



wwPDB EM Validation Summary Report ⓘ

Sep 29, 2026 – 10:03 PM JST

PDB ID : 8Z9D / pdb_00008z9d
EMDB ID : EMD-39860
Title : cryo-EM structure of PSII-LHCII megacomplex from spinach
Authors : Shan, J.Y.; Liu, Z.F.
Deposited on : 2024-04-23
Resolution : 3.22 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 Phenix2.2
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) : 2.51

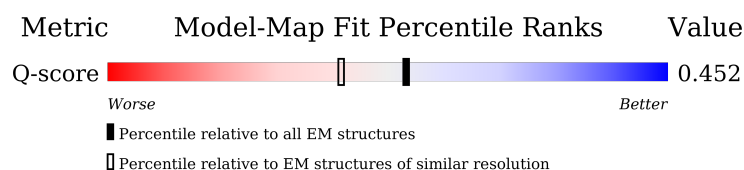
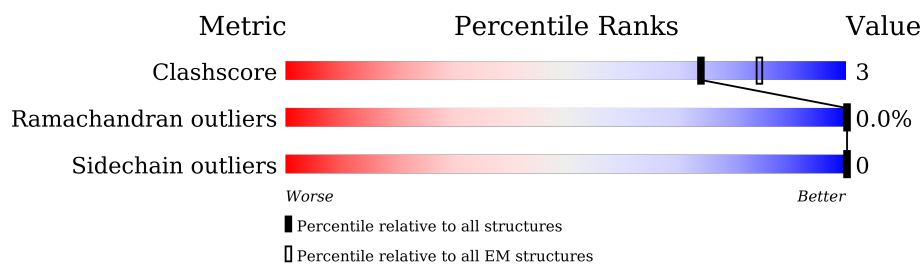
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 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.



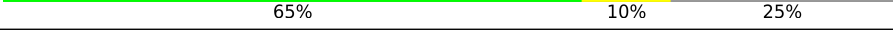
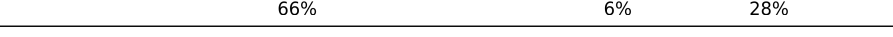
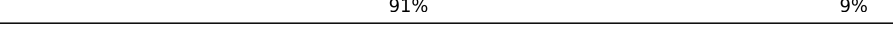
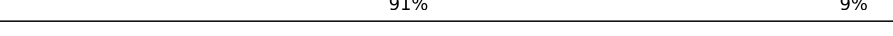
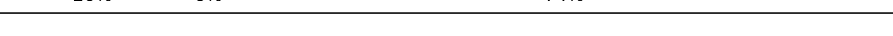
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.72 - 3.72)

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	A	351	
1	AA	351	
1	Aa	351	
1	a	351	

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Mol	Chain	Length	Quality of chain
2	O	332	
2	OO	332	
2	Oo	332	
2	o	332	
3	R	286	
3	RR	286	
3	Rr	286	
3	r	286	
4	S	295	
4	SS	295	
4	Ss	295	
4	s	295	
5	T	33	
5	TT	33	
5	Tt	33	
5	t	33	
6	U	99	
6	UU	99	
6	Uu	99	
6	u	99	
7	W	137	
7	WW	137	
7	Ww	137	
7	w	137	
8	X	117	

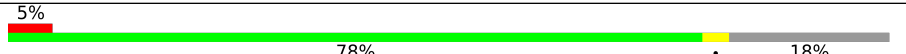
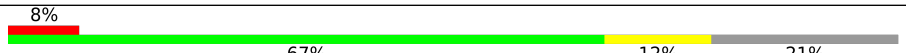
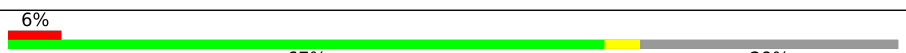
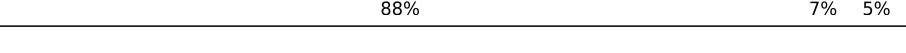
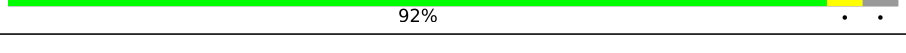
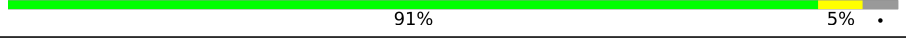
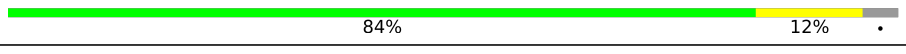
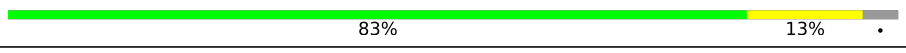
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Mol	Chain	Length	Quality of chain
8	XX	117	
8	Xx	117	
8	x	117	
9	G	267	
9	GG	267	
9	Gg	267	
9	N	267	
9	NN	267	
9	Nn	267	
9	Y	267	
9	YY	267	
9	Yy	267	
9	g	267	
9	n	267	
9	y	267	
10	Z	62	
10	ZZ	62	
10	Zz	62	
10	z	62	
11	4	259	
11	44	259	
12	P	267	
12	PP	267	
12	Pp	267	
12	p	267	

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Mol	Chain	Length	Quality of chain
13	Q	232	
13	QQ	232	
13	Qq	232	
13	q	232	
14	1	267	
14	11	267	
14	2	267	
14	22	267	
15	3	264	
15	33	264	
16	0	140	
16	00	140	
17	5	199	
17	55	199	
18	C	473	
18	CC	473	
18	Cc	473	
18	c	473	
19	D	352	
19	DD	352	
19	Dd	352	
19	d	352	
20	E	83	
20	EE	83	
20	Ee	83	

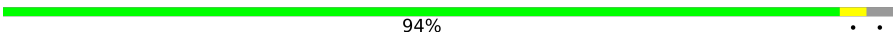
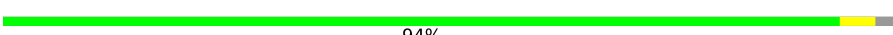
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Mol	Chain	Length	Quality of chain
20	e	83	
21	F	39	
21	FF	39	
21	Ff	39	
21	f	39	
22	H	73	
22	HH	73	
22	Hh	73	
22	h	73	
23	I	36	
23	II	36	
23	Ii	36	
23	i	36	
24	J	40	
24	JJ	40	
24	Jj	40	
24	j	40	
25	K	59	
25	KK	59	
25	Kk	59	
25	k	59	
26	L	38	
26	LL	38	
26	Ll	38	
26	l	38	

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Mol	Chain	Length	Quality of chain
27	M	34	 91% 6% .
27	MM	34	 94% . .
27	Mm	34	 91% . 6%
27	m	34	 85% 9% 6%
28	B	508	 92% 6% .
28	BB	508	 94% . .
28	Bb	508	 91% 5% .
28	b	508	 91% 5% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	PL9	A	410	-	X	-	-
35	PL9	AA	410	-	X	-	-
35	PL9	D	407	-	X	-	-
35	PL9	DD	406	-	X	-	-
35	PL9	Dd	404	-	X	-	-
35	PL9	d	404	-	X	-	-
45	BCT	D	403	-	-	X	-

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 339330 atoms, of which 168031 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	335	Total	C	H	N	O	S	0	0
			5145	1710	2526	431	465	13		
1	a	334	Total	C	H	N	O	S	0	0
			5134	1707	2521	430	463	13		
1	AA	335	Total	C	H	N	O	S	0	0
			5146	1710	2527	431	465	13		
1	Aa	334	Total	C	H	N	O	S	0	0
			5134	1707	2521	430	463	13		

- Molecule 2 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Oo	234	Total	C	H	N	O	S	0	0
			3524	1125	1748	289	359	3		
2	O	236	Total	C	H	N	O	S	0	0
			3559	1136	1765	292	363	3		
2	o	234	Total	C	H	N	O	S	0	0
			3524	1125	1748	289	359	3		
2	OO	236	Total	C	H	N	O	S	0	0
			3561	1136	1767	292	363	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	Rr	228	Total	C	H	N	O	S	0	0
			3541	1155	1763	289	330	4		
3	R	227	Total	C	H	N	O	S	0	0
			3526	1150	1753	290	329	4		
3	r	228	Total	C	H	N	O	S	0	0
			3541	1155	1763	289	330	4		
3	RR	227	Total	C	H	N	O	S	0	0
			3526	1150	1753	290	329	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Ss	213	Total	C	H	N	O	S	0	0
			3266	1078	1617	268	298	5		
4	S	222	Total	C	H	N	O	S	0	0
			3395	1117	1683	280	310	5		
4	s	213	Total	C	H	N	O	S	0	0
			3266	1078	1617	268	298	5		
4	SS	222	Total	C	H	N	O	S	0	0
			3395	1117	1683	280	310	5		

- Molecule 5 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	Tt	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	T	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	t	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	TT	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		

- Molecule 6 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Uu	26	Total	C	H	N	O	S	0	0
			420	129	218	37	33	3		
6	U	27	Total	C	H	N	O	S	0	0
			435	134	226	38	34	3		
6	u	26	Total	C	H	N	O	S	0	0
			420	129	218	37	33	3		
6	UU	27	Total	C	H	N	O	S	0	0
			435	134	226	38	34	3		

- Molecule 7 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Ww	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		
7	W	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		
7	w	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	WW	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		

- Molecule 8 is a protein called Photosystem II reaction center X protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Xx	34	Total	C	H	N	O		0	0
			487	158	250	37	42			
8	X	46	Total	C	H	N	O		0	0
			667	213	341	53	60			
8	x	34	Total	C	H	N	O		0	0
			487	158	250	37	42			
8	XX	48	Total	C	H	N	O	S	0	0
			701	223	359	55	62	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Xx	45	GLY	SER	conflict	UNP A0A9R0JQ89
X	45	GLY	SER	conflict	UNP A0A9R0JQ89
x	45	GLY	SER	conflict	UNP A0A9R0JQ89
XX	45	GLY	SER	conflict	UNP A0A9R0JQ89

- Molecule 9 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Yy	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	G	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	N	217	Total	C	H	N	O	S	0	0
			3245	1077	1589	269	303	7		
9	Y	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	g	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	n	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	y	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	GG	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	NN	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	YY	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	Gg	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	Nn	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Zz	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	Z	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	z	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	ZZ	61	Total	C	H	N	O	0	0
			933	306	479	68	80		

- Molecule 11 is a protein called Chlorophyll a-b binding protein CP24, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	44	186	Total	C	H	N	O	S	0	0
			2847	952	1395	234	262	4		
11	4	186	Total	C	H	N	O	S	0	0
			2847	952	1395	234	262	4		

- Molecule 12 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Pp	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0
12	p	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0
12	P	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0
12	PP	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0

- Molecule 13 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Qq	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	q	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	Q	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	QQ	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	11	206	Total	C	H	N	O	S	0	0
			3075	1021	1505	254	288	7		
14	22	218	Total	C	H	N	O	S	0	0
			3253	1079	1592	270	305	7		
14	1	207	Total	C	H	N	O	S	0	0
			3086	1024	1510	255	290	7		
14	2	218	Total	C	H	N	O	S	0	0
			3253	1079	1592	270	305	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	33	207	Total	C	H	N	O	S	0	0
			3189	1061	1575	258	290	5		
15	3	209	Total	C	H	N	O	S	0	0
			3195	1063	1573	260	294	5		

- Molecule 16 is a protein called Photosystem II 10 kDa polypeptide, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	0	99	Total	C	H	N	O	S	0	0
			1448	462	726	120	139	1		
16	00	99	Total	C	H	N	O	S	0	0
			1448	462	726	120	139	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	5	40	Total	C	H	N	O	S	0	0
			633	199	325	55	53	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
17	55	40	Total	C	H	N	O	S	0	0
			633	199	325	55	53	1		

- Molecule 18 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	C	449	Total	C	H	N	O	S	0	0
			6892	2284	3417	581	599	11		
18	c	449	Total	C	H	N	O	S	0	0
			6891	2284	3416	581	599	11		
18	CC	449	Total	C	H	N	O	S	0	0
			6892	2284	3417	581	599	11		
18	Cc	449	Total	C	H	N	O	S	0	0
			6891	2284	3416	581	599	11		

- Molecule 19 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	D	339	Total	C	H	N	O	S	0	0
			5274	1780	2580	441	461	12		
19	d	340	Total	C	H	N	O	S	0	0
			5295	1786	2592	443	462	12		
19	DD	339	Total	C	H	N	O	S	0	0
			5275	1780	2581	441	461	12		
19	Dd	340	Total	C	H	N	O	S	0	0
			5295	1786	2592	443	462	12		

- Molecule 20 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	80	Total	C	H	N	O	0	0
			1255	414	615	105	121		
20	e	75	Total	C	H	N	O	0	0
			1201	398	591	100	112		
20	EE	80	Total	C	H	N	O	0	0
			1255	414	615	105	121		
20	Ee	75	Total	C	H	N	O	0	0
			1201	398	591	100	112		

- Molecule 21 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	34	Total	C	H	N	O	S	
			558	187	282	45	43	1	0
21	f	31	Total	C	H	N	O	S	
			509	169	259	42	38	1	0
21	FF	34	Total	C	H	N	O	S	
			558	187	282	45	43	1	0
21	Ff	31	Total	C	H	N	O	S	
			509	169	259	42	38	1	0

- Molecule 22 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0
22	h	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0
22	HH	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0
22	Hh	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0

- Molecule 23 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	35	Total	C	H	N	O	S	
			581	195	295	44	46	1	0
23	i	33	Total	C	H	N	O	S	
			542	184	276	39	42	1	0
23	II	35	Total	C	H	N	O	S	
			581	195	295	44	46	1	0
23	Ii	33	Total	C	H	N	O	S	
			542	184	276	39	42	1	0

- Molecule 24 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	37	Total	C	H	N	O		
			552	182	283	41	46	0	0
24	j	34	Total	C	H	N	O		
			505	168	258	38	41	0	0
24	JJ	37	Total	C	H	N	O		
			552	182	283	41	46	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	Jj	34	Total	C	H	N	O	0	0
			505	168	258	38	41		

- Molecule 25 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	K	37	Total 617	C 217	H 310	N 43	O 46	S 1	0	0
25	k	37	Total 617	C 217	H 310	N 43	O 46	S 1	0	0
25	KK	37	Total 617	C 217	H 310	N 43	O 46	S 1	0	0
25	Kk	37	Total 616	C 217	H 310	N 43	O 45	S 1	0	0

- Molecule 26 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	35	Total 579	C 196	H 284	N 46	O 53	0	0
26	l	36	Total 596	C 201	H 292	N 48	O 55	0	0
26	LL	35	Total 579	C 196	H 284	N 46	O 53	0	0
26	Ll	36	Total 596	C 201	H 292	N 48	O 55	0	0

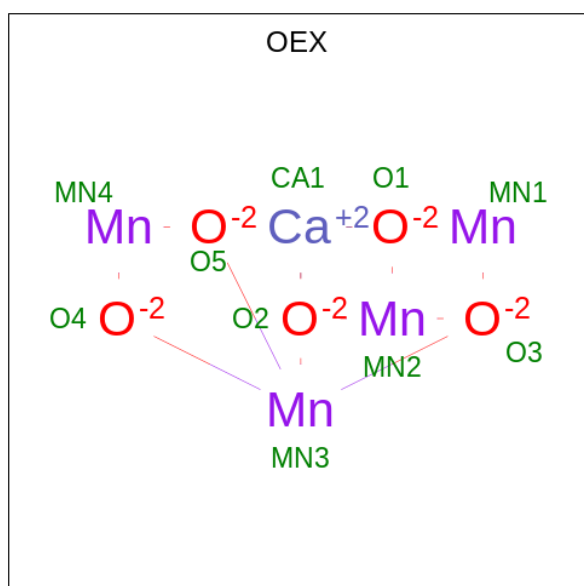
- Molecule 27 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	M	33	Total 543	C 177	H 285	N 37	O 43	S 1	0	0
27	m	32	Total 523	C 172	H 273	N 36	O 42		0	0
27	MM	33	Total 543	C 177	H 285	N 37	O 43	S 1	0	0
27	Mm	32	Total 523	C 172	H 273	N 36	O 42		0	0

- Molecule 28 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	487	Total	C	H	N	O	S	0	0
			7510	2501	3690	640	667	12		
28	BB	499	Total	C	H	N	O	S	0	0
			7692	2562	3778	655	685	12		
28	B	499	Total	C	H	N	O	S	0	0
			7692	2562	3778	655	685	12		
28	Bb	487	Total	C	H	N	O	S	0	0
			7510	2501	3690	640	667	12		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	AA	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	Cc	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Fe	0
			1	1	
30	a	1	Total	Fe	0
			1	1	

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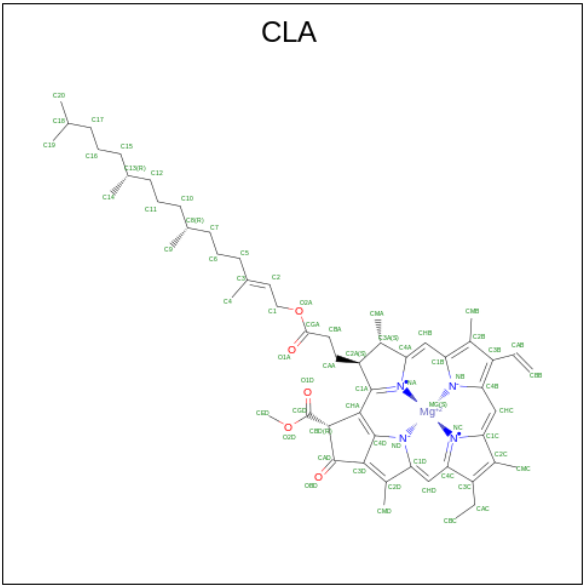
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Mol	Chain	Residues	Atoms		AltConf
30	AA	1	Total	Fe	0
			1	1	
30	Aa	1	Total	Fe	0
			1	1	

- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Cl	0
			2	2	
31	a	2	Total	Cl	0
			2	2	
31	AA	2	Total	Cl	0
			2	2	
31	Aa	2	Total	Cl	0
			2	2	

- Molecule 32 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						AltConf
32	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	A	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 73	C 34	H 31	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms						AltConf
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	G	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	G	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	G	1	Total 73	C 34	H 31	Mg 1	N 4	O 3	0
32	G	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	G	1	Total 95	C 42	H 43	Mg 1	N 4	O 5	0
32	G	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	G	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms						AltConf
32	G	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	S	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	S	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	S	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	S	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	S	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	S	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	S	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	S	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	X	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	Y	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Y	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	Y	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	Y	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Y	1	Total 73	C 34	H 31	Mg 1	N 4	O 3	0
32	Y	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Y	1	Total 114	C 49	H 55	Mg 1	N 4	O 5	0
32	Y	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	a	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	a	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
32	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	n	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	n	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	n	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	n	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	n	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	y	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	y	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	y	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	y	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	y	1	Total 73	C 34	H 31	Mg 1	N 4	O 3	0
32	y	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	y	1	Total 114	C 49	H 55	Mg 1	N 4	O 5	0
32	y	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	AA	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	AA	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	AA	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0



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Mol	Chain	Residues	Atoms						AltConf
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	DD	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	DD	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	DD	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	GG	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	SS	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	XX	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	YY	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	YY	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	YY	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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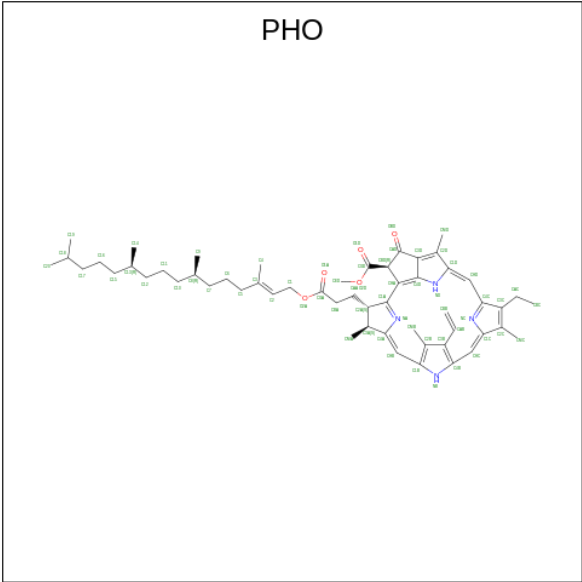
Mol	Chain	Residues	Atoms						AltConf
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
32	Dd	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Dd	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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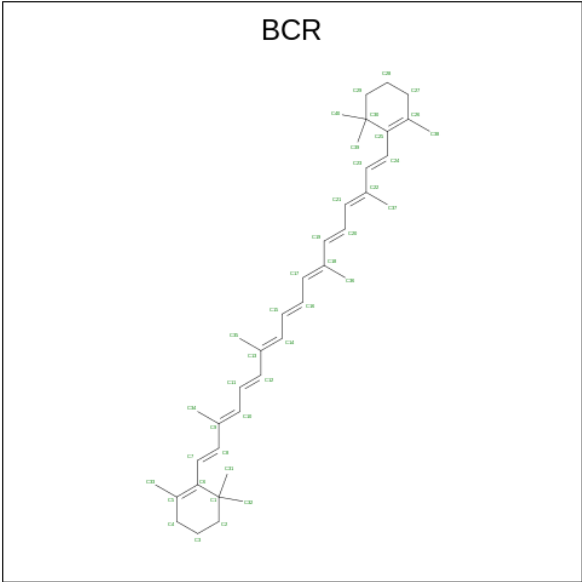
Mol	Chain	Residues	Atoms						AltConf
32	Gg	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	D	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	AA	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	DD	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	Aa	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	Aa	1	Total	C	H	N	O	0
			138	55	74	4	5	

- Molecule 34 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	D	1	Total	C	H	0
			96	40	56	
34	H	1	Total	C	H	0
			96	40	56	
34	K	1	Total	C	H	0
			96	40	56	
34	T	1	Total	C	H	0
			96	40	56	
34	a	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	c	1	Total	C	H	0
			96	40	56	
34	c	1	Total	C	H	0
			96	40	56	

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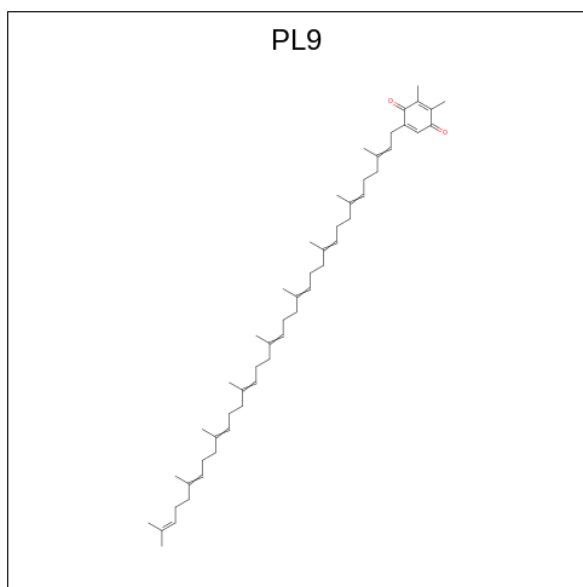
Mol	Chain	Residues	Atoms			AltConf
34	c	1	Total 96	C 40	H 56	0
34	d	1	Total 96	C 40	H 56	0
34	h	1	Total 96	C 40	H 56	0
34	k	1	Total 96	C 40	H 56	0
34	AA	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	CC	1	Total 96	C 40	H 56	0
34	CC	1	Total 96	C 40	H 56	0
34	CC	1	Total 96	C 40	H 56	0
34	DD	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	KK	1	Total 96	C 40	H 56	0
34	TT	1	Total 96	C 40	H 56	0
34	XX	1	Total 96	C 40	H 56	0
34	Aa	1	Total 96	C 40	H 56	0

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Mol	Chain	Residues	Atoms			AltConf
34	Bb	1	Total	C	H	0
			96	40	56	
34	Bb	1	Total	C	H	0
			96	40	56	
34	Bb	1	Total	C	H	0
			96	40	56	
34	Cc	1	Total	C	H	0
			96	40	56	
34	Cc	1	Total	C	H	0
			96	40	56	
34	Cc	1	Total	C	H	0
			96	40	56	
34	Dd	1	Total	C	H	0
			96	40	56	
34	Hh	1	Total	C	H	0
			96	40	56	
34	Kk	1	Total	C	H	0
			96	40	56	

- Molecule 35 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) (labeled as "Ligand of Interest" by depositor).



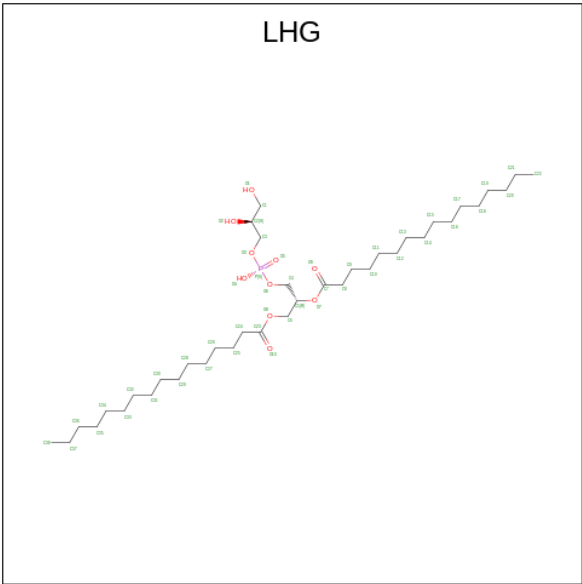
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			55	53	2	

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Mol	Chain	Residues	Atoms			AltConf
35	D	1	Total	C	O	0
			55	53	2	
35	d	1	Total	C	O	0
			55	53	2	
35	AA	1	Total	C	O	0
			55	53	2	
35	DD	1	Total	C	O	0
			55	53	2	
35	Dd	1	Total	C	O	0
			55	53	2	

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	A	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	A	1	Total	C	H	O	P	0
			108	34	63	10	1	
36	Rr	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Ss	1	Total	C	H	O	P	0
			117	37	69	10	1	
36	Yy	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
36	44	1	Total 33	C 10	H 12	O 10	P 1	0
36	44	1	Total 31	C 8	H 12	O 10	P 1	0
36	11	1	Total 72	C 23	H 38	O 10	P 1	0
36	22	1	Total 72	C 23	H 38	O 10	P 1	0
36	33	1	Total 72	C 23	H 38	O 10	P 1	0
36	1	1	Total 60	C 19	H 30	O 10	P 1	0
36	3	1	Total 72	C 23	H 38	O 10	P 1	0
36	0	1	Total 114	C 36	H 67	O 10	P 1	0
36	C	1	Total 63	C 20	H 32	O 10	P 1	0
36	D	1	Total 102	C 32	H 59	O 10	P 1	0
36	D	1	Total 123	C 38	H 74	O 10	P 1	0
36	D	1	Total 72	C 23	H 38	O 10	P 1	0
36	G	1	Total 72	C 23	H 38	O 10	P 1	0
36	J	1	Total 51	C 16	H 24	O 10	P 1	0
36	K	1	Total 72	C 23	H 38	O 10	P 1	0
36	N	1	Total 84	C 27	H 46	O 10	P 1	0
36	Y	1	Total 123	C 38	H 74	O 10	P 1	0
36	a	1	Total 81	C 26	H 44	O 10	P 1	0
36	d	1	Total 102	C 32	H 59	O 10	P 1	0
36	d	1	Total 123	C 38	H 74	O 10	P 1	0
36	g	1	Total 72	C 23	H 38	O 10	P 1	0

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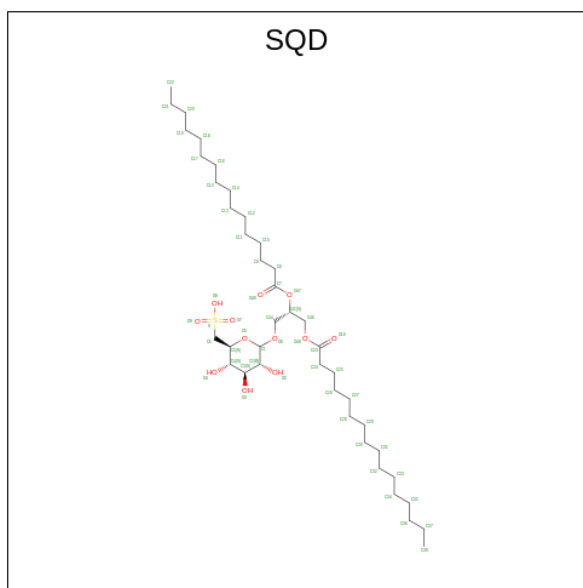
Mol	Chain	Residues	Atoms					AltConf
36	l	1	Total 123	C 38	H 74	O 10	P 1	0
36	n	1	Total 123	C 38	H 74	O 10	P 1	0
36	r	1	Total 123	C 38	H 74	O 10	P 1	0
36	s	1	Total 117	C 37	H 69	O 10	P 1	0
36	y	1	Total 123	C 38	H 74	O 10	P 1	0
36	4	1	Total 31	C 8	H 12	O 10	P 1	0
36	4	1	Total 33	C 10	H 12	O 10	P 1	0
36	AA	1	Total 72	C 23	H 38	O 10	P 1	0
36	AA	1	Total 108	C 34	H 63	O 10	P 1	0
36	BB	1	Total 72	C 23	H 38	O 10	P 1	0
36	CC	1	Total 72	C 23	H 38	O 10	P 1	0
36	CC	1	Total 81	C 26	H 44	O 10	P 1	0
36	DD	1	Total 102	C 32	H 59	O 10	P 1	0
36	DD	1	Total 123	C 38	H 74	O 10	P 1	0
36	EE	1	Total 93	C 29	H 53	O 10	P 1	0
36	GG	1	Total 72	C 23	H 38	O 10	P 1	0
36	II	1	Total 72	C 23	H 38	O 10	P 1	0
36	JJ	1	Total 69	C 22	H 36	O 10	P 1	0
36	KK	1	Total 72	C 23	H 38	O 10	P 1	0
36	NN	1	Total 84	C 27	H 46	O 10	P 1	0
36	SS	1	Total 48	C 15	H 22	O 10	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
36	YY	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Dd	1	Total	C	H	O	P	0
			102	32	59	10	1	
36	Dd	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Dd	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	Gg	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	Ll	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Nn	1	Total	C	H	O	P	0
			123	38	74	10	1	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



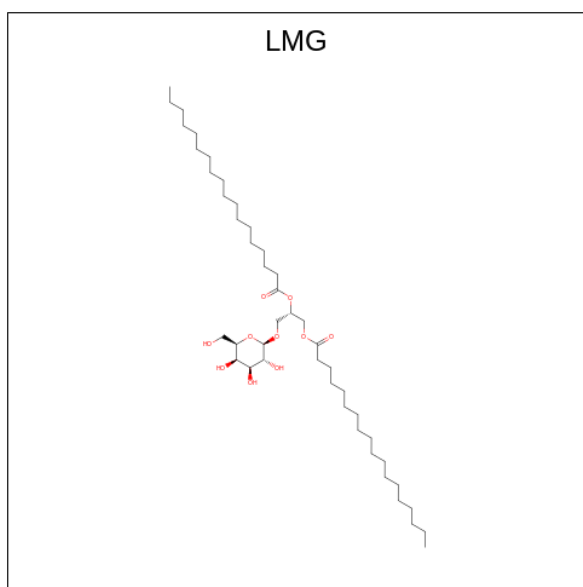
Mol	Chain	Residues	Atoms					AltConf
37	A	1	Total	C	H	O	S	0
			69	22	34	12	1	
37	C	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	L	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	L	1	Total	C	H	O	S	0
			72	23	36	12	1	

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Mol	Chain	Residues	Atoms					AltConf
37	l	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	AA	1	Total	C	H	O	S	0
			69	22	34	12	1	
37	BB	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	CC	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	B	1	Total	C	H	O	S	0
			108	34	61	12	1	
37	B	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	LL	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	LL	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	Aa	1	Total	C	H	O	S	0
			108	34	61	12	1	
37	Ll	1	Total	C	H	O	S	0
			132	41	78	12	1	

- Molecule 38 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



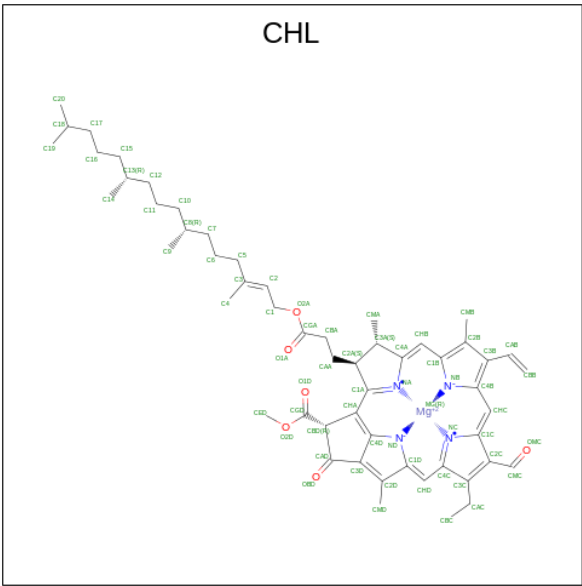
Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	H	O	0
			78	26	42	10	

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Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total 123	C 41	H 72	O 10	0
38	F	1	Total 108	C 36	H 62	O 10	0
38	W	1	Total 114	C 38	H 66	O 10	0
38	a	1	Total 97	C 33	H 54	O 10	0
38	b	1	Total 78	C 26	H 42	O 10	0
38	b	1	Total 78	C 26	H 42	O 10	0
38	c	1	Total 72	C 24	H 38	O 10	0
38	j	1	Total 108	C 36	H 62	O 10	0
38	m	1	Total 123	C 41	H 72	O 10	0
38	AA	1	Total 78	C 26	H 42	O 10	0
38	BB	1	Total 105	C 35	H 60	O 10	0
38	CC	1	Total 87	C 29	H 48	O 10	0
38	DD	1	Total 108	C 36	H 62	O 10	0
38	B	1	Total 105	C 35	H 60	O 10	0
38	WW	1	Total 114	C 38	H 66	O 10	0
38	Aa	1	Total 97	C 33	H 54	O 10	0
38	Bb	1	Total 78	C 26	H 42	O 10	0
38	Bb	1	Total 78	C 26	H 42	O 10	0
38	Cc	1	Total 72	C 24	H 38	O 10	0
38	Dd	1	Total 108	C 36	H 62	O 10	0
38	Mm	1	Total 123	C 41	H 72	O 10	0

- Molecule 39 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms						AltConf
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	Yy	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Yy	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
39	44	1	Total	C	H	Mg	N	O	0
			73	34	28	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	

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Mol	Chain	Residues	Atoms						AltConf
39	1	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	1	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	1	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	1	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	G	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	G	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	G	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	G	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
39	G	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	G	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	N	1	Total 75	C 35	H 31	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms						AltConf
39	N	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	N	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	N	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	N	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	N	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	R	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	R	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	R	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	S	1	Total 91	C 41	H 39	Mg 1	N 4	O 6	0
39	S	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	S	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	S	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	Y	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	Y	1	Total 81	C 37	H 33	Mg 1	N 4	O 6	0
39	Y	1	Total 75	C 35	H 31	Mg 1	N 4	O 4	0
39	Y	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	Y	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	Y	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	g	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	g	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	g	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms						AltConf
39	g	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	g	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	g	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	r	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	r	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	r	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	y	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	y	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	y	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	y	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
39	y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			73	34	28	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			86	39	36	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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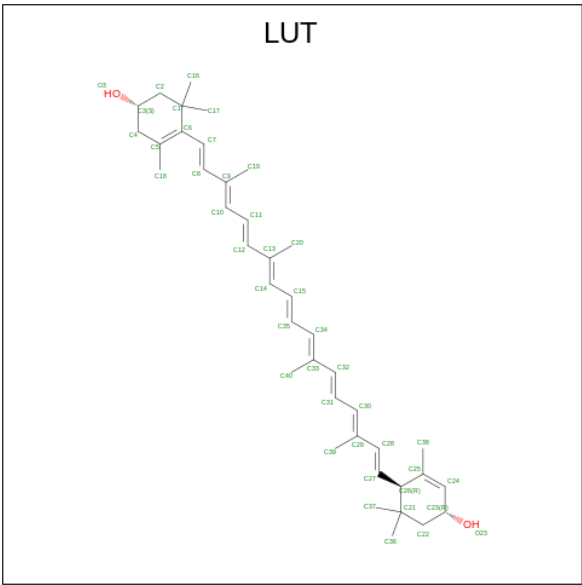
Mol	Chain	Residues	Atoms						AltConf
39	SS	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	SS	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	SS	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	SS	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	YY	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	YY	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
39	Nn	1	87	39	37	1	4	6	0

- Molecule 40 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
			Total	C	H	O	
40	Rr	1	98	40	56	2	0
40	Ss	1	98	40	56	2	0
40	Ss	1	98	40	56	2	0
40	Yy	1	98	40	56	2	0
40	Yy	1	98	40	56	2	0
40	44	1	98	40	56	2	0
40	22	1	98	40	56	2	0
40	2	1	98	40	56	2	0
40	G	1	98	40	56	2	0
40	G	1	98	40	56	2	0

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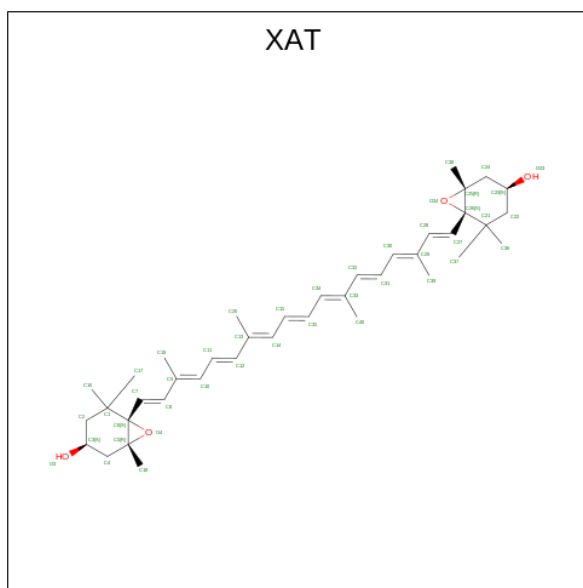
Mol	Chain	Residues	Atoms				AltConf
40	N	1	Total 98	C 40	H 56	O 2	0
40	N	1	Total 98	C 40	H 56	O 2	0
40	R	1	Total 98	C 40	H 56	O 2	0
40	S	1	Total 98	C 40	H 56	O 2	0
40	Y	1	Total 98	C 40	H 56	O 2	0
40	Y	1	Total 98	C 40	H 56	O 2	0
40	g	1	Total 98	C 40	H 56	O 2	0
40	g	1	Total 98	C 40	H 56	O 2	0
40	n	1	Total 98	C 40	H 56	O 2	0
40	n	1	Total 98	C 40	H 56	O 2	0
40	r	1	Total 98	C 40	H 56	O 2	0
40	s	1	Total 98	C 40	H 56	O 2	0
40	s	1	Total 98	C 40	H 56	O 2	0
40	y	1	Total 98	C 40	H 56	O 2	0
40	y	1	Total 98	C 40	H 56	O 2	0
40	4	1	Total 98	C 40	H 56	O 2	0
40	GG	1	Total 98	C 40	H 56	O 2	0
40	GG	1	Total 98	C 40	H 56	O 2	0
40	NN	1	Total 98	C 40	H 56	O 2	0
40	NN	1	Total 98	C 40	H 56	O 2	0
40	RR	1	Total 98	C 40	H 56	O 2	0

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Mol	Chain	Residues	Atoms				AltConf
40	SS	1	Total	C	H	O	0
			98	40	56	2	
40	YY	1	Total	C	H	O	0
			98	40	56	2	
40	YY	1	Total	C	H	O	0
			98	40	56	2	
40	Gg	1	Total	C	H	O	0
			98	40	56	2	
40	Gg	1	Total	C	H	O	0
			98	40	56	2	
40	Nn	1	Total	C	H	O	0
			98	40	56	2	
40	Nn	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 41 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).



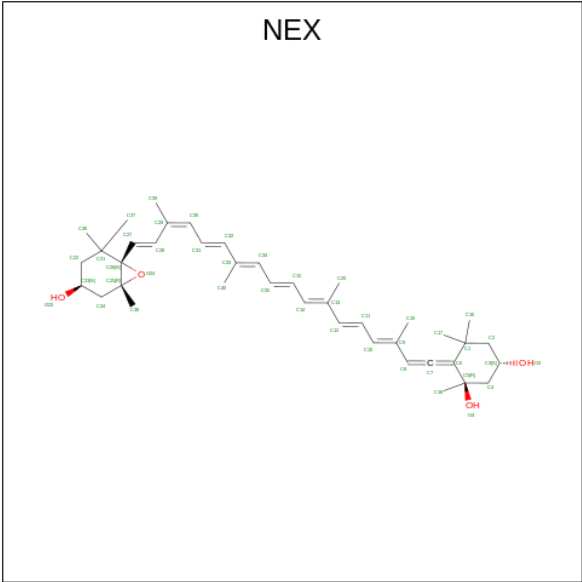
Mol	Chain	Residues	Atoms				AltConf
41	Rr	1	Total	C	H	O	0
			100	40	56	4	
41	Yy	1	Total	C	H	O	0
			100	40	56	4	
41	44	1	Total	C	H	O	0
			100	40	56	4	
41	G	1	Total	C	H	O	0
			100	40	56	4	

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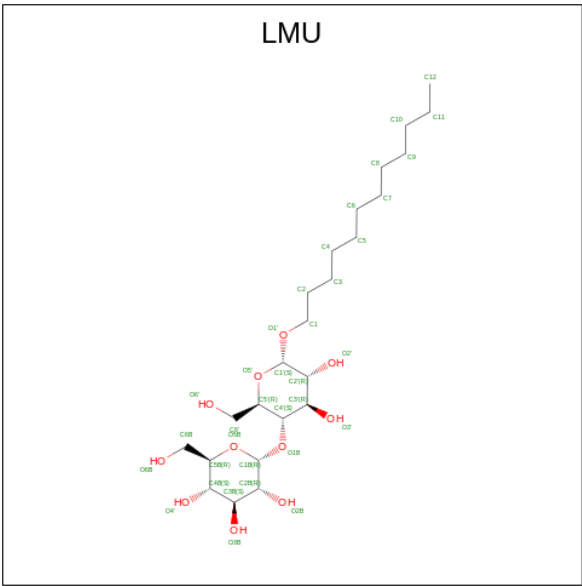
Mol	Chain	Residues	Atoms				AltConf
41	G	1	Total	C	H	O	0
			100	40	56	4	
41	N	1	Total	C	H	O	0
			100	40	56	4	
41	R	1	Total	C	H	O	0
			100	40	56	4	
41	g	1	Total	C	H	O	0
			100	40	56	4	
41	r	1	Total	C	H	O	0
			100	40	56	4	
41	y	1	Total	C	H	O	0
			100	40	56	4	
41	y	1	Total	C	H	O	0
			100	40	56	4	
41	4	1	Total	C	H	O	0
			100	40	56	4	
41	GG	1	Total	C	H	O	0
			100	40	56	4	
41	GG	1	Total	C	H	O	0
			100	40	56	4	
41	NN	1	Total	C	H	O	0
			100	40	56	4	
41	RR	1	Total	C	H	O	0
			100	40	56	4	
41	Gg	1	Total	C	H	O	0
			100	40	56	4	
41	Nn	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 42 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).



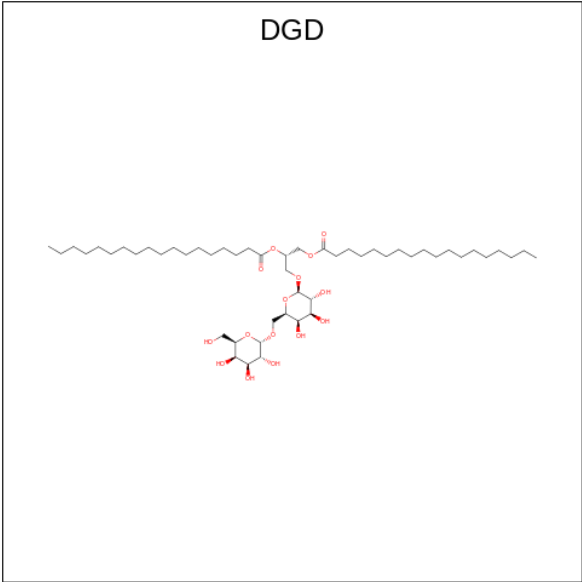
Mol	Chain	Residues	Atoms				AltConf
42	Rr	1	Total	C	H	O	0
			100	40	56	4	
42	Yy	1	Total	C	H	O	0
			100	40	56	4	
42	N	1	Total	C	H	O	0
			100	40	56	4	
42	R	1	Total	C	H	O	0
			100	40	56	4	
42	Y	1	Total	C	H	O	0
			100	40	56	4	
42	Y	1	Total	C	H	O	0
			100	40	56	4	
42	g	1	Total	C	H	O	0
			100	40	56	4	
42	n	1	Total	C	H	O	0
			100	40	56	4	
42	y	1	Total	C	H	O	0
			100	40	56	4	
42	NN	1	Total	C	H	O	0
			100	40	56	4	
42	RR	1	Total	C	H	O	0
			100	40	56	4	
42	YY	1	Total	C	H	O	0
			100	40	56	4	
42	Gg	1	Total	C	H	O	0
			100	40	56	4	
42	Nn	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 43 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				AltConf
43	C	1	Total	C	H	O	0
			54	16	27	11	
43	R	1	Total	C	H	O	0
			54	16	27	11	
43	KK	1	Total	C	H	O	0
			54	16	27	11	
43	RR	1	Total	C	H	O	0
			53	16	26	11	

- Molecule 44 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



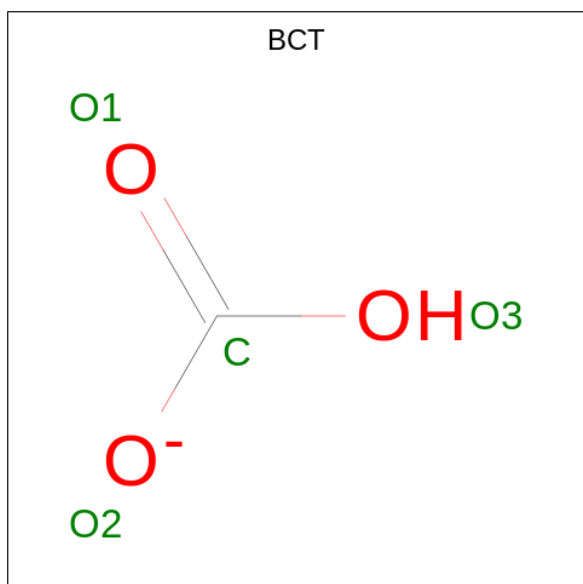
Mol	Chain	Residues	Atoms				AltConf
44	C	1	Total	C	H	O	0
			117	40	62	15	
44	C	1	Total	C	H	O	0
			132	47	70	15	
44	C	1	Total	C	H	O	0
			110	37	58	15	
44	D	1	Total	C	H	O	0
			132	47	70	15	
44	a	1	Total	C	H	O	0
			117	40	62	15	
44	c	1	Total	C	H	O	0
			117	40	62	15	
44	c	1	Total	C	H	O	0
			108	37	56	15	
44	h	1	Total	C	H	O	0
			132	47	70	15	
44	BB	1	Total	C	H	O	0
			132	47	70	15	
44	BB	1	Total	C	H	O	0
			117	40	62	15	
44	BB	1	Total	C	H	O	0
			121	42	64	15	
44	CC	1	Total	C	H	O	0
			117	40	62	15	
44	CC	1	Total	C	H	O	0
			132	47	70	15	
44	CC	1	Total	C	H	O	0
			117	40	62	15	

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Mol	Chain	Residues	Atoms				AltConf
44	B	1	Total	C	H	O	0
			117	40	62	15	
44	B	1	Total	C	H	O	0
			121	42	64	15	
44	Aa	1	Total	C	H	O	0
			117	40	62	15	
44	Cc	1	Total	C	H	O	0
			117	40	62	15	
44	Cc	1	Total	C	H	O	0
			108	37	56	15	
44	Hh	1	Total	C	H	O	0
			132	47	70	15	

- Molecule 45 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				AltConf
45	D	1	Total	C	O		0
			4	1	3		
45	a	1	Total	C	H	O	0
			5	1	1	3	
45	AA	1	Total	C	O		0
			4	1	3		
45	Aa	1	Total	C	H	O	0
			5	1	1	3	

- Molecule 46 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						AltConf
46	E	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
46	e	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
46	EE	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
46	Ee	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0

3 Residue-property plots

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

- Molecule 1: Photosystem II protein D1

Chain A: 



- Molecule 1: Photosystem II protein D1

Chain a: 



- Molecule 1: Photosystem II protein D1

Chain AA: 



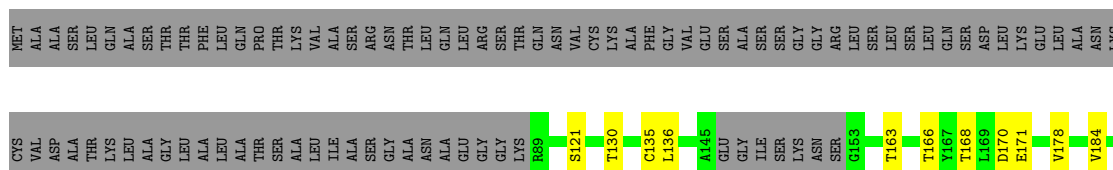
- Molecule 1: Photosystem II protein D1

Chain Aa: 



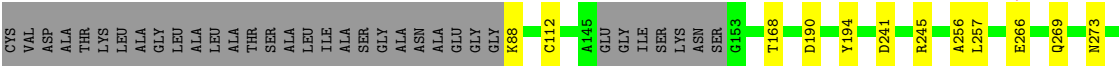
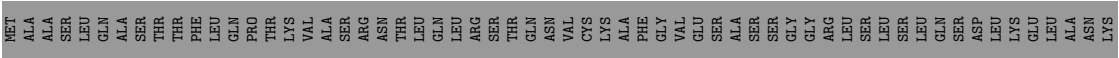
- Molecule 2: Oxygen-evolving enhancer protein 1, chloroplastic

Chain Oo: 

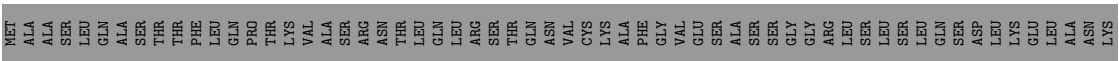




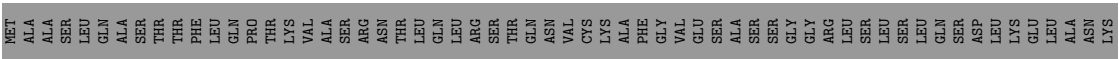
• Molecule 2: Oxygen-evolving enhancer protein 1, chloroplastic



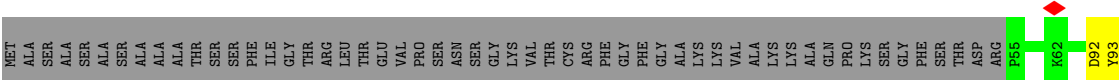
• Molecule 2: Oxygen-evolving enhancer protein 1, chloroplastic



• Molecule 2: Oxygen-evolving enhancer protein 1, chloroplastic

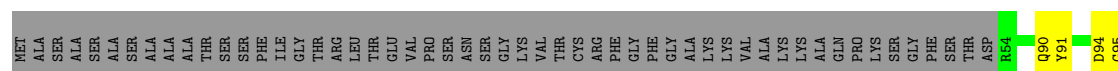
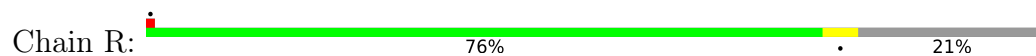


• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

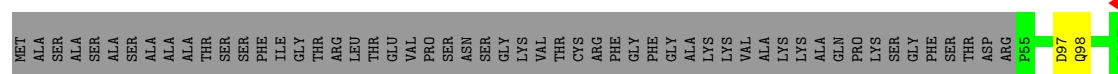




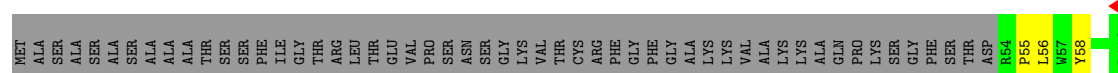
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



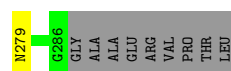
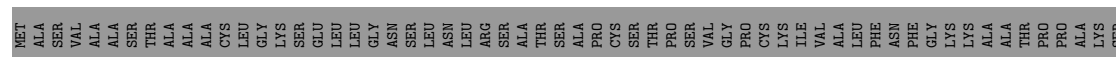
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



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



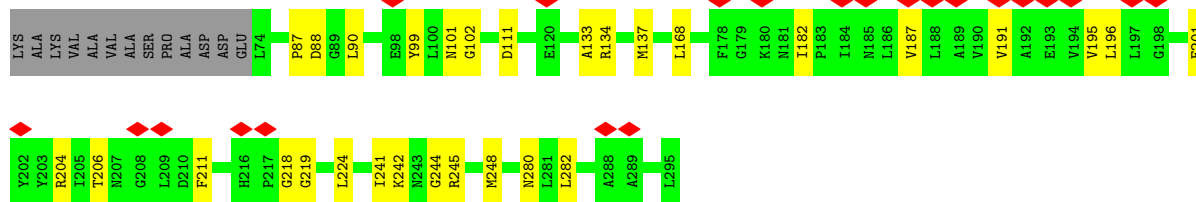
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic



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



MET ALA SER VAL ALA ALA SER THR ALA ALA ASP CYS LEU GLY LYS SER GLU LEU LEU GLY ASN SER LEU LEU ASN ARG SER SER ALA THR SER ALA PRO PRO SER THR PRO SER VAL GLY PRO CYS LYS LYS ILE VAL ALA LEU PHE PHE ASN PHE GLY LYS LYS ALA ALA THR PRO PRO ALA LYS SER



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



MET ALA SER VAL ALA ALA SER THR ALA ALA ASP CYS LEU GLY LYS SER GLU LEU LEU GLY ASN SER LEU LEU ARG SER SER ALA THR SER ALA PRO CYS SER THR PRO PRO SER VAL GLY PRO CYS LYS LYS ILE VAL ALA LEU PHE PHE ASN PHE GLY LYS LYS ALA ALA THR PRO PRO ALA LYS SER



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



MET ALA SER VAL ALA ALA SER THR ALA ALA ASP CYS LEU GLY LYS SER GLU LEU LEU GLY ASN SER LEU LEU ARG SER SER ALA THR SER ALA PRO CYS SER THR PRO PRO SER VAL GLY PRO CYS LYS LYS ILE VAL ALA LEU PHE PHE ASN PHE GLY LYS LYS ALA ALA THR PRO PRO ALA LYS SER



- Molecule 5: Photosystem II reaction center protein T



- Molecule 5: Photosystem II reaction center protein T

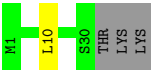


- Molecule 5: Photosystem II reaction center protein T

Chain t:

88%

9%



• Molecule 5: Photosystem II reaction center protein T

Chain TT:

91%

9%



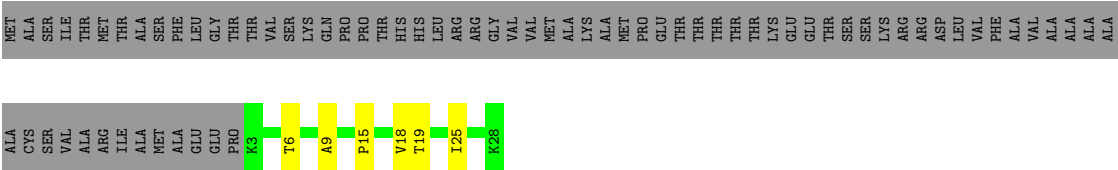
• Molecule 6: Photosystem II 5 kDa protein, chloroplastic

Chain Uu:

20%

6%

74%

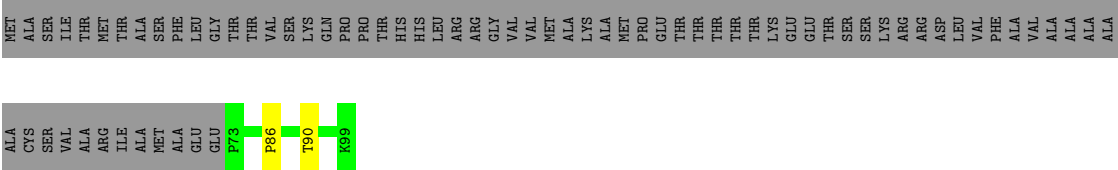


• Molecule 6: Photosystem II 5 kDa protein, chloroplastic

Chain U:

