



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 01:41 PM JST

PDB ID : 9LE7 / pdb_00009le7
EMDB ID : EMD-63017
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana C4S4M4-type PSII supercomplex
Authors : Chen, S.J.B.; Wu, C.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2025-01-07
Resolution : 3.80 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

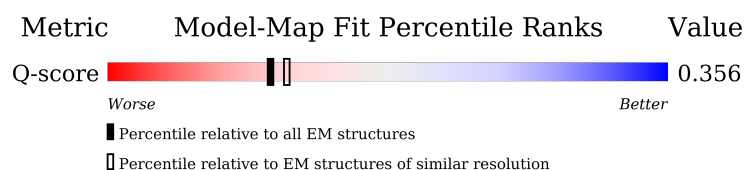
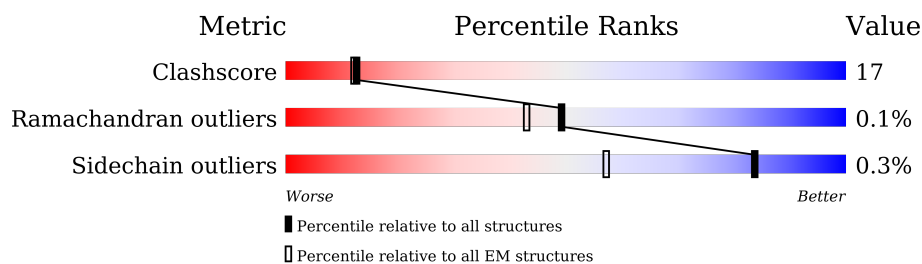
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



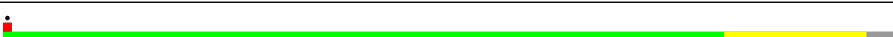
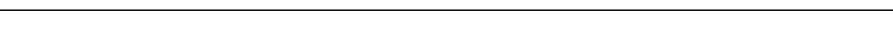
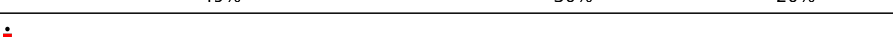
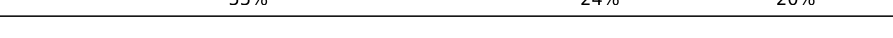
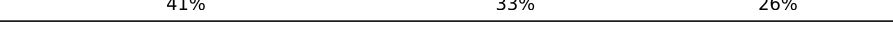
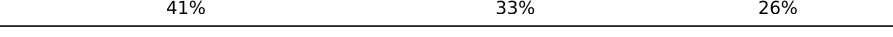
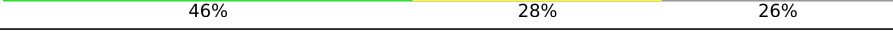
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	5	266	50% 25% 24%
1	7	266	49% 26% 24%
1	9	266	49% 27% 24%
1	AA	266	48% 27% 24%

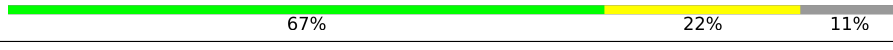
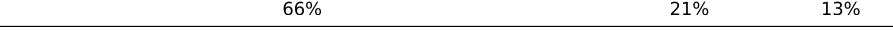
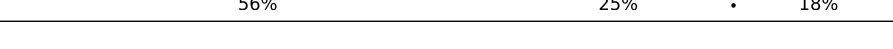
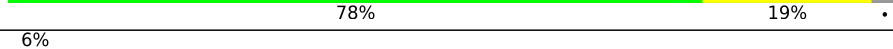
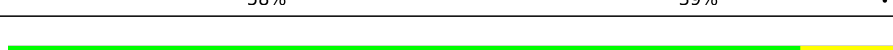
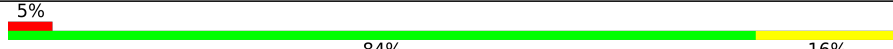
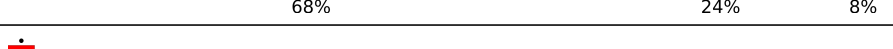
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Mol	Chain	Length	Quality of chain
2	0	243	
2	6	243	
3	8	212	
3	AB	212	
4	B	508	
4	BE	508	
4	b	508	
4	v	508	
5	2	352	
5	BG	352	
5	D	352	
5	d	352	
6	3	83	
6	BH	83	
6	E	83	
6	e	83	
7	4	39	
7	BI	39	
7	F	39	
7	f	39	
8	A2	232	
8	Au	232	
8	BB	232	
8	BJ	232	
8	BQ	232	

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Mol	Chain	Length	Quality of chain
8	Ba	232	
8	G	232	
8	N	232	
8	Y	232	
8	g	232	
8	n	232	
8	y	232	
9	Av	72	
9	BK	72	
9	H	72	
9	h	72	
10	Aw	36	
10	BL	36	
10	I	36	
10	i	36	
11	Ay	37	
11	BN	37	
11	K	37	
11	k	37	
12	Az	38	
12	BO	38	
12	L	38	
12	l	38	
13	A1	34	
13	BP	34	

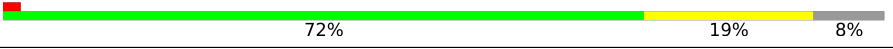
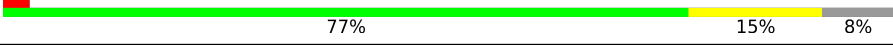
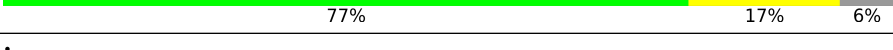
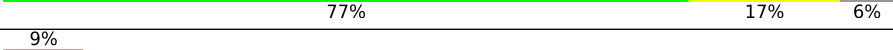
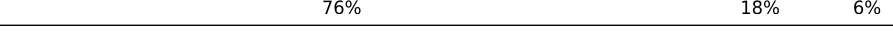
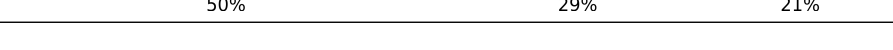
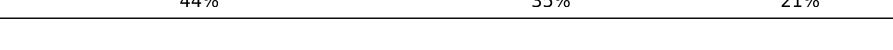
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Mol	Chain	Length	Quality of chain
13	M	34	
13	m	34	
14	A6	232	
14	BV	232	
14	S	232	
14	s	232	
15	A7	33	
15	BW	33	
15	T	33	
15	t	33	
16	A8	28	
16	BX	28	
16	U	28	
16	u	28	
17	A0	54	
17	BY	54	
17	W	54	
17	w	54	
18	BA	42	
18	BZ	42	
18	X	42	
18	x	42	
19	BC	62	
19	Bb	62	
19	Z	62	

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Mol	Chain	Length	Quality of chain
19	z	62	
20	A	352	
20	BD	352	
20	R	352	
20	a	352	
21	1	459	
21	BF	459	
21	C	459	
21	c	459	
22	BU	250	
22	r	250	

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 146846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	201	Total	C	N	O	S	0	0
			1529	991	249	285	4		
1	7	201	Total	C	N	O	S	0	0
			1530	991	249	285	5		
1	9	201	Total	C	N	O	S	0	0
			1529	991	249	285	4		
1	AA	201	Total	C	N	O	S	0	0
			1530	991	249	285	5		

- Molecule 2 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	222	Total	C	N	O	S	0	0
			1716	1120	280	311	5		
2	0	222	Total	C	N	O	S	0	0
			1716	1120	280	311	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	192	Total	C	N	O	S	0	0
			1512	993	245	270	4		
3	AB	192	Total	C	N	O	S	0	0
			1512	993	245	270	4		

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	479	Total	C	N	O	S	0	0
			3757	2462	636	647	12		
4	b	479	Total	C	N	O	S	0	0
			3757	2462	636	647	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	v	479	Total	C	N	O	S	0	0
			3757	2462	636	647	12		
4	BE	479	Total	C	N	O	S	0	0
			3757	2462	636	647	12		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	342	Total	C	N	O	S	0	0
			2723	1800	445	466	12		
5	d	342	Total	C	N	O	S	0	0
			2723	1800	445	466	12		
5	2	342	Total	C	N	O	S	0	0
			2723	1800	445	466	12		
5	BG	342	Total	C	N	O	S	0	0
			2723	1800	445	466	12		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	66	Total	C	N	O	0	0
			544	357	88	99		
6	e	66	Total	C	N	O	0	0
			544	357	88	99		
6	3	66	Total	C	N	O	0	0
			544	357	88	99		
6	BH	66	Total	C	N	O	0	0
			544	357	88	99		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	29	Total	C	N	O	S	0	0
			225	147	40	37	1		
7	f	29	Total	C	N	O	S	0	0
			225	147	40	37	1		
7	4	29	Total	C	N	O	S	0	0
			225	147	40	37	1		
7	BI	29	Total	C	N	O	S	0	0
			225	147	40	37	1		

- Molecule 8 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
8	N	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
8	Y	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		
8	g	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
8	n	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
8	y	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		
8	Au	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
8	A2	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
8	BB	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		
8	BJ	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
8	BQ	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
8	Ba	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		

- Molecule 9 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	59	Total	C	N	O	S	0	0
			438	289	68	79	2		
9	h	59	Total	C	N	O	S	0	0
			438	289	68	79	2		
9	Av	59	Total	C	N	O	S	0	0
			438	289	68	79	2		
9	BK	59	Total	C	N	O	S	0	0
			438	289	68	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	35	Total	C	N	O	S	0	0
			286	195	44	46	1		
10	i	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	Aw	35	Total	C	N	O	S	0	0
			286	195	44	46	1		
10	BL	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			302	211	44	46	1		
11	k	37	Total	C	N	O	S	0	0
			302	211	44	46	1		
11	Ay	37	Total	C	N	O	S	0	0
			302	211	44	46	1		
11	BN	37	Total	C	N	O	S	0	0
			302	211	44	46	1		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	35	Total	C	N	O		0	0
			293	195	45	53			
12	l	35	Total	C	N	O		0	0
			293	195	45	53			
12	Az	35	Total	C	N	O		0	0
			293	195	45	53			
12	BO	35	Total	C	N	O		0	0
			293	195	45	53			

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	32	Total	C	N	O	S	0	0
			250	173	35	41	1		
13	m	32	Total	C	N	O	S	0	0
			250	173	35	41	1		
13	A1	32	Total	C	N	O	S	0	0
			250	173	35	41	1		
13	BP	32	Total	C	N	O	S	0	0
			250	173	35	41	1		

- Molecule 14 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		
14	s	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		
14	A6	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		
14	BV	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
15	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
15	A7	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
15	BW	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 16 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	25	Total	C	N	O	S	0	0
			195	122	36	34	3		
16	u	25	Total	C	N	O	S	0	0
			195	122	36	34	3		
16	A8	25	Total	C	N	O	S	0	0
			195	122	36	34	3		
16	BX	25	Total	C	N	O	S	0	0
			195	122	36	34	3		

- Molecule 17 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	54	Total	C	N	O	S	0	0
			428	282	61	84	1		
17	w	54	Total	C	N	O	S	0	0
			428	282	61	84	1		
17	A0	54	Total	C	N	O	S	0	0
			428	282	61	84	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	BY	54	Total	C	N	O	S	0	0
			428	282	61	84	1		

- Molecule 18 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	36	Total	C	N	O		0	0
			248	162	39	47			
18	x	36	Total	C	N	O		0	0
			248	162	39	47			
18	BA	36	Total	C	N	O		0	0
			248	162	39	47			
18	BZ	36	Total	C	N	O		0	0
			248	162	39	47			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0
			465	313	69	82	1		
19	z	62	Total	C	N	O	S	0	0
			465	313	69	82	1		
19	BC	62	Total	C	N	O	S	0	0
			465	313	69	82	1		
19	Bb	62	Total	C	N	O	S	0	0
			465	313	69	82	1		

- Molecule 20 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A	323	Total	C	N	O	S	0	0
			2525	1652	415	445	13		
20	a	323	Total	C	N	O	S	0	0
			2525	1652	415	445	13		
20	R	323	Total	C	N	O	S	0	0
			2525	1652	415	445	13		
20	BD	323	Total	C	N	O	S	0	0
			2525	1652	415	445	13		

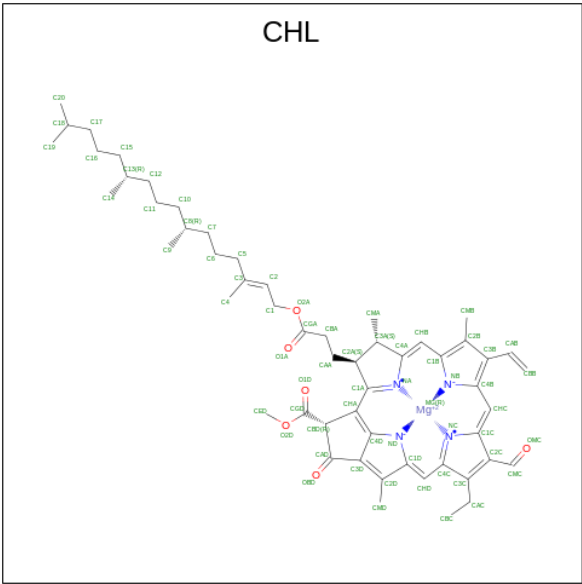
- Molecule 21 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
21	c	432	Total	C	N	O	S	0	0
			3365	2217	561	576	11		
21	1	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
21	BF	432	Total	C	N	O	S	0	0
			3365	2217	561	576	11		

- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	197	Total	C	N	O	S	0	0
			1539	1004	251	281	3		
22	BU	197	Total	C	N	O	S	0	0
			1539	1004	251	281	3		

- Molecule 23 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			62	51	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	5	1	Total 61	C 50	Mg 1	N 4	O 6	0
23	6	1	Total 63	C 52	Mg 1	N 4	O 6	0
23	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	6	1	Total 53	C 42	Mg 1	N 4	O 6	0
23	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	6	1	Total 60	C 49	Mg 1	N 4	O 6	0
23	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	7	1	Total 60	C 49	Mg 1	N 4	O 6	0
23	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	7	1	Total 60	C 49	Mg 1	N 4	O 6	0
23	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	G	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	G	1	Total 50	C 39	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
23	G	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	G	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	N	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
23	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	N	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	N	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	N	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	S	1	Total 57	C 46	Mg 1	N 4	O 6	0
23	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	Y	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	Y	1	Total 48	C 37	Mg 1	N 4	O 6	0
23	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	Y	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	Y	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	Y	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	e	1	Total 45	C 34	Mg 1	N 4	O 6	0
23	g	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
23	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	g	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	g	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	g	1	Total 60	C 49	Mg 1	N 4	O 6	0
23	n	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
23	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	n	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	n	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	n	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	s	1	Total 57	C 46	Mg 1	N 4	O 6	0
23	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	y	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	y	1	Total 48	C 37	Mg 1	N 4	O 6	0
23	y	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	y	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	y	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	y	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
23	r	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	r	1	Total 55	C 44	Mg 1	N 4	O 6	0
23	r	1	Total 60	C 49	Mg 1	N 4	O 6	0
23	r	1	Total 42	C 33	Mg 1	N 4	O 4	0
23	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	9	1	Total 62	C 51	Mg 1	N 4	O 6	0
23	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	9	1	Total 61	C 50	Mg 1	N 4	O 6	0
23	0	1	Total 63	C 52	Mg 1	N 4	O 6	0
23	0	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	0	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	0	1	Total 53	C 42	Mg 1	N 4	O 6	0
23	0	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	0	1	Total 60	C 49	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 60	C 49	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
23	AA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
23	AB	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	AB	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	AB	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	AB	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	Au	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	Au	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	Au	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
23	Au	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	Au	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	Au	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	A2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	A2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	A2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
23	A2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	A2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	A2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	A6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	A6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	A6	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
23	A6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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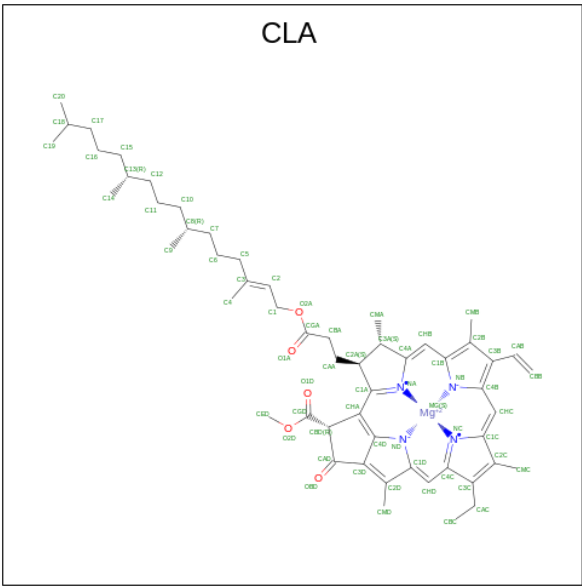
Mol	Chain	Residues	Atoms					AltConf
23	BB	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BB	1	Total 48	C 37	Mg 1	N 4	O 6	0
23	BB	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	BB	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BB	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BB	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BH	1	Total 45	C 34	Mg 1	N 4	O 6	0
23	BJ	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BJ	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	BJ	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	BJ	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BJ	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BJ	1	Total 60	C 49	Mg 1	N 4	O 6	0
23	BQ	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BQ	1	Total 48	C 37	Mg 1	N 4	O 6	0
23	BQ	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	BQ	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BQ	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BQ	1	Total 65	C 54	Mg 1	N 4	O 6	0
23	BV	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	BV	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
23	BV	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
23	BV	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	Ba	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	Ba	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	Ba	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
23	Ba	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	Ba	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	Ba	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	BU	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
23	BU	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
23	BU	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
23	BU	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
24	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			48	39	1	4	4	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	G	1	Total 64	C 54	Mg 1	N 4	O 5	0
24	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	G	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	N	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	N	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	S	1	Total 53	C 44	Mg 1	N 4	O 4	0
24	S	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Y	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	g	1	Total 64	C 54	Mg 1	N 4	O 5	0
24	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	g	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	n	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	s	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	y	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	r	1	Total 58	C 49	Mg 1	N 4	O 4	0
24	r	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	r	1	Total 37	C 31	Mg 1	N 4	O 1	0
24	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	9	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	0	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	0	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	0	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	AA	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	AA	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AA	1	Total 48	C 39	Mg 1	N 4	O 4	0
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Au	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Au	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Au	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	Au	1	Total 64	C 54	Mg 1	N 4	O 5	0
24	Au	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	Au	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	Au	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Au	1	Total 48	C 38	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	Aw	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A2	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A2	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A2	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A2	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A2	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	A6	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	A6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A6	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A6	1	Total 53	C 44	Mg 1	N 4	O 4	0
24	A6	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	A6	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	A6	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A6	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BB	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	BB	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BB	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BB	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BB	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BE	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	BG	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BG	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BJ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BJ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BJ	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	BJ	1	Total 64	C 54	Mg 1	N 4	O 5	0
24	BJ	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BJ	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BJ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BJ	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	BQ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BQ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BQ	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	BQ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BQ	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BQ	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BQ	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BQ	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BQ	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	BV	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	BV	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	BV	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	BV	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	BV	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	BV	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	BV	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	BV	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	BV	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	Ba	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Ba	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Ba	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	Ba	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	Ba	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	Ba	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	Ba	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Ba	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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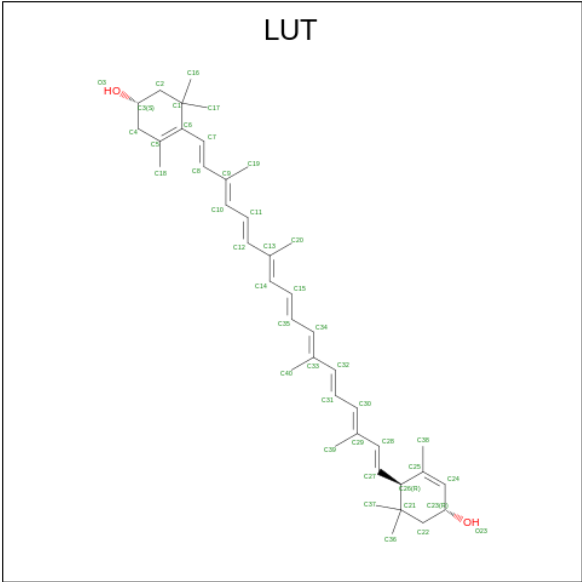
Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BD	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BD	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BD	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	BD	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BF	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BU	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	BU	1	Total 58	C 49	Mg 1	N 4	O 4	0
24	BU	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	BU	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	BU	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	BU	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	BU	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	BU	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	BU	1	Total 37	C 31	Mg 1	N 4	O 1	0
24	BU	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 25 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
25	5	1	Total	C	O	0
			42	40	2	
25	5	1	Total	C	O	0
			42	40	2	
25	6	1	Total	C	O	0
			42	40	2	
25	6	1	Total	C	O	0
			42	40	2	
25	7	1	Total	C	O	0
			42	40	2	
25	7	1	Total	C	O	0
			42	40	2	
25	8	1	Total	C	O	0
			42	40	2	
25	G	1	Total	C	O	0
			42	40	2	
25	G	1	Total	C	O	0
			42	40	2	
25	N	1	Total	C	O	0
			42	40	2	
25	N	1	Total	C	O	0
			42	40	2	
25	S	1	Total	C	O	0
			42	40	2	
25	S	1	Total	C	O	0
			42	40	2	
25	Y	1	Total	C	O	0
			42	40	2	

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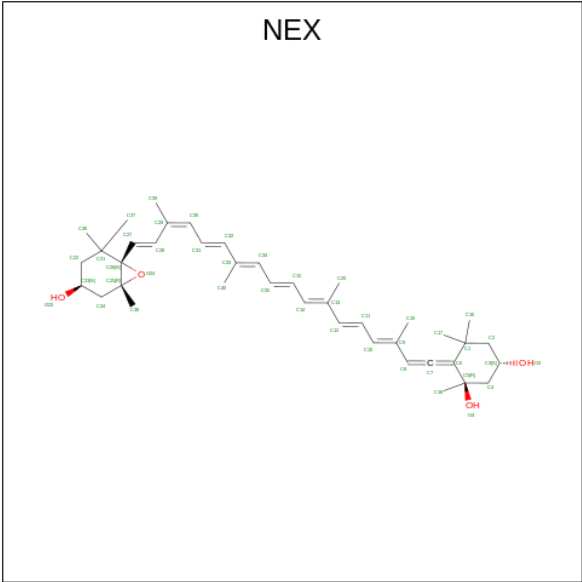
Mol	Chain	Residues	Atoms			AltConf
25	Y	1	Total	C	O	0
			42	40	2	
25	g	1	Total	C	O	0
			42	40	2	
25	g	1	Total	C	O	0
			42	40	2	
25	n	1	Total	C	O	0
			42	40	2	
25	n	1	Total	C	O	0
			42	40	2	
25	s	1	Total	C	O	0
			42	40	2	
25	s	1	Total	C	O	0
			42	40	2	
25	y	1	Total	C	O	0
			42	40	2	
25	y	1	Total	C	O	0
			42	40	2	
25	r	1	Total	C	O	0
			42	40	2	
25	9	1	Total	C	O	0
			42	40	2	
25	9	1	Total	C	O	0
			42	40	2	
25	0	1	Total	C	O	0
			42	40	2	
25	0	1	Total	C	O	0
			42	40	2	
25	AA	1	Total	C	O	0
			42	40	2	
25	AA	1	Total	C	O	0
			42	40	2	
25	AB	1	Total	C	O	0
			42	40	2	
25	Au	1	Total	C	O	0
			42	40	2	
25	Au	1	Total	C	O	0
			42	40	2	
25	A2	1	Total	C	O	0
			42	40	2	
25	A2	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
25	A6	1	Total	C	O	0
			42	40	2	
25	A6	1	Total	C	O	0
			42	40	2	
25	BB	1	Total	C	O	0
			42	40	2	
25	BB	1	Total	C	O	0
			42	40	2	
25	BJ	1	Total	C	O	0
			42	40	2	
25	BJ	1	Total	C	O	0
			42	40	2	
25	BQ	1	Total	C	O	0
			42	40	2	
25	BQ	1	Total	C	O	0
			42	40	2	
25	BV	1	Total	C	O	0
			42	40	2	
25	BV	1	Total	C	O	0
			42	40	2	
25	Ba	1	Total	C	O	0
			42	40	2	
25	Ba	1	Total	C	O	0
			42	40	2	
25	BU	1	Total	C	O	0
			42	40	2	

- Molecule 26 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



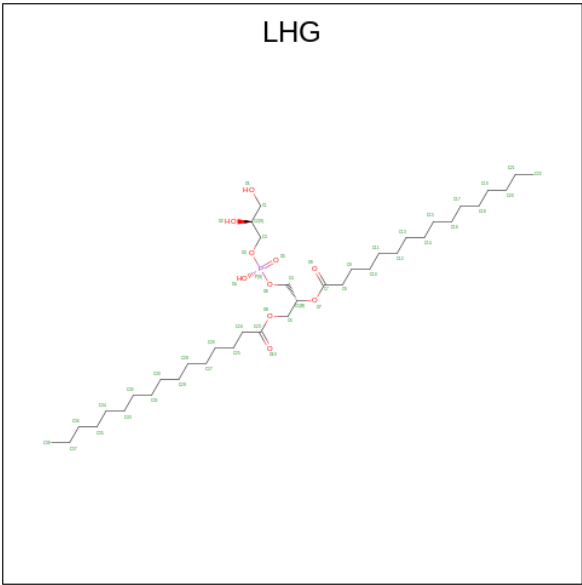
Mol	Chain	Residues	Atoms			AltConf
26	5	1	Total	C	O	0
			44	40	4	
26	7	1	Total	C	O	0
			44	40	4	
26	G	1	Total	C	O	0
			44	40	4	
26	N	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	Y	1	Total	C	O	0
			44	40	4	
26	g	1	Total	C	O	0
			44	40	4	
26	n	1	Total	C	O	0
			44	40	4	
26	s	1	Total	C	O	0
			44	40	4	
26	y	1	Total	C	O	0
			44	40	4	
26	r	1	Total	C	O	0
			44	40	4	
26	9	1	Total	C	O	0
			44	40	4	
26	AA	1	Total	C	O	0
			44	40	4	
26	Au	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
26	A2	1	Total	C	O	0
			44	40	4	
26	A6	1	Total	C	O	0
			44	40	4	
26	BB	1	Total	C	O	0
			44	40	4	
26	BB	1	Total	C	O	0
			44	40	4	
26	BJ	1	Total	C	O	0
			44	40	4	
26	BQ	1	Total	C	O	0
			44	40	4	
26	BV	1	Total	C	O	0
			44	40	4	
26	Ba	1	Total	C	O	0
			44	40	4	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
27	5	1	Total	C	O	P	0
			41	30	10	1	
27	6	1	Total	C	O	P	0
			47	36	10	1	
27	B	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
27	B	1	Total 46	C 35	O 10	P 1	0
27	D	1	Total 49	C 38	O 10	P 1	0
27	G	1	Total 49	C 38	O 10	P 1	0
27	L	1	Total 49	C 38	O 10	P 1	0
27	N	1	Total 49	C 38	O 10	P 1	0
27	W	1	Total 49	C 38	O 10	P 1	0
27	Y	1	Total 49	C 38	O 10	P 1	0
27	b	1	Total 49	C 38	O 10	P 1	0
27	b	1	Total 46	C 35	O 10	P 1	0
27	b	1	Total 49	C 38	O 10	P 1	0
27	d	1	Total 49	C 38	O 10	P 1	0
27	g	1	Total 49	C 38	O 10	P 1	0
27	n	1	Total 49	C 38	O 10	P 1	0
27	w	1	Total 49	C 38	O 10	P 1	0
27	y	1	Total 49	C 38	O 10	P 1	0
27	C	1	Total 49	C 38	O 10	P 1	0
27	C	1	Total 49	C 38	O 10	P 1	0
27	c	1	Total 49	C 38	O 10	P 1	0
27	c	1	Total 49	C 38	O 10	P 1	0
27	r	1	Total 42	C 31	O 10	P 1	0
27	9	1	Total 41	C 30	O 10	P 1	0

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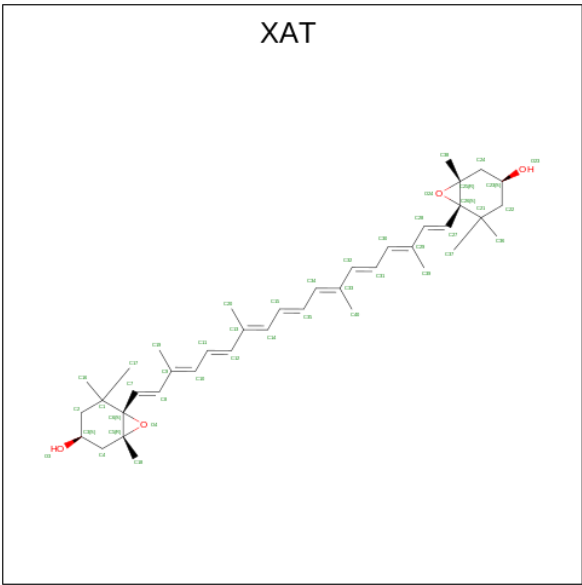
Mol	Chain	Residues	Atoms				AltConf
27	0	1	Total 47	C 36	O 10	P 1	0
27	v	1	Total 49	C 38	O 10	P 1	0
27	2	1	Total 46	C 35	O 10	P 1	0
27	2	1	Total 49	C 38	O 10	P 1	0
27	Au	1	Total 49	C 38	O 10	P 1	0
27	Az	1	Total 49	C 38	O 10	P 1	0
27	A2	1	Total 49	C 38	O 10	P 1	0
27	A0	1	Total 49	C 38	O 10	P 1	0
27	BB	1	Total 49	C 38	O 10	P 1	0
27	BE	1	Total 49	C 38	O 10	P 1	0
27	BE	1	Total 46	C 35	O 10	P 1	0
27	BE	1	Total 49	C 38	O 10	P 1	0
27	BG	1	Total 49	C 38	O 10	P 1	0
27	BJ	1	Total 49	C 38	O 10	P 1	0
27	BQ	1	Total 49	C 38	O 10	P 1	0
27	BY	1	Total 49	C 38	O 10	P 1	0
27	Ba	1	Total 49	C 38	O 10	P 1	0
27	1	1	Total 49	C 38	O 10	P 1	0
27	1	1	Total 49	C 38	O 10	P 1	0
27	BF	1	Total 49	C 38	O 10	P 1	0
27	BF	1	Total 49	C 38	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
27	BU	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 28 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).



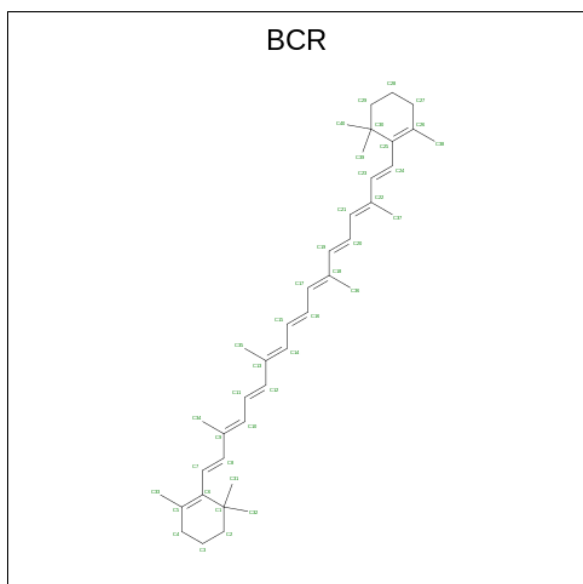
Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	O	0
			44	40	4	
28	7	1	Total	C	O	0
			44	40	4	
28	7	1	Total	C	O	0
			44	40	4	
28	8	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	Y	1	Total	C	O	0
			44	40	4	
28	g	1	Total	C	O	0
			44	40	4	
28	n	1	Total	C	O	0
			44	40	4	
28	y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
28	r	1	Total	C	O	0
			44	40	4	
28	9	1	Total	C	O	0
			44	40	4	
28	AA	1	Total	C	O	0
			44	40	4	
28	AA	1	Total	C	O	0
			44	40	4	
28	AB	1	Total	C	O	0
			44	40	4	
28	Au	1	Total	C	O	0
			44	40	4	
28	A2	1	Total	C	O	0
			44	40	4	
28	BB	1	Total	C	O	0
			44	40	4	
28	BJ	1	Total	C	O	0
			44	40	4	
28	BQ	1	Total	C	O	0
			44	40	4	
28	Ba	1	Total	C	O	0
			44	40	4	
28	BU	1	Total	C	O	0
			44	40	4	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
29	8	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	H	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	f	1	Total C 40 40	0
29	h	1	Total C 40 40	0
29	k	1	Total C 40 40	0
29	z	1	Total C 40 40	0
29	z	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	a	1	Total C 40 40	0

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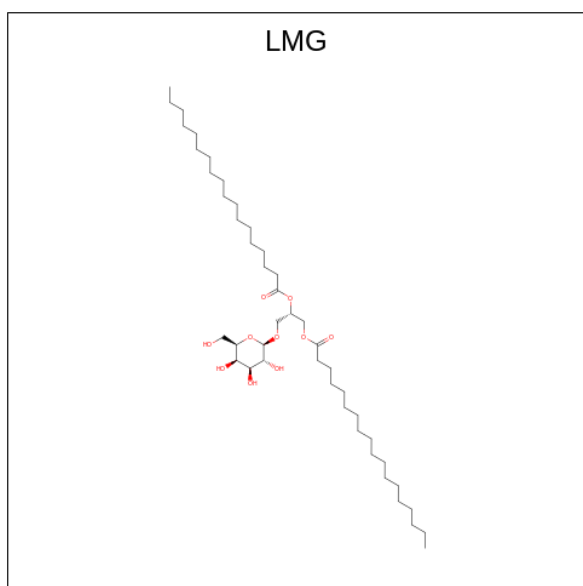
Mol	Chain	Residues	Atoms	AltConf
29	c	1	Total C 40 40	0
29	AB	1	Total C 40 40	0
29	v	1	Total C 40 40	0
29	v	1	Total C 40 40	0
29	v	1	Total C 40 40	0
29	v	1	Total C 40 40	0
29	4	1	Total C 40 40	0
29	Av	1	Total C 40 40	0
29	Ay	1	Total C 40 40	0
29	Ay	1	Total C 40 40	0
29	BE	1	Total C 40 40	0
29	BE	1	Total C 40 40	0
29	BE	1	Total C 40 40	0
29	BE	1	Total C 40 40	0
29	BI	1	Total C 40 40	0
29	BK	1	Total C 40 40	0
29	BN	1	Total C 40 40	0
29	Bb	1	Total C 40 40	0
29	R	1	Total C 40 40	0
29	1	1	Total C 40 40	0
29	1	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
29	BD	1	Total	C	0
			40	40	
29	BF	1	Total	C	0
			40	40	
29	BF	1	Total	C	0
			40	40	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



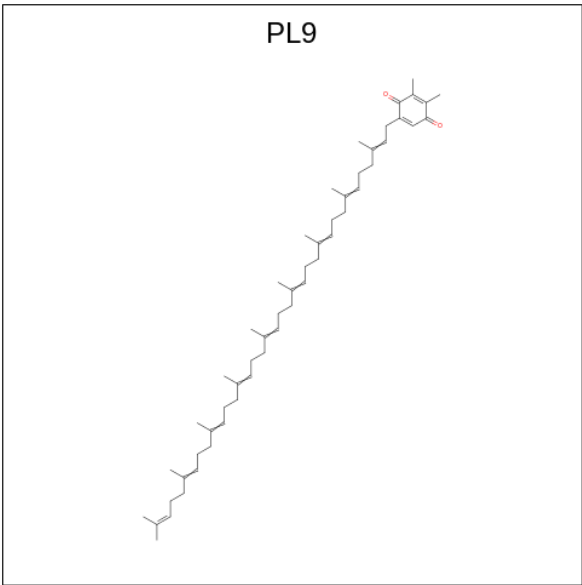
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			51	41	10	
30	B	1	Total	C	O	0
			40	30	10	
30	D	1	Total	C	O	0
			46	36	10	
30	I	1	Total	C	O	0
			40	30	10	
30	b	1	Total	C	O	0
			51	41	10	
30	d	1	Total	C	O	0
			46	36	10	
30	i	1	Total	C	O	0
			48	38	10	
30	A	1	Total	C	O	0
			48	38	10	

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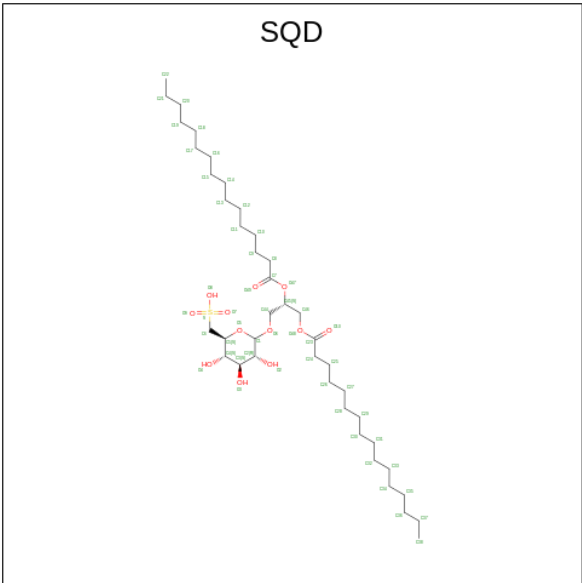
Mol	Chain	Residues	Atoms			AltConf
30	C	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			51	41	10	
30	v	1	Total	C	O	0
			51	41	10	
30	v	1	Total	C	O	0
			40	30	10	
30	2	1	Total	C	O	0
			46	36	10	
30	Aw	1	Total	C	O	0
			40	30	10	
30	A0	1	Total	C	O	0
			48	38	10	
30	BE	1	Total	C	O	0
			51	41	10	
30	BG	1	Total	C	O	0
			46	36	10	
30	BL	1	Total	C	O	0
			48	38	10	
30	1	1	Total	C	O	0
			51	41	10	
30	1	1	Total	C	O	0
			51	41	10	
30	BF	1	Total	C	O	0
			51	41	10	
30	BF	1	Total	C	O	0
			51	41	10	

- Molecule 31 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



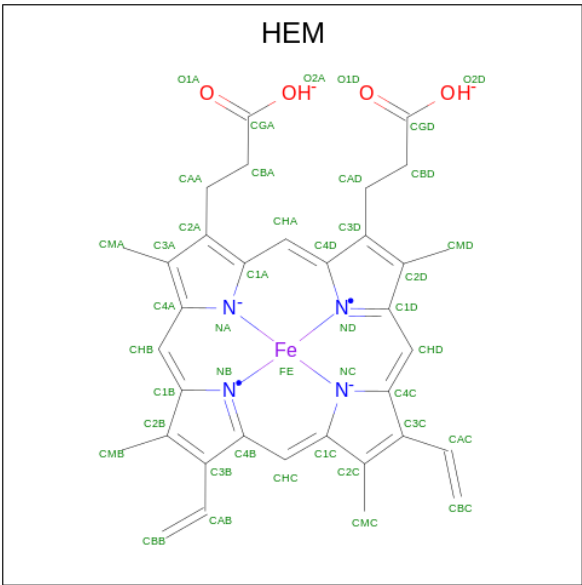
Mol	Chain	Residues	Atoms			AltConf
31	D	1	Total	C	O	0
			55	53	2	
31	d	1	Total	C	O	0
			55	53	2	
31	2	1	Total	C	O	0
			55	53	2	
31	BG	1	Total	C	O	0
			55	53	2	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



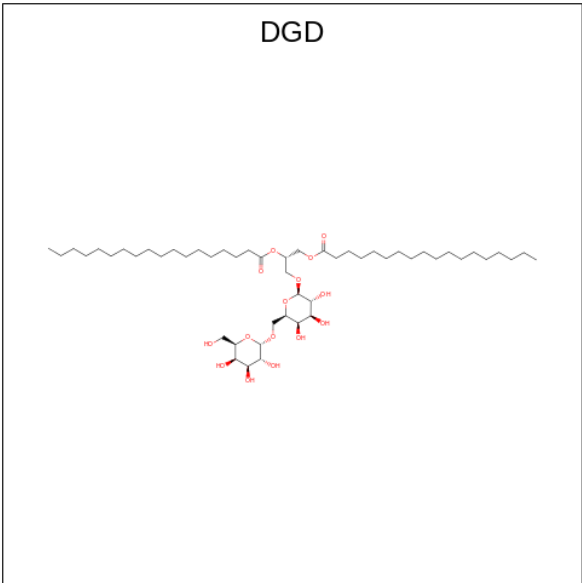
Mol	Chain	Residues	Atoms				AltConf
32	D	1	Total	C	O	S	0
			50	37	12	1	
32	L	1	Total	C	O	S	0
			42	29	12	1	
32	L	1	Total	C	O	S	0
			54	41	12	1	
32	d	1	Total	C	O	S	0
			50	37	12	1	
32	l	1	Total	C	O	S	0
			54	41	12	1	
32	l	1	Total	C	O	S	0
			42	29	12	1	
32	A	1	Total	C	O	S	0
			54	41	12	1	
32	a	1	Total	C	O	S	0
			54	41	12	1	
32	2	1	Total	C	O	S	0
			50	37	12	1	
32	Az	1	Total	C	O	S	0
			42	29	12	1	
32	A1	1	Total	C	O	S	0
			54	41	12	1	
32	BG	1	Total	C	O	S	0
			50	37	12	1	
32	BO	1	Total	C	O	S	0
			54	41	12	1	
32	BO	1	Total	C	O	S	0
			42	29	12	1	
32	R	1	Total	C	O	S	0
			54	41	12	1	
32	BD	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



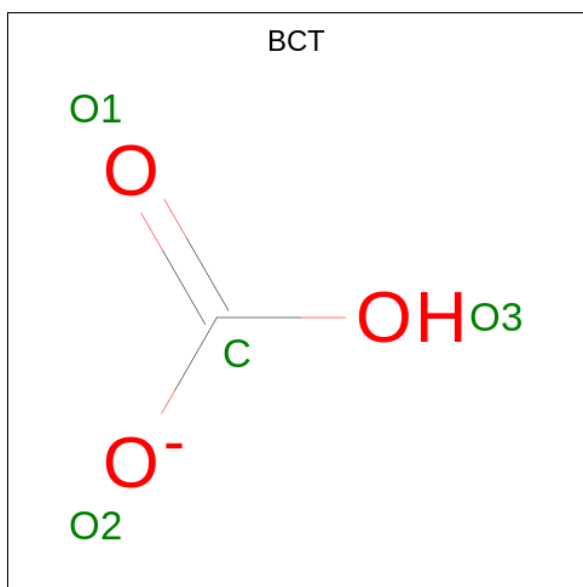
Mol	Chain	Residues	Atoms					AltConf
33	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
33	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
33	4	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
33	BI	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



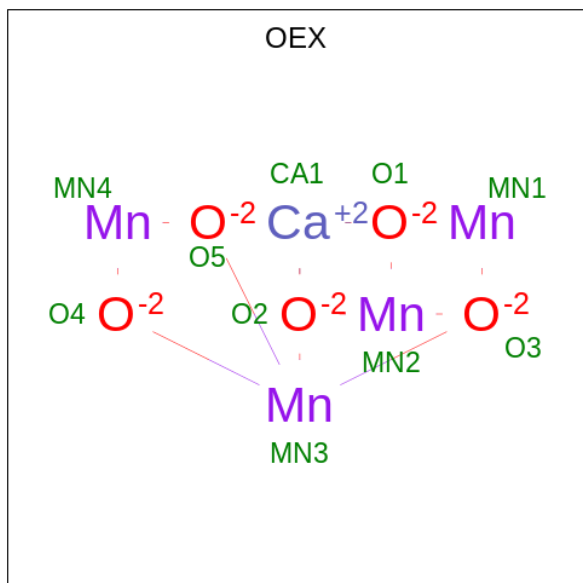
Mol	Chain	Residues	Atoms			AltConf
34	H	1	Total	C	O	0
			62	47	15	
34	h	1	Total	C	O	0
			62	47	15	
34	A	1	Total	C	O	0
			59	44	15	
34	C	1	Total	C	O	0
			55	40	15	
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			60	45	15	
34	a	1	Total	C	O	0
			59	44	15	
34	a	1	Total	C	O	0
			60	45	15	
34	c	1	Total	C	O	0
			55	40	15	
34	c	1	Total	C	O	0
			62	47	15	
34	Av	1	Total	C	O	0
			62	47	15	
34	BK	1	Total	C	O	0
			62	47	15	
34	R	1	Total	C	O	0
			59	44	15	
34	1	1	Total	C	O	0
			55	40	15	
34	1	1	Total	C	O	0
			62	47	15	
34	1	1	Total	C	O	0
			60	45	15	
34	BD	1	Total	C	O	0
			59	44	15	
34	BD	1	Total	C	O	0
			60	45	15	
34	BF	1	Total	C	O	0
			55	40	15	
34	BF	1	Total	C	O	0
			62	47	15	

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			4	1	3	
35	a	1	Total	C	O	0
			4	1	3	
35	2	1	Total	C	O	0
			4	1	3	
35	BD	1	Total	C	O	0
			4	1	3	

- Molecule 36 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

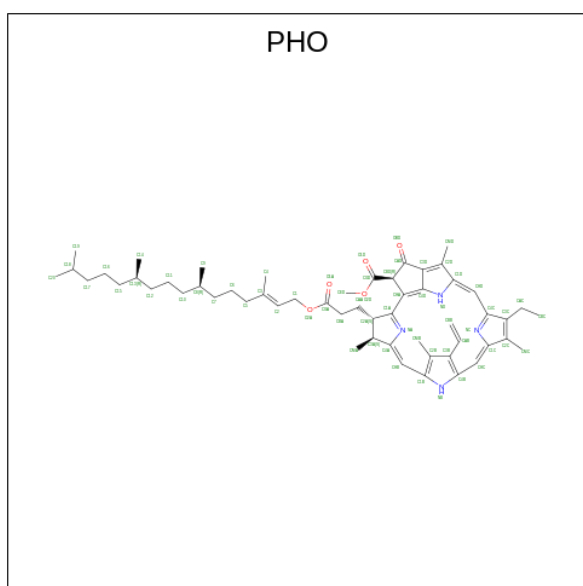


Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
36	a	1	Total	Ca	Mn	O	0
			10	1	4	5	
36	R	1	Total	Ca	Mn	O	0
			10	1	4	5	
36	BD	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 37 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
37	A	1	Total	Fe	0
			1	1	
37	a	1	Total	Fe	0
			1	1	
37	R	1	Total	Fe	0
			1	1	
37	BD	1	Total	Fe	0
			1	1	

- Molecule 38 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	N	O	0
			64	55	4	5	
38	A	1	Total	C	N	O	0
			64	55	4	5	

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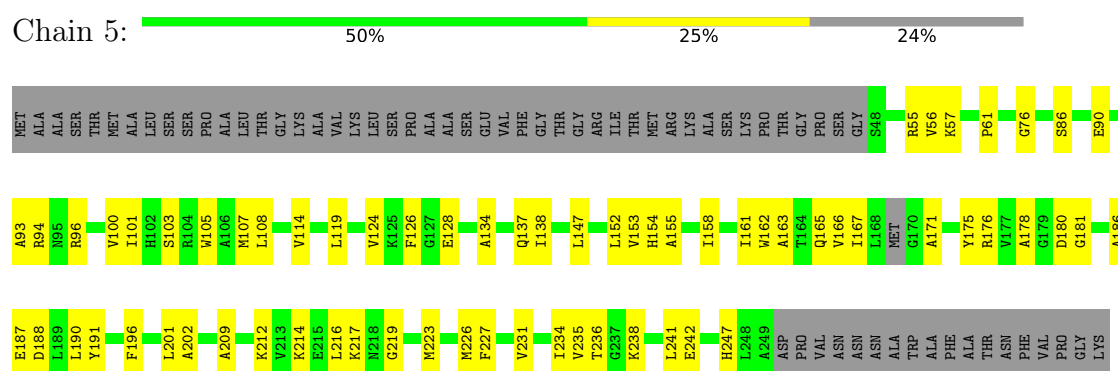
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Mol	Chain	Residues	Atoms				AltConf
38	a	1	Total 64	C 55	N 4	O 5	0
38	a	1	Total 64	C 55	N 4	O 5	0
38	R	1	Total 64	C 55	N 4	O 5	0
38	R	1	Total 64	C 55	N 4	O 5	0
38	BD	1	Total 64	C 55	N 4	O 5	0
38	BD	1	Total 64	C 55	N 4	O 5	0

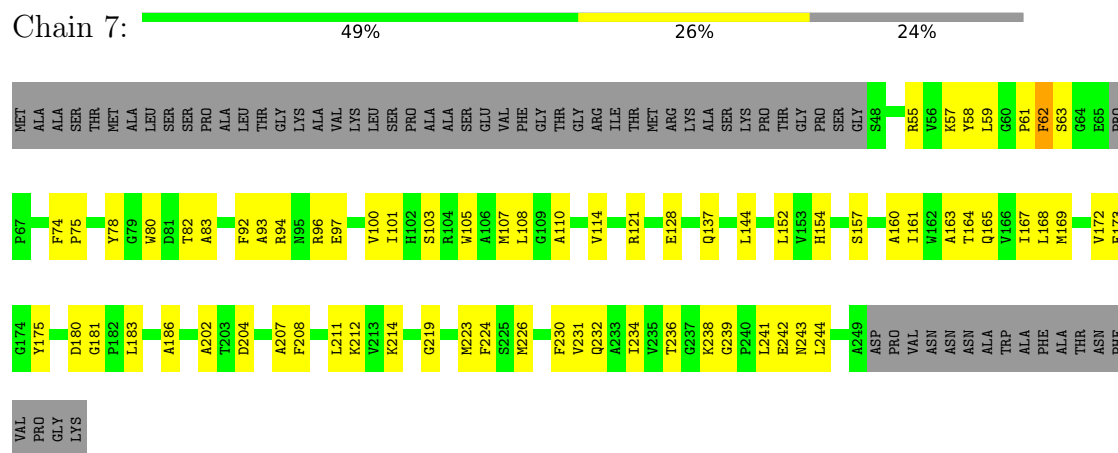
3 Residue-property plots

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.

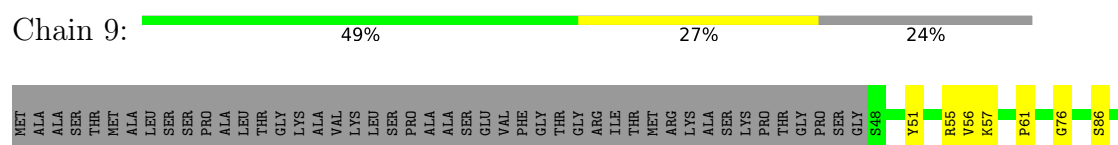
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

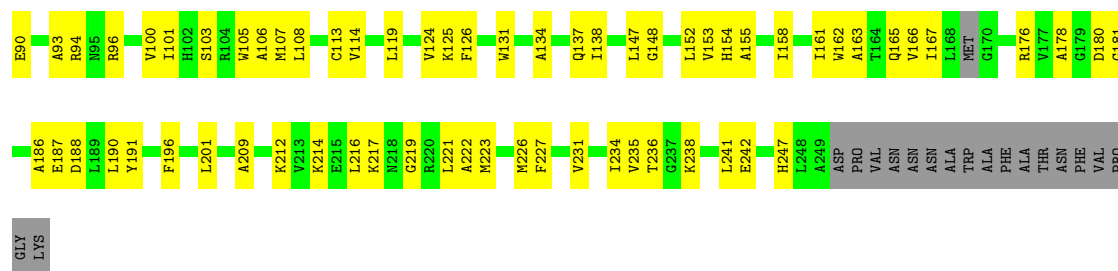


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

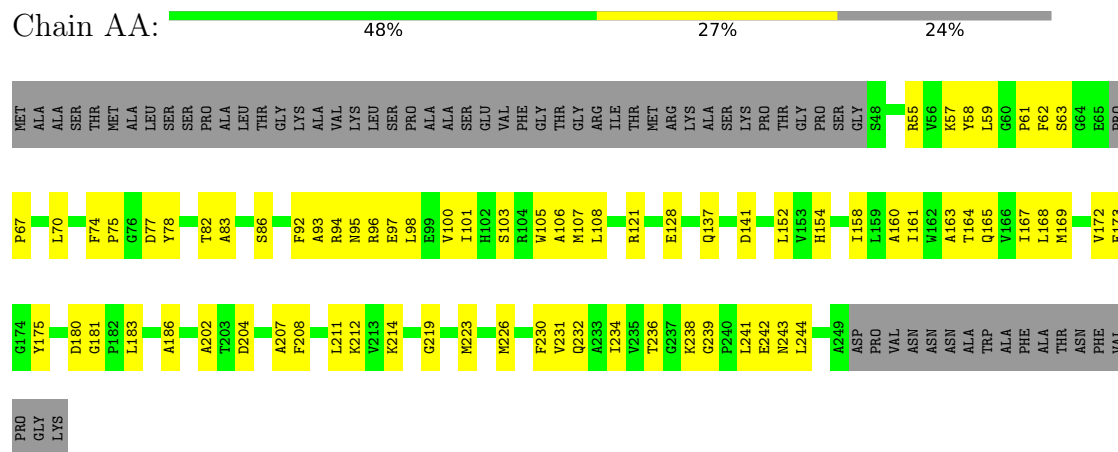


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

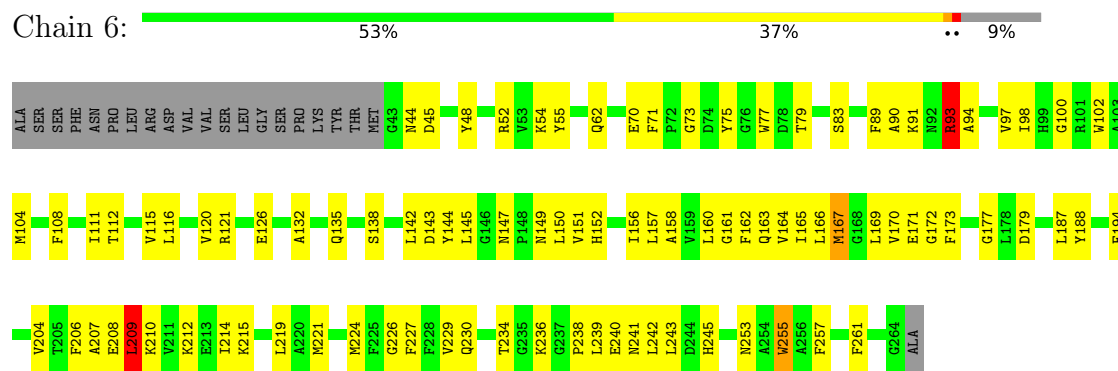




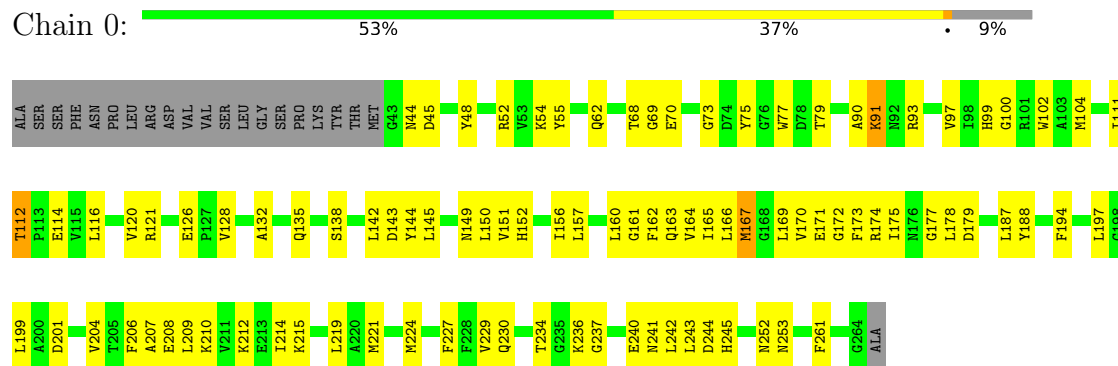
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



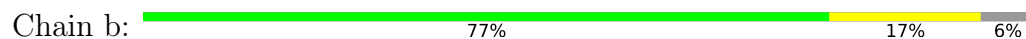
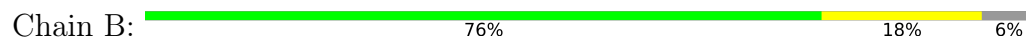
- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

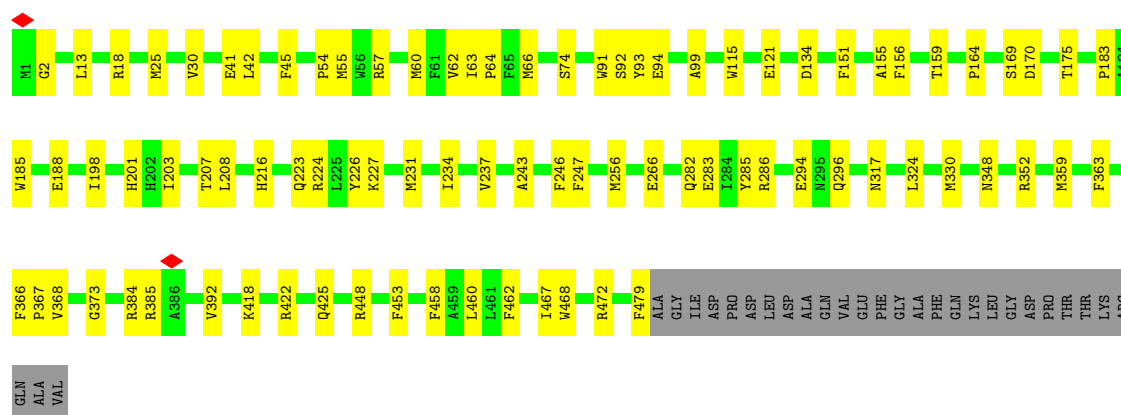


- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic



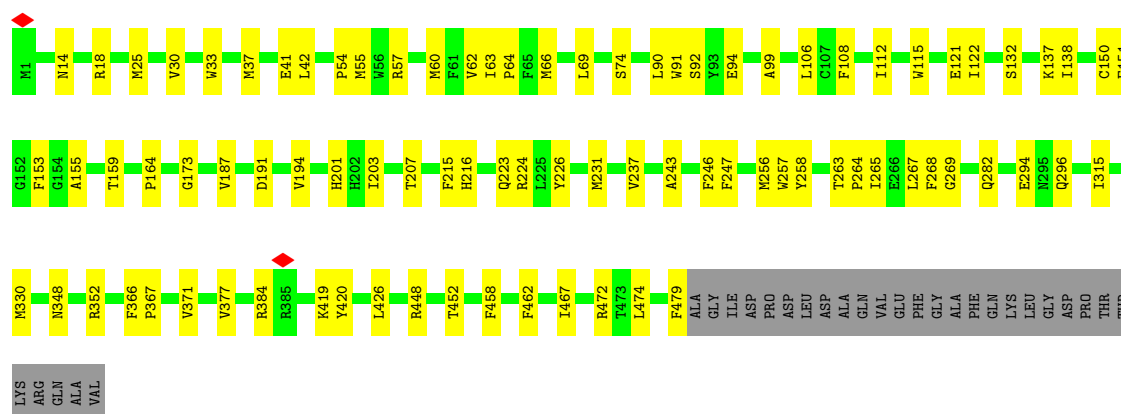
- Chain 8: 54% 36% 9%





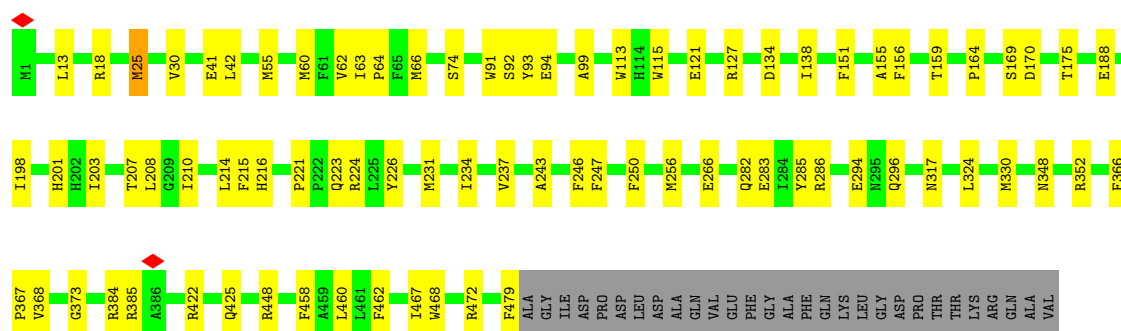
• Molecule 4: Photosystem II CP47 reaction center protein

Chain v: 77% 17% 6%



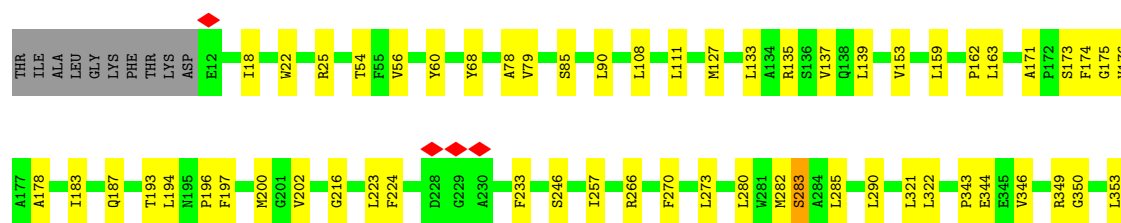
• Molecule 4: Photosystem II CP47 reaction center protein

Chain BE: 78% 16% 6%



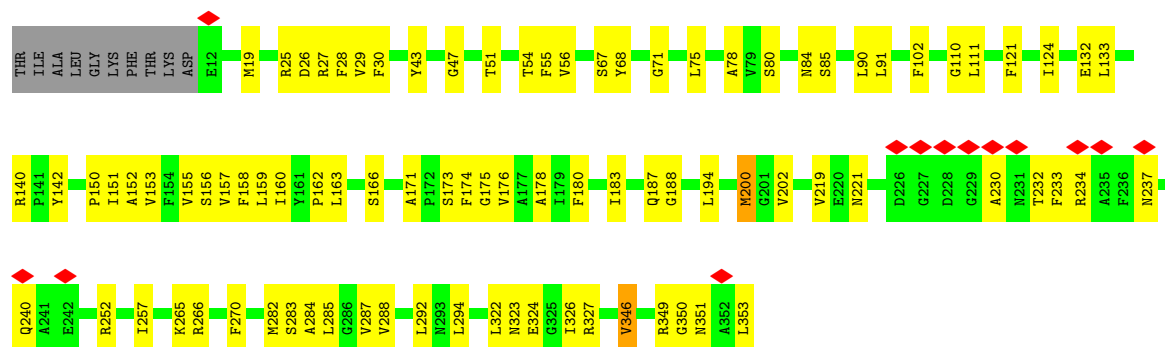
• Molecule 5: Photosystem II D2 protein

Chain D: 81% 16% 3%



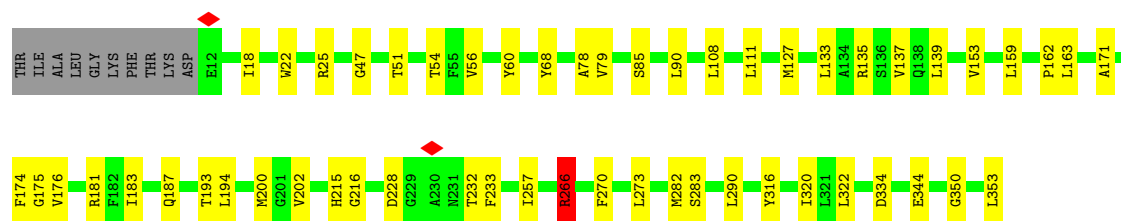
• Molecule 5: Photosystem II D2 protein

Chain d: 72% 25%



• Molecule 5: Photosystem II D2 protein

Chain 2: 82% 15%



• Molecule 5: Photosystem II D2 protein

Chain BG: 75% 21%



• Molecule 6: Cytochrome b559 subunit alpha



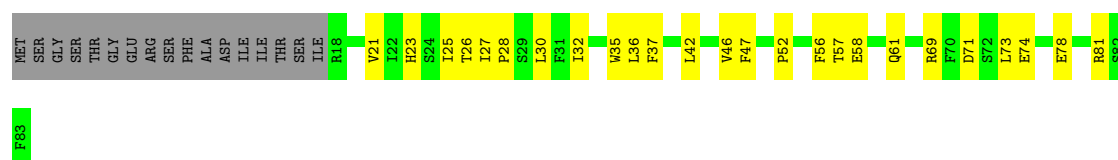
- Molecule 6: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit alpha



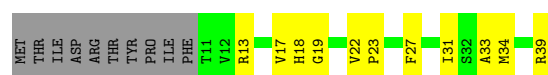
- Molecule 6: Cytochrome b559 subunit alpha



- Molecule 7: Cytochrome b559 subunit beta



- Molecule 7: Cytochrome b559 subunit beta

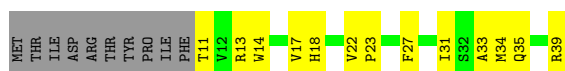


- Molecule 7: Cytochrome b559 subunit beta





- Molecule 7: Cytochrome b559 subunit beta



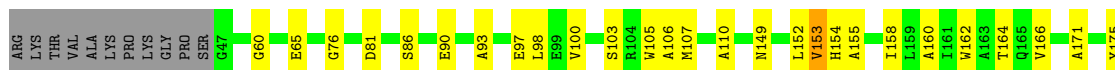
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic



- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

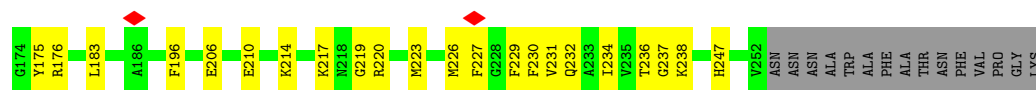


- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

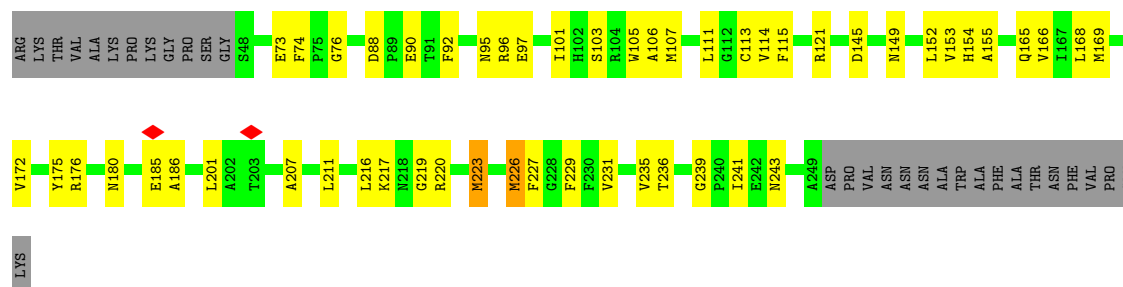


- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

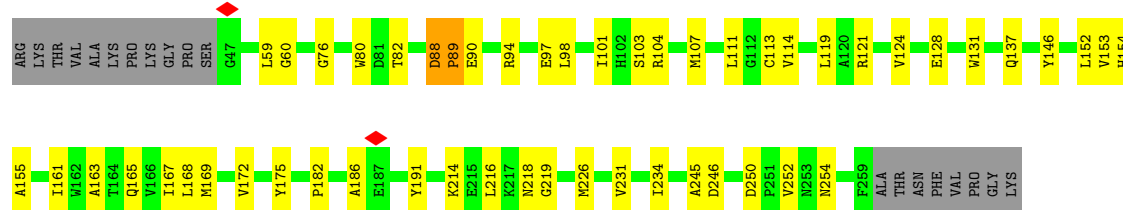




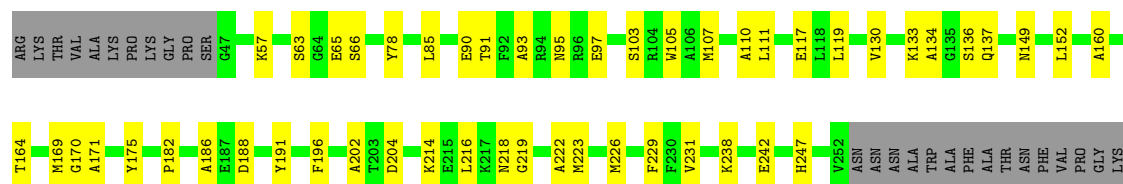
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic



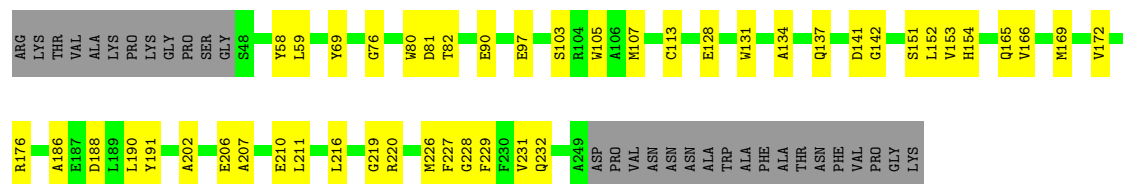
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic



- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

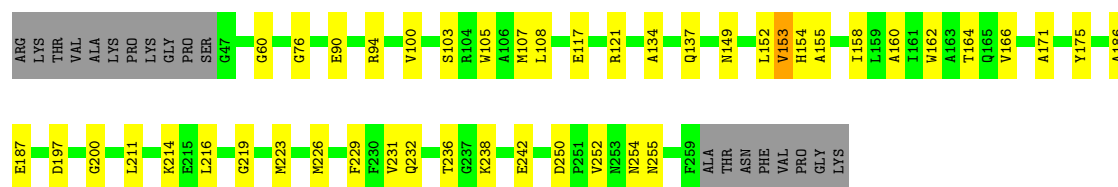


- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic



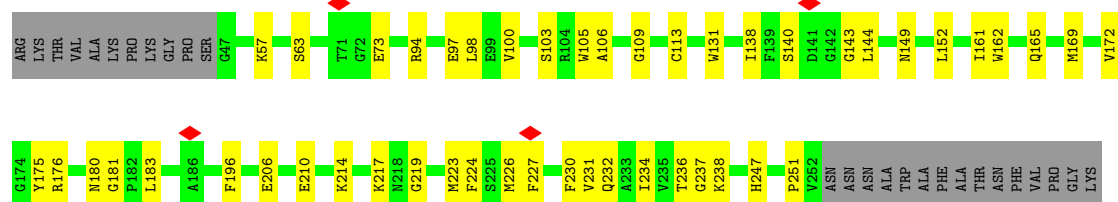
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain BB: 



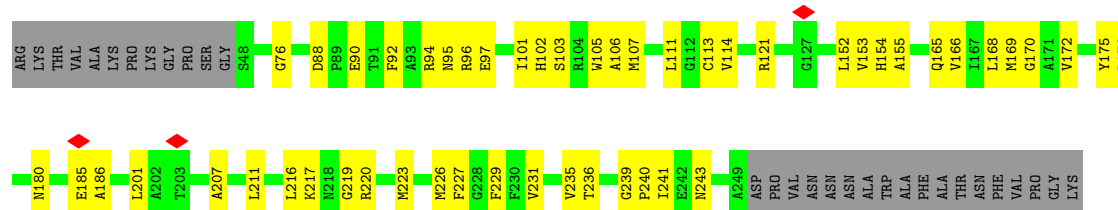
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain BJ: 



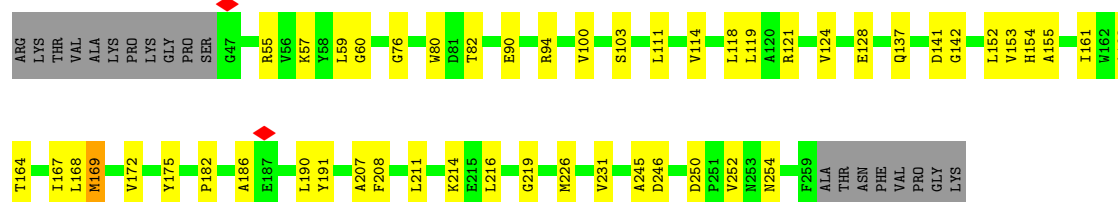
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain BQ: 



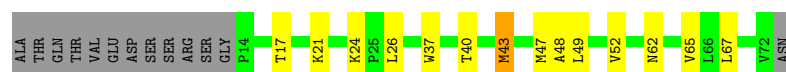
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain Ba: 

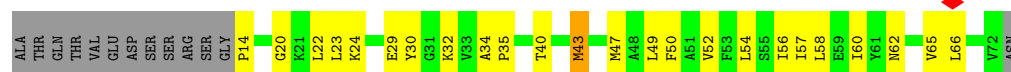


- Molecule 9: Photosystem II reaction center protein H

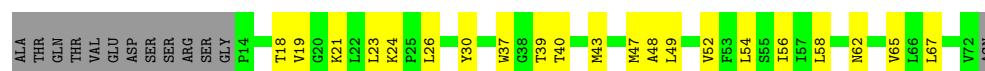
Chain H: 



- Molecule 9: Photosystem II reaction center protein H



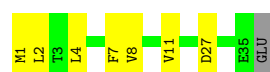
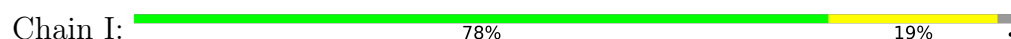
- Molecule 9: Photosystem II reaction center protein H



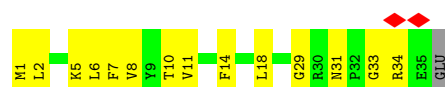
- Molecule 9: Photosystem II reaction center protein H



- Molecule 10: Photosystem II reaction center protein I



- Molecule 10: Photosystem II reaction center protein I



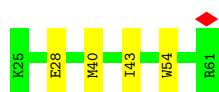
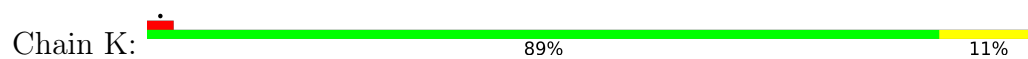
- Molecule 10: Photosystem II reaction center protein I



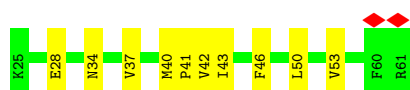
- Molecule 10: Photosystem II reaction center protein I



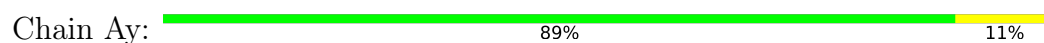
- Molecule 11: Photosystem II reaction center protein K



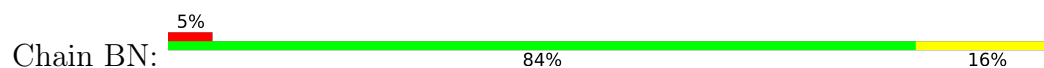
- Molecule 11: Photosystem II reaction center protein K



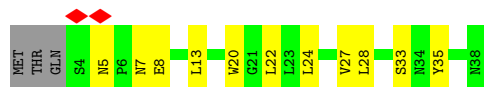
- Molecule 11: Photosystem II reaction center protein K



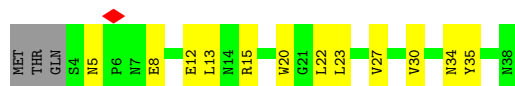
- Molecule 11: Photosystem II reaction center protein K



- Molecule 12: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein L

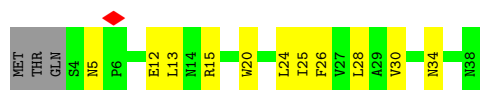


- Molecule 12: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein L

Chain BO:  63% 29% 8%



- Molecule 13: Photosystem II reaction center protein M

Chain M:  56% 32% 6% 6%



- Molecule 13: Photosystem II reaction center protein M

Chain m:  50% 41% 6% 6%



- Molecule 13: Photosystem II reaction center protein M

Chain A1:  50% 44% 6%



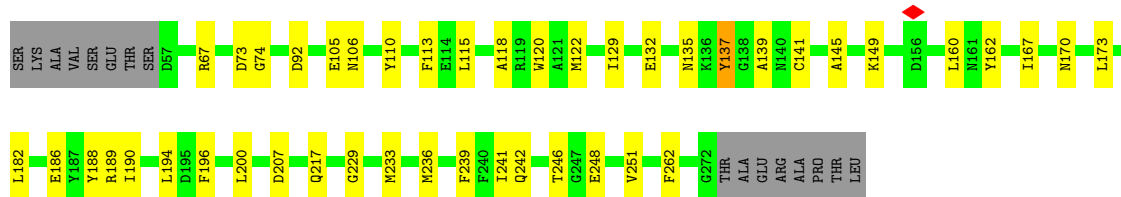
- Molecule 13: Photosystem II reaction center protein M

Chain BP:  56% 35% 6% 6%



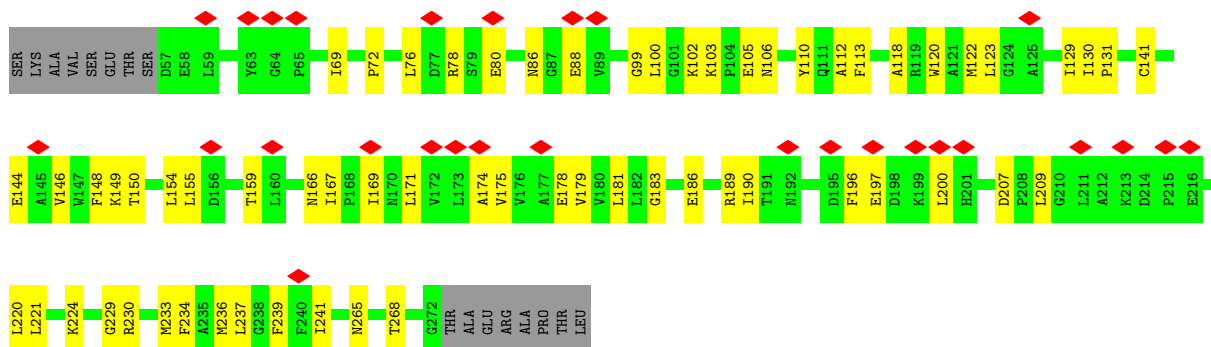
- Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic

Chain S:  74% 19% 7%

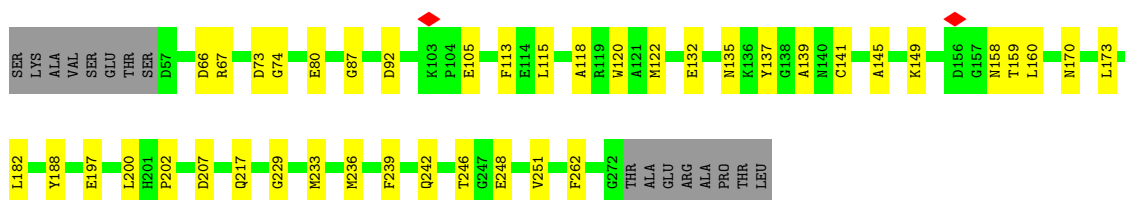
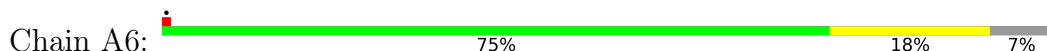


- Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic

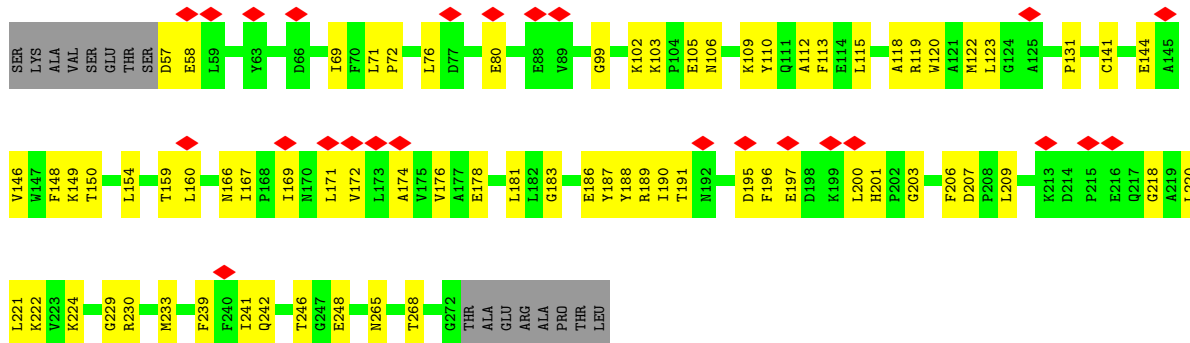
Chain s:  12% 66% 27% 7%



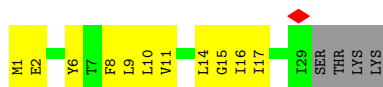
- Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic



- Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic



- Molecule 15: Photosystem II reaction center protein T

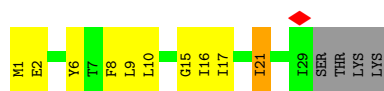


- Molecule 15: Photosystem II reaction center protein T





- Molecule 15: Photosystem II reaction center protein T



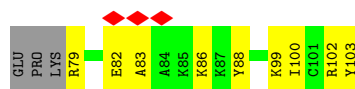
- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 5 kDa protein, chloroplastic



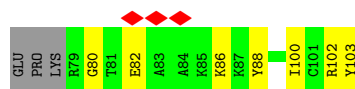
- Molecule 16: Photosystem II 5 kDa protein, chloroplastic



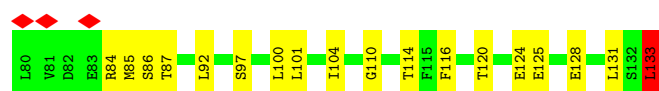
- Molecule 16: Photosystem II 5 kDa protein, chloroplastic



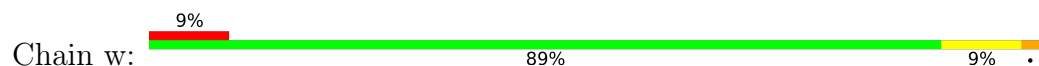
- Molecule 16: Photosystem II 5 kDa protein, chloroplastic



- Molecule 17: Photosystem II reaction center W protein, chloroplastic



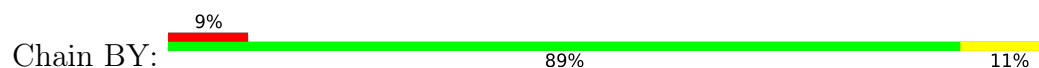
- Molecule 17: Photosystem II reaction center W protein, chloroplastic



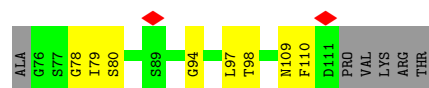
- Molecule 17: Photosystem II reaction center W protein, chloroplastic



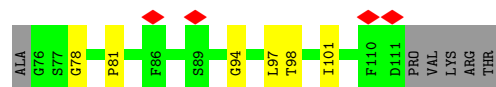
- Molecule 17: Photosystem II reaction center W protein, chloroplastic



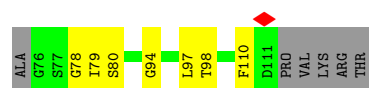
- Molecule 18: (thale cress) hypothetical protein



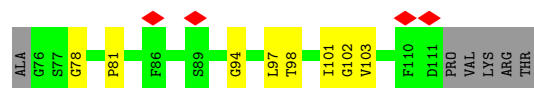
- Molecule 18: (thale cress) hypothetical protein



- Molecule 18: (thale cress) hypothetical protein



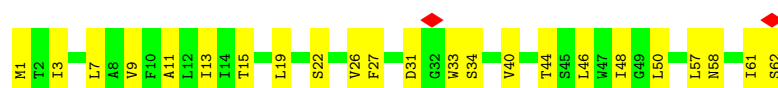
- Molecule 18: (thale cress) hypothetical protein



- Molecule 19: Photosystem II reaction center protein Z



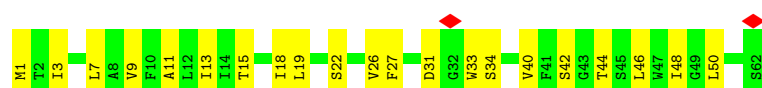
- Molecule 19: Photosystem II reaction center protein Z



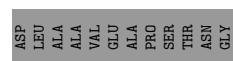
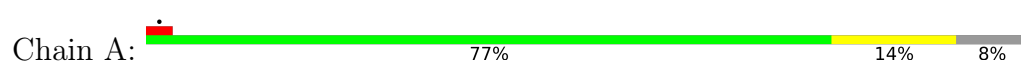
- Molecule 19: Photosystem II reaction center protein Z



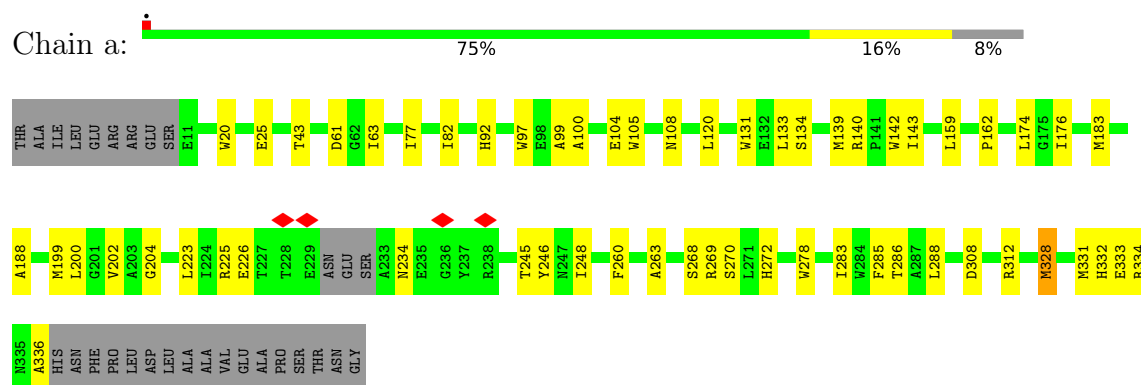
- Molecule 19: Photosystem II reaction center protein Z



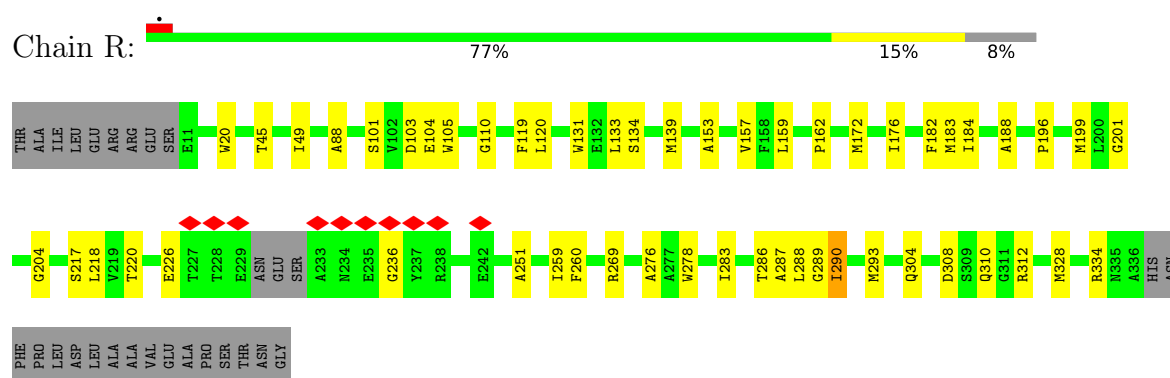
- Molecule 20: Photosystem II protein D1



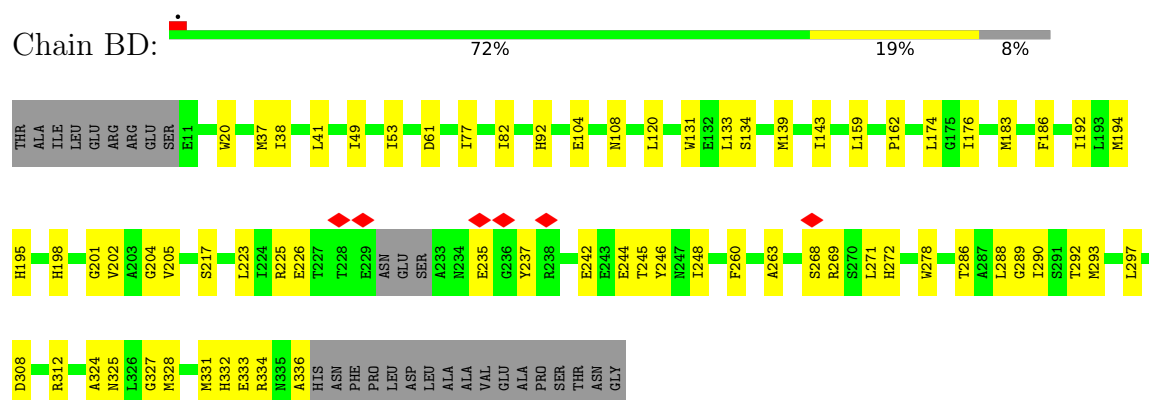
- Molecule 20: Photosystem II protein D1



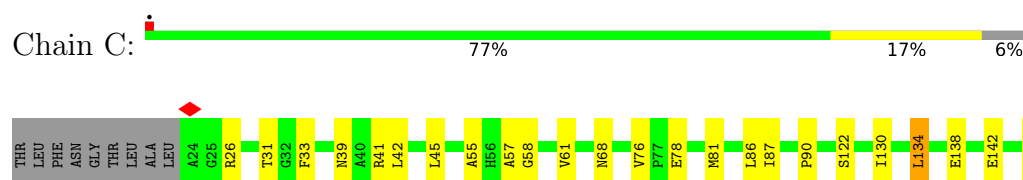
- Molecule 20: Photosystem II protein D1

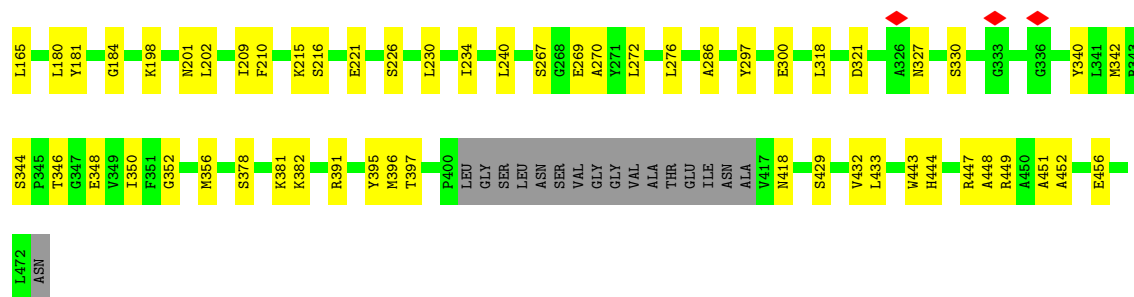


- Molecule 20: Photosystem II protein D1

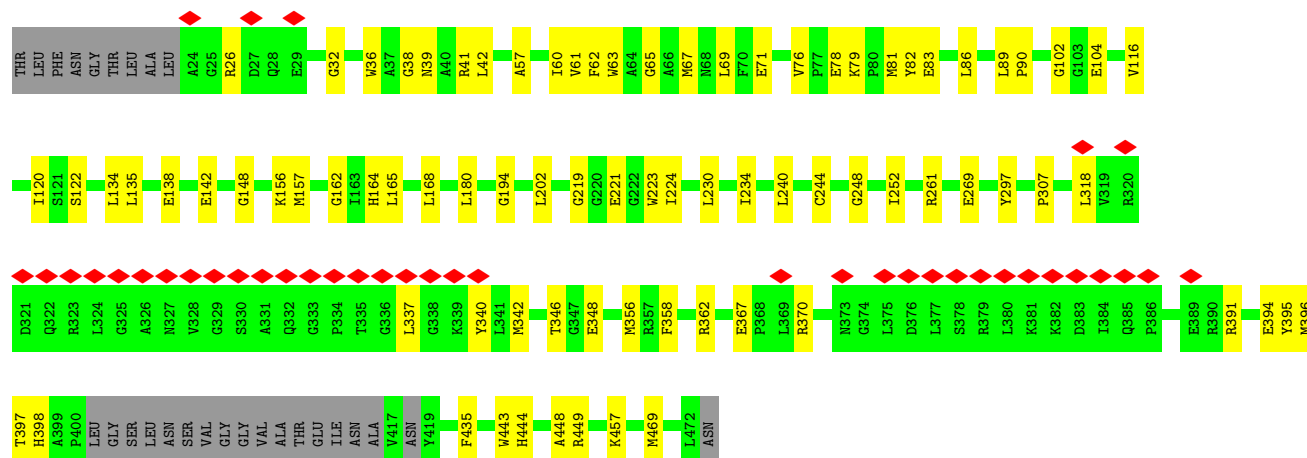
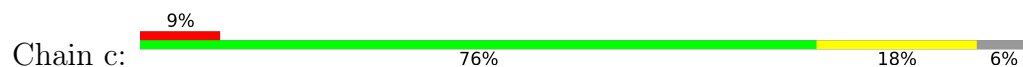


- Molecule 21: Photosystem II CP43 reaction center protein

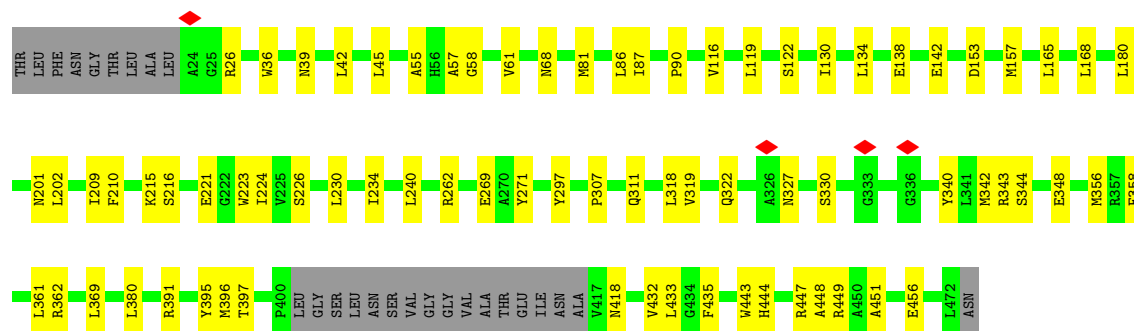
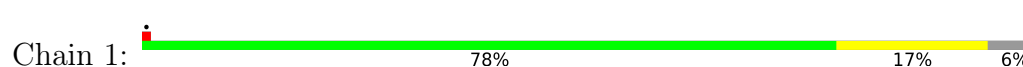




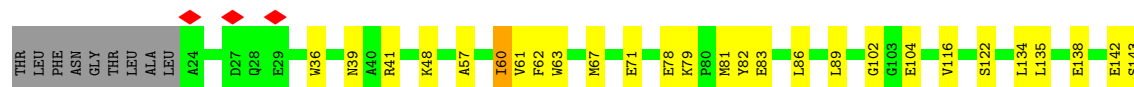
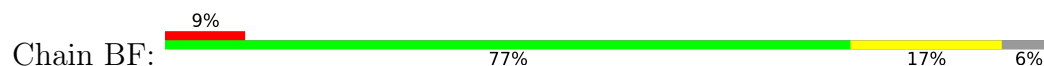
• Molecule 21: Photosystem II CP43 reaction center protein



• Molecule 21: Photosystem II CP43 reaction center protein



• Molecule 21: Photosystem II CP43 reaction center protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48981	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.874	Depositor
Minimum map value	-18.604	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	770.4, 770.4, 770.4	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, BCT, FE2, BCR, DGD, OEX, LMG, SQD, XAT, PL9, LHG, NEX, CHL, PHO, CLA, LUT

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	5	0.26	0/1573	0.44	0/2137
1	7	0.28	0/1573	0.45	0/2134
1	9	0.25	0/1573	0.38	0/2137
1	AA	0.31	0/1573	0.45	0/2134
2	0	0.34	0/1768	0.55	2/2405 (0.1%)
2	6	0.36	0/1768	0.58	3/2405 (0.1%)
3	8	0.27	0/1564	0.54	0/2123
3	AB	0.29	0/1564	0.55	0/2123
4	B	0.23	0/3886	0.34	1/5293 (0.0%)
4	BE	0.24	0/3886	0.36	1/5293 (0.0%)
4	b	0.22	0/3886	0.35	0/5293
4	v	0.23	0/3886	0.32	0/5293
5	2	0.35	0/2816	0.40	1/3837 (0.0%)
5	BG	0.32	1/2816 (0.0%)	0.41	0/3837
5	D	0.25	0/2816	0.35	0/3837
5	d	0.31	1/2816 (0.0%)	0.41	1/3837 (0.0%)
6	3	0.15	0/562	0.34	0/763
6	BH	0.17	0/562	0.33	0/763
6	E	0.15	0/562	0.34	0/763
6	e	0.15	0/562	0.30	0/763
7	4	0.17	0/230	0.34	0/311
7	BI	0.15	0/230	0.31	0/311
7	F	0.15	0/230	0.31	0/311
7	f	0.17	0/230	0.33	0/311
8	A2	0.29	0/1580	0.40	0/2146
8	Au	0.23	0/1607	0.33	0/2184
8	BB	0.31	0/1669	0.37	0/2270
8	BJ	0.15	0/1607	0.38	0/2184
8	BQ	0.19	0/1580	0.40	0/2146
8	Ba	0.19	0/1669	0.37	1/2270 (0.0%)
8	G	0.25	0/1607	0.38	1/2184 (0.0%)
8	N	0.28	0/1580	0.40	0/2146

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	Y	0.31	0/1669	0.39	1/2270 (0.0%)
8	g	0.15	0/1607	0.38	0/2184
8	n	0.26	0/1580	0.48	2/2146 (0.1%)
8	y	0.25	0/1669	0.46	1/2270 (0.0%)
9	Av	0.29	0/447	0.52	0/608
9	BK	0.27	0/447	0.48	0/608
9	H	0.28	0/447	0.48	1/608 (0.2%)
9	h	0.28	0/447	0.52	1/608 (0.2%)
10	Aw	0.28	0/294	0.41	0/397
10	BL	0.27	0/294	0.39	0/397
10	I	0.27	0/294	0.40	0/397
10	i	0.27	0/294	0.50	0/397
11	Ay	0.22	0/313	0.44	0/428
11	BN	0.22	0/313	0.45	0/428
11	K	0.20	0/313	0.40	0/428
11	k	0.21	0/313	0.45	0/428
12	Az	0.28	0/301	0.33	0/409
12	BO	0.25	0/301	0.30	0/409
12	L	0.25	0/301	0.39	0/409
12	l	0.26	0/301	0.33	0/409
13	A1	0.26	0/254	0.50	0/347
13	BP	0.27	0/254	0.53	0/347
13	M	0.31	0/254	0.53	0/347
13	m	0.26	0/254	0.53	0/347
14	A6	0.22	0/1715	0.37	0/2328
14	BV	0.17	0/1715	0.36	0/2328
14	S	0.19	0/1715	0.35	0/2328
14	s	0.16	0/1715	0.34	0/2328
15	A7	0.26	0/246	0.34	0/333
15	BW	0.29	0/246	0.36	0/333
15	T	0.33	0/246	0.43	0/333
15	t	0.21	0/246	0.33	0/333
16	A8	0.17	0/197	0.26	0/261
16	BX	0.15	0/197	0.36	0/261
16	U	0.16	0/197	0.28	0/261
16	u	0.16	0/197	0.34	0/261
17	A0	0.26	0/439	0.41	0/594
17	BY	0.21	0/439	0.33	0/594
17	W	0.26	0/439	0.43	1/594 (0.2%)
17	w	0.26	0/439	0.44	0/594
18	BA	0.15	0/250	0.42	0/339
18	BZ	0.16	0/250	0.39	0/339
18	X	0.15	0/250	0.42	0/339

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	x	0.16	0/250	0.44	0/339
19	BC	0.20	0/475	0.43	0/649
19	Bb	0.19	0/475	0.39	0/649
19	Z	0.23	0/475	0.49	0/649
19	z	0.19	0/475	0.37	0/649
20	A	0.27	0/2602	0.37	0/3546
20	BD	0.26	0/2602	0.37	0/3546
20	R	0.32	0/2602	0.42	1/3546 (0.0%)
20	a	0.25	0/2602	0.38	1/3546 (0.0%)
21	1	0.28	0/3487	0.37	0/4750
21	BF	0.27	0/3478	0.35	0/4736
21	C	0.24	0/3487	0.36	0/4750
21	c	0.26	0/3478	0.38	0/4736
22	BU	0.35	0/1585	0.48	0/2161
22	r	0.31	0/1585	0.52	0/2161
All	All	0.26	2/109588 (0.0%)	0.40	20/149064 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	6	0	1
3	8	0	1
5	2	0	1
17	w	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	d	346	VAL	CB-CG1	-5.66	1.33	1.52
5	BG	346	VAL	CB-CG1	-5.54	1.34	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	167	MET	CG-SD-CE	-9.25	80.54	100.90
8	y	89	PRO	CA-N-CD	-8.75	99.75	112.00
20	a	328	MET	CG-SD-CE	-7.01	85.48	100.90
8	n	226	MET	CG-SD-CE	-6.92	85.69	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	167	MET	CG-SD-CE	-6.76	86.02	100.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2	266	ARG	Sidechain
2	6	93	ARG	Sidechain
3	8	223	ARG	Sidechain
17	w	84	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	1529	0	1470	72	0
1	7	1530	0	1473	68	0
1	9	1529	0	1470	68	0
1	AA	1530	0	1473	82	0
2	0	1716	0	1658	115	0
2	6	1716	0	1658	113	0
3	8	1512	0	1444	81	0
3	AB	1512	0	1444	95	0
4	B	3757	0	3641	84	0
4	BE	3757	0	3641	88	0
4	b	3757	0	3641	93	0
4	v	3757	0	3641	83	0
5	2	2723	0	2615	68	0
5	BG	2723	0	2615	85	0
5	D	2723	0	2615	65	0
5	d	2723	0	2615	99	0
6	3	544	0	519	17	0
6	BH	544	0	519	20	0
6	E	544	0	519	18	0
6	e	544	0	519	21	0
7	4	225	0	233	10	0
7	BI	225	0	233	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	225	0	233	9	0
7	f	225	0	233	13	0
8	A2	1536	0	1480	44	0
8	Au	1562	0	1503	43	0
8	BB	1621	0	1550	36	0
8	BJ	1562	0	1503	47	0
8	BQ	1536	0	1480	49	0
8	Ba	1621	0	1550	35	0
8	G	1562	0	1503	52	0
8	N	1536	0	1480	42	0
8	Y	1621	0	1550	43	0
8	g	1562	0	1503	47	0
8	n	1536	0	1480	51	0
8	y	1621	0	1550	42	0
9	Av	438	0	465	27	0
9	BK	438	0	465	23	0
9	H	438	0	465	19	0
9	h	438	0	465	29	0
10	Aw	286	0	295	2	0
10	BL	286	0	295	7	0
10	I	286	0	295	7	0
10	i	286	0	295	10	0
11	Ay	302	0	313	5	0
11	BN	302	0	313	4	0
11	K	302	0	313	5	0
11	k	302	0	313	9	0
12	Az	293	0	283	11	0
12	BO	293	0	283	12	0
12	L	293	0	283	13	0
12	l	293	0	283	16	0
13	A1	250	0	279	16	0
13	BP	250	0	279	15	0
13	M	250	0	279	15	0
13	m	250	0	279	15	0
14	A6	1670	0	1649	36	0
14	BV	1670	0	1649	74	0
14	S	1670	0	1649	42	0
14	s	1670	0	1649	67	0
15	A7	239	0	255	9	0
15	BW	239	0	255	5	0
15	T	239	0	255	12	0
15	t	239	0	255	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A8	195	0	206	14	0
16	BX	195	0	206	8	0
16	U	195	0	206	16	0
16	u	195	0	206	11	0
17	A0	428	0	405	13	0
17	BY	428	0	405	4	0
17	W	428	0	405	17	0
17	w	428	0	405	8	0
18	BA	248	0	266	7	0
18	BZ	248	0	266	8	0
18	X	248	0	266	8	0
18	x	248	0	266	7	0
19	BC	465	0	495	16	0
19	Bb	465	0	495	15	0
19	Z	465	0	495	16	0
19	z	465	0	495	17	0
20	A	2525	0	2443	50	0
20	BD	2525	0	2443	68	0
20	R	2525	0	2443	58	0
20	a	2525	0	2443	65	0
21	1	3373	0	3302	58	0
21	BF	3365	0	3295	62	0
21	C	3373	0	3302	60	0
21	c	3365	0	3295	81	0
22	BU	1539	0	1502	75	0
22	r	1539	0	1502	93	0
23	0	314	0	238	35	0
23	5	307	0	228	43	0
23	6	314	0	238	42	0
23	7	304	0	222	32	0
23	8	184	0	124	10	0
23	9	307	0	228	40	0
23	A2	358	0	318	47	0
23	A6	195	0	136	15	0
23	AA	304	0	222	34	0
23	AB	184	0	124	15	0
23	Au	349	0	300	39	0
23	BB	358	0	318	48	0
23	BH	45	0	28	0	0
23	BJ	351	0	303	54	0
23	BQ	358	0	318	51	0
23	BU	222	0	179	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	BV	195	0	136	20	0
23	Ba	358	0	318	45	0
23	G	349	0	300	50	0
23	N	358	0	318	45	0
23	S	195	0	136	15	0
23	Y	358	0	318	47	0
23	e	45	0	28	0	0
23	g	351	0	303	52	0
23	n	358	0	318	54	0
23	r	222	0	179	35	0
23	s	195	0	136	20	0
23	y	358	0	318	45	0
24	0	426	0	373	37	0
24	1	780	0	864	34	0
24	2	130	0	144	8	0
24	5	412	0	348	41	0
24	6	426	0	373	43	0
24	7	389	0	311	28	0
24	8	266	0	194	20	0
24	9	412	0	348	37	0
24	A	240	0	242	14	0
24	A2	473	0	468	23	0
24	A6	463	0	390	14	0
24	AA	389	0	311	28	0
24	AB	266	0	194	25	0
24	Au	477	0	477	20	0
24	Aw	65	0	72	3	0
24	B	1040	0	1152	73	0
24	BB	473	0	468	18	0
24	BD	240	0	242	18	0
24	BE	1040	0	1152	69	0
24	BF	845	0	936	39	0
24	BG	130	0	144	8	0
24	BJ	477	0	477	25	0
24	BQ	473	0	468	27	0
24	BU	518	0	452	36	0
24	BV	465	0	393	29	0
24	Ba	473	0	468	21	0
24	C	780	0	864	36	0
24	D	130	0	144	7	0
24	G	477	0	477	21	0
24	I	65	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	N	473	0	468	23	0
24	R	240	0	242	12	0
24	S	463	0	390	20	0
24	Y	473	0	468	22	0
24	a	240	0	242	17	0
24	b	1040	0	1152	74	0
24	c	845	0	936	47	0
24	d	130	0	144	7	0
24	g	477	0	477	21	0
24	n	473	0	468	25	0
24	r	518	0	452	37	0
24	s	465	0	393	29	0
24	v	1040	0	1152	79	0
24	y	473	0	468	19	0
25	0	84	0	112	19	0
25	5	84	0	112	15	0
25	6	84	0	112	17	0
25	7	84	0	112	13	0
25	8	42	0	56	6	0
25	9	84	0	112	18	0
25	A2	84	0	112	12	0
25	A6	84	0	112	10	0
25	AA	84	0	112	14	0
25	AB	42	0	56	9	0
25	Au	84	0	112	12	0
25	BB	84	0	112	11	0
25	BJ	84	0	112	17	0
25	BQ	84	0	112	11	0
25	BU	42	0	56	10	0
25	BV	84	0	112	10	0
25	Ba	84	0	112	7	0
25	G	84	0	112	11	0
25	N	84	0	112	10	0
25	S	84	0	112	11	0
25	Y	84	0	112	9	0
25	g	84	0	112	16	0
25	n	84	0	112	11	0
25	r	42	0	56	9	0
25	s	84	0	112	16	0
25	y	84	0	112	9	0
26	5	44	0	56	1	0
26	7	44	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	9	44	0	56	1	0
26	A2	44	0	56	3	0
26	A6	44	0	56	2	0
26	AA	44	0	56	4	0
26	Au	44	0	56	1	0
26	BB	88	0	112	8	0
26	BJ	44	0	56	1	0
26	BQ	44	0	56	3	0
26	BV	44	0	56	5	0
26	Ba	44	0	56	2	0
26	G	44	0	56	1	0
26	N	44	0	56	3	0
26	S	44	0	56	3	0
26	Y	44	0	56	1	0
26	g	44	0	56	1	0
26	n	44	0	56	3	0
26	r	44	0	56	5	0
26	s	44	0	56	5	0
26	y	44	0	56	3	0
27	0	47	0	67	8	0
27	1	98	0	148	4	0
27	2	95	0	139	1	0
27	5	41	0	55	3	0
27	6	47	0	67	5	0
27	9	41	0	55	3	0
27	A0	49	0	74	1	0
27	A2	49	0	74	3	0
27	Au	49	0	74	4	0
27	Az	49	0	74	3	0
27	B	95	0	139	2	0
27	BB	49	0	74	7	0
27	BE	144	0	213	3	0
27	BF	98	0	148	3	0
27	BG	49	0	74	1	0
27	BJ	49	0	74	4	0
27	BQ	49	0	74	6	0
27	BU	42	0	57	5	0
27	BY	49	0	74	1	0
27	Ba	49	0	74	4	0
27	C	98	0	148	5	0
27	D	49	0	74	3	0
27	G	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	L	49	0	74	3	0
27	N	49	0	74	5	0
27	W	49	0	74	1	0
27	Y	49	0	74	6	0
27	b	144	0	213	6	0
27	c	98	0	148	3	0
27	d	49	0	74	1	0
27	g	49	0	74	4	0
27	n	49	0	74	5	0
27	r	42	0	57	6	0
27	v	49	0	74	2	0
27	w	49	0	74	1	0
27	y	49	0	74	5	0
28	5	44	0	56	11	0
28	7	88	0	112	4	0
28	8	44	0	56	6	0
28	9	44	0	56	11	0
28	A2	44	0	56	6	0
28	AA	88	0	112	6	0
28	AB	44	0	56	6	0
28	Au	44	0	56	4	0
28	BB	44	0	56	6	0
28	BJ	44	0	56	1	0
28	BQ	44	0	56	5	0
28	BU	44	0	56	4	0
28	Ba	44	0	56	2	0
28	G	44	0	56	4	0
28	N	44	0	56	5	0
28	Y	44	0	56	5	0
28	g	44	0	56	1	0
28	n	44	0	56	2	0
28	r	44	0	56	5	0
28	y	44	0	56	3	0
29	1	80	0	112	7	0
29	4	40	0	56	3	0
29	8	40	0	56	6	0
29	A	40	0	56	3	0
29	AB	40	0	56	5	0
29	Av	40	0	56	4	0
29	Ay	80	0	112	8	0
29	B	160	0	224	20	0
29	BD	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BE	160	0	224	15	0
29	BF	80	0	112	6	0
29	BI	40	0	56	2	0
29	BK	40	0	56	8	0
29	BN	40	0	56	2	0
29	Bb	40	0	56	3	0
29	C	80	0	112	5	0
29	F	40	0	56	1	0
29	H	40	0	56	5	0
29	K	80	0	112	5	0
29	R	40	0	56	1	0
29	a	40	0	56	3	0
29	b	160	0	224	16	0
29	c	40	0	56	3	0
29	f	40	0	56	2	0
29	h	40	0	56	7	0
29	k	40	0	56	1	0
29	v	160	0	224	16	0
29	z	80	0	112	8	0
30	1	102	0	144	5	0
30	2	46	0	62	0	0
30	A	48	0	66	1	0
30	A0	48	0	66	1	0
30	Aw	40	0	50	1	0
30	B	91	0	122	0	0
30	BE	51	0	72	1	0
30	BF	102	0	144	5	0
30	BG	46	0	62	0	0
30	BL	48	0	66	2	0
30	C	102	0	144	5	0
30	D	46	0	62	0	0
30	I	40	0	50	3	0
30	b	51	0	72	1	0
30	c	102	0	144	7	0
30	d	46	0	62	0	0
30	i	48	0	66	2	0
30	v	91	0	122	0	0
31	2	55	0	80	1	0
31	BG	55	0	80	2	0
31	D	55	0	80	1	0
31	d	55	0	80	3	0
32	2	50	0	67	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	A	54	0	78	8	0
32	A1	54	0	78	2	0
32	Az	42	0	48	3	0
32	BD	54	0	78	6	0
32	BG	50	0	67	4	0
32	BO	96	0	126	6	0
32	D	50	0	67	1	0
32	L	96	0	126	5	0
32	R	54	0	78	9	0
32	a	54	0	78	6	0
32	d	50	0	67	3	0
32	l	96	0	126	7	0
33	4	43	0	30	3	0
33	BI	43	0	30	2	0
33	F	43	0	30	1	0
33	f	43	0	30	2	0
34	1	177	0	228	7	0
34	A	59	0	76	2	0
34	Av	62	0	82	6	0
34	BD	119	0	154	2	0
34	BF	117	0	150	4	0
34	BK	62	0	82	6	0
34	C	177	0	228	5	0
34	H	62	0	82	6	0
34	R	59	0	76	2	0
34	a	119	0	154	3	0
34	c	117	0	150	4	0
34	h	62	0	82	4	0
35	2	4	0	1	0	0
35	A	4	0	1	0	0
35	BD	4	0	1	0	0
35	a	4	0	1	0	0
36	A	10	0	0	0	0
36	BD	10	0	0	1	0
36	R	10	0	0	0	0
36	a	10	0	0	1	0
37	A	1	0	0	0	0
37	BD	1	0	0	0	0
37	R	1	0	0	0	0
37	a	1	0	0	0	0
38	A	128	0	148	8	0
38	BD	128	0	148	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	R	128	0	148	7	0
38	a	128	0	148	4	0
All	All	146846	0	146920	4896	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 17.

The worst 5 of 4896 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)
8:n:103:SER:HA	8:n:223:MET:HE1	1.25	1.18
8:BJ:226:MET:HE1	25:BJ:616:LUT:H12	1.27	1.14
4:BE:223:GLN:HE22	9:BK:35:PRO:HA	0.97	1.11
5:d:326:ILE:HG12	20:a:328:MET:HE1	1.39	1.05
2:0:172:GLY:HA3	1:AA:62:PHE:CE1	1.96	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	197/266 (74%)	196 (100%)	0	1 (0%)	24	57
1	7	197/266 (74%)	193 (98%)	4 (2%)	0	100	100
1	9	197/266 (74%)	196 (100%)	0	1 (0%)	24	57
1	AA	197/266 (74%)	194 (98%)	3 (2%)	0	100	100
2	0	220/243 (90%)	211 (96%)	8 (4%)	1 (0%)	24	57
2	6	220/243 (90%)	212 (96%)	7 (3%)	1 (0%)	24	57
3	8	190/212 (90%)	184 (97%)	6 (3%)	0	100	100
3	AB	190/212 (90%)	182 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	477/508 (94%)	468 (98%)	9 (2%)	0	100	100
4	BE	477/508 (94%)	473 (99%)	4 (1%)	0	100	100
4	b	477/508 (94%)	473 (99%)	4 (1%)	0	100	100
4	v	477/508 (94%)	467 (98%)	10 (2%)	0	100	100
5	2	340/352 (97%)	336 (99%)	4 (1%)	0	100	100
5	BG	340/352 (97%)	336 (99%)	4 (1%)	0	100	100
5	D	340/352 (97%)	334 (98%)	6 (2%)	0	100	100
5	d	340/352 (97%)	335 (98%)	5 (2%)	0	100	100
6	3	64/83 (77%)	63 (98%)	1 (2%)	0	100	100
6	BH	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
6	E	64/83 (77%)	63 (98%)	1 (2%)	0	100	100
6	e	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
7	4	27/39 (69%)	27 (100%)	0	0	100	100
7	BI	27/39 (69%)	27 (100%)	0	0	100	100
7	F	27/39 (69%)	27 (100%)	0	0	100	100
7	f	27/39 (69%)	27 (100%)	0	0	100	100
8	A2	200/232 (86%)	198 (99%)	1 (0%)	1 (0%)	24	57
8	Au	204/232 (88%)	202 (99%)	2 (1%)	0	100	100
8	BB	211/232 (91%)	209 (99%)	1 (0%)	1 (0%)	24	57
8	BJ	204/232 (88%)	201 (98%)	3 (2%)	0	100	100
8	BQ	200/232 (86%)	199 (100%)	0	1 (0%)	24	57
8	Ba	211/232 (91%)	209 (99%)	1 (0%)	1 (0%)	24	57
8	G	204/232 (88%)	201 (98%)	3 (2%)	0	100	100
8	N	200/232 (86%)	199 (100%)	0	1 (0%)	24	57
8	Y	211/232 (91%)	209 (99%)	1 (0%)	1 (0%)	24	57
8	g	204/232 (88%)	202 (99%)	2 (1%)	0	100	100
8	n	200/232 (86%)	199 (100%)	0	1 (0%)	24	57
8	y	211/232 (91%)	209 (99%)	1 (0%)	1 (0%)	24	57
9	Av	57/72 (79%)	53 (93%)	4 (7%)	0	100	100
9	BK	57/72 (79%)	52 (91%)	5 (9%)	0	100	100
9	H	57/72 (79%)	53 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	h	57/72 (79%)	52 (91%)	5 (9%)	0	100	100
10	Aw	33/36 (92%)	33 (100%)	0	0	100	100
10	BL	33/36 (92%)	33 (100%)	0	0	100	100
10	I	33/36 (92%)	33 (100%)	0	0	100	100
10	i	33/36 (92%)	33 (100%)	0	0	100	100
11	Ay	35/37 (95%)	35 (100%)	0	0	100	100
11	BN	35/37 (95%)	35 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	Az	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
12	BO	33/38 (87%)	33 (100%)	0	0	100	100
12	L	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
12	l	33/38 (87%)	33 (100%)	0	0	100	100
13	A1	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	24
13	BP	30/34 (88%)	29 (97%)	0	1 (3%)	3	24
13	M	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	24
13	m	30/34 (88%)	29 (97%)	0	1 (3%)	3	24
14	A6	214/232 (92%)	211 (99%)	3 (1%)	0	100	100
14	BV	214/232 (92%)	210 (98%)	4 (2%)	0	100	100
14	S	214/232 (92%)	212 (99%)	2 (1%)	0	100	100
14	s	214/232 (92%)	211 (99%)	3 (1%)	0	100	100
15	A7	27/33 (82%)	27 (100%)	0	0	100	100
15	BW	27/33 (82%)	27 (100%)	0	0	100	100
15	T	27/33 (82%)	27 (100%)	0	0	100	100
15	t	27/33 (82%)	27 (100%)	0	0	100	100
16	A8	23/28 (82%)	23 (100%)	0	0	100	100
16	BX	23/28 (82%)	22 (96%)	1 (4%)	0	100	100
16	U	23/28 (82%)	23 (100%)	0	0	100	100
16	u	23/28 (82%)	22 (96%)	1 (4%)	0	100	100
17	A0	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
17	BY	52/54 (96%)	51 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	W	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
17	w	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
18	BA	34/42 (81%)	33 (97%)	0	1 (3%)	3	25
18	BZ	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
18	X	34/42 (81%)	33 (97%)	0	1 (3%)	3	25
18	x	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
19	BC	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	Bb	60/62 (97%)	60 (100%)	0	0	100	100
19	Z	60/62 (97%)	60 (100%)	0	0	100	100
19	z	60/62 (97%)	60 (100%)	0	0	100	100
20	A	319/352 (91%)	308 (97%)	11 (3%)	0	100	100
20	BD	319/352 (91%)	310 (97%)	9 (3%)	0	100	100
20	R	319/352 (91%)	309 (97%)	10 (3%)	0	100	100
20	a	319/352 (91%)	310 (97%)	9 (3%)	0	100	100
21	1	429/459 (94%)	428 (100%)	1 (0%)	0	100	100
21	BF	427/459 (93%)	425 (100%)	2 (0%)	0	100	100
21	C	429/459 (94%)	427 (100%)	2 (0%)	0	100	100
21	c	427/459 (93%)	425 (100%)	2 (0%)	0	100	100
22	BU	193/250 (77%)	189 (98%)	4 (2%)	0	100	100
22	r	193/250 (77%)	185 (96%)	8 (4%)	0	100	100
All	All	13466/15102 (89%)	13241 (98%)	207 (2%)	18 (0%)	49	79

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	m	3	VAL
13	A1	3	VAL
13	BP	3	VAL
13	M	3	VAL
18	BA	79	ILE

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	5	153/201 (76%)	153 (100%)	0	100	100
1	7	153/201 (76%)	152 (99%)	1 (1%)	76	77
1	9	153/201 (76%)	153 (100%)	0	100	100
1	AA	153/201 (76%)	153 (100%)	0	100	100
2	0	174/192 (91%)	173 (99%)	1 (1%)	78	79
2	6	174/192 (91%)	171 (98%)	3 (2%)	53	67
3	8	148/159 (93%)	147 (99%)	1 (1%)	76	77
3	AB	148/159 (93%)	146 (99%)	2 (1%)	59	70
4	B	379/402 (94%)	379 (100%)	0	100	100
4	BE	379/402 (94%)	379 (100%)	0	100	100
4	b	379/402 (94%)	379 (100%)	0	100	100
4	v	379/402 (94%)	379 (100%)	0	100	100
5	2	274/282 (97%)	274 (100%)	0	100	100
5	BG	274/282 (97%)	272 (99%)	2 (1%)	76	77
5	D	274/282 (97%)	273 (100%)	1 (0%)	84	83
5	d	274/282 (97%)	273 (100%)	1 (0%)	84	83
6	3	59/73 (81%)	59 (100%)	0	100	100
6	BH	59/73 (81%)	59 (100%)	0	100	100
6	E	59/73 (81%)	59 (100%)	0	100	100
6	e	59/73 (81%)	59 (100%)	0	100	100
7	4	24/34 (71%)	24 (100%)	0	100	100
7	BI	24/34 (71%)	24 (100%)	0	100	100
7	F	24/34 (71%)	23 (96%)	1 (4%)	26	50
7	f	24/34 (71%)	24 (100%)	0	100	100
8	A2	154/177 (87%)	154 (100%)	0	100	100
8	Au	157/177 (89%)	156 (99%)	1 (1%)	78	79
8	BB	162/177 (92%)	161 (99%)	1 (1%)	78	79
8	BJ	157/177 (89%)	157 (100%)	0	100	100
8	BQ	154/177 (87%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Ba	162/177 (92%)	162 (100%)	0	100	100
8	G	157/177 (89%)	157 (100%)	0	100	100
8	N	154/177 (87%)	154 (100%)	0	100	100
8	Y	162/177 (92%)	160 (99%)	2 (1%)	63	72
8	g	157/177 (89%)	157 (100%)	0	100	100
8	n	154/177 (87%)	154 (100%)	0	100	100
8	y	162/177 (92%)	161 (99%)	1 (1%)	78	79
9	Av	49/60 (82%)	49 (100%)	0	100	100
9	BK	49/60 (82%)	48 (98%)	1 (2%)	48	65
9	H	49/60 (82%)	49 (100%)	0	100	100
9	h	49/60 (82%)	49 (100%)	0	100	100
10	Aw	32/33 (97%)	32 (100%)	0	100	100
10	BL	32/33 (97%)	32 (100%)	0	100	100
10	I	32/33 (97%)	32 (100%)	0	100	100
10	i	32/33 (97%)	32 (100%)	0	100	100
11	Ay	32/32 (100%)	32 (100%)	0	100	100
11	BN	32/32 (100%)	32 (100%)	0	100	100
11	K	32/32 (100%)	32 (100%)	0	100	100
11	k	32/32 (100%)	32 (100%)	0	100	100
12	Az	33/36 (92%)	33 (100%)	0	100	100
12	BO	33/36 (92%)	33 (100%)	0	100	100
12	L	33/36 (92%)	32 (97%)	1 (3%)	36	57
12	l	33/36 (92%)	33 (100%)	0	100	100
13	A1	28/30 (93%)	28 (100%)	0	100	100
13	BP	28/30 (93%)	28 (100%)	0	100	100
13	M	28/30 (93%)	27 (96%)	1 (4%)	31	54
13	m	28/30 (93%)	28 (100%)	0	100	100
14	A6	167/180 (93%)	166 (99%)	1 (1%)	78	79
14	BV	167/180 (93%)	167 (100%)	0	100	100
14	S	167/180 (93%)	166 (99%)	1 (1%)	78	79
14	s	167/180 (93%)	166 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	A7	26/30 (87%)	25 (96%)	1 (4%)	29	53
15	BW	26/30 (87%)	26 (100%)	0	100	100
15	T	26/30 (87%)	26 (100%)	0	100	100
15	t	26/30 (87%)	26 (100%)	0	100	100
16	A8	20/23 (87%)	20 (100%)	0	100	100
16	BX	20/23 (87%)	20 (100%)	0	100	100
16	U	20/23 (87%)	20 (100%)	0	100	100
16	u	20/23 (87%)	20 (100%)	0	100	100
17	A0	47/47 (100%)	46 (98%)	1 (2%)	47	64
17	BY	47/47 (100%)	47 (100%)	0	100	100
17	W	47/47 (100%)	46 (98%)	1 (2%)	47	64
17	w	47/47 (100%)	47 (100%)	0	100	100
18	BA	29/34 (85%)	29 (100%)	0	100	100
18	BZ	29/34 (85%)	29 (100%)	0	100	100
18	X	29/34 (85%)	29 (100%)	0	100	100
18	x	29/34 (85%)	29 (100%)	0	100	100
19	BC	54/54 (100%)	54 (100%)	0	100	100
19	Bb	54/54 (100%)	54 (100%)	0	100	100
19	Z	54/54 (100%)	54 (100%)	0	100	100
19	z	54/54 (100%)	54 (100%)	0	100	100
20	A	260/284 (92%)	260 (100%)	0	100	100
20	BD	260/284 (92%)	260 (100%)	0	100	100
20	R	260/284 (92%)	259 (100%)	1 (0%)	84	83
20	a	260/284 (92%)	260 (100%)	0	100	100
21	1	340/359 (95%)	340 (100%)	0	100	100
21	BF	339/359 (94%)	338 (100%)	1 (0%)	86	84
21	C	340/359 (95%)	338 (99%)	2 (1%)	78	79
21	c	339/359 (94%)	339 (100%)	0	100	100
22	BU	159/201 (79%)	156 (98%)	3 (2%)	50	66
22	r	159/201 (79%)	159 (100%)	0	100	100
All	All	10876/12004 (91%)	10842 (100%)	34 (0%)	84	84

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	BK	57	ILE
20	R	290	ILE
22	BU	134	GLN
8	Y	226	MET
8	Y	158	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
14	A6	228	ASN
14	BV	242	GLN
4	BE	26	HIS
8	BJ	232	GLN
20	R	181	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 766 ligands modelled in this entry, 4 are monoatomic - leaving 762 for Mogul analysis.

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
24	CLA	y	311	8	64,68,73	1.30	10 (15%)	77,107,113	1.41	9 (11%)
24	CLA	BU	604	-	52,56,73	1.40	11 (21%)	62,92,113	1.55	7 (11%)
28	XAT	Y	301	-	39,47,47	6.16	21 (53%)	54,74,74	7.77	34 (62%)
25	LUT	n	615	-	42,43,43	1.68	8 (19%)	51,60,60	1.51	9 (17%)
23	CHL	n	608	-	67,71,74	1.99	19 (28%)	75,109,114	2.69	26 (34%)
27	LHG	BQ	618	24	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
23	CHL	5	607	-	64,68,74	1.99	20 (31%)	71,105,114	2.72	25 (35%)
24	CLA	BU	601	22	53,57,73	1.42	11 (20%)	62,93,113	1.55	7 (11%)
29	BCR	B	618	-	41,41,41	1.21	2 (4%)	56,56,56	1.23	5 (8%)
29	BCR	BI	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.21	5 (8%)
35	BCT	a	402	-	2,3,3	1.31	0	2,3,3	4.15	1 (50%)
23	CHL	G	608	-	67,71,74	1.95	20 (29%)	75,109,114	2.69	25 (33%)
24	CLA	B	602	4	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
24	CLA	BJ	613	-	69,73,73	1.27	7 (10%)	83,113,113	1.31	6 (7%)
25	LUT	y	317	-	42,43,43	1.61	8 (19%)	51,60,60	1.52	10 (19%)
24	CLA	c	512	21	69,73,73	1.26	11 (15%)	83,113,113	1.41	7 (8%)
23	CHL	n	605	8	52,56,74	2.19	16 (30%)	58,92,114	3.04	20 (34%)
24	CLA	BU	614	-	49,53,73	1.49	9 (18%)	59,89,113	1.51	6 (10%)
24	CLA	7	315	1	49,53,73	1.49	9 (18%)	59,89,113	1.47	5 (8%)
32	SQD	A1	101	-	53,54,54	1.52	7 (13%)	62,65,65	1.37	6 (9%)
23	CHL	BB	306	8	52,56,74	2.24	18 (34%)	58,92,114	2.94	23 (39%)
23	CHL	AA	302	1	50,54,74	2.36	19 (38%)	56,90,114	3.07	22 (39%)
23	CHL	A6	601	14	50,54,74	2.25	20 (40%)	56,90,114	3.04	23 (41%)
24	CLA	n	612	-	64,68,73	1.29	8 (12%)	77,107,113	1.36	7 (9%)
23	CHL	n	609	-	67,71,74	1.98	18 (26%)	75,109,114	2.70	26 (34%)
28	XAT	AB	312	-	39,47,47	6.08	19 (48%)	54,74,74	7.74	36 (66%)
24	CLA	C	511	21	69,73,73	1.30	11 (15%)	83,113,113	1.36	11 (13%)
28	XAT	8	312	-	39,47,47	6.10	19 (48%)	54,74,74	7.74	36 (66%)
26	NEX	BB	318	-	38,46,46	1.61	7 (18%)	50,70,70	1.66	9 (18%)
24	CLA	AB	309	-	49,53,73	1.49	7 (14%)	59,89,113	1.42	6 (10%)
26	NEX	AA	319	-	38,46,46	1.66	6 (15%)	50,70,70	1.69	10 (20%)
24	CLA	8	309	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	5 (8%)
34	DGD	h	102	-	63,63,67	0.89	2 (3%)	77,77,81	1.40	9 (11%)
38	PHO	a	408	-	58,69,69	2.00	11 (18%)	56,99,99	1.51	7 (12%)
23	CHL	Au	605	8	50,54,74	2.28	18 (36%)	56,90,114	3.09	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	NEX	BV	616	-	38,46,46	1.61	7 (18%)	50,70,70	1.61	9 (18%)
24	CLA	v	608	4	69,73,73	1.24	9 (13%)	83,113,113	1.35	7 (8%)
24	CLA	BV	610	-	60,64,73	1.34	9 (15%)	72,102,113	1.48	8 (11%)
25	LUT	S	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.50	10 (19%)
28	XAT	BU	616	-	39,47,47	6.03	19 (48%)	54,74,74	7.69	38 (70%)
24	CLA	v	602	4	69,73,73	1.23	9 (13%)	83,113,113	1.33	6 (7%)
24	CLA	C	510	21	69,73,73	1.25	9 (13%)	83,113,113	1.30	4 (4%)
24	CLA	D	401	5	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
29	BCR	BN	101	-	41,41,41	1.24	3 (7%)	56,56,56	1.32	6 (10%)
30	LMG	C	501	-	51,51,55	0.74	0	59,59,63	1.35	6 (10%)
24	CLA	S	609	14	57,61,73	1.37	10 (17%)	66,98,113	1.37	5 (7%)
24	CLA	Au	614	-	52,56,73	1.42	8 (15%)	62,92,113	1.46	6 (9%)
29	BCR	8	313	-	41,41,41	1.26	3 (7%)	56,56,56	1.29	7 (12%)
32	SQD	2	408	-	49,50,54	1.57	9 (18%)	58,61,65	1.52	8 (13%)
24	CLA	BE	603	4	69,73,73	1.26	10 (14%)	83,113,113	1.31	4 (4%)
23	CHL	BU	613	22	46,50,74	2.33	19 (41%)	51,85,114	3.21	24 (47%)
23	CHL	Au	609	8	60,64,74	1.94	20 (33%)	63,100,114	2.92	24 (38%)
23	CHL	7	309	-	50,54,74	2.26	19 (38%)	56,90,114	3.06	20 (35%)
29	BCR	C	514	-	41,41,41	1.27	2 (4%)	56,56,56	1.22	5 (8%)
27	LHG	C	520	-	48,48,48	0.58	0	51,54,54	1.25	6 (11%)
24	CLA	Au	612	-	64,68,73	1.30	9 (14%)	77,107,113	1.33	6 (7%)
25	LUT	Ba	317	-	42,43,43	1.61	8 (19%)	51,60,60	1.52	10 (19%)
23	CHL	BJ	608	-	67,71,74	1.93	17 (25%)	75,109,114	2.80	27 (36%)
24	CLA	y	312	27	64,68,73	1.31	9 (14%)	77,107,113	1.34	8 (10%)
38	PHO	a	409	-	58,69,69	2.01	11 (18%)	56,99,99	1.70	8 (14%)
24	CLA	v	604	4	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
24	CLA	BU	608	22	62,66,73	1.32	10 (16%)	74,104,113	1.41	6 (8%)
25	LUT	Au	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.54	9 (17%)
25	LUT	N	615	-	42,43,43	1.68	8 (19%)	51,60,60	1.53	9 (17%)
27	LHG	g	618	24	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	BJ	612	-	64,68,73	1.33	8 (12%)	77,107,113	1.27	5 (6%)
23	CHL	y	302	8	67,71,74	1.99	19 (28%)	75,109,114	2.76	26 (34%)
25	LUT	S	615	-	42,43,43	1.62	8 (19%)	51,60,60	1.75	15 (29%)
24	CLA	5	611	27	49,53,73	1.48	9 (18%)	59,89,113	1.44	5 (8%)
27	LHG	b	624	-	48,48,48	0.67	1 (2%)	51,54,54	1.28	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	e	601	-	48,53,74	2.24	17 (35%)	53,89,114	3.09	21 (39%)
23	CHL	g	608	-	67,71,74	1.93	17 (25%)	75,109,114	2.80	27 (36%)
24	CLA	b	602	-	69,73,73	1.25	7 (10%)	83,113,113	1.28	6 (7%)
36	OEX	A	403	20	0,14,14	-	-	-		
23	CHL	S	606	-	59,63,74	2.06	19 (32%)	64,99,114	3.02	25 (39%)
24	CLA	A2	610	-	69,73,73	1.25	10 (14%)	83,113,113	1.36	9 (10%)
23	CHL	9	606	1	50,54,74	2.25	19 (38%)	56,90,114	3.16	24 (42%)
27	LHG	A0	202	-	48,48,48	0.59	0	51,54,54	1.27	6 (11%)
24	CLA	Y	311	8	64,68,73	1.31	11 (17%)	77,107,113	1.37	6 (7%)
23	CHL	A2	605	8	52,56,74	2.15	18 (34%)	58,92,114	3.01	22 (37%)
24	CLA	b	617	4	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
24	CLA	v	616	4	69,73,73	1.26	9 (13%)	83,113,113	1.32	6 (7%)
26	NEX	Ba	318	-	38,46,46	1.64	7 (18%)	50,70,70	1.59	9 (18%)
23	CHL	N	605	8	52,56,74	2.16	19 (36%)	58,92,114	3.02	22 (37%)
24	CLA	N	603	8	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
23	CHL	BJ	601	8	67,71,74	1.94	17 (25%)	75,109,114	2.81	26 (34%)
25	LUT	5	615	-	42,43,43	1.70	8 (19%)	51,60,60	1.68	12 (23%)
27	LHG	w	201	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
23	CHL	8	305	-	50,54,74	2.27	20 (40%)	56,90,114	3.00	19 (33%)
24	CLA	BB	312	-	64,68,73	1.30	11 (17%)	77,107,113	1.39	9 (11%)
24	CLA	g	604	-	54,58,73	1.43	9 (16%)	65,95,113	1.43	6 (9%)
27	LHG	BJ	618	24	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	B	616	4	69,73,73	1.27	9 (13%)	83,113,113	1.31	6 (7%)
24	CLA	B	603	4	69,73,73	1.24	9 (13%)	83,113,113	1.30	4 (4%)
27	LHG	BF	521	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	N	607	-	67,71,74	1.92	20 (29%)	75,109,114	2.80	28 (37%)
24	CLA	A2	614	-	52,56,73	1.46	8 (15%)	62,92,113	1.48	6 (9%)
24	CLA	BQ	610	8	69,73,73	1.25	8 (11%)	83,113,113	1.46	8 (9%)
23	CHL	9	601	1	50,54,74	2.26	20 (40%)	56,90,114	3.16	20 (35%)
30	LMG	1	519	-	51,51,55	0.73	1 (1%)	59,59,63	1.32	4 (6%)
38	PHO	A	409	-	58,69,69	1.97	12 (20%)	56,99,99	1.61	7 (12%)
24	CLA	BQ	612	-	64,68,73	1.29	8 (12%)	77,107,113	1.36	7 (9%)
27	LHG	9	618	24	40,40,48	0.63	0	43,46,54	1.30	6 (13%)
29	BCR	AB	313	-	41,41,41	1.29	3 (7%)	56,56,56	1.30	7 (12%)
32	SQD	BD	412	-	53,54,54	1.52	7 (13%)	62,65,65	1.35	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	Au	601	8	67,71,74	1.92	20 (29%)	75,109,114	2.76	25 (33%)
24	CLA	c	507	21	69,73,73	1.25	11 (15%)	83,113,113	1.32	7 (8%)
24	CLA	C	508	21	69,73,73	1.24	11 (15%)	83,113,113	1.33	6 (7%)
23	CHL	Y	309	-	67,71,74	1.92	18 (26%)	75,109,114	2.74	24 (32%)
29	BCR	R	410	-	41,41,41	1.29	3 (7%)	56,56,56	1.25	5 (8%)
24	CLA	R	404	20	69,73,73	1.25	10 (14%)	83,113,113	1.32	7 (8%)
24	CLA	BF	507	21	69,73,73	1.26	11 (15%)	83,113,113	1.33	7 (8%)
29	BCR	BF	515	-	41,41,41	1.31	4 (9%)	56,56,56	1.26	5 (8%)
23	CHL	Y	310	8	67,71,74	1.96	20 (29%)	75,109,114	2.71	23 (30%)
24	CLA	BE	602	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	6 (7%)
24	CLA	AB	301	3	46,49,73	1.53	10 (21%)	55,83,113	1.48	5 (9%)
23	CHL	8	304	-	50,54,74	2.28	19 (38%)	56,90,114	2.97	22 (39%)
24	CLA	S	610	-	60,64,73	1.34	10 (16%)	72,102,113	1.37	5 (6%)
24	CLA	g	614	8	52,56,73	1.44	7 (13%)	62,92,113	1.46	4 (6%)
24	CLA	BU	603	22	64,68,73	1.30	10 (15%)	77,107,113	1.30	5 (6%)
25	LUT	A2	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.57	10 (19%)
32	SQD	BO	101	-	53,54,54	1.53	8 (15%)	62,65,65	1.36	6 (9%)
24	CLA	BE	615	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
24	CLA	y	313	-	64,68,73	1.31	9 (14%)	77,107,113	1.34	6 (7%)
26	NEX	7	319	-	38,46,46	1.65	7 (18%)	50,70,70	1.70	10 (20%)
24	CLA	1	510	21	69,73,73	1.26	11 (15%)	83,113,113	1.33	4 (4%)
24	CLA	D	402	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	5 (6%)
24	CLA	S	603	-	49,53,73	1.48	10 (20%)	59,89,113	1.49	4 (6%)
23	CHL	8	306	-	50,54,74	2.34	20 (40%)	56,90,114	2.95	24 (42%)
24	CLA	b	613	4	69,73,73	1.24	10 (14%)	83,113,113	1.31	7 (8%)
27	LHG	B	621	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	0	606	-	50,54,74	2.19	20 (40%)	56,90,114	3.12	21 (37%)
24	CLA	AB	302	-	49,53,73	1.50	8 (16%)	59,89,113	1.43	4 (6%)
25	LUT	5	616	-	42,43,43	1.69	8 (19%)	51,60,60	1.68	12 (23%)
24	CLA	Y	305	-	54,58,73	1.41	10 (18%)	65,95,113	1.45	7 (10%)
24	CLA	r	614	-	49,53,73	1.49	9 (18%)	59,89,113	1.53	6 (10%)
23	CHL	y	308	-	67,71,74	1.94	19 (28%)	75,109,114	2.78	25 (33%)
23	CHL	g	609	-	62,66,74	2.19	19 (30%)	68,103,114	2.86	24 (35%)
24	CLA	n	610	8	69,73,73	1.23	7 (10%)	83,113,113	1.42	10 (12%)
24	CLA	B	608	4	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	1	514	-	41,41,41	1.28	4 (9%)	56,56,56	1.22	6 (10%)
25	LUT	r	615	-	42,43,43	1.60	8 (19%)	51,60,60	1.55	11 (21%)
30	LMG	1	501	-	51,51,55	0.74	0	59,59,63	1.35	6 (10%)
30	LMG	A0	201	-	48,48,55	0.75	0	56,56,63	1.32	6 (10%)
24	CLA	6	602	2	64,68,73	1.30	9 (14%)	77,107,113	1.34	6 (7%)
24	CLA	I	102	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	7 (8%)
24	CLA	BV	604	-	54,58,73	1.47	10 (18%)	65,95,113	1.60	7 (10%)
24	CLA	Ba	303	8	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
24	CLA	c	503	21	69,73,73	1.26	11 (15%)	83,113,113	1.33	5 (6%)
23	CHL	r	605	22	67,71,74	1.84	18 (26%)	75,109,114	2.76	25 (33%)
24	CLA	5	614	1	49,53,73	1.47	8 (16%)	59,89,113	1.54	5 (8%)
24	CLA	Au	613	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
25	LUT	G	616	-	42,43,43	1.63	8 (19%)	51,60,60	1.53	10 (19%)
24	CLA	BE	613	-	69,73,73	1.24	11 (15%)	83,113,113	1.31	7 (8%)
24	CLA	5	602	1	65,69,73	1.28	10 (15%)	78,108,113	1.31	5 (6%)
24	CLA	v	605	4	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
24	CLA	AA	315	1	49,53,73	1.49	9 (18%)	59,89,113	1.46	5 (8%)
24	CLA	R	405	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	8 (9%)
24	CLA	BB	303	8	69,73,73	1.26	11 (15%)	83,113,113	1.35	5 (6%)
24	CLA	BE	617	4	69,73,73	1.24	9 (13%)	83,113,113	1.31	5 (6%)
27	LHG	c	520	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
34	DGD	a	401	-	60,60,67	0.94	2 (3%)	74,74,81	1.38	7 (9%)
24	CLA	s	610	-	60,64,73	1.33	9 (15%)	72,102,113	1.47	8 (11%)
24	CLA	1	511	21	69,73,73	1.26	11 (15%)	83,113,113	1.34	5 (6%)
23	CHL	7	302	1	50,54,74	2.35	20 (40%)	56,90,114	3.05	22 (39%)
24	CLA	g	610	8	68,72,73	1.27	8 (11%)	81,111,113	1.29	7 (8%)
24	CLA	7	304	-	59,63,73	1.36	9 (15%)	71,101,113	1.30	7 (9%)
24	CLA	BE	608	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	5 (6%)
29	BCR	b	618	-	41,41,41	1.18	2 (4%)	56,56,56	1.28	8 (14%)
23	CHL	G	605	8	50,54,74	2.28	18 (36%)	56,90,114	3.08	20 (35%)
23	CHL	s	606	-	59,63,74	2.06	17 (28%)	64,99,114	3.04	25 (39%)
29	BCR	f	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	5 (8%)
24	CLA	BV	603	14	49,53,73	1.49	7 (14%)	59,89,113	1.44	5 (8%)
24	CLA	Ba	311	8	64,68,73	1.30	10 (15%)	77,107,113	1.37	9 (11%)
24	CLA	C	505	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HEM	BI	102	6,7	50,50,50	1.33	8 (16%)	66,82,82	1.09	4 (6%)
24	CLA	9	614	1	49,53,73	1.47	7 (14%)	59,89,113	1.56	5 (8%)
30	LMG	I	101	-	40,40,55	0.81	0	48,48,63	1.31	6 (12%)
24	CLA	BD	407	-	54,58,73	1.39	9 (16%)	65,95,113	1.50	8 (12%)
24	CLA	G	614	-	52,56,73	1.42	8 (15%)	62,92,113	1.45	6 (9%)
30	LMG	d	405	-	46,46,55	0.77	1 (2%)	54,54,63	1.34	5 (9%)
24	CLA	A6	609	14	57,61,73	1.38	10 (17%)	66,98,113	1.38	6 (9%)
23	CHL	9	609	-	63,67,74	2.23	21 (33%)	70,104,114	2.97	27 (38%)
28	XAT	N	619	-	39,47,47	6.10	20 (51%)	54,74,74	7.74	35 (64%)
24	CLA	AA	314	1	49,53,73	1.47	9 (18%)	59,89,113	1.48	5 (8%)
25	LUT	N	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.55	9 (17%)
23	CHL	AA	307	1	50,54,74	2.26	19 (38%)	56,90,114	2.98	21 (37%)
24	CLA	Ba	312	27	64,68,73	1.30	9 (14%)	77,107,113	1.34	8 (10%)
24	CLA	R	409	-	64,68,73	1.29	9 (14%)	77,107,113	1.37	6 (7%)
24	CLA	b	603	4	69,73,73	1.25	10 (14%)	83,113,113	1.30	5 (6%)
29	BCR	4	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.21	5 (8%)
24	CLA	B	601	-	69,73,73	1.27	9 (13%)	83,113,113	1.28	7 (8%)
24	CLA	S	608	-	49,53,73	1.46	9 (18%)	59,89,113	1.41	5 (8%)
23	CHL	5	606	1	50,54,74	2.23	19 (38%)	56,90,114	3.22	23 (41%)
27	LHG	v	621	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
24	CLA	BF	503	21	69,73,73	1.27	11 (15%)	83,113,113	1.34	6 (7%)
29	BCR	BE	618	-	41,41,41	1.16	2 (4%)	56,56,56	1.41	10 (17%)
24	CLA	b	616	-	69,73,73	1.25	10 (14%)	83,113,113	1.30	5 (6%)
34	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	1.44	8 (10%)
24	CLA	Ba	305	-	54,58,73	1.41	9 (16%)	65,95,113	1.43	5 (7%)
30	LMG	BF	519	-	51,51,55	0.71	1 (1%)	59,59,63	1.33	4 (6%)
23	CHL	Au	608	-	67,71,74	1.94	20 (29%)	75,109,114	2.70	25 (33%)
25	LUT	6	615	-	42,43,43	1.59	9 (21%)	51,60,60	1.39	10 (19%)
24	CLA	A2	613	8	64,68,73	1.31	9 (14%)	77,107,113	1.40	6 (7%)
24	CLA	a	407	-	54,58,73	1.39	10 (18%)	65,95,113	1.50	7 (10%)
24	CLA	c	504	21	69,73,73	1.25	10 (14%)	83,113,113	1.34	6 (7%)
29	BCR	B	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.17	5 (8%)
24	CLA	8	302	-	49,53,73	1.50	9 (18%)	59,89,113	1.45	4 (6%)
24	CLA	b	612	4	69,73,73	1.24	10 (14%)	83,113,113	1.32	8 (9%)
24	CLA	BF	504	21	69,73,73	1.24	10 (14%)	83,113,113	1.35	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	PHO	BD	409	-	58,69,69	2.01	12 (20%)	56,99,99	1.69	9 (16%)
23	CHL	BH	601	-	48,53,74	2.24	16 (33%)	53,89,114	3.09	21 (39%)
25	LUT	0	616	-	42,43,43	1.70	8 (19%)	51,60,60	1.63	10 (19%)
24	CLA	5	613	1	59,63,73	1.34	8 (13%)	71,101,113	1.41	6 (8%)
24	CLA	a	405	20	69,73,73	1.25	11 (15%)	83,113,113	1.30	7 (8%)
24	CLA	Au	611	27	64,68,73	1.29	9 (14%)	77,107,113	1.30	5 (6%)
27	LHG	n	618	24	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
30	LMG	BL	101	-	48,48,55	0.74	1 (2%)	56,56,63	1.32	6 (10%)
23	CHL	AB	305	-	50,54,74	2.26	20 (40%)	56,90,114	3.00	19 (33%)
24	CLA	S	611	-	53,57,73	1.42	10 (18%)	62,93,113	1.42	5 (8%)
23	CHL	G	606	-	54,58,74	2.16	20 (37%)	59,94,114	3.00	22 (37%)
23	CHL	BQ	607	-	67,71,74	1.96	19 (28%)	75,109,114	2.78	24 (32%)
34	DGD	c	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.41	8 (10%)
23	CHL	AA	306	1	50,54,74	2.38	19 (38%)	56,90,114	2.94	21 (37%)
24	CLA	N	610	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	10 (12%)
28	XAT	Ba	301	-	39,47,47	6.12	22 (56%)	54,74,74	7.78	34 (62%)
31	PL9	BG	403	-	55,55,55	1.50	6 (10%)	68,69,69	1.54	14 (20%)
23	CHL	0	605	2	50,54,74	2.30	19 (38%)	56,90,114	3.01	24 (42%)
24	CLA	0	603	-	59,63,73	1.36	12 (20%)	71,101,113	1.36	8 (11%)
24	CLA	y	315	-	52,56,73	1.42	9 (17%)	62,92,113	1.45	5 (8%)
24	CLA	AB	310	-	49,53,73	1.49	9 (18%)	59,89,113	1.54	9 (15%)
24	CLA	BD	405	20	69,73,73	1.25	10 (14%)	83,113,113	1.33	6 (7%)
30	LMG	c	518	-	51,51,55	0.72	1 (1%)	59,59,63	1.33	5 (8%)
24	CLA	B	610	-	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
23	CHL	g	601	8	67,71,74	1.94	17 (25%)	75,109,114	2.81	26 (34%)
25	LUT	Y	316	-	42,43,43	1.65	8 (19%)	51,60,60	1.52	11 (21%)
24	CLA	Y	313	-	64,68,73	1.30	11 (17%)	77,107,113	1.33	6 (7%)
24	CLA	A6	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.45	5 (7%)
24	CLA	BV	608	-	49,53,73	1.50	8 (16%)	59,89,113	1.39	4 (6%)
24	CLA	BJ	602	8	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
23	CHL	0	607	-	57,61,74	2.12	20 (35%)	64,98,114	2.90	26 (40%)
24	CLA	BF	508	-	69,73,73	1.26	11 (15%)	83,113,113	1.30	6 (7%)
24	CLA	1	508	21	69,73,73	1.23	11 (15%)	83,113,113	1.33	6 (7%)
24	CLA	0	614	2	52,56,73	1.43	10 (19%)	62,92,113	1.40	7 (11%)
24	CLA	r	604	-	52,56,73	1.41	11 (21%)	62,92,113	1.50	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	6	608	2	50,54,74	2.27	18 (36%)	56,90,114	3.06	23 (41%)
24	CLA	BQ	602	8	69,73,73	1.26	8 (11%)	83,113,113	1.25	5 (6%)
30	LMG	v	623	-	40,40,55	0.85	1 (2%)	48,48,63	1.30	5 (10%)
27	LHG	Au	618	24	48,48,48	0.60	0	51,54,54	1.27	6 (11%)
26	NEX	5	617	-	38,46,46	1.66	7 (18%)	50,70,70	1.67	9 (18%)
23	CHL	AA	309	-	50,54,74	2.26	19 (38%)	56,90,114	3.05	20 (35%)
24	CLA	5	612	-	49,53,73	1.49	10 (20%)	59,89,113	1.49	5 (8%)
24	CLA	7	313	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	5 (8%)
24	CLA	Aw	102	-	69,73,73	1.24	11 (15%)	83,113,113	1.39	9 (10%)
24	CLA	S	613	14	53,57,73	1.40	9 (16%)	62,93,113	1.48	9 (14%)
24	CLA	r	601	22	53,57,73	1.40	10 (18%)	62,93,113	1.53	6 (9%)
27	LHG	A2	618	24	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
29	BCR	c	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.28	6 (10%)
24	CLA	s	604	-	54,58,73	1.45	10 (18%)	65,95,113	1.53	6 (9%)
24	CLA	A	410	-	64,68,73	1.29	8 (12%)	77,107,113	1.35	5 (6%)
27	LHG	BE	624	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	7 (13%)
24	CLA	v	614	-	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
24	CLA	Y	314	8	69,73,73	1.25	10 (14%)	83,113,113	1.33	4 (4%)
33	HEM	f	102	6,7	50,50,50	1.33	7 (14%)	66,82,82	1.10	4 (6%)
24	CLA	A	406	-	69,73,73	1.26	10 (14%)	83,113,113	1.38	8 (9%)
23	CHL	BJ	607	-	67,71,74	1.95	18 (26%)	75,109,114	2.78	26 (34%)
24	CLA	N	602	8	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
23	CHL	A2	608	-	67,71,74	1.95	19 (28%)	75,109,114	2.72	26 (34%)
23	CHL	7	306	1	50,54,74	2.38	18 (36%)	56,90,114	2.94	21 (37%)
24	CLA	c	506	-	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
25	LUT	BV	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.52	11 (21%)
26	NEX	9	617	-	38,46,46	1.66	7 (18%)	50,70,70	1.68	9 (18%)
27	LHG	2	406	-	48,48,48	0.65	1 (2%)	51,54,54	1.27	5 (9%)
24	CLA	BF	506	-	69,73,73	1.24	9 (13%)	83,113,113	1.41	7 (8%)
24	CLA	c	505	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	5 (6%)
24	CLA	b	615	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
24	CLA	8	301	3	46,49,73	1.53	11 (23%)	55,83,113	1.48	5 (9%)
26	NEX	s	616	-	38,46,46	1.61	7 (18%)	50,70,70	1.62	9 (18%)
23	CHL	y	309	-	67,71,74	2.08	19 (28%)	75,109,114	2.69	26 (34%)
34	DGD	BD	413	-	61,61,67	0.90	2 (3%)	75,75,81	1.41	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	7	307	1	50,54,74	2.26	19 (38%)	56,90,114	2.98	21 (37%)
27	LHG	L	102	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	7 (13%)
24	CLA	0	610	2	64,68,73	1.29	10 (15%)	77,107,113	1.48	12 (15%)
24	CLA	BE	605	4	69,73,73	1.24	9 (13%)	83,113,113	1.35	8 (9%)
27	LHG	BG	404	-	48,48,48	0.67	1 (2%)	51,54,54	1.26	6 (11%)
27	LHG	BY	201	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
38	PHO	R	407	-	58,69,69	1.99	11 (18%)	56,99,99	1.52	9 (16%)
24	CLA	c	514	21	69,73,73	1.24	11 (15%)	83,113,113	1.35	4 (4%)
29	BCR	v	618	-	41,41,41	1.22	2 (4%)	56,56,56	1.23	5 (8%)
24	CLA	v	601	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	7 (8%)
24	CLA	1	507	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	5 (6%)
29	BCR	Av	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.30	9 (16%)
24	CLA	BV	613	14	53,57,73	1.41	9 (16%)	62,93,113	1.47	7 (11%)
32	SQD	d	406	-	49,50,54	1.57	7 (14%)	58,61,65	1.44	7 (12%)
23	CHL	BU	605	22	67,71,74	1.84	18 (26%)	75,109,114	2.75	27 (36%)
23	CHL	A2	609	8	67,71,74	1.94	19 (28%)	75,109,114	2.73	21 (28%)
26	NEX	Y	318	-	38,46,46	1.63	7 (18%)	50,70,70	1.62	9 (18%)
27	LHG	B	622	-	45,45,48	0.66	1 (2%)	48,51,54	1.23	4 (8%)
30	LMG	A	412	-	48,48,55	0.75	0	56,56,63	1.32	5 (8%)
27	LHG	Az	102	-	48,48,48	0.67	1 (2%)	51,54,54	1.29	7 (13%)
24	CLA	y	305	-	54,58,73	1.41	10 (18%)	65,95,113	1.44	5 (7%)
29	BCR	Ay	102	-	41,41,41	1.25	4 (9%)	56,56,56	1.30	8 (14%)
23	CHL	g	607	-	67,71,74	1.96	18 (26%)	75,109,114	2.78	26 (34%)
35	BCT	A	401	-	2,3,3	1.30	0	2,3,3	4.03	1 (50%)
24	CLA	G	610	8	68,72,73	1.24	10 (14%)	81,111,113	1.35	7 (8%)
27	LHG	N	618	24	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	0	613	-	62,66,73	1.35	11 (17%)	74,104,113	1.50	9 (12%)
24	CLA	BB	314	8	69,73,73	1.25	11 (15%)	83,113,113	1.35	7 (8%)
24	CLA	BJ	611	27	64,68,73	1.31	8 (12%)	77,107,113	1.34	7 (9%)
23	CHL	N	606	8	54,58,74	2.17	19 (35%)	59,94,114	2.97	22 (37%)
24	CLA	v	613	4	69,73,73	1.24	10 (14%)	83,113,113	1.34	5 (6%)
24	CLA	A6	613	14	53,57,73	1.40	10 (18%)	62,93,113	1.50	9 (14%)
32	SQD	a	412	-	53,54,54	1.53	7 (13%)	62,65,65	1.34	6 (9%)
28	XAT	AA	318	-	39,47,47	6.12	21 (53%)	54,74,74	7.81	34 (62%)
24	CLA	BJ	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.43	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	r	613	22	46,50,74	2.33	19 (41%)	51,85,114	3.22	24 (47%)
24	CLA	9	610	1	60,64,73	1.33	11 (18%)	72,102,113	1.39	7 (9%)
27	LHG	6	617	24	46,46,48	0.66	1 (2%)	49,52,54	1.32	6 (12%)
24	CLA	d	402	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
30	LMG	C	519	-	51,51,55	0.72	1 (1%)	59,59,63	1.32	5 (8%)
24	CLA	v	615	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
24	CLA	BD	406	-	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
24	CLA	B	613	4	69,73,73	1.24	9 (13%)	83,113,113	1.33	5 (6%)
23	CHL	r	606	-	57,61,74	2.14	20 (35%)	64,98,114	2.94	26 (40%)
29	BCR	C	515	-	41,41,41	1.32	3 (7%)	56,56,56	1.28	6 (10%)
24	CLA	9	612	-	49,53,73	1.48	9 (18%)	59,89,113	1.50	5 (8%)
24	CLA	BU	612	22	40,44,73	1.55	11 (27%)	47,76,113	1.49	4 (8%)
24	CLA	0	611	27	59,63,73	1.33	10 (16%)	71,101,113	1.48	10 (14%)
23	CHL	Y	306	8	52,56,74	2.23	18 (34%)	58,92,114	2.95	23 (39%)
24	CLA	BF	511	21	69,73,73	1.26	11 (15%)	83,113,113	1.34	5 (6%)
24	CLA	y	304	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	5 (6%)
24	CLA	Au	602	8	69,73,73	1.24	10 (14%)	83,113,113	1.35	8 (9%)
24	CLA	BQ	611	27	64,68,73	1.30	7 (10%)	77,107,113	1.36	5 (6%)
23	CHL	s	601	-	50,54,74	2.30	18 (36%)	56,90,114	3.00	21 (37%)
24	CLA	Au	604	-	54,58,73	1.40	8 (14%)	65,95,113	1.43	7 (10%)
24	CLA	BQ	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	7 (10%)
27	LHG	G	618	24	48,48,48	0.60	0	51,54,54	1.27	6 (11%)
32	SQD	Az	101	-	41,42,54	1.59	8 (19%)	50,53,65	1.83	9 (18%)
23	CHL	y	310	-	67,71,74	2.08	19 (28%)	75,109,114	2.65	26 (34%)
24	CLA	8	303	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	4 (6%)
24	CLA	BF	513	-	69,73,73	1.24	11 (15%)	83,113,113	1.34	6 (7%)
23	CHL	S	601	14	50,54,74	2.26	19 (38%)	56,90,114	3.04	22 (39%)
23	CHL	BV	607	-	50,54,74	2.34	18 (36%)	56,90,114	2.96	23 (41%)
23	CHL	BQ	605	8	52,56,74	2.19	16 (30%)	58,92,114	3.03	20 (34%)
23	CHL	8	307	3	50,54,74	2.28	19 (38%)	56,90,114	3.06	25 (44%)
23	CHL	BU	606	-	57,61,74	2.15	20 (35%)	64,98,114	2.94	25 (39%)
23	CHL	Ba	308	-	67,71,74	1.95	19 (28%)	75,109,114	2.78	26 (34%)
24	CLA	A2	612	-	64,68,73	1.29	10 (15%)	77,107,113	1.37	4 (5%)
23	CHL	6	605	2	50,54,74	2.31	19 (38%)	56,90,114	3.02	22 (39%)
35	BCT	BD	402	-	2,3,3	1.33	0	2,3,3	4.13	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	509	21	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
24	CLA	7	312	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
26	NEX	r	617	-	38,46,46	1.61	7 (18%)	50,70,70	1.62	9 (18%)
24	CLA	BE	609	4	69,73,73	1.24	9 (13%)	83,113,113	1.44	8 (9%)
24	CLA	BG	402	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	5 (6%)
29	BCR	BD	411	-	41,41,41	1.25	2 (4%)	56,56,56	1.20	5 (8%)
34	DGD	BF	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.41	7 (9%)
24	CLA	Ba	313	-	64,68,73	1.31	9 (14%)	77,107,113	1.34	7 (9%)
29	BCR	F	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.21	5 (8%)
24	CLA	n	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	7 (10%)
26	NEX	n	617	-	38,46,46	1.62	7 (18%)	50,70,70	1.60	9 (18%)
27	LHG	Y	319	-	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	AA	303	1	65,69,73	1.26	9 (13%)	78,108,113	1.42	7 (8%)
26	NEX	N	617	-	38,46,46	1.57	7 (18%)	50,70,70	1.59	9 (18%)
24	CLA	Au	610	8	68,72,73	1.24	10 (14%)	81,111,113	1.37	7 (8%)
24	CLA	N	614	-	52,56,73	1.46	7 (13%)	62,92,113	1.48	6 (9%)
24	CLA	s	611	-	53,57,73	1.43	10 (18%)	62,93,113	1.45	5 (8%)
28	XAT	5	619	-	39,47,47	6.02	19 (48%)	54,74,74	7.65	35 (64%)
23	CHL	N	608	-	67,71,74	1.95	20 (29%)	75,109,114	2.72	26 (34%)
27	LHG	0	617	24	46,46,48	0.68	1 (2%)	49,52,54	1.33	6 (12%)
24	CLA	v	606	-	69,73,73	1.26	10 (14%)	83,113,113	1.32	7 (8%)
28	XAT	9	619	-	39,47,47	6.07	20 (51%)	54,74,74	7.51	33 (61%)
25	LUT	BV	614	-	42,43,43	1.66	8 (19%)	51,60,60	1.47	10 (19%)
36	OEX	BD	403	20	0,14,14	-	-	-	-	-
24	CLA	r	602	22	62,66,73	1.32	11 (17%)	72,104,113	1.39	6 (8%)
23	CHL	5	605	1	50,54,74	2.32	19 (38%)	56,90,114	2.99	21 (37%)
24	CLA	5	603	1	59,63,73	1.37	10 (16%)	71,101,113	1.31	8 (11%)
29	BCR	z	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.27	5 (8%)
24	CLA	g	611	27	64,68,73	1.31	8 (12%)	77,107,113	1.35	6 (7%)
24	CLA	C	507	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	5 (6%)
24	CLA	A2	602	8	69,73,73	1.25	10 (14%)	83,113,113	1.34	6 (7%)
27	LHG	D	404	-	48,48,48	0.63	1 (2%)	51,54,54	1.27	5 (9%)
29	BCR	z	102	-	41,41,41	1.27	3 (7%)	56,56,56	1.32	8 (14%)
23	CHL	0	601	2	65,69,74	2.02	19 (29%)	72,106,114	2.72	26 (36%)
24	CLA	C	502	21	69,73,73	1.25	10 (14%)	83,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	Y	307	-	54,58,74	2.08	18 (33%)	59,94,114	3.13	23 (38%)
25	LUT	BQ	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.52	11 (21%)
24	CLA	S	612	14	59,63,73	1.35	9 (15%)	71,101,113	1.41	6 (8%)
38	PHO	A	408	-	58,69,69	2.00	11 (18%)	56,99,99	1.53	9 (16%)
29	BCR	v	622	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	5 (8%)
28	XAT	BB	301	-	39,47,47	6.17	20 (51%)	54,74,74	7.80	34 (62%)
24	CLA	BE	612	4	69,73,73	1.25	10 (14%)	83,113,113	1.33	7 (8%)
29	BCR	BE	619	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	5 (8%)
24	CLA	v	610	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
24	CLA	b	610	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	5 (6%)
24	CLA	AA	311	1	52,56,73	1.44	11 (21%)	60,92,113	1.45	8 (13%)
23	CHL	0	608	2	50,54,74	2.27	18 (36%)	56,90,114	3.08	22 (39%)
30	LMG	B	620	-	51,51,55	0.72	0	59,59,63	1.37	7 (11%)
23	CHL	G	609	-	60,64,74	2.07	19 (31%)	63,100,114	2.78	23 (36%)
24	CLA	s	603	14	49,53,73	1.50	8 (16%)	59,89,113	1.45	5 (8%)
24	CLA	7	303	1	65,69,73	1.27	9 (13%)	78,108,113	1.41	5 (6%)
24	CLA	G	612	-	64,68,73	1.30	9 (14%)	77,107,113	1.31	6 (7%)
24	CLA	G	611	27	64,68,73	1.32	9 (14%)	77,107,113	1.39	9 (11%)
24	CLA	AA	304	-	59,63,73	1.37	9 (15%)	71,101,113	1.29	6 (8%)
24	CLA	s	602	14	65,69,73	1.30	9 (13%)	78,108,113	1.31	5 (6%)
24	CLA	G	604	-	54,58,73	1.40	8 (14%)	65,95,113	1.44	7 (10%)
24	CLA	Ba	315	-	52,56,73	1.43	9 (17%)	62,92,113	1.45	5 (8%)
23	CHL	A2	601	8	67,71,74	1.93	20 (29%)	75,109,114	2.74	25 (33%)
24	CLA	b	614	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	4 (4%)
24	CLA	Y	315	-	52,56,73	1.42	10 (19%)	62,92,113	1.50	8 (12%)
32	SQD	BO	102	-	41,42,54	1.63	7 (17%)	50,53,65	1.46	7 (14%)
23	CHL	S	605	14	50,54,74	2.21	17 (34%)	56,90,114	3.15	21 (37%)
34	DGD	Av	102	-	63,63,67	0.91	2 (3%)	77,77,81	1.38	9 (11%)
24	CLA	S	602	14	65,69,73	1.28	9 (13%)	78,108,113	1.35	6 (7%)
25	LUT	BJ	615	-	42,43,43	1.61	8 (19%)	51,60,60	1.52	9 (17%)
34	DGD	H	102	-	63,63,67	0.90	2 (3%)	77,77,81	1.38	7 (9%)
25	LUT	AA	316	-	42,43,43	1.64	8 (19%)	51,60,60	1.55	11 (21%)
34	DGD	A	402	-	60,60,67	0.93	2 (3%)	74,74,81	1.38	8 (10%)
24	CLA	BD	410	-	64,68,73	1.29	9 (14%)	77,107,113	1.38	7 (9%)
24	CLA	d	401	5	69,73,73	1.23	11 (15%)	83,113,113	1.33	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	1	502	21	69,73,73	1.25	10 (14%)	83,113,113	1.28	6 (7%)
28	XAT	BJ	619	-	39,47,47	6.17	22 (56%)	54,74,74	7.65	34 (62%)
24	CLA	BV	611	-	53,57,73	1.43	10 (18%)	62,93,113	1.44	5 (8%)
29	BCR	B	623	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	5 (8%)
24	CLA	C	512	-	69,73,73	1.24	11 (15%)	83,113,113	1.33	7 (8%)
27	LHG	b	623	-	45,45,48	0.66	1 (2%)	48,51,54	1.25	4 (8%)
30	LMG	Aw	101	-	40,40,55	0.81	0	48,48,63	1.34	7 (14%)
24	CLA	BB	311	8	64,68,73	1.31	10 (15%)	77,107,113	1.35	5 (6%)
23	CHL	7	308	-	62,66,74	1.99	20 (32%)	68,103,114	2.92	25 (36%)
24	CLA	v	609	4	69,73,73	1.23	11 (15%)	83,113,113	1.31	5 (6%)
24	CLA	b	609	4	69,73,73	1.23	8 (11%)	83,113,113	1.40	7 (8%)
30	LMG	B	624	-	40,40,55	0.84	1 (2%)	48,48,63	1.31	5 (10%)
24	CLA	9	603	-	59,63,73	1.37	10 (16%)	71,101,113	1.31	8 (11%)
28	XAT	BQ	619	-	39,47,47	6.12	21 (53%)	54,74,74	7.75	34 (62%)
25	LUT	6	616	-	42,43,43	1.71	7 (16%)	51,60,60	1.65	10 (19%)
24	CLA	9	602	1	65,69,73	1.29	10 (15%)	78,108,113	1.31	6 (7%)
25	LUT	y	316	-	42,43,43	1.62	8 (19%)	51,60,60	1.47	10 (19%)
26	NEX	A6	616	-	38,46,46	1.63	7 (18%)	50,70,70	1.64	9 (18%)
24	CLA	c	509	21	69,73,73	1.23	9 (13%)	83,113,113	1.33	6 (7%)
24	CLA	BF	512	21	69,73,73	1.26	11 (15%)	83,113,113	1.38	7 (8%)
24	CLA	s	608	-	49,53,73	1.51	8 (16%)	59,89,113	1.39	4 (6%)
23	CHL	5	609	-	63,67,74	2.17	21 (33%)	70,104,114	2.93	27 (38%)
24	CLA	BF	509	21	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
28	XAT	AA	301	-	39,47,47	6.20	22 (56%)	54,74,74	7.72	34 (62%)
24	CLA	g	602	8	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
25	LUT	BB	317	-	42,43,43	1.67	8 (19%)	51,60,60	1.54	9 (17%)
24	CLA	B	609	-	69,73,73	1.22	10 (14%)	83,113,113	1.31	5 (6%)
24	CLA	s	613	14	53,57,73	1.41	9 (16%)	62,93,113	1.46	6 (9%)
24	CLA	8	308	-	49,53,73	1.48	12 (24%)	59,89,113	1.78	12 (20%)
23	CHL	AB	307	3	50,54,74	2.32	19 (38%)	56,90,114	3.03	22 (39%)
29	BCR	H	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.29	9 (16%)
23	CHL	6	606	-	50,54,74	2.20	20 (40%)	56,90,114	3.11	21 (37%)
24	CLA	c	513	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	6 (7%)
24	CLA	N	613	8	64,68,73	1.30	9 (14%)	77,107,113	1.39	6 (7%)
24	CLA	y	314	8	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	6	613	-	62,66,73	1.35	11 (17%)	74,104,113	1.49	9 (12%)
25	LUT	Y	317	-	42,43,43	1.66	8 (19%)	51,60,60	1.54	10 (19%)
24	CLA	C	504	21	69,73,73	1.23	8 (11%)	83,113,113	1.33	6 (7%)
23	CHL	n	601	8	67,71,74	2.00	17 (25%)	75,109,114	2.68	24 (32%)
24	CLA	1	512	-	69,73,73	1.23	10 (14%)	83,113,113	1.34	8 (9%)
25	LUT	AB	311	-	42,43,43	1.64	8 (19%)	51,60,60	1.61	10 (19%)
28	XAT	n	619	-	39,47,47	6.12	21 (53%)	54,74,74	7.74	34 (62%)
26	NEX	BQ	617	-	38,46,46	1.68	7 (18%)	50,70,70	1.66	9 (18%)
24	CLA	0	612	-	49,53,73	1.49	9 (18%)	59,89,113	1.49	5 (8%)
26	NEX	G	617	-	38,46,46	1.64	7 (18%)	50,70,70	1.69	9 (18%)
24	CLA	B	606	-	69,73,73	1.26	10 (14%)	83,113,113	1.30	6 (7%)
31	PL9	2	404	-	55,55,55	1.68	10 (18%)	68,69,69	1.52	13 (19%)
34	DGD	1	518	-	61,61,67	0.90	2 (3%)	75,75,81	1.40	10 (13%)
27	LHG	Ba	319	24	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
24	CLA	N	612	-	64,68,73	1.29	10 (15%)	77,107,113	1.37	4 (5%)
23	CHL	BB	308	-	67,71,74	1.89	19 (28%)	75,109,114	2.81	26 (34%)
33	HEM	F	102	7	50,50,50	1.34	7 (14%)	66,82,82	1.18	6 (9%)
27	LHG	BF	520	-	48,48,48	0.55	0	51,54,54	1.27	6 (11%)
24	CLA	B	612	4	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
32	SQD	D	406	-	49,50,54	1.57	7 (14%)	58,61,65	1.45	7 (12%)
34	DGD	BD	401	-	60,60,67	0.94	2 (3%)	74,74,81	1.38	6 (8%)
23	CHL	BJ	605	8	50,54,74	2.25	16 (32%)	56,90,114	3.11	23 (41%)
23	CHL	g	606	-	54,58,74	2.19	17 (31%)	59,94,114	3.00	22 (37%)
23	CHL	Ba	309	-	67,71,74	2.01	19 (28%)	75,109,114	2.69	25 (33%)
24	CLA	6	612	-	49,53,73	1.49	9 (18%)	59,89,113	1.51	5 (8%)
24	CLA	9	613	1	59,63,73	1.35	9 (15%)	71,101,113	1.41	6 (8%)
26	NEX	BB	320	-	38,46,46	1.65	7 (18%)	50,70,70	1.63	10 (20%)
27	LHG	C	521	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
23	CHL	Ba	310	-	67,71,74	2.09	20 (29%)	75,109,114	2.65	26 (34%)
34	DGD	BF	517	-	56,56,67	0.96	2 (3%)	70,70,81	1.50	11 (15%)
27	LHG	d	404	-	48,48,48	0.65	1 (2%)	51,54,54	1.26	6 (11%)
26	NEX	y	318	-	38,46,46	1.65	7 (18%)	50,70,70	1.62	9 (18%)
24	CLA	BU	602	22	62,66,73	1.33	11 (17%)	72,104,113	1.39	6 (8%)
32	SQD	R	411	-	53,54,54	1.51	7 (13%)	62,65,65	1.34	6 (9%)
23	CHL	BQ	608	-	67,71,74	1.99	19 (28%)	75,109,114	2.69	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	BV	606	-	59,63,74	2.05	16 (27%)	64,99,114	3.04	25 (39%)
24	CLA	BV	602	14	65,69,73	1.30	9 (13%)	78,108,113	1.29	5 (6%)
30	LMG	BF	501	-	51,51,55	0.74	0	59,59,63	1.34	7 (11%)
25	LUT	g	615	-	42,43,43	1.61	8 (19%)	51,60,60	1.52	9 (17%)
24	CLA	n	611	27	64,68,73	1.30	7 (10%)	77,107,113	1.37	5 (6%)
24	CLA	BQ	603	8	69,73,73	1.26	10 (14%)	83,113,113	1.27	7 (8%)
24	CLA	BB	315	-	52,56,73	1.42	10 (19%)	62,92,113	1.50	8 (12%)
24	CLA	c	511	21	69,73,73	1.25	11 (15%)	83,113,113	1.34	5 (6%)
23	CHL	0	609	-	62,66,74	2.20	21 (33%)	68,103,114	3.06	25 (36%)
25	LUT	AA	317	-	42,43,43	1.61	8 (19%)	51,60,60	1.51	10 (19%)
32	SQD	L	103	-	53,54,54	1.52	8 (15%)	62,65,65	1.37	6 (9%)
23	CHL	Au	607	-	67,71,74	1.92	20 (29%)	75,109,114	2.79	27 (36%)
24	CLA	BQ	614	-	52,56,73	1.46	6 (11%)	62,92,113	1.50	8 (12%)
23	CHL	BV	601	-	50,54,74	2.29	18 (36%)	56,90,114	3.00	20 (35%)
24	CLA	9	611	27	49,53,73	1.48	9 (18%)	59,89,113	1.45	5 (8%)
24	CLA	BU	611	22	53,57,73	1.43	11 (20%)	62,93,113	1.42	5 (8%)
24	CLA	2	403	-	69,73,73	1.24	9 (13%)	83,113,113	1.31	5 (6%)
34	DGD	a	413	-	61,61,67	0.90	2 (3%)	75,75,81	1.41	9 (12%)
23	CHL	A6	607	14	50,54,74	2.36	19 (38%)	56,90,114	3.25	19 (33%)
23	CHL	y	306	8	52,56,74	2.25	19 (36%)	58,92,114	2.93	22 (37%)
24	CLA	1	513	21	69,73,73	1.24	9 (13%)	83,113,113	1.37	6 (7%)
23	CHL	A2	607	-	67,71,74	1.93	20 (29%)	75,109,114	2.82	29 (38%)
29	BCR	BE	620	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	4 (7%)
30	LMG	D	405	-	46,46,55	0.77	1 (2%)	54,54,63	1.35	5 (9%)
24	CLA	b	611	-	69,73,73	1.27	9 (13%)	83,113,113	1.61	11 (13%)
24	CLA	A	405	20	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
24	CLA	AA	313	-	49,53,73	1.47	9 (18%)	59,89,113	1.49	7 (11%)
28	XAT	7	301	-	39,47,47	6.21	21 (53%)	54,74,74	7.69	34 (62%)
24	CLA	C	506	21	69,73,73	1.26	11 (15%)	83,113,113	1.30	7 (8%)
24	CLA	g	612	-	64,68,73	1.33	8 (12%)	77,107,113	1.27	5 (6%)
23	CHL	BB	302	8	67,71,74	1.91	19 (28%)	75,109,114	2.81	28 (37%)
24	CLA	S	604	-	54,58,73	1.40	10 (18%)	65,95,113	1.46	5 (7%)
24	CLA	n	614	-	52,56,73	1.46	6 (11%)	62,92,113	1.50	8 (12%)
24	CLA	9	604	-	54,58,73	1.45	11 (20%)	65,95,113	1.55	9 (13%)
24	CLA	A6	602	14	65,69,73	1.27	9 (13%)	78,108,113	1.35	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	n	603	8	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
23	CHL	N	601	8	67,71,74	1.93	20 (29%)	75,109,114	2.74	24 (32%)
23	CHL	AA	308	-	62,66,74	2.00	20 (32%)	68,103,114	2.95	26 (38%)
24	CLA	AA	312	-	49,53,73	1.46	8 (16%)	59,89,113	1.49	6 (10%)
34	DGD	1	516	-	56,56,67	0.99	4 (7%)	70,70,81	1.50	11 (15%)
26	NEX	g	617	-	38,46,46	1.65	6 (15%)	50,70,70	1.68	9 (18%)
27	LHG	c	519	-	48,48,48	0.55	0	51,54,54	1.26	6 (11%)
24	CLA	2	402	5	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
24	CLA	Y	303	8	69,73,73	1.25	12 (17%)	83,113,113	1.33	4 (4%)
24	CLA	r	610	27	53,57,73	1.41	11 (20%)	62,93,113	1.44	6 (9%)
23	CHL	BB	309	-	67,71,74	1.92	19 (28%)	75,109,114	2.74	24 (32%)
25	LUT	7	317	-	42,43,43	1.64	8 (19%)	51,60,60	1.50	9 (17%)
26	NEX	S	616	-	38,46,46	1.65	7 (18%)	50,70,70	1.63	9 (18%)
25	LUT	7	316	-	42,43,43	1.68	8 (19%)	51,60,60	1.59	7 (13%)
24	CLA	r	612	22	40,44,73	1.56	11 (27%)	47,76,113	1.49	5 (10%)
23	CHL	6	609	-	62,66,74	2.19	22 (35%)	68,103,114	3.04	24 (35%)
38	PHO	R	408	-	58,69,69	1.95	11 (18%)	56,99,99	1.61	7 (12%)
25	LUT	n	616	-	42,43,43	1.62	8 (19%)	51,60,60	1.53	11 (21%)
24	CLA	v	607	-	69,73,73	1.24	9 (13%)	83,113,113	1.35	4 (4%)
28	XAT	Au	619	-	39,47,47	6.18	21 (53%)	54,74,74	7.66	34 (62%)
24	CLA	Au	603	8	69,73,73	1.23	10 (14%)	83,113,113	1.28	4 (4%)
27	LHG	y	319	24	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
24	CLA	C	513	21	69,73,73	1.24	9 (13%)	83,113,113	1.36	5 (6%)
27	LHG	r	618	24	41,41,48	0.72	1 (2%)	44,47,54	1.34	7 (15%)
23	CHL	S	607	-	50,54,74	2.23	18 (36%)	56,90,114	3.26	22 (39%)
24	CLA	s	609	14	59,63,73	1.35	9 (15%)	71,101,113	1.40	7 (9%)
29	BCR	1	515	-	41,41,41	1.35	4 (9%)	56,56,56	1.28	6 (10%)
24	CLA	A2	611	27	64,68,73	1.28	9 (14%)	77,107,113	1.35	7 (9%)
24	CLA	C	503	21	69,73,73	1.25	10 (14%)	83,113,113	1.33	6 (7%)
25	LUT	BB	316	-	42,43,43	1.66	8 (19%)	51,60,60	1.53	11 (21%)
23	CHL	AB	304	3	50,54,74	2.27	19 (38%)	56,90,114	2.98	22 (39%)
23	CHL	G	601	8	67,71,74	1.93	20 (29%)	75,109,114	2.77	28 (37%)
24	CLA	6	614	2	52,56,73	1.43	10 (19%)	62,92,113	1.39	6 (9%)
24	CLA	b	604	4	69,73,73	1.23	9 (13%)	83,113,113	1.30	4 (4%)
27	LHG	1	521	-	48,48,48	0.61	0	51,54,54	1.27	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	i	101	-	48,48,55	0.74	1 (2%)	56,56,63	1.32	6 (10%)
29	BCR	Bb	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.33	9 (16%)
32	SQD	A	413	-	53,54,54	1.51	7 (13%)	62,65,65	1.33	6 (9%)
29	BCR	B	617	-	41,41,41	1.22	2 (4%)	56,56,56	1.34	8 (14%)
24	CLA	c	508	-	69,73,73	1.25	11 (15%)	83,113,113	1.29	5 (6%)
25	LUT	8	311	-	42,43,43	1.59	8 (19%)	51,60,60	1.41	9 (17%)
26	NEX	BJ	617	-	38,46,46	1.66	6 (15%)	50,70,70	1.69	9 (18%)
24	CLA	0	604	-	49,53,73	1.47	9 (18%)	59,89,113	1.43	6 (10%)
32	SQD	BG	406	-	49,50,54	1.58	7 (14%)	58,61,65	1.44	7 (12%)
23	CHL	n	607	-	67,71,74	1.96	18 (26%)	75,109,114	2.78	24 (32%)
23	CHL	y	307	-	54,58,74	2.20	19 (35%)	59,94,114	2.96	23 (38%)
24	CLA	Ba	304	-	69,73,73	1.27	8 (11%)	83,113,113	1.25	5 (6%)
23	CHL	5	608	-	50,54,74	2.26	20 (40%)	56,90,114	3.03	20 (35%)
30	LMG	c	501	-	51,51,55	0.73	0	59,59,63	1.34	6 (10%)
25	LUT	s	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.52	11 (21%)
29	BCR	Ay	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	7 (12%)
23	CHL	9	607	-	64,68,74	1.96	19 (29%)	71,105,114	2.79	25 (35%)
24	CLA	A	407	-	54,58,73	1.41	11 (20%)	65,95,113	1.50	9 (13%)
24	CLA	r	609	22	69,73,73	1.24	11 (15%)	83,113,113	1.36	6 (7%)
23	CHL	9	608	-	50,54,74	2.26	20 (40%)	56,90,114	3.02	20 (35%)
23	CHL	s	607	-	50,54,74	2.34	18 (36%)	56,90,114	2.96	23 (41%)
24	CLA	6	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.69	11 (18%)
24	CLA	BU	610	27	53,57,73	1.40	11 (20%)	62,93,113	1.45	6 (9%)
24	CLA	n	602	8	69,73,73	1.26	8 (11%)	83,113,113	1.25	6 (7%)
25	LUT	Ba	316	-	42,43,43	1.62	8 (19%)	51,60,60	1.46	9 (17%)
27	LHG	1	520	-	48,48,48	0.57	0	51,54,54	1.26	6 (11%)
29	BCR	b	601	-	41,41,41	1.16	2 (4%)	56,56,56	1.31	8 (14%)
24	CLA	BF	514	-	69,73,73	1.23	10 (14%)	83,113,113	1.34	4 (4%)
24	CLA	BE	611	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
24	CLA	R	406	-	54,58,73	1.40	12 (22%)	65,95,113	1.49	8 (12%)
29	BCR	v	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.34	8 (14%)
24	CLA	Y	312	-	64,68,73	1.29	10 (15%)	77,107,113	1.38	9 (11%)
24	CLA	b	606	4	69,73,73	1.26	10 (14%)	83,113,113	1.27	6 (7%)
24	CLA	A2	604	-	54,58,73	1.39	10 (18%)	65,95,113	1.48	6 (9%)
24	CLA	BE	604	4	69,73,73	1.23	9 (13%)	83,113,113	1.31	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	AB	306	-	50,54,74	2.34	20 (40%)	56,90,114	2.95	23 (41%)
24	CLA	BJ	610	8	68,72,73	1.27	7 (10%)	81,111,113	1.29	7 (8%)
28	XAT	G	619	-	39,47,47	6.18	22 (56%)	54,74,74	7.66	34 (62%)
29	BCR	b	619	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	5 (8%)
34	DGD	R	401	-	60,60,67	0.92	2 (3%)	74,74,81	1.38	8 (10%)
24	CLA	y	303	8	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
24	CLA	s	612	14	59,63,73	1.36	9 (15%)	71,101,113	1.37	6 (8%)
23	CHL	Y	302	8	67,71,74	1.92	20 (29%)	75,109,114	2.79	27 (36%)
30	LMG	b	621	-	51,51,55	0.72	0	59,59,63	1.39	7 (11%)
23	CHL	BB	310	-	67,71,74	1.94	19 (28%)	75,109,114	2.71	23 (30%)
27	LHG	5	618	24	40,40,48	0.64	1 (2%)	43,46,54	1.30	6 (13%)
23	CHL	Ba	302	8	67,71,74	1.98	19 (28%)	75,109,114	2.74	27 (36%)
24	CLA	BB	305	-	54,58,73	1.42	10 (18%)	65,95,113	1.46	7 (10%)
24	CLA	A6	603	-	49,53,73	1.47	10 (20%)	59,89,113	1.50	4 (6%)
25	LUT	s	614	-	42,43,43	1.64	8 (19%)	51,60,60	1.46	11 (21%)
25	LUT	G	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.64	11 (21%)
24	CLA	8	310	-	49,53,73	1.51	9 (18%)	59,89,113	1.53	6 (10%)
23	CHL	A6	606	-	59,63,74	2.06	19 (32%)	64,99,114	3.02	25 (39%)
24	CLA	n	613	-	64,68,73	1.33	10 (15%)	77,107,113	1.34	6 (7%)
24	CLA	BE	614	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	4 (4%)
23	CHL	BB	307	-	54,58,74	2.08	18 (33%)	59,94,114	3.12	23 (38%)
24	CLA	G	603	8	69,73,73	1.24	9 (13%)	83,113,113	1.32	7 (8%)
28	XAT	g	619	-	39,47,47	6.17	22 (56%)	54,74,74	7.66	34 (62%)
24	CLA	5	604	-	54,58,73	1.44	10 (18%)	65,95,113	1.54	9 (13%)
31	PL9	D	403	-	55,55,55	1.80	9 (16%)	68,69,69	1.49	11 (16%)
24	CLA	BE	606	4	69,73,73	1.26	10 (14%)	83,113,113	1.28	6 (7%)
23	CHL	BJ	606	-	54,58,74	2.18	18 (33%)	59,94,114	3.00	24 (40%)
27	LHG	b	622	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
33	HEM	4	102	7	50,50,50	1.33	6 (12%)	66,82,82	1.18	6 (9%)
24	CLA	BQ	613	-	64,68,73	1.32	10 (15%)	77,107,113	1.34	6 (7%)
24	CLA	Ba	314	8	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
24	CLA	1	504	21	69,73,73	1.23	10 (14%)	83,113,113	1.34	5 (6%)
23	CHL	g	605	8	50,54,74	2.25	16 (32%)	56,90,114	3.12	23 (41%)
24	CLA	g	603	8	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
27	LHG	BE	623	-	45,45,48	0.68	1 (2%)	48,51,54	1.25	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	BE	621	-	51,51,55	0.72	1 (1%)	59,59,63	1.40	8 (13%)
24	CLA	6	610	2	64,68,73	1.30	10 (15%)	77,107,113	1.56	11 (14%)
24	CLA	a	410	-	64,68,73	1.29	9 (14%)	77,107,113	1.38	7 (9%)
23	CHL	AA	310	-	62,66,74	2.14	19 (30%)	68,103,114	2.89	27 (39%)
24	CLA	b	607	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	6 (7%)
29	BCR	A	411	-	41,41,41	1.27	3 (7%)	56,56,56	1.25	6 (10%)
24	CLA	a	406	-	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
23	CHL	s	605	14	50,54,74	2.28	18 (36%)	56,90,114	3.00	24 (42%)
24	CLA	5	610	1	60,64,73	1.35	12 (20%)	72,102,113	1.39	9 (12%)
36	OEX	a	403	20	0,14,14	-	-	-	-	-
32	SQD	l	101	-	53,54,54	1.53	8 (15%)	62,65,65	1.36	6 (9%)
24	CLA	b	608	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	5 (6%)
25	LUT	A6	615	-	42,43,43	1.62	8 (19%)	51,60,60	1.75	14 (27%)
34	DGD	c	516	-	56,56,67	0.97	2 (3%)	70,70,81	1.50	12 (17%)
24	CLA	1	505	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
25	LUT	Au	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.65	11 (21%)
24	CLA	r	603	22	64,68,73	1.31	10 (15%)	77,107,113	1.29	5 (6%)
24	CLA	BE	610	-	69,73,73	1.23	10 (14%)	83,113,113	1.32	5 (6%)
25	LUT	A2	615	-	42,43,43	1.67	8 (19%)	51,60,60	1.53	10 (19%)
27	LHG	BE	622	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	B	605	4	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
24	CLA	BB	313	-	64,68,73	1.30	11 (17%)	77,107,113	1.34	6 (7%)
23	CHL	Au	606	-	54,58,74	2.15	20 (37%)	59,94,114	2.99	23 (38%)
24	CLA	r	608	22	62,66,73	1.32	10 (16%)	74,104,113	1.41	4 (5%)
23	CHL	BQ	606	8	54,58,74	2.20	19 (35%)	59,94,114	2.94	23 (38%)
38	PHO	BD	408	-	58,69,69	2.00	11 (18%)	56,99,99	1.53	8 (14%)
23	CHL	A2	606	8	54,58,74	2.16	19 (35%)	59,94,114	3.00	22 (37%)
23	CHL	r	607	22	62,66,74	1.98	20 (32%)	68,103,114	2.90	26 (38%)
23	CHL	Ba	306	8	52,56,74	2.24	19 (36%)	58,92,114	2.93	21 (36%)
24	CLA	BV	609	14	59,63,73	1.35	8 (13%)	71,101,113	1.40	6 (8%)
24	CLA	AA	305	-	49,53,73	1.48	10 (20%)	59,89,113	1.42	7 (11%)
24	CLA	B	607	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	4 (4%)
24	CLA	c	510	21	69,73,73	1.26	11 (15%)	83,113,113	1.32	6 (7%)
24	CLA	B	615	-	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
36	OEX	R	402	20	0,14,14	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	6	611	27	59,63,73	1.33	10 (16%)	71,101,113	1.49	10 (14%)
24	CLA	A6	608	-	49,53,73	1.47	9 (18%)	59,89,113	1.42	6 (10%)
24	CLA	BJ	603	8	69,73,73	1.26	8 (11%)	83,113,113	1.29	4 (4%)
24	CLA	1	503	21	69,73,73	1.26	11 (15%)	83,113,113	1.34	6 (7%)
25	LUT	9	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.69	9 (17%)
23	CHL	n	606	8	54,58,74	2.18	19 (35%)	59,94,114	2.96	23 (38%)
23	CHL	BQ	601	8	67,71,74	1.99	17 (25%)	75,109,114	2.68	24 (32%)
24	CLA	N	611	27	64,68,73	1.29	9 (14%)	77,107,113	1.35	7 (9%)
25	LUT	BU	615	-	42,43,43	1.60	8 (19%)	51,60,60	1.55	11 (21%)
30	LMG	v	620	-	51,51,55	0.72	0	59,59,63	1.38	7 (11%)
32	SQD	l	102	-	41,42,54	1.63	7 (17%)	50,53,65	1.45	7 (14%)
29	BCR	h	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	8 (14%)
23	CHL	9	605	1	50,54,74	2.31	19 (38%)	56,90,114	3.00	21 (37%)
24	CLA	G	602	8	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
24	CLA	1	506	21	69,73,73	1.26	12 (17%)	83,113,113	1.30	7 (8%)
24	CLA	BF	505	-	69,73,73	1.25	10 (14%)	83,113,113	1.26	5 (6%)
24	CLA	B	611	4	69,73,73	1.24	10 (14%)	83,113,113	1.40	7 (8%)
24	CLA	v	603	4	69,73,73	1.23	9 (13%)	83,113,113	1.31	5 (6%)
24	CLA	BF	510	21	69,73,73	1.27	11 (15%)	83,113,113	1.33	7 (8%)
27	LHG	2	405	-	45,45,48	0.68	1 (2%)	48,51,54	1.23	4 (8%)
31	PL9	d	403	-	55,55,55	1.65	9 (16%)	68,69,69	1.66	14 (20%)
23	CHL	BV	605	14	50,54,74	2.27	18 (36%)	56,90,114	2.99	23 (41%)
24	CLA	B	604	4	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
28	XAT	r	616	-	39,47,47	6.05	20 (51%)	54,74,74	7.70	38 (70%)
24	CLA	v	611	4	69,73,73	1.24	10 (14%)	83,113,113	1.39	7 (8%)
23	CHL	BU	607	22	62,66,74	1.99	20 (32%)	68,103,114	2.91	26 (38%)
23	CHL	6	601	2	65,69,74	2.02	19 (29%)	72,106,114	2.72	27 (37%)
25	LUT	A6	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.50	10 (19%)
26	NEX	A2	617	-	38,46,46	1.85	9 (23%)	50,70,70	1.70	10 (20%)
24	CLA	BV	612	14	59,63,73	1.36	9 (15%)	71,101,113	1.37	6 (8%)
24	CLA	Y	304	8	69,73,73	1.26	11 (15%)	83,113,113	1.30	6 (7%)
26	NEX	Au	617	-	38,46,46	1.64	6 (15%)	50,70,70	1.69	9 (18%)
29	BCR	K	102	-	41,41,41	1.25	3 (7%)	56,56,56	1.30	8 (14%)
24	CLA	BU	609	22	69,73,73	1.24	11 (15%)	83,113,113	1.36	6 (7%)
23	CHL	7	310	-	62,66,74	2.13	19 (30%)	68,103,114	2.88	27 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AB	308	-	49,53,73	1.50	11 (22%)	59,89,113	1.72	13 (22%)
28	XAT	A2	619	-	39,47,47	6.09	20 (51%)	54,74,74	7.74	35 (64%)
24	CLA	BG	401	5	69,73,73	1.23	11 (15%)	83,113,113	1.35	7 (8%)
34	DGD	C	518	-	61,61,67	0.90	2 (3%)	75,75,81	1.40	10 (13%)
25	LUT	BJ	616	-	42,43,43	1.65	7 (16%)	51,60,60	1.65	9 (17%)
29	BCR	a	411	-	41,41,41	1.23	2 (4%)	56,56,56	1.19	5 (8%)
24	CLA	A2	603	8	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
23	CHL	G	607	-	67,71,74	1.93	20 (29%)	75,109,114	2.79	25 (33%)
29	BCR	BF	516	-	41,41,41	1.37	3 (7%)	56,56,56	1.31	8 (14%)
24	CLA	6	603	-	59,63,73	1.35	12 (20%)	71,101,113	1.35	7 (9%)
23	CHL	Y	308	-	67,71,74	1.89	19 (28%)	75,109,114	2.81	26 (34%)
23	CHL	BQ	609	-	67,71,74	1.99	18 (26%)	75,109,114	2.67	26 (34%)
24	CLA	7	311	1	52,56,73	1.42	11 (21%)	60,92,113	1.44	8 (13%)
30	LMG	2	407	-	46,46,55	0.78	1 (2%)	54,54,63	1.35	5 (9%)
23	CHL	5	601	1	50,54,74	2.27	20 (40%)	56,90,114	3.15	22 (39%)
24	CLA	1	509	21	69,73,73	1.25	11 (15%)	83,113,113	1.35	9 (10%)
24	CLA	B	614	-	69,73,73	1.24	9 (13%)	83,113,113	1.37	6 (7%)
25	LUT	9	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.65	11 (21%)
29	BCR	k	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.24	6 (10%)
32	SQD	L	101	-	41,42,54	1.62	7 (17%)	50,53,65	1.57	9 (18%)
24	CLA	7	314	1	49,53,73	1.48	10 (20%)	59,89,113	1.48	5 (8%)
24	CLA	BE	616	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)
28	XAT	y	301	-	39,47,47	6.11	22 (56%)	54,74,74	7.77	34 (62%)
24	CLA	BE	607	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
25	LUT	g	616	-	42,43,43	1.65	7 (16%)	51,60,60	1.59	10 (19%)
24	CLA	N	604	-	54,58,73	1.39	10 (18%)	65,95,113	1.48	6 (9%)
25	LUT	0	615	-	42,43,43	1.69	8 (19%)	51,60,60	1.48	10 (19%)
24	CLA	BJ	614	8	52,56,73	1.44	7 (13%)	62,92,113	1.46	4 (6%)
24	CLA	BB	304	8	69,73,73	1.26	11 (15%)	83,113,113	1.30	6 (7%)
29	BCR	BK	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	9 (16%)
23	CHL	Ba	307	-	54,58,74	2.19	19 (35%)	59,94,114	2.97	23 (38%)
23	CHL	N	609	8	67,71,74	1.94	19 (28%)	75,109,114	2.71	21 (28%)
24	CLA	A6	610	-	60,64,73	1.34	10 (16%)	72,102,113	1.38	5 (6%)
29	BCR	b	620	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	4 (7%)
24	CLA	G	613	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	BG	405	-	46,46,55	0.78	1 (2%)	54,54,63	1.34	5 (9%)
24	CLA	v	612	4	69,73,73	1.25	11 (15%)	83,113,113	1.35	8 (9%)
24	CLA	A6	612	14	59,63,73	1.34	9 (15%)	71,101,113	1.43	6 (8%)
27	LHG	BB	319	-	48,48,48	0.67	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	r	611	22	53,57,73	1.43	11 (20%)	62,93,113	1.42	5 (8%)
27	LHG	BU	617	24	41,41,48	0.74	1 (2%)	44,47,54	1.35	7 (15%)
27	LHG	W	201	-	48,48,48	0.60	0	51,54,54	1.26	6 (11%)
34	DGD	BK	102	-	63,63,67	0.95	3 (4%)	77,77,81	1.47	10 (12%)
34	DGD	1	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.44	8 (10%)
24	CLA	0	602	2	64,68,73	1.28	11 (17%)	77,107,113	1.35	8 (10%)
24	CLA	c	502	21	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
24	CLA	7	305	-	49,53,73	1.49	9 (18%)	59,89,113	1.42	7 (11%)
24	CLA	AB	303	-	49,53,73	1.46	9 (18%)	59,89,113	1.49	4 (6%)
24	CLA	A6	611	-	53,57,73	1.42	10 (18%)	62,93,113	1.41	5 (8%)
24	CLA	BF	502	21	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
24	CLA	g	613	-	69,73,73	1.27	8 (11%)	83,113,113	1.32	6 (7%)
28	XAT	7	318	-	39,47,47	6.13	21 (53%)	54,74,74	7.80	34 (62%)
23	CHL	BJ	609	-	62,66,74	2.19	20 (32%)	68,103,114	2.86	24 (35%)
29	BCR	K	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.34	5 (8%)
25	LUT	BQ	615	-	42,43,43	1.68	8 (19%)	51,60,60	1.51	9 (17%)
34	DGD	C	516	-	56,56,67	0.96	2 (3%)	70,70,81	1.49	10 (14%)
29	BCR	BE	601	-	41,41,41	1.18	2 (4%)	56,56,56	1.30	6 (10%)
23	CHL	6	607	-	57,61,74	2.11	20 (35%)	64,98,114	2.91	25 (39%)
24	CLA	b	605	4	69,73,73	1.24	9 (13%)	83,113,113	1.34	8 (9%)
35	BCT	2	401	-	2,3,3	1.31	0	2,3,3	3.99	1 (50%)
29	BCR	v	619	-	41,41,41	1.18	2 (4%)	56,56,56	1.23	6 (10%)
23	CHL	A6	605	14	50,54,74	2.20	19 (38%)	56,90,114	3.15	21 (37%)

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
24	CLA	y	311	8	-	12/33/109/115	-
24	CLA	BU	604	-	-	11/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	XAT	Y	301	-	-	18/31/93/93	0/4/4/4
25	LUT	n	615	-	-	1/29/67/67	0/2/2/2
23	CHL	n	608	-	-	13/35/111/117	-
27	LHG	BQ	618	24	-	20/53/53/53	-
23	CHL	5	607	-	-	19/32/108/117	-
24	CLA	BU	601	22	-	10/20/96/115	-
29	BCR	B	618	-	-	7/29/63/63	0/2/2/2
29	BCR	BI	101	-	-	11/29/63/63	0/2/2/2
23	CHL	G	608	-	-	23/35/111/117	-
24	CLA	B	602	4	-	15/39/115/115	-
24	CLA	BJ	613	-	-	13/39/115/115	-
25	LUT	y	317	-	-	1/29/67/67	0/2/2/2
24	CLA	c	512	21	-	12/39/115/115	-
23	CHL	n	605	8	-	6/20/96/117	-
24	CLA	BU	614	-	-	9/15/91/115	-
24	CLA	7	315	1	-	4/15/91/115	-
32	SQD	A1	101	-	-	19/49/69/69	0/1/1/1
23	CHL	BB	306	8	-	7/20/96/117	-
23	CHL	AA	302	1	-	6/17/93/117	-
23	CHL	A6	601	14	-	5/17/93/117	-
24	CLA	n	612	-	-	6/33/109/115	-
23	CHL	n	609	-	-	15/35/111/117	-
28	XAT	AB	312	-	-	16/31/93/93	0/4/4/4
24	CLA	C	511	21	-	13/39/115/115	-
28	XAT	8	312	-	-	16/31/93/93	0/4/4/4
26	NEX	BB	318	-	-	10/27/83/83	0/3/3/3
24	CLA	AB	309	-	-	5/15/91/115	-
26	NEX	AA	319	-	-	22/27/83/83	0/3/3/3
24	CLA	8	309	-	-	5/15/91/115	-
34	DGD	h	102	-	-	15/51/91/95	0/2/2/2
38	PHO	a	408	-	-	6/37/103/103	0/5/6/6
23	CHL	Au	605	8	-	7/17/93/117	-
26	NEX	BV	616	-	-	15/27/83/83	0/3/3/3
24	CLA	v	608	4	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BV	610	-	-	12/29/105/115	-
25	LUT	S	614	-	-	2/29/67/67	0/2/2/2
28	XAT	BU	616	-	-	17/31/93/93	0/4/4/4
24	CLA	v	602	4	-	15/39/115/115	-
24	CLA	C	510	21	-	16/39/115/115	-
24	CLA	D	401	5	-	18/39/115/115	-
29	BCR	BN	101	-	-	11/29/63/63	0/2/2/2
30	LMG	C	501	-	-	18/46/66/70	0/1/1/1
24	CLA	S	609	14	-	2/21/99/115	-
24	CLA	Au	614	-	-	5/19/95/115	-
29	BCR	8	313	-	-	16/29/63/63	0/2/2/2
32	SQD	2	408	-	-	24/45/65/69	0/1/1/1
24	CLA	BE	603	4	-	16/39/115/115	-
23	CHL	BU	613	22	-	4/12/88/117	-
23	CHL	Au	609	8	-	8/23/101/117	-
23	CHL	7	309	-	-	10/17/93/117	-
29	BCR	C	514	-	-	3/29/63/63	0/2/2/2
27	LHG	C	520	-	-	25/53/53/53	-
24	CLA	Au	612	-	-	10/33/109/115	-
25	LUT	Ba	317	-	-	1/29/67/67	0/2/2/2
23	CHL	BJ	608	-	-	21/35/111/117	-
24	CLA	y	312	27	-	13/33/109/115	-
38	PHO	a	409	-	-	15/37/103/103	0/5/6/6
24	CLA	v	604	4	-	14/39/115/115	-
24	CLA	BU	608	22	-	13/31/107/115	-
25	LUT	Au	616	-	-	2/29/67/67	0/2/2/2
25	LUT	N	615	-	-	1/29/67/67	0/2/2/2
27	LHG	g	618	24	-	18/53/53/53	-
24	CLA	BJ	612	-	-	6/33/109/115	-
23	CHL	y	302	8	-	14/35/111/117	-
25	LUT	S	615	-	-	0/29/67/67	0/2/2/2
24	CLA	5	611	27	-	8/15/91/115	-
27	LHG	b	624	-	-	19/53/53/53	-
23	CHL	e	601	-	-	3/15/91/117	-
23	CHL	g	608	-	-	21/35/111/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	602	-	-	16/39/115/115	-
23	CHL	S	606	-	-	8/26/102/117	-
24	CLA	A2	610	-	-	15/39/115/115	-
23	CHL	9	606	1	-	5/17/93/117	-
27	LHG	A0	202	-	-	14/53/53/53	-
24	CLA	Y	311	8	-	12/33/109/115	-
23	CHL	A2	605	8	-	9/20/96/117	-
24	CLA	b	617	4	-	18/39/115/115	-
24	CLA	v	616	4	-	17/39/115/115	-
26	NEX	Ba	318	-	-	13/27/83/83	0/3/3/3
23	CHL	N	605	8	-	9/20/96/117	-
24	CLA	N	603	8	-	13/39/115/115	-
23	CHL	BJ	601	8	-	17/35/111/117	-
25	LUT	5	615	-	-	3/29/67/67	0/2/2/2
27	LHG	w	201	-	-	16/53/53/53	-
23	CHL	8	305	-	-	9/17/93/117	-
24	CLA	BB	312	-	-	13/33/109/115	-
24	CLA	g	604	-	-	9/21/97/115	-
27	LHG	BJ	618	24	-	18/53/53/53	-
24	CLA	B	616	4	-	17/39/115/115	-
24	CLA	B	603	4	-	12/39/115/115	-
27	LHG	BF	521	-	-	22/53/53/53	-
23	CHL	N	607	-	-	14/35/111/117	-
24	CLA	A2	614	-	-	8/19/95/115	-
24	CLA	BQ	610	8	-	14/39/115/115	-
23	CHL	9	601	1	-	9/17/93/117	-
30	LMG	1	519	-	-	22/46/66/70	0/1/1/1
38	PHO	A	409	-	-	16/37/103/103	0/5/6/6
24	CLA	BQ	612	-	-	6/33/109/115	-
27	LHG	9	618	24	-	18/45/45/53	-
29	BCR	AB	313	-	-	16/29/63/63	0/2/2/2
32	SQD	BD	412	-	-	28/49/69/69	0/1/1/1
23	CHL	Au	601	8	-	17/35/111/117	-
24	CLA	c	507	21	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	508	21	-	15/39/115/115	-
23	CHL	Y	309	-	-	14/35/111/117	-
29	BCR	R	410	-	-	5/29/63/63	0/2/2/2
24	CLA	R	404	20	-	10/39/115/115	-
24	CLA	BF	507	21	-	19/39/115/115	-
29	BCR	BF	515	-	-	3/29/63/63	0/2/2/2
23	CHL	Y	310	8	-	17/35/111/117	-
24	CLA	BE	602	-	-	15/39/115/115	-
24	CLA	AB	301	3	-	5/9/81/115	-
23	CHL	8	304	-	-	9/17/93/117	-
24	CLA	S	610	-	-	11/29/105/115	-
24	CLA	g	614	8	-	5/19/95/115	-
24	CLA	BU	603	22	-	8/33/109/115	-
25	LUT	A2	616	-	-	1/29/67/67	0/2/2/2
32	SQD	BO	101	-	-	21/49/69/69	0/1/1/1
24	CLA	BE	615	-	-	18/39/115/115	-
24	CLA	y	313	-	-	12/33/109/115	-
26	NEX	7	319	-	-	22/27/83/83	0/3/3/3
24	CLA	1	510	21	-	16/39/115/115	-
24	CLA	D	402	-	-	12/39/115/115	-
24	CLA	S	603	-	-	5/15/91/115	-
23	CHL	8	306	-	-	6/17/93/117	-
24	CLA	b	613	4	-	15/39/115/115	-
27	LHG	B	621	-	-	23/53/53/53	-
23	CHL	0	606	-	-	7/17/93/117	-
24	CLA	AB	302	-	-	6/15/91/115	-
25	LUT	5	616	-	-	2/29/67/67	0/2/2/2
24	CLA	Y	305	-	-	11/21/97/115	-
24	CLA	r	614	-	-	9/15/91/115	-
23	CHL	y	308	-	-	20/35/111/117	-
23	CHL	g	609	-	-	10/29/105/117	-
24	CLA	n	610	8	-	14/39/115/115	-
24	CLA	B	608	4	-	13/39/115/115	-
29	BCR	1	514	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LUT	r	615	-	-	3/29/67/67	0/2/2/2
30	LMG	1	501	-	-	18/46/66/70	0/1/1/1
30	LMG	A0	201	-	-	16/43/63/70	0/1/1/1
24	CLA	6	602	2	-	18/33/109/115	-
24	CLA	I	102	-	-	14/39/115/115	-
24	CLA	BV	604	-	-	7/21/97/115	-
24	CLA	Ba	303	8	-	15/39/115/115	-
24	CLA	c	503	21	-	15/39/115/115	-
23	CHL	r	605	22	-	22/35/111/117	-
24	CLA	5	614	1	-	6/15/91/115	-
24	CLA	Au	613	-	-	12/39/115/115	-
25	LUT	G	616	-	-	2/29/67/67	0/2/2/2
24	CLA	BE	613	-	-	16/39/115/115	-
24	CLA	5	602	1	-	15/35/111/115	-
24	CLA	v	605	4	-	23/39/115/115	-
24	CLA	AA	315	1	-	3/15/91/115	-
24	CLA	R	405	-	-	6/39/115/115	-
24	CLA	BB	303	8	-	23/39/115/115	-
24	CLA	BE	617	4	-	17/39/115/115	-
27	LHG	c	520	-	-	22/53/53/53	-
34	DGD	a	401	-	-	21/48/88/95	0/2/2/2
24	CLA	s	610	-	-	12/29/105/115	-
24	CLA	1	511	21	-	14/39/115/115	-
23	CHL	7	302	1	-	6/17/93/117	-
24	CLA	g	610	8	-	20/38/114/115	-
24	CLA	7	304	-	-	12/27/103/115	-
24	CLA	BE	608	-	-	19/39/115/115	-
29	BCR	b	618	-	-	3/29/63/63	0/2/2/2
23	CHL	G	605	8	-	7/17/93/117	-
23	CHL	s	606	-	-	8/26/102/117	-
29	BCR	f	101	-	-	11/29/63/63	0/2/2/2
24	CLA	BV	603	14	-	6/15/91/115	-
24	CLA	Ba	311	8	-	12/33/109/115	-
24	CLA	C	505	-	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HEM	BI	102	6,7	-	3/14/54/54	-
24	CLA	9	614	1	-	6/15/91/115	-
30	LMG	I	101	-	-	12/35/55/70	0/1/1/1
24	CLA	BD	407	-	-	8/21/97/115	-
24	CLA	G	614	-	-	5/19/95/115	-
30	LMG	d	405	-	-	14/41/61/70	0/1/1/1
24	CLA	A6	609	14	-	3/21/99/115	-
23	CHL	9	609	-	-	13/31/107/117	-
28	XAT	N	619	-	-	17/31/93/93	0/4/4/4
24	CLA	AA	314	1	-	7/15/91/115	-
25	LUT	N	616	-	-	1/29/67/67	0/2/2/2
23	CHL	AA	307	1	-	6/17/93/117	-
24	CLA	Ba	312	27	-	14/33/109/115	-
24	CLA	R	409	-	-	11/33/109/115	-
24	CLA	b	603	4	-	14/39/115/115	-
29	BCR	4	101	-	-	8/29/63/63	0/2/2/2
24	CLA	B	601	-	-	15/39/115/115	-
24	CLA	S	608	-	-	6/15/91/115	-
23	CHL	5	606	1	-	6/17/93/117	-
27	LHG	v	621	-	-	23/53/53/53	-
24	CLA	BF	503	21	-	15/39/115/115	-
29	BCR	BE	618	-	-	4/29/63/63	0/2/2/2
24	CLA	b	616	-	-	12/39/115/115	-
34	DGD	C	517	-	-	20/51/91/95	0/2/2/2
24	CLA	Ba	305	-	-	9/21/97/115	-
30	LMG	BF	519	-	-	22/46/66/70	0/1/1/1
23	CHL	Au	608	-	-	22/35/111/117	-
25	LUT	6	615	-	-	2/29/67/67	0/2/2/2
24	CLA	A2	613	8	-	12/33/109/115	-
24	CLA	a	407	-	-	8/21/97/115	-
24	CLA	c	504	21	-	22/39/115/115	-
29	BCR	B	619	-	-	6/29/63/63	0/2/2/2
24	CLA	8	302	-	-	6/15/91/115	-
24	CLA	b	612	4	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BF	504	21	-	17/39/115/115	-
38	PHO	BD	409	-	-	15/37/103/103	0/5/6/6
23	CHL	BH	601	-	-	2/15/91/117	-
25	LUT	0	616	-	-	1/29/67/67	0/2/2/2
24	CLA	5	613	1	-	8/27/103/115	-
24	CLA	a	405	20	-	9/39/115/115	-
24	CLA	Au	611	27	-	11/33/109/115	-
27	LHG	n	618	24	-	20/53/53/53	-
30	LMG	BL	101	-	-	17/43/63/70	0/1/1/1
23	CHL	AB	305	-	-	9/17/93/117	-
24	CLA	S	611	-	-	6/20/96/115	-
23	CHL	G	606	-	-	9/22/98/117	-
23	CHL	BQ	607	-	-	16/35/111/117	-
34	DGD	c	517	-	-	21/51/91/95	0/2/2/2
23	CHL	AA	306	1	-	5/17/93/117	-
24	CLA	N	610	-	-	16/39/115/115	-
28	XAT	Ba	301	-	-	15/31/93/93	0/4/4/4
31	PL9	BG	403	-	-	8/53/73/73	0/1/1/1
23	CHL	0	605	2	-	5/17/93/117	-
24	CLA	0	603	-	-	8/27/103/115	-
24	CLA	y	315	-	-	6/19/95/115	-
24	CLA	AB	310	-	-	5/15/91/115	-
24	CLA	BD	405	20	-	9/39/115/115	-
30	LMG	c	518	-	-	23/46/66/70	0/1/1/1
24	CLA	B	610	-	-	15/39/115/115	-
23	CHL	g	601	8	-	16/35/111/117	-
25	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
24	CLA	Y	313	-	-	11/33/109/115	-
24	CLA	A6	604	-	-	9/21/97/115	-
24	CLA	BV	608	-	-	7/15/91/115	-
24	CLA	BJ	602	8	-	15/39/115/115	-
23	CHL	0	607	-	-	12/26/102/117	-
24	CLA	BF	508	-	-	15/39/115/115	-
24	CLA	1	508	21	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	0	614	2	-	11/19/95/115	-
24	CLA	r	604	-	-	9/19/95/115	-
23	CHL	6	608	2	-	7/17/93/117	-
24	CLA	BQ	602	8	-	16/39/115/115	-
30	LMG	v	623	-	-	16/35/55/70	0/1/1/1
27	LHG	Au	618	24	-	17/53/53/53	-
26	NEX	5	617	-	-	17/27/83/83	0/3/3/3
23	CHL	AA	309	-	-	10/17/93/117	-
24	CLA	5	612	-	-	8/15/91/115	-
24	CLA	7	313	-	-	6/15/91/115	-
24	CLA	Aw	102	-	-	14/39/115/115	-
24	CLA	S	613	14	-	9/20/96/115	-
24	CLA	r	601	22	-	10/20/96/115	-
27	LHG	A2	618	24	-	17/53/53/53	-
29	BCR	c	515	-	-	6/29/63/63	0/2/2/2
24	CLA	s	604	-	-	7/21/97/115	-
24	CLA	A	410	-	-	10/33/109/115	-
27	LHG	BE	624	-	-	19/53/53/53	-
24	CLA	v	614	-	-	20/39/115/115	-
24	CLA	Y	314	8	-	14/39/115/115	-
33	HEM	f	102	6,7	-	3/14/54/54	-
24	CLA	A	406	-	-	6/39/115/115	-
23	CHL	BJ	607	-	-	18/35/111/117	-
24	CLA	N	602	8	-	15/39/115/115	-
23	CHL	A2	608	-	-	14/35/111/117	-
23	CHL	7	306	1	-	5/17/93/117	-
24	CLA	c	506	-	-	13/39/115/115	-
25	LUT	BV	615	-	-	1/29/67/67	0/2/2/2
26	NEX	9	617	-	-	17/27/83/83	0/3/3/3
27	LHG	2	406	-	-	18/53/53/53	-
24	CLA	BF	506	-	-	14/39/115/115	-
24	CLA	c	505	-	-	10/39/115/115	-
24	CLA	b	615	-	-	18/39/115/115	-
24	CLA	8	301	3	-	5/9/81/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	NEX	s	616	-	-	15/27/83/83	0/3/3/3
23	CHL	y	309	-	-	14/35/111/117	-
34	DGD	BD	413	-	-	26/49/89/95	0/2/2/2
23	CHL	7	307	1	-	6/17/93/117	-
27	LHG	L	102	-	-	19/53/53/53	-
24	CLA	0	610	2	-	11/33/109/115	-
24	CLA	BE	605	4	-	19/39/115/115	-
27	LHG	BG	404	-	-	18/53/53/53	-
27	LHG	BY	201	-	-	16/53/53/53	-
38	PHO	R	407	-	-	7/37/103/103	0/5/6/6
24	CLA	c	514	21	-	16/39/115/115	-
29	BCR	v	618	-	-	7/29/63/63	0/2/2/2
24	CLA	v	601	-	-	15/39/115/115	-
24	CLA	1	507	-	-	18/39/115/115	-
29	BCR	Av	101	-	-	4/29/63/63	0/2/2/2
24	CLA	BV	613	14	-	8/20/96/115	-
32	SQD	d	406	-	-	21/45/65/69	0/1/1/1
23	CHL	BU	605	22	-	22/35/111/117	-
23	CHL	A2	609	8	-	11/35/111/117	-
26	NEX	Y	318	-	-	12/27/83/83	0/3/3/3
27	LHG	B	622	-	-	16/50/50/53	-
30	LMG	A	412	-	-	16/43/63/70	0/1/1/1
27	LHG	Az	102	-	-	19/53/53/53	-
24	CLA	y	305	-	-	10/21/97/115	-
29	BCR	Ay	102	-	-	6/29/63/63	0/2/2/2
23	CHL	g	607	-	-	18/35/111/117	-
24	CLA	G	610	8	-	21/38/114/115	-
27	LHG	N	618	24	-	16/53/53/53	-
24	CLA	0	613	-	-	13/31/107/115	-
24	CLA	BB	314	8	-	13/39/115/115	-
24	CLA	BJ	611	27	-	11/33/109/115	-
23	CHL	N	606	8	-	10/22/98/117	-
24	CLA	v	613	4	-	14/39/115/115	-
24	CLA	A6	613	14	-	9/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	a	412	-	-	28/49/69/69	0/1/1/1
28	XAT	AA	318	-	-	12/31/93/93	0/4/4/4
24	CLA	BJ	604	-	-	9/21/97/115	-
23	CHL	r	613	22	-	2/12/88/117	-
24	CLA	9	610	1	-	8/29/105/115	-
27	LHG	6	617	24	-	13/51/51/53	-
24	CLA	d	402	-	-	13/39/115/115	-
30	LMG	C	519	-	-	22/46/66/70	0/1/1/1
24	CLA	v	615	-	-	19/39/115/115	-
24	CLA	BD	406	-	-	8/39/115/115	-
24	CLA	B	613	4	-	13/39/115/115	-
23	CHL	r	606	-	-	6/26/102/117	-
29	BCR	C	515	-	-	5/29/63/63	0/2/2/2
24	CLA	9	612	-	-	8/15/91/115	-
24	CLA	BU	612	22	-	0/4/72/115	-
24	CLA	0	611	27	-	14/27/103/115	-
23	CHL	Y	306	8	-	7/20/96/117	-
24	CLA	BF	511	21	-	15/39/115/115	-
24	CLA	y	304	-	-	9/39/115/115	-
24	CLA	Au	602	8	-	13/39/115/115	-
24	CLA	BQ	611	27	-	14/33/109/115	-
23	CHL	s	601	-	-	6/17/93/117	-
24	CLA	Au	604	-	-	6/21/97/115	-
24	CLA	BQ	604	-	-	9/21/97/115	-
27	LHG	G	618	24	-	17/53/53/53	-
32	SQD	Az	101	-	-	18/37/57/69	0/1/1/1
23	CHL	y	310	-	-	20/35/111/117	-
24	CLA	8	303	-	-	7/15/91/115	-
24	CLA	BF	513	-	-	15/39/115/115	-
23	CHL	S	601	14	-	5/17/93/117	-
23	CHL	BV	607	-	-	10/17/93/117	-
23	CHL	BQ	605	8	-	7/20/96/117	-
23	CHL	8	307	3	-	8/17/93/117	-
23	CHL	BU	606	-	-	6/26/102/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	Ba	308	-	-	20/35/111/117	-
24	CLA	A2	612	-	-	6/33/109/115	-
23	CHL	6	605	2	-	5/17/93/117	-
24	CLA	C	509	21	-	8/39/115/115	-
24	CLA	7	312	-	-	11/15/91/115	-
26	NEX	r	617	-	-	17/27/83/83	0/3/3/3
24	CLA	BE	609	4	-	13/39/115/115	-
24	CLA	BG	402	-	-	12/39/115/115	-
29	BCR	BD	411	-	-	5/29/63/63	0/2/2/2
34	DGD	BF	518	-	-	21/51/91/95	0/2/2/2
24	CLA	Ba	313	-	-	12/33/109/115	-
29	BCR	F	101	-	-	8/29/63/63	0/2/2/2
24	CLA	n	604	-	-	10/21/97/115	-
26	NEX	n	617	-	-	15/27/83/83	0/3/3/3
27	LHG	Y	319	-	-	20/53/53/53	-
24	CLA	AA	303	1	-	6/35/111/115	-
26	NEX	N	617	-	-	15/27/83/83	0/3/3/3
24	CLA	Au	610	8	-	21/38/114/115	-
24	CLA	N	614	-	-	8/19/95/115	-
24	CLA	s	611	-	-	4/20/96/115	-
28	XAT	5	619	-	-	15/31/93/93	0/4/4/4
23	CHL	N	608	-	-	14/35/111/117	-
27	LHG	0	617	24	-	12/51/51/53	-
24	CLA	v	606	-	-	17/39/115/115	-
28	XAT	9	619	-	-	16/31/93/93	0/4/4/4
25	LUT	BV	614	-	-	2/29/67/67	0/2/2/2
24	CLA	r	602	22	-	8/27/105/115	-
23	CHL	5	605	1	-	7/17/93/117	-
24	CLA	5	603	1	-	12/27/103/115	-
29	BCR	z	101	-	-	3/29/63/63	0/2/2/2
24	CLA	g	611	27	-	11/33/109/115	-
24	CLA	C	507	-	-	16/39/115/115	-
24	CLA	A2	602	8	-	15/39/115/115	-
27	LHG	D	404	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	z	102	-	-	7/29/63/63	0/2/2/2
23	CHL	0	601	2	-	15/33/109/117	-
24	CLA	C	502	21	-	16/39/115/115	-
23	CHL	Y	307	-	-	9/22/98/117	-
25	LUT	BQ	616	-	-	1/29/67/67	0/2/2/2
24	CLA	S	612	14	-	10/27/103/115	-
38	PHO	A	408	-	-	7/37/103/103	0/5/6/6
29	BCR	v	622	-	-	13/29/63/63	0/2/2/2
28	XAT	BB	301	-	-	17/31/93/93	0/4/4/4
24	CLA	BE	612	4	-	11/39/115/115	-
29	BCR	BE	619	-	-	7/29/63/63	0/2/2/2
24	CLA	v	610	-	-	15/39/115/115	-
24	CLA	b	610	-	-	12/39/115/115	-
24	CLA	AA	311	1	-	6/15/93/115	-
23	CHL	0	608	2	-	7/17/93/117	-
30	LMG	B	620	-	-	18/46/66/70	0/1/1/1
23	CHL	G	609	-	-	8/23/101/117	-
24	CLA	s	603	14	-	6/15/91/115	-
24	CLA	7	303	1	-	8/35/111/115	-
24	CLA	G	612	-	-	11/33/109/115	-
24	CLA	G	611	27	-	11/33/109/115	-
24	CLA	AA	304	-	-	12/27/103/115	-
24	CLA	s	602	14	-	12/35/111/115	-
24	CLA	G	604	-	-	6/21/97/115	-
24	CLA	Ba	315	-	-	6/19/95/115	-
23	CHL	A2	601	8	-	17/35/111/117	-
24	CLA	b	614	-	-	12/39/115/115	-
24	CLA	Y	315	-	-	6/19/95/115	-
32	SQD	BO	102	-	-	21/37/57/69	0/1/1/1
23	CHL	S	605	14	-	11/17/93/117	-
34	DGD	Av	102	-	-	14/51/91/95	0/2/2/2
24	CLA	S	602	14	-	13/35/111/115	-
25	LUT	BJ	615	-	-	2/29/67/67	0/2/2/2
34	DGD	H	102	-	-	14/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LUT	AA	316	-	-	3/29/67/67	0/2/2/2
34	DGD	A	402	-	-	24/48/88/95	0/2/2/2
24	CLA	BD	410	-	-	9/33/109/115	-
24	CLA	d	401	5	-	16/39/115/115	-
24	CLA	1	502	21	-	15/39/115/115	-
28	XAT	BJ	619	-	-	12/31/93/93	0/4/4/4
24	CLA	BV	611	-	-	5/20/96/115	-
29	BCR	B	623	-	-	13/29/63/63	0/2/2/2
24	CLA	C	512	-	-	11/39/115/115	-
27	LHG	b	623	-	-	15/50/50/53	-
30	LMG	Aw	101	-	-	12/35/55/70	0/1/1/1
24	CLA	BB	311	8	-	12/33/109/115	-
23	CHL	7	308	-	-	15/29/105/117	-
24	CLA	v	609	4	-	13/39/115/115	-
24	CLA	b	609	4	-	13/39/115/115	-
30	LMG	B	624	-	-	17/35/55/70	0/1/1/1
24	CLA	9	603	-	-	9/27/103/115	-
28	XAT	BQ	619	-	-	19/31/93/93	0/4/4/4
25	LUT	6	616	-	-	1/29/67/67	0/2/2/2
24	CLA	9	602	1	-	14/35/111/115	-
25	LUT	y	316	-	-	2/29/67/67	0/2/2/2
26	NEX	A6	616	-	-	13/27/83/83	0/3/3/3
24	CLA	c	509	21	-	16/39/115/115	-
24	CLA	BF	512	21	-	13/39/115/115	-
24	CLA	s	608	-	-	7/15/91/115	-
23	CHL	5	609	-	-	12/31/107/117	-
24	CLA	BF	509	21	-	16/39/115/115	-
28	XAT	AA	301	-	-	11/31/93/93	0/4/4/4
24	CLA	g	602	8	-	15/39/115/115	-
25	LUT	BB	317	-	-	1/29/67/67	0/2/2/2
24	CLA	B	609	-	-	13/39/115/115	-
24	CLA	s	613	14	-	9/20/96/115	-
24	CLA	8	308	-	-	5/15/91/115	-
23	CHL	AB	307	3	-	8/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	H	101	-	-	5/29/63/63	0/2/2/2
23	CHL	6	606	-	-	7/17/93/117	-
24	CLA	c	513	-	-	14/39/115/115	-
24	CLA	N	613	8	-	11/33/109/115	-
24	CLA	y	314	8	-	15/39/115/115	-
24	CLA	6	613	-	-	15/31/107/115	-
25	LUT	Y	317	-	-	1/29/67/67	0/2/2/2
24	CLA	C	504	21	-	14/39/115/115	-
23	CHL	n	601	8	-	19/35/111/117	-
24	CLA	1	512	-	-	11/39/115/115	-
25	LUT	AB	311	-	-	1/29/67/67	0/2/2/2
28	XAT	n	619	-	-	19/31/93/93	0/4/4/4
26	NEX	BQ	617	-	-	16/27/83/83	0/3/3/3
24	CLA	0	612	-	-	8/15/91/115	-
26	NEX	G	617	-	-	19/27/83/83	0/3/3/3
24	CLA	B	606	-	-	17/39/115/115	-
31	PL9	2	404	-	-	5/53/73/73	0/1/1/1
34	DGD	1	518	-	-	20/49/89/95	0/2/2/2
27	LHG	Ba	319	24	-	20/53/53/53	-
24	CLA	N	612	-	-	6/33/109/115	-
23	CHL	BB	308	-	-	15/35/111/117	-
33	HEM	F	102	7	-	5/14/54/54	-
27	LHG	BF	520	-	-	27/53/53/53	-
24	CLA	B	612	4	-	13/39/115/115	-
32	SQD	D	406	-	-	21/45/65/69	0/1/1/1
34	DGD	BD	401	-	-	21/48/88/95	0/2/2/2
23	CHL	BJ	605	8	-	7/17/93/117	-
23	CHL	g	606	-	-	6/22/98/117	-
23	CHL	Ba	309	-	-	15/35/111/117	-
24	CLA	6	612	-	-	8/15/91/115	-
24	CLA	9	613	1	-	9/27/103/115	-
26	NEX	BB	320	-	-	17/27/83/83	0/3/3/3
27	LHG	C	521	-	-	23/53/53/53	-
23	CHL	Ba	310	-	-	19/35/111/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	BF	517	-	-	14/44/84/95	0/2/2/2
27	LHG	d	404	-	-	16/53/53/53	-
26	NEX	y	318	-	-	13/27/83/83	0/3/3/3
24	CLA	BU	602	22	-	8/27/105/115	-
32	SQD	R	411	-	-	26/49/69/69	0/1/1/1
23	CHL	BQ	608	-	-	13/35/111/117	-
23	CHL	BV	606	-	-	8/26/102/117	-
24	CLA	BV	602	14	-	9/35/111/115	-
30	LMG	BF	501	-	-	22/46/66/70	0/1/1/1
25	LUT	g	615	-	-	2/29/67/67	0/2/2/2
24	CLA	n	611	27	-	14/33/109/115	-
24	CLA	BQ	603	8	-	14/39/115/115	-
24	CLA	BB	315	-	-	6/19/95/115	-
24	CLA	c	511	21	-	15/39/115/115	-
23	CHL	0	609	-	-	9/29/105/117	-
25	LUT	AA	317	-	-	1/29/67/67	0/2/2/2
32	SQD	L	103	-	-	18/49/69/69	0/1/1/1
23	CHL	Au	607	-	-	15/35/111/117	-
24	CLA	BQ	614	-	-	7/19/95/115	-
23	CHL	BV	601	-	-	6/17/93/117	-
24	CLA	9	611	27	-	8/15/91/115	-
24	CLA	BU	611	22	-	6/20/96/115	-
24	CLA	2	403	-	-	12/39/115/115	-
34	DGD	a	413	-	-	26/49/89/95	0/2/2/2
23	CHL	A6	607	14	-	14/17/93/117	-
23	CHL	y	306	8	-	7/20/96/117	-
24	CLA	1	513	21	-	15/39/115/115	-
23	CHL	A2	607	-	-	16/35/111/117	-
29	BCR	BE	620	-	-	5/29/63/63	0/2/2/2
30	LMG	D	405	-	-	13/41/61/70	0/1/1/1
24	CLA	b	611	-	-	13/39/115/115	-
24	CLA	A	405	20	-	10/39/115/115	-
24	CLA	AA	313	-	-	4/15/91/115	-
28	XAT	7	301	-	-	11/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	506	21	-	17/39/115/115	-
24	CLA	g	612	-	-	6/33/109/115	-
23	CHL	BB	302	8	-	16/35/111/117	-
24	CLA	S	604	-	-	9/21/97/115	-
24	CLA	n	614	-	-	7/19/95/115	-
24	CLA	9	604	-	-	12/21/97/115	-
24	CLA	A6	602	14	-	13/35/111/115	-
24	CLA	n	603	8	-	16/39/115/115	-
23	CHL	N	601	8	-	17/35/111/117	-
23	CHL	AA	308	-	-	17/29/105/117	-
24	CLA	AA	312	-	-	11/15/91/115	-
34	DGD	l	516	-	-	12/44/84/95	0/2/2/2
26	NEX	g	617	-	-	17/27/83/83	0/3/3/3
27	LHG	c	519	-	-	26/53/53/53	-
24	CLA	2	402	5	-	17/39/115/115	-
24	CLA	Y	303	8	-	22/39/115/115	-
24	CLA	r	610	27	-	11/20/96/115	-
23	CHL	BB	309	-	-	14/35/111/117	-
25	LUT	7	317	-	-	1/29/67/67	0/2/2/2
26	NEX	S	616	-	-	15/27/83/83	0/3/3/3
25	LUT	7	316	-	-	3/29/67/67	0/2/2/2
24	CLA	r	612	22	-	0/4/72/115	-
23	CHL	6	609	-	-	10/29/105/117	-
38	PHO	R	408	-	-	15/37/103/103	0/5/6/6
25	LUT	n	616	-	-	1/29/67/67	0/2/2/2
24	CLA	v	607	-	-	20/39/115/115	-
28	XAT	Au	619	-	-	14/31/93/93	0/4/4/4
24	CLA	Au	603	8	-	14/39/115/115	-
27	LHG	y	319	24	-	20/53/53/53	-
24	CLA	C	513	21	-	14/39/115/115	-
27	LHG	r	618	24	-	12/46/46/53	-
23	CHL	S	607	-	-	11/17/93/117	-
24	CLA	s	609	14	-	8/27/103/115	-
29	BCR	1	515	-	-	5/29/63/63	0/2/2/2
24	CLA	A2	611	27	-	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	503	21	-	16/39/115/115	-
25	LUT	BB	316	-	-	3/29/67/67	0/2/2/2
23	CHL	AB	304	3	-	10/17/93/117	-
23	CHL	G	601	8	-	16/35/111/117	-
24	CLA	6	614	2	-	12/19/95/115	-
24	CLA	b	604	4	-	13/39/115/115	-
27	LHG	1	521	-	-	23/53/53/53	-
30	LMG	i	101	-	-	17/43/63/70	0/1/1/1
29	BCR	Bb	101	-	-	7/29/63/63	0/2/2/2
32	SQD	A	413	-	-	26/49/69/69	0/1/1/1
29	BCR	B	617	-	-	5/29/63/63	0/2/2/2
24	CLA	c	508	-	-	14/39/115/115	-
25	LUT	8	311	-	-	1/29/67/67	0/2/2/2
26	NEX	BJ	617	-	-	17/27/83/83	0/3/3/3
24	CLA	0	604	-	-	8/15/91/115	-
32	SQD	BG	406	-	-	23/45/65/69	0/1/1/1
23	CHL	n	607	-	-	16/35/111/117	-
23	CHL	y	307	-	-	7/22/98/117	-
24	CLA	Ba	304	-	-	9/39/115/115	-
23	CHL	5	608	-	-	7/17/93/117	-
30	LMG	c	501	-	-	23/46/66/70	0/1/1/1
25	LUT	s	615	-	-	1/29/67/67	0/2/2/2
29	BCR	Ay	101	-	-	11/29/63/63	0/2/2/2
23	CHL	9	607	-	-	18/32/108/117	-
24	CLA	A	407	-	-	7/21/97/115	-
24	CLA	r	609	22	-	12/39/115/115	-
23	CHL	9	608	-	-	7/17/93/117	-
23	CHL	s	607	-	-	9/17/93/117	-
24	CLA	6	604	-	-	10/15/91/115	-
24	CLA	BU	610	27	-	10/20/96/115	-
24	CLA	n	602	8	-	16/39/115/115	-
25	LUT	Ba	316	-	-	2/29/67/67	0/2/2/2
27	LHG	1	520	-	-	25/53/53/53	-
29	BCR	b	601	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BF	514	-	-	15/39/115/115	-
24	CLA	BE	611	-	-	14/39/115/115	-
24	CLA	R	406	-	-	7/21/97/115	-
29	BCR	v	617	-	-	5/29/63/63	0/2/2/2
24	CLA	Y	312	-	-	13/33/109/115	-
24	CLA	b	606	4	-	17/39/115/115	-
24	CLA	A2	604	-	-	9/21/97/115	-
24	CLA	BE	604	4	-	13/39/115/115	-
23	CHL	AB	306	-	-	5/17/93/117	-
24	CLA	BJ	610	8	-	21/38/114/115	-
28	XAT	G	619	-	-	14/31/93/93	0/4/4/4
29	BCR	b	619	-	-	7/29/63/63	0/2/2/2
34	DGD	R	401	-	-	24/48/88/95	0/2/2/2
24	CLA	y	303	8	-	16/39/115/115	-
24	CLA	s	612	14	-	10/27/103/115	-
23	CHL	Y	302	8	-	15/35/111/117	-
30	LMG	b	621	-	-	25/46/66/70	0/1/1/1
23	CHL	BB	310	-	-	17/35/111/117	-
27	LHG	5	618	24	-	18/45/45/53	-
23	CHL	Ba	302	8	-	14/35/111/117	-
24	CLA	BB	305	-	-	11/21/97/115	-
24	CLA	A6	603	-	-	5/15/91/115	-
25	LUT	s	614	-	-	2/29/67/67	0/2/2/2
25	LUT	G	615	-	-	1/29/67/67	0/2/2/2
24	CLA	8	310	-	-	4/15/91/115	-
23	CHL	A6	606	-	-	7/26/102/117	-
24	CLA	n	613	-	-	11/33/109/115	-
24	CLA	BE	614	-	-	12/39/115/115	-
23	CHL	BB	307	-	-	8/22/98/117	-
24	CLA	G	603	8	-	14/39/115/115	-
28	XAT	g	619	-	-	12/31/93/93	0/4/4/4
24	CLA	5	604	-	-	12/21/97/115	-
31	PL9	D	403	-	-	5/53/73/73	0/1/1/1
24	CLA	BE	606	4	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	BJ	606	-	-	6/22/98/117	-
27	LHG	b	622	-	-	24/53/53/53	-
33	HEM	4	102	7	-	6/14/54/54	-
24	CLA	BQ	613	-	-	11/33/109/115	-
24	CLA	Ba	314	8	-	15/39/115/115	-
24	CLA	1	504	21	-	14/39/115/115	-
23	CHL	g	605	8	-	7/17/93/117	-
24	CLA	g	603	8	-	13/39/115/115	-
27	LHG	BE	623	-	-	15/50/50/53	-
30	LMG	BE	621	-	-	23/46/66/70	0/1/1/1
24	CLA	6	610	2	-	10/33/109/115	-
24	CLA	a	410	-	-	9/33/109/115	-
23	CHL	AA	310	-	-	12/29/105/117	-
24	CLA	b	607	-	-	14/39/115/115	-
29	BCR	A	411	-	-	5/29/63/63	0/2/2/2
24	CLA	a	406	-	-	7/39/115/115	-
23	CHL	s	605	14	-	11/17/93/117	-
24	CLA	5	610	1	-	8/29/105/115	-
32	SQD	l	101	-	-	21/49/69/69	0/1/1/1
24	CLA	b	608	-	-	19/39/115/115	-
25	LUT	A6	615	-	-	1/29/67/67	0/2/2/2
34	DGD	c	516	-	-	14/44/84/95	0/2/2/2
24	CLA	1	505	-	-	9/39/115/115	-
25	LUT	Au	615	-	-	1/29/67/67	0/2/2/2
24	CLA	r	603	22	-	7/33/109/115	-
24	CLA	BE	610	-	-	14/39/115/115	-
25	LUT	A2	615	-	-	1/29/67/67	0/2/2/2
27	LHG	BE	622	-	-	24/53/53/53	-
24	CLA	B	605	4	-	22/39/115/115	-
24	CLA	BB	313	-	-	11/33/109/115	-
23	CHL	Au	606	-	-	9/22/98/117	-
24	CLA	r	608	22	-	13/31/107/115	-
23	CHL	BQ	606	8	-	11/22/98/117	-
38	PHO	BD	408	-	-	7/37/103/103	0/5/6/6
23	CHL	A2	606	8	-	10/22/98/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	r	607	22	-	19/29/105/117	-
23	CHL	Ba	306	8	-	7/20/96/117	-
24	CLA	BV	609	14	-	9/27/103/115	-
24	CLA	AA	305	-	-	7/15/91/115	-
24	CLA	B	607	-	-	20/39/115/115	-
24	CLA	c	510	21	-	8/39/115/115	-
24	CLA	B	615	-	-	19/39/115/115	-
24	CLA	6	611	27	-	14/27/103/115	-
24	CLA	A6	608	-	-	6/15/91/115	-
24	CLA	BJ	603	8	-	13/39/115/115	-
24	CLA	1	503	21	-	13/39/115/115	-
25	LUT	9	615	-	-	3/29/67/67	0/2/2/2
23	CHL	n	606	8	-	11/22/98/117	-
23	CHL	BQ	601	8	-	18/35/111/117	-
24	CLA	N	611	27	-	15/33/109/115	-
25	LUT	BU	615	-	-	3/29/67/67	0/2/2/2
30	LMG	v	620	-	-	18/46/66/70	0/1/1/1
32	SQD	l	102	-	-	21/37/57/69	0/1/1/1
29	BCR	h	101	-	-	5/29/63/63	0/2/2/2
23	CHL	9	605	1	-	7/17/93/117	-
24	CLA	G	602	8	-	13/39/115/115	-
24	CLA	1	506	21	-	17/39/115/115	-
24	CLA	BF	505	-	-	8/39/115/115	-
24	CLA	B	611	4	-	11/39/115/115	-
24	CLA	v	603	4	-	13/39/115/115	-
24	CLA	BF	510	21	-	8/39/115/115	-
27	LHG	2	405	-	-	15/50/50/53	-
31	PL9	d	403	-	-	10/53/73/73	0/1/1/1
23	CHL	BV	605	14	-	10/17/93/117	-
24	CLA	B	604	4	-	14/39/115/115	-
28	XAT	r	616	-	-	17/31/93/93	0/4/4/4
24	CLA	v	611	4	-	11/39/115/115	-
23	CHL	BU	607	22	-	18/29/105/117	-
23	CHL	6	601	2	-	16/33/109/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LUT	A6	614	-	-	2/29/67/67	0/2/2/2
26	NEX	A2	617	-	-	15/27/83/83	0/3/3/3
24	CLA	BV	612	14	-	10/27/103/115	-
24	CLA	Y	304	8	-	11/39/115/115	-
26	NEX	Au	617	-	-	19/27/83/83	0/3/3/3
29	BCR	K	102	-	-	6/29/63/63	0/2/2/2
24	CLA	BU	609	22	-	12/39/115/115	-
23	CHL	7	310	-	-	14/29/105/117	-
24	CLA	AB	308	-	-	6/15/91/115	-
28	XAT	A2	619	-	-	17/31/93/93	0/4/4/4
24	CLA	BG	401	5	-	16/39/115/115	-
34	DGD	C	518	-	-	20/49/89/95	0/2/2/2
25	LUT	BJ	616	-	-	1/29/67/67	0/2/2/2
29	BCR	a	411	-	-	5/29/63/63	0/2/2/2
24	CLA	A2	603	8	-	13/39/115/115	-
23	CHL	G	607	-	-	15/35/111/117	-
29	BCR	BF	516	-	-	6/29/63/63	0/2/2/2
24	CLA	6	603	-	-	9/27/103/115	-
23	CHL	Y	308	-	-	15/35/111/117	-
23	CHL	BQ	609	-	-	15/35/111/117	-
24	CLA	7	311	1	-	6/15/93/115	-
30	LMG	2	407	-	-	13/41/61/70	0/1/1/1
23	CHL	5	601	1	-	9/17/93/117	-
24	CLA	1	509	21	-	8/39/115/115	-
24	CLA	B	614	-	-	19/39/115/115	-
25	LUT	9	616	-	-	1/29/67/67	0/2/2/2
29	BCR	k	101	-	-	11/29/63/63	0/2/2/2
32	SQD	L	101	-	-	19/37/57/69	0/1/1/1
24	CLA	7	314	1	-	7/15/91/115	-
24	CLA	BE	616	-	-	12/39/115/115	-
28	XAT	y	301	-	-	15/31/93/93	0/4/4/4
24	CLA	BE	607	-	-	14/39/115/115	-
25	LUT	g	616	-	-	1/29/67/67	0/2/2/2
24	CLA	N	604	-	-	9/21/97/115	-
25	LUT	0	615	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BJ	614	8	-	5/19/95/115	-
24	CLA	BB	304	8	-	11/39/115/115	-
29	BCR	BK	101	-	-	6/29/63/63	0/2/2/2
23	CHL	Ba	307	-	-	8/22/98/117	-
23	CHL	N	609	8	-	12/35/111/117	-
24	CLA	A6	610	-	-	10/29/105/115	-
29	BCR	b	620	-	-	4/29/63/63	0/2/2/2
24	CLA	G	613	-	-	12/39/115/115	-
30	LMG	BG	405	-	-	14/41/61/70	0/1/1/1
24	CLA	v	612	4	-	13/39/115/115	-
24	CLA	A6	612	14	-	11/27/103/115	-
27	LHG	BB	319	-	-	18/53/53/53	-
24	CLA	r	611	22	-	6/20/96/115	-
27	LHG	BU	617	24	-	12/46/46/53	-
27	LHG	W	201	-	-	15/53/53/53	-
34	DGD	BK	102	-	-	18/51/91/95	0/2/2/2
34	DGD	1	517	-	-	21/51/91/95	0/2/2/2
24	CLA	0	602	2	-	16/33/109/115	-
24	CLA	c	502	21	-	14/39/115/115	-
24	CLA	7	305	-	-	7/15/91/115	-
24	CLA	AB	303	-	-	7/15/91/115	-
24	CLA	A6	611	-	-	6/20/96/115	-
24	CLA	BF	502	21	-	14/39/115/115	-
24	CLA	g	613	-	-	13/39/115/115	-
28	XAT	7	318	-	-	12/31/93/93	0/4/4/4
23	CHL	BJ	609	-	-	10/29/105/117	-
29	BCR	K	101	-	-	11/29/63/63	0/2/2/2
25	LUT	BQ	615	-	-	1/29/67/67	0/2/2/2
34	DGD	C	516	-	-	13/44/84/95	0/2/2/2
29	BCR	BE	601	-	-	15/29/63/63	0/2/2/2
23	CHL	6	607	-	-	12/26/102/117	-
24	CLA	b	605	4	-	19/39/115/115	-
29	BCR	v	619	-	-	7/29/63/63	0/2/2/2
23	CHL	A6	605	14	-	11/17/93/117	-

The worst 5 of 7506 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	7	301	XAT	C10-C9	15.13	1.55	1.35
28	AA	301	XAT	C10-C9	15.11	1.55	1.35
28	Au	619	XAT	C10-C9	15.10	1.55	1.35
28	G	619	XAT	C10-C9	15.07	1.55	1.35
28	AA	318	XAT	C10-C9	15.04	1.55	1.35

The worst 5 of 8154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BB	301	XAT	O24-C25-C24	33.02	138.19	113.38
28	AA	301	XAT	O24-C25-C24	32.93	138.12	113.38
28	N	619	XAT	O24-C25-C24	32.85	138.06	113.38
28	5	619	XAT	O4-C5-C4	32.85	138.06	113.38
28	A2	619	XAT	O24-C25-C24	32.82	138.04	113.38

There are no chirality outliers.

5 of 8915 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	5	601	CHL	C1A-C2A-CAA-CBA
23	5	601	CHL	C3A-C2A-CAA-CBA
23	5	601	CHL	CBD-CGD-O2D-CED
23	5	605	CHL	C1A-C2A-CAA-CBA
23	5	606	CHL	C2B-C3B-CAB-CBB

There are no ring outliers.

