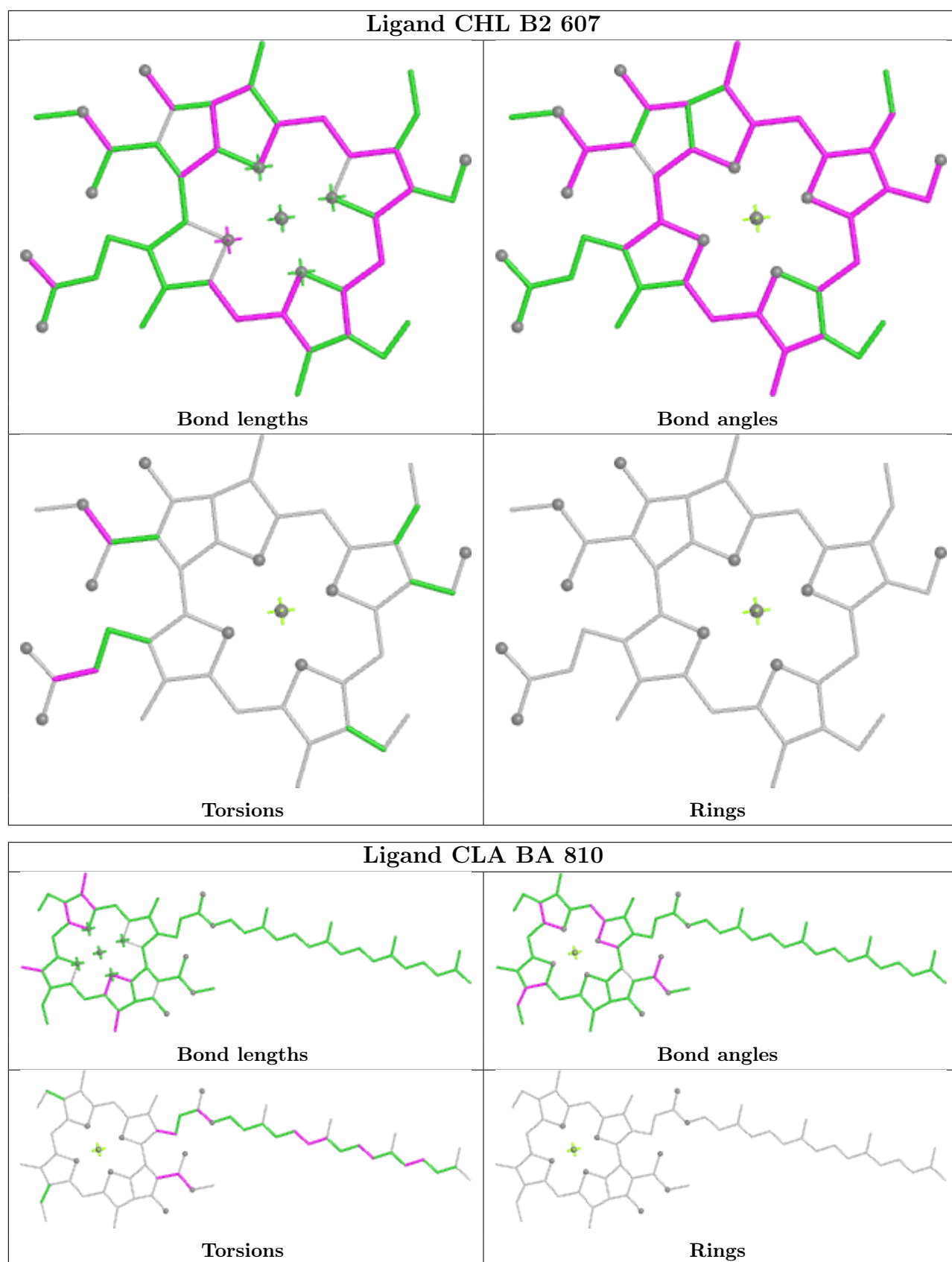
Bond angles



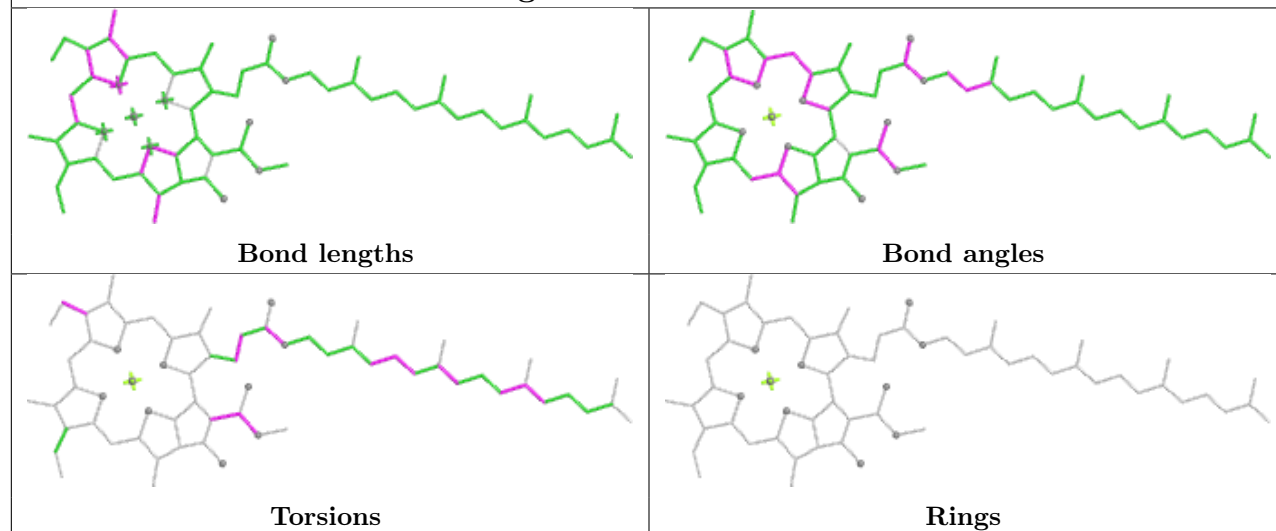
Torsions



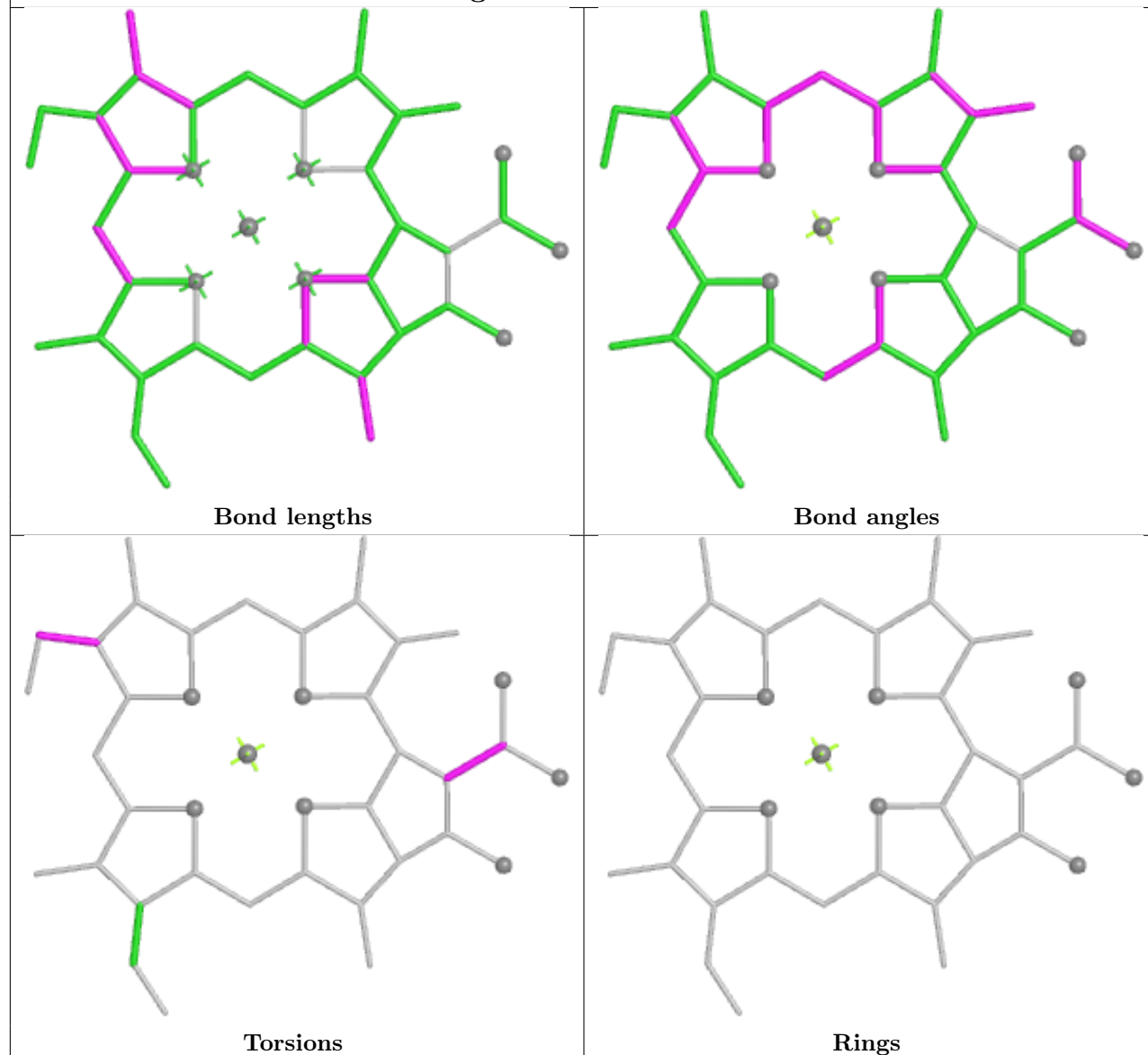
Rings

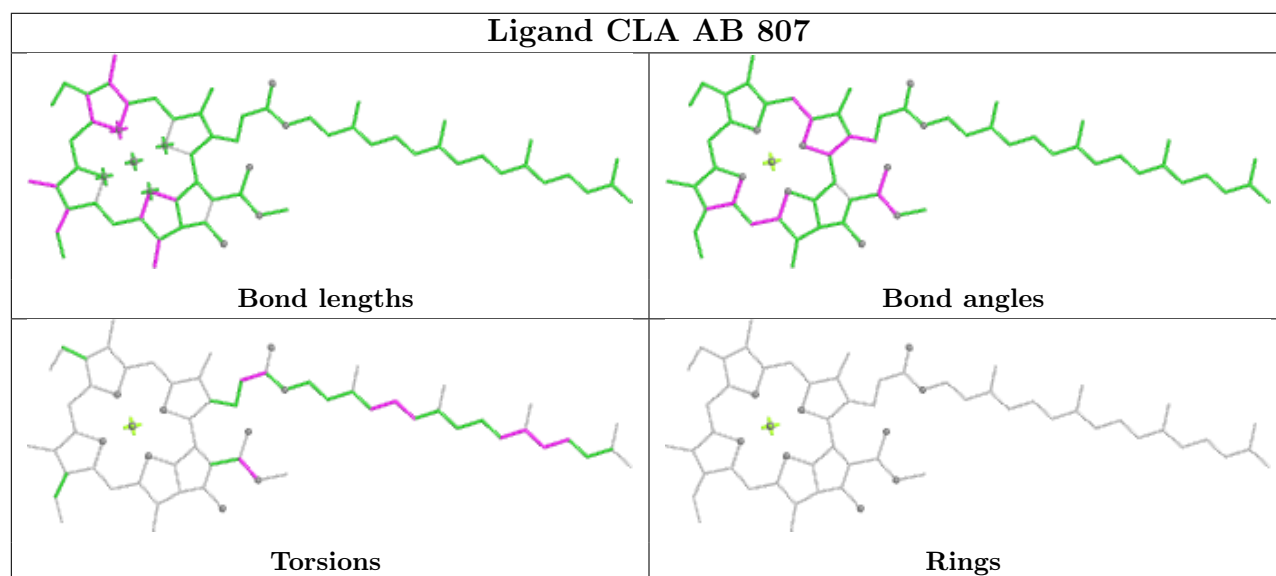
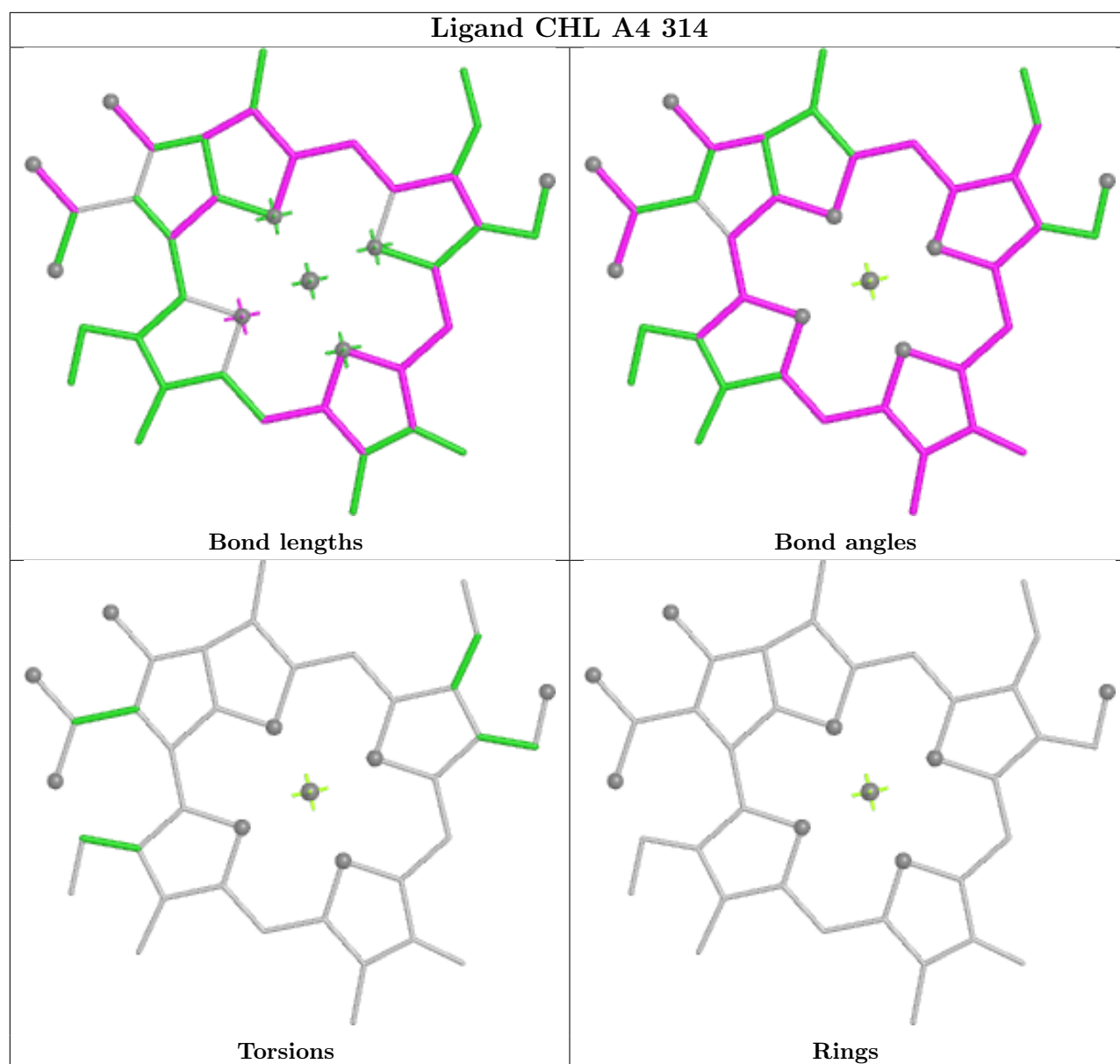


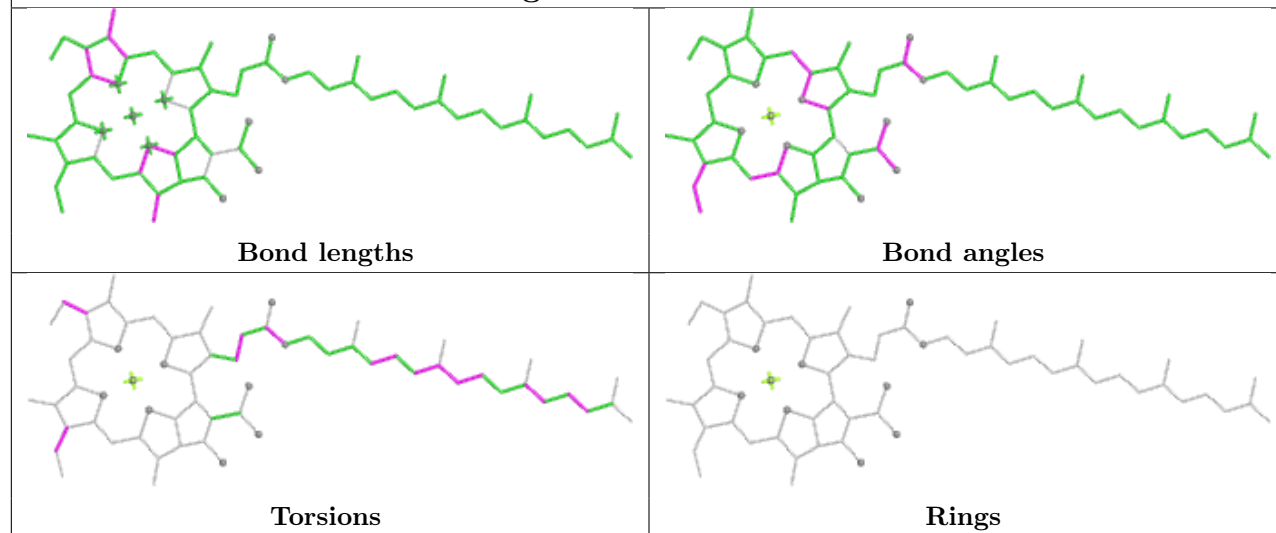
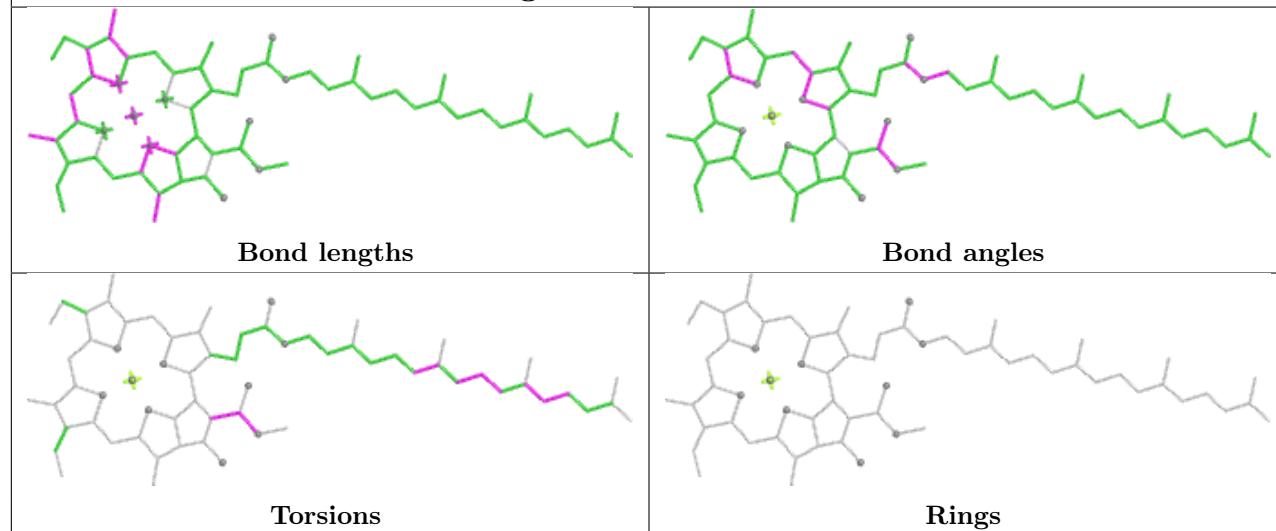
Ligand CLA AA 840



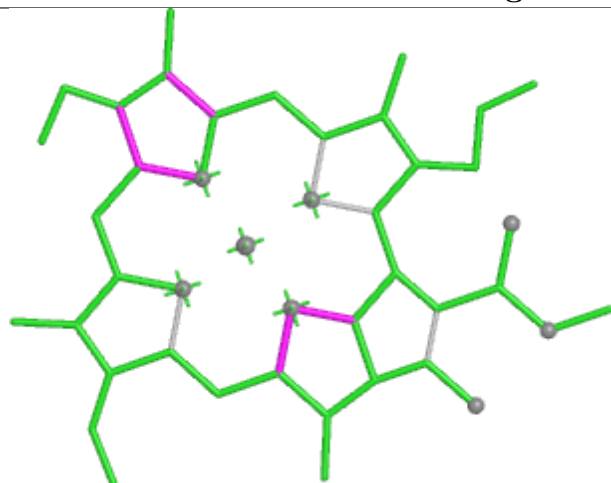
Ligand CLA A3 313



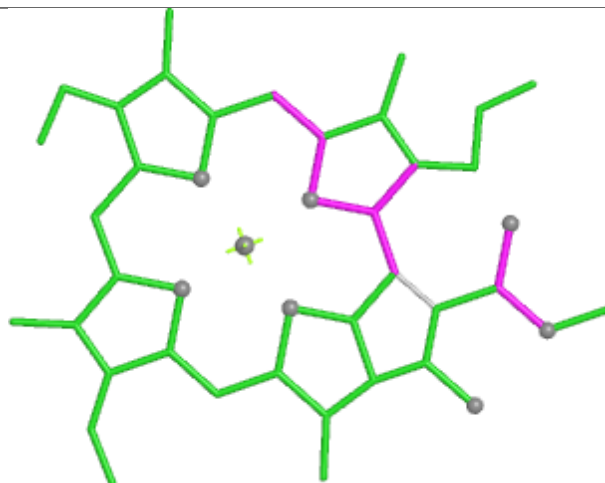


Ligand CLA A1 314**Ligand CLA BB 826**

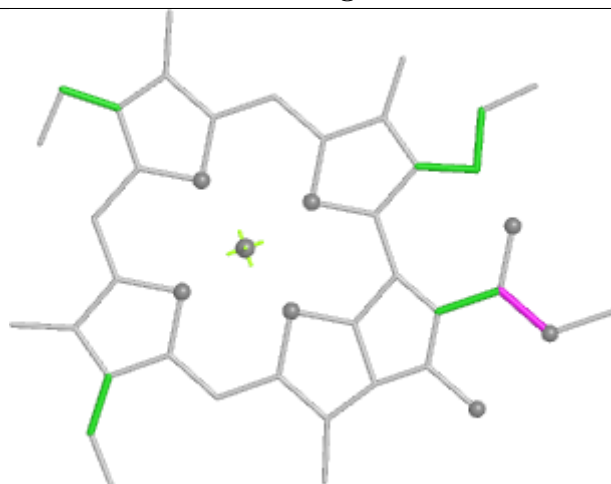
Ligand CLA B3 310



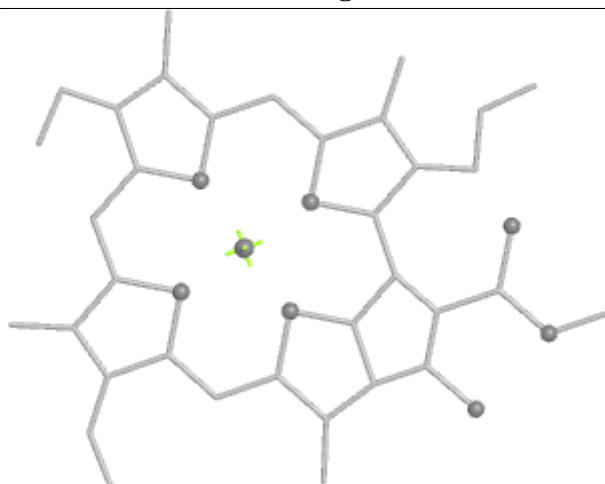
Bond lengths



Bond angles

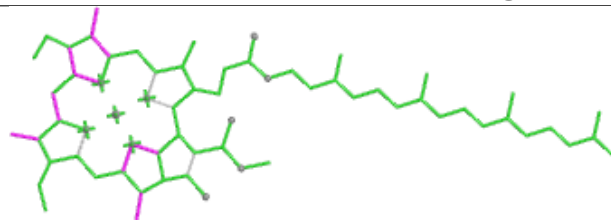


Torsions

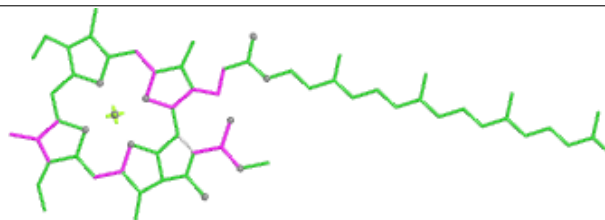


Rings

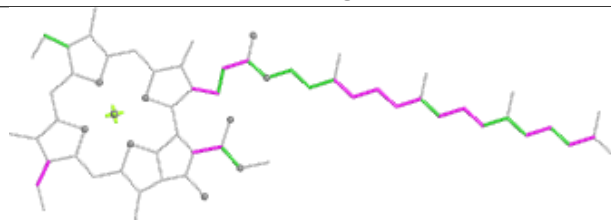
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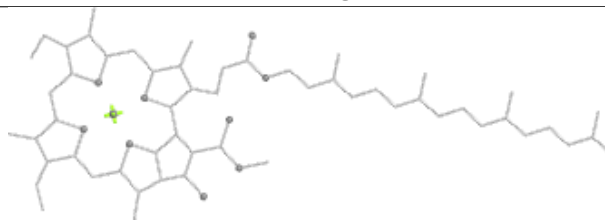
Bond lengths



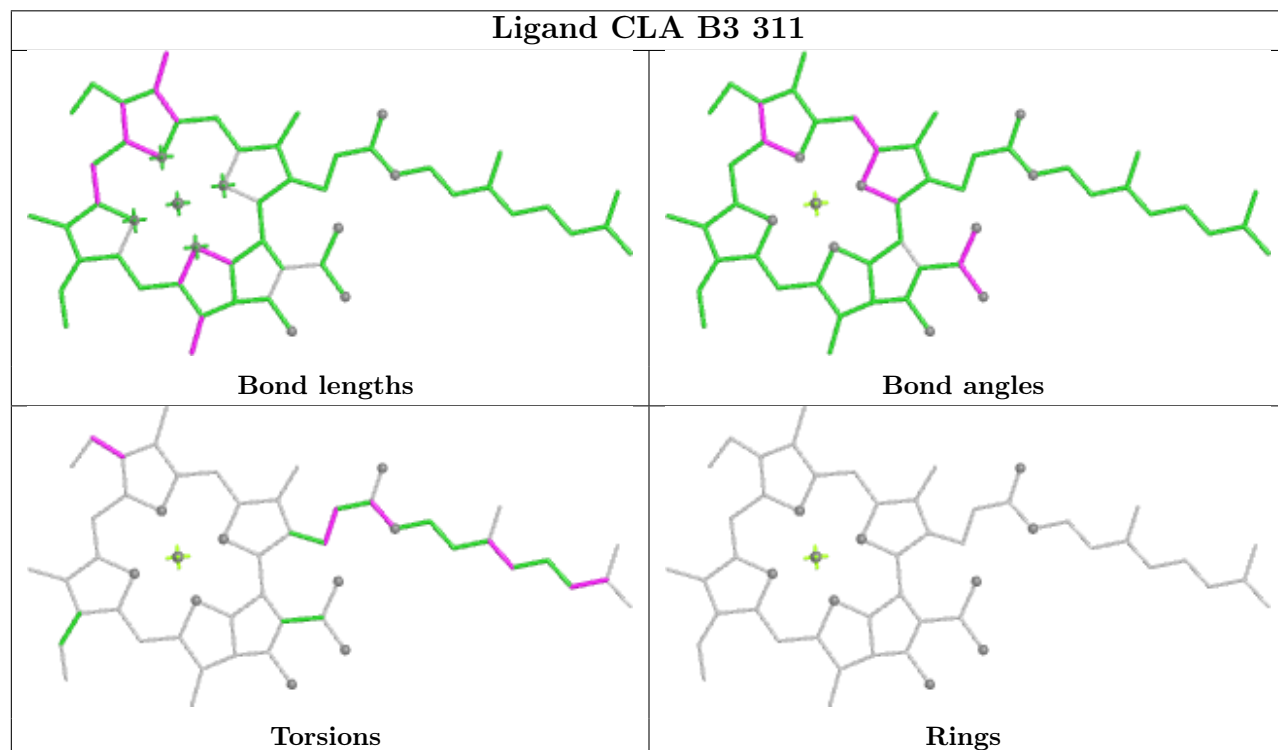
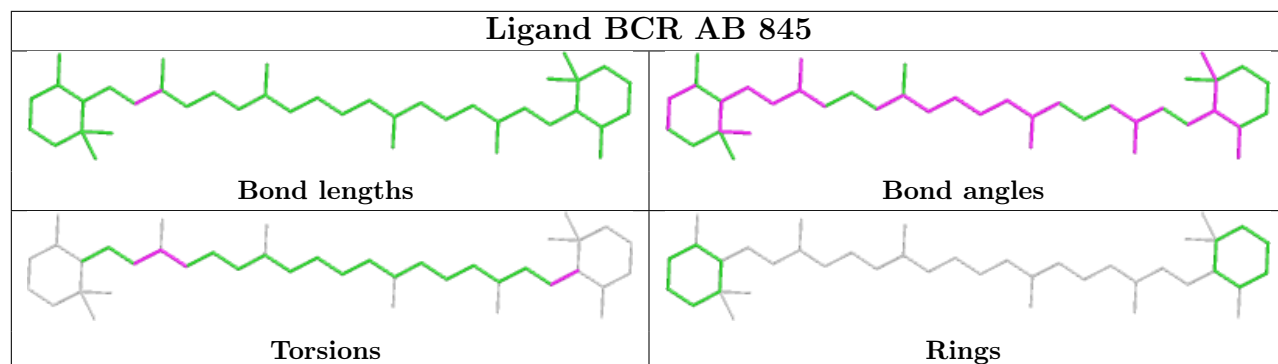
Bond angles



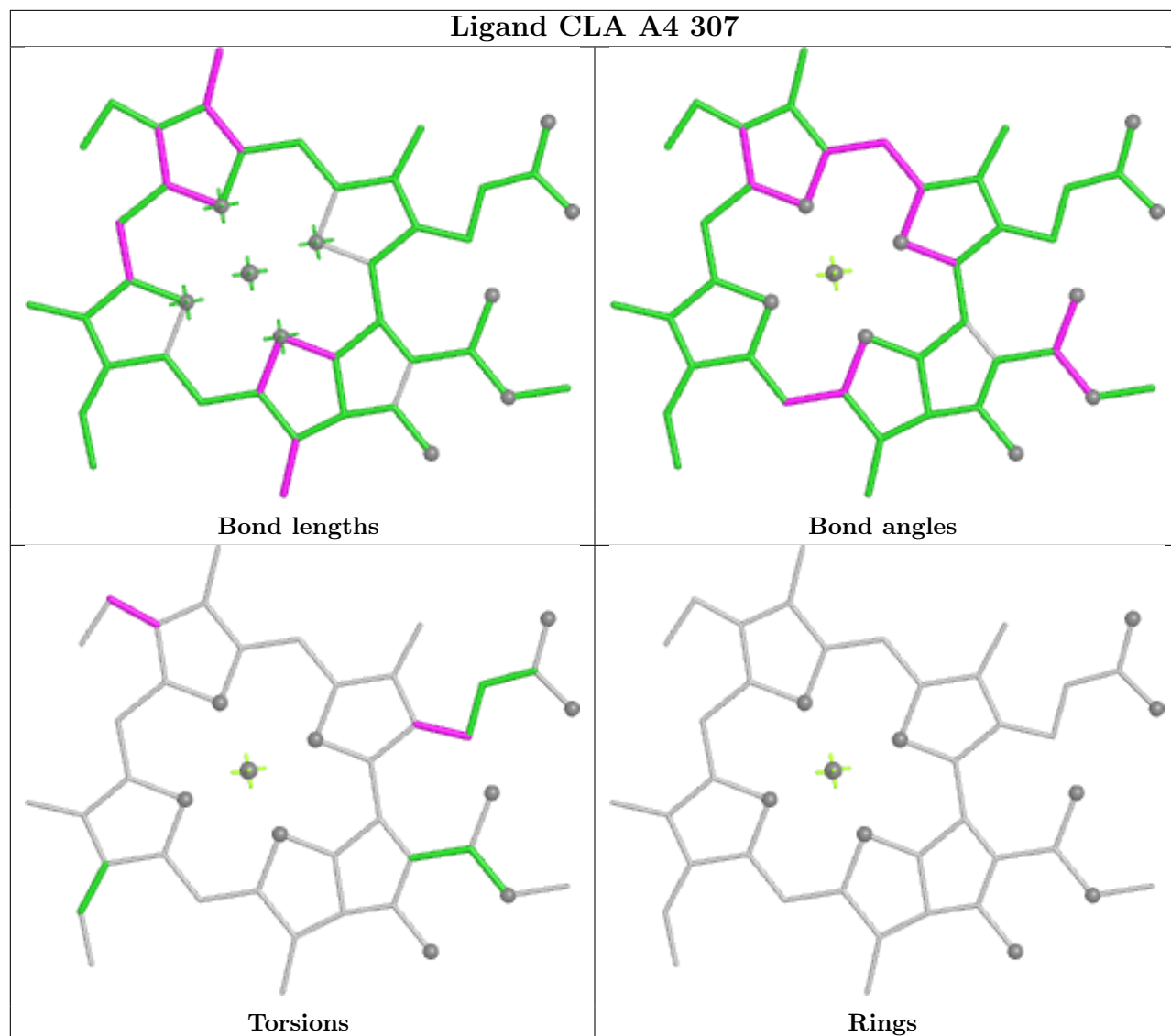
Torsions



Rings



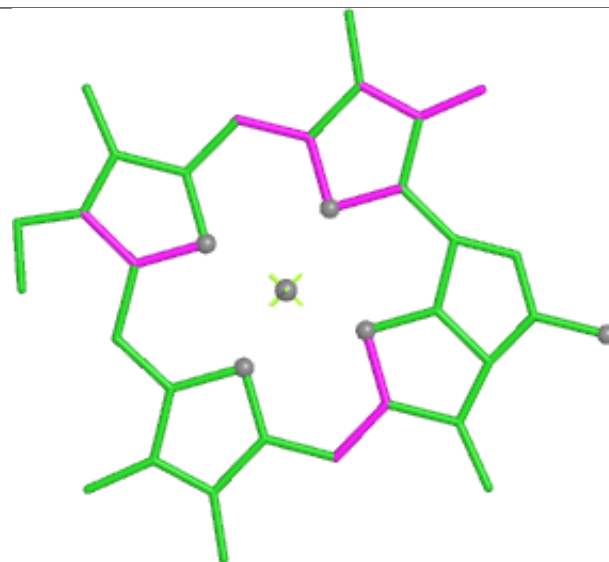
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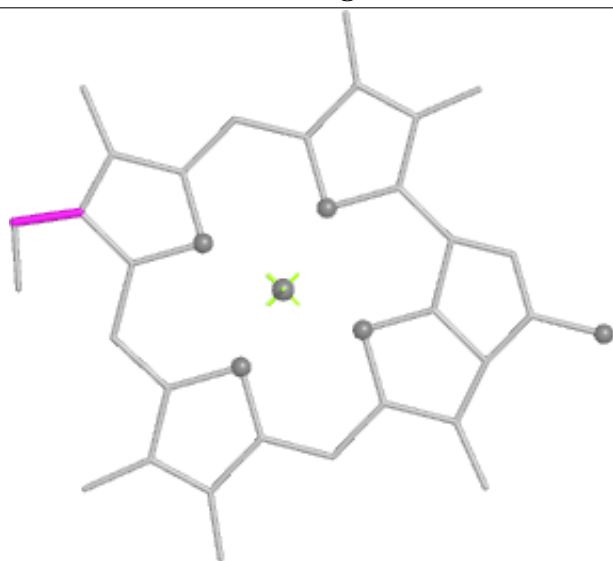
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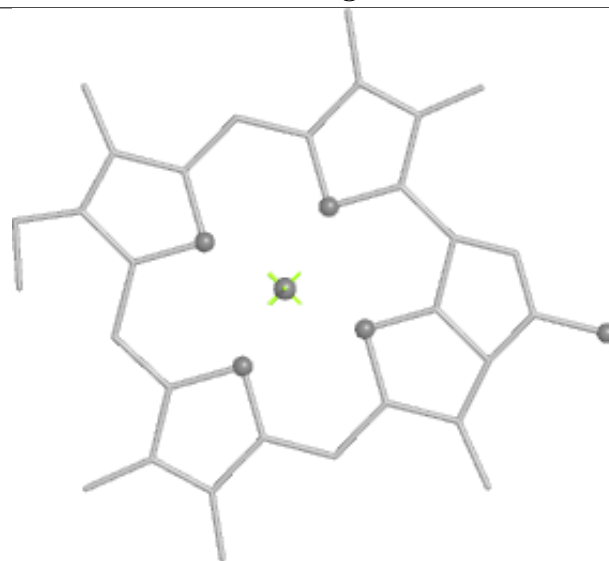
Bond lengths



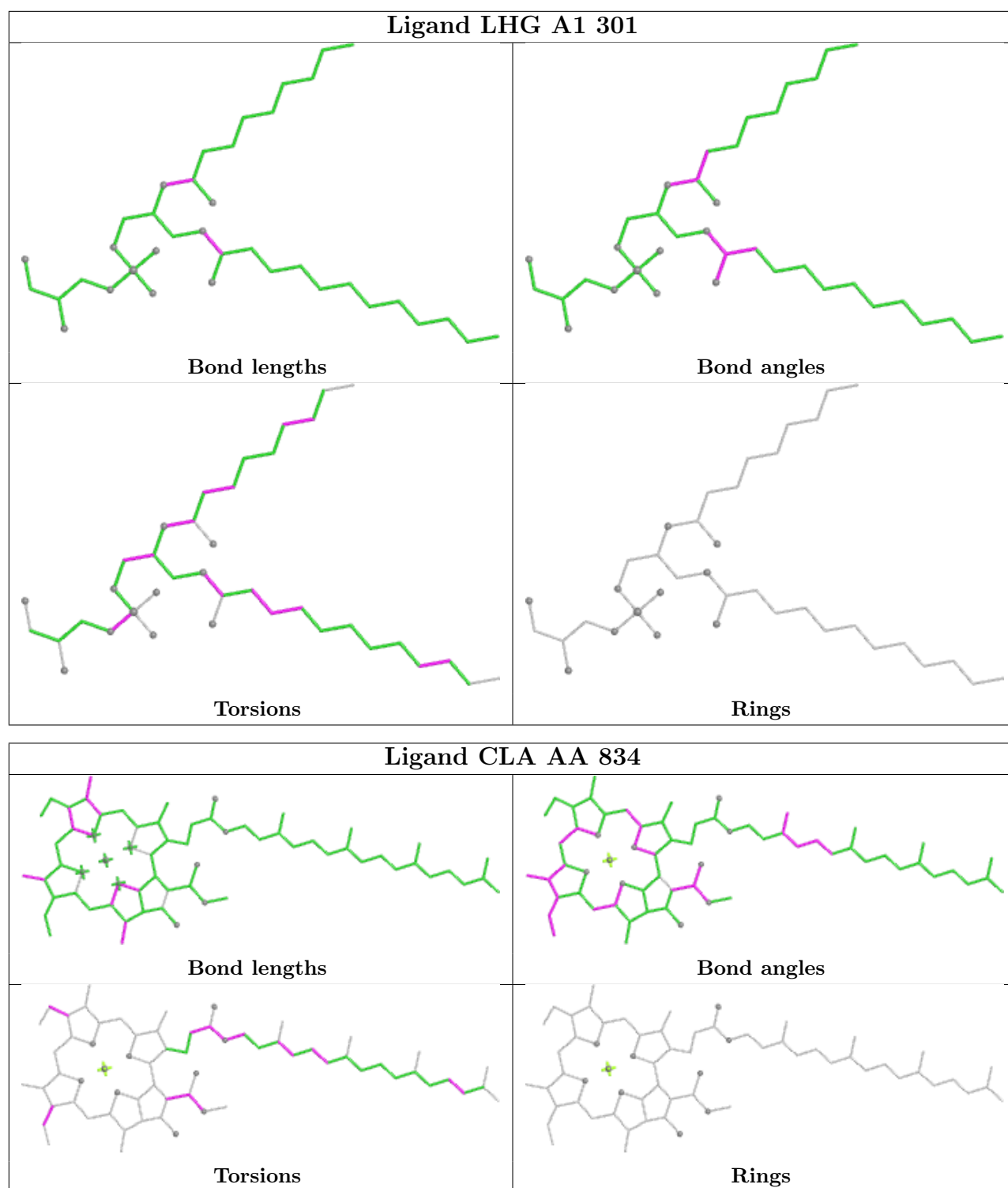
Bond angles



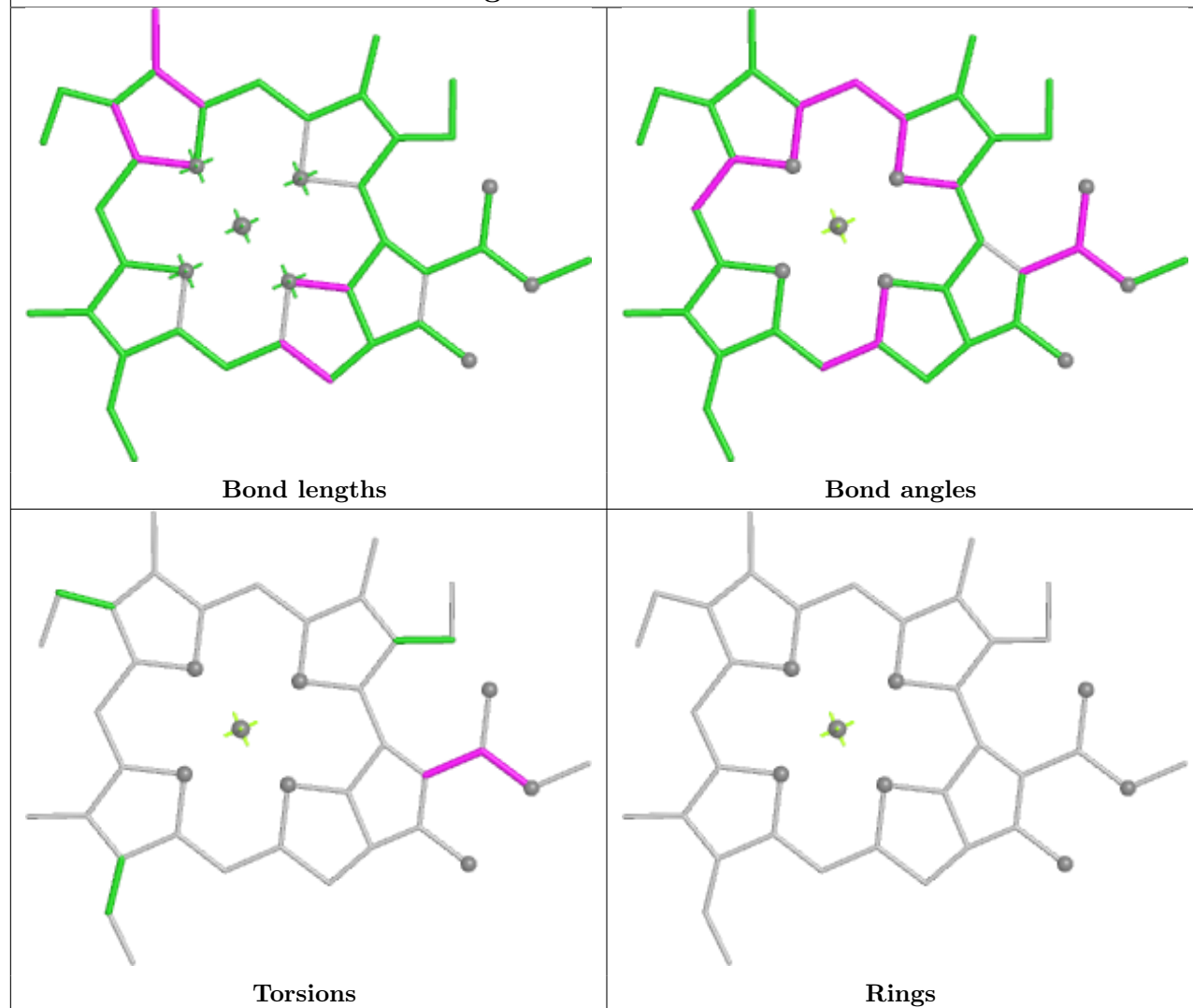
Torsions



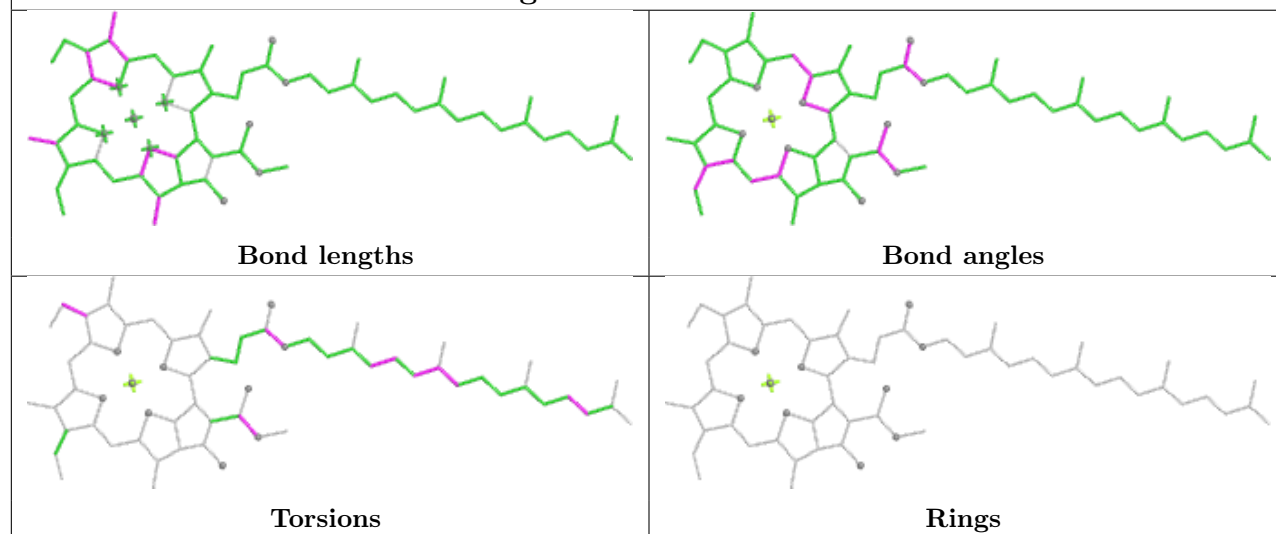
Rings



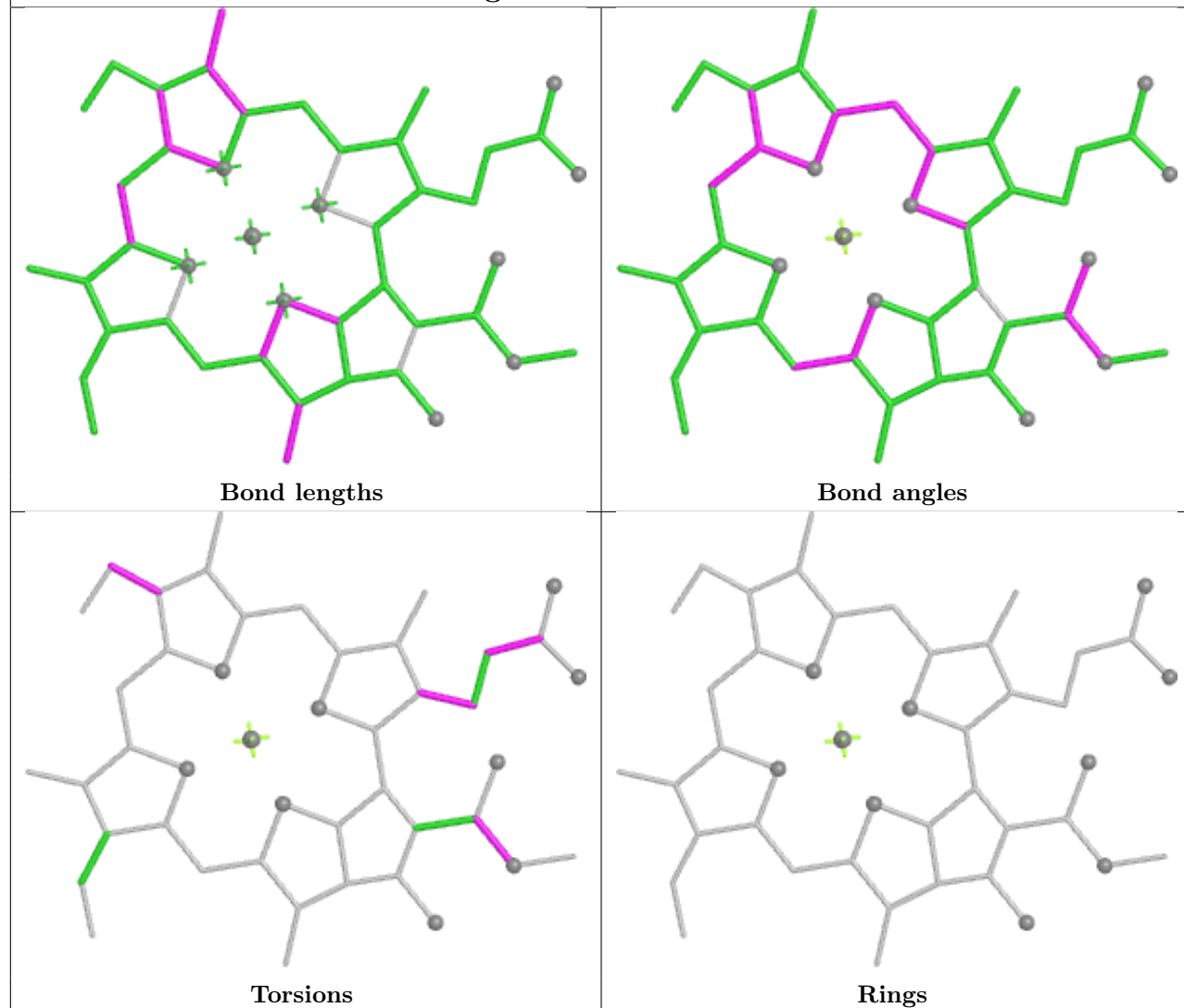
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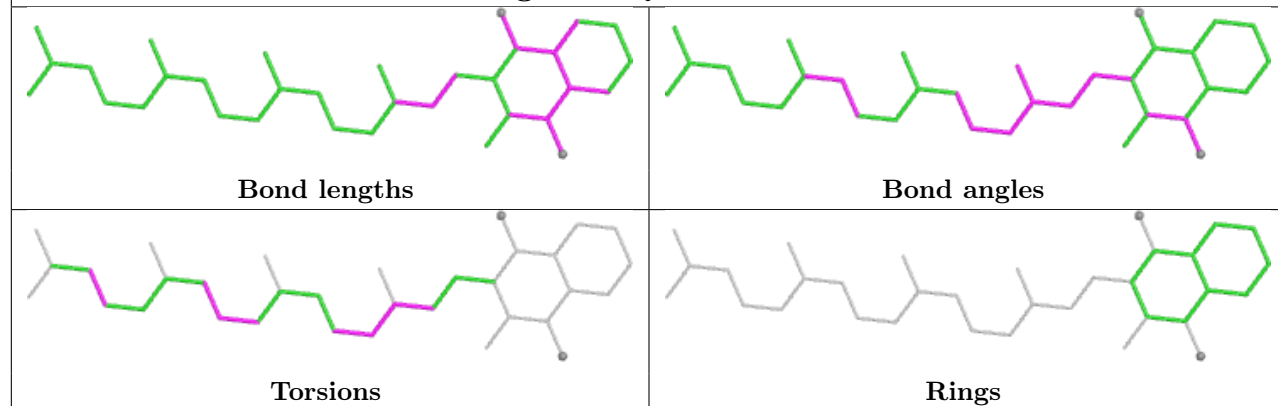
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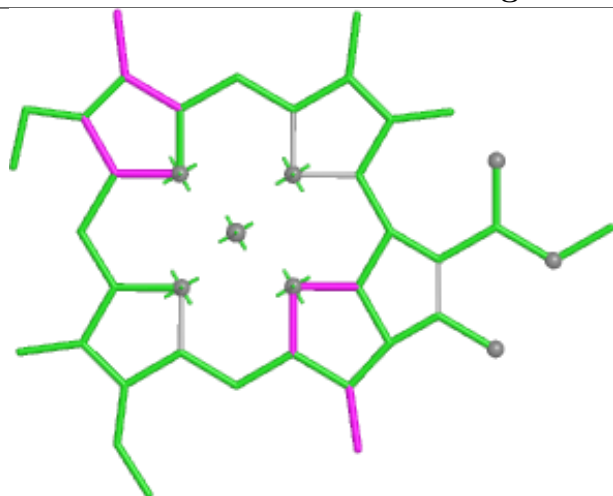
Ligand CLA B5 613



Ligand PQN AA 843



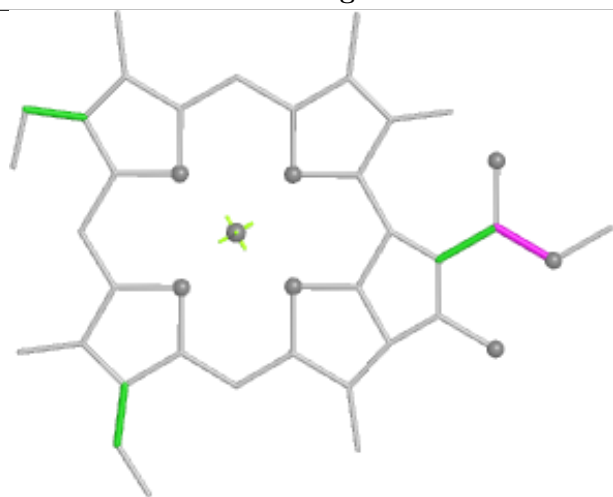
Ligand CLA AB 805



Bond lengths



Bond angles

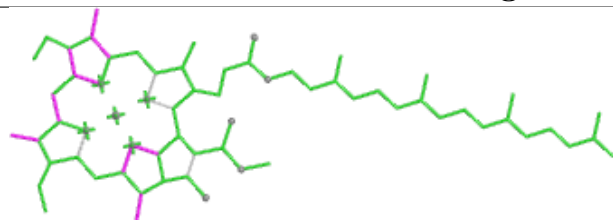


Torsions

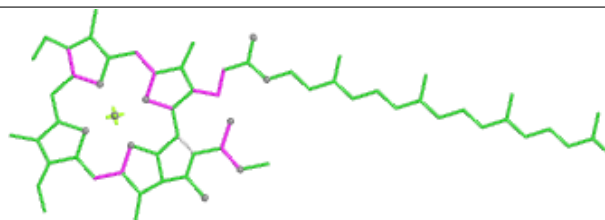


Rings

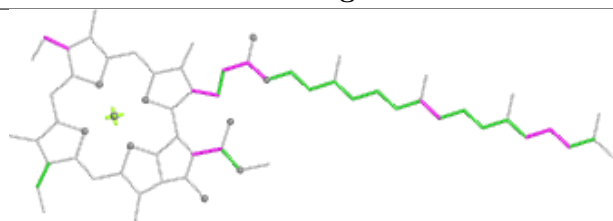
Ligand CLA AA 841



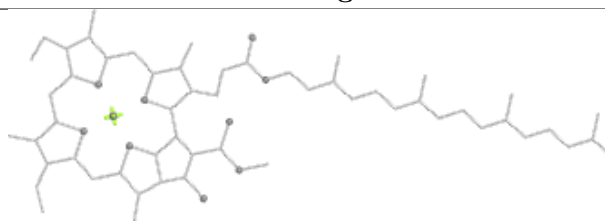
Bond lengths



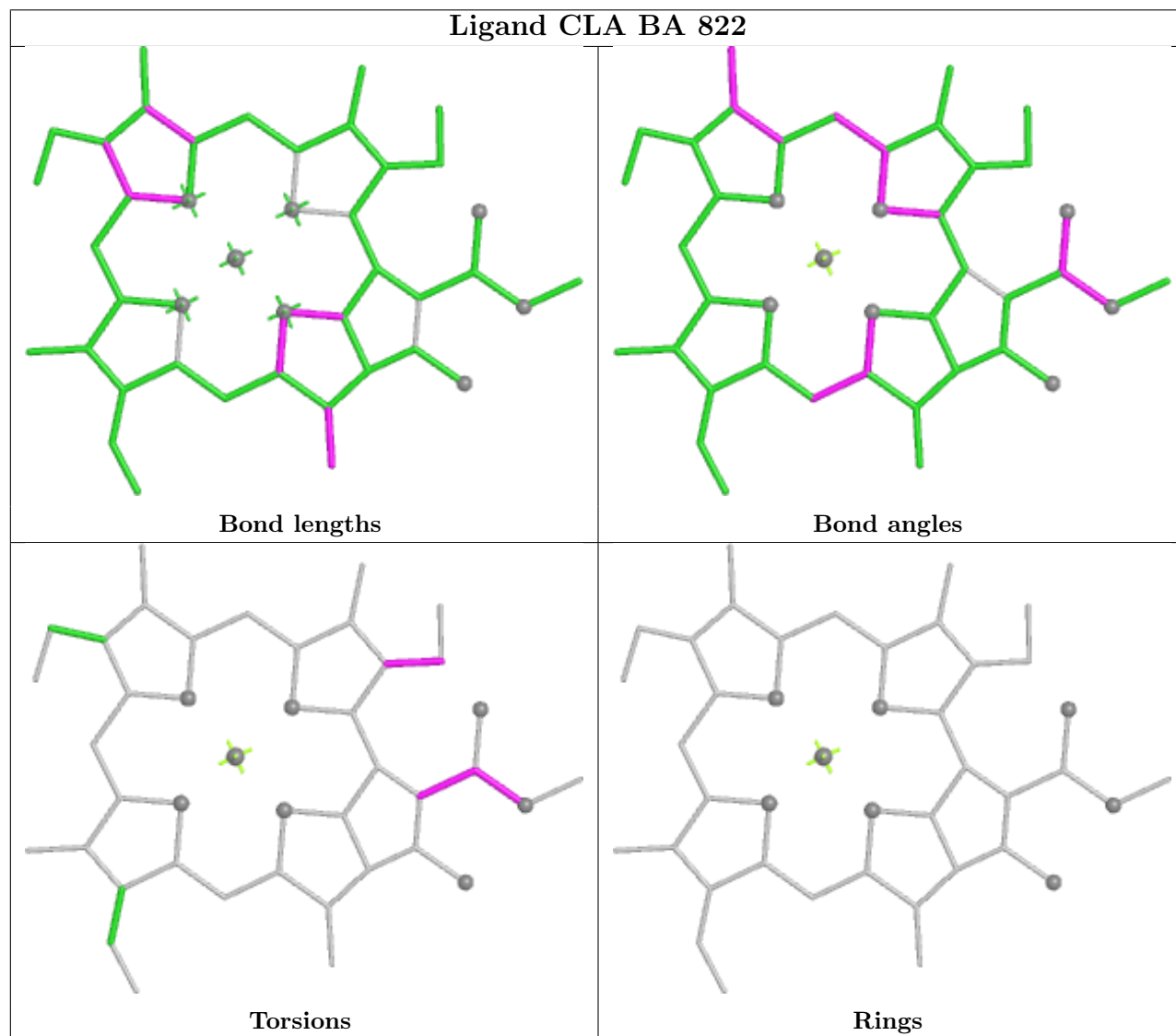
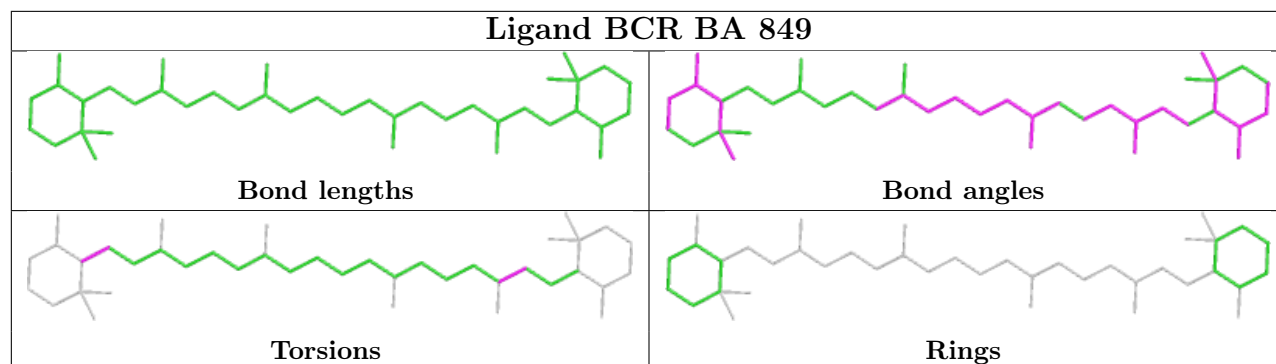
Bond angles

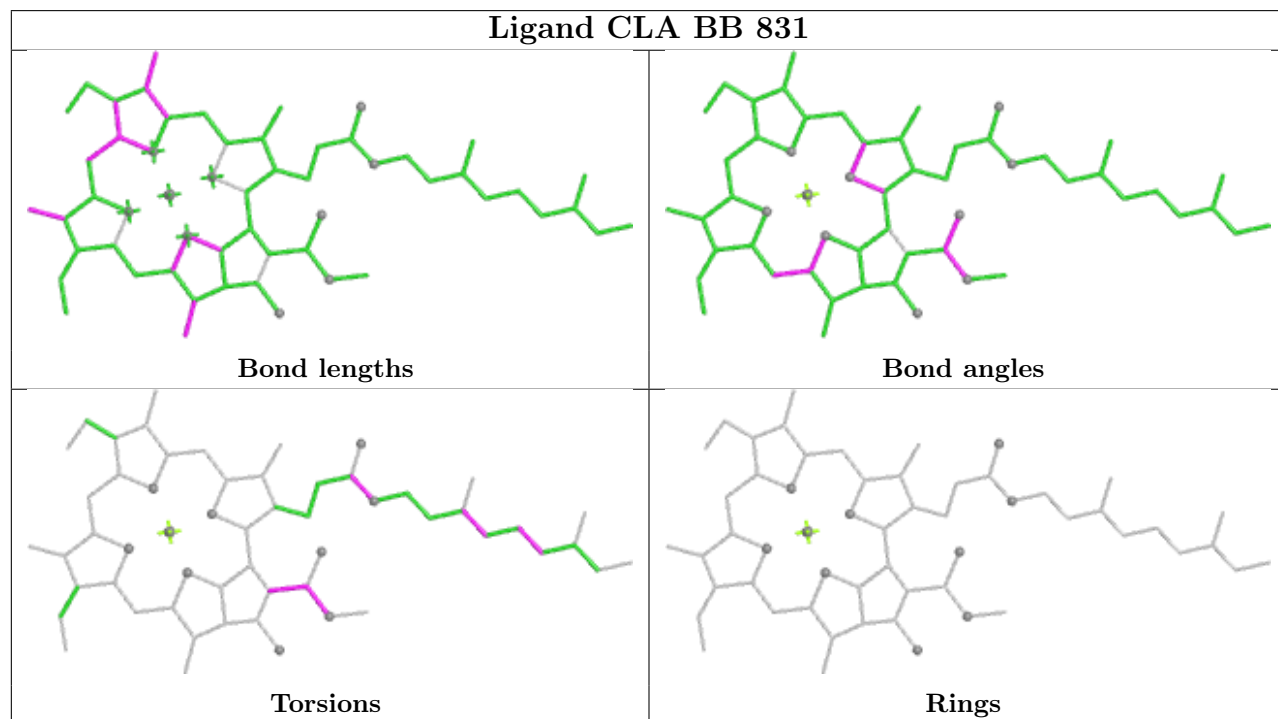
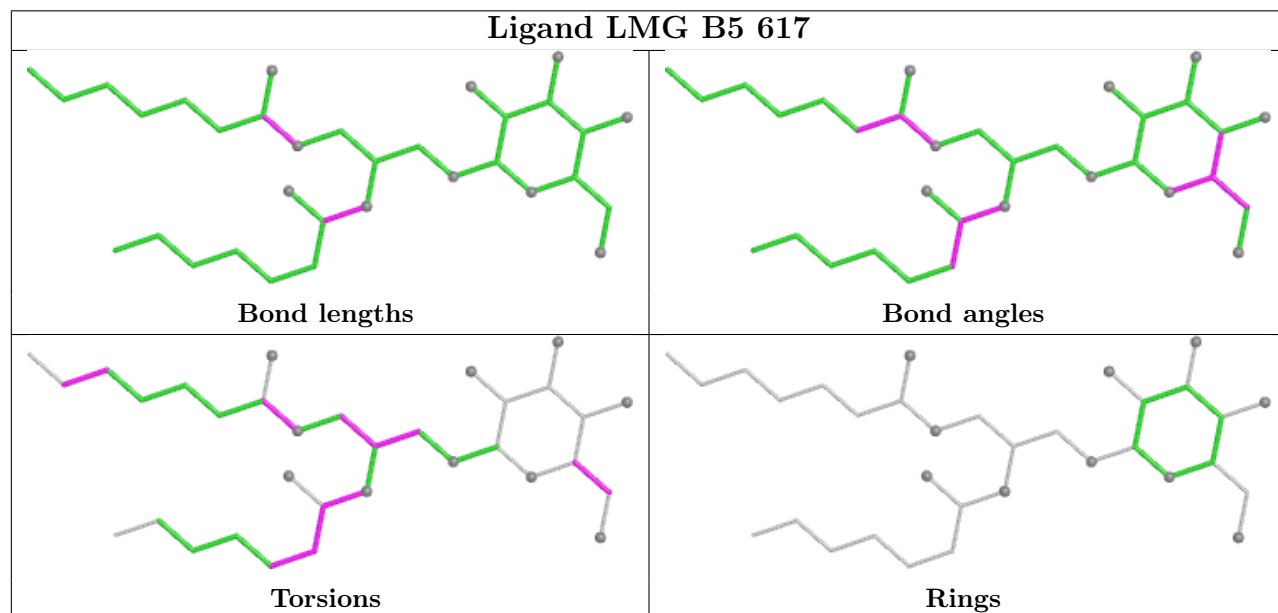
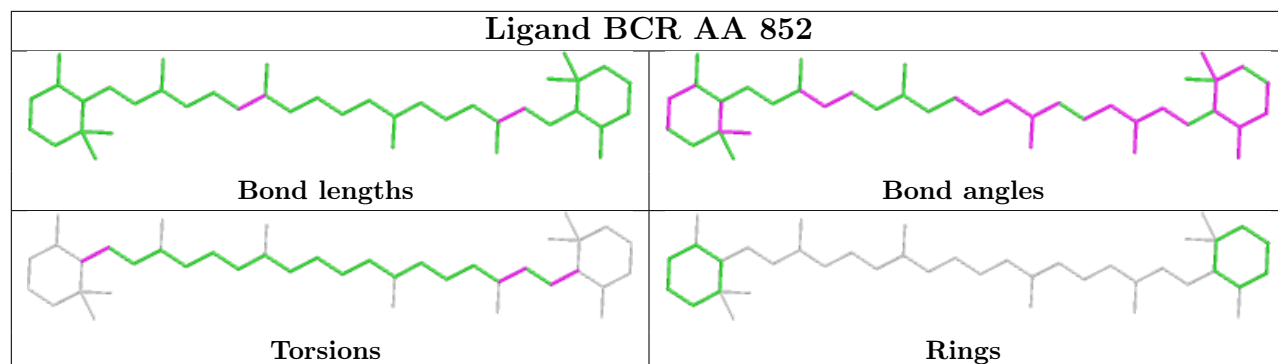


Torsions

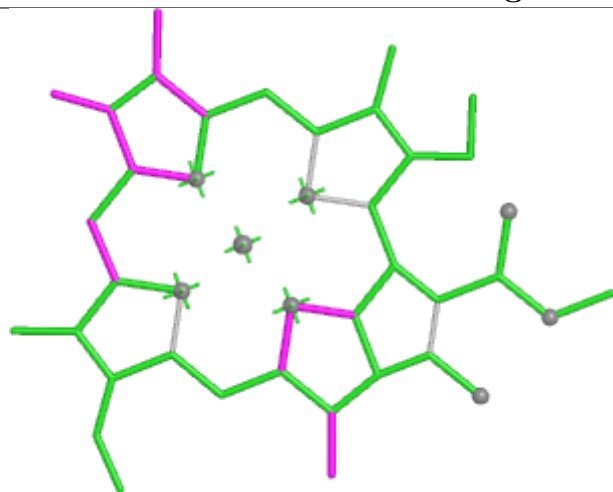


Rings

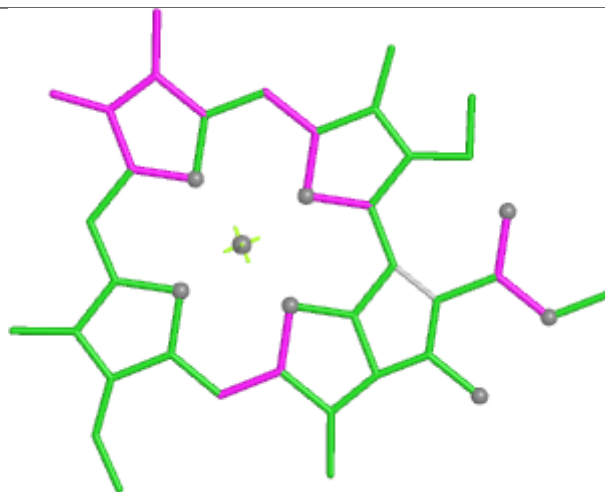




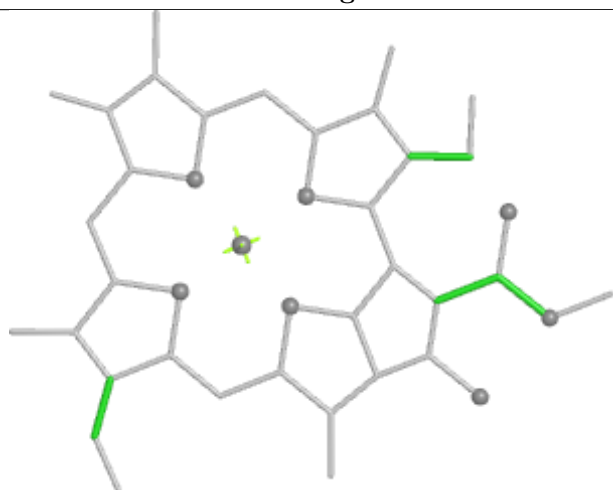
Ligand CLA A3 306



Bond lengths



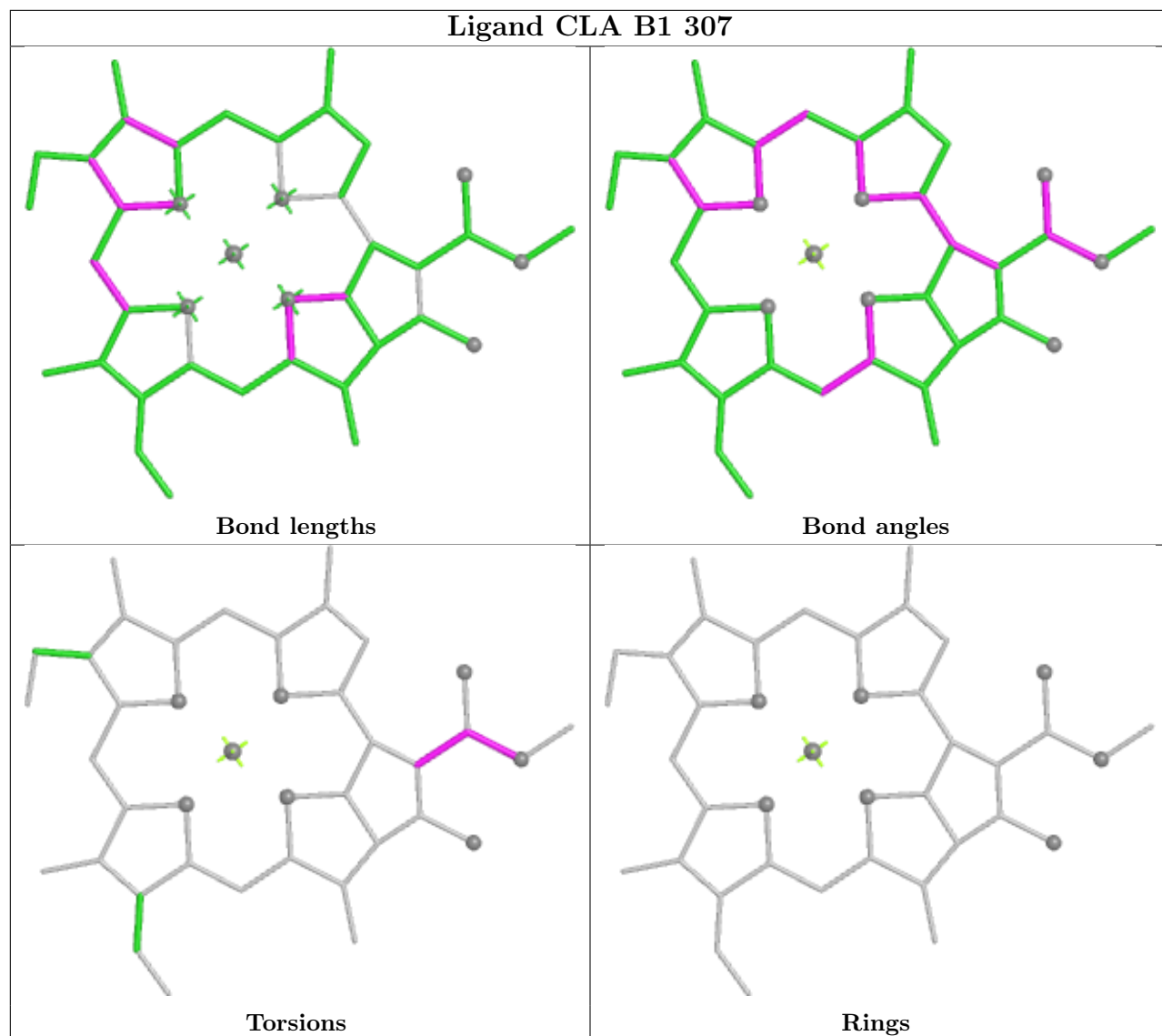
Bond angles

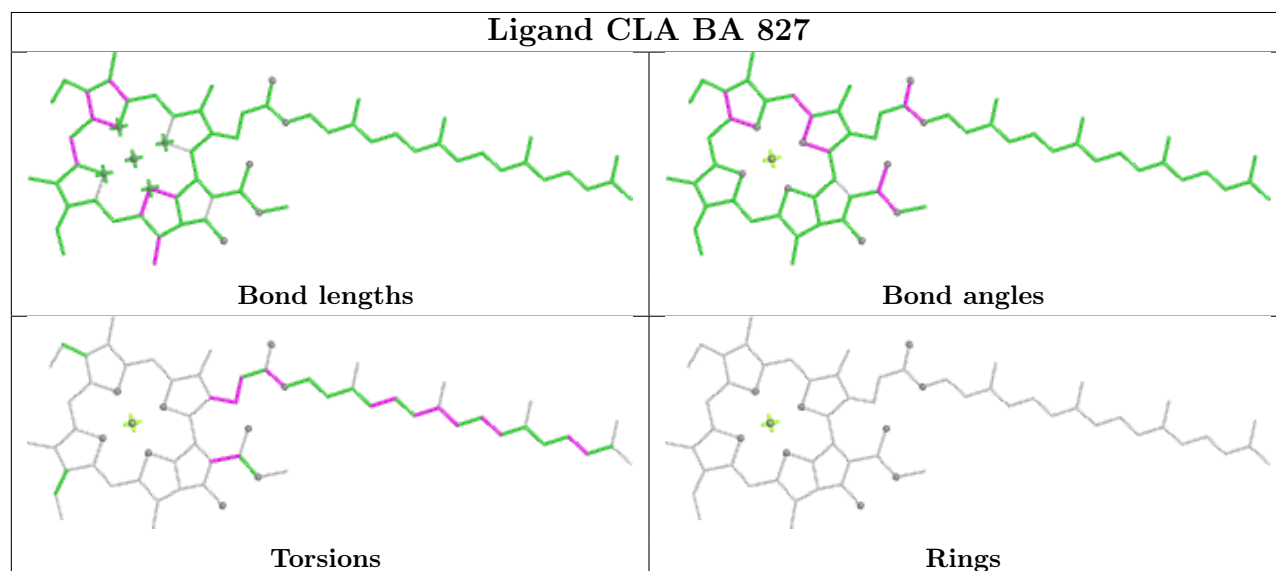
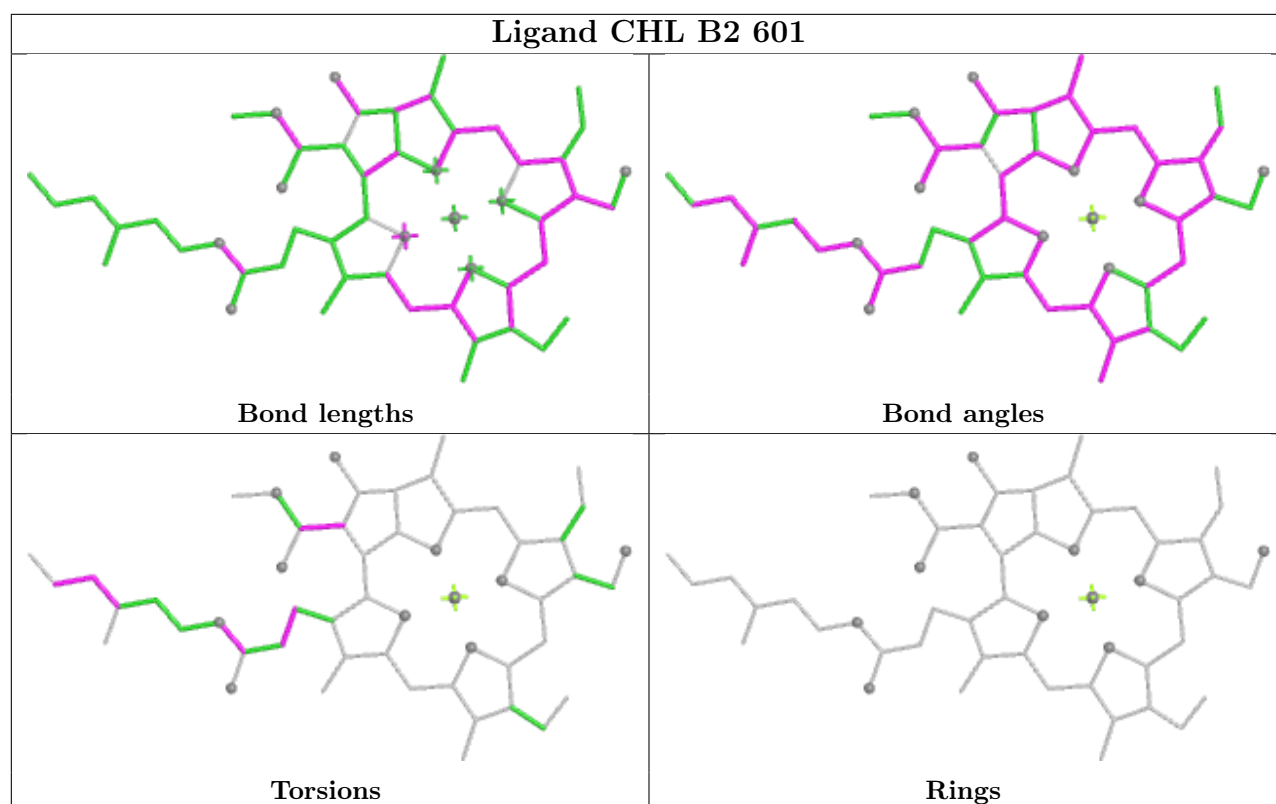


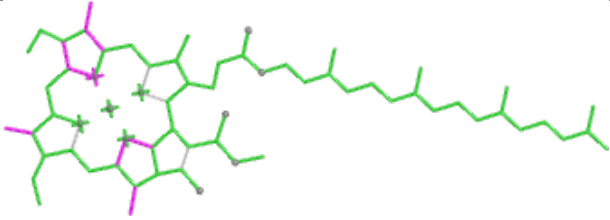
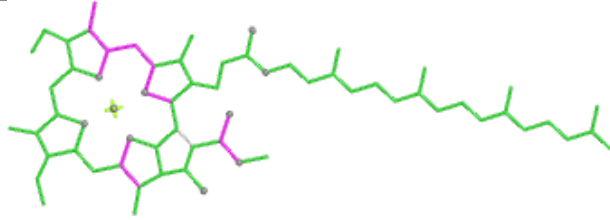
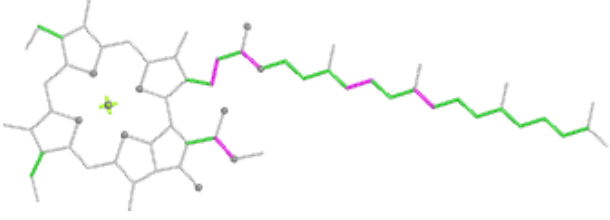
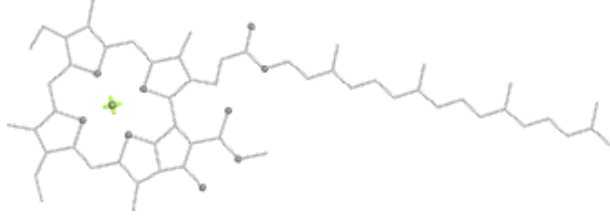
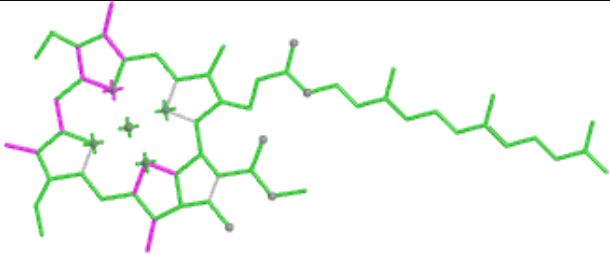
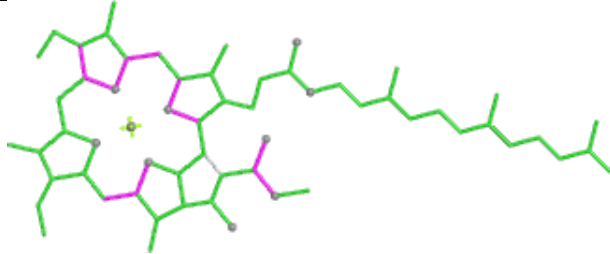
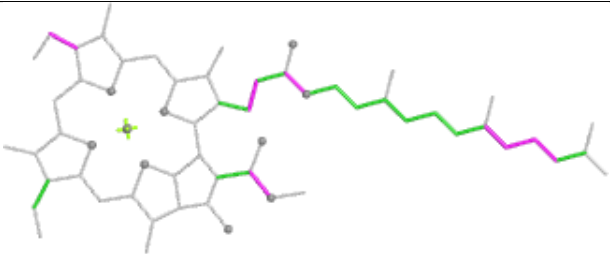
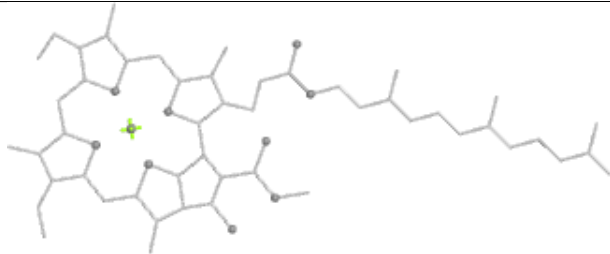
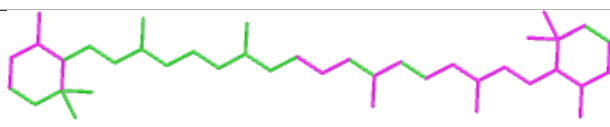
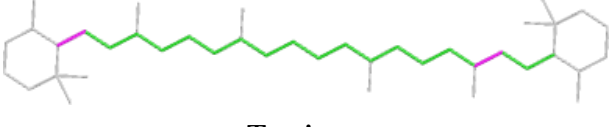
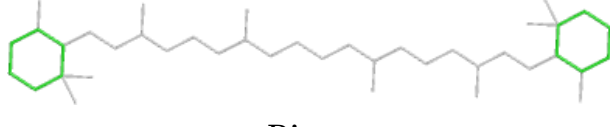
Torsions



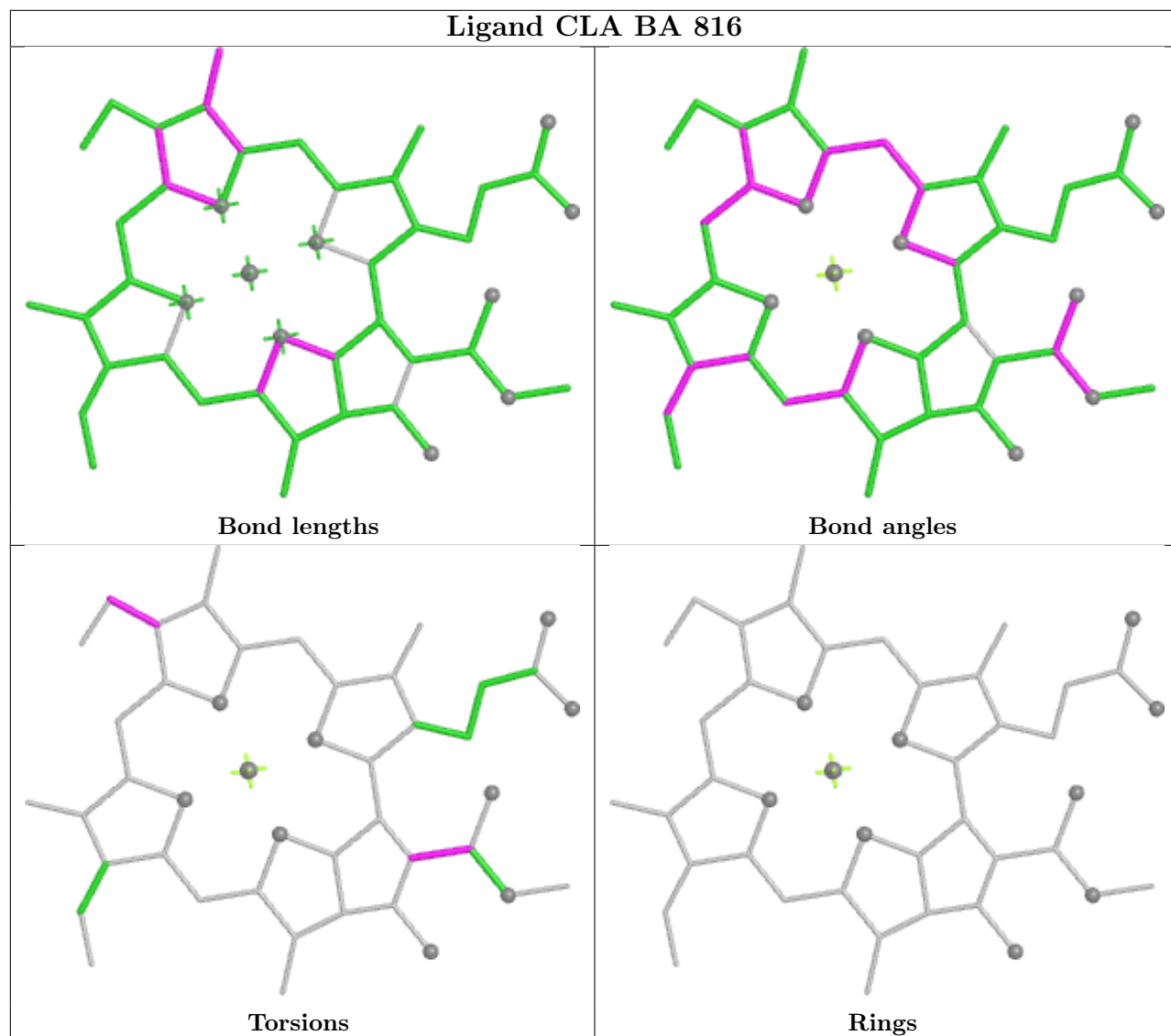
Rings



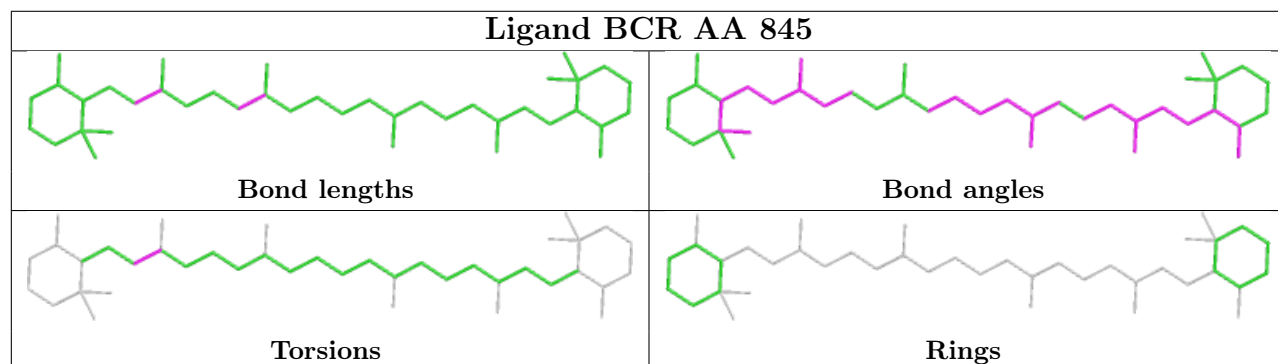


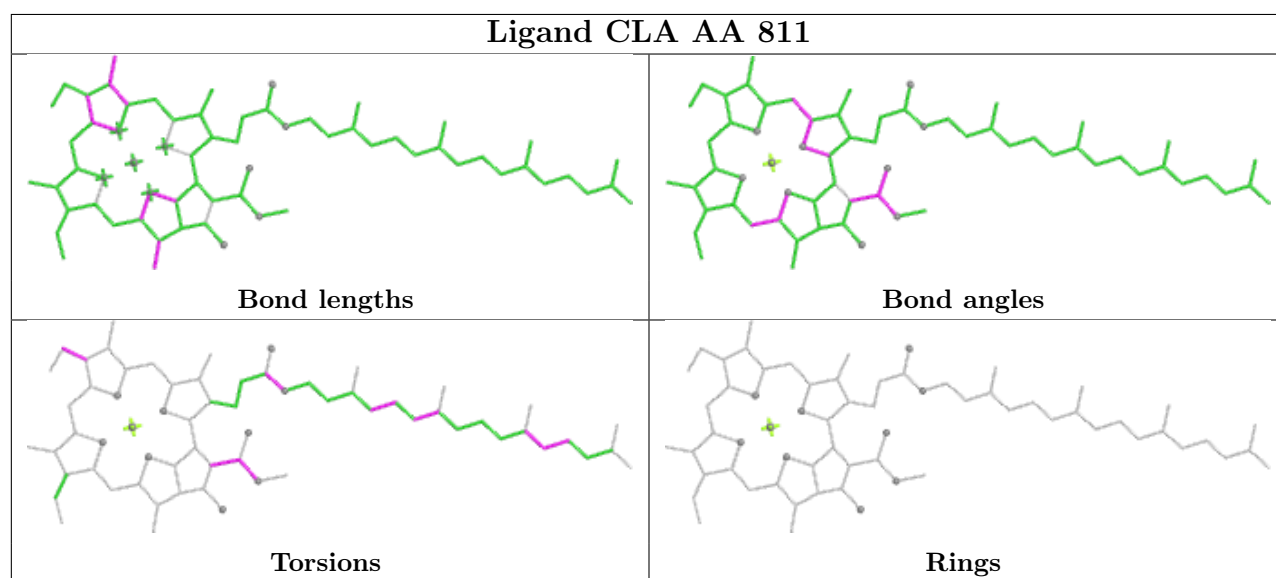
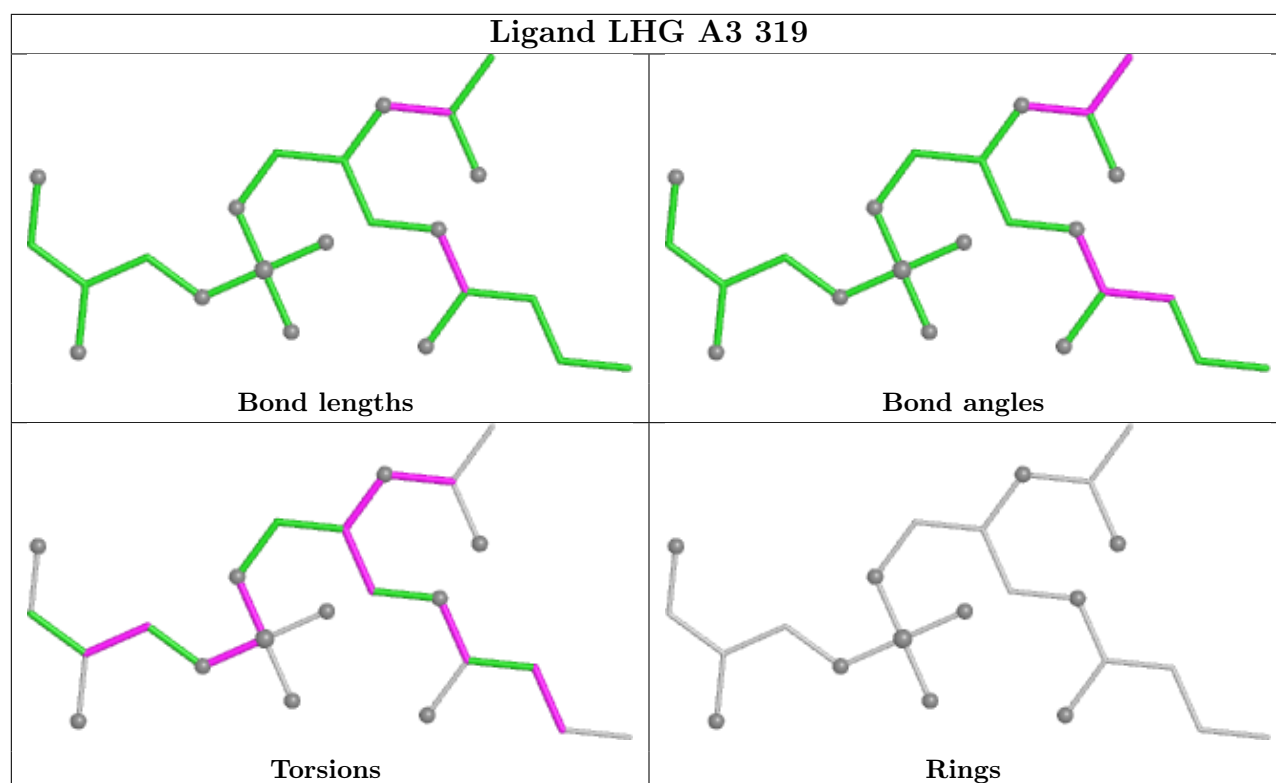
Ligand CLA AB 840	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B5 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A3 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

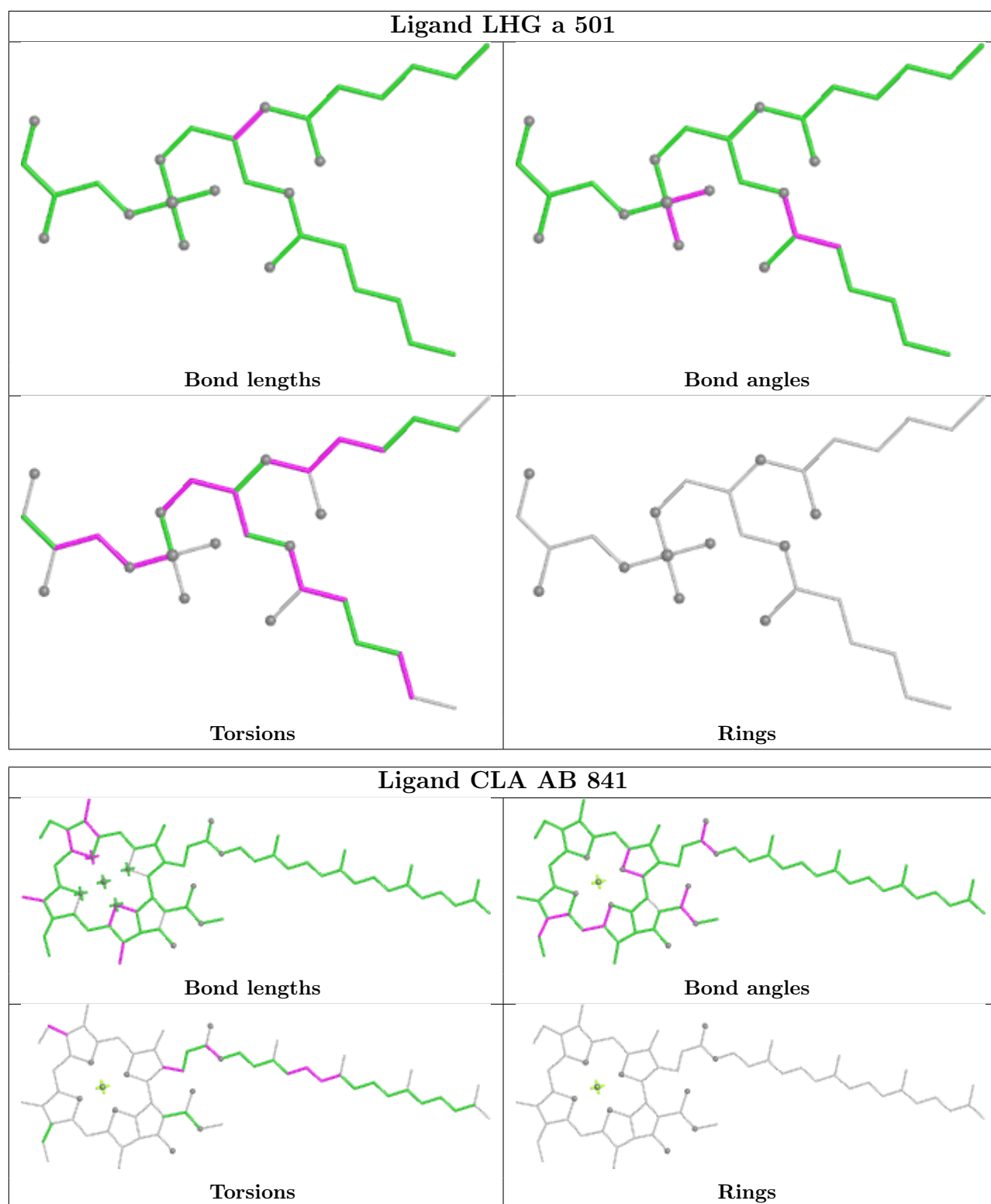
Ligand CLA BA 816



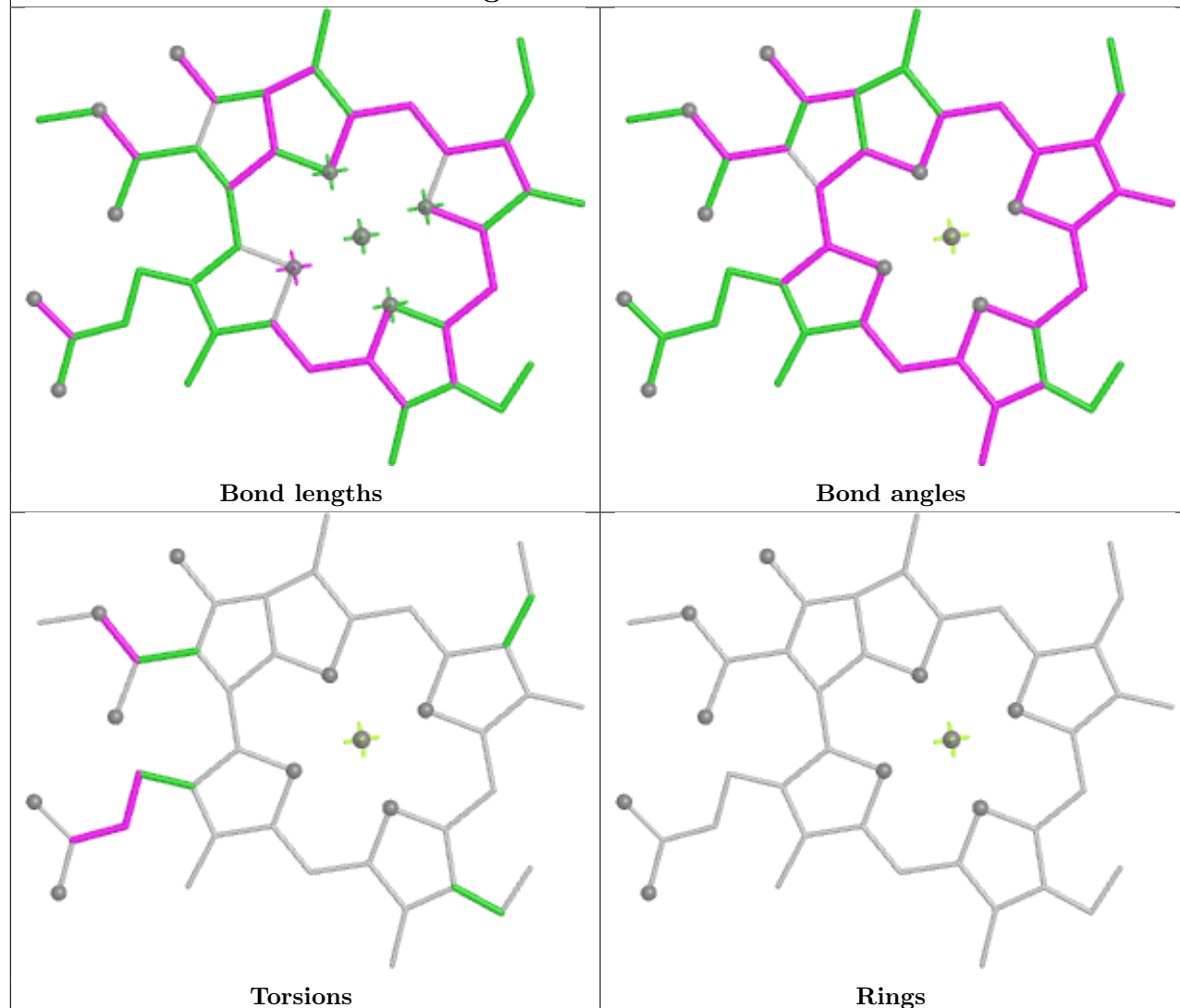
Ligand BCR AA 845



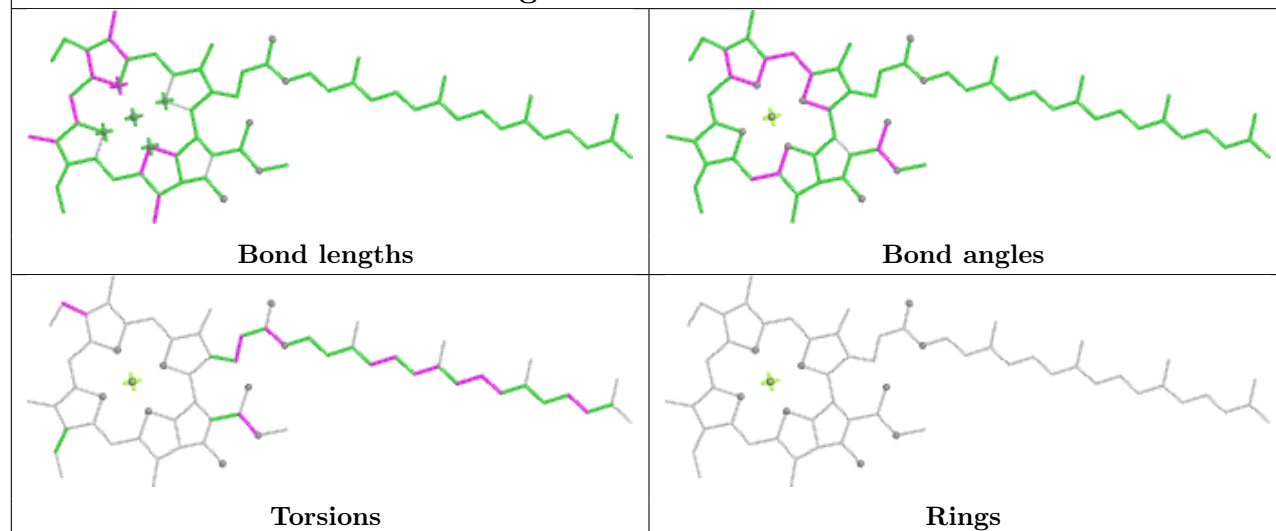


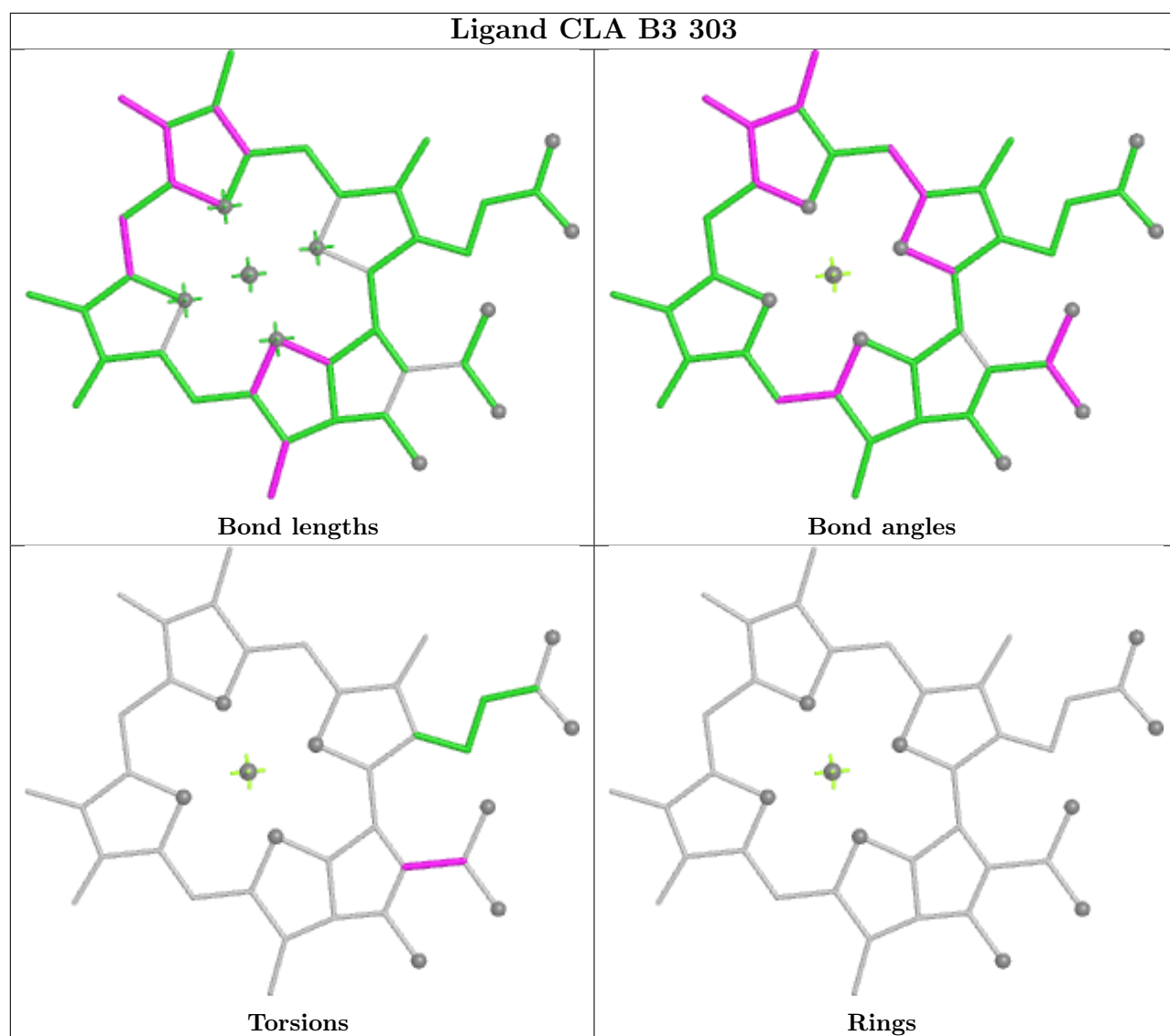


Ligand CHL B3 306

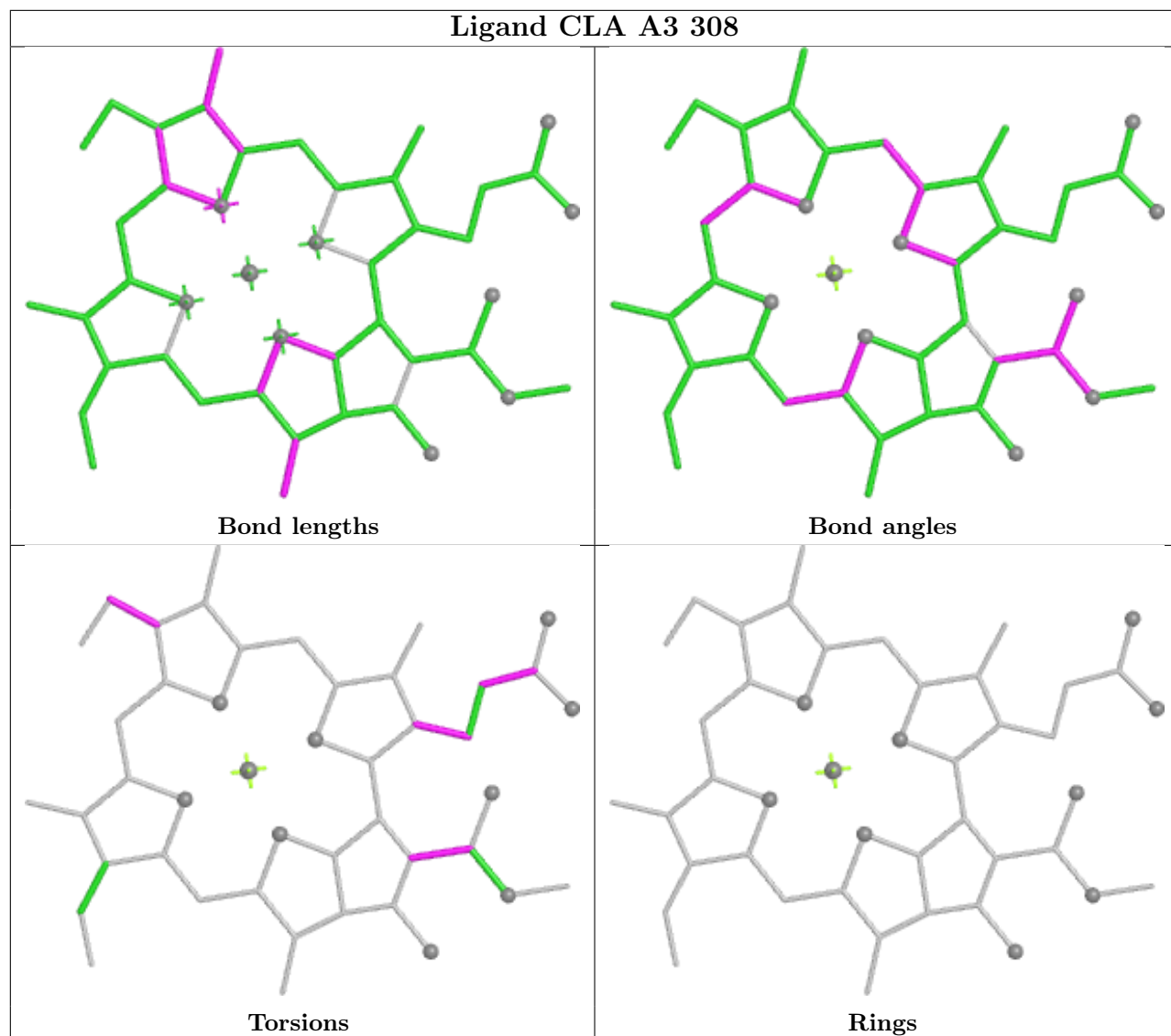


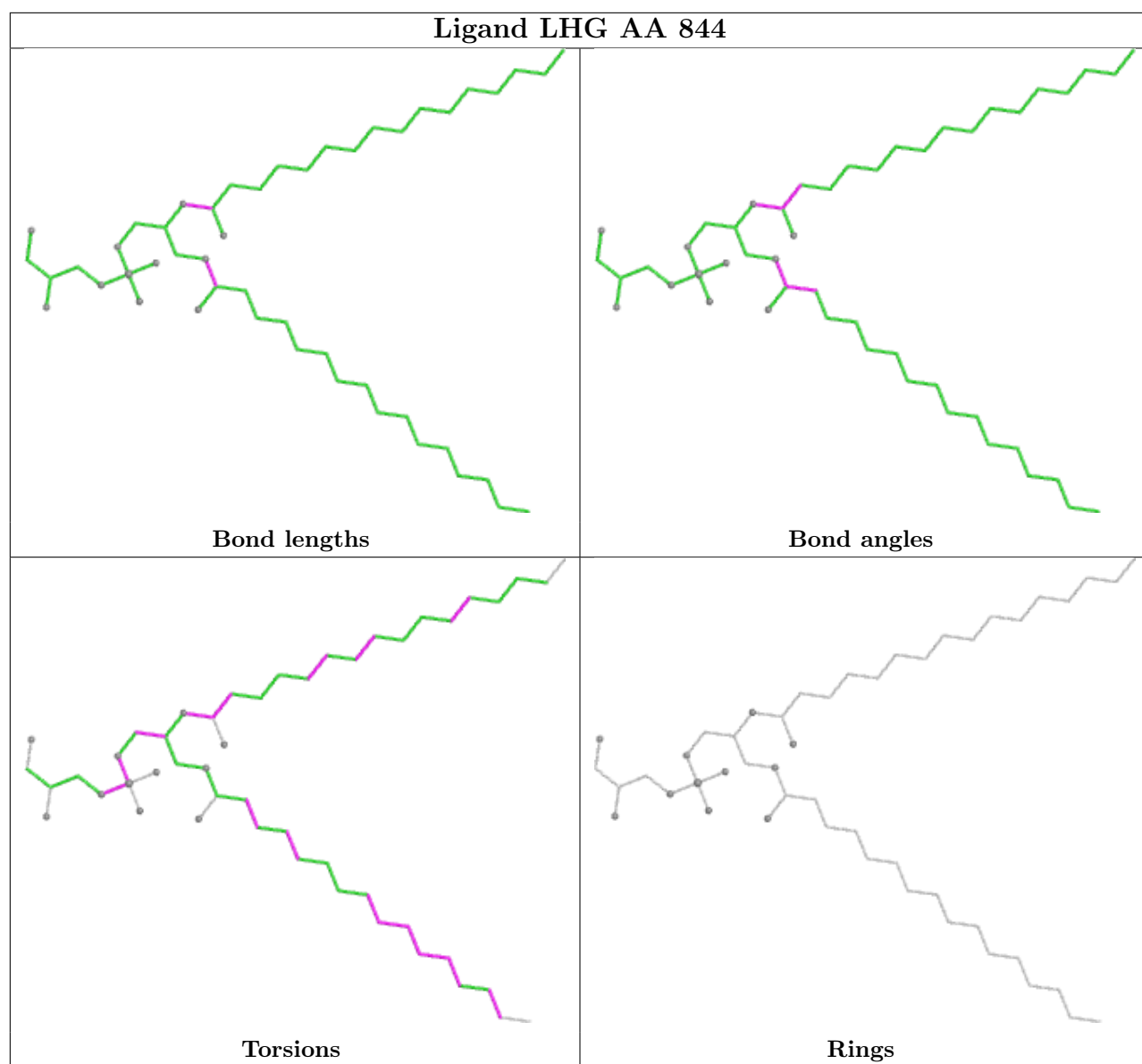
Ligand CLA BB 843



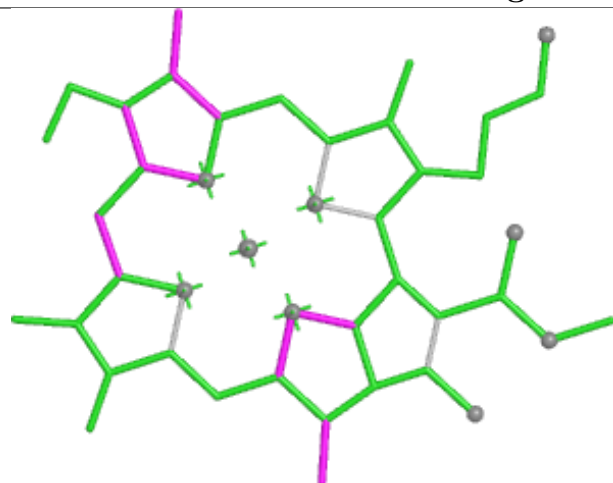


Ligand CLA A3 308

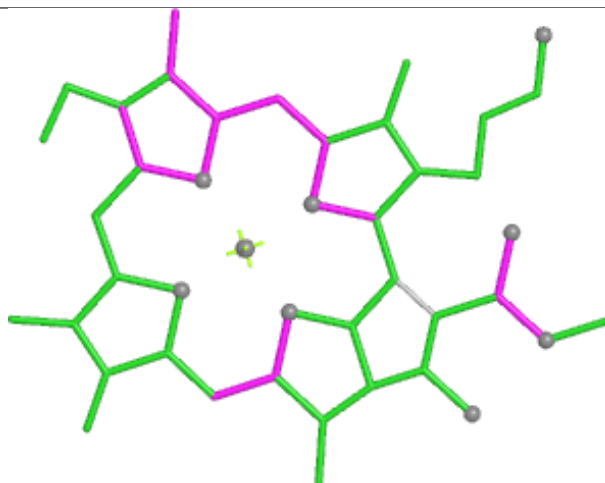




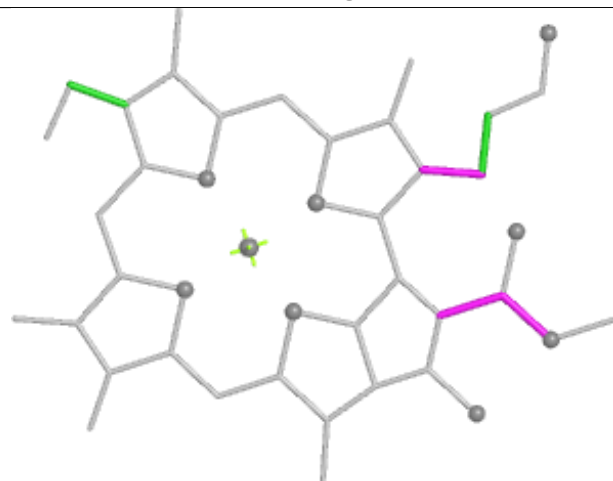
Ligand CLA B2 604



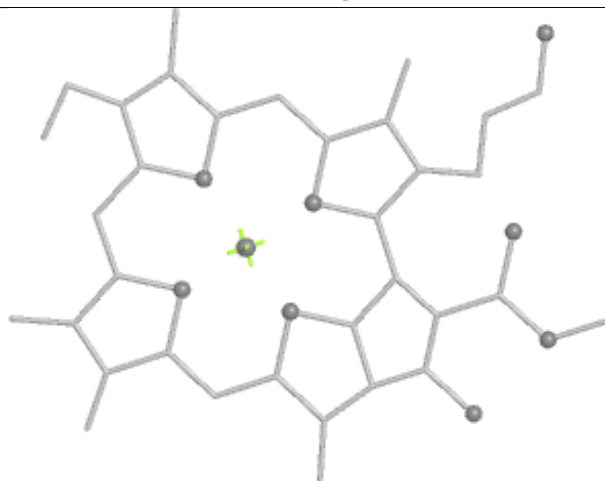
Bond lengths



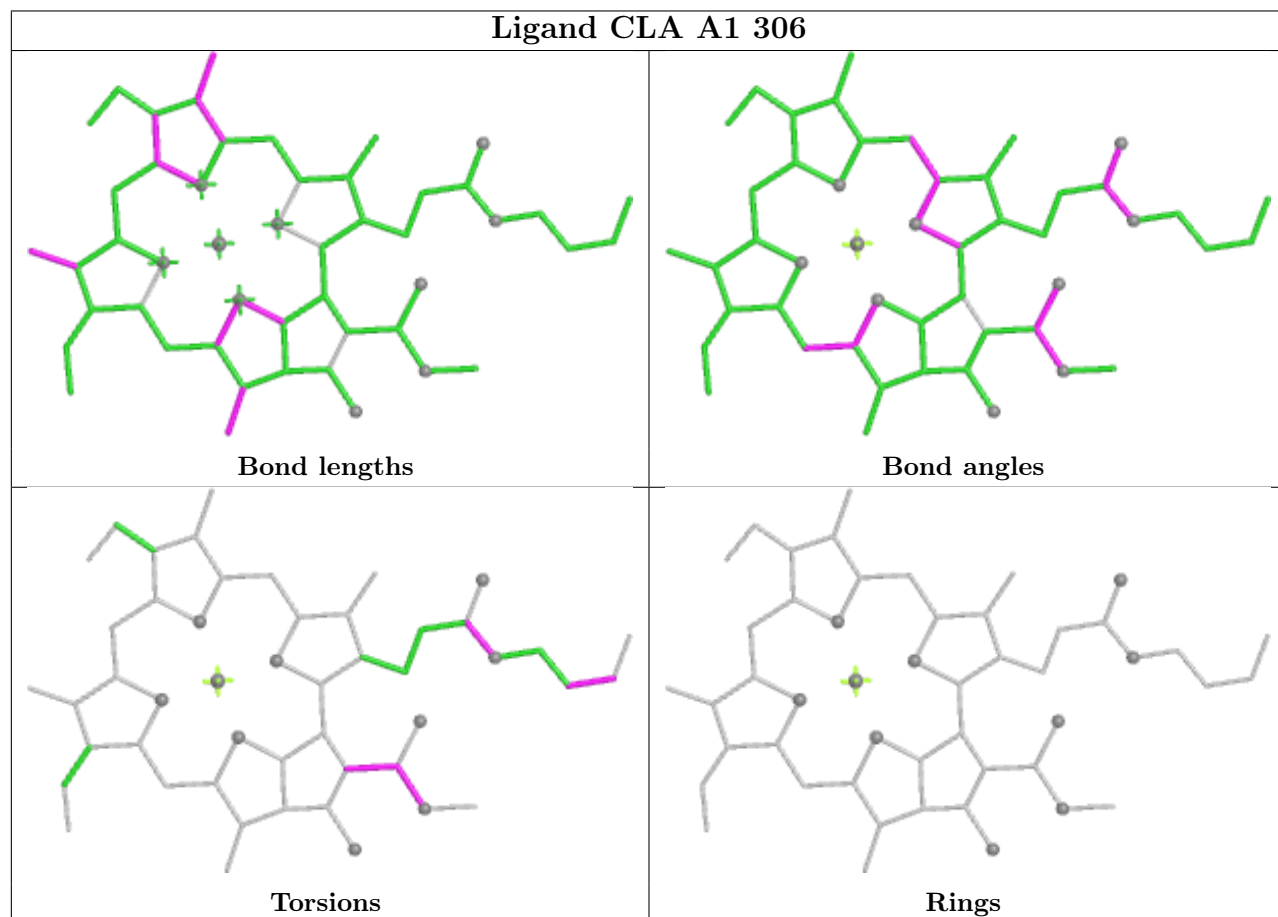
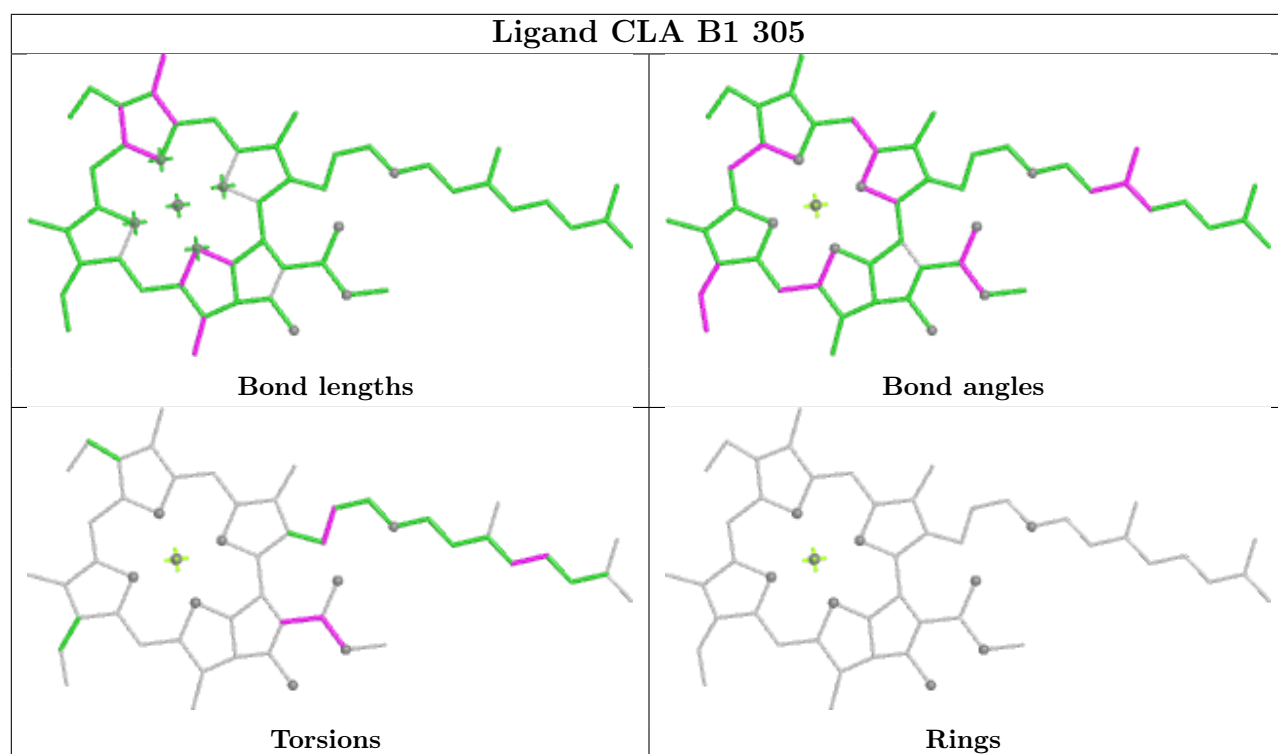
Bond angles