25%

73%



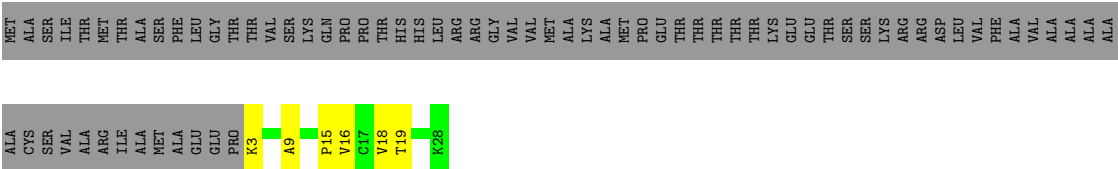
• Molecule 6: Photosystem II 5 kDa protein, chloroplastic

Chain u:

20%

6%

74%

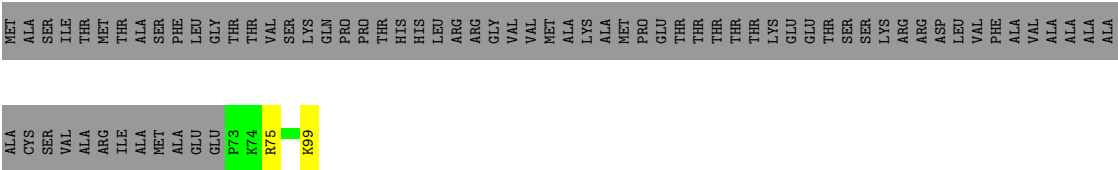


• Molecule 6: Photosystem II 5 kDa protein, chloroplastic

Chain UU:

25%

73%



- Chain Ww:**
- 38%
- 61%
- MET ALA THR ILE THR SER SER SER LEU VAL ARG ALA SER LEU HIS ASN SER VAL GLY VAL SER PRO ILE LEU GLY LEU PRO SER MET THR LYS ARG SER LYS VAL THR CYS ILE GLU ASN LYS PRO SER THR THR GLU THR THR THR
- ASN LYS SER MET GLY ALA SER LEU ALA ALA THR ILE SER ASN PRO ALA MET ALA L84 S136 L137

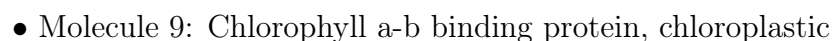
- Chain W:  38% 61%
- ASN LYS SER MET GLY ALA SER LEU LEU ALA ALA ALA THR ILE SER ASN PRO MET ALA ALA L84 E87 L109 L137

- Chain w:
-
- | Amino Acid | Frequency (%) |
|------------|---------------|
| MET | 38% |
| THR | 61% |
| ASN | L84 |
| LYS | L105 |
| SER | E129 |
| GLY | L137 |

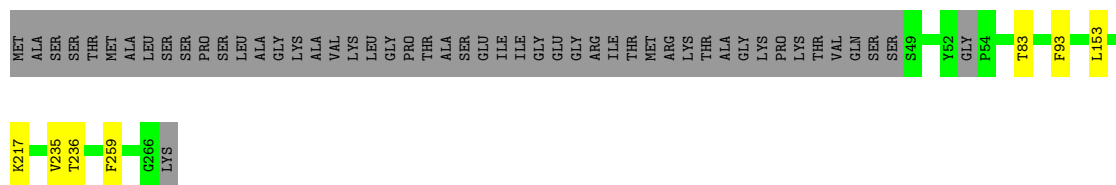
- Chain WW:
-
- | Amino Acid | Frequency (%) |
|------------|---------------|
| MET | 39% |
| THR | 61% |
| ASN | |
| LYS | |
| SER | |
| MET | |
| GLY | |
| ALA | |
| LEU | |
| PRO | |
| ARG | |
| THR | |
| ILE | |
| VAL | |
| ASP | |
| L137 | |

- Chain Xx:
- MET ALA SER ILE SER ALA VAL SER MET ALA THR PRO ILE THR THR THR THR LYS THR PHE PHE SER PRO LEU PRO VAL VAL LYS PRO GLN ARG ALA THR LEU MET MET GLY LYS VAL GLN ALA SER LEU LYS GLU LYS ALA VAL THR MET
- THR ALA ALA ALA LEU THR ALA SER MET MET VAL PRO ASP VAL ALA ALA GLU ALA ALA L80 F113 VAL LYS ARG ALA

- 

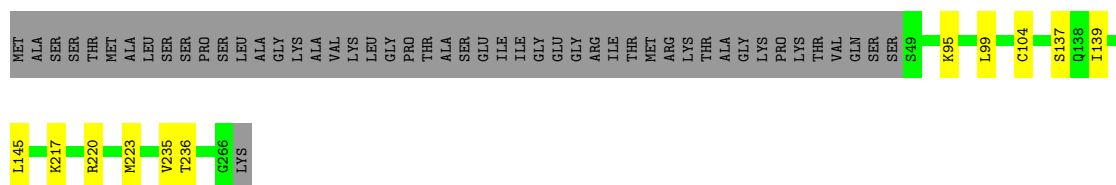


Chain N:  79% 19%



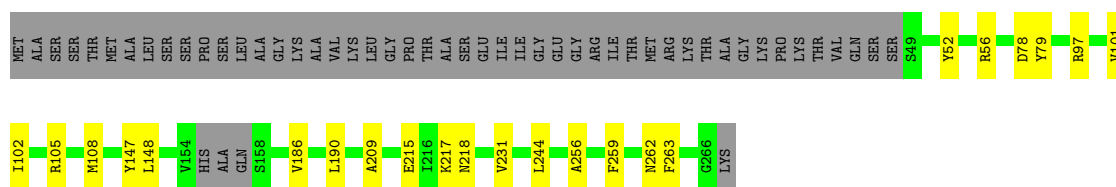
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain Y:  78% 18%



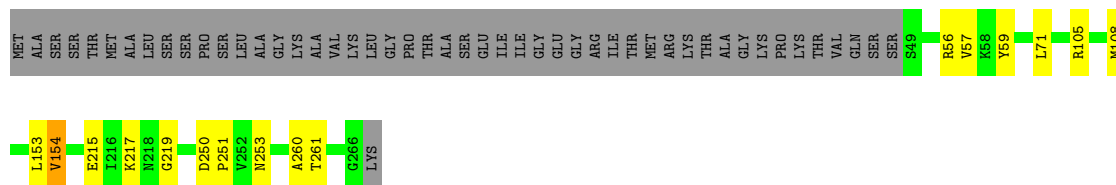
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain g:  72% 19%



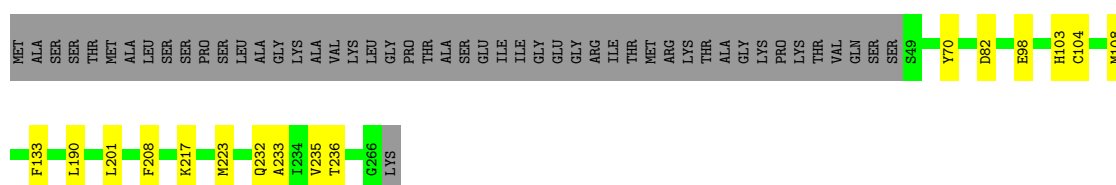
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain n:  76% 18%



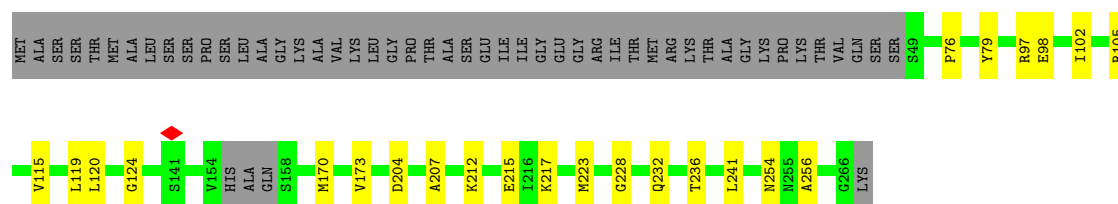
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain y:  76% 18%



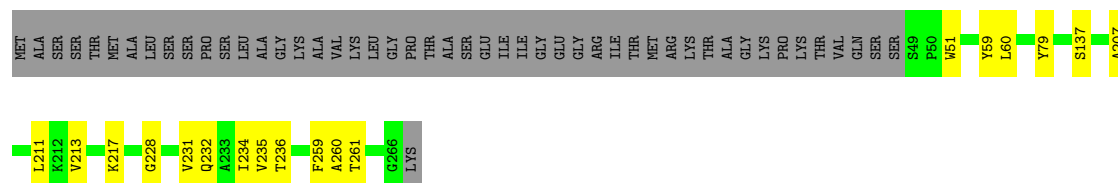
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain GG:  72% 9% 19%



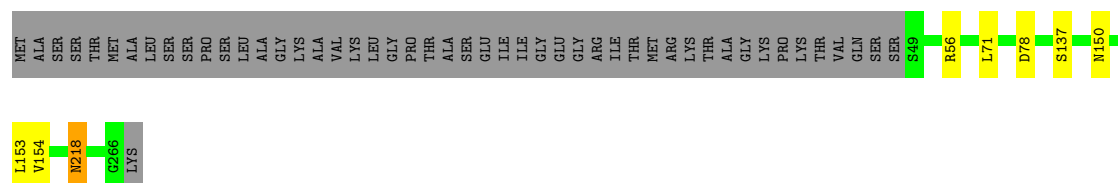
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain NN:  75% 7% 18%



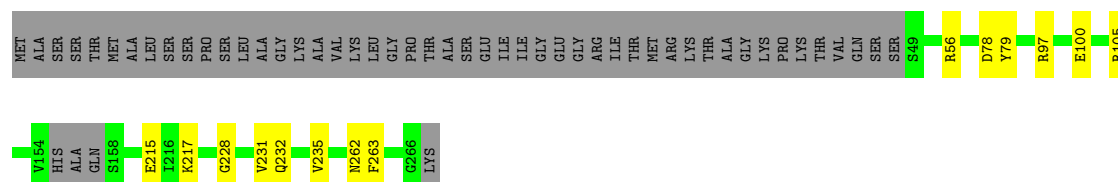
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain YY:  79% 1% 18%



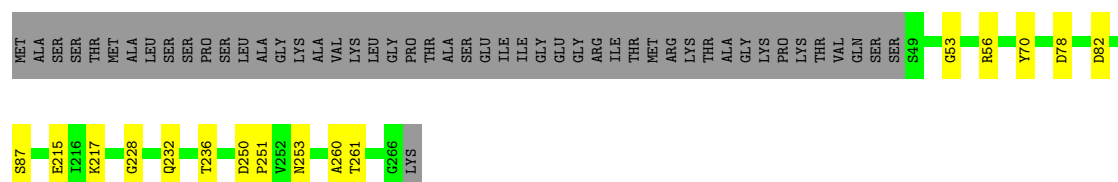
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain Gg:  75% 5% 19%

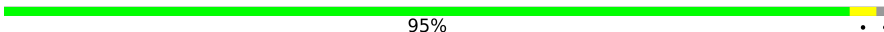


- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain Nn:  76% 6% 18%



- Molecule 10: Photosystem II reaction center protein Z

Chain Zz:  95%



- Molecule 10: Photosystem II reaction center protein Z

Chain Z:  89%



- Molecule 10: Photosystem II reaction center protein Z

Chain z:  89%



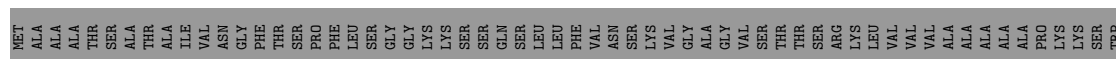
- Molecule 10: Photosystem II reaction center protein Z

Chain ZZ:  92%



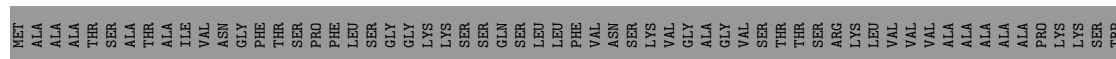
- Molecule 11: Chlorophyll a-b binding protein CP24, chloroplastic

Chain 44:  68%



- Molecule 11: Chlorophyll a-b binding protein CP24, chloroplastic

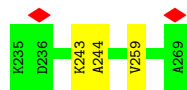
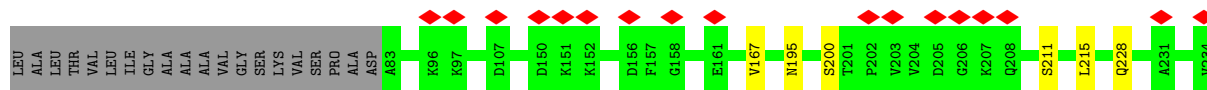
Chain 4:  65%



- Molecule 12: Oxygen-evolving enhancer protein 2, chloroplastic



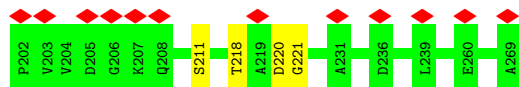
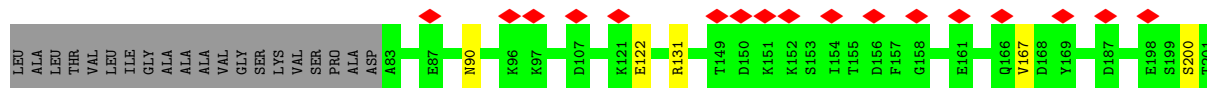
MET ALA ALA SER THR THR ALA ALA CYS PHE LEU LEU HIS HIS HIS ALA ALA VAL ILE SER LYS SER PRO ALA ALA GLY ARG GLY SER SER ALA ALA GLN ARG TYR TYR GLN ALA VAL SER ILE ILE LYS PRO ASN GLN GLN VAL CYS LYS ALA GLN LYS LYS ASP ASP ASN ASN GLU GLU ALA ASN VAL LEU SER GLY VAL SER ARG ARG



- Molecule 12: Oxygen-evolving enhancer protein 2, chloroplastic



MET ALA ALA SER THR THR ALA ALA CYS PHE LEU LEU HIS HIS HIS ALA ALA VAL GLY SER LYS SER PRO ALA ALA GLY ARG GLY SER SER ALA ALA GLN TYR TYR GLN ALA VAL SER ILE ILE LYS PRO ASN GLN GLN VAL CYS LYS ALA GLN LYS LYS ASP ASP ASN ASN GLU GLU ALA ASN VAL LEU SER GLY VAL SER ARG ARG



- Molecule 12: Oxygen-evolving enhancer protein 2, chloroplastic



MET ALA ALA SER THR THR ALA ALA CYS PHE LEU LEU HIS HIS HIS ALA ALA VAL GLY SER LYS SER PRO ALA ALA GLY ARG GLY SER SER ALA ALA GLN TYR TYR GLN ALA VAL SER ILE ILE LYS PRO ASN GLN GLN VAL CYS LYS ALA GLN LYS LYS ASP ASP ASN ASN GLU GLU ALA ASN VAL LEU SER GLY VAL SER ARG ARG



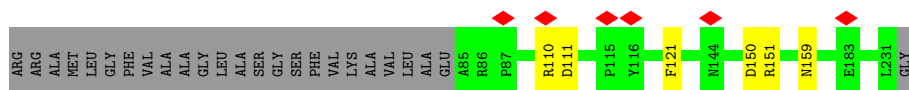
- Molecule 12: Oxygen-evolving enhancer protein 2, chloroplastic



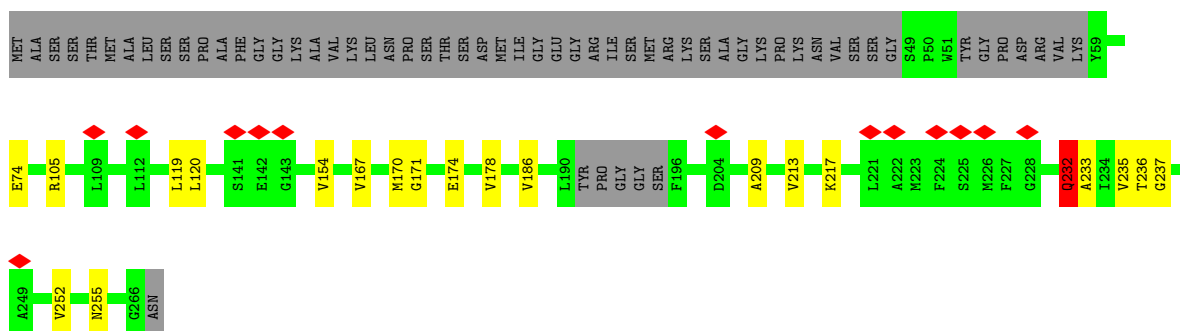
MET ALA ALA SER THR THR ALA ALA CYS PHE LEU LEU HIS HIS HIS ALA ALA VAL GLY SER LYS SER PRO ALA ALA GLY ARG GLY SER SER ALA ALA GLN ARG TYR TYR GLN ALA VAL SER ILE ILE LYS PRO ASN GLN GLN VAL CYS LYS ALA GLN LYS LYS ASP ASP ASN ASN GLU GLU ALA ASN VAL LEU SER GLY VAL SER ARG ARG



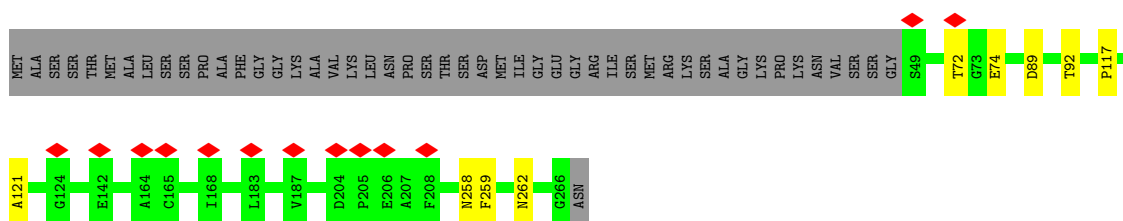
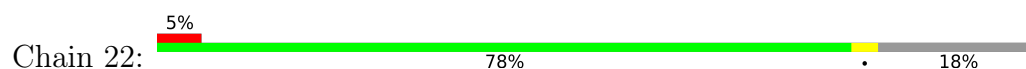




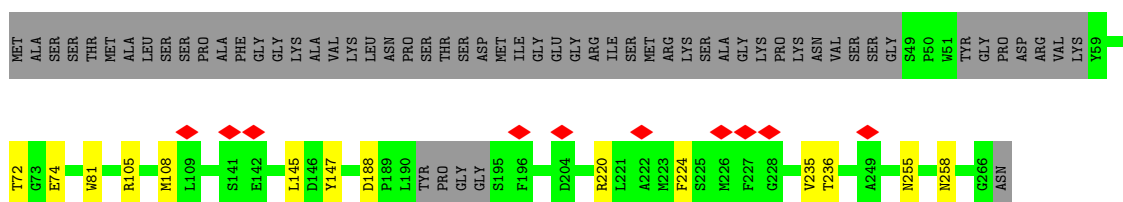
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



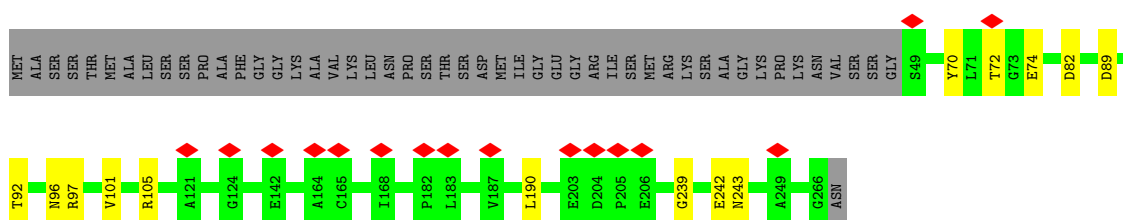
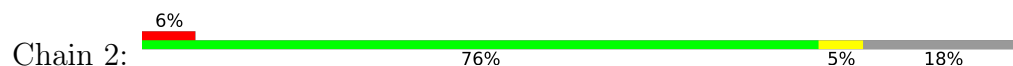
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



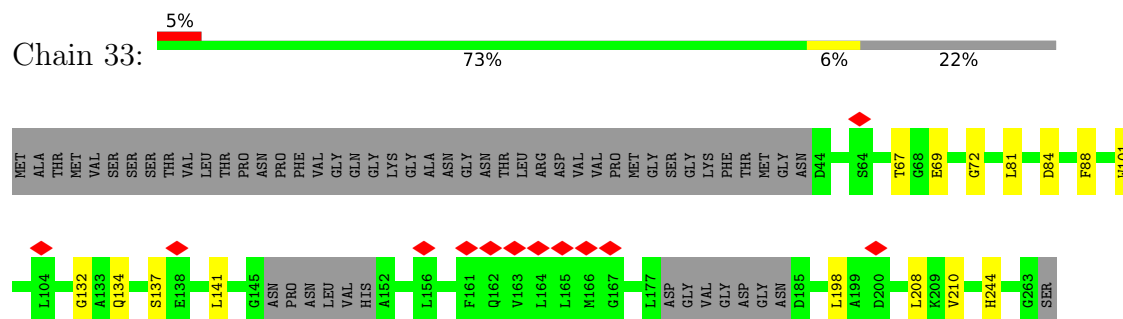
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



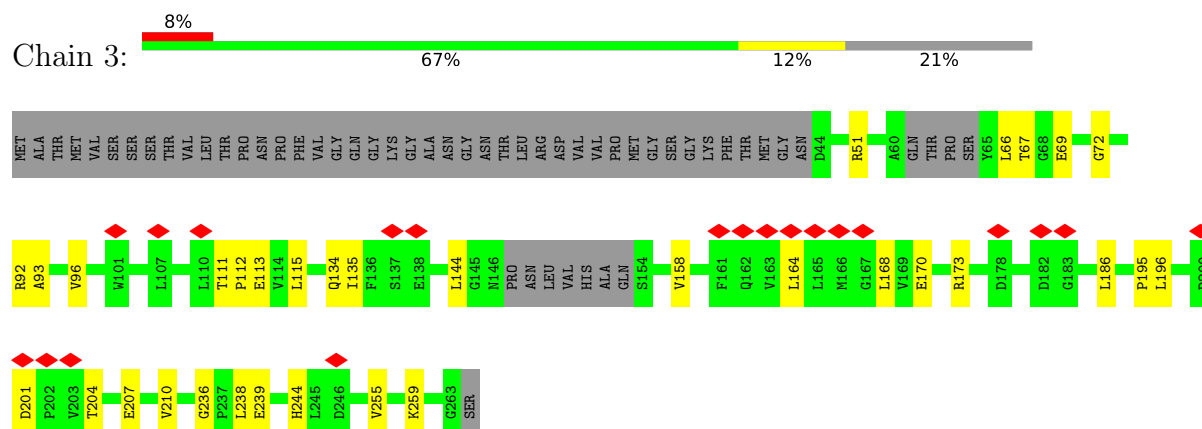
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



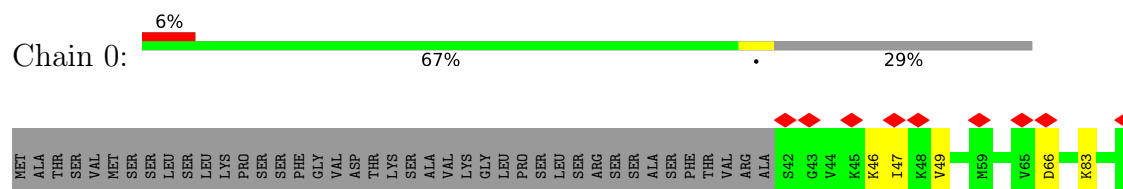
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



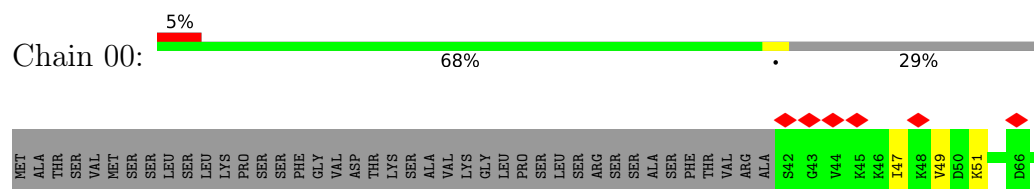
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



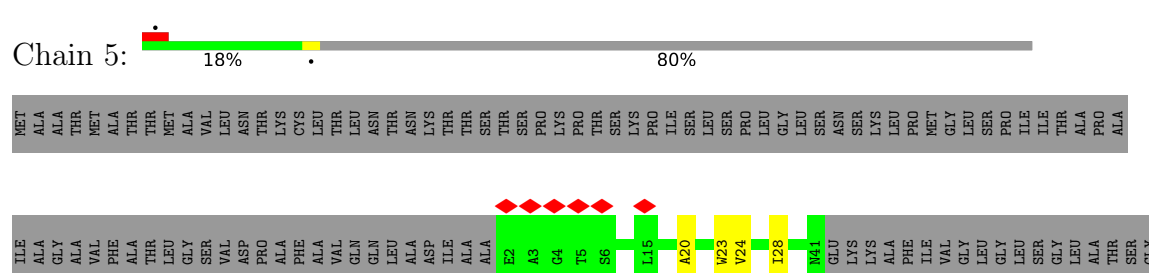
- Molecule 16: Photosystem II 10 kDa polypeptide, chloroplastic



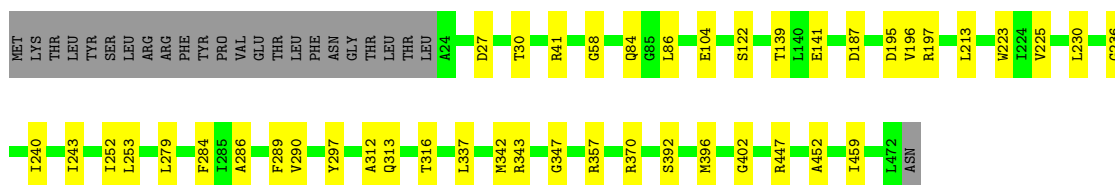
- Molecule 16: Photosystem II 10 kDa polypeptide, chloroplastic



- Molecule 17: Photosystem II reaction center proteins PsbY, chloroplastic



Chain Cc: 86% 9% 5%



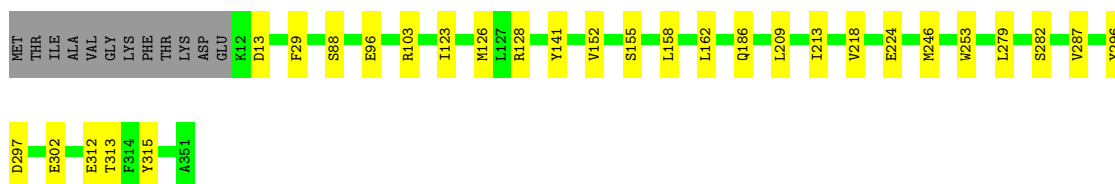
- Molecule 19: Photosystem II D2 protein

Chain D: 92%



- Molecule 19: Photosystem II D2 protein

Chain d: 88%



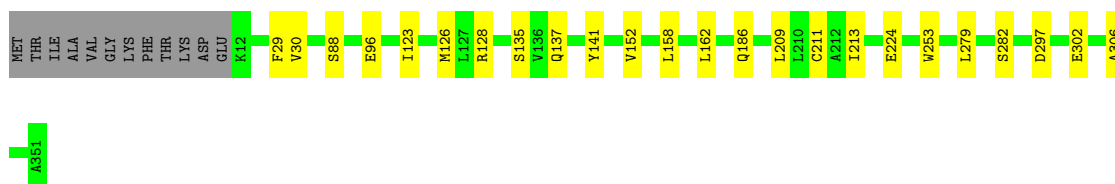
- Molecule 19: Photosystem II D2 protein

Chain DD: 91%



- Molecule 19: Photosystem II D2 protein

Chain Dd: 90%



- Molecule 20: Cytochrome b559 subunit alpha

Chain E: 84%



- Molecule 20: Cytochrome b559 subunit alpha

Chain e:  82% 8% 10%



- Molecule 20: Cytochrome b559 subunit alpha

Chain EE:  83% 13%



- Molecule 20: Cytochrome b559 subunit alpha

Chain Ee:  88% 10%



- Molecule 21: Cytochrome b559 subunit beta

Chain F:  74% 13% 13%



- Molecule 21: Cytochrome b559 subunit beta

Chain f:  67% 13% 21%



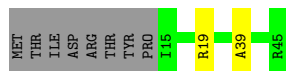
- Molecule 21: Cytochrome b559 subunit beta

Chain FF:  77% 10% 13%



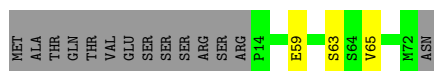
- Molecule 21: Cytochrome b559 subunit beta

Chain Ff:  74% 5% 21%



- Molecule 22: Photosystem II reaction center protein H

Chain H:  77% 19%



- Molecule 22: Photosystem II reaction center protein H

Chain h:  74% 7% 19%



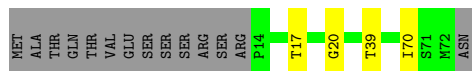
- Molecule 22: Photosystem II reaction center protein H

Chain HH:  70% 11% 19%



- Molecule 22: Photosystem II reaction center protein H

Chain Hh:  75% 5% 19%



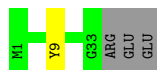
- Molecule 23: Photosystem II reaction center protein I

Chain I:  94% 2% 4%



- Molecule 23: Photosystem II reaction center protein I

Chain i:  89% 3% 8%



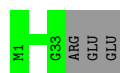
- Molecule 23: Photosystem II reaction center protein I

Chain II:  94% 2% 4%



- Molecule 23: Photosystem II reaction center protein I

Chain Ii:  92% 8%



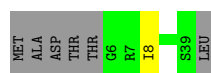
- Molecule 24: Photosystem II reaction center protein J

Chain J:  88% 5% 8%



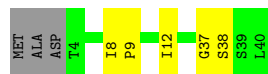
- Molecule 24: Photosystem II reaction center protein J

Chain j:  82% 15%



- Molecule 24: Photosystem II reaction center protein J

Chain JJ:  80% 12% 8%



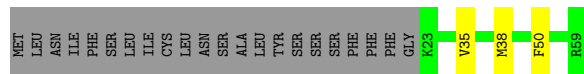
- Molecule 24: Photosystem II reaction center protein J

Chain Jj:  78% 8% 15%



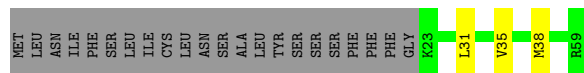
- Molecule 25: Photosystem II reaction center protein K

Chain K:  58% 5% 37%



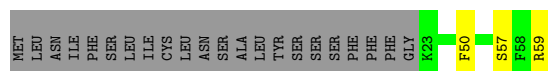
- Molecule 25: Photosystem II reaction center protein K

Chain k:  58% 5% 37%



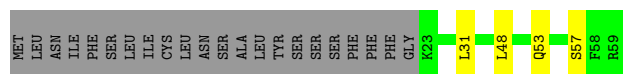
- Molecule 25: Photosystem II reaction center protein K

Chain KK:  58% 5% 37%



- Molecule 25: Photosystem II reaction center protein K

Chain Kk:  56% 7% 37%



- Molecule 26: Photosystem II reaction center protein L

Chain L:  84% 8% 8%



- Molecule 26: Photosystem II reaction center protein L

Chain l:  89% 5% 5%

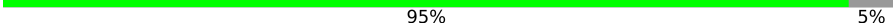


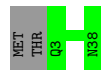
- Molecule 26: Photosystem II reaction center protein L

Chain LL:  84% 8% 8%



- Molecule 26: Photosystem II reaction center protein L

Chain Ll:  95% 5%



- Molecule 27: Photosystem II reaction center protein M

Chain M:  91% 6% 3%



- Molecule 27: Photosystem II reaction center protein M

Chain m:  85% 9% 6%



- Molecule 27: Photosystem II reaction center protein M

Chain MM:  94% . .



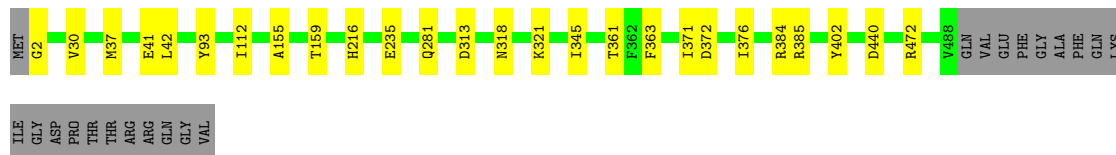
- Molecule 27: Photosystem II reaction center protein M

Chain Mm:  91% . 6%

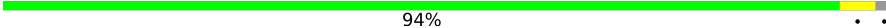


- Molecule 28: Photosystem II CP47 reaction center protein

Chain b:  91% 5% .



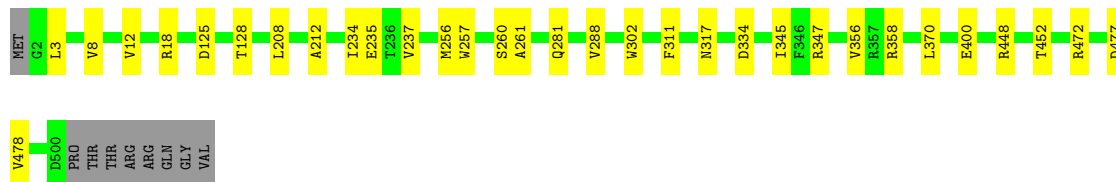
- Molecule 28: Photosystem II CP47 reaction center protein

Chain BB:  94% . .



- Molecule 28: Photosystem II CP47 reaction center protein

Chain B:  92% 6% .



- Molecule 28: Photosystem II CP47 reaction center protein

Chain Bb:  91% 5% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93684	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	34.286	Depositor
Minimum map value	-20.735	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	648.0, 648.0, 648.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/2700	0.43	0/3682
1	AA	0.22	0/2700	0.40	0/3682
1	Aa	0.21	0/2694	0.39	0/3674
1	a	0.22	0/2694	0.41	0/3674
2	O	0.18	0/1829	0.39	0/2471
2	OO	0.18	0/1829	0.40	0/2471
2	Oo	0.18	0/1811	0.40	0/2448
2	o	0.18	0/1811	0.39	0/2448
3	R	0.18	0/1819	0.42	0/2475
3	RR	0.20	0/1819	0.45	0/2475
3	Rr	0.17	0/1824	0.38	0/2481
3	r	0.18	0/1824	0.38	0/2481
4	S	0.21	0/1760	0.46	0/2393
4	SS	0.20	0/1760	0.45	0/2393
4	Ss	0.17	0/1696	0.41	0/2305
4	s	0.18	0/1696	0.42	0/2305
5	T	0.21	0/252	0.39	0/341
5	TT	0.19	0/252	0.32	0/341
5	Tt	0.20	0/252	0.35	0/341
5	t	0.20	0/252	0.40	0/341
6	U	0.23	0/214	0.56	0/286
6	UU	0.18	0/214	0.40	0/286
6	Uu	0.25	0/206	0.62	0/275
6	u	0.28	0/206	0.67	0/275
7	W	0.20	0/429	0.45	0/582
7	WW	0.19	0/429	0.40	0/582
7	Ww	0.18	0/429	0.36	0/582
7	w	0.19	0/429	0.43	0/582
8	X	0.19	0/331	0.41	0/453
8	XX	0.19	0/347	0.45	0/473
8	Xx	0.16	0/241	0.35	0/330

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	x	0.20	0/241	0.42	0/330
9	G	0.23	0/1686	0.56	0/2295
9	GG	0.19	0/1686	0.45	0/2295
9	Gg	0.19	0/1686	0.45	0/2295
9	N	0.22	0/1707	0.49	0/2323
9	NN	0.20	0/1712	0.46	0/2332
9	Nn	0.19	0/1712	0.43	0/2332
9	Y	0.21	0/1712	0.44	0/2332
9	YY	0.18	0/1712	0.41	0/2332
9	Yy	0.19	0/1712	0.42	0/2332
9	g	0.22	0/1686	0.48	0/2295
9	n	0.23	0/1712	0.52	0/2332
9	y	0.22	0/1712	0.44	0/2332
10	Z	0.18	0/464	0.40	0/636
10	ZZ	0.16	0/464	0.38	0/636
10	Zz	0.15	0/464	0.37	0/636
10	z	0.23	0/464	0.57	0/636
11	4	0.21	0/1501	0.53	1/2043 (0.0%)
11	44	0.19	0/1501	0.46	0/2043
12	P	0.21	0/1465	0.47	0/1978
12	PP	0.18	0/1465	0.38	0/1978
12	Pp	0.17	0/1465	0.37	0/1978
12	p	0.16	0/1465	0.36	0/1978
13	Q	0.25	0/1177	0.51	0/1597
13	QQ	0.20	0/1177	0.42	0/1597
13	Qq	0.23	0/1177	0.50	1/1597 (0.1%)
13	q	0.19	0/1177	0.46	0/1597
14	1	0.21	0/1622	0.47	0/2206
14	11	0.20	0/1616	0.48	1/2198 (0.0%)
14	2	0.20	0/1713	0.43	0/2333
14	22	0.17	0/1713	0.37	0/2333
15	3	0.20	0/1668	0.46	0/2265
15	33	0.17	0/1661	0.38	0/2257
16	0	0.20	0/736	0.46	0/997
16	00	0.17	0/736	0.41	0/997
17	5	0.23	0/313	0.47	0/426
17	55	0.21	0/313	0.52	0/426
18	C	0.22	0/3589	0.42	0/4891
18	CC	0.20	0/3589	0.35	0/4891
18	Cc	0.18	0/3589	0.36	0/4891
18	c	0.20	0/3589	0.40	0/4891
19	D	0.22	0/2787	0.41	0/3800
19	DD	0.21	0/2787	0.37	0/3800

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Dd	0.18	0/2796	0.34	0/3811
19	d	0.20	0/2796	0.37	0/3811
20	E	0.23	0/658	0.47	0/894
20	EE	0.19	0/658	0.39	0/894
20	Ee	0.16	0/628	0.36	0/854
20	e	0.20	0/628	0.43	0/854
21	F	0.22	0/285	0.52	0/387
21	FF	0.21	0/285	0.44	0/387
21	Ff	0.21	0/257	0.50	0/347
21	f	0.21	0/257	0.46	0/347
22	H	0.20	0/444	0.43	0/605
22	HH	0.18	0/444	0.39	0/605
22	Hh	0.18	0/444	0.42	0/605
22	h	0.19	0/444	0.48	0/605
23	I	0.23	0/294	0.42	0/397
23	II	0.21	0/294	0.35	0/397
23	Ii	0.22	0/274	0.34	0/371
23	i	0.24	0/274	0.44	0/371
24	J	0.18	0/275	0.41	0/374
24	JJ	0.19	0/275	0.36	0/374
24	Jj	0.18	0/253	0.38	0/343
24	j	0.17	0/253	0.41	0/343
25	K	0.25	0/320	0.47	0/436
25	KK	0.22	0/320	0.50	0/436
25	Kk	0.20	0/319	0.44	0/436
25	k	0.25	0/320	0.55	0/436
26	L	0.25	0/303	0.40	0/412
26	LL	0.21	0/303	0.31	0/412
26	Ll	0.21	0/312	0.32	0/424
26	l	0.21	0/312	0.34	0/424
27	M	0.21	0/262	0.46	0/358
27	MM	0.19	0/262	0.42	0/358
27	Mm	0.20	0/254	0.38	0/348
27	m	0.25	0/254	0.51	0/348
28	B	0.21	0/4047	0.40	0/5507
28	BB	0.20	0/4047	0.37	0/5507
28	Bb	0.20	0/3951	0.37	0/5379
28	b	0.21	0/3951	0.42	0/5379
All	All	0.20	0/137625	0.42	3/187193 (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	O	0	1
2	OO	0	1
9	YY	0	2
9	n	0	2
14	11	0	2
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Qq	93	PRO	CA-N-CD	-7.17	101.97	112.00
14	11	232	GLN	CB-CG-CD	6.65	123.91	112.60
11	4	152	GLN	CA-CB-CG	6.13	126.36	114.10

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	11	154	VAL	Peptide
14	11	232	GLN	Peptide
2	O	266	GLU	Peptide
9	n	153	LEU	Peptide
9	n	154	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2619	2526	2526	14	0
1	AA	2619	2527	2526	16	0
1	Aa	2613	2521	2521	16	0
1	a	2613	2521	2521	15	0
2	O	1794	1765	1767	7	0
2	OO	1794	1767	1767	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Oo	1776	1748	1748	16	0
2	o	1776	1748	1748	18	0
3	R	1773	1753	1753	7	0
3	RR	1773	1753	1753	11	0
3	Rr	1778	1763	1763	12	0
3	r	1778	1763	1763	13	0
4	S	1712	1683	1683	22	0
4	SS	1712	1683	1683	12	0
4	Ss	1649	1617	1617	14	0
4	s	1649	1617	1617	9	0
5	T	245	260	260	0	0
5	TT	245	260	260	0	0
5	Tt	245	260	260	1	0
5	t	245	260	260	1	0
6	U	209	226	226	1	0
6	UU	209	226	226	1	0
6	Uu	202	218	218	4	0
6	u	202	218	218	4	0
7	W	419	401	401	3	0
7	WW	419	401	401	0	0
7	Ww	419	401	401	3	0
7	w	419	401	401	2	0
8	X	326	341	341	0	0
8	XX	342	359	359	1	0
8	Xx	237	250	250	0	0
8	x	237	250	250	2	0
9	G	1636	1571	1571	11	0
9	GG	1636	1571	1571	16	0
9	Gg	1636	1571	1571	9	0
9	N	1656	1589	1589	6	0
9	NN	1660	1592	1592	11	0
9	Nn	1660	1592	1592	11	0
9	Y	1660	1592	1592	8	0
9	YY	1660	1592	1592	6	0
9	Yy	1660	1592	1592	7	0
9	g	1636	1571	1571	17	0
9	n	1660	1592	1592	11	0
9	y	1660	1592	1592	12	0
10	Z	454	479	479	4	0
10	ZZ	454	479	479	4	0
10	Zz	454	479	479	3	0
10	z	454	479	479	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	4	1452	1395	1395	13	0
11	44	1452	1395	1394	5	0
12	P	1433	1394	1394	14	0
12	PP	1433	1394	1394	12	0
12	Pp	1433	1394	1394	5	0
12	p	1433	1394	1394	9	0
13	Q	1153	1181	1181	5	0
13	QQ	1153	1181	1181	5	0
13	Qq	1153	1181	1181	3	0
13	q	1153	1181	1181	7	0
14	1	1576	1510	1510	9	0
14	11	1570	1505	1505	14	0
14	2	1661	1592	1592	9	0
14	22	1661	1592	1592	6	0
15	3	1622	1573	1573	23	0
15	33	1614	1575	1575	14	0
16	0	722	726	726	3	0
16	00	722	726	726	3	0
17	5	308	325	325	6	0
17	55	308	325	325	3	0
18	C	3475	3417	3416	26	0
18	CC	3475	3417	3416	26	0
18	Cc	3475	3416	3416	33	0
18	c	3475	3416	3416	34	0
19	D	2694	2580	2579	13	0
19	DD	2694	2581	2579	15	0
19	Dd	2703	2592	2592	18	0
19	d	2703	2592	2592	23	0
20	E	640	615	615	11	0
20	EE	640	615	615	9	0
20	Ee	610	591	591	2	0
20	e	610	591	591	5	0
21	F	276	282	282	6	0
21	FF	276	282	282	4	0
21	Ff	250	259	259	2	0
21	f	250	259	259	4	0
22	H	434	459	459	2	0
22	HH	434	459	459	6	0
22	Hh	434	459	459	3	0
22	h	434	459	459	3	0
23	I	286	295	295	2	0
23	II	286	295	295	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Ii	266	276	276	0	0
23	i	266	276	276	1	0
24	J	269	283	283	2	0
24	JJ	269	283	283	3	0
24	Jj	247	258	258	2	0
24	j	247	258	258	1	0
25	K	307	310	310	2	0
25	KK	307	310	310	3	0
25	Kk	306	310	310	3	0
25	k	307	310	310	2	0
26	L	295	284	284	3	0
26	LL	295	284	284	3	0
26	Ll	304	292	292	0	0
26	l	304	292	292	3	0
27	M	258	285	285	2	0
27	MM	258	285	285	1	0
27	Mm	250	273	273	1	0
27	m	250	273	273	3	0
28	B	3914	3778	3778	20	0
28	BB	3914	3778	3778	15	0
28	Bb	3820	3690	3690	20	0
28	b	3820	3690	3690	22	0
29	A	10	0	0	0	0
29	AA	10	0	0	0	0
29	Cc	10	0	0	0	0
29	a	10	0	0	0	0
30	A	1	0	0	0	0
30	AA	1	0	0	0	0
30	Aa	1	0	0	0	0
30	a	1	0	0	0	0
31	A	2	0	0	1	0
31	AA	2	0	0	1	0
31	Aa	2	0	0	0	0
31	a	2	0	0	0	0
32	1	320	224	224	4	0
32	11	320	224	224	5	0
32	2	320	224	224	1	0
32	22	322	227	227	0	0
32	3	320	224	224	2	0
32	33	320	224	224	4	0
32	4	270	198	198	3	0
32	44	319	237	237	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	A	174	170	170	0	0
32	AA	174	170	170	0	0
32	Aa	239	242	242	4	0
32	B	946	1024	1024	4	0
32	BB	946	1024	1024	2	0
32	Bb	1040	1152	1152	6	0
32	C	829	903	903	8	0
32	CC	829	903	903	8	0
32	Cc	808	861	861	4	0
32	D	195	216	216	2	0
32	DD	195	216	216	3	0
32	Dd	130	144	144	2	0
32	G	387	320	320	3	0
32	GG	387	320	320	5	0
32	Gg	408	359	359	3	0
32	N	394	342	342	4	0
32	NN	394	342	342	2	0
32	Nn	424	378	378	5	0
32	R	556	477	477	0	0
32	RR	507	438	438	5	0
32	Rr	522	456	456	4	0
32	S	417	319	319	5	0
32	SS	421	325	325	4	0
32	Ss	441	351	351	4	0
32	X	41	29	29	1	0
32	XX	41	29	29	0	0
32	Y	443	419	422	2	0
32	YY	436	402	405	1	0
32	Yy	443	419	422	0	0
32	a	239	242	242	2	0
32	b	1040	1152	1152	7	0
32	c	808	861	861	6	0
32	d	130	144	144	2	0
32	g	408	359	359	5	0
32	n	424	378	378	6	0
32	r	522	456	456	6	0
32	s	441	351	351	3	0
32	y	443	419	422	3	0
33	A	64	74	74	0	0
33	AA	64	74	74	0	0
33	Aa	128	148	148	0	0
33	D	64	74	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DD	64	74	74	0	0
33	a	128	148	148	0	0
34	A	40	56	56	1	0
34	AA	40	56	56	1	0
34	Aa	40	56	56	2	0
34	B	160	224	224	3	0
34	BB	160	224	224	2	0
34	Bb	120	168	168	4	0
34	C	120	168	168	6	0
34	CC	120	168	168	3	0
34	Cc	120	168	168	5	0
34	D	40	56	56	1	0
34	DD	40	56	56	1	0
34	Dd	40	56	56	0	0
34	H	40	56	56	4	0
34	Hh	40	56	56	3	0
34	K	40	56	56	1	0
34	KK	40	56	56	3	0
34	Kk	40	56	56	5	0
34	T	40	56	56	0	0
34	TT	40	56	56	1	0
34	XX	40	56	56	2	0
34	a	40	56	56	3	0
34	b	120	168	168	4	0
34	c	120	168	168	7	0
34	d	40	56	56	0	0
34	h	40	56	56	3	0
34	k	40	56	56	1	0
35	A	55	0	80	10	0
35	AA	55	0	80	4	0
35	D	55	0	80	3	0
35	DD	55	0	80	7	0
35	Dd	55	0	80	6	0
35	d	55	0	80	10	0
36	0	47	67	67	2	0
36	1	30	30	30	0	0
36	11	34	38	38	0	0
36	22	34	38	38	0	0
36	3	34	38	38	0	0
36	33	34	38	38	0	0
36	4	40	24	24	0	0
36	44	40	24	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	A	116	145	145	2	0
36	AA	79	101	101	1	0
36	BB	34	38	38	0	0
36	C	31	32	32	0	0
36	CC	71	82	82	1	0
36	D	126	171	171	0	0
36	DD	92	133	133	1	0
36	Dd	129	177	177	3	0
36	EE	40	53	53	0	0
36	G	34	38	38	0	0
36	GG	34	38	38	0	0
36	Gg	34	38	38	0	0
36	II	34	38	38	0	0
36	J	27	24	24	0	0
36	JJ	33	36	36	0	0
36	K	34	38	38	0	0
36	KK	34	38	38	1	0
36	Ll	49	74	74	1	0
36	N	38	46	46	0	0
36	NN	38	46	46	1	0
36	Nn	49	74	74	0	0
36	Rr	49	74	74	0	0
36	SS	26	22	22	0	0
36	Ss	48	69	69	1	0
36	Y	49	74	74	0	0
36	YY	49	74	74	0	0
36	Yy	49	74	74	0	0
36	a	37	44	44	2	0
36	d	92	133	133	1	0
36	g	34	38	38	0	0
36	l	49	74	74	2	0
36	n	49	74	74	0	0
36	r	49	74	74	0	0
36	s	48	69	69	1	0
36	y	49	74	74	0	0
37	A	35	34	34	0	0
37	AA	35	34	34	2	0
37	Aa	47	61	61	0	0
37	B	83	97	97	0	0
37	BB	36	36	36	0	0
37	C	54	78	78	1	0
37	CC	54	78	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	L	90	114	114	0	0
37	LL	90	114	114	0	0
37	Ll	54	78	78	0	0
37	l	54	78	78	0	0
38	A	36	42	42	0	0
38	AA	36	42	42	0	0
38	Aa	43	54	54	1	0
38	B	45	60	60	0	0
38	BB	45	60	60	0	0
38	Bb	72	84	84	1	0
38	C	51	72	72	0	0
38	CC	39	48	48	0	0
38	Cc	34	38	38	1	0
38	DD	46	62	62	0	0
38	Dd	46	62	62	0	0
38	F	46	62	62	0	0
38	Mm	51	72	72	0	0
38	W	48	66	66	1	0
38	WW	48	66	66	1	0
38	a	43	54	54	0	0
38	b	72	84	84	0	0
38	c	34	38	38	1	0
38	j	46	62	62	1	0
38	m	51	72	72	1	0
39	1	205	130	130	6	0
39	11	205	130	130	6	0
39	2	205	130	130	3	0
39	22	205	130	130	3	0
39	3	205	130	130	3	0
39	33	205	130	130	5	0
39	4	229	152	152	4	0
39	44	229	152	152	2	0
39	G	283	215	215	7	0
39	GG	283	215	215	4	0
39	Gg	287	221	221	5	0
39	N	286	219	219	5	0
39	NN	286	219	219	4	0
39	Nn	314	251	251	4	0
39	R	150	111	111	3	0
39	RR	150	110	111	1	0
39	Rr	150	111	111	3	0
39	S	179	122	122	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	SS	185	127	127	3	0
39	Ss	201	147	147	2	0
39	Y	317	270	270	7	0
39	YY	317	270	270	6	0
39	Yy	317	270	270	6	0
39	g	287	221	221	6	0
39	n	314	251	251	8	0
39	r	150	111	111	1	0
39	s	201	147	147	3	0
39	y	317	270	270	5	0
40	2	42	56	56	0	0
40	22	42	56	56	0	0
40	4	42	56	56	0	0
40	44	42	56	56	0	0
40	G	84	112	112	0	0
40	GG	84	112	112	0	0
40	Gg	84	112	112	0	0
40	N	84	112	112	1	0
40	NN	84	112	112	0	0
40	Nn	84	112	112	3	0
40	R	42	56	56	0	0
40	RR	42	56	56	0	0
40	Rr	42	56	56	0	0
40	S	42	56	56	0	0
40	SS	42	56	56	0	0
40	Ss	84	112	112	3	0
40	Y	84	112	112	0	0
40	YY	84	112	112	0	0
40	Yy	84	112	112	1	0
40	g	84	112	112	1	0
40	n	84	112	112	3	0
40	r	42	56	56	0	0
40	s	84	112	112	0	0
40	y	84	112	112	2	0
41	4	44	56	56	0	0
41	44	44	56	56	0	0
41	G	88	112	112	0	0
41	GG	88	112	112	0	0
41	Gg	44	56	56	0	0
41	N	44	56	56	0	0
41	NN	44	56	56	1	0
41	Nn	44	56	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	R	44	56	56	0	0
41	RR	44	56	56	2	0
41	Rr	44	56	56	1	0
41	Yy	44	56	56	0	0
41	g	44	56	56	0	0
41	r	44	56	56	2	0
41	y	88	112	112	1	0
42	Gg	44	56	56	0	0
42	N	44	56	56	1	0
42	NN	44	56	56	1	0
42	Nn	44	56	56	1	0
42	R	44	56	56	4	0
42	RR	44	56	56	1	0
42	Rr	44	56	56	1	0
42	Y	88	112	112	1	0
42	YY	44	56	56	1	0
42	Yy	44	56	56	1	0
42	g	44	56	56	0	0
42	n	44	56	56	0	0
42	y	44	56	56	1	0
43	C	27	27	27	0	0
43	KK	27	27	27	0	0
43	R	27	27	27	0	0
43	RR	27	26	27	0	0
44	Aa	55	62	68	1	0
44	B	112	126	136	1	0
44	BB	174	196	218	4	0
44	C	169	190	212	4	0
44	CC	172	194	218	2	0
44	Cc	107	118	130	4	0
44	D	62	70	82	1	0
44	Hh	62	70	82	2	0
44	a	55	62	68	0	0
44	c	107	118	130	2	0
44	h	62	70	82	1	0
45	AA	4	0	0	1	0
45	Aa	4	1	1	0	0
45	D	4	0	0	2	0
45	a	4	1	1	0	0
46	E	43	30	30	1	0
46	EE	43	30	30	1	0
46	Ee	43	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	e	43	30	30	1	0
All	All	171299	168031	168670	1035	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 3.