699 monomers are involved in 2718 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	y	311	CLA	4	0
24	BU	604	CLA	3	0
28	Y	301	XAT	5	0
25	n	615	LUT	5	0
23	n	608	CHL	10	0
27	BQ	618	LHG	6	0
23	5	607	CHL	11	0
24	BU	601	CLA	3	0
29	B	618	BCR	1	0
29	BI	101	BCR	2	0
23	G	608	CHL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	602	CLA	6	0
24	BJ	613	CLA	6	0
25	y	317	LUT	4	0
24	c	512	CLA	5	0
23	n	605	CHL	2	0
24	BU	614	CLA	1	0
32	A1	101	SQD	2	0
23	BB	306	CHL	5	0
23	AA	302	CHL	11	0
23	A6	601	CHL	2	0
24	n	612	CLA	3	0
23	n	609	CHL	15	0
28	AB	312	XAT	6	0
24	C	511	CLA	5	0
28	8	312	XAT	6	0
26	BB	318	NEX	3	0
24	AB	309	CLA	1	0
26	AA	319	NEX	4	0
24	8	309	CLA	1	0
34	h	102	DGD	4	0
38	a	408	PHO	4	0
26	BV	616	NEX	5	0
24	v	608	CLA	5	0
24	BV	610	CLA	2	0
25	S	614	LUT	4	0
28	BU	616	XAT	4	0
24	v	602	CLA	6	0
24	C	510	CLA	1	0
24	D	401	CLA	7	0
29	BN	101	BCR	2	0
30	C	501	LMG	2	0
24	S	609	CLA	4	0
29	8	313	BCR	6	0
32	2	408	SQD	3	0
24	BE	603	CLA	13	0
23	BU	613	CHL	2	0
23	Au	609	CHL	8	0
23	7	309	CHL	5	0
29	C	514	BCR	2	0
27	C	520	LHG	2	0
24	Au	612	CLA	3	0
25	Ba	317	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	BJ	608	CHL	7	0
24	y	312	CLA	1	0
24	v	604	CLA	6	0
24	BU	608	CLA	3	0
25	Au	616	LUT	5	0
25	N	615	LUT	4	0
27	g	618	LHG	4	0
24	BJ	612	CLA	3	0
23	y	302	CHL	11	0
25	S	615	LUT	7	0
24	5	611	CLA	2	0
27	b	624	LHG	4	0
23	g	608	CHL	6	0
24	b	602	CLA	4	0
23	S	606	CHL	7	0
24	A2	610	CLA	6	0
23	9	606	CHL	5	0
27	A0	202	LHG	1	0
24	Y	311	CLA	5	0
23	A2	605	CHL	2	0
24	b	617	CLA	3	0
24	v	616	CLA	3	0
26	Ba	318	NEX	2	0
23	N	605	CHL	2	0
24	N	603	CLA	1	0
23	BJ	601	CHL	15	0
25	5	615	LUT	6	0
27	w	201	LHG	1	0
23	8	305	CHL	2	0
24	BB	312	CLA	3	0
24	g	604	CLA	2	0
27	BJ	618	LHG	4	0
24	B	616	CLA	3	0
24	B	603	CLA	4	0
27	BF	521	LHG	3	0
23	N	607	CHL	8	0
24	A2	614	CLA	3	0
24	BQ	610	CLA	12	0
23	9	601	CHL	6	0
30	1	519	LMG	3	0
38	A	409	PHO	2	0
24	BQ	612	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	9	618	LHG	3	0
29	AB	313	BCR	5	0
32	BD	412	SQD	6	0
23	Au	601	CHL	14	0
24	c	507	CLA	4	0
24	C	508	CLA	5	0
23	Y	309	CHL	5	0
29	R	410	BCR	1	0
24	R	404	CLA	5	0
24	BF	507	CLA	4	0
29	BF	515	BCR	4	0
23	Y	310	CHL	12	0
24	BE	602	CLA	5	0
24	AB	301	CLA	6	0
23	8	304	CHL	2	0
24	S	610	CLA	1	0
24	BU	603	CLA	3	0
25	A2	616	LUT	7	0
32	BO	101	SQD	5	0
24	BE	615	CLA	4	0
24	y	313	CLA	3	0
26	7	319	NEX	5	0
24	1	510	CLA	1	0
23	8	306	CHL	3	0
24	b	613	CLA	5	0
27	B	621	LHG	2	0
23	0	606	CHL	5	0
24	AB	302	CLA	2	0
25	5	616	LUT	9	0
24	r	614	CLA	3	0
23	y	308	CHL	6	0
23	g	609	CHL	16	0
24	n	610	CLA	10	0
24	B	608	CLA	5	0
29	1	514	BCR	3	0
25	r	615	LUT	9	0
30	1	501	LMG	2	0
30	A0	201	LMG	1	0
24	6	602	CLA	12	0
24	I	102	CLA	3	0
24	BV	604	CLA	6	0
24	Ba	303	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	503	CLA	1	0
23	r	605	CHL	17	0
24	5	614	CLA	1	0
24	Au	613	CLA	6	0
25	G	616	LUT	5	0
24	BE	613	CLA	4	0
24	5	602	CLA	8	0
24	v	605	CLA	9	0
24	R	405	CLA	6	0
24	BB	303	CLA	3	0
24	BE	617	CLA	3	0
27	c	520	LHG	3	0
34	a	401	DGD	2	0
24	s	610	CLA	3	0
24	1	511	CLA	3	0
23	7	302	CHL	9	0
24	g	610	CLA	2	0
24	7	304	CLA	5	0
24	BE	608	CLA	3	0
29	b	618	BCR	3	0
23	G	605	CHL	1	0
23	s	606	CHL	11	0
29	f	101	BCR	2	0
24	BV	603	CLA	1	0
24	Ba	311	CLA	4	0
24	C	505	CLA	3	0
33	BI	102	HEM	2	0
24	9	614	CLA	1	0
30	I	101	LMG	3	0
24	BD	407	CLA	3	0
24	A6	609	CLA	3	0
23	9	609	CHL	15	0
28	N	619	XAT	5	0
24	AA	314	CLA	3	0
25	N	616	LUT	6	0
23	AA	307	CHL	2	0
24	Ba	312	CLA	1	0
24	b	603	CLA	10	0
29	4	101	BCR	3	0
24	B	601	CLA	4	0
24	S	608	CLA	3	0
23	5	606	CHL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	v	621	LHG	2	0
29	BE	618	BCR	4	0
24	b	616	CLA	4	0
34	C	517	DGD	4	0
24	Ba	305	CLA	2	0
30	BF	519	LMG	4	0
23	Au	608	CHL	6	0
25	6	615	LUT	8	0
24	A2	613	CLA	5	0
24	a	407	CLA	6	0
24	c	504	CLA	4	0
29	B	619	BCR	6	0
24	8	302	CLA	2	0
24	b	612	CLA	3	0
24	BF	504	CLA	2	0
38	BD	409	PHO	1	0
25	0	616	LUT	9	0
24	5	613	CLA	7	0
24	a	405	CLA	5	0
24	Au	611	CLA	3	0
27	n	618	LHG	5	0
30	BL	101	LMG	2	0
23	AB	305	CHL	2	0
23	G	606	CHL	3	0
23	BQ	607	CHL	10	0
34	c	517	DGD	4	0
24	N	610	CLA	9	0
28	Ba	301	XAT	2	0
31	BG	403	PL9	2	0
24	0	603	CLA	1	0
24	AB	310	CLA	2	0
24	BD	405	CLA	8	0
30	c	518	LMG	4	0
24	B	610	CLA	2	0
23	g	601	CHL	14	0
25	Y	316	LUT	4	0
24	Y	313	CLA	1	0
24	A6	604	CLA	3	0
24	BV	608	CLA	6	0
24	BJ	602	CLA	6	0
23	0	607	CHL	6	0
24	BF	508	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	508	CLA	7	0
24	0	614	CLA	4	0
24	r	604	CLA	3	0
23	6	608	CHL	2	0
24	BQ	602	CLA	6	0
27	Au	618	LHG	4	0
26	5	617	NEX	1	0
23	AA	309	CHL	4	0
24	5	612	CLA	1	0
24	7	313	CLA	3	0
24	Aw	102	CLA	3	0
24	r	601	CLA	4	0
27	A2	618	LHG	3	0
29	c	515	BCR	3	0
24	s	604	CLA	6	0
24	A	410	CLA	1	0
27	BE	624	LHG	2	0
24	v	614	CLA	8	0
24	Y	314	CLA	5	0
33	f	102	HEM	2	0
24	A	406	CLA	5	0
23	BJ	607	CHL	10	0
24	N	602	CLA	2	0
23	A2	608	CHL	11	0
24	c	506	CLA	3	0
25	BV	615	LUT	4	0
26	9	617	NEX	1	0
24	BF	506	CLA	3	0
24	c	505	CLA	5	0
24	b	615	CLA	4	0
24	8	301	CLA	6	0
26	s	616	NEX	5	0
23	y	309	CHL	8	0
23	7	307	CHL	2	0
27	L	102	LHG	3	0
24	0	610	CLA	10	0
24	BE	605	CLA	5	0
27	BG	404	LHG	1	0
27	BY	201	LHG	1	0
38	R	407	PHO	7	0
24	c	514	CLA	7	0
24	v	601	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	507	CLA	4	0
29	Av	101	BCR	4	0
32	d	406	SQD	3	0
23	BU	605	CHL	17	0
23	A2	609	CHL	10	0
26	Y	318	NEX	1	0
30	A	412	LMG	1	0
27	Az	102	LHG	3	0
24	y	305	CLA	2	0
29	Ay	102	BCR	5	0
23	g	607	CHL	8	0
24	G	610	CLA	4	0
27	N	618	LHG	5	0
24	0	613	CLA	10	0
24	BB	314	CLA	5	0
24	BJ	611	CLA	3	0
23	N	606	CHL	5	0
24	v	613	CLA	2	0
32	a	412	SQD	6	0
28	AA	318	XAT	3	0
24	BJ	604	CLA	2	0
23	r	613	CHL	3	0
24	9	610	CLA	9	0
27	6	617	LHG	5	0
24	d	402	CLA	1	0
30	C	519	LMG	3	0
24	v	615	CLA	4	0
24	BD	406	CLA	8	0
24	B	613	CLA	2	0
23	r	606	CHL	13	0
29	C	515	BCR	3	0
24	9	612	CLA	2	0
24	BU	612	CLA	4	0
24	0	611	CLA	6	0
23	Y	306	CHL	6	0
24	BF	511	CLA	5	0
24	y	304	CLA	3	0
24	Au	602	CLA	6	0
24	BQ	611	CLA	2	0
23	s	601	CHL	3	0
27	G	618	LHG	3	0
32	Az	101	SQD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	y	310	CHL	12	0
24	8	303	CLA	2	0
24	BF	513	CLA	3	0
23	S	601	CHL	2	0
23	BV	607	CHL	5	0
23	BQ	605	CHL	2	0
23	8	307	CHL	4	0
23	BU	606	CHL	12	0
23	Ba	308	CHL	8	0
24	A2	612	CLA	1	0
24	C	509	CLA	2	0
24	7	312	CLA	2	0
26	r	617	NEX	5	0
24	BE	609	CLA	4	0
24	BG	402	CLA	1	0
29	BD	411	BCR	2	0
34	BF	518	DGD	4	0
24	Ba	313	CLA	2	0
29	F	101	BCR	1	0
26	n	617	NEX	3	0
27	Y	319	LHG	6	0
24	AA	303	CLA	11	0
26	N	617	NEX	3	0
24	Au	610	CLA	3	0
24	N	614	CLA	3	0
24	s	611	CLA	2	0
28	5	619	XAT	11	0
23	N	608	CHL	12	0
27	0	617	LHG	8	0
24	v	606	CLA	9	0
28	9	619	XAT	11	0
25	BV	614	LUT	6	0
36	BD	403	OEX	1	0
24	r	602	CLA	10	0
23	5	605	CHL	2	0
24	5	603	CLA	3	0
29	z	101	BCR	5	0
24	g	611	CLA	3	0
24	C	507	CLA	2	0
24	A2	602	CLA	2	0
27	D	404	LHG	3	0
29	z	102	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	0	601	CHL	12	0
24	C	502	CLA	3	0
23	Y	307	CHL	5	0
25	BQ	616	LUT	6	0
24	S	612	CLA	1	0
38	A	408	PHO	6	0
29	v	622	BCR	5	0
28	BB	301	XAT	6	0
24	BE	612	CLA	3	0
24	v	610	CLA	2	0
24	b	610	CLA	12	0
24	AA	311	CLA	4	0
23	0	608	CHL	2	0
23	G	609	CHL	18	0
24	s	603	CLA	1	0
24	7	303	CLA	8	0
24	G	612	CLA	3	0
24	G	611	CLA	4	0
24	AA	304	CLA	4	0
24	s	602	CLA	6	0
23	A2	601	CHL	9	0
24	b	614	CLA	2	0
24	Y	315	CLA	1	0
32	BO	102	SQD	1	0
23	S	605	CHL	1	0
34	Av	102	DGD	6	0
24	S	602	CLA	8	0
25	BJ	615	LUT	7	0
34	H	102	DGD	6	0
25	AA	316	LUT	7	0
34	A	402	DGD	2	0
24	BD	410	CLA	1	0
24	d	401	CLA	6	0
24	1	502	CLA	2	0
28	BJ	619	XAT	1	0
24	BV	611	CLA	2	0
29	B	623	BCR	8	0
24	C	512	CLA	3	0
27	b	623	LHG	2	0
30	Aw	101	LMG	1	0
24	BB	311	CLA	3	0
23	7	308	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	v	609	CLA	12	0
24	b	609	CLA	5	0
24	9	603	CLA	4	0
28	BQ	619	XAT	5	0
25	6	616	LUT	9	0
24	9	602	CLA	7	0
25	y	316	LUT	5	0
26	A6	616	NEX	2	0
24	c	509	CLA	5	0
24	BF	512	CLA	3	0
24	s	608	CLA	6	0
23	5	609	CHL	15	0
24	BF	509	CLA	9	0
28	AA	301	XAT	3	0
24	g	602	CLA	5	0
25	BB	317	LUT	6	0
24	B	609	CLA	11	0
24	8	308	CLA	7	0
23	AB	307	CHL	8	0
29	H	101	BCR	5	0
23	6	606	CHL	7	0
24	c	513	CLA	3	0
24	N	613	CLA	5	0
24	y	314	CLA	3	0
24	6	613	CLA	11	0
25	Y	317	LUT	5	0
24	C	504	CLA	2	0
23	n	601	CHL	12	0
24	1	512	CLA	2	0
25	AB	311	LUT	9	0
28	n	619	XAT	2	0
26	BQ	617	NEX	3	0
24	0	612	CLA	3	0
26	G	617	NEX	1	0
24	B	606	CLA	8	0
31	2	404	PL9	1	0
34	1	518	DGD	2	0
27	Ba	319	LHG	4	0
24	N	612	CLA	1	0
23	BB	308	CHL	9	0
33	F	102	HEM	1	0
24	B	612	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	D	406	SQD	1	0
34	BD	401	DGD	2	0
23	BJ	605	CHL	3	0
23	g	606	CHL	7	0
23	Ba	309	CHL	8	0
24	6	612	CLA	3	0
24	9	613	CLA	7	0
26	BB	320	NEX	5	0
27	C	521	LHG	3	0
23	Ba	310	CHL	12	0
27	d	404	LHG	1	0
26	y	318	NEX	3	0
24	BU	602	CLA	12	0
32	R	411	SQD	9	0
23	BQ	608	CHL	9	0
23	BV	606	CHL	10	0
24	BV	602	CLA	4	0
30	BF	501	LMG	1	0
25	g	615	LUT	7	0
24	n	611	CLA	2	0
24	BQ	603	CLA	1	0
24	BB	315	CLA	1	0
24	c	511	CLA	3	0
23	0	609	CHL	12	0
25	AA	317	LUT	7	0
32	L	103	SQD	2	0
23	Au	607	CHL	10	0
24	BQ	614	CLA	2	0
23	BV	601	CHL	3	0
24	9	611	CLA	2	0
24	2	403	CLA	1	0
34	a	413	DGD	1	0
23	A6	607	CHL	6	0
23	y	306	CHL	3	0
24	1	513	CLA	7	0
23	A2	607	CHL	11	0
29	BE	620	BCR	5	0
24	b	611	CLA	6	0
24	A	405	CLA	6	0
24	AA	313	CLA	2	0
28	7	301	XAT	3	0
24	C	506	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	g	612	CLA	3	0
23	BB	302	CHL	14	0
24	S	604	CLA	3	0
24	n	614	CLA	2	0
24	9	604	CLA	5	0
24	A6	602	CLA	5	0
24	n	603	CLA	1	0
23	N	601	CHL	10	0
23	AA	308	CHL	7	0
24	AA	312	CLA	1	0
34	1	516	DGD	1	0
26	g	617	NEX	1	0
24	2	402	CLA	7	0
24	Y	303	CLA	3	0
24	r	610	CLA	3	0
23	BB	309	CHL	7	0
25	7	317	LUT	7	0
26	S	616	NEX	3	0
25	7	316	LUT	6	0
24	r	612	CLA	4	0
23	6	609	CHL	13	0
25	n	616	LUT	6	0
24	v	607	CLA	5	0
28	Au	619	XAT	4	0
27	y	319	LHG	5	0
24	C	513	CLA	6	0
27	r	618	LHG	6	0
23	S	607	CHL	6	0
24	s	609	CLA	4	0
29	1	515	BCR	4	0
24	A2	611	CLA	3	0
24	C	503	CLA	1	0
25	BB	316	LUT	5	0
23	AB	304	CHL	3	0
23	G	601	CHL	13	0
24	6	614	CLA	4	0
24	b	604	CLA	1	0
27	1	521	LHG	3	0
30	i	101	LMG	2	0
29	Bb	101	BCR	3	0
32	A	413	SQD	8	0
29	B	617	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	508	CLA	5	0
25	8	311	LUT	6	0
26	BJ	617	NEX	1	0
24	0	604	CLA	2	0
32	BG	406	SQD	4	0
23	n	607	CHL	10	0
23	y	307	CHL	7	0
24	Ba	304	CLA	3	0
23	5	608	CHL	4	0
30	c	501	LMG	3	0
25	s	615	LUT	9	0
29	Ay	101	BCR	3	0
23	9	607	CHL	8	0
24	A	407	CLA	3	0
24	r	609	CLA	6	0
23	9	608	CHL	4	0
23	s	607	CHL	4	0
24	6	604	CLA	6	0
24	BU	610	CLA	3	0
24	n	602	CLA	5	0
25	Ba	316	LUT	4	0
27	1	520	LHG	1	0
29	b	601	BCR	7	0
24	BF	514	CLA	7	0
24	BE	611	CLA	3	0
24	R	406	CLA	2	0
29	v	617	BCR	5	0
24	Y	312	CLA	6	0
24	b	606	CLA	5	0
24	A2	604	CLA	1	0
24	BE	604	CLA	1	0
23	AB	306	CHL	3	0
24	BJ	610	CLA	3	0
28	G	619	XAT	4	0
29	b	619	BCR	3	0
34	R	401	DGD	2	0
24	y	303	CLA	3	0
24	s	612	CLA	1	0
23	Y	302	CHL	12	0
30	b	621	LMG	1	0
23	BB	310	CHL	10	0
27	5	618	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Ba	302	CHL	10	0
24	BB	305	CLA	1	0
25	s	614	LUT	7	0
25	G	615	LUT	6	0
24	8	310	CLA	2	0
23	A6	606	CHL	7	0
24	n	613	CLA	5	0
24	BE	614	CLA	2	0
23	BB	307	CHL	4	0
24	G	603	CLA	1	0
28	g	619	XAT	1	0
24	5	604	CLA	6	0
31	D	403	PL9	1	0
24	BE	606	CLA	5	0
23	BJ	606	CHL	6	0
33	4	102	HEM	3	0
24	BQ	613	CLA	4	0
24	Ba	314	CLA	7	0
24	1	504	CLA	2	0
23	g	605	CHL	3	0
24	g	603	CLA	2	0
27	BE	623	LHG	1	0
30	BE	621	LMG	1	0
24	6	610	CLA	5	0
24	a	410	CLA	1	0
23	AA	310	CHL	10	0
24	b	607	CLA	9	0
29	A	411	BCR	3	0
24	a	406	CLA	7	0
23	s	605	CHL	5	0
24	5	610	CLA	13	0
36	a	403	OEX	1	0
32	l	101	SQD	5	0
24	b	608	CLA	3	0
25	A6	615	LUT	8	0
24	1	505	CLA	2	0
25	Au	615	LUT	7	0
24	r	603	CLA	1	0
24	BE	610	CLA	11	0
25	A2	615	LUT	5	0
24	B	605	CLA	10	0
24	BB	313	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Au	606	CHL	2	0
24	r	608	CLA	2	0
23	BQ	606	CHL	7	0
38	BD	408	PHO	5	0
23	A2	606	CHL	5	0
23	r	607	CHL	10	0
23	Ba	306	CHL	3	0
24	BV	609	CLA	7	0
24	AA	305	CLA	4	0
24	B	607	CLA	2	0
24	c	510	CLA	2	0
24	B	615	CLA	4	0
24	6	611	CLA	5	0
24	A6	608	CLA	2	0
24	BJ	603	CLA	3	0
24	1	503	CLA	1	0
25	9	615	LUT	8	0
23	n	606	CHL	8	0
23	BQ	601	CHL	11	0
24	N	611	CLA	3	0
25	BU	615	LUT	10	0
32	l	102	SQD	2	0
29	h	101	BCR	7	0
23	9	605	CHL	2	0
24	G	602	CLA	4	0
24	1	506	CLA	5	0
24	BF	505	CLA	2	0
24	B	611	CLA	5	0
24	v	603	CLA	3	0
24	BF	510	CLA	3	0
27	2	405	LHG	1	0
31	d	403	PL9	3	0
23	BV	605	CHL	5	0
24	B	604	CLA	6	0
28	r	616	XAT	5	0
24	v	611	CLA	5	0
23	BU	607	CHL	12	0
23	6	601	CHL	16	0
25	A6	614	LUT	2	0
26	A2	617	NEX	3	0
24	BV	612	CLA	1	0
24	Y	304	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Au	617	NEX	1	0
29	K	102	BCR	2	0
24	BU	609	CLA	5	0
23	7	310	CHL	11	0
24	AB	308	CLA	11	0
28	A2	619	XAT	6	0
24	BG	401	CLA	7	0
34	C	518	DGD	1	0
25	BJ	616	LUT	10	0
29	a	411	BCR	3	0
24	A2	603	CLA	3	0
23	G	607	CHL	11	0
29	BF	516	BCR	2	0
24	6	603	CLA	1	0
23	Y	308	CHL	9	0
23	BQ	609	CHL	15	0
24	7	311	CLA	4	0
23	5	601	CHL	5	0
24	1	509	CLA	1	0
24	B	614	CLA	7	0
25	9	616	LUT	10	0
29	k	101	BCR	1	0
32	L	101	SQD	3	0
24	7	314	CLA	3	0
24	BE	616	CLA	2	0
28	y	301	XAT	3	0
24	BE	607	CLA	8	0
25	g	616	LUT	9	0
25	0	615	LUT	10	0
24	BB	304	CLA	1	0
29	BK	101	BCR	8	0
23	Ba	307	CHL	6	0
23	N	609	CHL	9	0
24	A6	610	CLA	1	0
29	b	620	BCR	3	0
24	G	613	CLA	6	0
24	v	612	CLA	4	0
27	BB	319	LHG	7	0
24	r	611	CLA	1	0
27	BU	617	LHG	5	0
27	W	201	LHG	1	0
34	BK	102	DGD	6	0

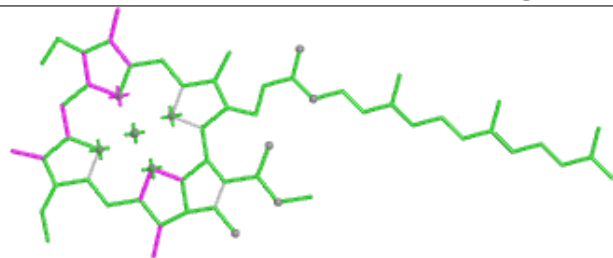
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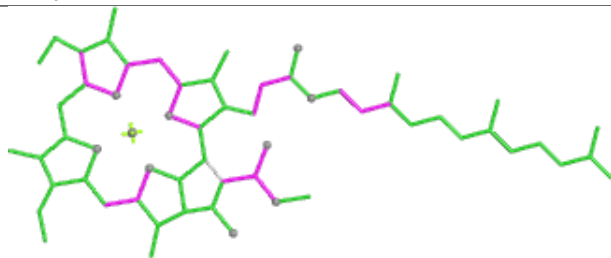
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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24	0	602	CLA	5	0
24	c	502	CLA	4	0
24	7	305	CLA	4	0
24	AB	303	CLA	3	0
24	BF	502	CLA	2	0
24	g	613	CLA	5	0
28	7	318	XAT	1	0
23	BJ	609	CHL	15	0
29	K	101	BCR	3	0
25	BQ	615	LUT	5	0
29	BE	601	BCR	6	0
23	6	607	CHL	7	0
24	b	605	CLA	6	0
29	v	619	BCR	6	0
23	A6	605	CHL	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.

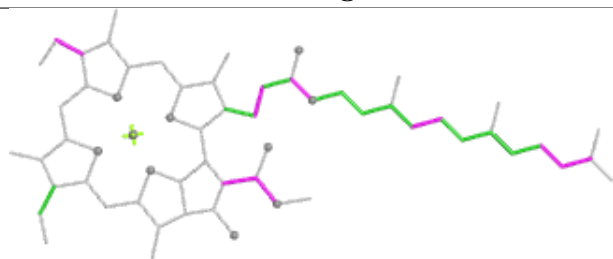
Ligand CLA y 311



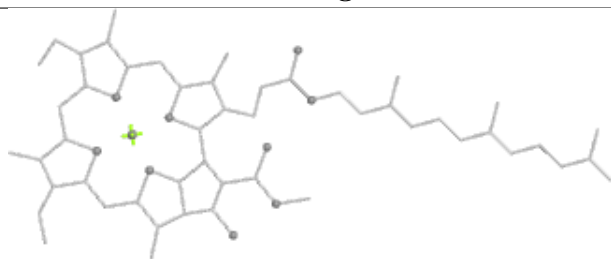
Bond lengths



Bond angles

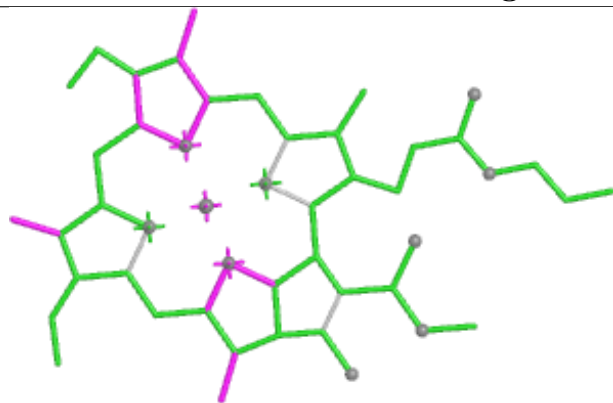


Torsions

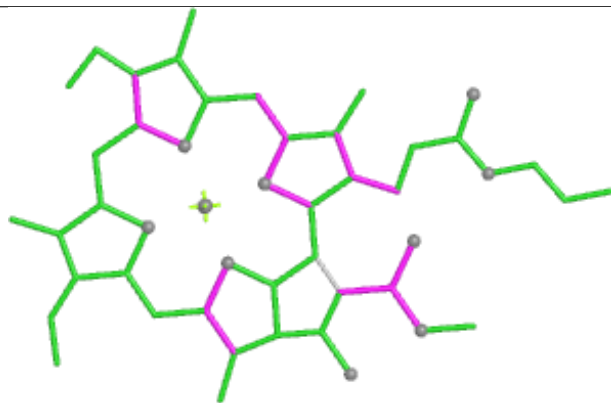


Rings

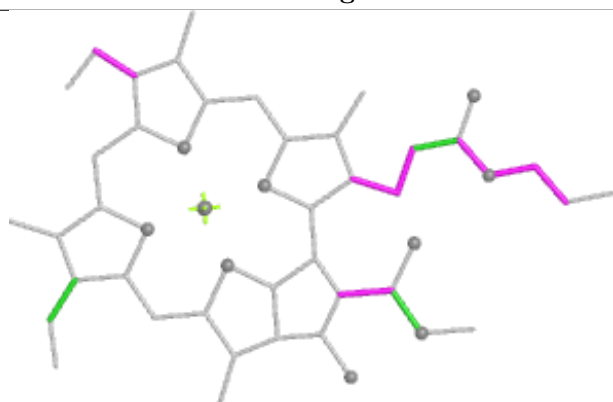
Ligand CLA BU 604



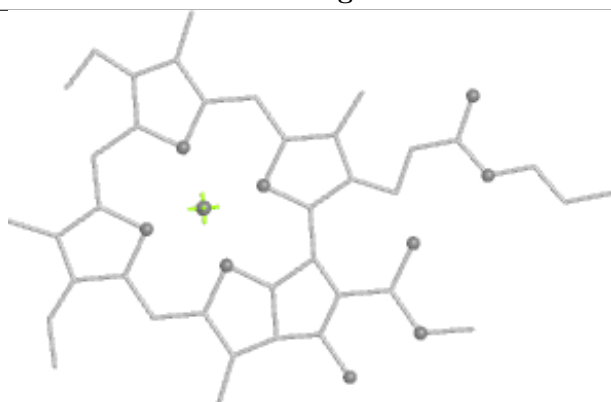
Bond lengths



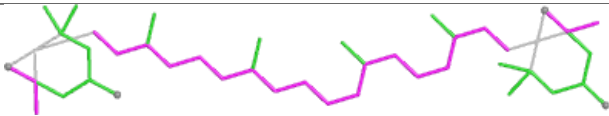
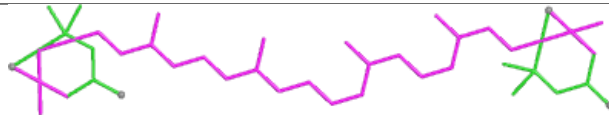
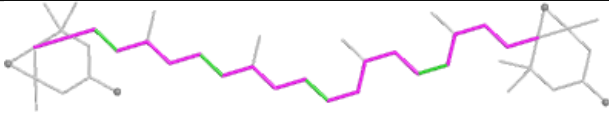
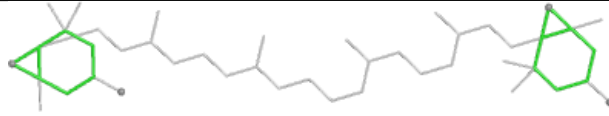
Bond angles

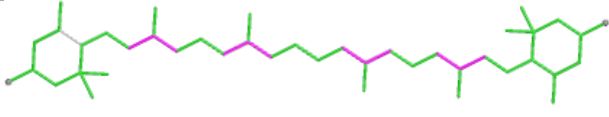
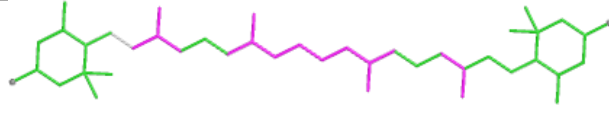
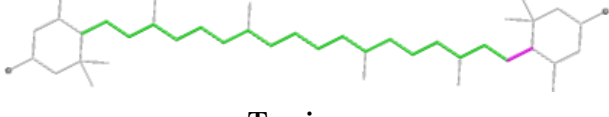
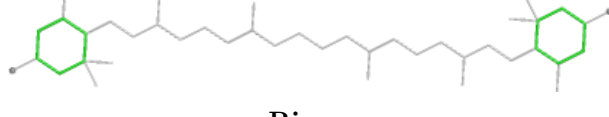


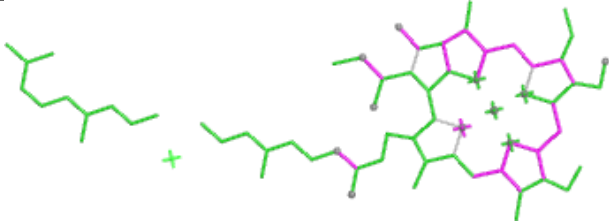
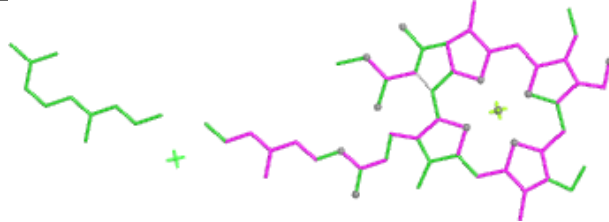
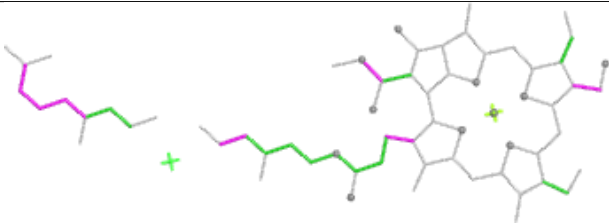
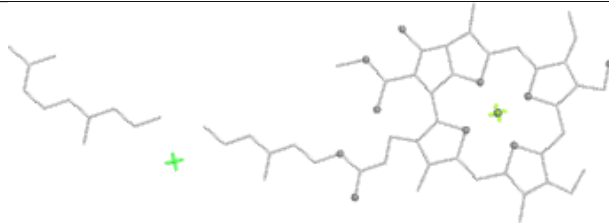
Torsions

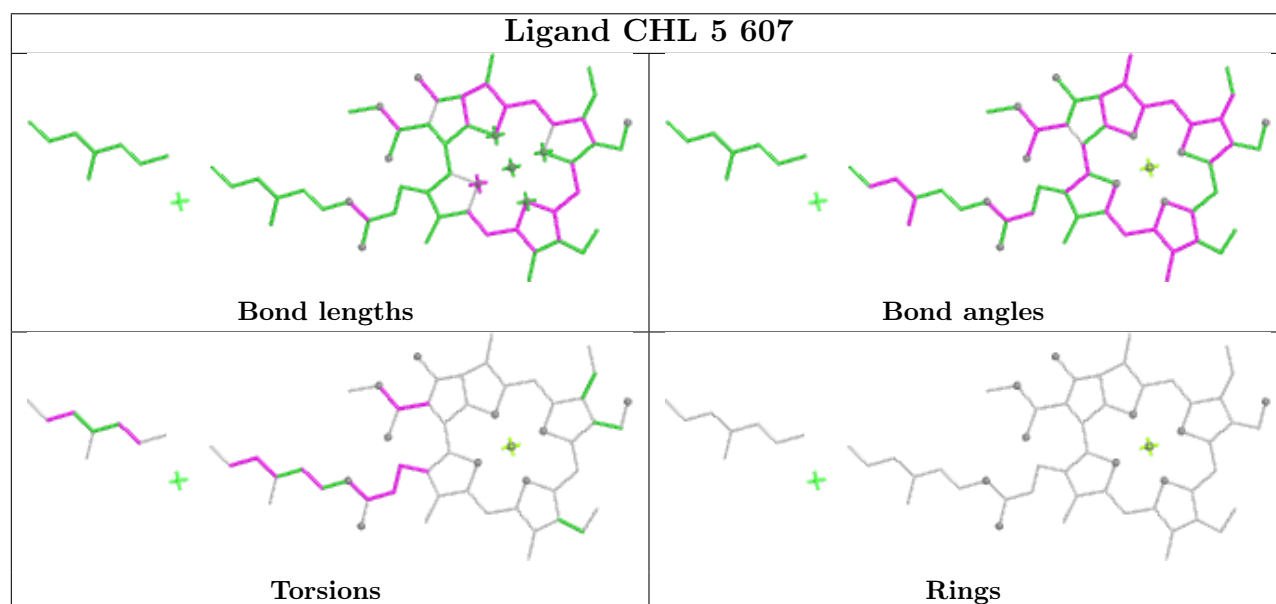
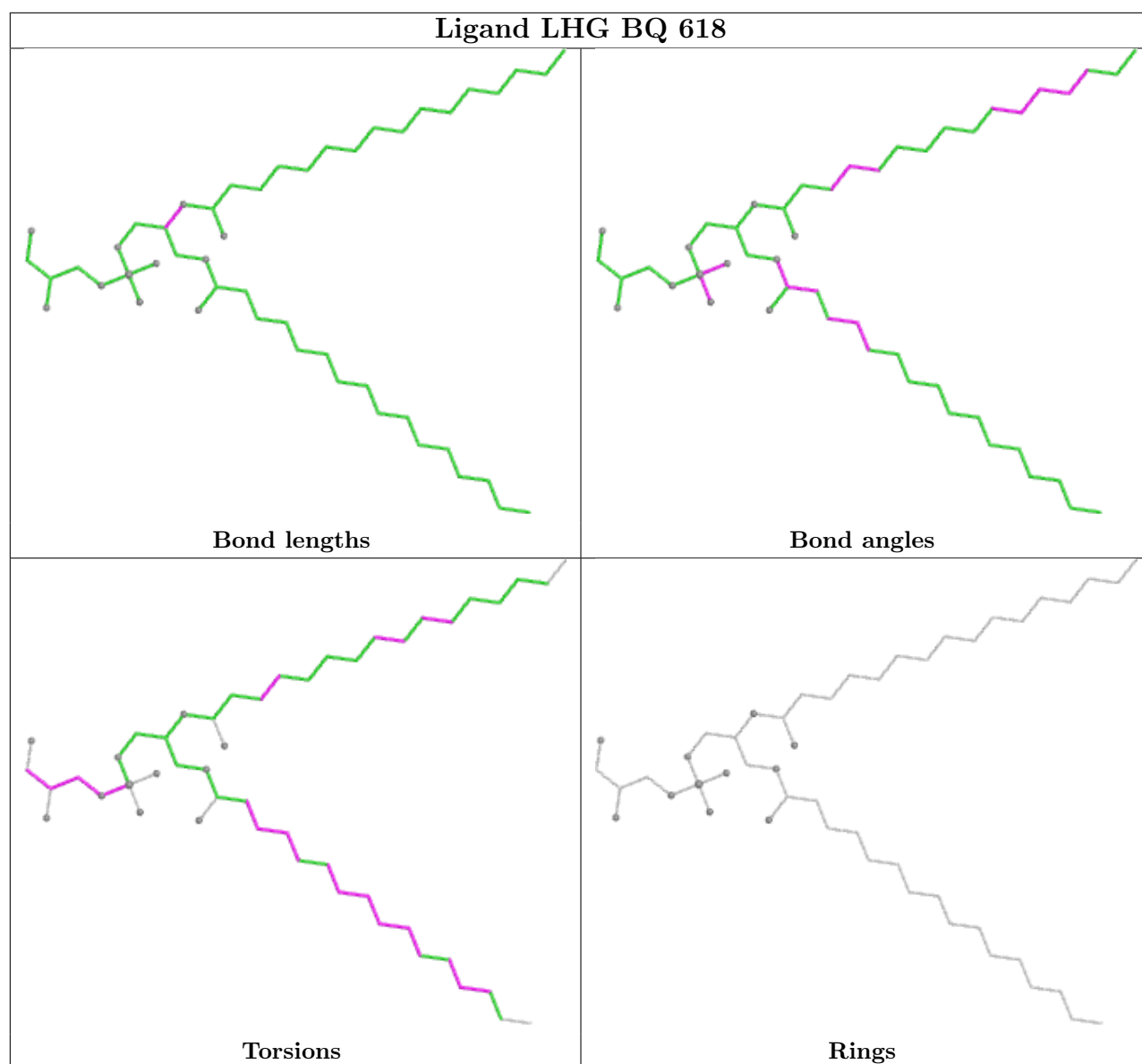


Rings

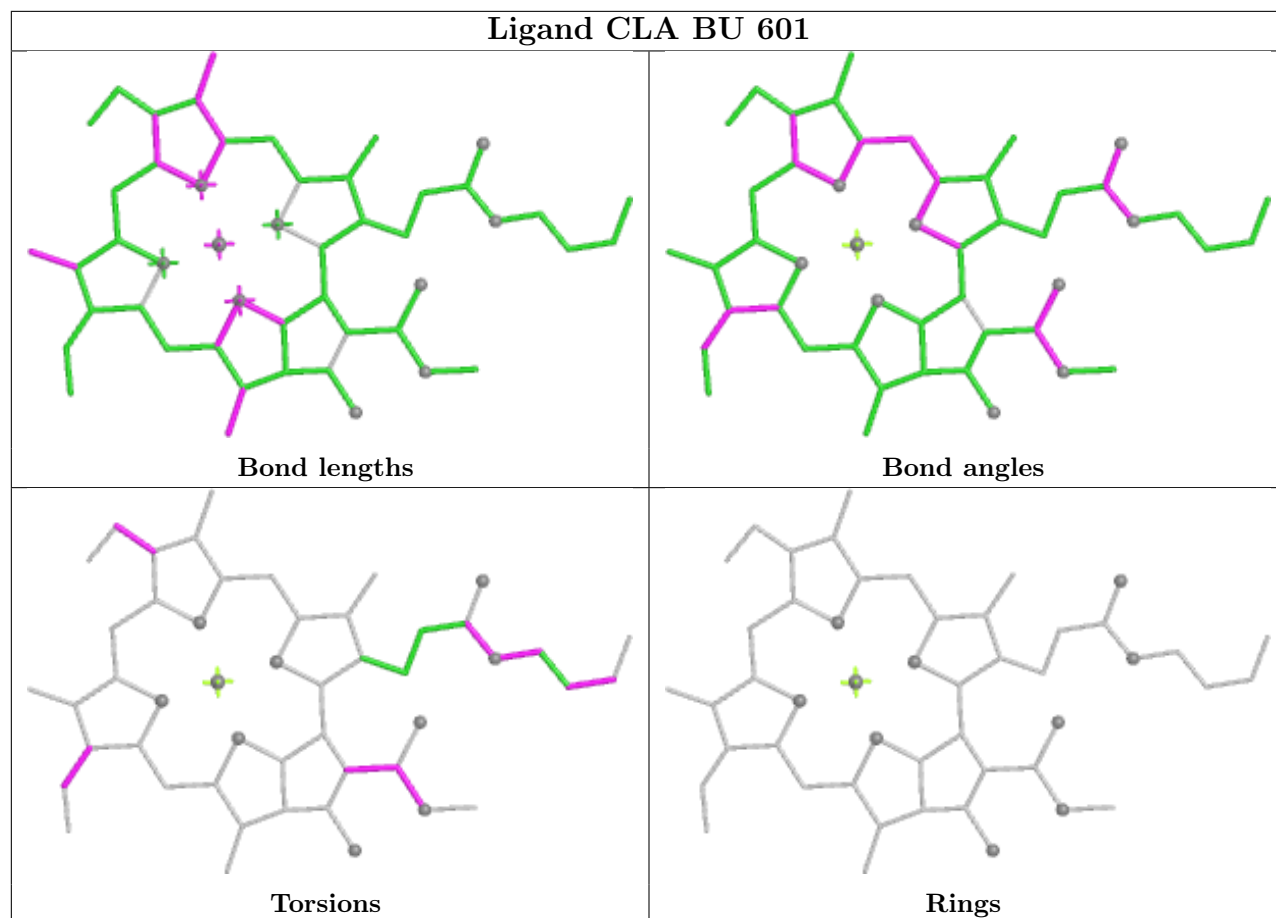
Ligand XAT Y 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT n 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

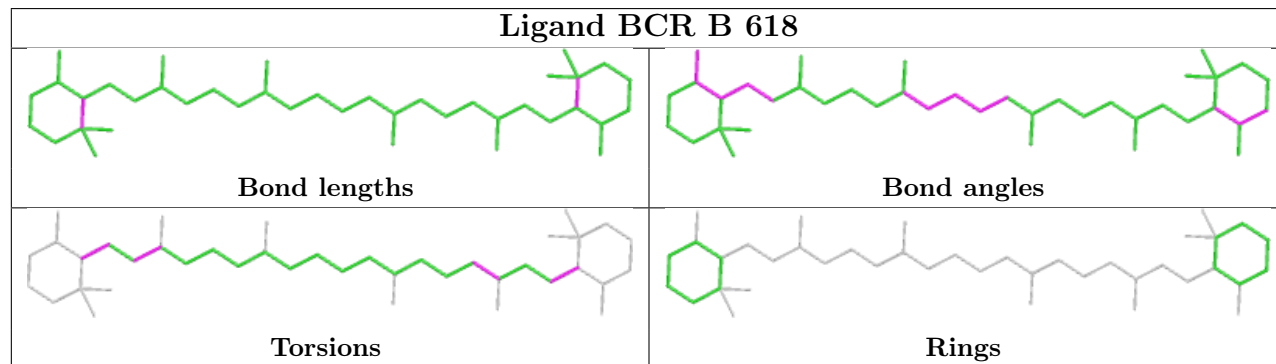
Ligand CHL n 608	
	
Bond lengths	Bond angles
	
Torsions	Rings



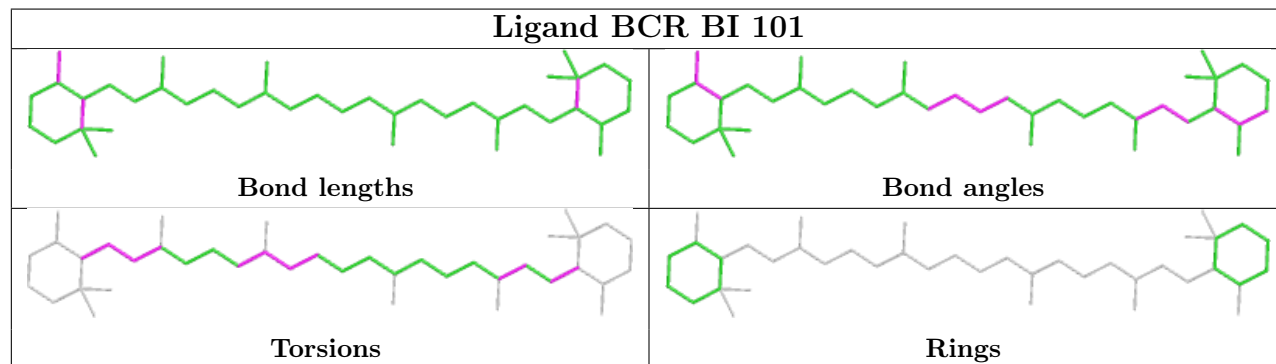
Ligand CLA BU 601

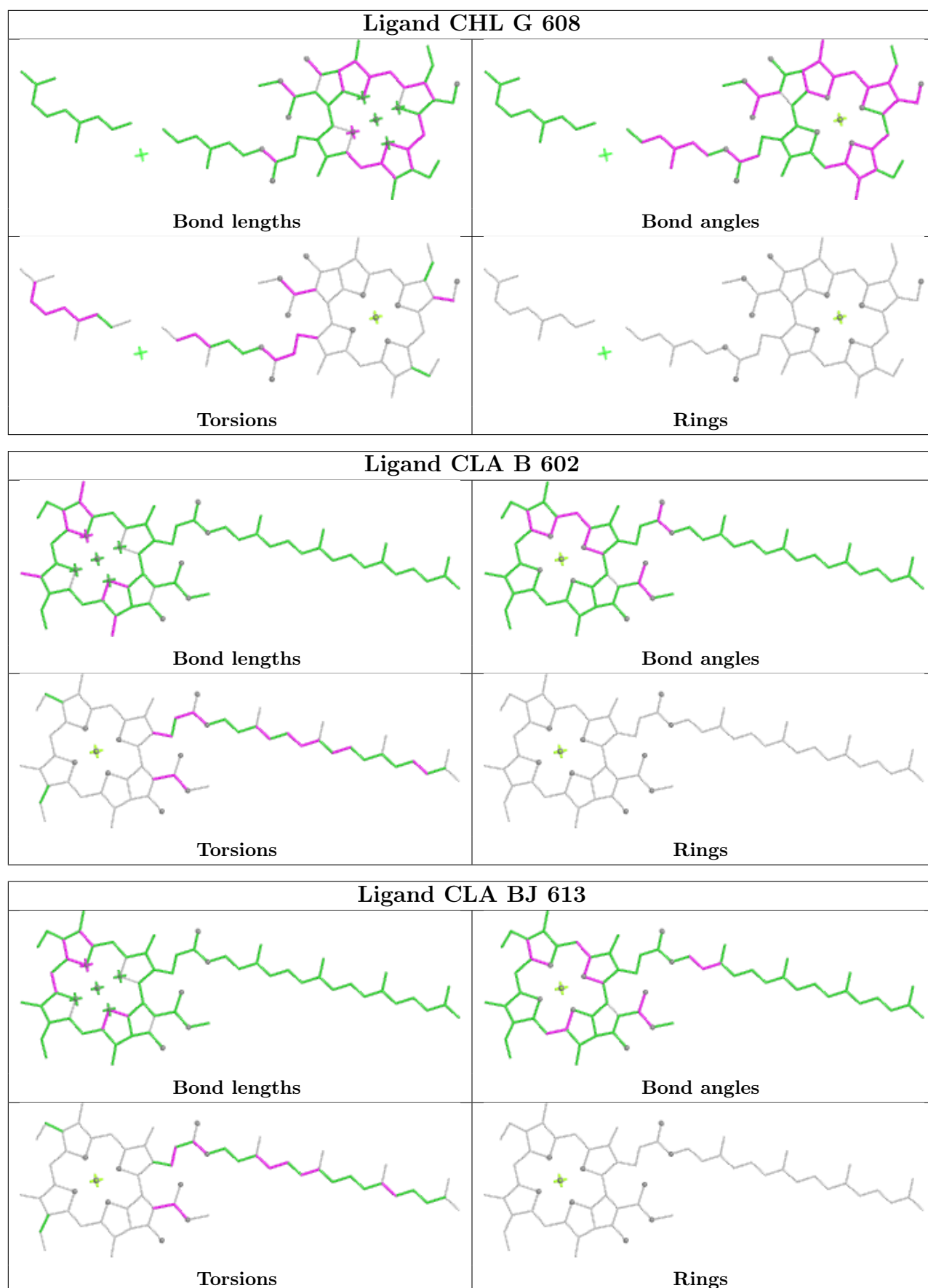


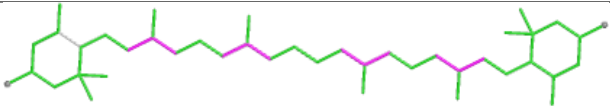
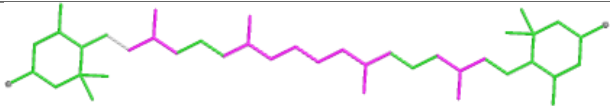
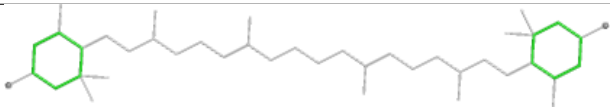
Ligand BCR B 618

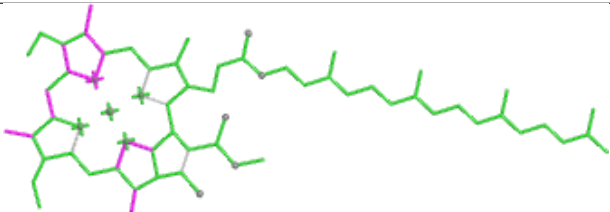
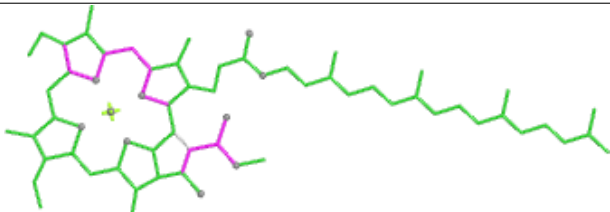
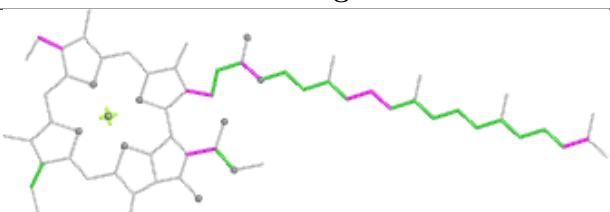
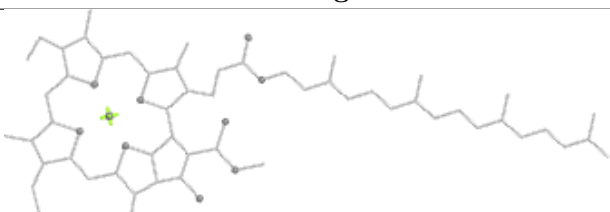


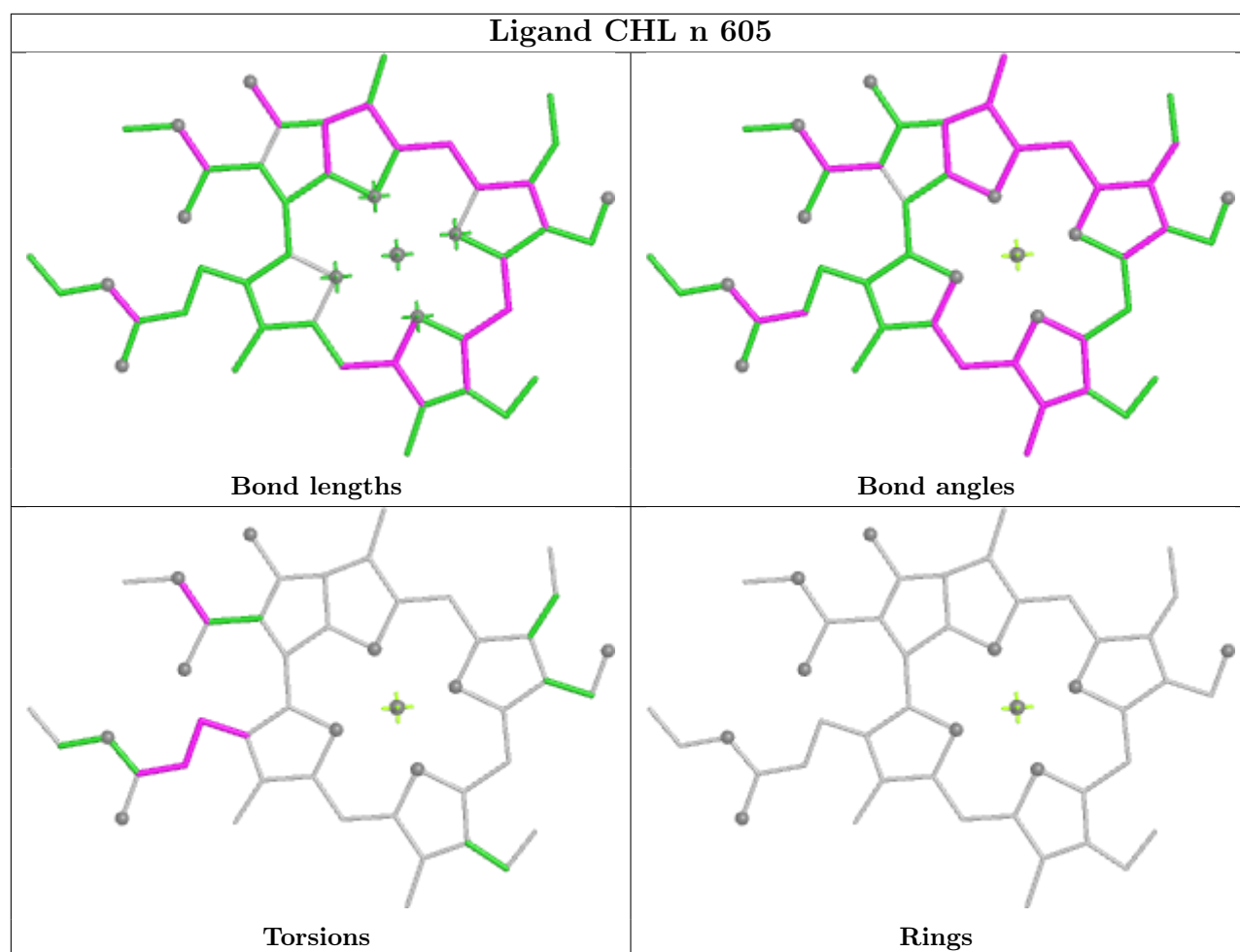
Ligand BCR BI 101



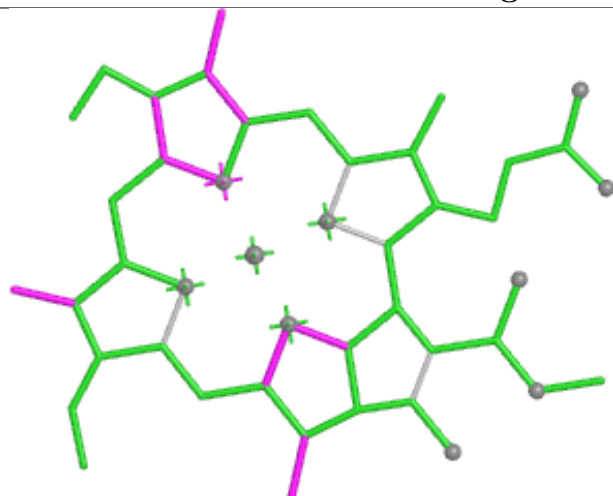


Ligand LUT y 317			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

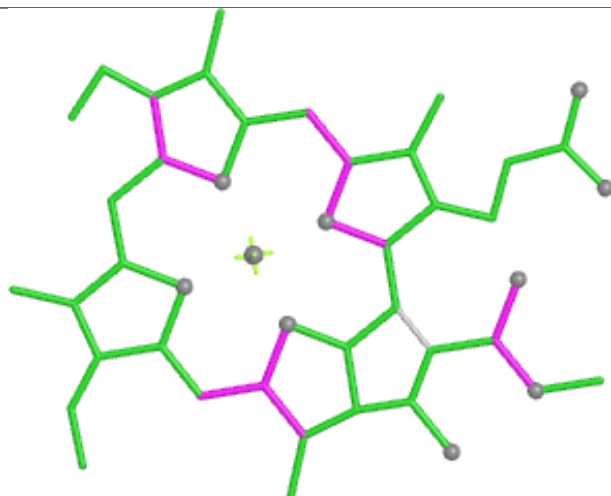
Ligand CLA c 512			
			
Bond lengths	Bond angles		
			
Torsions	Rings		



Ligand CLA BU 614



Bond lengths



Bond angles

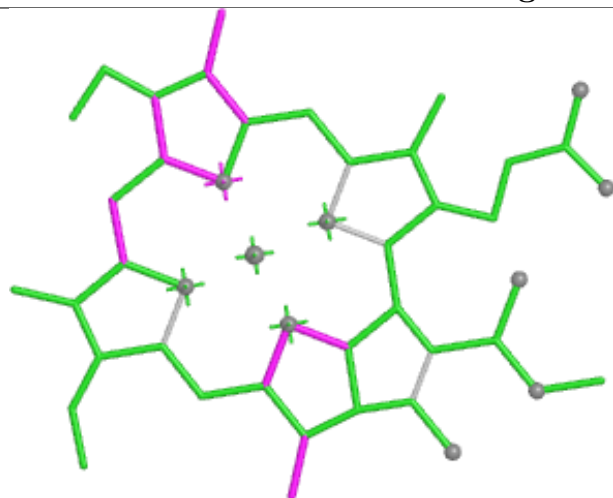


Torsions

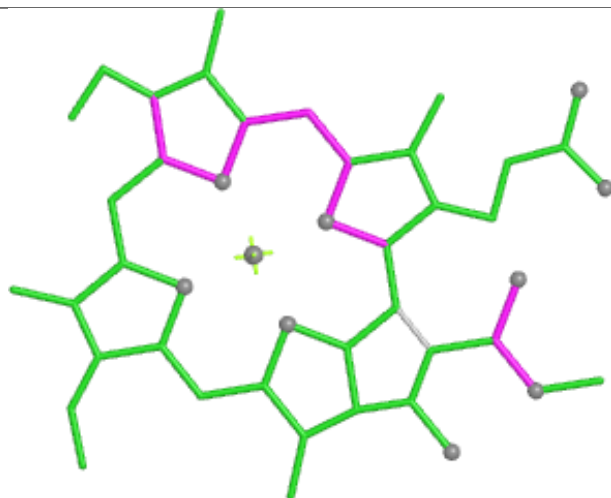


Rings

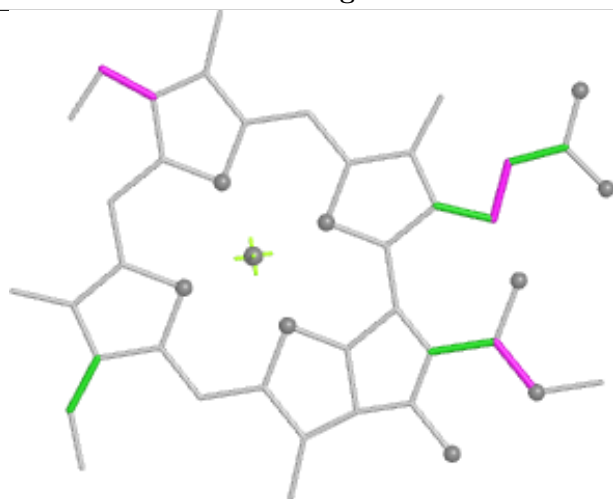
Ligand CLA 7 315



Bond lengths



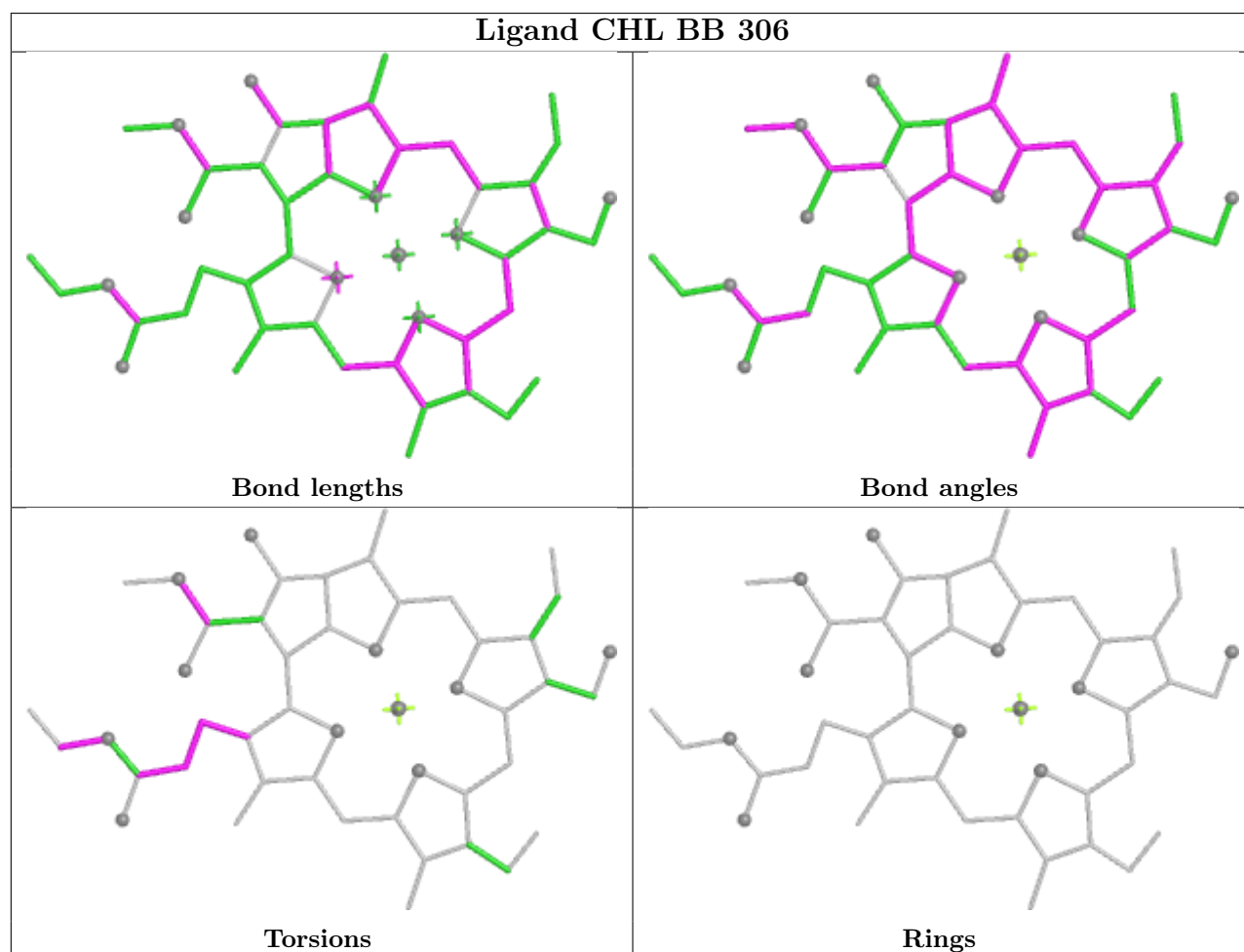
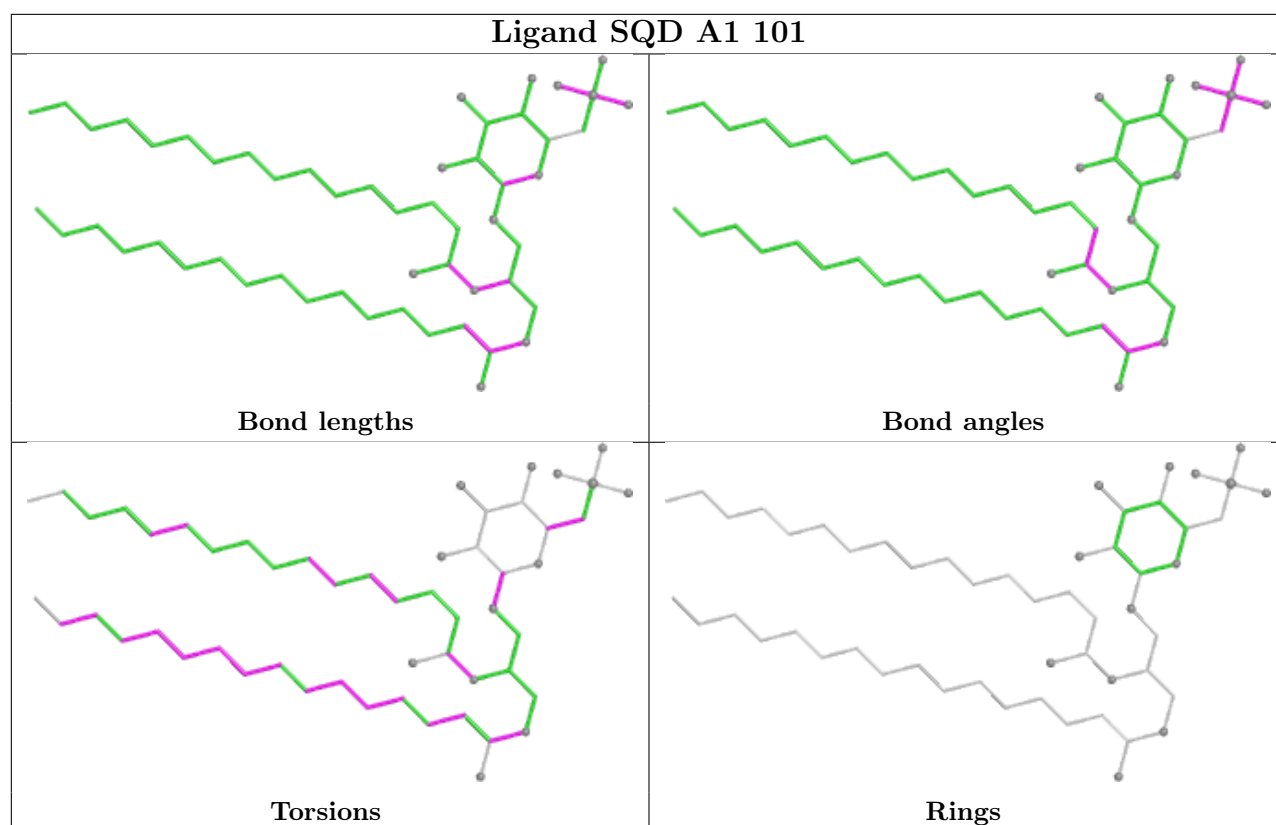
Bond angles



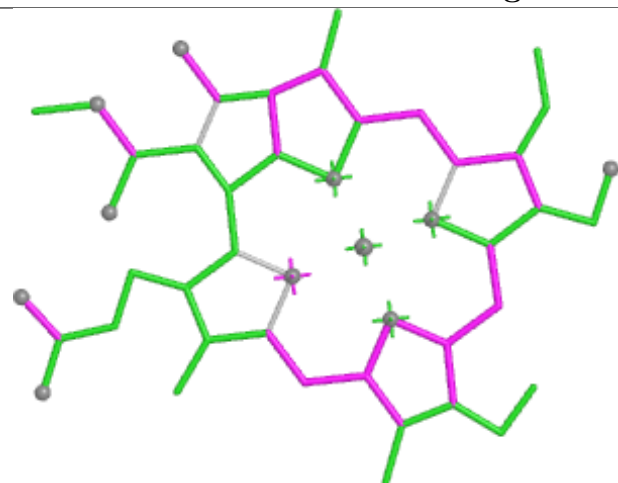
Torsions



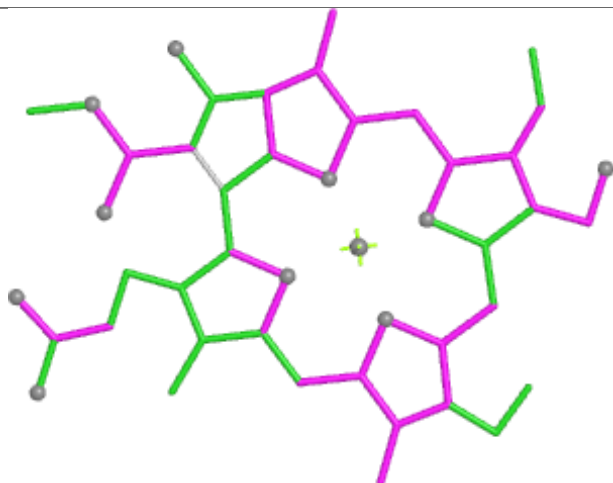
Rings



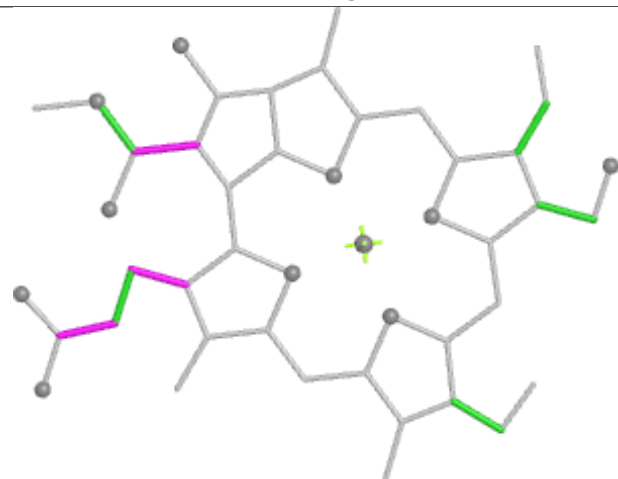
Ligand CHL AA 302



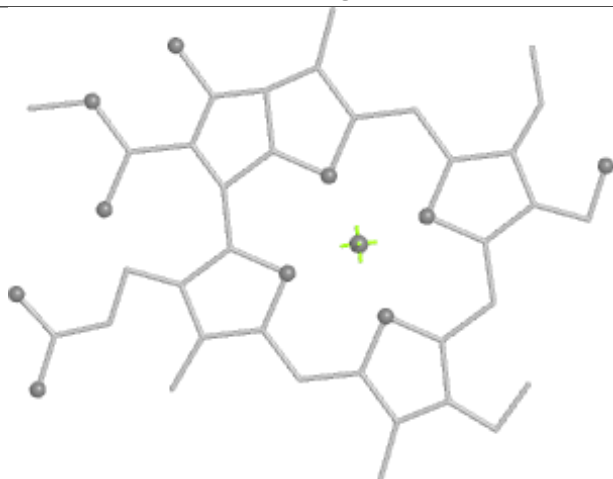
Bond lengths



Bond angles

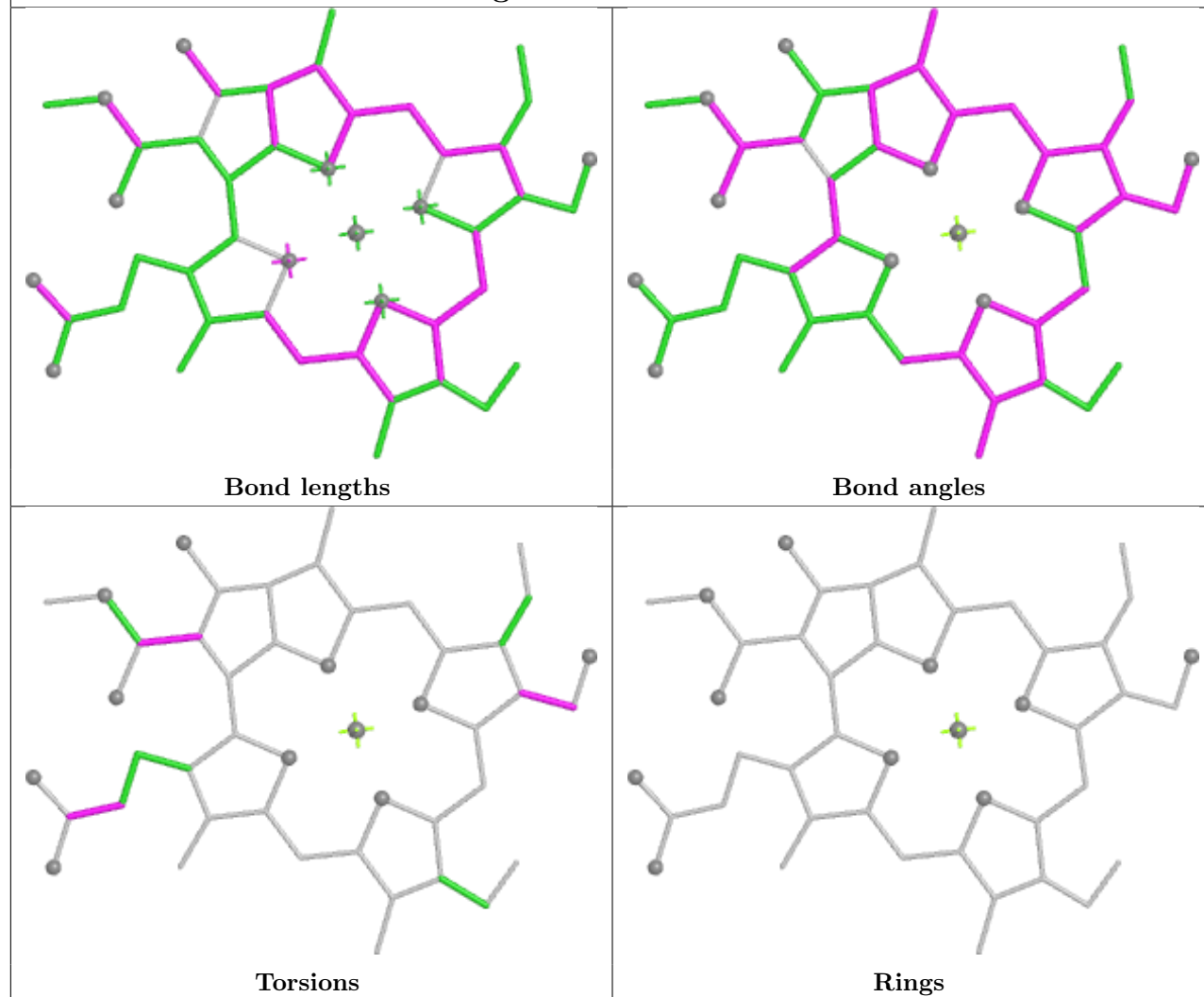


Torsions

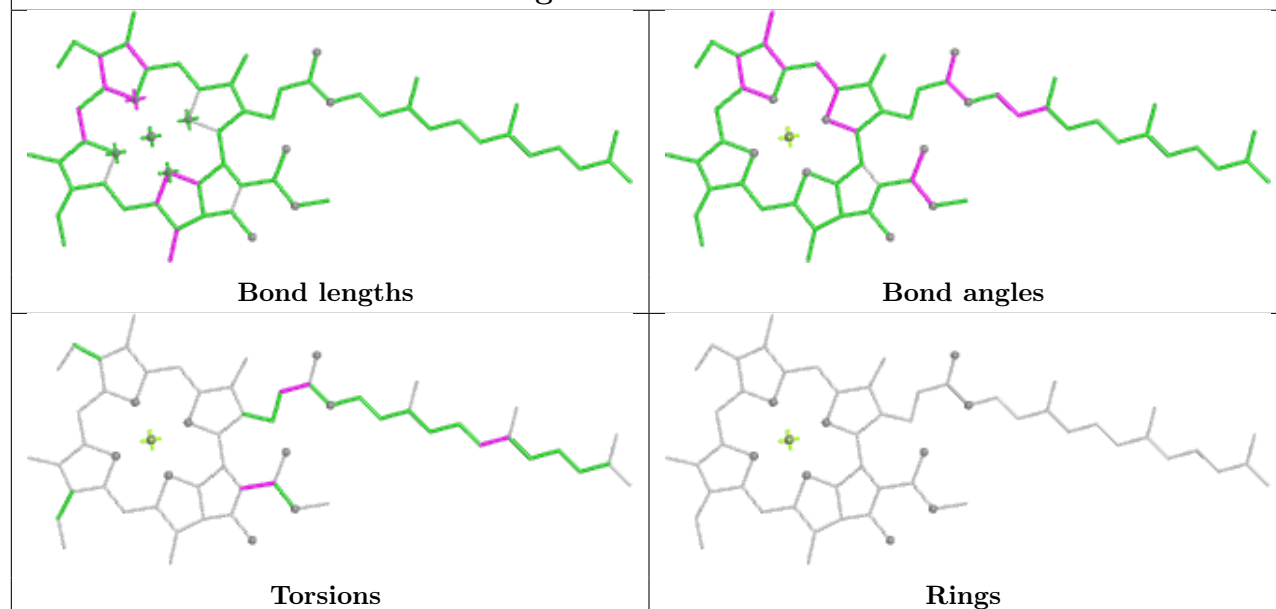


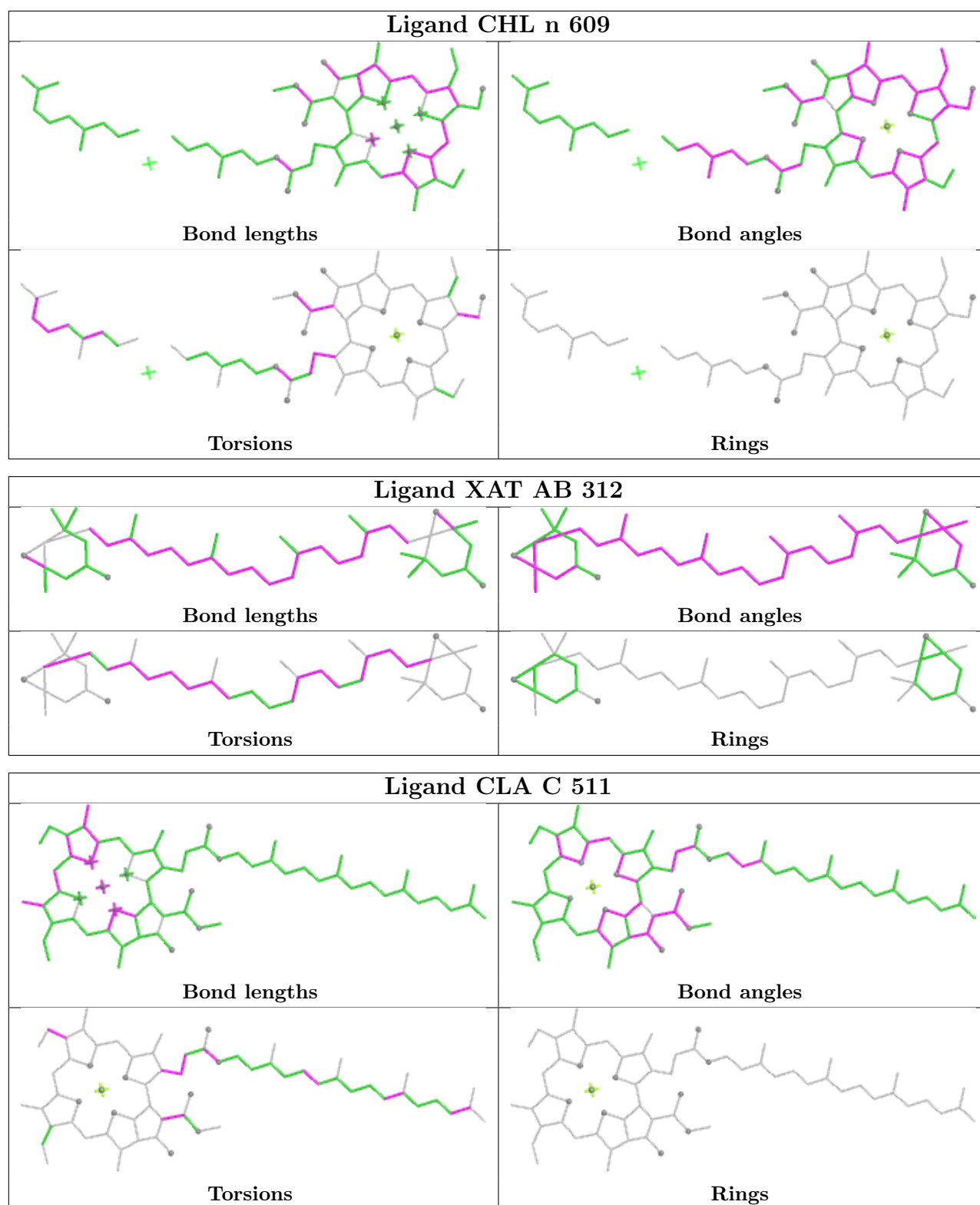
Rings

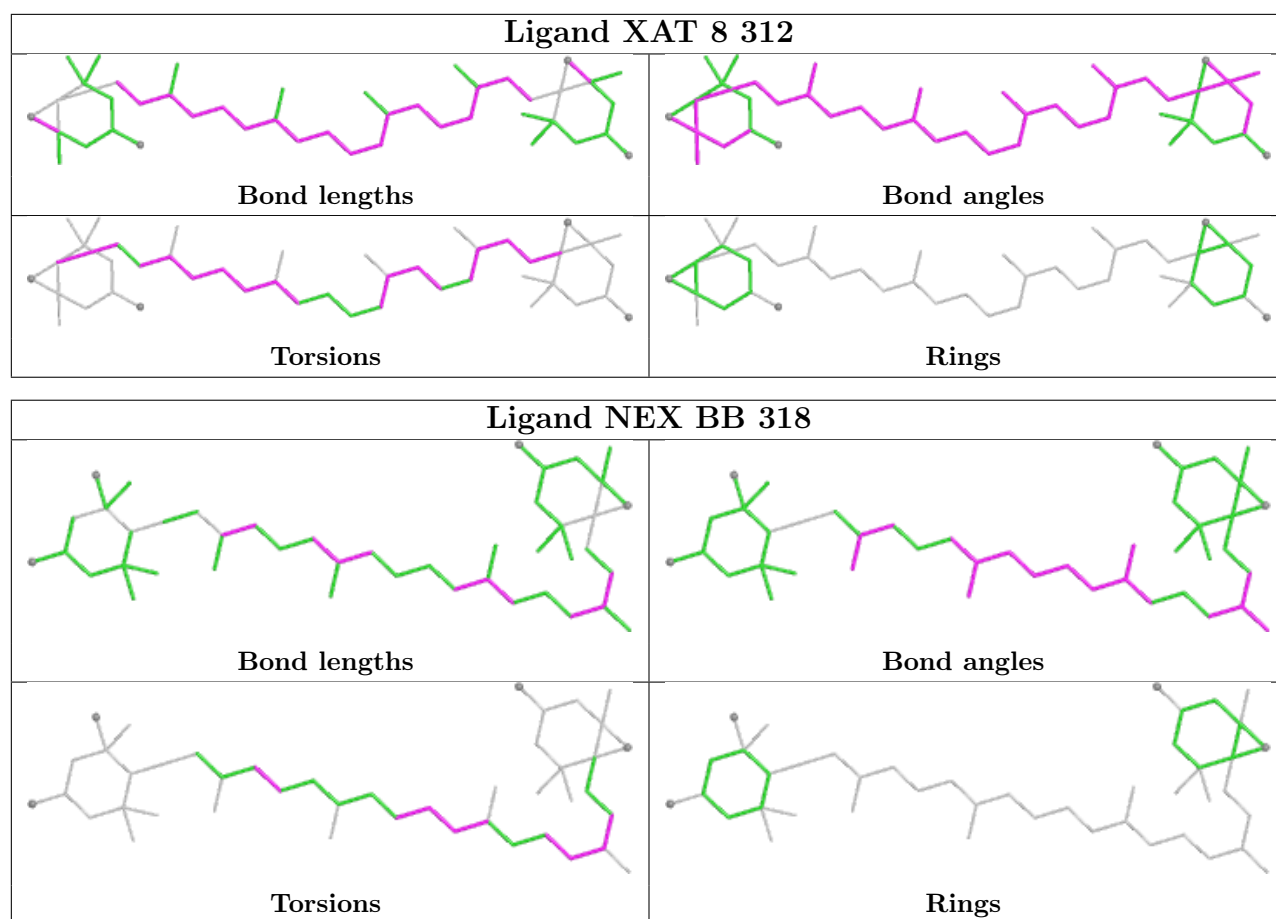
Ligand CHL A6 601



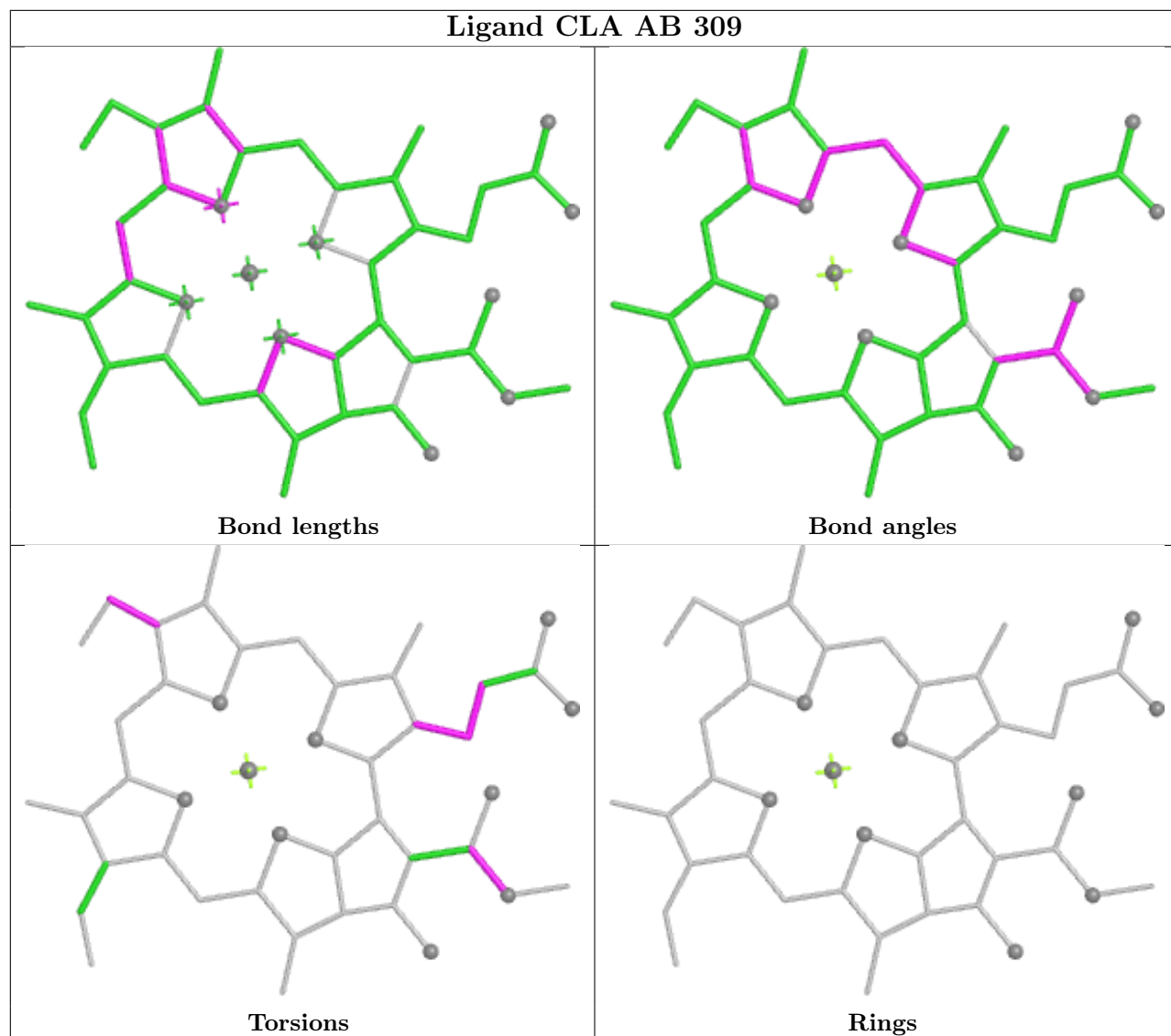
Ligand CLA n 612



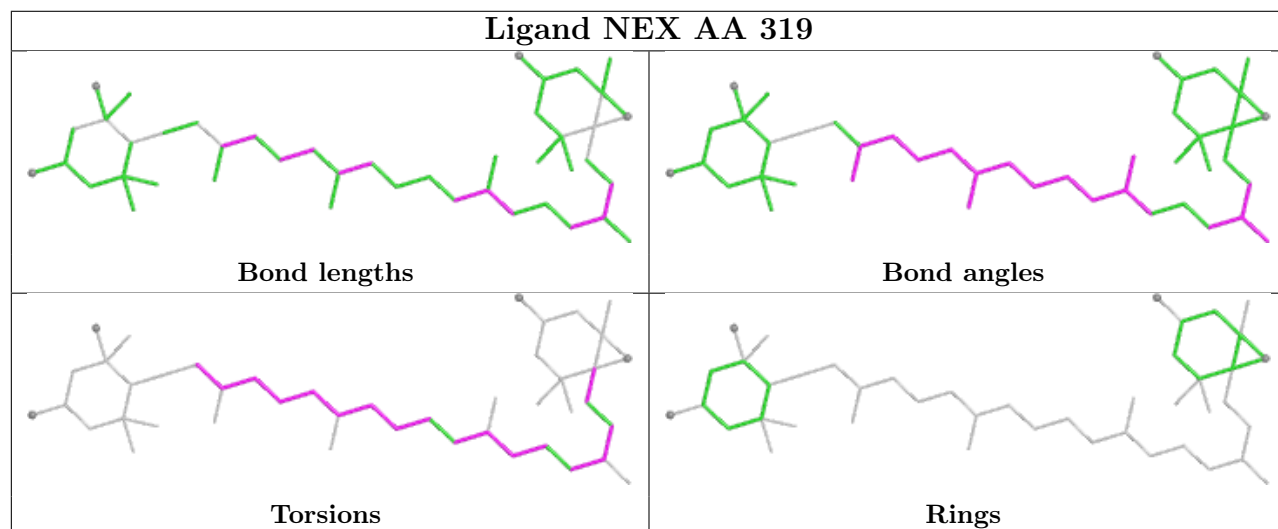




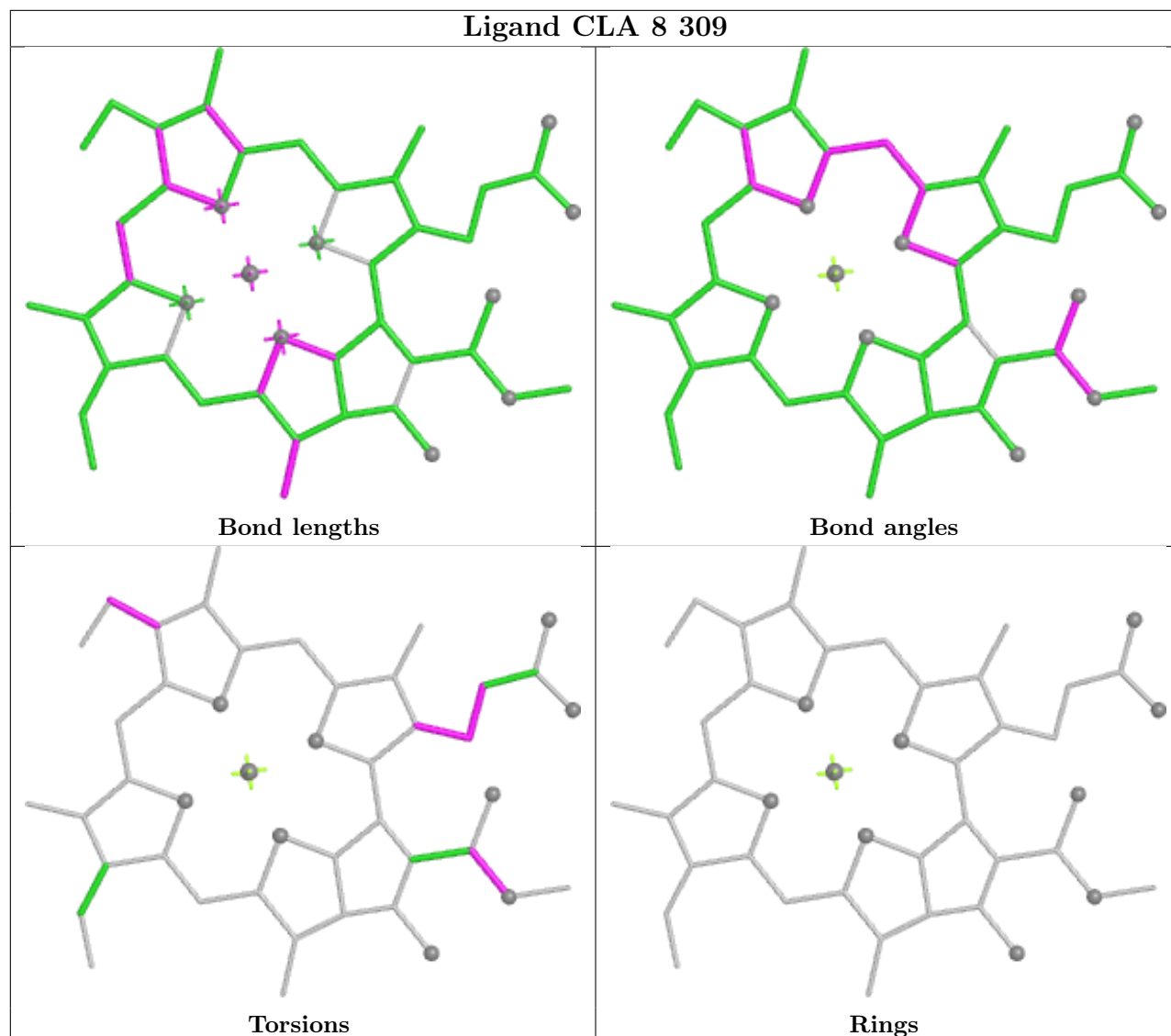
Ligand CLA AB 309



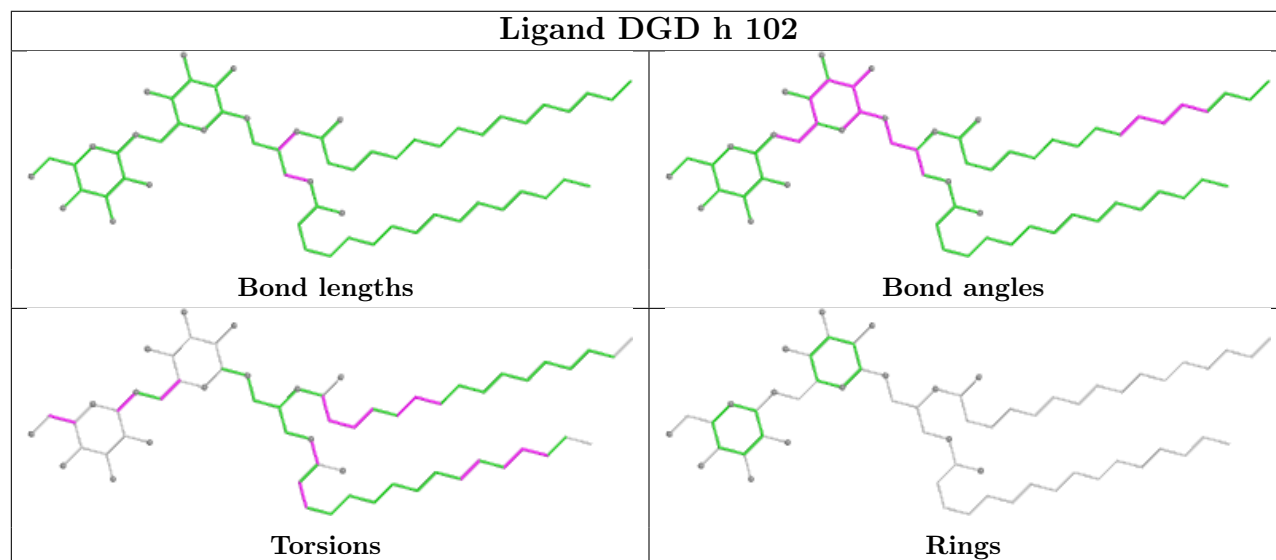
Ligand NEX AA 319

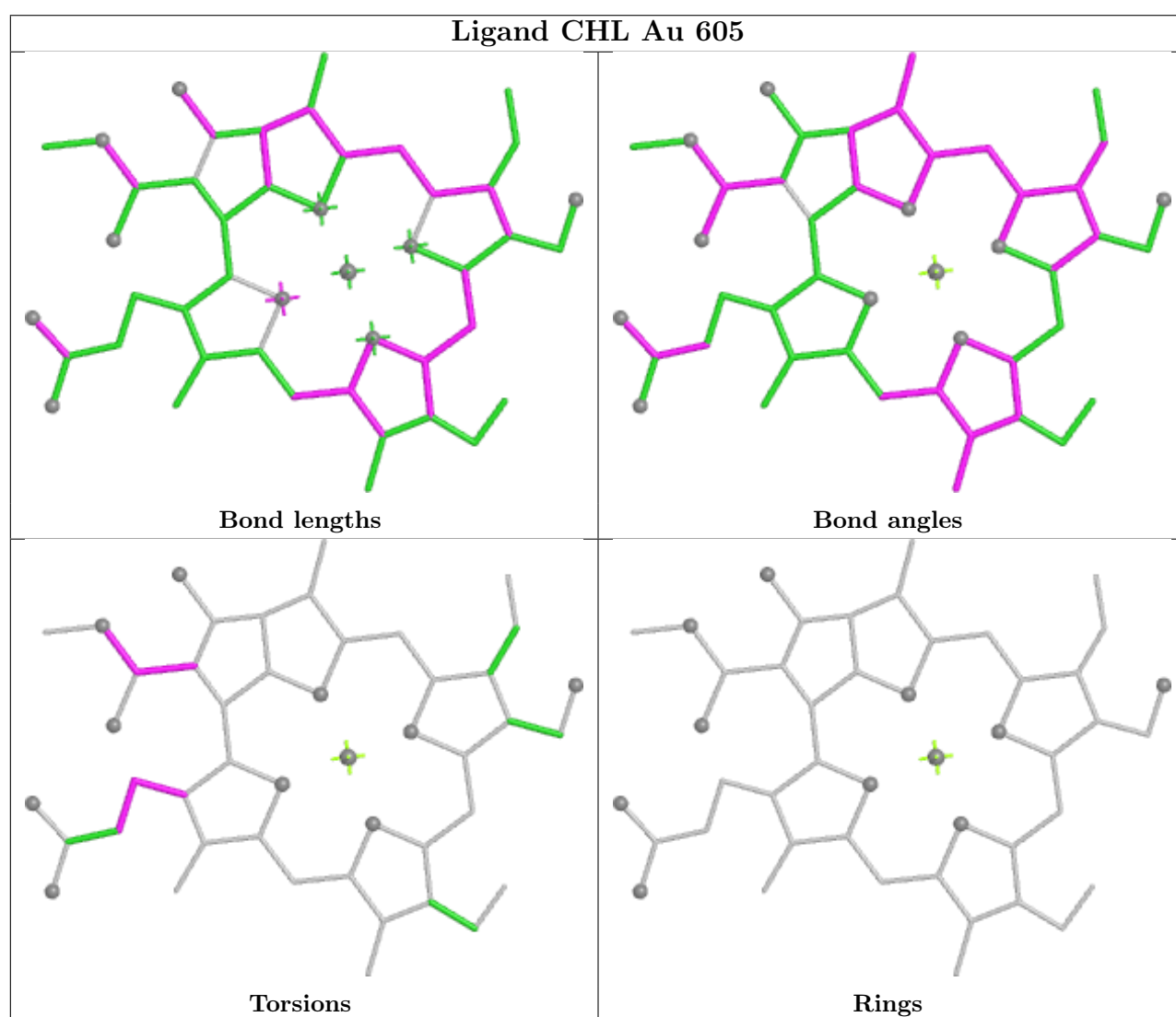
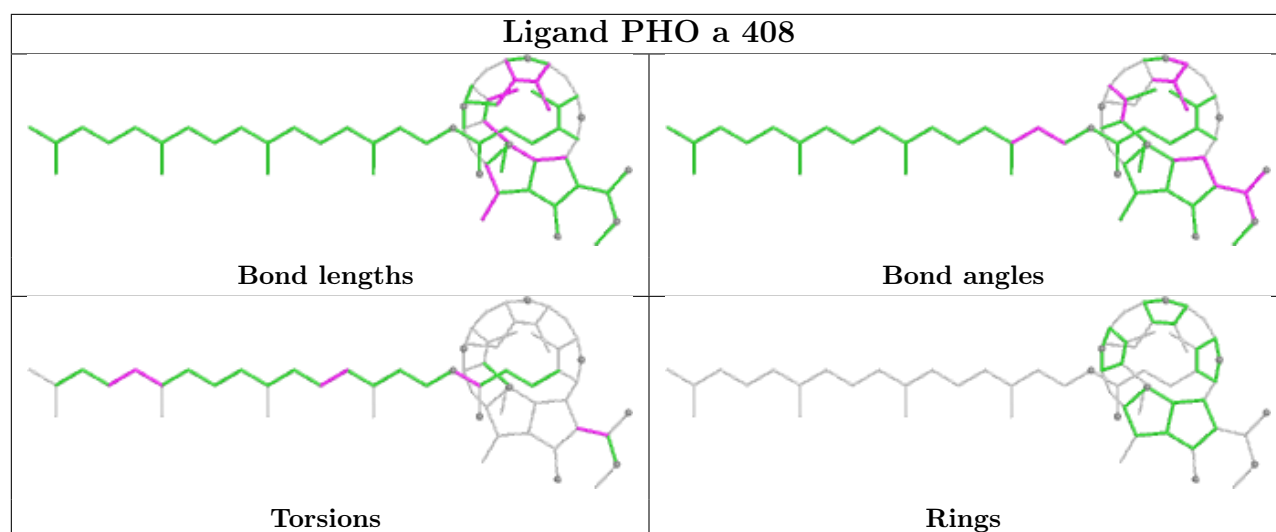


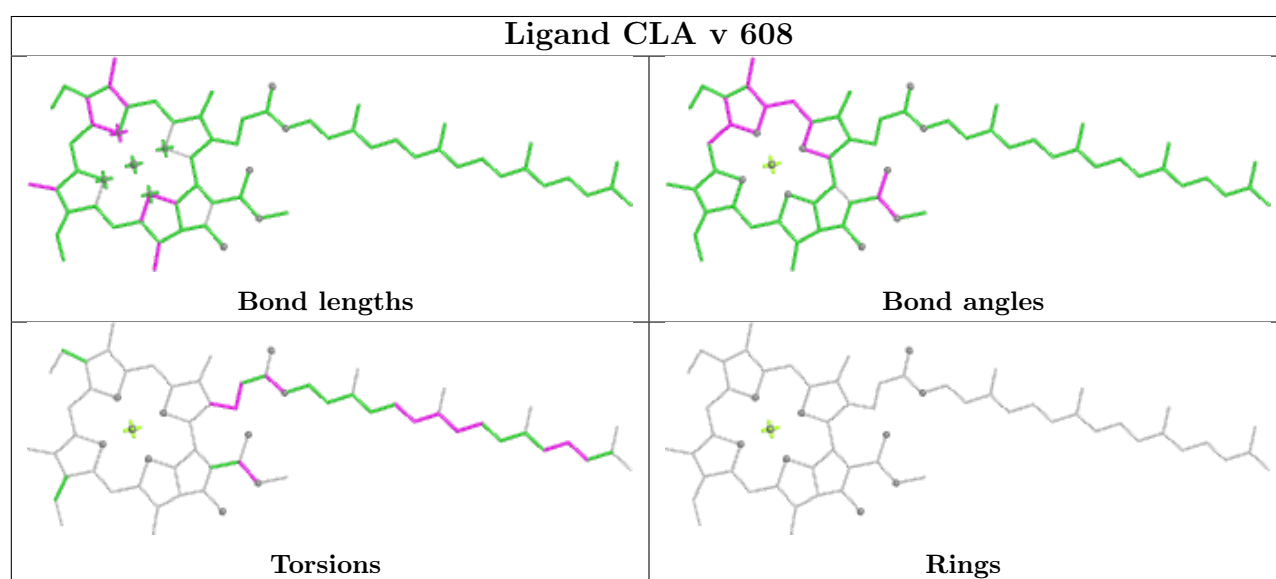
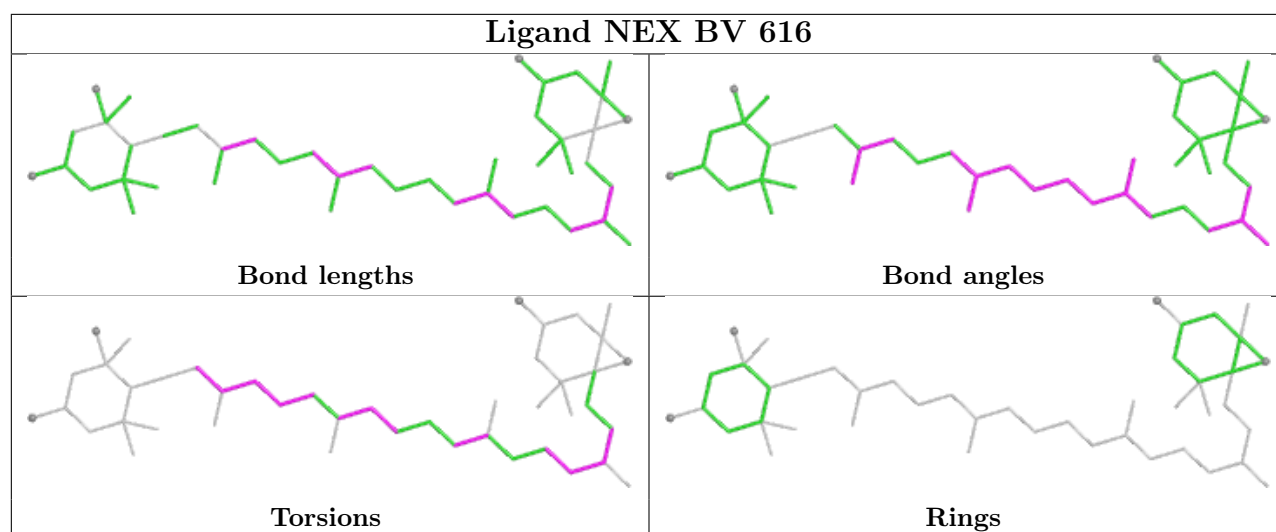
Ligand CLA 8 309

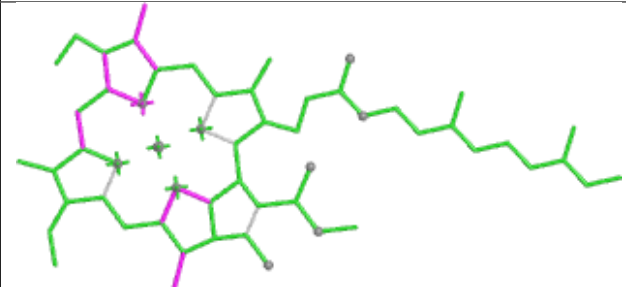
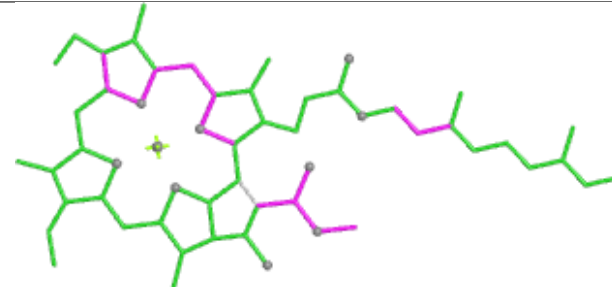
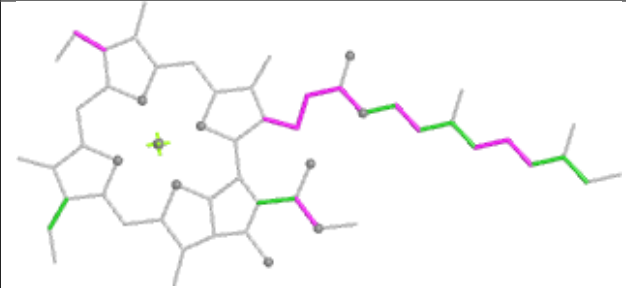
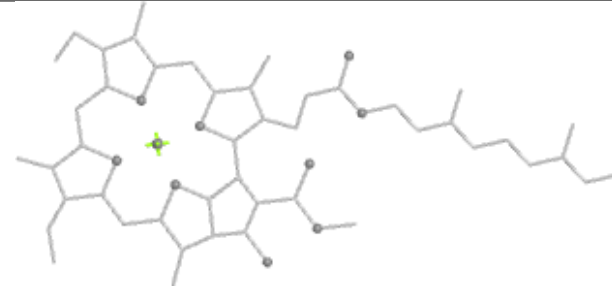


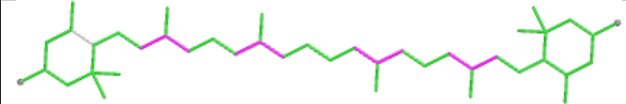
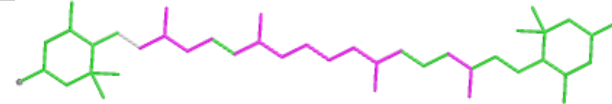
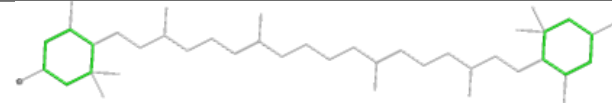
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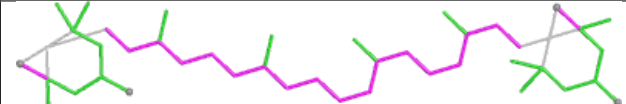
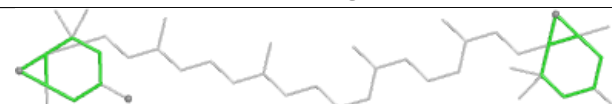


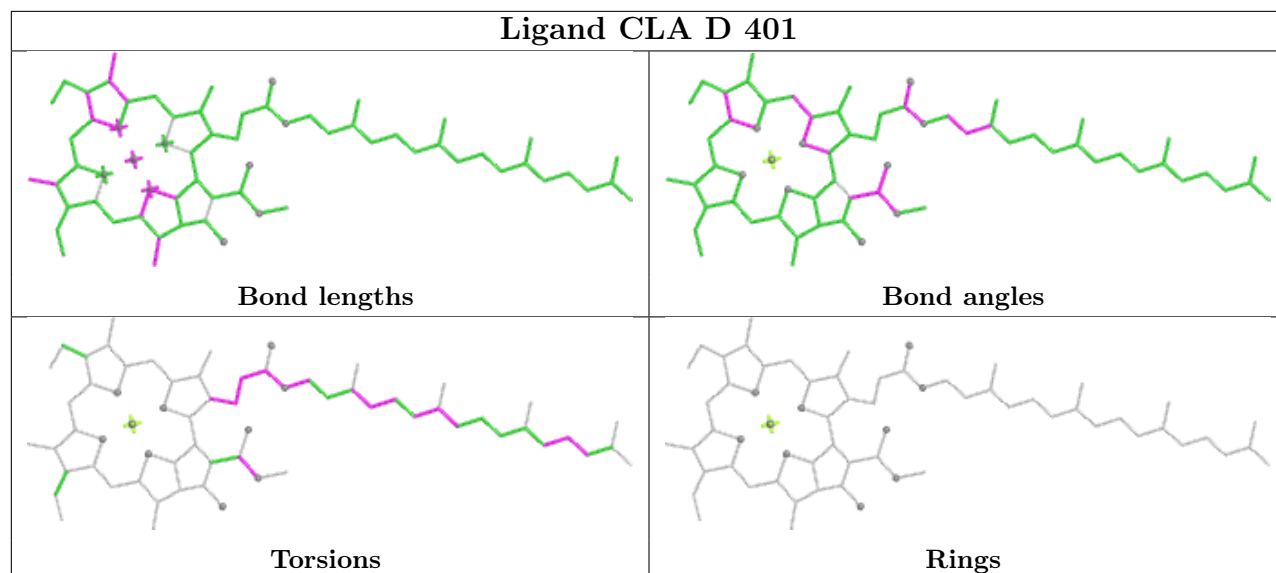
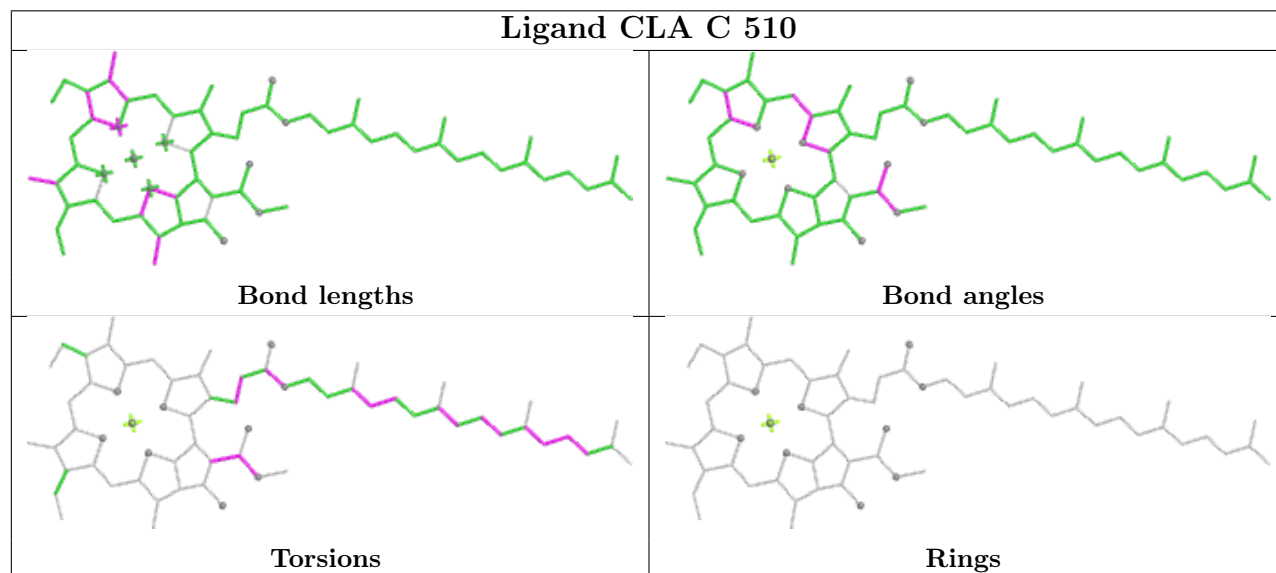
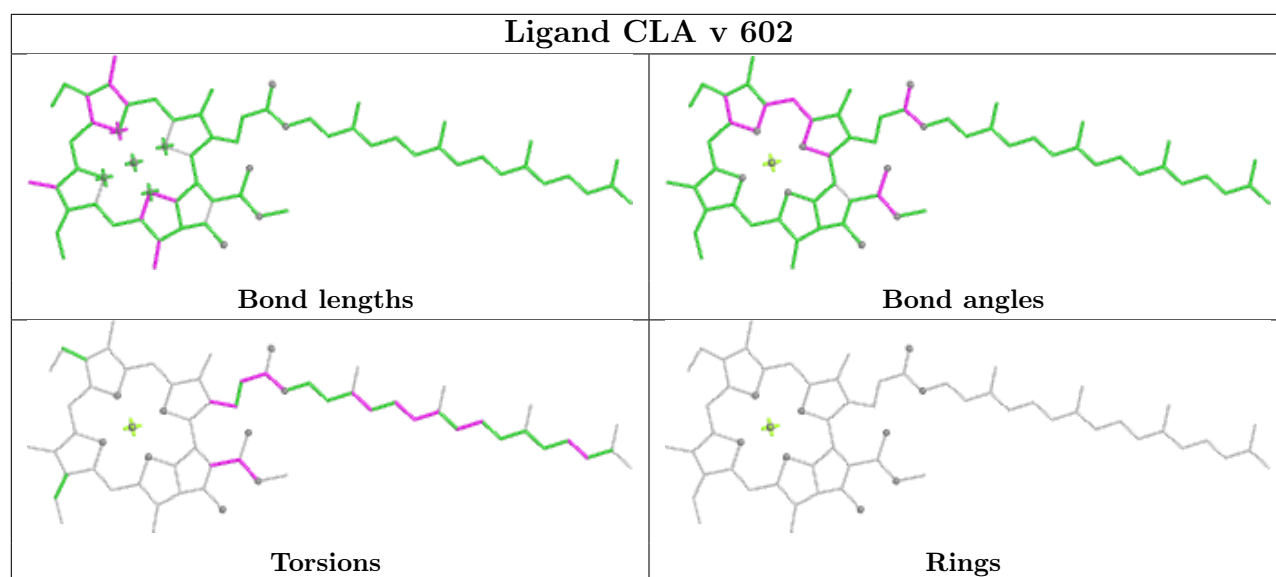


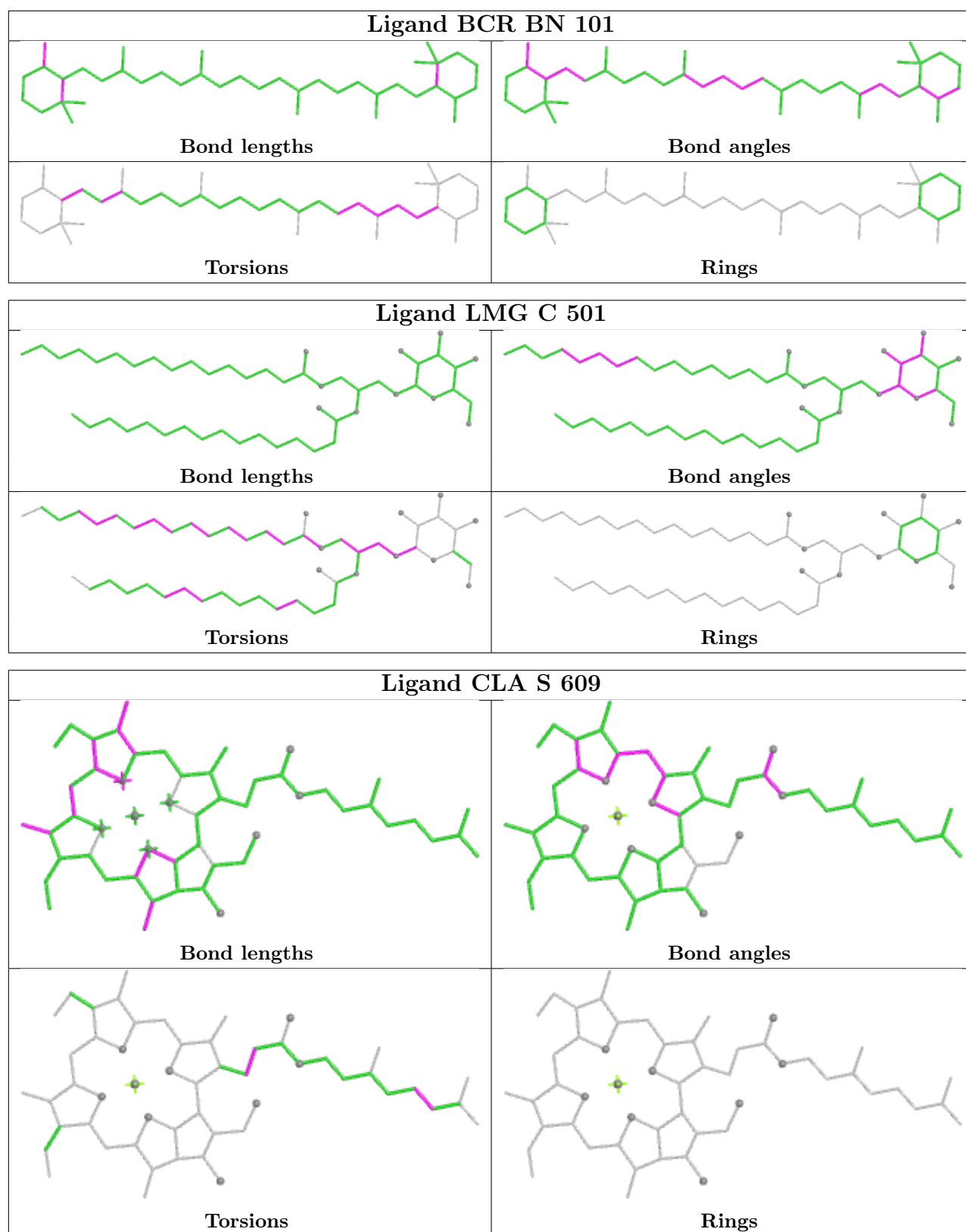


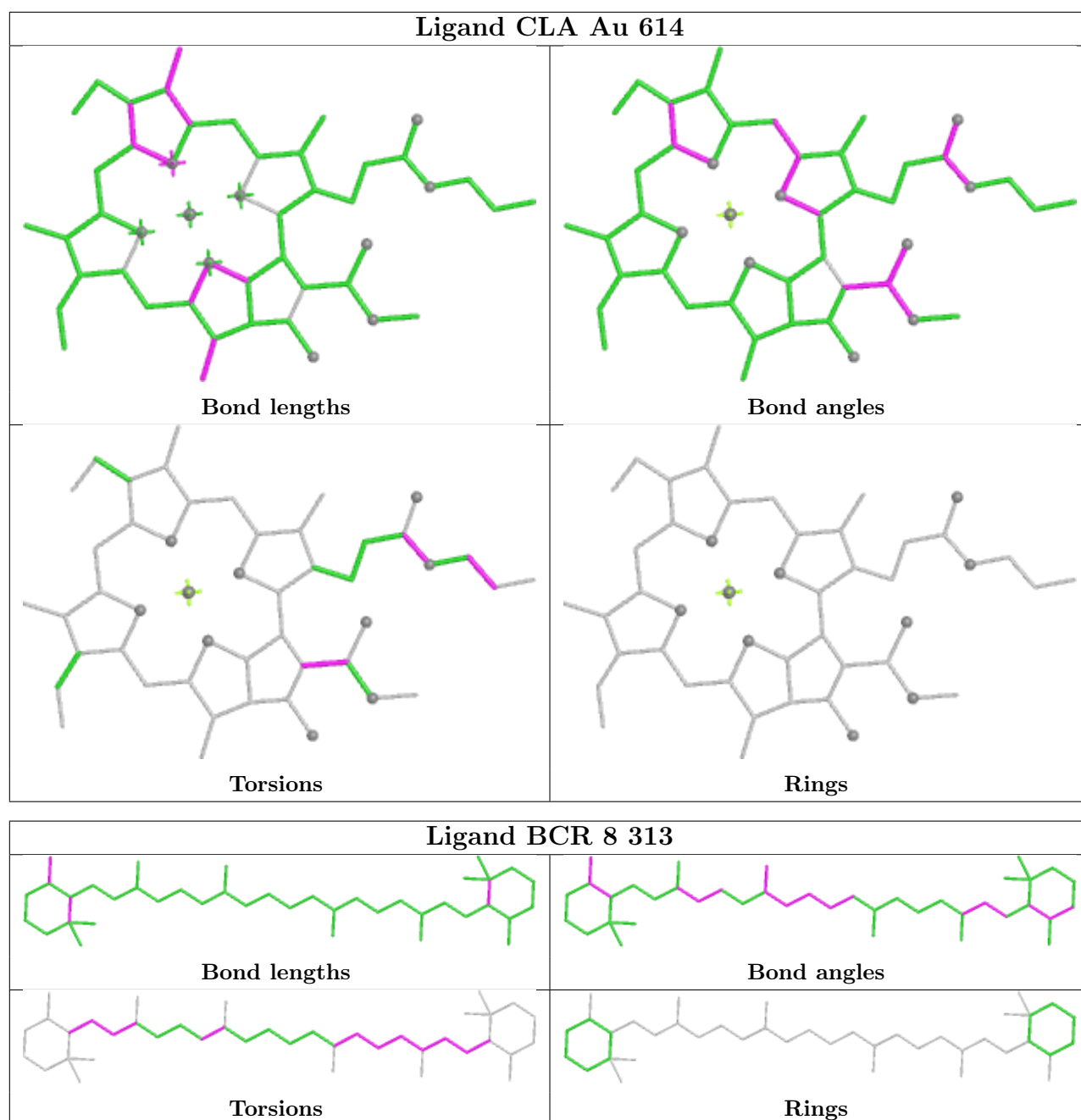
Ligand CLA BV 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

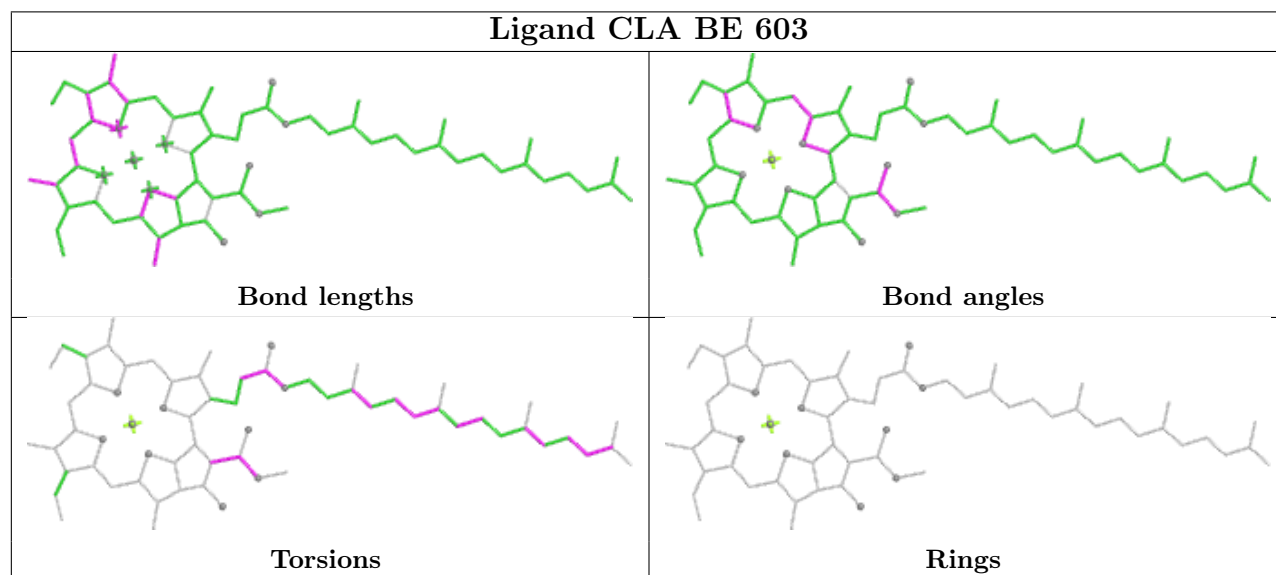
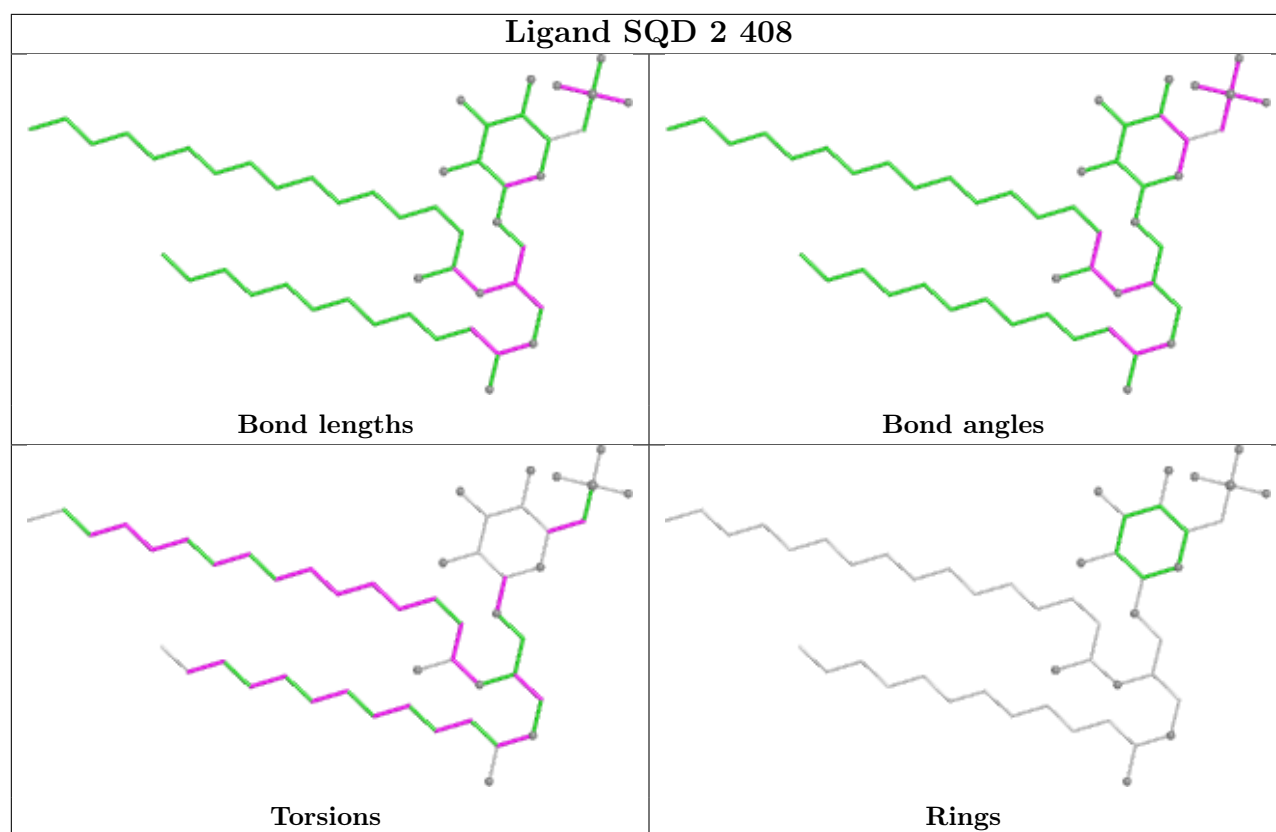
Ligand LUT S 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT BU 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

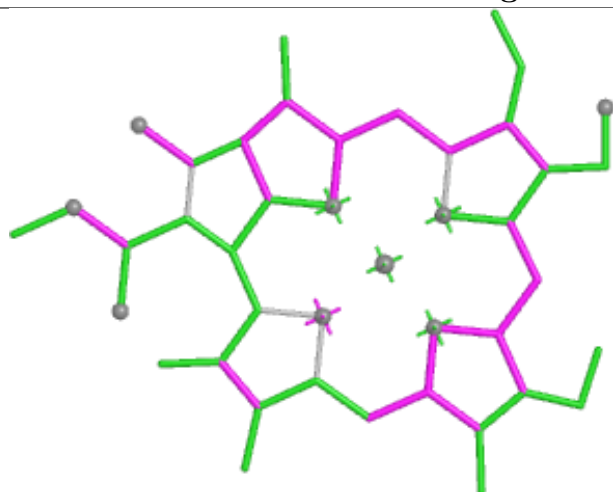








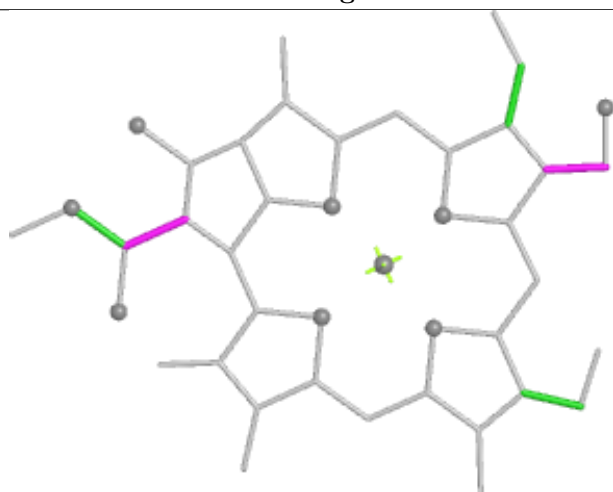
Ligand CHL BU 613



Bond lengths



Bond angles

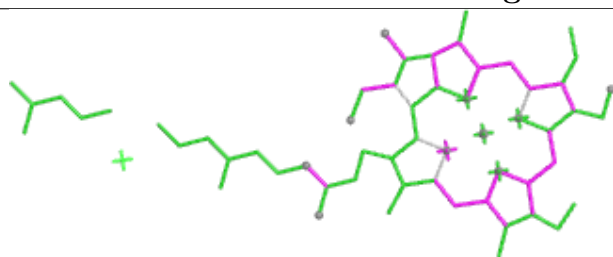


Torsions

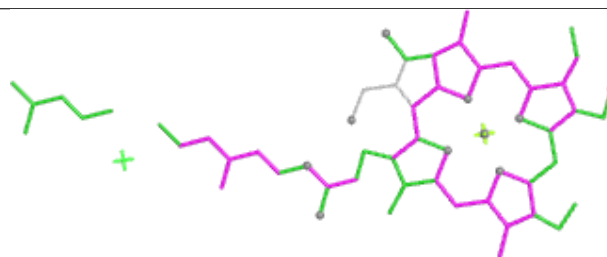


Rings

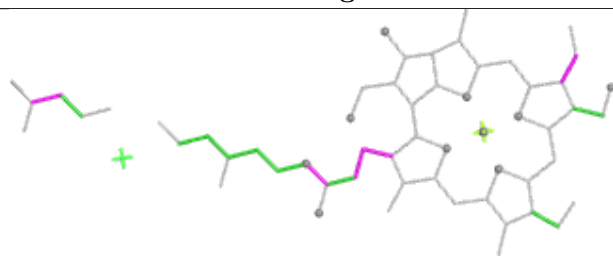
Ligand CHL Au 609



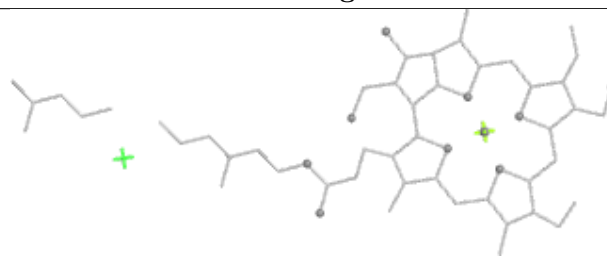
Bond lengths



Bond angles

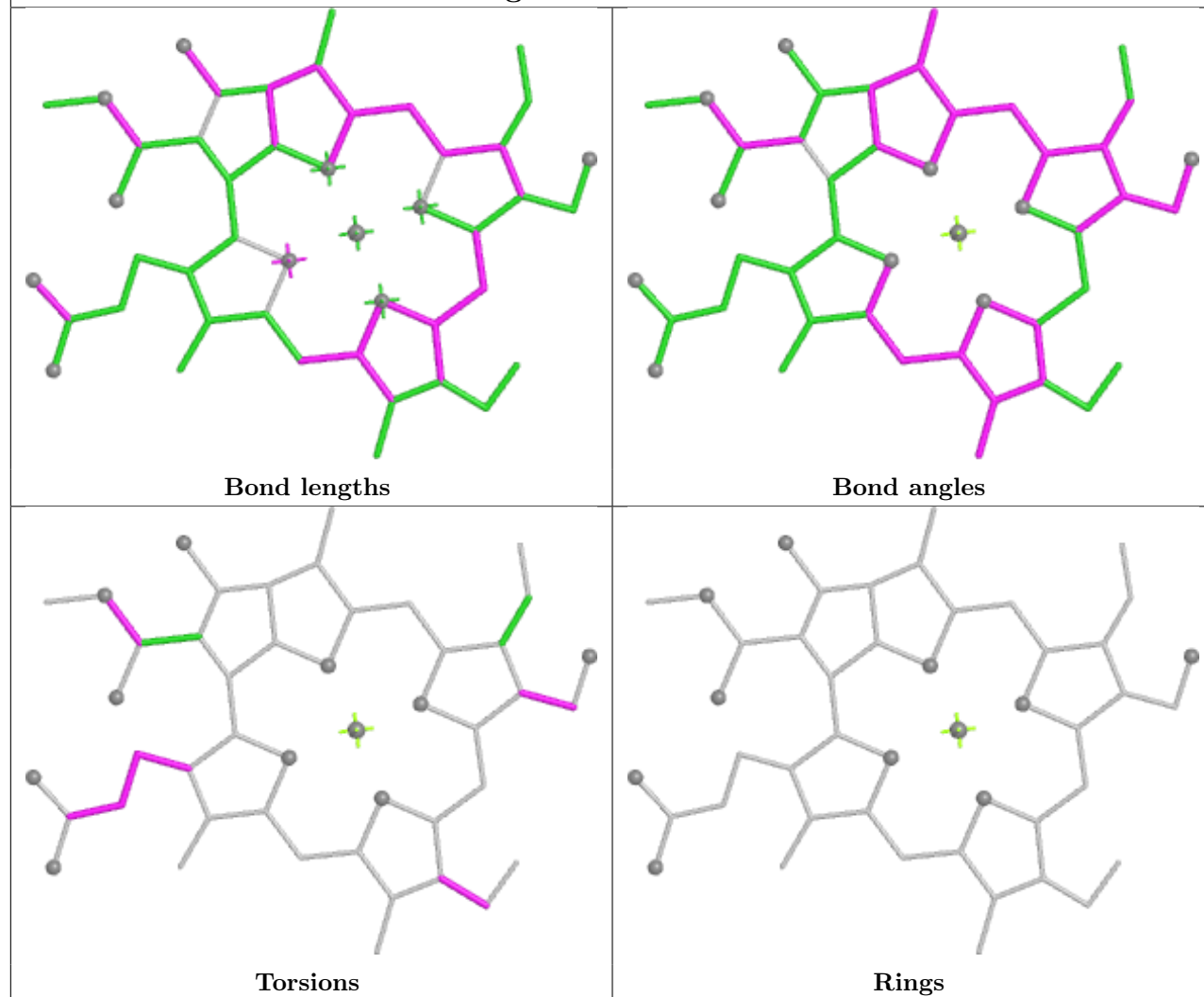


Torsions

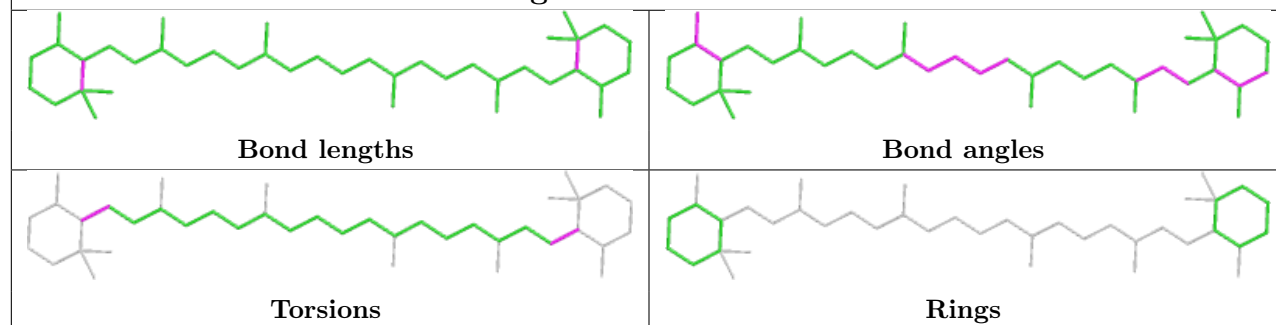


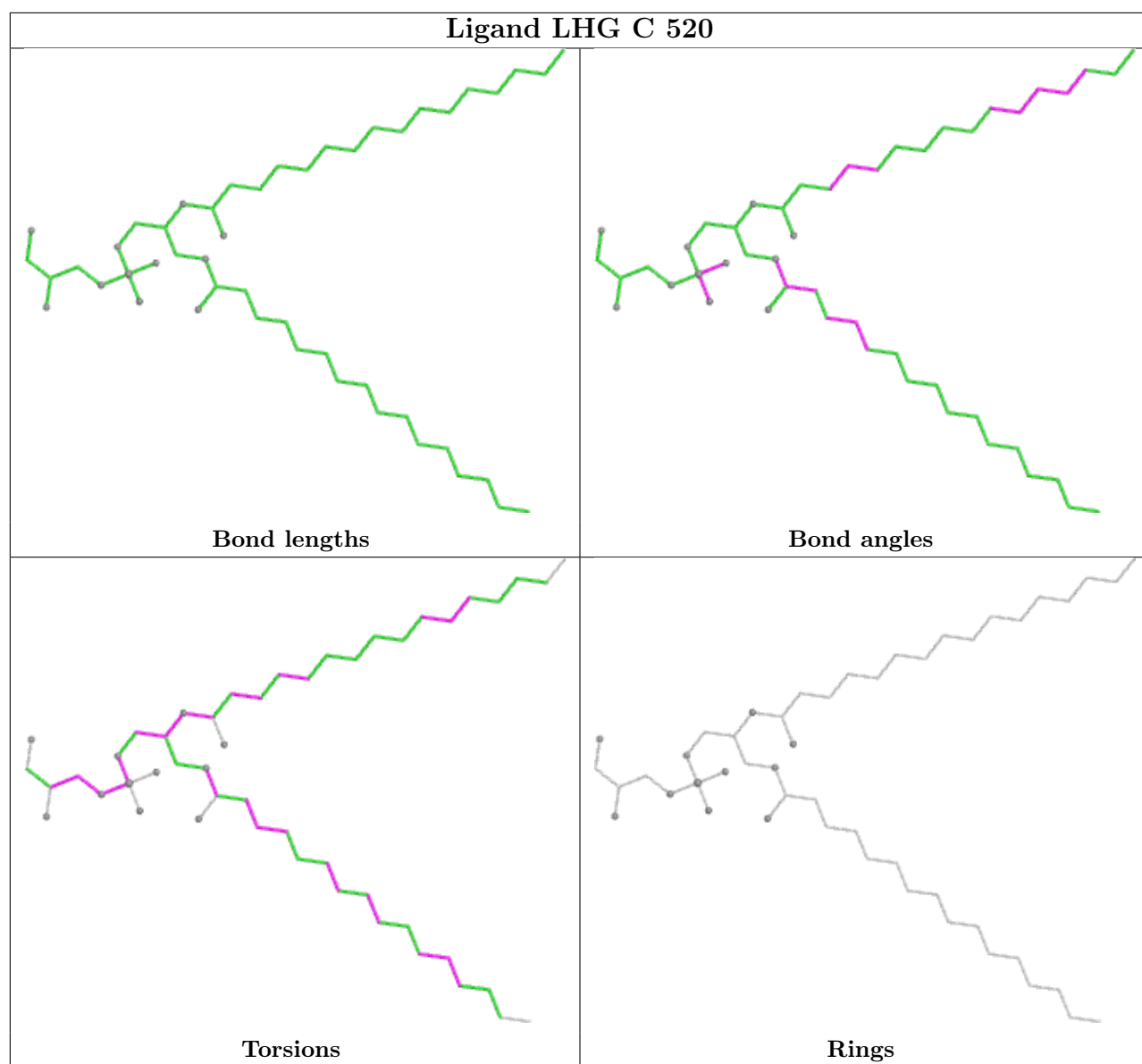
Rings

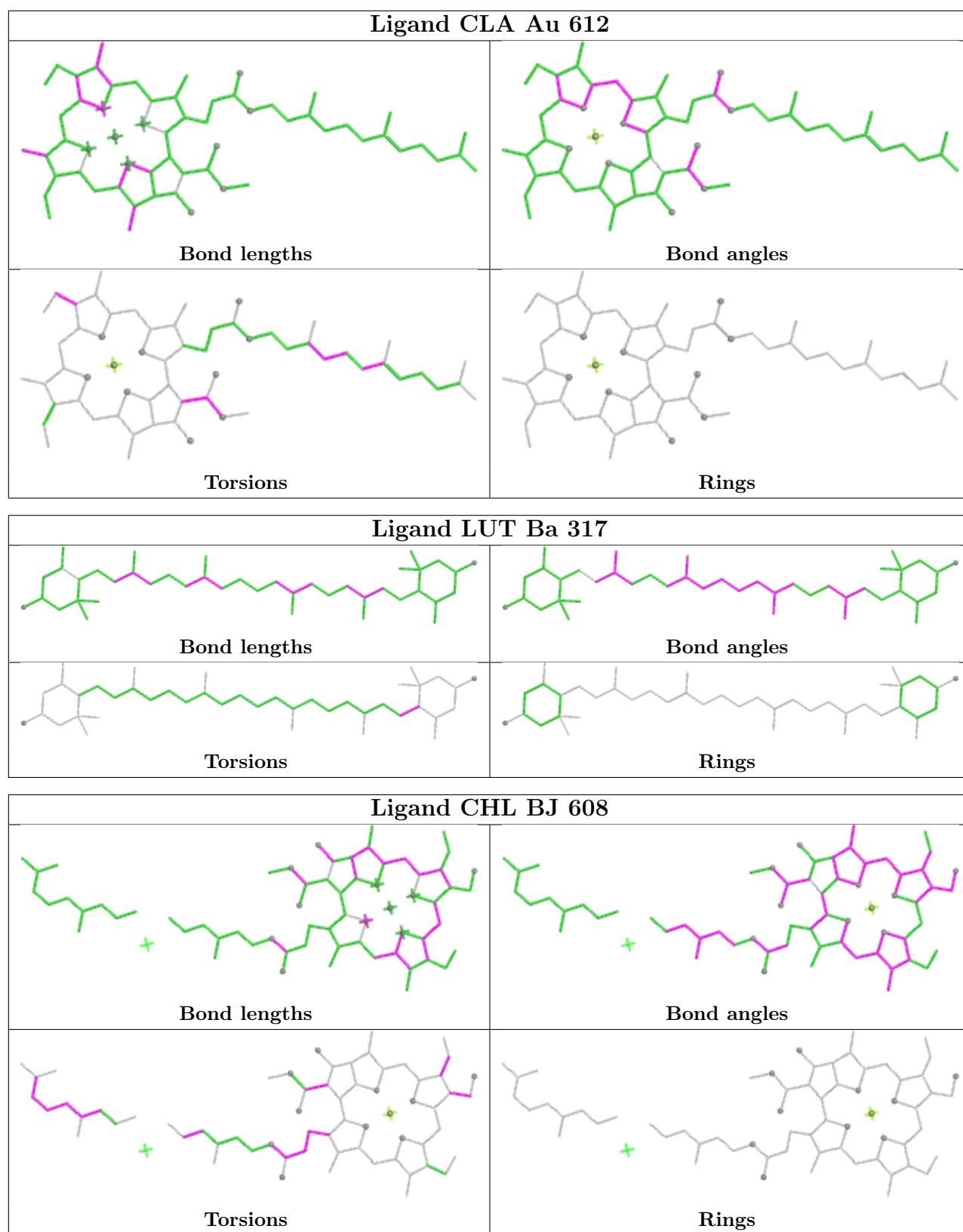
Ligand CHL 7 309



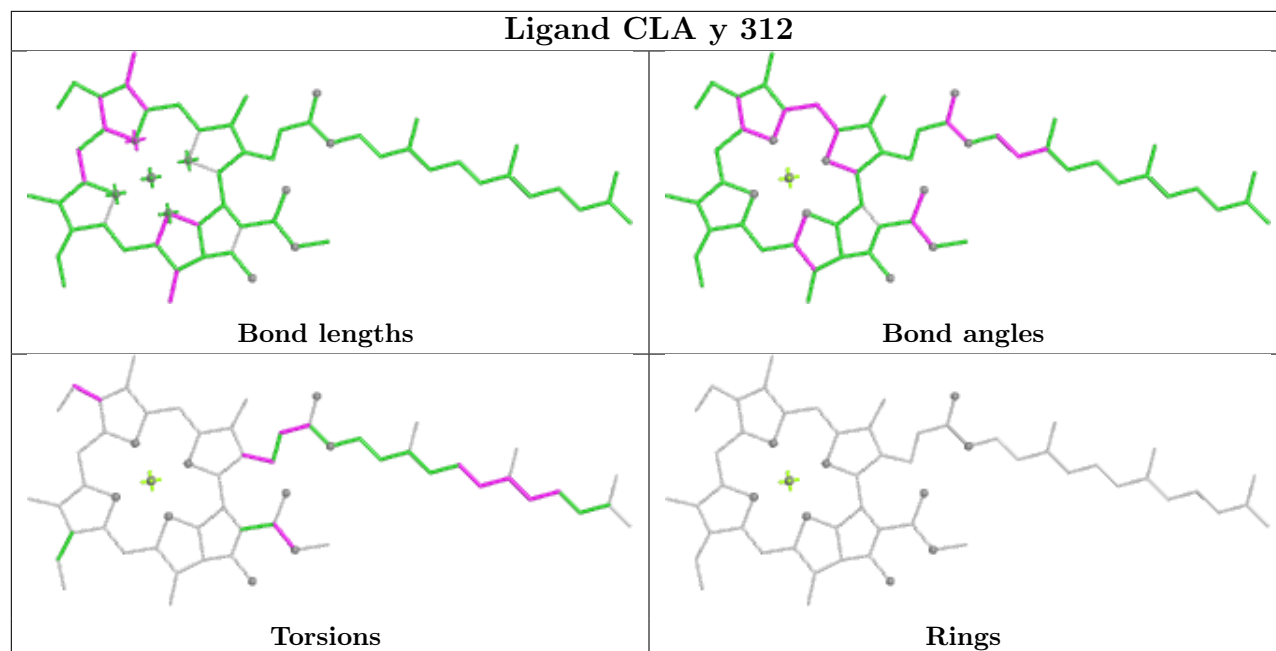
Ligand BCR C 514



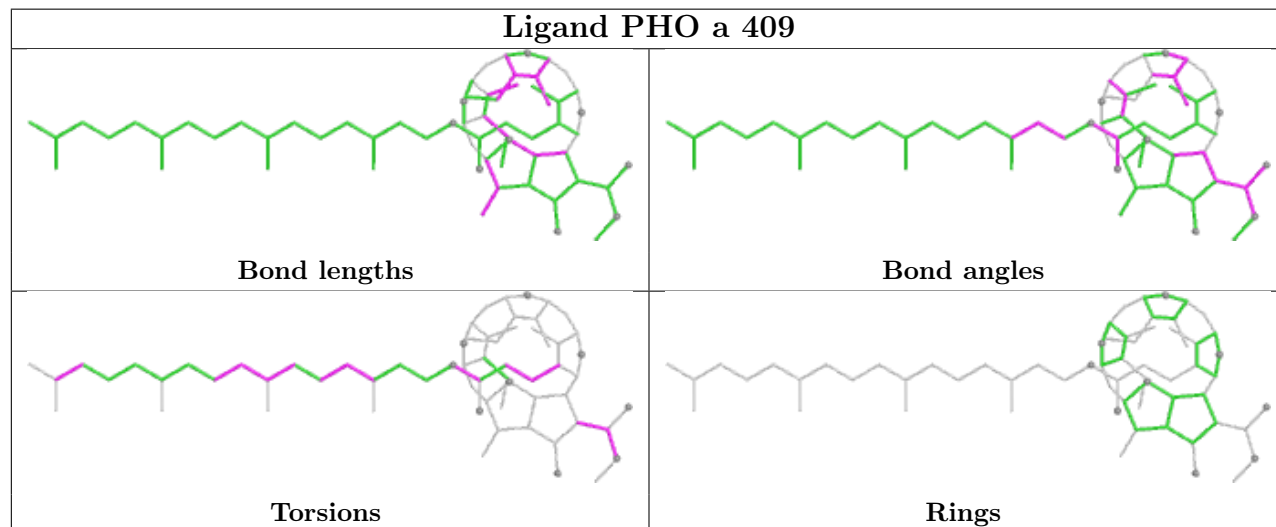




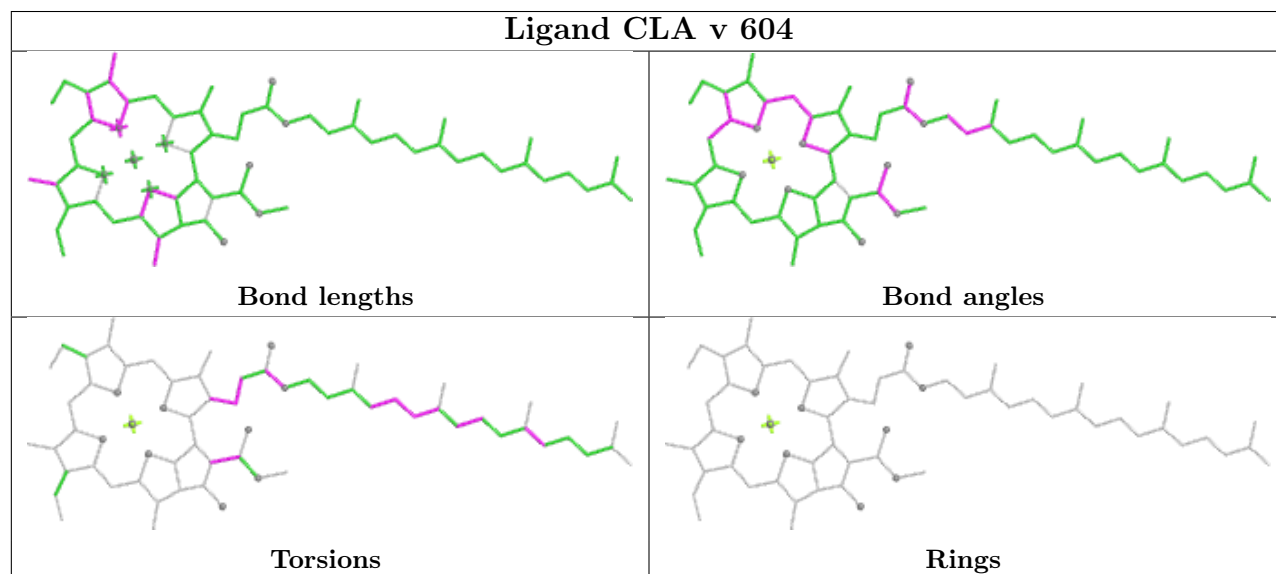
Ligand CLA y 312

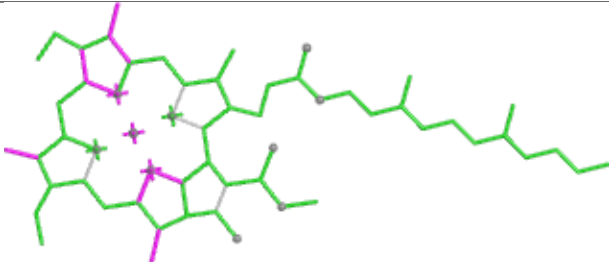
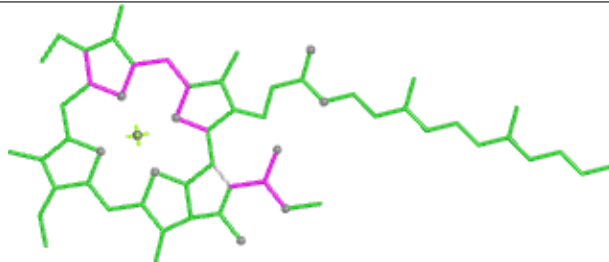
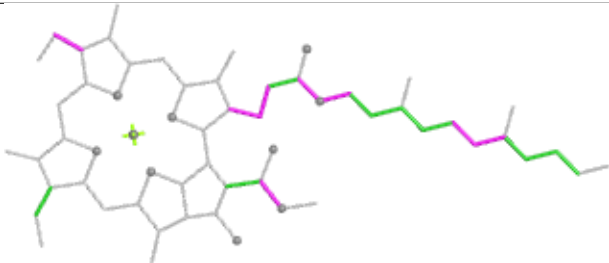
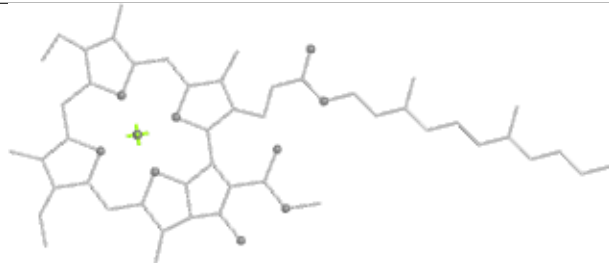


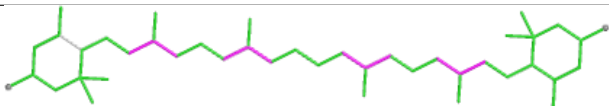
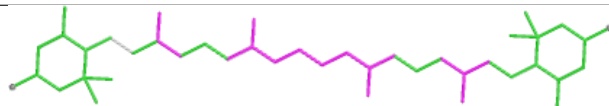
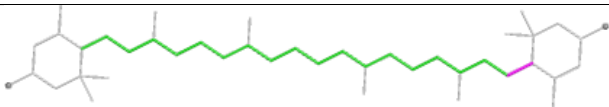
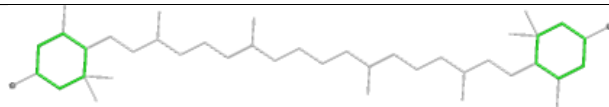
Ligand PHO a 409

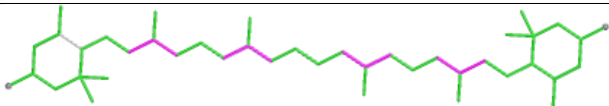
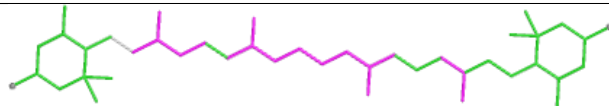
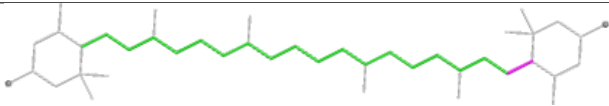
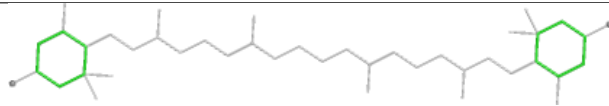


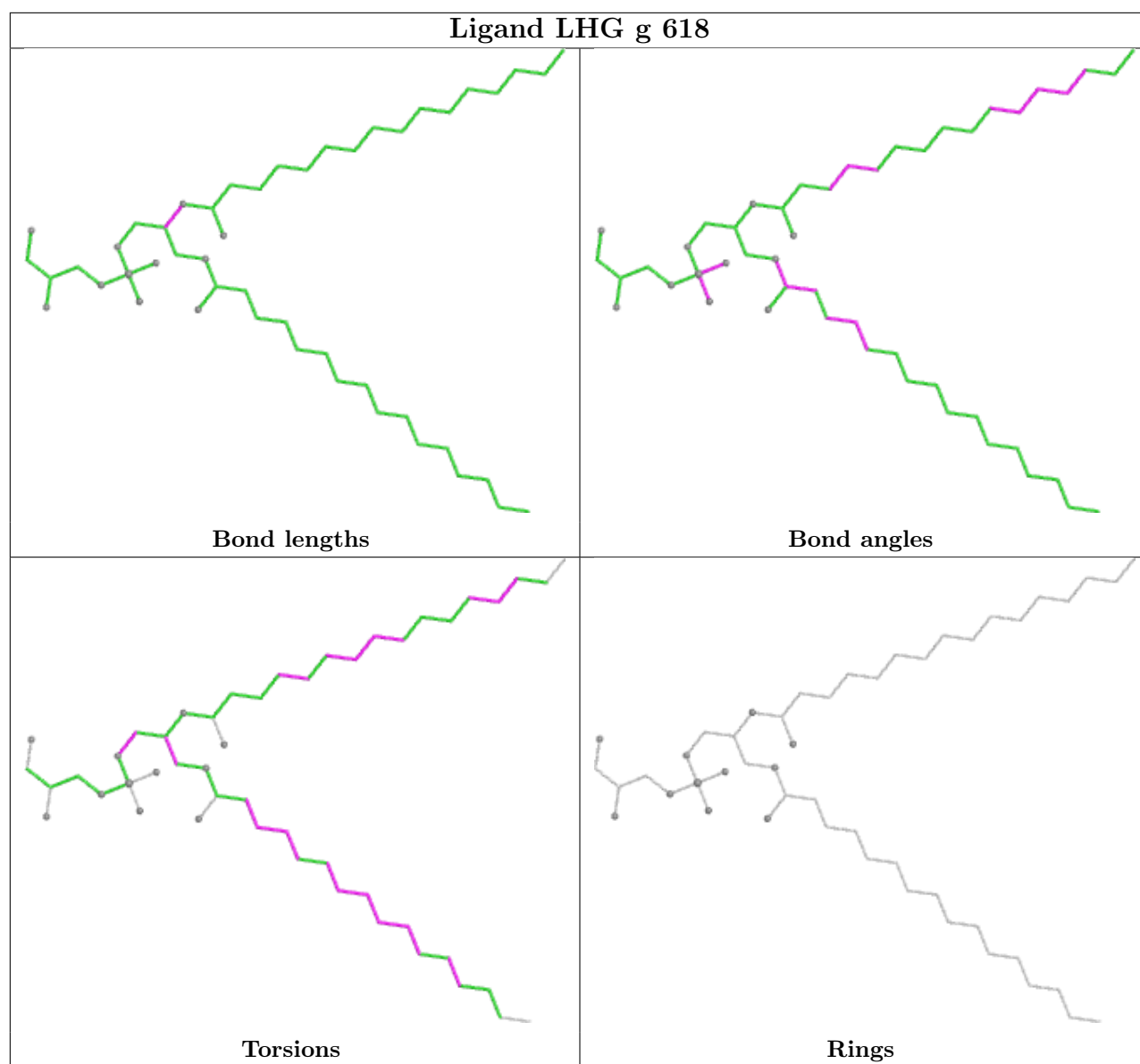
Ligand CLA v 604

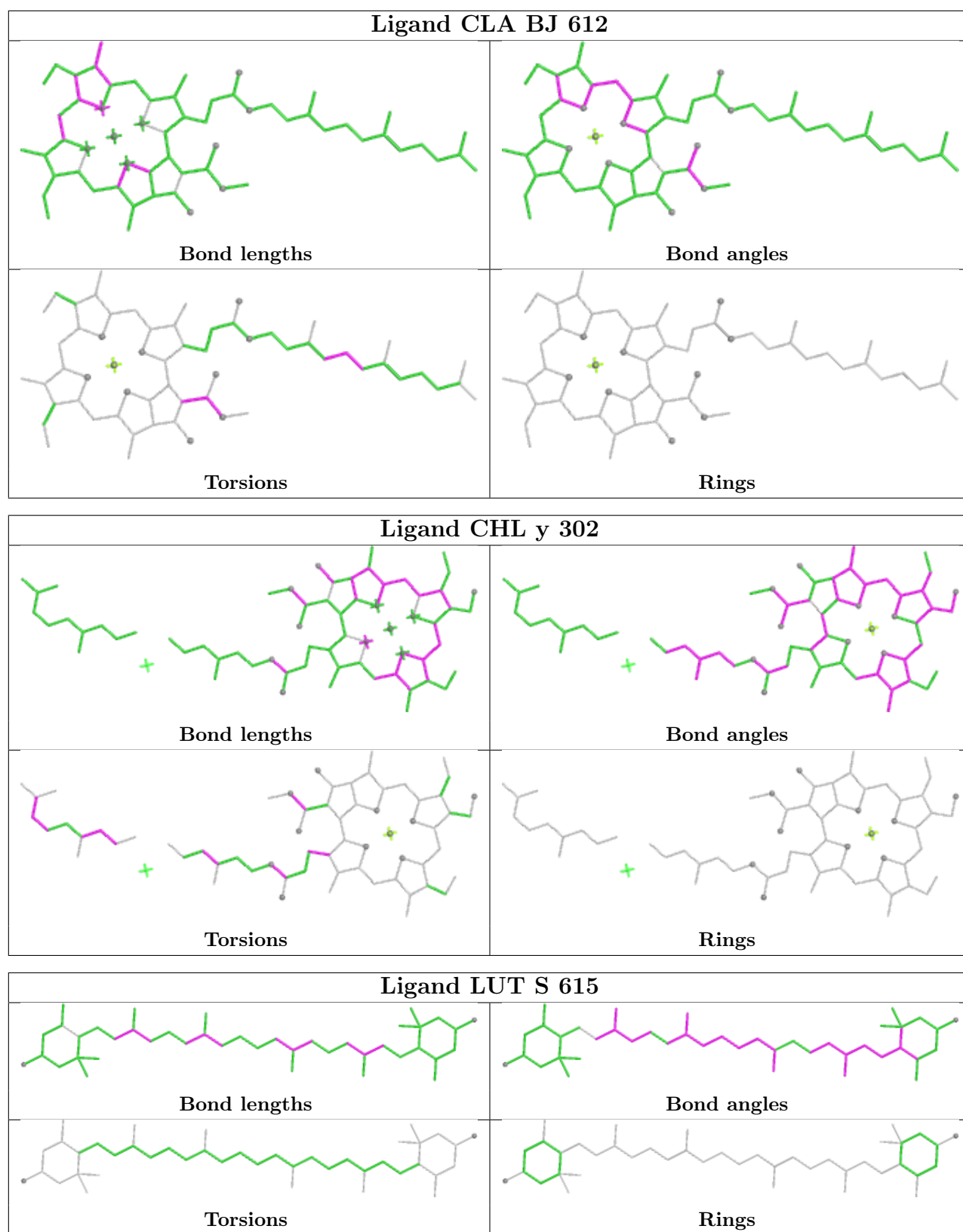


Ligand CLA BU 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

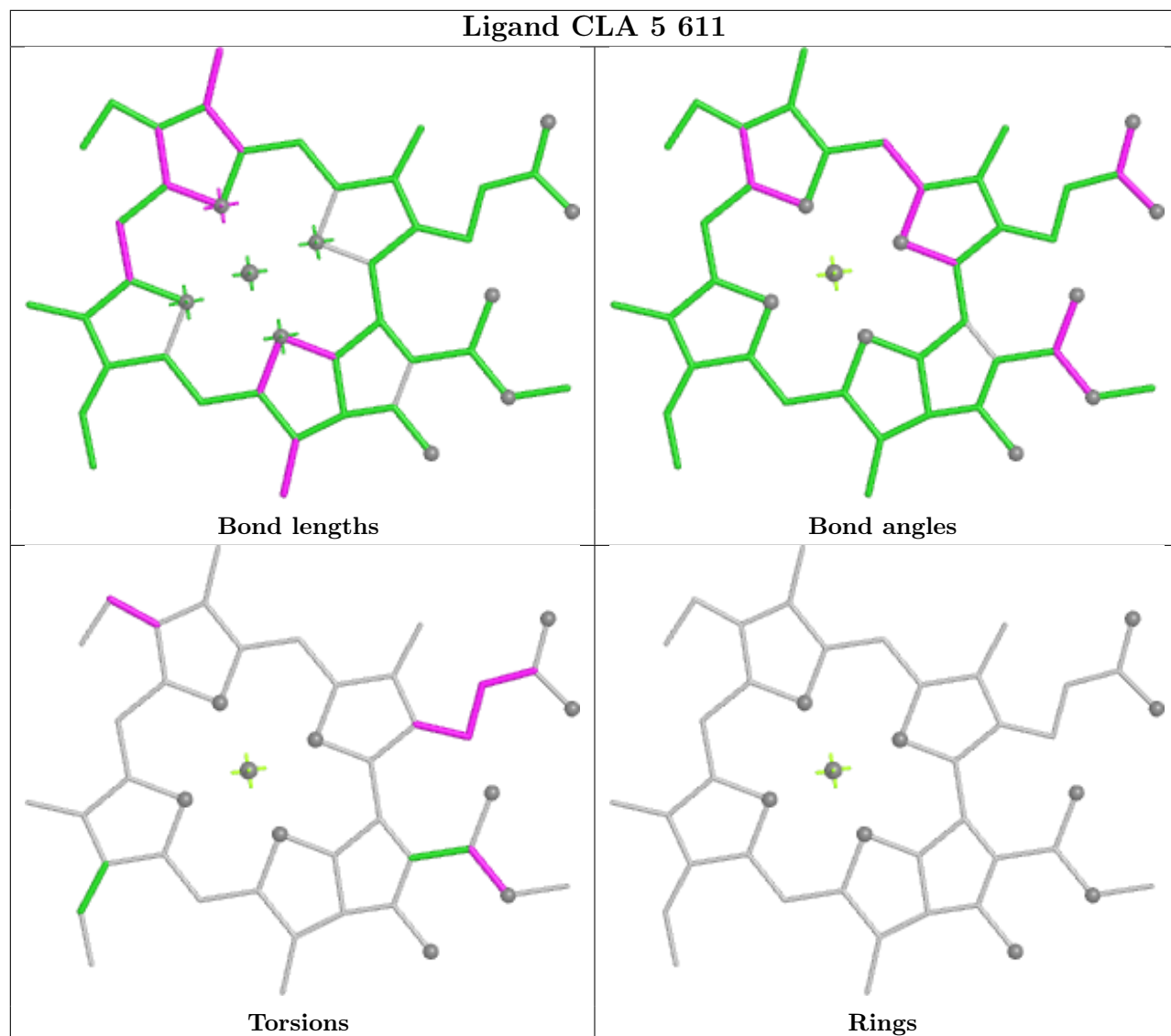
Ligand LUT Au 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

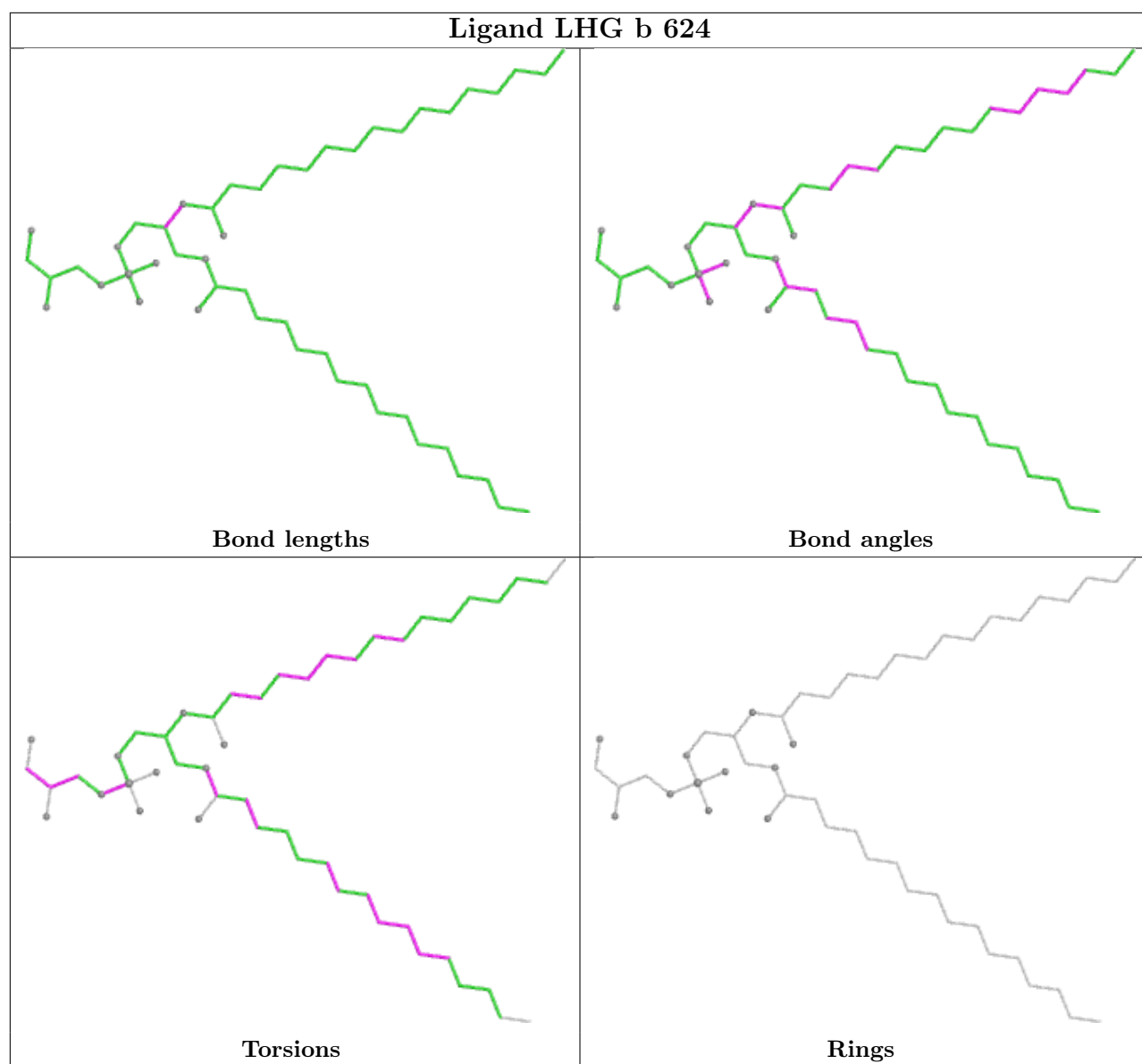
Ligand LUT N 615	
	
Bond lengths	Bond angles
	
Torsions	Rings



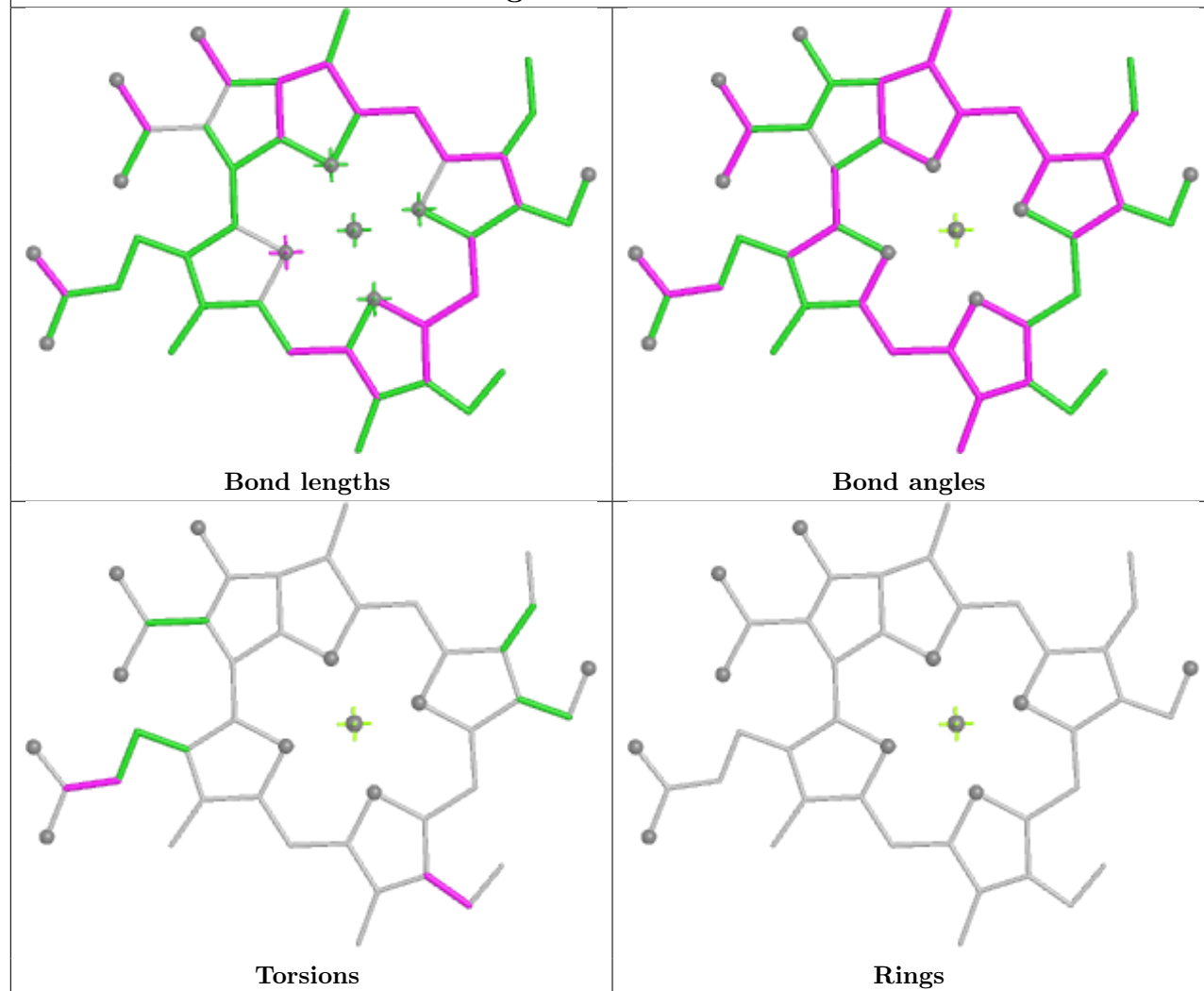


Ligand CLA 5 611

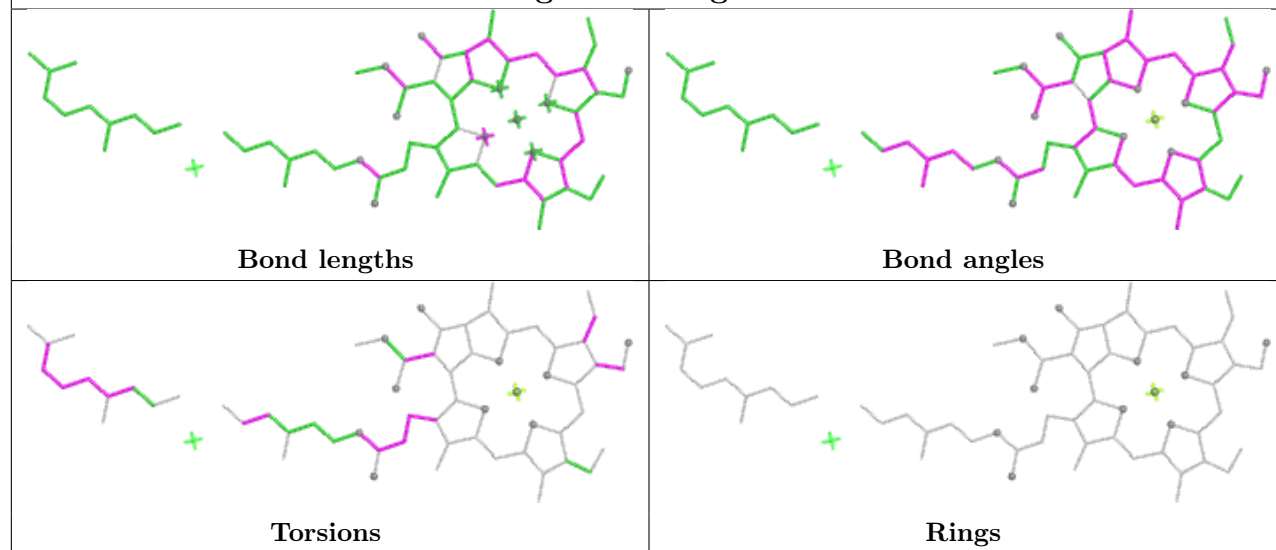


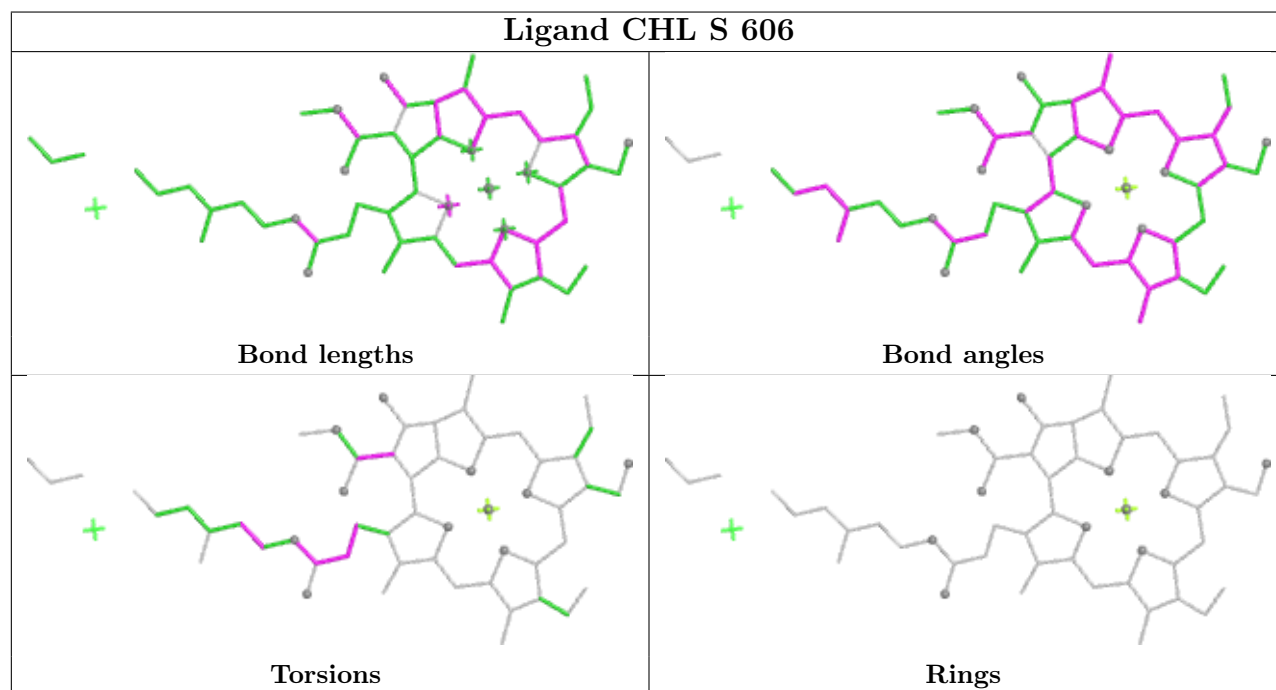
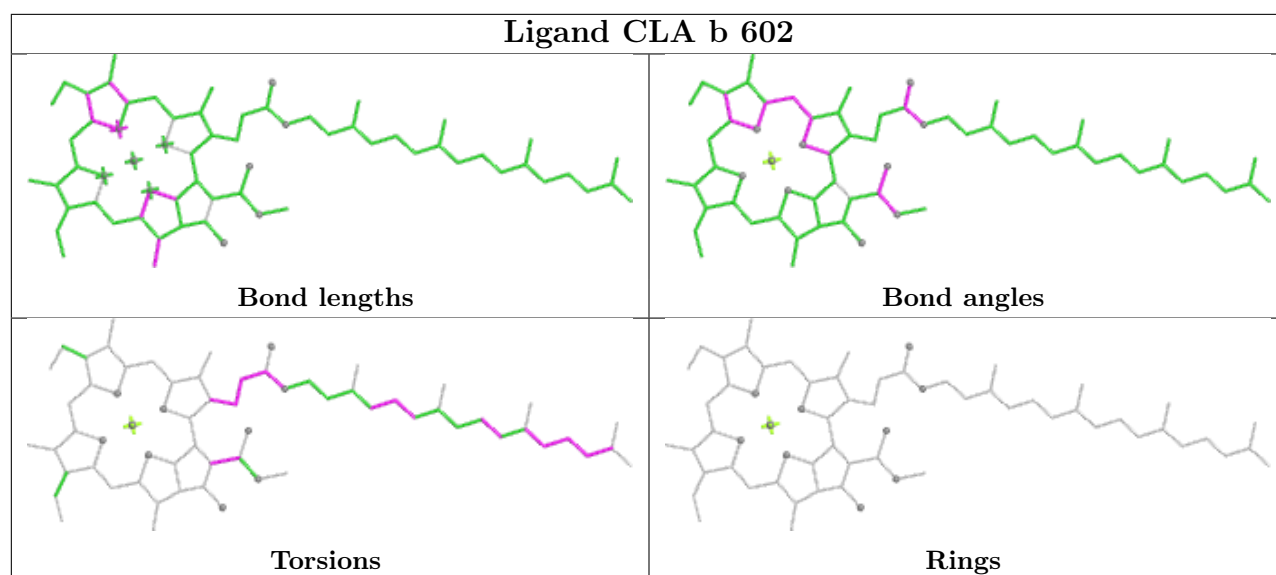


Ligand CHL e 601

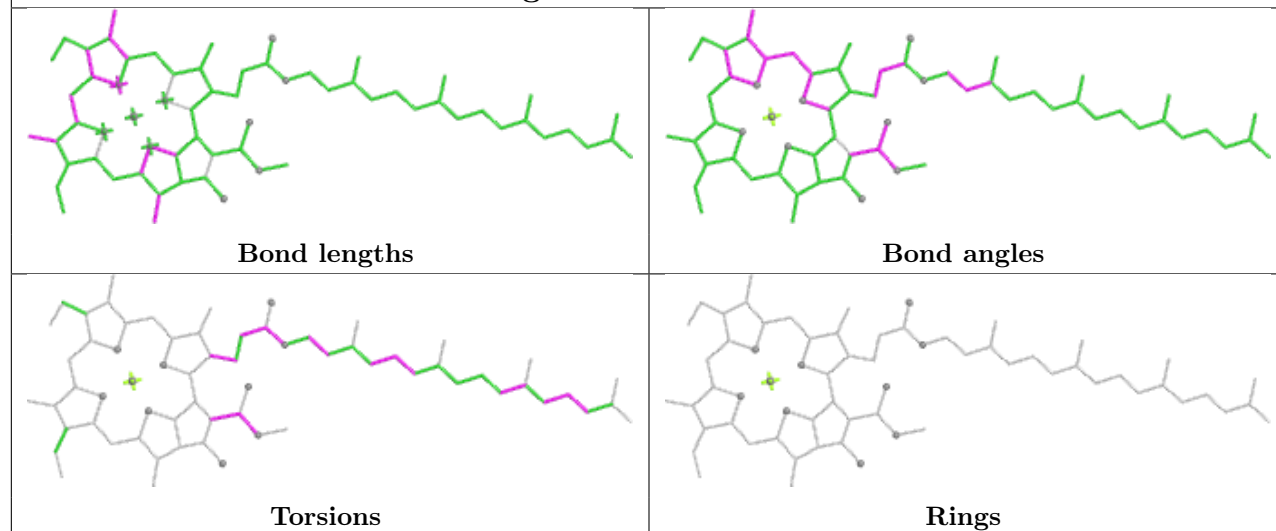


Ligand CHL g 608

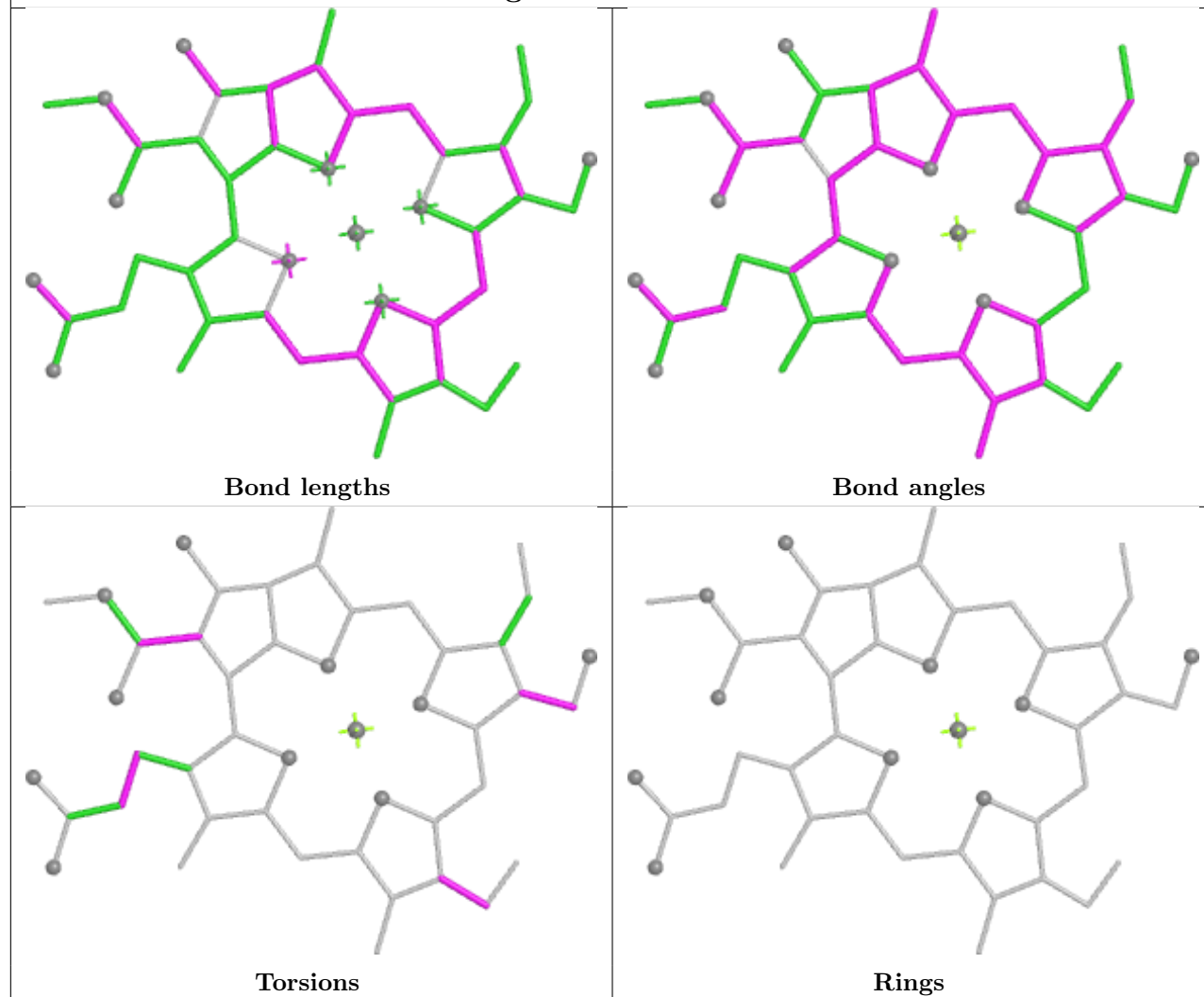


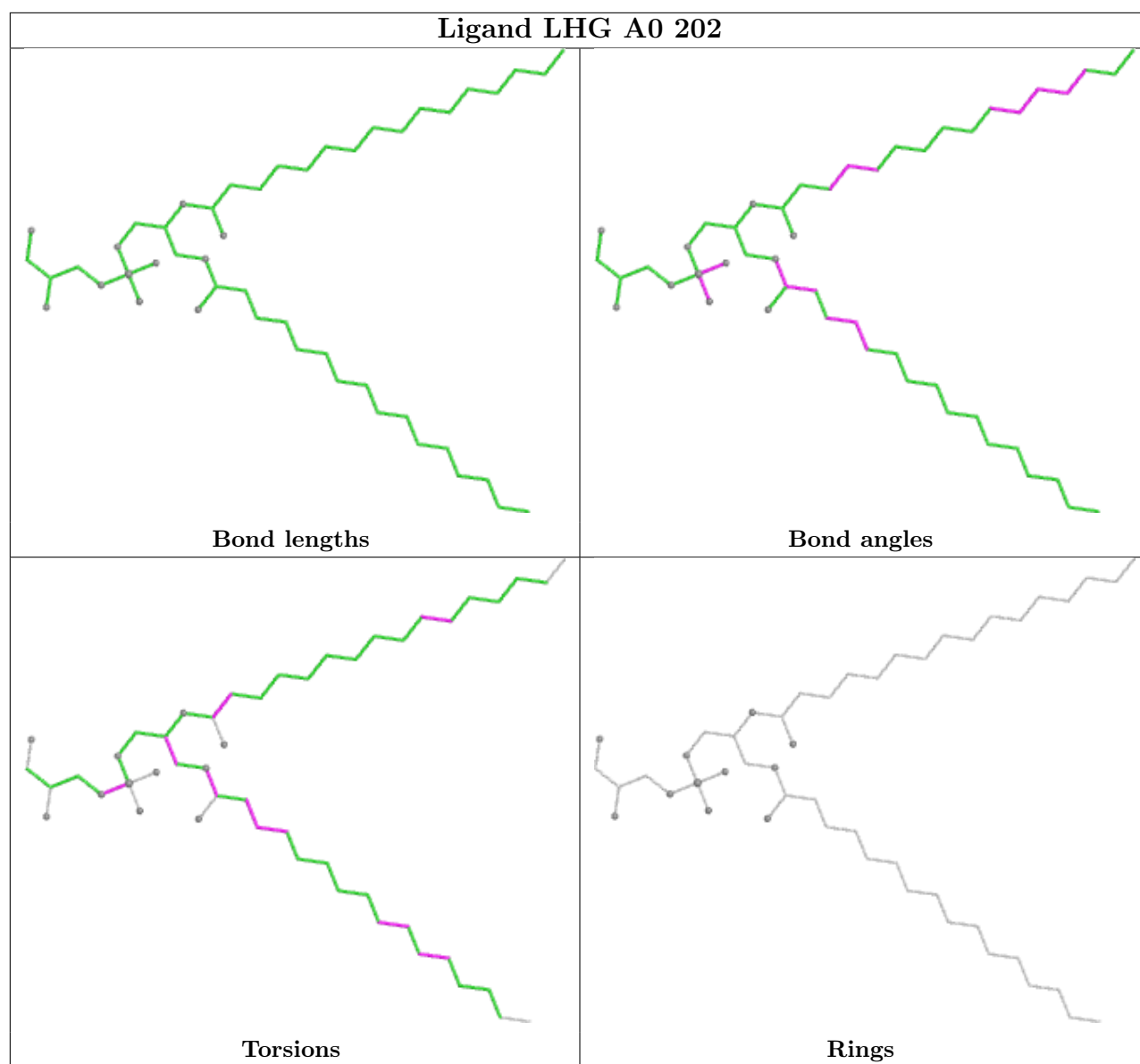


Ligand CLA A2 610

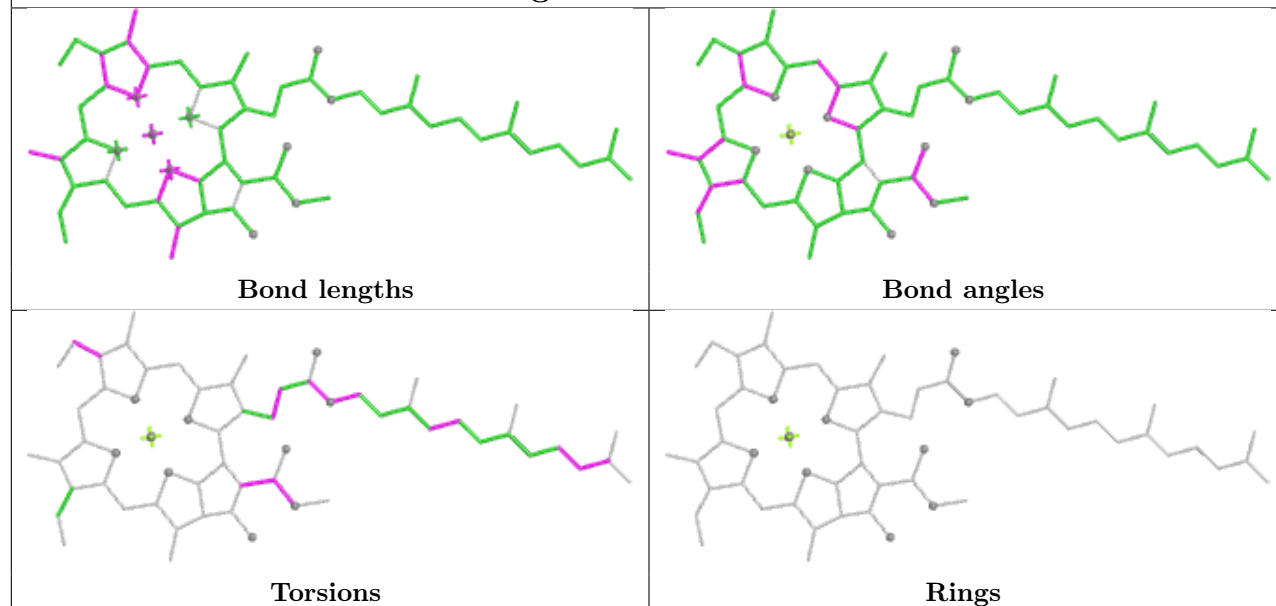


Ligand CHL 9 606

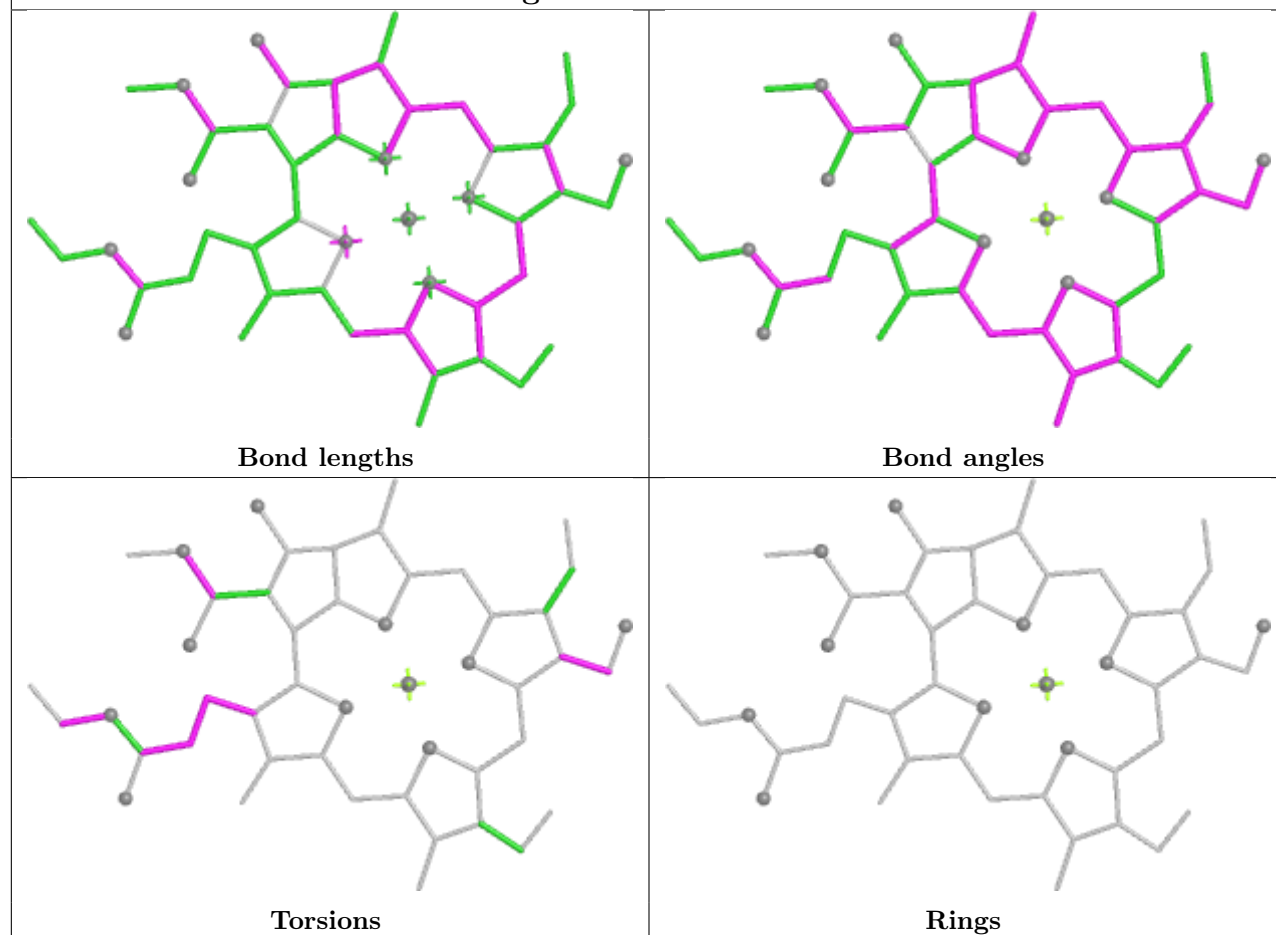


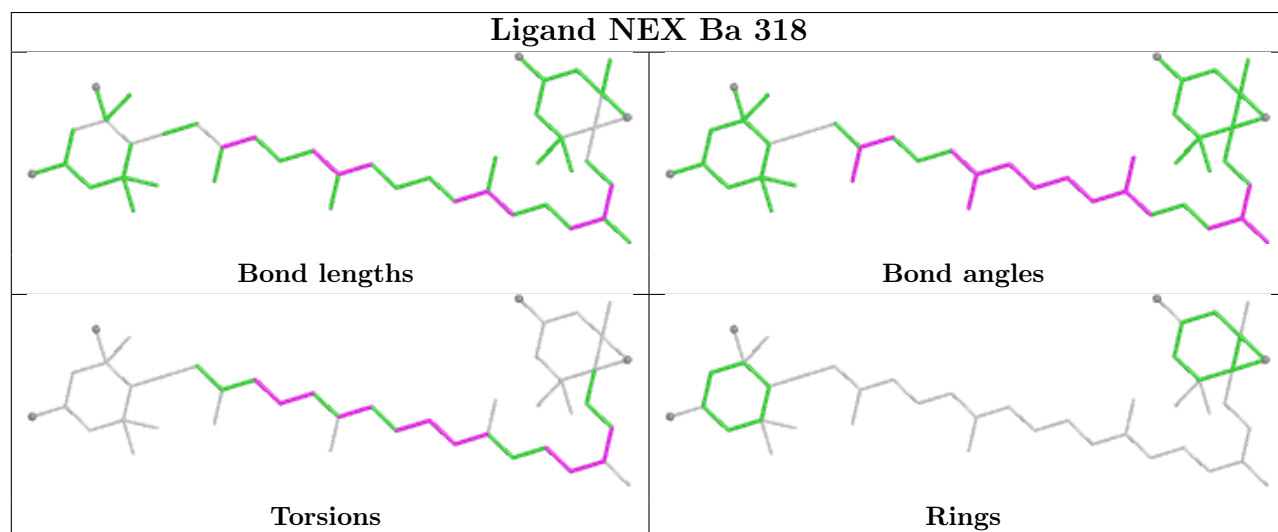
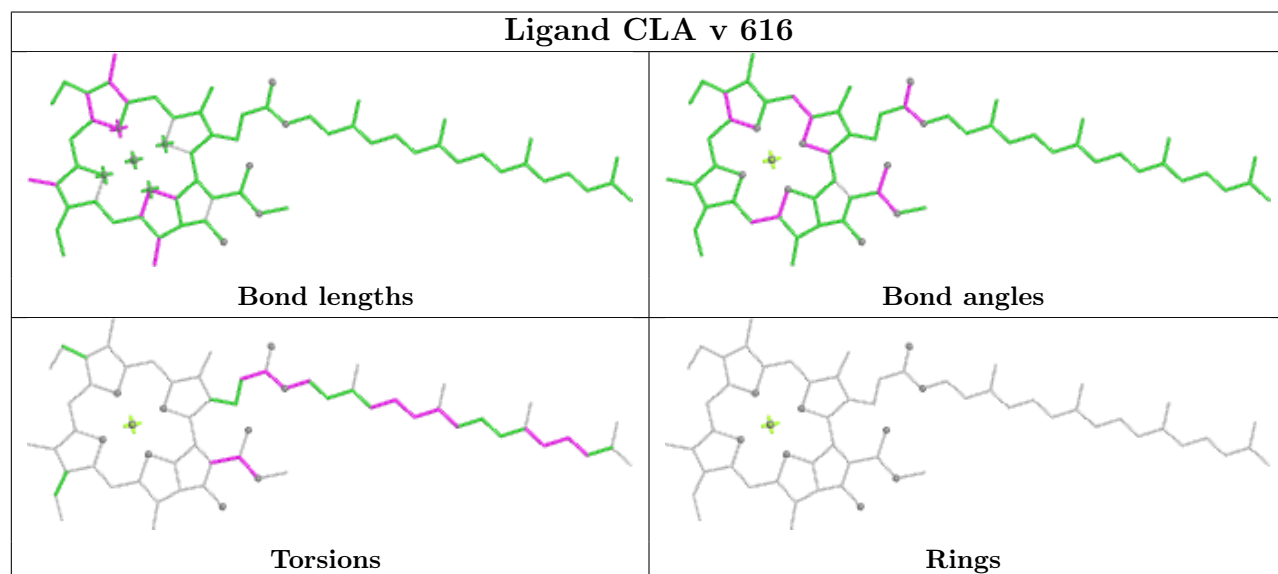
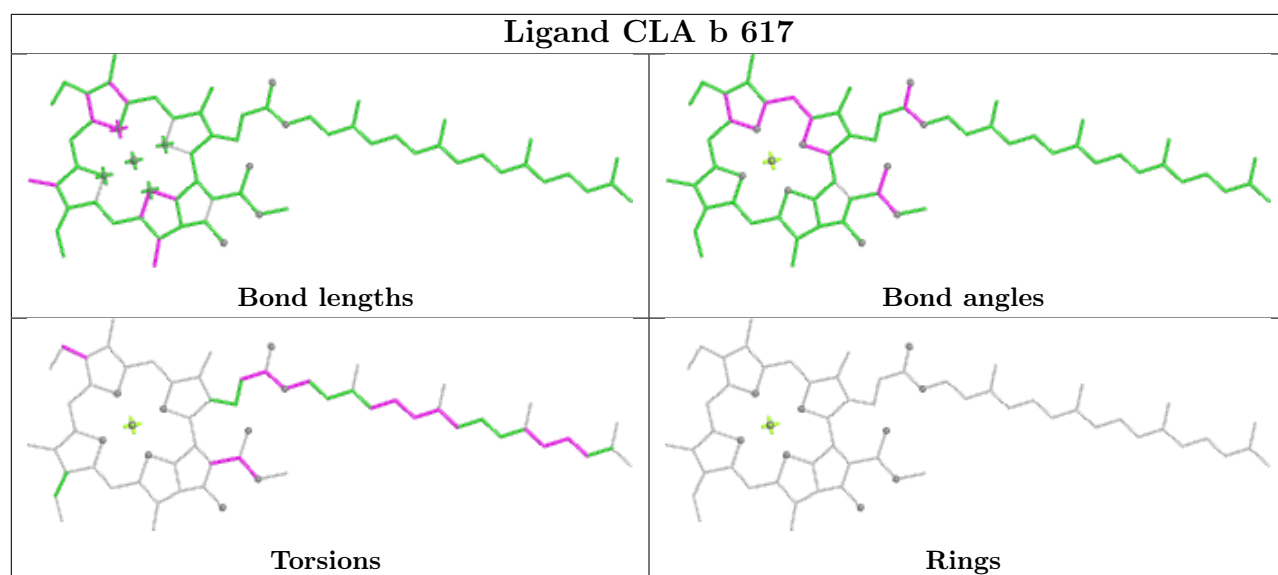


Ligand CLA Y 311

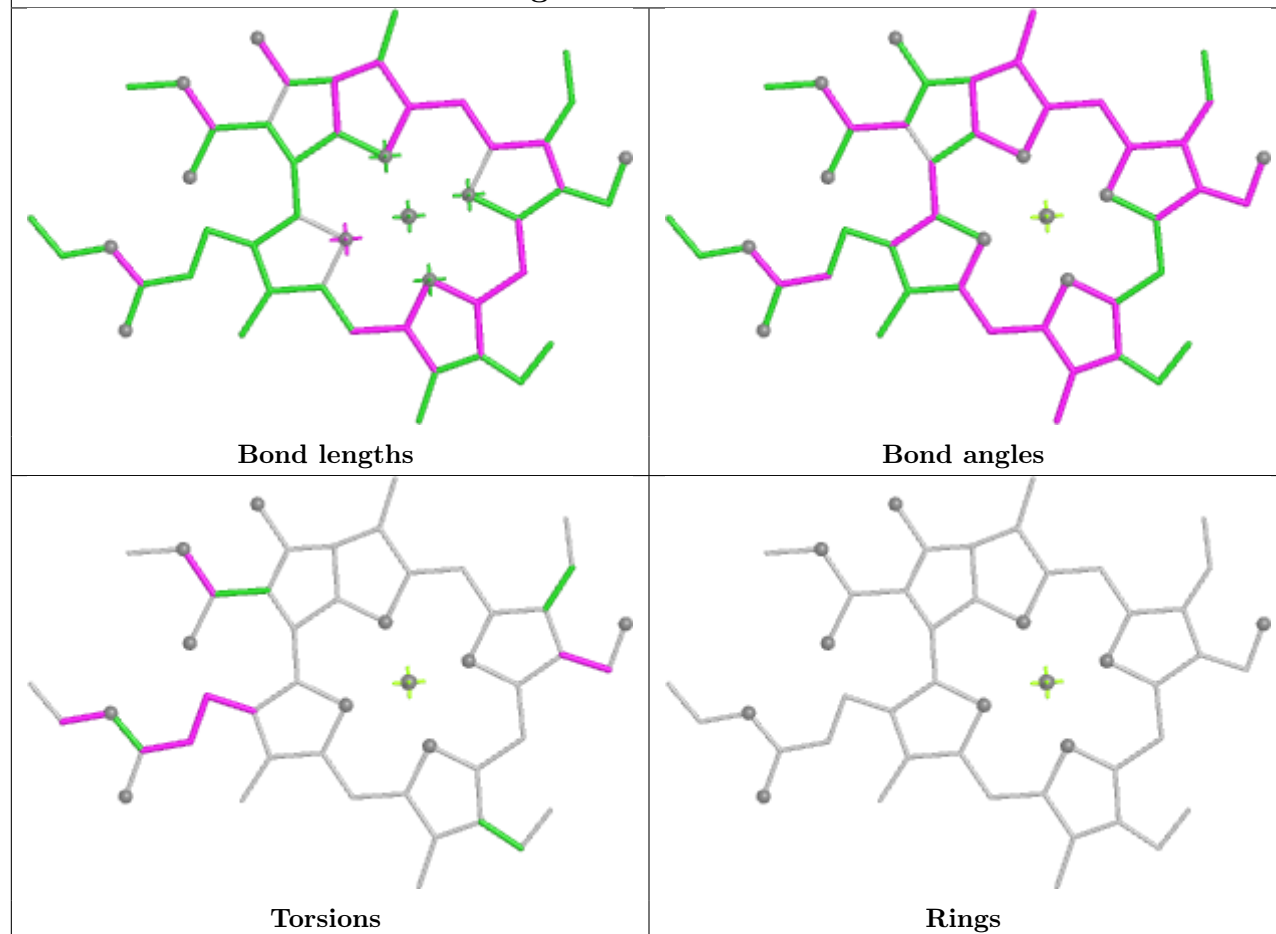


Ligand CHL A2 605

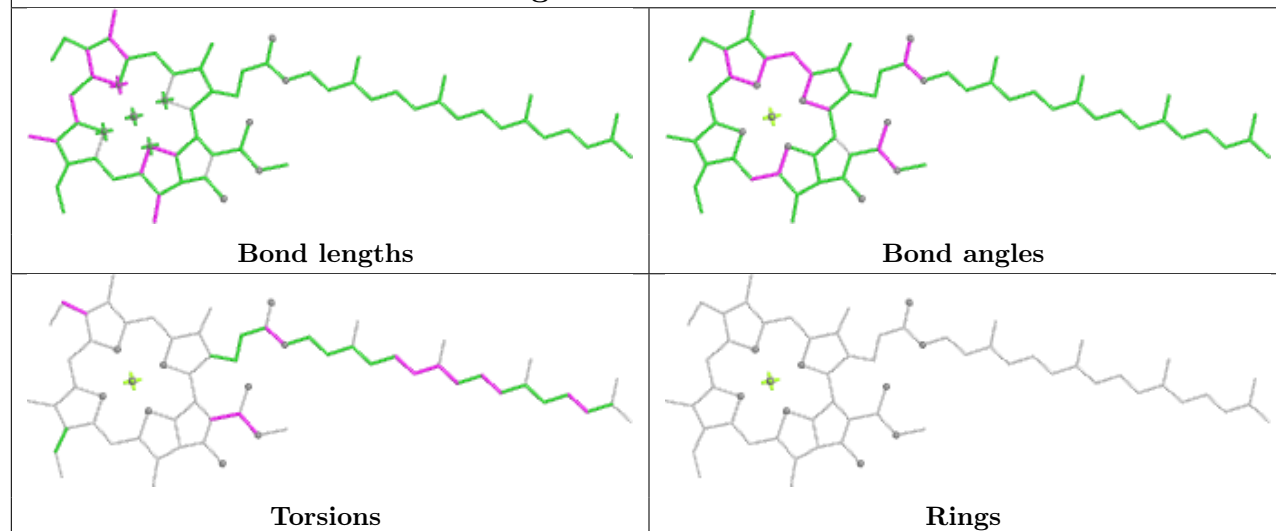


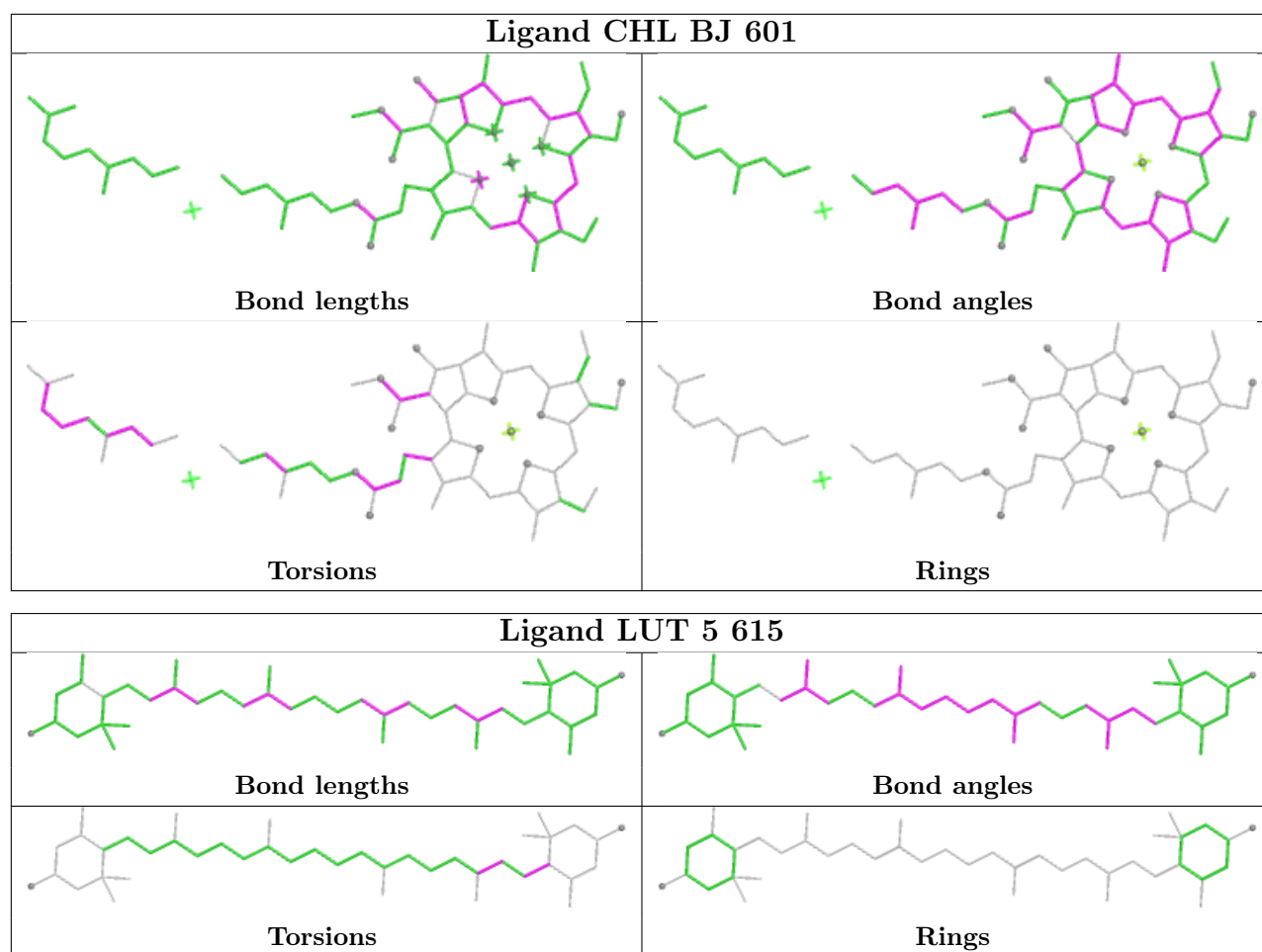


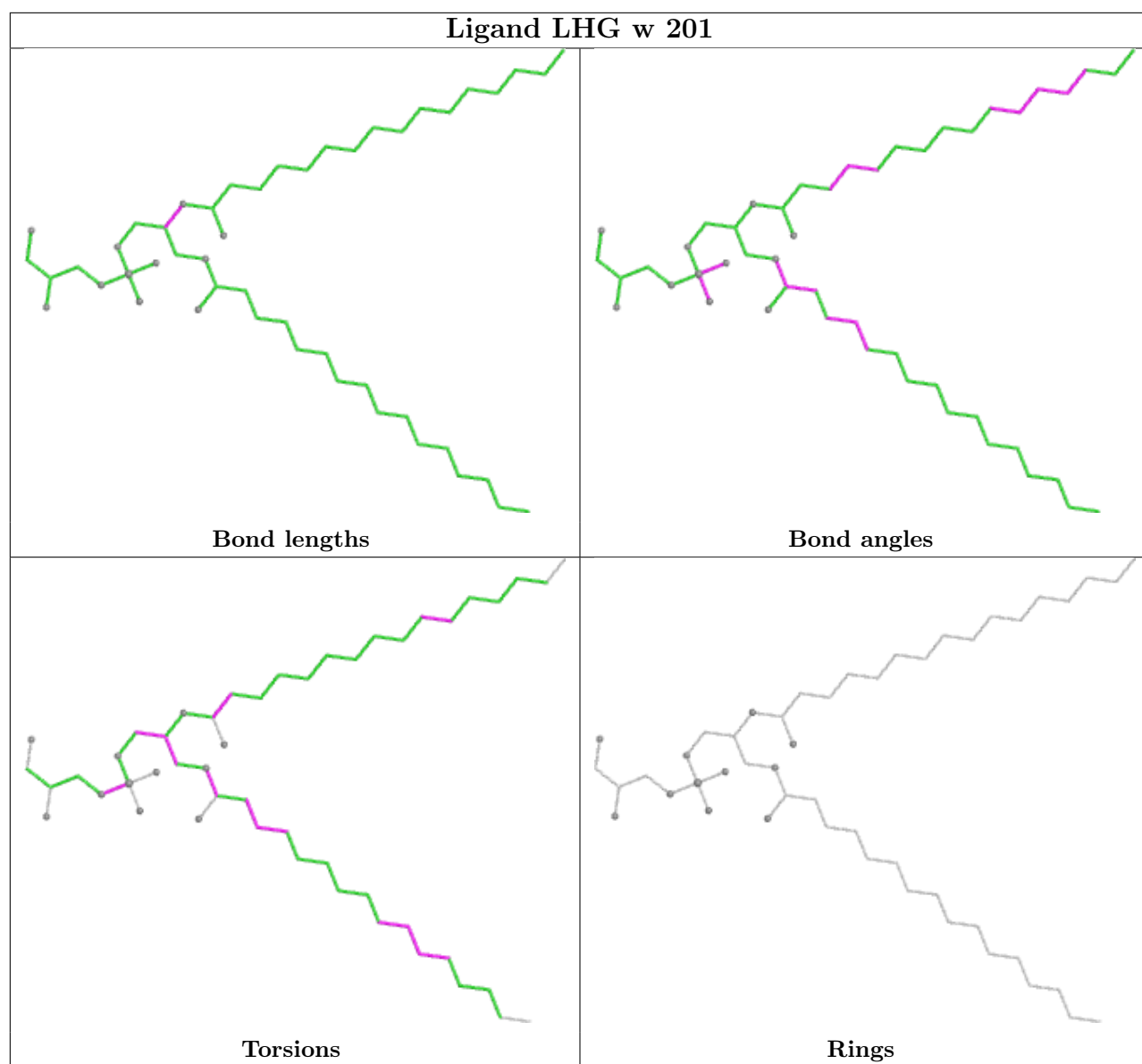
Ligand CHL N 605



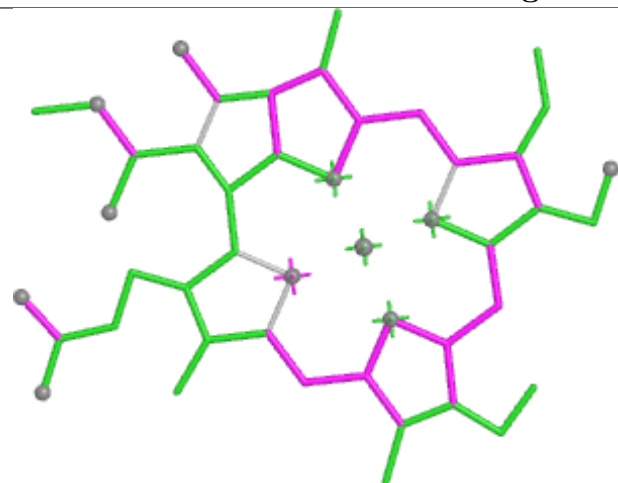
Ligand CLA N 603



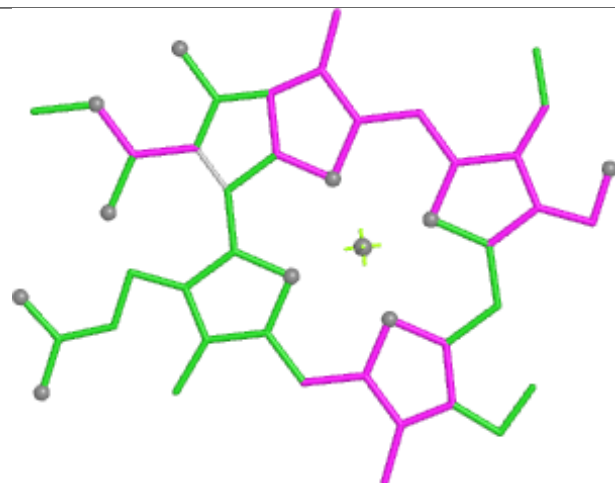




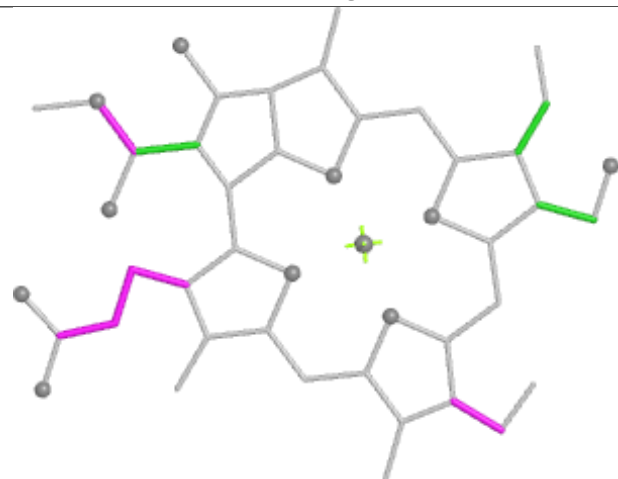
Ligand CHL 8 305



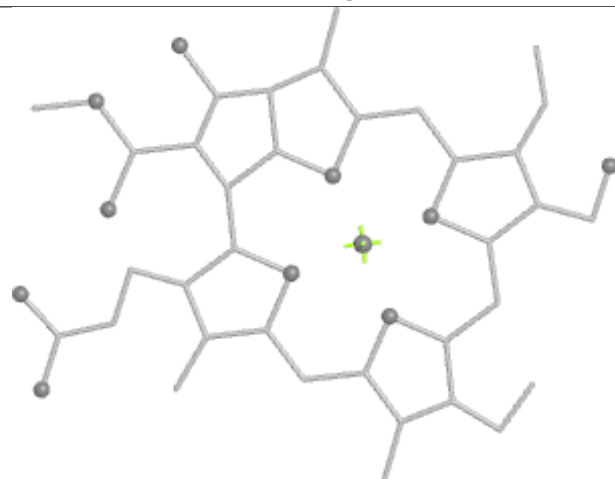
Bond lengths



Bond angles

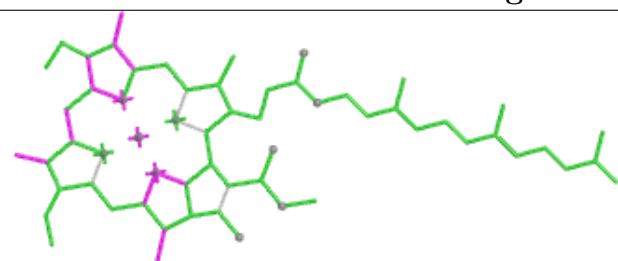


Torsions

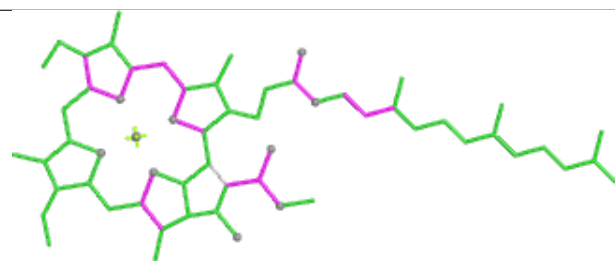


Rings

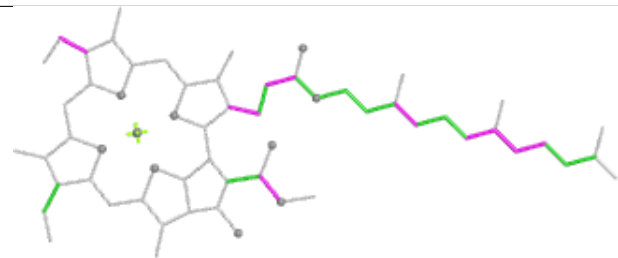
Ligand CLA BB 312



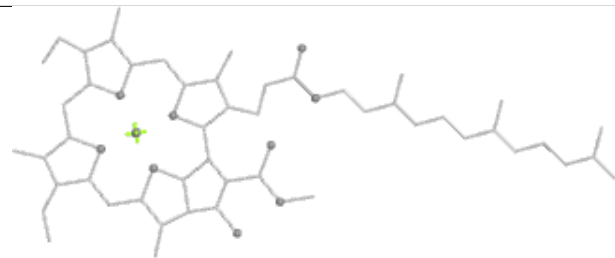
Bond lengths



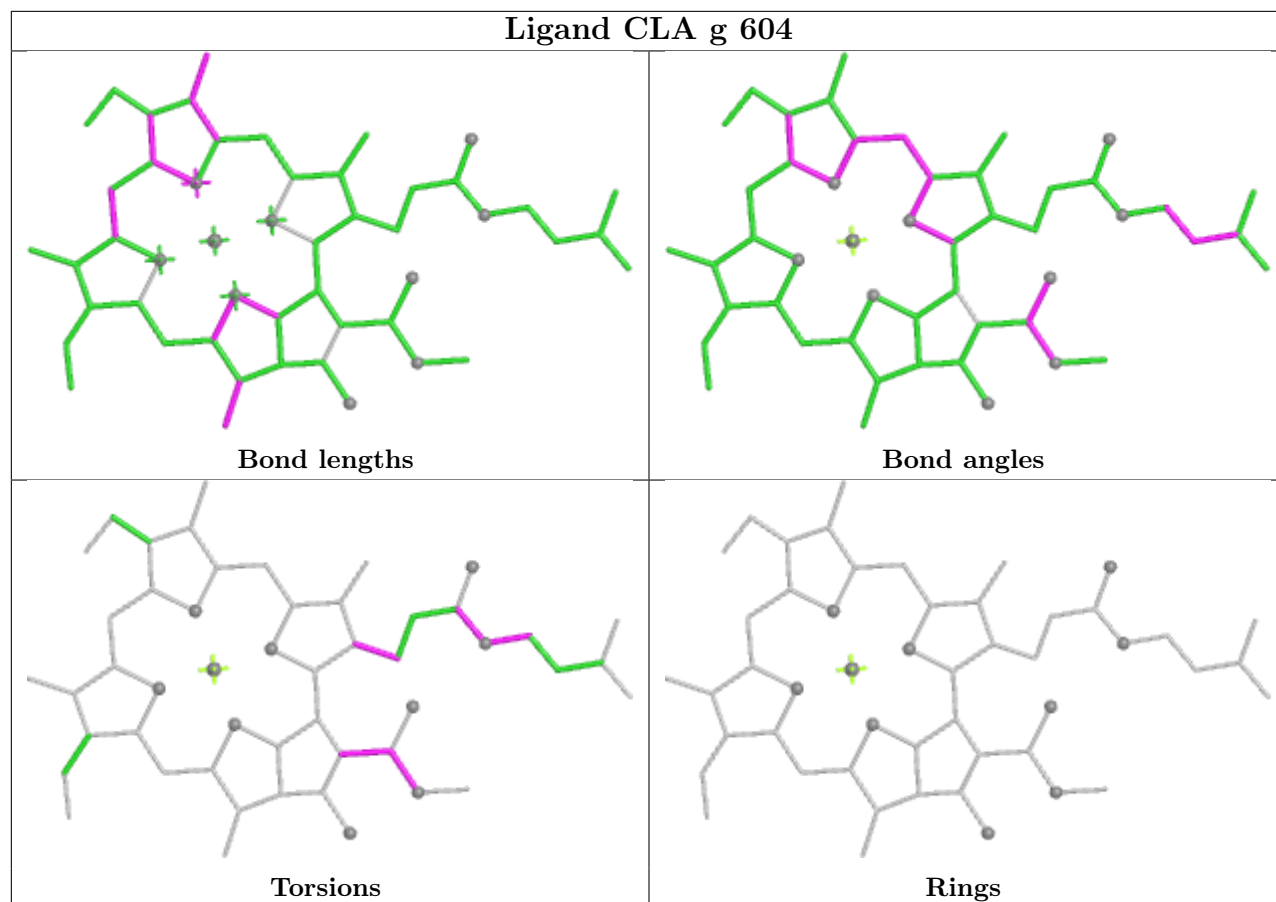
Bond angles

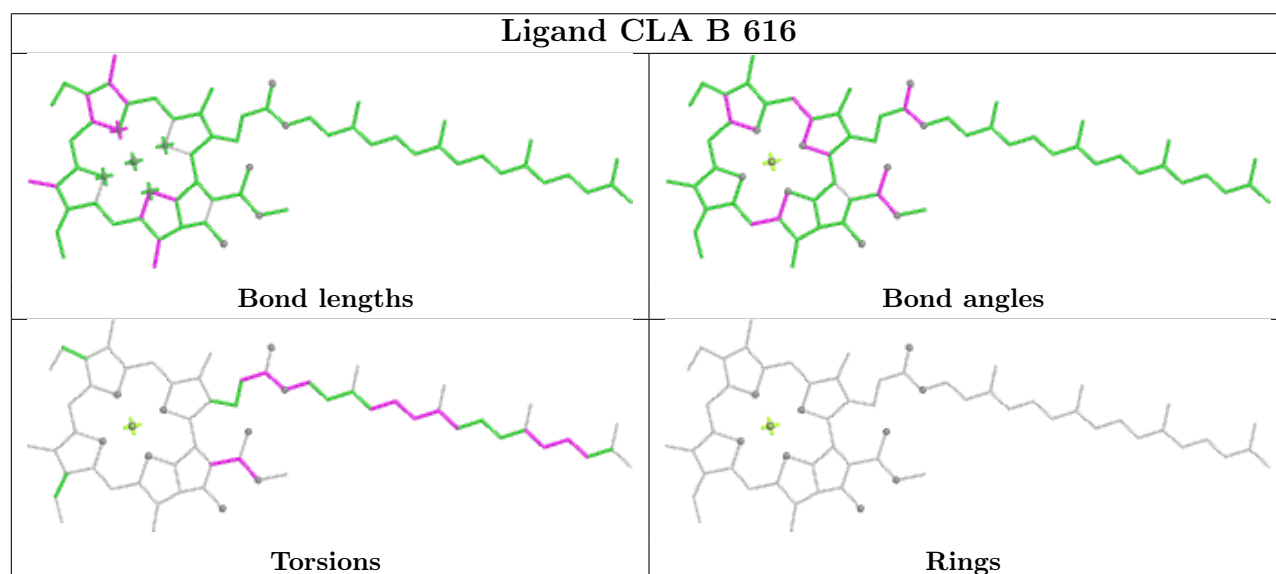
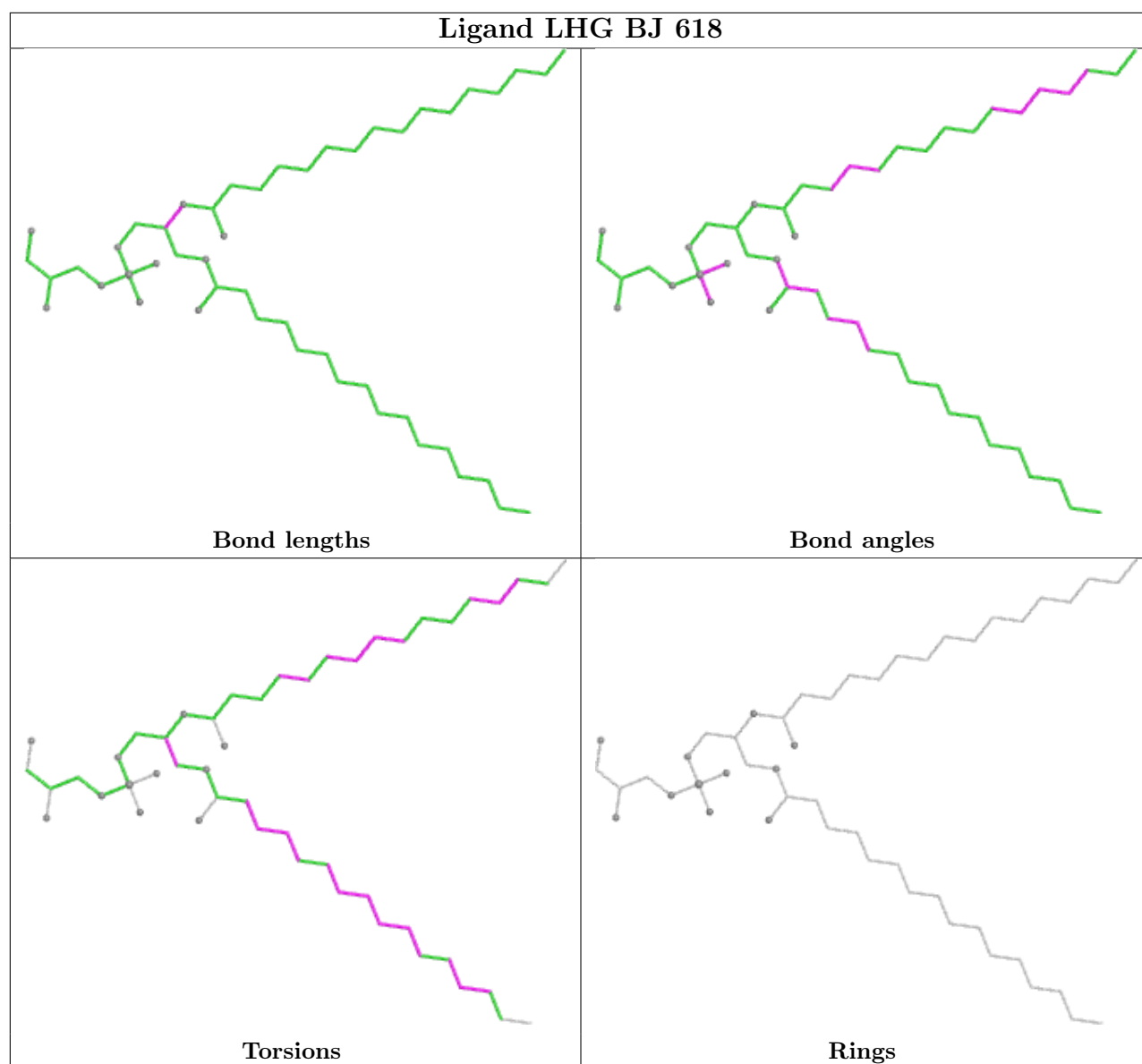


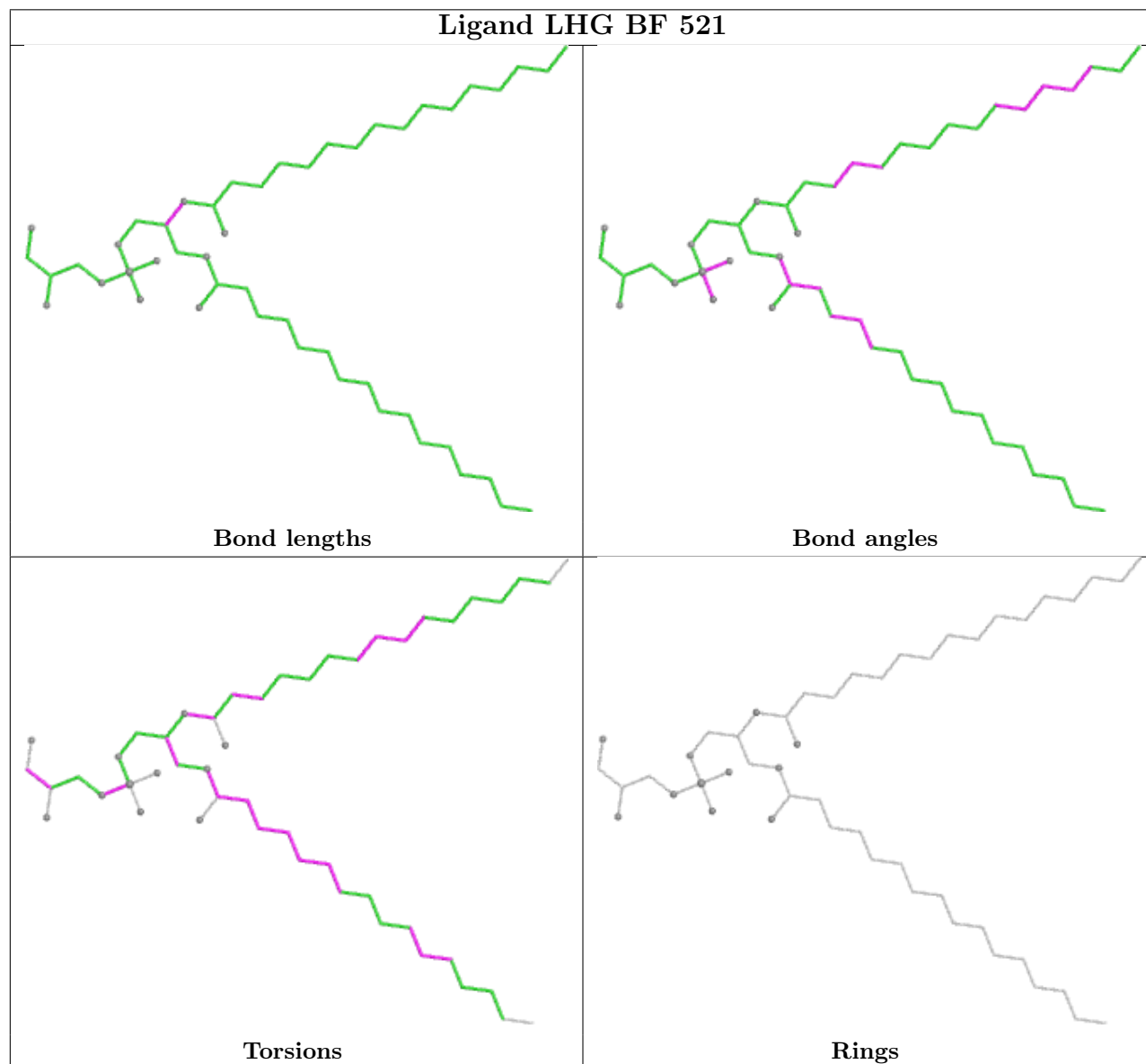
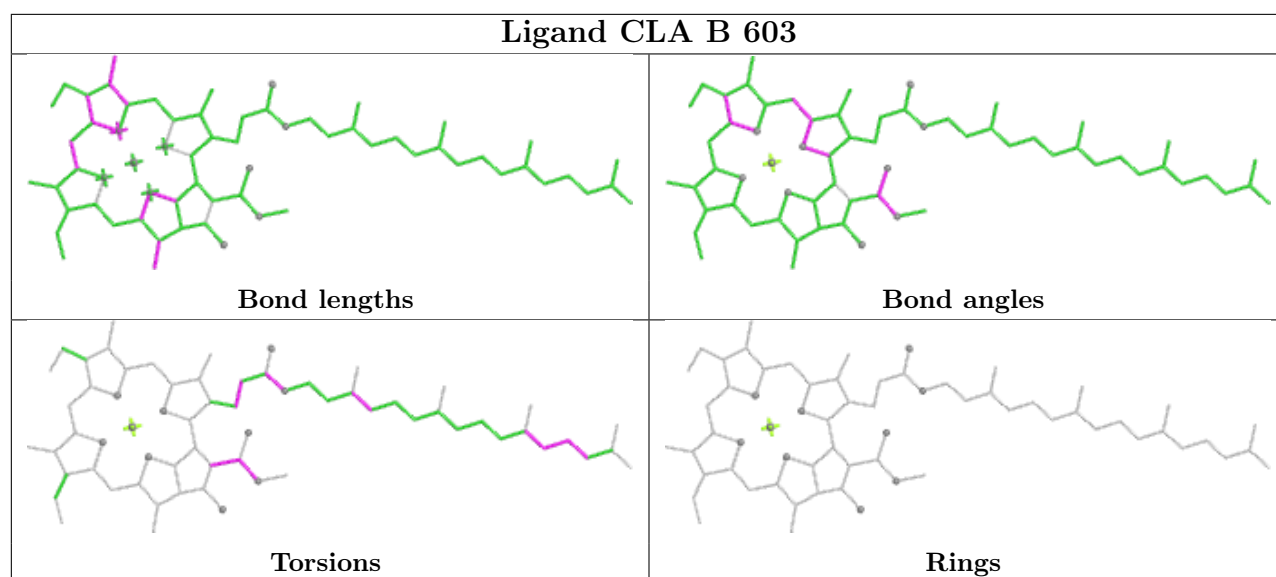
Torsions

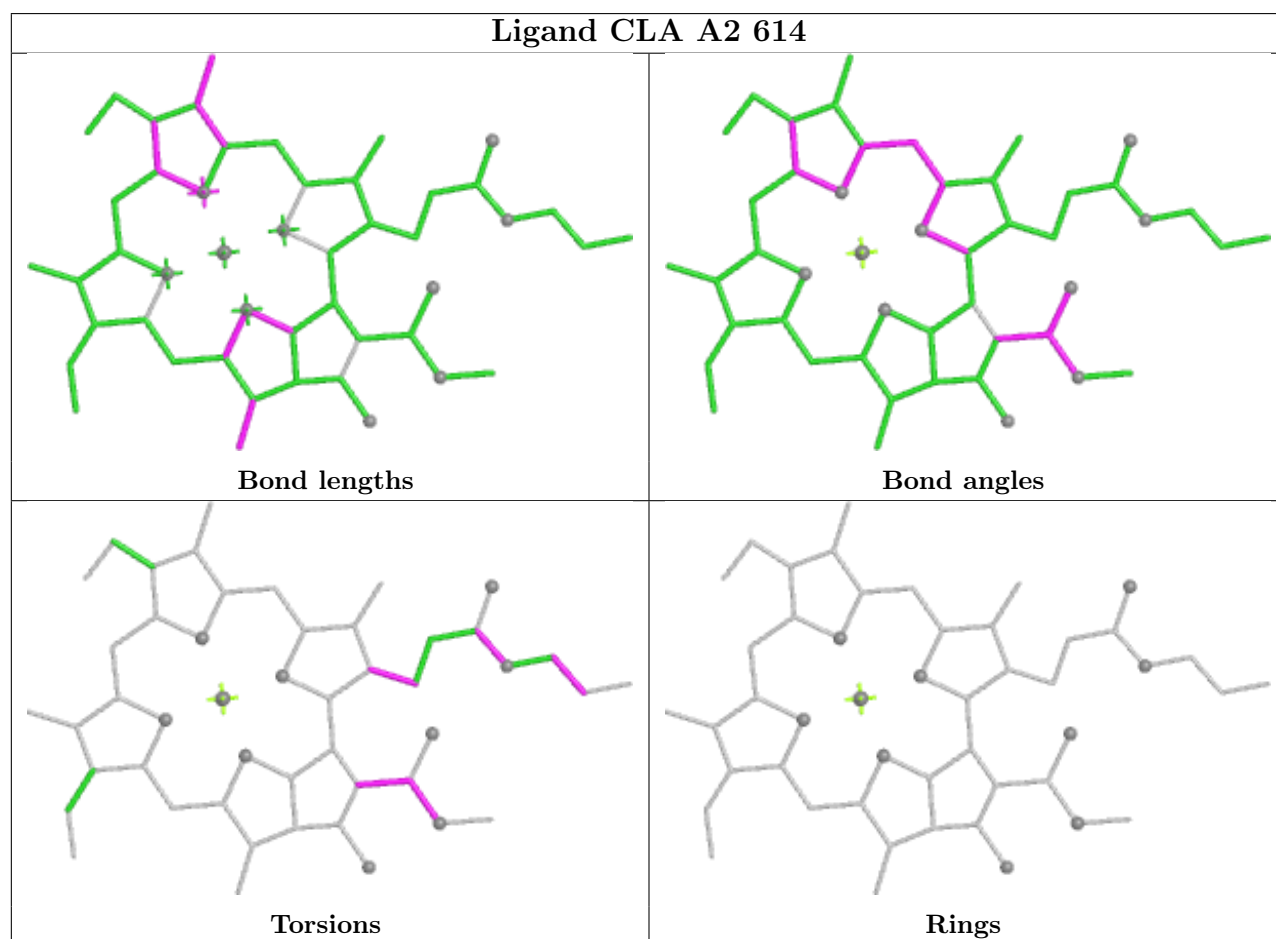
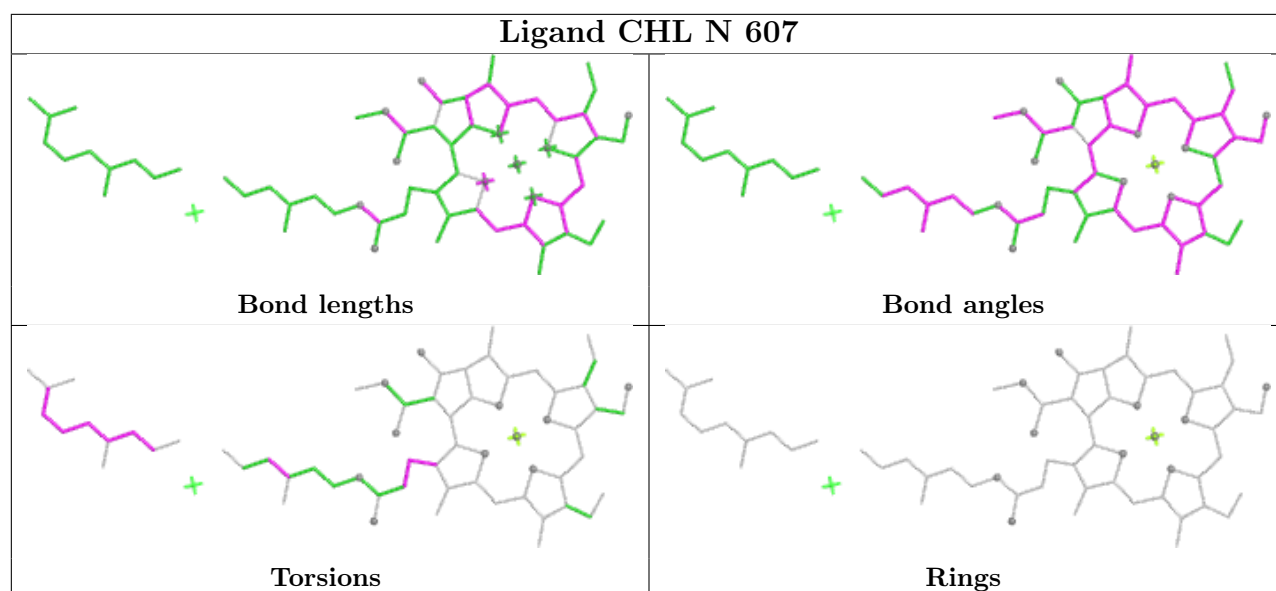


Rings

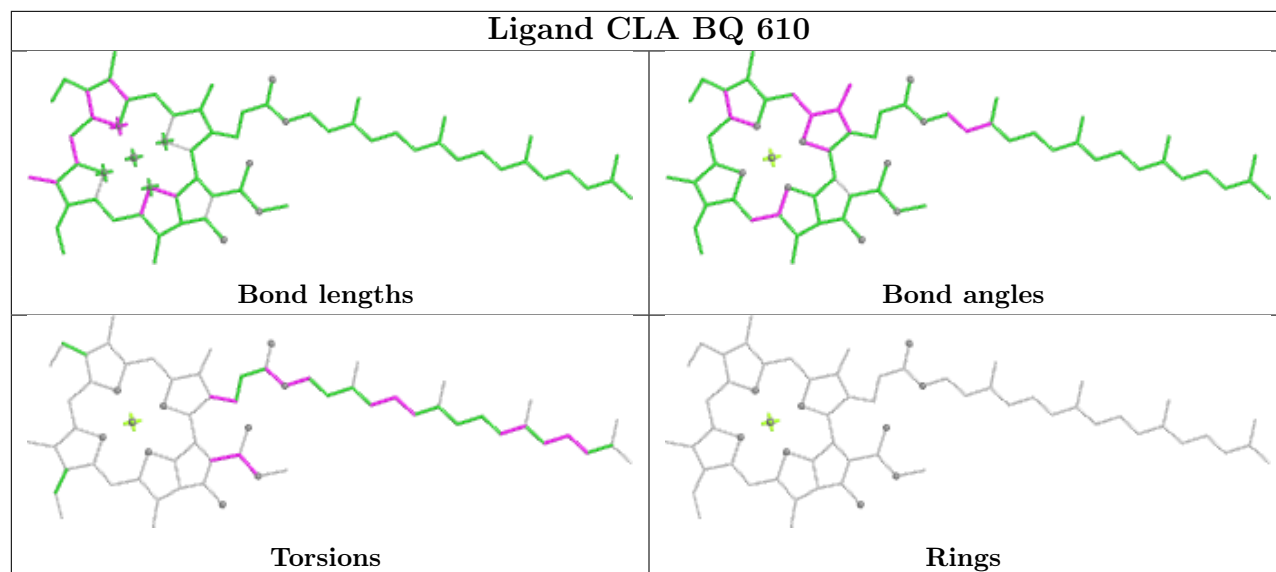




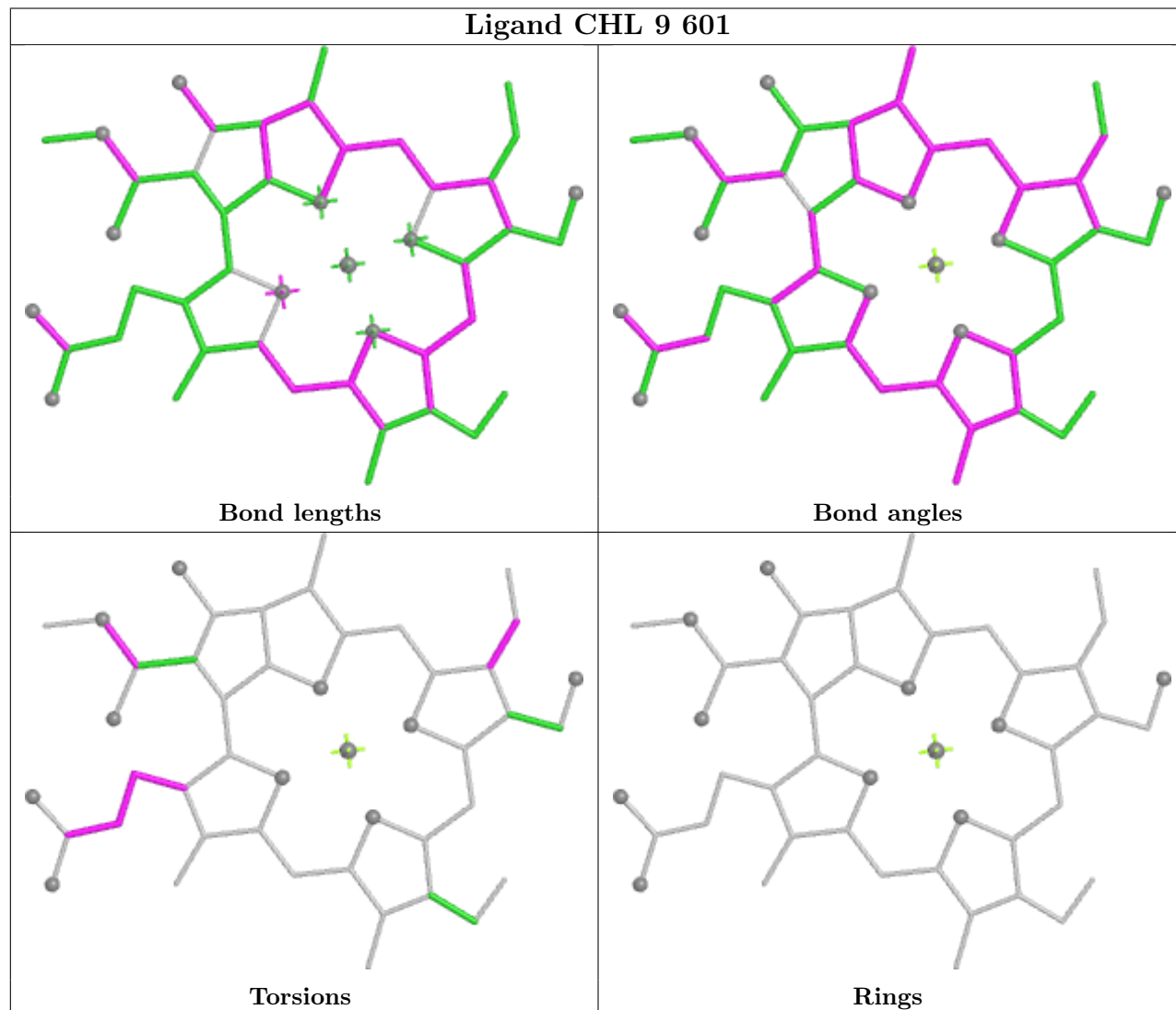


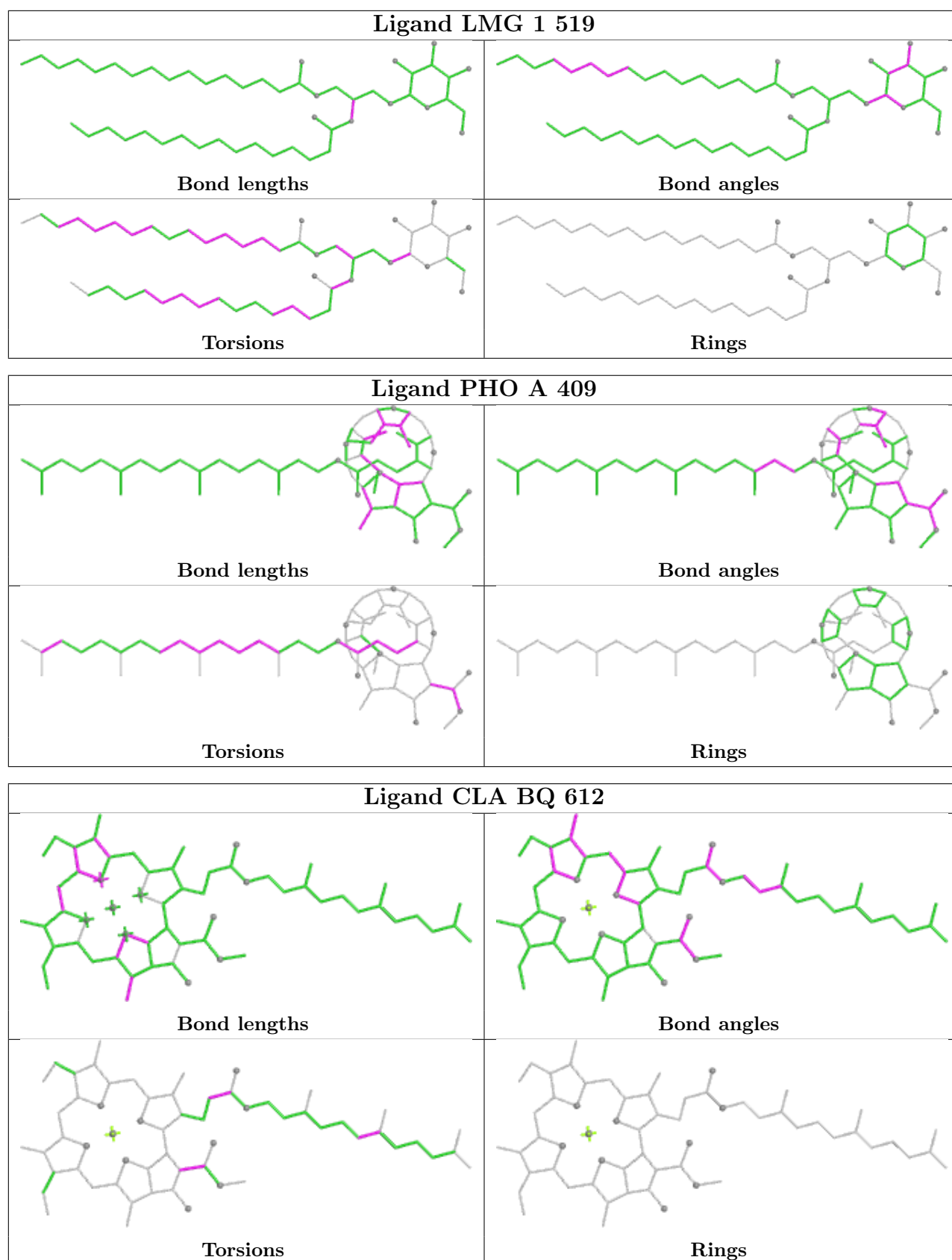


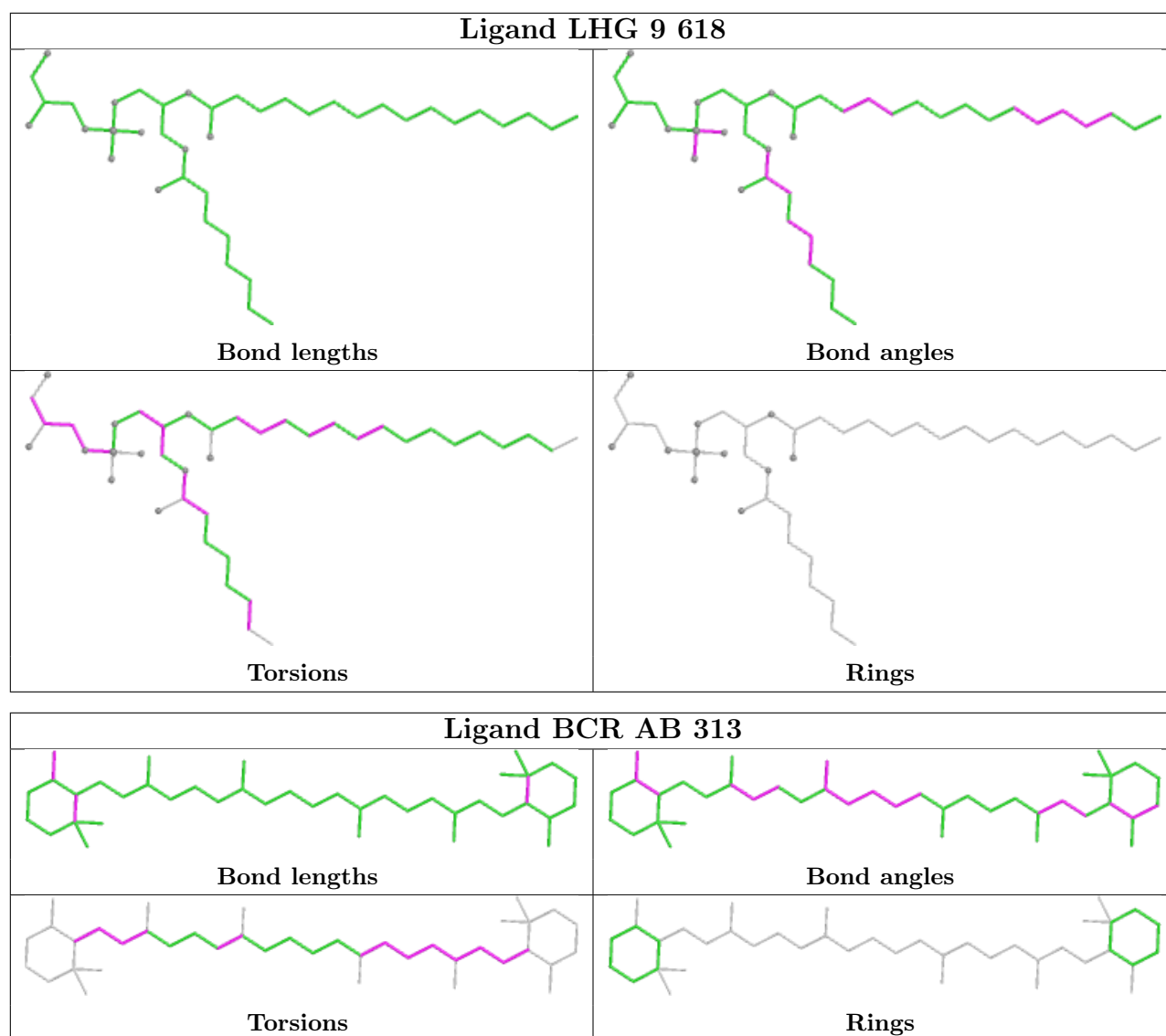
Ligand CLA BQ 610

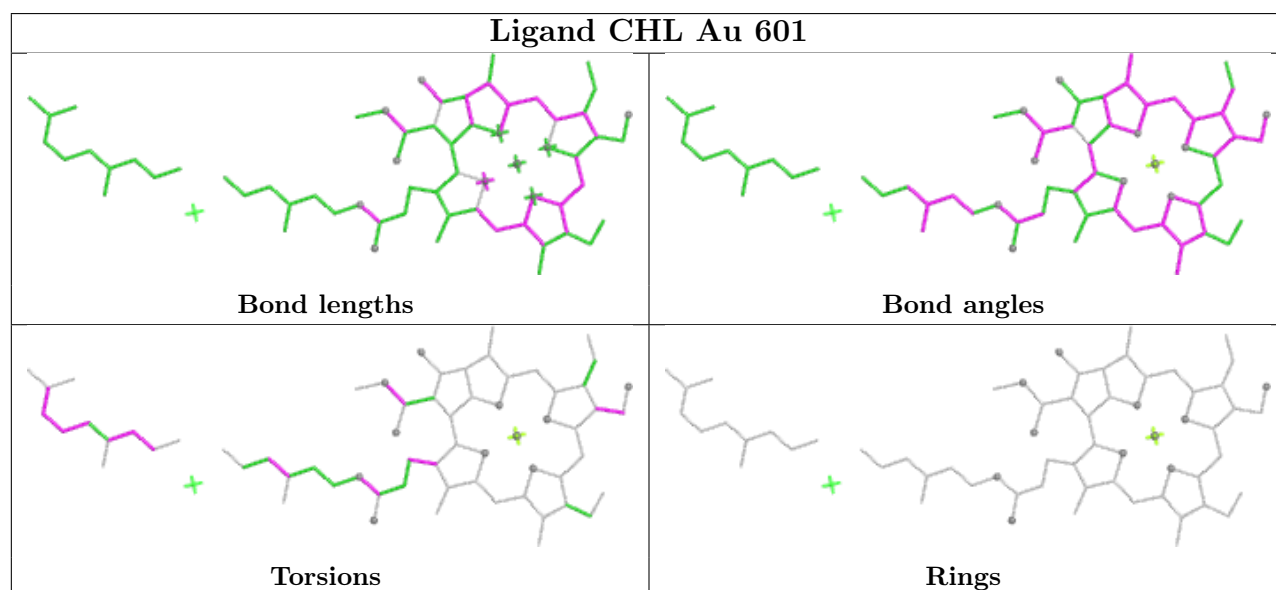
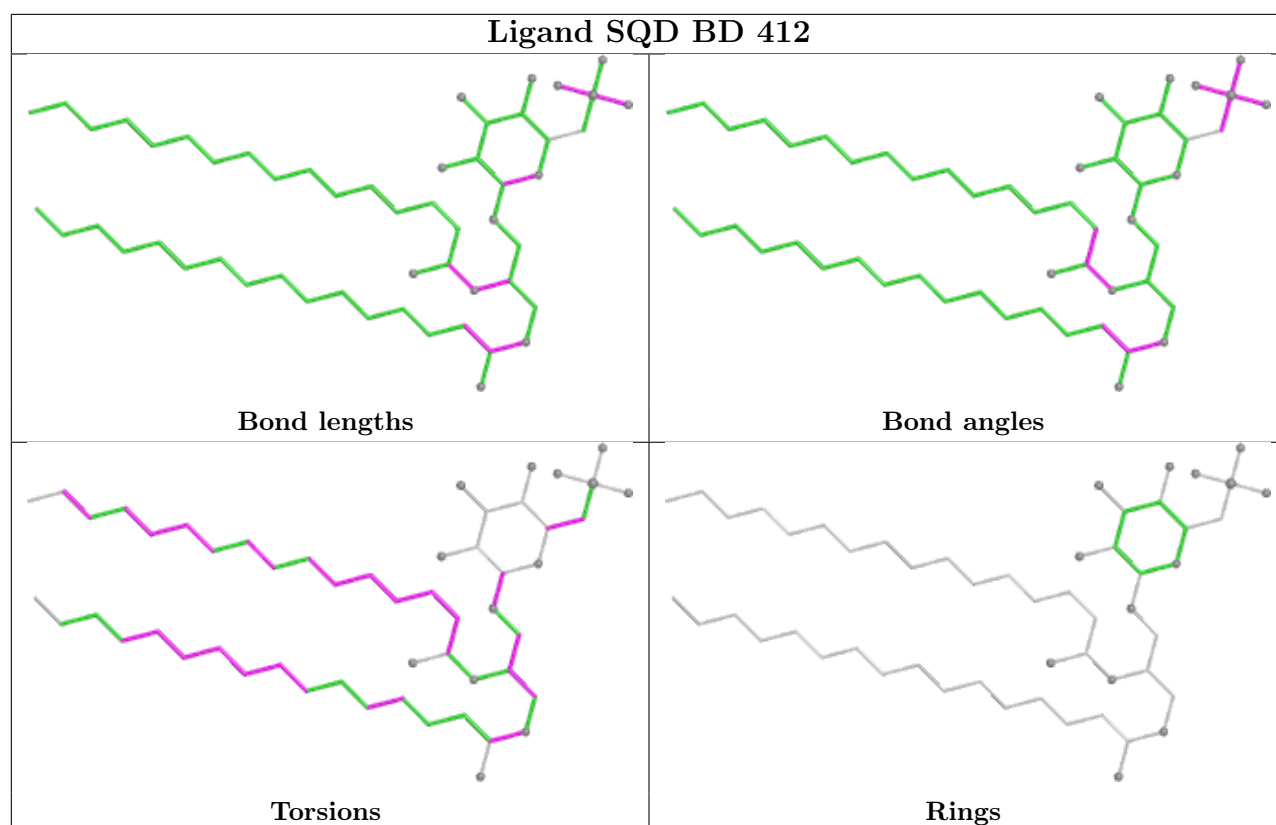


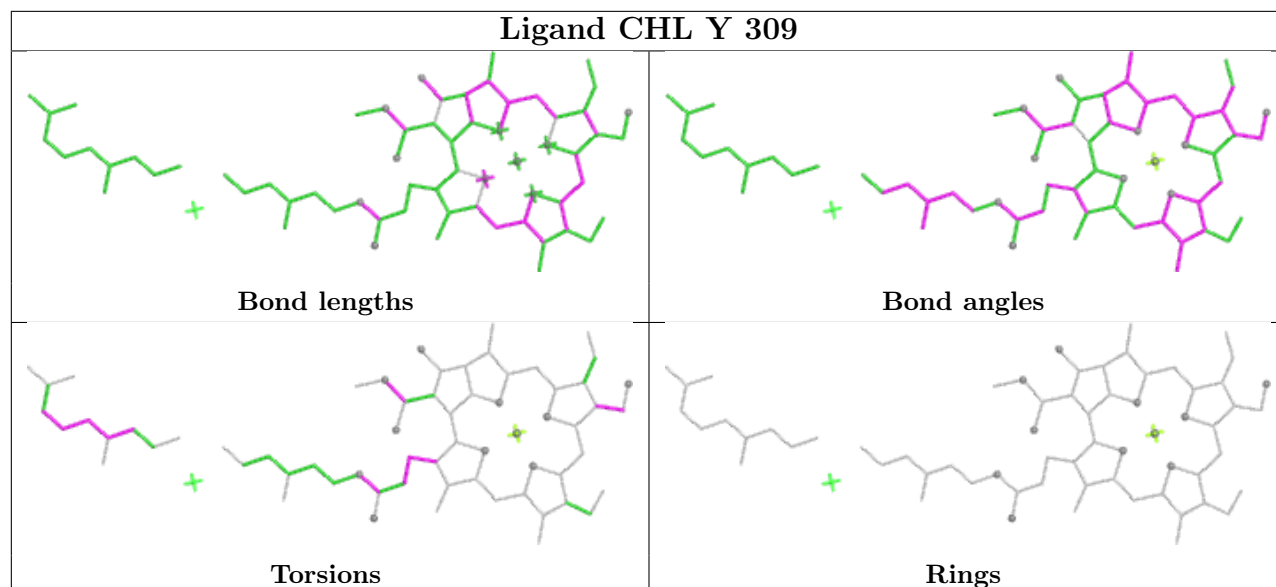
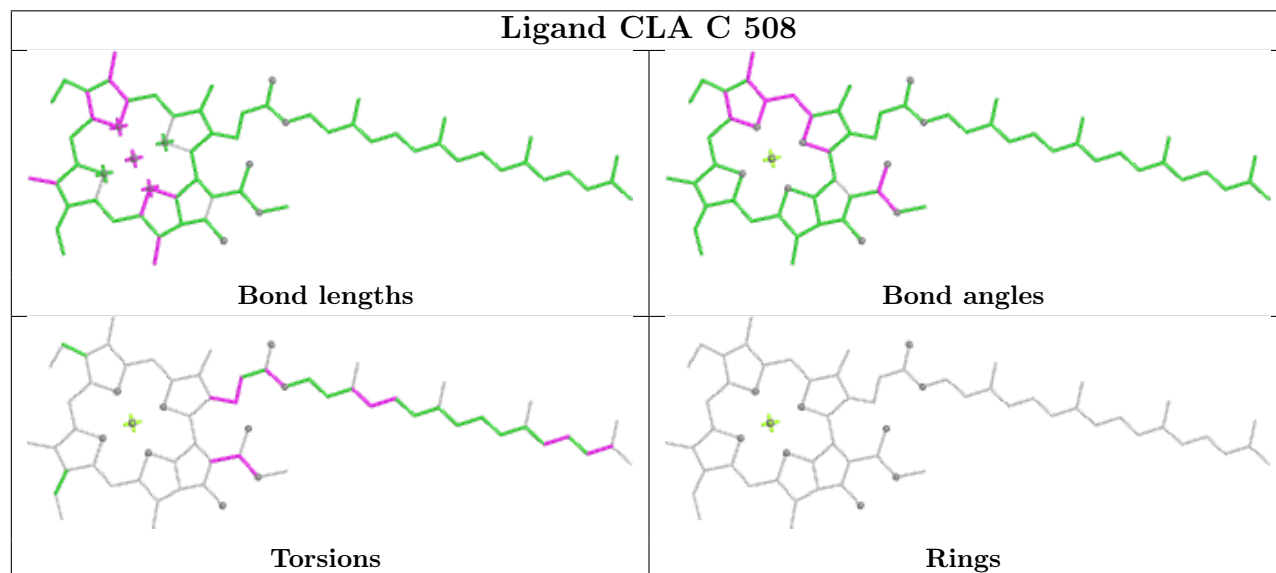
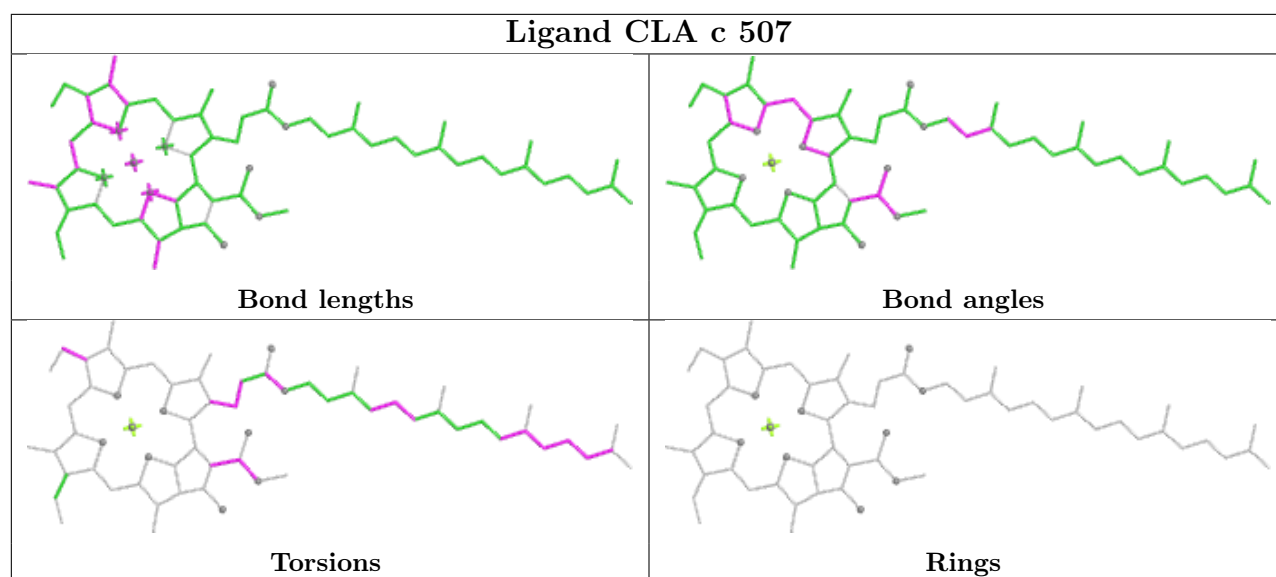
Ligand CHL 9 601