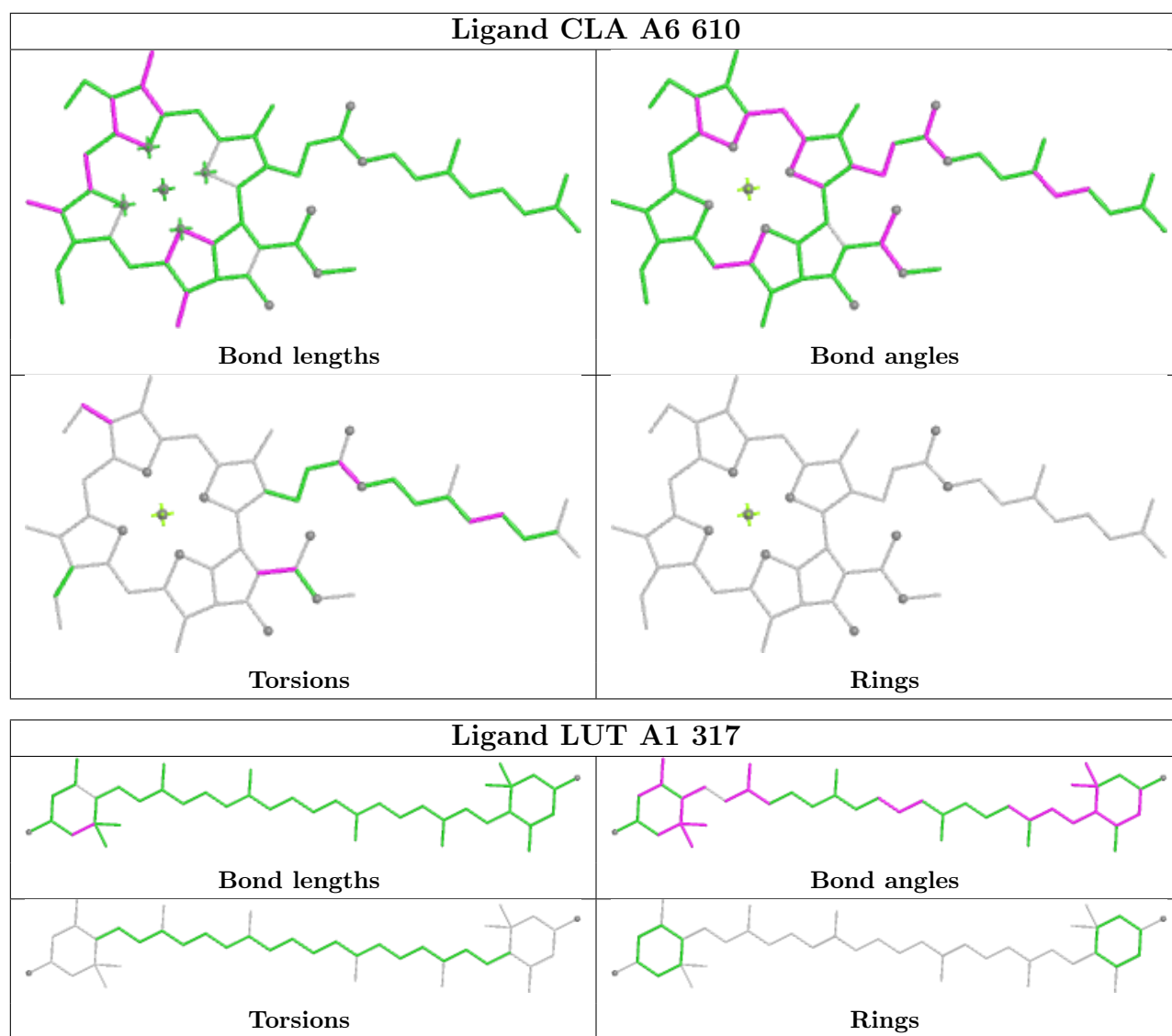


Torsions

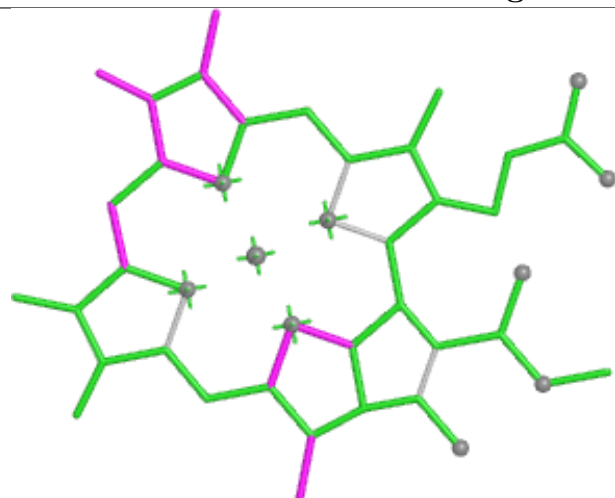


Rings

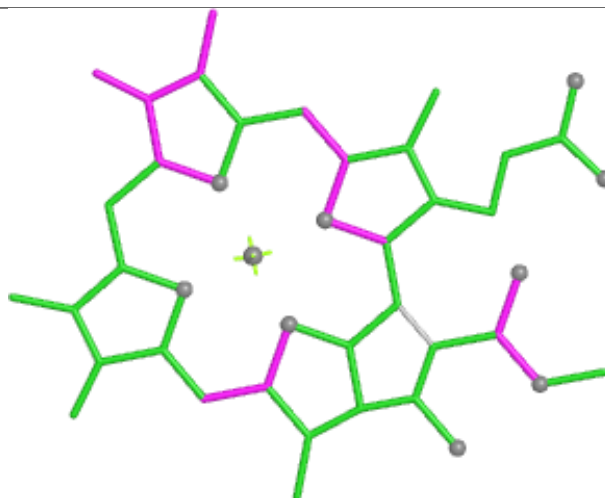




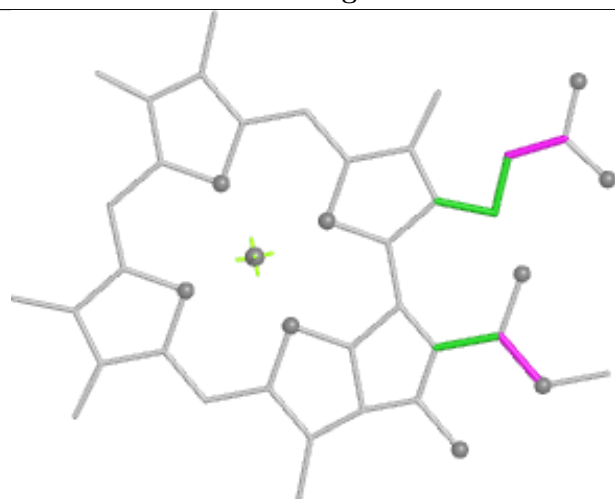
Ligand CLA A4 303



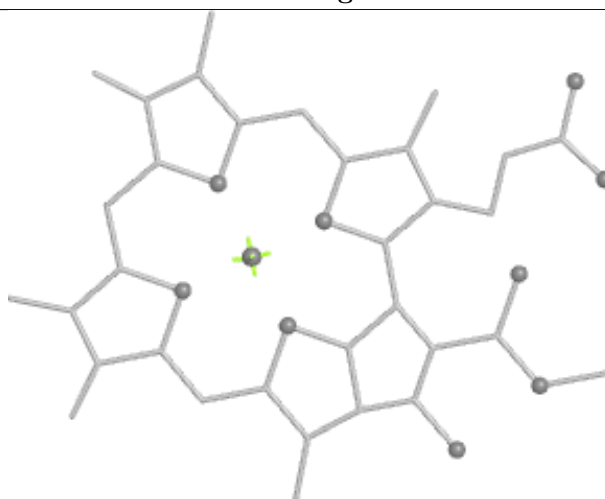
Bond lengths



Bond angles

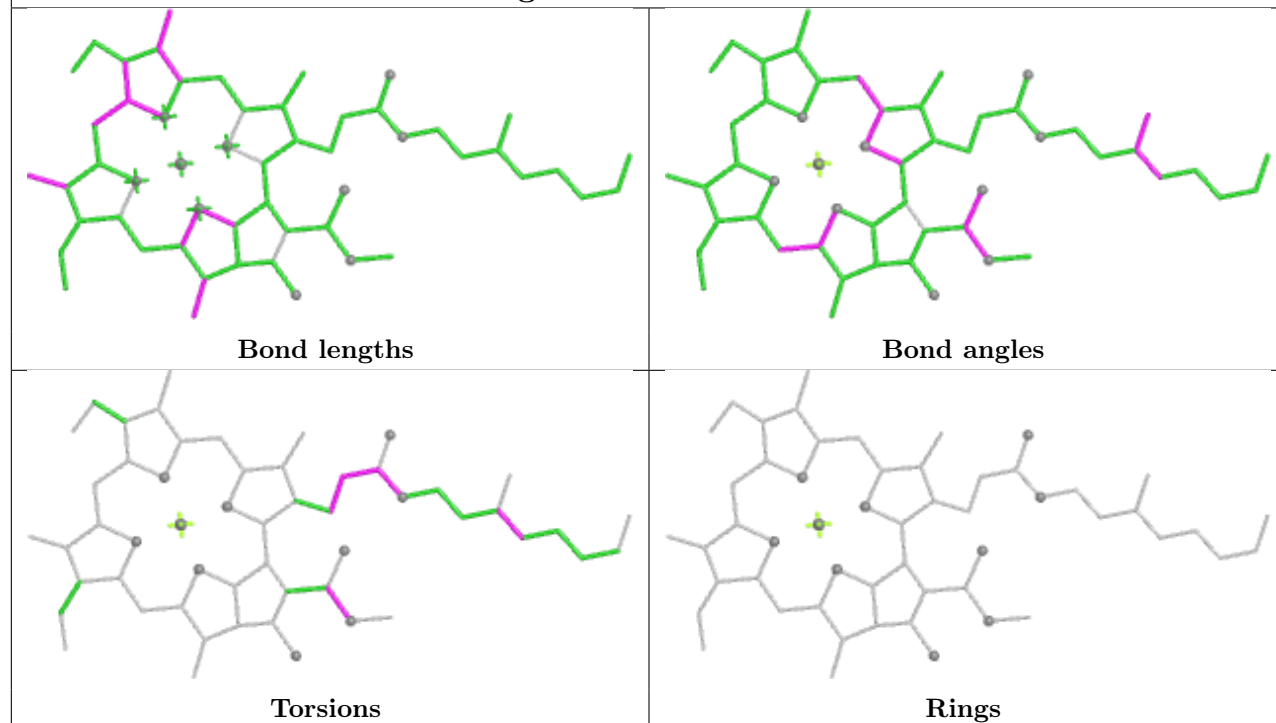


Torsions

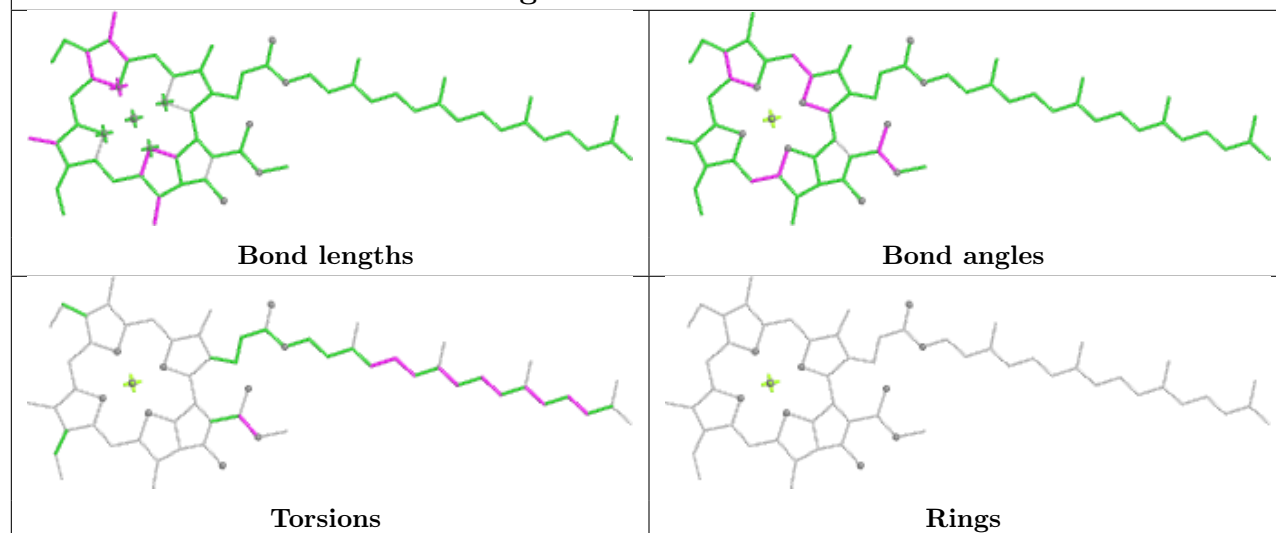


Rings

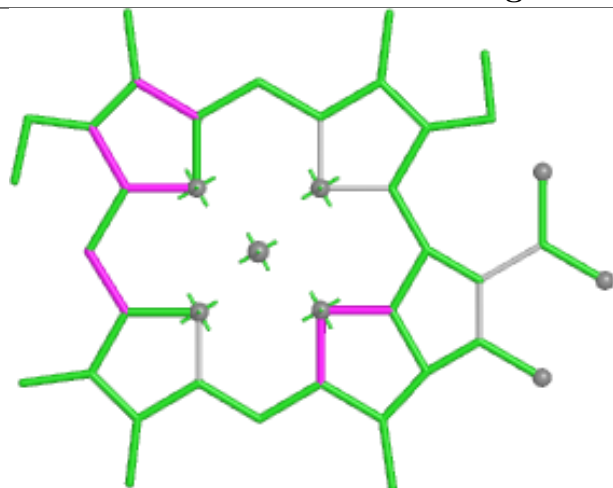
Ligand CLA AA 812



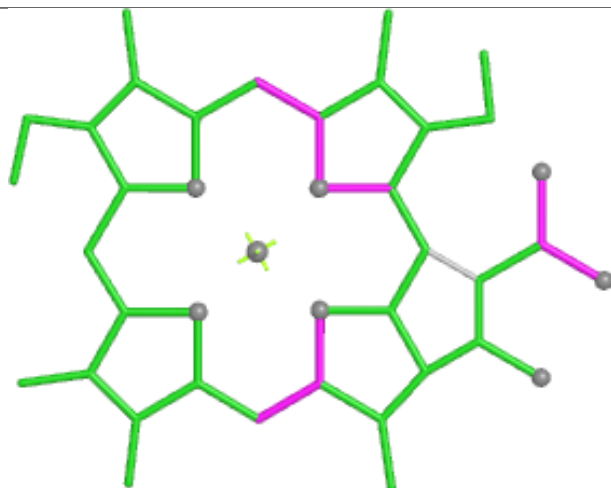
Ligand CLA BB 808



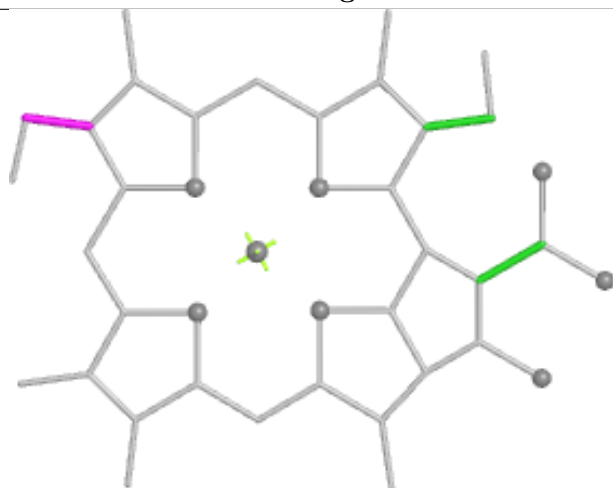
Ligand CLA B3 309



Bond lengths



Bond angles

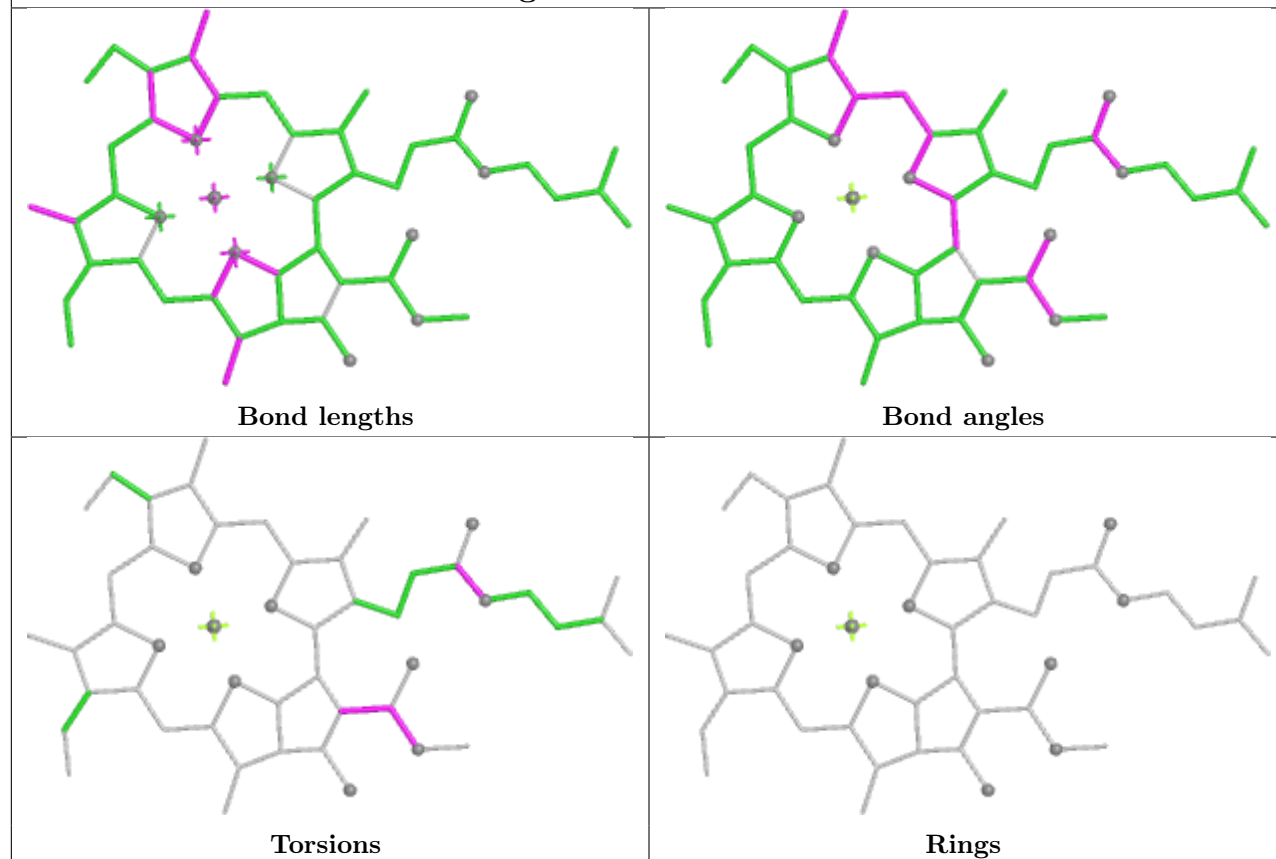


Torsions

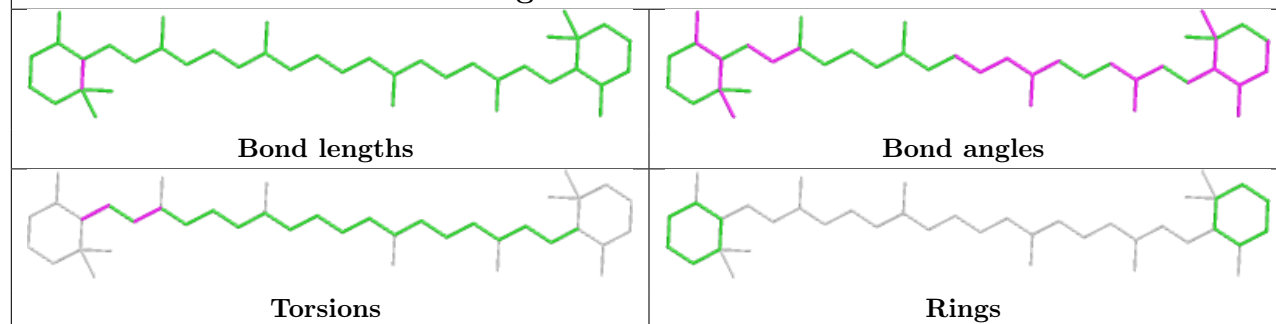


Rings

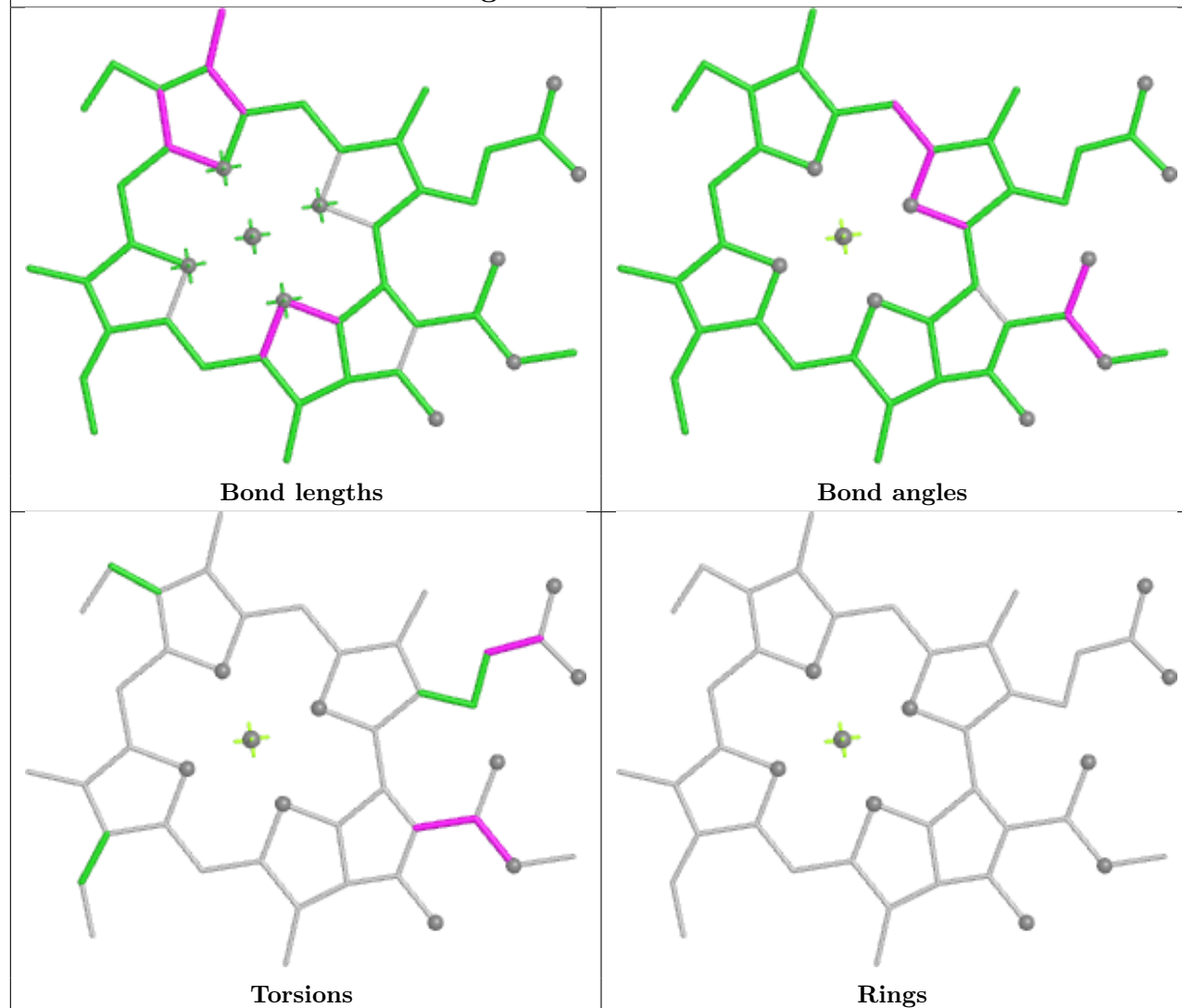
Ligand CLA AB 837



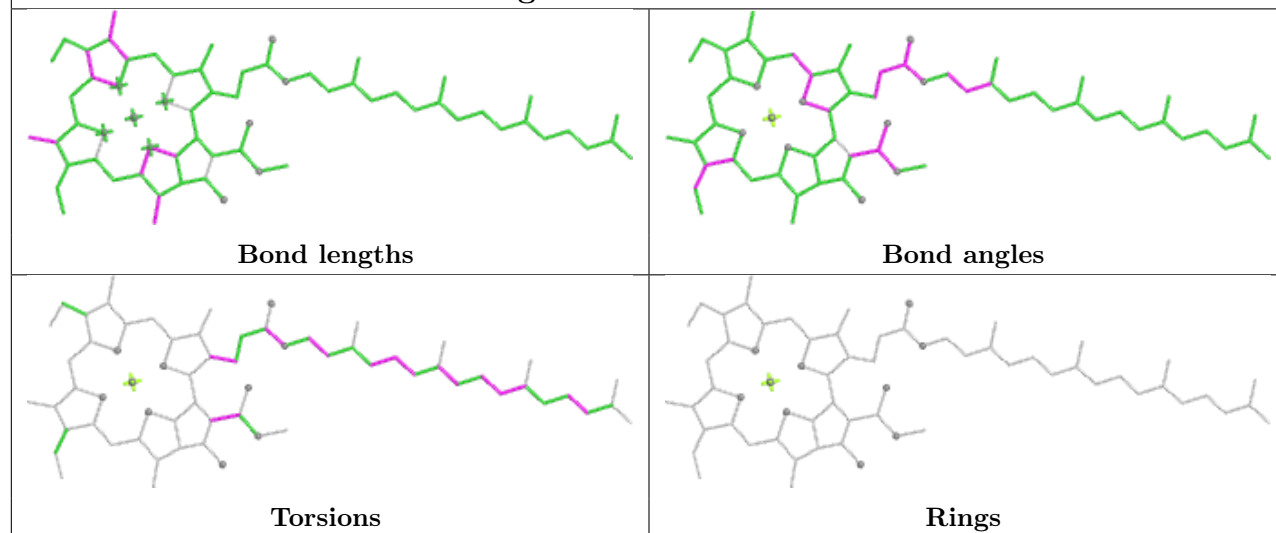
Ligand BCR AA 848



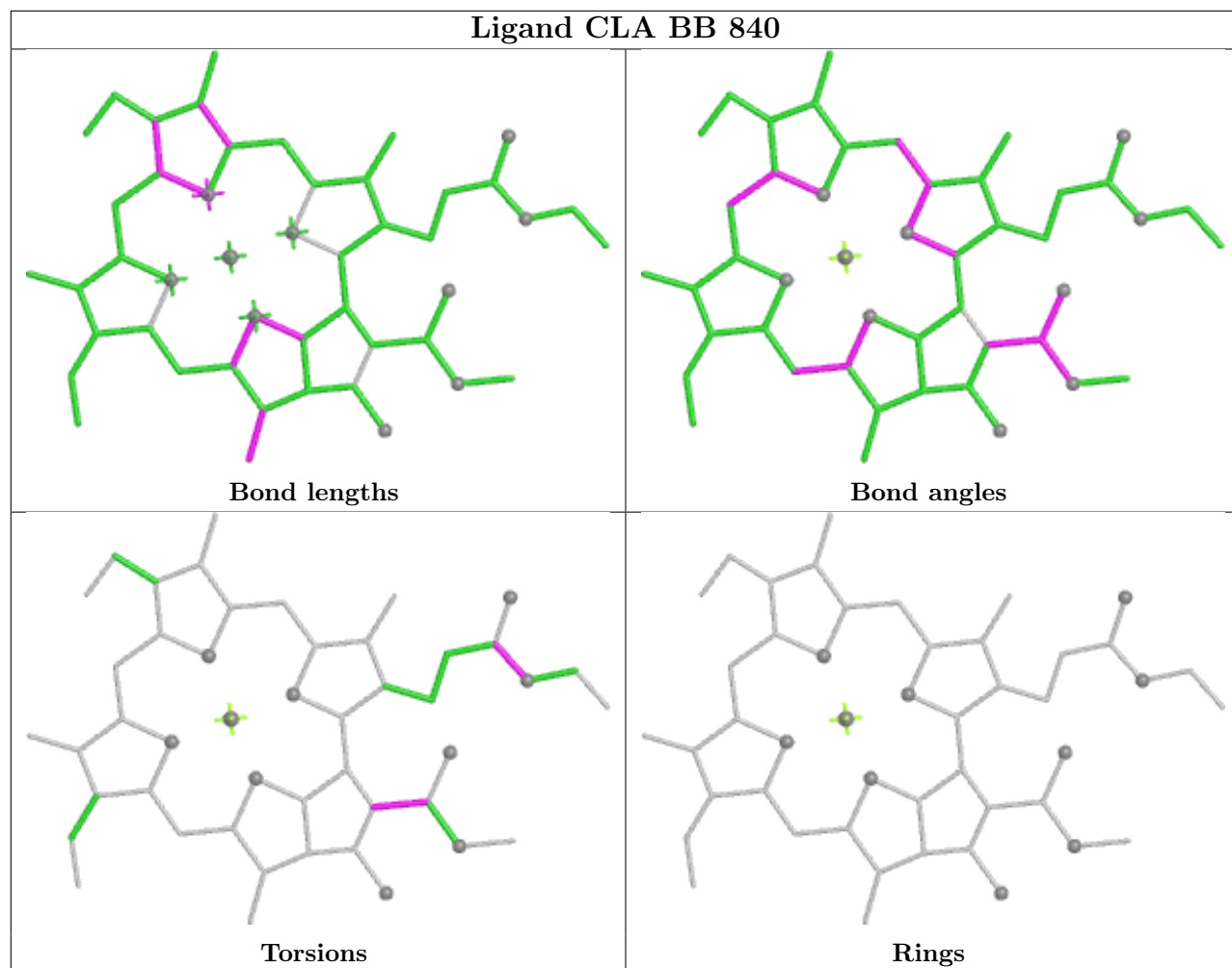
Ligand CLA BA 835



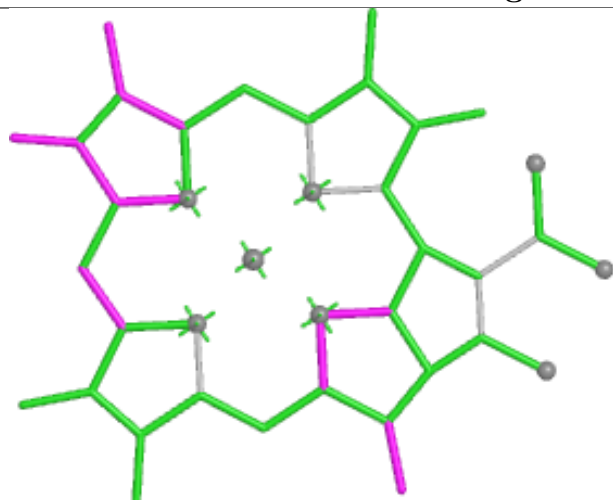
Ligand CLA AA 803



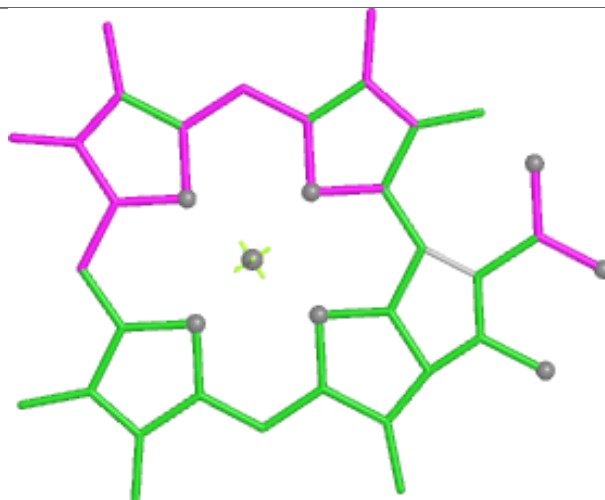
Ligand CLA BB 840



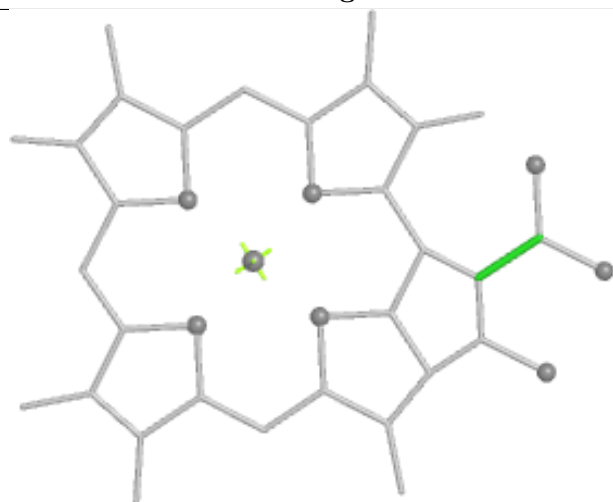
Ligand CLA B1 315



Bond lengths



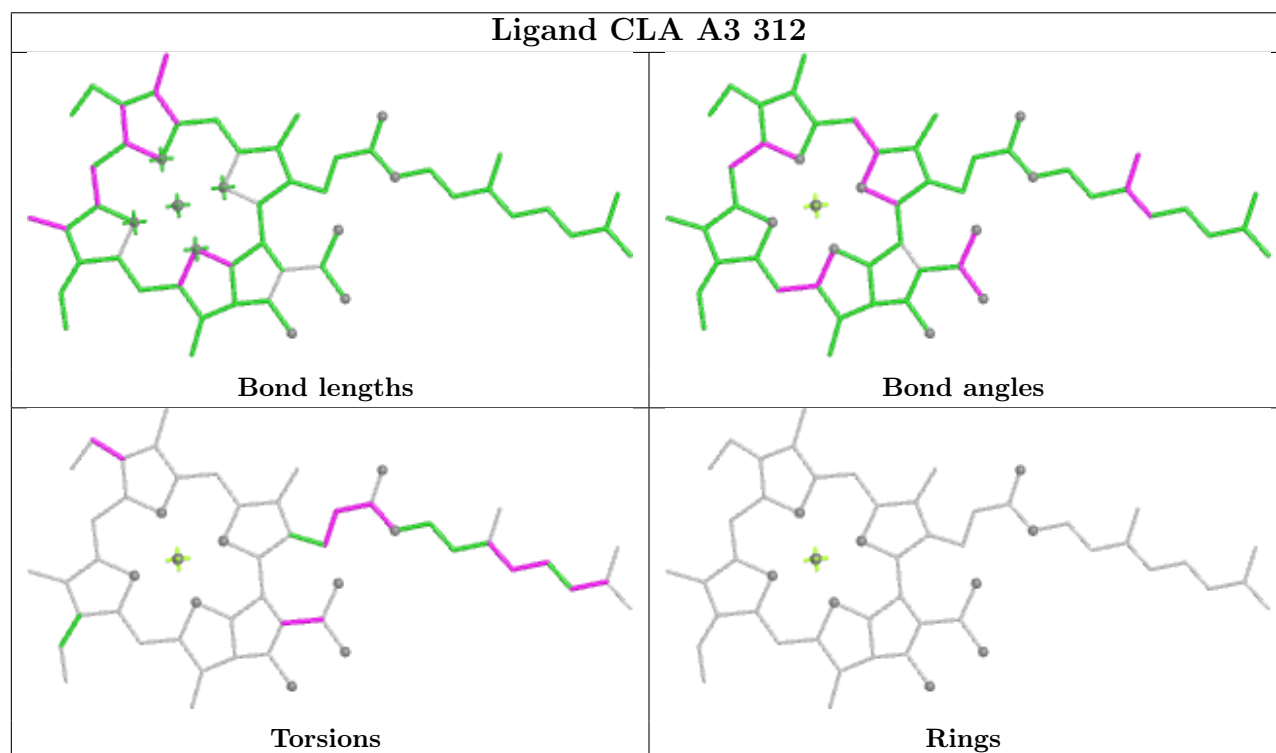
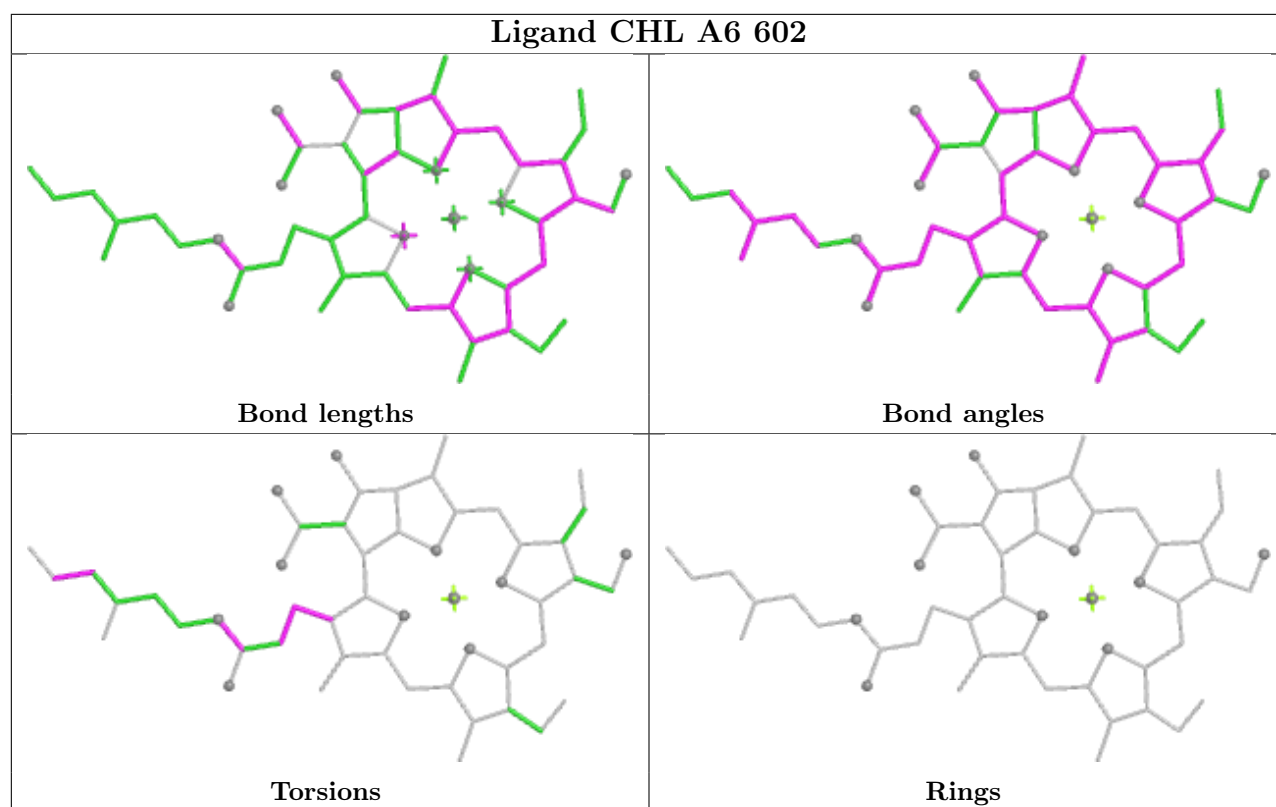
Bond angles

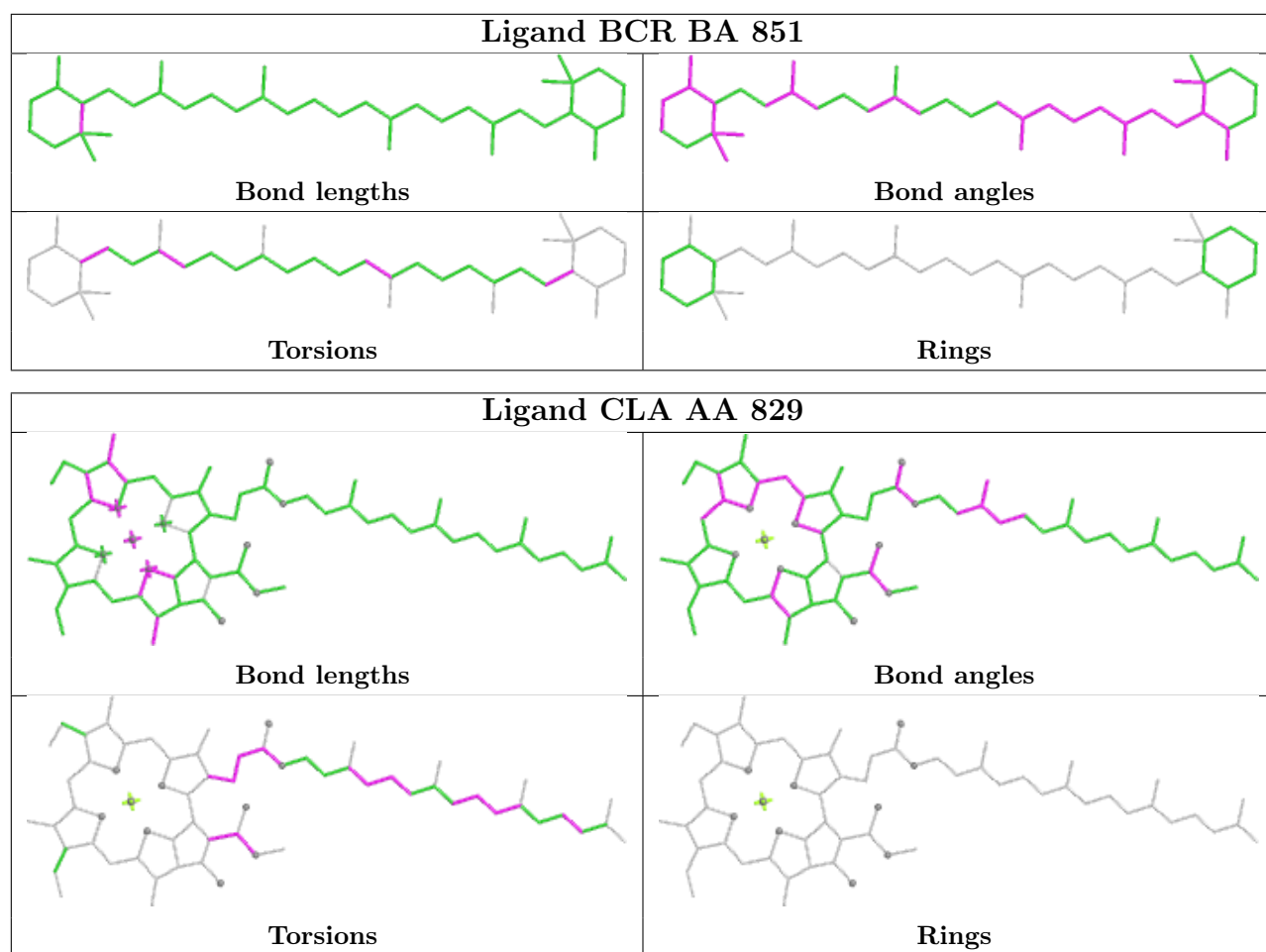


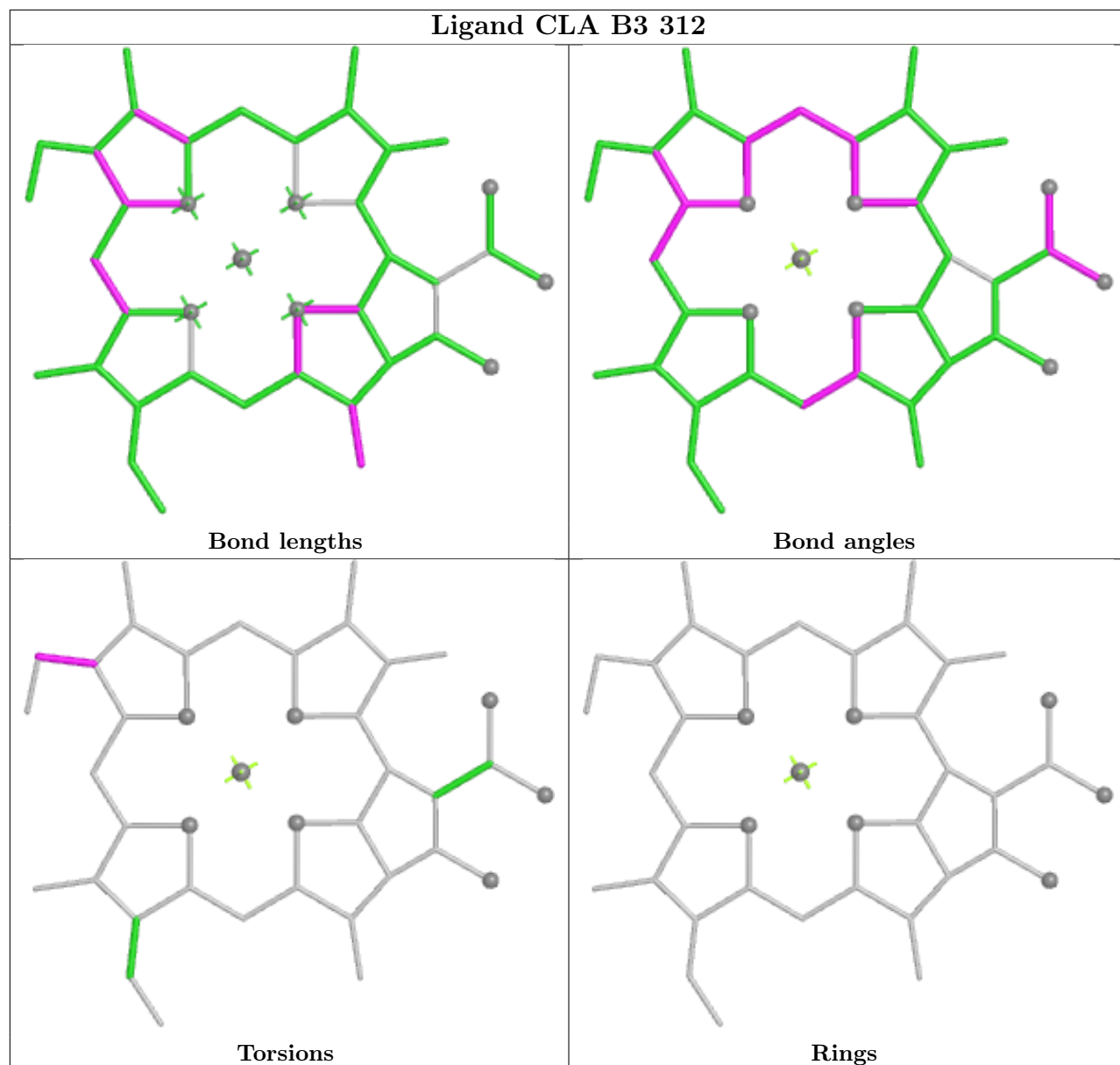
Torsions



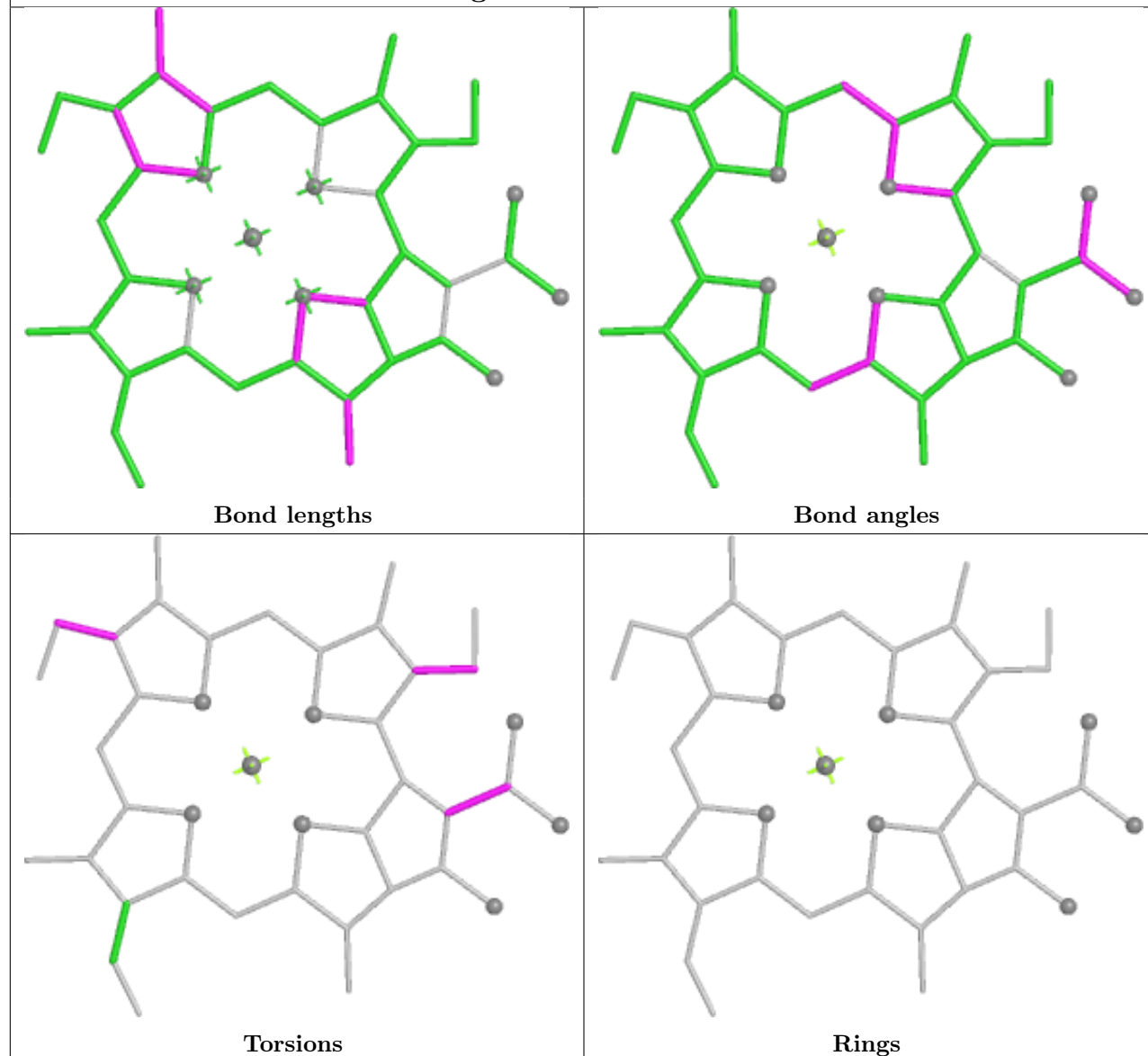
Rings



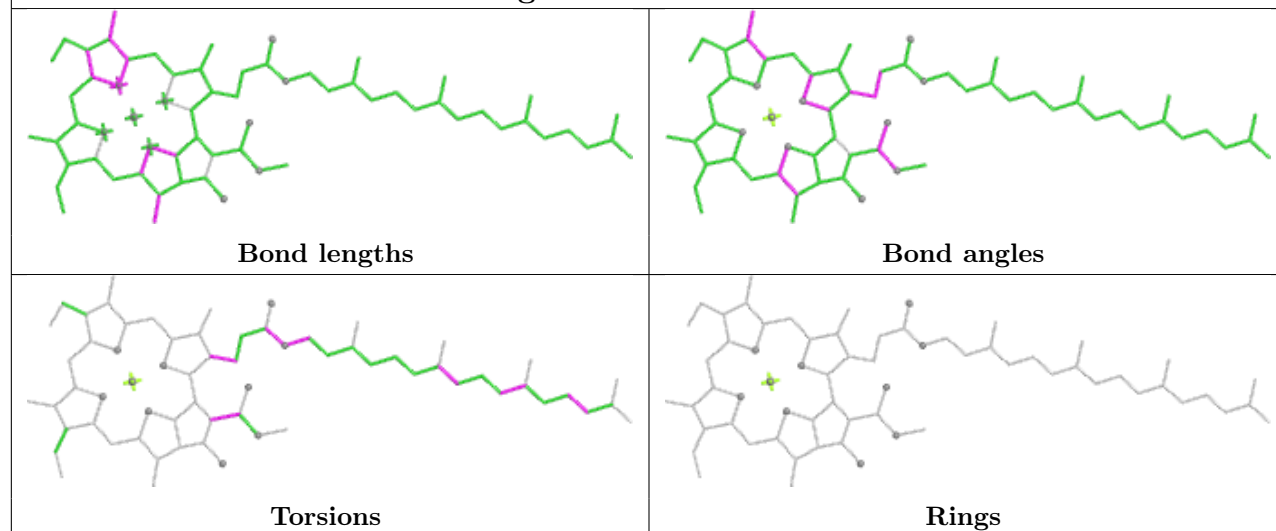


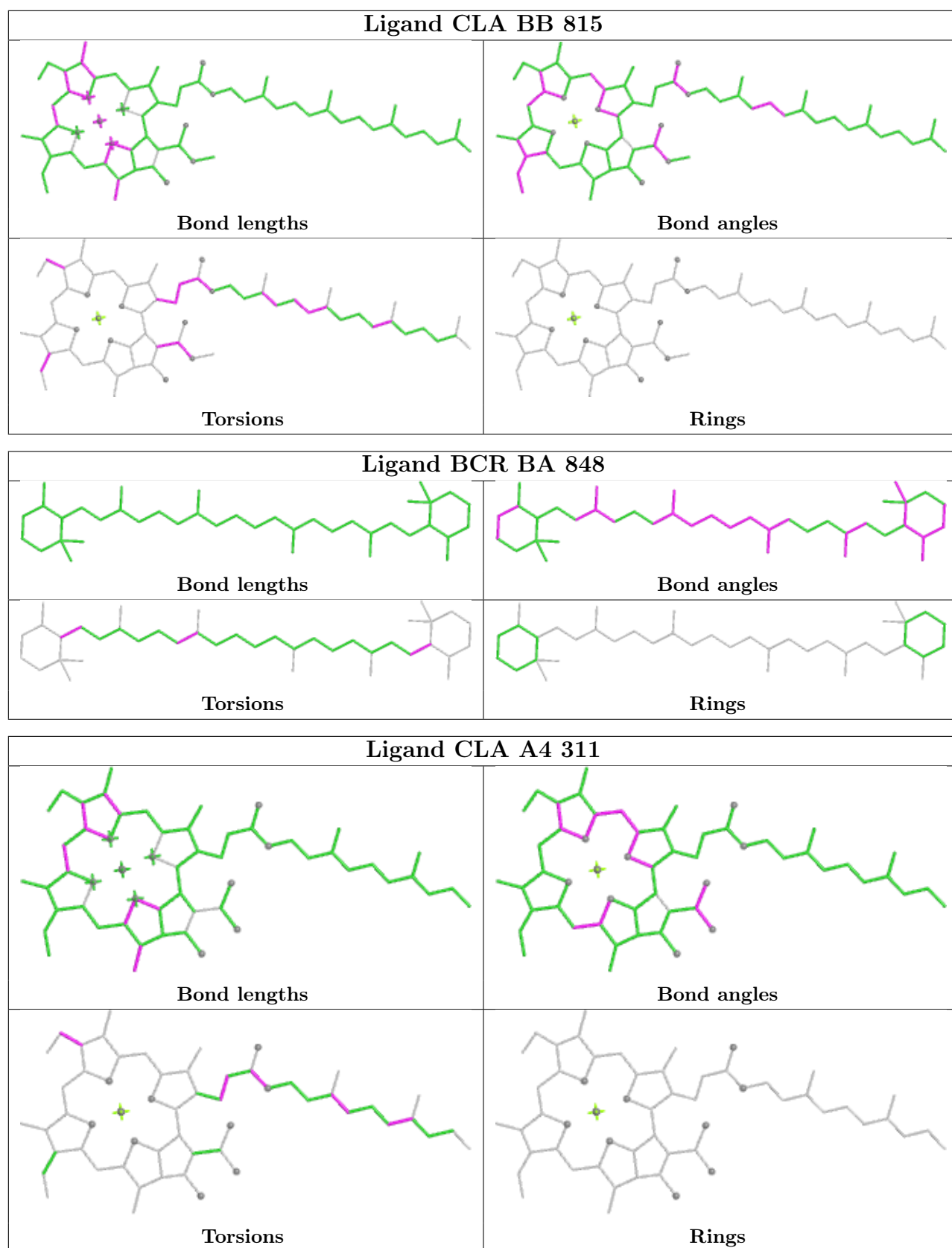


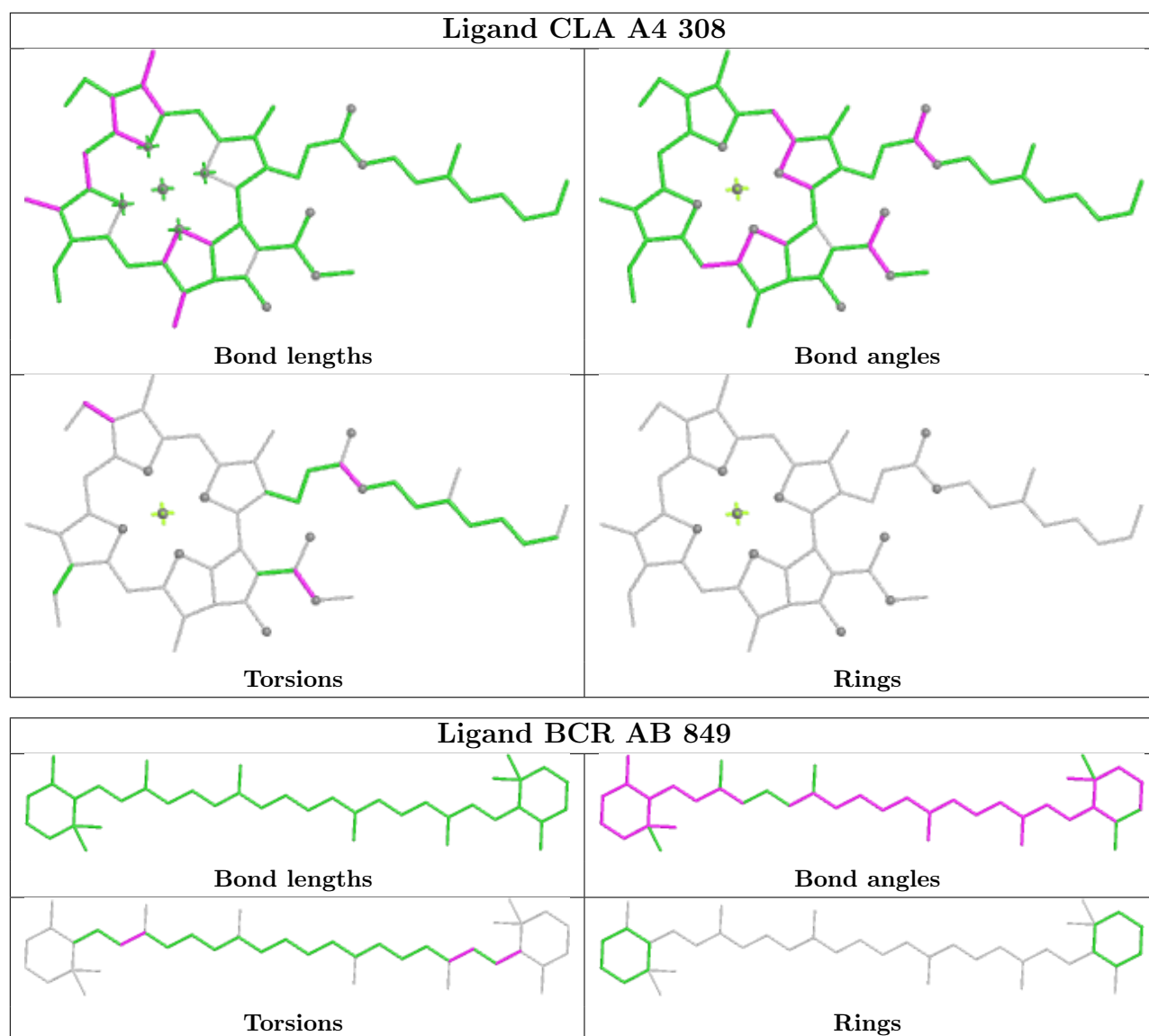
Ligand CLA B3 304



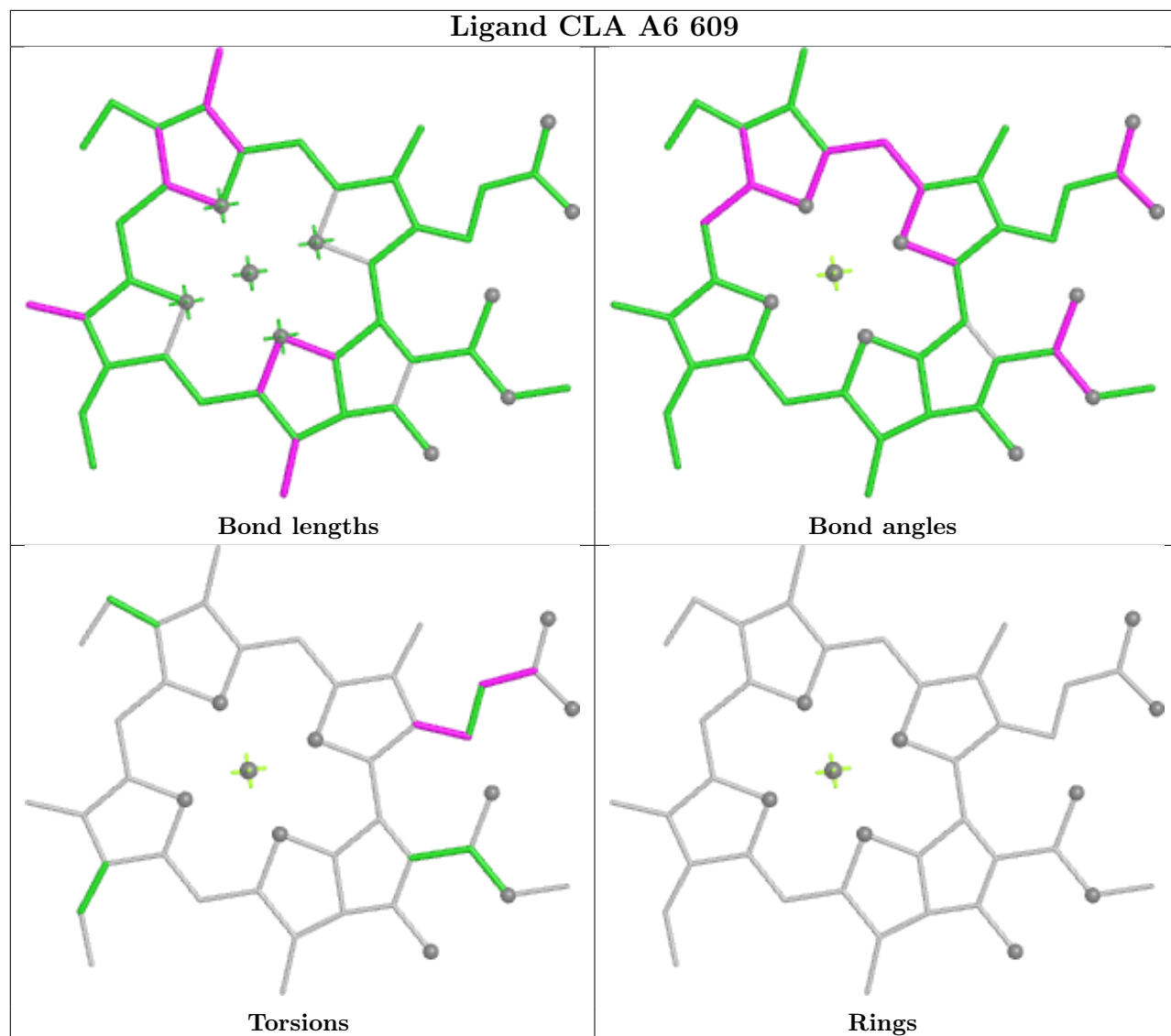
Ligand CLA AA 825



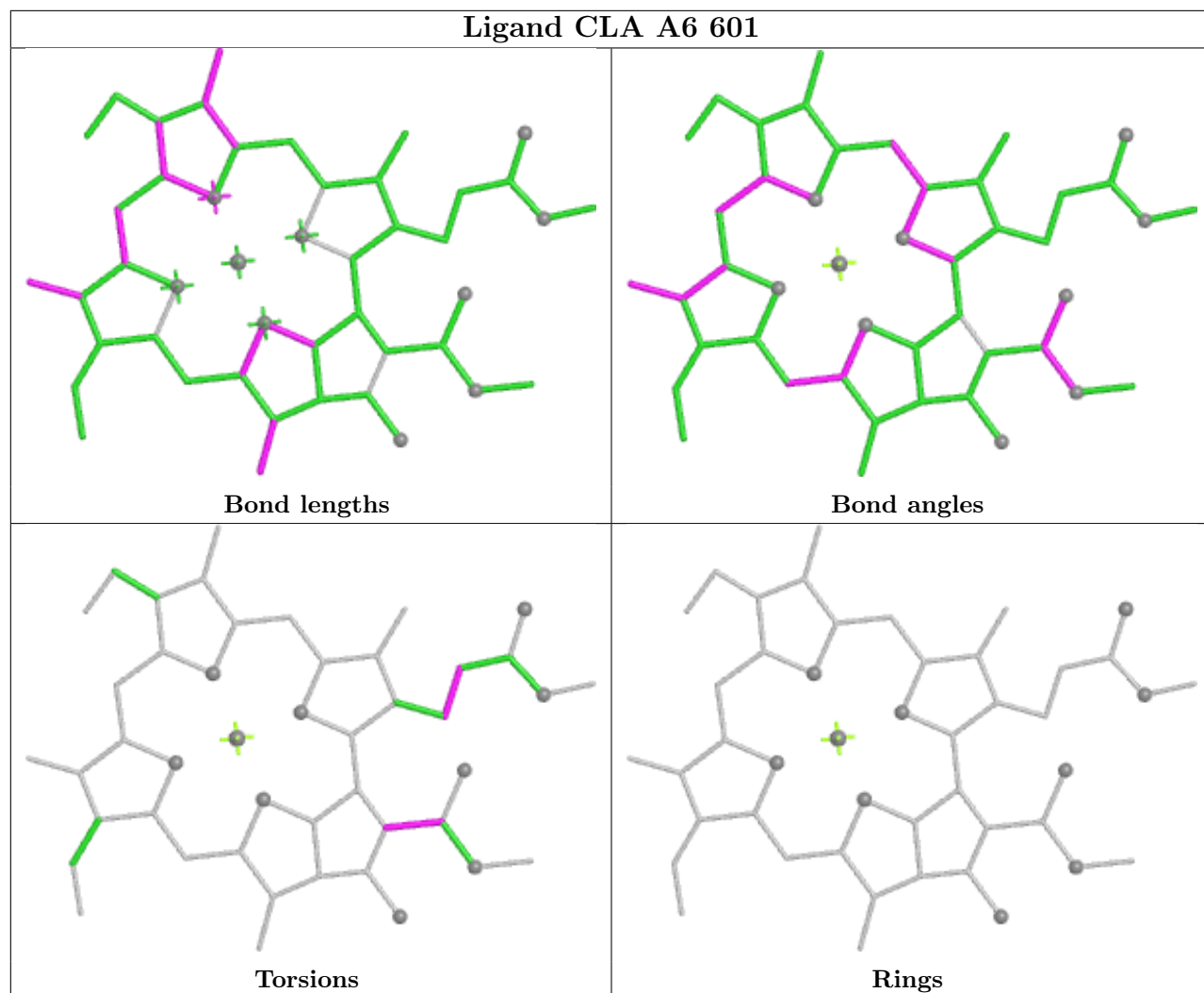




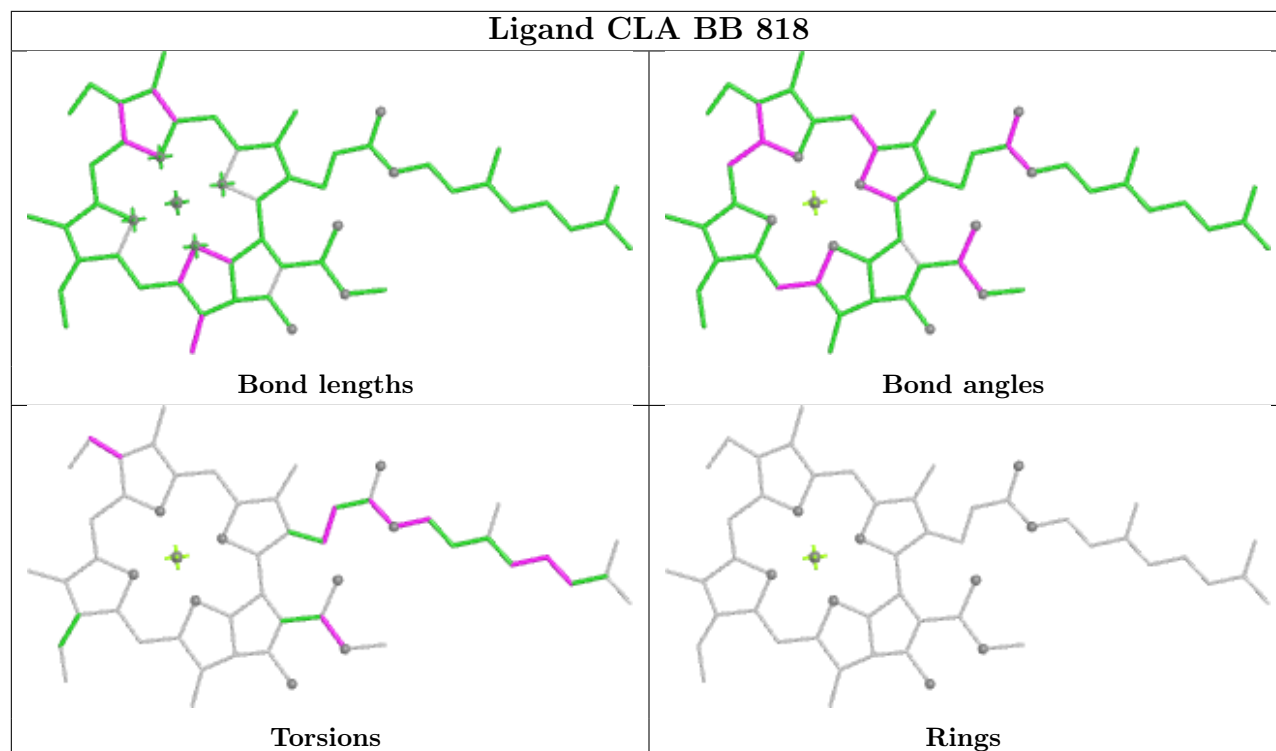
Ligand CLA A6 609



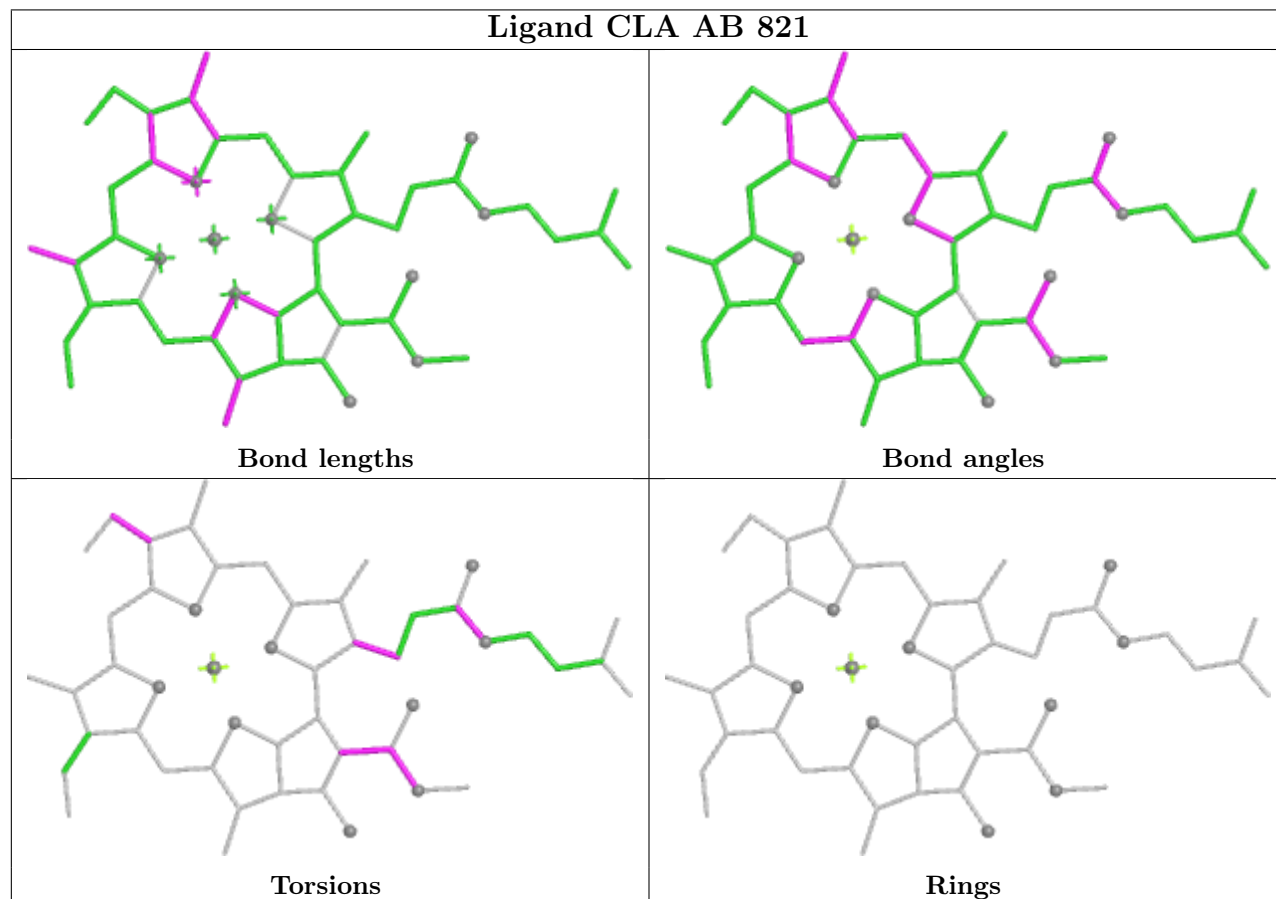
Ligand CLA A6 601

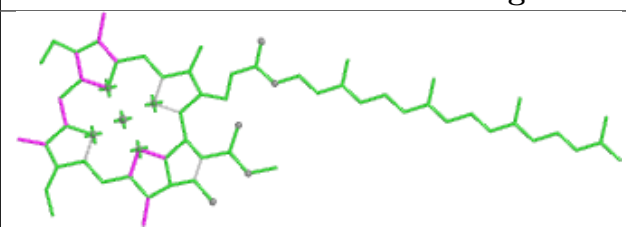
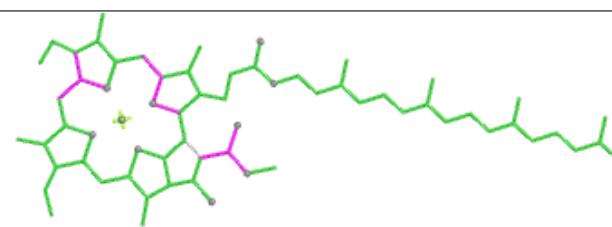
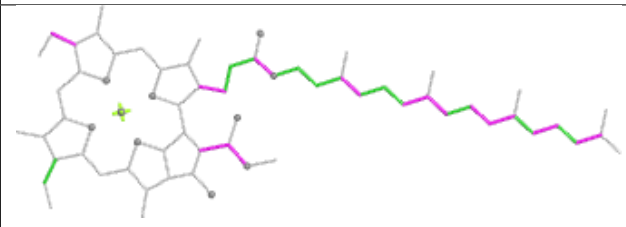
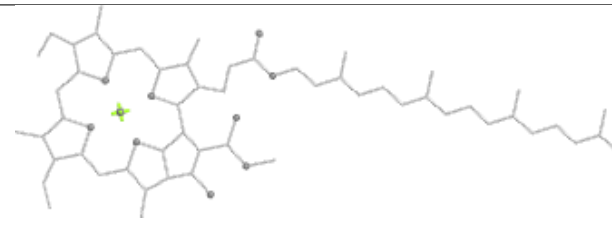


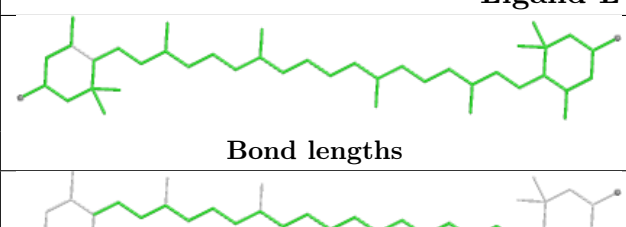
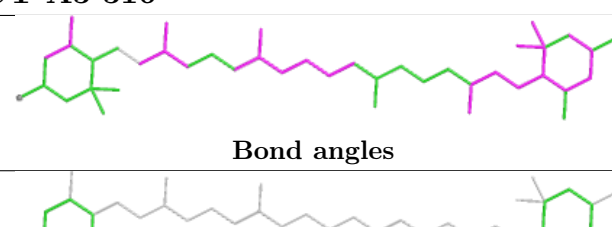
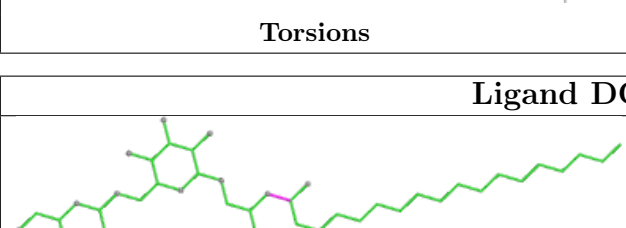
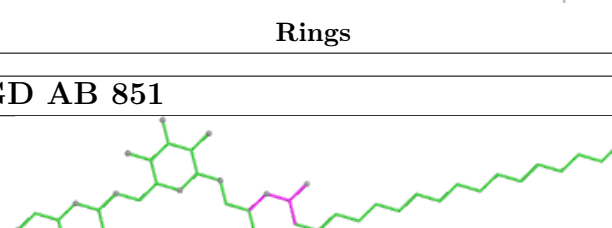
Ligand CLA BB 818

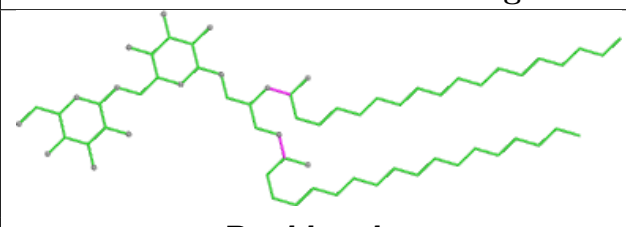
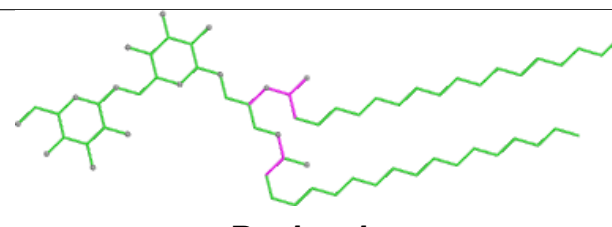
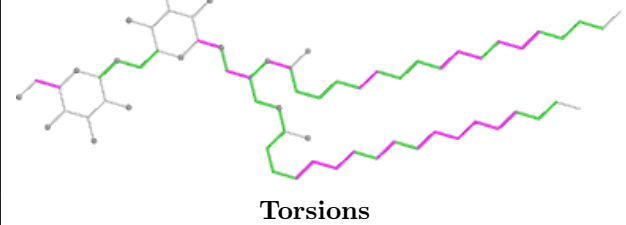
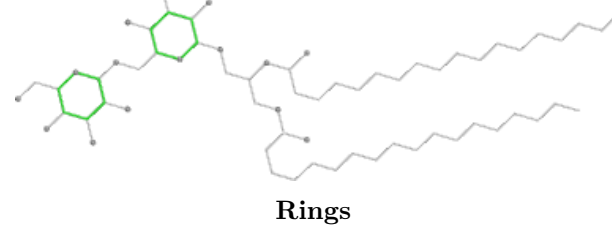


Ligand CLA AB 821

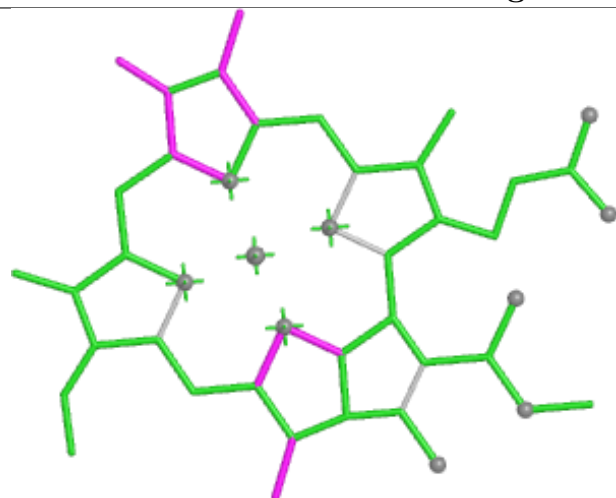


Ligand CLA AB 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

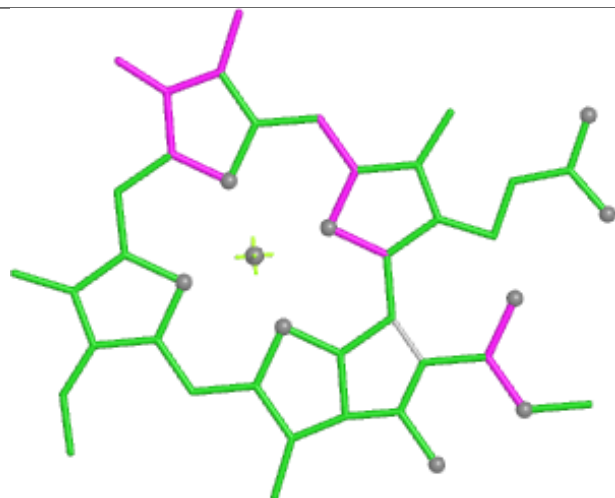
Ligand LUT A3 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD AB 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

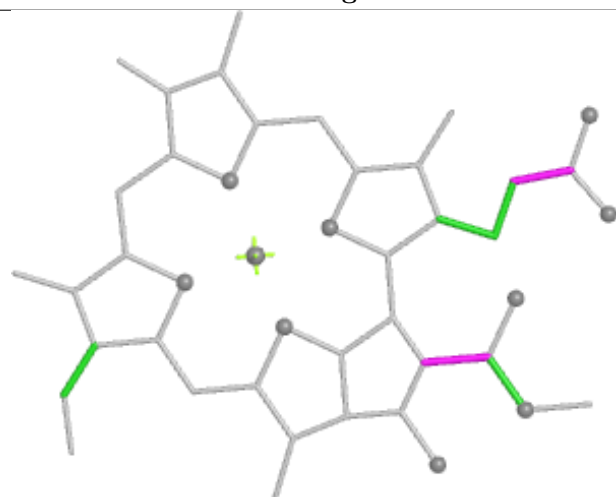
Ligand CLA B5 603



Bond lengths



Bond angles

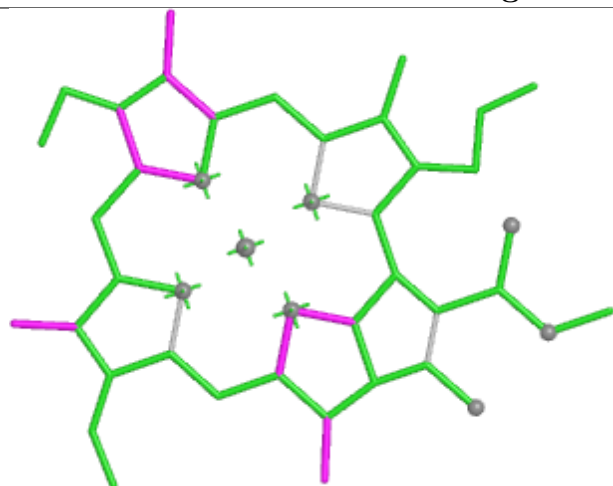


Torsions

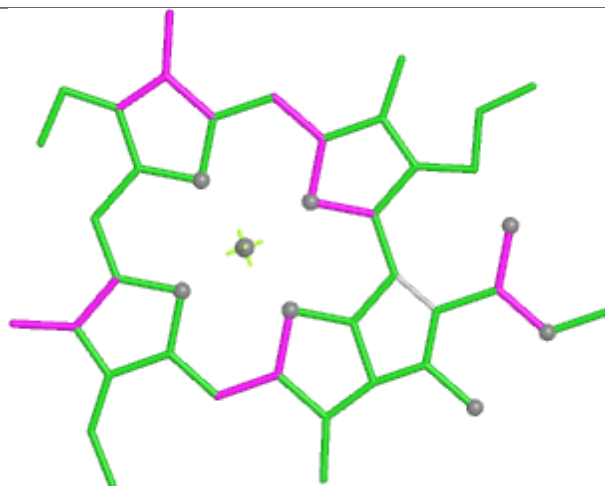


Rings

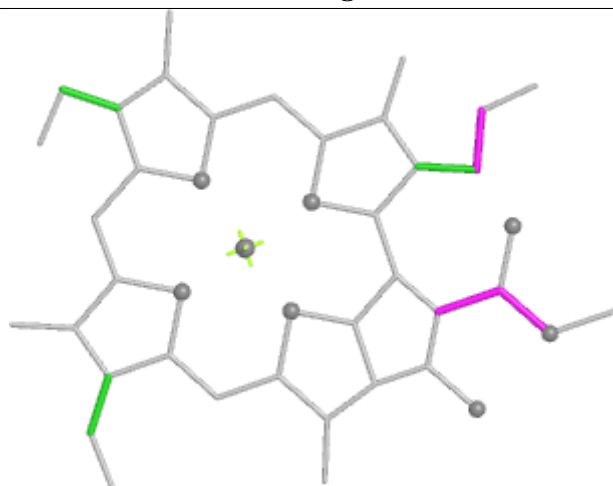
Ligand CLA BB 833



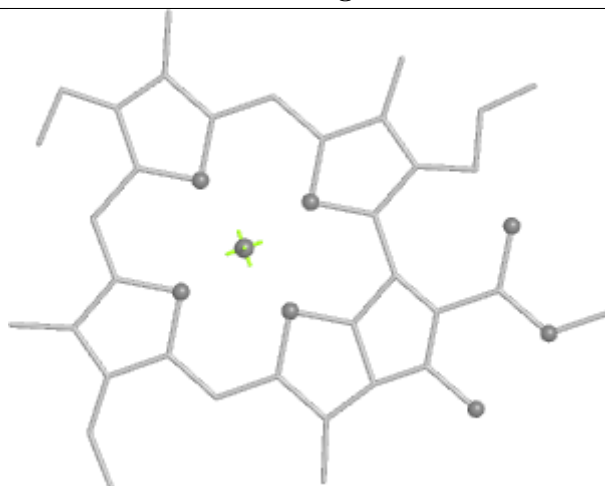
Bond lengths



Bond angles

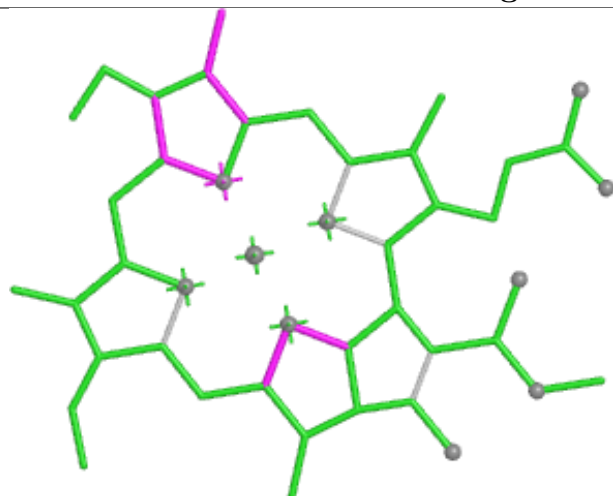


Torsions

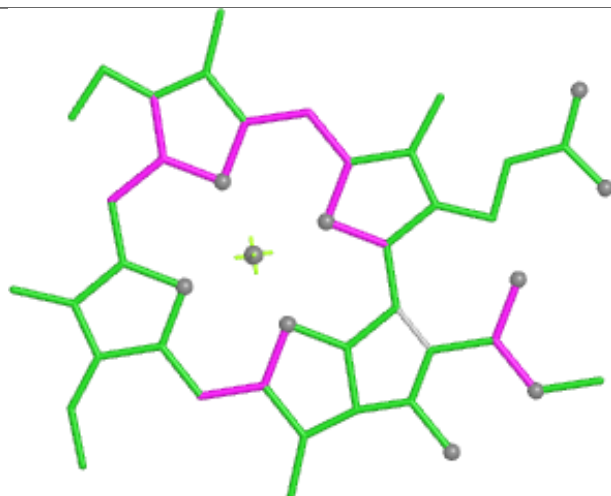


Rings

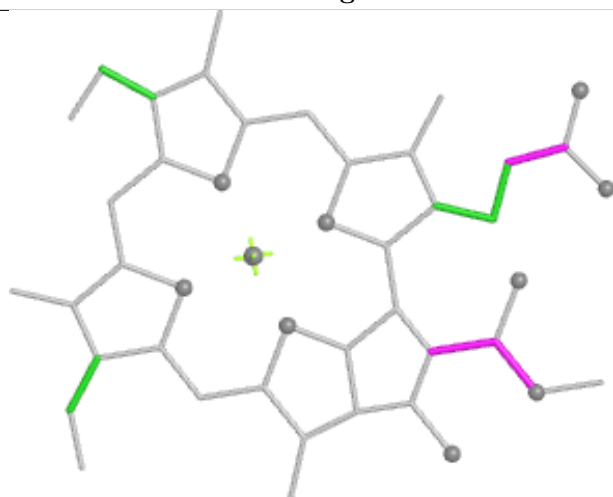
Ligand CLA BG 202



Bond lengths



Bond angles

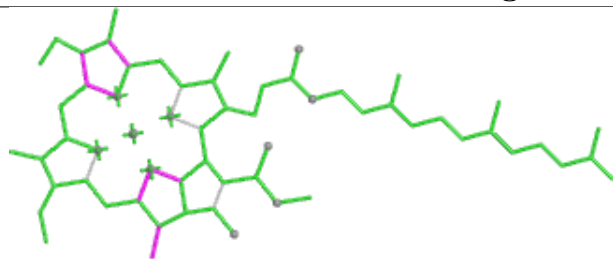


Torsions

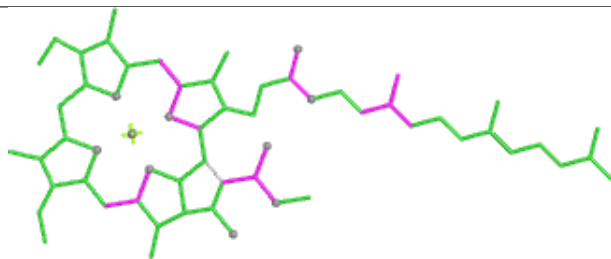


Rings

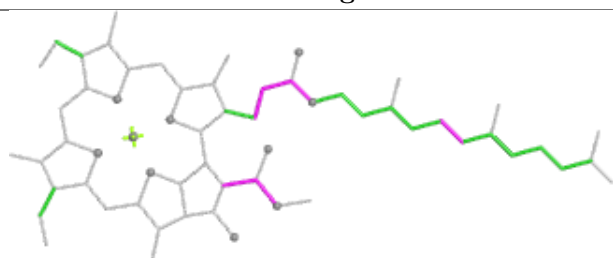
Ligand CLA BA 817



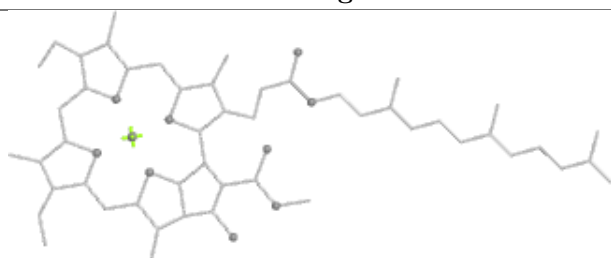
Bond lengths



Bond angles

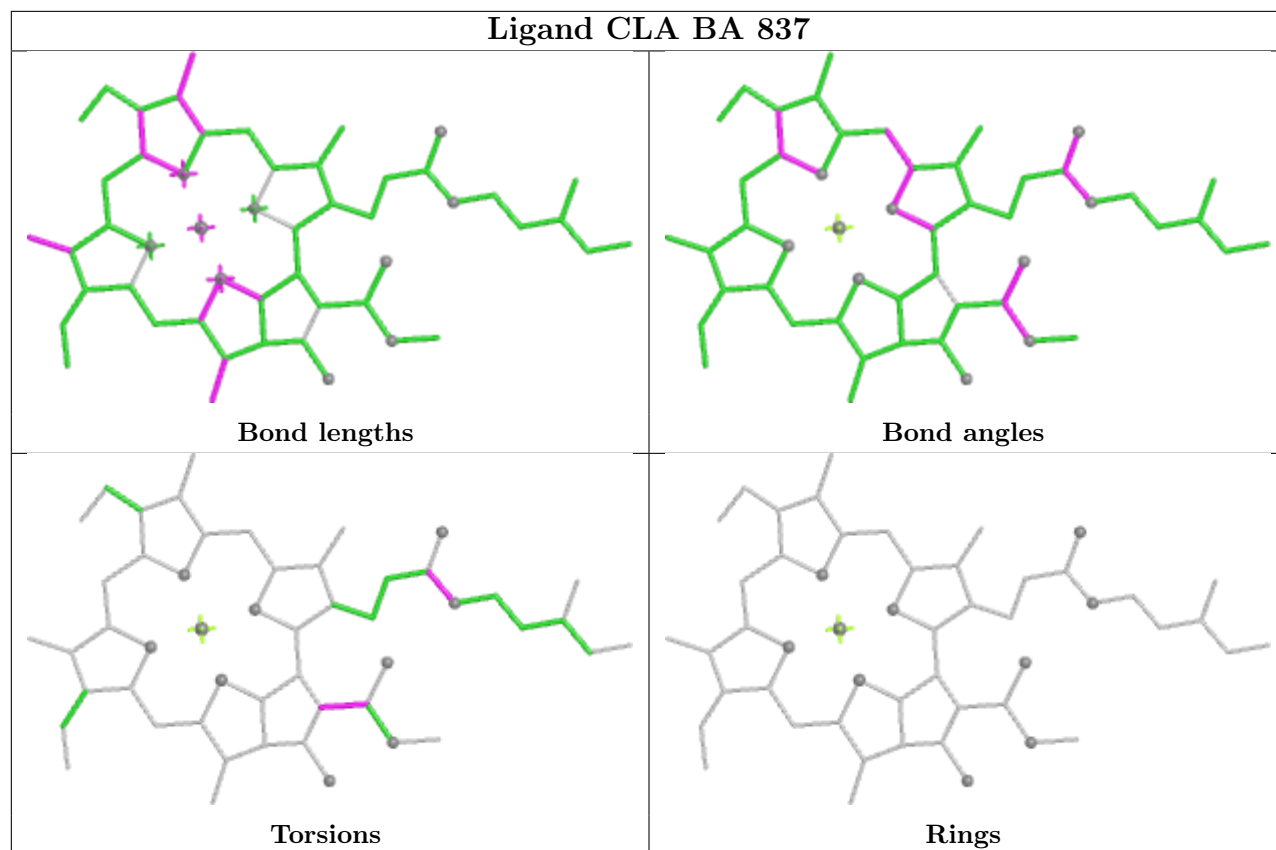


Torsions

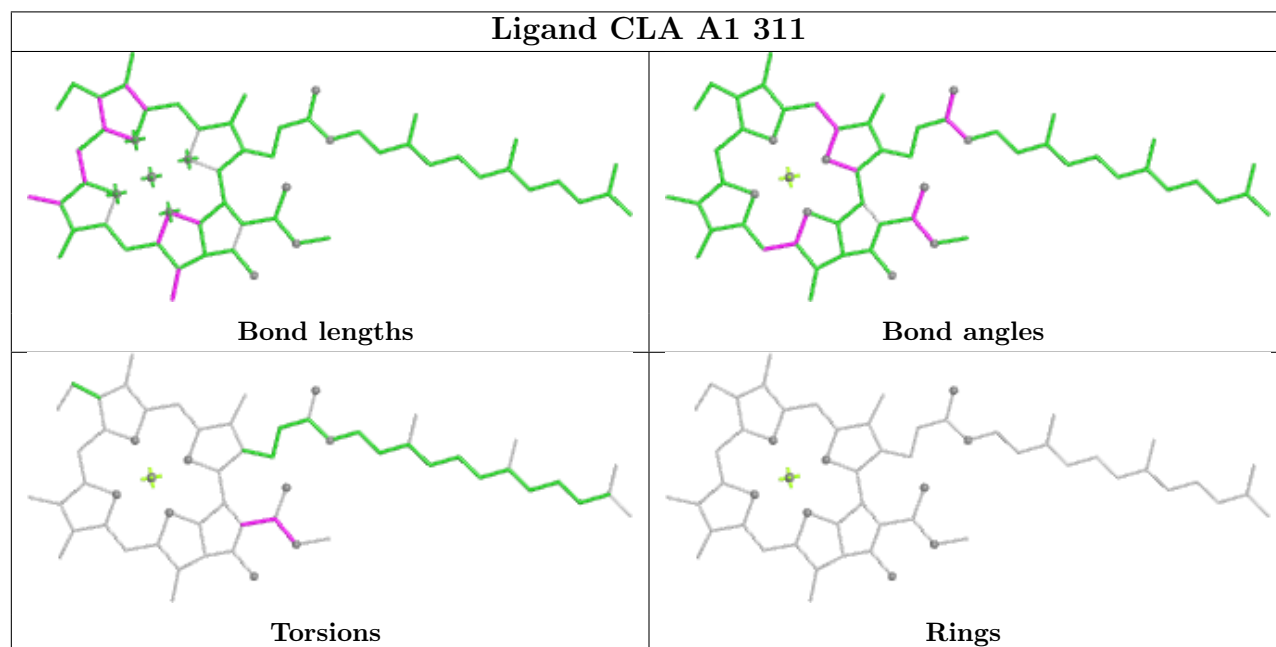


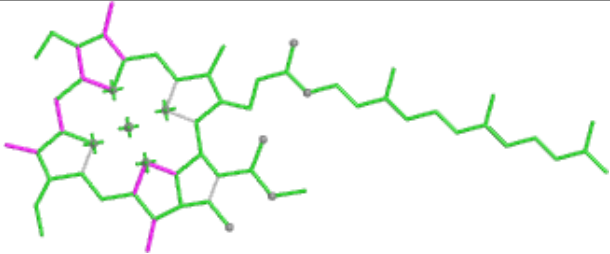
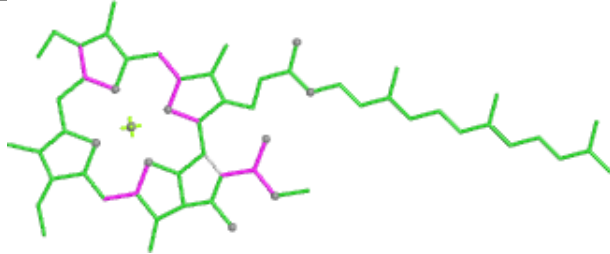
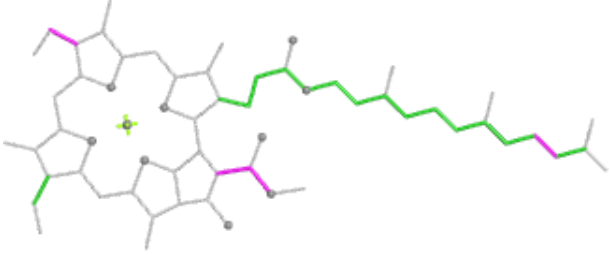
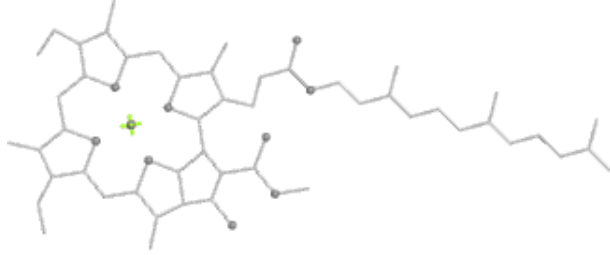
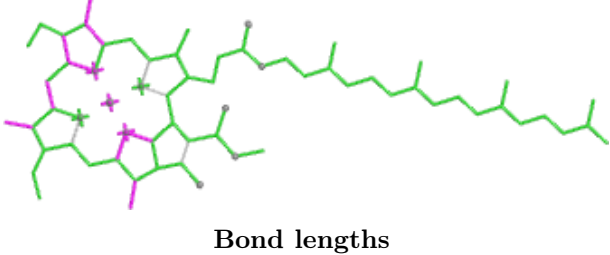
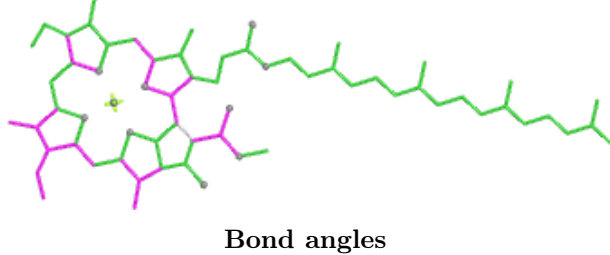
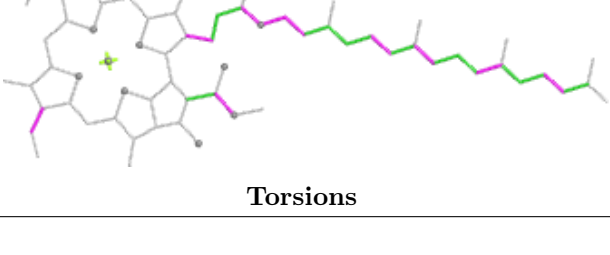
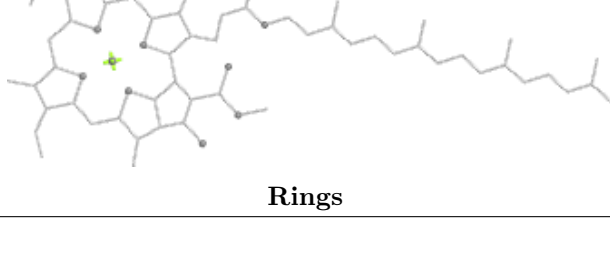
Rings

Ligand CLA BA 837

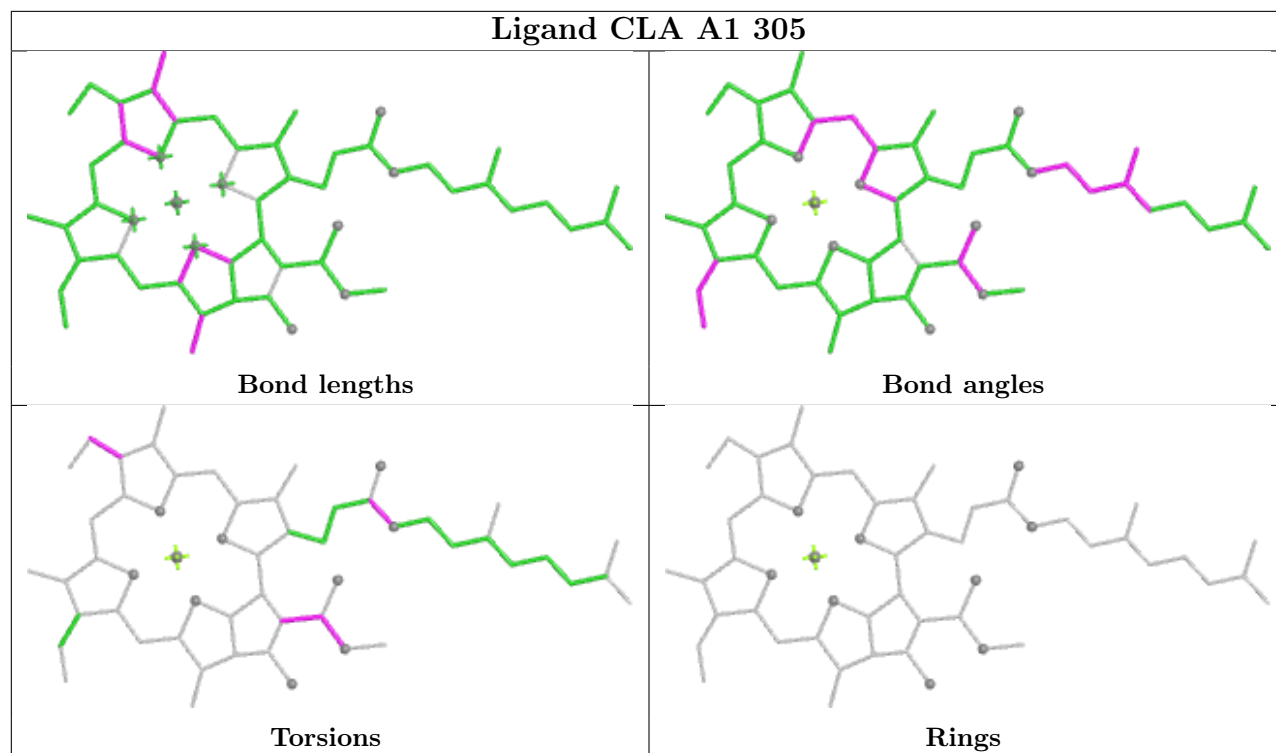


Ligand CLA A1 311

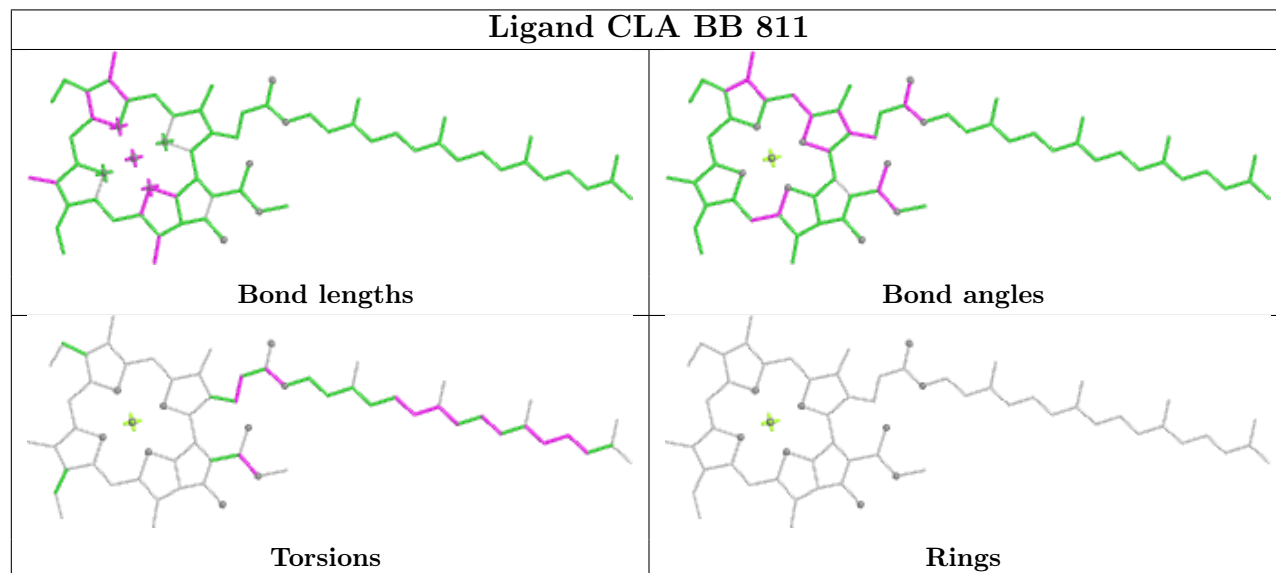


Ligand CLA B3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA AB 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

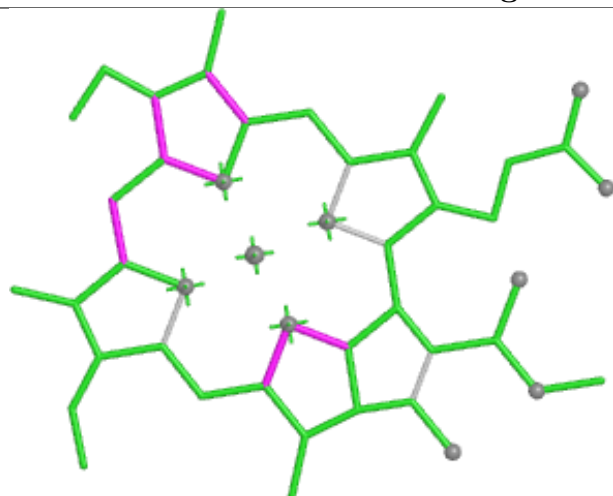
Ligand CLA A1 305



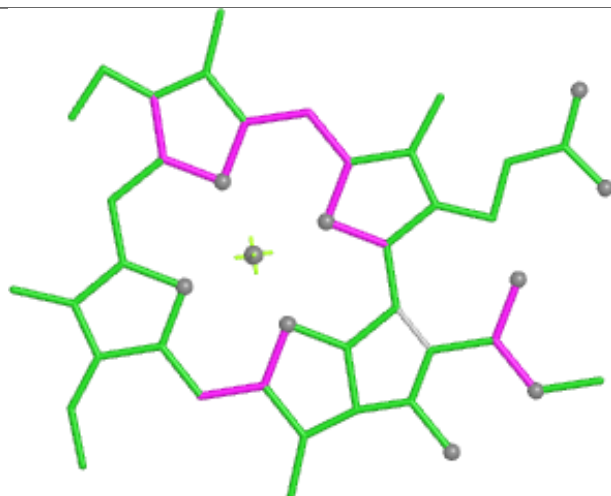
Ligand CLA BB 811



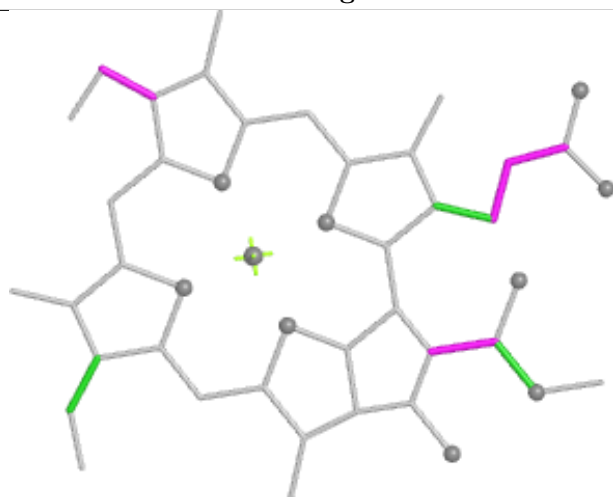
Ligand CLA BK 202



Bond lengths



Bond angles

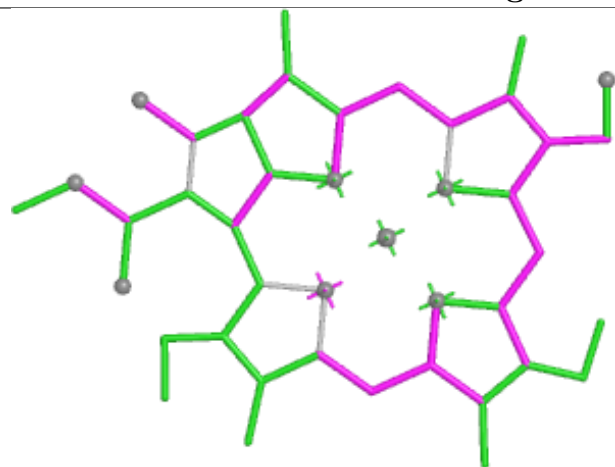


Torsions

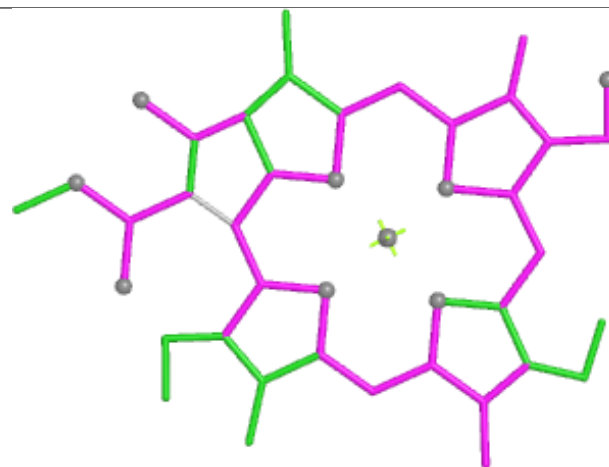


Rings

Ligand CHL A6 606



Bond lengths



Bond angles

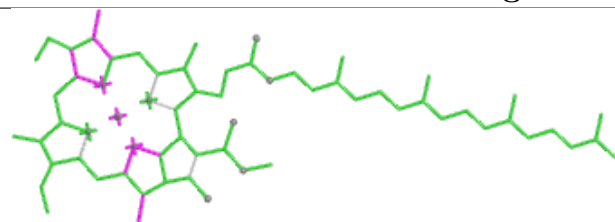


Torsions

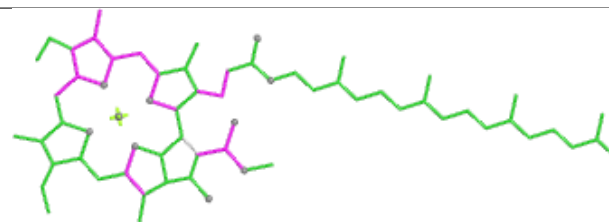


Rings

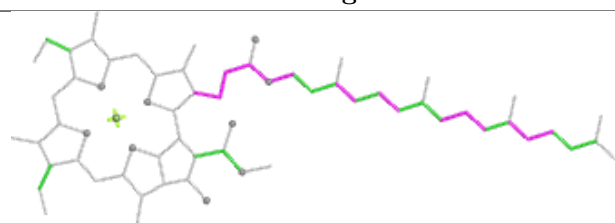
Ligand CLA AB 829



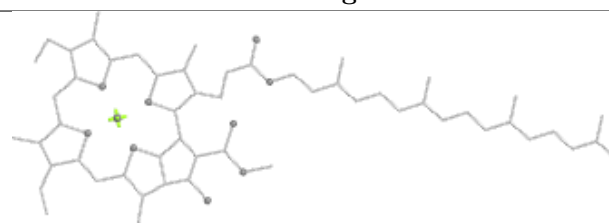
Bond lengths



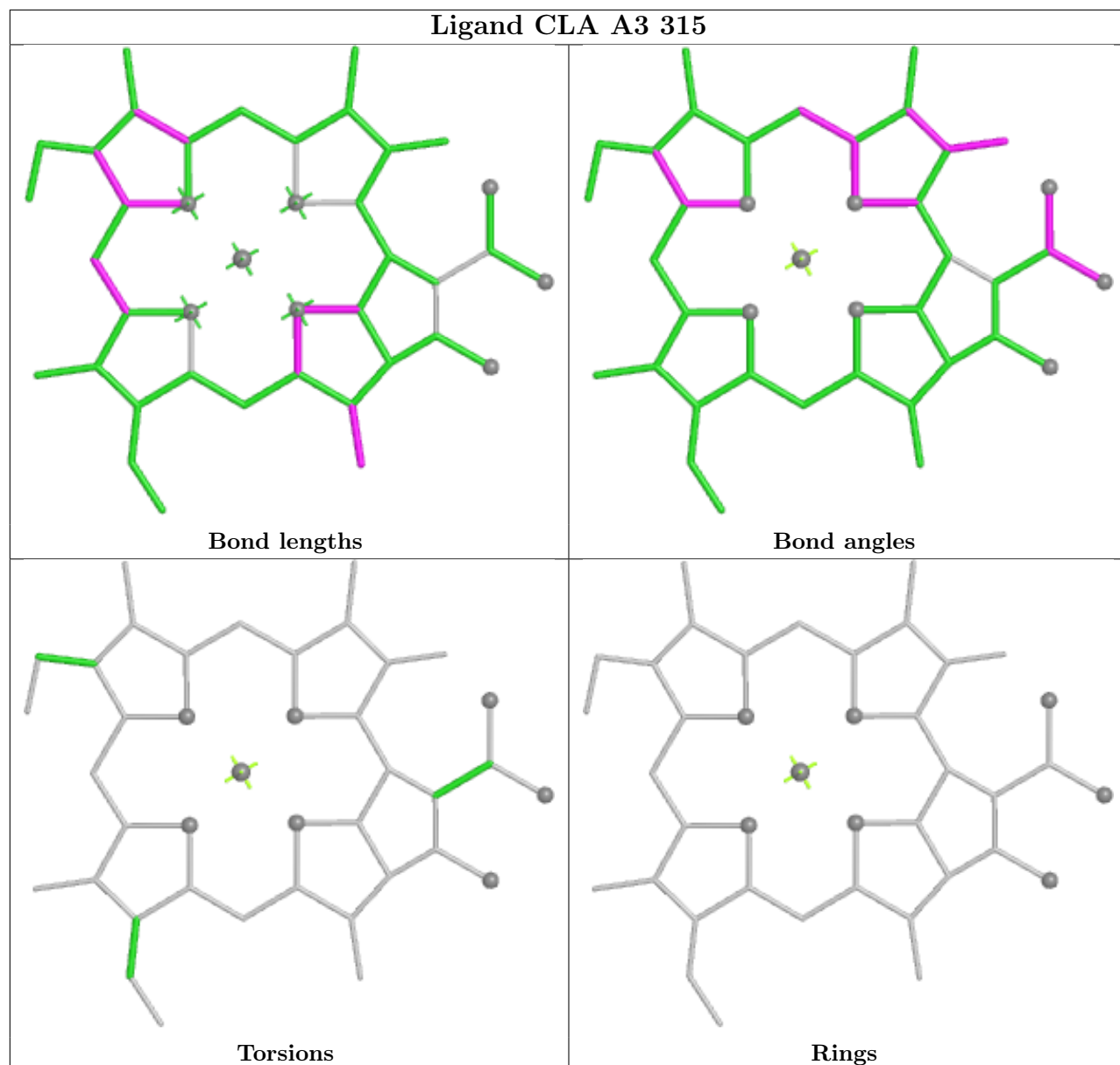
Bond angles



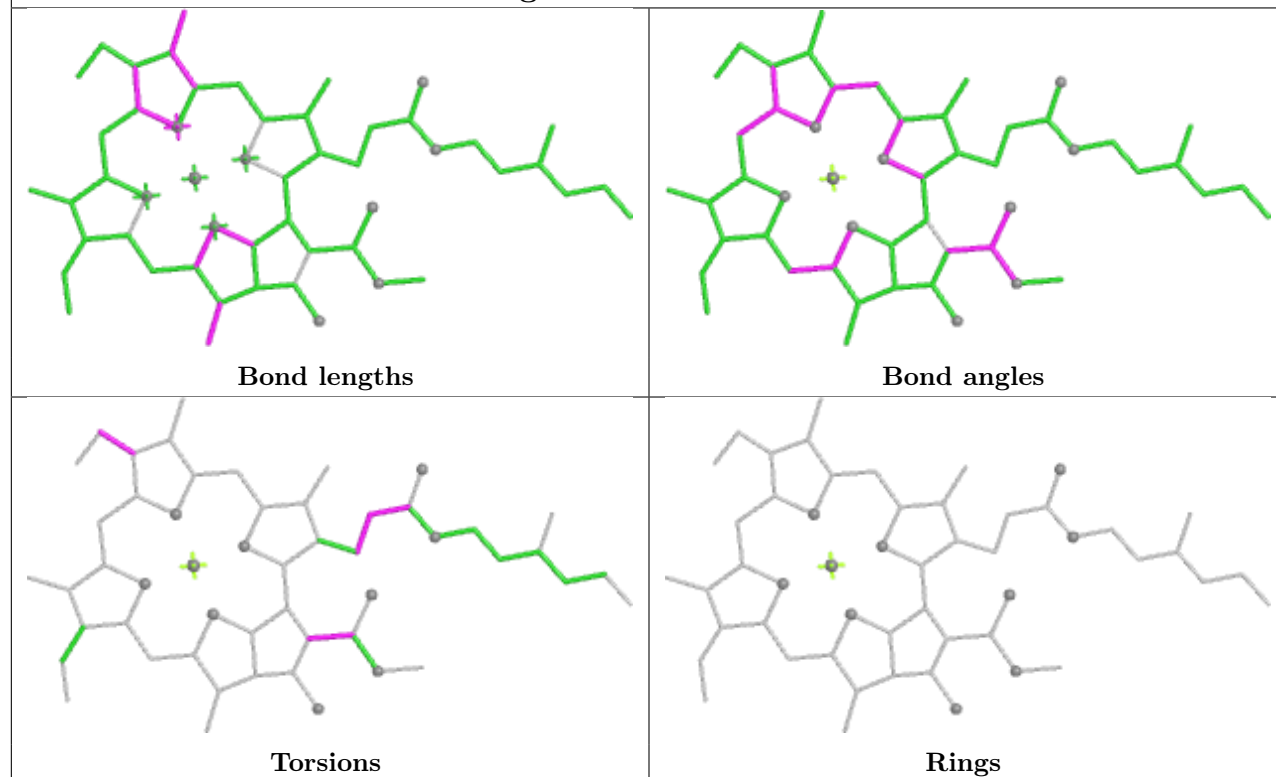
Torsions



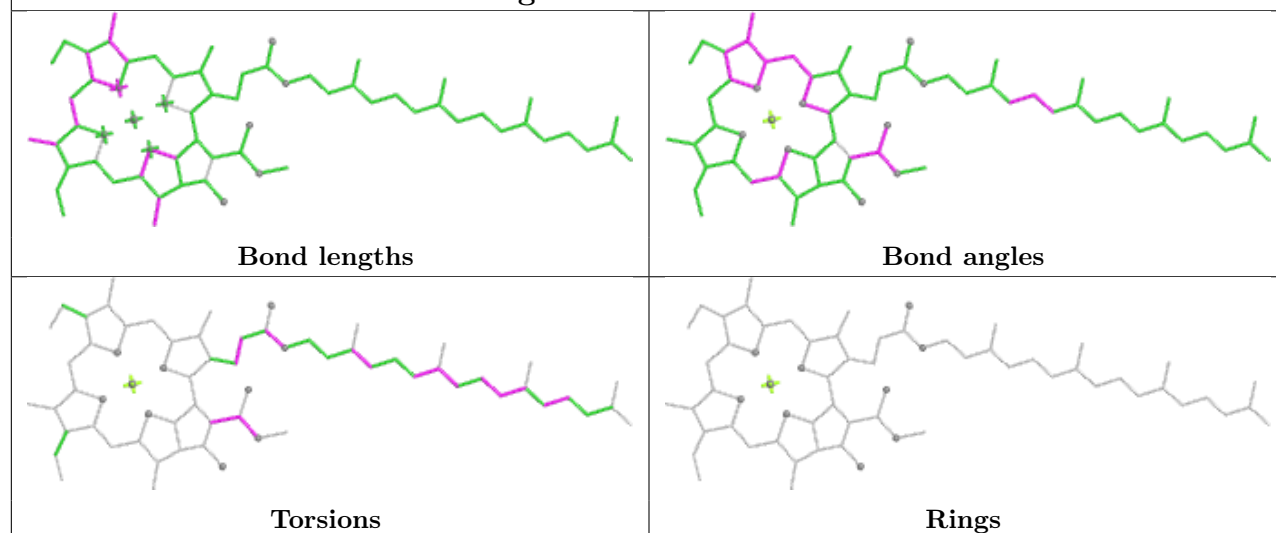
Rings



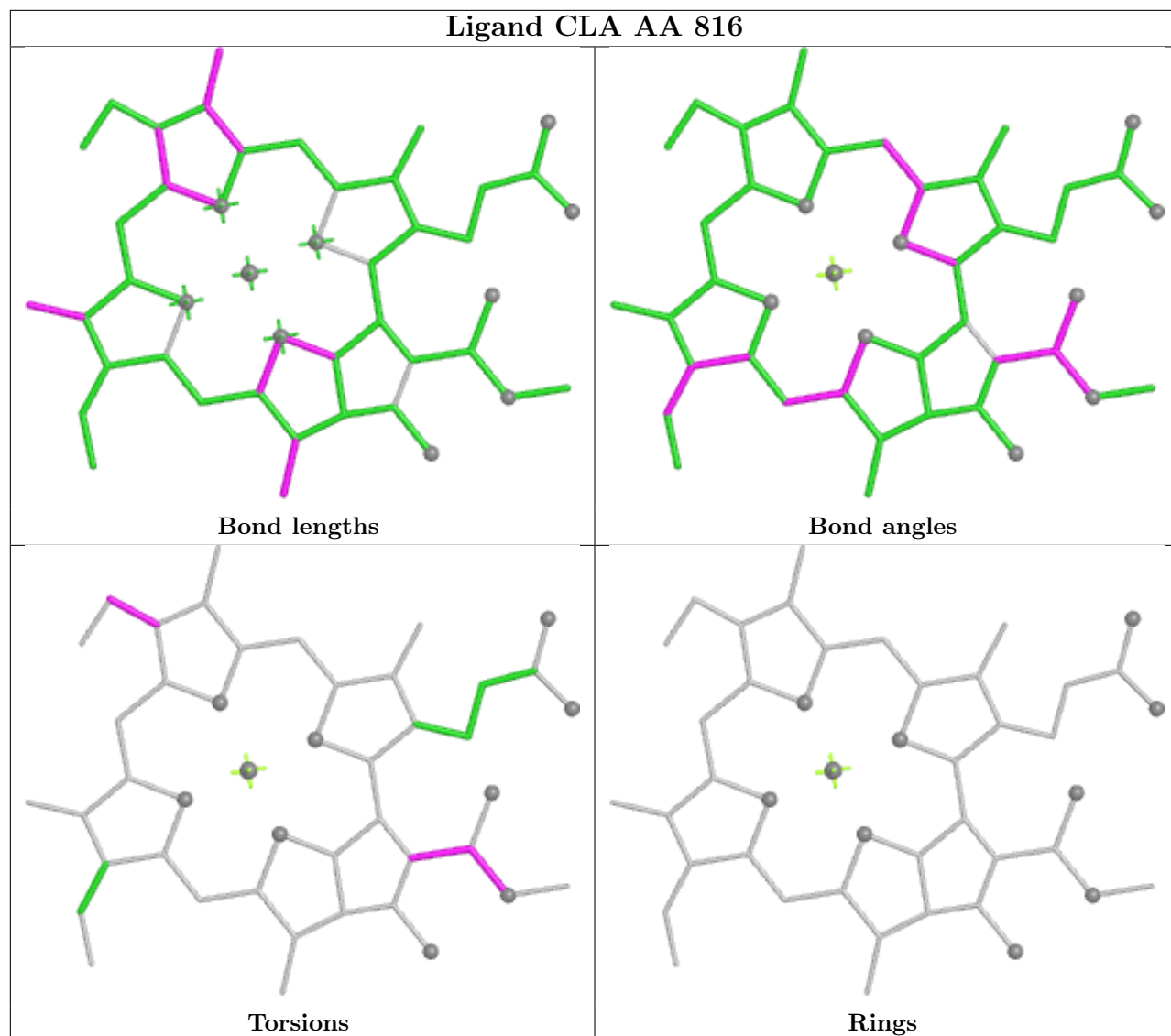
Ligand CLA BB 809

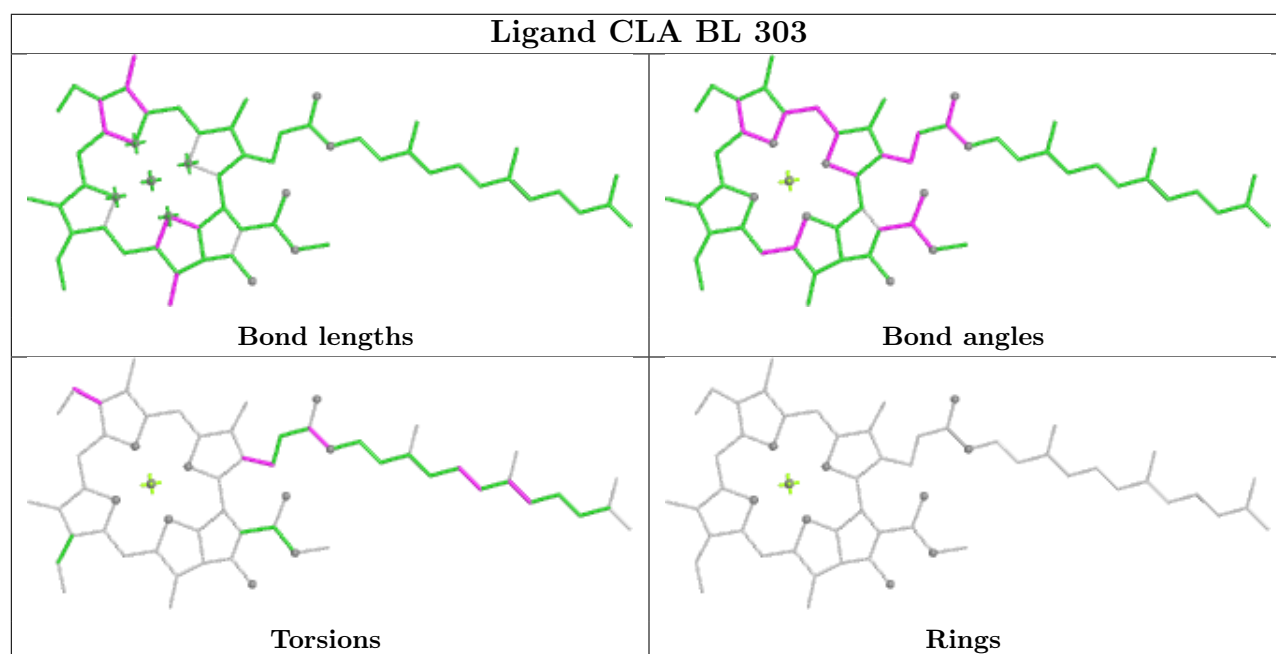
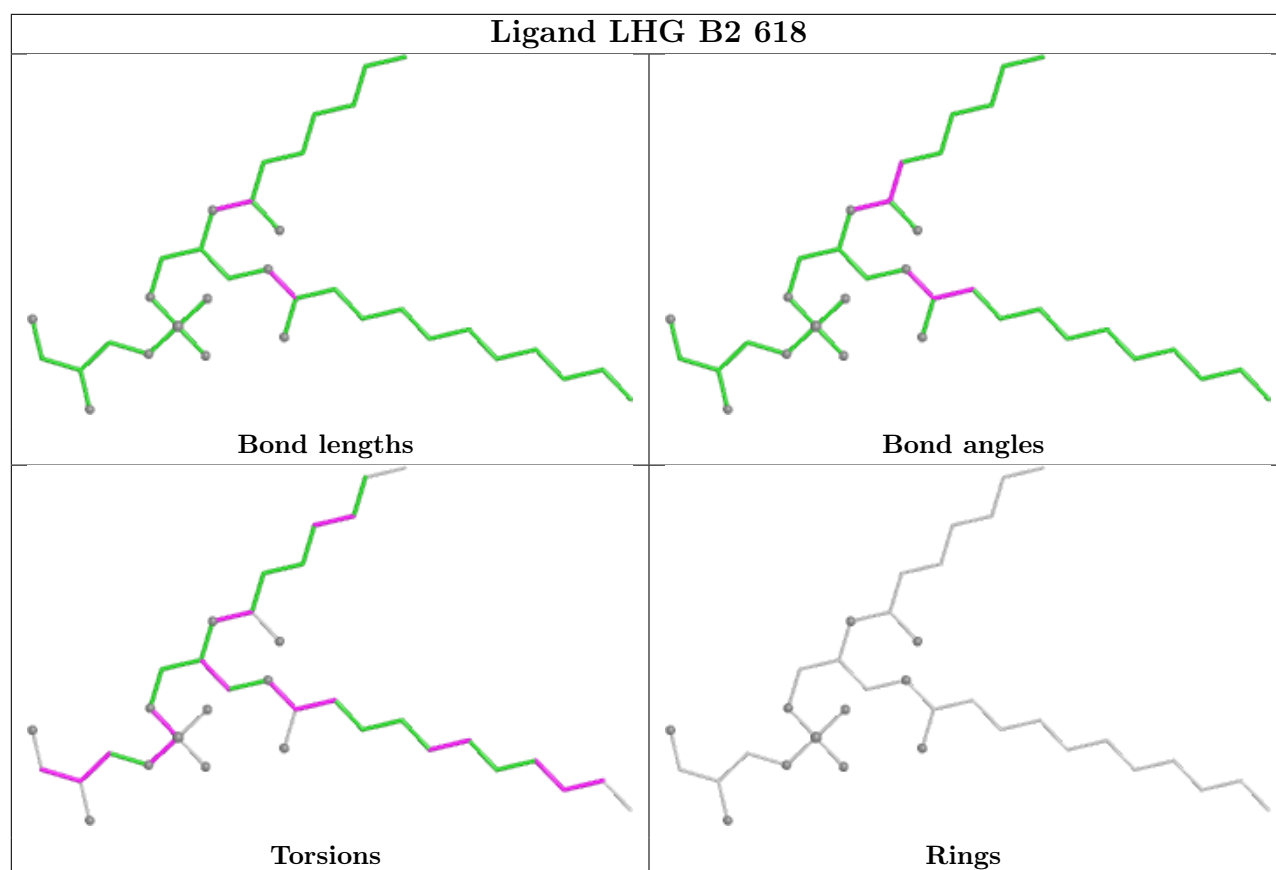


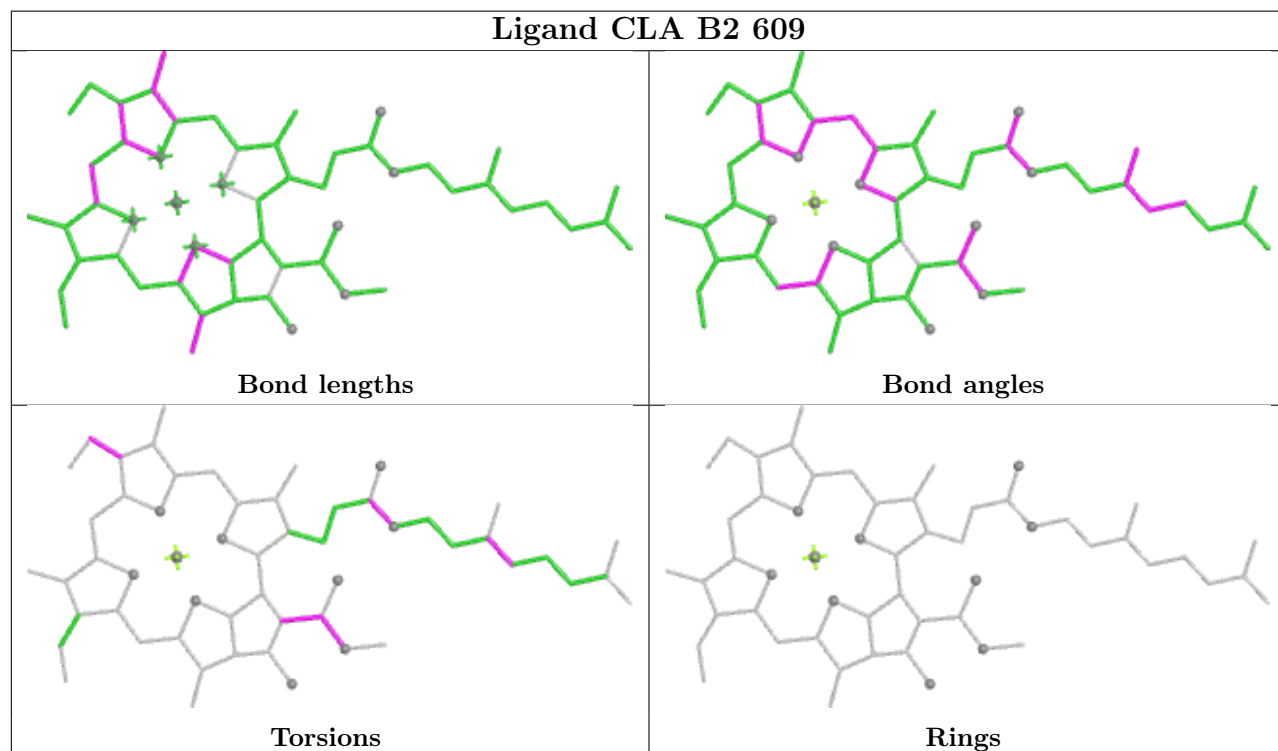
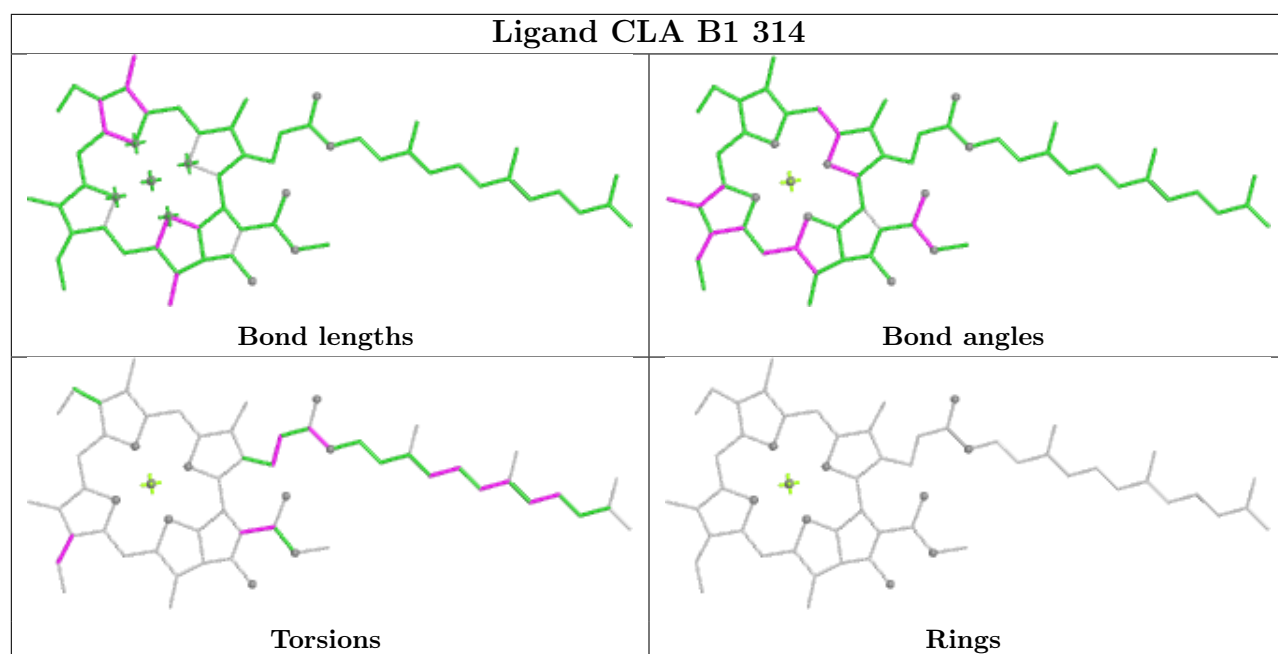
Ligand CLA AA 821