The worst 5 of 1035 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)
4:Ss:257:GLN:OE1	32:Ss:612:CLA:ND	1.93	1.00
10:Zz:20:LEU:HD21	34:Kk:101:BCR:H343	1.46	0.98
38:c:519:LMG:HO5	38:c:519:LMG:HO4	1.17	0.93
9:Nn:70:TYR:OH	9:Nn:82:ASP:OD2	1.96	0.83
12:p:200:SER:HG	12:p:211:SER:HG	1.26	0.80

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	A	333/351 (95%)	313 (94%)	20 (6%)	0	100	100
1	AA	333/351 (95%)	305 (92%)	28 (8%)	0	100	100
1	Aa	332/351 (95%)	317 (96%)	14 (4%)	1 (0%)	36	67
1	a	332/351 (95%)	318 (96%)	14 (4%)	0	100	100
2	O	232/332 (70%)	219 (94%)	13 (6%)	0	100	100
2	OO	232/332 (70%)	216 (93%)	16 (7%)	0	100	100
2	Oo	230/332 (69%)	206 (90%)	24 (10%)	0	100	100
2	o	230/332 (69%)	210 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	223/286 (78%)	215 (96%)	8 (4%)	0	100	100
3	RR	223/286 (78%)	212 (95%)	10 (4%)	1 (0%)	30	61
3	Rr	224/286 (78%)	216 (96%)	8 (4%)	0	100	100
3	r	224/286 (78%)	216 (96%)	8 (4%)	0	100	100
4	S	220/295 (75%)	205 (93%)	14 (6%)	1 (0%)	24	58
4	SS	220/295 (75%)	201 (91%)	19 (9%)	0	100	100
4	Ss	211/295 (72%)	196 (93%)	15 (7%)	0	100	100
4	s	211/295 (72%)	199 (94%)	12 (6%)	0	100	100
5	T	28/33 (85%)	28 (100%)	0	0	100	100
5	TT	28/33 (85%)	28 (100%)	0	0	100	100
5	Tt	28/33 (85%)	28 (100%)	0	0	100	100
5	t	28/33 (85%)	28 (100%)	0	0	100	100
6	U	25/99 (25%)	25 (100%)	0	0	100	100
6	UU	25/99 (25%)	24 (96%)	1 (4%)	0	100	100
6	Uu	24/99 (24%)	22 (92%)	2 (8%)	0	100	100
6	u	24/99 (24%)	24 (100%)	0	0	100	100
7	W	52/137 (38%)	51 (98%)	1 (2%)	0	100	100
7	WW	52/137 (38%)	52 (100%)	0	0	100	100
7	Ww	52/137 (38%)	50 (96%)	2 (4%)	0	100	100
7	w	52/137 (38%)	48 (92%)	4 (8%)	0	100	100
8	X	44/117 (38%)	43 (98%)	1 (2%)	0	100	100
8	XX	46/117 (39%)	46 (100%)	0	0	100	100
8	Xx	32/117 (27%)	32 (100%)	0	0	100	100
8	x	32/117 (27%)	32 (100%)	0	0	100	100
9	G	211/267 (79%)	198 (94%)	13 (6%)	0	100	100
9	GG	211/267 (79%)	200 (95%)	11 (5%)	0	100	100
9	Gg	211/267 (79%)	197 (93%)	14 (7%)	0	100	100
9	N	213/267 (80%)	196 (92%)	17 (8%)	0	100	100
9	NN	216/267 (81%)	203 (94%)	13 (6%)	0	100	100
9	Nn	216/267 (81%)	195 (90%)	21 (10%)	0	100	100
9	Y	216/267 (81%)	207 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	YY	216/267 (81%)	205 (95%)	11 (5%)	0	100	100
9	Yy	216/267 (81%)	204 (94%)	12 (6%)	0	100	100
9	g	211/267 (79%)	197 (93%)	14 (7%)	0	100	100
9	n	216/267 (81%)	195 (90%)	20 (9%)	1 (0%)	24	58
9	y	216/267 (81%)	206 (95%)	10 (5%)	0	100	100
10	Z	59/62 (95%)	59 (100%)	0	0	100	100
10	ZZ	59/62 (95%)	59 (100%)	0	0	100	100
10	Zz	59/62 (95%)	59 (100%)	0	0	100	100
10	z	59/62 (95%)	59 (100%)	0	0	100	100
11	4	184/259 (71%)	172 (94%)	12 (6%)	0	100	100
11	44	184/259 (71%)	174 (95%)	8 (4%)	2 (1%)	11	42
12	P	185/267 (69%)	169 (91%)	16 (9%)	0	100	100
12	PP	185/267 (69%)	171 (92%)	14 (8%)	0	100	100
12	Pp	185/267 (69%)	176 (95%)	9 (5%)	0	100	100
12	p	185/267 (69%)	178 (96%)	7 (4%)	0	100	100
13	Q	145/232 (62%)	135 (93%)	10 (7%)	0	100	100
13	QQ	145/232 (62%)	134 (92%)	11 (8%)	0	100	100
13	Qq	145/232 (62%)	138 (95%)	7 (5%)	0	100	100
13	q	145/232 (62%)	141 (97%)	4 (3%)	0	100	100
14	1	201/267 (75%)	191 (95%)	9 (4%)	1 (0%)	24	58
14	11	200/267 (75%)	189 (94%)	11 (6%)	0	100	100
14	2	216/267 (81%)	203 (94%)	13 (6%)	0	100	100
14	22	216/267 (81%)	206 (95%)	10 (5%)	0	100	100
15	3	203/264 (77%)	195 (96%)	8 (4%)	0	100	100
15	33	201/264 (76%)	190 (94%)	11 (6%)	0	100	100
16	0	97/140 (69%)	90 (93%)	7 (7%)	0	100	100
16	00	97/140 (69%)	90 (93%)	7 (7%)	0	100	100
17	5	38/199 (19%)	38 (100%)	0	0	100	100
17	55	38/199 (19%)	36 (95%)	2 (5%)	0	100	100
18	C	447/473 (94%)	429 (96%)	17 (4%)	1 (0%)	43	73
18	CC	447/473 (94%)	433 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Cc	447/473 (94%)	423 (95%)	24 (5%)	0	100	100
18	c	447/473 (94%)	421 (94%)	26 (6%)	0	100	100
19	D	337/352 (96%)	322 (96%)	15 (4%)	0	100	100
19	DD	337/352 (96%)	323 (96%)	14 (4%)	0	100	100
19	Dd	338/352 (96%)	328 (97%)	10 (3%)	0	100	100
19	d	338/352 (96%)	328 (97%)	10 (3%)	0	100	100
20	E	78/83 (94%)	75 (96%)	3 (4%)	0	100	100
20	EE	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
20	Ee	73/83 (88%)	72 (99%)	1 (1%)	0	100	100
20	e	73/83 (88%)	72 (99%)	1 (1%)	0	100	100
21	F	32/39 (82%)	31 (97%)	1 (3%)	0	100	100
21	FF	32/39 (82%)	30 (94%)	2 (6%)	0	100	100
21	Ff	29/39 (74%)	29 (100%)	0	0	100	100
21	f	29/39 (74%)	29 (100%)	0	0	100	100
22	H	57/73 (78%)	54 (95%)	3 (5%)	0	100	100
22	HH	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
22	Hh	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
22	h	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
23	I	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
23	II	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
23	Ii	31/36 (86%)	31 (100%)	0	0	100	100
23	i	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
24	J	35/40 (88%)	35 (100%)	0	0	100	100
24	JJ	35/40 (88%)	35 (100%)	0	0	100	100
24	Jj	32/40 (80%)	31 (97%)	1 (3%)	0	100	100
24	j	32/40 (80%)	31 (97%)	1 (3%)	0	100	100
25	K	35/59 (59%)	34 (97%)	1 (3%)	0	100	100
25	KK	35/59 (59%)	34 (97%)	1 (3%)	0	100	100
25	Kk	35/59 (59%)	31 (89%)	4 (11%)	0	100	100
25	k	35/59 (59%)	34 (97%)	1 (3%)	0	100	100
26	L	33/38 (87%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	LL	33/38 (87%)	33 (100%)	0	0	100	100
26	Ll	34/38 (90%)	34 (100%)	0	0	100	100
26	l	34/38 (90%)	34 (100%)	0	0	100	100
27	M	31/34 (91%)	31 (100%)	0	0	100	100
27	MM	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
27	Mm	30/34 (88%)	30 (100%)	0	0	100	100
27	m	30/34 (88%)	30 (100%)	0	0	100	100
28	B	497/508 (98%)	472 (95%)	25 (5%)	0	100	100
28	BB	497/508 (98%)	477 (96%)	20 (4%)	0	100	100
28	Bb	485/508 (96%)	471 (97%)	14 (3%)	0	100	100
28	b	485/508 (96%)	471 (97%)	14 (3%)	0	100	100
All	All	16994/21780 (78%)	16158 (95%)	828 (5%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	44	171	ASP
14	1	147	TYR
9	n	57	VAL
3	RR	58	TYR
1	Aa	334	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/284 (95%)	271 (100%)	0	100	100
1	AA	271/284 (95%)	271 (100%)	0	100	100
1	Aa	270/284 (95%)	270 (100%)	0	100	100
1	a	270/284 (95%)	270 (100%)	0	100	100
2	O	196/269 (73%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	OO	196/269 (73%)	196 (100%)	0	100	100
2	Oo	194/269 (72%)	194 (100%)	0	100	100
2	o	194/269 (72%)	194 (100%)	0	100	100
3	R	185/229 (81%)	185 (100%)	0	100	100
3	RR	185/229 (81%)	185 (100%)	0	100	100
3	Rr	186/229 (81%)	186 (100%)	0	100	100
3	r	186/229 (81%)	186 (100%)	0	100	100
4	S	173/226 (76%)	173 (100%)	0	100	100
4	SS	173/226 (76%)	173 (100%)	0	100	100
4	Ss	167/226 (74%)	167 (100%)	0	100	100
4	s	167/226 (74%)	167 (100%)	0	100	100
5	T	27/30 (90%)	27 (100%)	0	100	100
5	TT	27/30 (90%)	27 (100%)	0	100	100
5	Tt	27/30 (90%)	27 (100%)	0	100	100
5	t	27/30 (90%)	27 (100%)	0	100	100
6	U	23/80 (29%)	23 (100%)	0	100	100
6	UU	23/80 (29%)	23 (100%)	0	100	100
6	Uu	22/80 (28%)	22 (100%)	0	100	100
6	u	22/80 (28%)	22 (100%)	0	100	100
7	W	44/110 (40%)	44 (100%)	0	100	100
7	WW	44/110 (40%)	44 (100%)	0	100	100
7	Ww	44/110 (40%)	44 (100%)	0	100	100
7	w	44/110 (40%)	44 (100%)	0	100	100
8	X	34/90 (38%)	34 (100%)	0	100	100
8	XX	36/90 (40%)	36 (100%)	0	100	100
8	Xx	25/90 (28%)	25 (100%)	0	100	100
8	x	25/90 (28%)	25 (100%)	0	100	100
9	G	165/205 (80%)	165 (100%)	0	100	100
9	GG	165/205 (80%)	165 (100%)	0	100	100
9	Gg	165/205 (80%)	165 (100%)	0	100	100
9	N	167/205 (82%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	NN	167/205 (82%)	167 (100%)	0	100	100
9	Nn	167/205 (82%)	167 (100%)	0	100	100
9	Y	167/205 (82%)	167 (100%)	0	100	100
9	YY	167/205 (82%)	167 (100%)	0	100	100
9	Yy	167/205 (82%)	167 (100%)	0	100	100
9	g	165/205 (80%)	165 (100%)	0	100	100
9	n	167/205 (82%)	167 (100%)	0	100	100
9	y	167/205 (82%)	167 (100%)	0	100	100
10	Z	52/53 (98%)	52 (100%)	0	100	100
10	ZZ	52/53 (98%)	52 (100%)	0	100	100
10	Zz	52/53 (98%)	52 (100%)	0	100	100
10	z	52/53 (98%)	52 (100%)	0	100	100
11	4	145/198 (73%)	145 (100%)	0	100	100
11	44	145/198 (73%)	145 (100%)	0	100	100
12	P	153/212 (72%)	153 (100%)	0	100	100
12	PP	153/212 (72%)	153 (100%)	0	100	100
12	Pp	153/212 (72%)	153 (100%)	0	100	100
12	p	153/212 (72%)	153 (100%)	0	100	100
13	Q	128/187 (68%)	128 (100%)	0	100	100
13	QQ	128/187 (68%)	128 (100%)	0	100	100
13	Qq	128/187 (68%)	128 (100%)	0	100	100
13	q	128/187 (68%)	128 (100%)	0	100	100
14	1	160/206 (78%)	160 (100%)	0	100	100
14	11	159/206 (77%)	159 (100%)	0	100	100
14	2	168/206 (82%)	168 (100%)	0	100	100
14	22	168/206 (82%)	168 (100%)	0	100	100
15	3	164/209 (78%)	164 (100%)	0	100	100
15	33	164/209 (78%)	164 (100%)	0	100	100
16	0	72/107 (67%)	72 (100%)	0	100	100
16	00	72/107 (67%)	72 (100%)	0	100	100
17	5	33/158 (21%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	55	33/158 (21%)	33 (100%)	0	100	100
18	C	351/374 (94%)	351 (100%)	0	100	100
18	CC	351/374 (94%)	351 (100%)	0	100	100
18	Cc	351/374 (94%)	351 (100%)	0	100	100
18	c	351/374 (94%)	351 (100%)	0	100	100
19	D	271/282 (96%)	271 (100%)	0	100	100
19	DD	271/282 (96%)	271 (100%)	0	100	100
19	Dd	272/282 (96%)	272 (100%)	0	100	100
19	d	272/282 (96%)	272 (100%)	0	100	100
20	E	70/73 (96%)	70 (100%)	0	100	100
20	EE	70/73 (96%)	70 (100%)	0	100	100
20	Ee	67/73 (92%)	67 (100%)	0	100	100
20	e	67/73 (92%)	67 (100%)	0	100	100
21	F	29/34 (85%)	29 (100%)	0	100	100
21	FF	29/34 (85%)	29 (100%)	0	100	100
21	Ff	26/34 (76%)	26 (100%)	0	100	100
21	f	26/34 (76%)	26 (100%)	0	100	100
22	H	48/61 (79%)	48 (100%)	0	100	100
22	HH	48/61 (79%)	48 (100%)	0	100	100
22	Hh	48/61 (79%)	48 (100%)	0	100	100
22	h	48/61 (79%)	48 (100%)	0	100	100
23	I	32/33 (97%)	32 (100%)	0	100	100
23	II	32/33 (97%)	32 (100%)	0	100	100
23	Ii	30/33 (91%)	30 (100%)	0	100	100
23	i	30/33 (91%)	30 (100%)	0	100	100
24	J	28/30 (93%)	28 (100%)	0	100	100
24	JJ	28/30 (93%)	28 (100%)	0	100	100
24	Jj	25/30 (83%)	25 (100%)	0	100	100
24	j	25/30 (83%)	25 (100%)	0	100	100
25	K	32/52 (62%)	32 (100%)	0	100	100
25	KK	32/52 (62%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Kk	32/52 (62%)	32 (100%)	0	100	100
25	k	32/52 (62%)	32 (100%)	0	100	100
26	L	33/36 (92%)	33 (100%)	0	100	100
26	LL	33/36 (92%)	33 (100%)	0	100	100
26	Ll	34/36 (94%)	34 (100%)	0	100	100
26	l	34/36 (94%)	34 (100%)	0	100	100
27	M	29/30 (97%)	29 (100%)	0	100	100
27	MM	29/30 (97%)	29 (100%)	0	100	100
27	Mm	28/30 (93%)	28 (100%)	0	100	100
27	m	28/30 (93%)	28 (100%)	0	100	100
28	B	398/406 (98%)	398 (100%)	0	100	100
28	BB	398/406 (98%)	398 (100%)	0	100	100
28	Bb	389/406 (96%)	389 (100%)	0	100	100
28	b	389/406 (96%)	389 (100%)	0	100	100
All	All	13835/17352 (80%)	13835 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
10	ZZ	38	ASN
1	Aa	165	GLN
19	Dd	255	GLN
27	M	4	ASN
9	G	218	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 781 ligands modelled in this entry, 12 are monoatomic - leaving 769 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$
32	CLA	g	604	42	46,50,73	1.51	7 (15%)	55,85,113	1.24	5 (9%)
32	CLA	A	405	1	69,73,73	1.24	7 (10%)	83,113,113	1.12	6 (7%)
40	LUT	RR	315	-	42,43,43	0.88	1 (2%)	51,60,60	1.54	13 (25%)
36	LHG	G	618	32	33,33,48	1.12	2 (6%)	36,39,54	1.14	3 (8%)
32	CLA	D	405	19	69,73,73	1.25	7 (10%)	83,113,113	1.07	5 (6%)
32	CLA	Cc	512	18	69,73,73	1.24	6 (8%)	83,113,113	1.12	5 (6%)
32	CLA	YY	613	9	63,67,73	1.30	6 (9%)	75,105,113	1.13	5 (6%)
39	CHL	N	608	-	46,50,74	1.55	7 (15%)	51,85,114	1.19	4 (7%)
32	CLA	1	610	36	43,48,73	1.56	5 (11%)	52,82,113	1.27	4 (7%)
32	CLA	Ss	603	4	53,57,73	1.43	6 (11%)	62,93,113	1.18	5 (8%)
32	CLA	Y	612	9	69,73,73	1.26	7 (10%)	83,113,113	1.10	7 (8%)
38	LMG	WW	201	-	48,48,55	0.98	3 (6%)	56,56,63	1.06	2 (3%)
32	CLA	r	601	3	53,57,73	1.43	6 (11%)	62,93,113	1.17	4 (6%)
32	CLA	NN	611	36	53,57,73	1.41	7 (13%)	62,93,113	1.30	6 (9%)
32	CLA	S	613	4	49,53,73	1.47	5 (10%)	59,89,113	1.20	6 (10%)
38	LMG	Aa	412	-	42,42,55	1.05	3 (7%)	50,50,63	1.09	4 (8%)
39	CHL	33	608	15	44,49,74	1.59	7 (15%)	49,83,114	1.42	8 (16%)
32	CLA	c	502	18	69,73,73	1.25	7 (10%)	83,113,113	1.17	9 (10%)
39	CHL	NN	601	9	48,52,74	1.52	7 (14%)	53,87,114	1.30	6 (11%)
34	BCR	B	613	-	41,41,41	0.98	3 (7%)	56,56,56	1.78	12 (21%)
36	LHG	a	414	-	36,36,48	1.07	2 (5%)	39,42,54	0.92	2 (5%)
46	HEM	EE	102	20,21	50,50,50	1.39	7 (14%)	66,82,82	1.11	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	RR	312	3	46,50,73	1.51	6 (13%)	55,85,113	1.19	4 (7%)
32	CLA	GG	612	9	53,57,73	1.43	6 (11%)	62,93,113	1.29	5 (8%)
32	CLA	Rr	608	3	53,57,73	1.40	6 (11%)	62,93,113	1.22	6 (9%)
32	CLA	Yy	602	9	69,73,73	1.24	8 (11%)	83,113,113	1.13	5 (6%)
32	CLA	C	503	18	69,73,73	1.24	7 (10%)	83,113,113	1.12	6 (7%)
32	CLA	g	612	9	53,57,73	1.43	7 (13%)	62,93,113	1.24	6 (9%)
34	BCR	B	614	-	41,41,41	0.96	2 (4%)	56,56,56	1.85	13 (23%)
40	LUT	r	614	-	42,43,43	0.94	1 (2%)	51,60,60	1.38	7 (13%)
44	DGD	Hh	102	-	63,63,67	0.89	2 (3%)	77,77,81	0.92	2 (2%)
32	CLA	R	603	3	53,57,73	1.41	6 (11%)	62,93,113	1.30	5 (8%)
32	CLA	Cc	509	-	69,73,73	1.24	6 (8%)	83,113,113	1.21	6 (7%)
33	PHO	a	409	-	58,69,69	2.07	9 (15%)	56,99,99	1.53	8 (14%)
39	CHL	N	606	-	46,50,74	1.54	7 (15%)	51,85,114	1.25	5 (9%)
32	CLA	11	612	14	43,48,73	1.58	10 (23%)	52,82,113	1.63	11 (21%)
32	CLA	s	603	4	53,57,73	1.43	6 (11%)	62,93,113	1.18	4 (6%)
32	CLA	11	609	14	43,48,73	1.56	6 (13%)	52,82,113	1.25	4 (7%)
39	CHL	2	607	-	44,49,74	1.60	6 (13%)	49,83,114	1.26	5 (10%)
32	CLA	RR	313	3	45,49,73	1.52	6 (13%)	54,84,113	1.26	5 (9%)
32	CLA	r	608	3	53,57,73	1.41	6 (11%)	62,93,113	1.21	4 (6%)
32	CLA	CC	510	18	69,73,73	1.24	8 (11%)	83,113,113	1.15	6 (7%)
36	LHG	EE	101	-	39,39,48	1.05	2 (5%)	42,45,54	0.90	2 (4%)
32	CLA	Y	611	36	46,50,73	1.48	6 (13%)	55,85,113	1.26	4 (7%)
39	CHL	g	608	-	46,50,74	1.54	7 (15%)	51,85,114	1.20	4 (7%)
32	CLA	n	612	9	53,57,73	1.42	8 (15%)	62,93,113	1.19	4 (6%)
41	XAT	g	619	-	39,47,47	1.22	4 (10%)	54,74,74	2.84	11 (20%)
32	CLA	R	612	3	46,50,73	1.50	6 (13%)	55,85,113	1.19	4 (7%)
39	CHL	YY	606	-	48,52,74	1.50	7 (14%)	53,87,114	1.19	4 (7%)
32	CLA	Nn	301	9	69,73,73	1.24	8 (11%)	83,113,113	1.09	8 (9%)
32	CLA	YY	604	-	53,57,73	1.39	6 (11%)	62,93,113	1.29	7 (11%)
37	SQD	LL	102	-	53,54,54	1.19	4 (7%)	62,65,65	1.10	6 (9%)
39	CHL	44	605	11	50,54,74	1.52	6 (12%)	56,90,114	1.37	6 (10%)
32	CLA	Bb	616	28	69,73,73	1.23	6 (8%)	83,113,113	1.12	5 (6%)
39	CHL	22	607	-	44,49,74	1.61	6 (13%)	49,83,114	1.26	6 (12%)
45	BCT	Aa	414	30	2,3,3	1.27	0	2,3,3	3.93	2 (100%)
32	CLA	RR	308	3	53,57,73	1.41	8 (15%)	62,93,113	1.31	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	CC	505	-	69,73,73	1.24	7 (10%)	83,113,113	1.13	7 (8%)
38	LMG	B	615	-	45,45,55	0.98	2 (4%)	53,53,63	0.93	2 (3%)
32	CLA	11	603	14	43,48,73	1.56	7 (16%)	52,82,113	1.21	4 (7%)
32	CLA	Bb	605	28	69,73,73	1.23	7 (10%)	83,113,113	1.13	6 (7%)
39	CHL	G	607	-	50,54,74	1.50	7 (14%)	56,90,114	1.24	5 (8%)
39	CHL	22	601	14	44,49,74	1.60	6 (13%)	49,83,114	1.26	5 (10%)
42	NEX	Gg	318	-	38,46,46	1.10	3 (7%)	50,70,70	2.44	14 (28%)
36	LHG	n	618	32	48,48,48	0.95	2 (4%)	51,54,54	1.01	2 (3%)
32	CLA	Y	613	9	63,67,73	1.30	6 (9%)	75,105,113	1.15	4 (5%)
32	CLA	BB	605	28	69,73,73	1.23	7 (10%)	83,113,113	1.17	7 (8%)
29	OEX	Cc	502	1,18	0,14,14	-	-	-	-	-
32	CLA	1	611	14	43,48,73	1.56	6 (13%)	52,82,113	1.27	5 (9%)
39	CHL	4	307	-	50,54,74	1.52	7 (14%)	56,90,114	1.20	4 (7%)
39	CHL	NN	607	-	70,74,74	1.26	7 (10%)	80,114,114	1.11	5 (6%)
40	LUT	SS	315	-	42,43,43	1.00	1 (2%)	51,60,60	1.31	7 (13%)
39	CHL	2	608	14	44,49,74	1.60	6 (13%)	49,83,114	1.23	5 (10%)
39	CHL	YY	601	9	70,74,74	1.26	7 (10%)	80,114,114	1.07	3 (3%)
32	CLA	SS	314	4	53,57,73	1.41	8 (15%)	62,93,113	1.18	7 (11%)
32	CLA	Bb	601	-	69,73,73	1.26	9 (13%)	83,113,113	1.20	7 (8%)
32	CLA	NN	603	9	46,50,73	1.47	7 (15%)	55,85,113	1.31	5 (9%)
44	DGD	BB	624	-	56,56,67	0.92	2 (3%)	70,70,81	0.98	4 (5%)
44	DGD	CC	518	-	56,56,67	0.92	2 (3%)	70,70,81	0.95	4 (5%)
38	LMG	CC	520	-	39,39,55	1.06	2 (5%)	47,47,63	0.95	2 (4%)
32	CLA	g	614	9	53,57,73	1.41	6 (11%)	62,93,113	1.15	5 (8%)
32	CLA	C	510	18	69,73,73	1.23	7 (10%)	83,113,113	1.17	5 (6%)
32	CLA	b	602	28	69,73,73	1.24	7 (10%)	83,113,113	1.11	7 (8%)
36	LHG	AA	411	-	33,33,48	1.12	2 (6%)	36,39,54	1.22	4 (11%)
32	CLA	GG	610	9	53,57,73	1.41	7 (13%)	62,93,113	1.16	6 (9%)
32	CLA	GG	604	-	46,50,73	1.50	7 (15%)	55,85,113	1.18	4 (7%)
41	XAT	N	617	-	39,47,47	1.13	3 (7%)	54,74,74	2.50	14 (25%)
32	CLA	Rr	610	36	53,57,73	1.44	6 (11%)	62,93,113	1.25	3 (4%)
32	CLA	4	311	36	49,53,73	1.48	7 (14%)	59,89,113	1.20	4 (6%)
45	BCT	AA	413	30	2,3,3	1.26	0	2,3,3	4.14	2 (100%)
40	LUT	n	616	-	42,43,43	0.99	0	51,60,60	1.50	8 (15%)
32	CLA	S	610	-	53,57,73	1.41	7 (13%)	62,93,113	1.28	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	3	603	15	43,48,73	1.56	5 (11%)	52,82,113	1.25	5 (9%)
32	CLA	Yy	613	9	63,67,73	1.31	6 (9%)	75,105,113	1.20	5 (6%)
32	CLA	BB	603	28	69,73,73	1.22	8 (11%)	83,113,113	1.16	5 (6%)
40	LUT	n	615	-	42,43,43	0.97	0	51,60,60	1.30	5 (9%)
32	CLA	22	611	14	43,48,73	1.56	7 (16%)	52,82,113	1.32	5 (9%)
34	BCR	Hh	101	-	41,41,41	1.06	4 (9%)	56,56,56	2.42	22 (39%)
32	CLA	2	604	-	43,48,73	1.57	7 (16%)	52,82,113	1.35	5 (9%)
32	CLA	4	304	11	49,53,73	1.48	6 (12%)	59,89,113	1.40	6 (10%)
38	LMG	Bb	621	-	36,36,55	1.11	2 (5%)	44,44,63	1.10	5 (11%)
39	CHL	22	608	14	44,49,74	1.61	6 (13%)	49,83,114	1.24	5 (10%)
39	CHL	Nn	315	9	52,56,74	1.47	7 (13%)	58,92,114	1.39	6 (10%)
34	BCR	CC	515	-	41,41,41	0.97	1 (2%)	56,56,56	2.02	17 (30%)
40	LUT	N	615	-	42,43,43	0.98	2 (4%)	51,60,60	1.48	8 (15%)
39	CHL	SS	308	4	53,57,74	1.49	6 (11%)	59,93,114	1.14	4 (6%)
36	LHG	11	614	32	33,33,48	1.14	2 (6%)	36,39,54	1.11	3 (8%)
32	CLA	a	405	1	69,73,73	1.25	7 (10%)	83,113,113	1.13	5 (6%)
32	CLA	S	611	4	53,57,73	1.41	6 (11%)	62,93,113	1.31	4 (6%)
32	CLA	r	610	36	53,57,73	1.43	5 (9%)	62,93,113	1.26	4 (6%)
32	CLA	N	610	9	69,73,73	1.24	7 (10%)	83,113,113	1.07	6 (7%)
35	PL9	A	410	-	55,55,55	4.31	22 (40%)	68,69,69	3.77	38 (55%)
32	CLA	c	507	-	69,73,73	1.24	6 (8%)	83,113,113	1.22	7 (8%)
36	LHG	Y	618	32	48,48,48	0.93	2 (4%)	51,54,54	0.85	2 (3%)
32	CLA	R	608	3	53,57,73	1.41	8 (15%)	62,93,113	1.29	4 (6%)
40	LUT	y	317	-	42,43,43	0.96	1 (2%)	51,60,60	2.02	11 (21%)
35	PL9	DD	406	-	55,55,55	4.25	19 (34%)	68,69,69	3.82	37 (54%)
39	CHL	YY	608	-	54,58,74	1.44	7 (12%)	59,94,114	1.18	5 (8%)
32	CLA	B	604	28	69,73,73	1.26	8 (11%)	83,113,113	1.11	6 (7%)
39	CHL	S	601	4	56,60,74	1.43	7 (12%)	63,97,114	1.11	5 (7%)
32	CLA	Gg	315	9	53,57,73	1.40	7 (13%)	62,93,113	1.15	6 (9%)
39	CHL	RR	307	-	54,58,74	1.45	7 (12%)	59,94,114	1.26	5 (8%)
41	XAT	GG	617	-	39,47,47	1.07	2 (5%)	54,74,74	2.51	16 (29%)
32	CLA	c	509	18	69,73,73	1.24	7 (10%)	83,113,113	1.07	5 (6%)
38	LMG	Bb	620	-	36,36,55	1.11	2 (5%)	44,44,63	0.95	2 (4%)
32	CLA	44	611	11	49,53,73	1.47	6 (12%)	59,89,113	1.24	3 (5%)
40	LUT	YY	615	-	42,43,43	0.96	1 (2%)	51,60,60	1.78	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Bb	603	28	69,73,73	1.25	9 (13%)	83,113,113	1.09	7 (8%)
32	CLA	RR	309	3	69,73,73	1.25	8 (11%)	83,113,113	1.08	7 (8%)
32	CLA	33	611	15	43,48,73	1.55	6 (13%)	52,82,113	1.31	5 (9%)
36	LHG	NN	619	32	37,37,48	1.08	2 (5%)	40,43,54	1.03	2 (5%)
32	CLA	4	303	11	49,53,73	1.46	6 (12%)	59,89,113	1.22	5 (8%)
44	DGD	c	518	-	53,53,67	0.95	2 (3%)	67,67,81	0.89	2 (2%)
36	LHG	r	616	32	48,48,48	0.97	2 (4%)	51,54,54	0.92	2 (3%)
39	CHL	RR	305	-	54,58,74	1.41	6 (11%)	59,94,114	1.55	13 (22%)
39	CHL	Gg	310	9	47,51,74	1.53	7 (14%)	52,86,114	1.38	7 (13%)
32	CLA	Cc	503	18	69,73,73	1.23	6 (8%)	83,113,113	1.23	6 (7%)
32	CLA	Bb	608	28	69,73,73	1.22	8 (11%)	83,113,113	1.13	8 (9%)
32	CLA	22	612	14	43,48,73	1.55	5 (11%)	52,82,113	1.28	4 (7%)
42	NEX	R	617	-	38,46,46	1.09	2 (5%)	50,70,70	2.01	13 (26%)
37	SQD	B	602	-	46,47,54	1.28	4 (8%)	55,58,65	1.05	5 (9%)
32	CLA	11	613	14	43,48,73	1.57	6 (13%)	52,82,113	1.24	4 (7%)
40	LUT	Ss	615	-	42,43,43	0.99	1 (2%)	51,60,60	1.69	13 (25%)
32	CLA	Gg	304	9	69,73,73	1.25	6 (8%)	83,113,113	1.06	5 (6%)
44	DGD	CC	522	-	56,56,67	0.92	3 (5%)	70,70,81	1.11	5 (7%)
32	CLA	C	505	18	69,73,73	1.24	6 (8%)	83,113,113	1.16	7 (8%)
32	CLA	YY	612	9	62,66,73	1.33	5 (8%)	74,104,113	1.36	13 (17%)
39	CHL	44	608	11	50,54,74	1.53	6 (12%)	56,90,114	1.36	7 (12%)
32	CLA	C	506	-	69,73,73	1.24	7 (10%)	83,113,113	1.13	5 (6%)
32	CLA	R	613	3	45,49,73	1.53	6 (13%)	54,84,113	1.24	5 (9%)
32	CLA	d	402	19	69,73,73	1.24	7 (10%)	83,113,113	1.03	5 (6%)
38	LMG	BB	619	-	45,45,55	0.98	2 (4%)	53,53,63	0.93	2 (3%)
32	CLA	Y	602	9	69,73,73	1.24	7 (10%)	83,113,113	1.11	7 (8%)
32	CLA	RR	302	3	69,73,73	1.24	9 (13%)	83,113,113	1.18	7 (8%)
32	CLA	s	608	4	53,57,73	1.41	7 (13%)	62,93,113	1.25	6 (9%)
36	LHG	4	301	32	18,18,48	1.77	3 (16%)	17,22,54	1.48	1 (5%)
39	CHL	2	606	-	44,49,74	1.62	6 (13%)	49,83,114	1.36	7 (14%)
39	CHL	Yy	605	9	52,56,74	1.46	7 (13%)	58,92,114	1.17	6 (10%)
32	CLA	BB	604	28	69,73,73	1.24	7 (10%)	83,113,113	1.08	8 (9%)
32	CLA	N	611	36	53,57,73	1.42	6 (11%)	62,93,113	1.28	7 (11%)
32	CLA	Bb	610	-	69,73,73	1.25	8 (11%)	83,113,113	1.13	7 (8%)
32	CLA	Yy	610	9	69,73,73	1.24	9 (13%)	83,113,113	1.04	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	SS	304	4	49,53,73	1.47	6 (12%)	59,89,113	1.25	5 (8%)
32	CLA	CC	502	-	69,73,73	1.22	8 (11%)	83,113,113	1.27	7 (8%)
32	CLA	Gg	303	9	53,57,73	1.45	6 (11%)	62,93,113	1.53	7 (11%)
32	CLA	AA	408	1	64,68,73	1.29	7 (10%)	77,107,113	1.13	7 (9%)
32	CLA	Nn	302	36	53,57,73	1.42	7 (13%)	62,93,113	1.23	4 (6%)
42	NEX	Y	617	-	38,46,46	1.08	2 (5%)	50,70,70	2.12	13 (26%)
42	NEX	g	617	32	38,46,46	1.09	3 (7%)	50,70,70	2.61	16 (32%)
32	CLA	BB	607	28	69,73,73	1.22	8 (11%)	83,113,113	1.20	7 (8%)
32	CLA	G	613	9	43,48,73	1.54	6 (13%)	52,82,113	1.36	7 (13%)
32	CLA	y	315	9	63,67,73	1.30	6 (9%)	75,105,113	1.17	5 (6%)
32	CLA	A	406	-	53,57,73	1.40	7 (13%)	62,93,113	1.21	5 (8%)
32	CLA	Yy	614	9	53,57,73	1.39	6 (11%)	62,93,113	1.23	5 (8%)
39	CHL	GG	609	9	47,51,74	1.55	7 (14%)	52,86,114	1.38	7 (13%)
32	CLA	Cc	511	18	69,73,73	1.24	7 (10%)	83,113,113	1.08	6 (7%)
34	BCR	H	101	-	41,41,41	0.99	2 (4%)	56,56,56	2.17	21 (37%)
39	CHL	n	607	-	70,74,74	1.26	7 (10%)	80,114,114	1.14	6 (7%)
39	CHL	r	606	-	54,58,74	1.47	6 (11%)	59,94,114	1.29	8 (13%)
39	CHL	YY	607	-	47,51,74	1.55	7 (14%)	52,86,114	1.32	7 (13%)
41	XAT	NN	617	-	39,47,47	1.15	4 (10%)	54,74,74	2.50	13 (24%)
32	CLA	Cc	507	18	69,73,73	1.23	7 (10%)	83,113,113	1.08	7 (8%)
39	CHL	n	601	9	54,58,74	1.44	7 (12%)	59,94,114	1.19	3 (5%)
39	CHL	4	306	11	50,54,74	1.53	6 (12%)	56,90,114	1.46	6 (10%)
32	CLA	Y	604	-	53,57,73	1.40	6 (11%)	62,93,113	1.23	6 (9%)
33	PHO	A	407	-	58,69,69	2.05	9 (15%)	56,99,99	1.66	10 (17%)
32	CLA	G	610	9	53,57,73	1.42	8 (15%)	62,93,113	1.37	5 (8%)
36	LHG	3	614	32	33,33,48	1.13	2 (6%)	36,39,54	1.14	3 (8%)
37	SQD	CC	501	-	53,54,54	1.16	5 (9%)	62,65,65	1.23	5 (8%)
32	CLA	CC	512	18	69,73,73	1.24	8 (11%)	83,113,113	1.13	5 (6%)
32	CLA	CC	506	18	69,73,73	1.22	7 (10%)	83,113,113	1.15	7 (8%)
39	CHL	n	609	9	54,58,74	1.44	7 (12%)	59,94,114	1.32	9 (15%)
39	CHL	y	303	9	70,74,74	1.28	7 (10%)	80,114,114	1.04	4 (5%)
32	CLA	NN	610	9	69,73,73	1.24	7 (10%)	83,113,113	1.09	8 (9%)
33	PHO	Aa	408	-	58,69,69	2.07	10 (17%)	56,99,99	1.56	9 (16%)
44	DGD	a	415	-	56,56,67	0.97	2 (3%)	70,70,81	0.91	3 (4%)
32	CLA	b	611	28	69,73,73	1.23	6 (8%)	83,113,113	1.07	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	S	609	4	45,49,73	1.52	7 (15%)	54,84,113	1.29	4 (7%)
38	LMG	A	415	-	36,36,55	1.10	2 (5%)	44,44,63	1.11	3 (6%)
29	OEX	AA	401	1,18	0,14,14	-	-	-	-	-
32	CLA	B	606	28	69,73,73	1.23	7 (10%)	83,113,113	1.16	5 (6%)
46	HEM	Ee	101	20,21	50,50,50	1.40	7 (14%)	66,82,82	1.17	5 (7%)
32	CLA	1	613	14	43,48,73	1.55	6 (13%)	52,82,113	1.25	4 (7%)
32	CLA	S	602	4	53,57,73	1.39	6 (11%)	62,93,113	1.21	7 (11%)
34	BCR	Cc	517	-	41,41,41	1.03	2 (4%)	56,56,56	1.79	14 (25%)
36	LHG	g	618	32	33,33,48	1.13	2 (6%)	36,39,54	1.16	3 (8%)
32	CLA	1	604	-	43,48,73	1.57	7 (16%)	52,82,113	1.35	8 (15%)
32	CLA	YY	611	36	46,50,73	1.51	9 (19%)	55,85,113	1.29	6 (10%)
32	CLA	Rr	609	3	69,73,73	1.23	7 (10%)	83,113,113	1.13	4 (4%)
32	CLA	B	622	28	69,73,73	1.24	7 (10%)	83,113,113	1.18	8 (9%)
34	BCR	Bb	618	-	41,41,41	0.89	1 (2%)	56,56,56	1.94	12 (21%)
36	LHG	A	411	-	33,33,48	1.12	2 (6%)	36,39,54	1.22	3 (8%)
36	LHG	D	409	-	48,48,48	0.90	2 (4%)	51,54,54	0.91	2 (3%)
32	CLA	YY	603	9	53,57,73	1.40	7 (13%)	62,93,113	1.30	4 (6%)
40	LUT	S	614	-	42,43,43	0.89	0	51,60,60	1.51	8 (15%)
32	CLA	33	610	36	43,48,73	1.55	5 (11%)	52,82,113	1.32	5 (9%)
32	CLA	r	602	3	69,73,73	1.24	7 (10%)	83,113,113	1.09	6 (7%)
32	CLA	DD	401	-	69,73,73	1.23	8 (11%)	83,113,113	1.16	8 (9%)
36	LHG	1	614	32	29,29,48	1.21	2 (6%)	32,35,54	1.12	2 (6%)
32	CLA	Yy	612	9	69,73,73	1.22	6 (8%)	83,113,113	1.16	6 (7%)
32	CLA	CC	513	18	69,73,73	1.24	6 (8%)	83,113,113	1.17	3 (3%)
42	NEX	y	319	-	38,46,46	1.07	1 (2%)	50,70,70	2.01	11 (22%)
39	CHL	Yy	606	-	48,52,74	1.50	6 (12%)	53,87,114	1.24	5 (9%)
39	CHL	Y	608	-	54,58,74	1.43	7 (12%)	59,94,114	1.20	5 (8%)
32	CLA	RR	303	3	53,57,73	1.40	6 (11%)	62,93,113	1.31	4 (6%)
39	CHL	2	601	14	44,49,74	1.60	6 (13%)	49,83,114	1.29	5 (10%)
39	CHL	R	607	-	54,58,74	1.45	7 (12%)	59,94,114	1.26	5 (8%)
40	LUT	g	616	-	42,43,43	0.87	1 (2%)	51,60,60	1.59	9 (17%)
32	CLA	Aa	406	1	69,73,73	1.27	9 (13%)	83,113,113	1.18	9 (10%)
39	CHL	Gg	307	-	47,51,74	1.54	7 (14%)	52,86,114	1.19	4 (7%)
32	CLA	22	610	36	46,50,73	1.51	6 (13%)	55,85,113	1.20	4 (7%)
39	CHL	n	606	-	54,58,74	1.45	7 (12%)	59,94,114	1.27	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Bb	614	28	69,73,73	1.22	6 (8%)	83,113,113	1.11	4 (4%)
40	LUT	s	614	-	42,43,43	1.05	2 (4%)	51,60,60	1.49	8 (15%)
36	LHG	AA	414	-	44,44,48	0.97	2 (4%)	47,50,54	0.89	2 (4%)
32	CLA	C	514	18	69,73,73	1.24	7 (10%)	83,113,113	1.19	4 (4%)
32	CLA	Cc	513	18	69,73,73	1.25	6 (8%)	83,113,113	1.09	5 (6%)
42	NEX	n	617	-	38,46,46	1.08	1 (2%)	50,70,70	2.13	13 (26%)
39	CHL	NN	606	-	46,50,74	1.54	7 (15%)	51,85,114	1.26	4 (7%)
32	CLA	YY	614	9	53,57,73	1.40	7 (13%)	62,93,113	1.20	5 (8%)
37	SQD	B	617	-	35,36,54	1.48	4 (11%)	44,47,65	4.31	10 (22%)
32	CLA	3	613	15	43,48,73	1.55	6 (13%)	52,82,113	1.31	6 (11%)
32	CLA	g	610	9	53,57,73	1.41	8 (15%)	62,93,113	1.13	6 (9%)
32	CLA	G	611	36	56,60,73	1.39	6 (10%)	67,97,113	1.18	4 (5%)
32	CLA	c	511	18	69,73,73	1.27	6 (8%)	83,113,113	1.06	3 (3%)
32	CLA	B	624	28	69,73,73	1.23	8 (11%)	83,113,113	1.18	8 (9%)
36	LHG	Dd	405	-	42,42,48	0.98	2 (4%)	45,48,54	0.95	2 (4%)
32	CLA	y	304	9	69,73,73	1.24	9 (13%)	83,113,113	1.11	4 (4%)
36	LHG	d	405	-	42,42,48	0.99	2 (4%)	45,48,54	0.97	2 (4%)
32	CLA	Rr	602	3	69,73,73	1.25	8 (11%)	83,113,113	1.11	5 (6%)
39	CHL	Ss	607	-	53,57,74	1.48	6 (11%)	59,93,114	1.14	5 (8%)
35	PL9	d	404	-	55,55,55	4.25	19 (34%)	68,69,69	3.83	37 (54%)
39	CHL	11	607	-	44,49,74	1.60	6 (13%)	49,83,114	1.48	9 (18%)
32	CLA	S	608	4	45,49,73	1.53	7 (15%)	54,84,113	1.23	7 (12%)
39	CHL	G	601	9	70,74,74	1.28	6 (8%)	80,114,114	1.00	4 (5%)
34	BCR	BB	618	-	41,41,41	0.92	1 (2%)	56,56,56	1.87	13 (23%)
41	XAT	Nn	308	-	39,47,47	1.16	3 (7%)	54,74,74	2.78	16 (29%)
32	CLA	B	605	-	69,73,73	1.24	8 (11%)	83,113,113	1.26	10 (12%)
32	CLA	33	604	-	43,48,73	1.56	6 (13%)	52,82,113	1.30	5 (9%)
29	OEX	A	401	1,18	0,14,14	-	-	-	-	-
40	LUT	22	614	-	42,43,43	1.12	4 (9%)	51,60,60	1.77	11 (21%)
40	LUT	G	616	-	42,43,43	0.93	0	51,60,60	1.59	9 (17%)
32	CLA	Cc	508	18	69,73,73	1.23	7 (10%)	83,113,113	1.19	9 (10%)
39	CHL	G	609	9	47,51,74	1.55	7 (14%)	52,86,114	1.30	6 (11%)
32	CLA	N	602	9	69,73,73	1.23	7 (10%)	83,113,113	1.17	8 (9%)
38	LMG	AA	415	-	36,36,55	1.10	2 (5%)	44,44,63	1.13	3 (6%)
39	CHL	y	308	-	48,52,74	1.51	7 (14%)	53,87,114	1.22	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	BCR	d	403	-	41,41,41	0.87	0	56,56,56	2.03	18 (32%)
40	LUT	G	615	-	42,43,43	0.94	0	51,60,60	1.49	6 (11%)
32	CLA	2	609	14	43,48,73	1.55	5 (11%)	52,82,113	1.25	4 (7%)
32	CLA	SS	309	4	45,49,73	1.52	7 (15%)	54,84,113	1.25	5 (9%)
32	CLA	R	602	3	69,73,73	1.25	9 (13%)	83,113,113	1.16	7 (8%)
32	CLA	Ss	612	4	53,57,73	1.40	6 (11%)	62,93,113	1.19	4 (6%)
40	LUT	Nn	306	-	42,43,43	0.97	0	51,60,60	1.30	5 (9%)
39	CHL	NN	609	9	54,58,74	1.42	7 (12%)	59,94,114	1.32	8 (13%)
36	LHG	J	101	-	26,26,48	1.33	2 (7%)	29,32,54	1.36	3 (10%)
32	CLA	Cc	510	18	64,68,73	1.28	7 (10%)	77,107,113	1.07	4 (5%)
36	LHG	Dd	406	-	48,48,48	0.91	2 (4%)	51,54,54	0.95	2 (3%)
32	CLA	c	510	18	69,73,73	1.25	6 (8%)	83,113,113	1.16	5 (6%)
35	PL9	Dd	404	-	55,55,55	4.25	19 (34%)	68,69,69	3.86	37 (54%)
40	LUT	g	615	-	42,43,43	0.94	1 (2%)	51,60,60	1.45	5 (9%)
32	CLA	Nn	313	9	53,57,73	1.41	6 (11%)	62,93,113	1.28	5 (8%)
32	CLA	Rr	613	3	53,57,73	1.42	7 (13%)	62,93,113	1.24	6 (9%)
32	CLA	B	609	28	64,68,73	1.28	6 (9%)	77,107,113	1.16	6 (7%)
32	CLA	S	603	4	49,53,73	1.49	6 (12%)	59,89,113	1.25	4 (6%)
35	PL9	D	407	-	55,55,55	4.24	19 (34%)	68,69,69	3.87	37 (54%)
32	CLA	NN	614	9	45,49,73	1.51	6 (13%)	54,84,113	1.22	4 (7%)
39	CHL	s	607	-	53,57,74	1.49	6 (11%)	59,93,114	1.14	5 (8%)
42	NEX	Rr	616	-	38,46,46	1.07	1 (2%)	50,70,70	2.22	16 (32%)
38	LMG	m	101	-	51,51,55	0.94	2 (3%)	59,59,63	0.82	2 (3%)
34	BCR	Aa	411	-	41,41,41	1.00	3 (7%)	56,56,56	1.60	10 (17%)
36	LHG	Gg	319	32	33,33,48	1.12	2 (6%)	36,39,54	1.17	3 (8%)
39	CHL	11	608	14	44,49,74	1.57	7 (15%)	49,83,114	1.37	9 (18%)
39	CHL	RR	306	-	54,58,74	1.38	7 (12%)	59,94,114	1.45	10 (16%)
36	LHG	SS	301	-	25,25,48	1.30	2 (8%)	28,31,54	1.09	2 (7%)
32	CLA	GG	602	9	53,57,73	1.43	7 (13%)	62,93,113	1.40	7 (11%)
32	CLA	r	613	3	53,57,73	1.41	7 (13%)	62,93,113	1.24	6 (9%)
32	CLA	N	613	9	53,57,73	1.42	7 (13%)	62,93,113	1.26	4 (6%)
32	CLA	b	605	28	69,73,73	1.23	7 (10%)	83,113,113	1.12	6 (7%)
39	CHL	1	601	14	44,49,74	1.60	7 (15%)	49,83,114	1.27	5 (10%)
39	CHL	GG	605	9	47,51,74	1.54	6 (12%)	52,86,114	1.12	5 (9%)
34	BCR	TT	101	-	41,41,41	0.98	1 (2%)	56,56,56	2.04	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	XAT	4	314	-	39,47,47	1.00	0	54,74,74	2.62	15 (27%)
39	CHL	SS	307	-	46,50,74	1.55	7 (15%)	51,85,114	1.22	4 (7%)
32	CLA	b	615	28	69,73,73	1.24	6 (8%)	83,113,113	1.10	4 (4%)
39	CHL	Rr	607	-	54,58,74	1.47	7 (12%)	59,94,114	1.26	7 (11%)
32	CLA	n	610	9	69,73,73	1.24	7 (10%)	83,113,113	1.06	8 (9%)
39	CHL	3	606	-	44,49,74	1.60	6 (13%)	49,83,114	1.28	6 (12%)
32	CLA	C	513	18	69,73,73	1.24	7 (10%)	83,113,113	1.16	4 (4%)
32	CLA	b	603	28	69,73,73	1.25	7 (10%)	83,113,113	1.07	7 (8%)
34	BCR	c	514	-	41,41,41	0.93	2 (4%)	56,56,56	2.15	18 (32%)
44	DGD	C	520	-	63,63,67	0.86	2 (3%)	77,77,81	0.86	2 (2%)
32	CLA	Nn	312	9	69,73,73	1.23	8 (11%)	83,113,113	1.20	7 (8%)
38	LMG	DD	409	-	46,46,55	0.98	2 (4%)	54,54,63	0.89	1 (1%)
32	CLA	3	610	36	43,48,73	1.55	5 (11%)	52,82,113	1.36	6 (11%)
32	CLA	r	609	3	69,73,73	1.23	7 (10%)	83,113,113	1.09	3 (3%)
34	BCR	B	612	-	41,41,41	0.95	0	56,56,56	1.75	13 (23%)
39	CHL	GG	606	-	47,51,74	1.52	7 (14%)	52,86,114	1.18	5 (9%)
39	CHL	y	309	-	47,51,74	1.53	7 (14%)	52,86,114	1.31	5 (9%)
39	CHL	Rr	606	-	54,58,74	1.46	6 (11%)	59,94,114	1.14	4 (6%)
34	BCR	Cc	518	-	41,41,41	0.89	1 (2%)	56,56,56	1.90	11 (19%)
37	SQD	BB	621	-	35,36,54	1.48	5 (14%)	44,47,65	4.32	10 (22%)
43	LMU	R	618	-	28,28,36	0.79	0	39,39,47	0.98	3 (7%)
32	CLA	s	602	4	53,57,73	1.40	7 (13%)	62,93,113	1.21	5 (8%)
44	DGD	Cc	519	-	56,56,67	0.91	2 (3%)	70,70,81	1.11	7 (10%)
41	XAT	GG	619	-	39,47,47	1.19	3 (7%)	54,74,74	2.94	12 (22%)
39	CHL	S	605	-	46,50,74	1.57	6 (13%)	51,85,114	1.41	4 (7%)
39	CHL	3	607	-	44,49,74	1.61	6 (13%)	49,83,114	1.37	5 (10%)
42	NEX	YY	617	-	38,46,46	1.08	2 (5%)	50,70,70	2.07	13 (26%)
42	NEX	Nn	309	-	38,46,46	1.06	1 (2%)	50,70,70	2.10	12 (24%)
32	CLA	2	602	14	43,48,73	1.57	6 (13%)	52,82,113	1.24	5 (9%)
32	CLA	Y	603	9	53,57,73	1.41	7 (13%)	62,93,113	1.27	4 (6%)
34	BCR	h	101	-	41,41,41	1.04	3 (7%)	56,56,56	2.51	23 (41%)
32	CLA	BB	609	-	69,73,73	1.25	8 (11%)	83,113,113	1.25	10 (12%)
38	LMG	b	621	-	36,36,55	1.11	2 (5%)	44,44,63	1.11	4 (9%)
32	CLA	s	609	4	53,57,73	1.40	7 (13%)	62,93,113	1.22	7 (11%)
37	SQD	AA	412	-	34,35,54	1.46	4 (11%)	43,46,65	1.16	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	N	604	-	45,49,73	1.50	6 (13%)	54,84,113	1.22	5 (9%)
32	CLA	b	604	28	69,73,73	1.24	7 (10%)	83,113,113	1.20	6 (7%)
39	CHL	r	605	3	54,58,74	1.44	7 (12%)	59,94,114	1.25	5 (8%)
39	CHL	Nn	317	-	70,74,74	1.25	7 (10%)	80,114,114	1.18	7 (8%)
39	CHL	1	606	-	44,49,74	1.61	6 (13%)	49,83,114	1.28	5 (10%)
32	CLA	Dd	401	19	69,73,73	1.25	8 (11%)	83,113,113	1.16	5 (6%)
36	LHG	YY	618	32	48,48,48	0.93	2 (4%)	51,54,54	0.84	2 (3%)
39	CHL	4	309	11	50,54,74	1.54	7 (14%)	56,90,114	1.45	9 (16%)
32	CLA	Gg	314	9	43,48,73	1.54	6 (13%)	52,82,113	1.33	7 (13%)
45	BCT	a	413	30	2,3,3	1.28	0	2,3,3	3.84	2 (100%)
33	PHO	Aa	409	-	58,69,69	2.06	10 (17%)	56,99,99	1.54	8 (14%)
32	CLA	44	609	11	49,53,73	1.46	7 (14%)	59,89,113	1.20	3 (5%)
39	CHL	g	607	-	54,58,74	1.44	7 (12%)	59,94,114	1.15	5 (8%)
32	CLA	22	602	14	43,48,73	1.55	6 (13%)	52,82,113	1.26	6 (11%)
39	CHL	4	302	-	48,53,74	1.54	6 (12%)	53,89,114	1.15	4 (7%)
32	CLA	G	614	9	45,49,73	1.50	6 (13%)	54,84,113	1.18	4 (7%)
41	XAT	y	302	-	39,47,47	1.17	3 (7%)	54,74,74	2.73	17 (31%)
32	CLA	G	602	9	53,57,73	1.43	7 (13%)	62,93,113	1.28	5 (8%)
29	OEX	a	401	1,18	0,14,14	-	-	-	-	-
32	CLA	1	603	14	43,48,73	1.54	6 (13%)	52,82,113	1.22	4 (7%)
32	CLA	44	603	11	49,53,73	1.48	6 (12%)	59,89,113	1.33	5 (8%)
32	CLA	S	604	-	53,57,73	1.41	6 (11%)	62,93,113	1.24	5 (8%)
39	CHL	GG	601	9	70,74,74	1.28	7 (10%)	80,114,114	1.02	5 (6%)
32	CLA	Bb	609	28	69,73,73	1.23	8 (11%)	83,113,113	1.23	7 (8%)
39	CHL	3	605	-	44,49,74	1.60	6 (13%)	49,83,114	1.28	6 (12%)
32	CLA	n	611	36	53,57,73	1.41	7 (13%)	62,93,113	1.25	5 (8%)
39	CHL	Yy	609	9	70,74,74	1.29	7 (10%)	80,114,114	1.29	9 (11%)
32	CLA	NN	602	9	69,73,73	1.23	7 (10%)	83,113,113	1.18	8 (9%)
32	CLA	GG	613	9	43,48,73	1.55	6 (13%)	52,82,113	1.45	7 (13%)
36	LHG	N	619	32	37,37,48	1.07	2 (5%)	40,43,54	1.06	3 (7%)
39	CHL	Ss	606	-	54,58,74	1.46	6 (11%)	59,94,114	1.35	6 (10%)
32	CLA	r	604	-	53,57,73	1.40	6 (11%)	62,93,113	1.24	6 (9%)
39	CHL	11	606	-	44,49,74	1.62	6 (13%)	49,83,114	1.27	5 (10%)
46	HEM	e	101	20,21	50,50,50	1.41	7 (14%)	66,82,82	1.16	5 (7%)
39	CHL	S	606	-	46,50,74	1.56	7 (15%)	51,85,114	1.23	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LHG	BB	622	-	33,33,48	1.12	2 (6%)	36,39,54	1.01	2 (5%)
39	CHL	GG	608	-	46,50,74	1.54	7 (15%)	51,85,114	1.23	5 (9%)
32	CLA	Ss	608	4	53,57,73	1.41	7 (13%)	62,93,113	1.27	7 (11%)
39	CHL	G	608	-	46,50,74	1.54	6 (13%)	51,85,114	1.26	6 (11%)
39	CHL	Y	601	9	70,74,74	1.27	7 (10%)	80,114,114	1.08	4 (5%)
39	CHL	3	601	15	44,49,74	1.61	6 (13%)	49,83,114	1.29	4 (8%)
39	CHL	g	606	-	47,51,74	1.54	7 (14%)	52,86,114	1.21	4 (7%)
32	CLA	Ss	610	36	53,57,73	1.41	6 (11%)	62,93,113	1.27	4 (6%)
37	SQD	Aa	413	-	46,47,54	1.27	4 (8%)	55,58,65	1.04	5 (9%)
32	CLA	s	613	4	53,57,73	1.42	7 (13%)	62,93,113	1.21	6 (9%)
36	LHG	Ll	102	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	3 (5%)
39	CHL	Rr	605	3	54,58,74	1.44	7 (12%)	59,94,114	1.30	6 (10%)
32	CLA	a	410	1	64,68,73	1.29	7 (10%)	77,107,113	1.15	6 (7%)
32	CLA	n	613	9	53,57,73	1.42	7 (13%)	62,93,113	1.22	4 (6%)
32	CLA	s	604	-	53,57,73	1.42	7 (13%)	62,93,113	1.17	4 (6%)
39	CHL	y	307	9	52,56,74	1.45	7 (13%)	58,92,114	1.19	6 (10%)
32	CLA	BB	614	28	69,73,73	1.23	6 (8%)	83,113,113	1.18	8 (9%)
34	BCR	BB	617	-	41,41,41	0.97	2 (4%)	56,56,56	1.75	12 (21%)
39	CHL	1l	605	14	44,49,74	1.61	6 (13%)	49,83,114	1.26	5 (10%)
32	CLA	a	406	1	69,73,73	1.27	9 (13%)	83,113,113	1.20	11 (13%)
32	CLA	1	609	14	43,48,73	1.53	6 (13%)	52,82,113	1.38	6 (11%)
32	CLA	c	506	18	69,73,73	1.23	7 (10%)	83,113,113	1.17	9 (10%)
32	CLA	B	608	28	69,73,73	1.24	6 (8%)	83,113,113	1.07	3 (3%)
36	LHG	K	101	-	33,33,48	1.12	2 (6%)	36,39,54	1.08	2 (5%)
40	LUT	N	616	-	42,43,43	0.97	1 (2%)	51,60,60	1.64	10 (19%)
32	CLA	Bb	615	28	69,73,73	1.24	6 (8%)	83,113,113	1.13	4 (4%)
34	BCR	Kk	101	-	41,41,41	0.85	0	56,56,56	1.98	13 (23%)
32	CLA	AA	405	1	69,73,73	1.23	7 (10%)	83,113,113	1.13	6 (7%)
32	CLA	Dd	402	19	69,73,73	1.24	7 (10%)	83,113,113	1.09	6 (7%)
38	LMG	c	519	-	34,34,55	1.14	3 (8%)	42,42,63	1.20	6 (14%)
39	CHL	N	609	9	54,58,74	1.42	7 (12%)	59,94,114	1.37	10 (16%)
39	CHL	N	605	9	46,50,74	1.55	7 (15%)	51,85,114	1.31	4 (7%)
32	CLA	S	612	4	53,57,73	1.42	6 (11%)	62,93,113	1.20	6 (9%)
36	LHG	Yy	618	32	48,48,48	0.91	2 (4%)	51,54,54	0.99	4 (7%)
32	CLA	BB	615	28	45,49,73	1.49	6 (13%)	54,84,113	1.34	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Yy	611	36	46,50,73	1.50	7 (15%)	55,85,113	1.30	4 (7%)
32	CLA	b	601	-	69,73,73	1.26	9 (13%)	83,113,113	1.18	8 (9%)
39	CHL	s	606	-	54,58,74	1.46	6 (11%)	59,94,114	1.33	6 (10%)
39	CHL	R	605	-	54,58,74	1.42	7 (12%)	59,94,114	1.53	12 (20%)
39	CHL	44	601	-	48,53,74	1.54	6 (12%)	53,89,114	1.16	4 (7%)
32	CLA	Cc	504	18	69,73,73	1.24	8 (11%)	83,113,113	1.16	7 (8%)
39	CHL	11	601	14	44,49,74	1.61	7 (15%)	49,83,114	1.27	6 (12%)
39	CHL	Gg	308	-	54,58,74	1.43	6 (11%)	59,94,114	1.15	5 (8%)
38	LMG	W	201	-	48,48,55	0.98	3 (6%)	56,56,63	1.05	2 (3%)
43	LMU	RR	301	-	28,28,36	0.76	0	39,39,47	0.75	0
32	CLA	R	610	36	53,57,73	1.43	7 (13%)	62,93,113	1.15	5 (8%)
39	CHL	G	606	-	47,51,74	1.53	7 (14%)	52,86,114	1.18	5 (9%)
40	LUT	Y	616	-	42,43,43	0.99	0	51,60,60	1.57	11 (21%)
35	PL9	AA	410	-	55,55,55	4.33	23 (41%)	68,69,69	3.71	38 (55%)
40	LUT	Y	615	-	42,43,43	0.94	1 (2%)	51,60,60	1.88	12 (23%)
32	CLA	Cc	514	18	69,73,73	1.23	6 (8%)	83,113,113	1.14	5 (6%)
32	CLA	c	504	-	59,63,73	1.32	6 (10%)	71,101,113	1.14	5 (7%)
39	CHL	Y	606	-	48,52,74	1.53	7 (14%)	53,87,114	1.14	4 (7%)
32	CLA	R	614	3	53,57,73	1.45	6 (11%)	62,93,113	1.28	7 (11%)
32	CLA	RR	310	36	53,57,73	1.41	5 (9%)	62,93,113	1.18	5 (8%)
32	CLA	Gg	313	9	53,57,73	1.41	6 (11%)	62,93,113	1.25	5 (8%)
32	CLA	SS	303	4	53,57,73	1.40	7 (13%)	62,93,113	1.25	7 (11%)
32	CLA	1	602	14	43,48,73	1.54	6 (13%)	52,82,113	1.31	5 (9%)
32	CLA	3	612	15	43,48,73	1.56	6 (13%)	52,82,113	1.24	4 (7%)
34	BCR	Cc	516	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	18 (32%)
41	XAT	G	619	-	39,47,47	1.19	2 (5%)	54,74,74	2.93	13 (24%)
39	CHL	N	601	9	48,52,74	1.53	7 (14%)	53,87,114	1.21	5 (9%)
39	CHL	22	606	-	44,49,74	1.62	6 (13%)	49,83,114	1.41	7 (14%)
32	CLA	22	604	-	43,48,73	1.55	6 (13%)	52,82,113	1.31	5 (9%)
32	CLA	NN	613	9	53,57,73	1.42	8 (15%)	62,93,113	1.21	5 (8%)
41	XAT	Gg	301	-	39,47,47	1.22	4 (10%)	54,74,74	2.84	11 (20%)
46	HEM	E	101	20,21	50,50,50	1.38	6 (12%)	66,82,82	1.14	5 (7%)
32	CLA	R	604	-	53,57,73	1.41	7 (13%)	62,93,113	1.31	5 (8%)
37	SQD	L	101	-	53,54,54	1.19	4 (7%)	62,65,65	1.10	6 (9%)
44	DGD	Aa	401	-	56,56,67	0.96	2 (3%)	70,70,81	0.90	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Rr	601	3	53,57,73	1.43	6 (11%)	62,93,113	1.18	5 (8%)
32	CLA	SS	312	4	53,57,73	1.41	6 (11%)	62,93,113	1.27	4 (6%)
38	LMG	C	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.01	3 (5%)
32	CLA	11	610	36	43,48,73	1.55	5 (11%)	52,82,113	1.28	5 (9%)
32	CLA	GG	611	36	56,60,73	1.38	7 (12%)	67,97,113	1.16	3 (4%)
39	CHL	g	609	9	47,51,74	1.52	7 (14%)	52,86,114	1.34	6 (11%)
32	CLA	3	609	15	43,48,73	1.55	6 (13%)	52,82,113	1.28	5 (9%)
39	CHL	Y	605	9	52,56,74	1.46	7 (13%)	58,92,114	1.16	5 (8%)
32	CLA	4	310	-	49,53,73	1.46	7 (14%)	59,89,113	1.20	3 (5%)
32	CLA	Rr	611	3	53,57,73	1.42	6 (11%)	62,93,113	1.19	3 (4%)
32	CLA	Yy	604	-	53,57,73	1.38	7 (13%)	62,93,113	1.22	6 (9%)
32	CLA	GG	603	9	69,73,73	1.24	6 (8%)	83,113,113	1.07	4 (4%)
39	CHL	g	605	9	47,51,74	1.53	7 (14%)	52,86,114	1.21	5 (9%)
39	CHL	y	310	-	54,58,74	1.43	8 (14%)	59,94,114	1.19	5 (8%)
44	DGD	c	517	-	56,56,67	0.91	2 (3%)	70,70,81	1.11	6 (8%)
32	CLA	Rr	603	3	53,57,73	1.42	7 (13%)	62,93,113	1.25	3 (4%)
32	CLA	n	604	-	53,57,73	1.41	7 (13%)	62,93,113	1.16	6 (9%)
36	LHG	D	410	-	33,33,48	1.12	2 (6%)	36,39,54	1.11	3 (8%)
32	CLA	RR	304	-	53,57,73	1.42	8 (15%)	62,93,113	1.30	7 (11%)
32	CLA	11	611	14	43,48,73	1.55	6 (13%)	52,82,113	1.30	5 (9%)
36	LHG	D	408	-	42,42,48	1.00	2 (4%)	45,48,54	1.02	2 (4%)
34	BCR	b	618	-	41,41,41	0.90	1 (2%)	56,56,56	1.92	12 (21%)
32	CLA	4	305	-	49,53,73	1.46	6 (12%)	59,89,113	1.25	5 (8%)
32	CLA	c	508	18	64,68,73	1.28	6 (9%)	77,107,113	1.11	5 (6%)
34	BCR	K	102	-	41,41,41	0.81	0	56,56,56	2.18	18 (32%)
36	LHG	C	522	-	30,30,48	1.16	2 (6%)	33,36,54	1.06	2 (6%)
39	CHL	SS	306	4	46,50,74	1.56	7 (15%)	51,85,114	1.47	5 (9%)
32	CLA	C	515	18	53,57,73	1.40	7 (13%)	62,93,113	1.23	5 (8%)
32	CLA	r	611	3	53,57,73	1.44	6 (11%)	62,93,113	1.15	4 (6%)
36	LHG	44	614	32	20,20,48	1.30	2 (10%)	23,26,54	1.50	2 (8%)
37	SQD	LL	101	-	35,36,54	1.45	4 (11%)	44,47,65	1.15	5 (11%)
36	LHG	DD	407	-	42,42,48	0.99	2 (4%)	45,48,54	1.02	2 (4%)
39	CHL	g	601	9	70,74,74	1.27	7 (10%)	80,114,114	1.04	5 (6%)
32	CLA	B	623	-	69,73,73	1.23	6 (8%)	83,113,113	1.05	4 (4%)
32	CLA	RR	314	3	53,57,73	1.43	6 (11%)	62,93,113	1.28	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Aa	410	1	64,68,73	1.29	7 (10%)	77,107,113	1.16	7 (9%)
36	LHG	Nn	310	32	48,48,48	0.95	2 (4%)	51,54,54	1.05	2 (3%)
32	CLA	N	603	9	46,50,73	1.48	7 (15%)	55,85,113	1.29	5 (9%)
32	CLA	Aa	405	1	69,73,73	1.24	7 (10%)	83,113,113	1.19	7 (8%)
40	LUT	44	612	-	42,43,43	0.91	0	51,60,60	1.38	6 (11%)
34	BCR	D	406	-	41,41,41	0.83	0	56,56,56	1.92	16 (28%)
32	CLA	R	611	3	53,57,73	1.41	6 (11%)	62,93,113	1.21	3 (4%)
39	CHL	Nn	316	-	54,58,74	1.45	7 (12%)	59,94,114	1.26	5 (8%)
32	CLA	2	611	14	43,48,73	1.56	6 (13%)	52,82,113	1.29	5 (9%)
32	CLA	Gg	312	36	69,73,73	1.24	7 (10%)	83,113,113	1.25	7 (8%)
39	CHL	3	608	15	44,49,74	1.58	6 (13%)	49,83,114	1.20	5 (10%)
39	CHL	s	605	-	54,58,74	1.46	6 (11%)	59,94,114	1.24	4 (6%)
33	PHO	AA	407	-	58,69,69	2.05	10 (17%)	56,99,99	1.66	9 (16%)
37	SQD	C	501	-	53,54,54	1.17	4 (7%)	62,65,65	1.07	5 (8%)
39	CHL	Y	609	9	70,74,74	1.28	7 (10%)	80,114,114	1.12	7 (8%)
38	LMG	a	412	-	42,42,55	1.03	2 (4%)	50,50,63	1.10	4 (8%)
34	BCR	KK	103	-	41,41,41	0.82	0	56,56,56	2.18	19 (33%)
38	LMG	j	101	-	46,46,55	0.98	2 (4%)	54,54,63	1.04	3 (5%)
39	CHL	Gg	309	-	46,50,74	1.54	7 (15%)	51,85,114	1.18	4 (7%)
32	CLA	c	512	18	69,73,73	1.23	7 (10%)	83,113,113	1.12	5 (6%)
40	LUT	Gg	317	-	42,43,43	0.89	1 (2%)	51,60,60	1.64	10 (19%)
32	CLA	33	603	15	43,48,73	1.56	5 (11%)	52,82,113	1.27	5 (9%)
32	CLA	B	607	28	69,73,73	1.24	9 (13%)	83,113,113	1.12	4 (4%)
36	LHG	A	413	-	36,36,48	1.07	2 (5%)	39,42,54	1.01	3 (7%)
39	CHL	2	605	-	44,49,74	1.62	6 (13%)	49,83,114	1.39	6 (12%)
39	CHL	Gg	302	9	70,74,74	1.28	7 (10%)	80,114,114	1.03	4 (5%)
32	CLA	C	508	18	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)
32	CLA	b	606	28	69,73,73	1.23	7 (10%)	83,113,113	1.13	6 (7%)
39	CHL	R	606	-	54,58,74	1.43	7 (12%)	59,94,114	1.38	9 (15%)
42	NEX	Yy	617	-	38,46,46	1.07	1 (2%)	50,70,70	2.02	13 (26%)
32	CLA	3	611	15	43,48,73	1.55	6 (13%)	52,82,113	1.25	5 (9%)
36	LHG	CC	523	-	36,36,48	1.05	2 (5%)	39,42,54	1.03	3 (7%)
32	CLA	b	612	28	69,73,73	1.24	7 (10%)	83,113,113	1.19	4 (4%)
39	CHL	Gg	306	9	47,51,74	1.53	7 (14%)	52,86,114	1.22	5 (9%)
39	CHL	s	601	4	56,60,74	1.44	7 (12%)	63,97,114	1.26	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	22	613	14	43,48,73	1.55	5 (11%)	52,82,113	1.26	4 (7%)
32	CLA	n	614	9	53,57,73	1.41	5 (9%)	62,93,113	1.16	5 (8%)
41	XAT	RR	316	-	39,47,47	1.01	2 (5%)	54,74,74	2.30	16 (29%)
36	LHG	y	320	32	48,48,48	0.92	2 (4%)	51,54,54	0.95	2 (3%)
32	CLA	NN	604	-	45,49,73	1.50	6 (13%)	54,84,113	1.22	5 (9%)
32	CLA	44	615	3	53,57,73	1.42	6 (11%)	62,93,113	1.26	3 (4%)
37	SQD	Ll	101	-	53,54,54	1.18	4 (7%)	62,65,65	1.02	4 (6%)
32	CLA	n	602	9	69,73,73	1.24	9 (13%)	83,113,113	1.21	10 (12%)
32	CLA	D	401	-	69,73,73	1.23	7 (10%)	83,113,113	1.16	8 (9%)
32	CLA	X	201	-	45,49,73	1.53	8 (17%)	54,84,113	1.27	5 (9%)
32	CLA	33	612	15	43,48,73	1.55	7 (16%)	52,82,113	1.25	4 (7%)
32	CLA	C	511	18	69,73,73	1.25	8 (11%)	83,113,113	1.15	5 (6%)
34	BCR	b	619	-	41,41,41	0.89	1 (2%)	56,56,56	1.93	12 (21%)
32	CLA	Ss	611	4	53,57,73	1.42	6 (11%)	62,93,113	1.29	9 (14%)
40	LUT	Rr	614	-	42,43,43	0.92	0	51,60,60	1.38	8 (15%)
41	XAT	Yy	619	-	39,47,47	1.05	2 (5%)	54,74,74	2.45	19 (35%)
32	CLA	c	503	18	69,73,73	1.25	7 (10%)	83,113,113	1.09	6 (7%)
32	CLA	44	610	36	49,53,73	1.48	6 (12%)	59,89,113	1.19	4 (6%)
33	PHO	D	402	-	58,69,69	2.05	9 (15%)	56,99,99	1.58	8 (14%)
32	CLA	SS	313	4	53,57,73	1.41	6 (11%)	62,93,113	1.19	7 (11%)
32	CLA	BB	606	-	69,73,73	1.23	6 (8%)	83,113,113	1.06	4 (4%)
32	CLA	Bb	604	28	69,73,73	1.25	7 (10%)	83,113,113	1.22	7 (8%)
32	CLA	Bb	607	-	69,73,73	1.25	6 (8%)	83,113,113	1.06	5 (6%)
39	CHL	YY	609	9	70,74,74	1.27	7 (10%)	80,114,114	1.05	7 (8%)
32	CLA	CC	509	18	69,73,73	1.23	7 (10%)	83,113,113	1.16	5 (6%)
32	CLA	33	609	15	43,48,73	1.55	6 (13%)	52,82,113	1.27	4 (7%)
32	CLA	c	513	18	47,51,73	1.47	7 (14%)	56,86,113	1.26	5 (8%)
39	CHL	GG	607	-	50,54,74	1.50	7 (14%)	56,90,114	1.20	4 (7%)
32	CLA	y	305	9	53,57,73	1.41	7 (13%)	62,93,113	1.21	3 (4%)
41	XAT	y	301	-	39,47,47	1.06	3 (7%)	54,74,74	2.48	19 (35%)
39	CHL	NN	605	9	46,50,74	1.54	7 (15%)	51,85,114	1.38	6 (11%)
44	DGD	CC	519	-	63,63,67	0.86	2 (3%)	77,77,81	0.93	3 (3%)
39	CHL	Nn	311	9	54,58,74	1.44	7 (12%)	59,94,114	1.16	4 (6%)
44	DGD	D	411	-	63,63,67	0.87	2 (3%)	77,77,81	0.88	3 (3%)
41	XAT	r	615	-	39,47,47	1.02	1 (2%)	54,74,74	2.49	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	R	601	3	53,57,73	1.43	7 (13%)	62,93,113	1.27	4 (6%)
34	BCR	T	101	-	41,41,41	0.97	1 (2%)	56,56,56	2.06	19 (33%)
32	CLA	4	312	11	49,53,73	1.48	6 (12%)	59,89,113	1.24	3 (5%)
43	LMU	C	502	-	28,28,36	0.77	0	39,39,47	0.95	1 (2%)
39	CHL	n	608	-	54,58,74	1.45	7 (12%)	59,94,114	1.20	5 (8%)
32	CLA	B	611	28	45,49,73	1.48	6 (13%)	54,84,113	1.33	5 (9%)
34	BCR	DD	405	-	41,41,41	0.83	0	56,56,56	1.91	15 (26%)
32	CLA	D	404	19	69,73,73	1.24	8 (11%)	83,113,113	1.19	5 (6%)
39	CHL	1	605	14	44,49,74	1.60	6 (13%)	49,83,114	1.44	5 (10%)
32	CLA	SS	305	-	53,57,73	1.41	6 (11%)	62,93,113	1.25	5 (8%)
32	CLA	C	512	18	69,73,73	1.24	8 (11%)	83,113,113	1.18	5 (6%)
32	CLA	s	611	4	53,57,73	1.42	7 (13%)	62,93,113	1.29	8 (12%)
32	CLA	R	609	3	69,73,73	1.25	7 (10%)	83,113,113	1.09	6 (7%)
38	LMG	b	620	-	36,36,55	1.11	2 (5%)	44,44,63	0.95	2 (4%)
39	CHL	Nn	318	-	54,58,74	1.45	7 (12%)	59,94,114	1.21	4 (6%)
32	CLA	Bb	606	28	69,73,73	1.23	7 (10%)	83,113,113	1.13	7 (8%)
32	CLA	Gg	311	9	53,57,73	1.39	7 (13%)	62,93,113	1.24	6 (9%)
38	LMG	F	101	-	46,46,55	0.98	2 (4%)	54,54,63	0.90	2 (3%)
32	CLA	Yy	603	9	53,57,73	1.40	7 (13%)	62,93,113	1.29	5 (8%)
36	LHG	Ss	616	32	47,47,48	0.94	2 (4%)	50,53,54	0.89	2 (4%)
44	DGD	Cc	520	-	53,53,67	0.95	2 (3%)	67,67,81	0.88	1 (1%)
32	CLA	G	604	-	46,50,73	1.49	6 (13%)	55,85,113	1.18	4 (7%)
32	CLA	2	603	14	43,48,73	1.56	7 (16%)	52,82,113	1.26	5 (9%)
32	CLA	b	608	28	69,73,73	1.23	7 (10%)	83,113,113	1.13	7 (8%)
32	CLA	2	612	14	43,48,73	1.54	5 (11%)	52,82,113	1.30	6 (11%)
32	CLA	33	602	15	43,48,73	1.55	5 (11%)	52,82,113	1.27	5 (9%)
32	CLA	RR	311	3	53,57,73	1.42	6 (11%)	62,93,113	1.19	3 (4%)
36	LHG	s	616	32	47,47,48	0.95	2 (4%)	50,53,54	0.90	2 (4%)
36	LHG	CC	521	-	33,33,48	1.12	2 (6%)	36,39,54	1.03	2 (5%)
39	CHL	NN	608	-	46,50,74	1.55	7 (15%)	51,85,114	1.20	4 (7%)
32	CLA	b	613	28	69,73,73	1.24	7 (10%)	83,113,113	1.23	7 (8%)
39	CHL	Yy	608	-	54,58,74	1.43	7 (12%)	59,94,114	1.19	5 (8%)
40	LUT	NN	616	-	42,43,43	0.94	1 (2%)	51,60,60	1.67	10 (19%)
36	LHG	KK	101	-	33,33,48	1.12	2 (6%)	36,39,54	1.10	3 (8%)
32	CLA	44	604	-	49,53,73	1.46	6 (12%)	59,89,113	1.25	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Bb	612	28	69,73,73	1.24	8 (11%)	83,113,113	1.20	4 (4%)
40	LUT	NN	615	-	42,43,43	0.98	2 (4%)	51,60,60	1.34	8 (15%)
39	CHL	SS	302	4	56,60,74	1.42	7 (12%)	63,97,114	1.12	5 (7%)
32	CLA	y	316	9	53,57,73	1.40	6 (11%)	62,93,113	1.22	6 (9%)
32	CLA	BB	612	28	69,73,73	1.24	6 (8%)	83,113,113	1.07	3 (3%)
32	CLA	33	613	15	43,48,73	1.55	6 (13%)	52,82,113	1.33	6 (11%)
32	CLA	s	612	4	53,57,73	1.40	6 (11%)	62,93,113	1.20	4 (6%)
34	BCR	B	616	-	41,41,41	0.85	0	56,56,56	1.97	19 (33%)
36	LHG	GG	618	32	33,33,48	1.12	2 (6%)	36,39,54	1.14	3 (8%)
34	BCR	BB	616	-	41,41,41	0.95	1 (2%)	56,56,56	1.89	13 (23%)
36	LHG	Dd	407	-	36,36,48	1.07	2 (5%)	39,42,54	0.91	2 (5%)
32	CLA	G	603	9	69,73,73	1.24	6 (8%)	83,113,113	1.08	5 (6%)
39	CHL	y	311	9	70,74,74	1.27	7 (10%)	80,114,114	1.08	6 (7%)
36	LHG	A	414	-	44,44,48	0.97	2 (4%)	47,50,54	0.89	2 (4%)
32	CLA	B	619	28	69,73,73	1.23	7 (10%)	83,113,113	1.11	7 (8%)
36	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
44	DGD	h	102	-	63,63,67	0.90	2 (3%)	77,77,81	0.80	2 (2%)
42	NEX	RR	317	-	38,46,46	1.08	2 (5%)	50,70,70	2.03	13 (26%)
32	CLA	Ss	602	4	53,57,73	1.41	7 (13%)	62,93,113	1.22	5 (8%)
34	BCR	Bb	619	-	41,41,41	0.90	1 (2%)	56,56,56	2.04	15 (26%)
32	CLA	11	602	14	43,48,73	1.56	6 (13%)	52,82,113	1.29	5 (9%)
32	CLA	y	314	9	69,73,73	1.23	6 (8%)	83,113,113	1.12	6 (7%)
32	CLA	B	610	28	69,73,73	1.23	6 (8%)	83,113,113	1.16	7 (8%)
37	SQD	L	102	-	35,36,54	1.45	4 (11%)	44,47,65	1.23	5 (11%)
39	CHL	Yy	601	9	70,74,74	1.28	7 (10%)	80,114,114	1.04	4 (5%)
32	CLA	BB	601	28	69,73,73	1.24	6 (8%)	83,113,113	1.09	7 (8%)
40	LUT	GG	616	-	42,43,43	0.95	1 (2%)	51,60,60	1.54	8 (15%)
32	CLA	GG	614	9	45,49,73	1.51	6 (13%)	54,84,113	1.19	4 (7%)
32	CLA	Ss	609	4	53,57,73	1.42	7 (13%)	62,93,113	1.19	6 (9%)
34	BCR	AA	409	-	41,41,41	1.01	3 (7%)	56,56,56	1.97	14 (25%)
32	CLA	Cc	505	18	69,73,73	1.24	7 (10%)	83,113,113	1.15	6 (7%)
32	CLA	BB	611	28	69,73,73	1.24	8 (11%)	83,113,113	1.13	5 (6%)
40	LUT	GG	615	-	42,43,43	0.93	0	51,60,60	1.45	7 (13%)
39	CHL	n	605	9	52,56,74	1.45	7 (13%)	58,92,114	1.23	6 (10%)
38	LMG	Dd	408	-	46,46,55	0.97	2 (4%)	54,54,63	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LHG	22	615	32	33,33,48	1.13	2 (6%)	36,39,54	0.94	2 (5%)
32	CLA	DD	404	19	69,73,73	1.24	7 (10%)	83,113,113	1.07	4 (4%)
39	CHL	44	606	-	50,54,74	1.50	7 (14%)	56,90,114	1.18	4 (7%)
32	CLA	AA	406	-	53,57,73	1.40	8 (15%)	62,93,113	1.24	7 (11%)
34	BCR	Dd	403	-	41,41,41	0.86	0	56,56,56	2.03	18 (32%)
34	BCR	CC	517	-	41,41,41	0.91	1 (2%)	56,56,56	2.00	14 (25%)
44	DGD	B	601	-	56,56,67	0.92	2 (3%)	70,70,81	0.97	4 (5%)
32	CLA	b	609	28	69,73,73	1.23	7 (10%)	83,113,113	1.25	6 (7%)
32	CLA	c	505	18	69,73,73	1.22	7 (10%)	83,113,113	1.03	6 (7%)
34	BCR	c	515	-	41,41,41	1.01	3 (7%)	56,56,56	1.69	12 (21%)
34	BCR	Bb	617	-	41,41,41	1.05	2 (4%)	56,56,56	2.11	16 (28%)
32	CLA	b	614	28	69,73,73	1.23	6 (8%)	83,113,113	1.11	4 (4%)
32	CLA	Ss	613	4	53,57,73	1.41	7 (13%)	62,93,113	1.20	6 (9%)
32	CLA	3	602	15	43,48,73	1.55	5 (11%)	52,82,113	1.29	5 (9%)
32	CLA	g	611	36	69,73,73	1.25	7 (10%)	83,113,113	1.25	7 (8%)
32	CLA	BB	602	28	69,73,73	1.23	7 (10%)	83,113,113	1.12	7 (8%)
32	CLA	Aa	407	-	53,57,73	1.41	8 (15%)	62,93,113	1.31	7 (11%)
32	CLA	C	509	-	69,73,73	1.24	8 (11%)	83,113,113	1.25	7 (8%)
39	CHL	4	308	-	50,54,74	1.49	7 (14%)	56,90,114	1.36	8 (14%)
41	XAT	R	616	-	39,47,47	0.98	2 (5%)	54,74,74	2.29	16 (29%)
42	NEX	N	618	-	38,46,46	1.13	2 (5%)	50,70,70	2.22	15 (30%)
39	CHL	Y	607	-	47,51,74	1.55	7 (14%)	52,86,114	1.34	7 (13%)
32	CLA	YY	610	9	69,73,73	1.24	7 (10%)	83,113,113	1.10	5 (6%)
32	CLA	Bb	611	28	69,73,73	1.23	6 (8%)	83,113,113	1.09	4 (4%)
40	LUT	y	318	-	42,43,43	0.91	0	51,60,60	1.55	10 (19%)
44	DGD	C	519	-	56,56,67	0.94	2 (3%)	70,70,81	0.94	3 (4%)
32	CLA	22	603	14	43,48,73	1.56	6 (13%)	52,82,113	1.28	7 (13%)
32	CLA	G	612	9	53,57,73	1.42	7 (13%)	62,93,113	1.23	5 (8%)
34	BCR	BB	620	-	41,41,41	0.83	0	56,56,56	1.99	18 (32%)
32	CLA	A	408	1	64,68,73	1.29	6 (9%)	77,107,113	1.12	7 (9%)
32	CLA	Nn	304	9	53,57,73	1.43	7 (13%)	62,93,113	1.23	5 (8%)
38	LMG	Mm	101	-	51,51,55	0.94	2 (3%)	59,59,63	0.83	2 (3%)
39	CHL	33	606	-	44,49,74	1.60	6 (13%)	49,83,114	1.27	7 (14%)
32	CLA	SS	311	-	53,57,73	1.41	7 (13%)	62,93,113	1.28	4 (6%)
44	DGD	BB	623	-	63,63,67	0.89	3 (4%)	77,77,81	0.93	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	BCR	k	101	-	41,41,41	0.88	0	56,56,56	1.92	15 (26%)
32	CLA	XX	201	-	45,49,73	1.52	7 (15%)	54,84,113	1.21	5 (9%)
32	CLA	b	607	-	69,73,73	1.25	6 (8%)	83,113,113	1.06	6 (7%)
32	CLA	3	604	-	43,48,73	1.57	6 (13%)	52,82,113	1.26	4 (7%)
36	LHG	44	616	32	18,18,48	1.77	3 (16%)	17,22,54	1.42	1 (5%)
32	CLA	g	603	9	69,73,73	1.25	6 (8%)	83,113,113	1.04	5 (6%)
39	CHL	YY	605	9	52,56,74	1.47	6 (11%)	58,92,114	1.10	3 (5%)
32	CLA	22	609	14	43,48,73	1.54	7 (16%)	52,82,113	1.32	5 (9%)
37	SQD	l	102	-	53,54,54	1.18	4 (7%)	62,65,65	1.03	4 (6%)
39	CHL	1	607	-	44,49,74	1.61	6 (13%)	49,83,114	1.39	5 (10%)
39	CHL	44	607	-	50,54,74	1.49	7 (14%)	56,90,114	1.20	4 (7%)
34	BCR	C	518	-	41,41,41	0.88	0	56,56,56	2.07	17 (30%)
39	CHL	33	605	-	44,49,74	1.61	6 (13%)	49,83,114	1.27	6 (12%)
32	CLA	SS	310	4	45,49,73	1.53	7 (15%)	54,84,113	1.22	4 (7%)
32	CLA	y	312	9	69,73,73	1.23	7 (10%)	83,113,113	1.04	4 (4%)
32	CLA	g	613	9	43,48,73	1.54	6 (13%)	52,82,113	1.37	7 (13%)
36	LHG	Rr	617	32	48,48,48	0.98	2 (4%)	51,54,54	0.97	2 (3%)
39	CHL	Nn	319	9	54,58,74	1.43	8 (14%)	59,94,114	1.30	7 (11%)
36	LHG	0	201	-	46,46,48	0.97	2 (4%)	49,52,54	0.84	2 (4%)
32	CLA	Cc	506	-	59,63,73	1.32	6 (10%)	71,101,113	1.17	6 (8%)
34	BCR	A	409	-	41,41,41	1.00	3 (7%)	56,56,56	1.98	14 (25%)
32	CLA	Ss	604	-	53,57,73	1.43	6 (11%)	62,93,113	1.19	5 (8%)
32	CLA	CC	507	18	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
32	CLA	CC	514	18	53,57,73	1.39	6 (11%)	62,93,113	1.22	5 (8%)
32	CLA	2	610	-	43,48,73	1.55	7 (16%)	52,82,113	1.30	7 (13%)
34	BCR	b	617	-	41,41,41	1.00	2 (4%)	56,56,56	2.10	16 (28%)
36	LHG	JJ	101	-	32,32,48	1.13	2 (6%)	35,38,54	1.13	3 (8%)
36	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	3 (5%)
39	CHL	33	601	15	44,49,74	1.59	6 (13%)	49,83,114	1.26	5 (10%)
32	CLA	1	612	14	43,48,73	1.56	6 (13%)	52,82,113	1.34	4 (7%)
32	CLA	Rr	604	-	53,57,73	1.40	6 (11%)	62,93,113	1.22	7 (11%)
32	CLA	CC	508	-	69,73,73	1.23	7 (10%)	83,113,113	1.27	8 (9%)
41	XAT	44	613	-	39,47,47	0.97	2 (5%)	54,74,74	2.56	12 (22%)
39	CHL	S	607	-	47,51,74	1.57	6 (12%)	52,86,114	1.13	4 (7%)
32	CLA	BB	608	28	69,73,73	1.25	8 (11%)	83,113,113	1.10	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Bb	613	28	69,73,73	1.24	7 (10%)	83,113,113	1.25	7 (8%)
34	BCR	XX	202	-	41,41,41	0.92	1 (2%)	56,56,56	2.14	16 (28%)
40	LUT	s	615	-	42,43,43	0.92	0	51,60,60	1.59	12 (23%)
39	CHL	22	605	-	44,49,74	1.62	6 (13%)	49,83,114	1.40	7 (14%)
32	CLA	BB	610	28	69,73,73	1.23	7 (10%)	83,113,113	1.19	6 (7%)
32	CLA	s	610	36	53,57,73	1.42	6 (11%)	62,93,113	1.26	4 (6%)
32	CLA	2	613	14	43,48,73	1.53	7 (16%)	52,82,113	1.25	4 (7%)
39	CHL	1	608	14	44,49,74	1.54	7 (15%)	49,83,114	1.46	10 (20%)
32	CLA	Nn	303	9	53,57,73	1.42	6 (11%)	62,93,113	1.25	5 (8%)
32	CLA	Gg	305	-	46,50,73	1.50	6 (13%)	55,85,113	1.23	5 (9%)
34	BCR	CC	516	-	41,41,41	0.95	1 (2%)	56,56,56	1.89	13 (23%)
32	CLA	g	602	9	53,57,73	1.46	8 (15%)	62,93,113	1.88	10 (16%)
32	CLA	Y	614	9	53,57,73	1.40	7 (13%)	62,93,113	1.18	5 (8%)
40	LUT	Nn	307	-	42,43,43	0.99	0	51,60,60	1.52	7 (13%)
32	CLA	CC	511	18	69,73,73	1.24	7 (10%)	83,113,113	1.18	5 (6%)
32	CLA	44	602	11	49,53,73	1.47	8 (16%)	59,89,113	1.23	6 (10%)
32	CLA	a	407	-	53,57,73	1.42	7 (13%)	62,93,113	1.28	7 (11%)
32	CLA	DD	403	19	69,73,73	1.24	9 (13%)	83,113,113	1.19	6 (7%)
40	LUT	Ss	614	-	42,43,43	1.08	2 (4%)	51,60,60	1.46	10 (19%)
40	LUT	R	615	-	42,43,43	0.89	0	51,60,60	1.57	12 (23%)
32	CLA	n	603	9	53,57,73	1.41	6 (11%)	62,93,113	1.26	5 (8%)
32	CLA	y	306	-	53,57,73	1.38	7 (13%)	62,93,113	1.22	7 (11%)
34	BCR	C	517	-	41,41,41	0.93	1 (2%)	56,56,56	1.88	12 (21%)
43	LMU	KK	102	-	28,28,36	0.76	0	39,39,47	0.88	1 (2%)
36	LHG	DD	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.92	2 (3%)
32	CLA	CC	503	18	69,73,73	1.23	7 (10%)	83,113,113	1.21	7 (8%)
40	LUT	2	614	-	42,43,43	1.08	4 (9%)	51,60,60	1.84	12 (23%)
36	LHG	33	614	32	33,33,48	1.13	2 (6%)	36,39,54	1.10	2 (5%)
41	XAT	Rr	615	-	39,47,47	1.03	1 (2%)	54,74,74	2.46	21 (38%)
38	LMG	Cc	501	-	34,34,55	1.14	3 (8%)	42,42,63	1.27	6 (14%)
32	CLA	b	616	28	69,73,73	1.23	6 (8%)	83,113,113	1.10	5 (6%)
44	DGD	B	603	-	57,57,67	0.92	2 (3%)	70,70,81	0.93	3 (4%)
32	CLA	y	313	36	46,50,73	1.50	7 (15%)	55,85,113	1.29	4 (7%)
34	BCR	C	516	-	41,41,41	0.95	1 (2%)	56,56,56	2.07	17 (30%)
40	LUT	YY	616	-	42,43,43	0.94	0	51,60,60	1.46	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	DGD	C	523	-	53,53,67	0.93	2 (3%)	67,67,81	0.93	2 (2%)
39	CHL	Ss	605	-	54,58,74	1.46	7 (12%)	59,94,114	1.22	4 (6%)
40	LUT	Gg	316	-	42,43,43	0.94	0	51,60,60	1.41	6 (11%)
32	CLA	B	618	28	69,73,73	1.24	7 (10%)	83,113,113	1.07	7 (8%)
41	XAT	G	617	-	39,47,47	1.10	2 (5%)	54,74,74	2.50	14 (25%)
36	LHG	II	101	-	33,33,48	1.13	2 (6%)	36,39,54	1.01	2 (5%)
32	CLA	d	401	19	69,73,73	1.26	7 (10%)	83,113,113	1.20	6 (7%)
32	CLA	Nn	305	9	53,57,73	1.41	5 (9%)	62,93,113	1.18	6 (9%)
42	NEX	Y	619	-	38,46,46	1.08	1 (2%)	50,70,70	2.23	15 (30%)
32	CLA	BB	613	28	64,68,73	1.28	6 (9%)	77,107,113	1.15	6 (7%)
42	NEX	NN	618	-	38,46,46	1.12	2 (5%)	50,70,70	2.22	14 (28%)
32	CLA	B	621	28	69,73,73	1.24	7 (10%)	83,113,113	1.13	8 (9%)
32	CLA	Cc	515	18	47,51,73	1.47	7 (14%)	56,86,113	1.25	5 (8%)
32	CLA	b	610	-	69,73,73	1.26	6 (8%)	83,113,113	1.10	5 (6%)
32	CLA	Nn	314	-	53,57,73	1.41	7 (13%)	62,93,113	1.20	6 (9%)
40	LUT	4	313	-	42,43,43	0.93	0	51,60,60	1.38	6 (11%)
39	CHL	Ss	601	4	56,60,74	1.43	7 (12%)	63,97,114	1.13	5 (7%)
32	CLA	c	501	18	69,73,73	1.22	7 (10%)	83,113,113	1.23	7 (8%)
34	BCR	c	516	-	41,41,41	0.89	1 (2%)	56,56,56	2.02	15 (26%)
33	PHO	DD	402	-	58,69,69	2.05	10 (17%)	56,99,99	1.63	8 (14%)
32	CLA	Bb	602	28	69,73,73	1.24	7 (10%)	83,113,113	1.09	6 (7%)
34	BCR	a	411	-	41,41,41	0.99	3 (7%)	56,56,56	1.64	10 (17%)
39	CHL	r	607	-	54,58,74	1.46	7 (12%)	59,94,114	1.25	5 (8%)
33	PHO	a	408	-	58,69,69	2.07	10 (17%)	56,99,99	1.56	9 (16%)
39	CHL	N	607	-	70,74,74	1.26	7 (10%)	80,114,114	1.10	6 (7%)
32	CLA	r	603	3	53,57,73	1.43	7 (13%)	62,93,113	1.29	4 (6%)
37	SQD	A	412	-	34,35,54	1.47	4 (11%)	43,46,65	1.16	4 (9%)
45	BCT	D	403	30	2,3,3	1.26	0	2,3,3	4.02	2 (100%)
32	CLA	Rr	612	3	53,57,73	1.41	6 (11%)	62,93,113	1.22	4 (6%)
32	CLA	YY	602	9	69,73,73	1.24	7 (10%)	83,113,113	1.09	6 (7%)
32	CLA	C	504	18	69,73,73	1.23	7 (10%)	83,113,113	1.22	5 (6%)
32	CLA	NN	612	9	46,50,73	1.49	6 (13%)	55,85,113	1.25	5 (9%)
36	LHG	4	315	32	20,20,48	1.35	2 (10%)	23,26,54	1.40	2 (8%)
32	CLA	Y	610	9	69,73,73	1.22	7 (10%)	83,113,113	1.13	7 (8%)
40	LUT	Yy	616	-	42,43,43	0.91	0	51,60,60	1.55	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	11	604	-	43,48,73	1.56	6 (13%)	52,82,113	1.46	7 (13%)
39	CHL	Yy	607	-	47,51,74	1.51	7 (14%)	52,86,114	1.33	6 (11%)
39	CHL	33	607	-	44,49,74	1.61	7 (15%)	49,83,114	1.40	6 (12%)
40	LUT	Yy	615	-	42,43,43	0.98	1 (2%)	51,60,60	2.06	12 (23%)
32	CLA	N	614	9	45,49,73	1.51	6 (13%)	54,84,113	1.22	4 (7%)
32	CLA	CC	504	18	69,73,73	1.24	7 (10%)	83,113,113	1.10	6 (7%)
32	CLA	B	620	28	69,73,73	1.23	8 (11%)	83,113,113	1.15	5 (6%)
32	CLA	C	507	18	69,73,73	1.21	6 (8%)	83,113,113	1.11	7 (8%)
39	CHL	G	605	9	47,51,74	1.55	6 (12%)	52,86,114	1.11	4 (7%)
44	DGD	BB	625	-	57,57,67	0.91	2 (3%)	70,70,81	0.94	3 (4%)
32	CLA	r	612	3	53,57,73	1.43	6 (11%)	62,93,113	1.27	7 (11%)
32	CLA	N	612	9	46,50,73	1.50	6 (13%)	55,85,113	1.24	5 (9%)