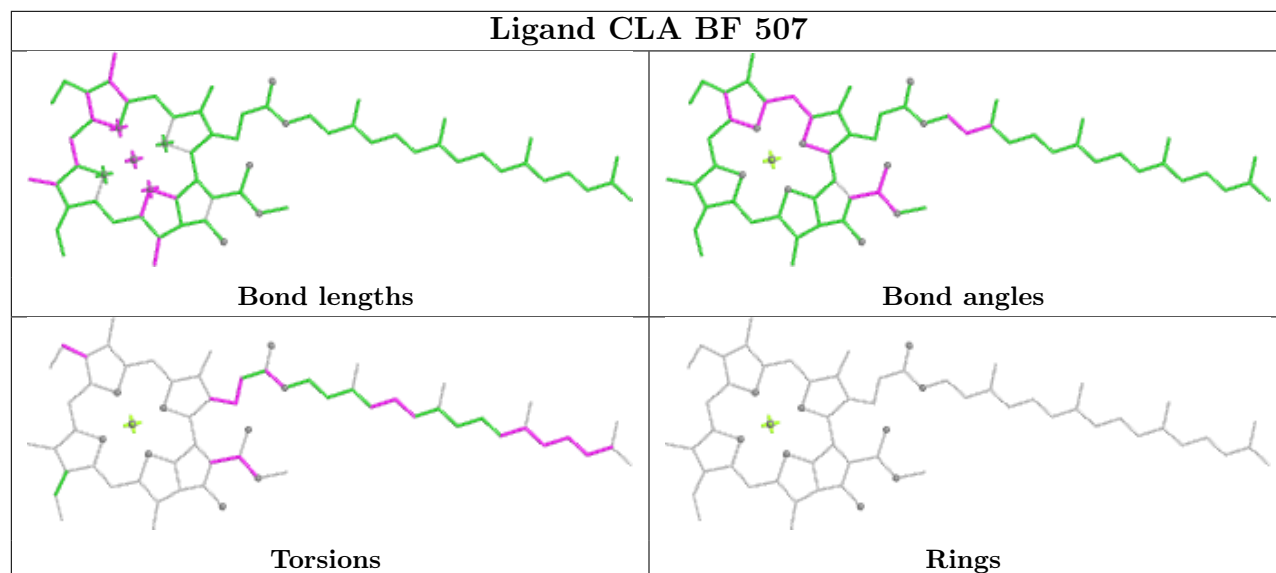
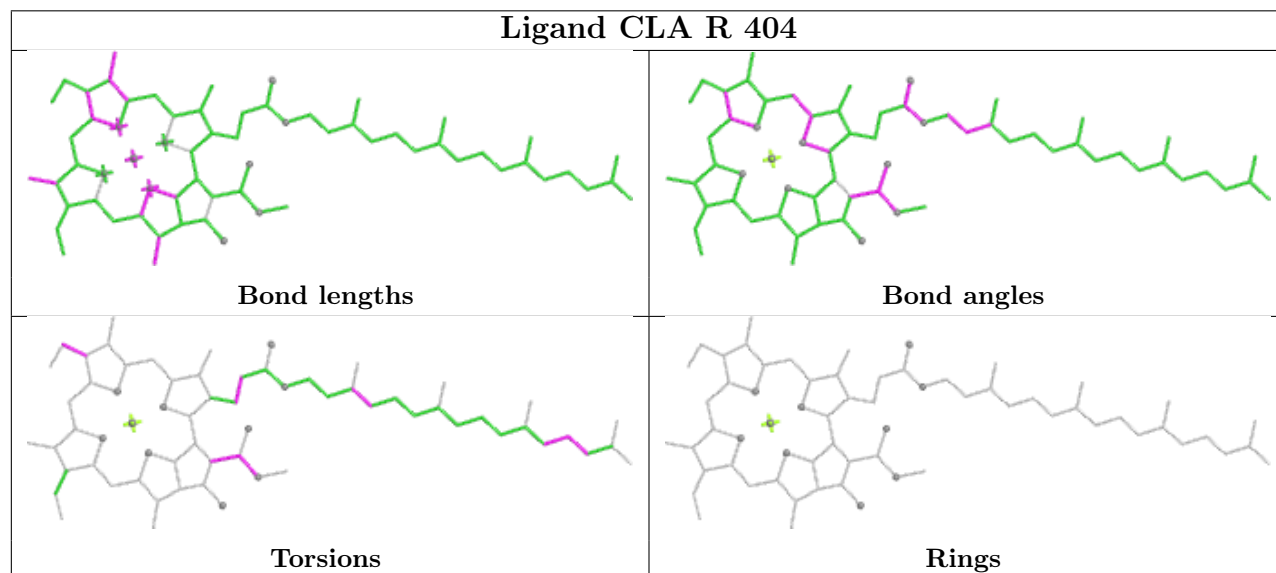
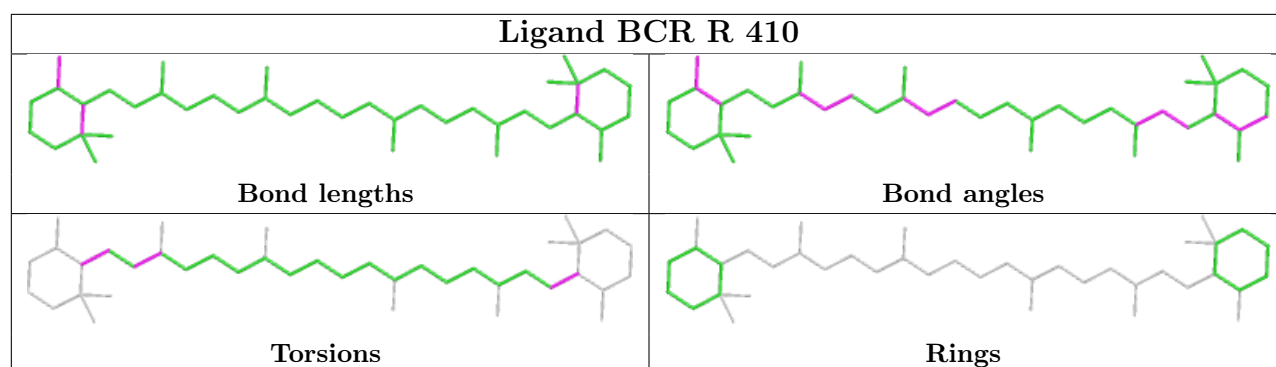


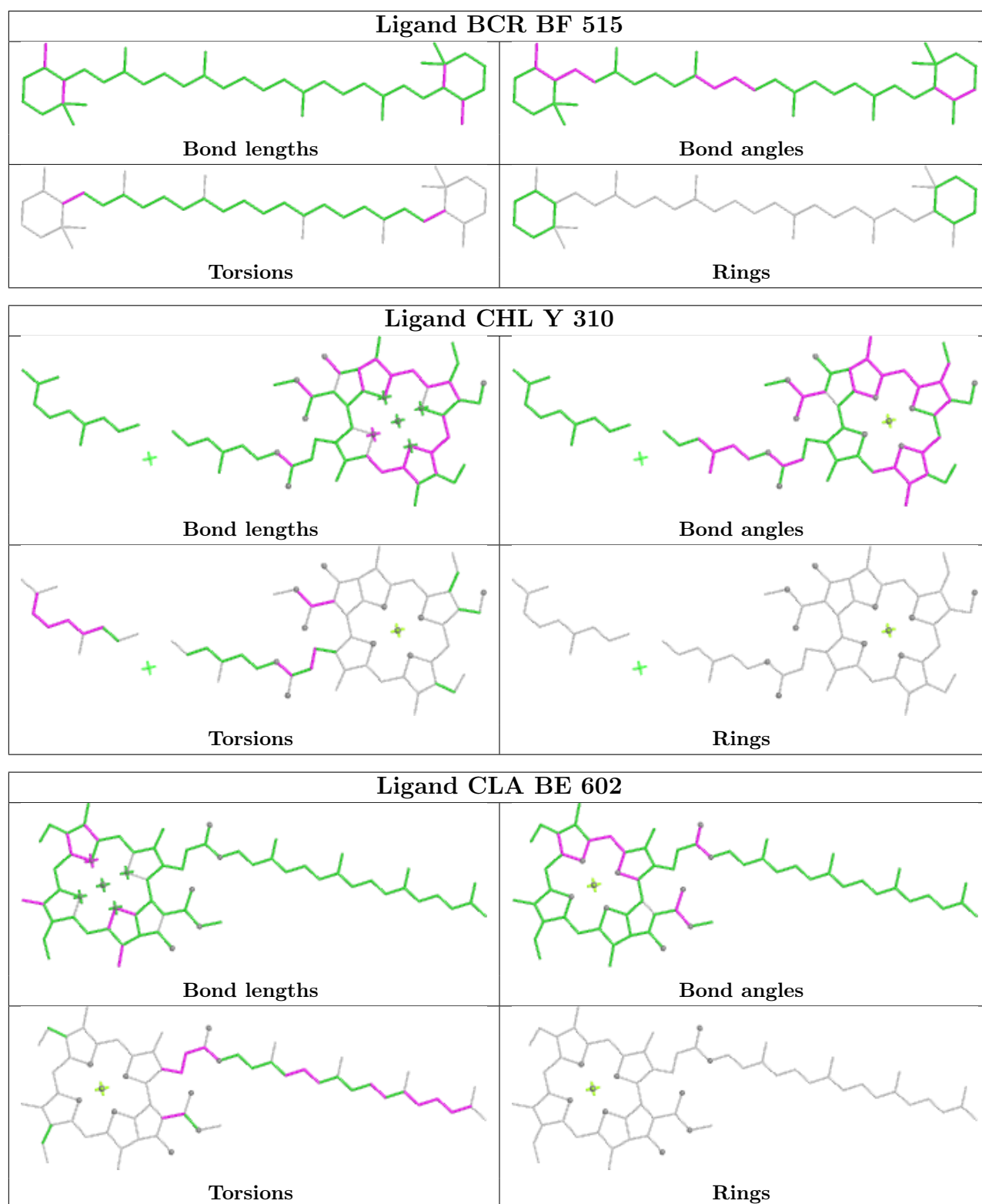


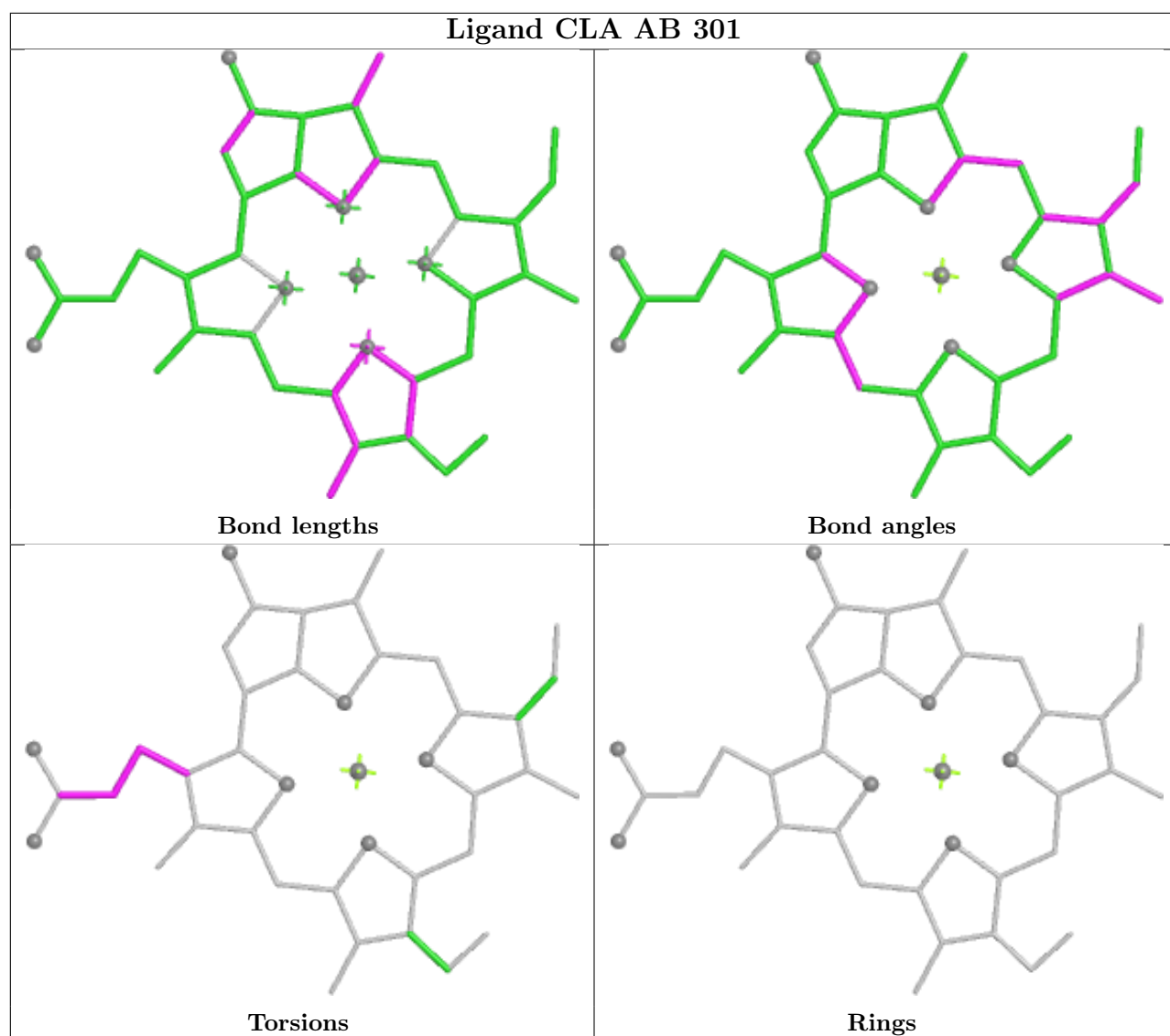




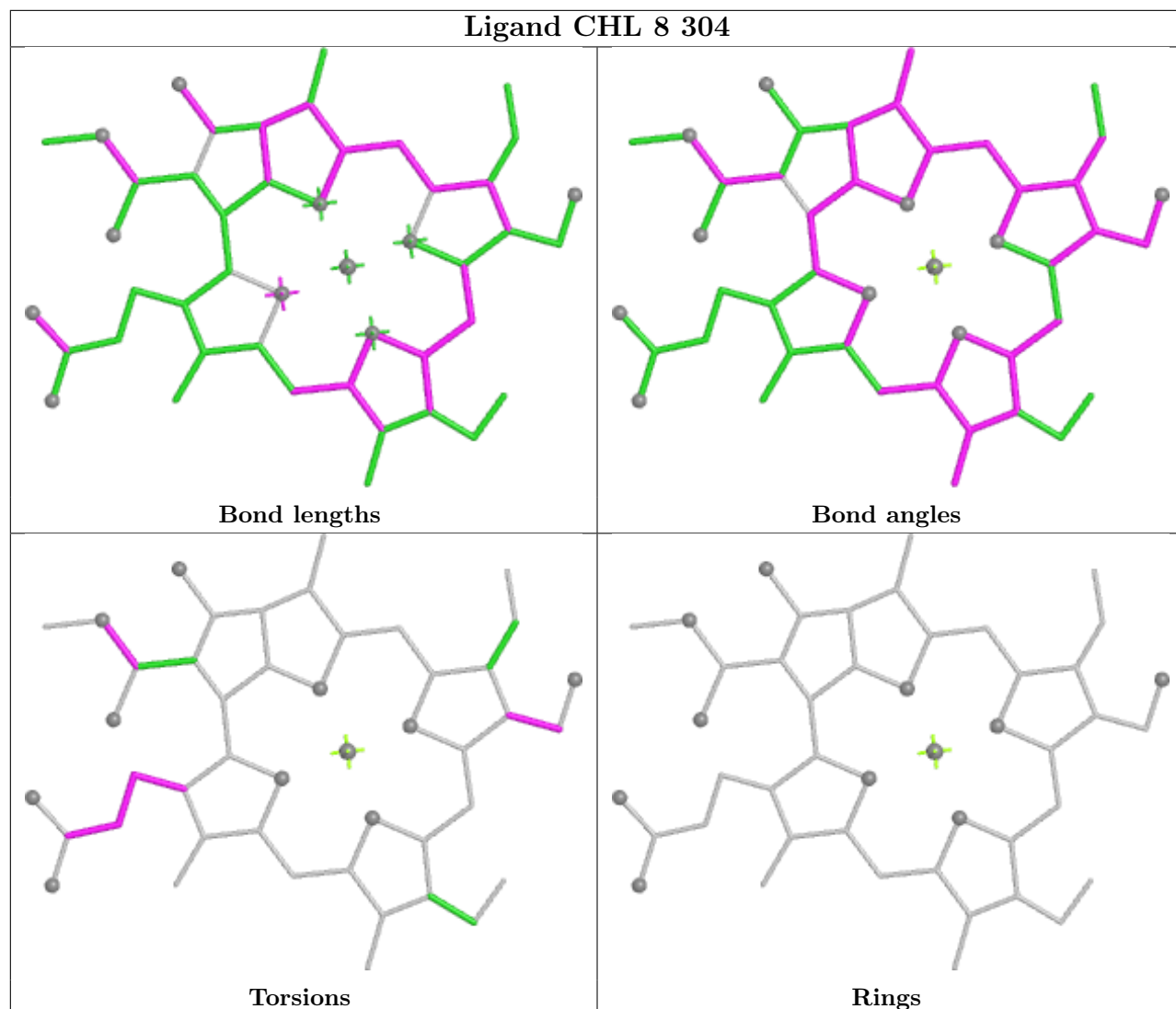


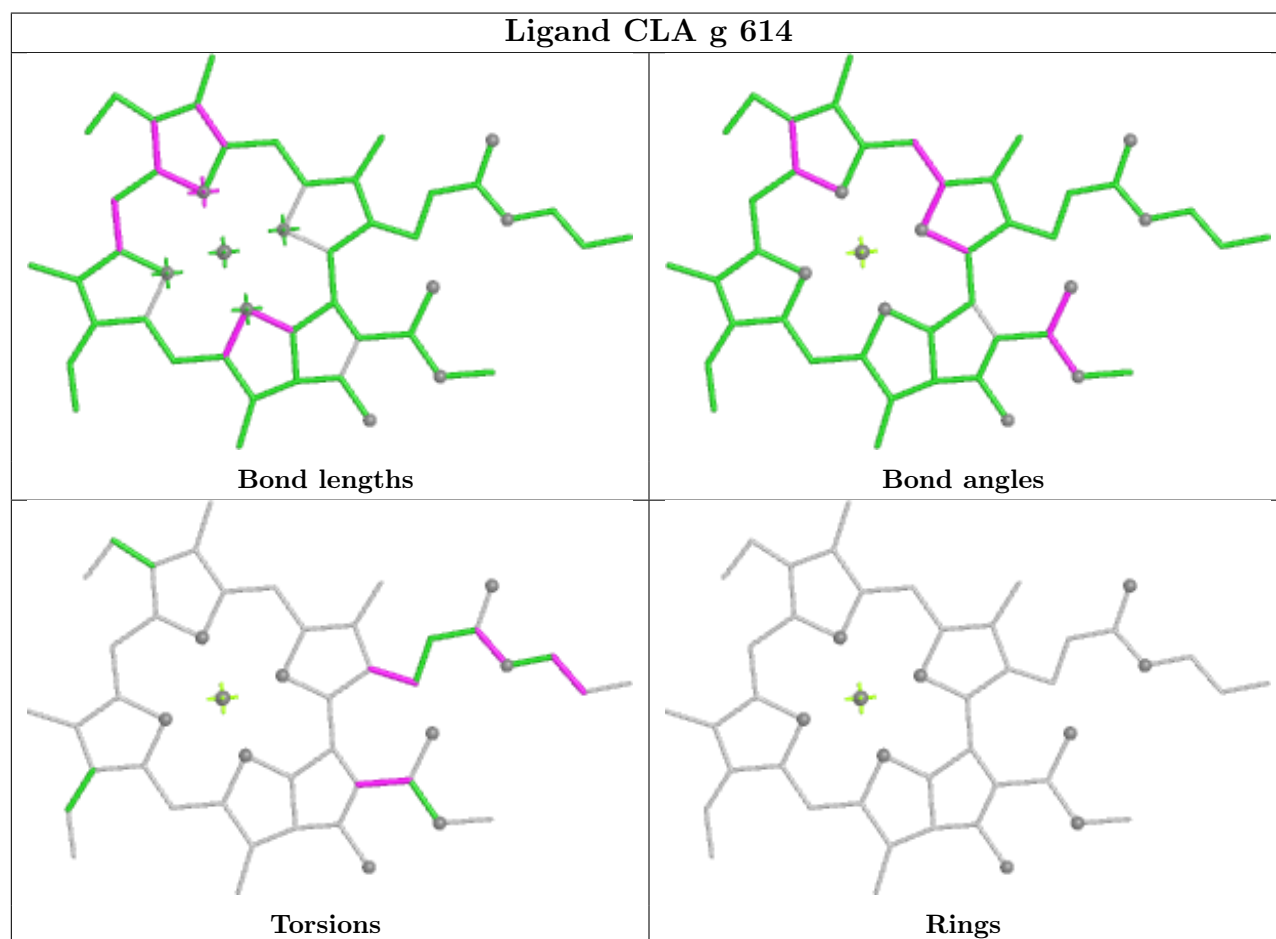
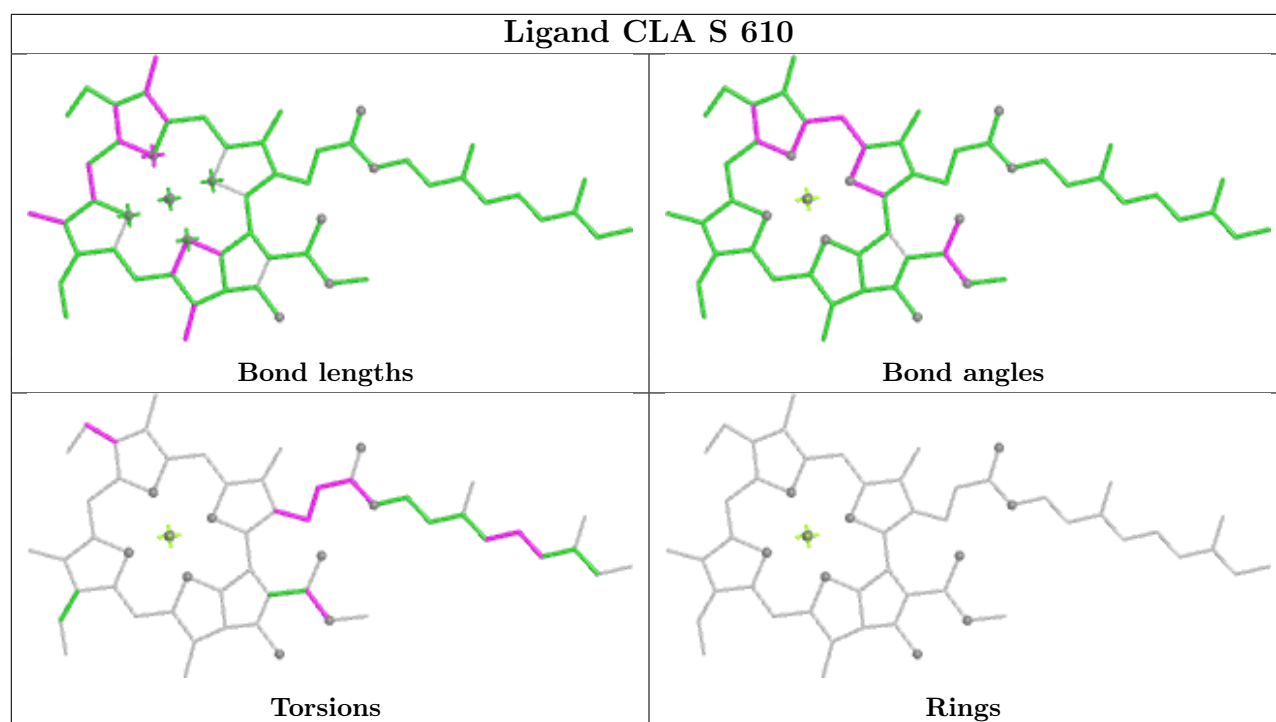


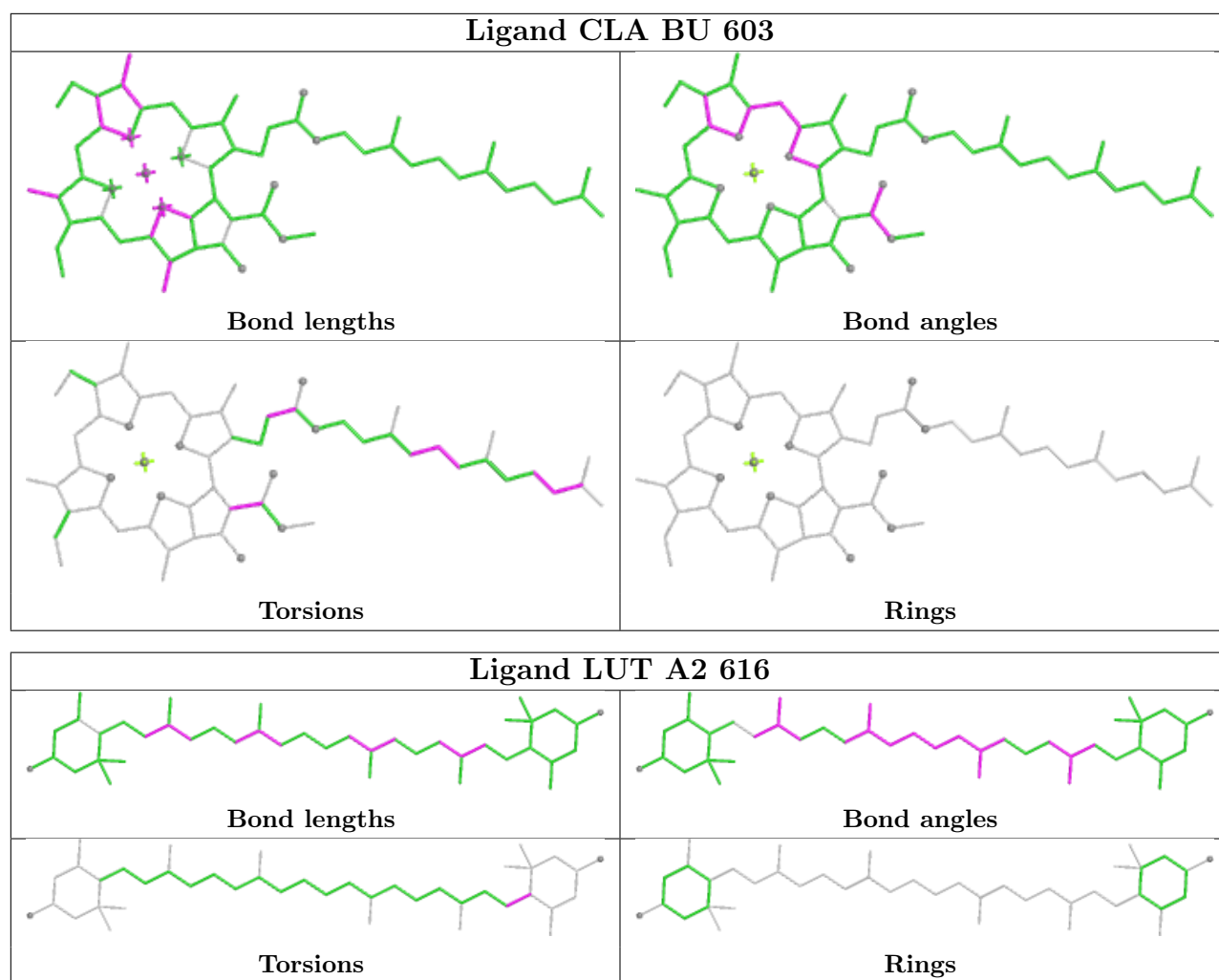


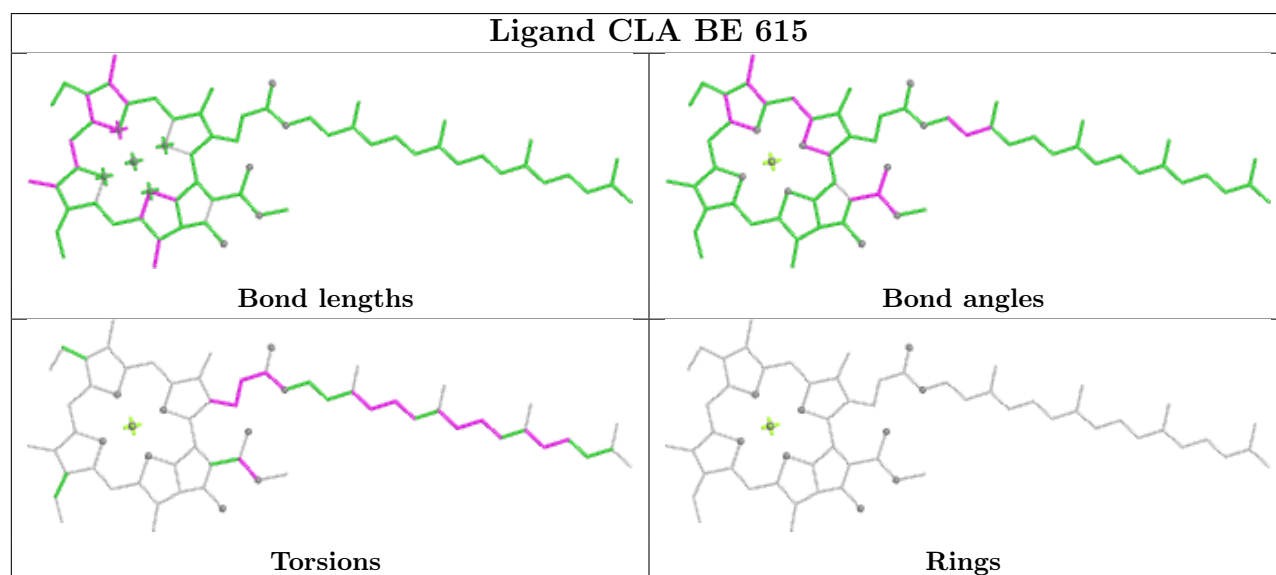
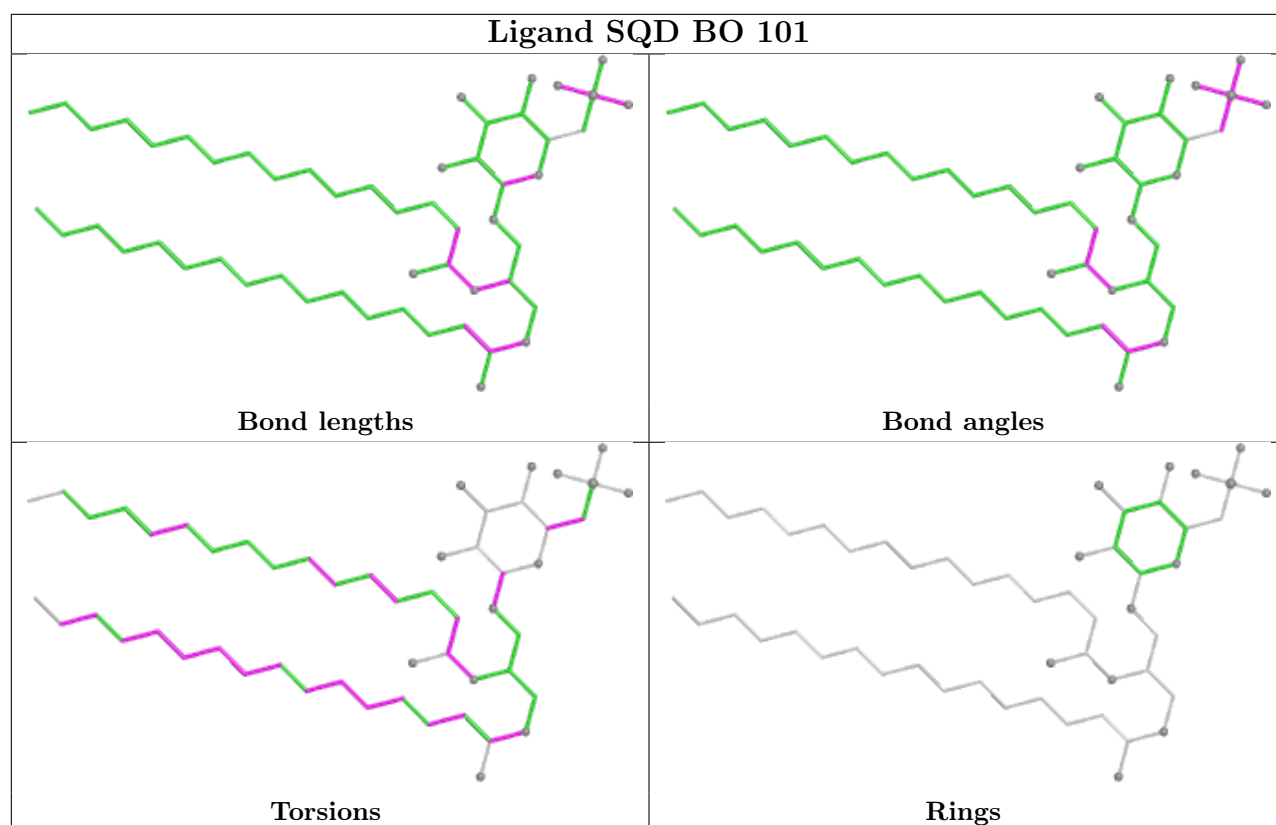


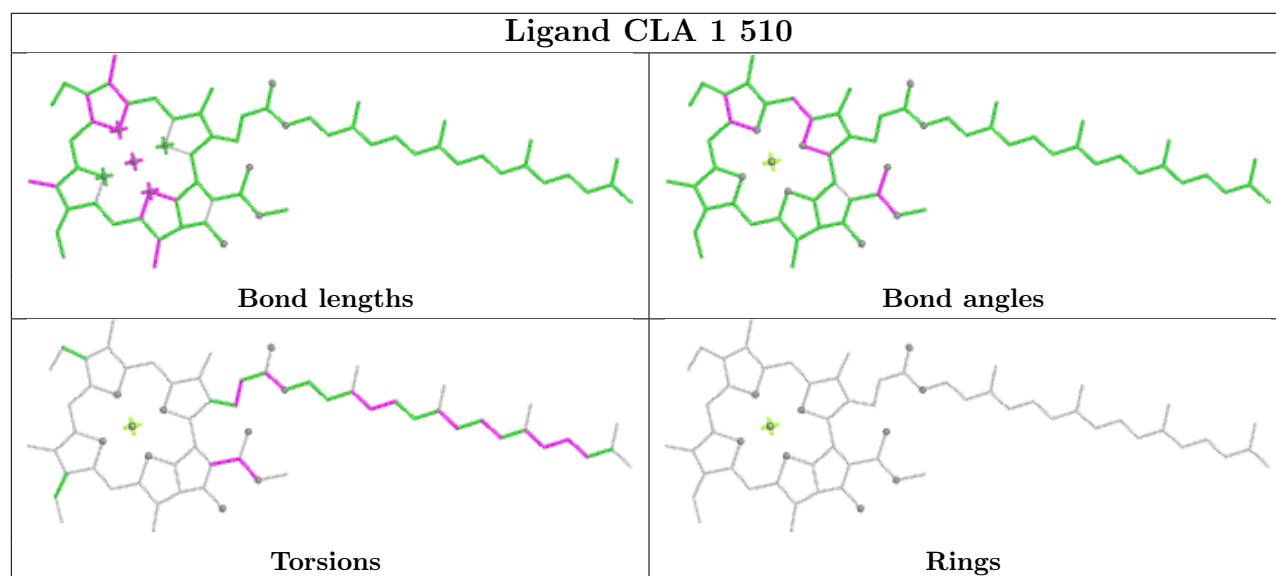
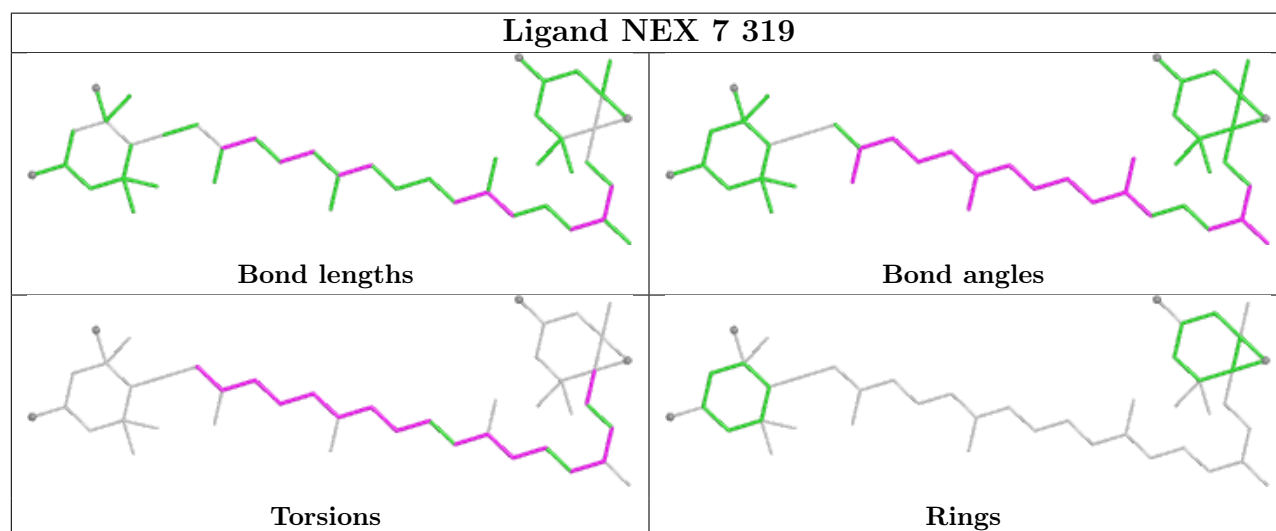
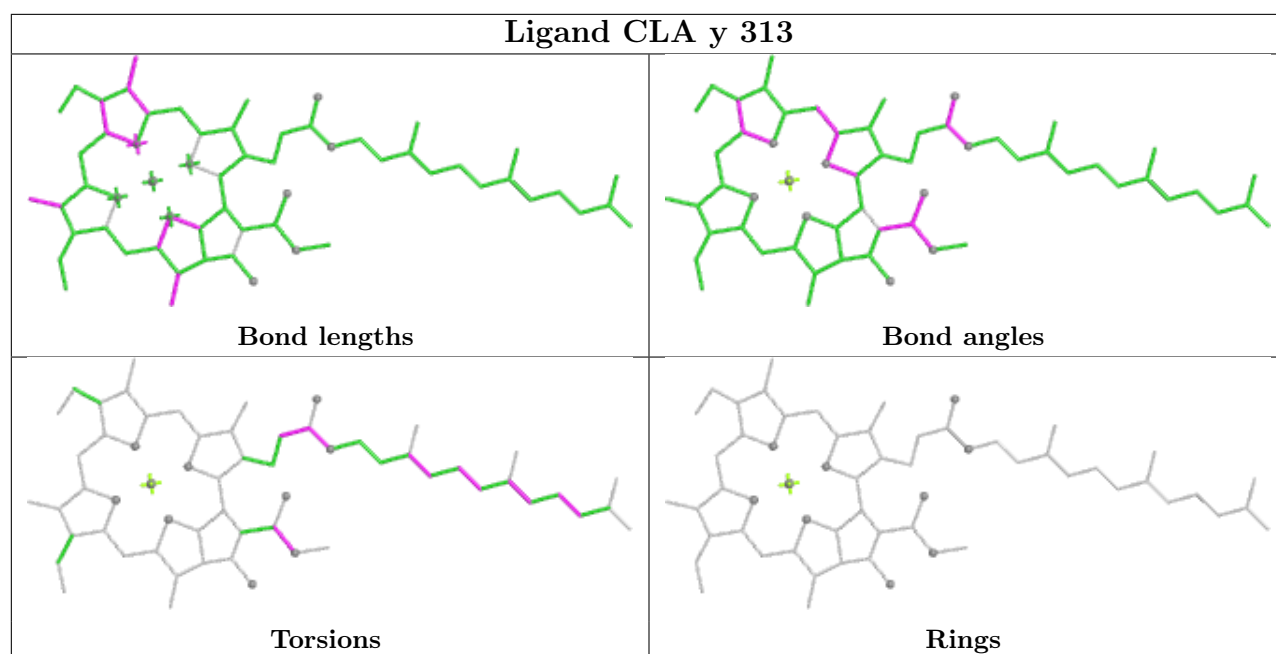
Ligand CHL 8 304

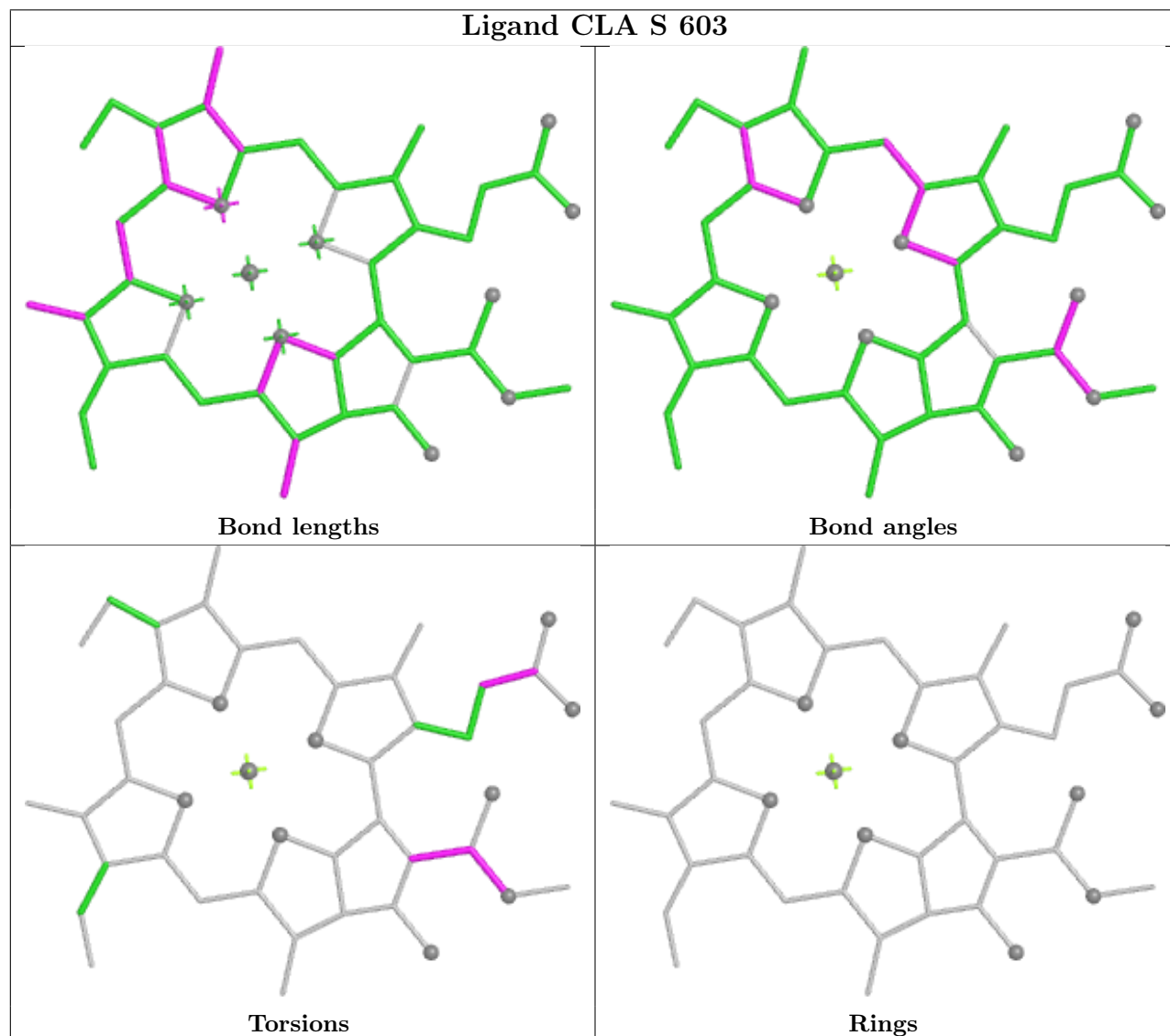
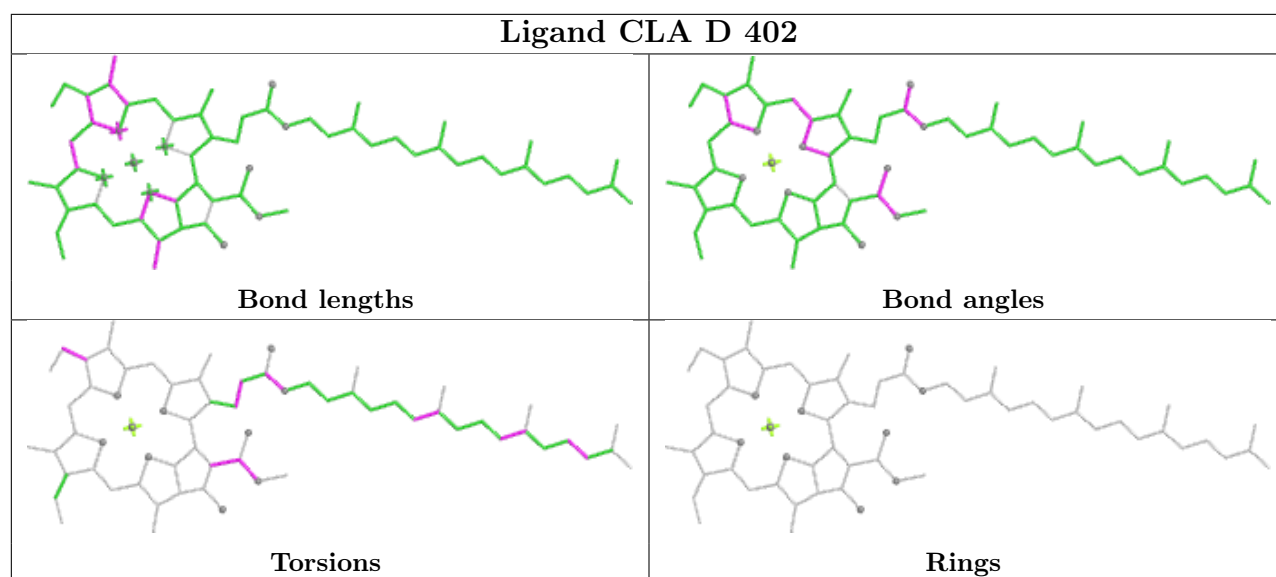




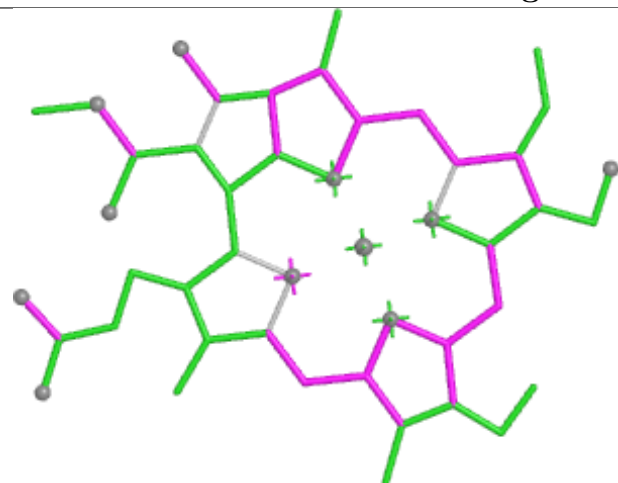




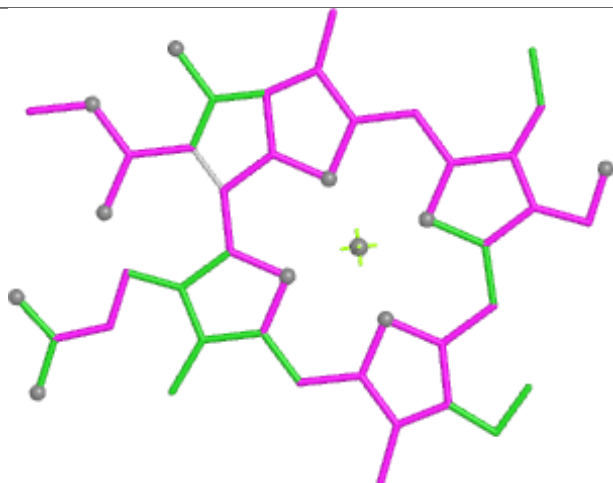




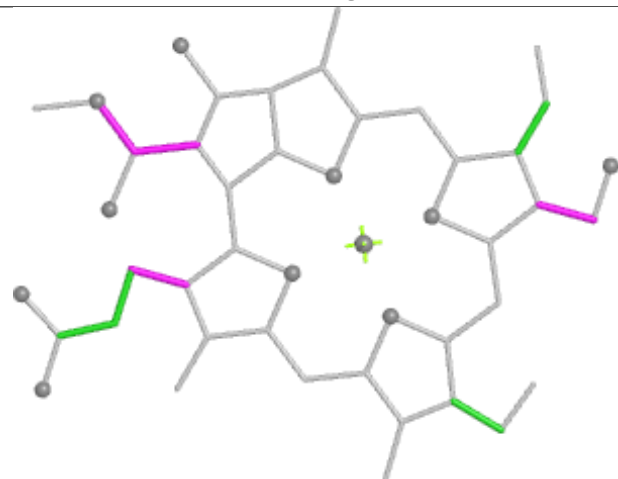
Ligand CHL 8 306



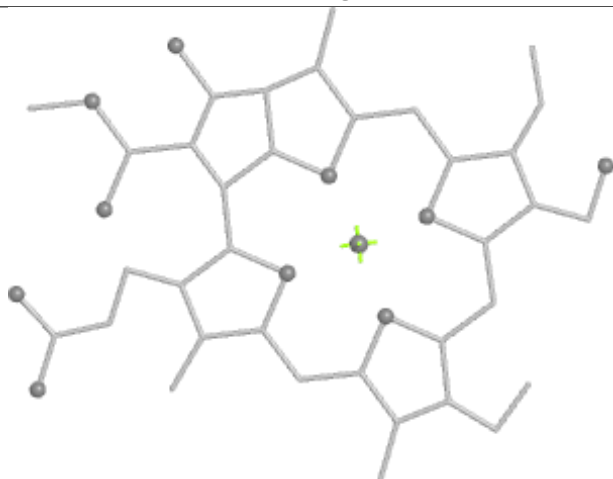
Bond lengths



Bond angles

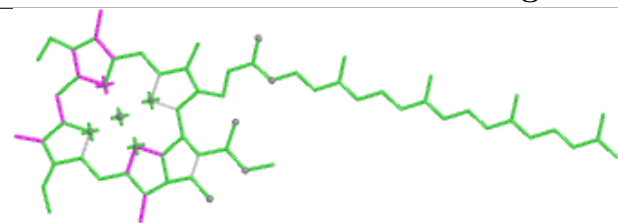


Torsions

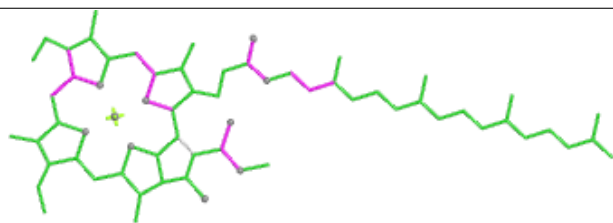


Rings

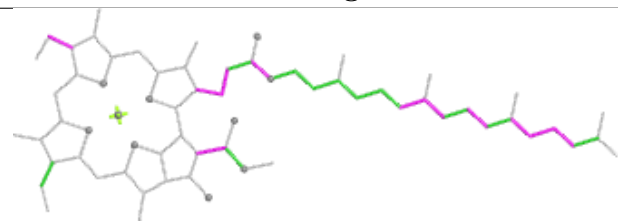
Ligand CLA b 613



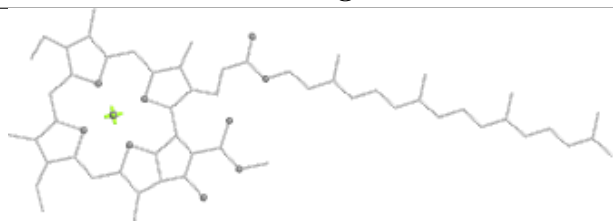
Bond lengths



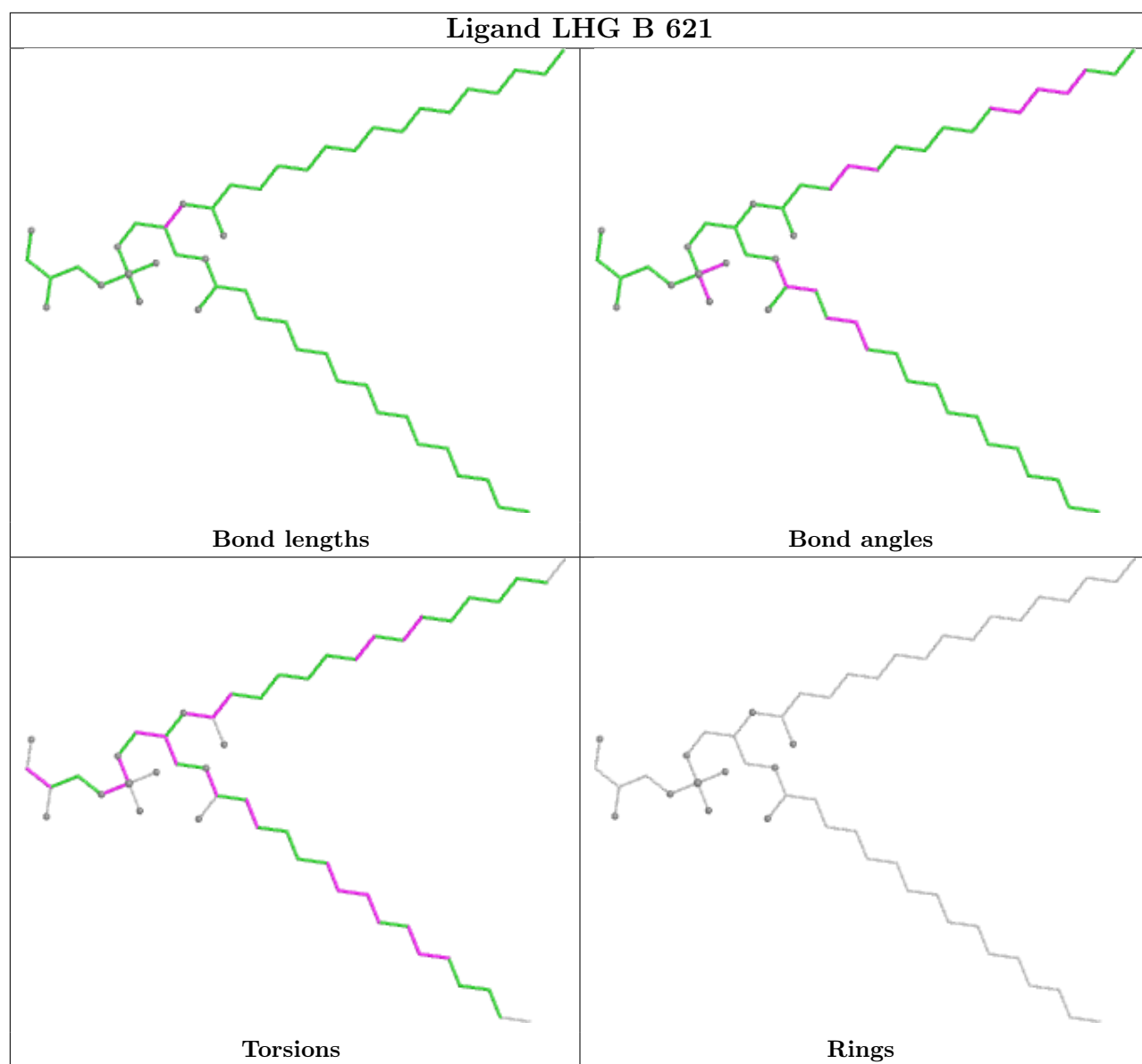
Bond angles



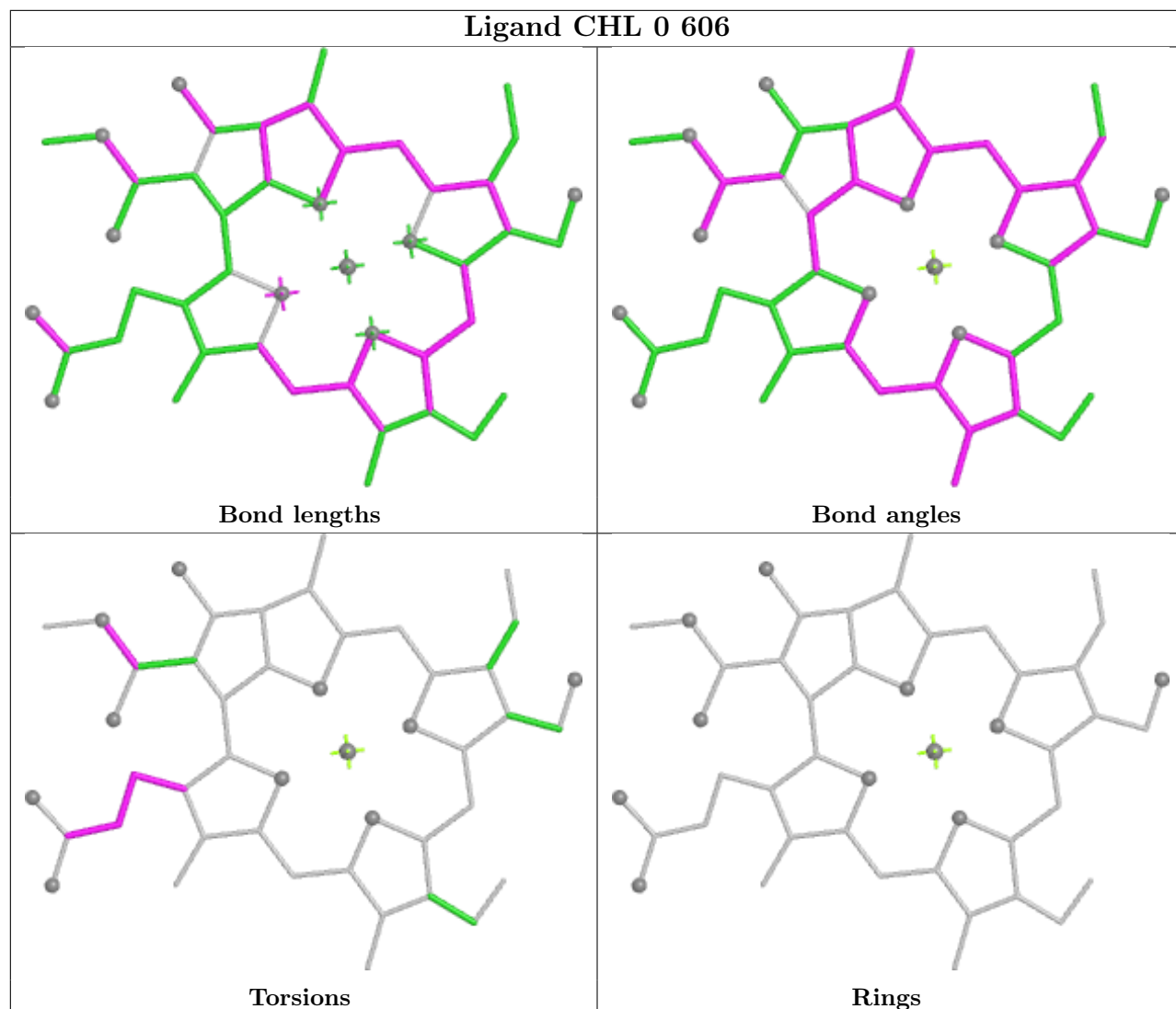
Torsions



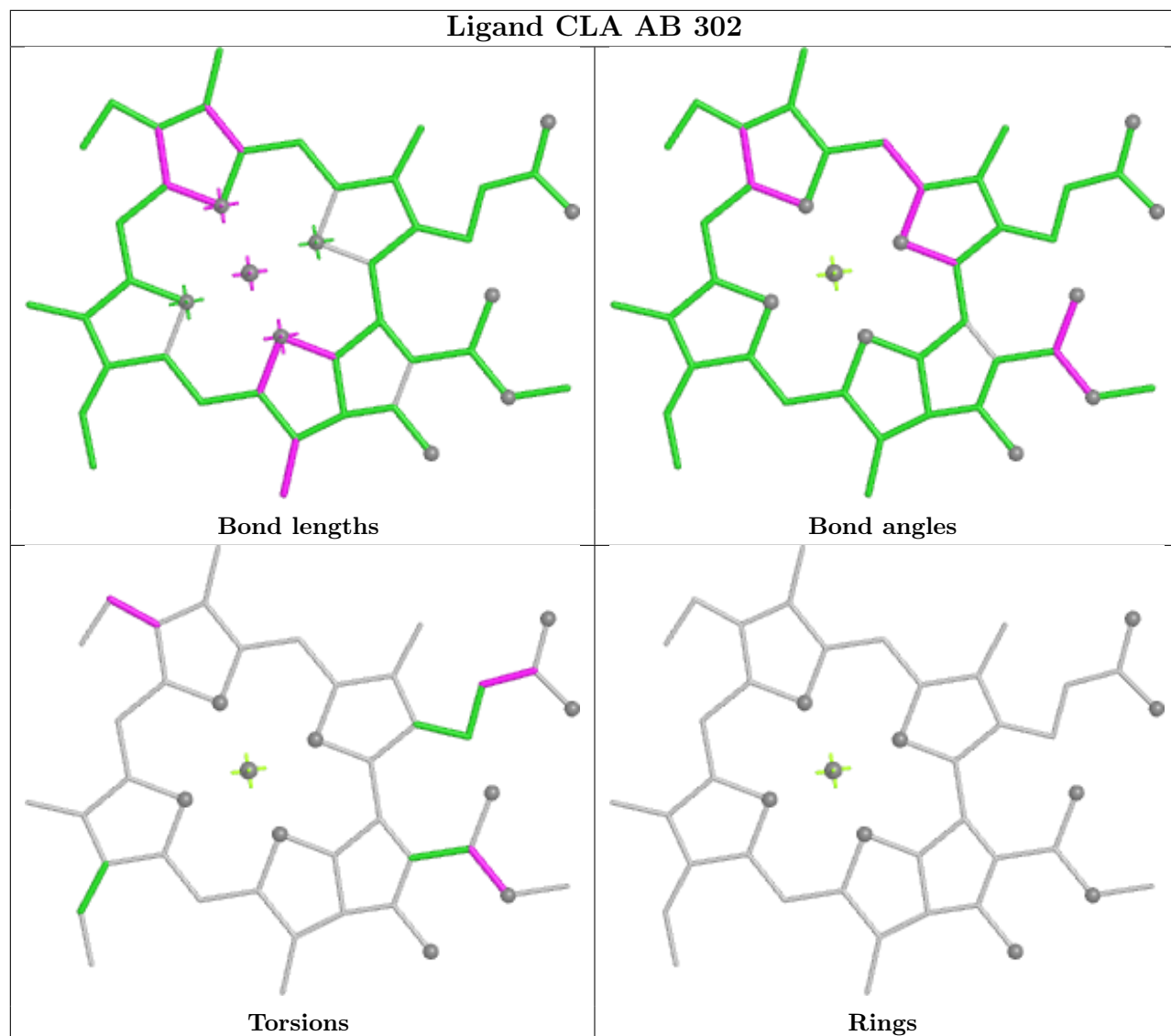
Rings



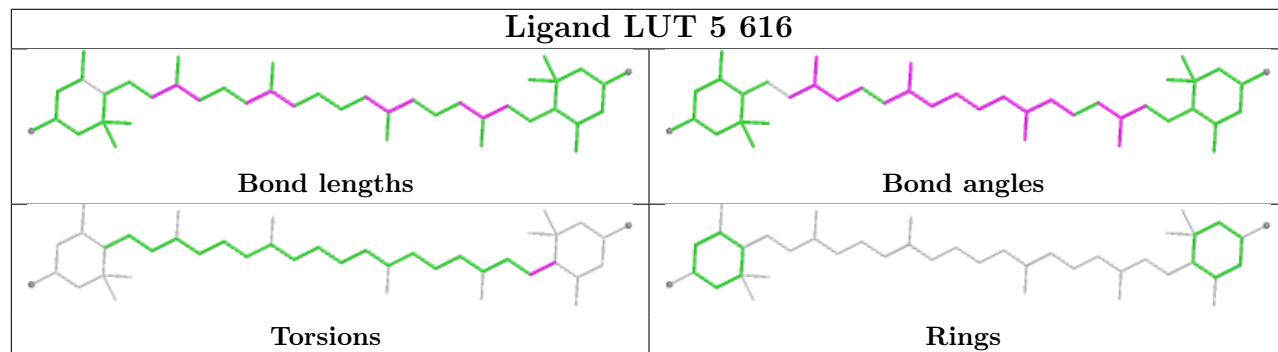
Ligand CHL 0 606

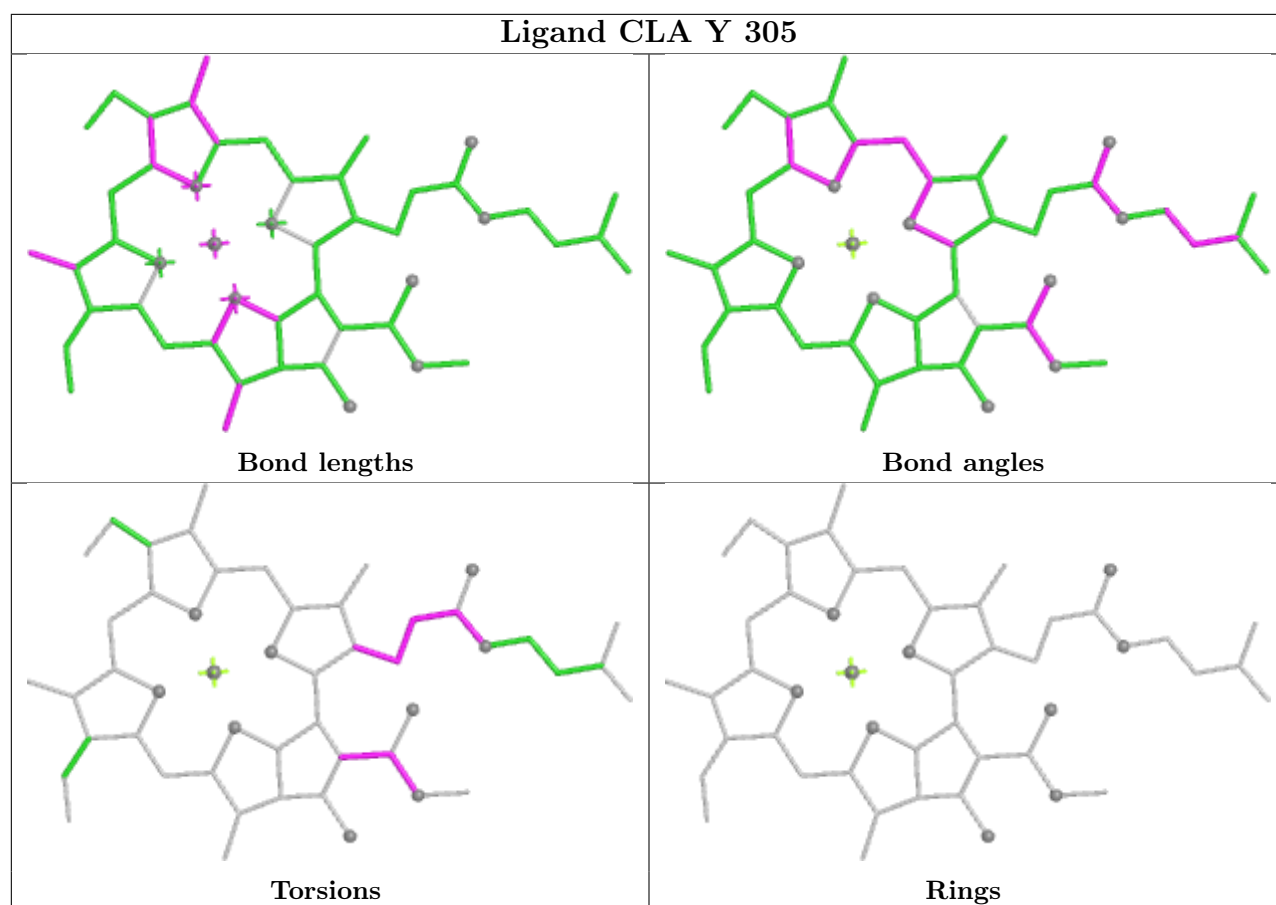


Ligand CLA AB 302

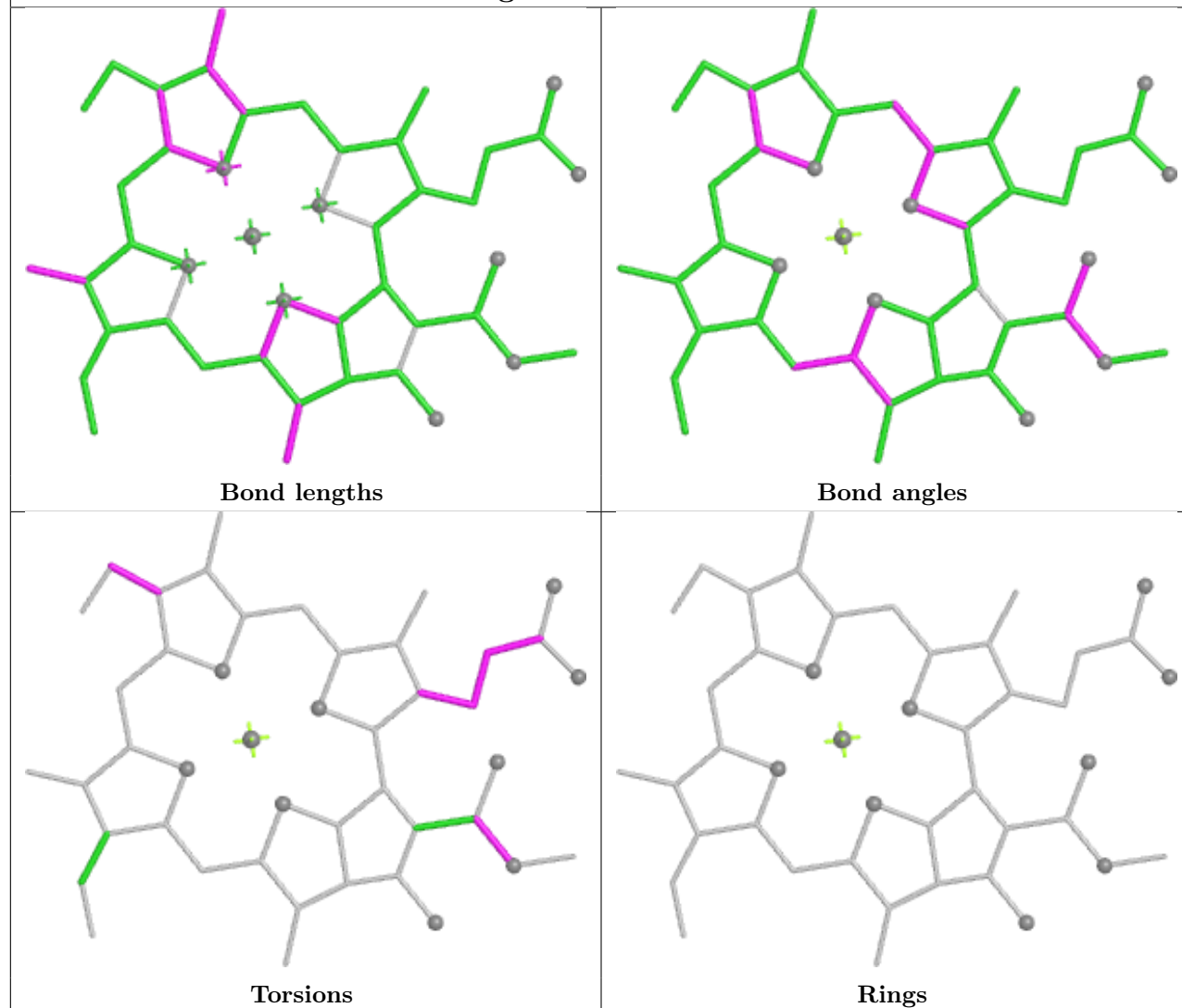


Ligand LUT 5 616

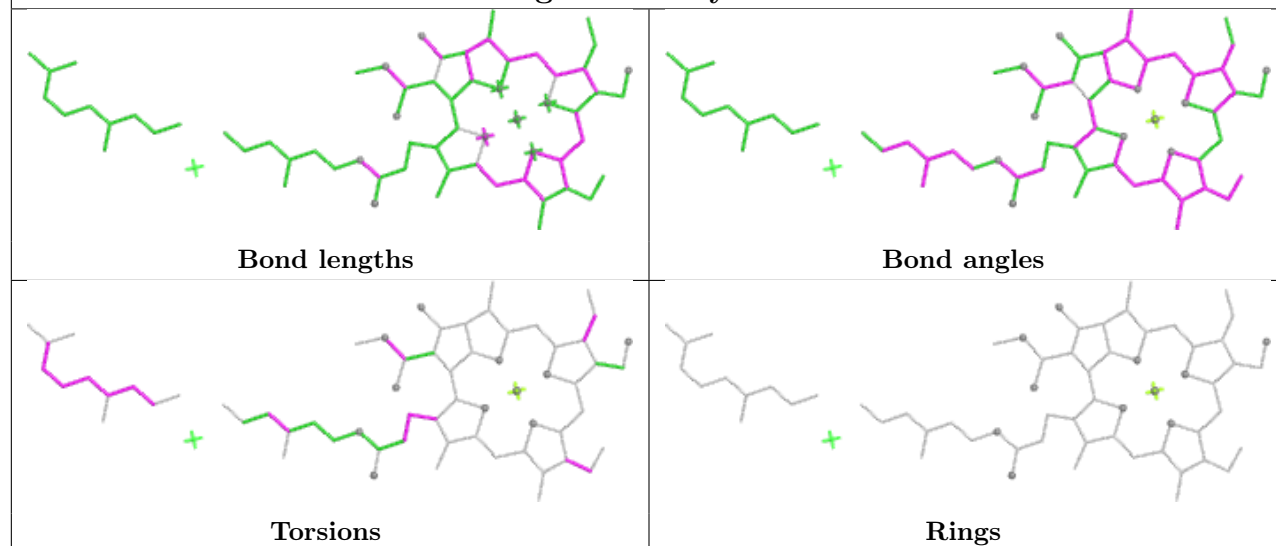


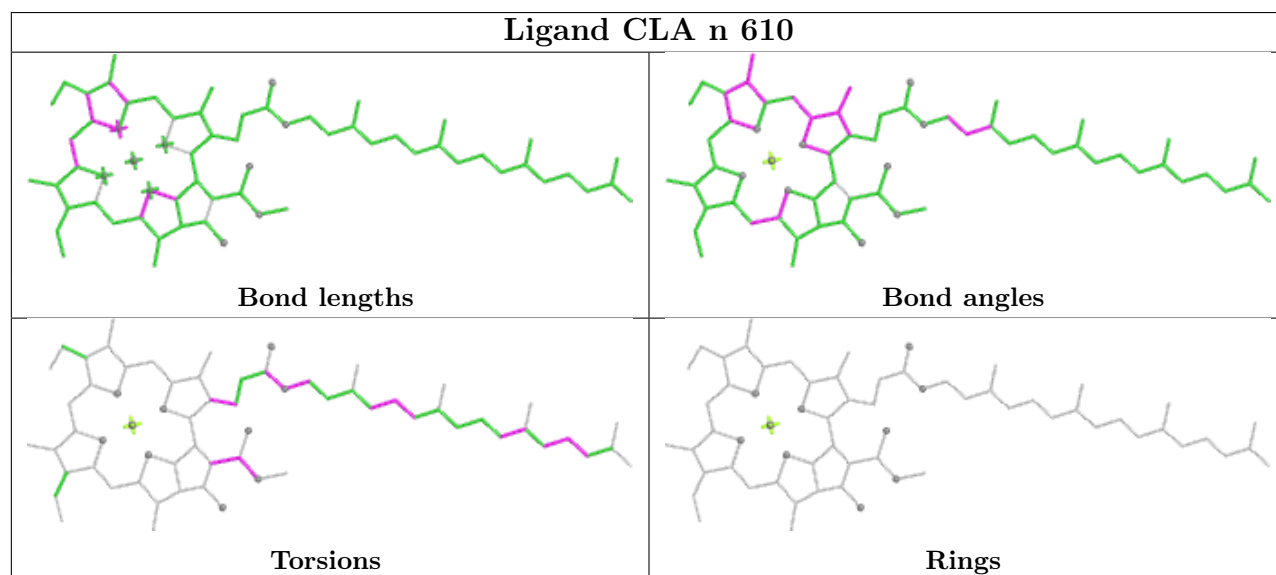
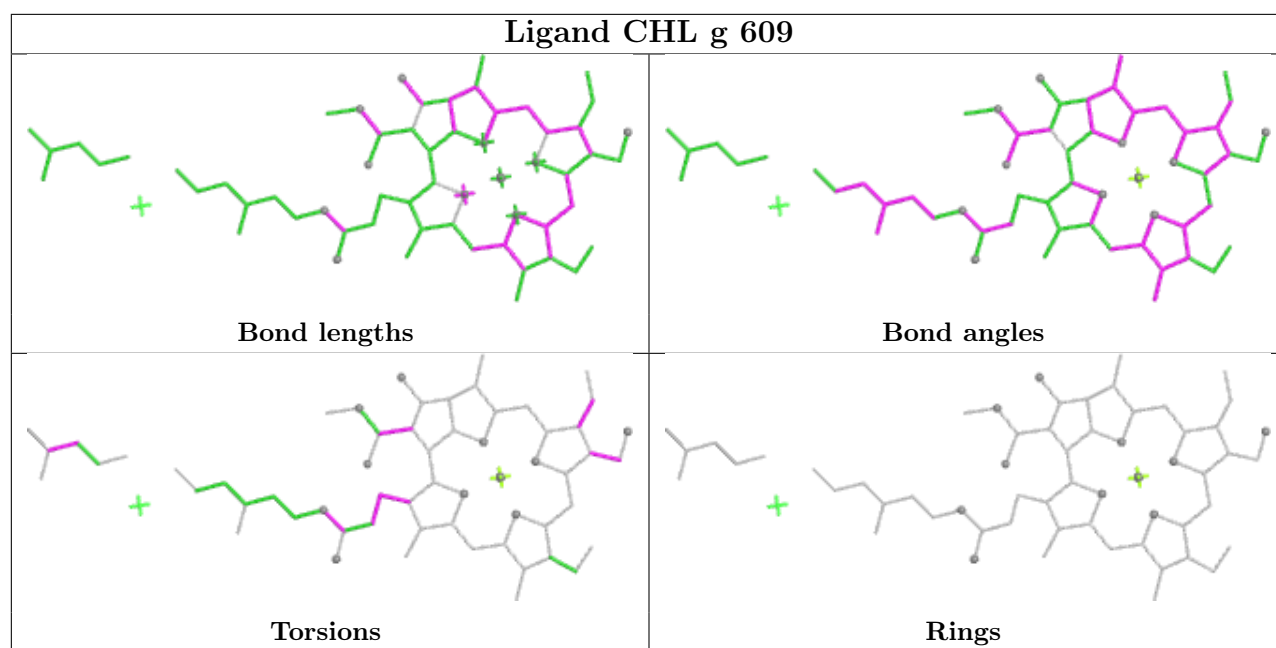


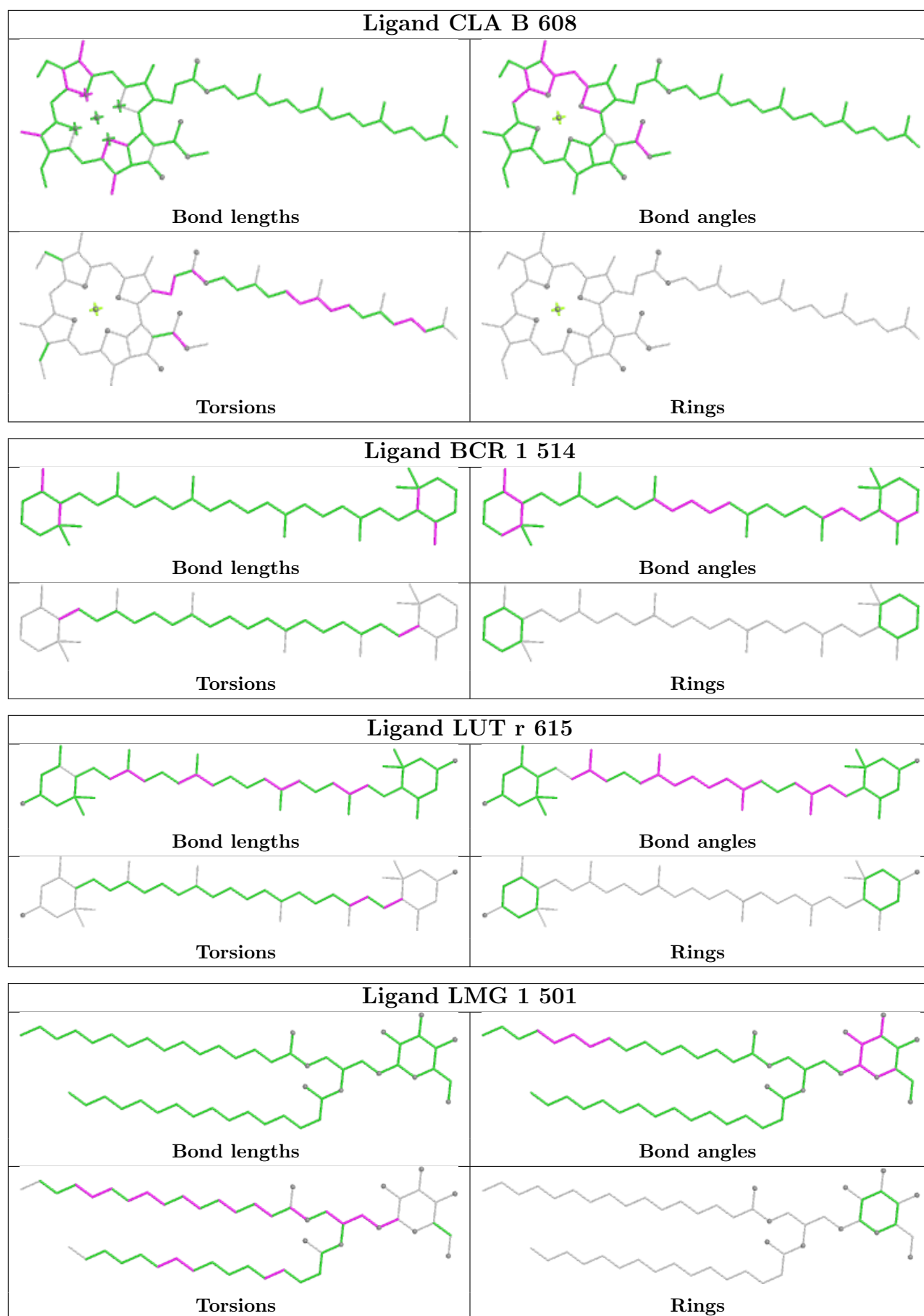
Ligand CLA r 614

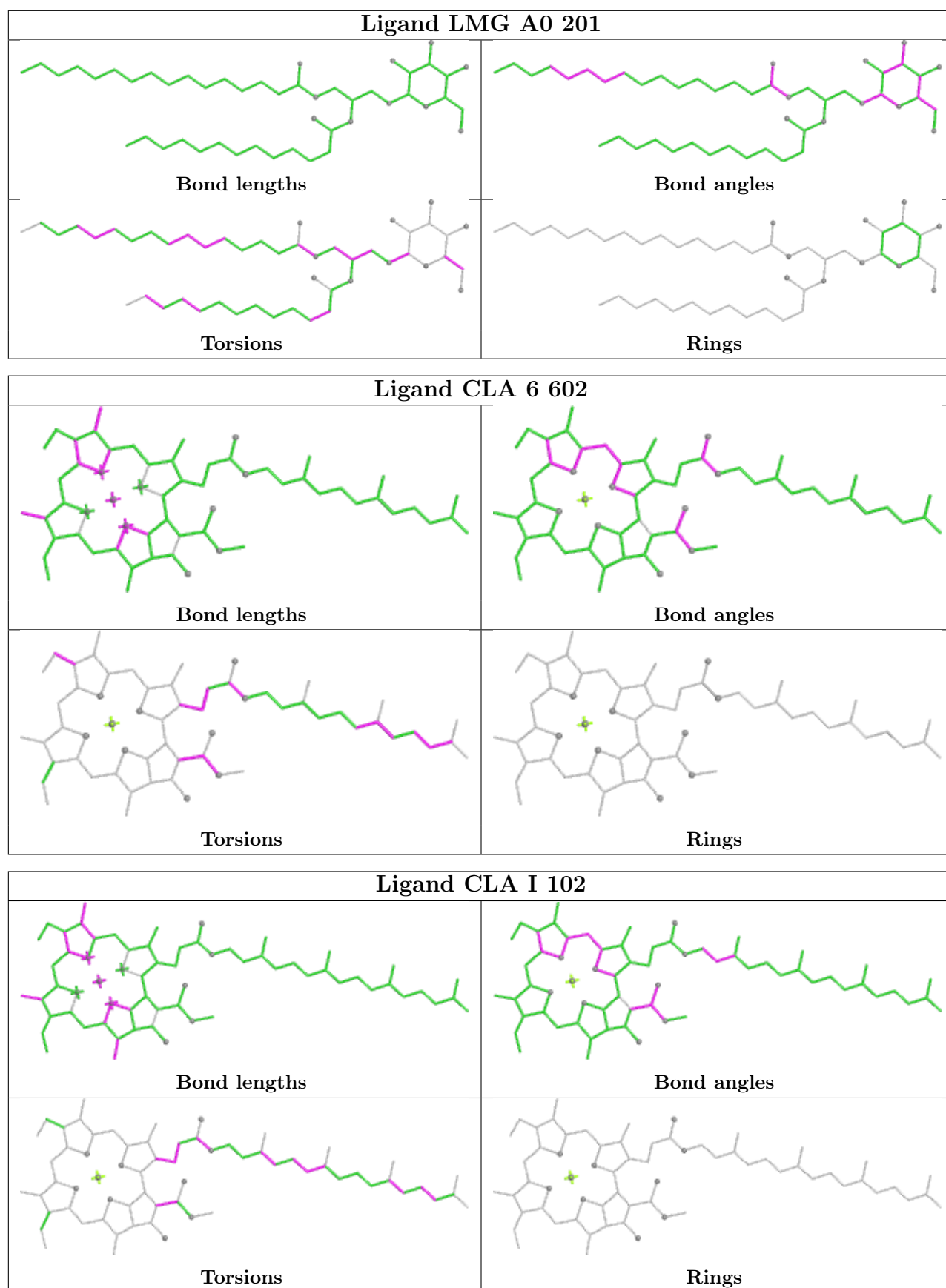


Ligand CHL y 308

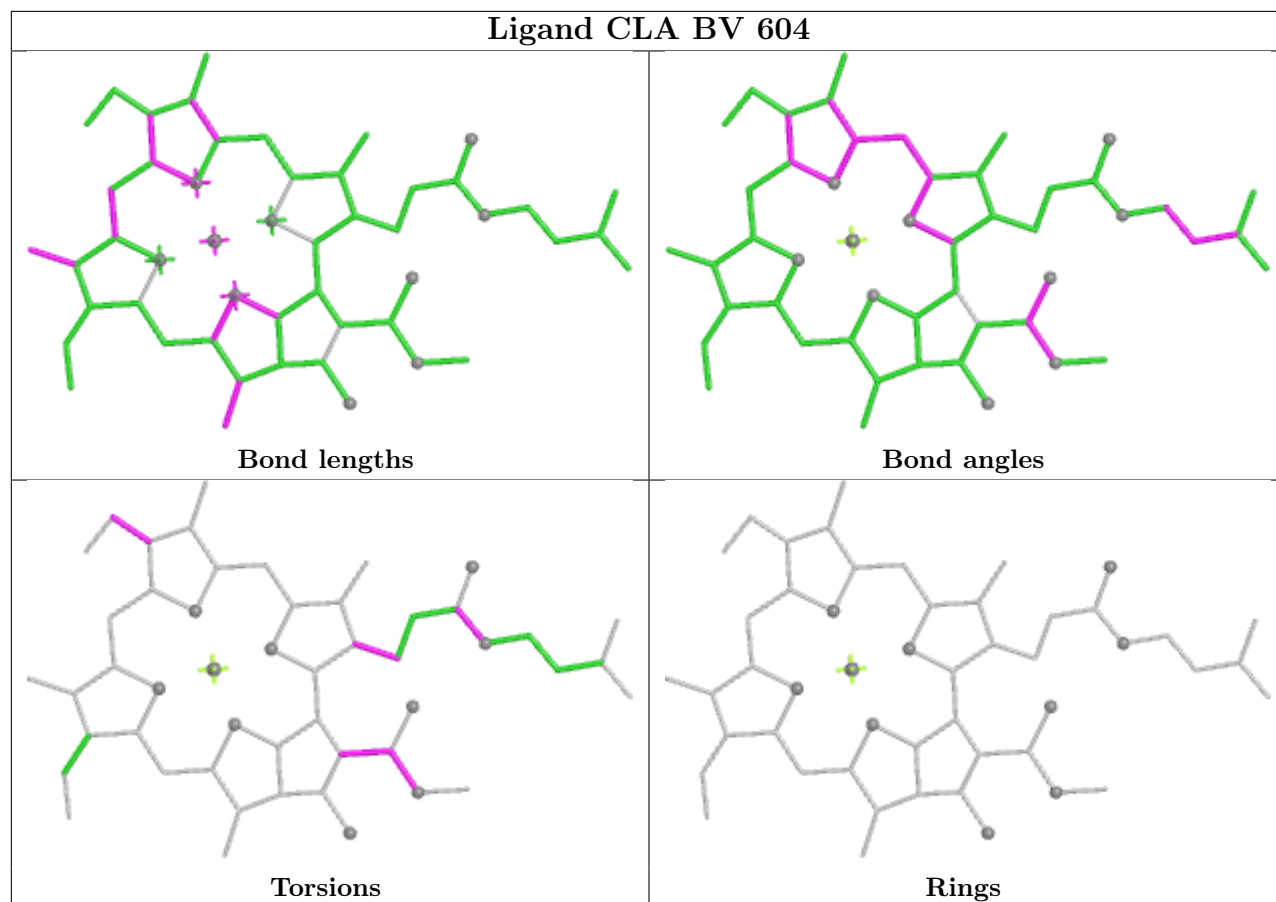




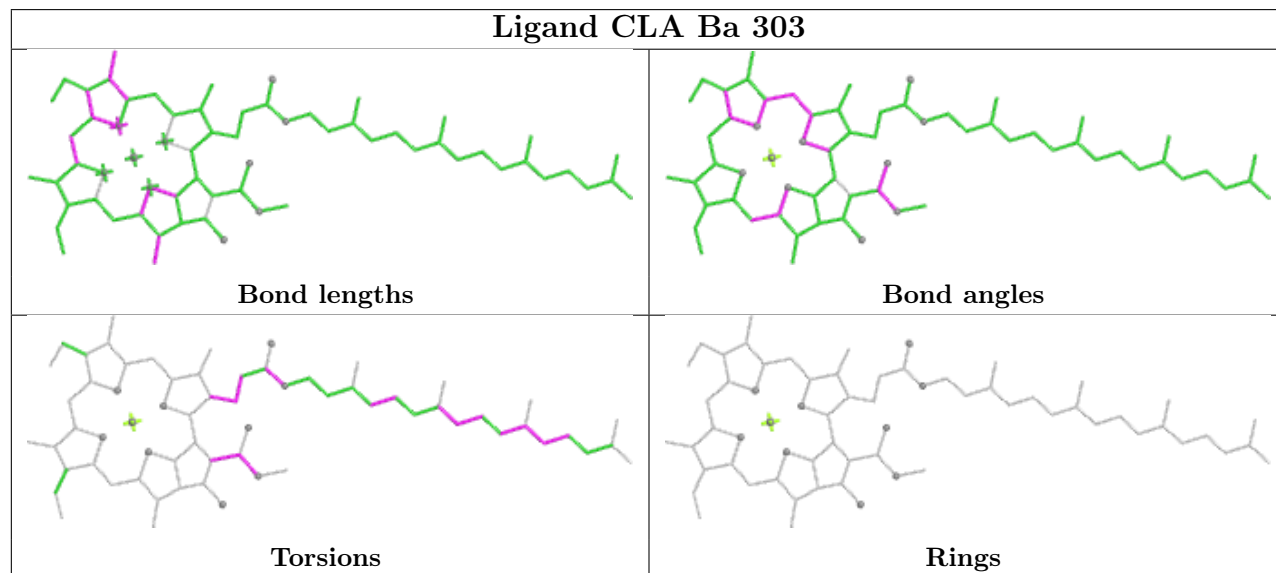


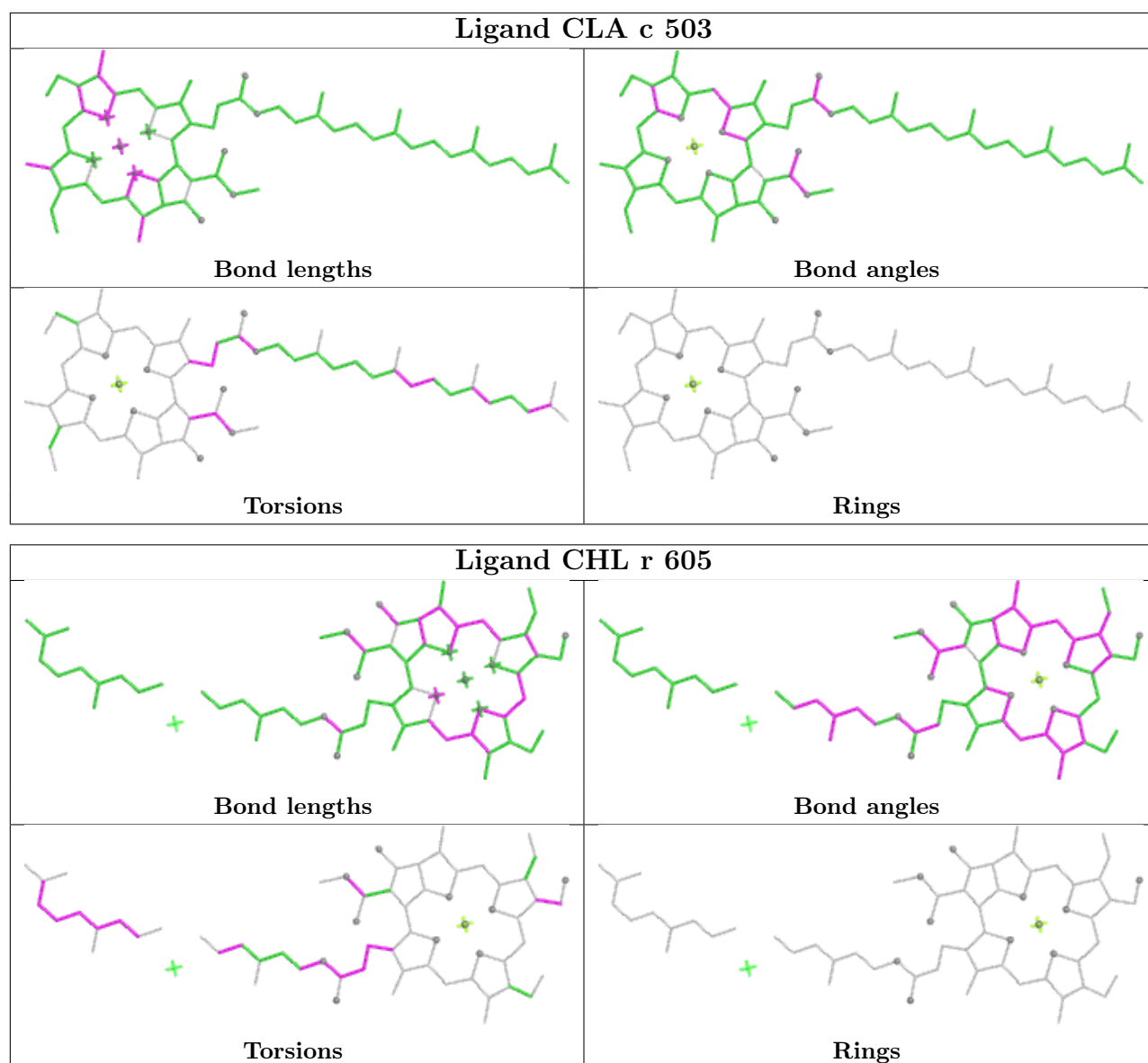


Ligand CLA BV 604

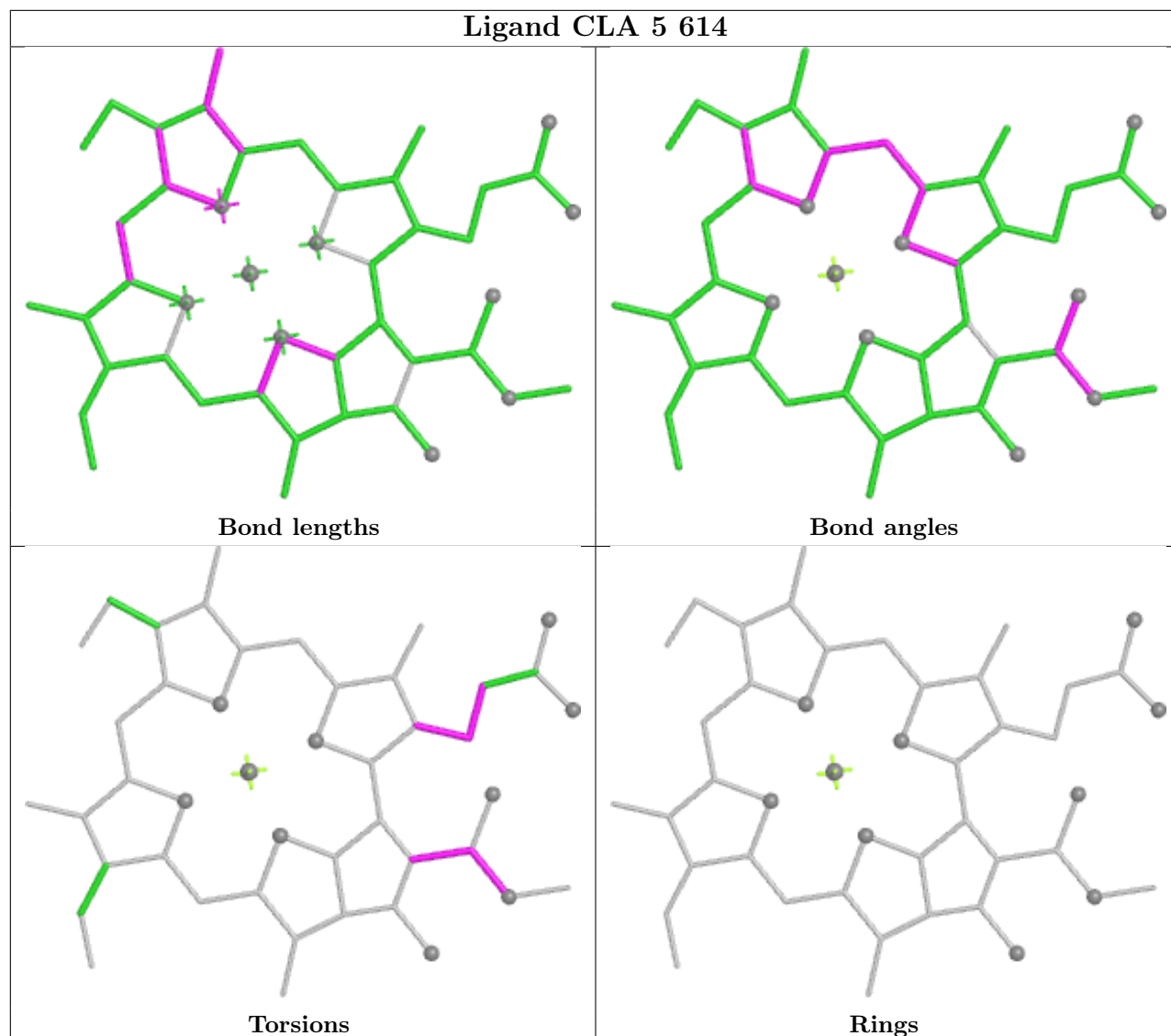


Ligand CLA Ba 303

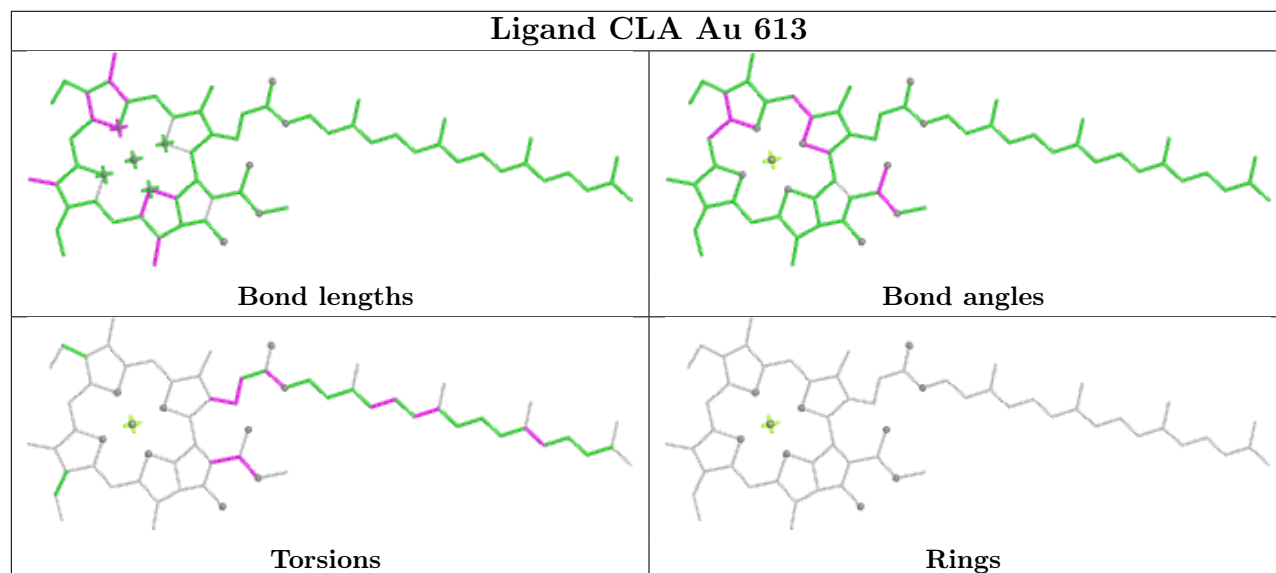


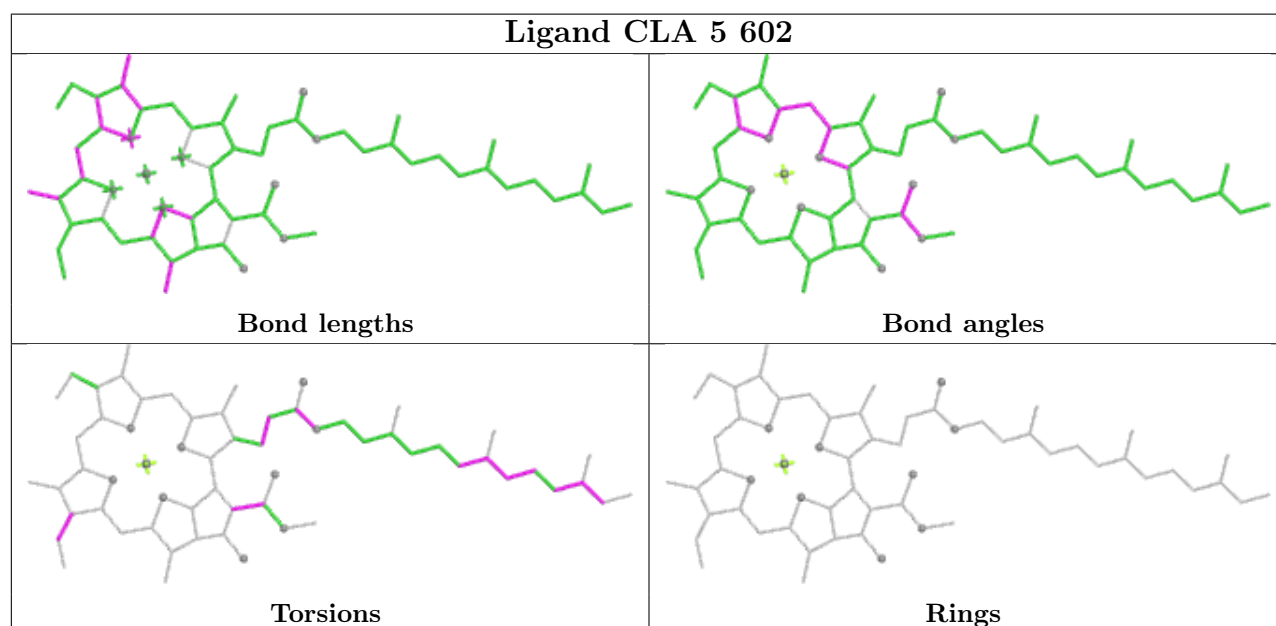
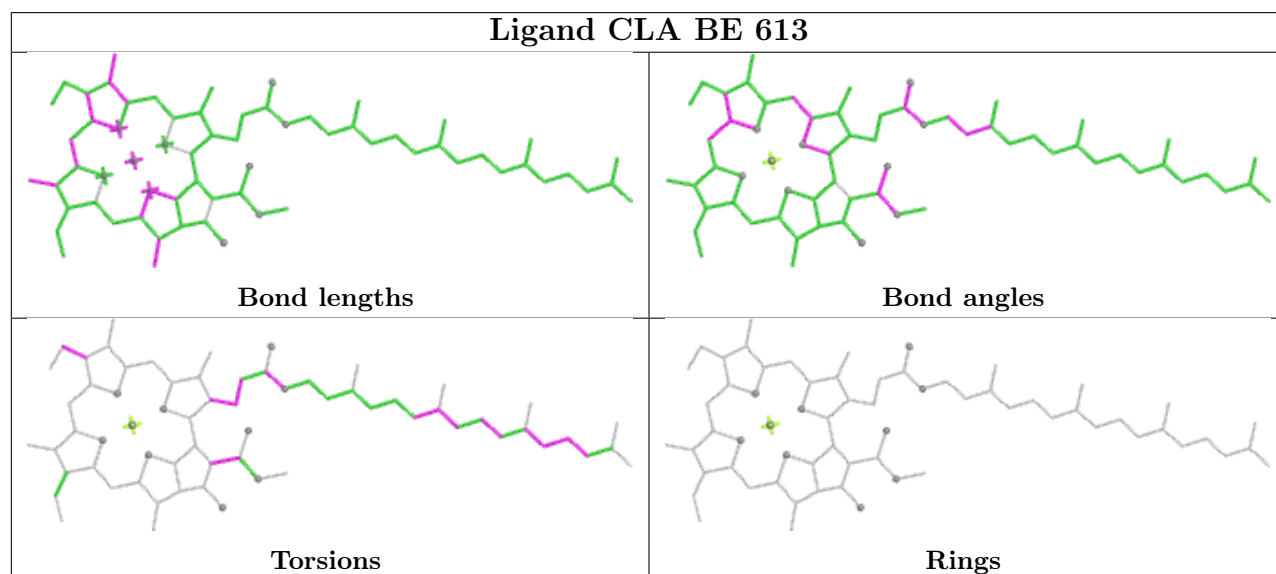
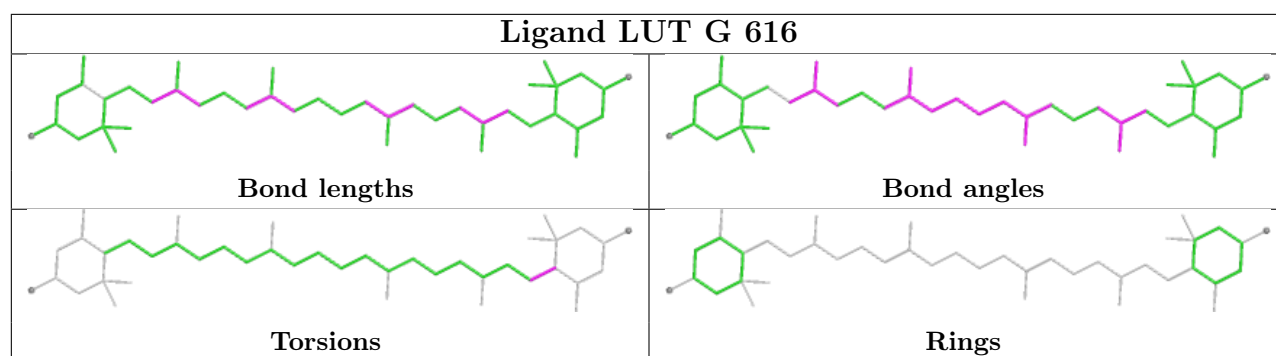


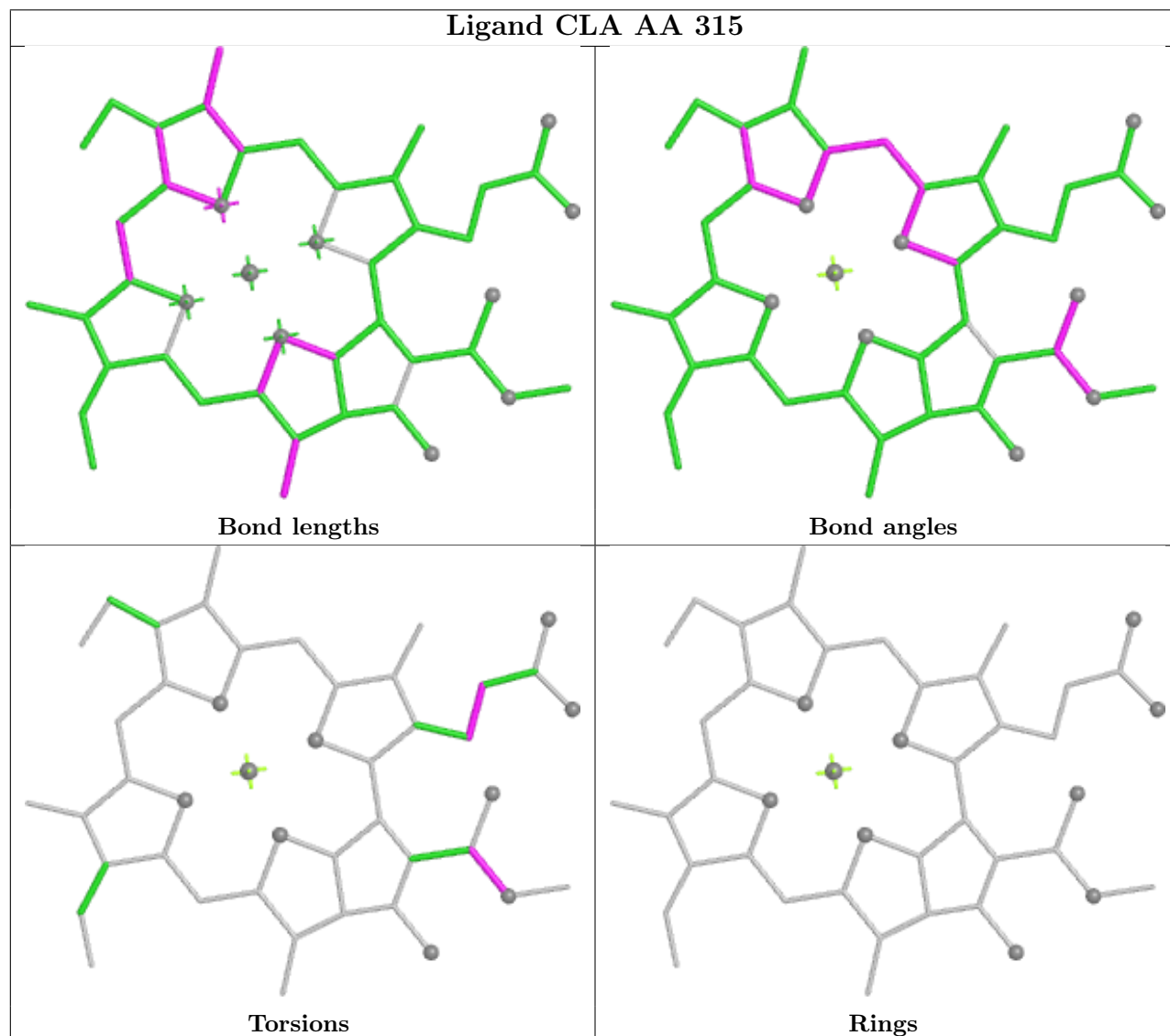
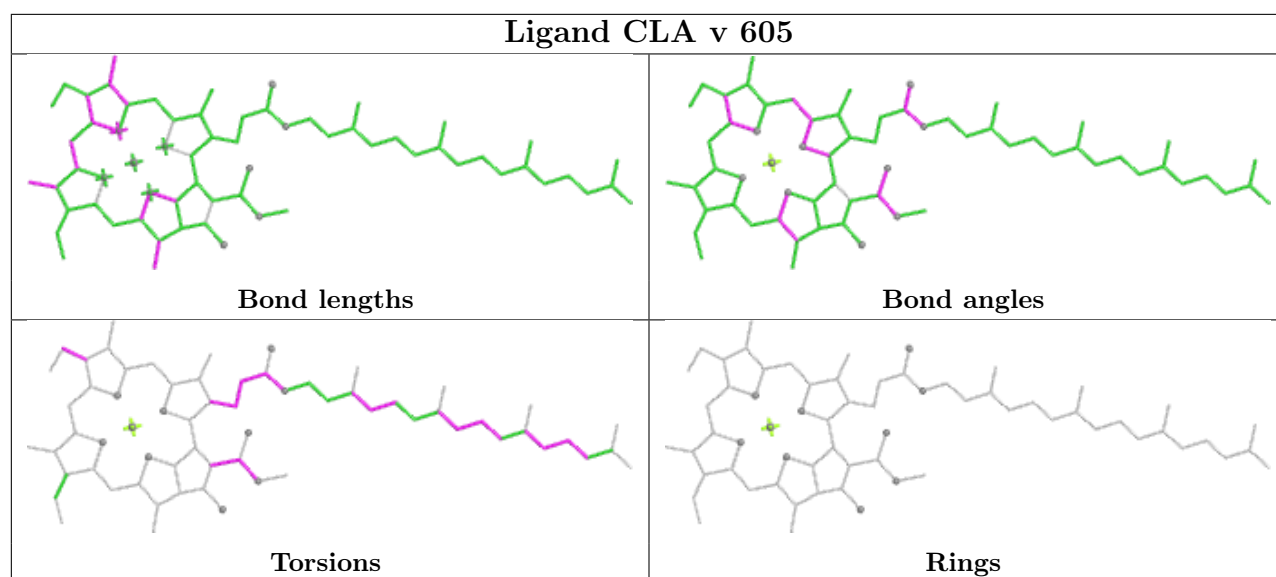
Ligand CLA 5 614

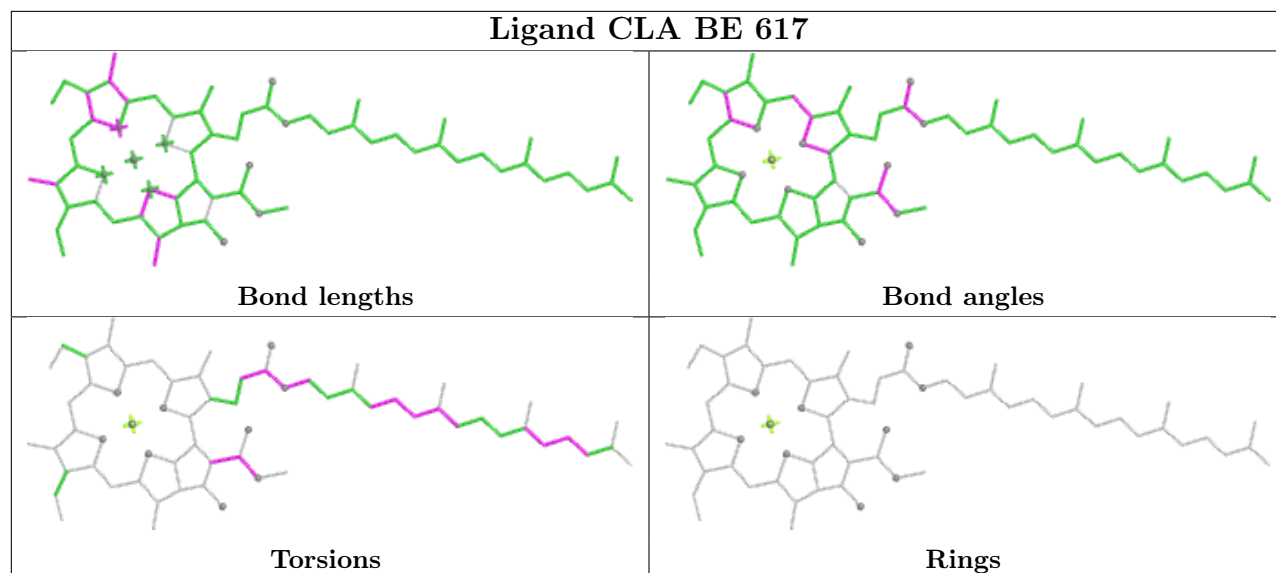
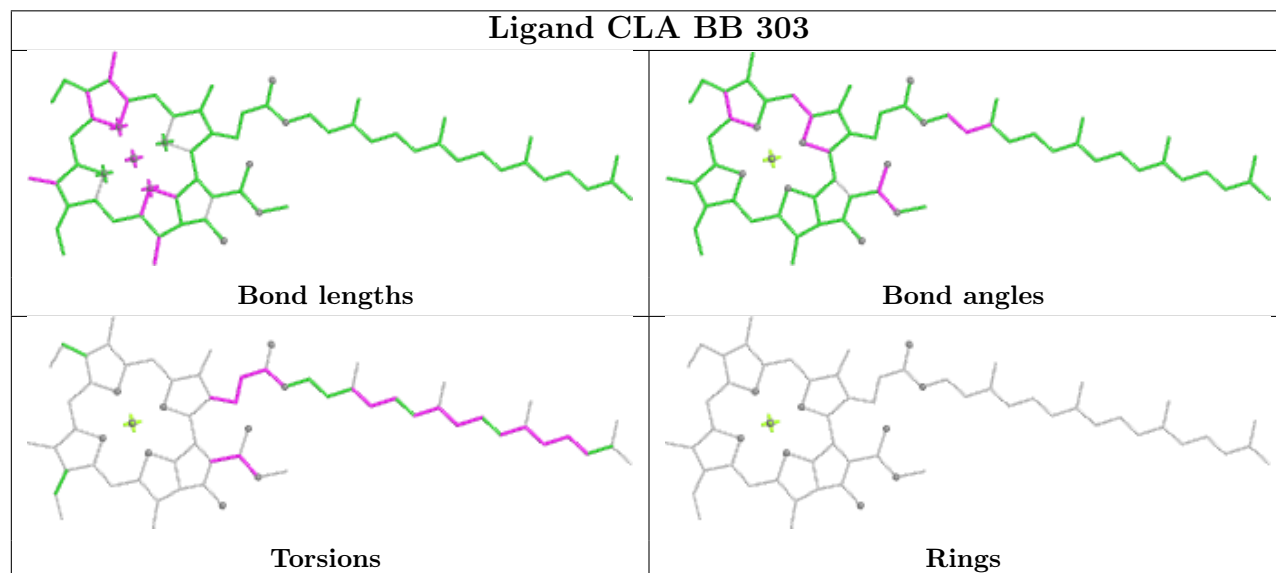
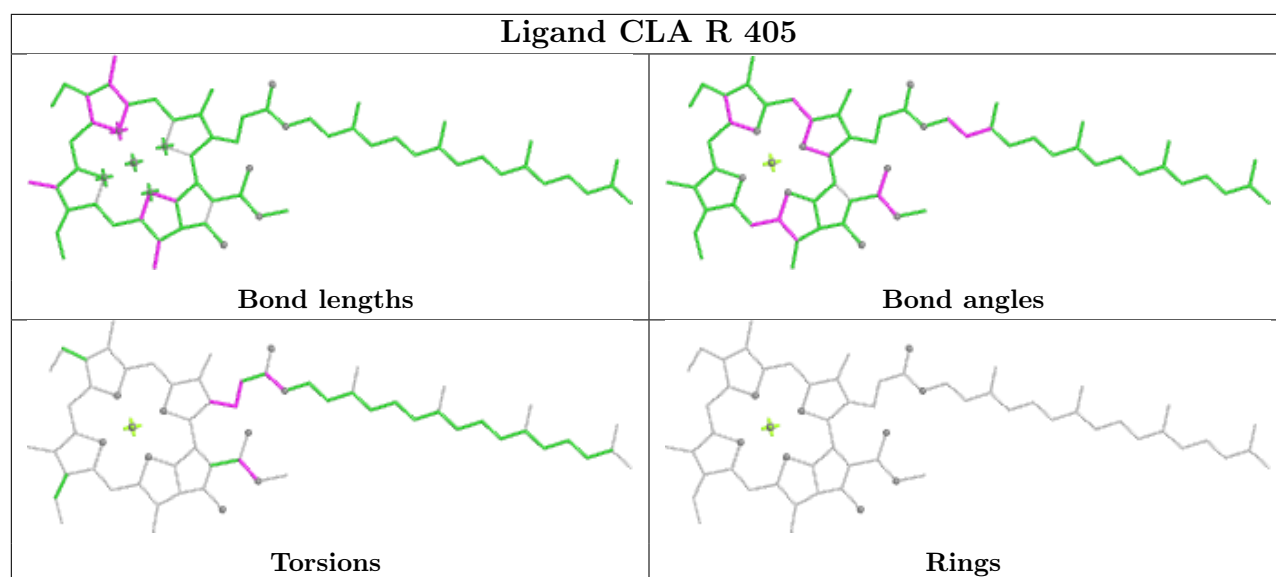


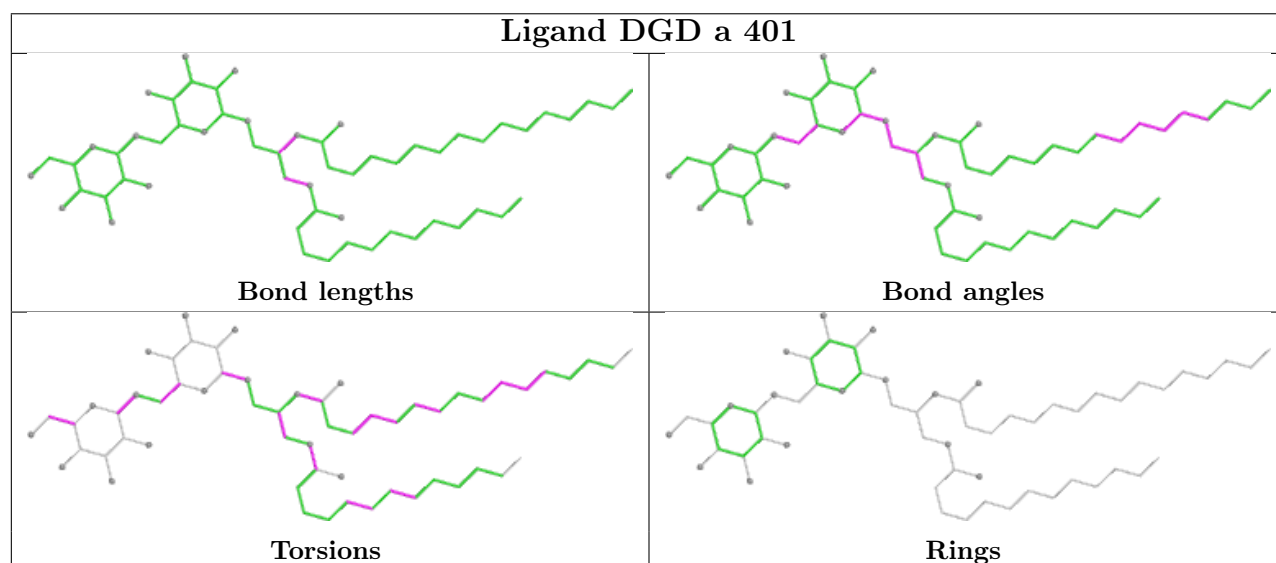
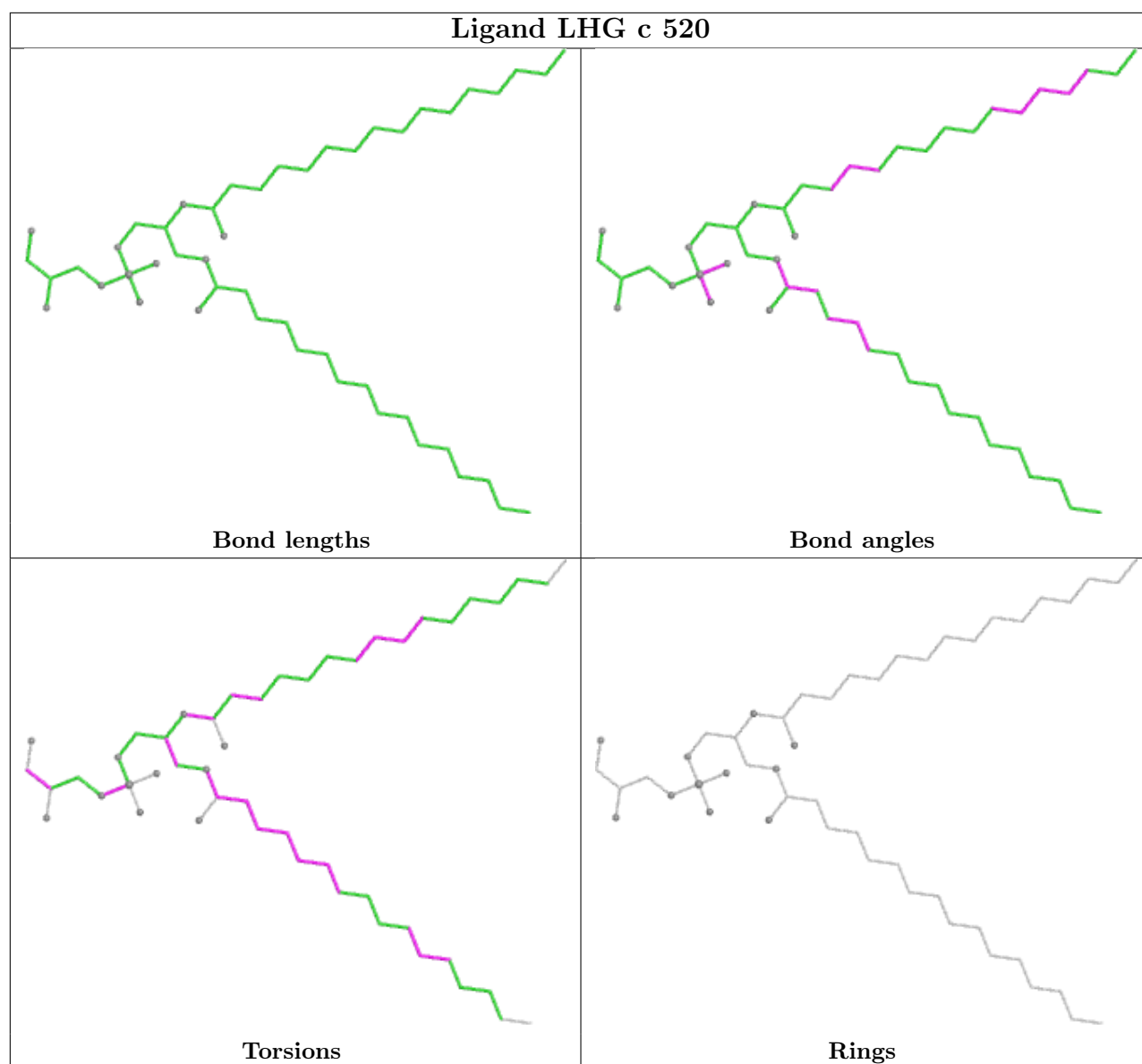
Ligand CLA Au 613

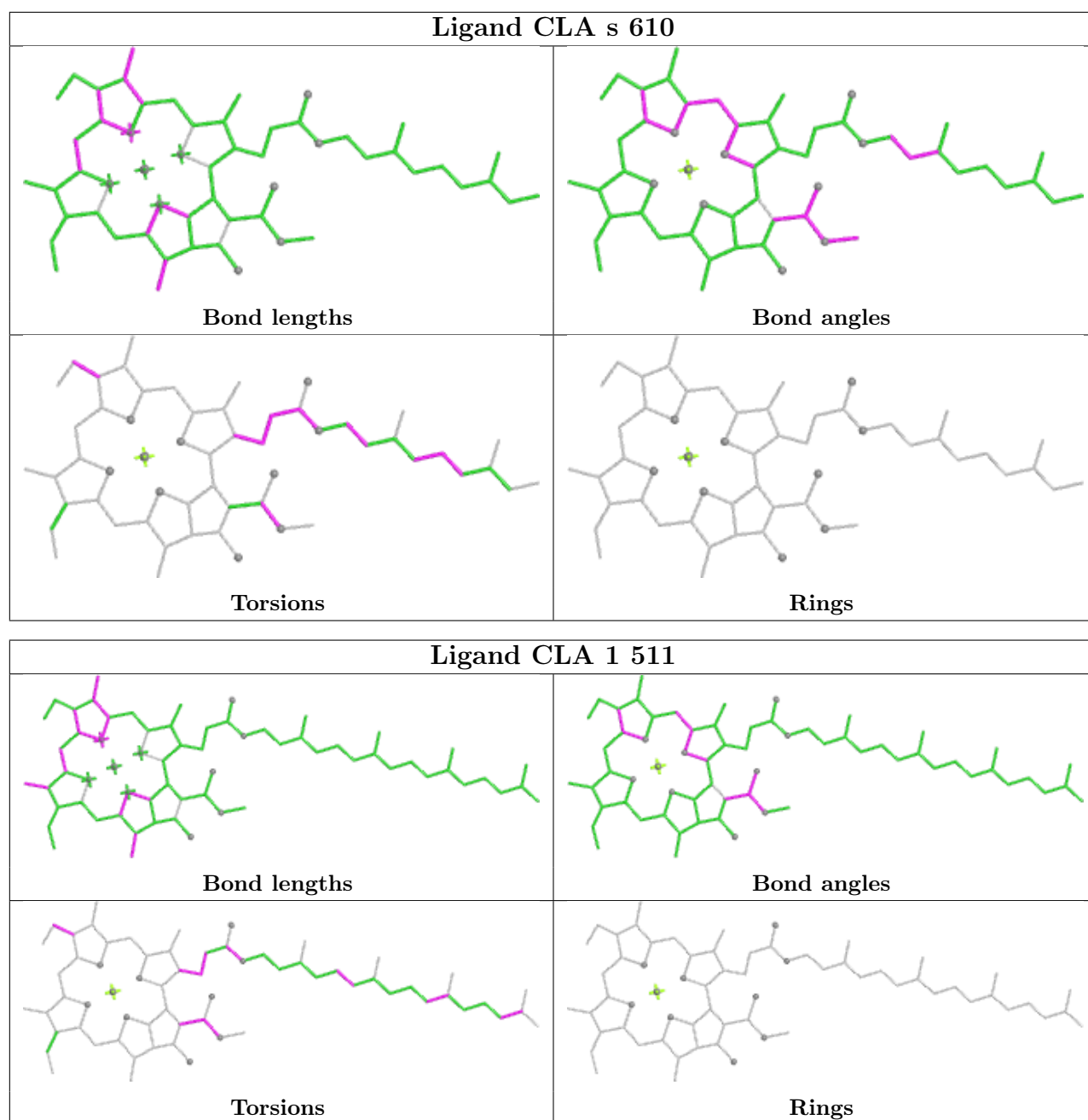




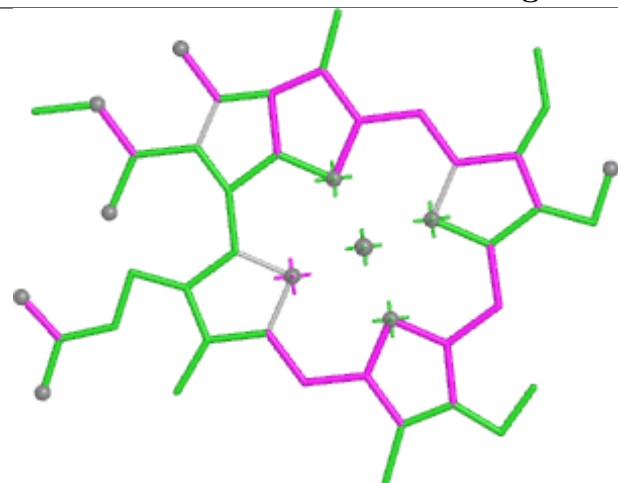




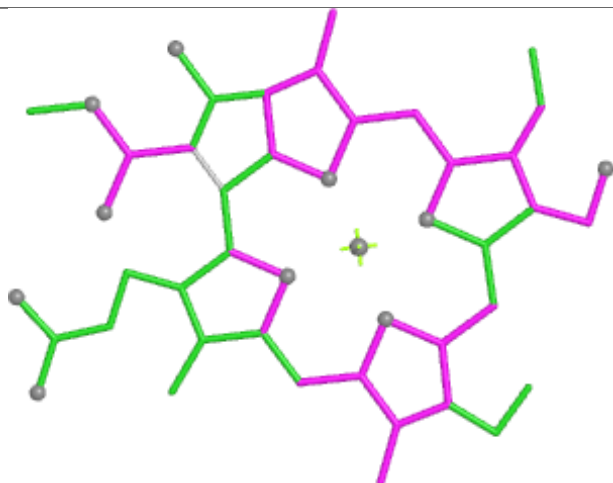




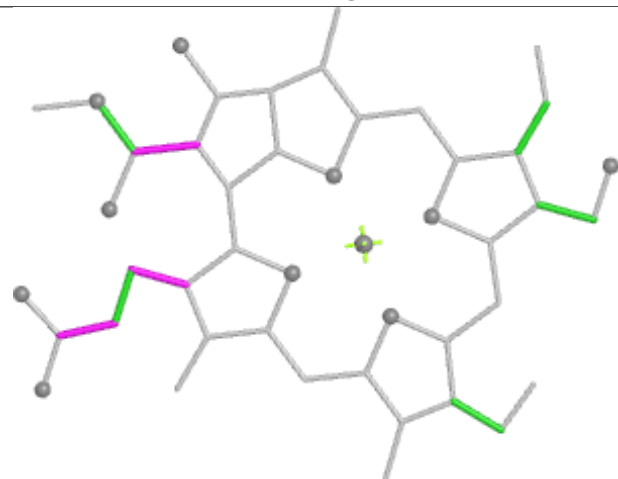
Ligand CHL 7 302



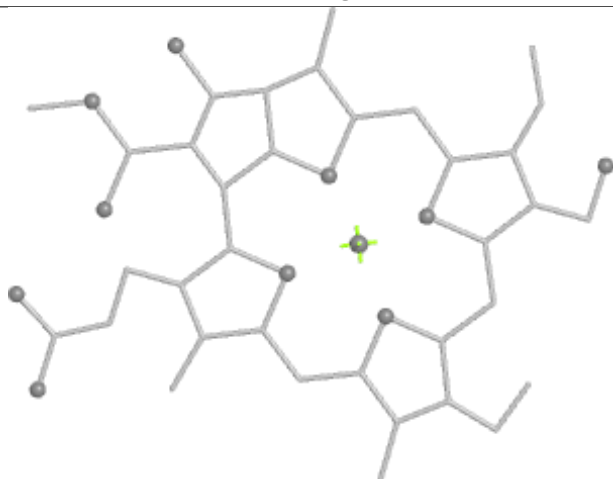
Bond lengths



Bond angles

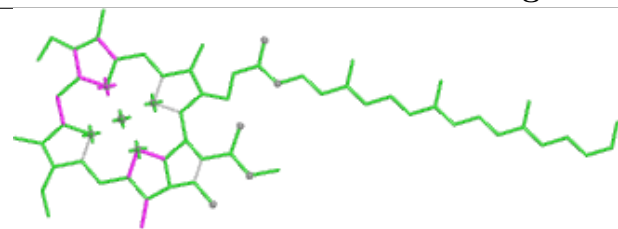


Torsions

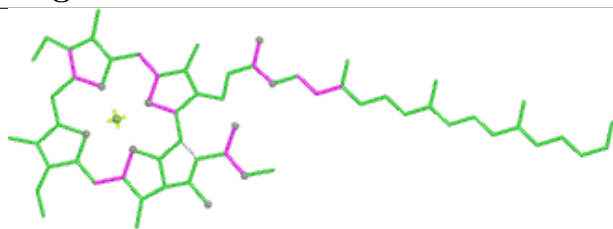


Rings

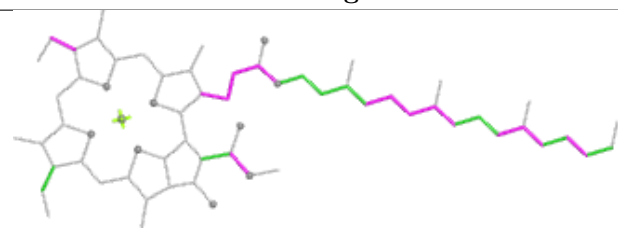
Ligand CLA g 610



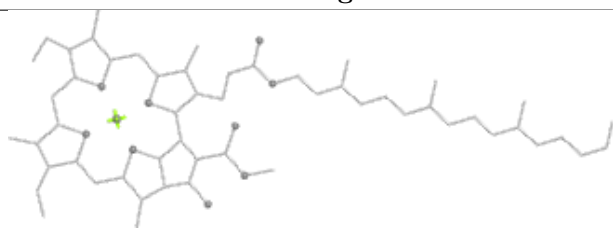
Bond lengths



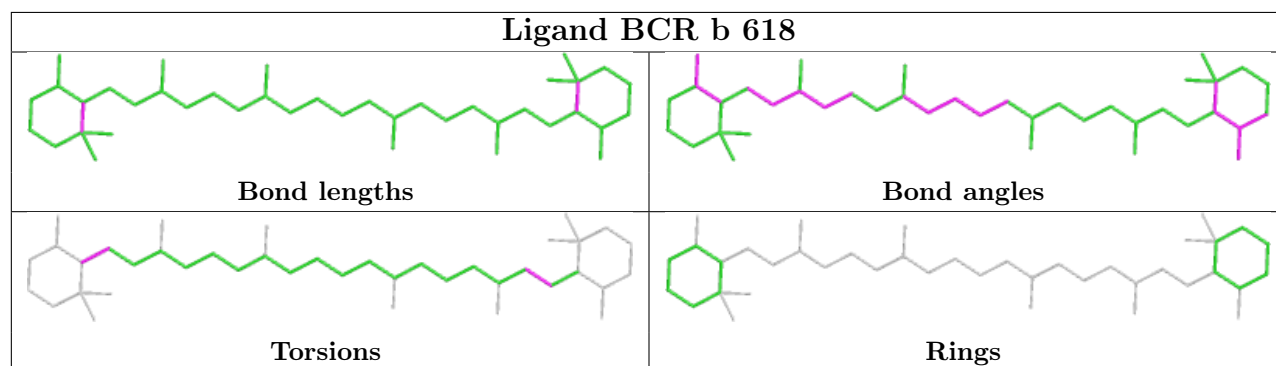
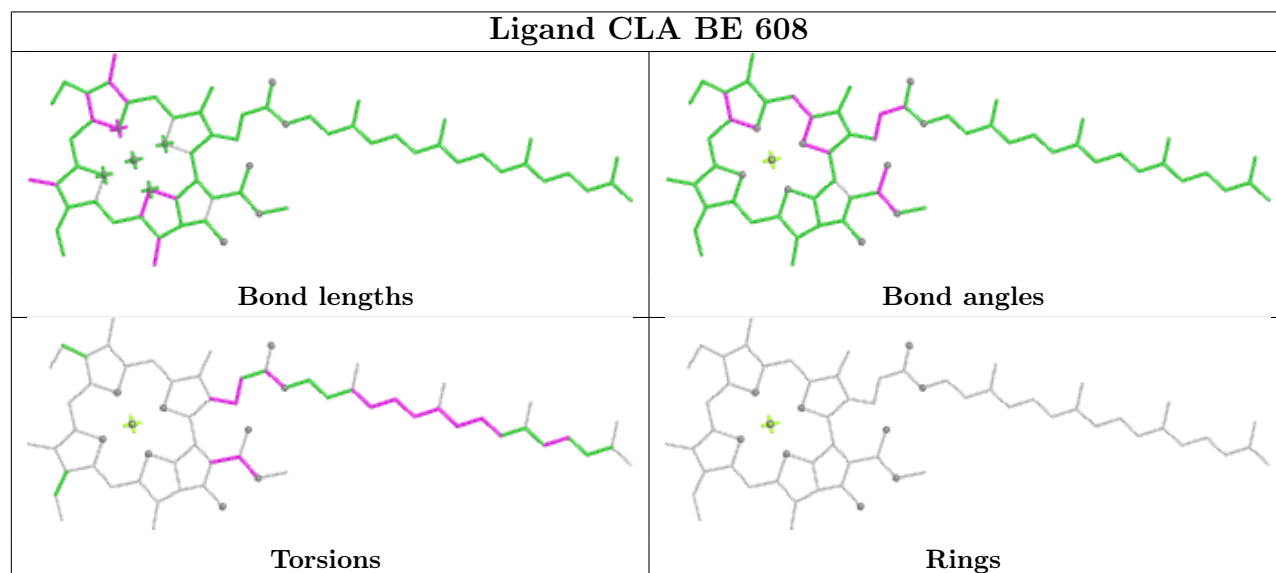
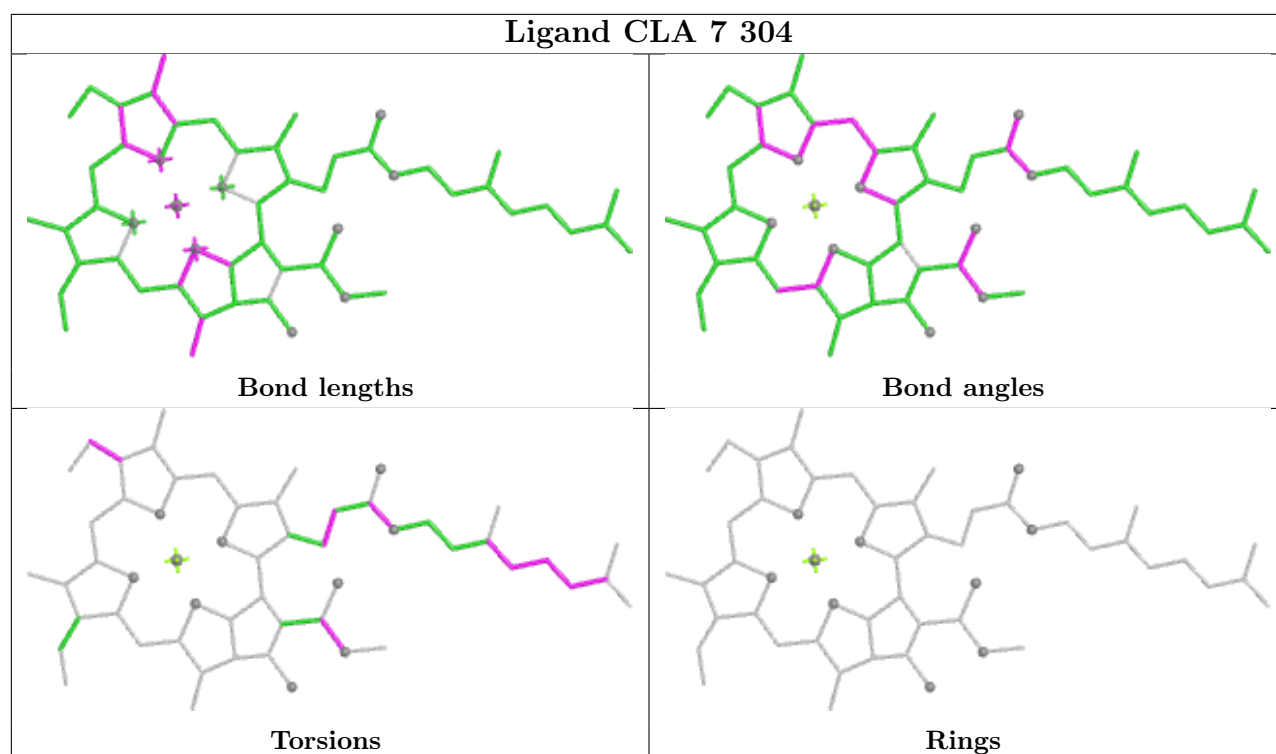
Bond angles

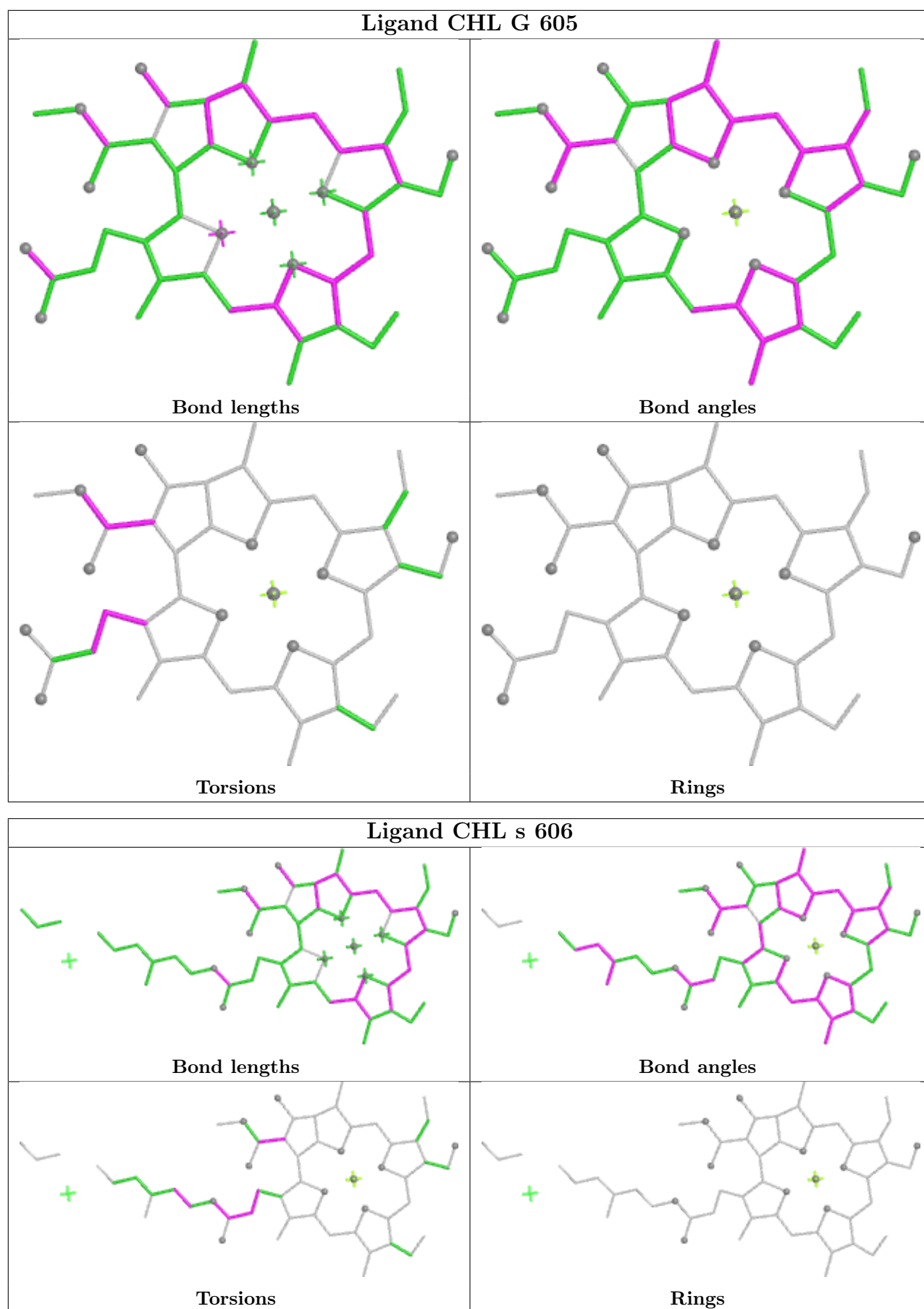


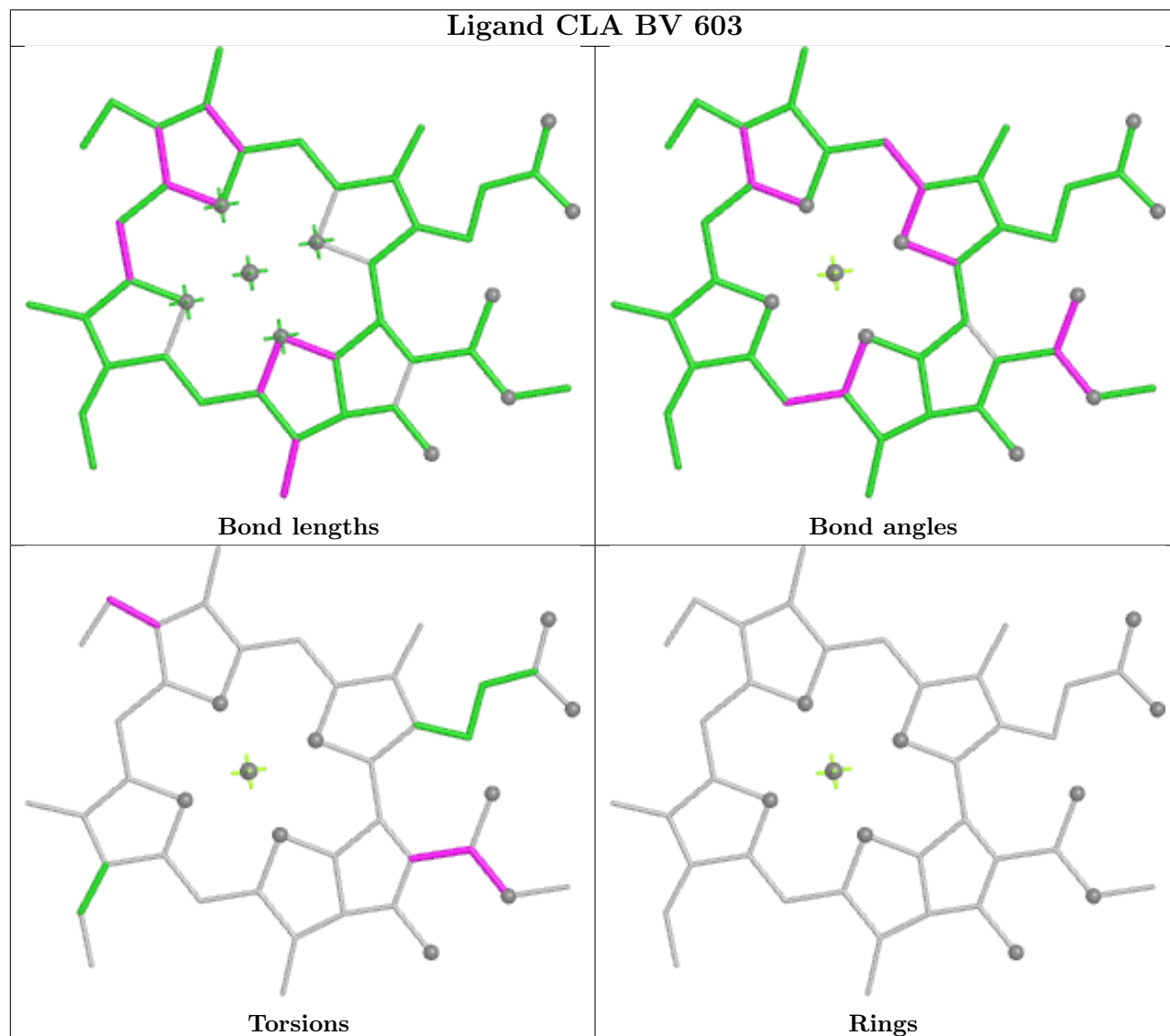
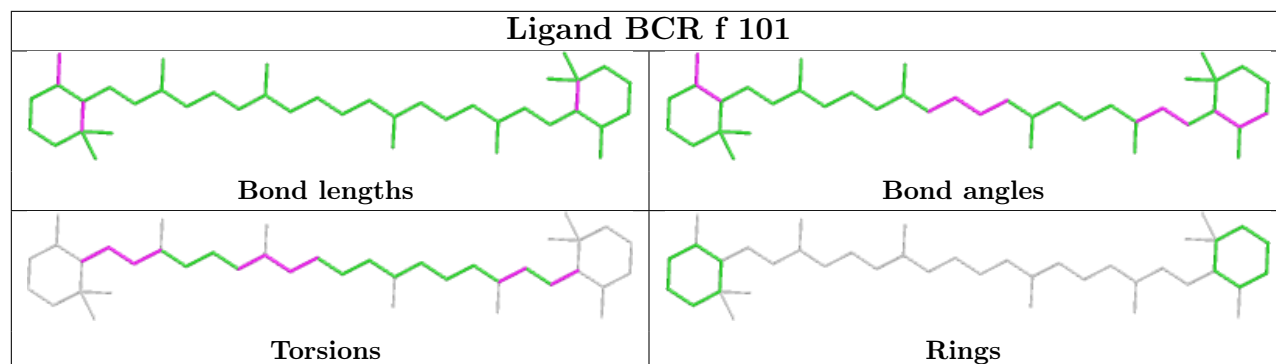
Torsions

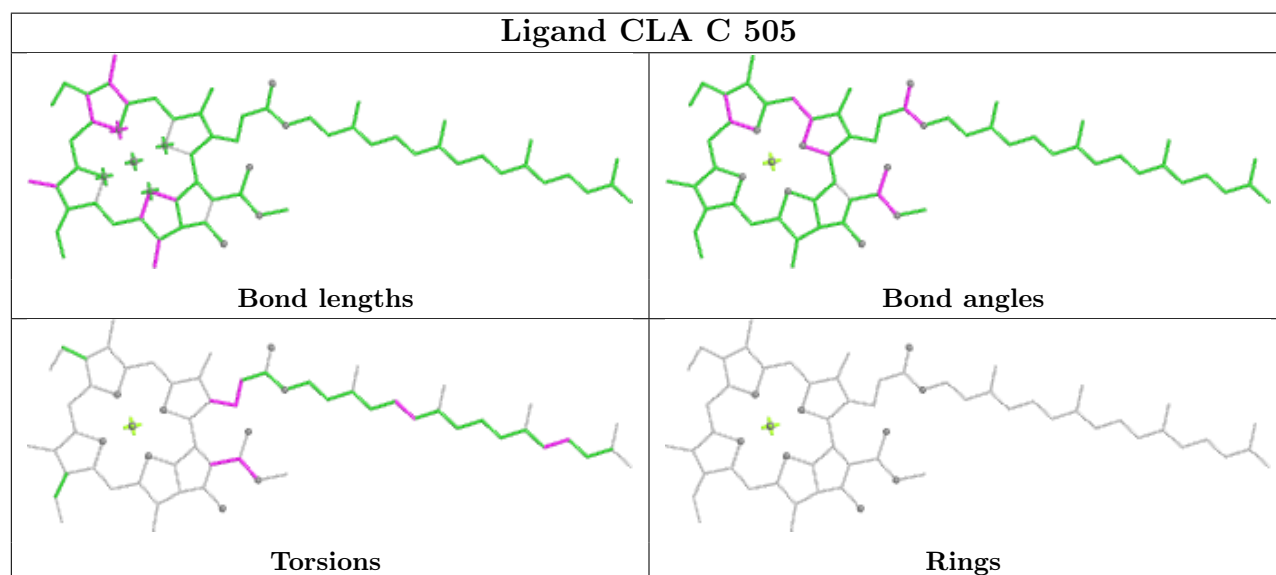
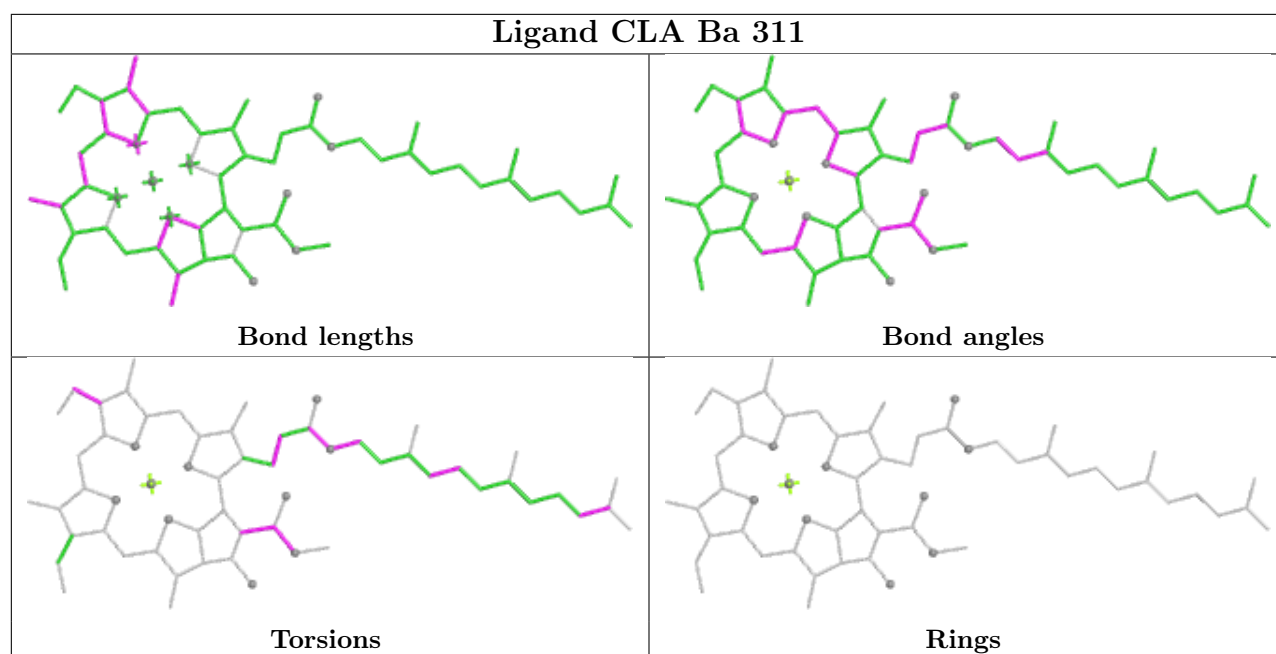


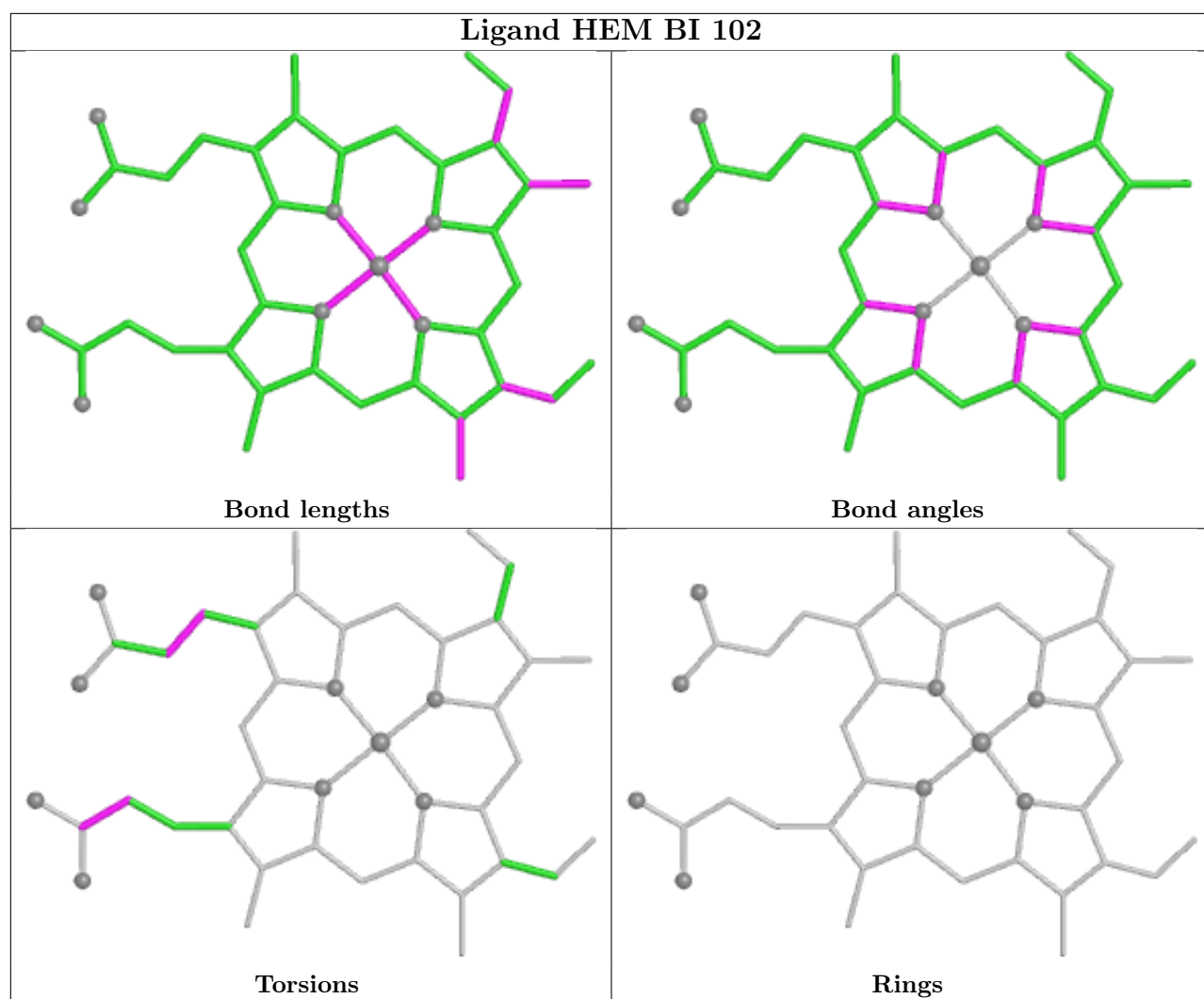
Rings

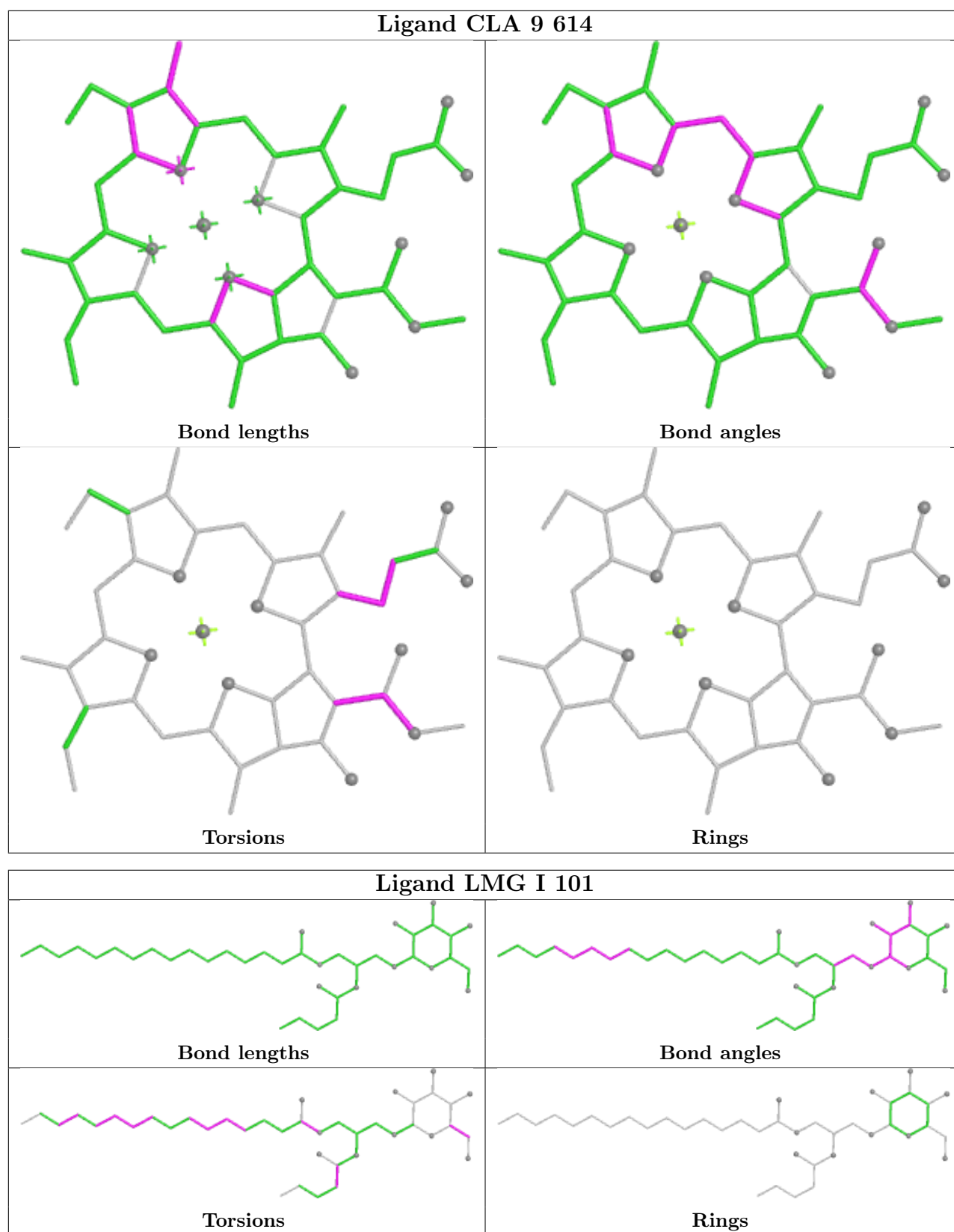


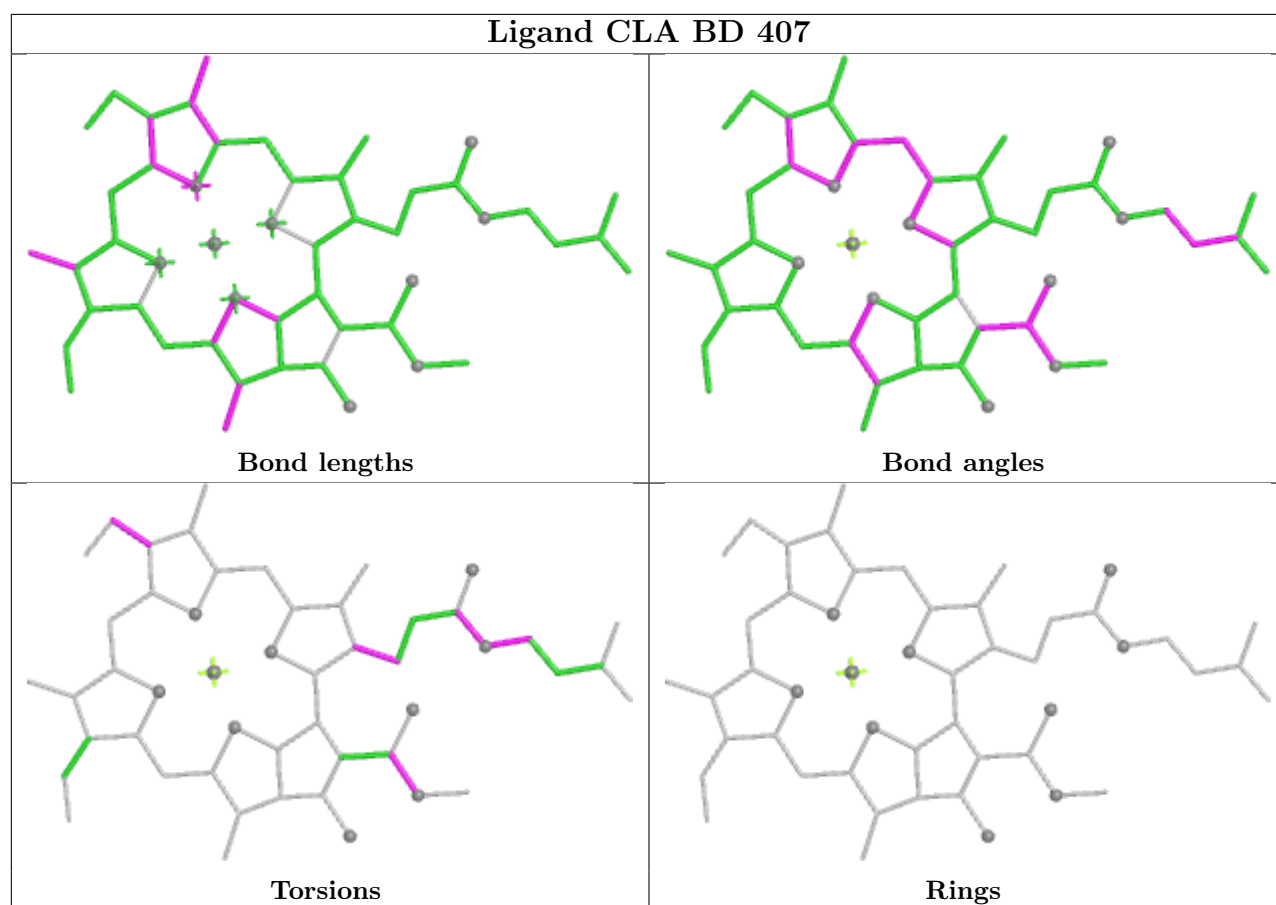




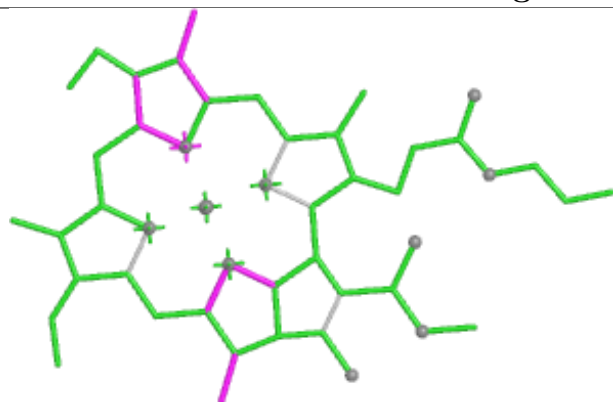




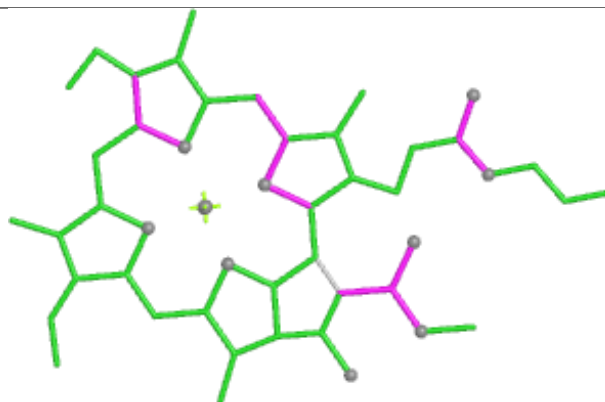




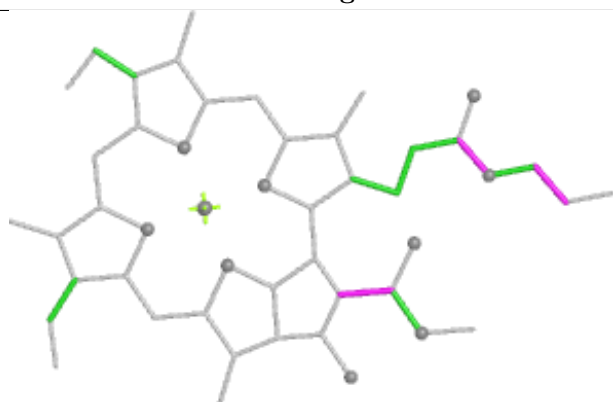
Ligand CLA G 614



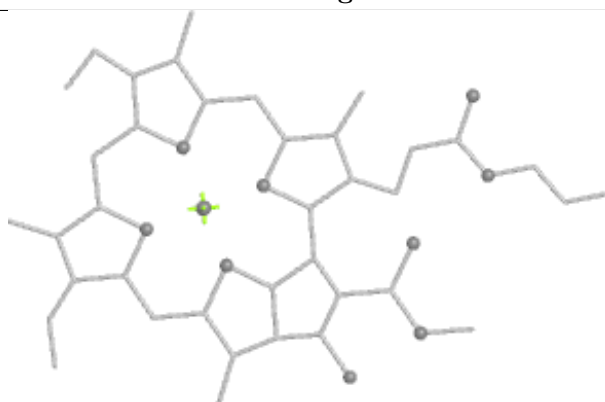
Bond lengths



Bond angles

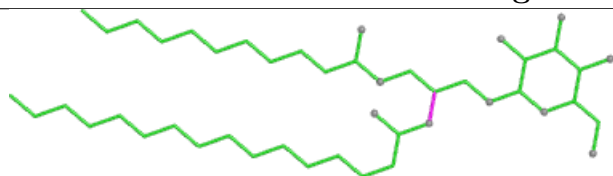


Torsions

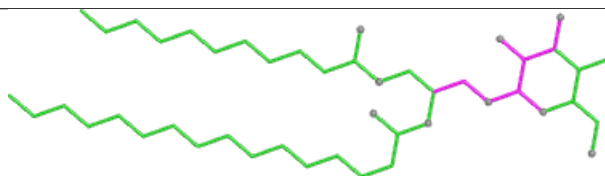


Rings

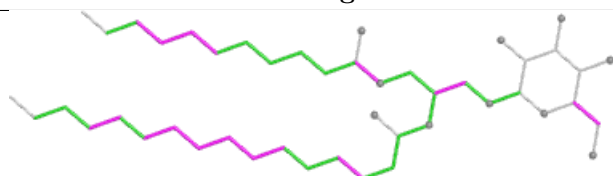
Ligand LMG d 405



Bond lengths



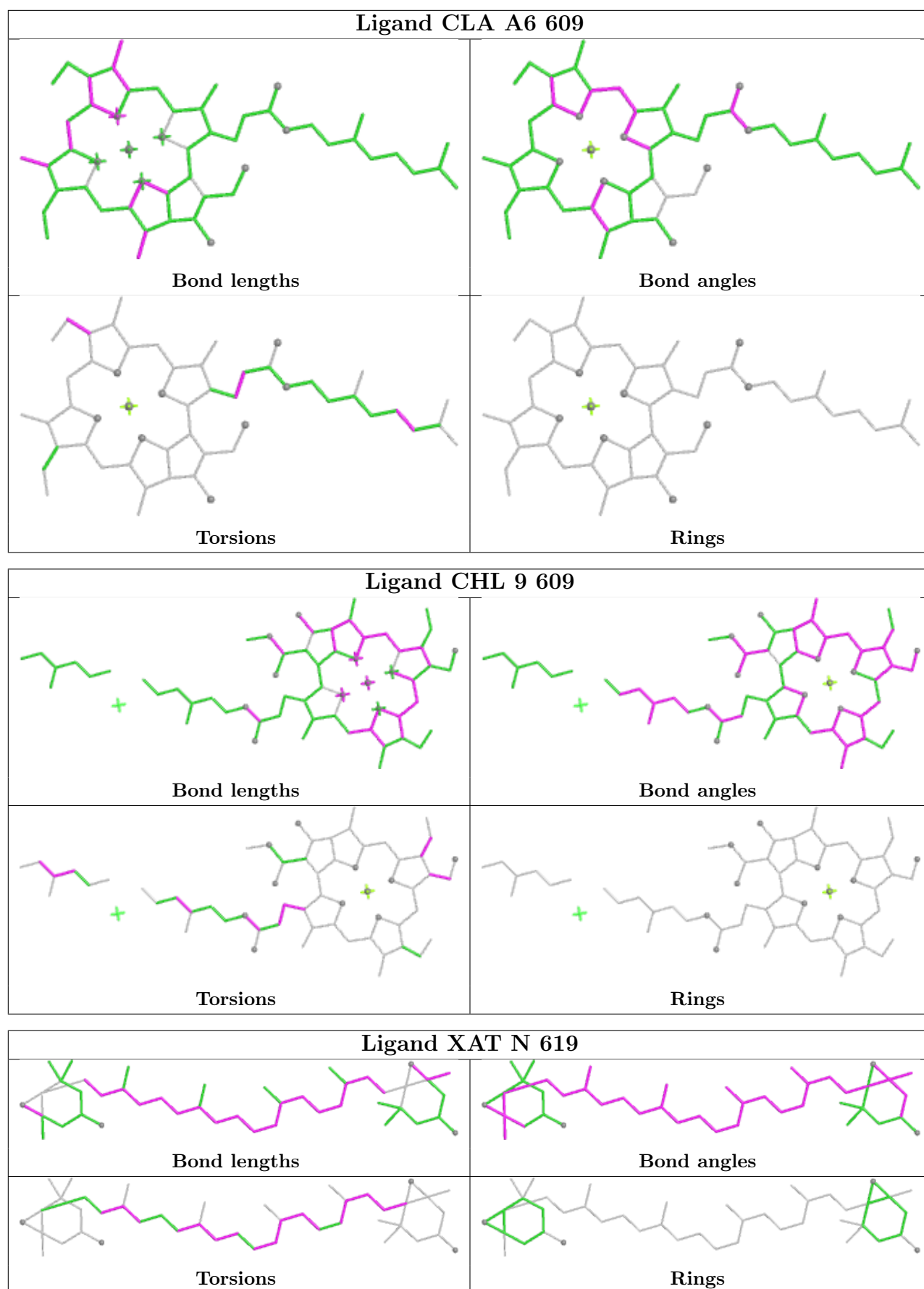
Bond angles



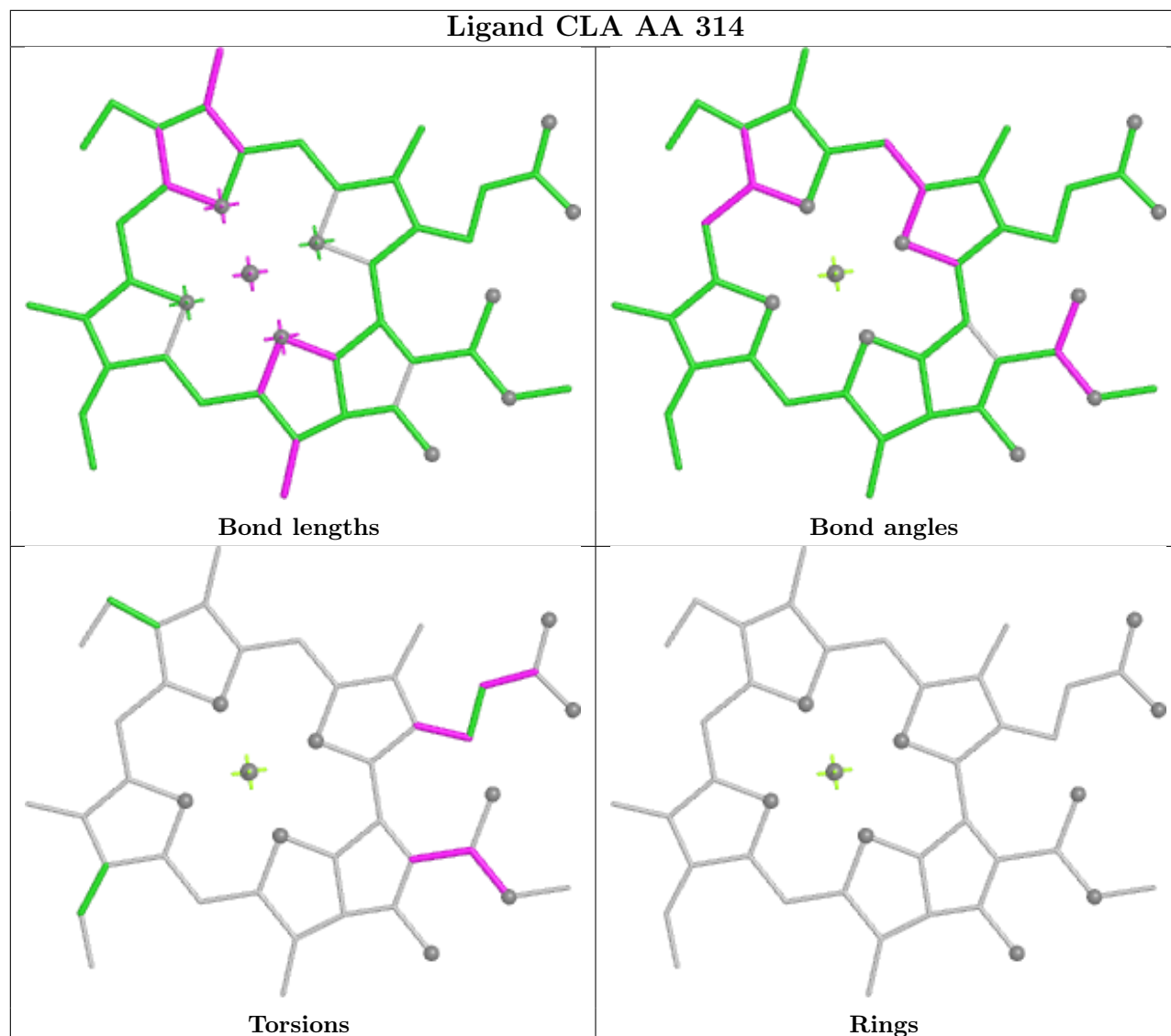
Torsions



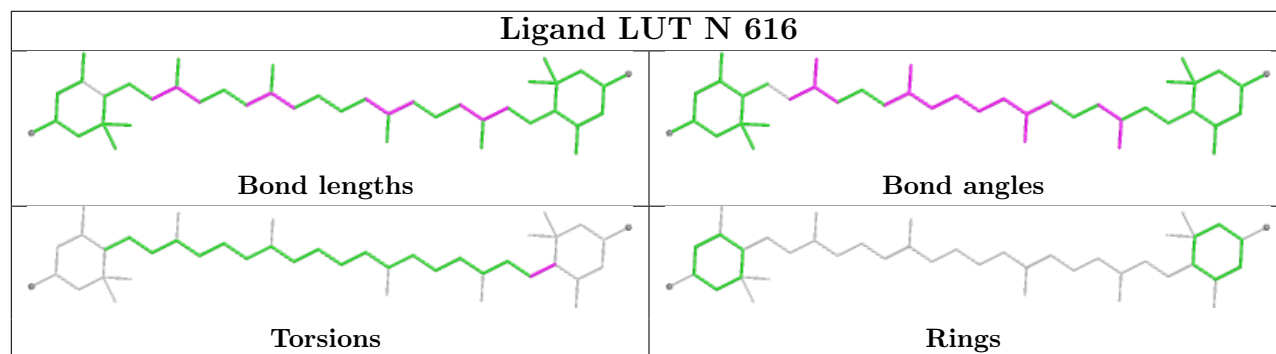
Rings



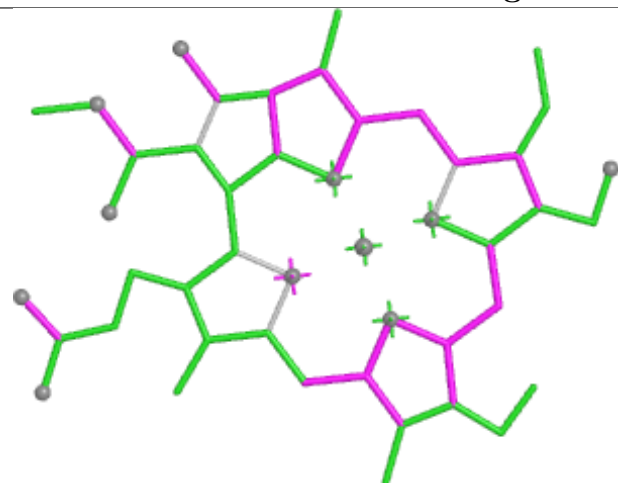
Ligand CLA AA 314



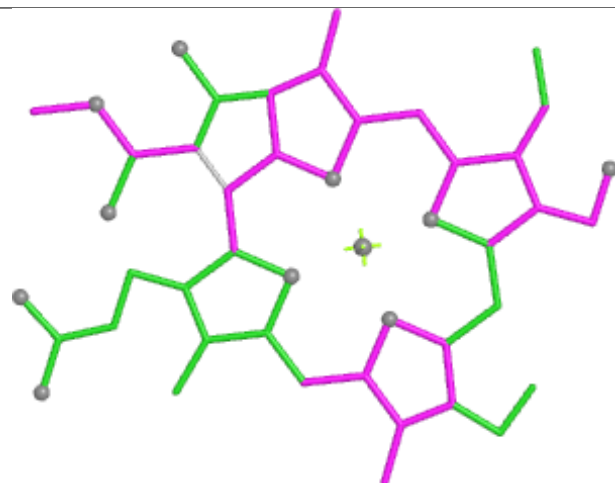
Ligand LUT N 616



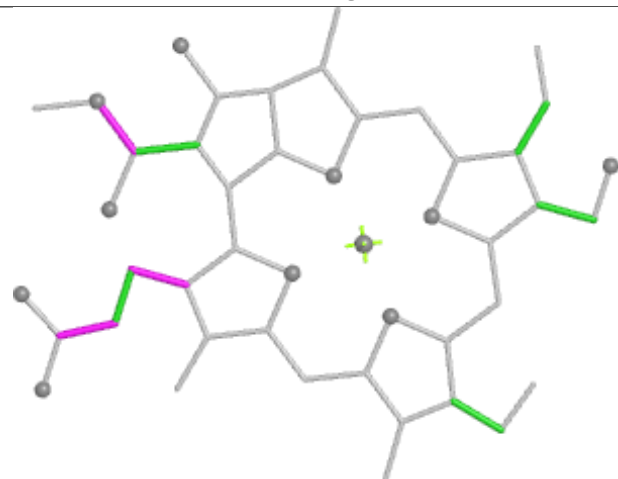
Ligand CHL AA 307



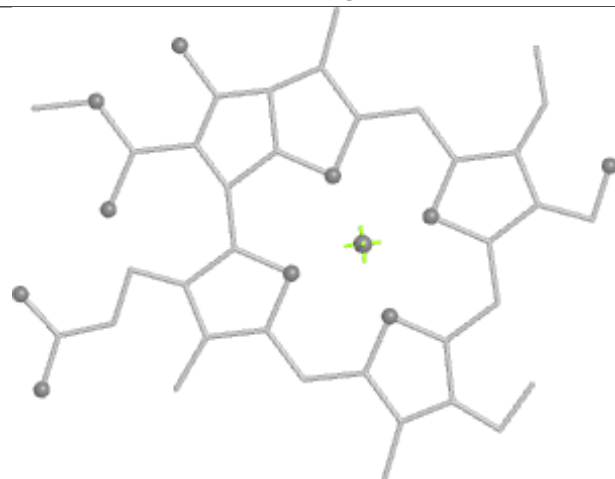
Bond lengths



Bond angles

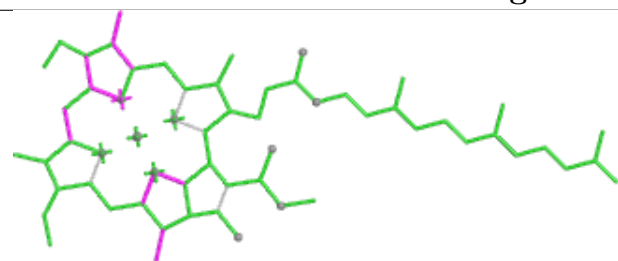


Torsions

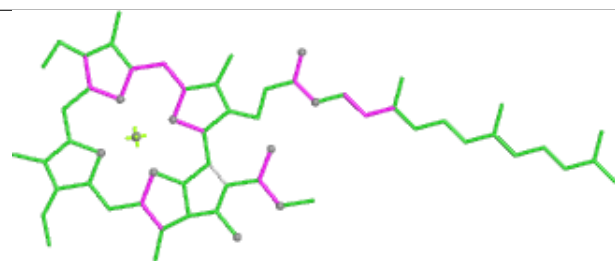


Rings

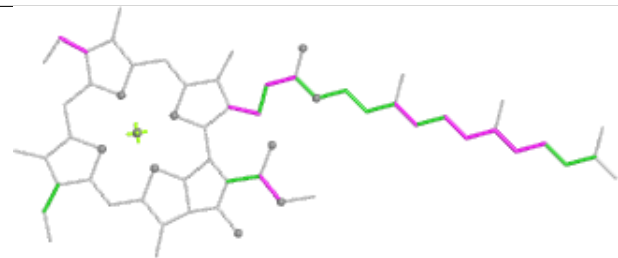
Ligand CLA Ba 312



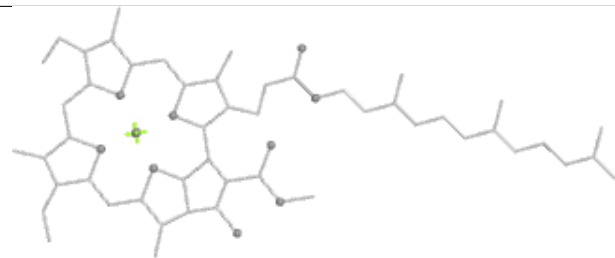
Bond lengths



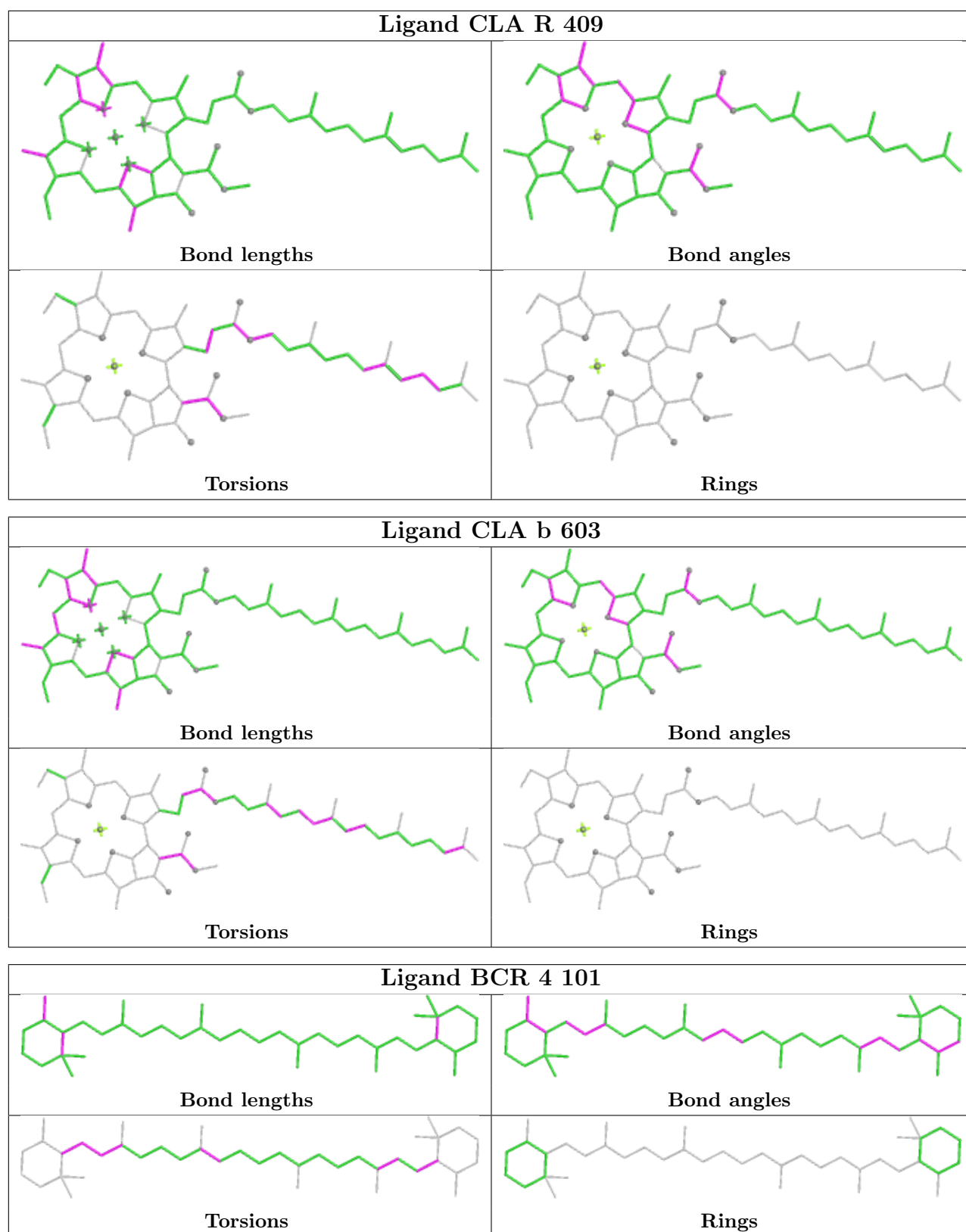
Bond angles



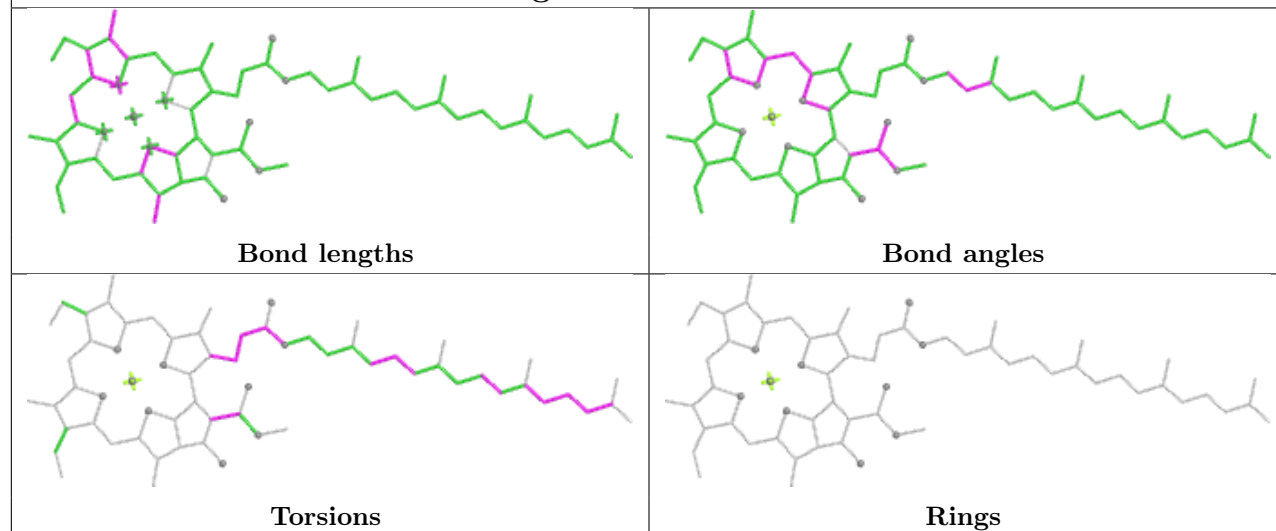
Torsions



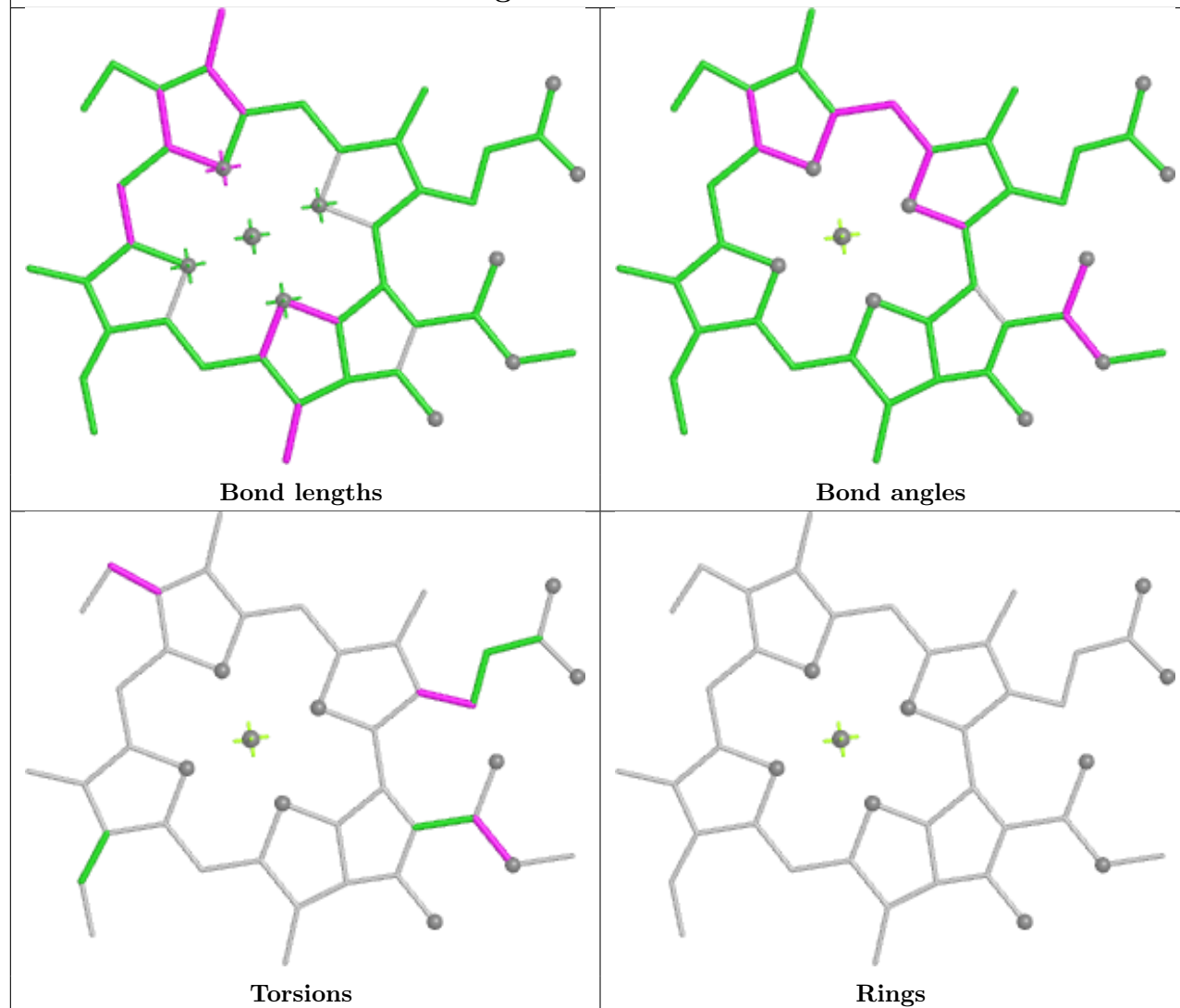
Rings



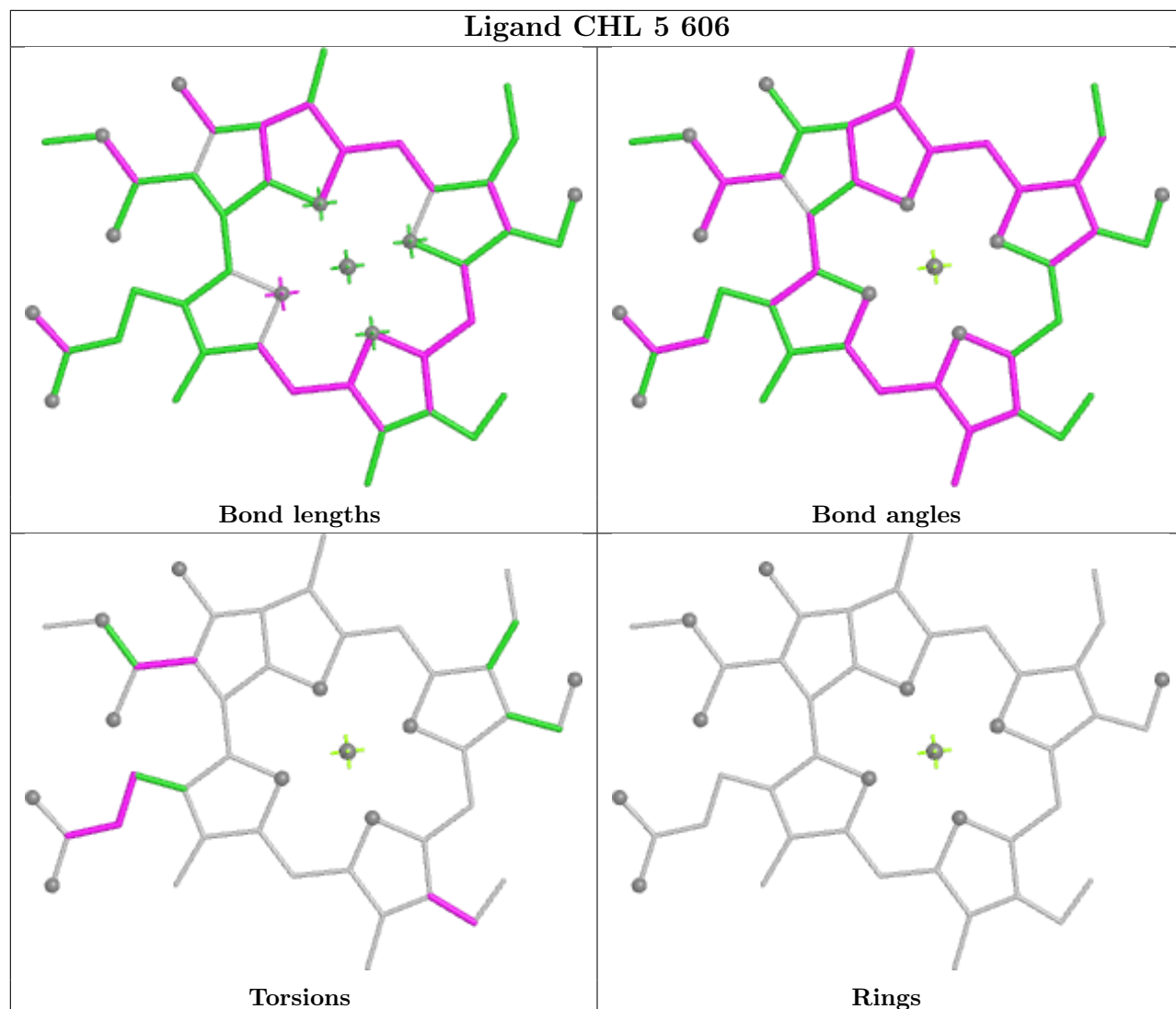
Ligand CLA B 601

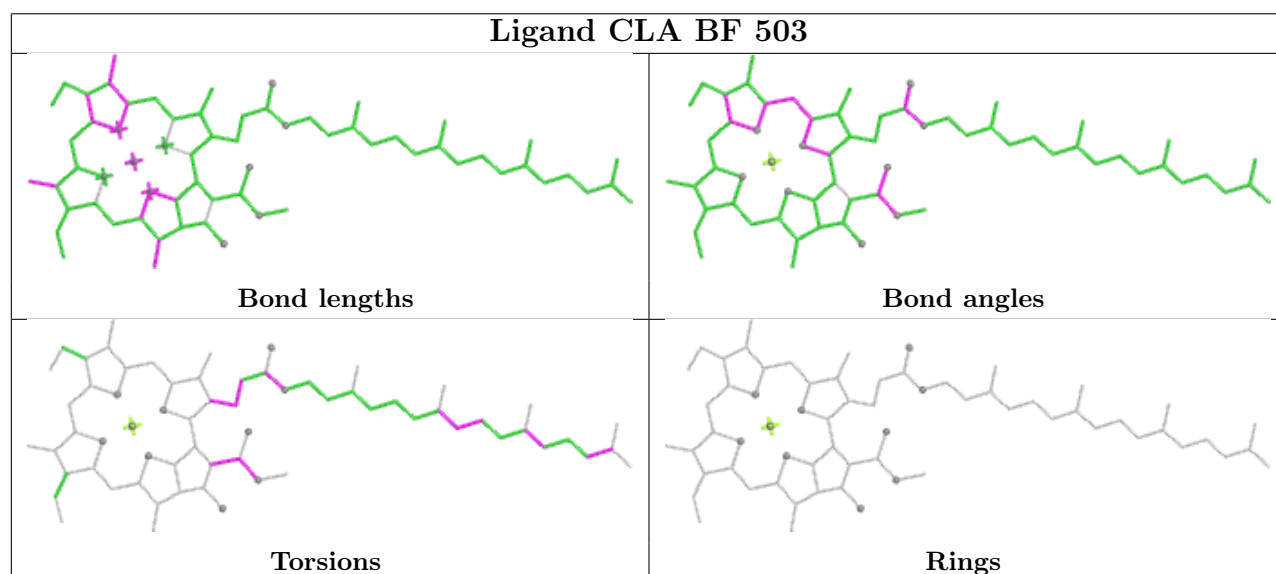
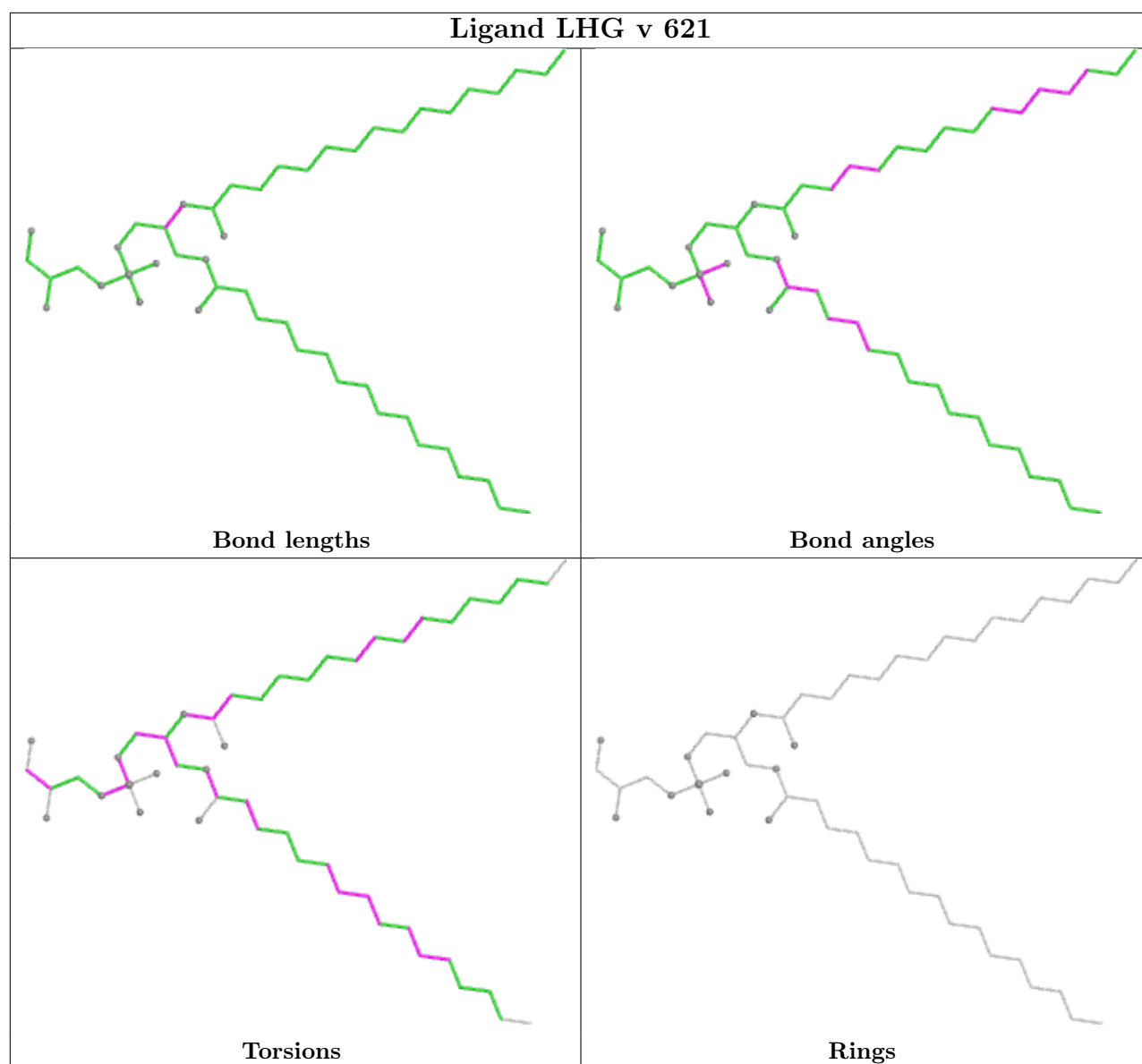


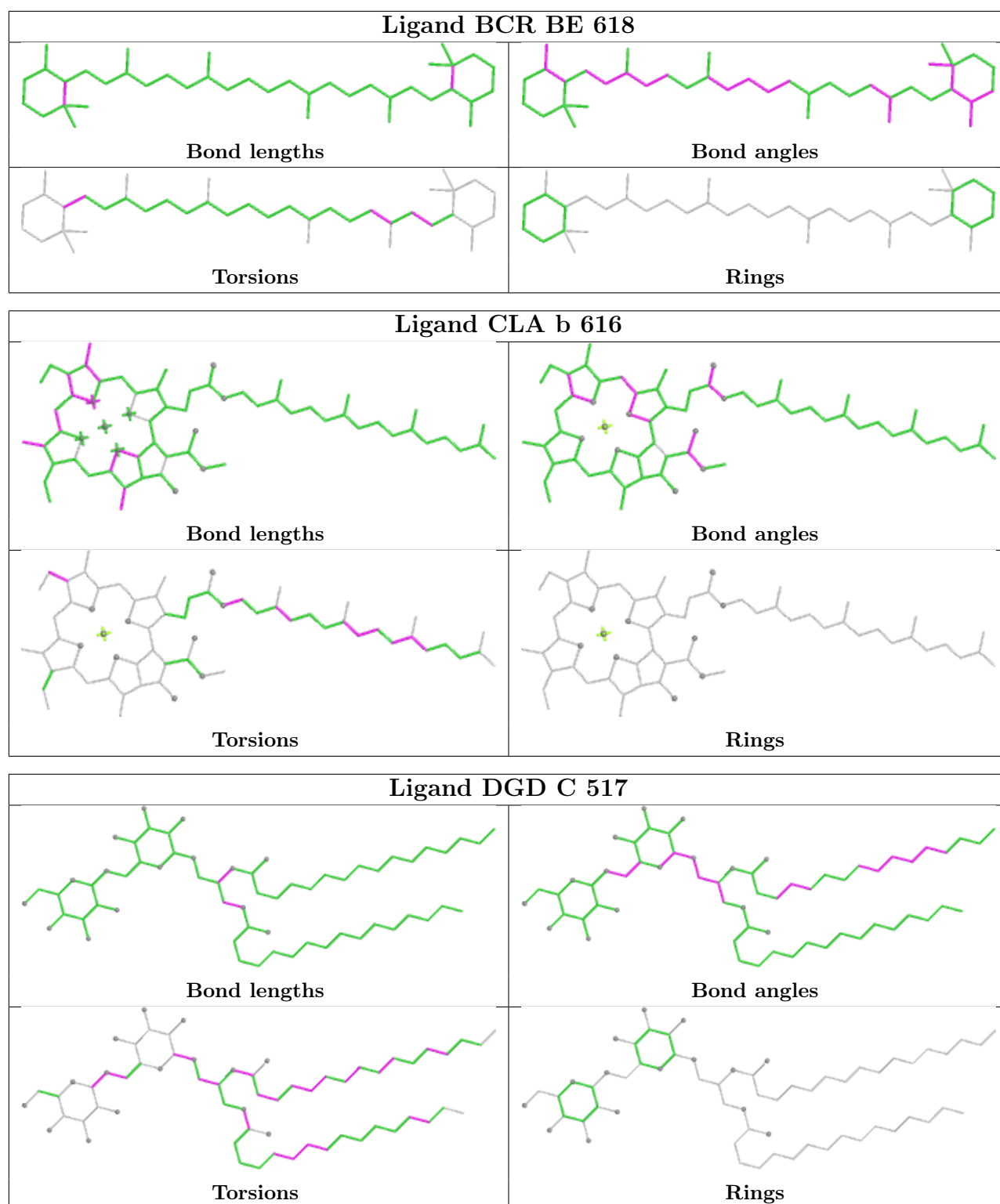
Ligand CLA S 608

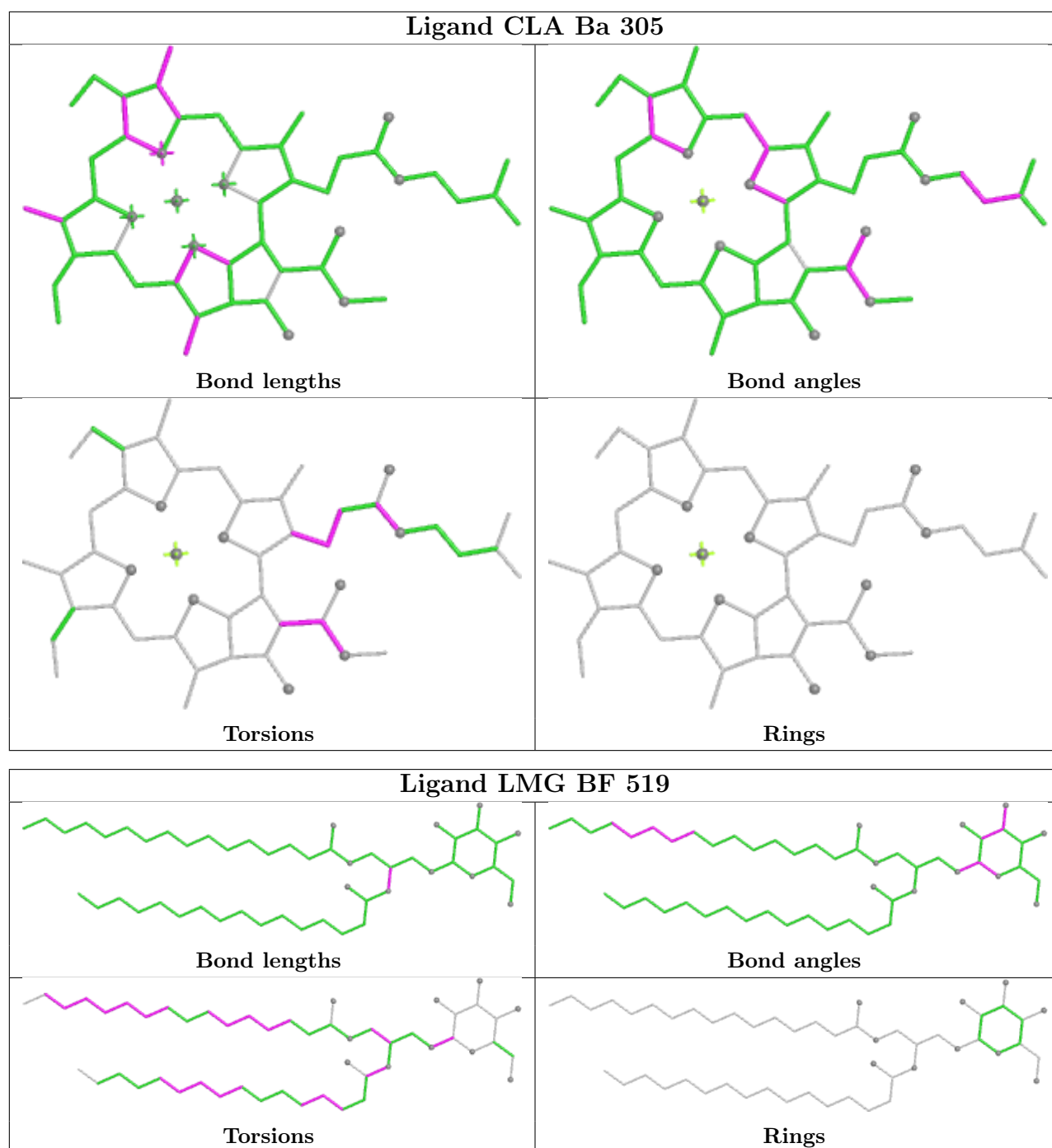


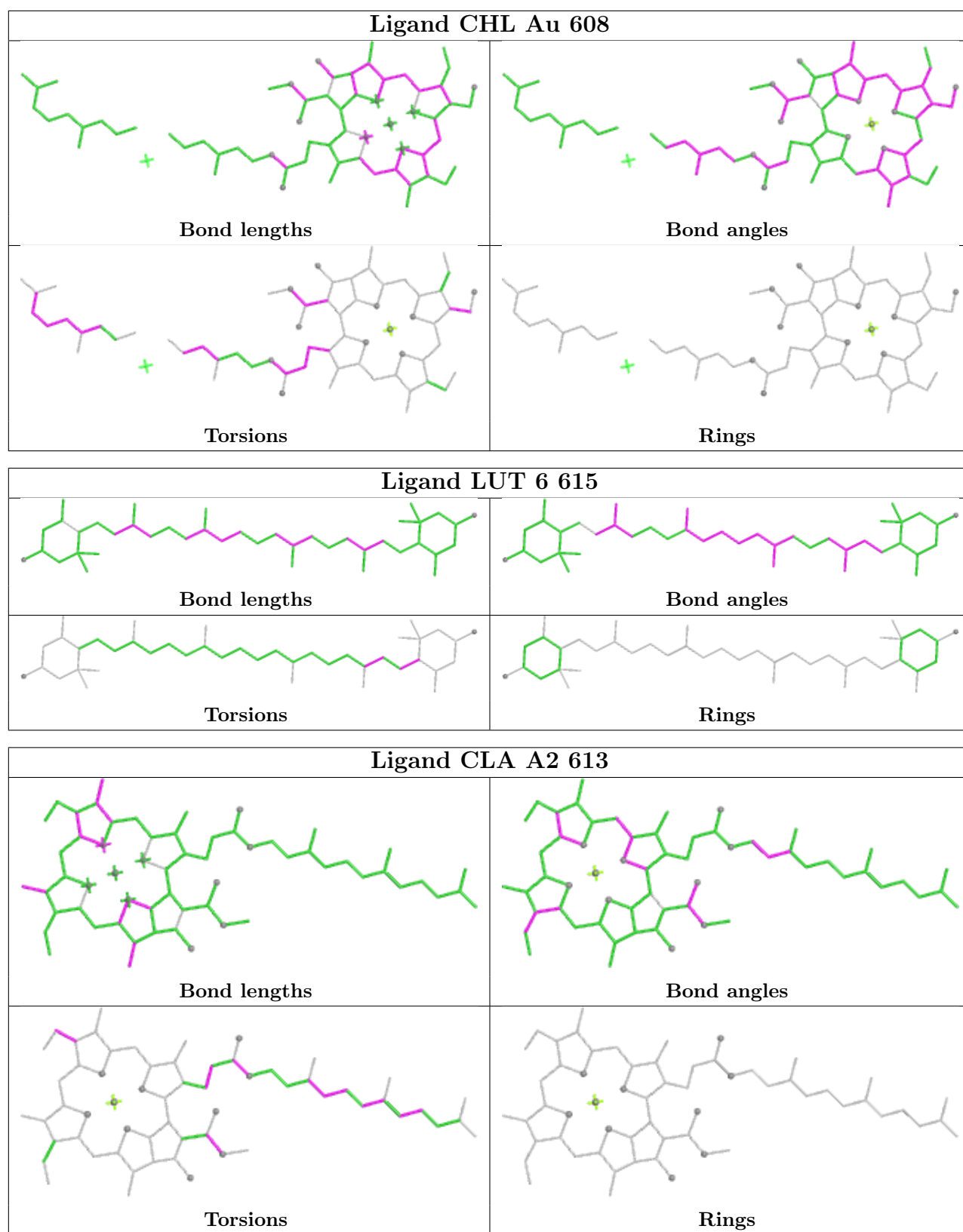
Ligand CHL 5 606



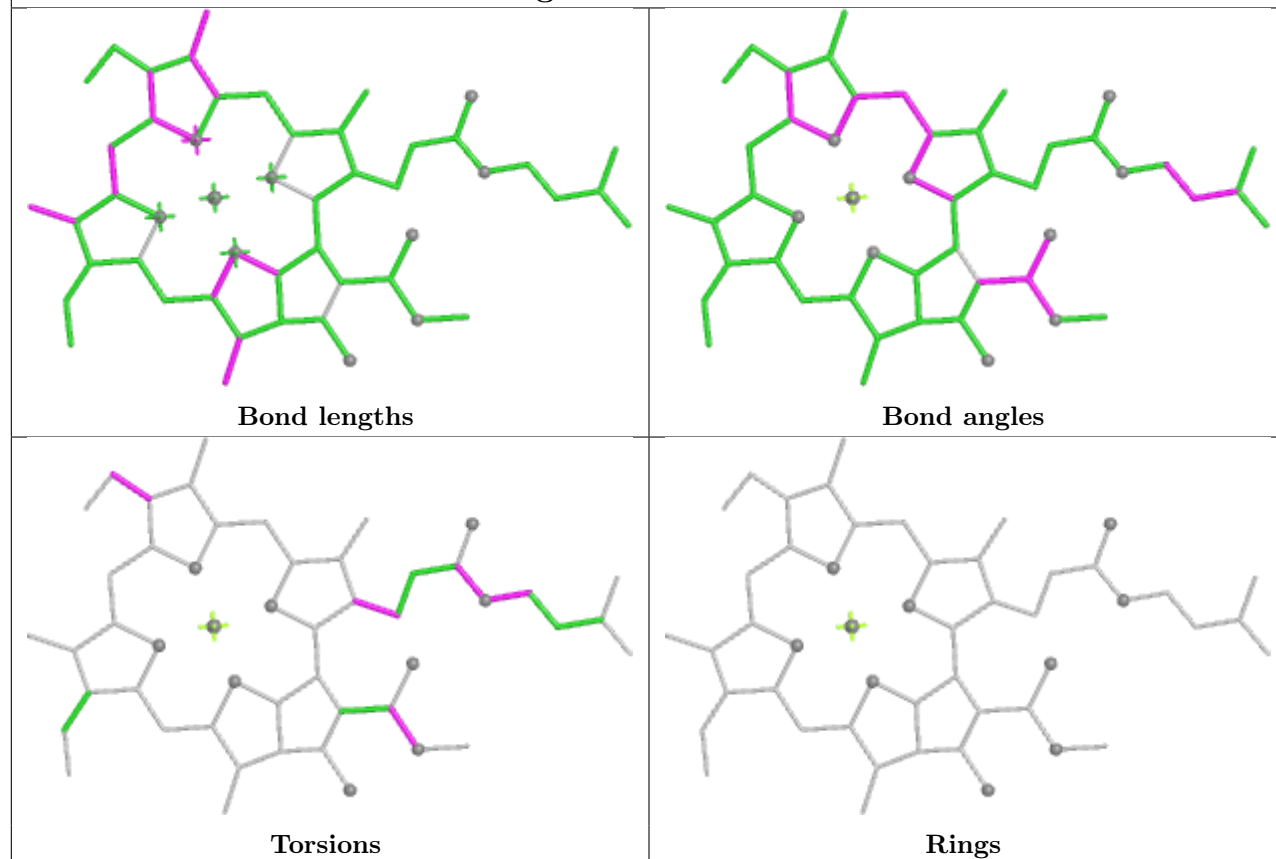




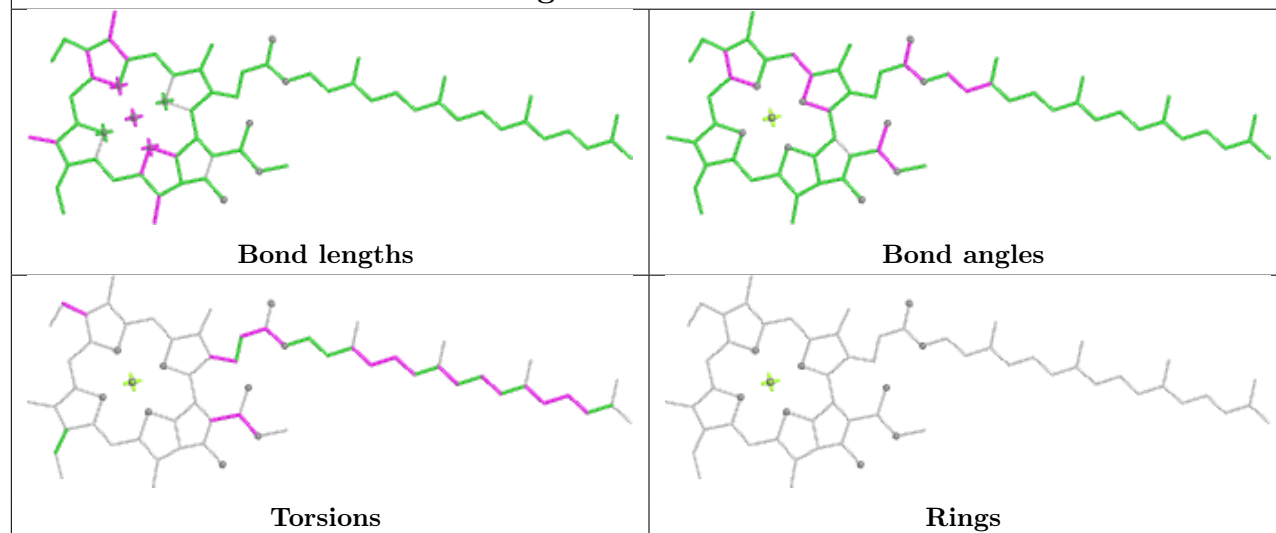


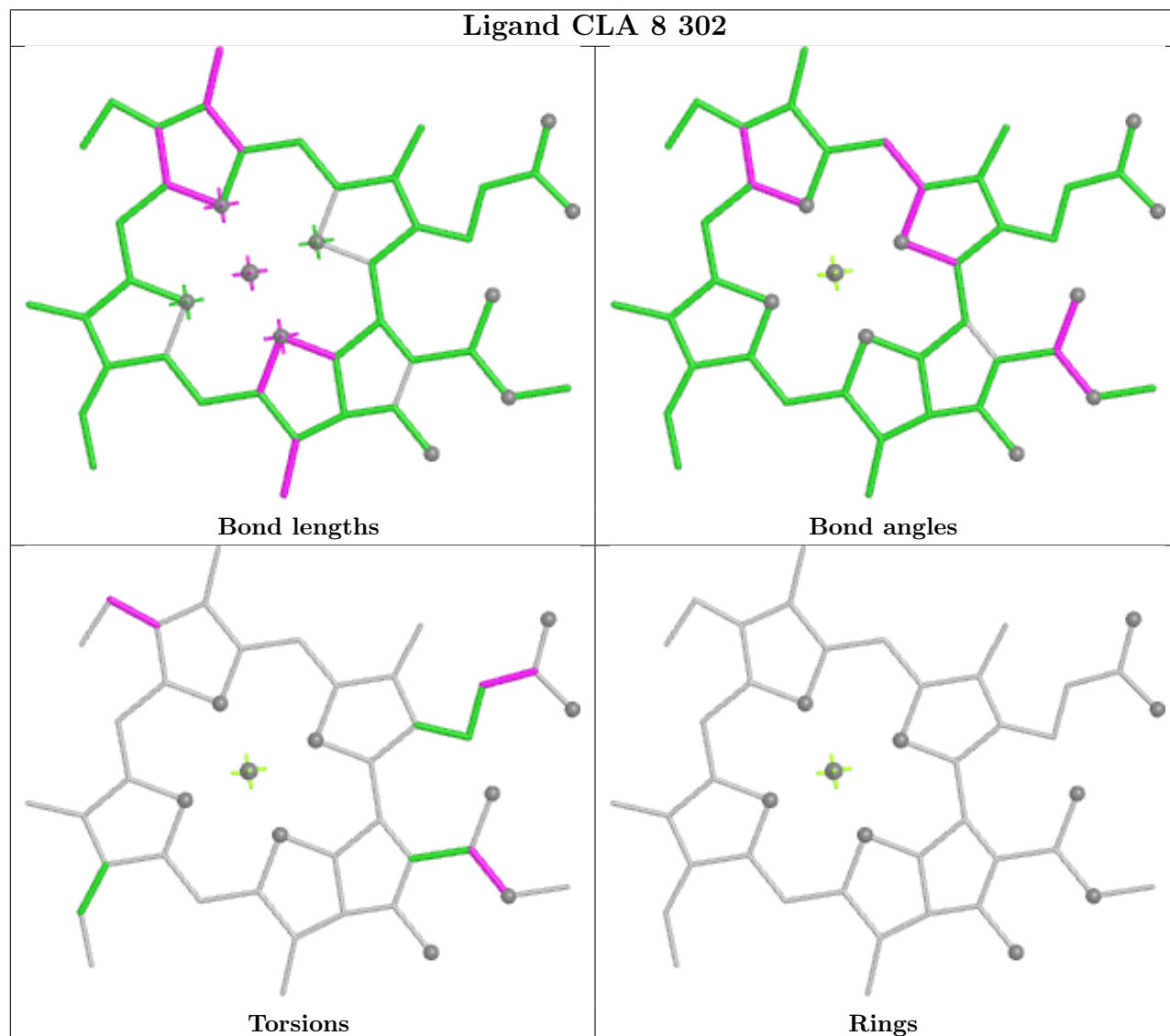
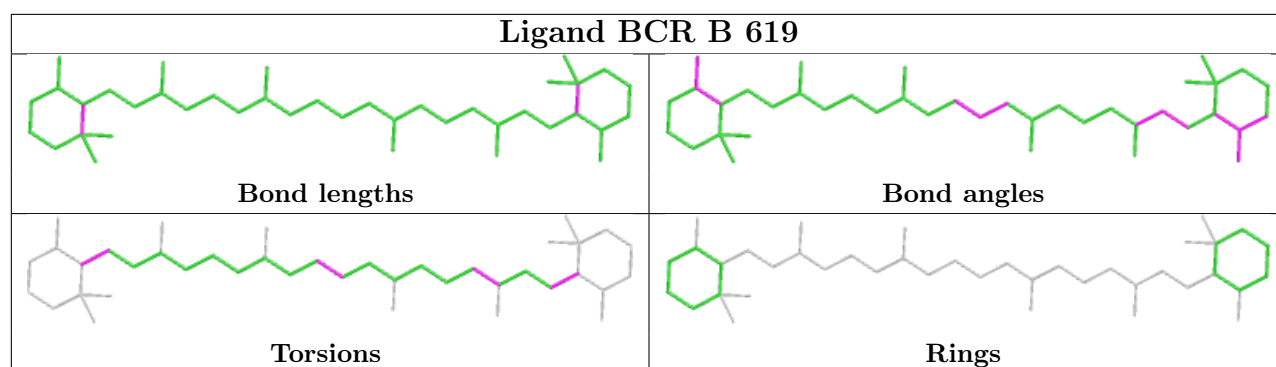


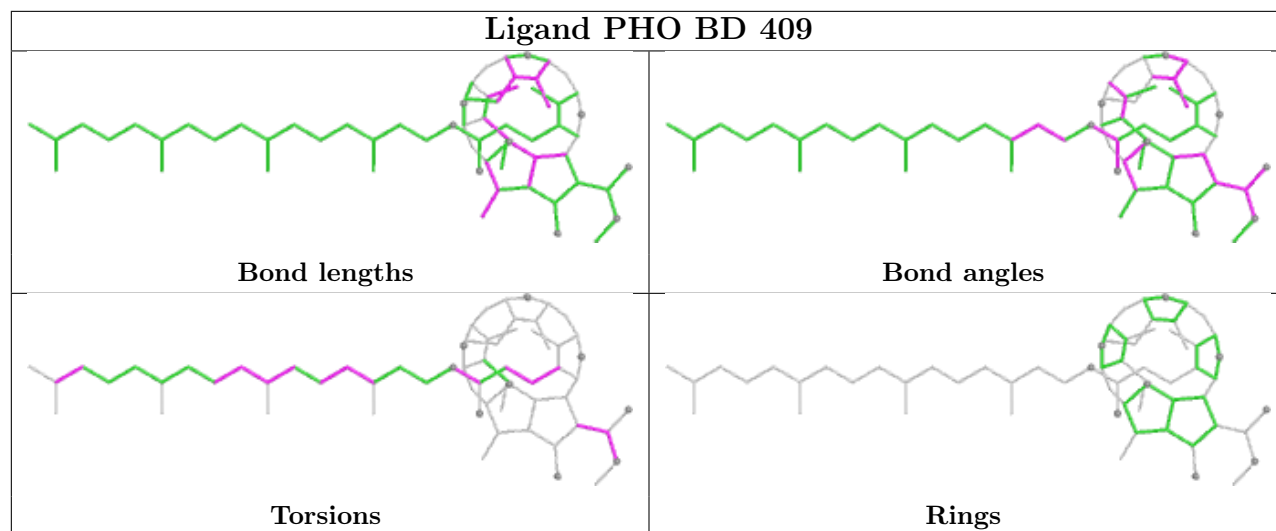
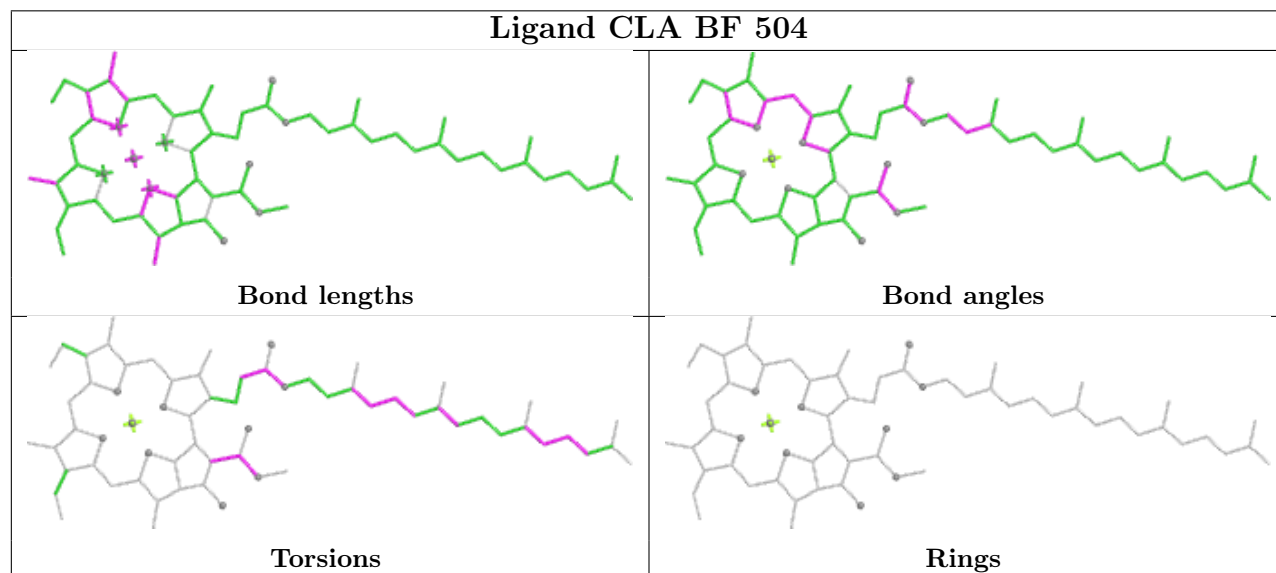
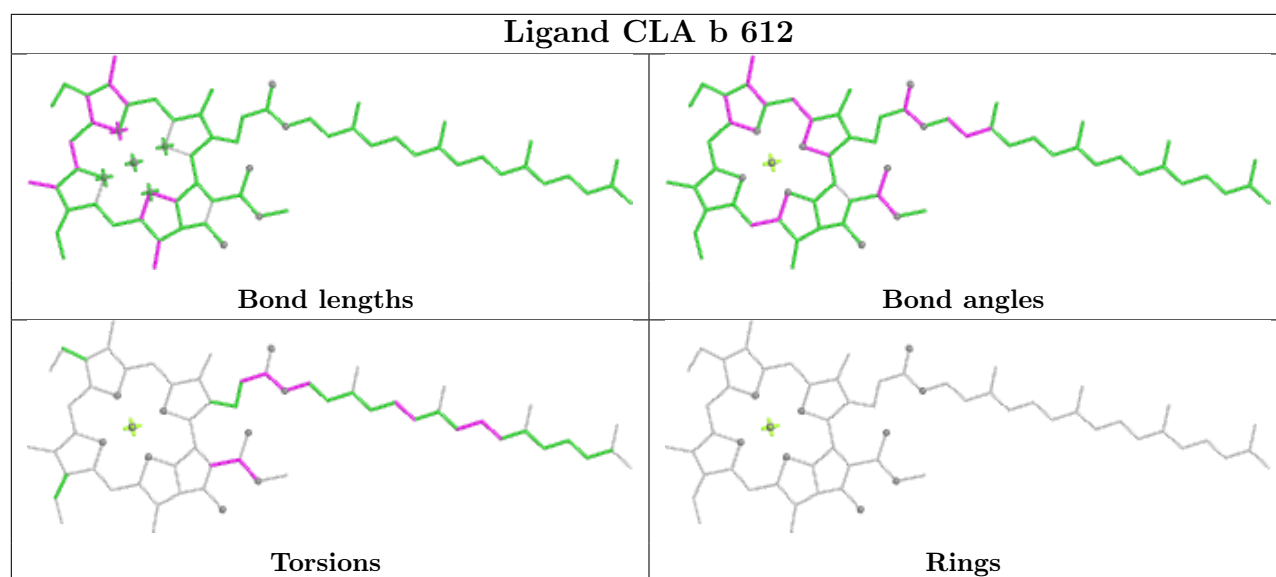
Ligand CLA a 407



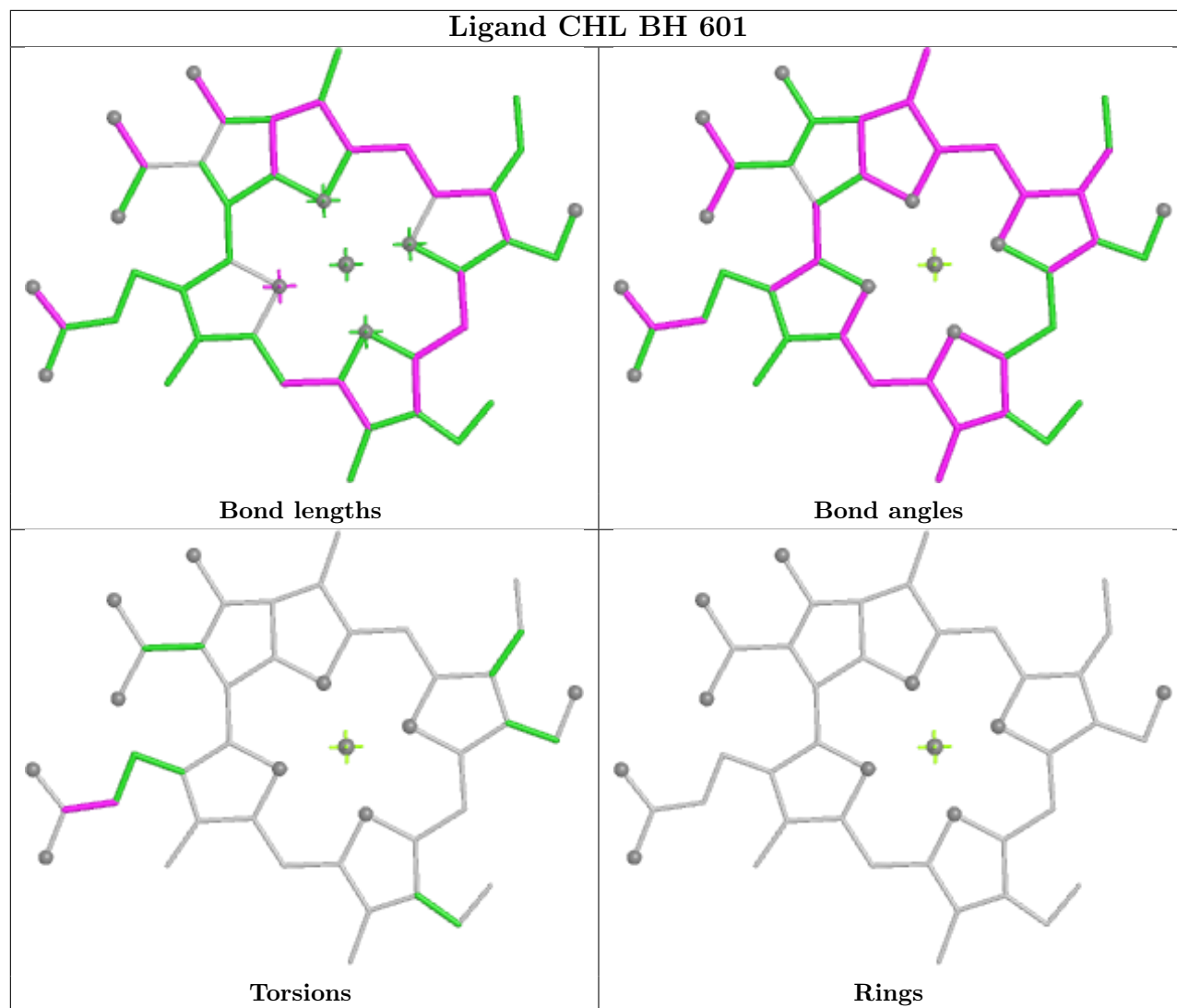
Ligand CLA c 504



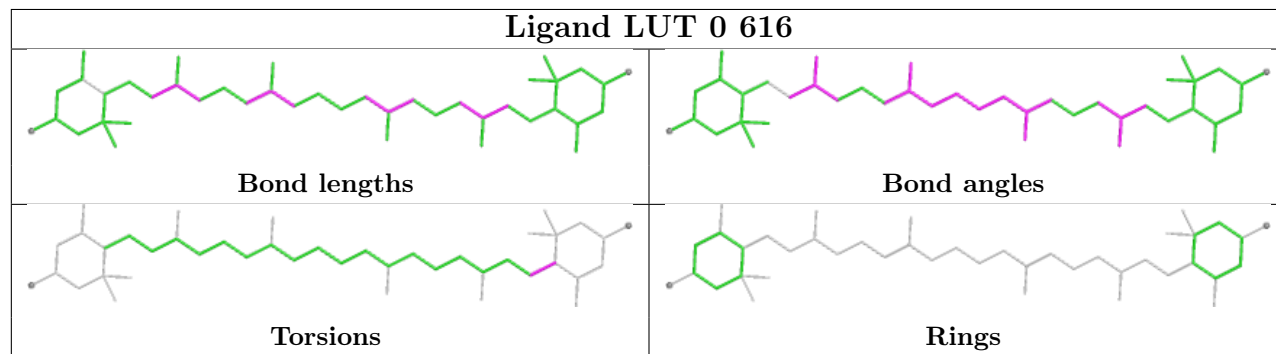


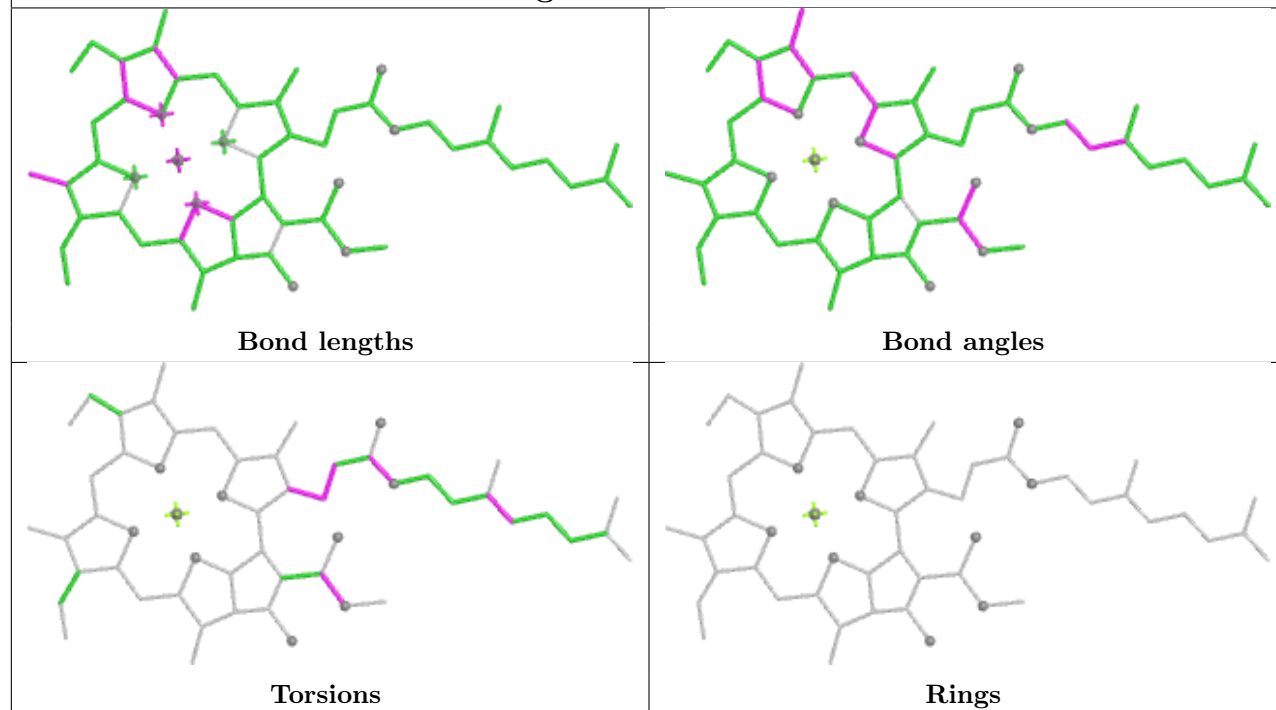
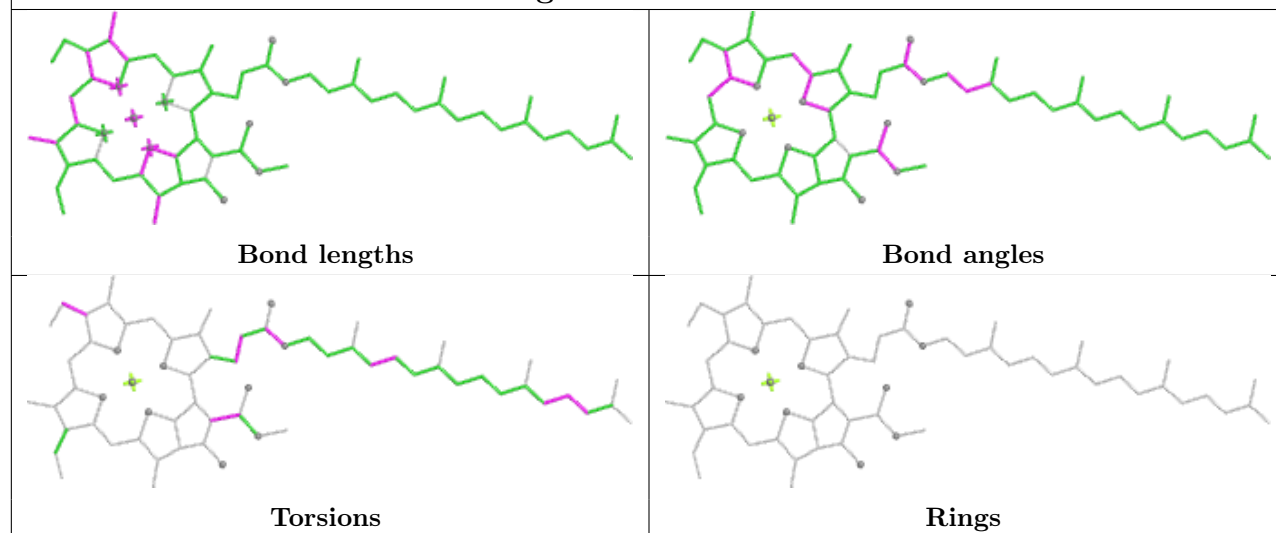


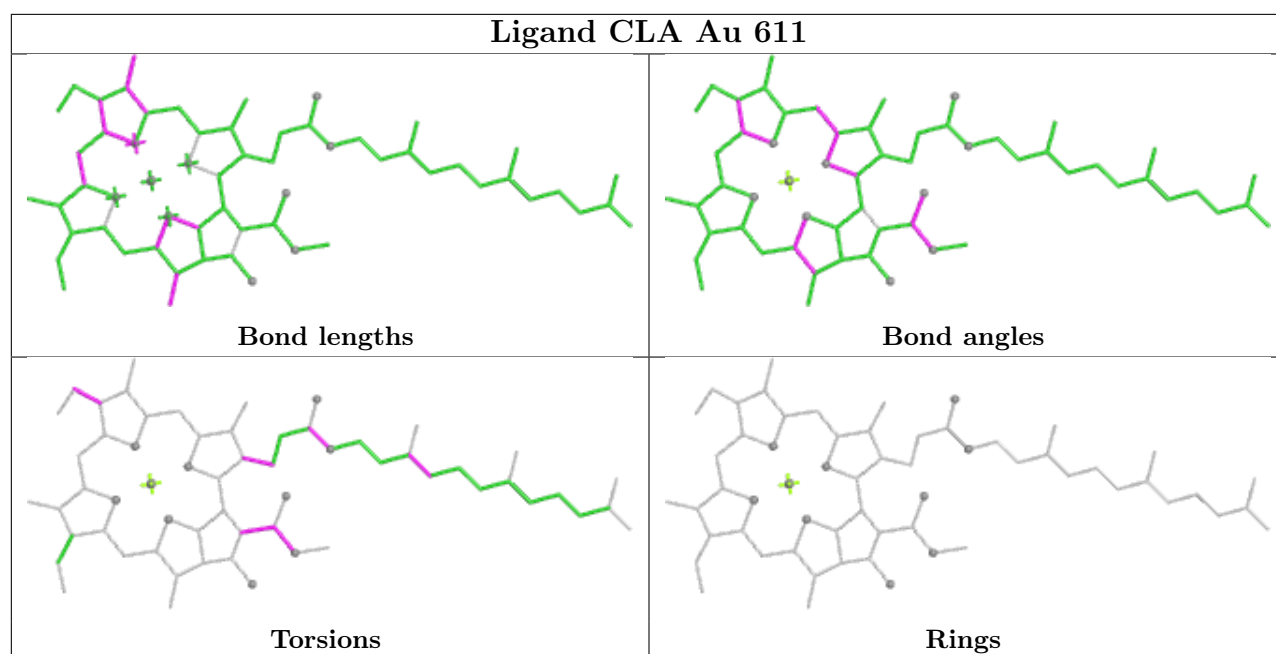
Ligand CHL BH 601

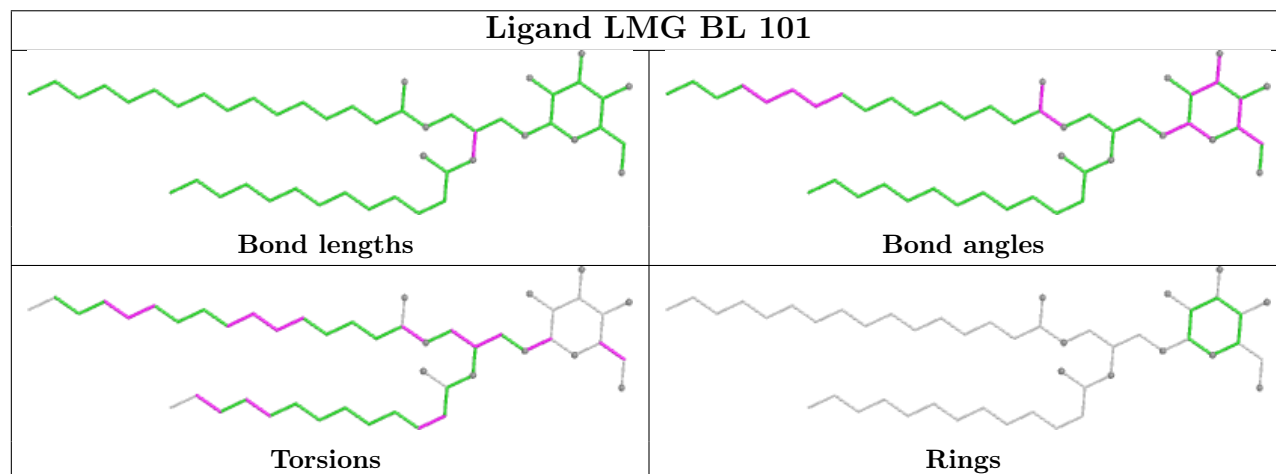
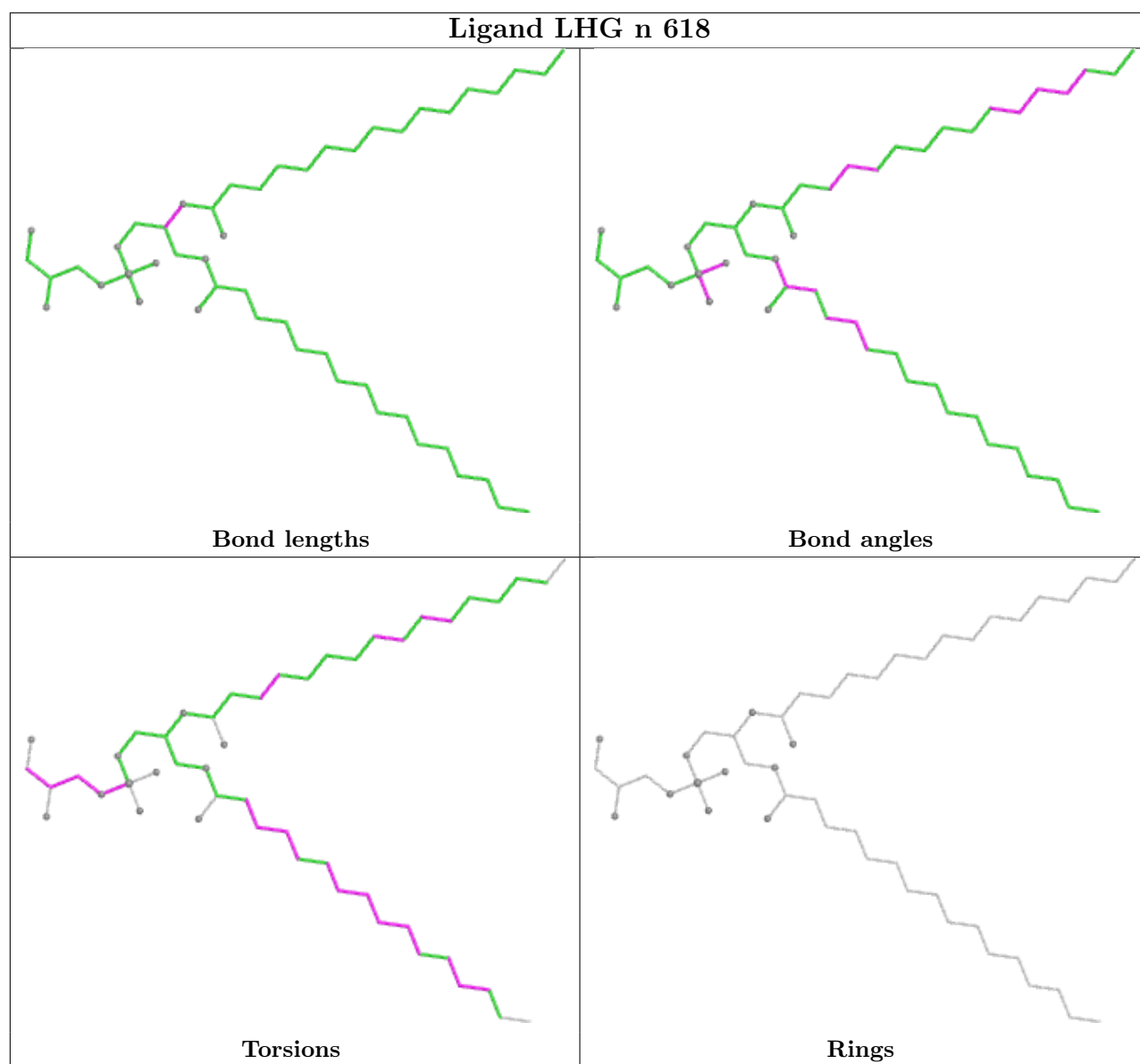