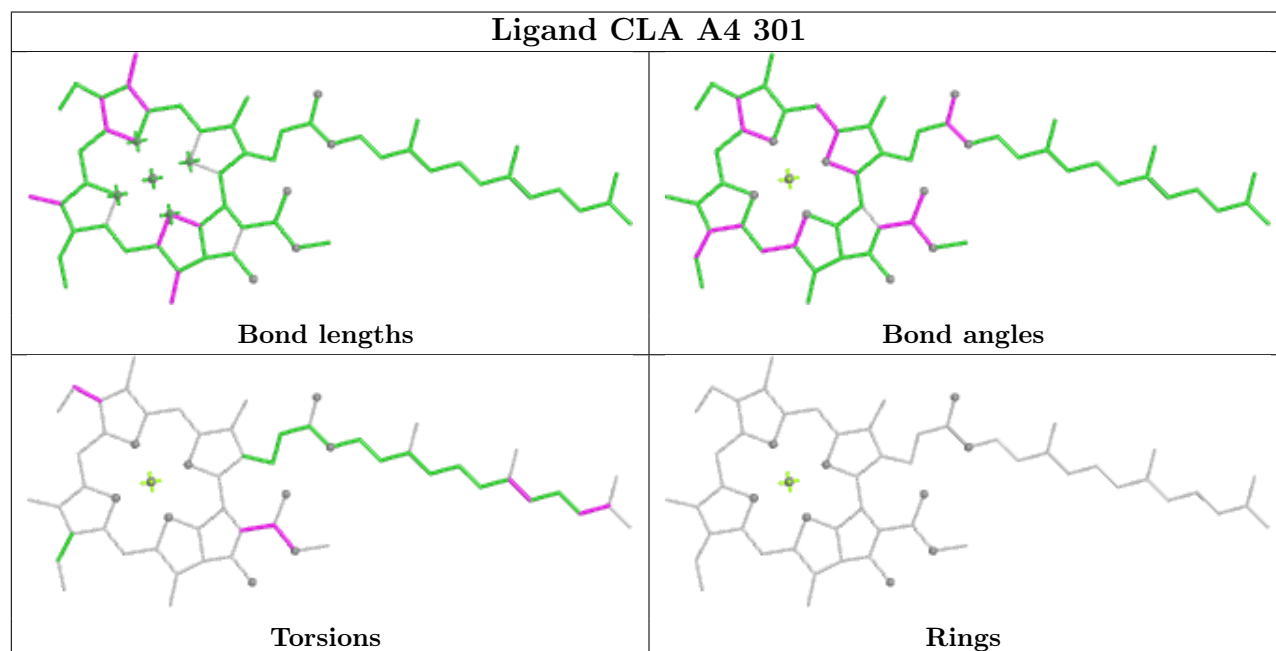
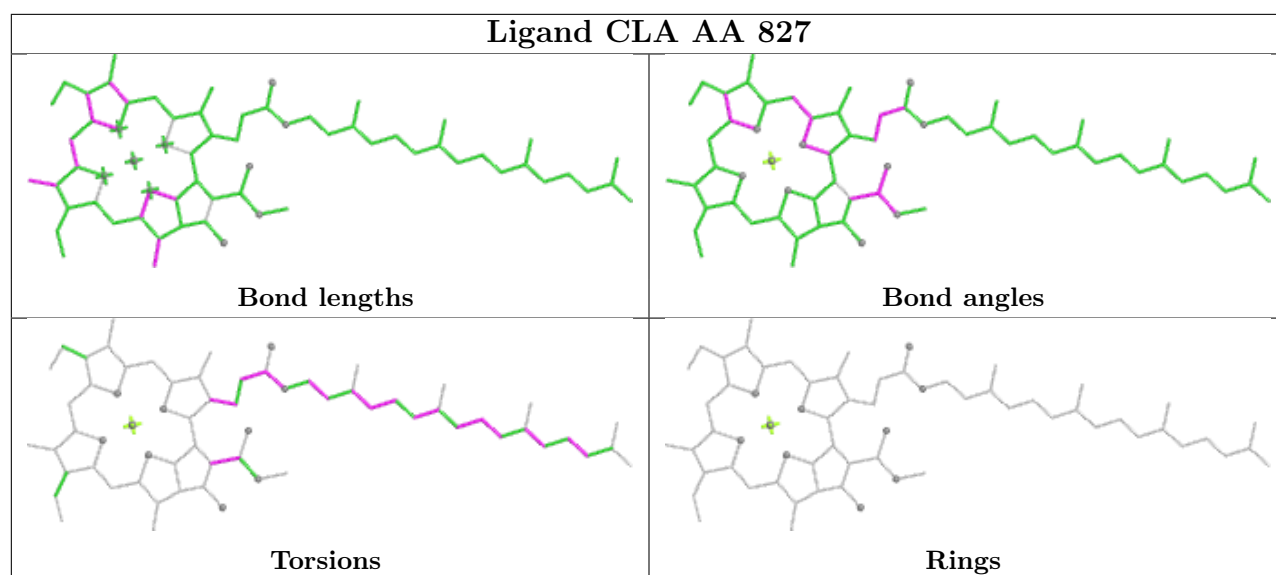


Ligand CLA AA 816

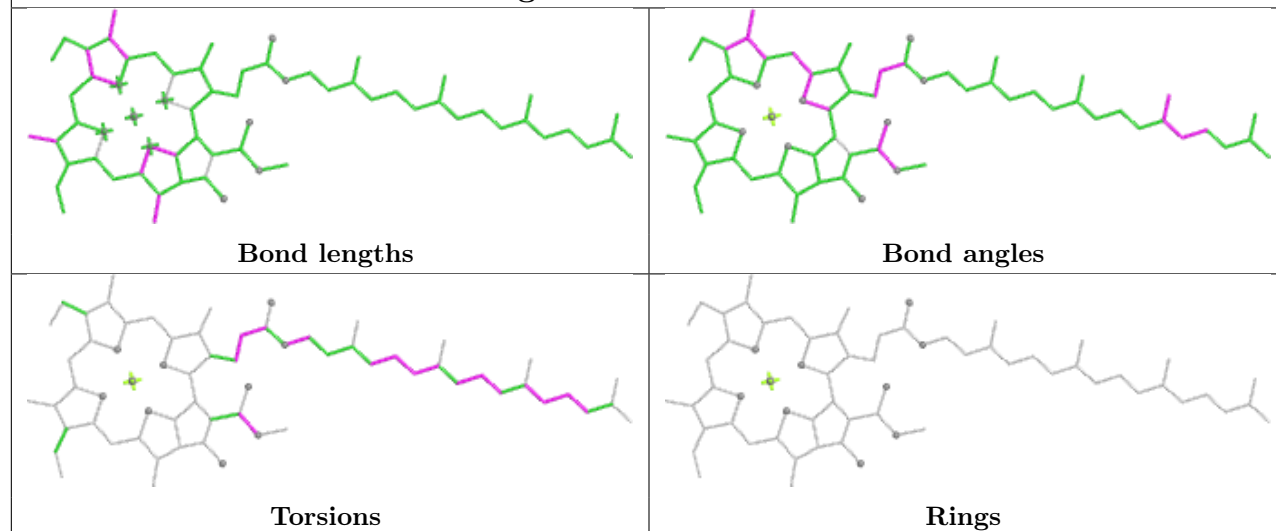




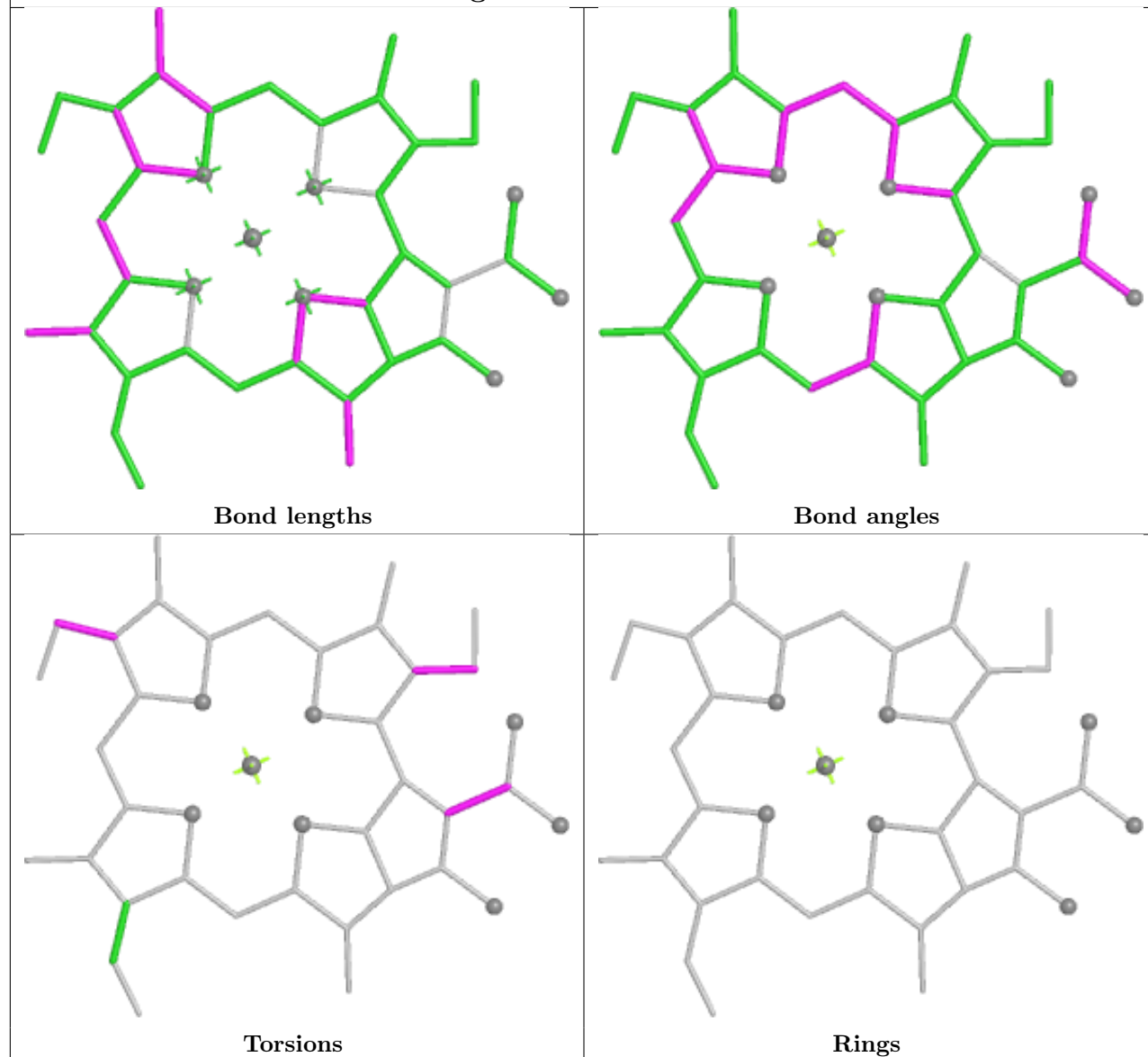




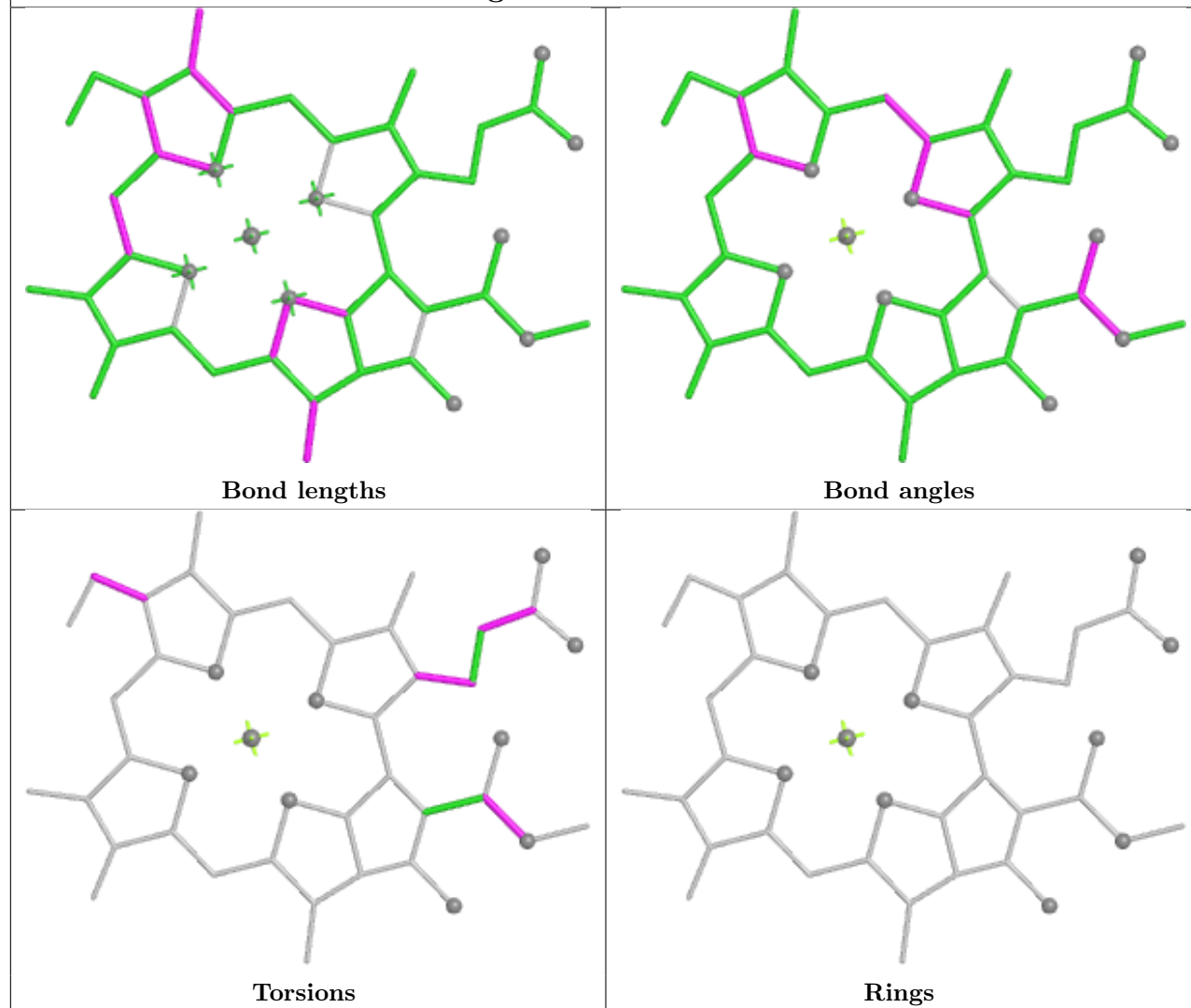
Ligand CLA AA 828



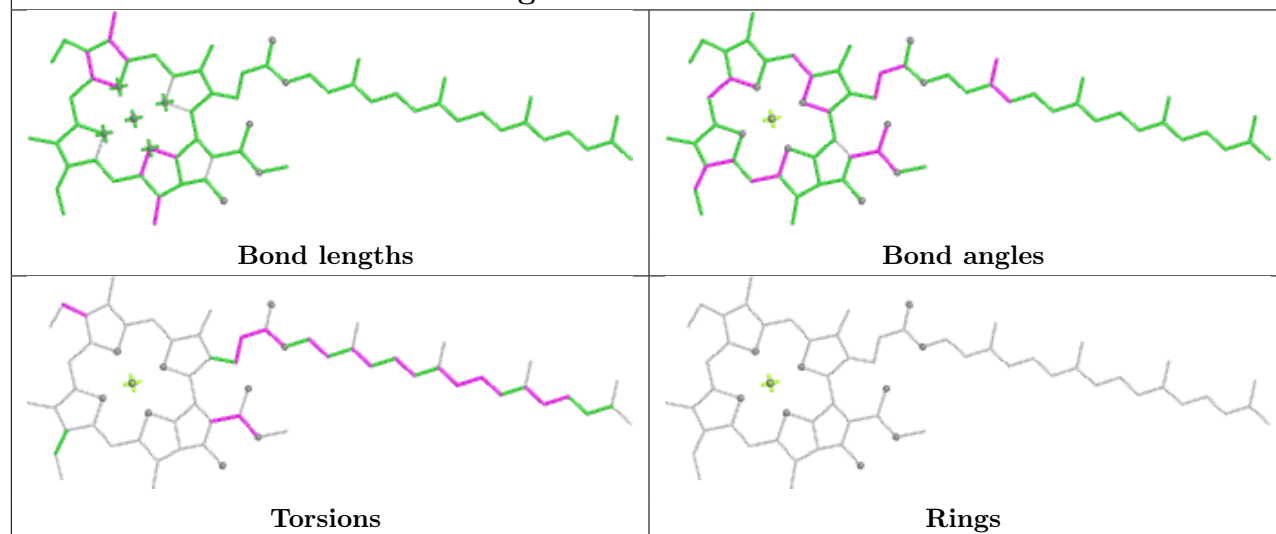
Ligand CLA A4 310

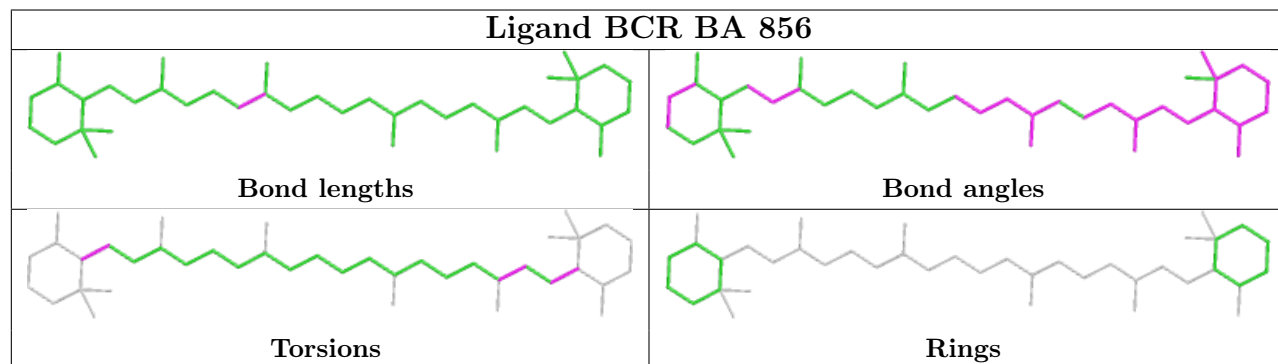
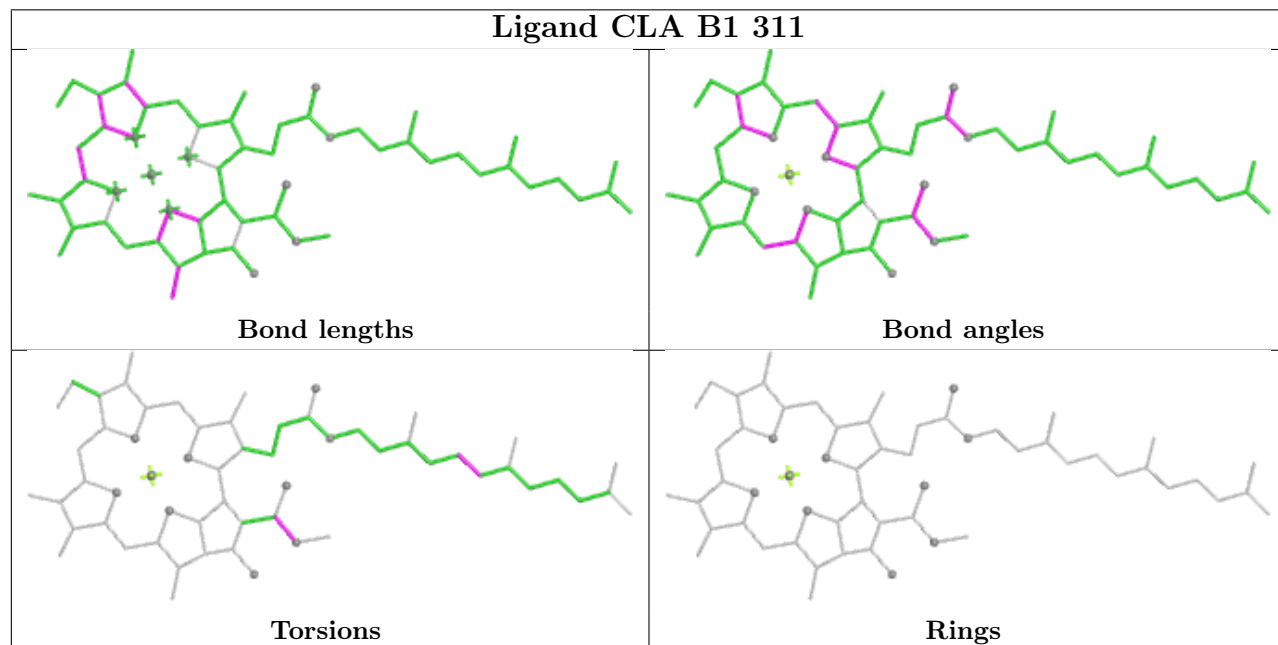
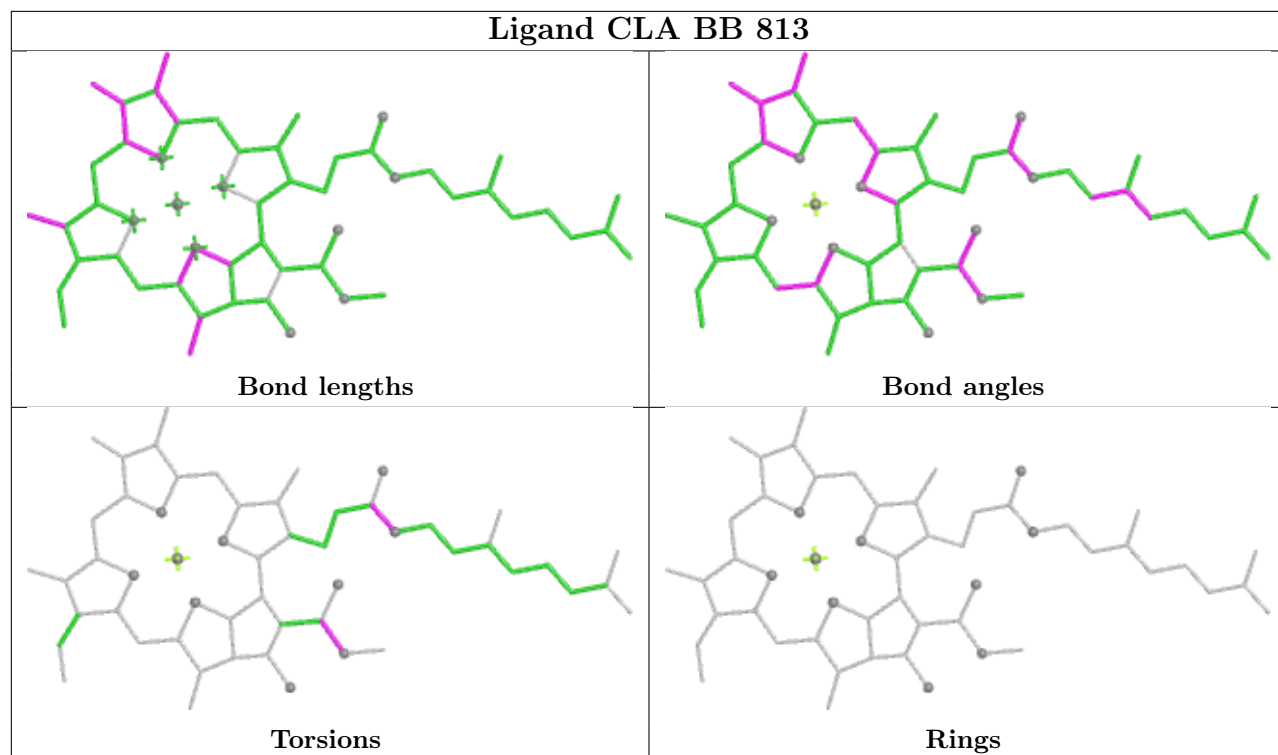


Ligand CLA A6 612

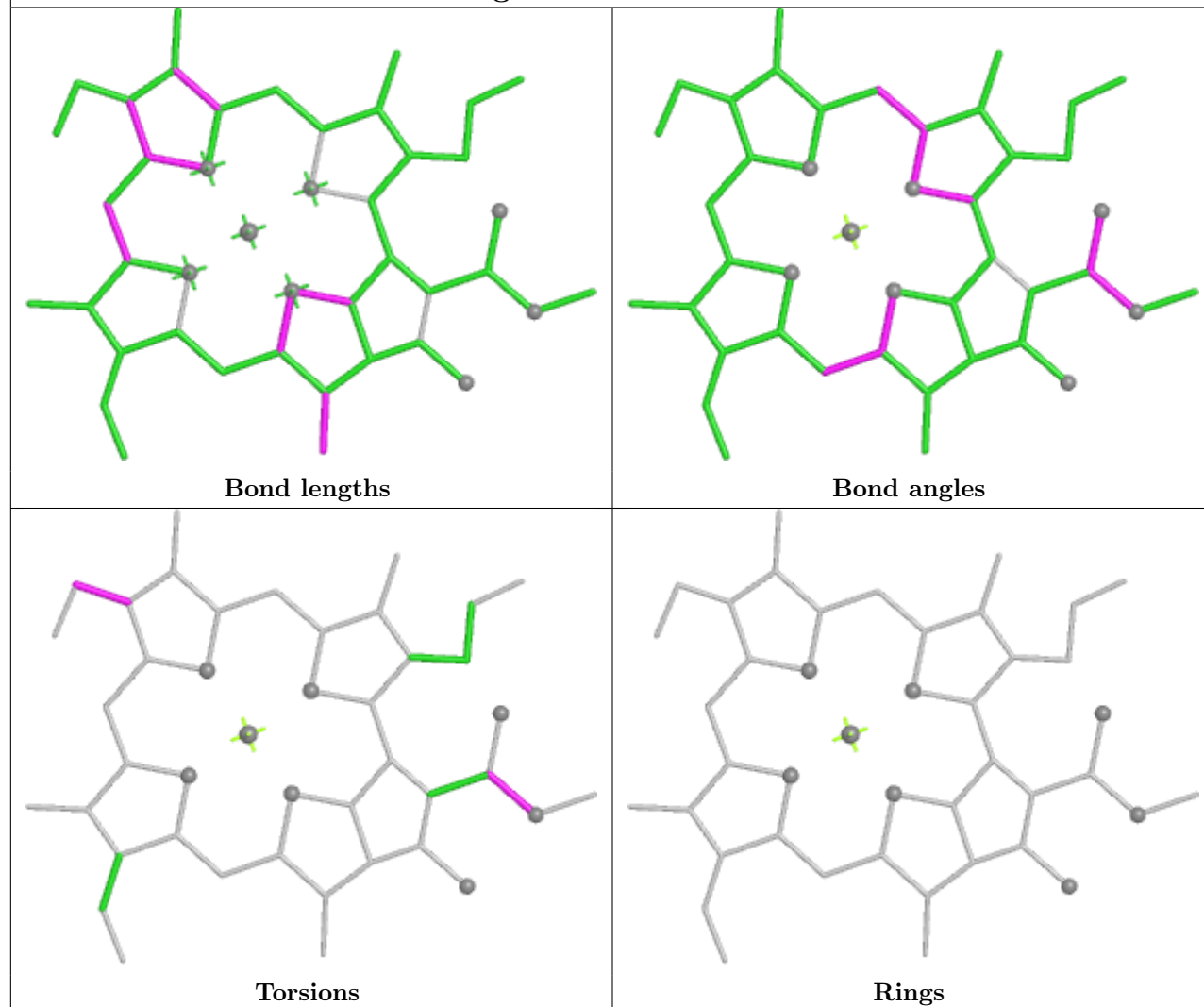


Ligand CLA AA 842

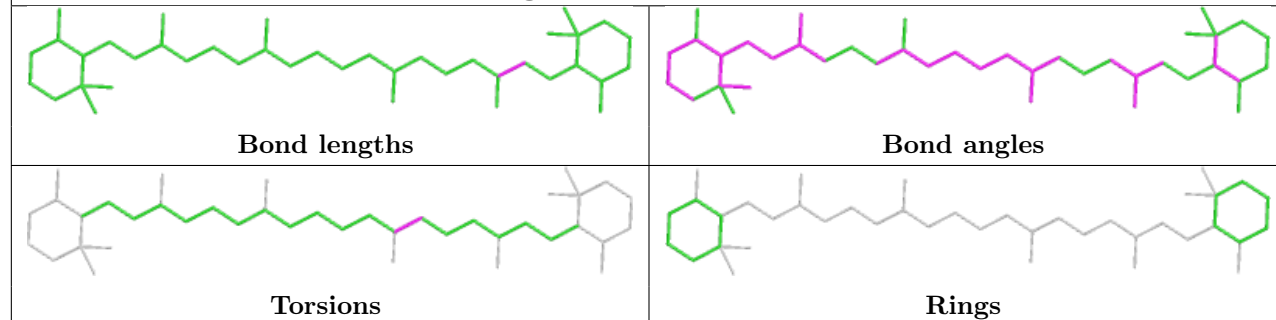




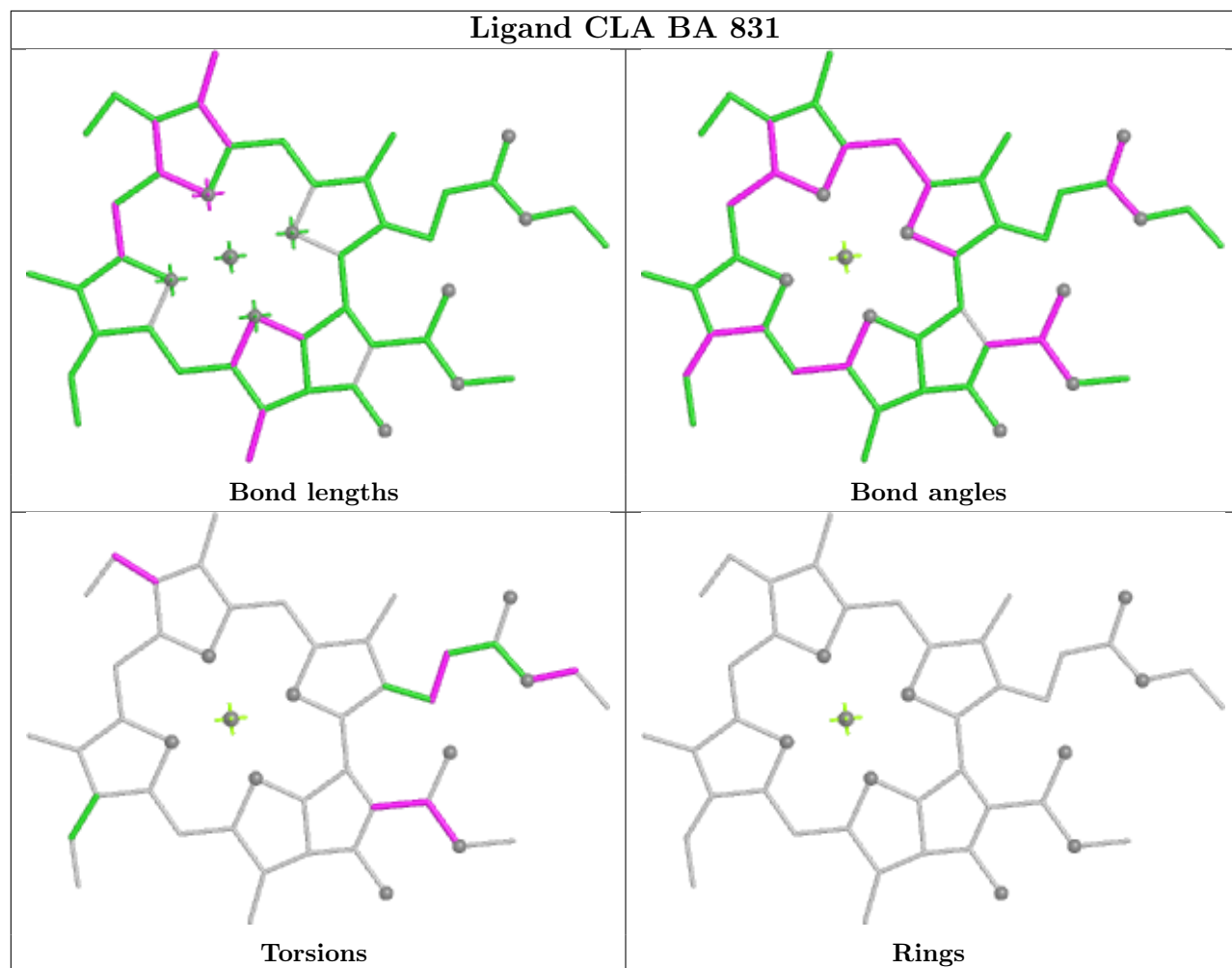
Ligand CLA A6 614



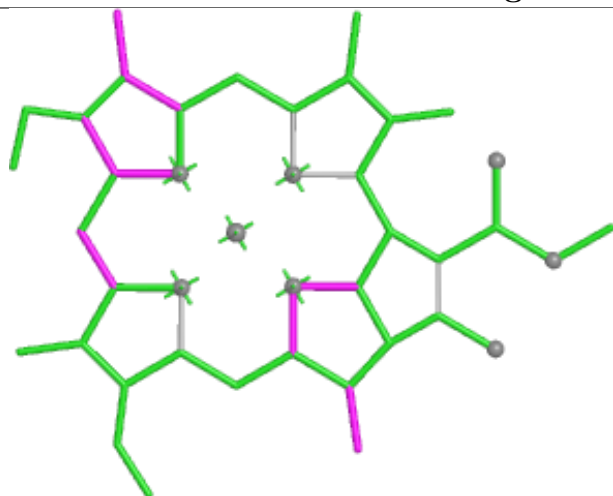
Ligand BCR AJ 101



Ligand CLA BA 831



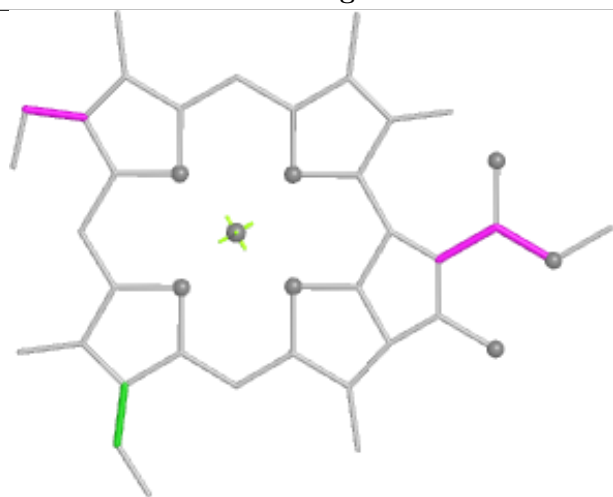
Ligand CLA A3 309



Bond lengths



Bond angles

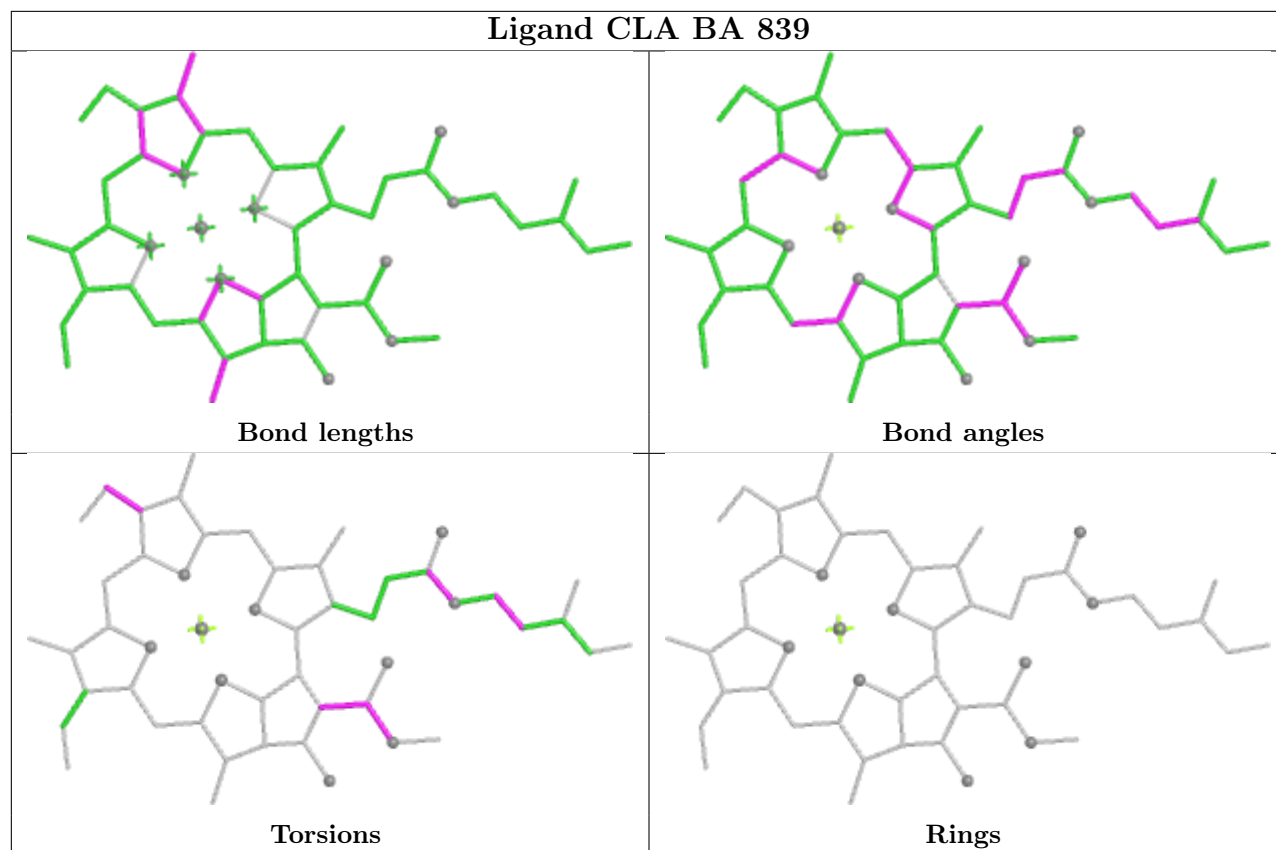


Torsions

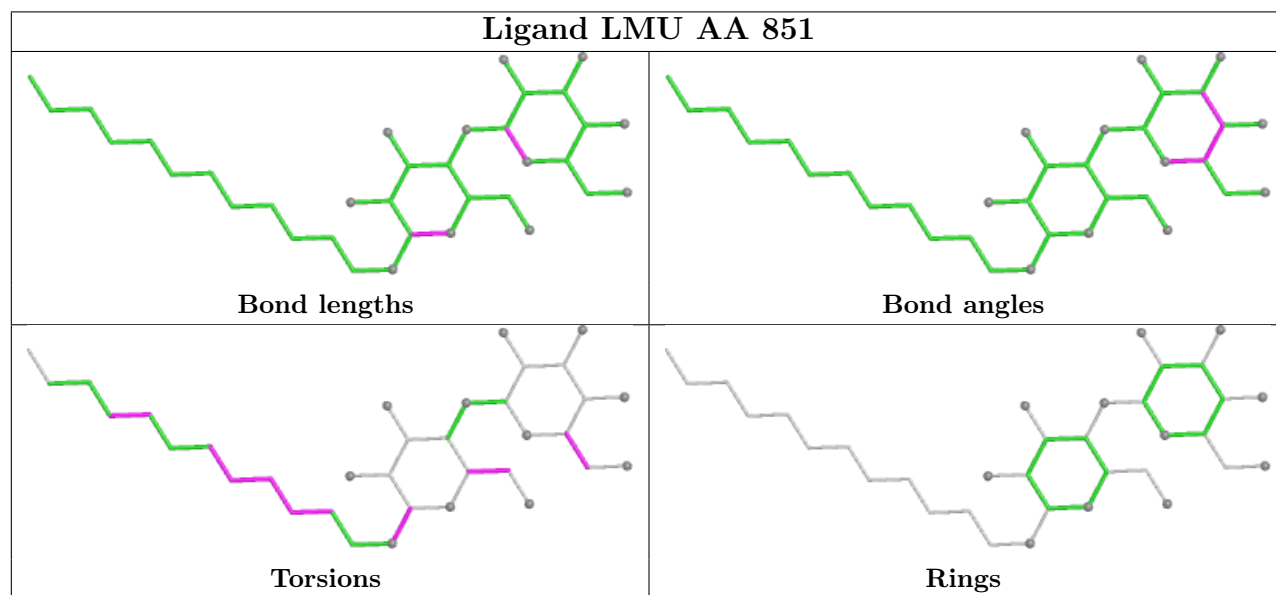


Rings

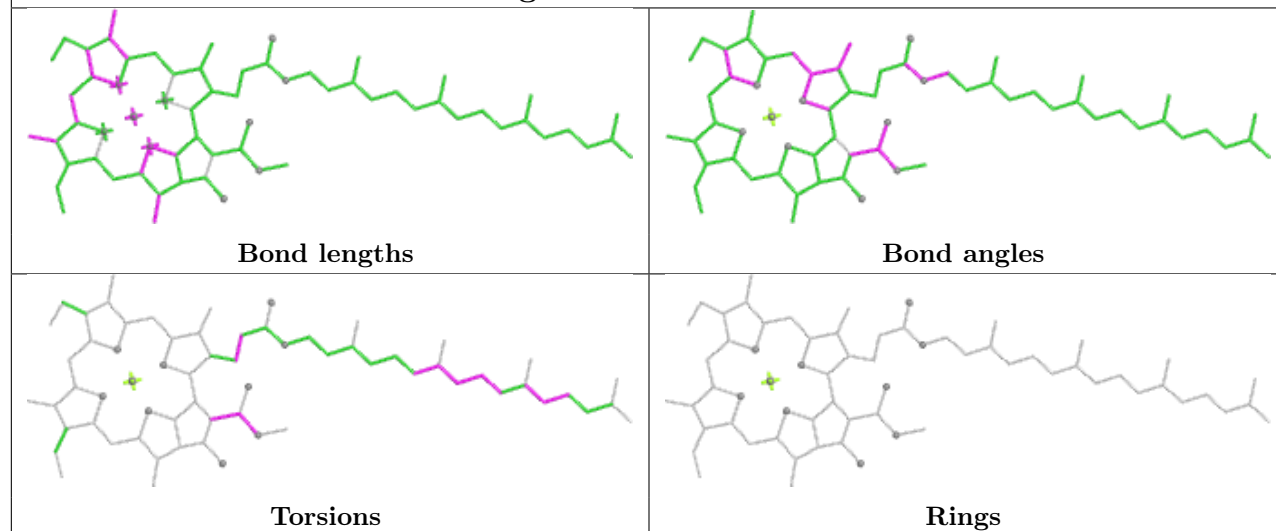
Ligand CLA BA 839



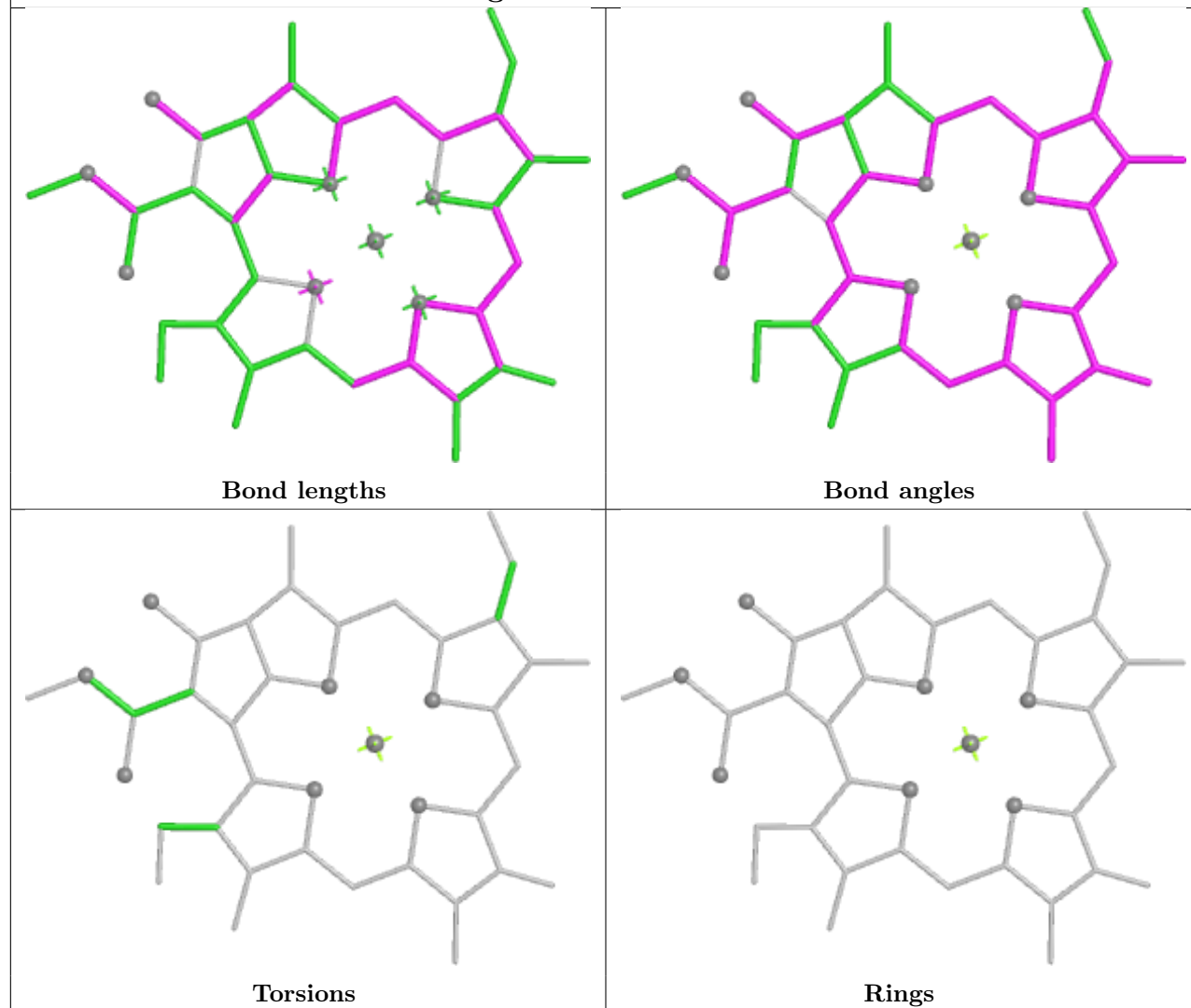
Ligand LMU AA 851

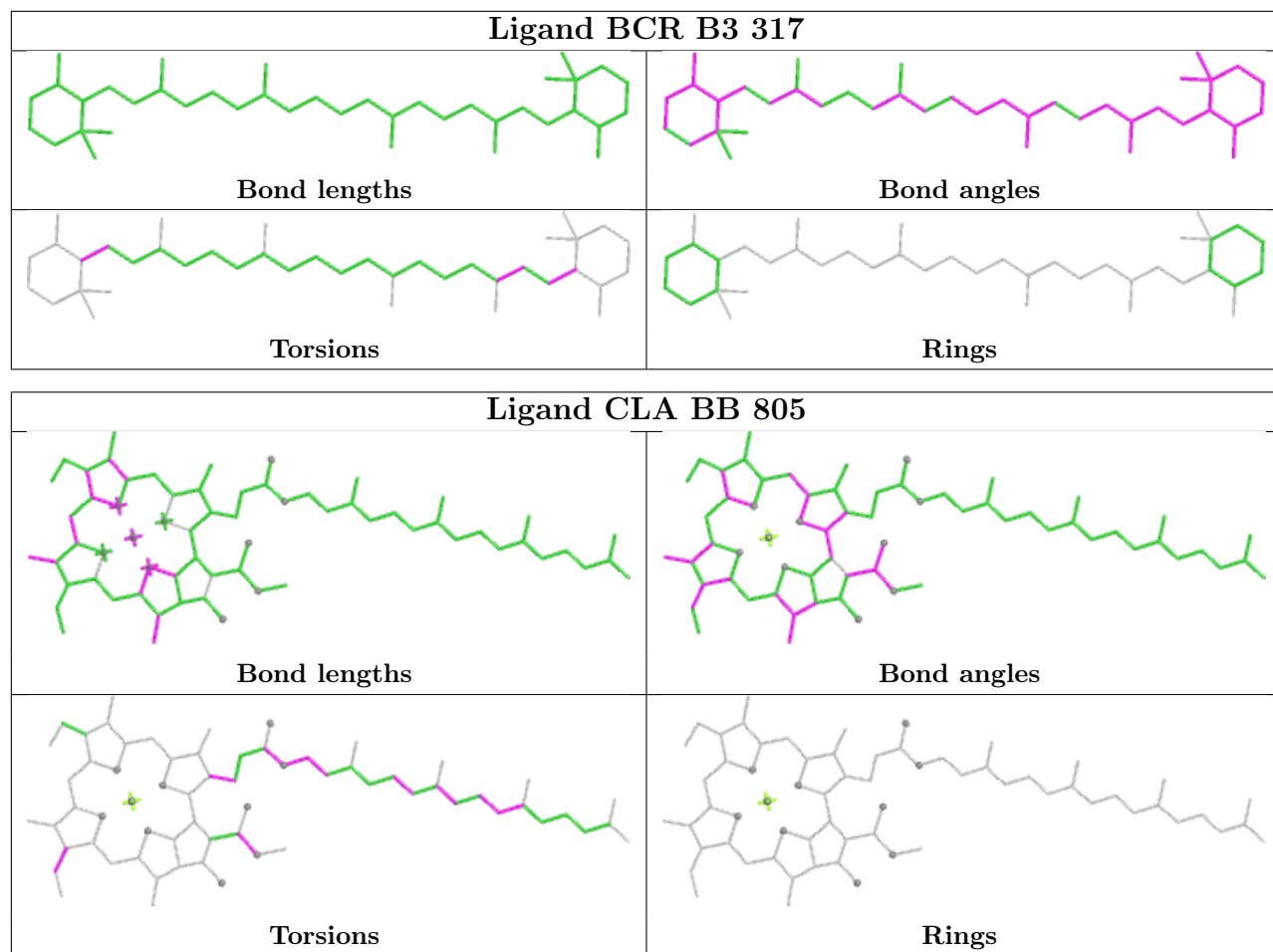


Ligand CLA AB 825

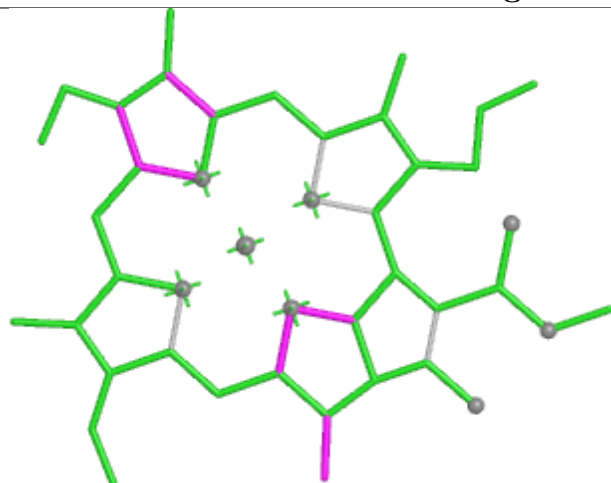


Ligand CHL A4 305

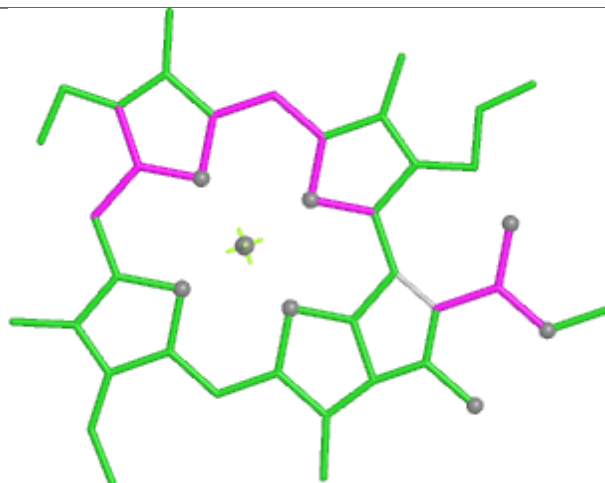




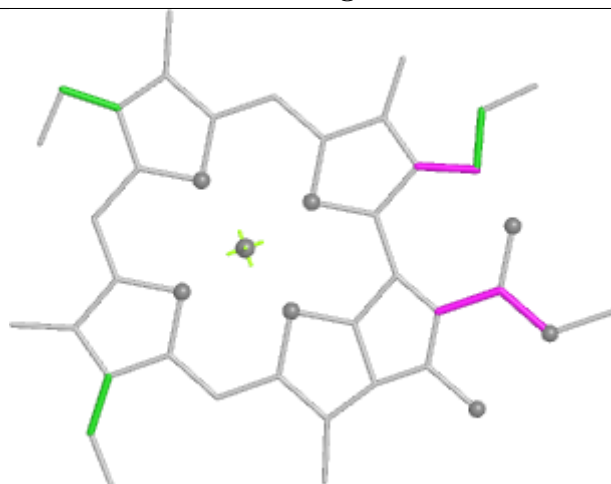
Ligand CLA BL 304



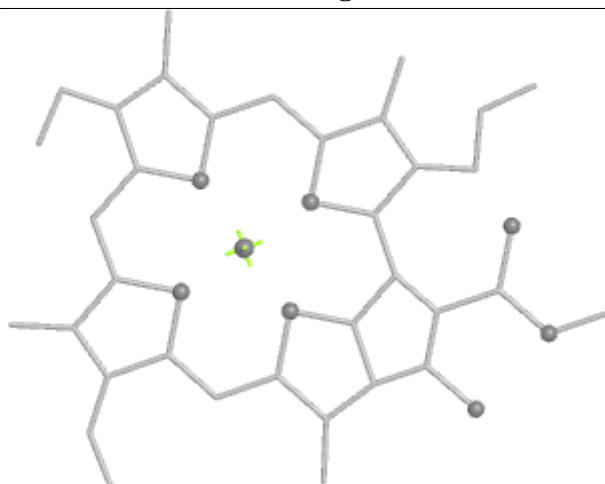
Bond lengths



Bond angles

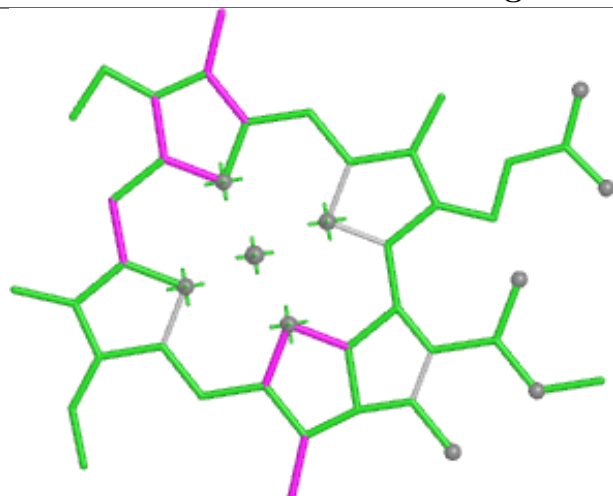


Torsions

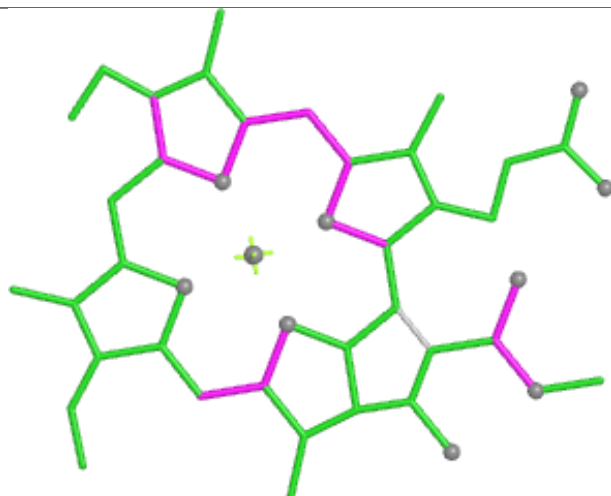


Rings

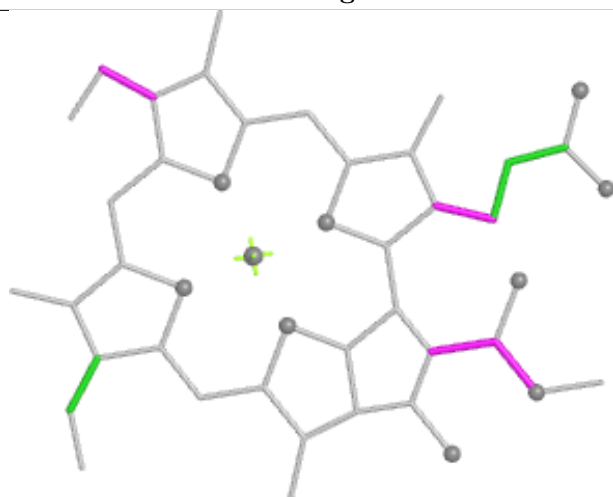
Ligand CLA A4 312



Bond lengths



Bond angles

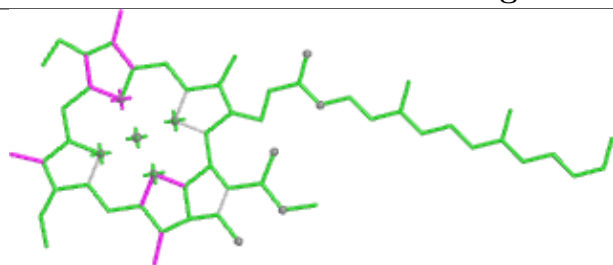


Torsions

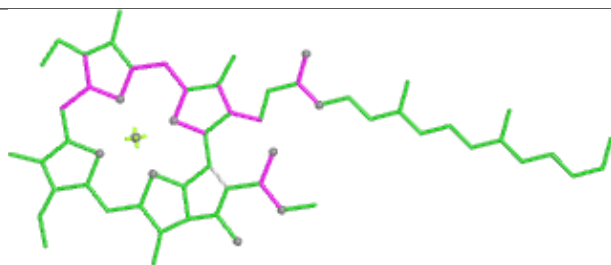


Rings

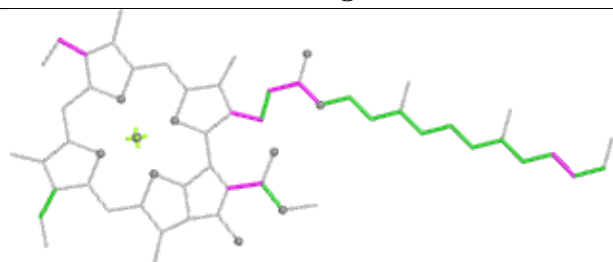
Ligand CLA AA 818



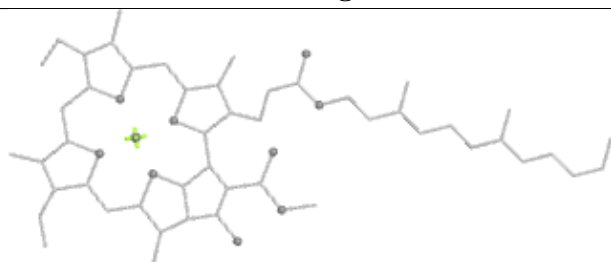
Bond lengths



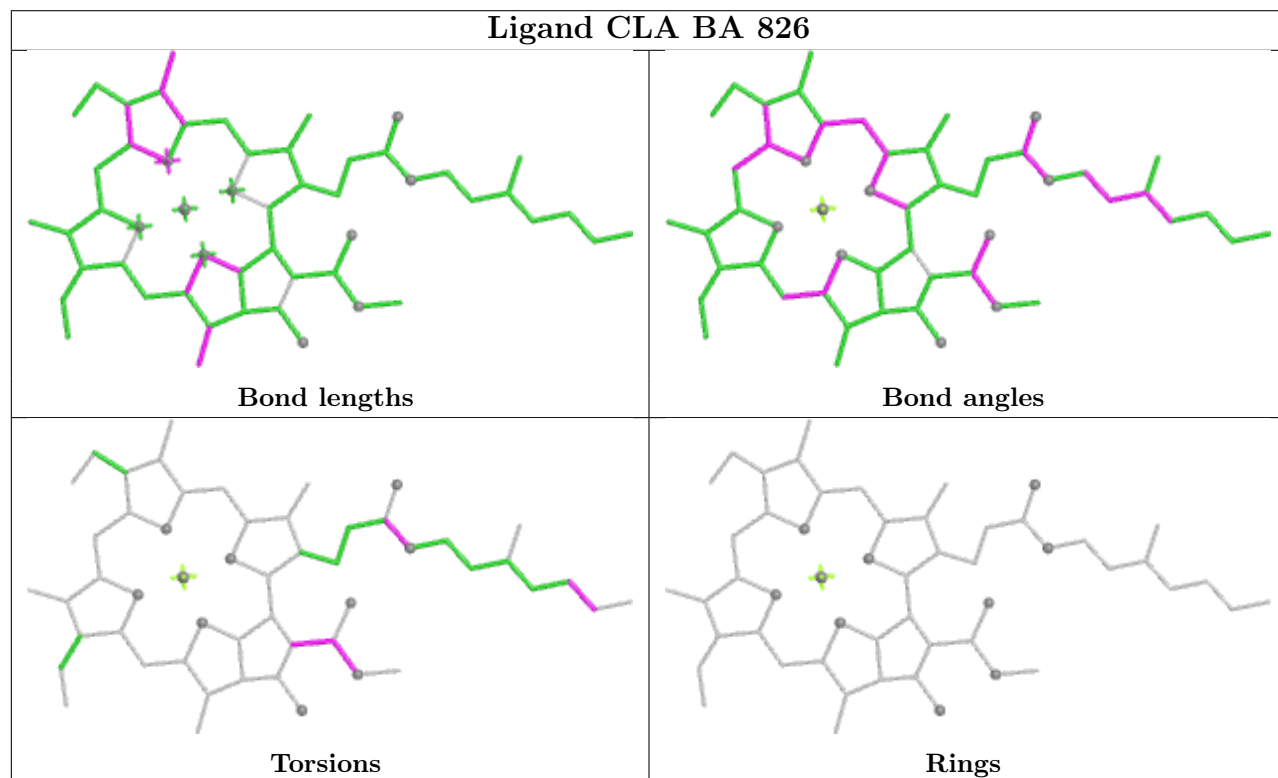
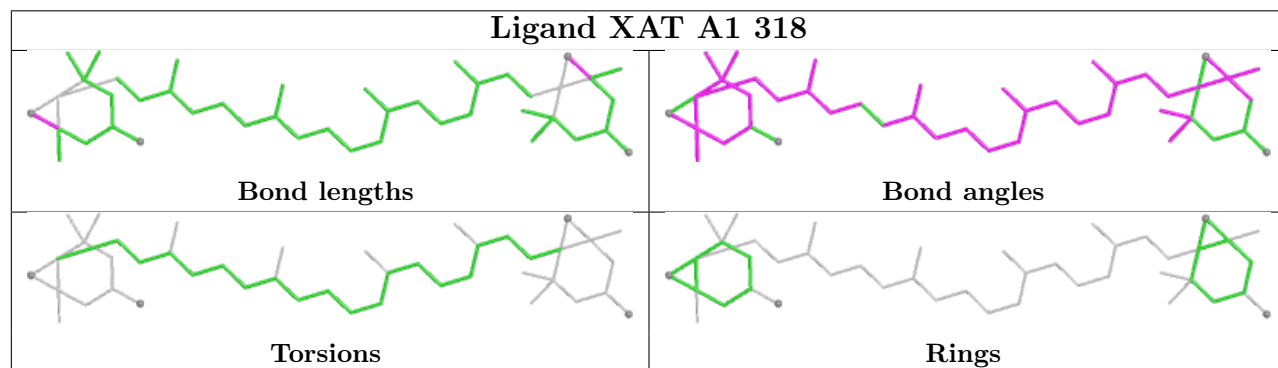
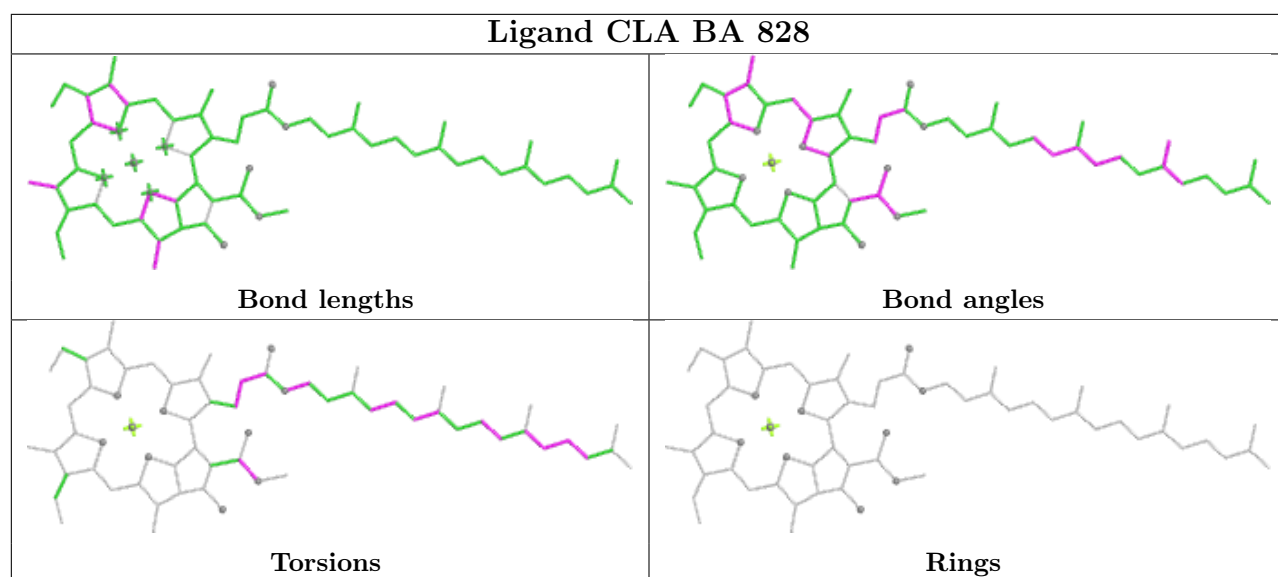
Bond angles

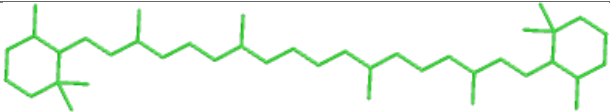
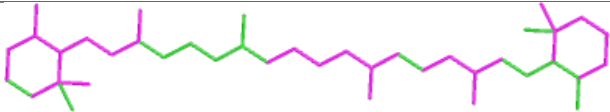
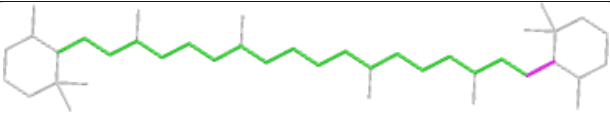
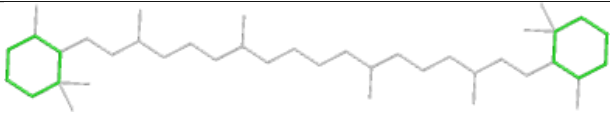


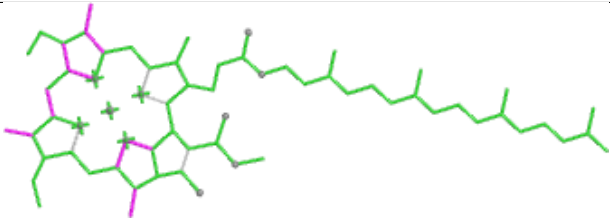
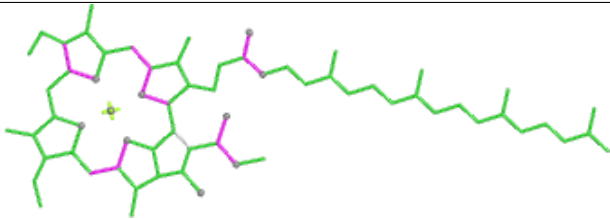
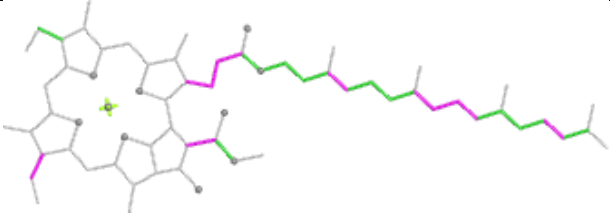
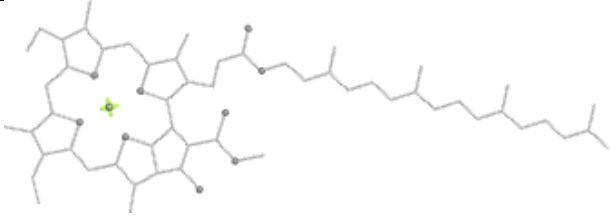
Torsions



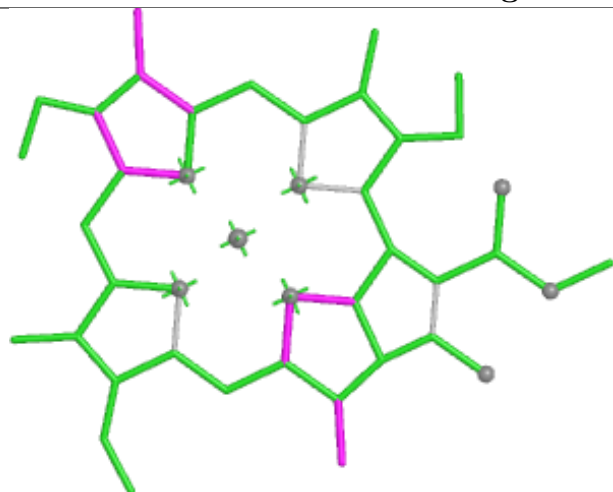
Rings



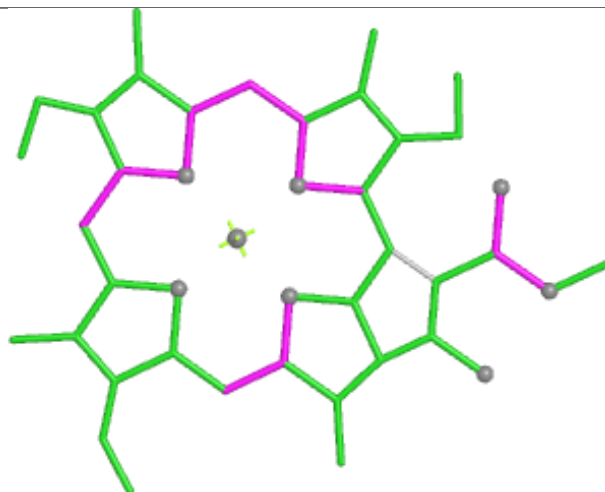
Ligand BCR AG 205			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand CLA AB 828			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand CLA AB 836



Bond lengths



Bond angles

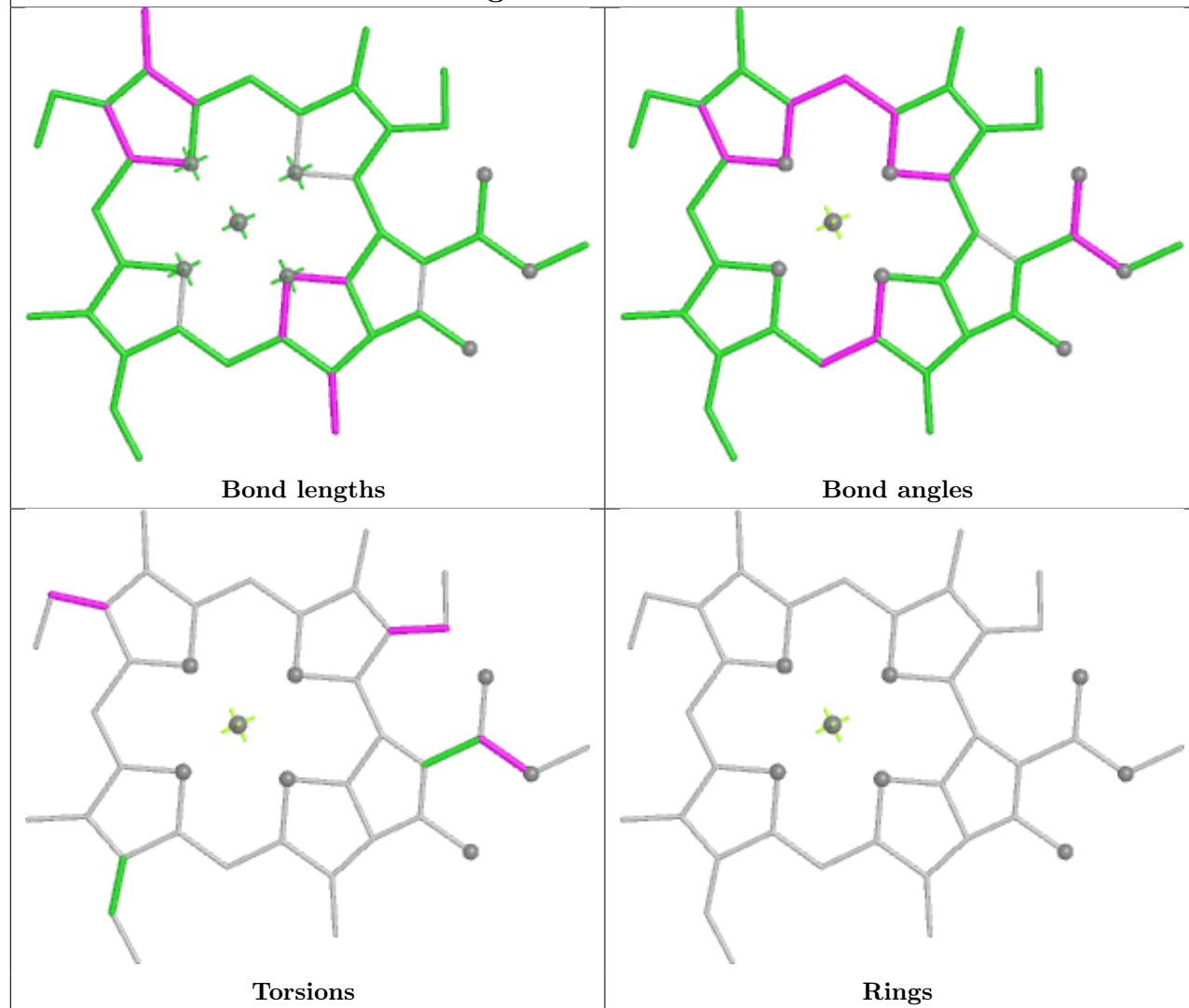


Torsions

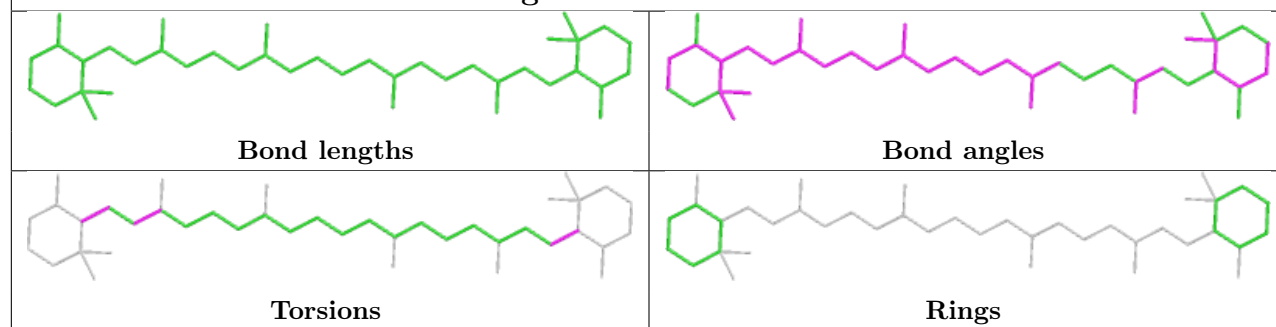


Rings

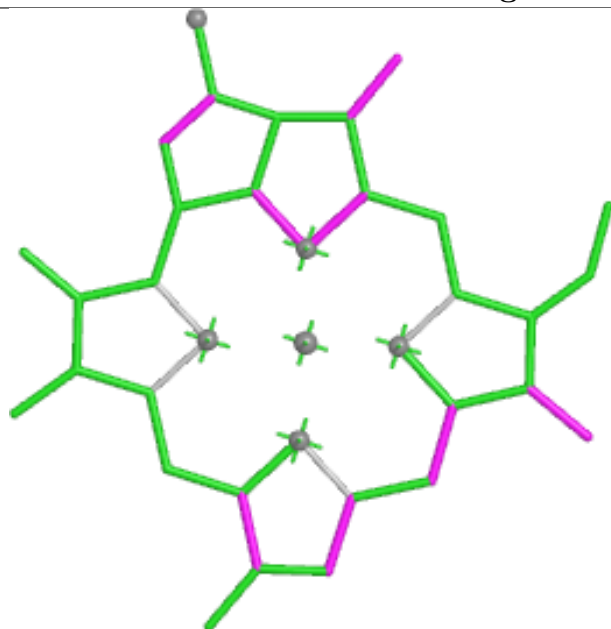
Ligand CLA B5 610



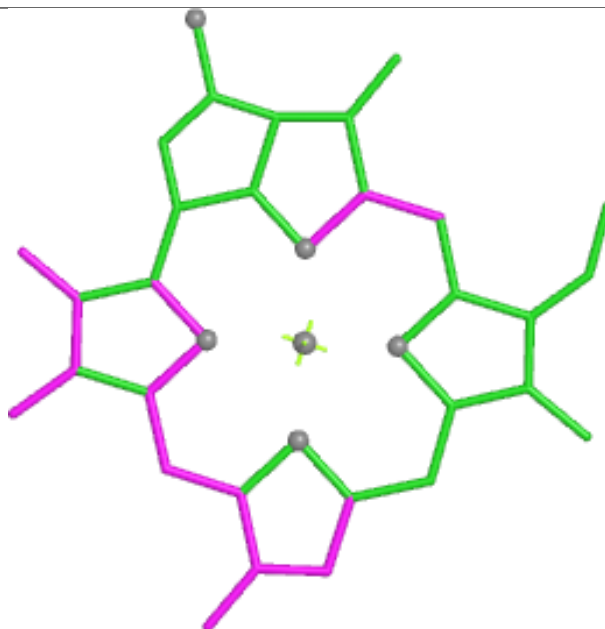
Ligand BCR BJ 103



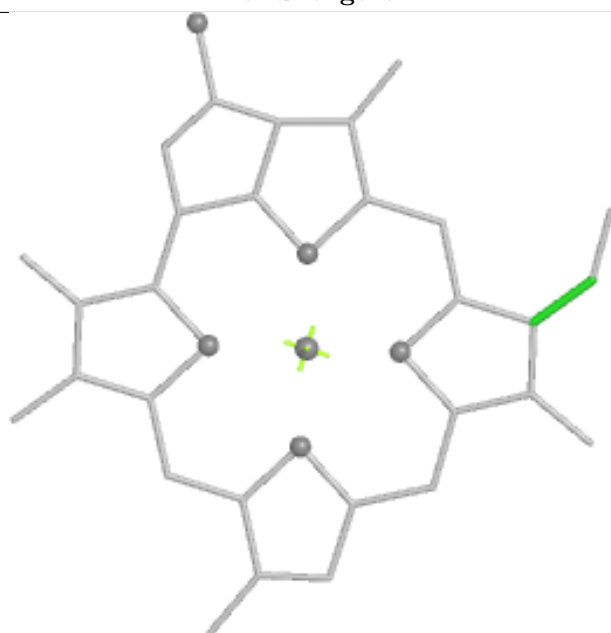
Ligand CLA AK 201



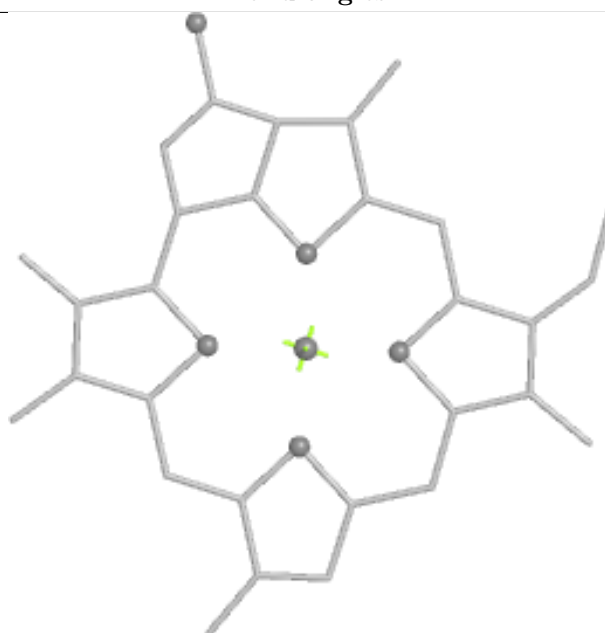
Bond lengths



Bond angles

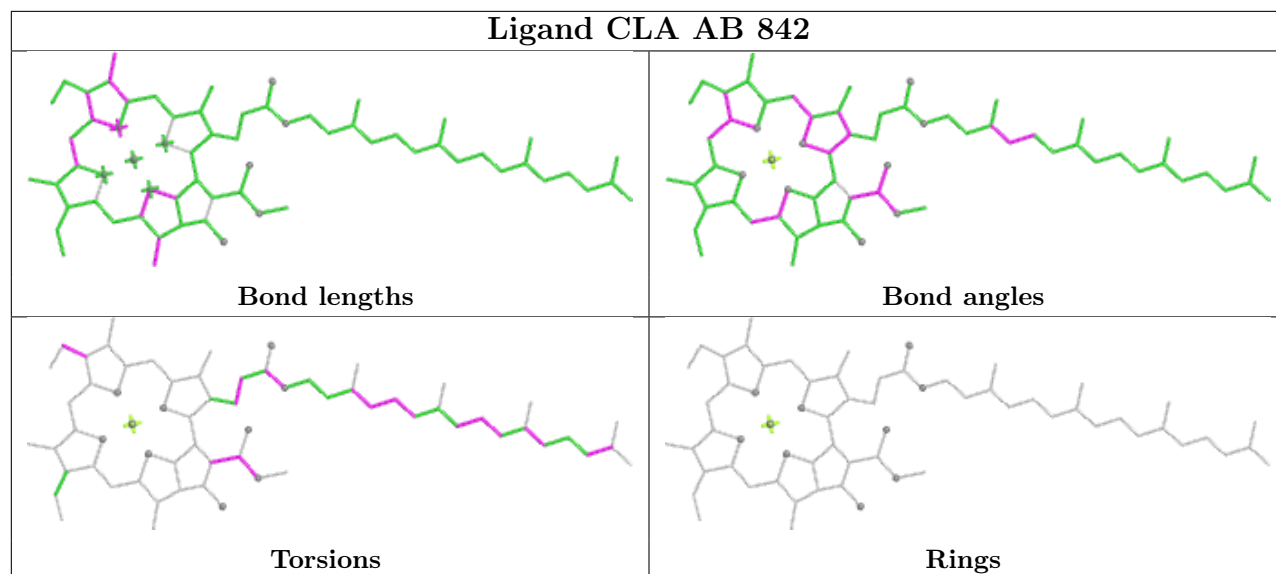


Torsions

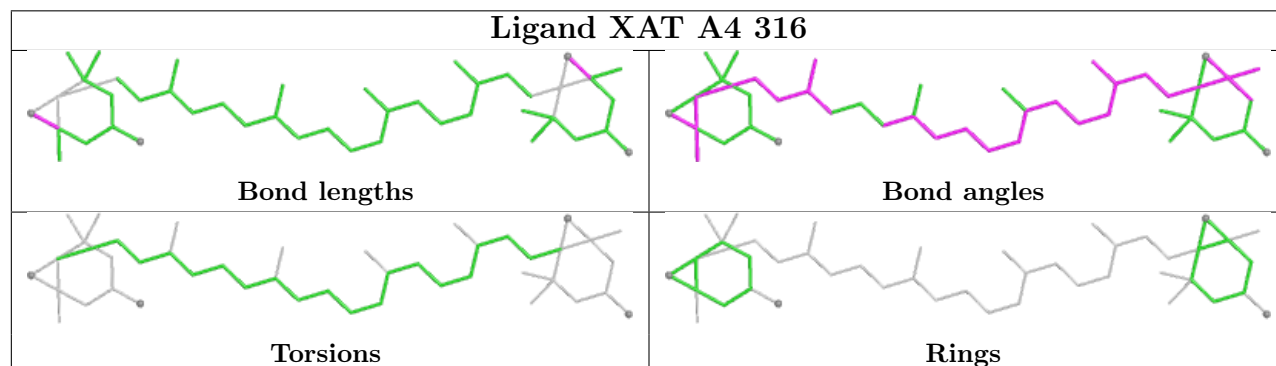


Rings

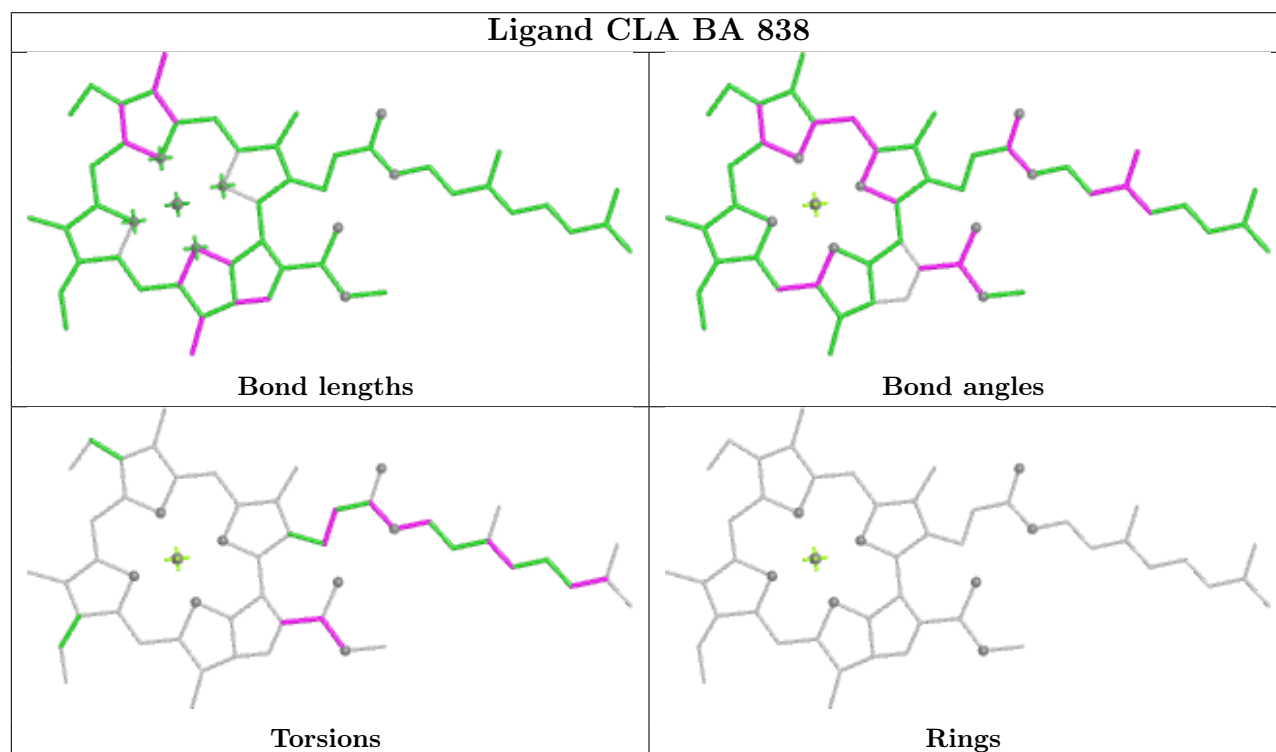
Ligand CLA AB 842

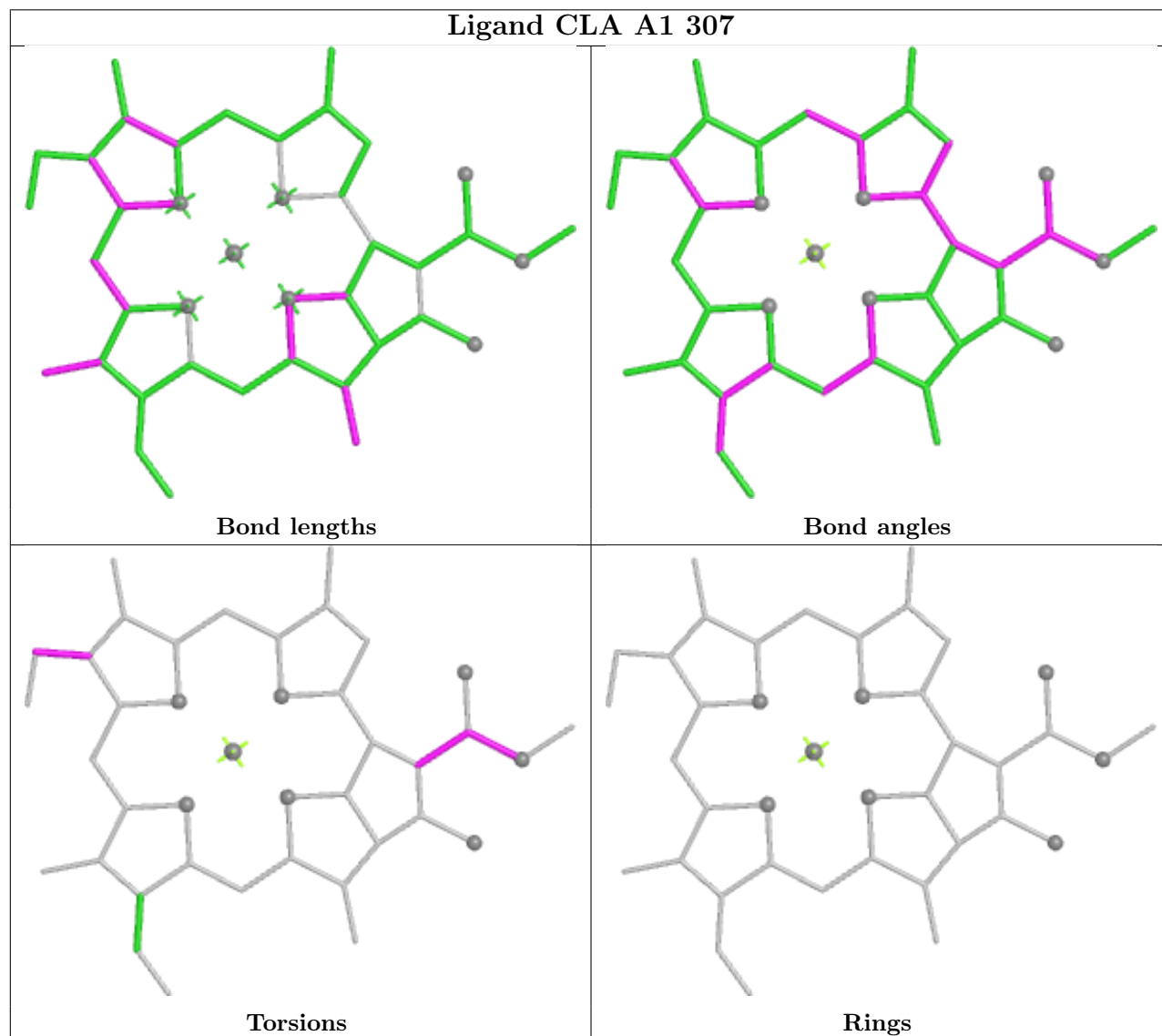
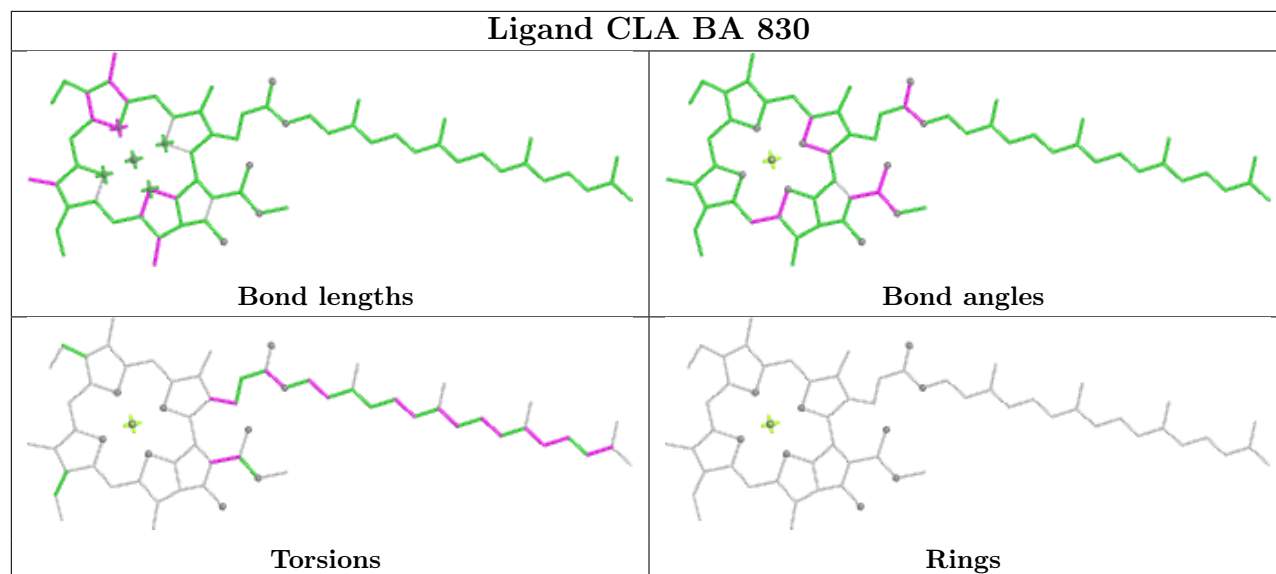


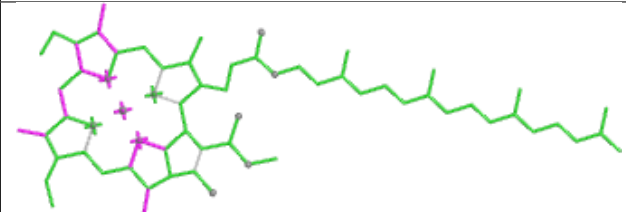
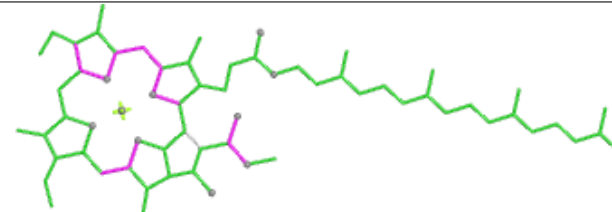
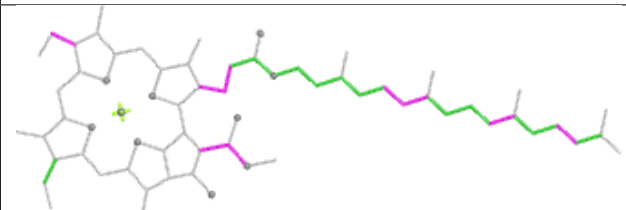
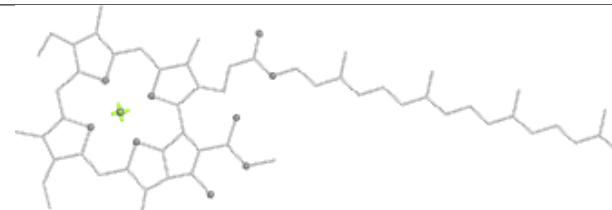
Ligand XAT A4 316

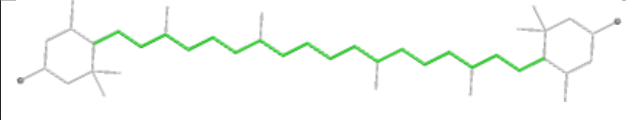
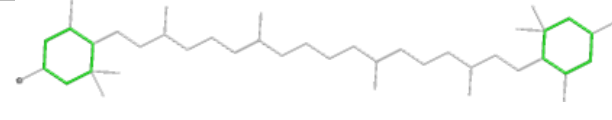


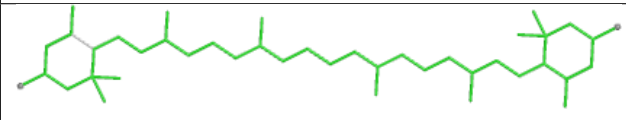
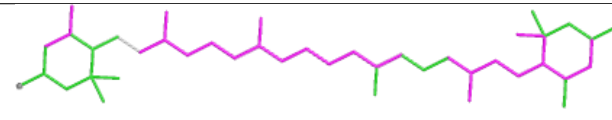
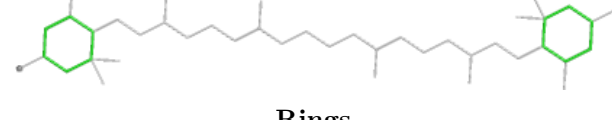
Ligand CLA BA 838



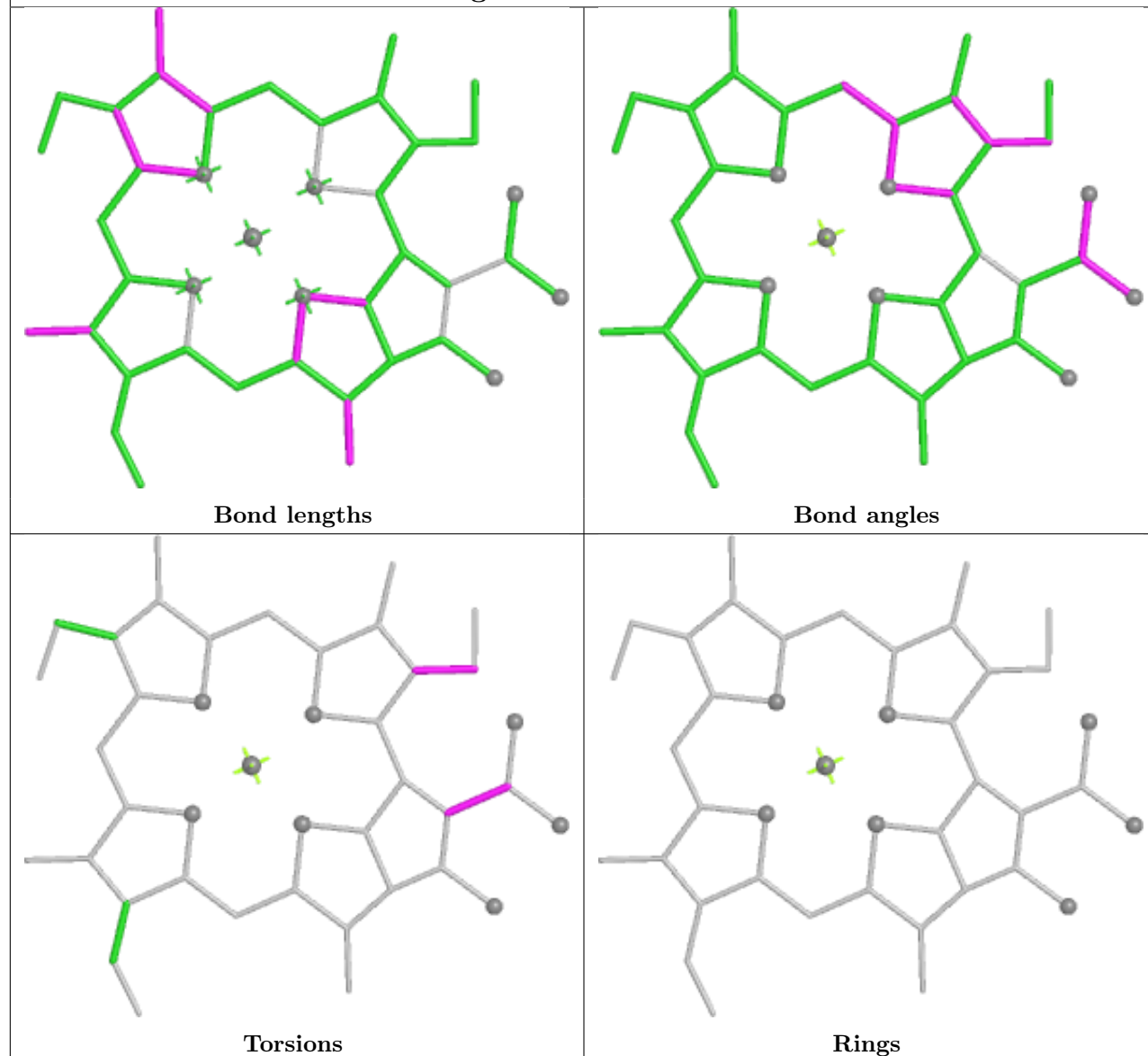


Ligand CLA AB 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

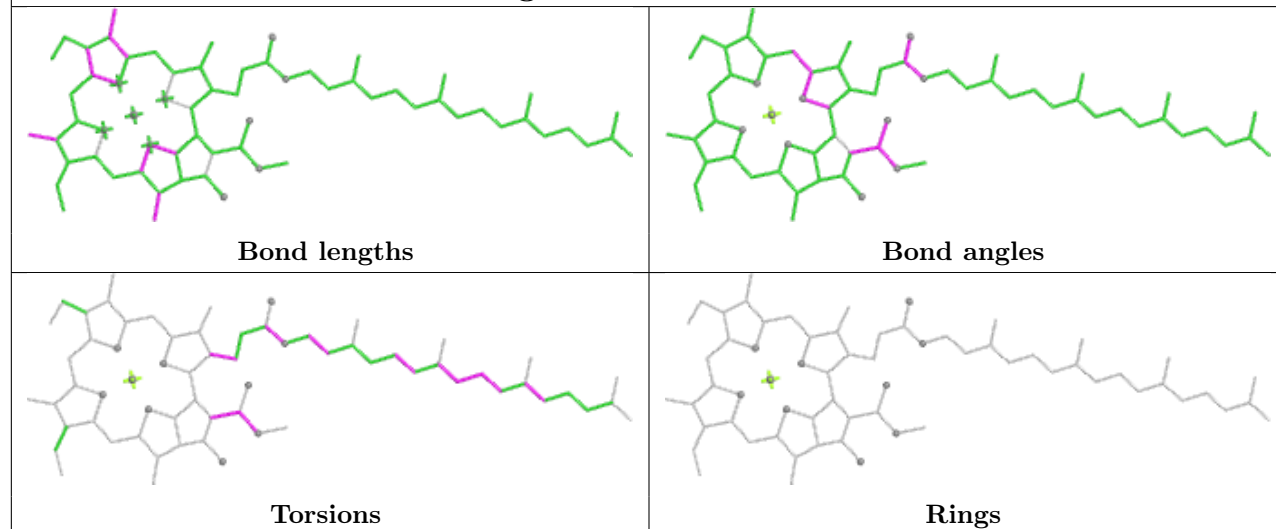
Ligand LUT A6 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

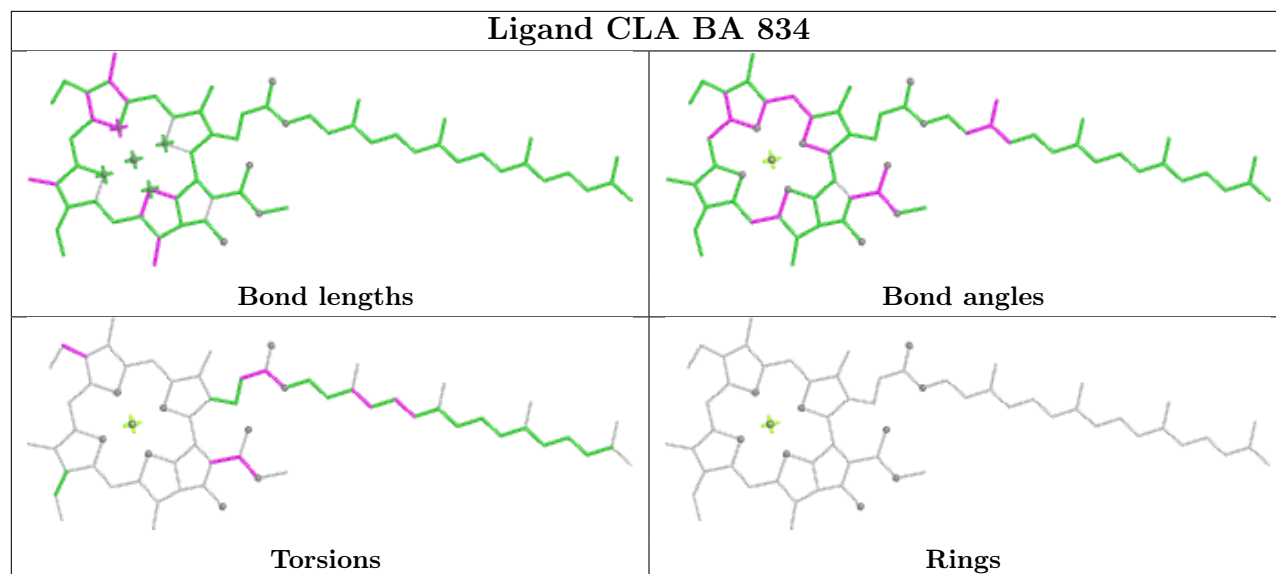
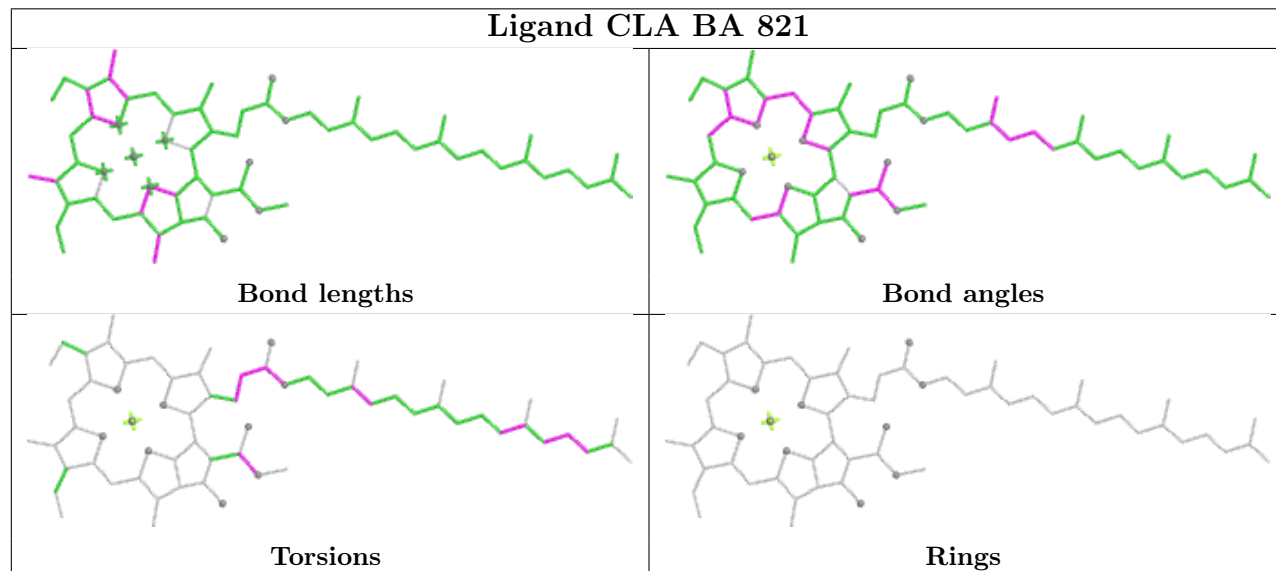
Ligand LUT B2 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B5 611

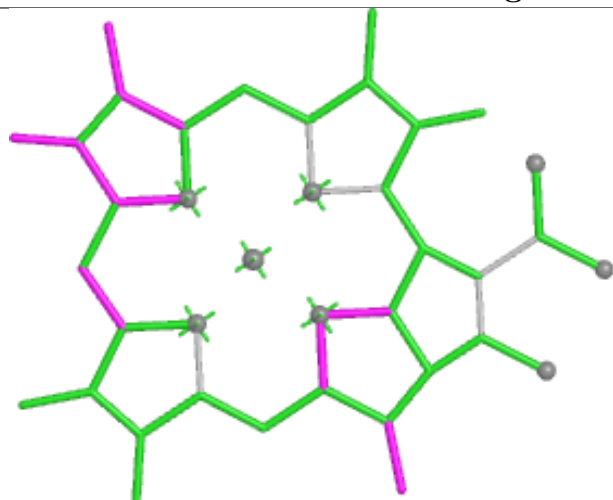


Ligand CLA AA 830

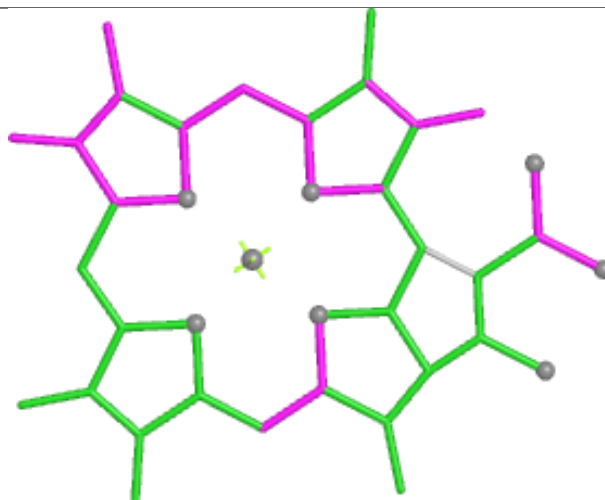


Ligand CLA BA 834**Ligand CLA BA 821**

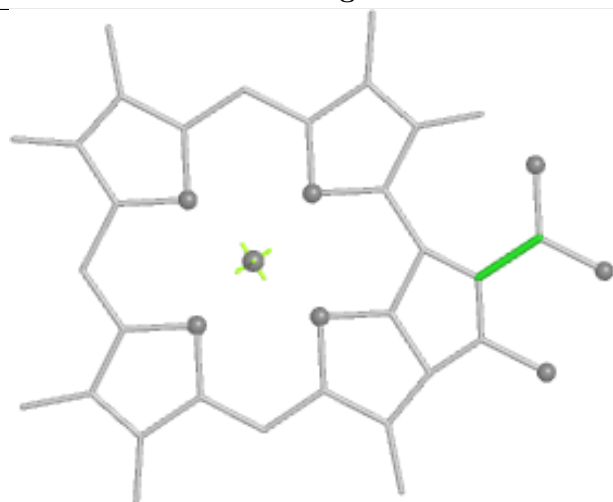
Ligand CLA A1 312



Bond lengths



Bond angles

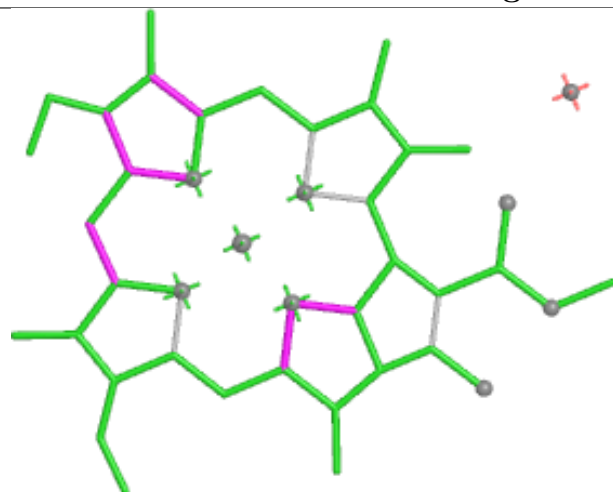


Torsions



Rings

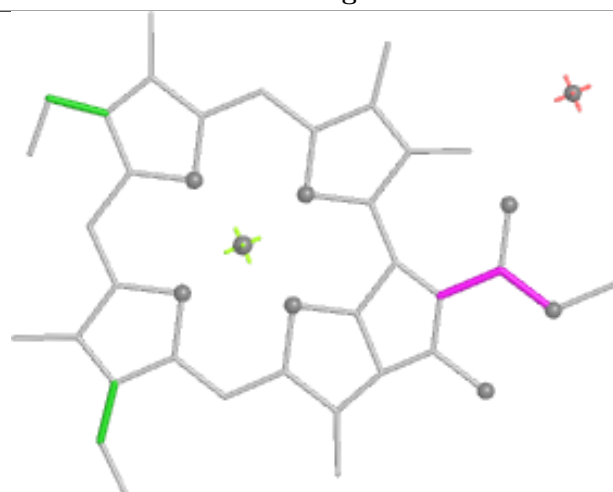
Ligand CLA BA 844



Bond lengths



Bond angles

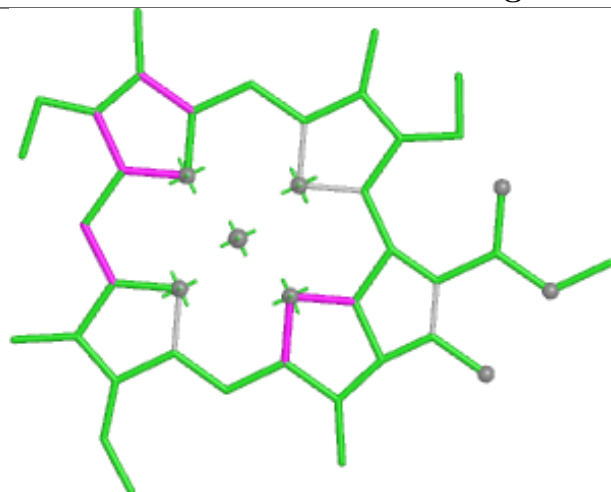


Torsions

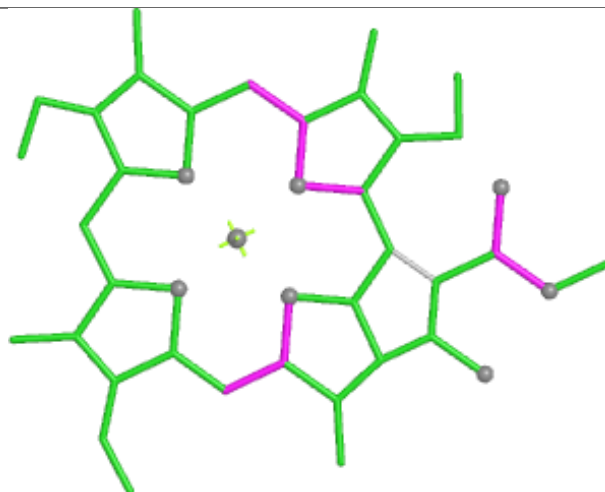


Rings

Ligand CLA AJ 102



Bond lengths



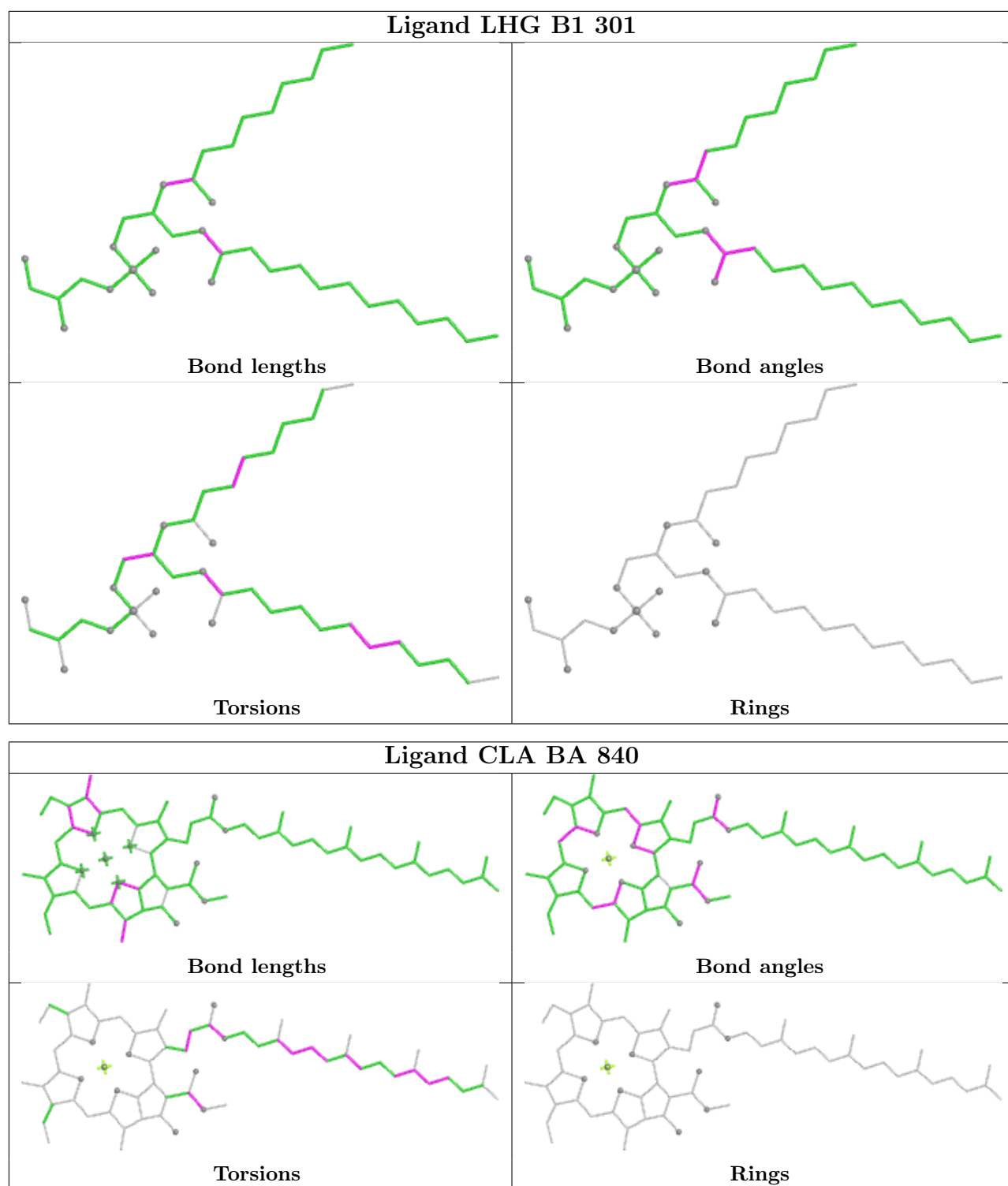
Bond angles

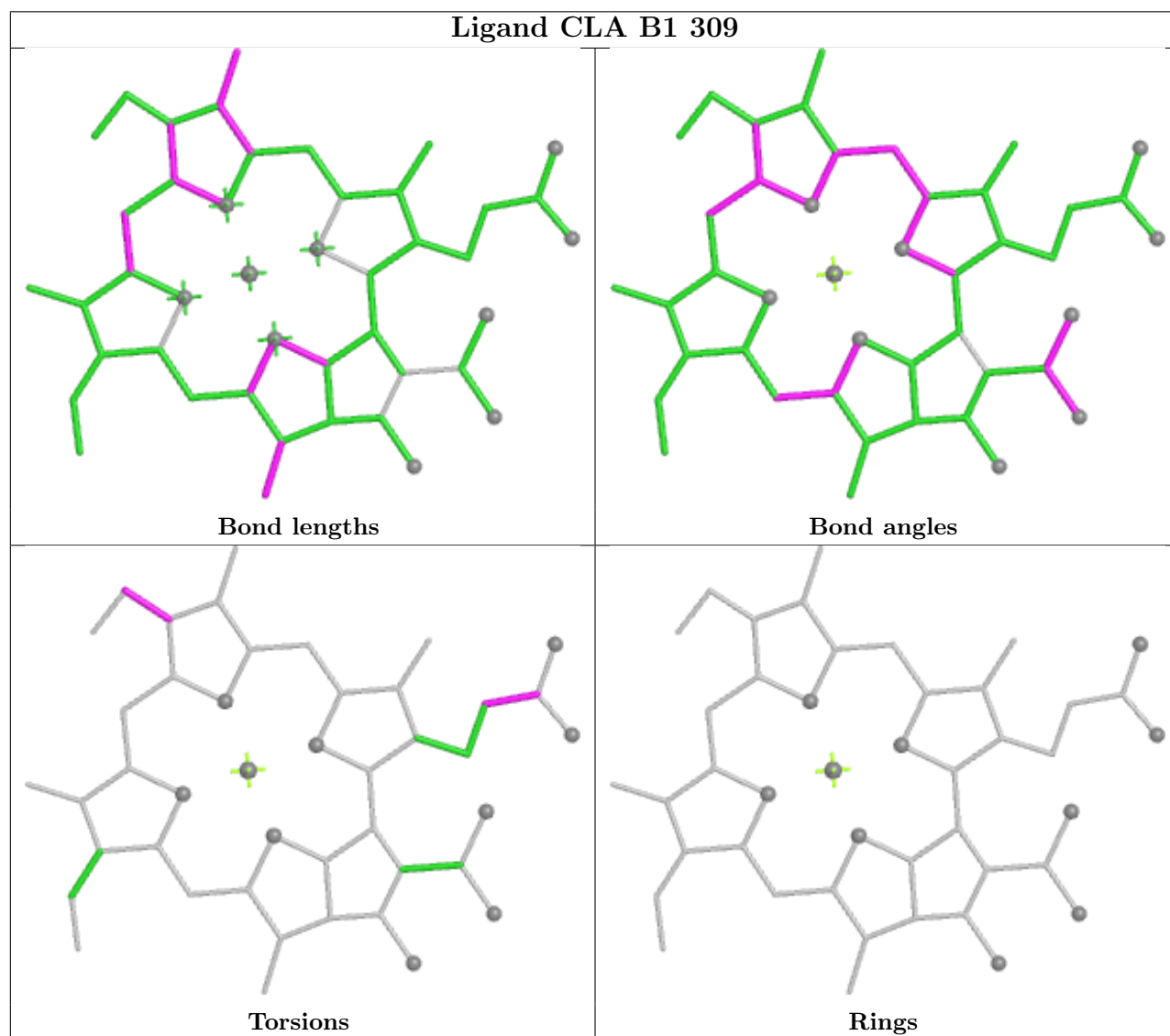
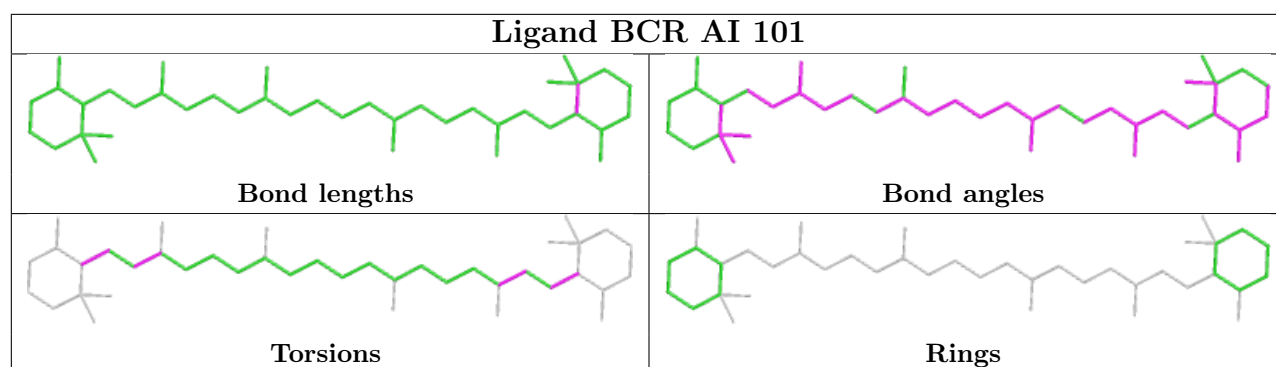


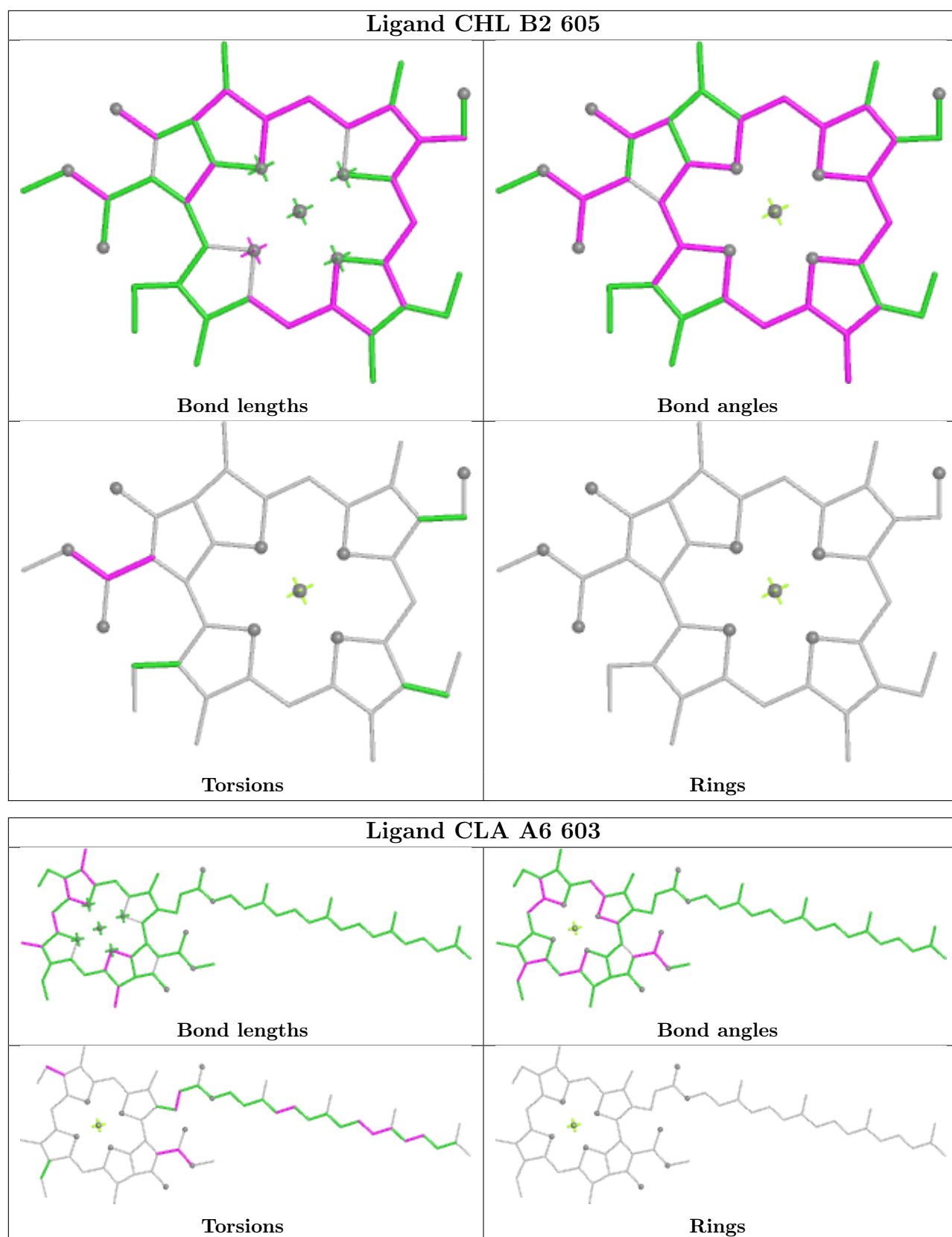
Torsions

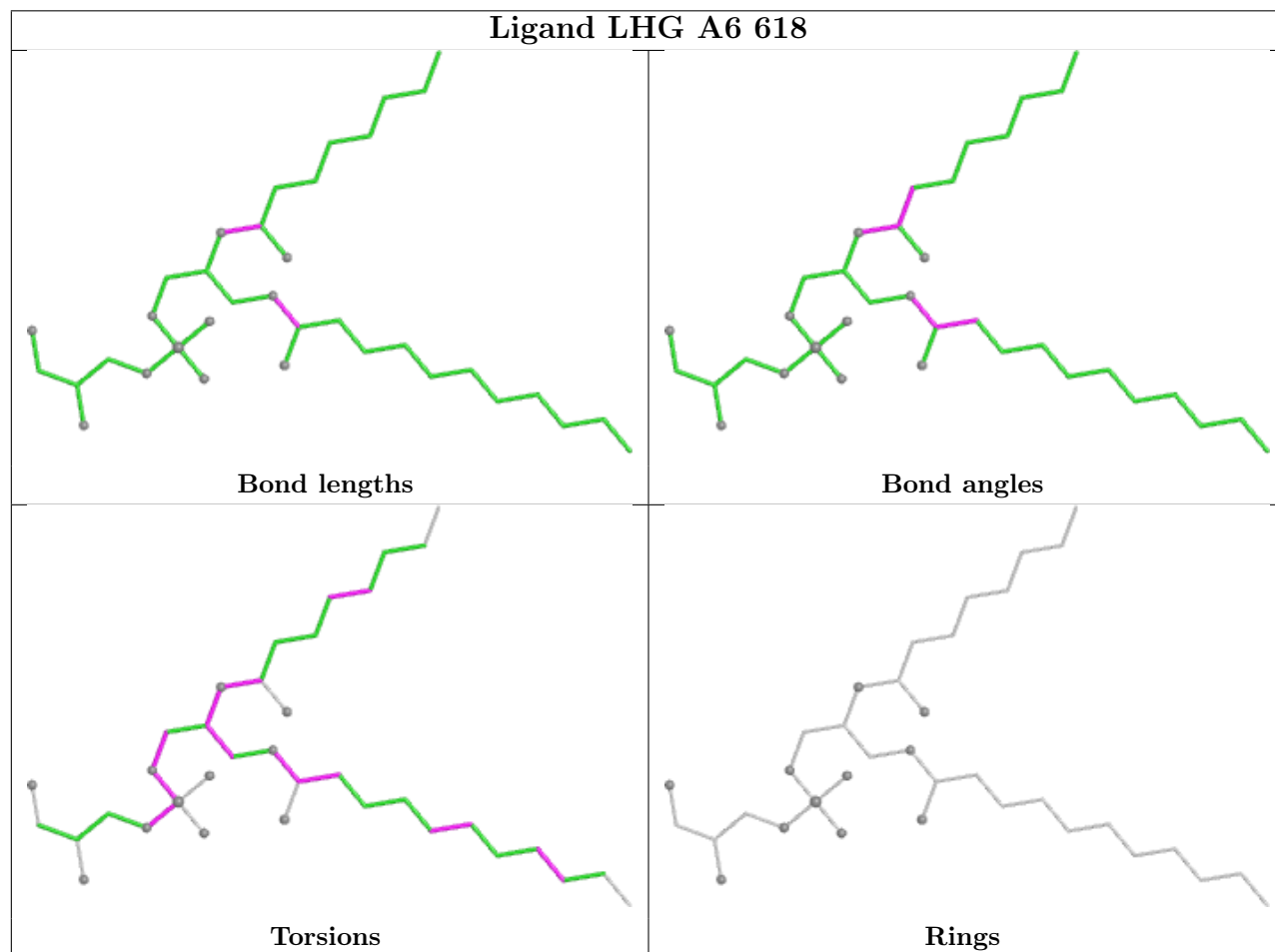
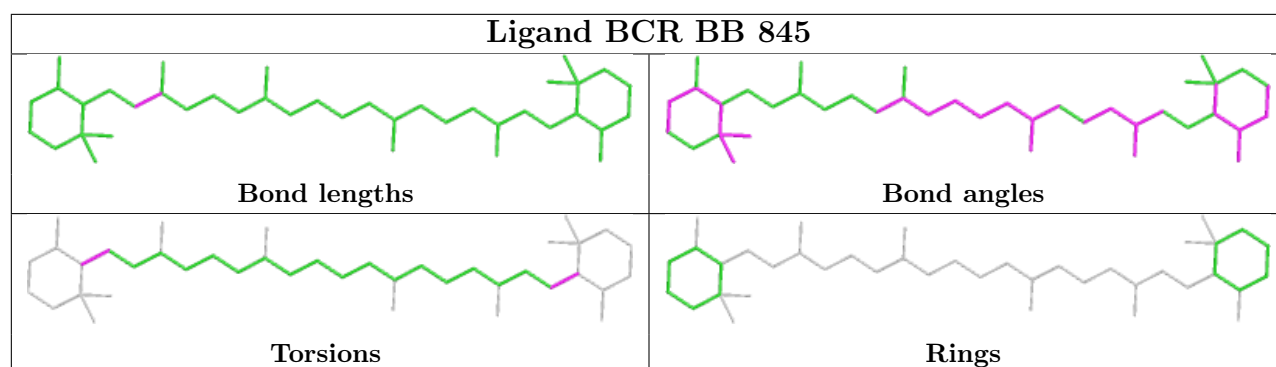