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
32	CLA	g	604	42	-	6/12/88/115	-
32	CLA	A	405	1	-	16/39/115/115	-
40	LUT	RR	315	-	-	2/29/67/67	0/2/2/2
36	LHG	G	618	32	-	7/38/38/53	-
32	CLA	D	405	19	-	8/39/115/115	-
32	CLA	Cc	512	18	-	15/39/115/115	-
32	CLA	YY	613	9	-	9/32/108/115	-
39	CHL	N	608	-	-	3/12/88/117	-
32	CLA	1	610	36	-	7/10/82/115	-
32	CLA	Ss	603	4	-	11/20/96/115	-
32	CLA	Y	612	9	-	13/39/115/115	-
38	LMG	WW	201	-	-	8/43/63/70	0/1/1/1
32	CLA	r	601	3	-	12/20/96/115	-
32	CLA	NN	611	36	-	14/20/96/115	-
32	CLA	S	613	4	-	4/15/91/115	-
38	LMG	Aa	412	-	-	7/37/57/70	0/1/1/1
39	CHL	33	608	15	-	3/12/84/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	c	502	18	-	9/39/115/115	-
39	CHL	NN	601	9	-	3/15/91/117	-
34	BCR	B	613	-	-	4/29/63/63	0/2/2/2
36	LHG	a	414	-	-	5/41/41/53	-
46	HEM	EE	102	20,21	-	1/14/54/54	-
32	CLA	RR	312	3	-	3/12/88/115	-
32	CLA	GG	612	9	-	10/20/96/115	-
32	CLA	Rr	608	3	-	14/20/96/115	-
32	CLA	Yy	602	9	-	15/39/115/115	-
32	CLA	C	503	18	-	13/39/115/115	-
32	CLA	g	612	9	-	12/20/96/115	-
34	BCR	B	614	-	-	4/29/63/63	0/2/2/2
40	LUT	r	614	-	-	2/29/67/67	0/2/2/2
44	DGD	Hh	102	-	-	12/51/91/95	0/2/2/2
32	CLA	R	603	3	-	3/20/96/115	-
32	CLA	Cc	509	-	-	14/39/115/115	-
33	PHO	a	409	-	-	16/37/103/103	0/5/6/6
39	CHL	N	606	-	-	1/12/88/117	-
32	CLA	11	612	14	-	5/10/82/115	-
32	CLA	s	603	4	-	11/20/96/115	-
32	CLA	11	609	14	-	4/10/82/115	-
39	CHL	2	607	-	-	5/12/84/117	-
32	CLA	RR	313	3	-	6/10/86/115	-
32	CLA	r	608	3	-	11/20/96/115	-
32	CLA	CC	510	18	-	15/39/115/115	-
36	LHG	EE	101	-	-	9/44/44/53	-
32	CLA	Y	611	36	-	5/12/88/115	-
39	CHL	g	608	-	-	2/12/88/117	-
32	CLA	n	612	9	-	7/20/96/115	-
41	XAT	g	619	-	-	1/31/93/93	0/4/4/4
32	CLA	R	612	3	-	3/12/88/115	-
39	CHL	YY	606	-	-	5/15/91/117	-
32	CLA	Nn	301	9	-	12/39/115/115	-
32	CLA	YY	604	-	-	13/20/96/115	-
37	SQD	LL	102	-	-	16/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	44	605	11	-	5/17/93/117	-
32	CLA	Bb	616	28	-	12/39/115/115	-
39	CHL	22	607	-	-	4/12/84/117	-
32	CLA	RR	308	3	-	10/20/96/115	-
32	CLA	CC	505	-	-	9/39/115/115	-
38	LMG	B	615	-	-	8/40/60/70	0/1/1/1
32	CLA	11	603	14	-	5/10/82/115	-
32	CLA	Bb	605	28	-	13/39/115/115	-
39	CHL	G	607	-	-	6/17/93/117	-
39	CHL	22	601	14	-	3/12/84/117	-
42	NEX	Gg	318	-	-	3/27/83/83	0/3/3/3
36	LHG	n	618	32	-	12/53/53/53	-
32	CLA	Y	613	9	-	13/32/108/115	-
32	CLA	BB	605	28	-	16/39/115/115	-
32	CLA	1	611	14	-	2/10/82/115	-
39	CHL	4	307	-	-	5/17/93/117	-
39	CHL	NN	607	-	-	12/41/117/117	-
40	LUT	SS	315	-	-	3/29/67/67	0/2/2/2
39	CHL	2	608	14	-	3/12/84/117	-
39	CHL	YY	601	9	-	15/41/117/117	-
32	CLA	SS	314	4	-	7/20/96/115	-
32	CLA	Bb	601	-	-	16/39/115/115	-
32	CLA	NN	603	9	-	6/12/88/115	-
44	DGD	BB	624	-	-	9/44/84/95	0/2/2/2
44	DGD	CC	518	-	-	11/44/84/95	0/2/2/2
38	LMG	CC	520	-	-	3/34/54/70	0/1/1/1
32	CLA	g	614	9	-	11/20/96/115	-
32	CLA	C	510	18	-	13/39/115/115	-
32	CLA	b	602	28	-	14/39/115/115	-
36	LHG	AA	411	-	-	13/38/38/53	-
32	CLA	GG	610	9	-	7/20/96/115	-
32	CLA	GG	604	-	-	5/12/88/115	-
41	XAT	N	617	-	-	0/31/93/93	0/4/4/4
32	CLA	Rr	610	36	-	13/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	4	311	36	-	8/15/91/115	-
40	LUT	n	616	-	-	3/29/67/67	0/2/2/2
32	CLA	S	610	-	-	9/20/96/115	-
32	CLA	3	603	15	-	5/10/82/115	-
32	CLA	Yy	613	9	-	9/32/108/115	-
32	CLA	BB	603	28	-	13/39/115/115	-
40	LUT	n	615	-	-	2/29/67/67	0/2/2/2
32	CLA	22	611	14	-	4/10/82/115	-
34	BCR	Hh	101	-	-	8/29/63/63	0/2/2/2
32	CLA	2	604	-	-	5/10/82/115	-
32	CLA	4	304	11	-	7/15/91/115	-
38	LMG	Bb	621	-	-	8/31/51/70	0/1/1/1
39	CHL	22	608	14	-	3/12/84/117	-
39	CHL	Nn	315	9	-	6/20/96/117	-
34	BCR	CC	515	-	-	6/29/63/63	0/2/2/2
40	LUT	N	615	-	-	1/29/67/67	0/2/2/2
39	CHL	SS	308	4	-	6/21/97/117	-
36	LHG	11	614	32	-	16/38/38/53	-
32	CLA	a	405	1	-	15/39/115/115	-
32	CLA	S	611	4	-	9/20/96/115	-
32	CLA	r	610	36	-	10/20/96/115	-
32	CLA	N	610	9	-	15/39/115/115	-
35	PL9	A	410	-	-	24/53/73/73	0/1/1/1
32	CLA	c	507	-	-	12/39/115/115	-
36	LHG	Y	618	32	-	18/53/53/53	-
32	CLA	R	608	3	-	11/20/96/115	-
40	LUT	y	317	-	-	3/29/67/67	0/2/2/2
35	PL9	DD	406	-	-	27/53/73/73	0/1/1/1
39	CHL	YY	608	-	-	6/22/98/117	-
32	CLA	B	604	28	-	11/39/115/115	-
39	CHL	S	601	4	-	9/25/101/117	-
32	CLA	Gg	315	9	-	11/20/96/115	-
39	CHL	RR	307	-	-	8/22/98/117	-
41	XAT	GG	617	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	c	509	18	-	13/39/115/115	-
38	LMG	Bb	620	-	-	4/31/51/70	0/1/1/1
32	CLA	44	611	11	-	7/15/91/115	-
40	LUT	YY	615	-	-	4/29/67/67	0/2/2/2
32	CLA	Bb	603	28	-	19/39/115/115	-
32	CLA	RR	309	3	-	12/39/115/115	-
32	CLA	33	611	15	-	6/10/82/115	-
36	LHG	NN	619	32	-	10/42/42/53	-
32	CLA	4	303	11	-	8/15/91/115	-
44	DGD	c	518	-	-	6/41/81/95	0/2/2/2
36	LHG	r	616	32	-	13/53/53/53	-
39	CHL	RR	305	-	-	8/22/98/117	-
39	CHL	Gg	310	9	-	6/14/90/117	-
32	CLA	Cc	503	18	-	18/39/115/115	-
32	CLA	Bb	608	28	-	11/39/115/115	-
32	CLA	22	612	14	-	3/10/82/115	-
42	NEX	R	617	-	-	2/27/83/83	0/3/3/3
37	SQD	B	602	-	-	10/42/62/69	0/1/1/1
32	CLA	11	613	14	-	4/10/82/115	-
40	LUT	Ss	615	-	-	0/29/67/67	0/2/2/2
32	CLA	Gg	304	9	-	14/39/115/115	-
44	DGD	CC	522	-	-	11/44/84/95	0/2/2/2
32	CLA	C	505	18	-	18/39/115/115	-
32	CLA	YY	612	9	-	12/31/107/115	-
39	CHL	44	608	11	-	4/17/93/117	-
32	CLA	C	506	-	-	9/39/115/115	-
32	CLA	R	613	3	-	8/10/86/115	-
32	CLA	d	402	19	-	12/39/115/115	-
38	LMG	BB	619	-	-	10/40/60/70	0/1/1/1
32	CLA	Y	602	9	-	18/39/115/115	-
32	CLA	RR	302	3	-	19/39/115/115	-
32	CLA	s	608	4	-	9/20/96/115	-
36	LHG	4	301	32	-	9/21/21/53	-
39	CHL	2	606	-	-	2/12/84/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	Yy	605	9	-	9/20/96/117	-
32	CLA	BB	604	28	-	14/39/115/115	-
32	CLA	N	611	36	-	11/20/96/115	-
32	CLA	Bb	610	-	-	16/39/115/115	-
32	CLA	Yy	610	9	-	12/39/115/115	-
32	CLA	SS	304	4	-	5/15/91/115	-
32	CLA	CC	502	-	-	15/39/115/115	-
32	CLA	Gg	303	9	-	12/20/96/115	-
32	CLA	AA	408	1	-	8/33/109/115	-
32	CLA	Nn	302	36	-	5/20/96/115	-
42	NEX	Y	617	-	-	2/27/83/83	0/3/3/3
42	NEX	g	617	32	-	3/27/83/83	0/3/3/3
32	CLA	BB	607	28	-	12/39/115/115	-
32	CLA	G	613	9	-	7/10/82/115	-
32	CLA	y	315	9	-	11/32/108/115	-
32	CLA	A	406	-	-	11/20/96/115	-
32	CLA	Yy	614	9	-	10/20/96/115	-
39	CHL	GG	609	9	-	4/14/90/117	-
32	CLA	Cc	511	18	-	17/39/115/115	-
34	BCR	H	101	-	-	3/29/63/63	0/2/2/2
39	CHL	n	607	-	-	18/41/117/117	-
39	CHL	r	606	-	-	4/22/98/117	-
39	CHL	YY	607	-	-	2/14/90/117	-
41	XAT	NN	617	-	-	0/31/93/93	0/4/4/4
32	CLA	Cc	507	18	-	12/39/115/115	-
39	CHL	n	601	9	-	6/22/98/117	-
39	CHL	4	306	11	-	5/17/93/117	-
32	CLA	Y	604	-	-	13/20/96/115	-
33	PHO	A	407	-	-	11/37/103/103	0/5/6/6
32	CLA	G	610	9	-	9/20/96/115	-
36	LHG	3	614	32	-	11/38/38/53	-
37	SQD	CC	501	-	-	11/49/69/69	0/1/1/1
32	CLA	CC	512	18	-	16/39/115/115	-
32	CLA	CC	506	18	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	n	609	9	-	6/22/98/117	-
39	CHL	y	303	9	-	14/41/117/117	-
32	CLA	NN	610	9	-	14/39/115/115	-
33	PHO	Aa	408	-	-	7/37/103/103	0/5/6/6
44	DGD	a	415	-	-	9/44/84/95	0/2/2/2
32	CLA	b	611	28	-	7/39/115/115	-
32	CLA	S	609	4	-	2/10/86/115	-
38	LMG	A	415	-	-	4/31/51/70	0/1/1/1
32	CLA	B	606	28	-	16/39/115/115	-
46	HEM	Ee	101	20,21	-	6/14/54/54	-
32	CLA	l	613	14	-	4/10/82/115	-
32	CLA	S	602	4	-	9/20/96/115	-
34	BCR	Cc	517	-	-	5/29/63/63	0/2/2/2
36	LHG	g	618	32	-	9/38/38/53	-
32	CLA	l	604	-	-	5/10/82/115	-
32	CLA	YY	611	36	-	4/12/88/115	-
32	CLA	Rr	609	3	-	14/39/115/115	-
32	CLA	B	622	28	-	19/39/115/115	-
34	BCR	Bb	618	-	-	4/29/63/63	0/2/2/2
36	LHG	A	411	-	-	12/38/38/53	-
36	LHG	D	409	-	-	7/53/53/53	-
32	CLA	YY	603	9	-	8/20/96/115	-
40	LUT	S	614	-	-	2/29/67/67	0/2/2/2
32	CLA	33	610	36	-	5/10/82/115	-
32	CLA	r	602	3	-	16/39/115/115	-
32	CLA	DD	401	-	-	8/39/115/115	-
36	LHG	l	614	32	-	8/34/34/53	-
32	CLA	Yy	612	9	-	10/39/115/115	-
32	CLA	CC	513	18	-	9/39/115/115	-
42	NEX	y	319	-	-	3/27/83/83	0/3/3/3
39	CHL	Yy	606	-	-	4/15/91/117	-
39	CHL	Y	608	-	-	6/22/98/117	-
32	CLA	RR	303	3	-	3/20/96/115	-
39	CHL	2	601	14	-	2/12/84/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	R	607	-	-	8/22/98/117	-
40	LUT	g	616	-	-	2/29/67/67	0/2/2/2
32	CLA	Aa	406	1	-	13/39/115/115	-
39	CHL	Gg	307	-	-	6/14/90/117	-
32	CLA	22	610	36	-	8/12/88/115	-
39	CHL	n	606	-	-	1/22/98/117	-
32	CLA	Bb	614	28	-	8/39/115/115	-
40	LUT	s	614	-	-	2/29/67/67	0/2/2/2
36	LHG	AA	414	-	-	10/49/49/53	-
32	CLA	C	514	18	-	8/39/115/115	-
32	CLA	Cc	513	18	-	11/39/115/115	-
42	NEX	n	617	-	-	3/27/83/83	0/3/3/3
39	CHL	NN	606	-	-	3/12/88/117	-
32	CLA	YY	614	9	-	13/20/96/115	-
37	SQD	B	617	-	-	5/31/51/69	0/1/1/1
32	CLA	3	613	15	-	6/10/82/115	-
32	CLA	g	610	9	-	8/20/96/115	-
32	CLA	G	611	36	-	10/24/100/115	-
32	CLA	c	511	18	-	12/39/115/115	-
32	CLA	B	624	28	-	11/39/115/115	-
36	LHG	Dd	405	-	-	9/47/47/53	-
32	CLA	y	304	9	-	13/39/115/115	-
36	LHG	d	405	-	-	9/47/47/53	-
32	CLA	Rr	602	3	-	14/39/115/115	-
39	CHL	Ss	607	-	-	7/21/97/117	-
35	PL9	d	404	-	-	28/53/73/73	0/1/1/1
39	CHL	11	607	-	-	2/12/84/117	-
32	CLA	S	608	4	-	8/10/86/115	-
39	CHL	G	601	9	-	14/41/117/117	-
34	BCR	BB	618	-	-	4/29/63/63	0/2/2/2
41	XAT	Nn	308	-	-	1/31/93/93	0/4/4/4
32	CLA	B	605	-	-	17/39/115/115	-
32	CLA	33	604	-	-	5/10/82/115	-
40	LUT	22	614	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LUT	G	616	-	-	2/29/67/67	0/2/2/2
32	CLA	Cc	508	18	-	20/39/115/115	-
39	CHL	G	609	9	-	3/14/90/117	-
32	CLA	N	602	9	-	16/39/115/115	-
38	LMG	AA	415	-	-	4/31/51/70	0/1/1/1
39	CHL	y	308	-	-	2/15/91/117	-
34	BCR	d	403	-	-	4/29/63/63	0/2/2/2
40	LUT	G	615	-	-	2/29/67/67	0/2/2/2
32	CLA	2	609	14	-	4/10/82/115	-
32	CLA	SS	309	4	-	7/10/86/115	-
32	CLA	R	602	3	-	20/39/115/115	-
32	CLA	Ss	612	4	-	9/20/96/115	-
40	LUT	Nn	306	-	-	1/29/67/67	0/2/2/2
39	CHL	NN	609	9	-	6/22/98/117	-
36	LHG	J	101	-	-	10/30/30/53	-
32	CLA	Cc	510	18	-	8/33/109/115	-
36	LHG	Dd	406	-	-	10/53/53/53	-
32	CLA	c	510	18	-	17/39/115/115	-
35	PL9	Dd	404	-	-	28/53/73/73	0/1/1/1
40	LUT	g	615	-	-	1/29/67/67	0/2/2/2
32	CLA	Nn	313	9	-	10/20/96/115	-
32	CLA	Rr	613	3	-	10/20/96/115	-
32	CLA	B	609	28	-	7/33/109/115	-
32	CLA	S	603	4	-	6/15/91/115	-
35	PL9	D	407	-	-	28/53/73/73	0/1/1/1
32	CLA	NN	614	9	-	5/10/86/115	-
39	CHL	s	607	-	-	7/21/97/117	-
42	NEX	Rr	616	-	-	3/27/83/83	0/3/3/3
38	LMG	m	101	-	-	13/46/66/70	0/1/1/1
34	BCR	Aa	411	-	-	4/29/63/63	0/2/2/2
36	LHG	Gg	319	32	-	7/38/38/53	-
39	CHL	11	608	14	-	2/12/84/117	-
39	CHL	RR	306	-	-	11/22/98/117	-
36	LHG	SS	301	-	-	4/30/30/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	GG	602	9	-	9/20/96/115	-
32	CLA	r	613	3	-	11/20/96/115	-
32	CLA	N	613	9	-	10/20/96/115	-
32	CLA	b	605	28	-	11/39/115/115	-
39	CHL	1	601	14	-	5/12/84/117	-
39	CHL	GG	605	9	-	4/14/90/117	-
34	BCR	TT	101	-	-	5/29/63/63	0/2/2/2
41	XAT	4	314	-	-	0/31/93/93	0/4/4/4
39	CHL	SS	307	-	-	2/12/88/117	-
32	CLA	b	615	28	-	16/39/115/115	-
39	CHL	Rr	607	-	-	9/22/98/117	-
32	CLA	n	610	9	-	13/39/115/115	-
39	CHL	3	606	-	-	5/12/84/117	-
32	CLA	C	513	18	-	18/39/115/115	-
32	CLA	b	603	28	-	18/39/115/115	-
34	BCR	c	514	-	-	4/29/63/63	0/2/2/2
44	DGD	C	520	-	-	4/51/91/95	0/2/2/2
32	CLA	Nn	312	9	-	15/39/115/115	-
38	LMG	DD	409	-	-	4/41/61/70	0/1/1/1
32	CLA	3	610	36	-	6/10/82/115	-
32	CLA	r	609	3	-	13/39/115/115	-
34	BCR	B	612	-	-	4/29/63/63	0/2/2/2
39	CHL	GG	606	-	-	5/14/90/117	-
39	CHL	y	309	-	-	4/14/90/117	-
39	CHL	Rr	606	-	-	6/22/98/117	-
34	BCR	Cc	518	-	-	3/29/63/63	0/2/2/2
37	SQD	BB	621	-	-	5/31/51/69	0/1/1/1
43	LMU	R	618	-	-	5/13/53/61	0/2/2/2
32	CLA	s	602	4	-	13/20/96/115	-
44	DGD	Cc	519	-	-	8/44/84/95	0/2/2/2
41	XAT	GG	619	-	-	1/31/93/93	0/4/4/4
39	CHL	S	605	-	-	4/12/88/117	-
39	CHL	3	607	-	-	2/12/84/117	-
42	NEX	YY	617	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	NEX	Nn	309	-	-	2/27/83/83	0/3/3/3
32	CLA	2	602	14	-	6/10/82/115	-
32	CLA	Y	603	9	-	10/20/96/115	-
34	BCR	h	101	-	-	7/29/63/63	0/2/2/2
32	CLA	BB	609	-	-	14/39/115/115	-
38	LMG	b	621	-	-	9/31/51/70	0/1/1/1
32	CLA	s	609	4	-	10/20/96/115	-
37	SQD	AA	412	-	-	7/30/50/69	0/1/1/1
32	CLA	N	604	-	-	5/10/86/115	-
32	CLA	b	604	28	-	11/39/115/115	-
39	CHL	r	605	3	-	8/22/98/117	-
39	CHL	Nn	317	-	-	14/41/117/117	-
39	CHL	l	606	-	-	5/12/84/117	-
32	CLA	Dd	401	19	-	14/39/115/115	-
36	LHG	YY	618	32	-	19/53/53/53	-
39	CHL	4	309	11	-	7/17/93/117	-
32	CLA	Gg	314	9	-	3/10/82/115	-
33	PHO	Aa	409	-	-	16/37/103/103	0/5/6/6
32	CLA	44	609	11	-	5/15/91/115	-
39	CHL	g	607	-	-	6/22/98/117	-
32	CLA	22	602	14	-	4/10/82/115	-
39	CHL	4	302	-	-	2/15/91/117	-
32	CLA	G	614	9	-	4/10/86/115	-
41	XAT	y	302	-	-	1/31/93/93	0/4/4/4
32	CLA	G	602	9	-	10/20/96/115	-
32	CLA	1	603	14	-	7/10/82/115	-
32	CLA	44	603	11	-	10/15/91/115	-
32	CLA	S	604	-	-	7/20/96/115	-
39	CHL	GG	601	9	-	11/41/117/117	-
32	CLA	Bb	609	28	-	17/39/115/115	-
39	CHL	3	605	-	-	5/12/84/117	-
32	CLA	n	611	36	-	7/20/96/115	-
39	CHL	Yy	609	9	-	11/41/117/117	-
32	CLA	NN	602	9	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	GG	613	9	-	6/10/82/115	-
36	LHG	N	619	32	-	11/42/42/53	-
39	CHL	Ss	606	-	-	11/22/98/117	-
32	CLA	r	604	-	-	16/20/96/115	-
39	CHL	11	606	-	-	5/12/84/117	-
46	HEM	e	101	20,21	-	3/14/54/54	-
39	CHL	S	606	-	-	2/12/88/117	-
36	LHG	BB	622	-	-	9/38/38/53	-
39	CHL	GG	608	-	-	7/12/88/117	-
32	CLA	Ss	608	4	-	11/20/96/115	-
39	CHL	G	608	-	-	6/12/88/117	-
39	CHL	Y	601	9	-	15/41/117/117	-
39	CHL	3	601	15	-	5/12/84/117	-
39	CHL	g	606	-	-	6/14/90/117	-
32	CLA	Ss	610	36	-	10/20/96/115	-
37	SQD	Aa	413	-	-	10/42/62/69	0/1/1/1
32	CLA	s	613	4	-	6/20/96/115	-
36	LHG	Ll	102	-	-	15/53/53/53	-
39	CHL	Rr	605	3	-	8/22/98/117	-
32	CLA	a	410	1	-	11/33/109/115	-
32	CLA	n	613	9	-	11/20/96/115	-
32	CLA	s	604	-	-	11/20/96/115	-
39	CHL	y	307	9	-	8/20/96/117	-
32	CLA	BB	614	28	-	8/39/115/115	-
34	BCR	BB	617	-	-	4/29/63/63	0/2/2/2
39	CHL	11	605	14	-	5/12/84/117	-
32	CLA	a	406	1	-	13/39/115/115	-
32	CLA	1	609	14	-	4/10/82/115	-
32	CLA	c	506	18	-	20/39/115/115	-
32	CLA	B	608	28	-	14/39/115/115	-
36	LHG	K	101	-	-	11/38/38/53	-
40	LUT	N	616	-	-	3/29/67/67	0/2/2/2
32	CLA	Bb	615	28	-	16/39/115/115	-
34	BCR	Kk	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	AA	405	1	-	14/39/115/115	-
32	CLA	Dd	402	19	-	16/39/115/115	-
38	LMG	c	519	-	-	7/29/49/70	0/1/1/1
39	CHL	N	609	9	-	6/22/98/117	-
39	CHL	N	605	9	-	4/12/88/117	-
32	CLA	S	612	4	-	8/20/96/115	-
36	LHG	Yy	618	32	-	19/53/53/53	-
32	CLA	BB	615	28	-	3/10/86/115	-
32	CLA	Yy	611	36	-	5/12/88/115	-
32	CLA	b	601	-	-	18/39/115/115	-
39	CHL	s	606	-	-	11/22/98/117	-
39	CHL	R	605	-	-	7/22/98/117	-
39	CHL	44	601	-	-	2/15/91/117	-
32	CLA	Cc	504	18	-	14/39/115/115	-
39	CHL	11	601	14	-	4/12/84/117	-
39	CHL	Gg	308	-	-	6/22/98/117	-
38	LMG	W	201	-	-	6/43/63/70	0/1/1/1
43	LMU	RR	301	-	-	3/13/53/61	0/2/2/2
32	CLA	R	610	36	-	11/20/96/115	-
39	CHL	G	606	-	-	5/14/90/117	-
40	LUT	Y	616	-	-	2/29/67/67	0/2/2/2
35	PL9	AA	410	-	-	27/53/73/73	0/1/1/1
40	LUT	Y	615	-	-	4/29/67/67	0/2/2/2
32	CLA	Cc	514	18	-	10/39/115/115	-
32	CLA	c	504	-	-	6/27/103/115	-
39	CHL	Y	606	-	-	4/15/91/117	-
32	CLA	R	614	3	-	8/20/96/115	-
32	CLA	RR	310	36	-	12/20/96/115	-
32	CLA	Gg	313	9	-	14/20/96/115	-
32	CLA	SS	303	4	-	10/20/96/115	-
32	CLA	1	602	14	-	3/10/82/115	-
32	CLA	3	612	15	-	6/10/82/115	-
34	BCR	Cc	516	-	-	4/29/63/63	0/2/2/2
41	XAT	G	619	-	-	1/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	N	601	9	-	3/15/91/117	-
39	CHL	22	606	-	-	2/12/84/117	-
32	CLA	22	604	-	-	4/10/82/115	-
32	CLA	NN	613	9	-	11/20/96/115	-
41	XAT	Gg	301	-	-	1/31/93/93	0/4/4/4
46	HEM	E	101	20,21	-	1/14/54/54	-
32	CLA	R	604	-	-	6/20/96/115	-
37	SQD	L	101	-	-	16/49/69/69	0/1/1/1
44	DGD	Aa	401	-	-	9/44/84/95	0/2/2/2
32	CLA	Rr	601	3	-	13/20/96/115	-
32	CLA	SS	312	4	-	8/20/96/115	-
38	LMG	C	521	-	-	10/46/66/70	0/1/1/1
32	CLA	11	610	36	-	5/10/82/115	-
32	CLA	GG	611	36	-	10/24/100/115	-
39	CHL	g	609	9	-	7/14/90/117	-
32	CLA	3	609	15	-	3/10/82/115	-
39	CHL	Y	605	9	-	6/20/96/117	-
32	CLA	4	310	-	-	6/15/91/115	-
32	CLA	Rr	611	3	-	13/20/96/115	-
32	CLA	Yy	604	-	-	10/20/96/115	-
32	CLA	GG	603	9	-	12/39/115/115	-
39	CHL	g	605	9	-	6/14/90/117	-
39	CHL	y	310	-	-	6/22/98/117	-
44	DGD	c	517	-	-	5/44/84/95	0/2/2/2
32	CLA	Rr	603	3	-	8/20/96/115	-
32	CLA	n	604	-	-	6/20/96/115	-
36	LHG	D	410	-	-	10/38/38/53	-
32	CLA	RR	304	-	-	6/20/96/115	-
32	CLA	11	611	14	-	2/10/82/115	-
36	LHG	D	408	-	-	13/47/47/53	-
34	BCR	b	618	-	-	4/29/63/63	0/2/2/2
32	CLA	4	305	-	-	6/15/91/115	-
32	CLA	c	508	18	-	11/33/109/115	-
34	BCR	K	102	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	C	522	-	-	9/35/35/53	-
39	CHL	SS	306	4	-	3/12/88/117	-
32	CLA	C	515	18	-	8/20/96/115	-
32	CLA	r	611	3	-	13/20/96/115	-
36	LHG	44	614	32	-	7/23/23/53	-
37	SQD	LL	101	-	-	9/31/51/69	0/1/1/1
36	LHG	DD	407	-	-	14/47/47/53	-
39	CHL	g	601	9	-	12/41/117/117	-
32	CLA	B	623	-	-	11/39/115/115	-
32	CLA	RR	314	3	-	11/20/96/115	-
32	CLA	Aa	410	1	-	12/33/109/115	-
36	LHG	Nn	310	32	-	16/53/53/53	-
32	CLA	N	603	9	-	6/12/88/115	-
32	CLA	Aa	405	1	-	14/39/115/115	-
40	LUT	44	612	-	-	2/29/67/67	0/2/2/2
34	BCR	D	406	-	-	2/29/63/63	0/2/2/2
32	CLA	R	611	3	-	8/20/96/115	-
39	CHL	Nn	316	-	-	2/22/98/117	-
32	CLA	2	611	14	-	5/10/82/115	-
32	CLA	Gg	312	36	-	19/39/115/115	-
39	CHL	3	608	15	-	3/12/84/117	-
39	CHL	s	605	-	-	9/22/98/117	-
33	PHO	AA	407	-	-	7/37/103/103	0/5/6/6
37	SQD	C	501	-	-	16/49/69/69	0/1/1/1
39	CHL	Y	609	9	-	10/41/117/117	-
38	LMG	a	412	-	-	10/37/57/70	0/1/1/1
34	BCR	KK	103	-	-	4/29/63/63	0/2/2/2
38	LMG	j	101	-	-	3/41/61/70	0/1/1/1
39	CHL	Gg	309	-	-	3/12/88/117	-
32	CLA	c	512	18	-	10/39/115/115	-
40	LUT	Gg	317	-	-	1/29/67/67	0/2/2/2
32	CLA	33	603	15	-	6/10/82/115	-
32	CLA	B	607	28	-	8/39/115/115	-
36	LHG	A	413	-	-	11/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	2	605	-	-	2/12/84/117	-
39	CHL	Gg	302	9	-	13/41/117/117	-
32	CLA	C	508	18	-	14/39/115/115	-
32	CLA	b	606	28	-	9/39/115/115	-
39	CHL	R	606	-	-	8/22/98/117	-
42	NEX	Yy	617	-	-	3/27/83/83	0/3/3/3
32	CLA	3	611	15	-	6/10/82/115	-
36	LHG	CC	523	-	-	10/41/41/53	-
32	CLA	b	612	28	-	13/39/115/115	-
39	CHL	Gg	306	9	-	6/14/90/117	-
39	CHL	s	601	4	-	10/25/101/117	-
32	CLA	22	613	14	-	6/10/82/115	-
32	CLA	n	614	9	-	8/20/96/115	-
41	XAT	RR	316	-	-	0/31/93/93	0/4/4/4
36	LHG	y	320	32	-	23/53/53/53	-
32	CLA	NN	604	-	-	5/10/86/115	-
32	CLA	44	615	3	-	11/20/96/115	-
37	SQD	Ll	101	-	-	9/49/69/69	0/1/1/1
32	CLA	n	602	9	-	15/39/115/115	-
32	CLA	D	401	-	-	10/39/115/115	-
32	CLA	X	201	-	-	3/10/86/115	-
32	CLA	33	612	15	-	7/10/82/115	-
32	CLA	C	511	18	-	14/39/115/115	-
34	BCR	b	619	-	-	4/29/63/63	0/2/2/2
32	CLA	Ss	611	4	-	10/20/96/115	-
40	LUT	Rr	614	-	-	2/29/67/67	0/2/2/2
41	XAT	Yy	619	-	-	3/31/93/93	0/4/4/4
32	CLA	c	503	18	-	9/39/115/115	-
32	CLA	44	610	36	-	8/15/91/115	-
33	PHO	D	402	-	-	9/37/103/103	0/5/6/6
32	CLA	SS	313	4	-	10/20/96/115	-
32	CLA	BB	606	-	-	12/39/115/115	-
32	CLA	Bb	604	28	-	9/39/115/115	-
32	CLA	Bb	607	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	YY	609	9	-	10/41/117/117	-
32	CLA	CC	509	18	-	16/39/115/115	-
32	CLA	33	609	15	-	3/10/82/115	-
32	CLA	c	513	18	-	11/13/89/115	-
39	CHL	GG	607	-	-	7/17/93/117	-
32	CLA	y	305	9	-	6/20/96/115	-
41	XAT	y	301	-	-	3/31/93/93	0/4/4/4
39	CHL	NN	605	9	-	5/12/88/117	-
44	DGD	CC	519	-	-	5/51/91/95	0/2/2/2
39	CHL	Nn	311	9	-	6/22/98/117	-
44	DGD	D	411	-	-	7/51/91/95	0/2/2/2
41	XAT	r	615	-	-	1/31/93/93	0/4/4/4
32	CLA	R	601	3	-	9/20/96/115	-
34	BCR	T	101	-	-	3/29/63/63	0/2/2/2
32	CLA	4	312	11	-	9/15/91/115	-
43	LMU	C	502	-	-	4/13/53/61	0/2/2/2
39	CHL	n	608	-	-	9/22/98/117	-
32	CLA	B	611	28	-	3/10/86/115	-
34	BCR	DD	405	-	-	2/29/63/63	0/2/2/2
32	CLA	D	404	19	-	16/39/115/115	-
39	CHL	1	605	14	-	5/12/84/117	-
32	CLA	SS	305	-	-	8/20/96/115	-
32	CLA	C	512	18	-	10/39/115/115	-
32	CLA	s	611	4	-	10/20/96/115	-
32	CLA	R	609	3	-	12/39/115/115	-
38	LMG	b	620	-	-	4/31/51/70	0/1/1/1
39	CHL	Nn	318	-	-	7/22/98/117	-
32	CLA	Bb	606	28	-	8/39/115/115	-
32	CLA	Gg	311	9	-	11/20/96/115	-
38	LMG	F	101	-	-	3/41/61/70	0/1/1/1
32	CLA	Yy	603	9	-	7/20/96/115	-
36	LHG	Ss	616	32	-	9/52/52/53	-
44	DGD	Cc	520	-	-	7/41/81/95	0/2/2/2
32	CLA	G	604	-	-	8/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	2	603	14	-	5/10/82/115	-
32	CLA	b	608	28	-	10/39/115/115	-
32	CLA	2	612	14	-	2/10/82/115	-
32	CLA	33	602	15	-	4/10/82/115	-
32	CLA	RR	311	3	-	8/20/96/115	-
36	LHG	s	616	32	-	9/52/52/53	-
36	LHG	CC	521	-	-	7/38/38/53	-
39	CHL	NN	608	-	-	3/12/88/117	-
32	CLA	b	613	28	-	14/39/115/115	-
39	CHL	Yy	608	-	-	6/22/98/117	-
40	LUT	NN	616	-	-	2/29/67/67	0/2/2/2
36	LHG	KK	101	-	-	8/38/38/53	-
32	CLA	44	604	-	-	8/15/91/115	-
32	CLA	Bb	612	28	-	15/39/115/115	-
40	LUT	NN	615	-	-	2/29/67/67	0/2/2/2
39	CHL	SS	302	4	-	9/25/101/117	-
32	CLA	y	316	9	-	10/20/96/115	-
32	CLA	BB	612	28	-	14/39/115/115	-
32	CLA	33	613	15	-	6/10/82/115	-
32	CLA	s	612	4	-	9/20/96/115	-
34	BCR	B	616	-	-	4/29/63/63	0/2/2/2
36	LHG	GG	618	32	-	7/38/38/53	-
34	BCR	BB	616	-	-	4/29/63/63	0/2/2/2
36	LHG	Dd	407	-	-	5/41/41/53	-
32	CLA	G	603	9	-	13/39/115/115	-
39	CHL	y	311	9	-	12/41/117/117	-
36	LHG	A	414	-	-	10/49/49/53	-
32	CLA	B	619	28	-	23/39/115/115	-
36	LHG	d	406	-	-	10/53/53/53	-
44	DGD	h	102	-	-	8/51/91/95	0/2/2/2
42	NEX	RR	317	-	-	3/27/83/83	0/3/3/3
32	CLA	Ss	602	4	-	13/20/96/115	-
34	BCR	Bb	619	-	-	2/29/63/63	0/2/2/2
32	CLA	11	602	14	-	2/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	y	314	9	-	13/39/115/115	-
32	CLA	B	610	28	-	11/39/115/115	-
37	SQD	L	102	-	-	10/31/51/69	0/1/1/1
39	CHL	Yy	601	9	-	15/41/117/117	-
32	CLA	BB	601	28	-	10/39/115/115	-
40	LUT	GG	616	-	-	2/29/67/67	0/2/2/2
32	CLA	GG	614	9	-	5/10/86/115	-
32	CLA	Ss	609	4	-	10/20/96/115	-
34	BCR	AA	409	-	-	5/29/63/63	0/2/2/2
32	CLA	Cc	505	18	-	13/39/115/115	-
32	CLA	BB	611	28	-	6/39/115/115	-
40	LUT	GG	615	-	-	2/29/67/67	0/2/2/2
39	CHL	n	605	9	-	9/20/96/117	-
38	LMG	Dd	408	-	-	6/41/61/70	0/1/1/1
36	LHG	22	615	32	-	9/38/38/53	-
32	CLA	DD	404	19	-	10/39/115/115	-
39	CHL	44	606	-	-	5/17/93/117	-
32	CLA	AA	406	-	-	9/20/96/115	-
34	BCR	Dd	403	-	-	4/29/63/63	0/2/2/2
34	BCR	CC	517	-	-	2/29/63/63	0/2/2/2
44	DGD	B	601	-	-	6/44/84/95	0/2/2/2
32	CLA	b	609	28	-	17/39/115/115	-
32	CLA	c	505	18	-	12/39/115/115	-
34	BCR	c	515	-	-	5/29/63/63	0/2/2/2
34	BCR	Bb	617	-	-	5/29/63/63	0/2/2/2
32	CLA	b	614	28	-	7/39/115/115	-
32	CLA	Ss	613	4	-	7/20/96/115	-
32	CLA	3	602	15	-	4/10/82/115	-
32	CLA	g	611	36	-	19/39/115/115	-
32	CLA	BB	602	28	-	23/39/115/115	-
32	CLA	Aa	407	-	-	10/20/96/115	-
32	CLA	C	509	-	-	12/39/115/115	-
39	CHL	4	308	-	-	6/17/93/117	-
41	XAT	R	616	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	NEX	N	618	-	-	2/27/83/83	0/3/3/3
39	CHL	Y	607	-	-	2/14/90/117	-
32	CLA	YY	610	9	-	16/39/115/115	-
32	CLA	Bb	611	28	-	7/39/115/115	-
40	LUT	y	318	-	-	2/29/67/67	0/2/2/2
44	DGD	C	519	-	-	9/44/84/95	0/2/2/2
32	CLA	22	603	14	-	2/10/82/115	-
32	CLA	G	612	9	-	10/20/96/115	-
34	BCR	BB	620	-	-	5/29/63/63	0/2/2/2
32	CLA	A	408	1	-	9/33/109/115	-
32	CLA	Nn	304	9	-	9/20/96/115	-
38	LMG	Mm	101	-	-	10/46/66/70	0/1/1/1
39	CHL	33	606	-	-	5/12/84/117	-
32	CLA	SS	311	-	-	7/20/96/115	-
44	DGD	BB	623	-	-	8/51/91/95	0/2/2/2
34	BCR	k	101	-	-	6/29/63/63	0/2/2/2
32	CLA	XX	201	-	-	2/10/86/115	-
32	CLA	b	607	-	-	13/39/115/115	-
32	CLA	3	604	-	-	4/10/82/115	-
36	LHG	44	616	32	-	8/21/21/53	-
32	CLA	g	603	9	-	18/39/115/115	-
39	CHL	YY	605	9	-	6/20/96/117	-
32	CLA	22	609	14	-	7/10/82/115	-
37	SQD	l	102	-	-	10/49/69/69	0/1/1/1
39	CHL	1	607	-	-	2/12/84/117	-
39	CHL	44	607	-	-	7/17/93/117	-
34	BCR	C	518	-	-	2/29/63/63	0/2/2/2
39	CHL	33	605	-	-	4/12/84/117	-
32	CLA	SS	310	4	-	3/10/86/115	-
32	CLA	y	312	9	-	14/39/115/115	-
32	CLA	g	613	9	-	8/10/82/115	-
36	LHG	Rr	617	32	-	11/53/53/53	-
39	CHL	Nn	319	9	-	7/22/98/117	-
36	LHG	0	201	-	-	11/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Cc	506	-	-	9/27/103/115	-
34	BCR	A	409	-	-	5/29/63/63	0/2/2/2
32	CLA	Ss	604	-	-	12/20/96/115	-
32	CLA	CC	507	18	-	13/39/115/115	-
32	CLA	CC	514	18	-	8/20/96/115	-
32	CLA	2	610	-	-	5/10/82/115	-
34	BCR	b	617	-	-	4/29/63/63	0/2/2/2
36	LHG	JJ	101	-	-	9/37/37/53	-
36	LHG	l	101	-	-	13/53/53/53	-
39	CHL	33	601	15	-	5/12/84/117	-
32	CLA	1	612	14	-	1/10/82/115	-
32	CLA	Rr	604	-	-	13/20/96/115	-
32	CLA	CC	508	-	-	12/39/115/115	-
41	XAT	44	613	-	-	0/31/93/93	0/4/4/4
39	CHL	S	607	-	-	2/14/90/117	-
32	CLA	BB	608	28	-	13/39/115/115	-
32	CLA	Bb	613	28	-	14/39/115/115	-
34	BCR	XX	202	-	-	6/29/63/63	0/2/2/2
40	LUT	s	615	-	-	2/29/67/67	0/2/2/2
39	CHL	22	605	-	-	2/12/84/117	-
32	CLA	BB	610	28	-	15/39/115/115	-
32	CLA	s	610	36	-	10/20/96/115	-
32	CLA	2	613	14	-	4/10/82/115	-
39	CHL	1	608	14	-	3/12/84/117	-
32	CLA	Nn	303	9	-	6/20/96/115	-
32	CLA	Gg	305	-	-	6/12/88/115	-
34	BCR	CC	516	-	-	5/29/63/63	0/2/2/2
32	CLA	g	602	9	-	9/20/96/115	-
32	CLA	Y	614	9	-	13/20/96/115	-
40	LUT	Nn	307	-	-	2/29/67/67	0/2/2/2
32	CLA	CC	511	18	-	8/39/115/115	-
32	CLA	44	602	11	-	8/15/91/115	-
32	CLA	a	407	-	-	8/20/96/115	-
32	CLA	DD	403	19	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LUT	Ss	614	-	-	2/29/67/67	0/2/2/2
40	LUT	R	615	-	-	0/29/67/67	0/2/2/2
32	CLA	n	603	9	-	10/20/96/115	-
32	CLA	y	306	-	-	8/20/96/115	-
34	BCR	C	517	-	-	5/29/63/63	0/2/2/2
43	LMU	KK	102	-	-	5/13/53/61	0/2/2/2
36	LHG	DD	408	-	-	10/53/53/53	-
32	CLA	CC	503	18	-	16/39/115/115	-
40	LUT	2	614	-	-	4/29/67/67	0/2/2/2
36	LHG	33	614	32	-	11/38/38/53	-
41	XAT	Rr	615	-	-	2/31/93/93	0/4/4/4
38	LMG	Cc	501	-	-	7/29/49/70	0/1/1/1
32	CLA	b	616	28	-	12/39/115/115	-
44	DGD	B	603	-	-	6/43/83/95	0/2/2/2
32	CLA	y	313	36	-	5/12/88/115	-
34	BCR	C	516	-	-	6/29/63/63	0/2/2/2
40	LUT	YY	616	-	-	2/29/67/67	0/2/2/2
44	DGD	C	523	-	-	9/41/81/95	0/2/2/2
39	CHL	Ss	605	-	-	12/22/98/117	-
40	LUT	Gg	316	-	-	2/29/67/67	0/2/2/2
32	CLA	B	618	28	-	10/39/115/115	-
41	XAT	G	617	-	-	2/31/93/93	0/4/4/4
36	LHG	II	101	-	-	11/38/38/53	-
32	CLA	d	401	19	-	11/39/115/115	-
32	CLA	Nn	305	9	-	9/20/96/115	-
42	NEX	Y	619	-	-	3/27/83/83	0/3/3/3
32	CLA	BB	613	28	-	8/33/109/115	-
42	NEX	NN	618	-	-	2/27/83/83	0/3/3/3
32	CLA	B	621	28	-	14/39/115/115	-
32	CLA	Cc	515	18	-	9/13/89/115	-
32	CLA	b	610	-	-	11/39/115/115	-
32	CLA	Nn	314	-	-	4/20/96/115	-
40	LUT	4	313	-	-	2/29/67/67	0/2/2/2
39	CHL	Ss	601	4	-	7/25/101/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	c	501	18	-	20/39/115/115	-
34	BCR	c	516	-	-	4/29/63/63	0/2/2/2
33	PHO	DD	402	-	-	11/37/103/103	0/5/6/6
32	CLA	Bb	602	28	-	11/39/115/115	-
34	BCR	a	411	-	-	4/29/63/63	0/2/2/2
39	CHL	r	607	-	-	8/22/98/117	-
33	PHO	a	408	-	-	8/37/103/103	0/5/6/6
39	CHL	N	607	-	-	12/41/117/117	-
32	CLA	r	603	3	-	9/20/96/115	-
37	SQD	A	412	-	-	6/30/50/69	0/1/1/1
32	CLA	Rr	612	3	-	7/20/96/115	-
32	CLA	YY	602	9	-	15/39/115/115	-
32	CLA	C	504	18	-	16/39/115/115	-
32	CLA	NN	612	9	-	4/12/88/115	-
36	LHG	4	315	32	-	8/23/23/53	-
32	CLA	Y	610	9	-	19/39/115/115	-
40	LUT	Yy	616	-	-	3/29/67/67	0/2/2/2
32	CLA	11	604	-	-	4/10/82/115	-
39	CHL	Yy	607	-	-	4/14/90/117	-
39	CHL	33	607	-	-	3/12/84/117	-
40	LUT	Yy	615	-	-	3/29/67/67	0/2/2/2
32	CLA	N	614	9	-	5/10/86/115	-
32	CLA	CC	504	18	-	16/39/115/115	-
32	CLA	B	620	28	-	10/39/115/115	-
32	CLA	C	507	18	-	13/39/115/115	-
39	CHL	G	605	9	-	5/14/90/117	-
44	DGD	BB	625	-	-	3/43/83/95	0/2/2/2
32	CLA	r	612	3	-	4/20/96/115	-
32	CLA	N	612	9	-	3/12/88/115	-