Ligand LUT 0 616

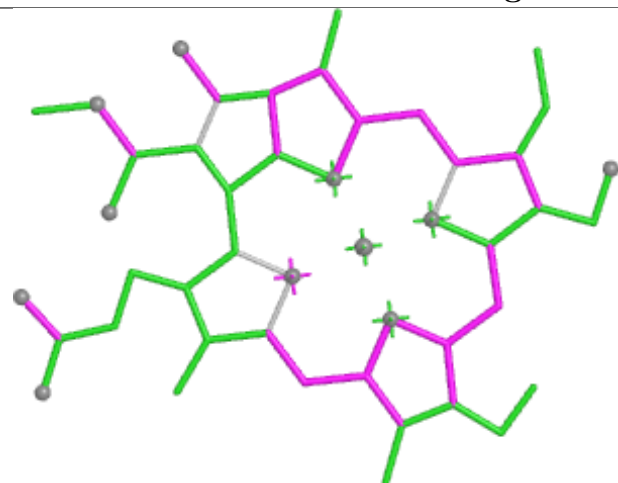


Ligand CLA 5 613**Ligand CLA a 405**

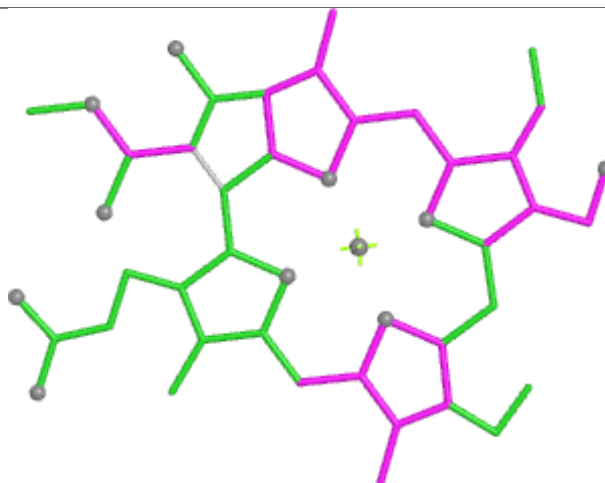




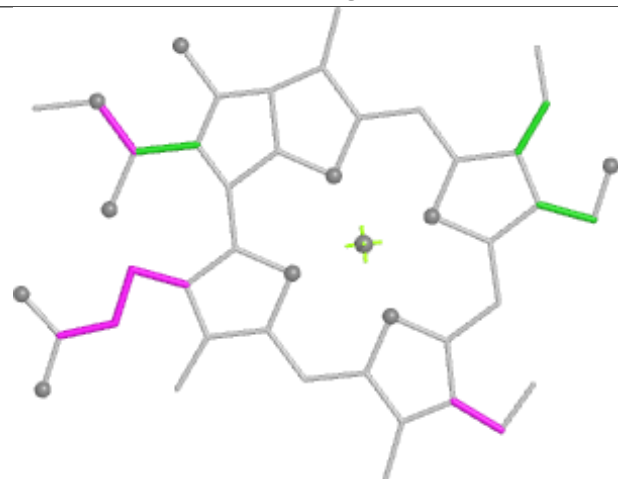
Ligand CHL AB 305



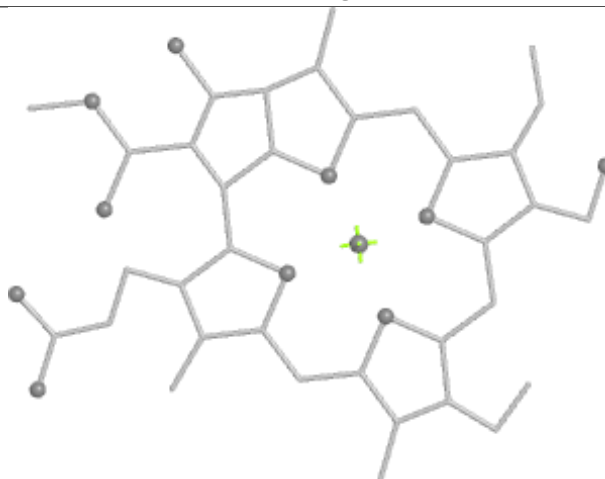
Bond lengths



Bond angles

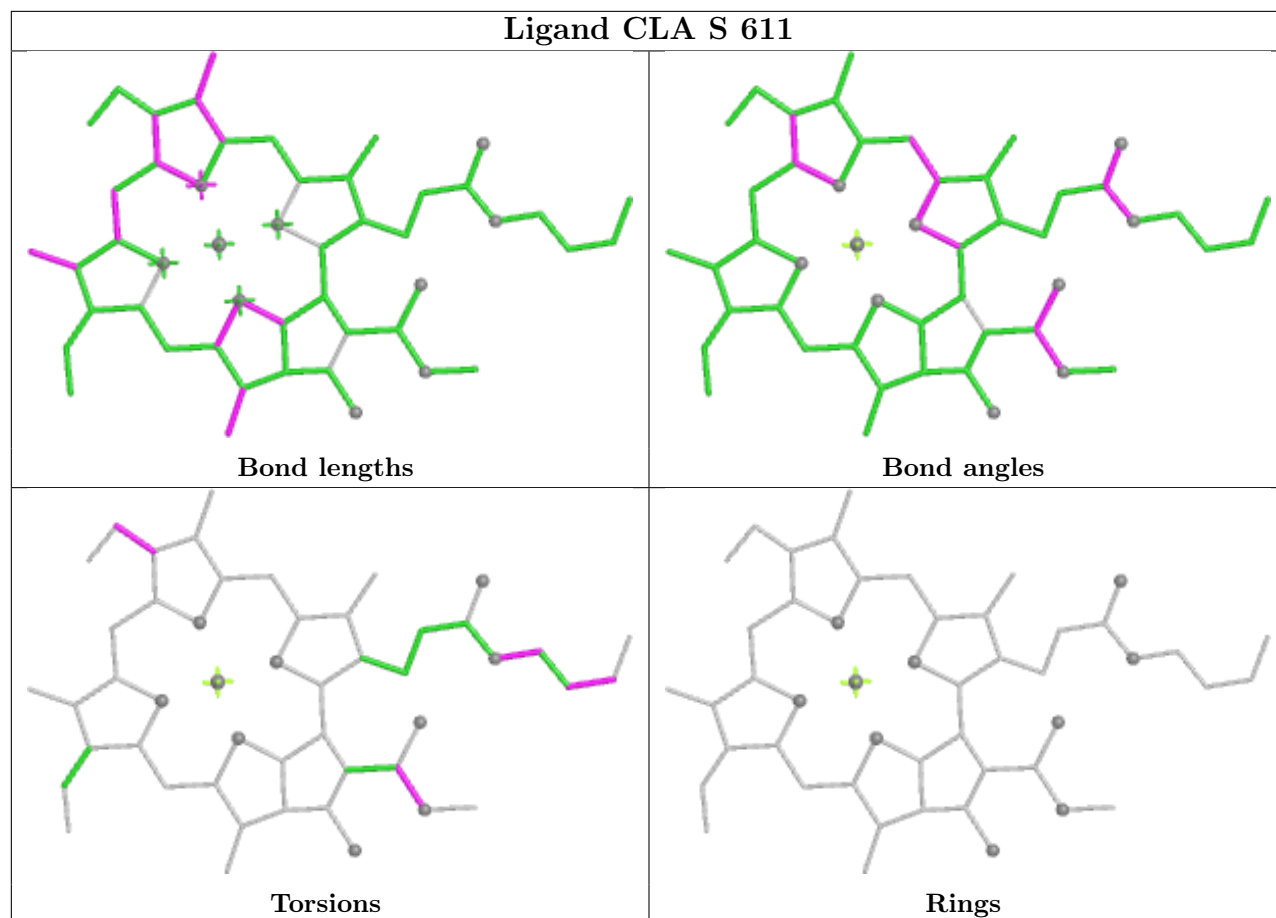


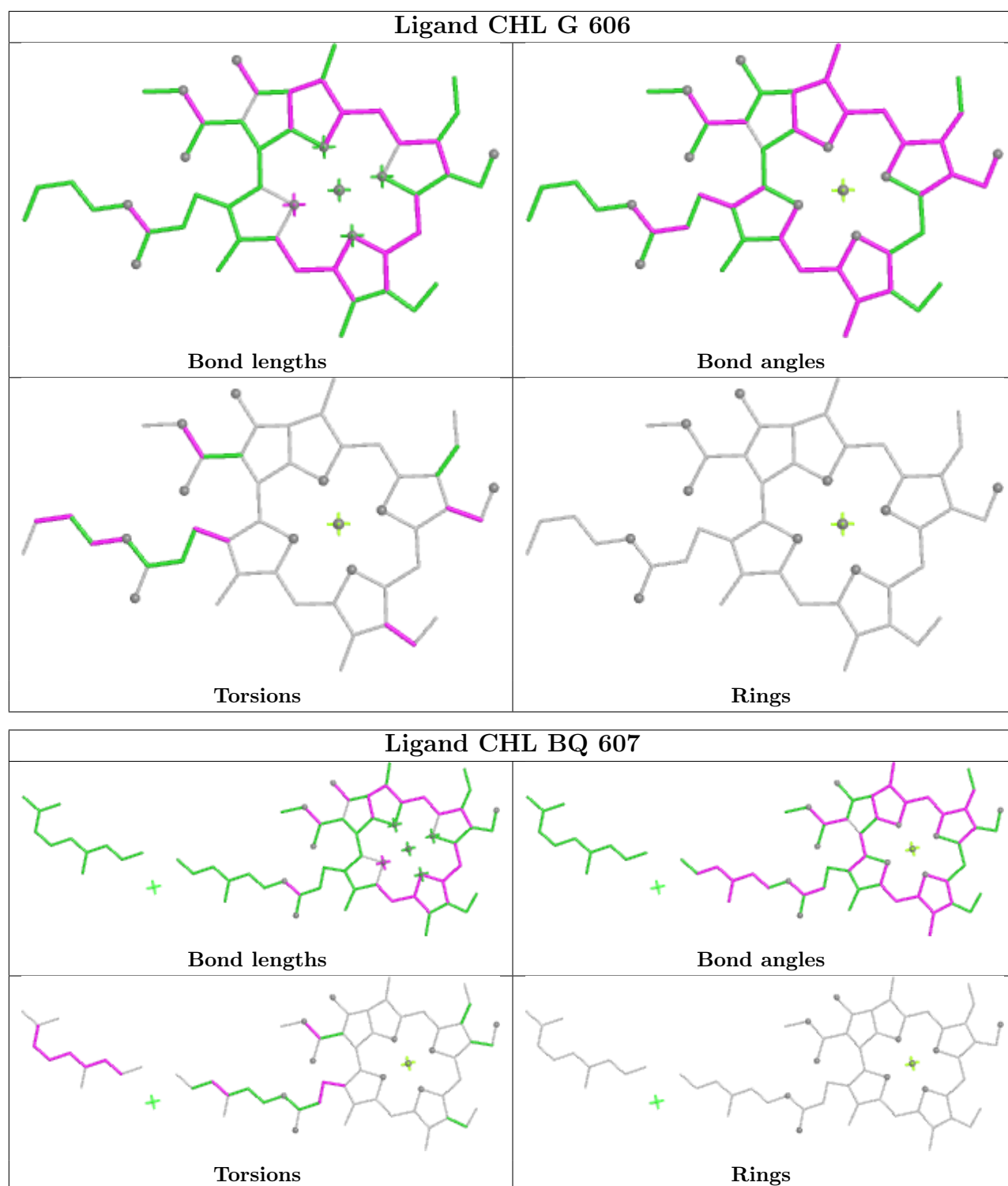
Torsions

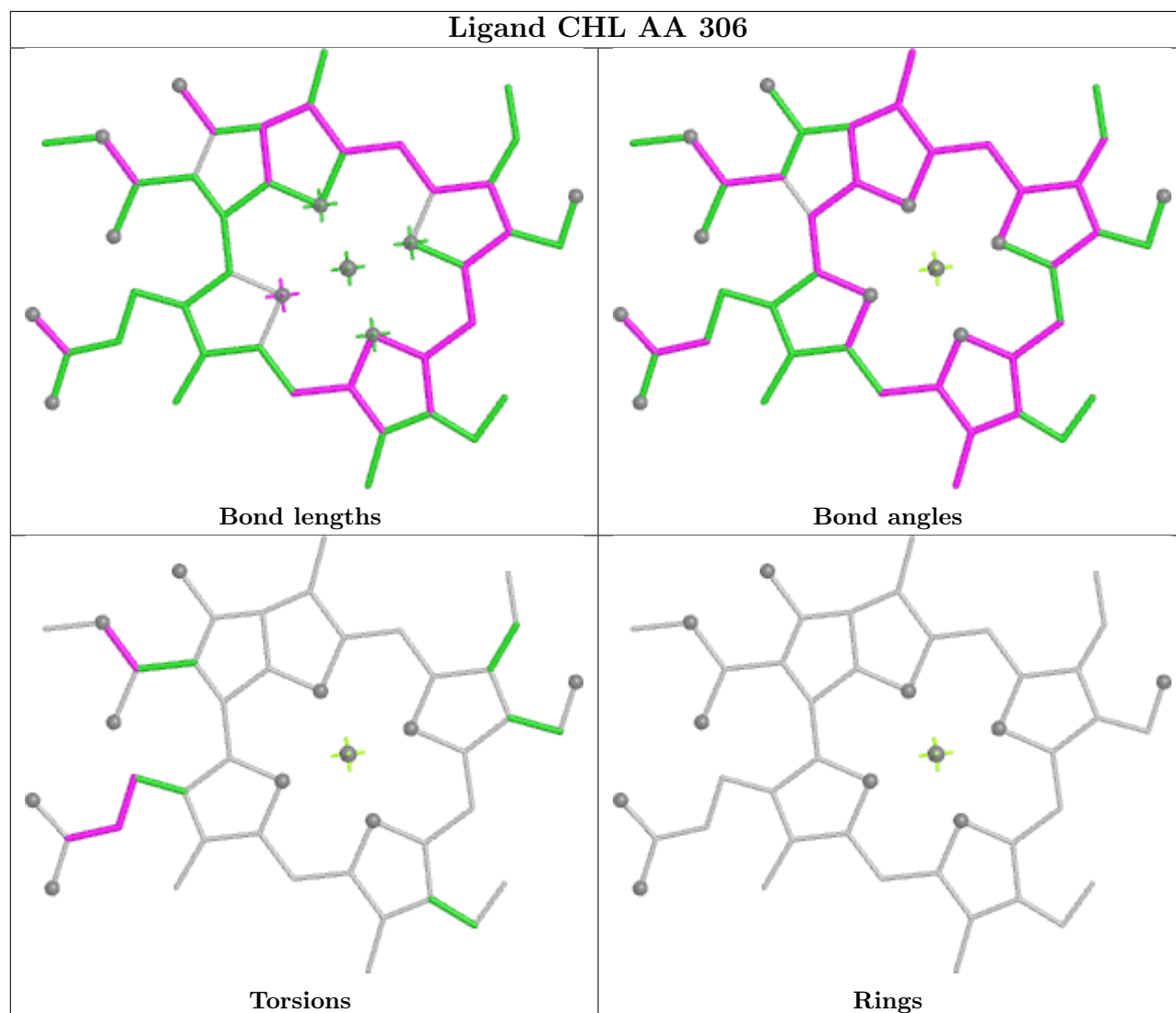
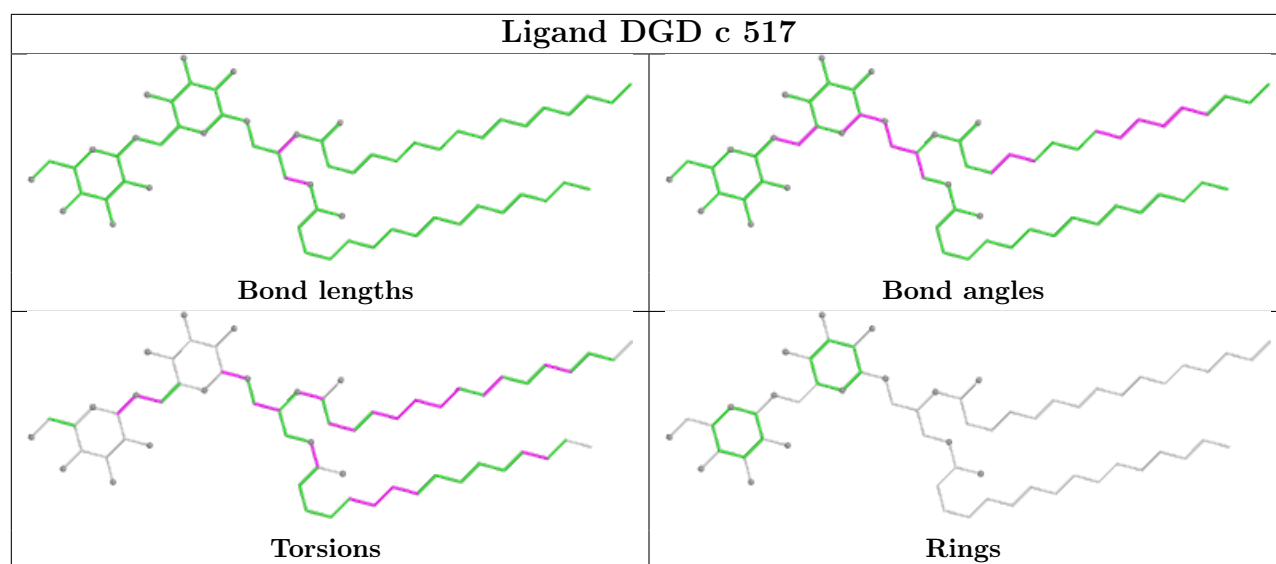


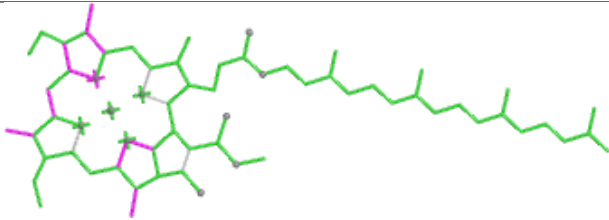
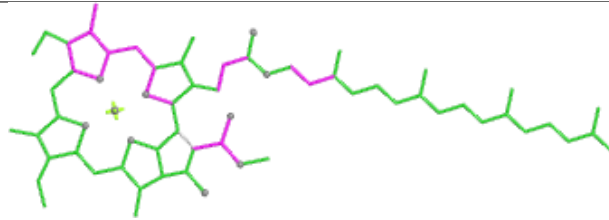
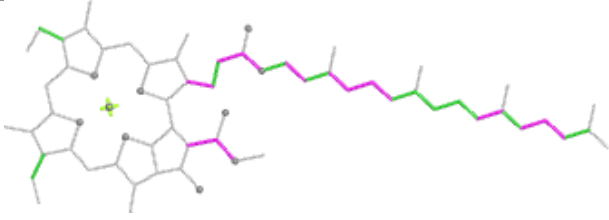
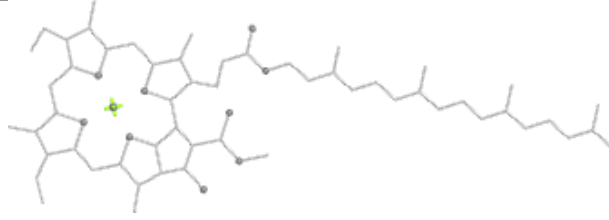
Rings

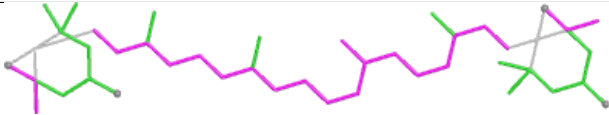
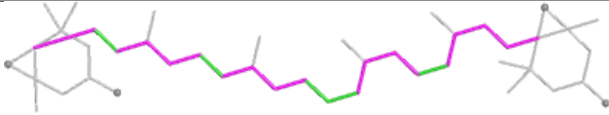
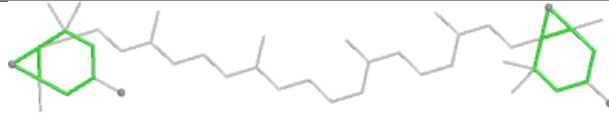
Ligand CLA S 611

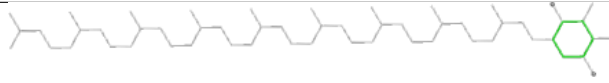




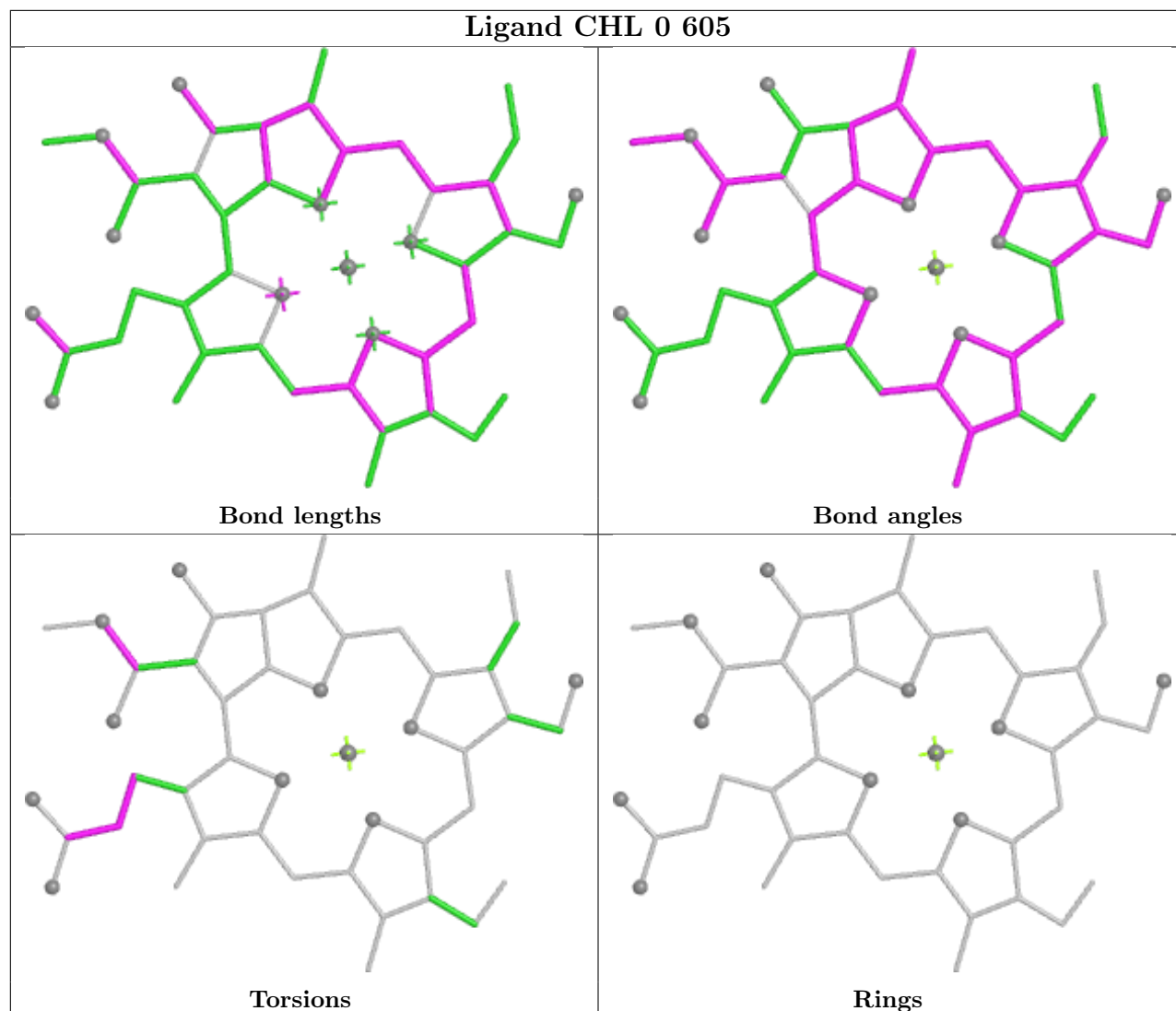


Ligand CLA N 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

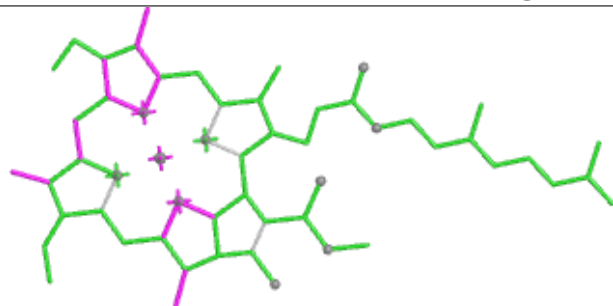
Ligand XAT Ba 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 BG 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

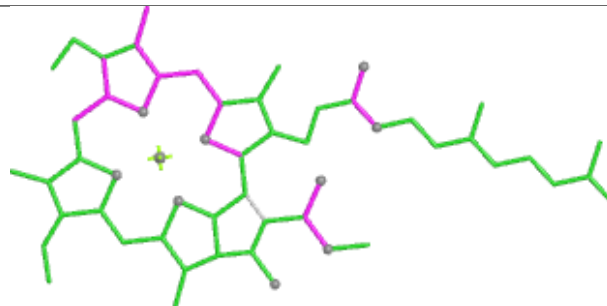
Ligand CHL 0 605



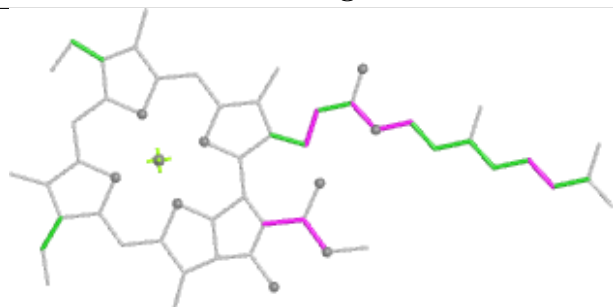
Ligand CLA 0 603



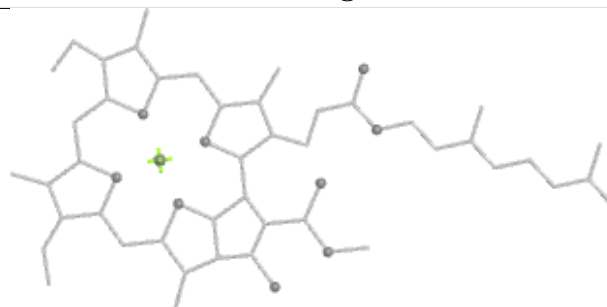
Bond lengths



Bond angles

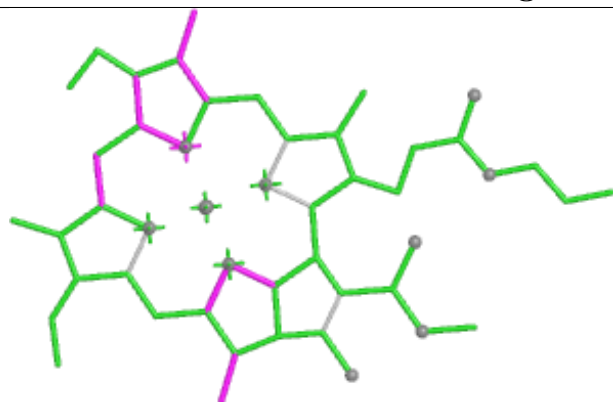


Torsions

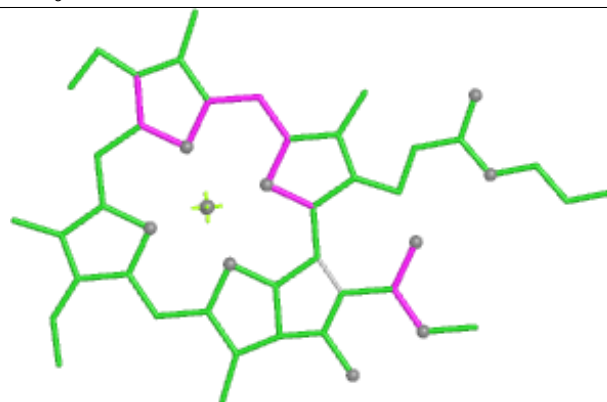


Rings

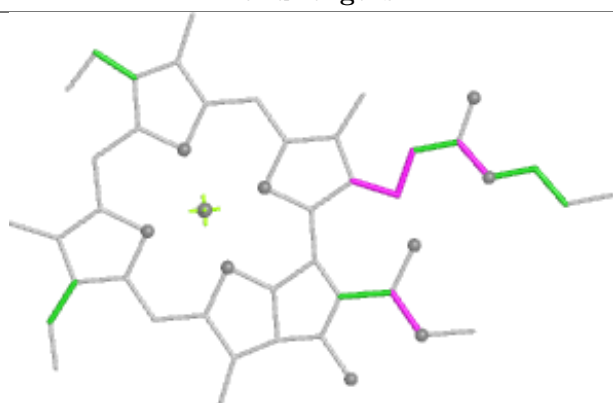
Ligand CLA y 315



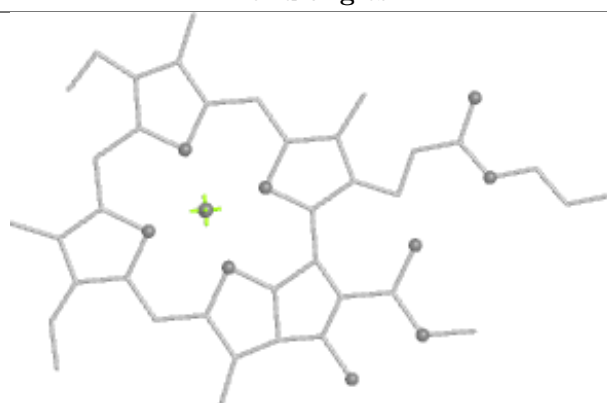
Bond lengths



Bond angles

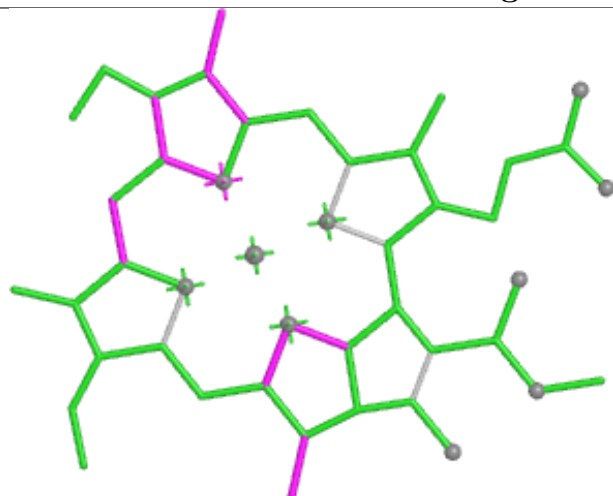


Torsions

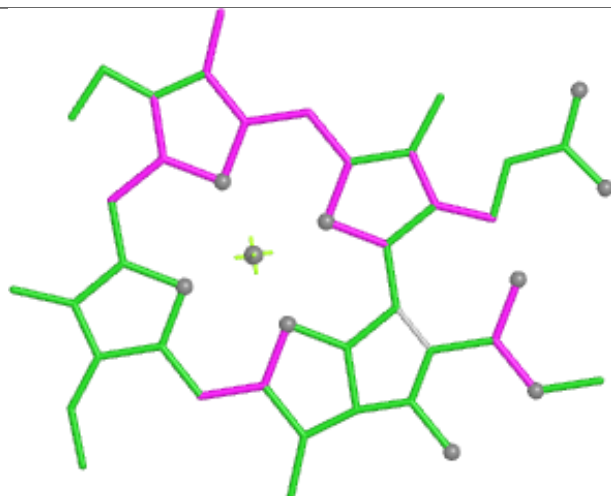


Rings

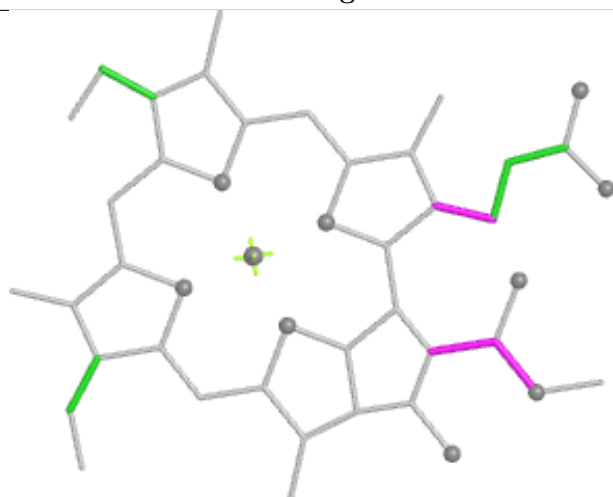
Ligand CLA AB 310



Bond lengths



Bond angles

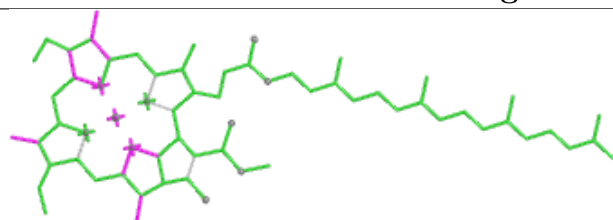


Torsions

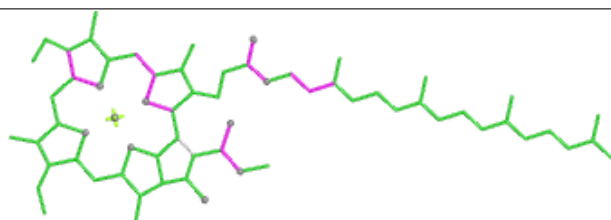


Rings

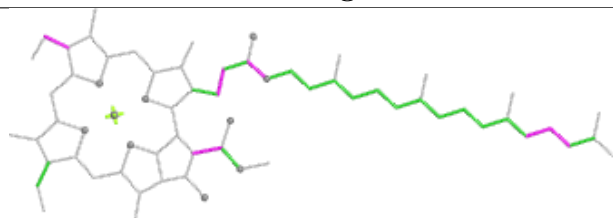
Ligand CLA BD 405



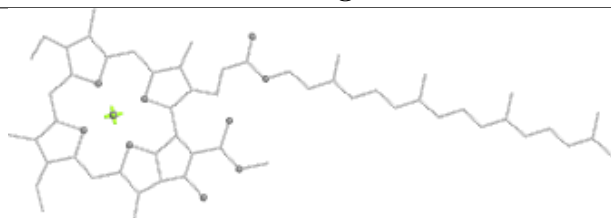
Bond lengths



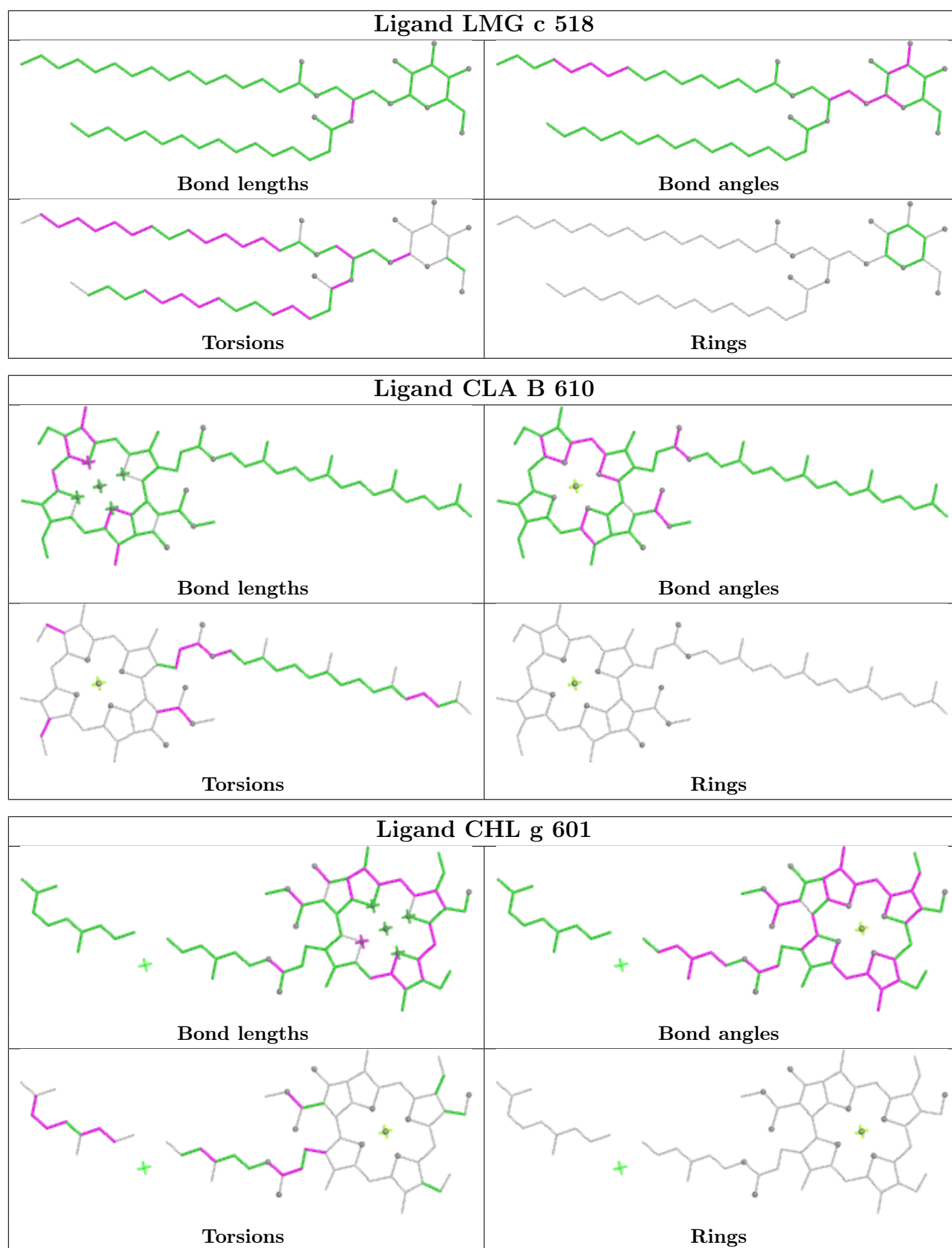
Bond angles

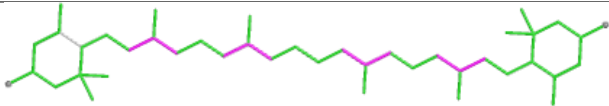
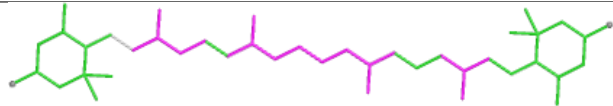
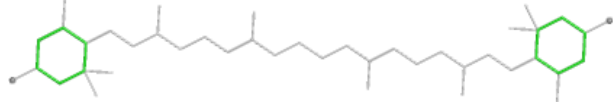


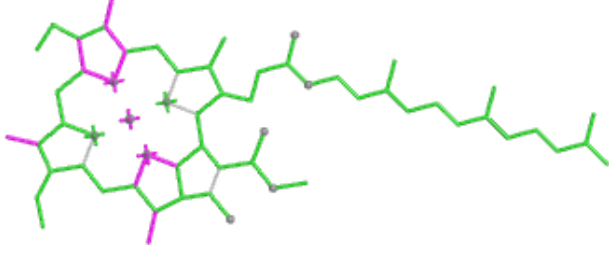
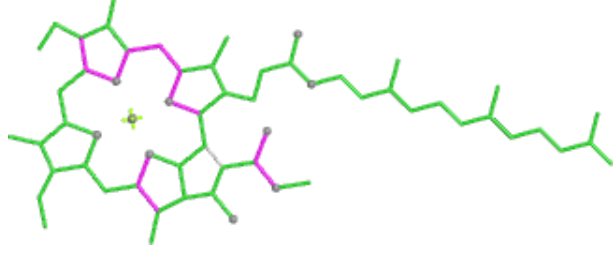
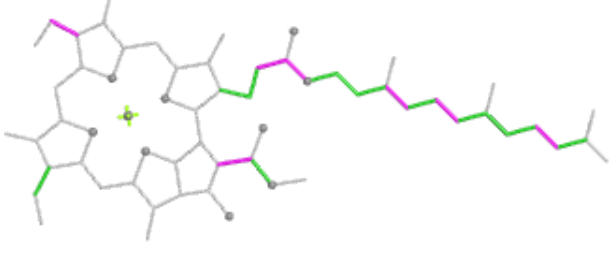
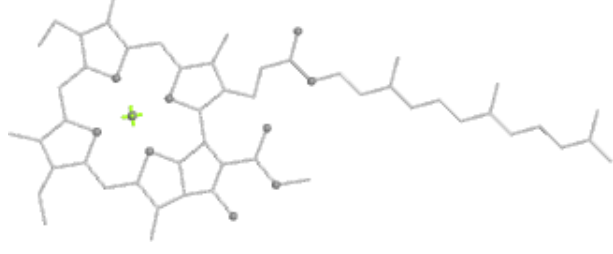
Torsions

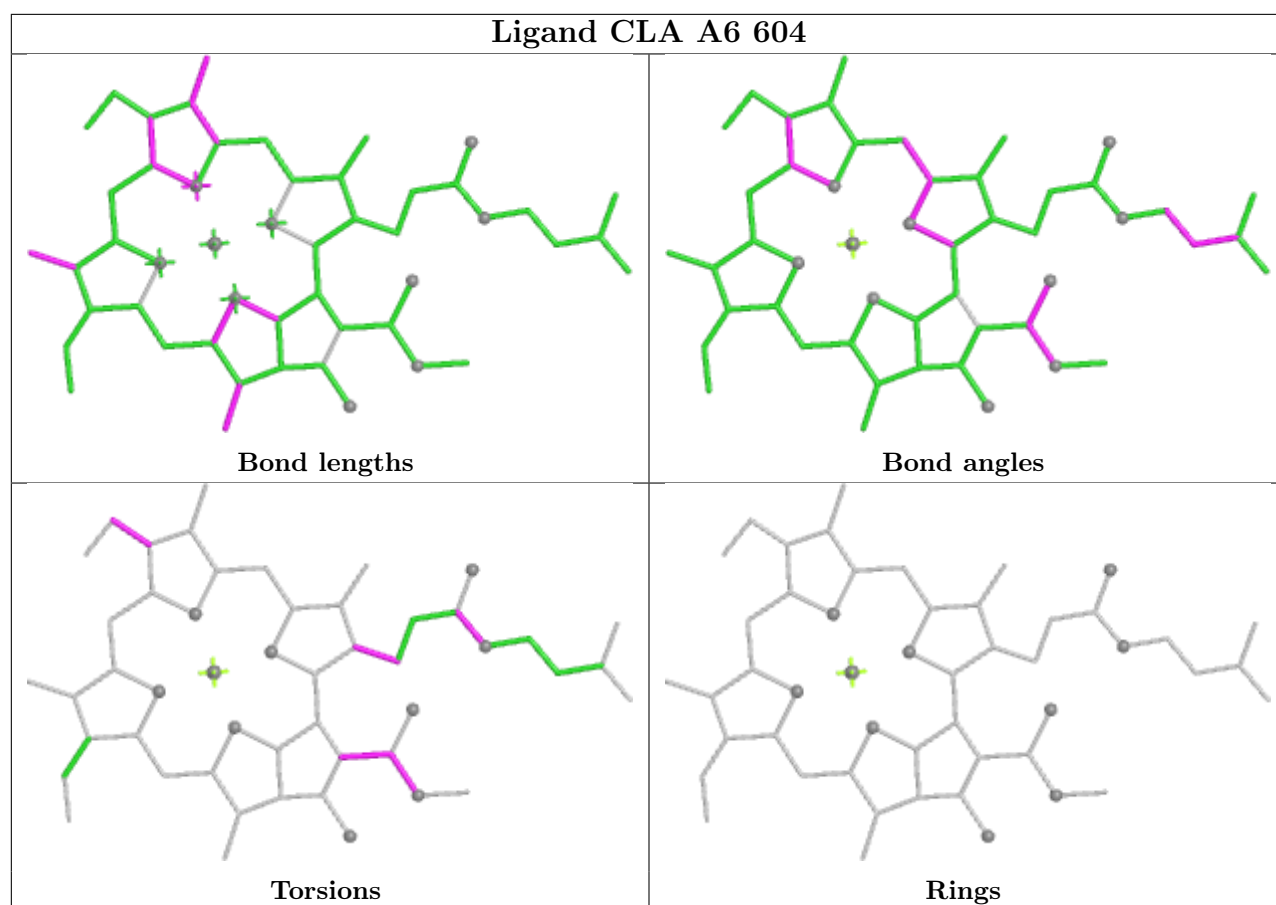


Rings

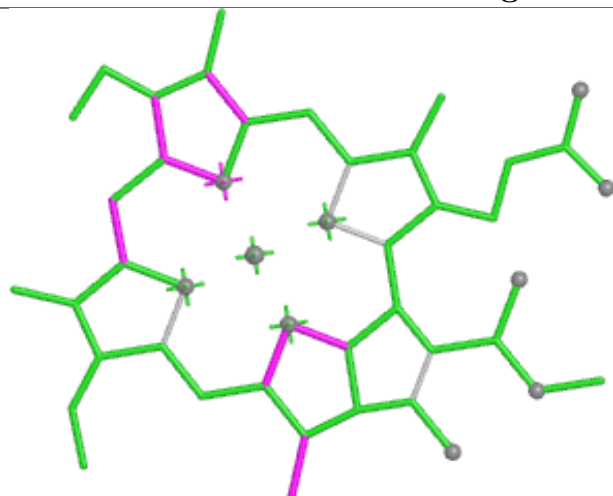


Ligand LUT Y 316	
	Bond lengths
	Bond angles
	Torsions
	Rings

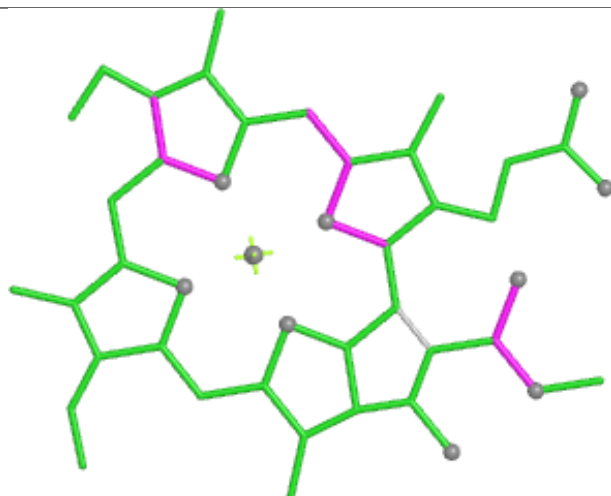
Ligand CLA Y 313	
	Bond lengths
	Bond angles
	Torsions
	Rings



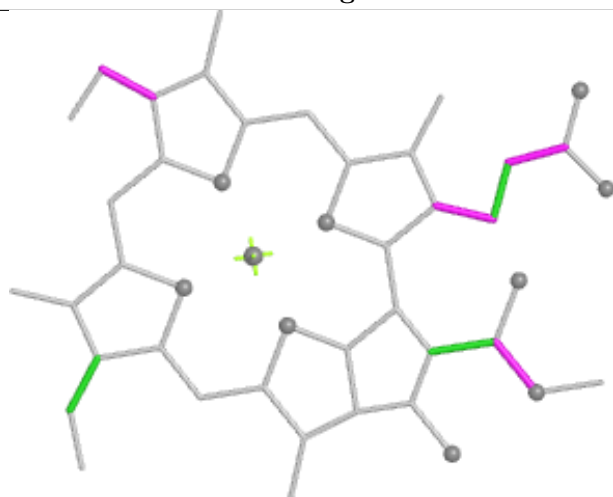
Ligand CLA BV 608



Bond lengths



Bond angles

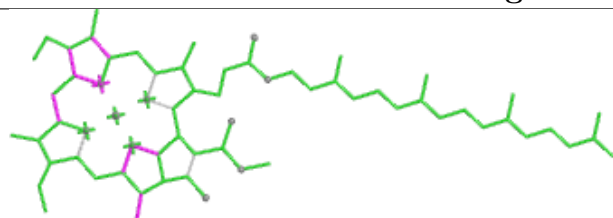


Torsions

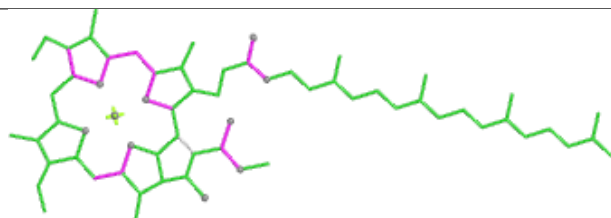


Rings

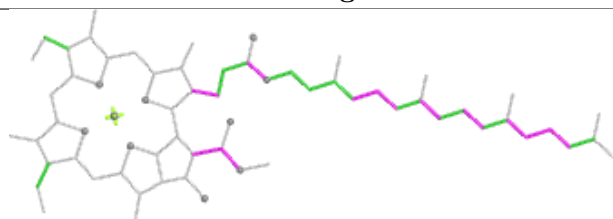
Ligand CLA BJ 602



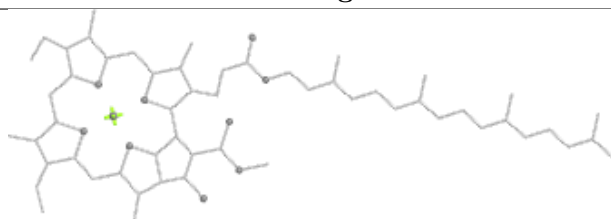
Bond lengths



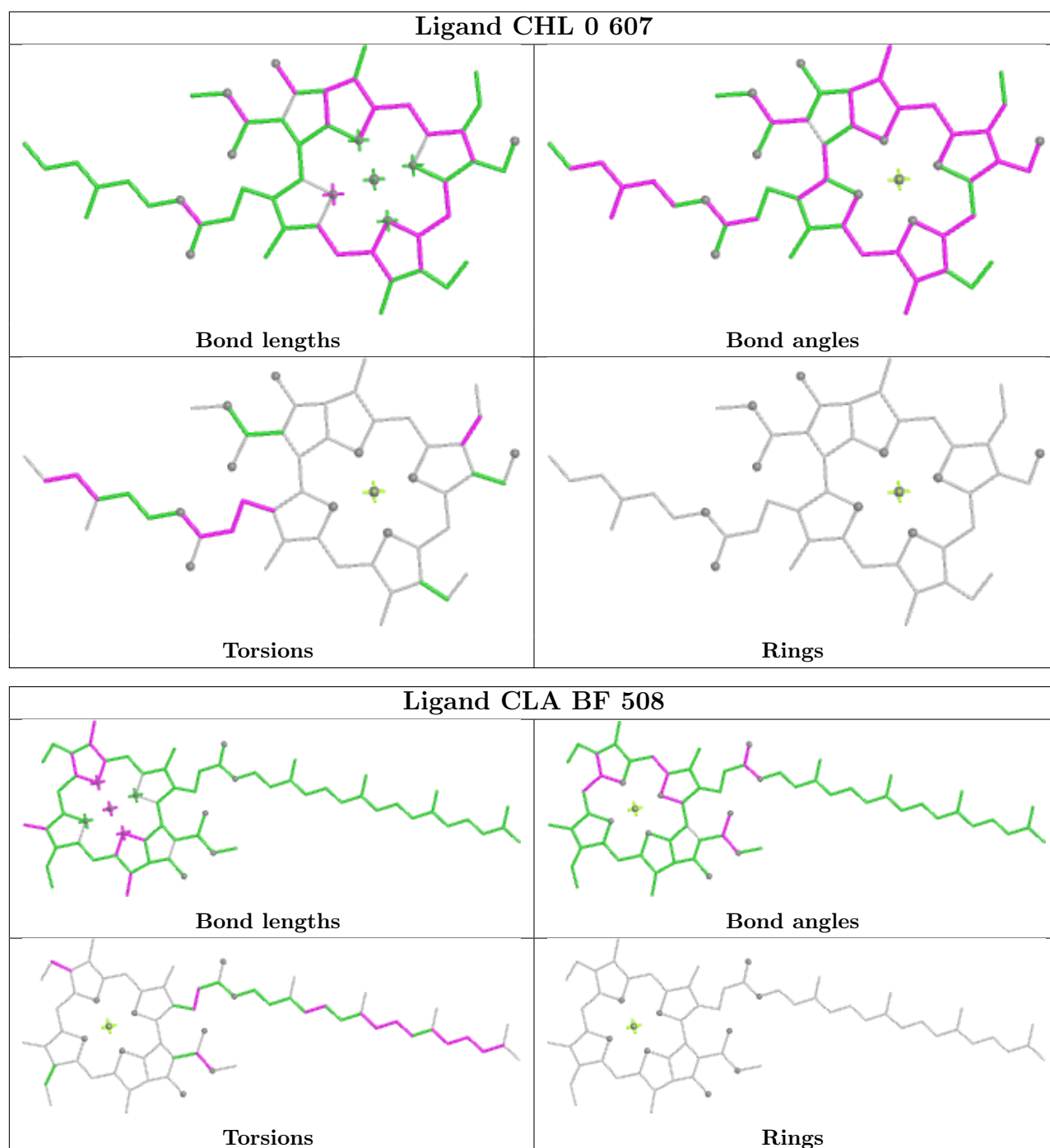
Bond angles



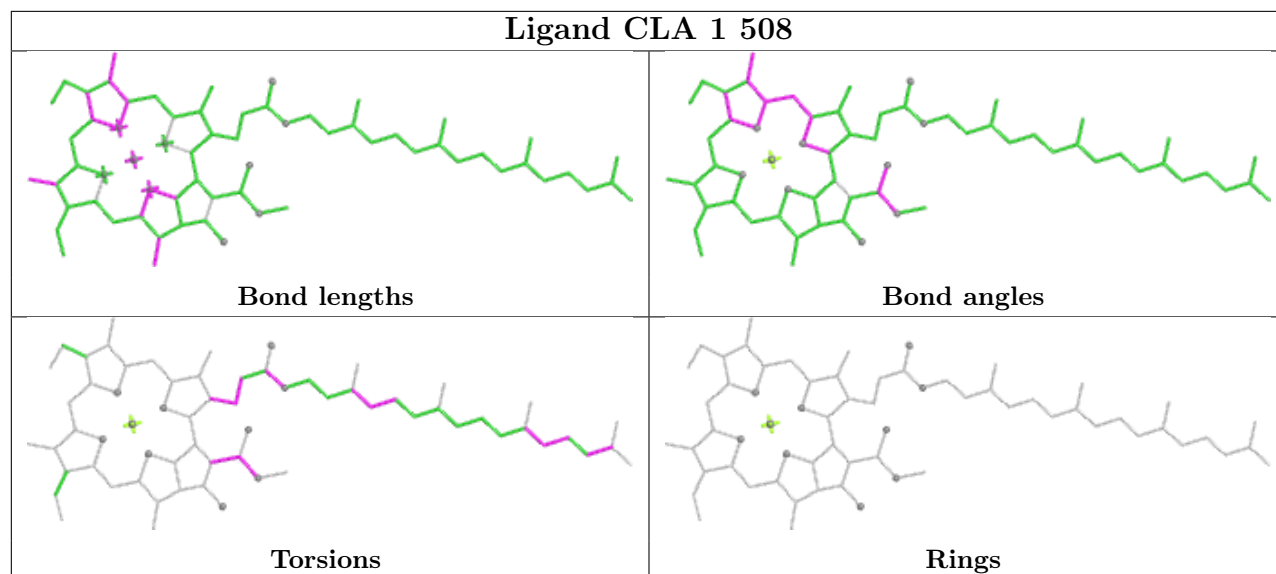
Torsions



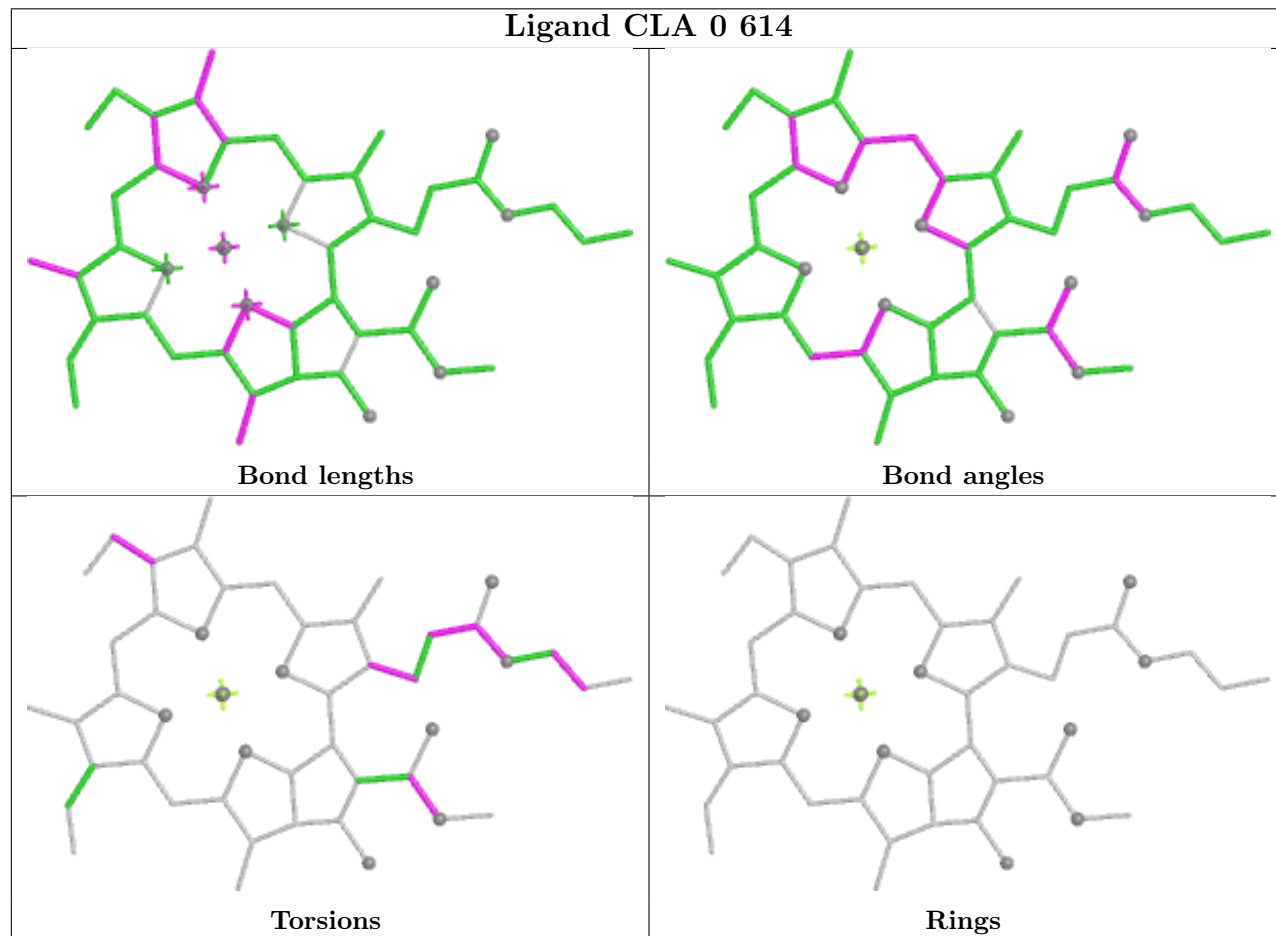
Rings

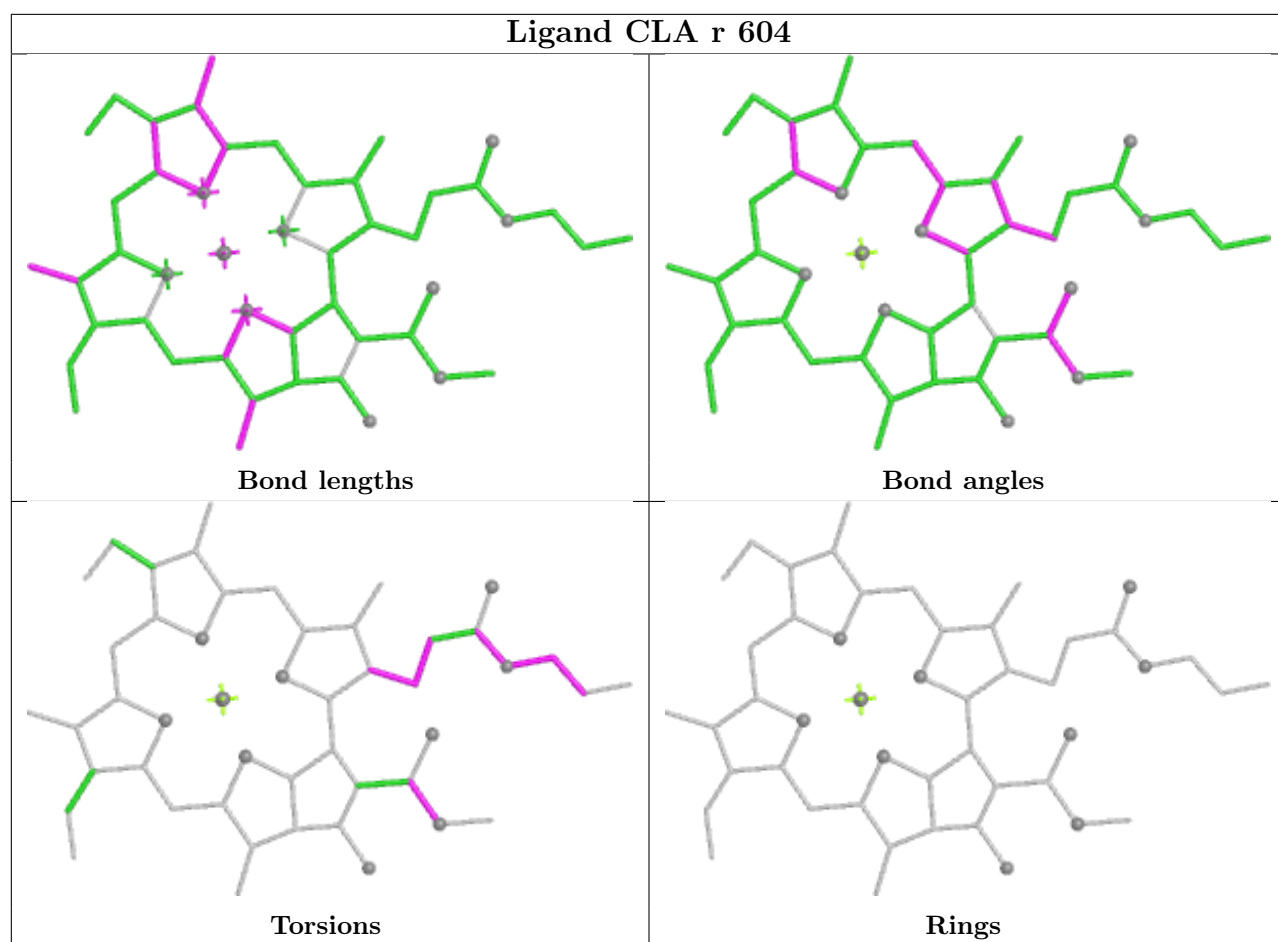


Ligand CLA 1 508

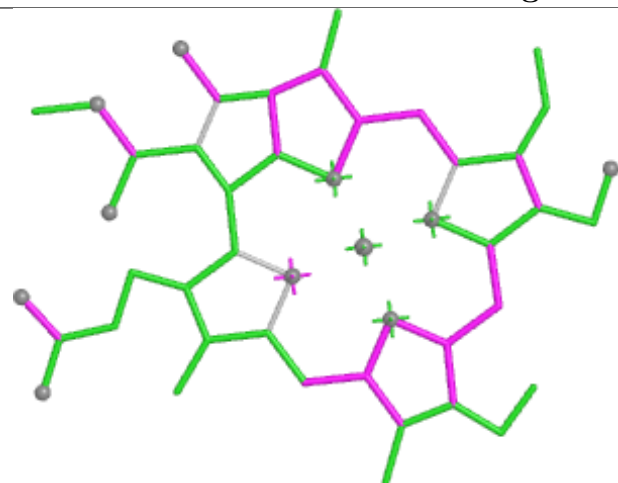


Ligand CLA 0 614

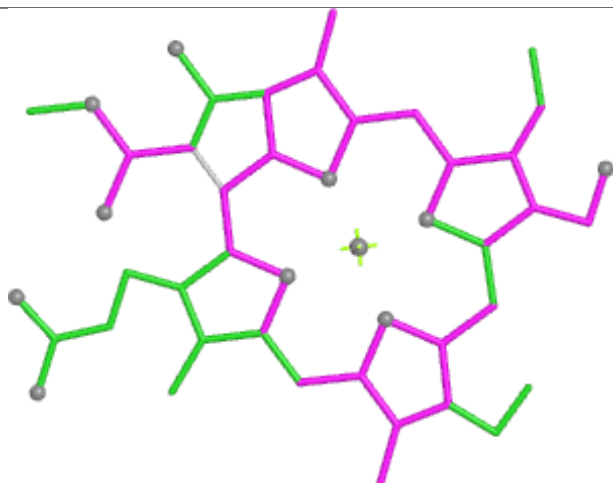




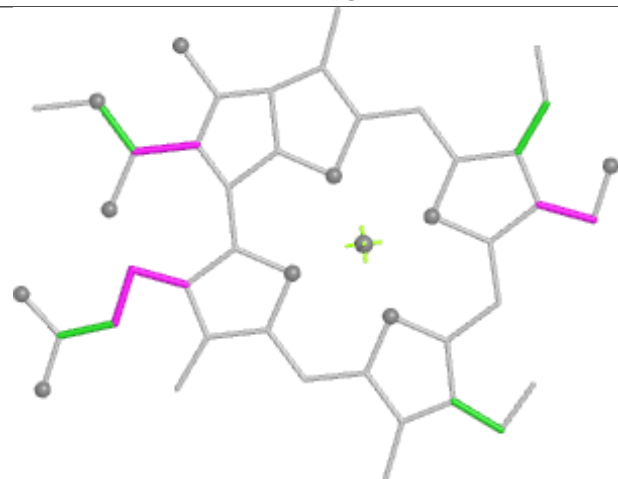
Ligand CHL 6 608



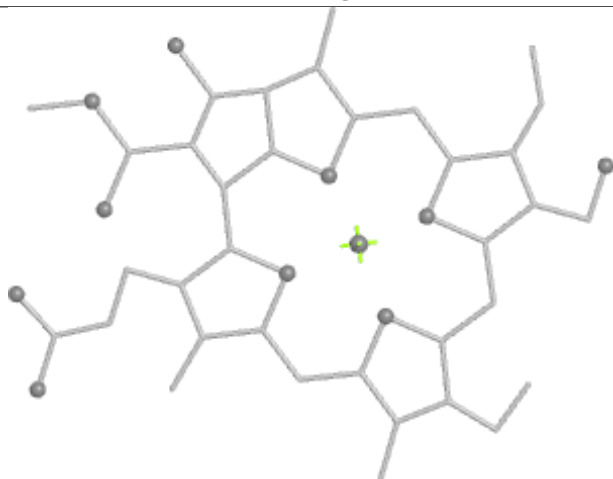
Bond lengths



Bond angles

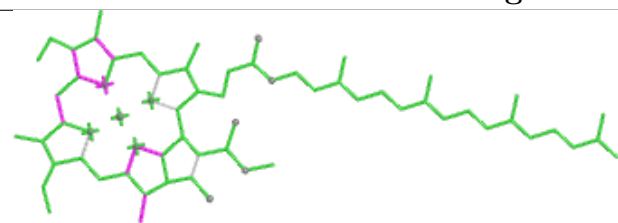


Torsions

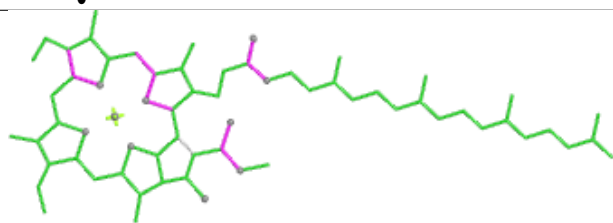


Rings

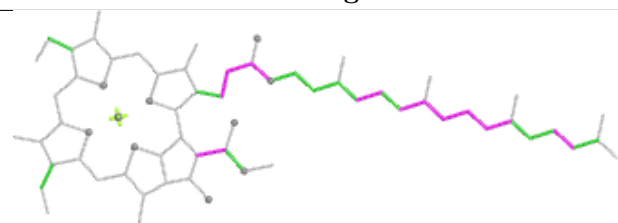
Ligand CLA BQ 602



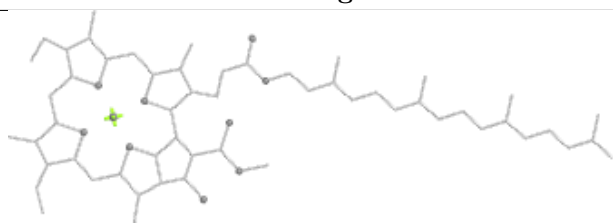
Bond lengths



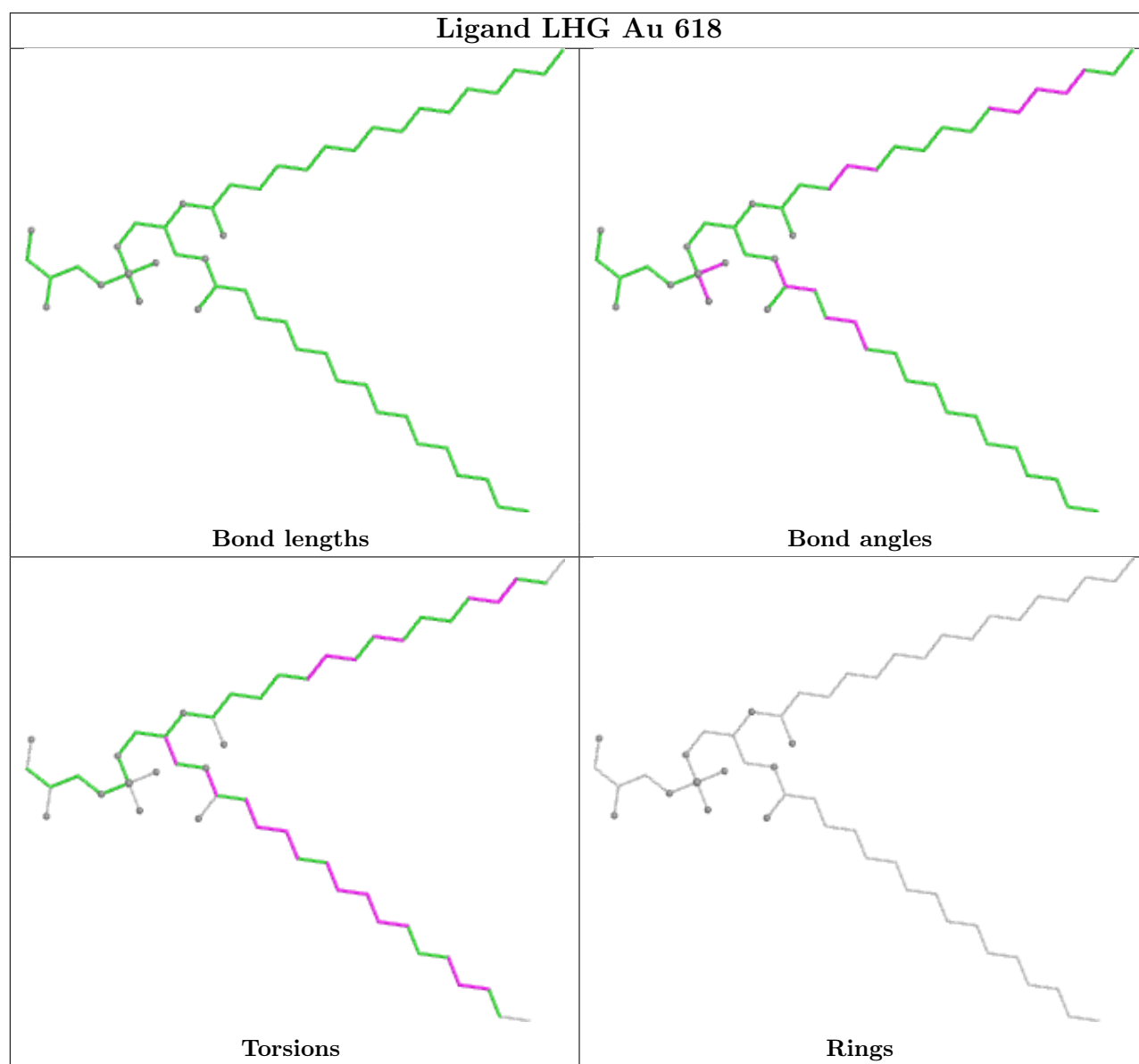
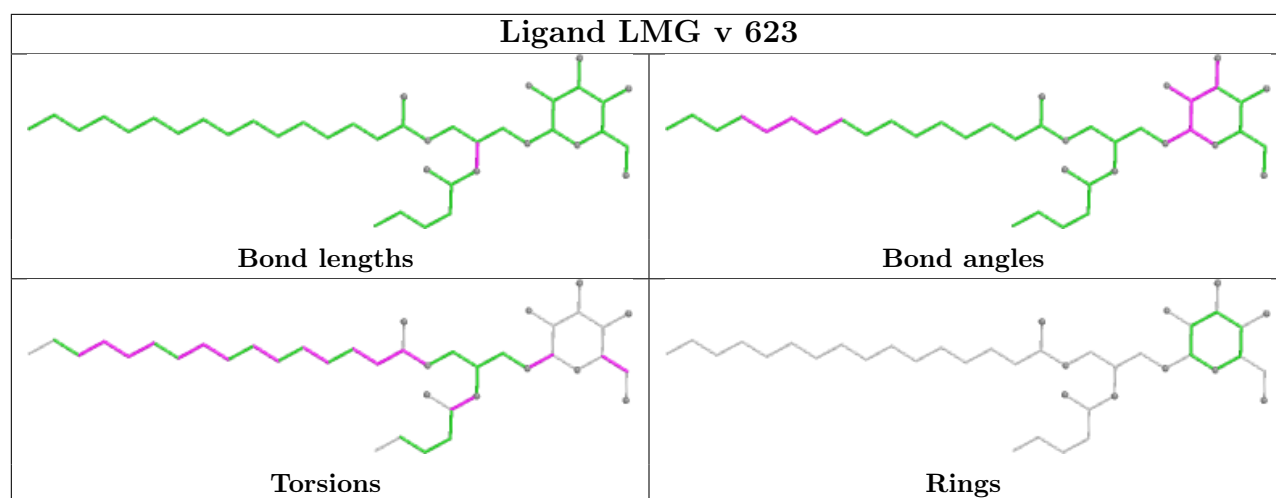
Bond angles

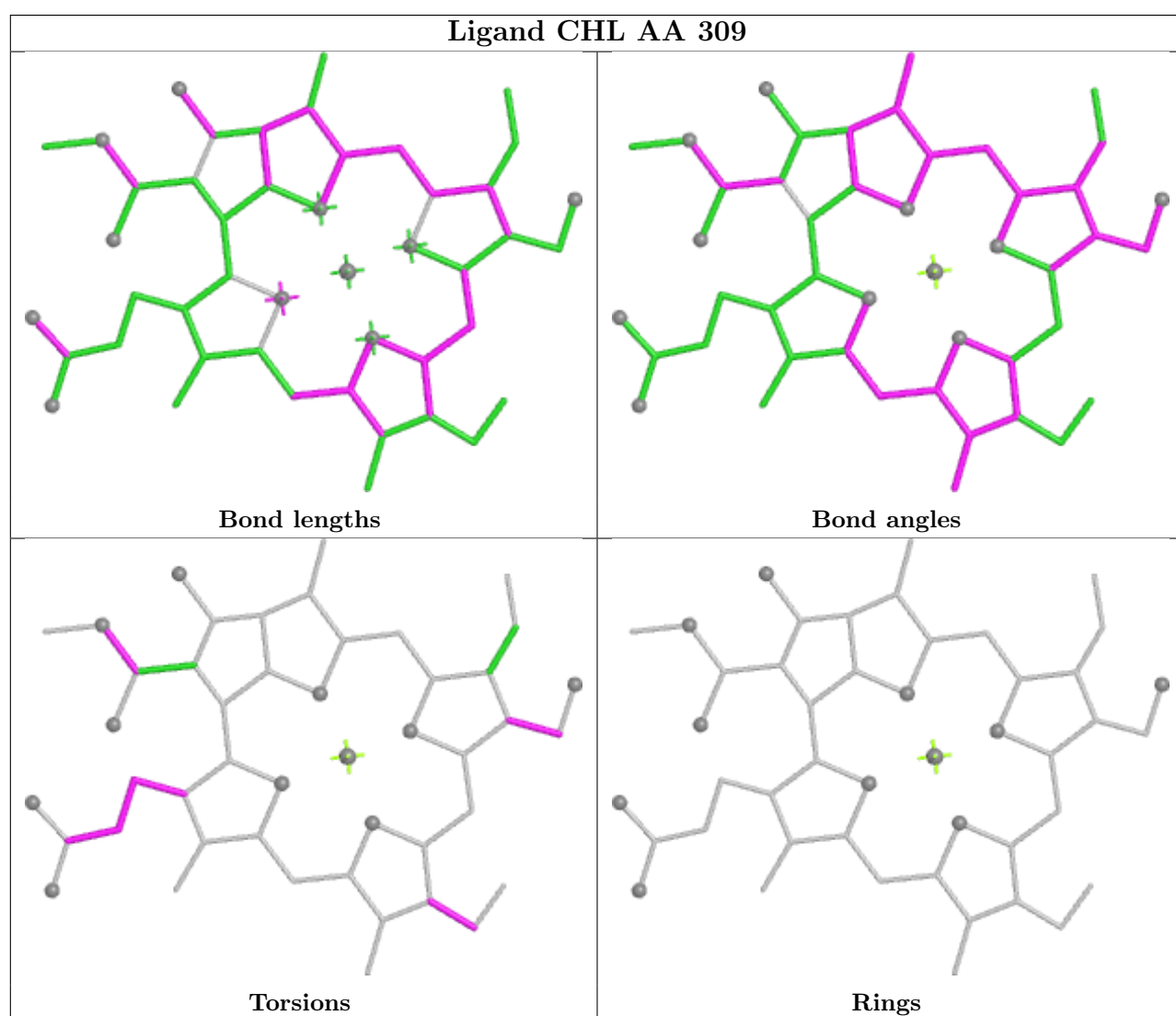
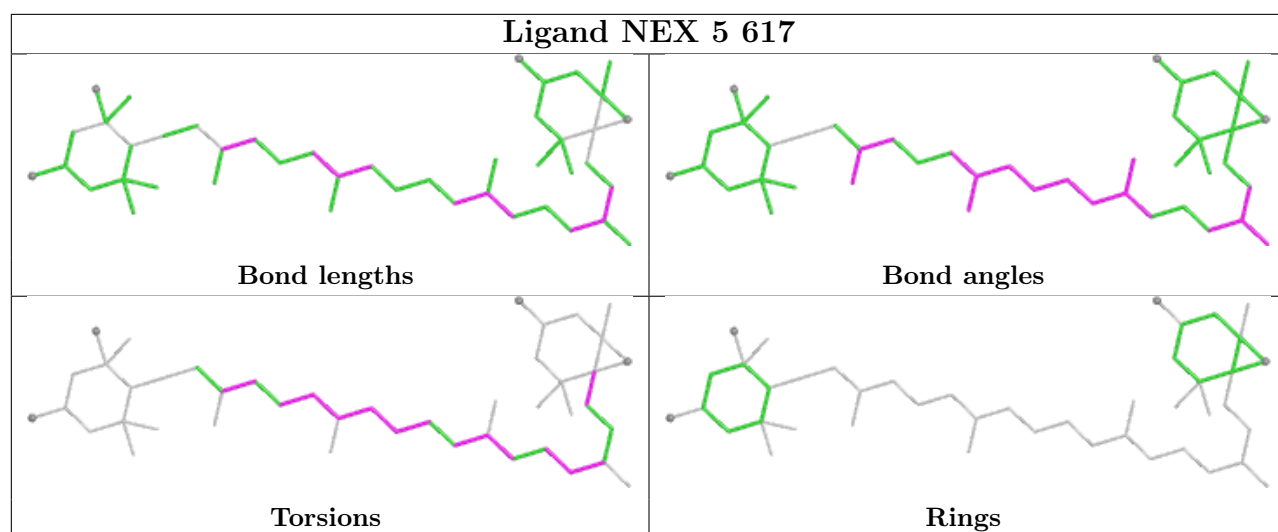


Torsions

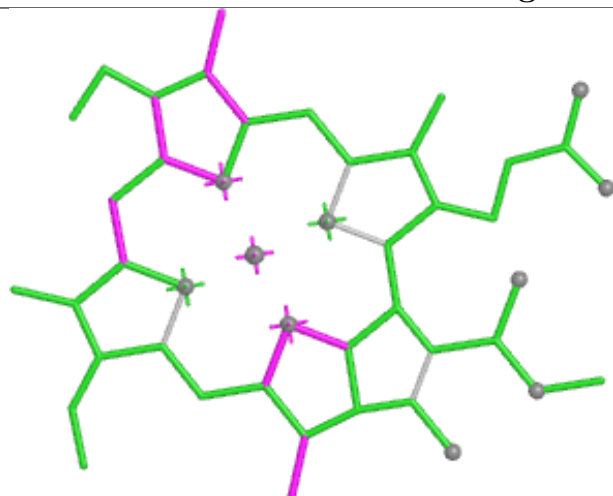


Rings

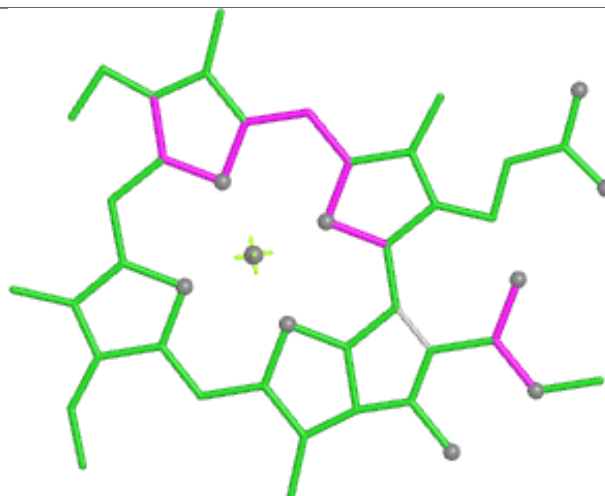




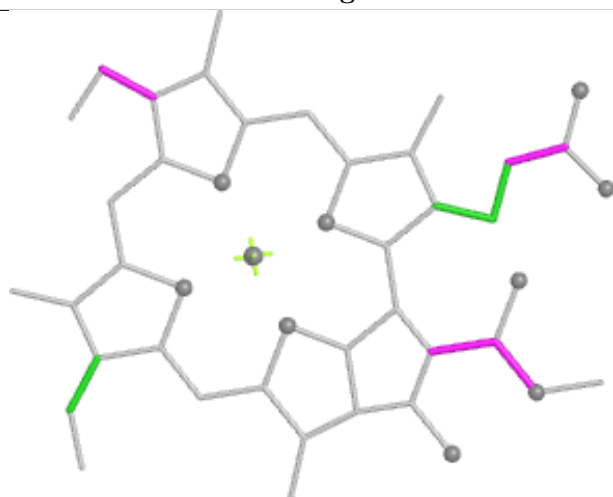
Ligand CLA 5 612



Bond lengths



Bond angles

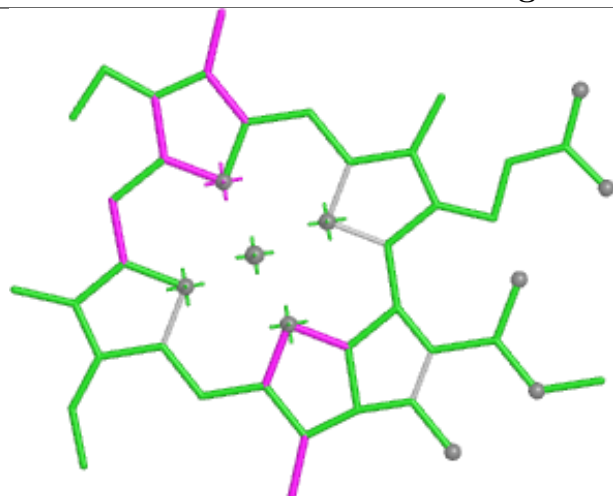


Torsions

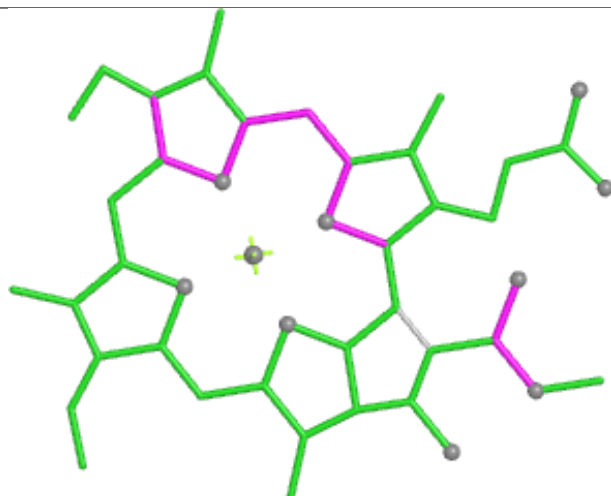


Rings

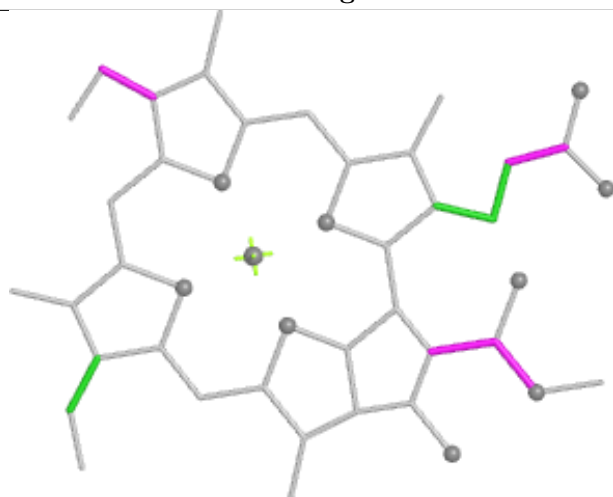
Ligand CLA 7 313



Bond lengths



Bond angles

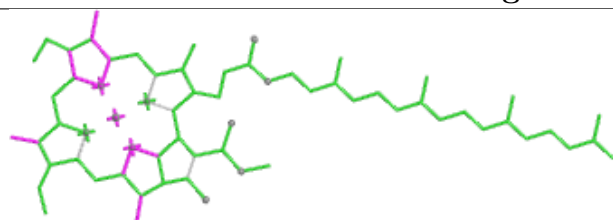


Torsions

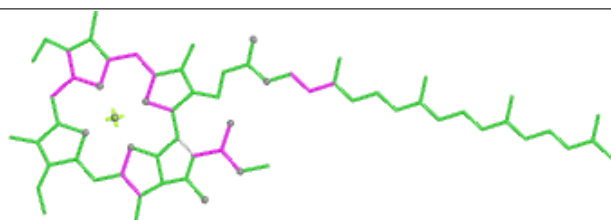


Rings

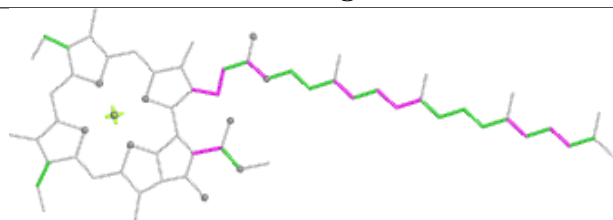
Ligand CLA Aw 102



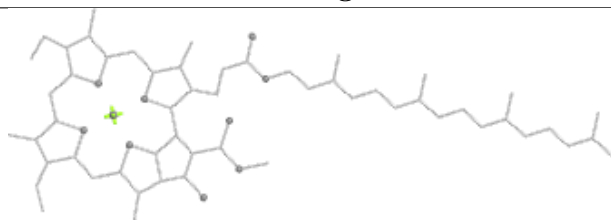
Bond lengths



Bond angles

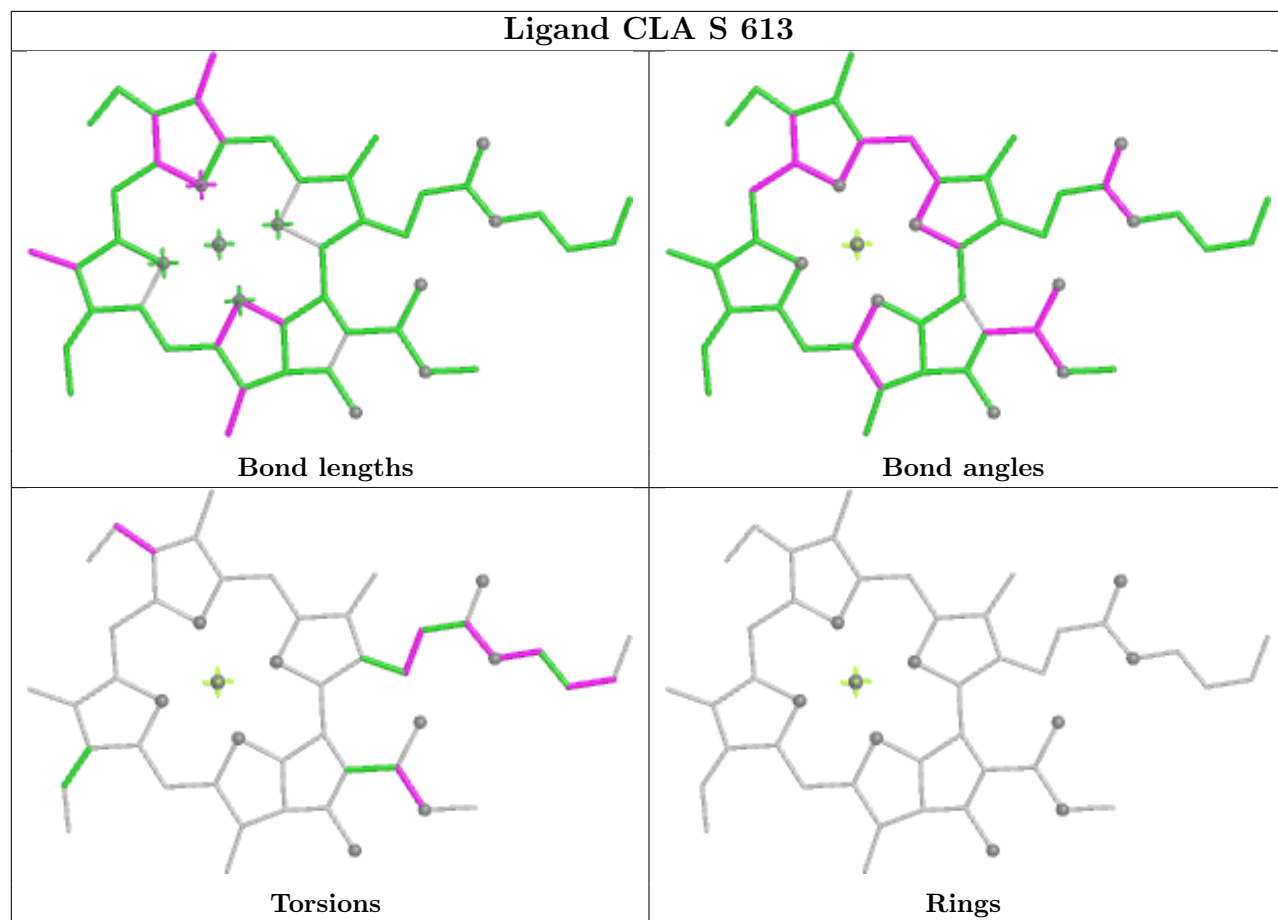


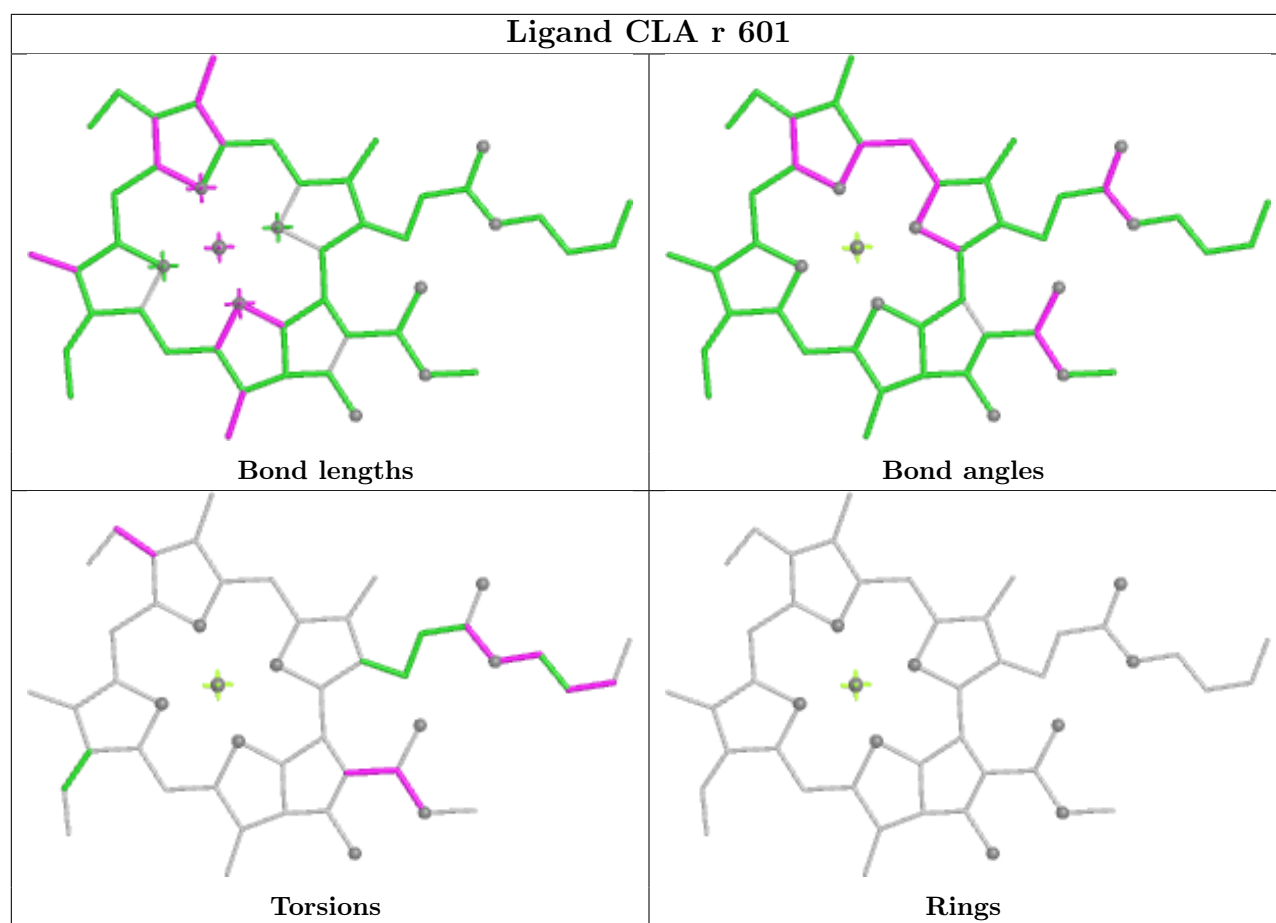
Torsions

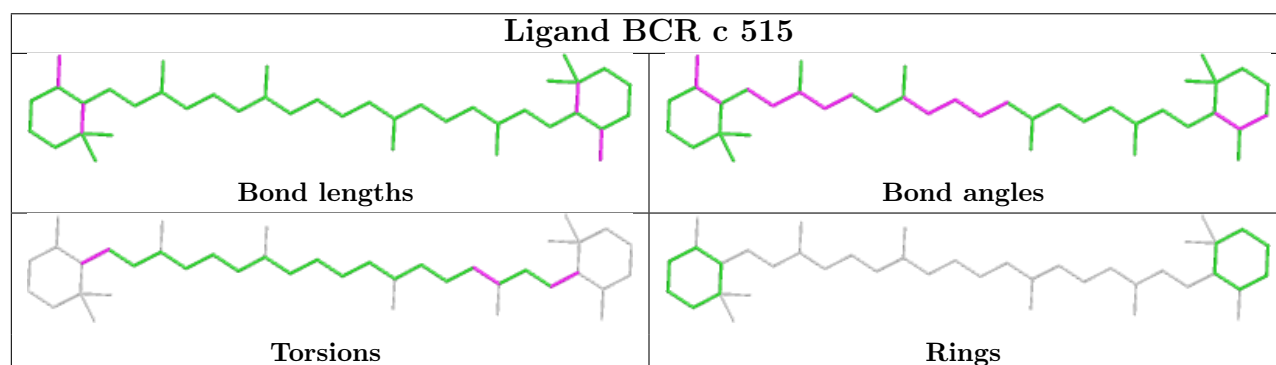
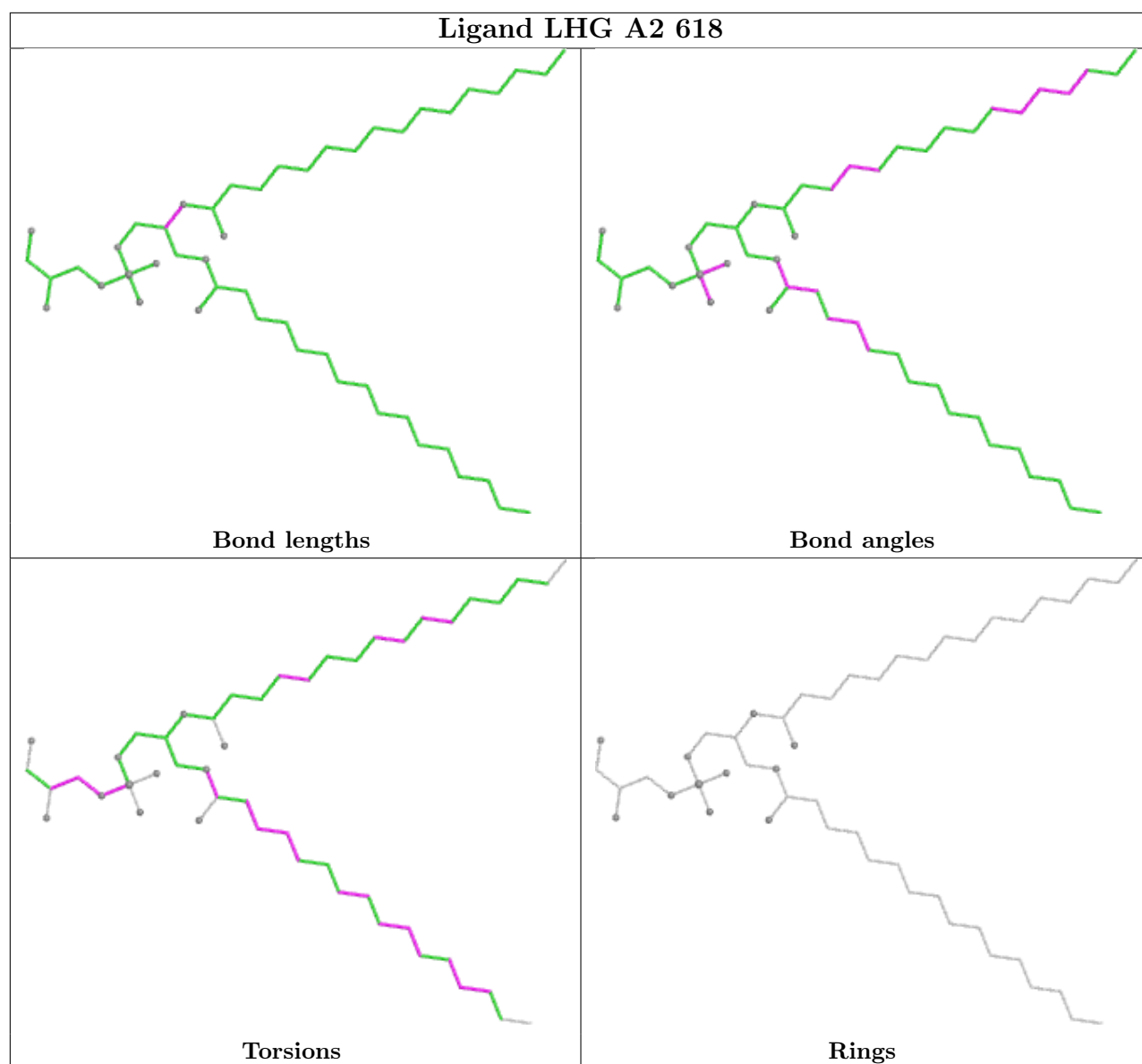


Rings

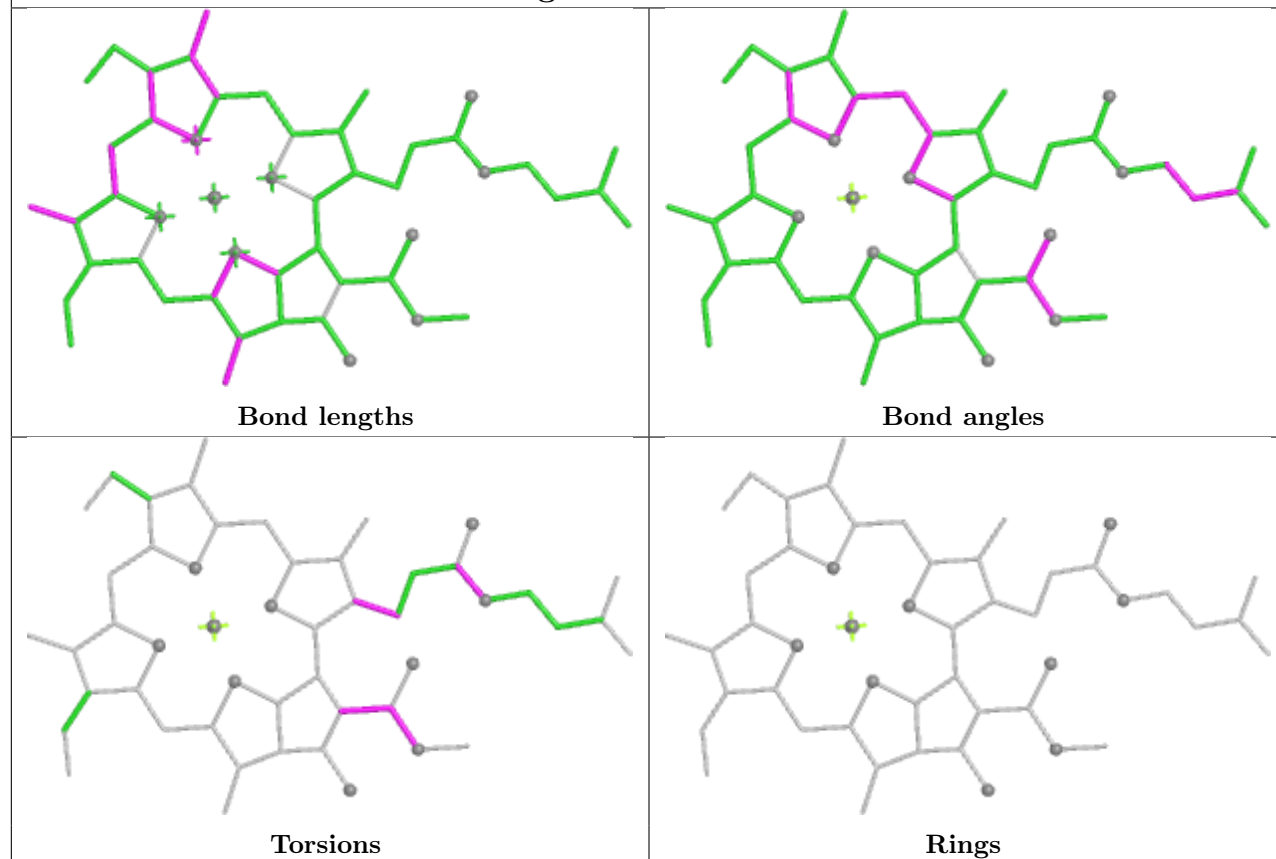
Ligand CLA S 613



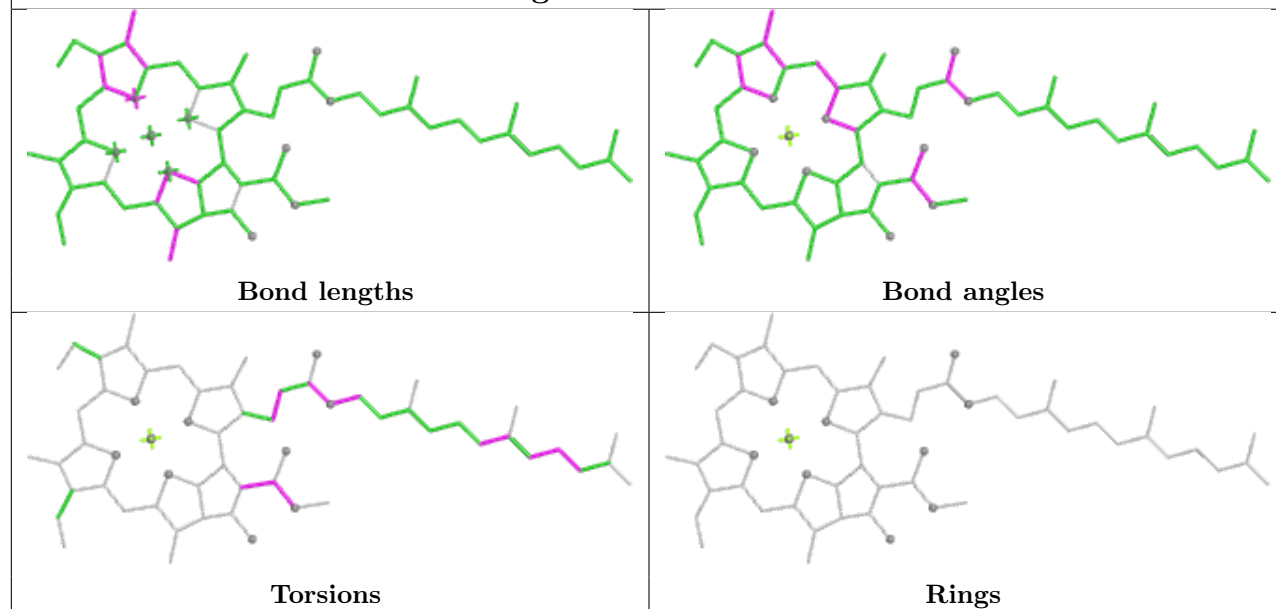


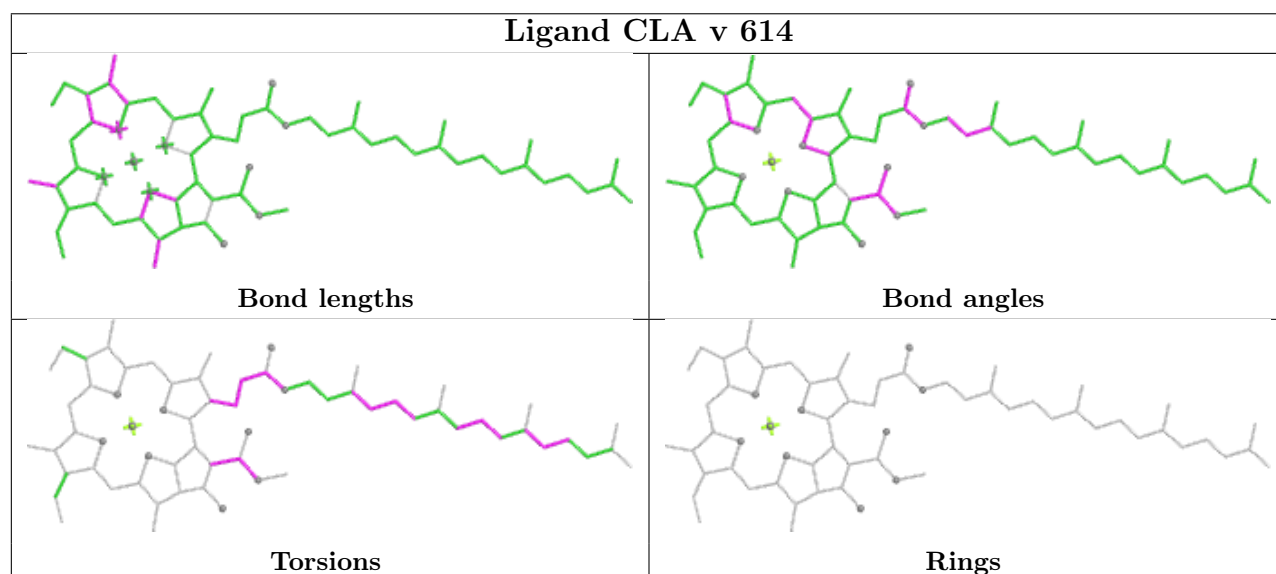
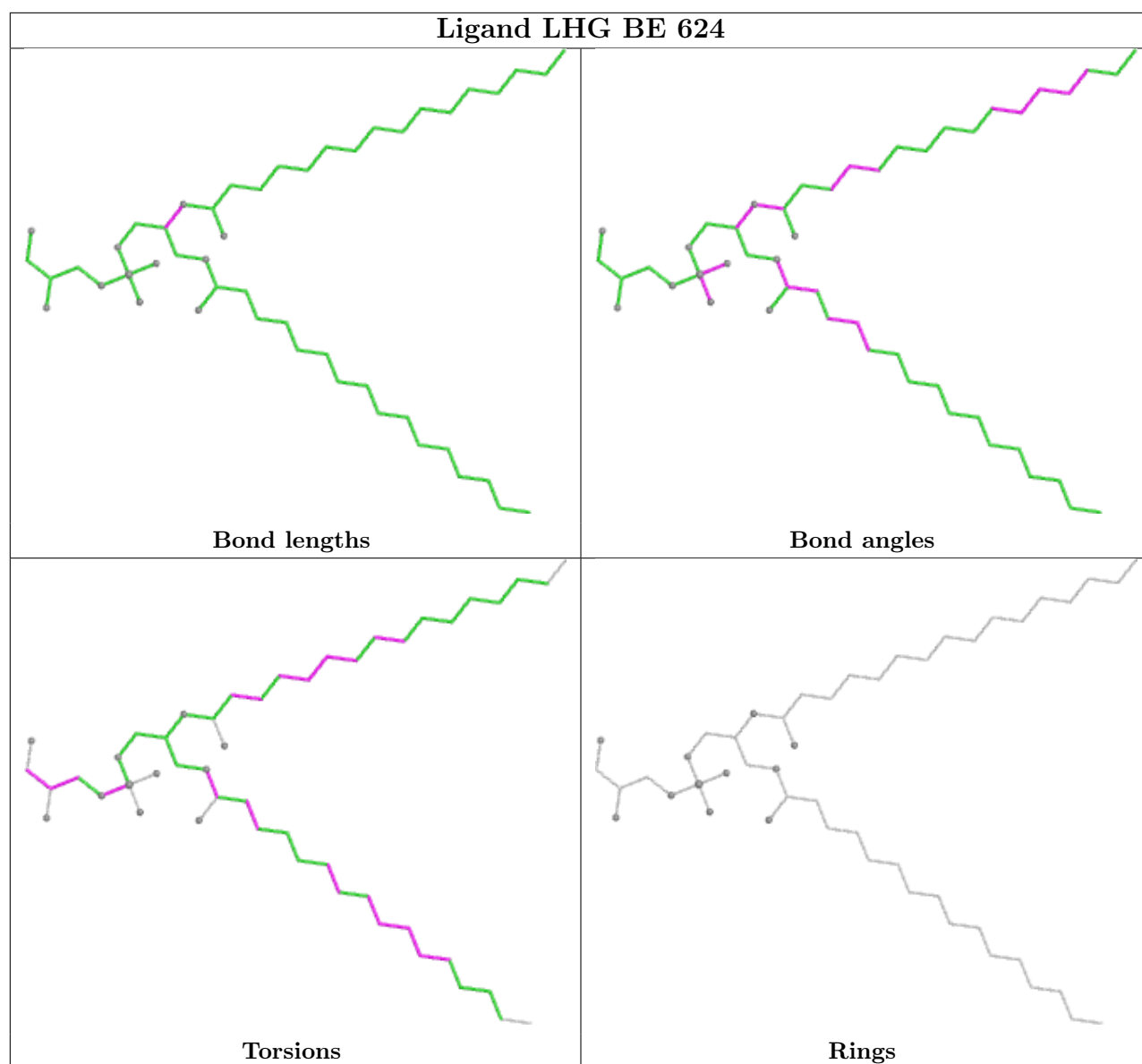


Ligand CLA s 604

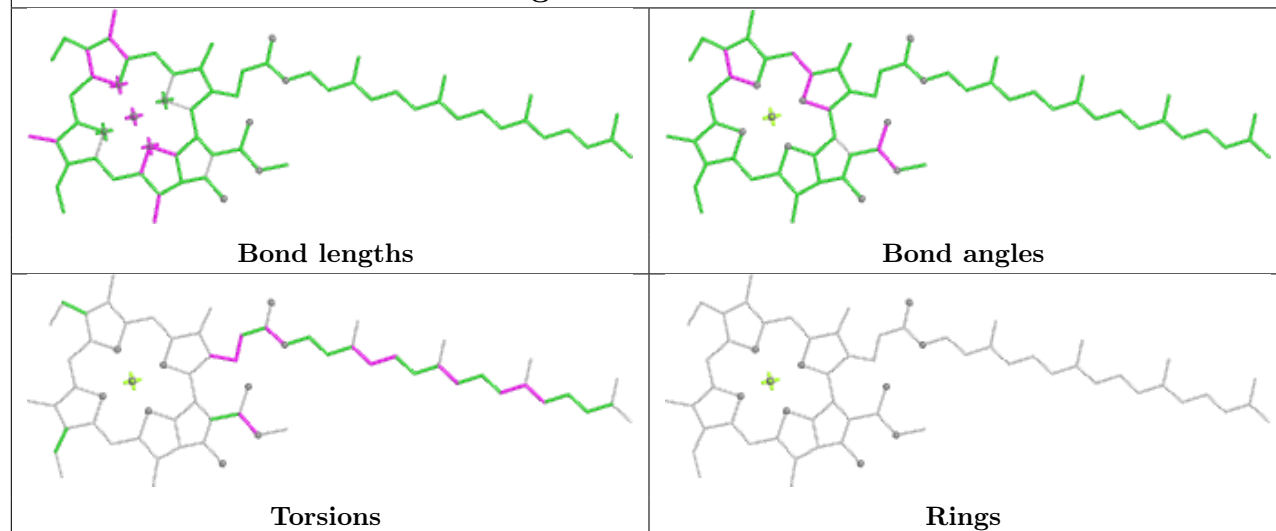


Ligand CLA A 410

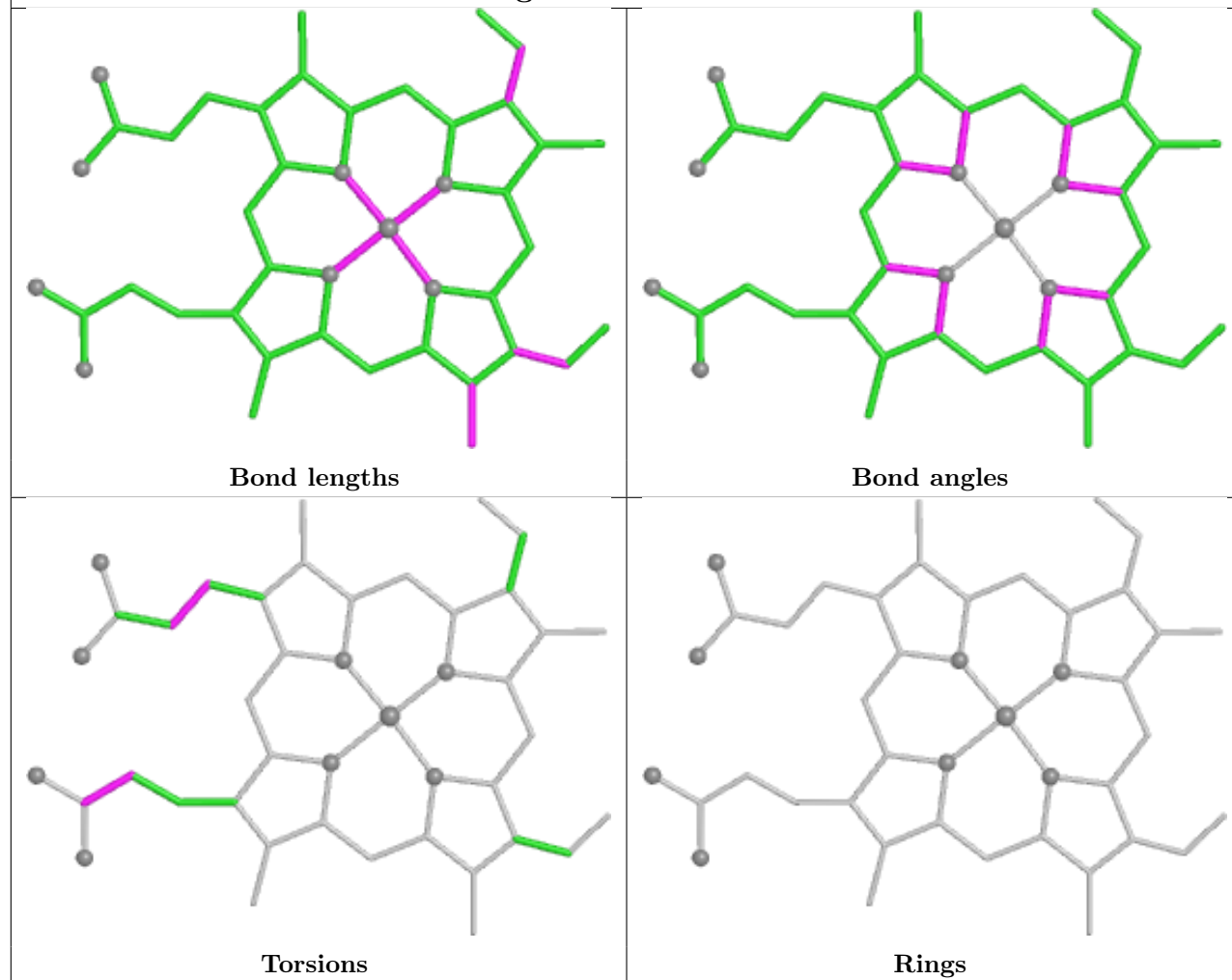


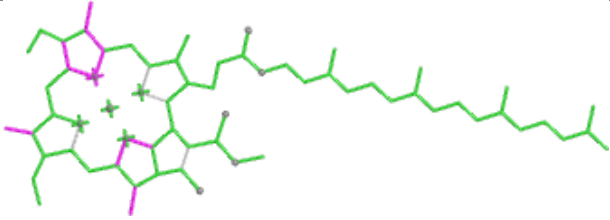
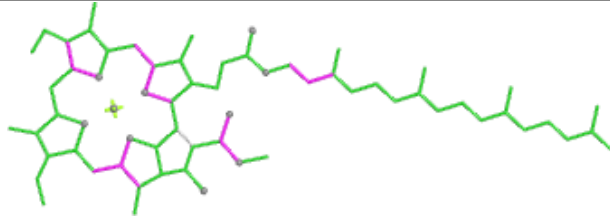
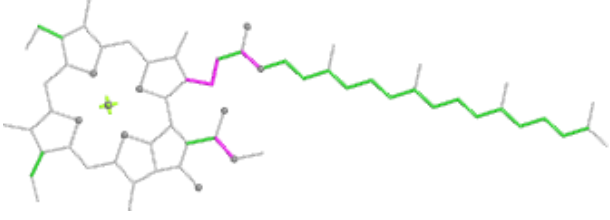
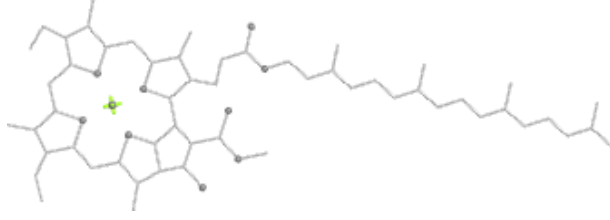
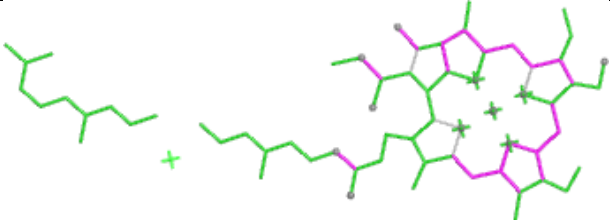
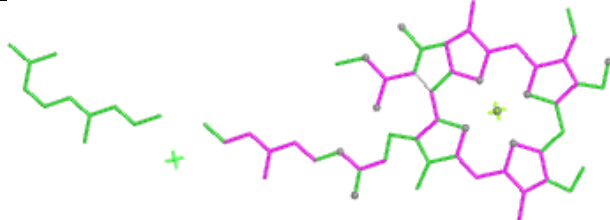
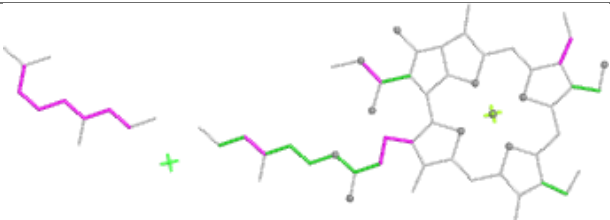
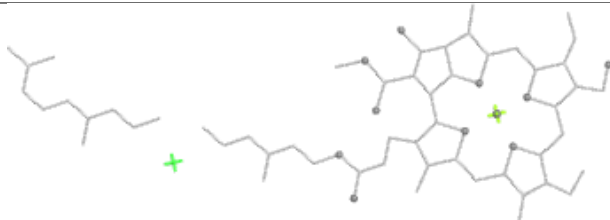
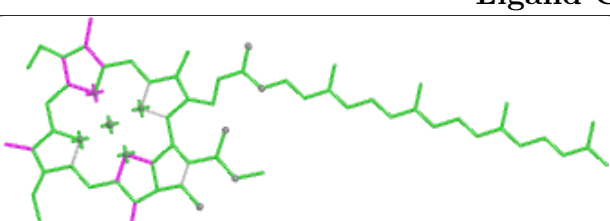
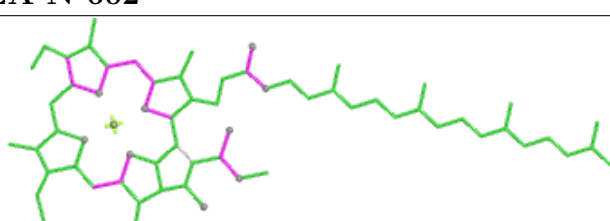
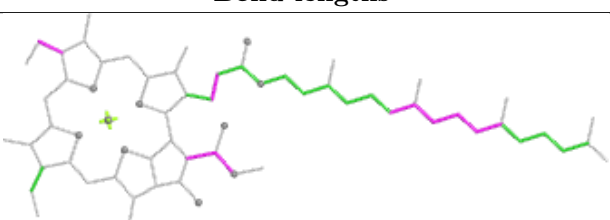
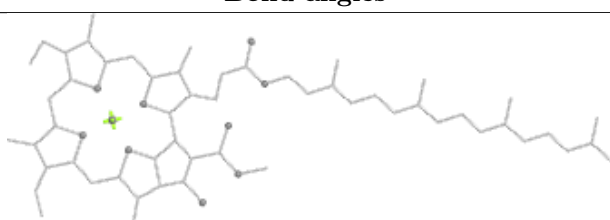


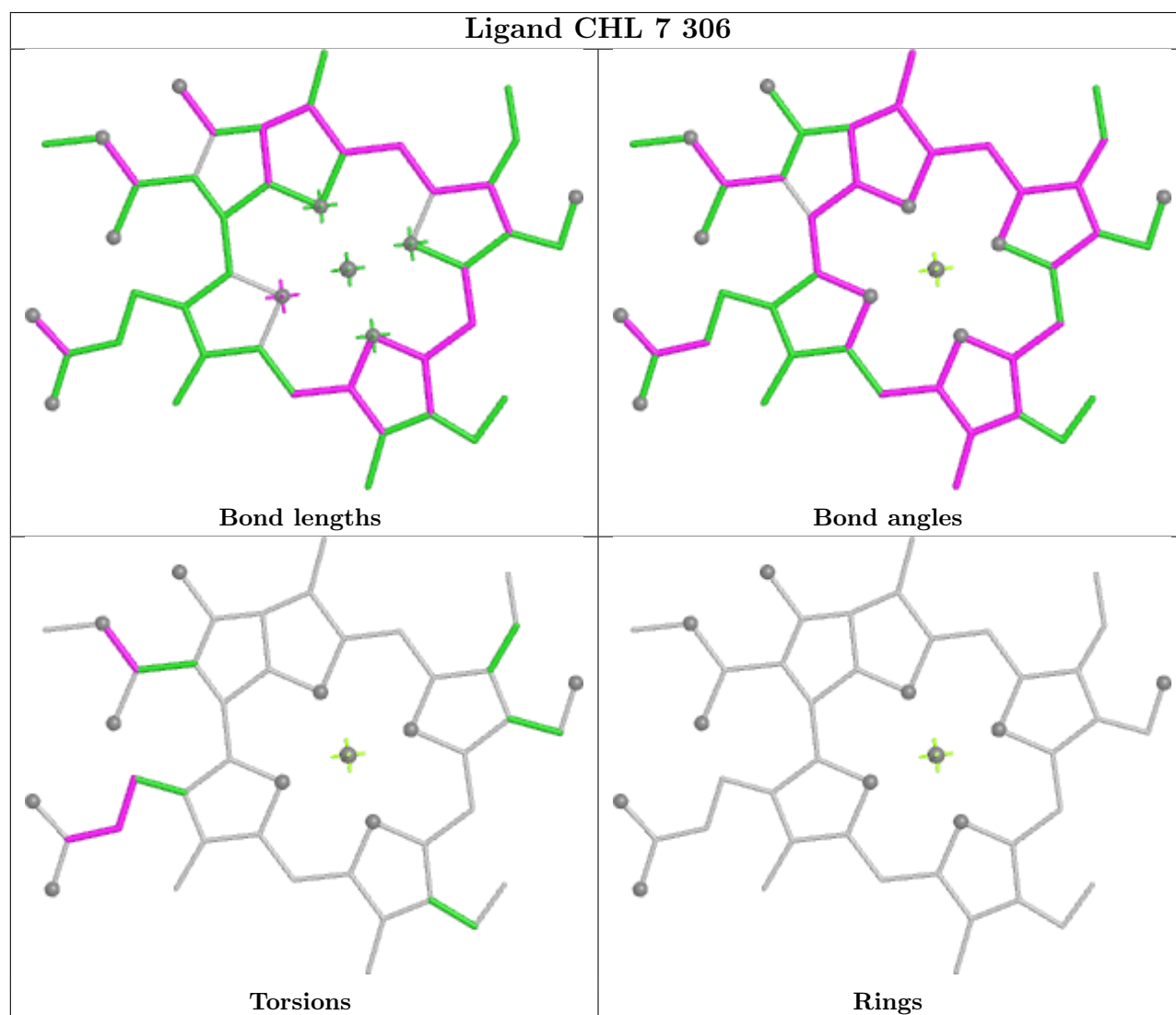
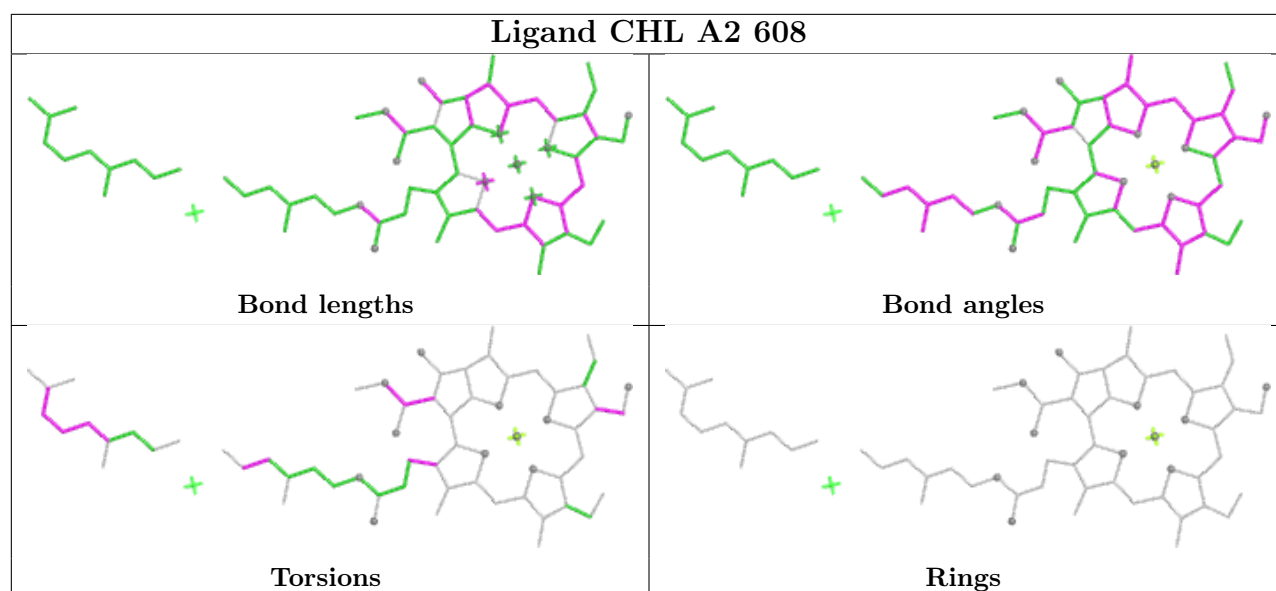
Ligand CLA Y 314

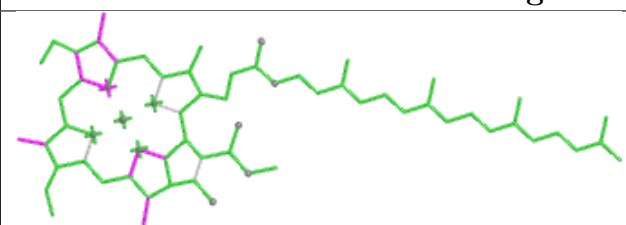
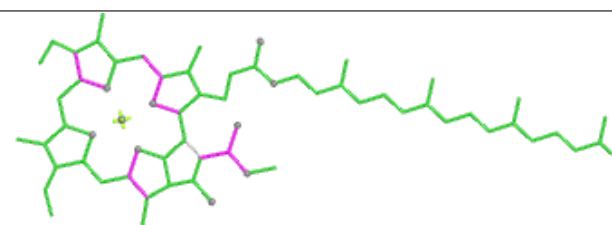
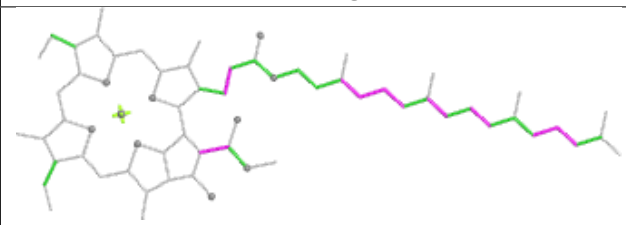
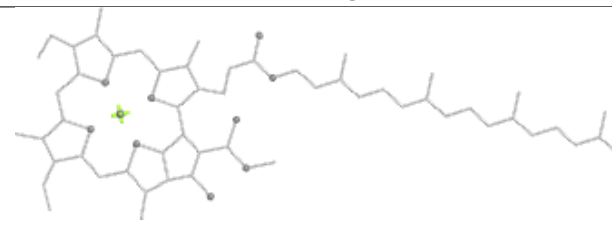


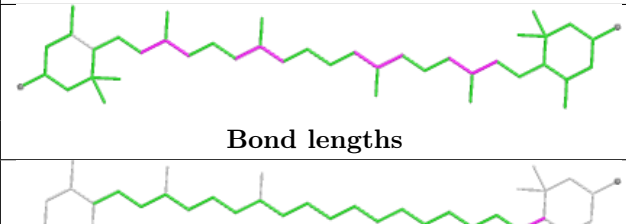
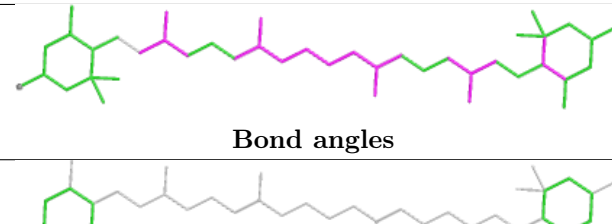
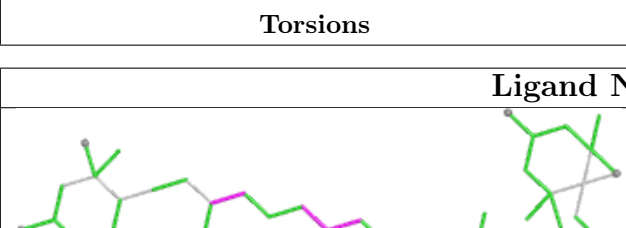
Ligand HEM f 102

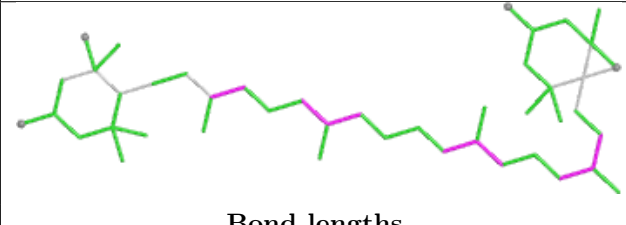
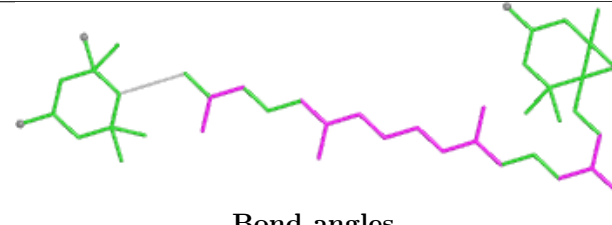
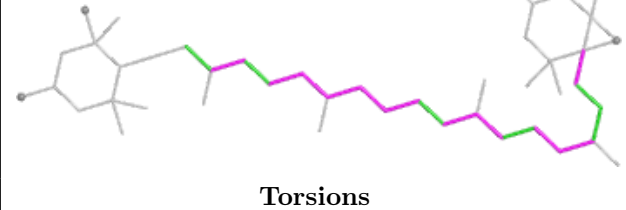
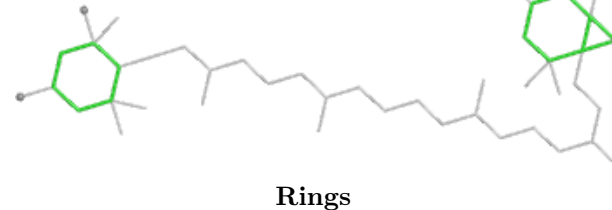


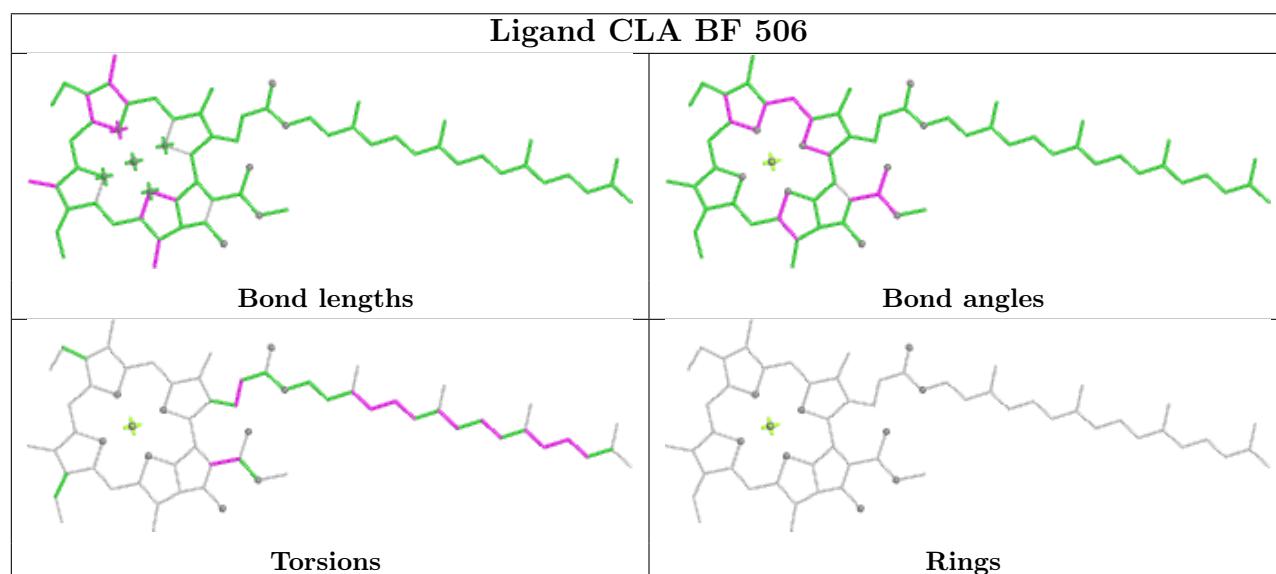
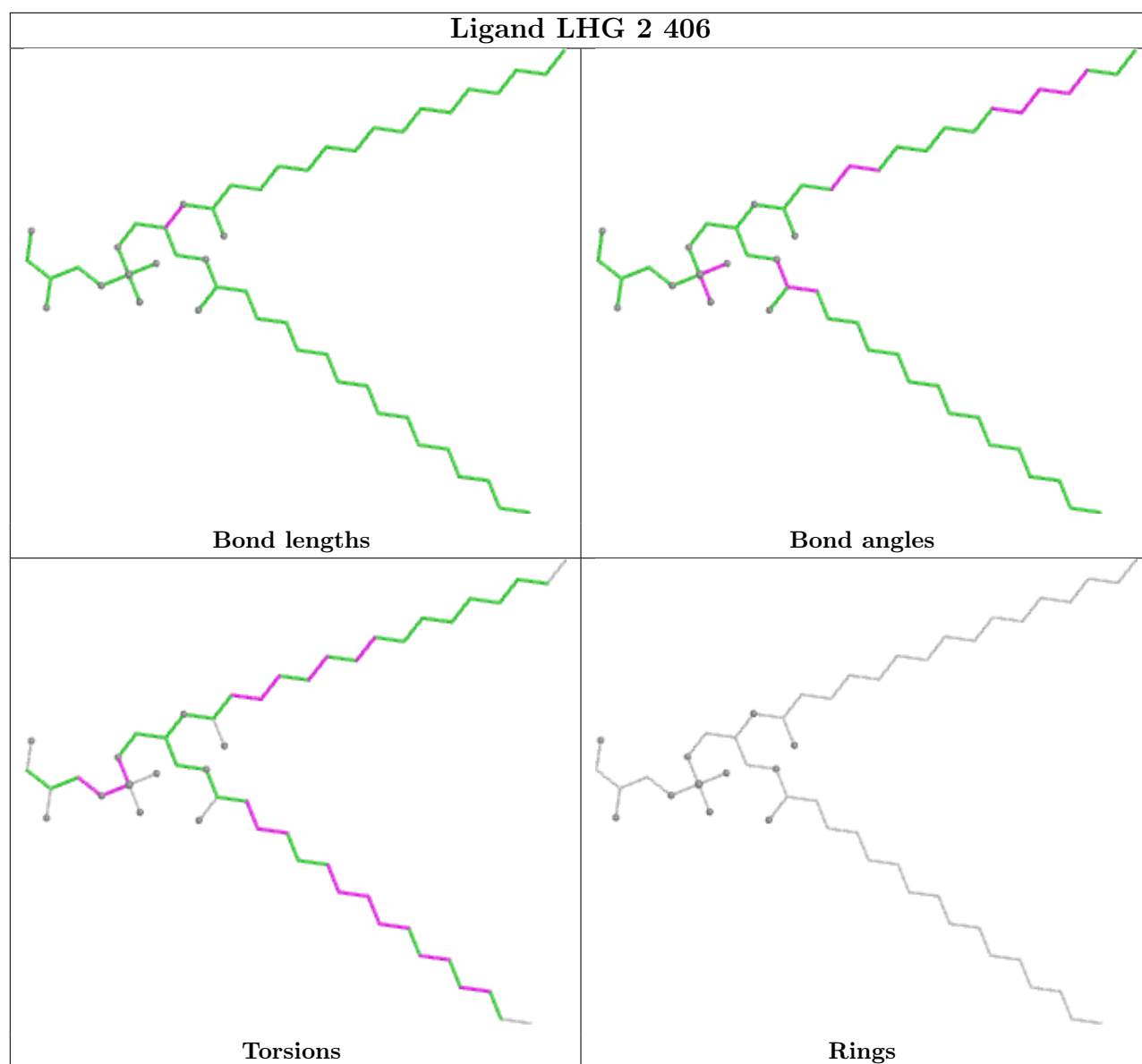
Ligand CLA A 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL BJ 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA N 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

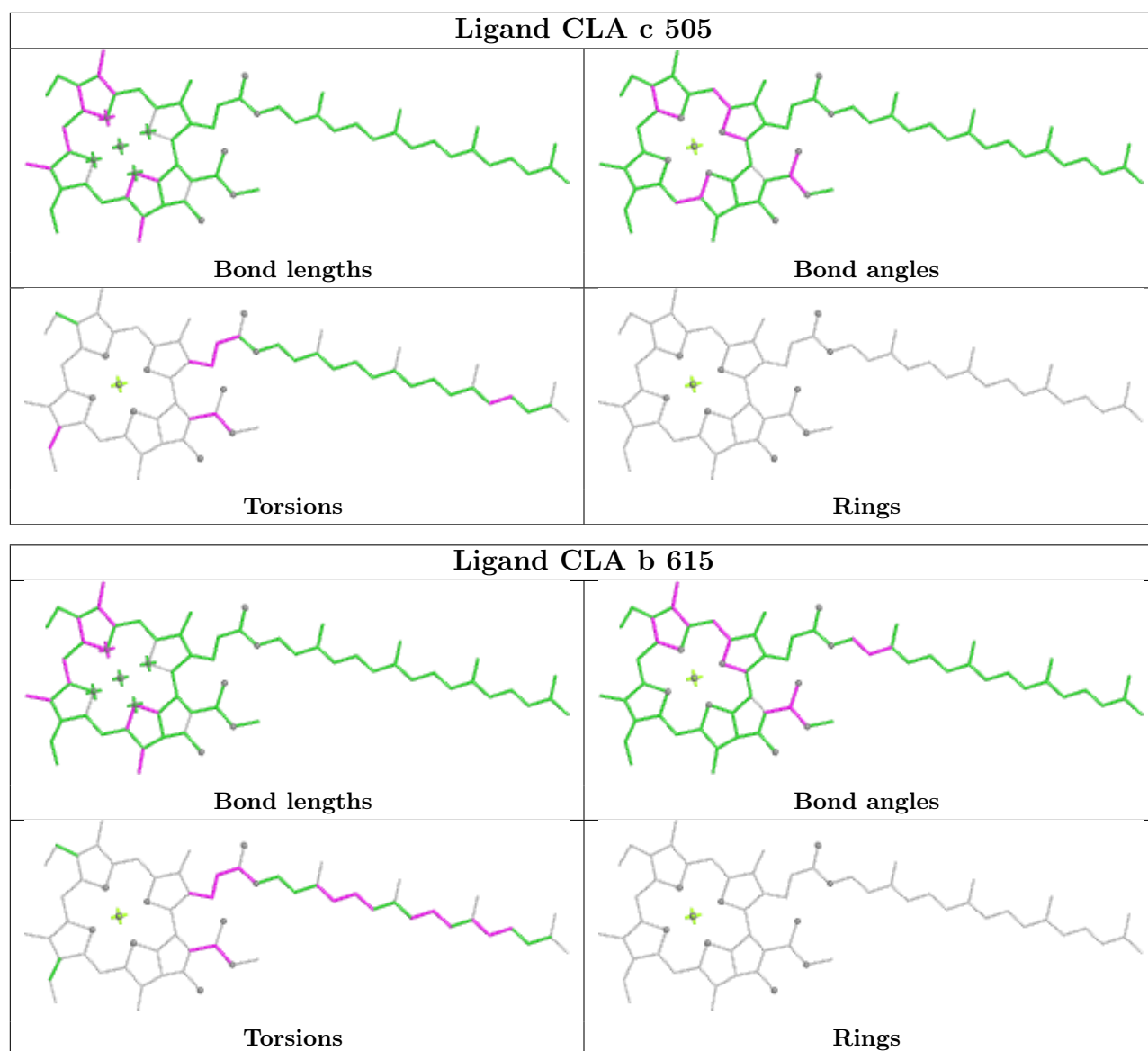


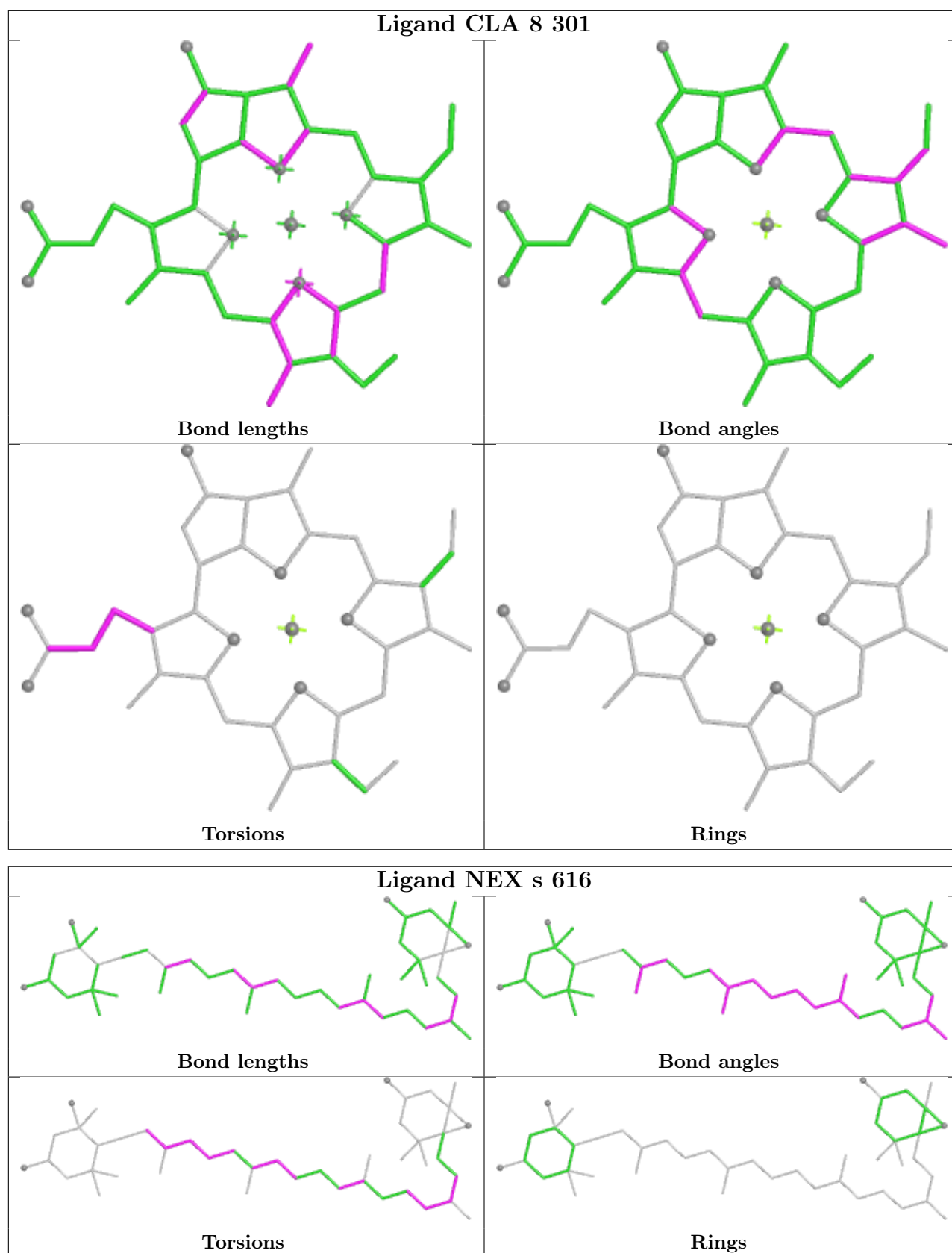
Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

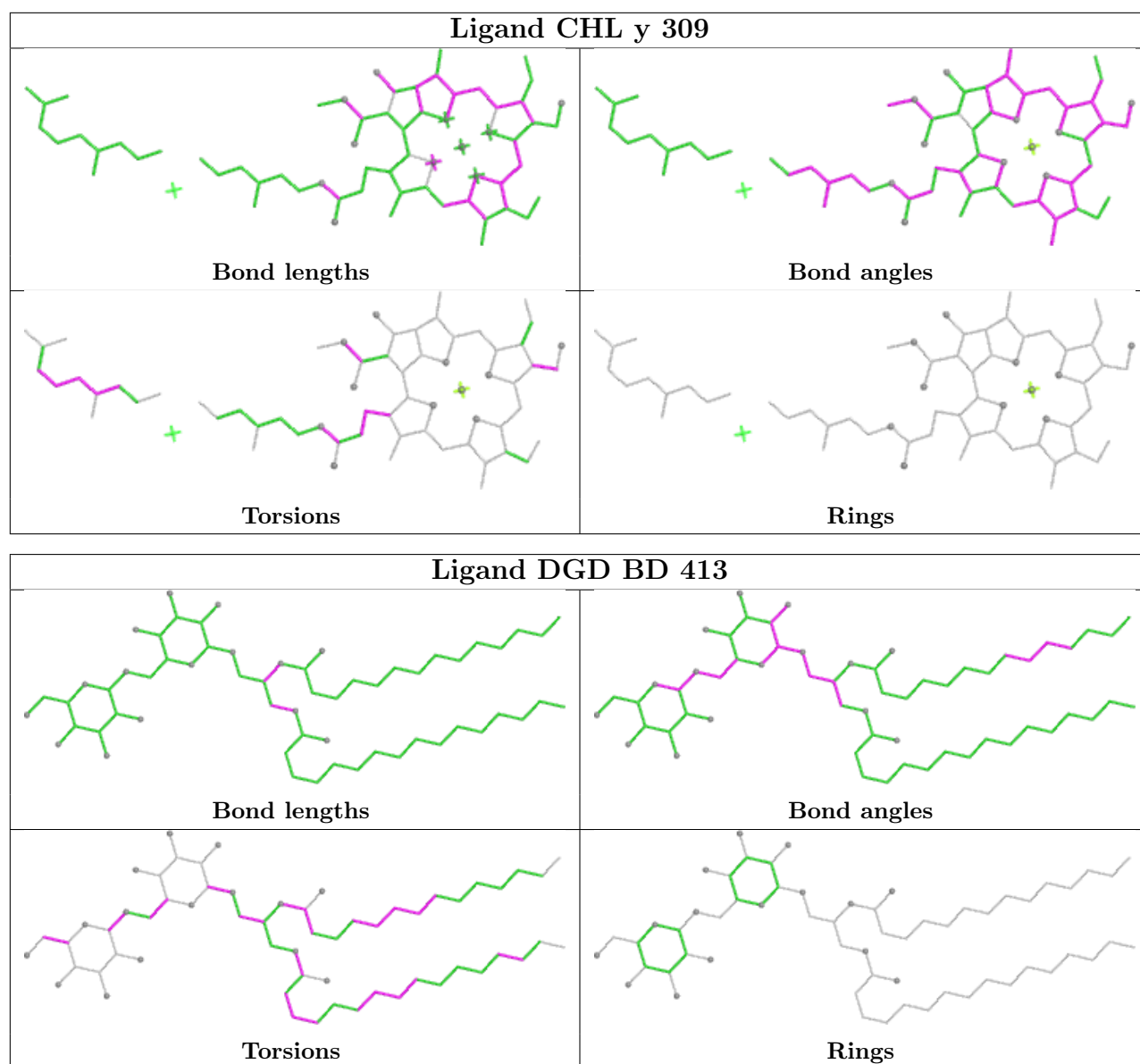
Ligand LUT BV 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX 9 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

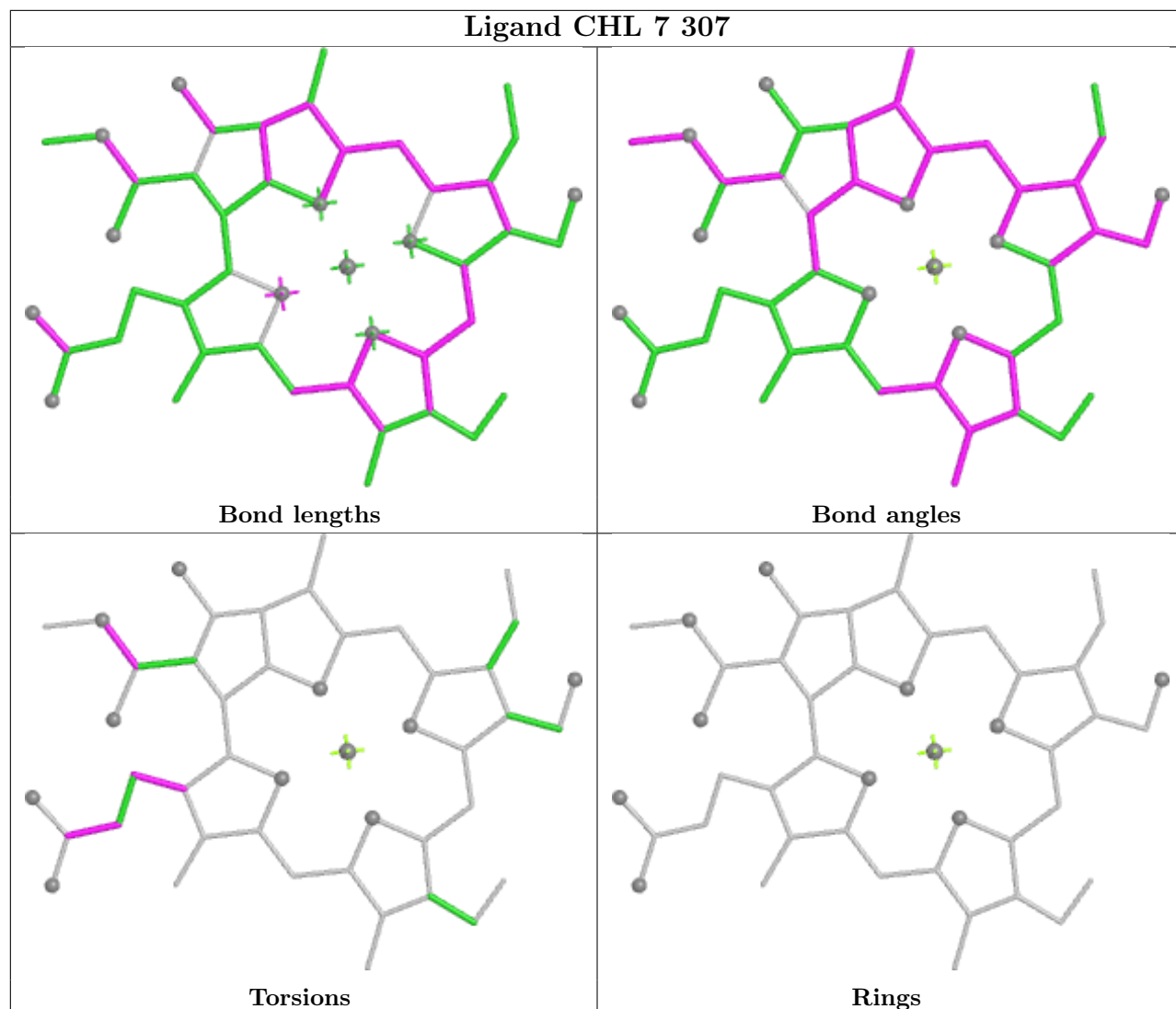


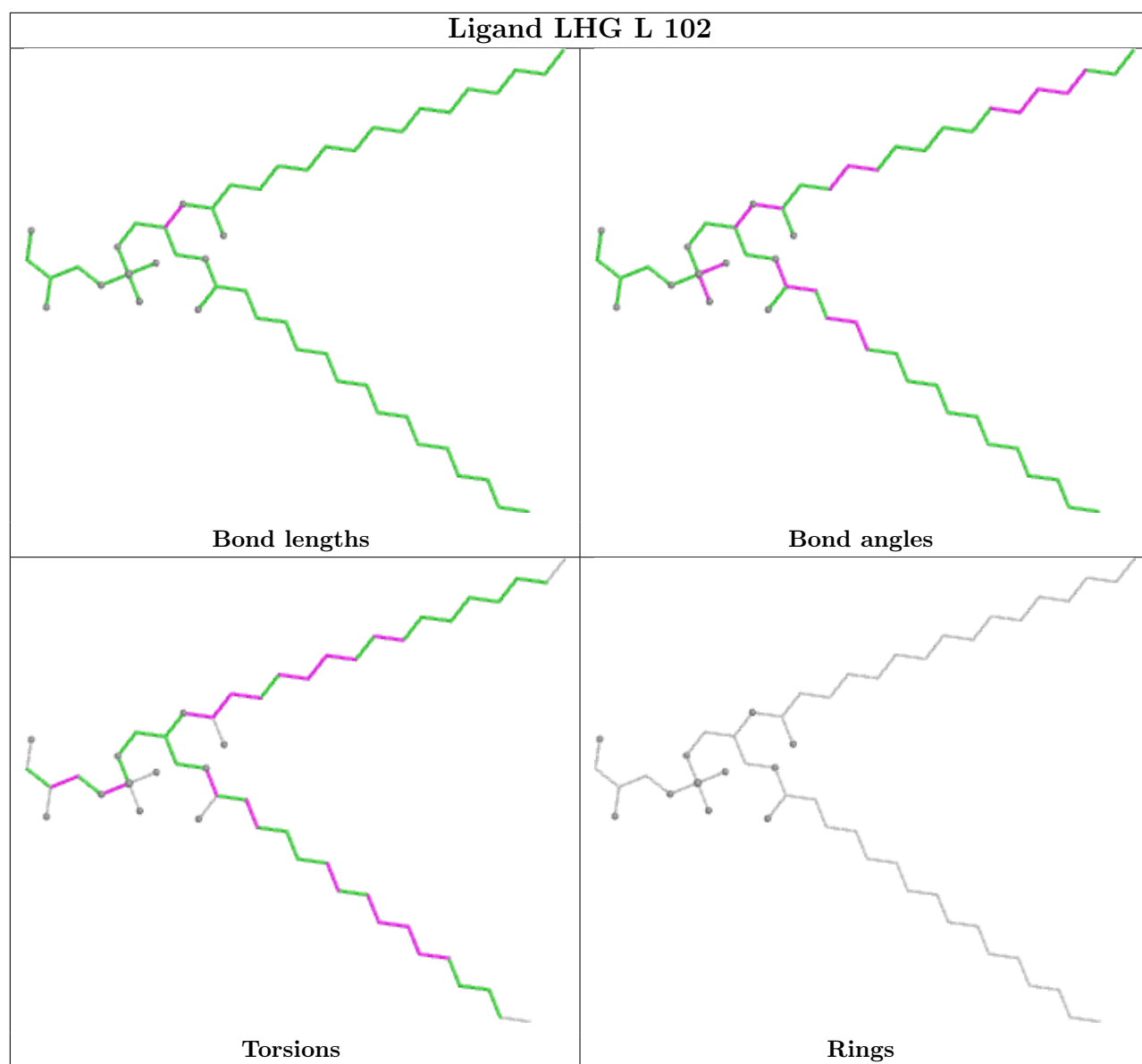


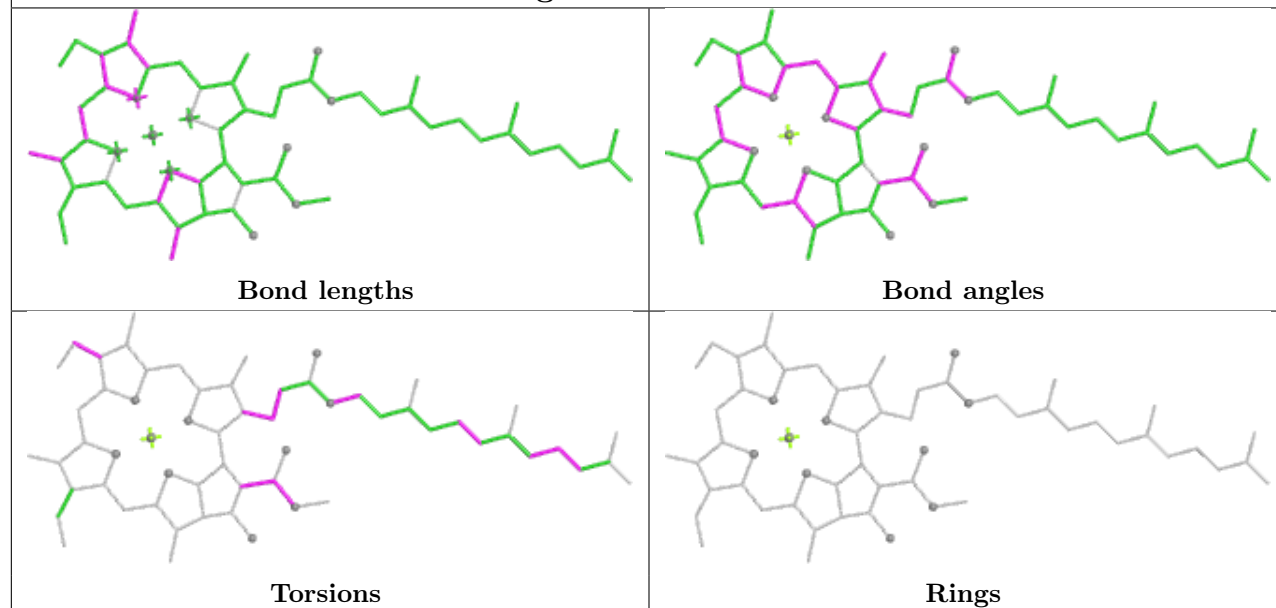
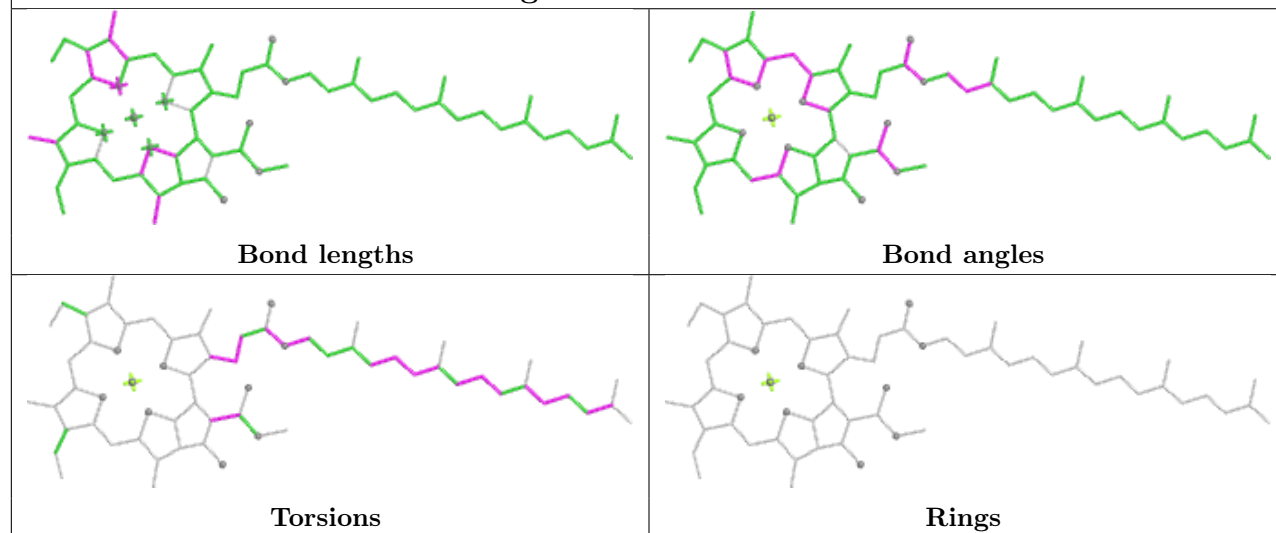


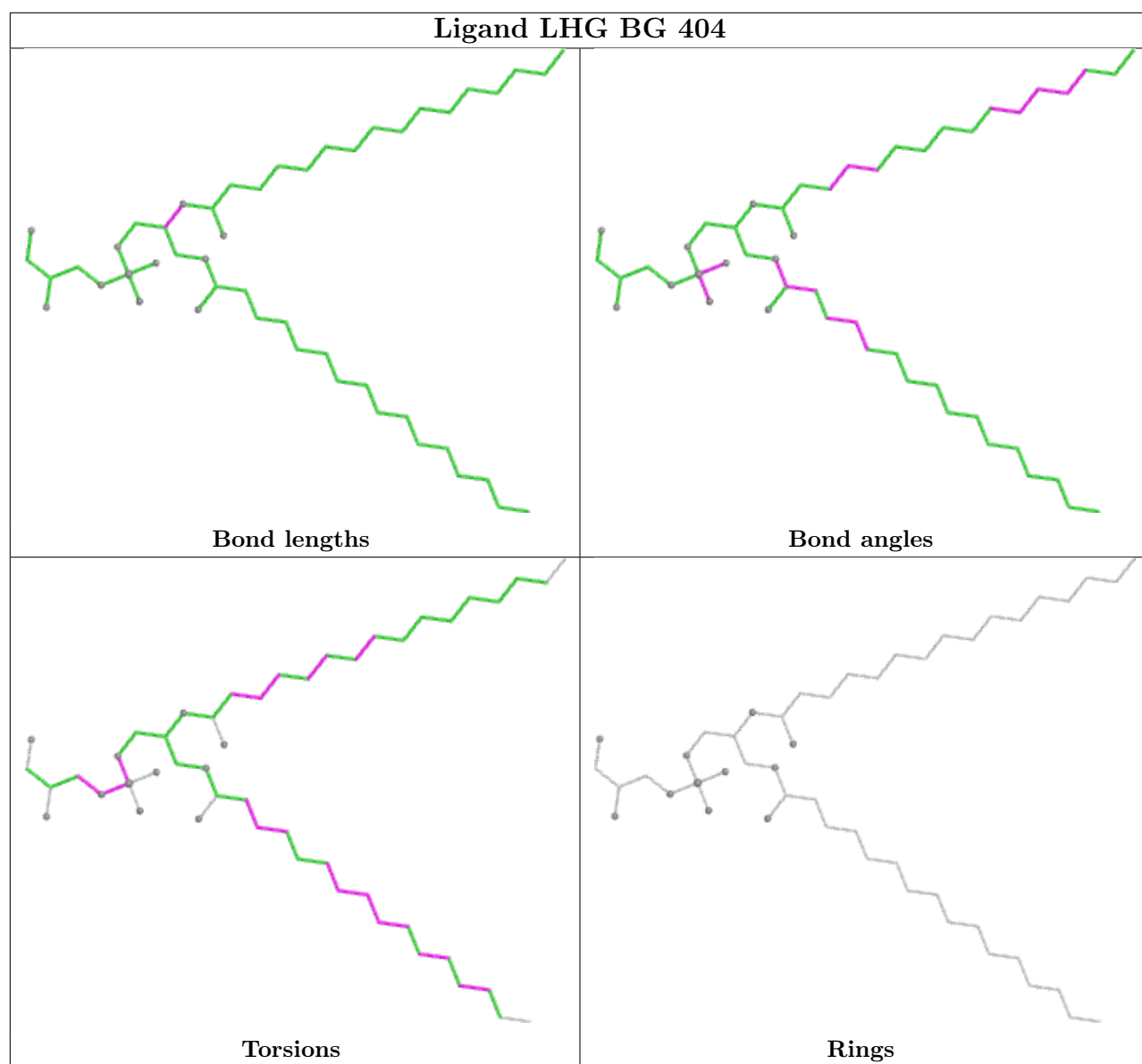


Ligand CHL 7 307

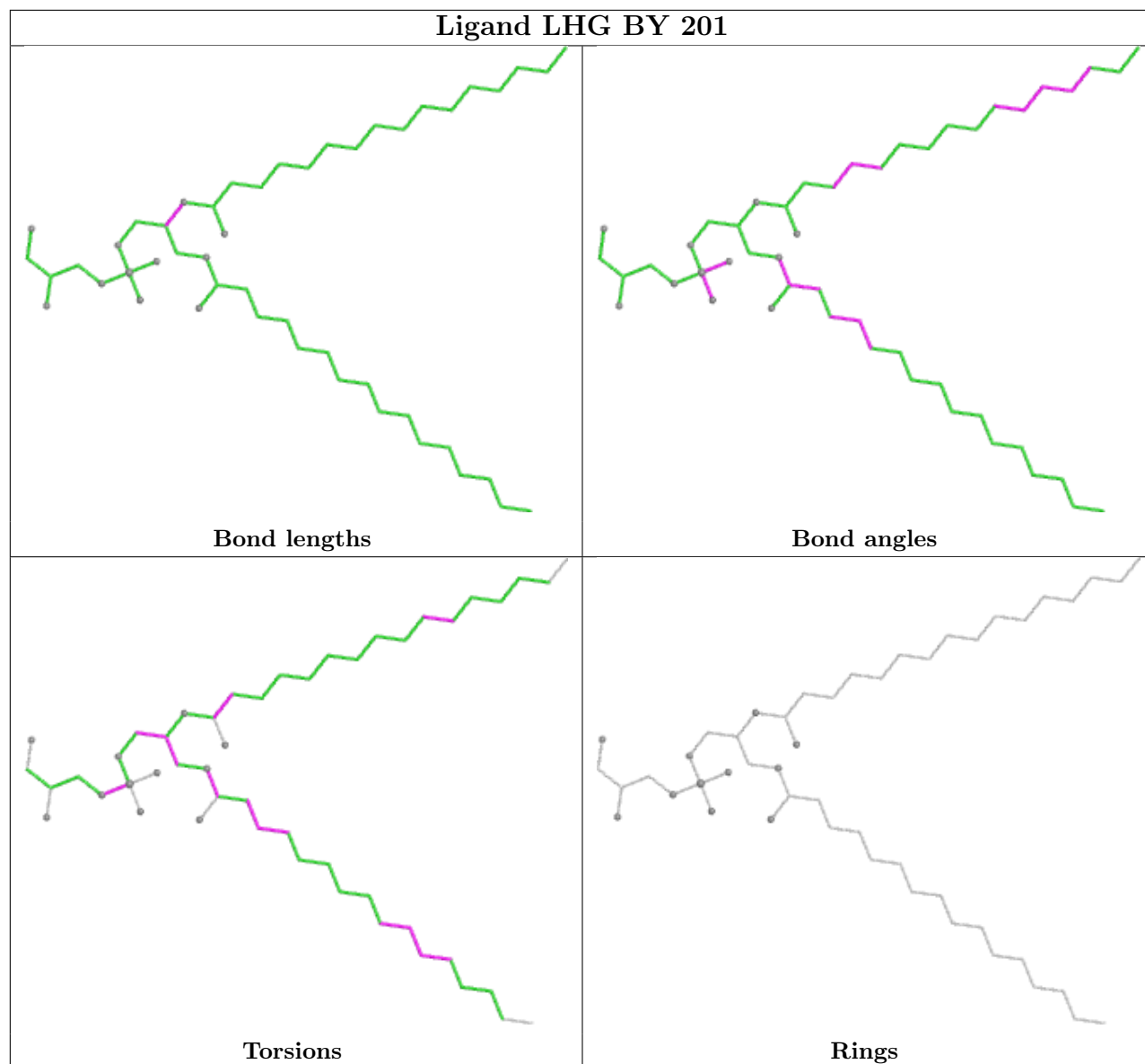




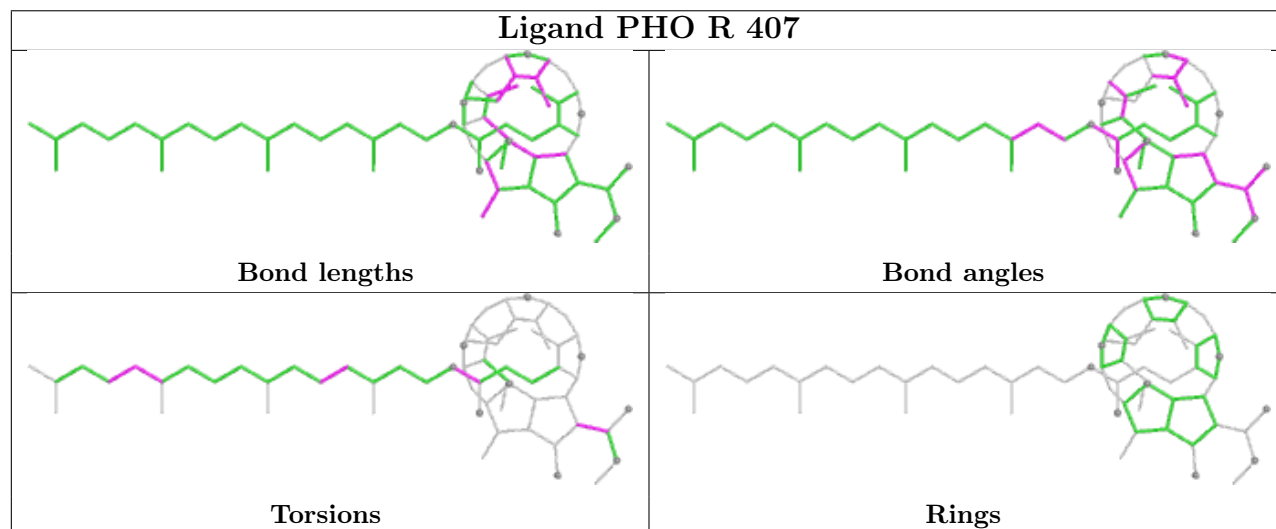
Ligand CLA 0 610**Ligand CLA BE 605**

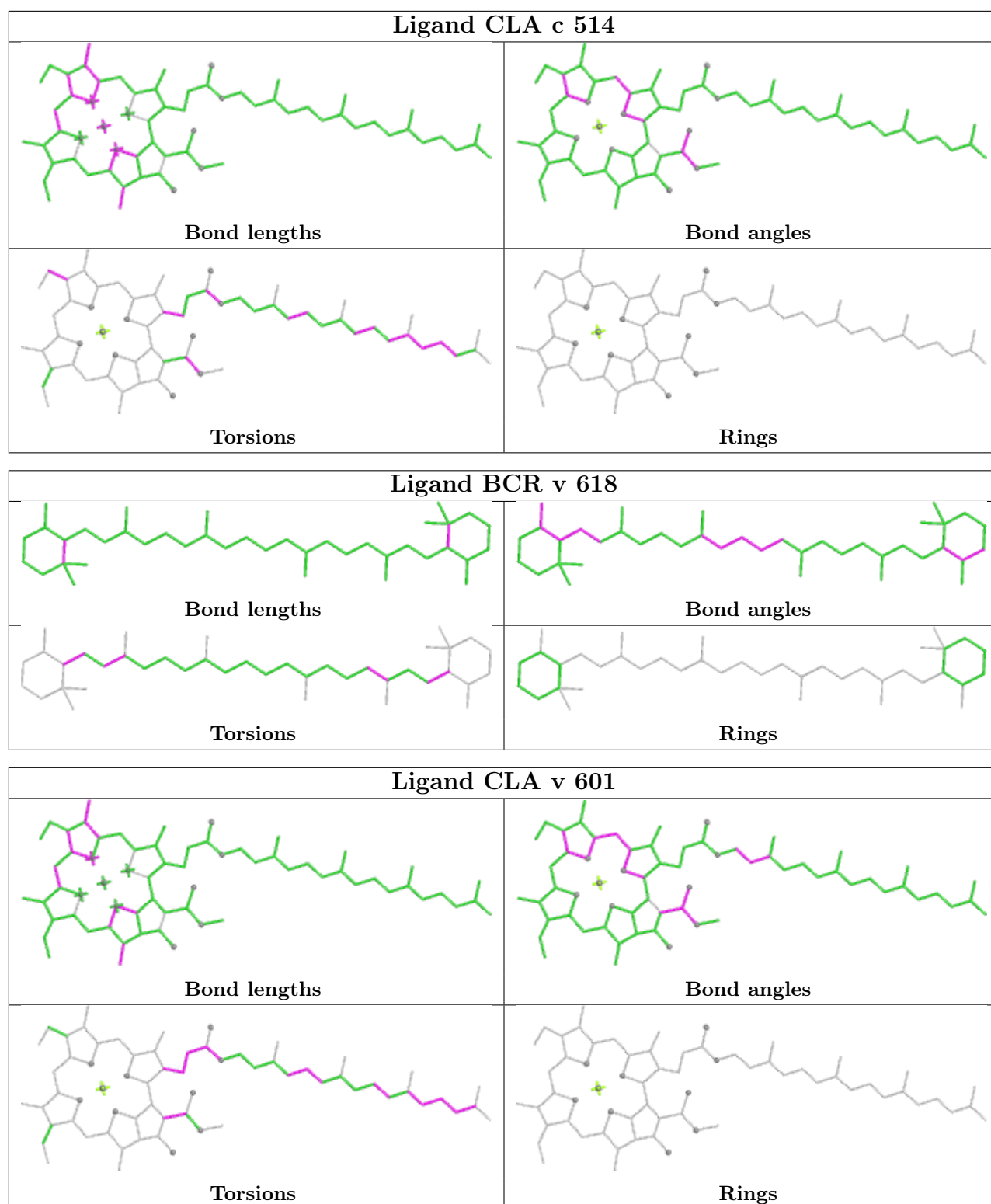


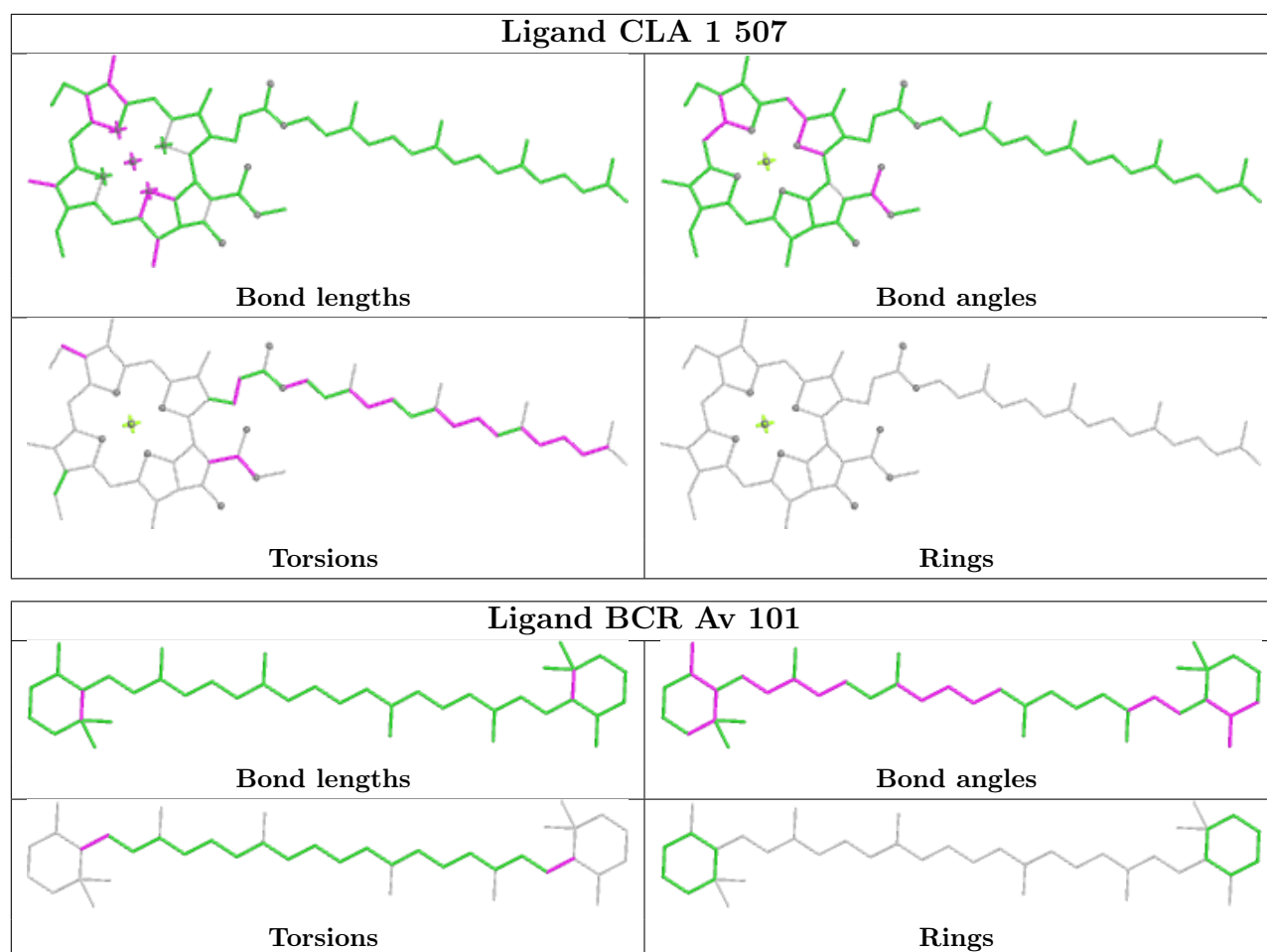
Ligand LHG BY 201



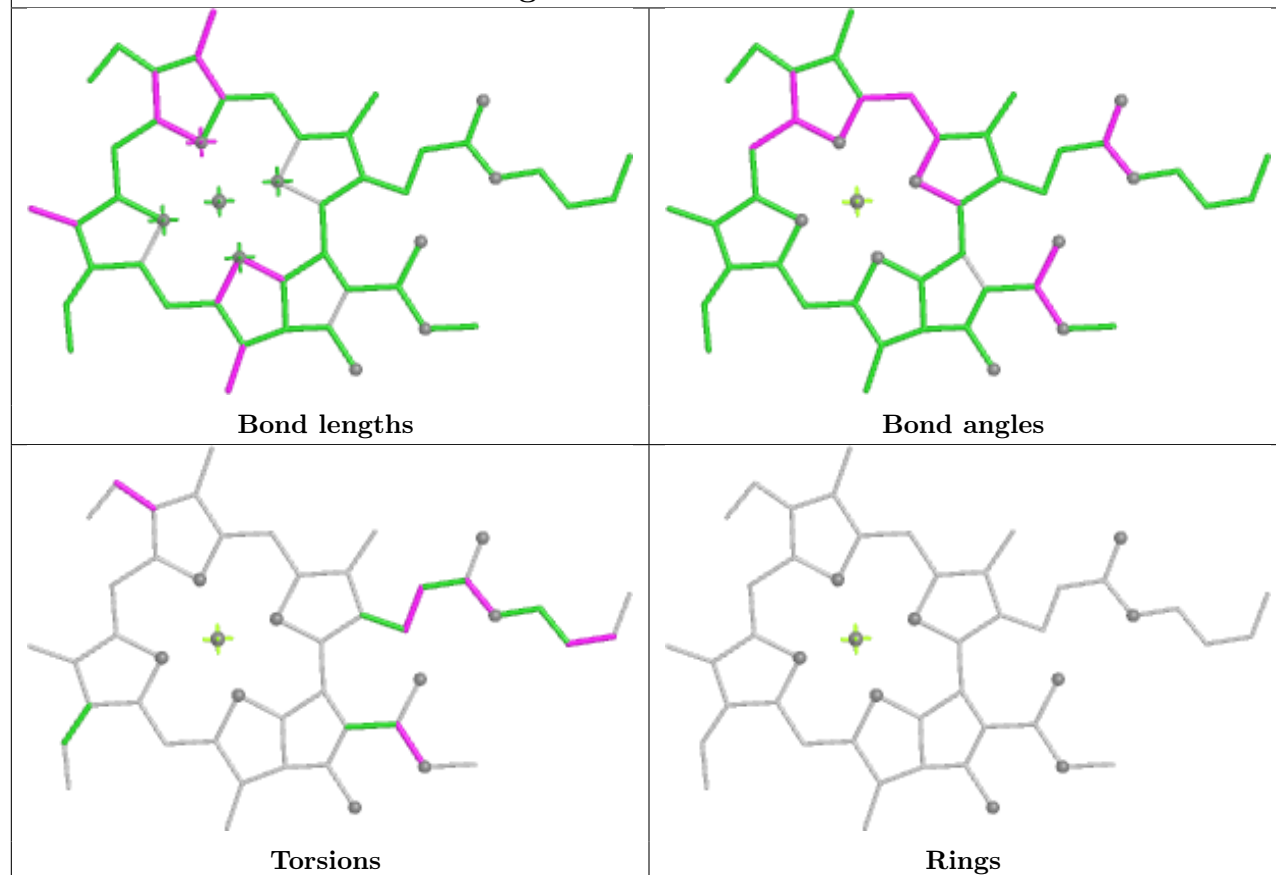
Ligand PHO R 407



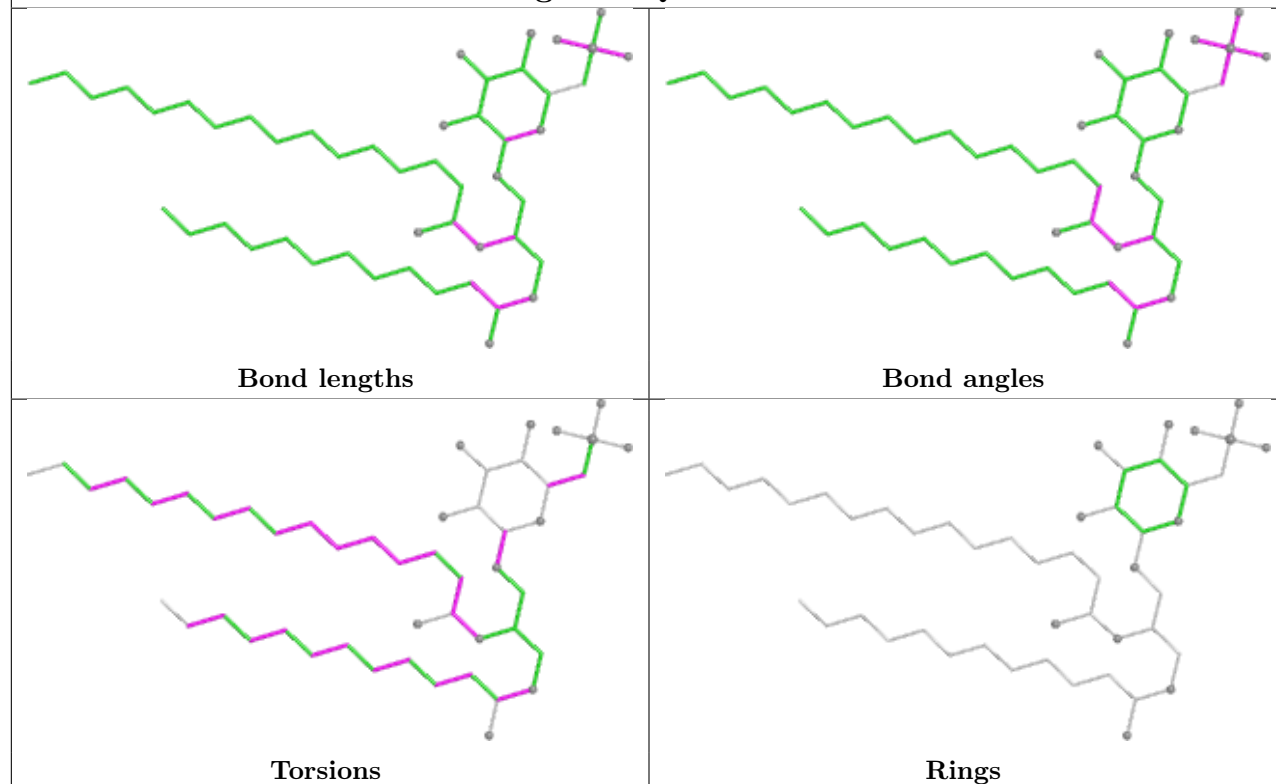


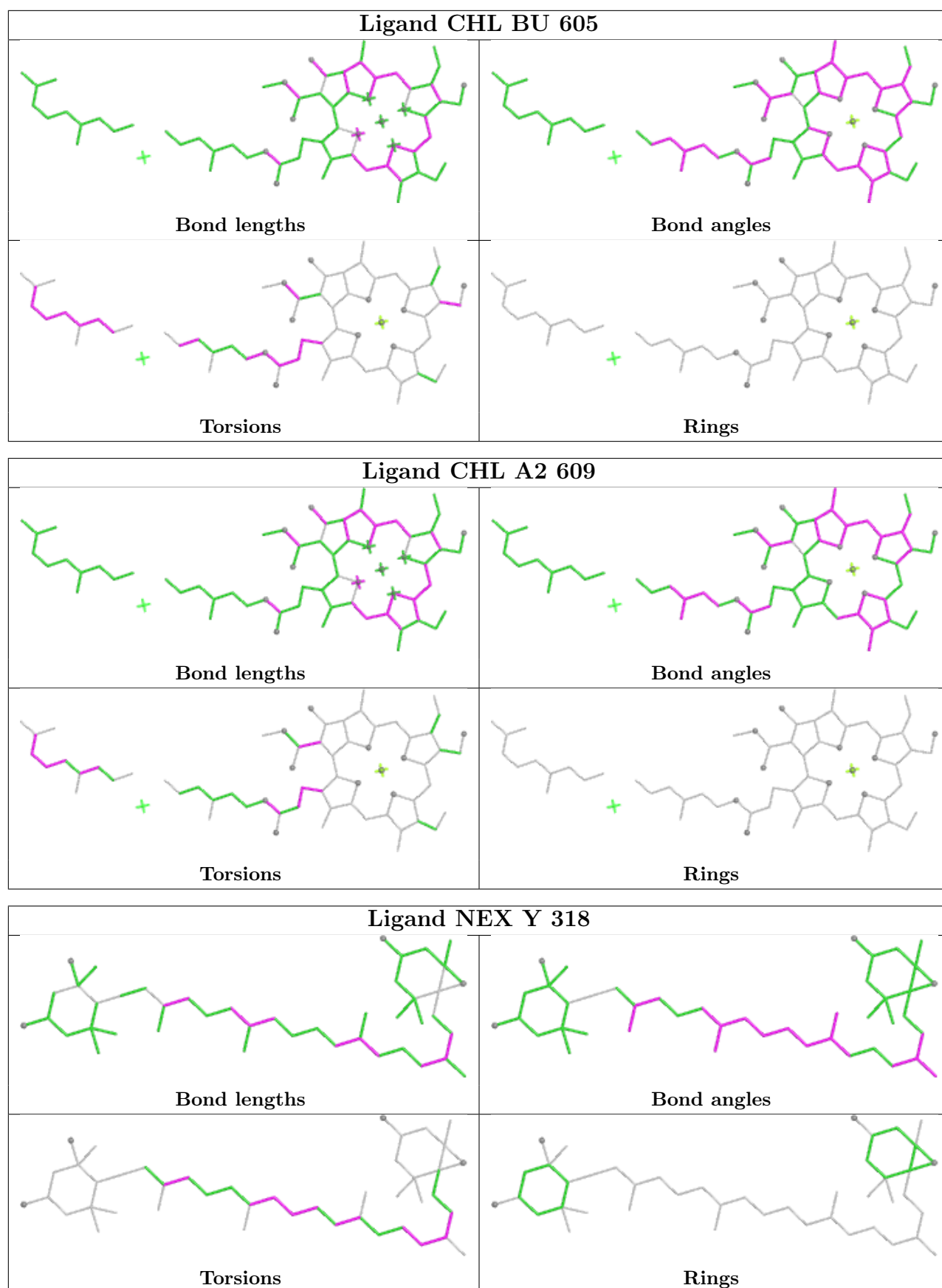


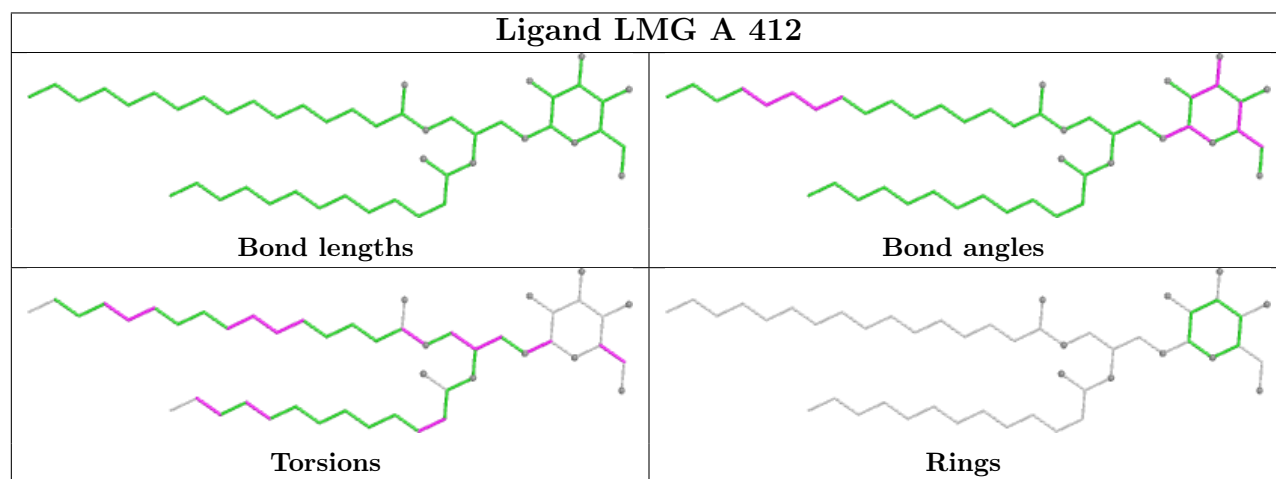
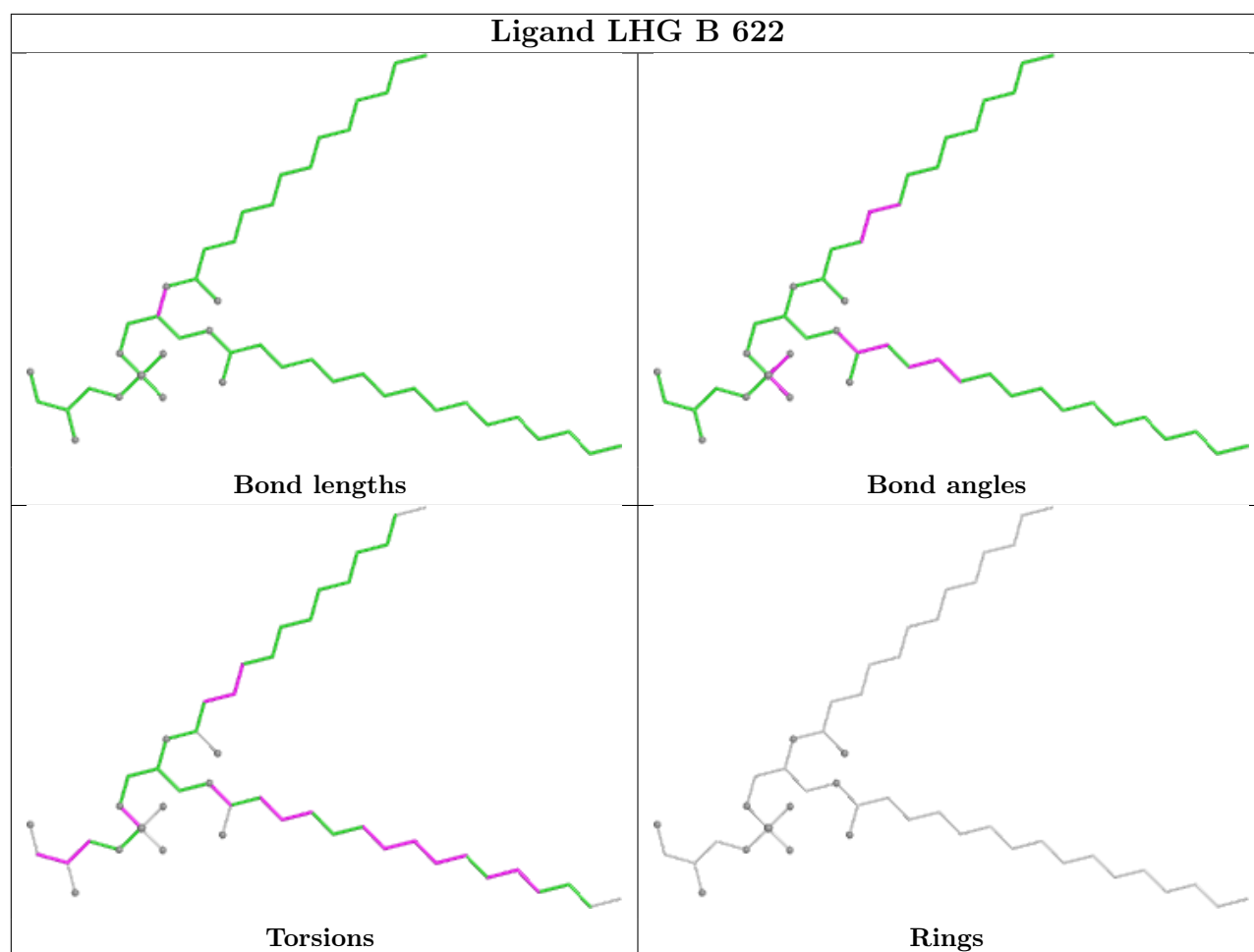
Ligand CLA BV 613

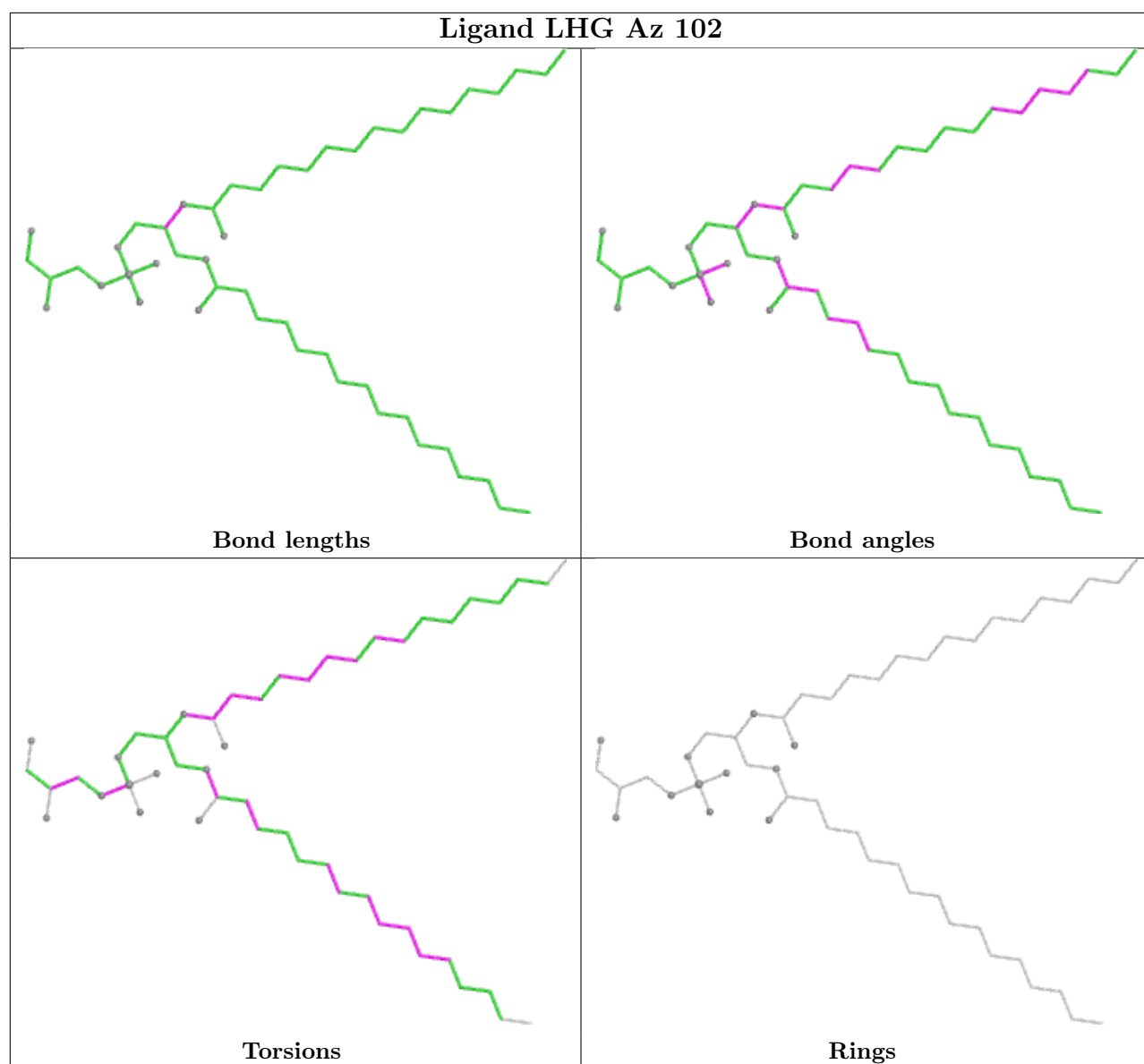


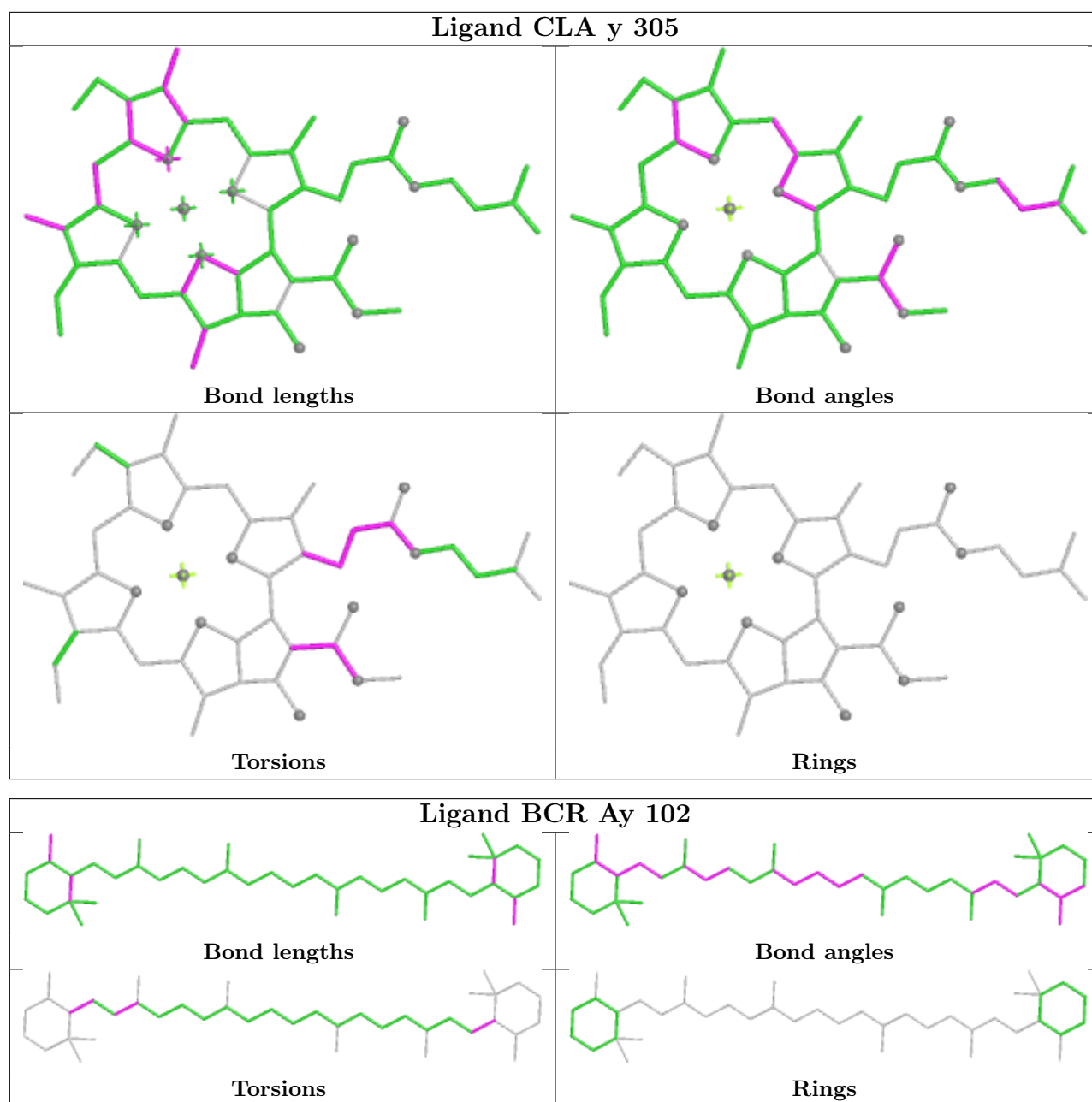
Ligand SQD d 406

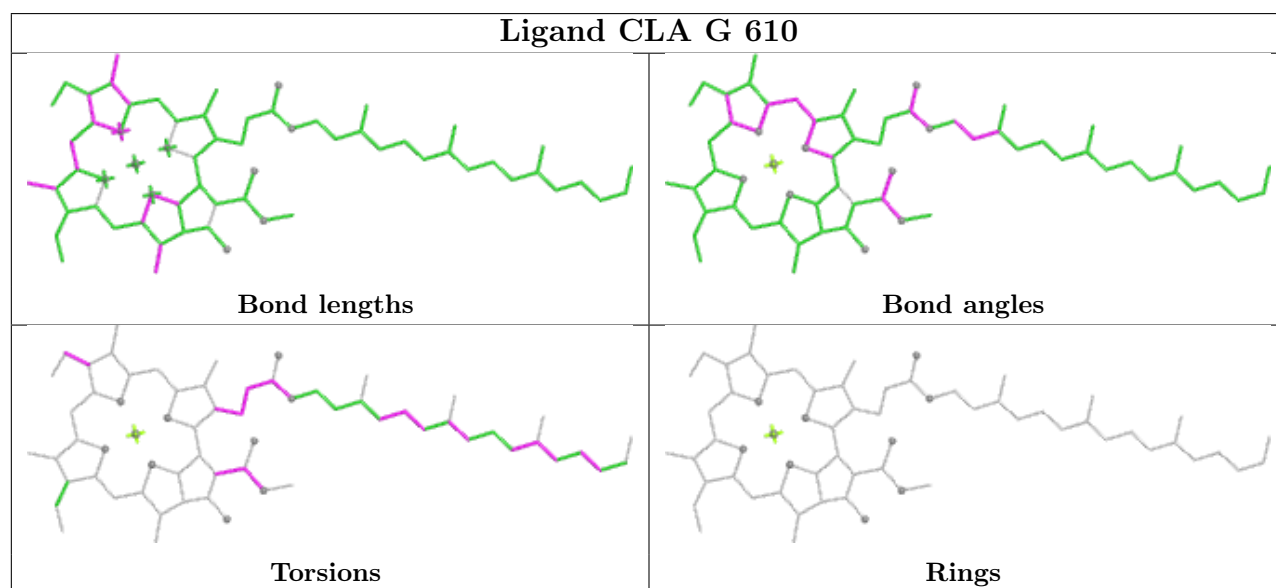
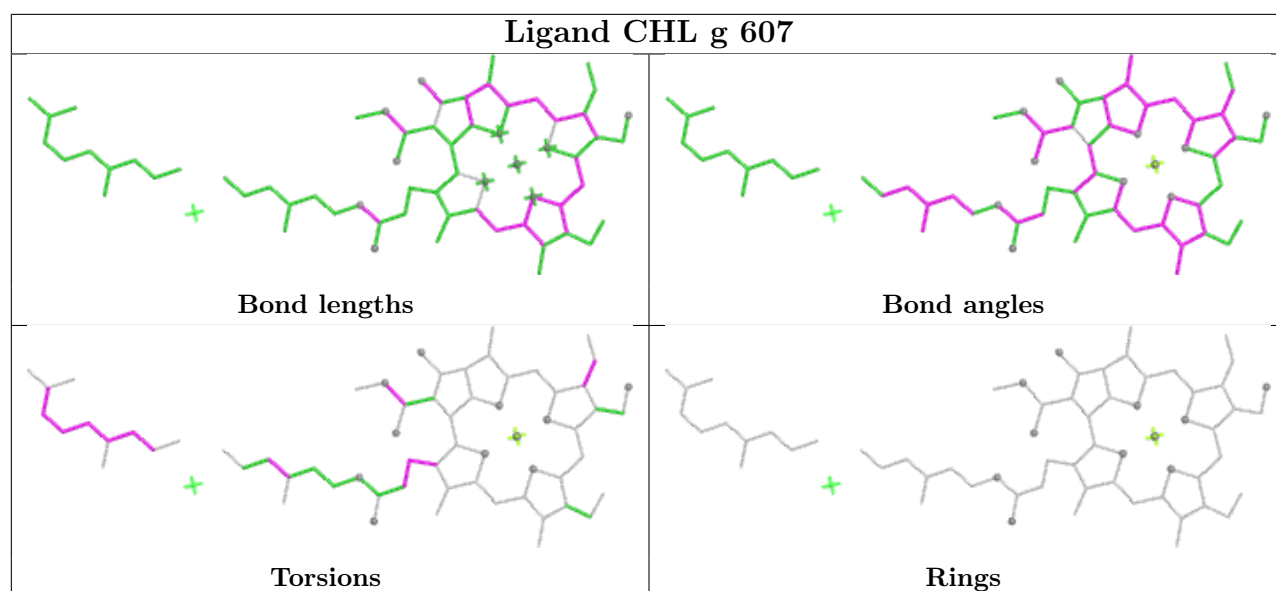


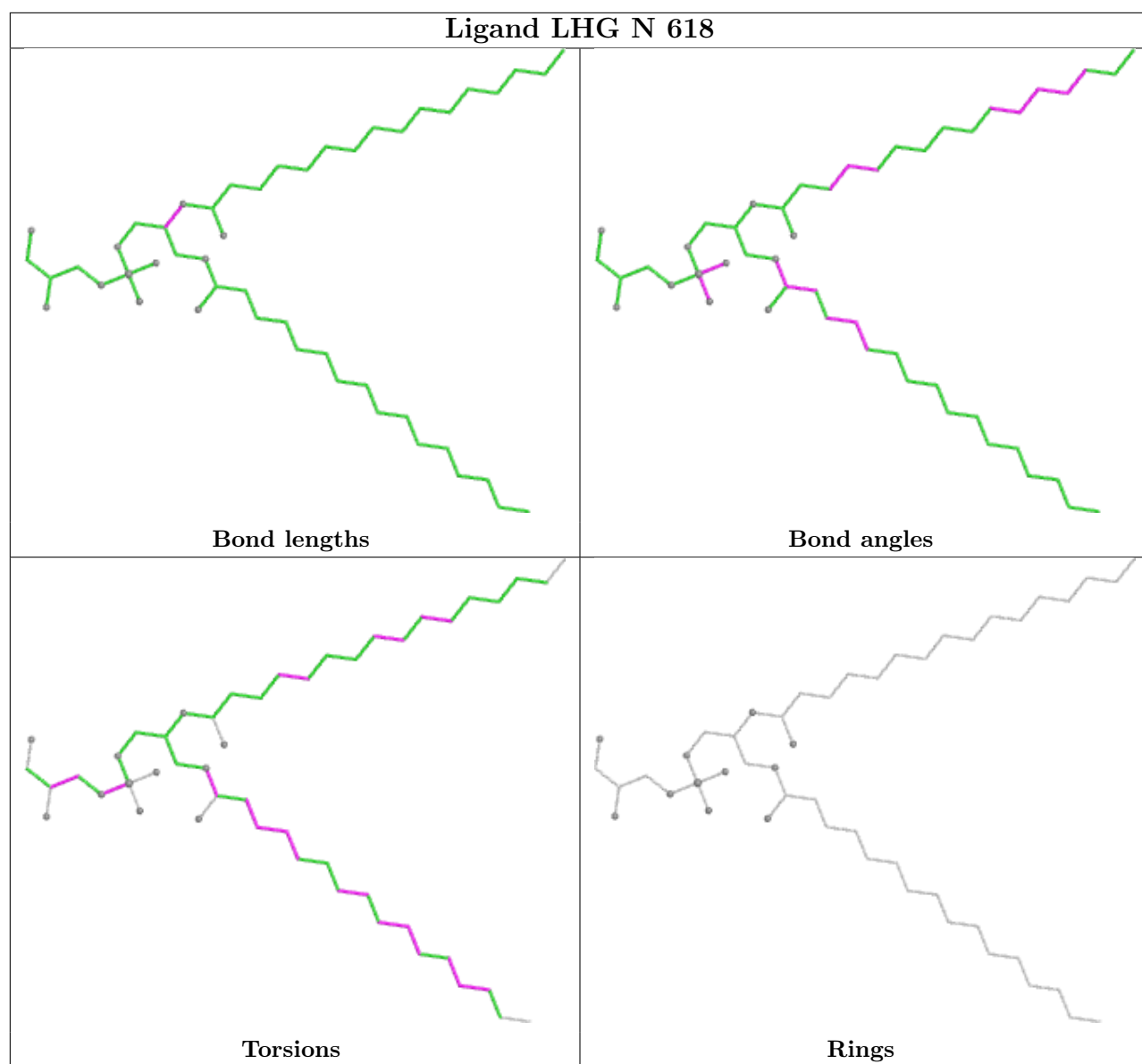


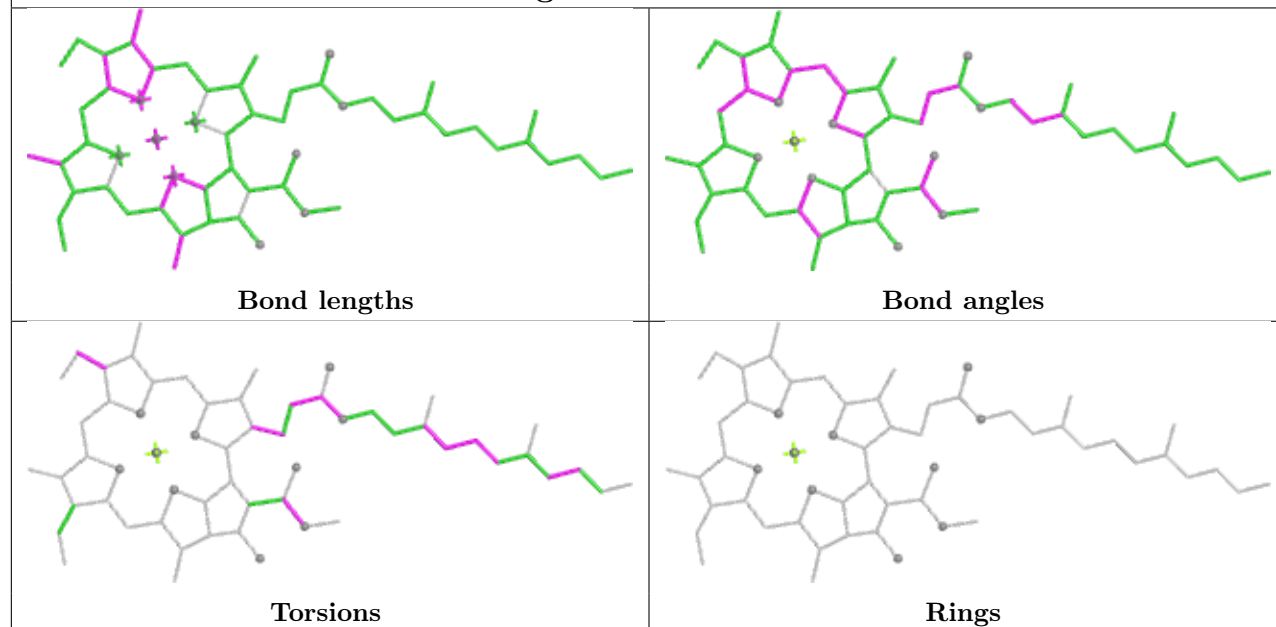
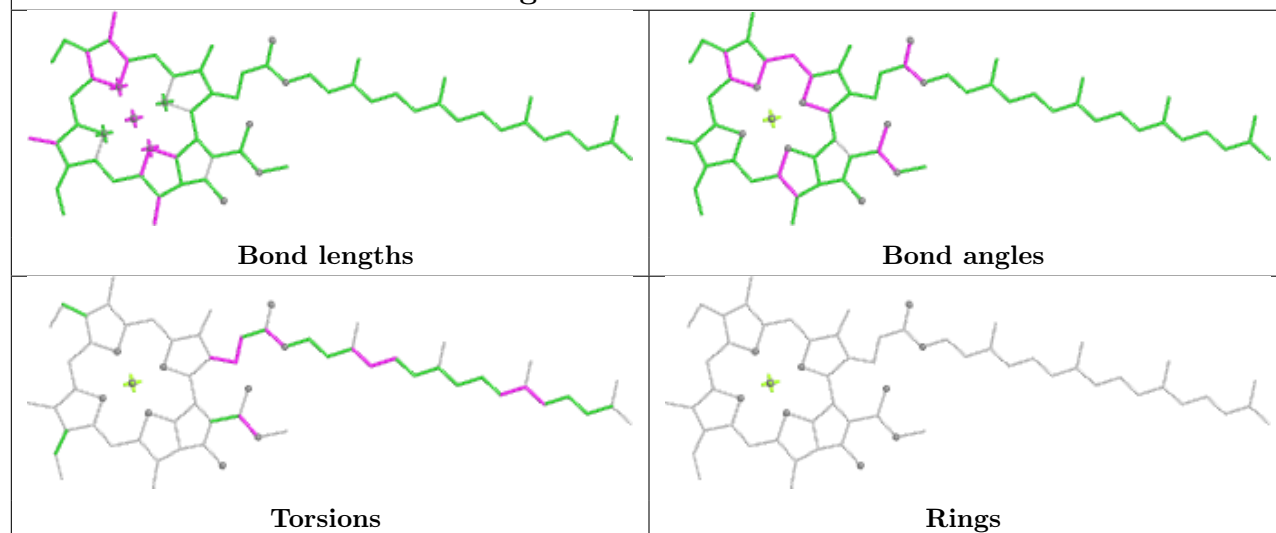




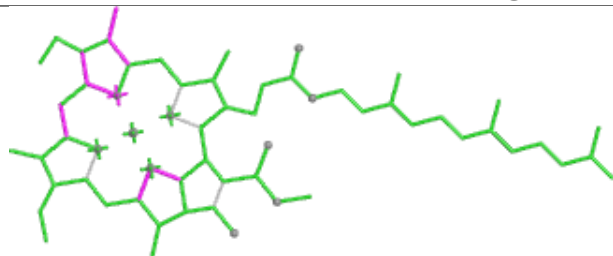




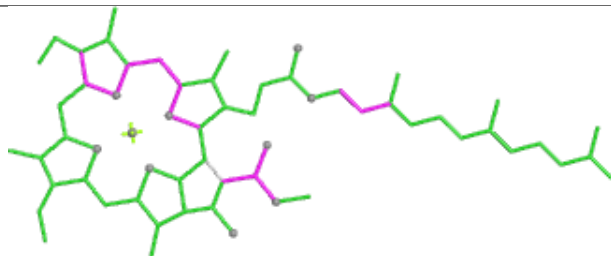


Ligand CLA 0 613**Ligand CLA BB 314**

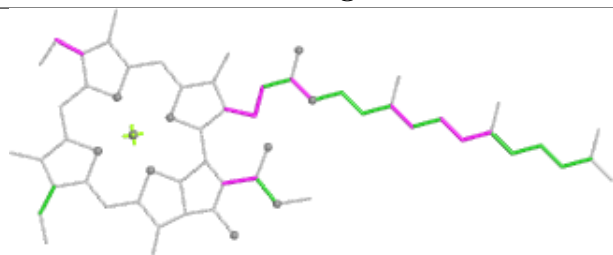
Ligand CLA BJ 611



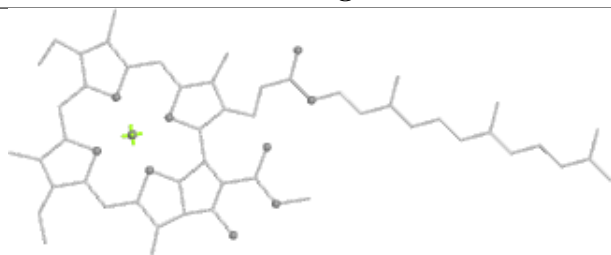
Bond lengths



Bond angles

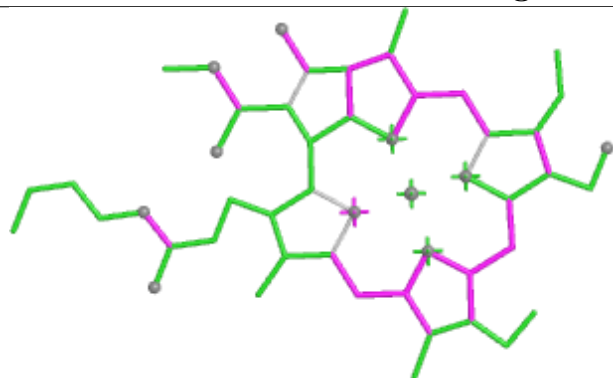


Torsions

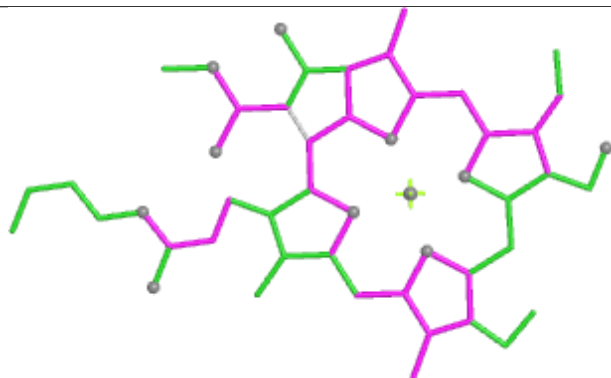


Rings

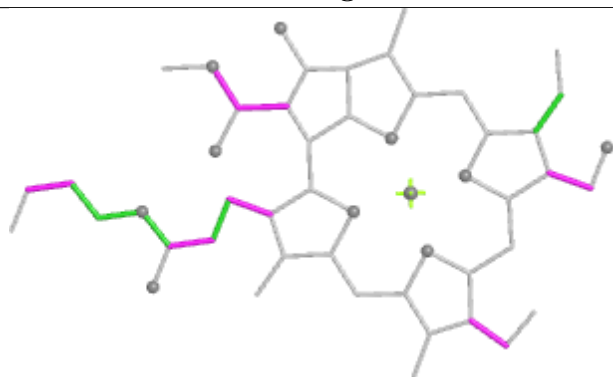
Ligand CHL N 606



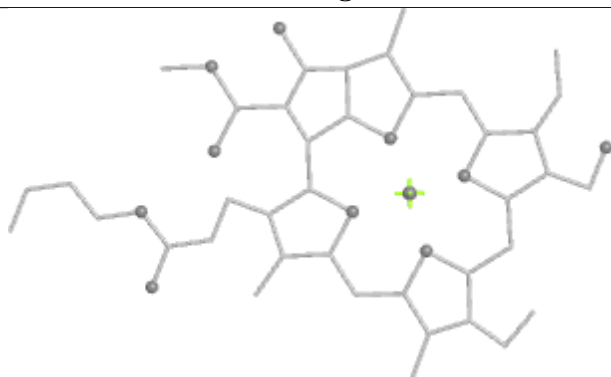
Bond lengths



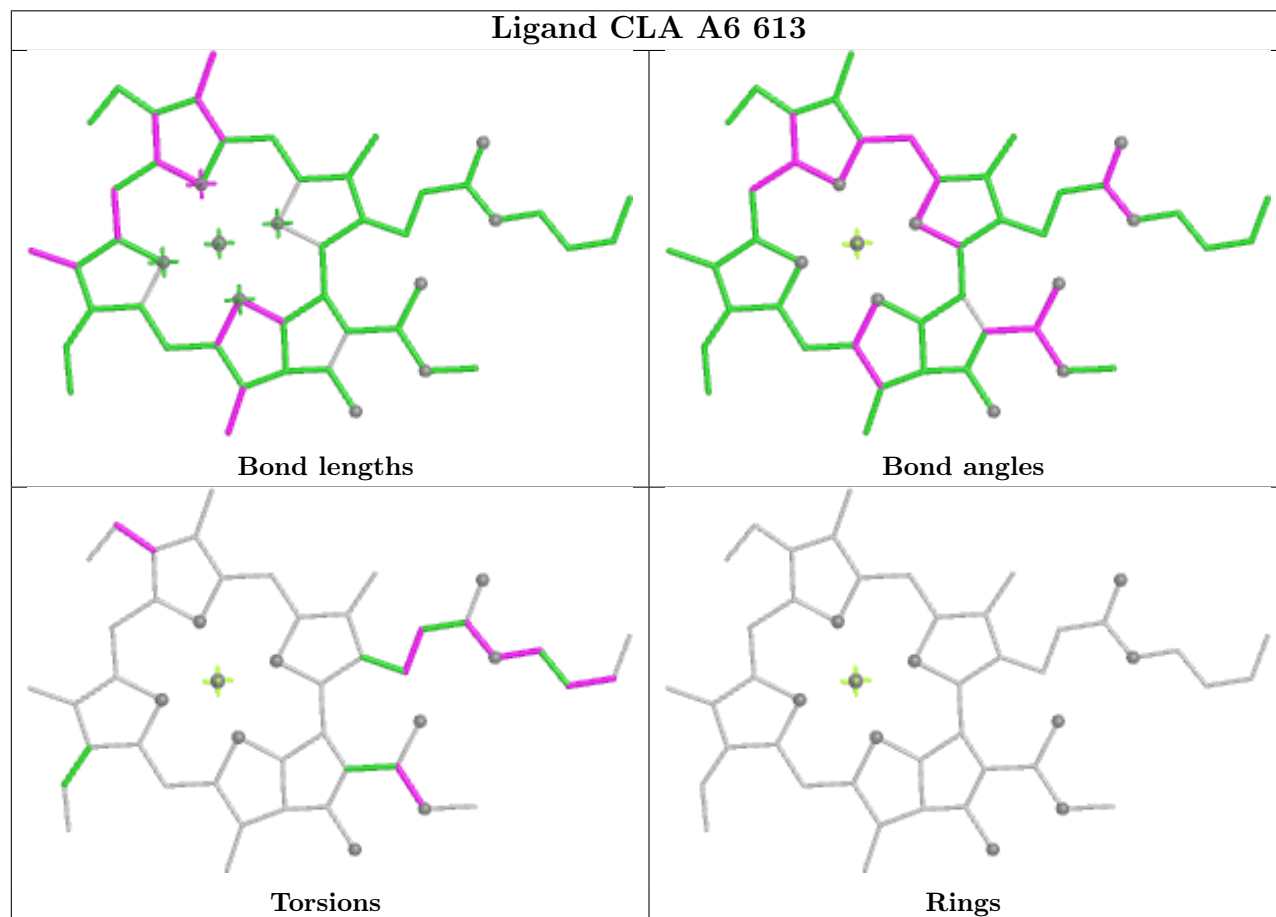
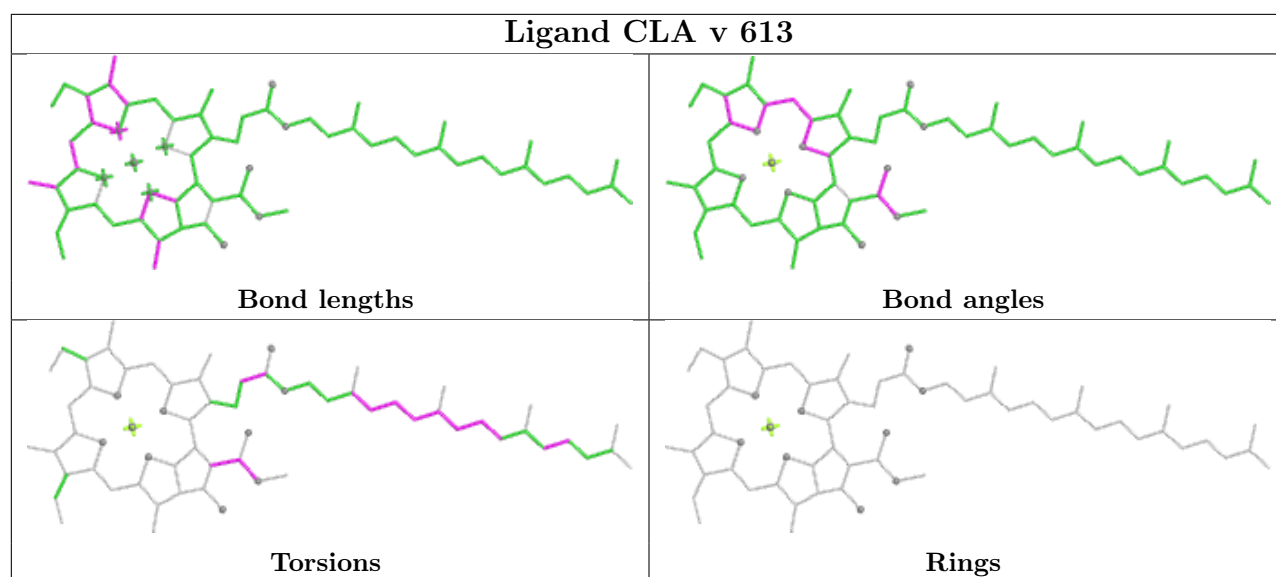
Bond angles

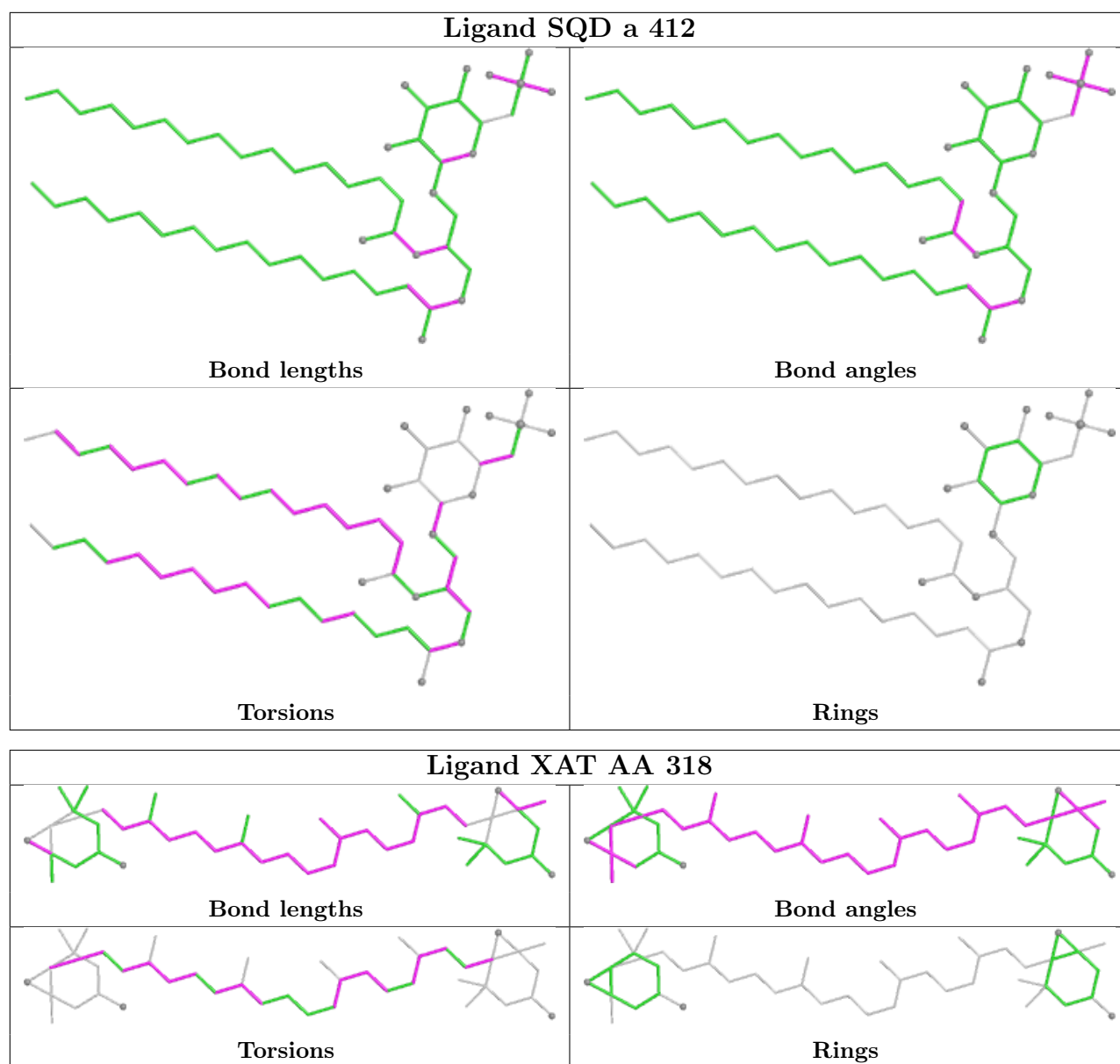


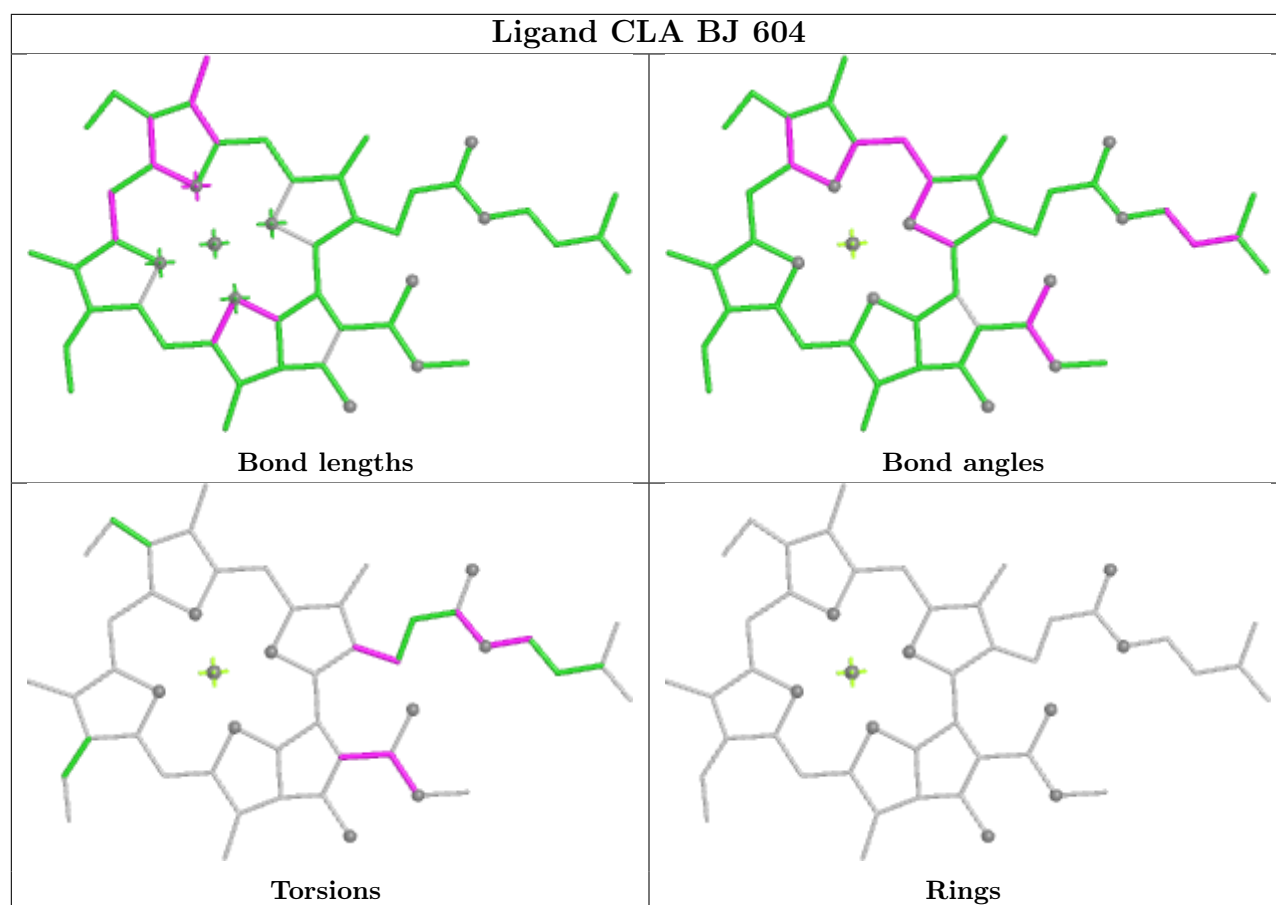
Torsions



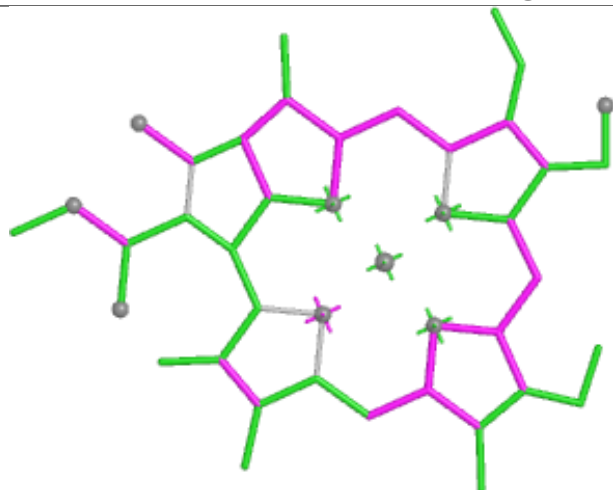
Rings



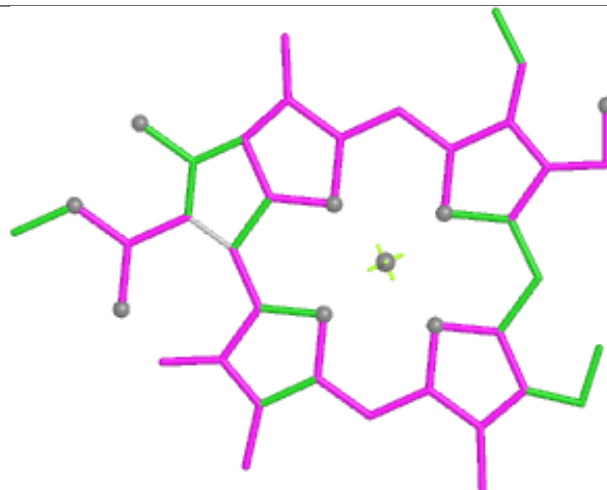




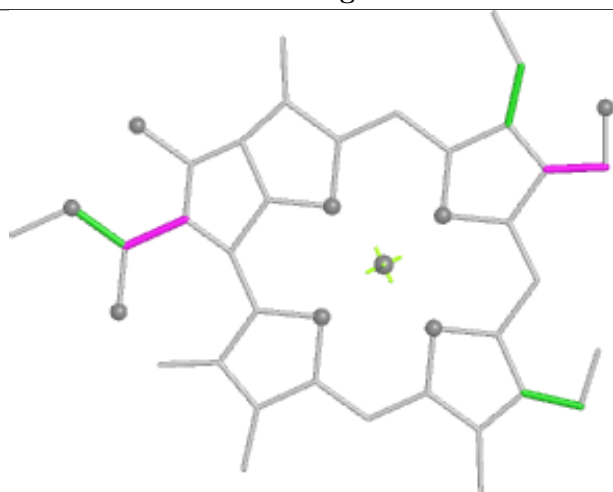
Ligand CHL r 613



Bond lengths



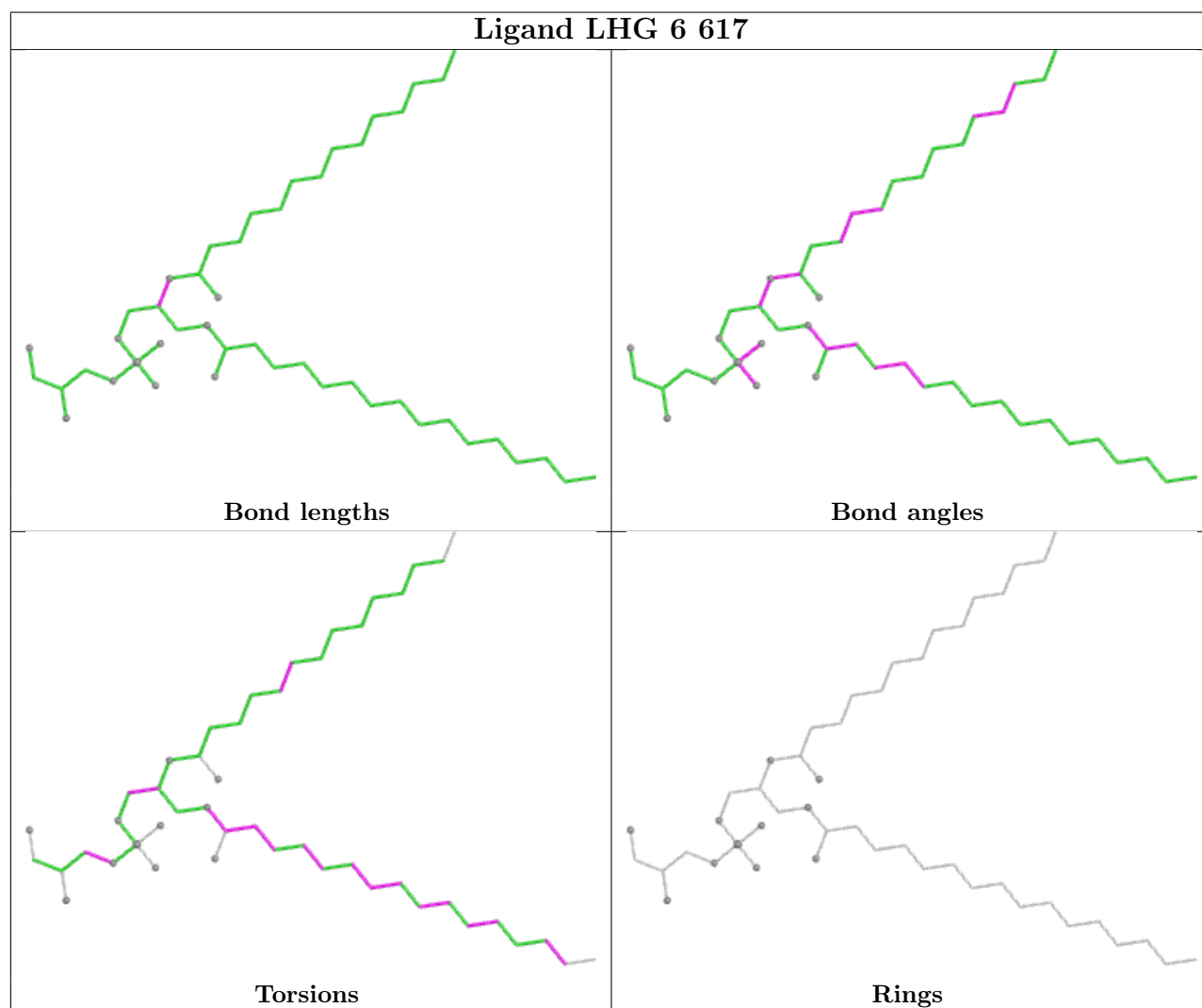
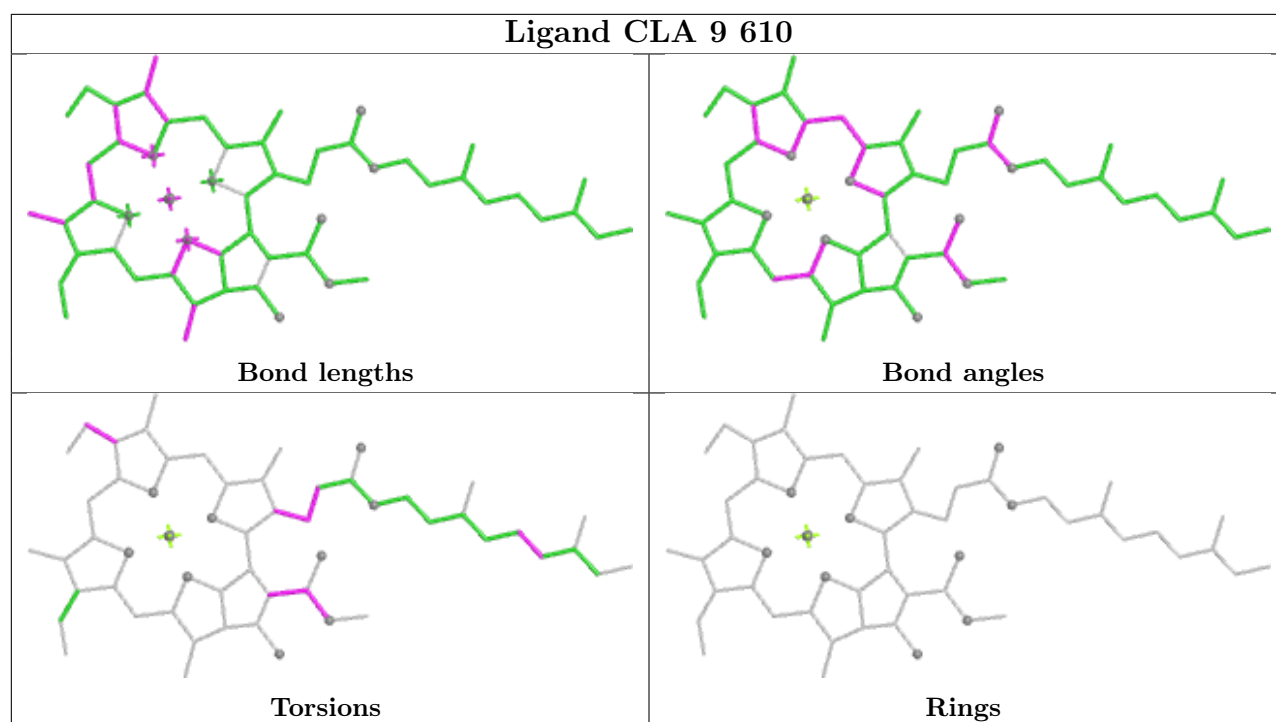
Bond angles

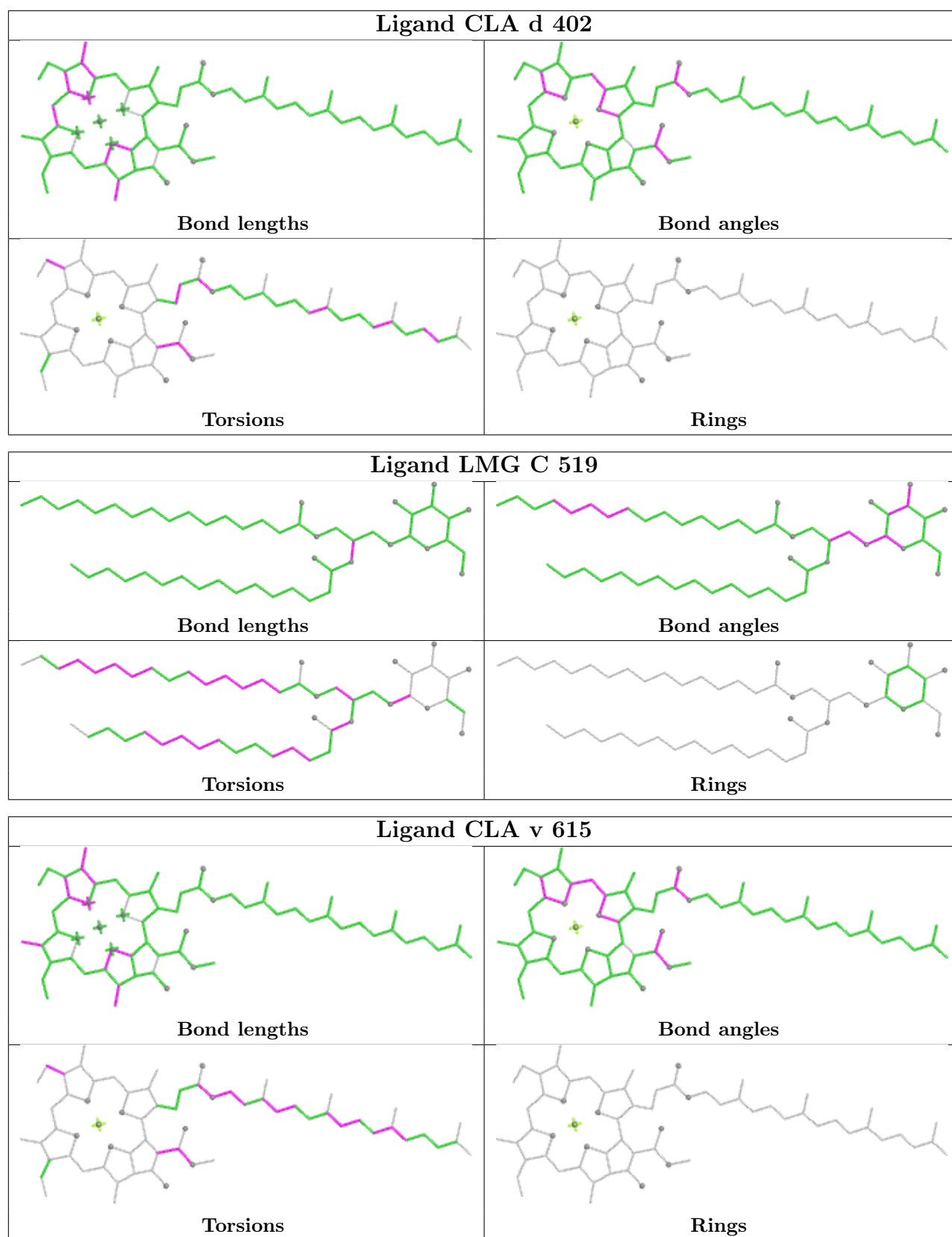


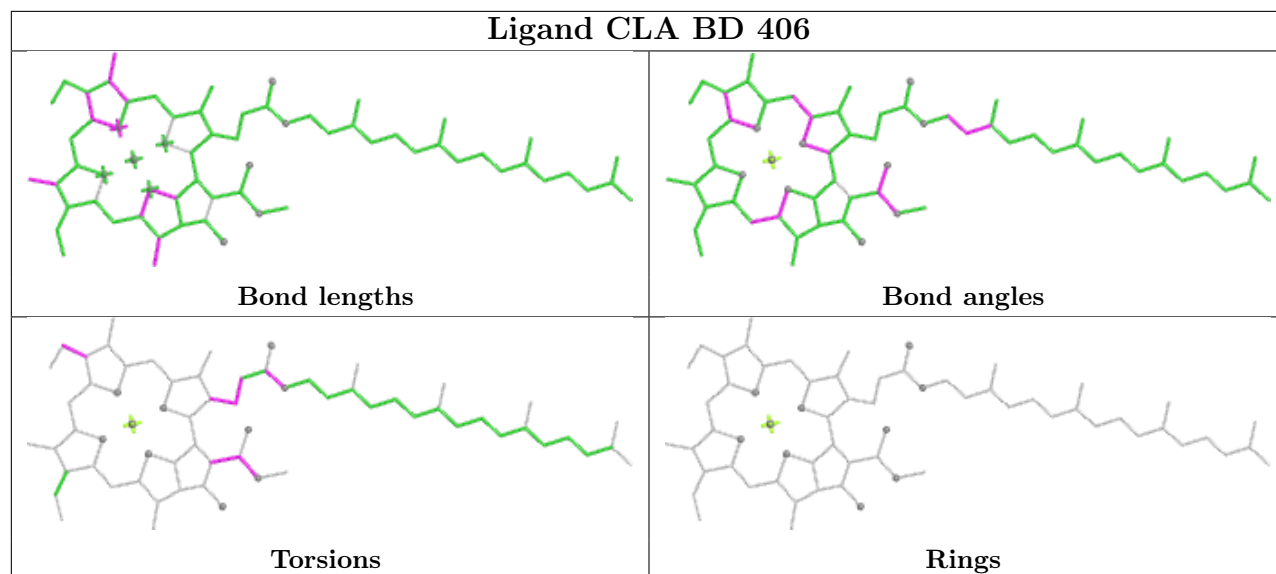
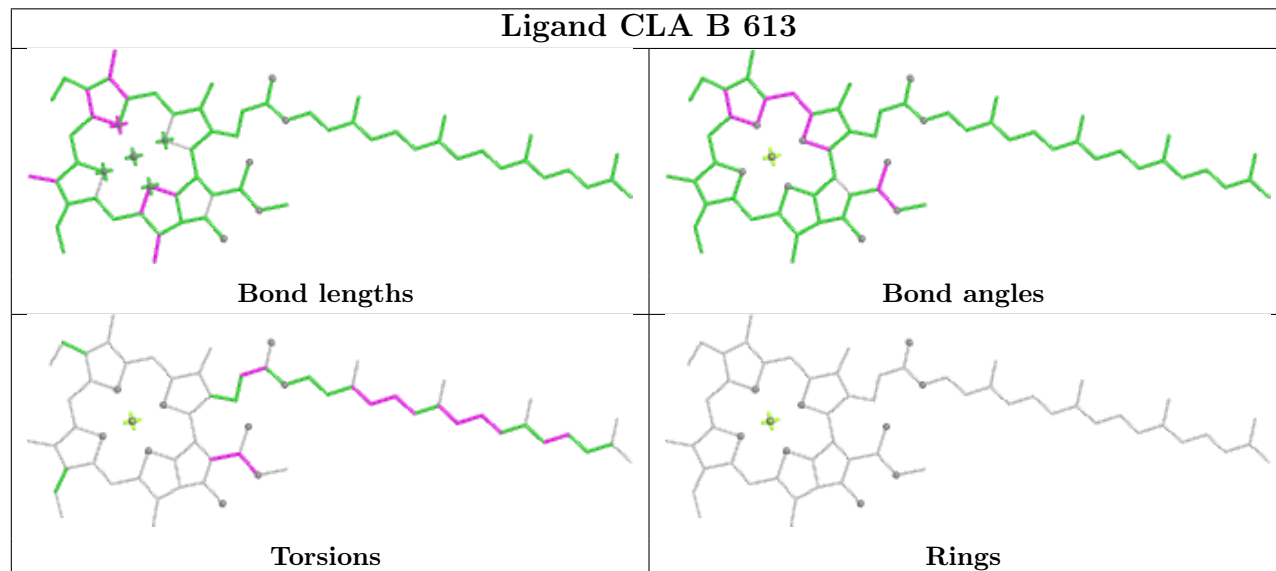
Torsions

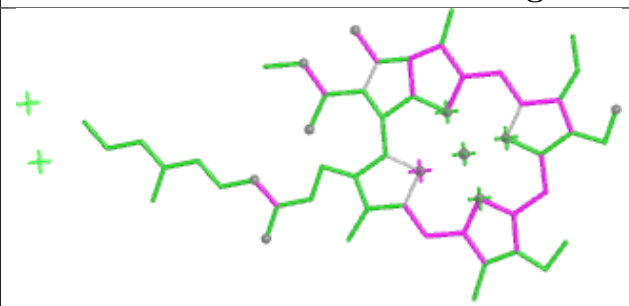
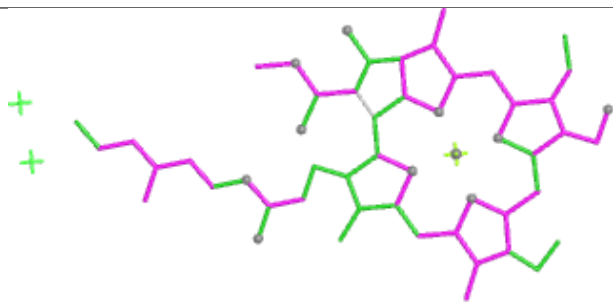
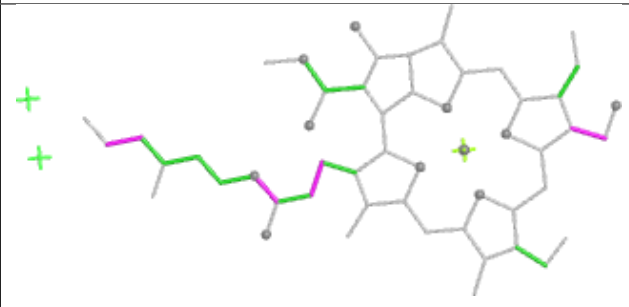
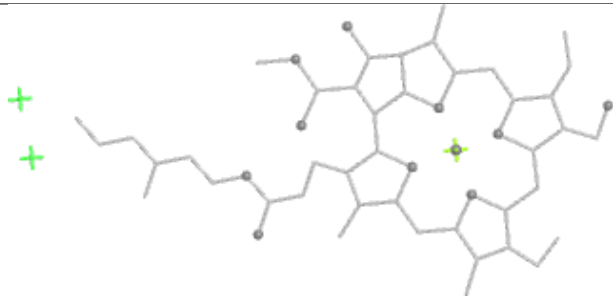
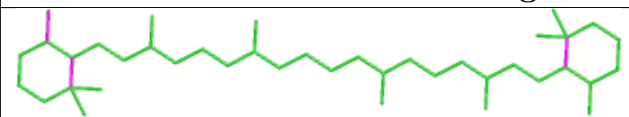
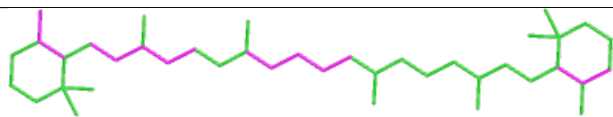
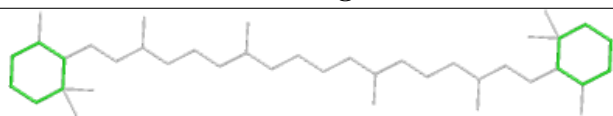