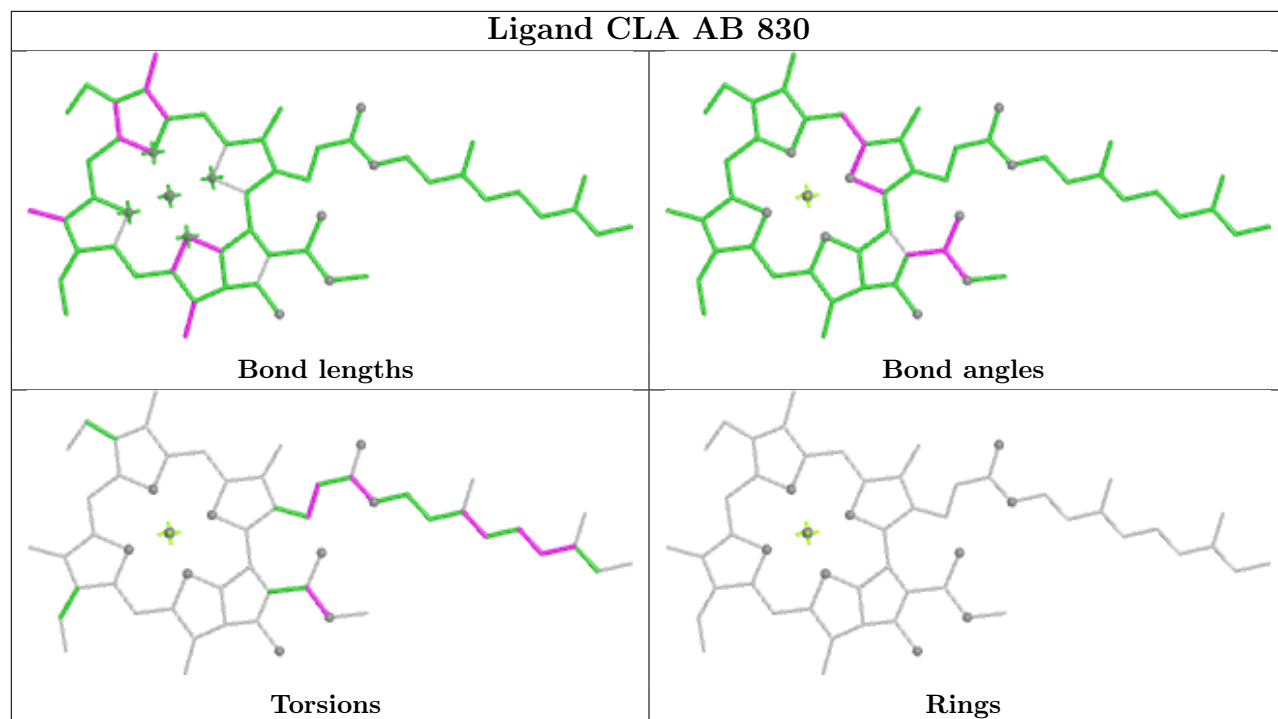
Rings



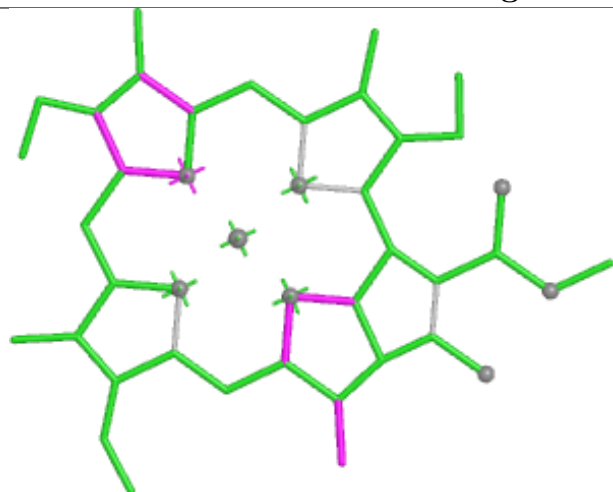




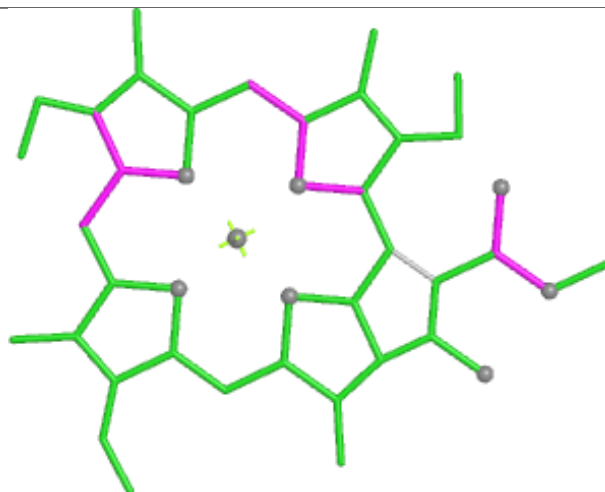




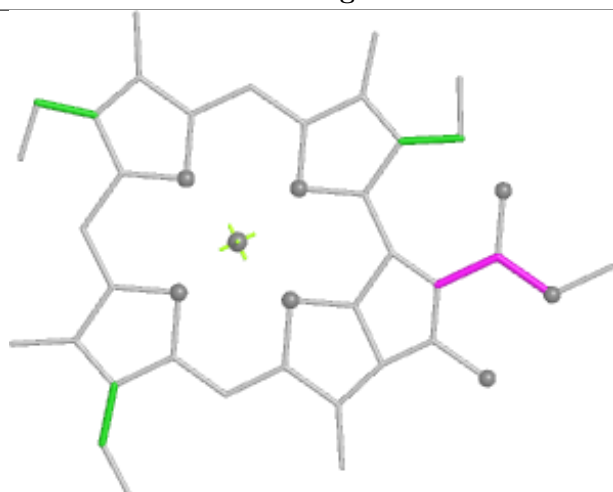
Ligand CLA BA 815



Bond lengths



Bond angles

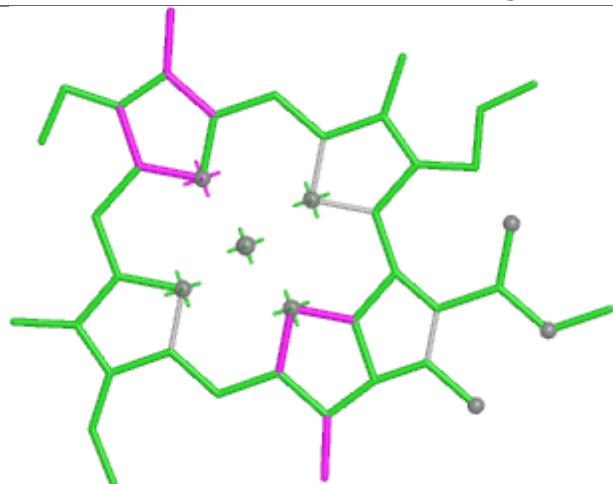


Torsions

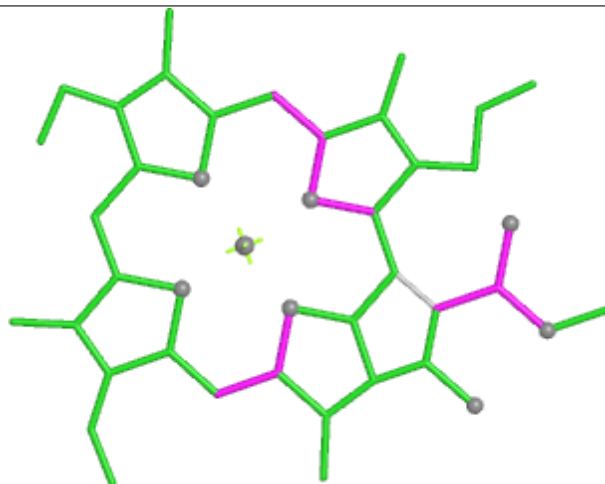


Rings

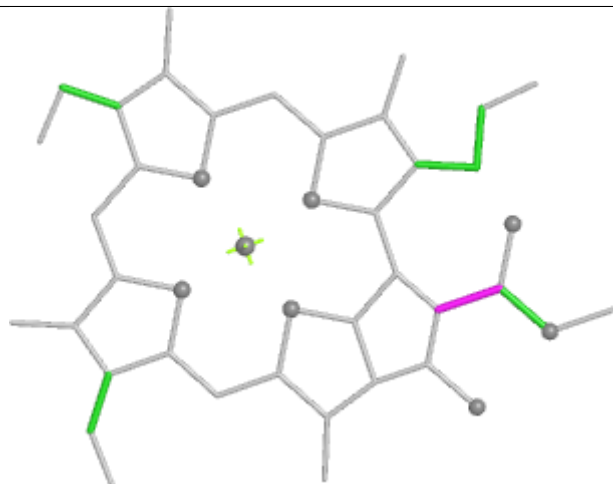
Ligand CLA BB 814



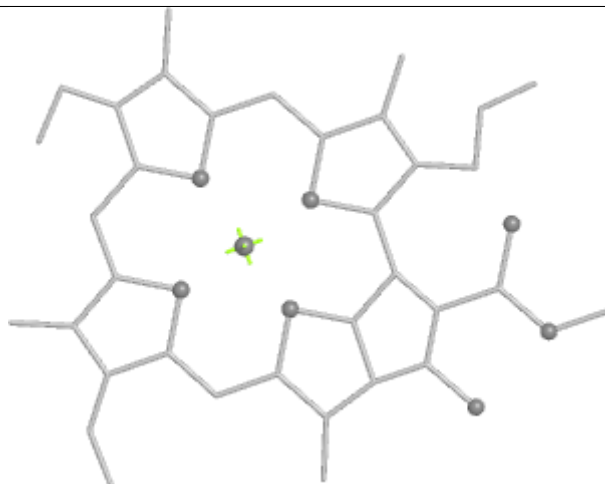
Bond lengths



Bond angles

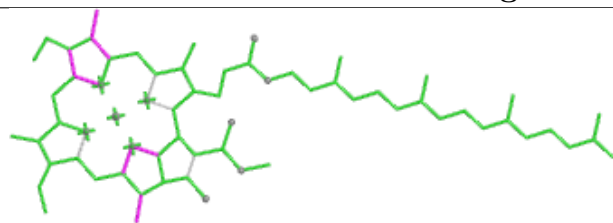


Torsions

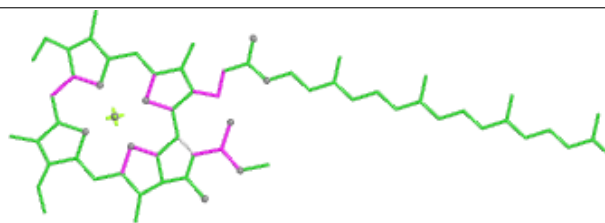


Rings

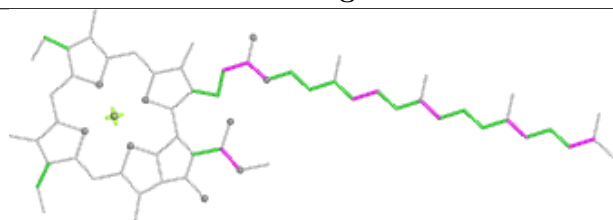
Ligand CLA AA 801



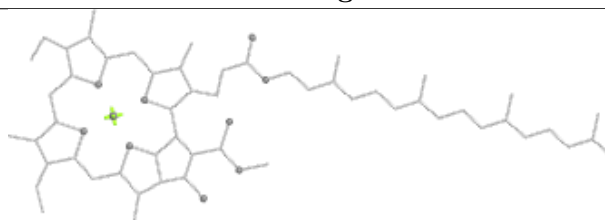
Bond lengths



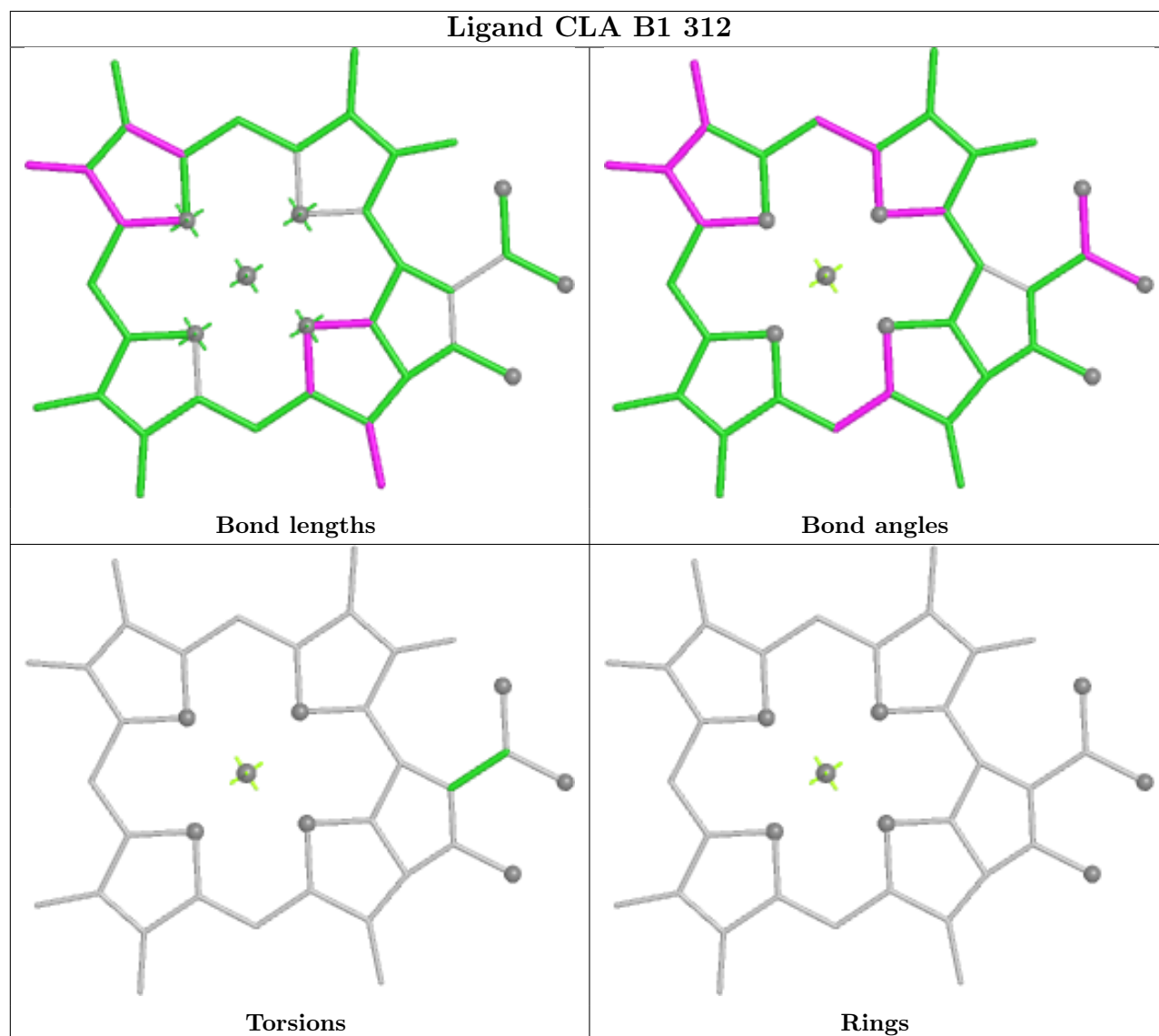
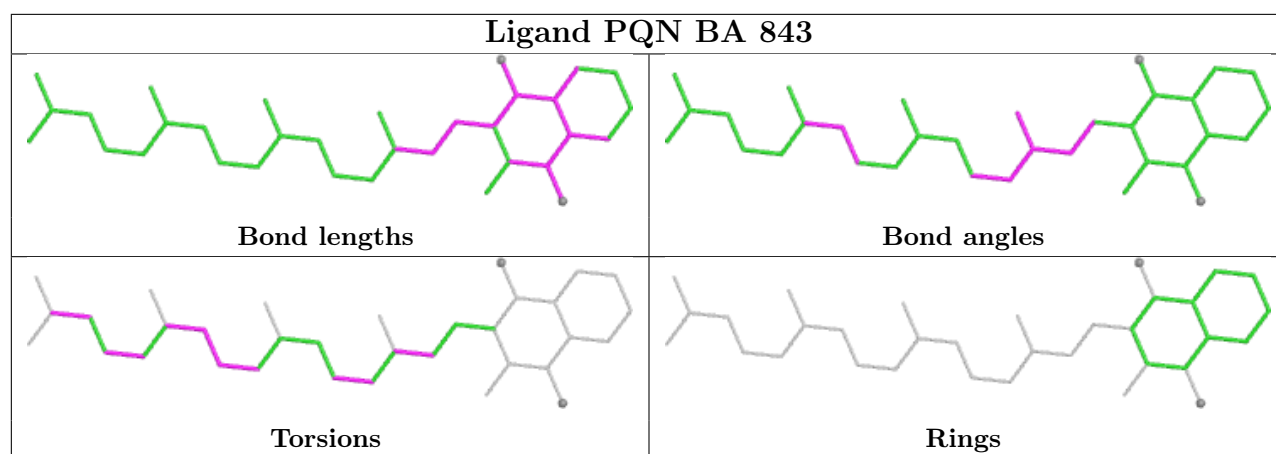
Bond angles

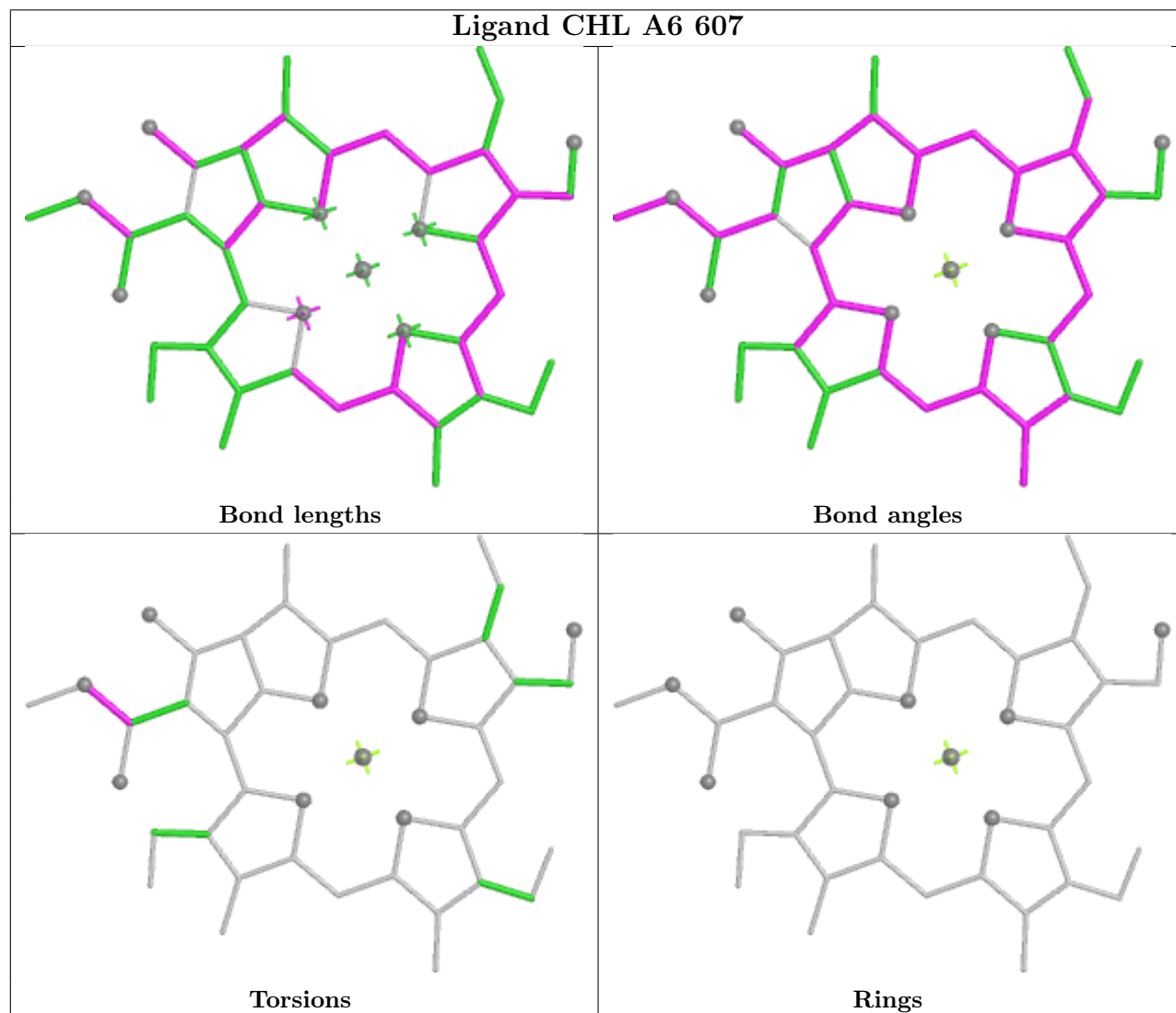
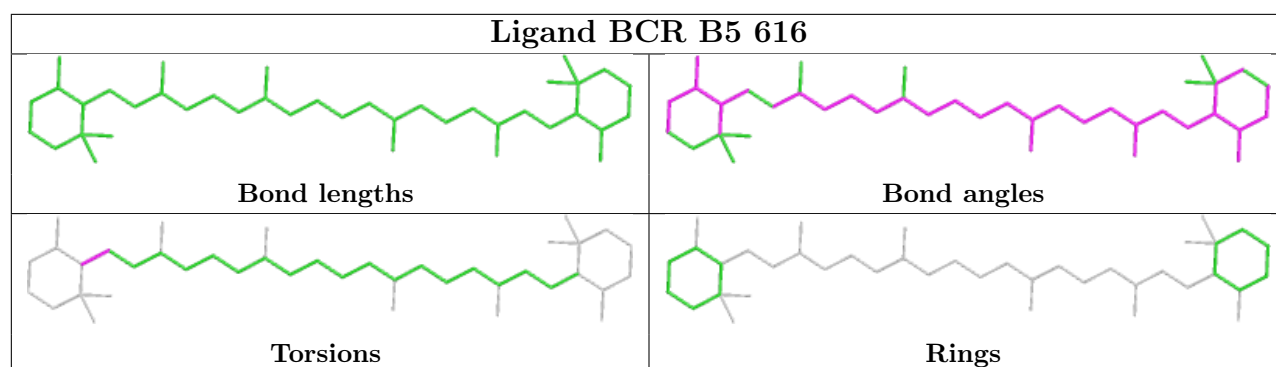


Torsions

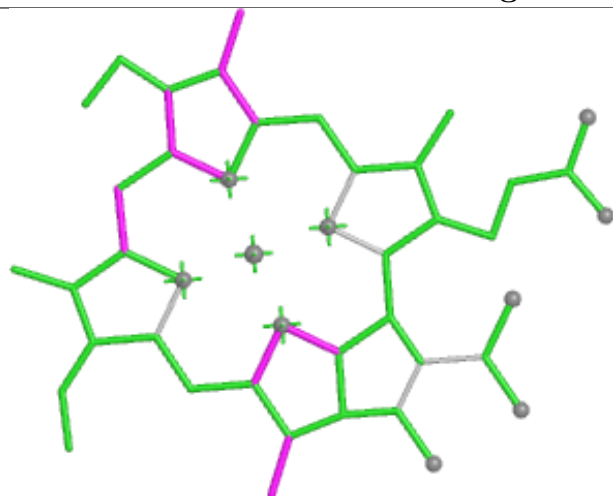


Rings

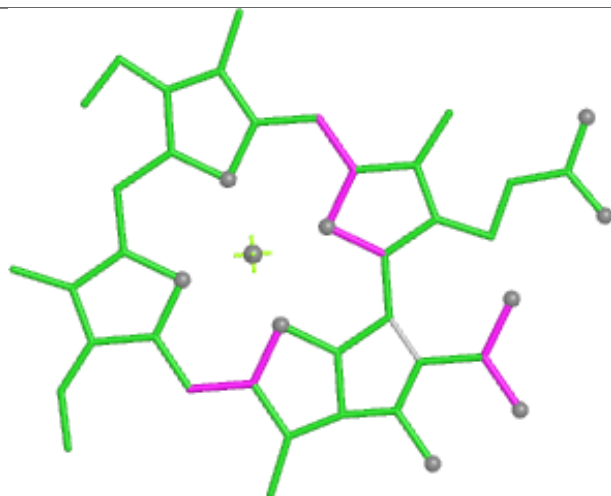




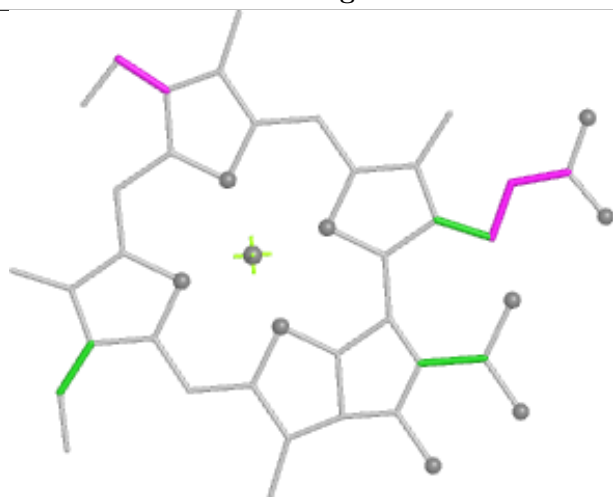
Ligand CLA AG 201



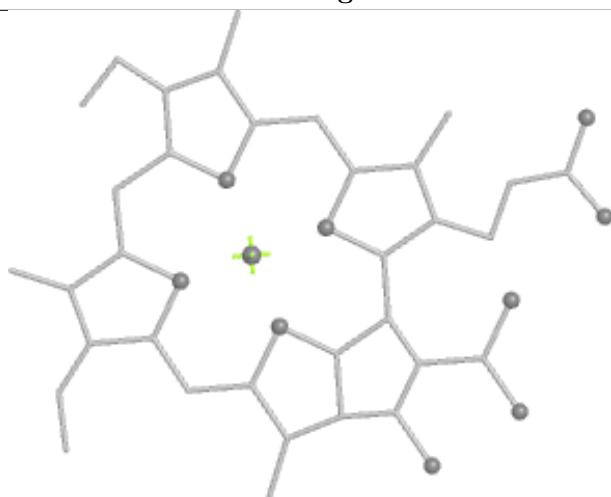
Bond lengths



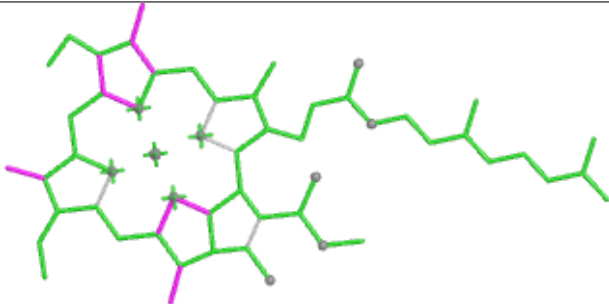
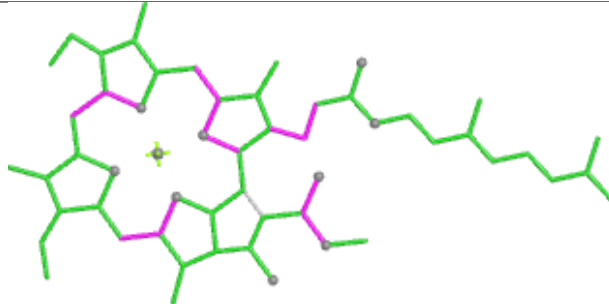
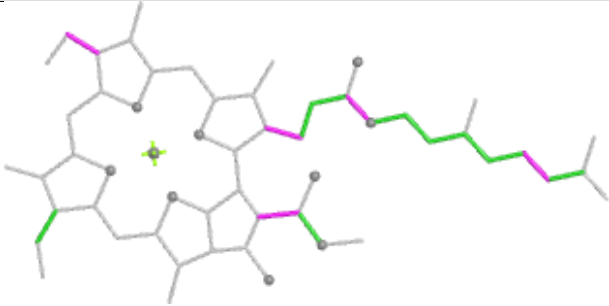
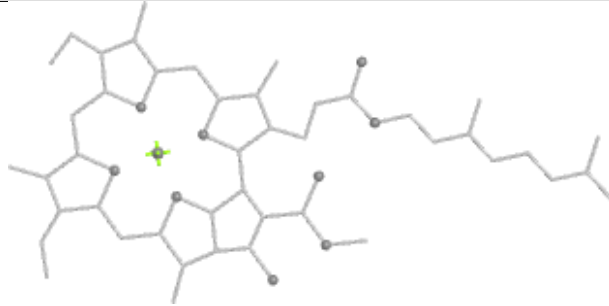
Bond angles

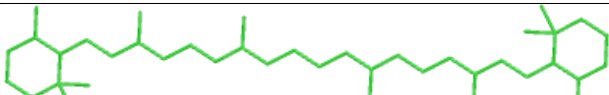
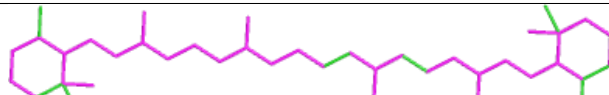
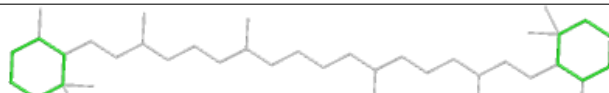


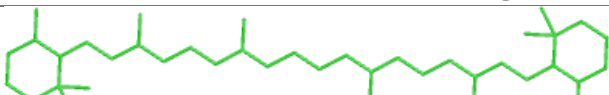
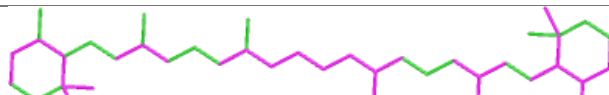
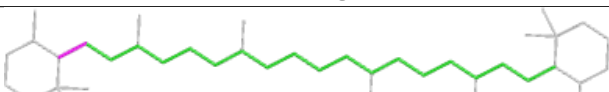
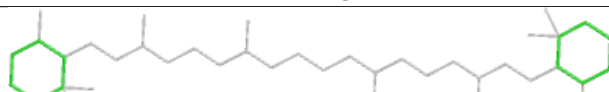
Torsions



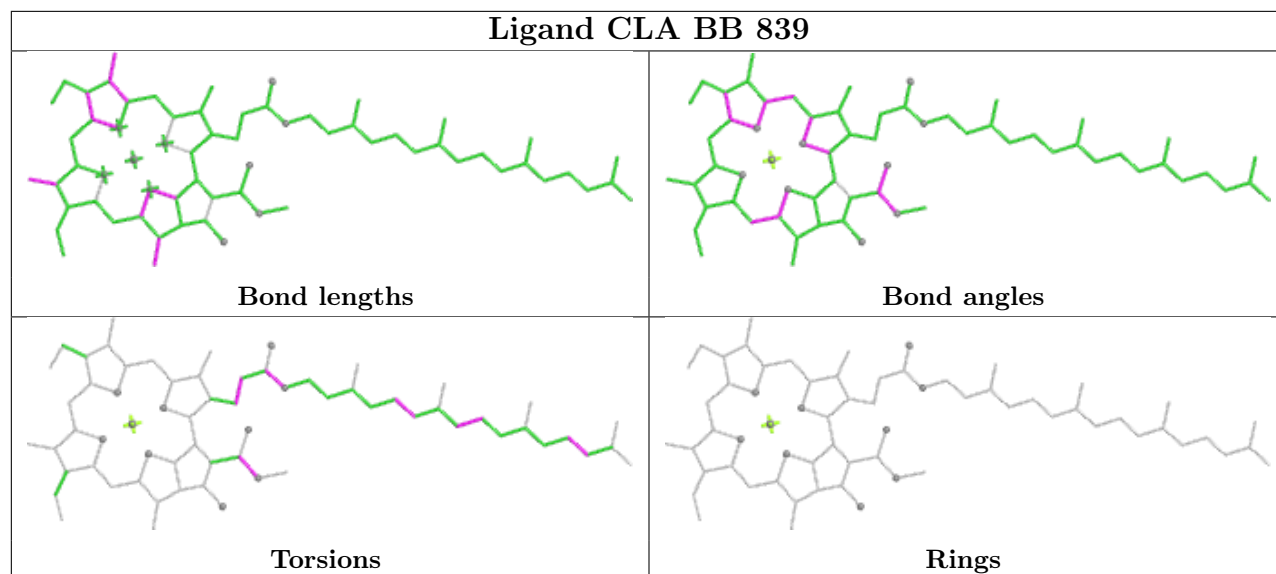
Rings

Ligand CLA BA 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

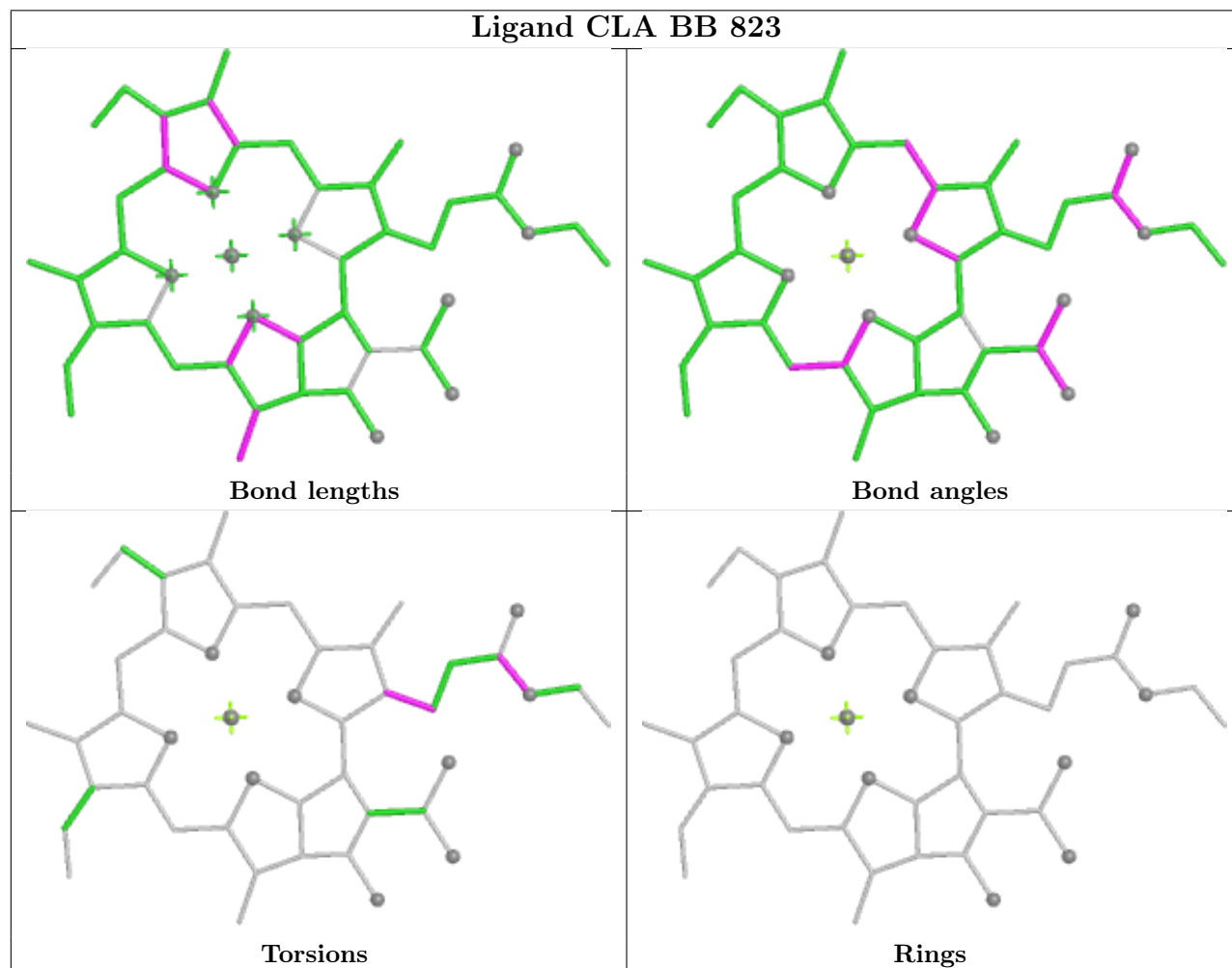
Ligand BCR BA 855	
	
Bond lengths	Bond angles
	
Torsions	Rings

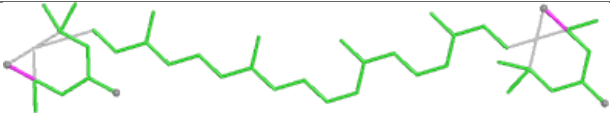
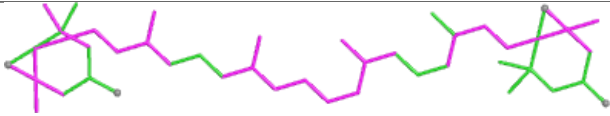
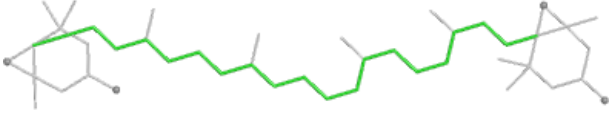
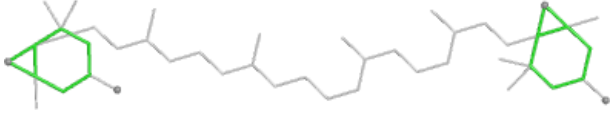
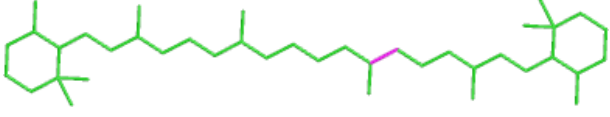
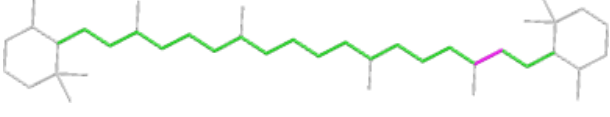
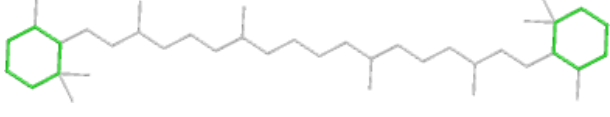
Ligand BCR BL 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

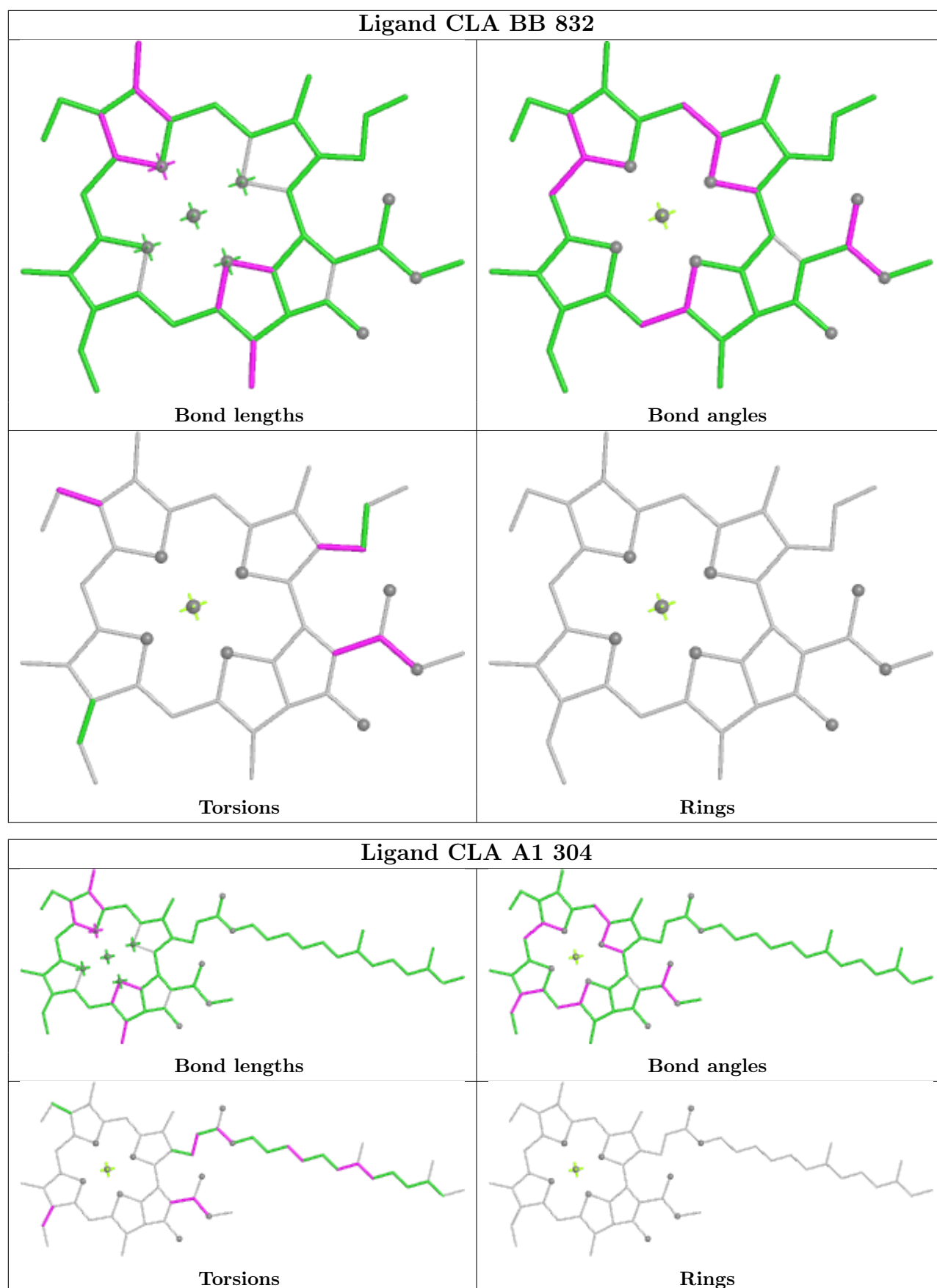
Ligand CLA BB 839



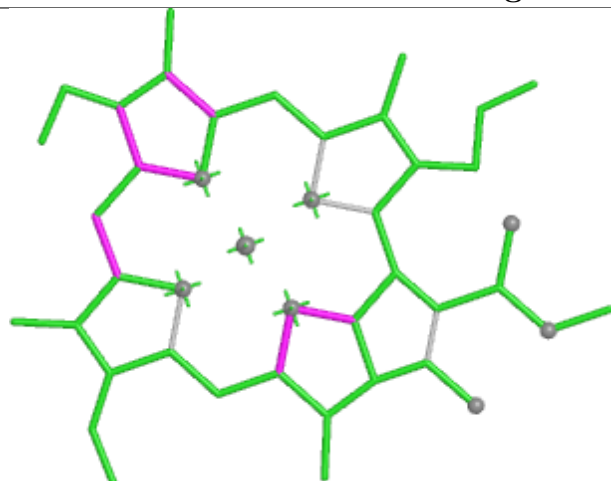
Ligand CLA BB 823



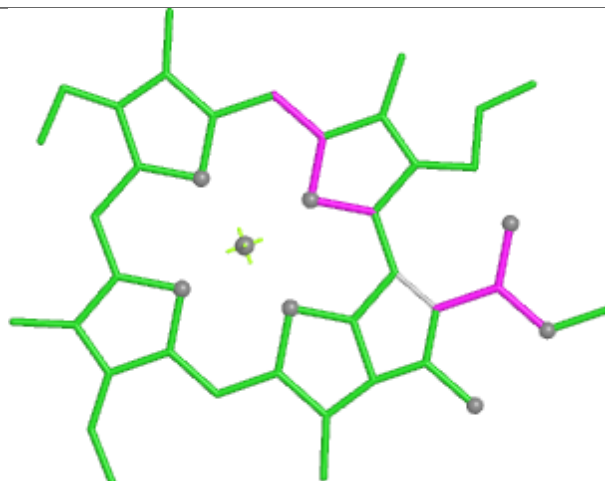
Ligand XAT B1 317	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR AB 848	
 Bond lengths	 Bond angles
 Torsions	 Rings



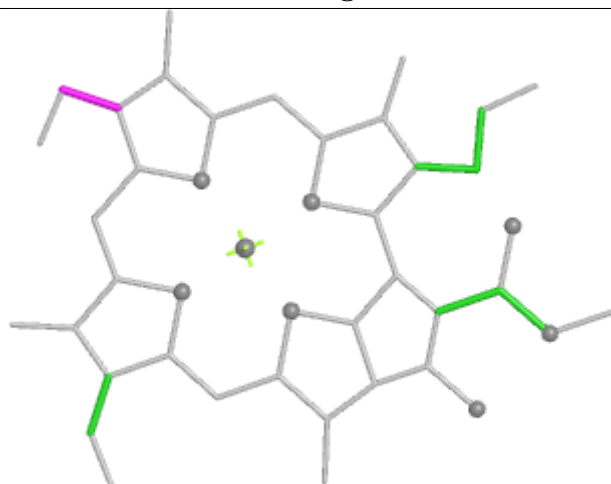
Ligand CLA A3 311



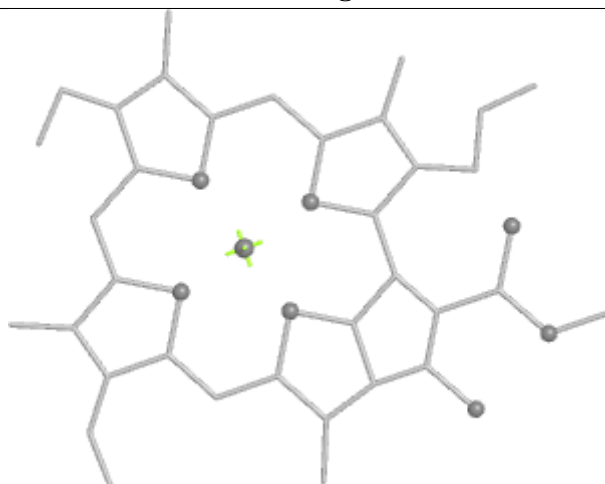
Bond lengths



Bond angles

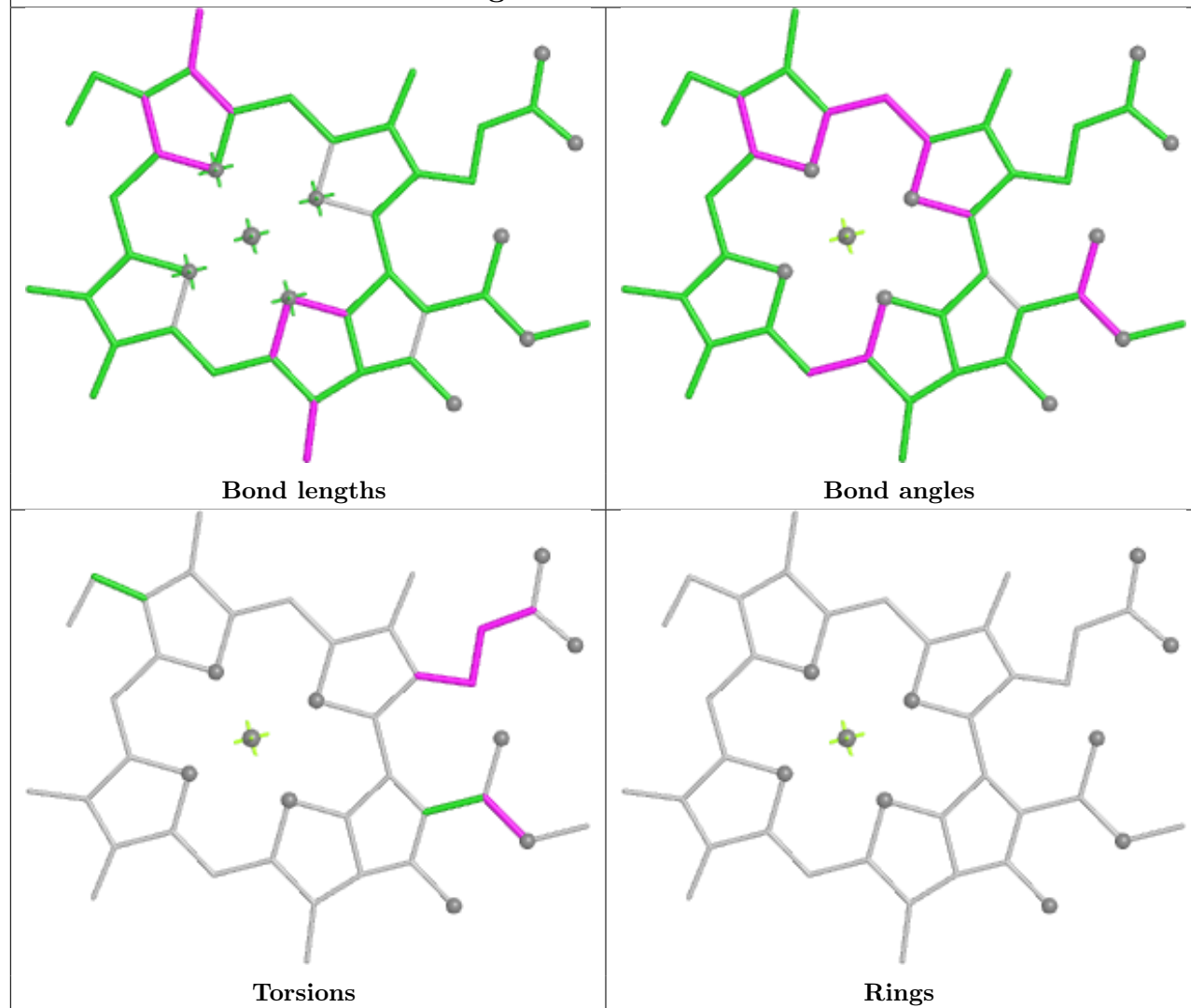


Torsions

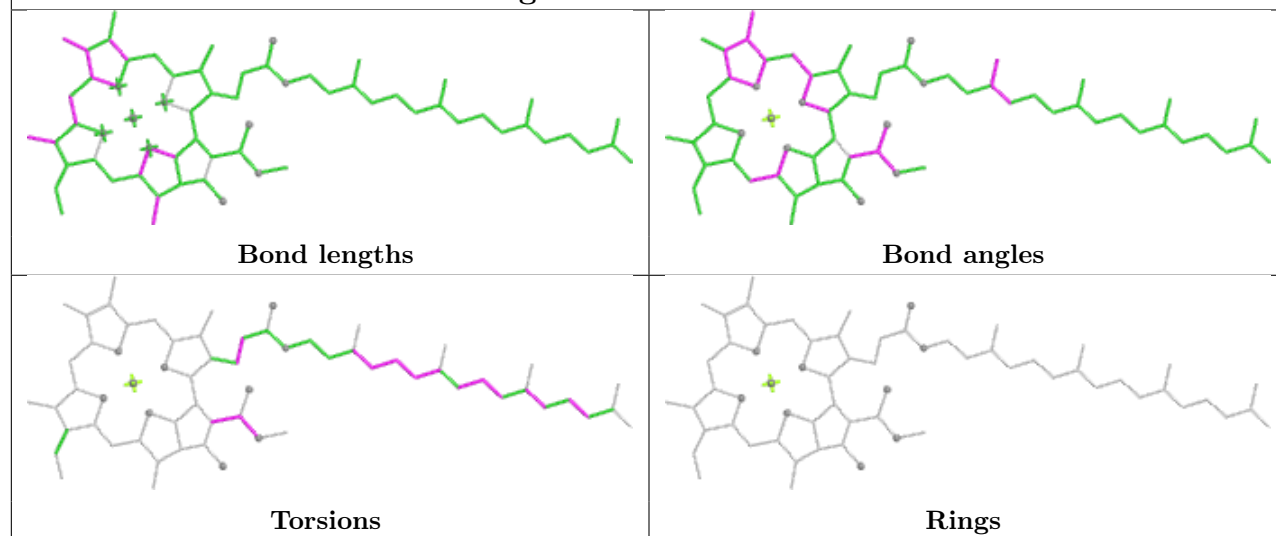


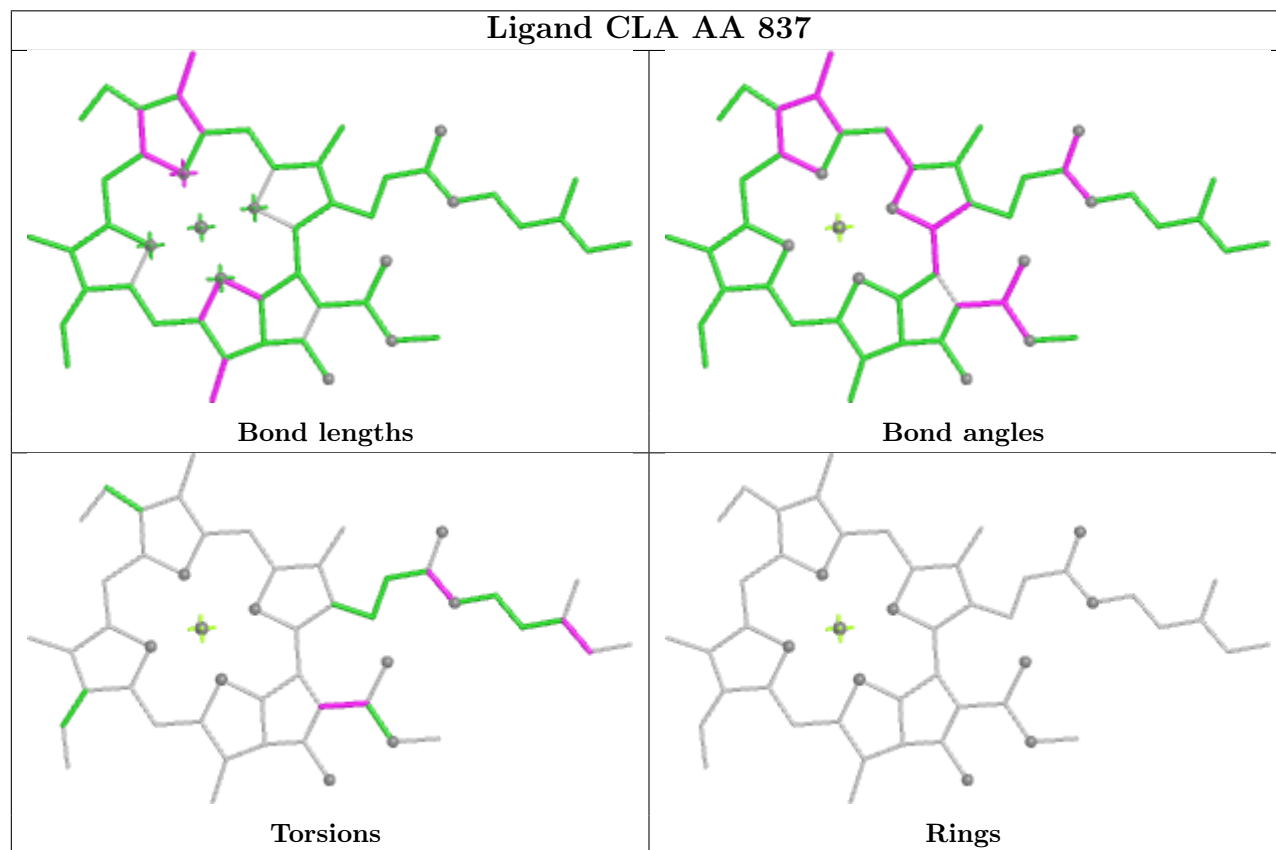
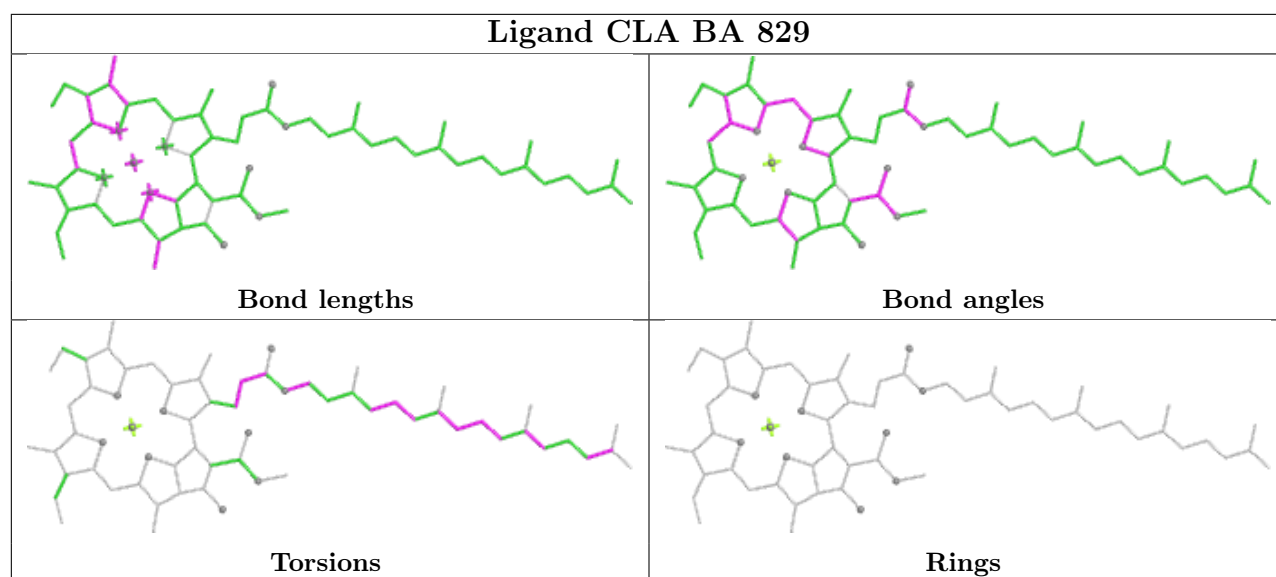
Rings

Ligand CLA B2 611

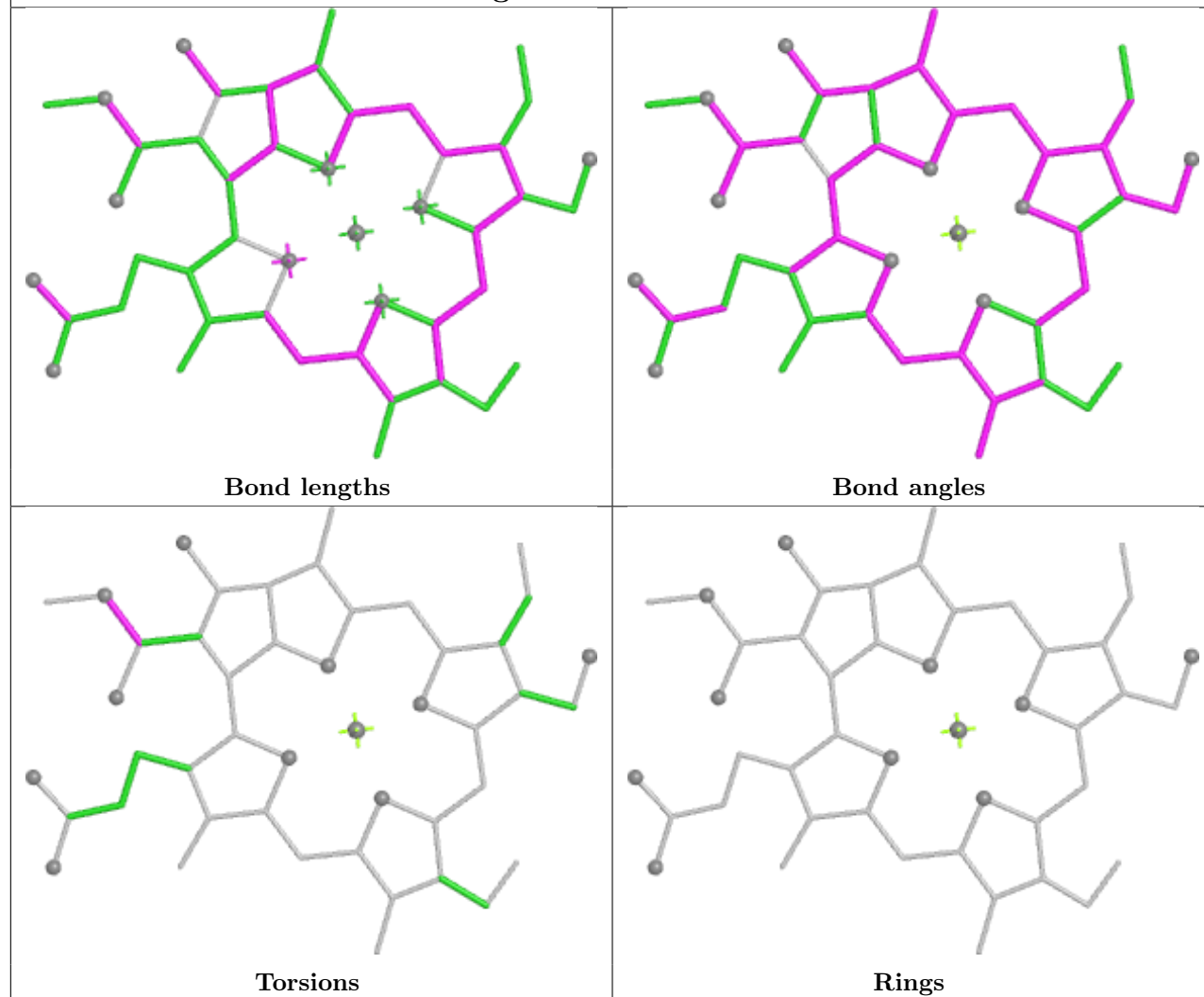


Ligand CLA AB 802

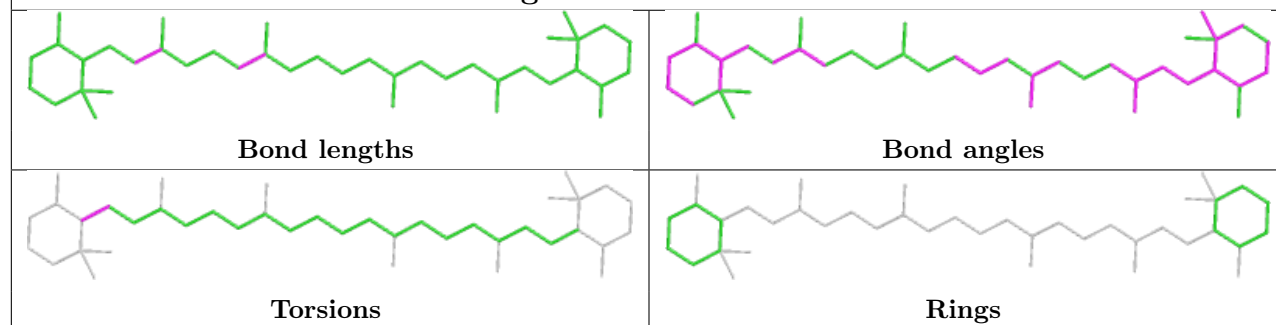


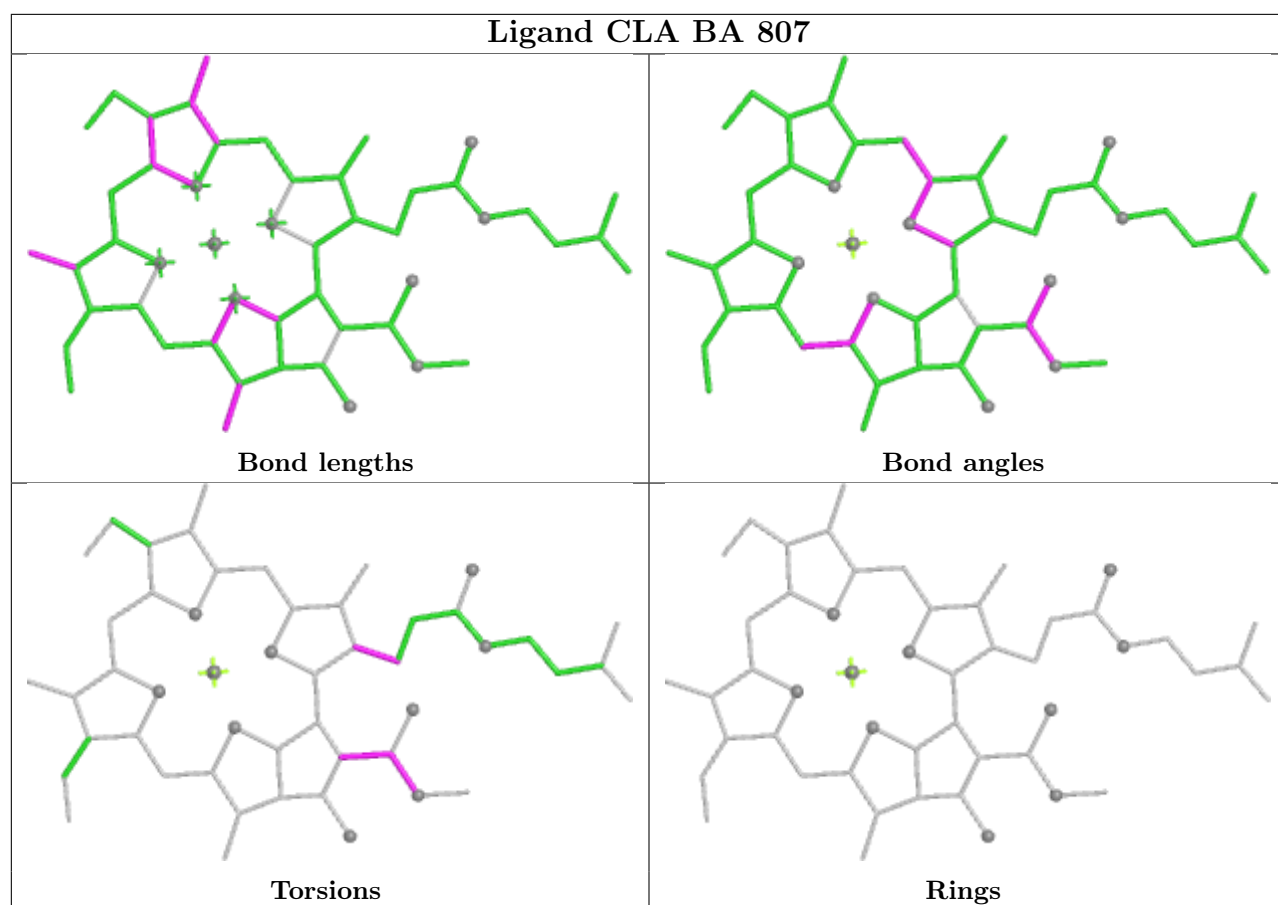


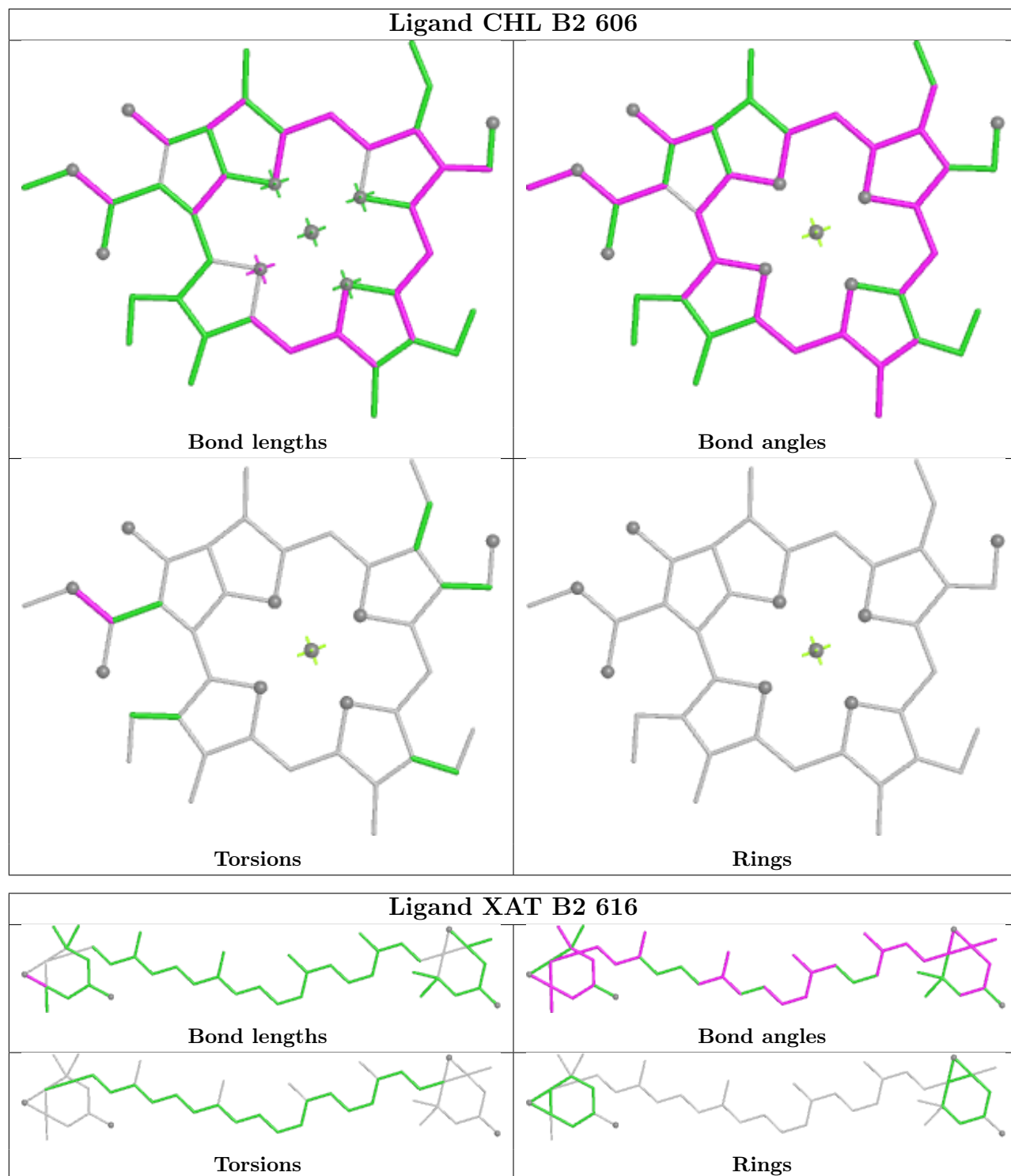
Ligand CHL A4 306

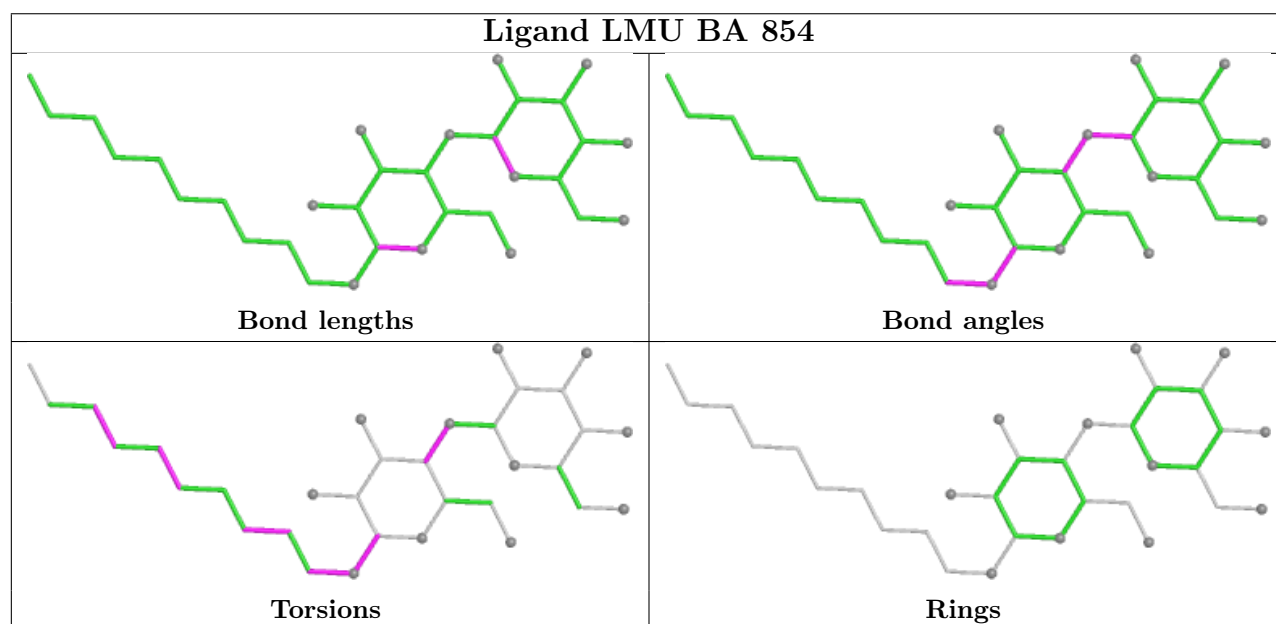
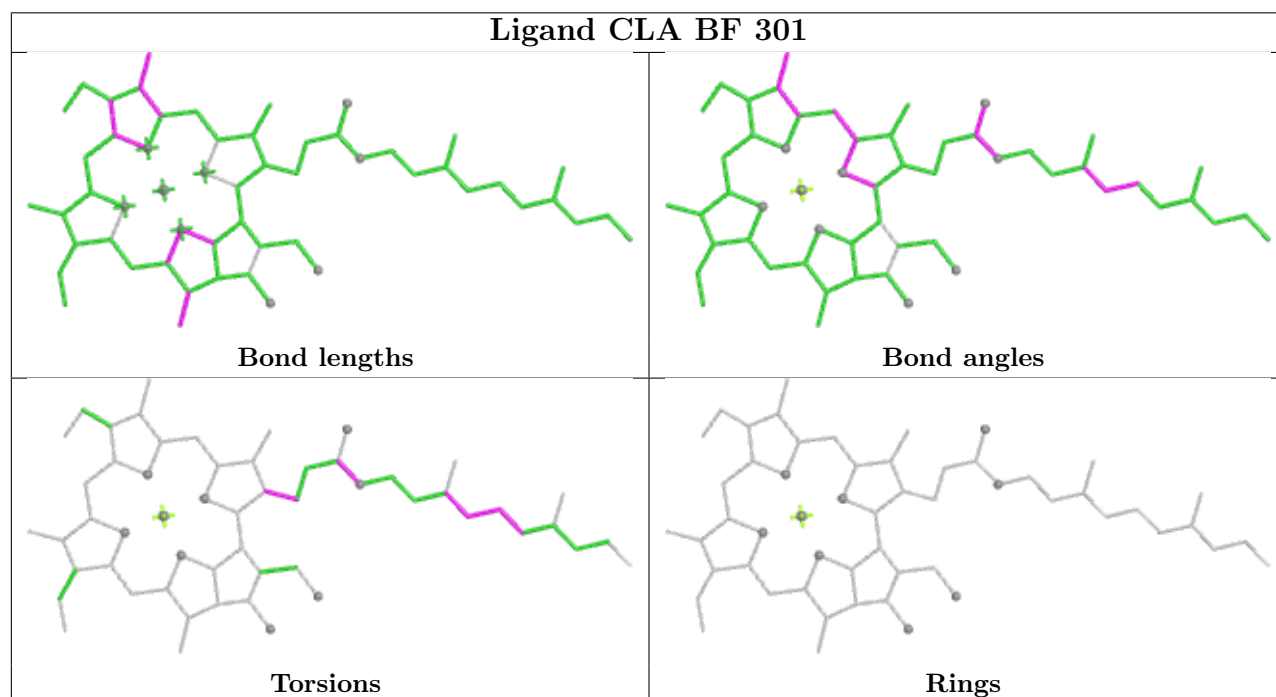
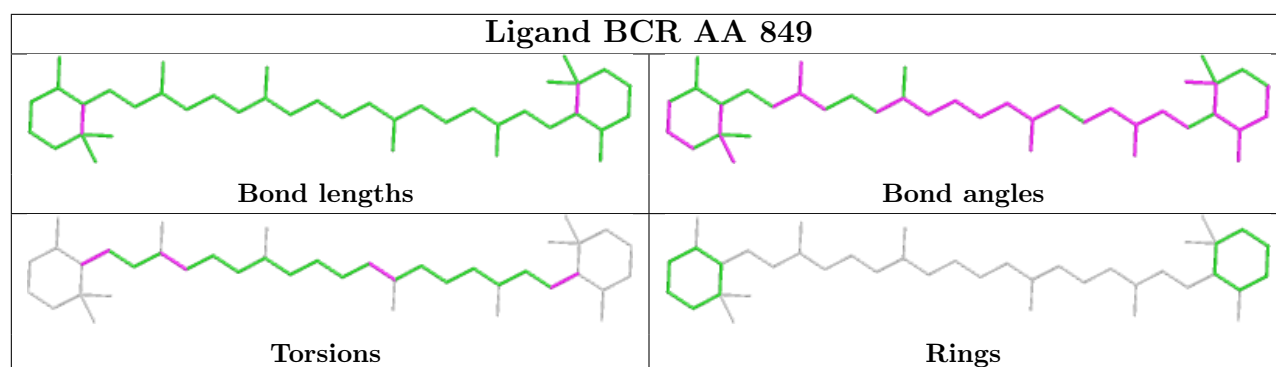


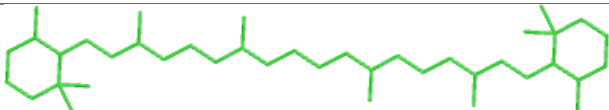
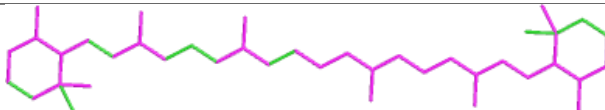
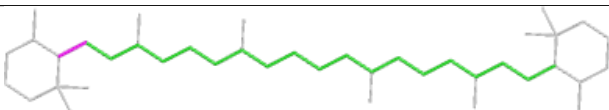
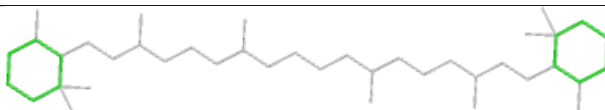
Ligand BCR A6 617

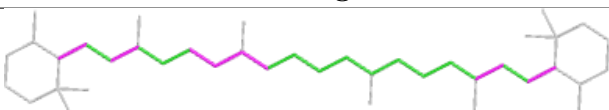
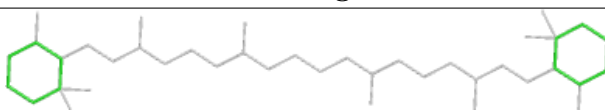


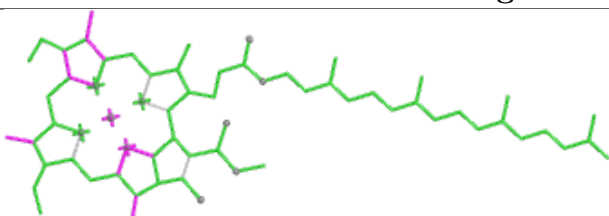
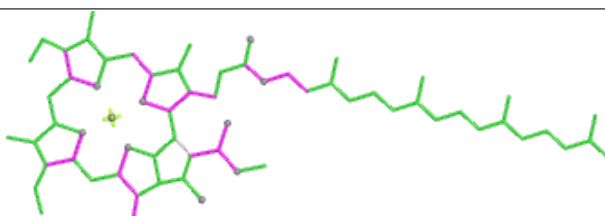
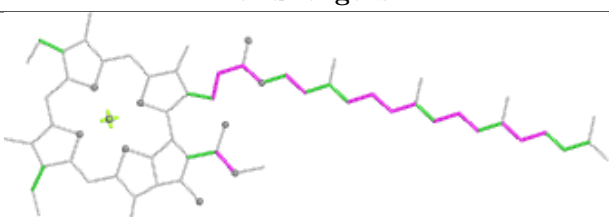
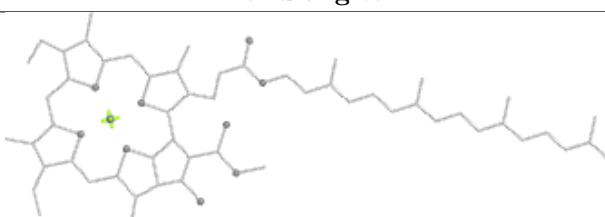




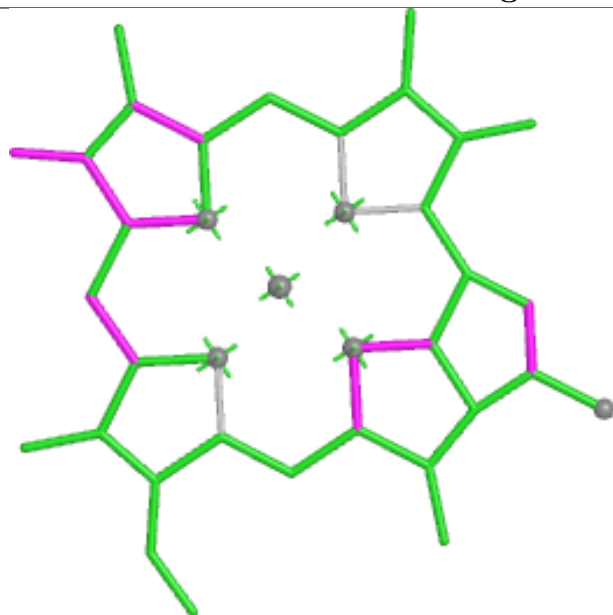


Ligand BCR A4 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR AA 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BB 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

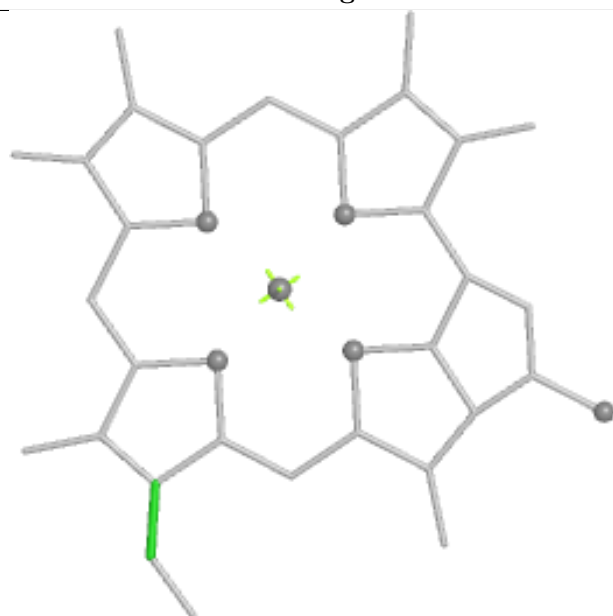
Ligand CLA BK 201



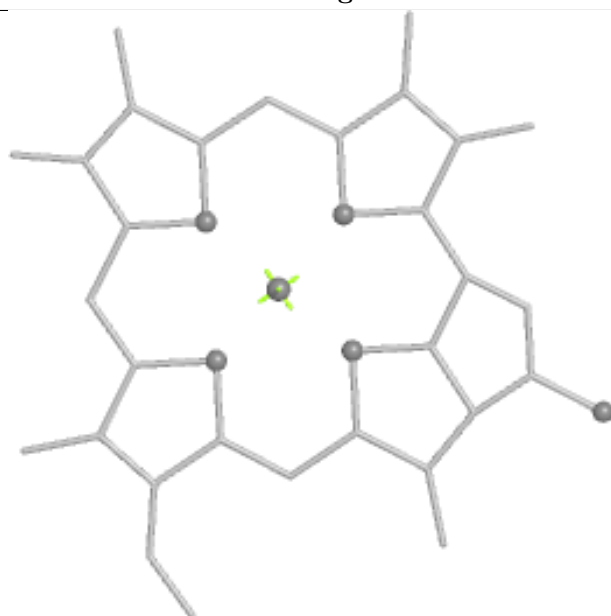
Bond lengths



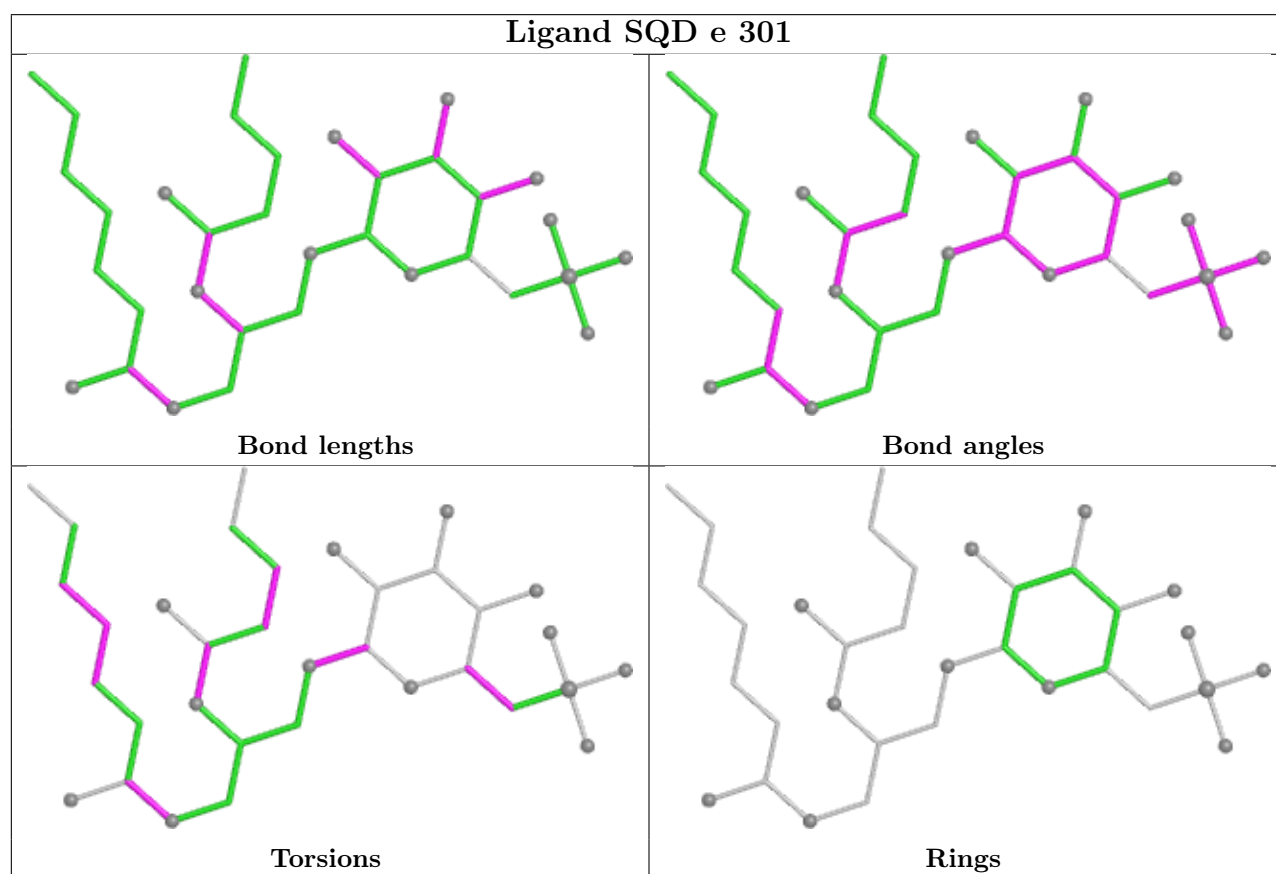
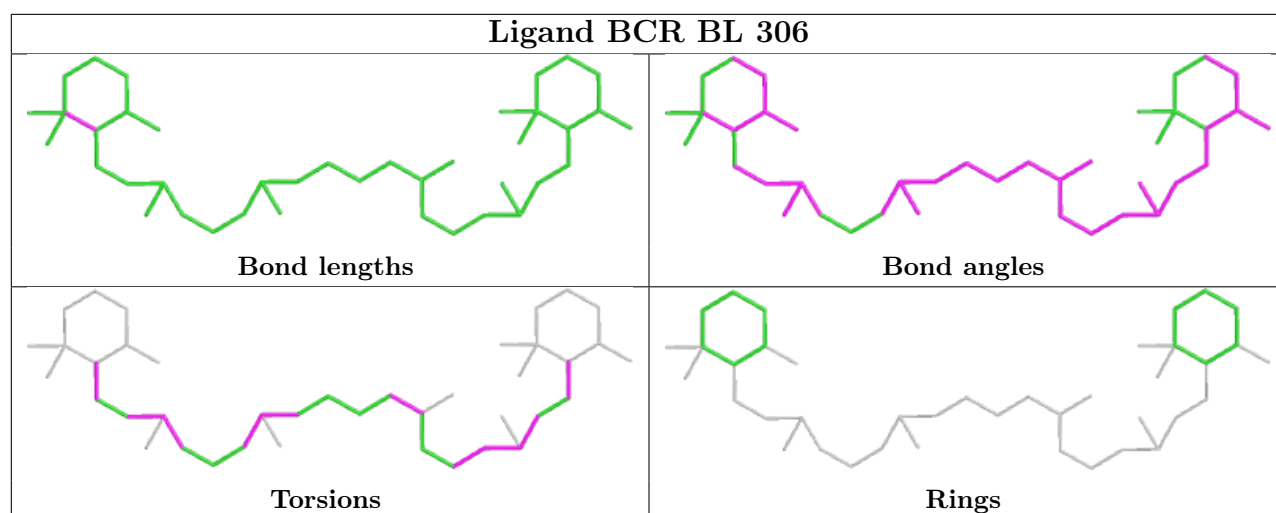
Bond angles



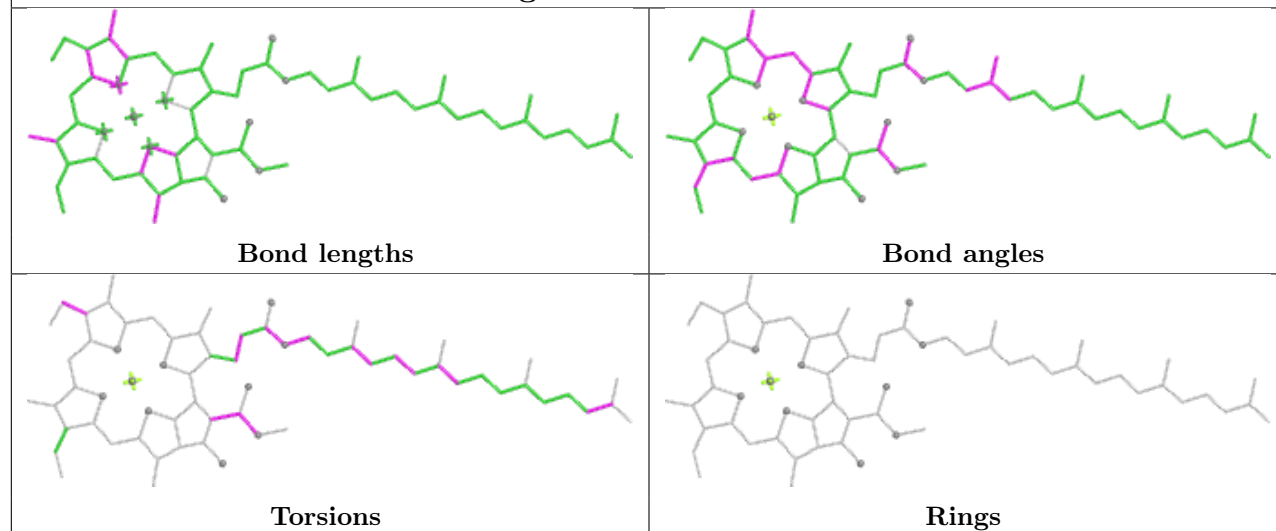
Torsions



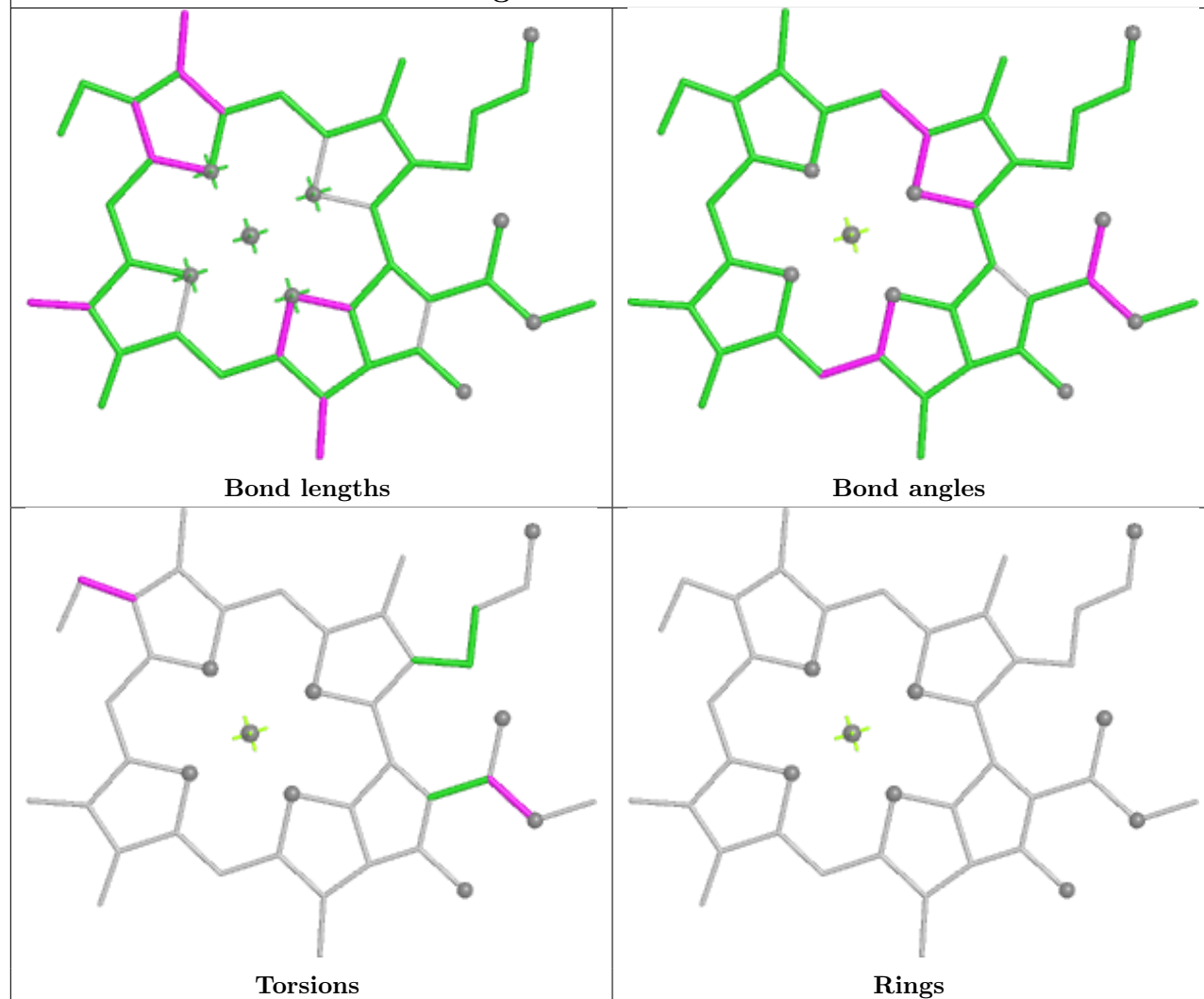
Rings

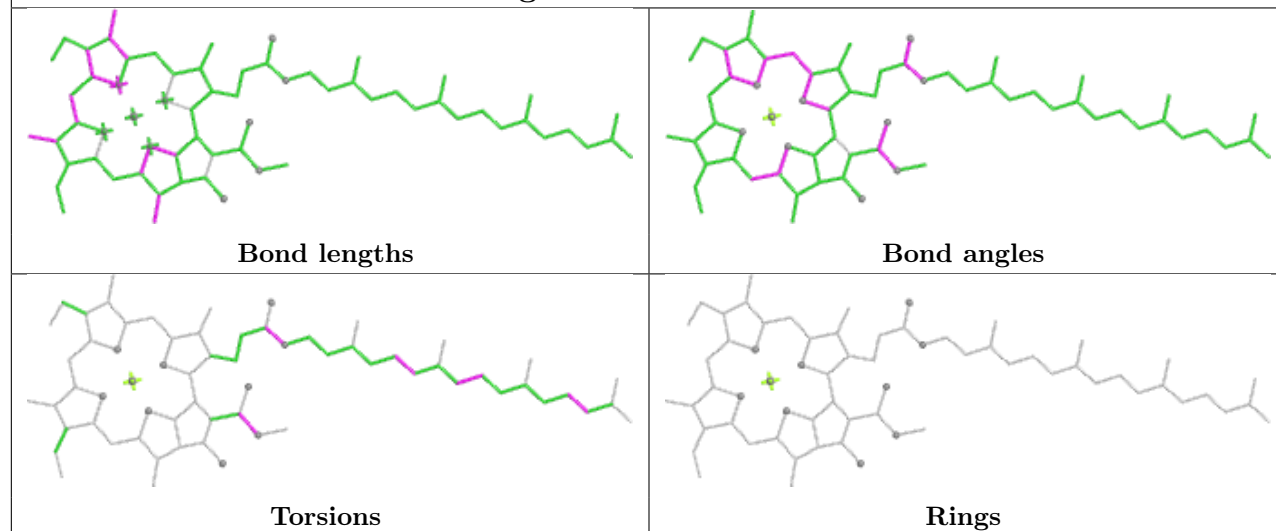
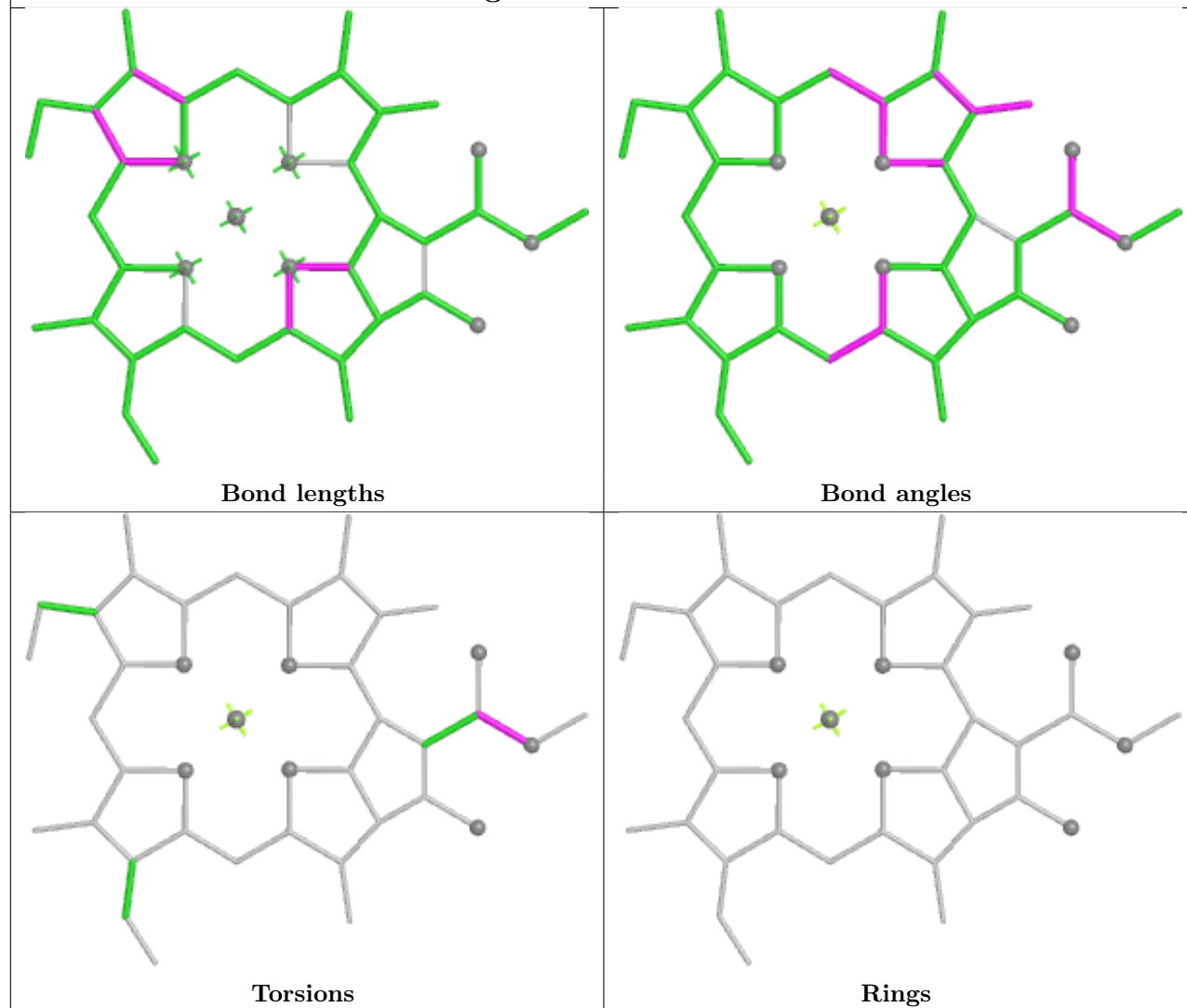


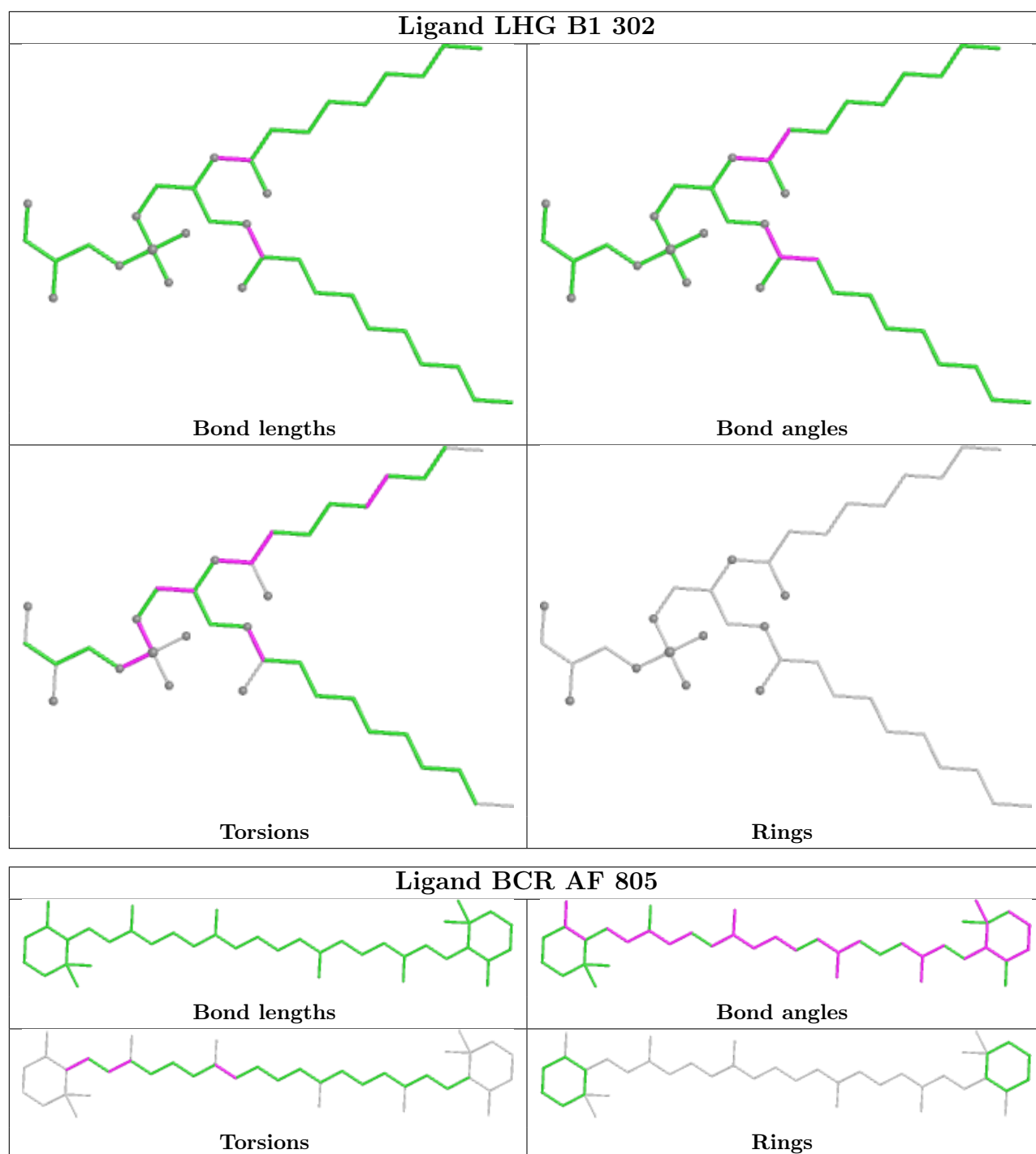
Ligand CLA BA 841

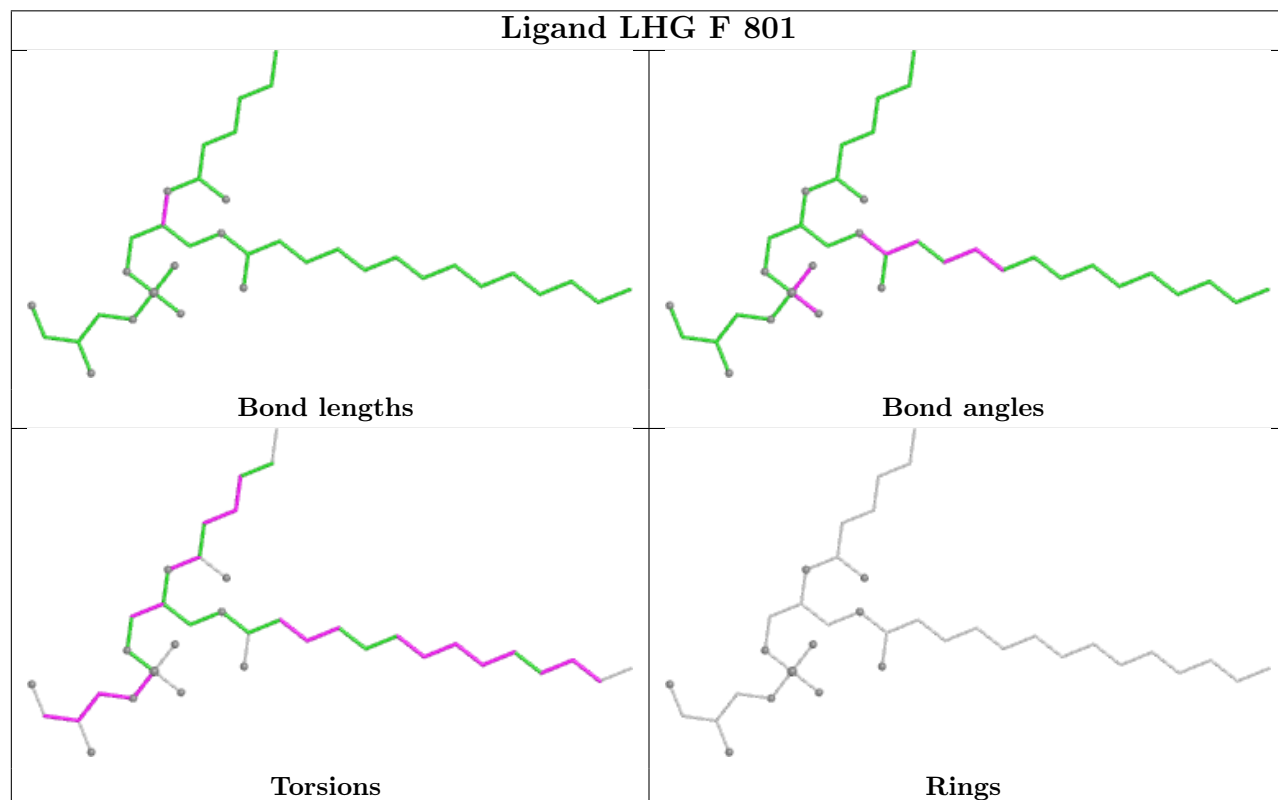
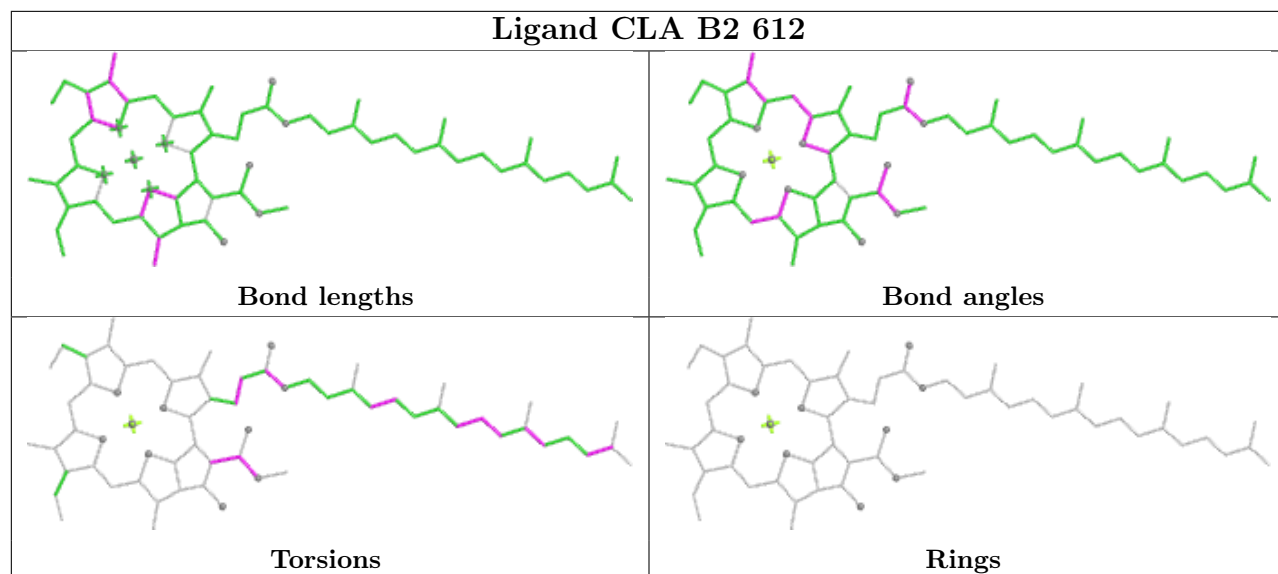


Ligand CLA A6 605

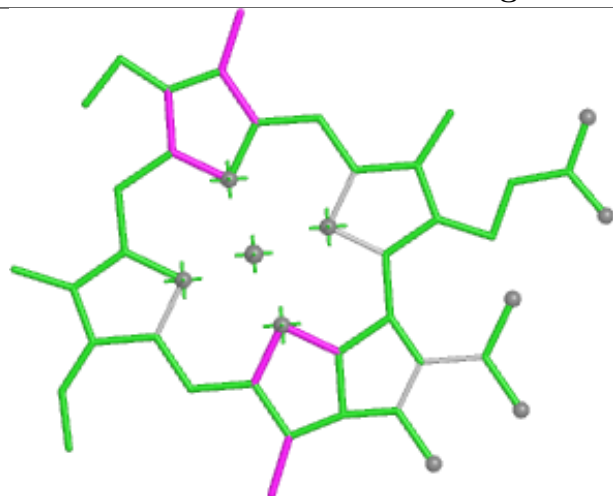


Ligand CLA AB 838**Ligand CLA BF 303**

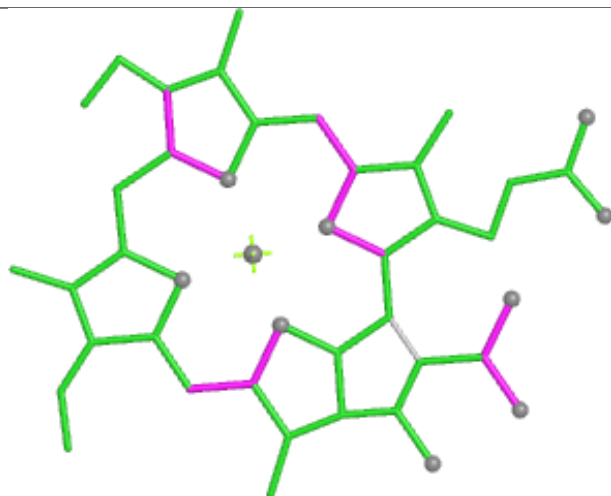




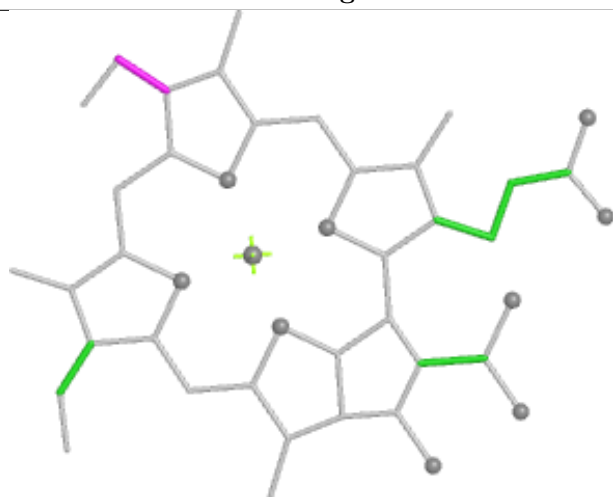
Ligand CLA AA 835



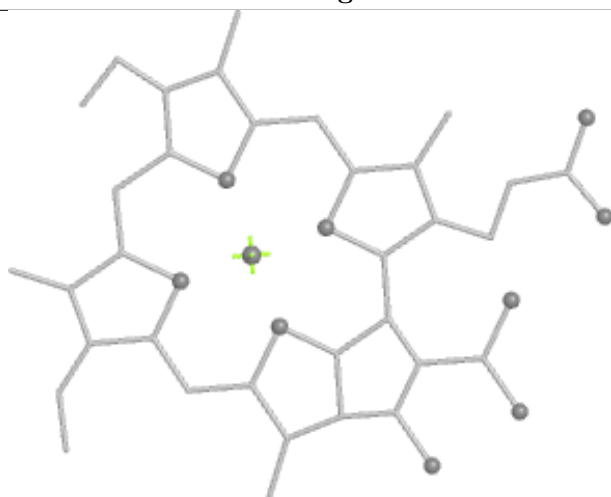
Bond lengths



Bond angles

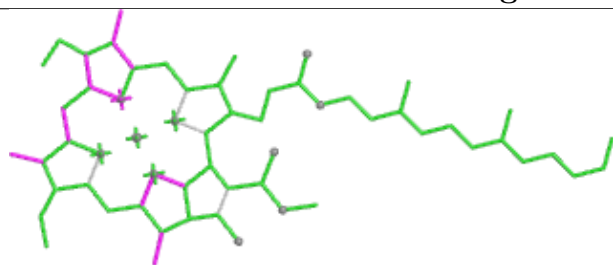


Torsions

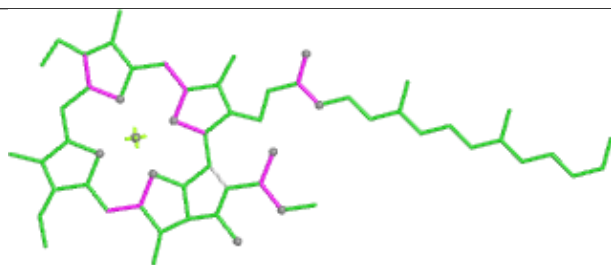


Rings

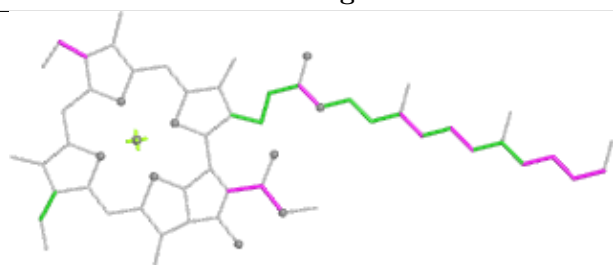
Ligand CLA AA 826



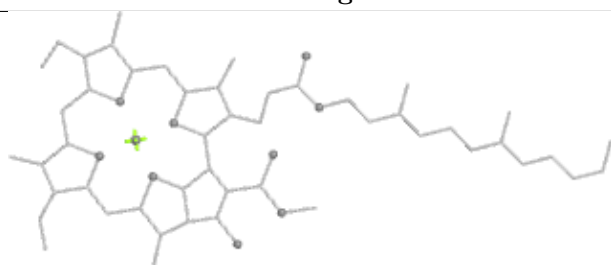
Bond lengths



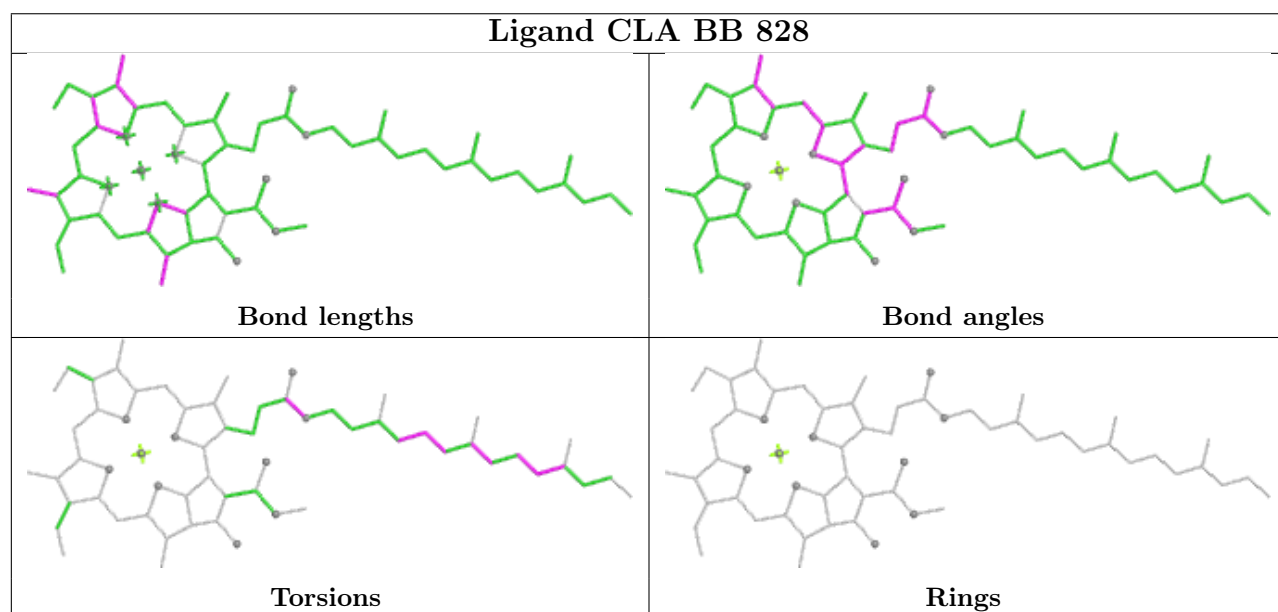
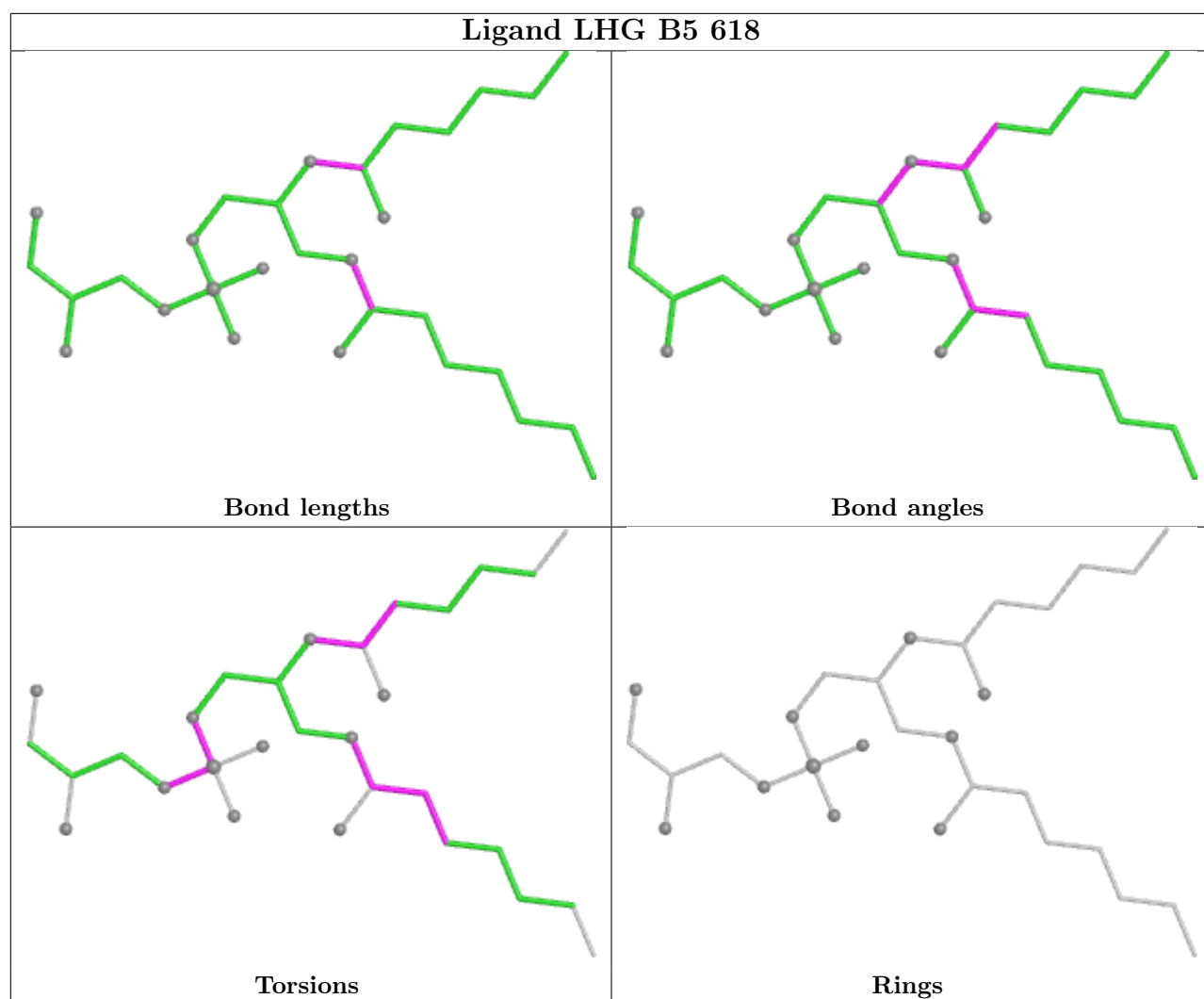
Bond angles



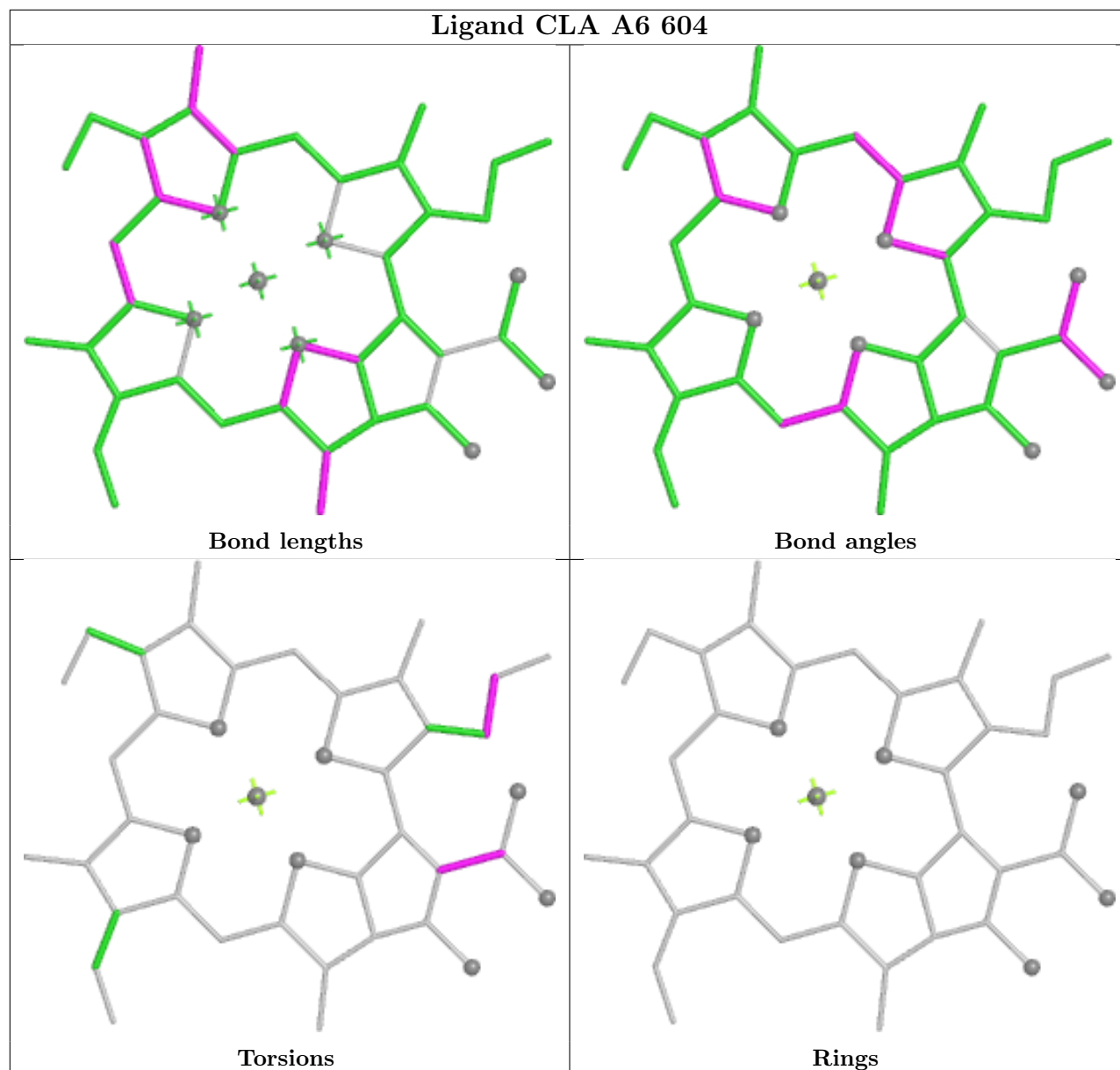
Torsions

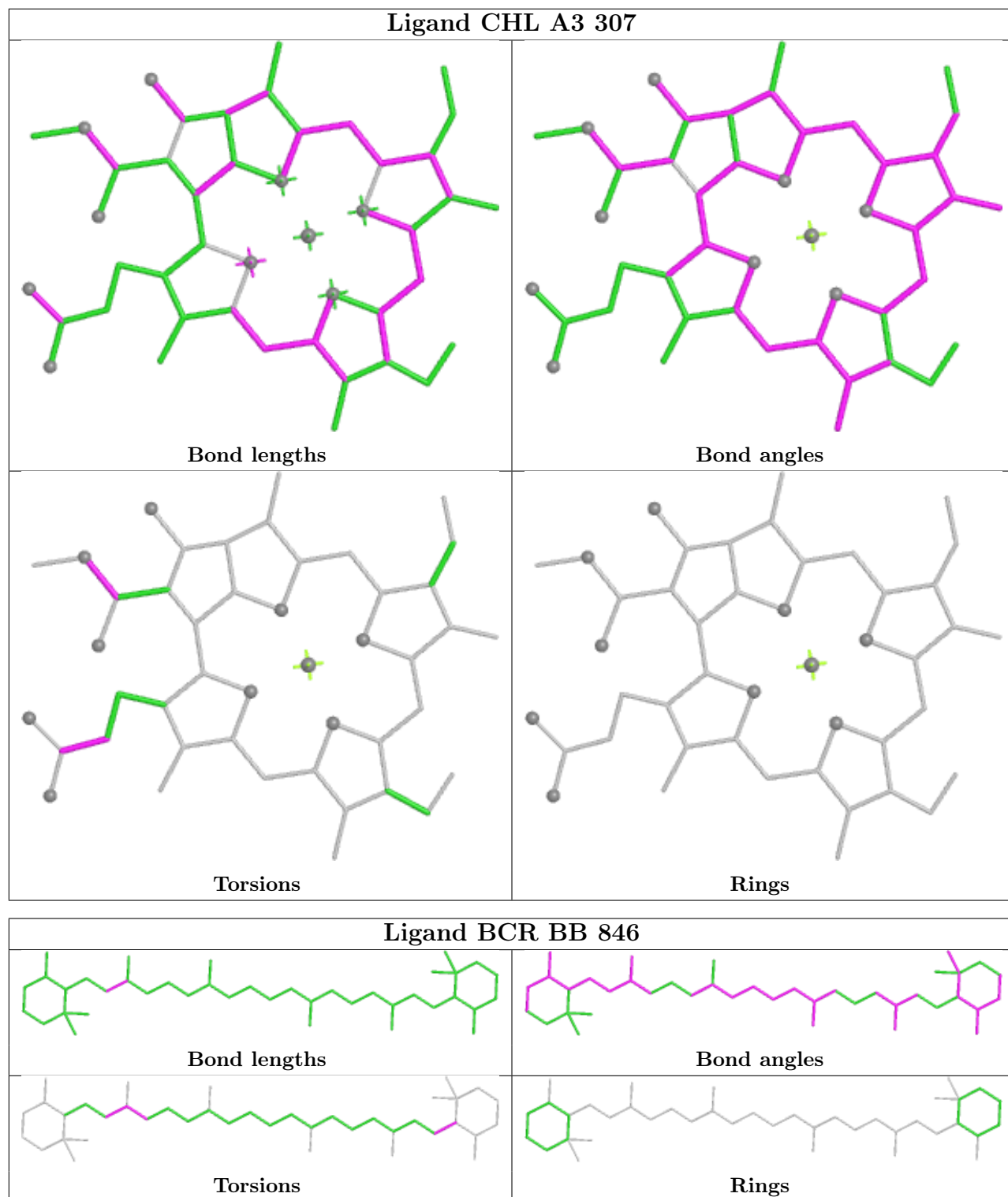


Rings

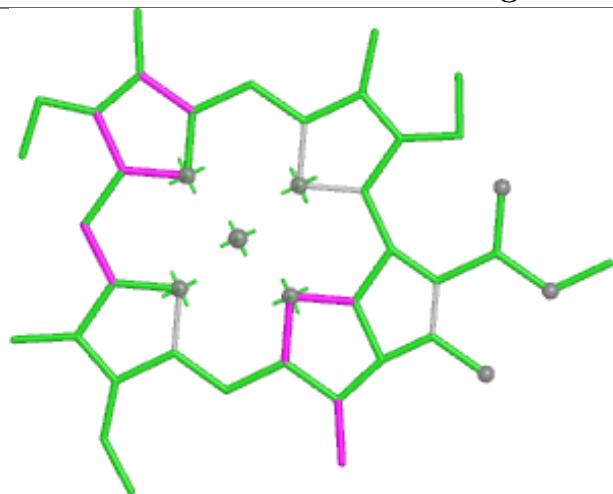


Ligand CLA A6 604

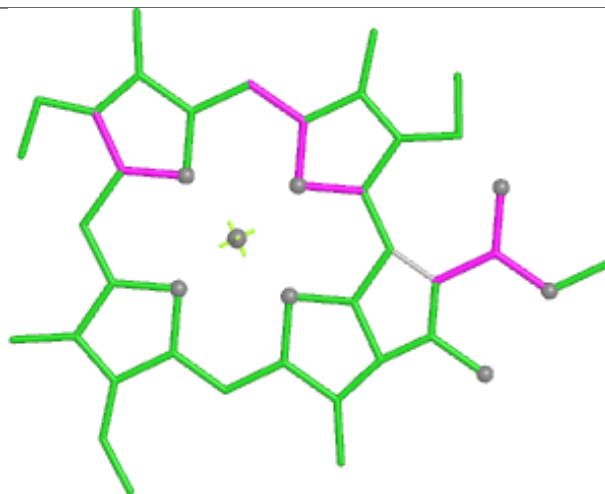




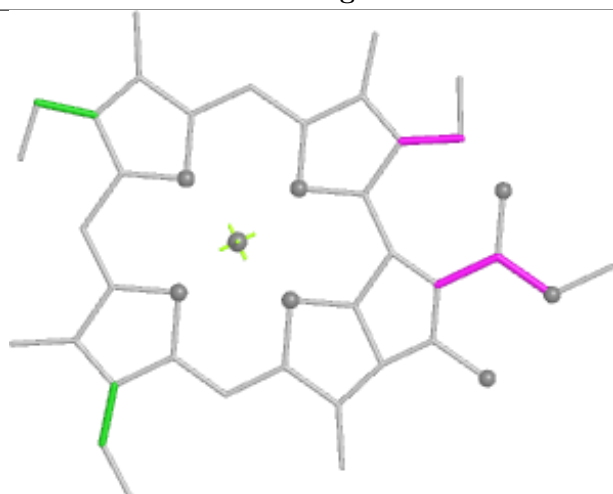
Ligand CLA BG 201



Bond lengths



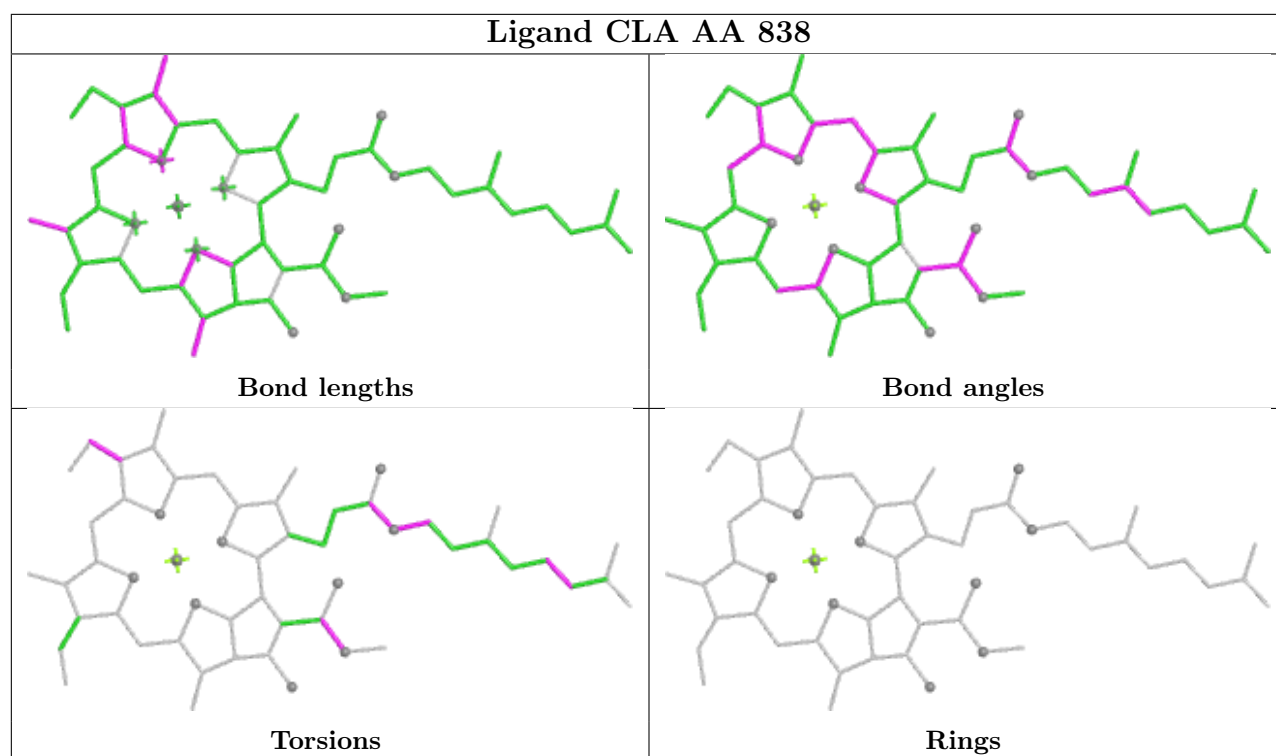
Bond angles

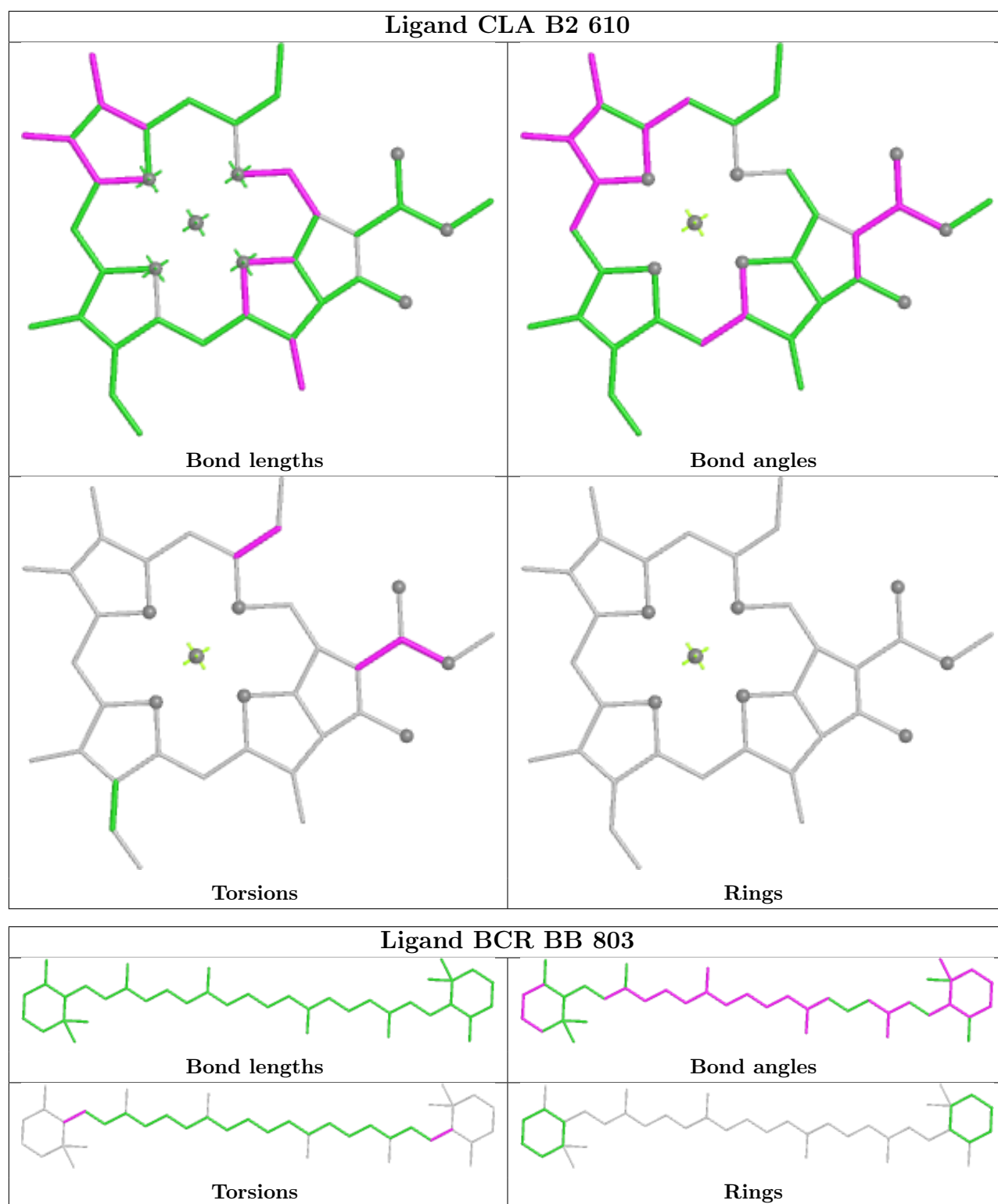


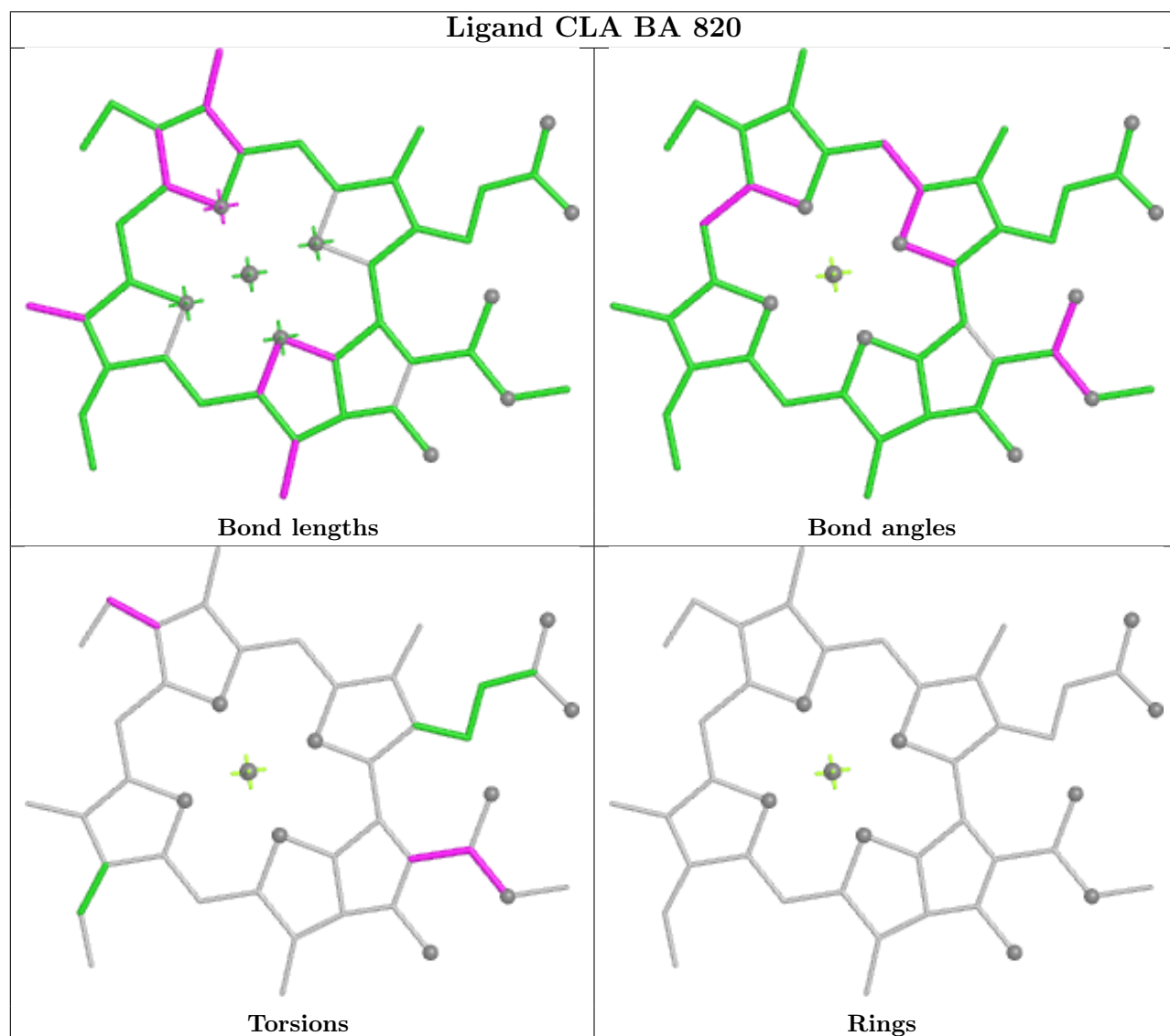
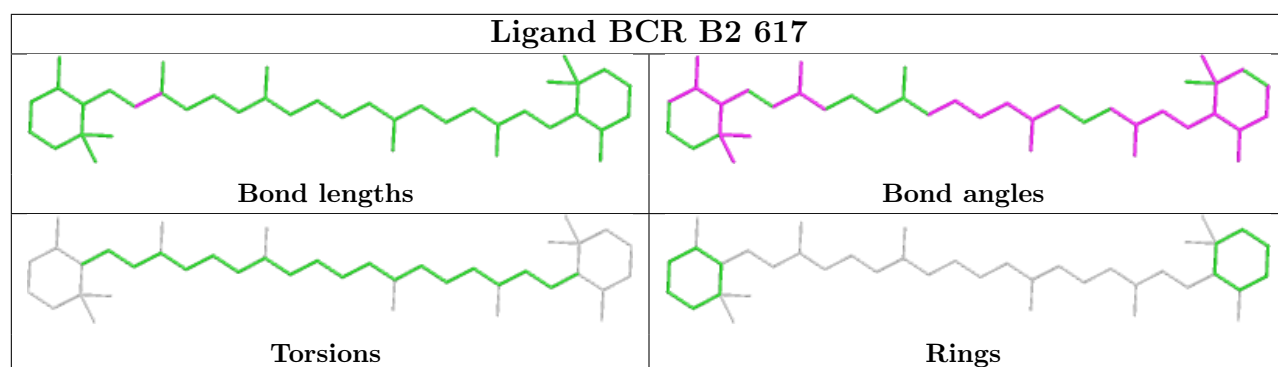
Torsions