The worst 5 of 4081 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	AA	410	PL9	C23-C24	10.46	1.58	1.33
35	A	410	PL9	C23-C24	10.36	1.57	1.33
35	d	404	PL9	C23-C24	10.20	1.57	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	Dd	404	PL9	C23-C24	10.20	1.57	1.33
35	DD	406	PL9	C23-C24	10.17	1.57	1.33

The worst 5 of 4988 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BB	621	SQD	O9-S-C6	-19.31	83.99	106.94
37	B	617	SQD	O9-S-C6	-19.24	84.07	106.94
41	G	619	XAT	O24-C25-C24	14.32	124.14	113.38
41	GG	619	XAT	O24-C25-C24	14.28	124.11	113.38
41	g	619	XAT	O24-C25-C24	13.93	123.85	113.38

There are no chirality outliers.

5 of 6209 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	406	CLA	CHA-CBD-CGD-O1D
32	A	406	CLA	CHA-CBD-CGD-O2D
32	A	408	CLA	CHA-CBD-CGD-O1D
32	A	408	CLA	CHA-CBD-CGD-O2D
32	A	408	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

336 monomers are involved in 452 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	N	608	CHL	1	0
38	WW	201	LMG	1	0
32	NN	611	CLA	2	0
38	Aa	412	LMG	1	0
39	33	608	CHL	1	0
34	B	613	BCR	2	0
36	a	414	LHG	2	0
46	EE	102	HEM	1	0
32	Rr	608	CLA	2	0
34	B	614	BCR	1	0
44	Hh	102	DGD	2	0
39	N	606	CHL	1	0
32	11	612	CLA	2	0
32	11	609	CLA	2	0
39	2	607	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	RR	313	CLA	1	0
32	r	608	CLA	2	0
32	Y	611	CLA	1	0
39	g	608	CHL	1	0
39	YY	606	CHL	1	0
32	Nn	301	CLA	1	0
39	22	607	CHL	1	0
32	RR	308	CLA	3	0
32	CC	505	CLA	2	0
39	G	607	CHL	1	0
39	22	601	CHL	1	0
32	Y	613	CLA	1	0
39	4	307	CHL	1	0
39	NN	607	CHL	2	0
39	2	608	CHL	1	0
39	YY	601	CHL	1	0
32	Bb	601	CLA	1	0
44	BB	624	DGD	1	0
44	CC	518	DGD	1	0
32	C	510	CLA	1	0
32	GG	610	CLA	1	0
32	4	311	CLA	1	0
45	AA	413	BCT	1	0
32	S	610	CLA	1	0
32	BB	603	CLA	1	0
40	n	615	LUT	3	0
34	Hh	101	BCR	3	0
39	22	608	CHL	1	0
40	N	615	LUT	1	0
39	SS	308	CHL	1	0
35	A	410	PL9	10	0
32	c	507	CLA	1	0
40	y	317	LUT	2	0
35	DD	406	PL9	7	0
39	YY	608	CHL	1	0
32	B	604	CLA	2	0
39	S	601	CHL	1	0
32	c	509	CLA	1	0
38	Bb	620	LMG	1	0
32	44	611	CLA	1	0
36	NN	619	LHG	1	0
44	c	518	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	RR	305	CHL	1	0
32	Bb	608	CLA	1	0
42	R	617	NEX	4	0
40	Ss	615	LUT	3	0
44	CC	522	DGD	1	0
32	C	505	CLA	2	0
32	C	506	CLA	1	0
32	s	608	CLA	1	0
39	Yy	605	CHL	1	0
32	N	611	CLA	1	0
32	Gg	303	CLA	3	0
32	Nn	302	CLA	1	0
42	Y	617	NEX	1	0
32	y	315	CLA	1	0
32	Cc	511	CLA	1	0
34	H	101	BCR	4	0
39	n	607	CHL	1	0
39	YY	607	CHL	1	0
41	NN	617	XAT	1	0
39	n	601	CHL	2	0
39	4	306	CHL	1	0
32	G	610	CLA	1	0
37	CC	501	SQD	1	0
39	y	303	CHL	1	0
32	S	609	CLA	4	0
46	Ee	101	HEM	2	0
34	Cc	517	BCR	2	0
32	YY	611	CLA	1	0
34	Bb	618	BCR	1	0
32	r	602	CLA	2	0
32	DD	401	CLA	2	0
42	y	319	NEX	1	0
39	Yy	606	CHL	1	0
39	Y	608	CHL	1	0
39	2	601	CHL	1	0
32	Aa	406	CLA	4	0
39	Gg	307	CHL	1	0
39	n	606	CHL	1	0
36	AA	414	LHG	1	0
32	Cc	513	CLA	1	0
39	NN	606	CHL	1	0
32	3	613	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	c	511	CLA	1	0
36	Dd	405	LHG	1	0
36	d	405	LHG	1	0
32	Rr	602	CLA	1	0
39	Ss	607	CHL	1	0
35	d	404	PL9	10	0
39	11	607	CHL	2	0
39	G	601	CHL	1	0
41	Nn	308	XAT	2	0
32	33	604	CLA	1	0
39	G	609	CHL	2	0
32	N	602	CLA	2	0
39	y	308	CHL	1	0
32	SS	309	CLA	1	0
32	Ss	612	CLA	2	0
40	Nn	306	LUT	2	0
35	Dd	404	PL9	6	0
40	g	615	LUT	1	0
32	Nn	313	CLA	1	0
35	D	407	PL9	3	0
39	s	607	CHL	1	0
42	Rr	616	NEX	1	0
38	m	101	LMG	1	0
34	Aa	411	BCR	2	0
39	11	608	CHL	1	0
32	GG	602	CLA	2	0
32	b	605	CLA	1	0
39	1	601	CHL	2	0
39	GG	605	CHL	1	0
34	TT	101	BCR	1	0
39	SS	307	CHL	1	0
39	Rr	607	CHL	1	0
32	n	610	CLA	3	0
39	3	606	CHL	1	0
34	c	514	BCR	1	0
44	C	520	DGD	1	0
32	Nn	312	CLA	2	0
39	Rr	606	CHL	1	0
34	Cc	518	BCR	2	0
44	Cc	519	DGD	2	0
39	S	605	CHL	1	0
42	YY	617	NEX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	Nn	309	NEX	1	0
34	h	101	BCR	3	0
32	s	609	CLA	1	0
37	AA	412	SQD	2	0
39	Nn	317	CHL	1	0
39	1	606	CHL	1	0
32	Dd	401	CLA	2	0
39	4	309	CHL	1	0
39	g	607	CHL	1	0
39	4	302	CHL	1	0
41	y	302	XAT	1	0
32	G	602	CLA	2	0
32	1	603	CLA	1	0
39	GG	601	CHL	1	0
32	Bb	609	CLA	2	0
39	3	605	CHL	1	0
32	n	611	CLA	1	0
32	GG	613	CLA	2	0
32	r	604	CLA	1	0
39	11	606	CHL	1	0
46	e	101	HEM	1	0
39	S	606	CHL	1	0
39	GG	608	CHL	1	0
32	Ss	608	CLA	1	0
39	G	608	CHL	1	0
39	Y	601	CHL	2	0
39	3	601	CHL	1	0
39	g	606	CHL	1	0
32	Ss	610	CLA	1	0
36	Ll	102	LHG	1	0
39	Rr	605	CHL	1	0
39	y	307	CHL	1	0
34	BB	617	BCR	2	0
39	11	605	CHL	1	0
32	a	406	CLA	2	0
32	1	609	CLA	1	0
32	B	608	CLA	1	0
34	Kk	101	BCR	5	0
38	c	519	LMG	1	0
39	N	609	CHL	1	0
39	N	605	CHL	1	0
32	b	601	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	s	606	CHL	1	0
39	R	605	CHL	2	0
32	Cc	504	CLA	2	0
39	11	601	CHL	1	0
39	Gg	308	CHL	1	0
38	W	201	LMG	1	0
39	G	606	CHL	1	0
35	AA	410	PL9	4	0
39	Y	606	CHL	1	0
32	RR	310	CLA	1	0
32	1	602	CLA	3	0
34	Cc	516	BCR	1	0
46	E	101	HEM	1	0
44	Aa	401	DGD	1	0
32	11	610	CLA	1	0
39	g	609	CHL	1	0
39	Y	605	CHL	1	0
32	4	310	CLA	2	0
39	g	605	CHL	1	0
39	y	310	CHL	1	0
44	c	517	DGD	1	0
34	b	618	BCR	1	0
34	K	102	BCR	1	0
32	C	515	CLA	1	0
39	g	601	CHL	1	0
32	RR	314	CLA	1	0
32	N	603	CLA	1	0
34	D	406	BCR	1	0
39	Nn	316	CHL	1	0
37	C	501	SQD	1	0
39	Y	609	CHL	1	0
34	KK	103	BCR	3	0
38	j	101	LMG	1	0
39	Gg	309	CHL	1	0
32	B	607	CLA	1	0
36	A	413	LHG	1	0
39	Gg	302	CHL	1	0
39	R	606	CHL	2	0
42	Yy	617	NEX	1	0
36	CC	523	LHG	1	0
39	Gg	306	CHL	1	0
39	s	601	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	n	614	CLA	1	0
41	RR	316	XAT	2	0
32	n	602	CLA	1	0
32	D	401	CLA	1	0
32	X	201	CLA	1	0
34	b	619	BCR	2	0
32	c	503	CLA	2	0
33	D	402	PHO	1	0
32	Bb	607	CLA	1	0
39	YY	609	CHL	1	0
32	CC	509	CLA	1	0
32	33	609	CLA	1	0
39	GG	607	CHL	1	0
39	Nn	311	CHL	1	0
44	D	411	DGD	1	0
41	r	615	XAT	2	0
39	n	608	CHL	2	0
34	DD	405	BCR	1	0
32	D	404	CLA	1	0
39	1	605	CHL	2	0
32	SS	305	CLA	2	0
39	Nn	318	CHL	1	0
36	Ss	616	LHG	1	0
44	Cc	520	DGD	2	0
32	b	608	CLA	1	0
32	2	612	CLA	1	0
32	33	602	CLA	1	0
36	s	616	LHG	1	0
39	NN	608	CHL	1	0
32	b	613	CLA	1	0
39	Yy	608	CHL	1	0
36	KK	101	LHG	1	0
39	SS	302	CHL	1	0
32	y	316	CLA	1	0
32	BB	612	CLA	1	0
32	33	613	CLA	1	0
32	s	612	CLA	1	0
36	Dd	407	LHG	2	0
39	y	311	CHL	1	0
36	A	414	LHG	1	0
44	h	102	DGD	1	0
42	RR	317	NEX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	Bb	619	BCR	2	0
39	Yy	601	CHL	1	0
34	AA	409	BCR	1	0
32	BB	611	CLA	1	0
39	n	605	CHL	2	0
39	44	606	CHL	1	0
34	CC	517	BCR	2	0
44	B	601	DGD	1	0
32	b	609	CLA	3	0
34	c	515	BCR	3	0
34	Bb	617	BCR	1	0
42	N	618	NEX	1	0
39	Y	607	CHL	1	0
44	C	519	DGD	2	0
39	33	606	CHL	2	0
44	BB	623	DGD	3	0
34	k	101	BCR	1	0
32	3	604	CLA	1	0
36	44	616	LHG	1	0
39	YY	605	CHL	1	0
39	1	607	CHL	1	0
39	44	607	CHL	1	0
34	C	518	BCR	2	0
39	33	605	CHL	1	0
32	SS	310	CLA	1	0
32	g	613	CLA	3	0
36	0	201	LHG	2	0
34	A	409	BCR	1	0
32	CC	507	CLA	1	0
32	CC	514	CLA	1	0
34	b	617	BCR	1	0
36	l	101	LHG	2	0
39	33	601	CHL	1	0
32	Rr	604	CLA	1	0
39	S	607	CHL	1	0
32	Bb	613	CLA	1	0
34	XX	202	BCR	2	0
34	CC	516	BCR	1	0
32	g	602	CLA	2	0
40	Nn	307	LUT	1	0
32	DD	403	CLA	1	0
32	n	603	CLA	1	0

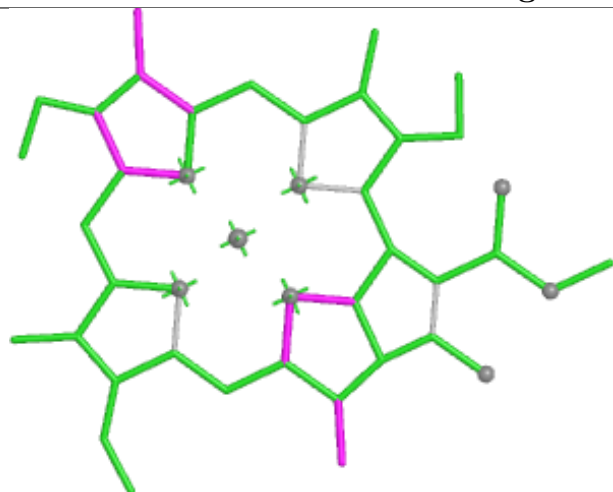
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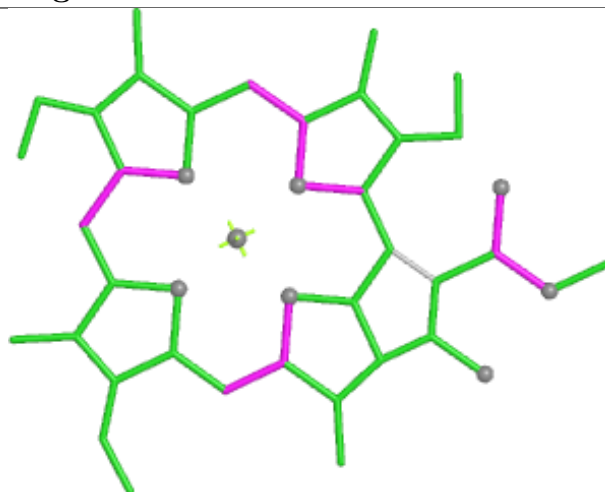
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	517	BCR	3	0
36	DD	408	LHG	1	0
32	CC	503	CLA	2	0
41	Rr	615	XAT	1	0
38	Cc	501	LMG	1	0
32	y	313	CLA	1	0
34	C	516	BCR	1	0
44	C	523	DGD	1	0
32	d	401	CLA	2	0
32	Nn	305	CLA	1	0
42	NN	618	NEX	1	0
32	b	610	CLA	1	0
39	Ss	601	CHL	1	0
32	c	501	CLA	2	0
34	c	516	BCR	3	0
34	a	411	BCR	3	0
39	r	607	CHL	1	0
39	N	607	CHL	1	0
45	D	403	BCT	2	0
32	C	504	CLA	3	0
40	Yy	616	LUT	1	0
39	Yy	607	CHL	2	0
32	CC	504	CLA	1	0
32	B	620	CLA	1	0
39	G	605	CHL	1	0
32	r	612	CLA	1	0
32	N	612	CLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

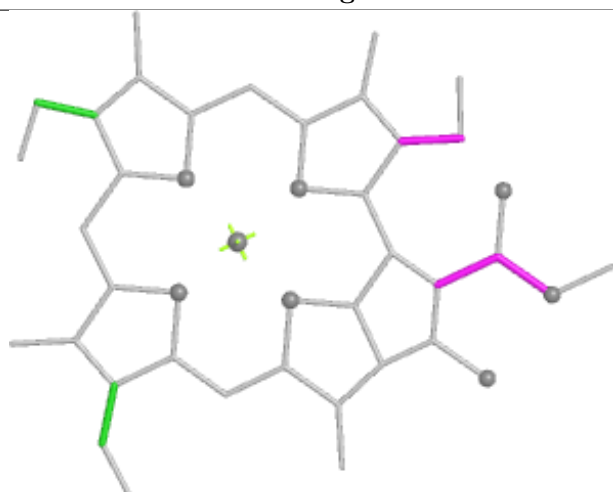
Ligand CLA g 604



Bond lengths



Bond angles

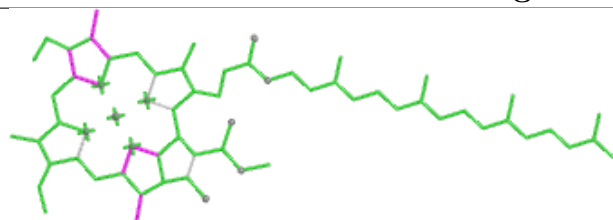


Torsions

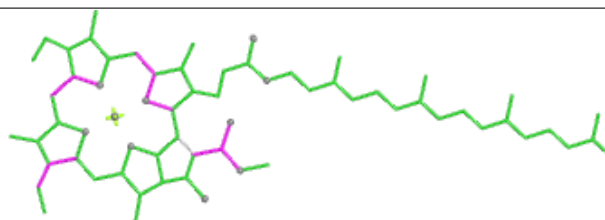


Rings

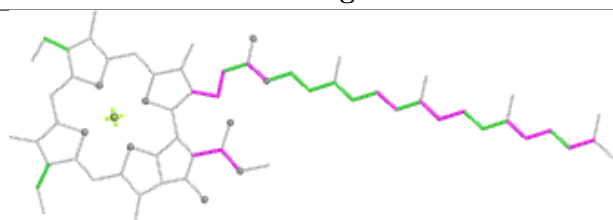
Ligand CLA A 405



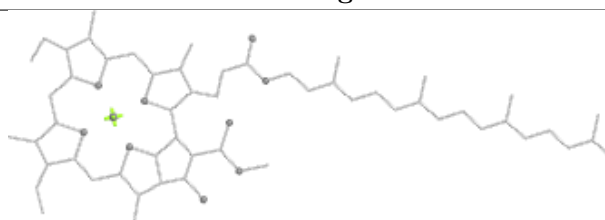
Bond lengths



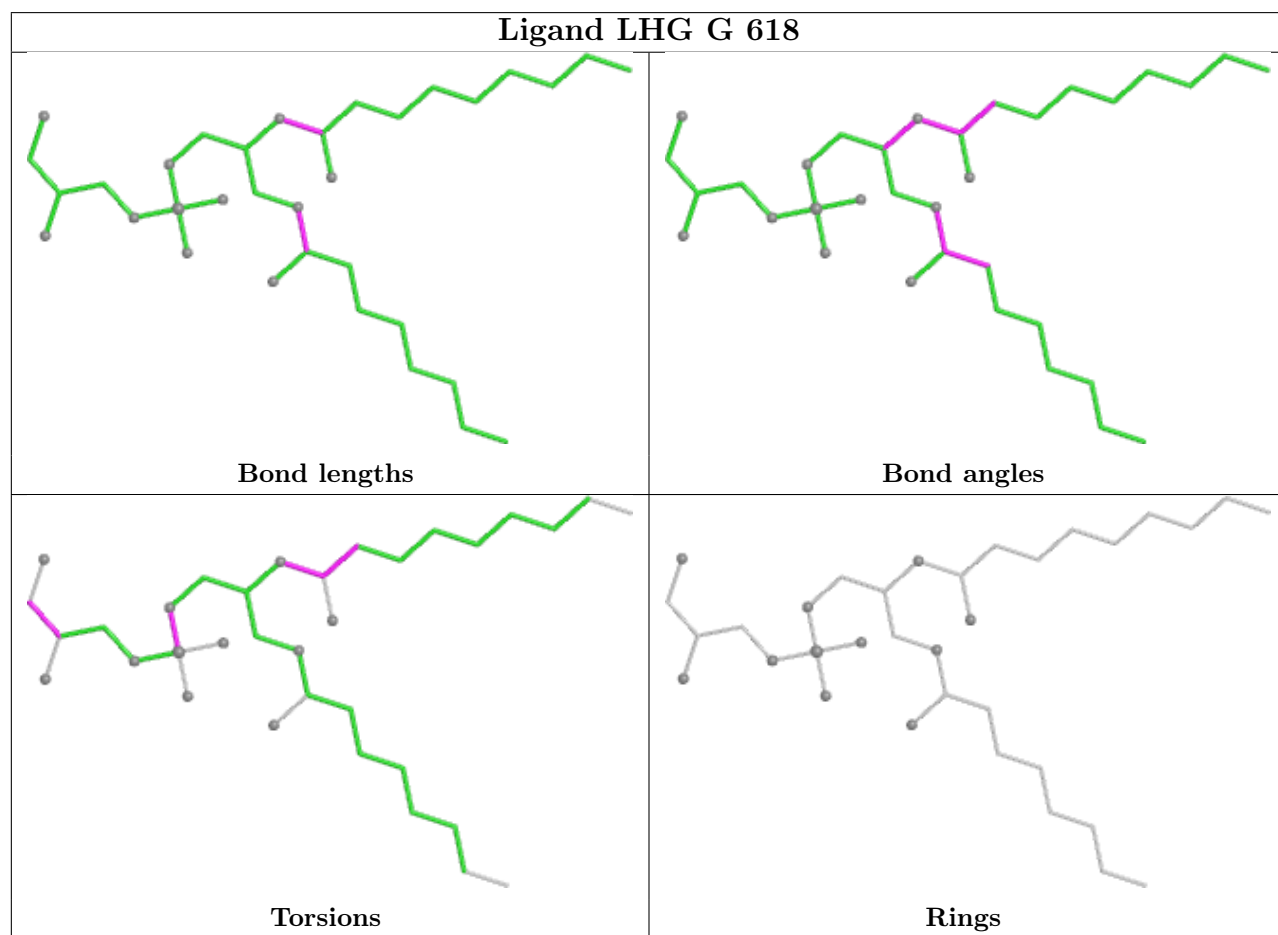
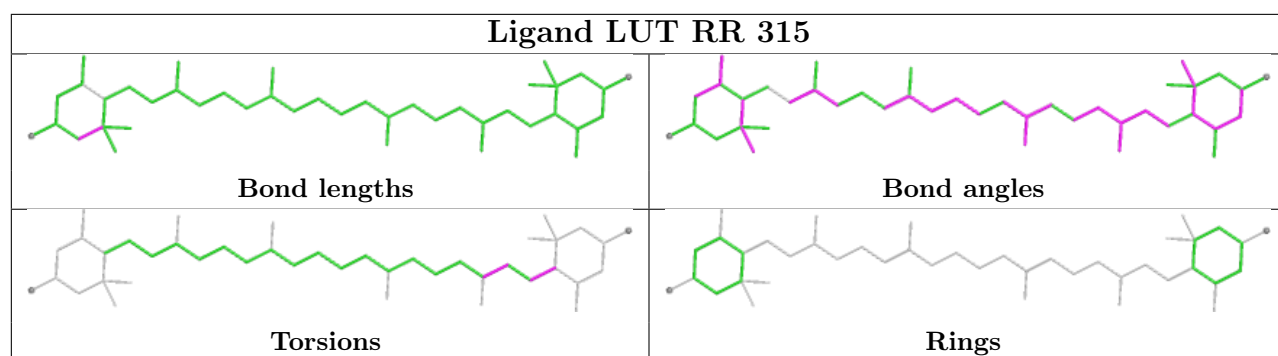
Bond angles

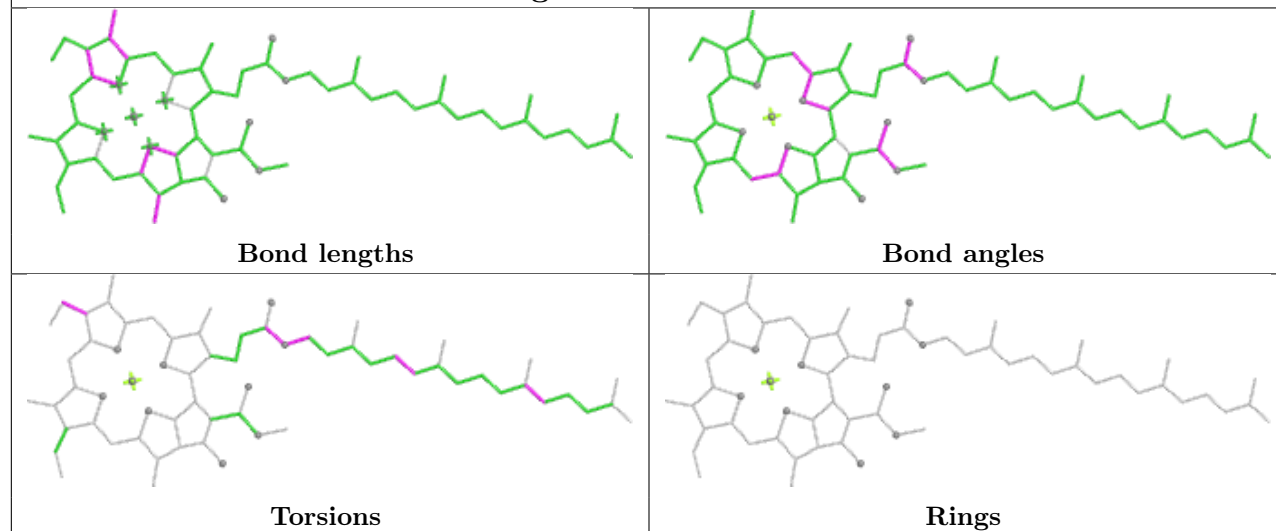
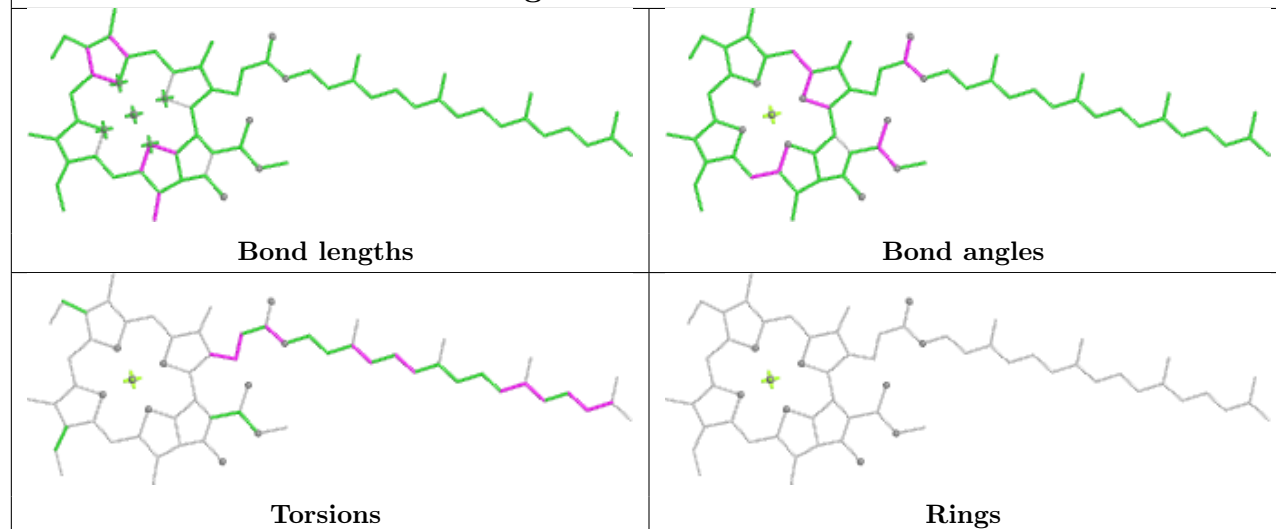