Rings

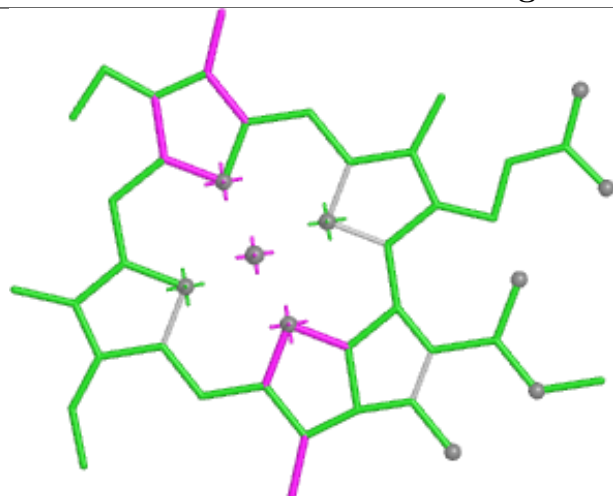




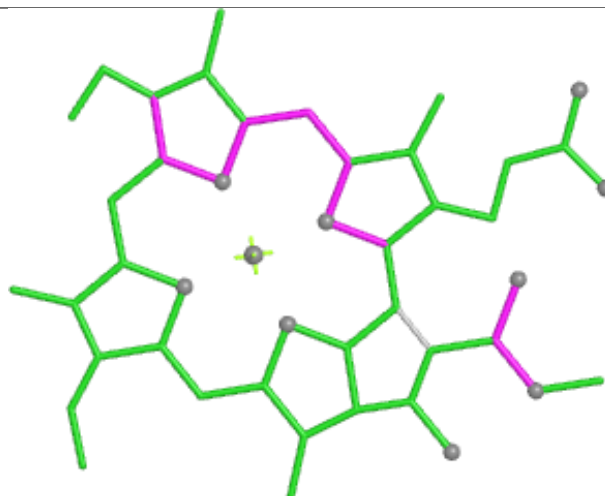
Ligand CLA BD 406**Ligand CLA B 613**

Ligand CHL r 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

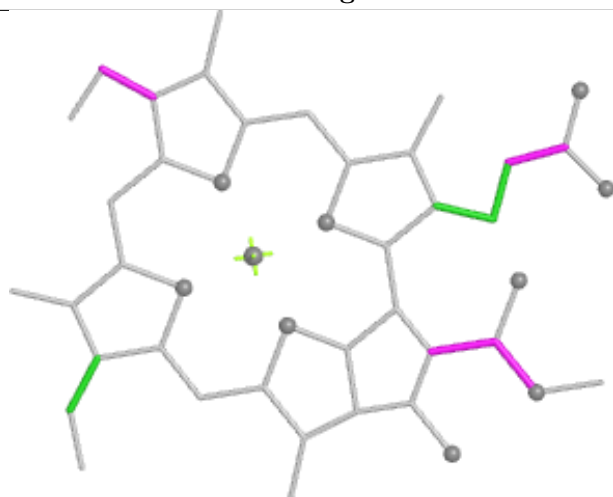
Ligand CLA 9 612



Bond lengths



Bond angles

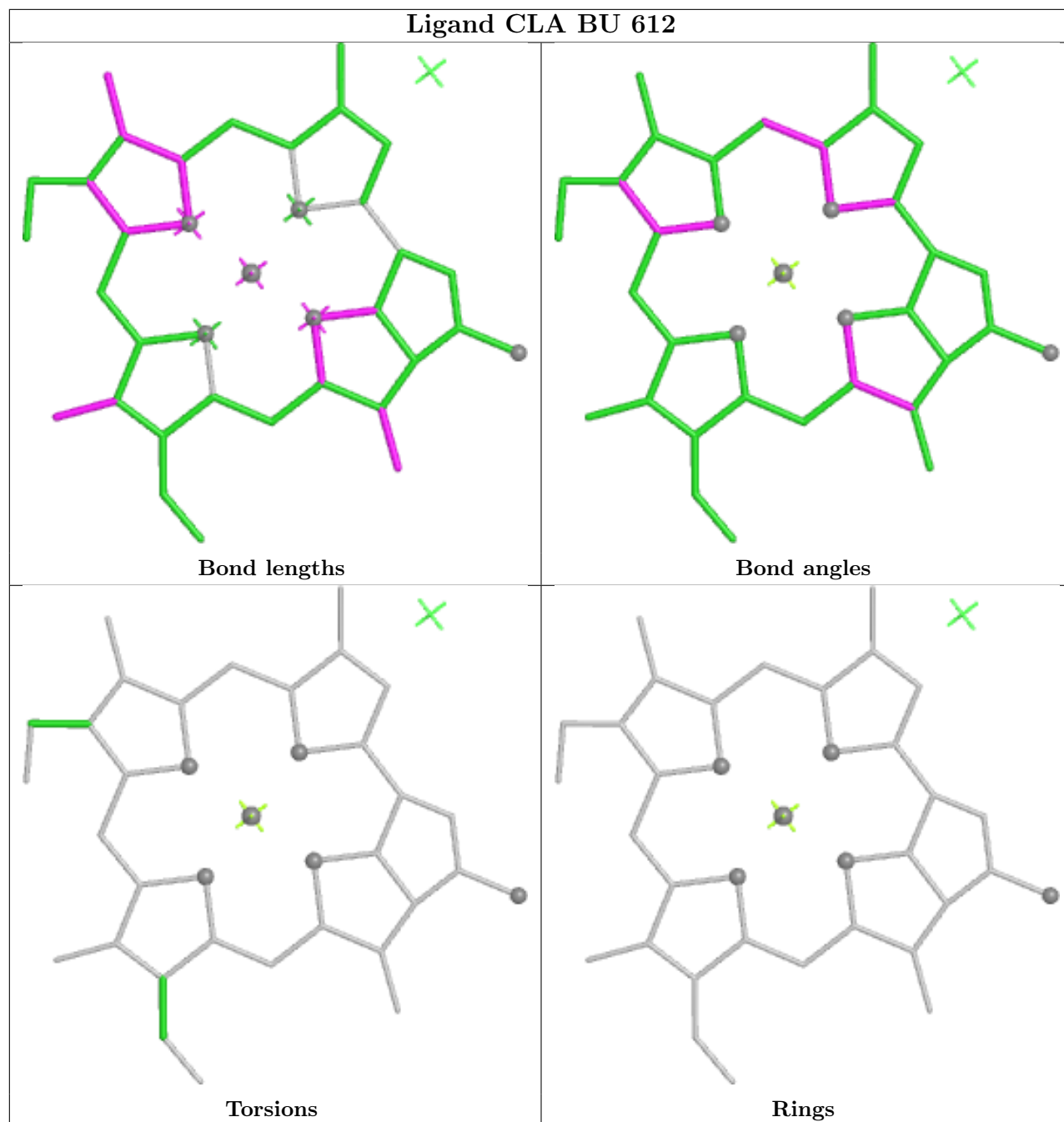


Torsions

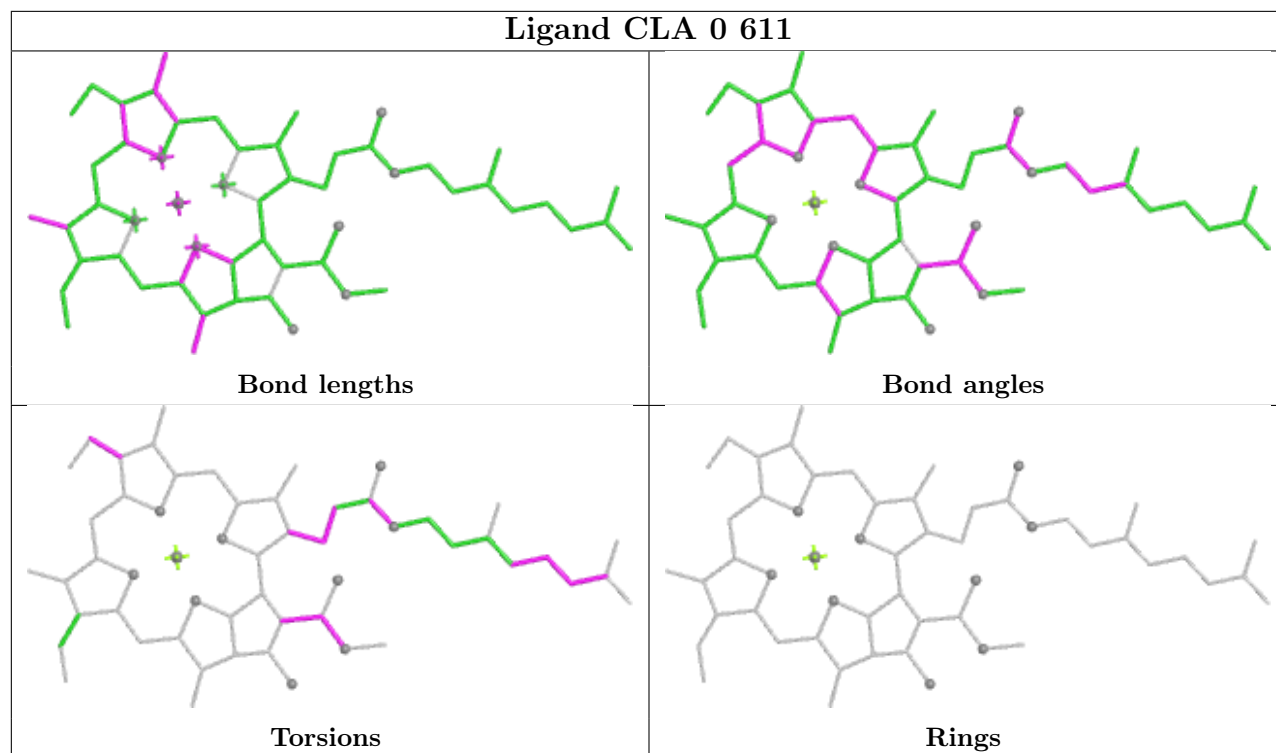


Rings

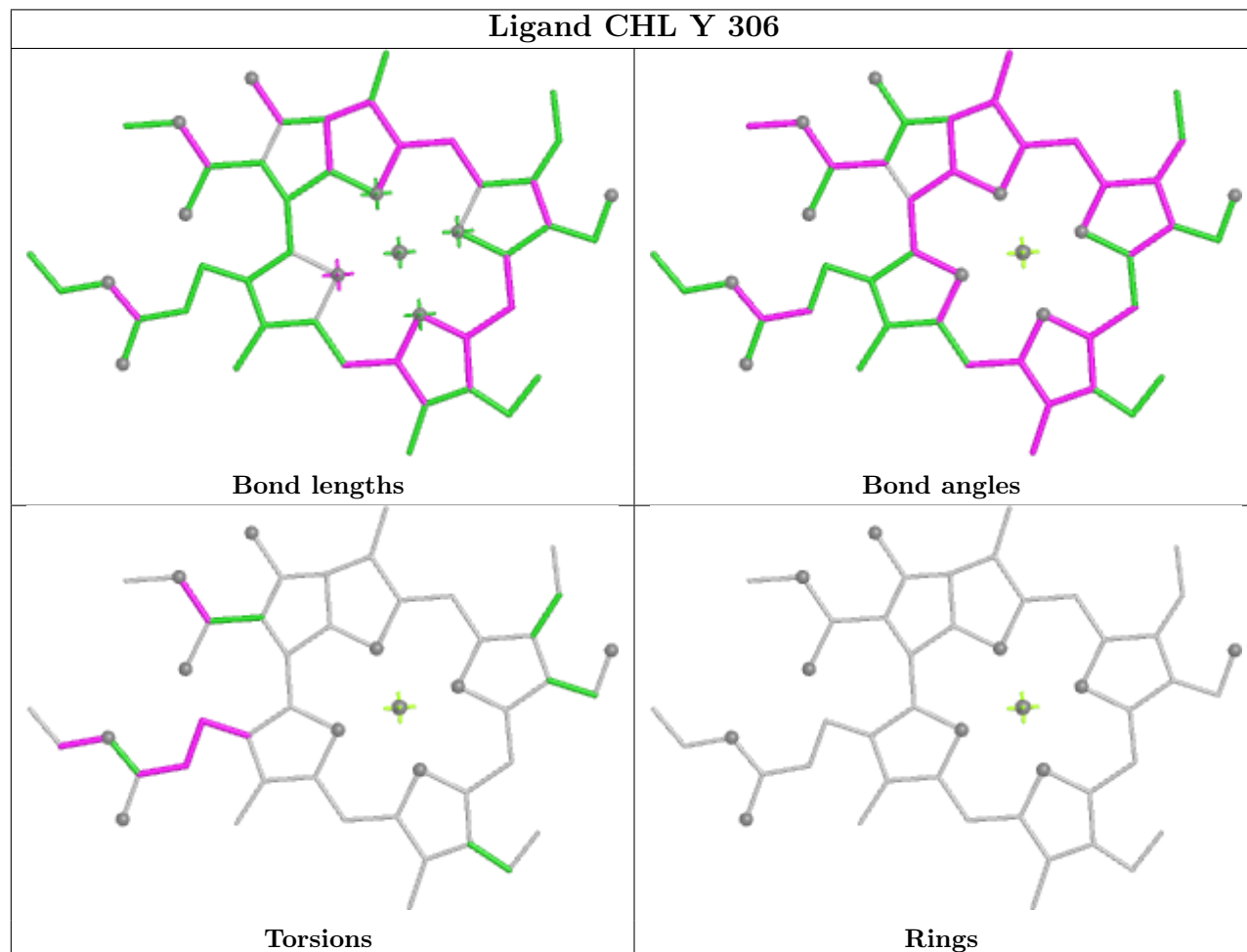
Ligand CLA BU 612

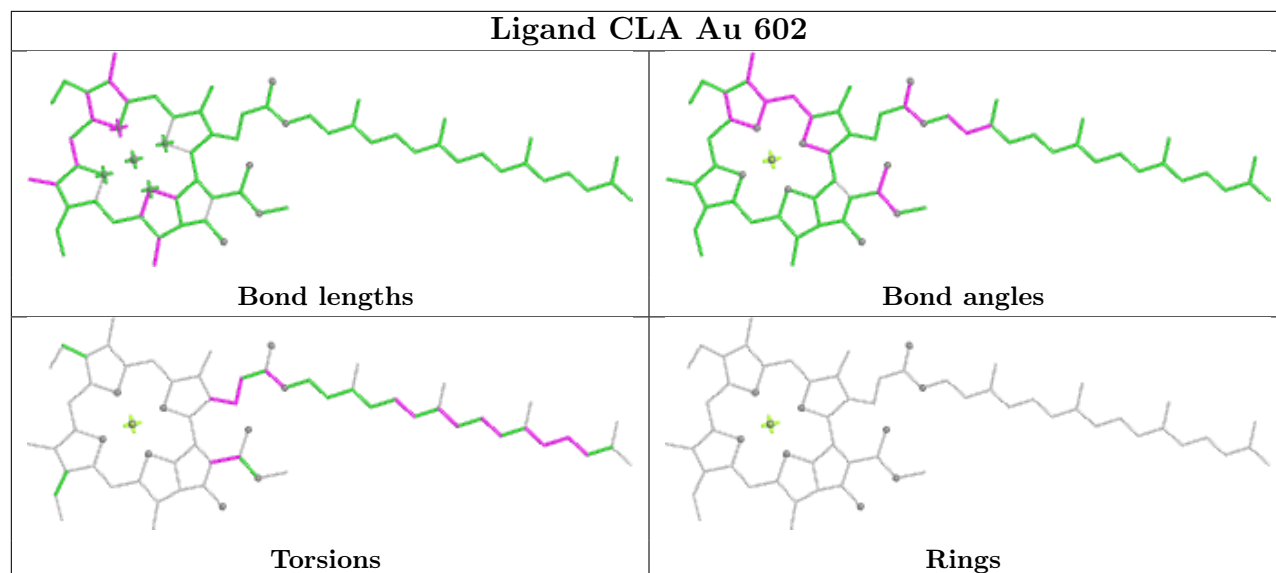
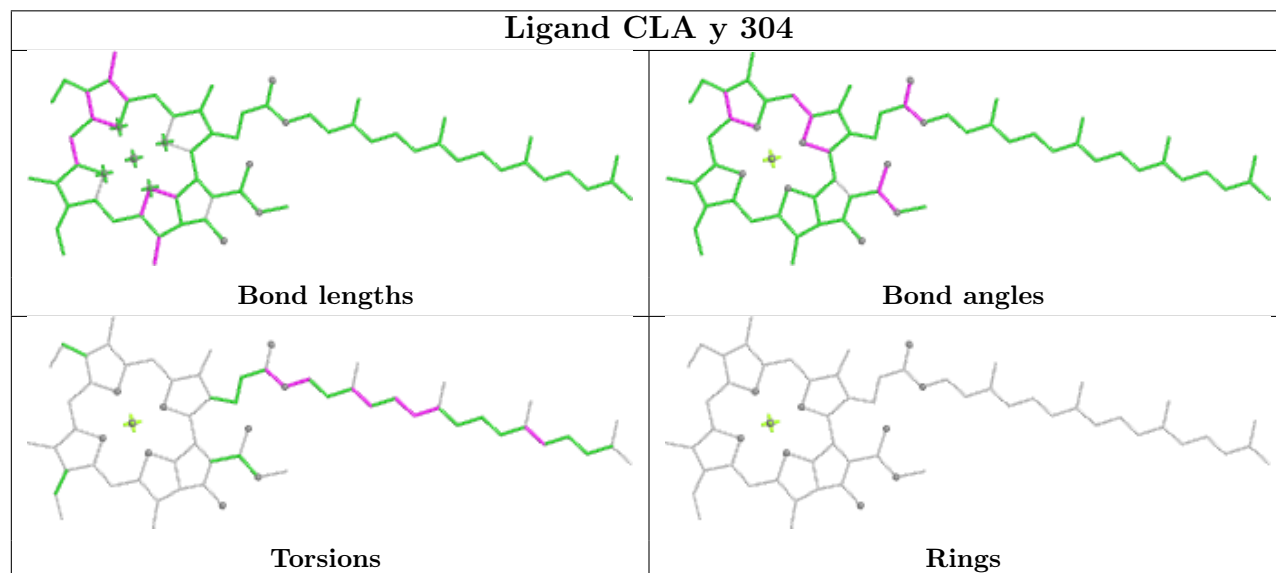
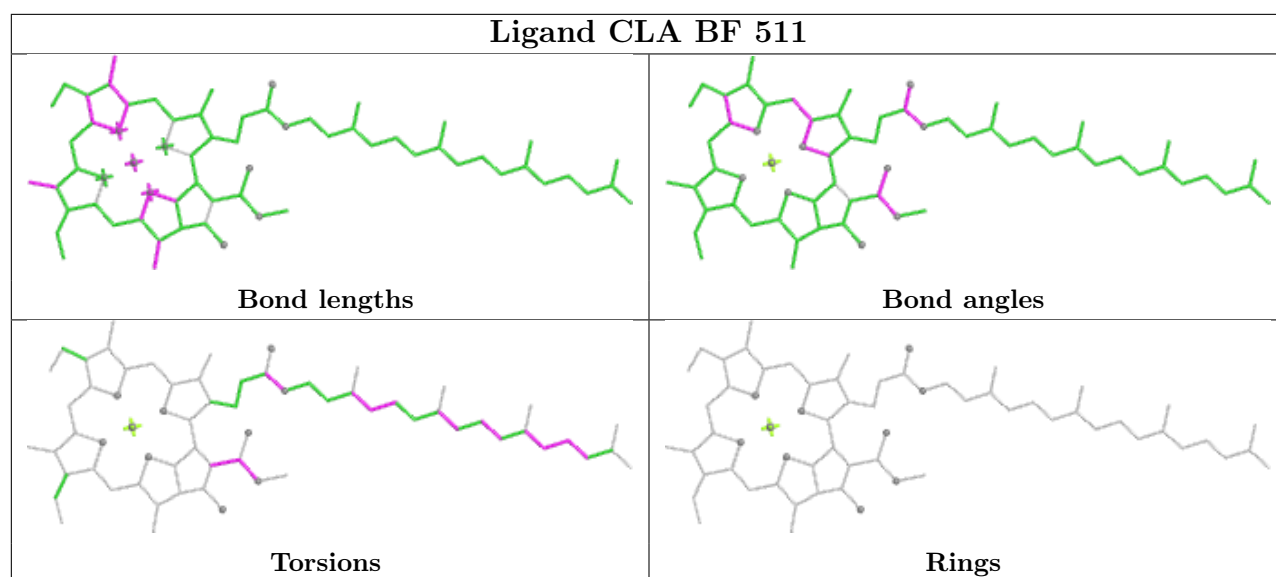


Ligand CLA 0 611

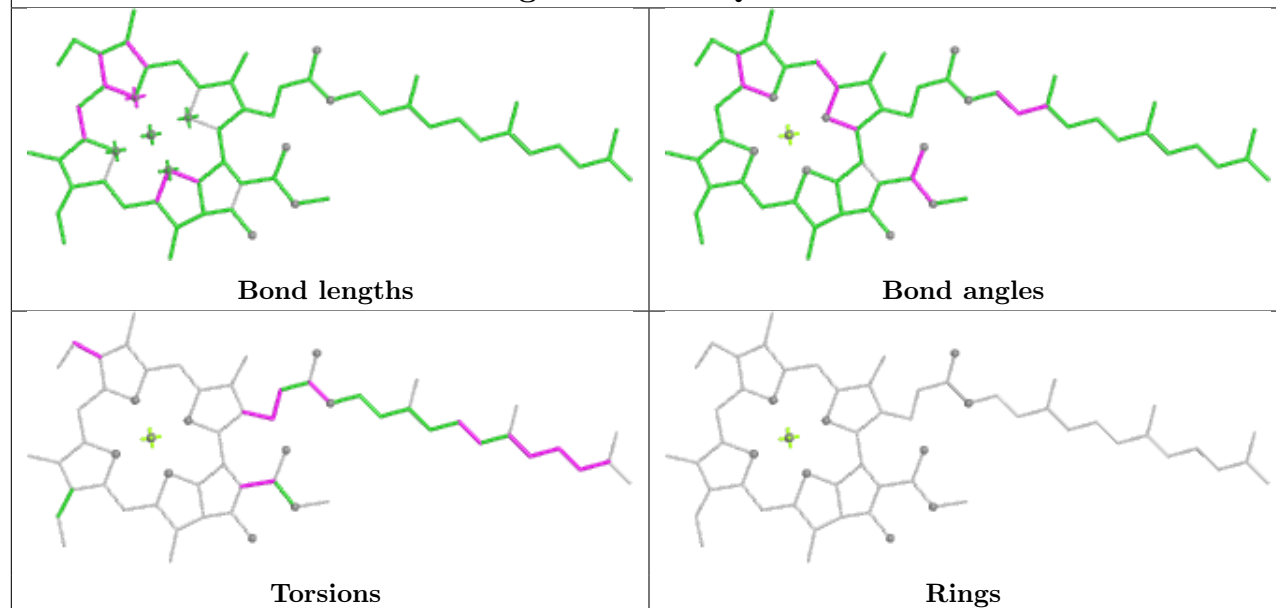


Ligand CHL Y 306

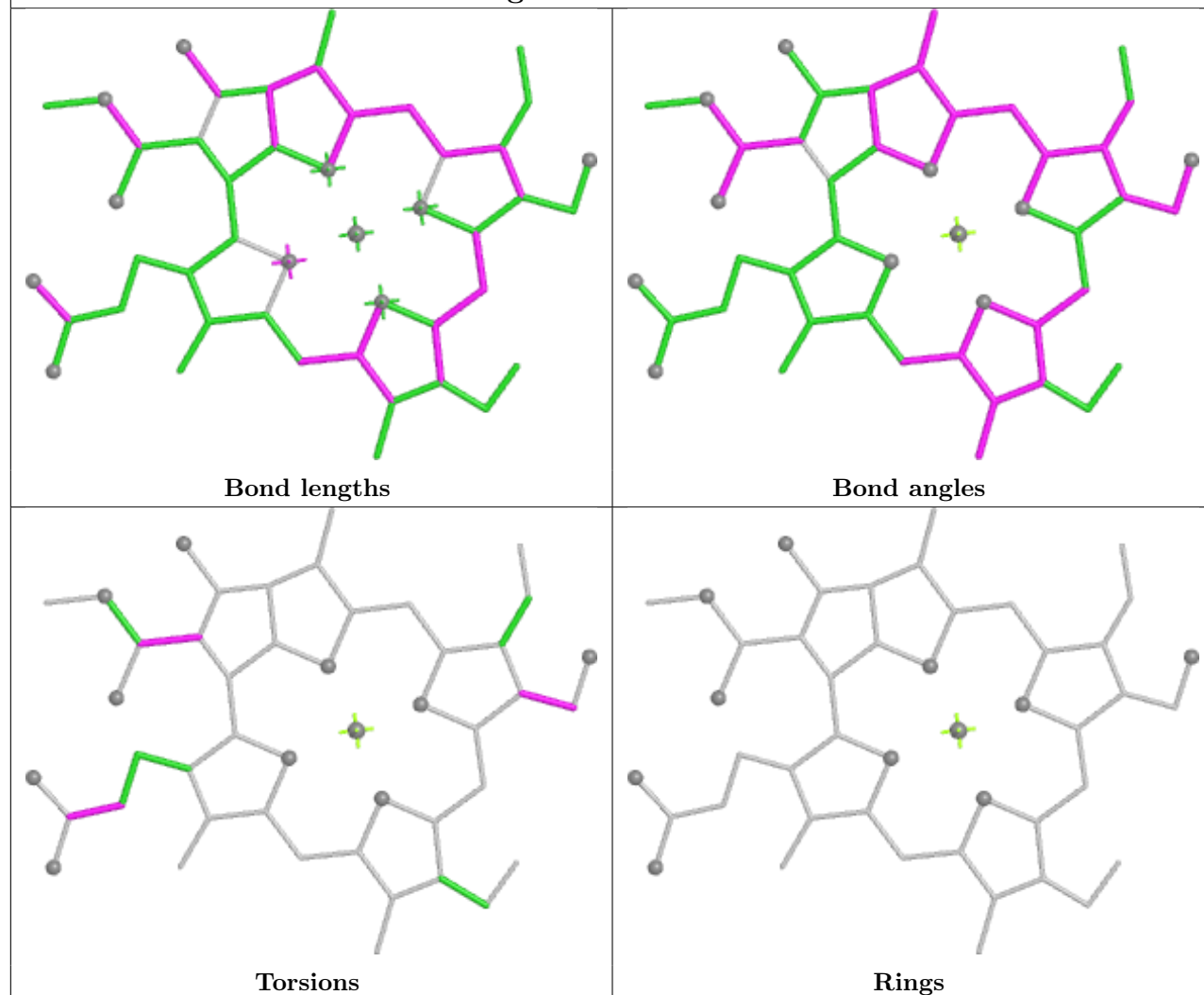


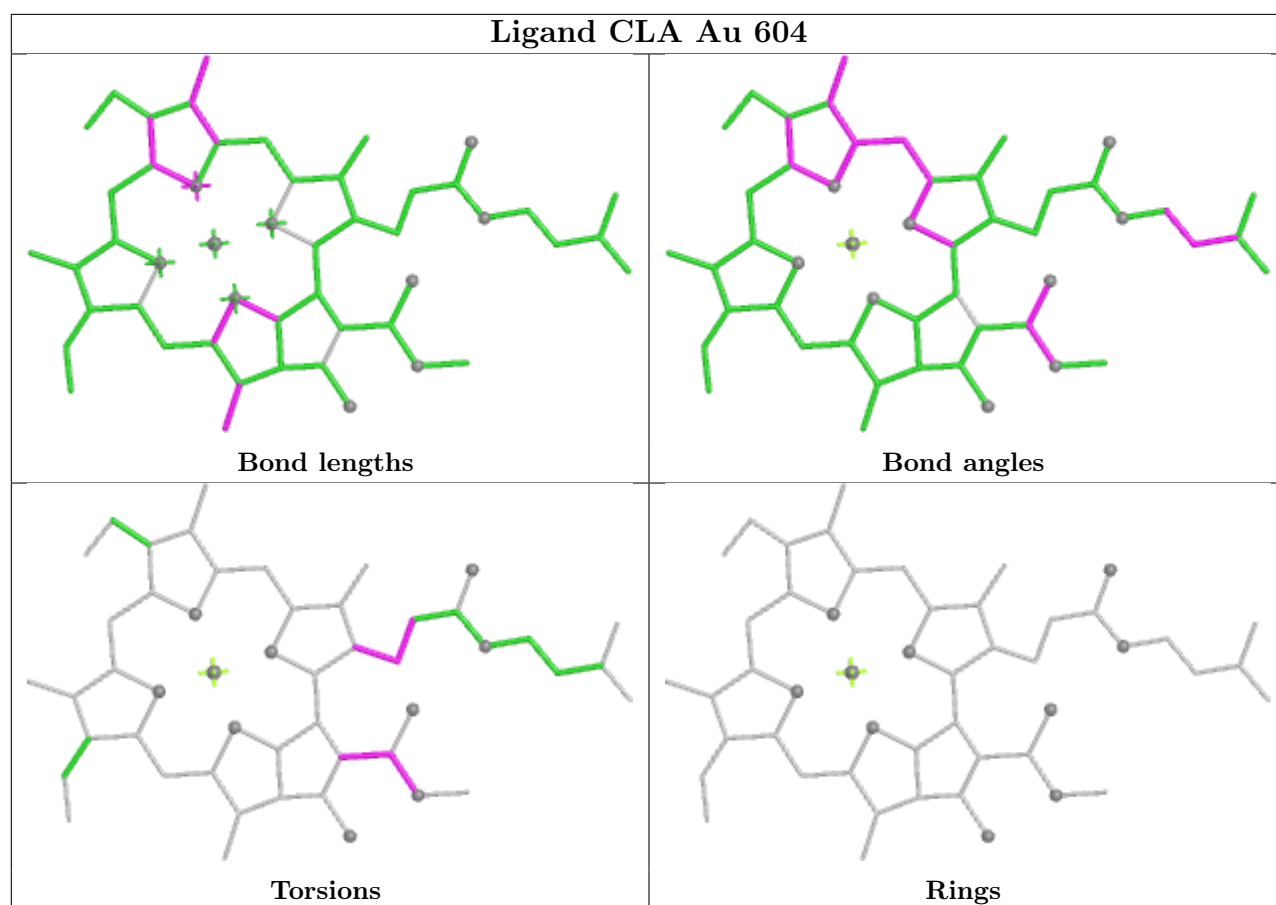


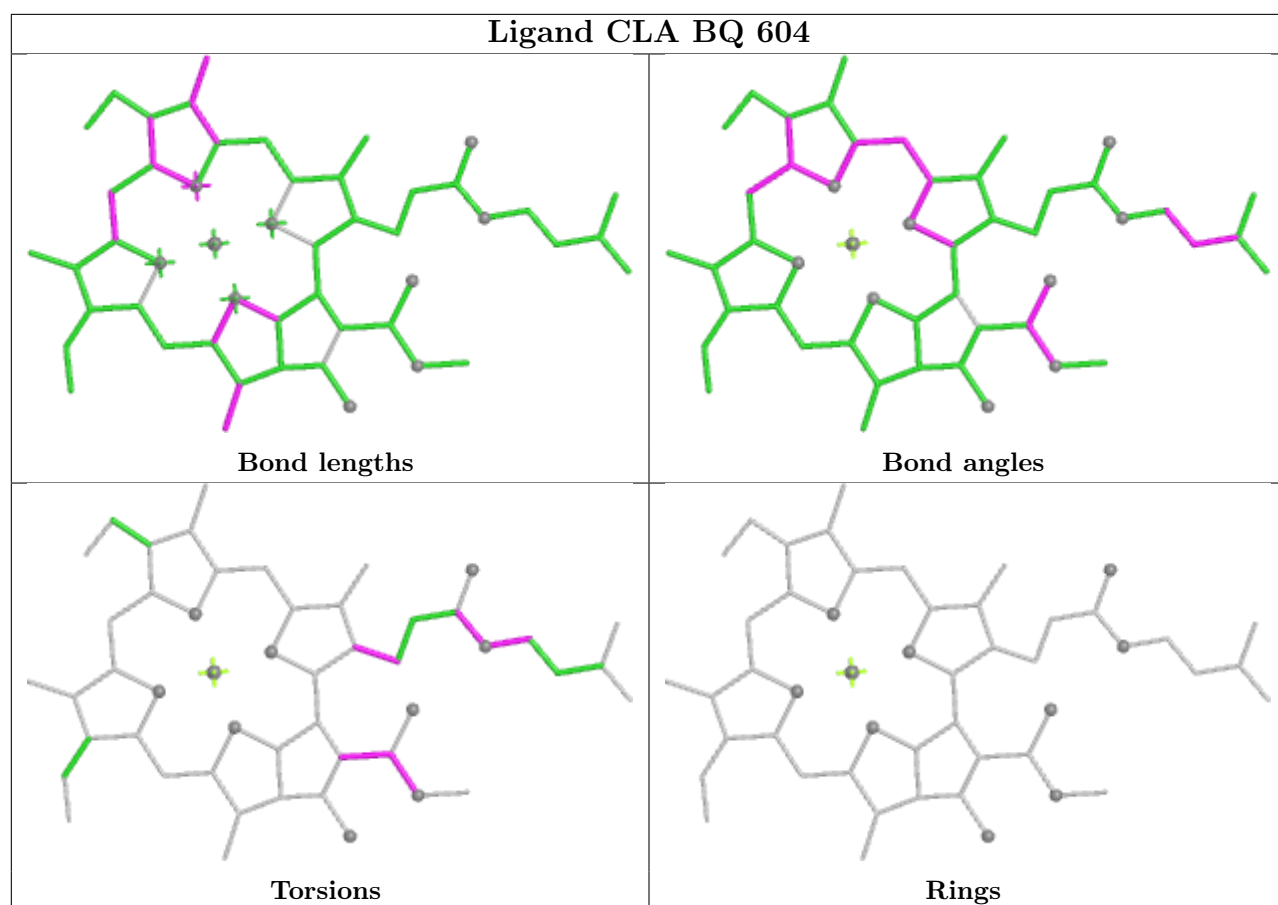
Ligand CLA BQ 611

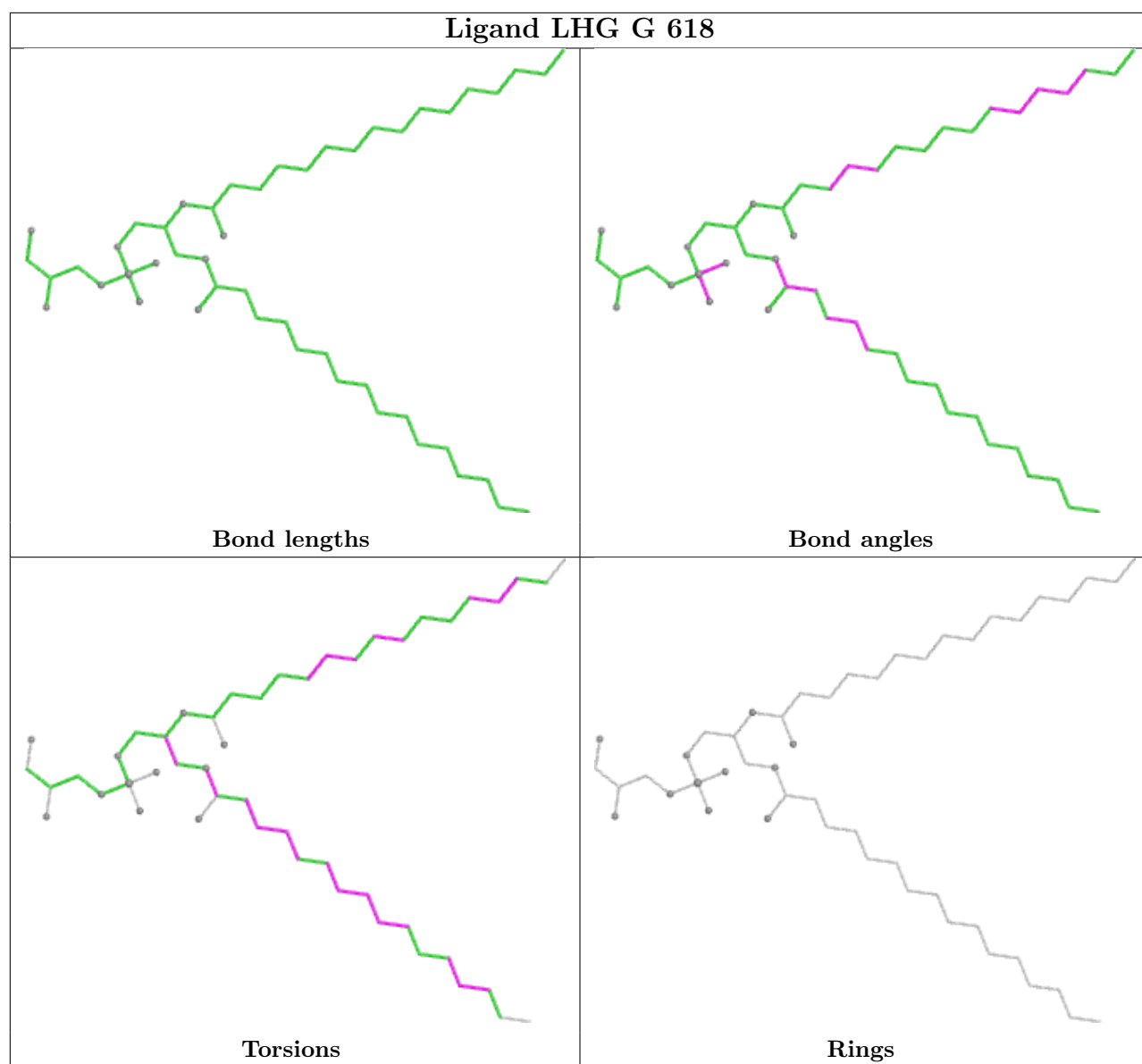


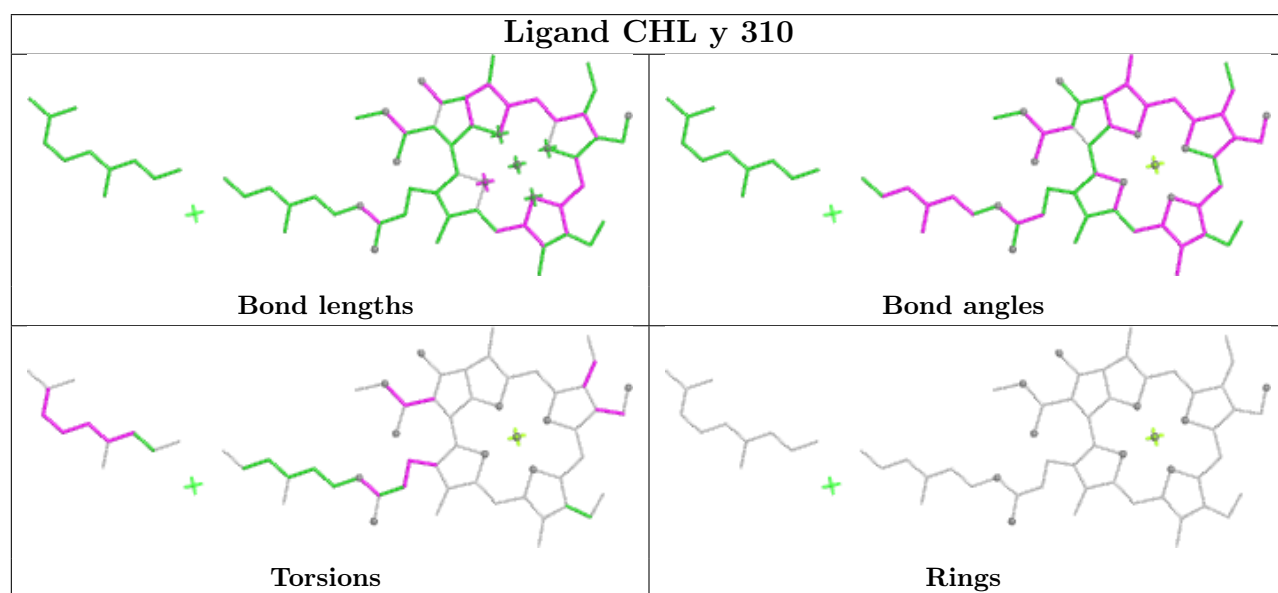
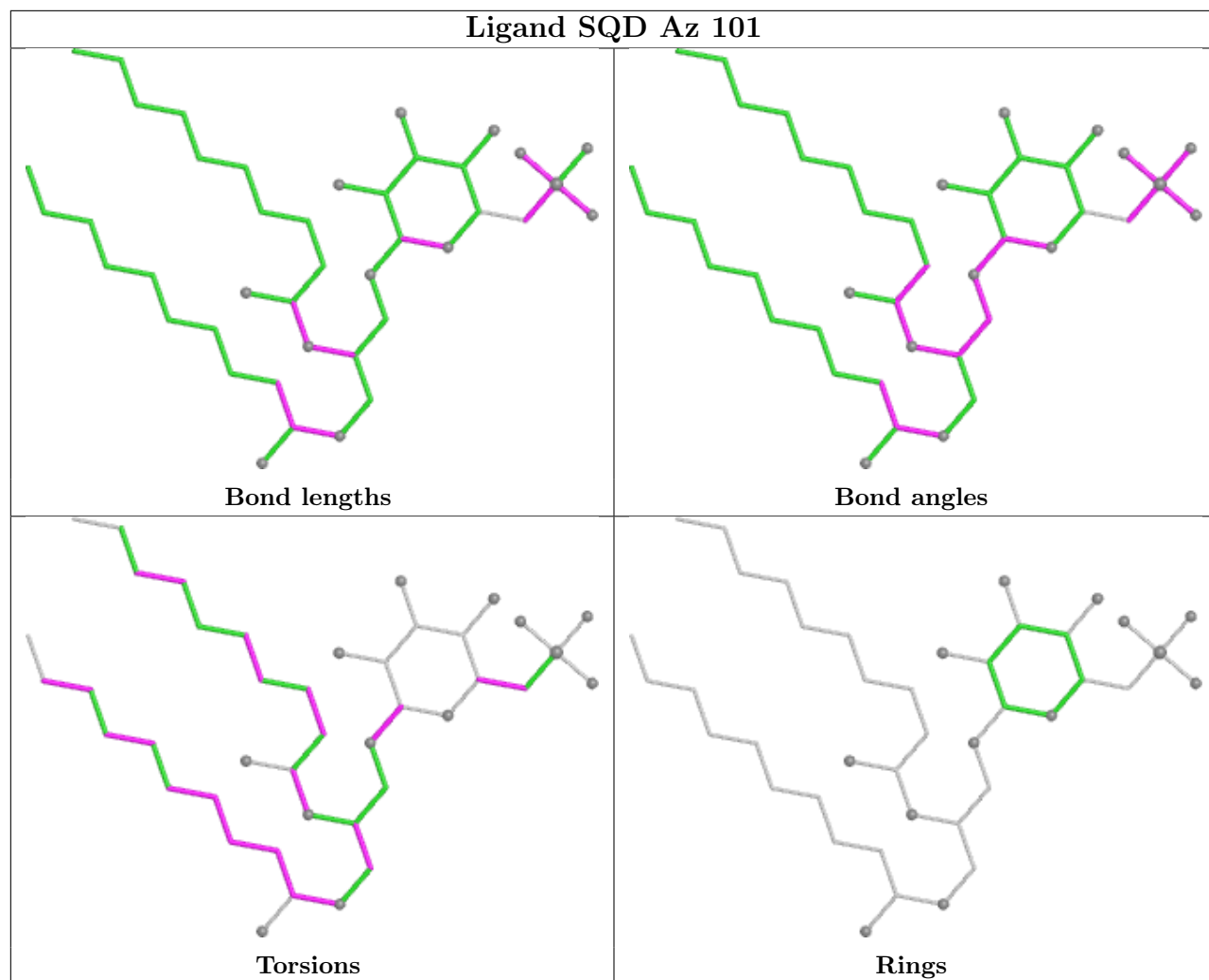
Ligand CHL s 601



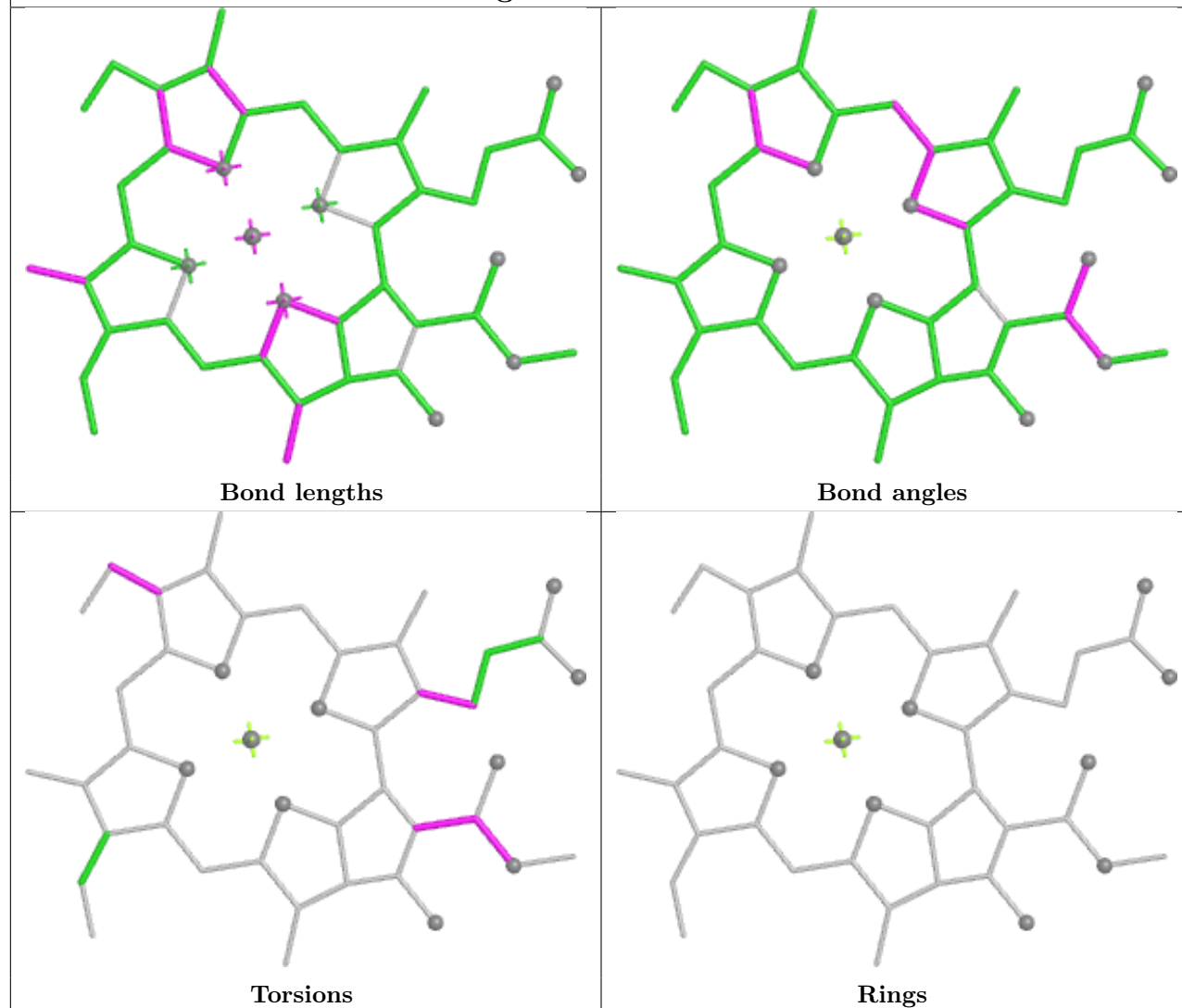




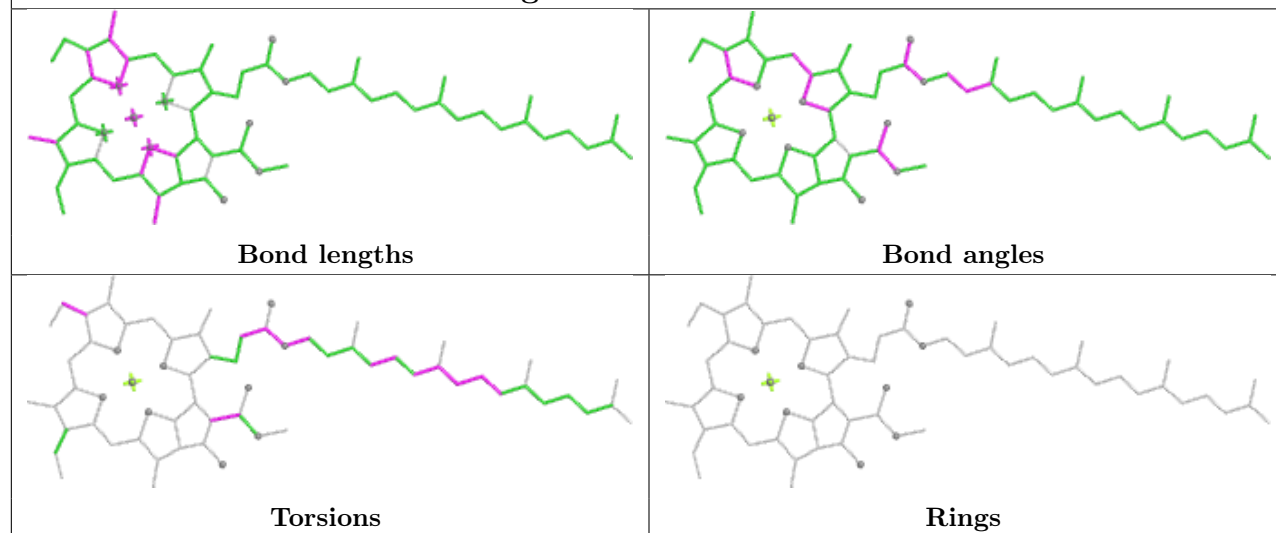




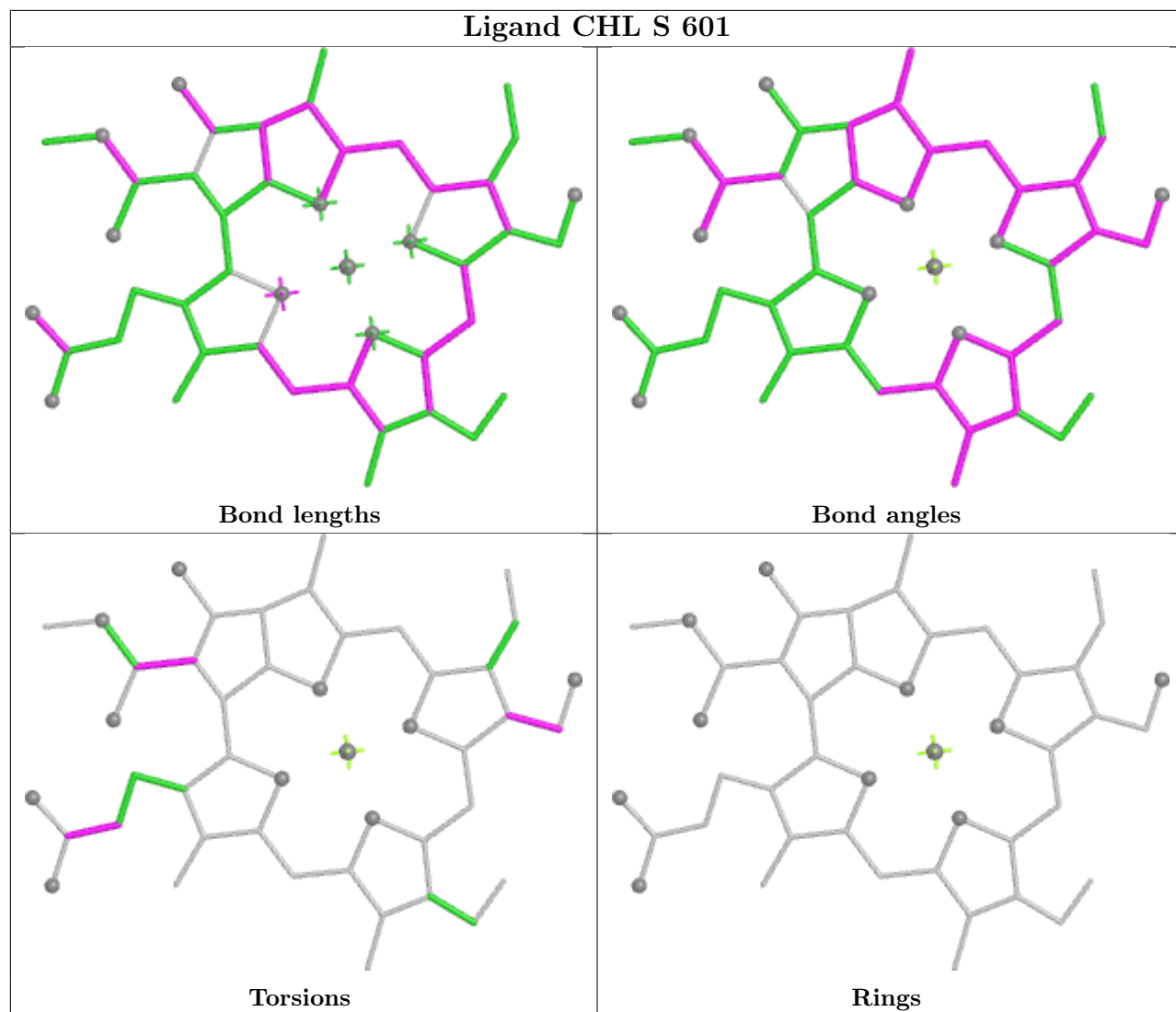
Ligand CLA 8 303



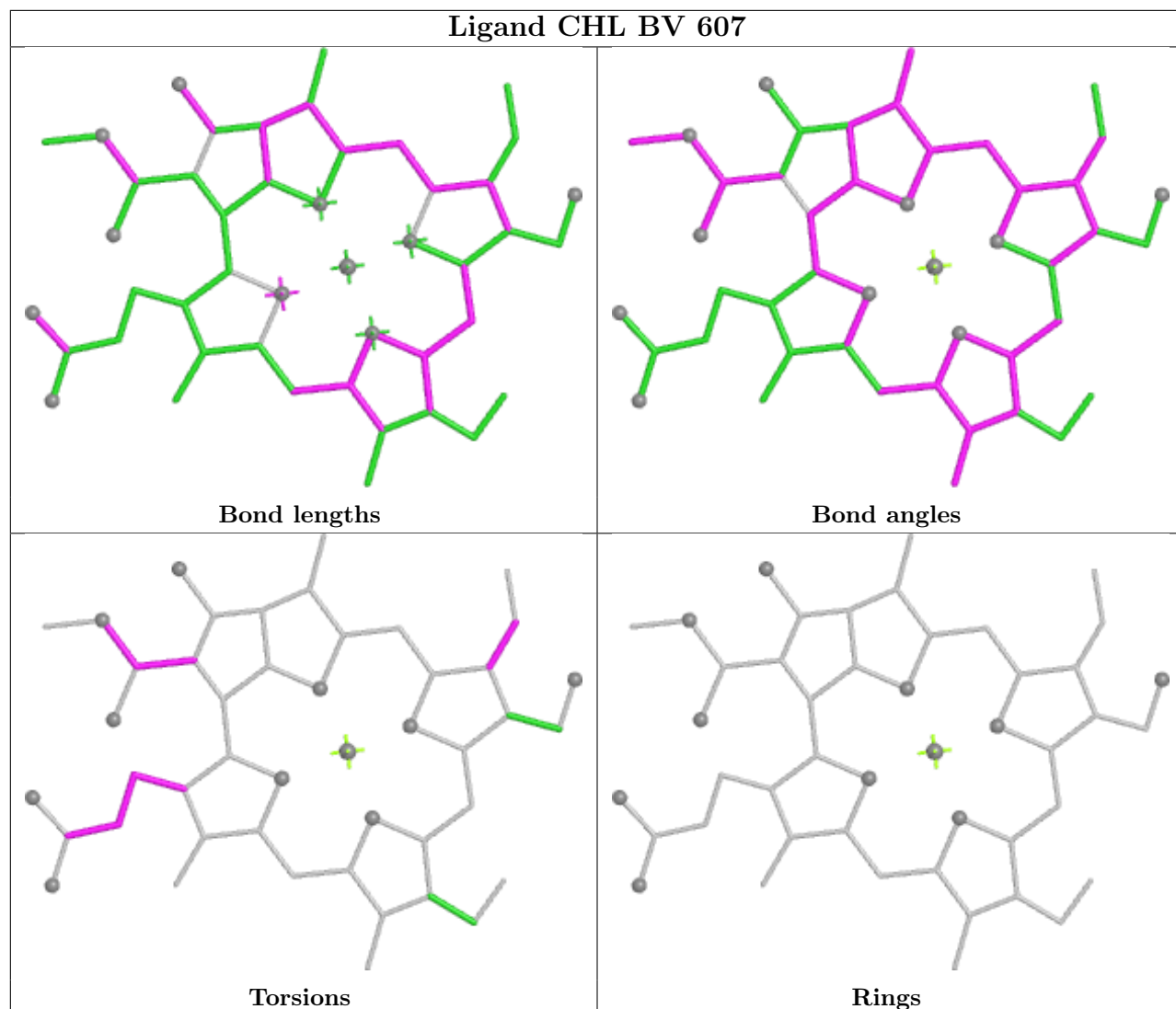
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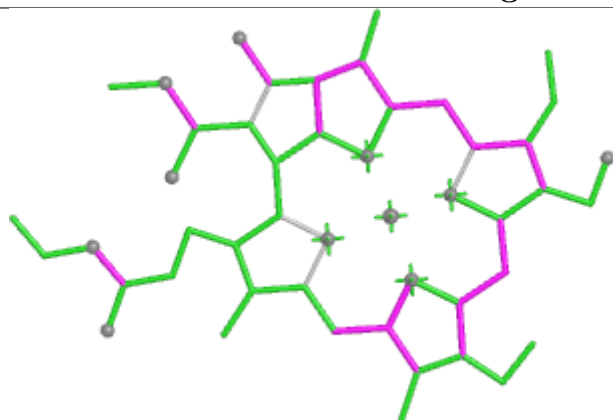
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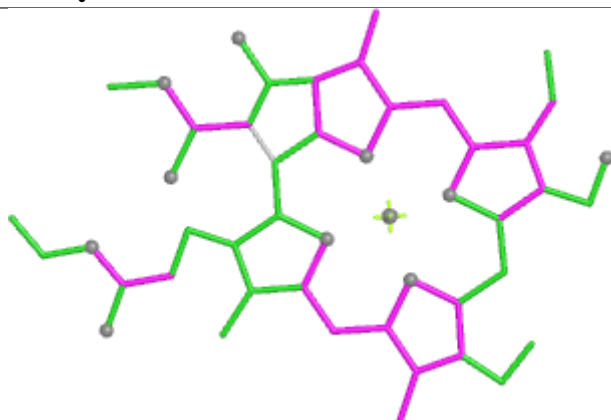
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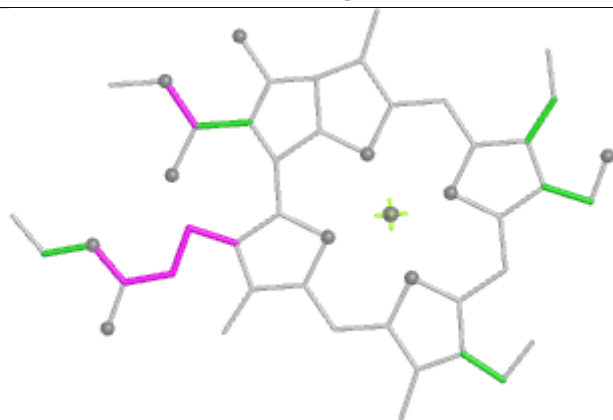
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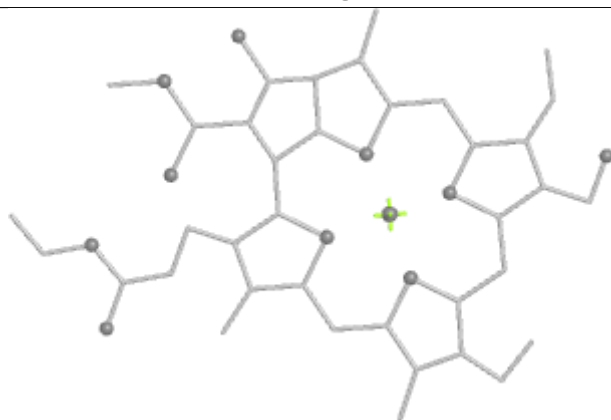
Bond lengths



Bond angles

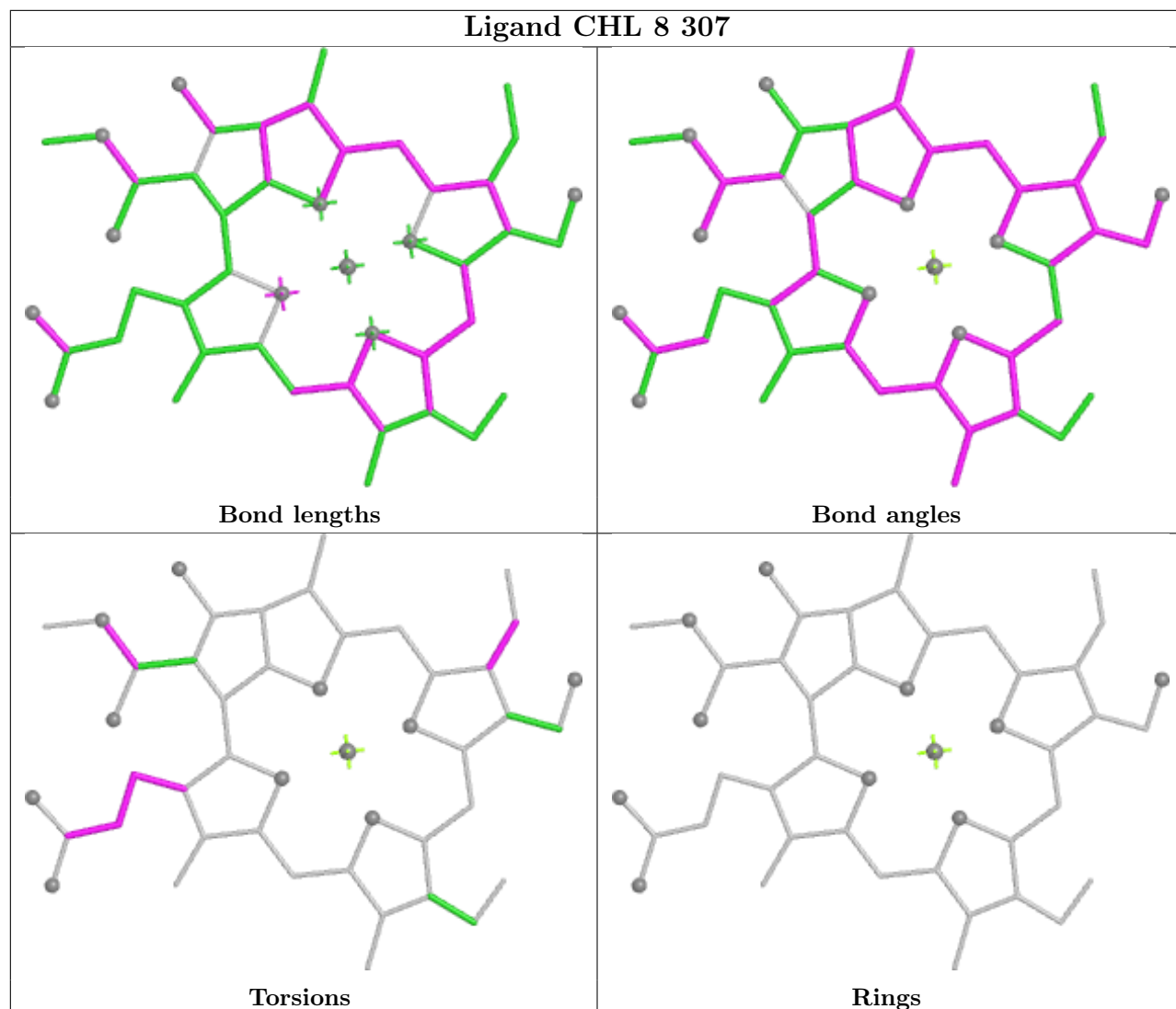


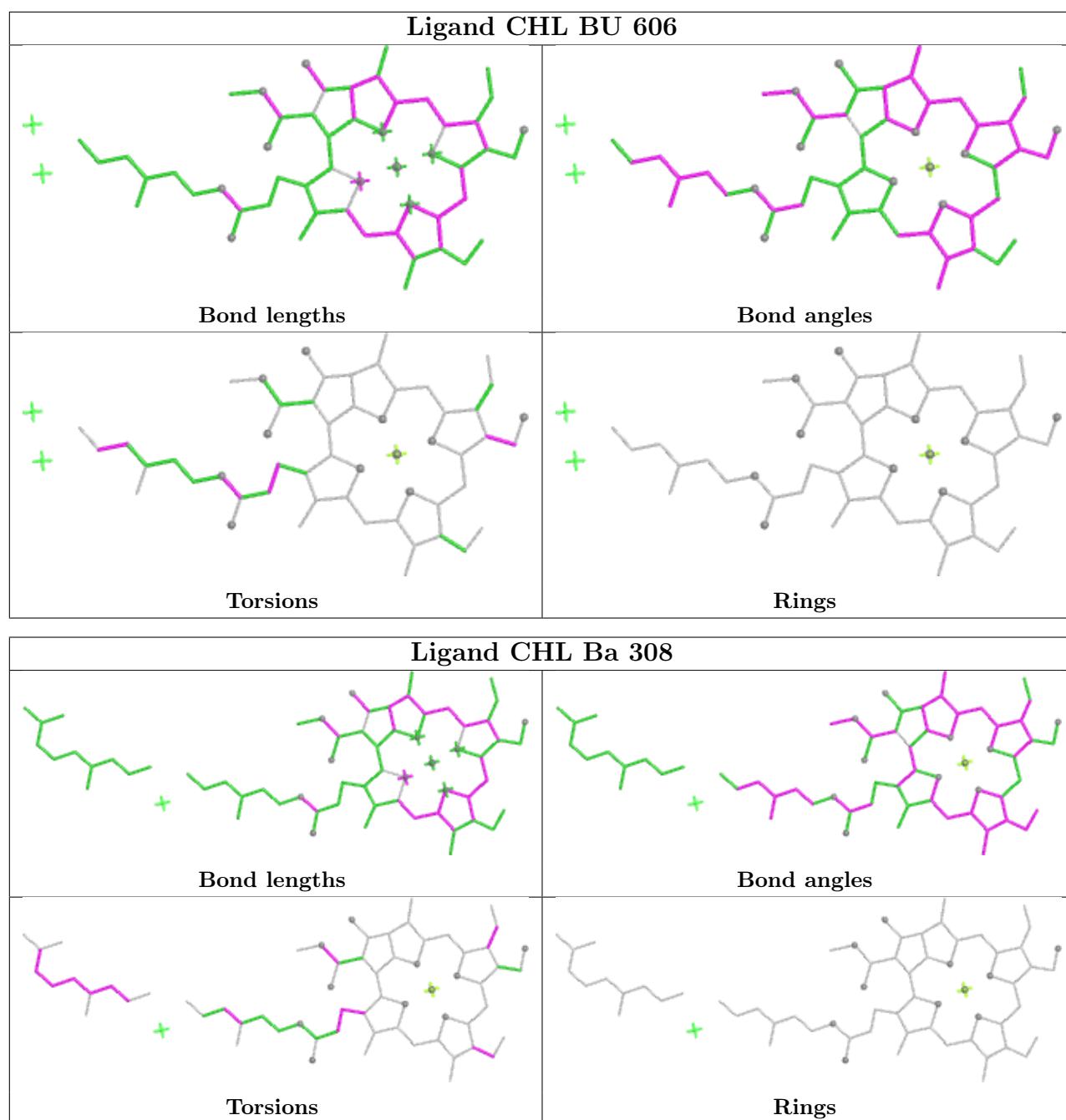
Torsions



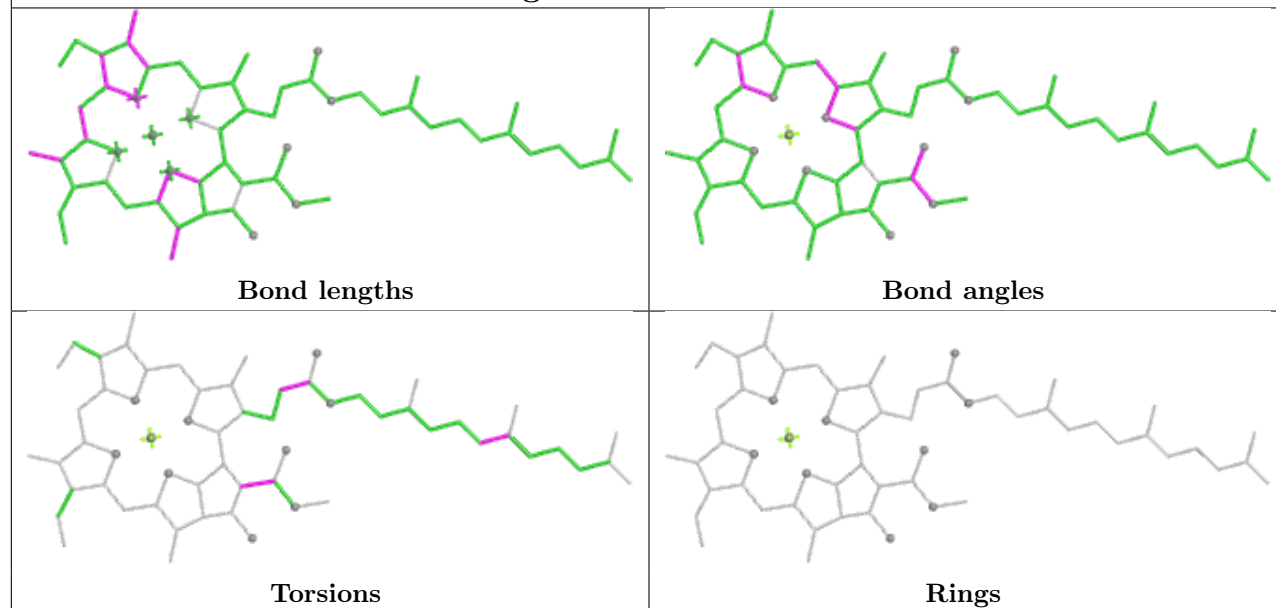
Rings

Ligand CHL 8 307

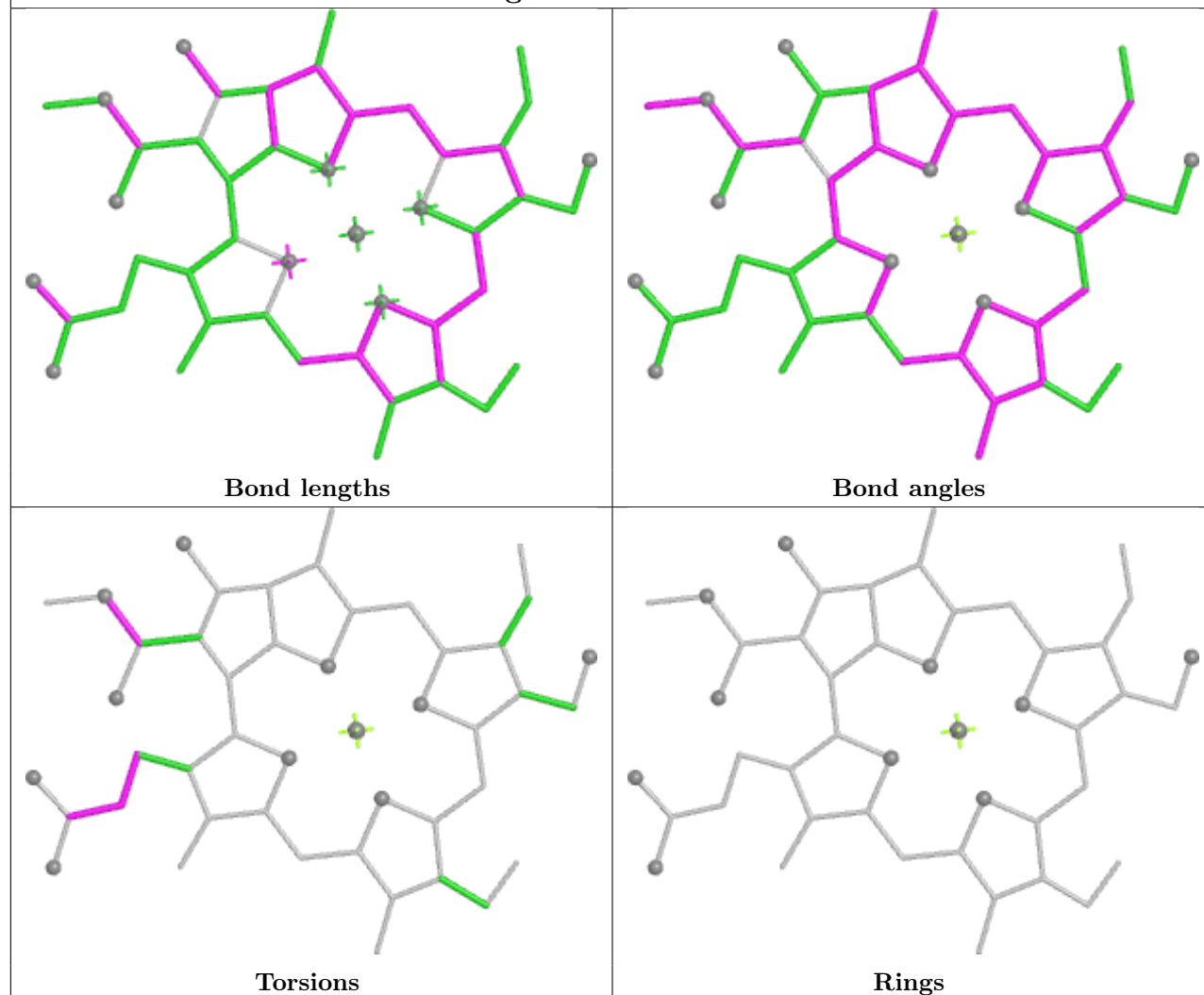




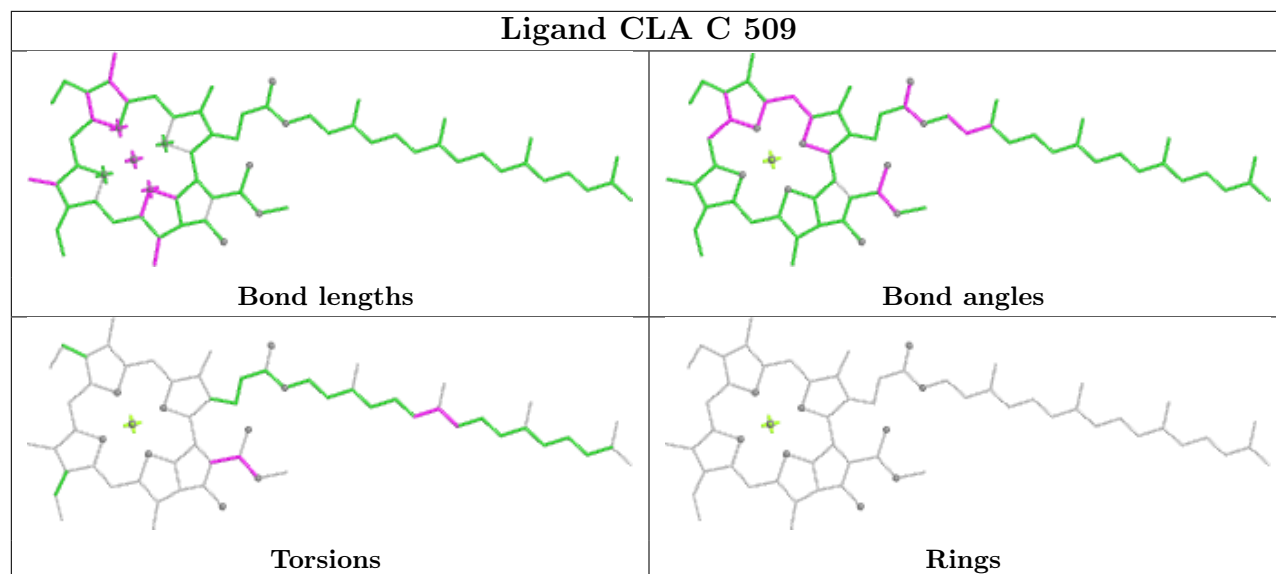
Ligand CLA A2 612



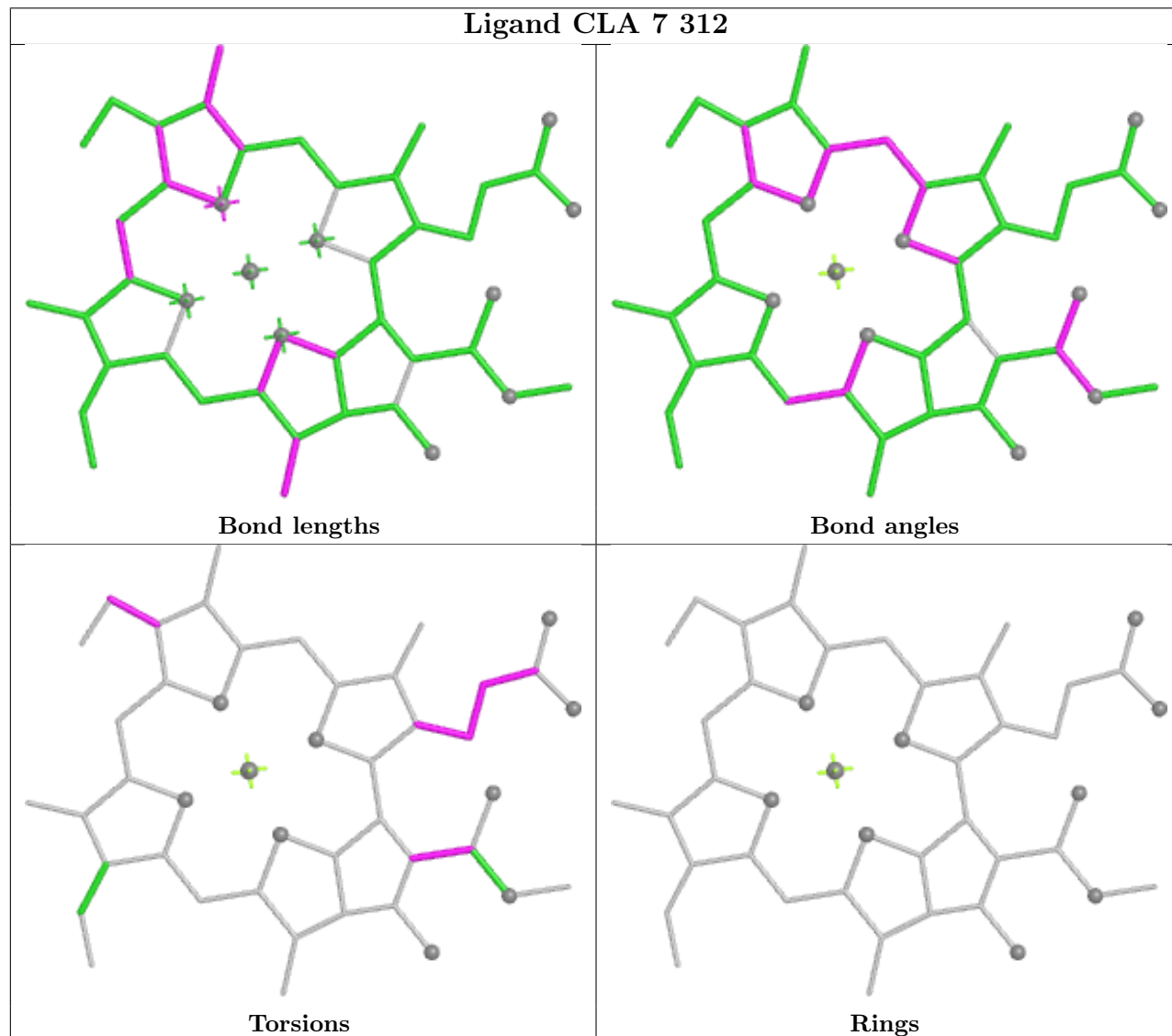
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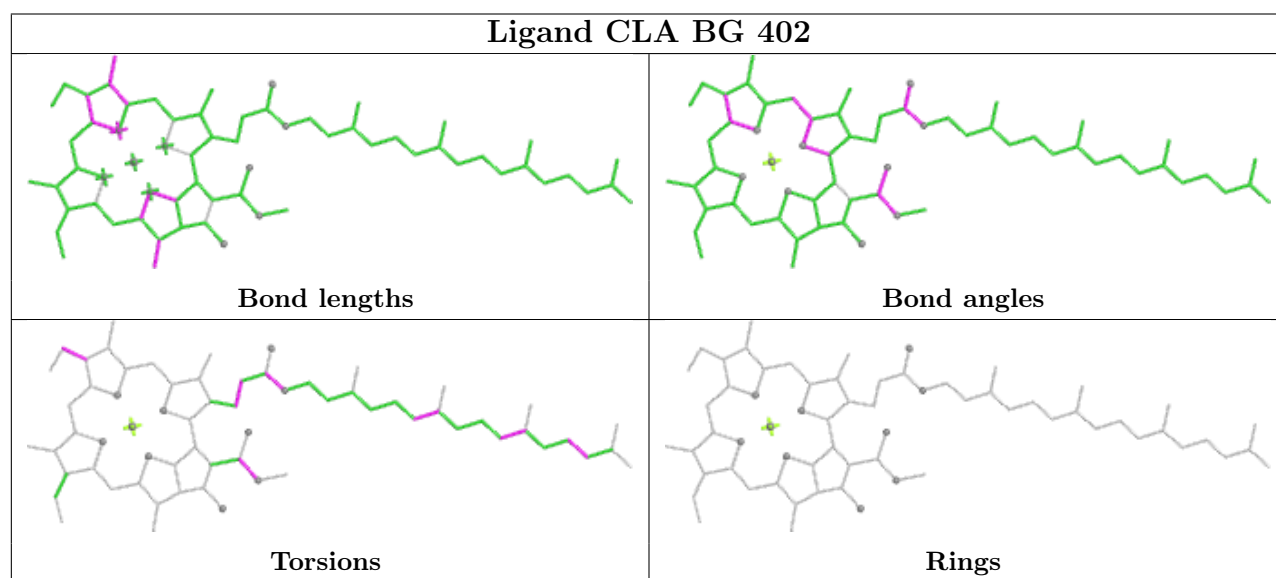
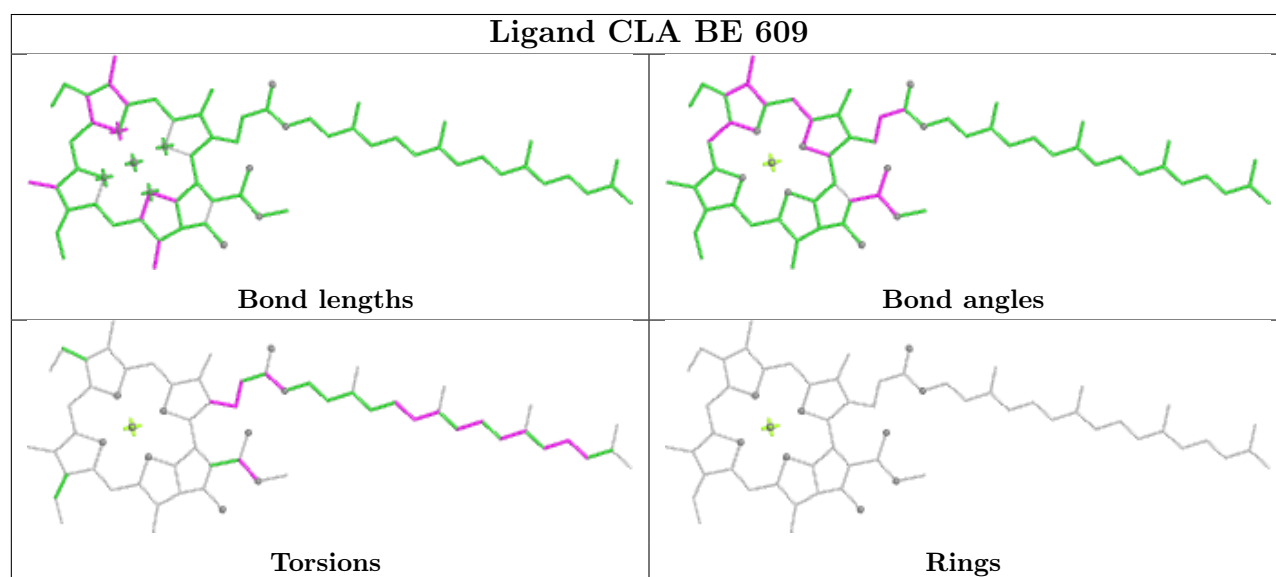
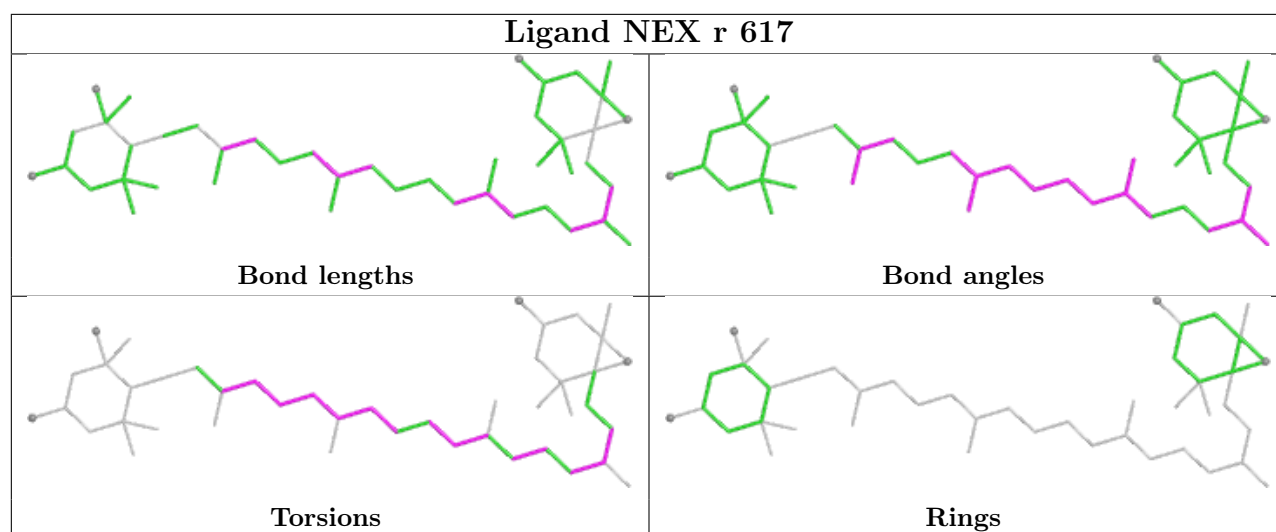


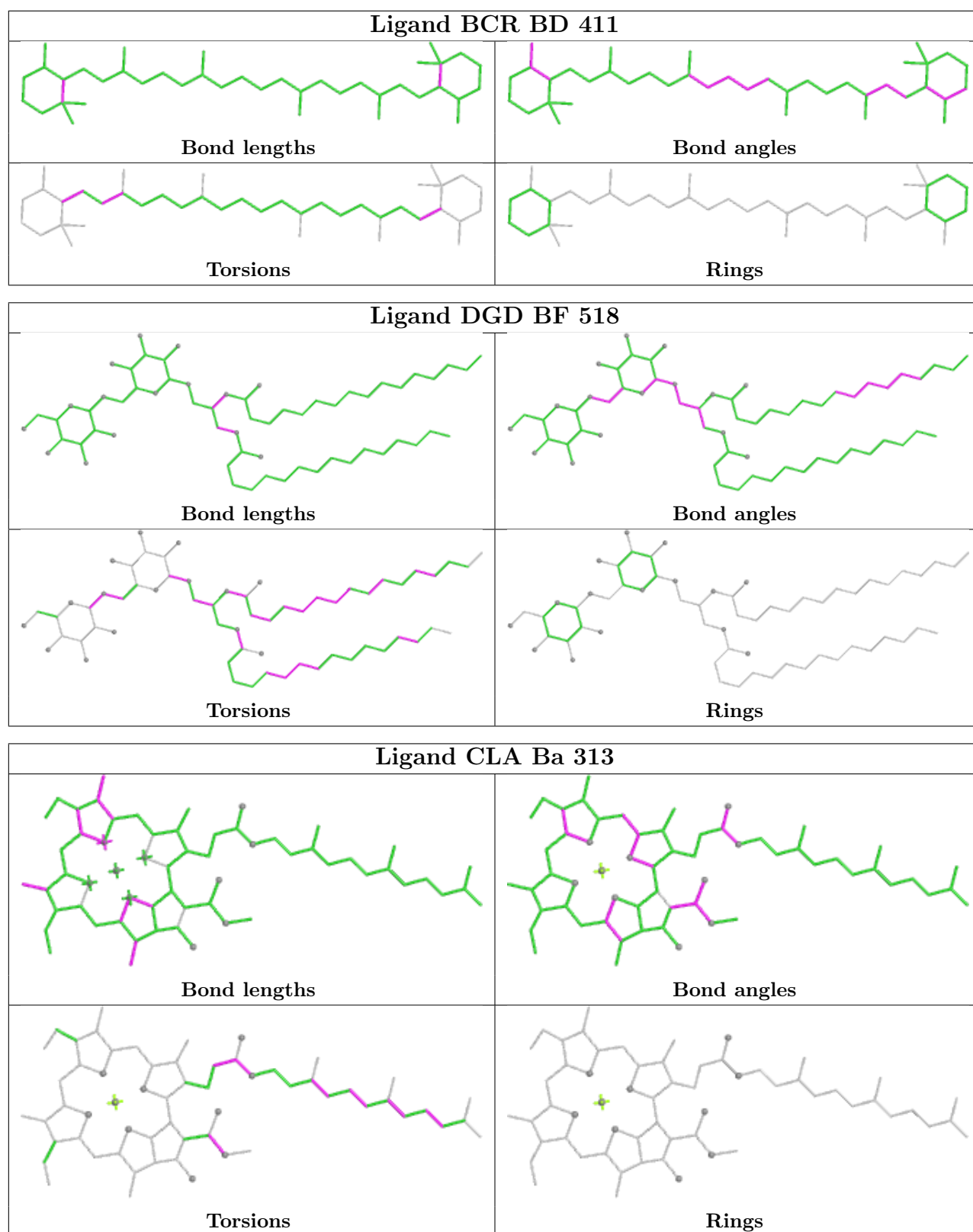
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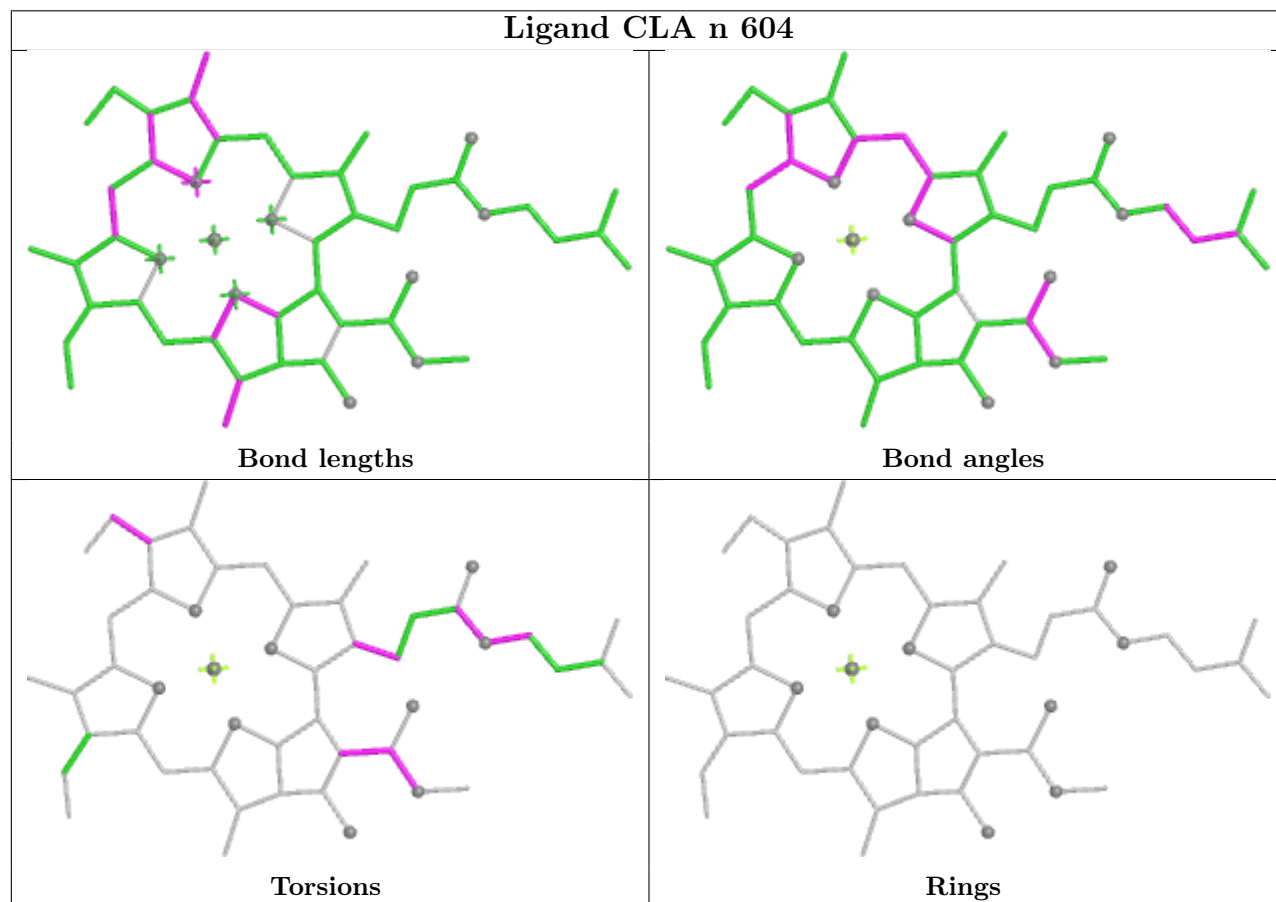
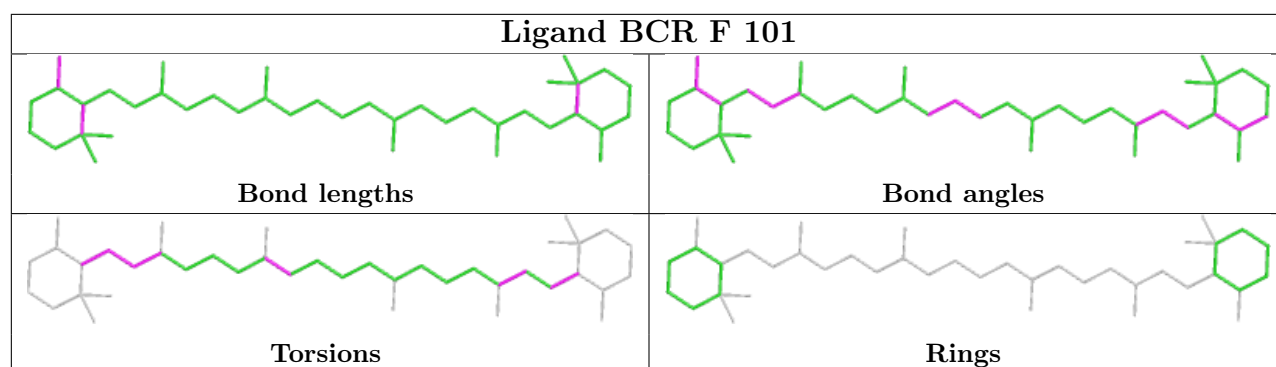


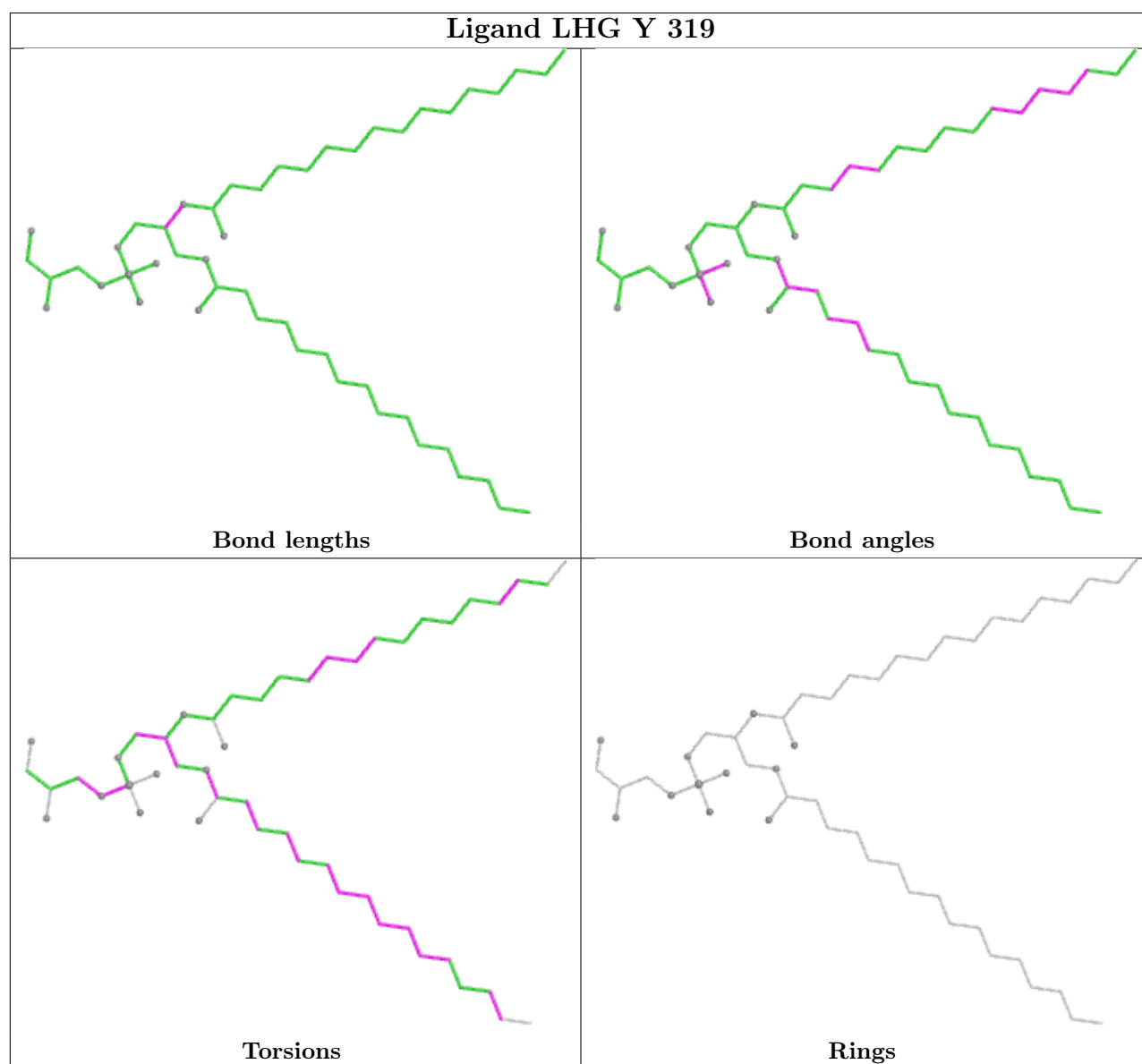
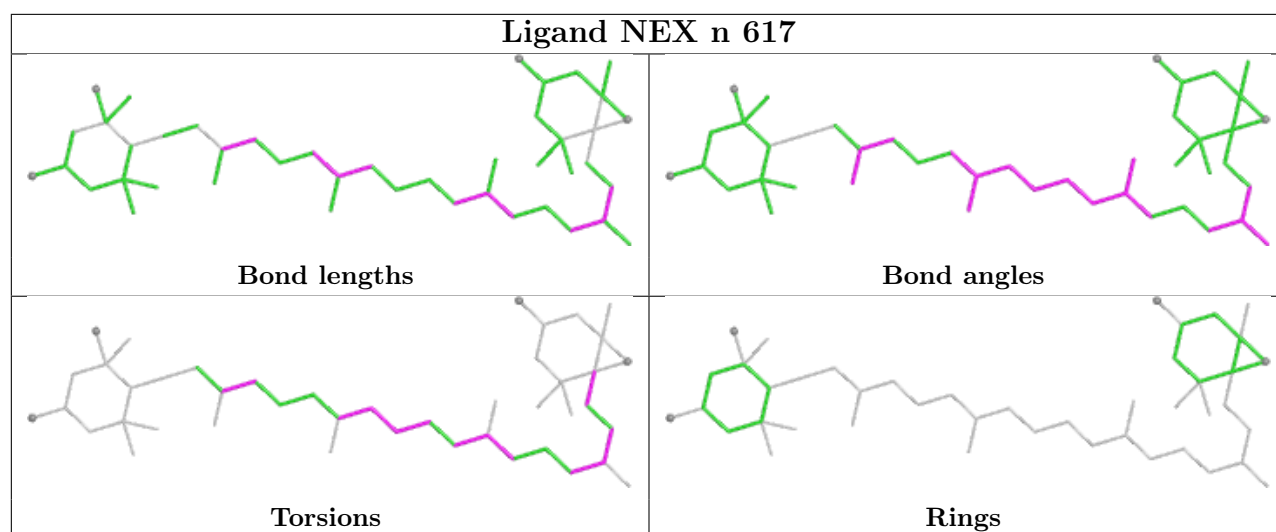
Ligand CLA 7 312

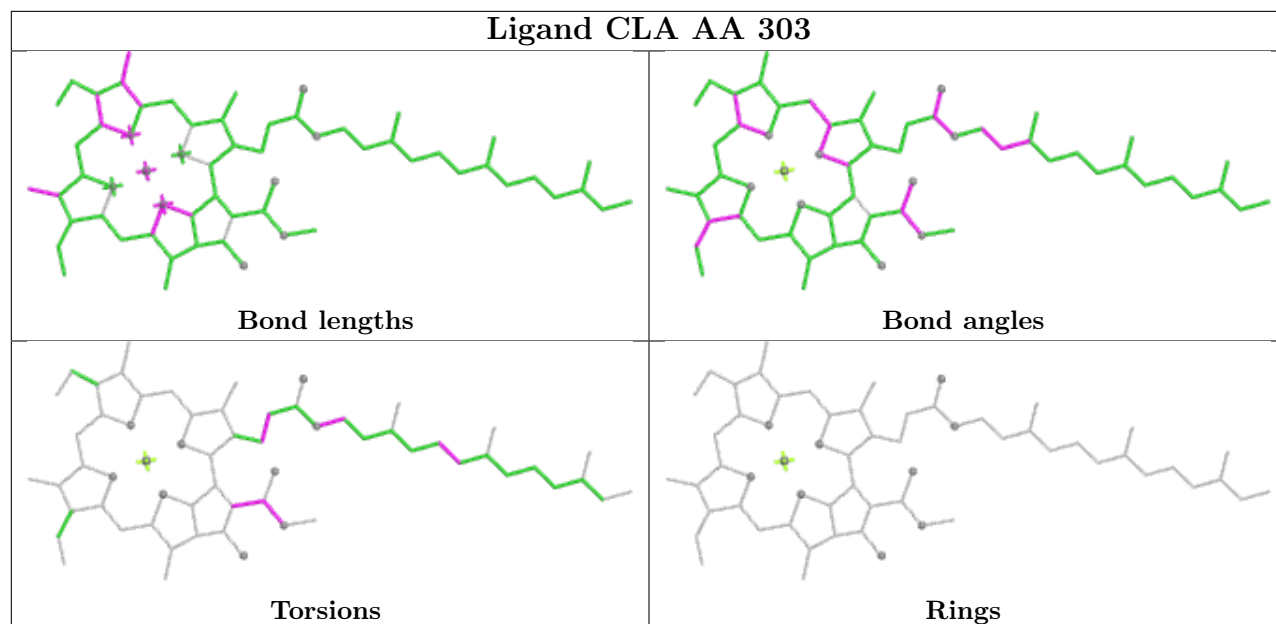
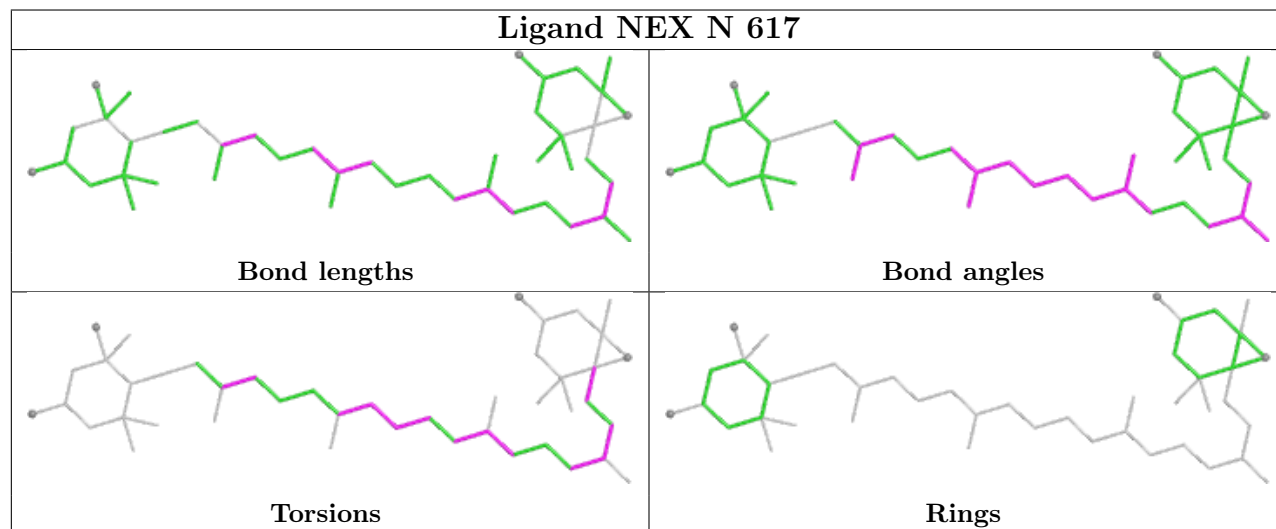
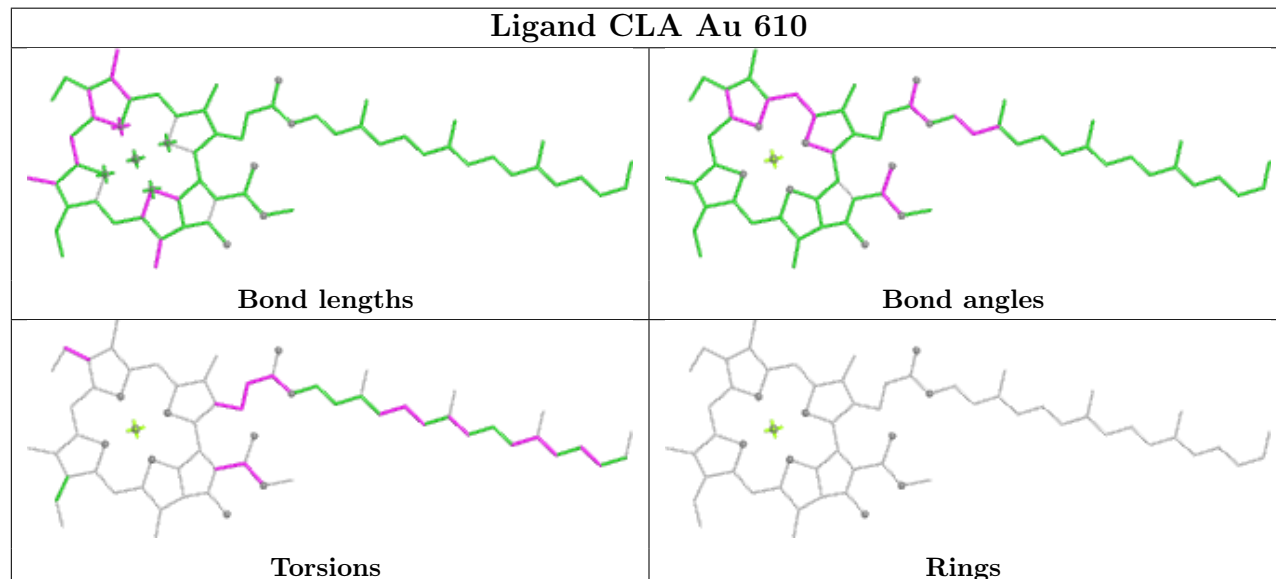


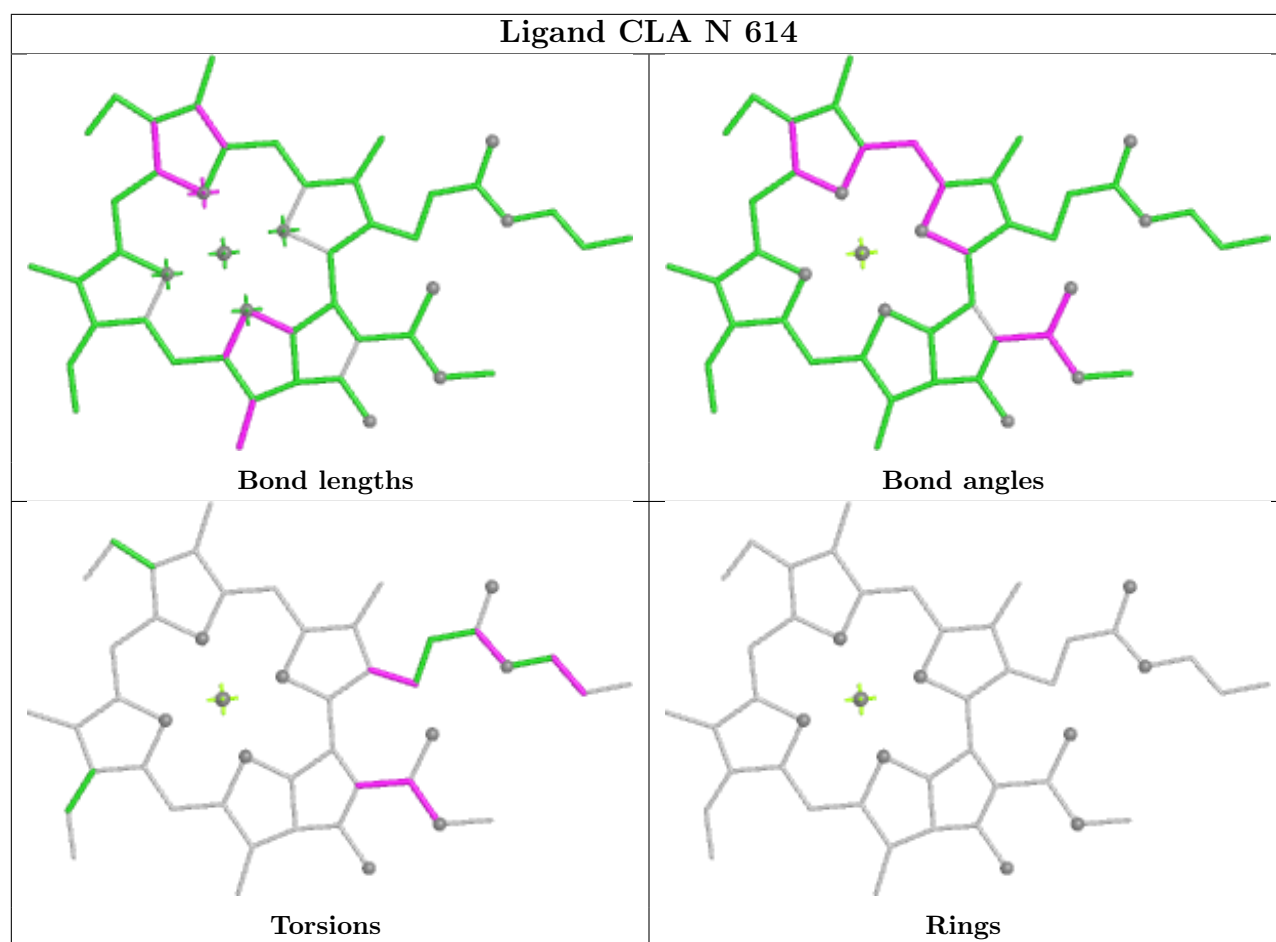




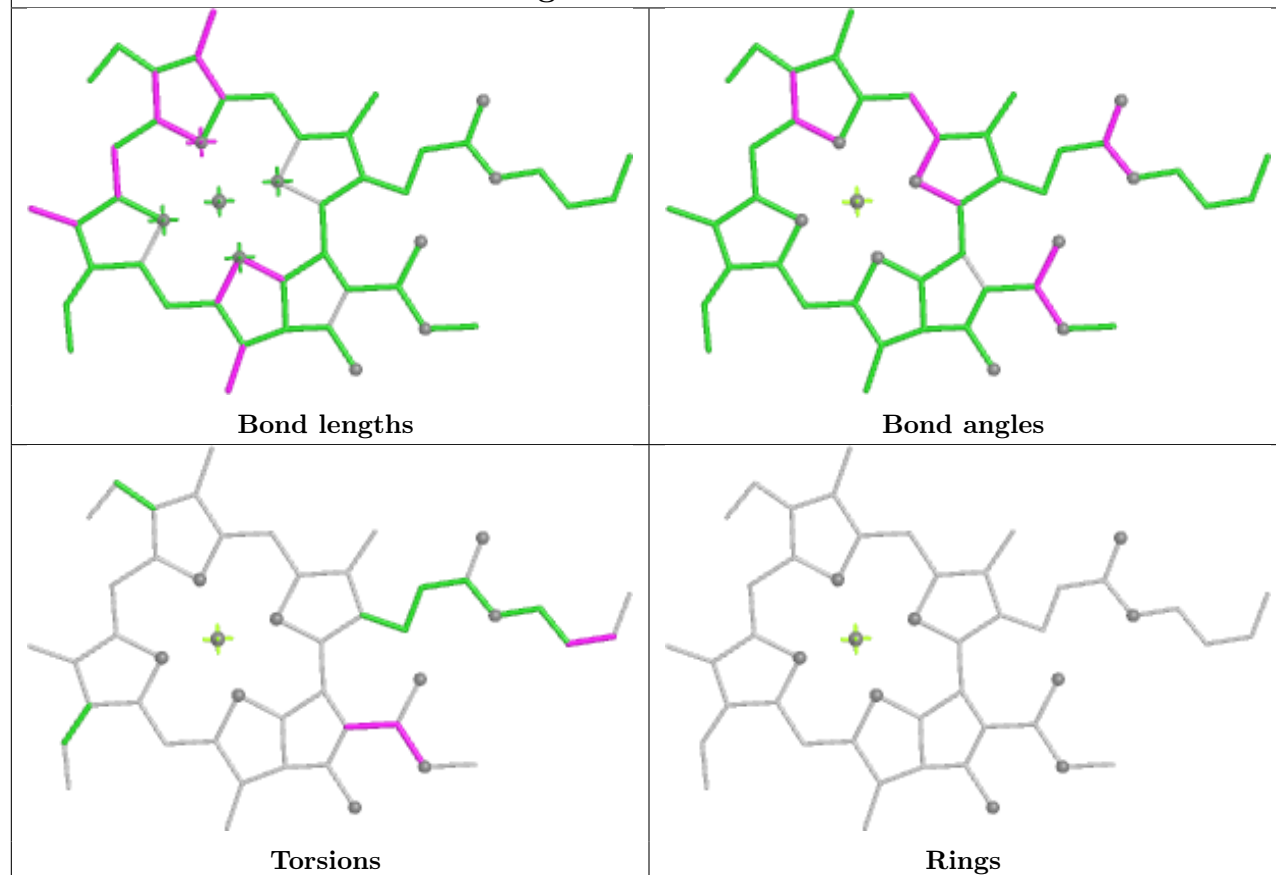




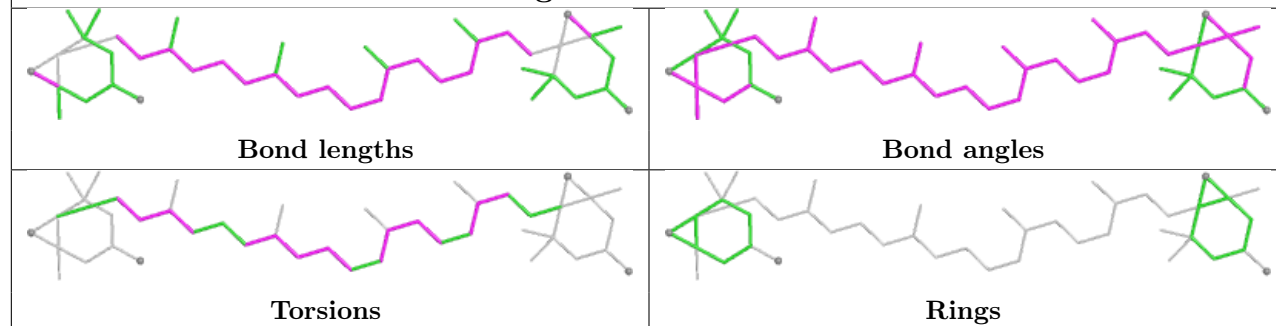
Ligand CLA AA 303**Ligand NEX N 617****Ligand CLA Au 610**

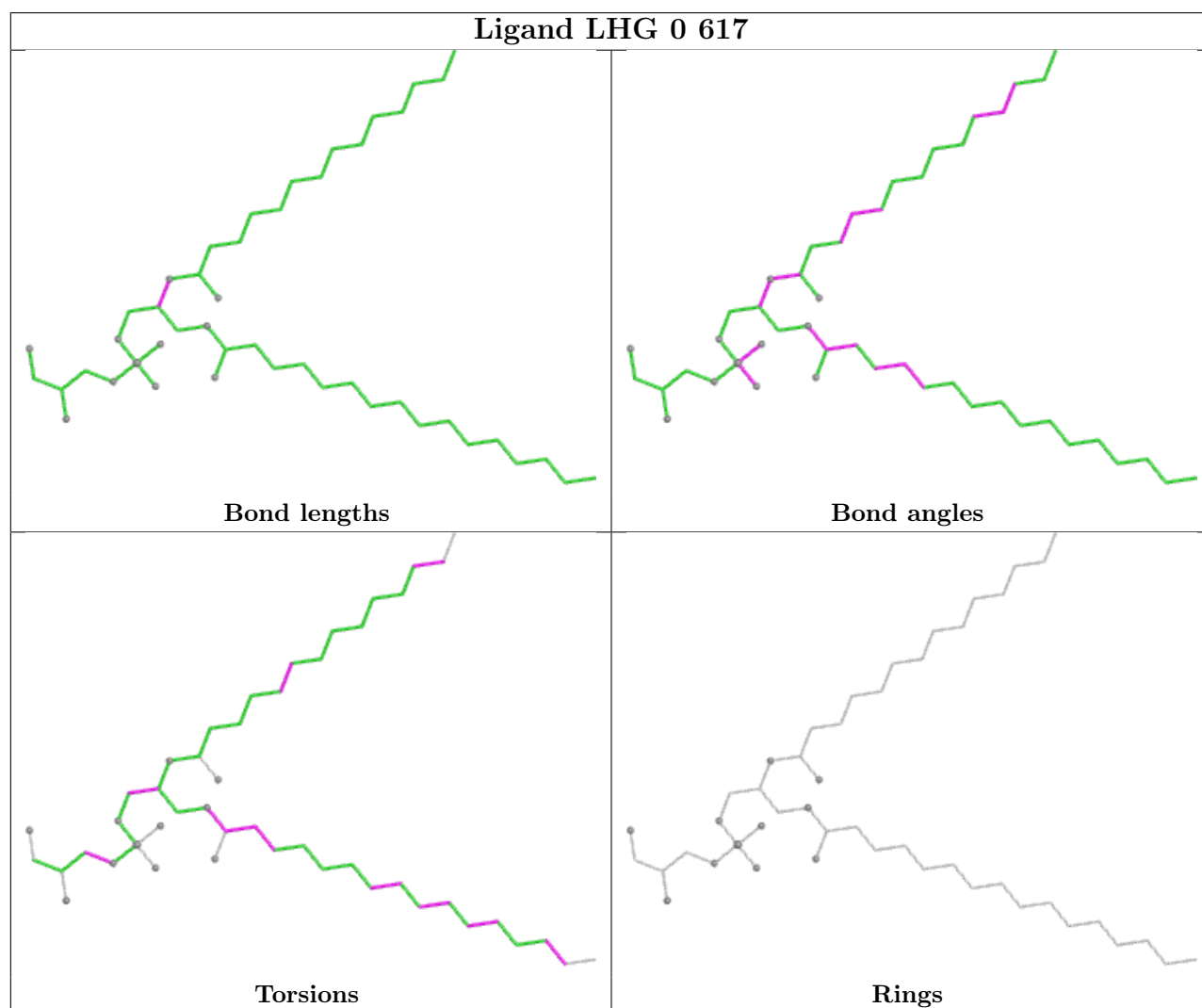
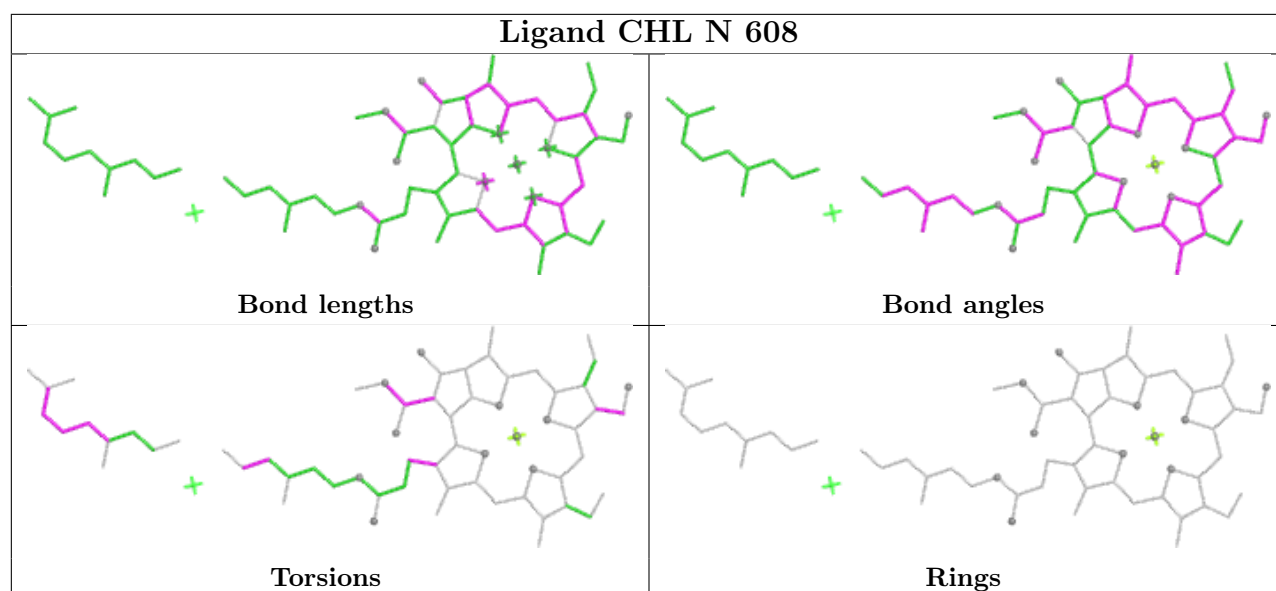


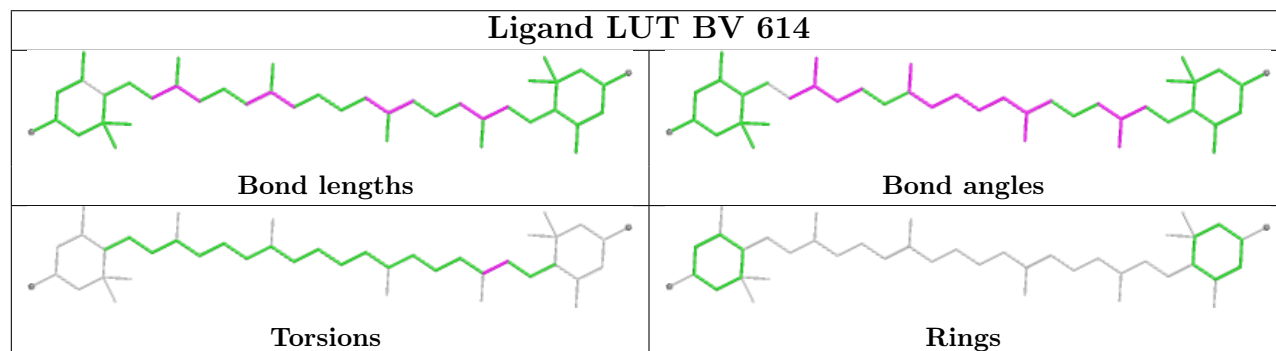
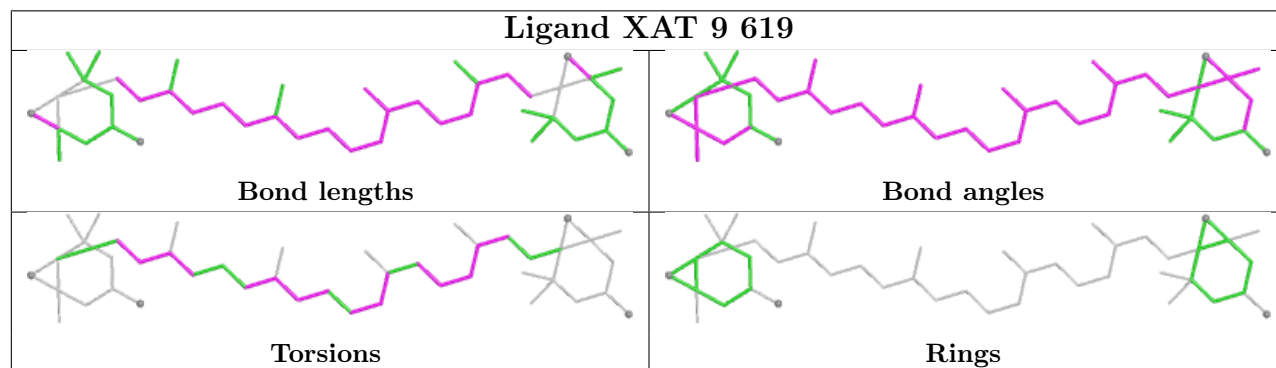
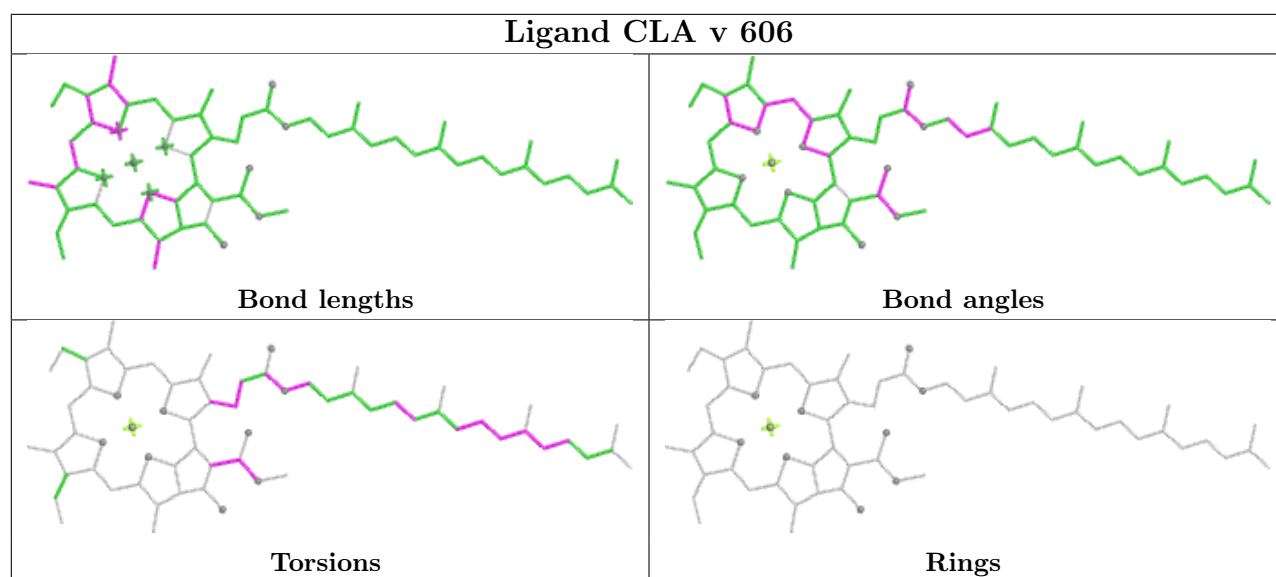
Ligand CLA s 611



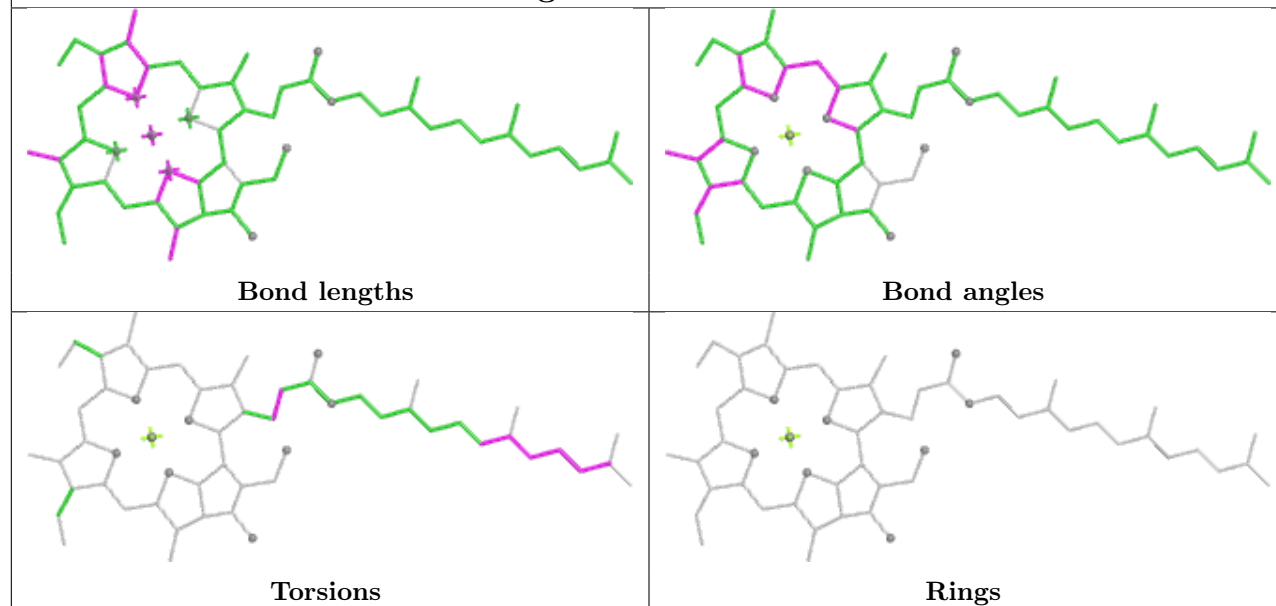
Ligand XAT 5 619



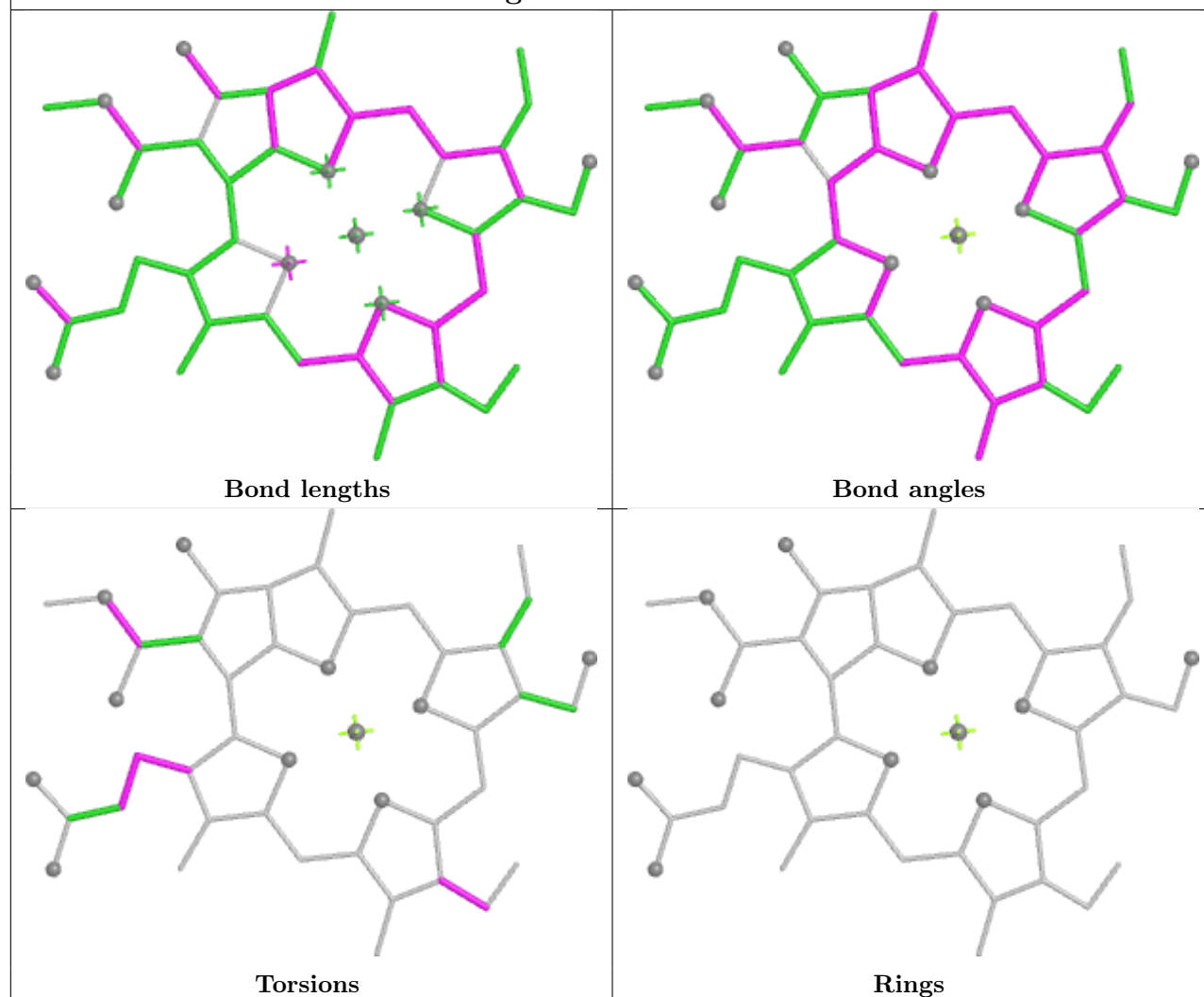


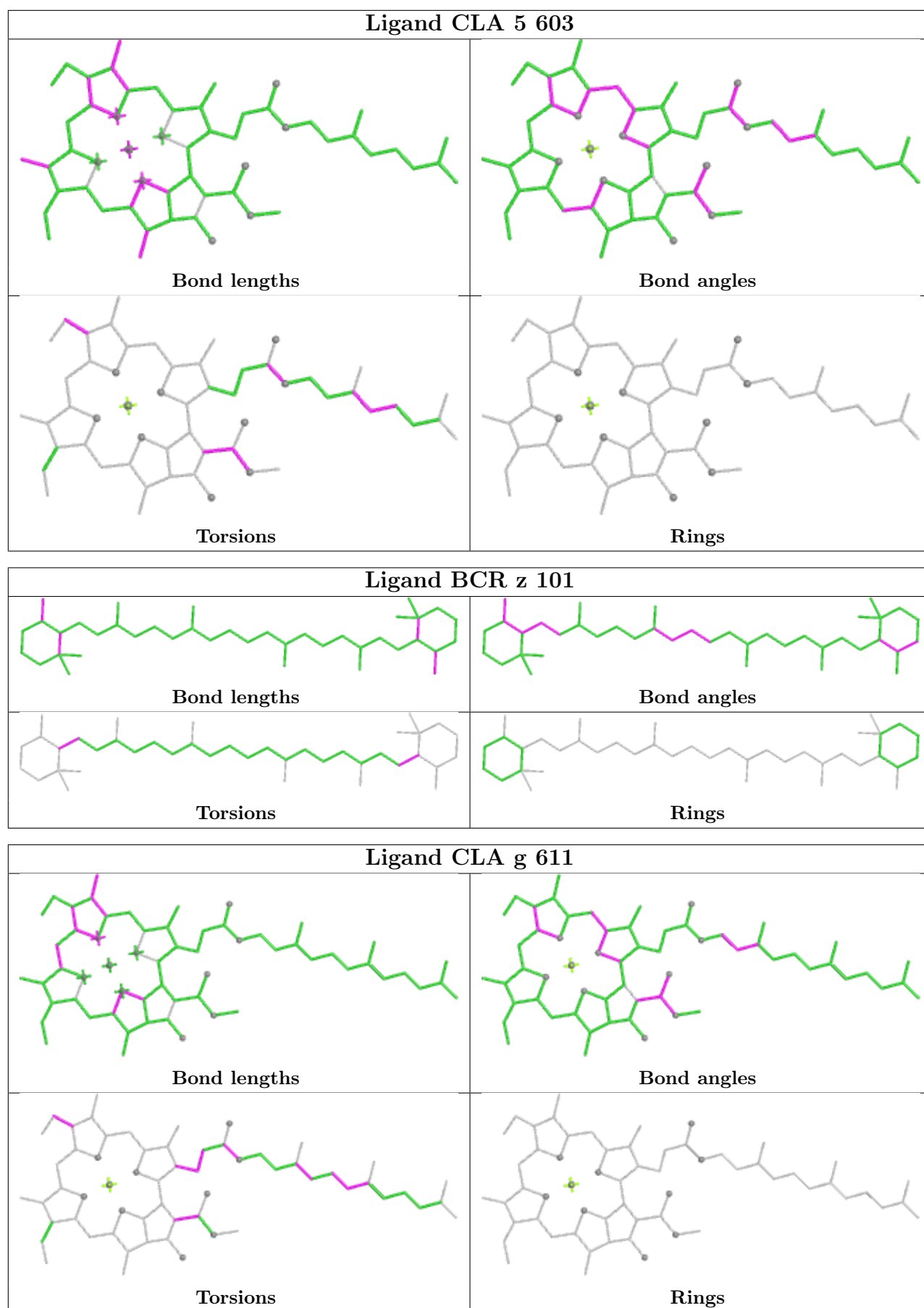


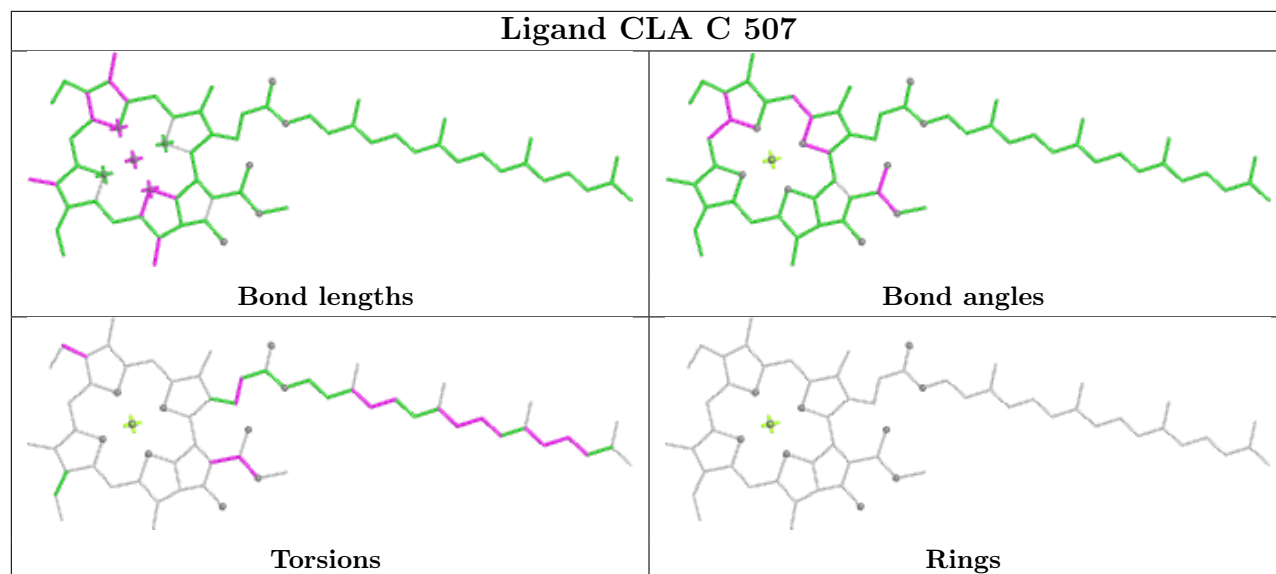
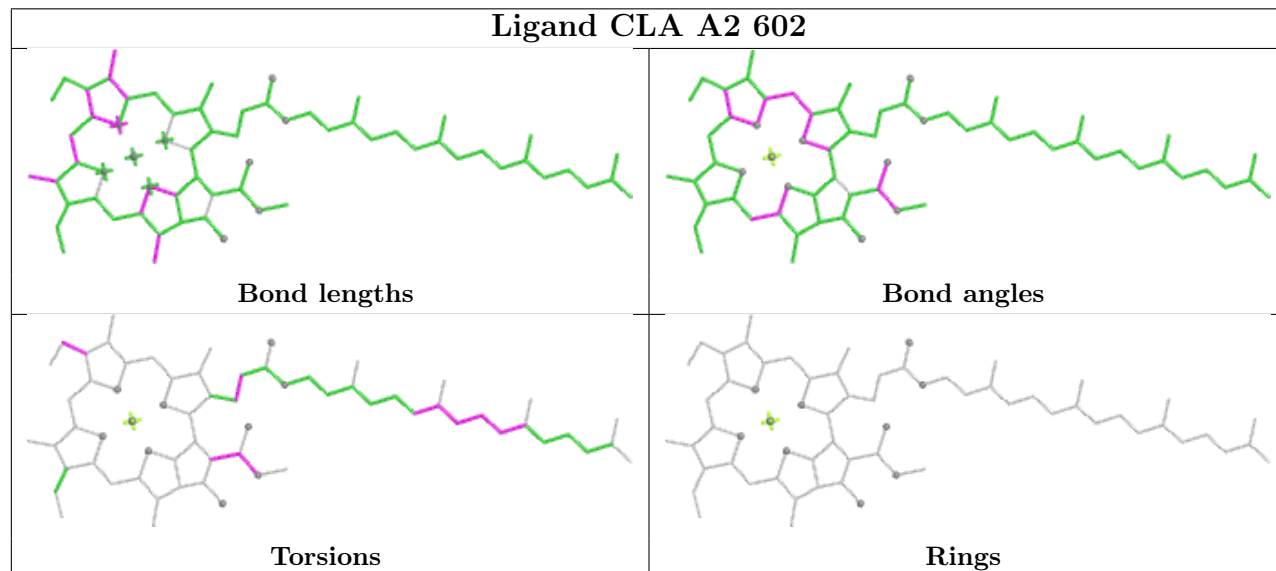
Ligand CLA r 602

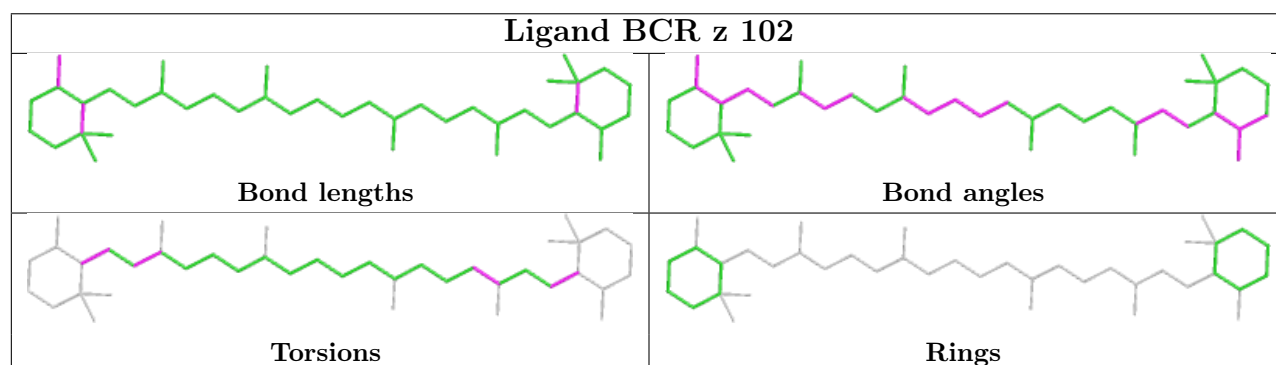
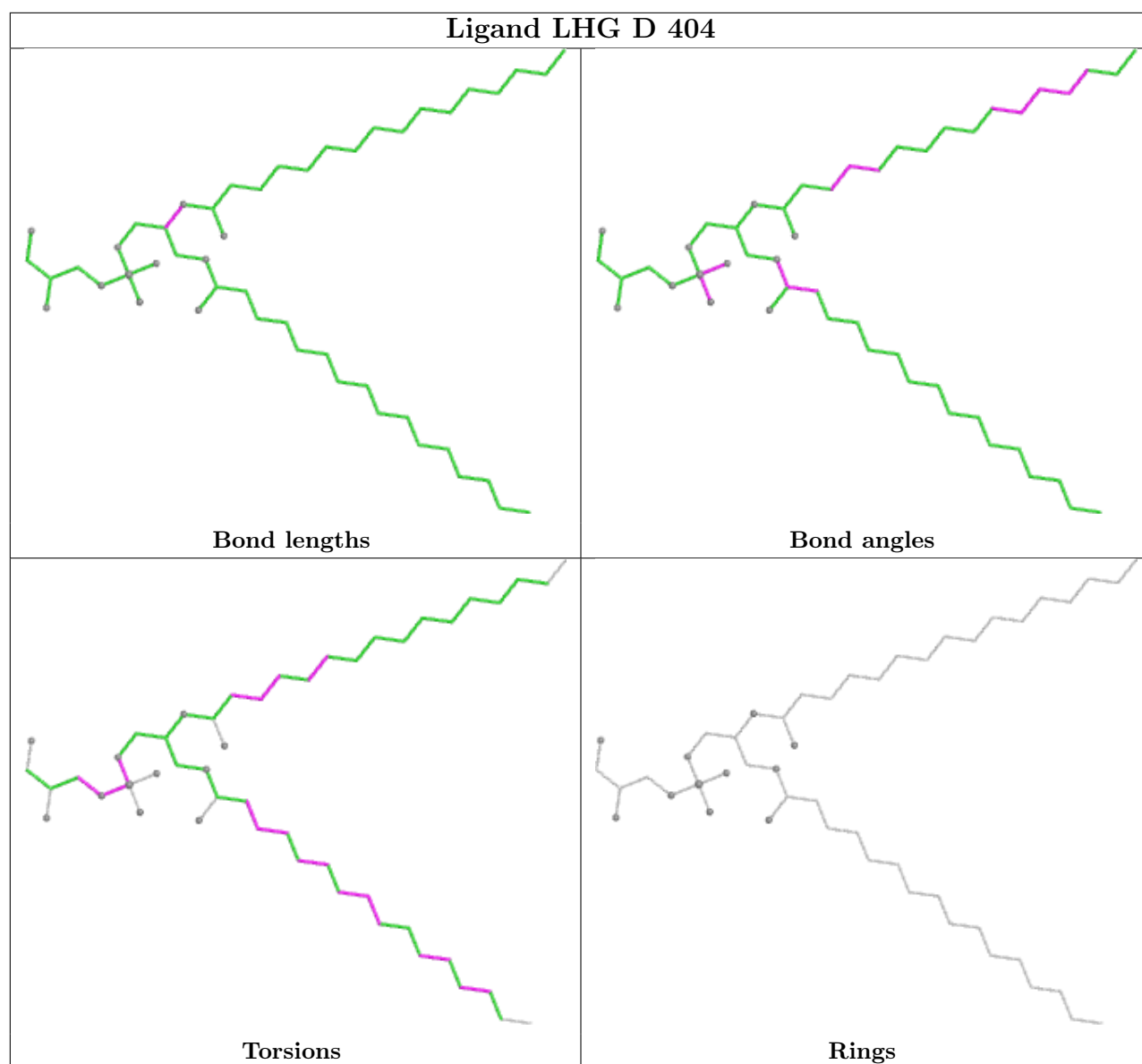


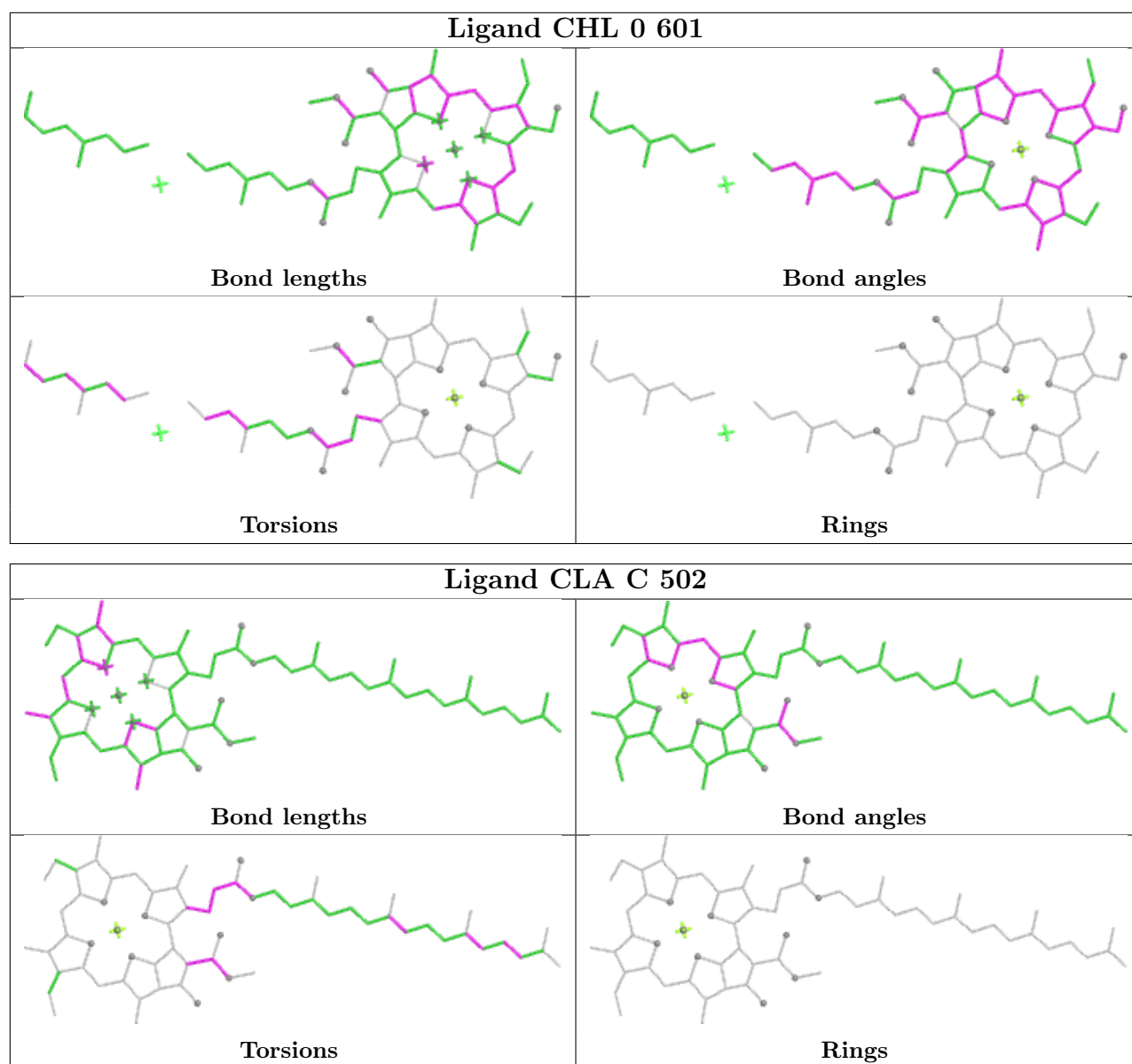
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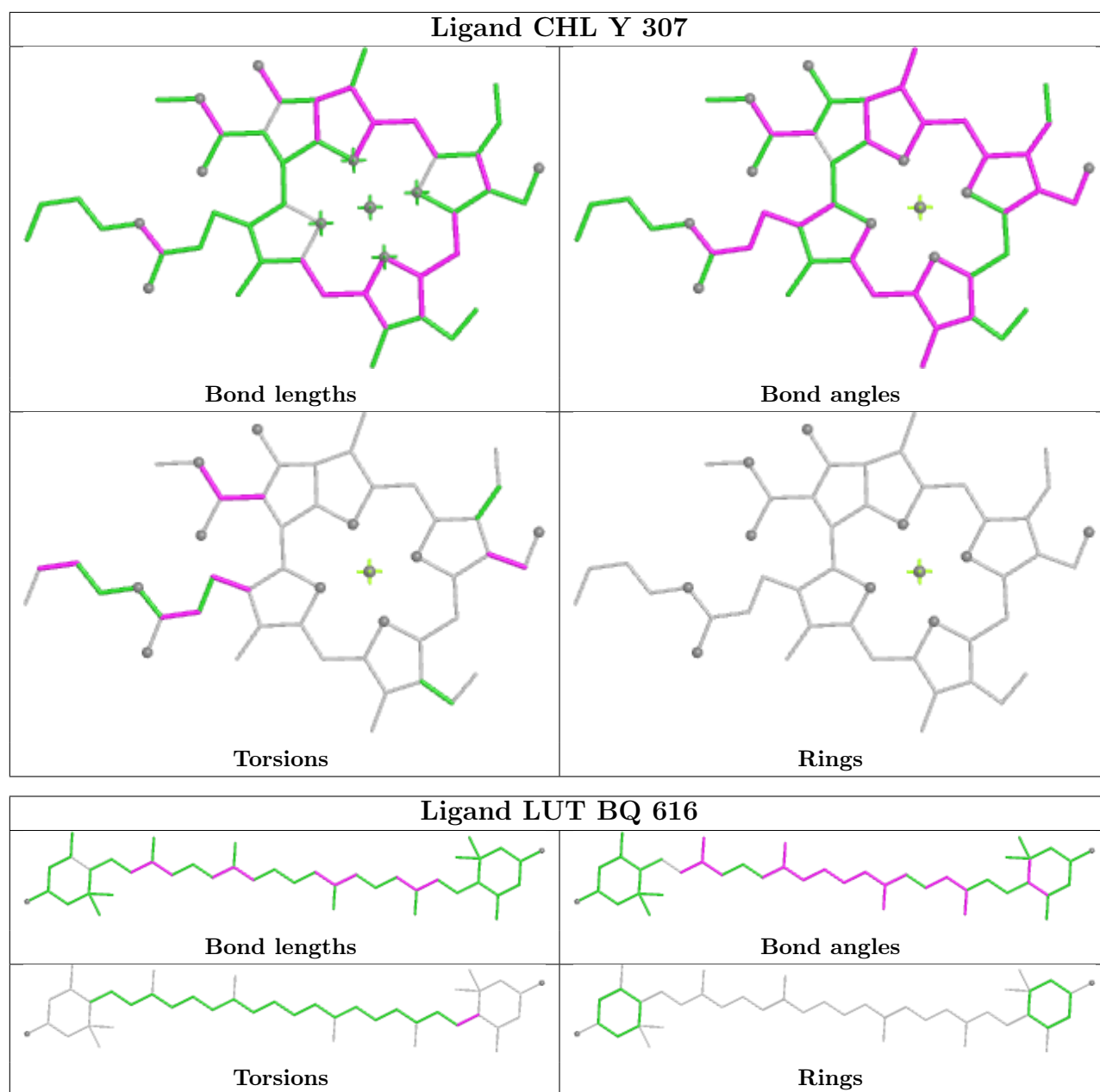




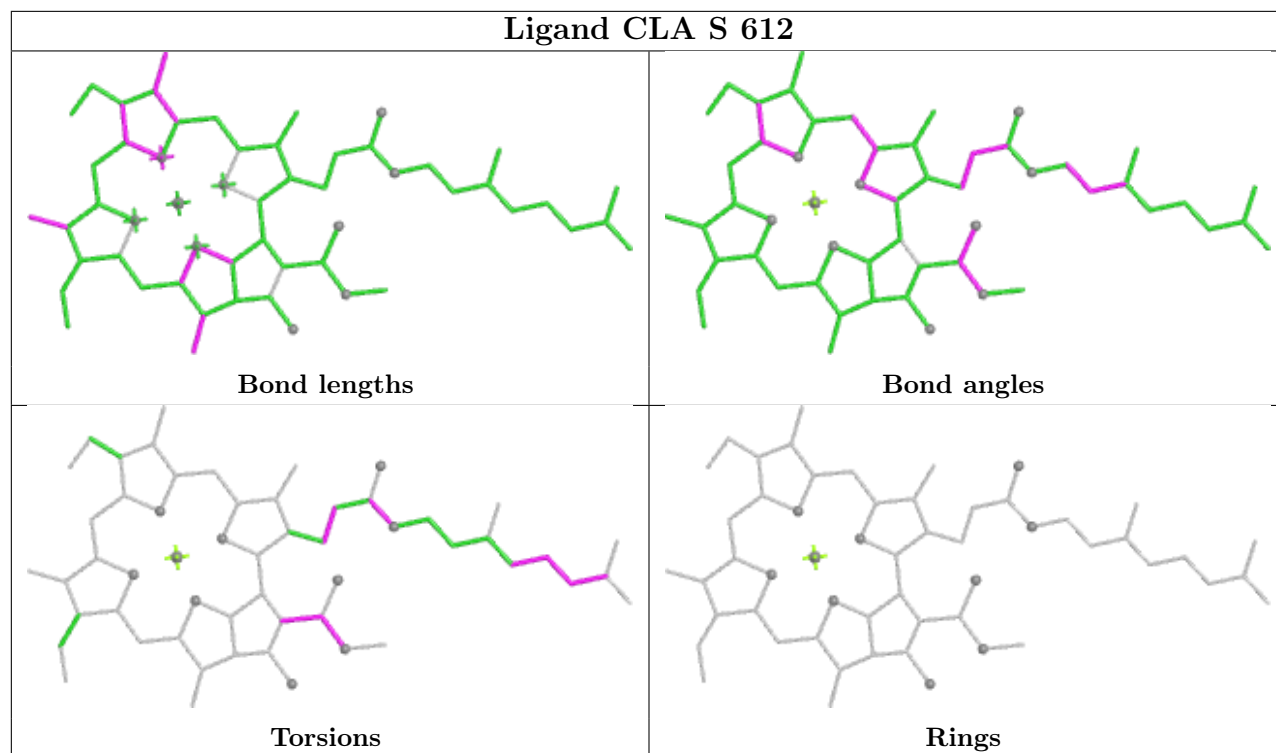
Ligand CLA C 507**Ligand CLA A2 602**



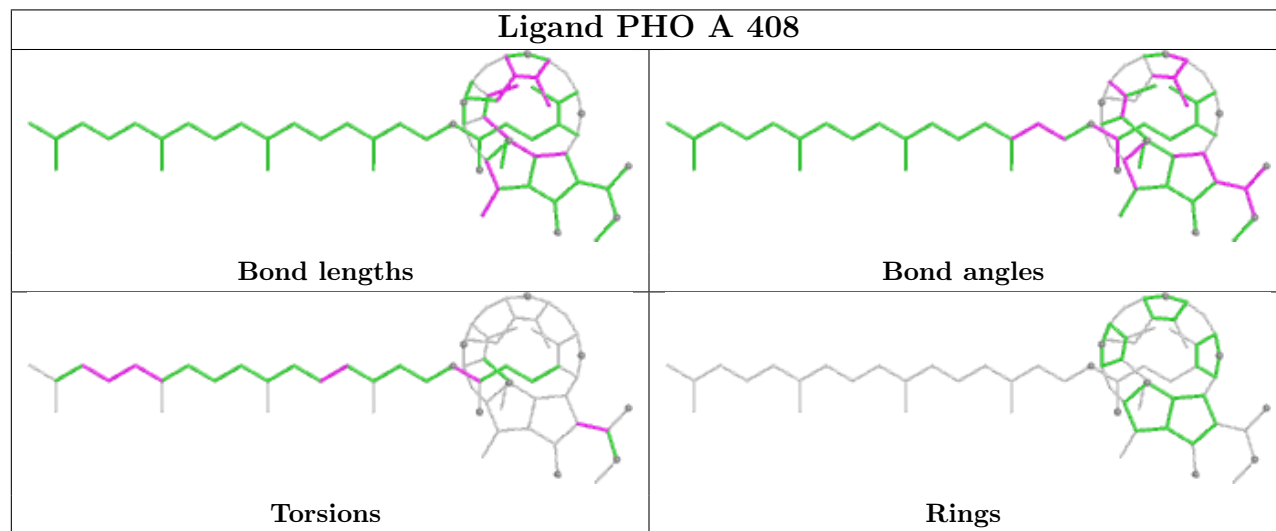




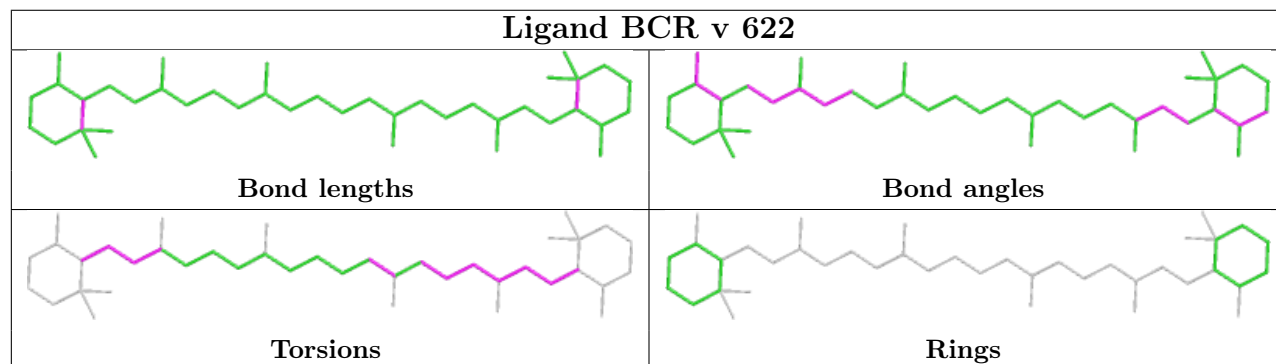
Ligand CLA S 612

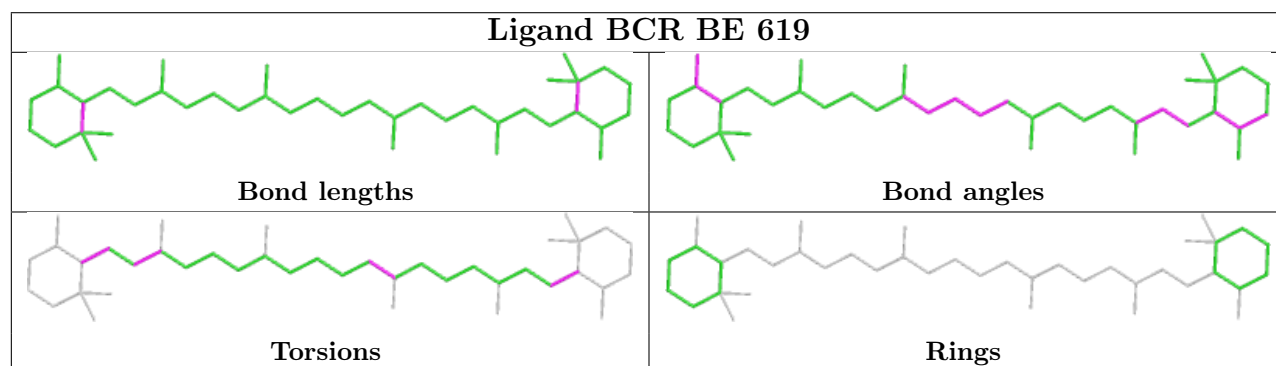
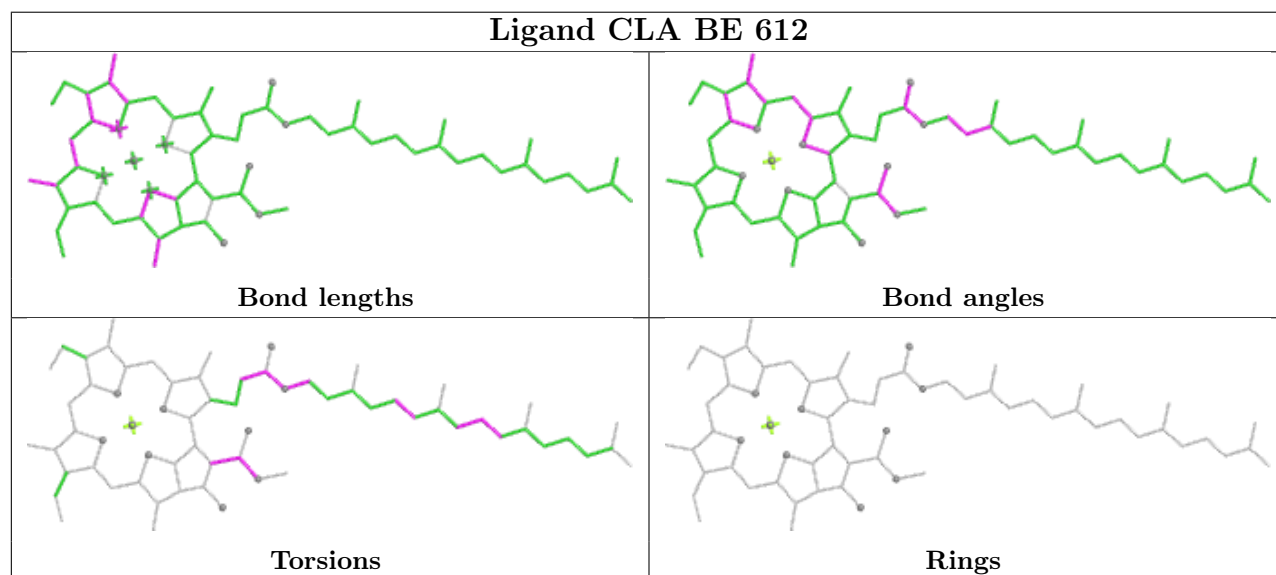
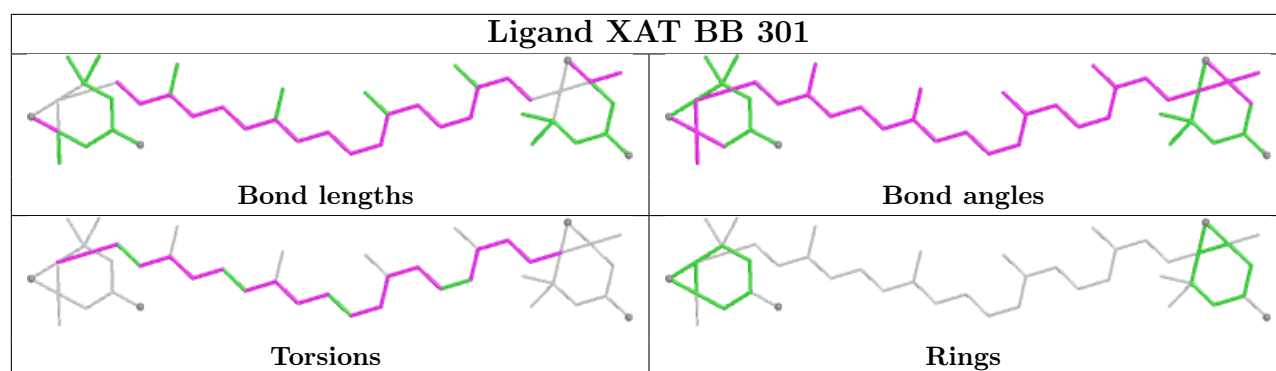


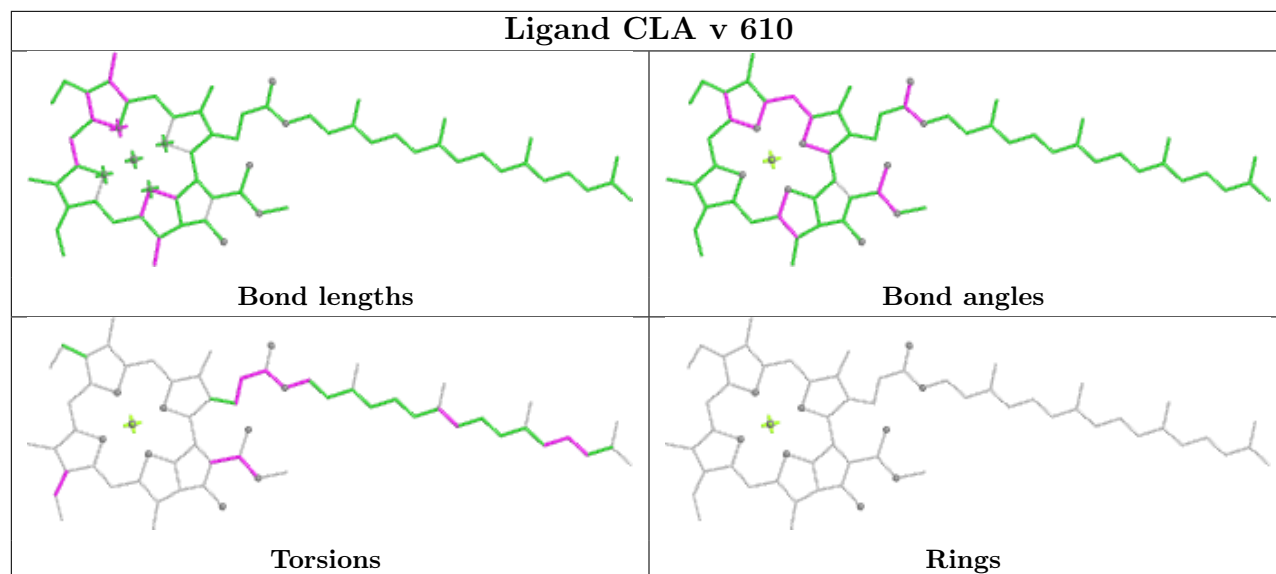
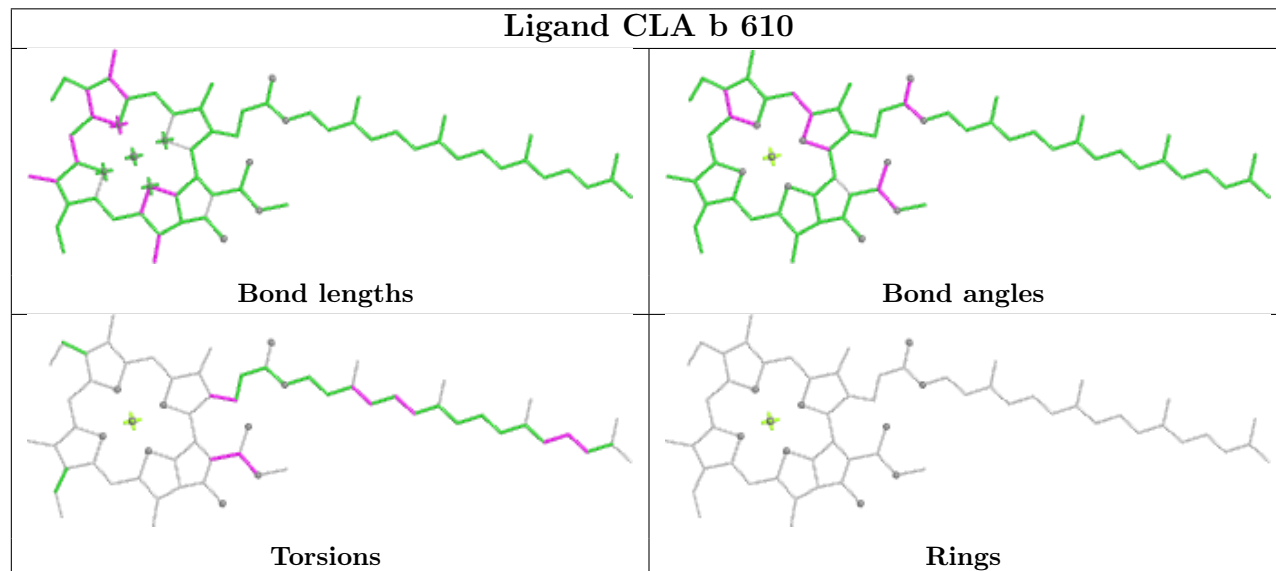
Ligand PHO A 408



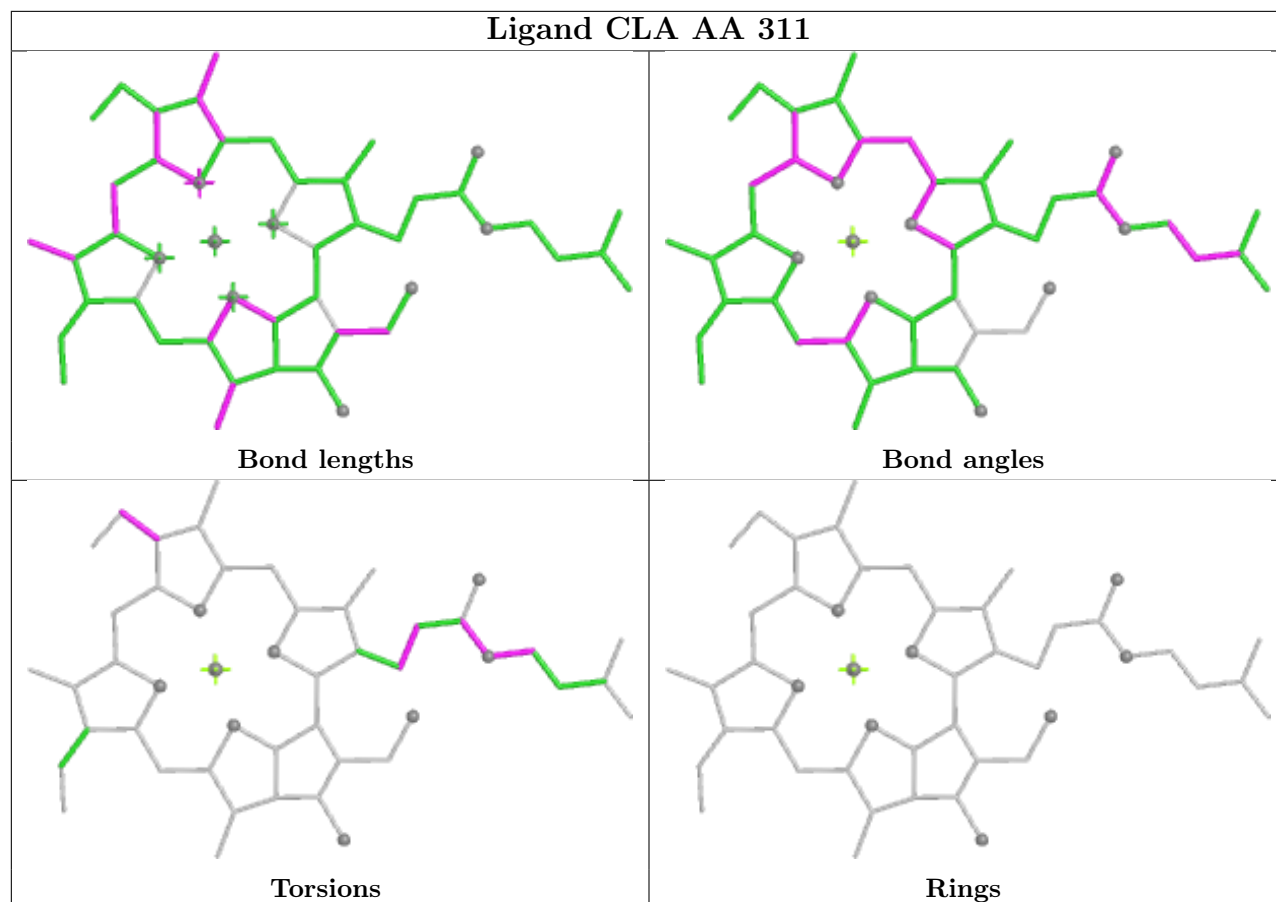
Ligand BCR v 622



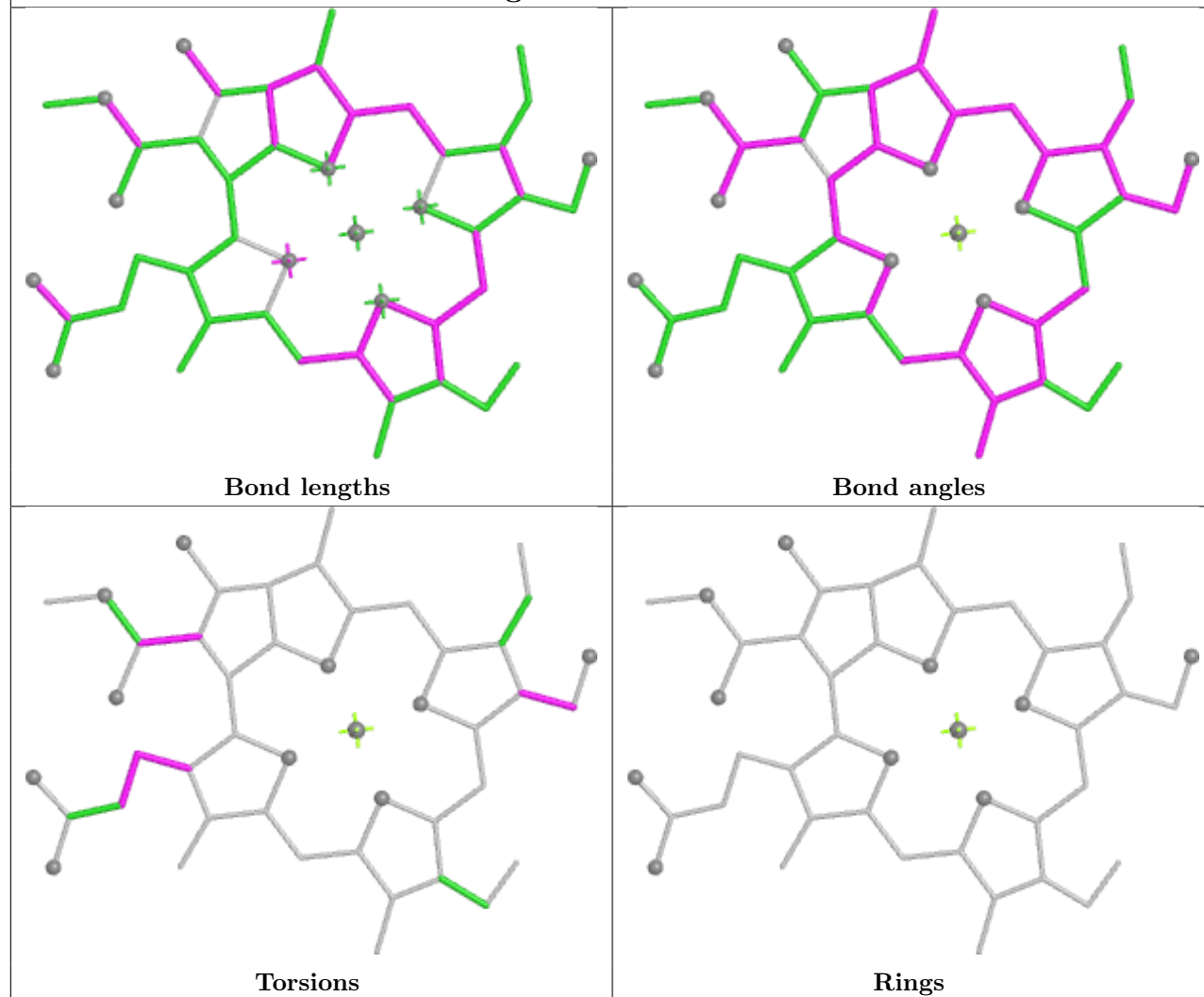


Ligand CLA v 610**Ligand CLA b 610**

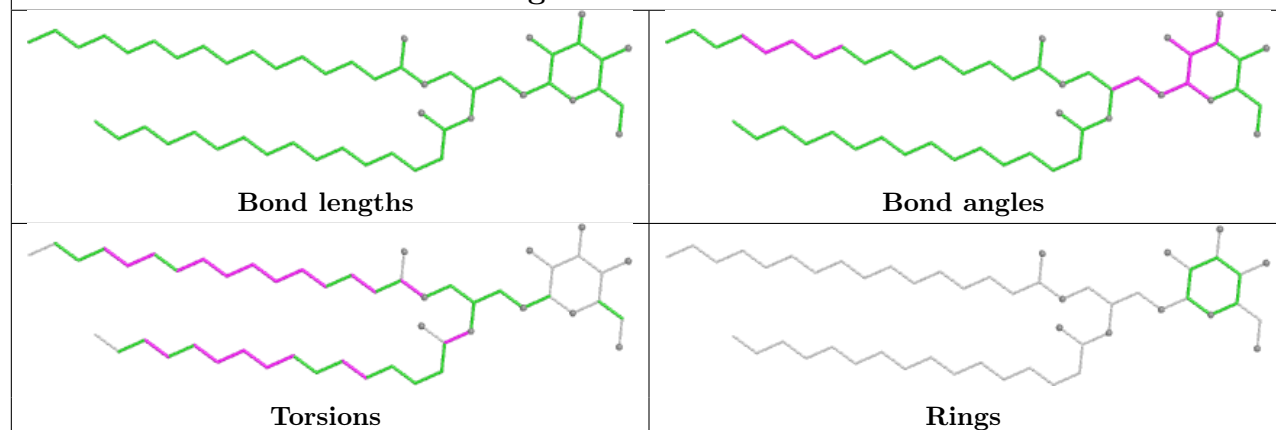
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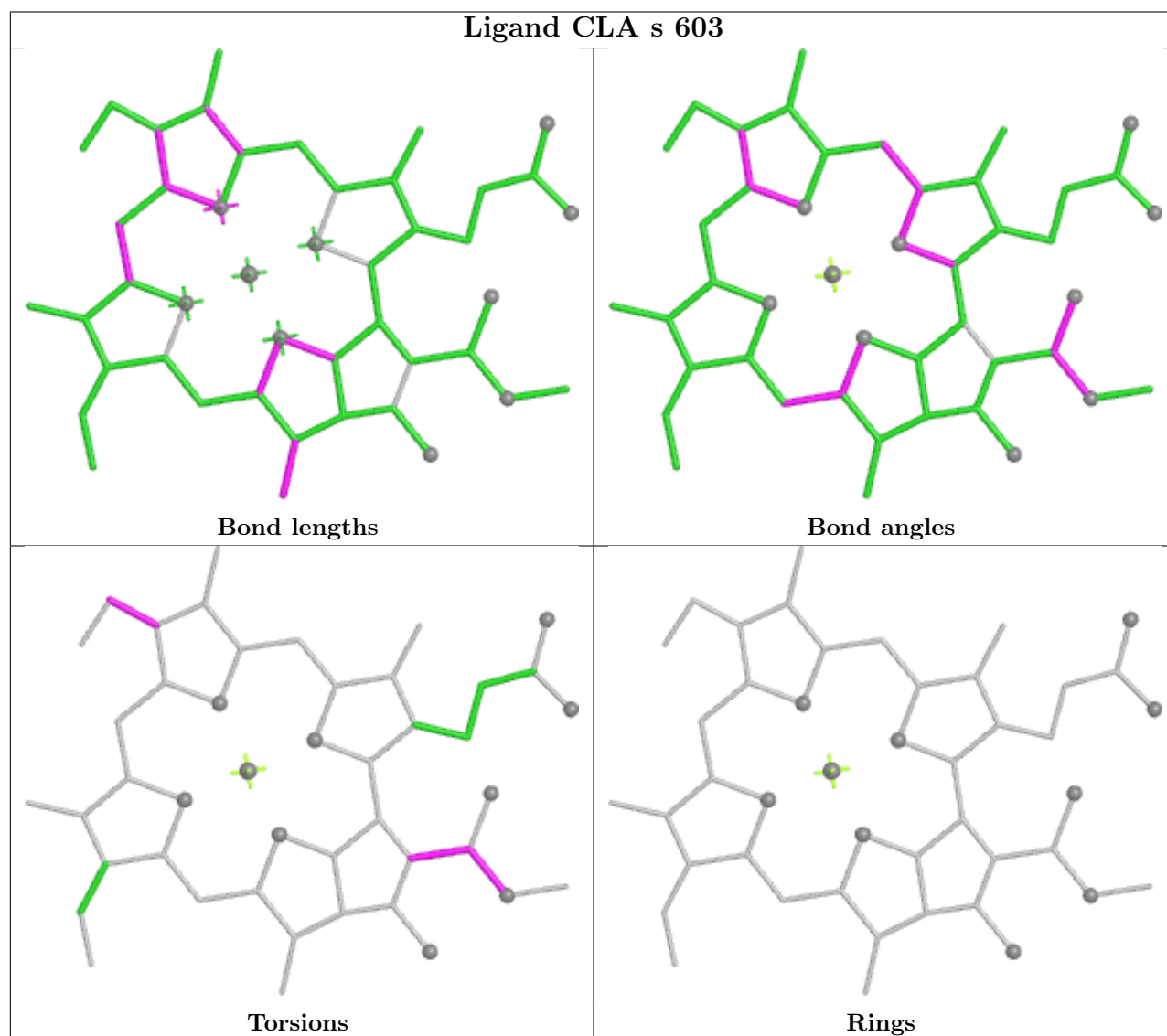
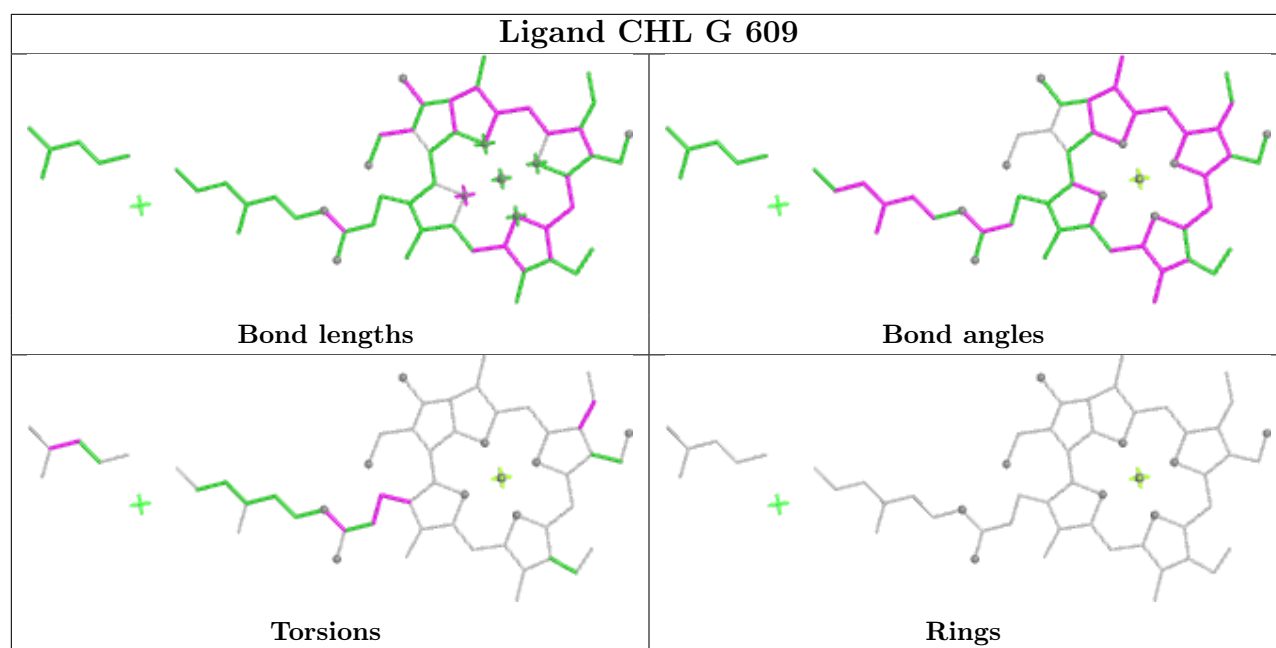


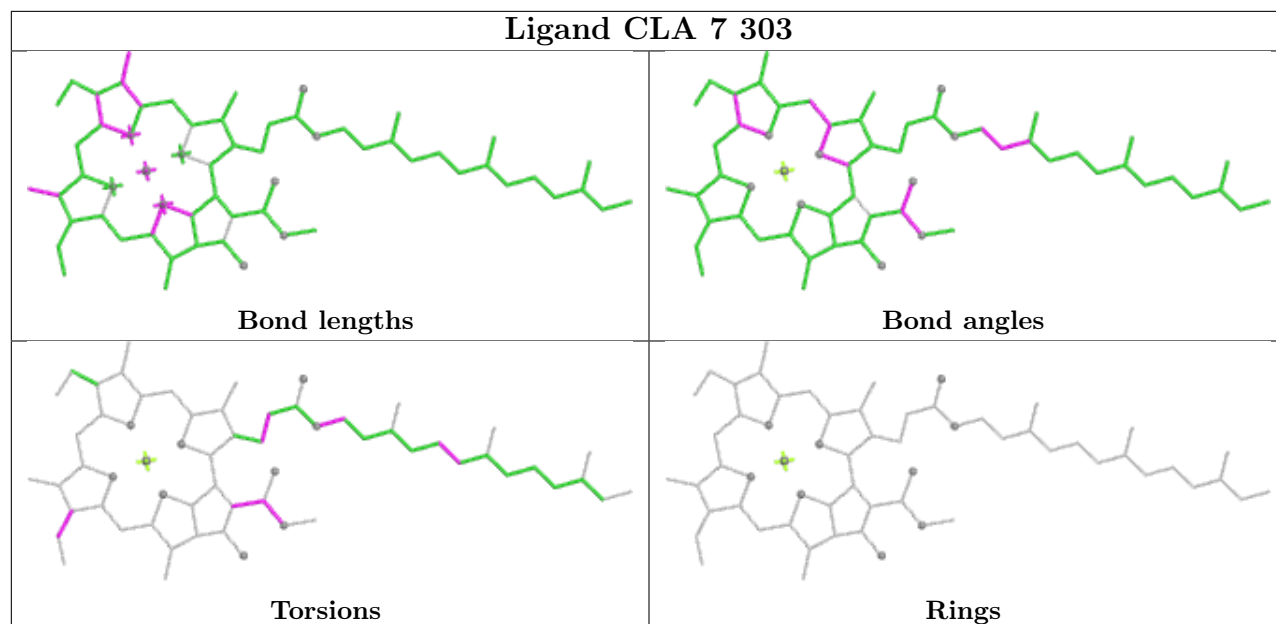
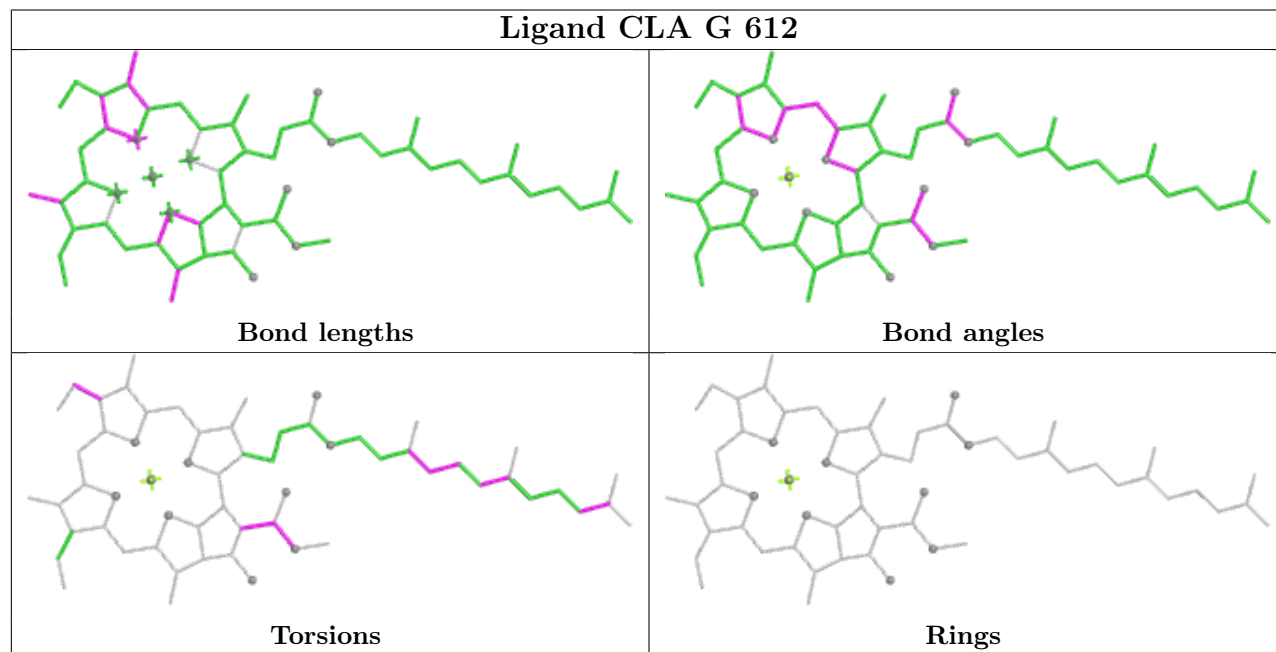
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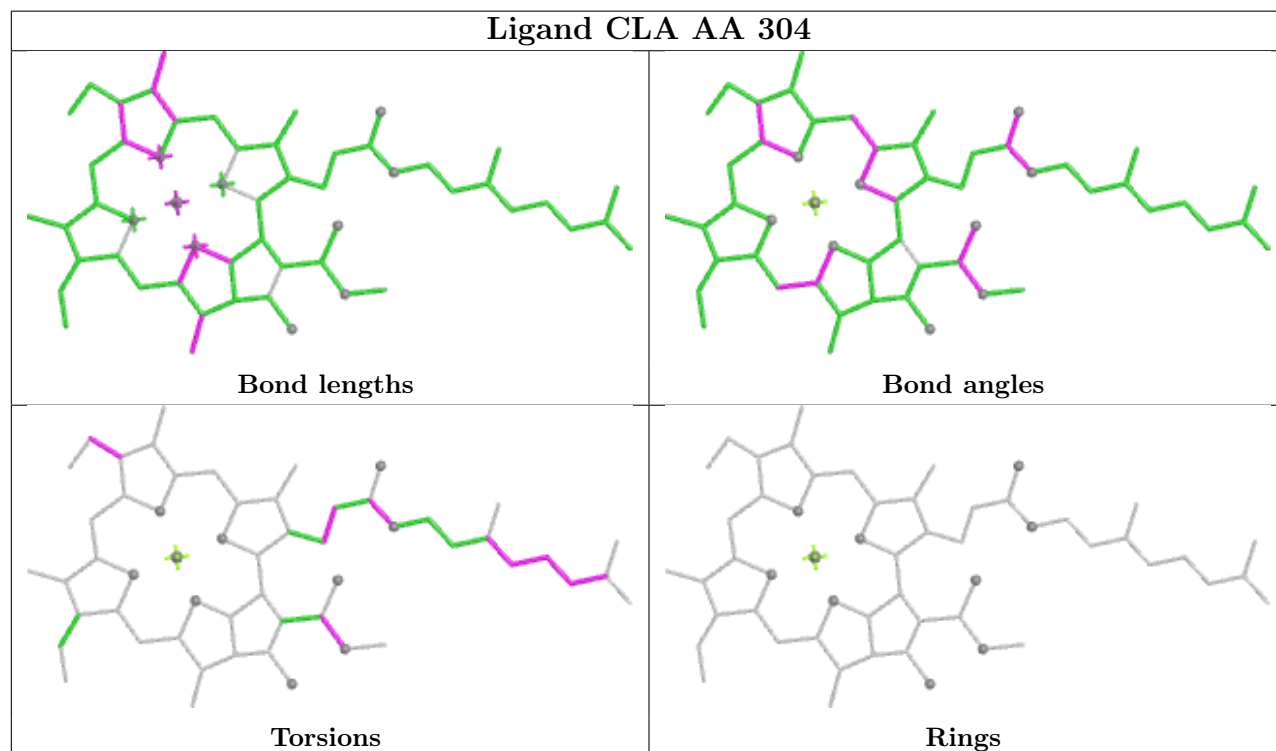
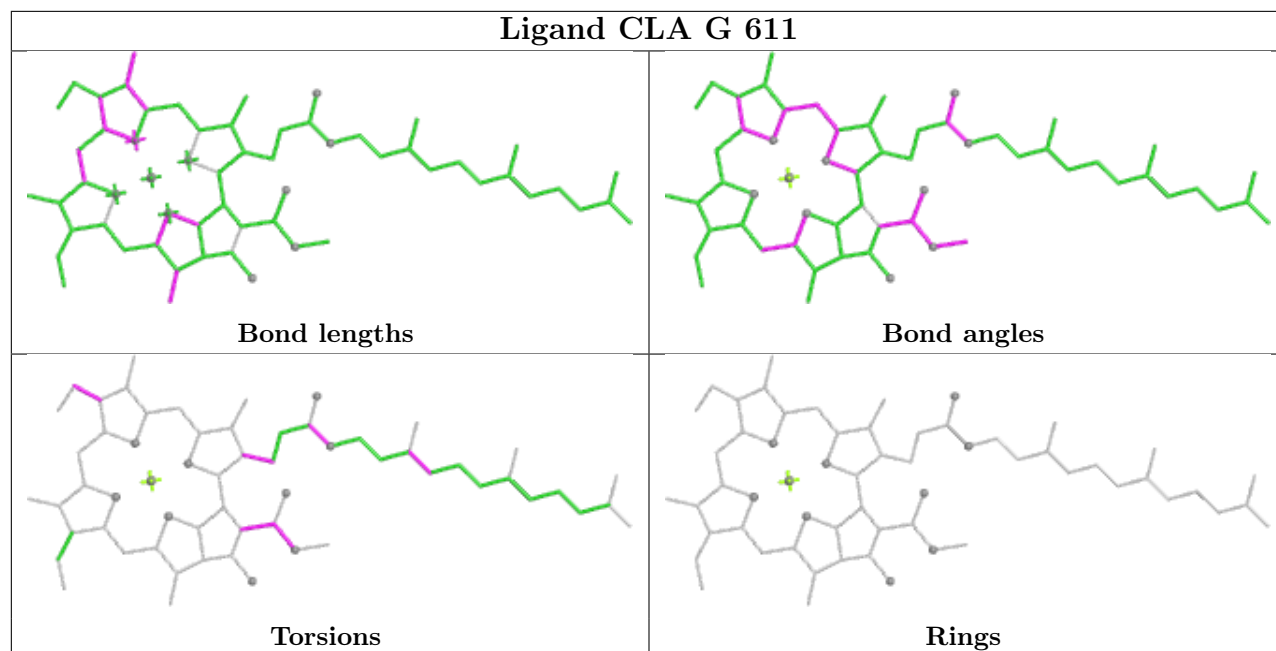


Ligand LMG B 620

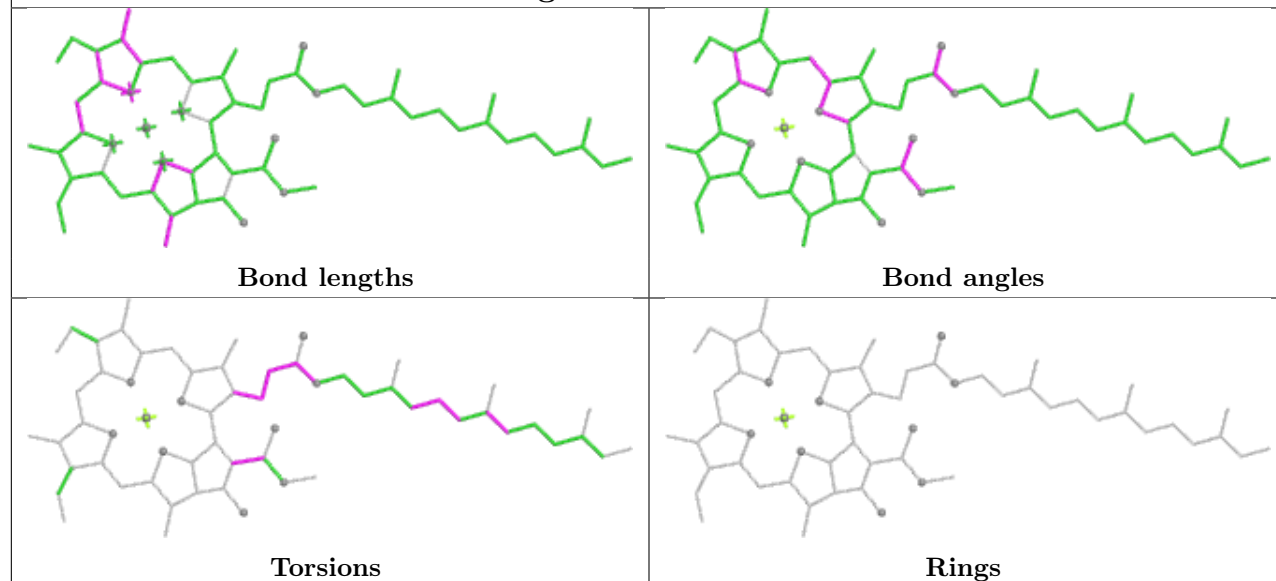




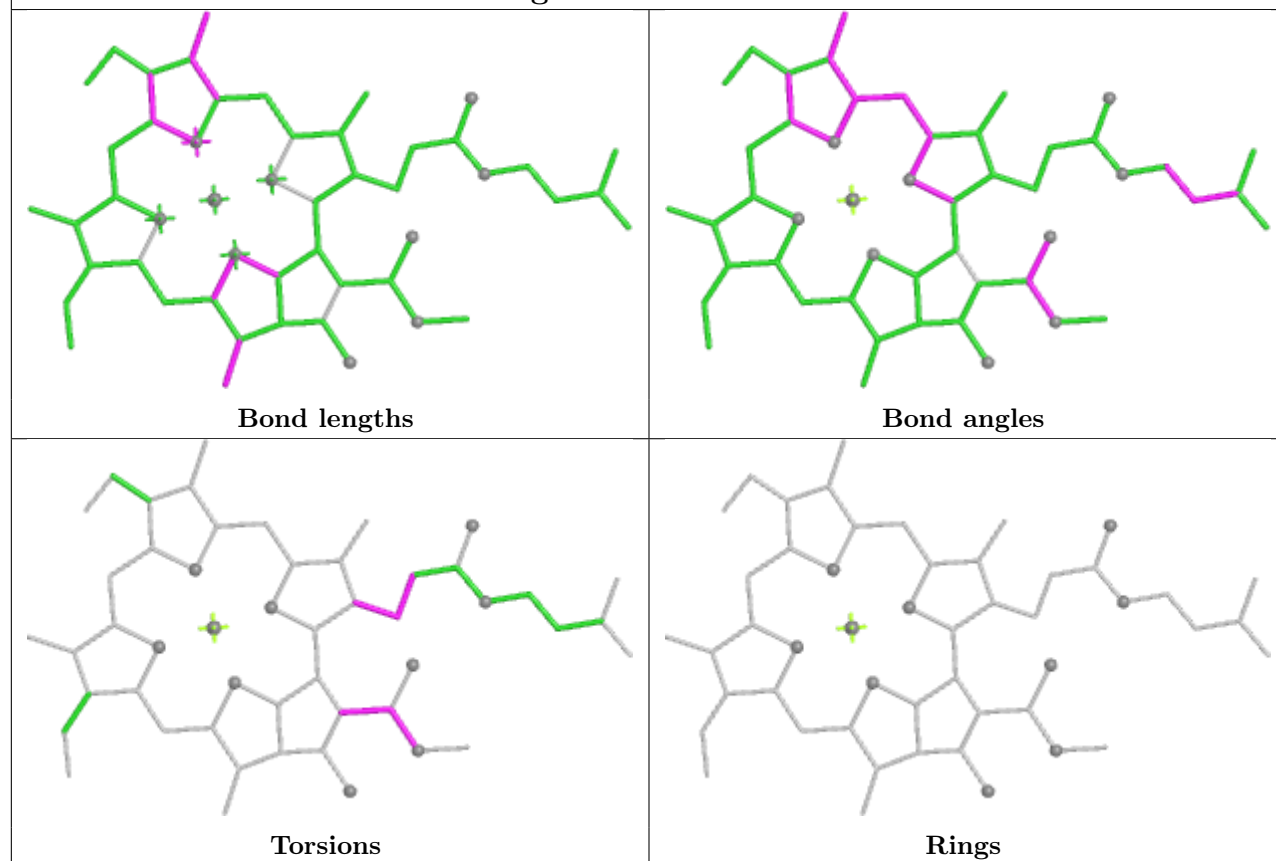
Ligand CLA 7 303**Ligand CLA G 612**

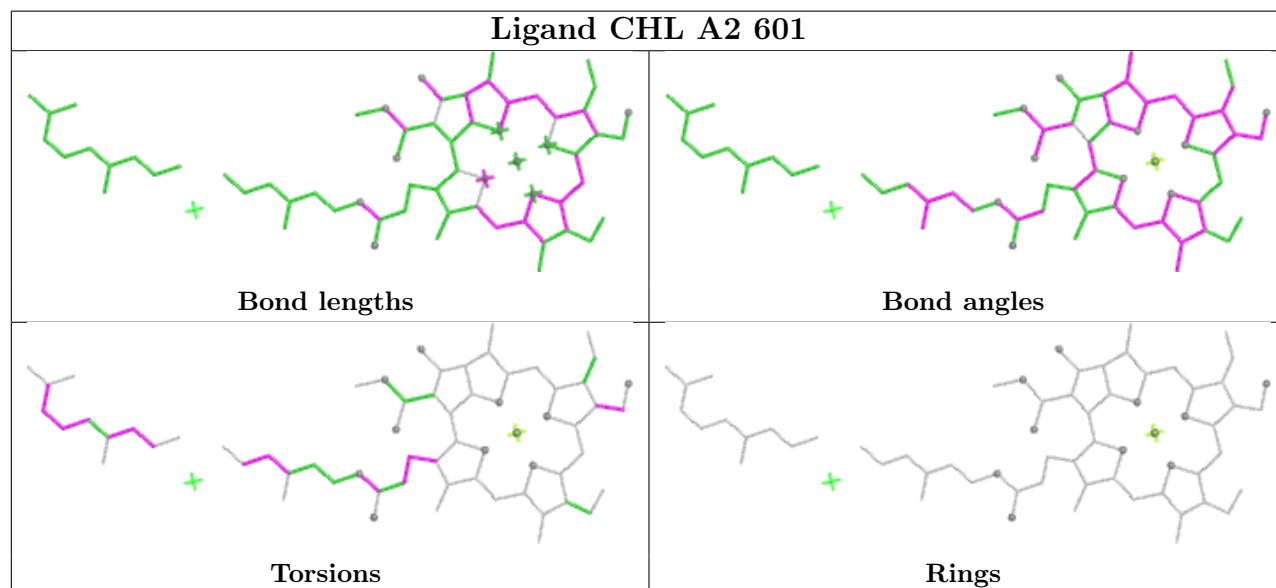
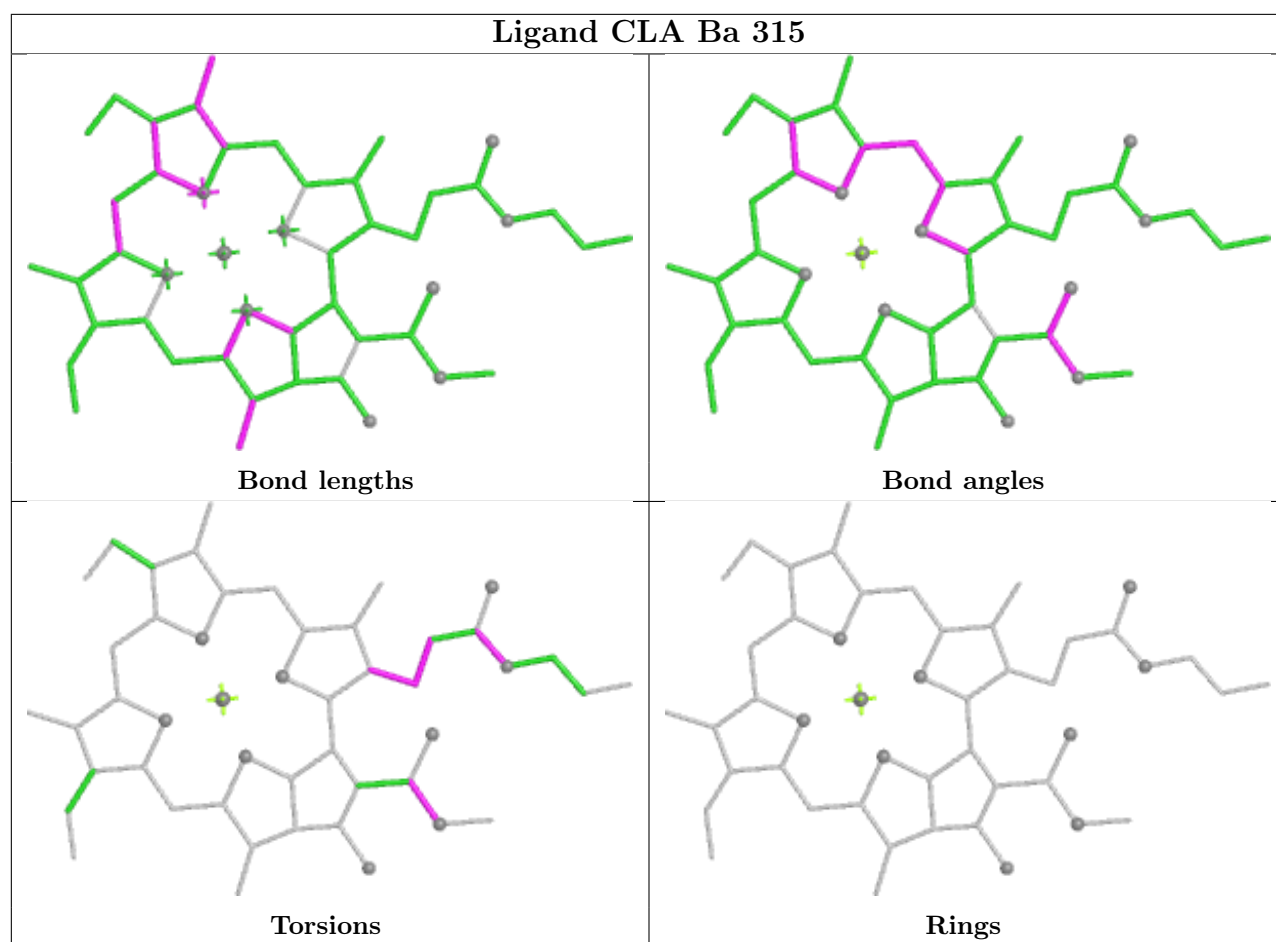


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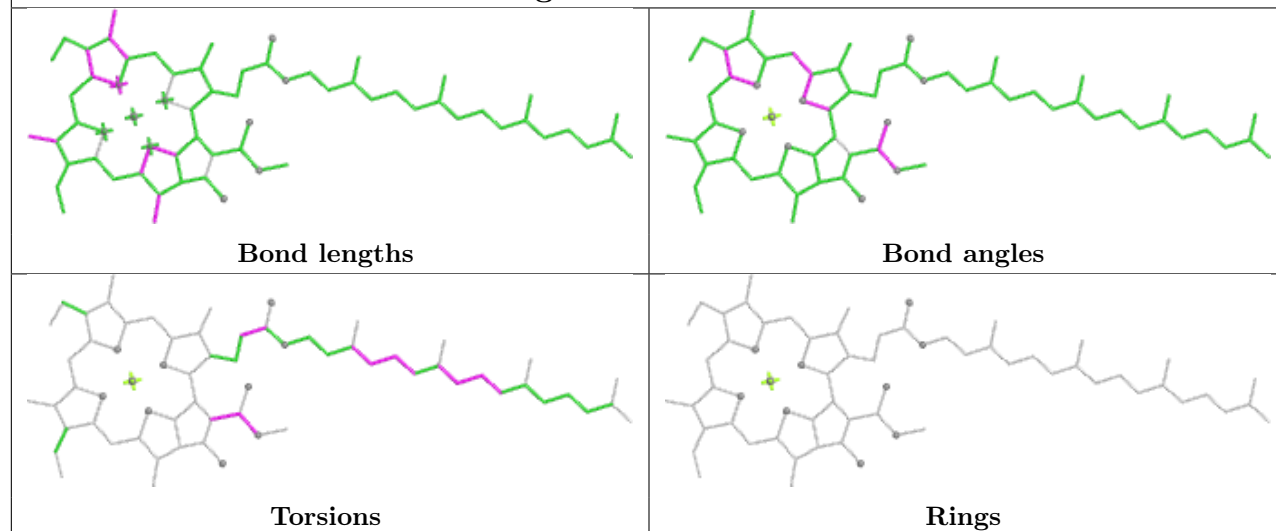


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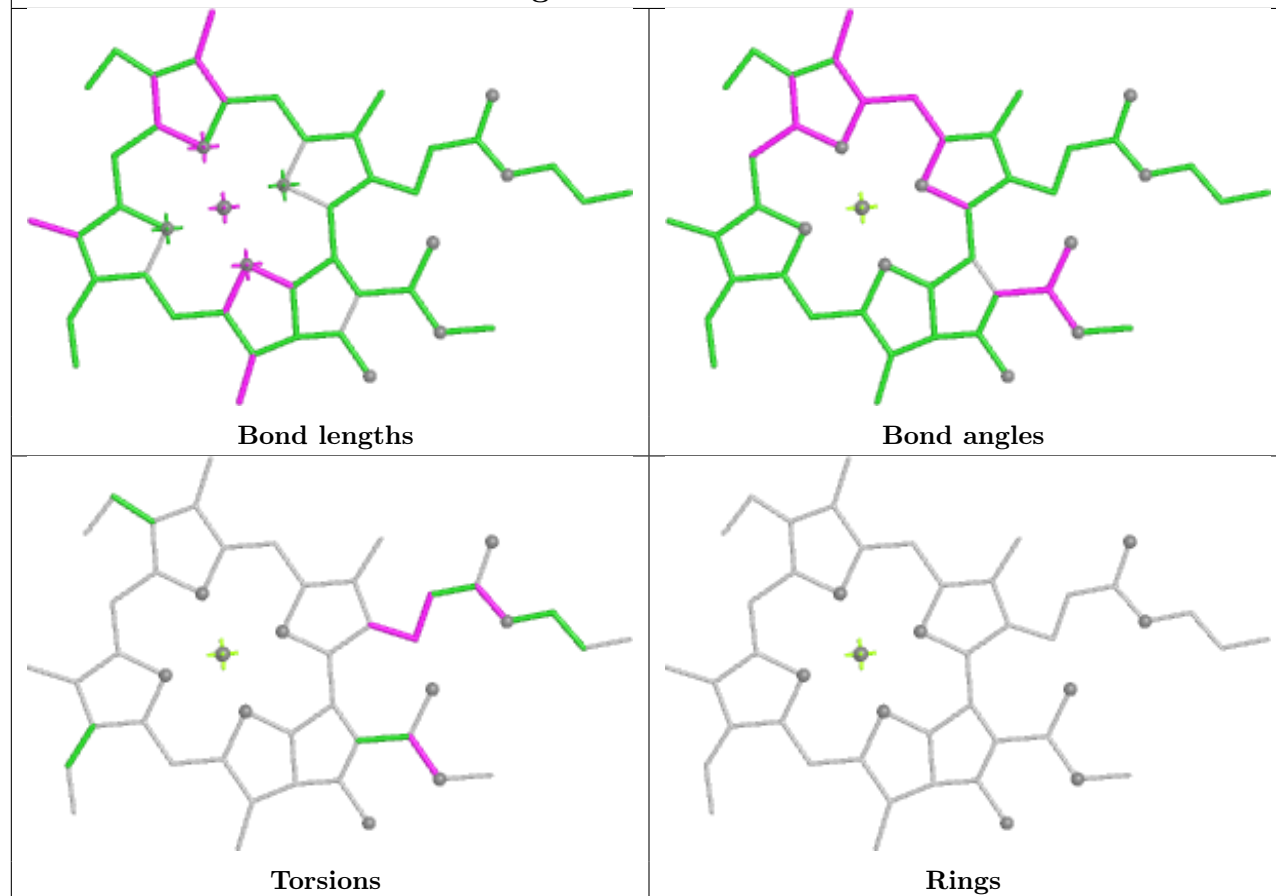




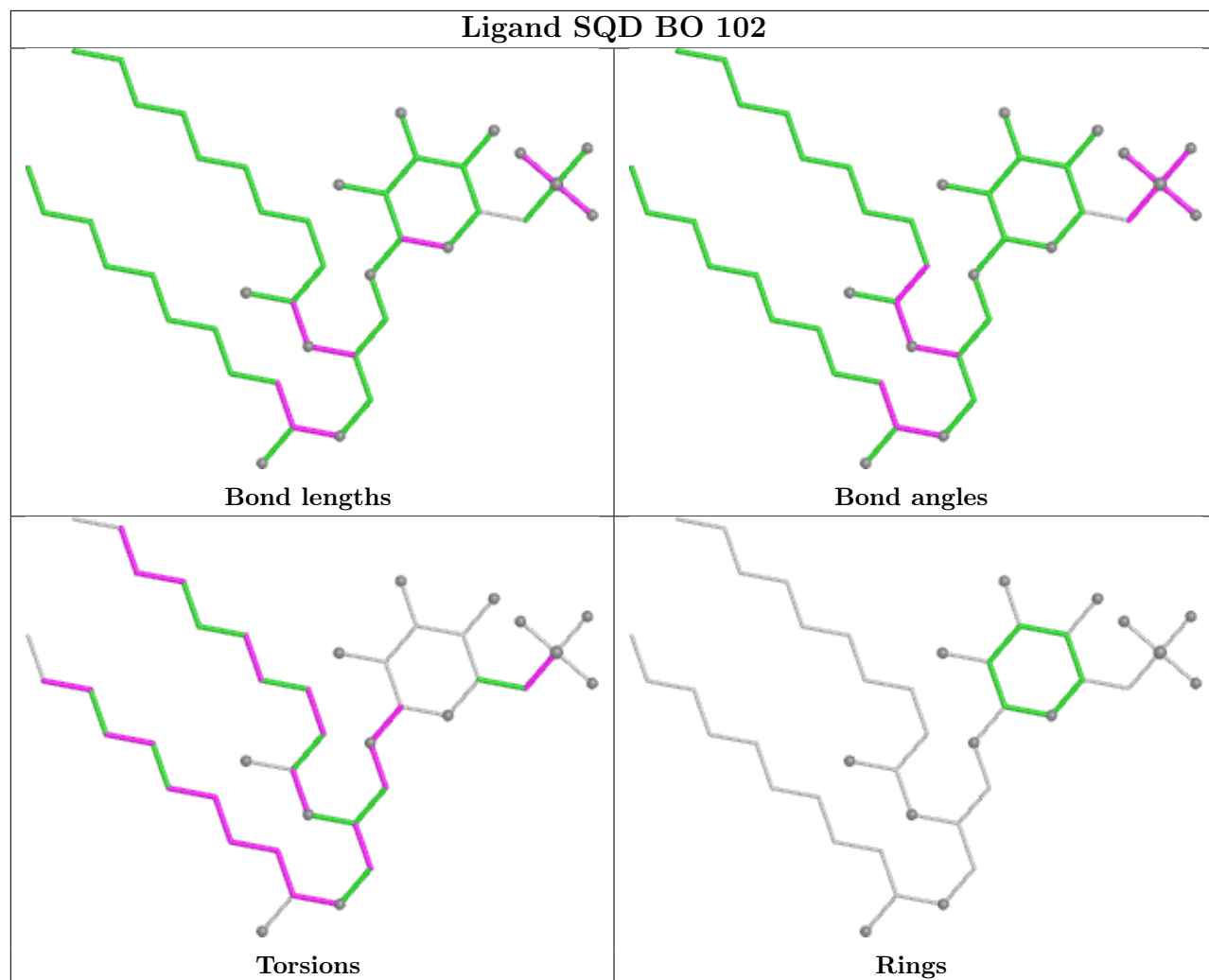
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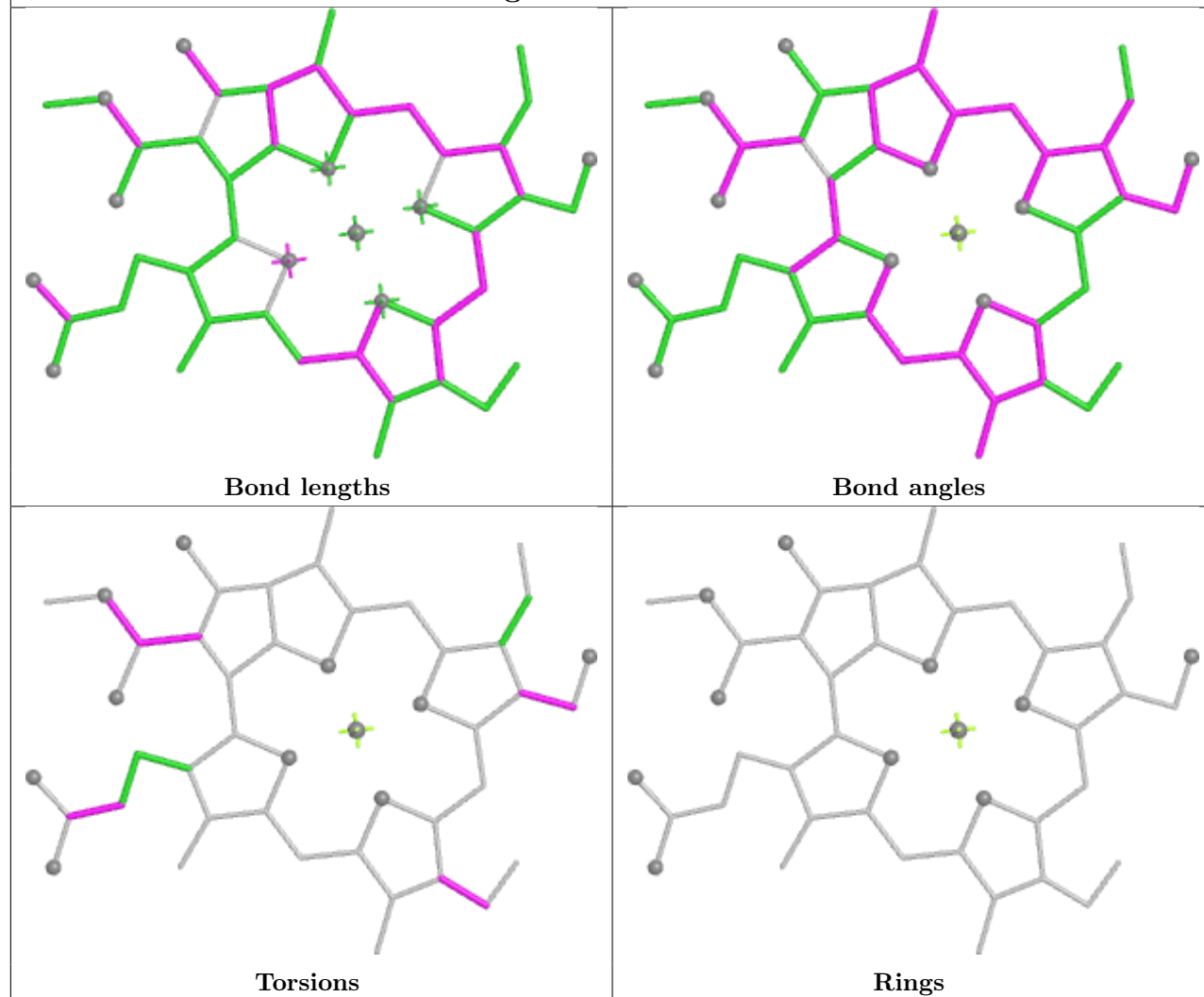
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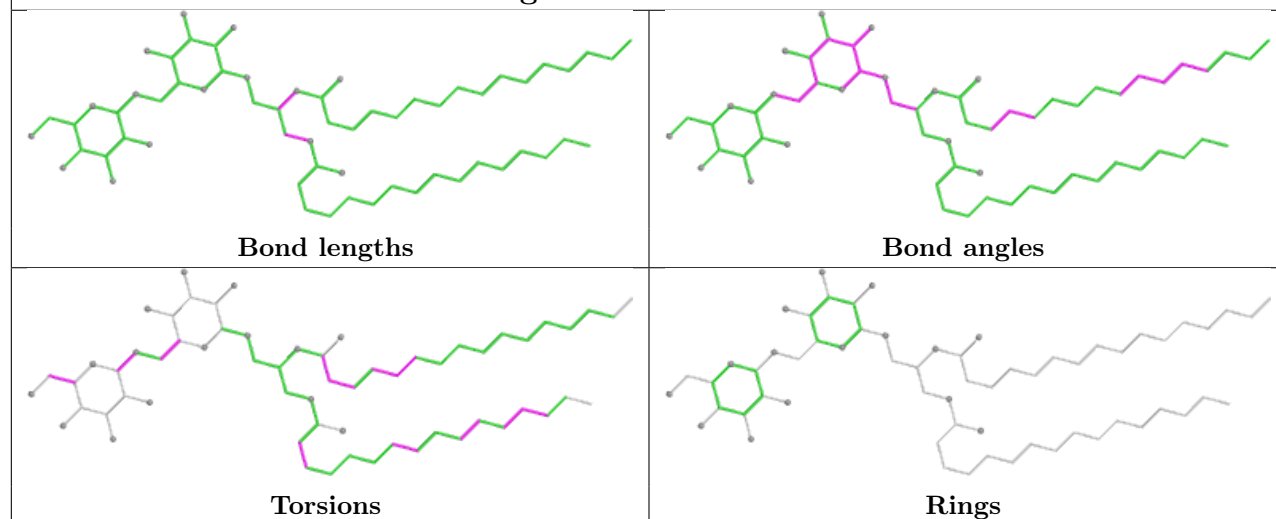
Ligand SQD BO 102

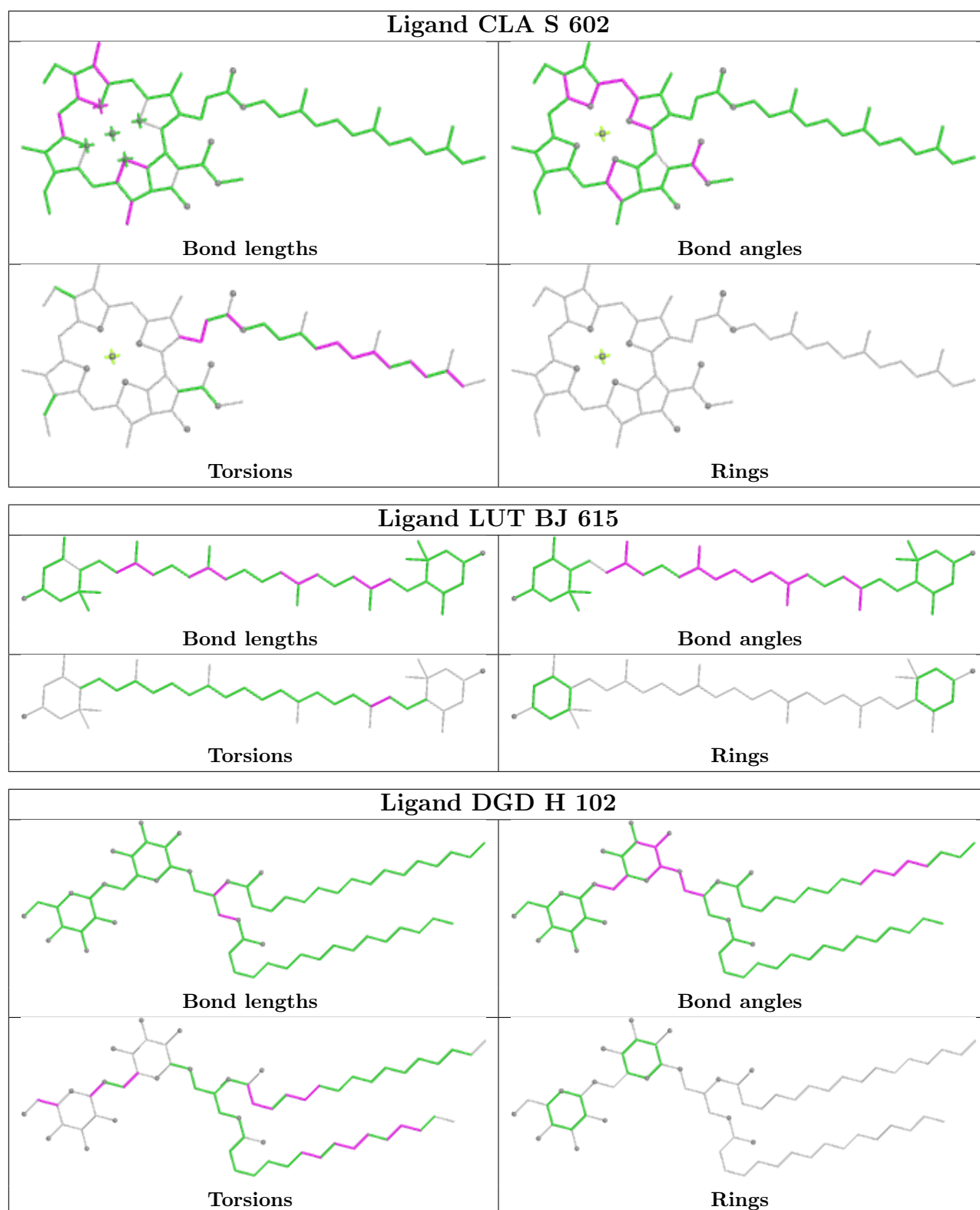


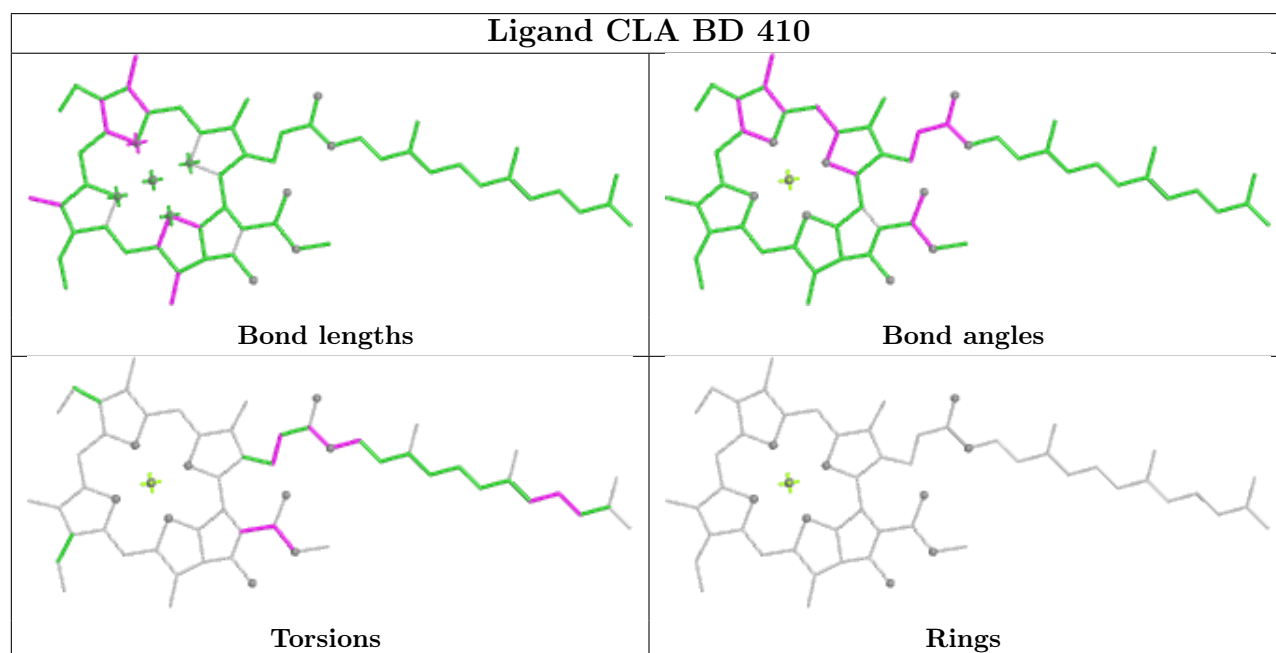
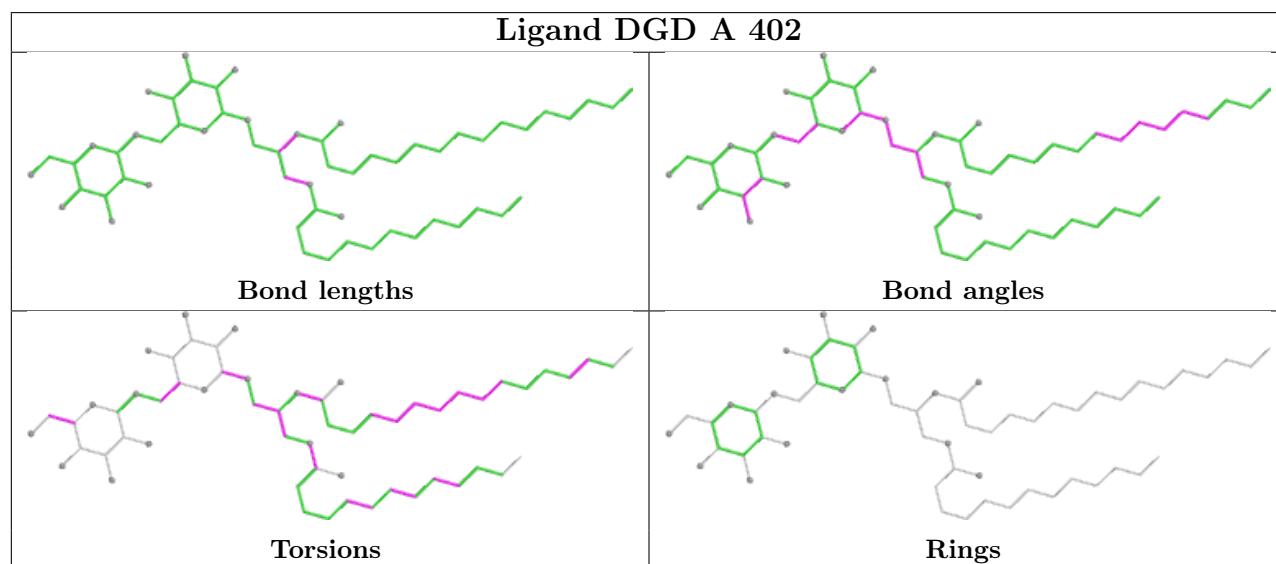
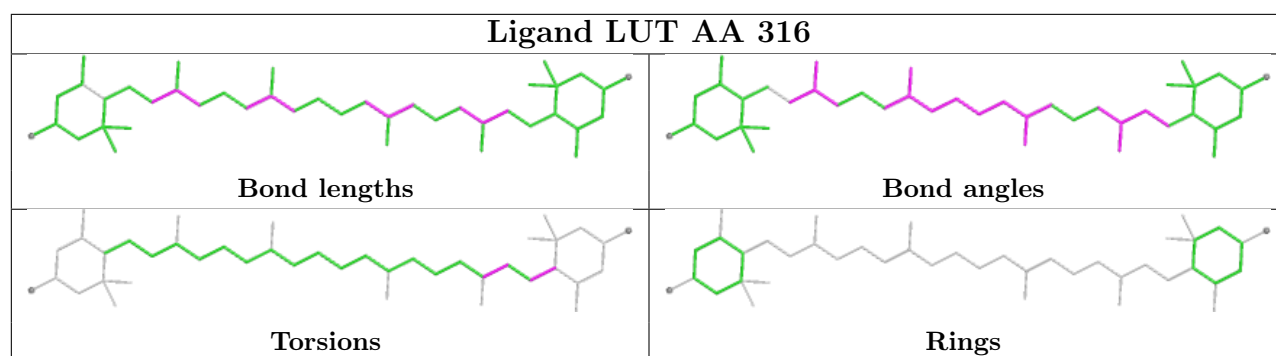
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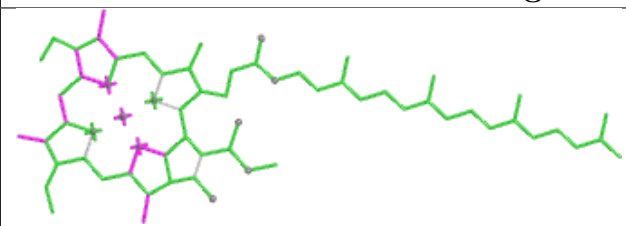
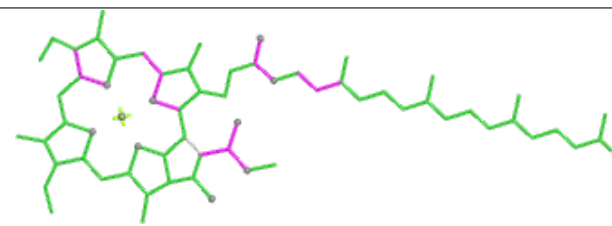
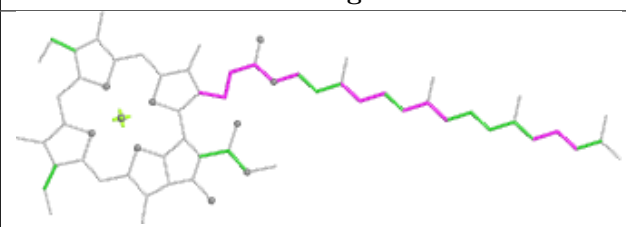
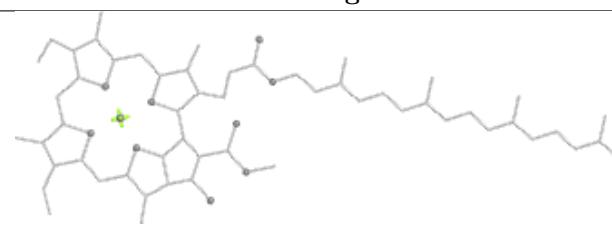


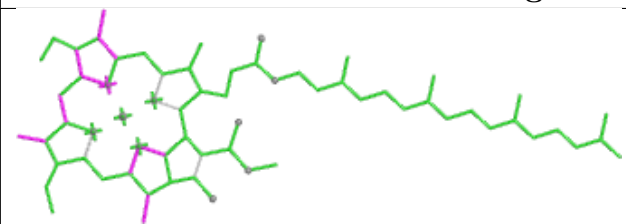
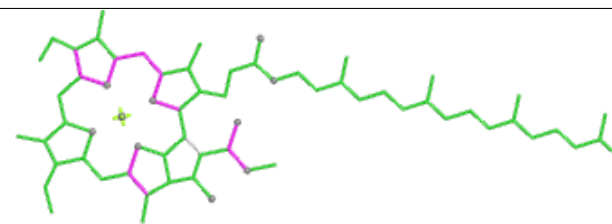
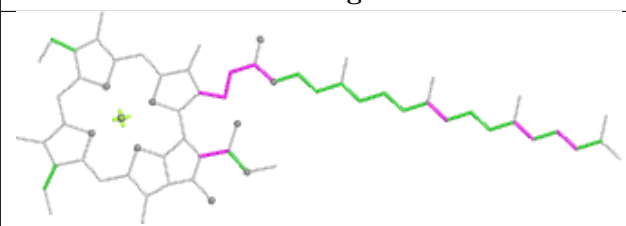
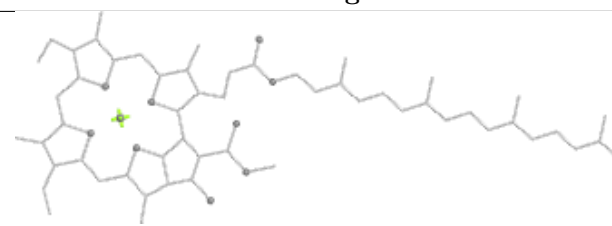
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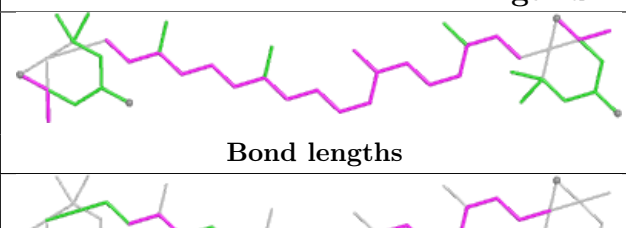
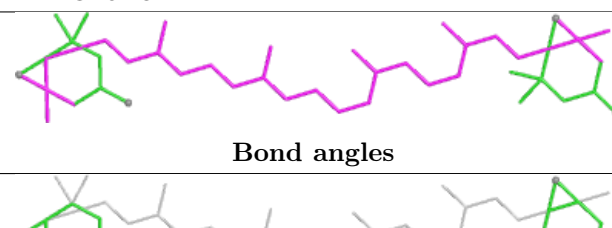




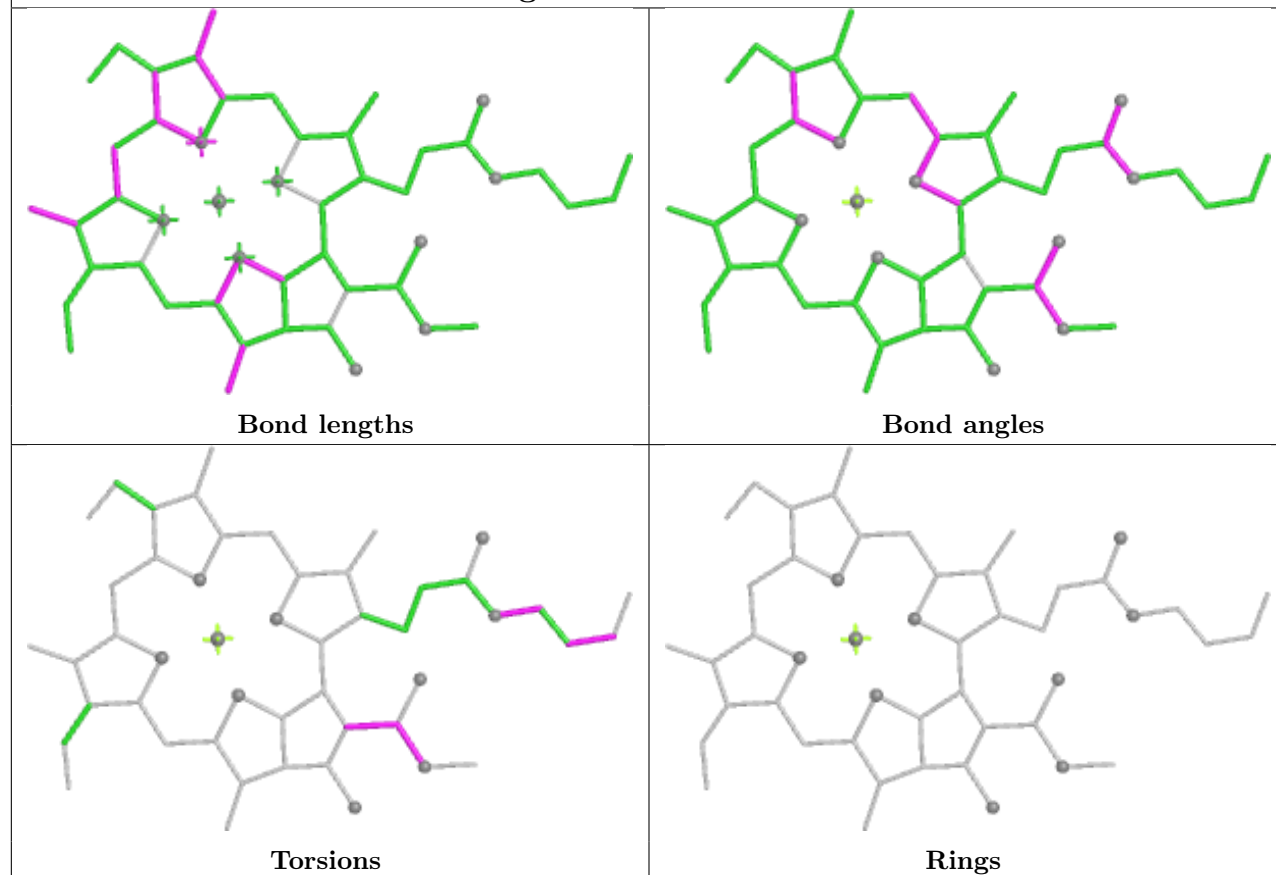


Ligand CLA d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

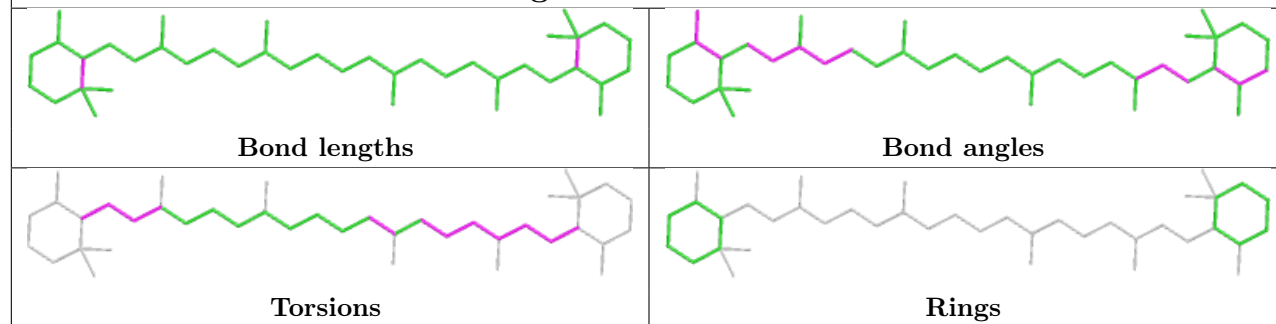
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Bond lengths	Bond angles
	
Torsions	Rings

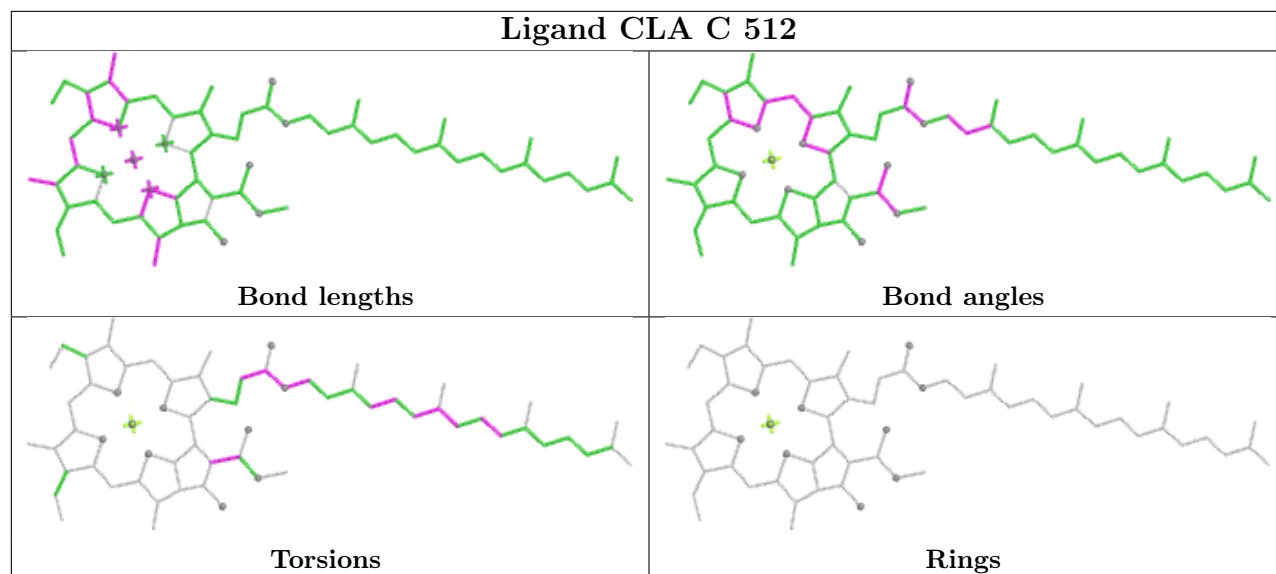
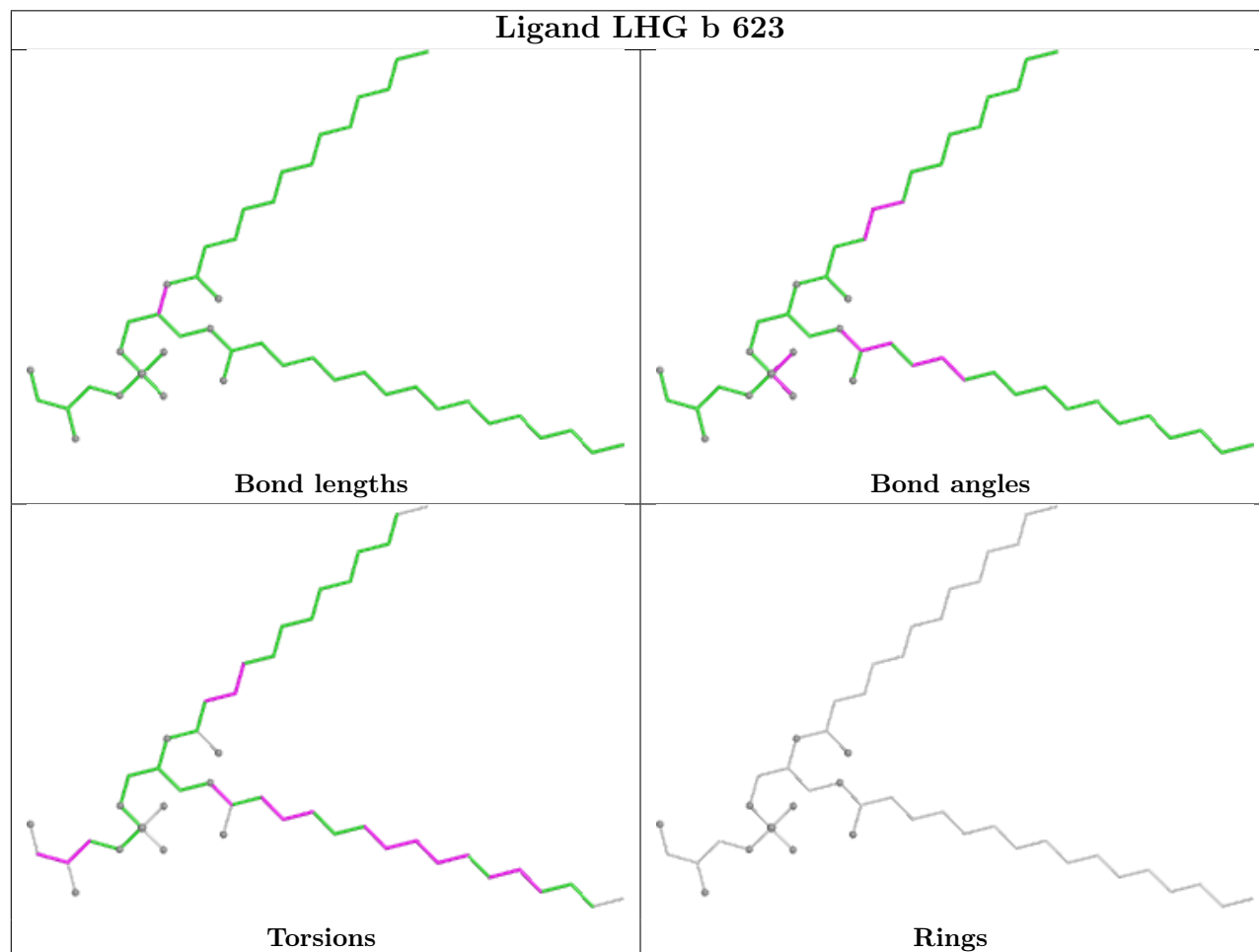
Ligand XAT BJ 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

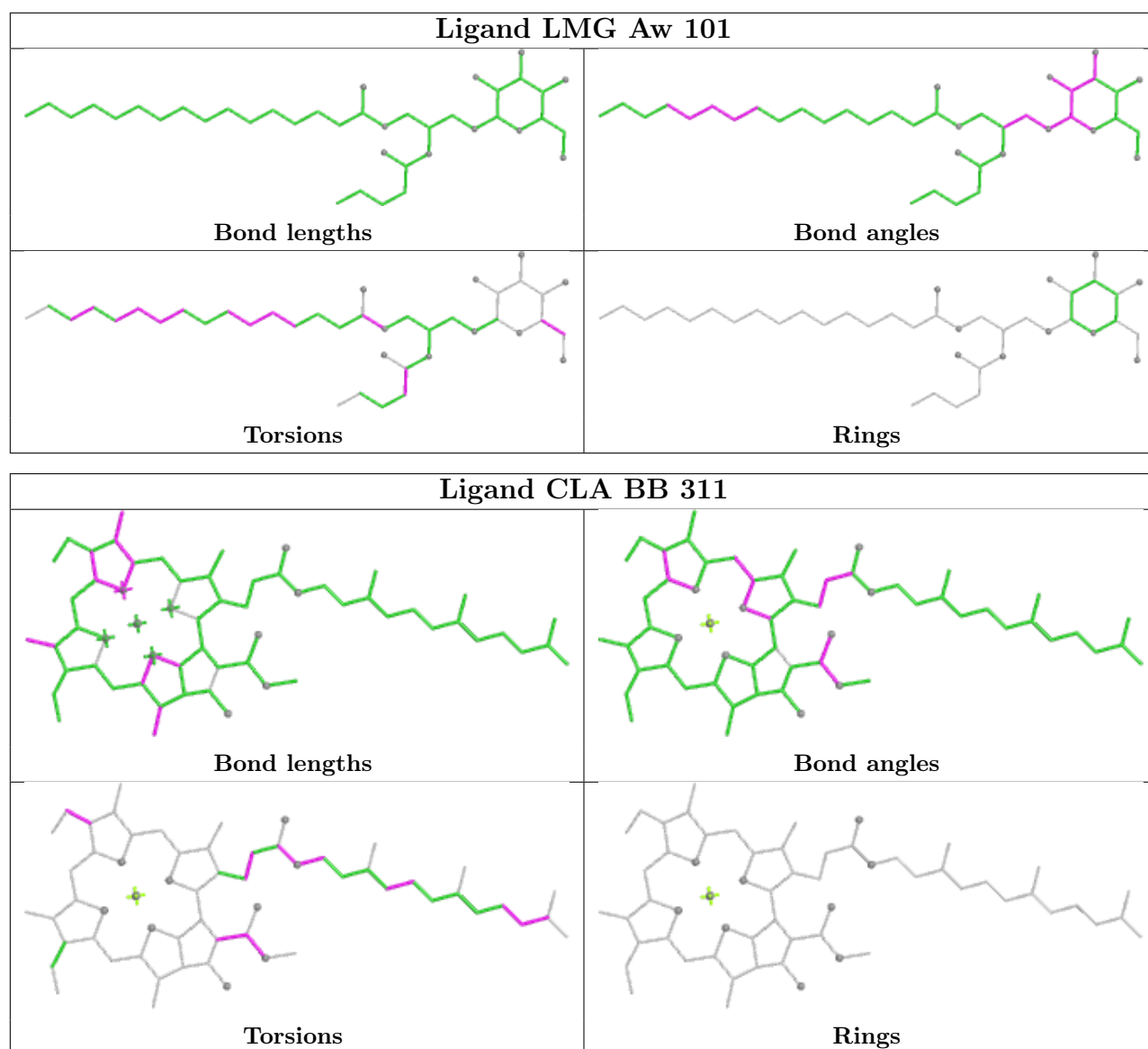
Ligand CLA BV 611

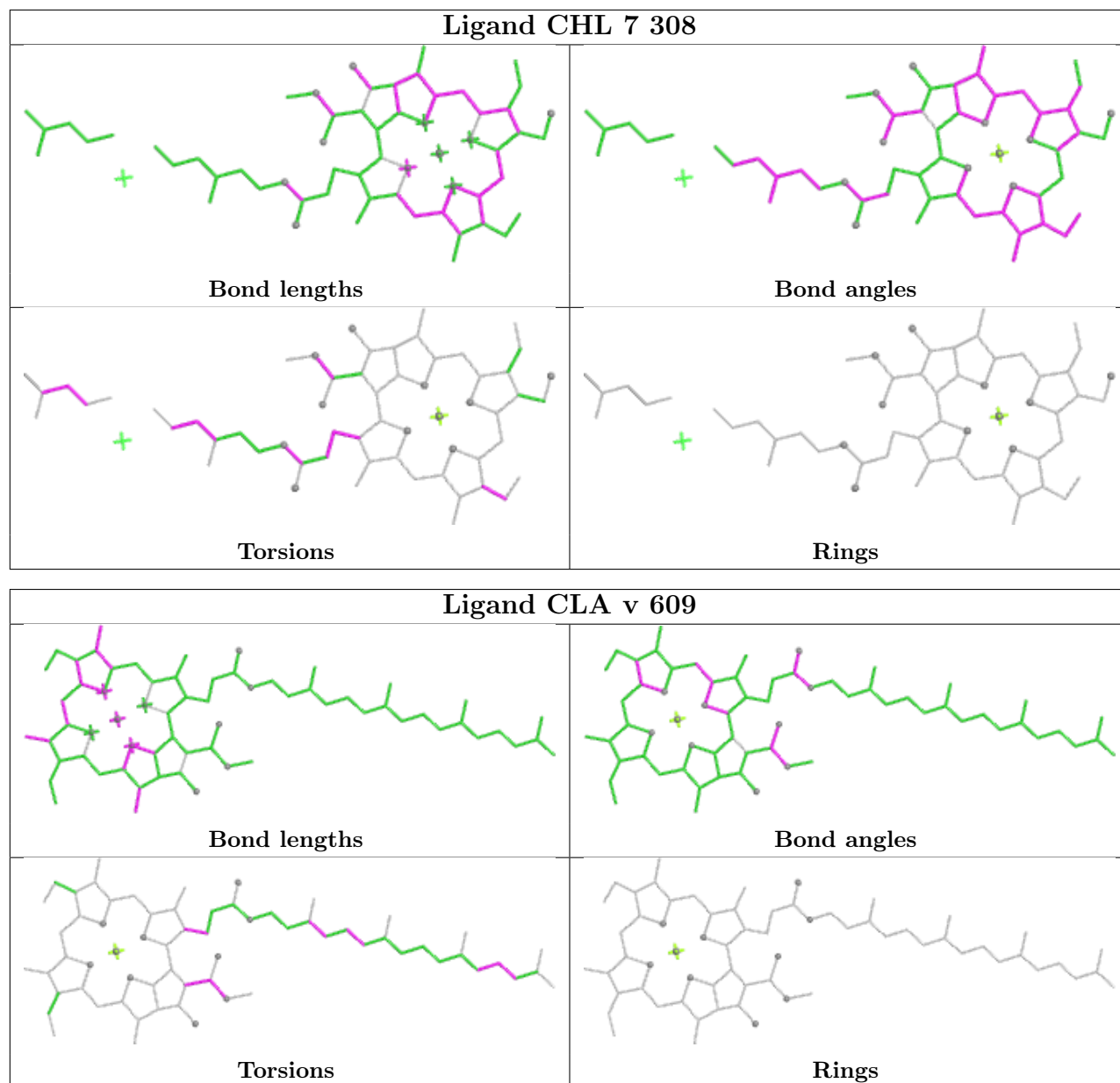


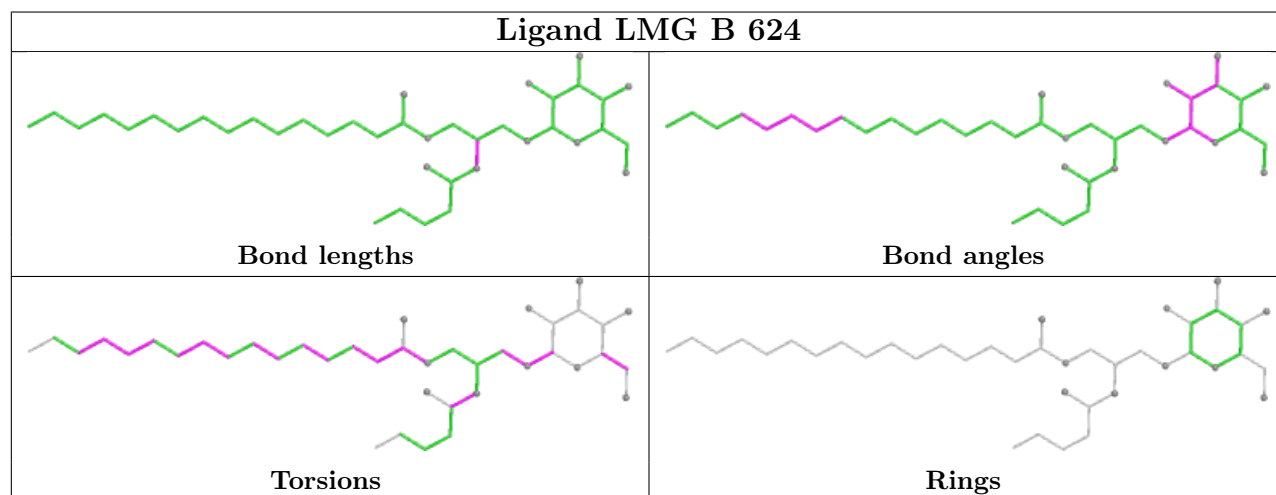
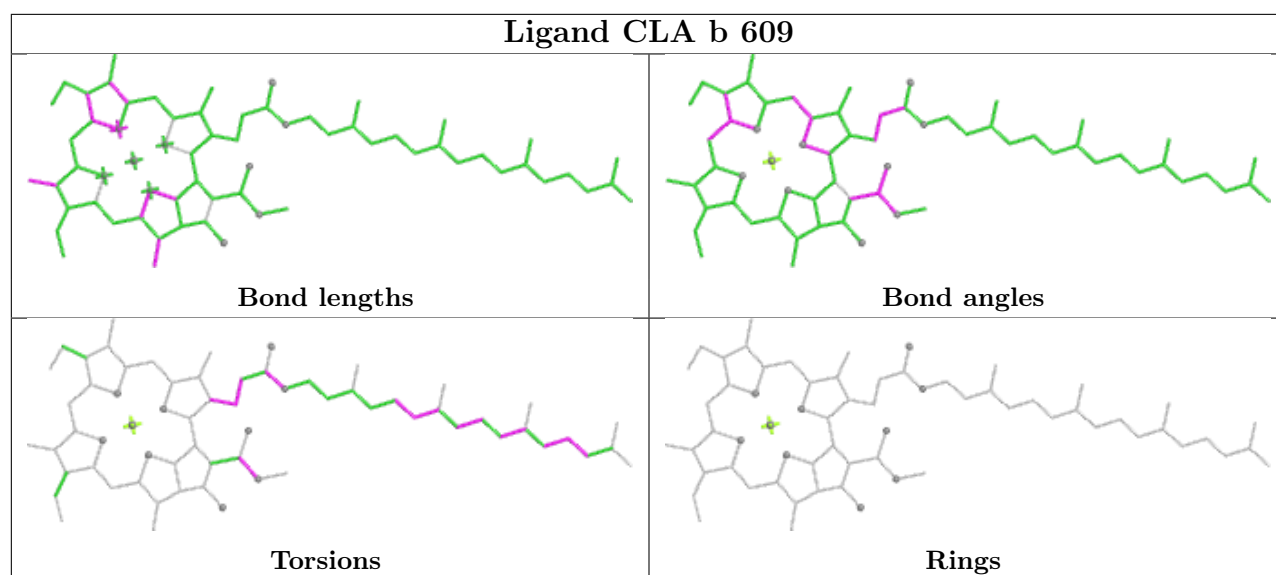
Ligand BCR B 623