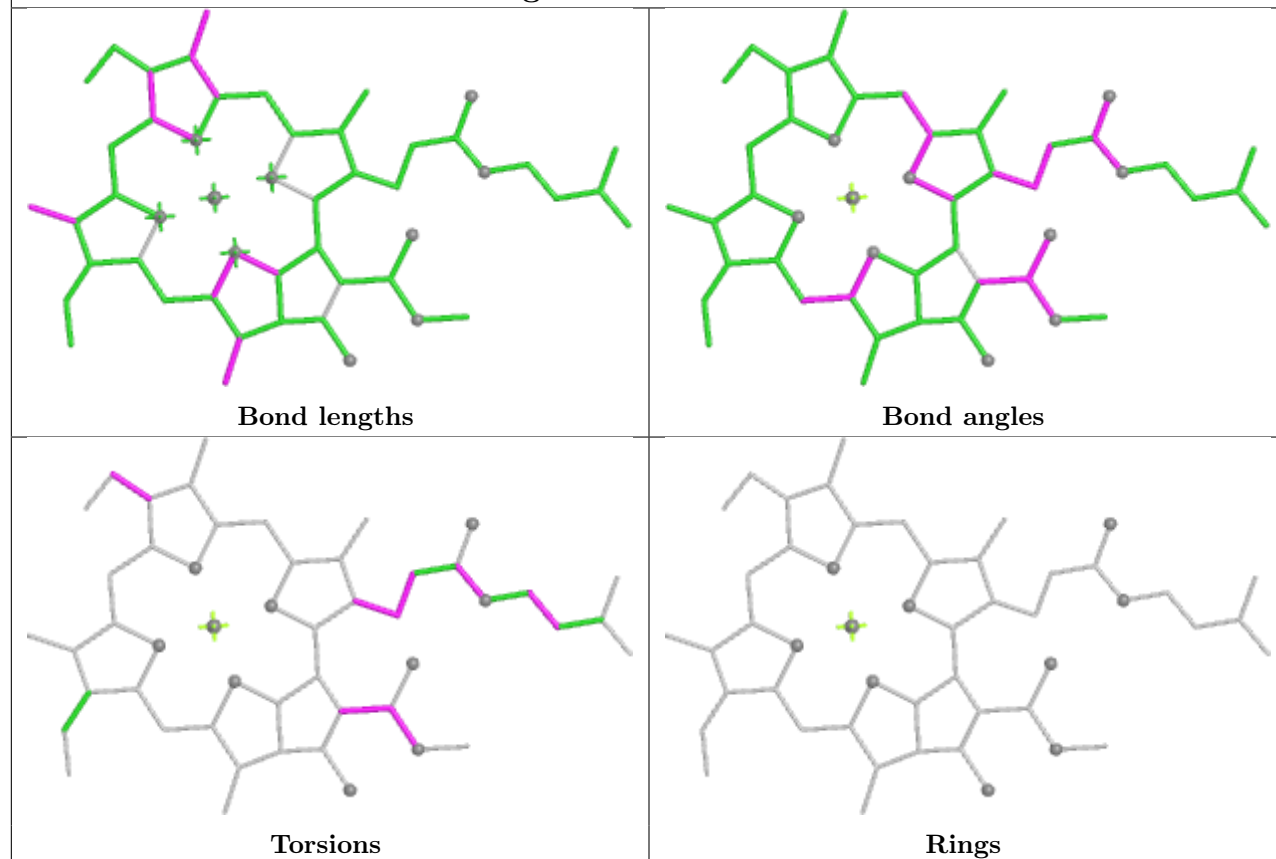
Rings



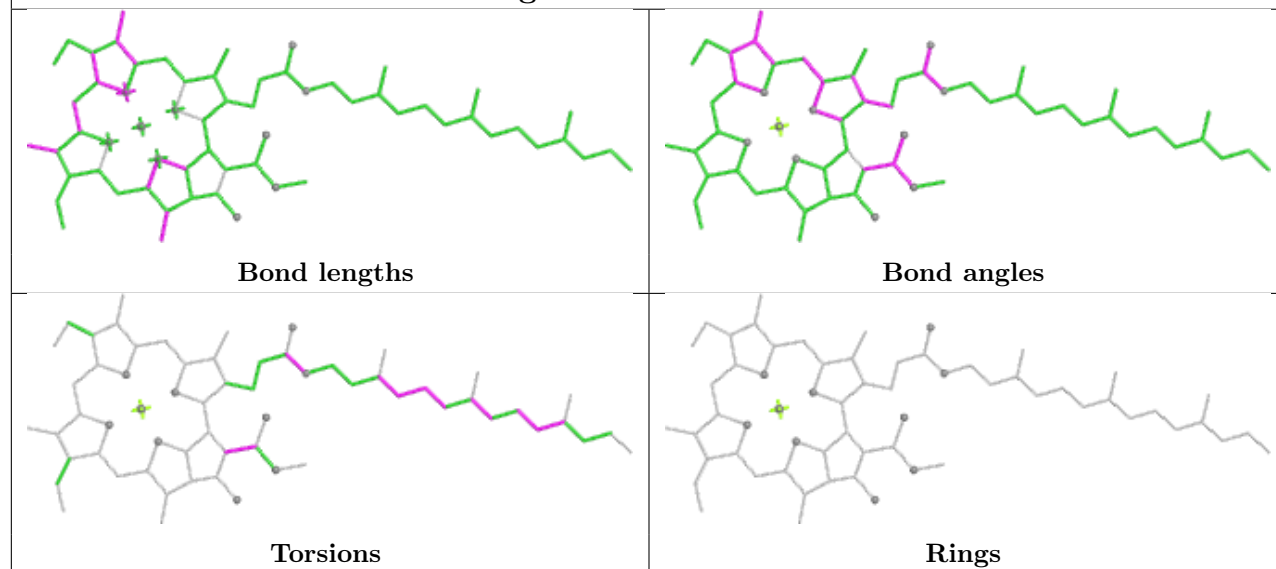




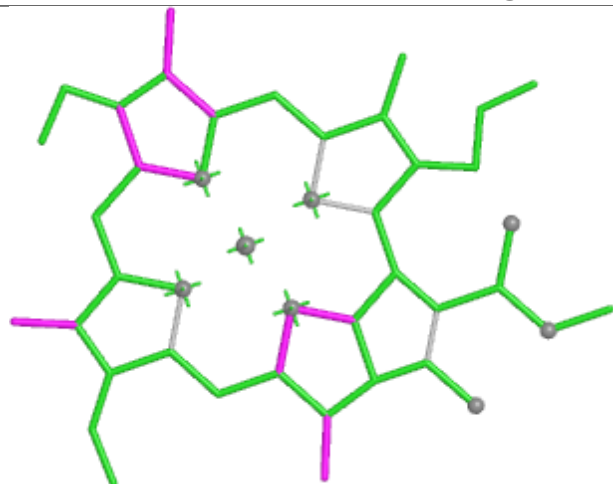
Ligand CLA A4 313



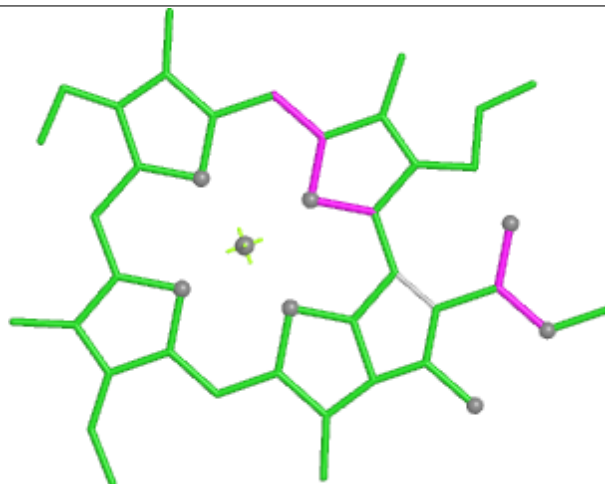
Ligand CLA AB 827



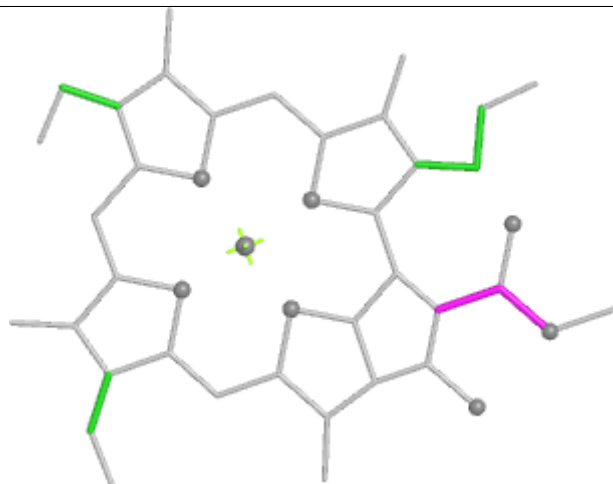
Ligand CLA AB 816



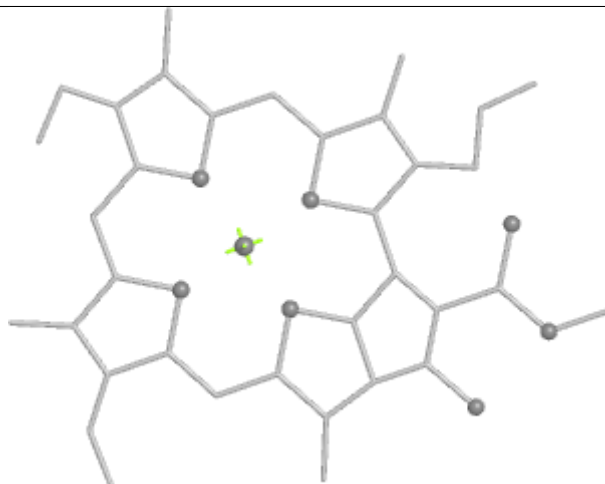
Bond lengths



Bond angles

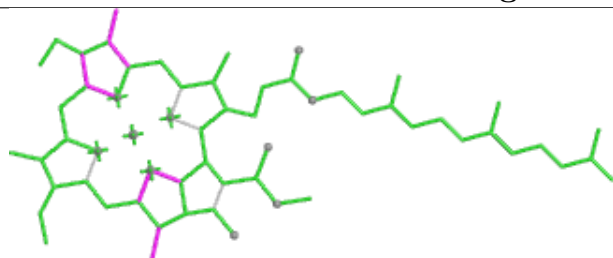


Torsions

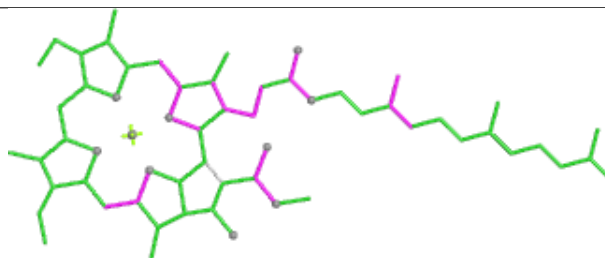


Rings

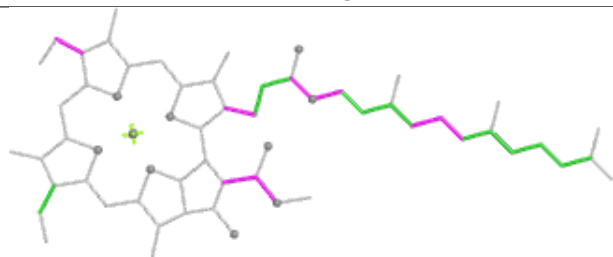
Ligand CLA AH 201



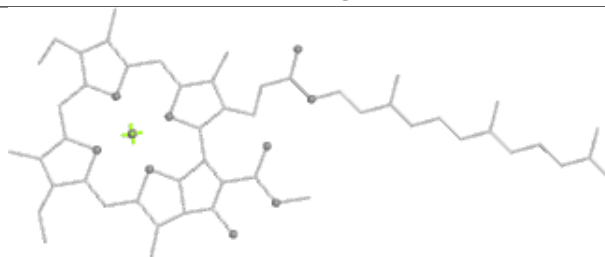
Bond lengths



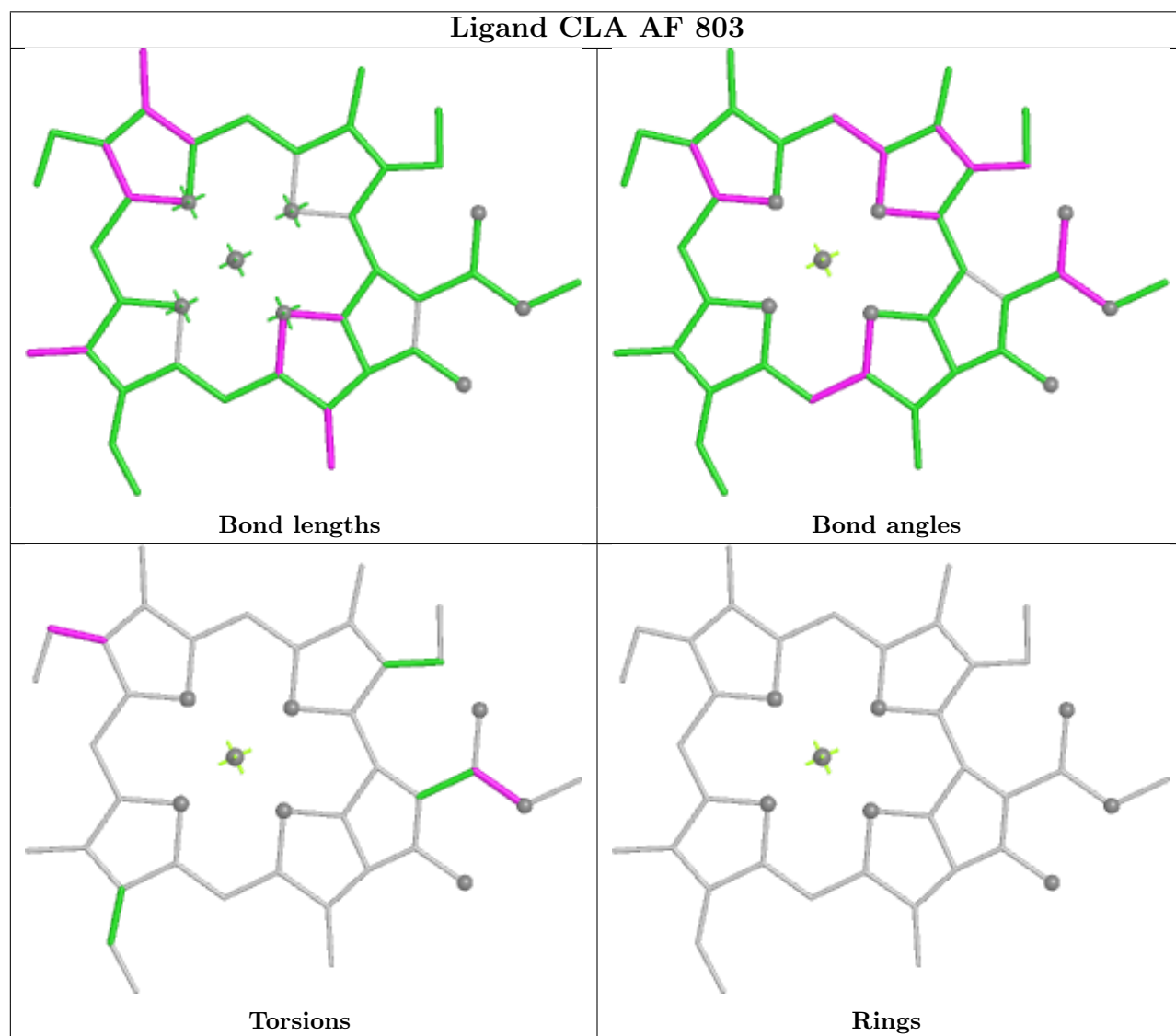
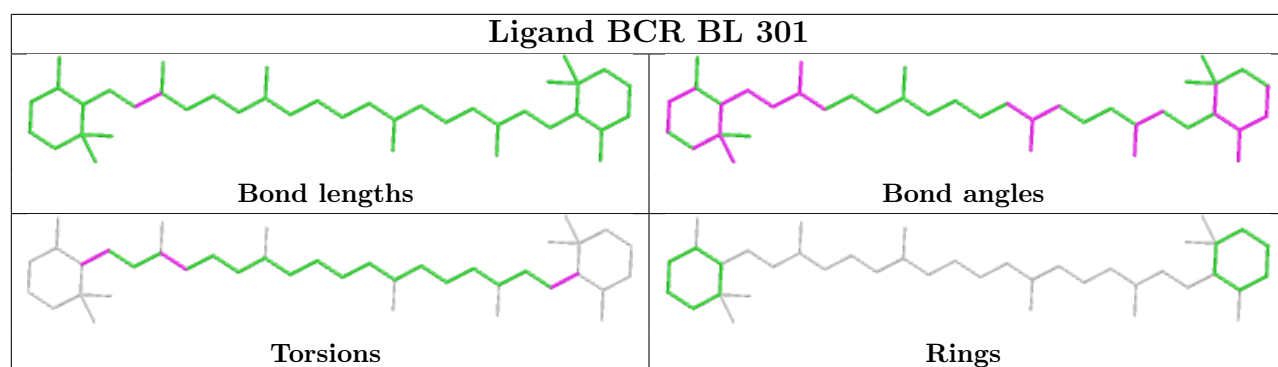
Bond angles



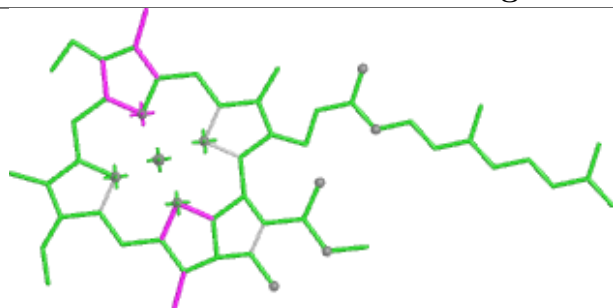
Torsions



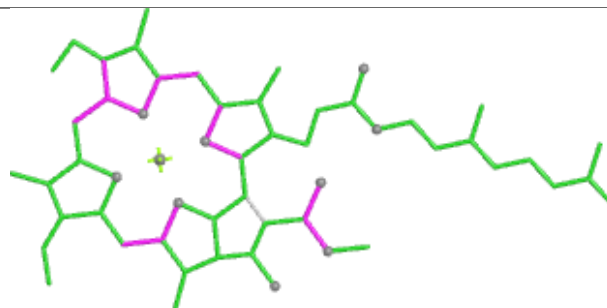
Rings



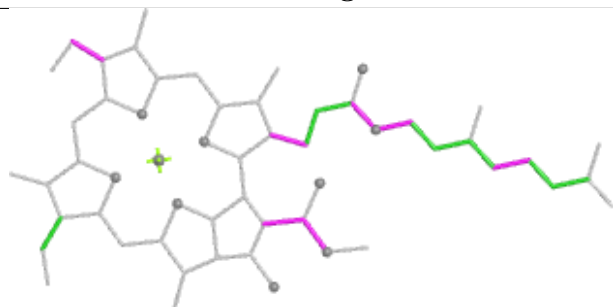
Ligand CLA AB 820



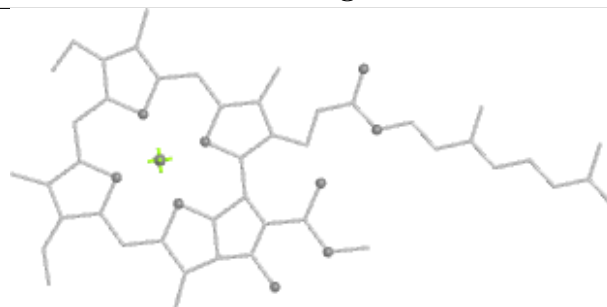
Bond lengths



Bond angles

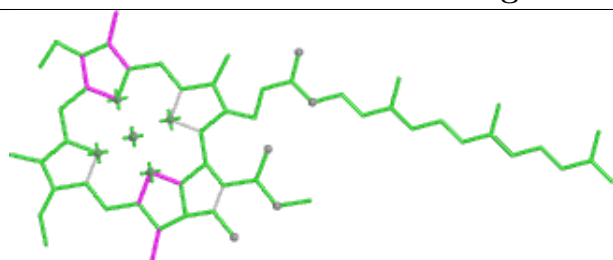


Torsions

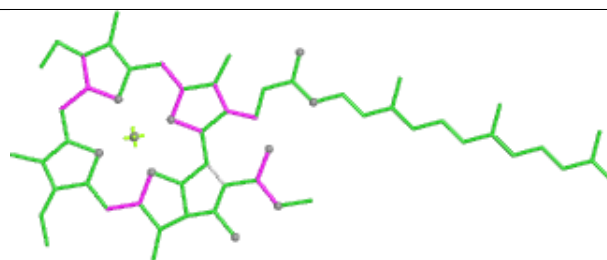


Rings

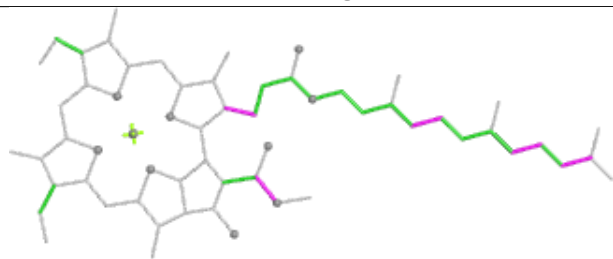
Ligand CLA AB 835



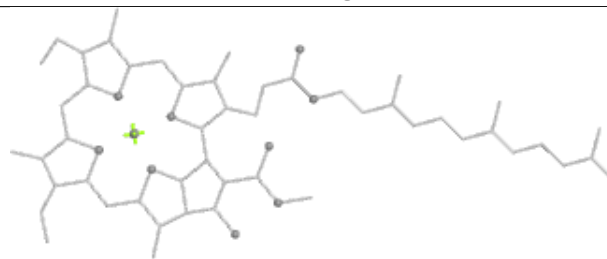
Bond lengths



Bond angles

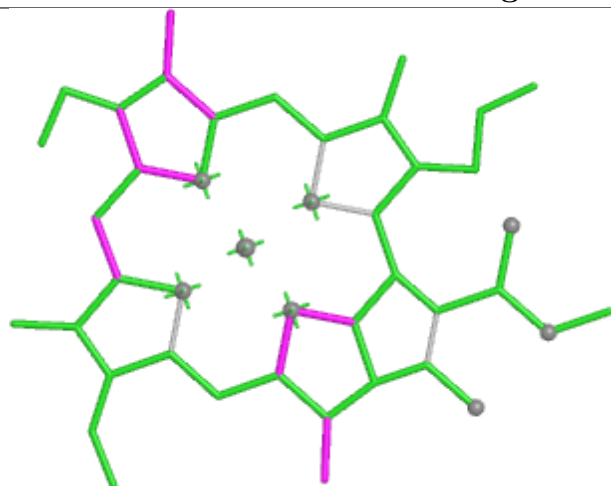


Torsions

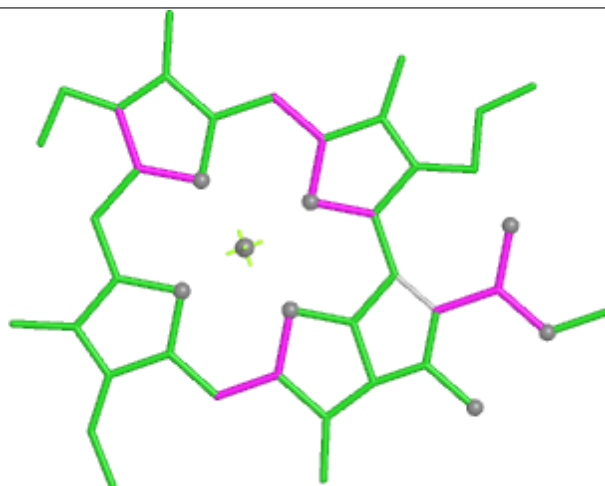


Rings

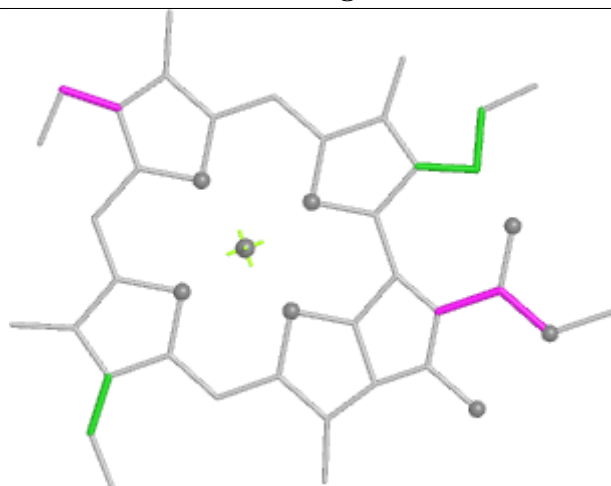
Ligand CLA AB 813



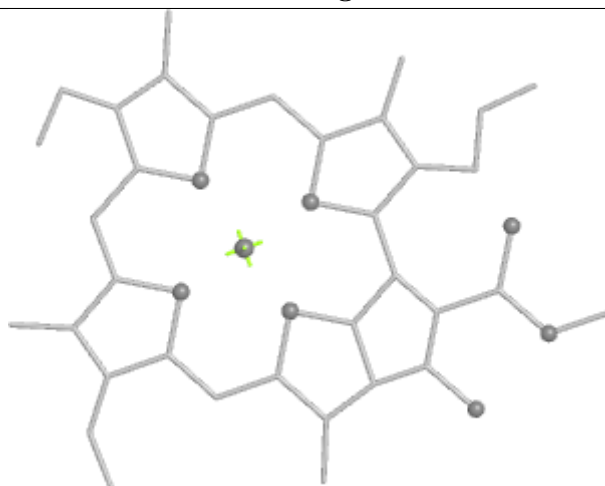
Bond lengths



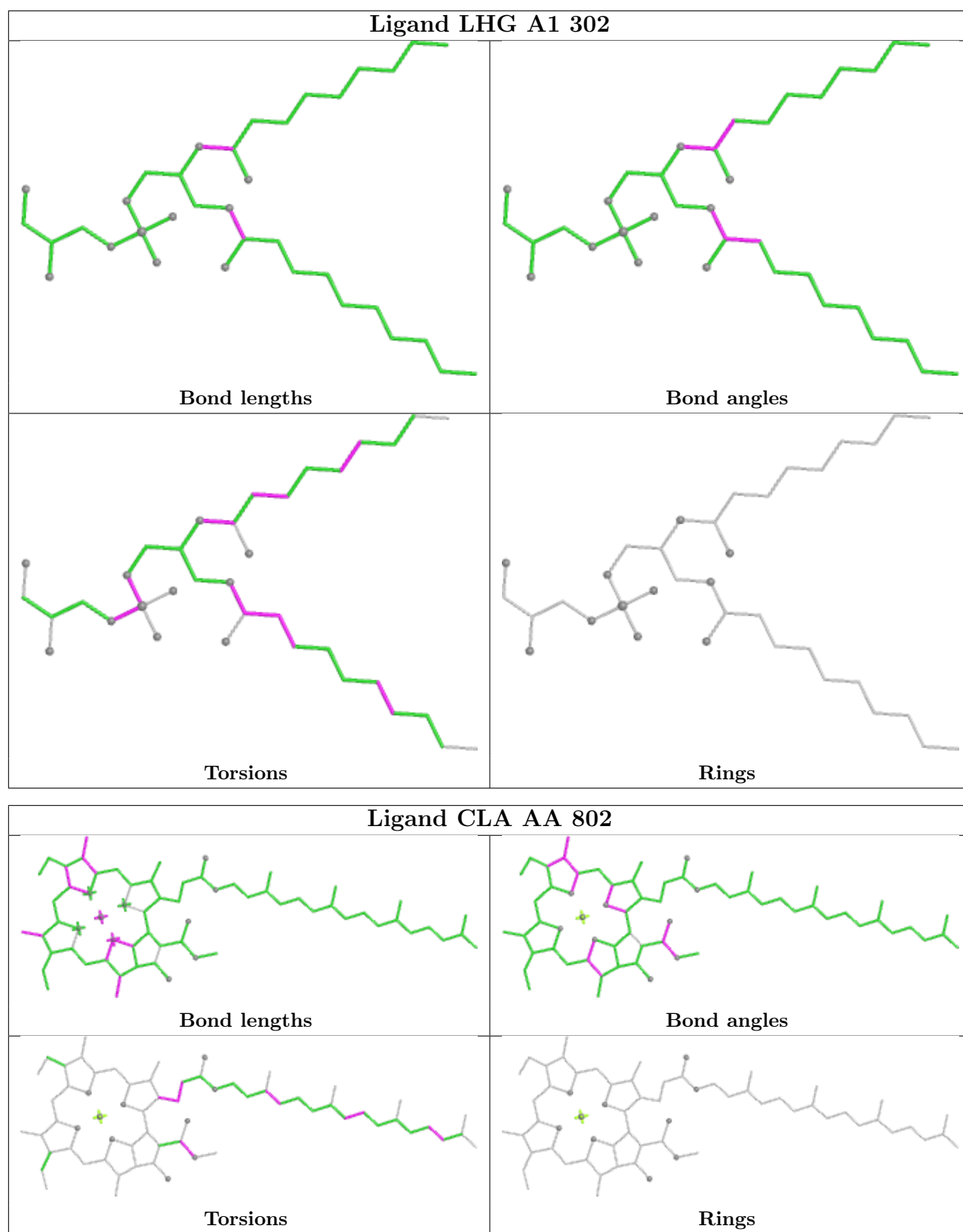
Bond angles



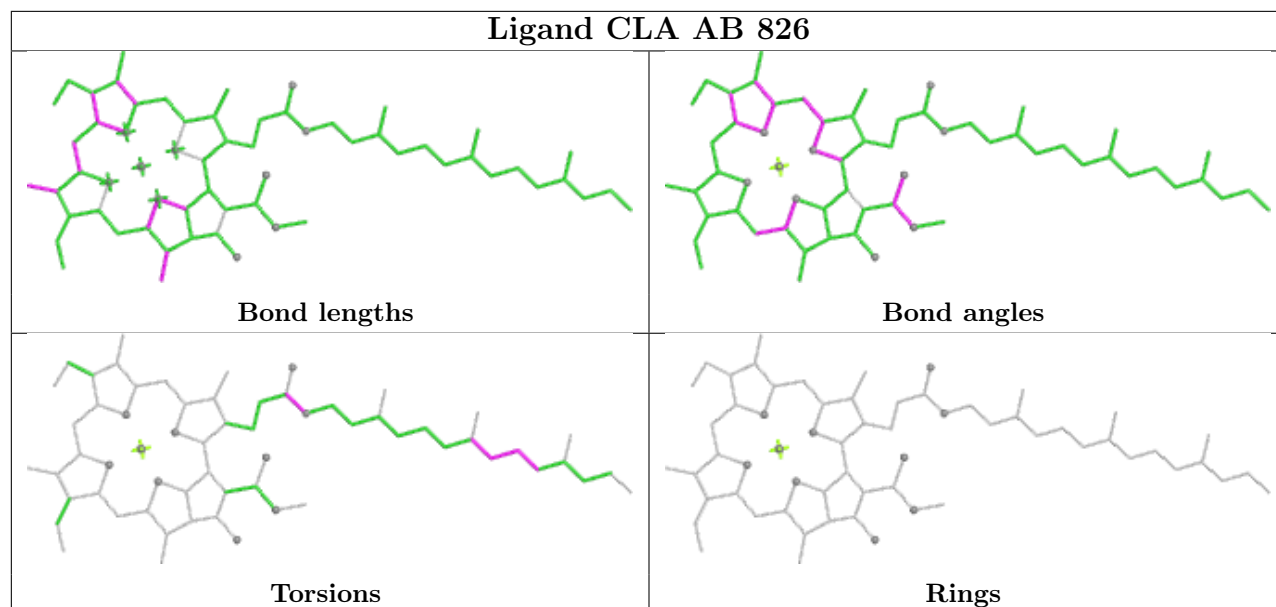
Torsions



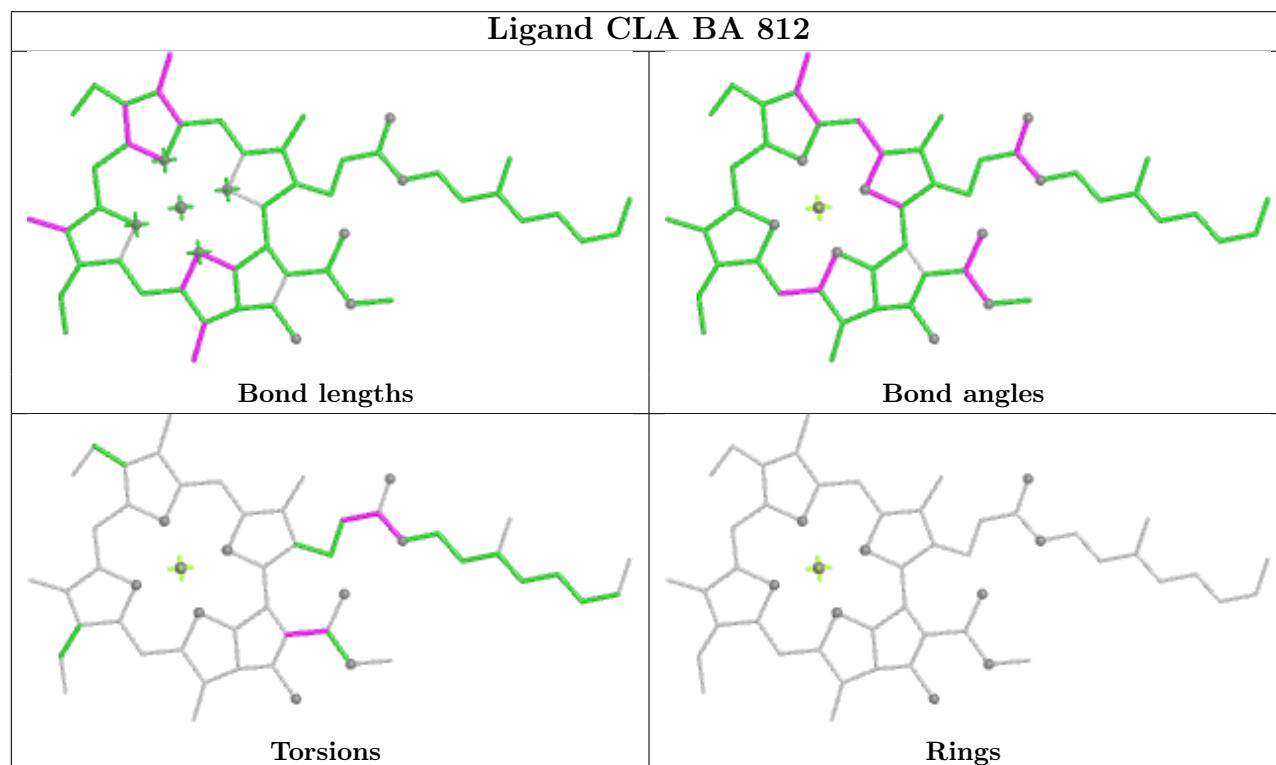
Rings

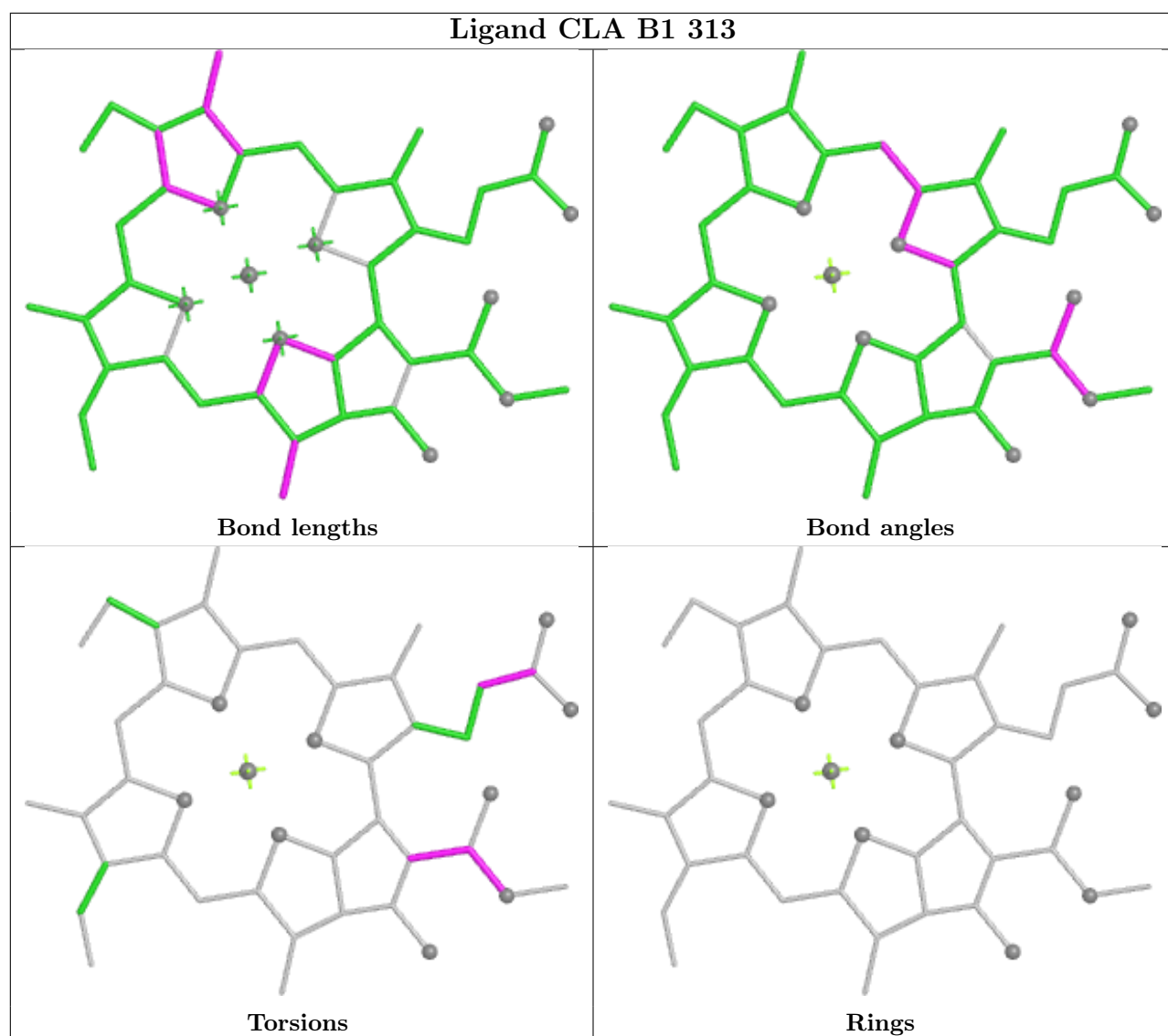


Ligand CLA AB 826

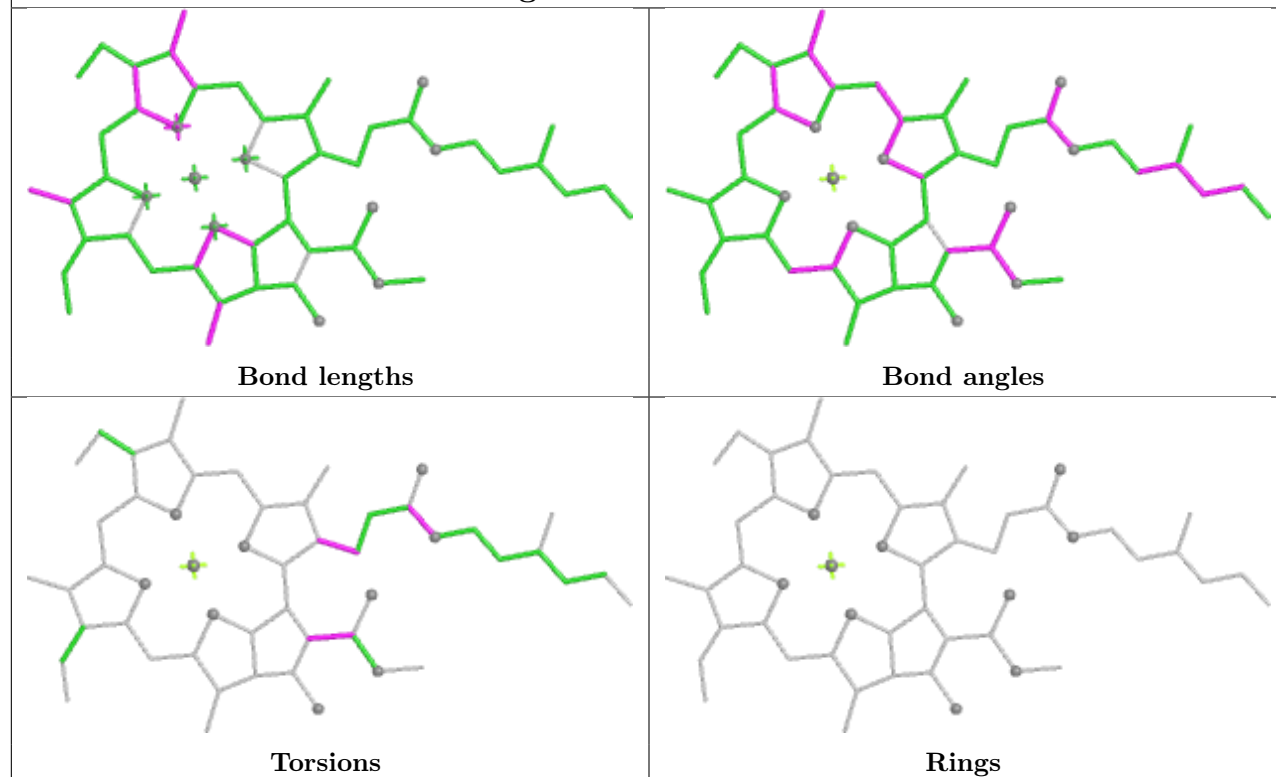


Ligand CLA BA 812

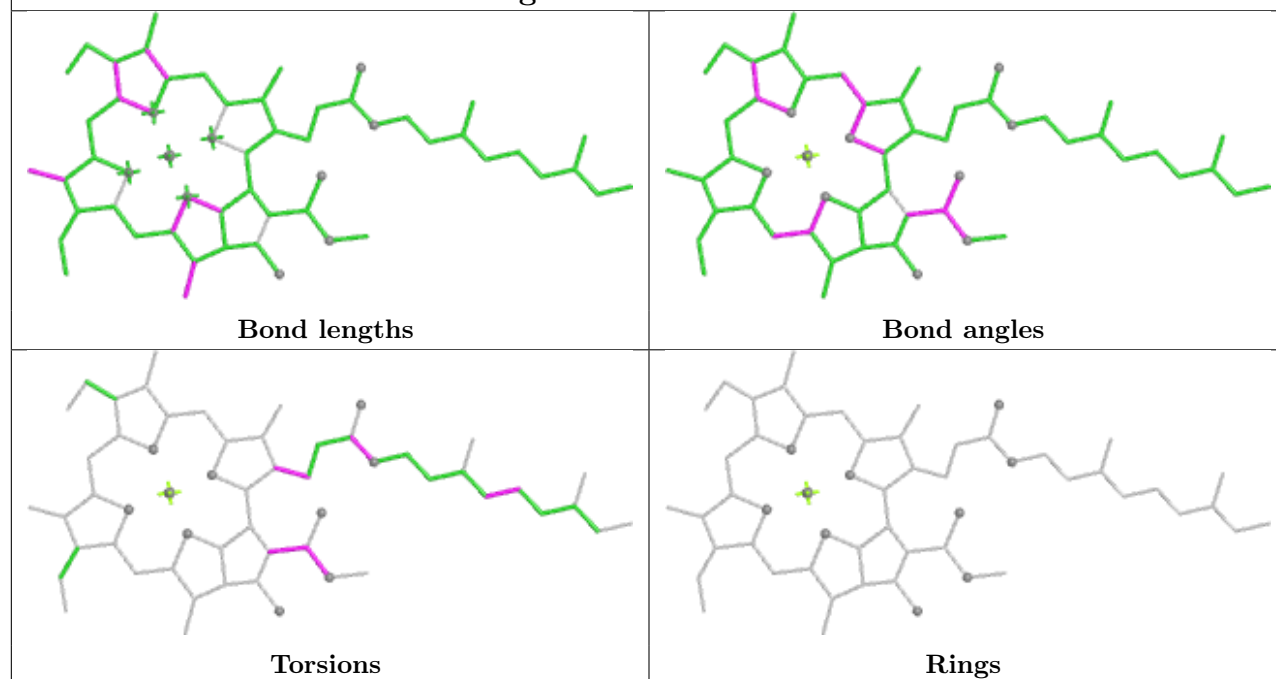




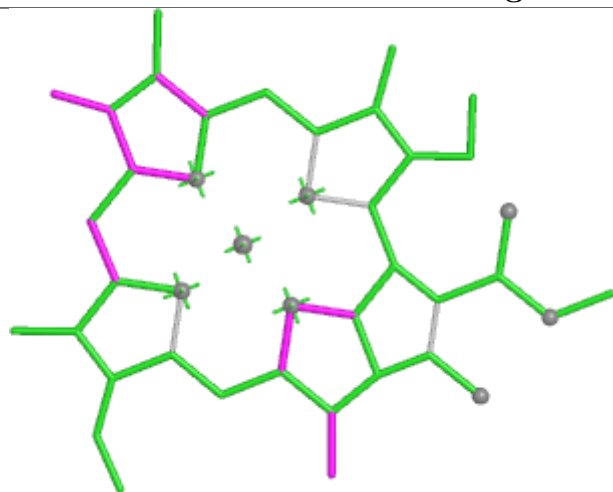
Ligand CLA BA 804



Ligand CLA BA 832



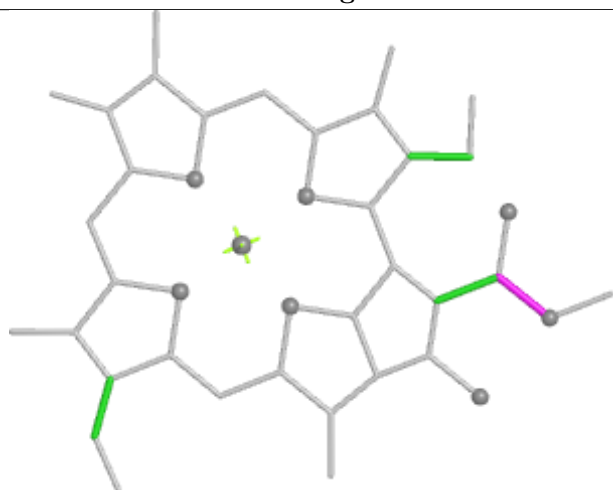
Ligand CLA B3 305



Bond lengths



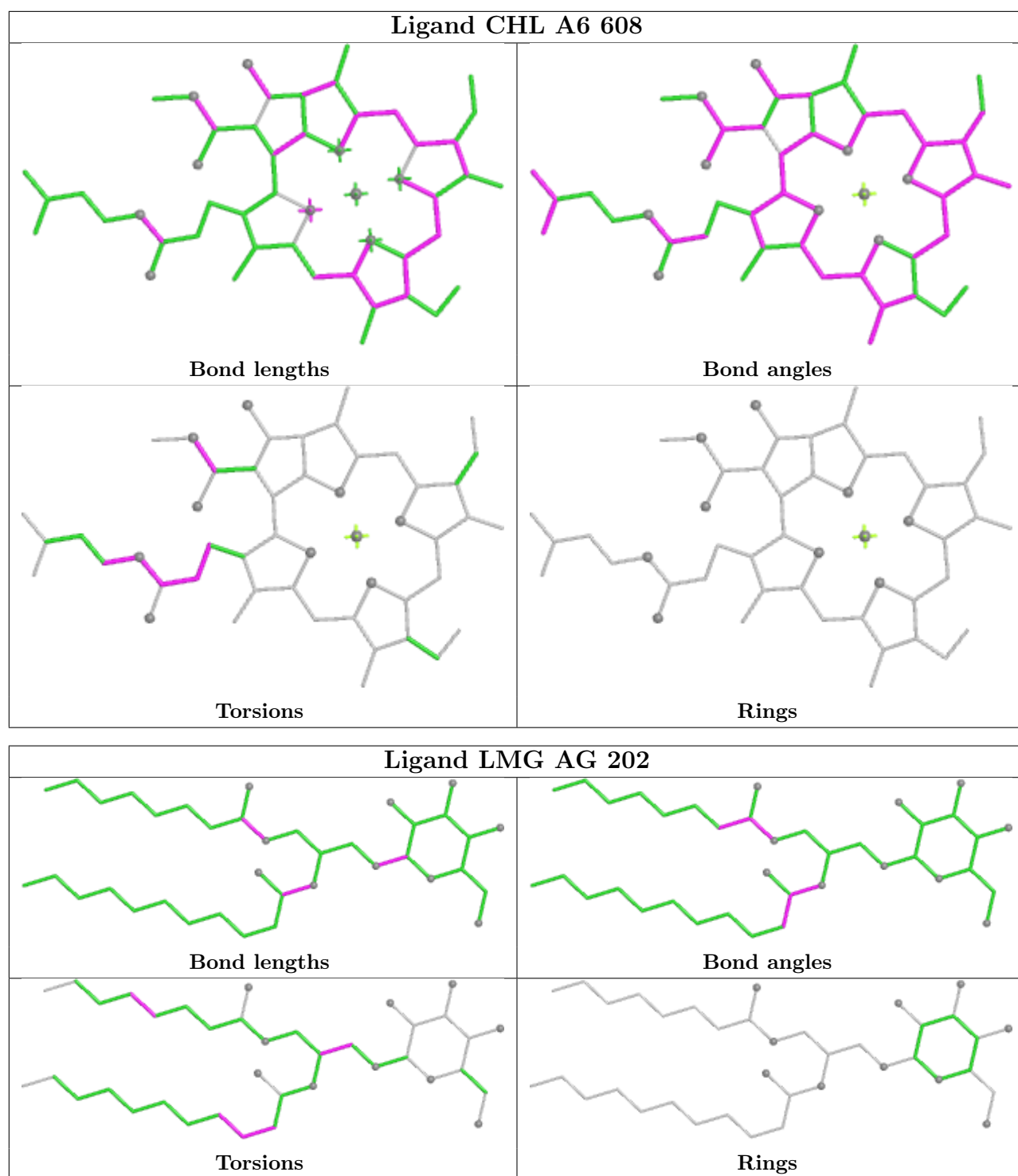
Bond angles

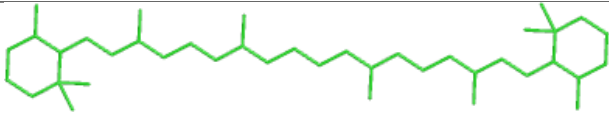
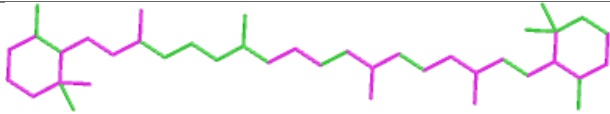
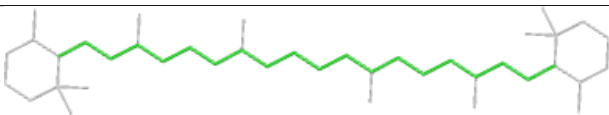
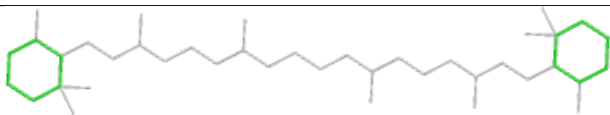


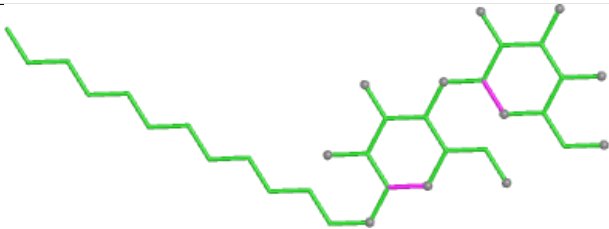
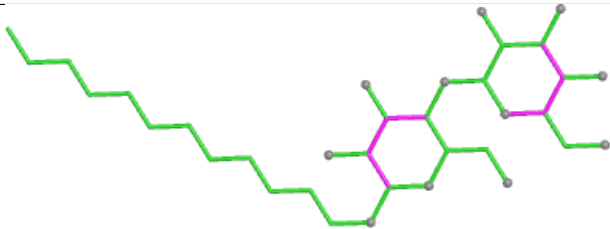
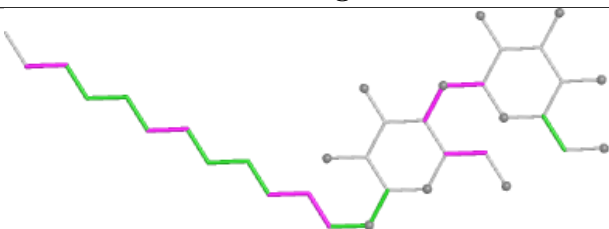
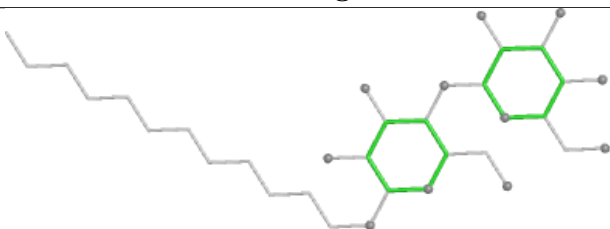
Torsions

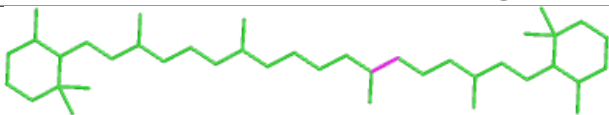
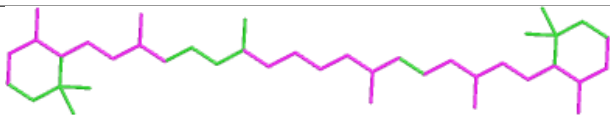
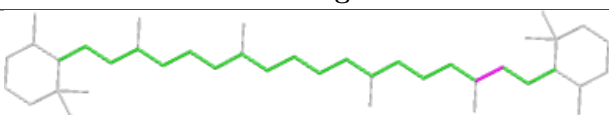
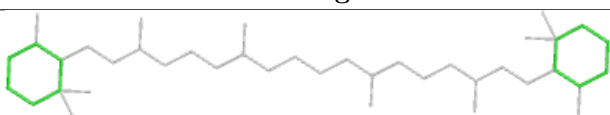


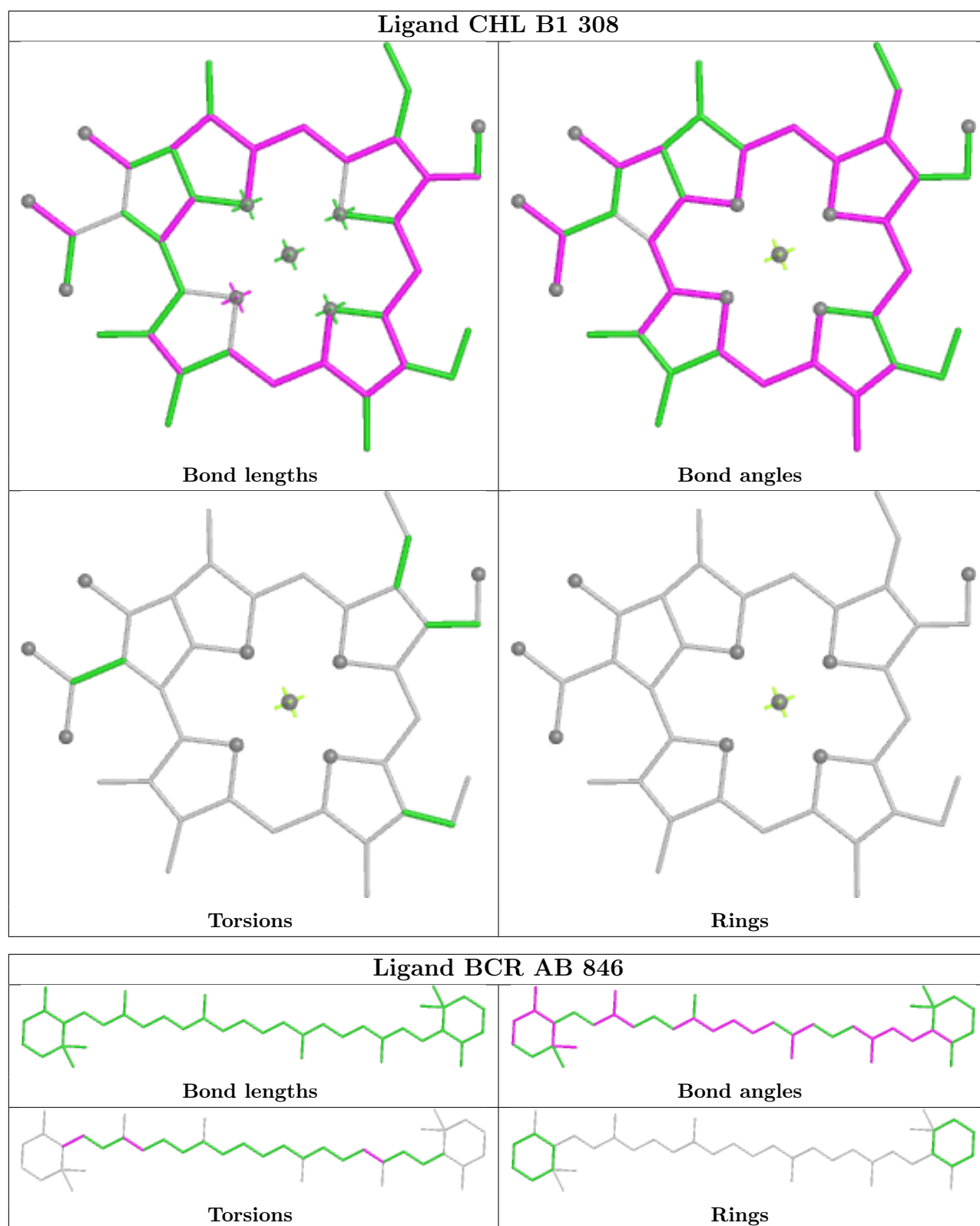
Rings



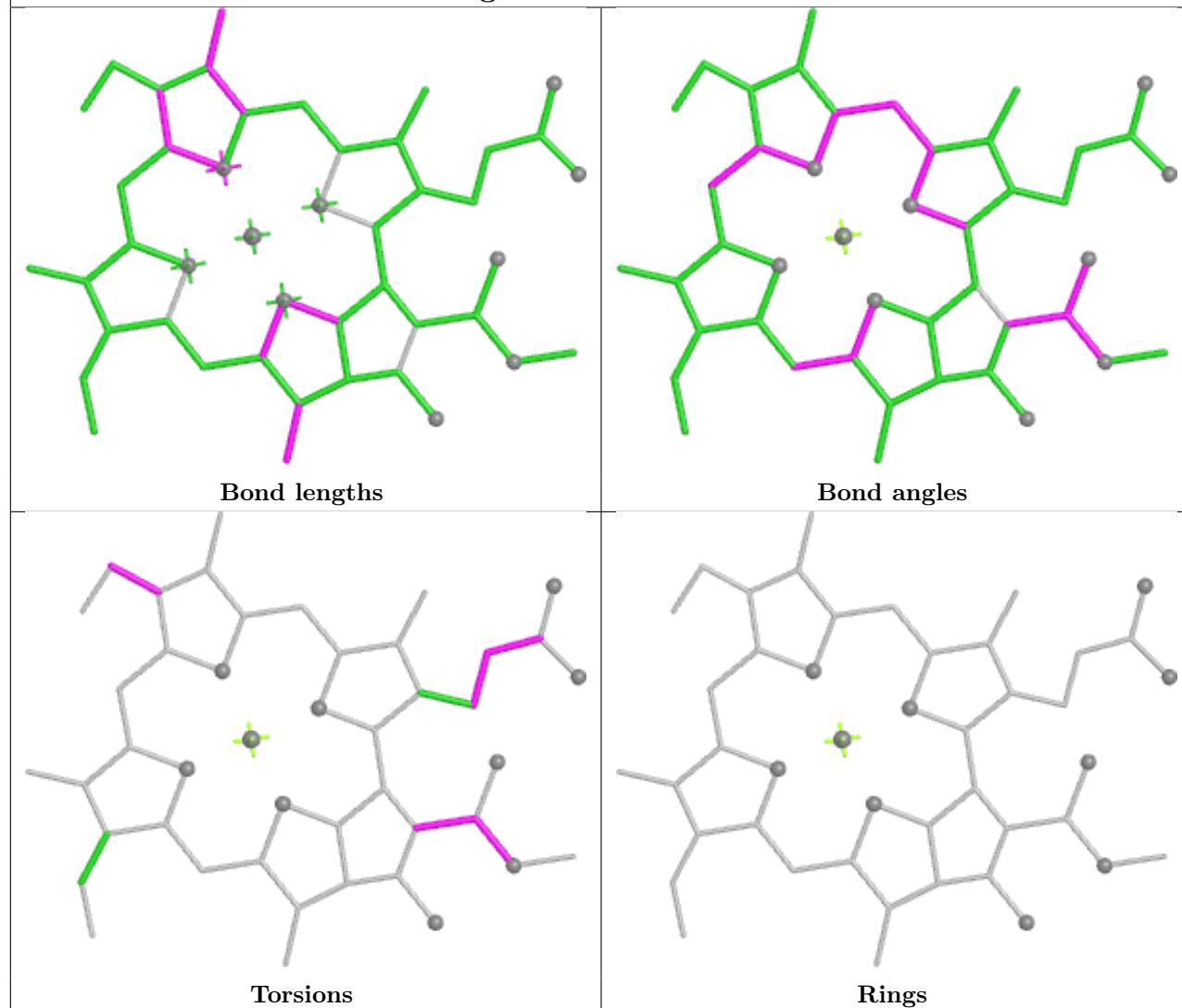
Ligand BCR BJ 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMU AB 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

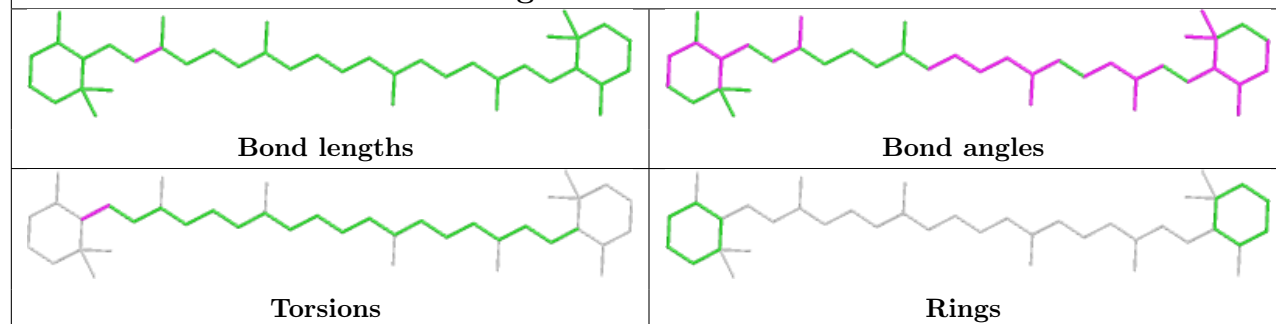
Ligand BCR BB 849	
	
Bond lengths	Bond angles
	
Torsions	Rings



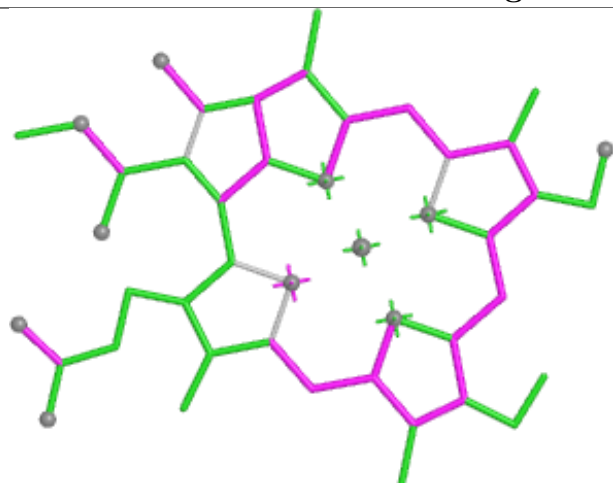
Ligand CLA AA 836



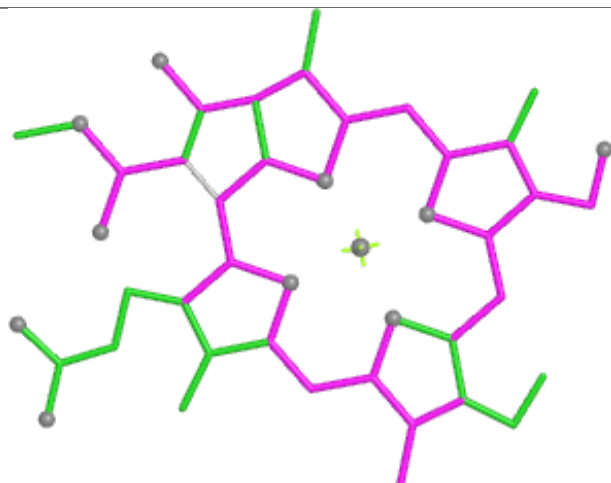
Ligand BCR BK 204



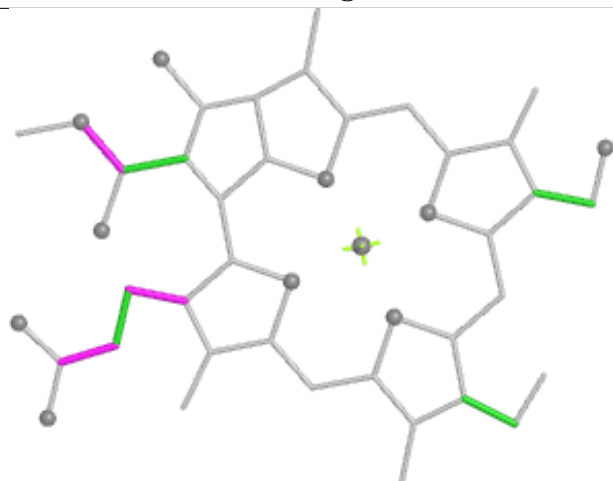
Ligand CHL B5 607



Bond lengths



Bond angles

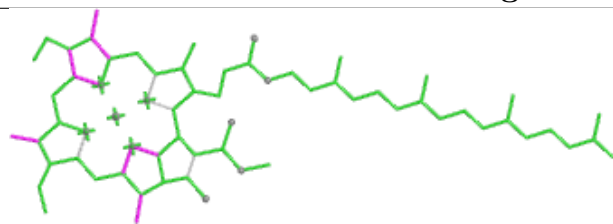


Torsions

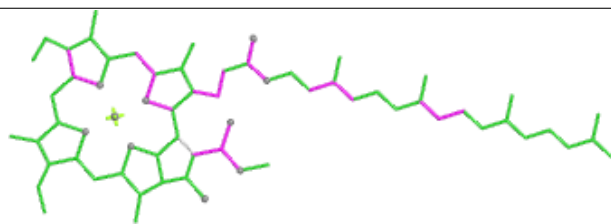


Rings

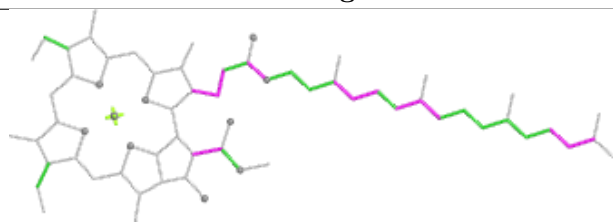
Ligand CLA AB 809



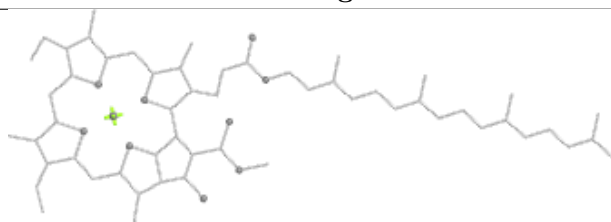
Bond lengths



Bond angles

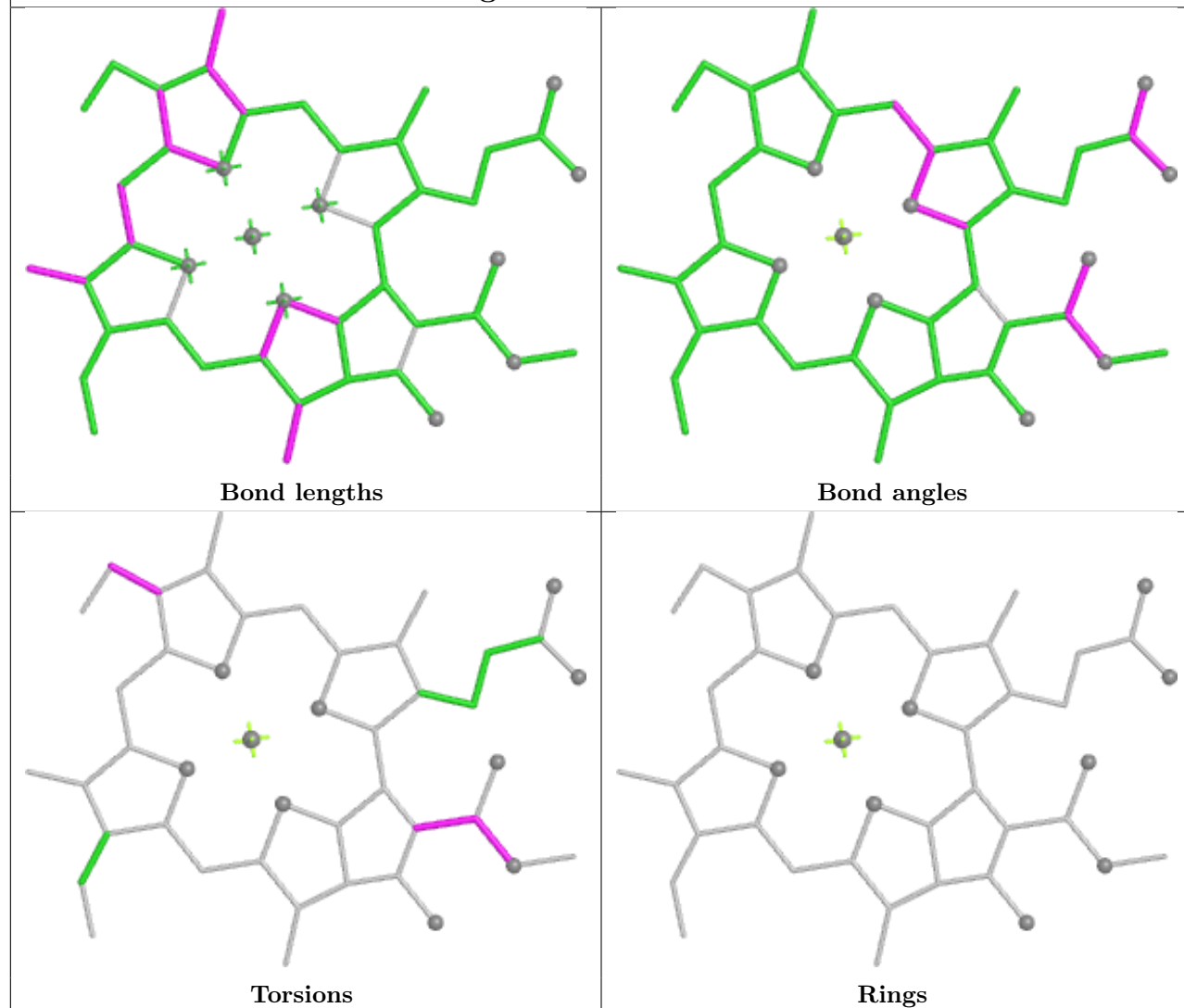


Torsions

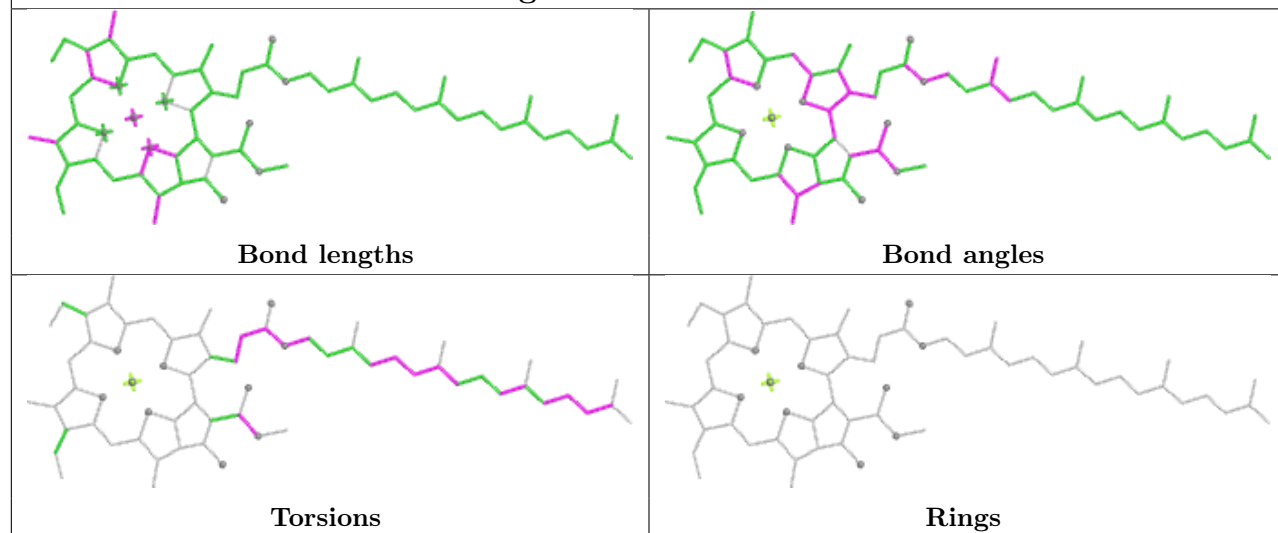


Rings

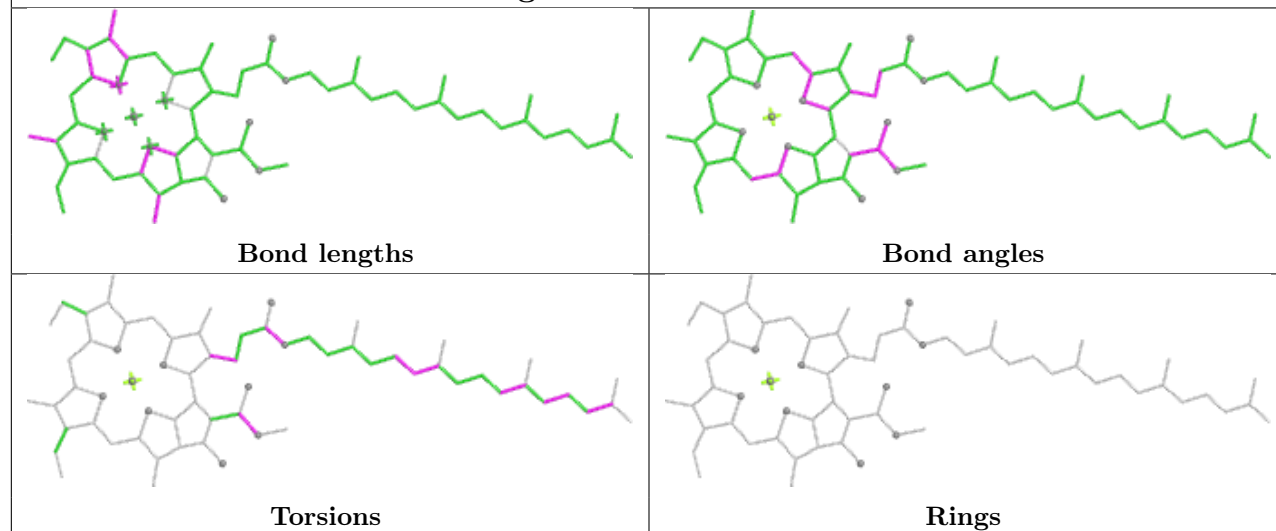
Ligand CLA AA 820



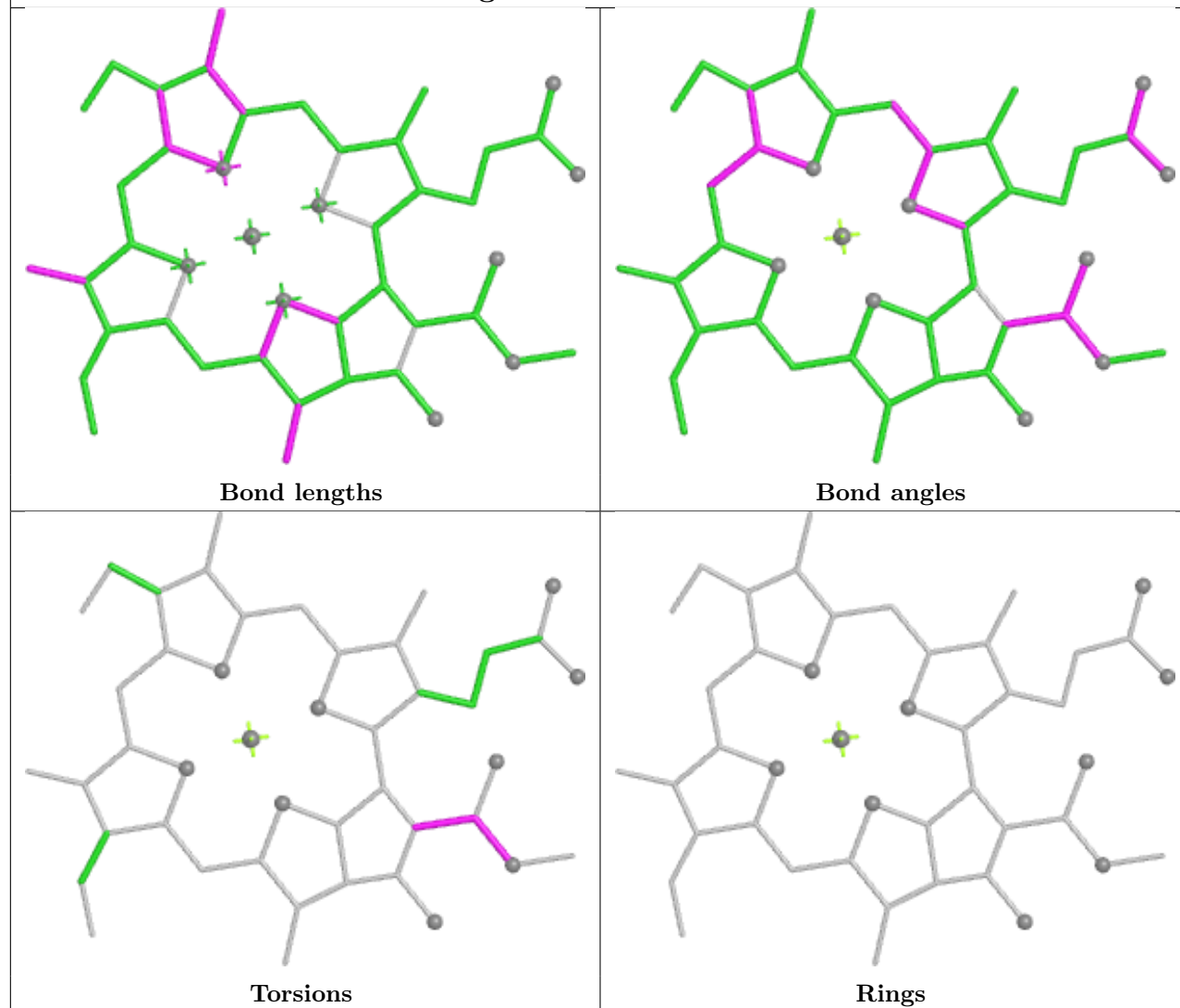
Ligand CLA AB 801



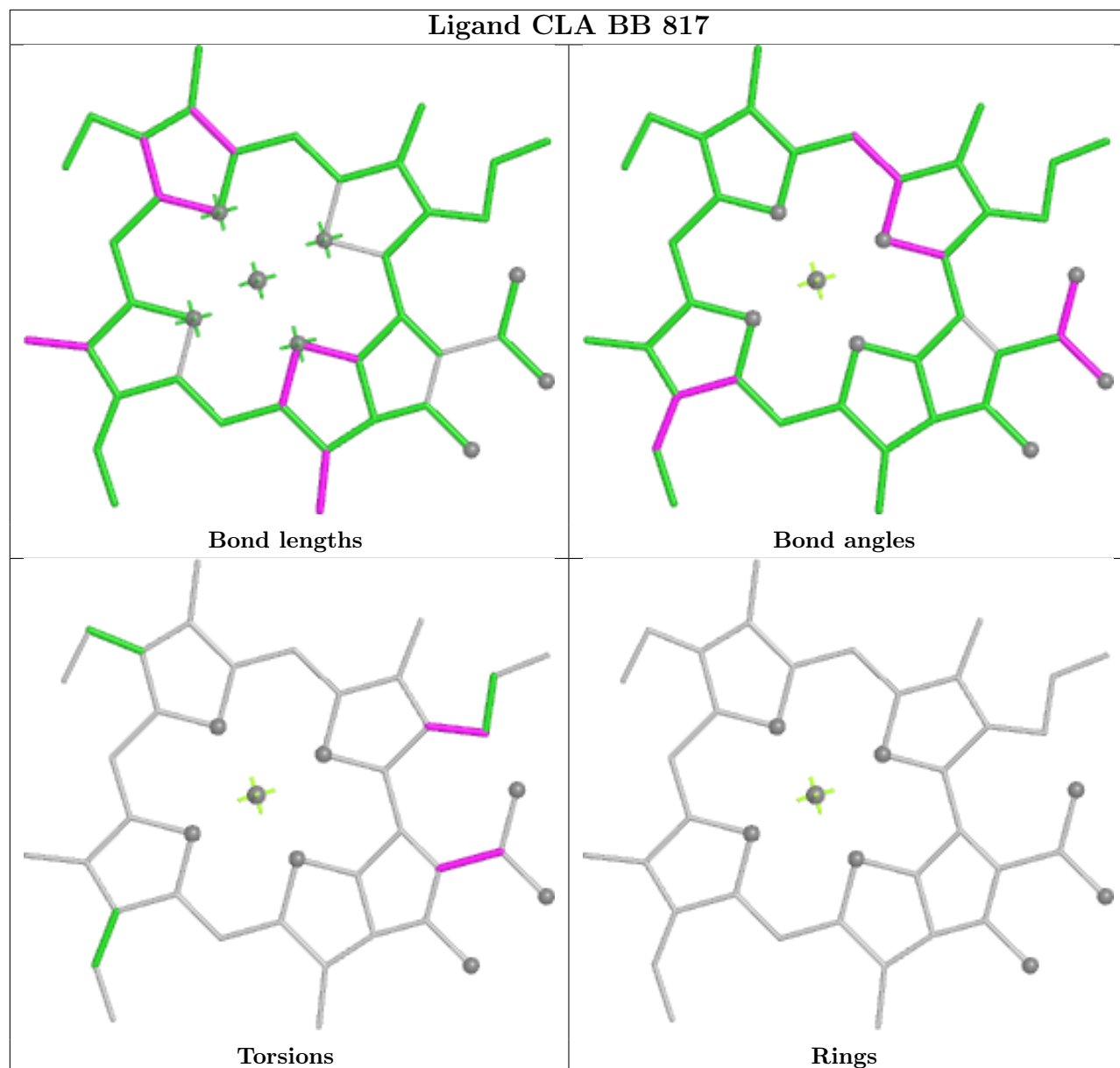
Ligand CLA AA 819

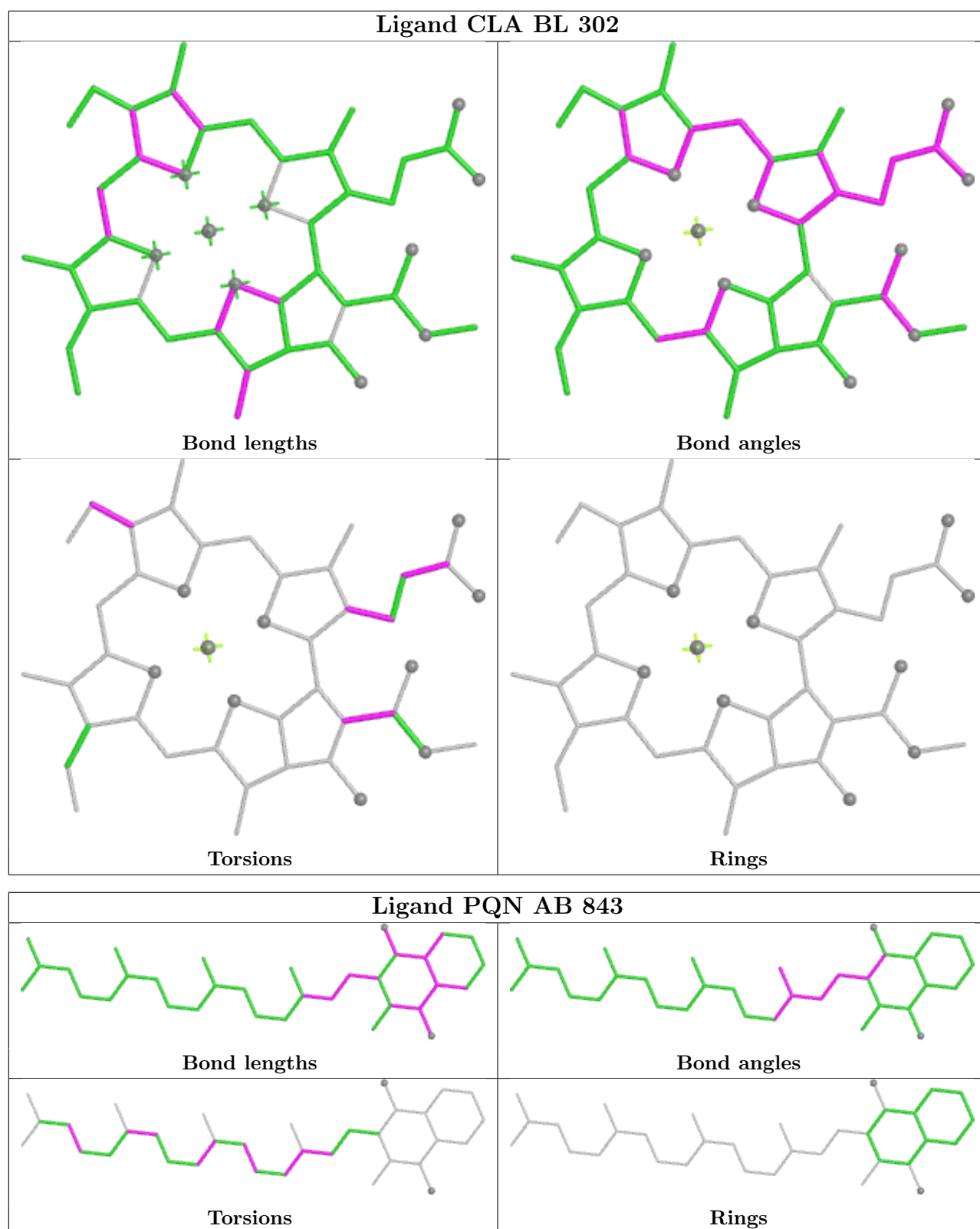


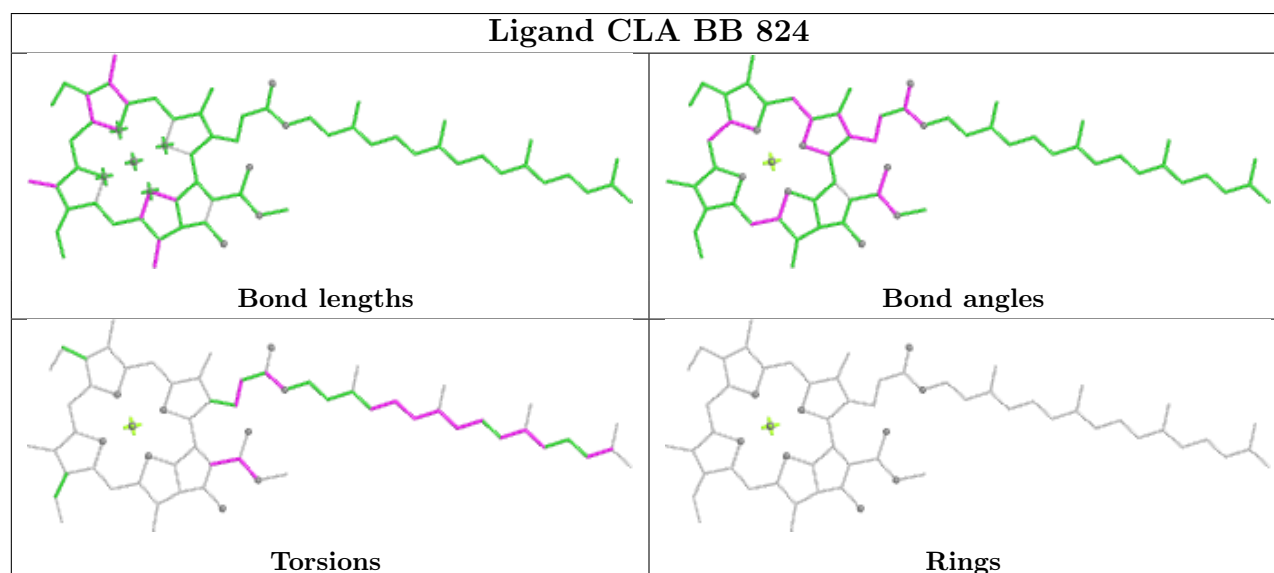
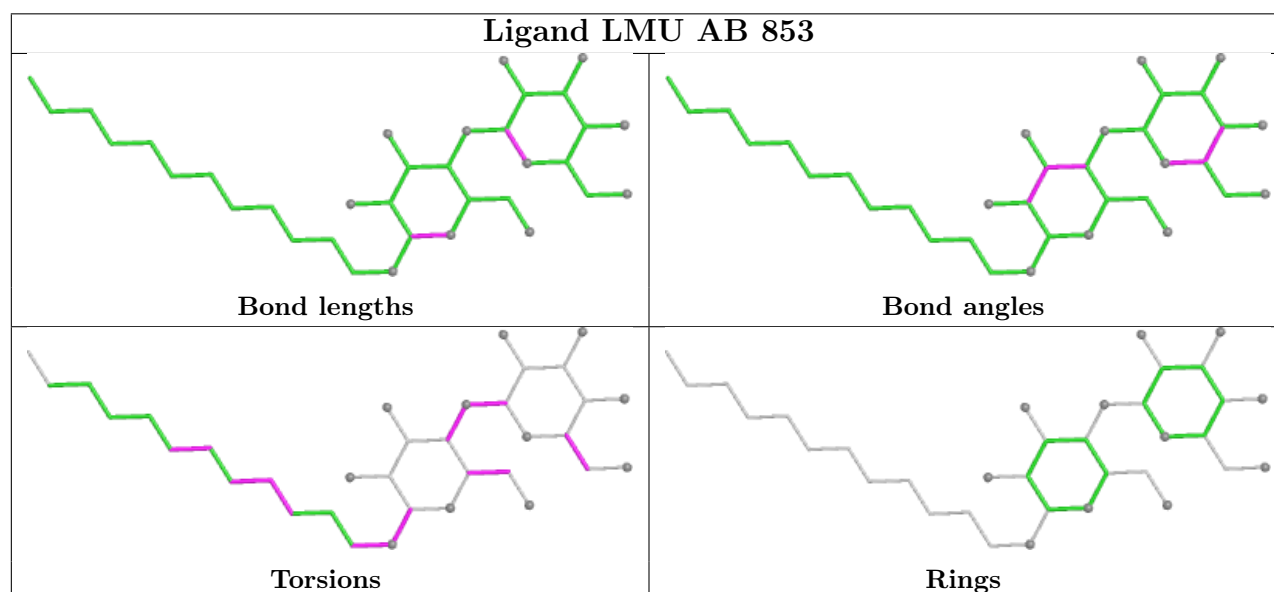
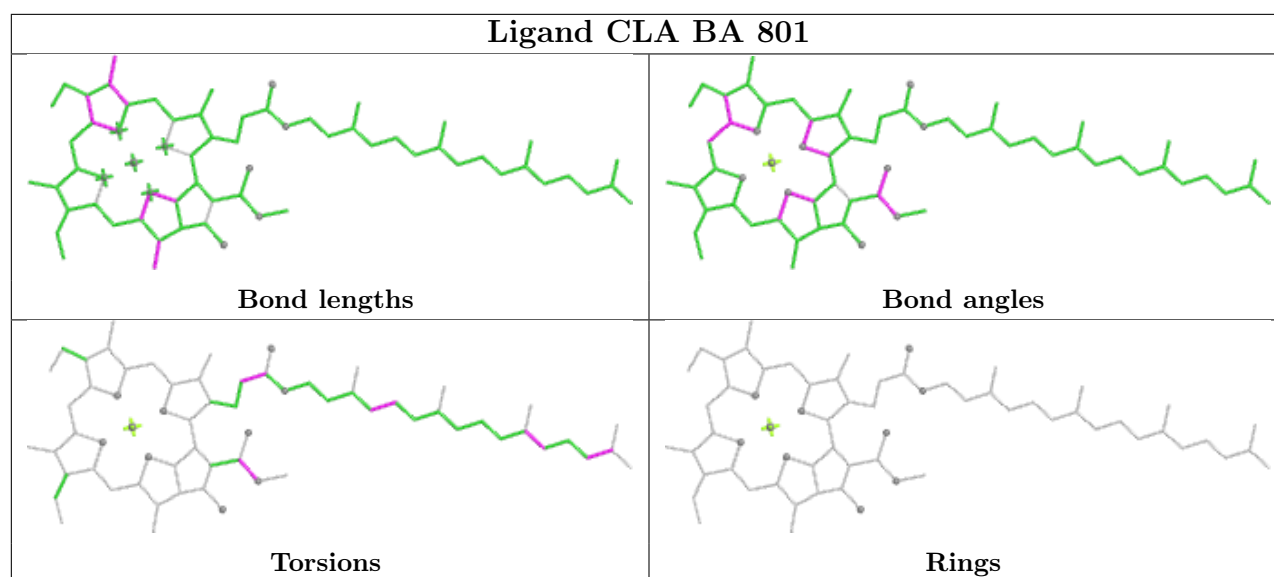
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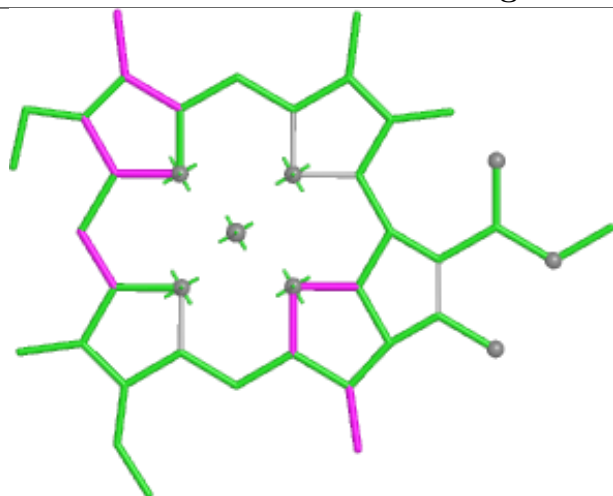
Ligand CLA BB 817







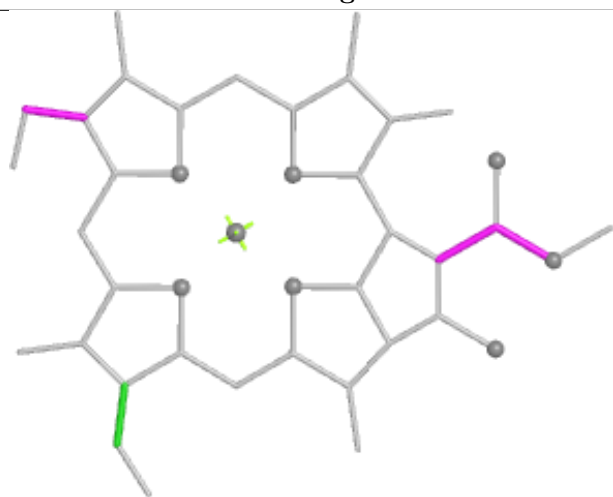
Ligand CLA AA 823



Bond lengths



Bond angles

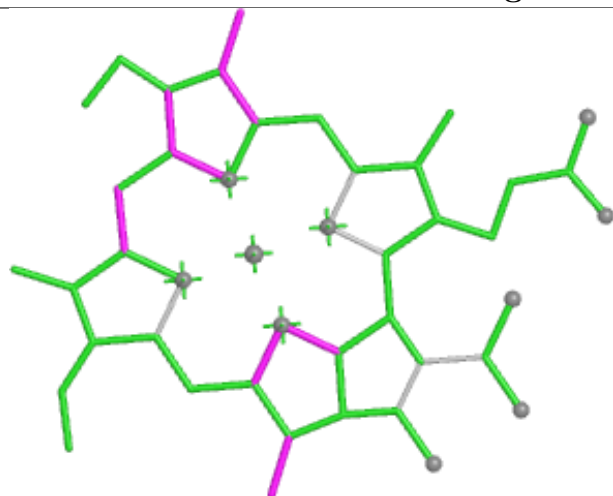


Torsions

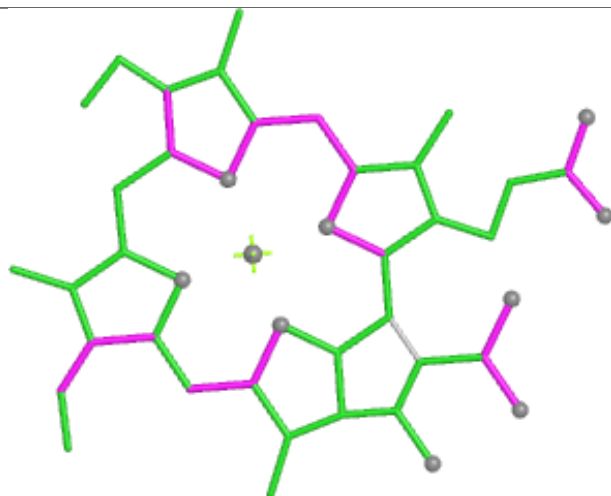


Rings

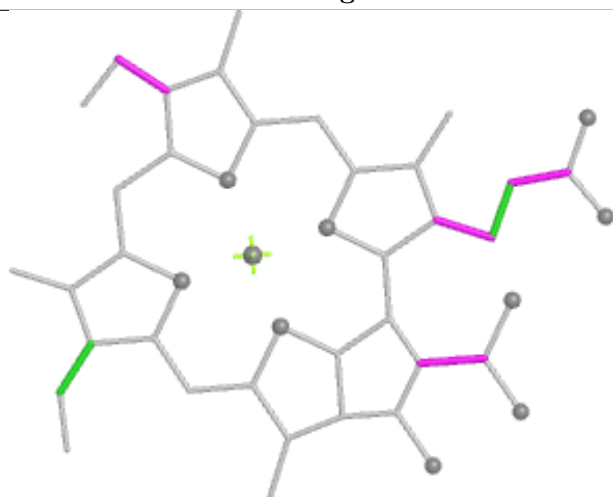
Ligand CLA A1 309



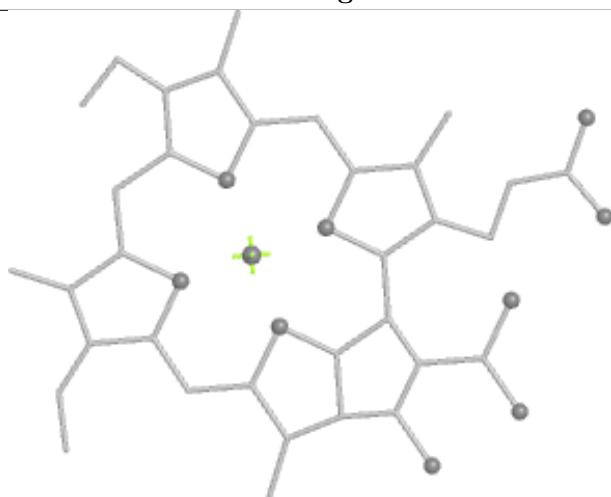
Bond lengths



Bond angles

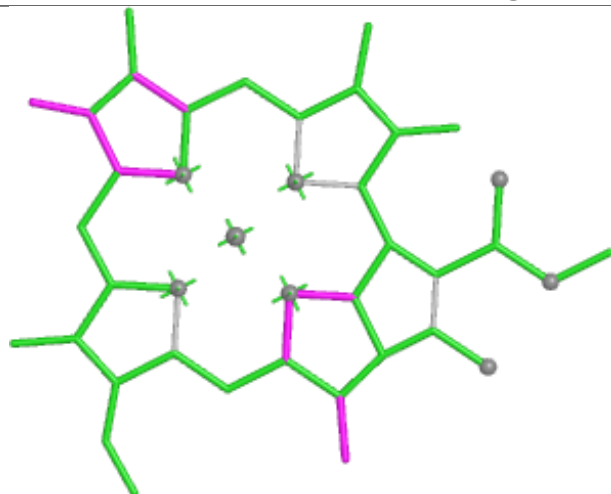


Torsions



Rings

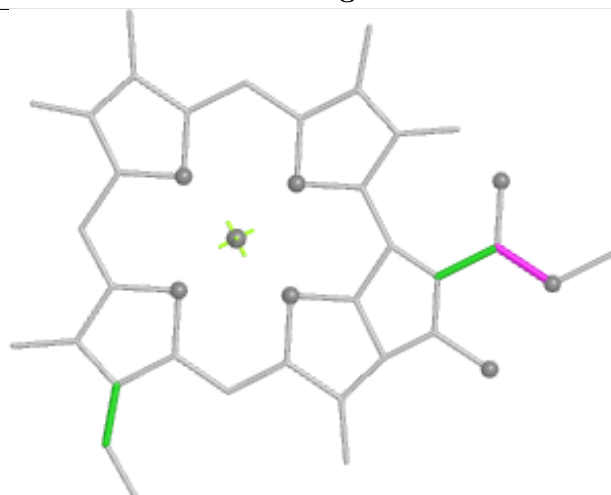
Ligand CLA A1 310



Bond lengths



Bond angles

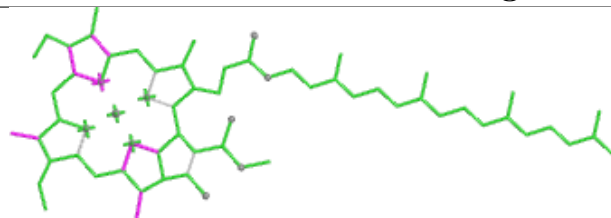


Torsions

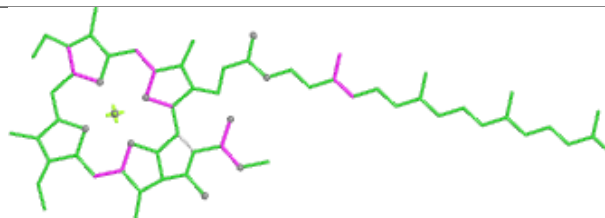


Rings

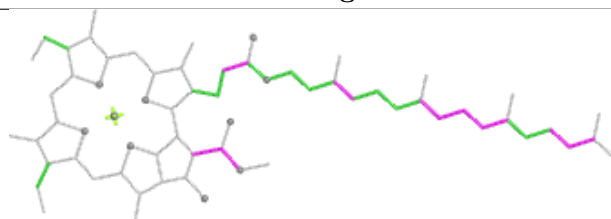
Ligand CLA BA 813



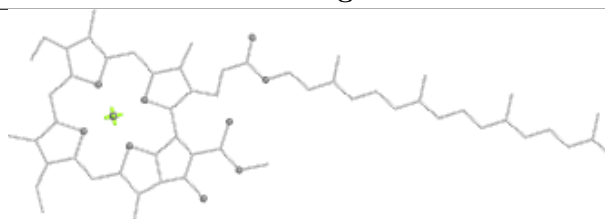
Bond lengths



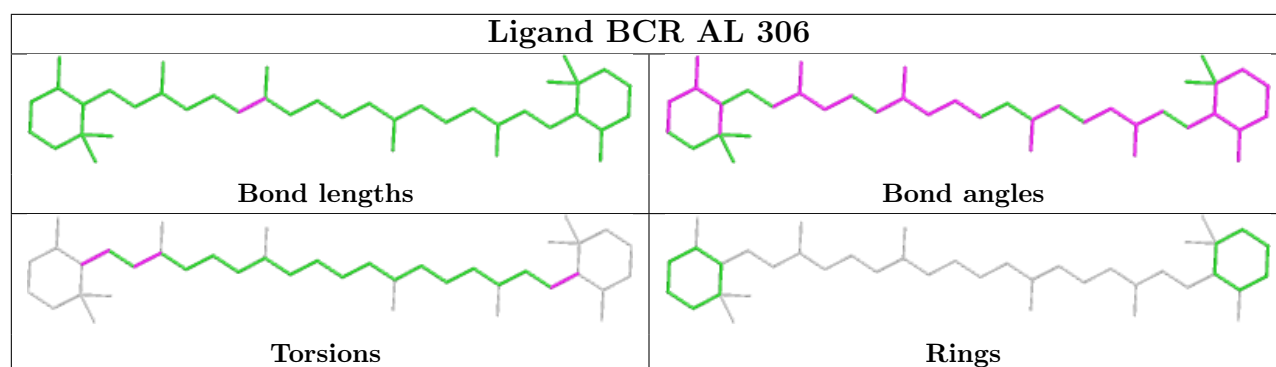
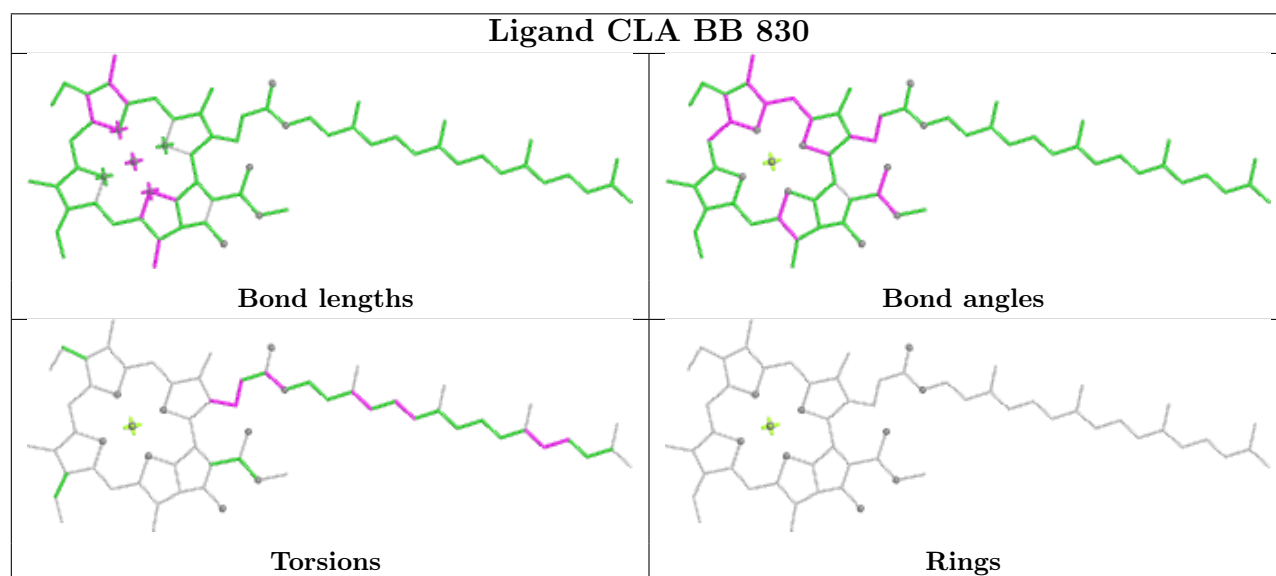
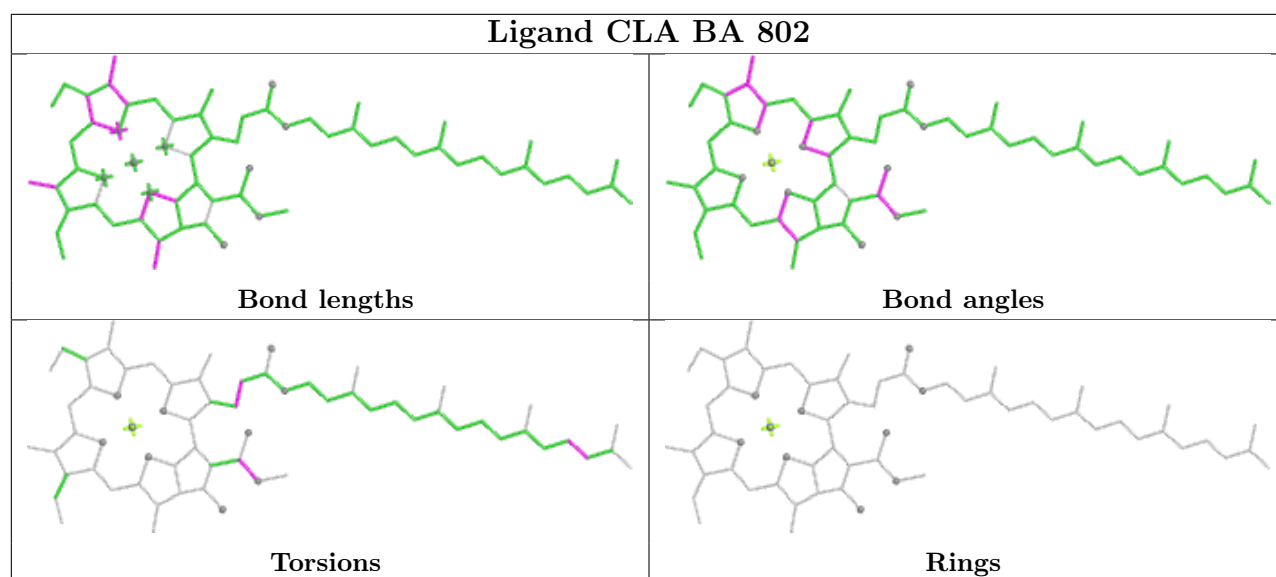
Bond angles

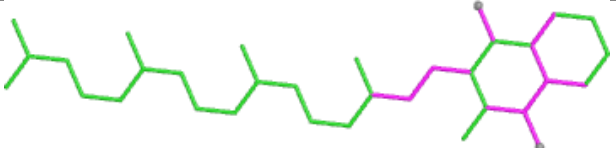
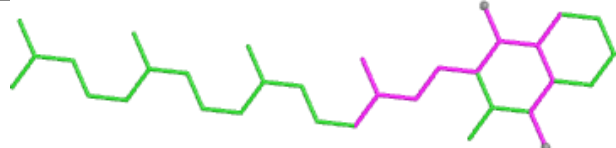
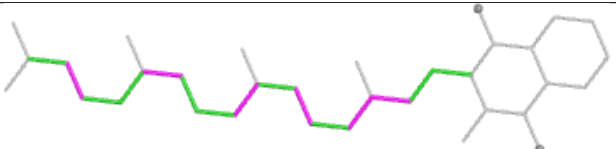
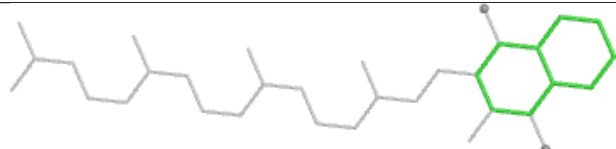


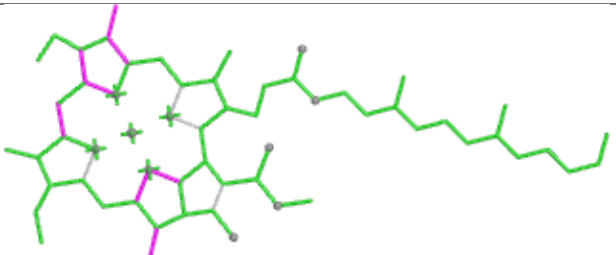
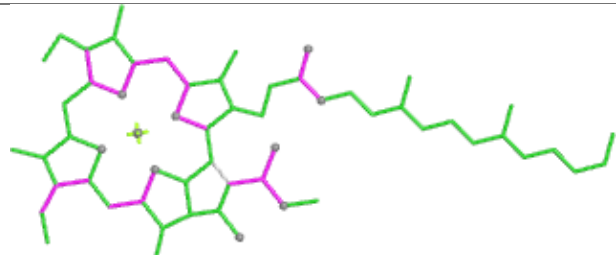
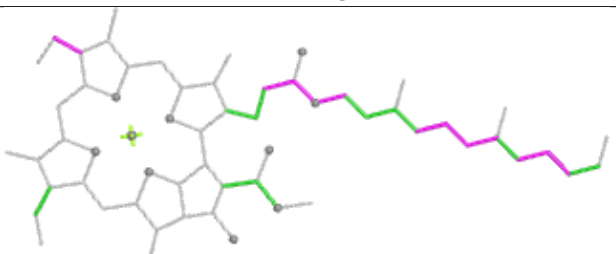
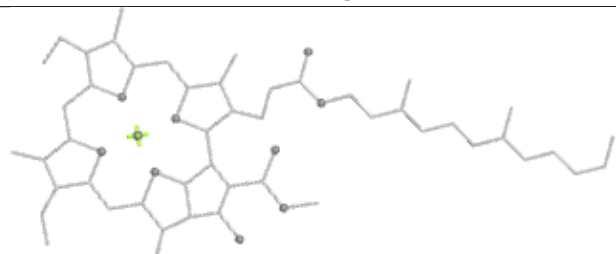
Torsions

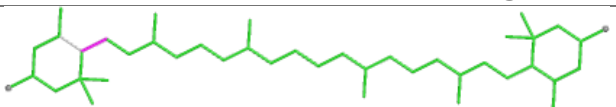
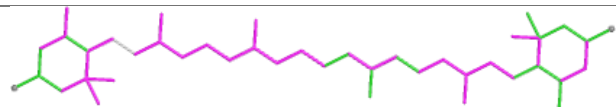
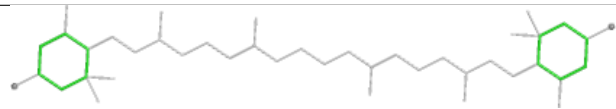


Rings

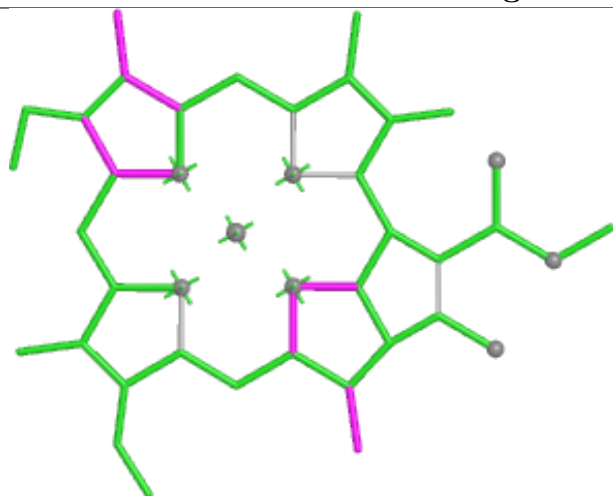


Ligand PQN BB 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AB 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT B3 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

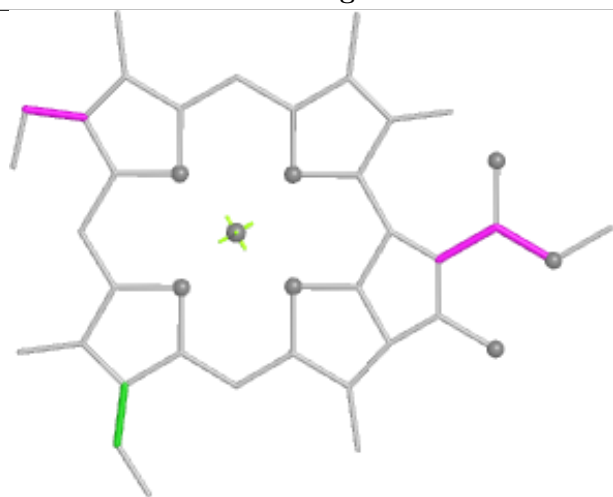
Ligand CLA AL 303



Bond lengths



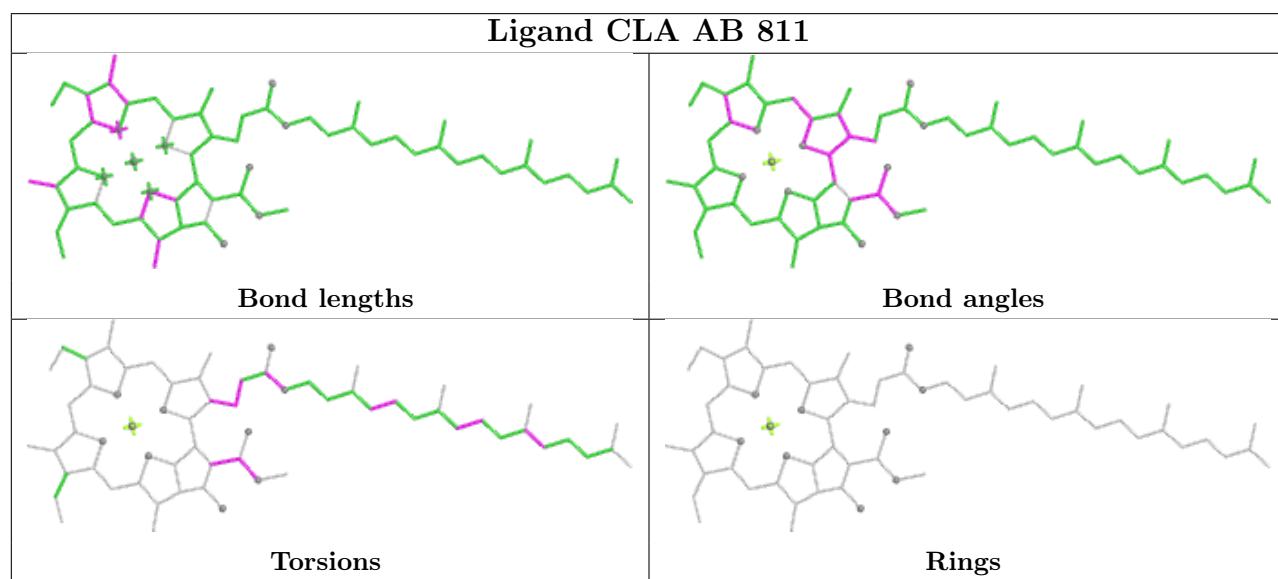
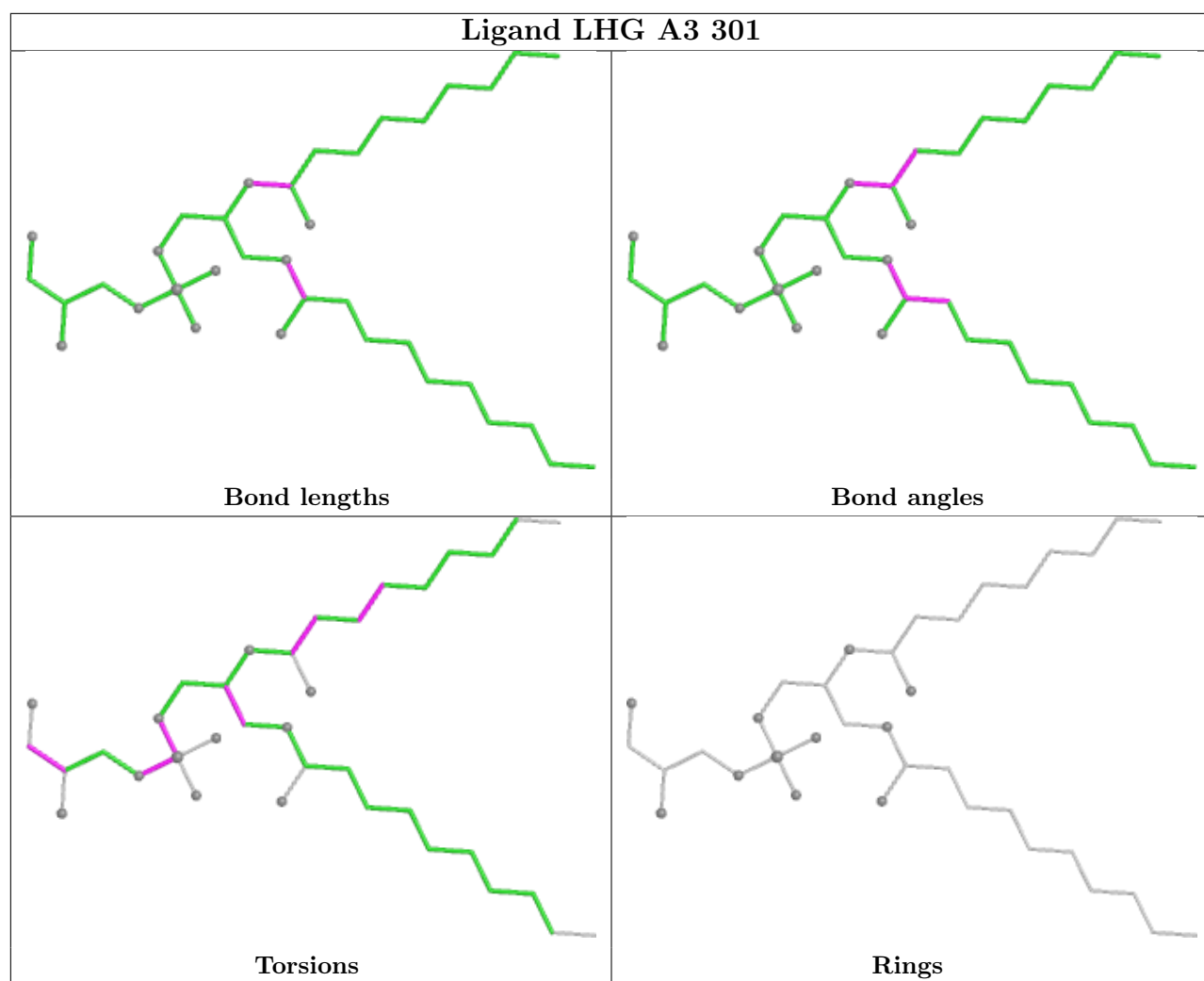
Bond angles