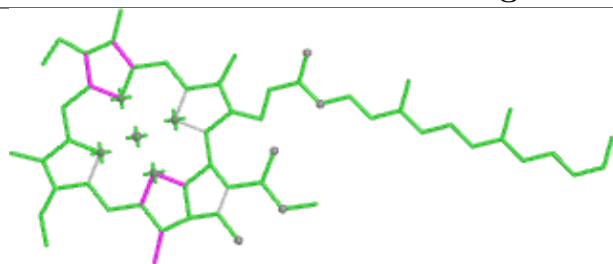
Torsions



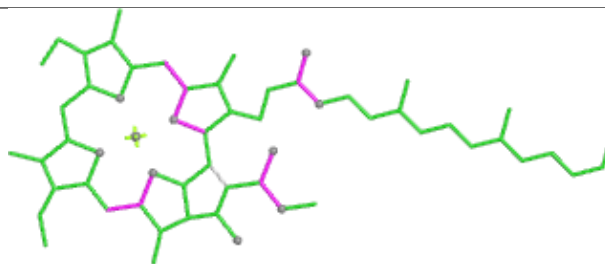
Rings



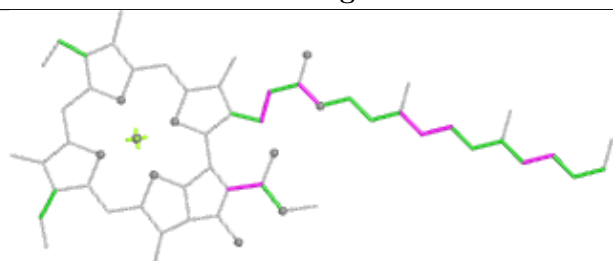
Ligand CLA D 405**Ligand CLA Cc 512**

Ligand CLA YY 613

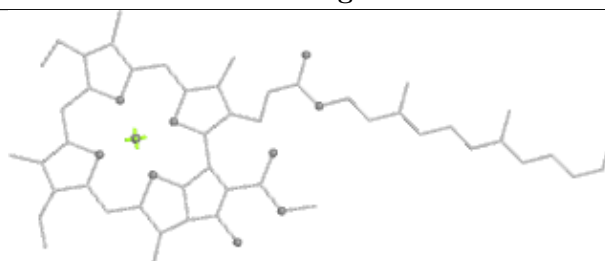
Bond lengths



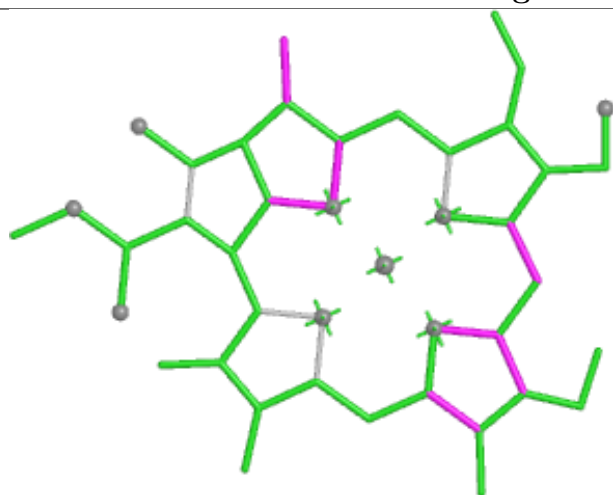
Bond angles



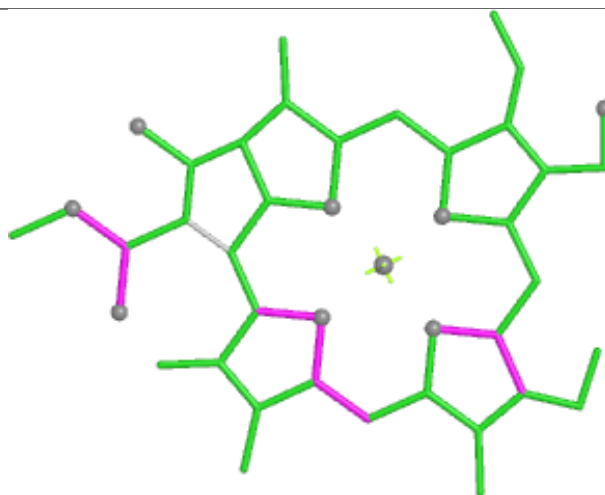
Torsions



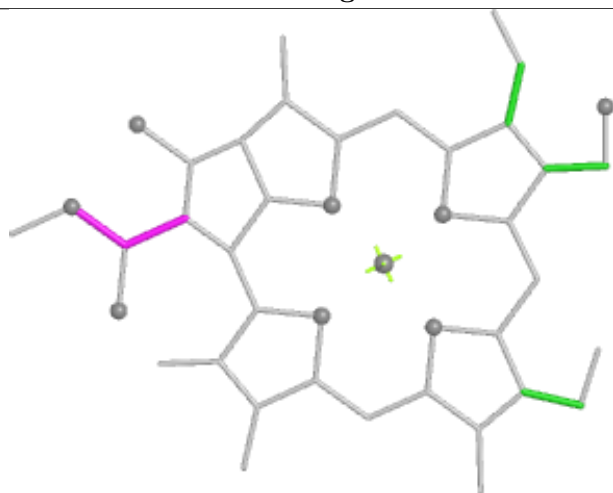
Rings

Ligand CHL N 608

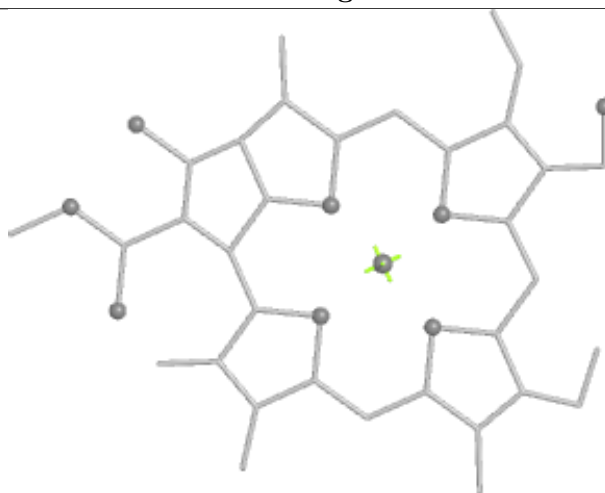
Bond lengths



Bond angles

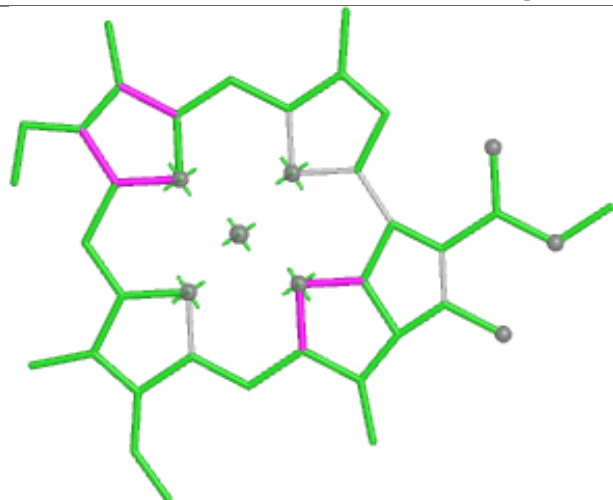


Torsions

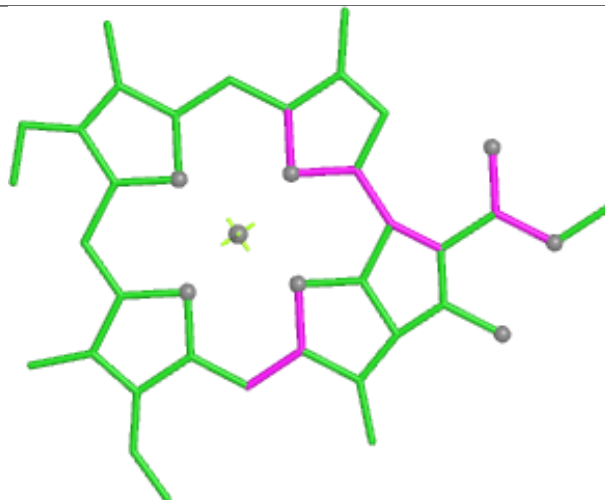


Rings

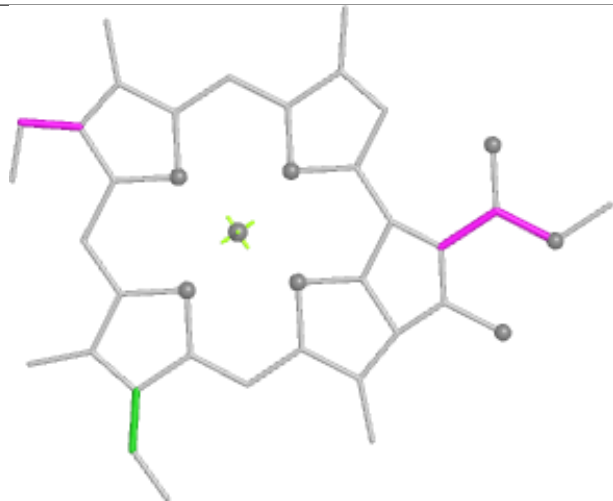
Ligand CLA 1 610



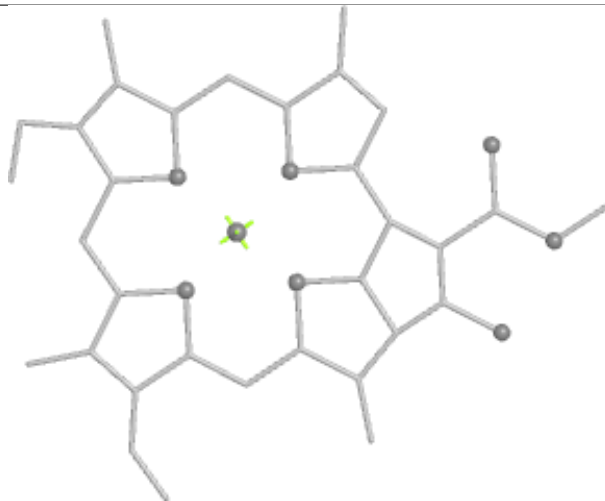
Bond lengths



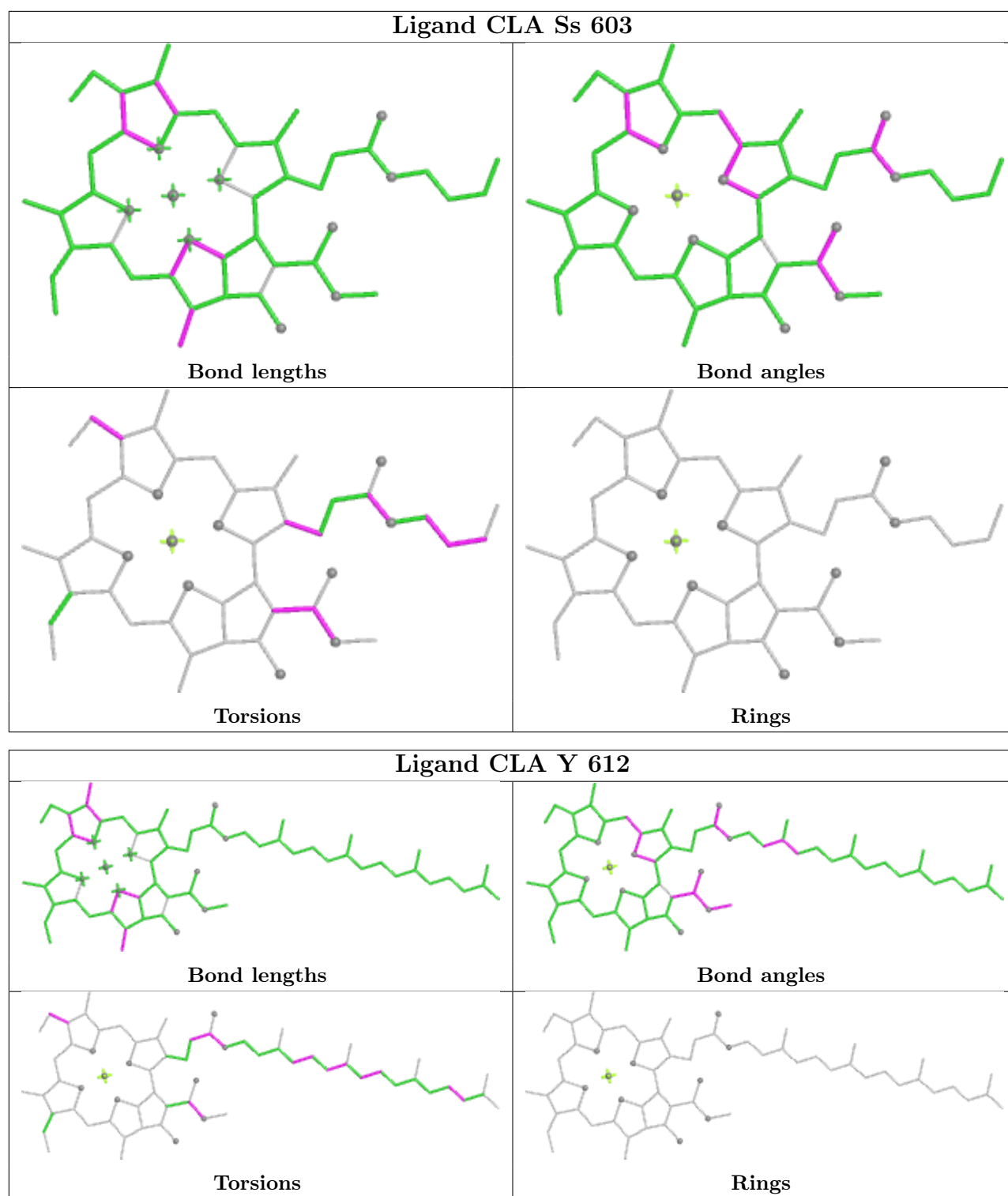
Bond angles

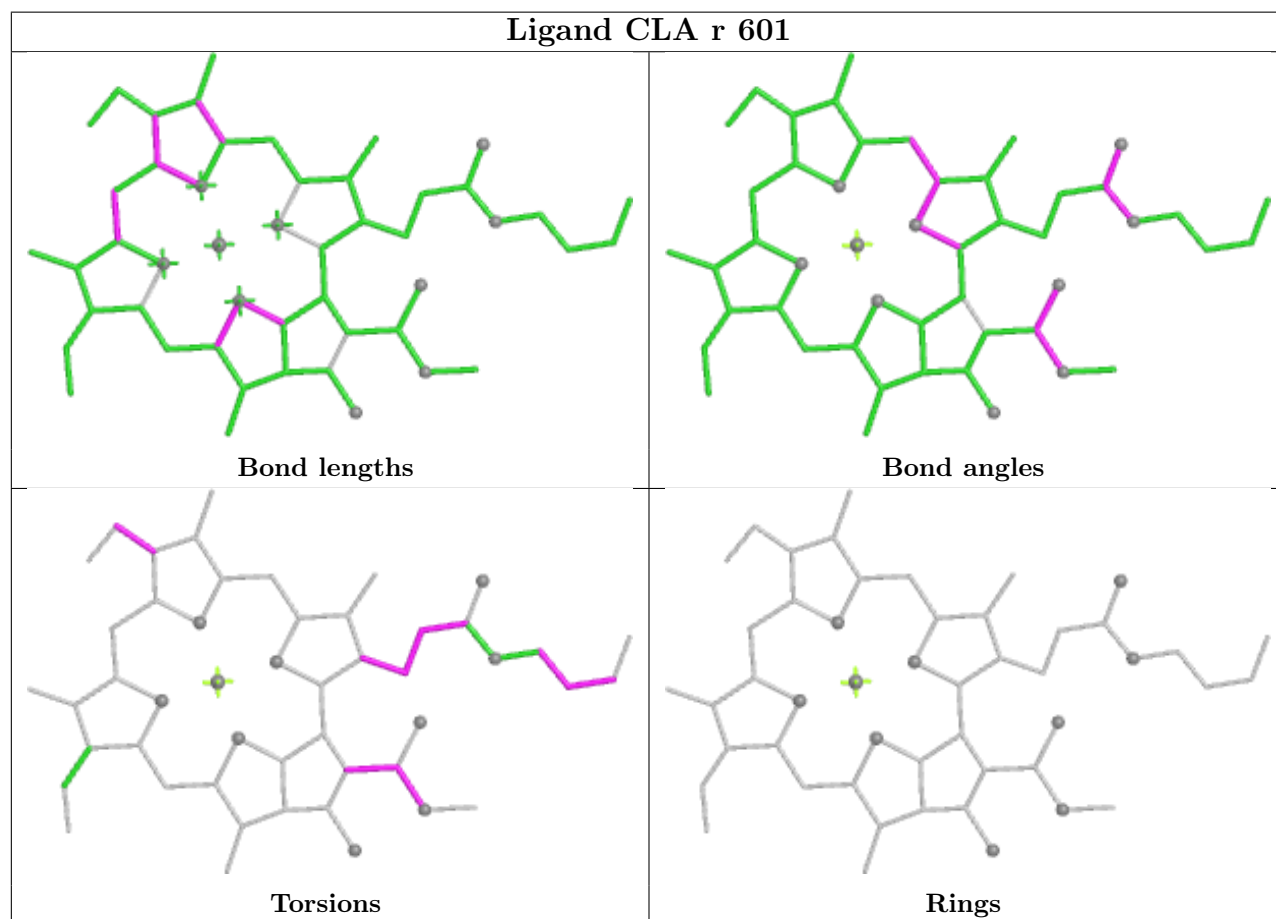
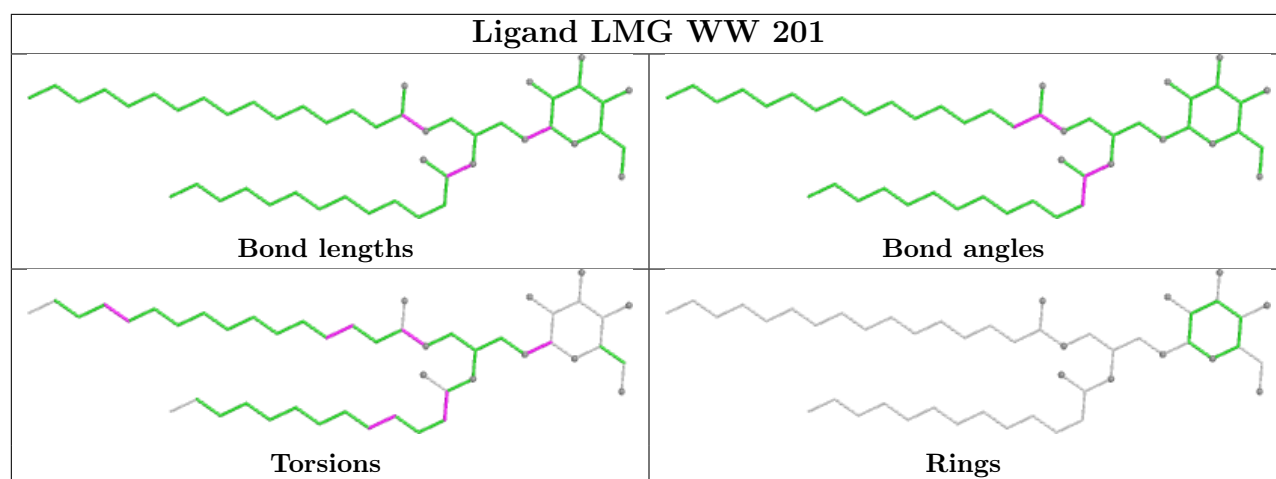


Torsions

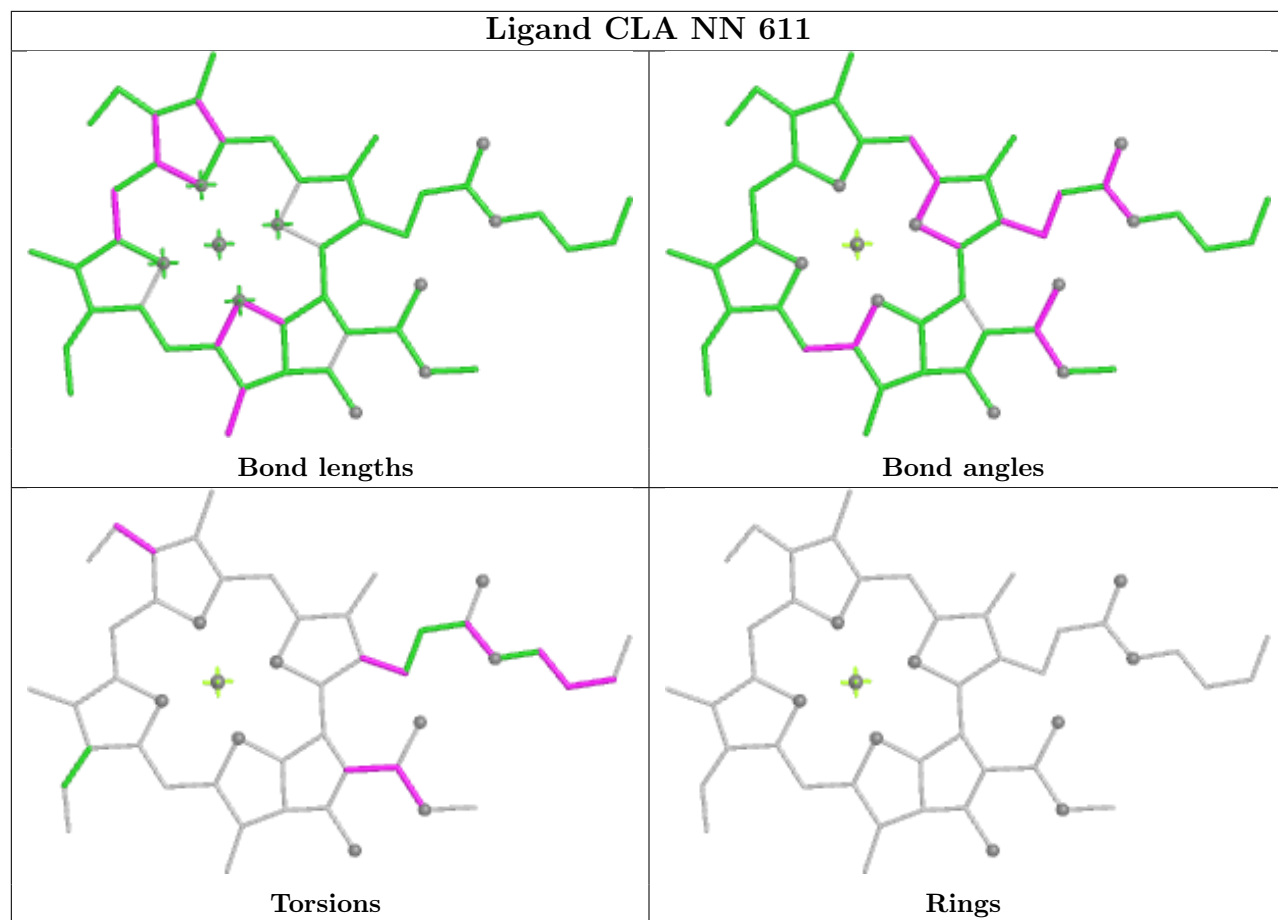


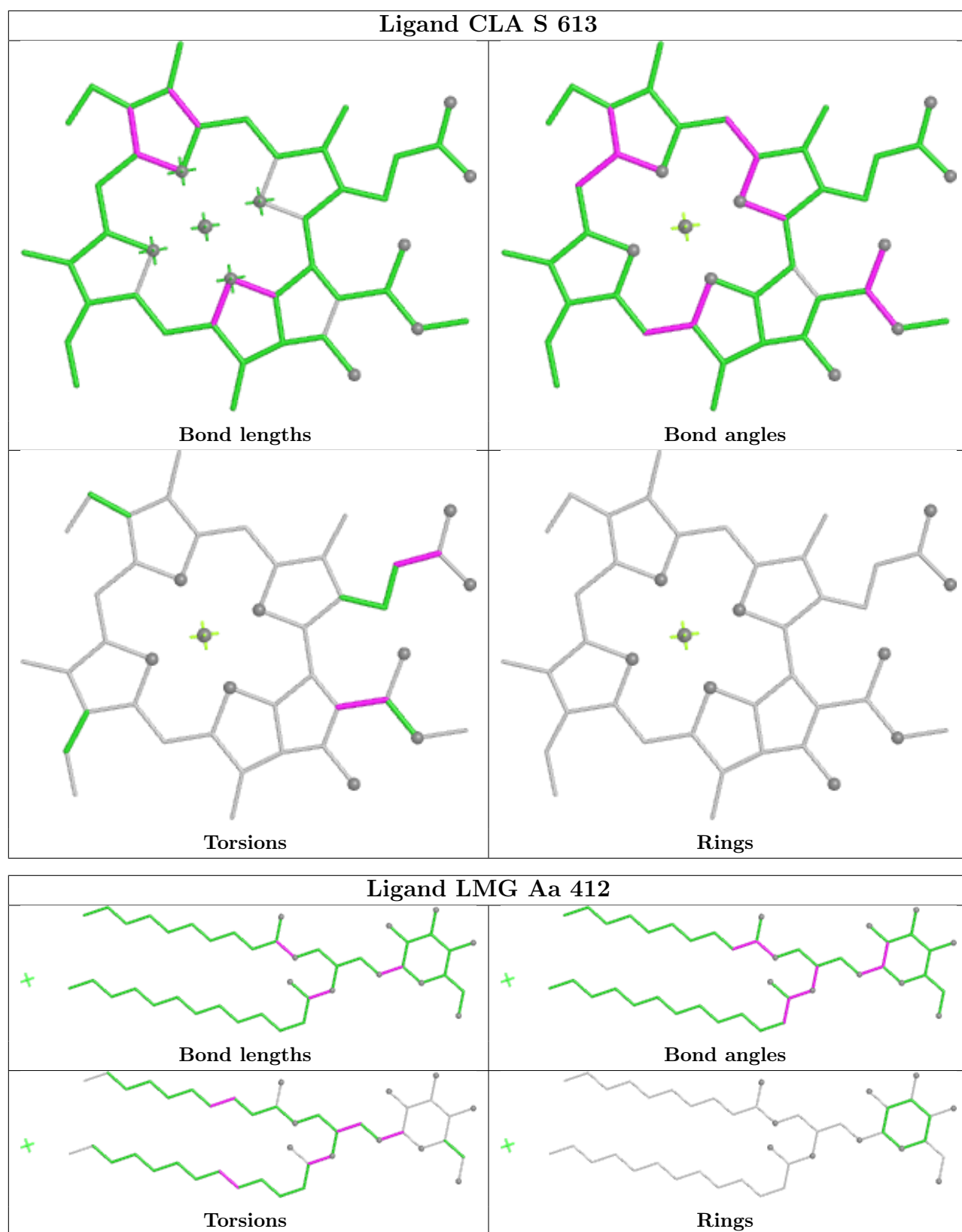
Rings

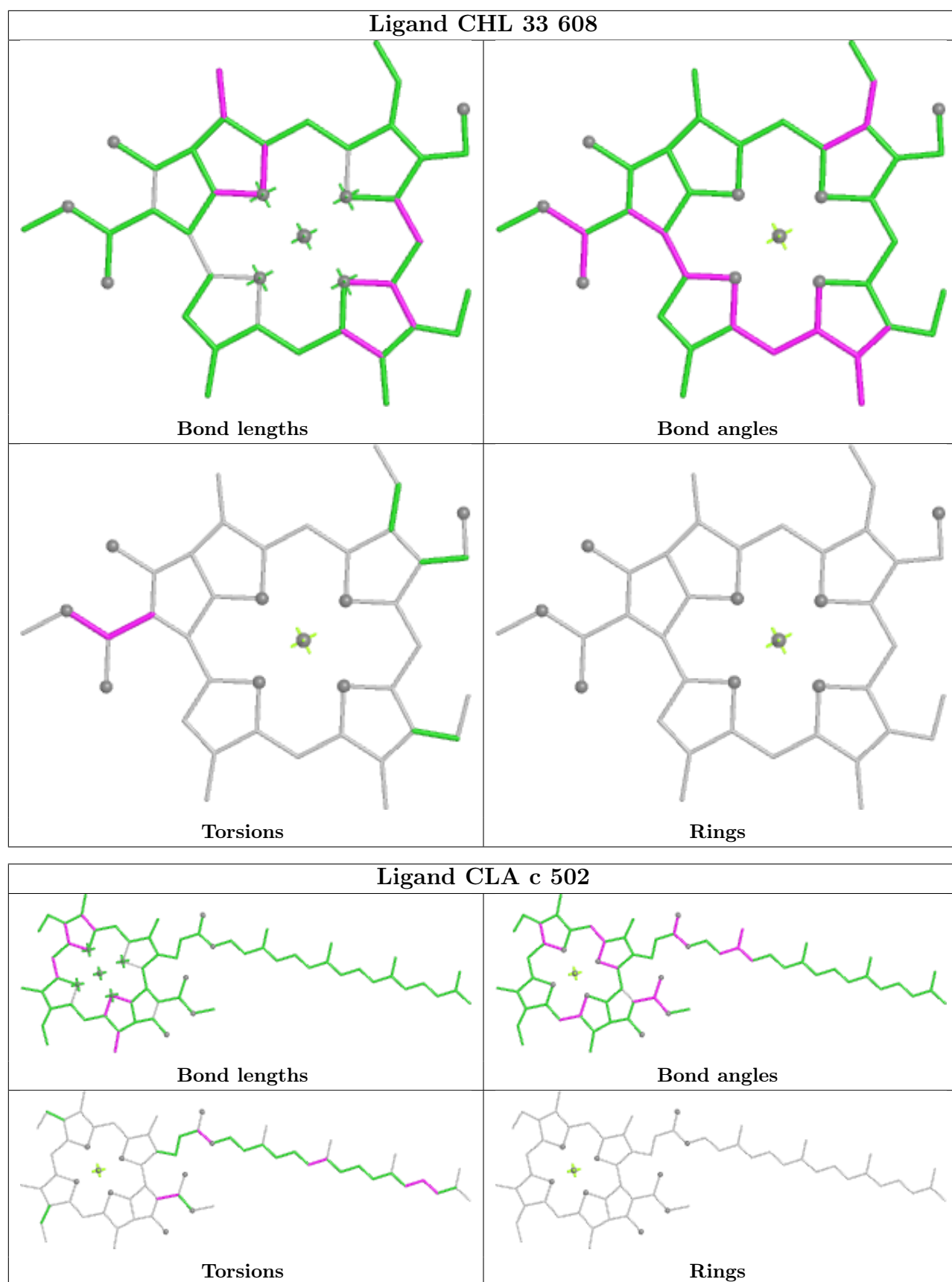


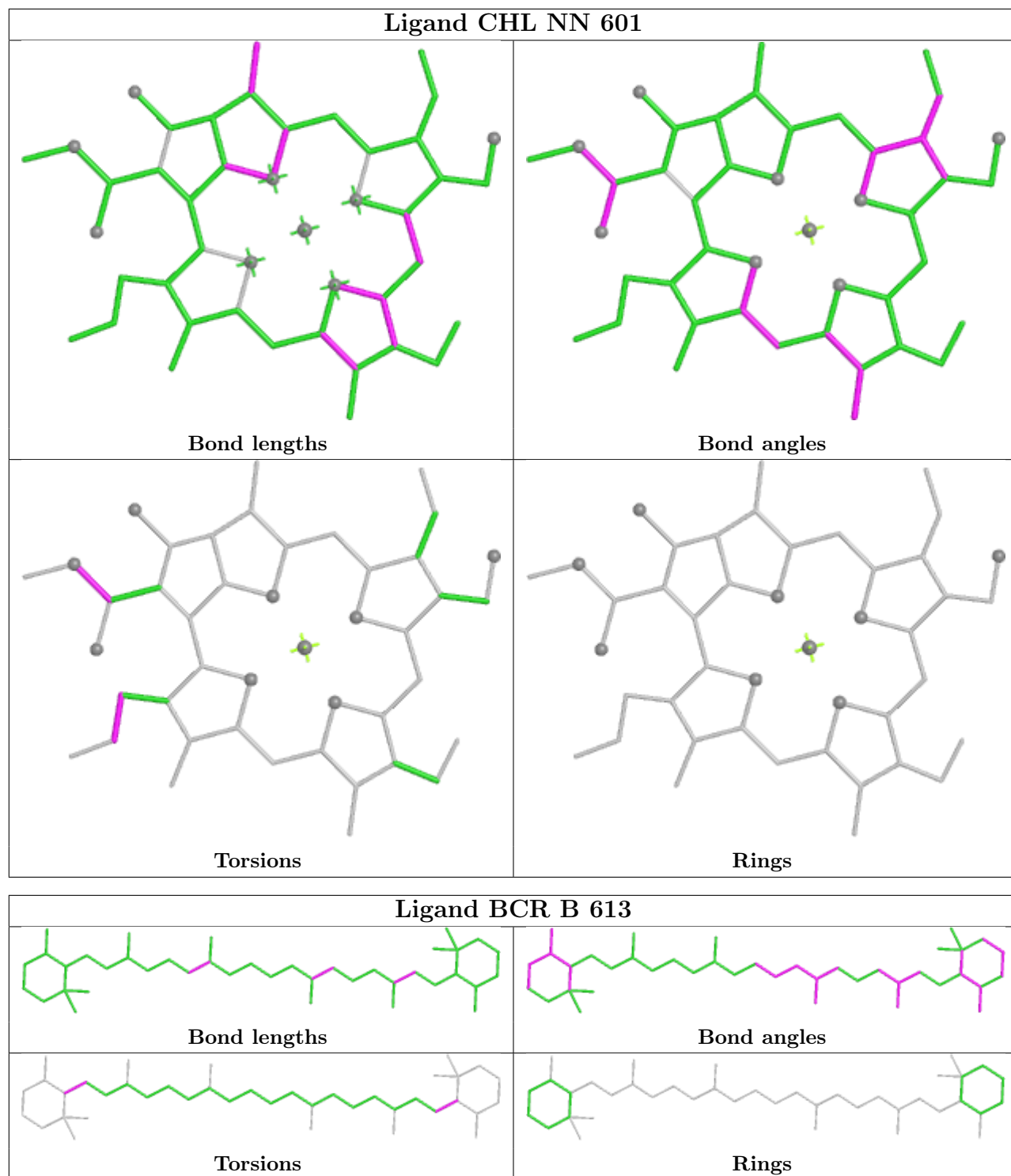


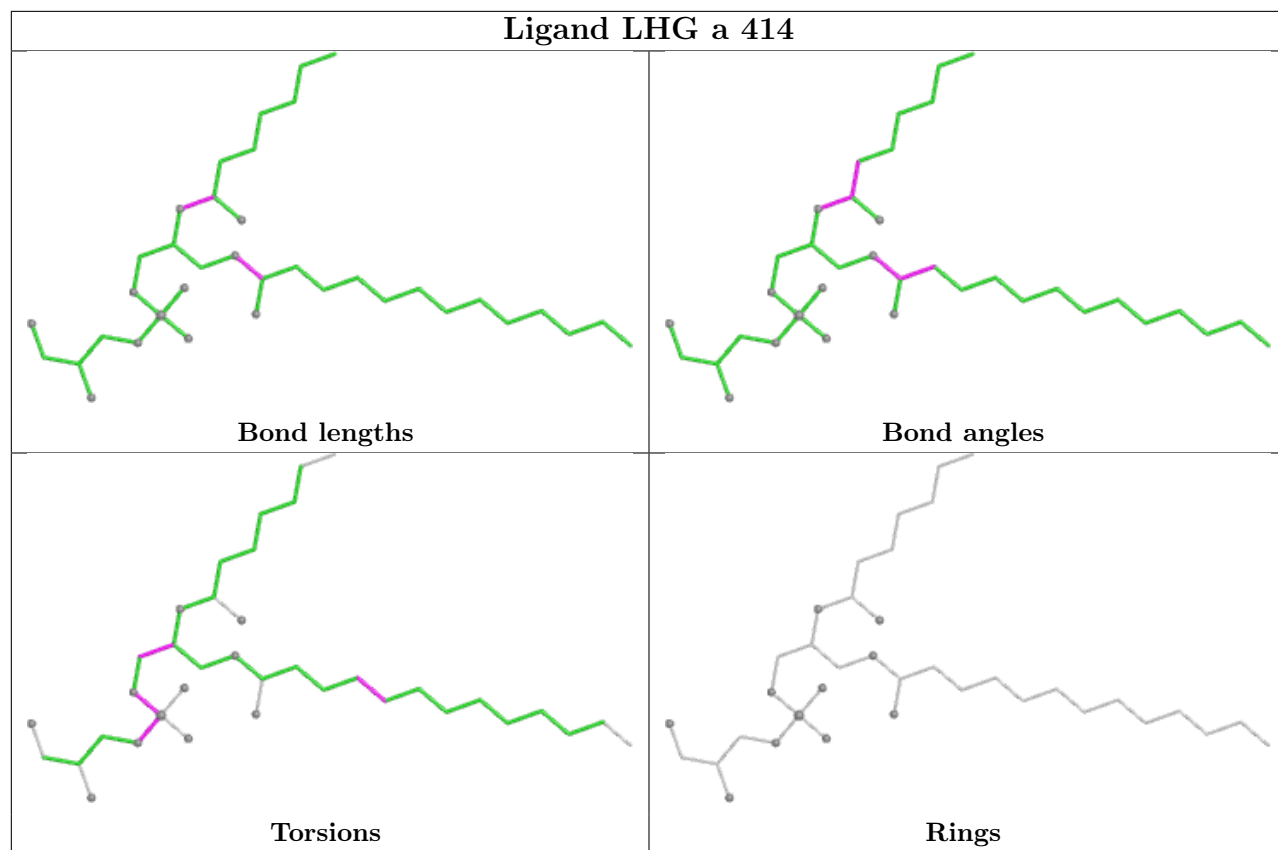
Ligand CLA NN 611



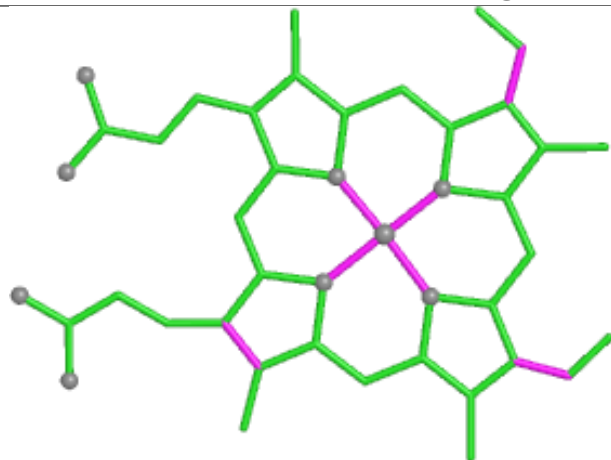




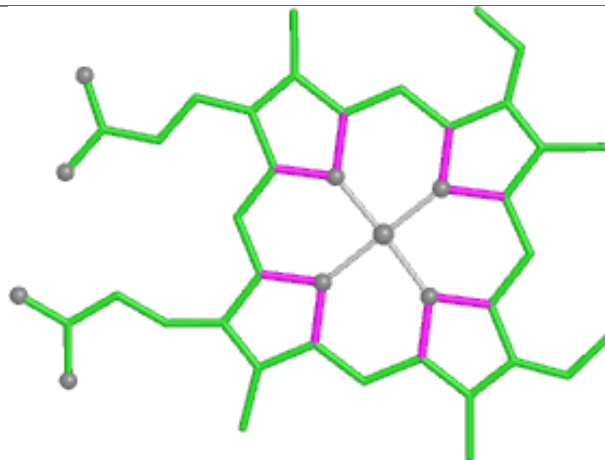




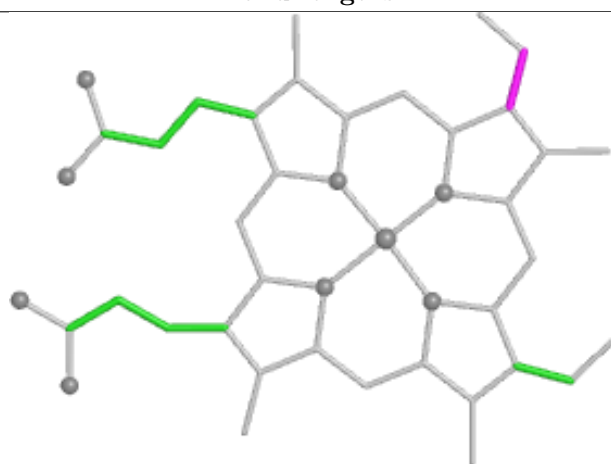
Ligand HEM EE 102



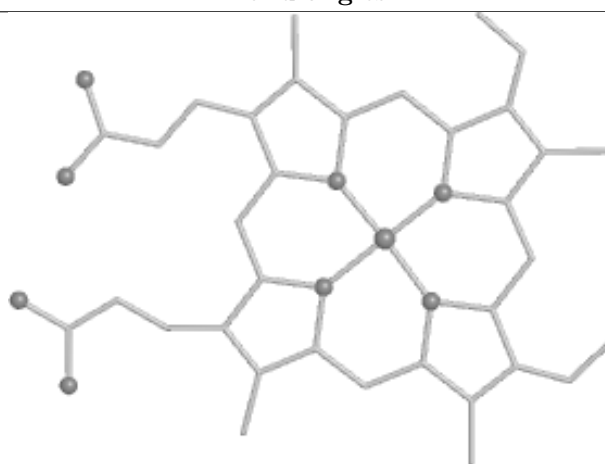
Bond lengths



Bond angles

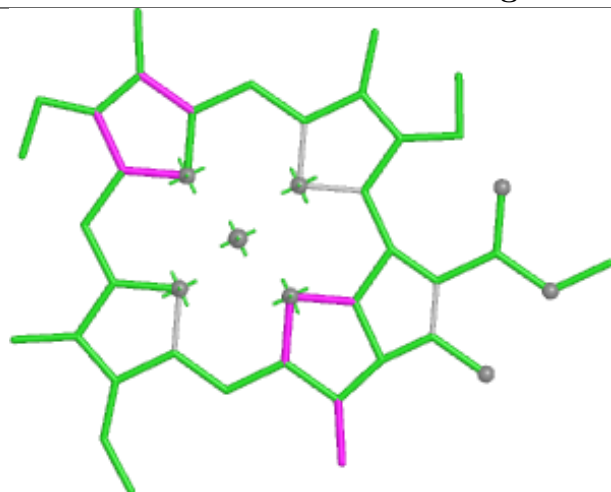


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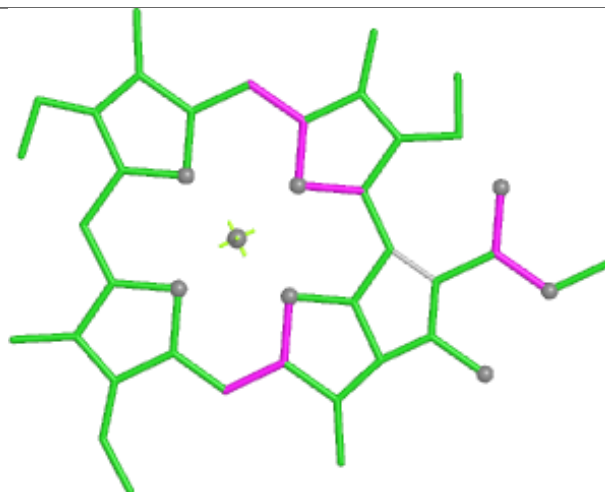


Rings

Ligand CLA RR 312



Bond lengths



Bond angles

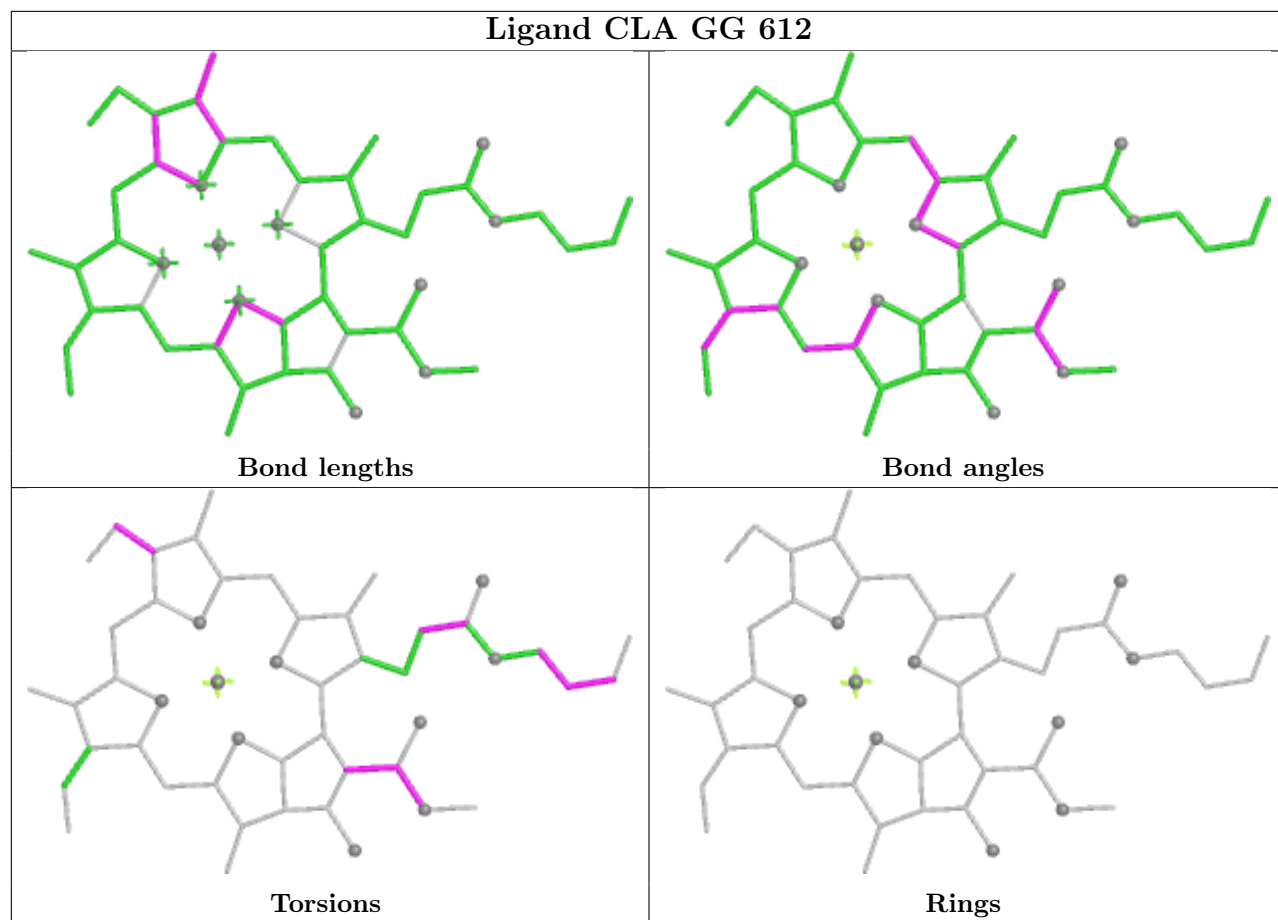


Torsions

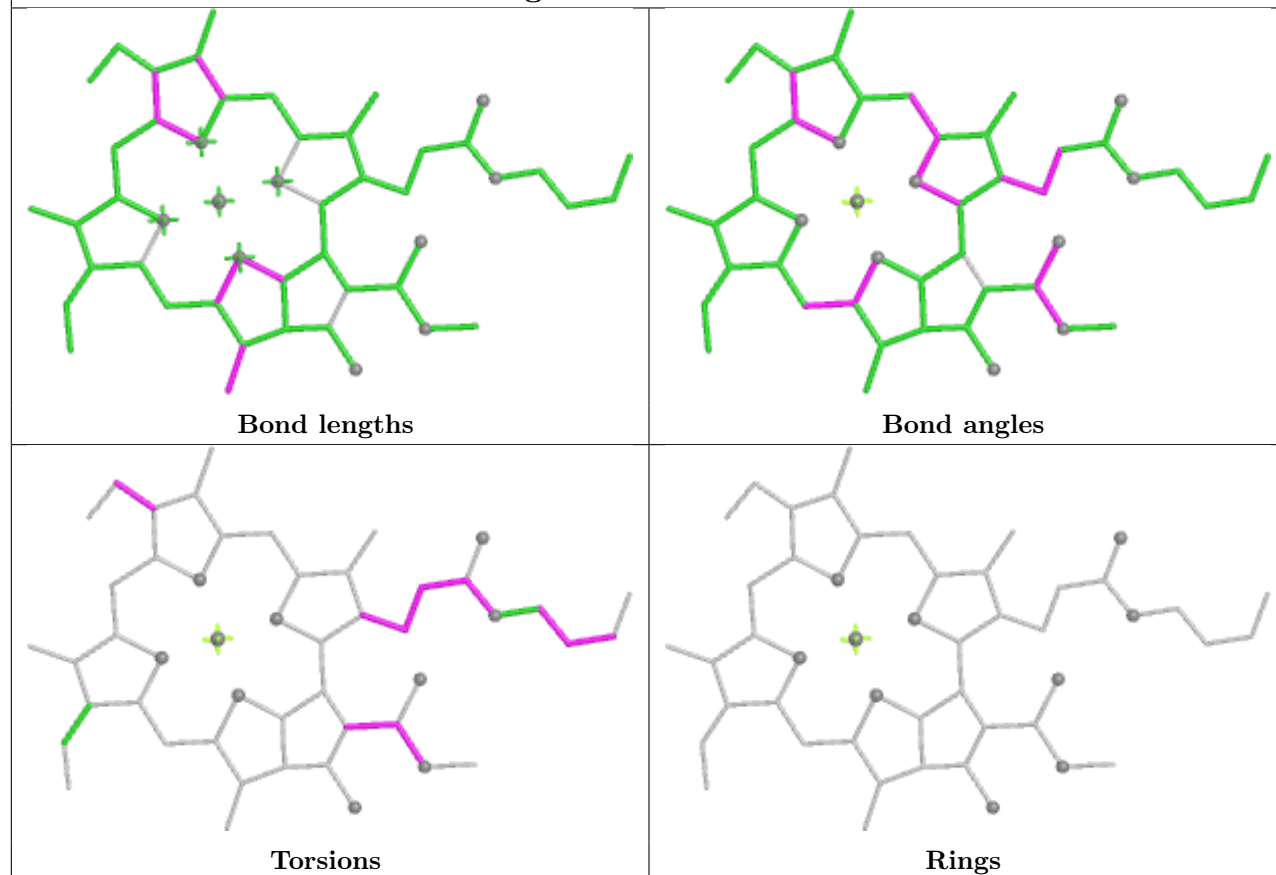


Rings

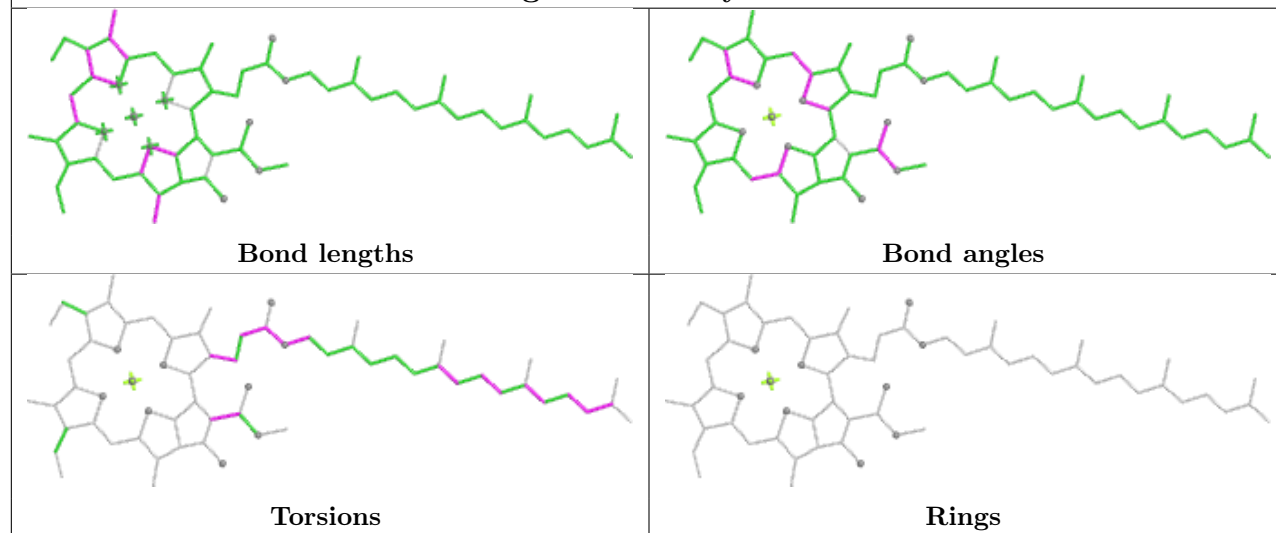
Ligand CLA GG 612

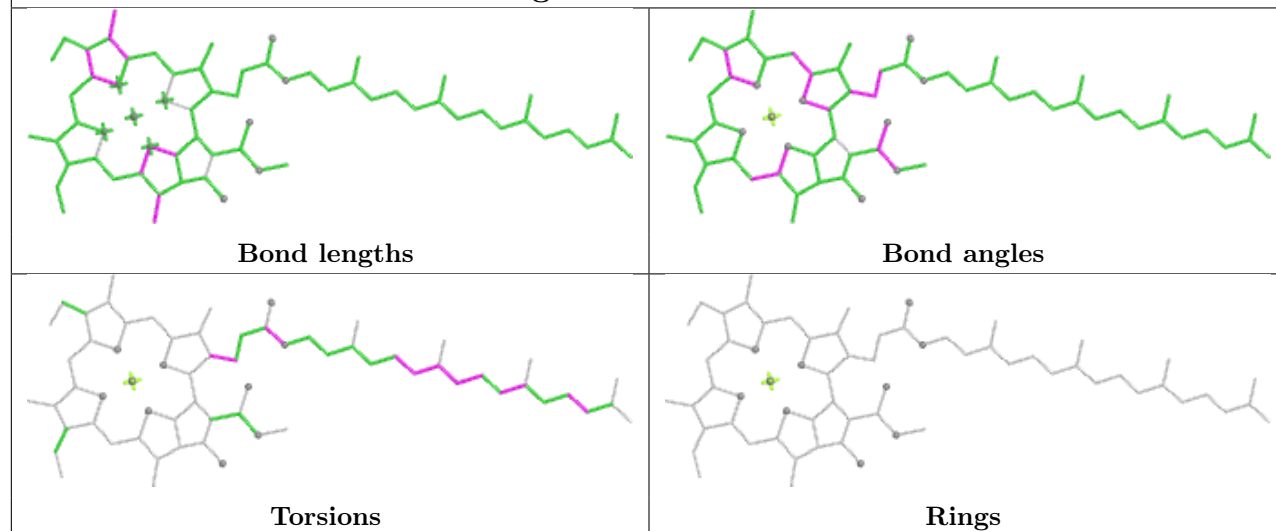
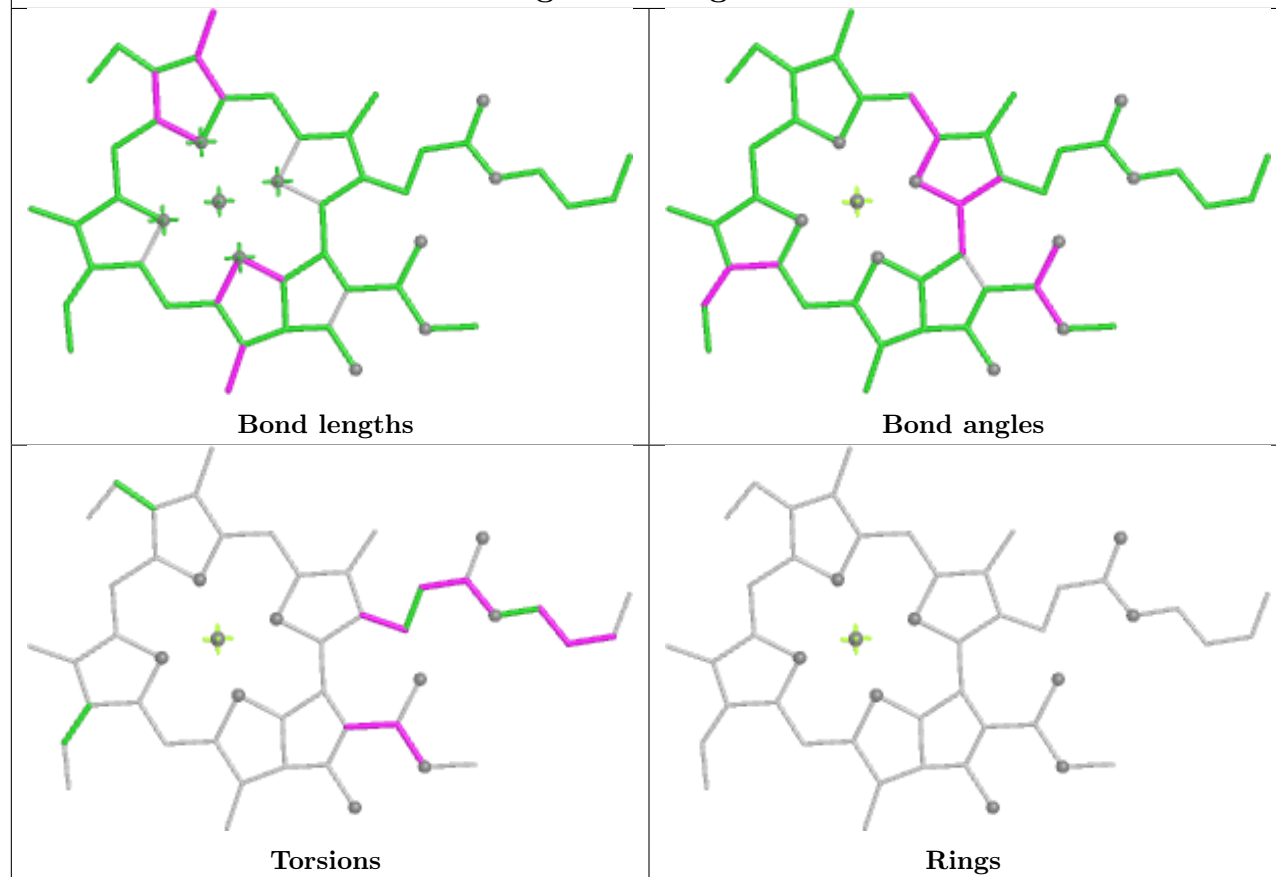