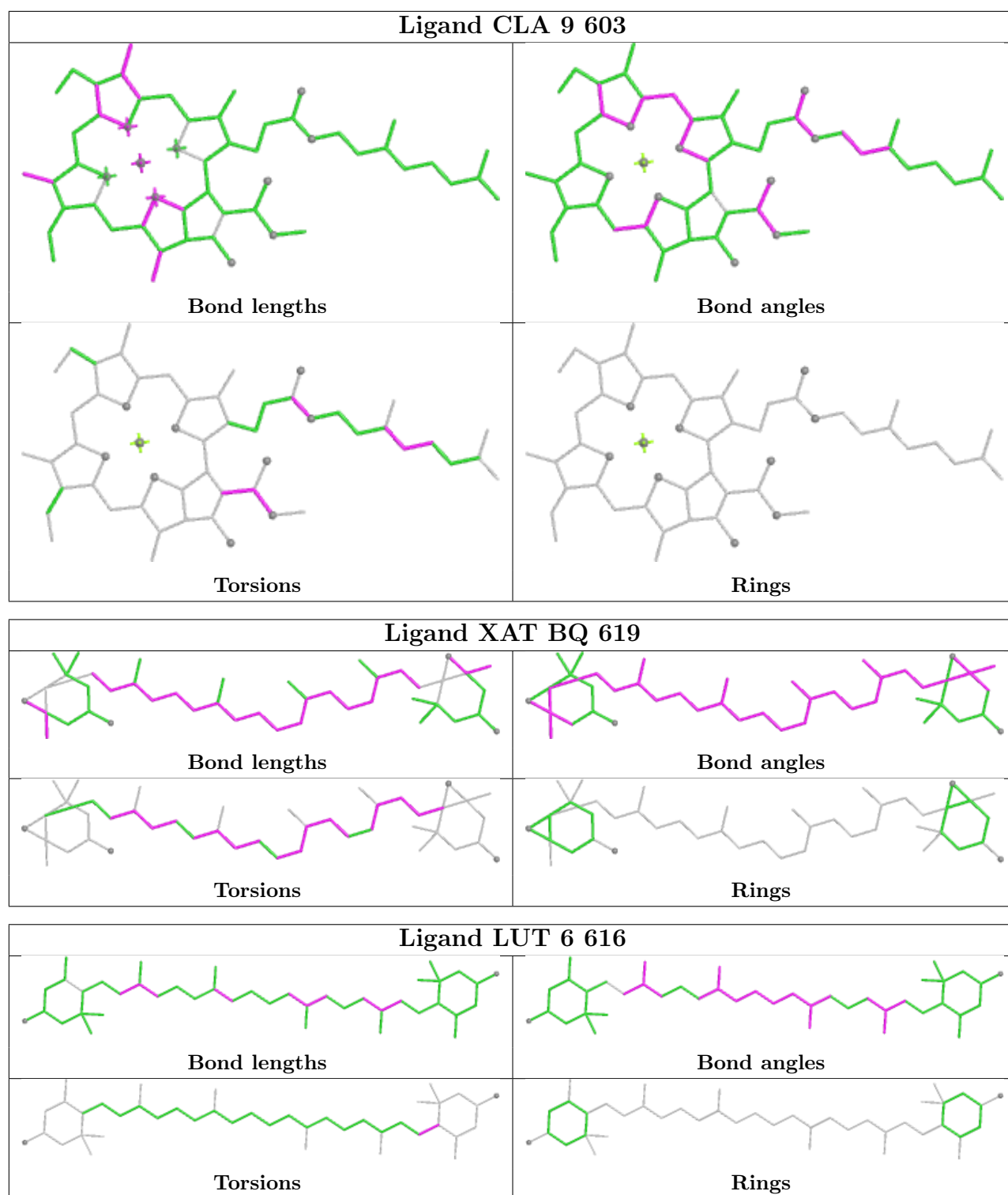


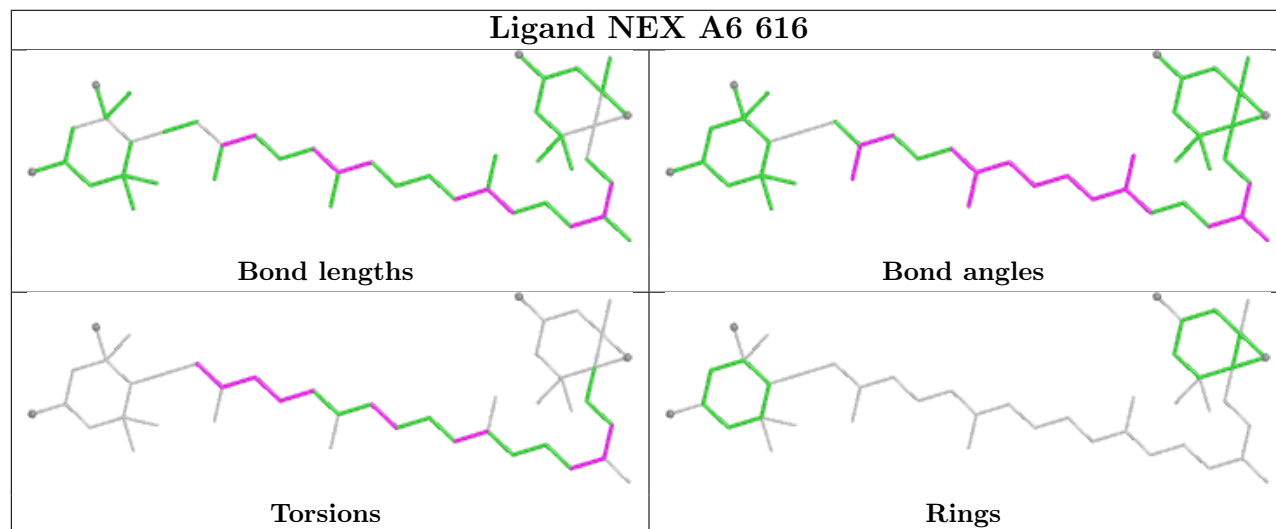
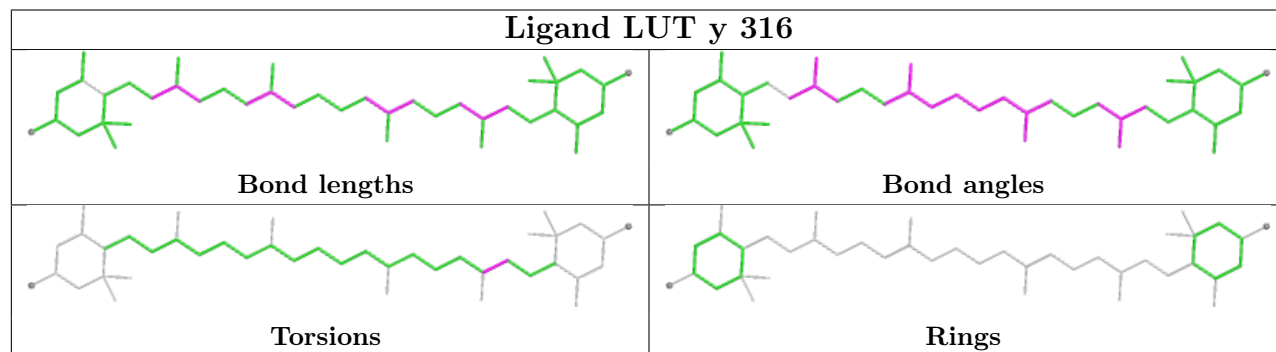
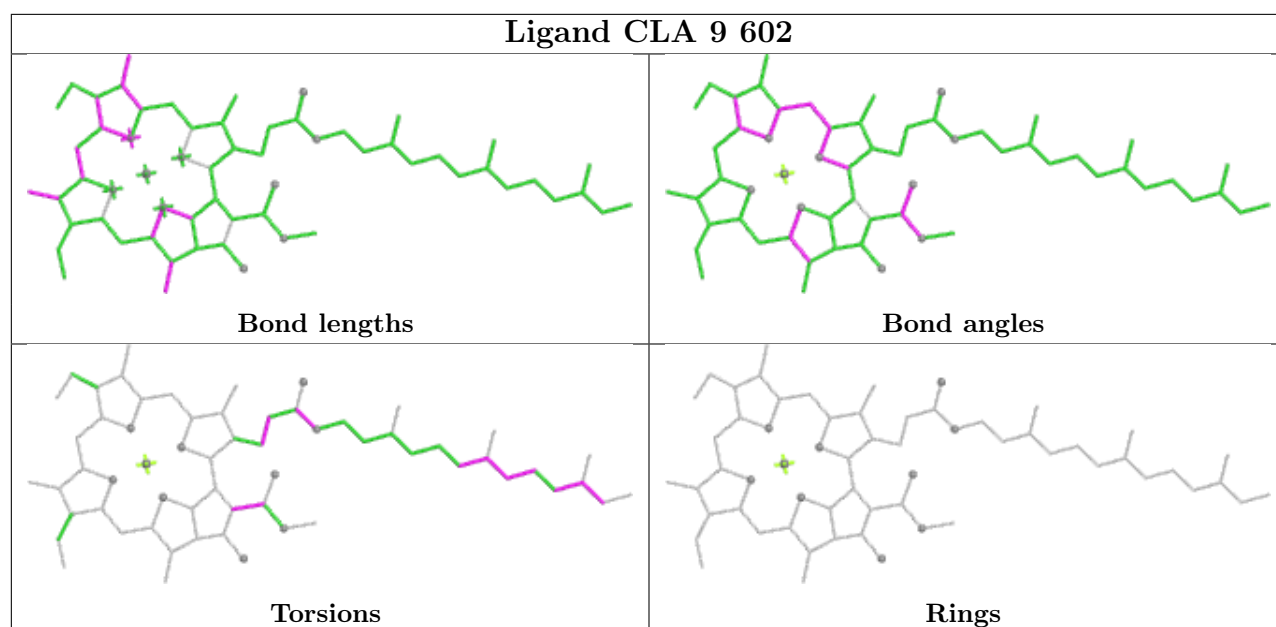
Ligand CLA C 512**Ligand LHG b 623**

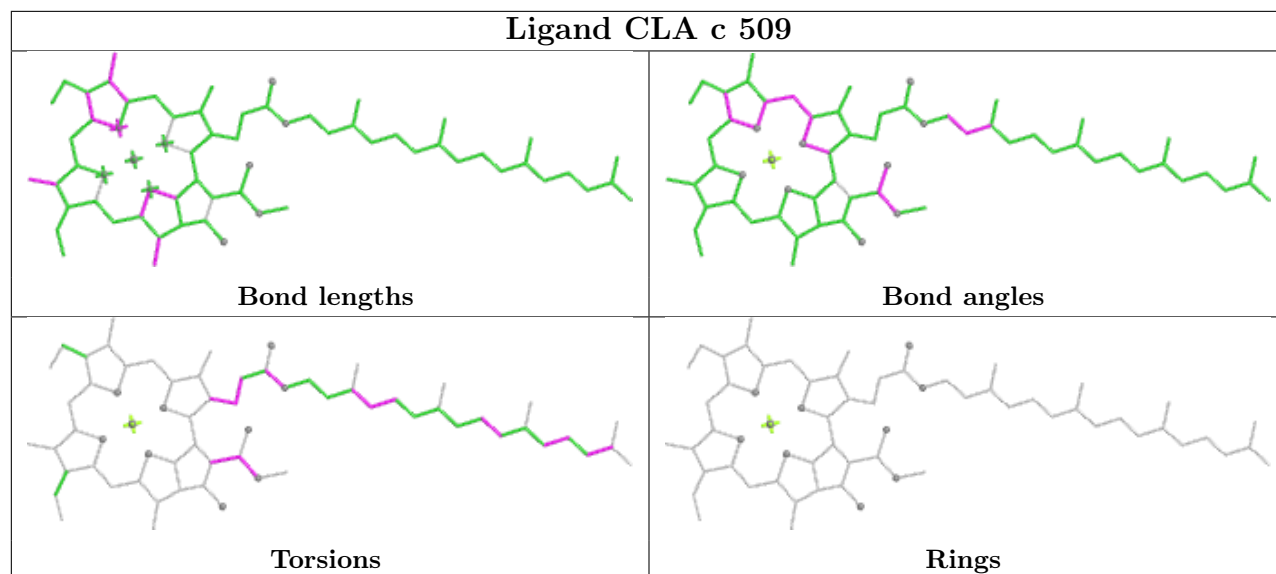
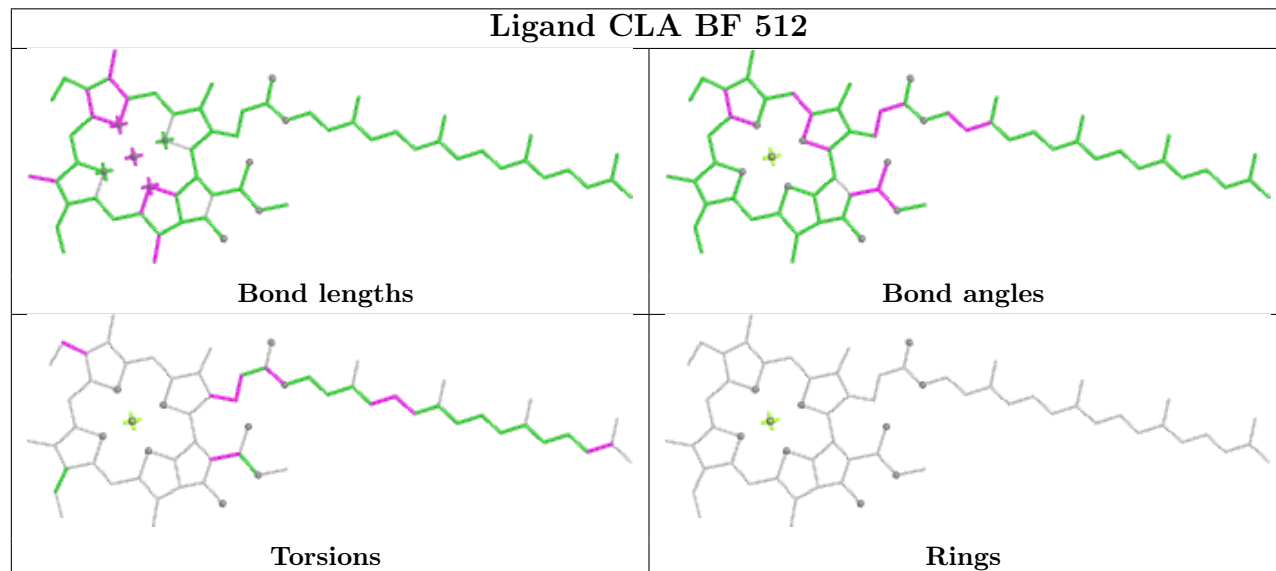




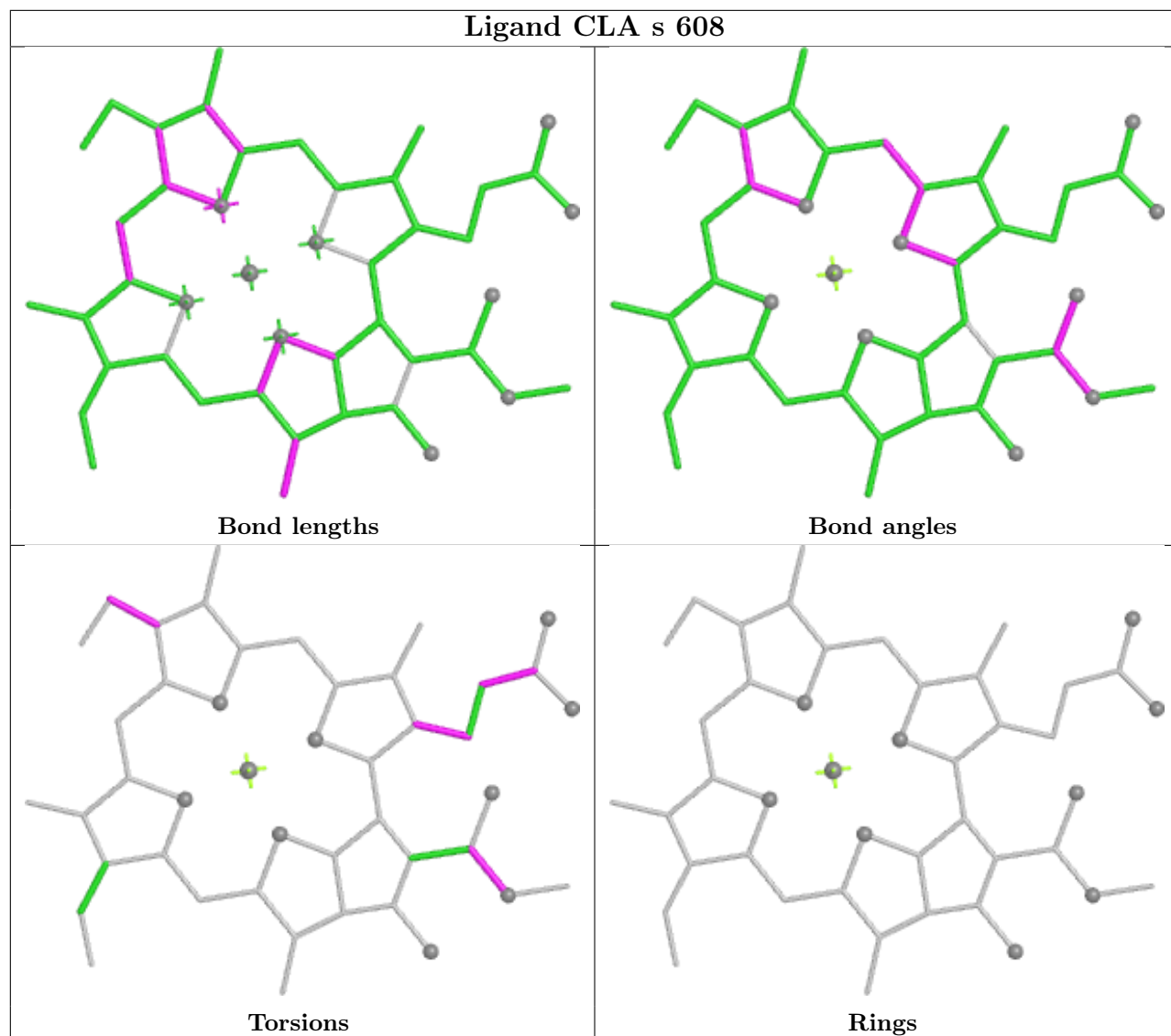




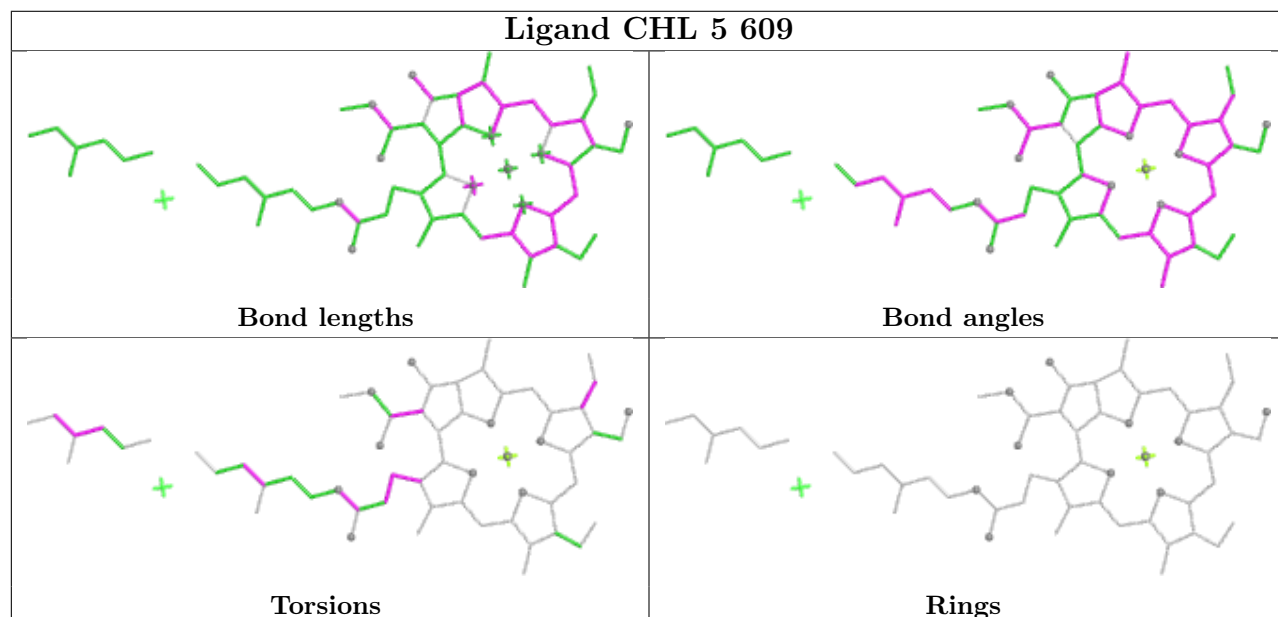


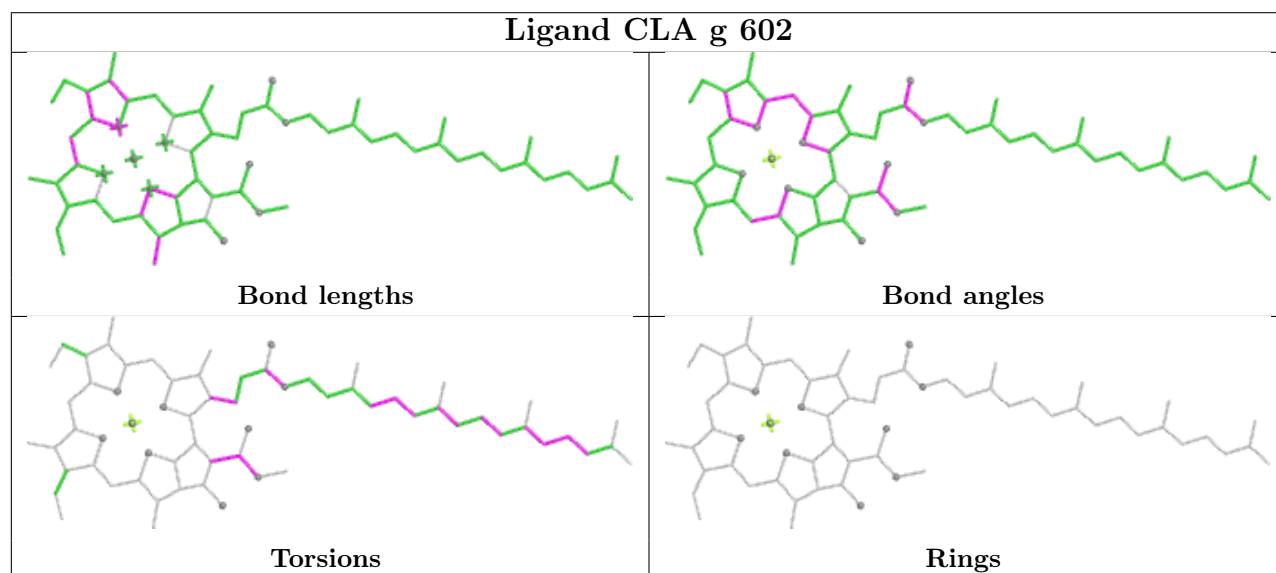
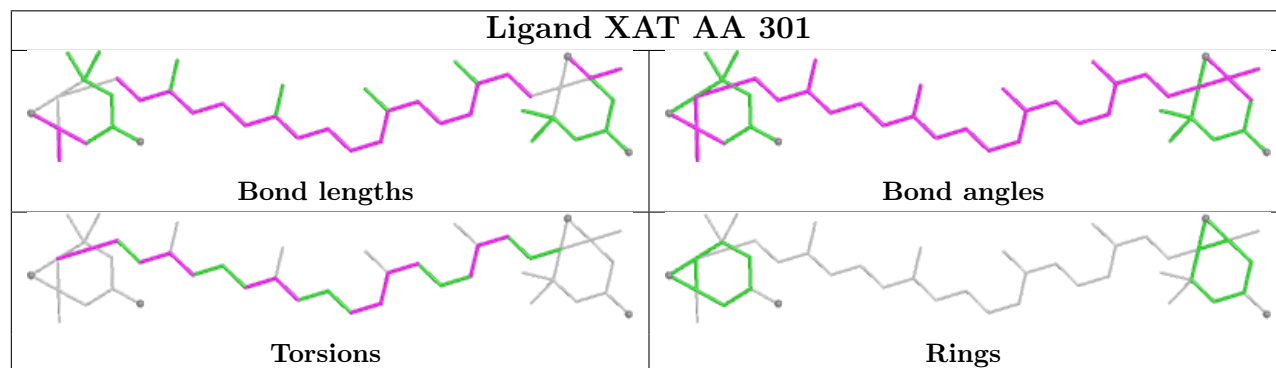
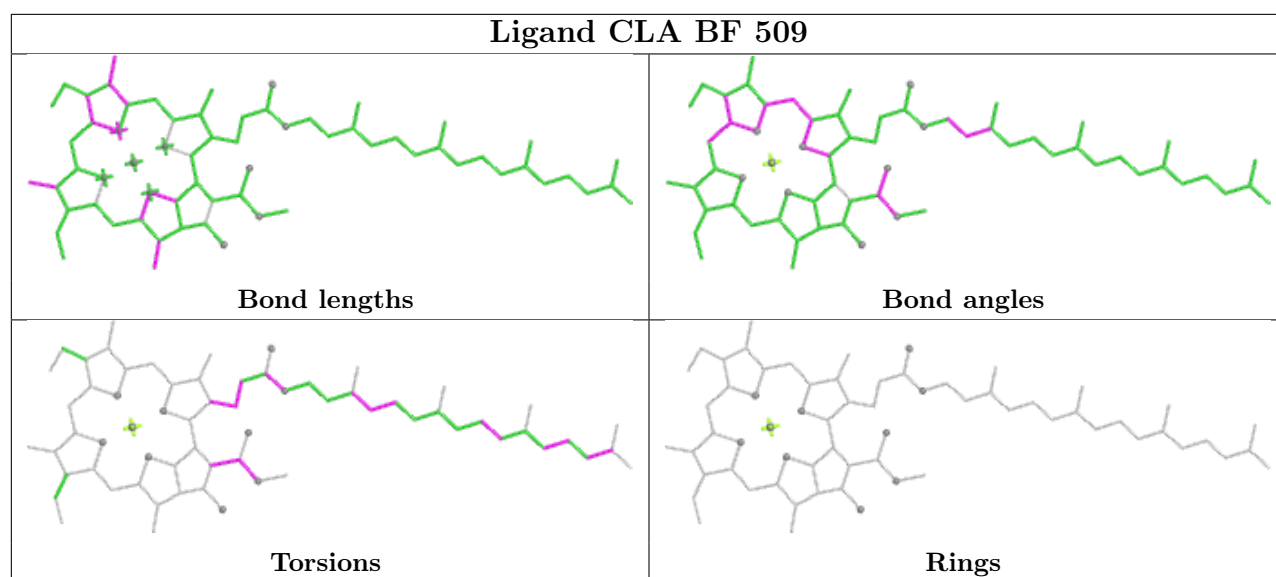
Ligand CLA c 509**Ligand CLA BF 512**

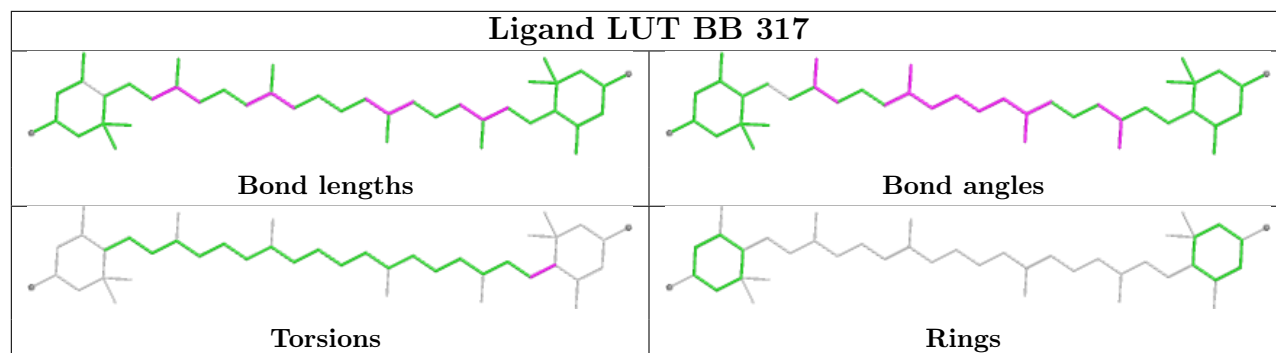
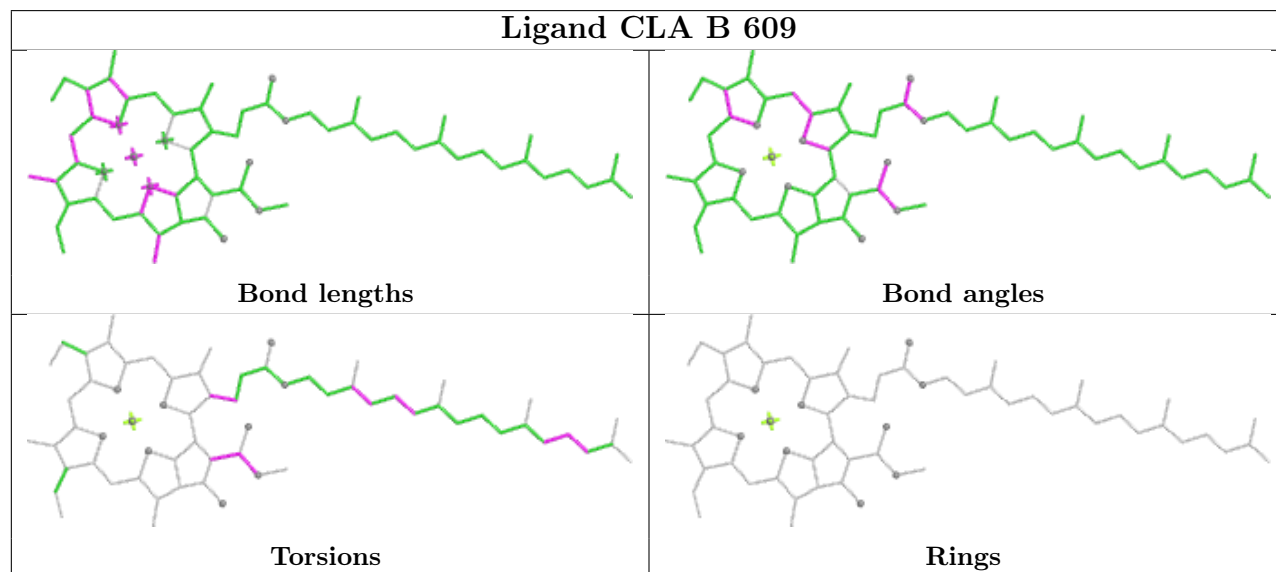
Ligand CLA s 608

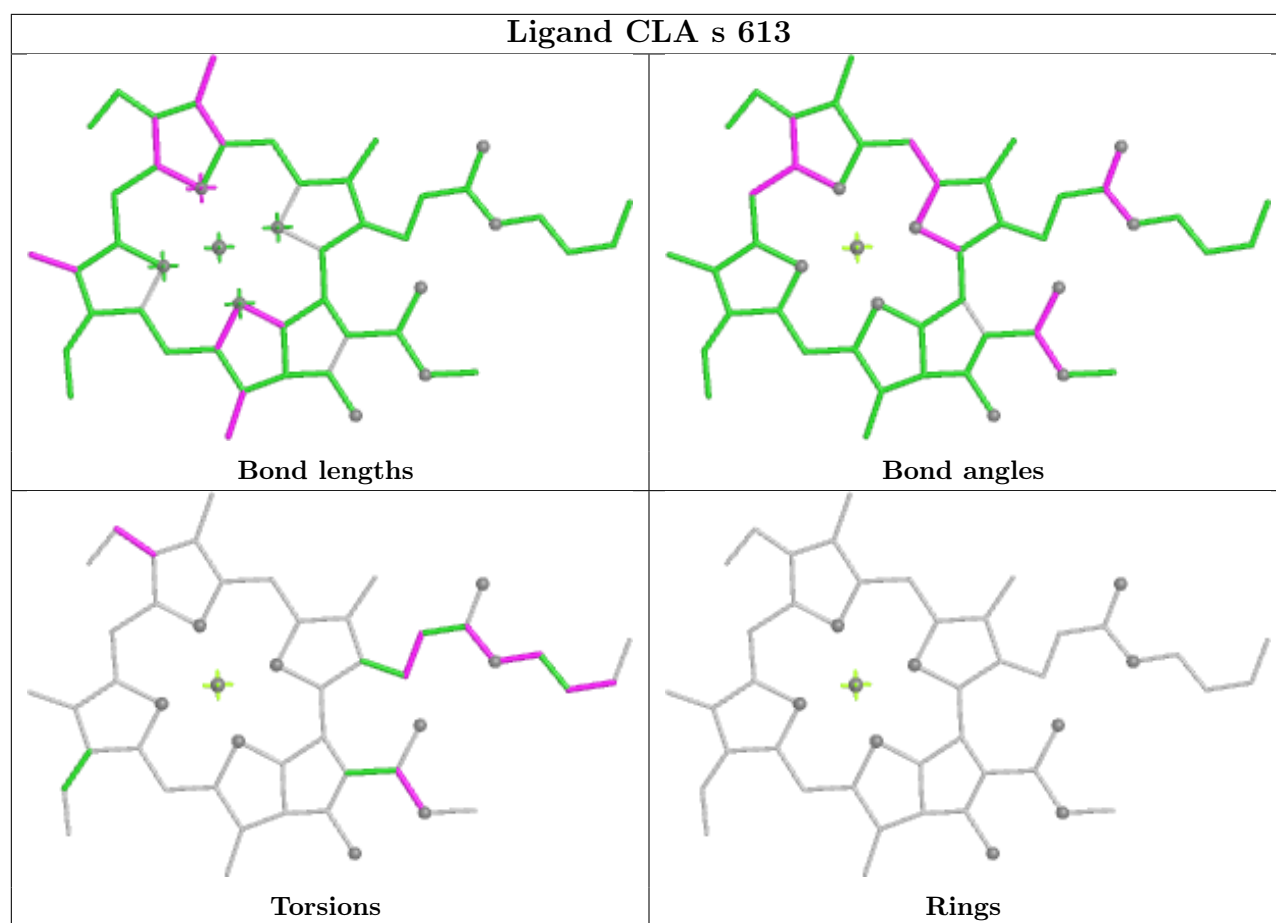


Ligand CHL 5 609

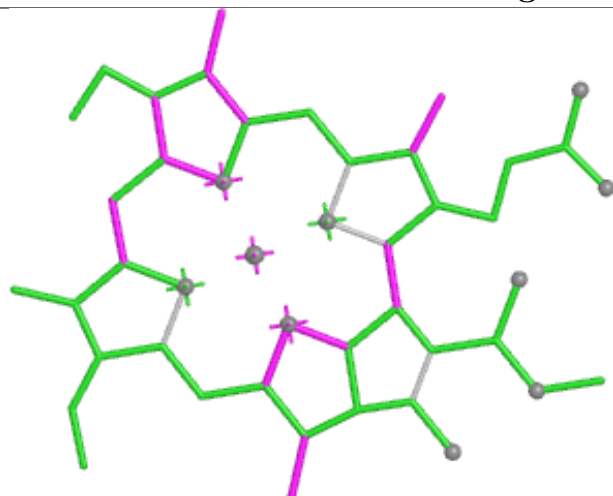




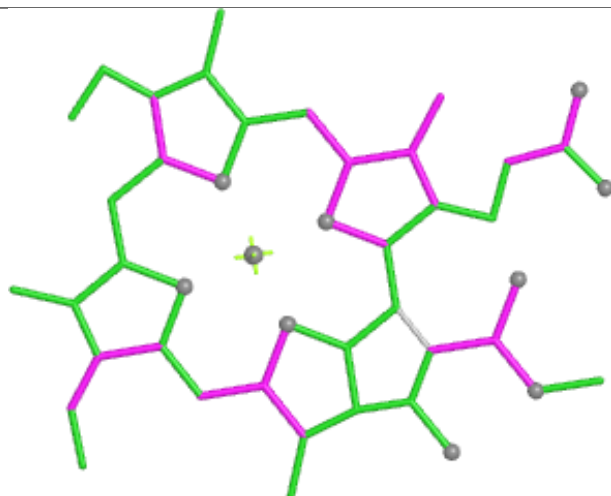
Ligand LUT BB 317**Ligand CLA B 609**



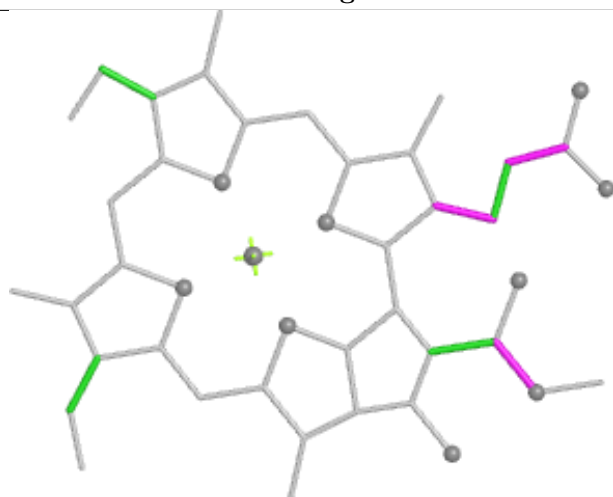
Ligand CLA 8 308



Bond lengths



Bond angles

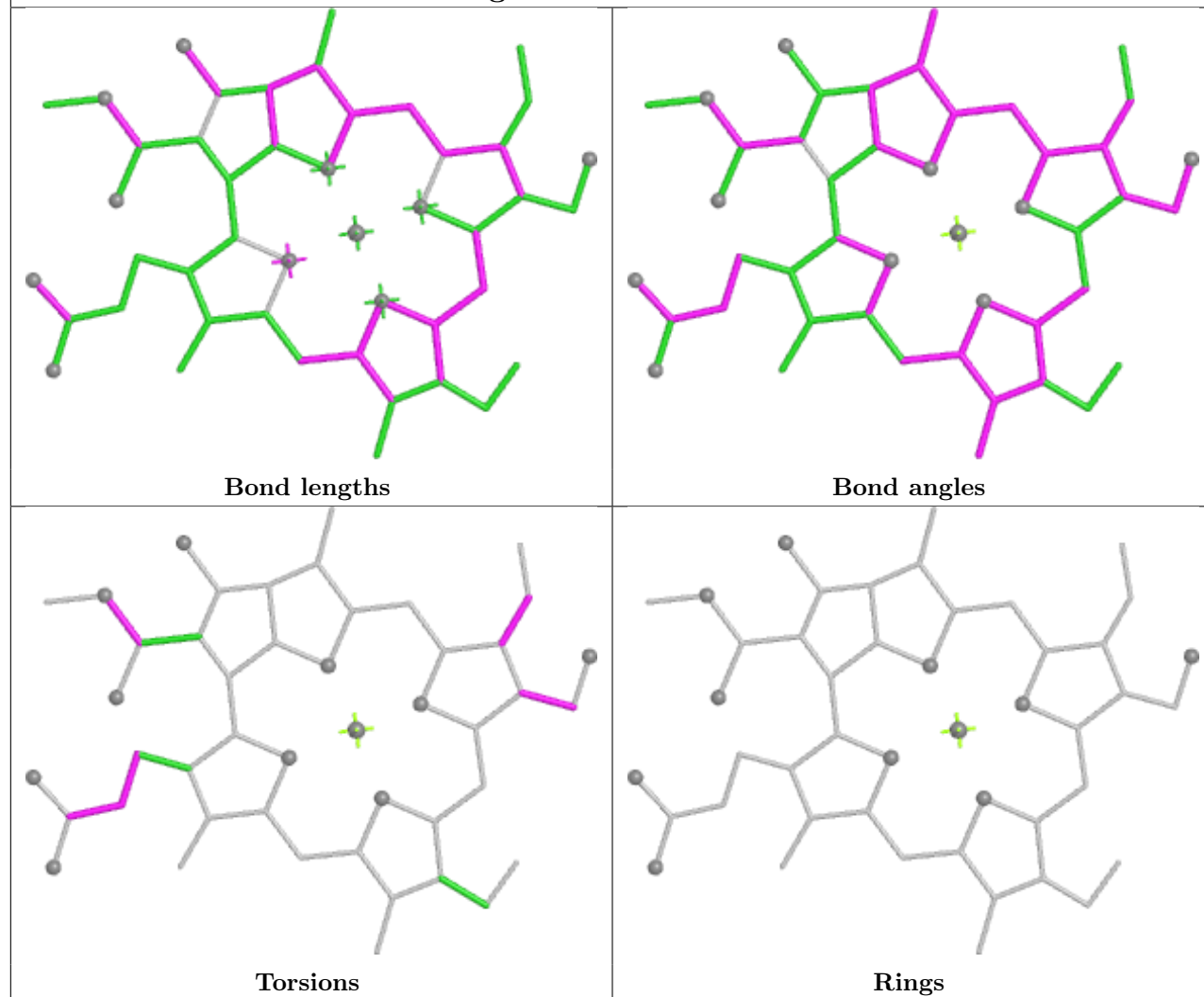


Torsions

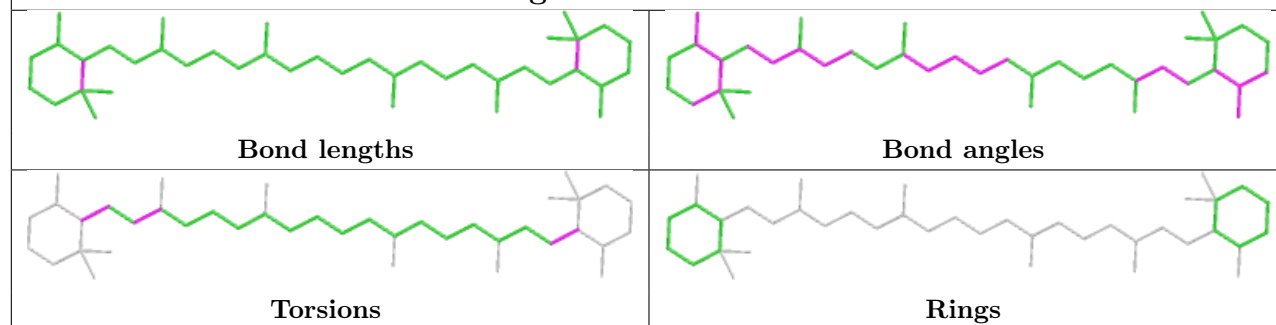


Rings

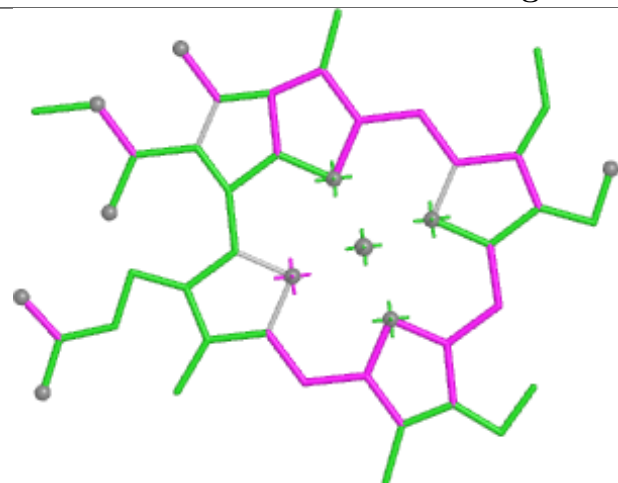
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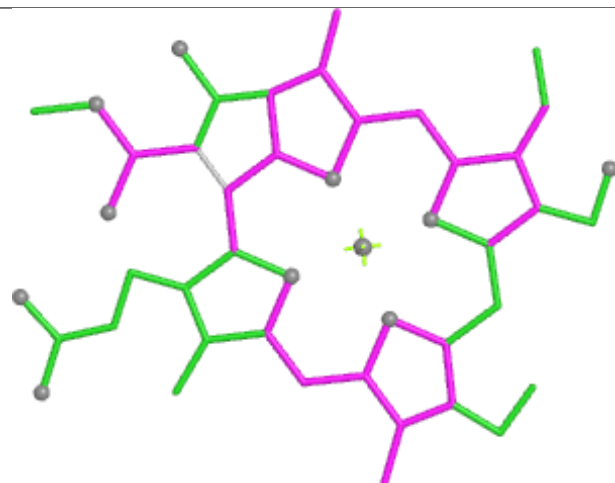
Ligand BCR H 101



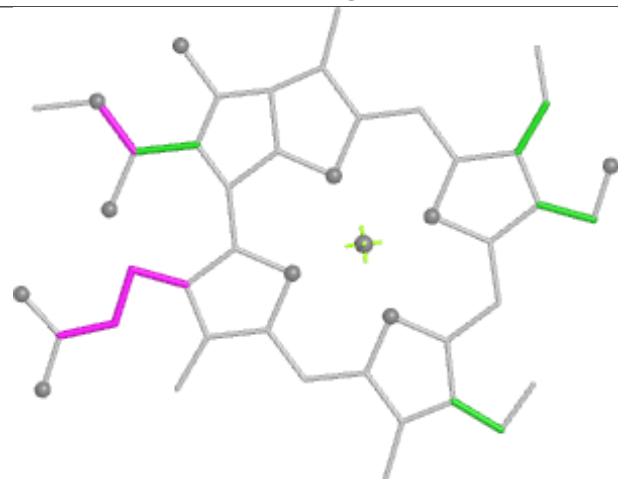
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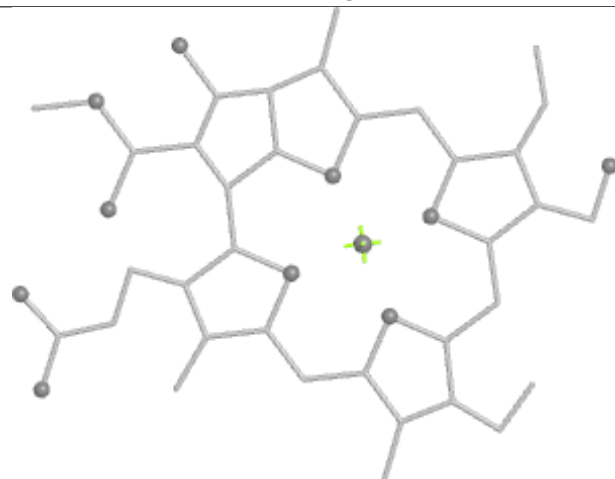
Bond lengths



Bond angles

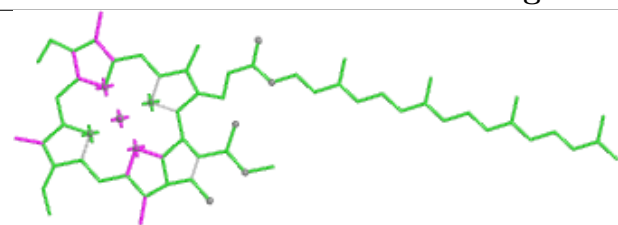


Torsions

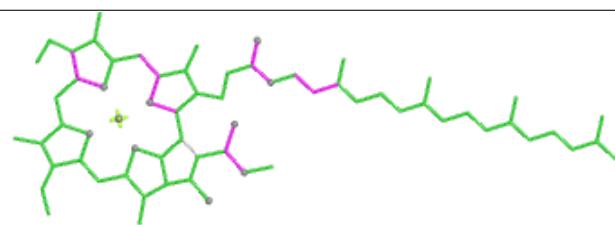


Rings

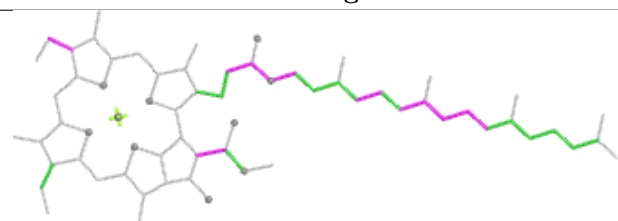
Ligand CLA c 513



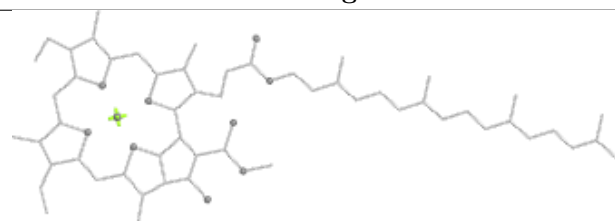
Bond lengths



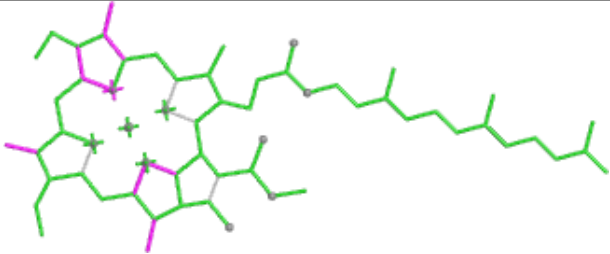
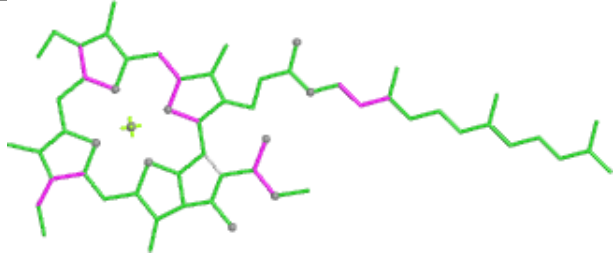
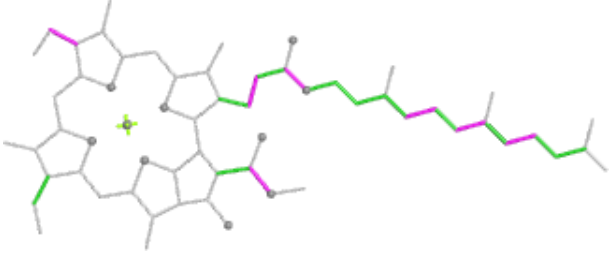
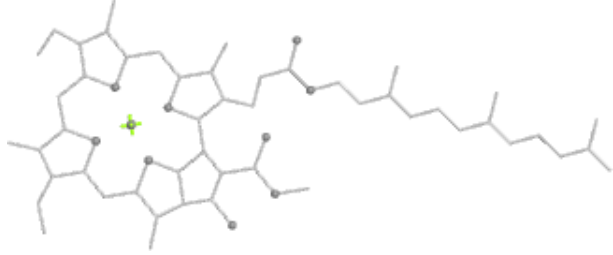
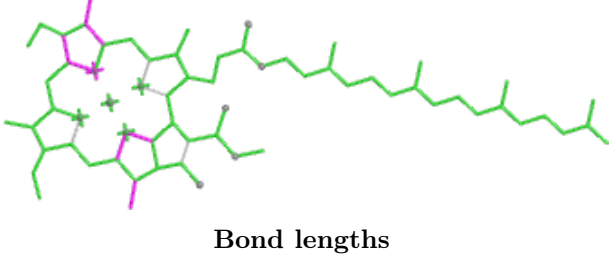
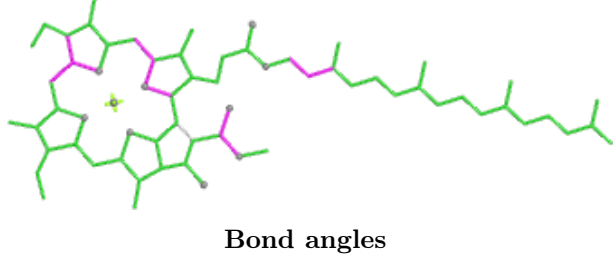
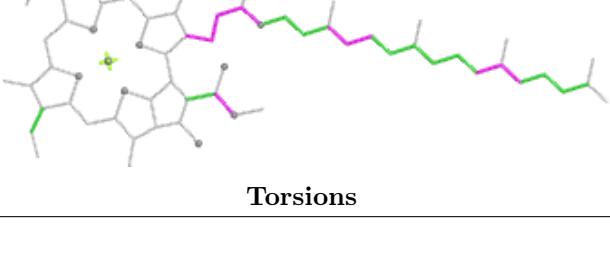
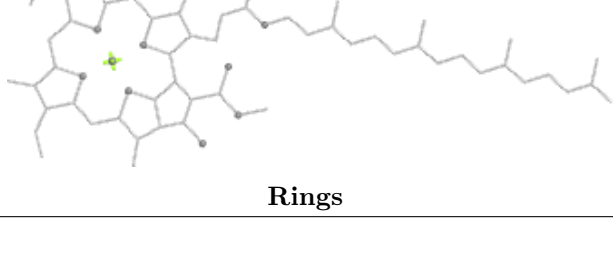
Bond angles



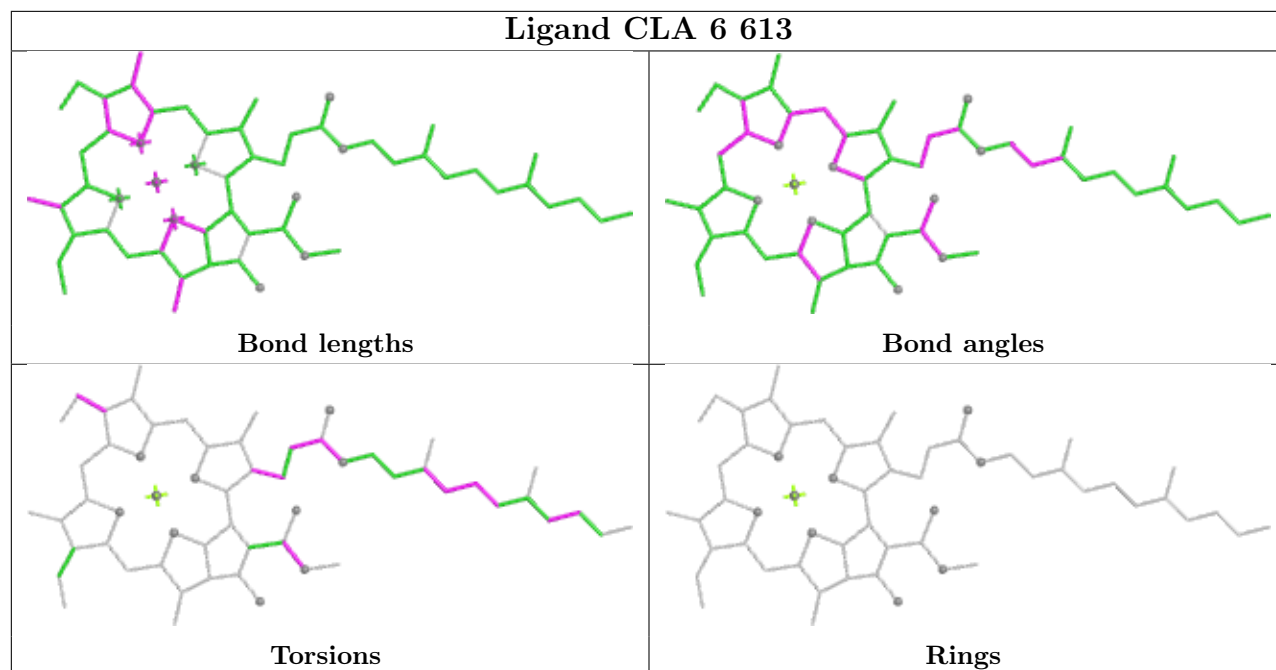
Torsions



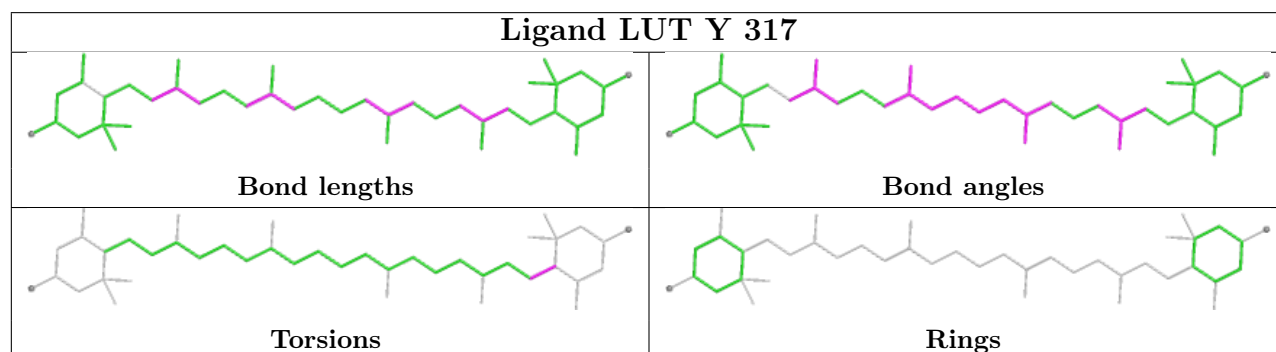
Rings

Ligand CLA N 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA y 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

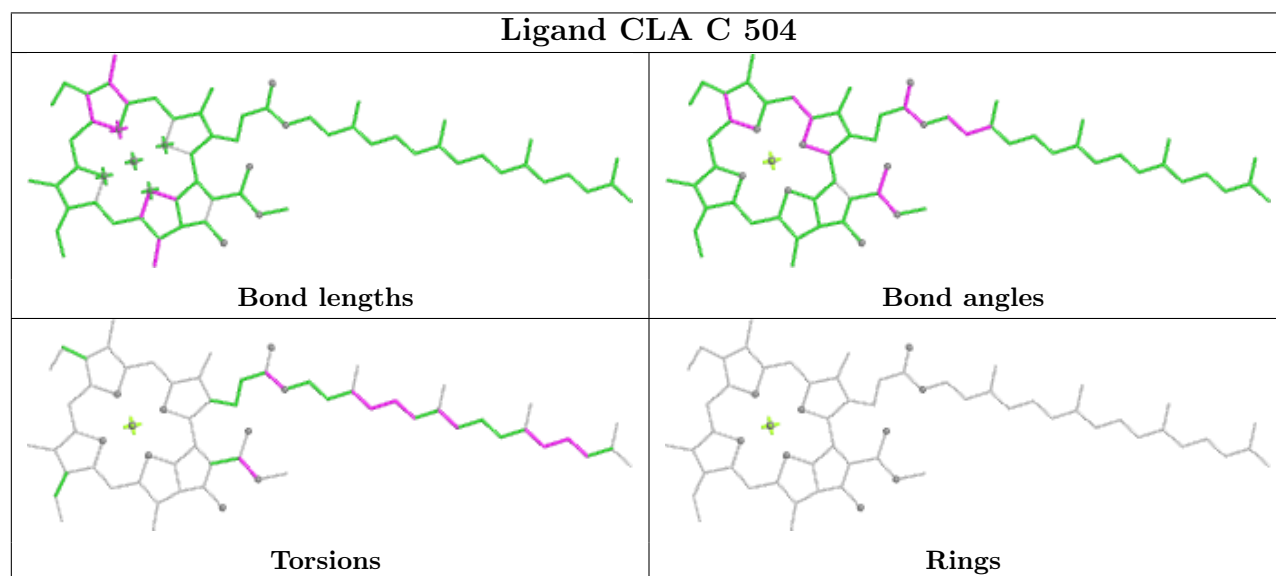
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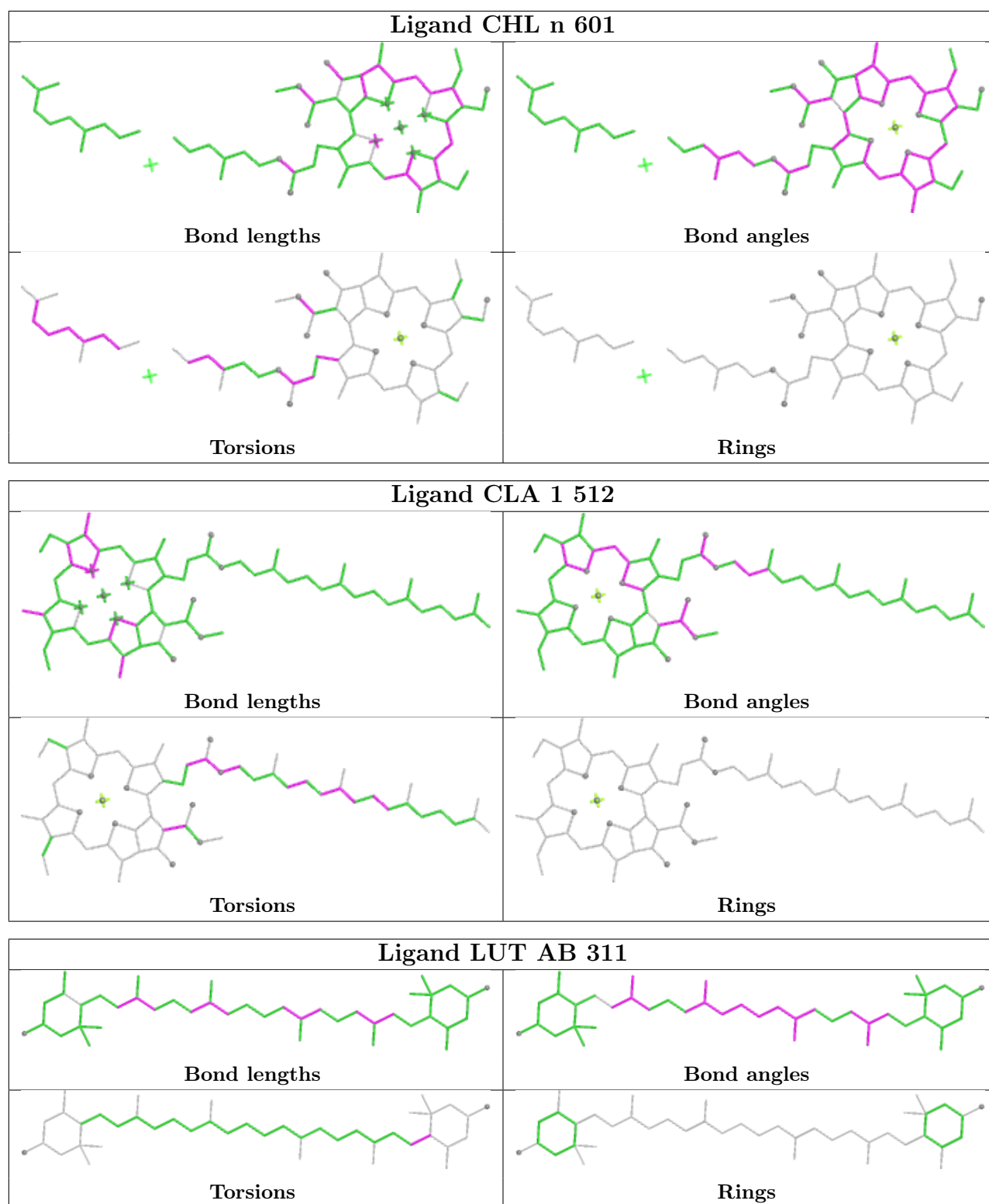


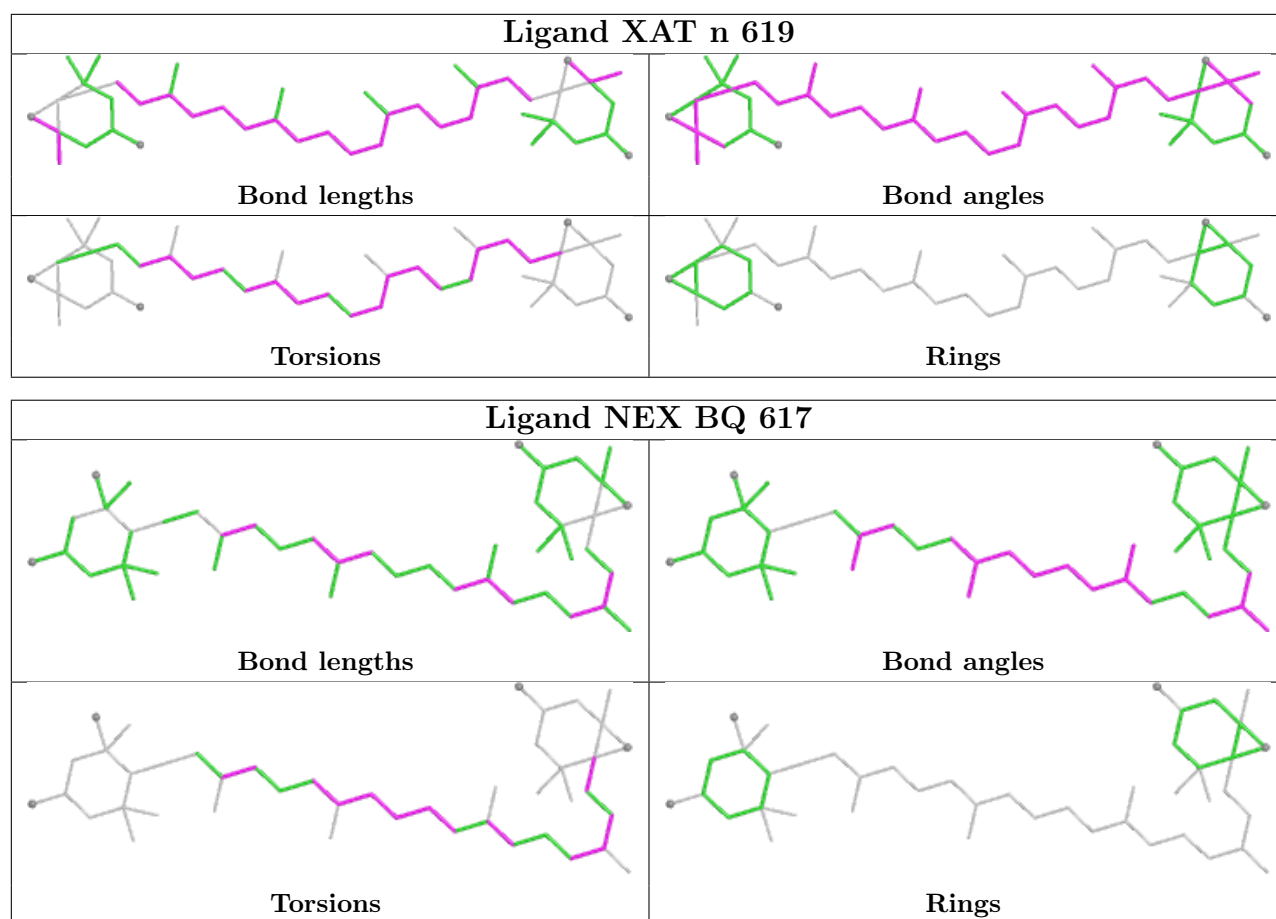
Ligand LUT Y 317



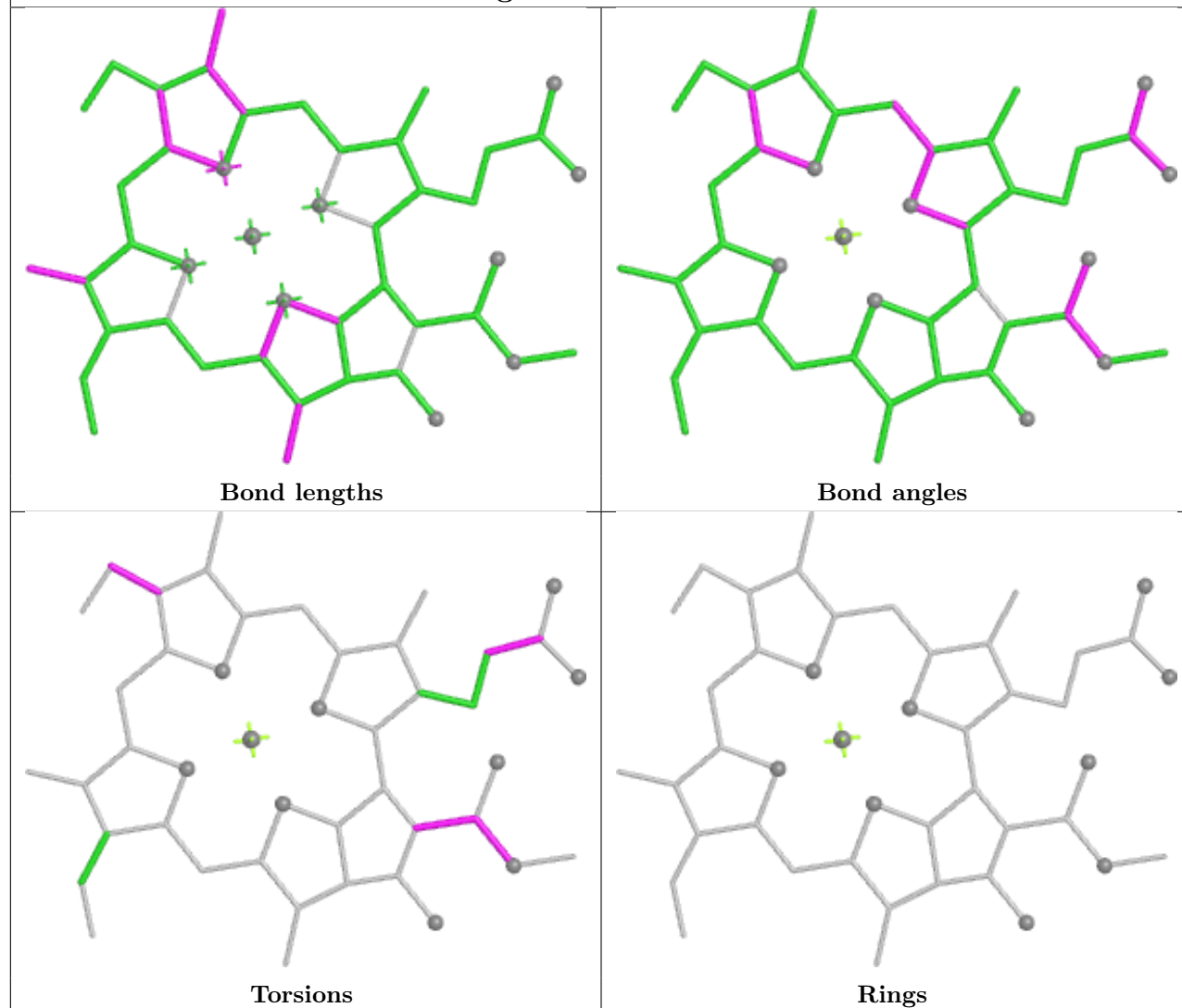
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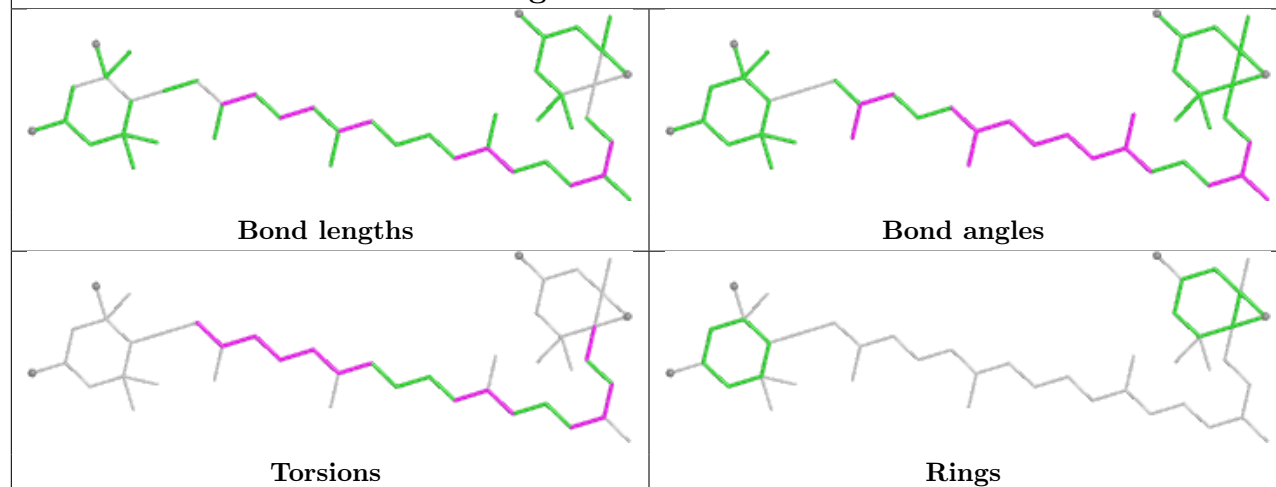


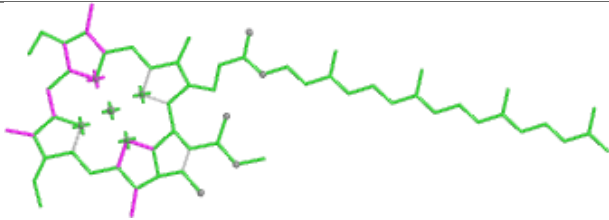
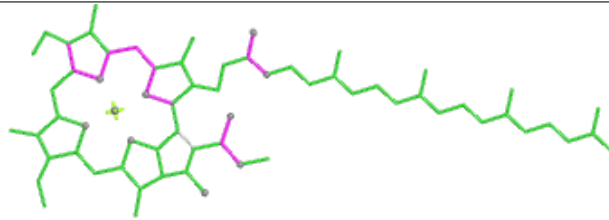
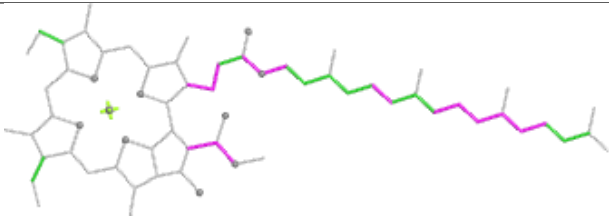
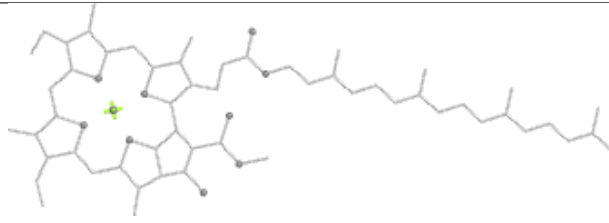


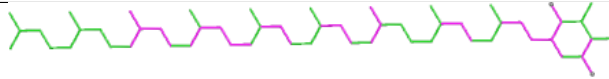
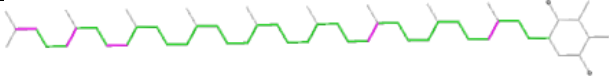
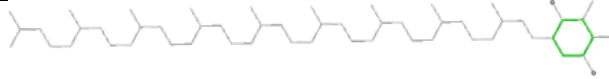
Ligand CLA 0 612

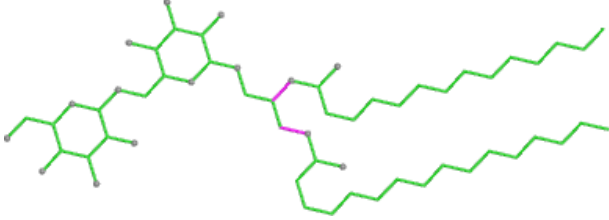
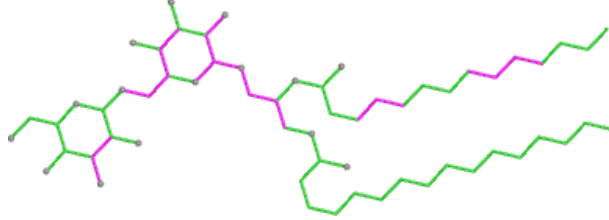
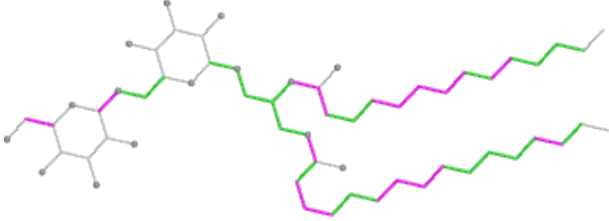
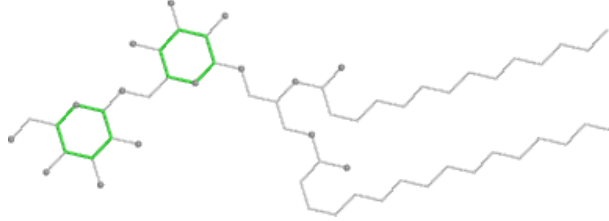


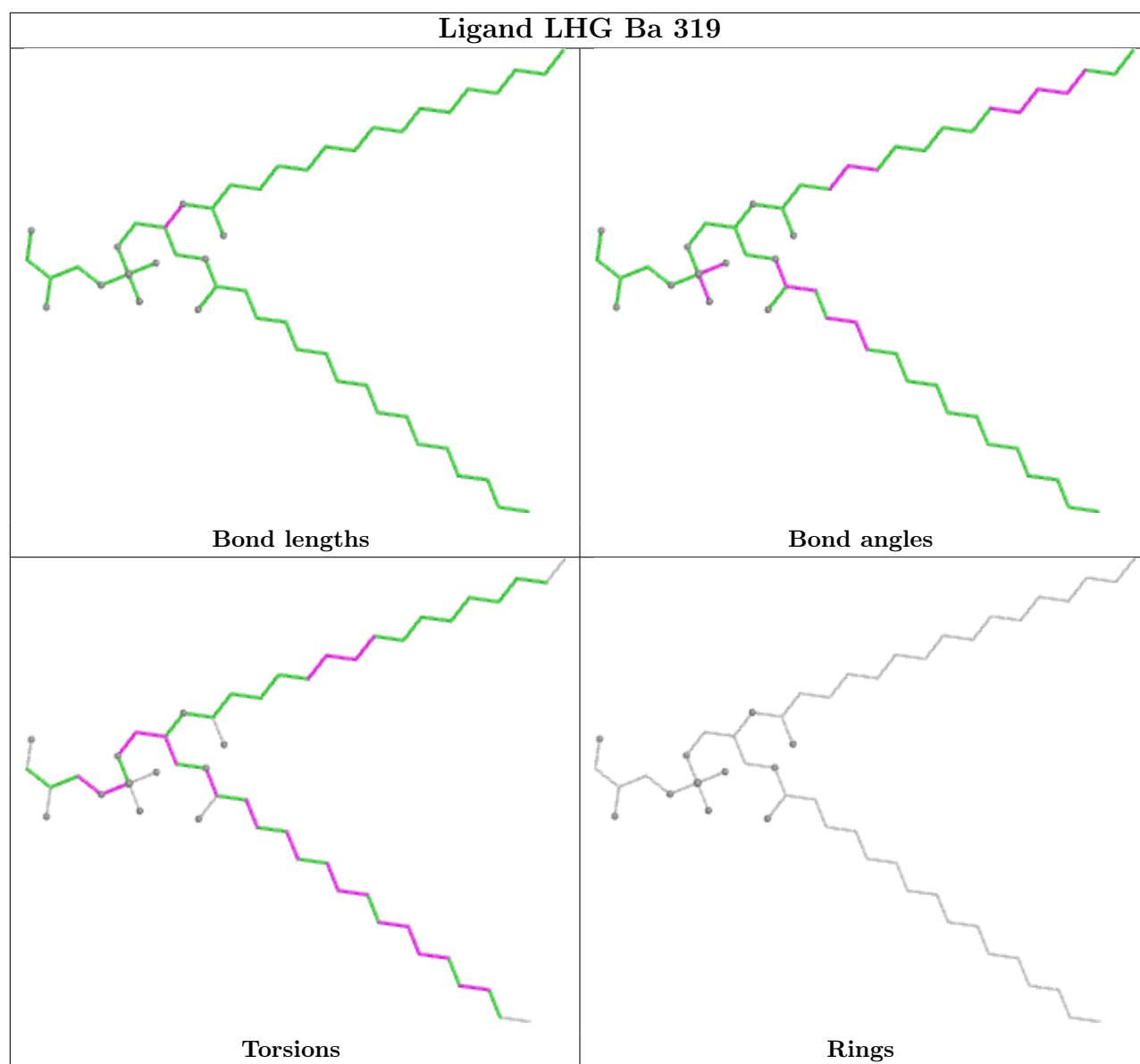
Ligand NEX G 617

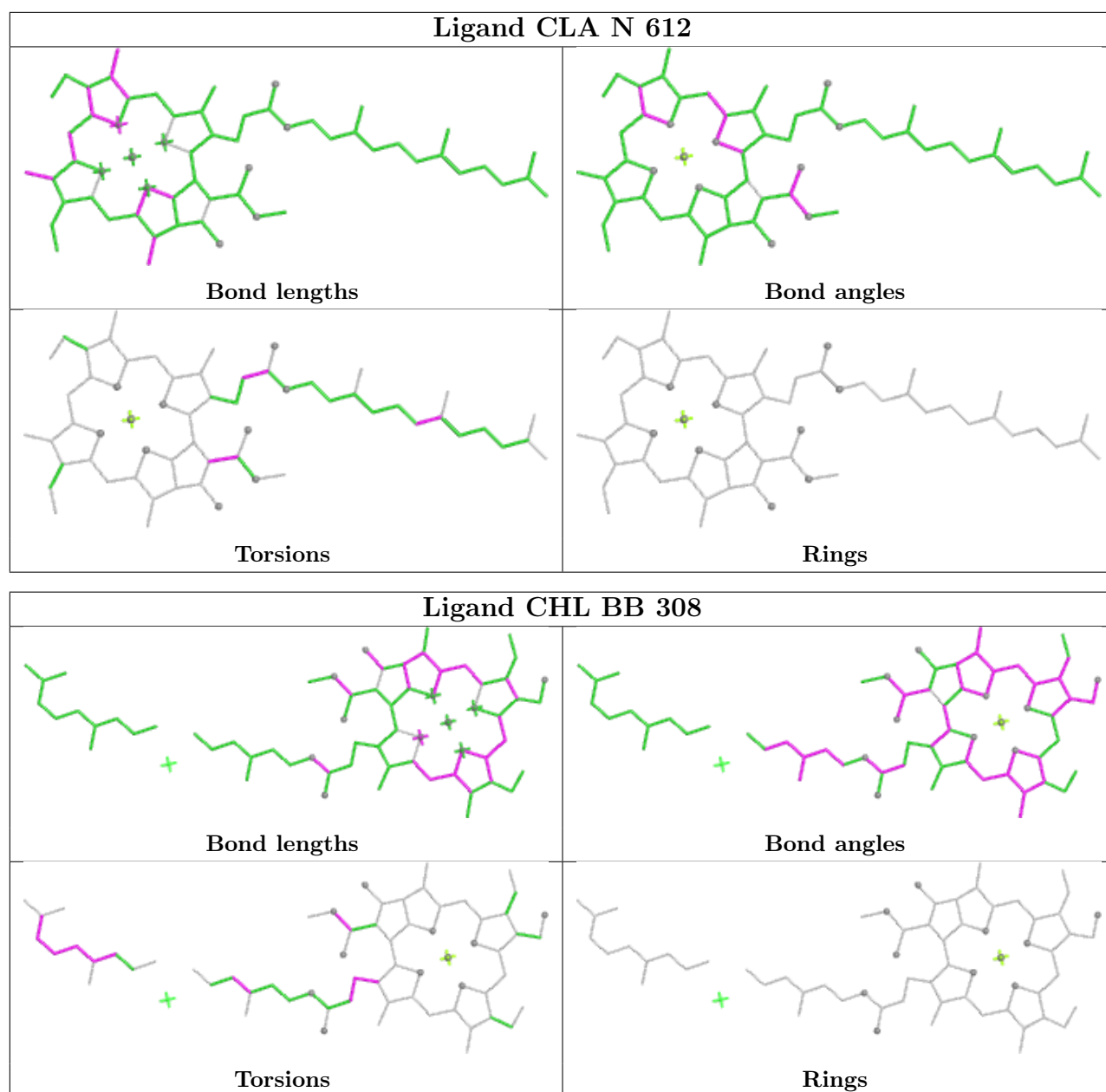


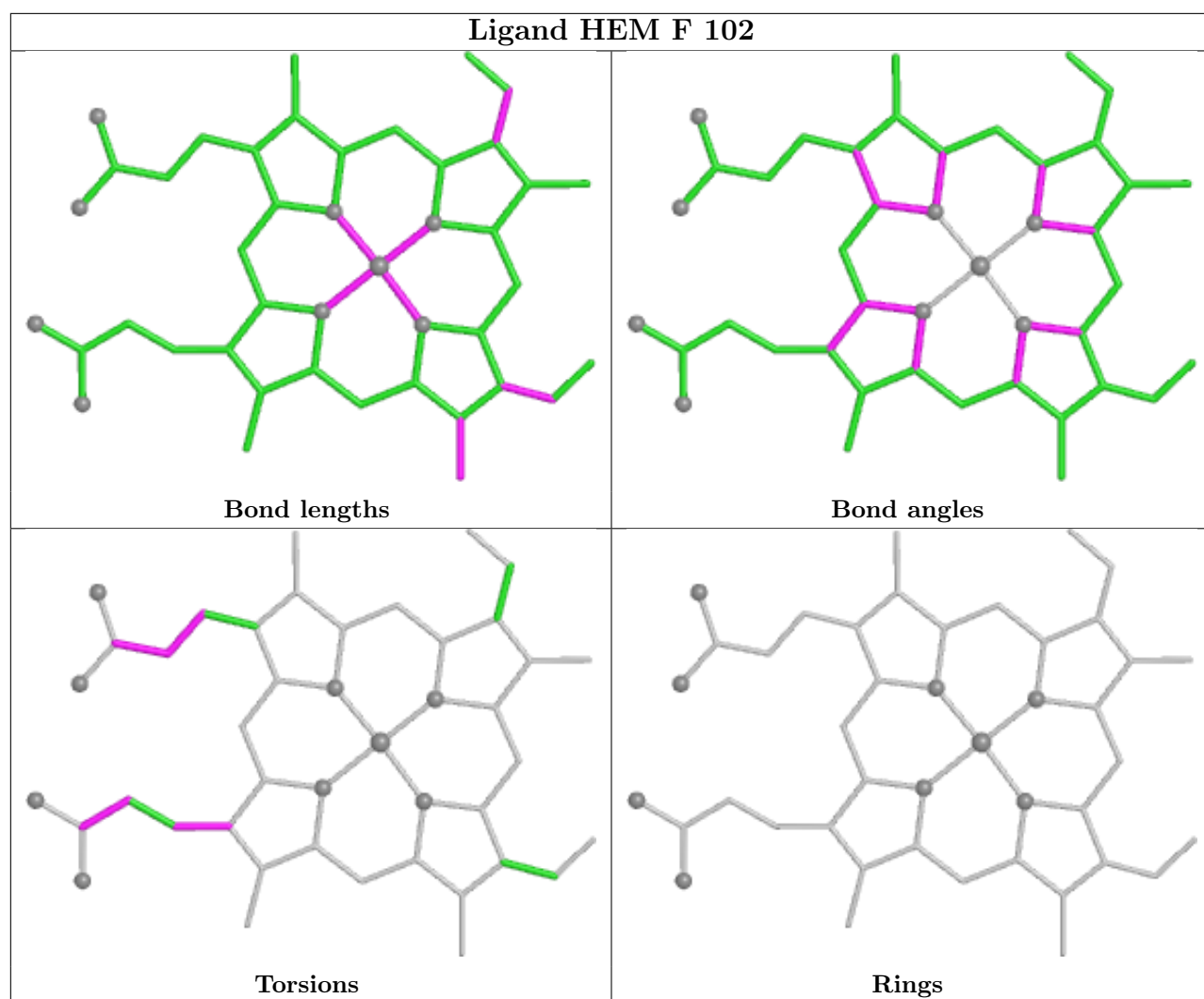
Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

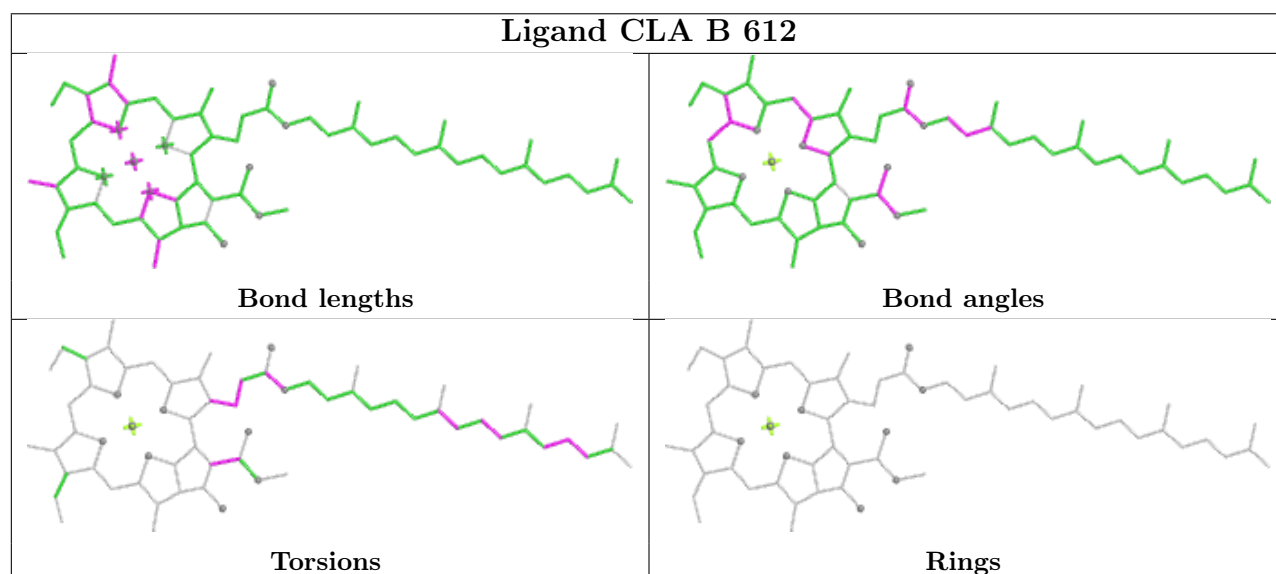
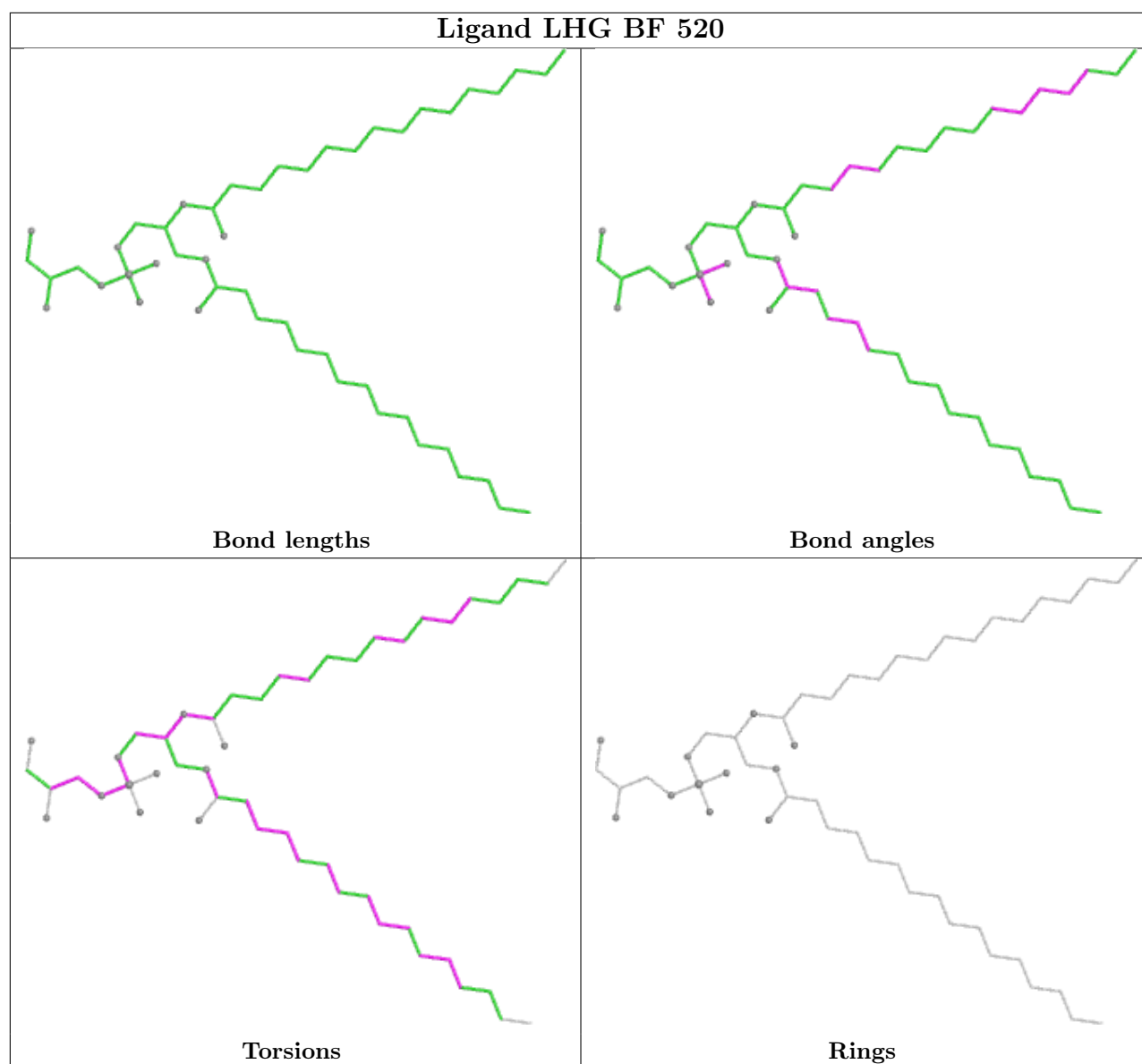
Ligand PL9 2 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

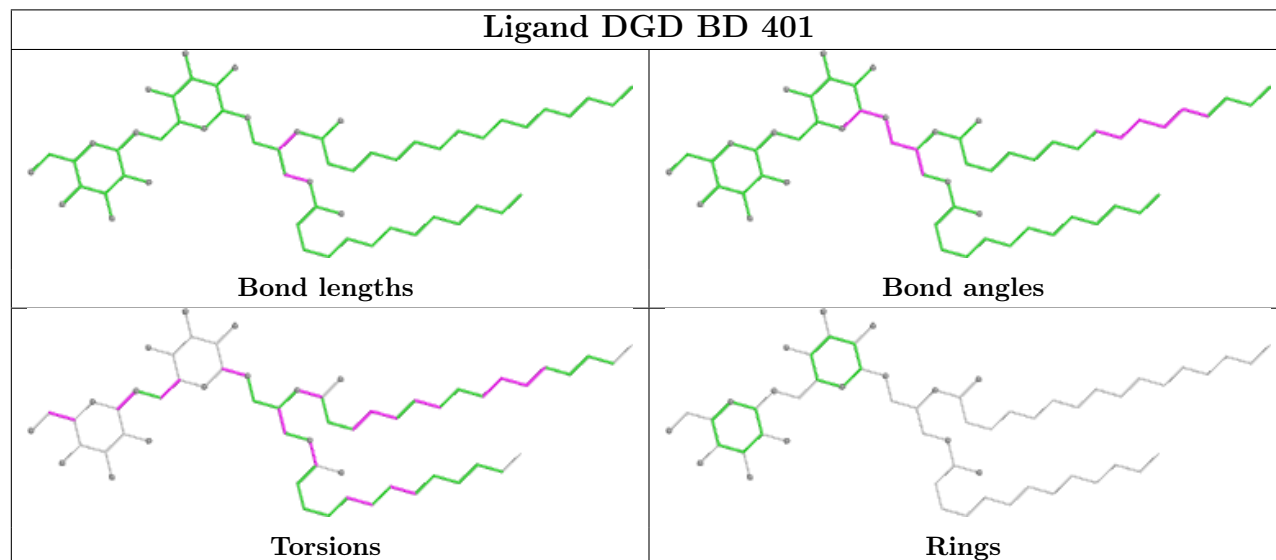
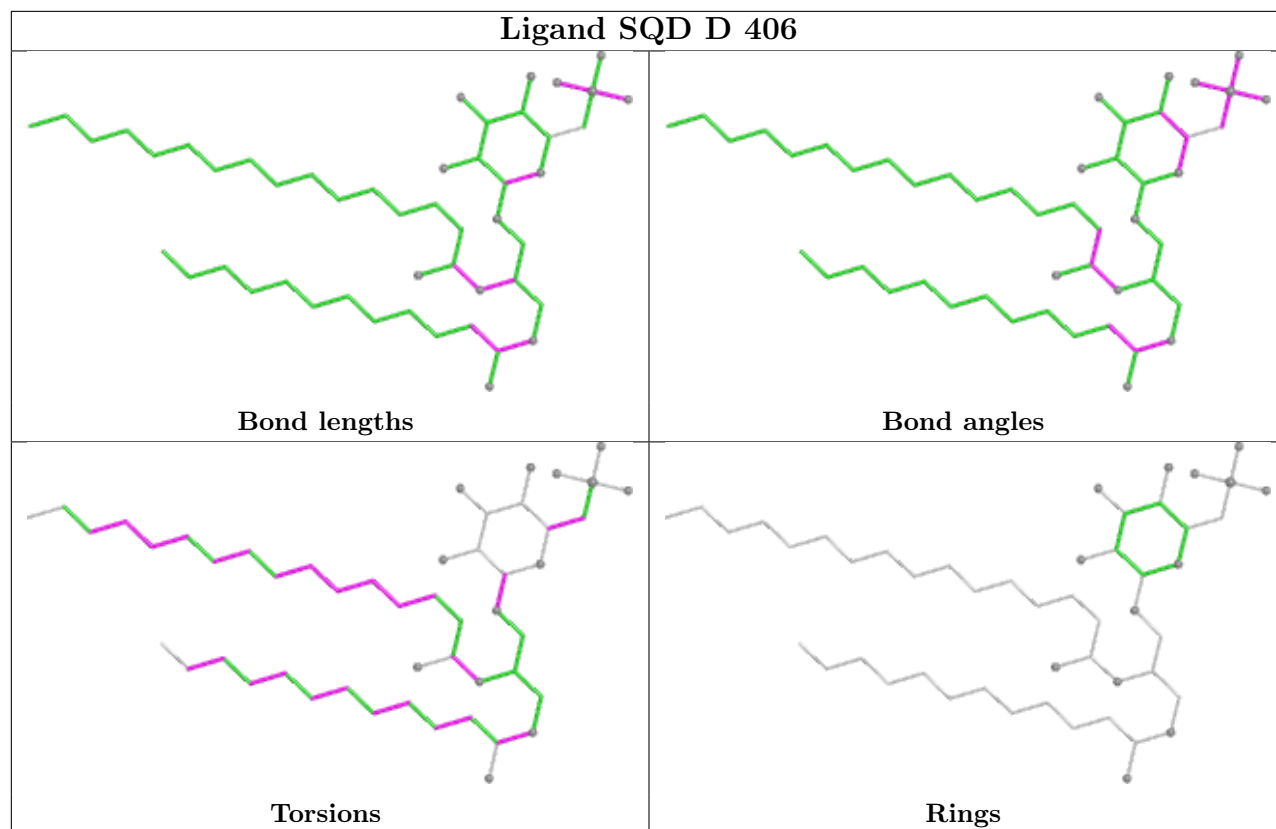
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Bond lengths	Bond angles
	
Torsions	Rings



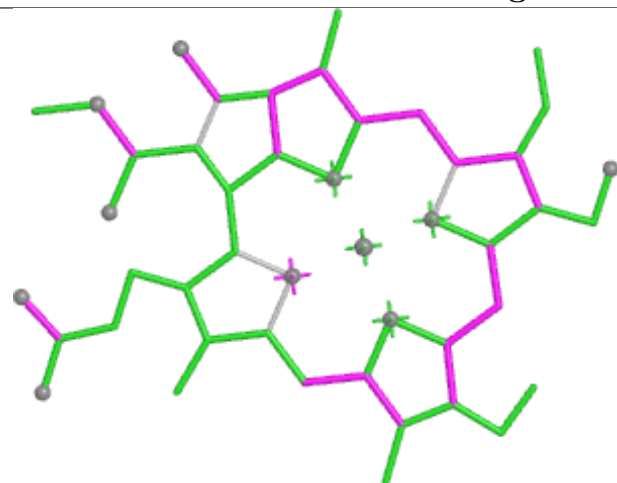




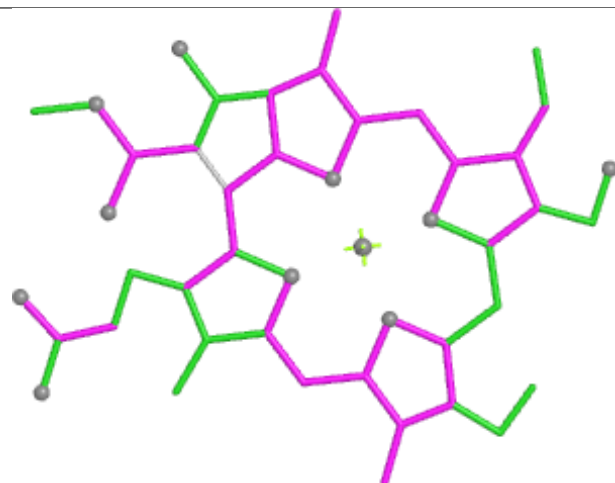




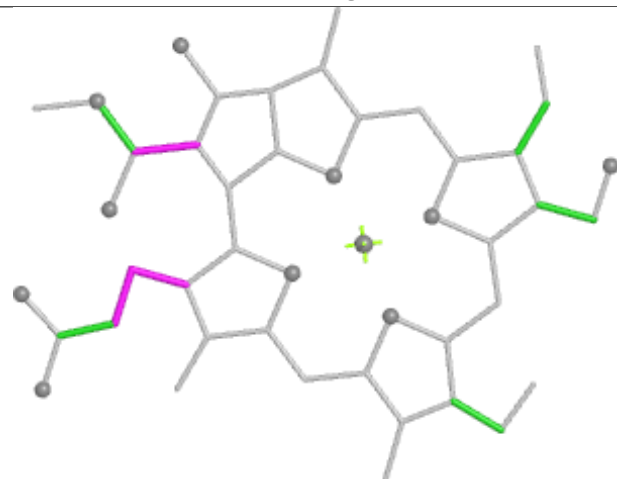
Ligand CHL BJ 605



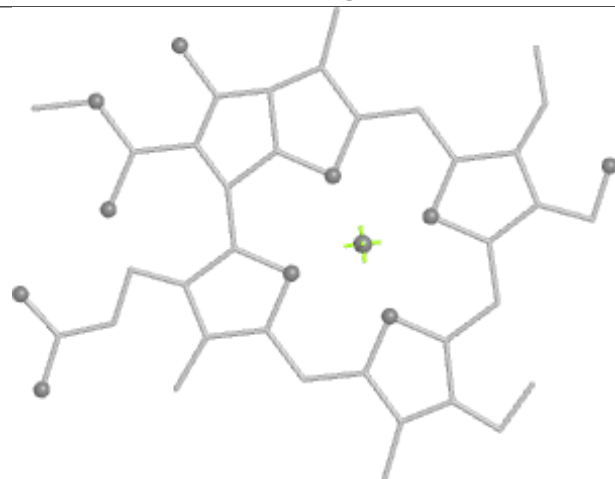
Bond lengths



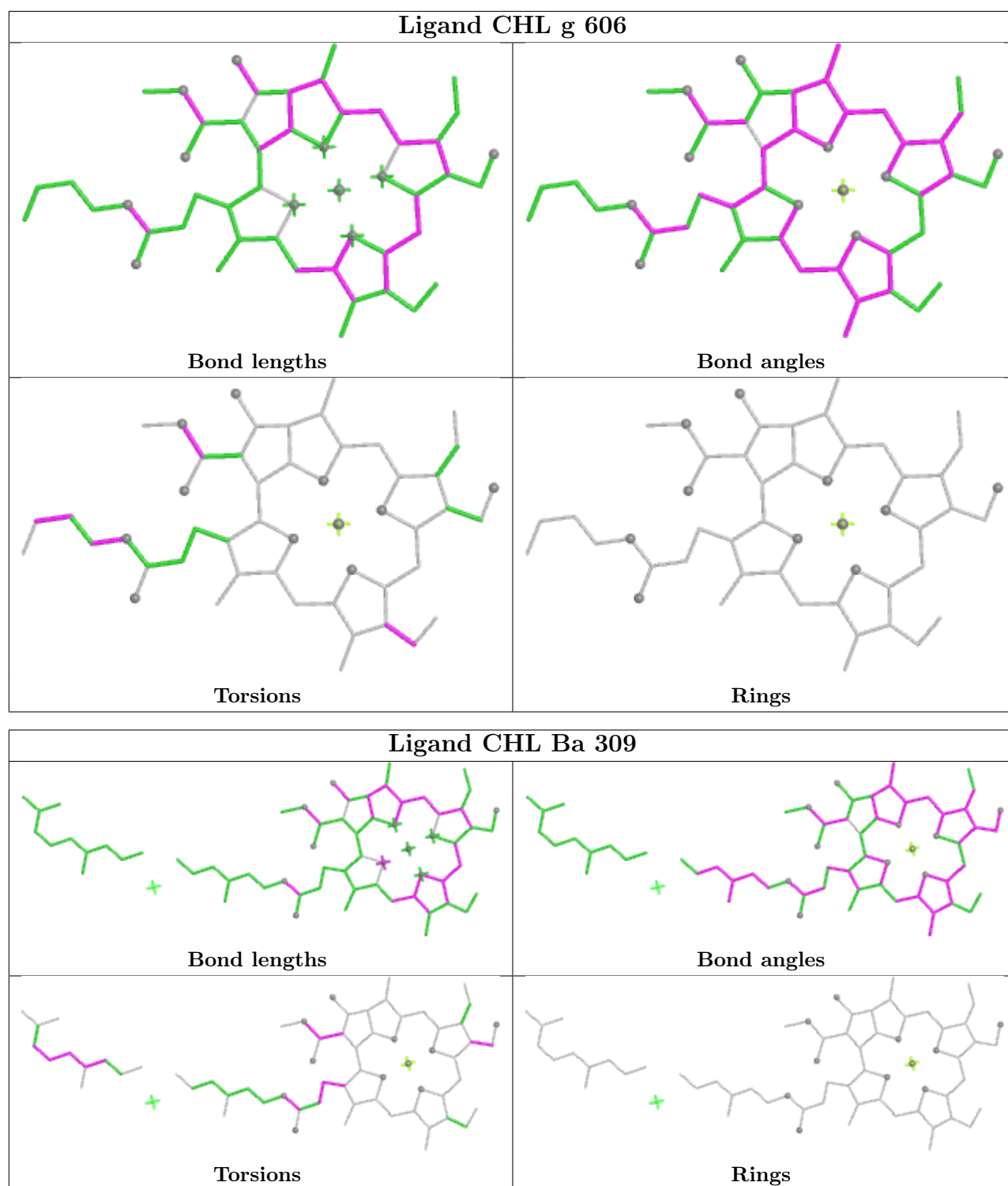
Bond angles



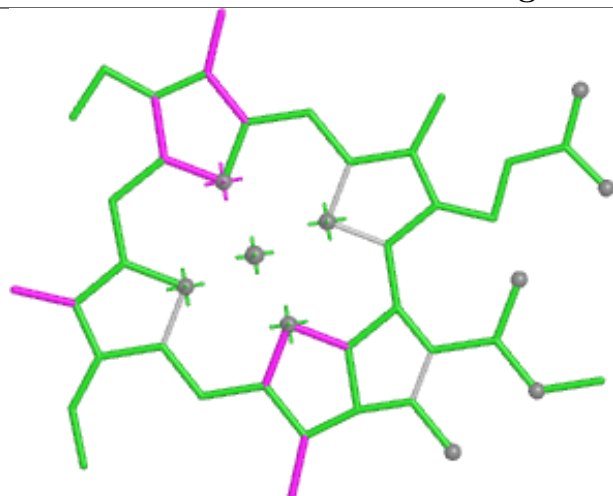
Torsions



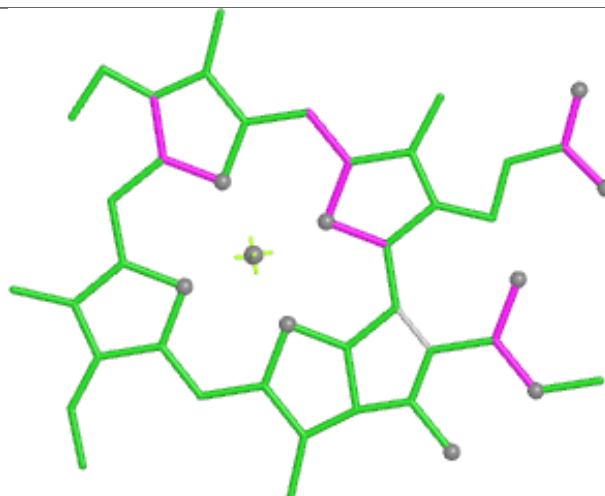
Rings



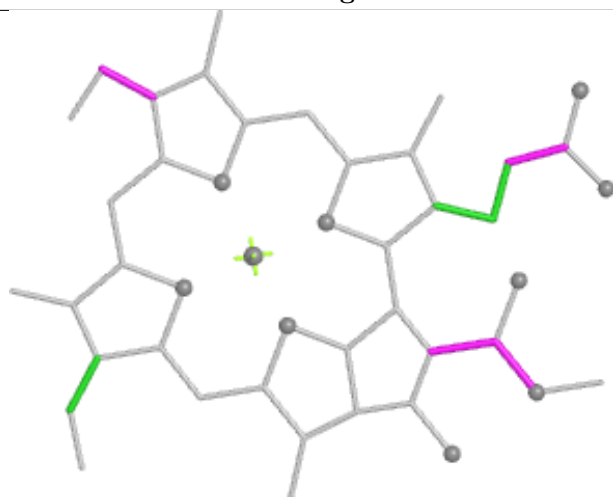
Ligand CLA 6 612



Bond lengths



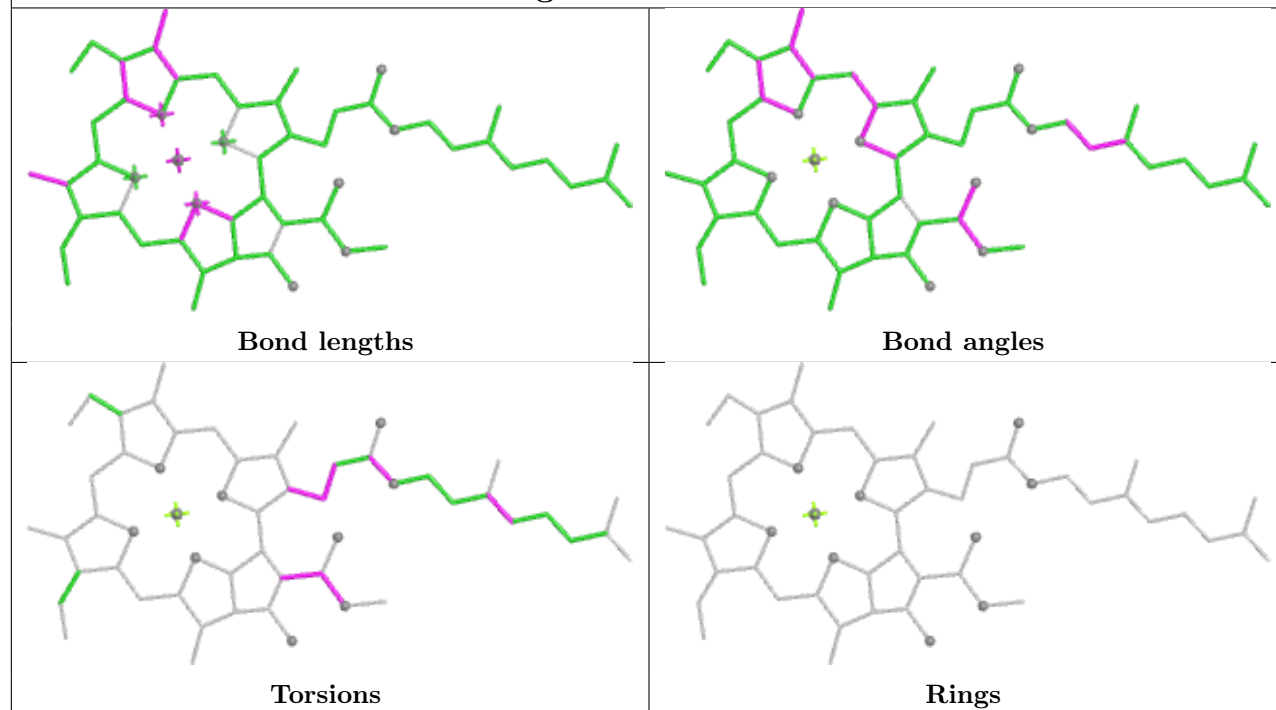
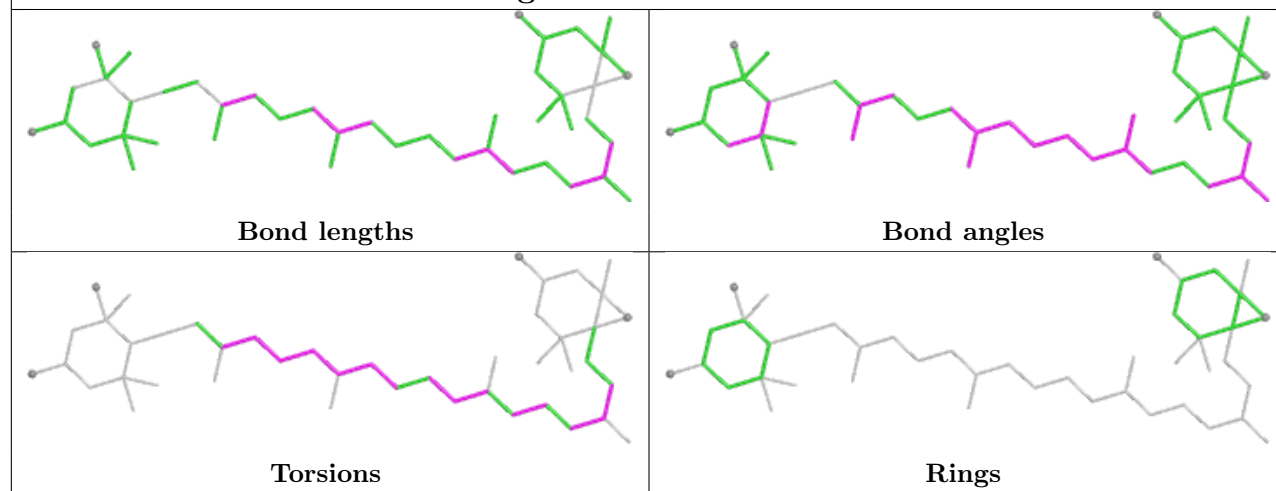
Bond angles

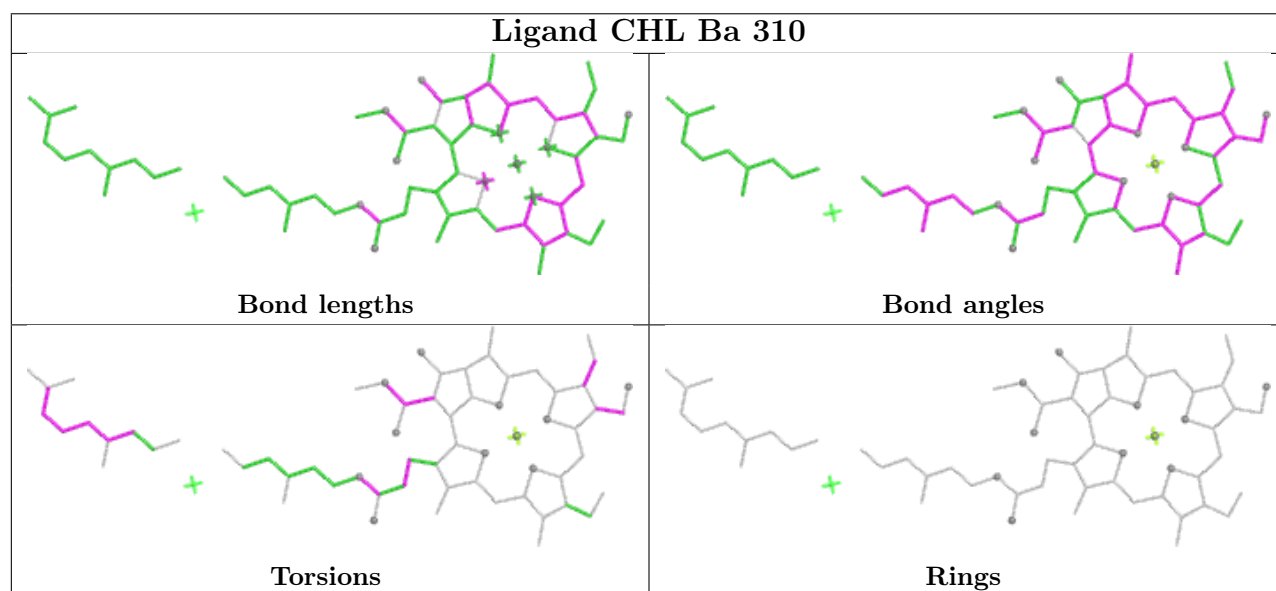
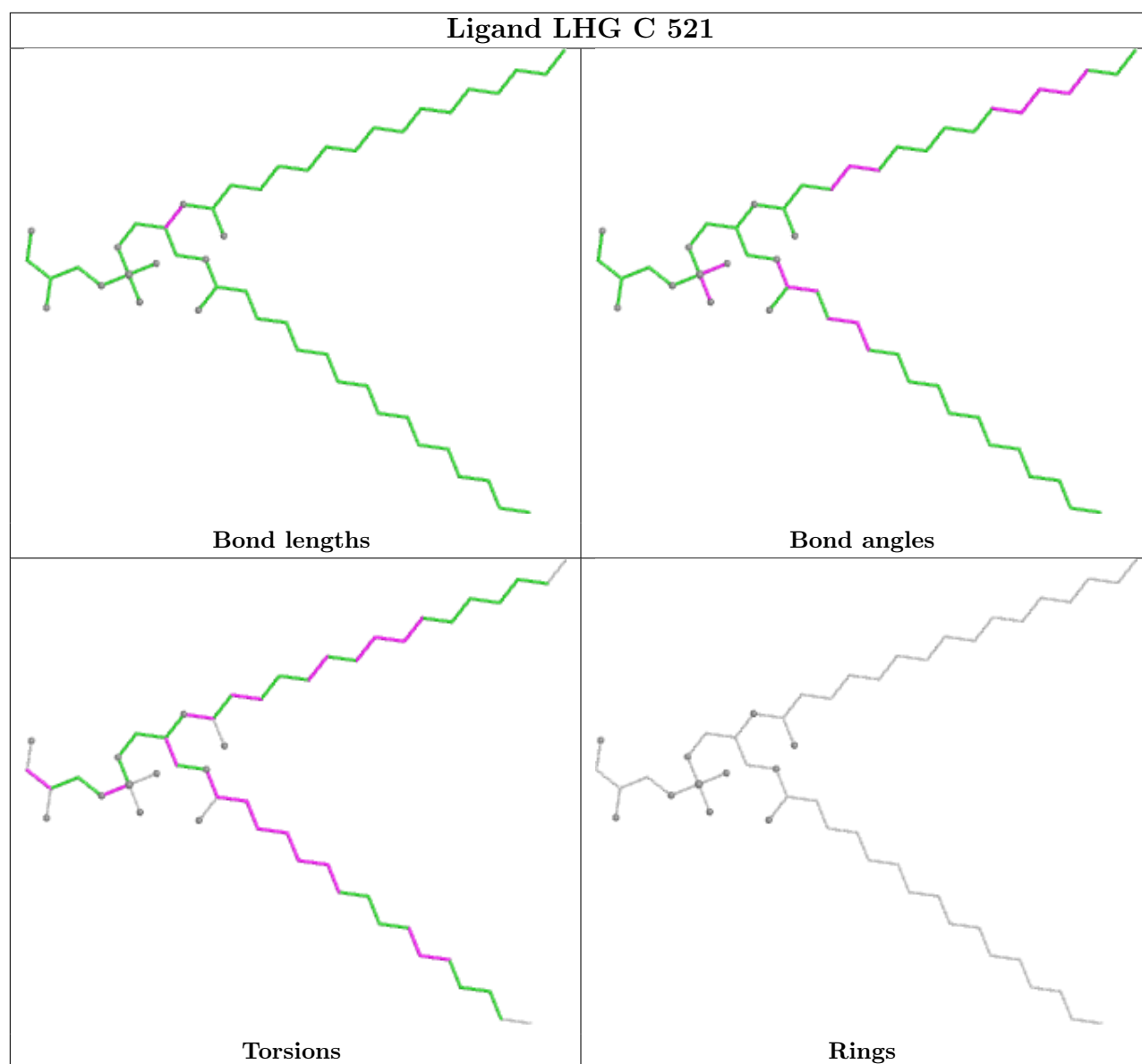


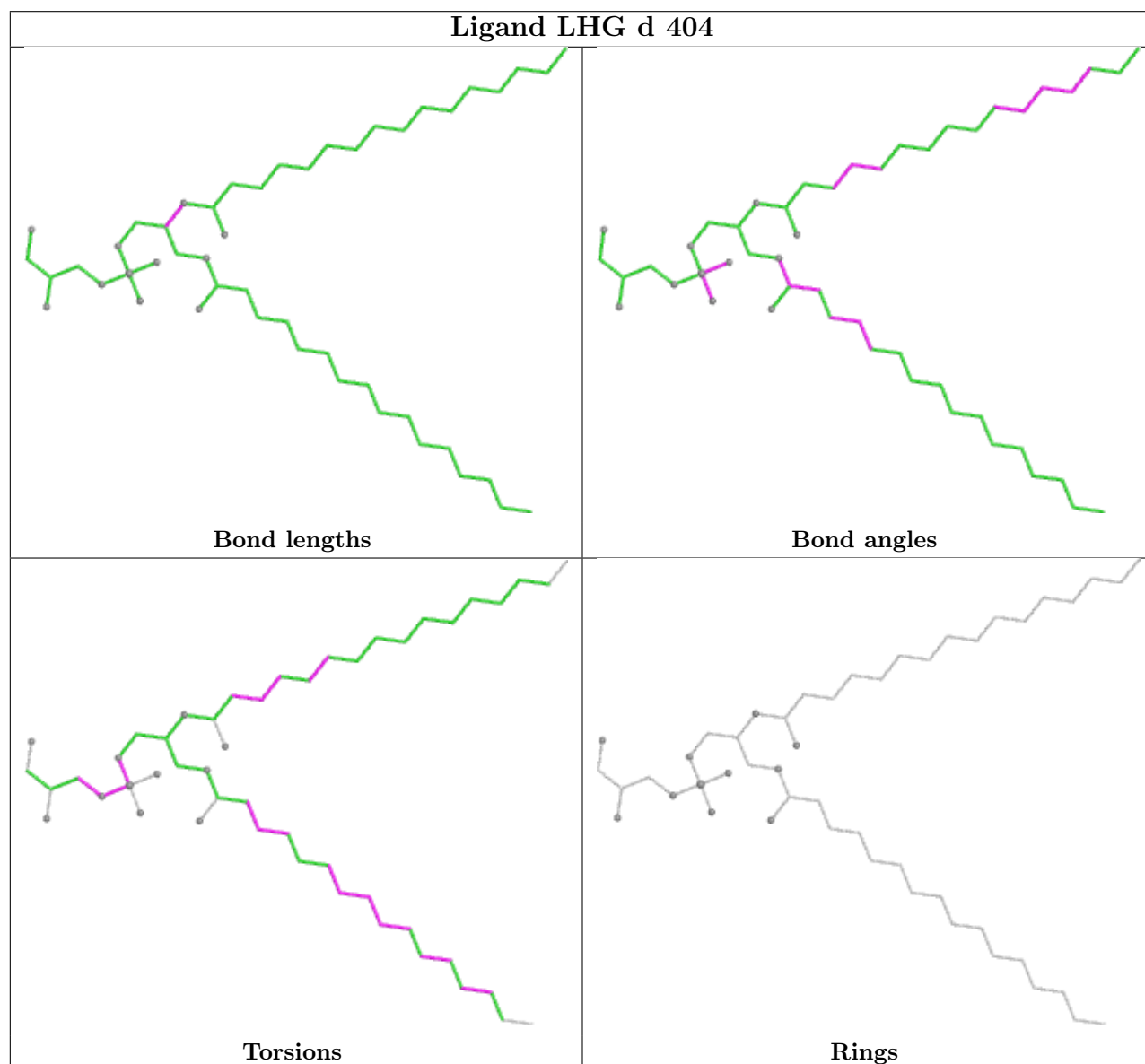
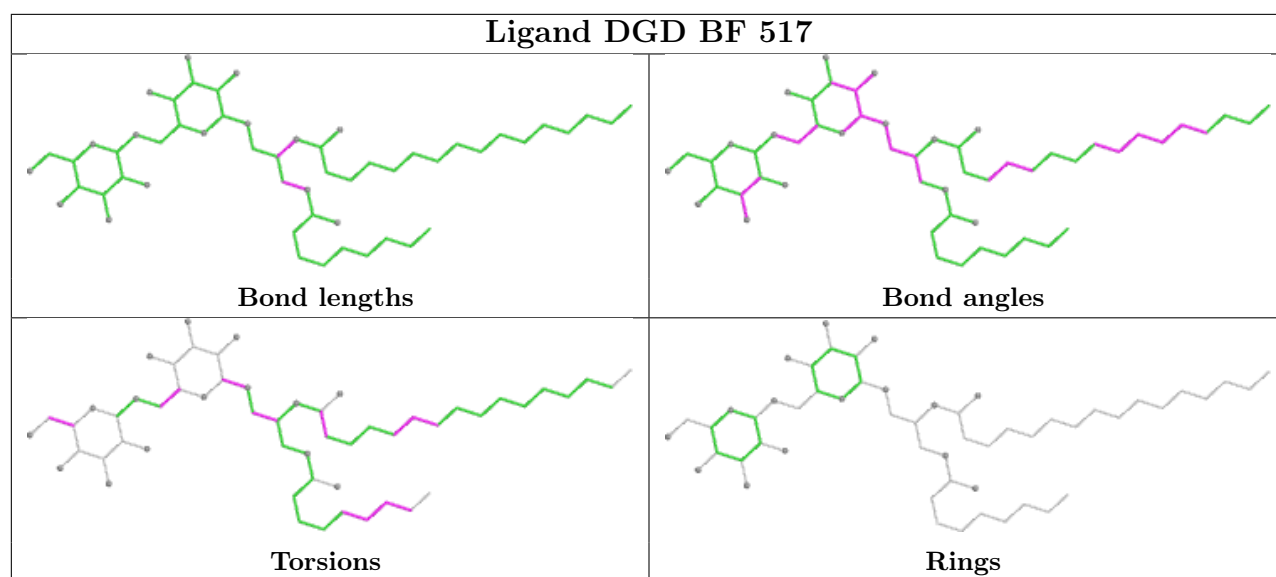
Torsions

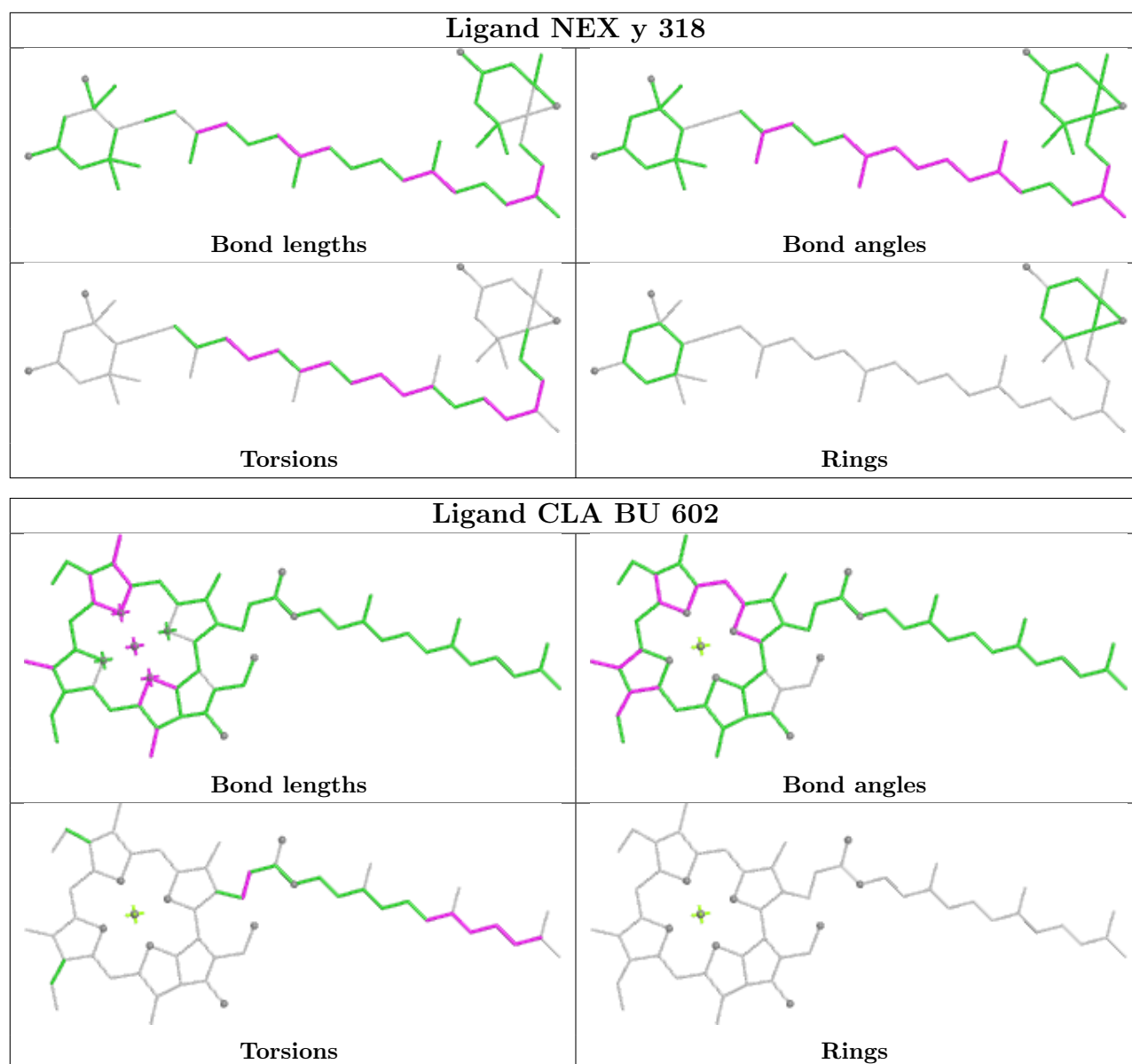


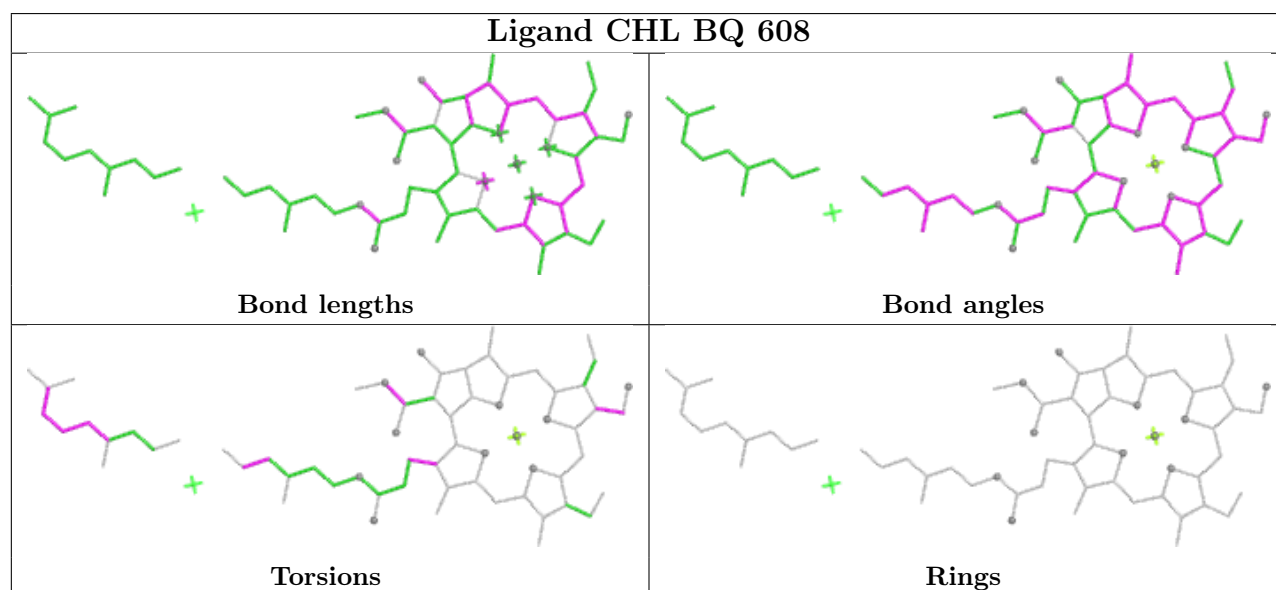
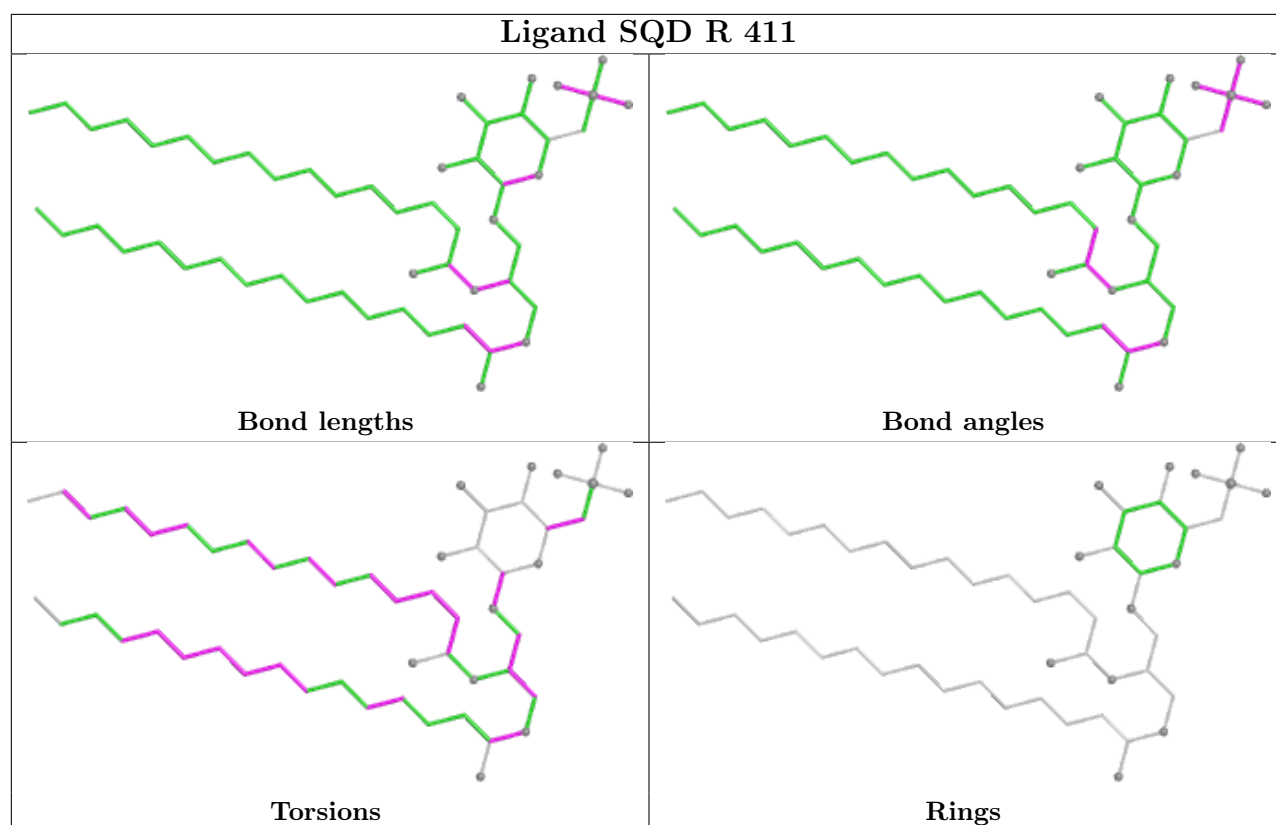
Rings

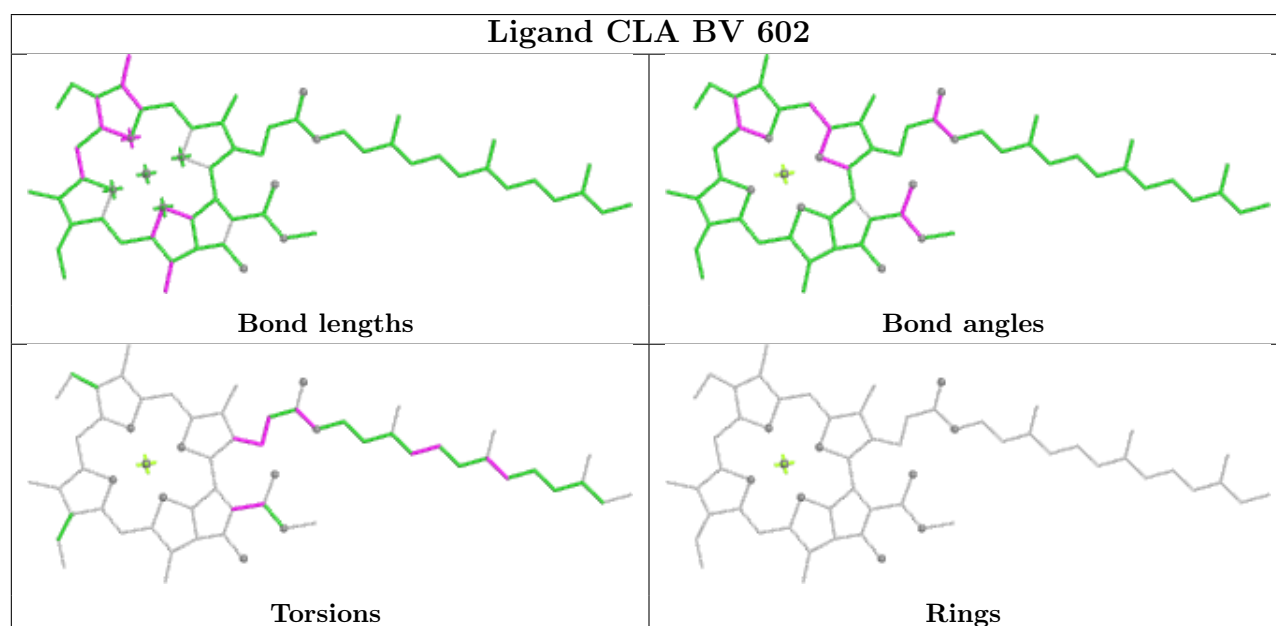
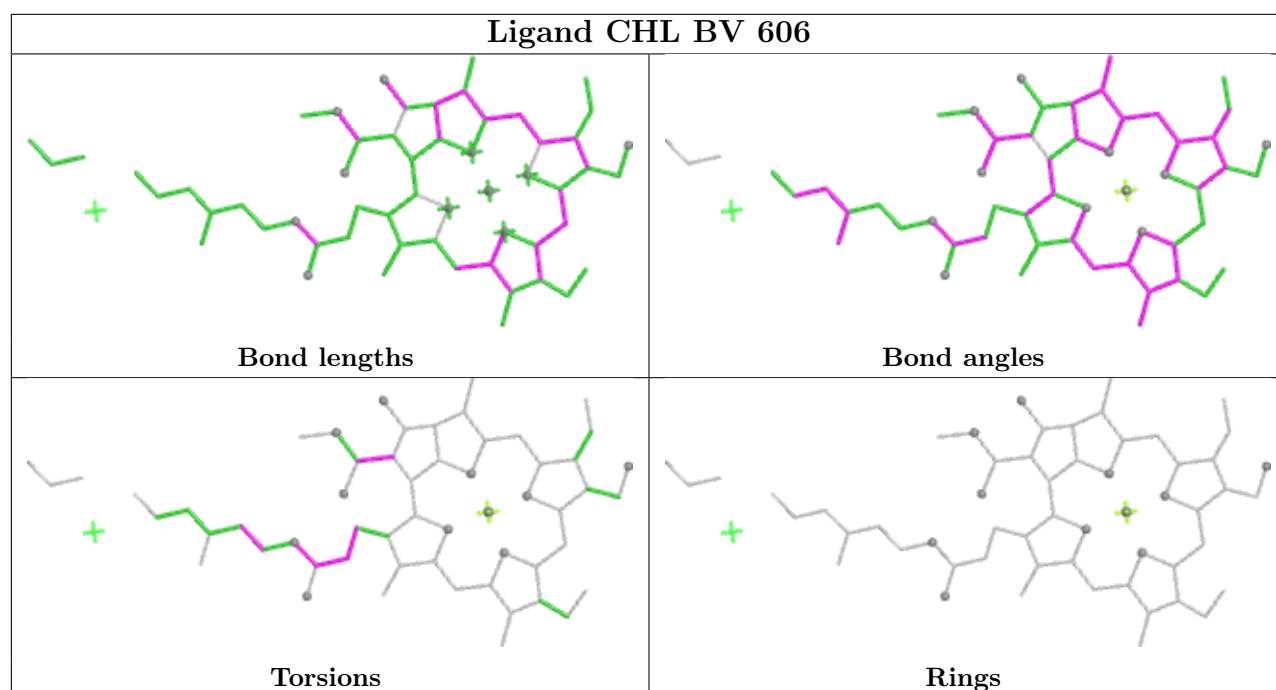
Ligand CLA 9 613**Ligand NEX BB 320**

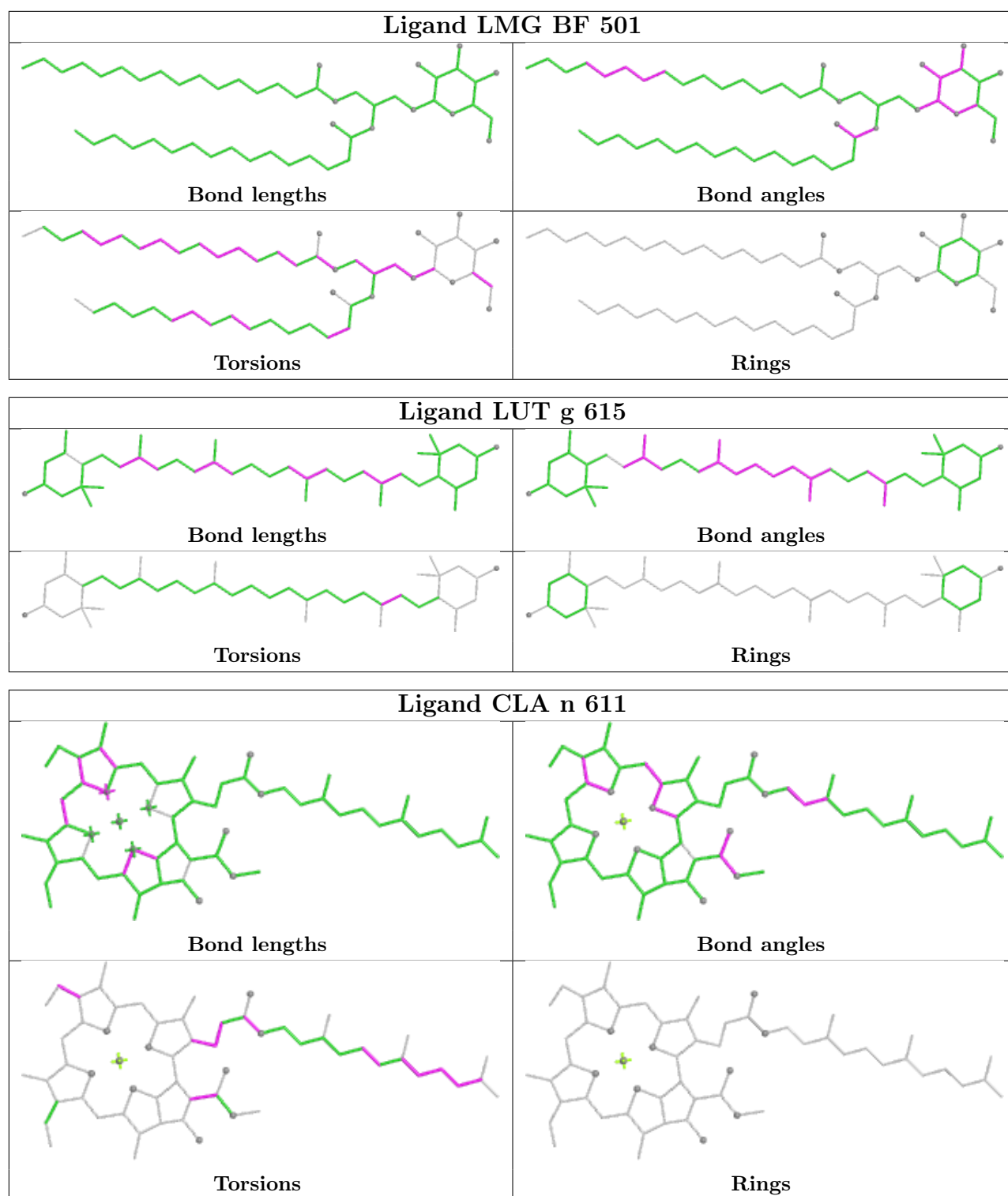


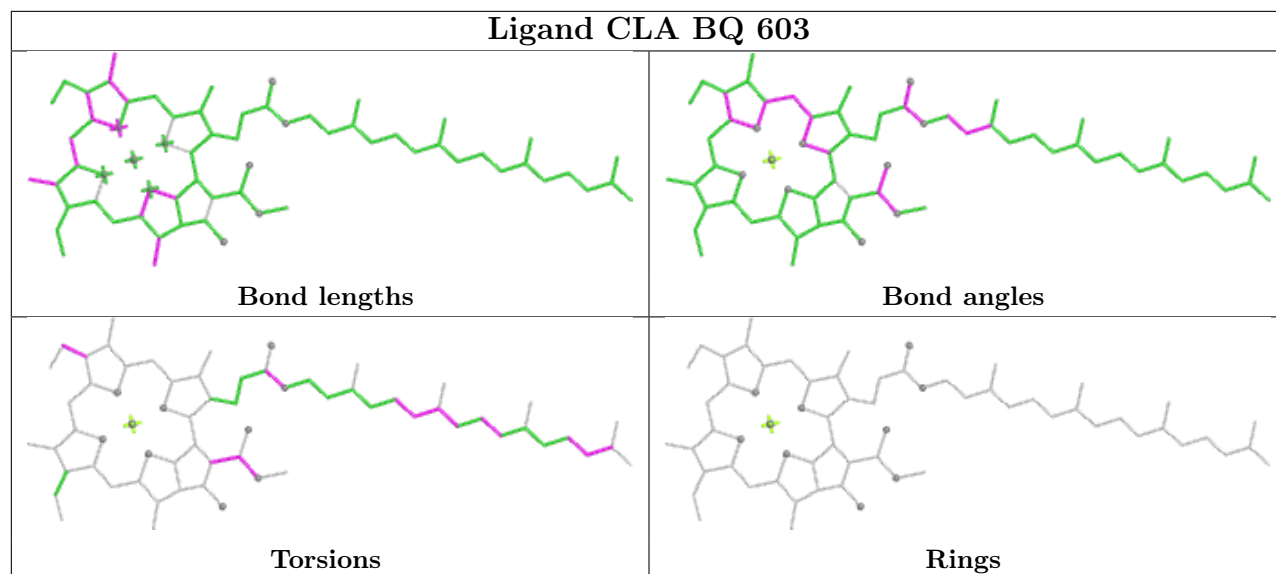
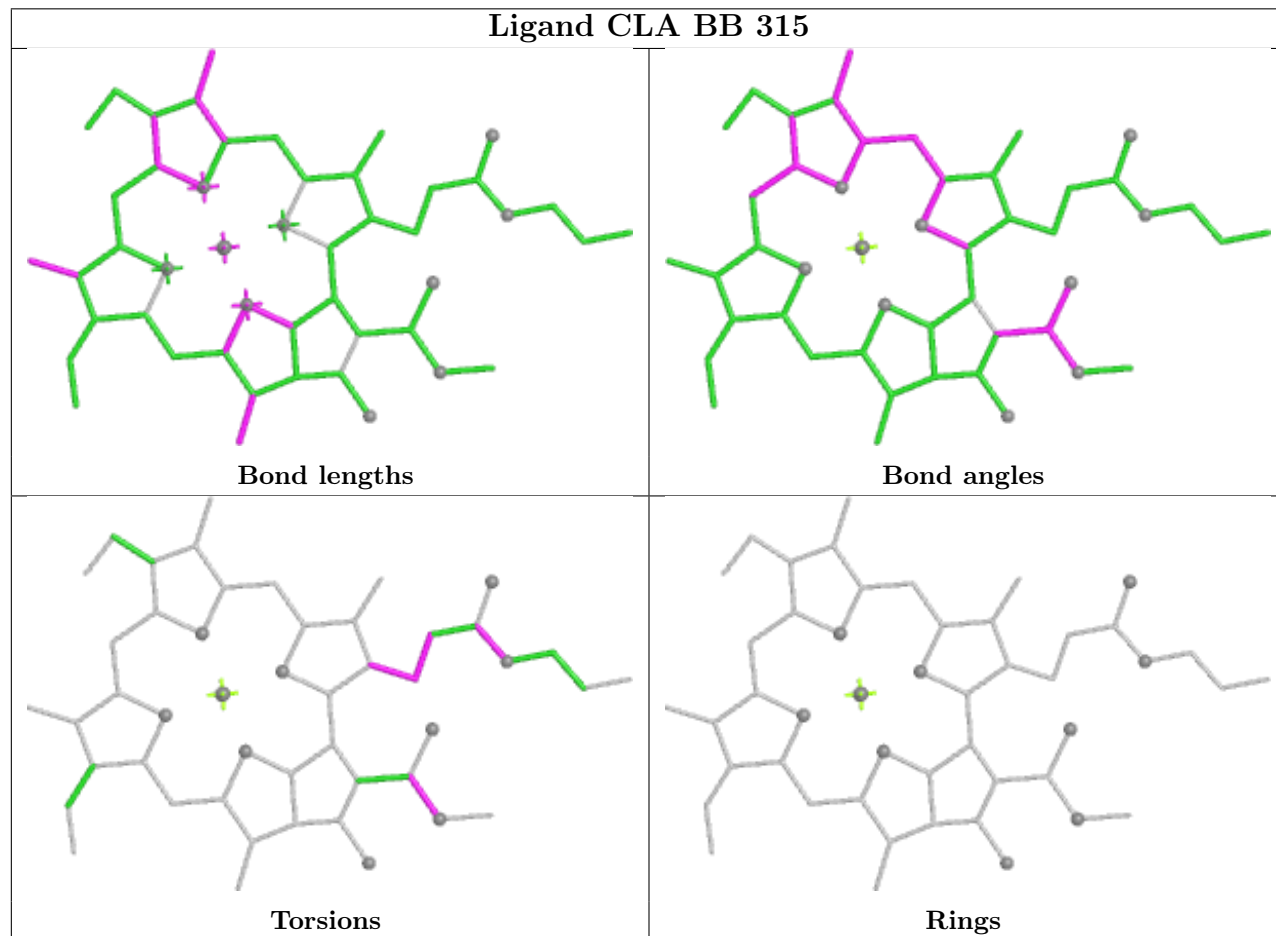


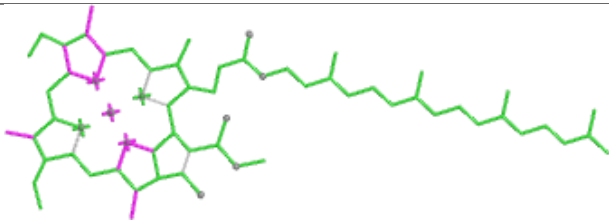
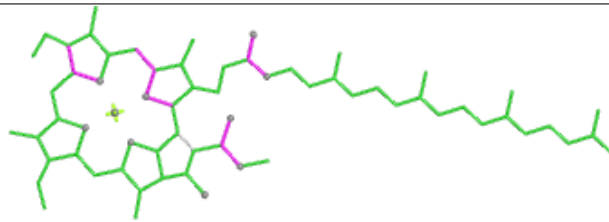
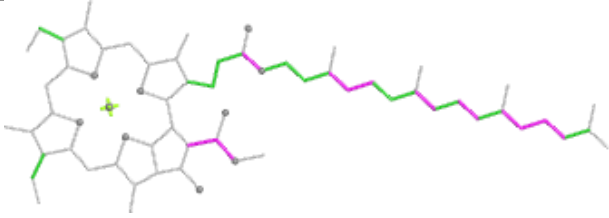
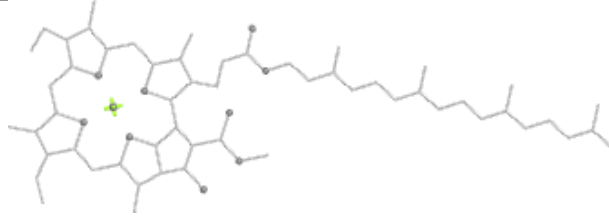
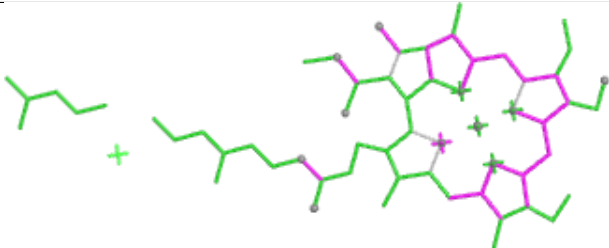
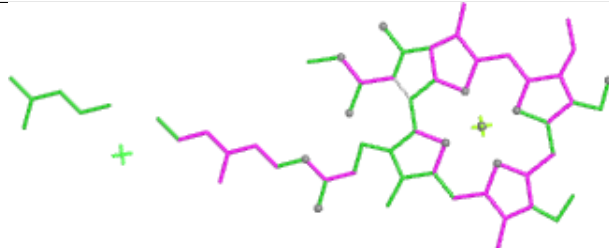
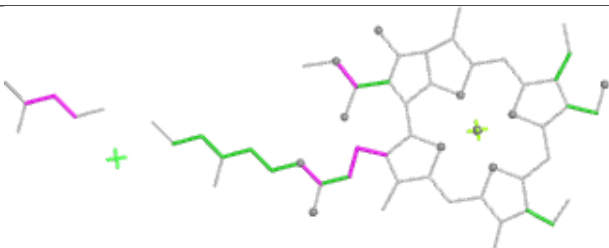
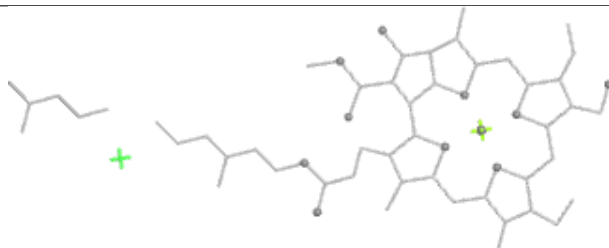
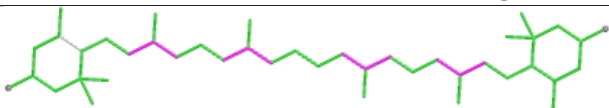
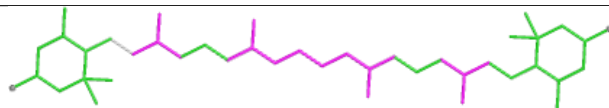
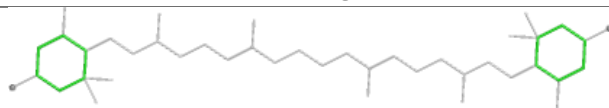


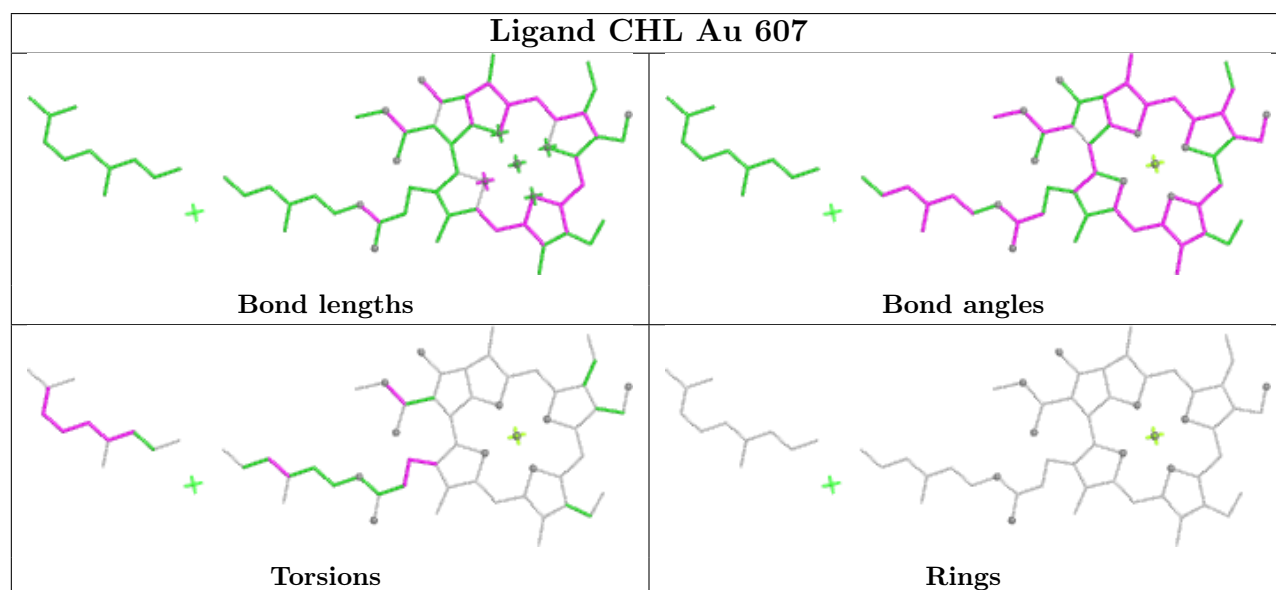
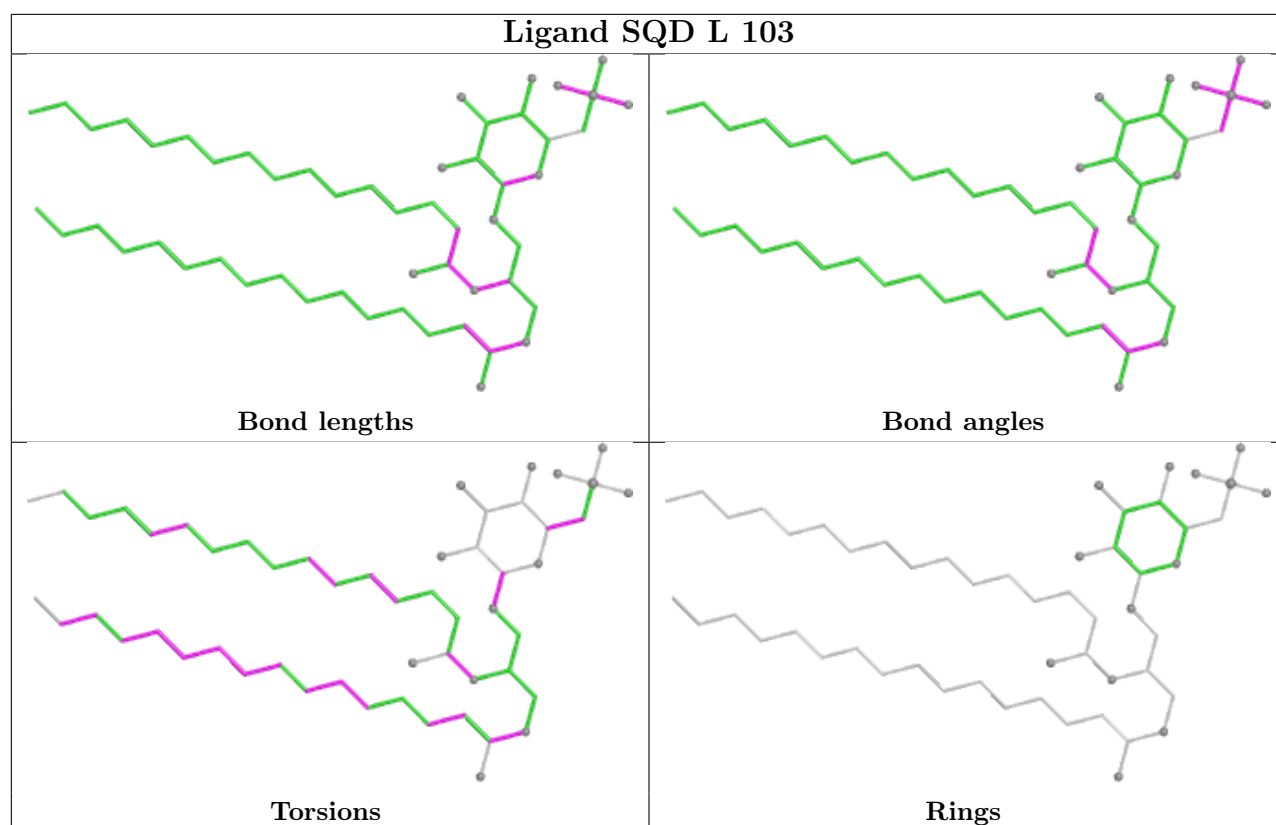


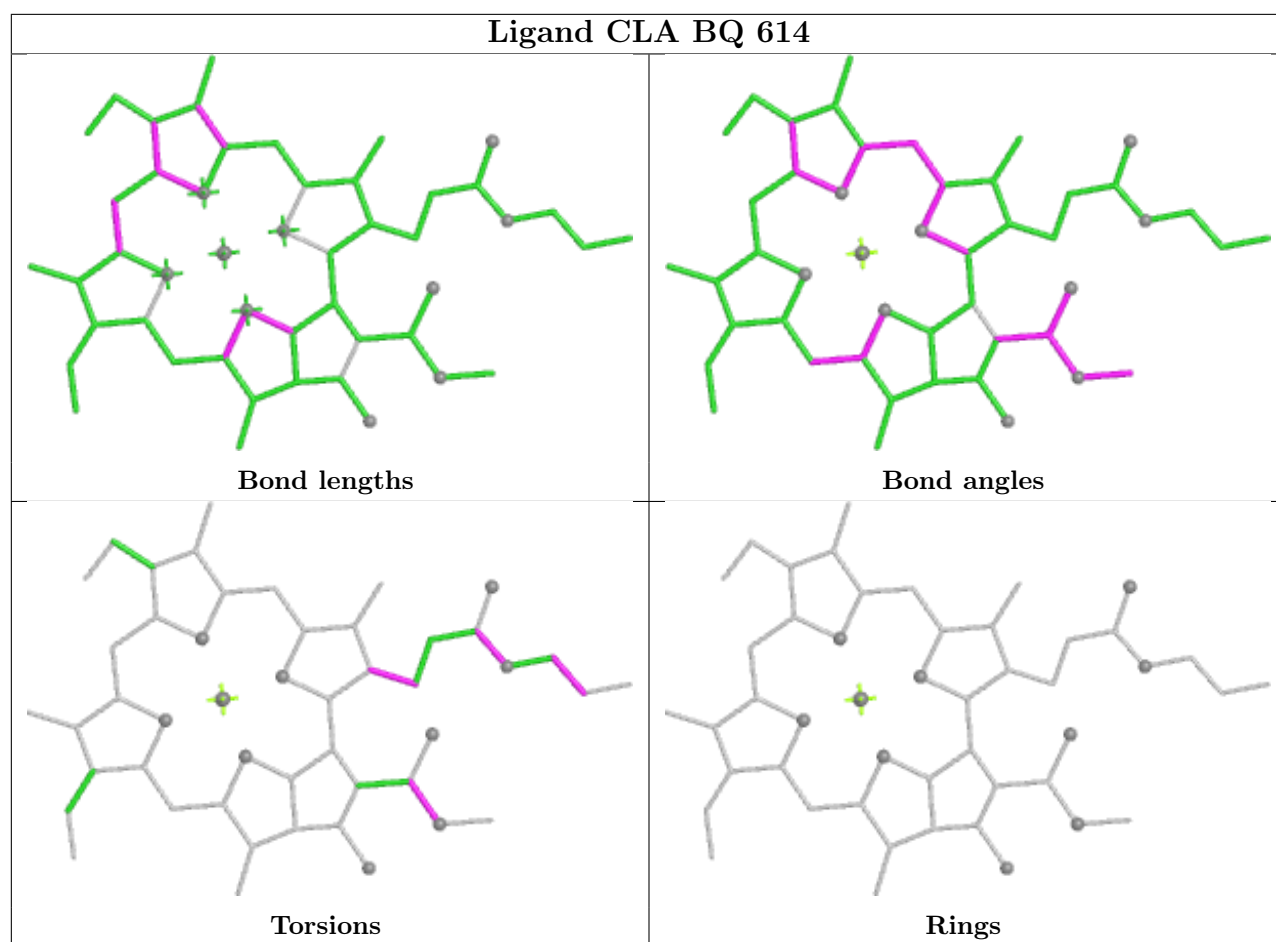




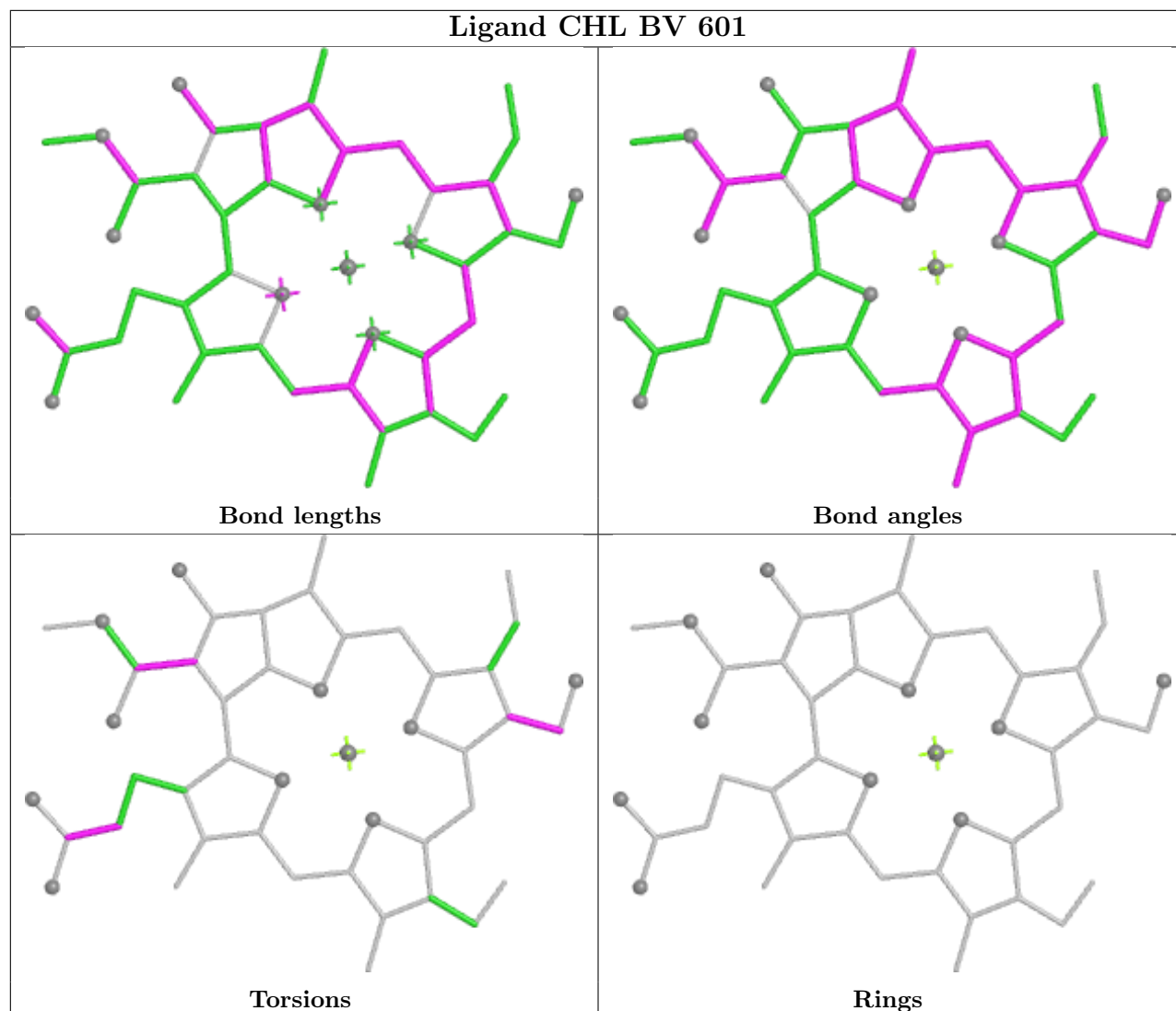
Ligand CLA BQ 603**Ligand CLA BB 315**

Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CHL 0 609	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LUT AA 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

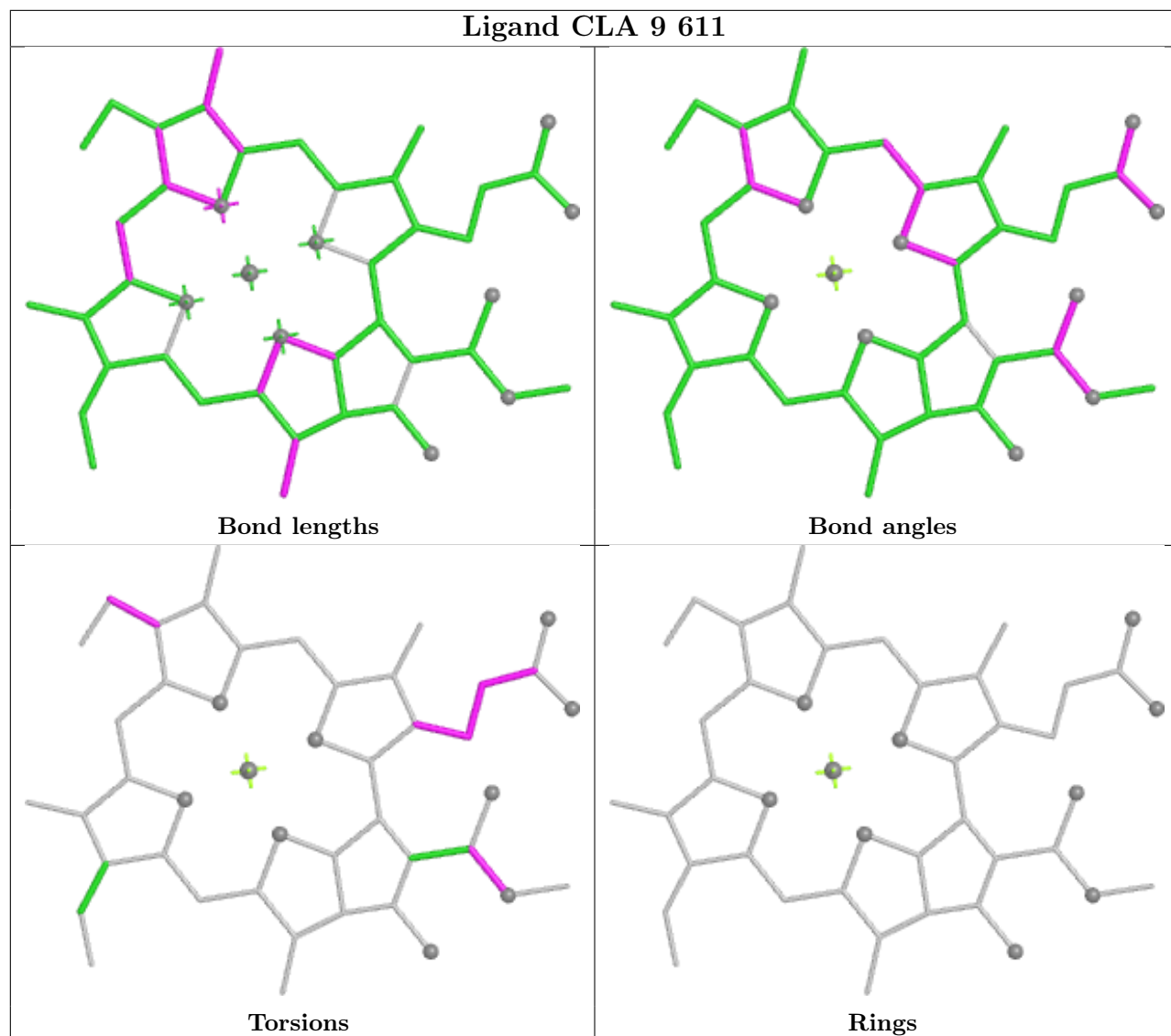


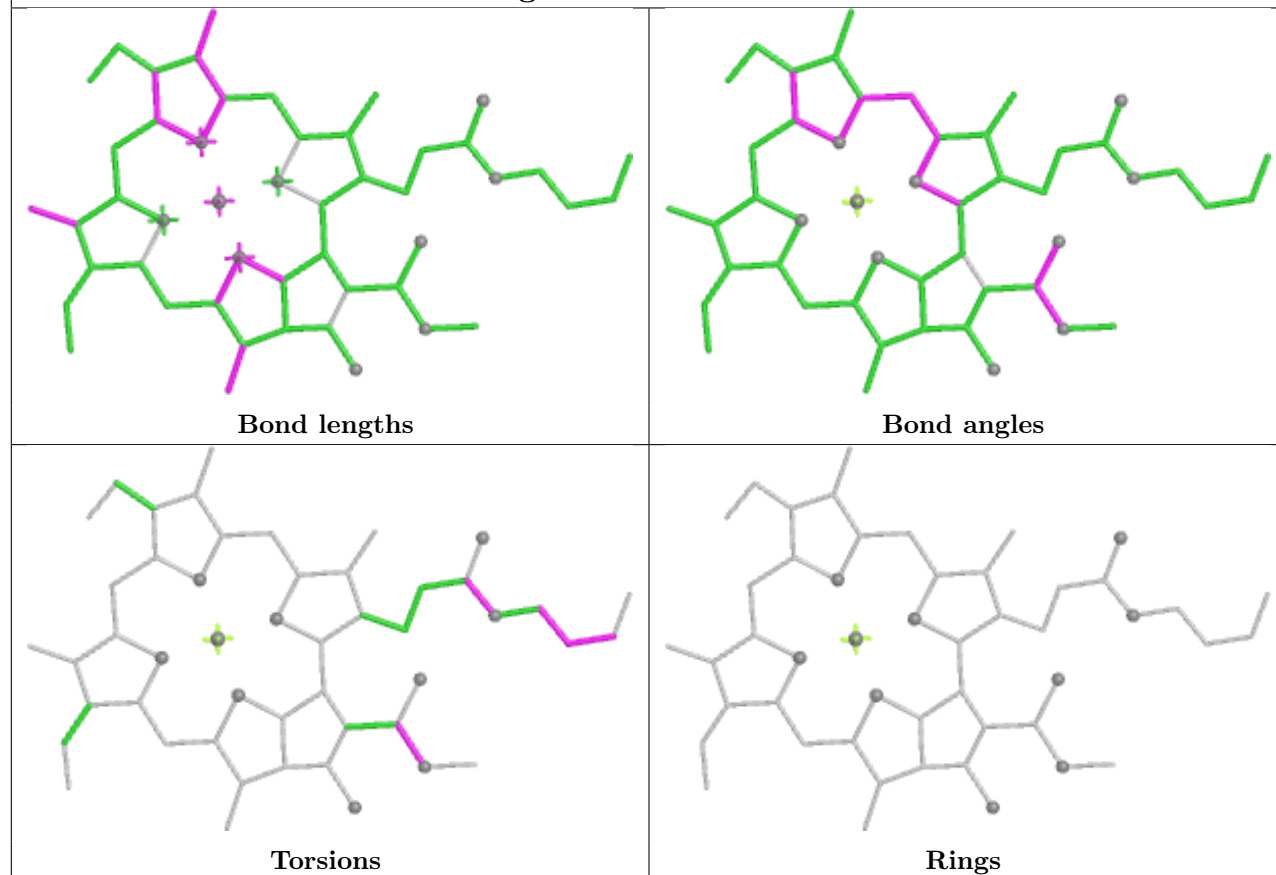
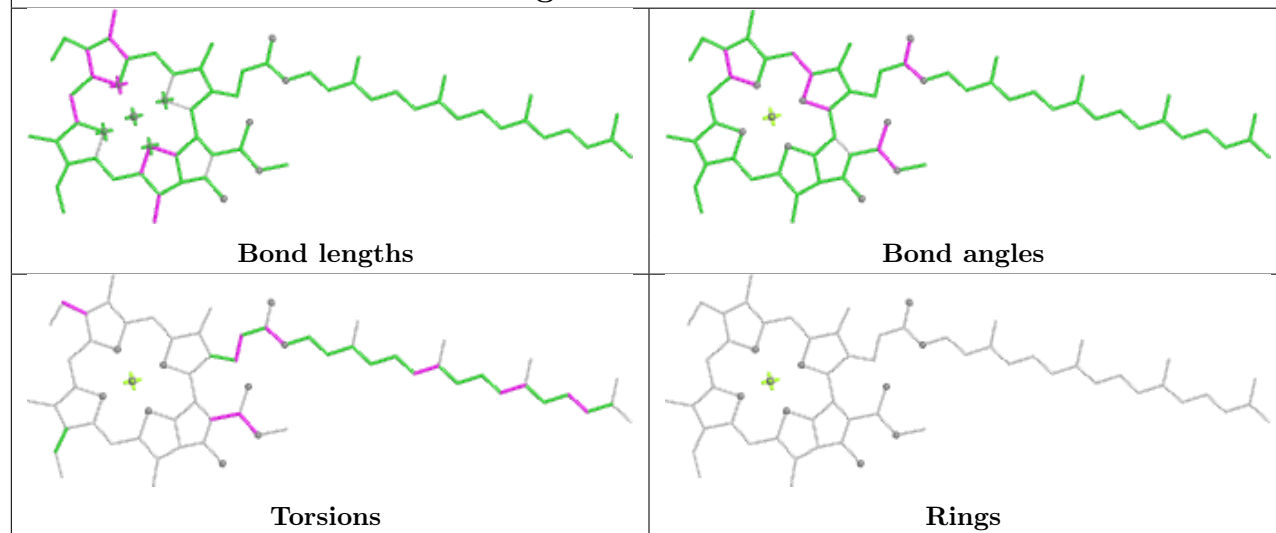


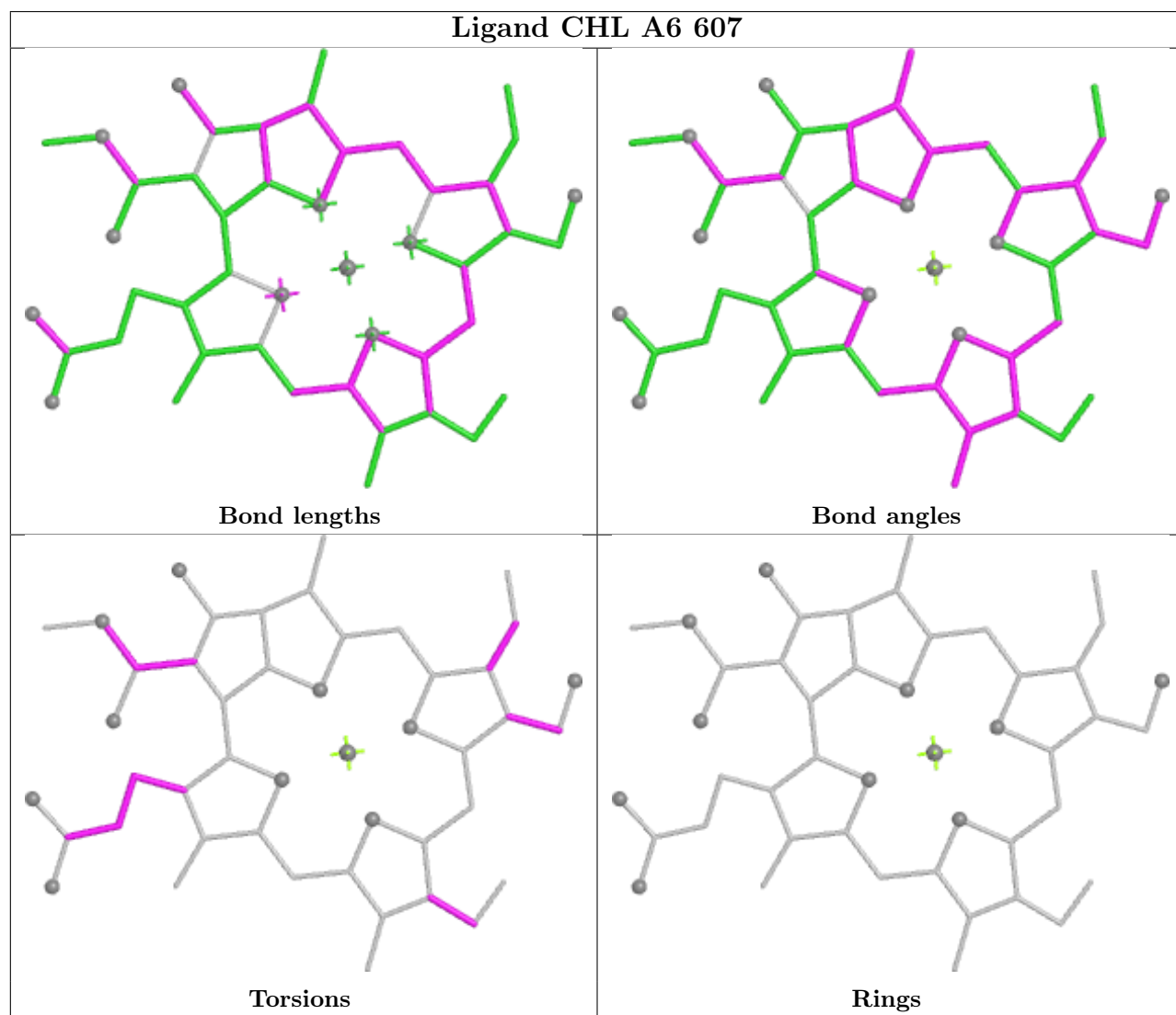
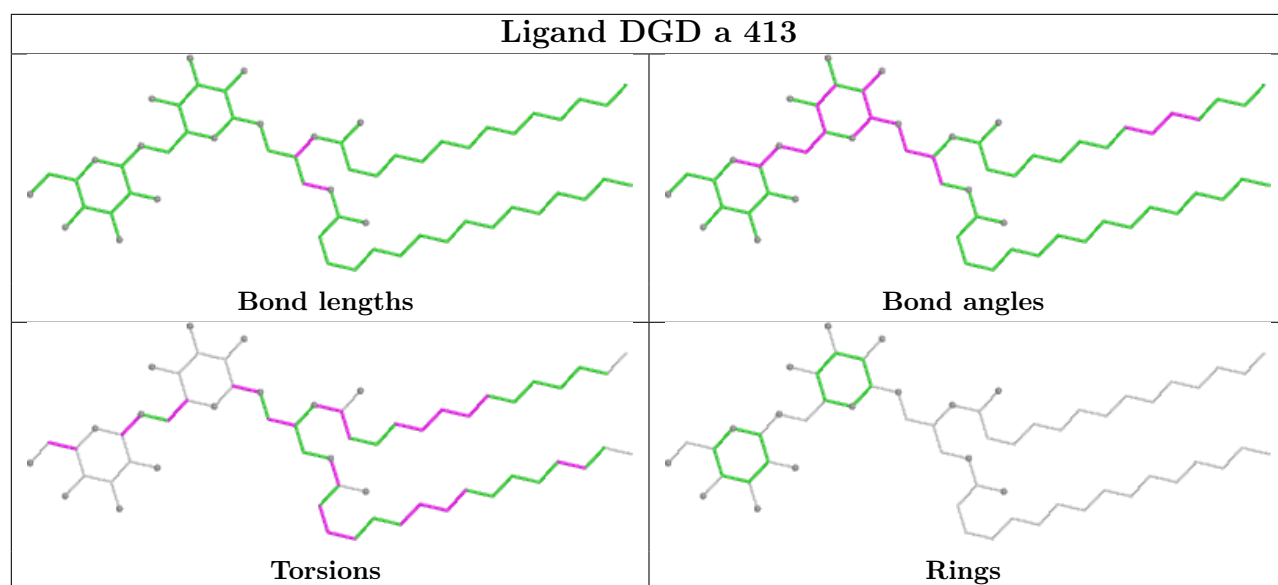
Ligand CHL BV 601



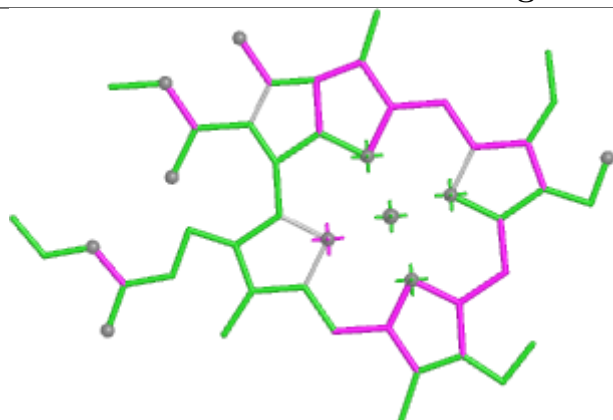
Ligand CLA 9 611



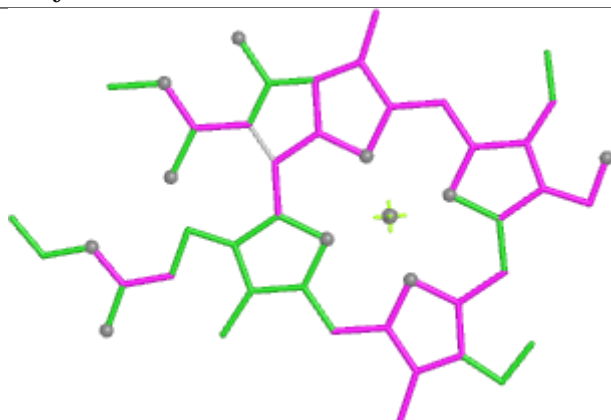
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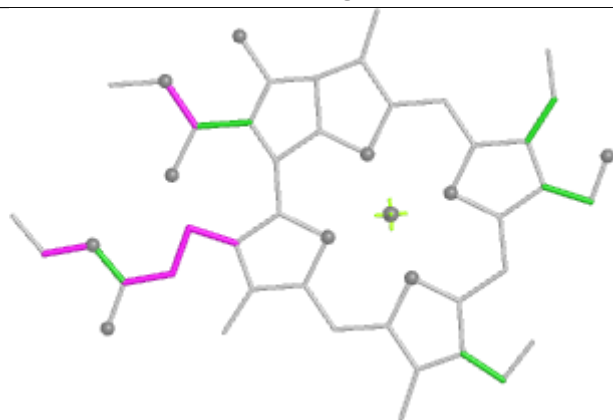
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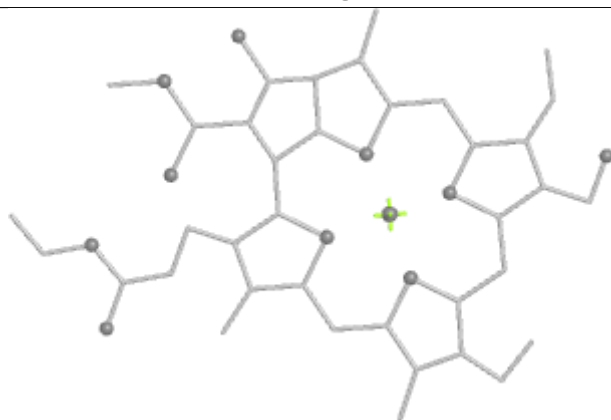
Bond lengths



Bond angles

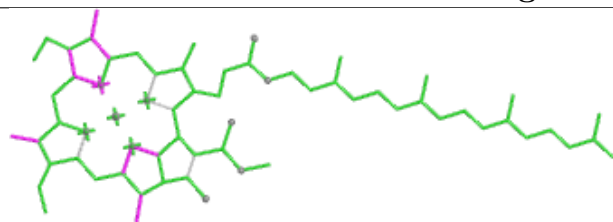


Torsions

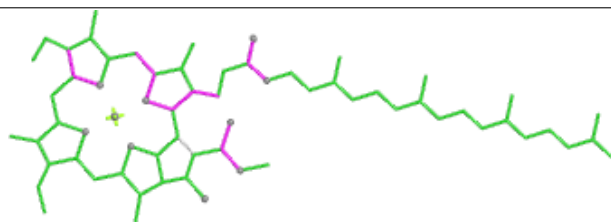


Rings

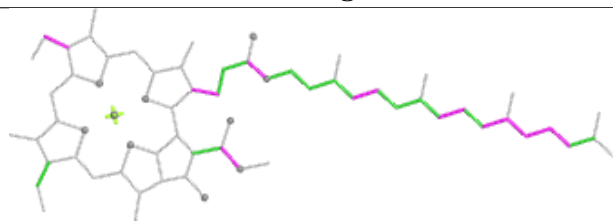
Ligand CLA 1 513



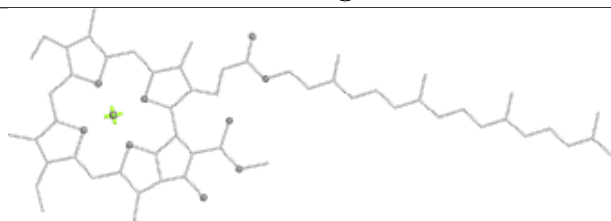
Bond lengths



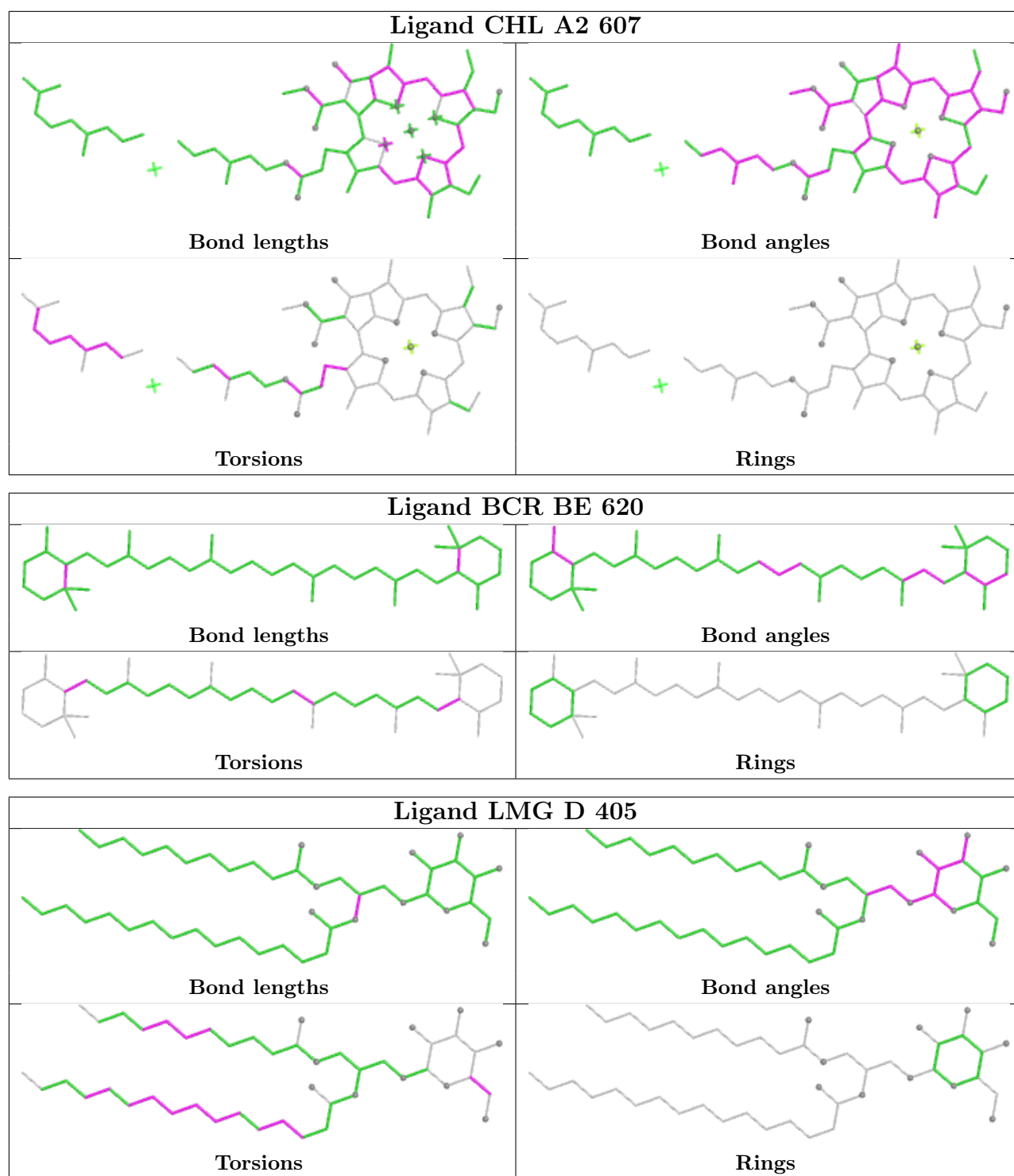
Bond angles

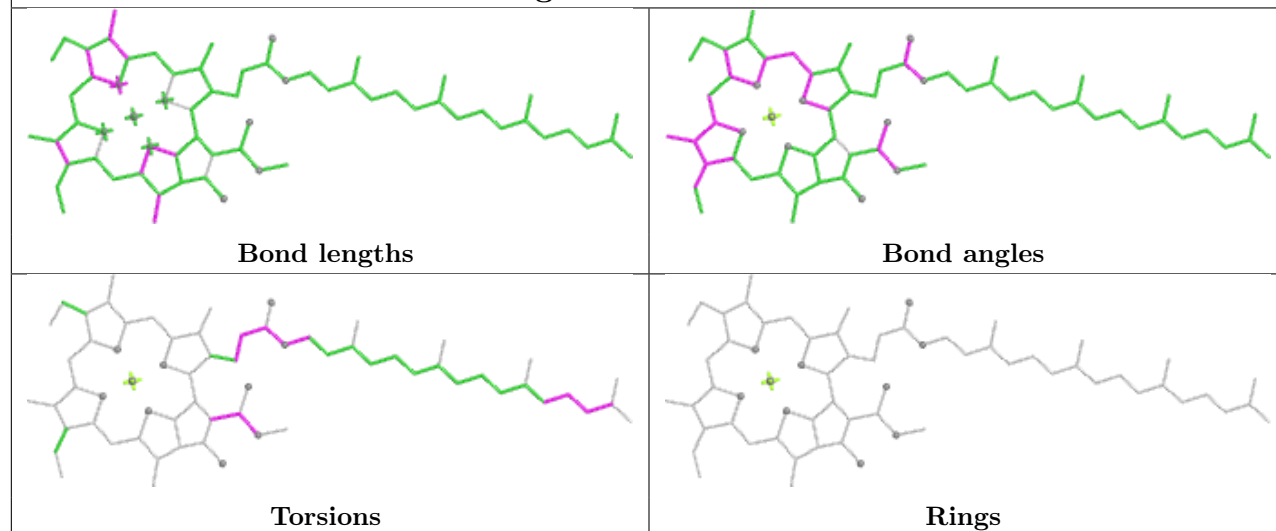
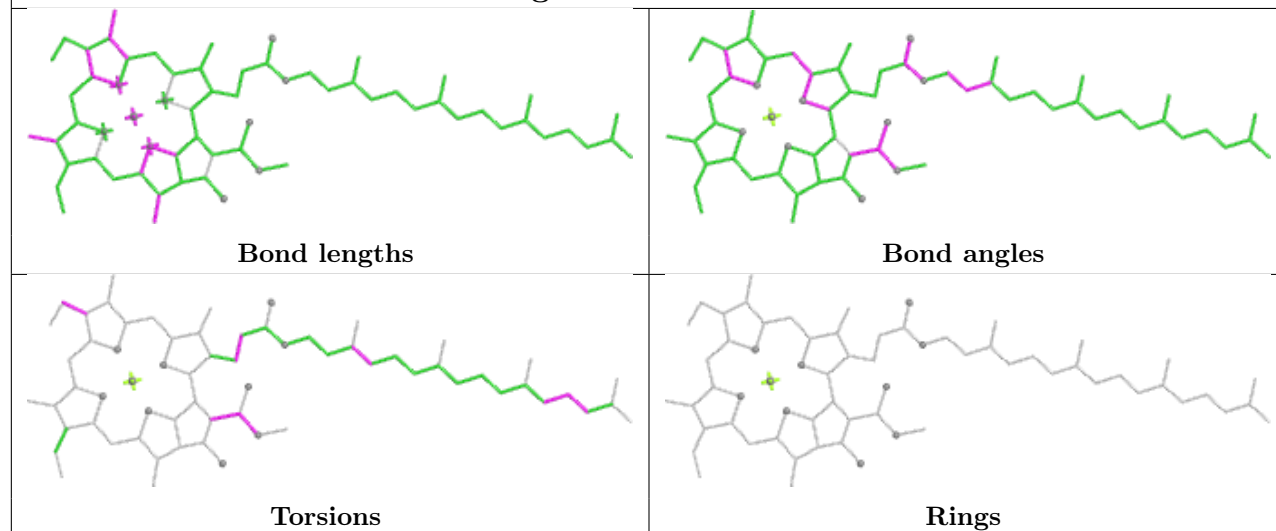


Torsions

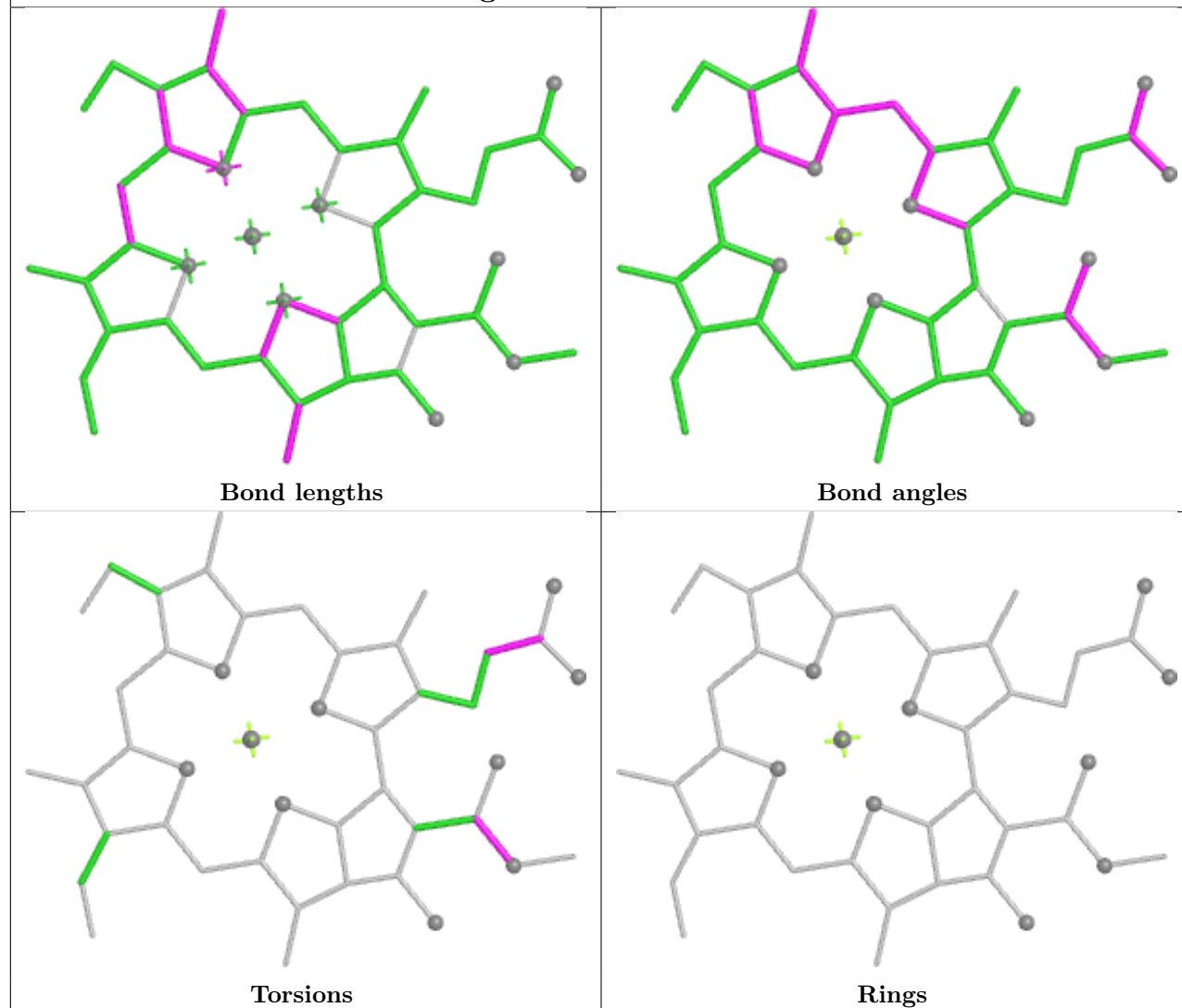


Rings

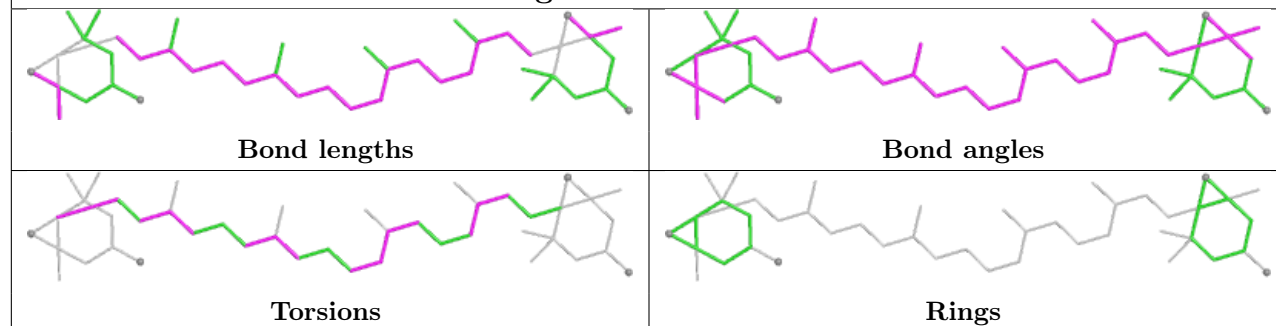


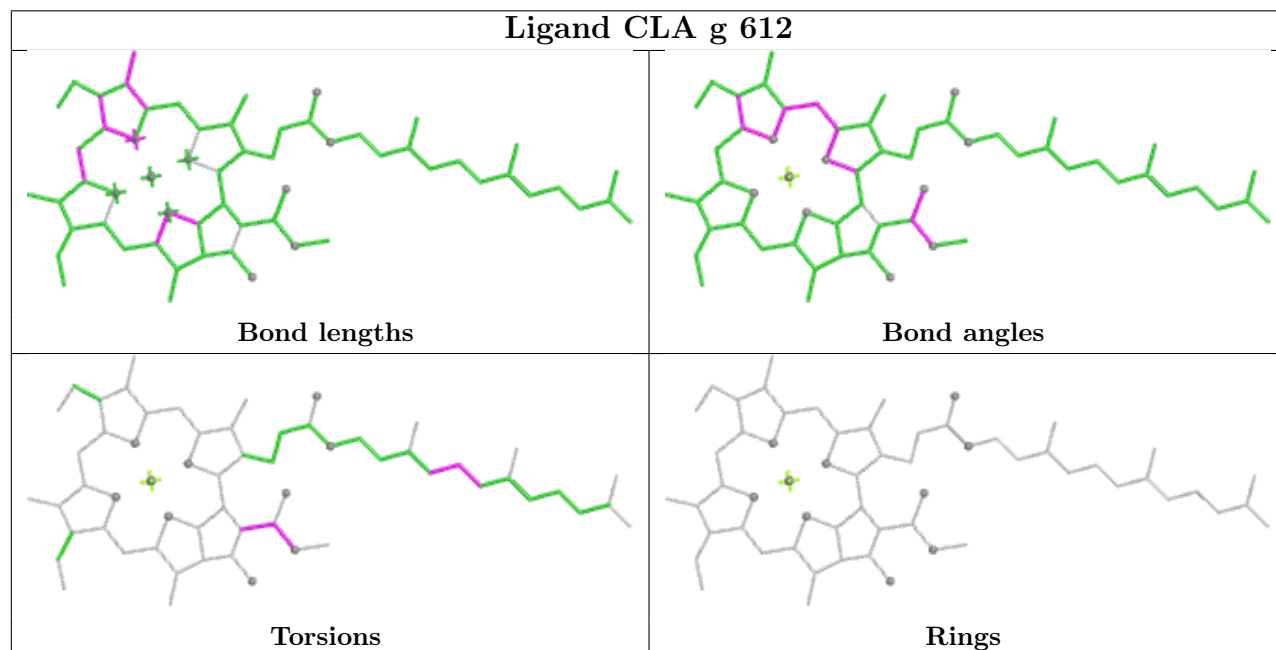
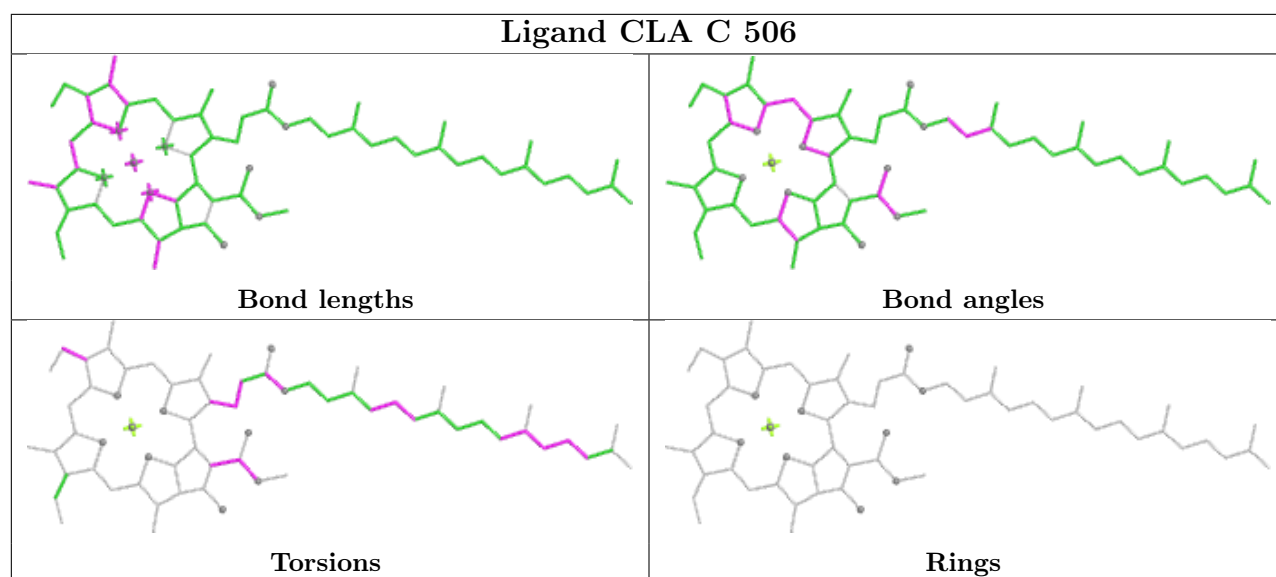
Ligand CLA b 611**Ligand CLA A 405**

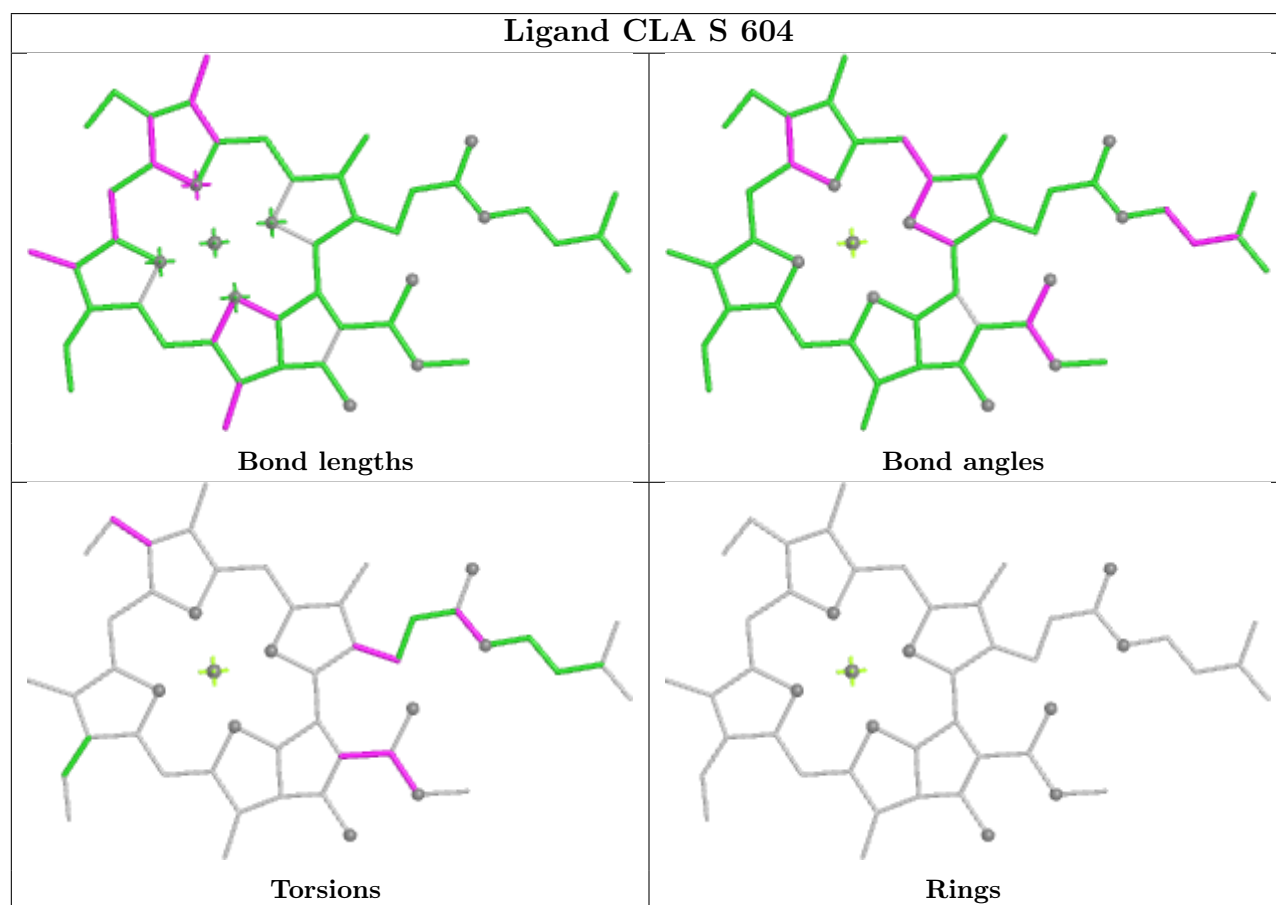
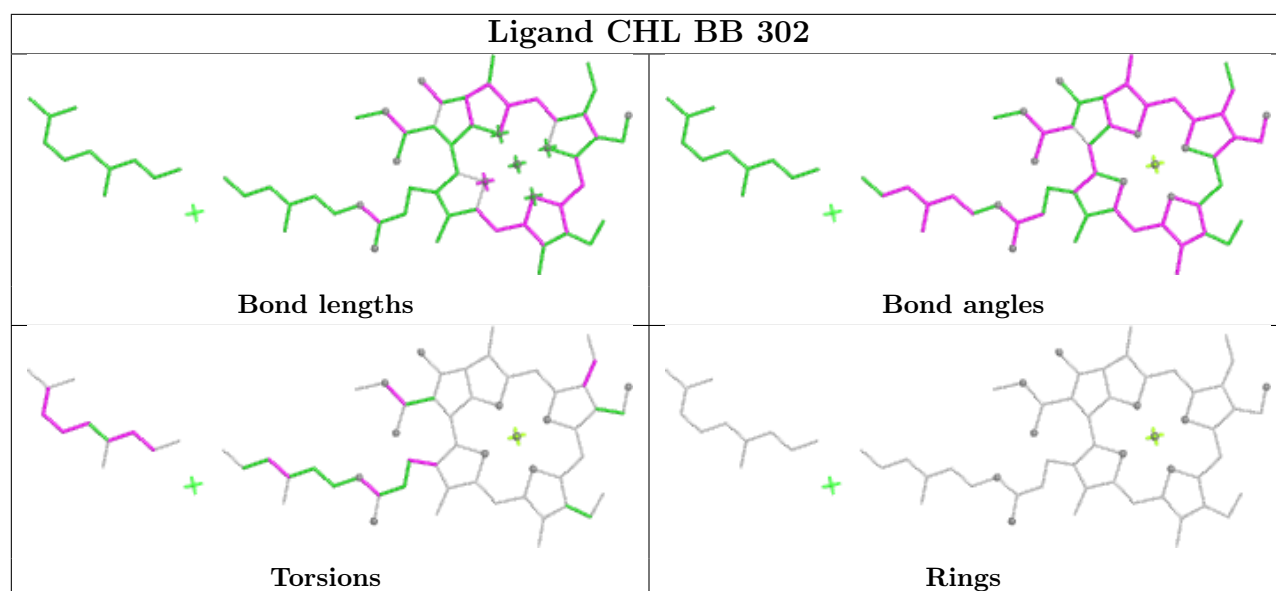
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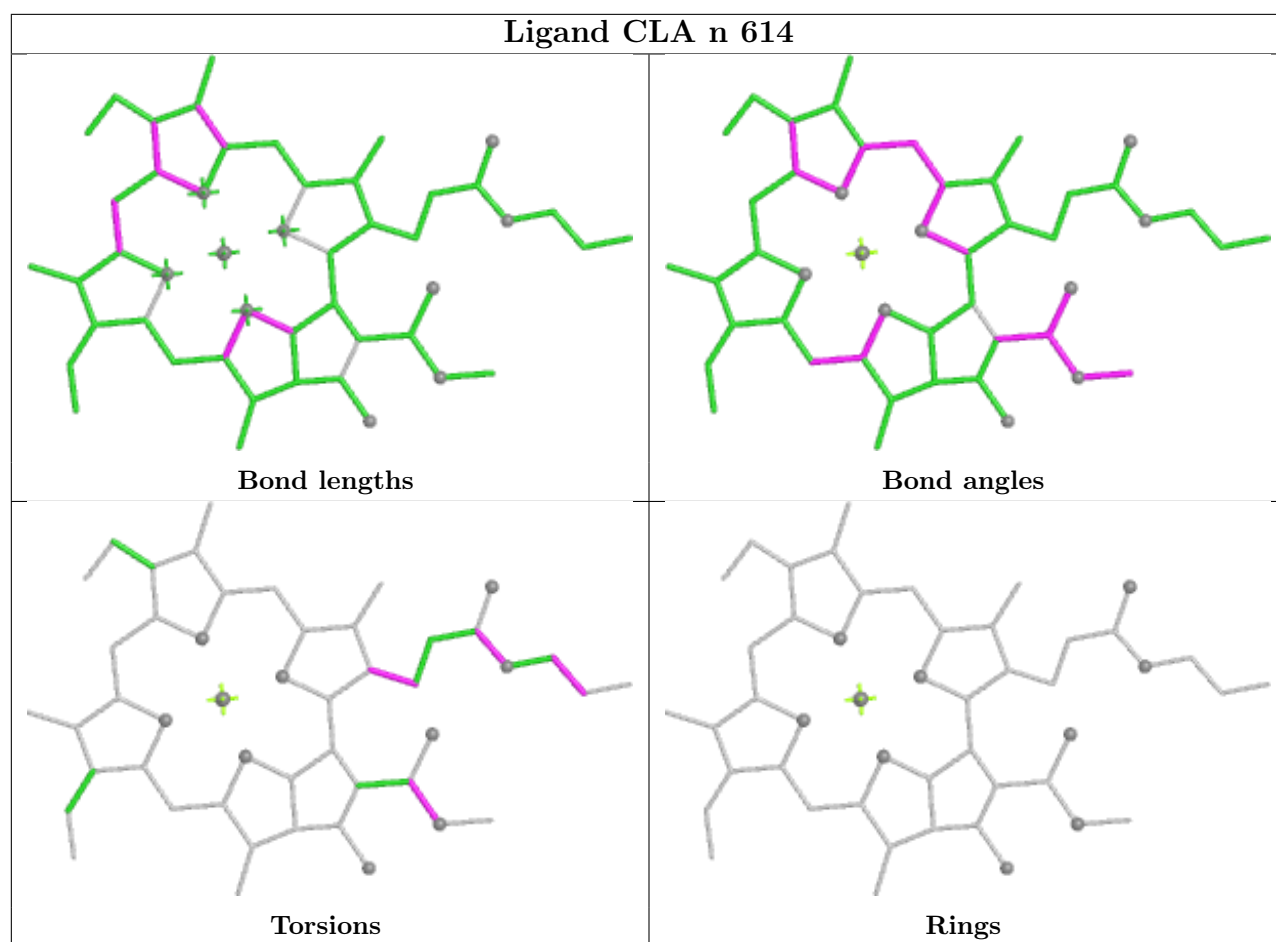


Ligand XAT 7 301

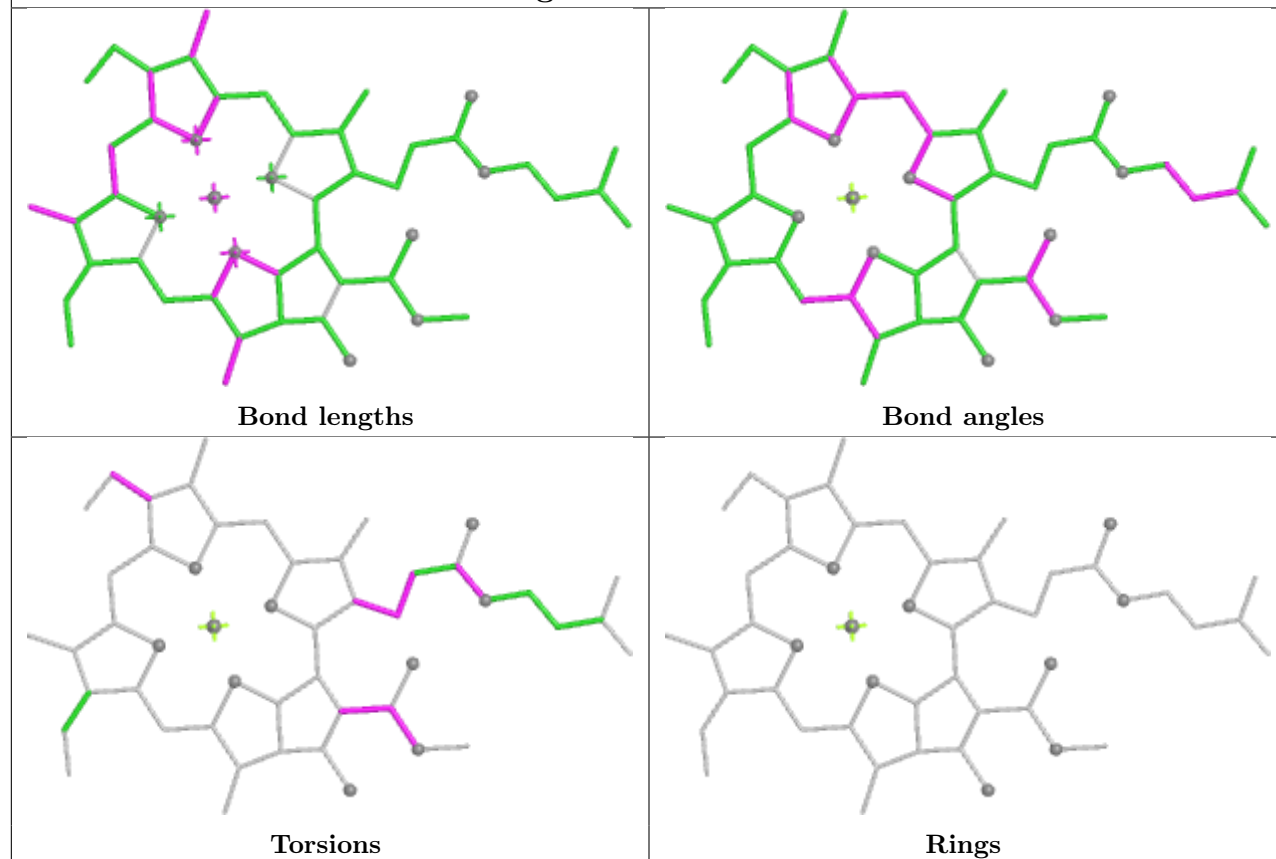




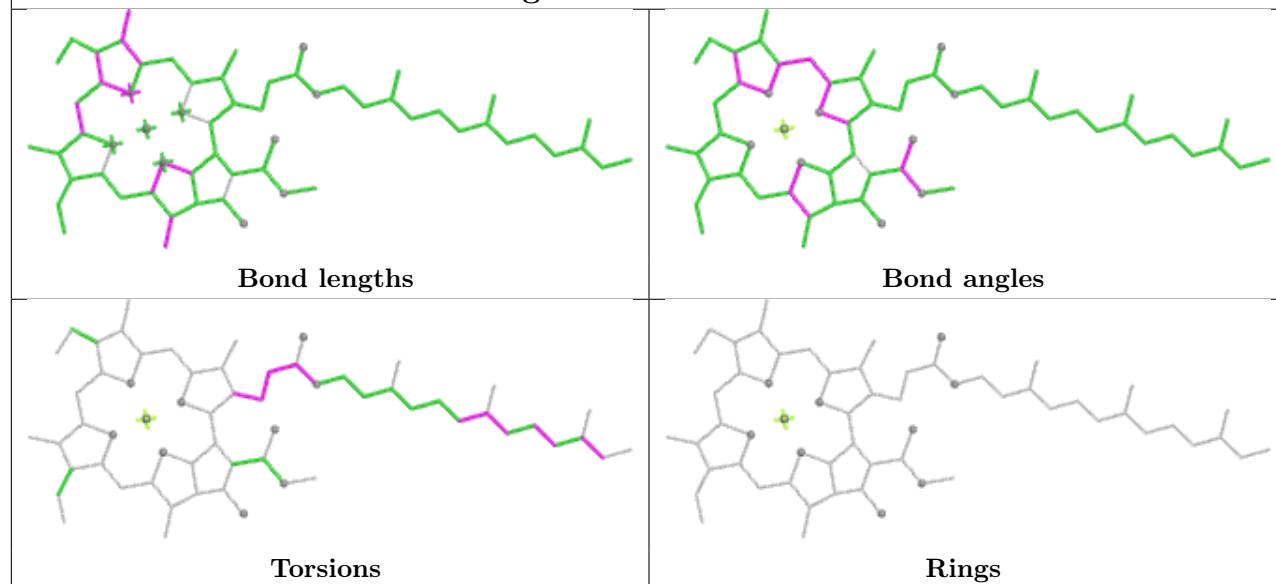


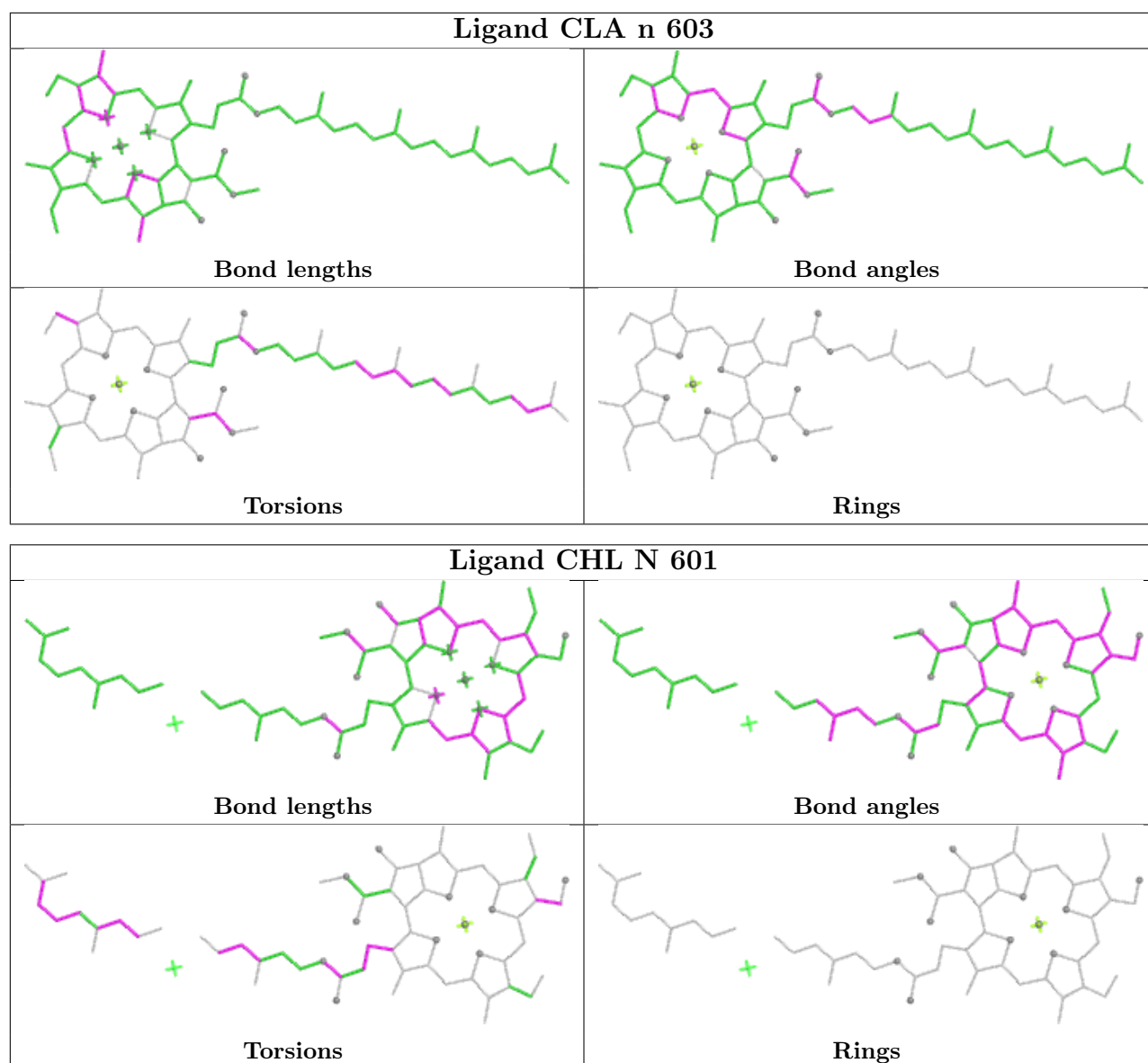


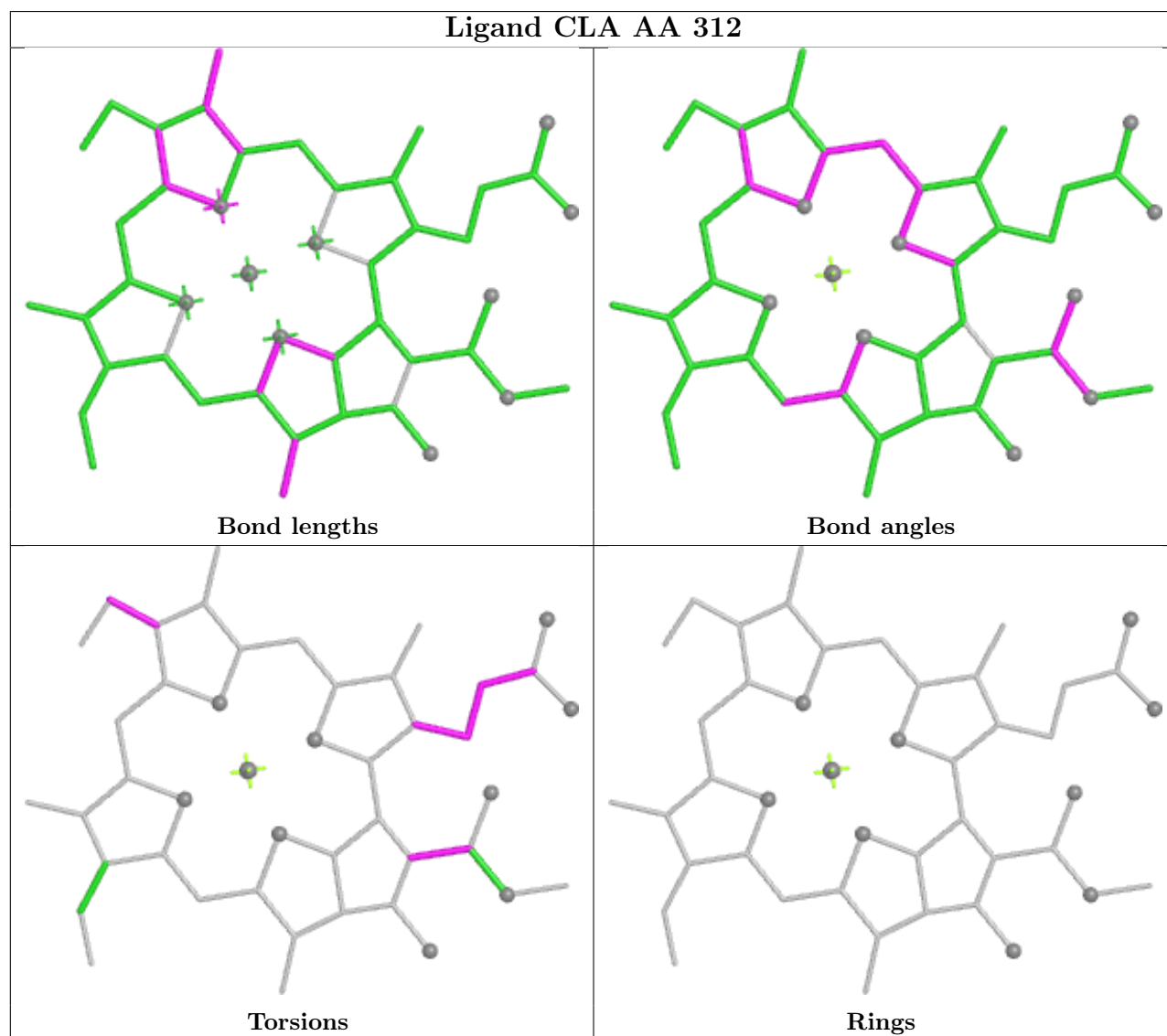
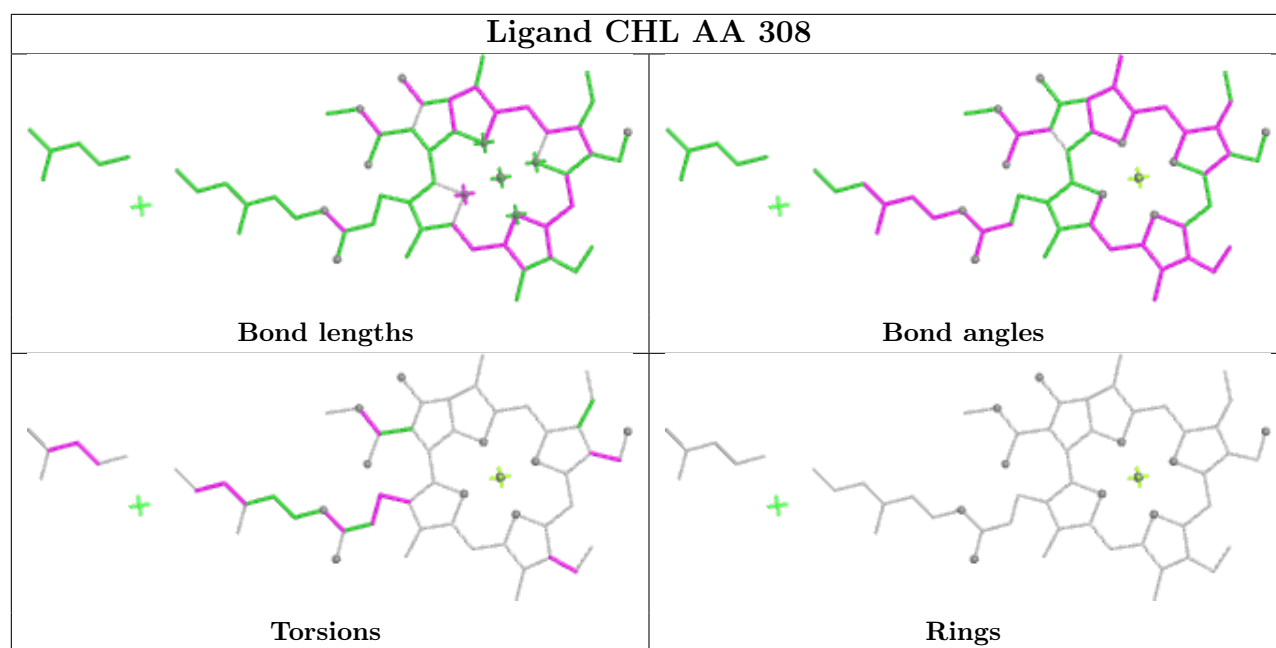
Ligand CLA 9 604

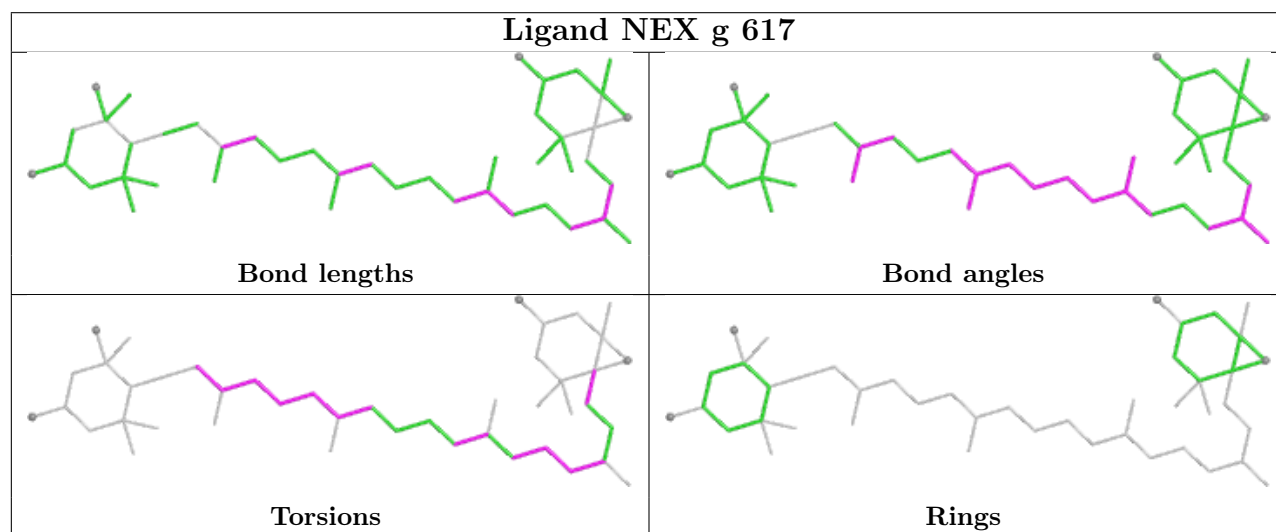
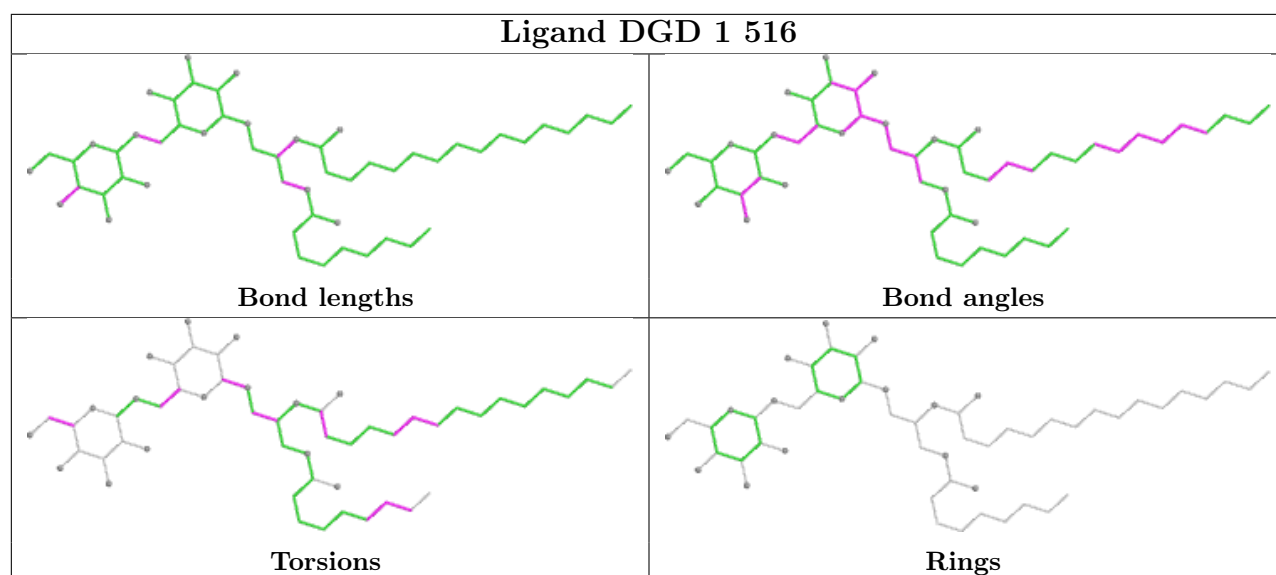


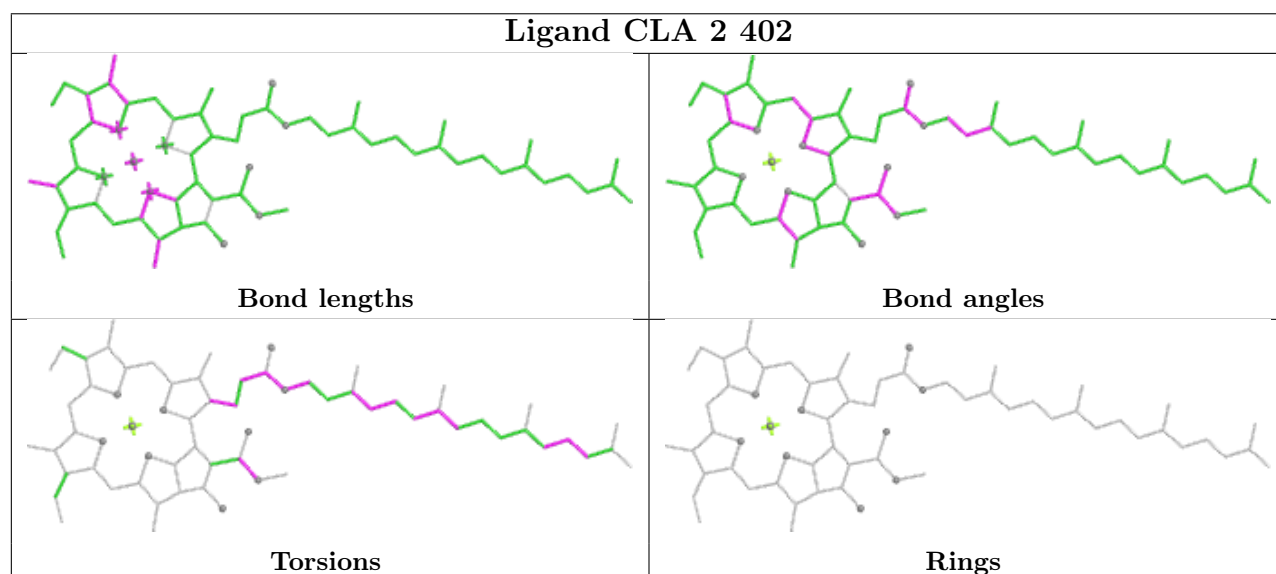
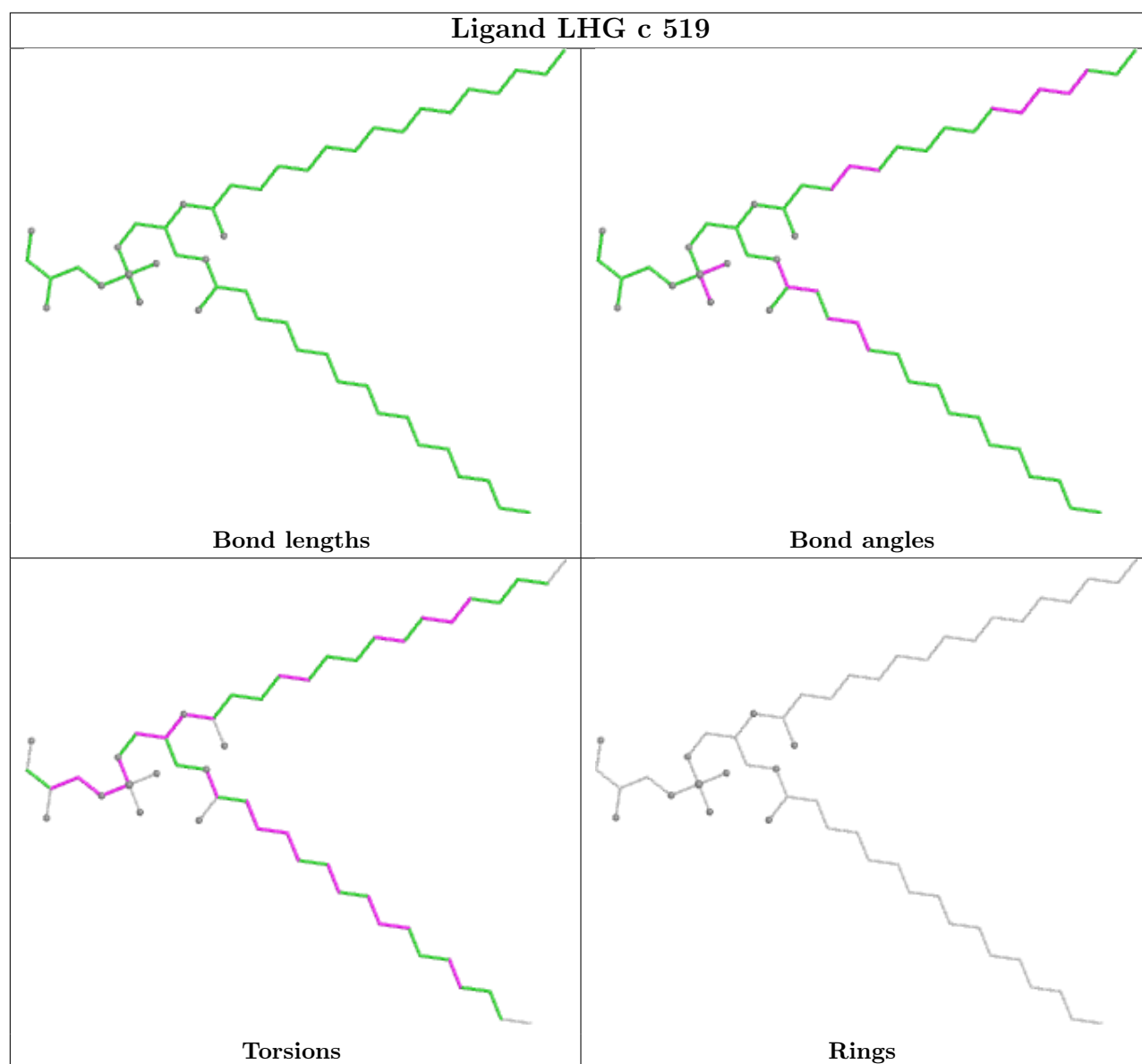
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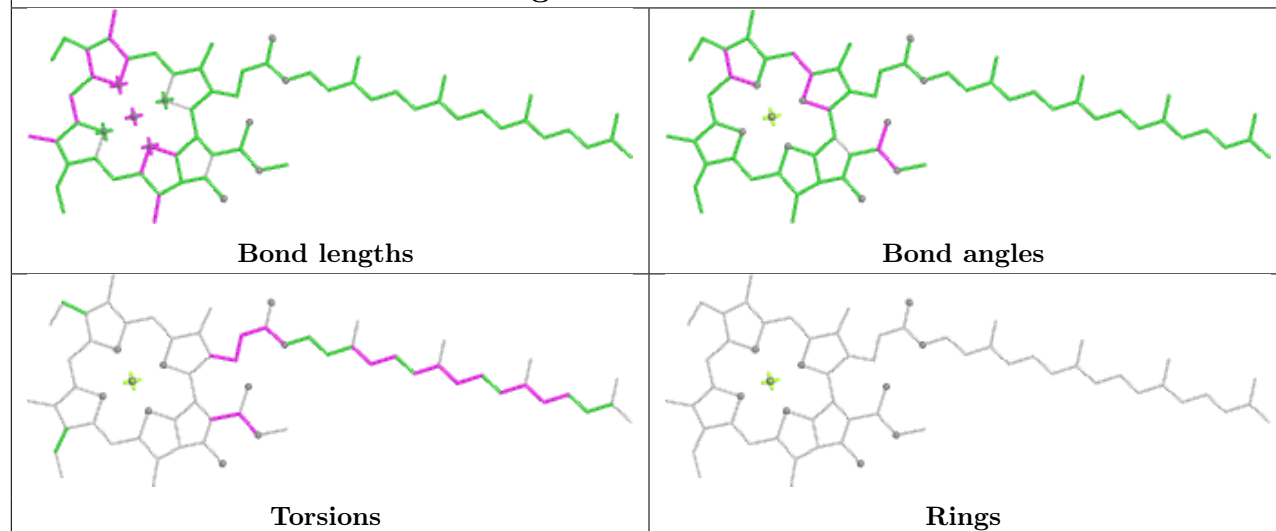
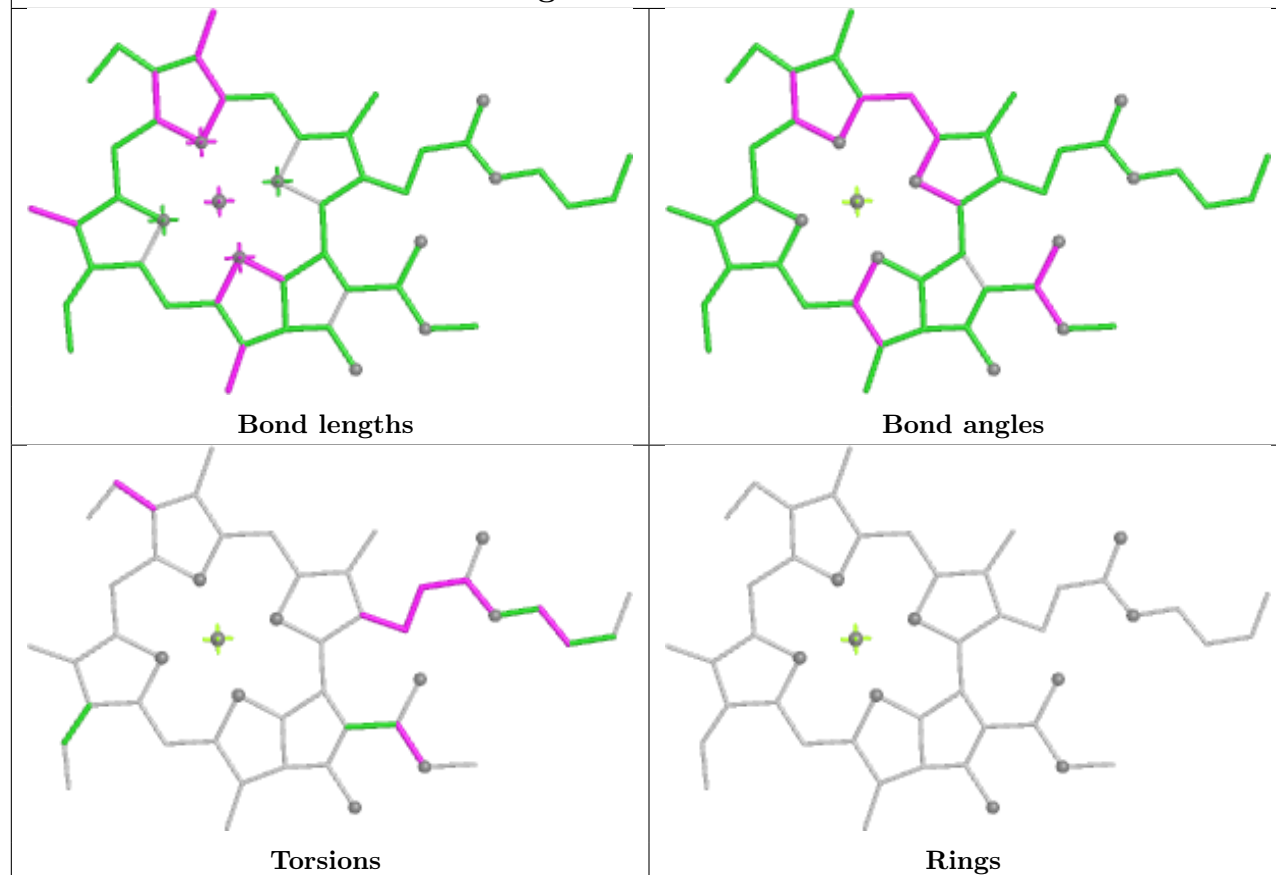


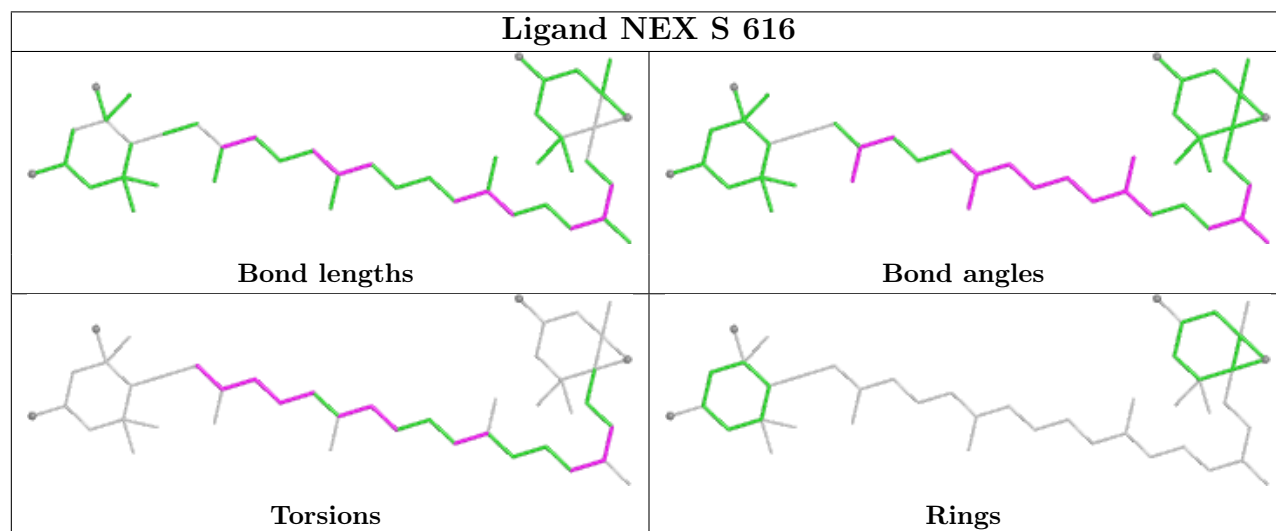
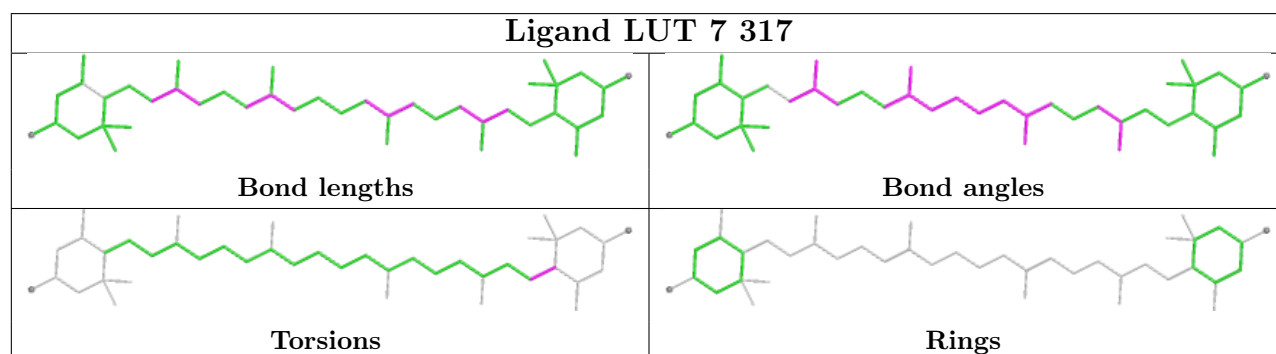
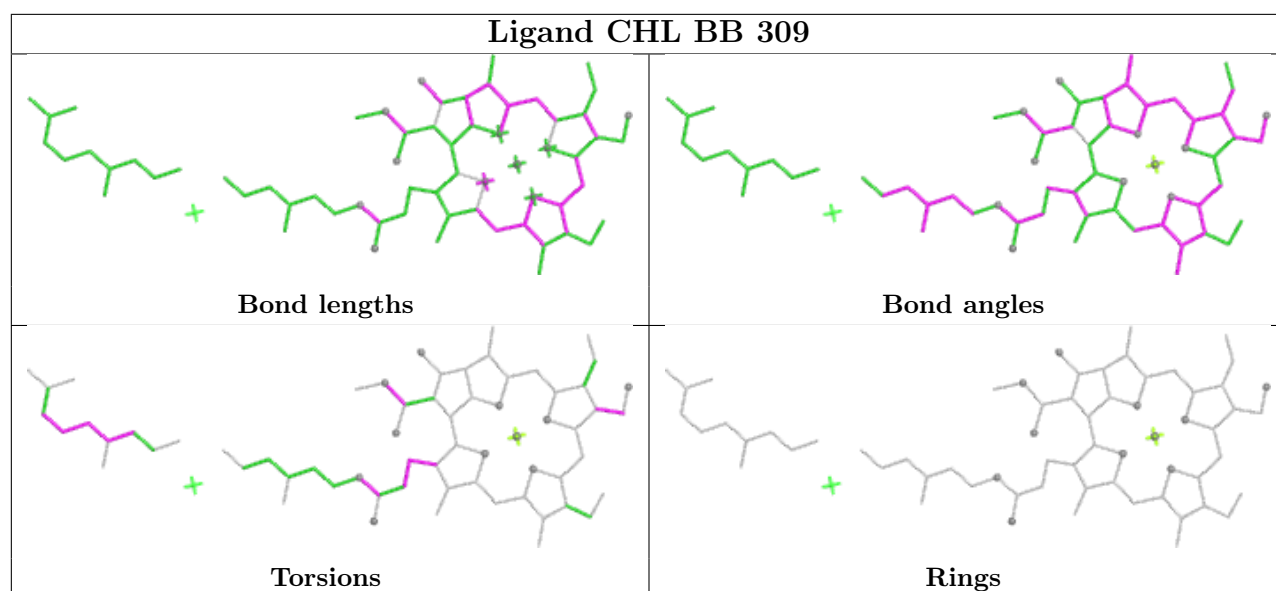


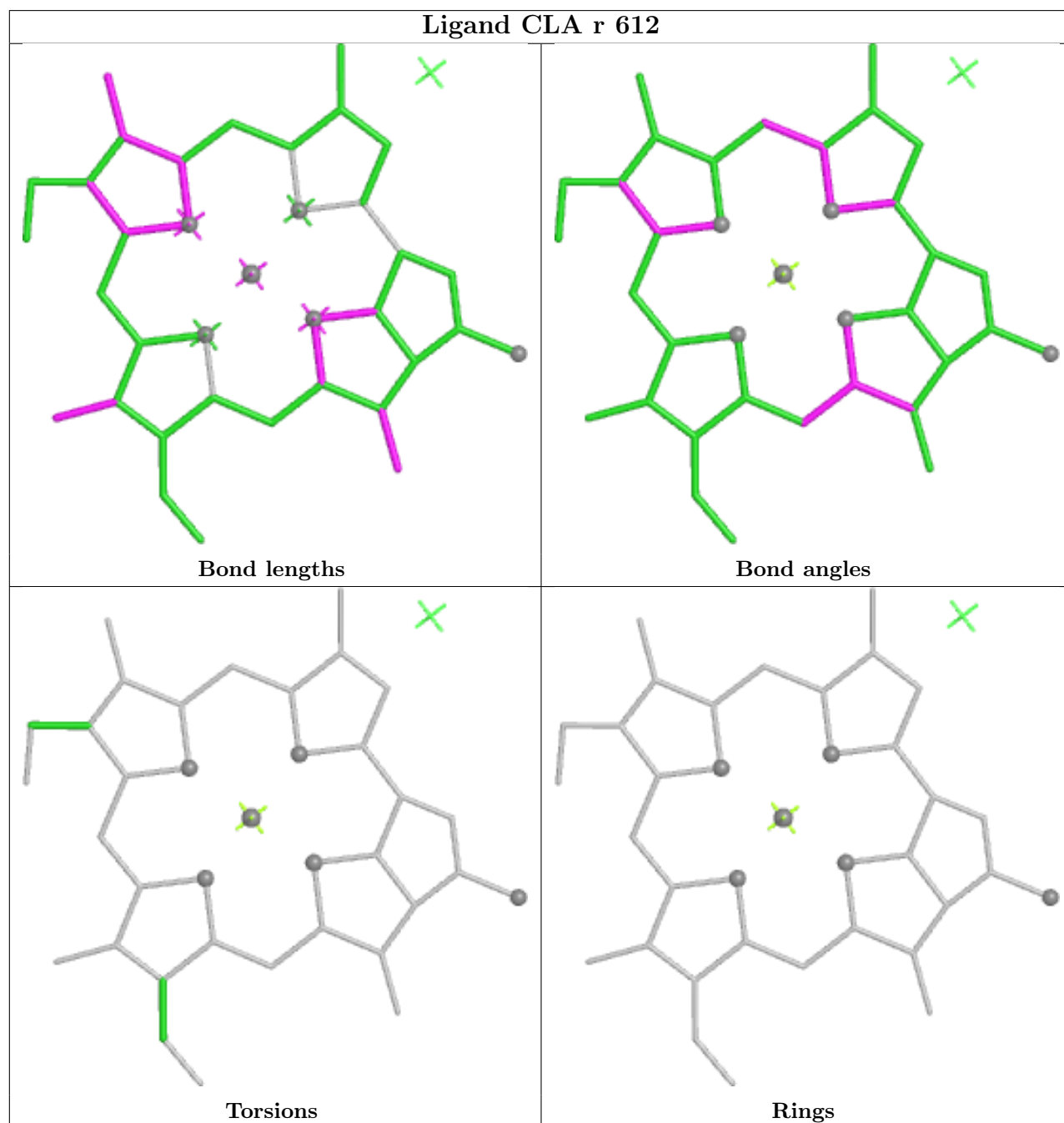
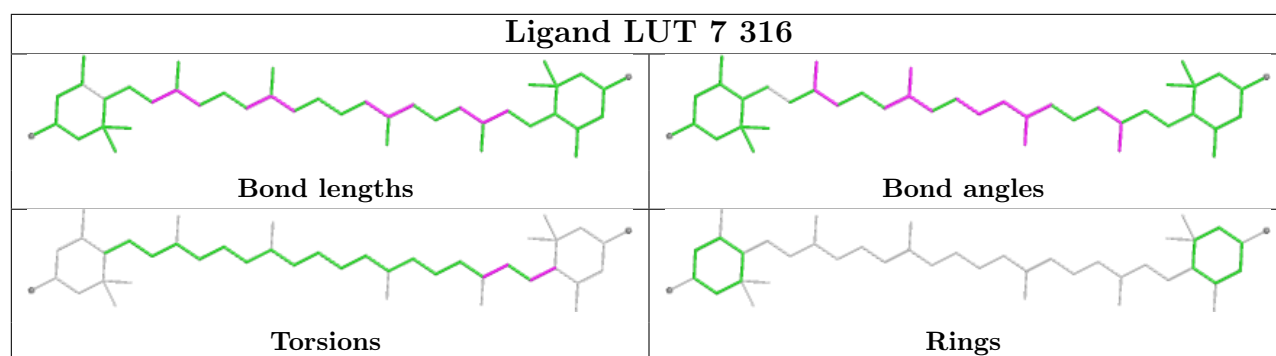