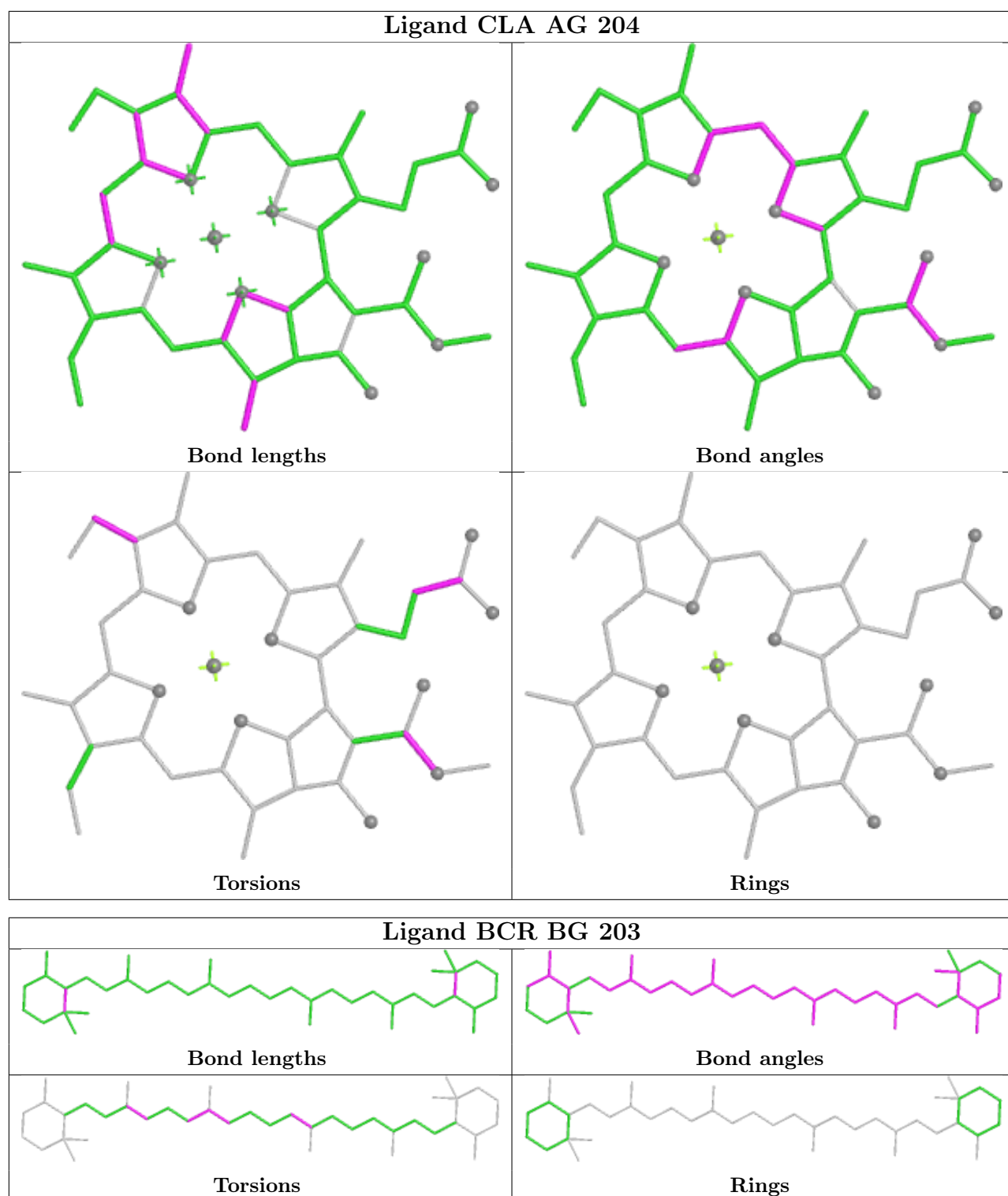


Torsions

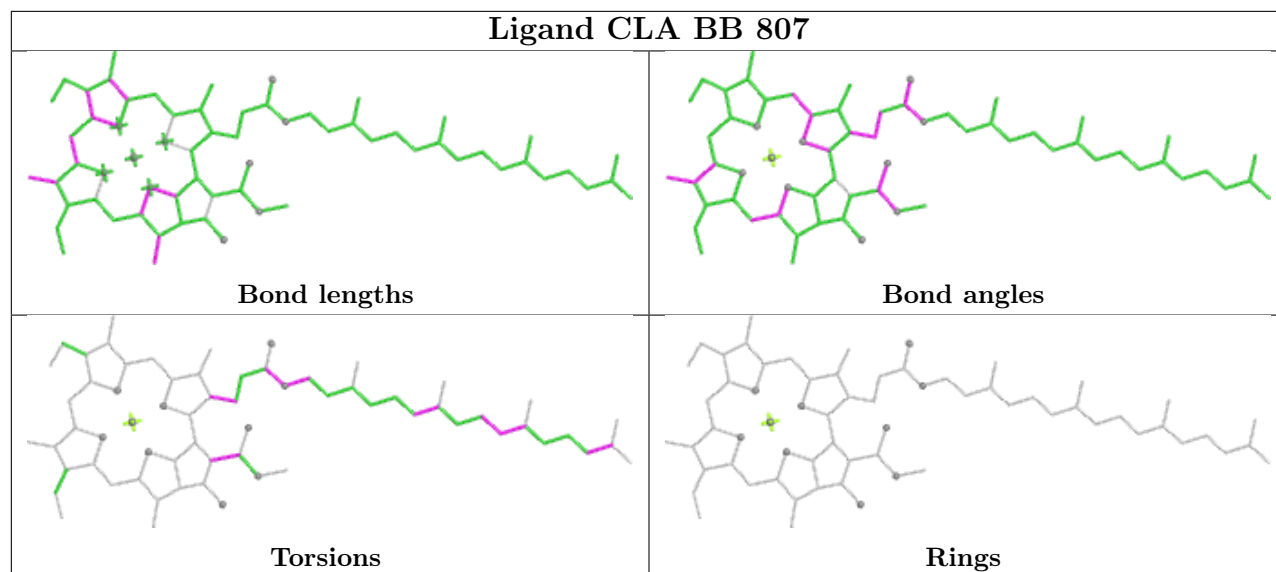


Rings

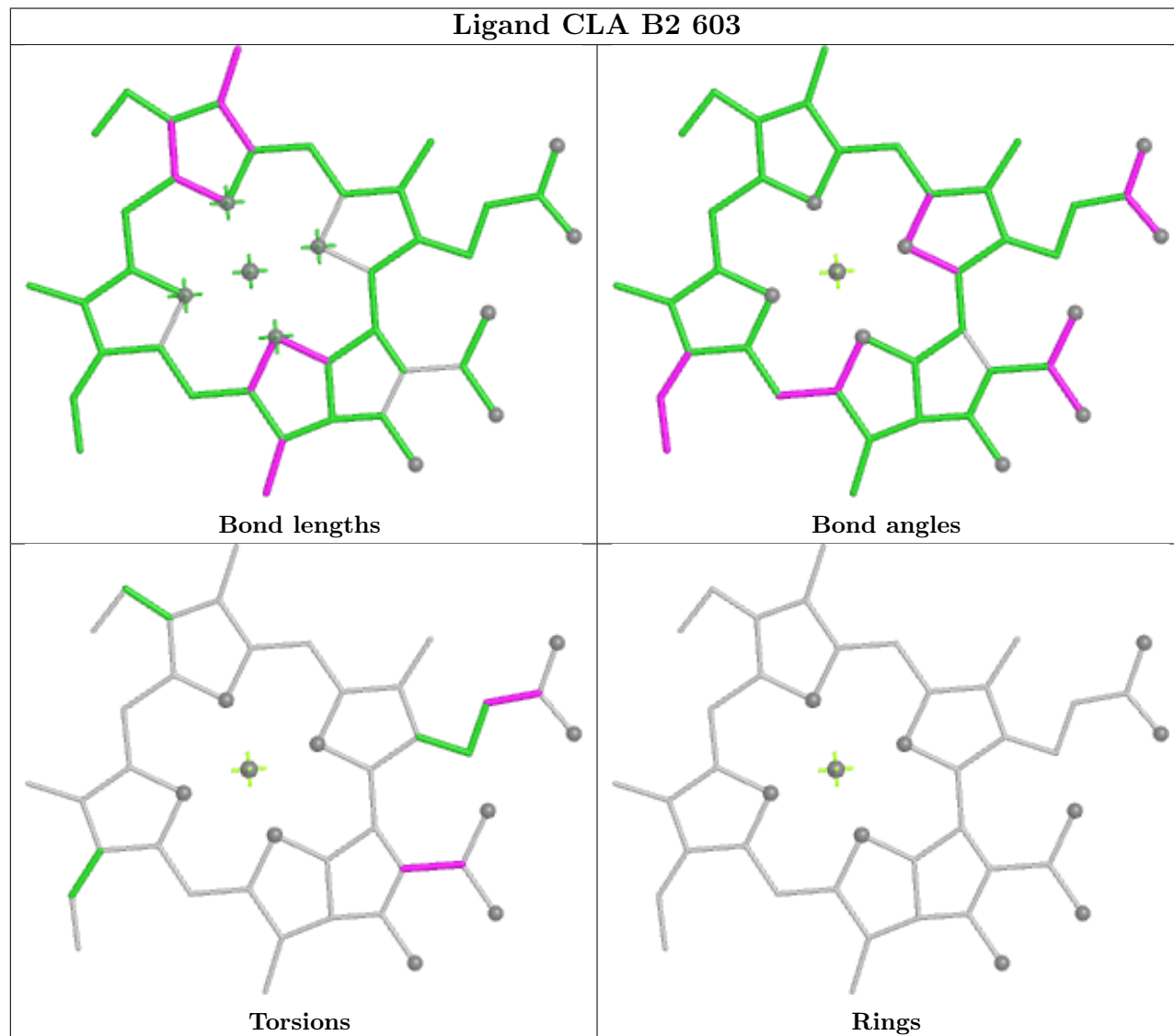




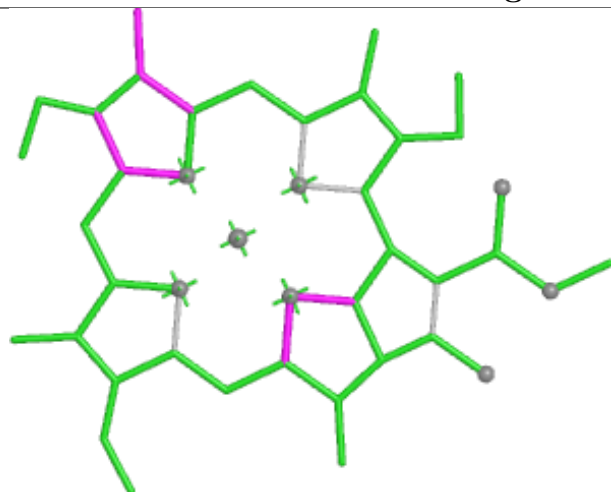
Ligand CLA BB 807



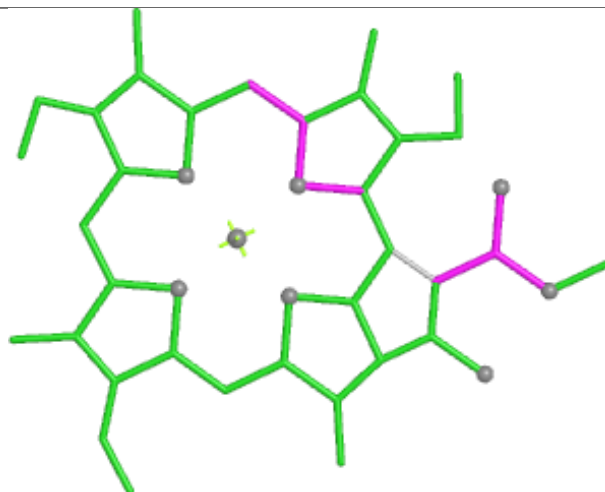
Ligand CLA B2 603



Ligand CLA A4 309



Bond lengths



Bond angles

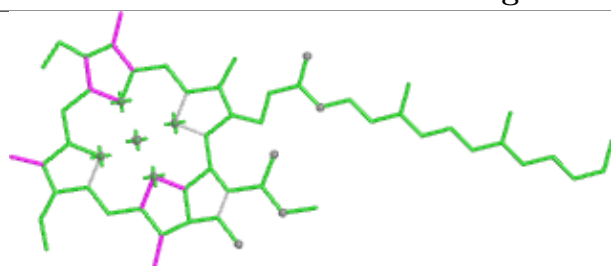


Torsions

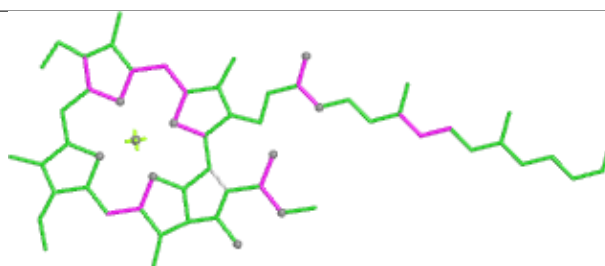


Rings

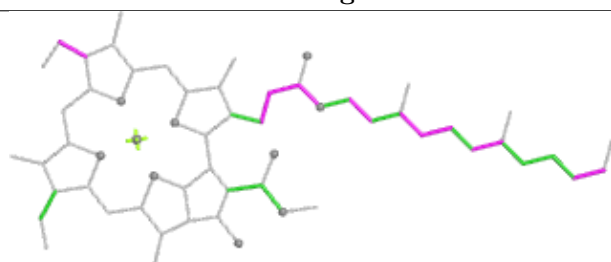
Ligand CLA BB 819



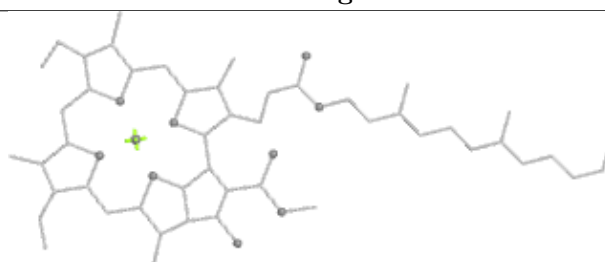
Bond lengths



Bond angles

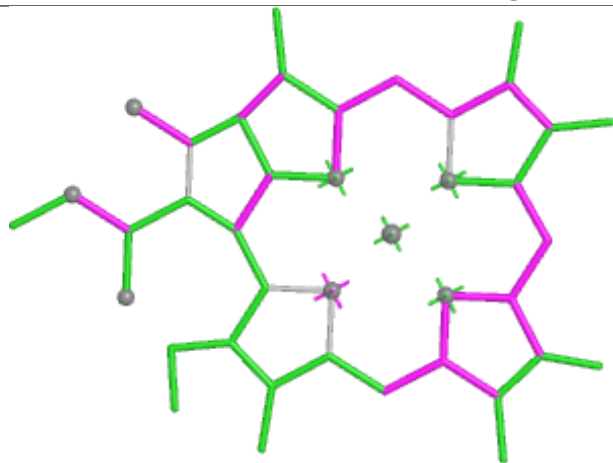


Torsions

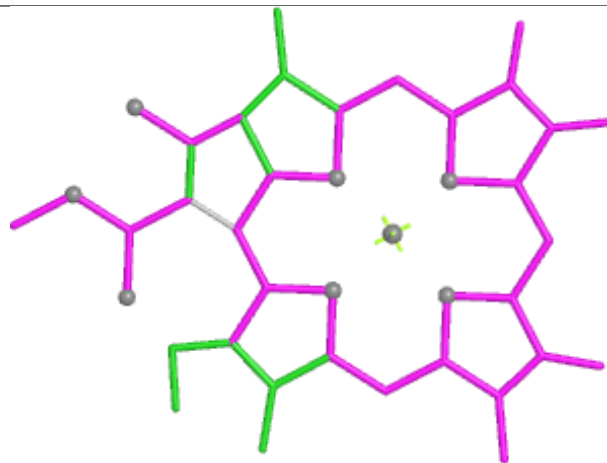


Rings

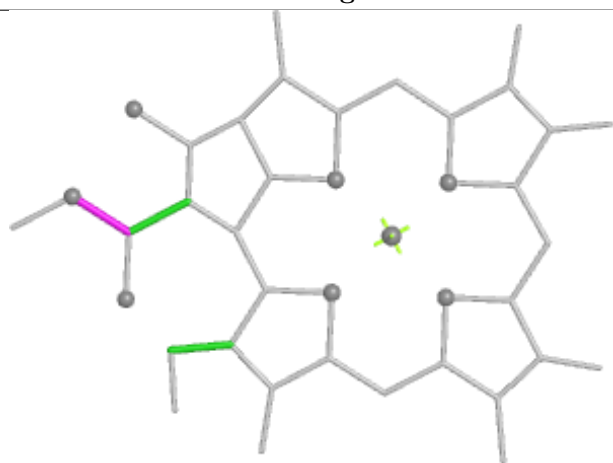
Ligand CHL B5 606



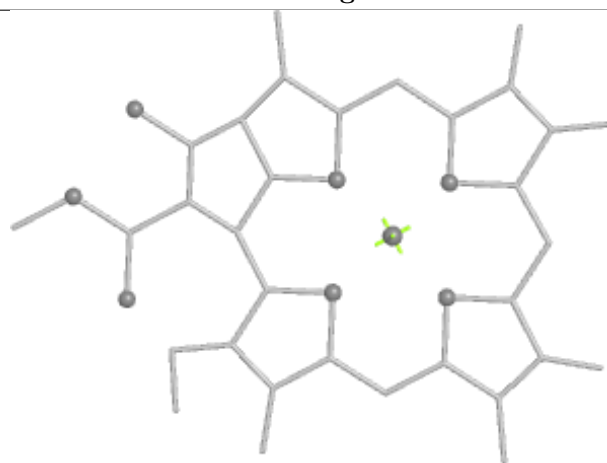
Bond lengths



Bond angles

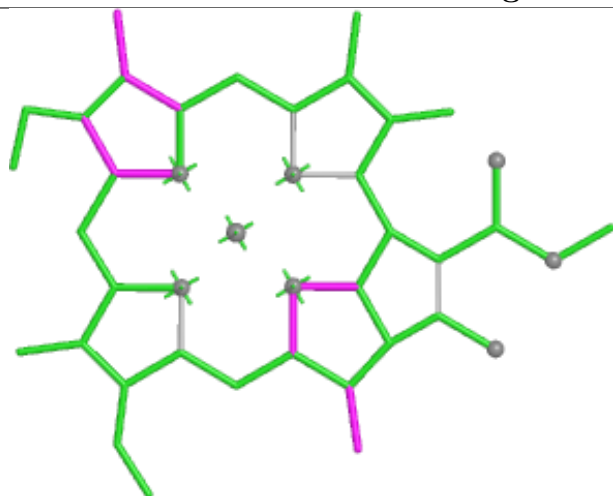


Torsions



Rings

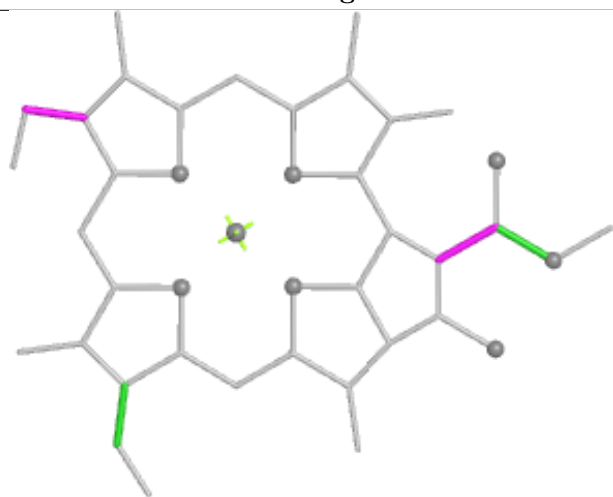
Ligand CLA AF 804



Bond lengths



Bond angles

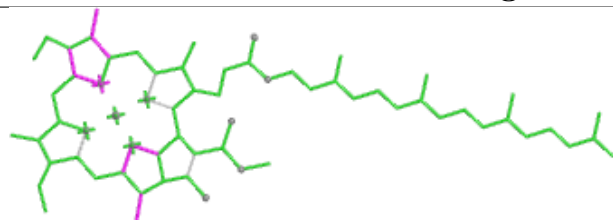


Torsions

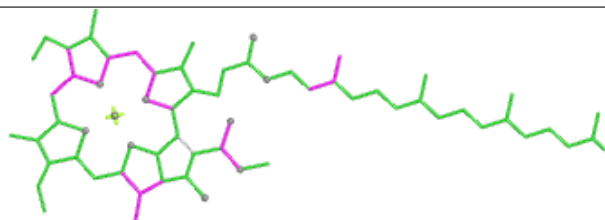


Rings

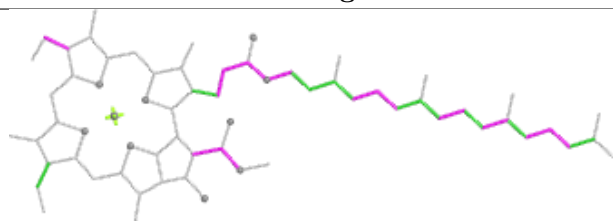
Ligand CLA AA 833



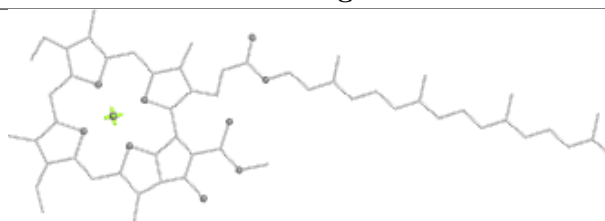
Bond lengths



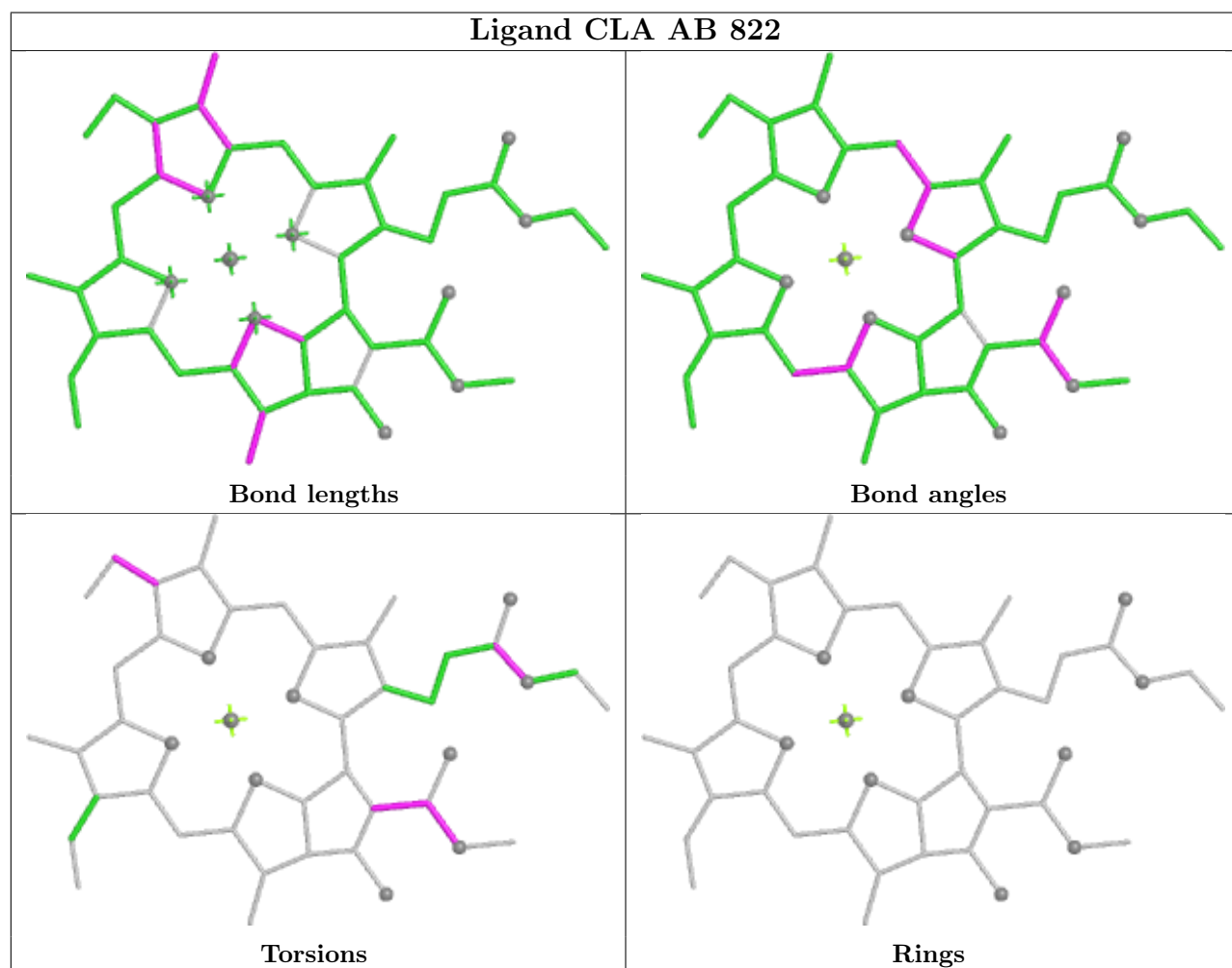
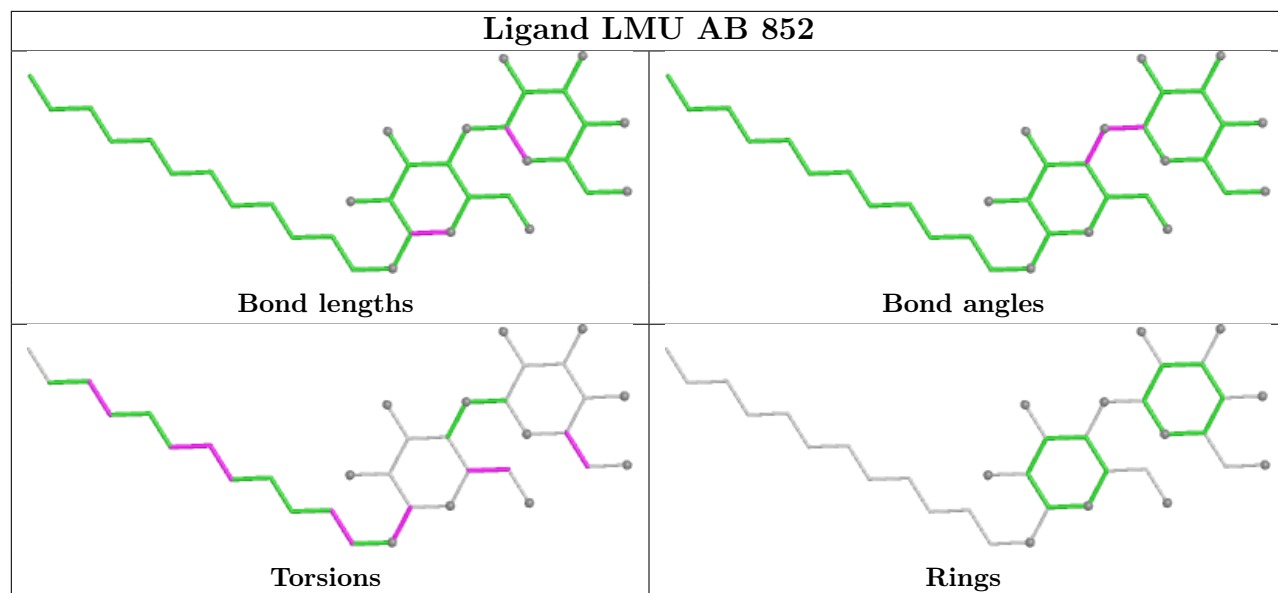
Bond angles

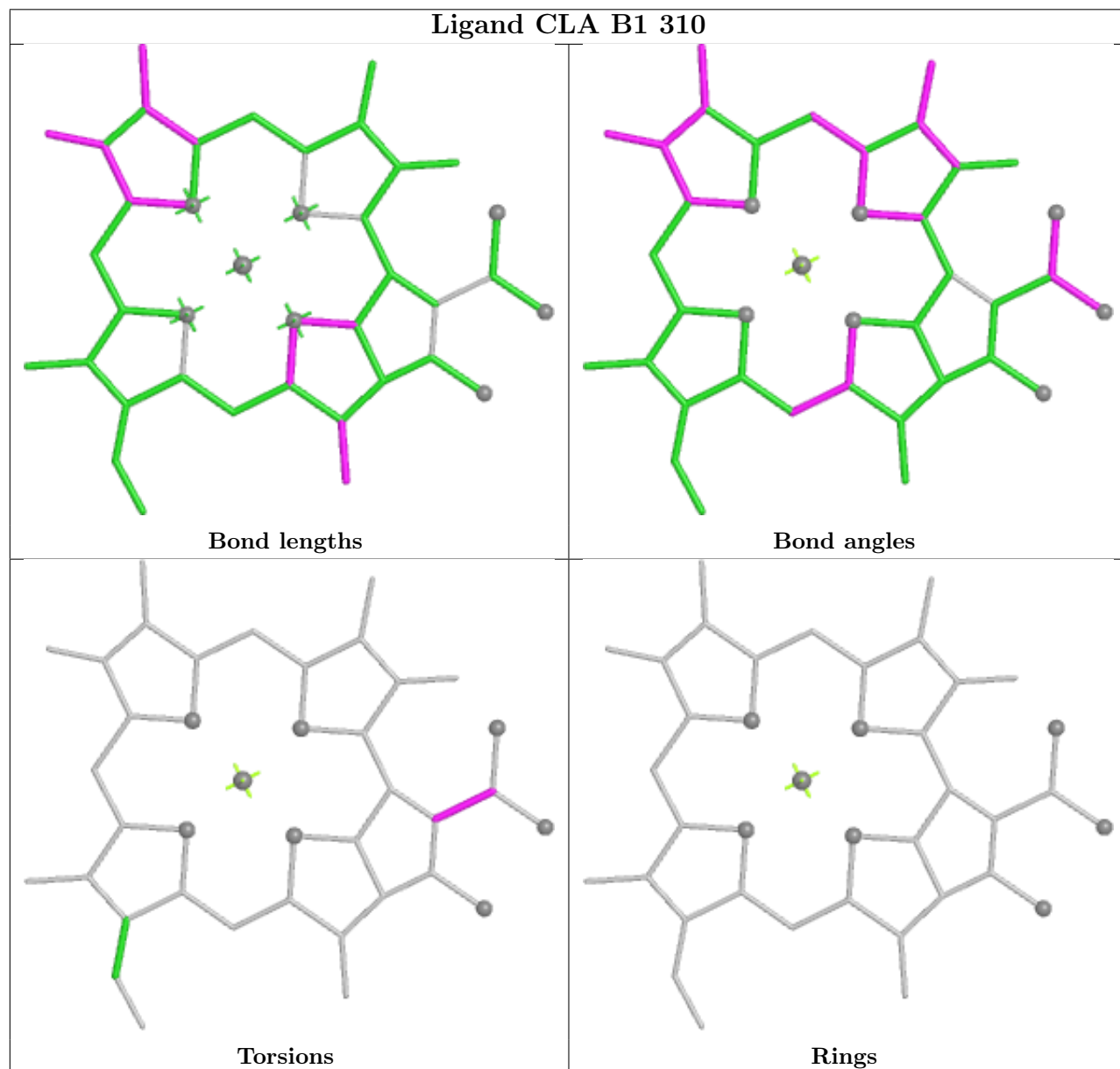
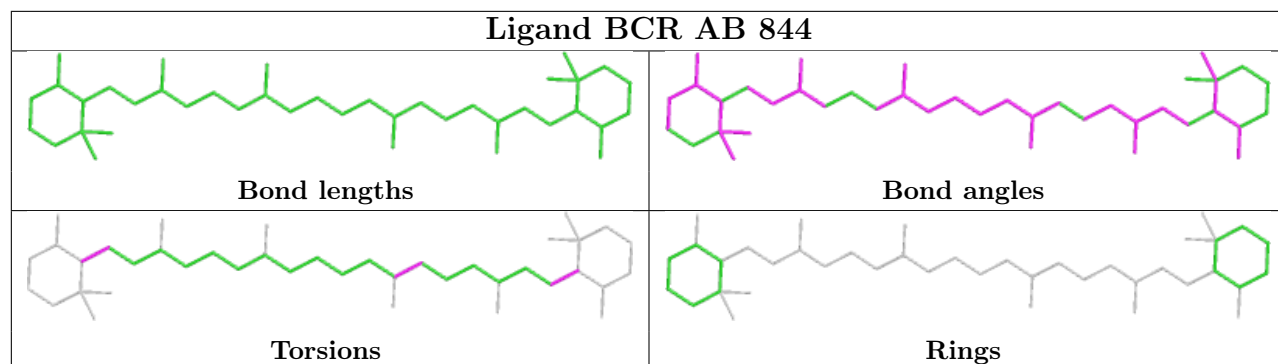


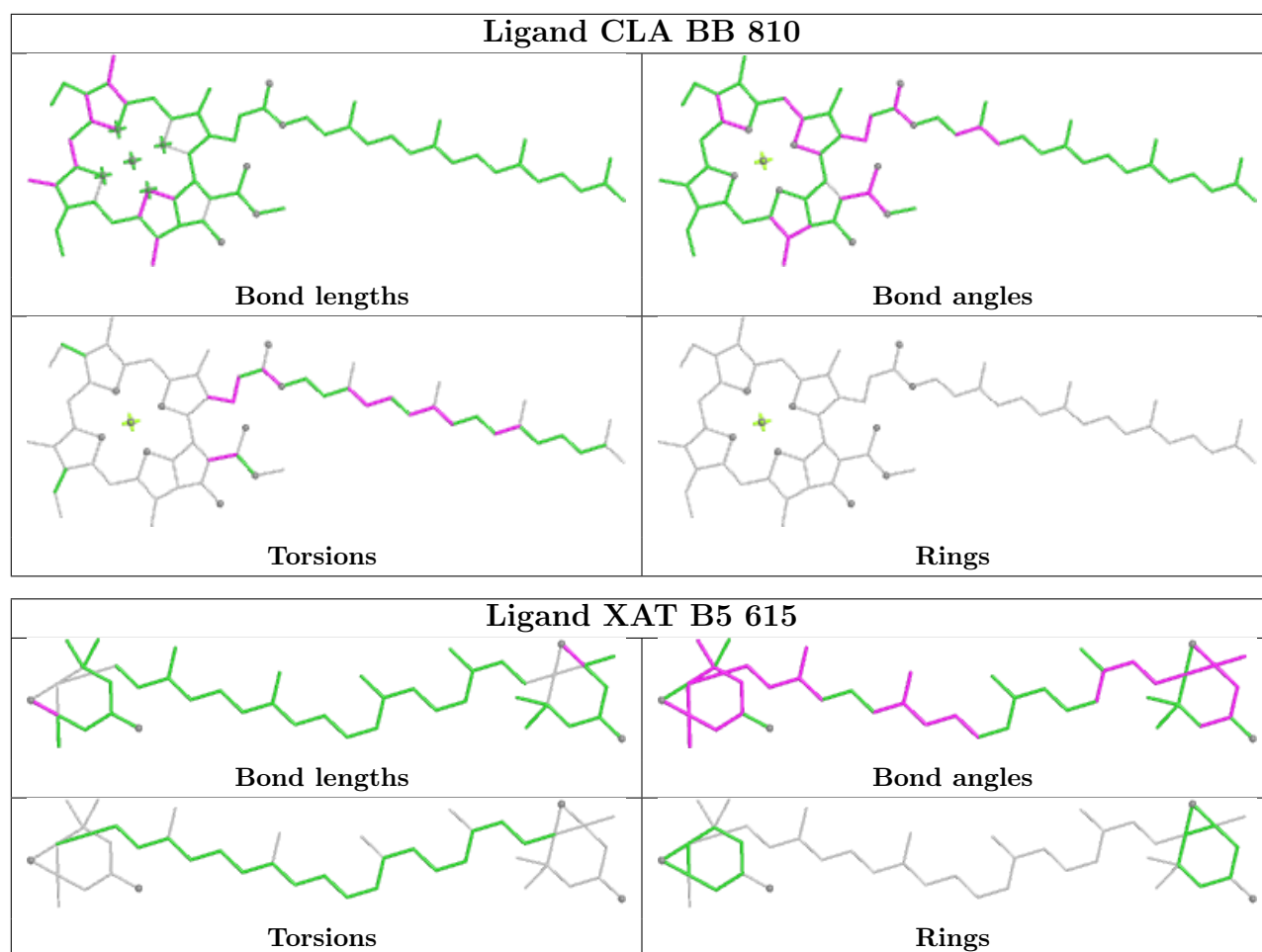
Torsions



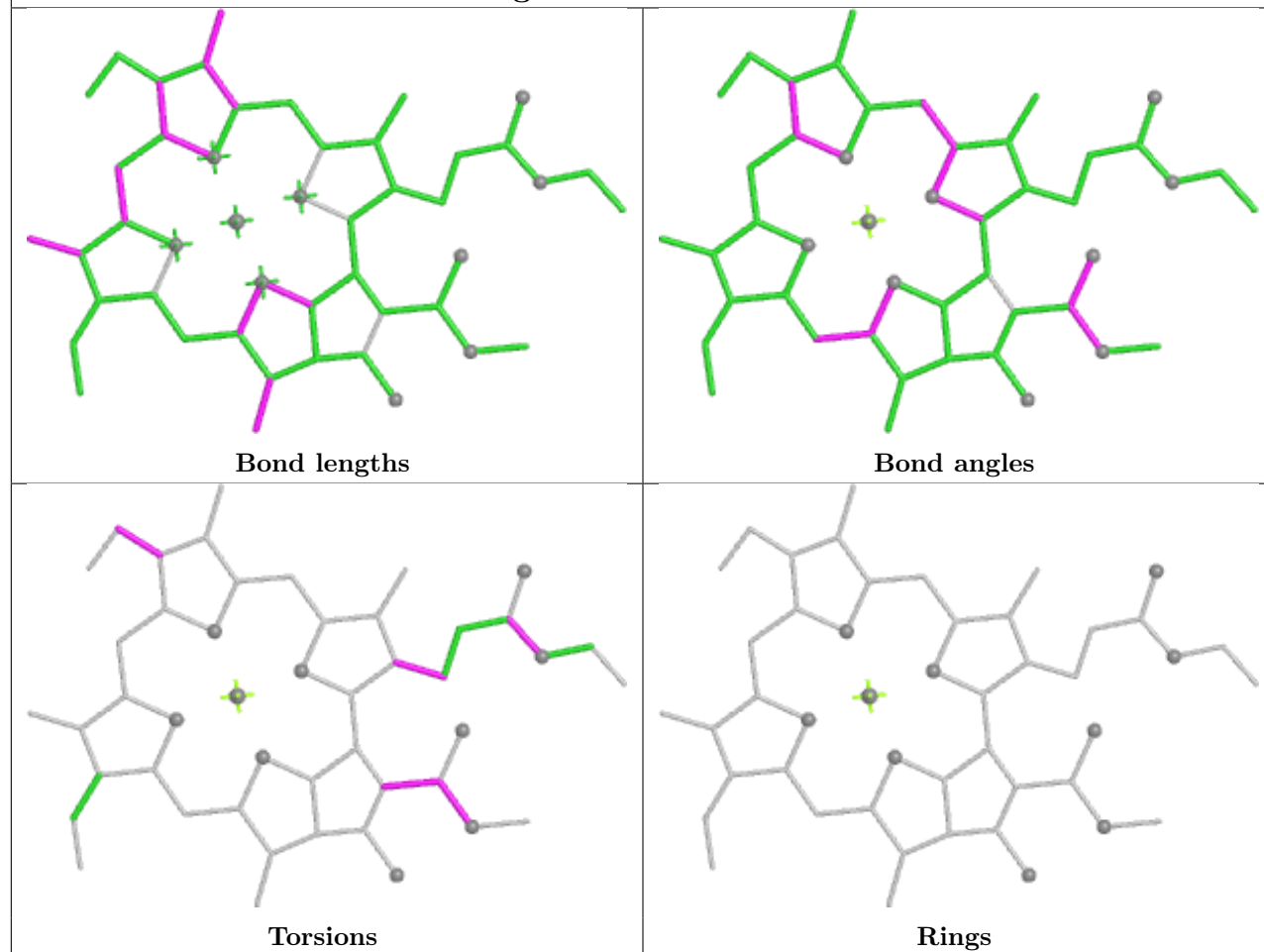
Rings



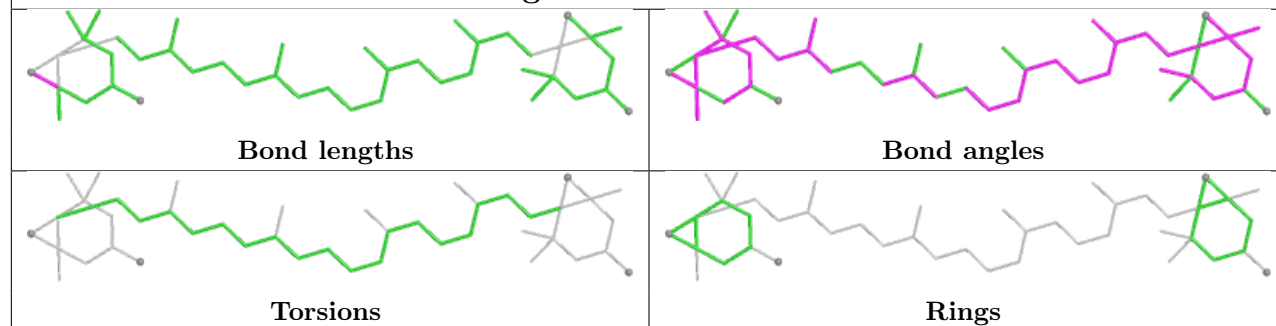


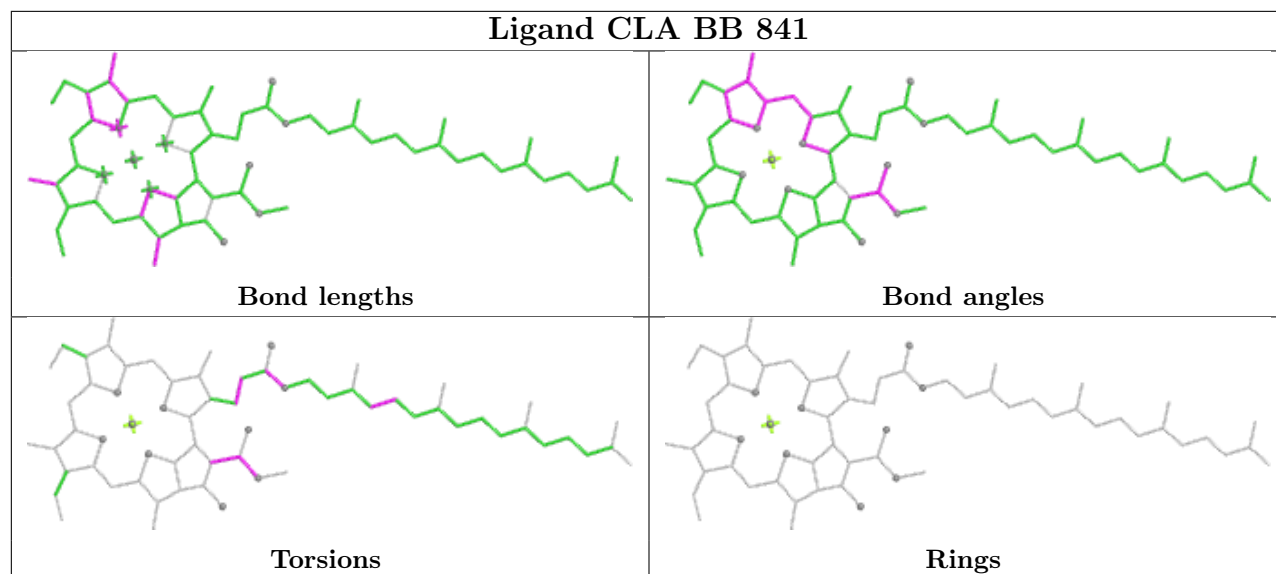
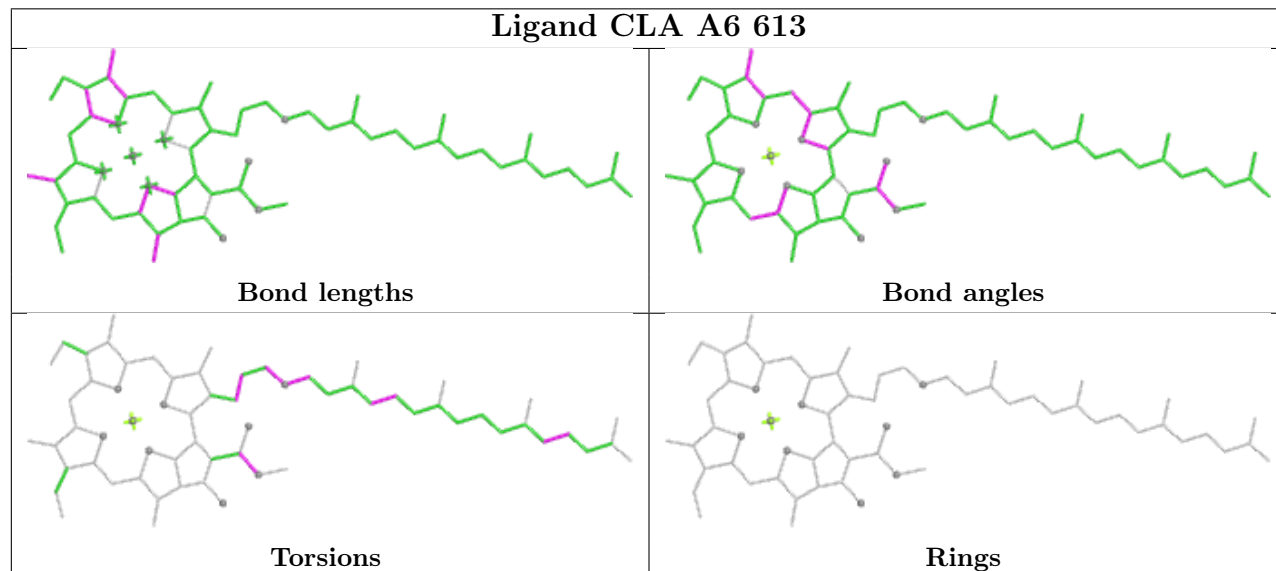


Ligand CLA AA 831

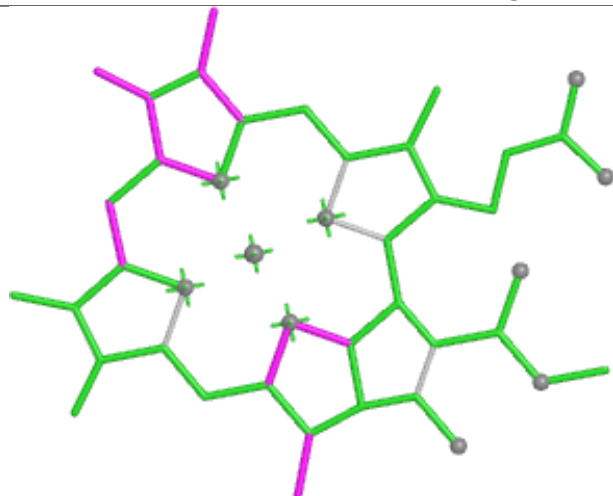


Ligand XAT B3 316

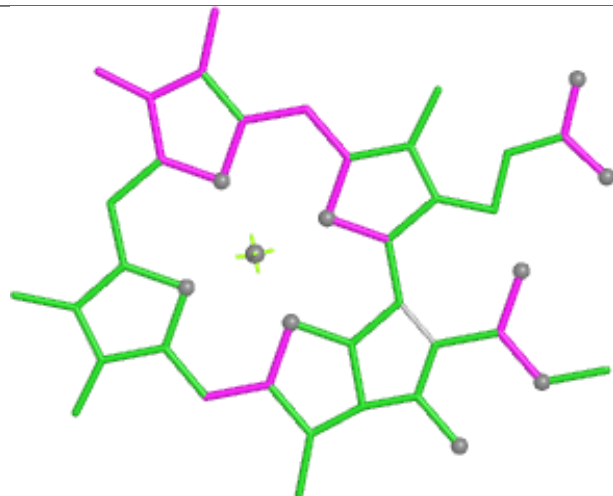


Ligand CLA BB 841**Ligand CLA A6 613**

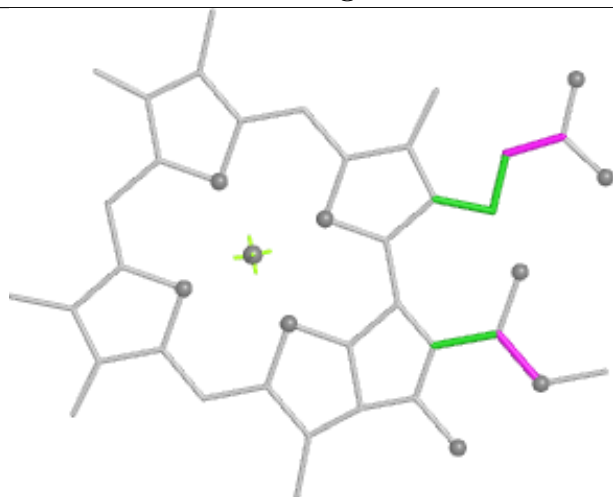
Ligand CLA B5 604



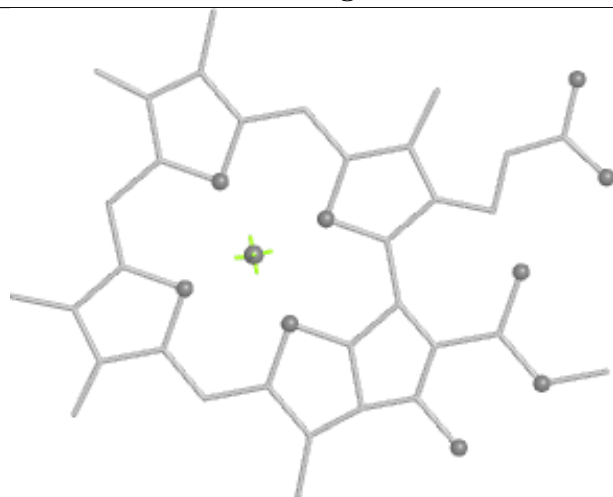
Bond lengths



Bond angles

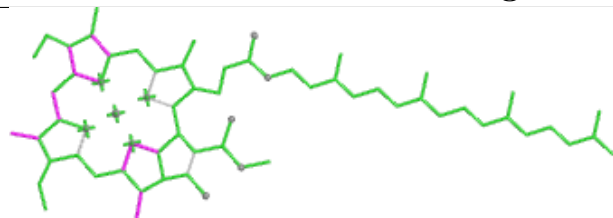


Torsions

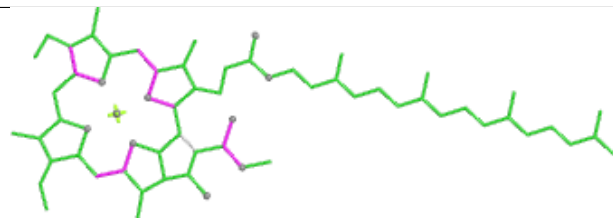


Rings

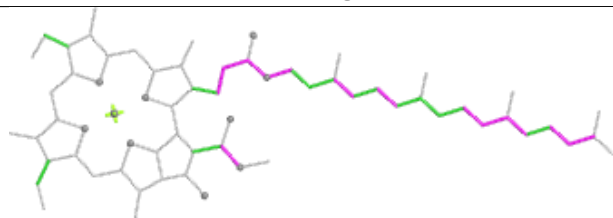
Ligand CLA BA 806



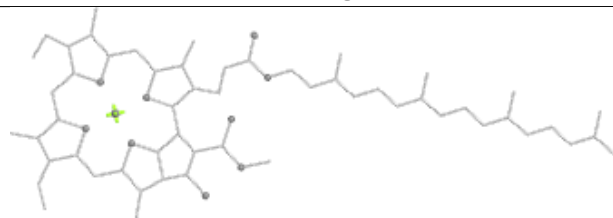
Bond lengths



Bond angles

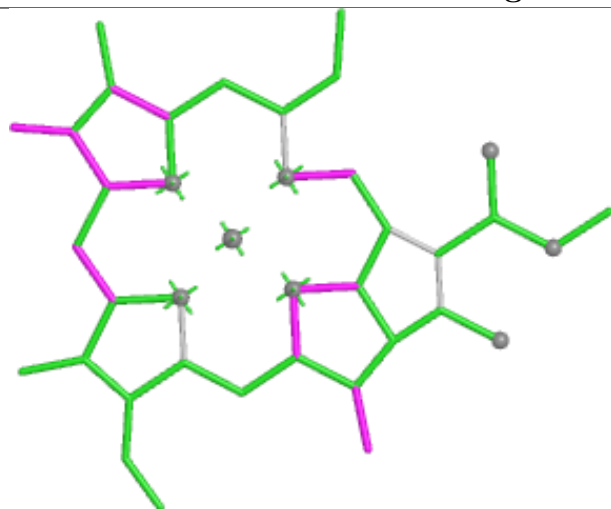


Torsions

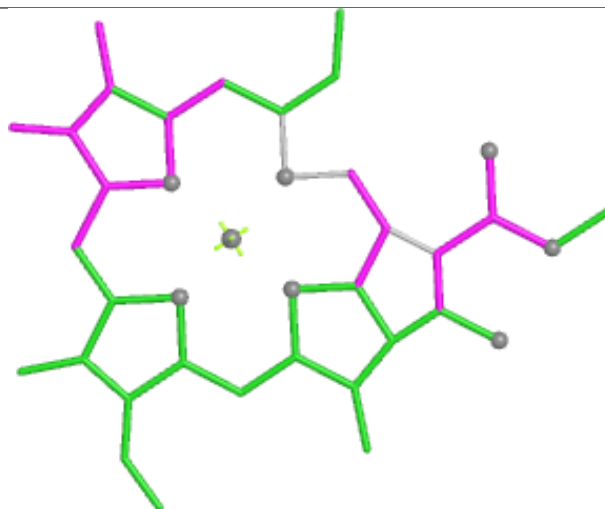


Rings

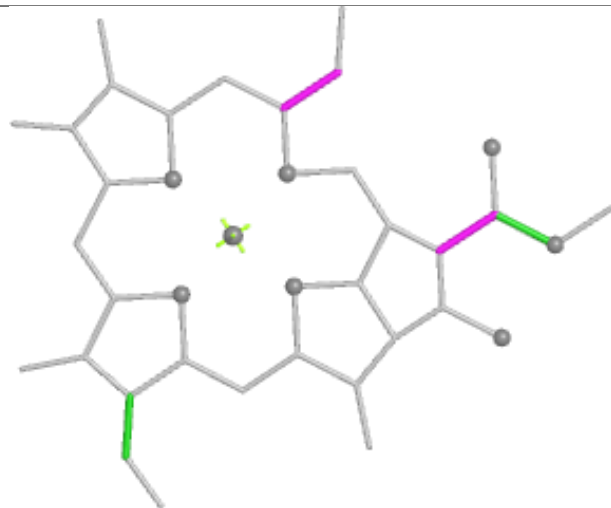
Ligand CLA A6 611



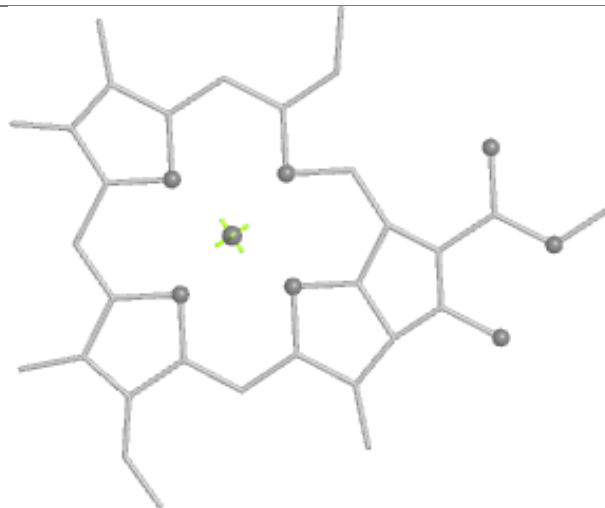
Bond lengths



Bond angles

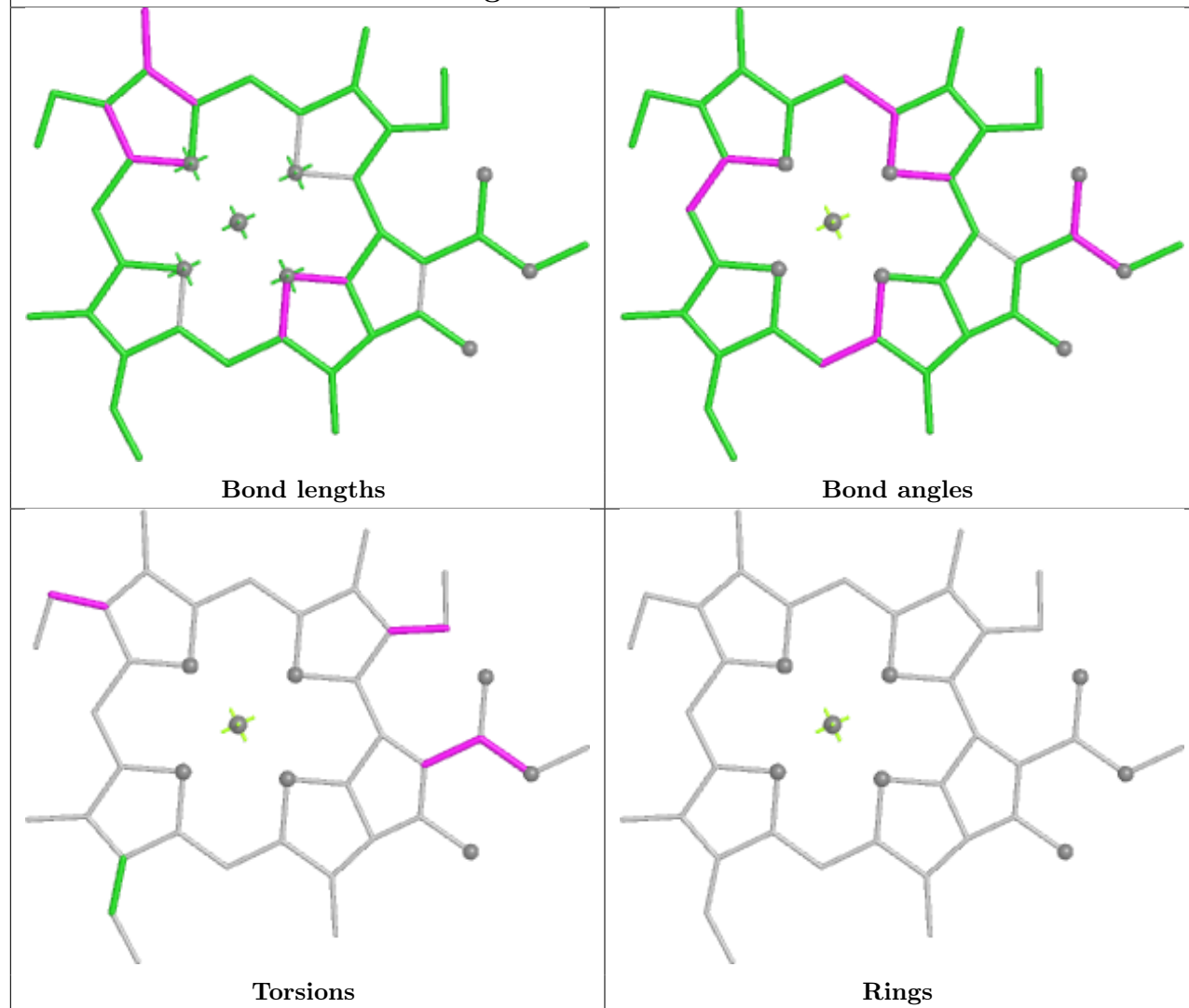


Torsions

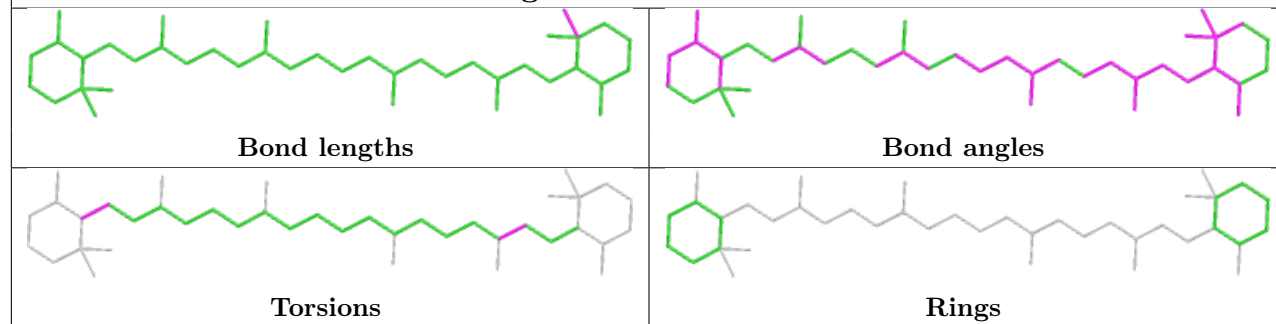


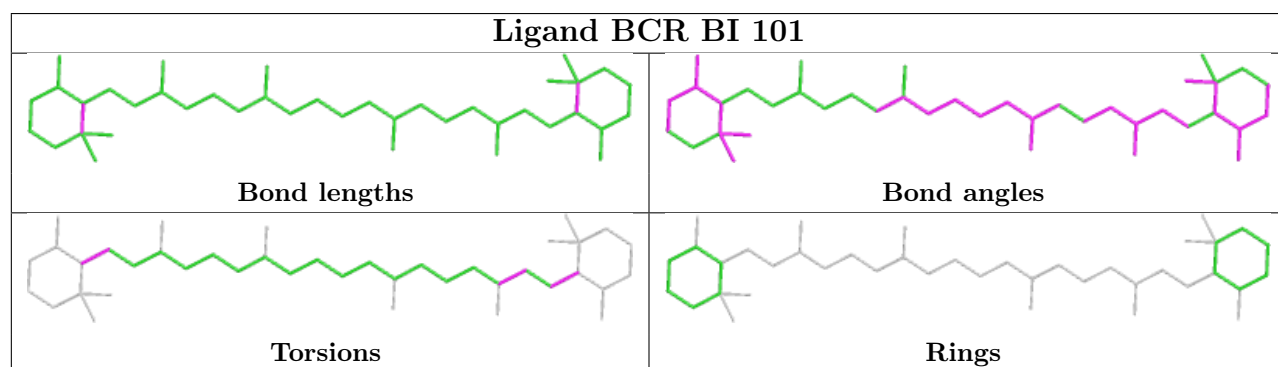
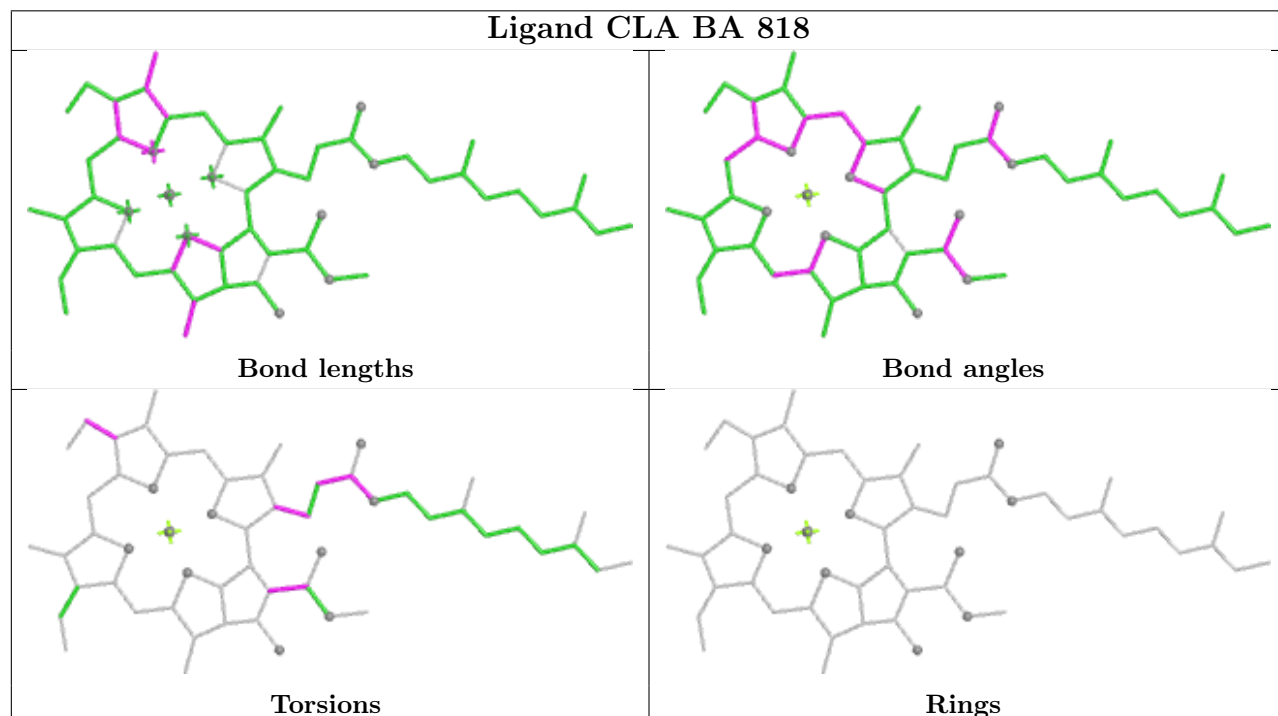
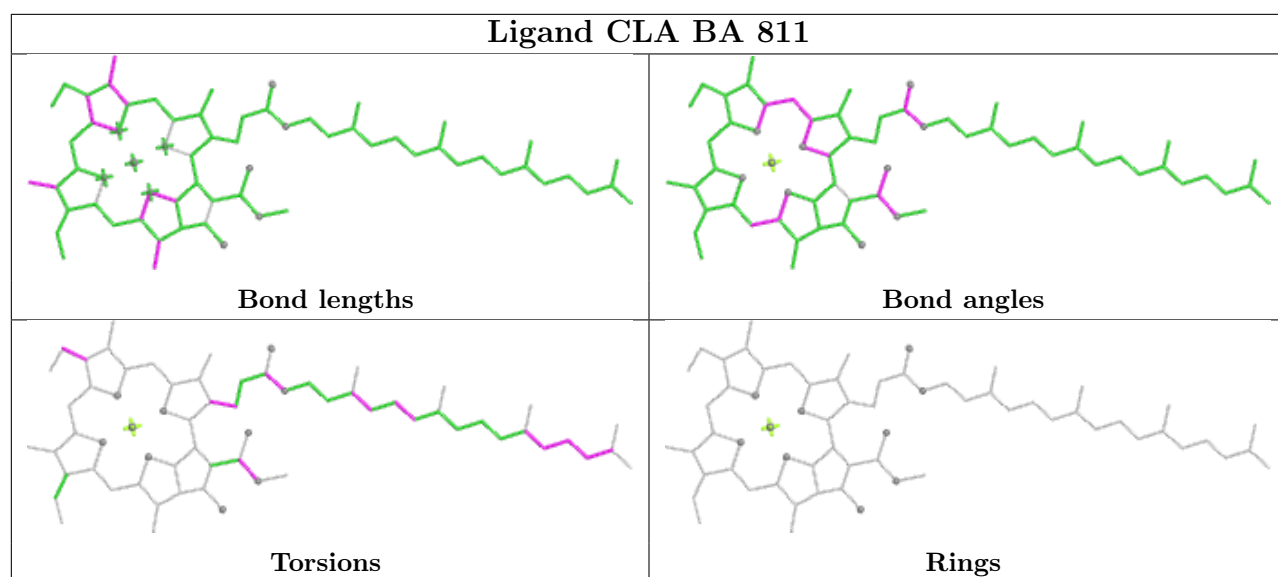
Rings

Ligand CLA BB 837

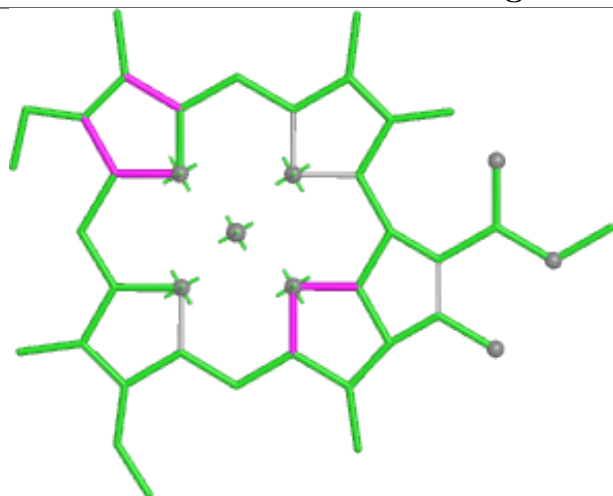


Ligand BCR A1 319





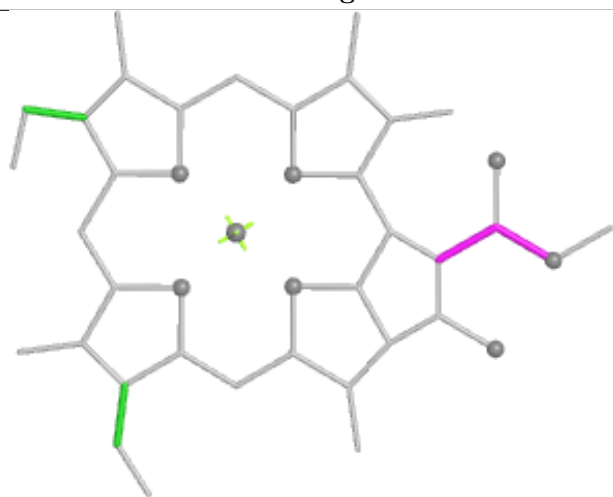
Ligand CLA B1 306



Bond lengths



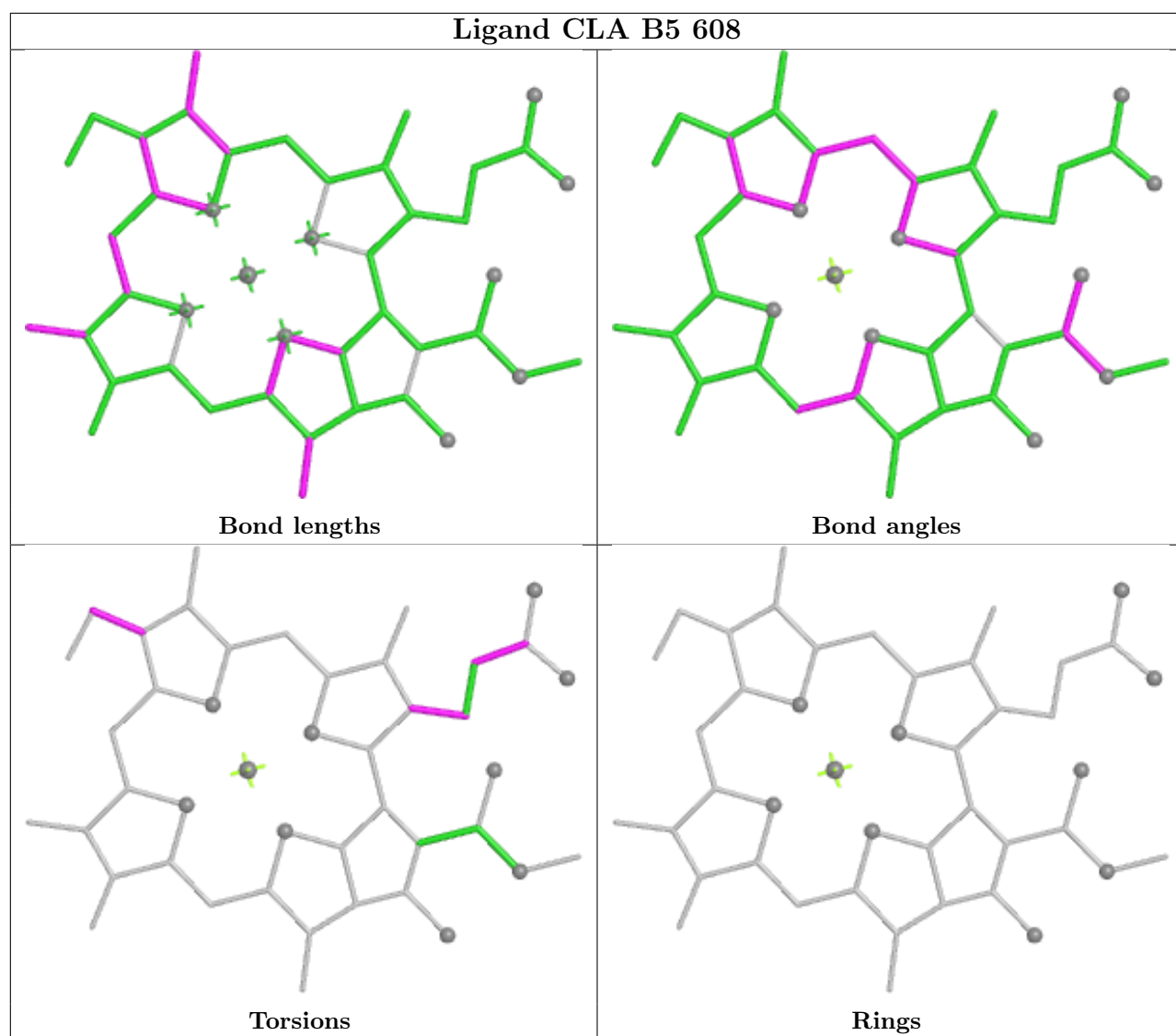
Bond angles

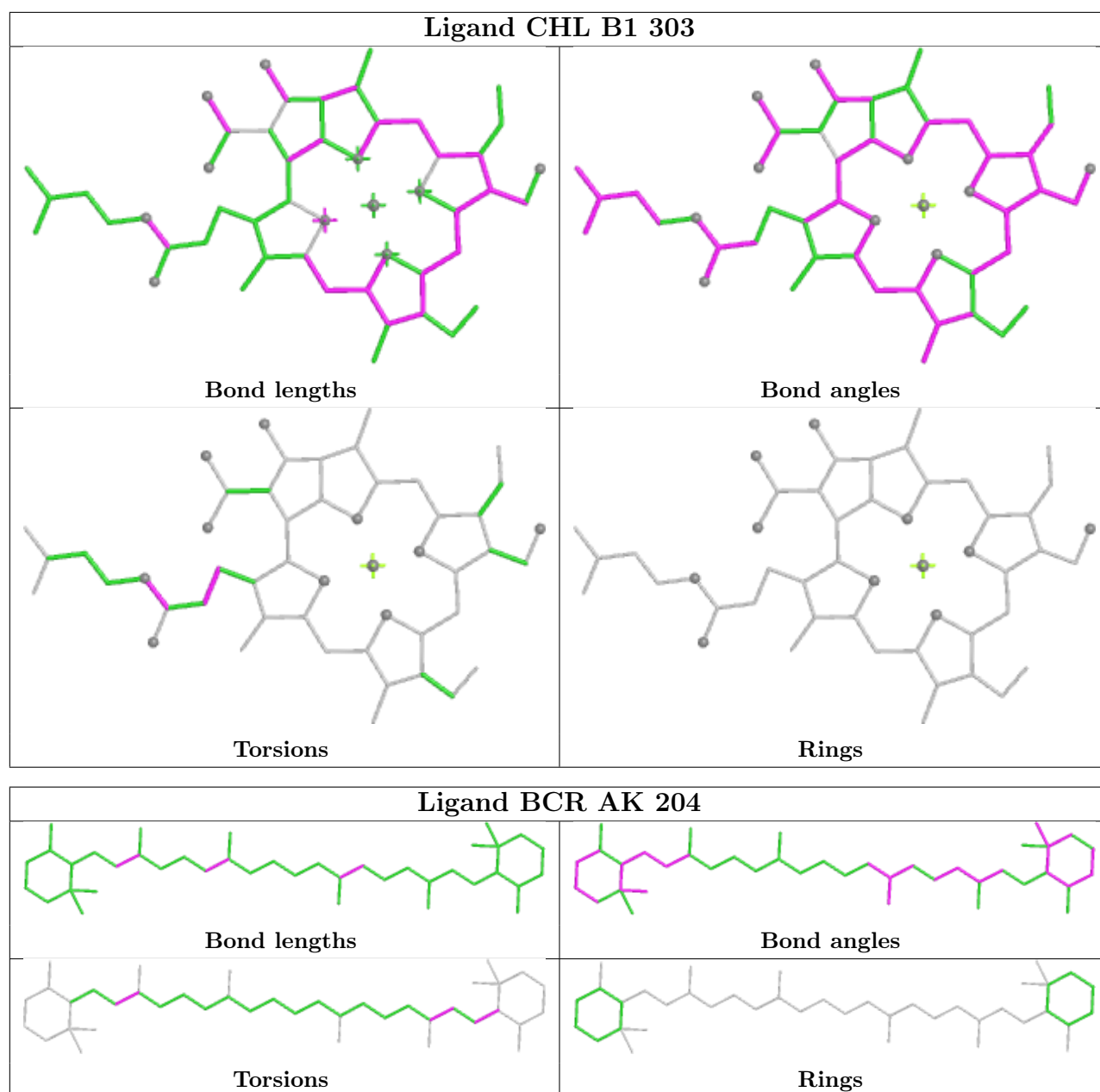


Torsions

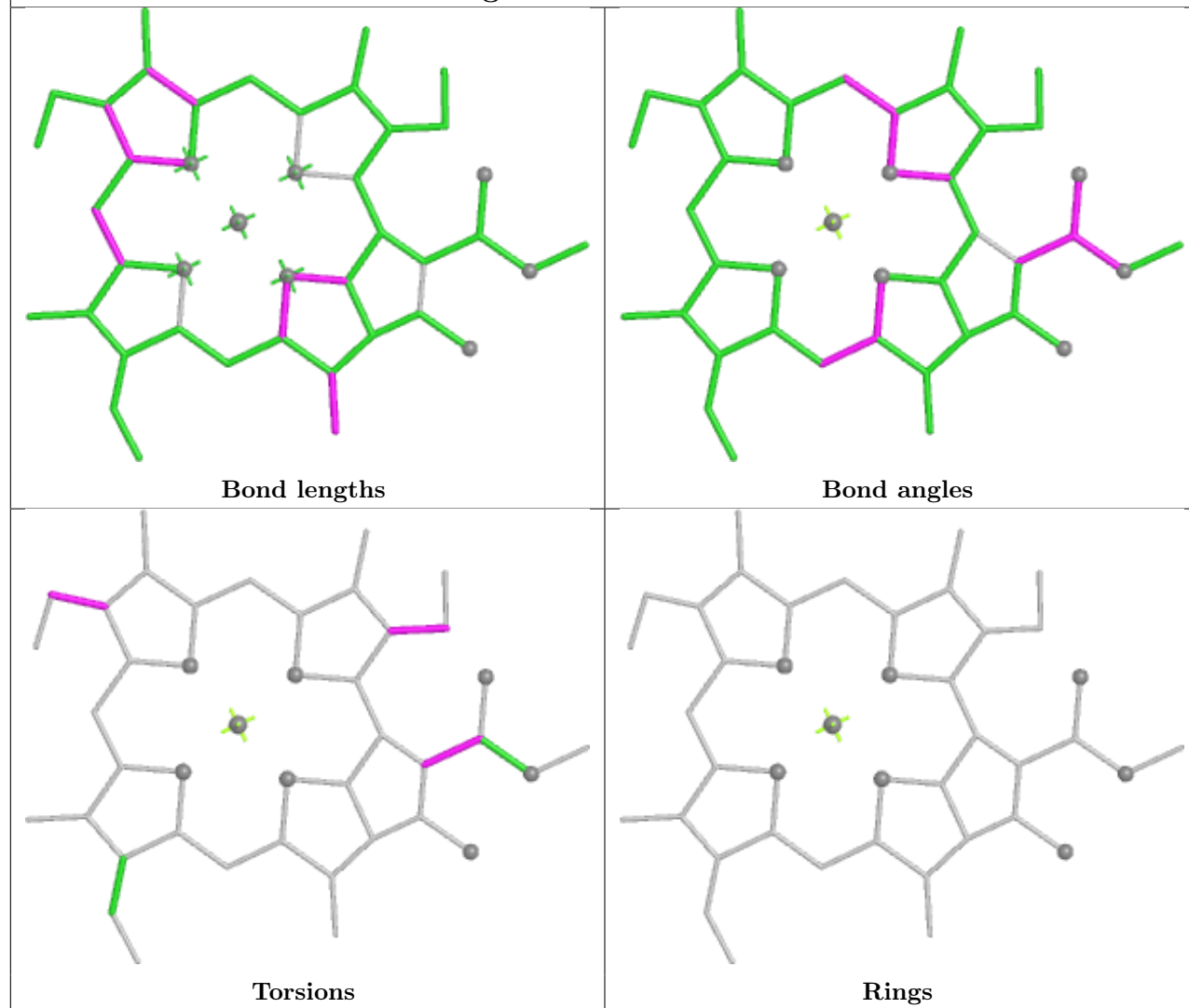


Rings

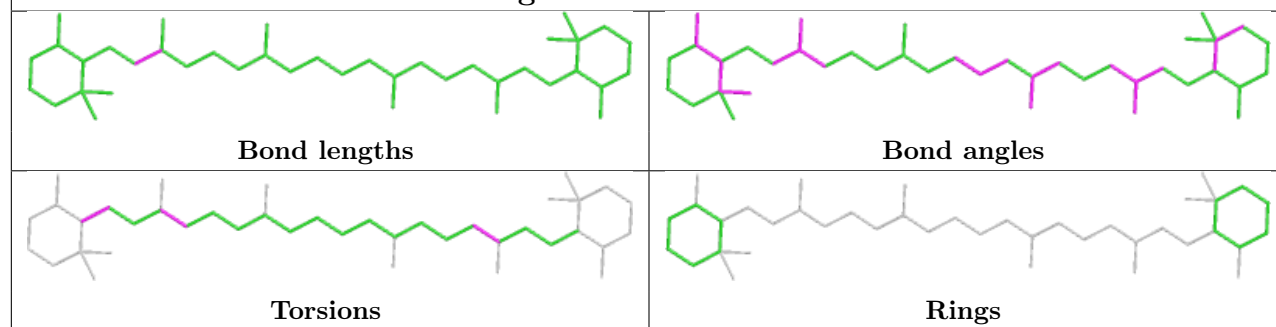


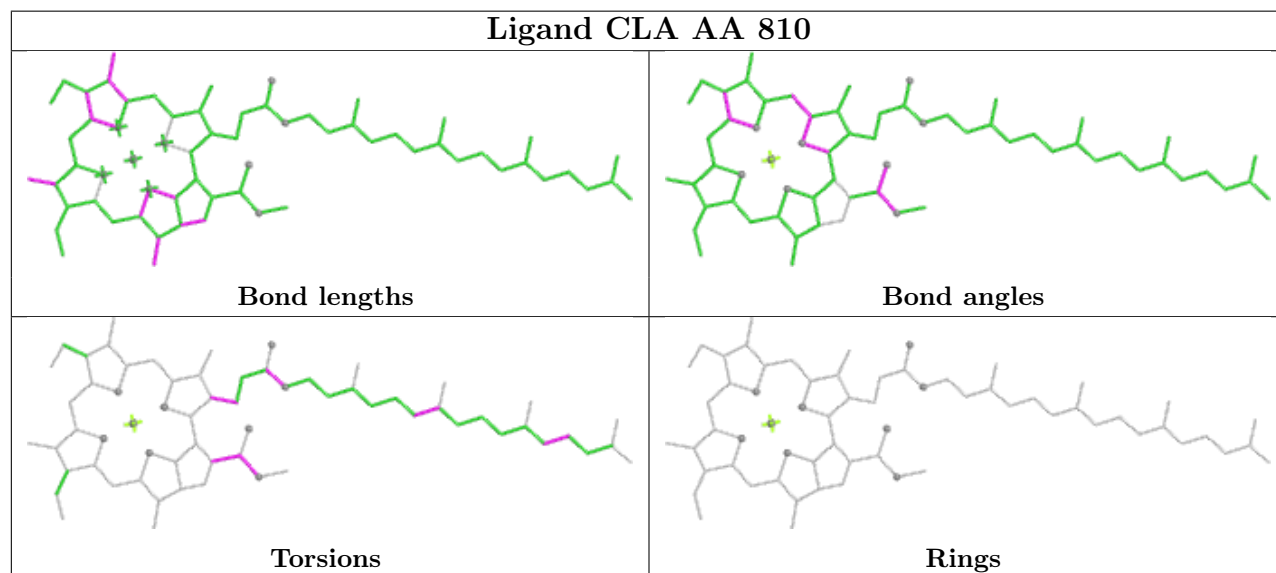
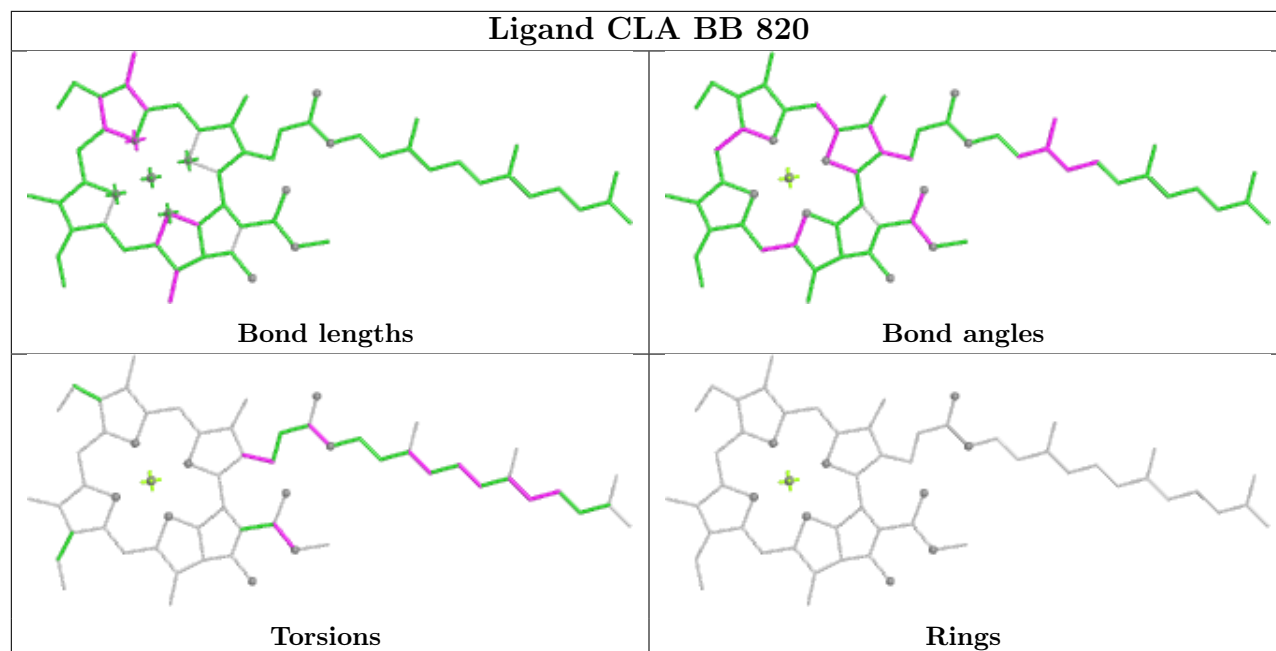


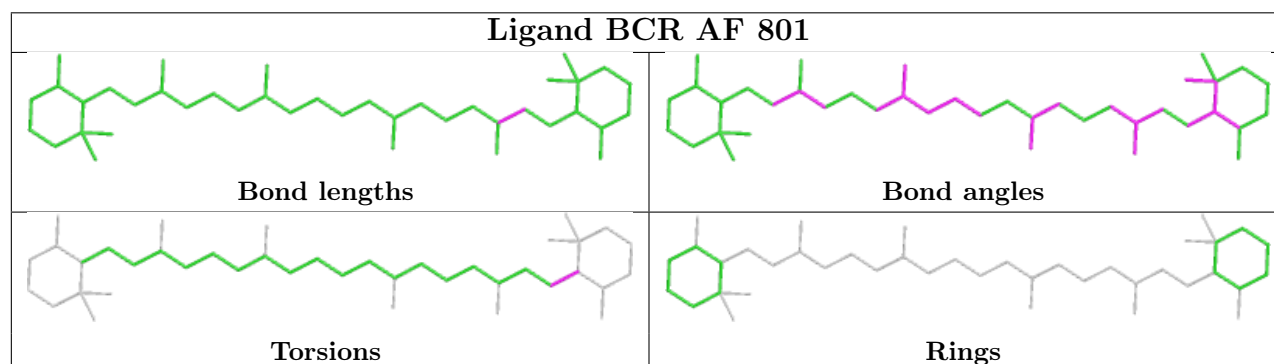
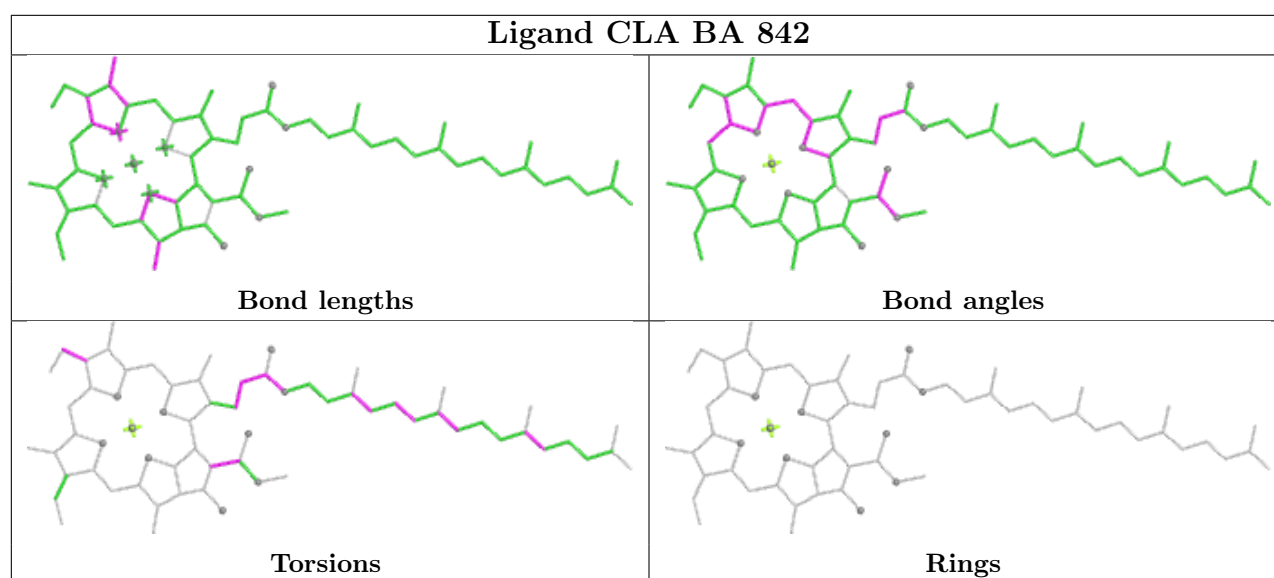
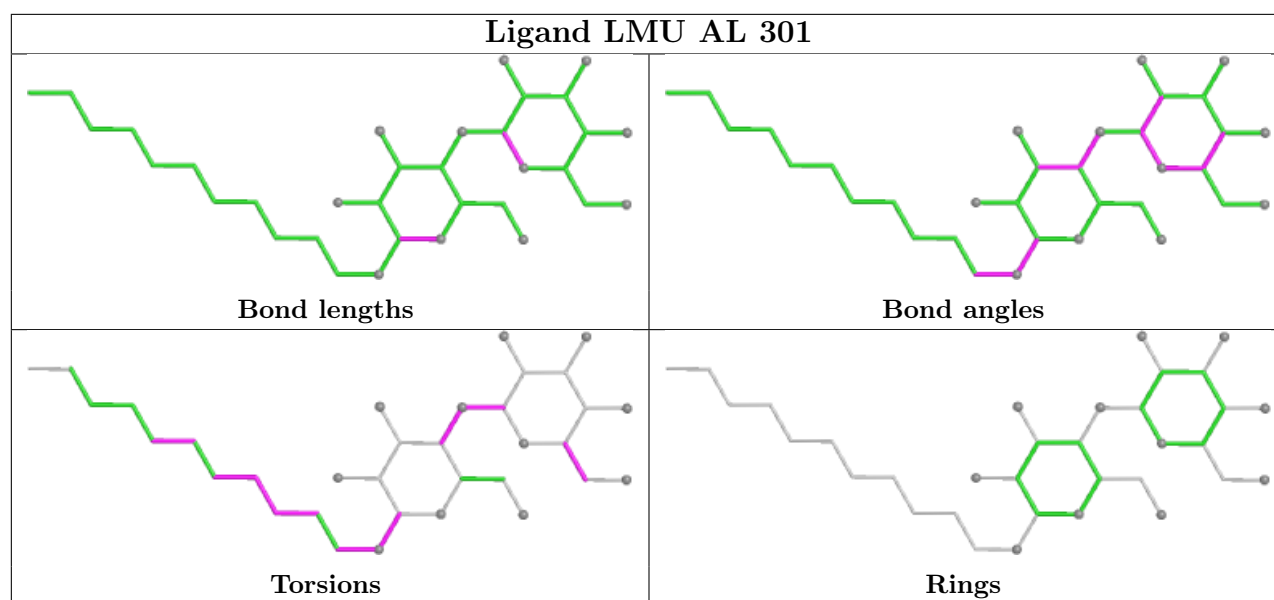
Ligand CLA AA 822



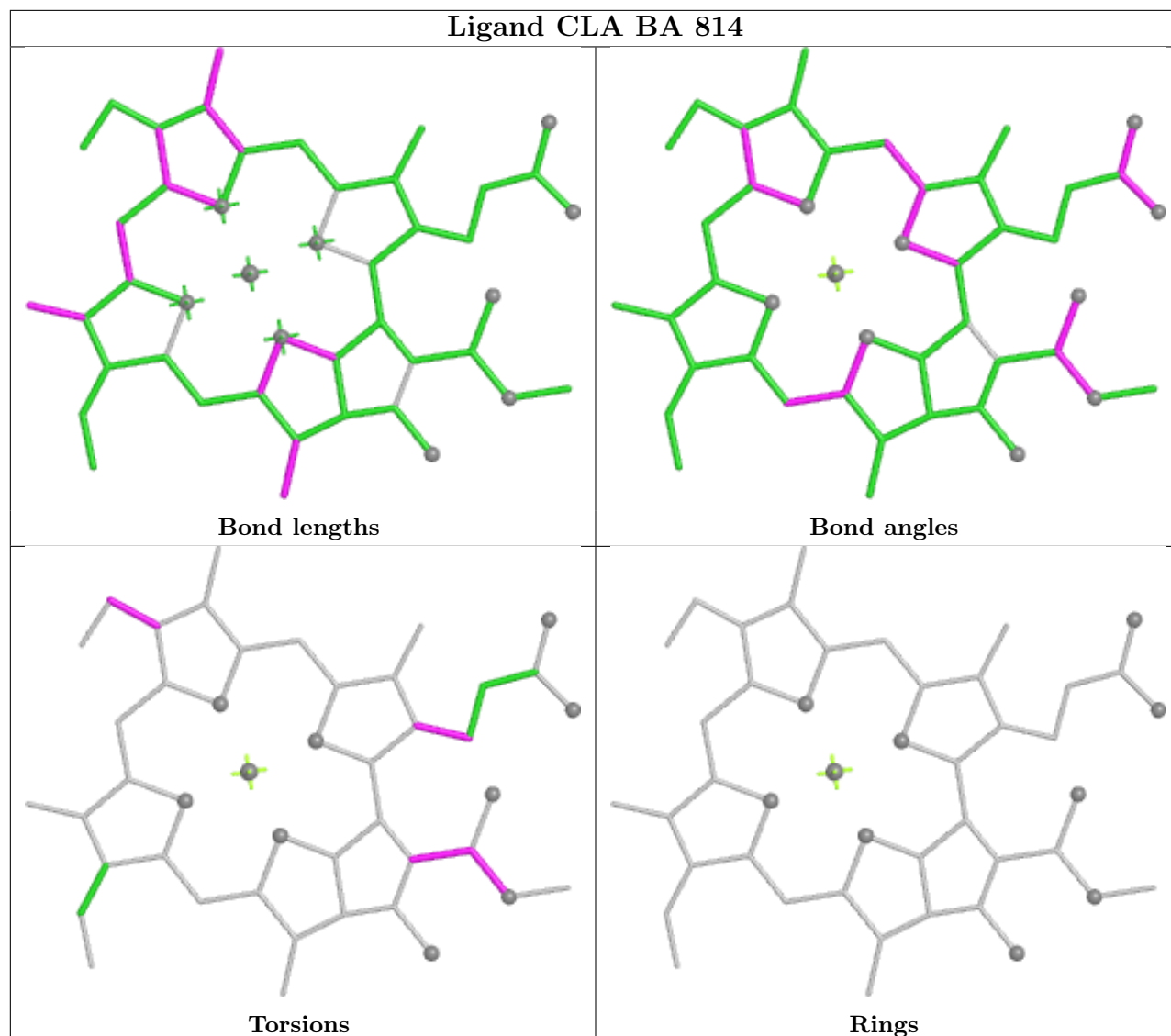
Ligand BCR BB 847



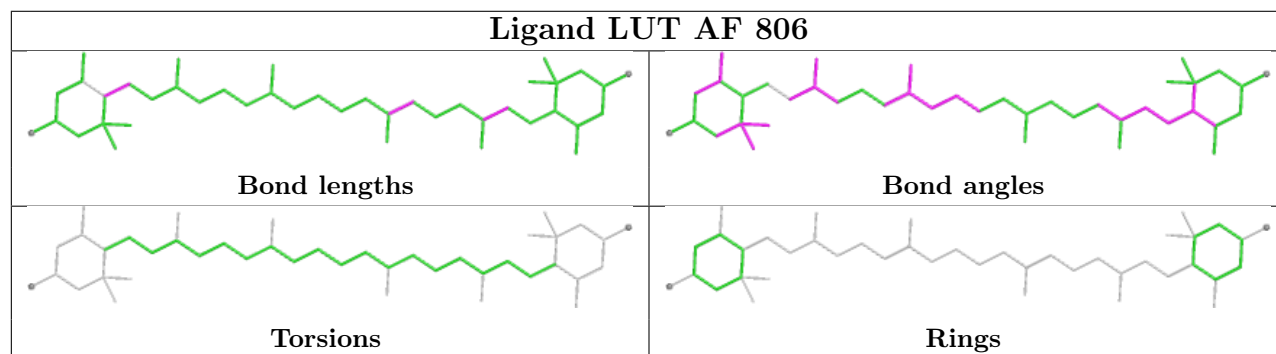


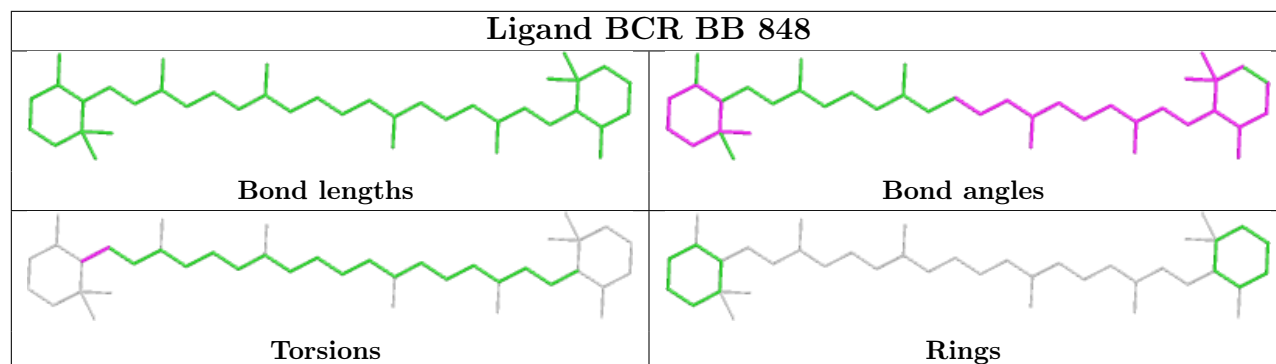
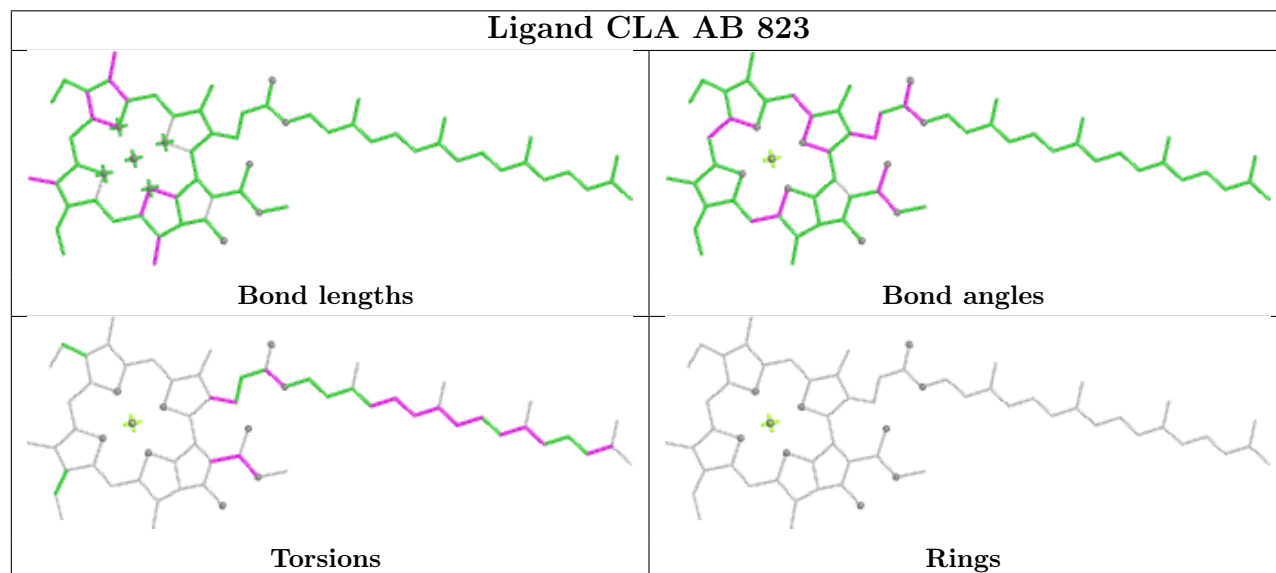
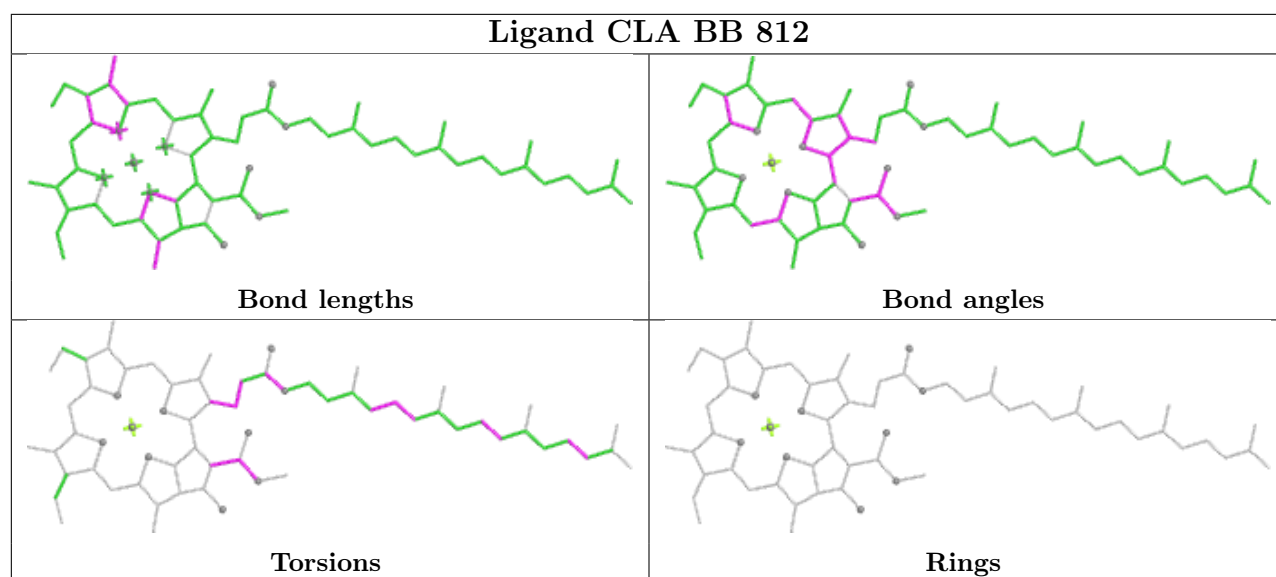


Ligand CLA BA 814

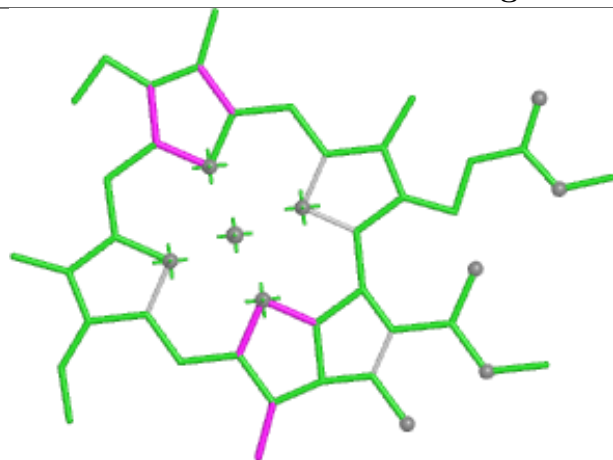


Ligand LUT AF 806

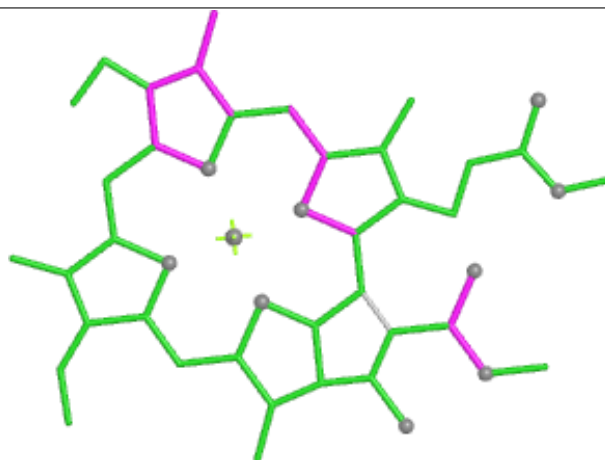




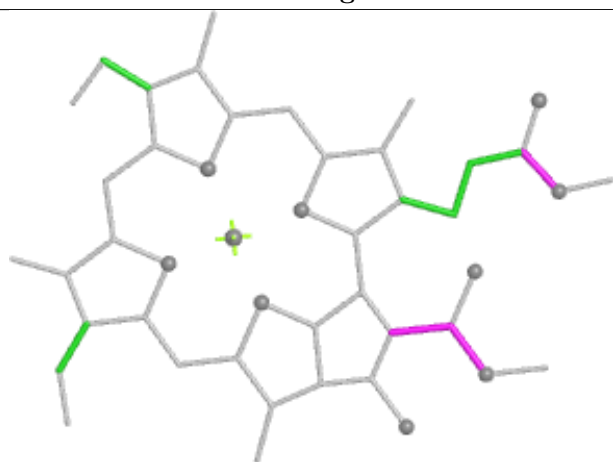
Ligand CLA BK 203



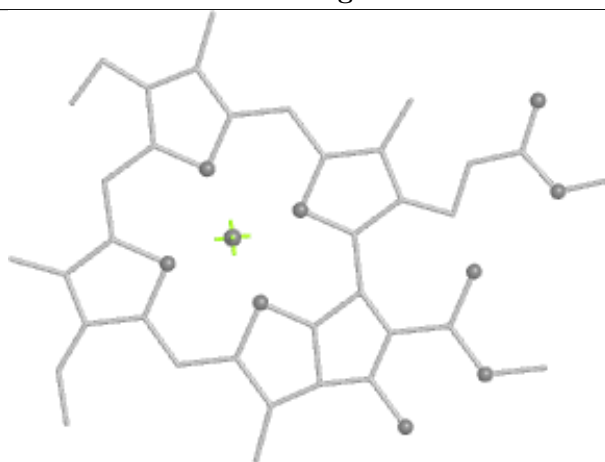
Bond lengths



Bond angles

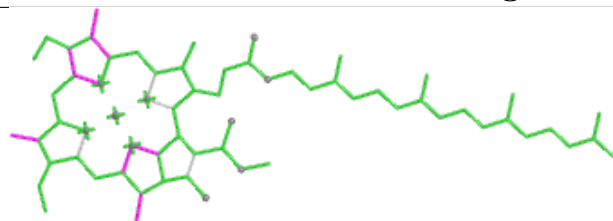


Torsions

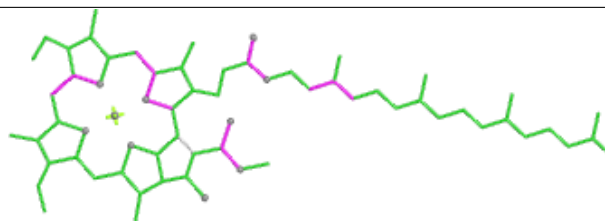


Rings

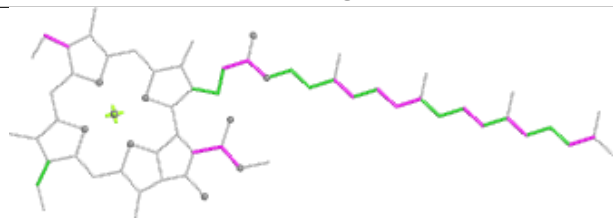
Ligand CLA BB 804



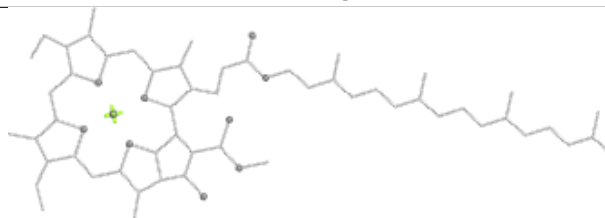
Bond lengths



Bond angles

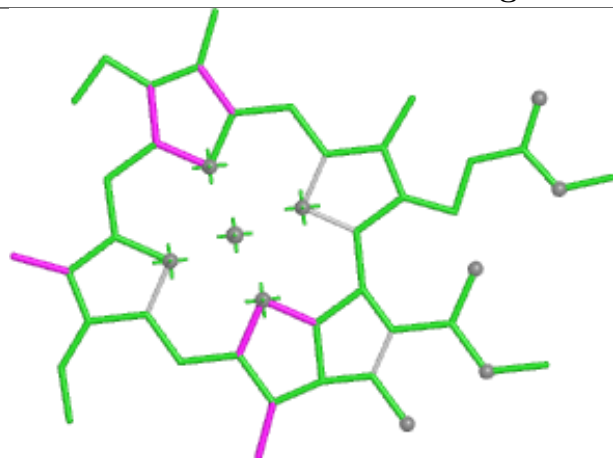


Torsions

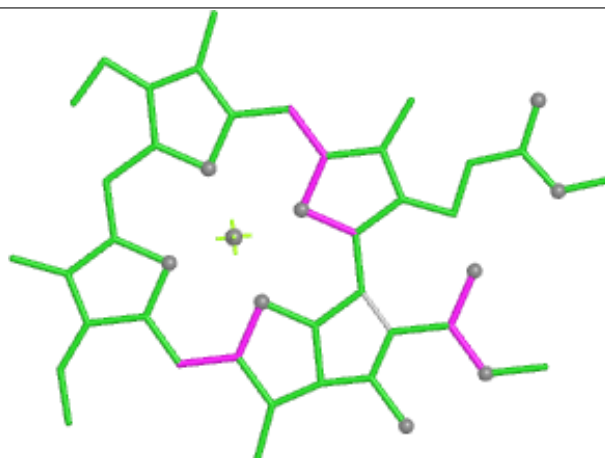


Rings

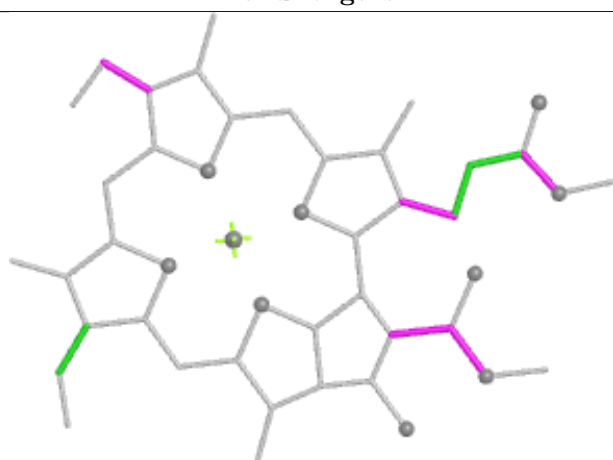
Ligand CLA AK 203



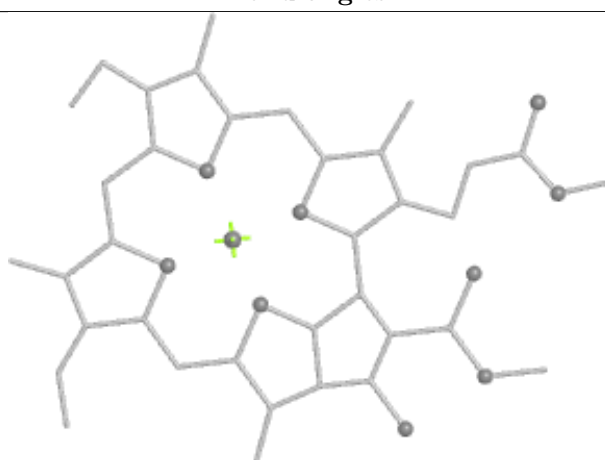
Bond lengths



Bond angles

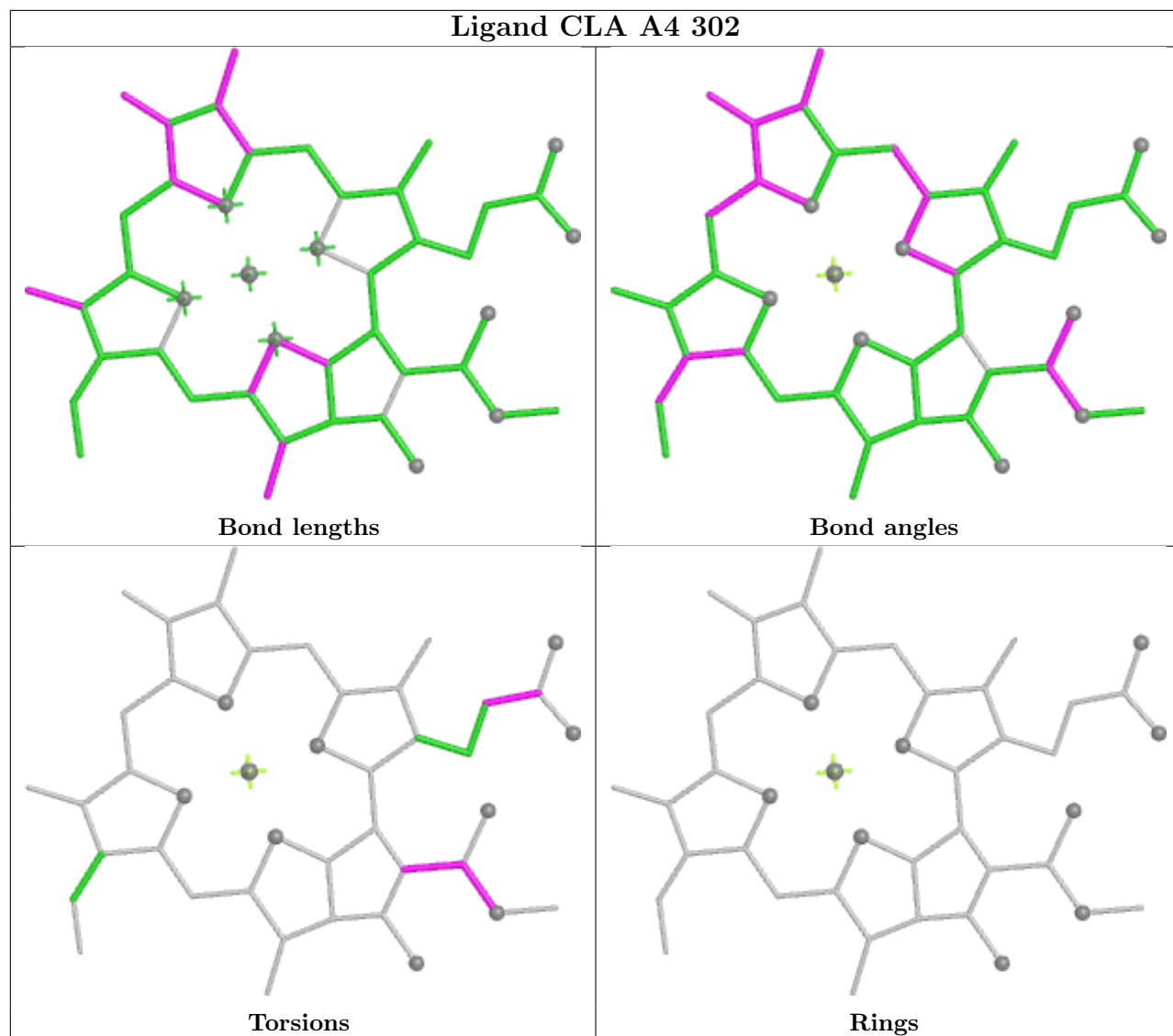


Torsions

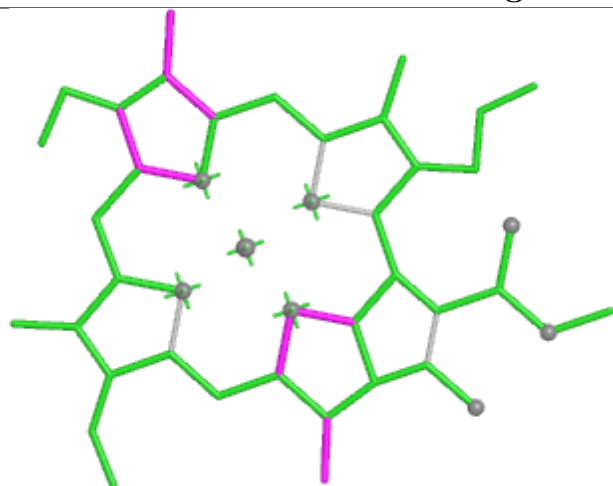


Rings

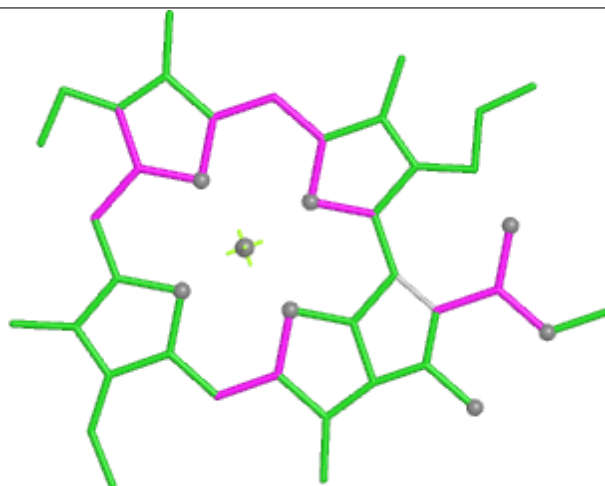
Ligand CLA A4 302



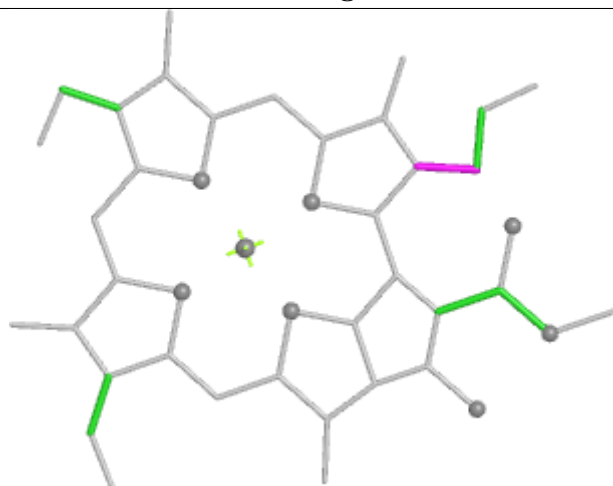
Ligand CLA B2 613



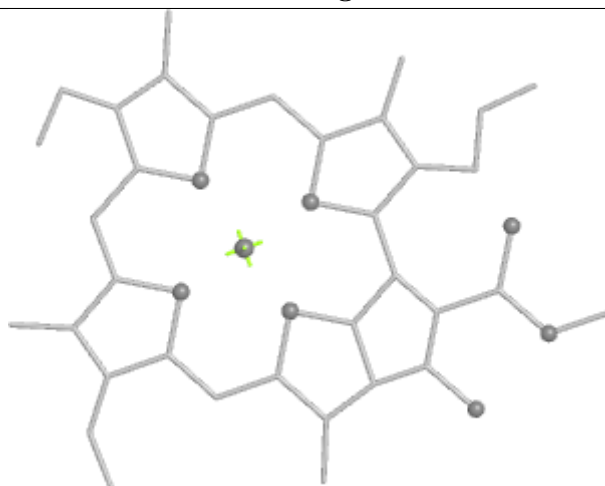
Bond lengths



Bond angles

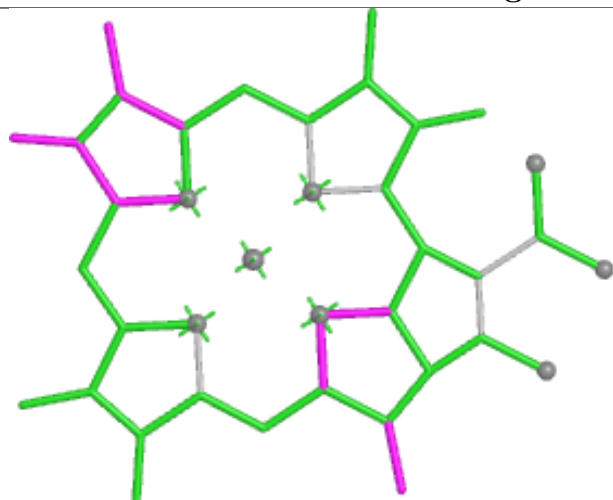


Torsions

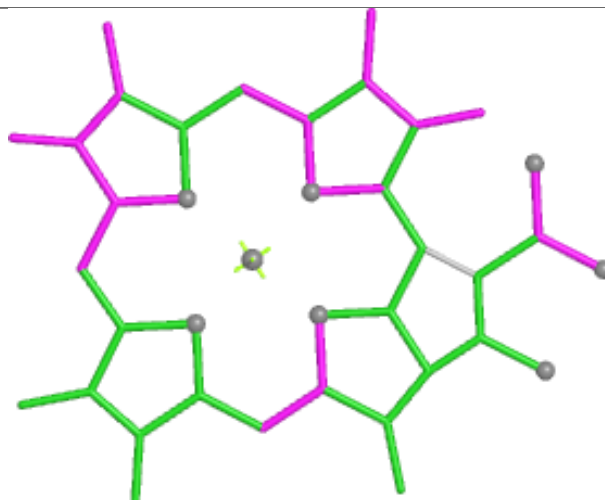


Rings

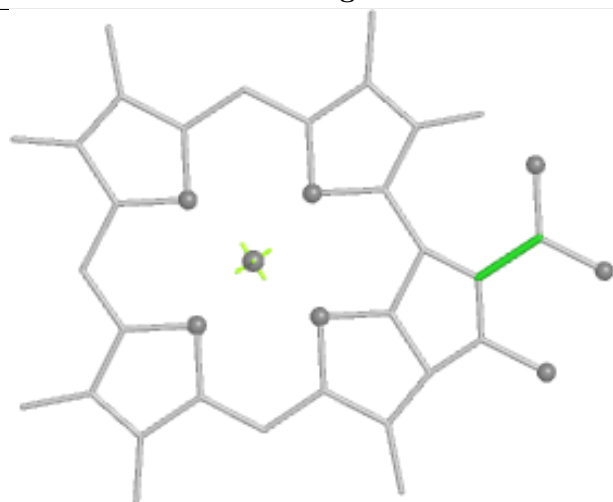
Ligand CLA A1 315



Bond lengths



Bond angles

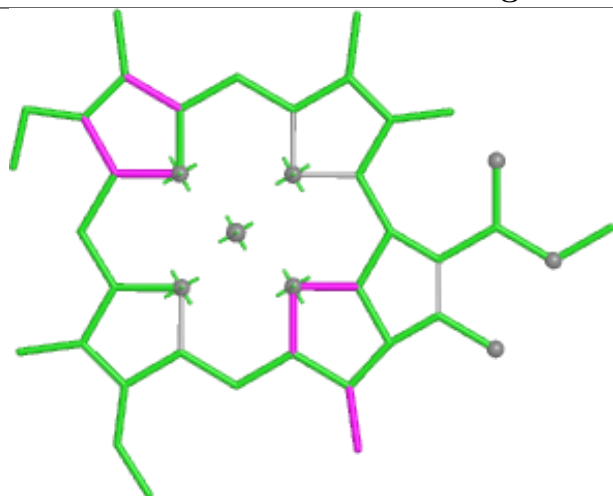


Torsions

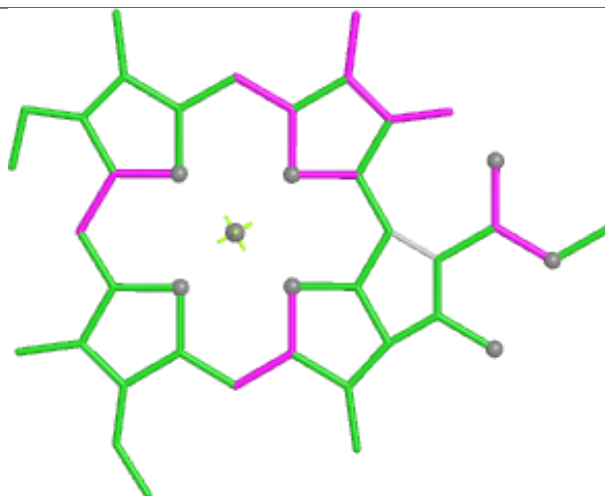


Rings

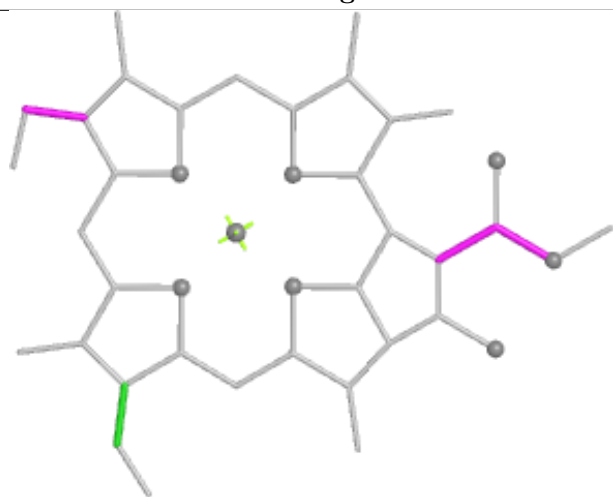
Ligand CLA BA 823



Bond lengths



Bond angles

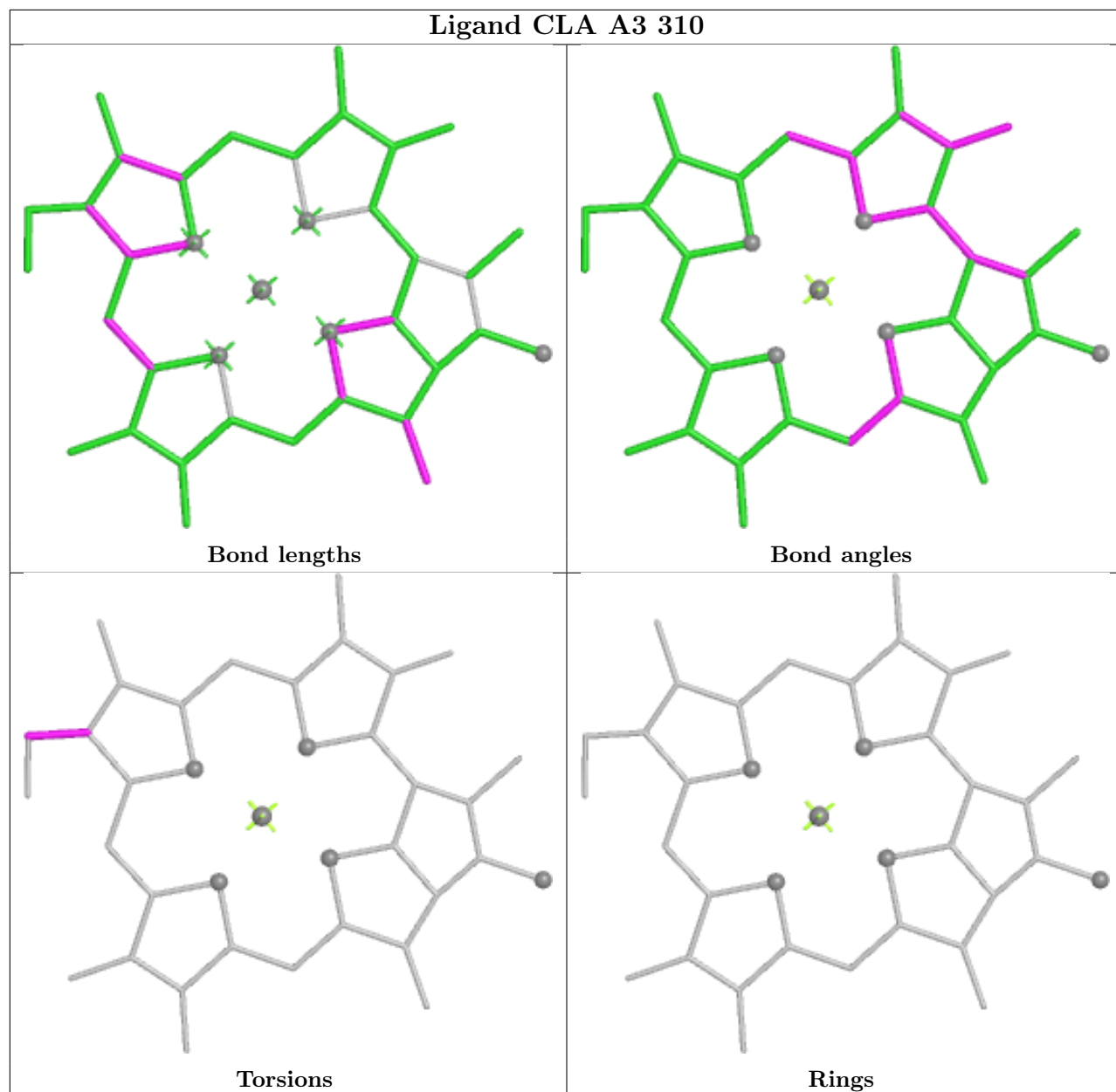


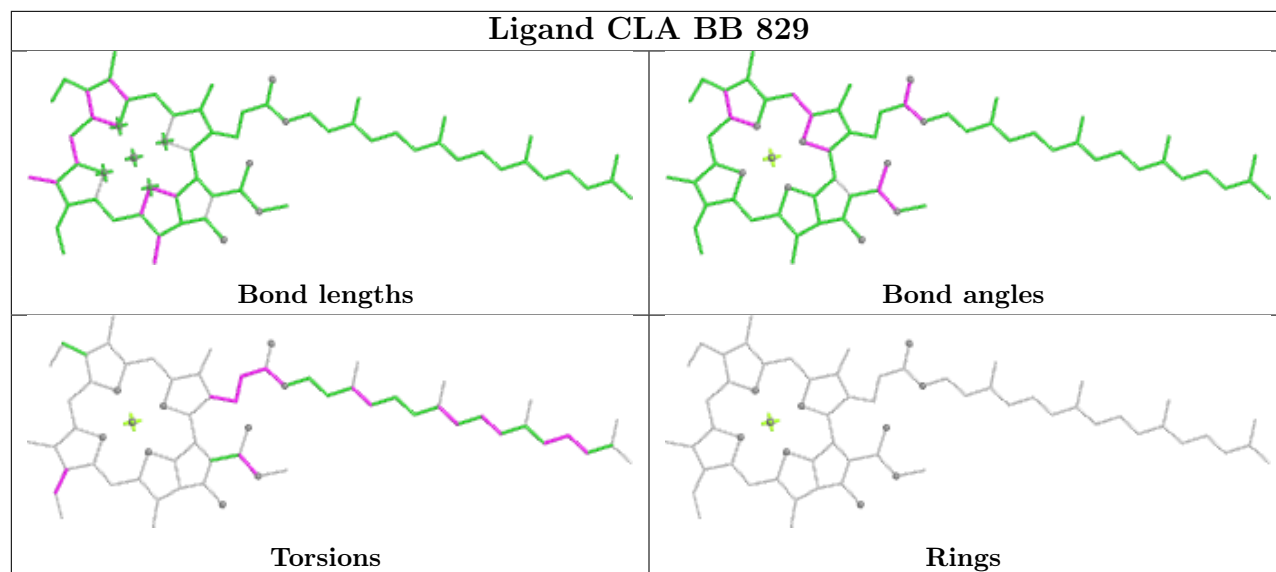
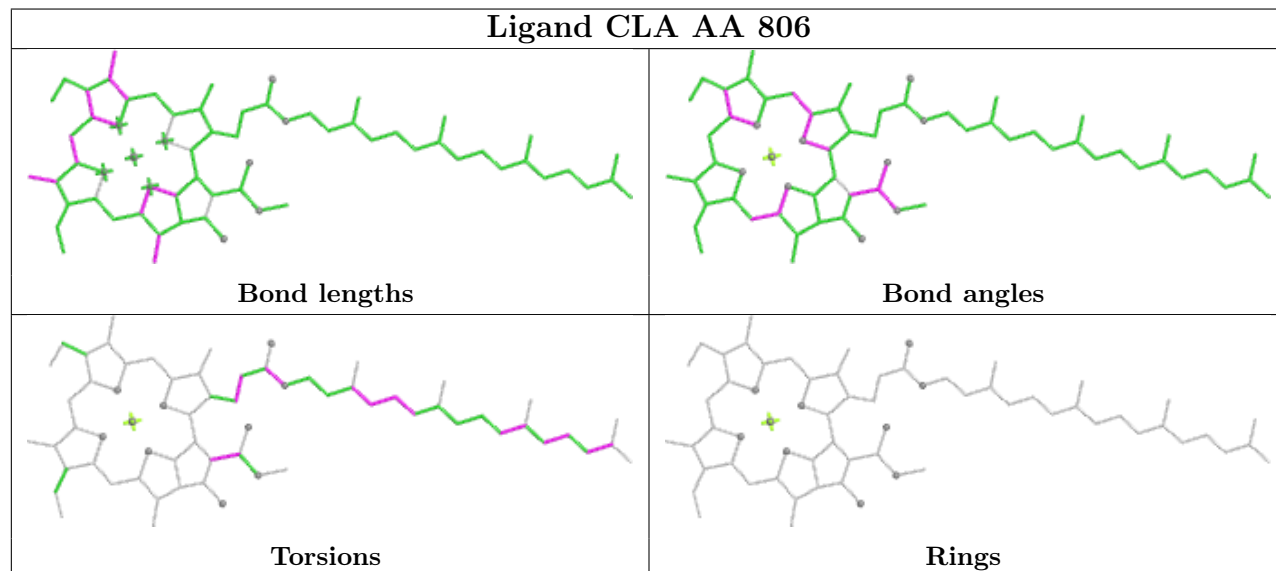
Torsions