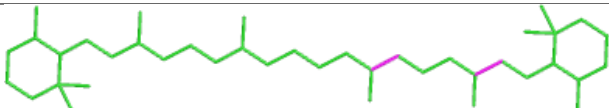
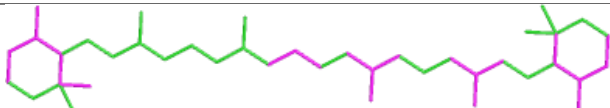
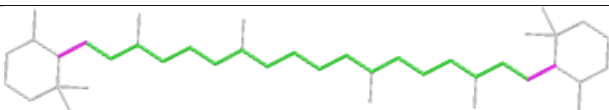
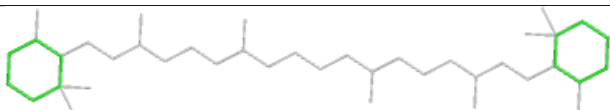
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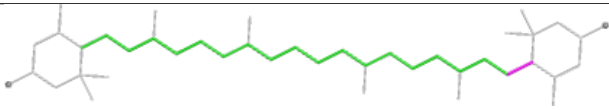
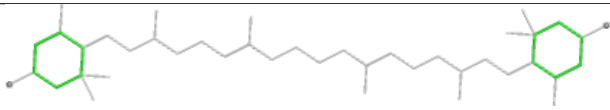


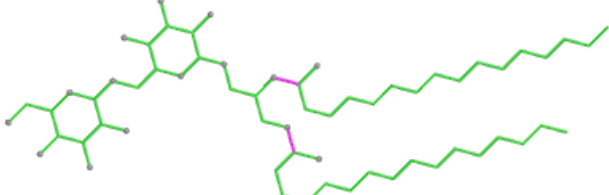
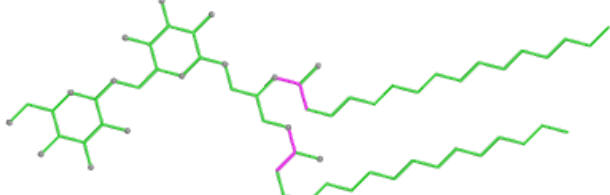
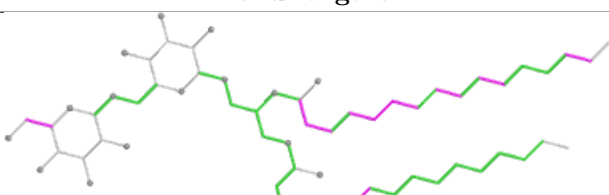
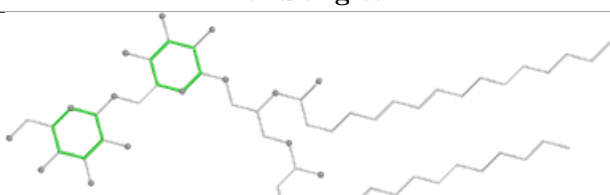
Ligand CLA Yy 602



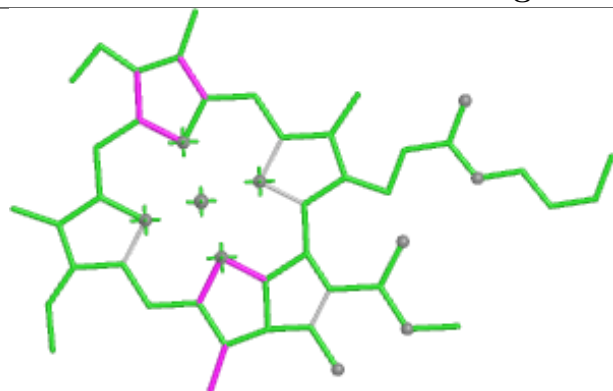
Ligand CLA C 503**Ligand CLA g 612**

Ligand BCR B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

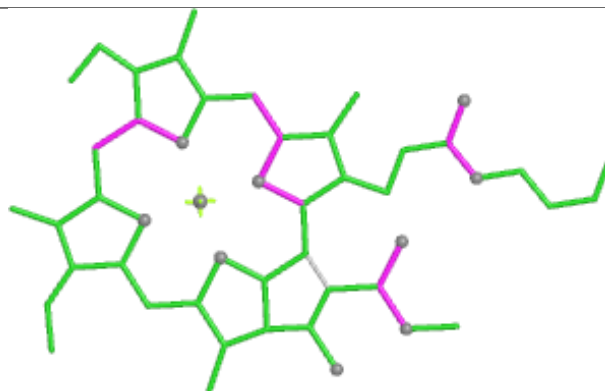
Ligand LUT r 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD Hh 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

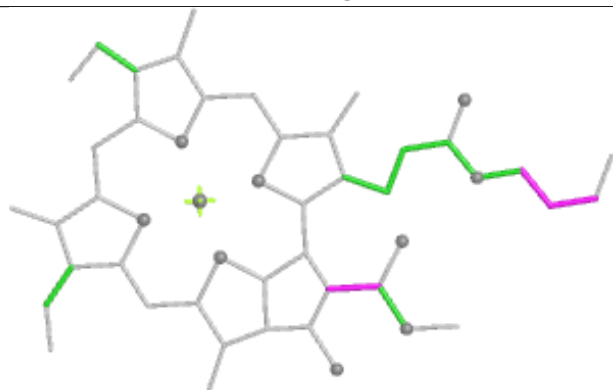
Ligand CLA R 603



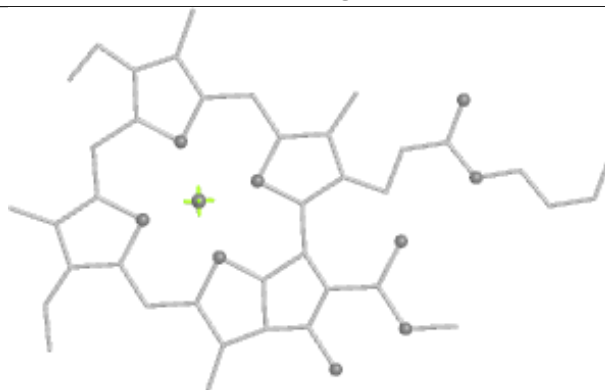
Bond lengths



Bond angles

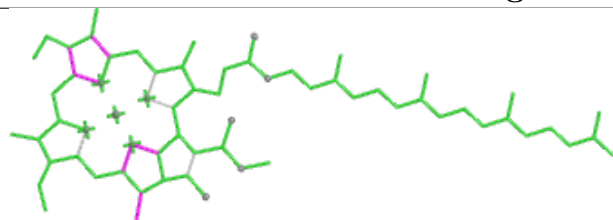


Torsions

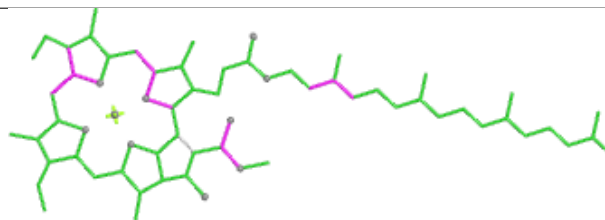


Rings

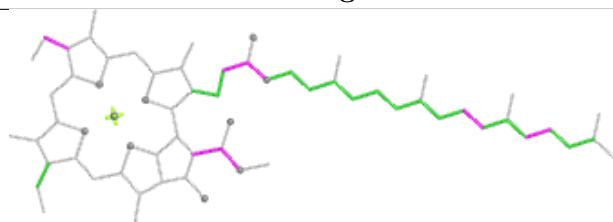
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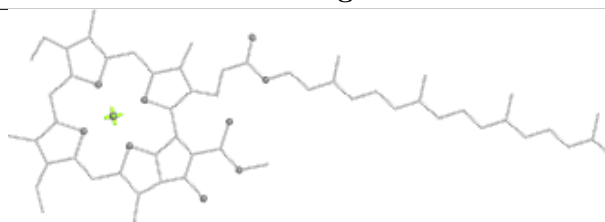
Bond lengths



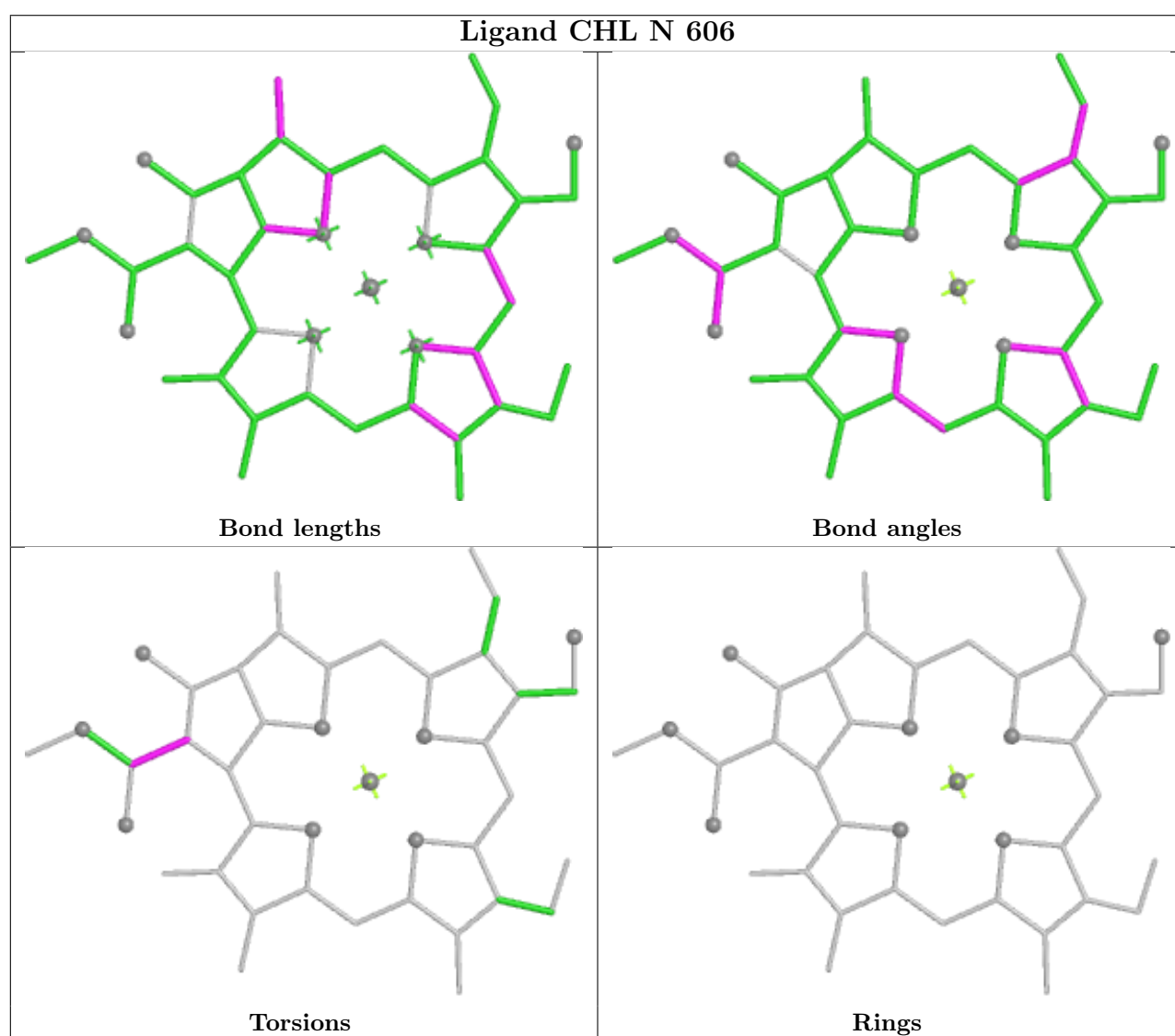
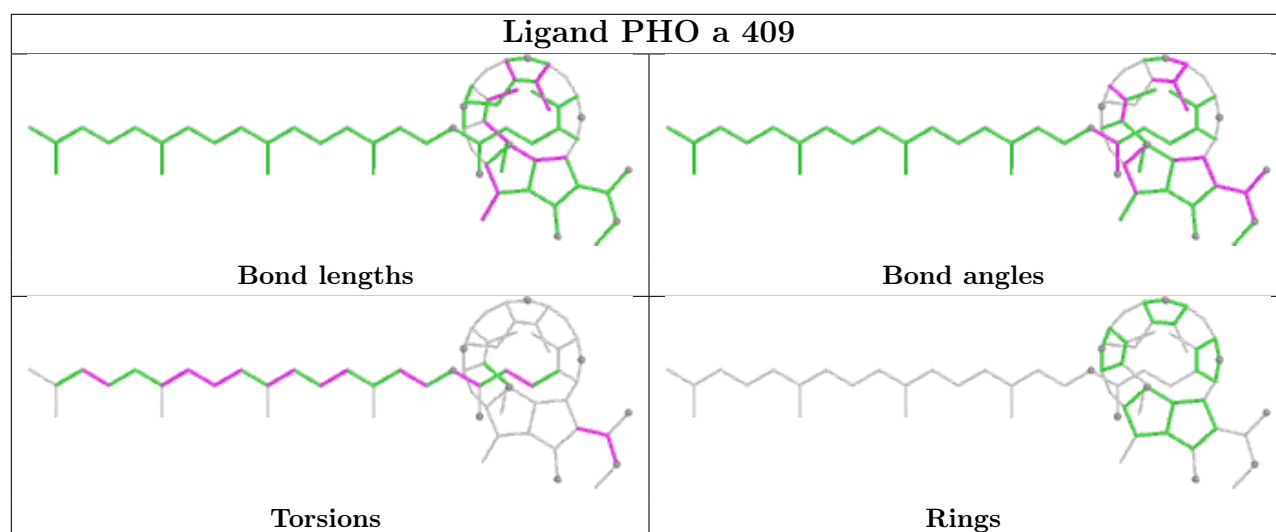
Bond angles

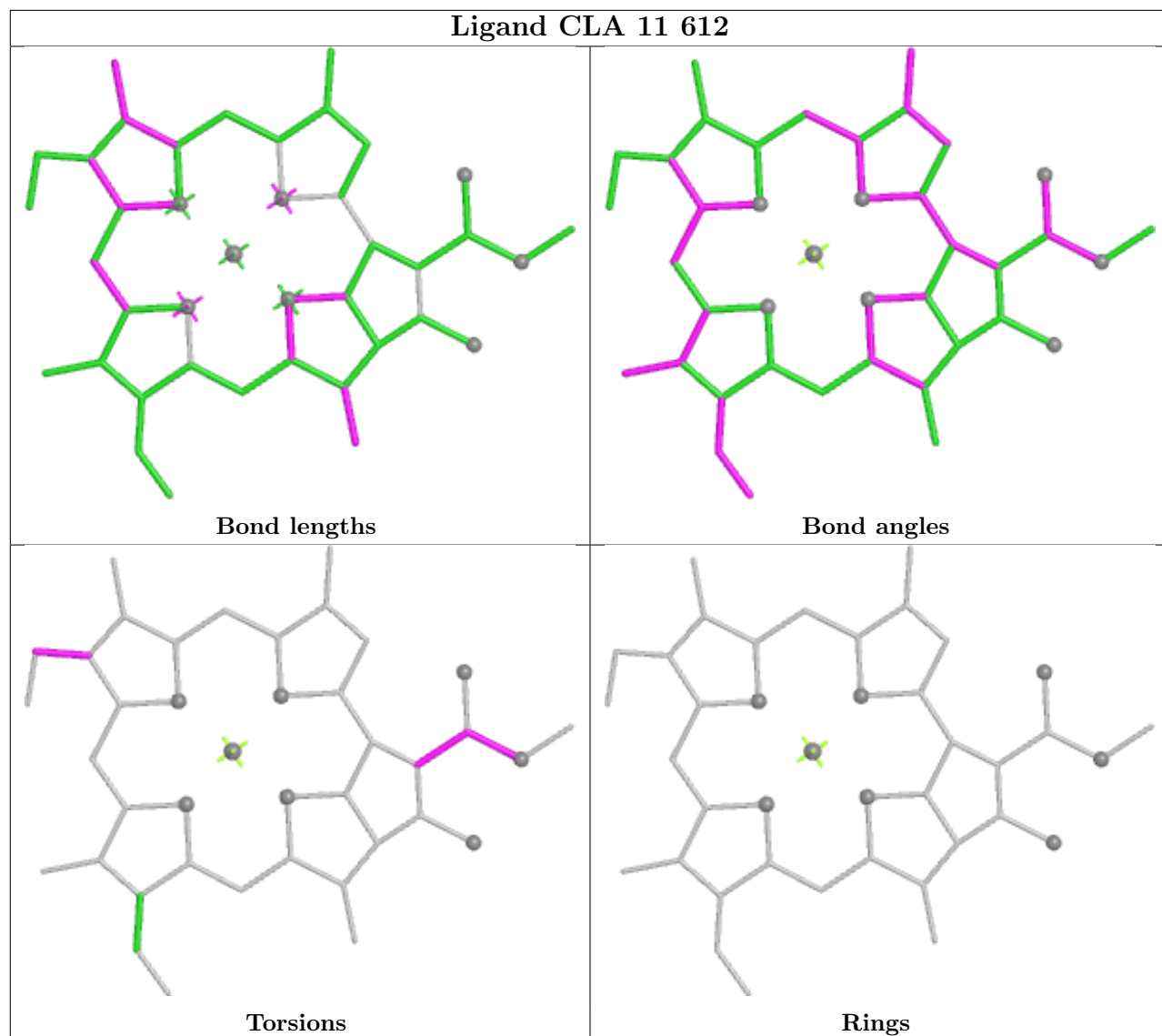


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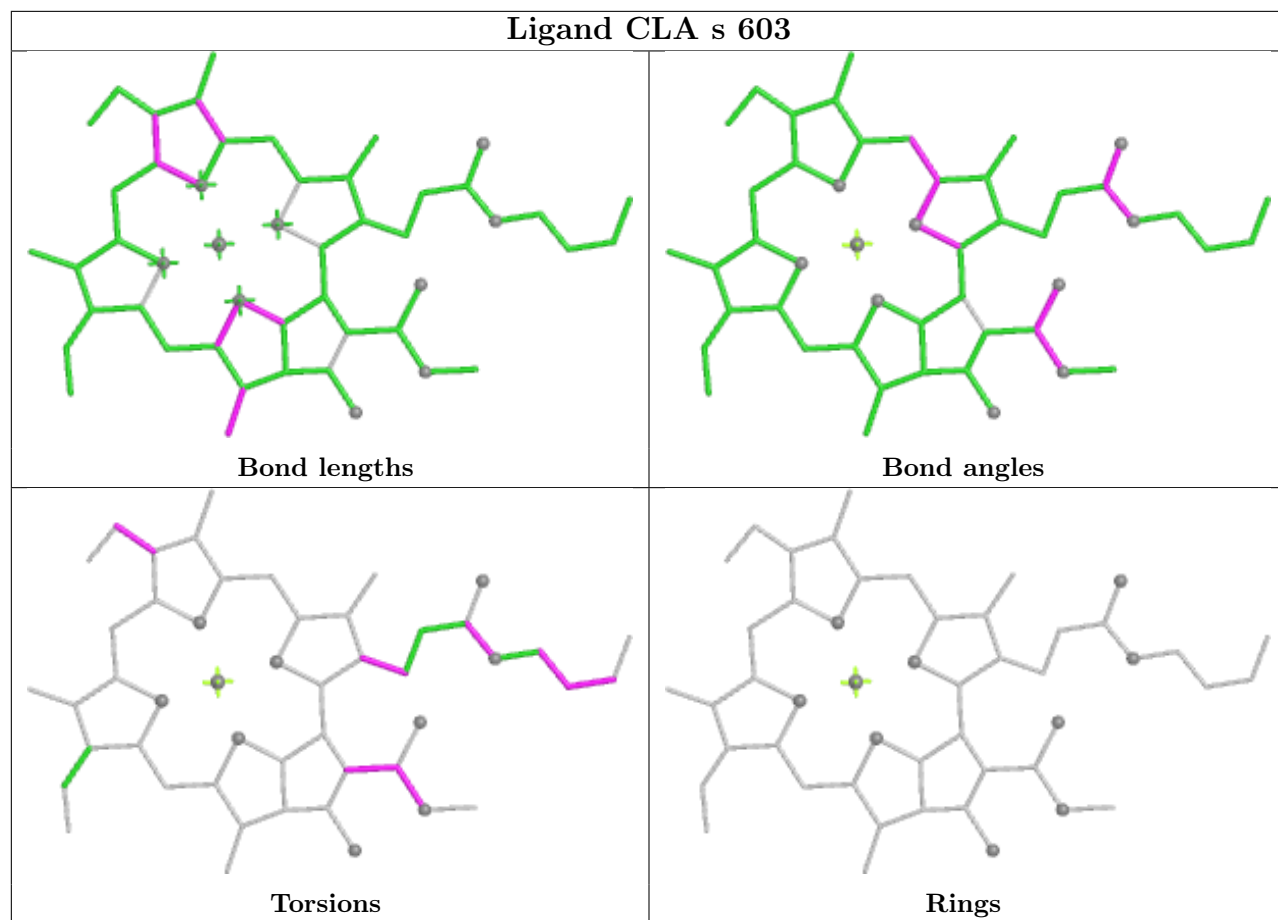


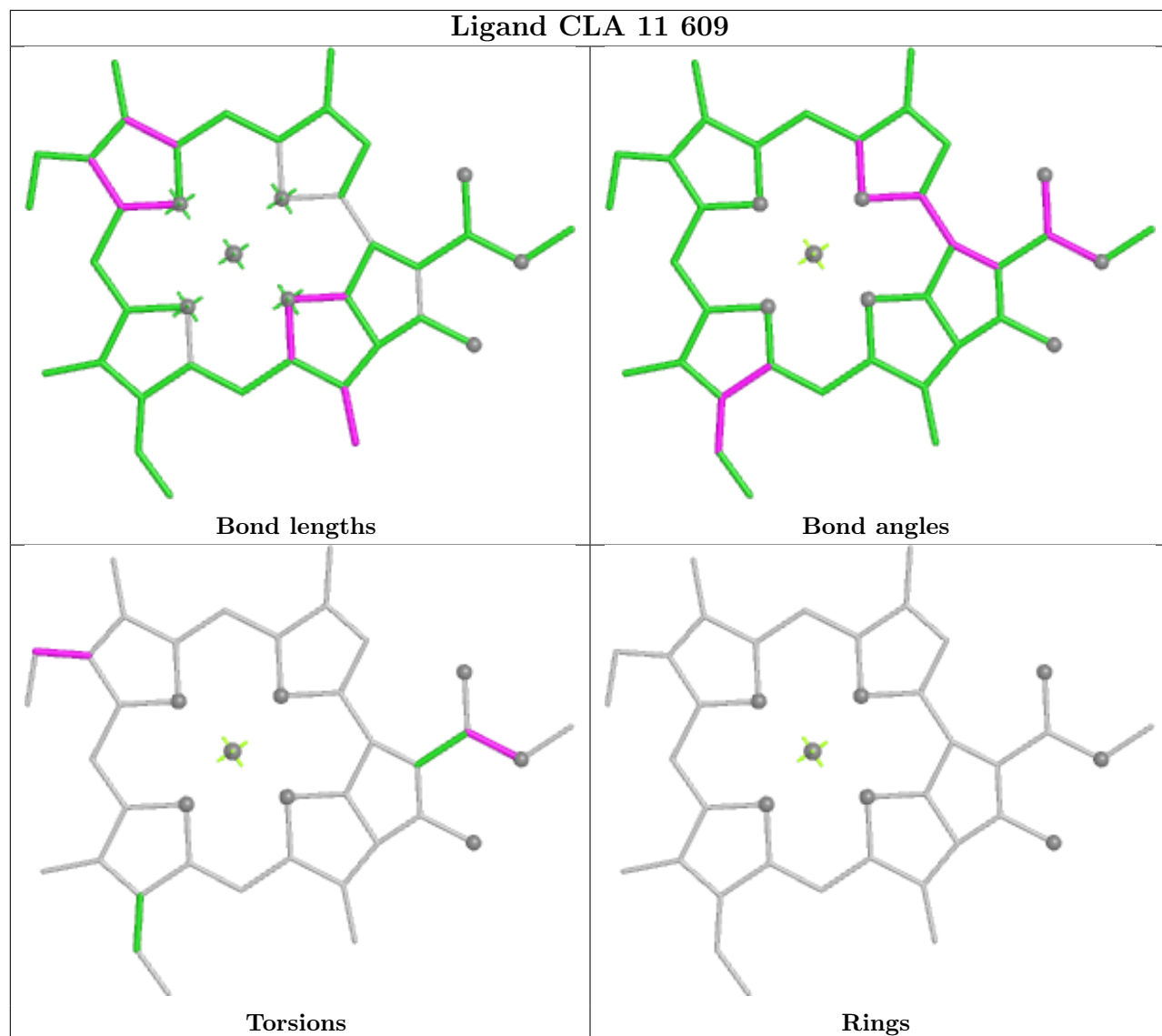
Rings



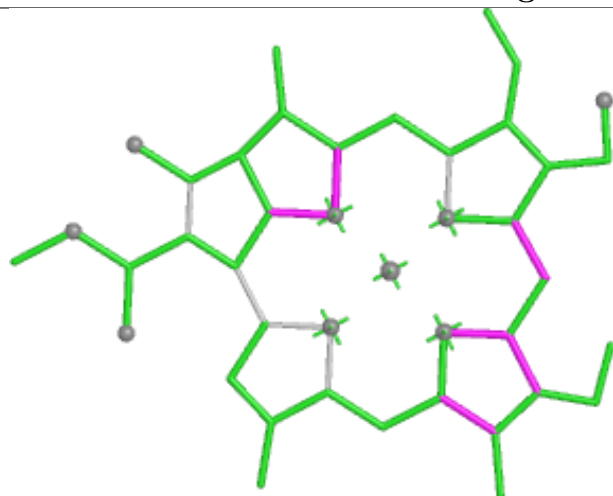


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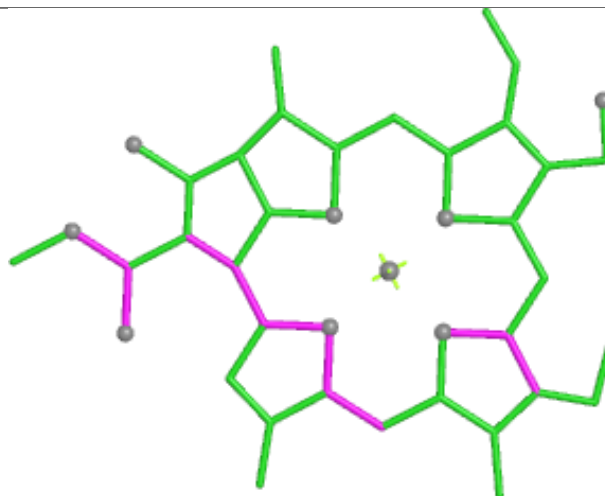




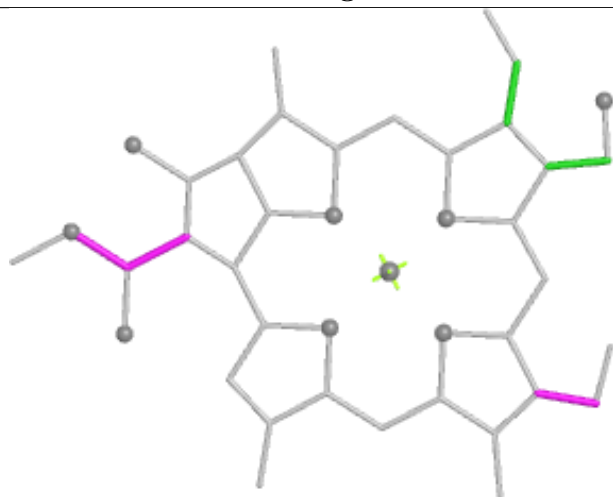
Ligand CHL 2 607



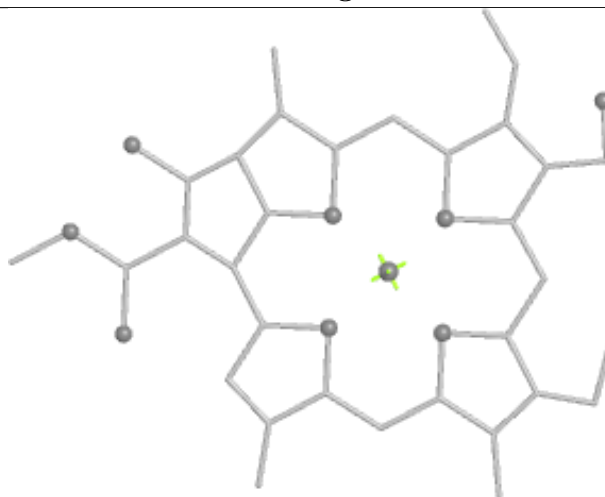
Bond lengths



Bond angles

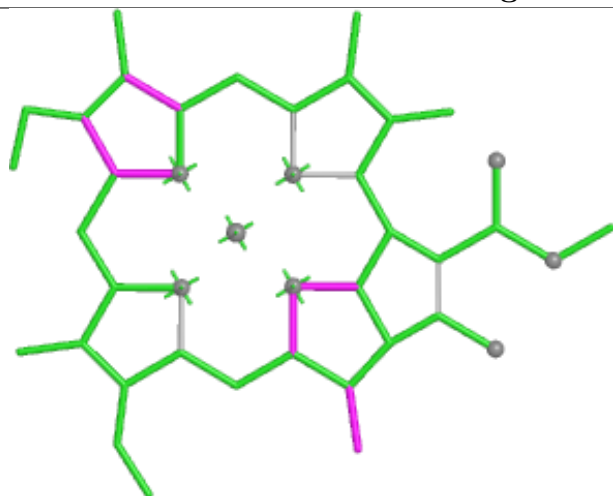


Torsions



Rings

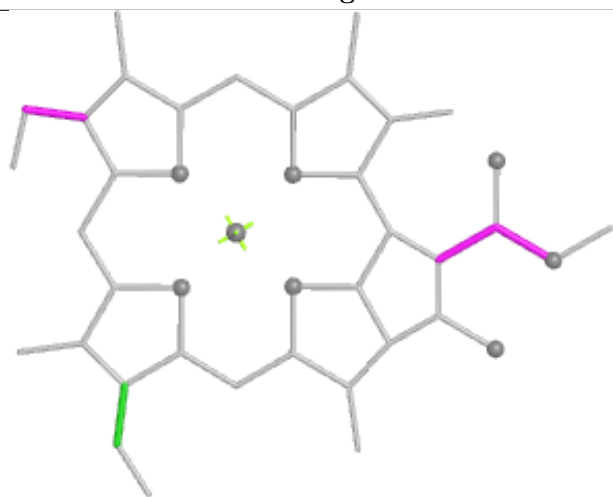
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Bond lengths



Bond angles

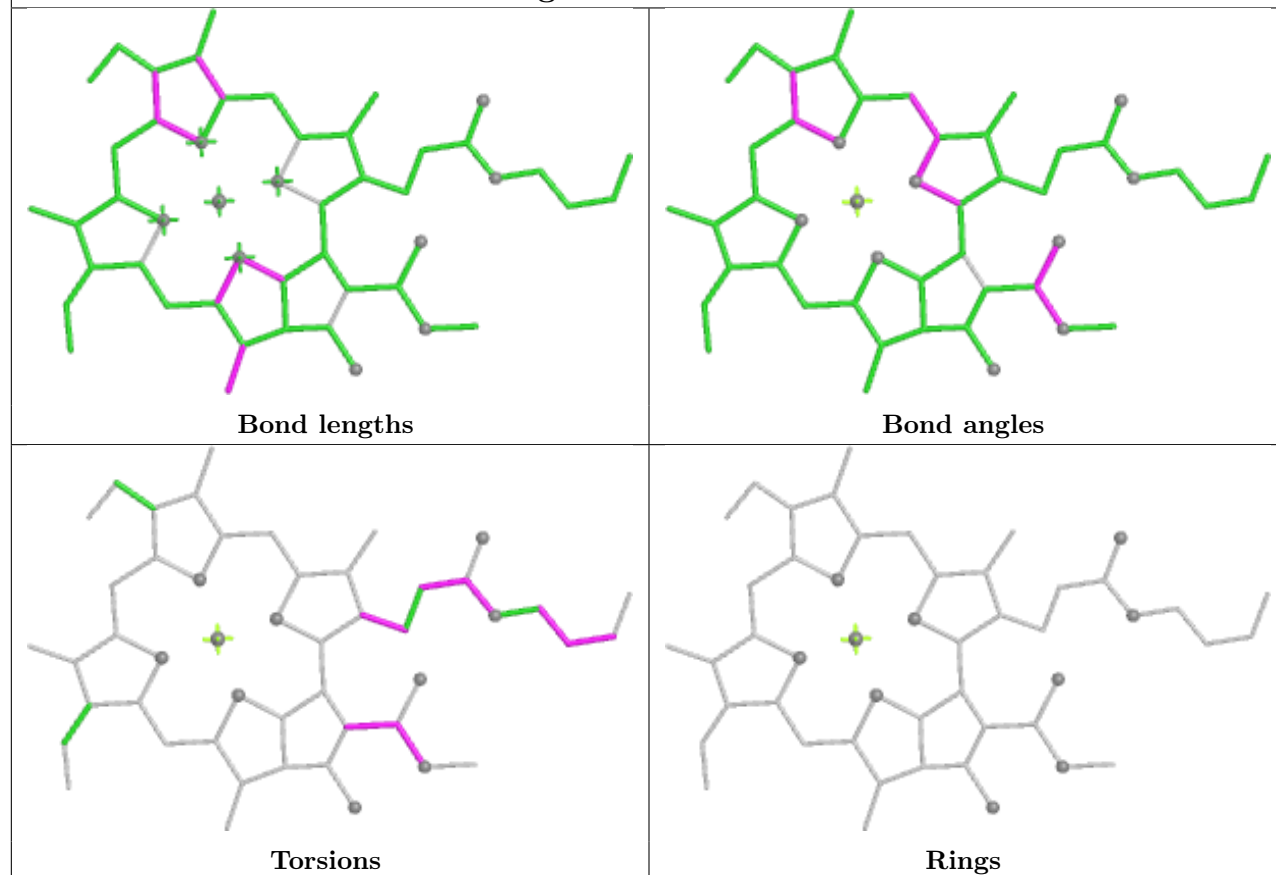


Torsions

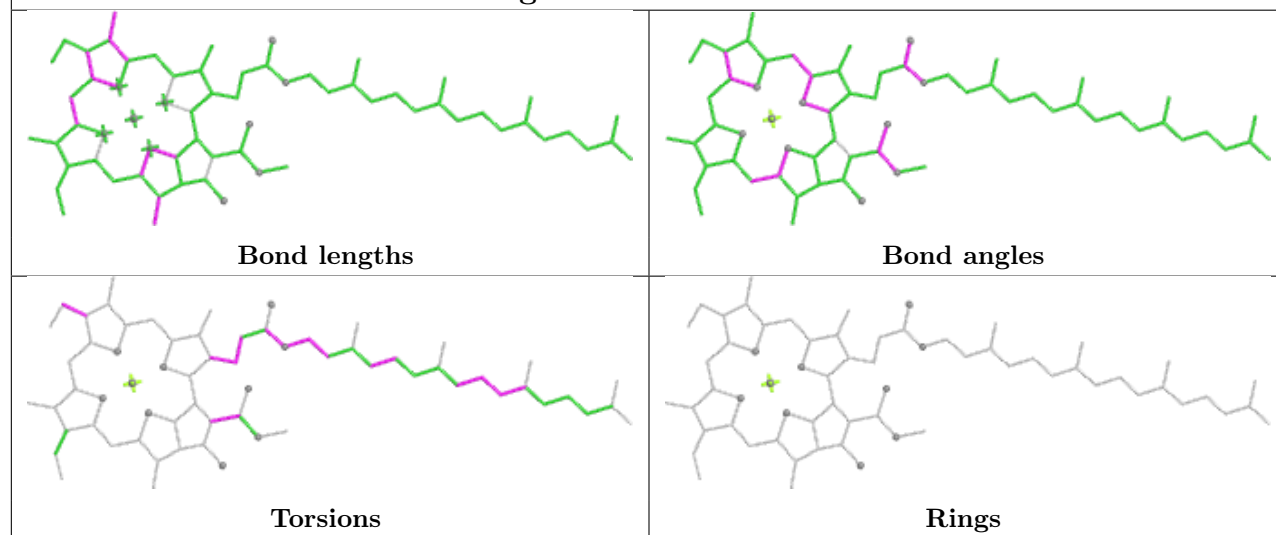


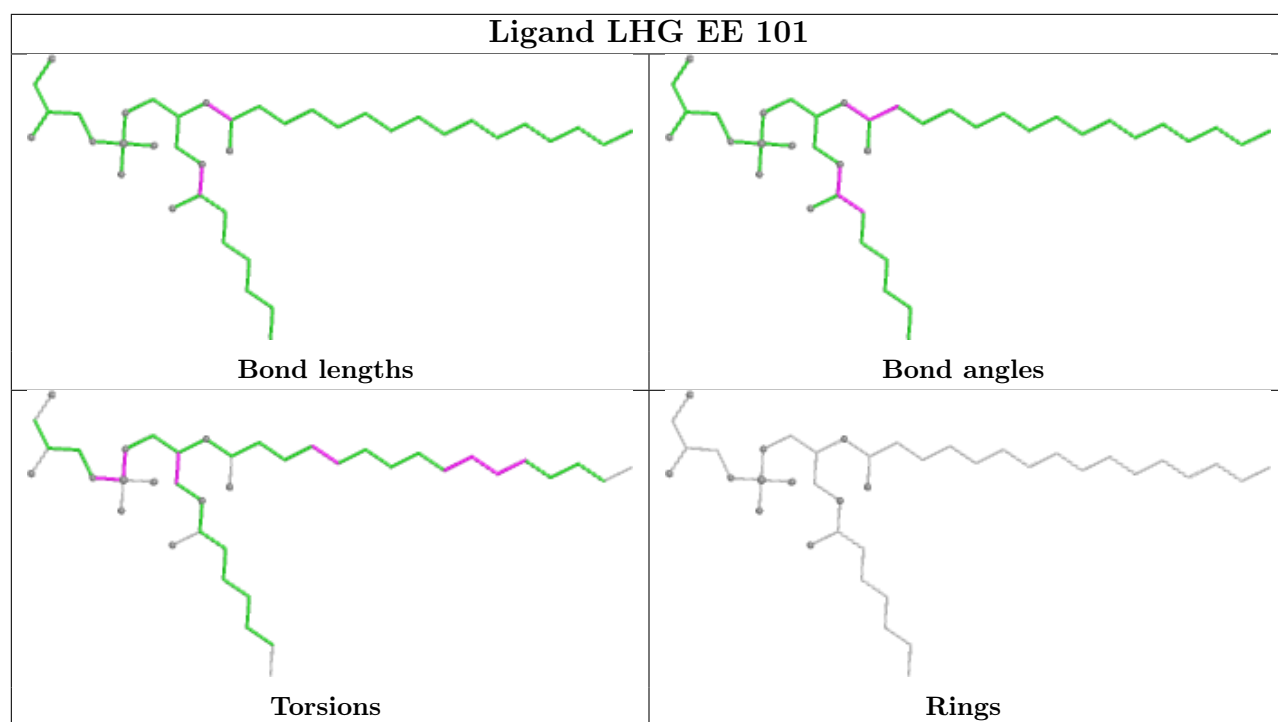
Rings

Ligand CLA r 608

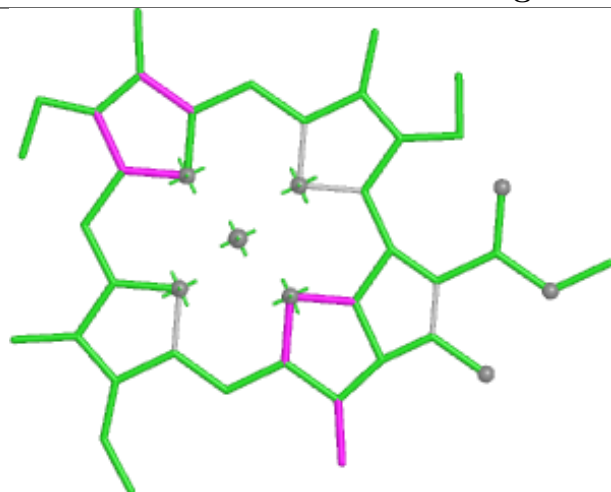


Ligand CLA CC 510

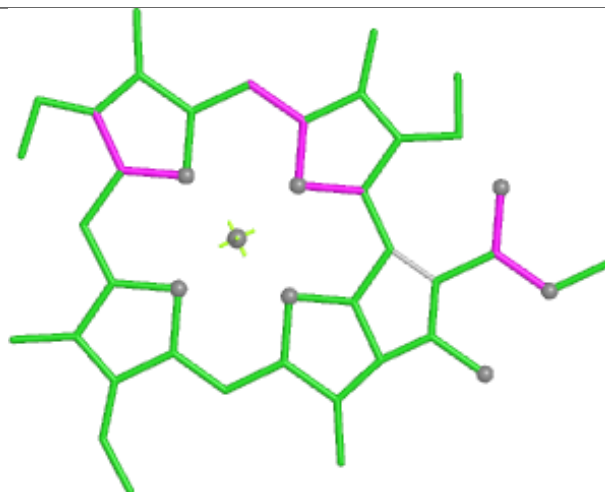




Ligand CLA Y 611



Bond lengths



Bond angles

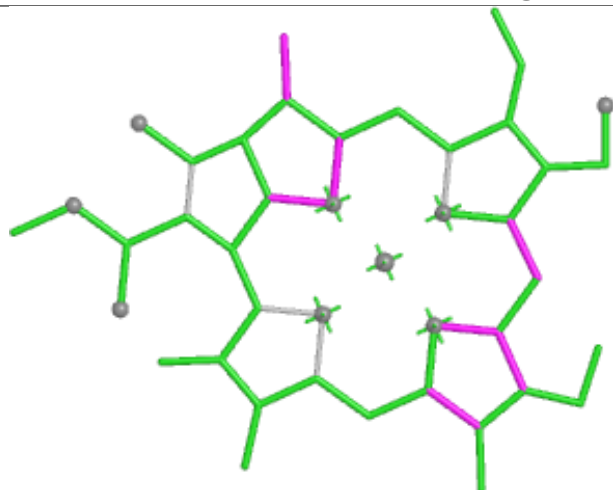


Torsions

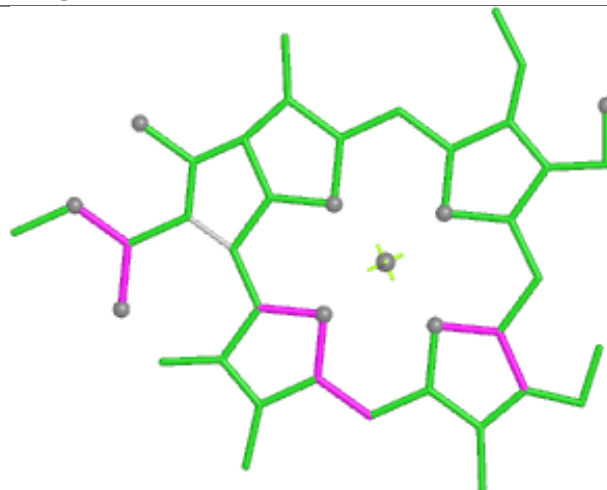


Rings

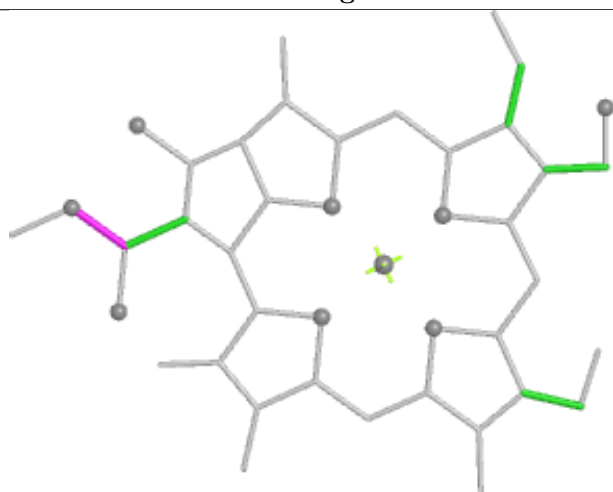
Ligand CHL g 608



Bond lengths



Bond angles

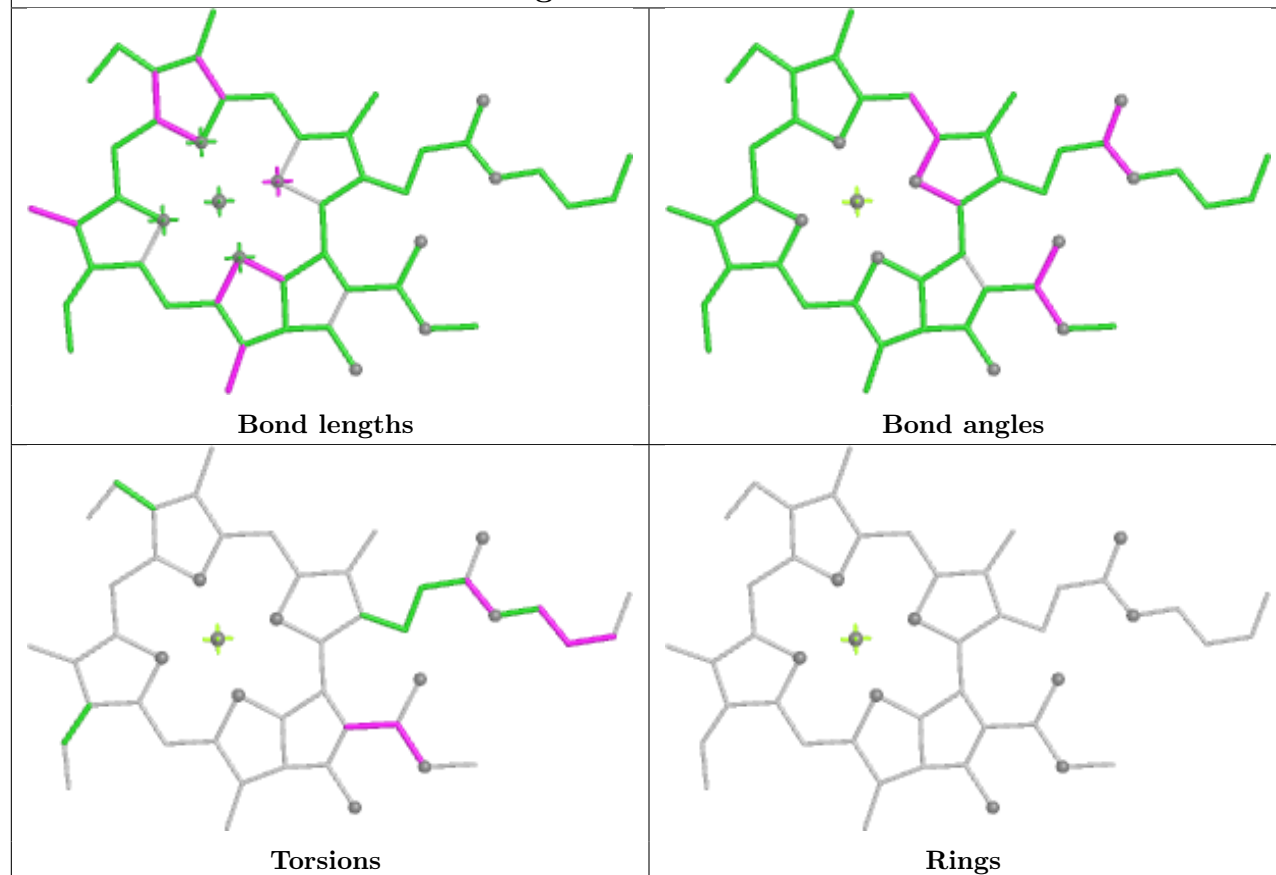


Torsions

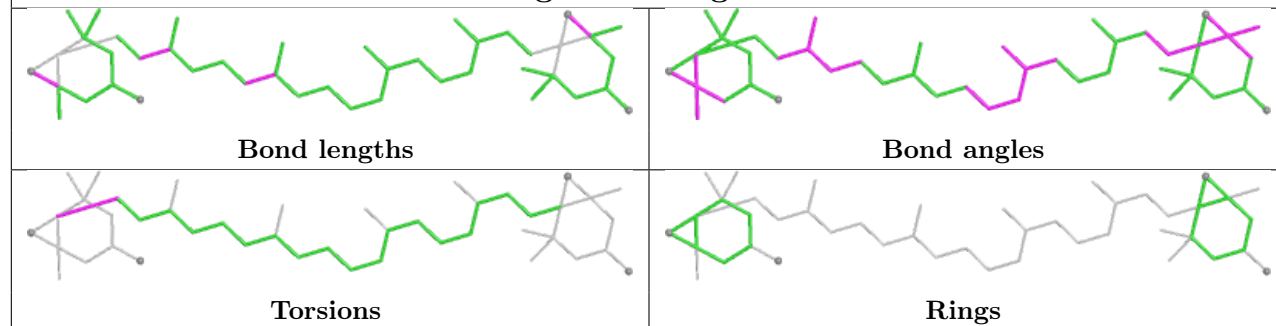


Rings

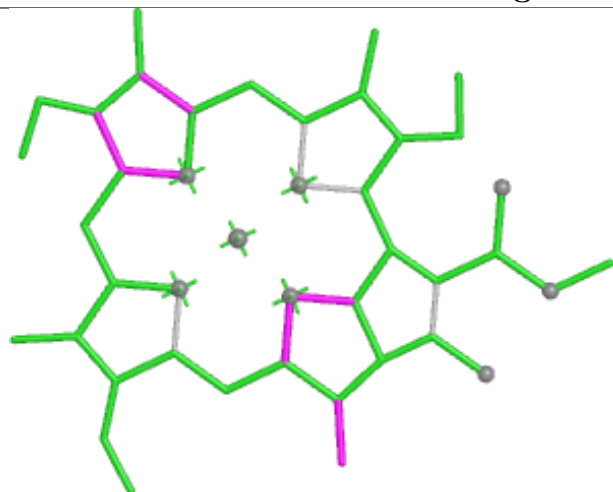
Ligand CLA n 612



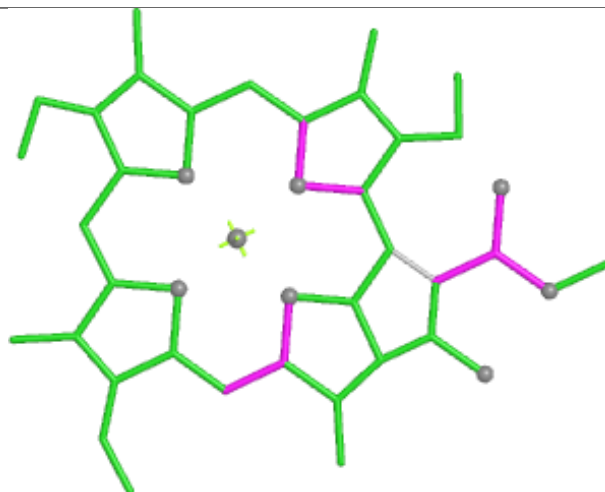
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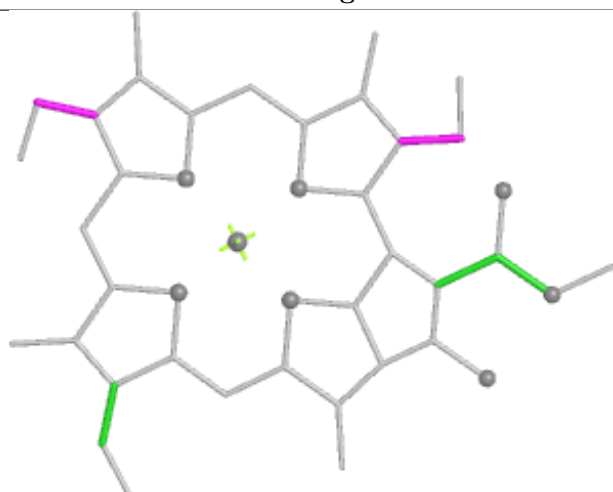
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Bond lengths