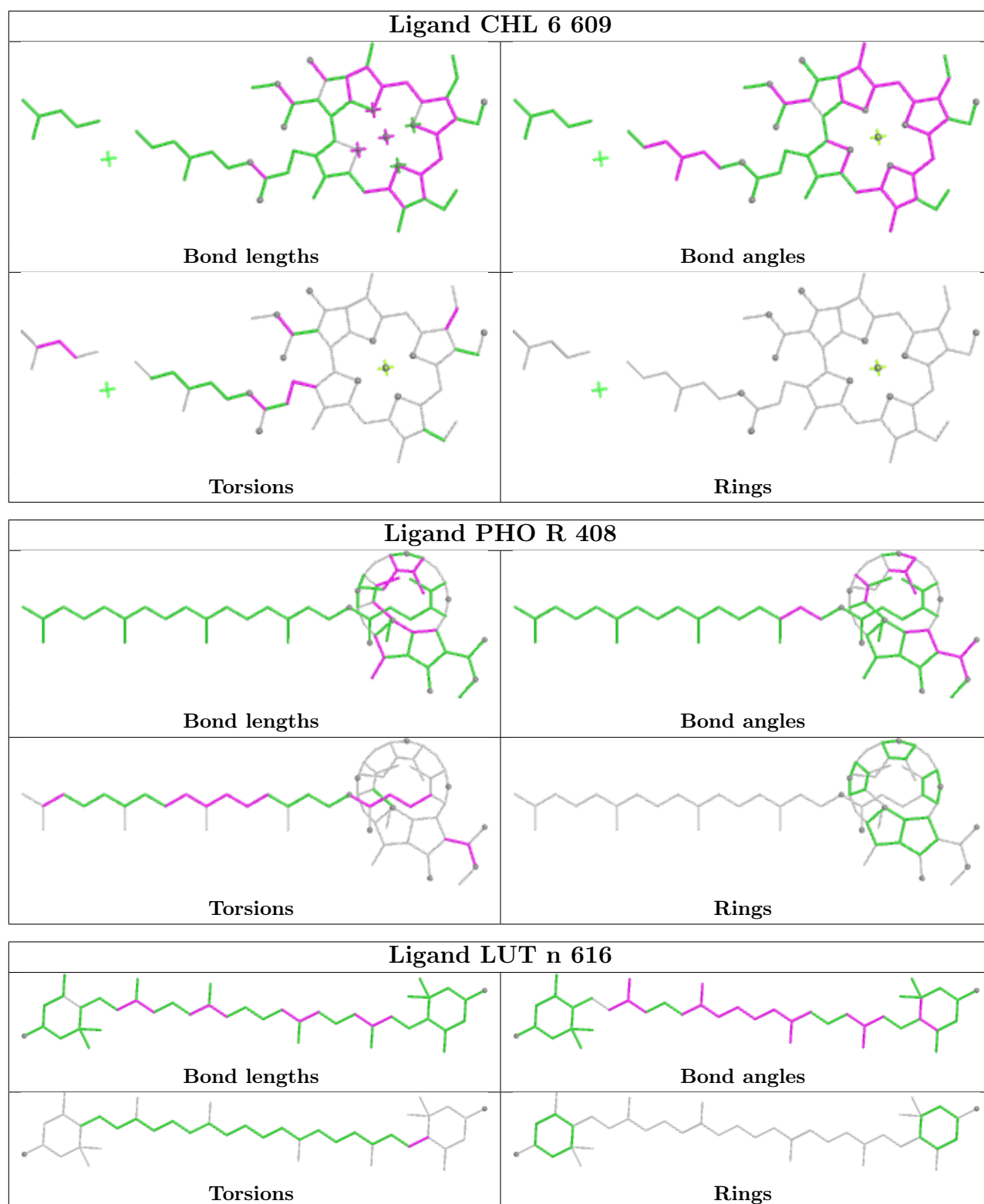


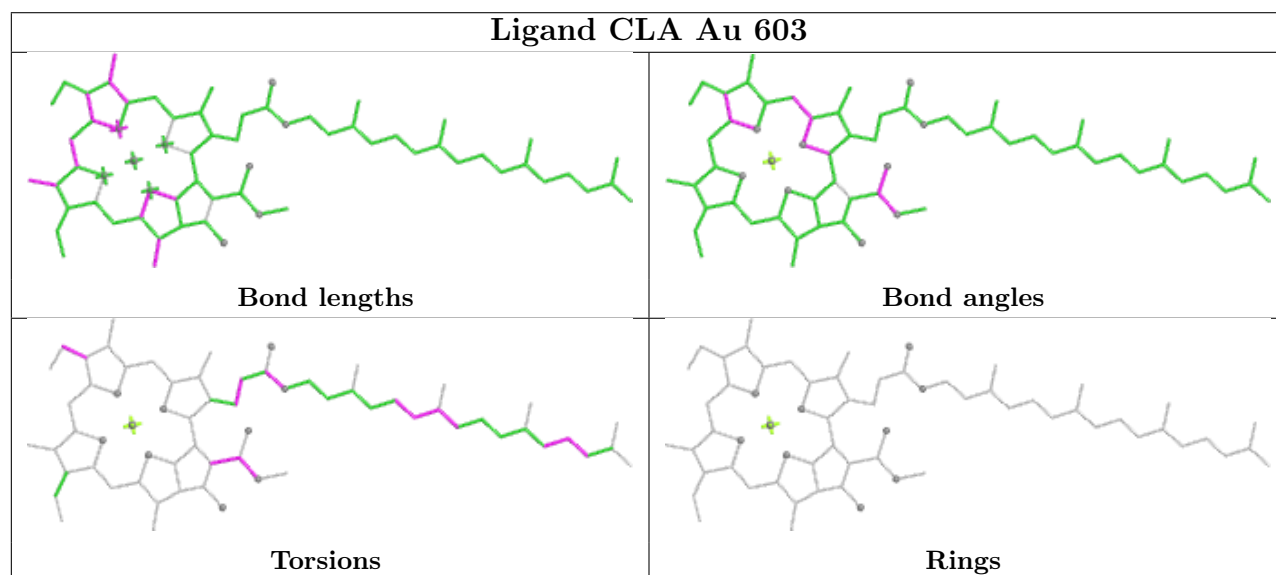
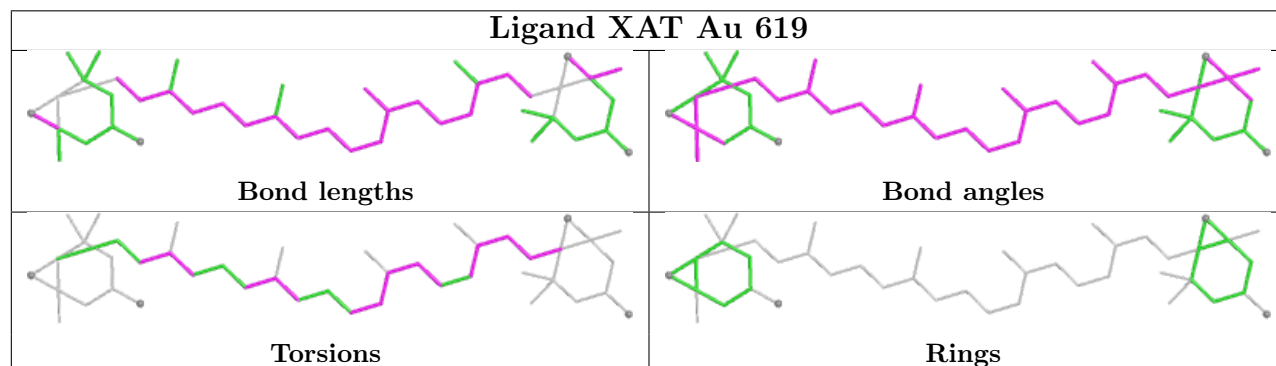
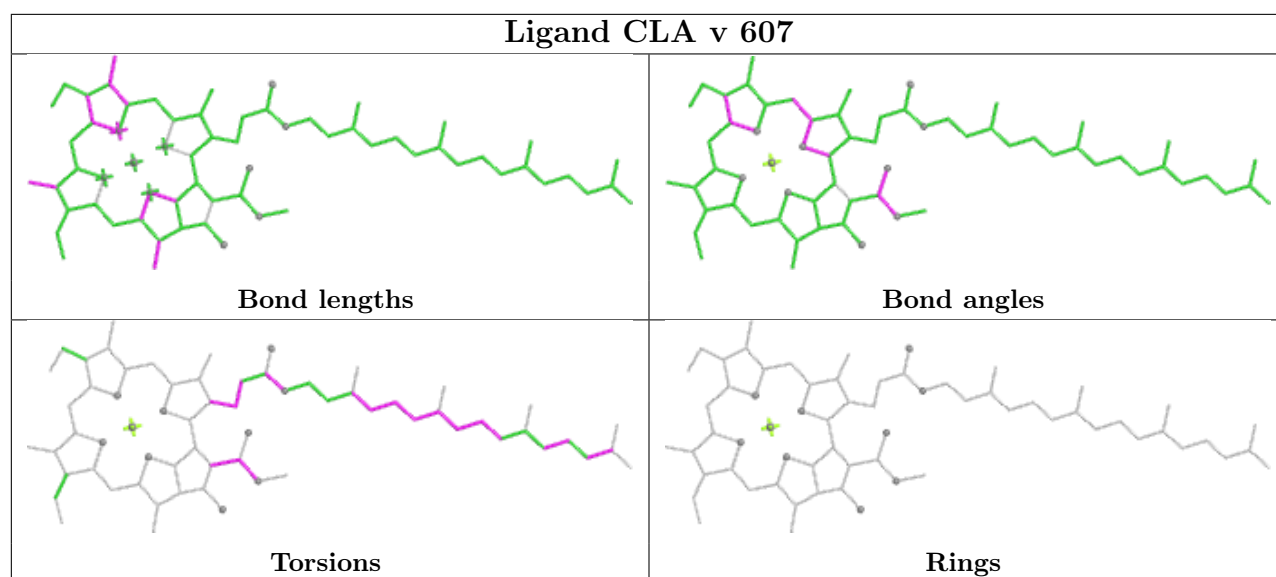


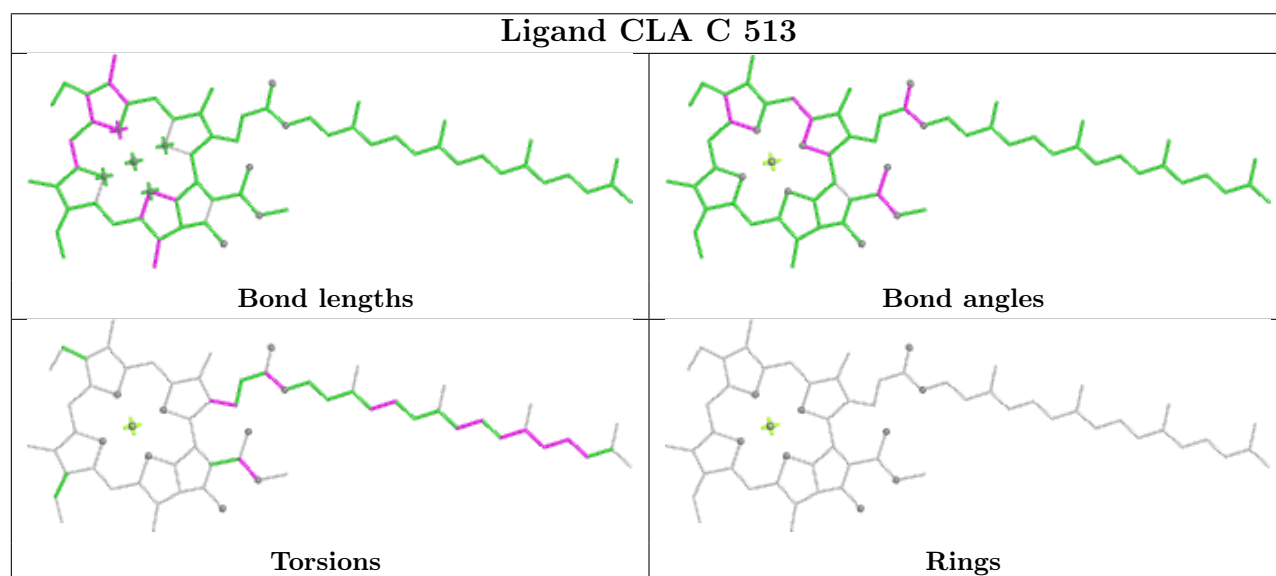
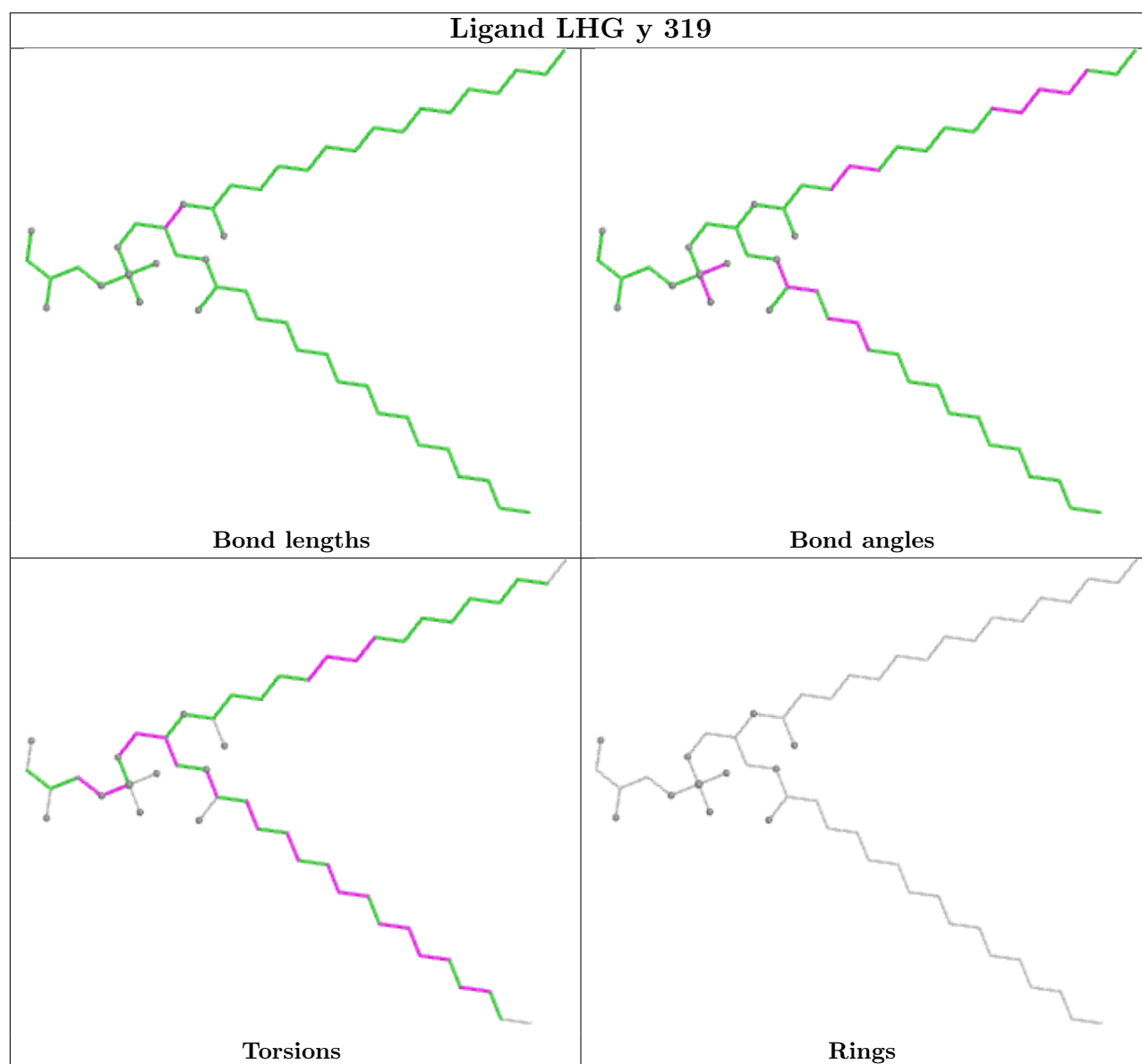
Ligand CLA Y 303**Ligand CLA r 610**

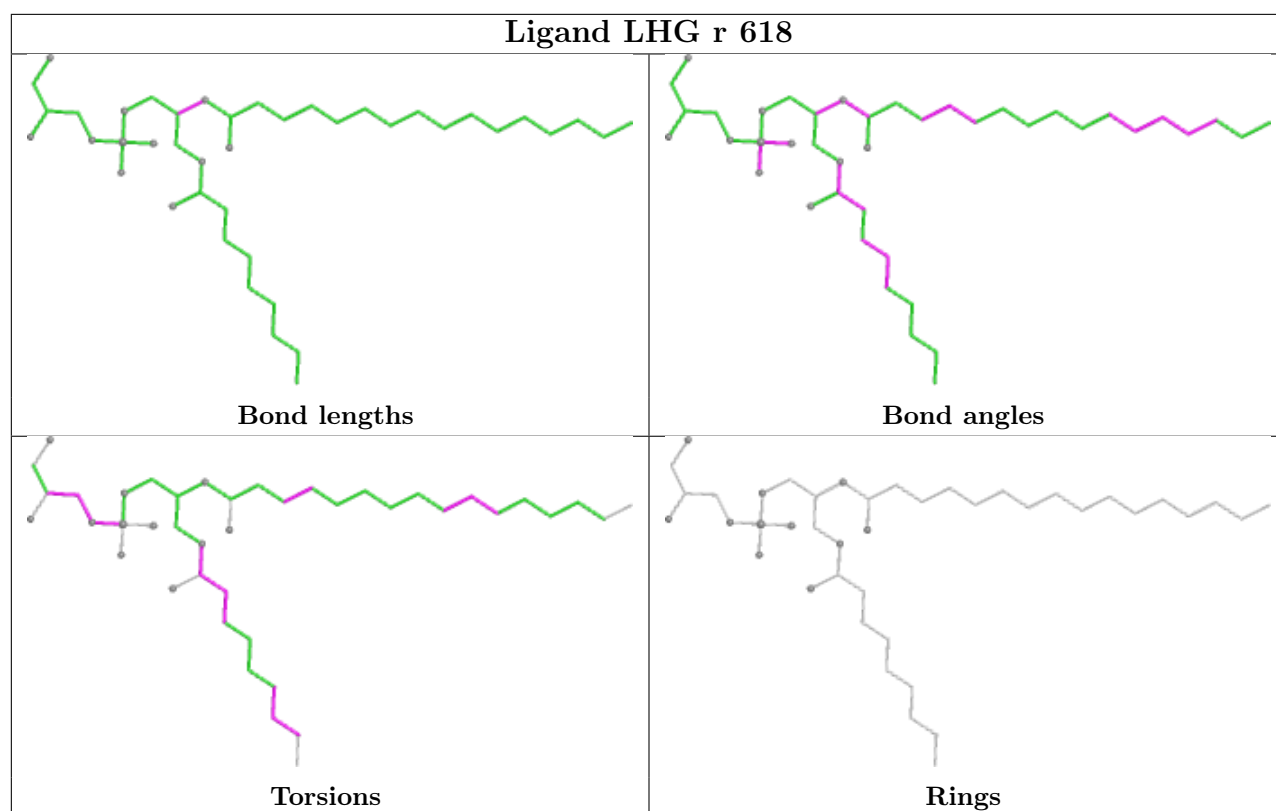




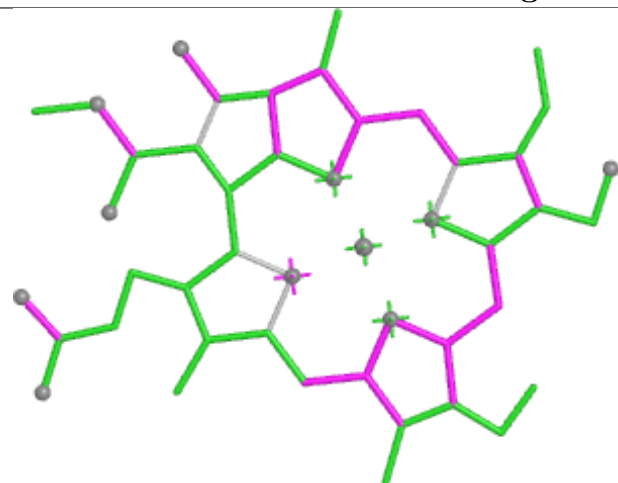




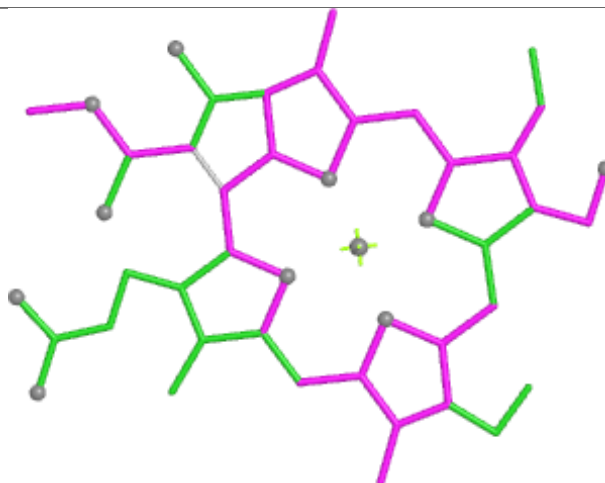




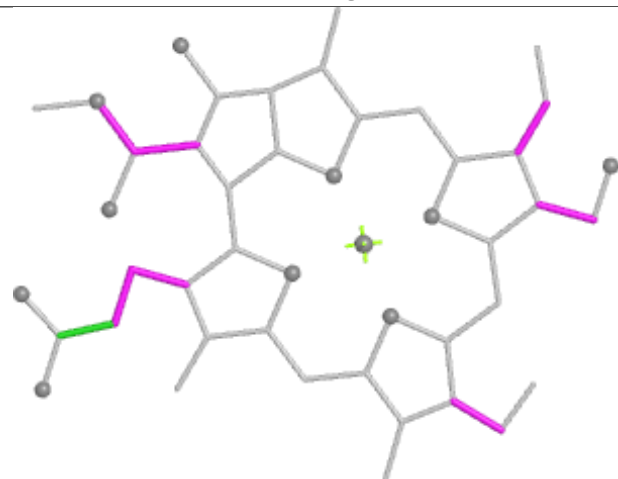
Ligand CHL S 607



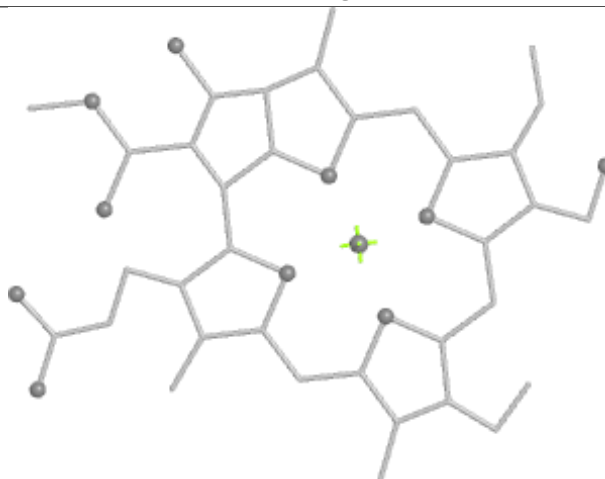
Bond lengths



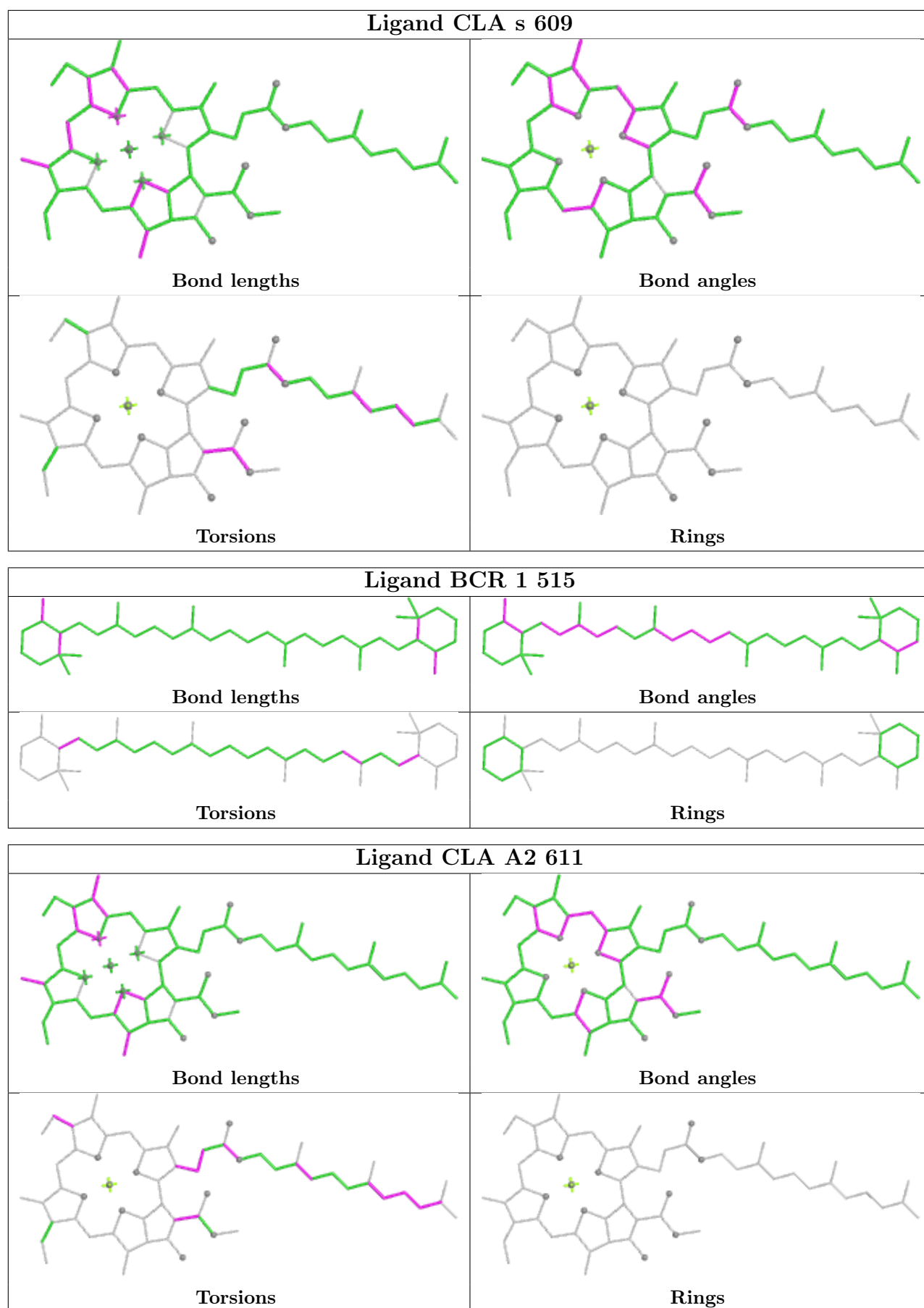
Bond angles

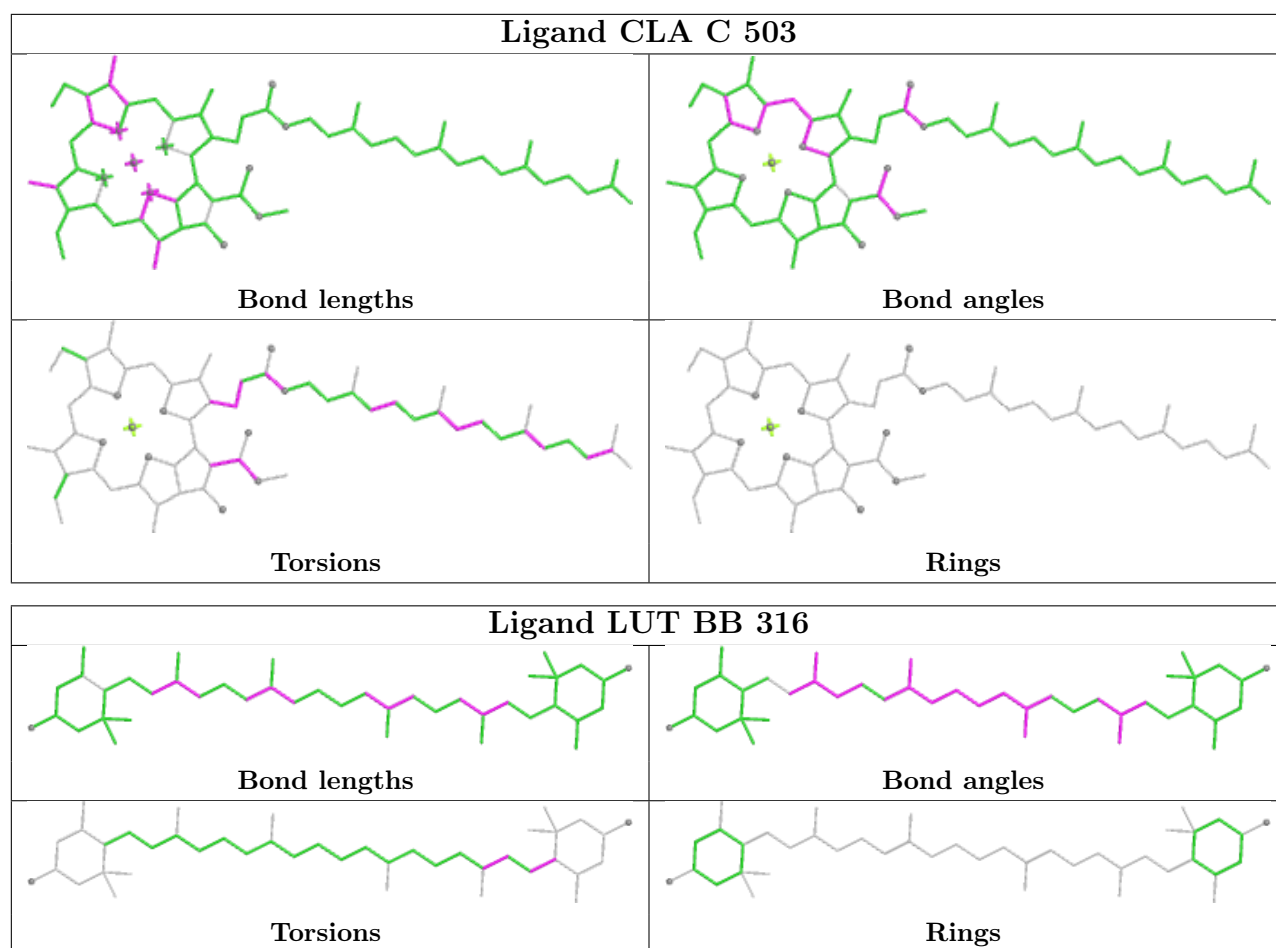


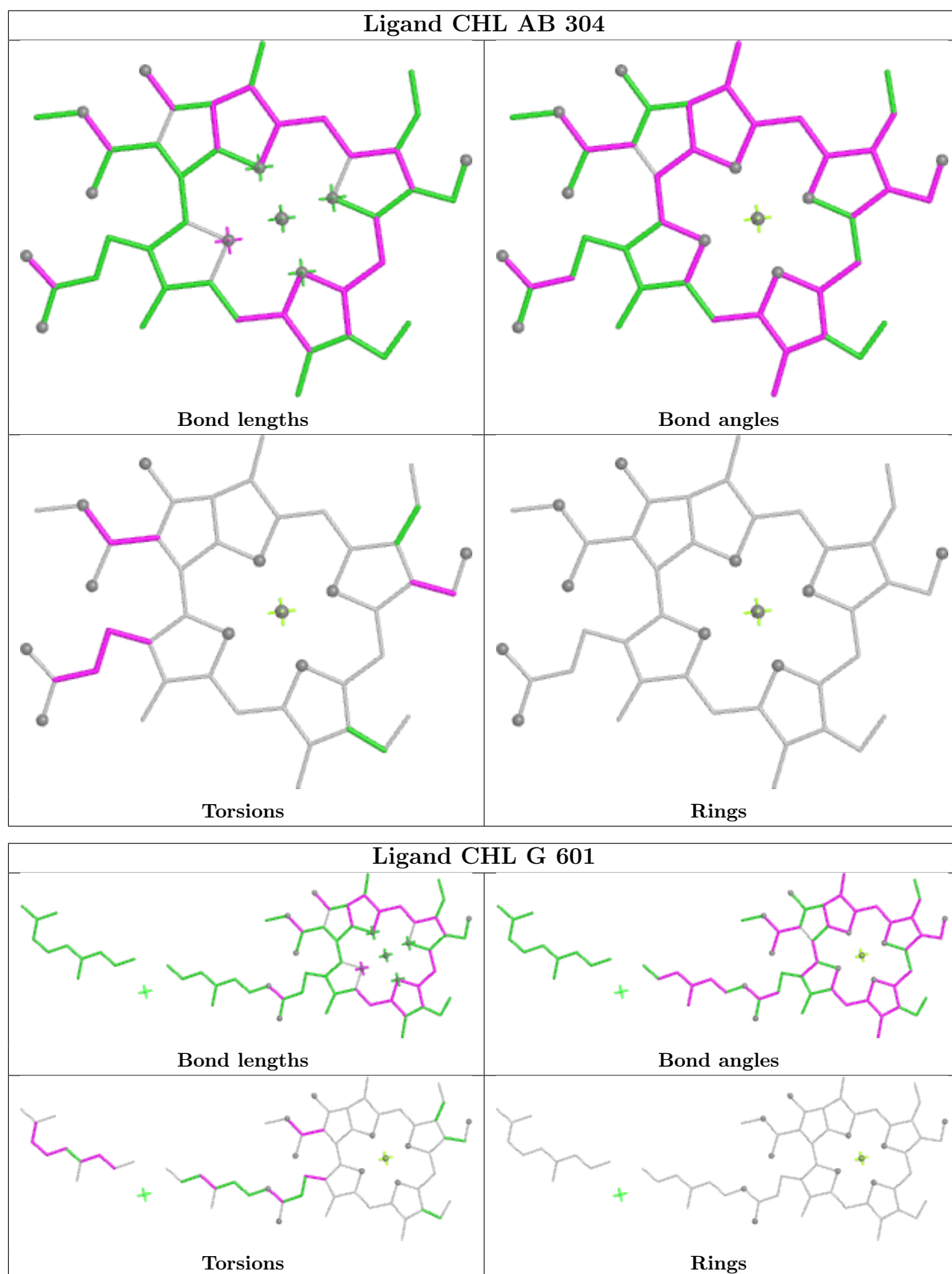
Torsions



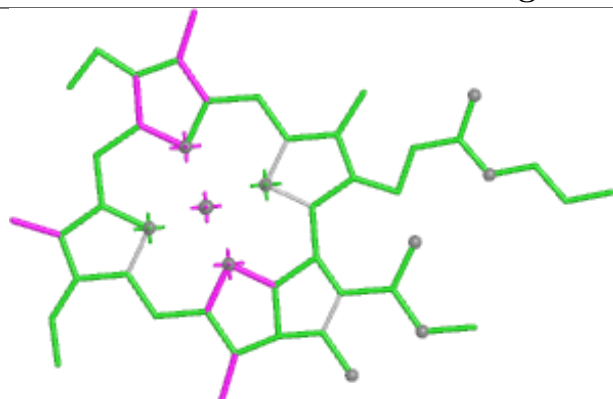
Rings



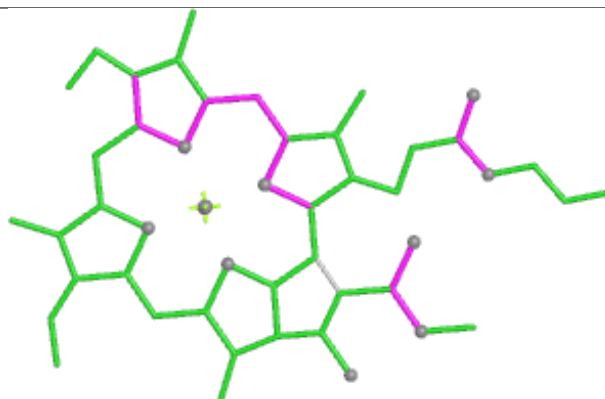




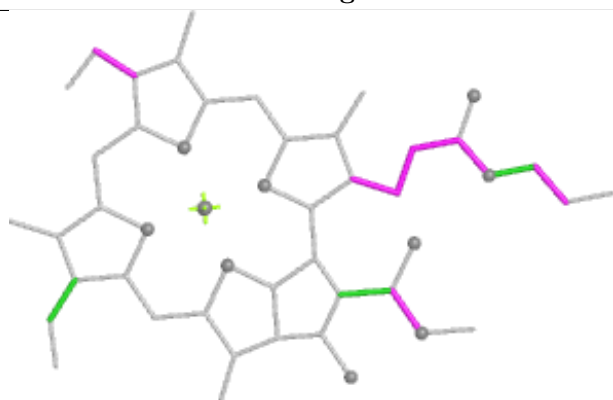
Ligand CLA 6 614



Bond lengths



Bond angles

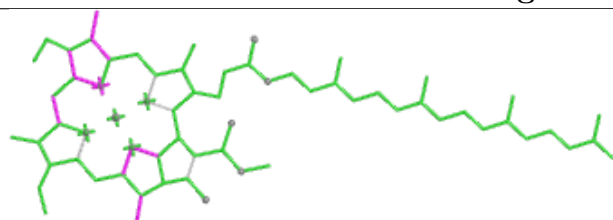


Torsions

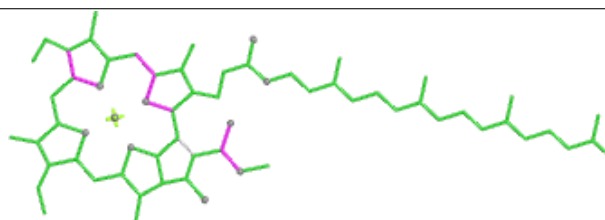


Rings

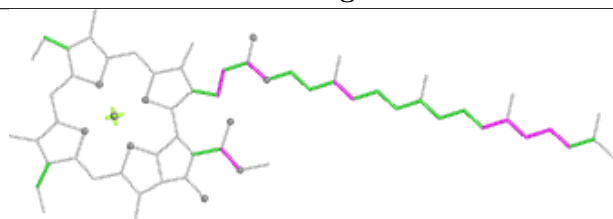
Ligand CLA b 604



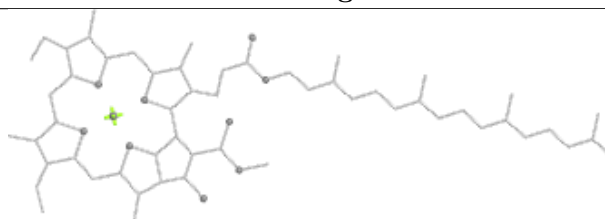
Bond lengths



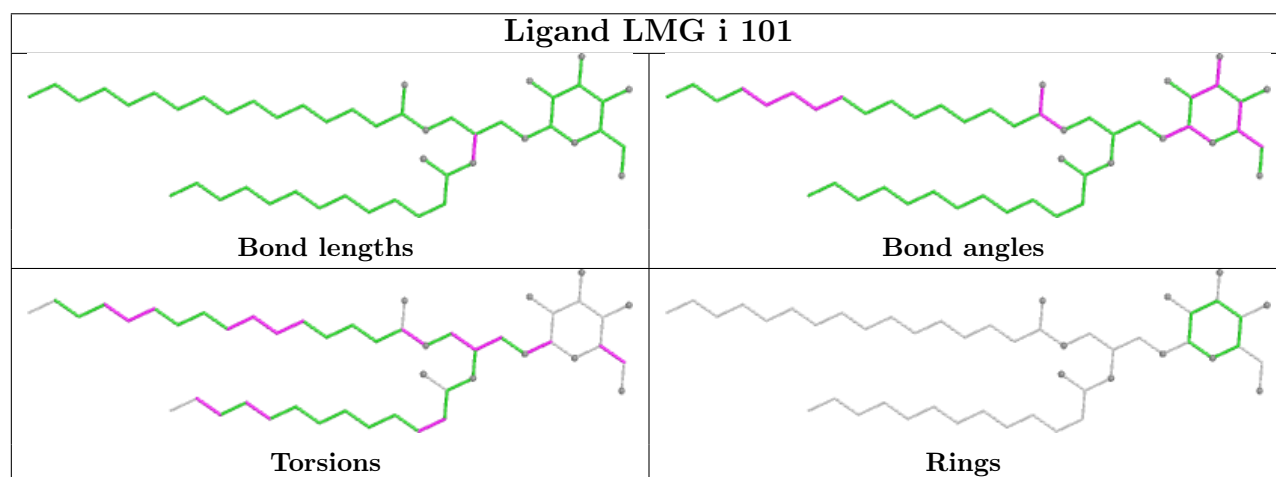
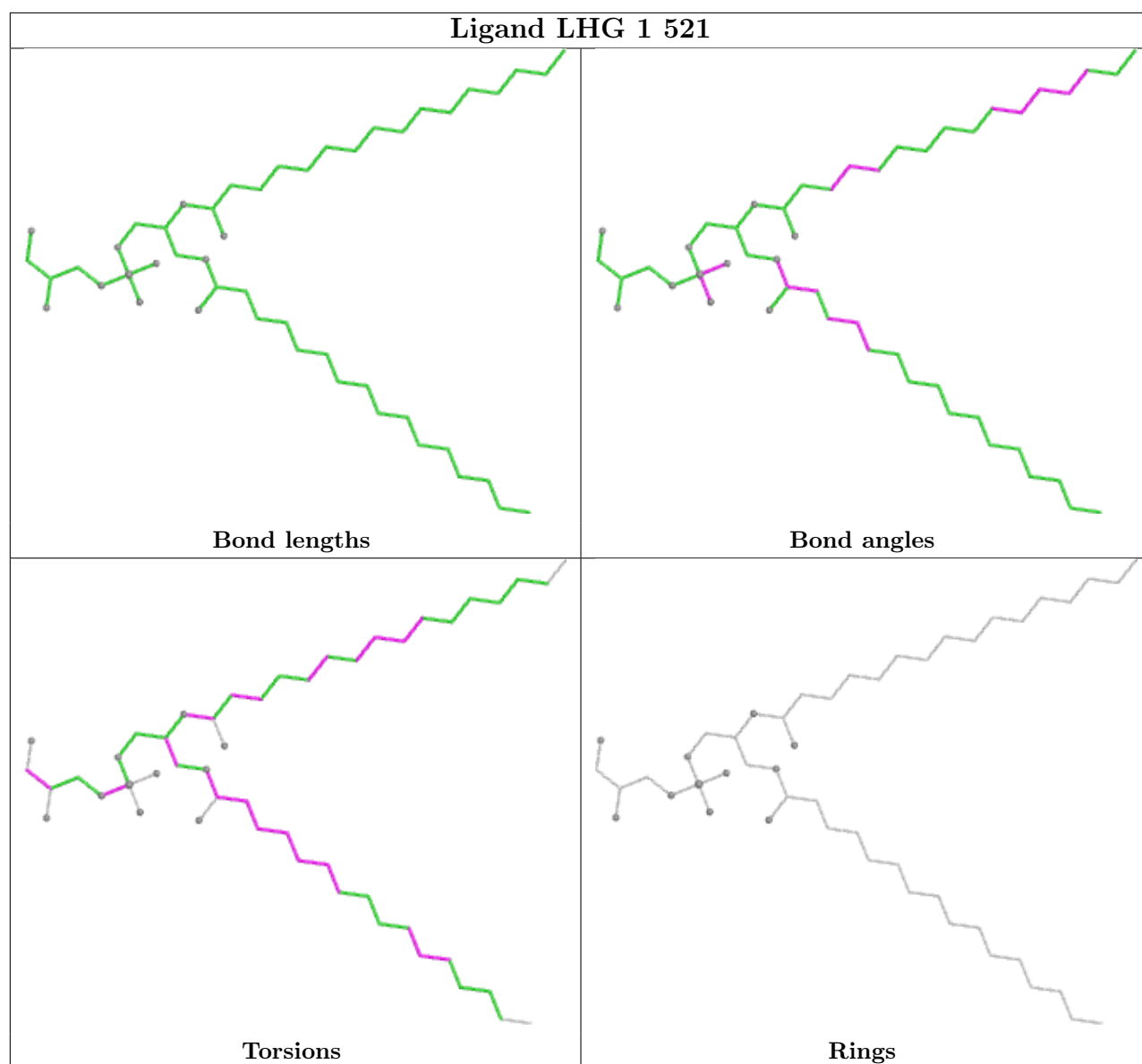
Bond angles

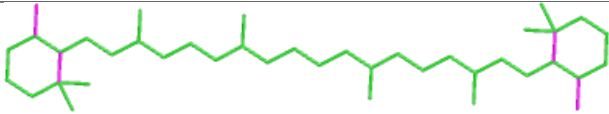
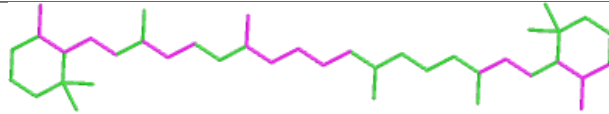
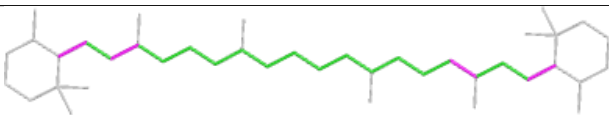
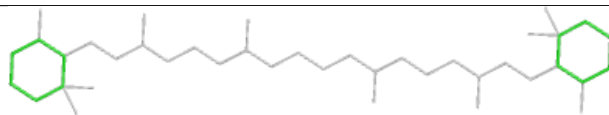


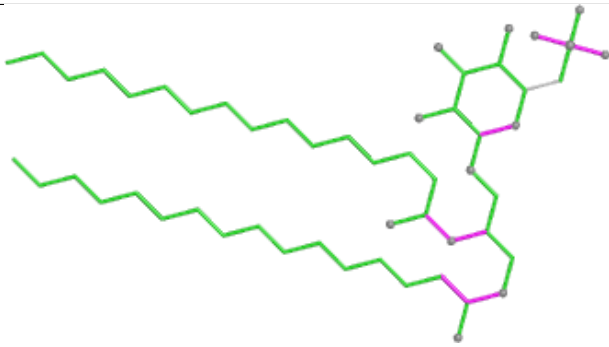
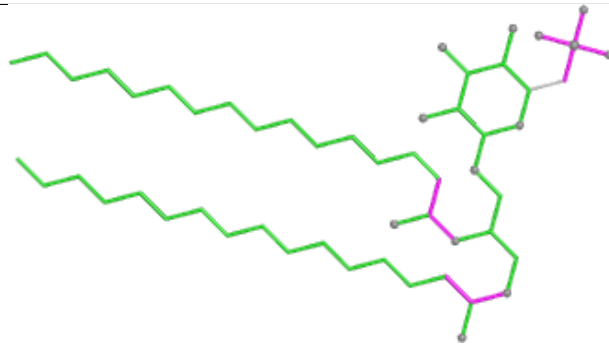
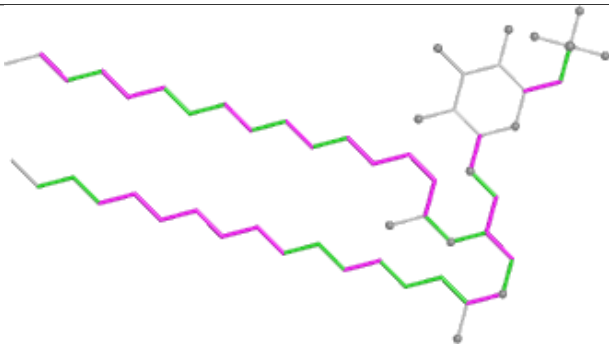
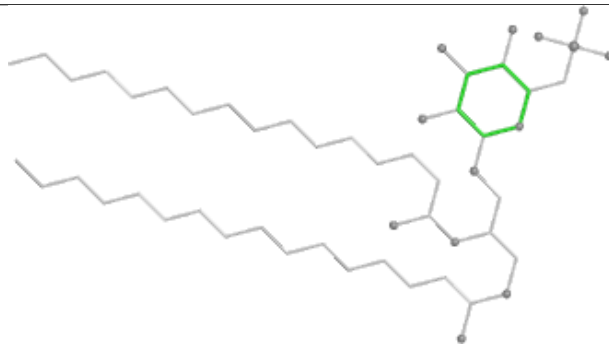
Torsions

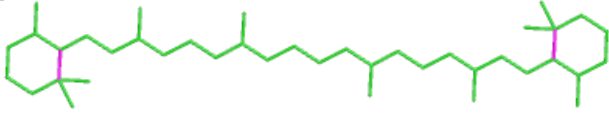
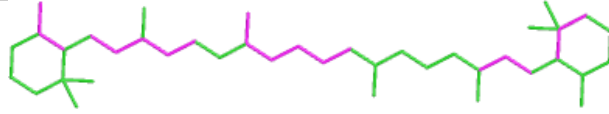
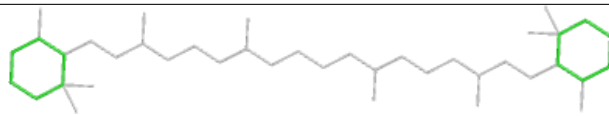


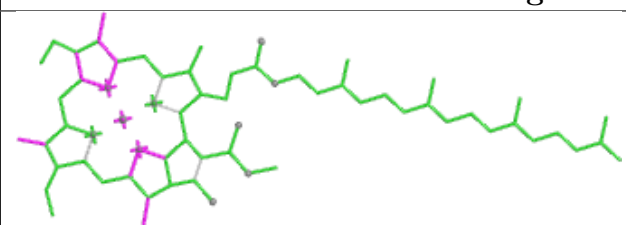
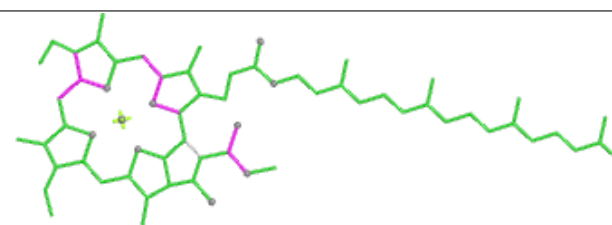
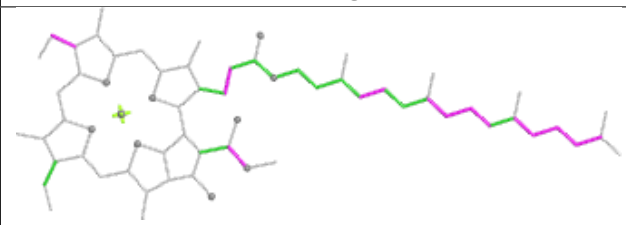
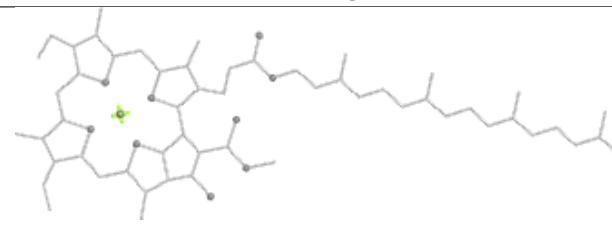
Rings

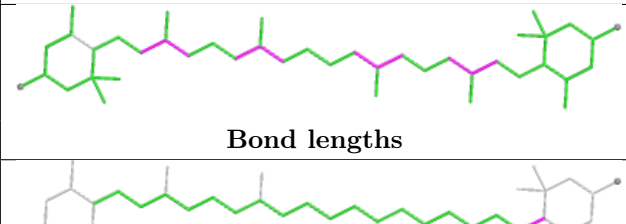
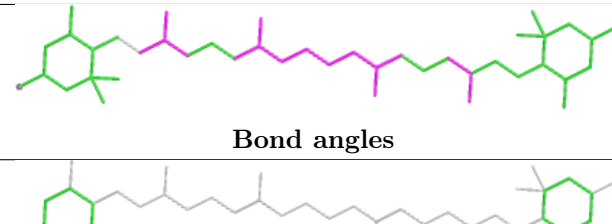
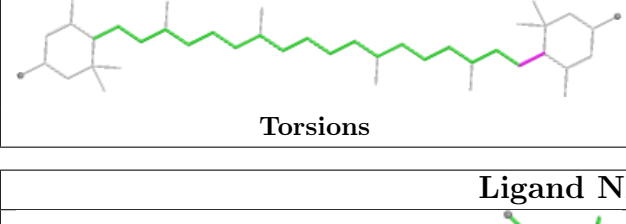
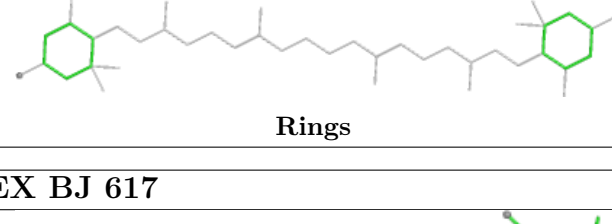


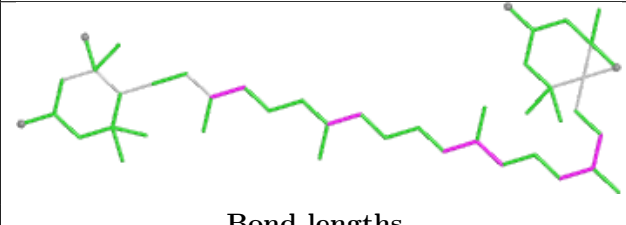
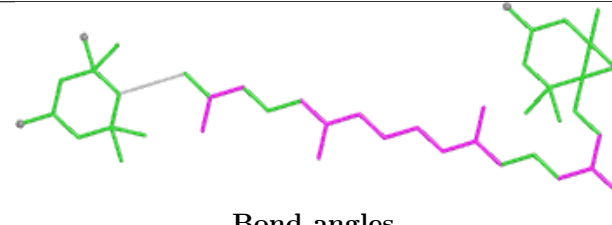
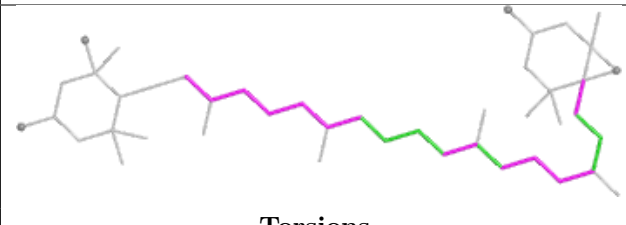
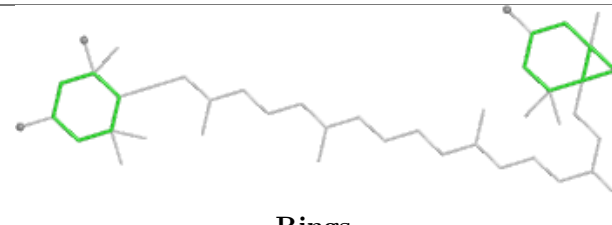
Ligand BCR Bb 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SQD A 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

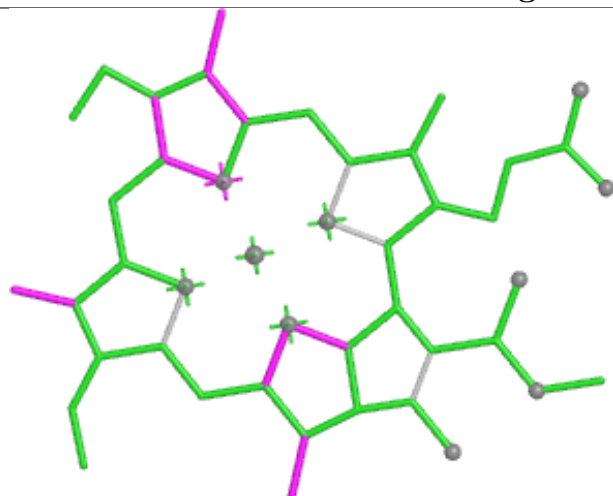
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

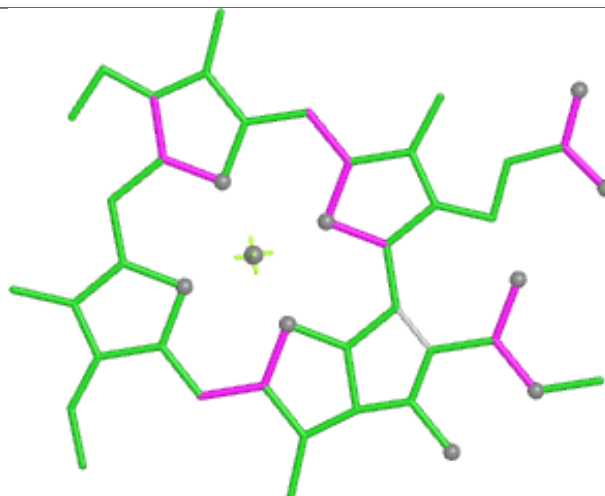
Ligand LUT 8 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX BJ 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

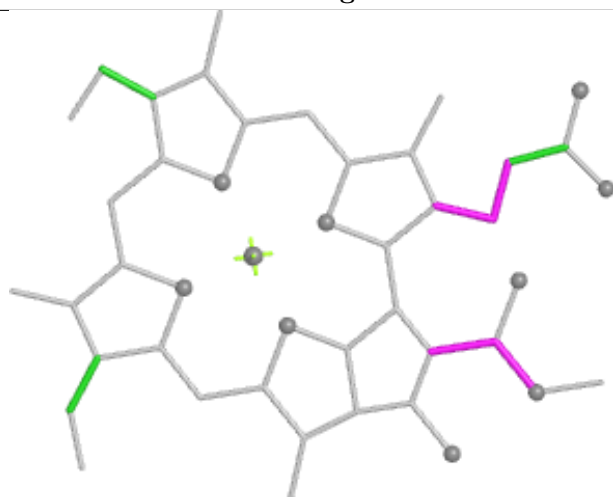
Ligand CLA 0 604



Bond lengths



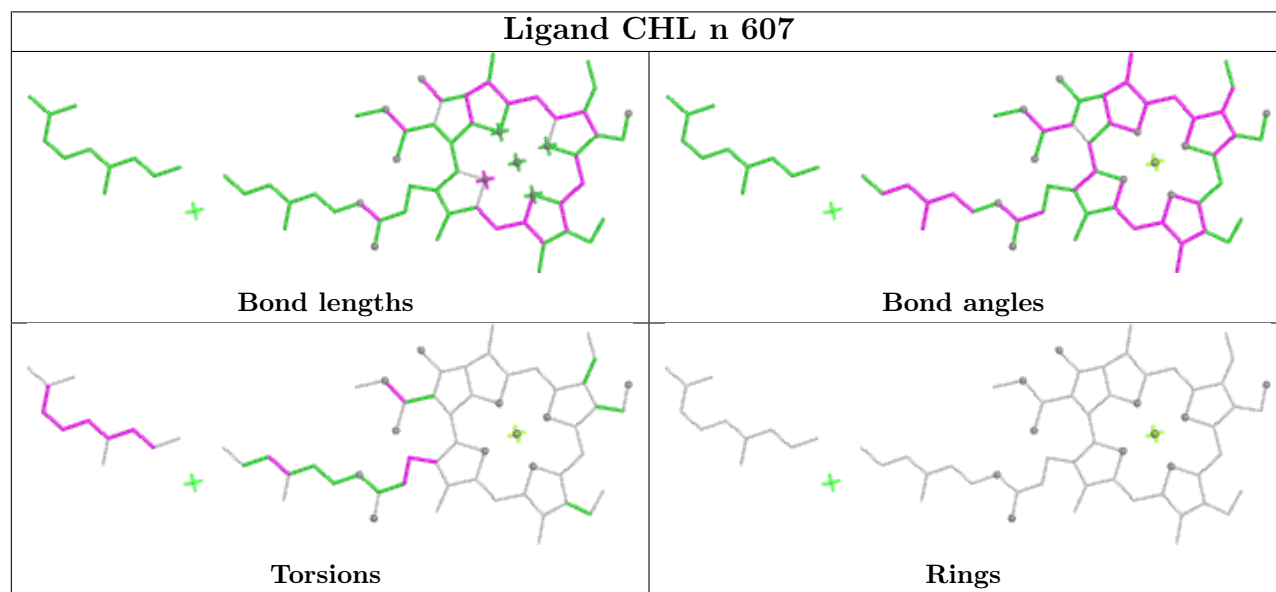
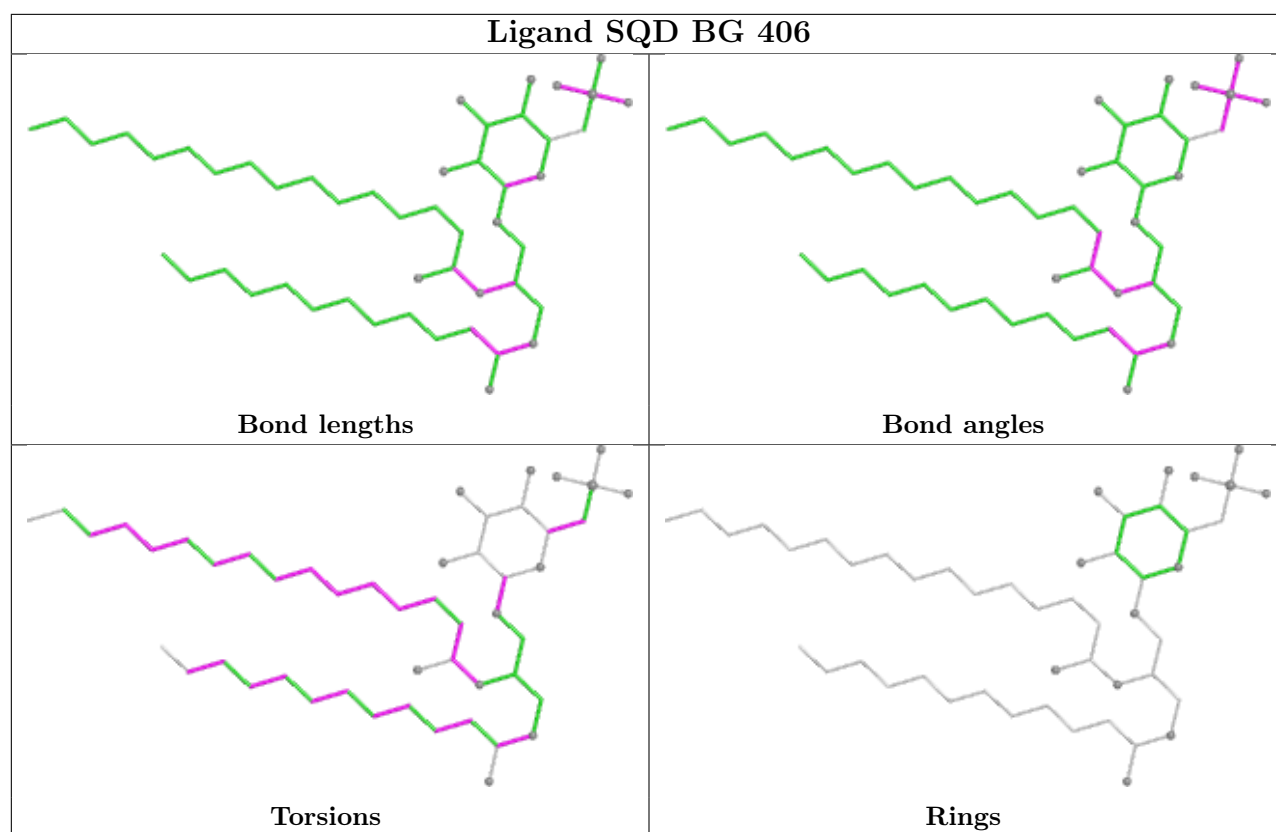
Bond angles

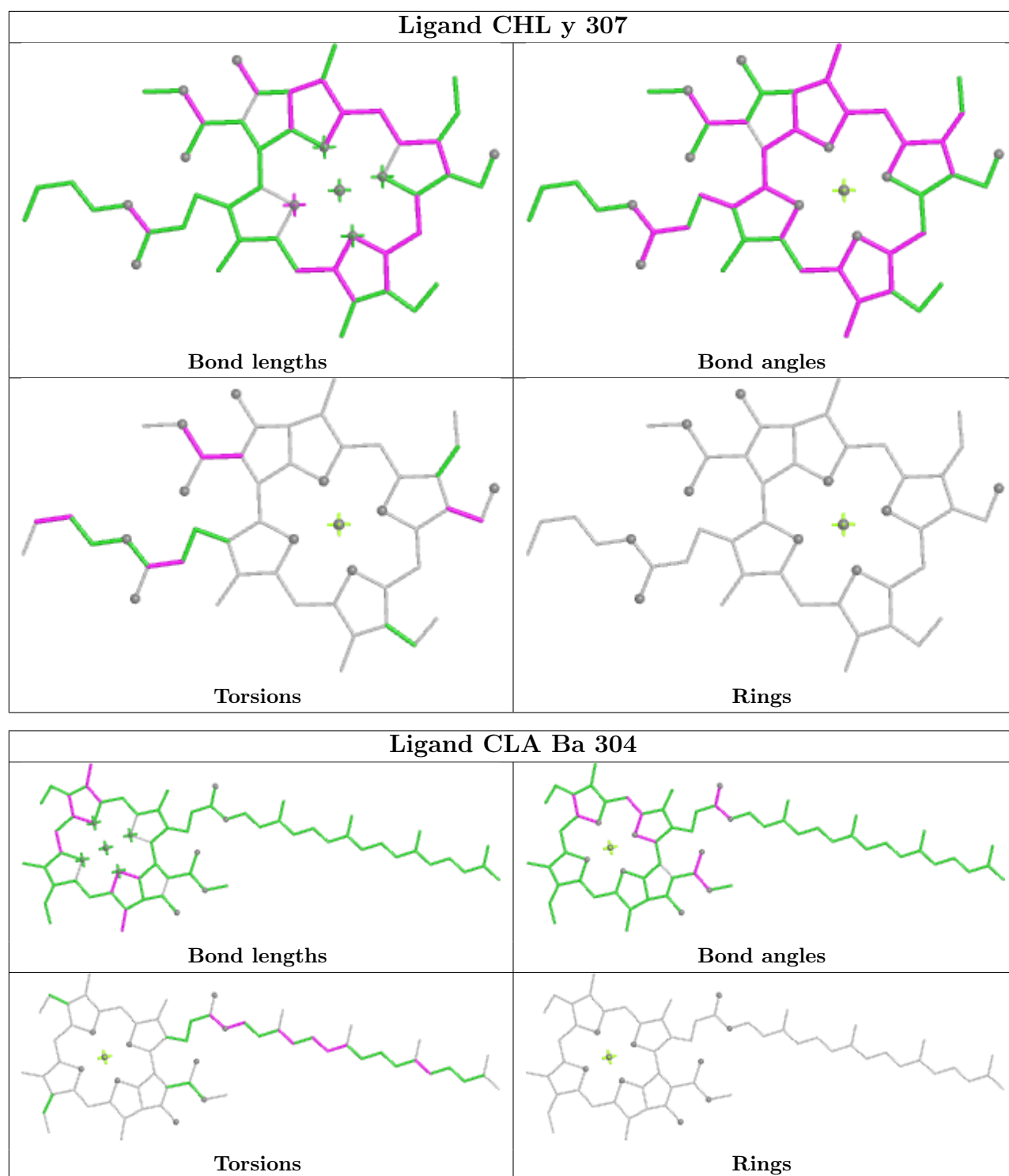


Torsions

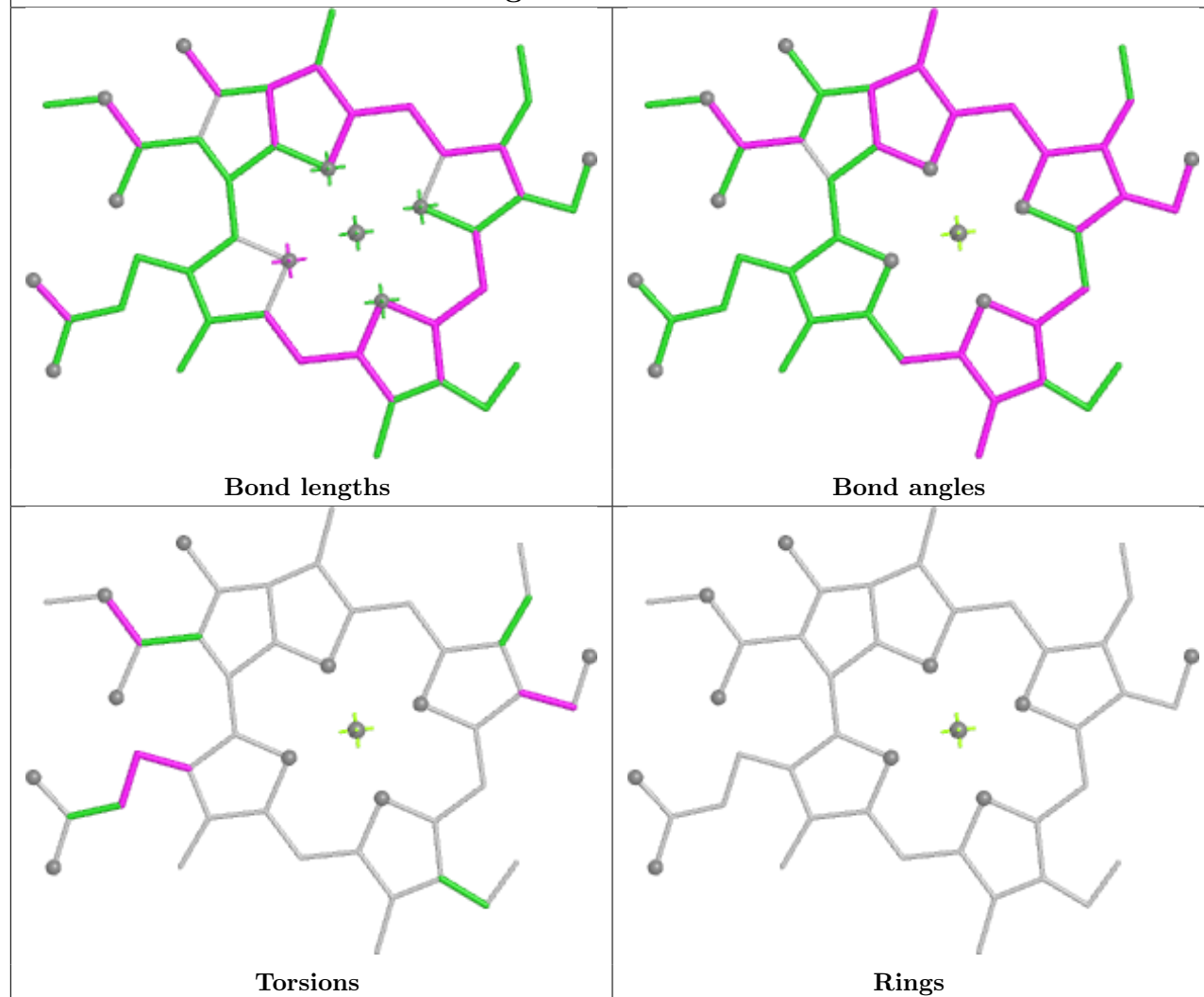


Rings

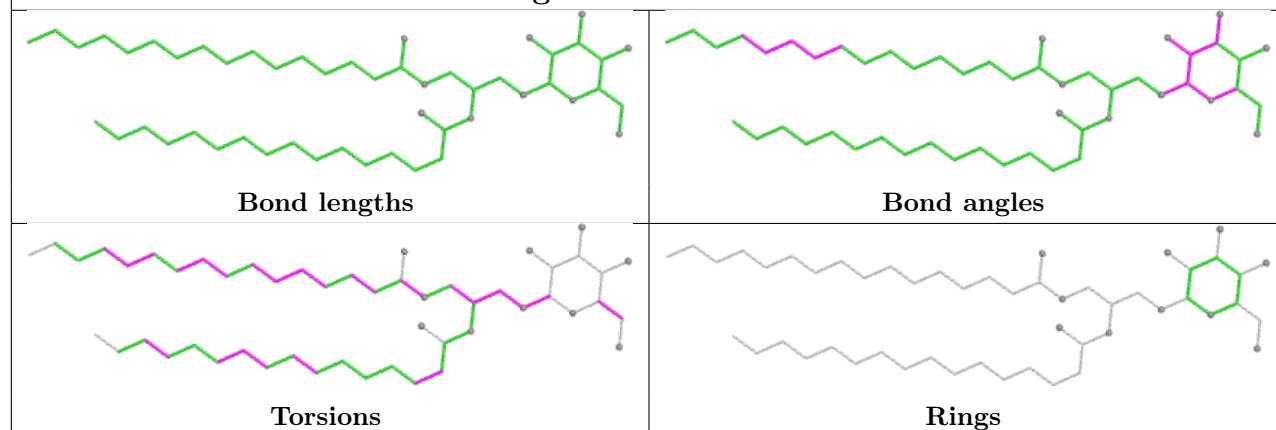


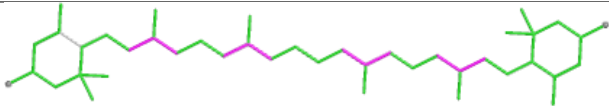
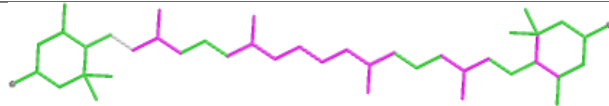
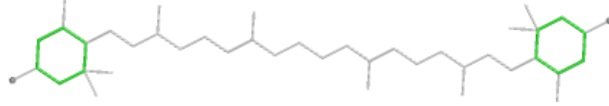


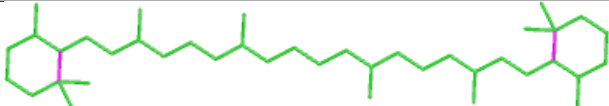
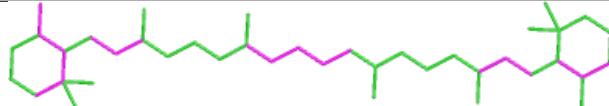
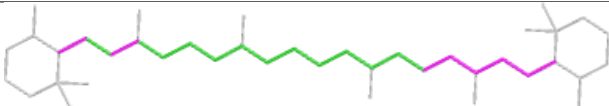
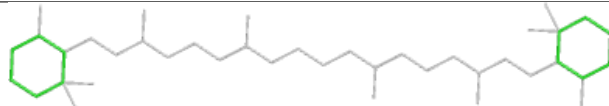
Ligand CHL 5 608

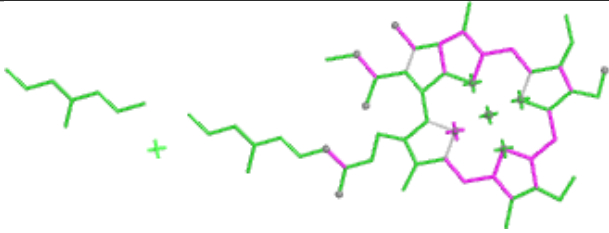
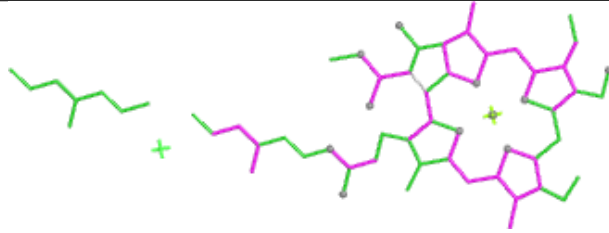
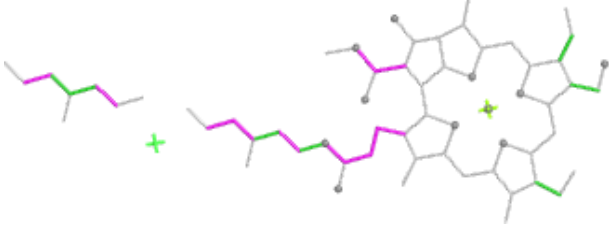
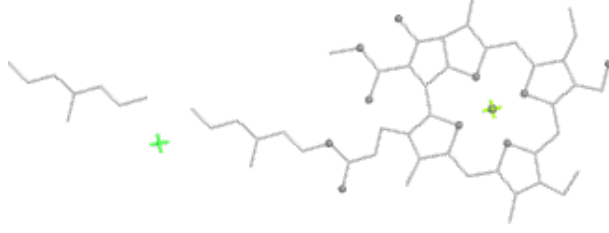


Ligand LMG c 501

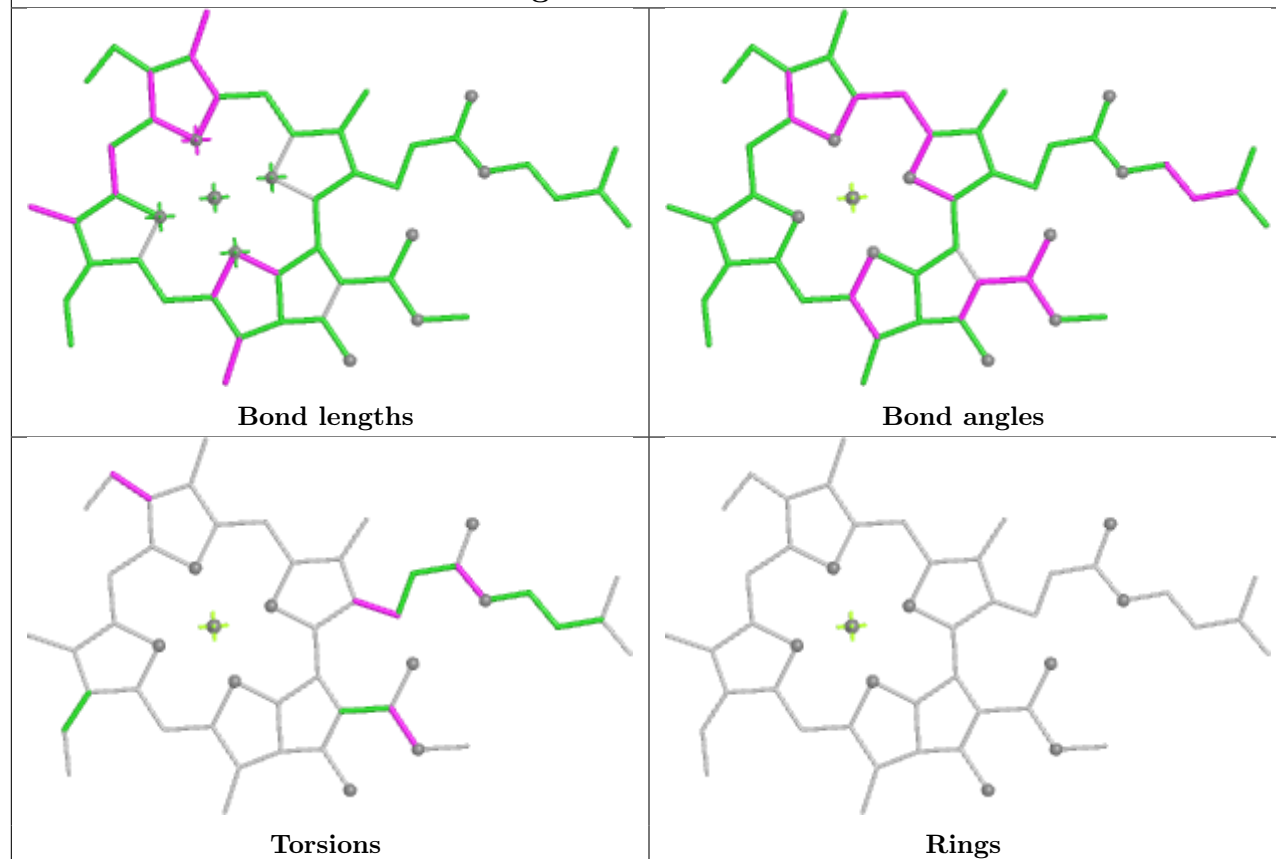


Ligand LUT s 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

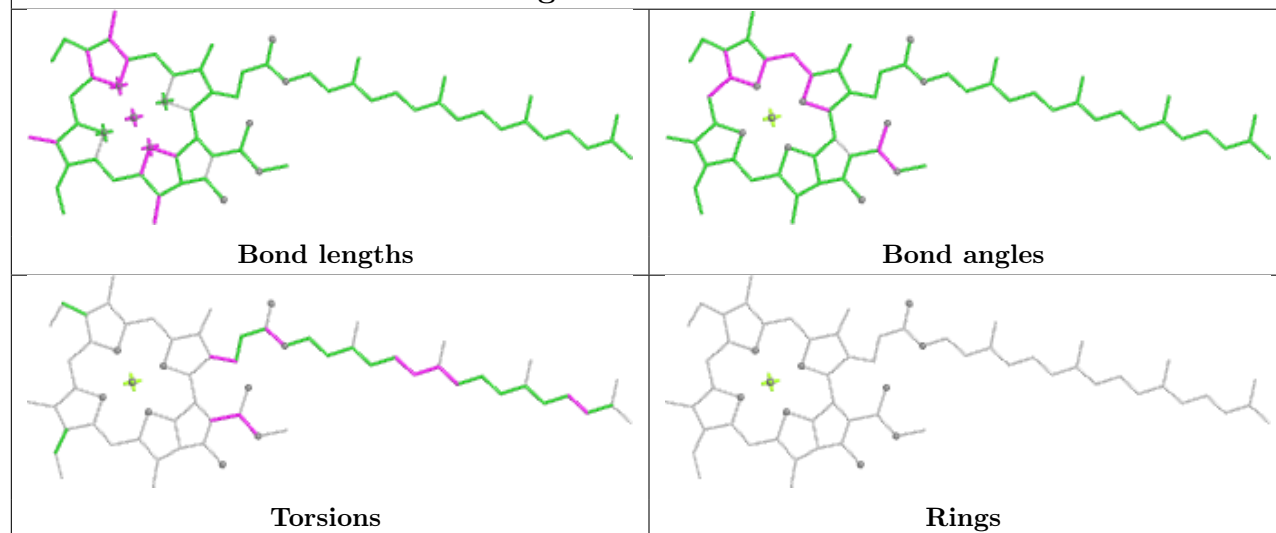
Ligand BCR Ay 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 9 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

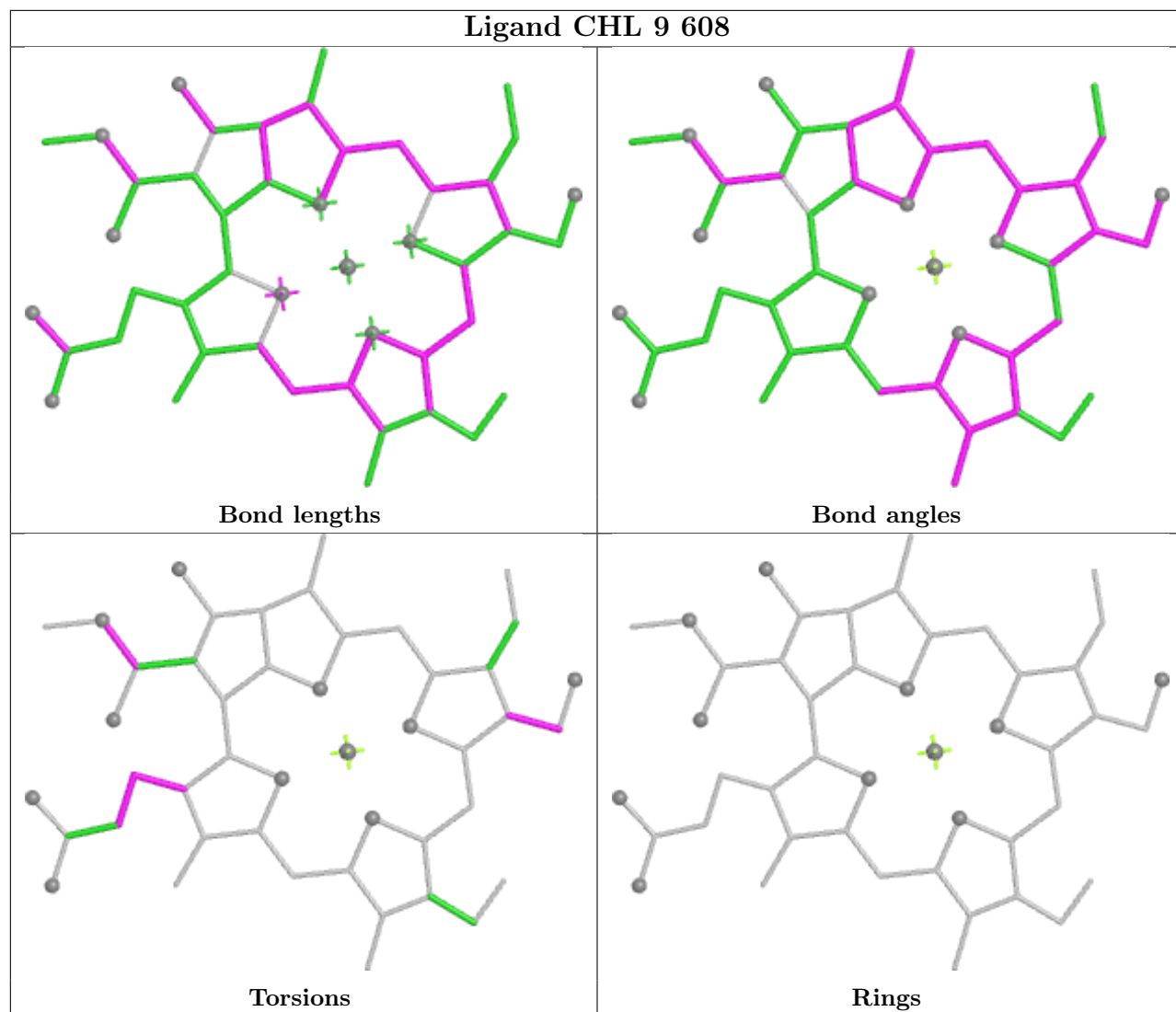
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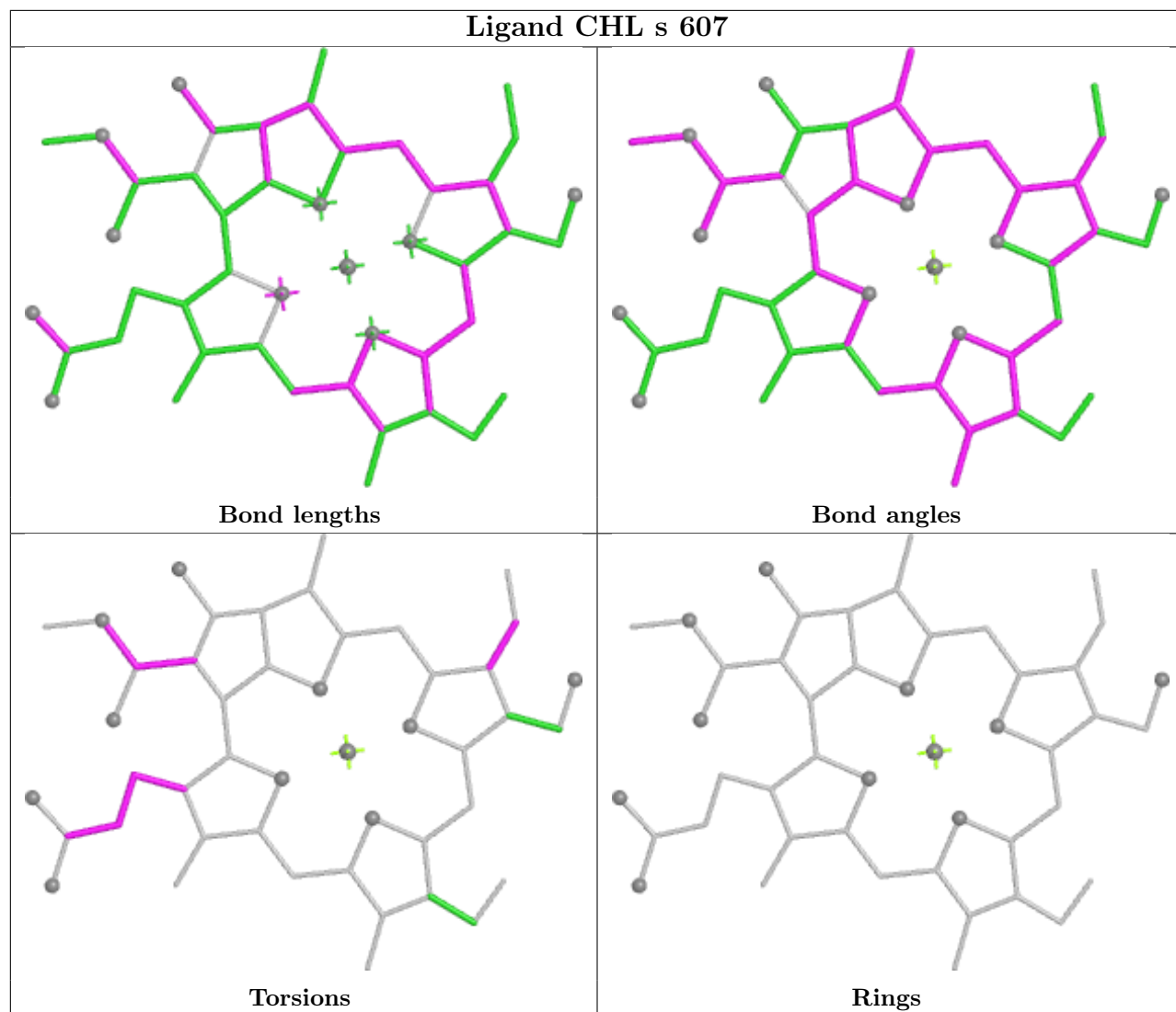
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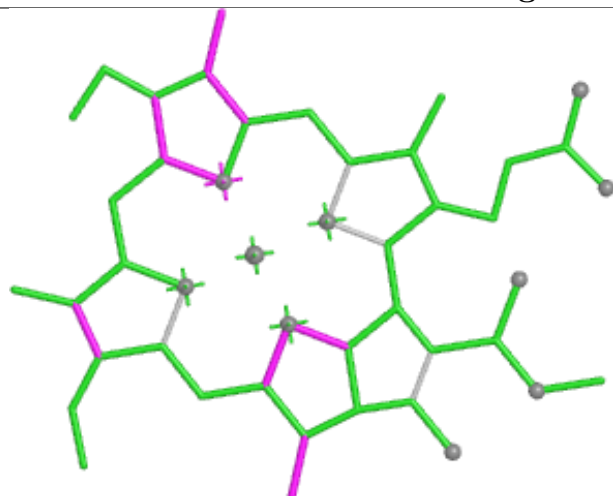
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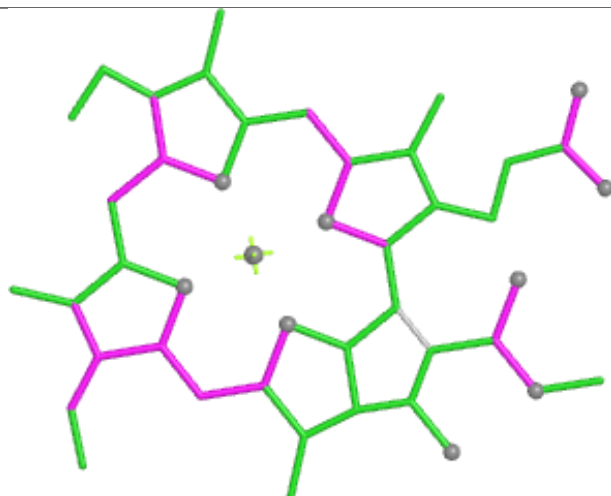
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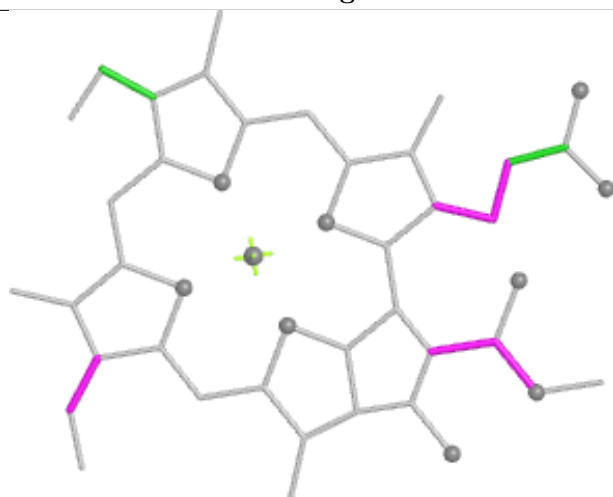
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Bond lengths



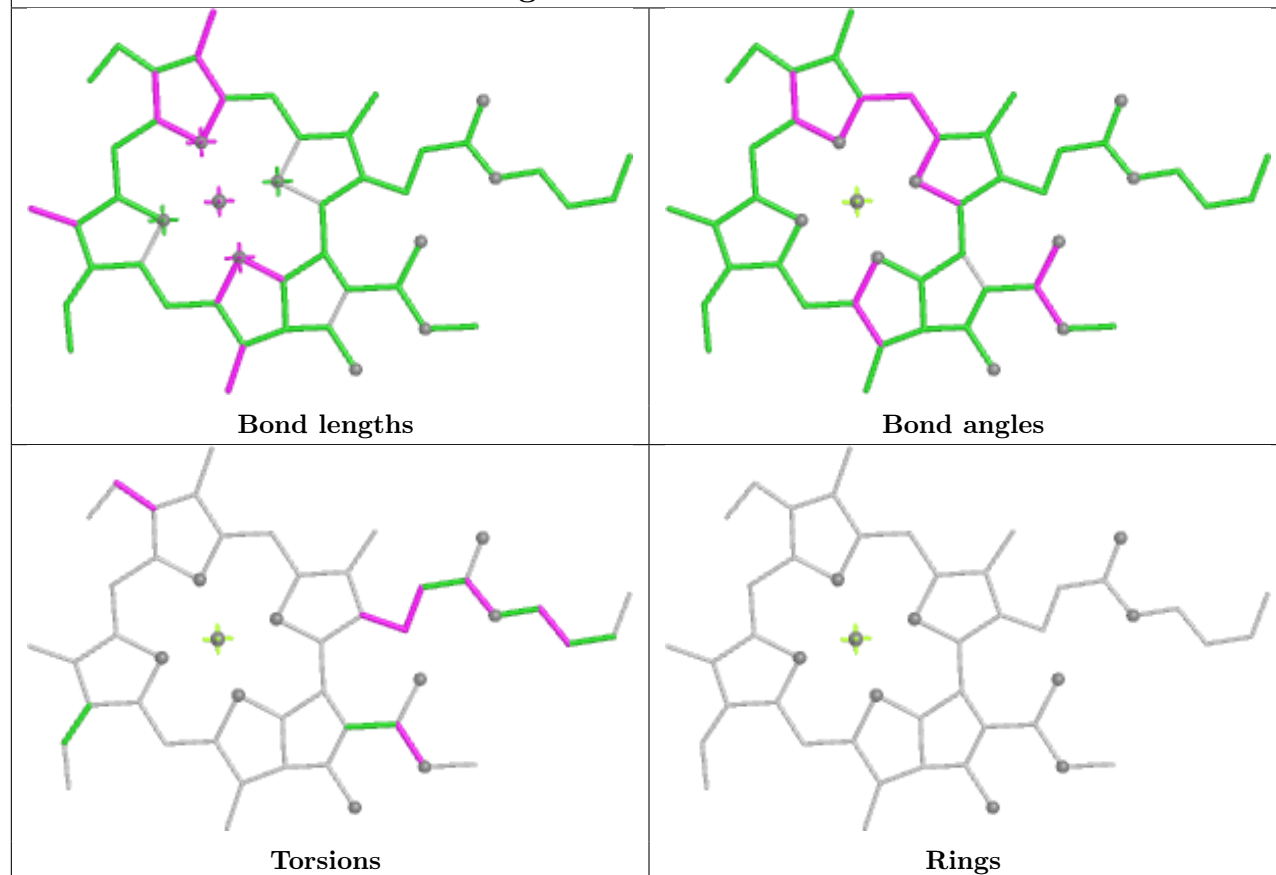
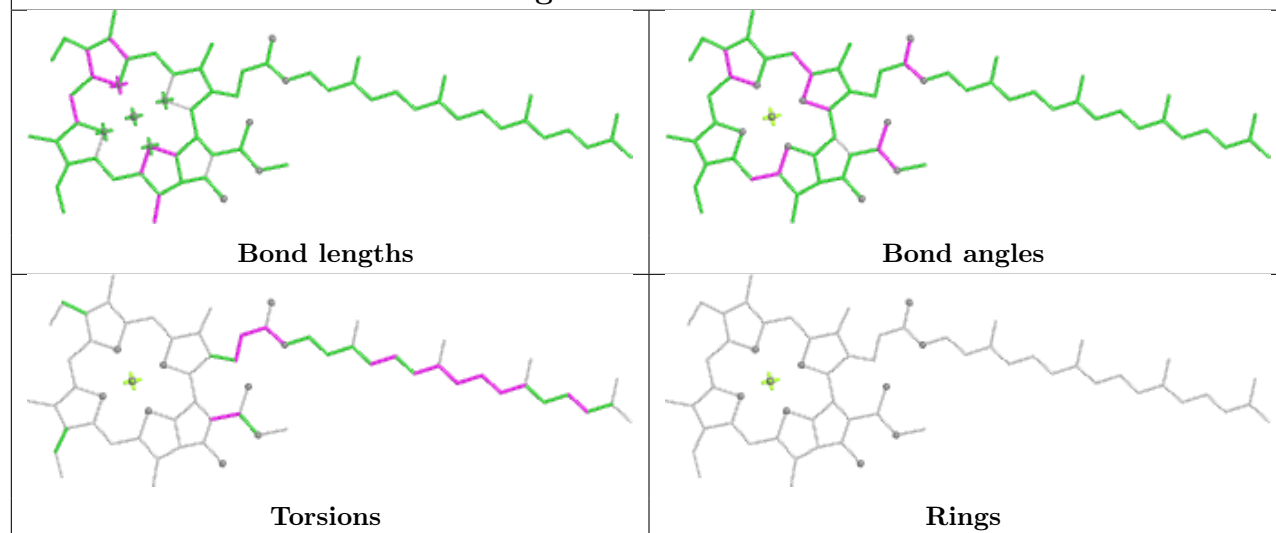
Bond angles

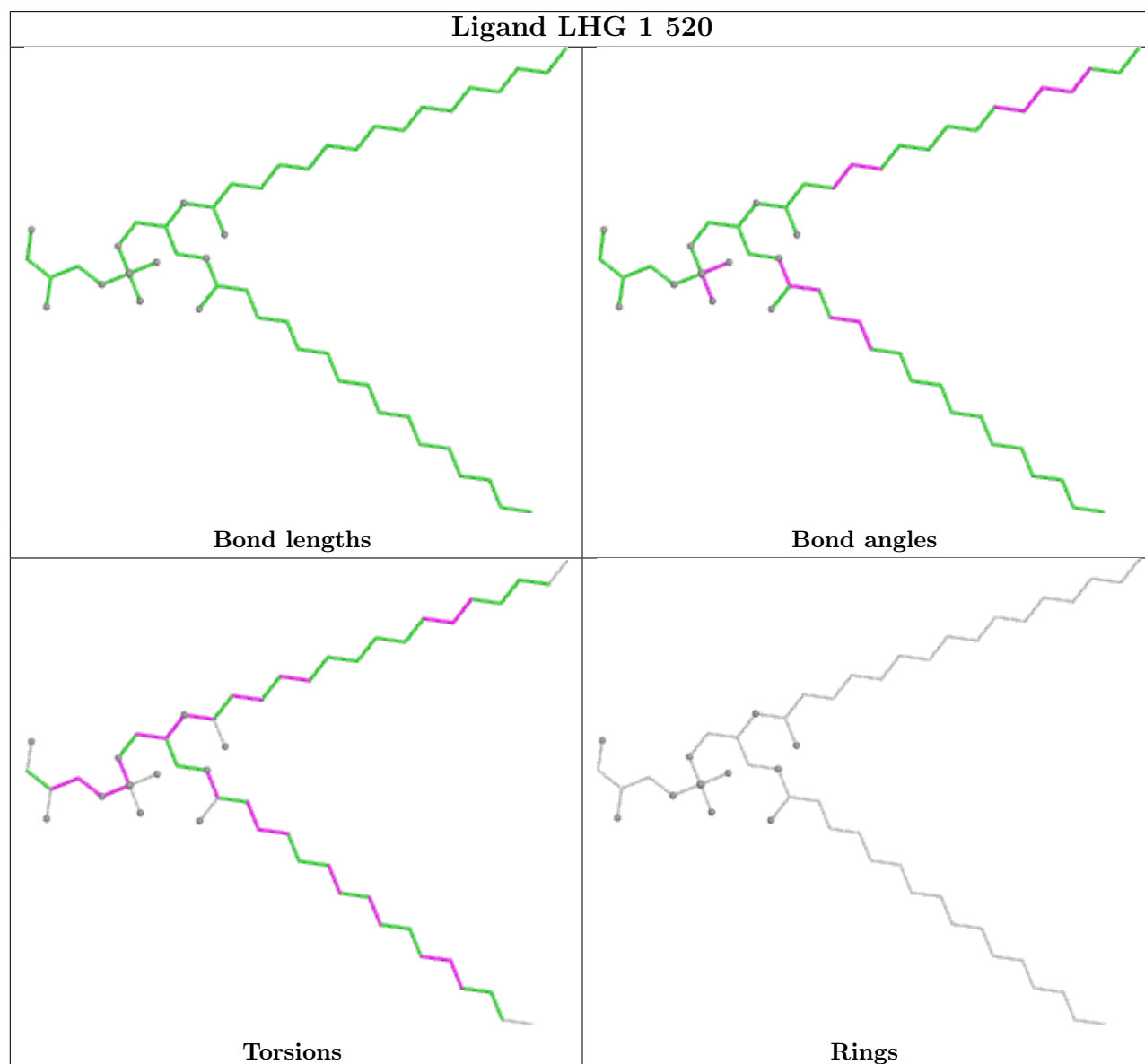
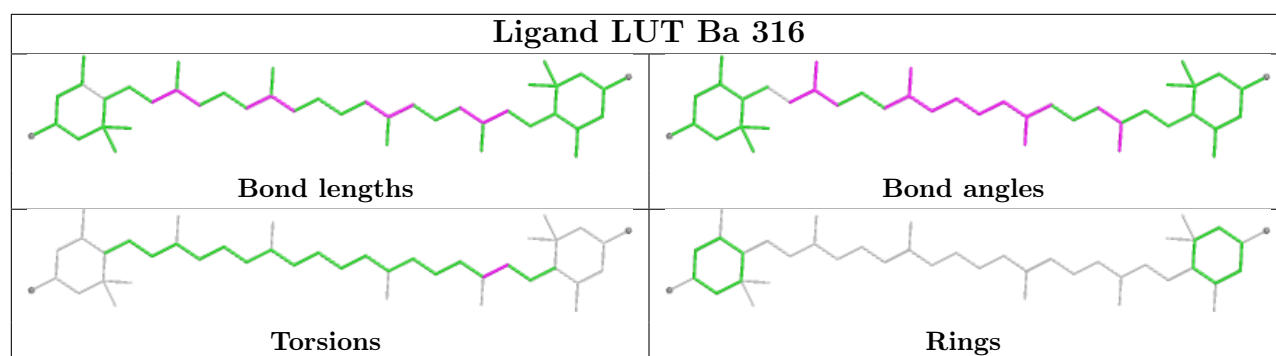


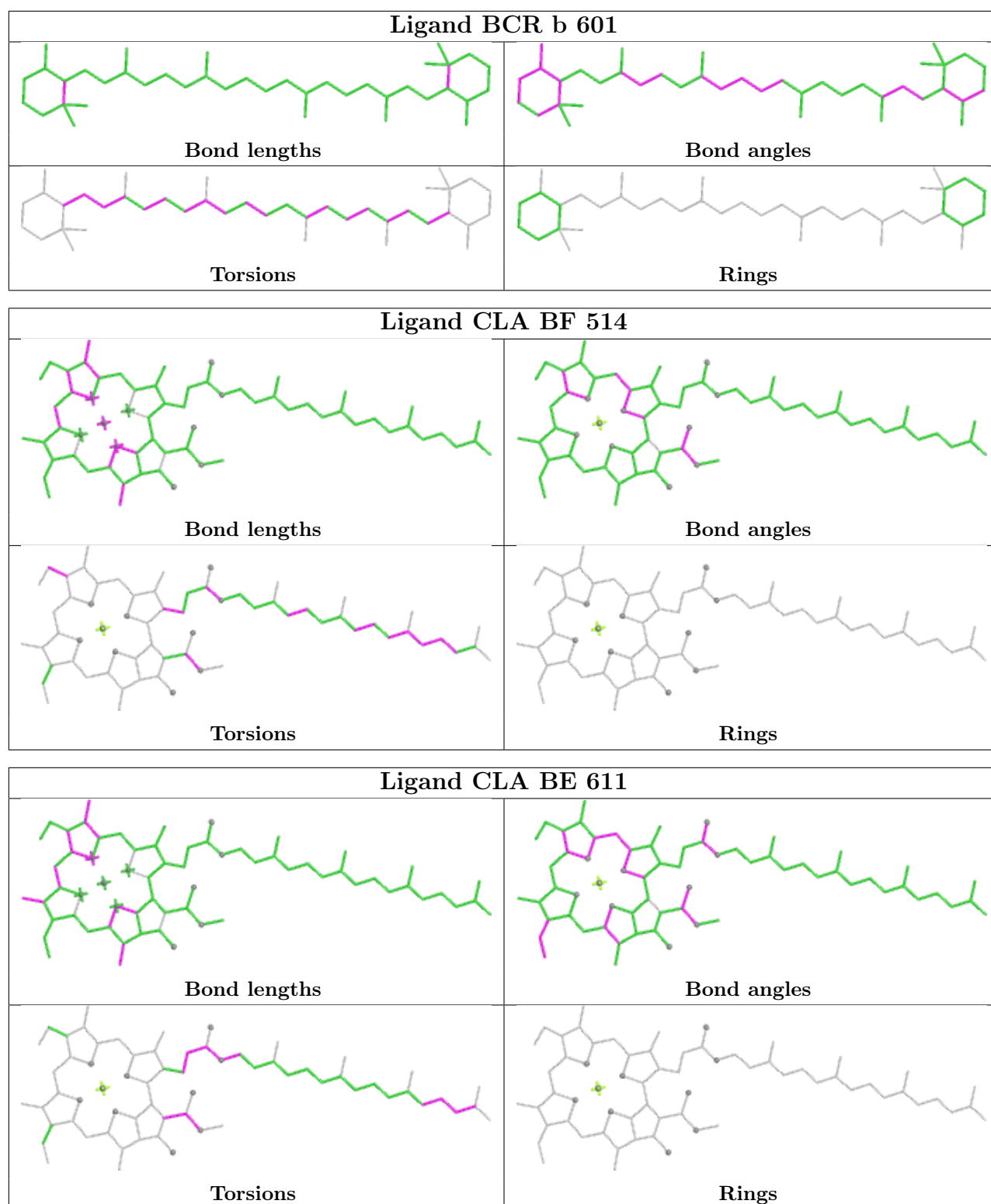
Torsions

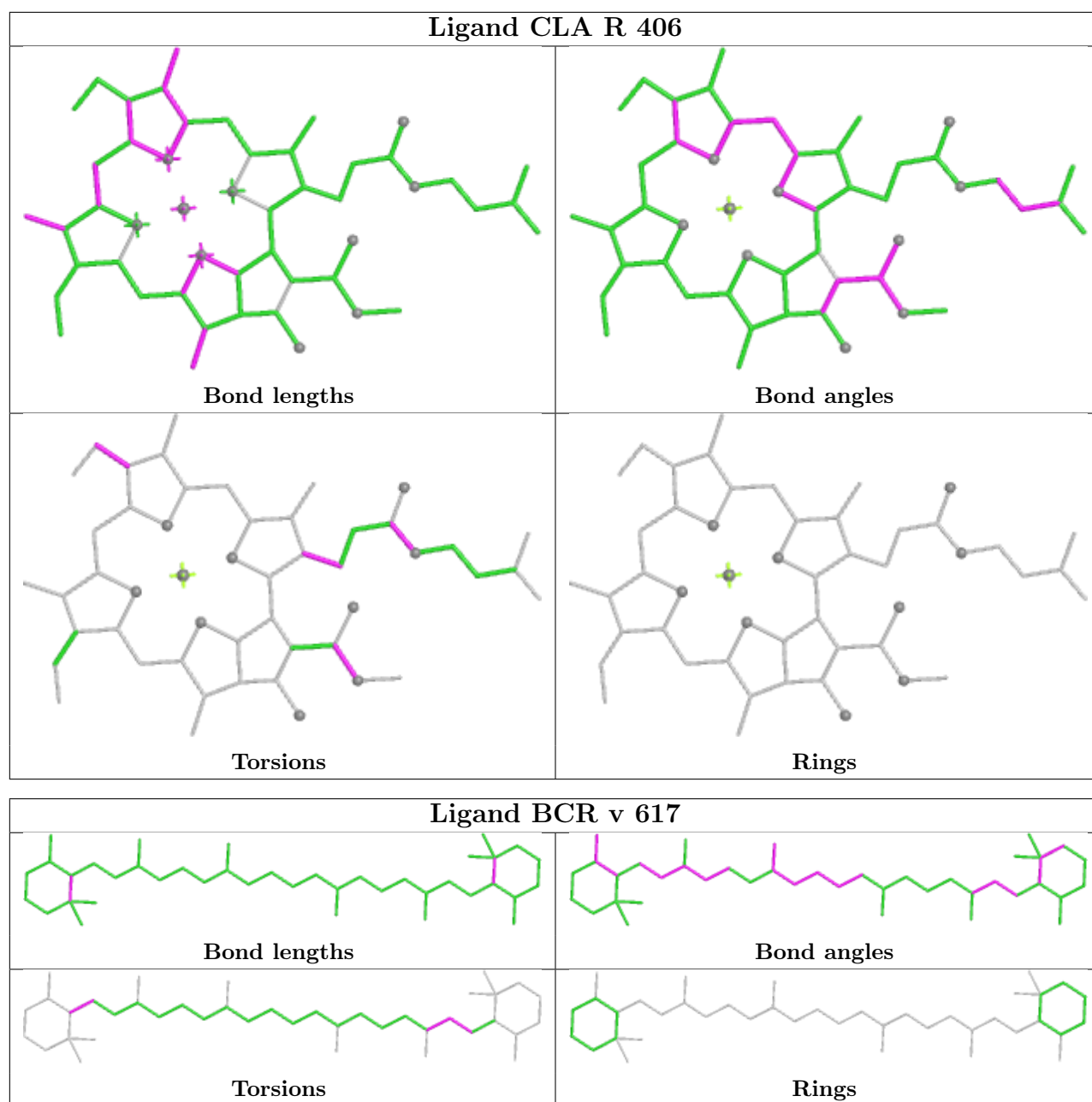


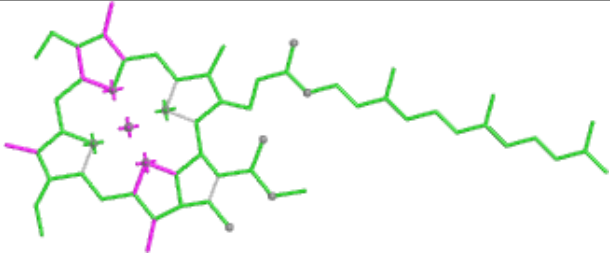
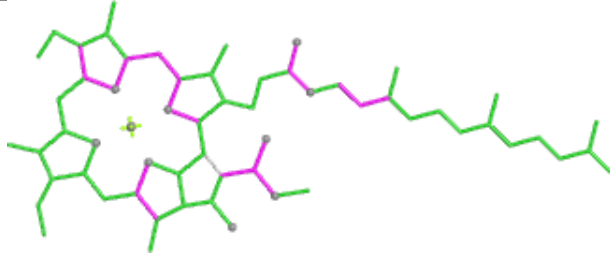
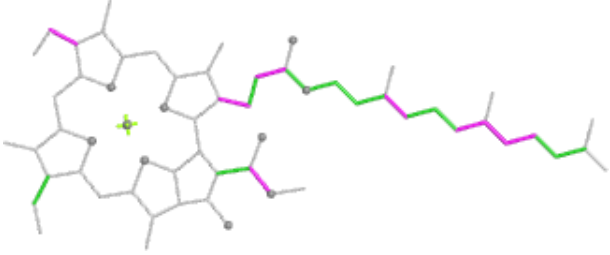
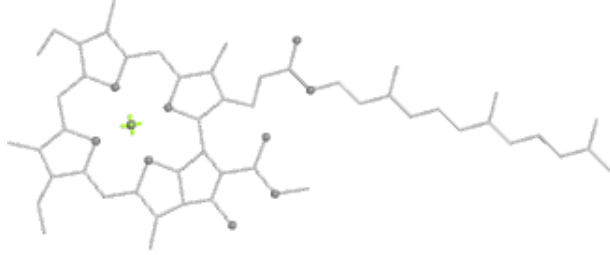
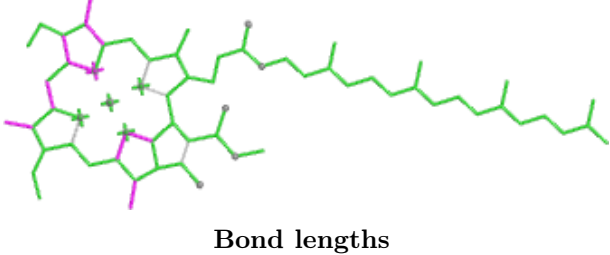
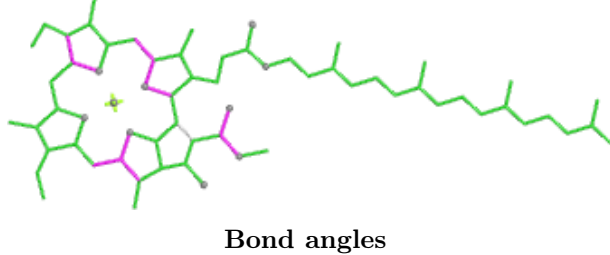
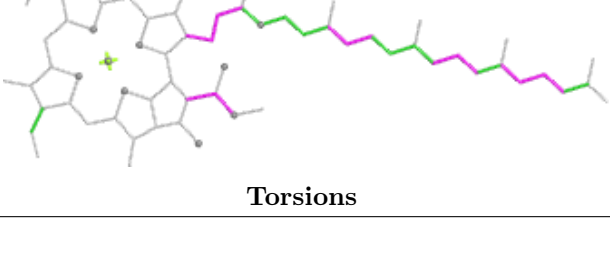
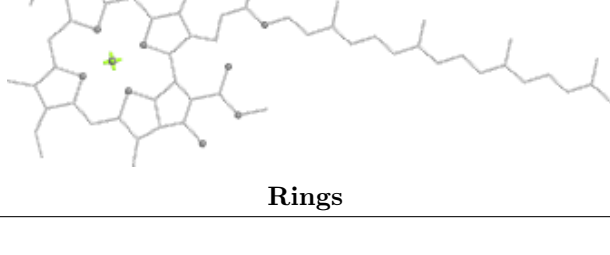
Rings

Ligand CLA BU 610**Ligand CLA n 602**

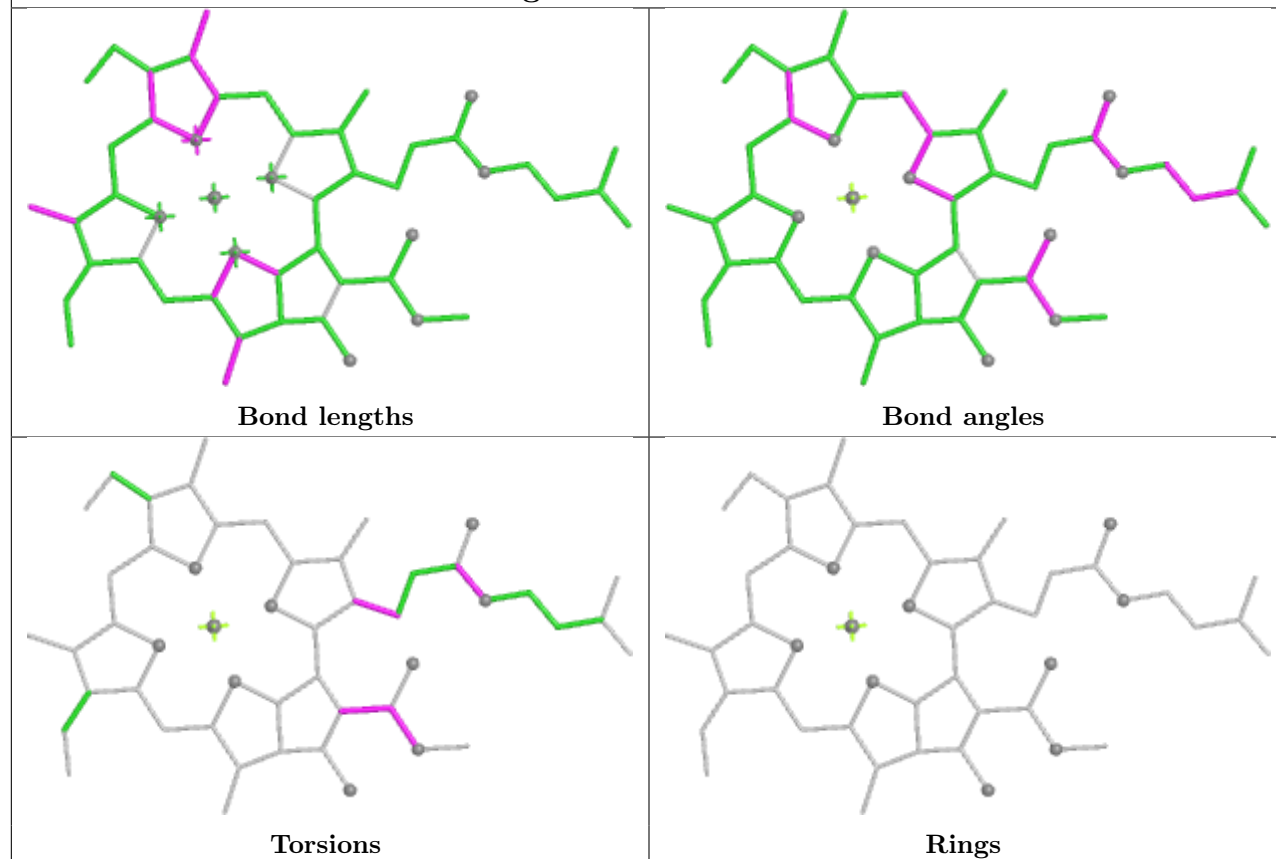




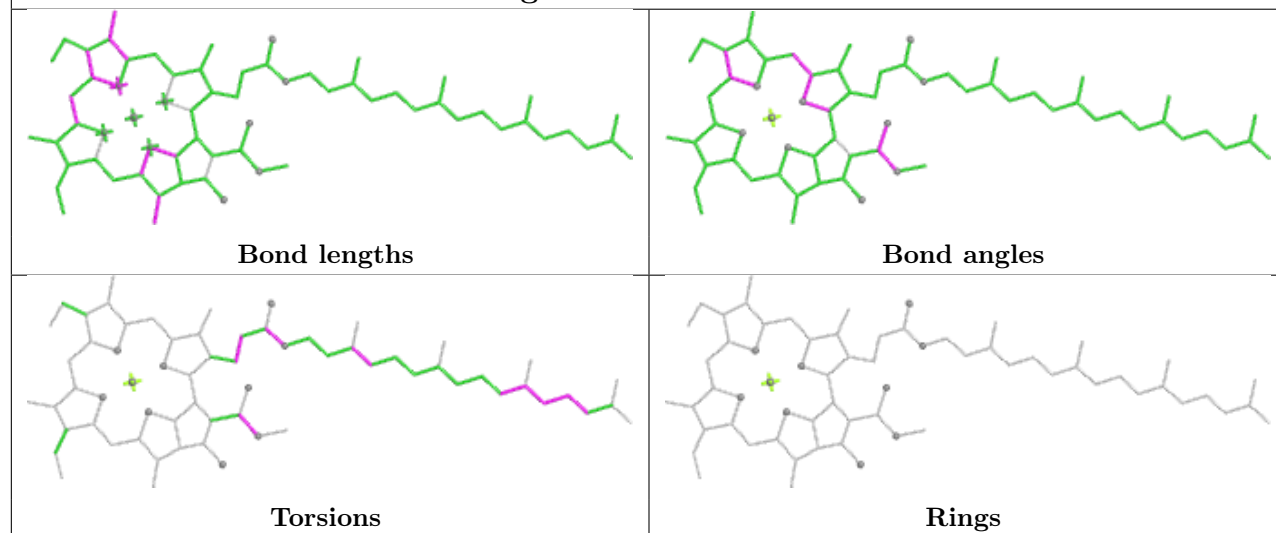


Ligand CLA Y 312	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

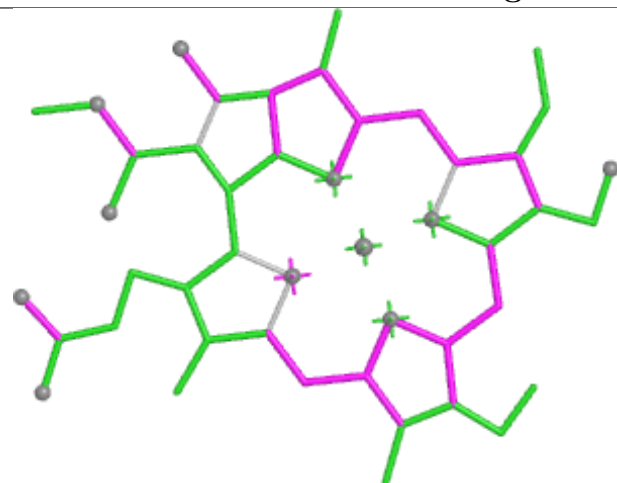
Ligand CLA A2 604



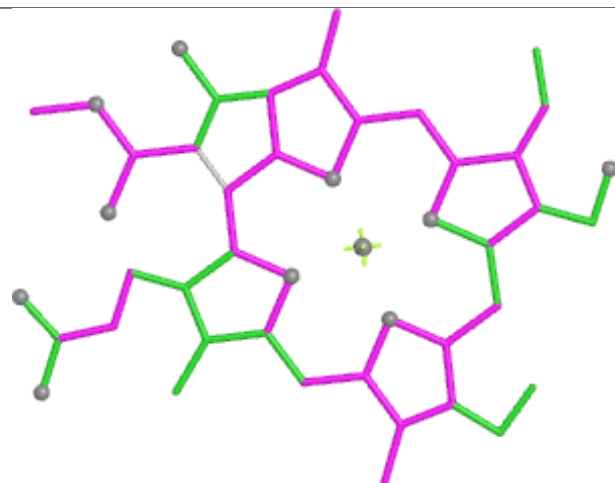
Ligand CLA BE 604



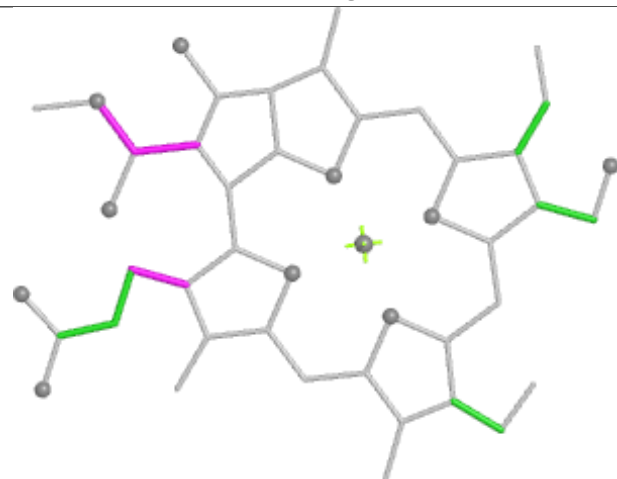
Ligand CHL AB 306



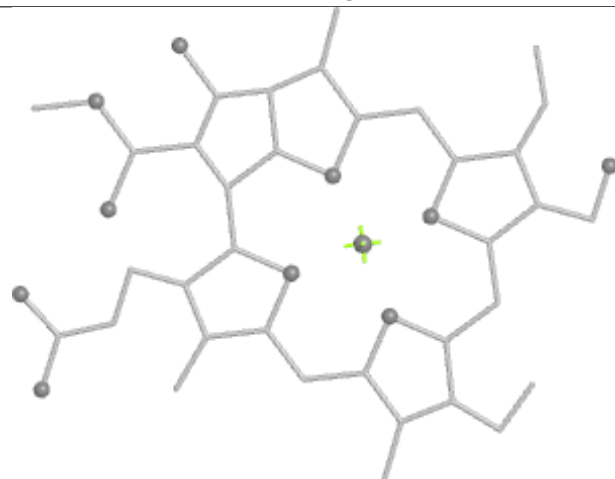
Bond lengths



Bond angles

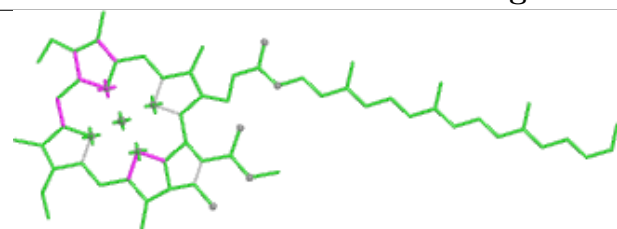


Torsions

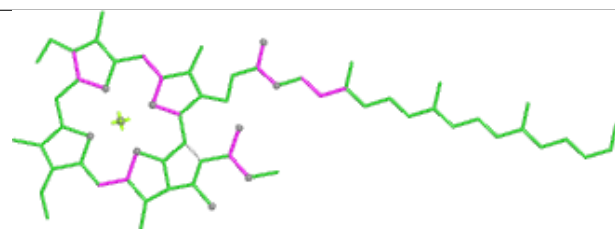


Rings

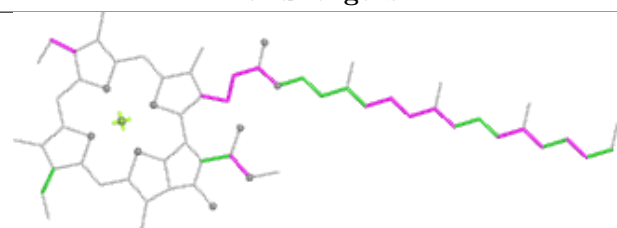
Ligand CLA BJ 610



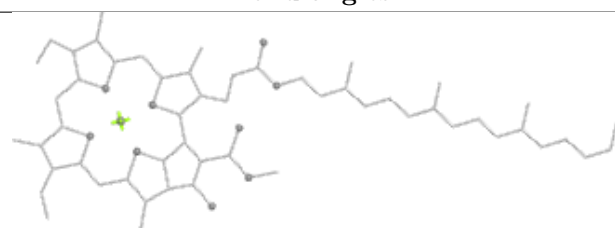
Bond lengths



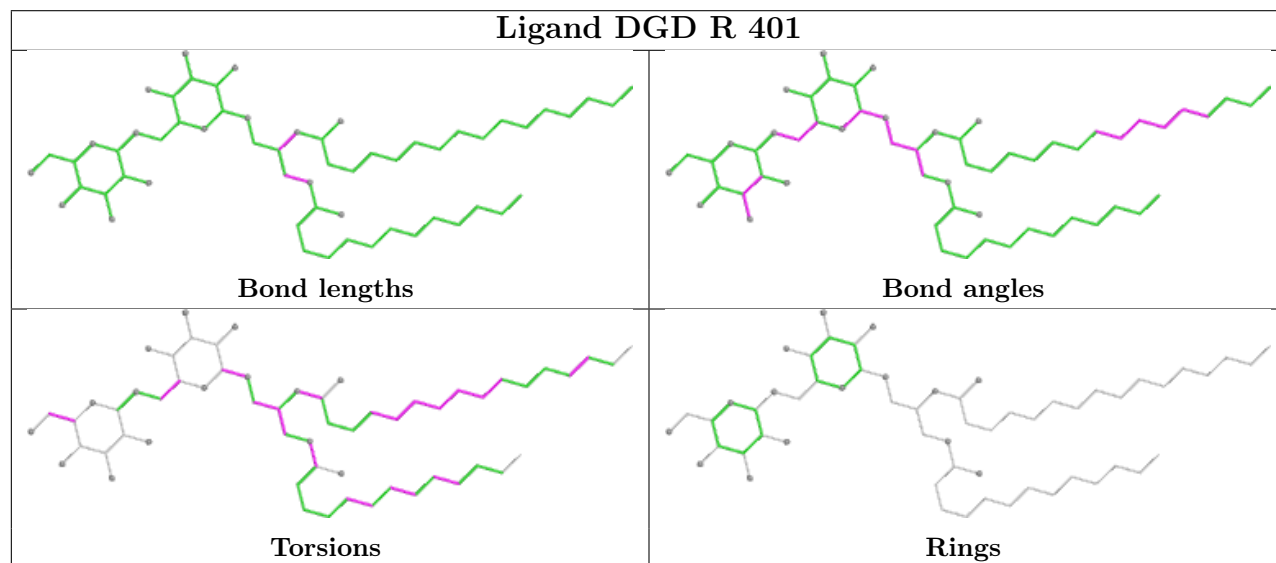
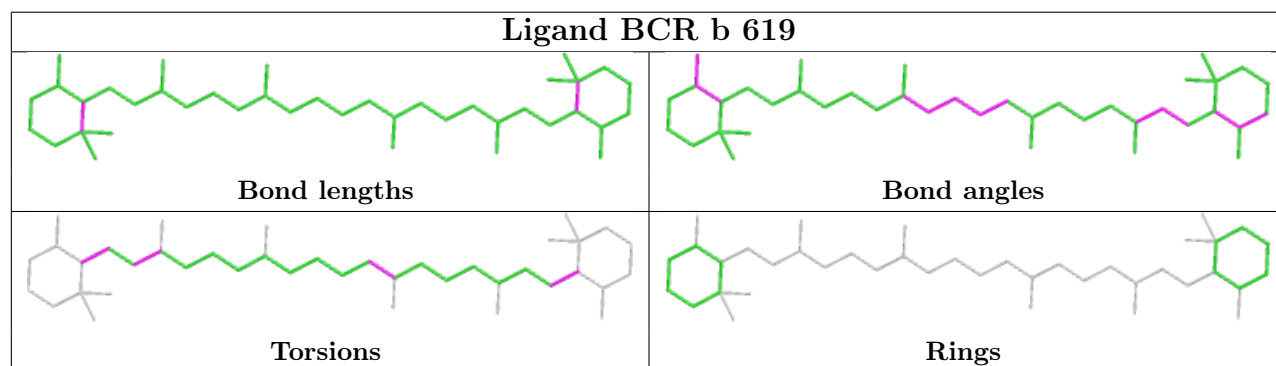
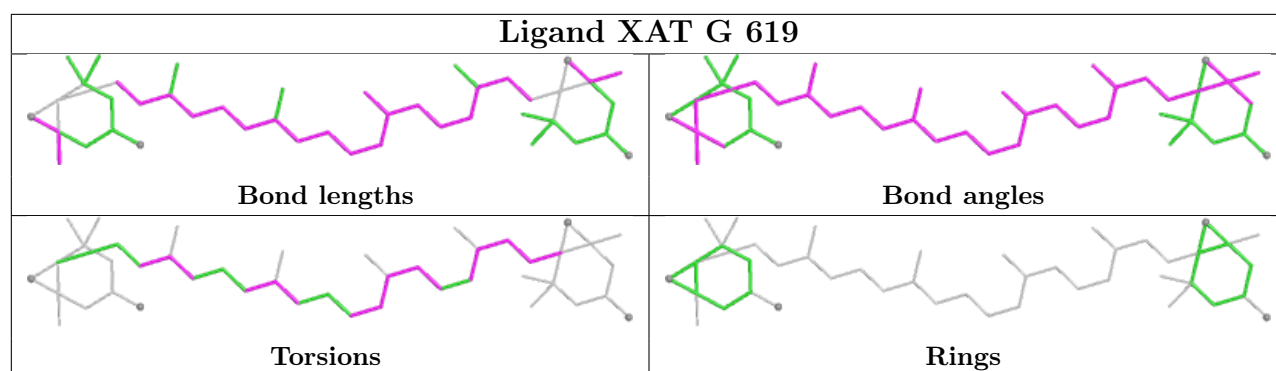
Bond angles

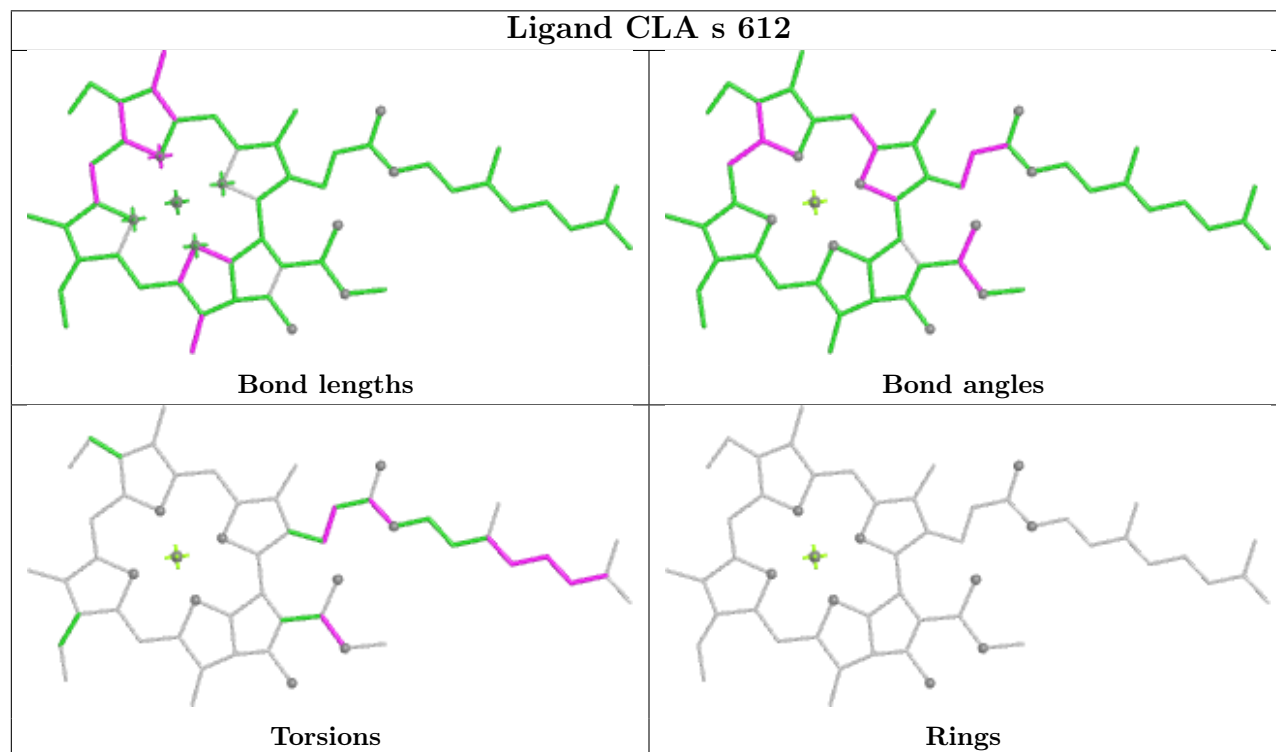
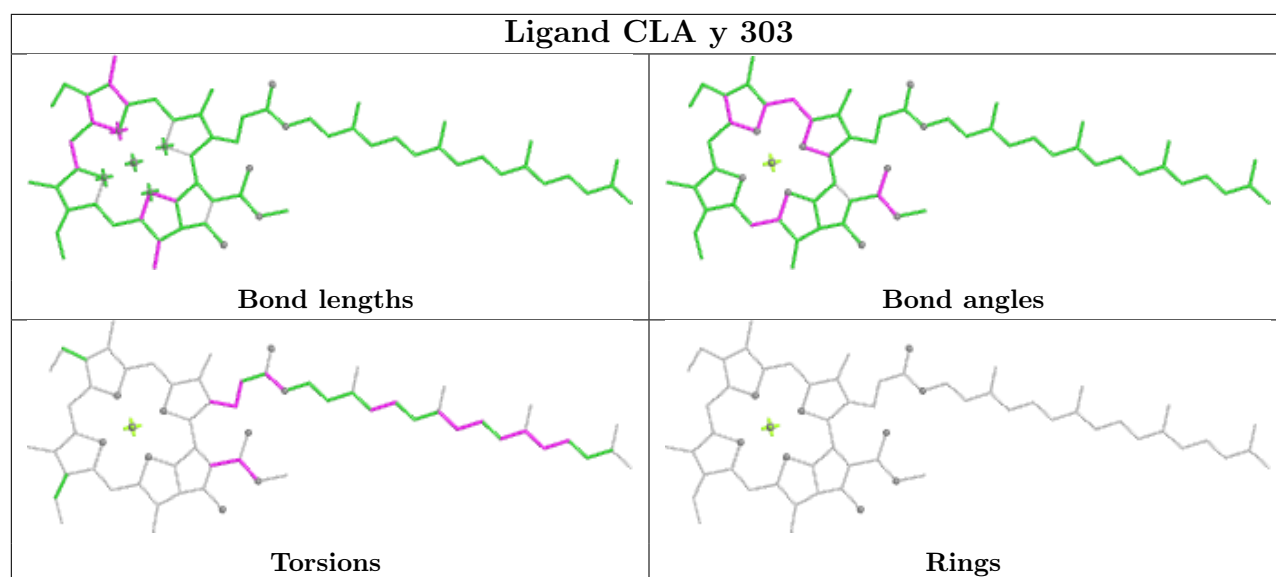


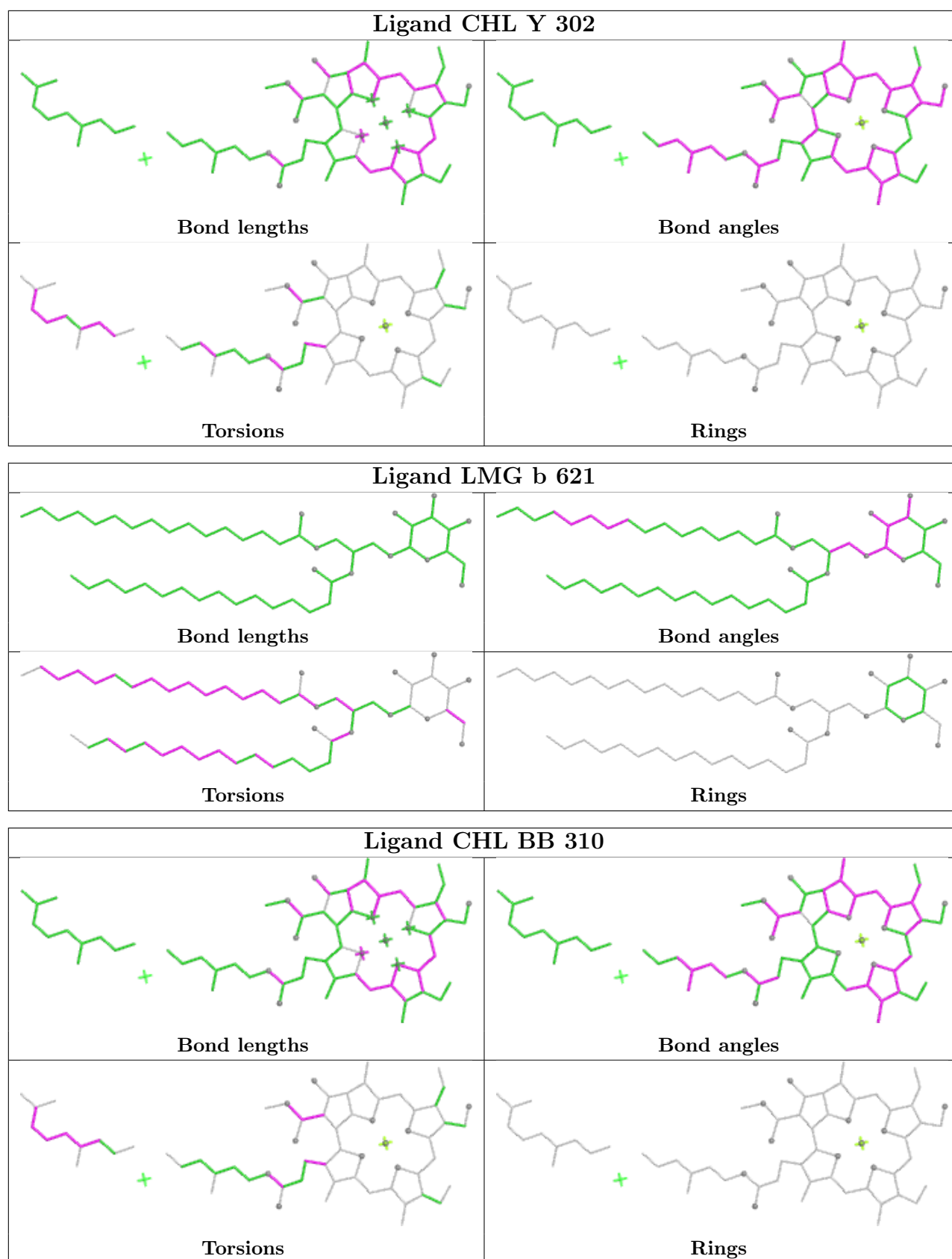
Torsions

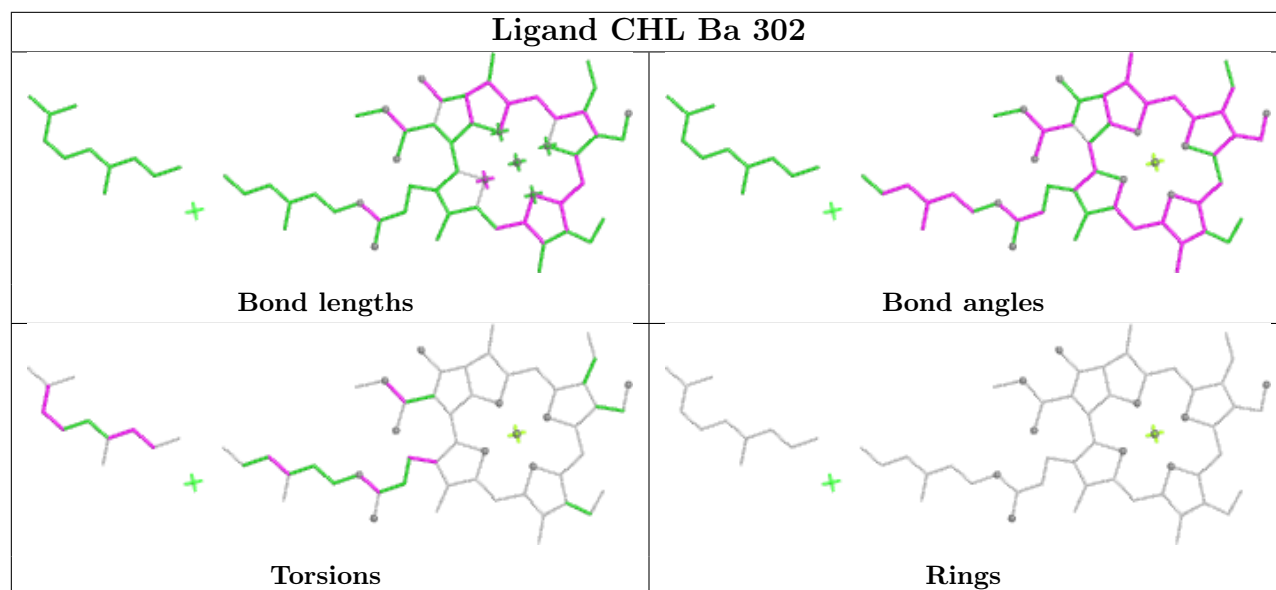
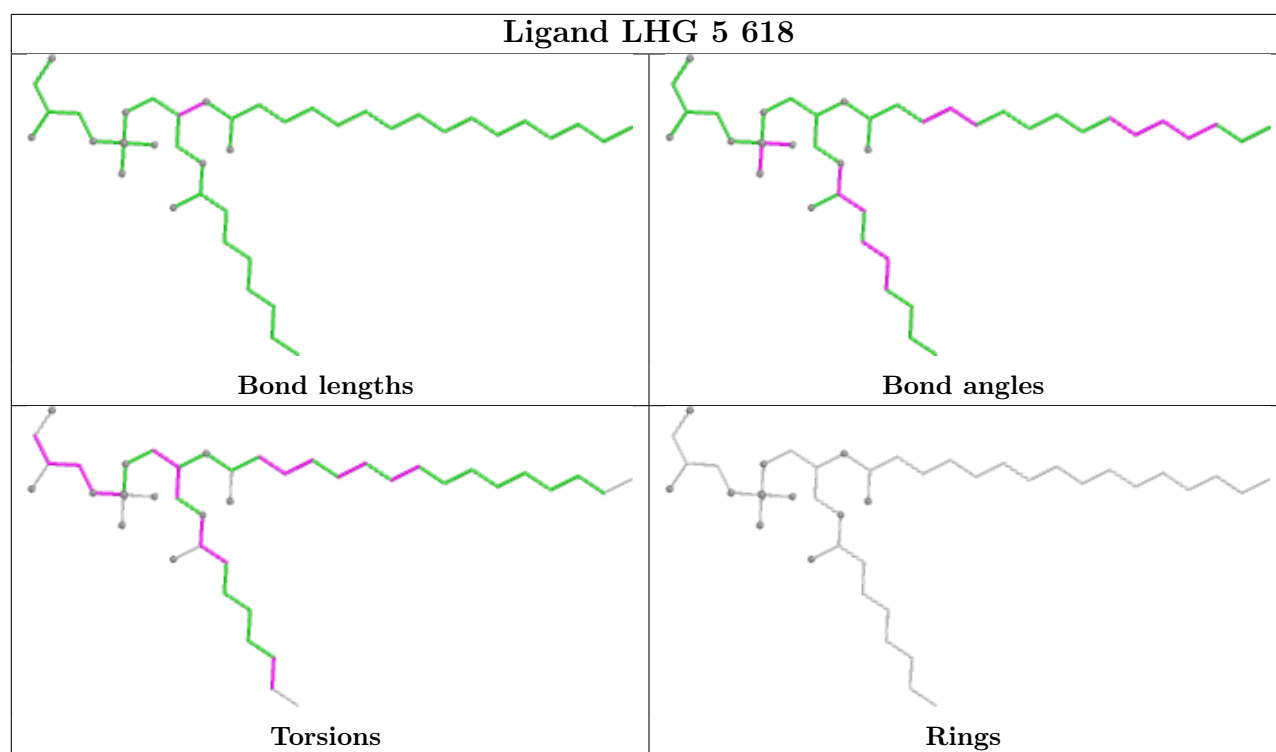


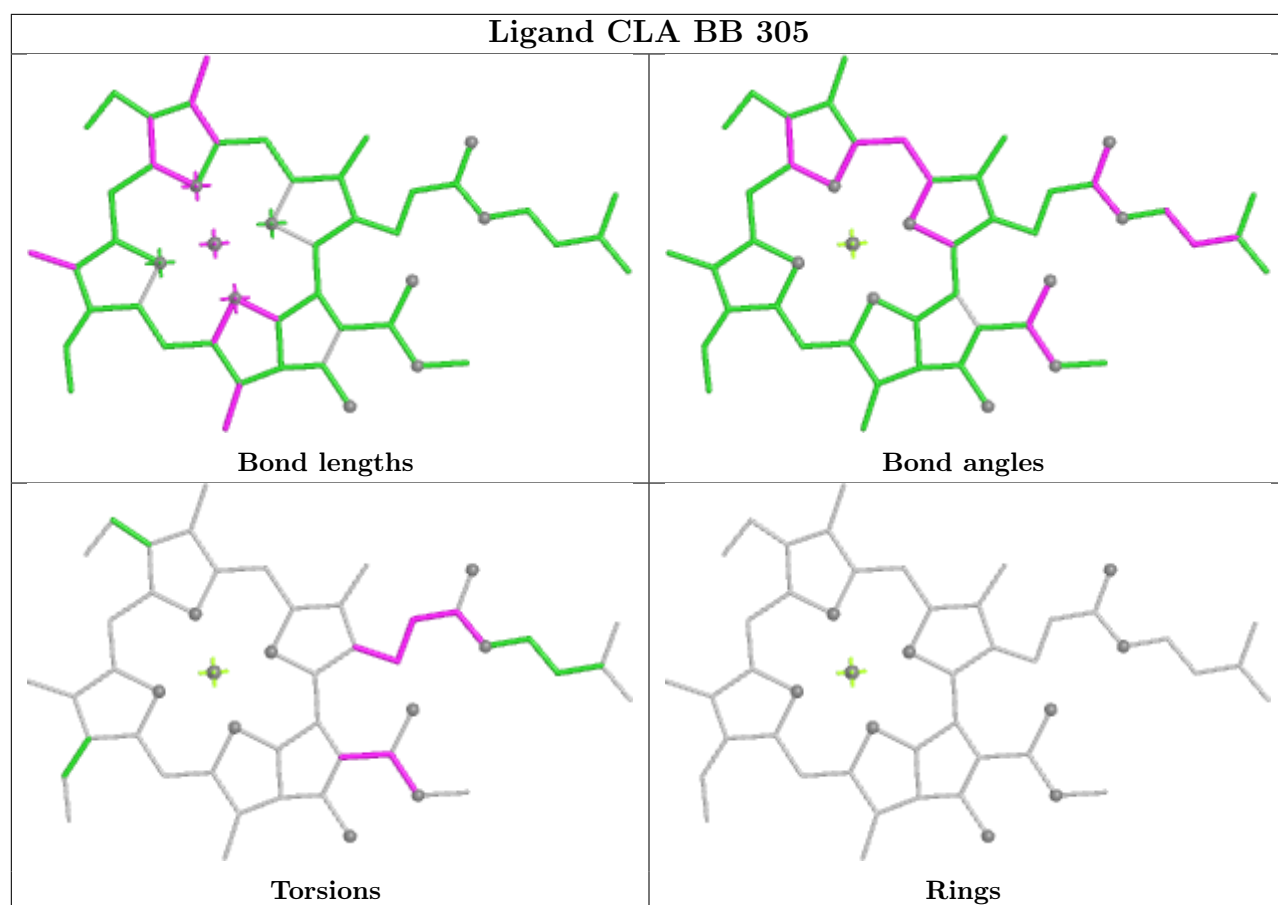
Rings

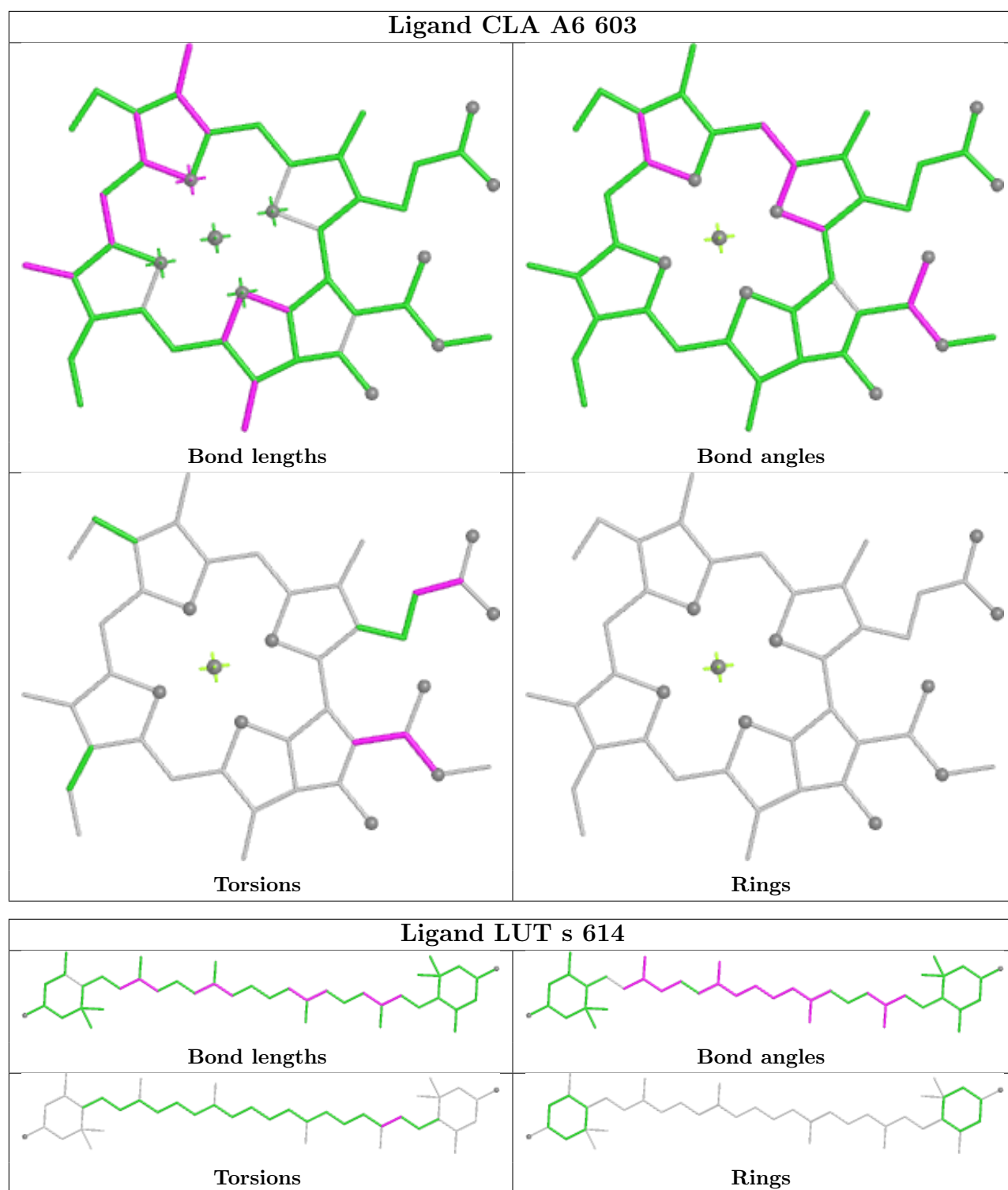


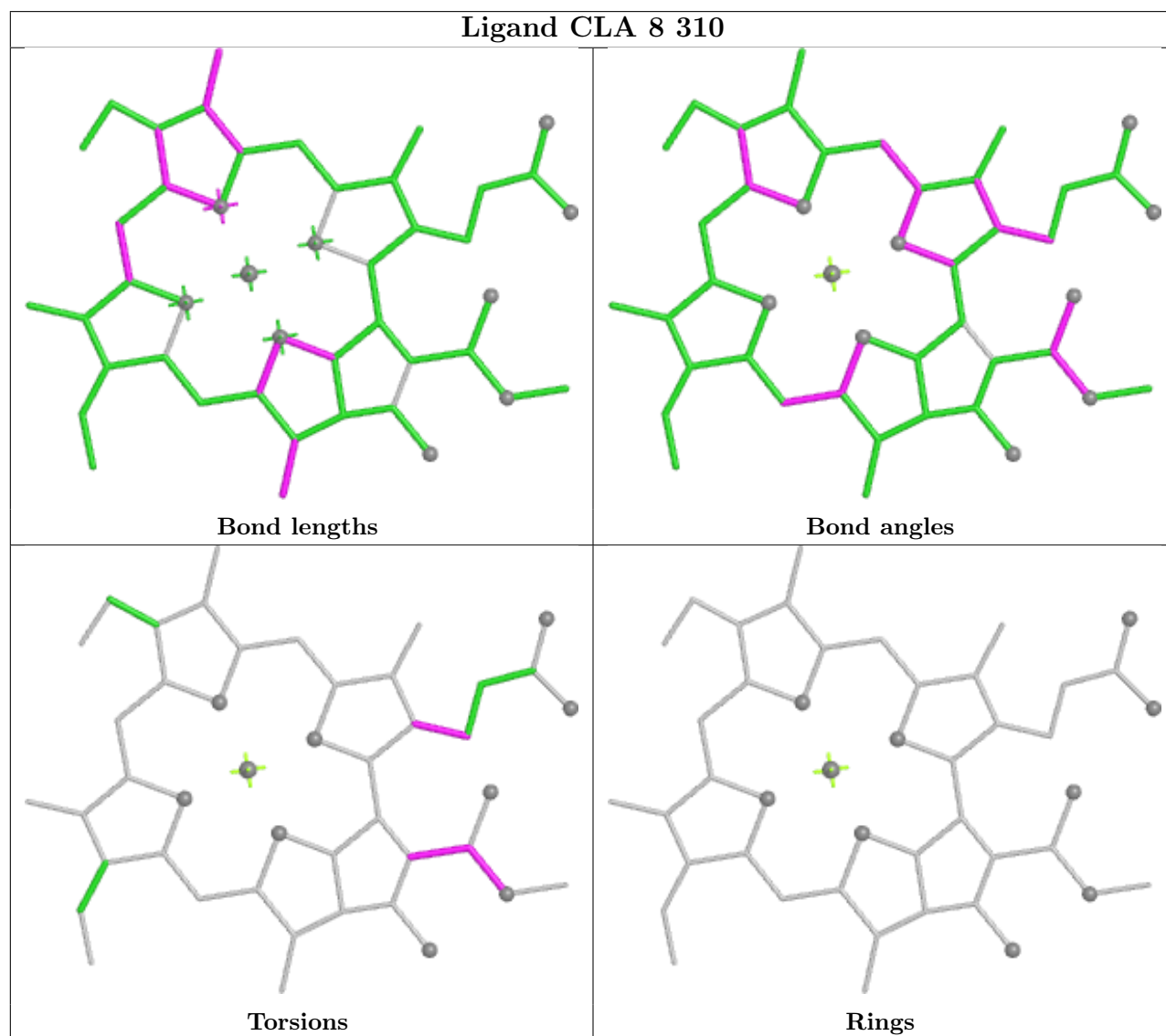
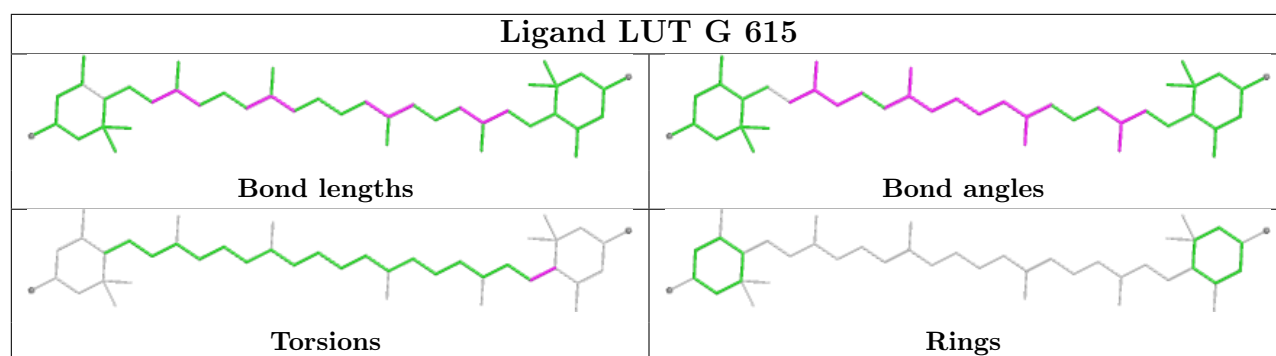


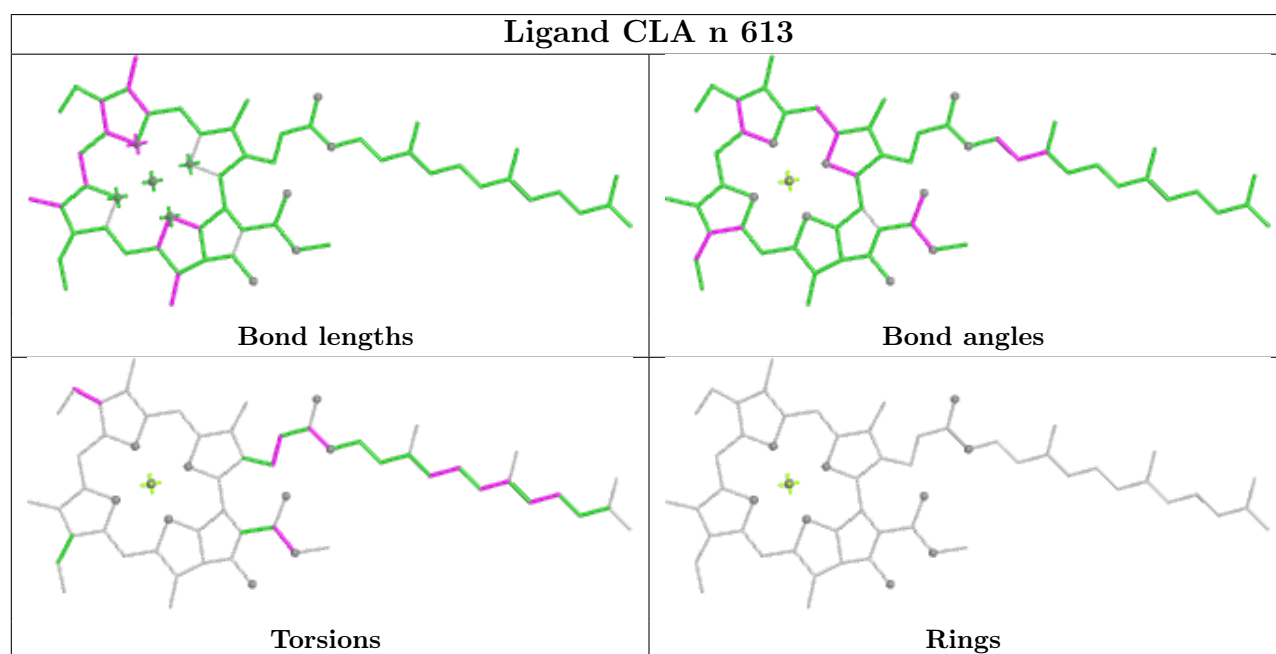
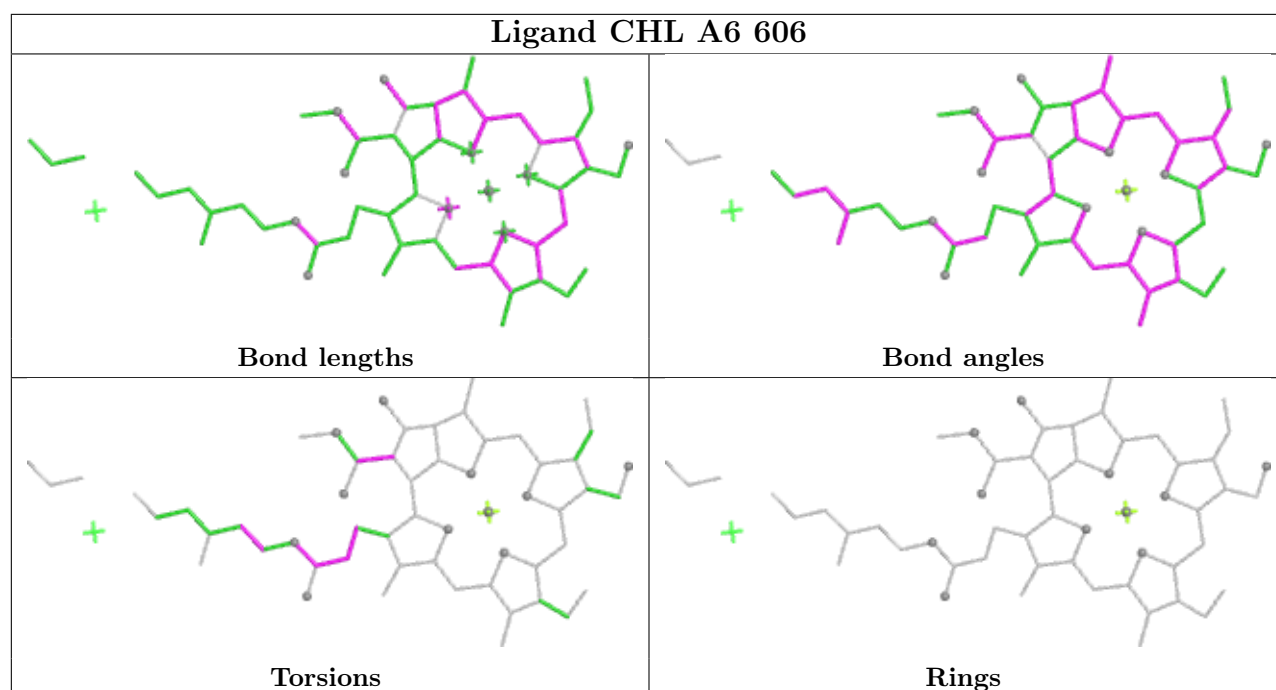


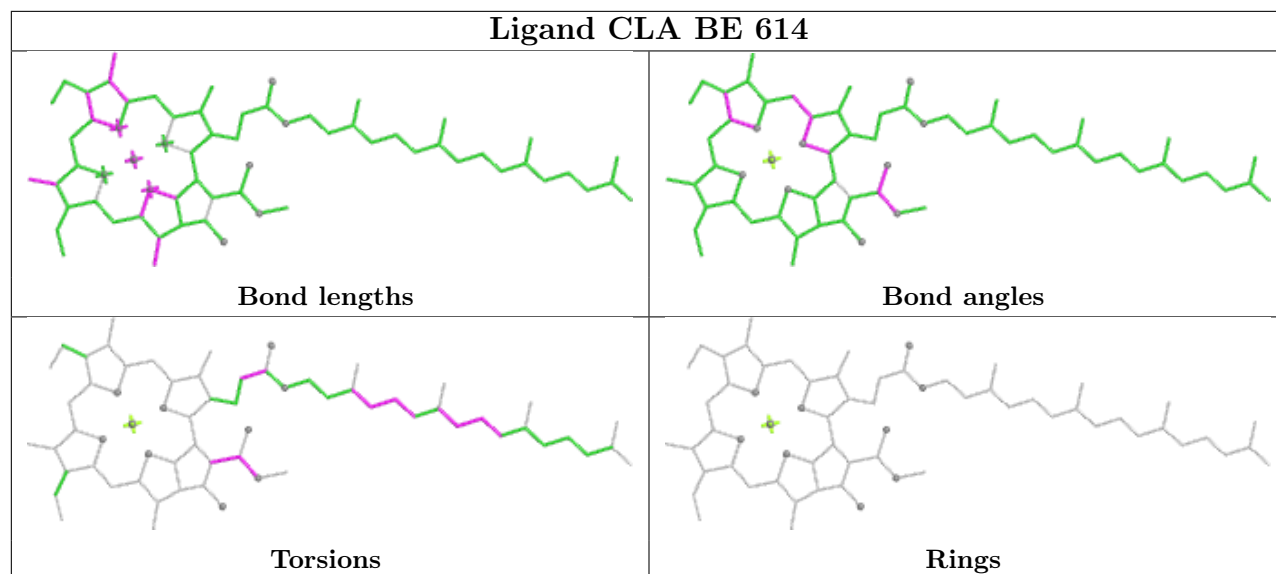
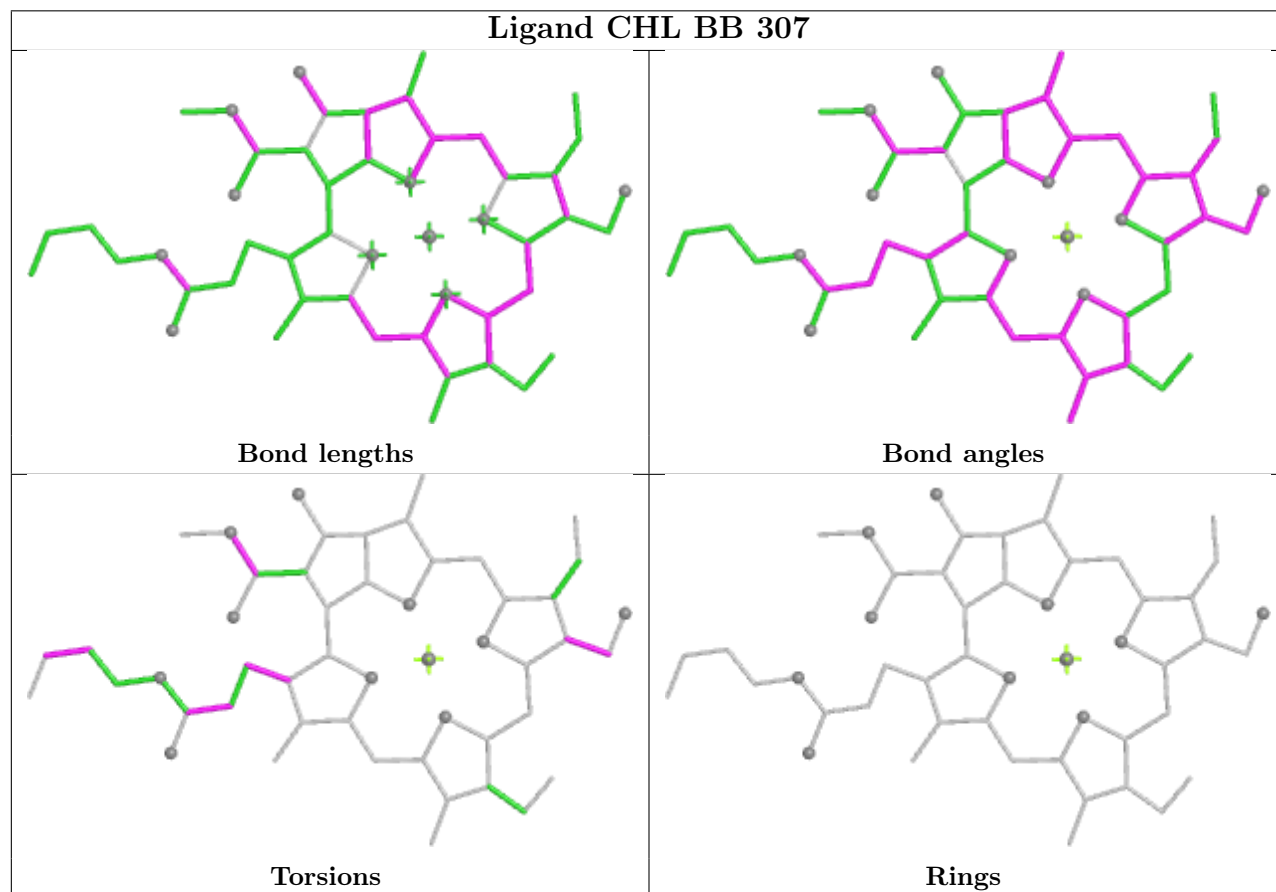


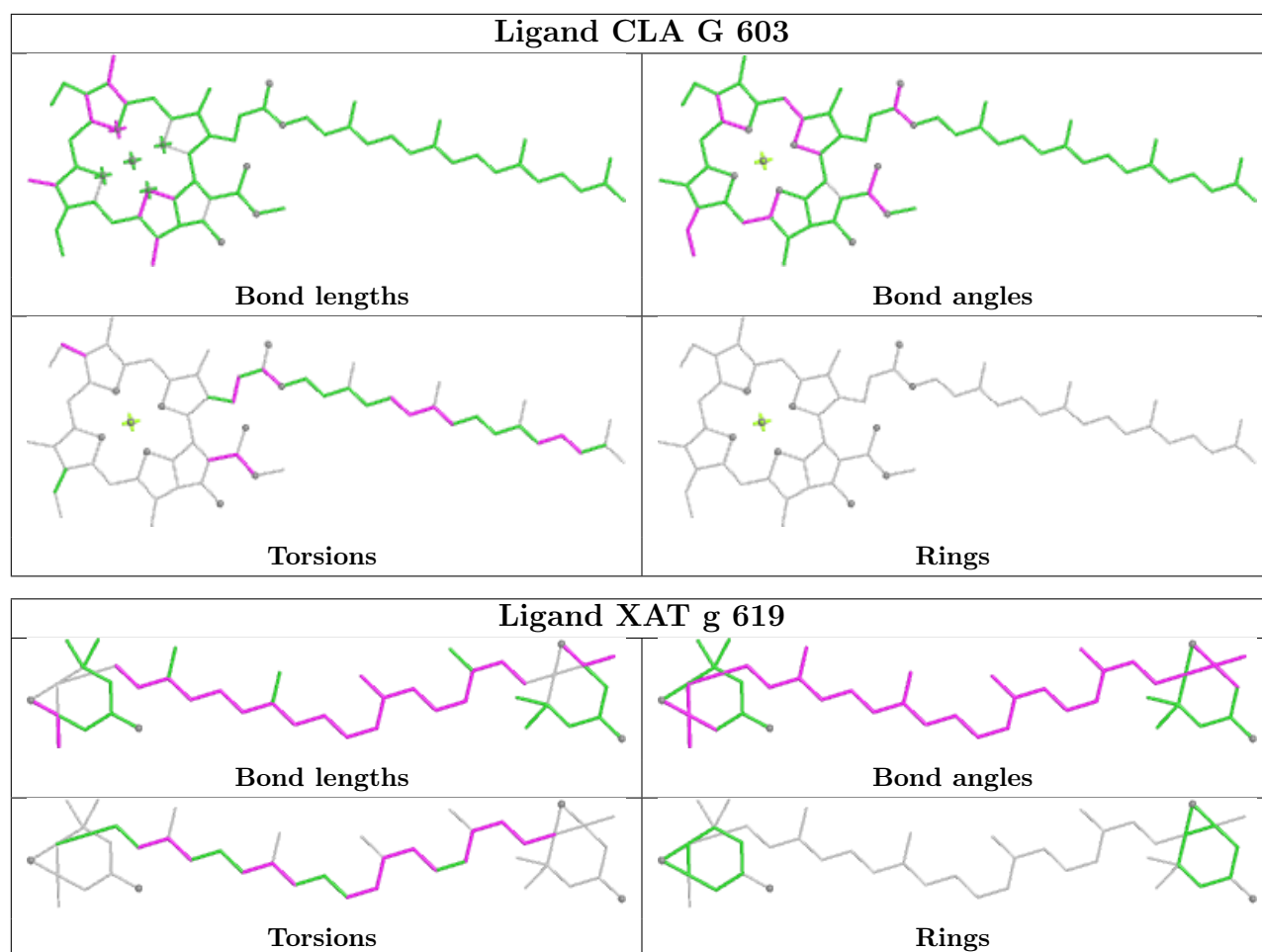




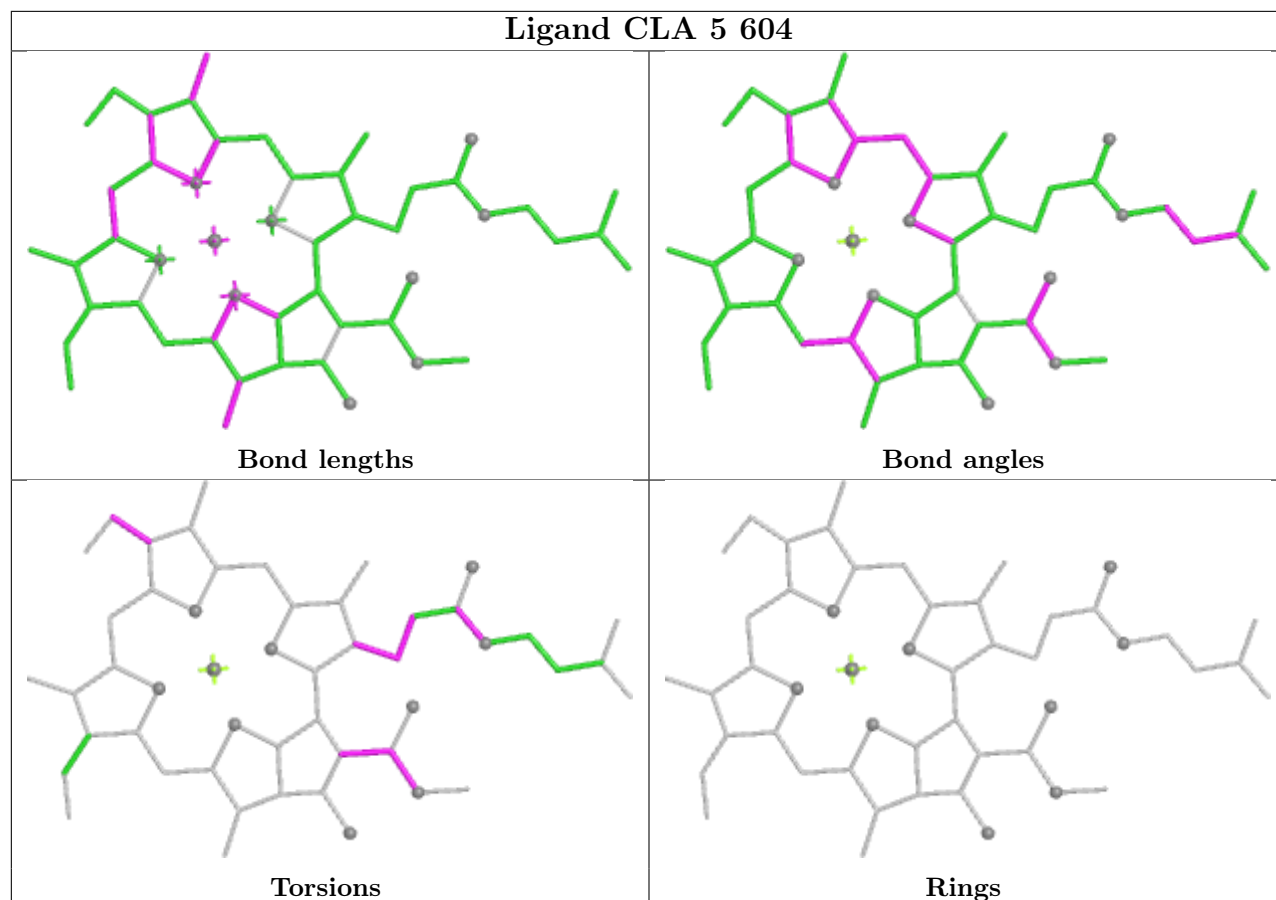




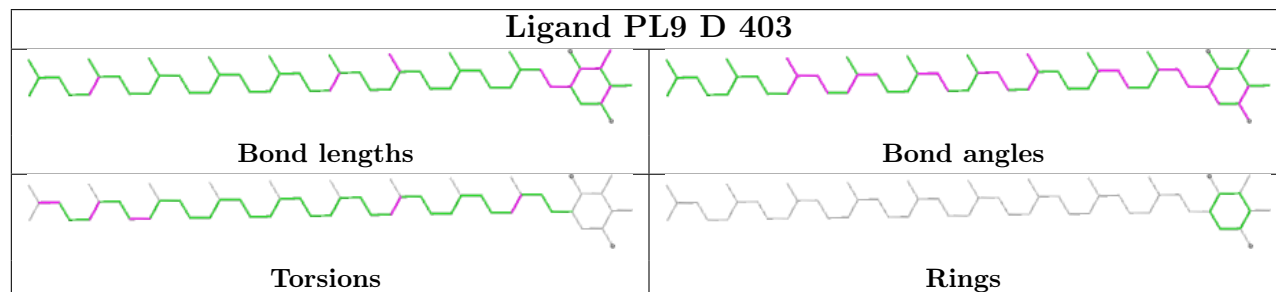
Ligand CLA BE 614**Ligand CHL BB 307**



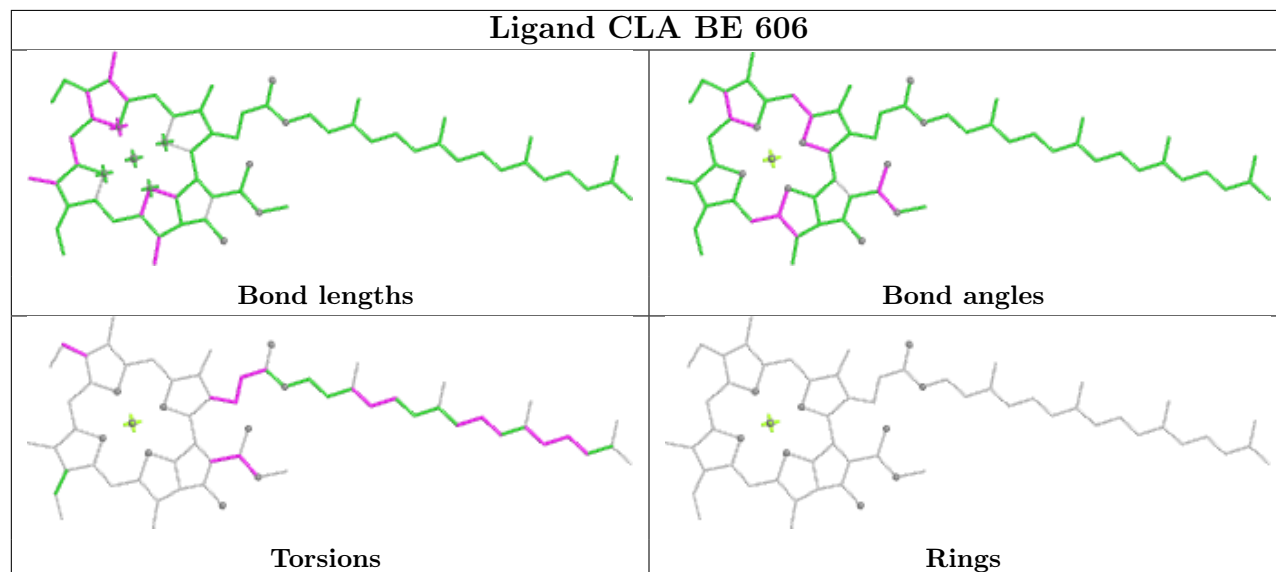
Ligand CLA 5 604

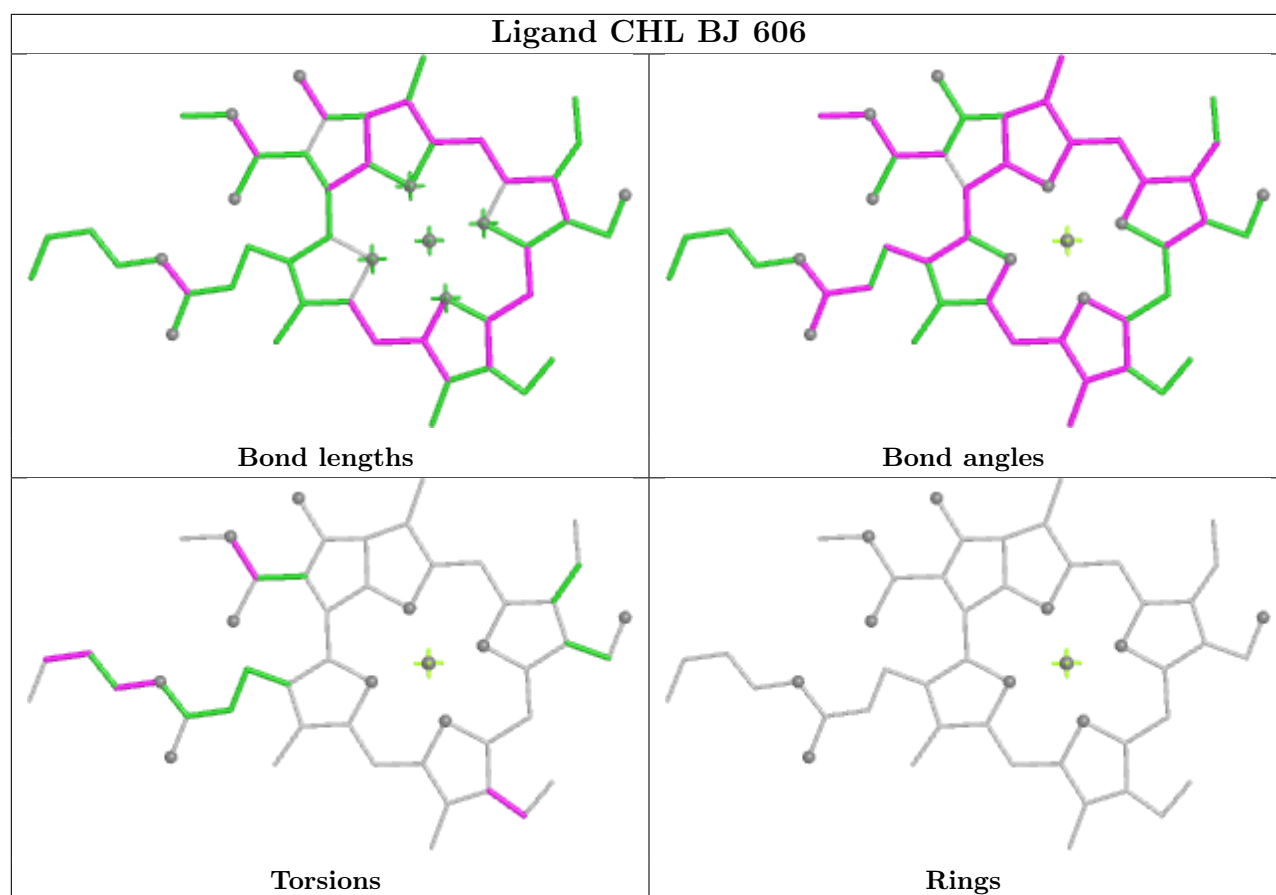


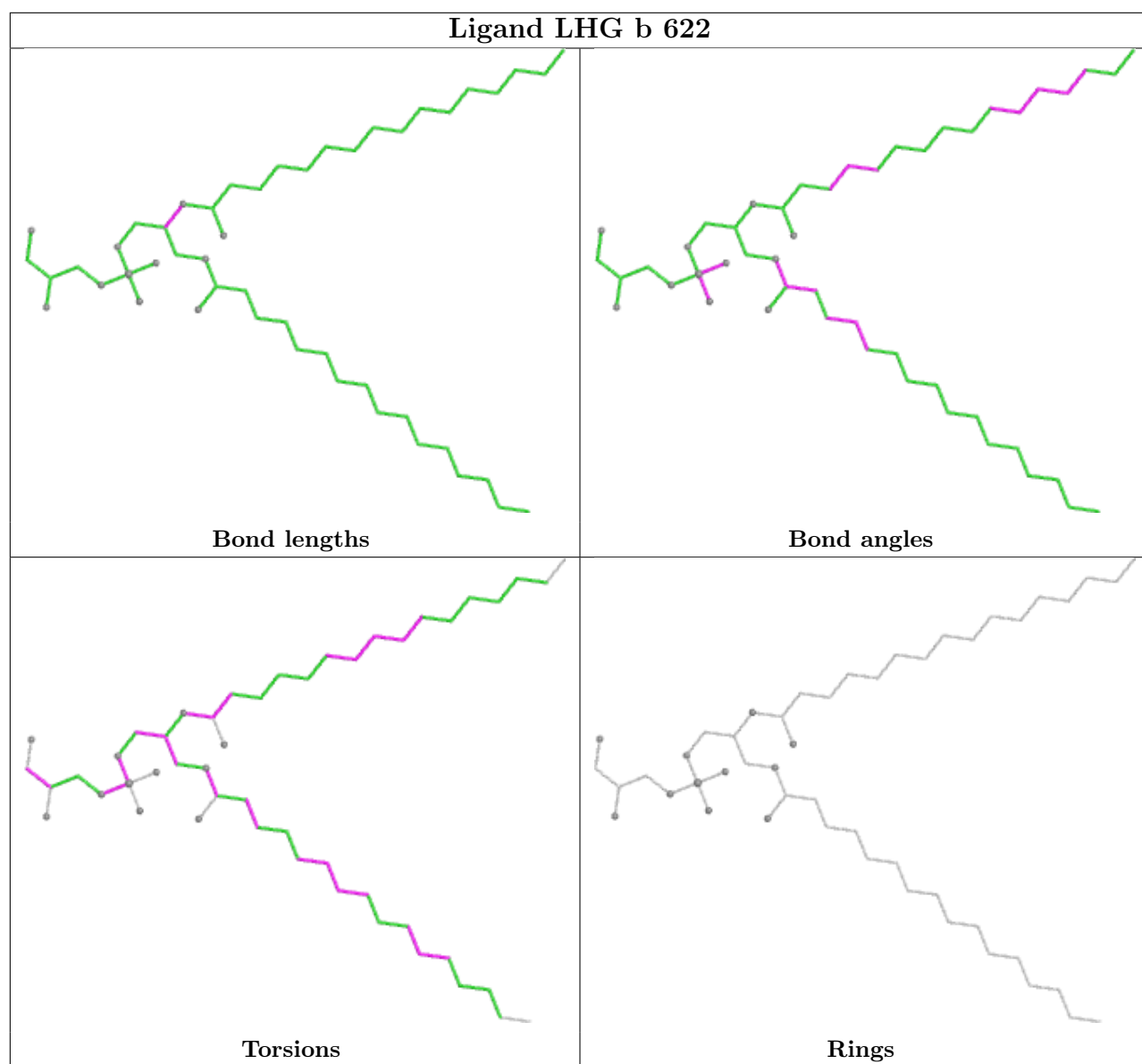
Ligand PL9 D 403

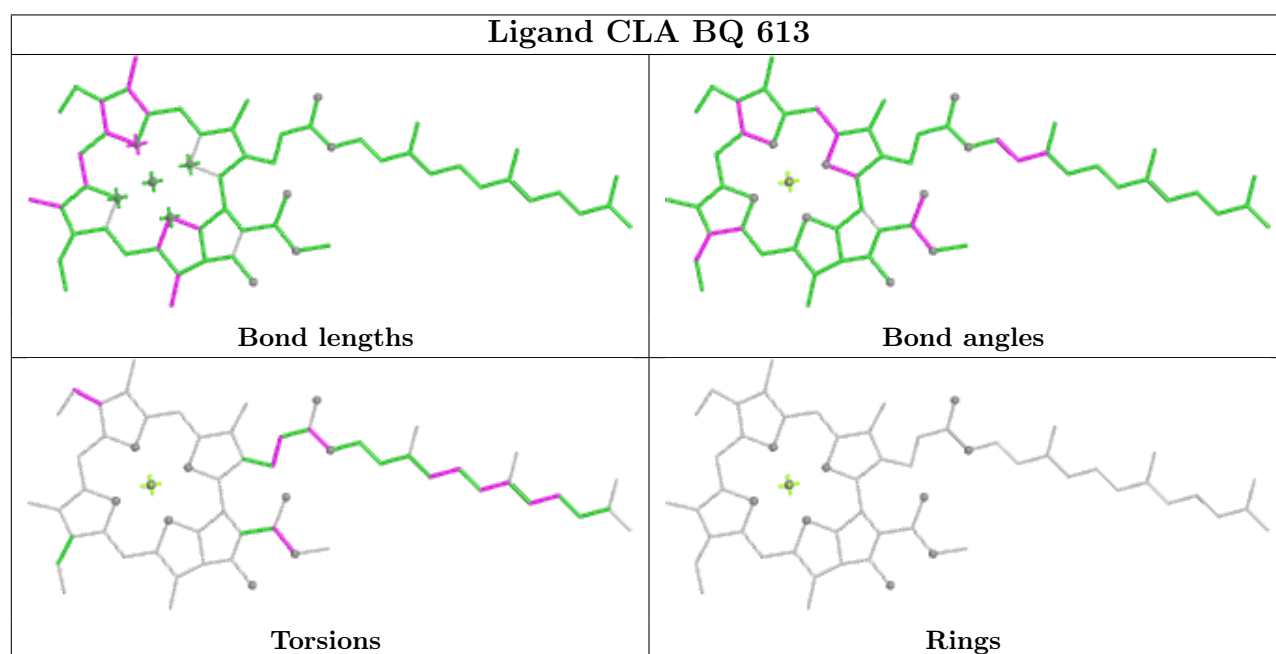
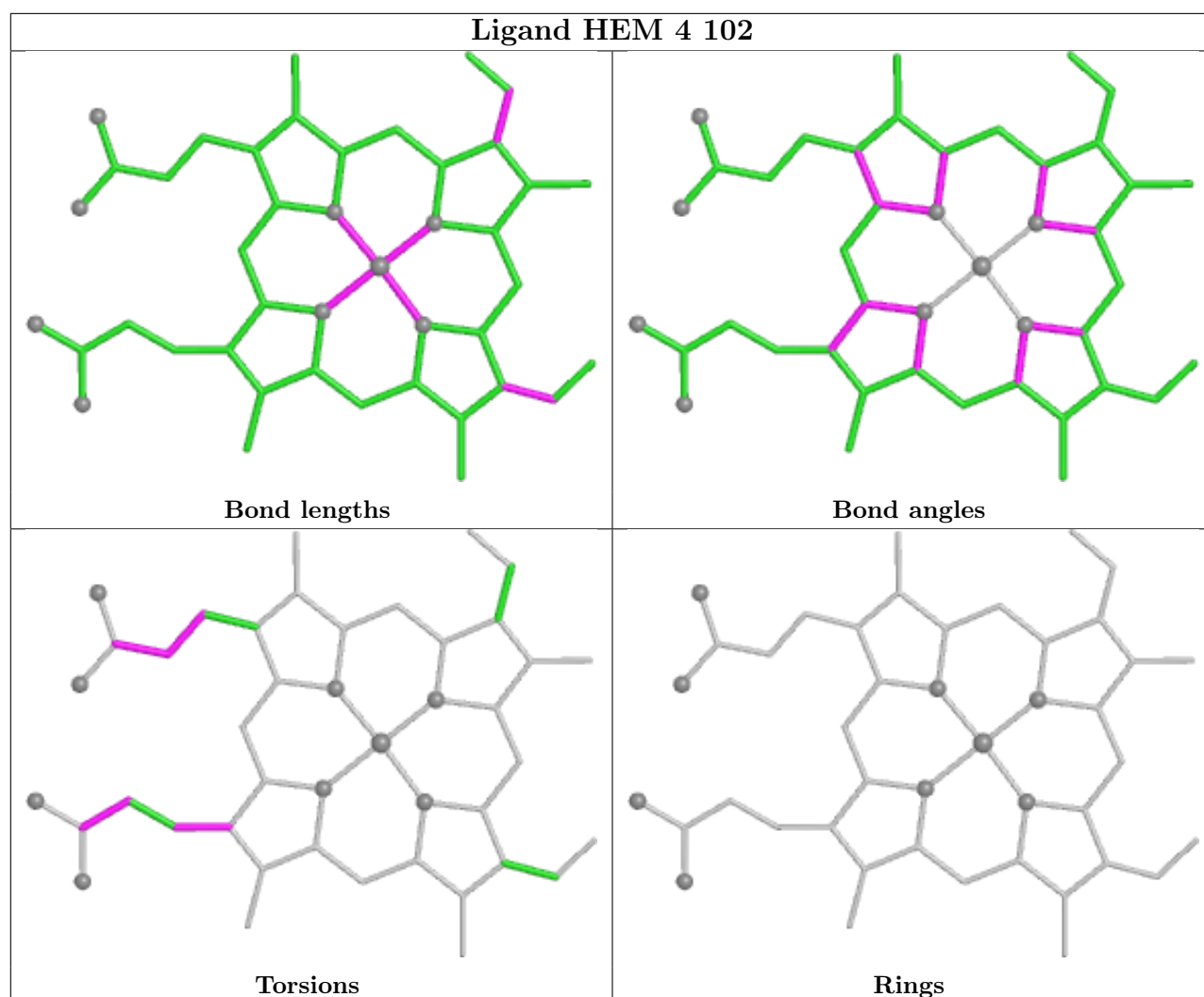


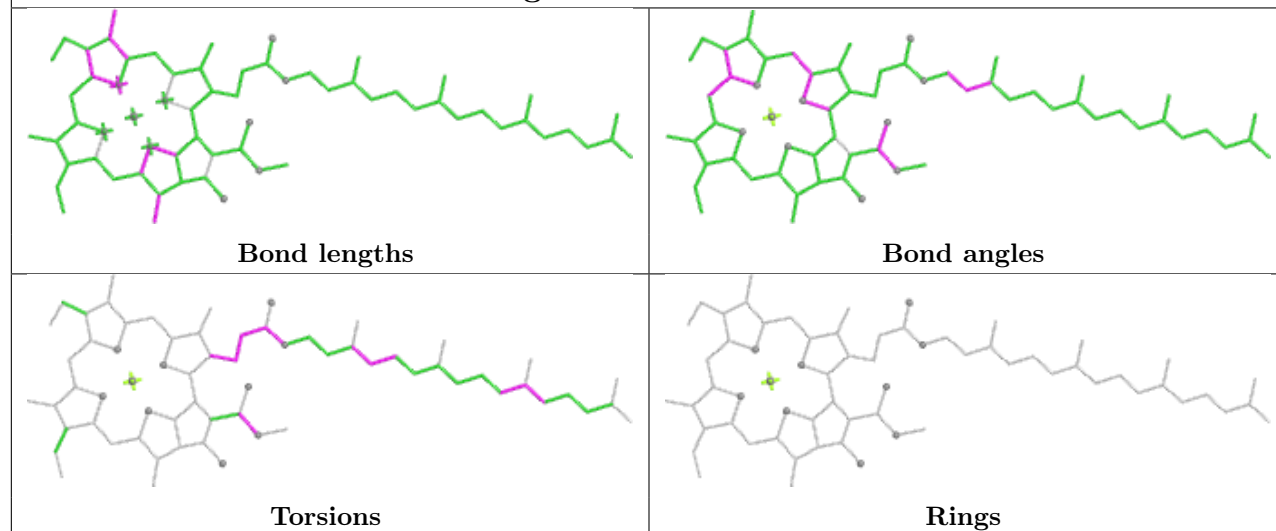
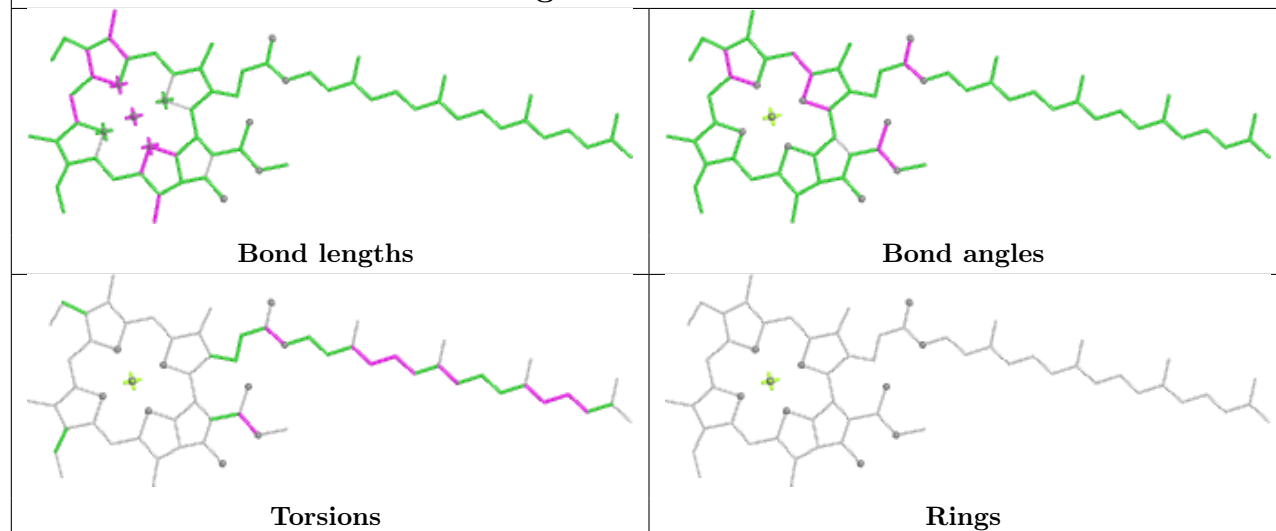
Ligand CLA BE 606

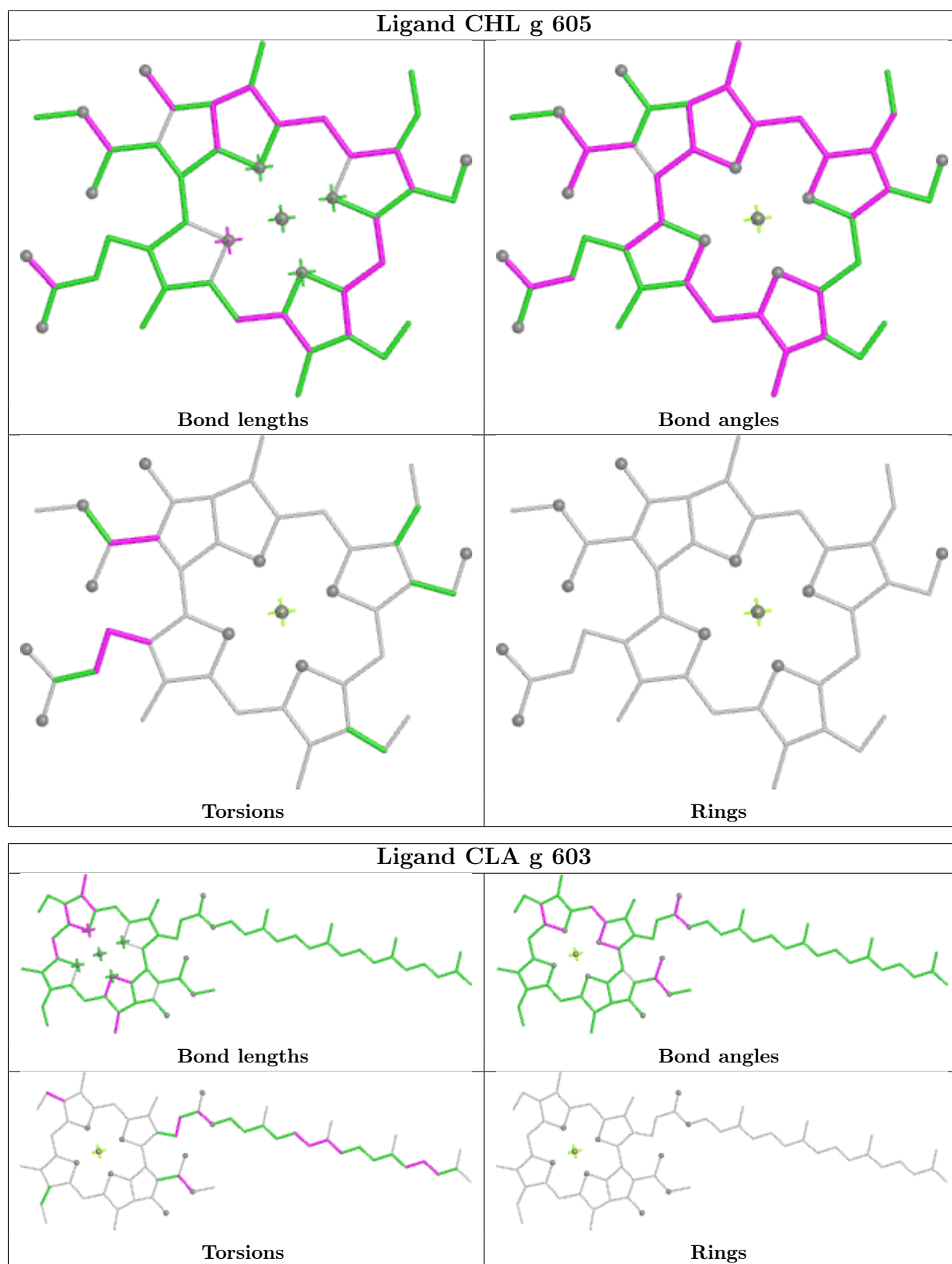


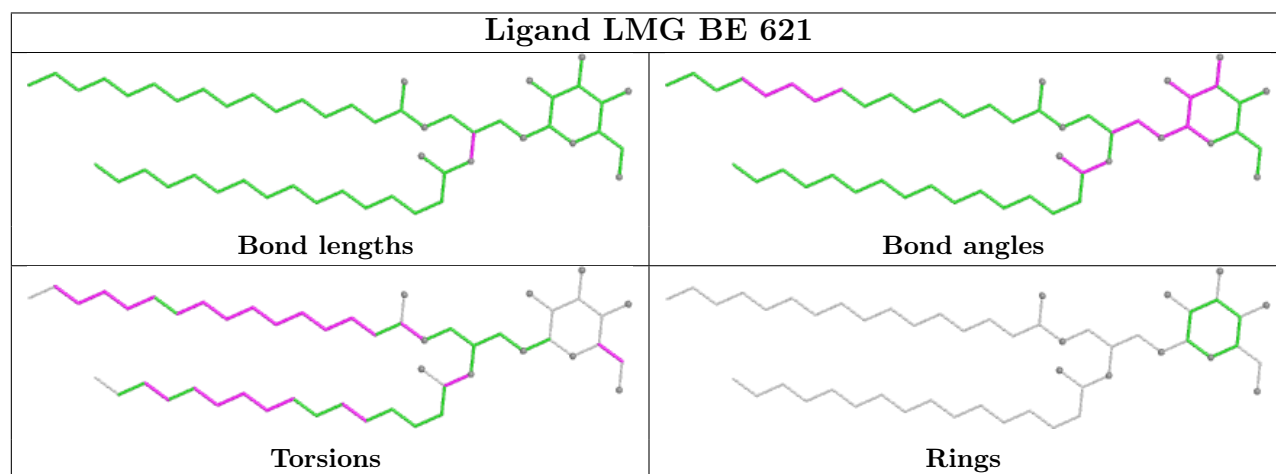
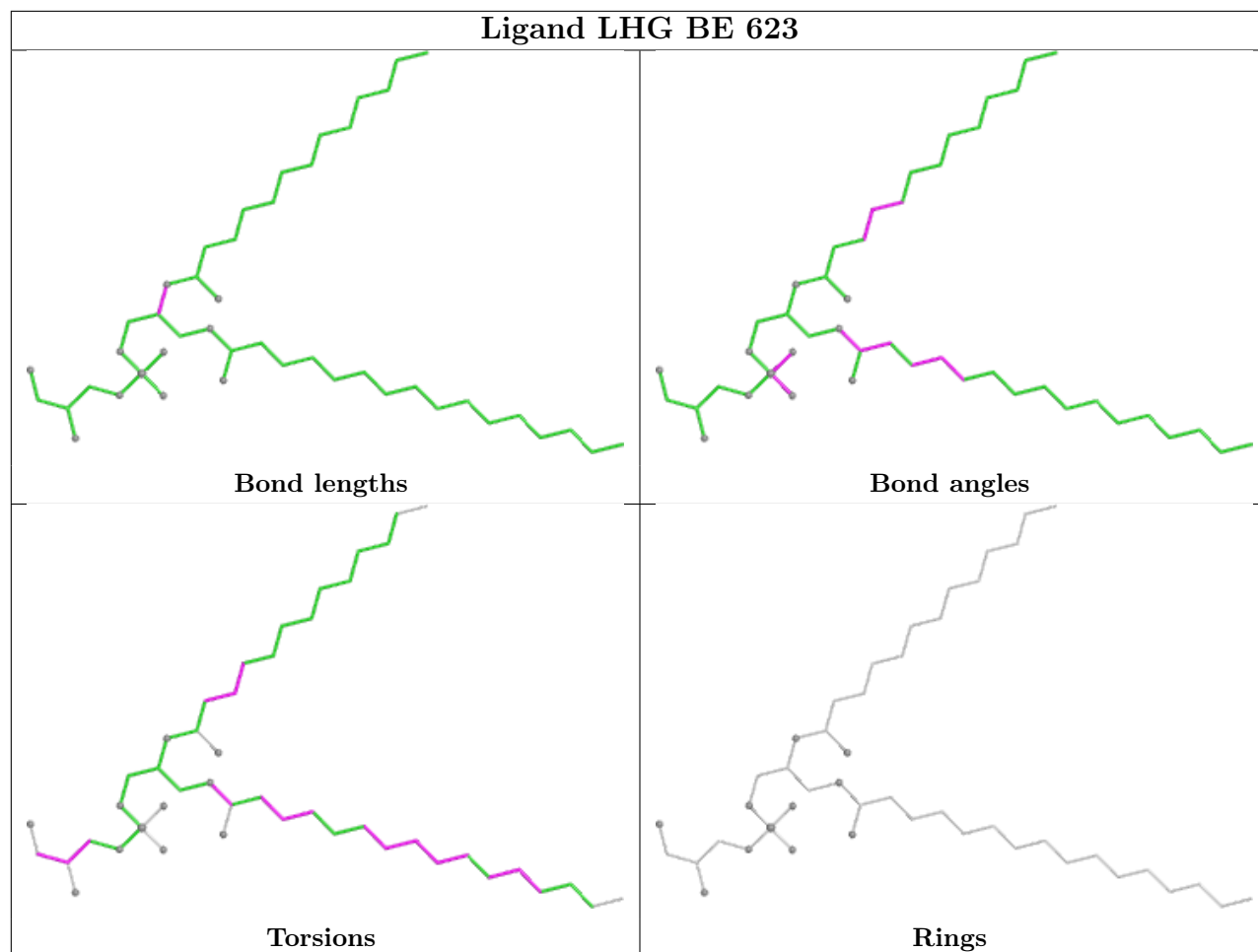


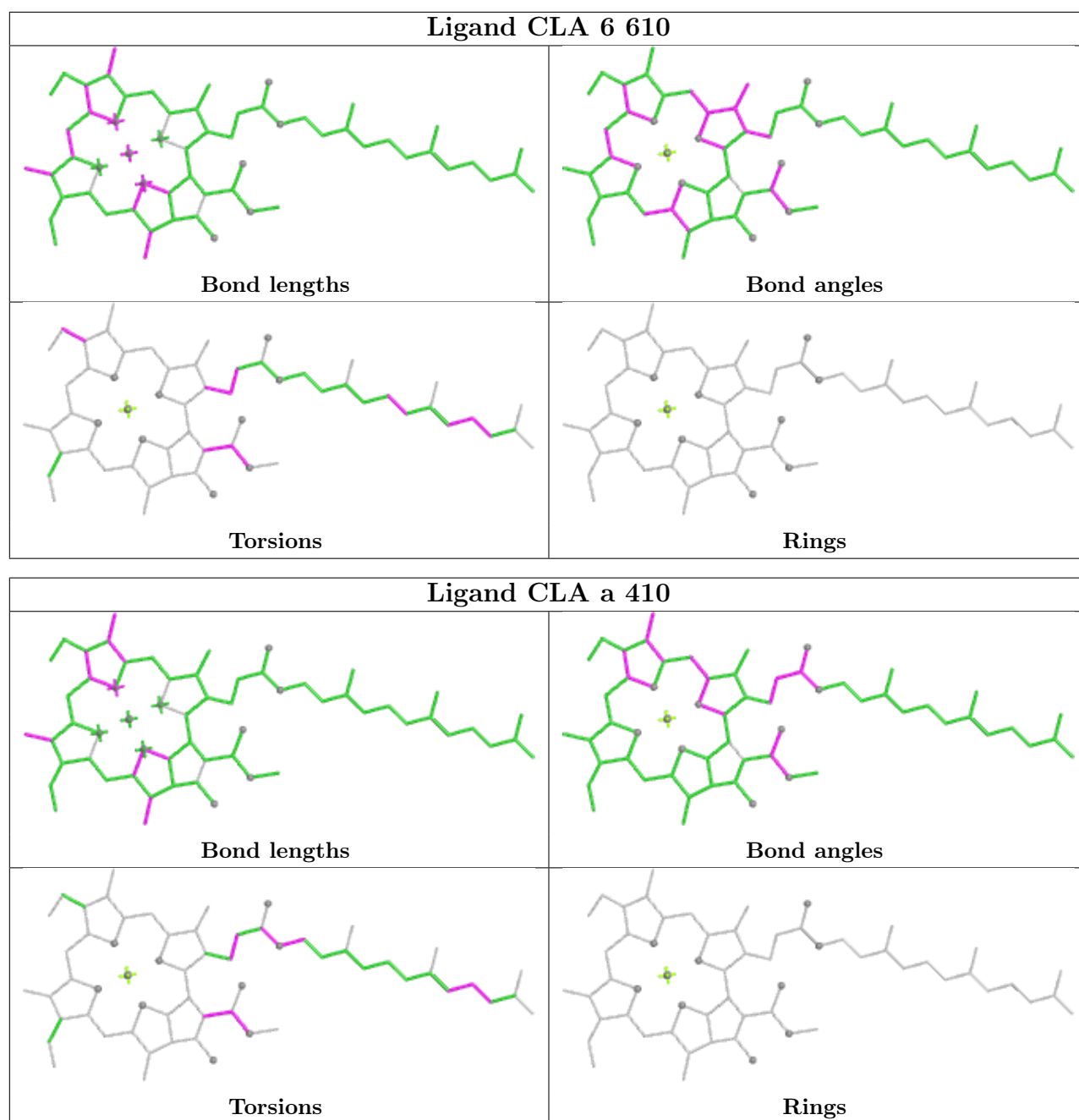


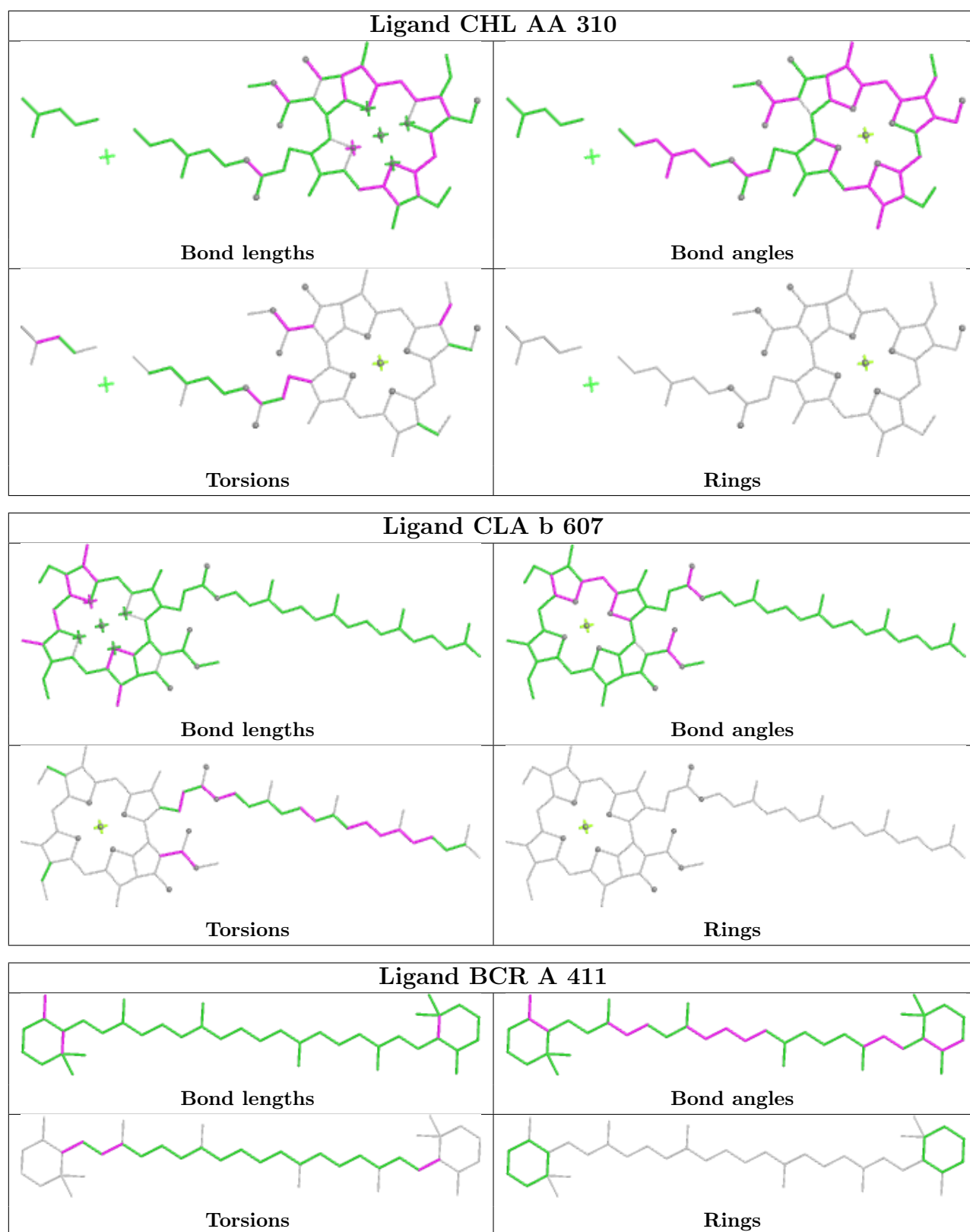


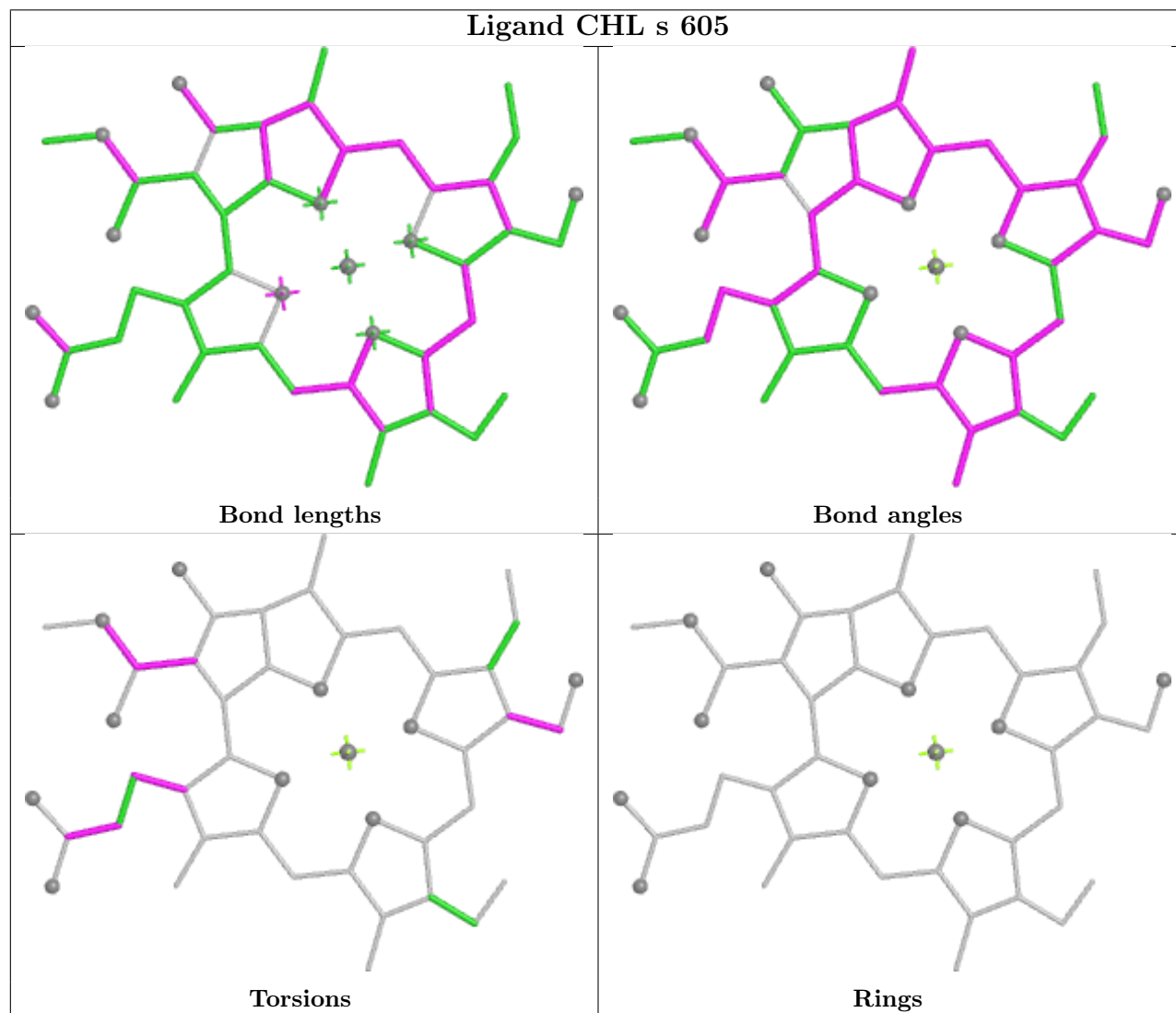
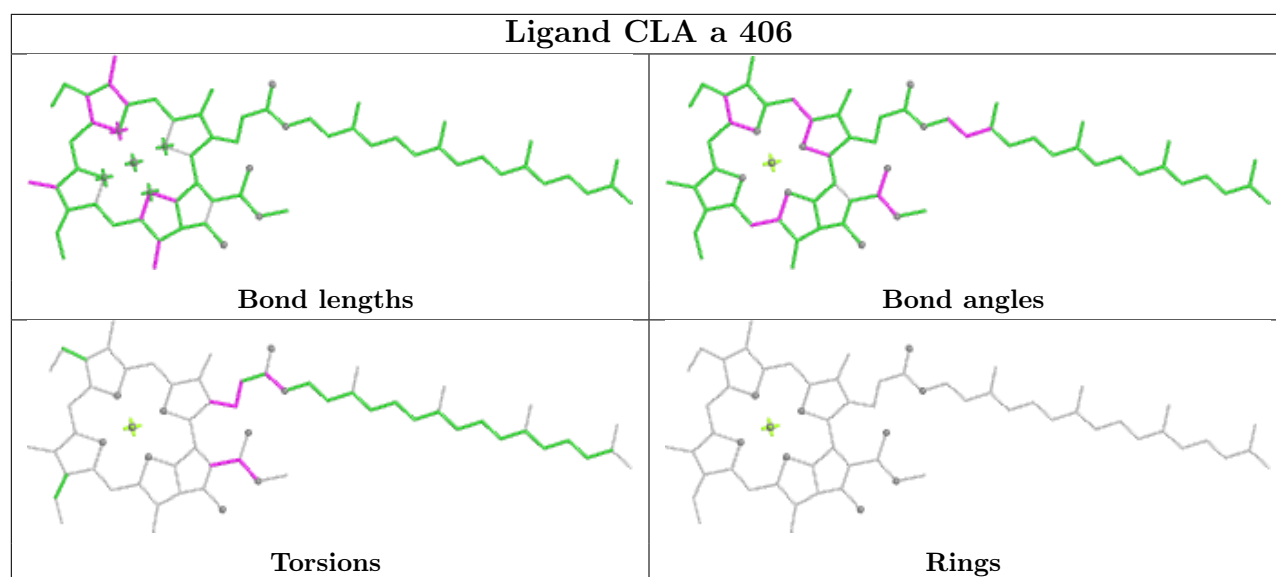
Ligand CLA Ba 314**Ligand CLA 1 504**



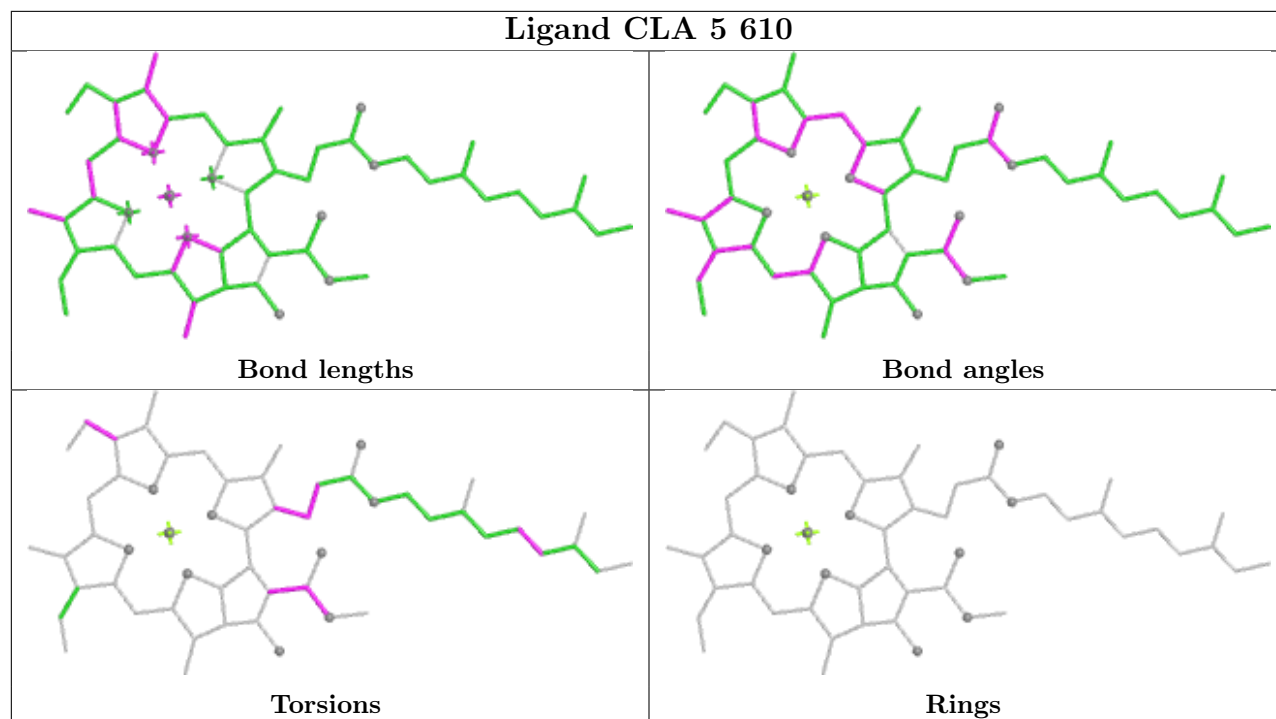




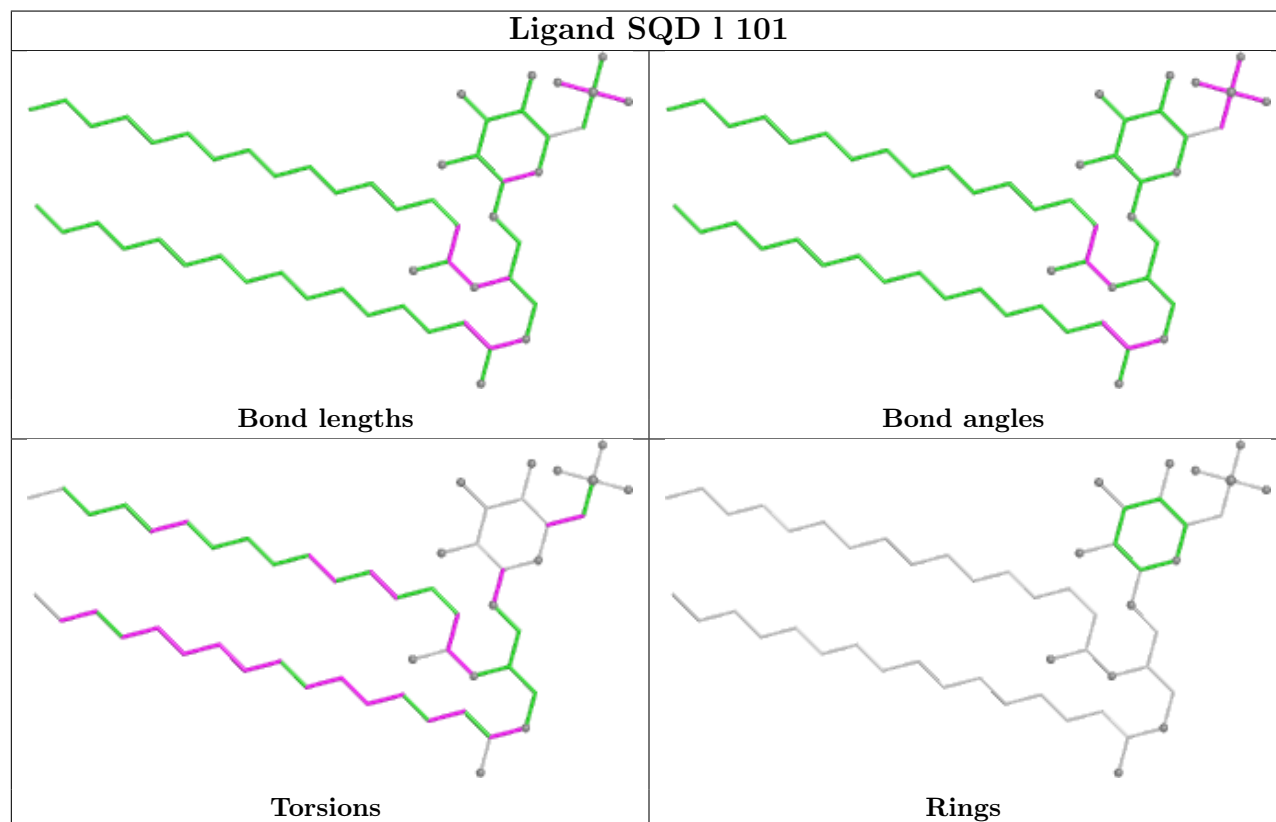


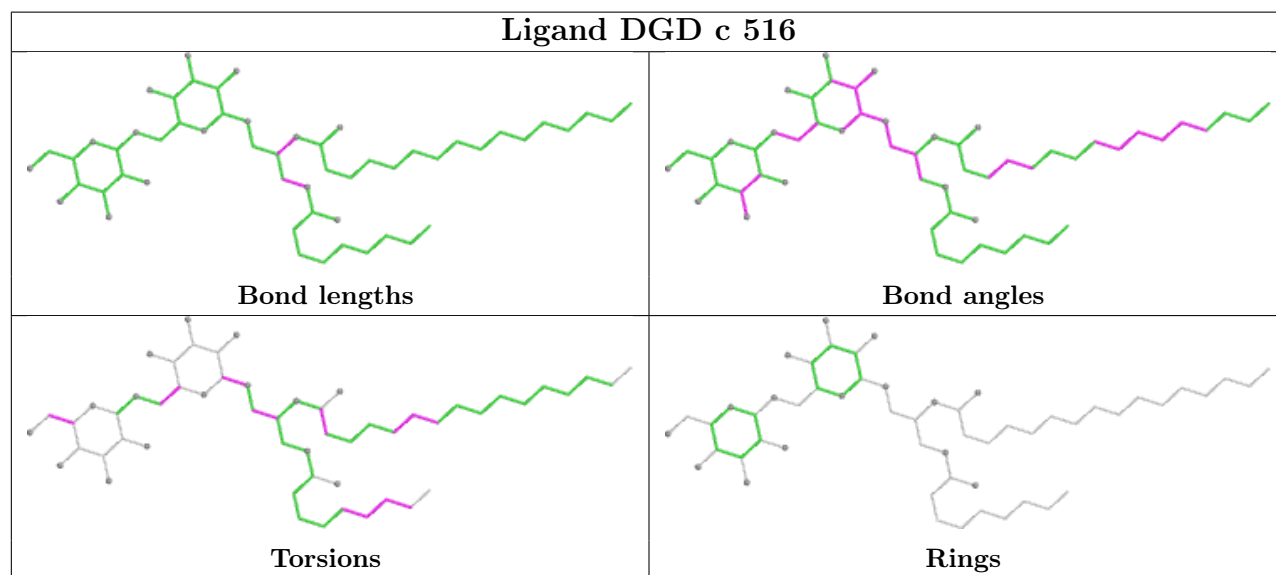
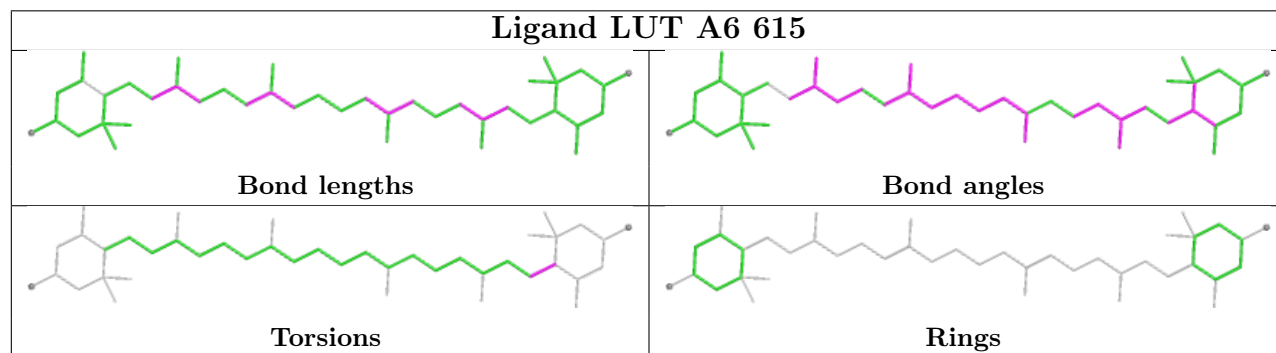
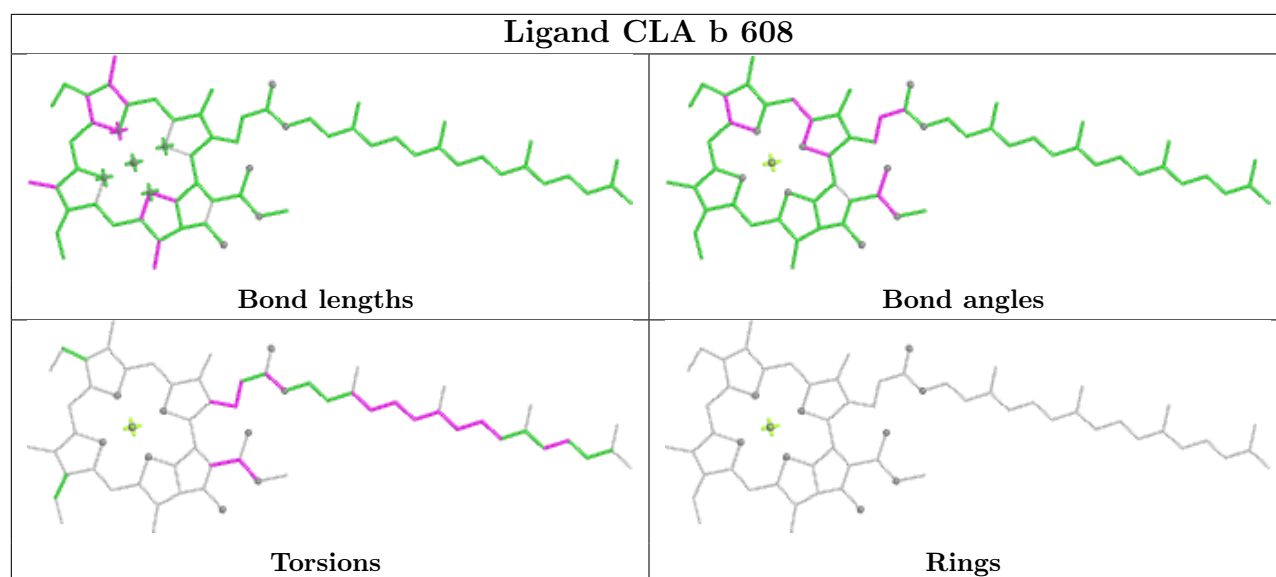


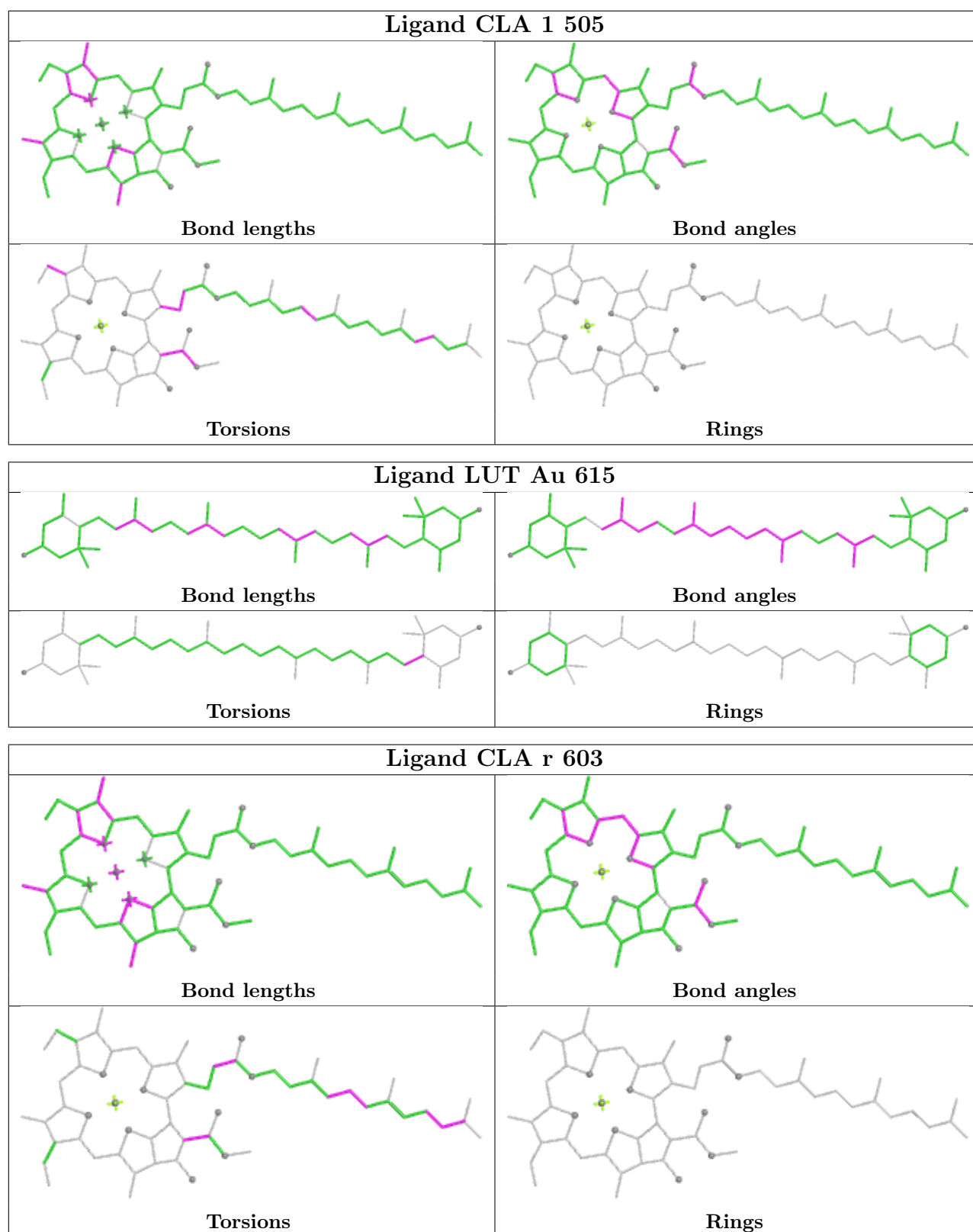
Ligand CLA 5 610

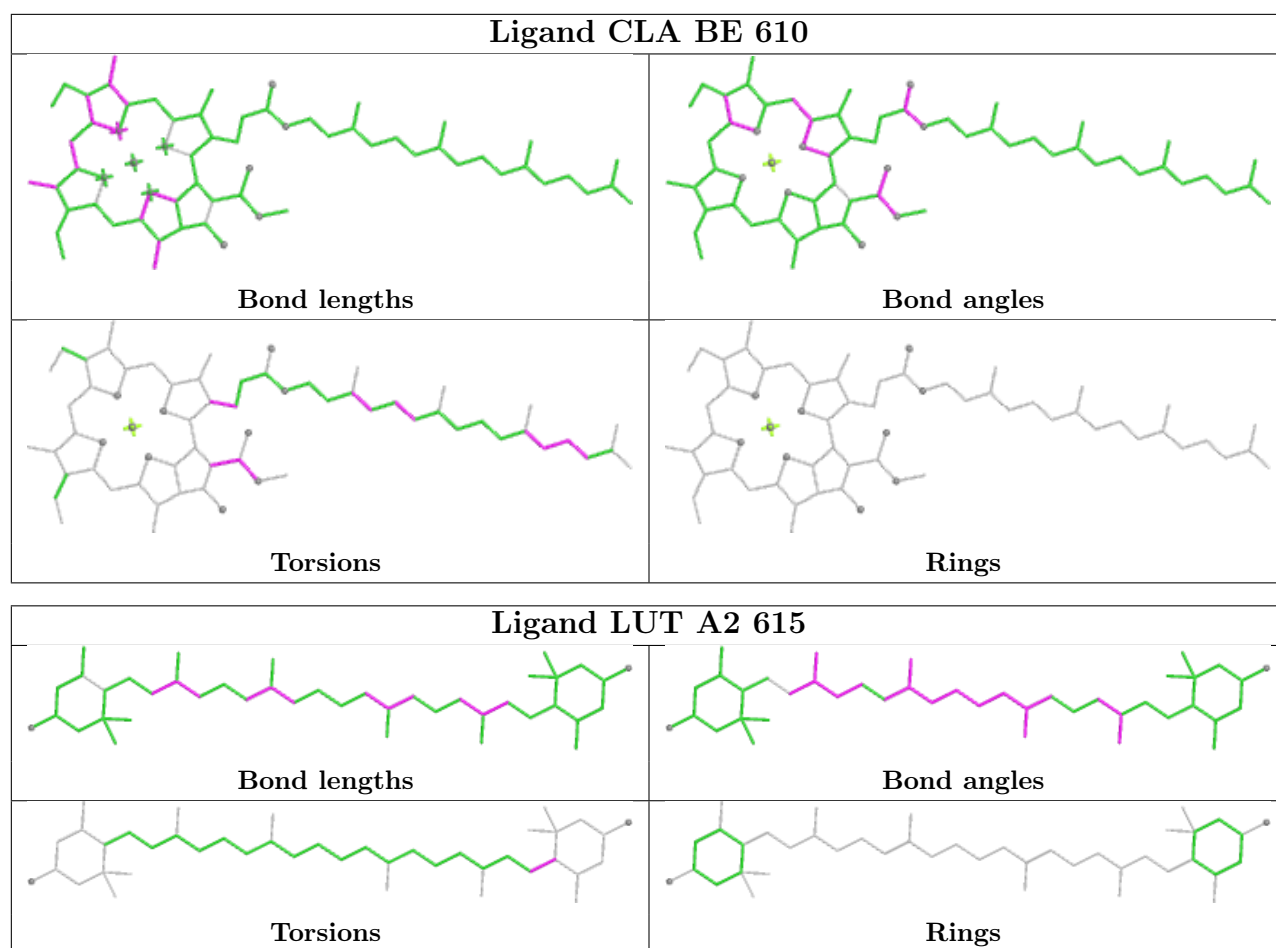


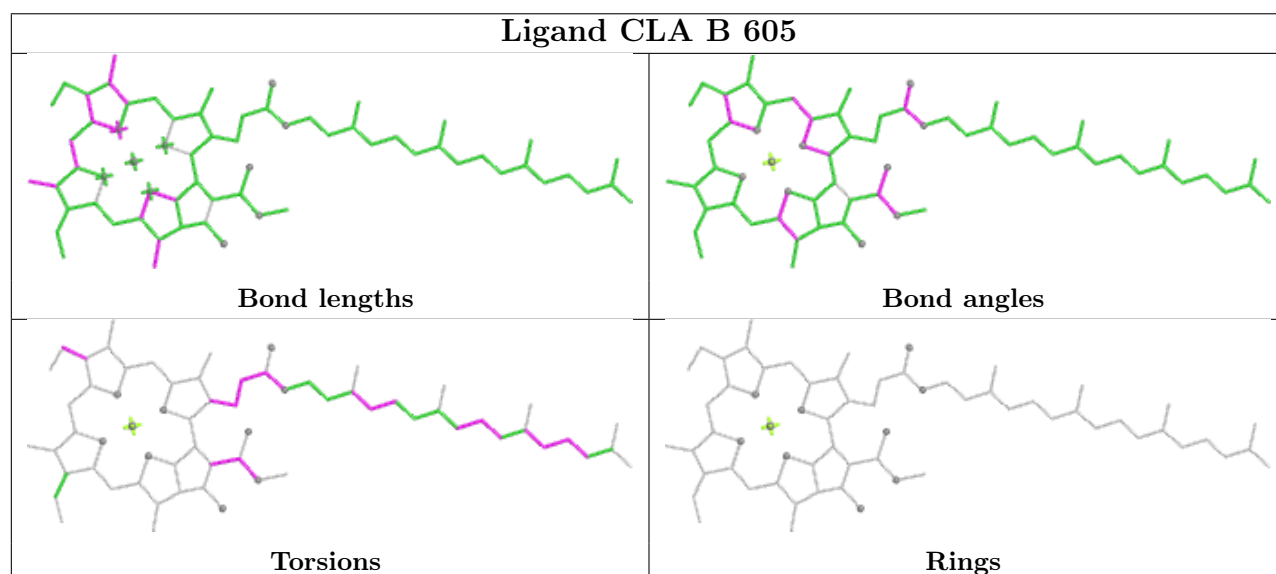
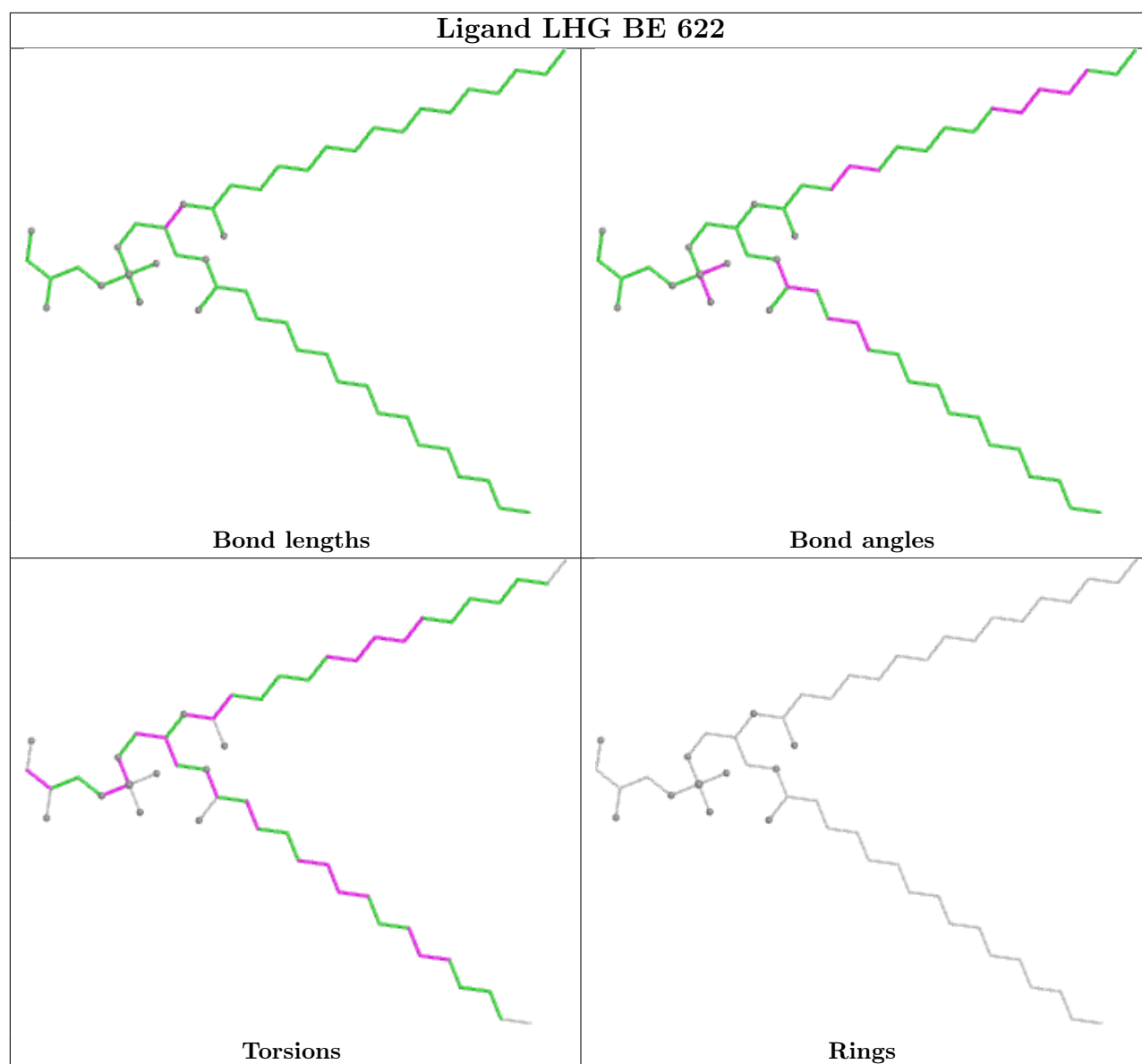
Ligand SQD 1 101

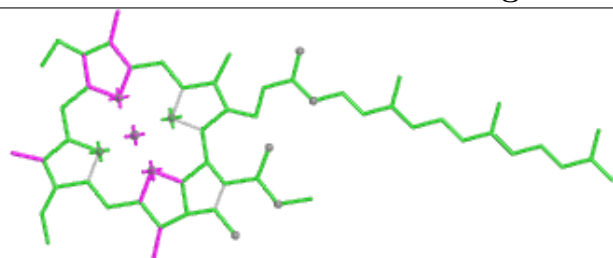




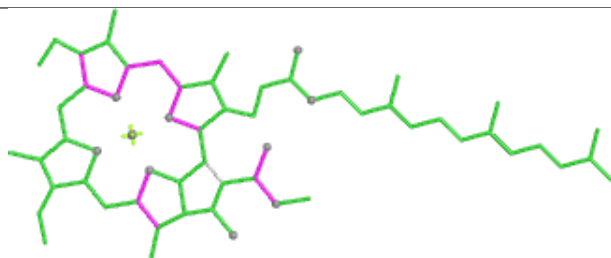




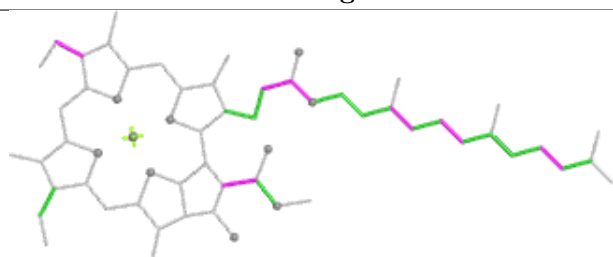


Ligand CLA BB 313

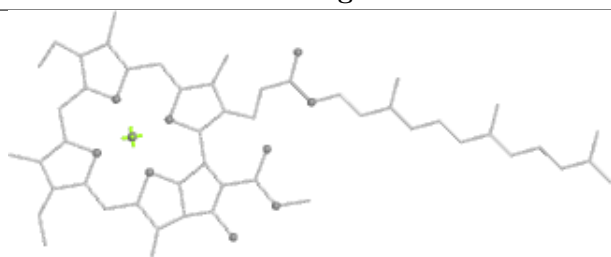
Bond lengths



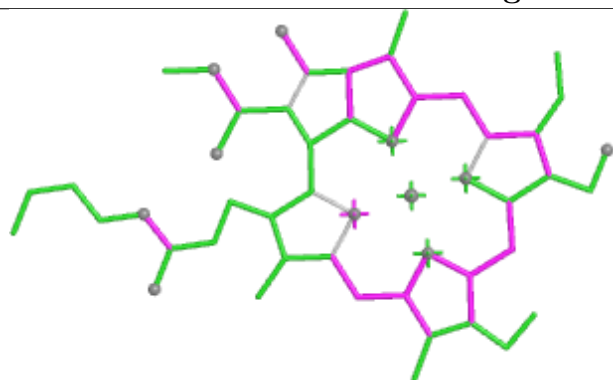
Bond angles



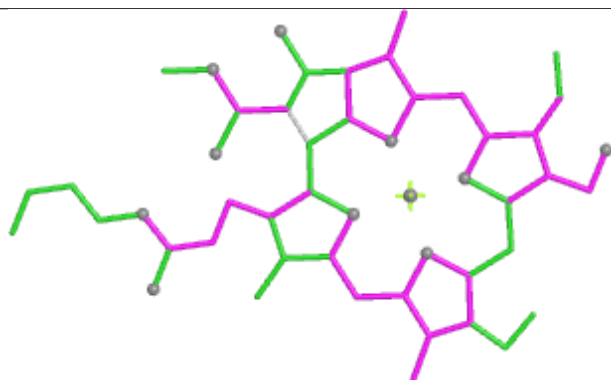
Torsions



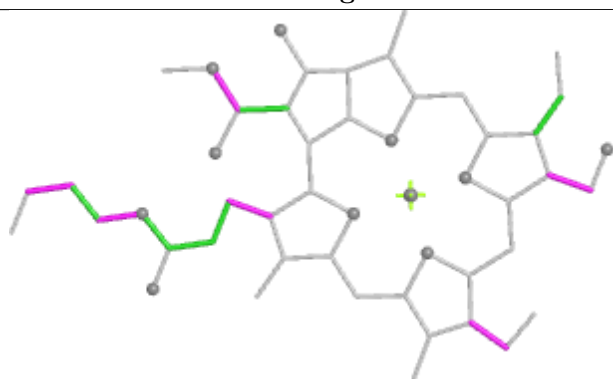
Rings

Ligand CHL Au 606

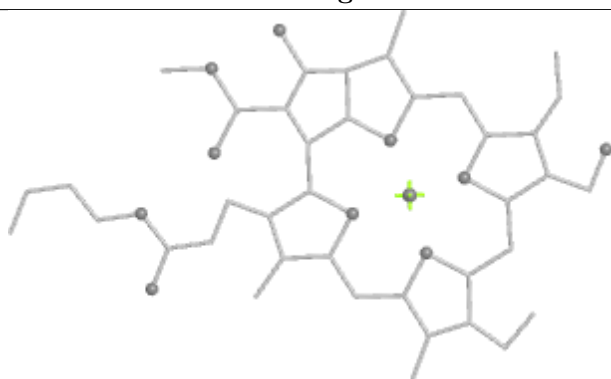
Bond lengths



Bond angles

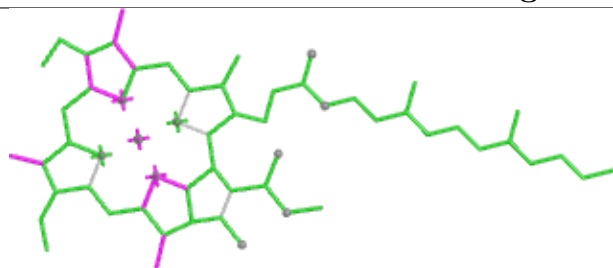


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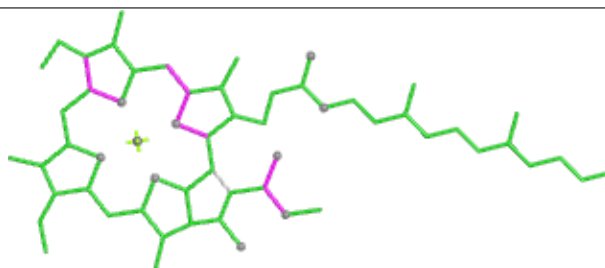


Rings

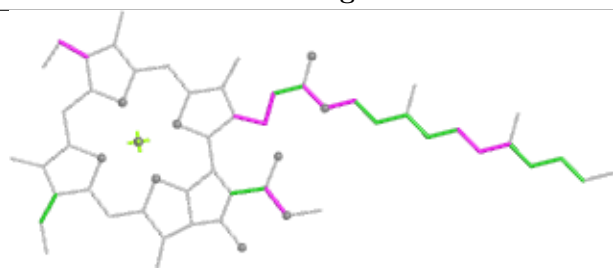
Ligand CLA r 608



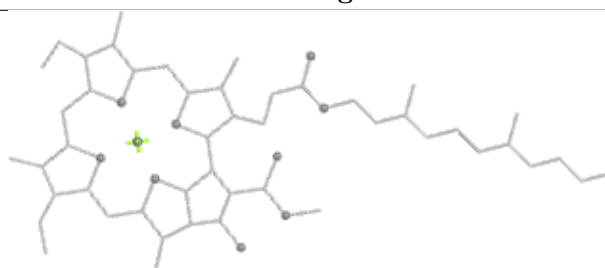
Bond lengths



Bond angles

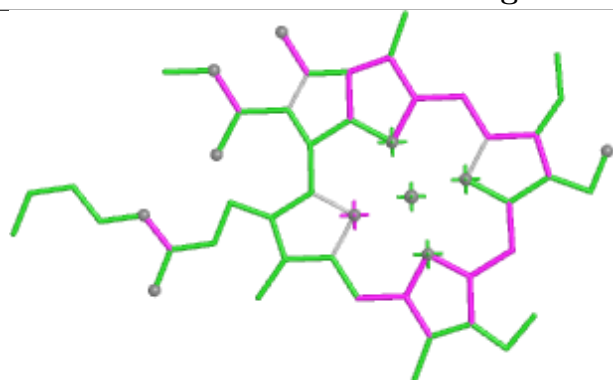


Torsions

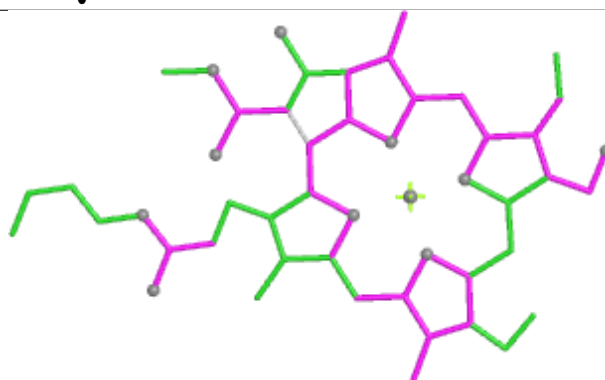


Rings

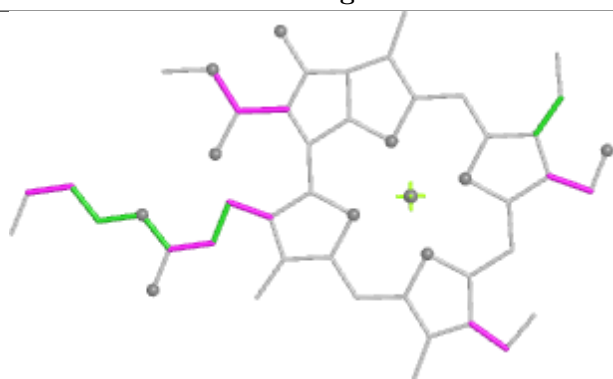
Ligand CHL BQ 606



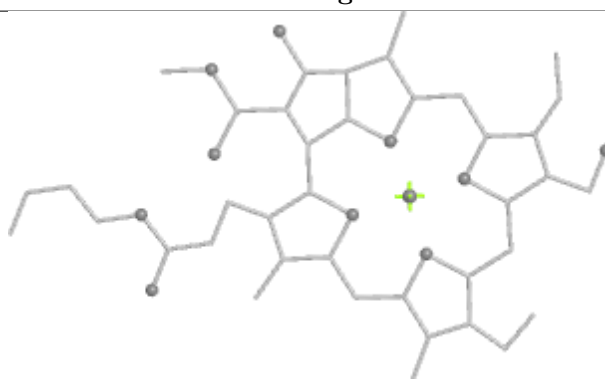
Bond lengths



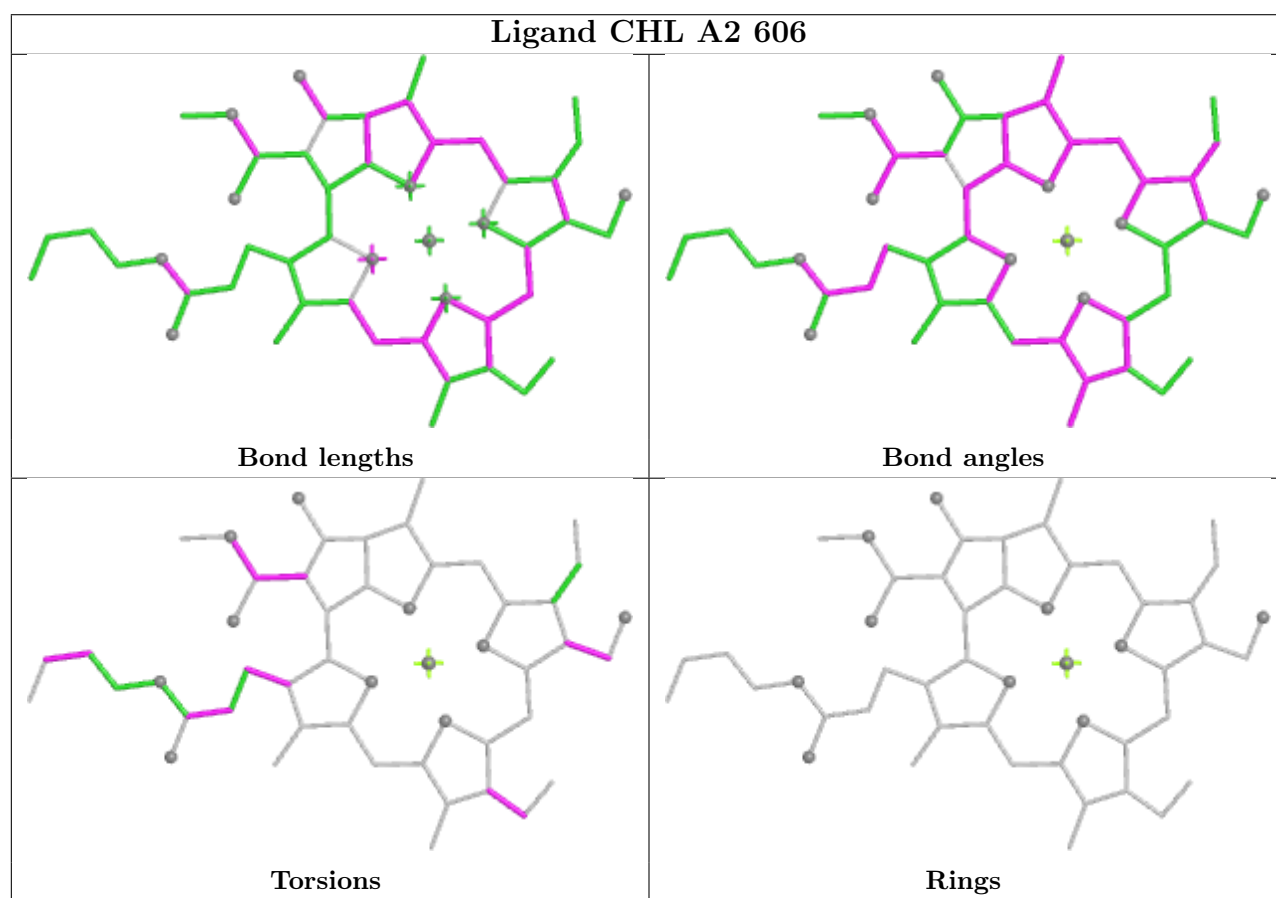
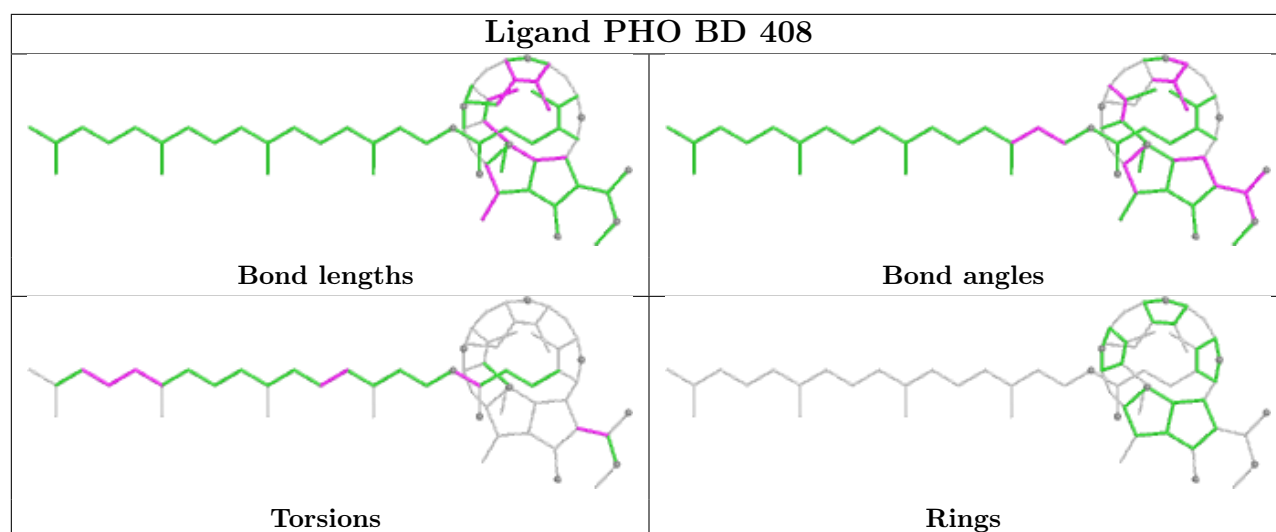
Bond angles