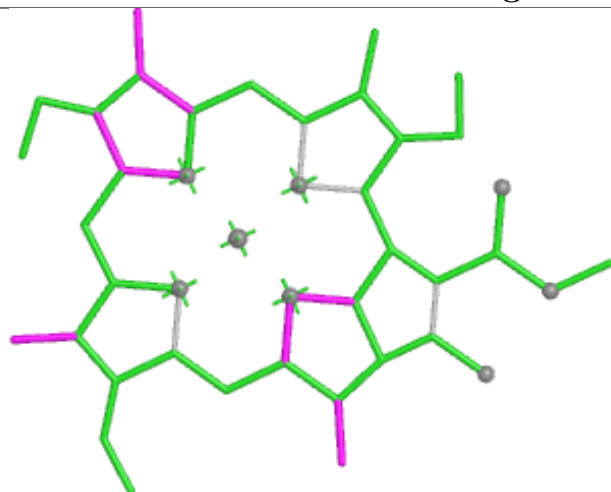
Rings

Ligand CLA A3 310

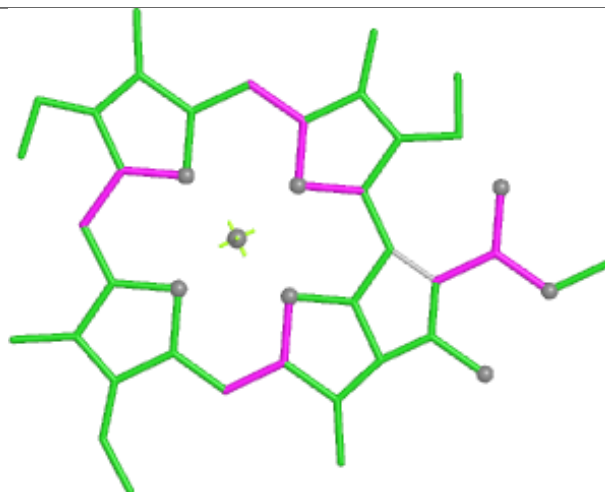


Ligand CLA BB 829**Ligand CLA AA 806**

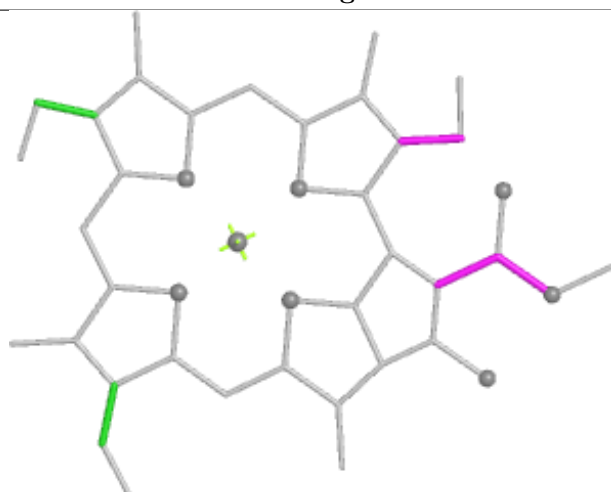
Ligand CLA AL 305



Bond lengths



Bond angles

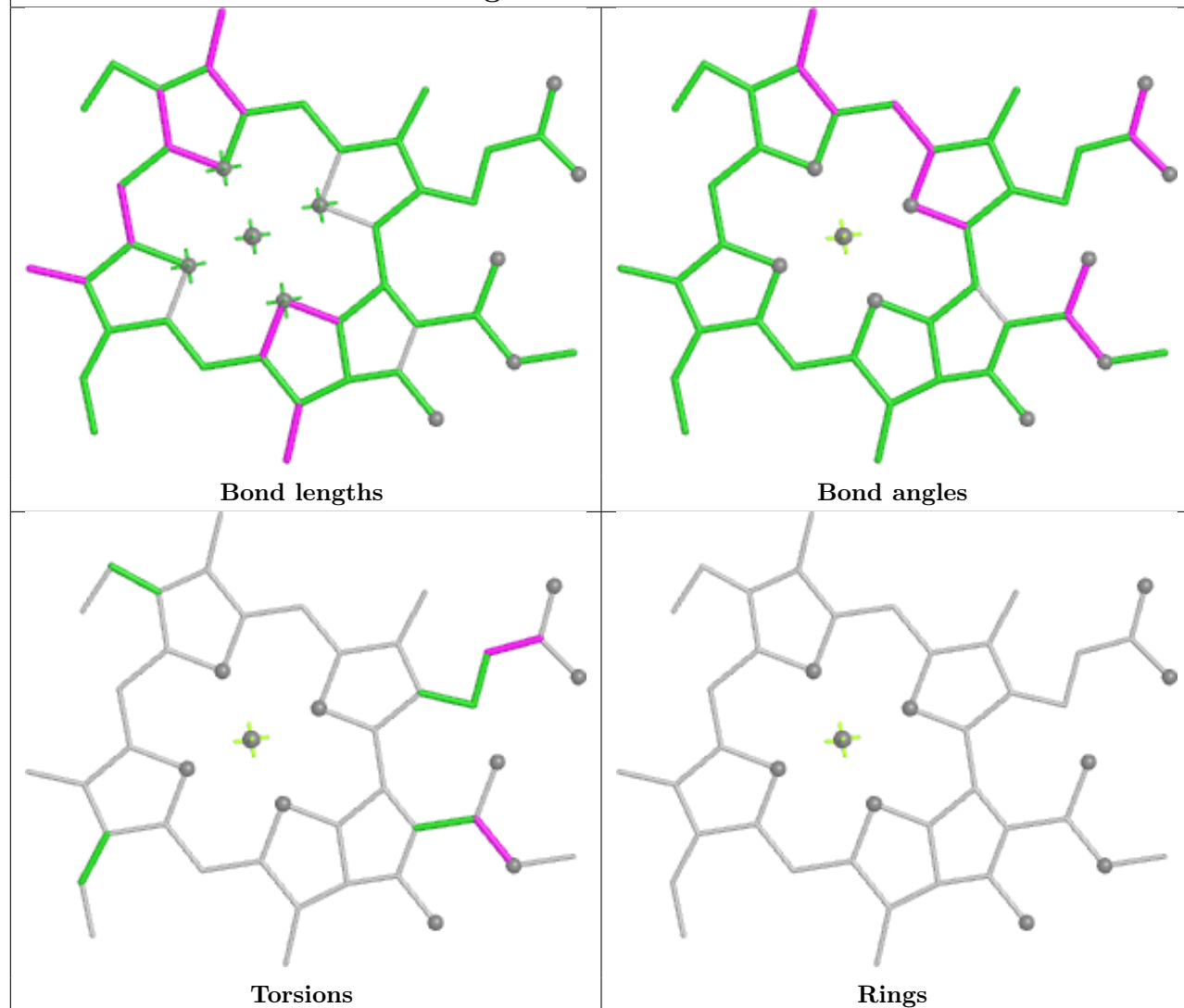


Torsions

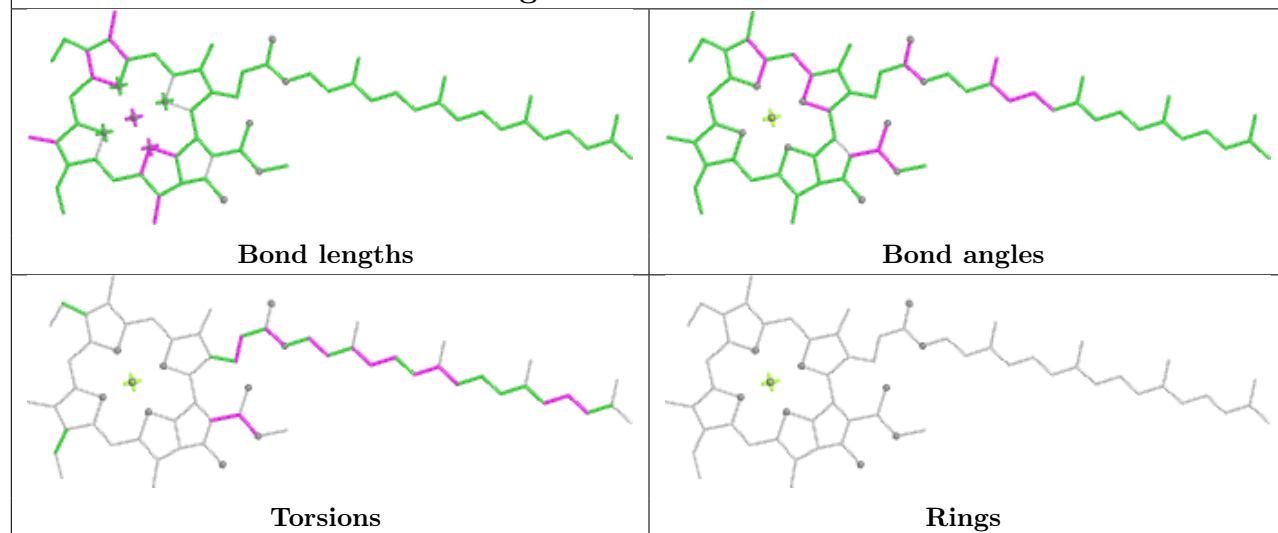


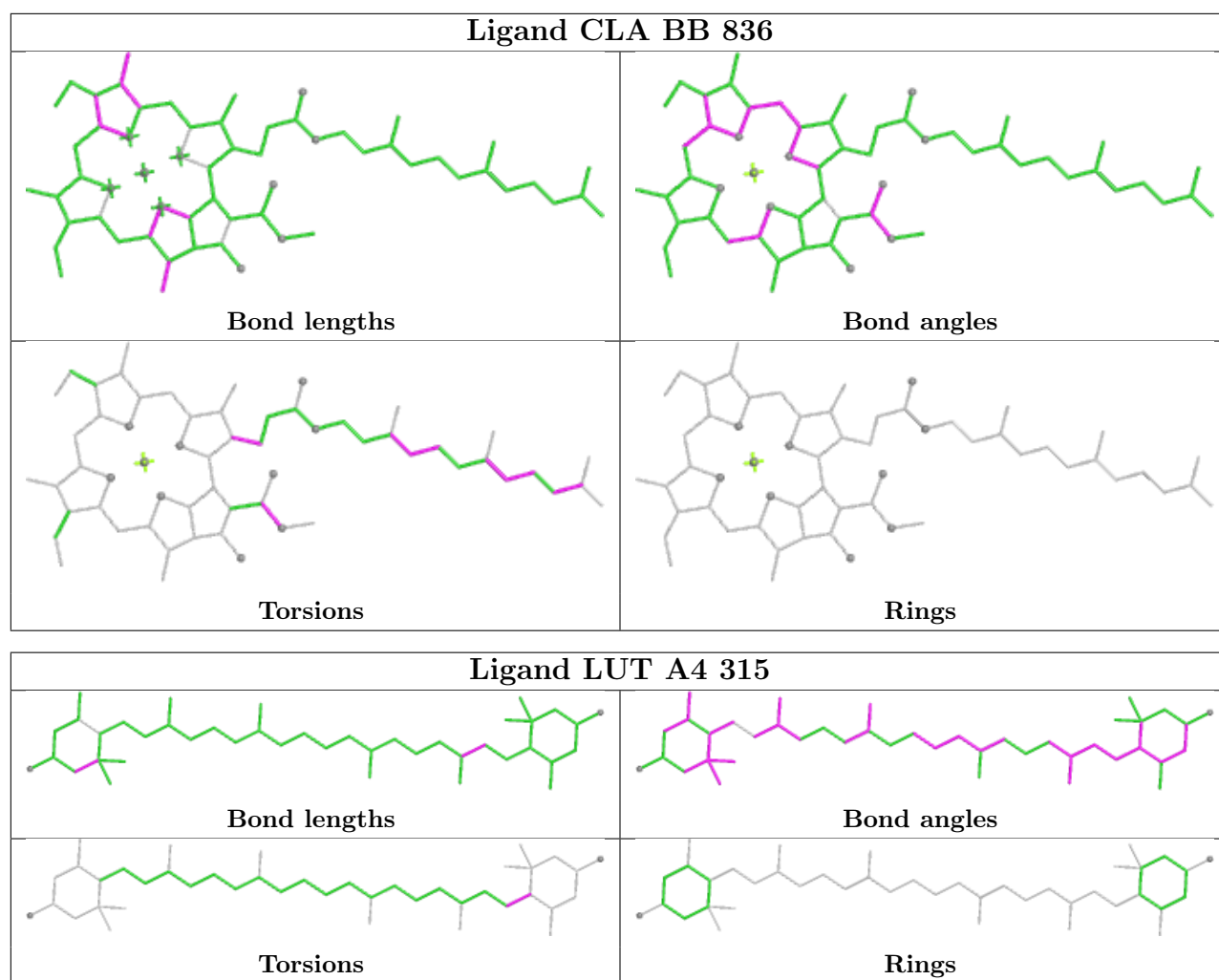
Rings

Ligand CLA A1 313

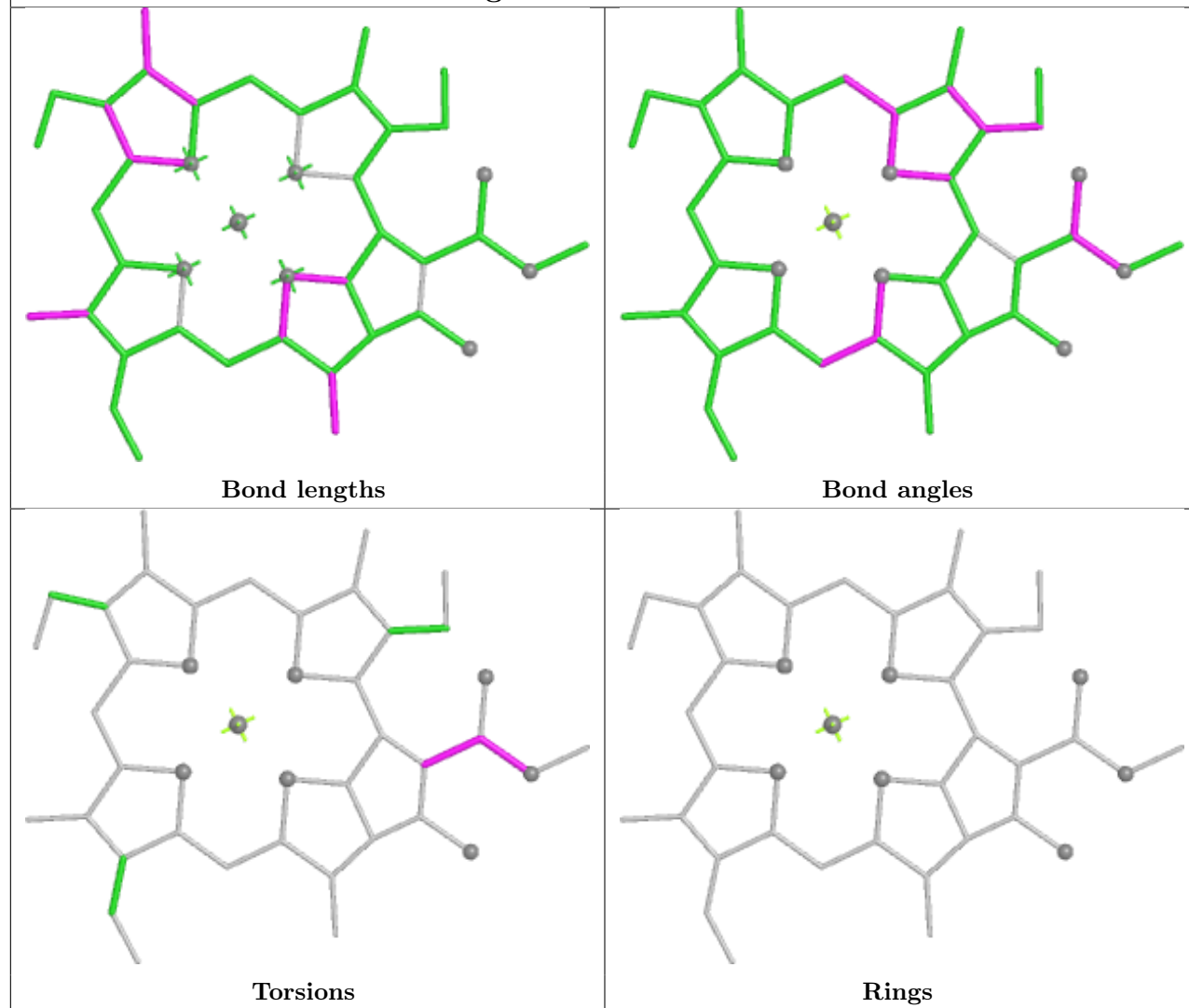


Ligand CLA BB 802

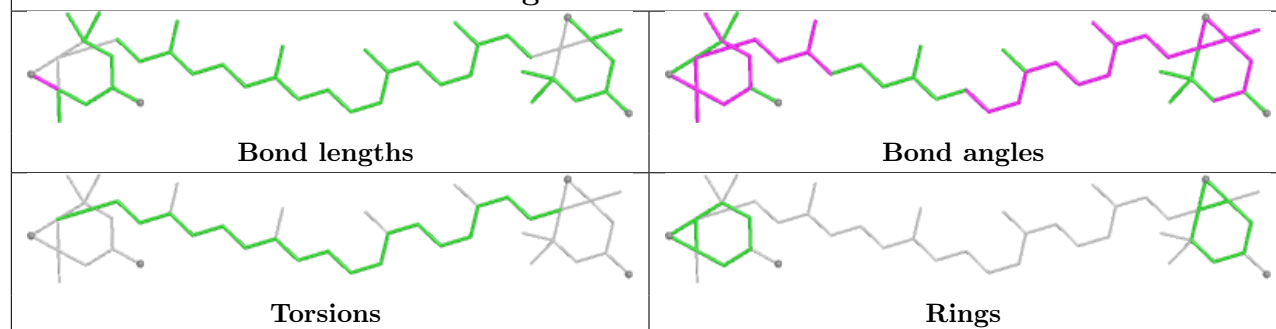




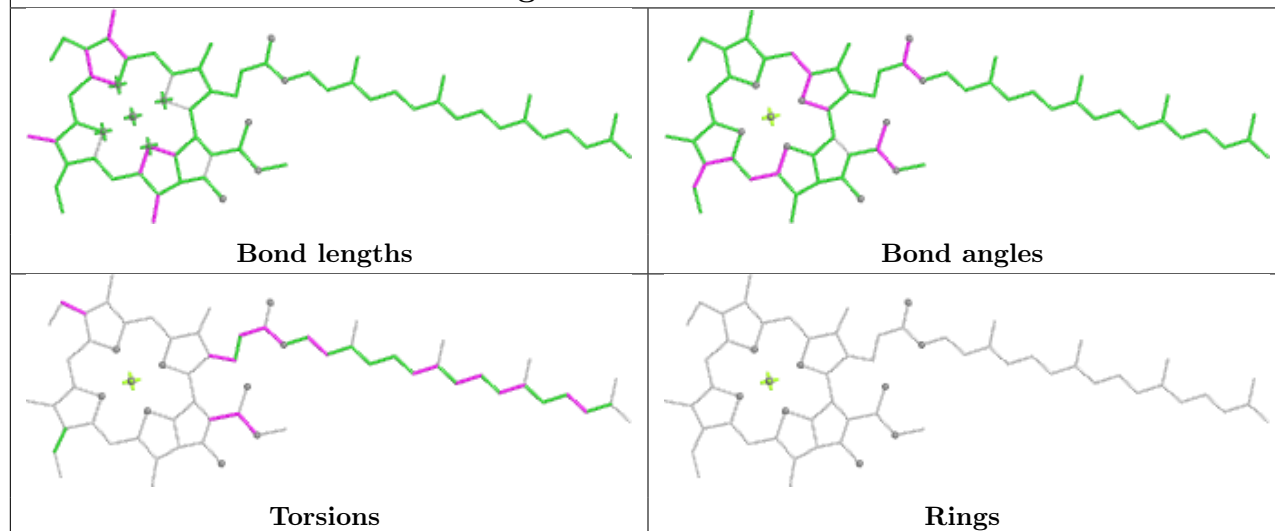
Ligand CLA BF 302



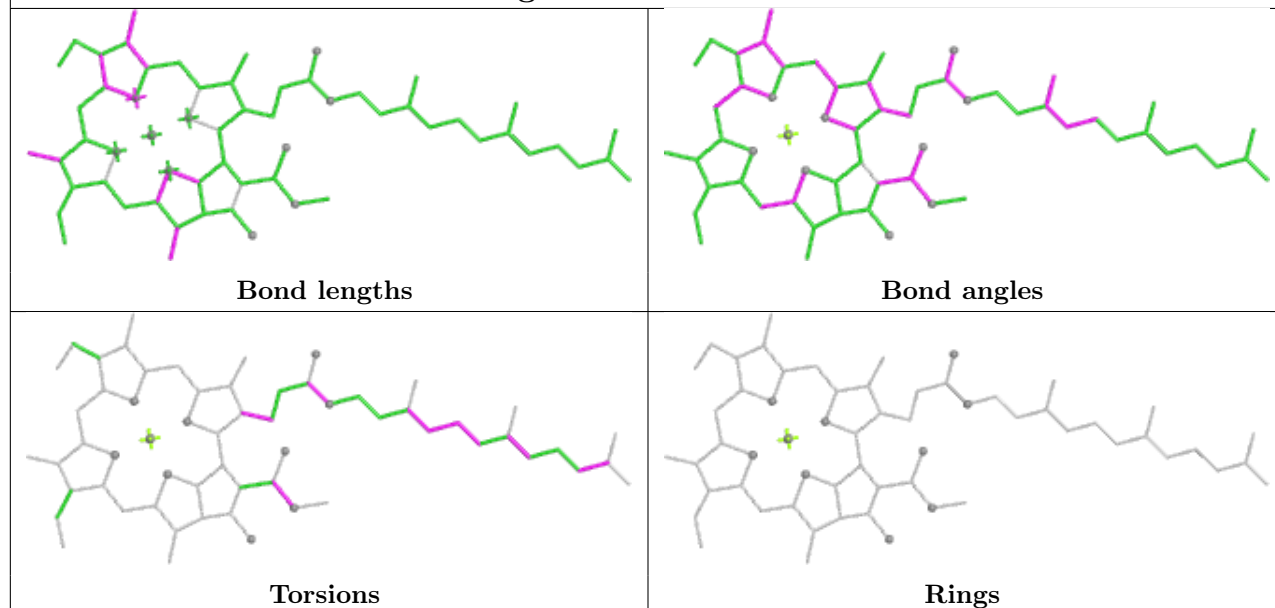
Ligand XAT A3 317



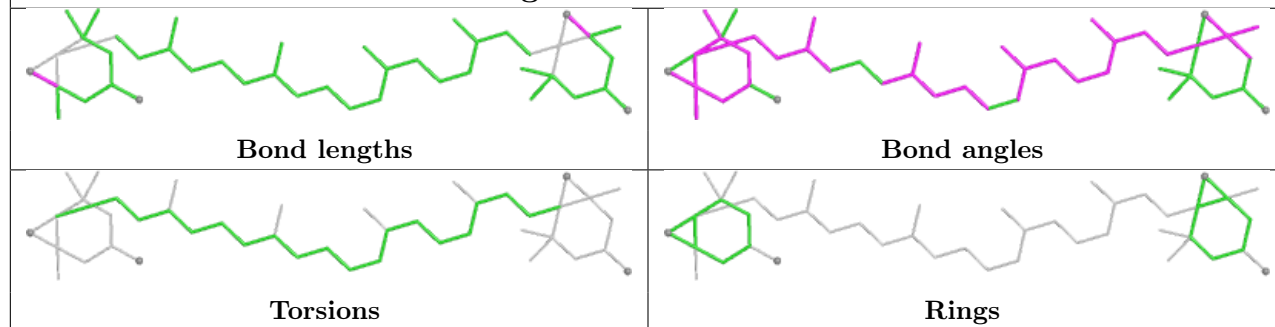
Ligand CLA AB 834



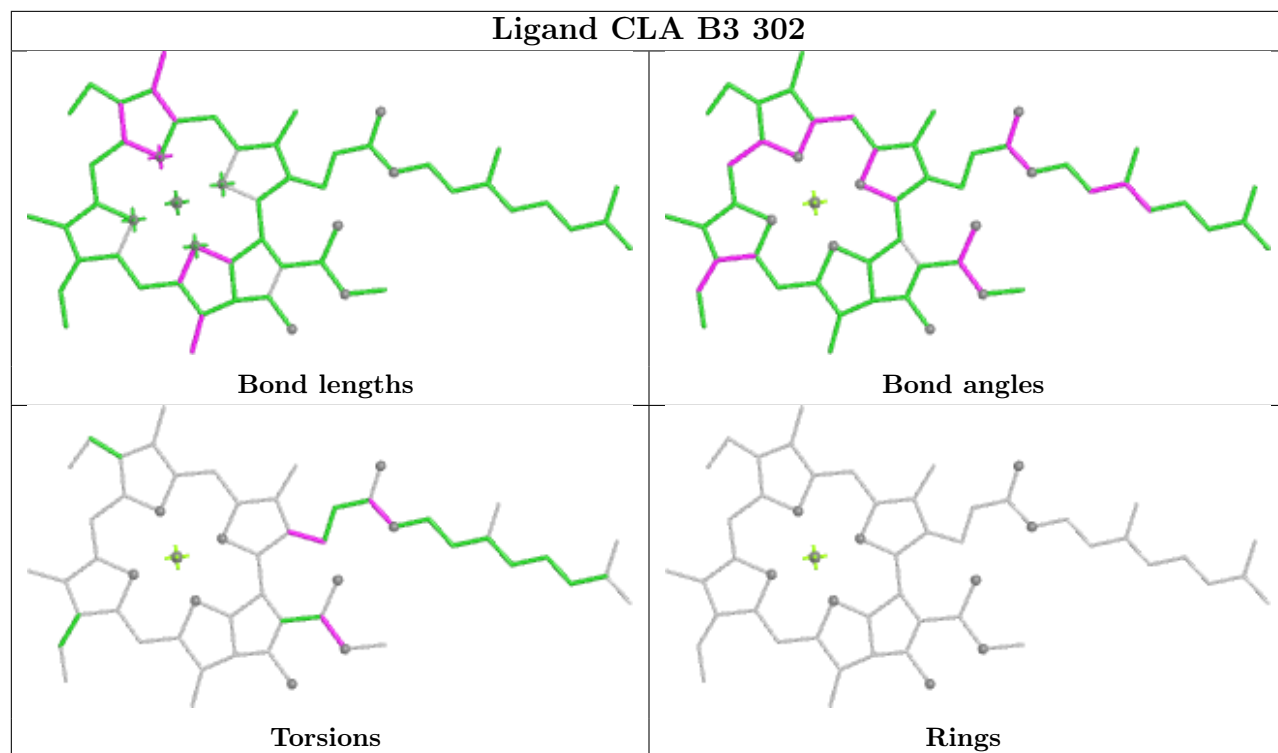
Ligand CLA AB 819



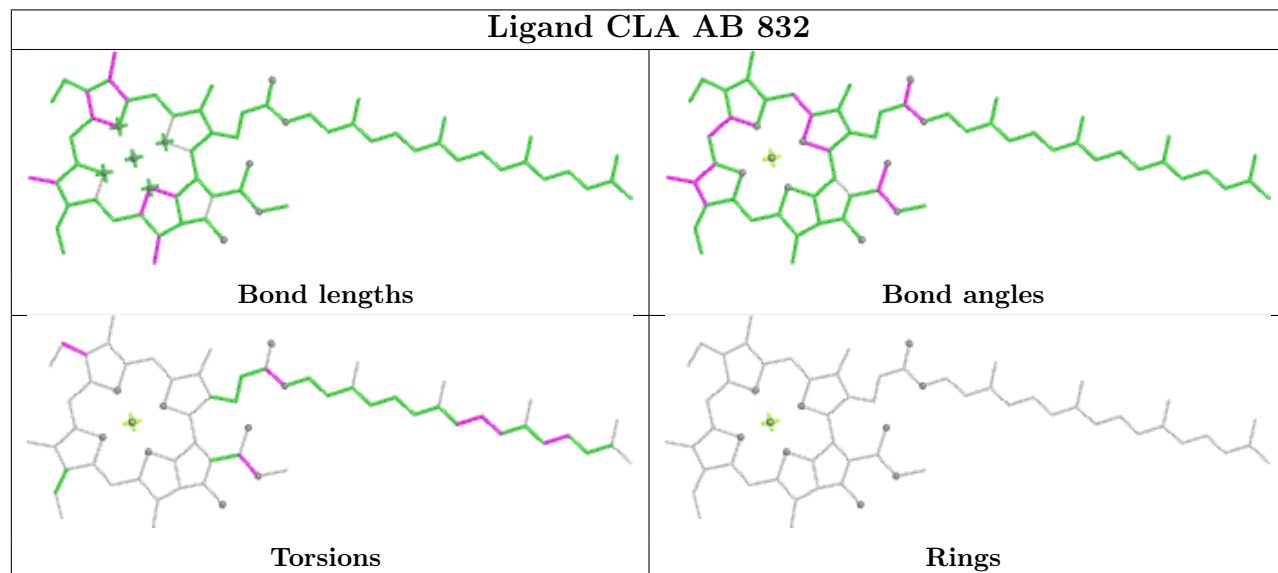
Ligand XAT A6 616

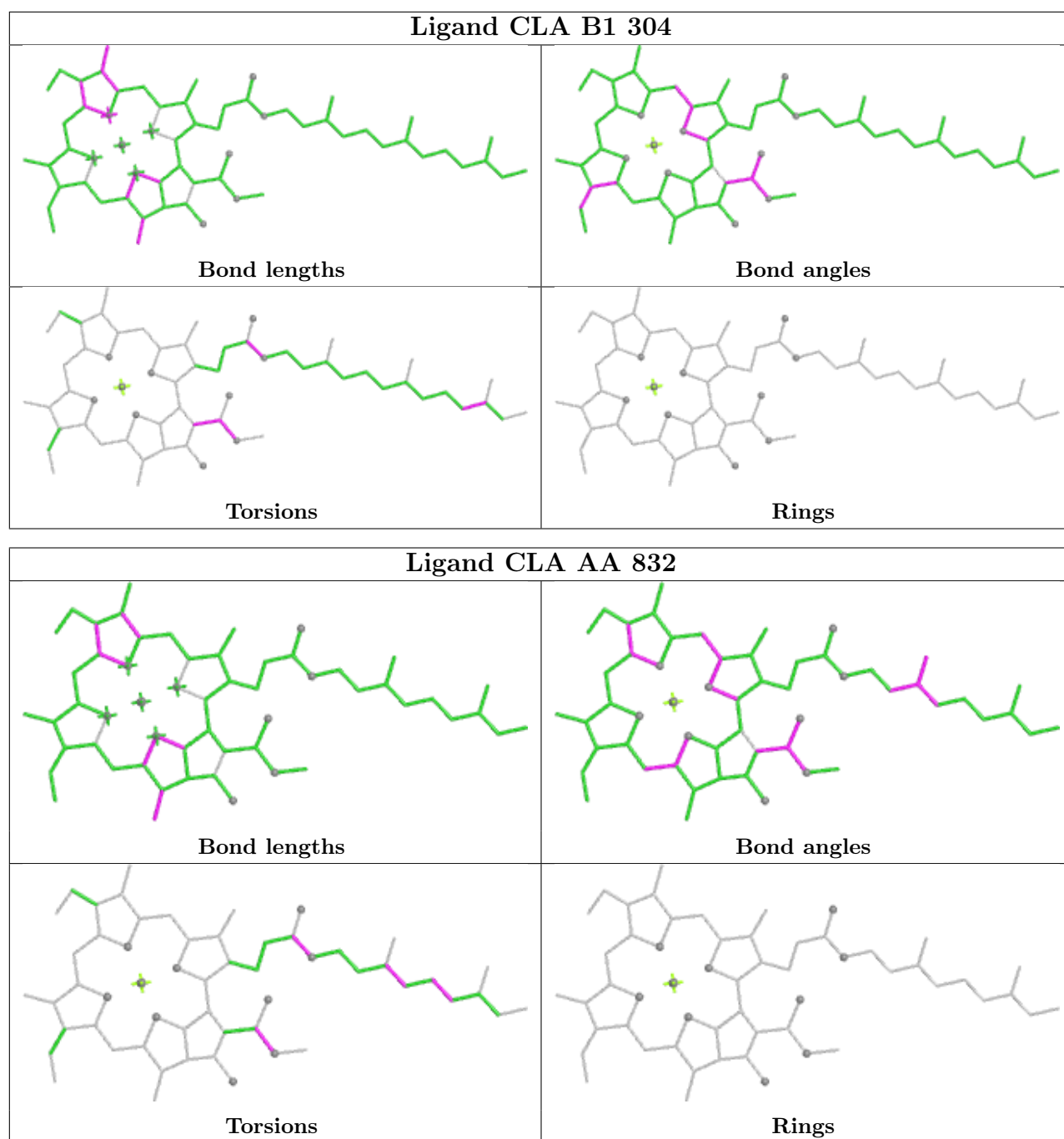


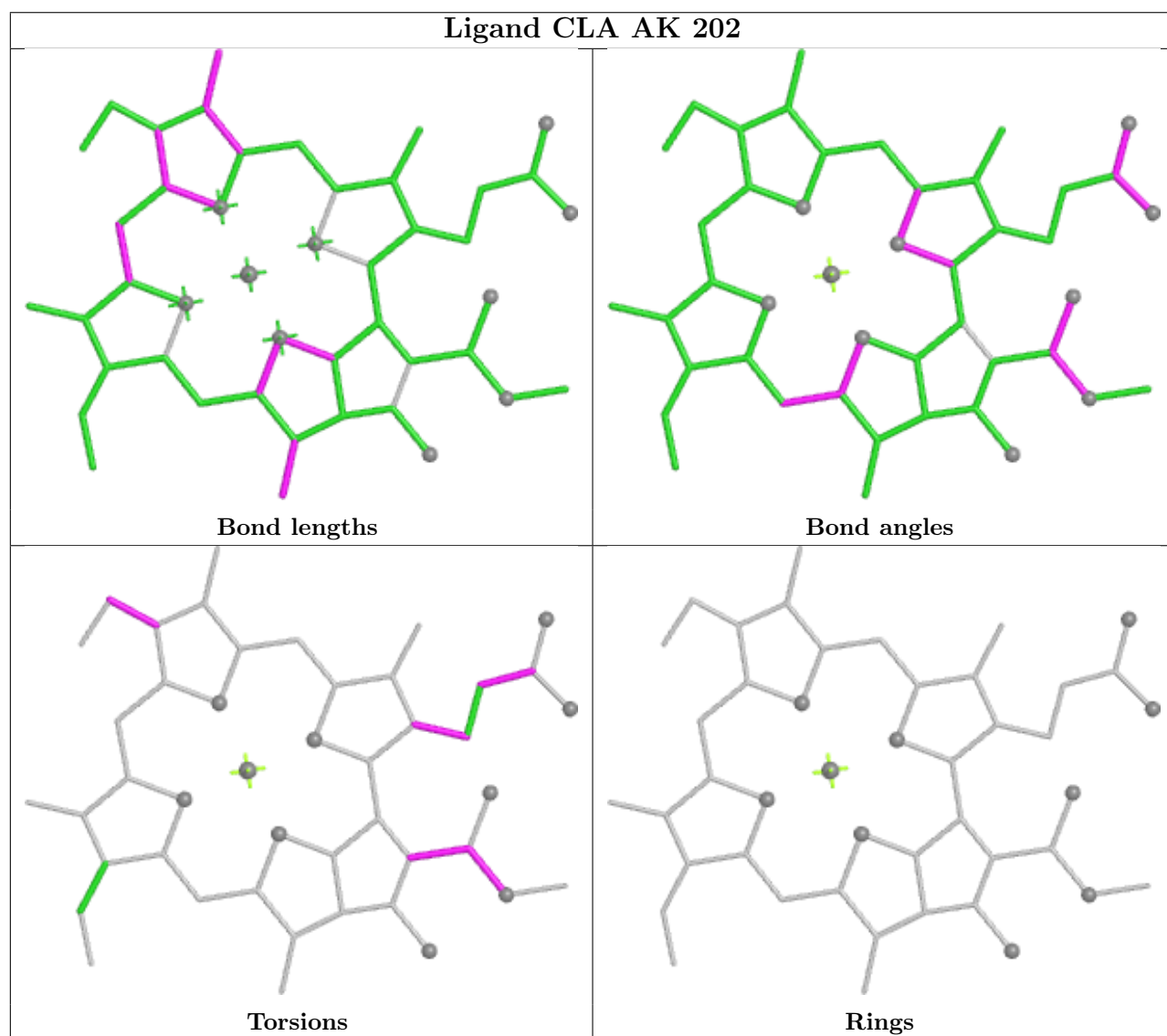
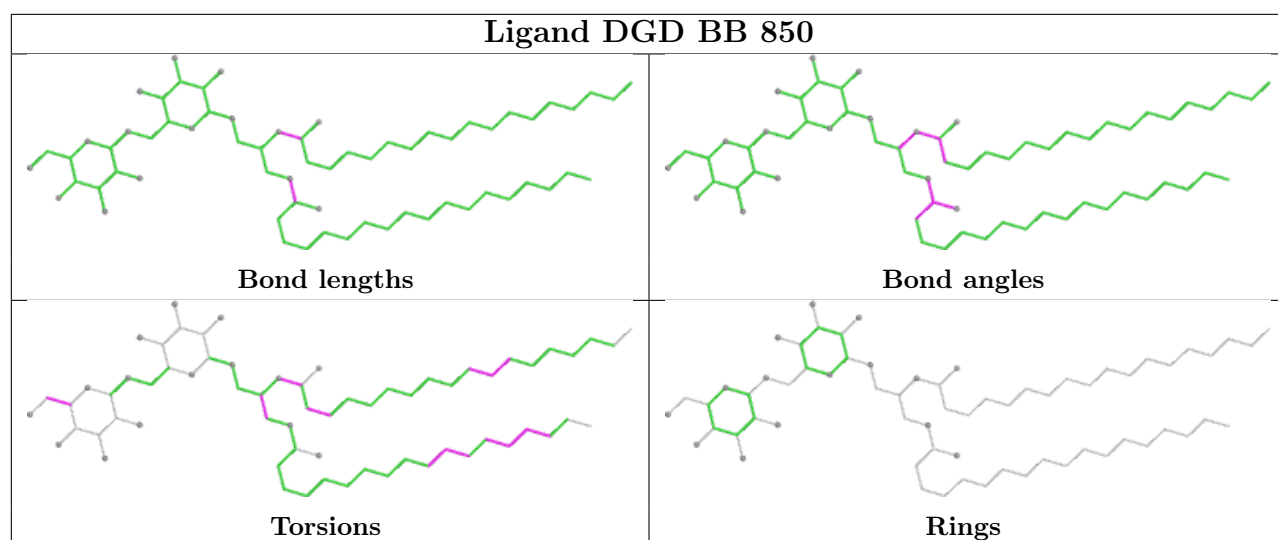
Ligand CLA B3 302

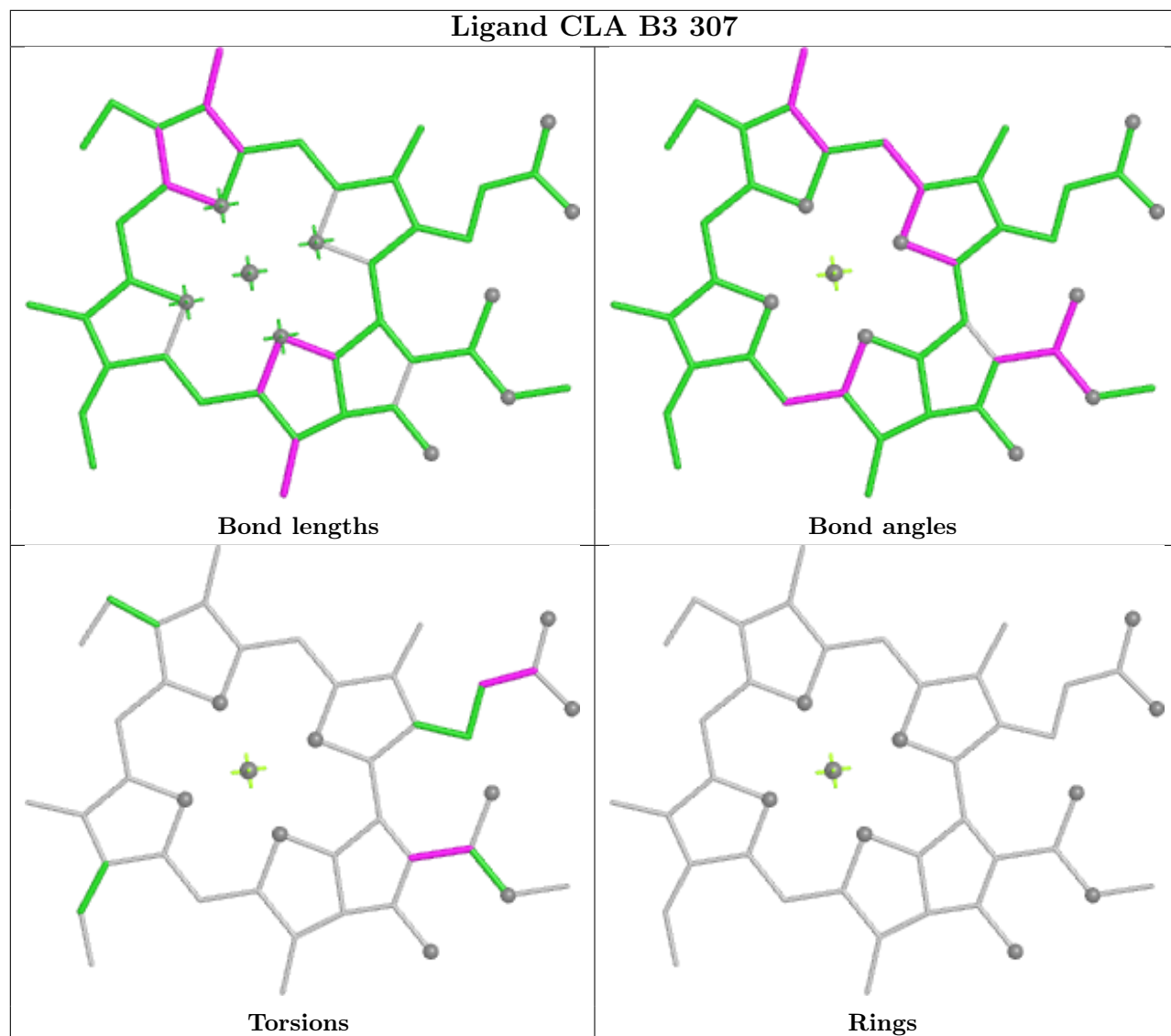


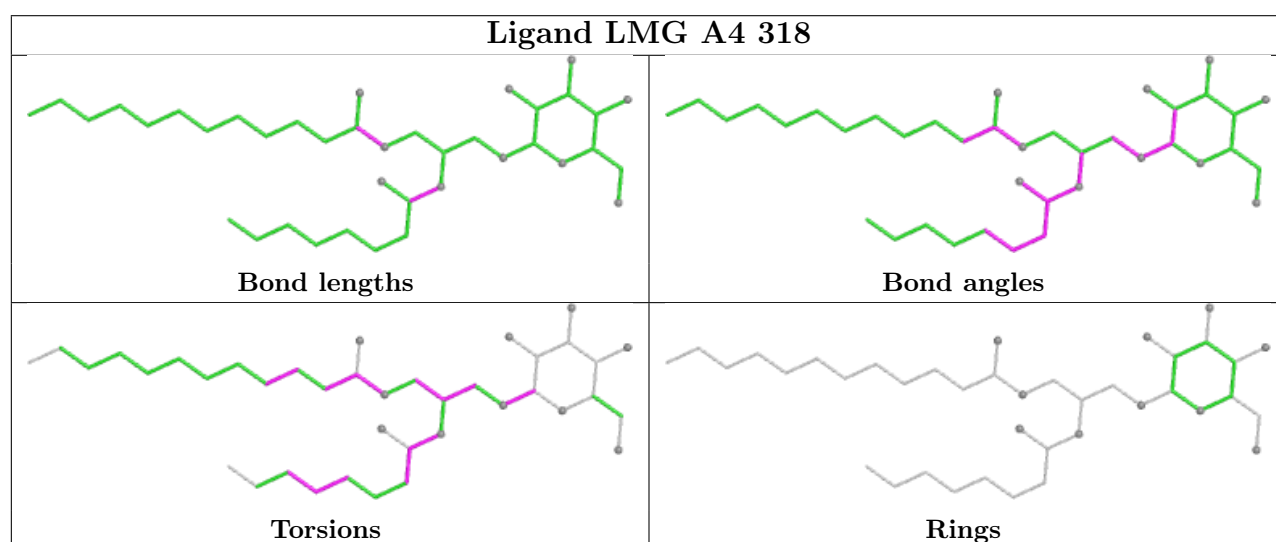
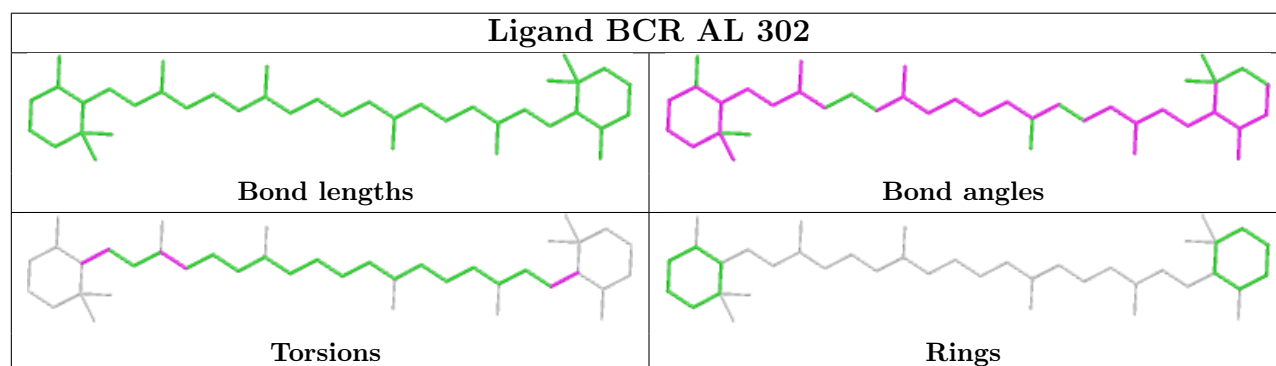
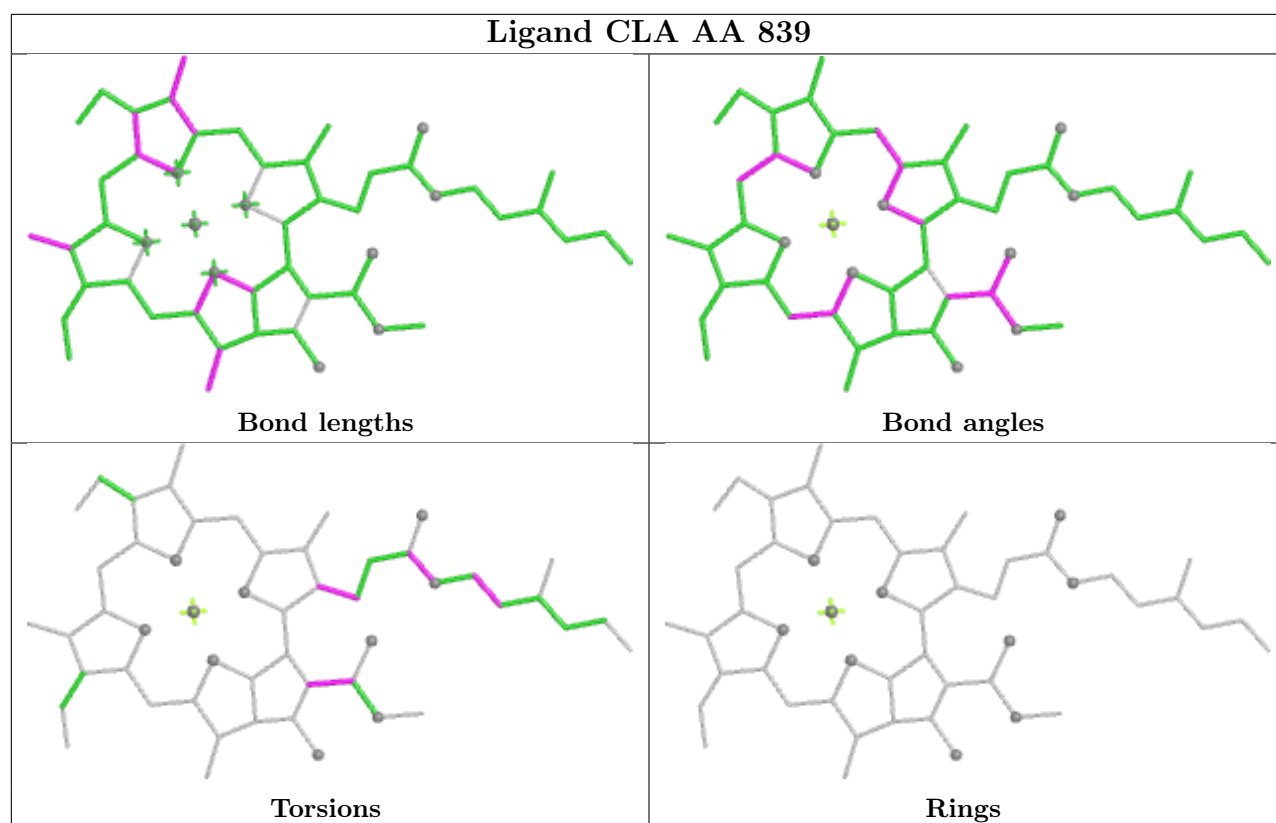
Ligand CLA AB 832

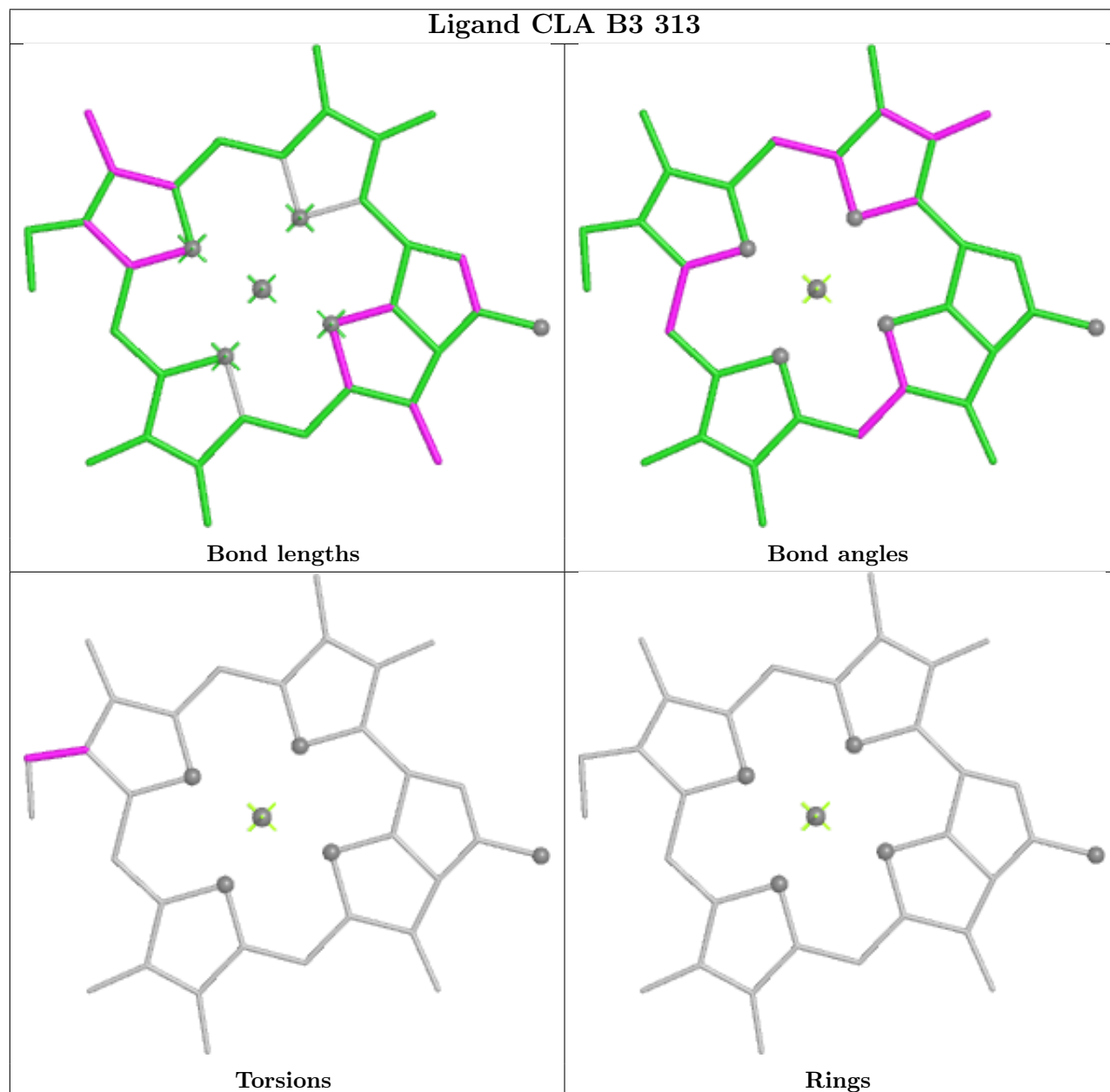
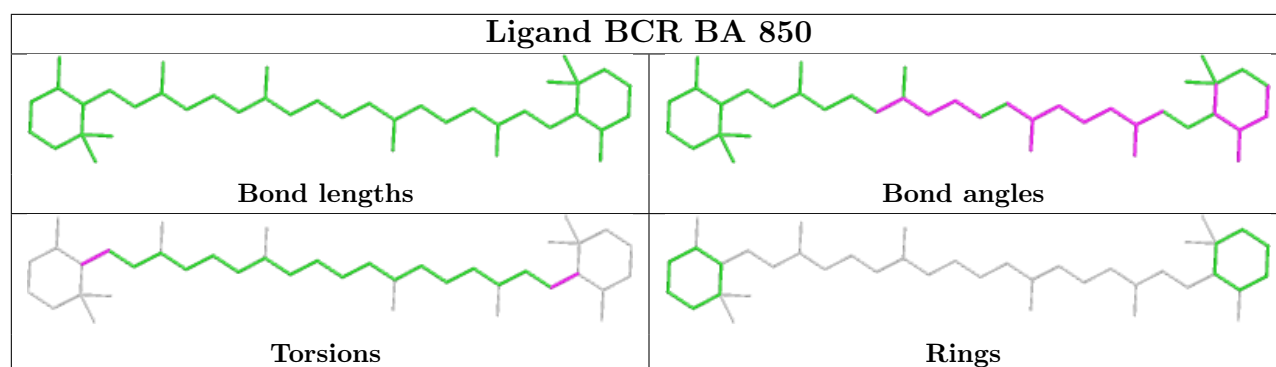




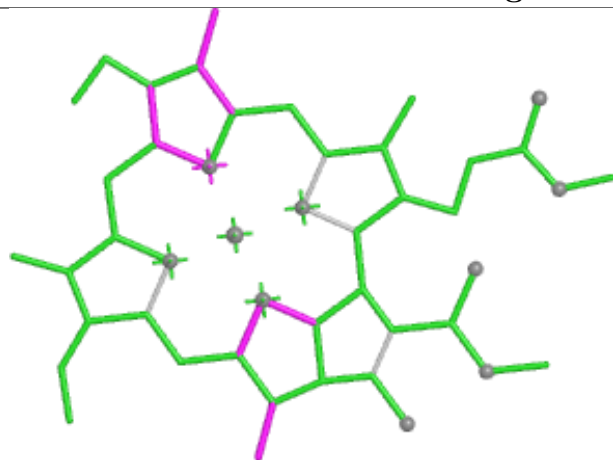




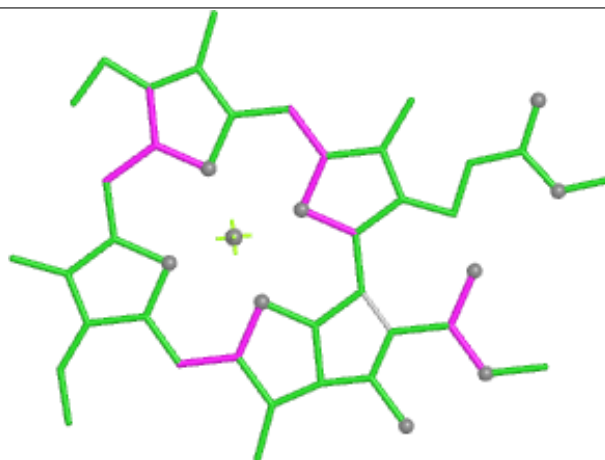




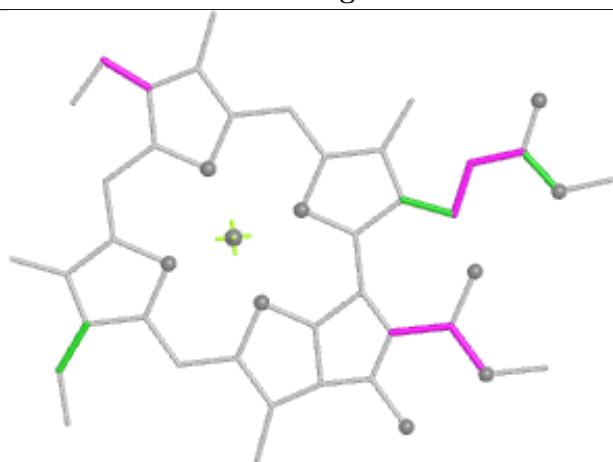
Ligand CLA B5 601



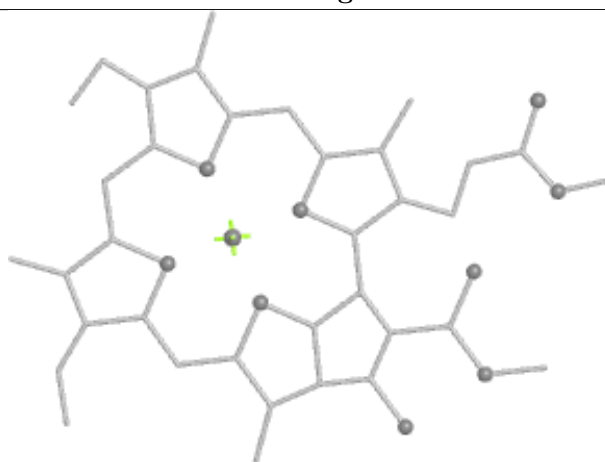
Bond lengths



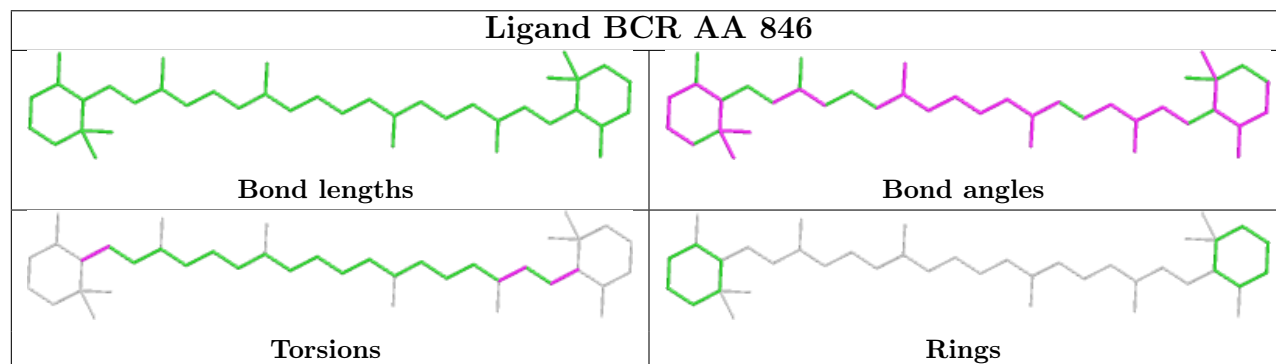
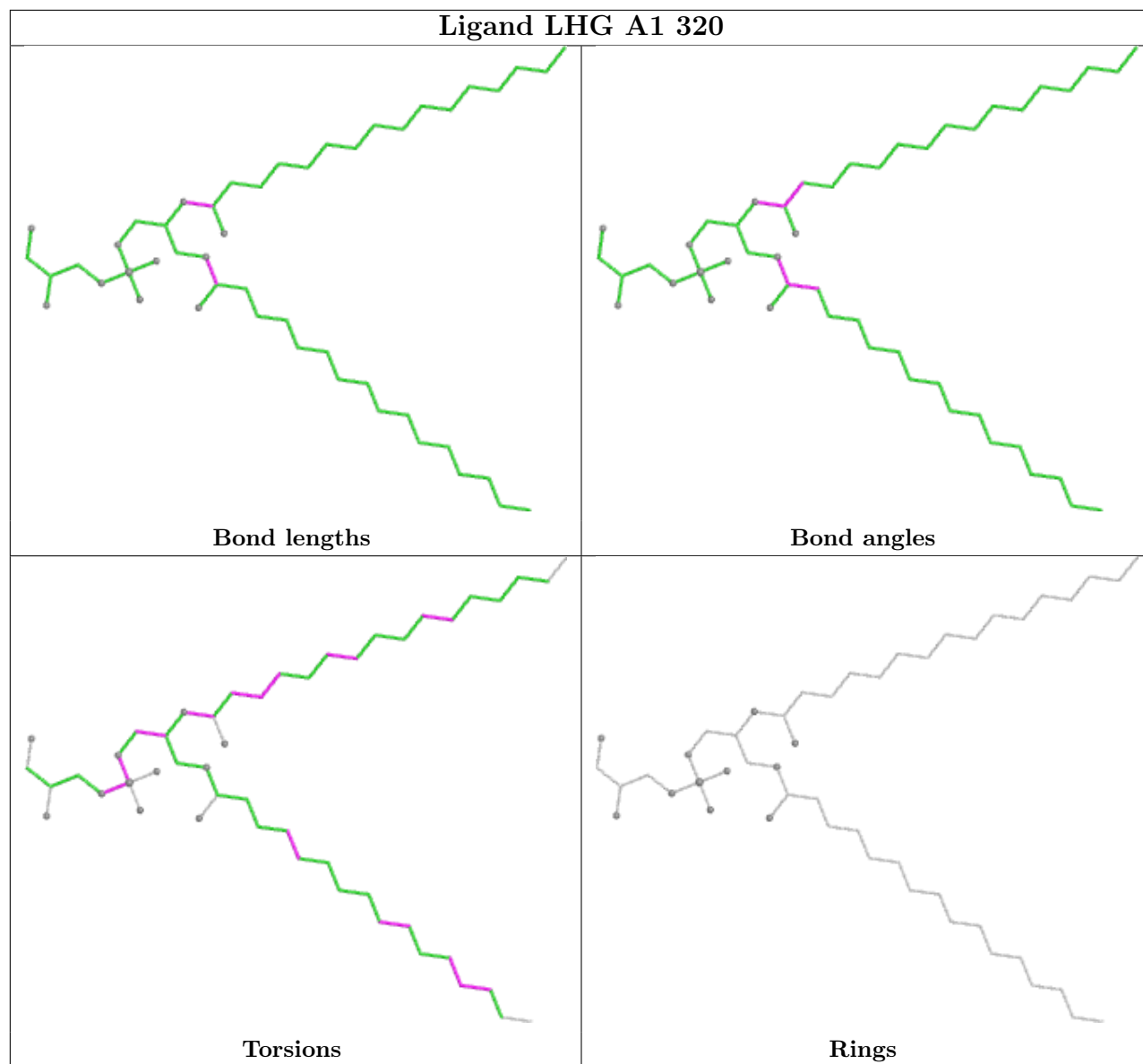
Bond angles



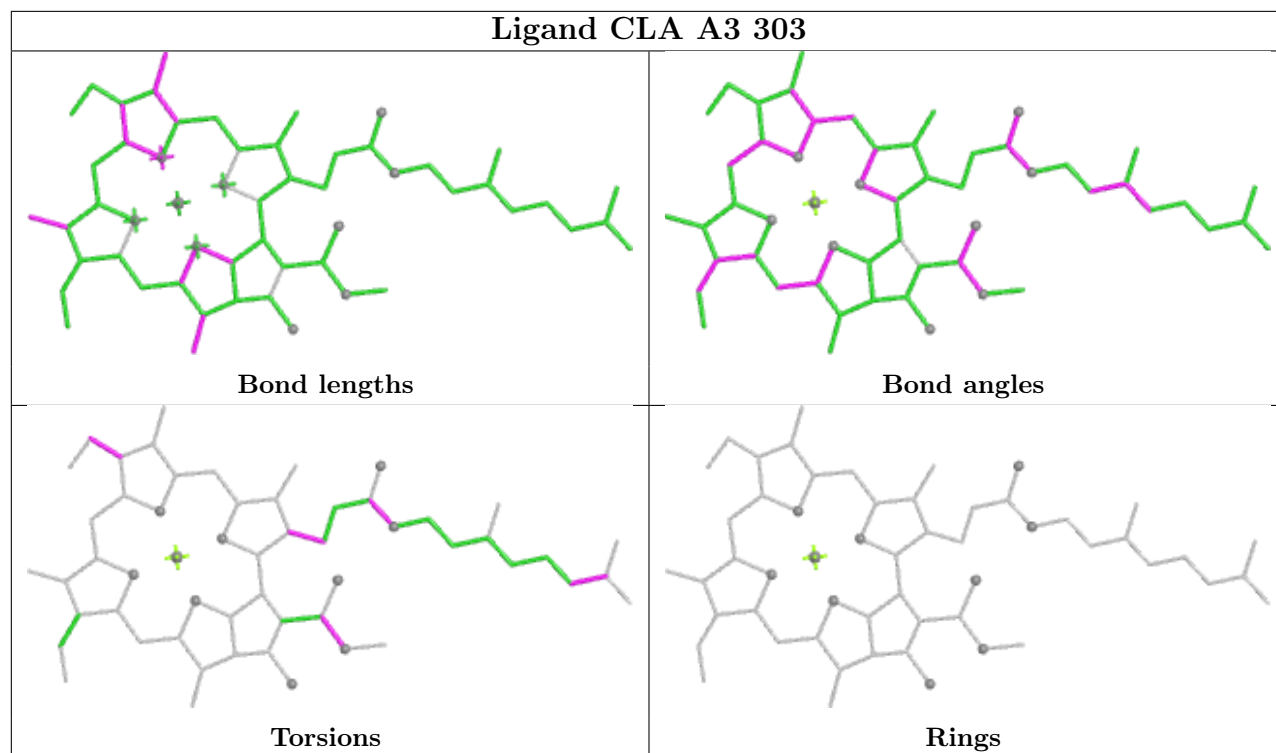
Torsions



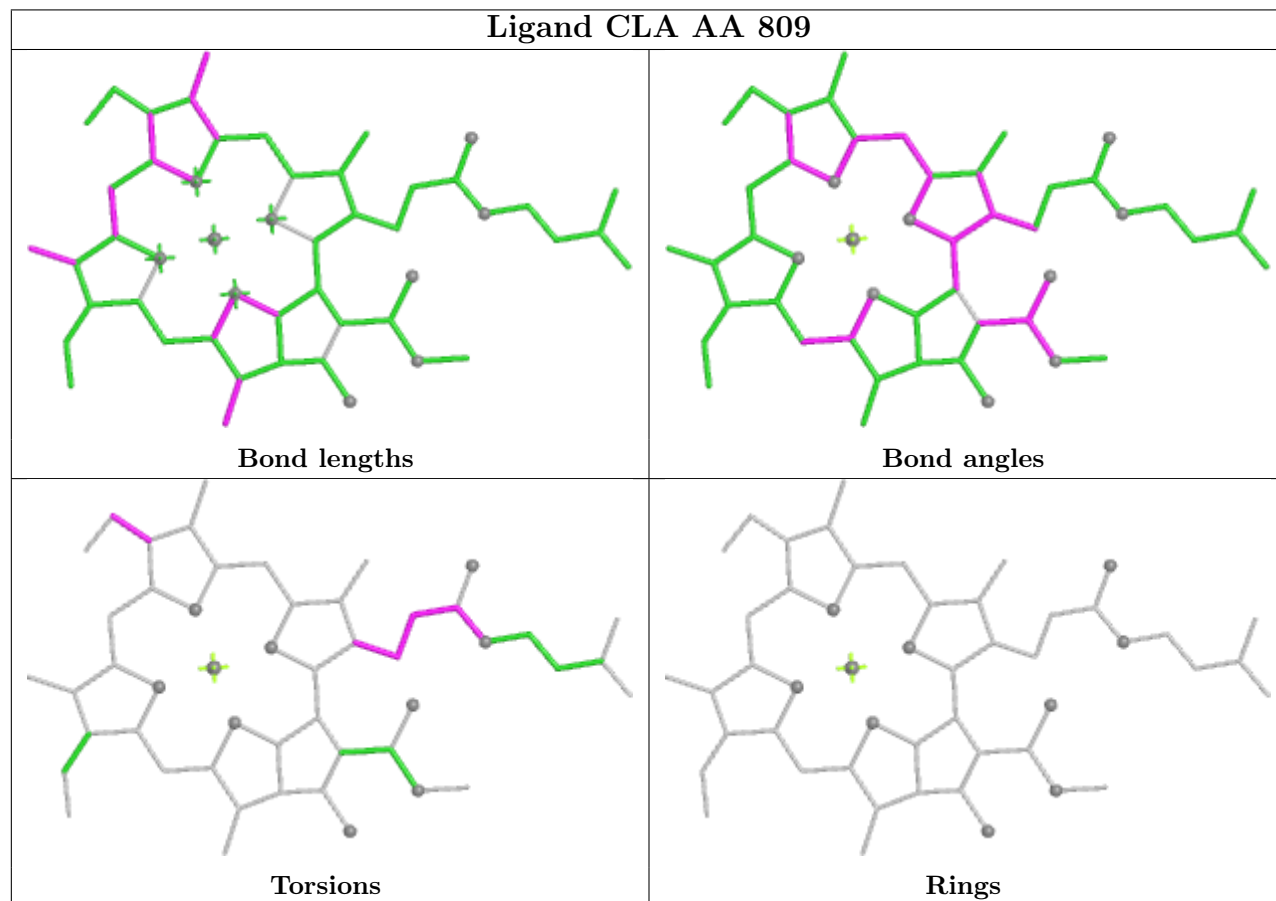
Rings

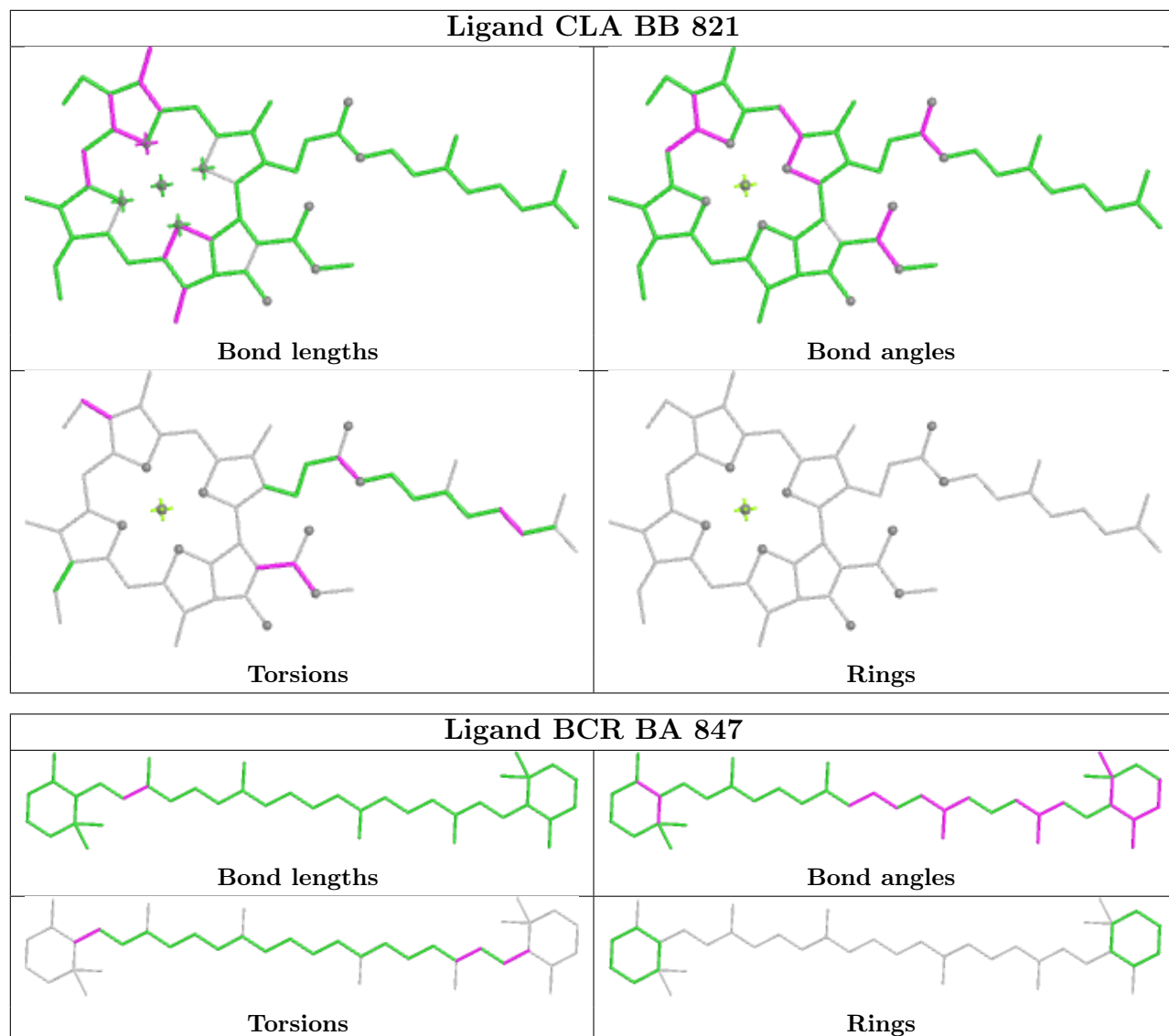


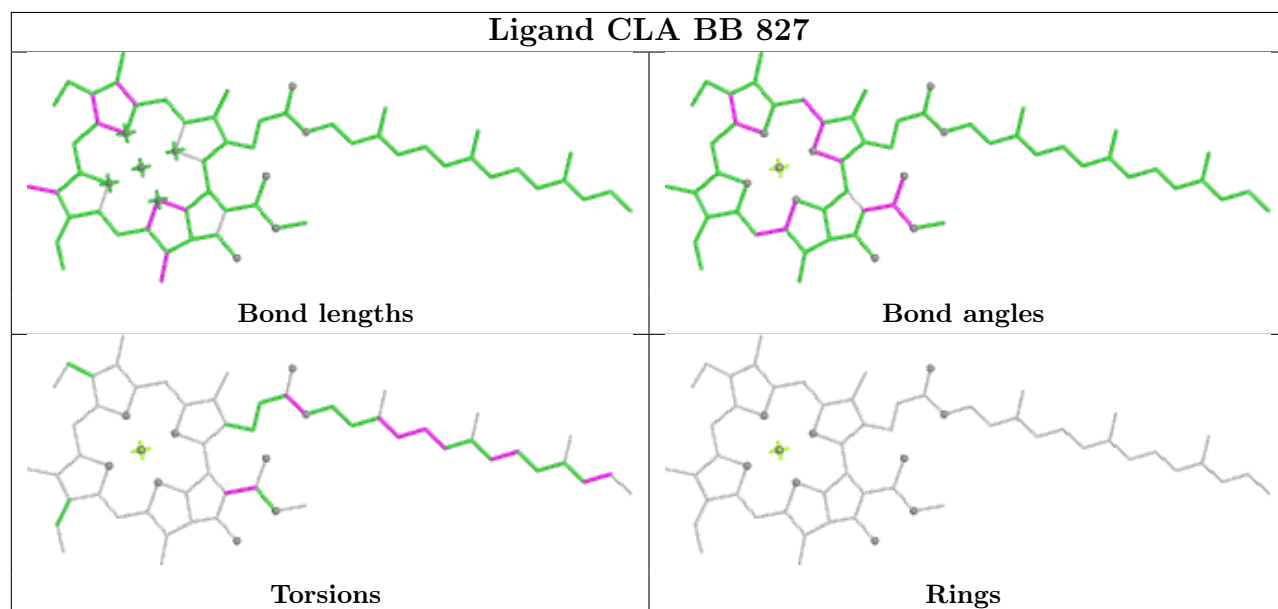
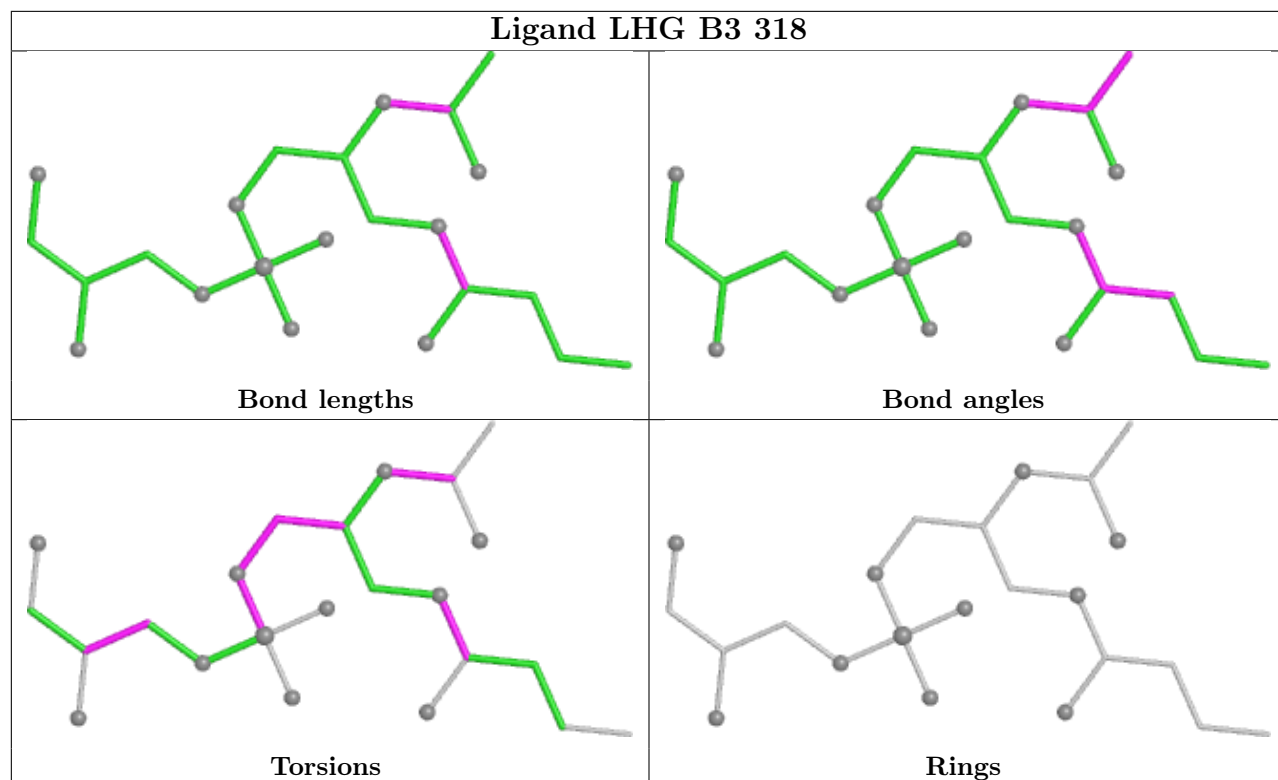
Ligand CLA A3 303



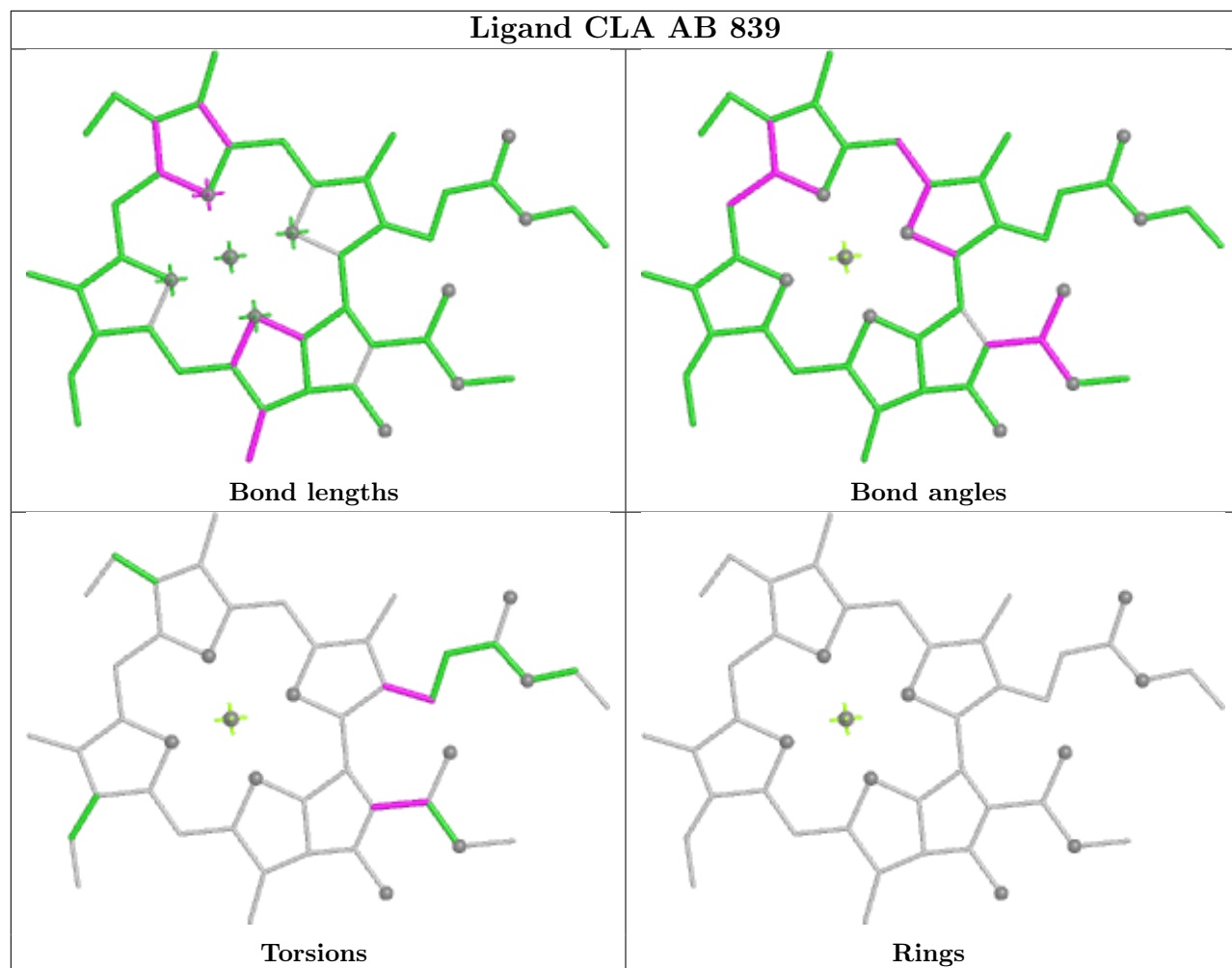
Ligand CLA AA 809



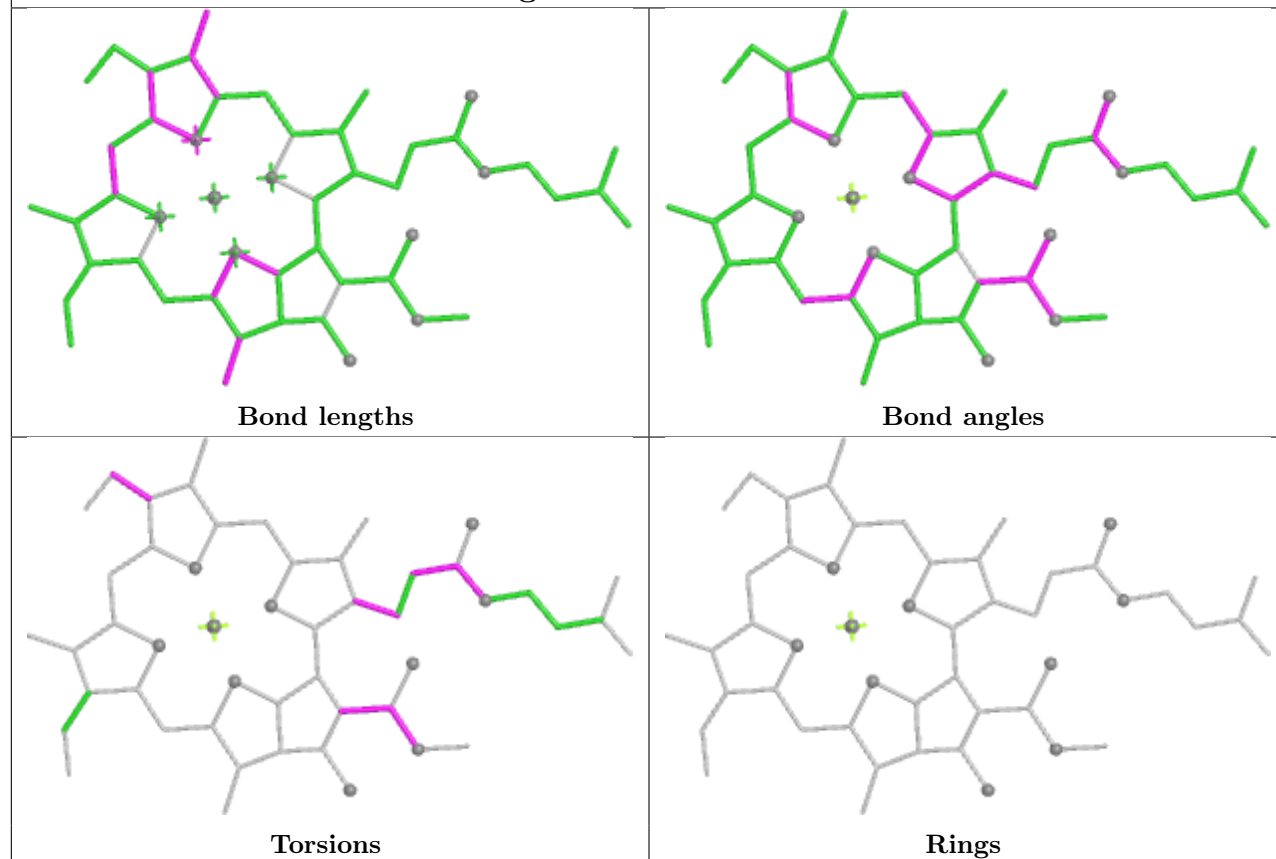




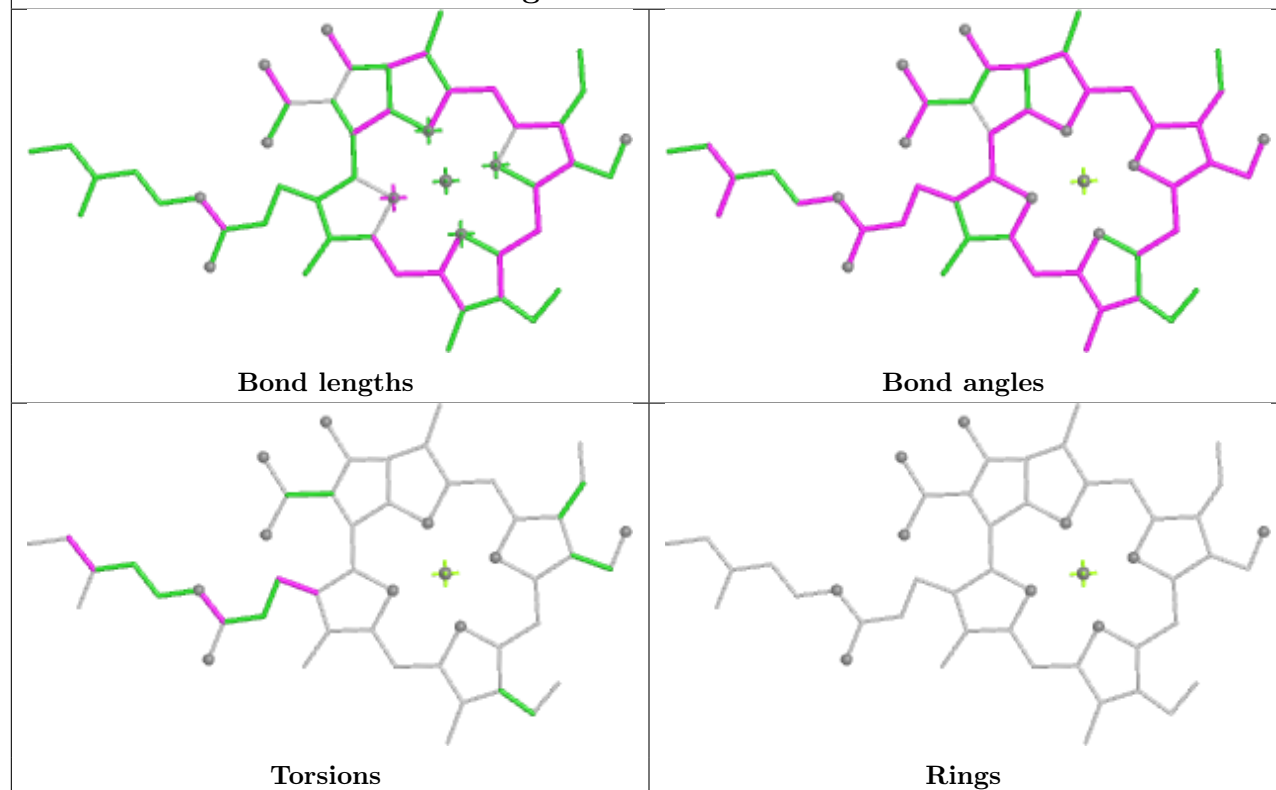
Ligand CLA AB 839



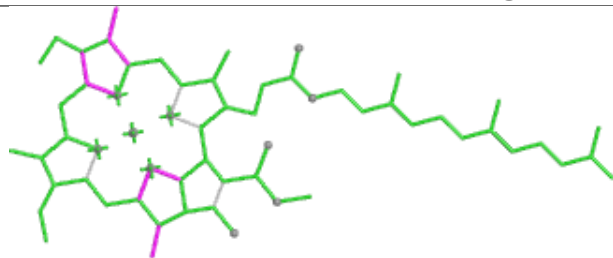
Ligand CLA BA 809



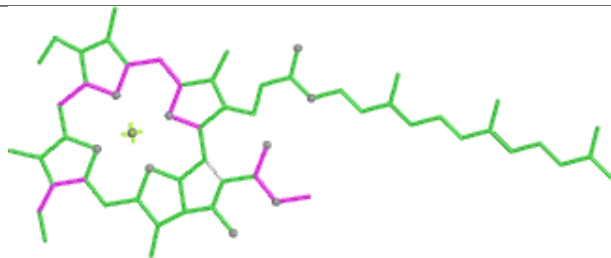
Ligand CHL A1 303



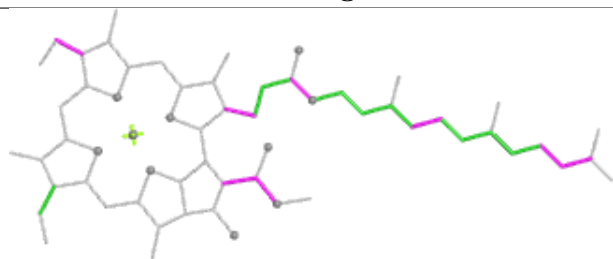
Ligand CLA BH 201



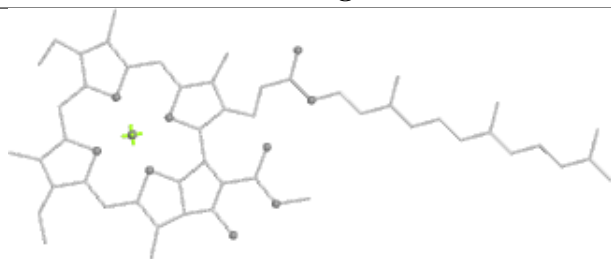
Bond lengths



Bond angles

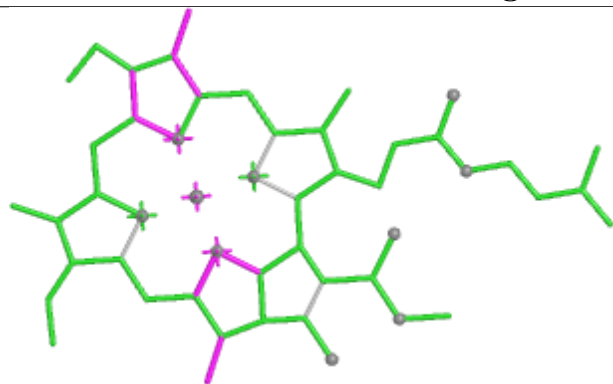


Torsions

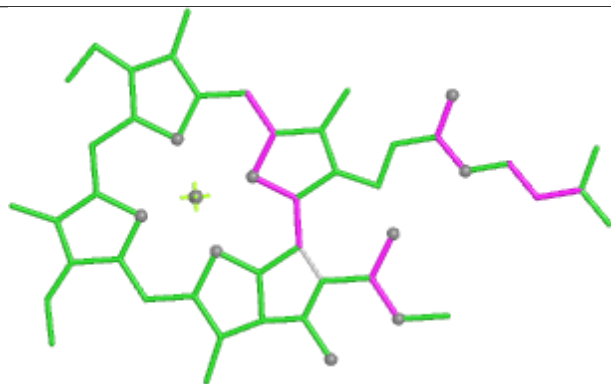


Rings

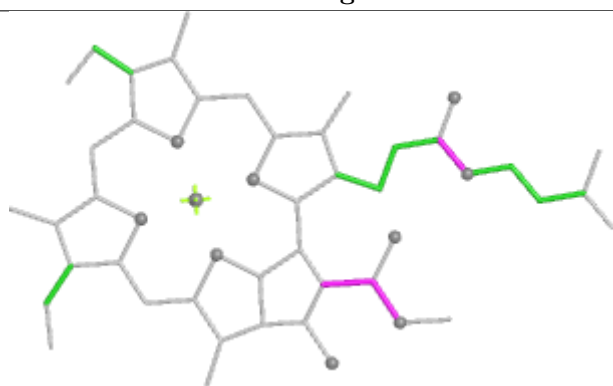
Ligand CLA BB 838



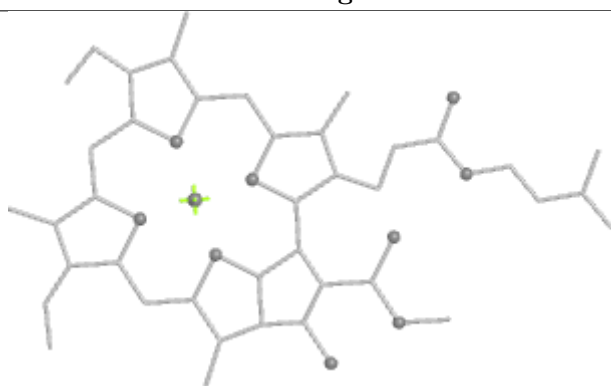
Bond lengths



Bond angles

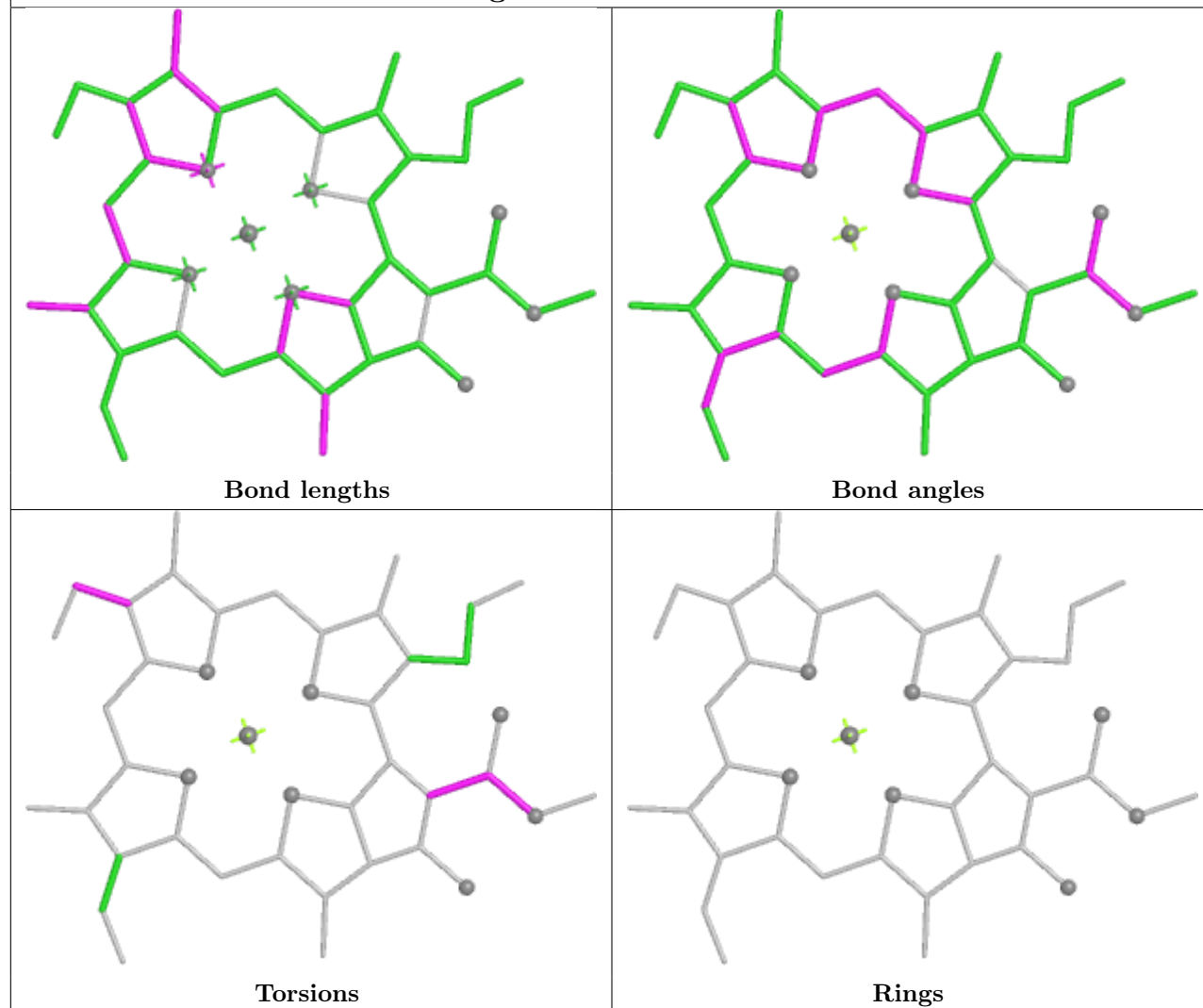


Torsions

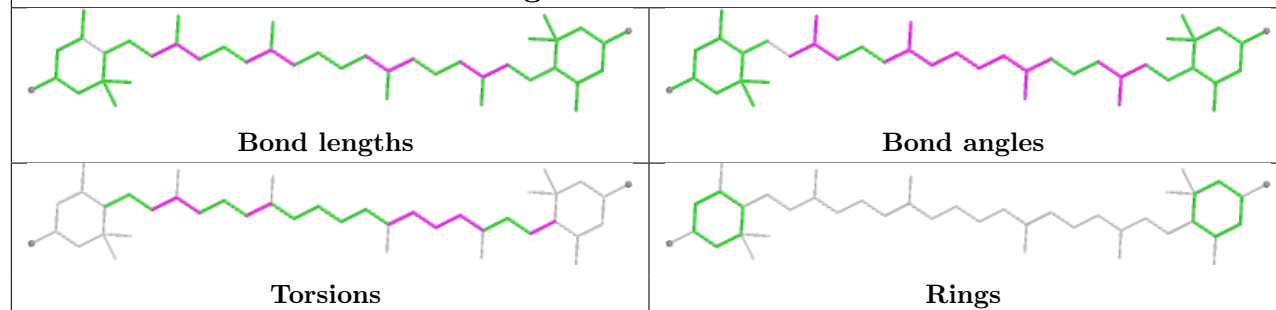


Rings

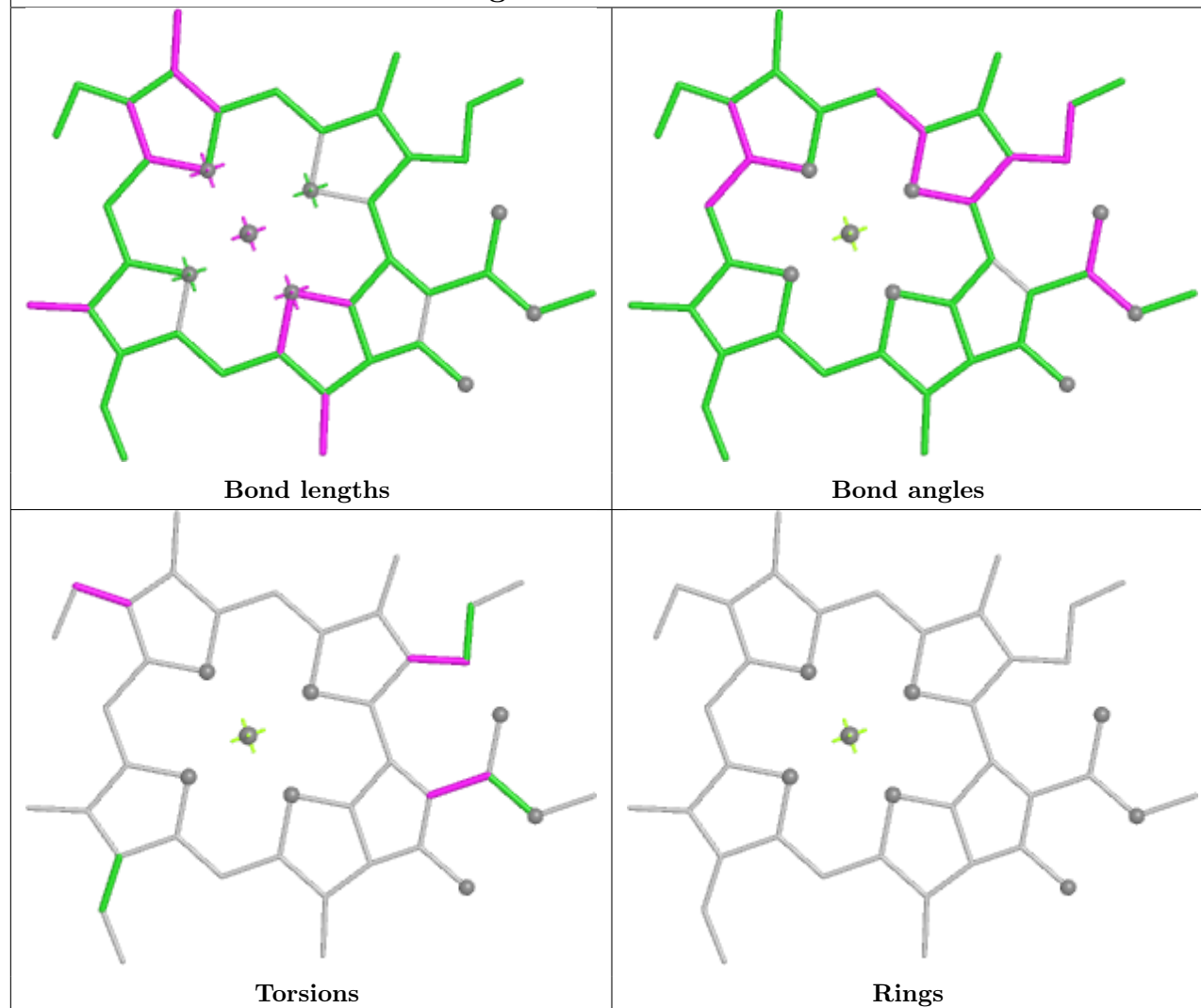
Ligand CLA AB 831



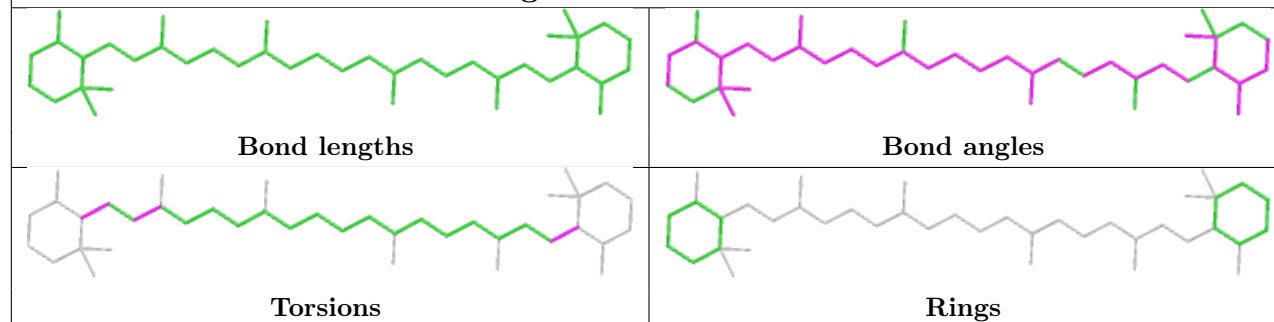
Ligand LUT B1 316



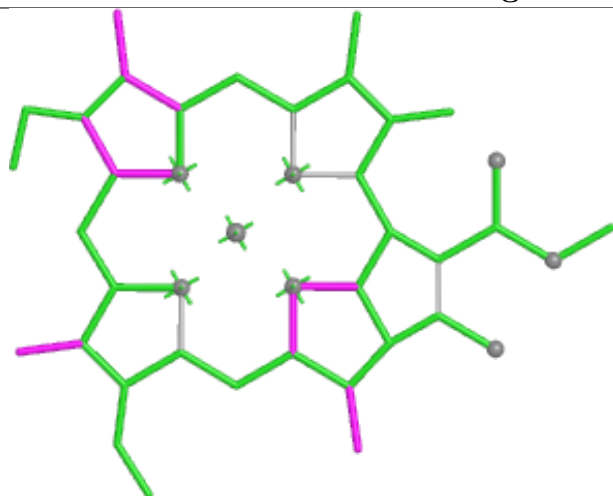
Ligand CLA AB 824



Ligand BCR AJ 103



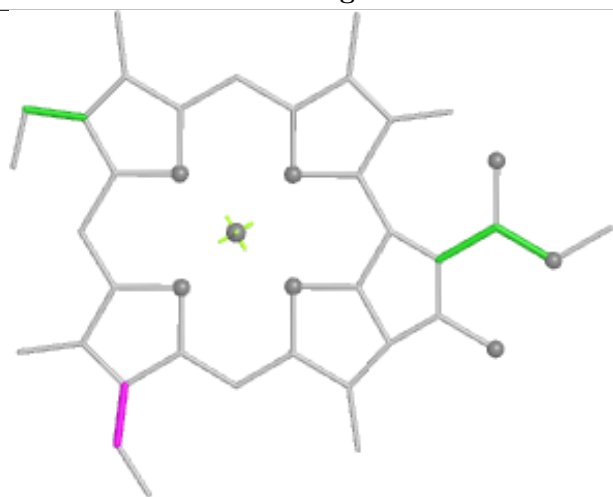
Ligand CLA BB 806



Bond lengths



Bond angles

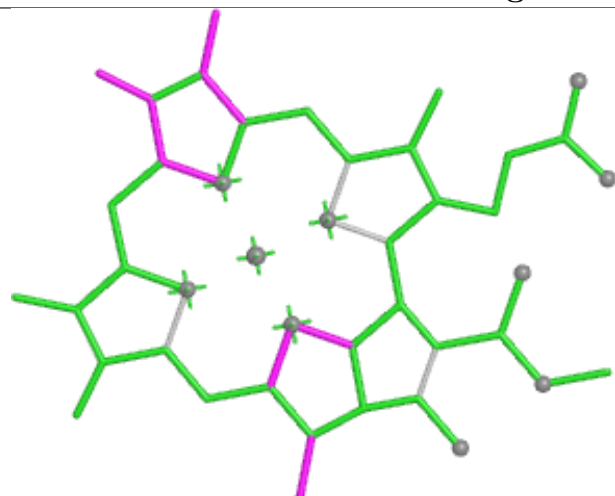


Torsions

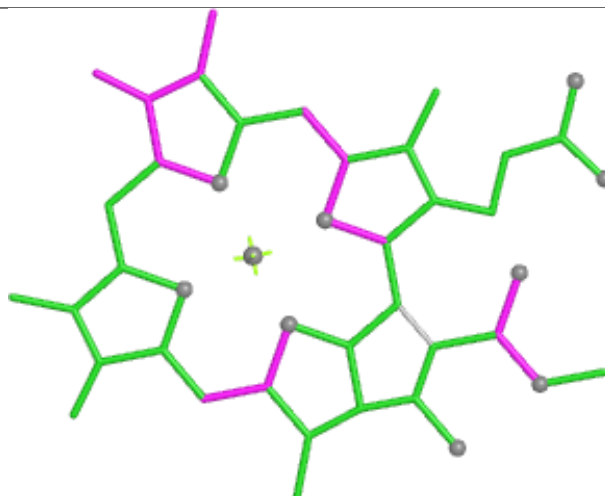


Rings

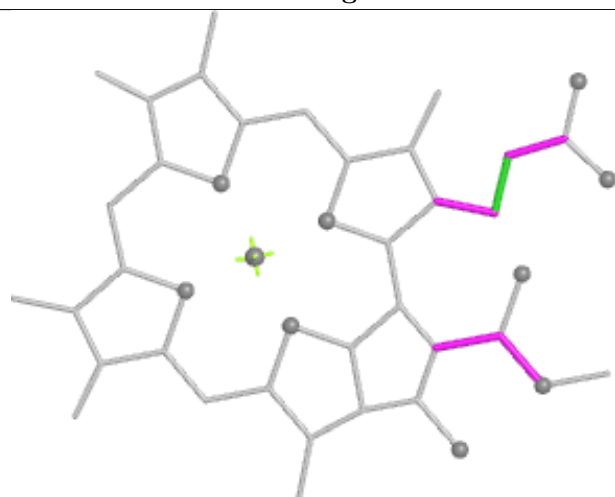
Ligand CLA A1 316



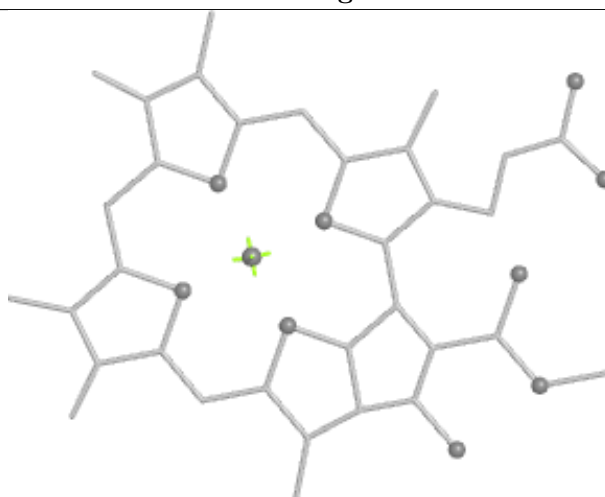
Bond lengths



Bond angles

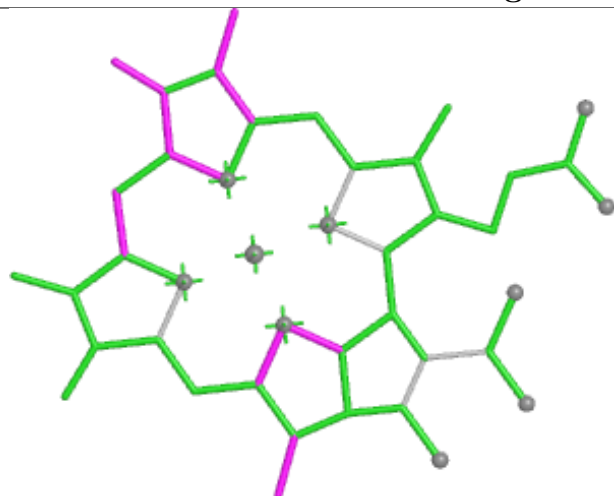


Torsions

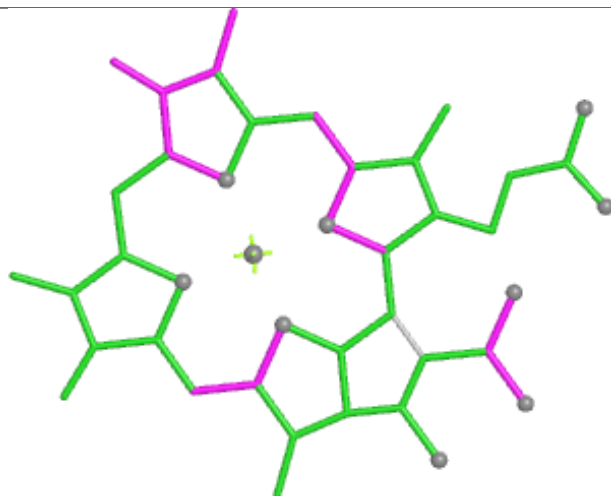


Rings

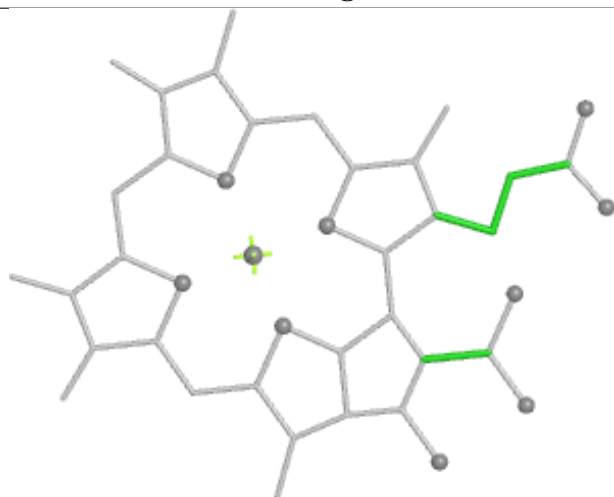
Ligand CLA A3 304



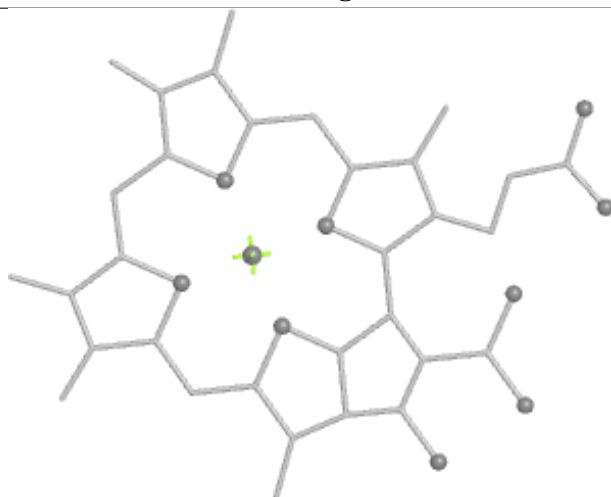
Bond lengths



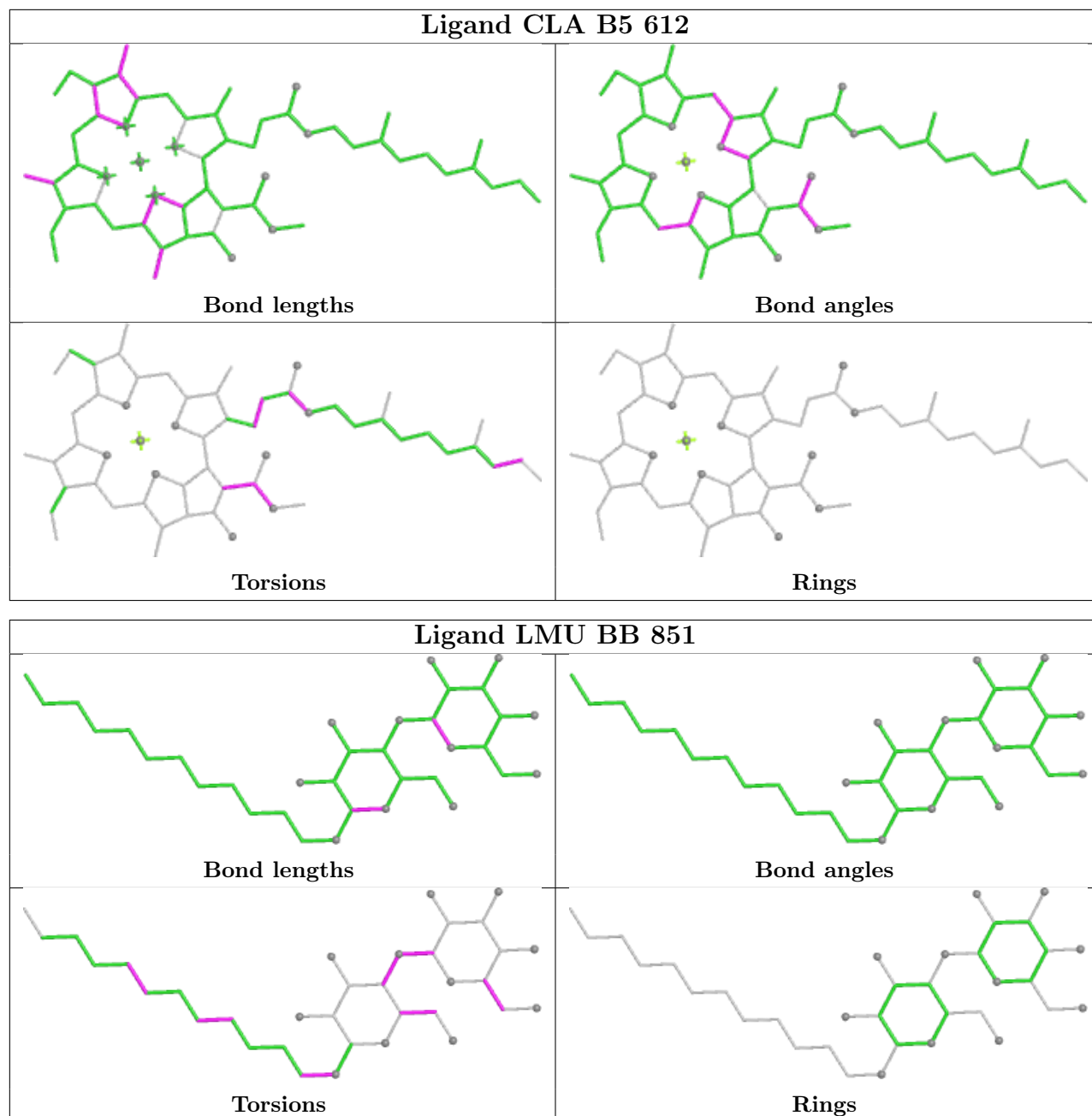
Bond angles

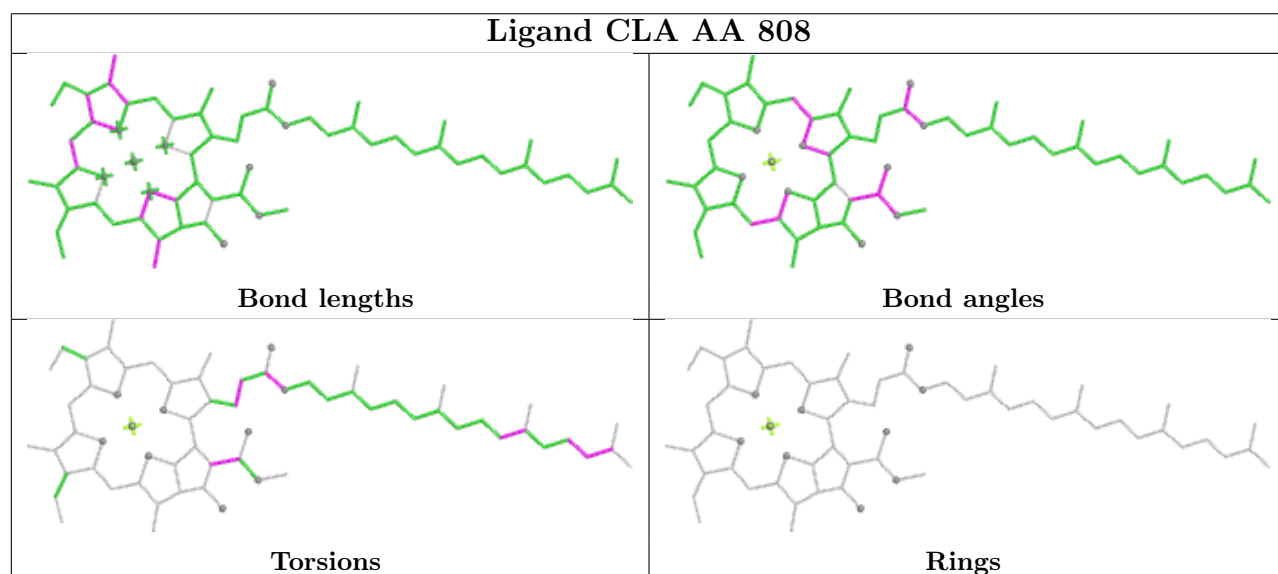
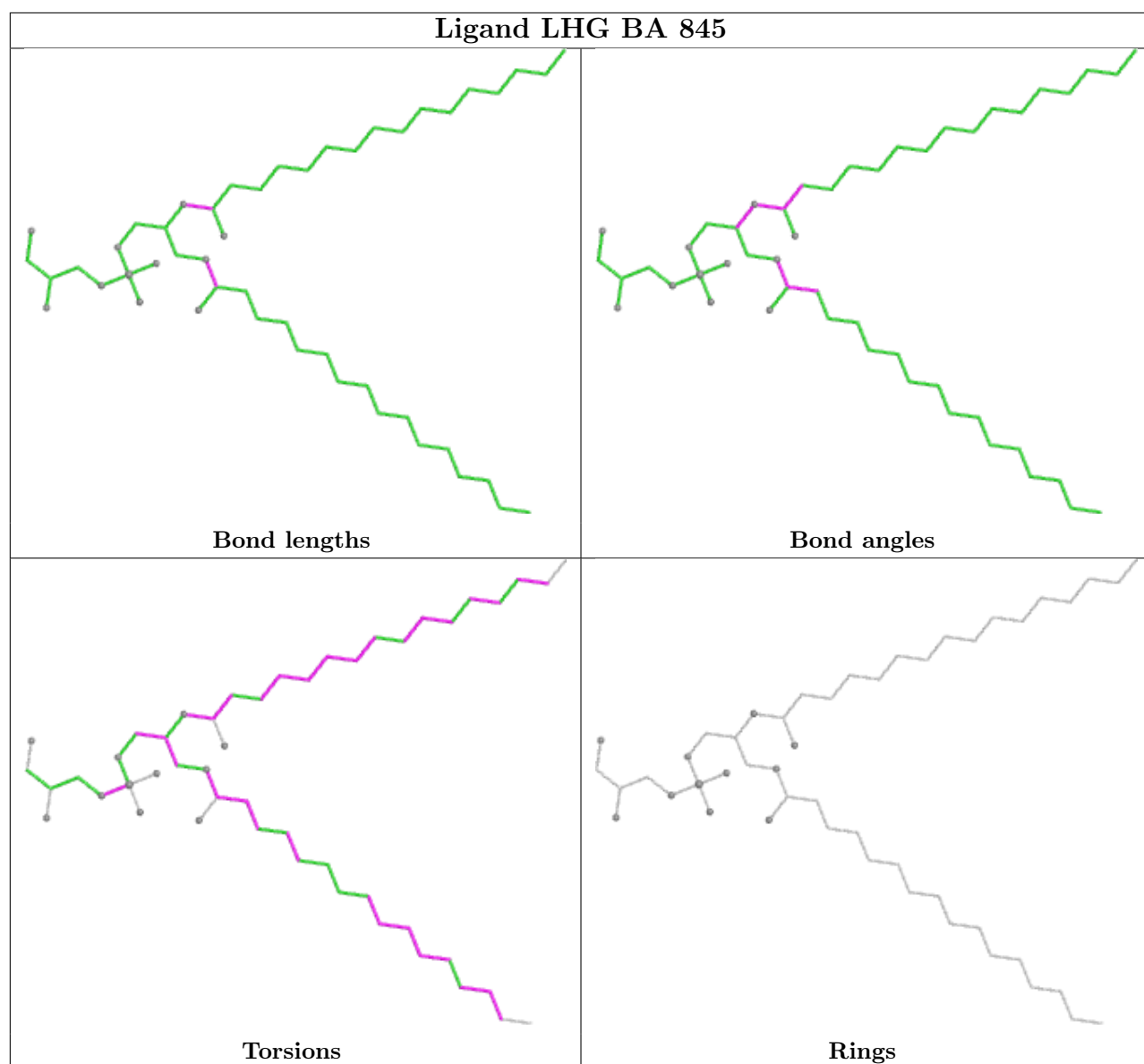


Torsions

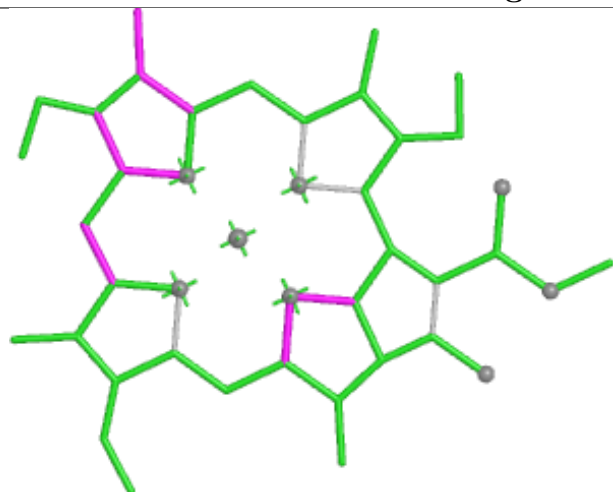


Rings

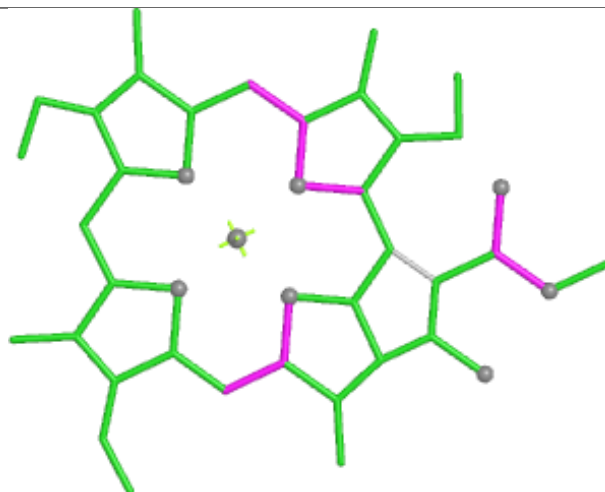




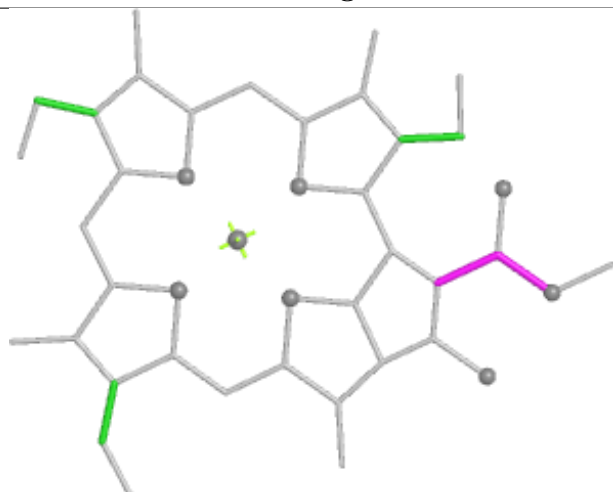
Ligand CLA BJ 102



Bond lengths



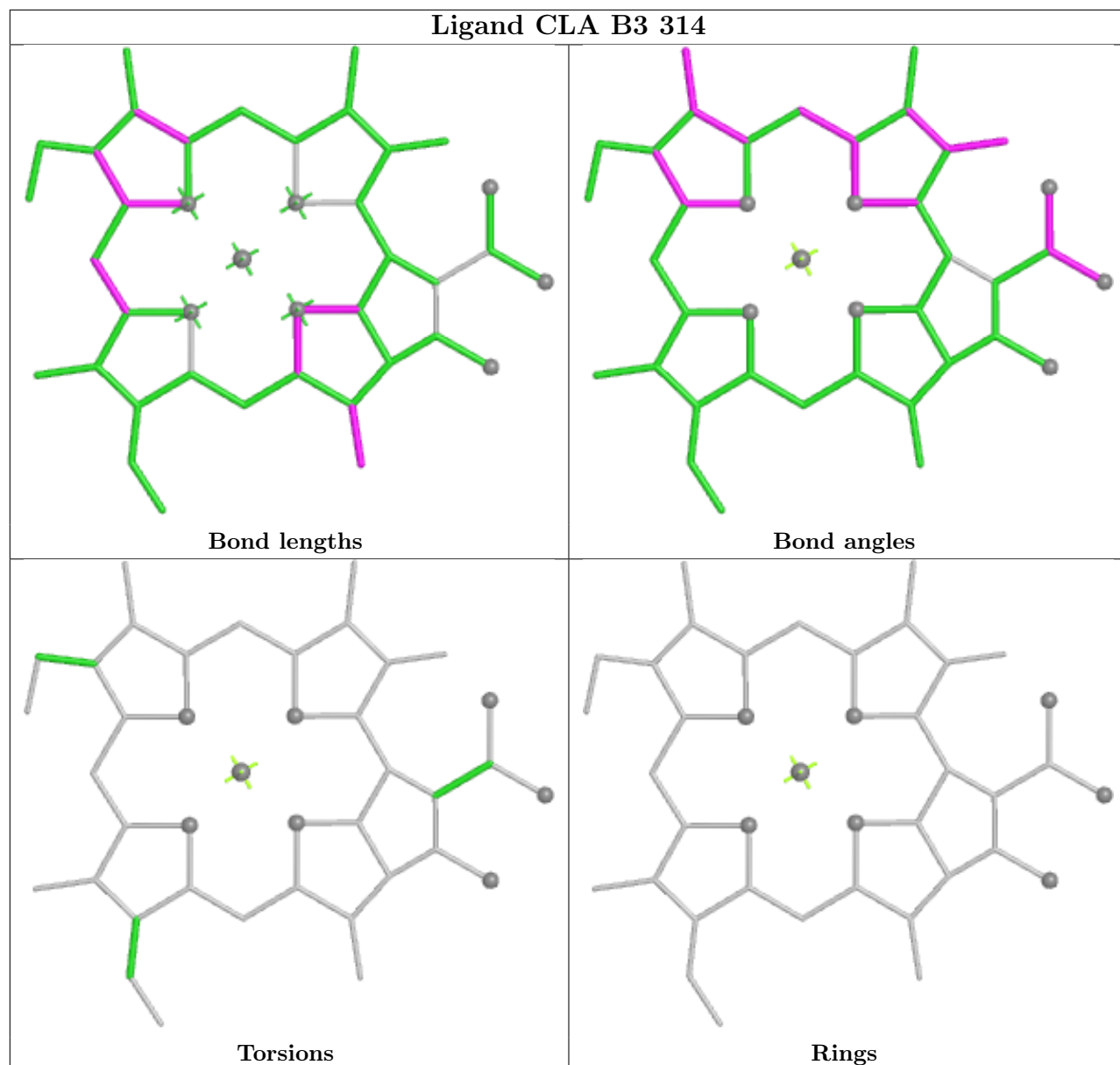
Bond angles



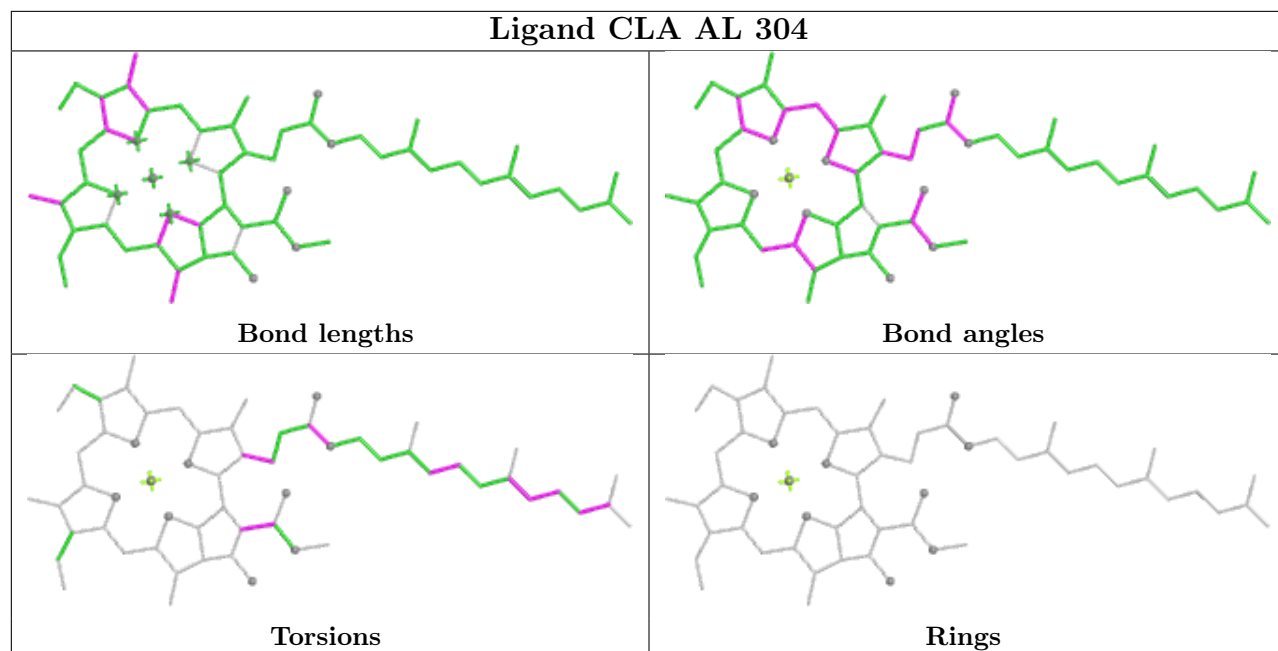
Torsions



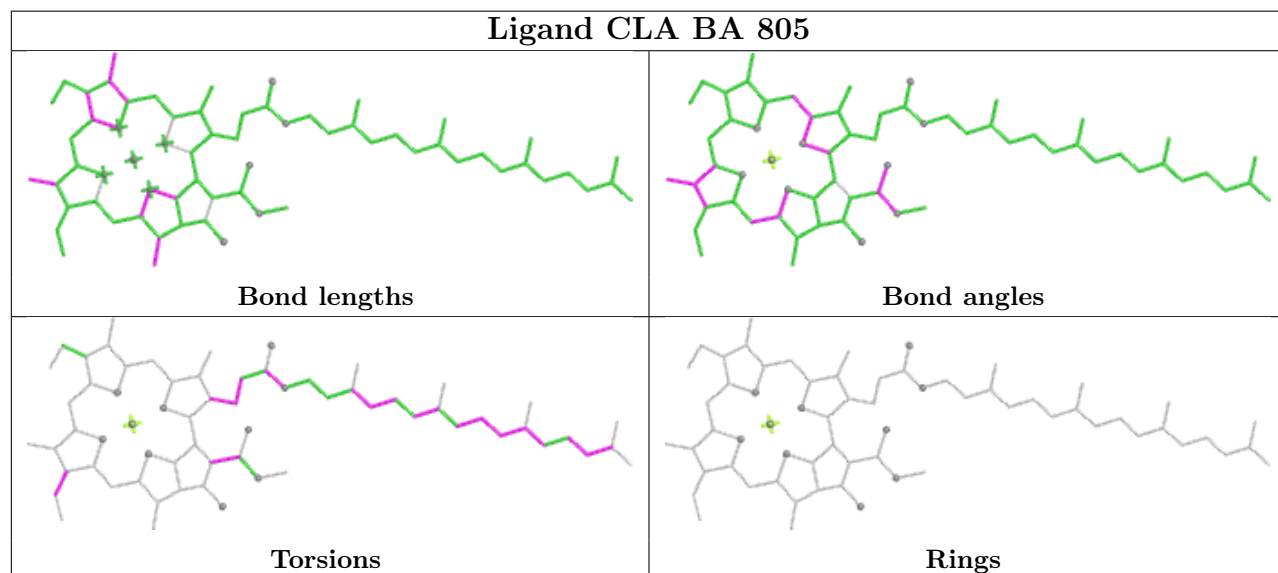
Rings



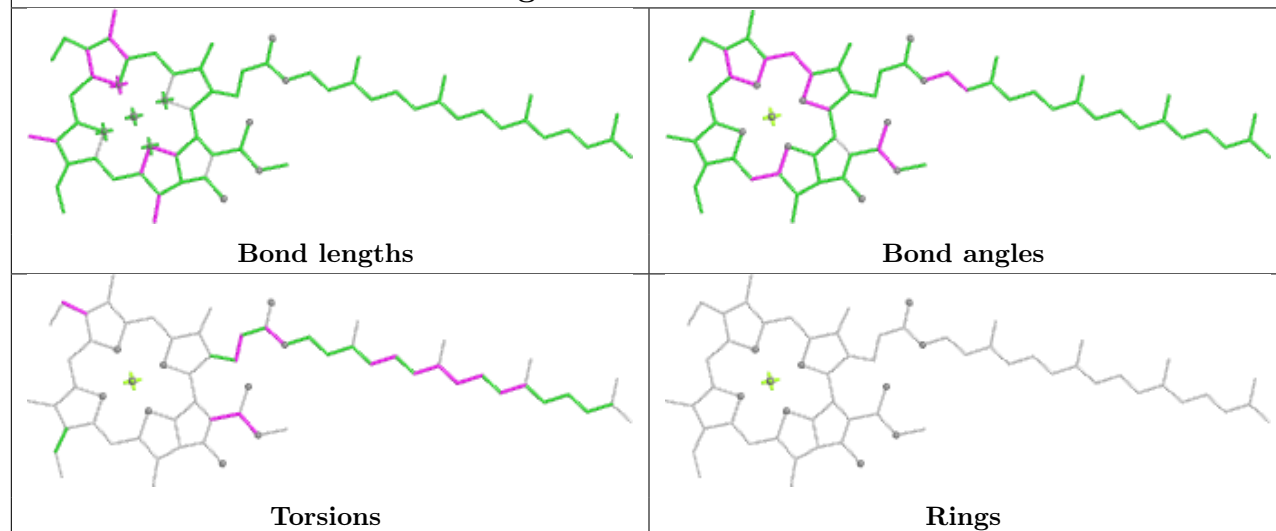
Ligand CLA AL 304



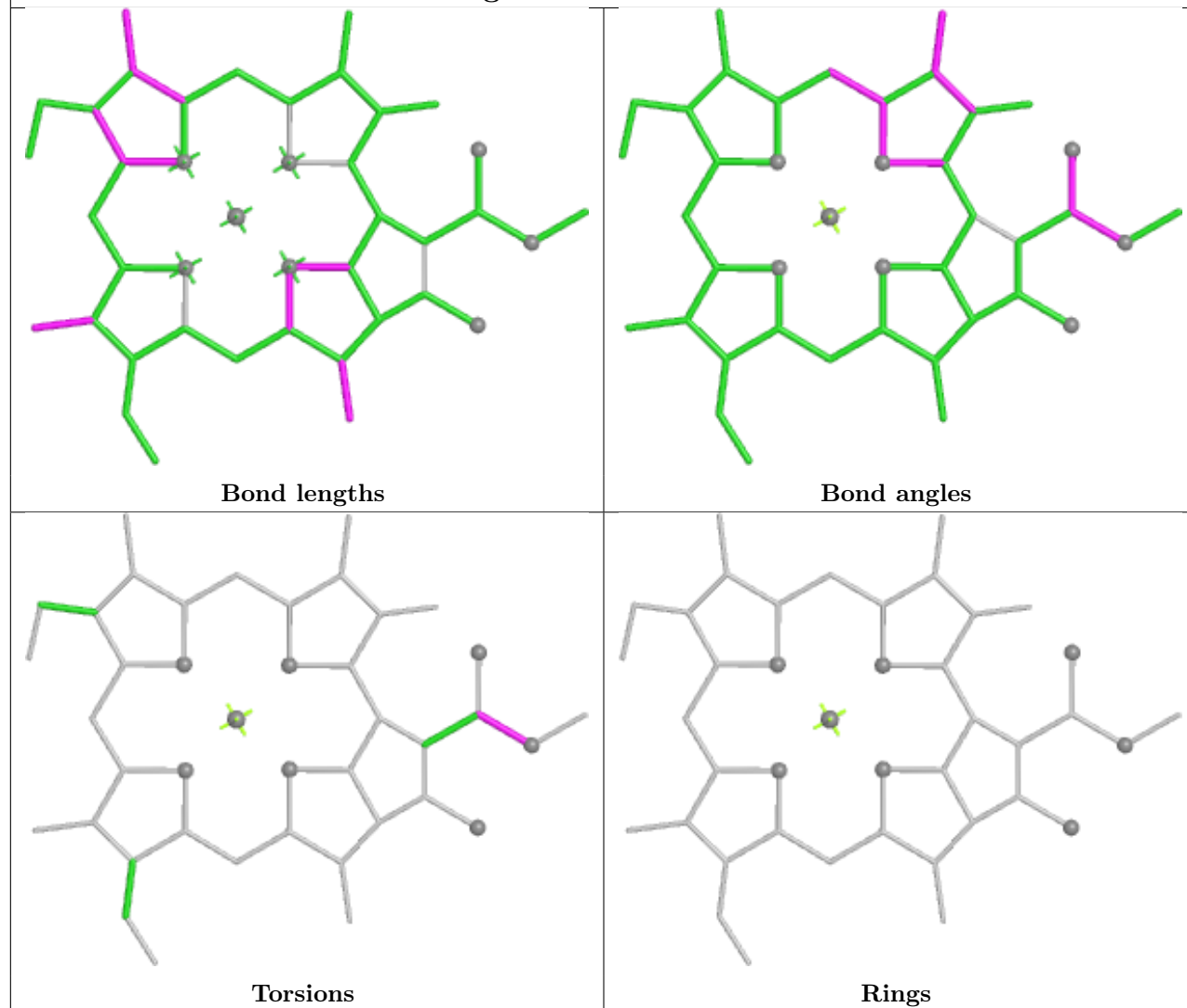
Ligand CLA BA 805

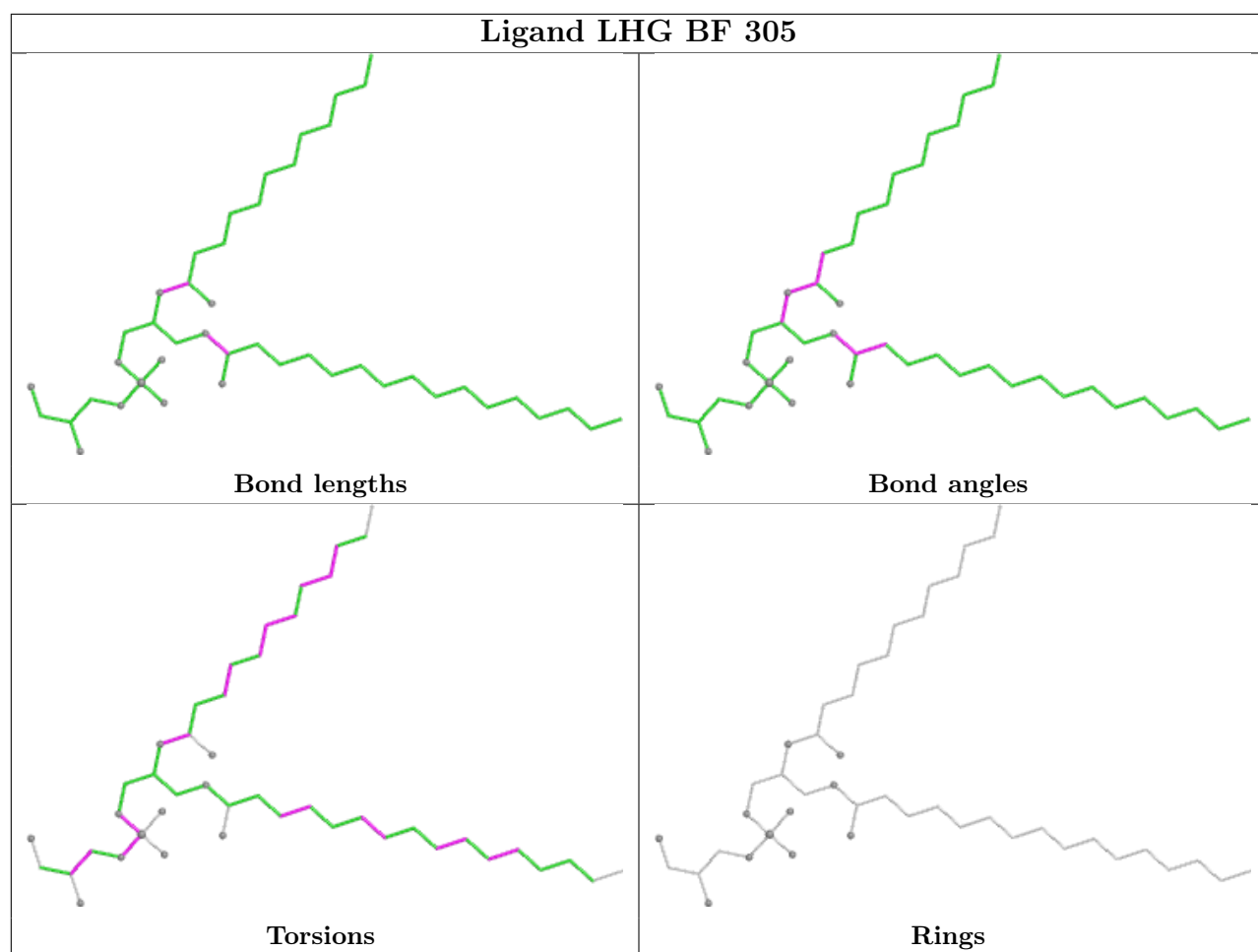


Ligand CLA AA 813

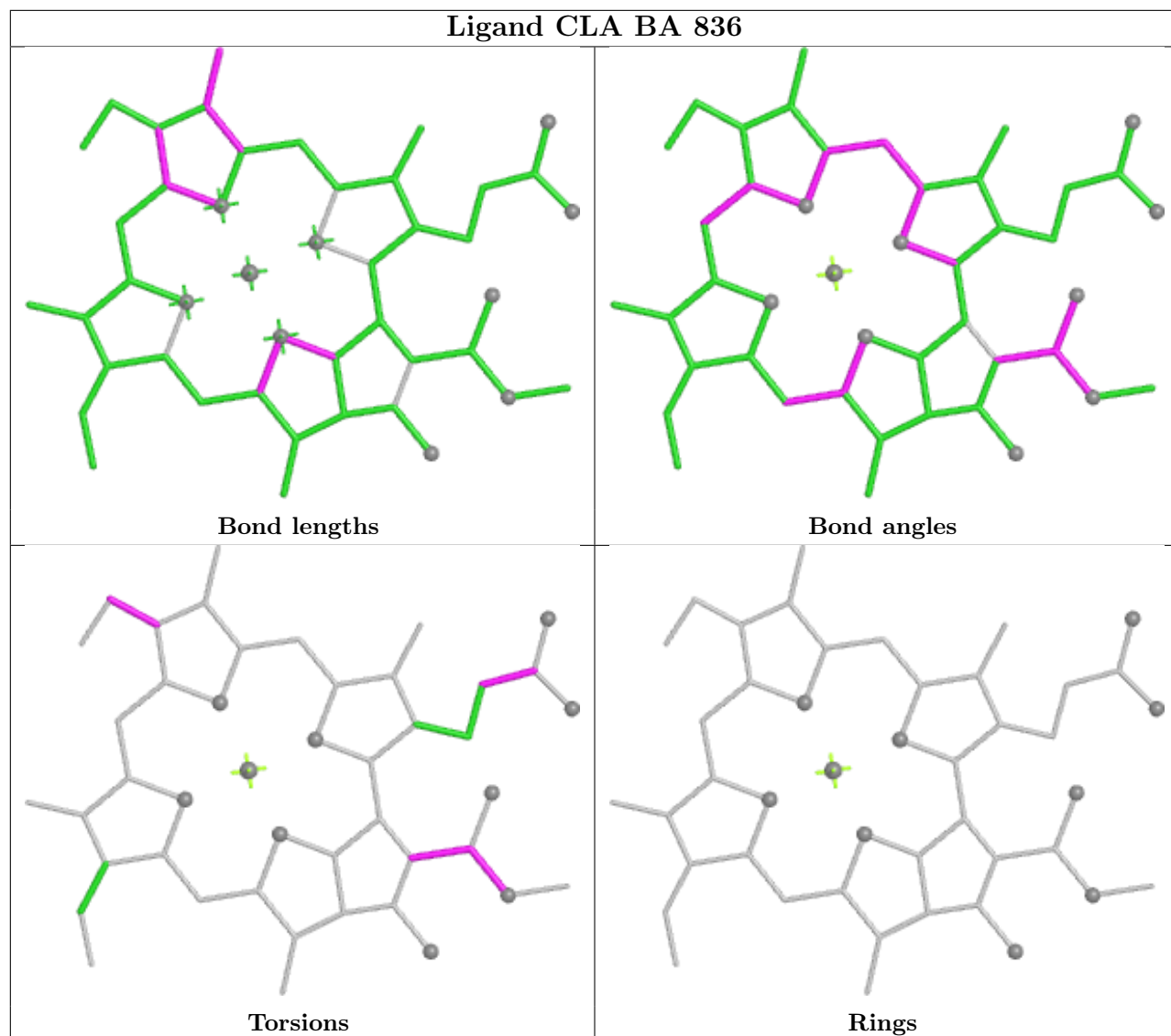


Ligand CLA BB 822

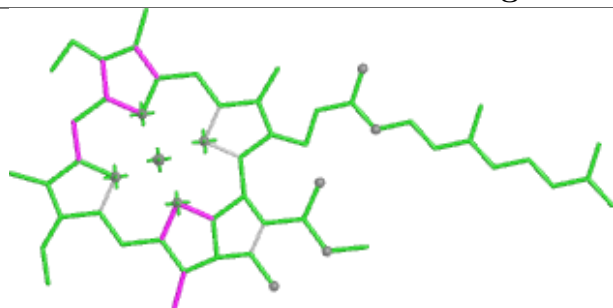




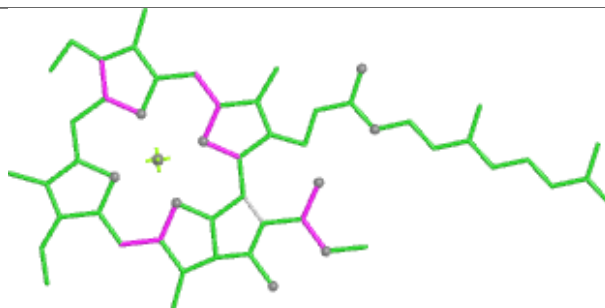
Ligand CLA BA 836



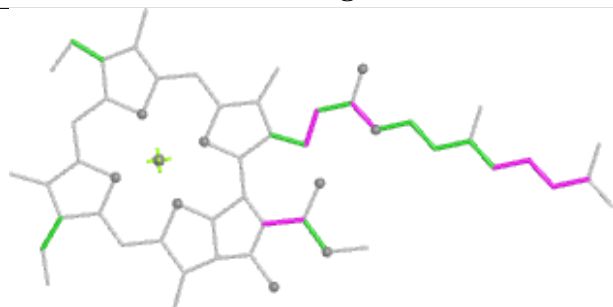
Ligand CLA AB 817



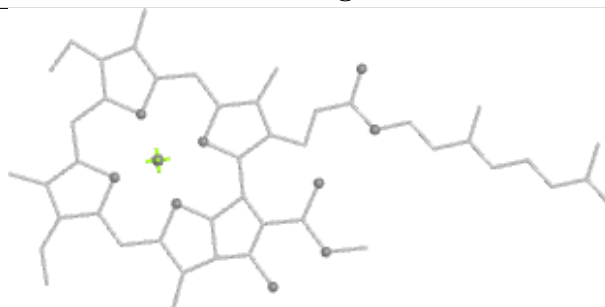
Bond lengths



Bond angles

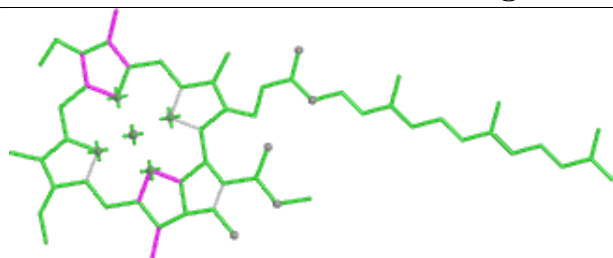


Torsions

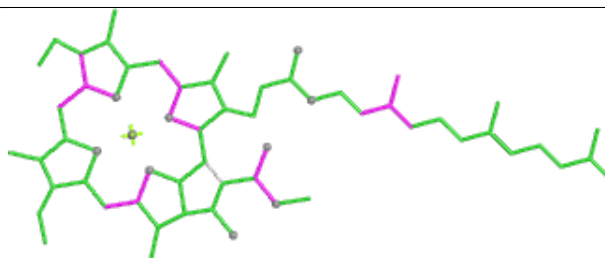


Rings

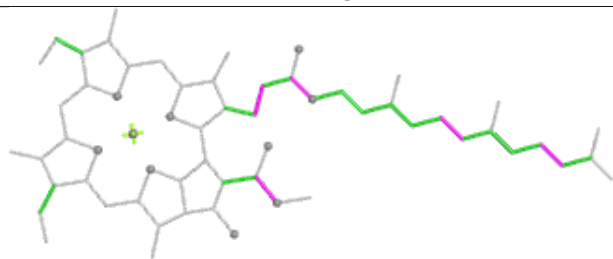
Ligand CLA AA 817



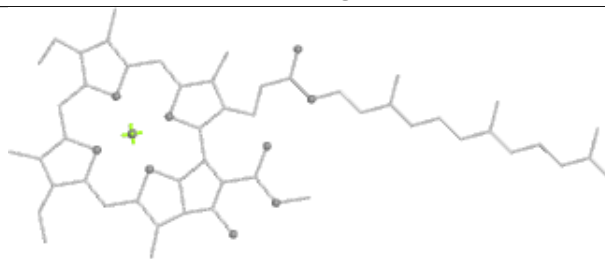
Bond lengths



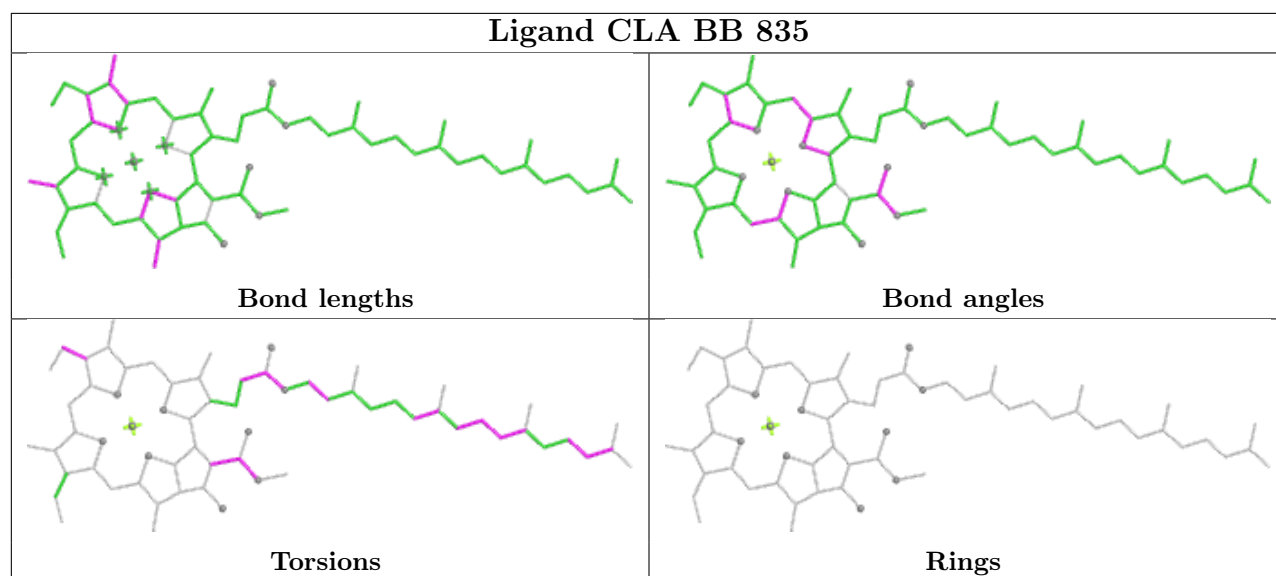
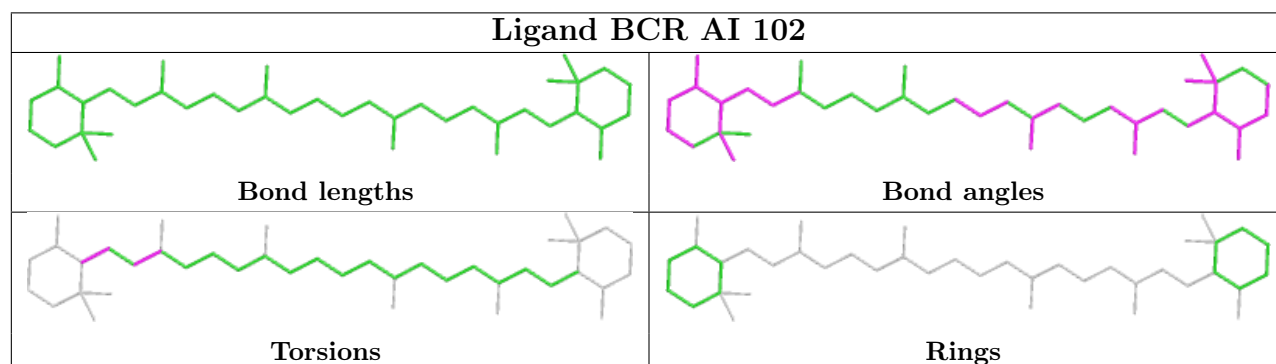
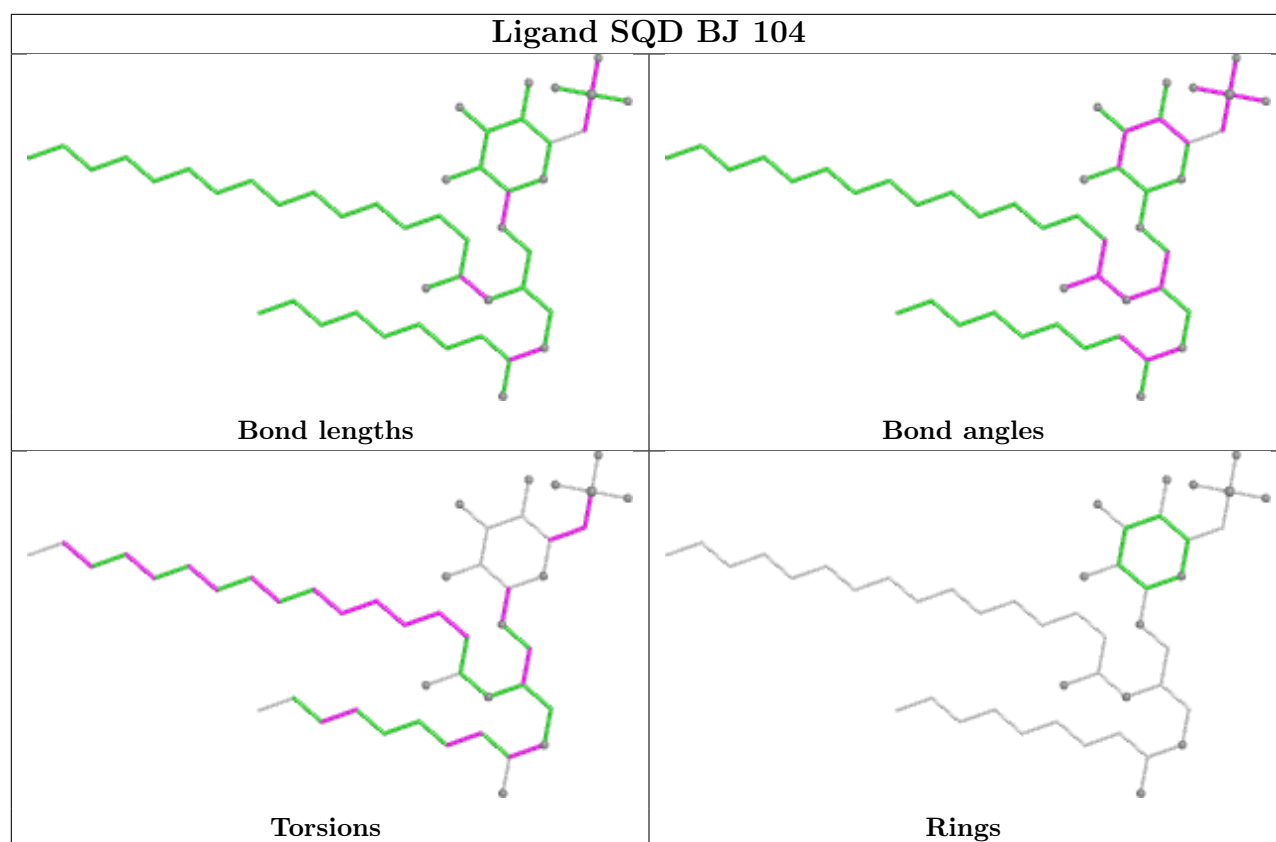
Bond angles



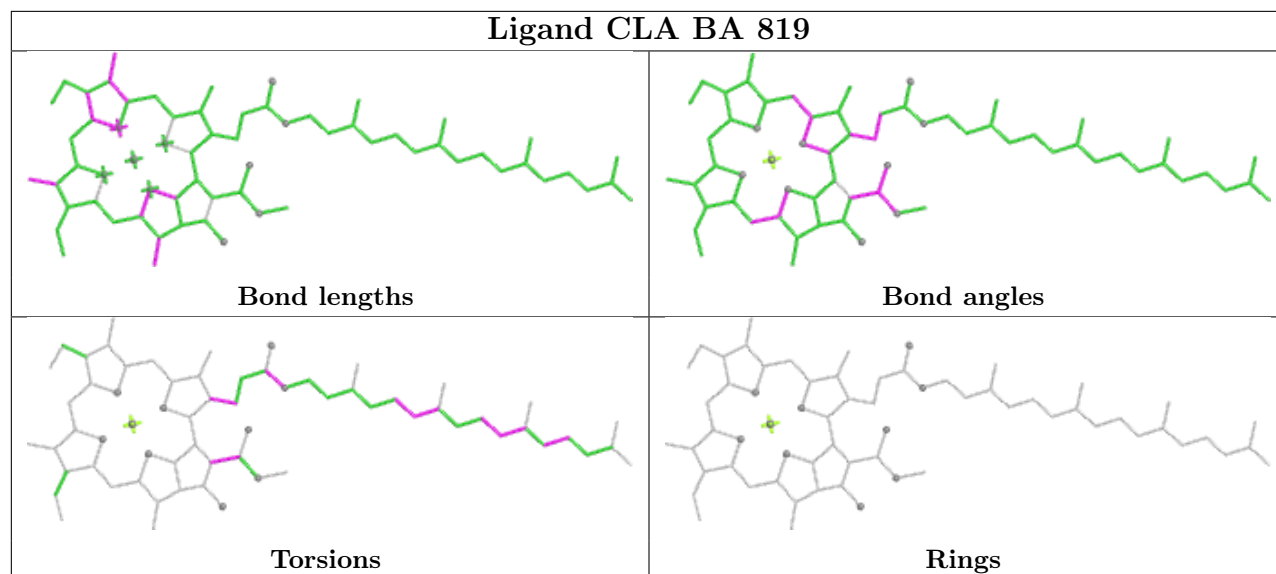
Torsions



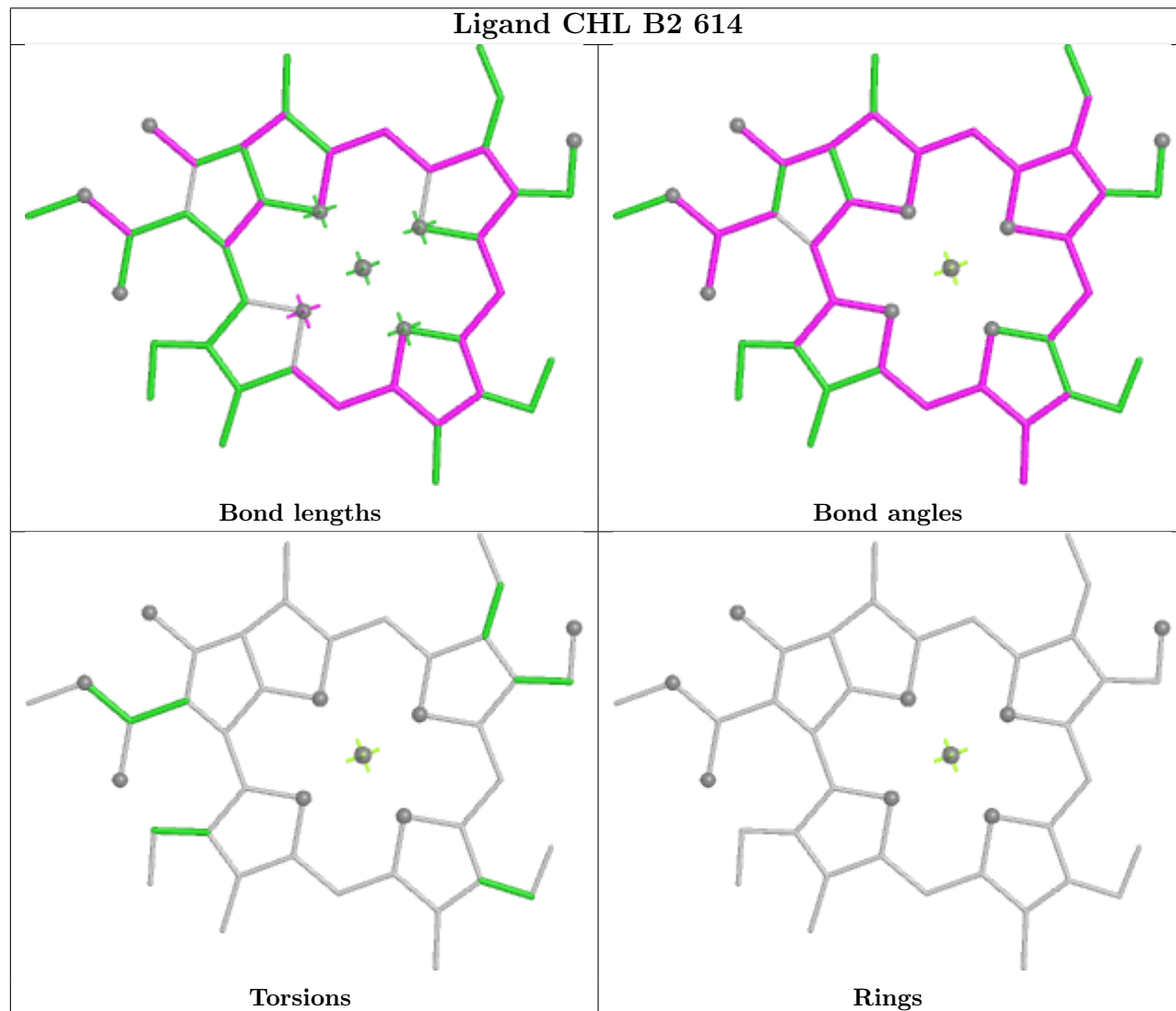
Rings

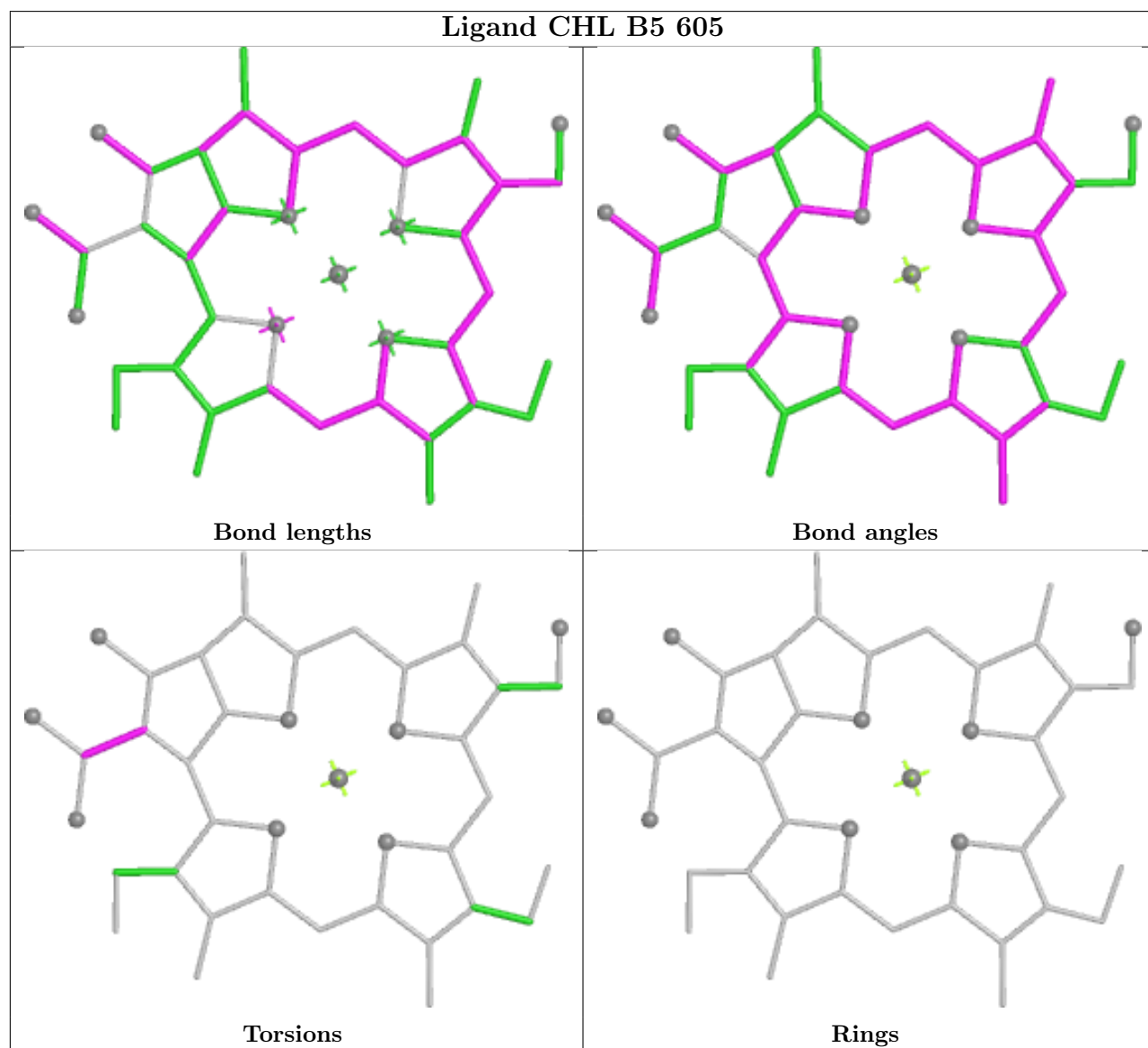
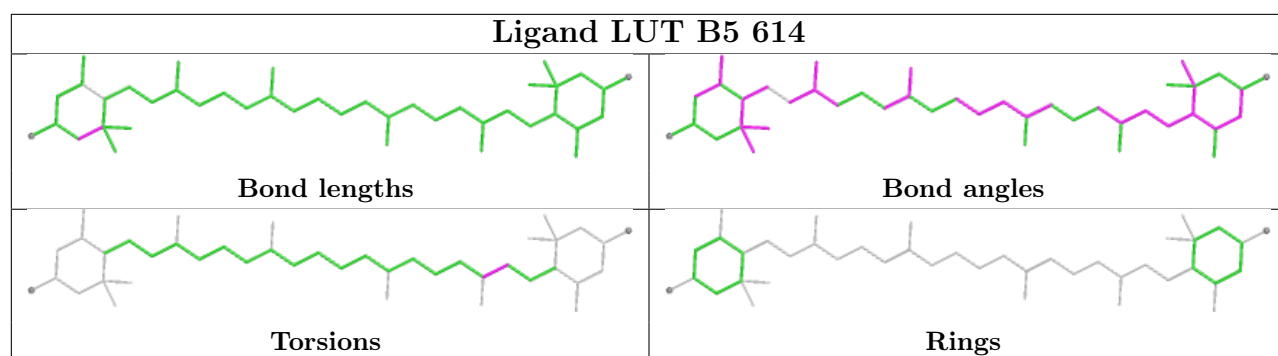


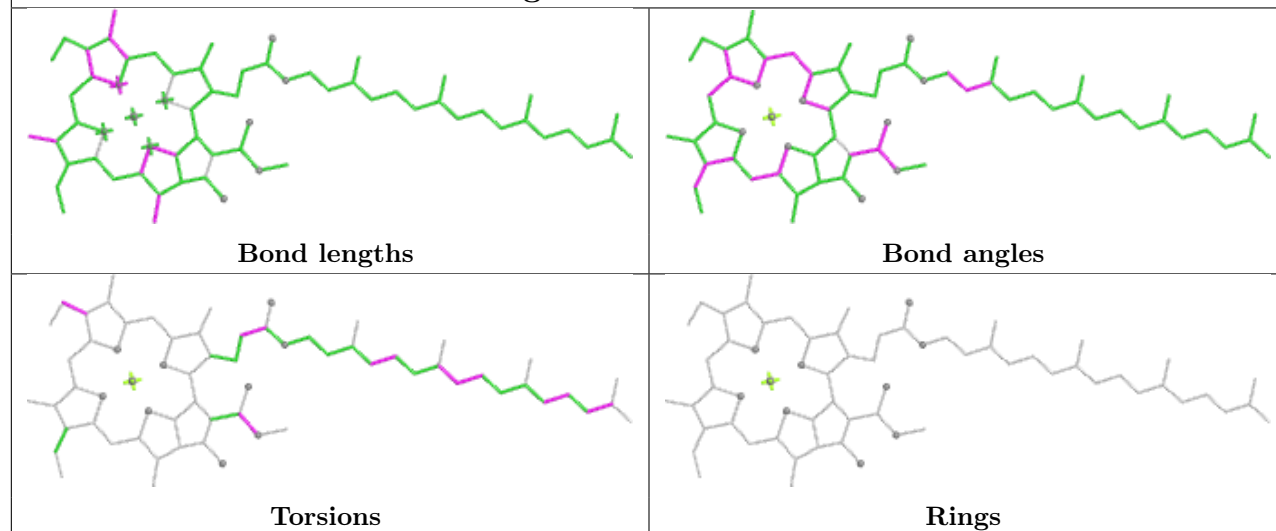
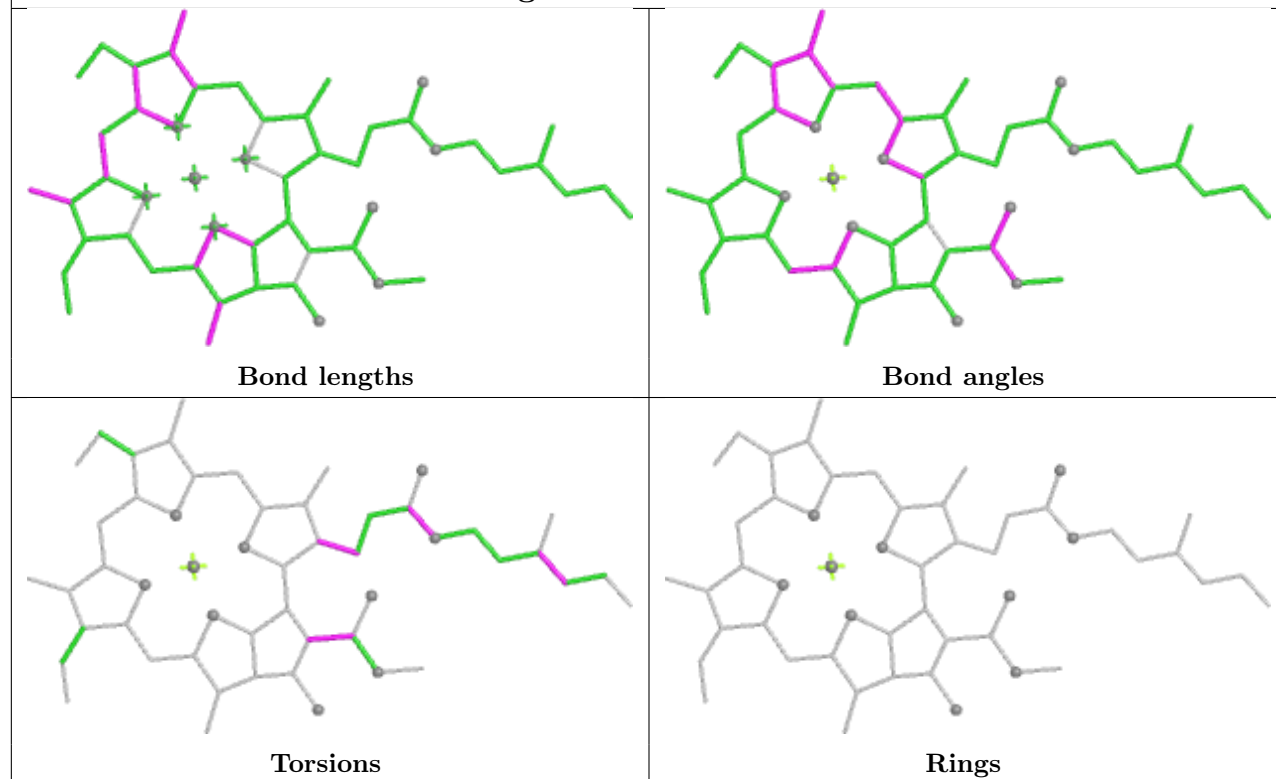
Ligand CLA BA 819

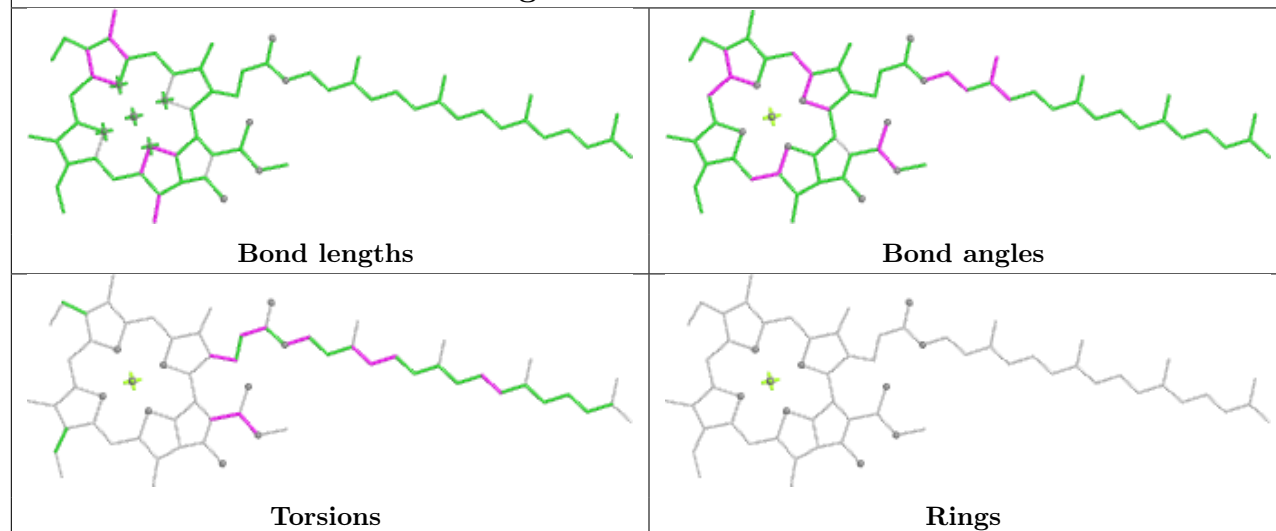
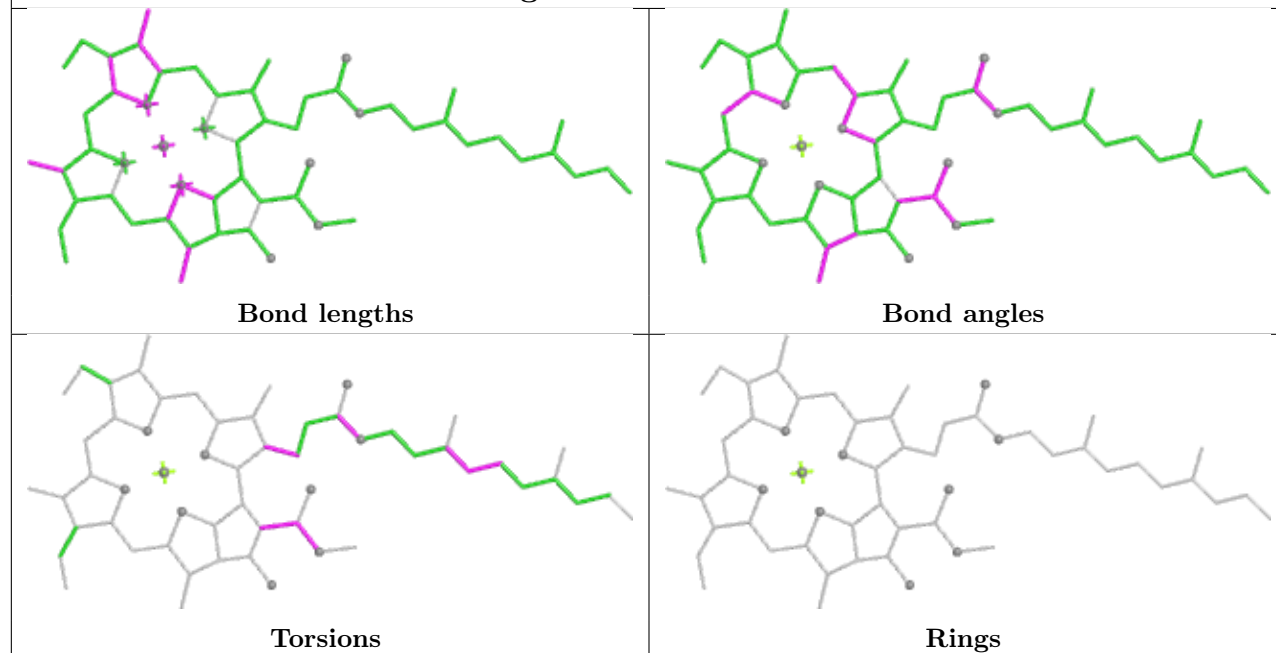


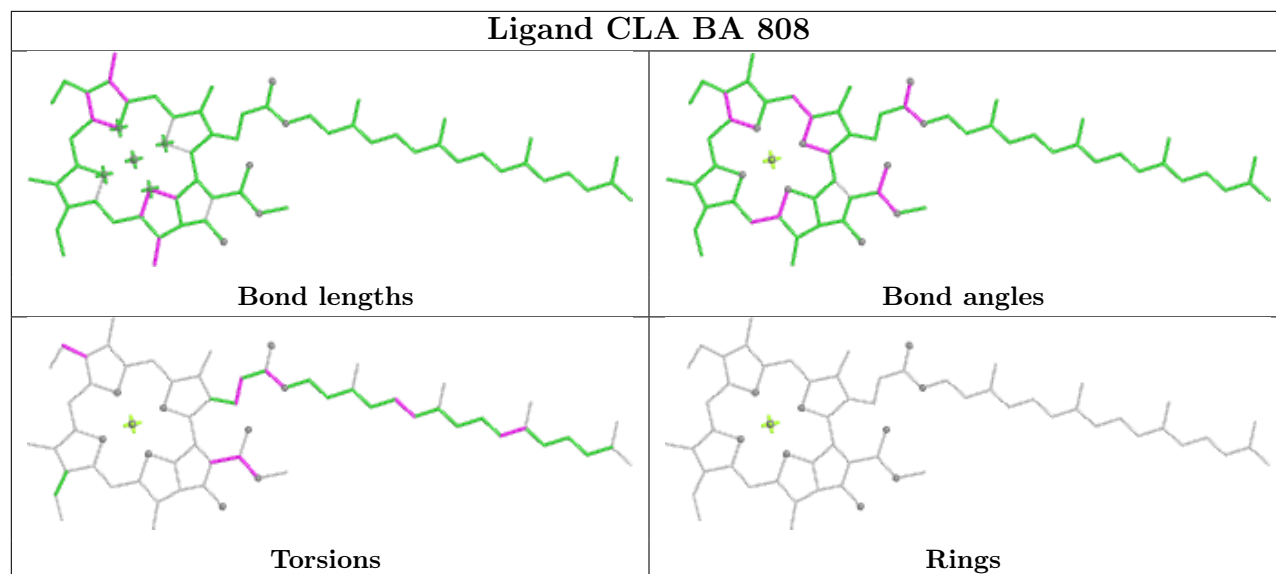
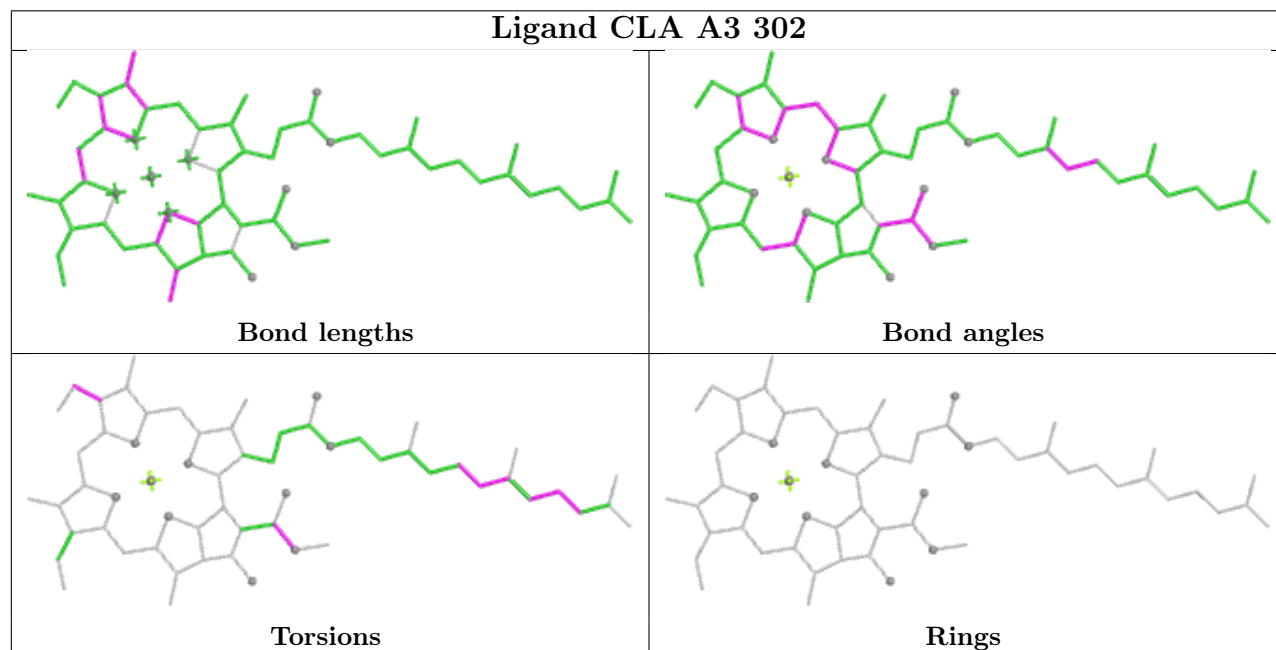
Ligand CHL B2 614

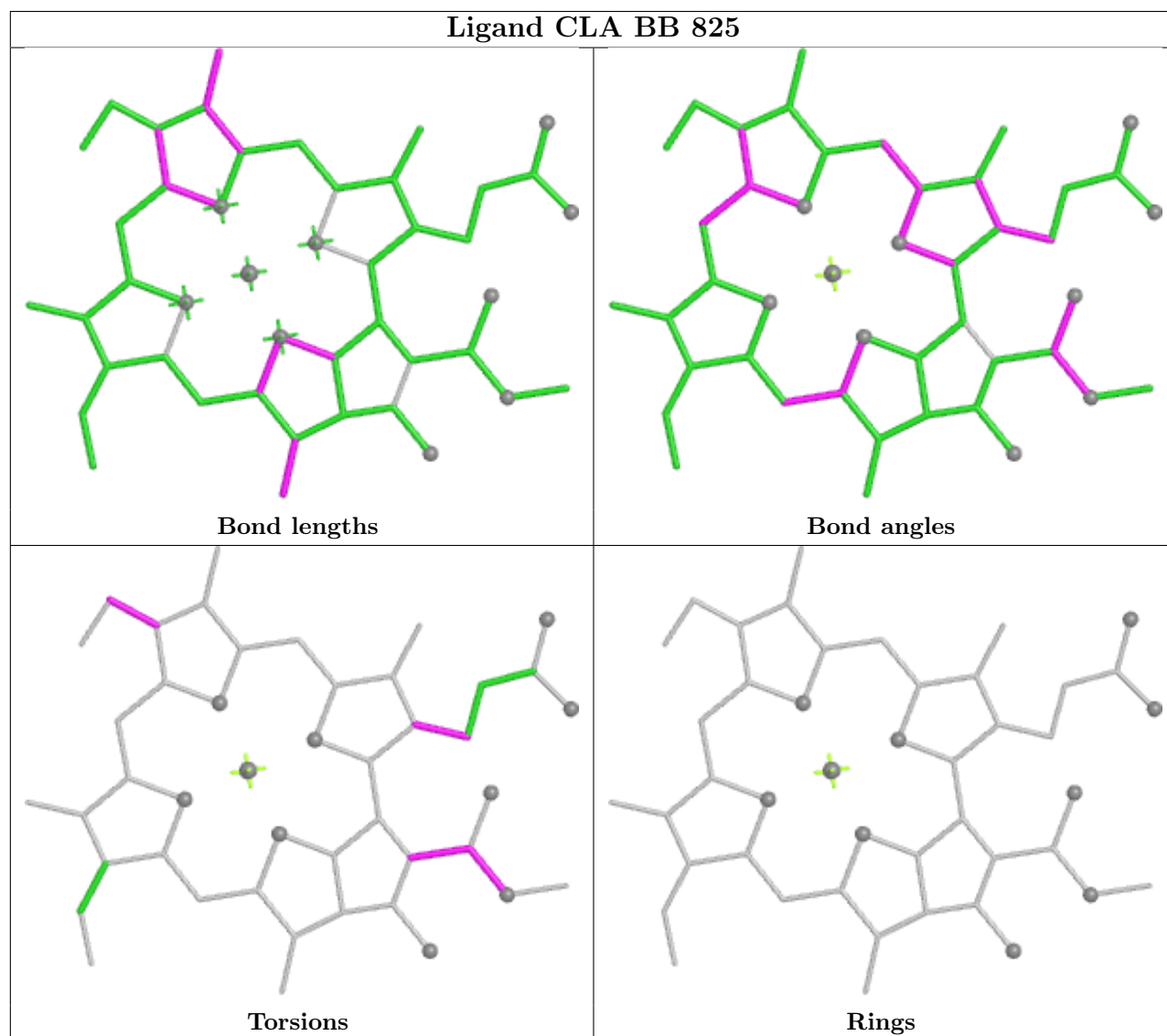
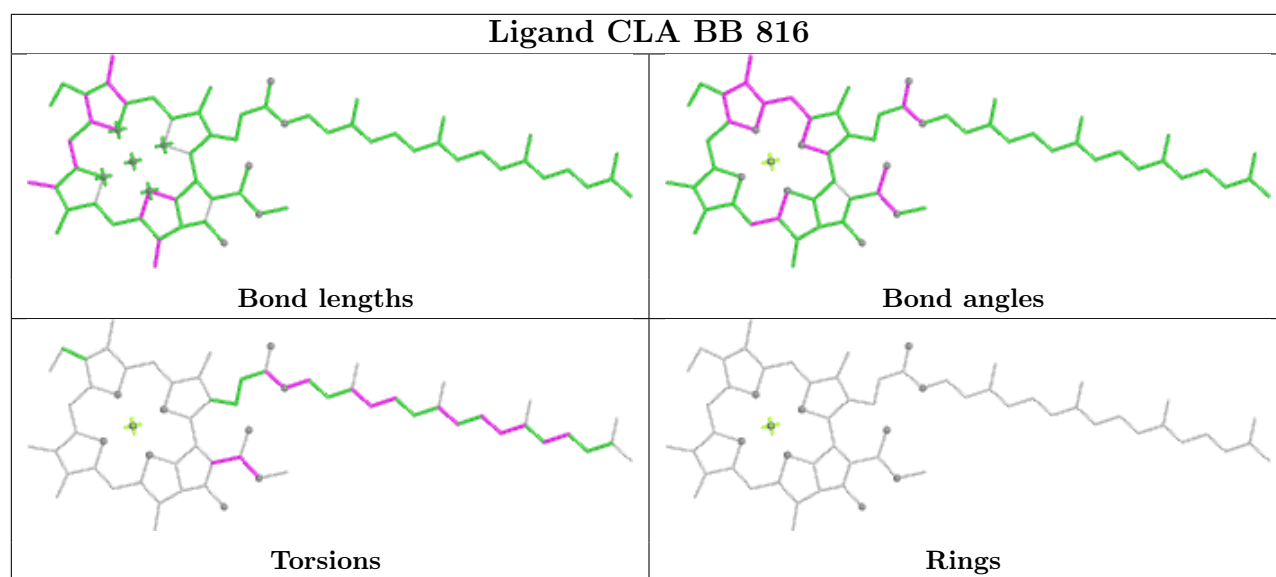


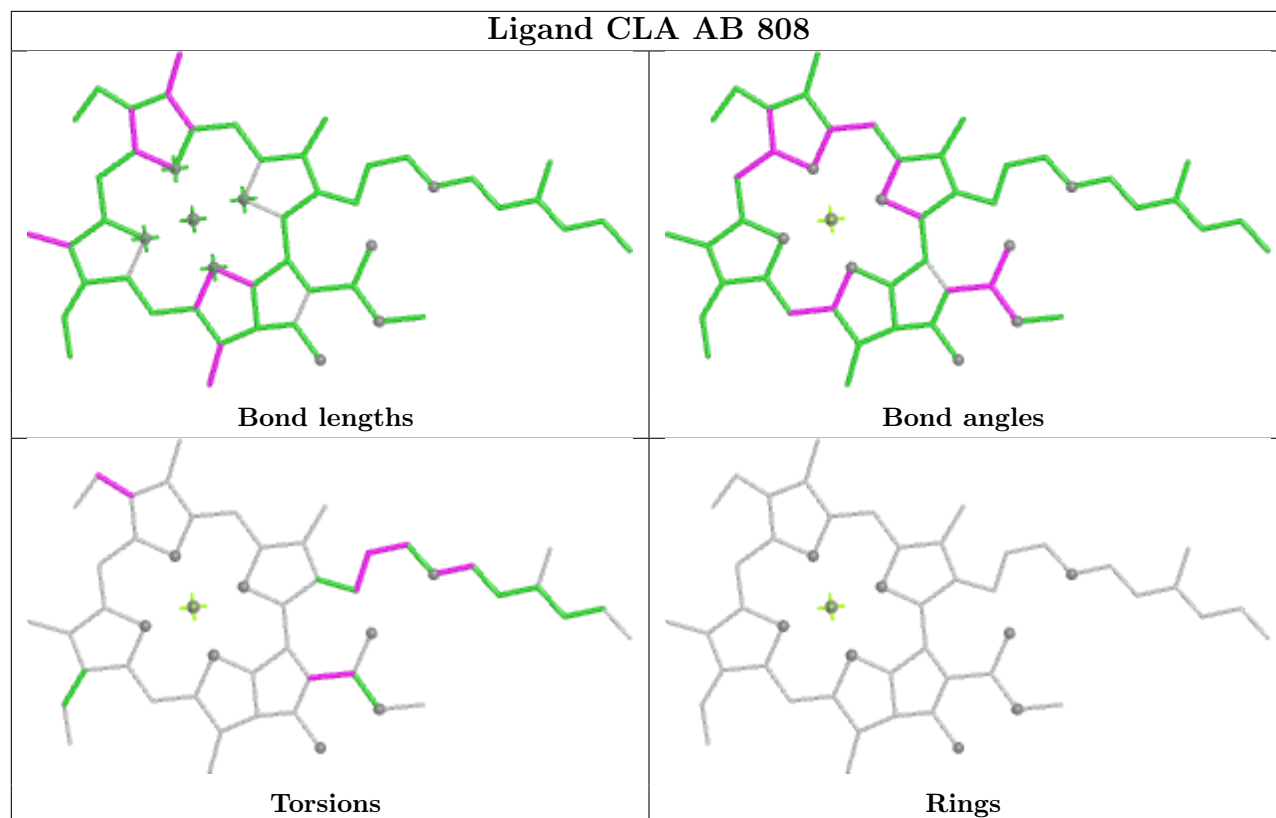


Ligand CLA B2 602**Ligand CLA AA 804**

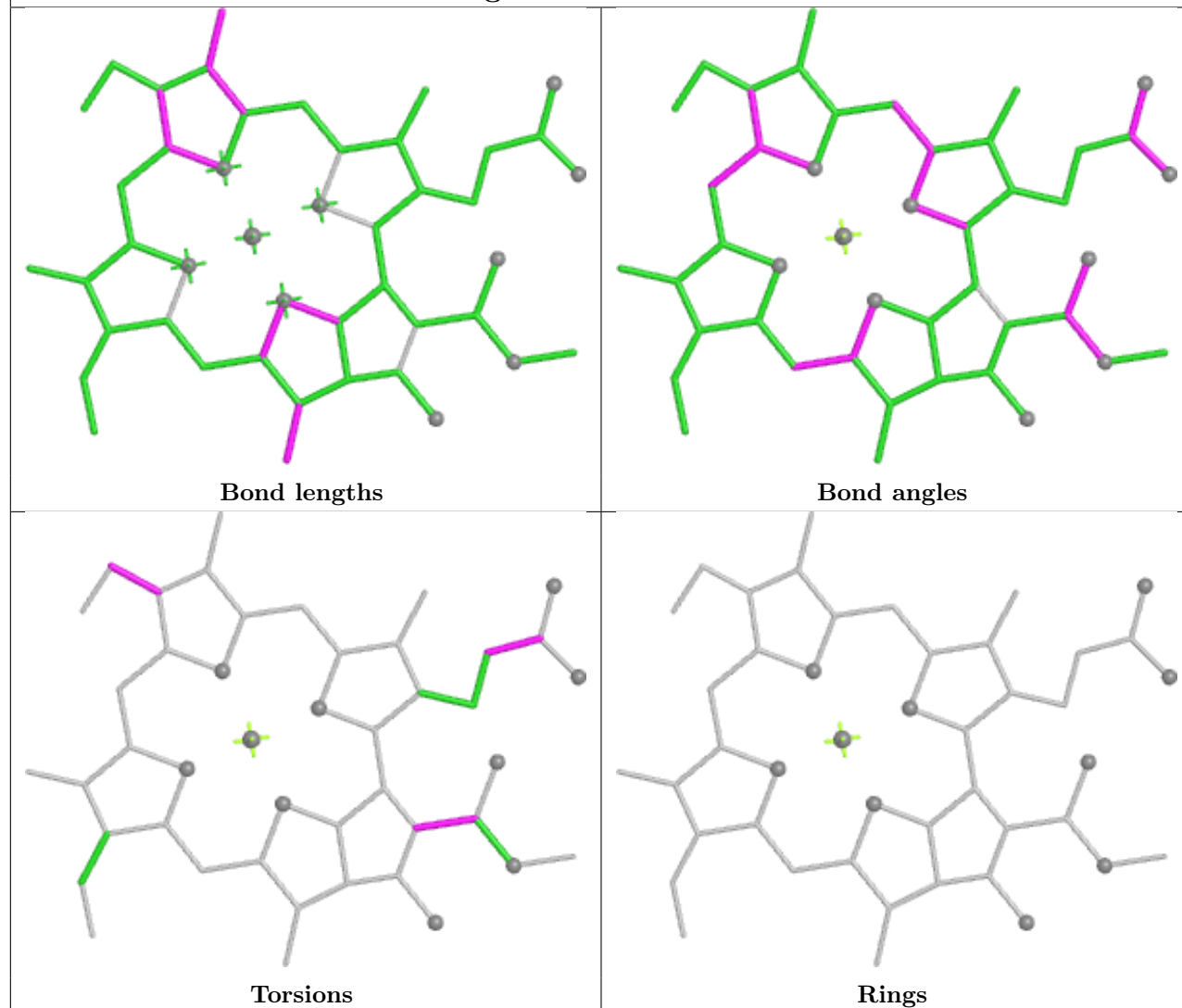
Ligand CLA AB 833**Ligand CLA AF 802**

Ligand CLA BA 808**Ligand CLA A3 302**

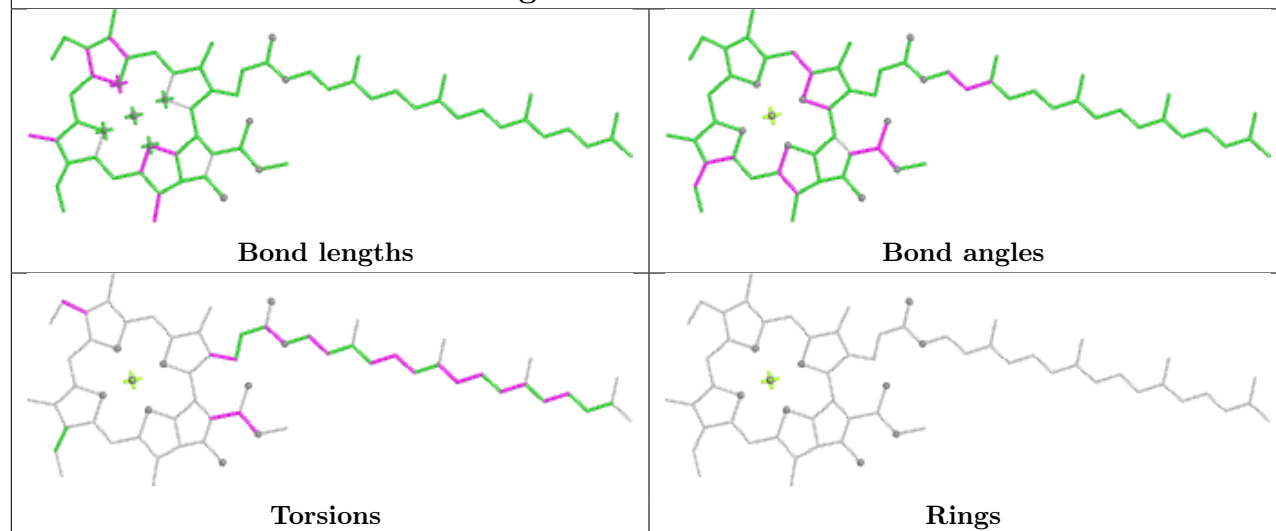


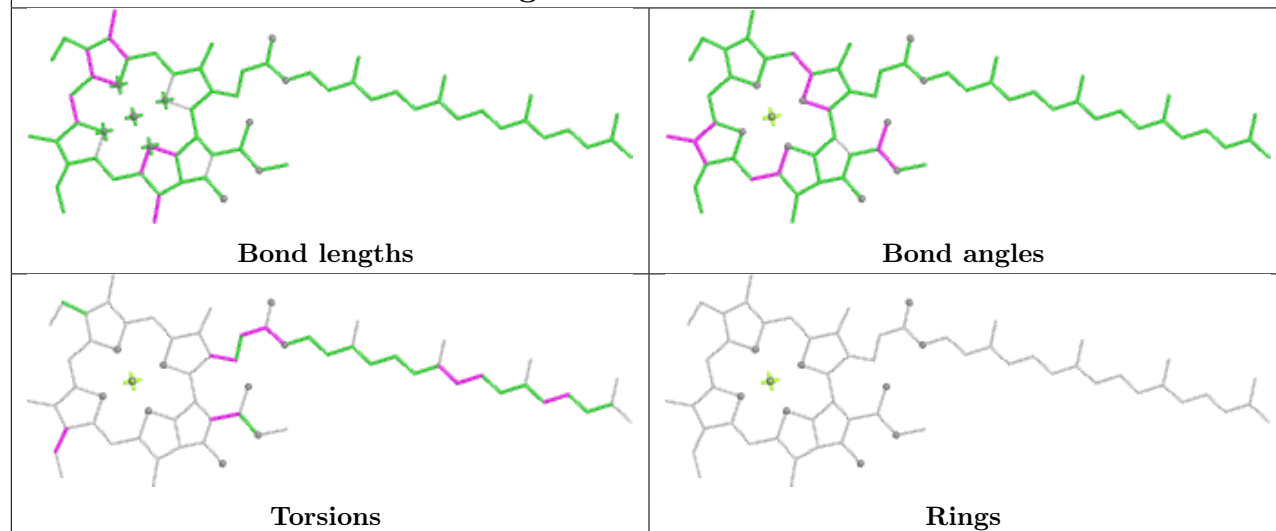
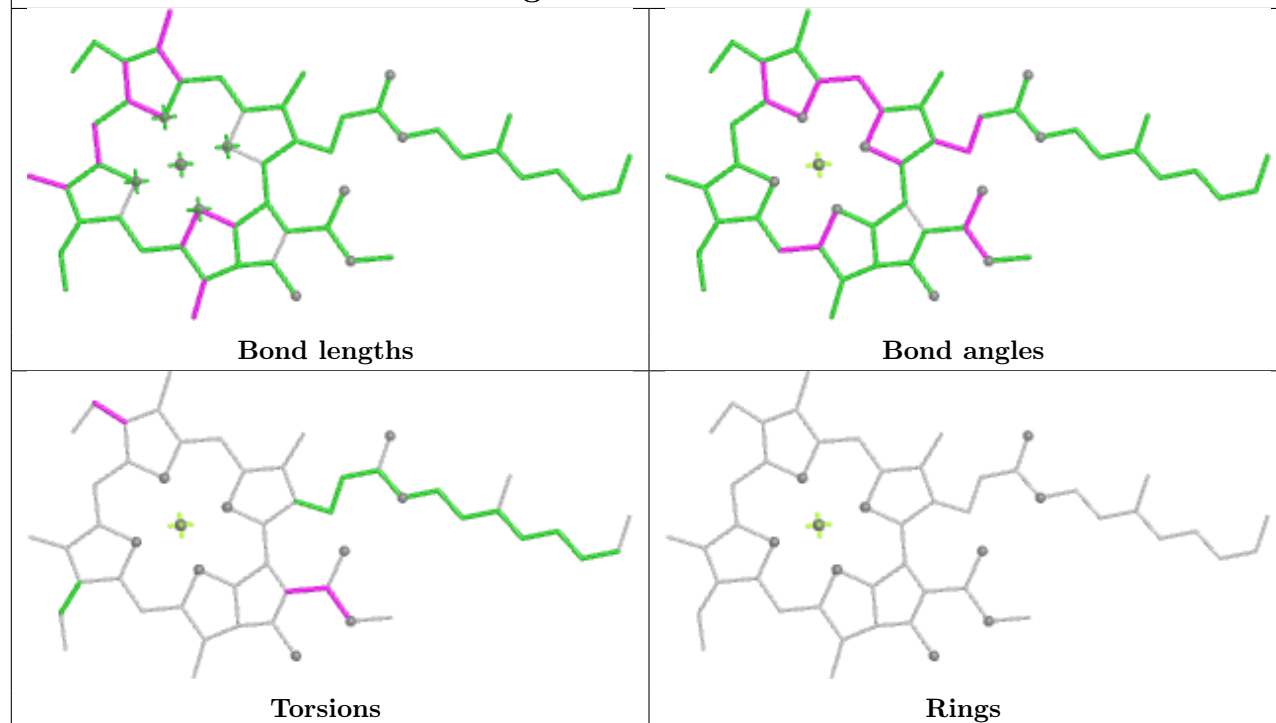


Ligand CLA B2 608

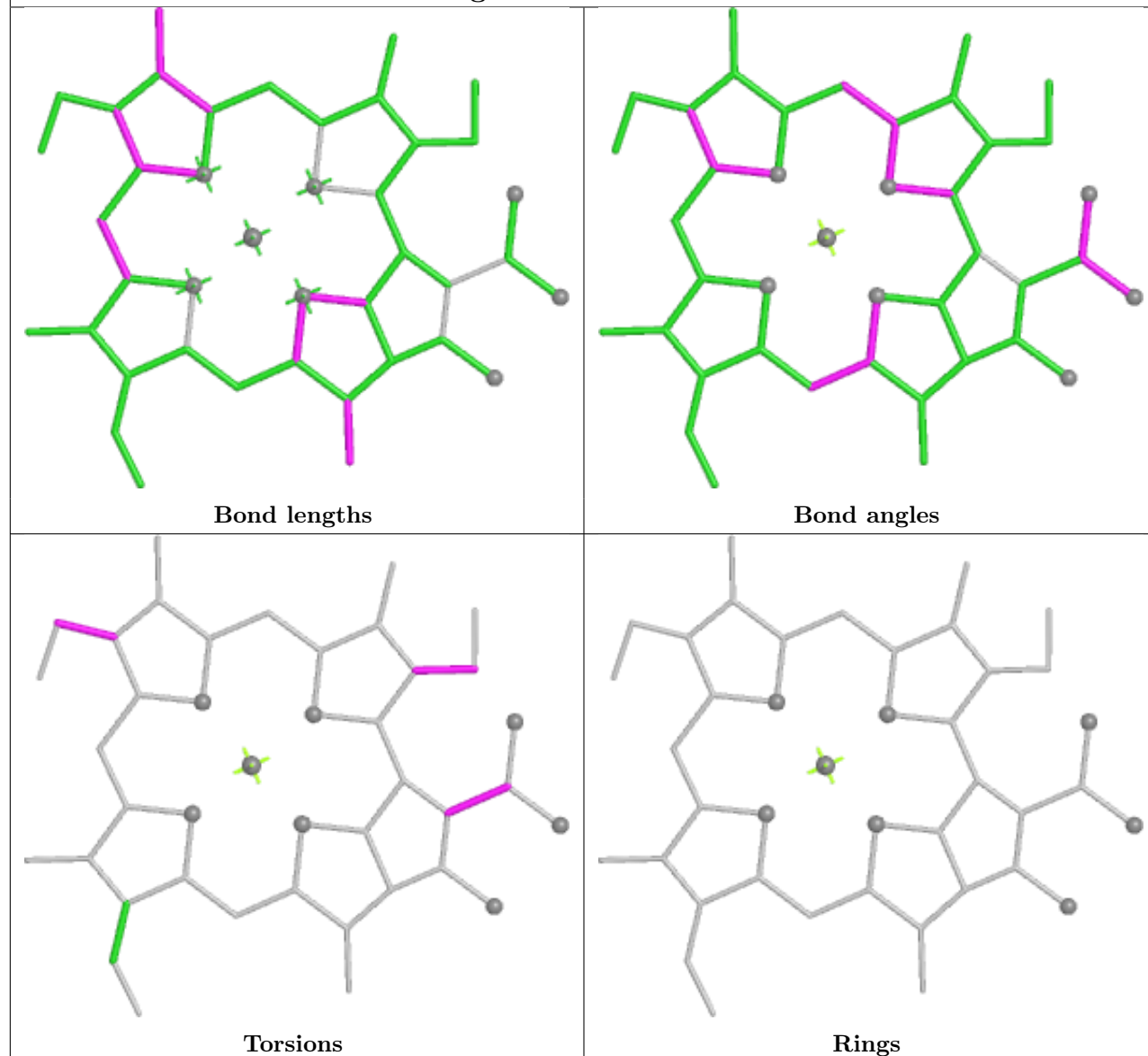


Ligand CLA BA 803

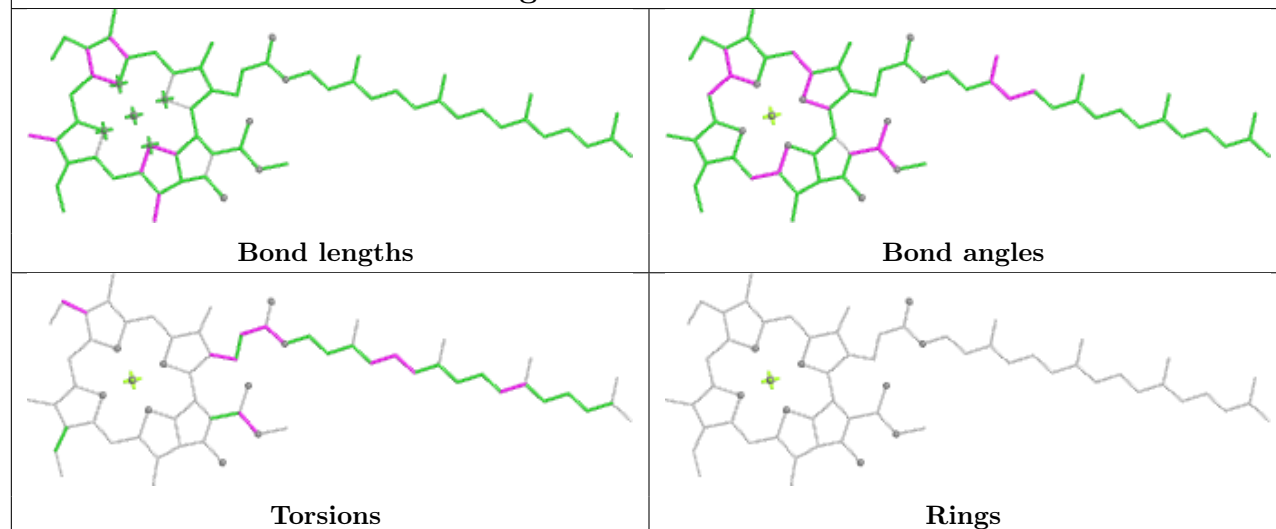


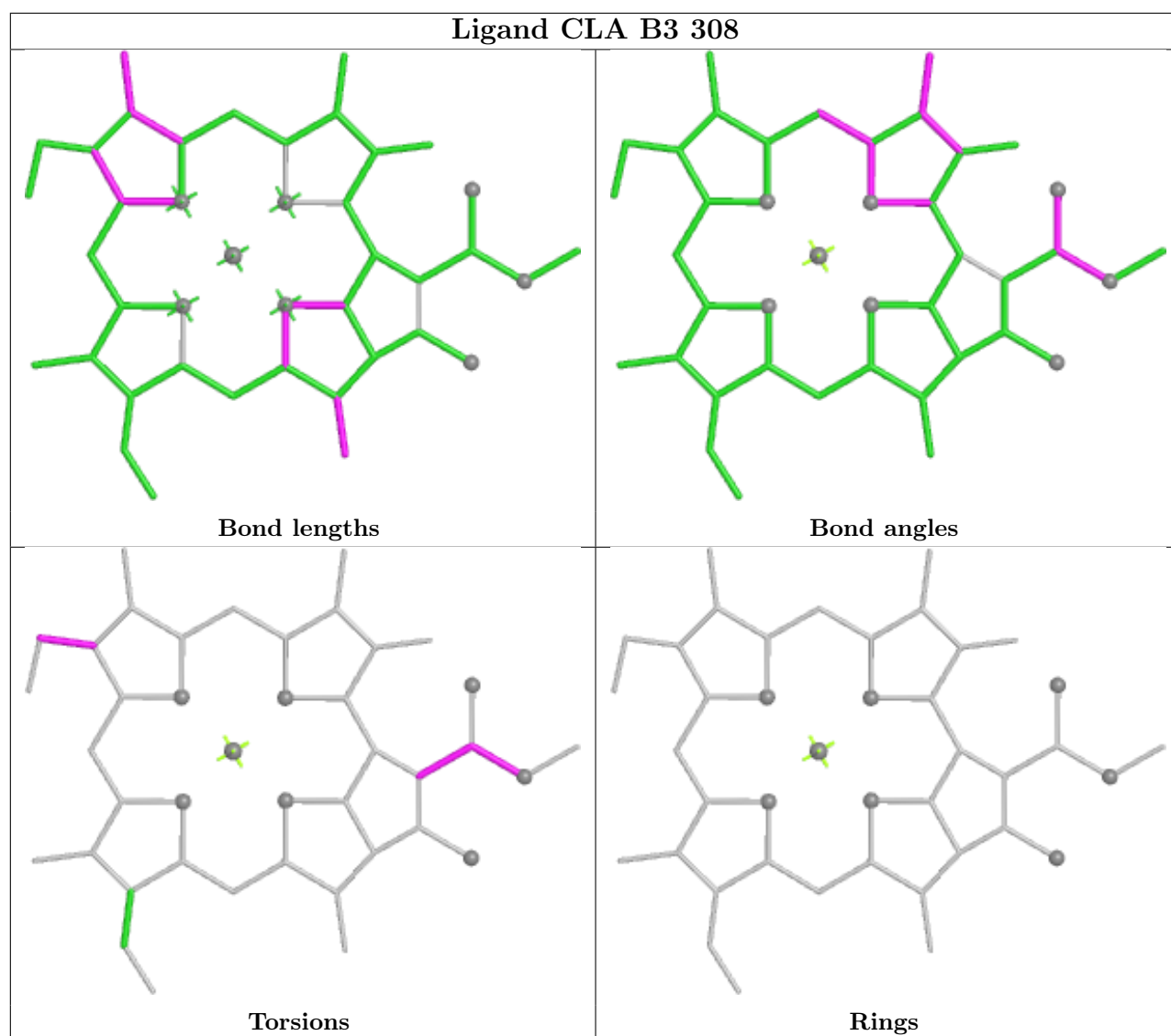
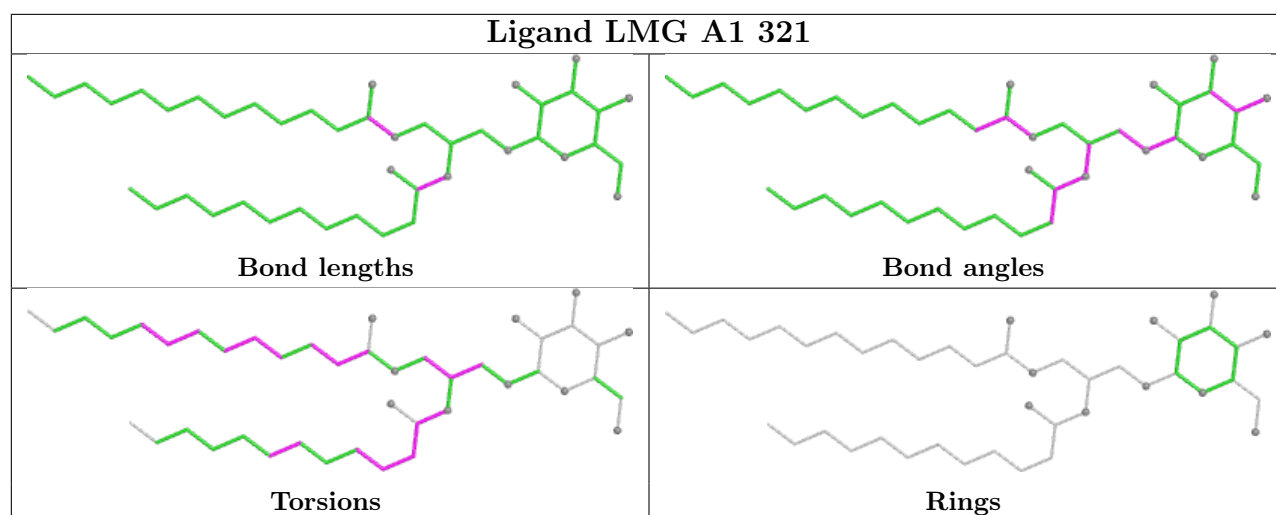
Ligand CLA AB 806**Ligand CLA B5 609**

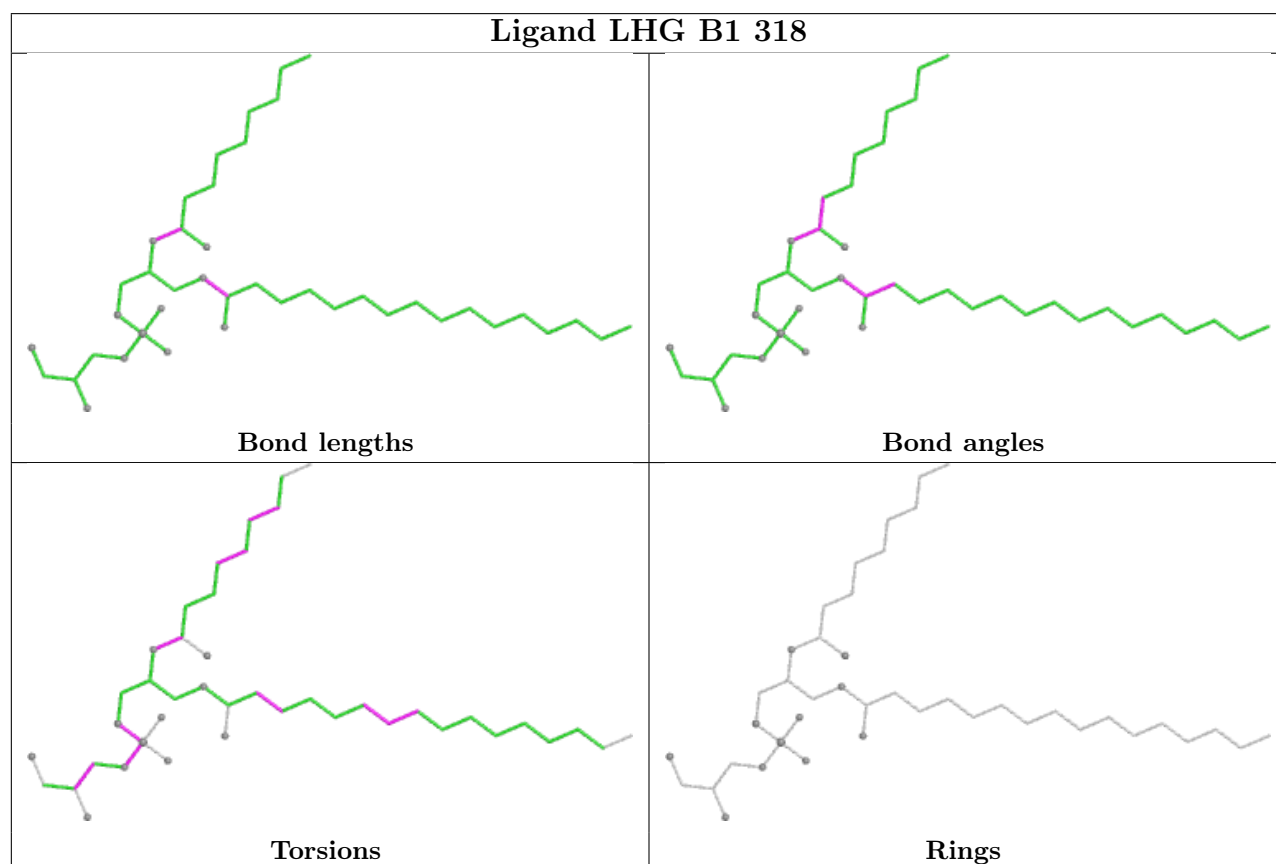
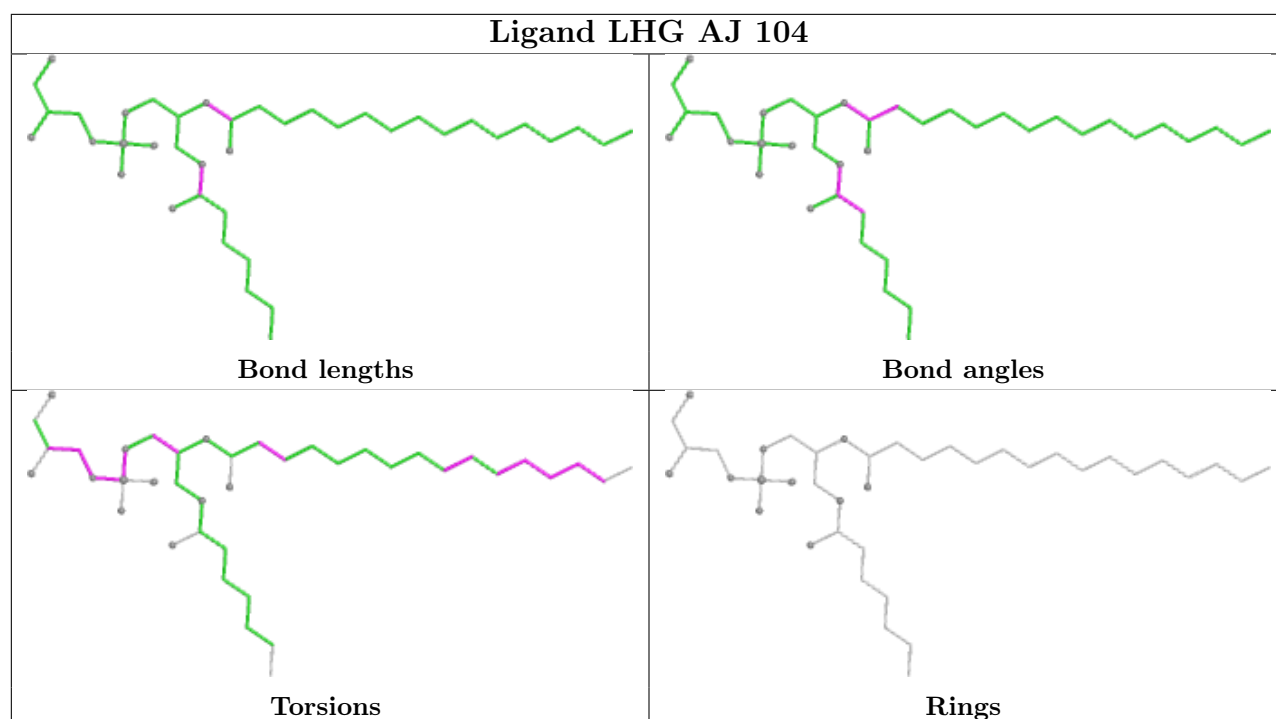
Ligand CLA A3 305



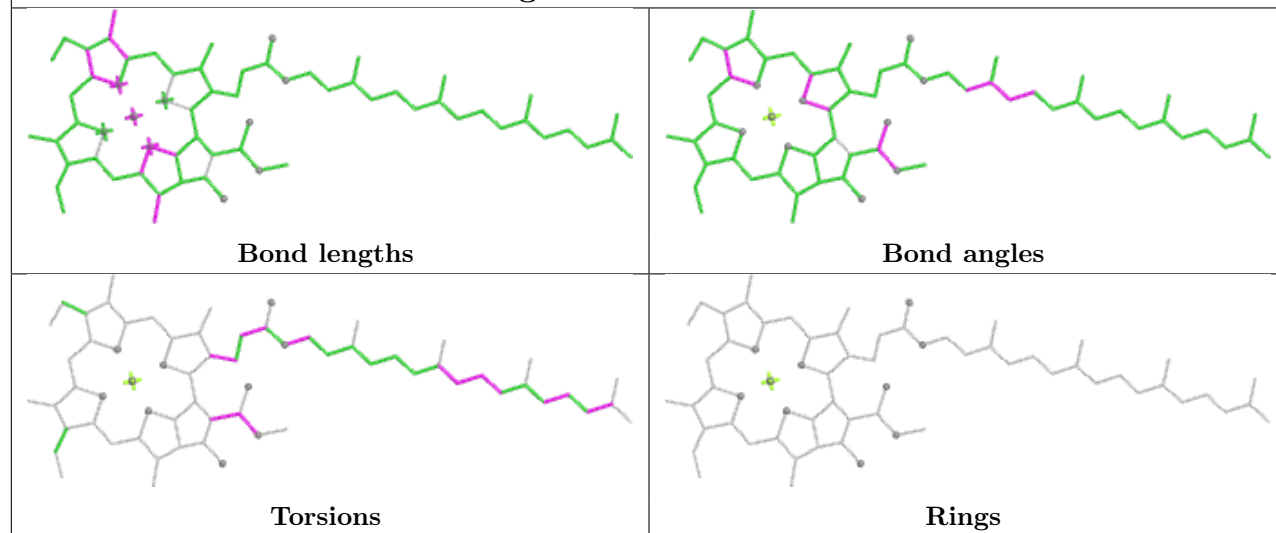
Ligand CLA BB 834



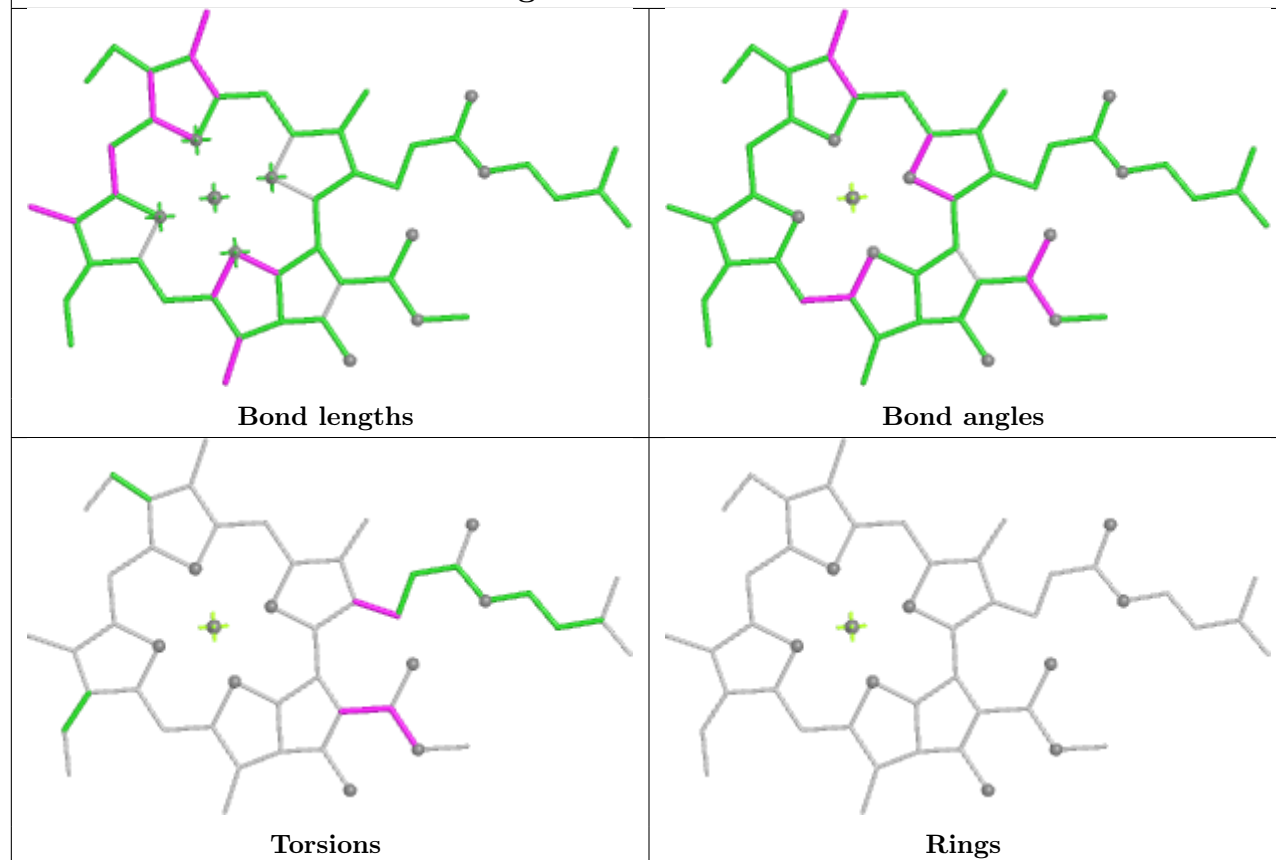


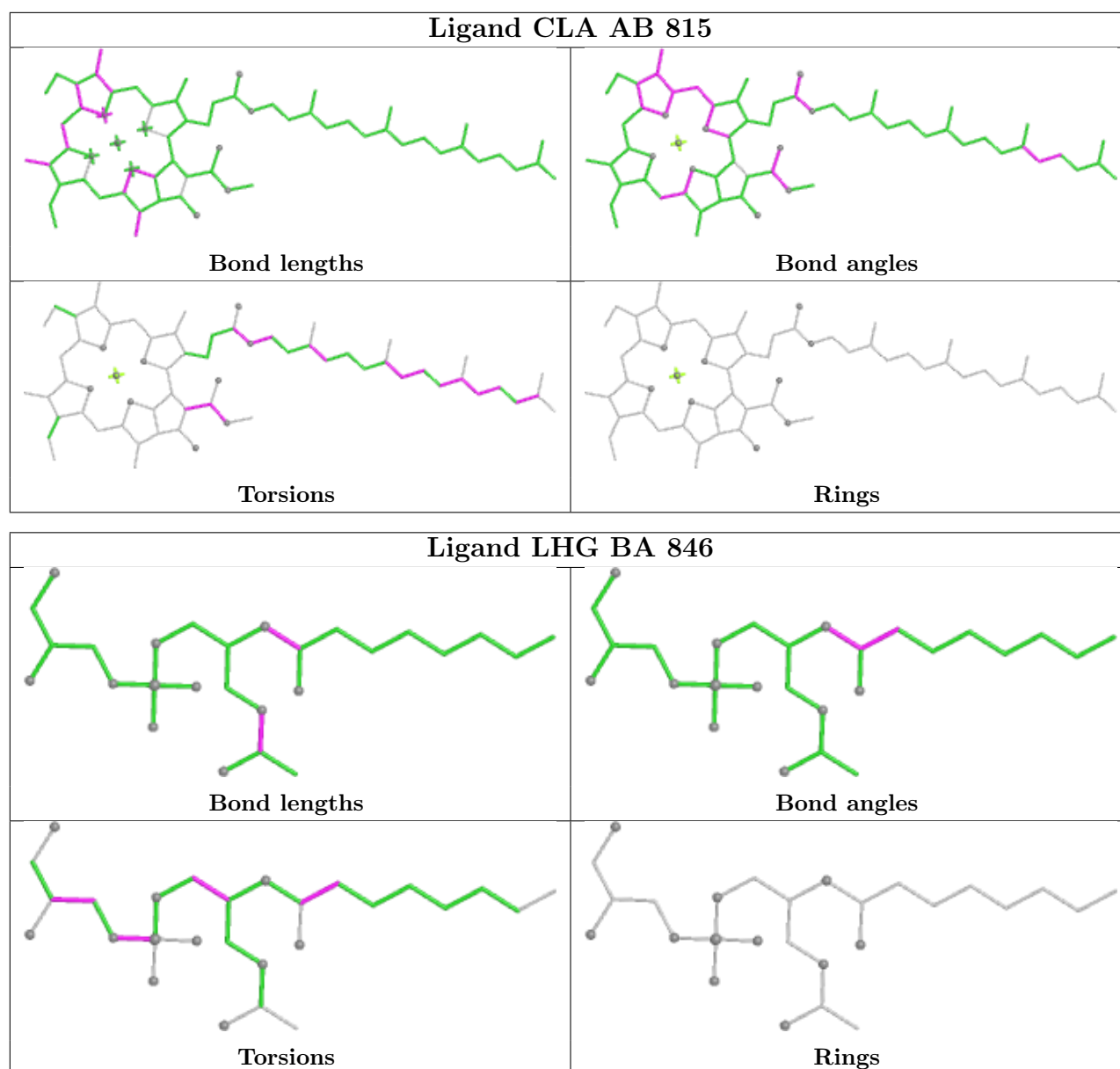


Ligand CLA BA 825



Ligand CLA AA 807





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.

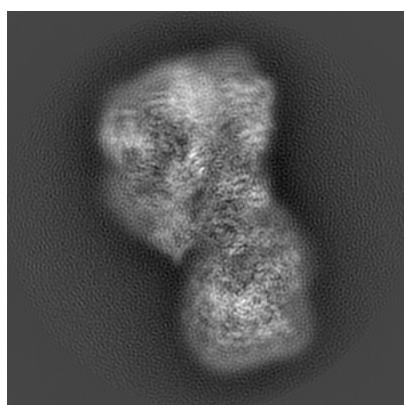
6 Map visualisation [i](#)

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.

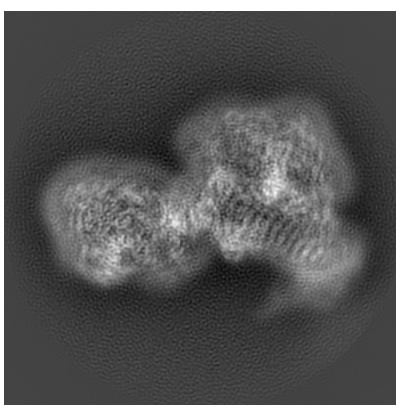
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

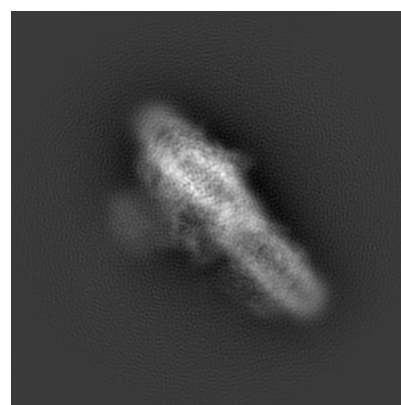
6.1.1 Primary map



X



Y

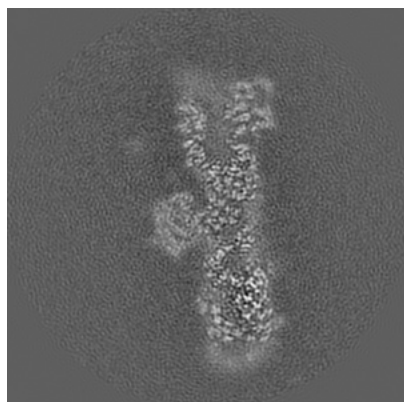


Z

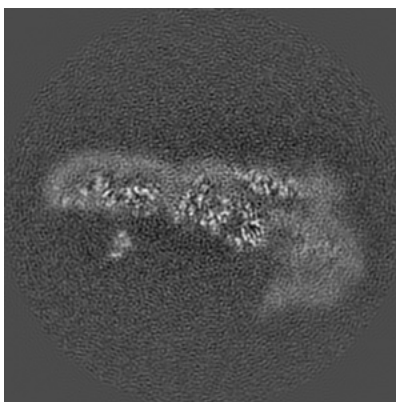
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

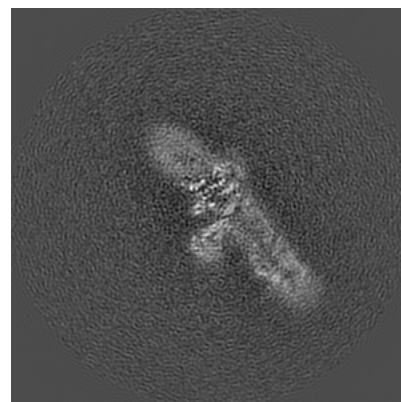
6.2.1 Primary map



X Index: 200



Y Index: 200

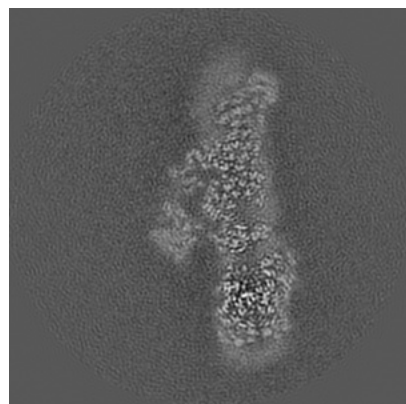


Z Index: 200

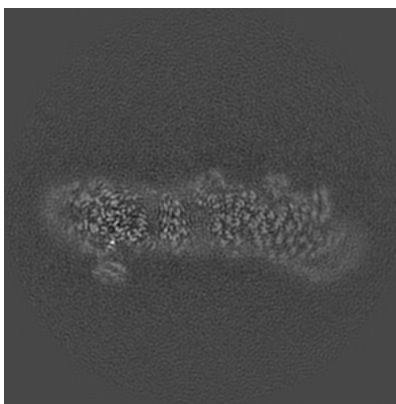
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

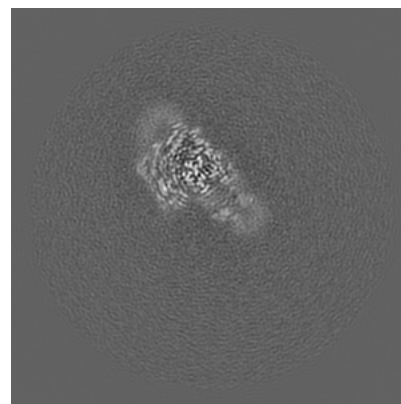
6.3.1 Primary map



X Index: 185



Y Index: 235

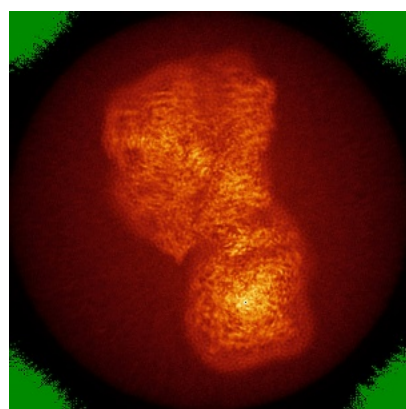


Z Index: 112

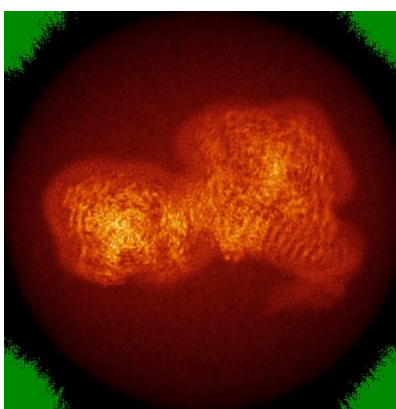
The images above show the largest variance slices of the map in three orthogonal directions.

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

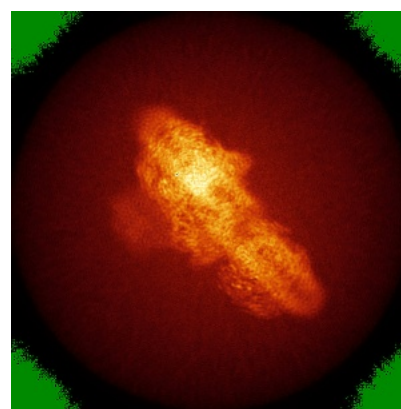
6.4.1 Primary map



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.

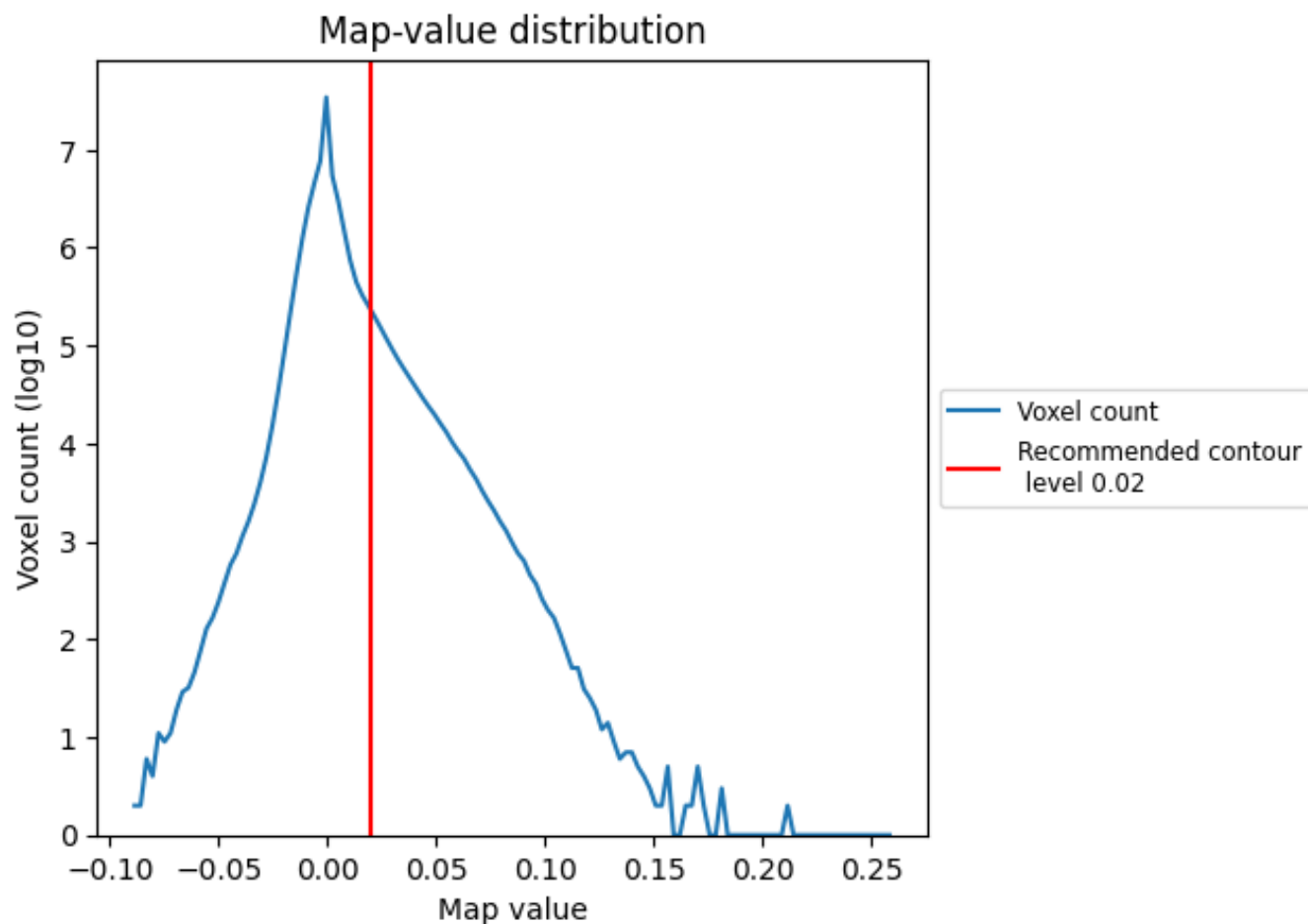
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

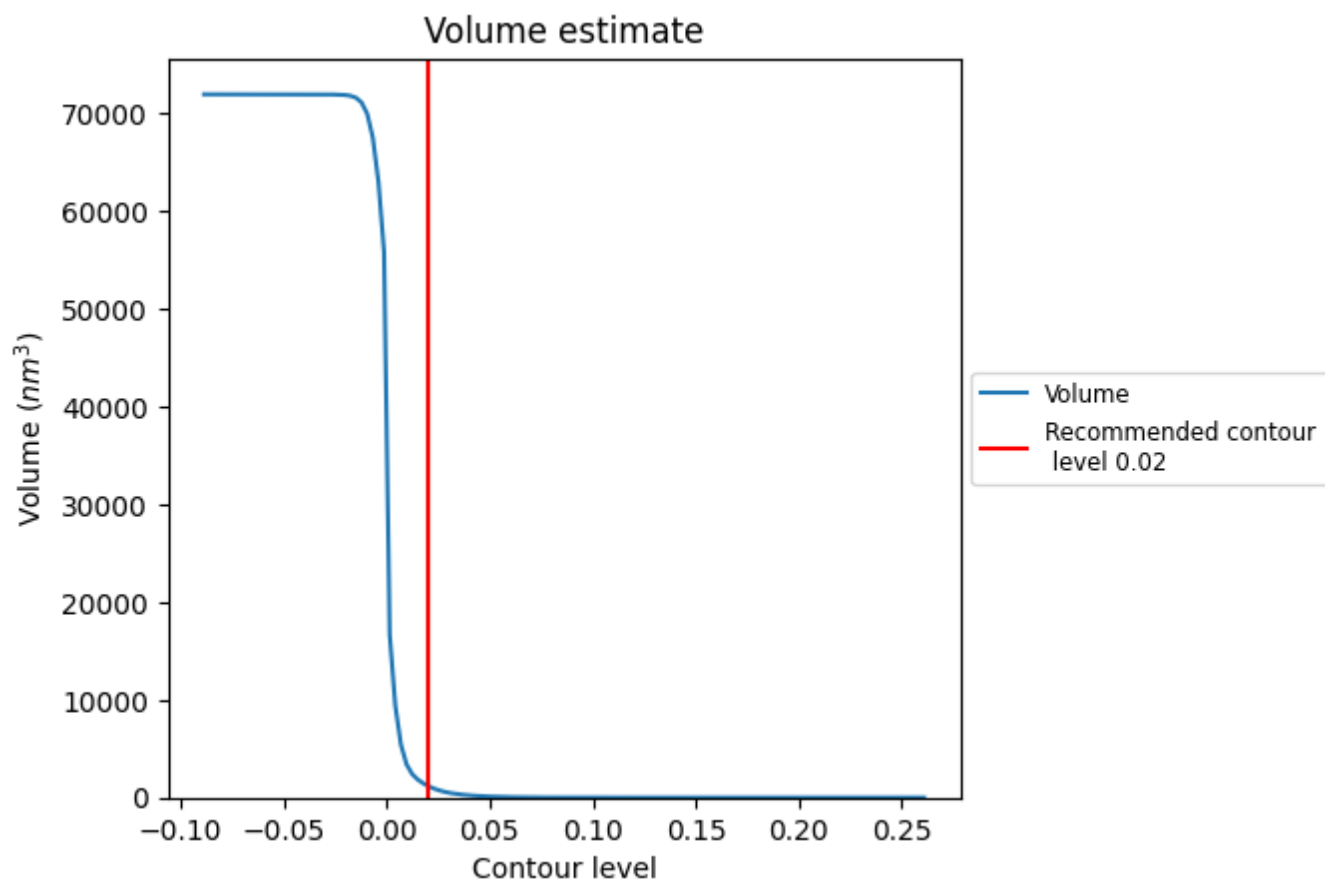
This section contains the results of statistical analysis of the map.

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.

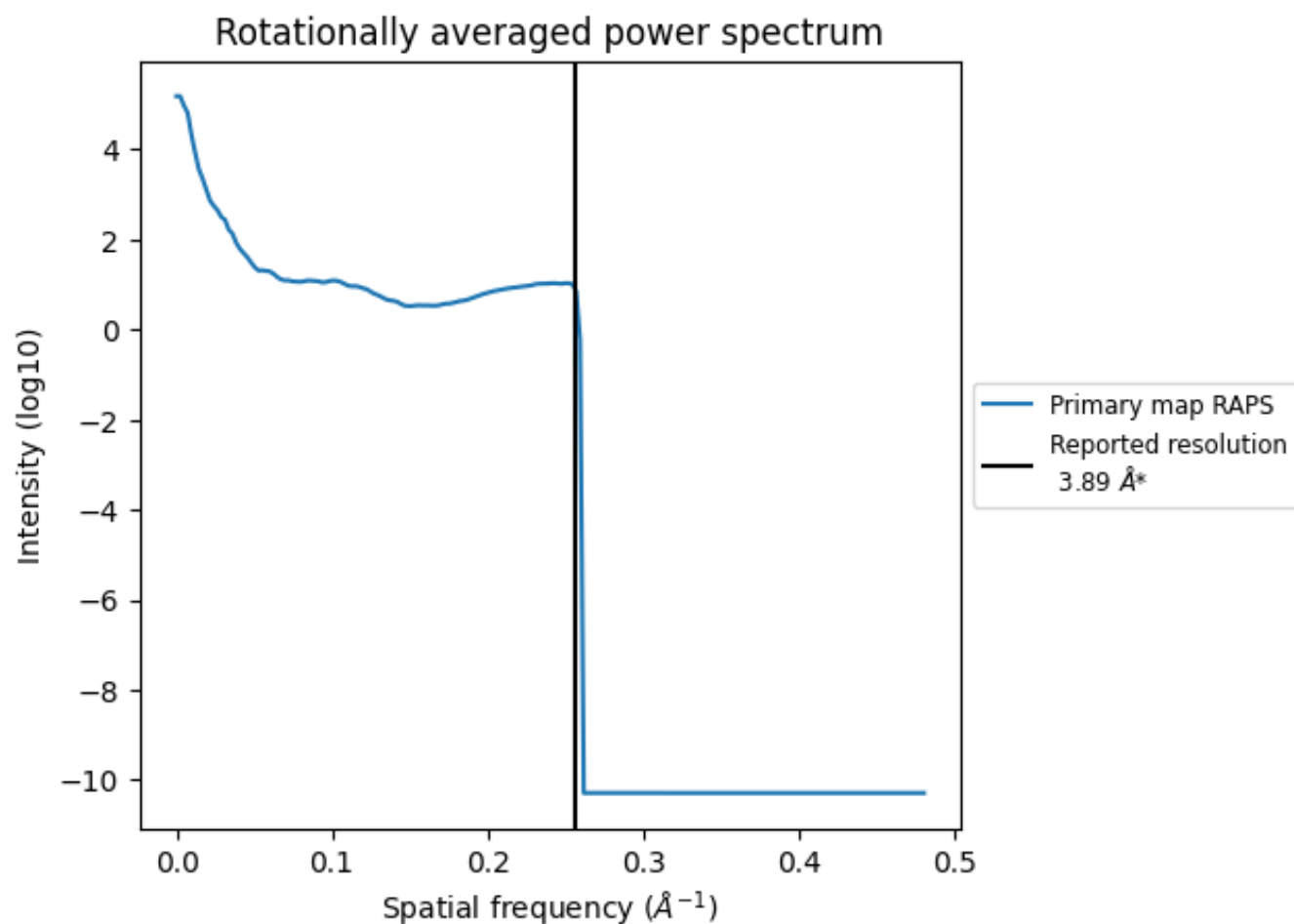
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1193 nm³; 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

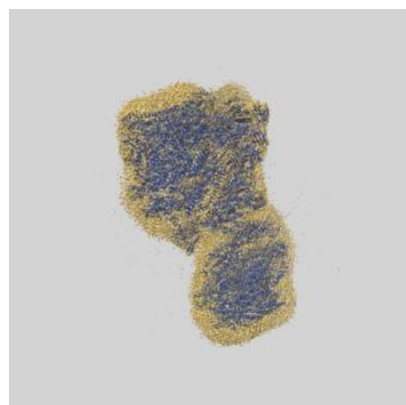
8 Fourier-Shell correlation

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

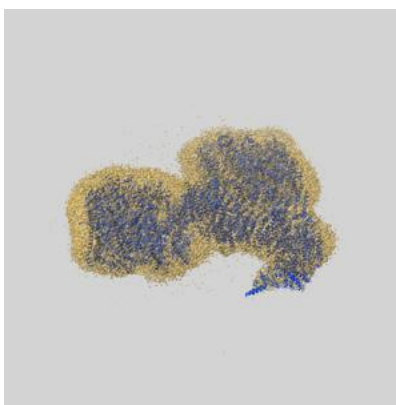
9 Map-model fit [i](#)

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 40](#).

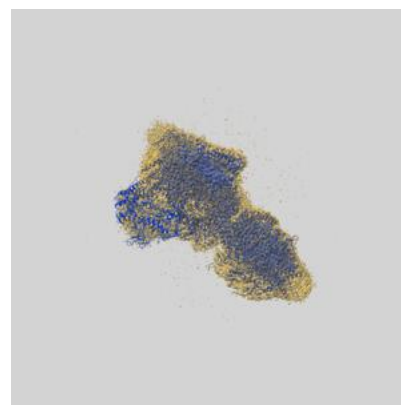
9.1 Map-model overlay [i](#)



X



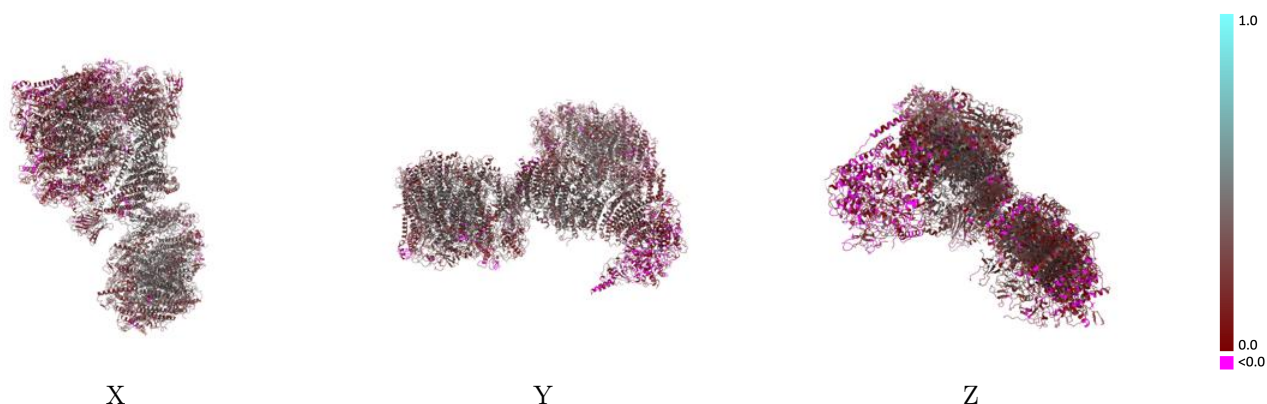
Y



Z

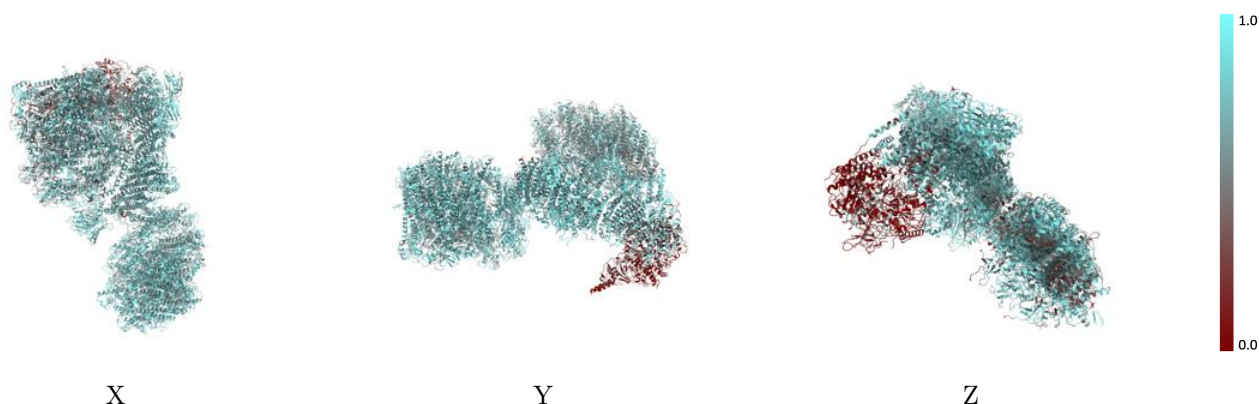
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



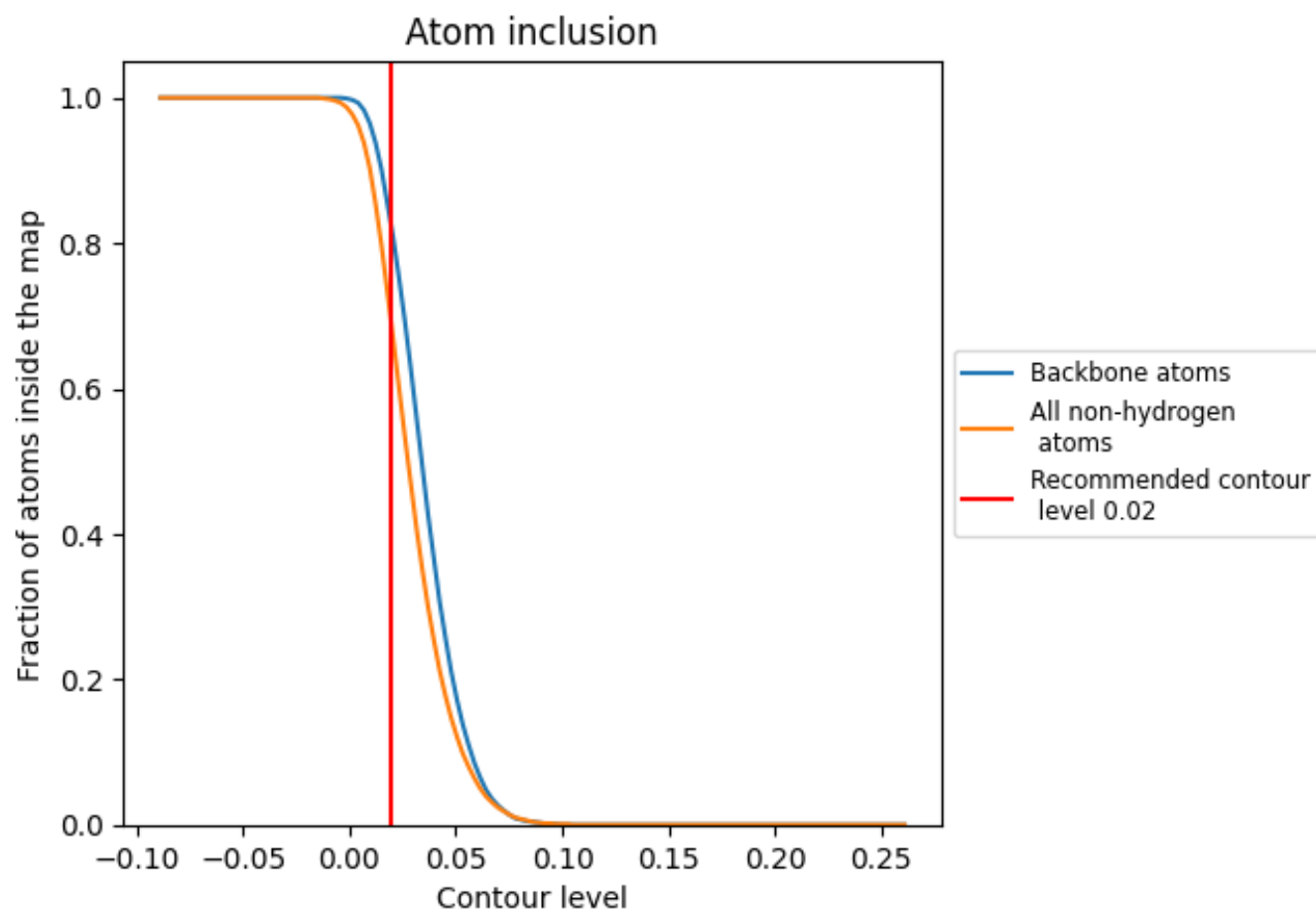
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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



Continued on next page...

Continued from previous page...

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