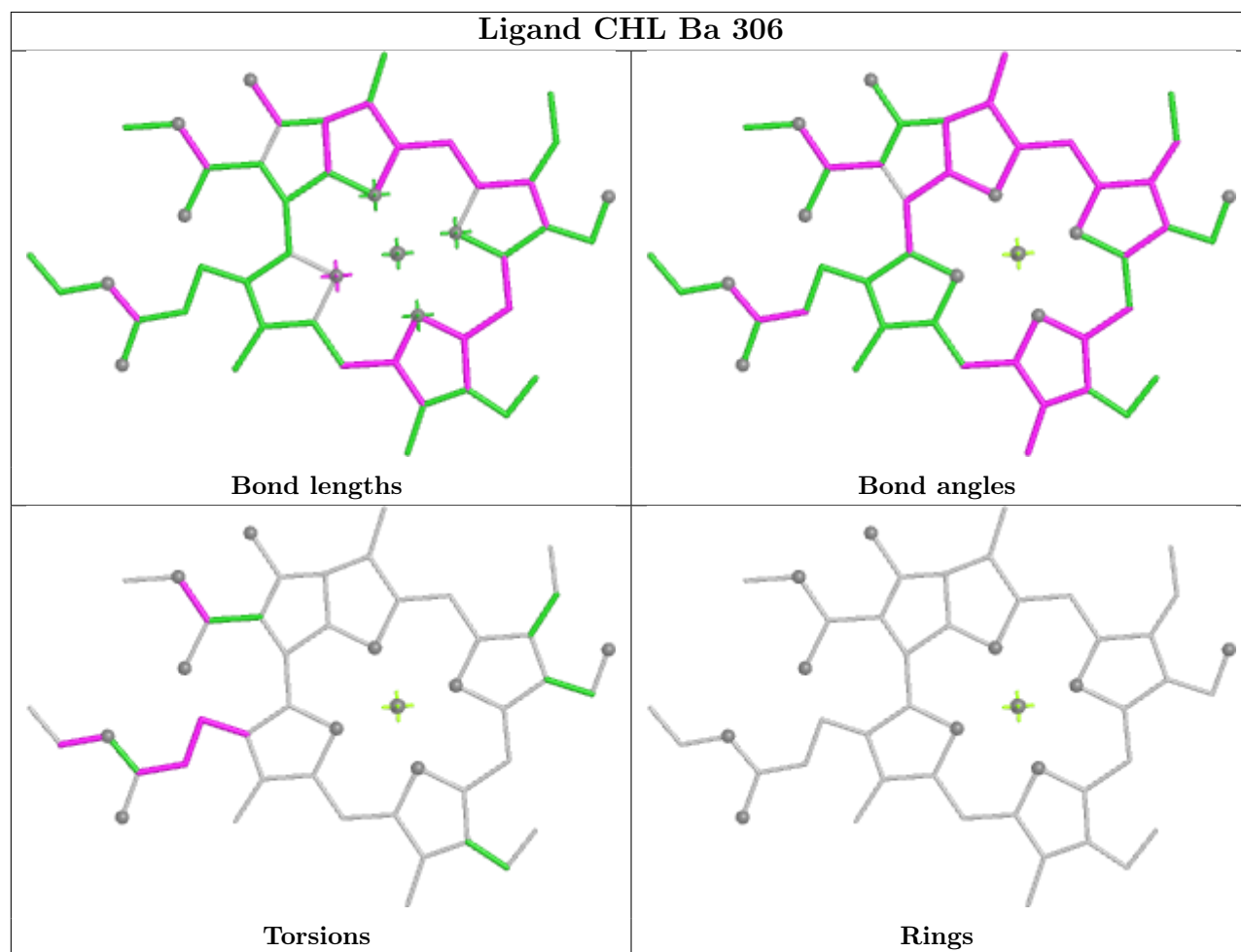
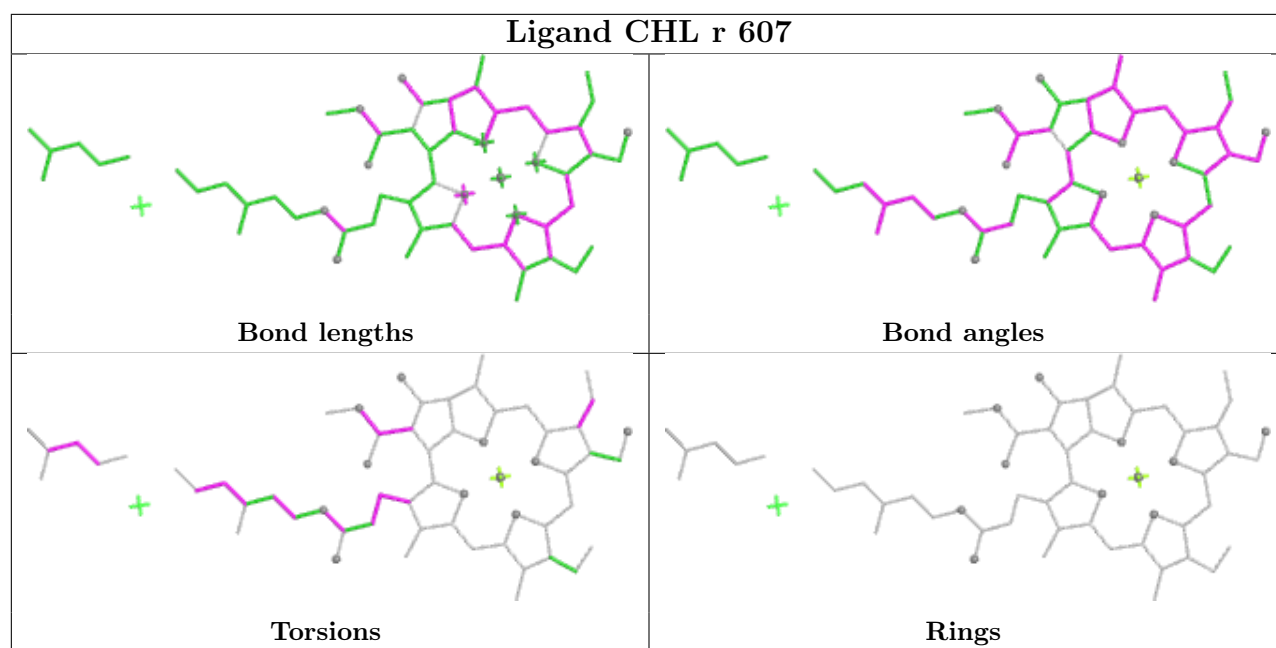


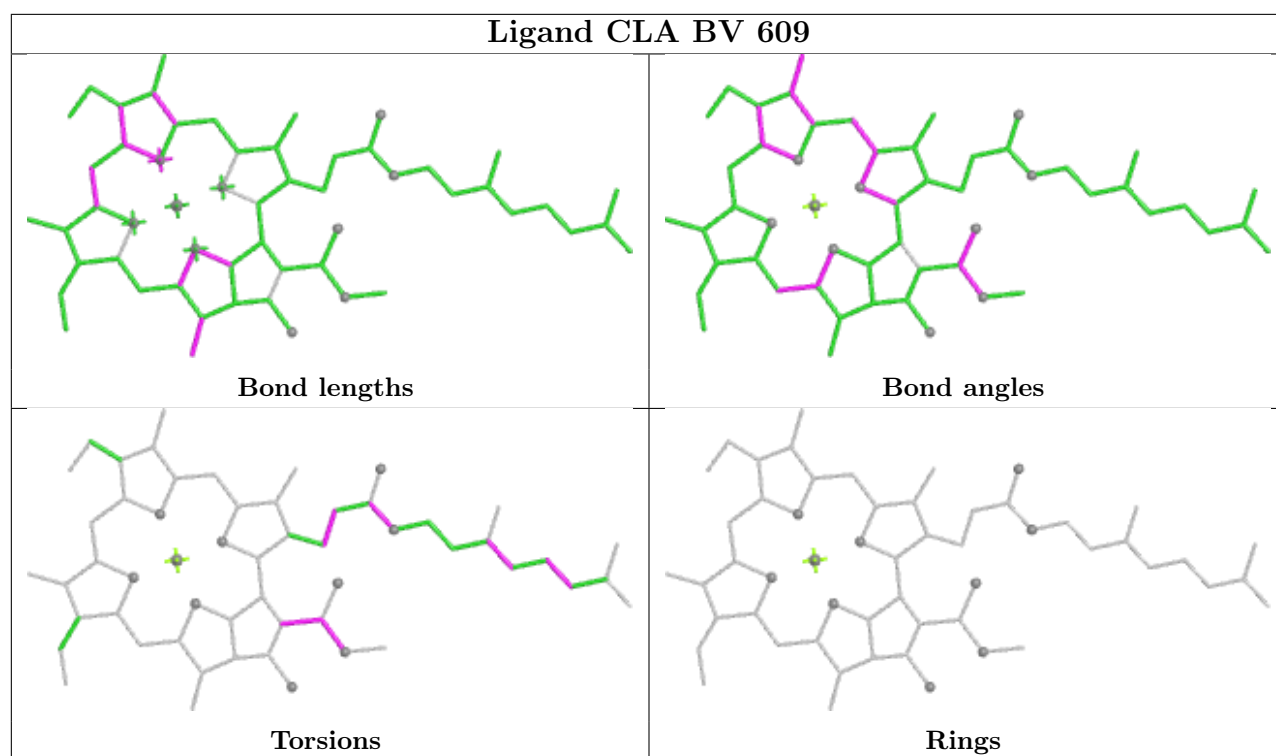
Torsions



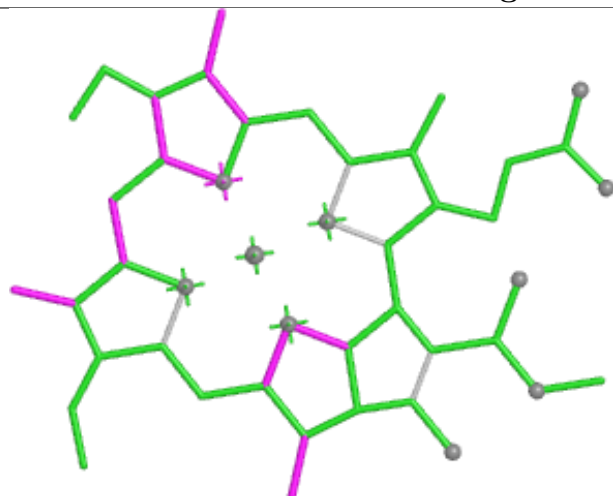
Rings



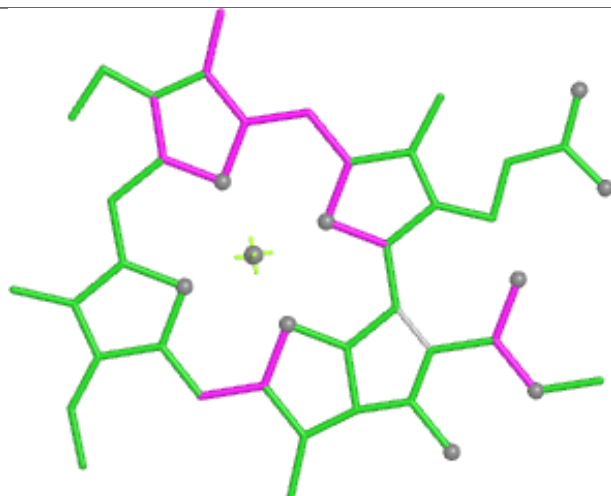




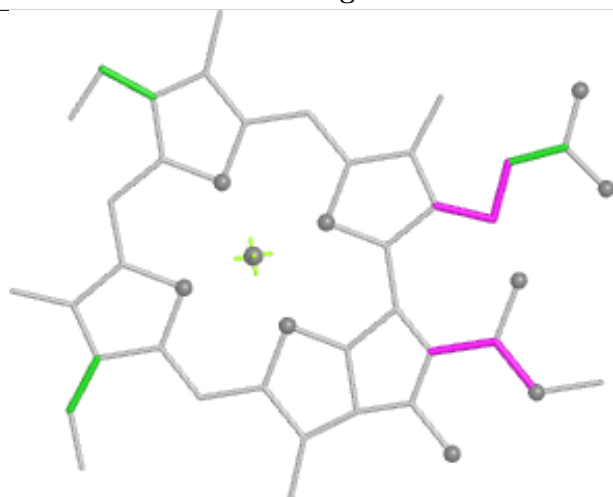
Ligand CLA AA 305



Bond lengths



Bond angles

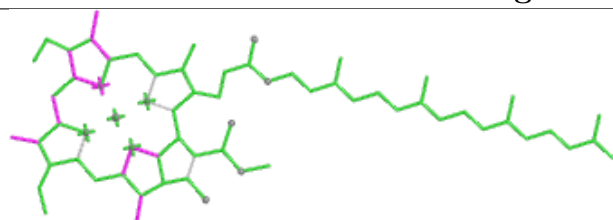


Torsions

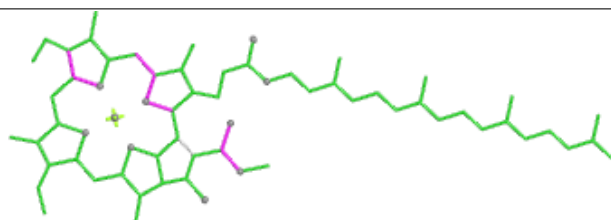


Rings

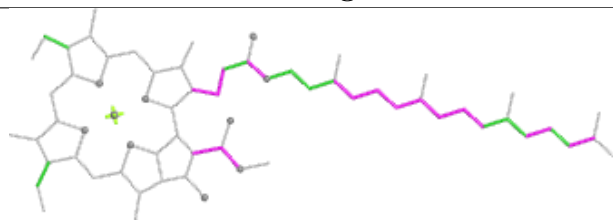
Ligand CLA B 607



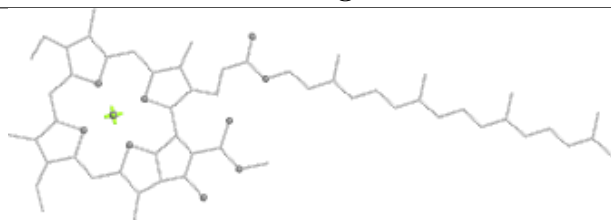
Bond lengths



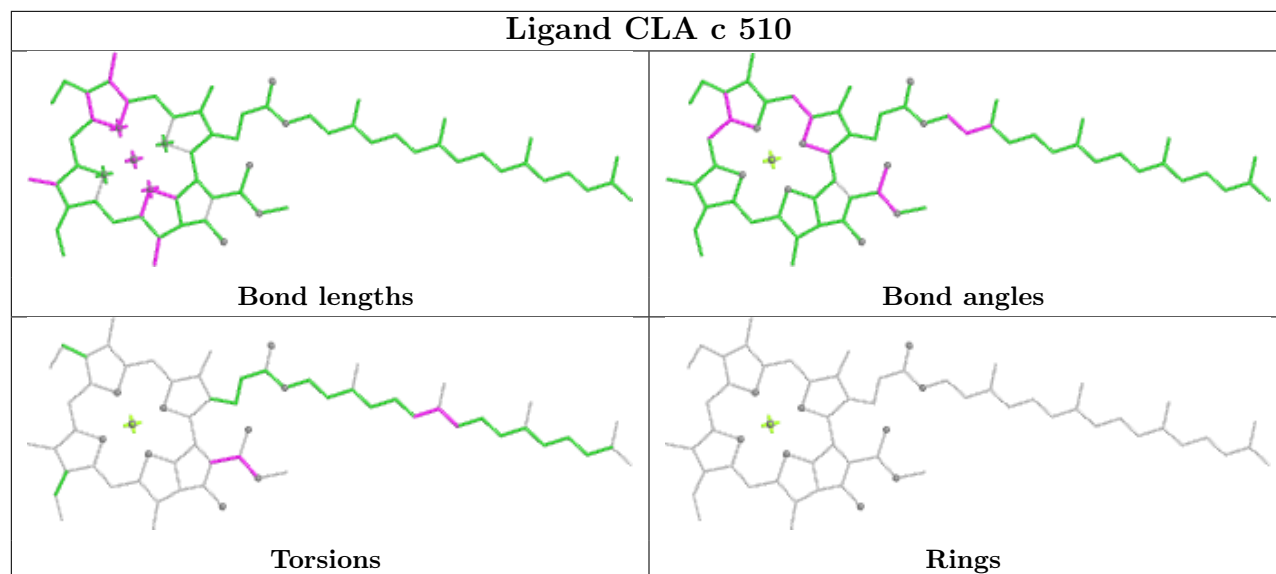
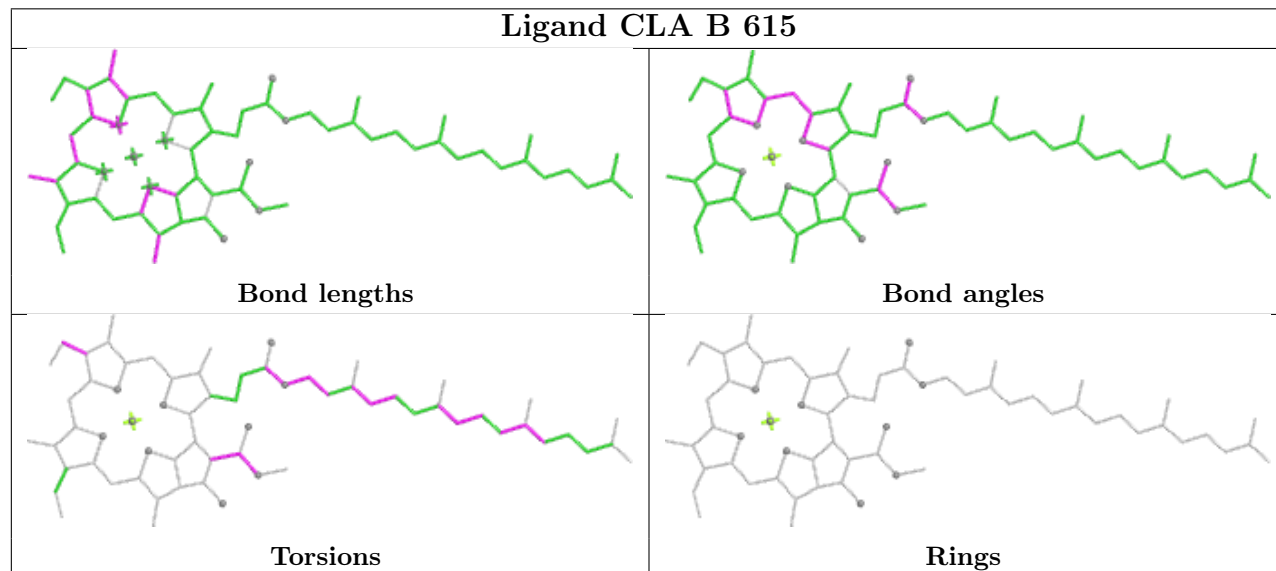
Bond angles

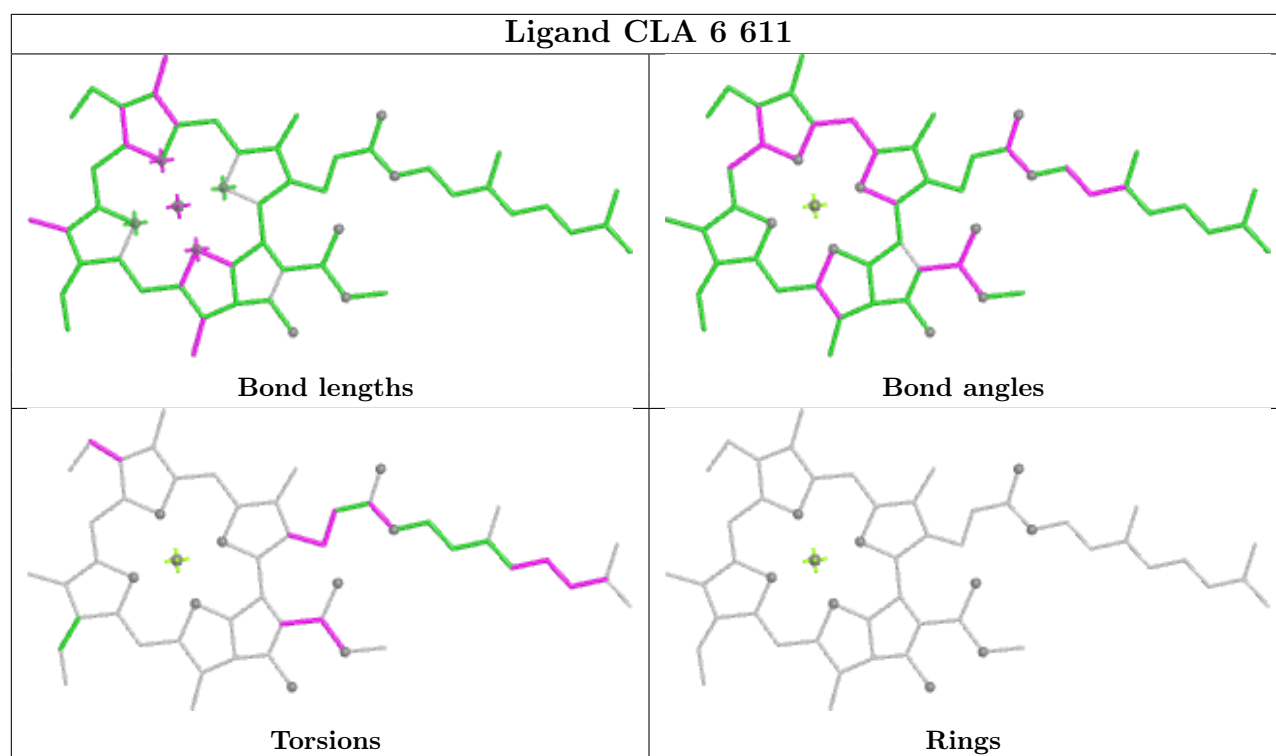


Torsions

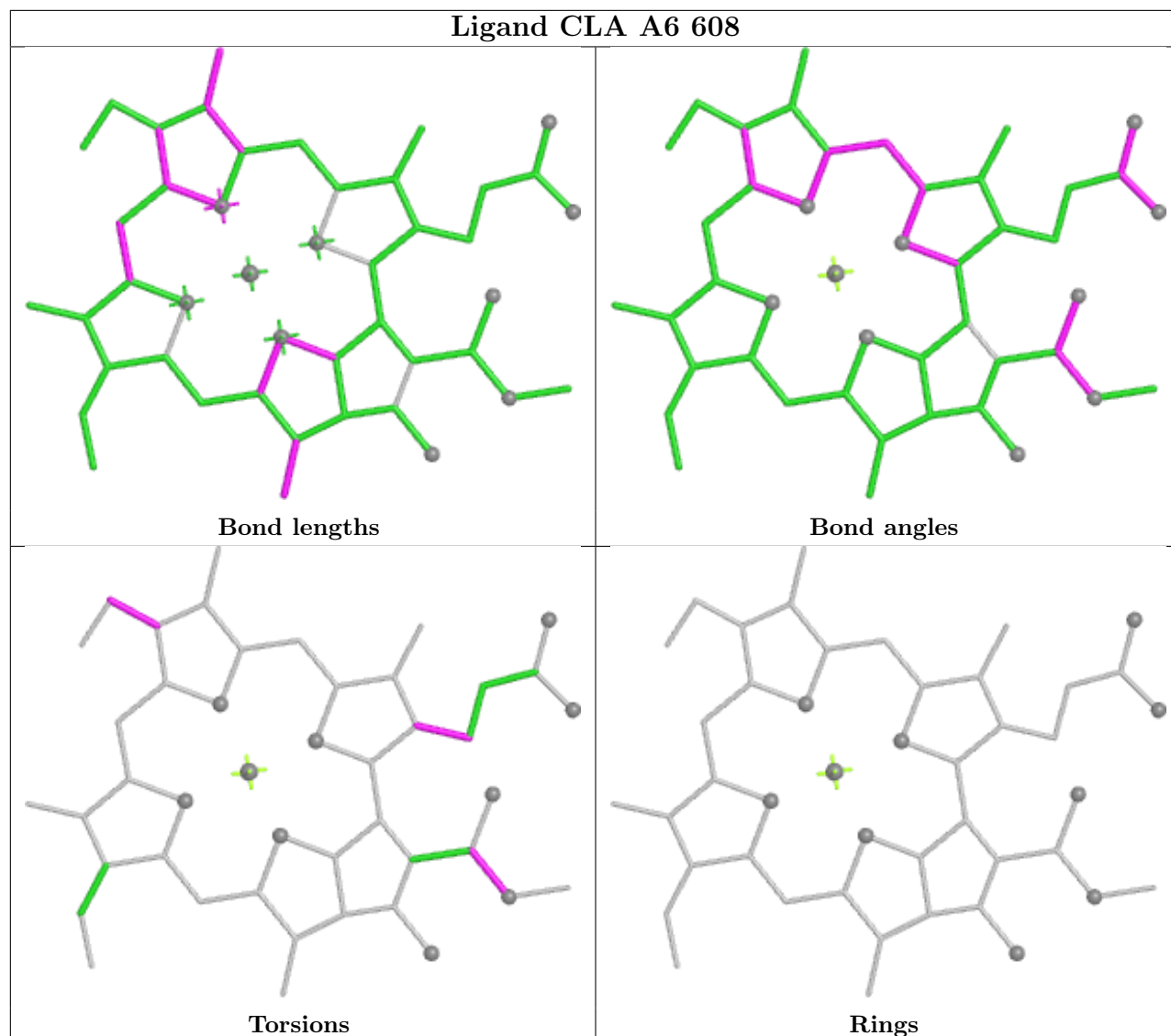


Rings

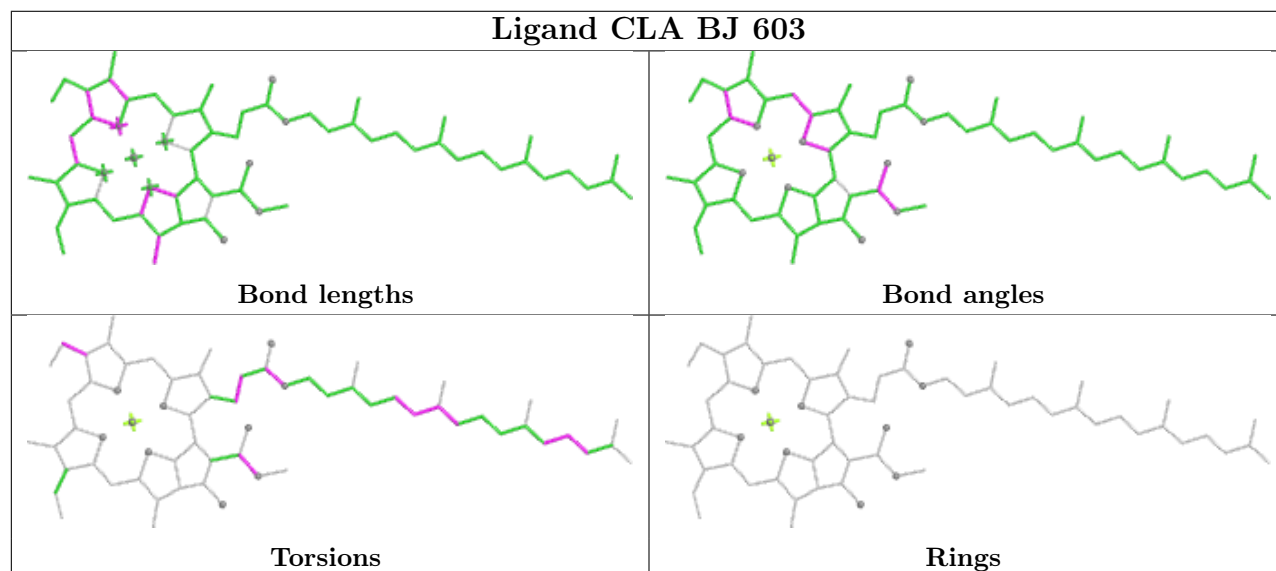
Ligand CLA c 510**Ligand CLA B 615**

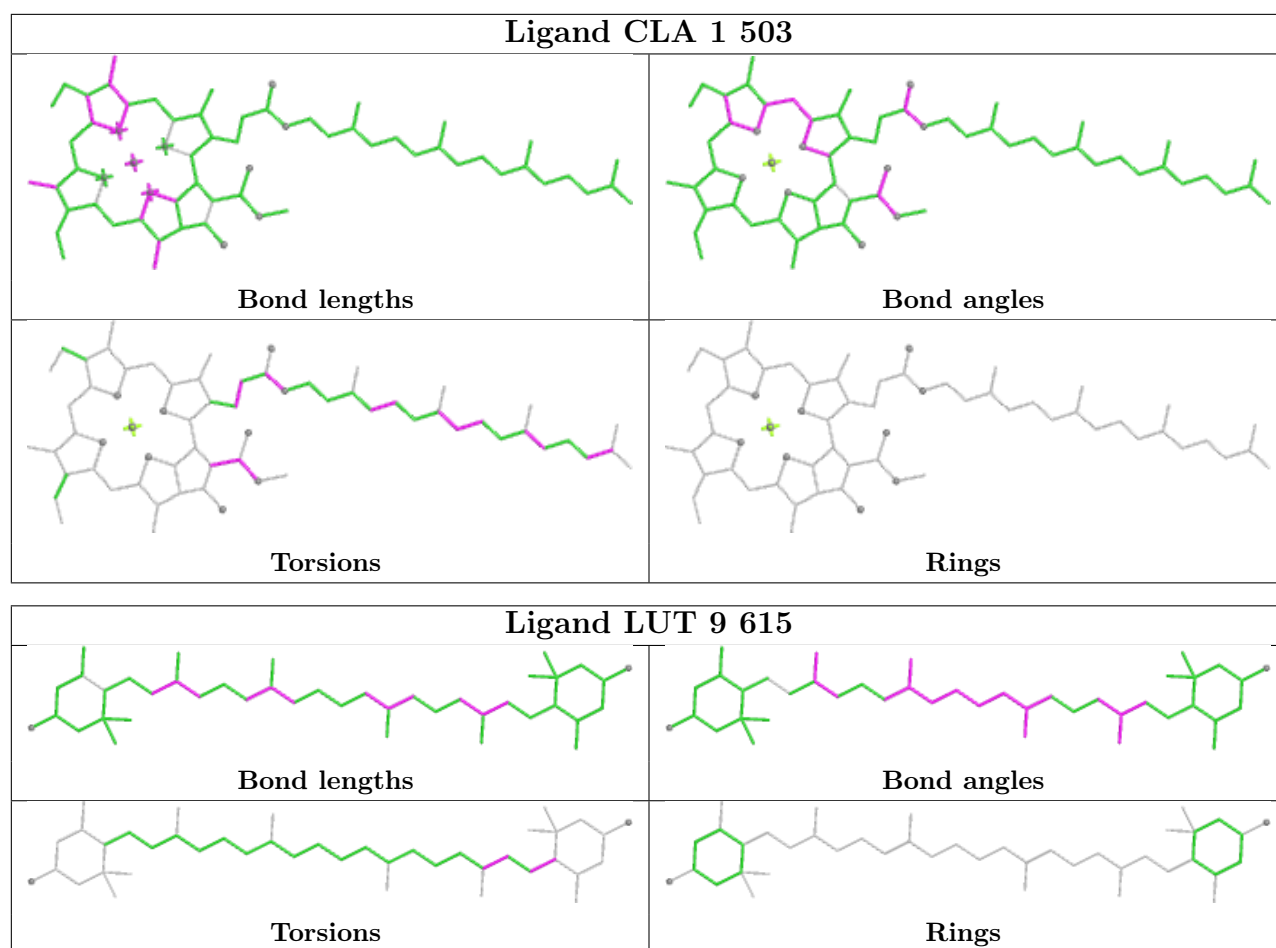


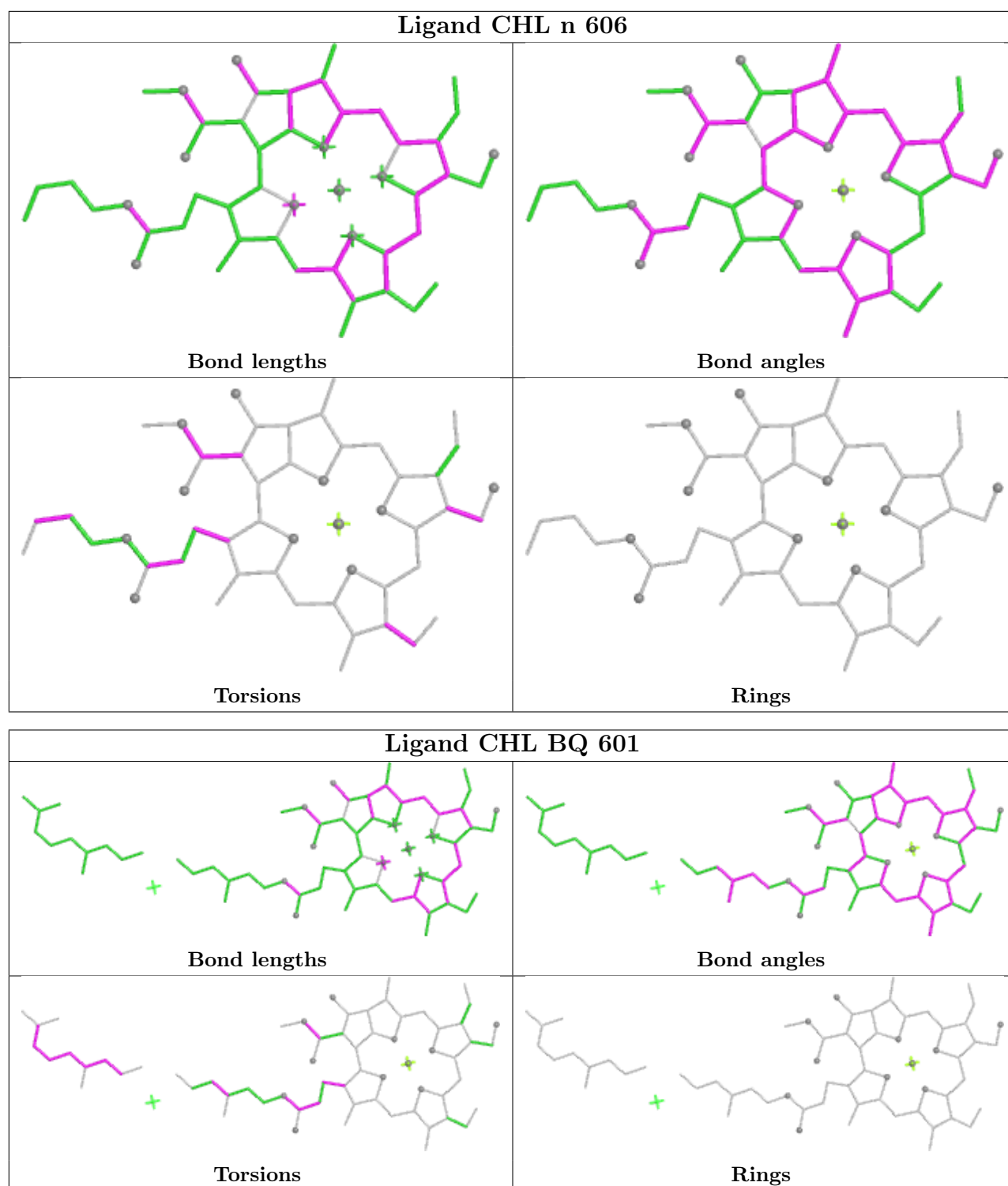
Ligand CLA A6 608

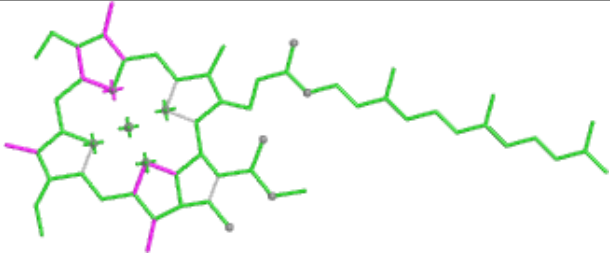
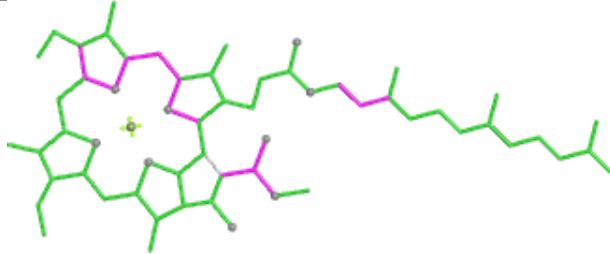
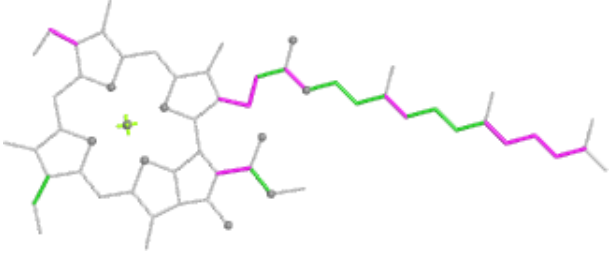
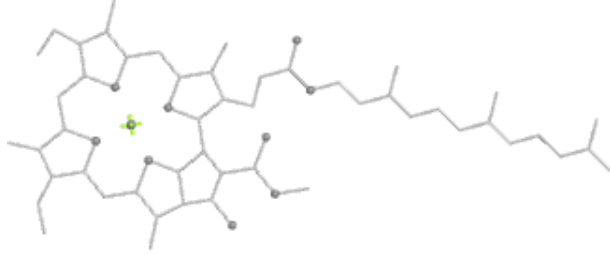
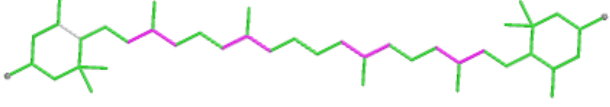
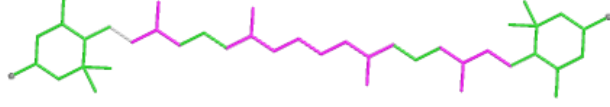
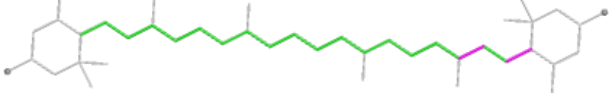
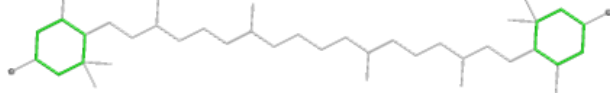
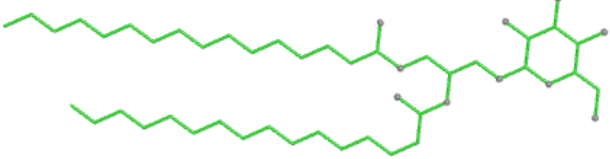
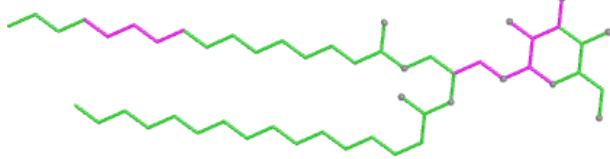
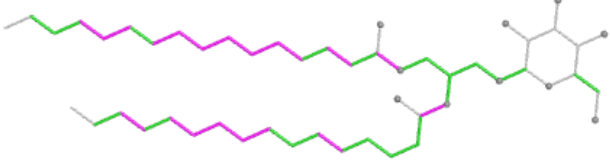
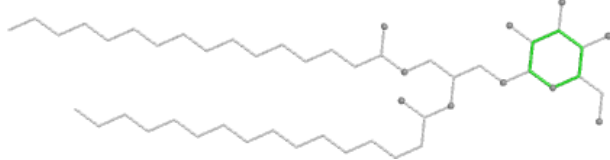


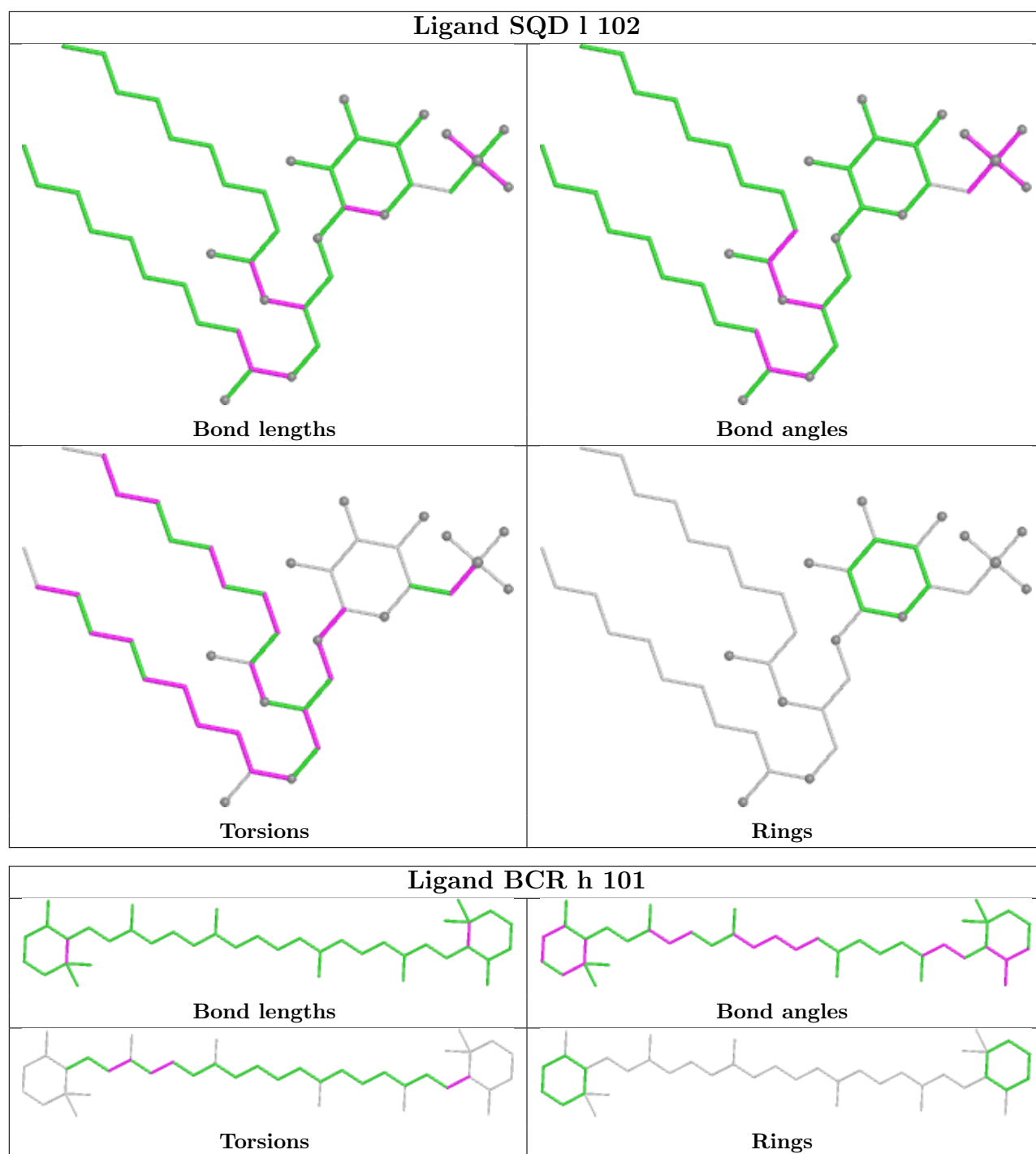
Ligand CLA BJ 603



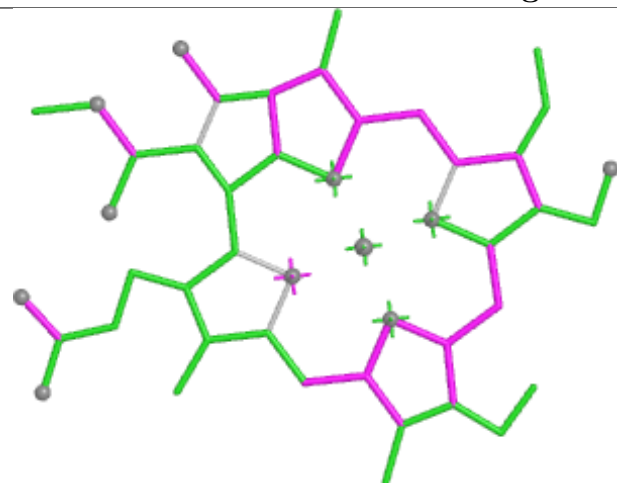




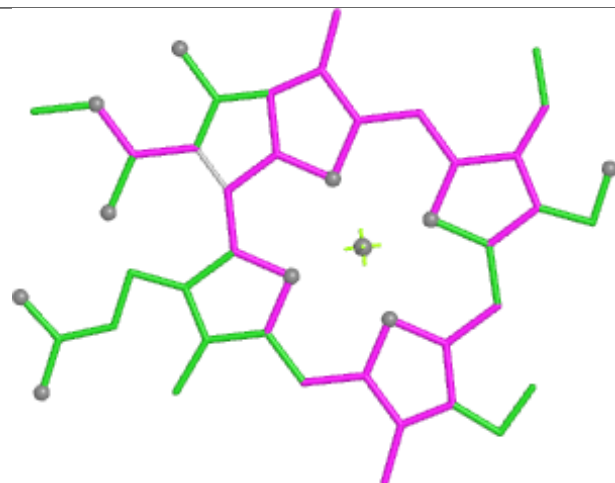
Ligand CLA N 611	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT BU 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG v 620	
 Bond lengths	 Bond angles
 Torsions	 Rings



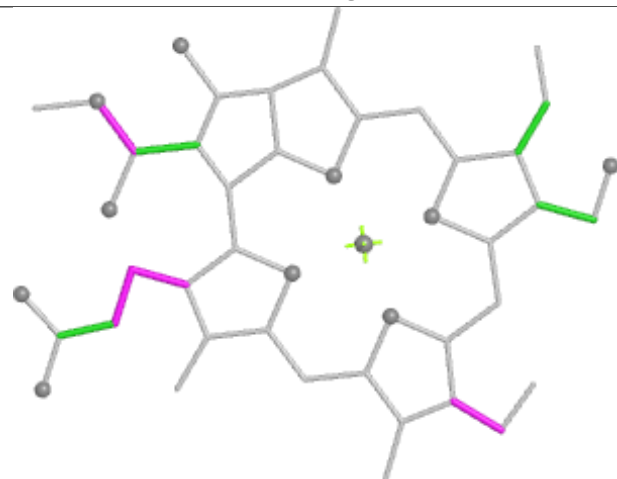
Ligand CHL 9 605



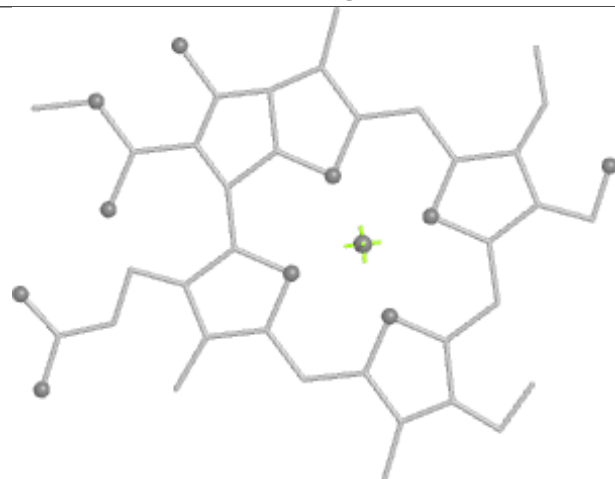
Bond lengths



Bond angles

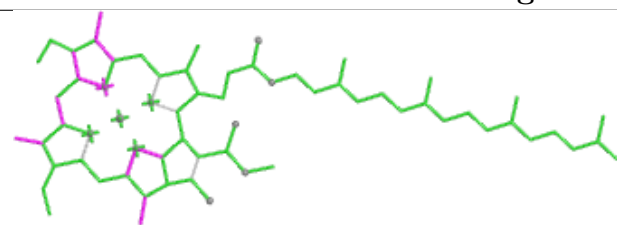


Torsions

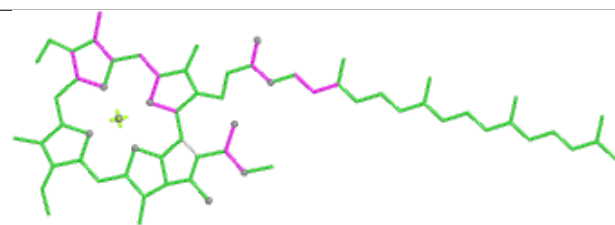


Rings

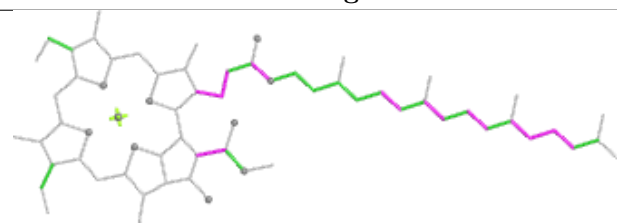
Ligand CLA G 602



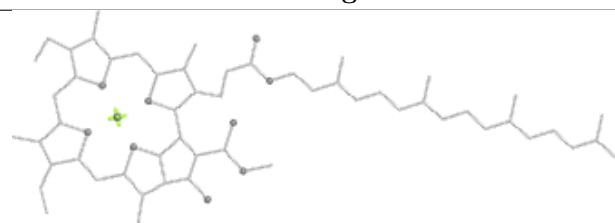
Bond lengths



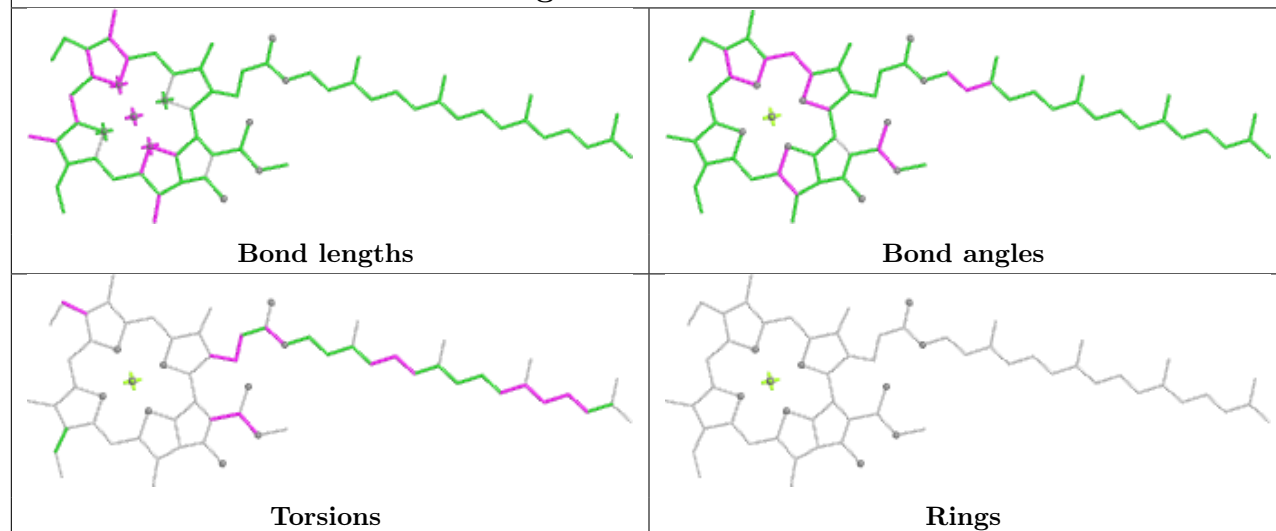
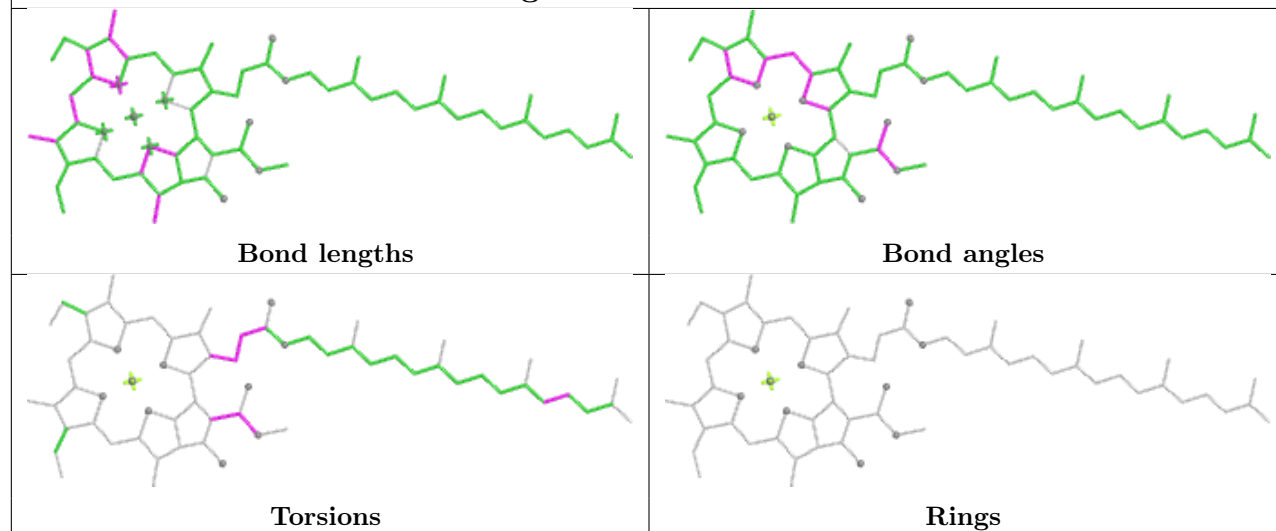
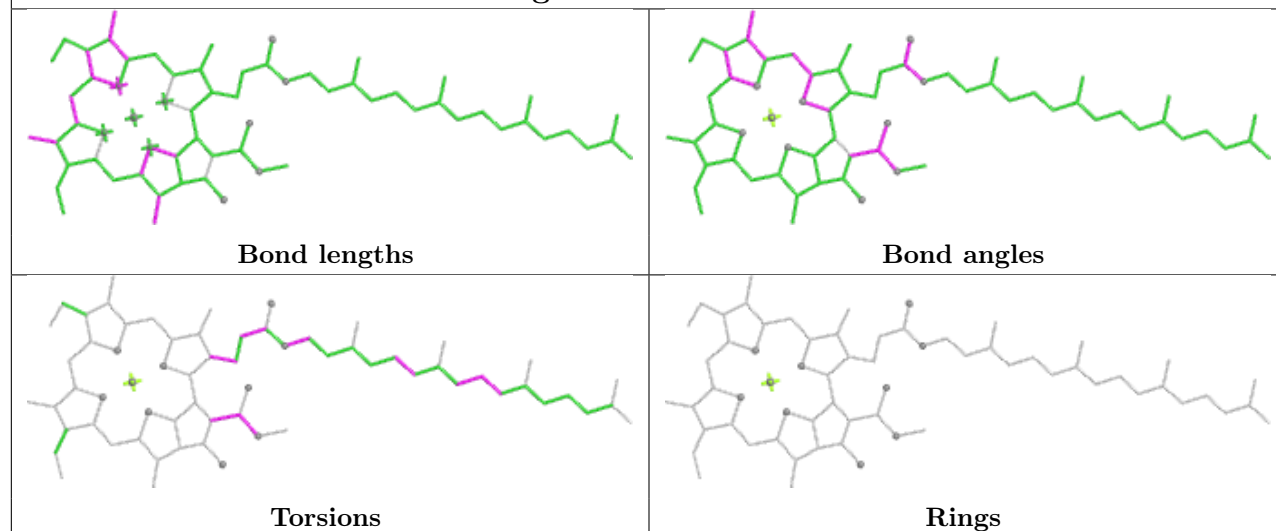
Bond angles

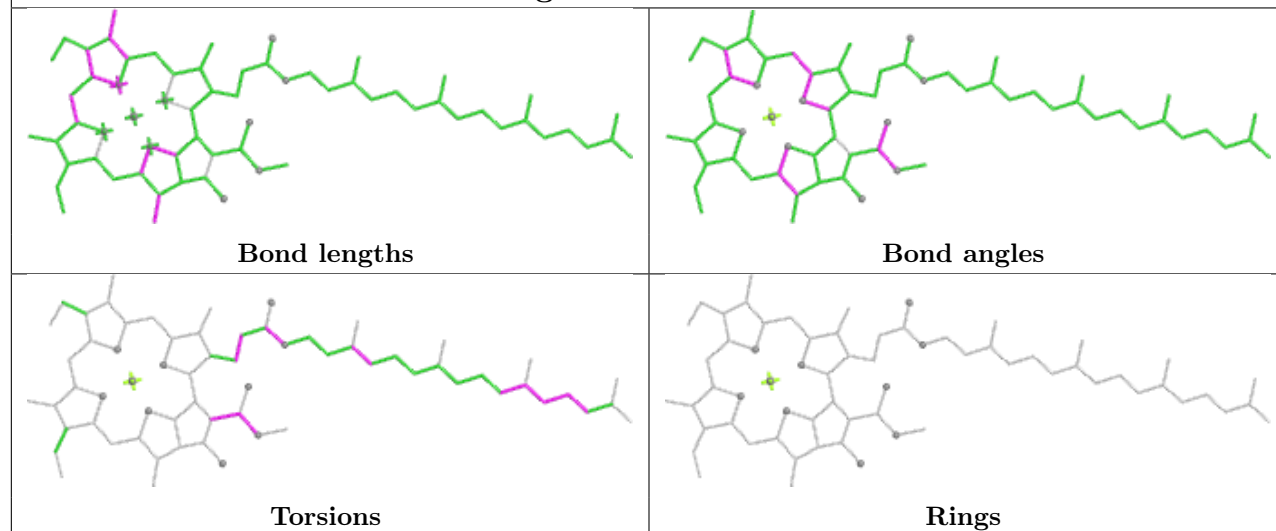
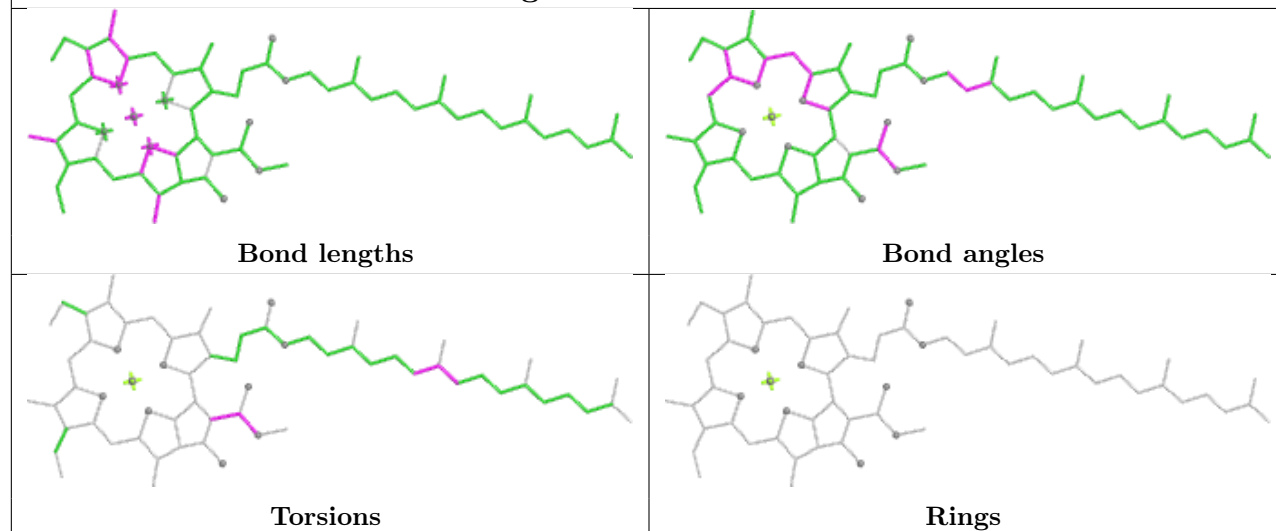


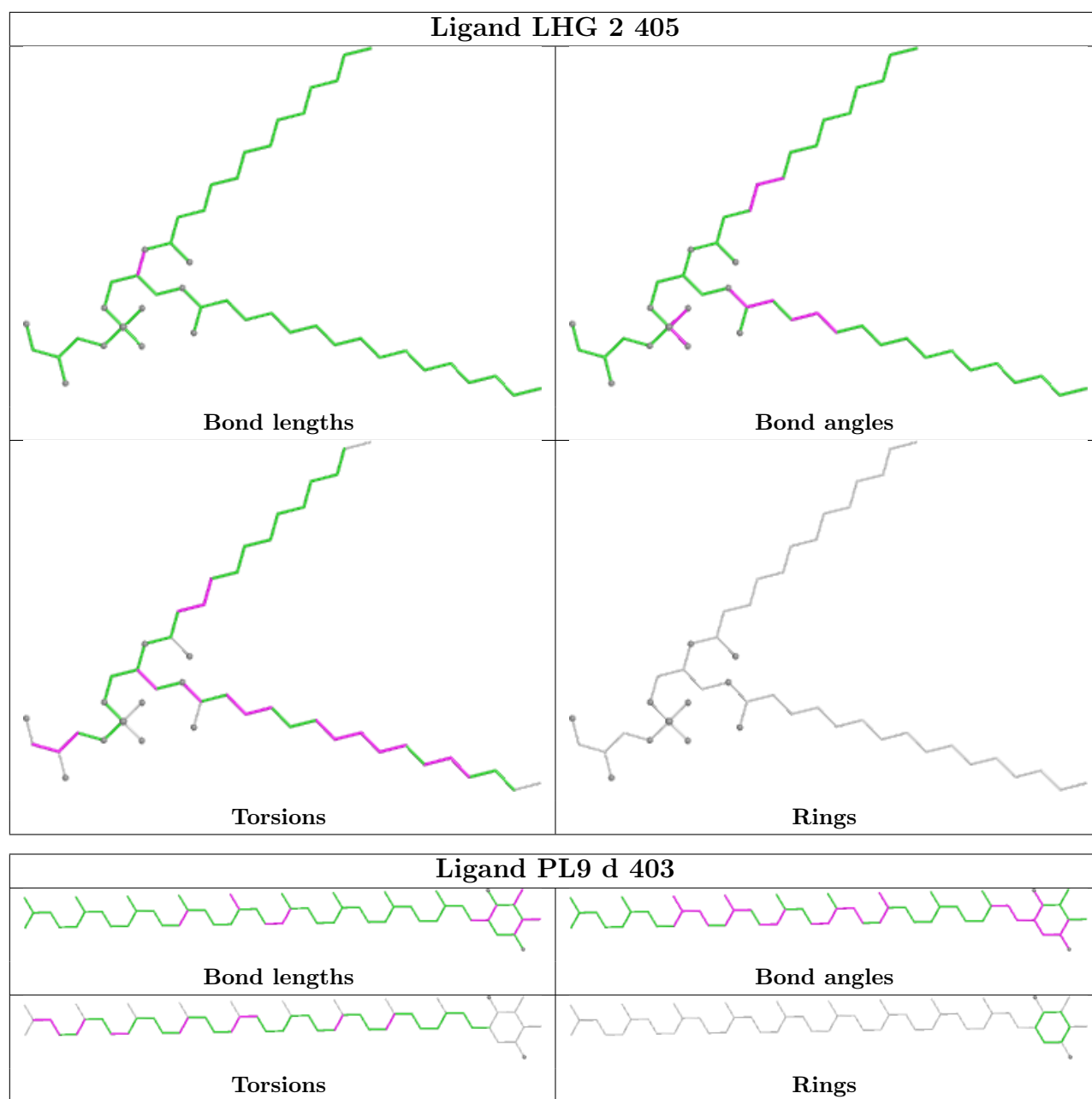
Torsions



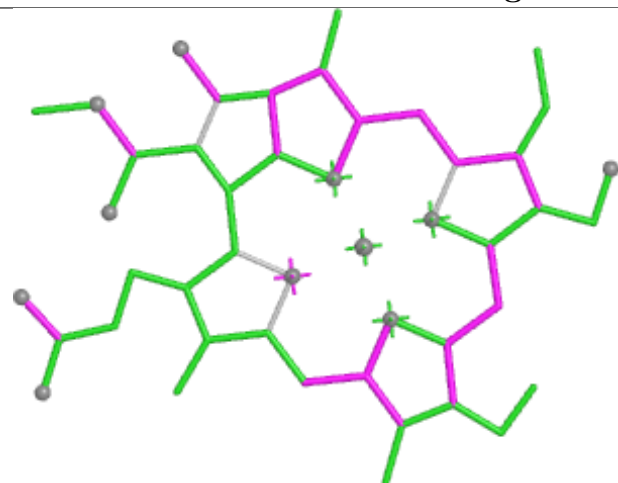
Rings

Ligand CLA 1 506**Ligand CLA BF 505****Ligand CLA B 611**

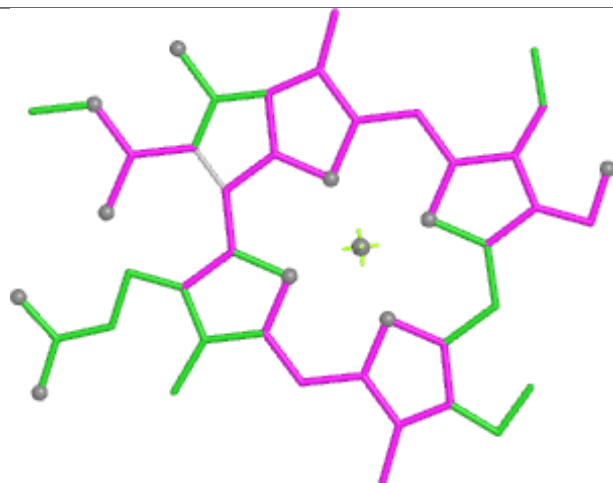
Ligand CLA v 603**Ligand CLA BF 510**



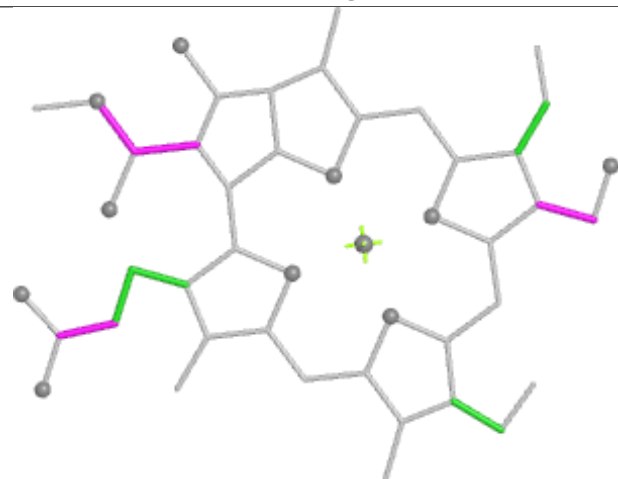
Ligand CHL BV 605



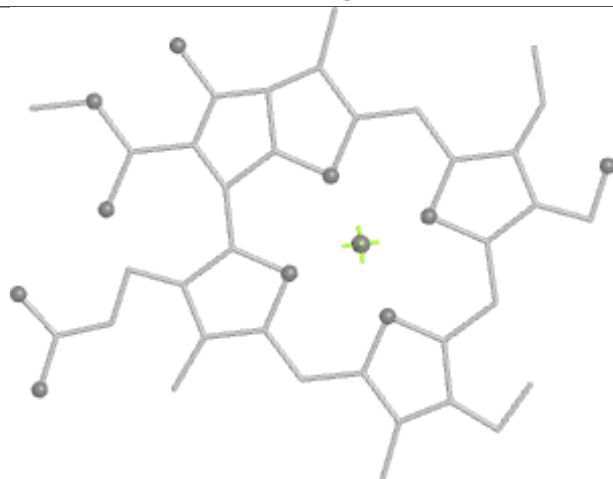
Bond lengths



Bond angles

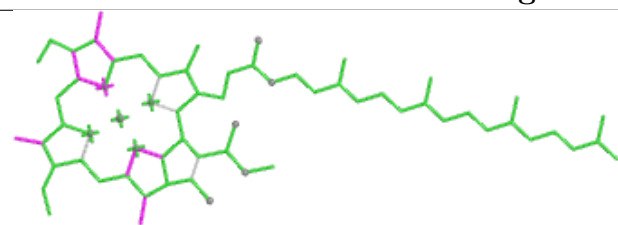


Torsions

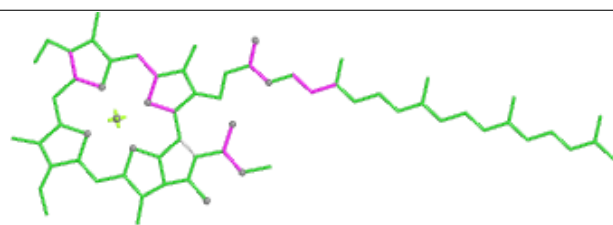


Rings

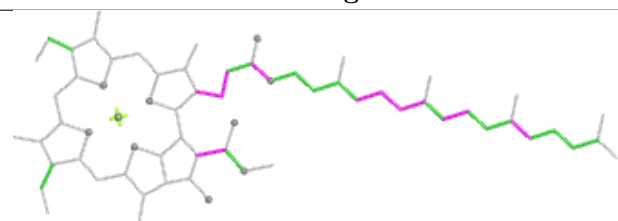
Ligand CLA B 604



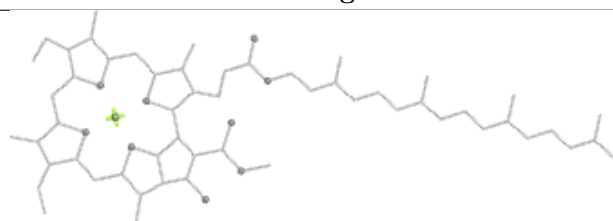
Bond lengths



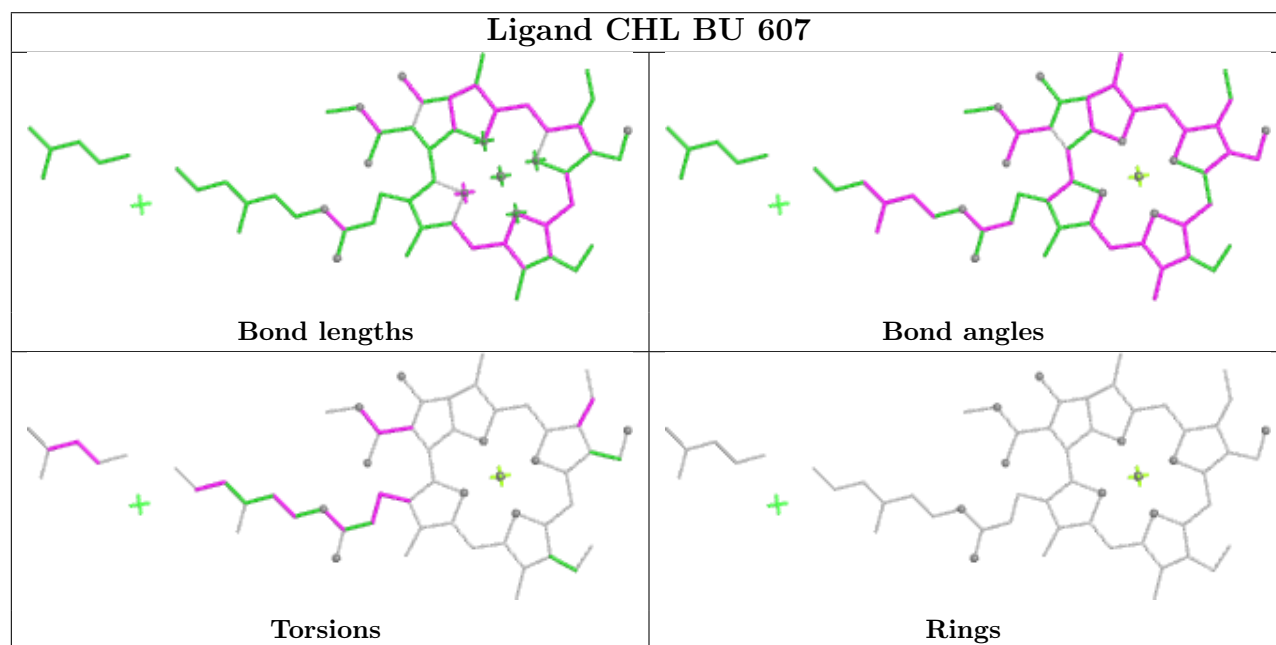
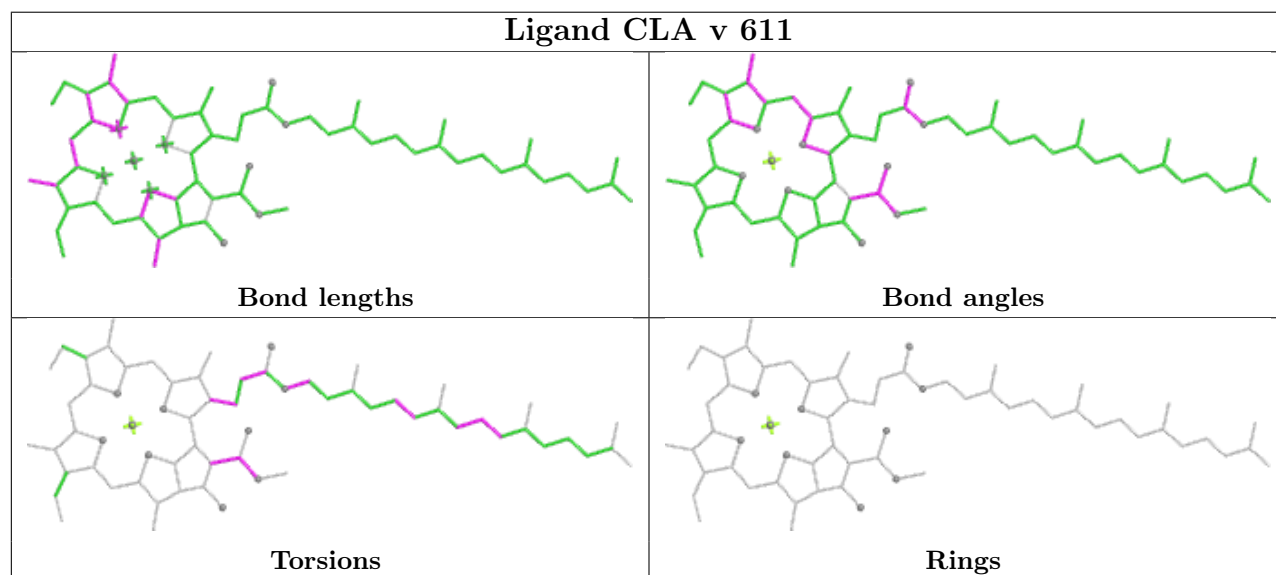
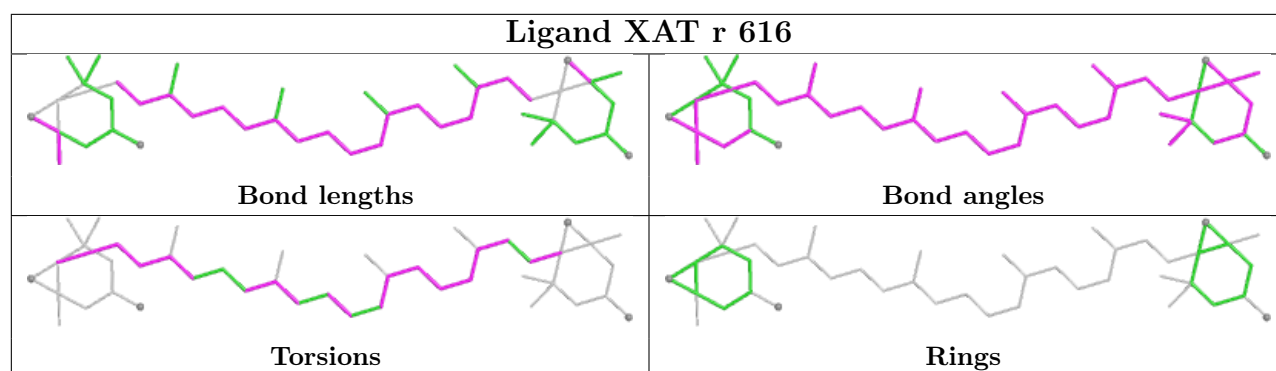
Bond angles

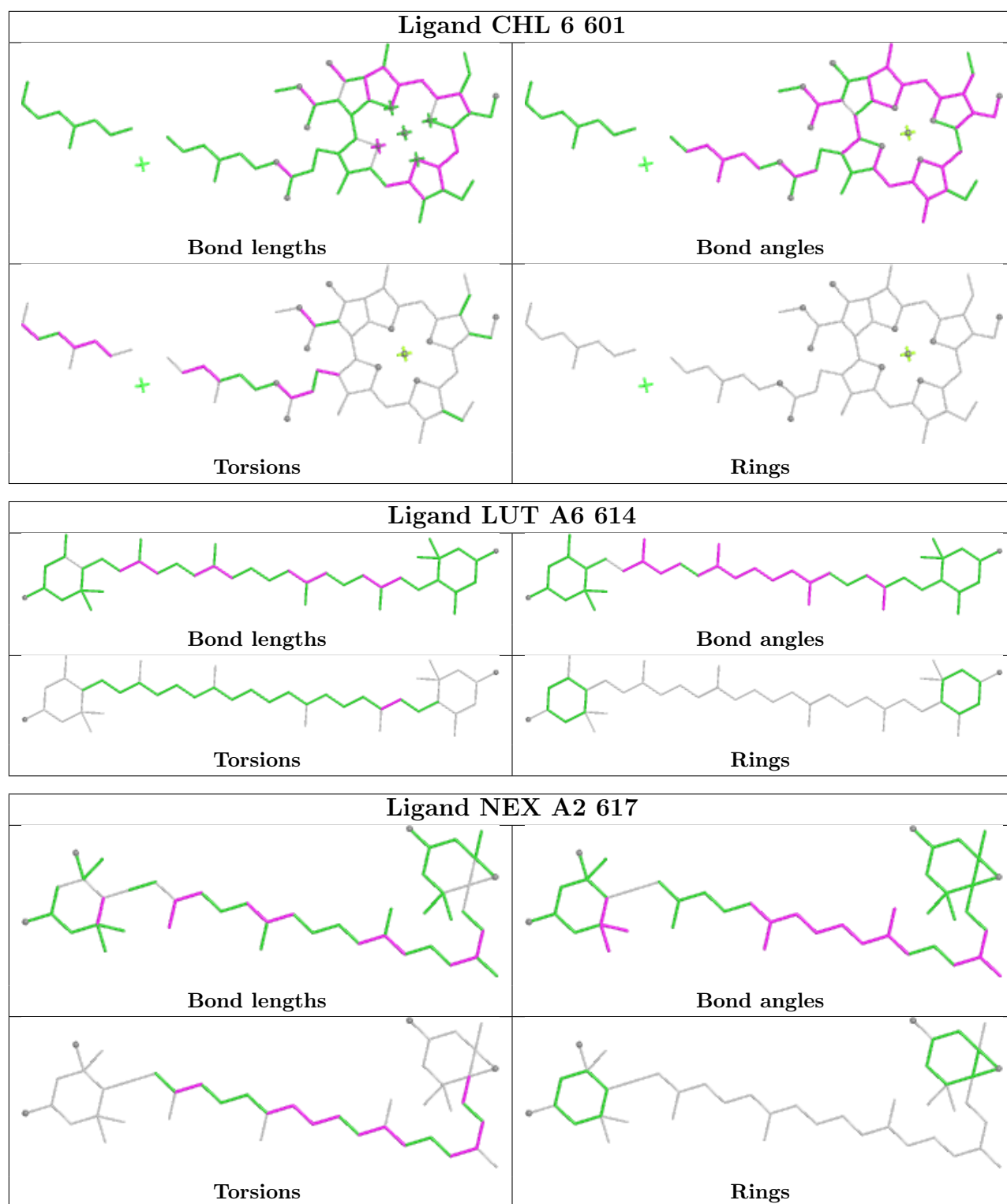


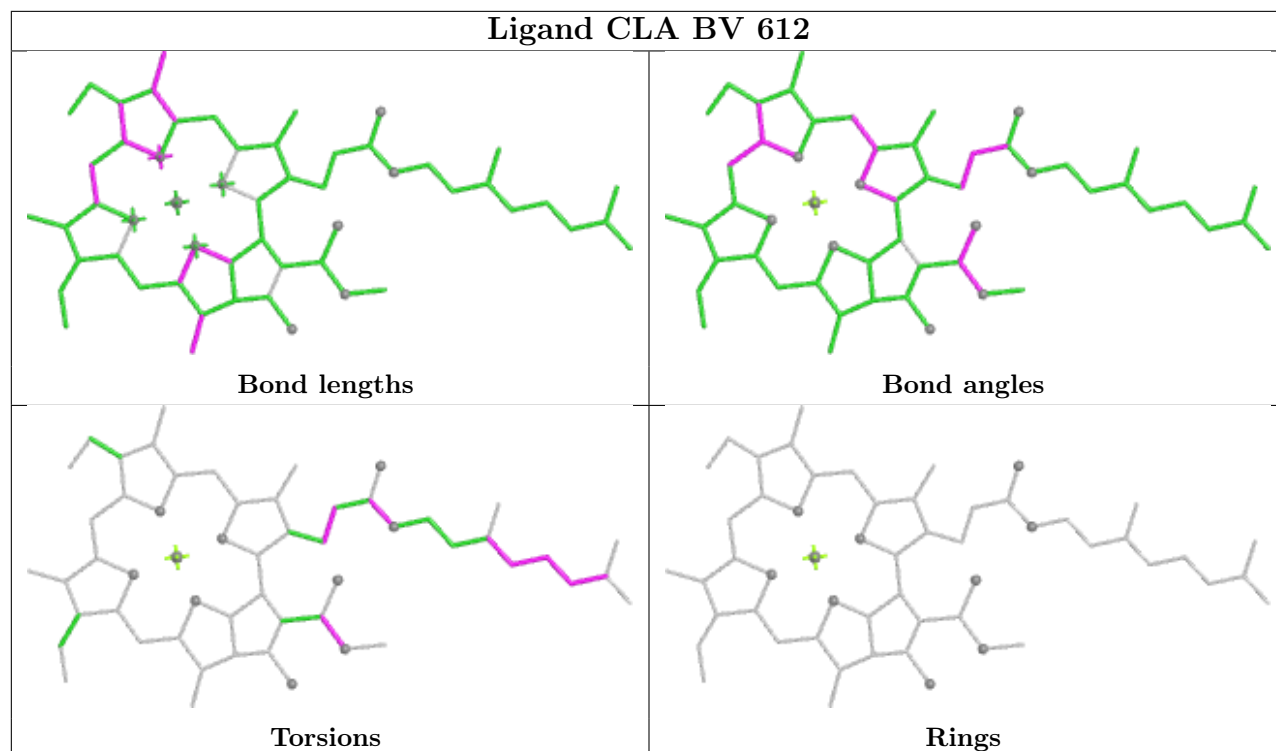
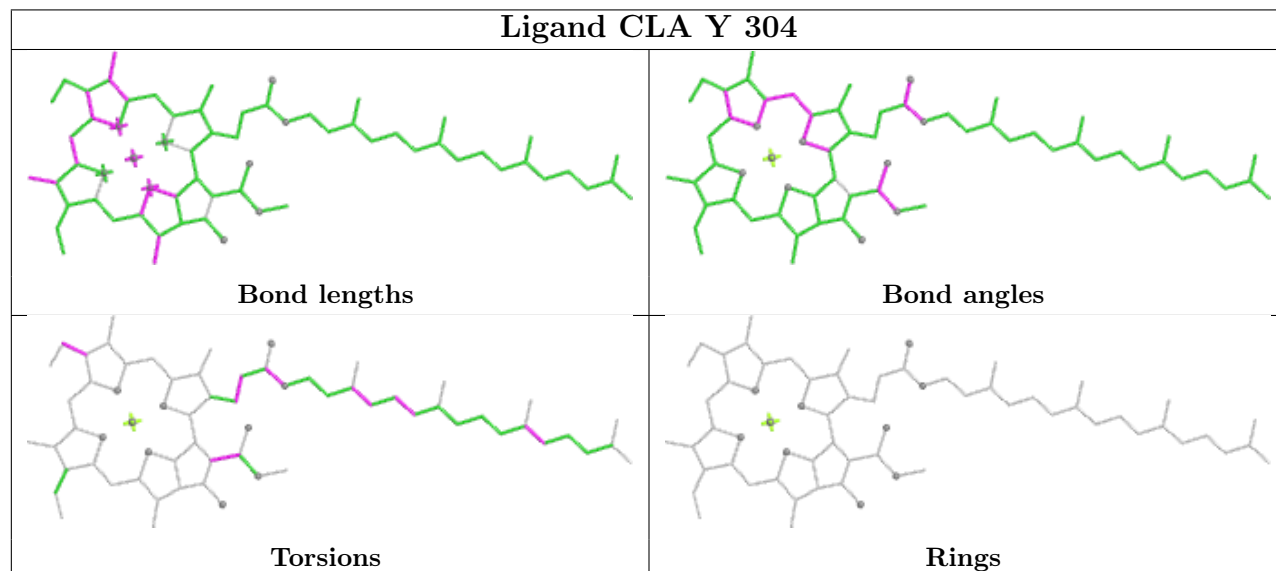
Torsions

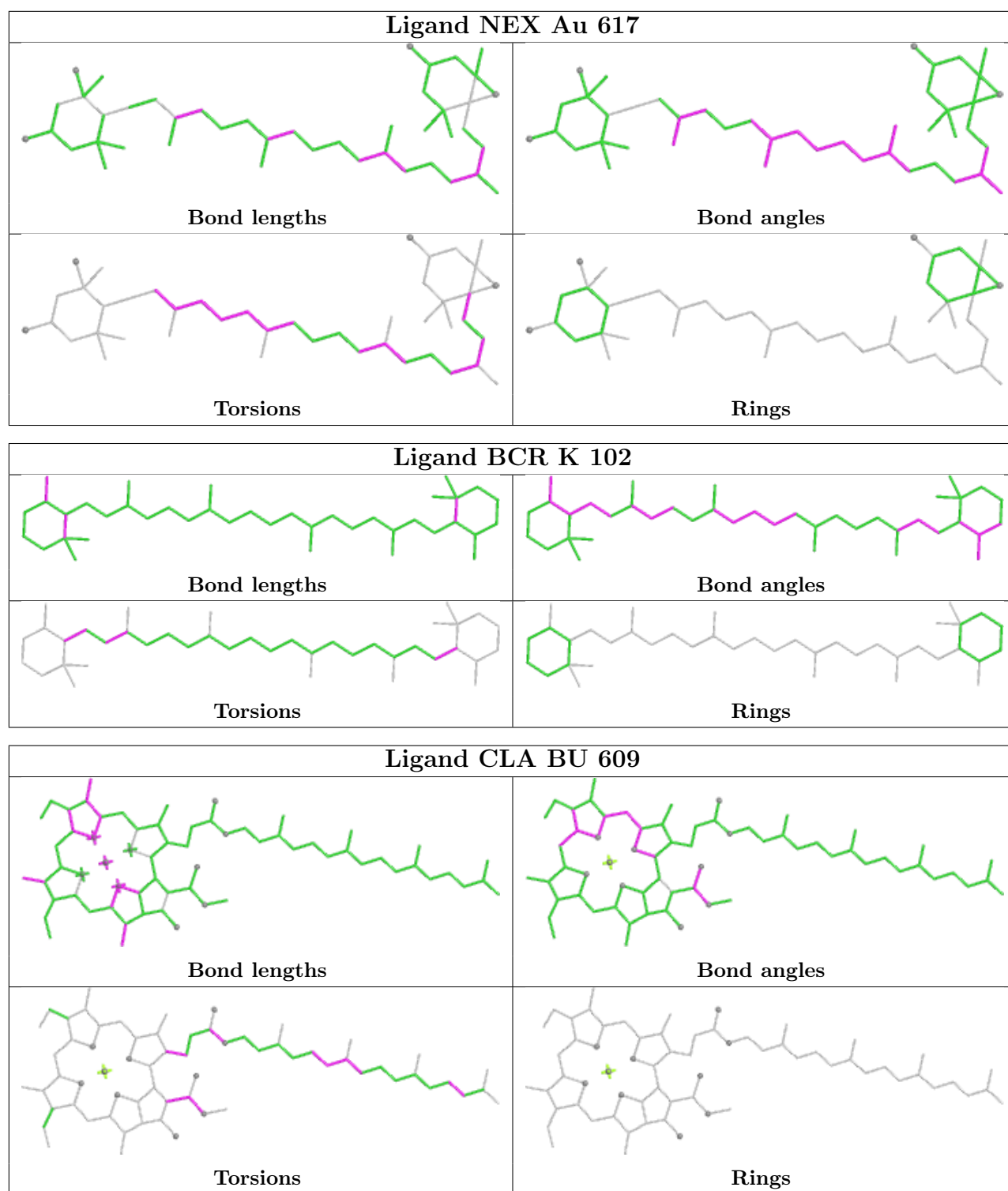


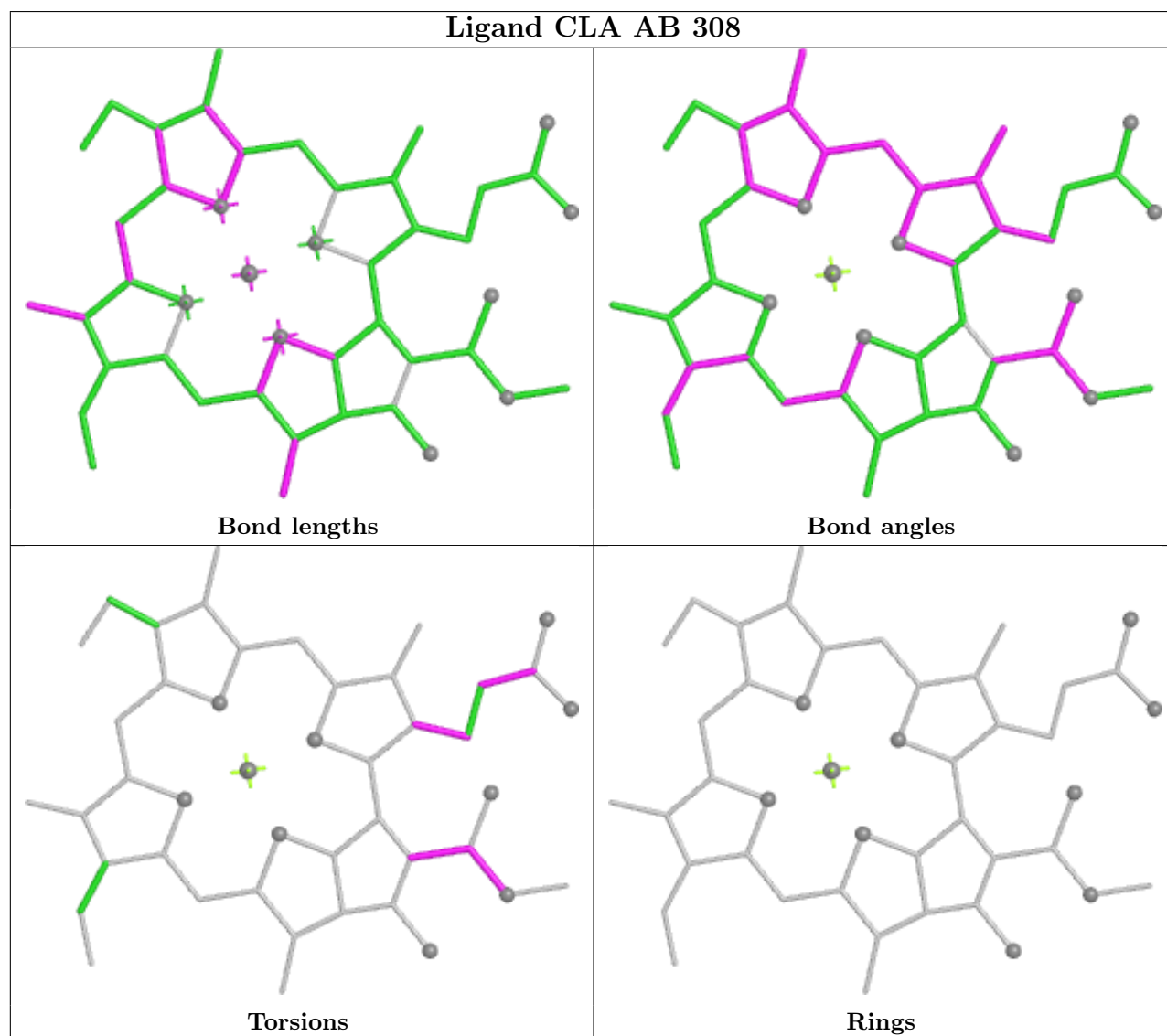
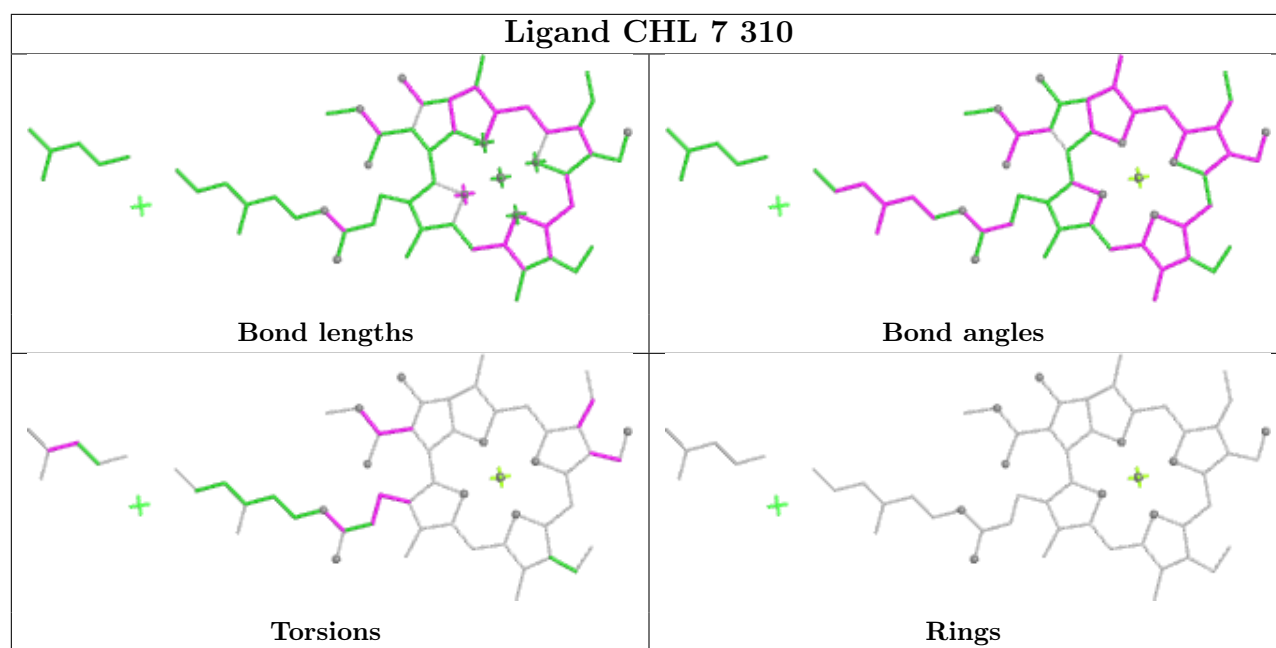
Rings

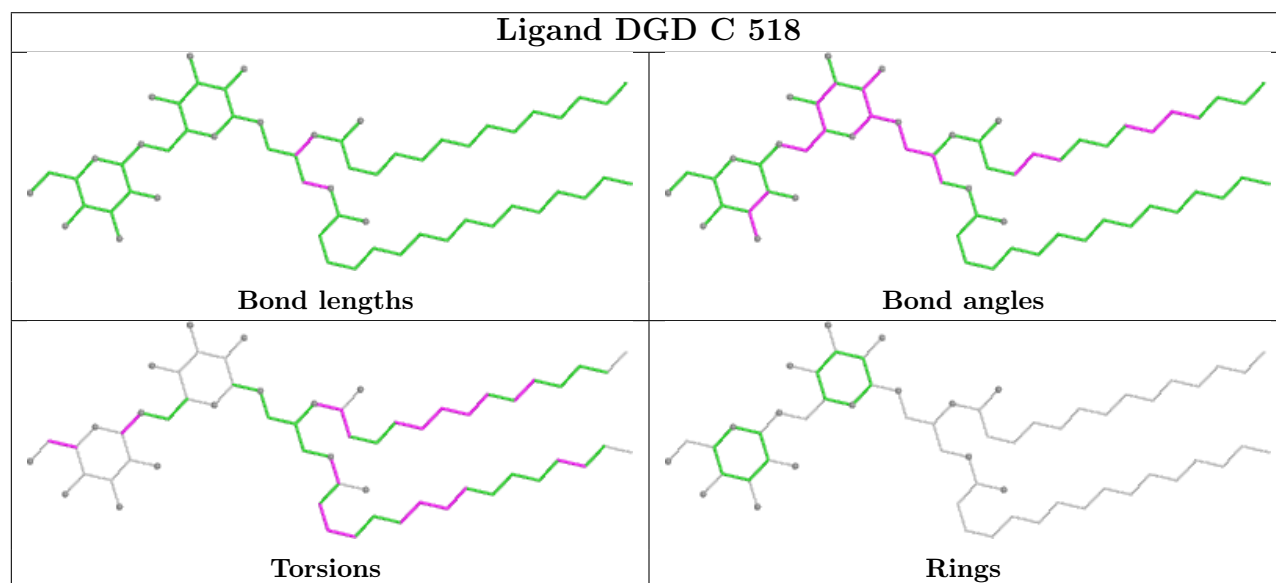
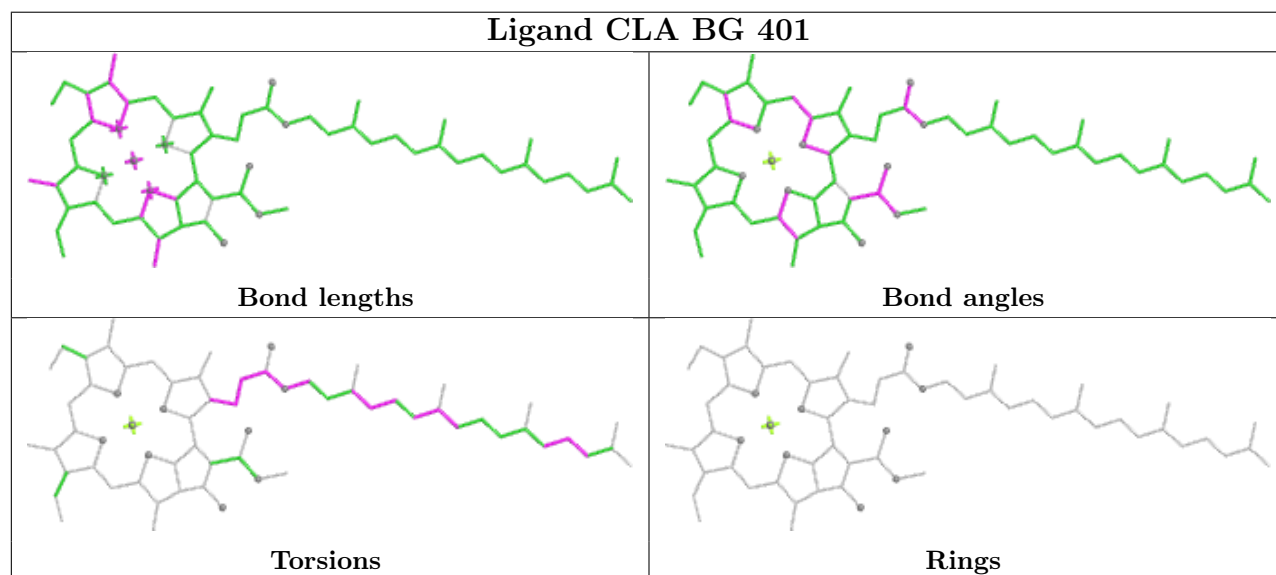
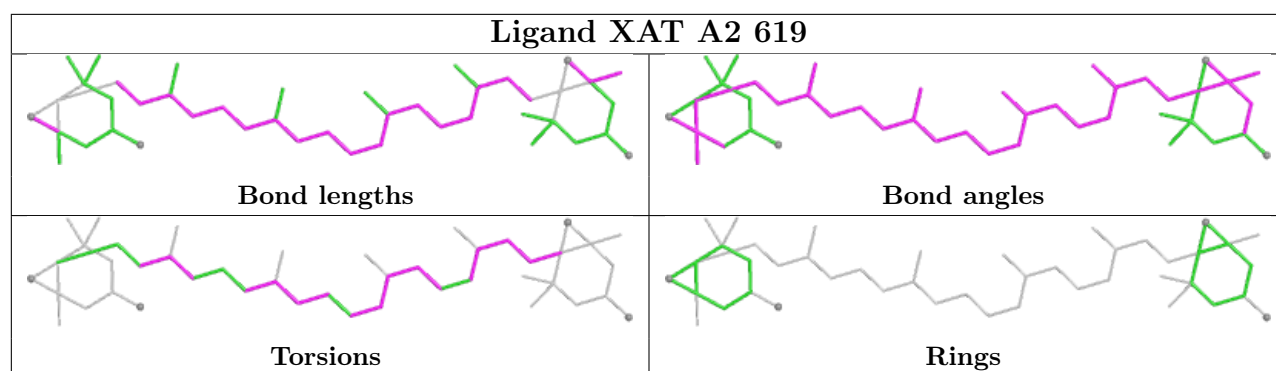


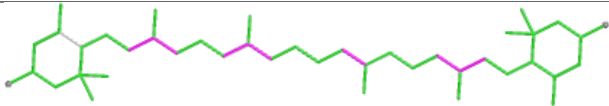
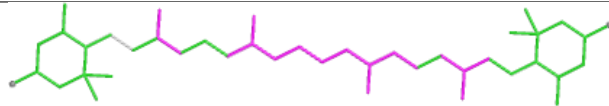
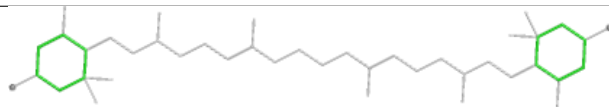


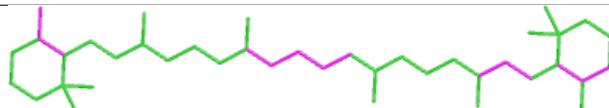
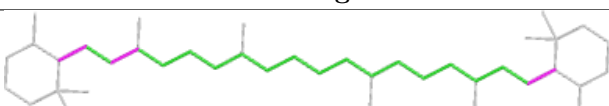
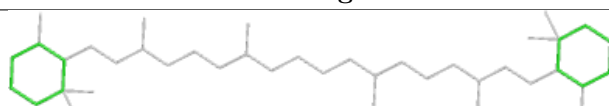
Ligand CLA BV 612**Ligand CLA Y 304**

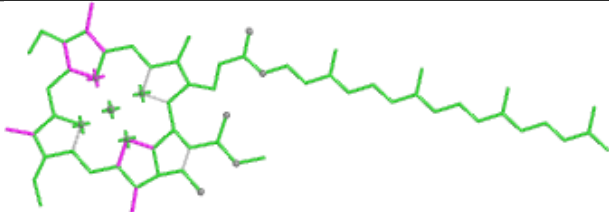
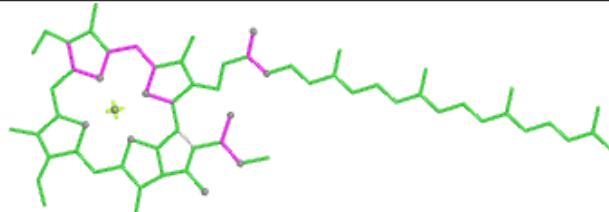
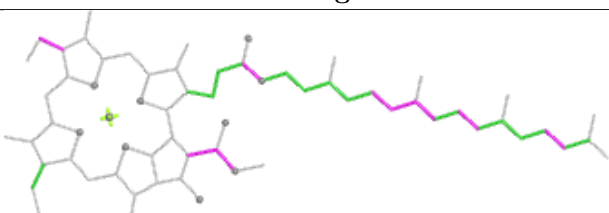
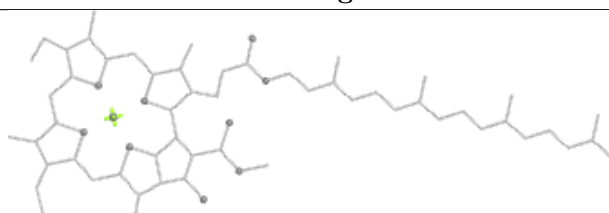


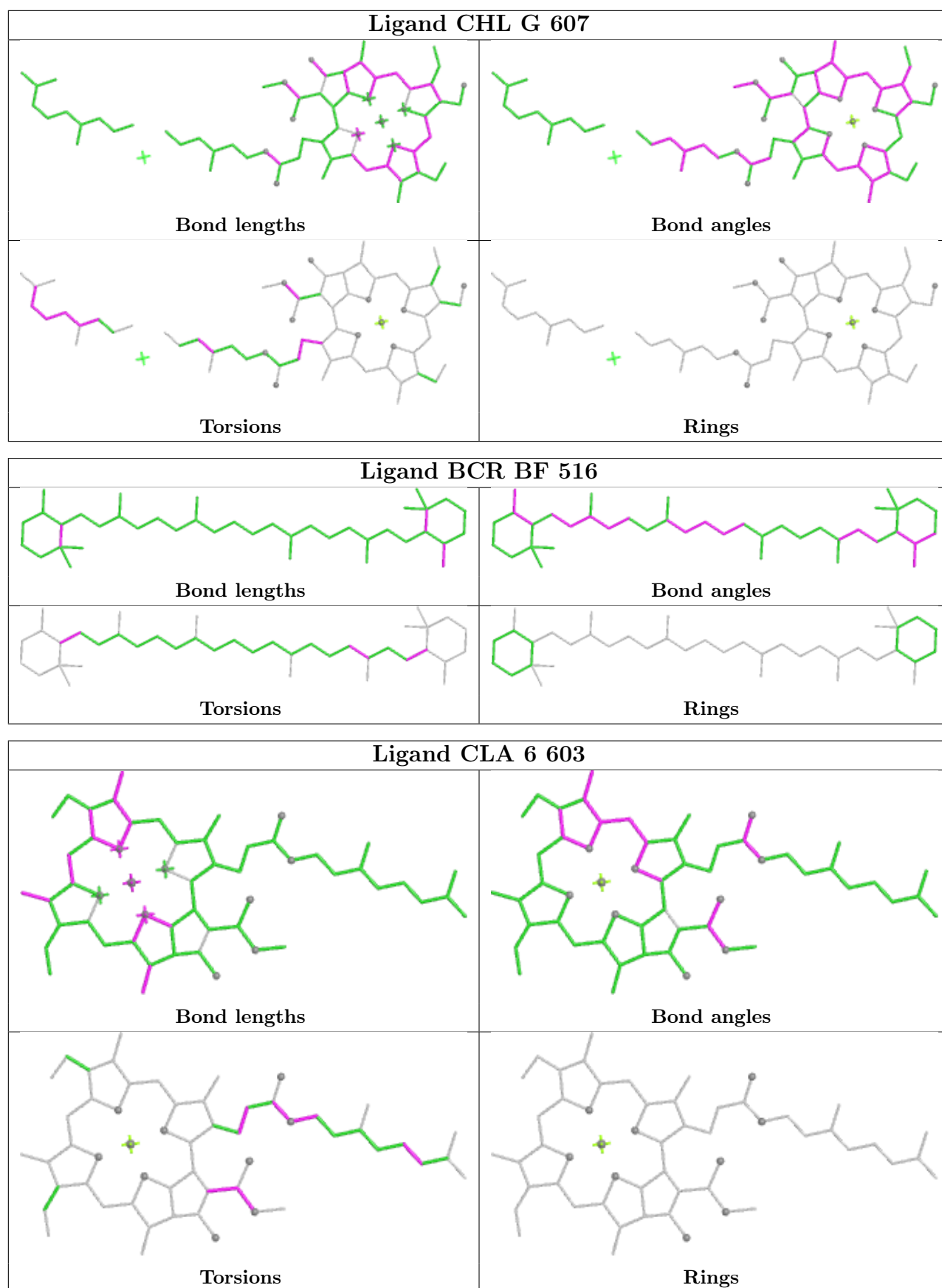


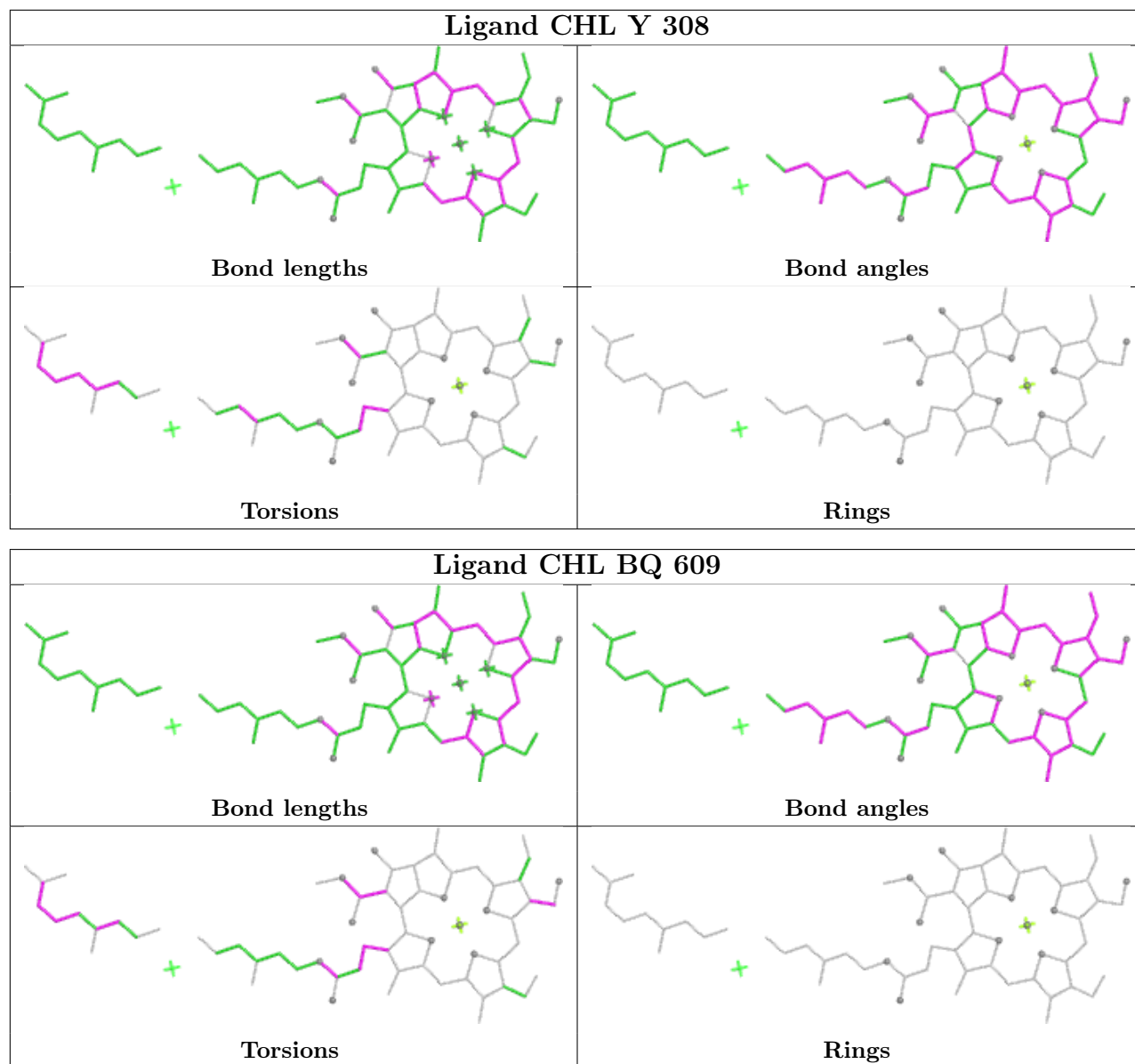


Ligand LUT BJ 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

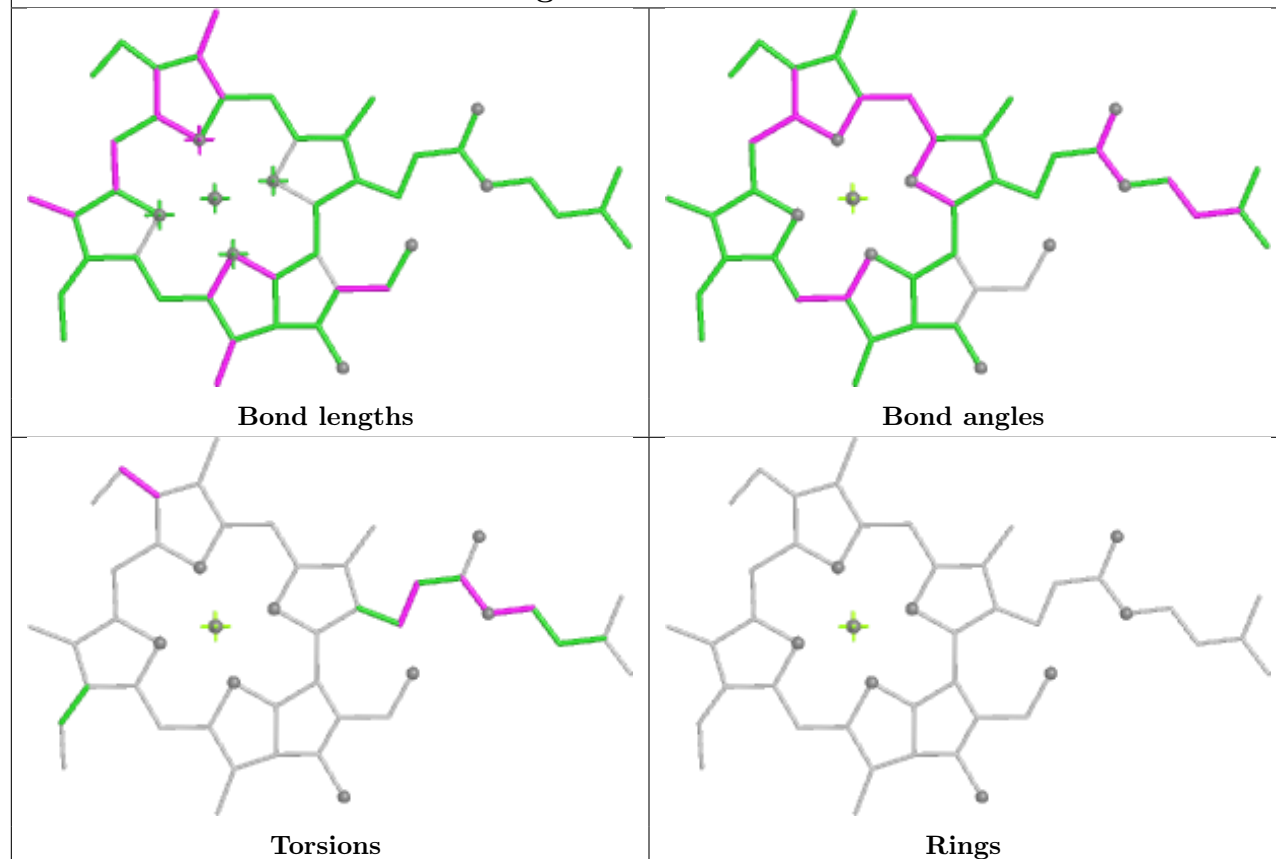
Ligand BCR a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

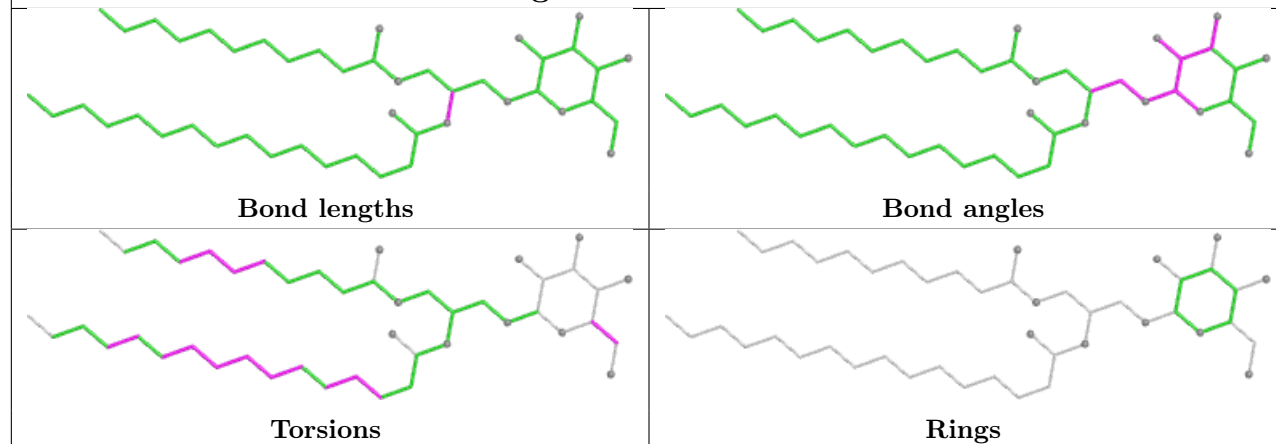




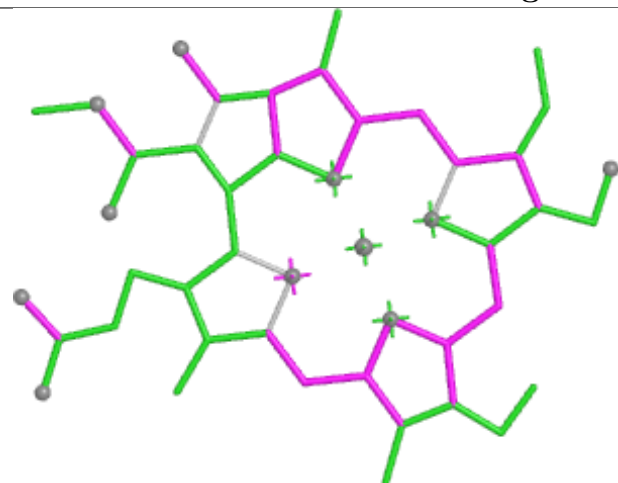
Ligand CLA 7 311



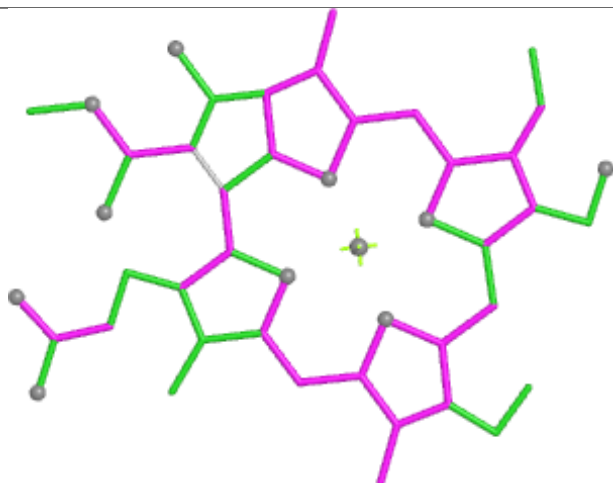
Ligand LMG 2 407



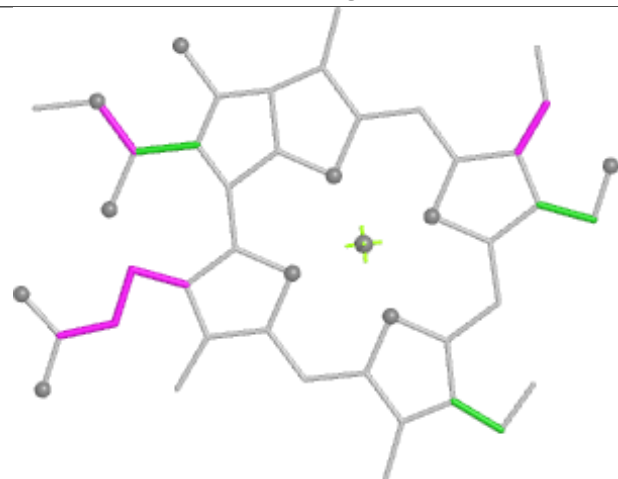
Ligand CHL 5 601



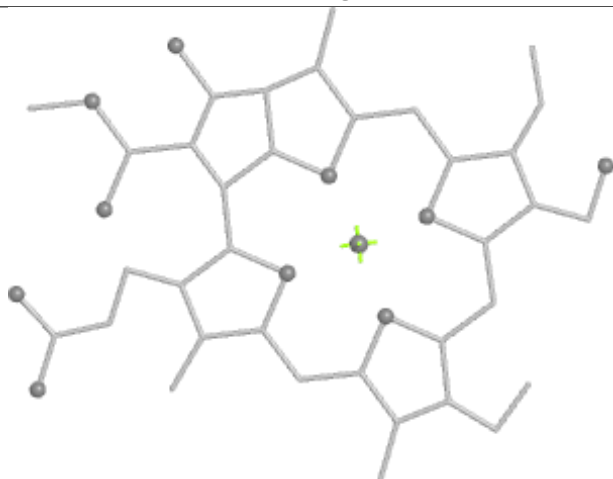
Bond lengths



Bond angles

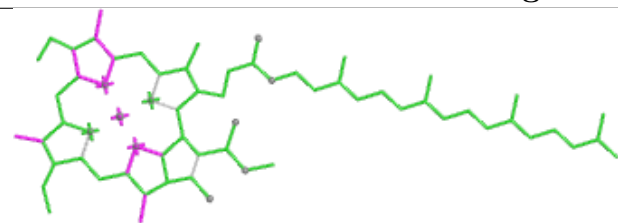


Torsions

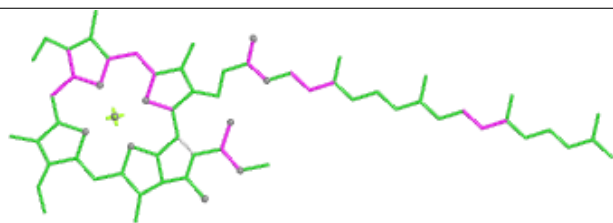


Rings

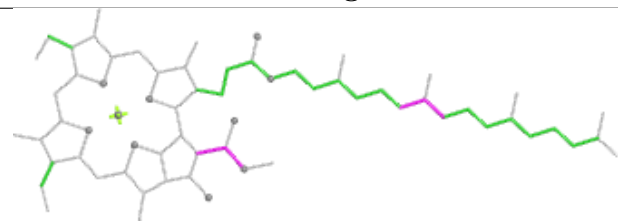
Ligand CLA 1 509



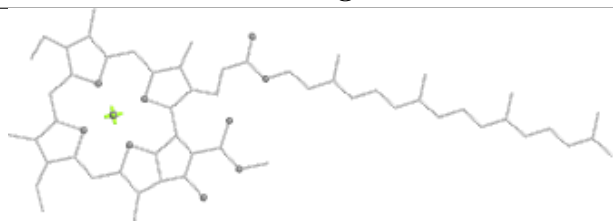
Bond lengths



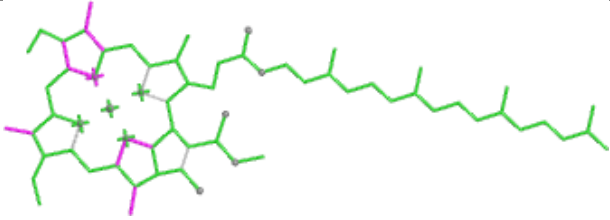
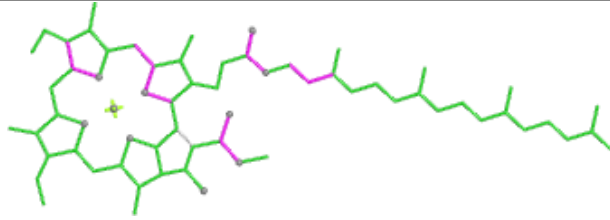
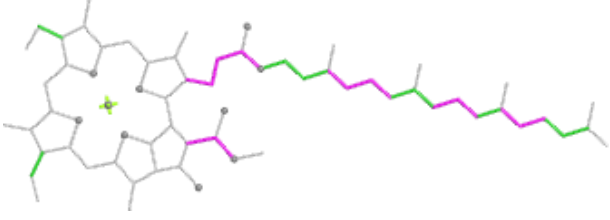
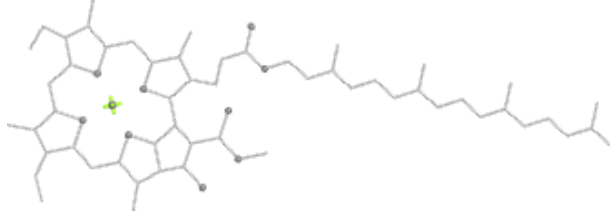
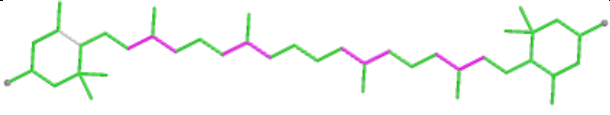
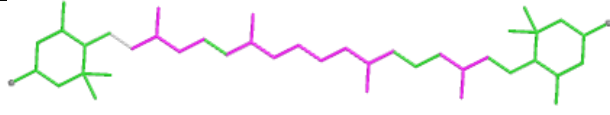
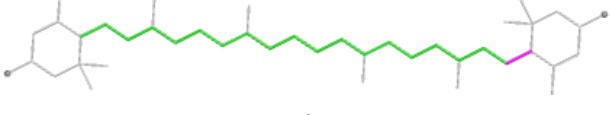
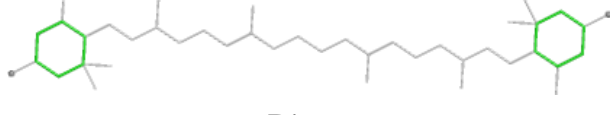
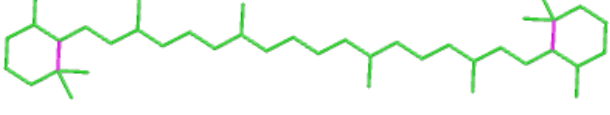
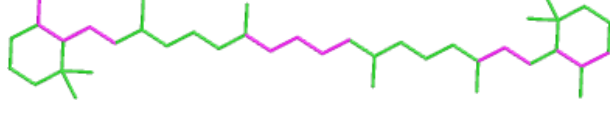
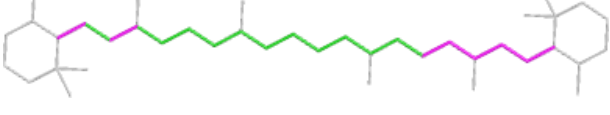
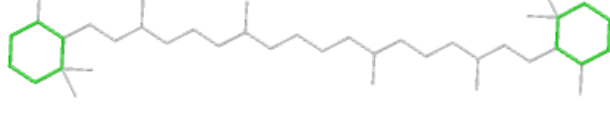
Bond angles

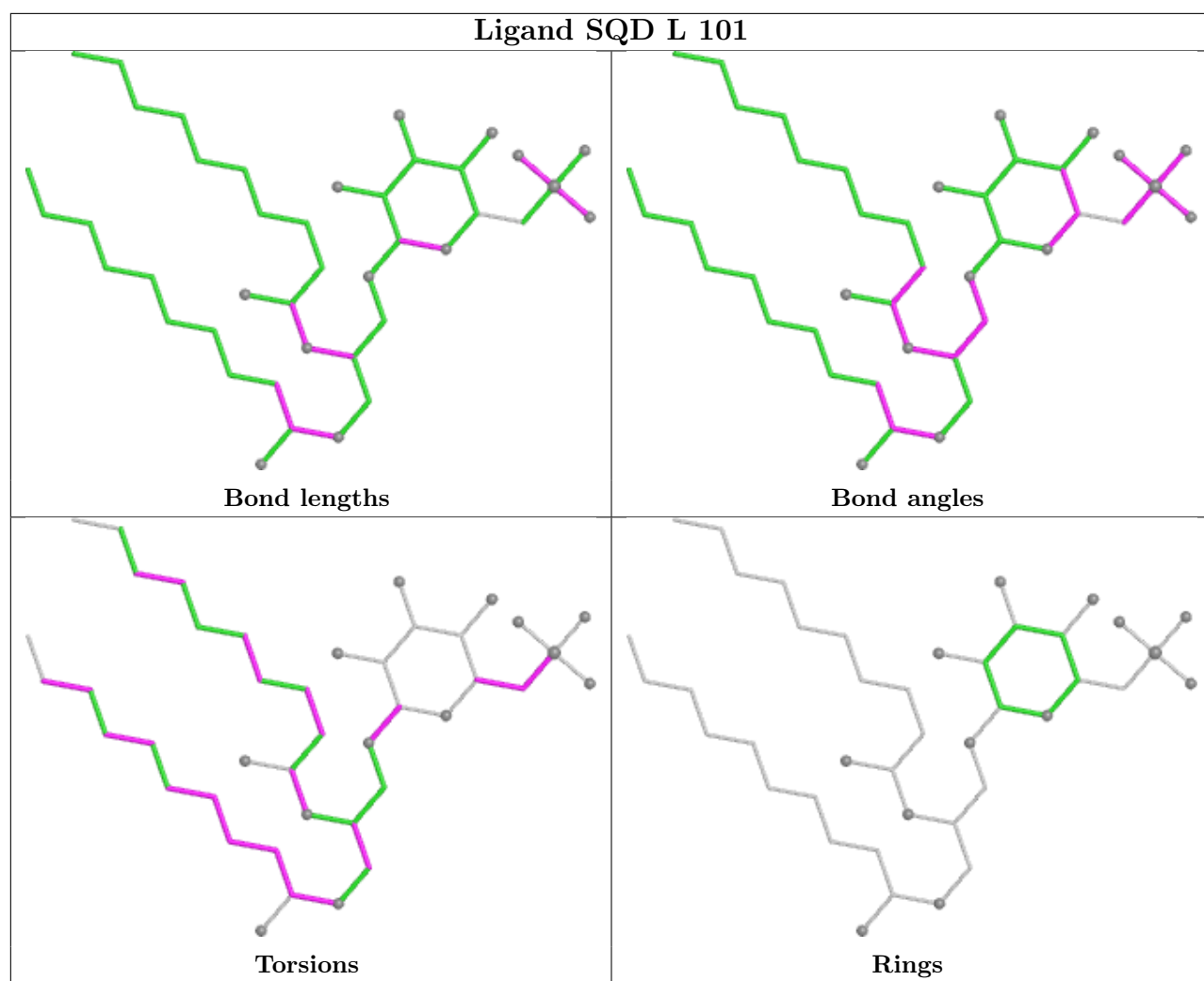


Torsions

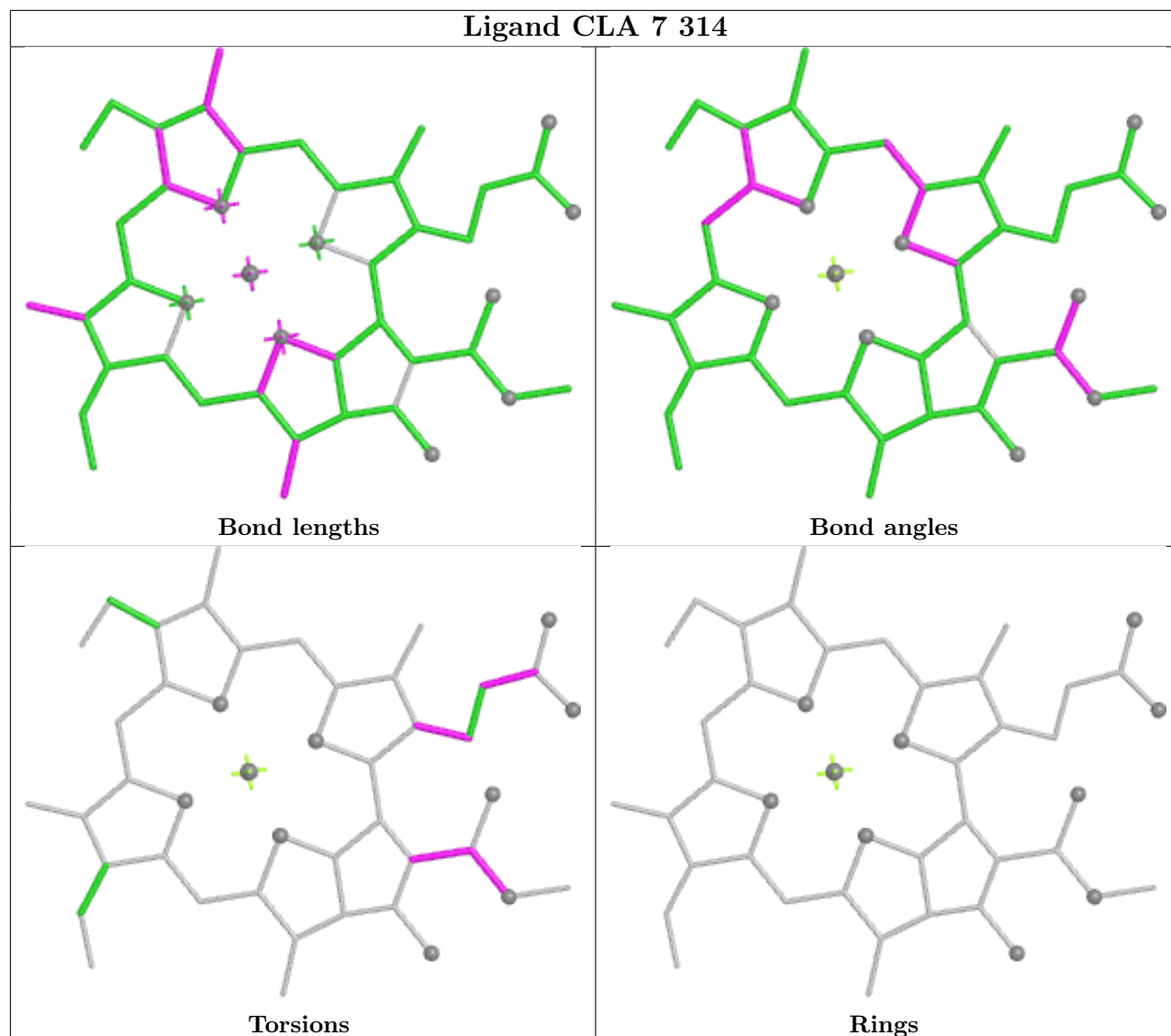


Rings

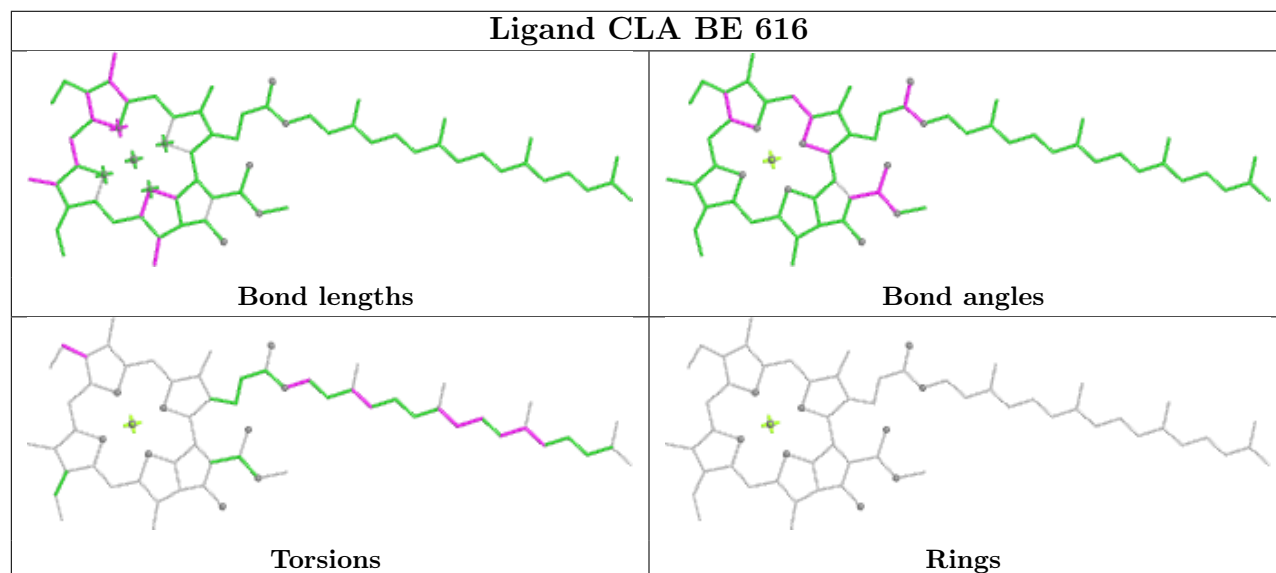
Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 9 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

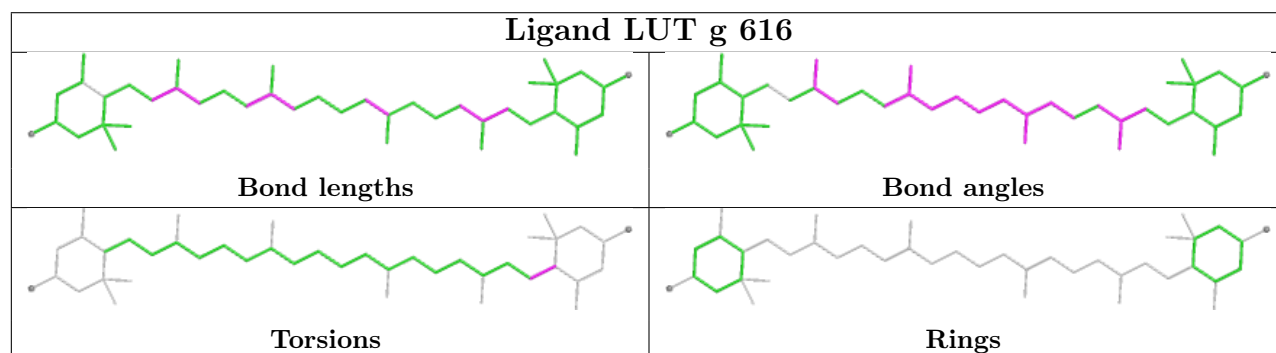
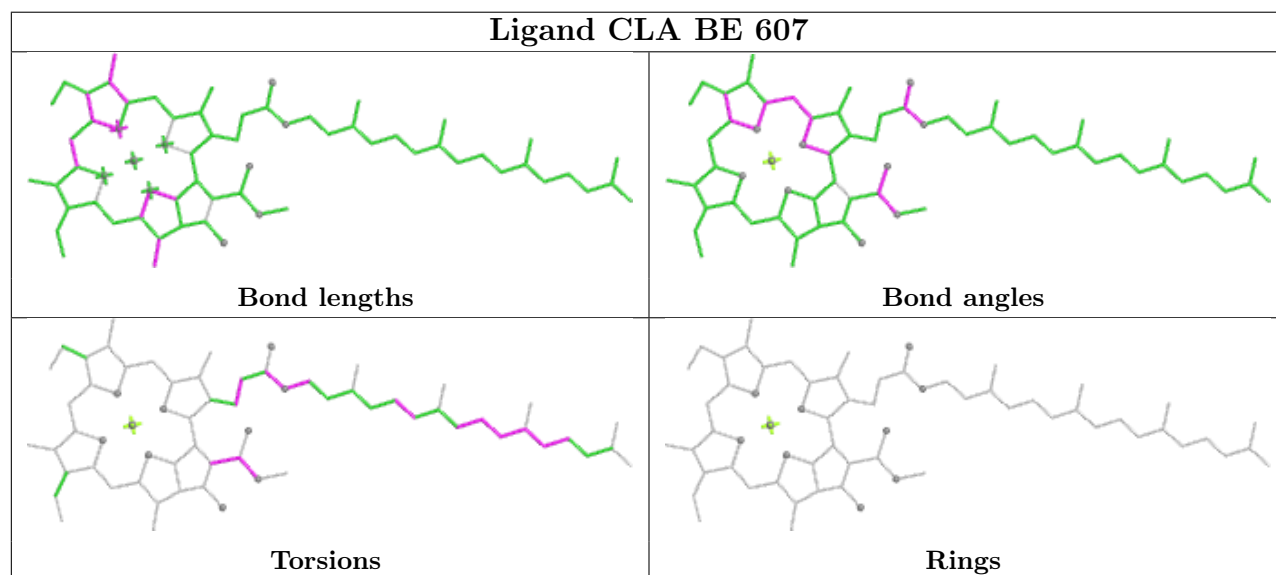
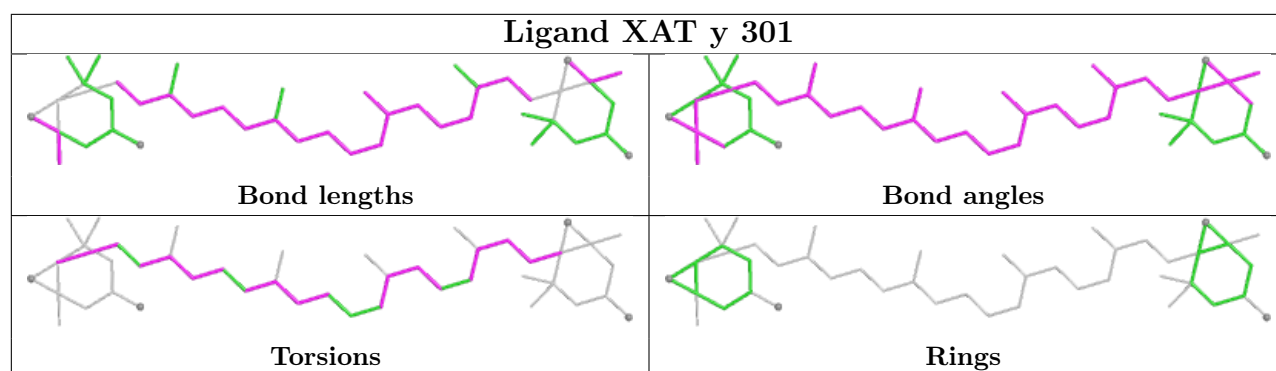


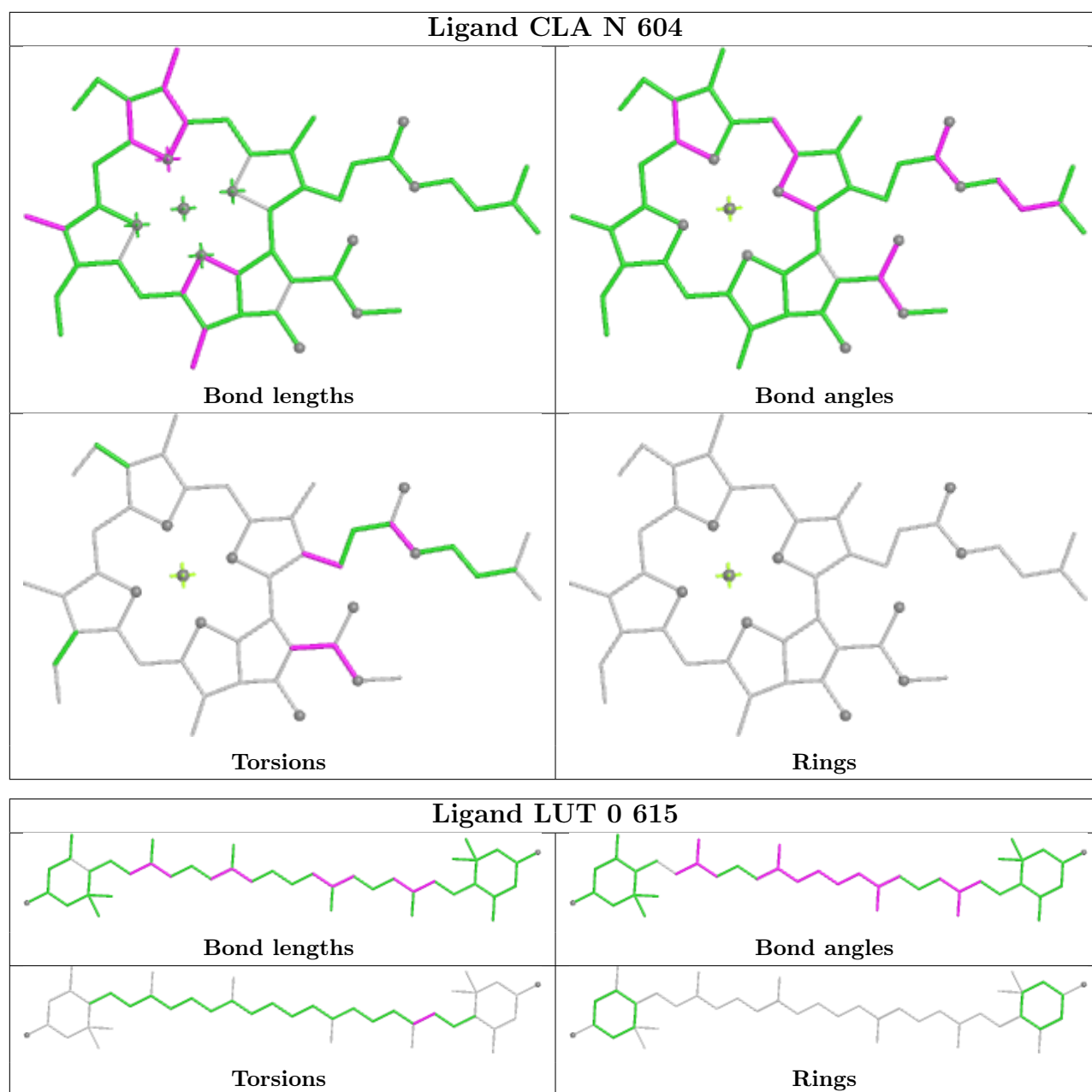
Ligand CLA 7 314



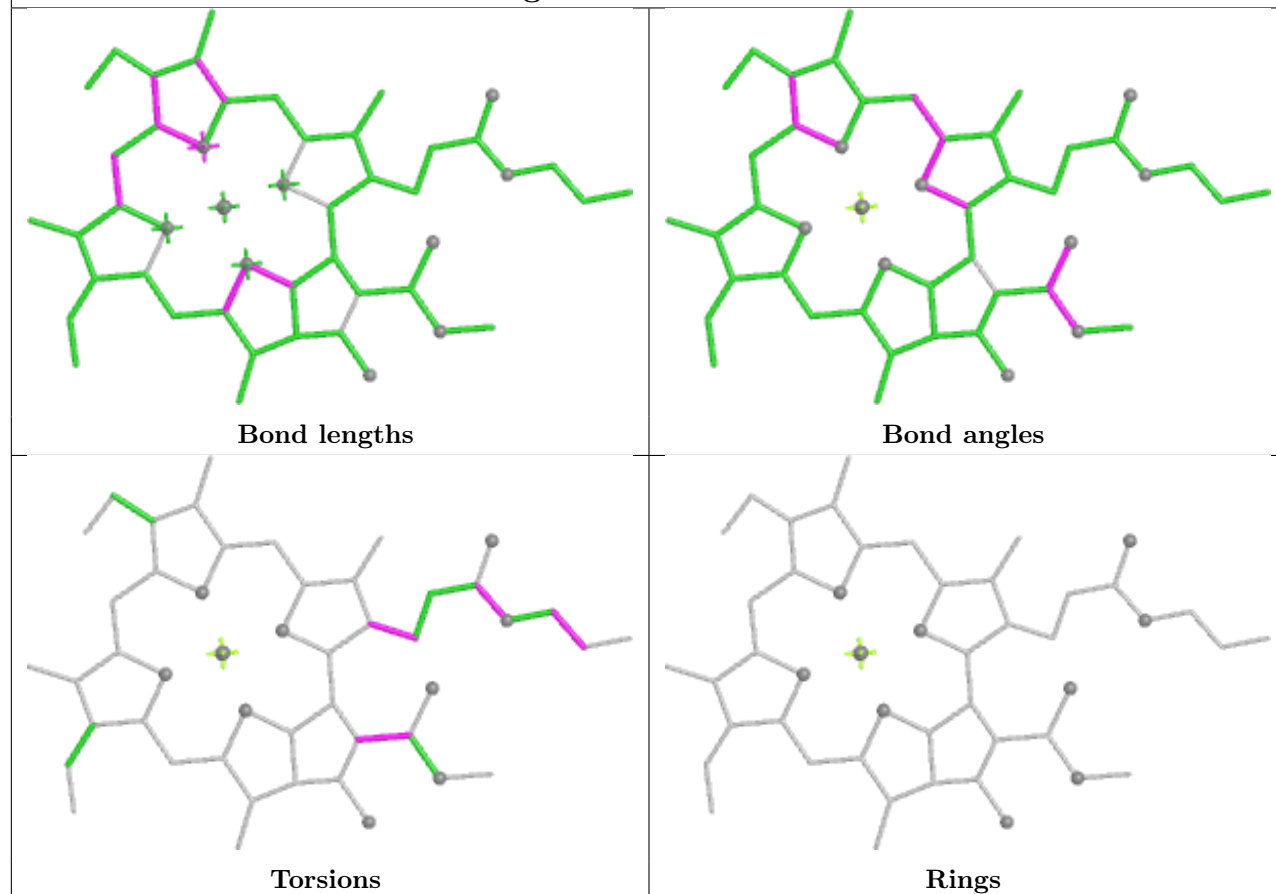
Ligand CLA BE 616



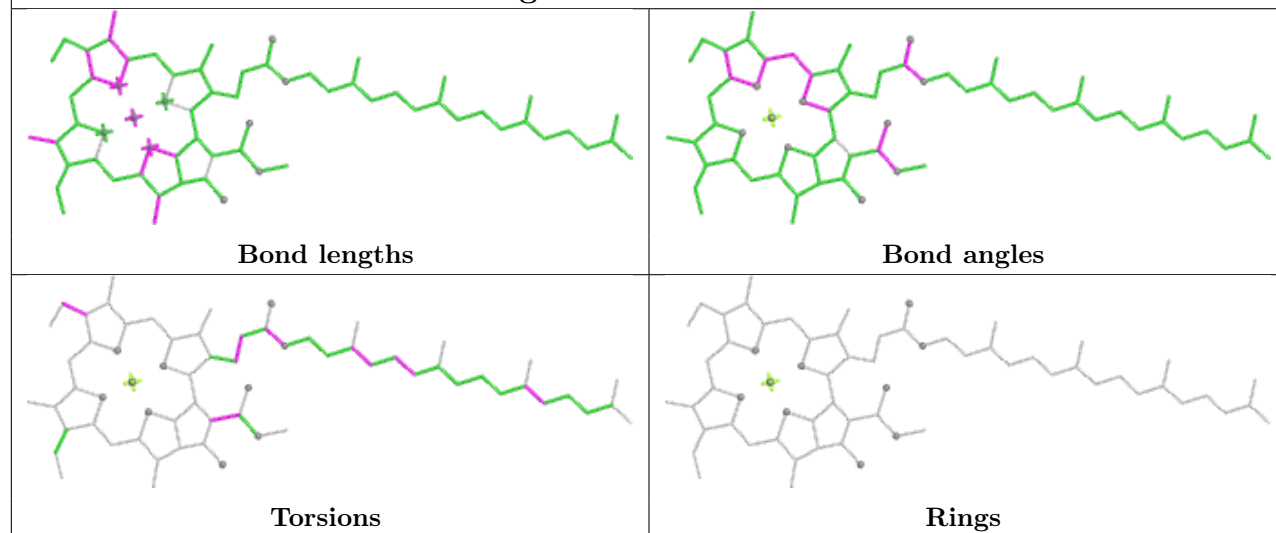


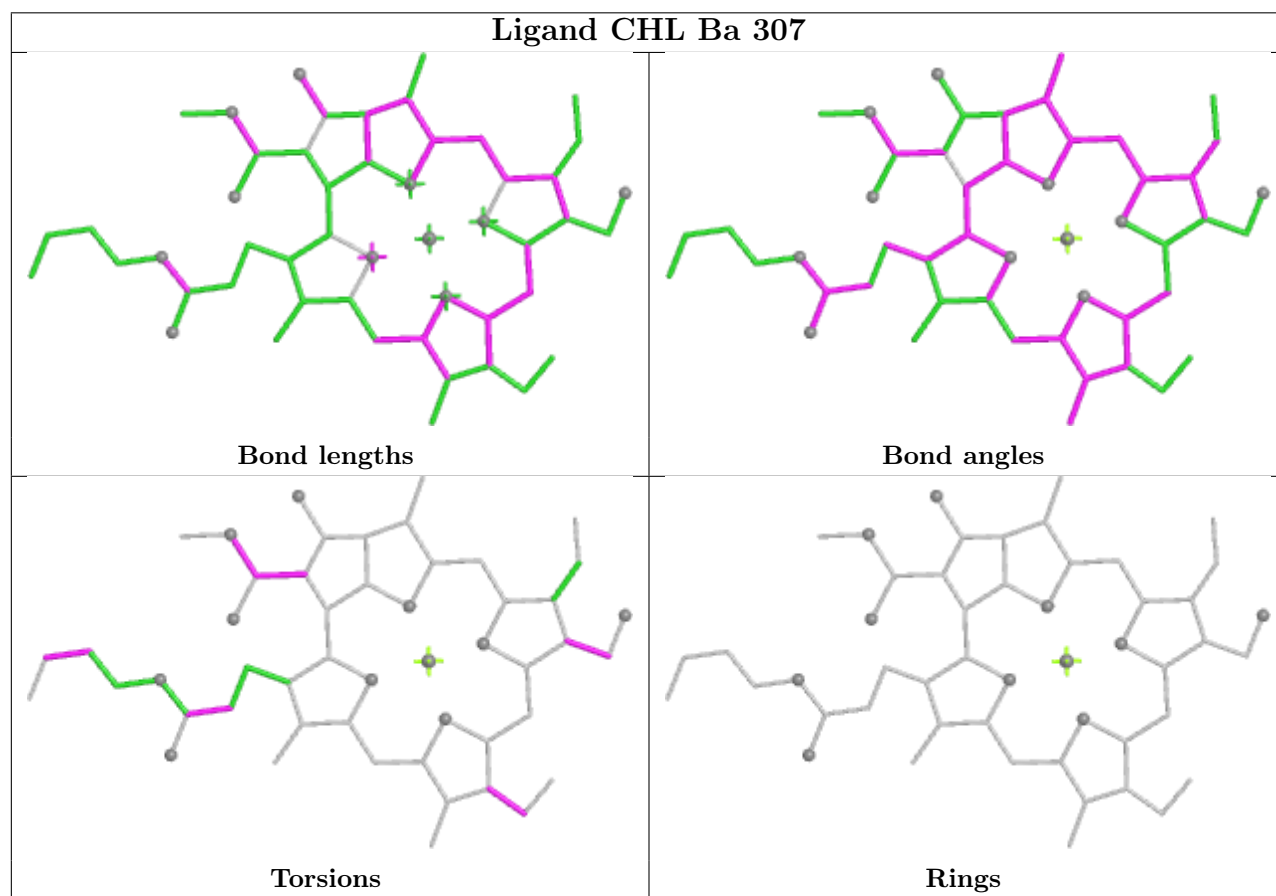
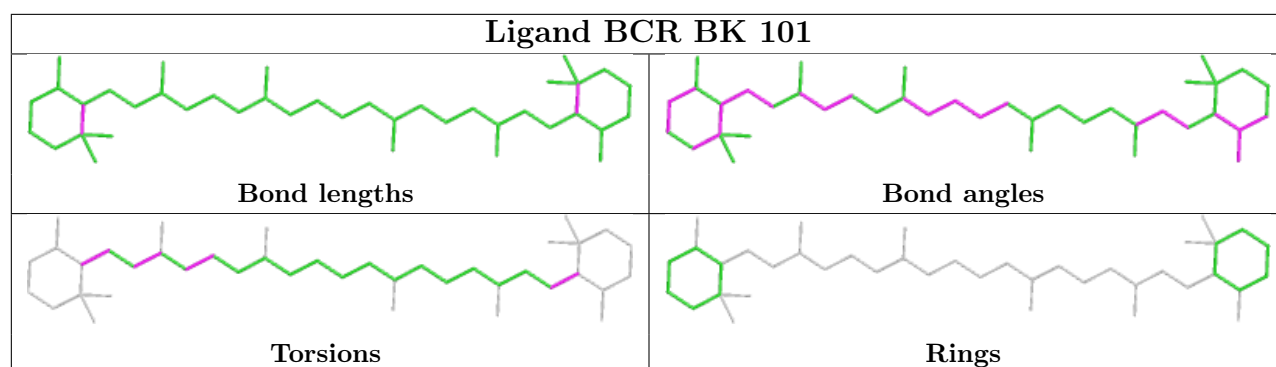


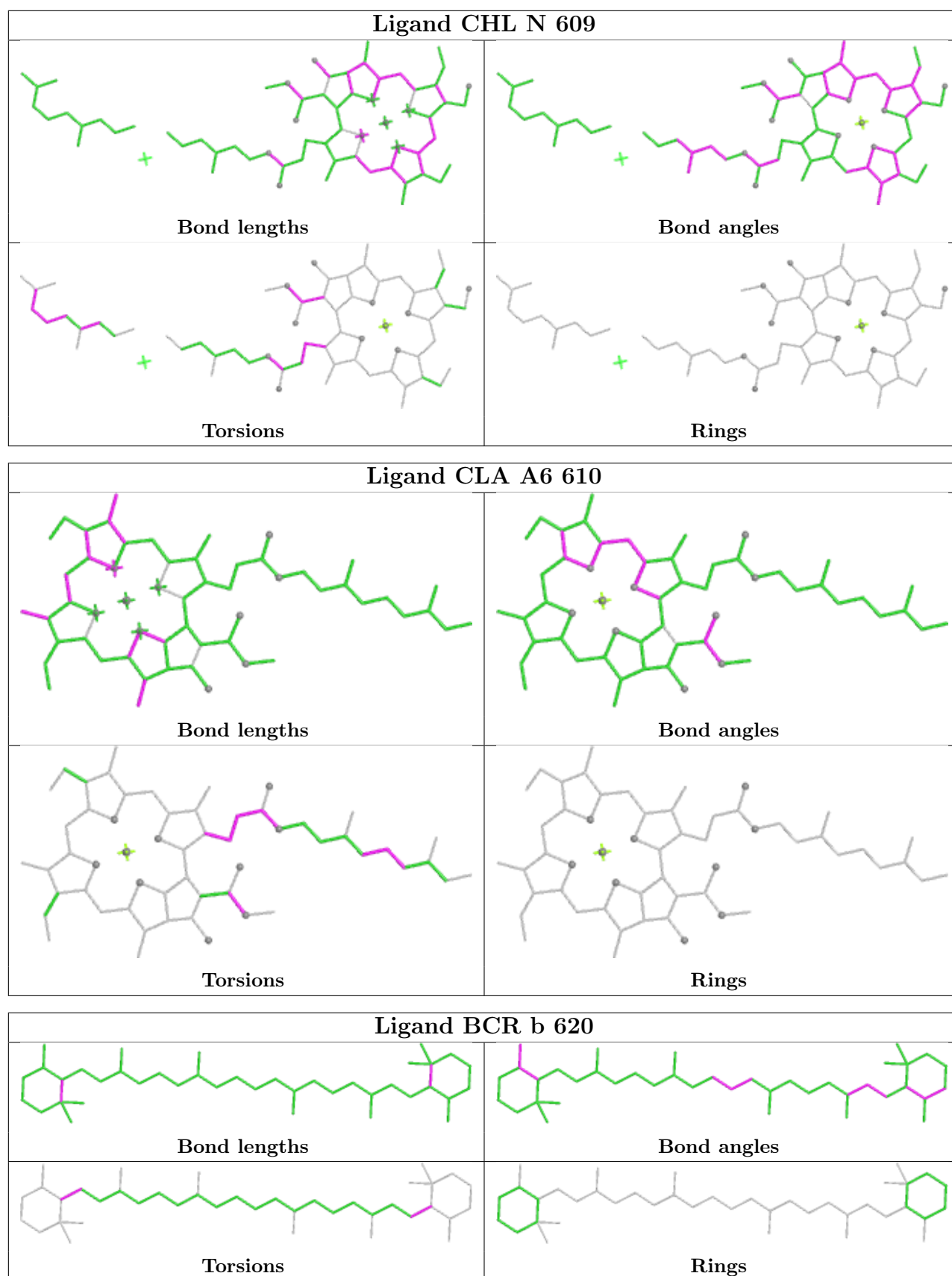
Ligand CLA BJ 614

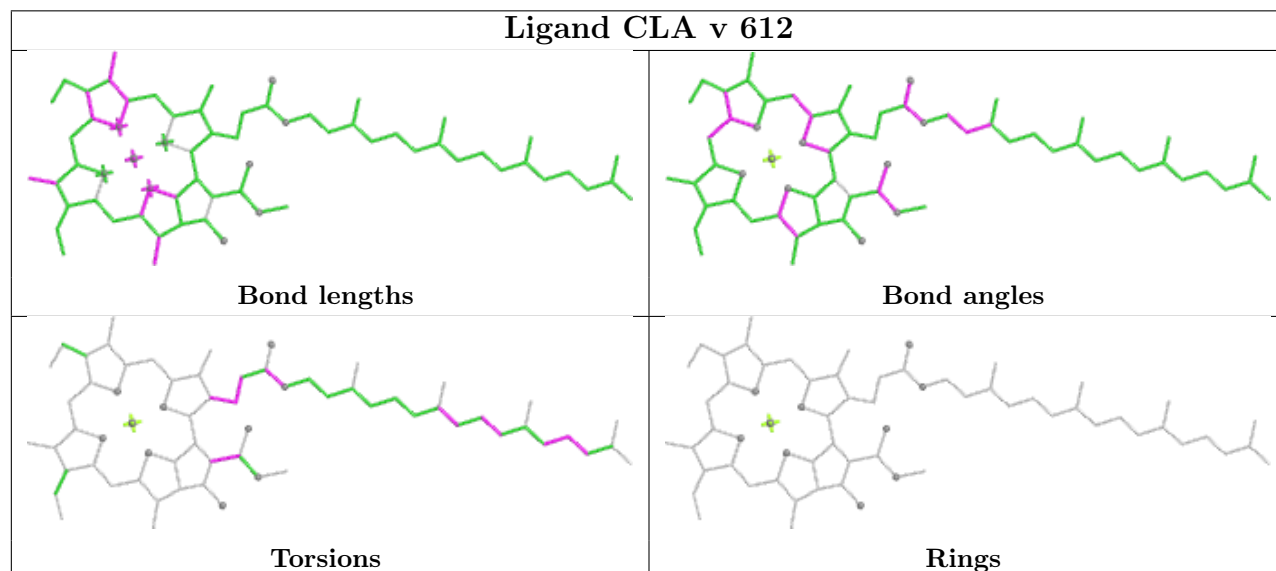
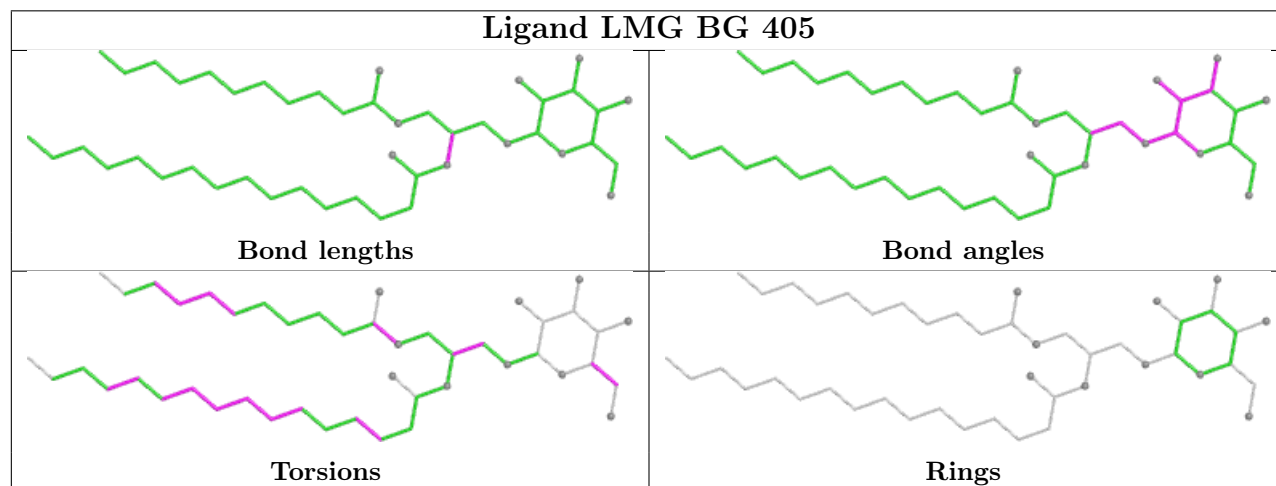
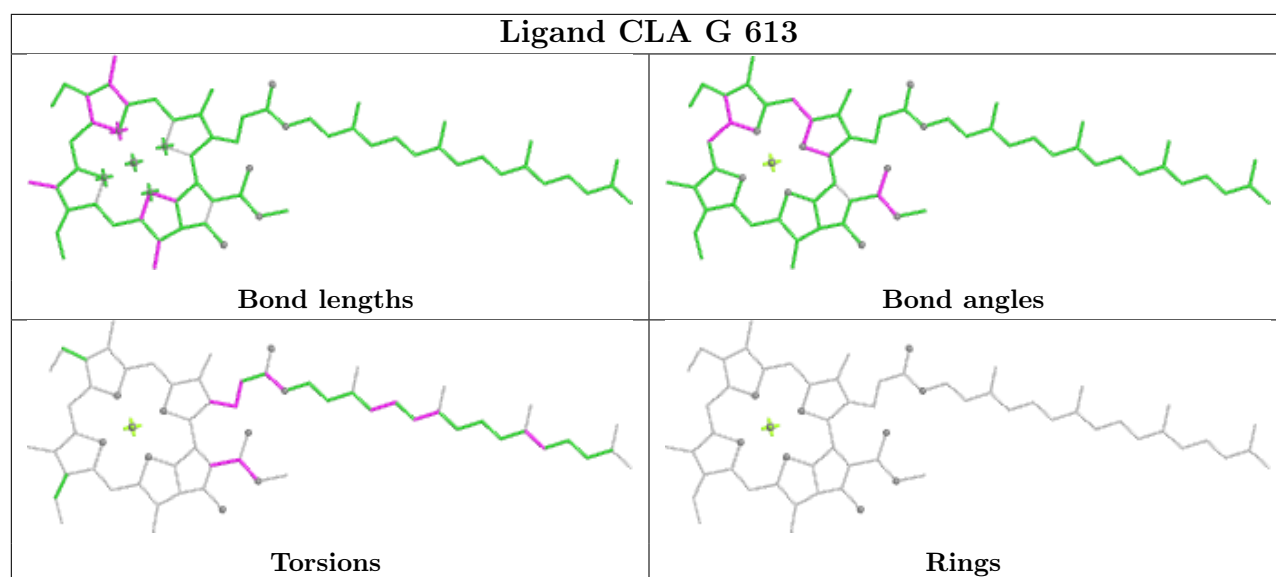


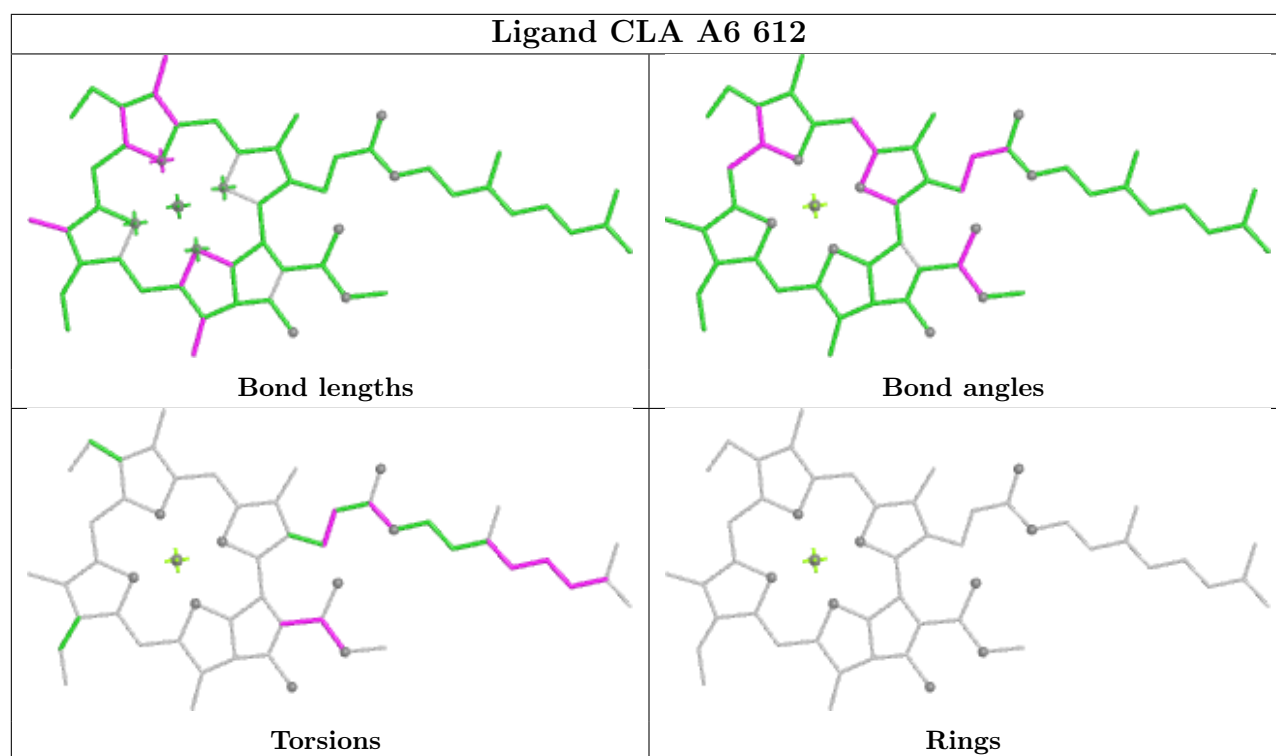
Ligand CLA BB 304

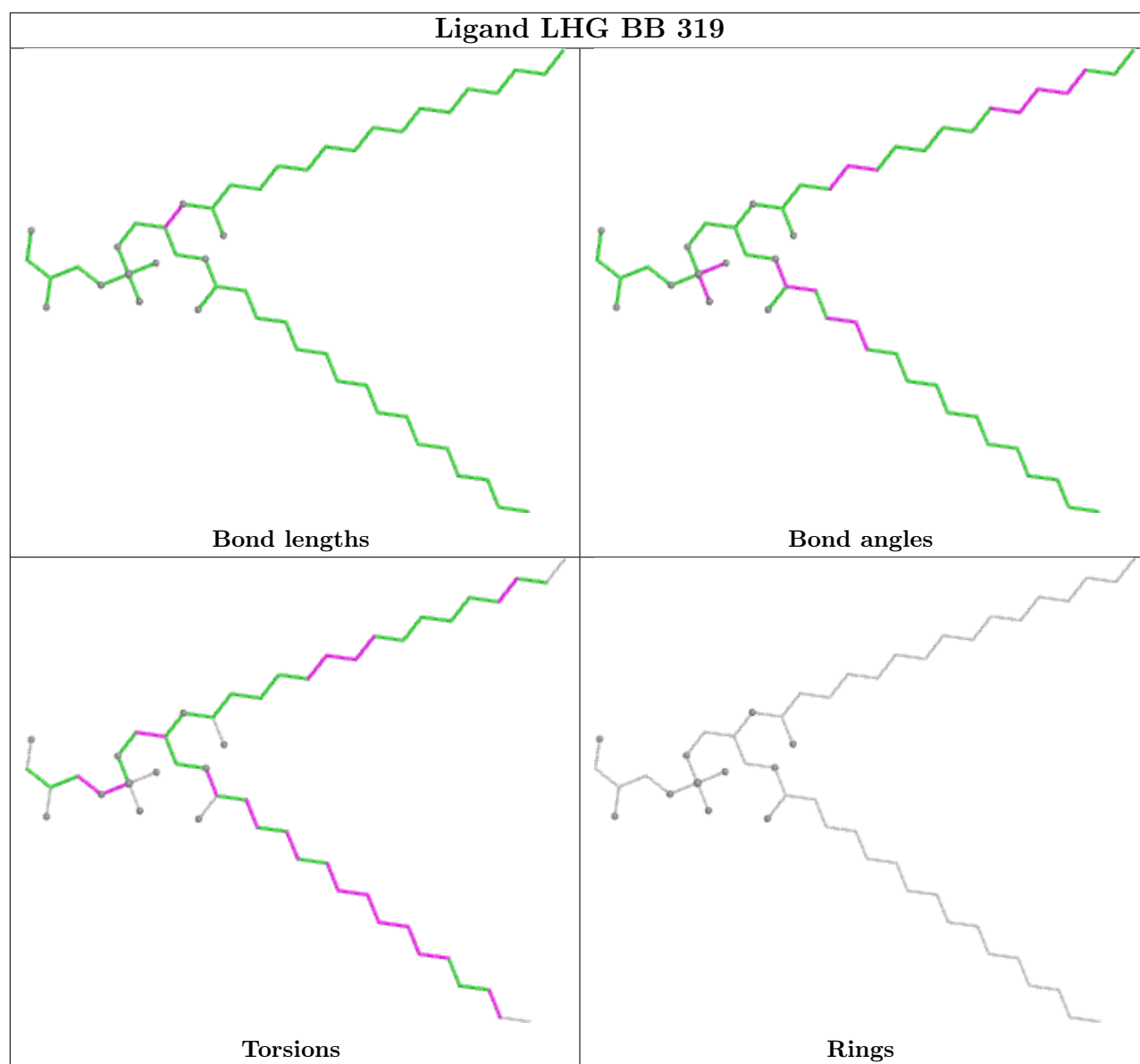




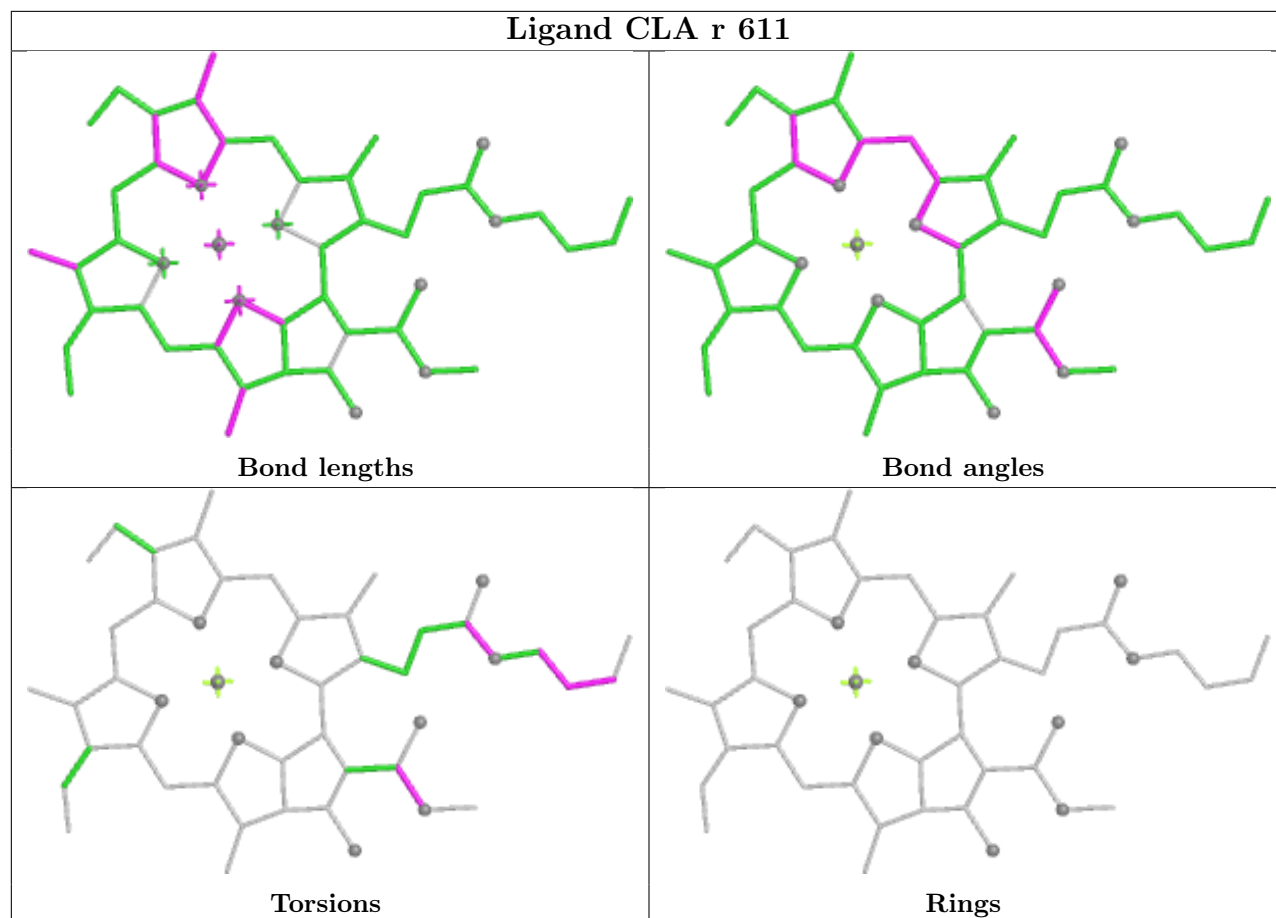




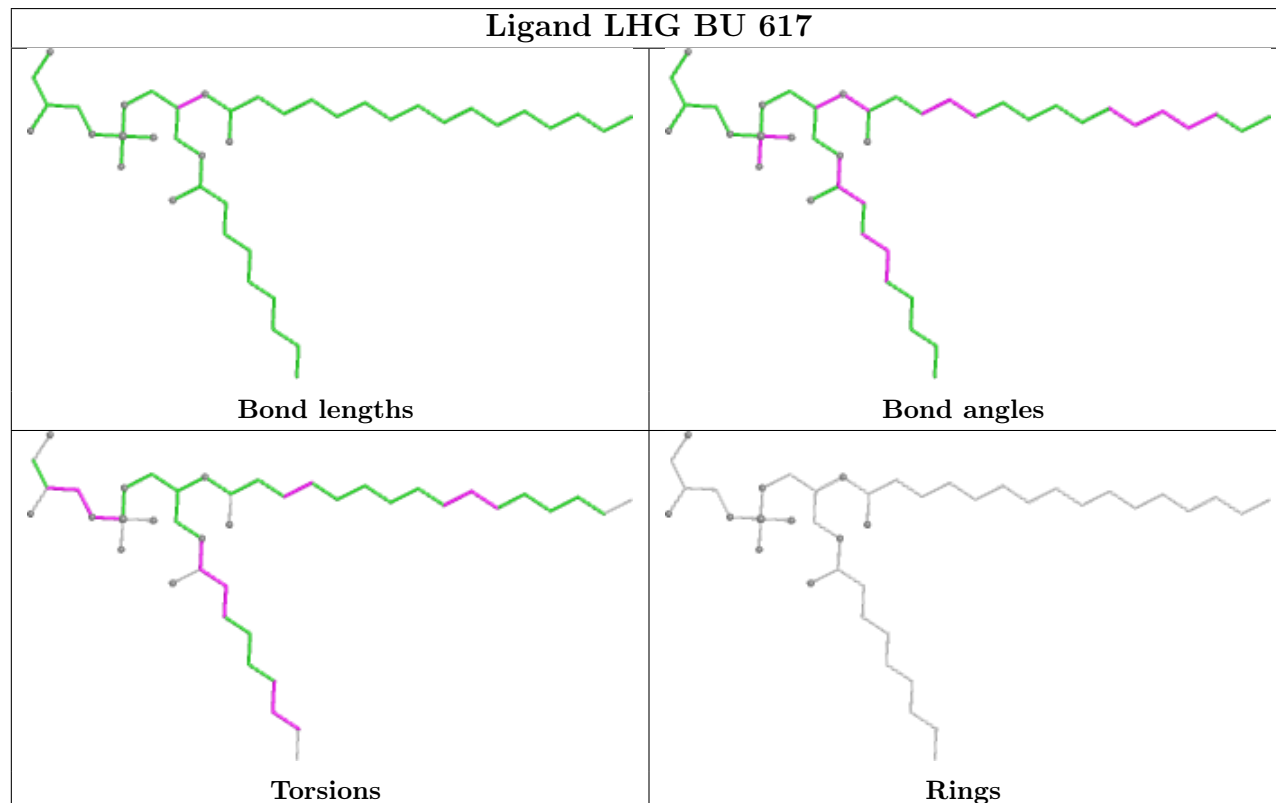


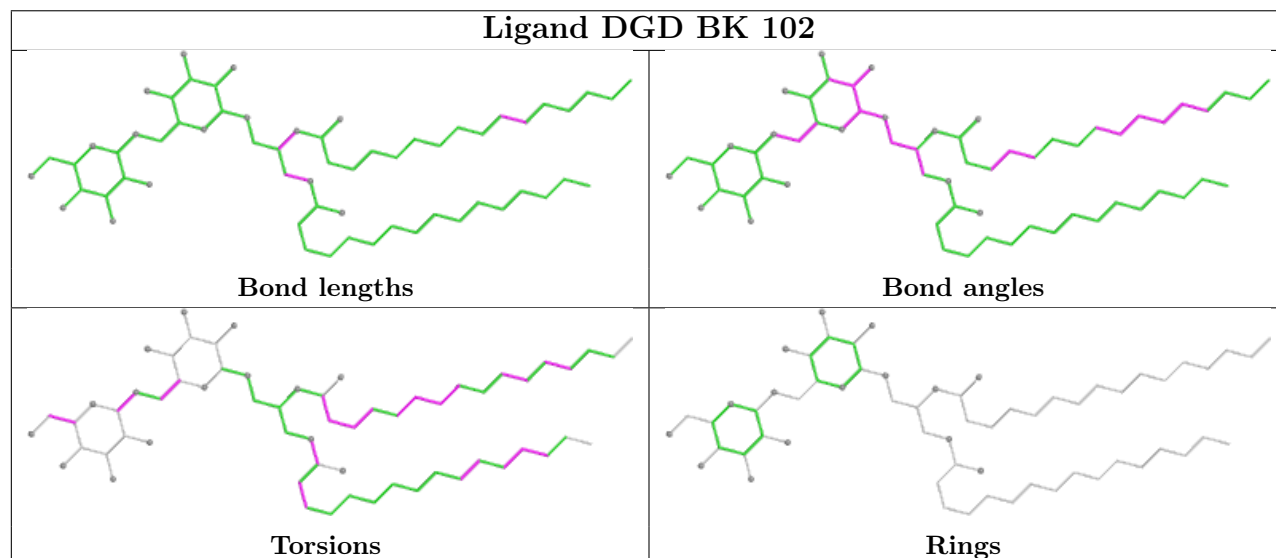
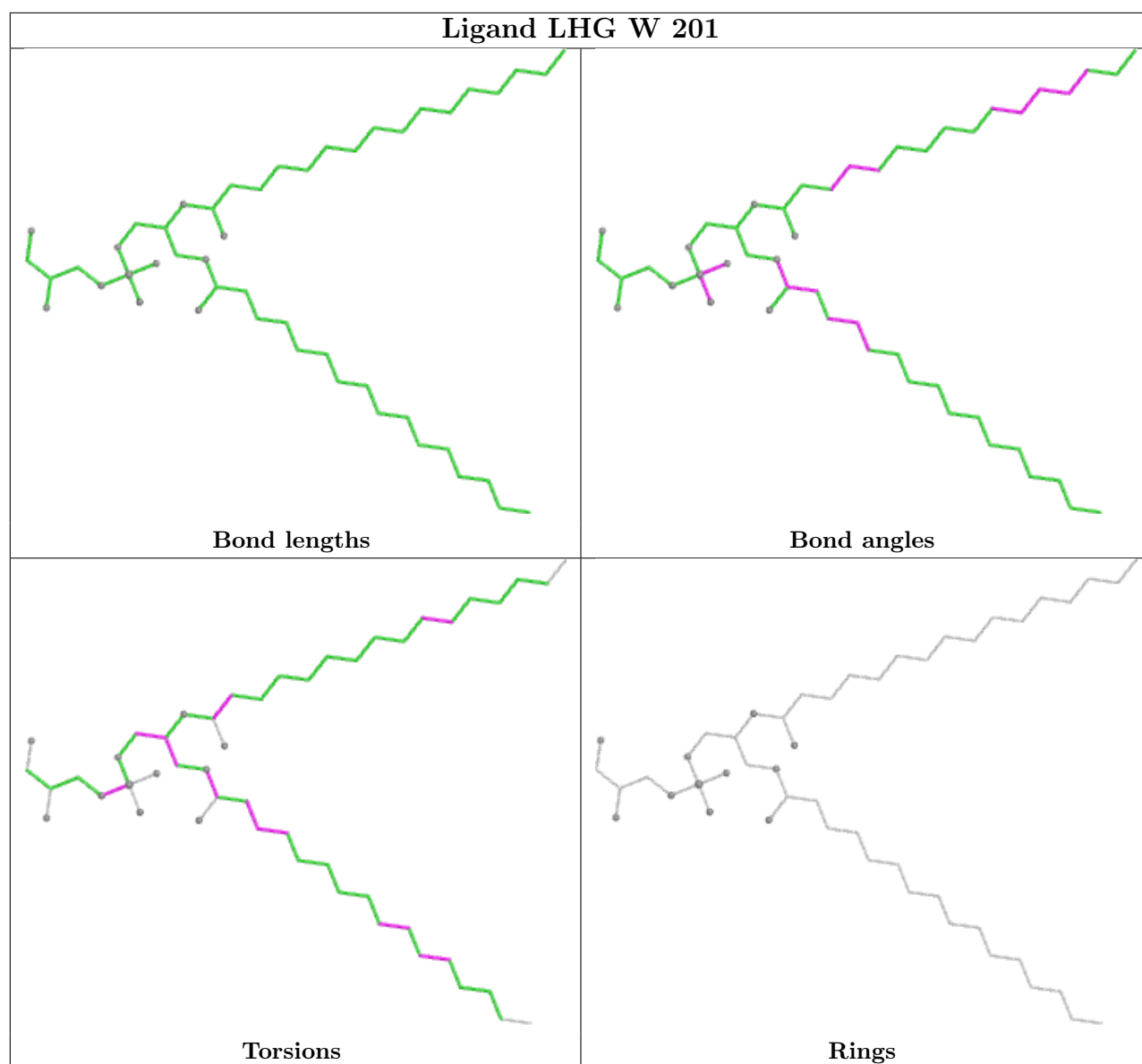


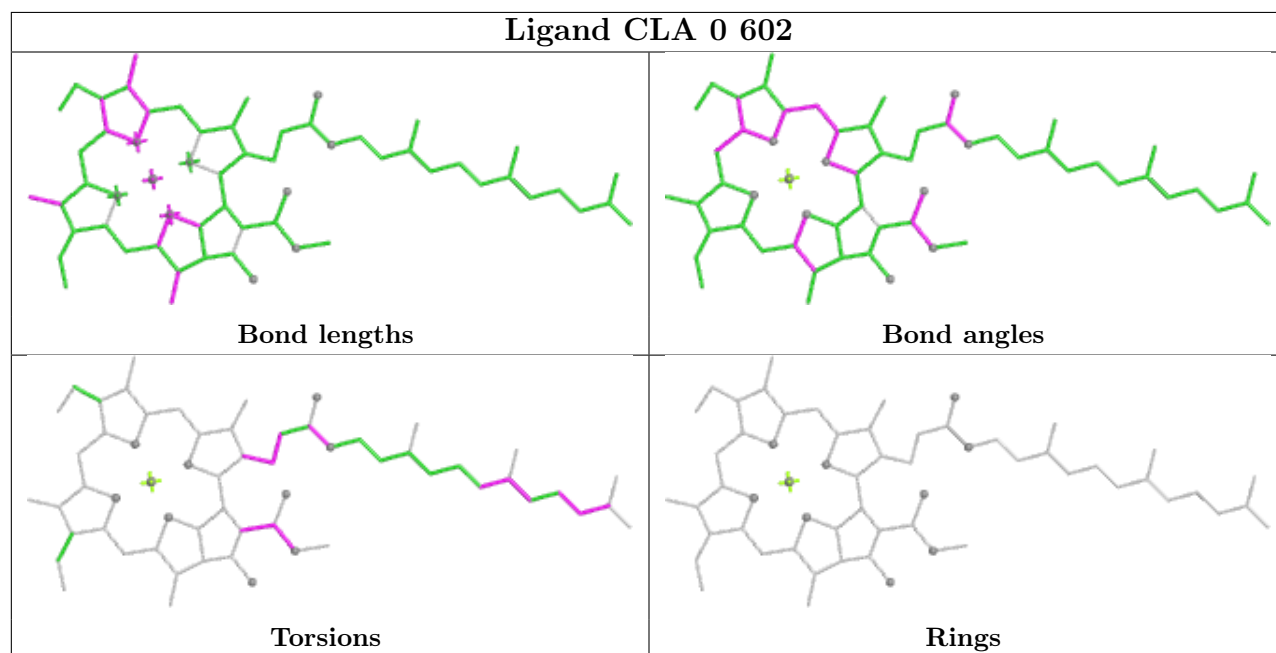
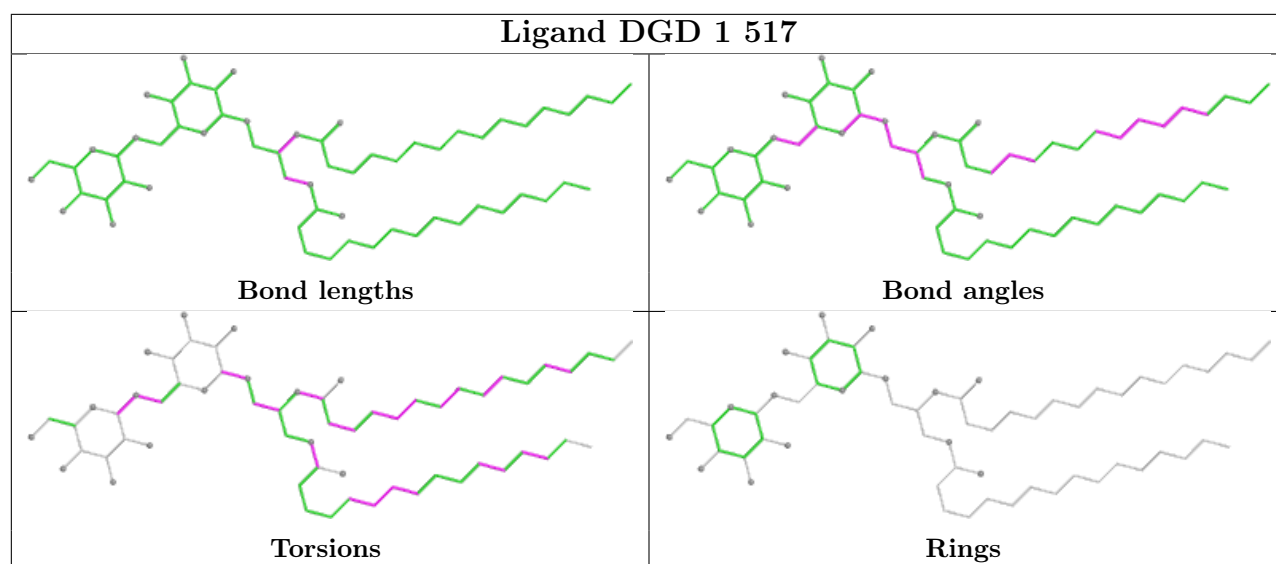
Ligand CLA r 611



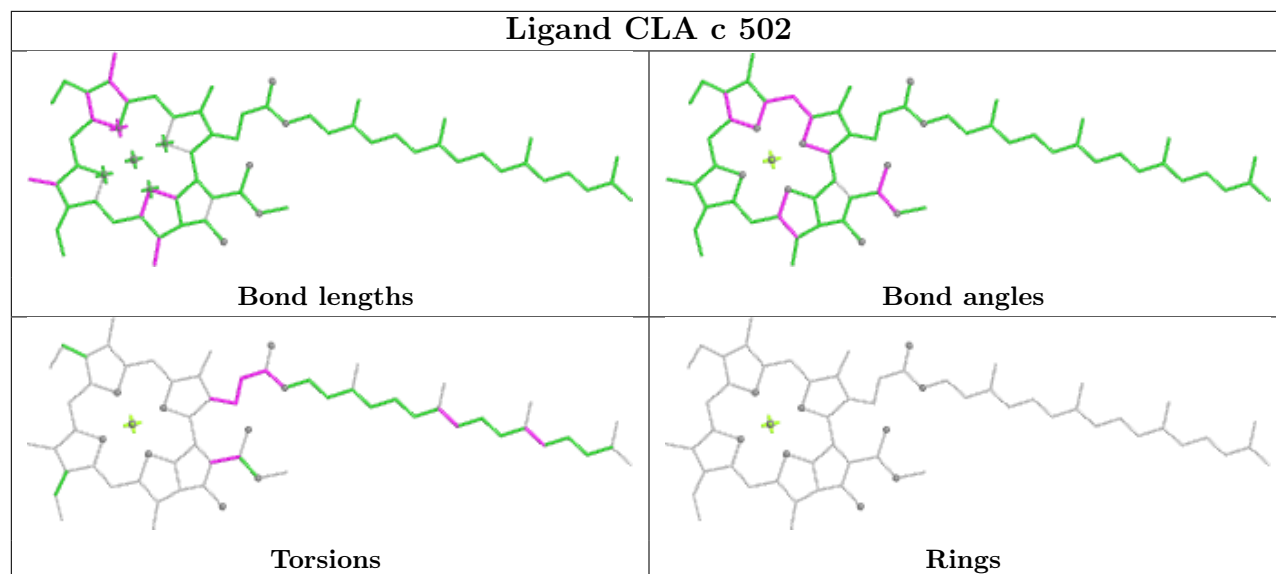
Ligand LHG BU 617



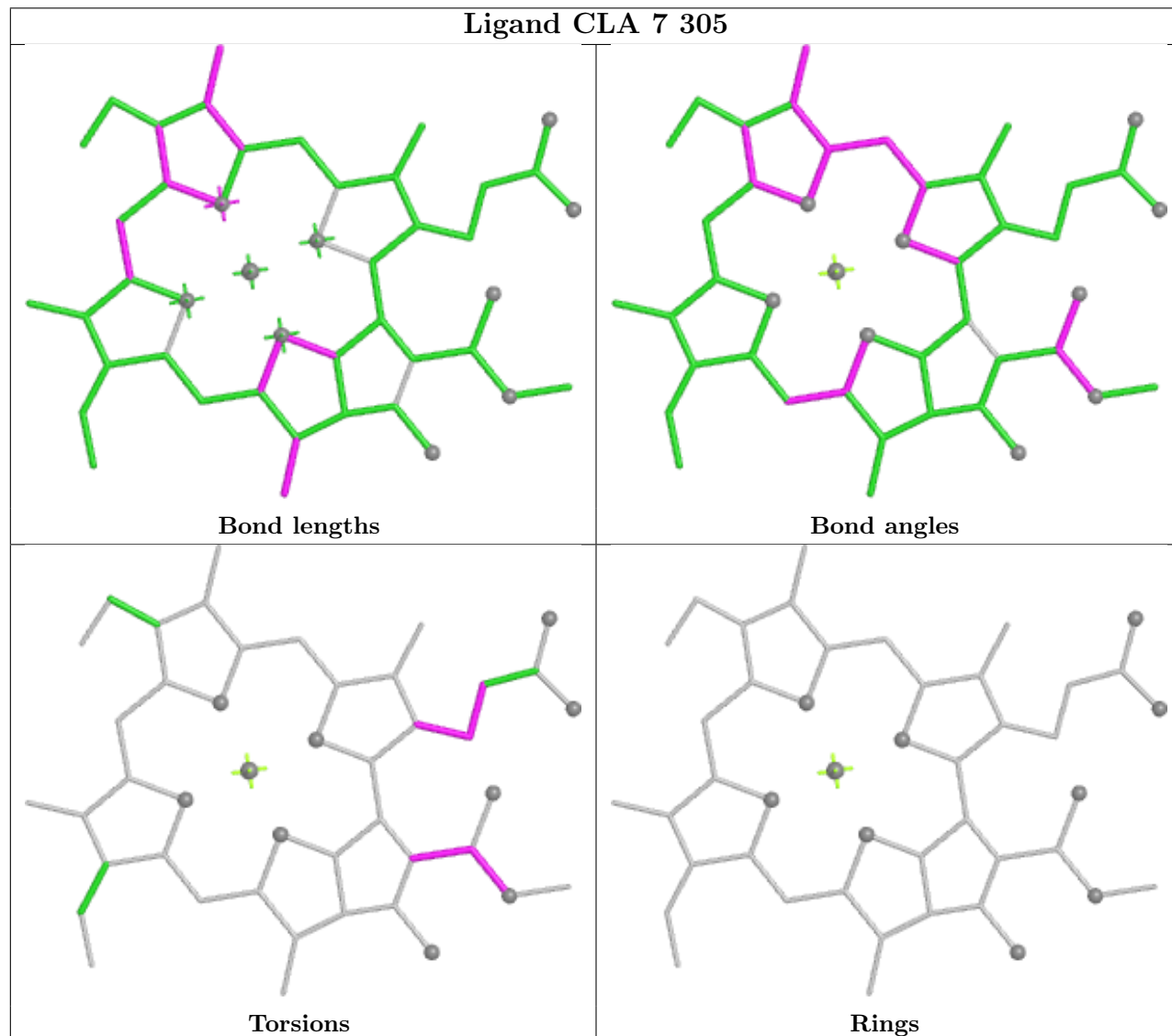




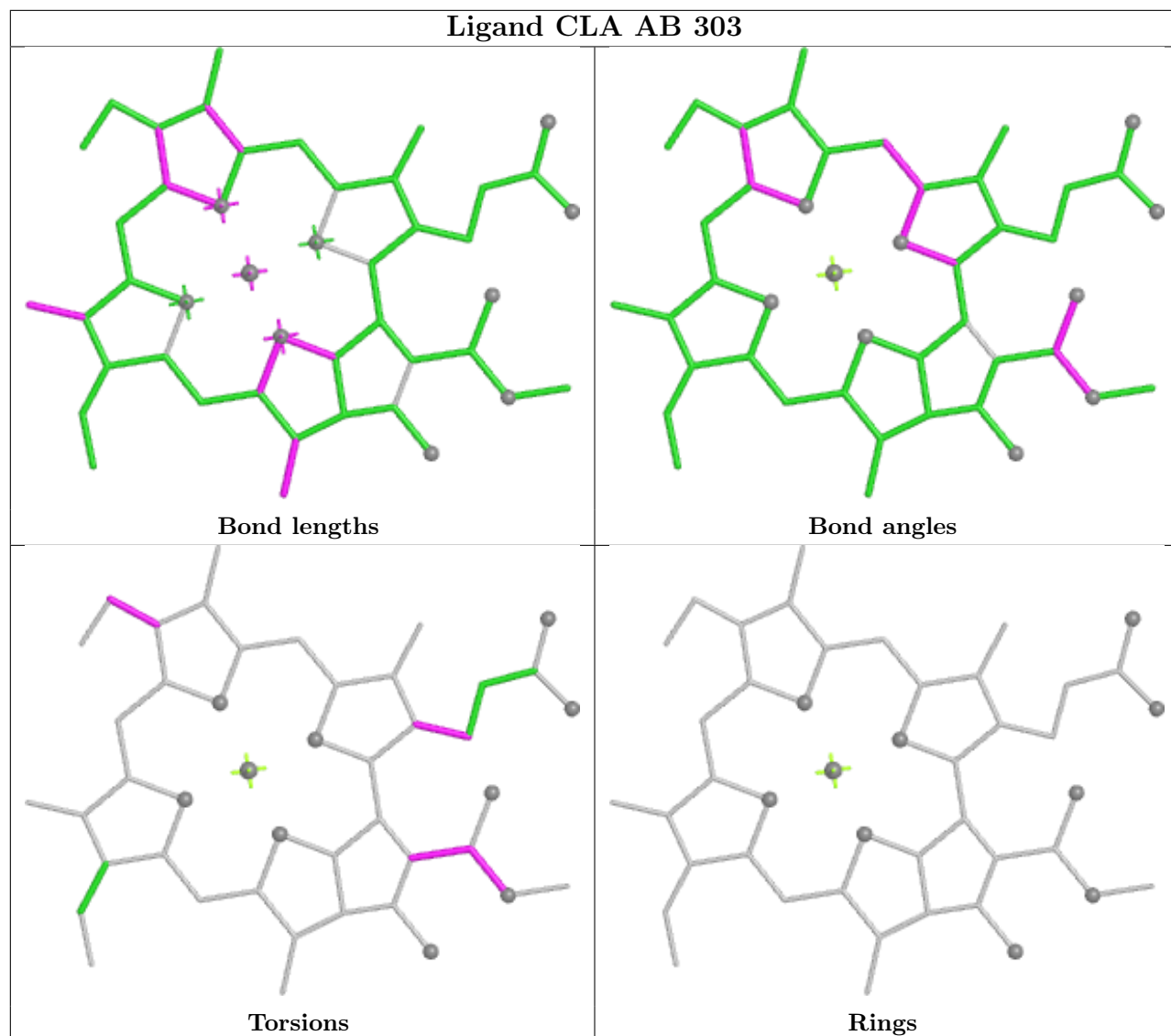
Ligand CLA c 502



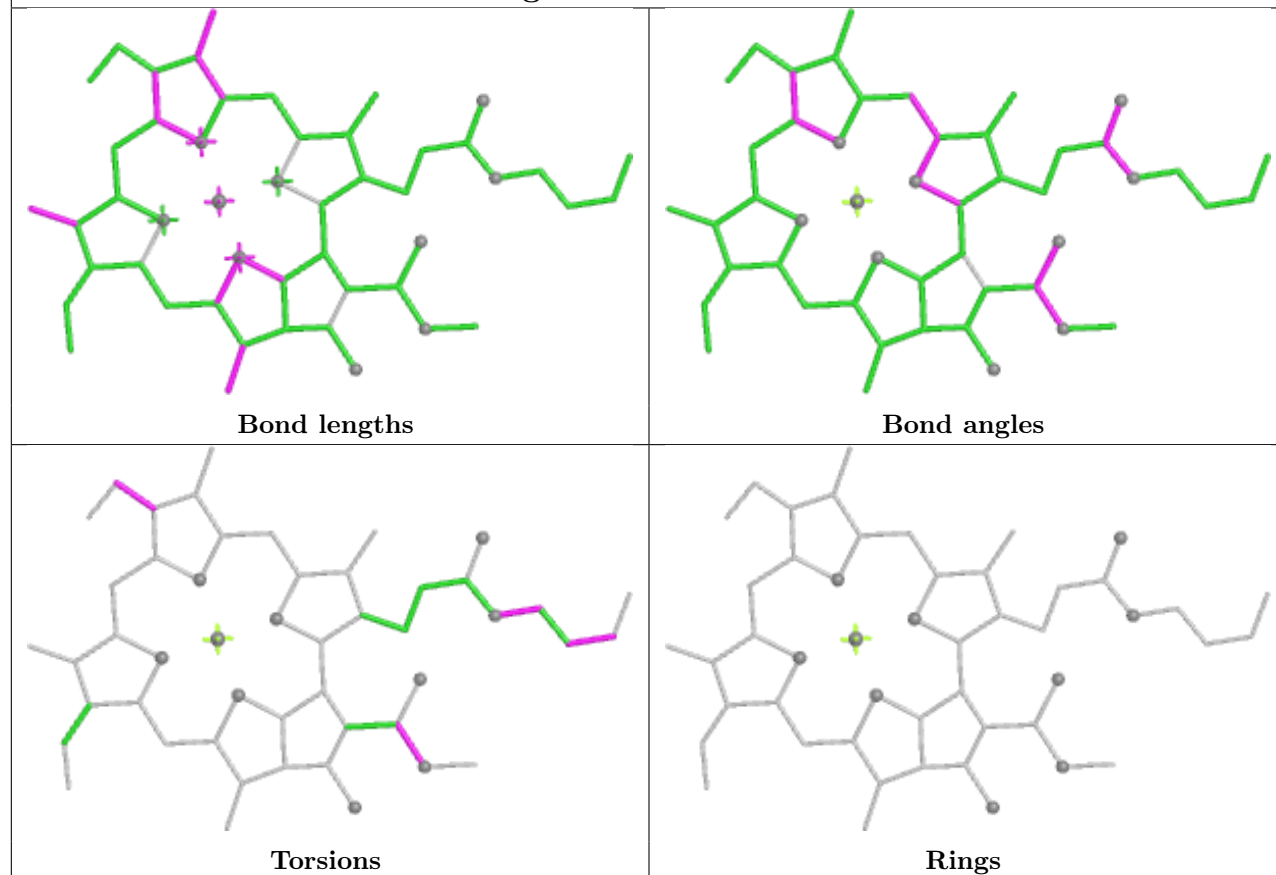
Ligand CLA 7 305



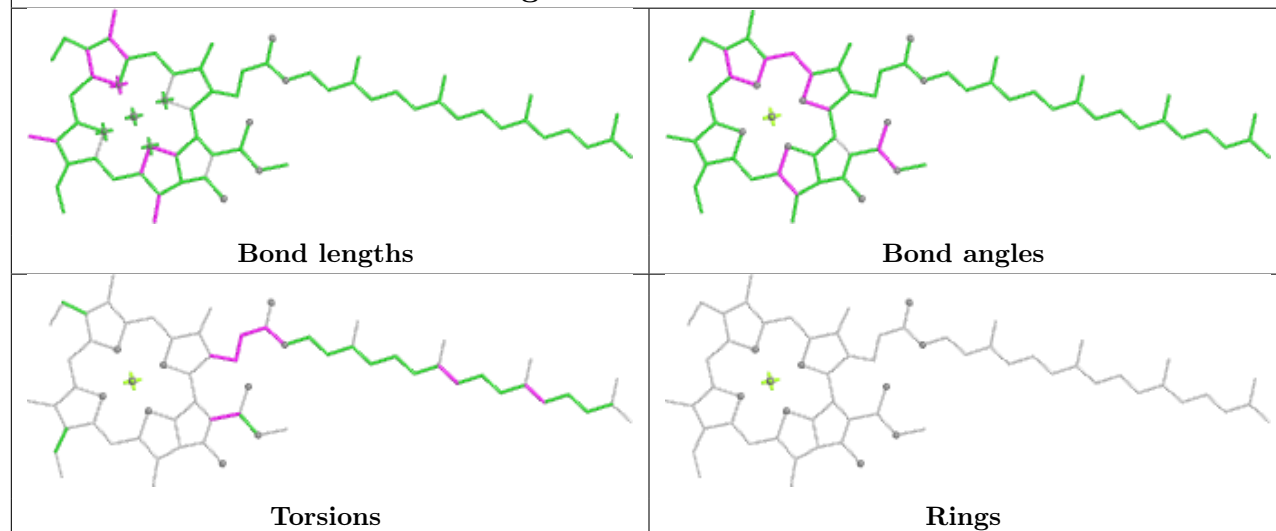
Ligand CLA AB 303

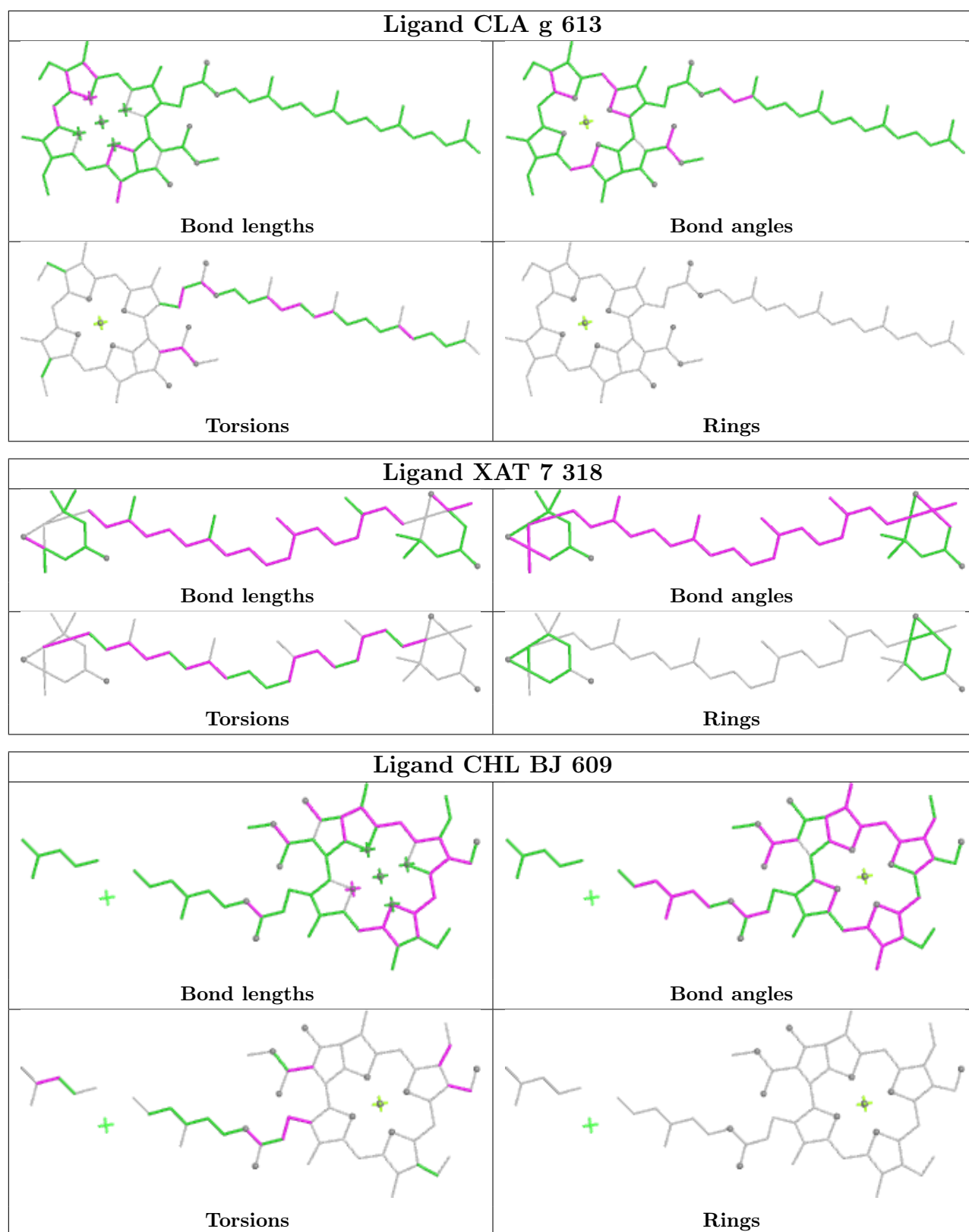


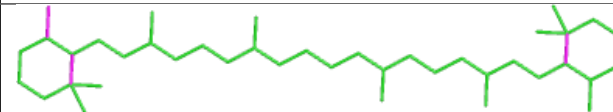
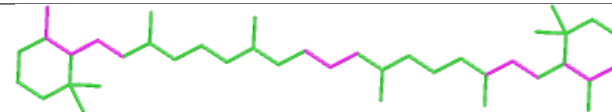
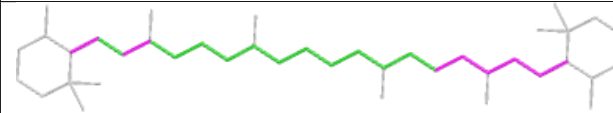
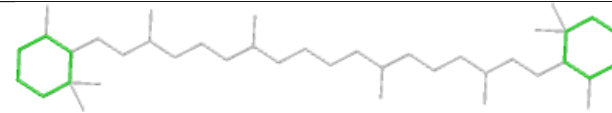
Ligand CLA A6 611

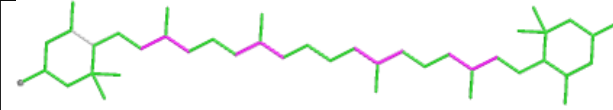
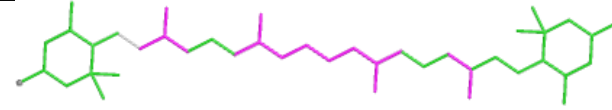
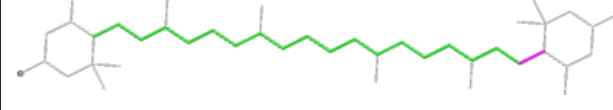
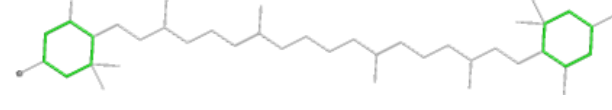


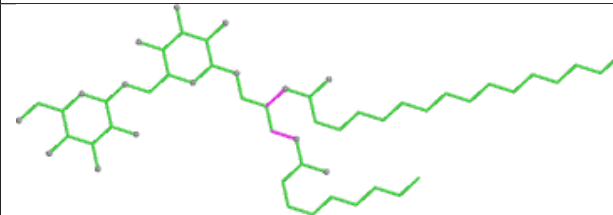
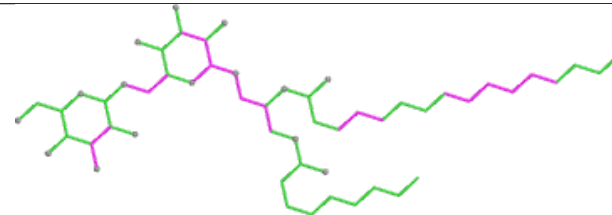
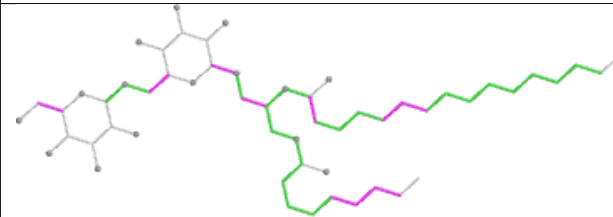
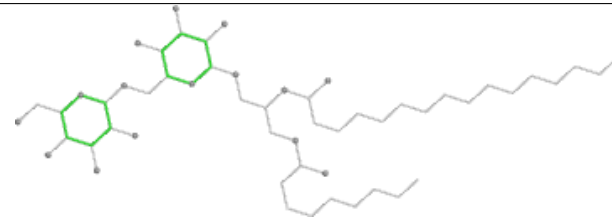
Ligand CLA BF 502

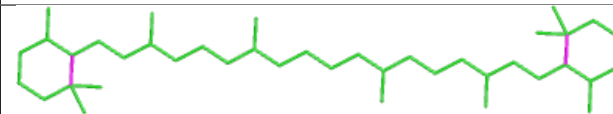
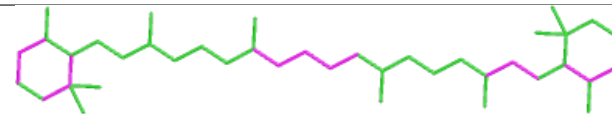
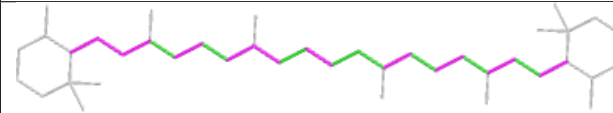
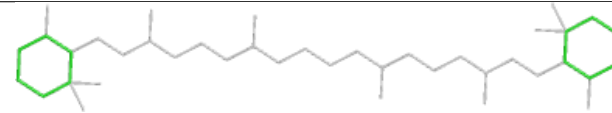


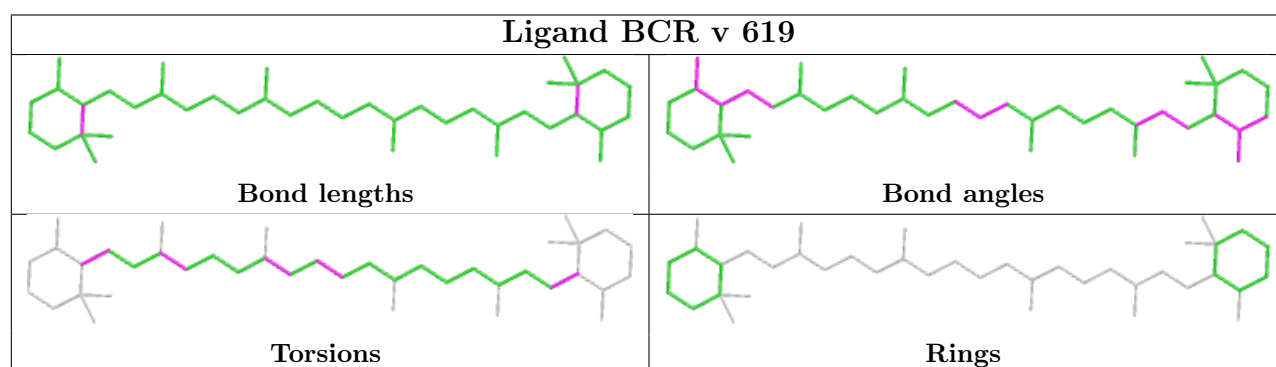
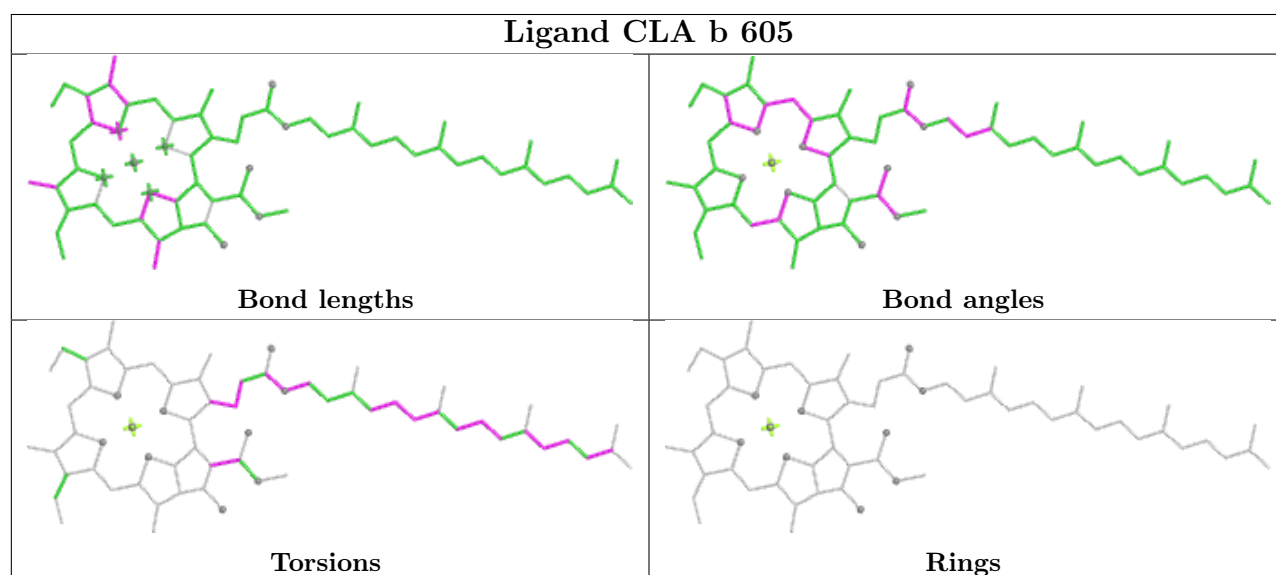
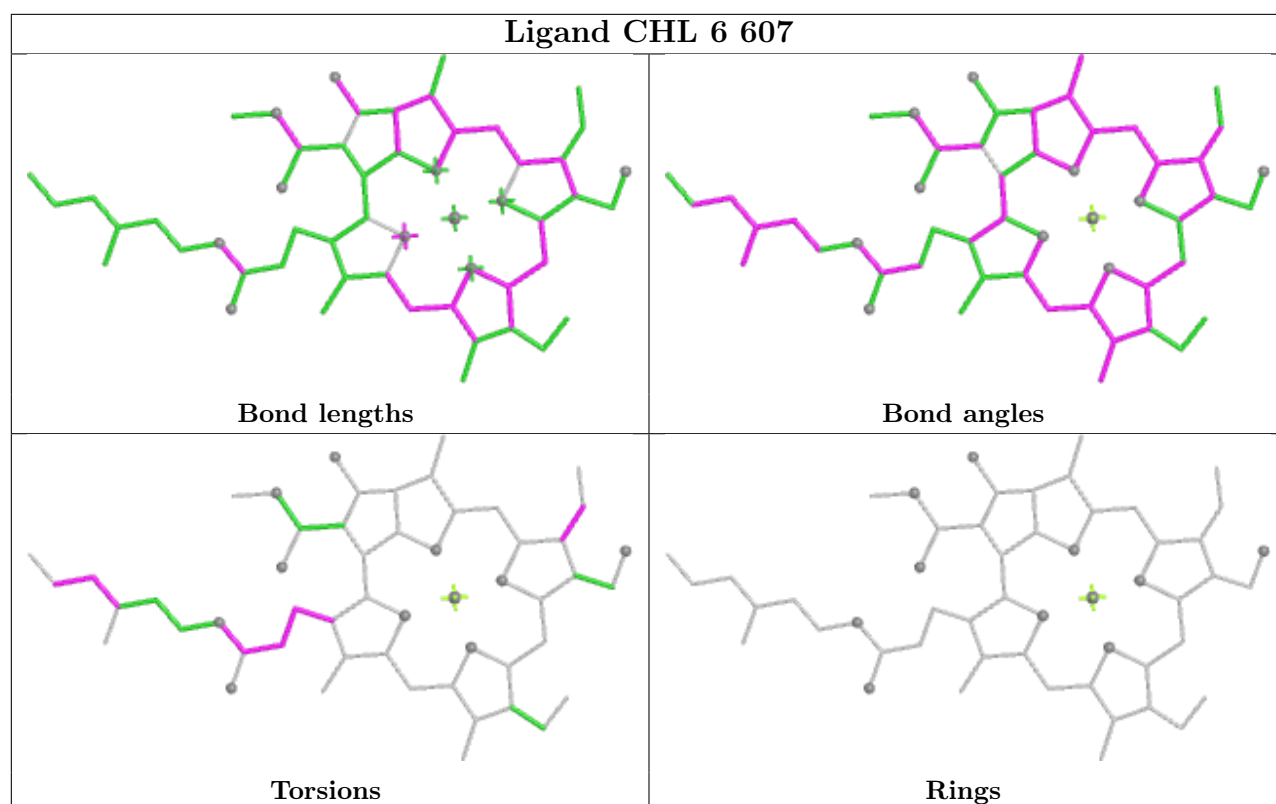


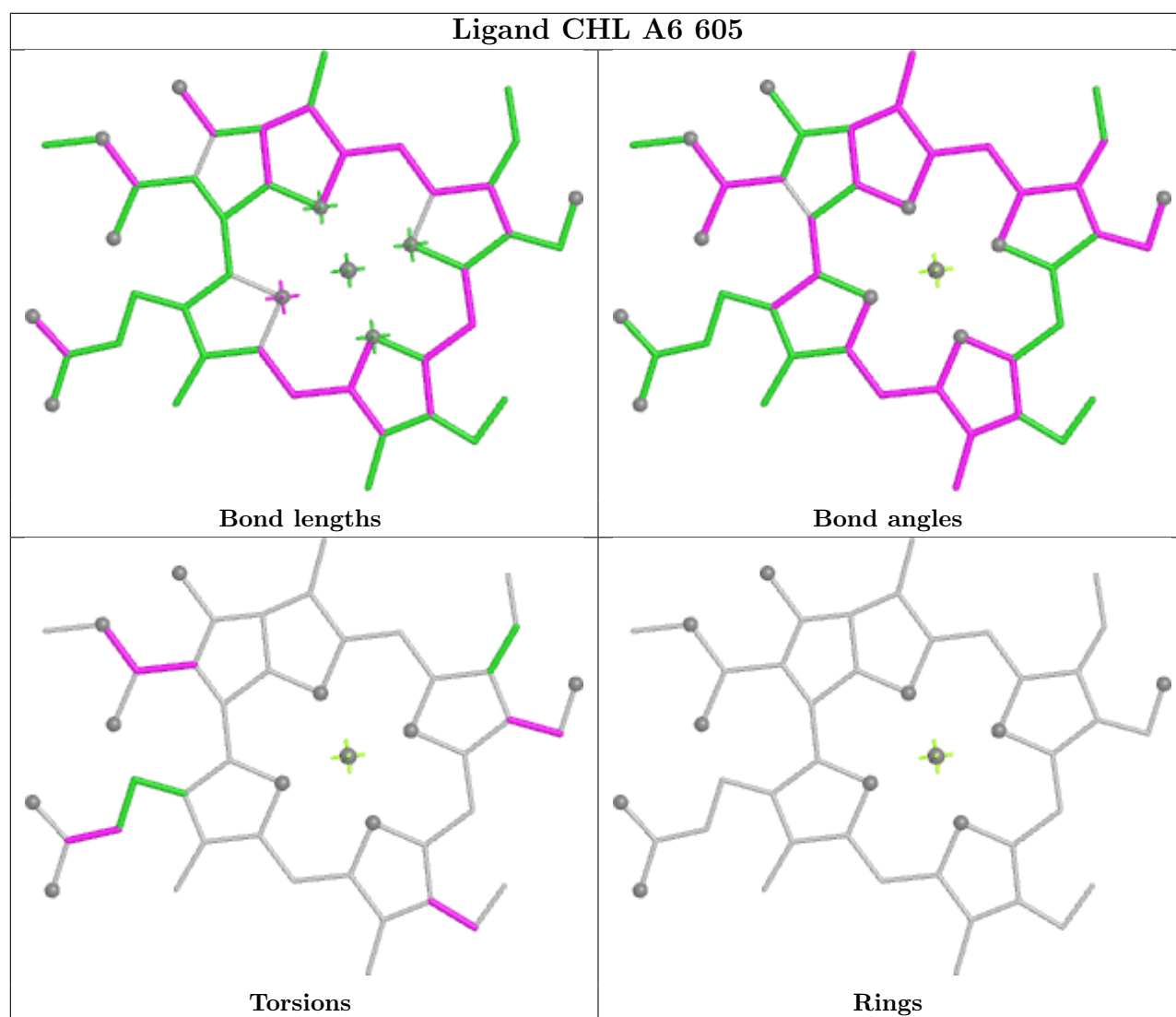
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT BQ 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR BE 601	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

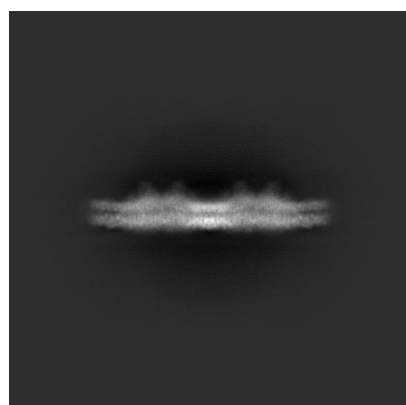
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63017. 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](#)

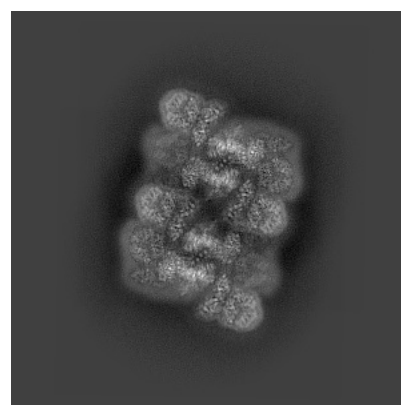
6.1.1 Primary map



X



Y

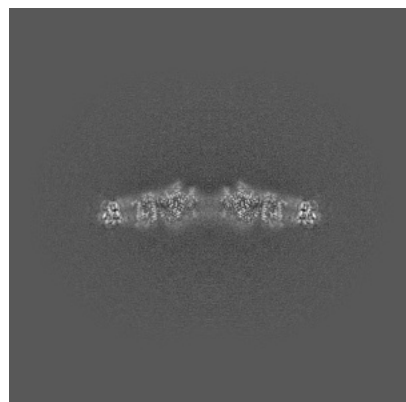


Z

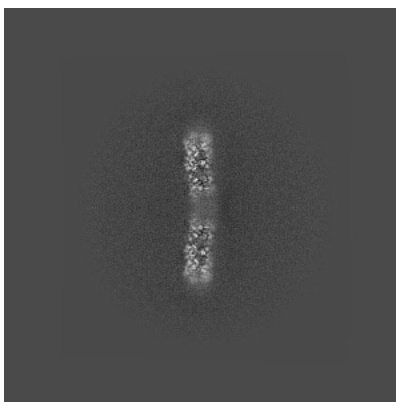
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

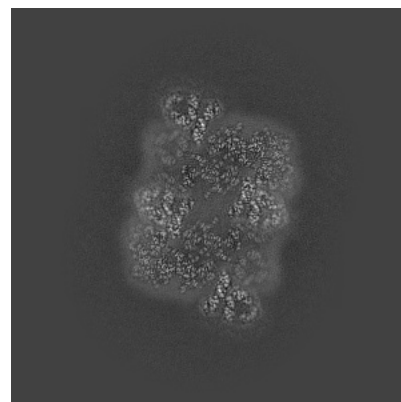
6.2.1 Primary map



X Index: 360



Y Index: 360

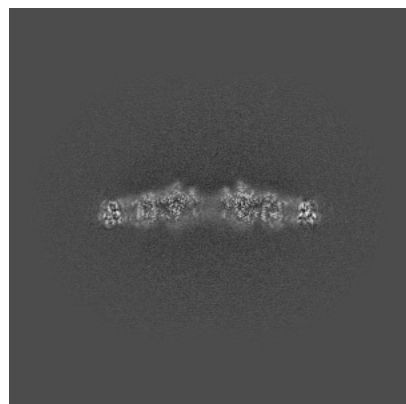


Z Index: 360

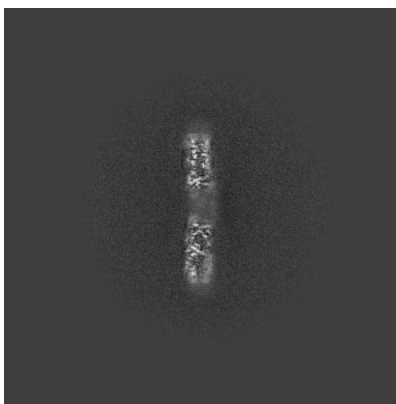
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

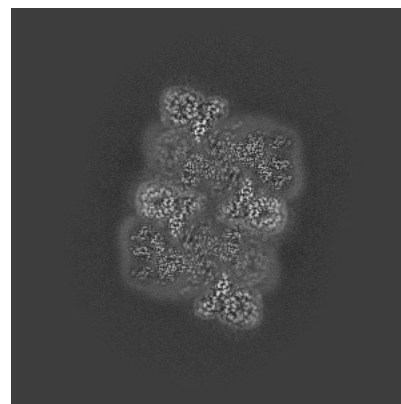
6.3.1 Primary map



X Index: 361



Y Index: 367

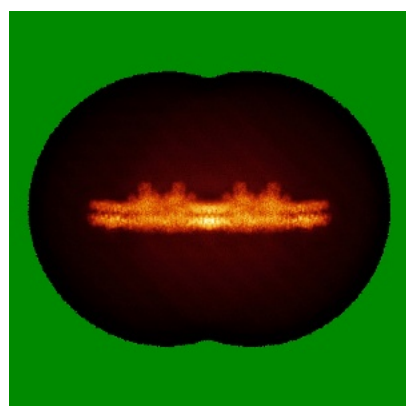


Z Index: 342

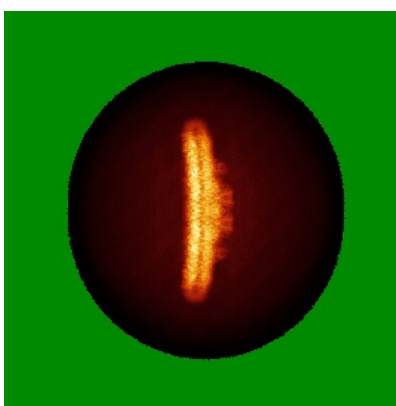
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

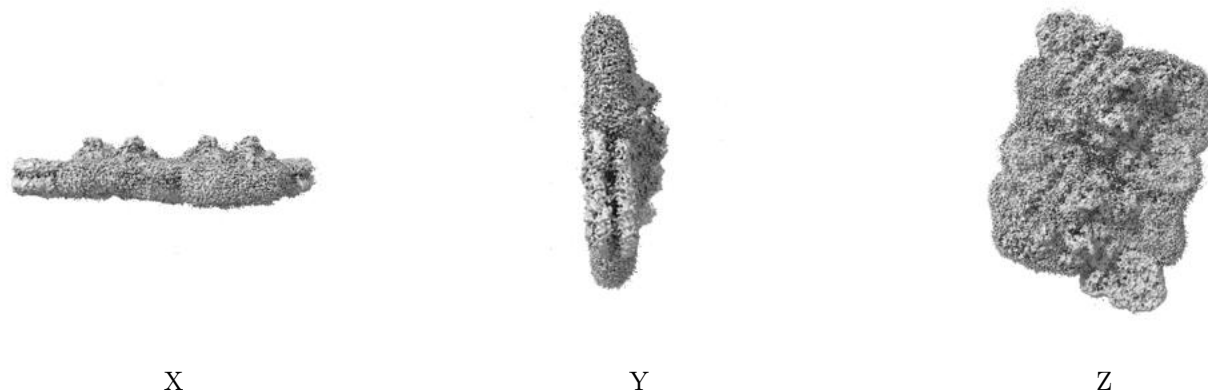


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

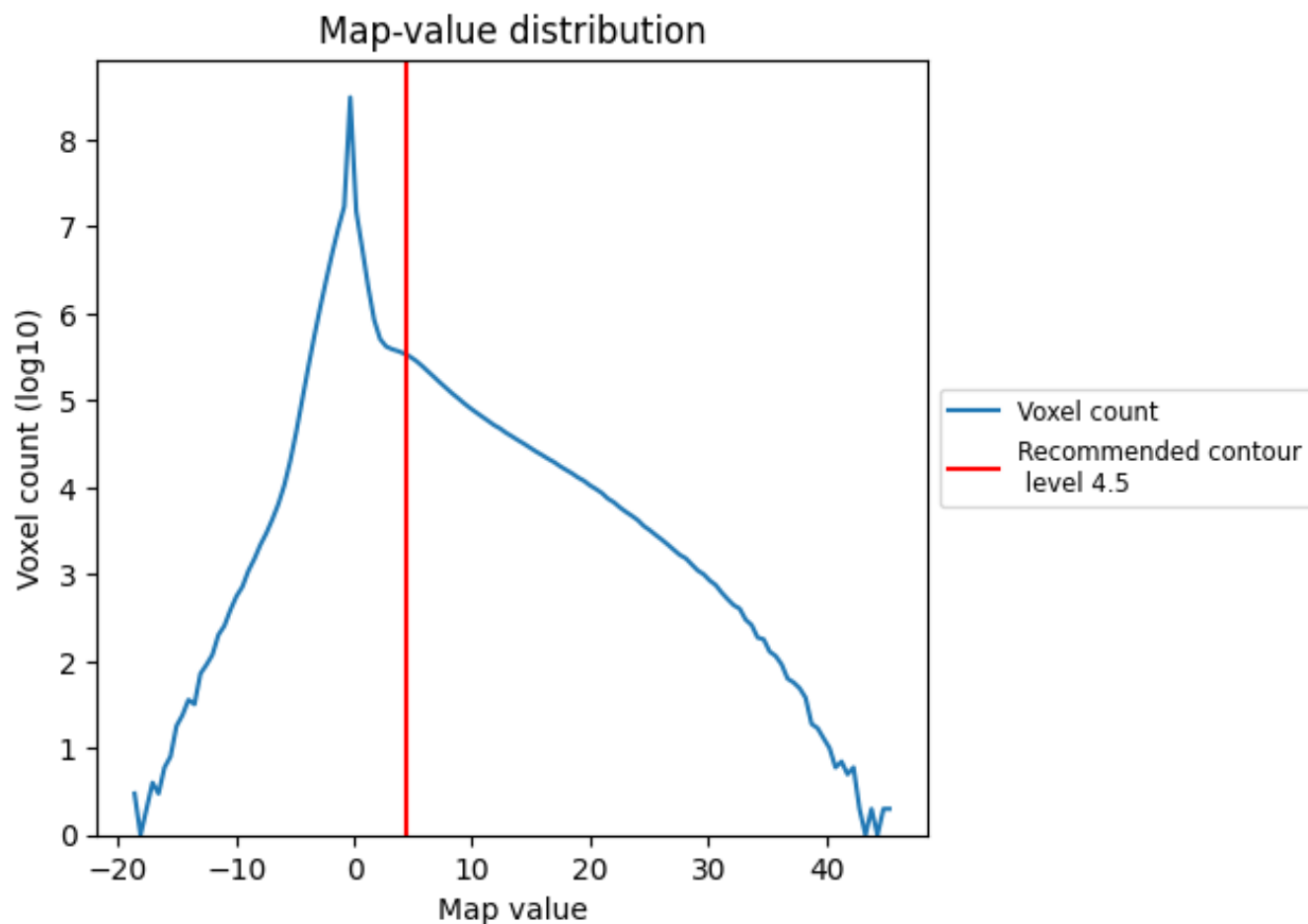
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

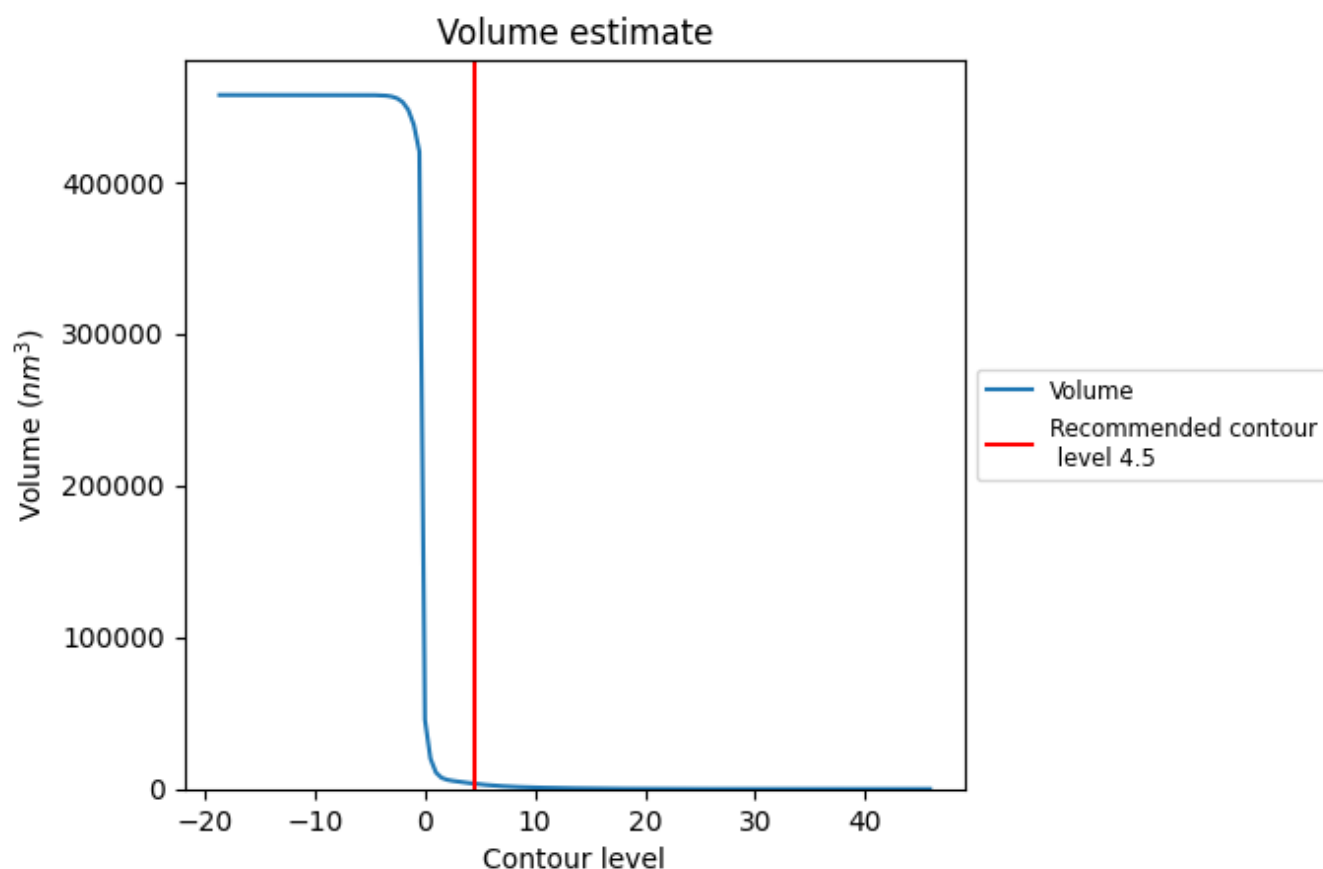
This section contains the results of statistical analysis of the map.

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.

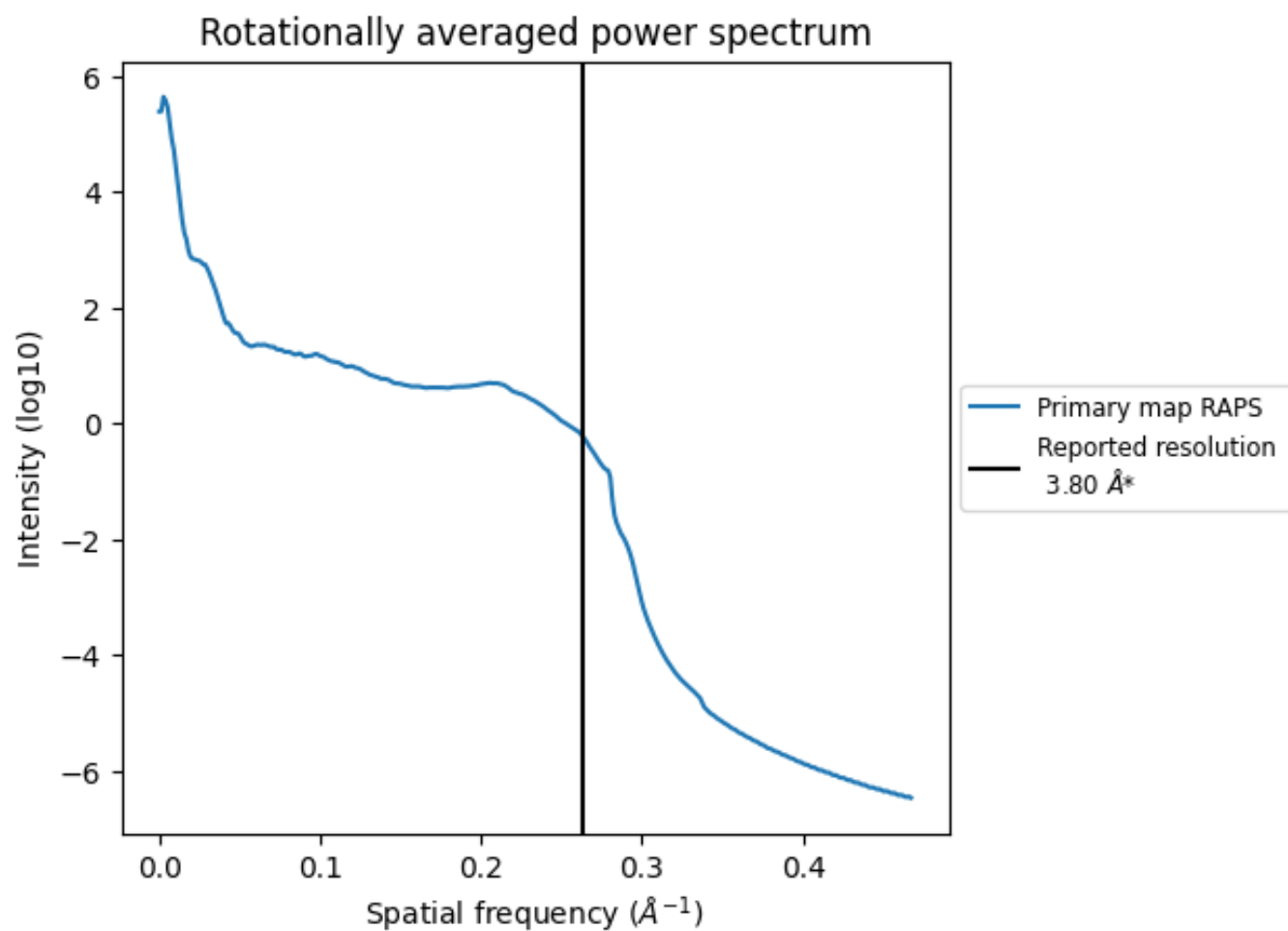
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3500 nm^3 ; this corresponds to an approximate mass of 3162 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 0.263 Å⁻¹

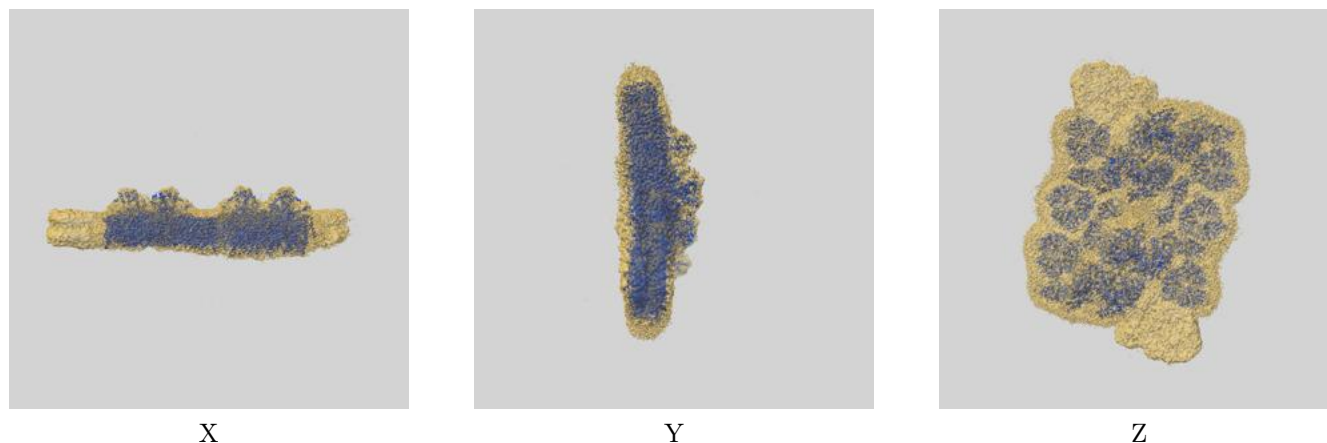
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

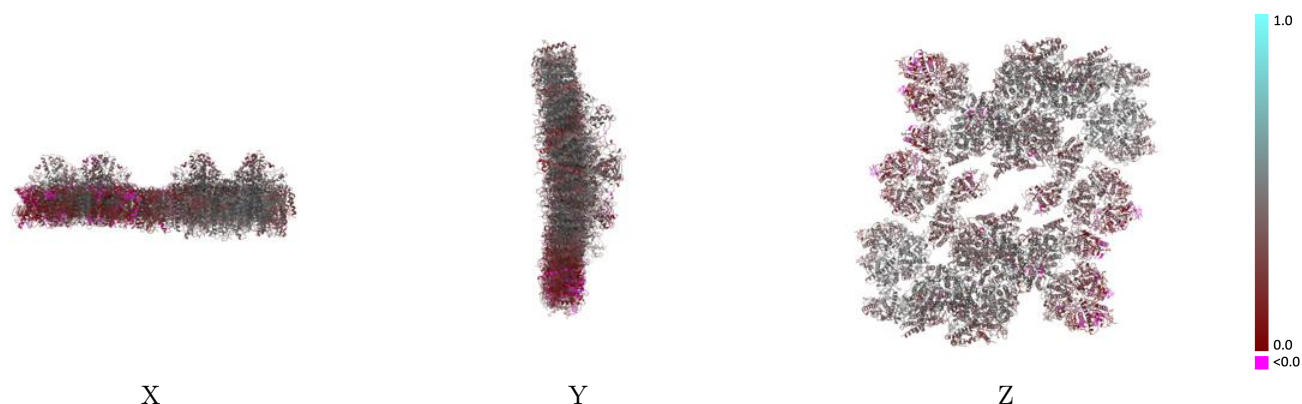
This section contains information regarding the fit between EMDB map EMD-63017 and PDB model 9LE7. Per-residue inclusion information can be found in [section 3](#) on [page 58](#).

9.1 Map-model overlay [i](#)



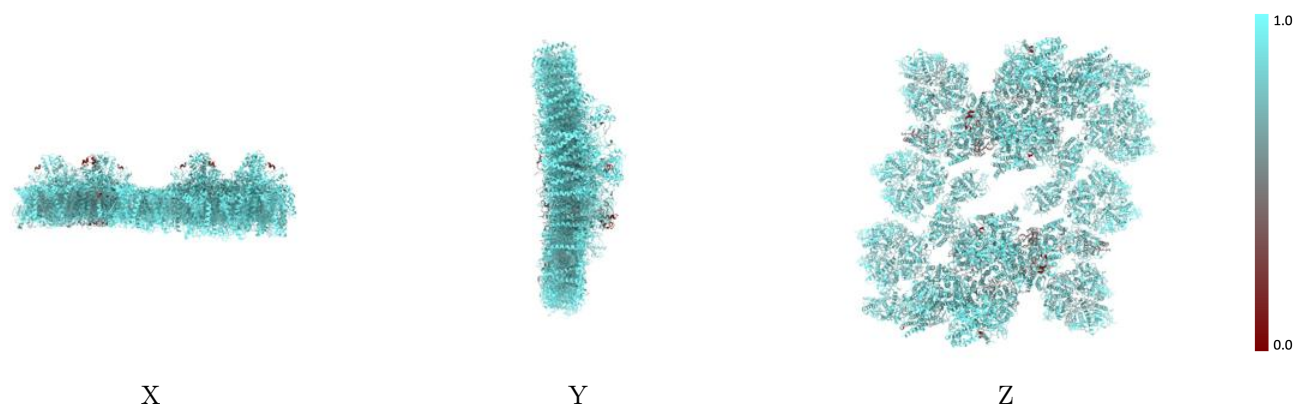
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



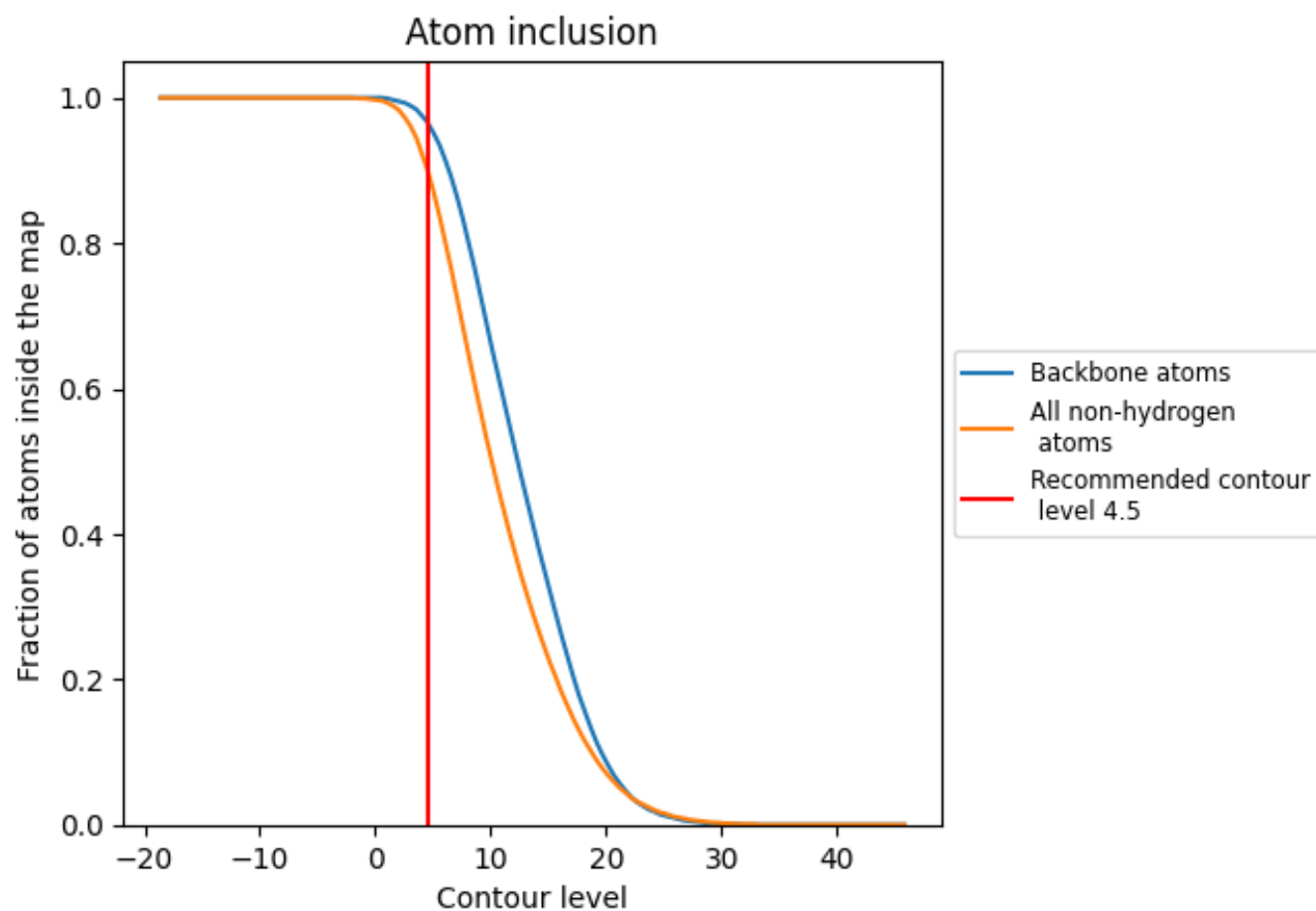
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 90% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.3560
0	 0.9480	 0.3160
1	 0.9370	 0.4360
2	 0.9520	 0.4400
3	 0.9320	 0.3050
4	 0.8930	 0.3100
5	 0.9690	 0.2760
6	 0.9510	 0.3040
7	 0.9720	 0.1710
8	 0.9130	 0.2480
9	 0.9670	 0.2830
A	 0.9210	 0.4230
A0	 0.8670	 0.3990
A1	 0.8980	 0.3770
A2	 0.9450	 0.4500
A6	 0.8890	 0.4040
A7	 0.8350	 0.4330
A8	 0.6400	 0.2120
AA	 0.9690	 0.1720
AB	 0.9110	 0.2560
Au	 0.9410	 0.3990
Av	 0.9380	 0.3490
Aw	 0.9420	 0.4570
Ay	 0.9050	 0.4320
Az	 0.8940	 0.4450
B	 0.9210	 0.4060
BA	 0.8270	 0.2090
BB	 0.9290	 0.4590
BC	 0.8680	 0.3250
BD	 0.9040	 0.4230
BE	 0.9140	 0.3960
BF	 0.8370	 0.4210
BG	 0.9130	 0.4230
BH	 0.9210	 0.2950
BI	 0.8260	 0.3230



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Chain	Atom inclusion	Q-score
BJ	 0.8500	 0.1420
BK	 0.8970	 0.3390
BL	 0.8870	 0.4330
BN	 0.8080	 0.3960
BO	 0.9110	 0.4230
BP	 0.9160	 0.3920
BQ	 0.8550	 0.1890
BU	 0.9390	 0.3370
BV	 0.7600	 0.2290
BW	 0.8640	 0.4060
BX	 0.7990	 0.2080
BY	 0.8310	 0.3500
BZ	 0.7580	 0.2340
Ba	 0.8710	 0.3090
Bb	 0.9200	 0.3420
C	 0.9310	 0.4240
D	 0.9480	 0.4270
E	 0.9320	 0.2950
F	 0.8800	 0.2980
G	 0.9380	 0.3880
H	 0.9210	 0.3270
I	 0.9320	 0.4500
K	 0.8860	 0.4190
L	 0.8960	 0.4270
M	 0.8550	 0.3610
N	 0.9350	 0.4410
R	 0.9280	 0.4320
S	 0.8790	 0.3960
T	 0.8390	 0.4080
U	 0.6450	 0.2100
W	 0.8690	 0.3810
X	 0.8270	 0.2140
Y	 0.9250	 0.4470
Z	 0.8600	 0.3170
a	 0.8980	 0.4140
b	 0.9080	 0.3850
c	 0.8280	 0.4060
d	 0.9010	 0.4090
e	 0.9230	 0.2840
f	 0.8130	 0.3050
g	 0.8530	 0.1340
h	 0.8620	 0.3220

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Chain	Atom inclusion	Q-score
i	 0.8690	 0.4210
k	 0.7780	 0.3800
l	 0.8880	 0.4130
m	 0.9080	 0.3870
n	 0.8570	 0.1790
r	 0.9370	 0.3280
s	 0.7480	 0.2090
t	 0.8520	 0.3960
u	 0.8040	 0.2000
v	 0.9260	 0.4160
w	 0.8310	 0.3380
x	 0.7420	 0.2240
y	 0.8680	 0.2970
z	 0.9120	 0.3420