Bond angles

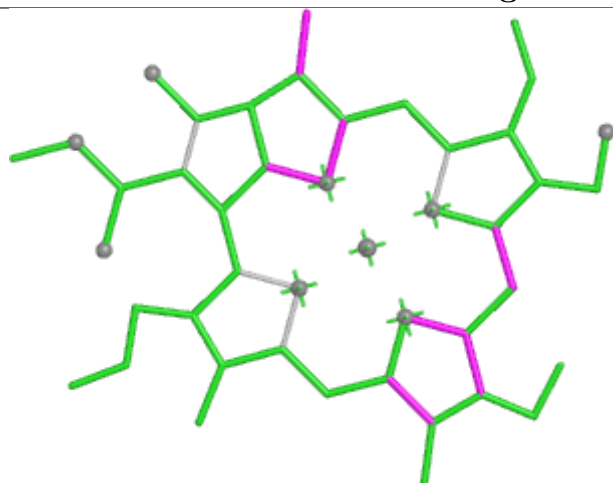


Torsions

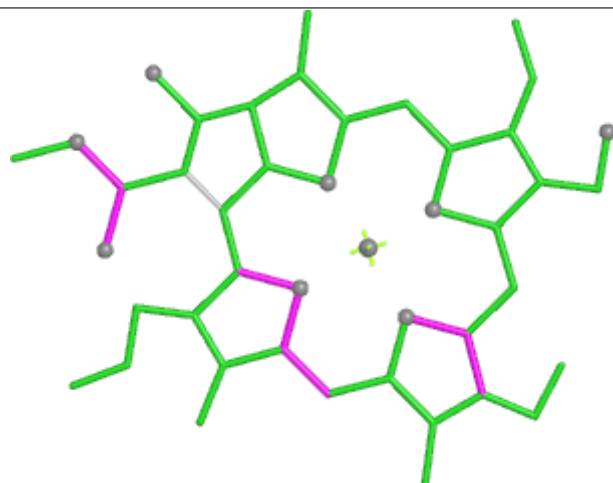


Rings

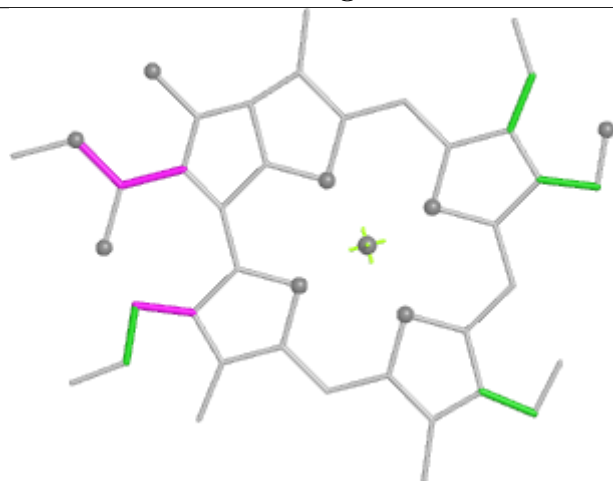
Ligand CHL YY 606



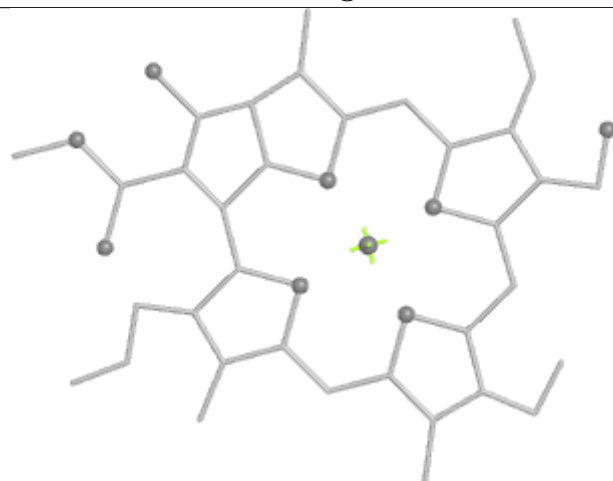
Bond lengths



Bond angles

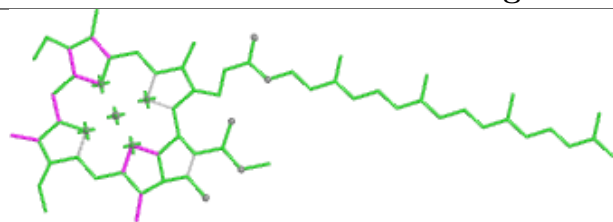


Torsions

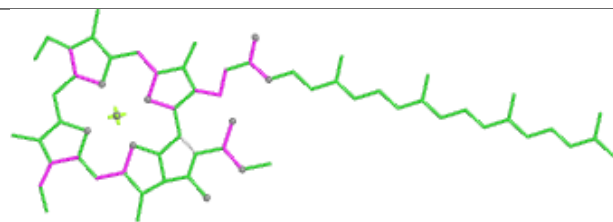


Rings

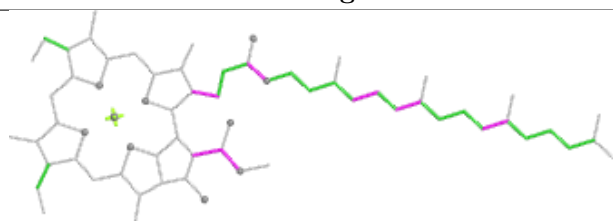
Ligand CLA Nn 301



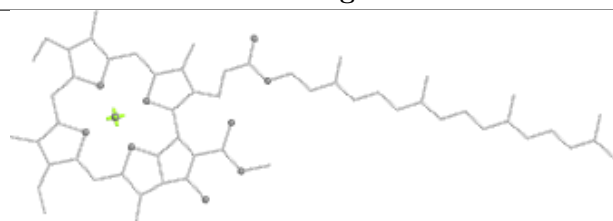
Bond lengths



Bond angles

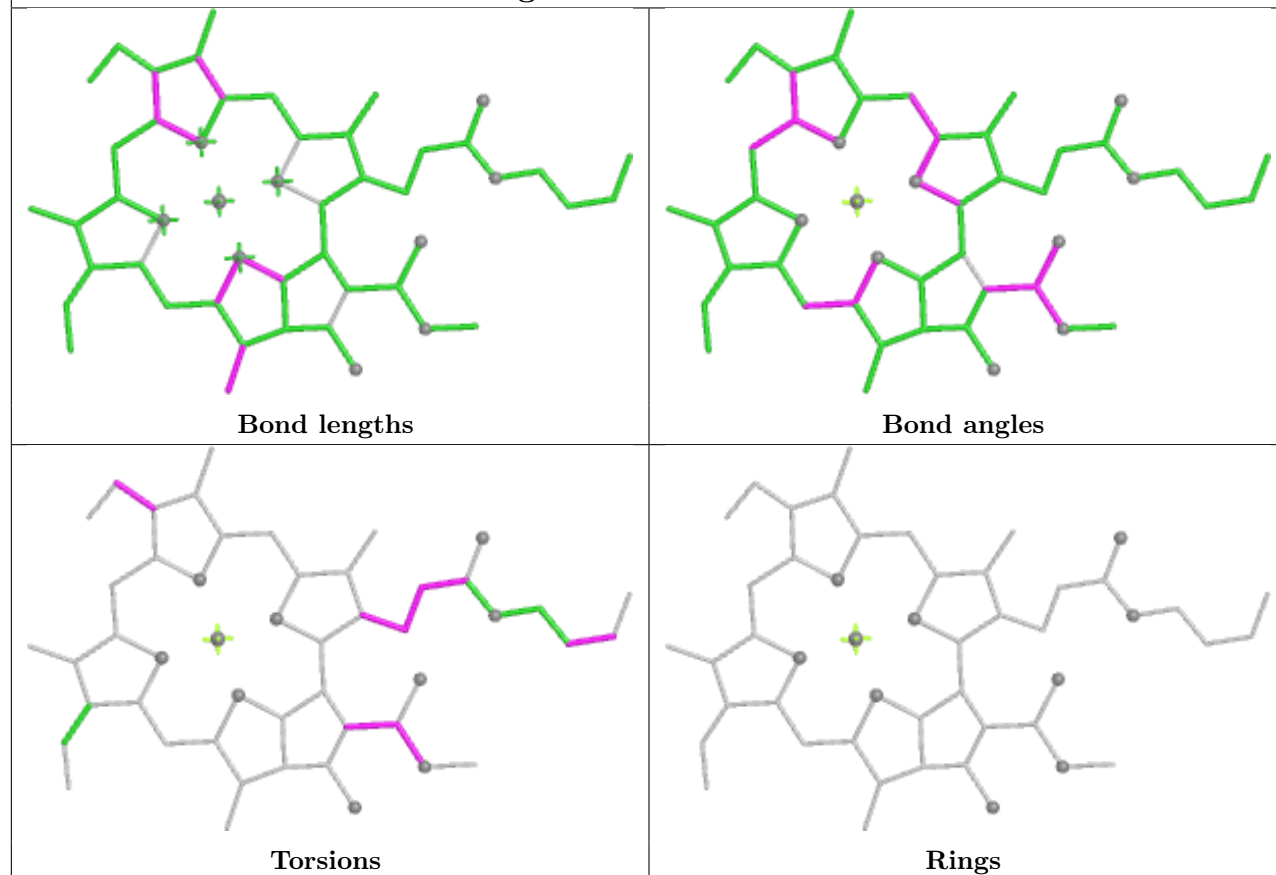


Torsions

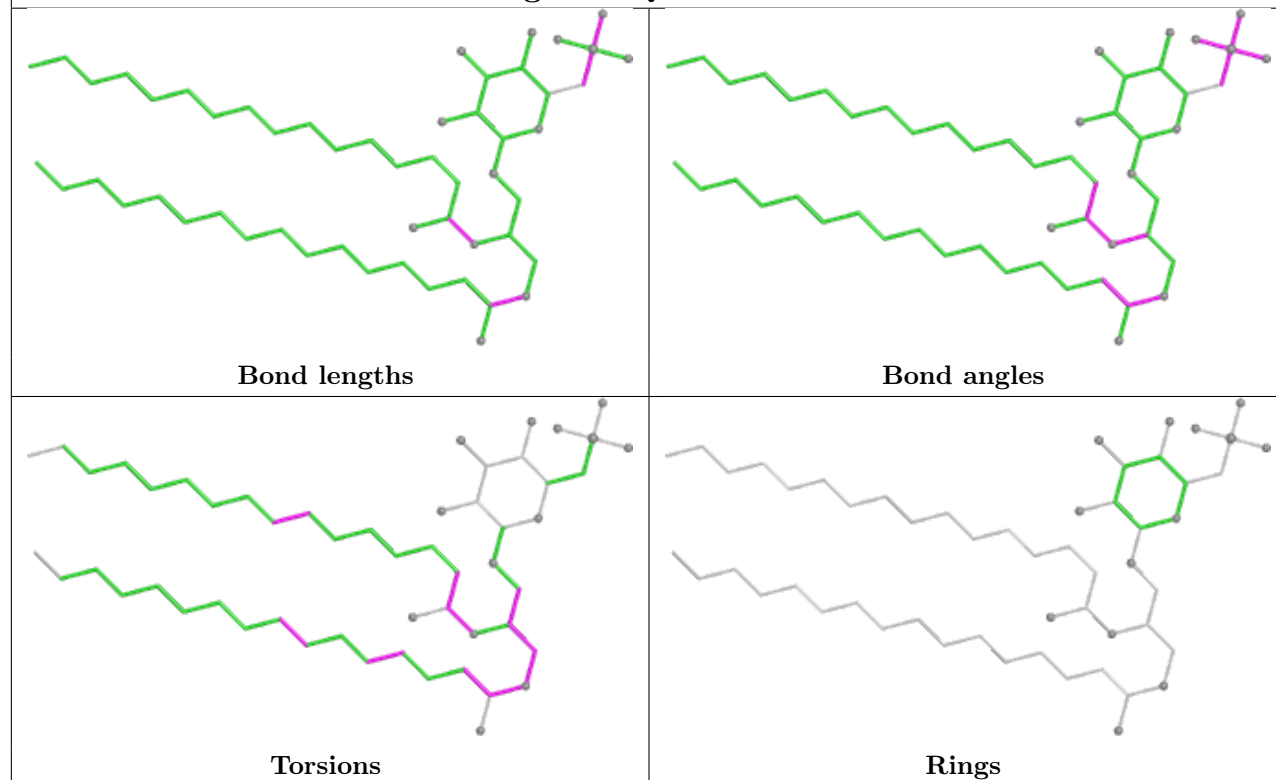


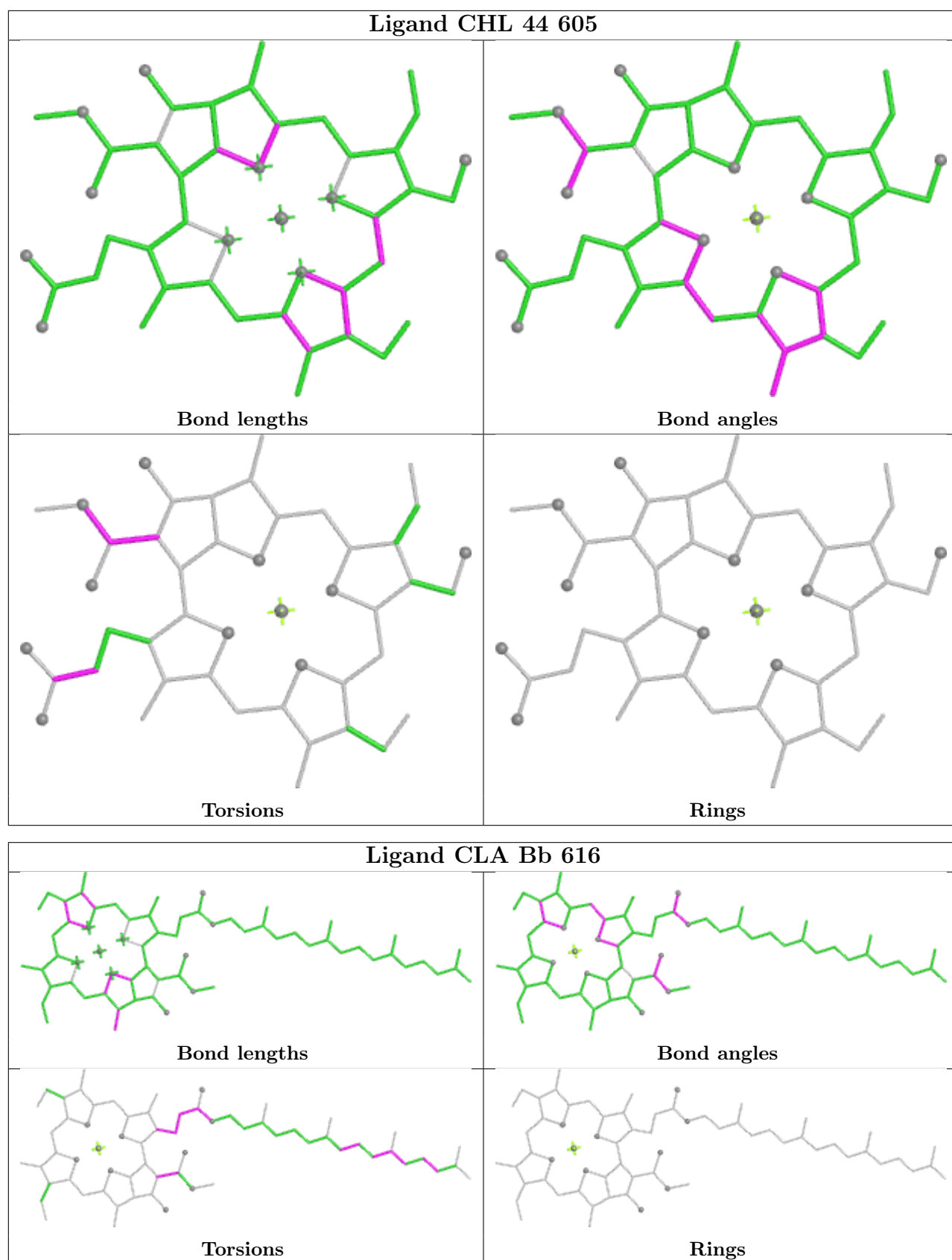
Rings

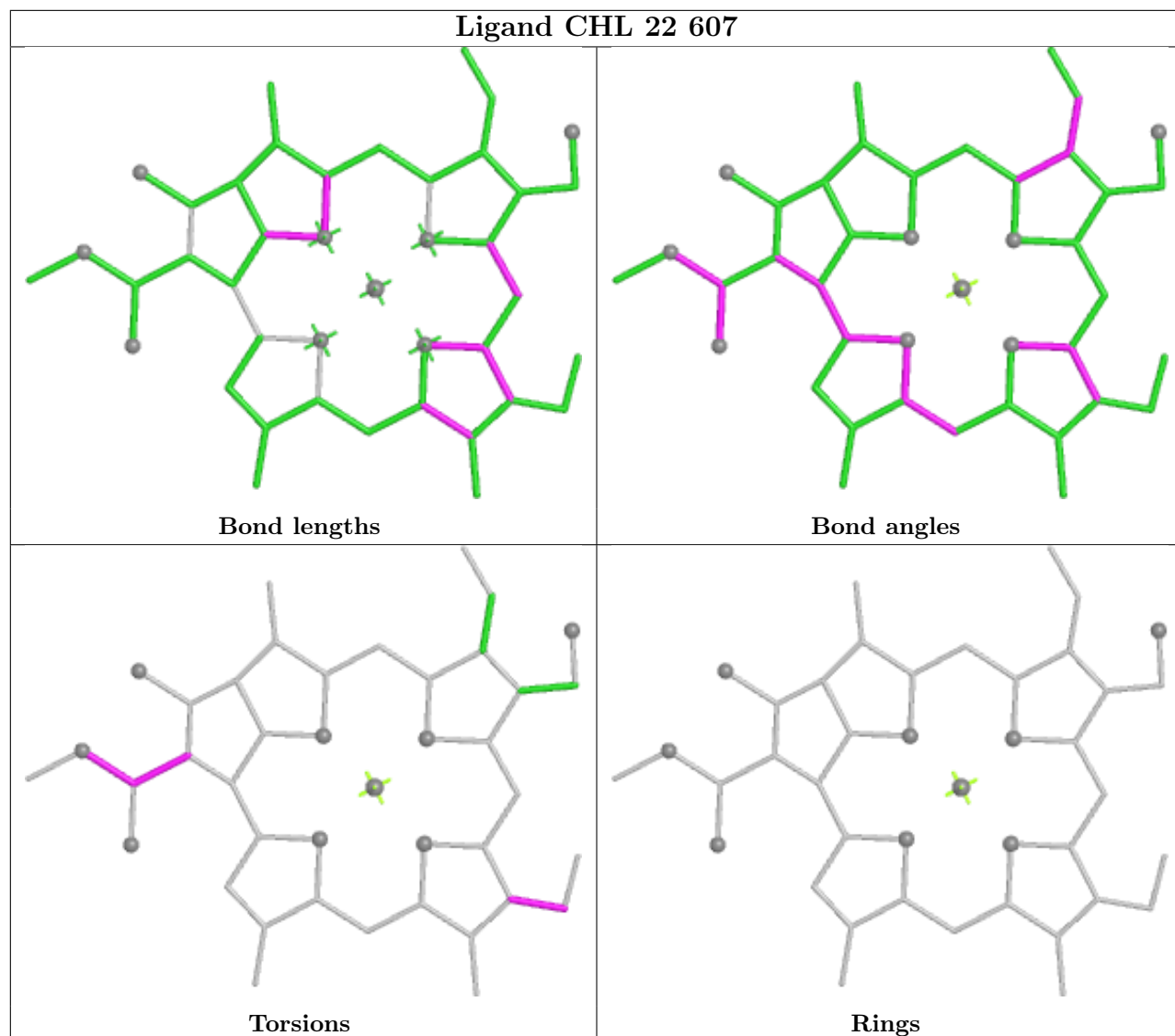
Ligand CLA YY 604



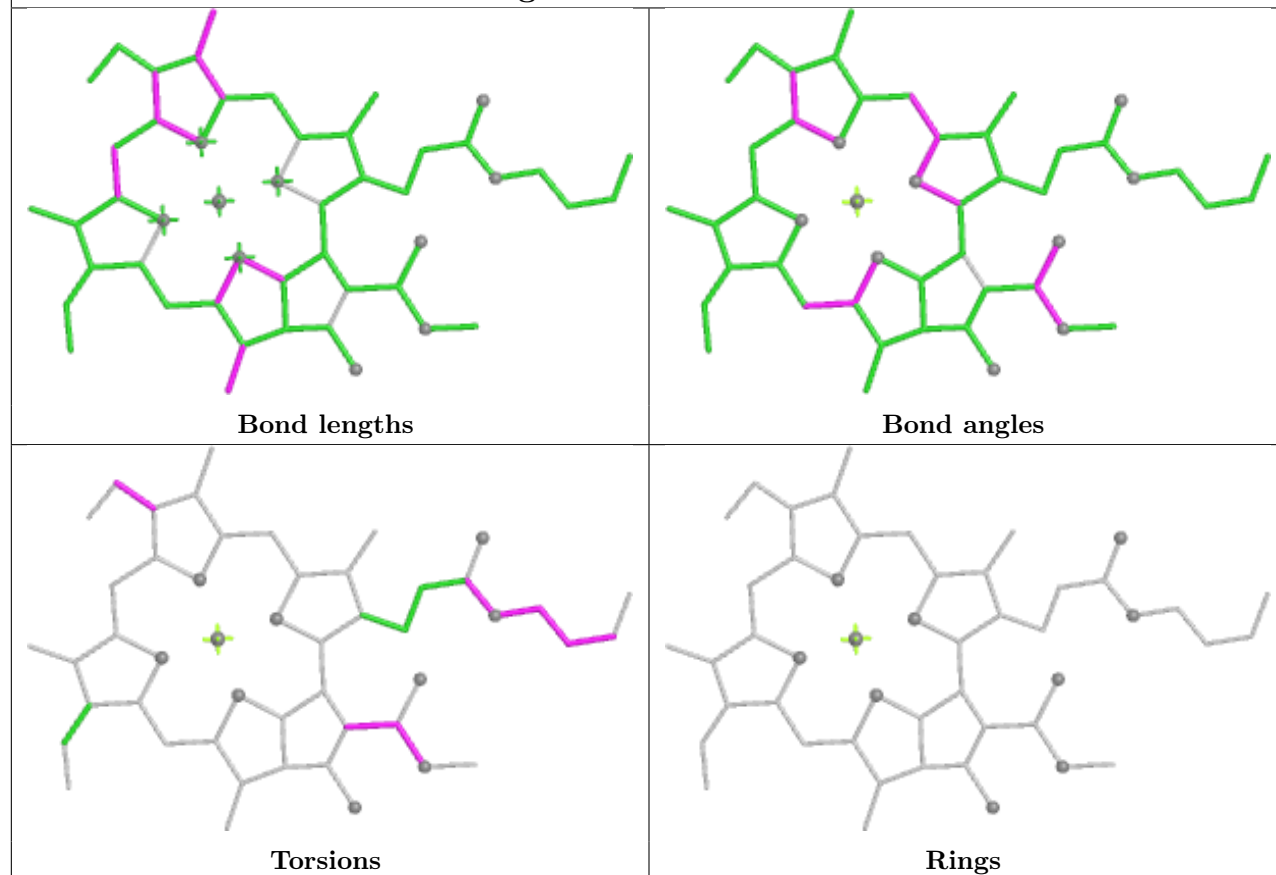
Ligand SQD LL 102



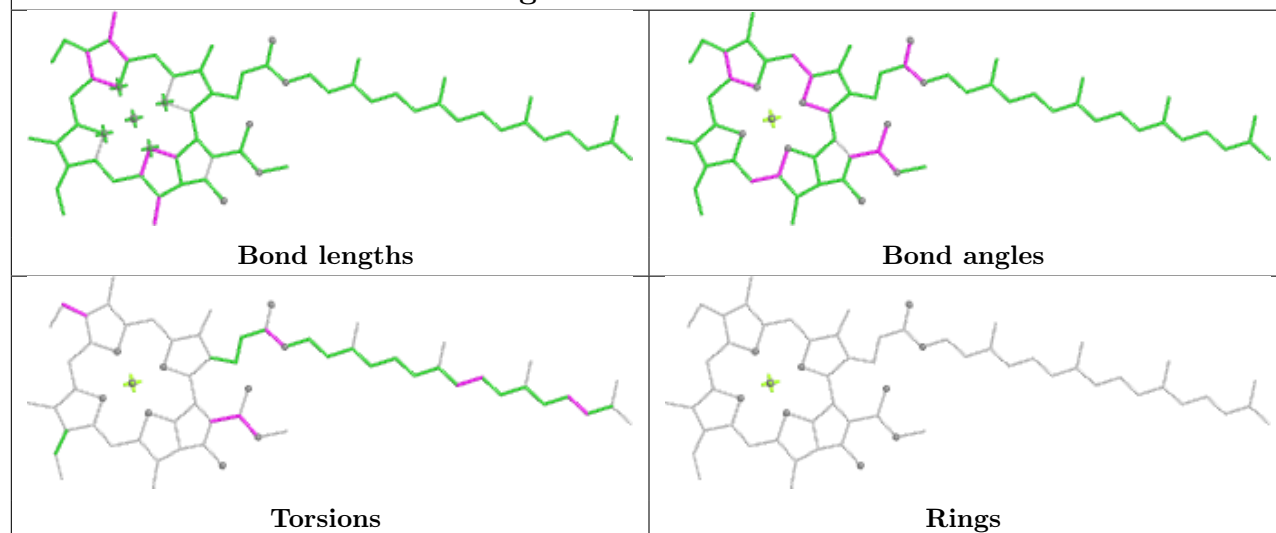


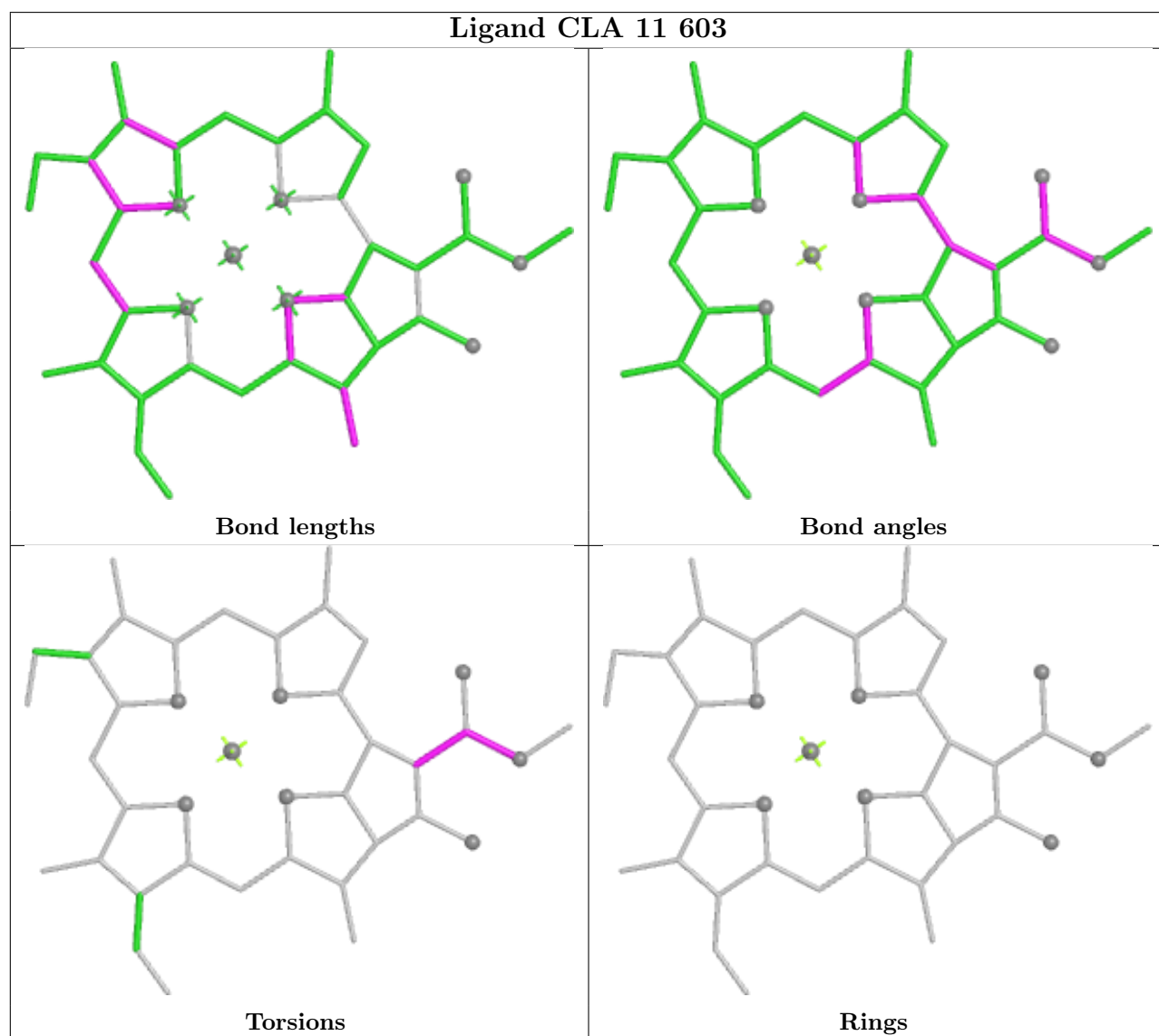
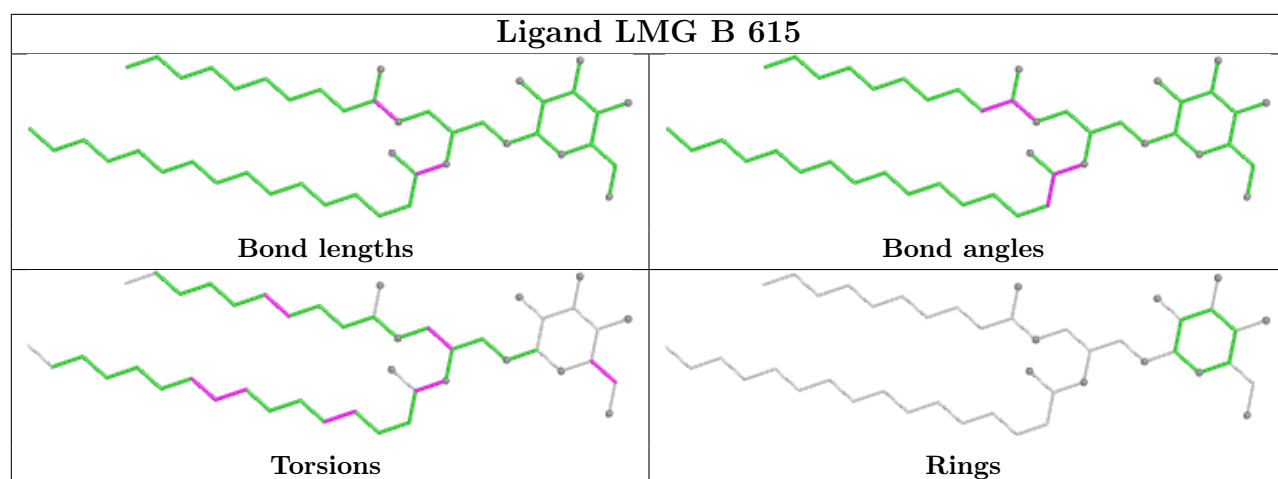


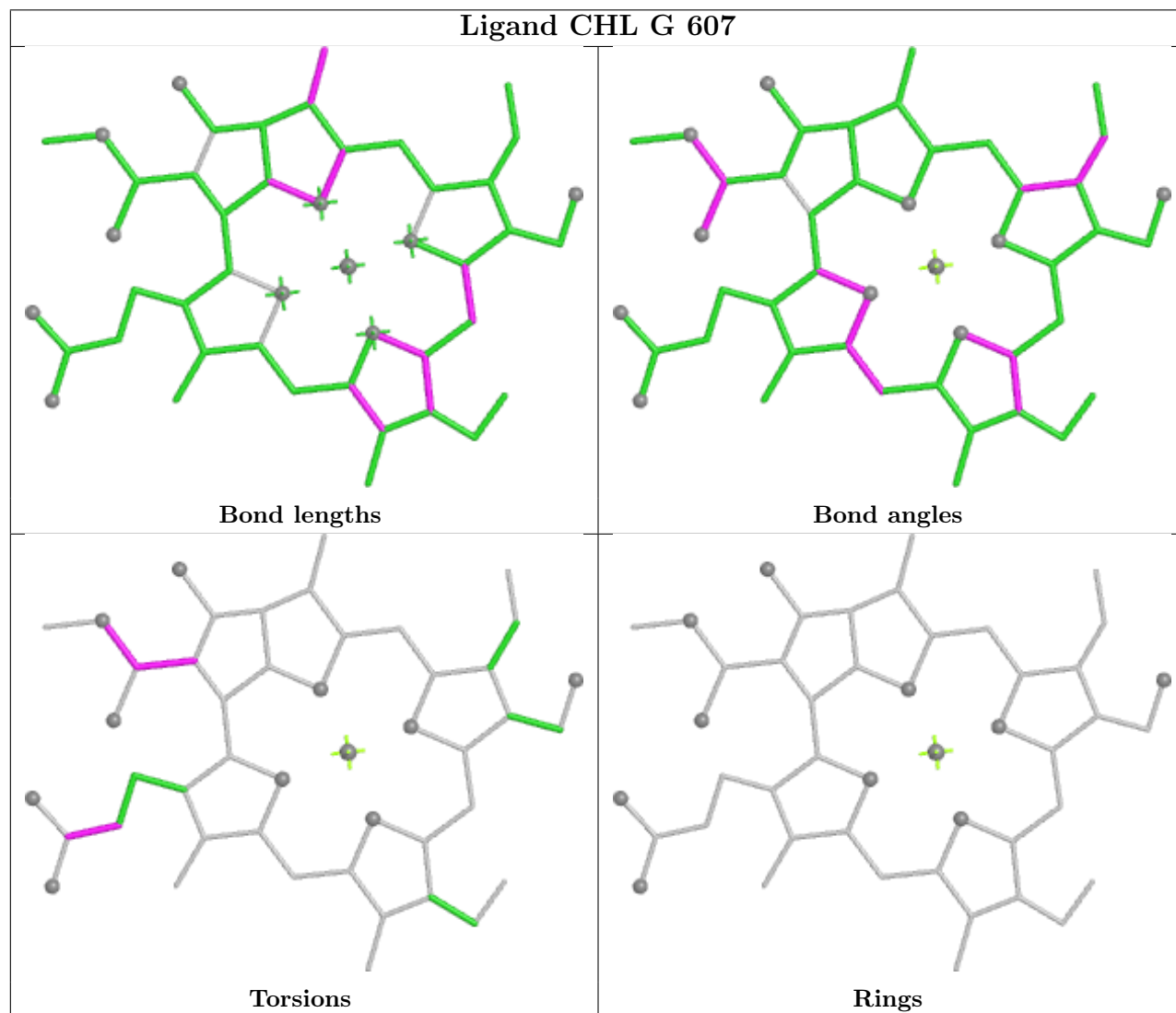
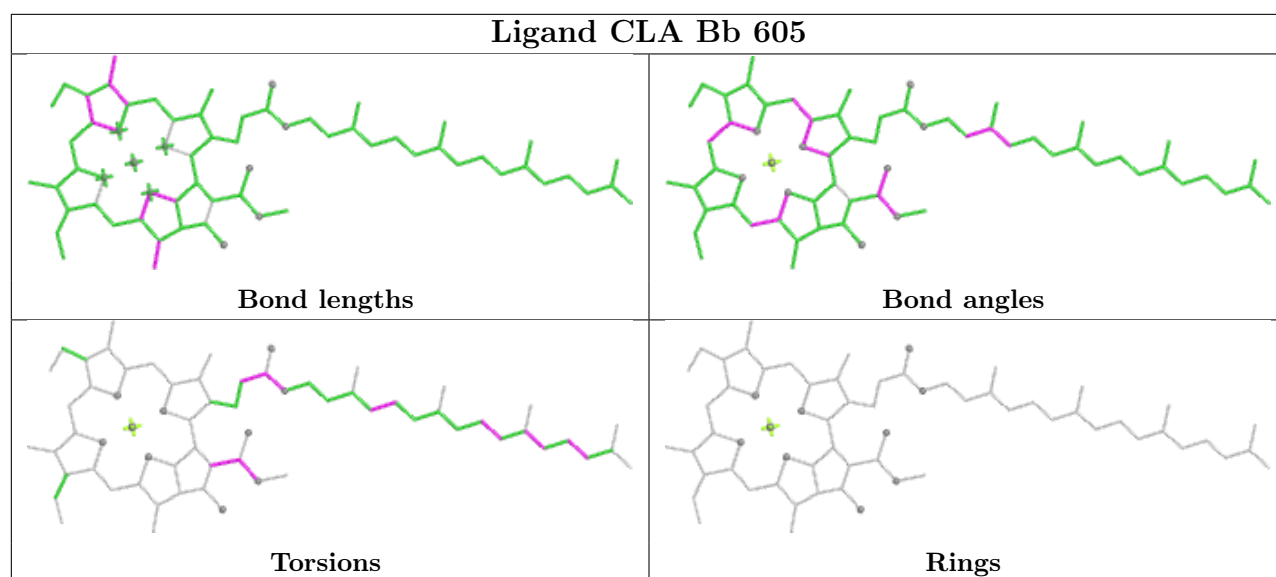
Ligand CLA RR 308

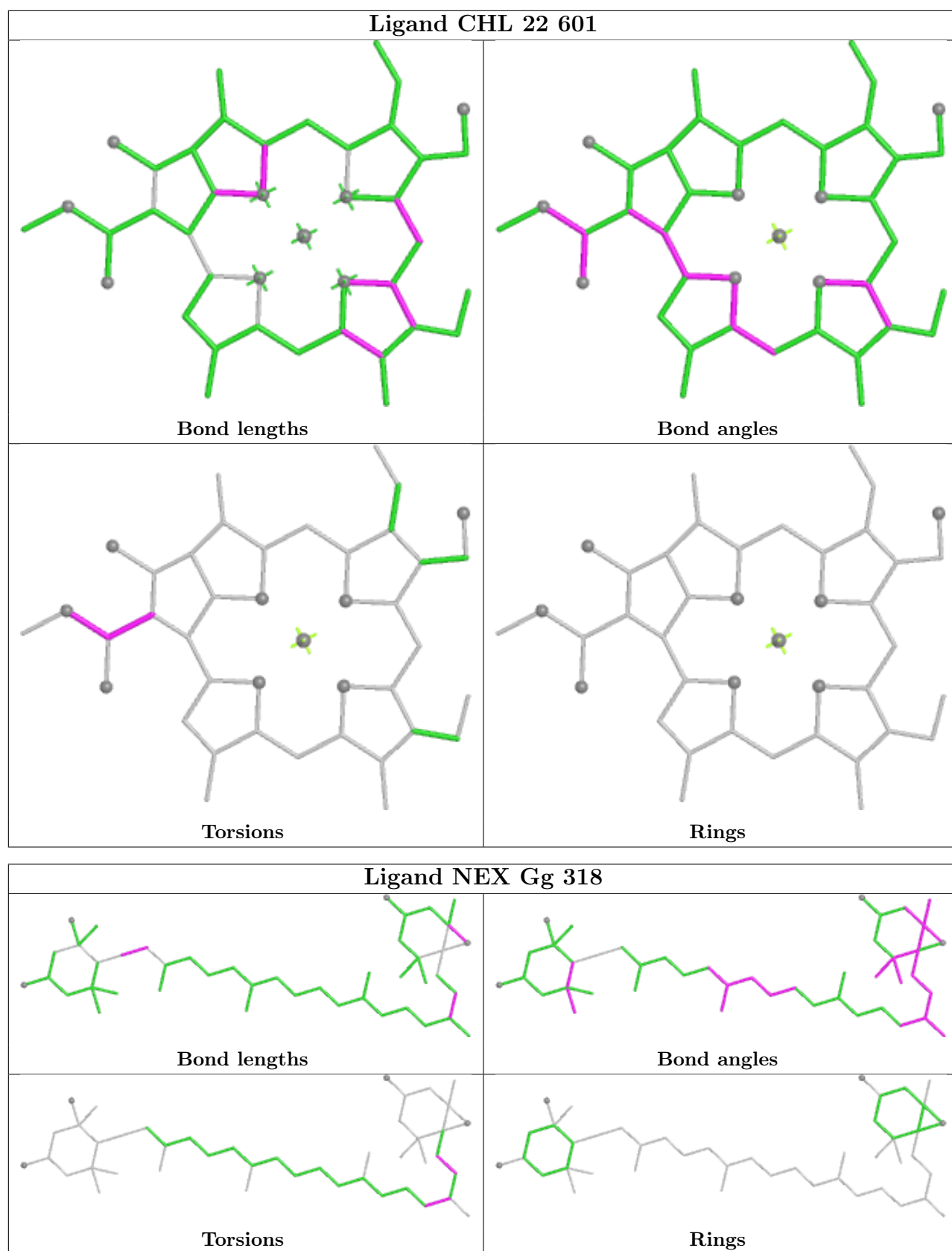


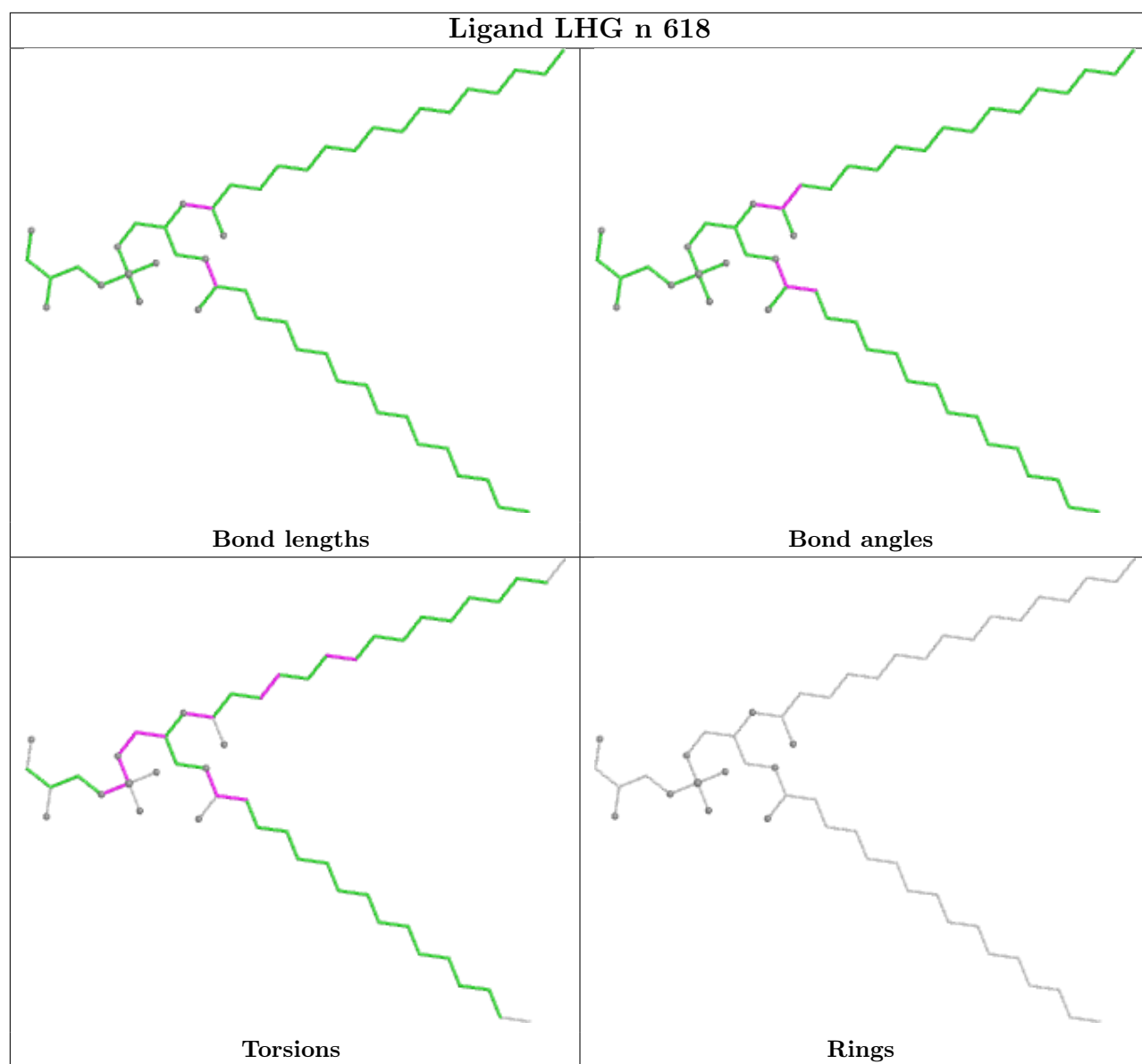
Ligand CLA CC 505

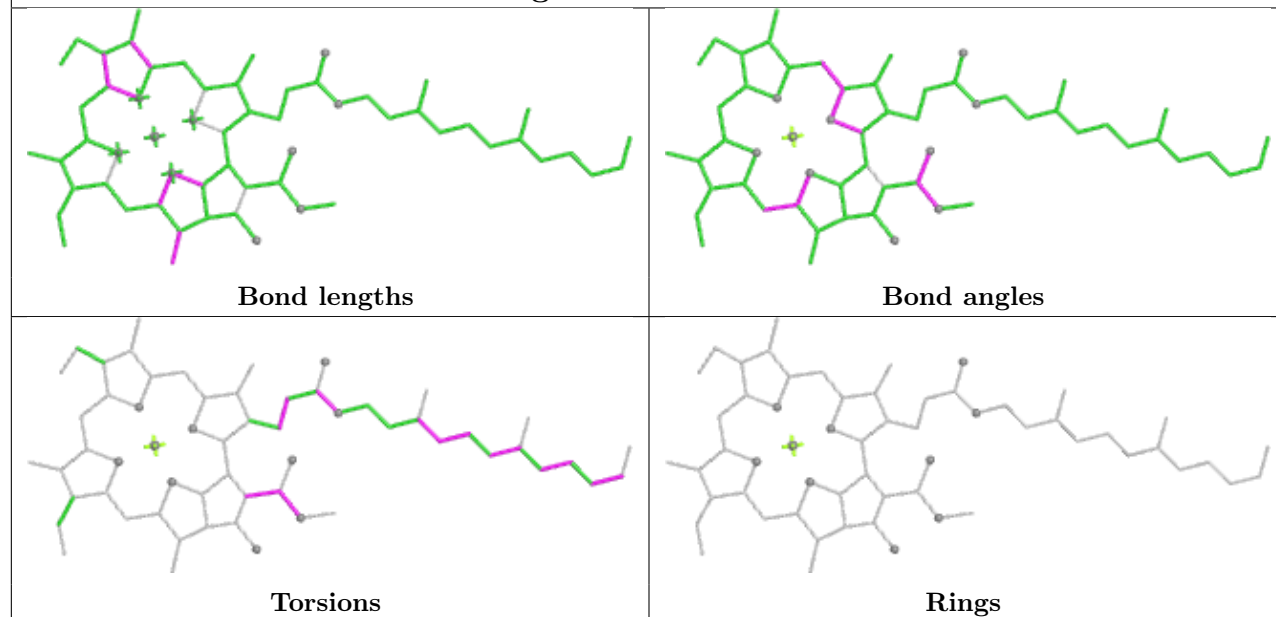
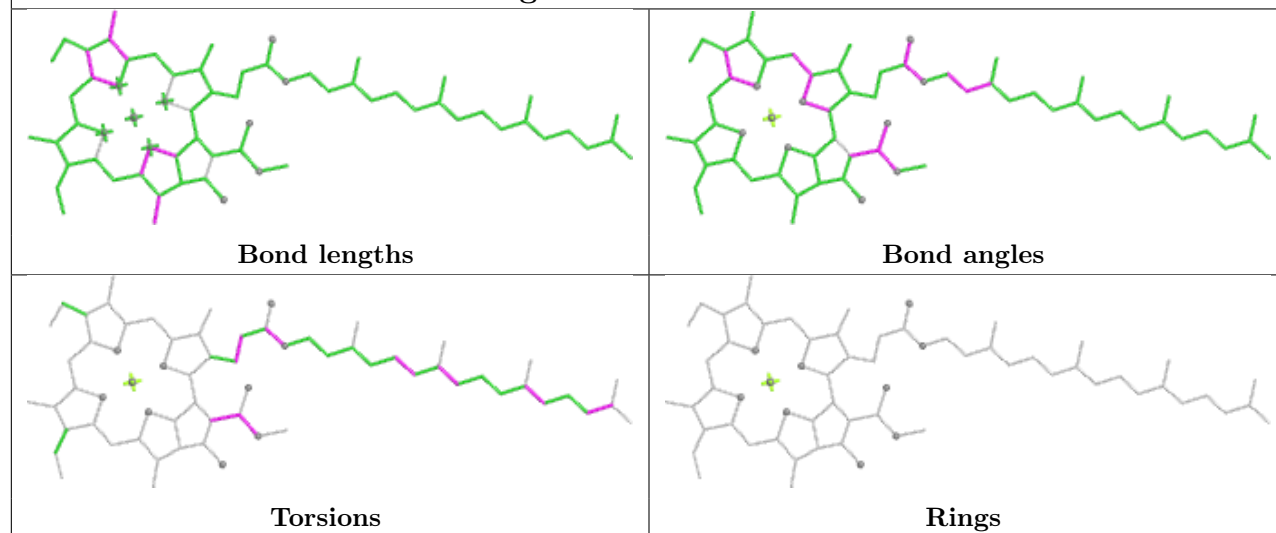




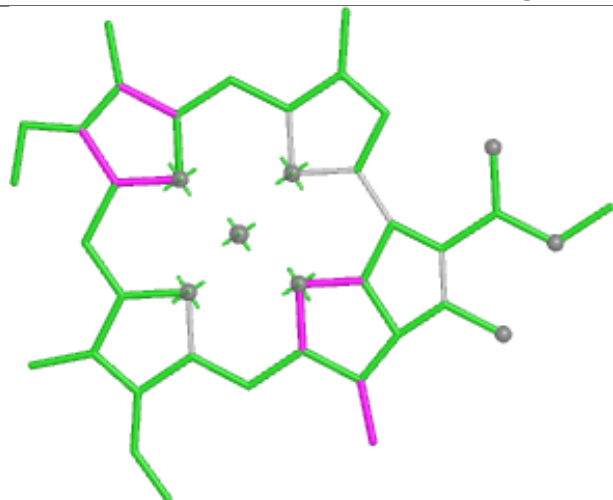




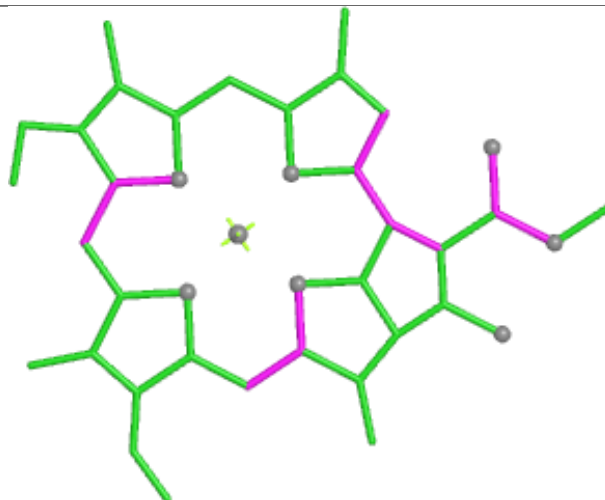


Ligand CLA Y 613**Ligand CLA BB 605**

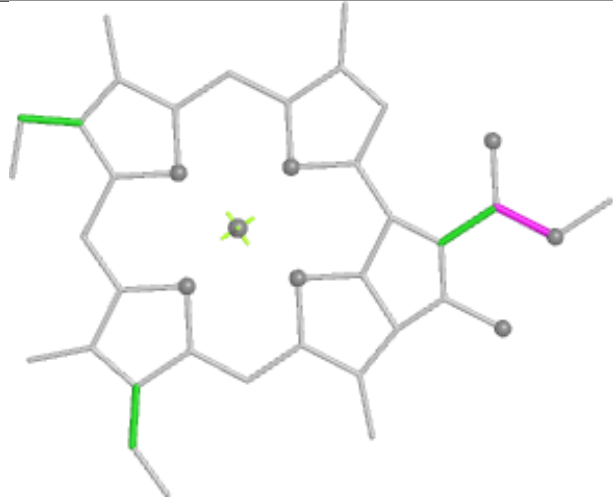
Ligand CLA 1 611



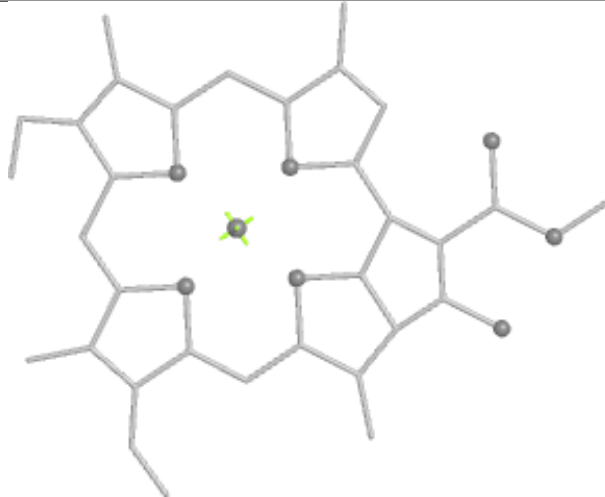
Bond lengths



Bond angles

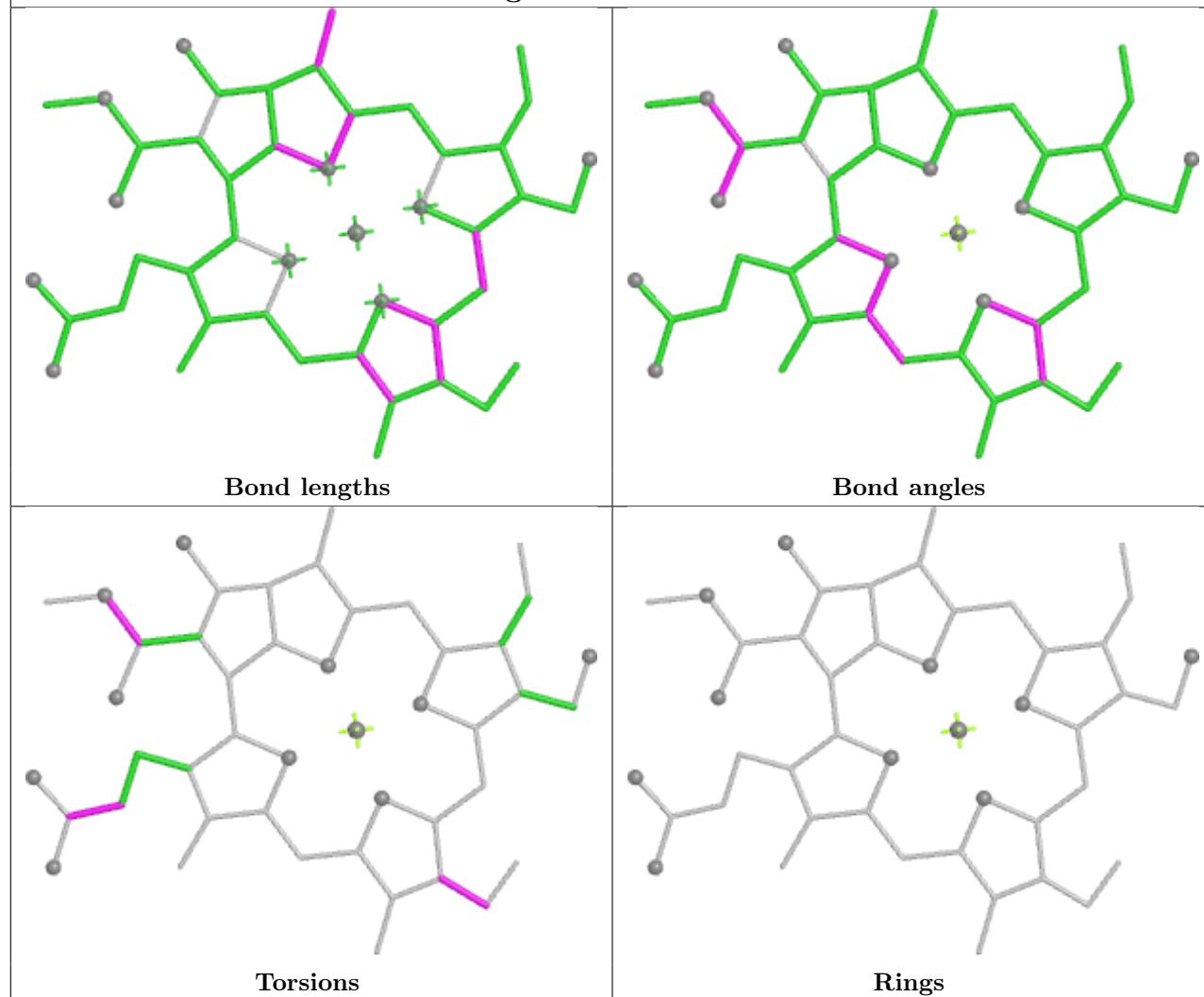


Torsions

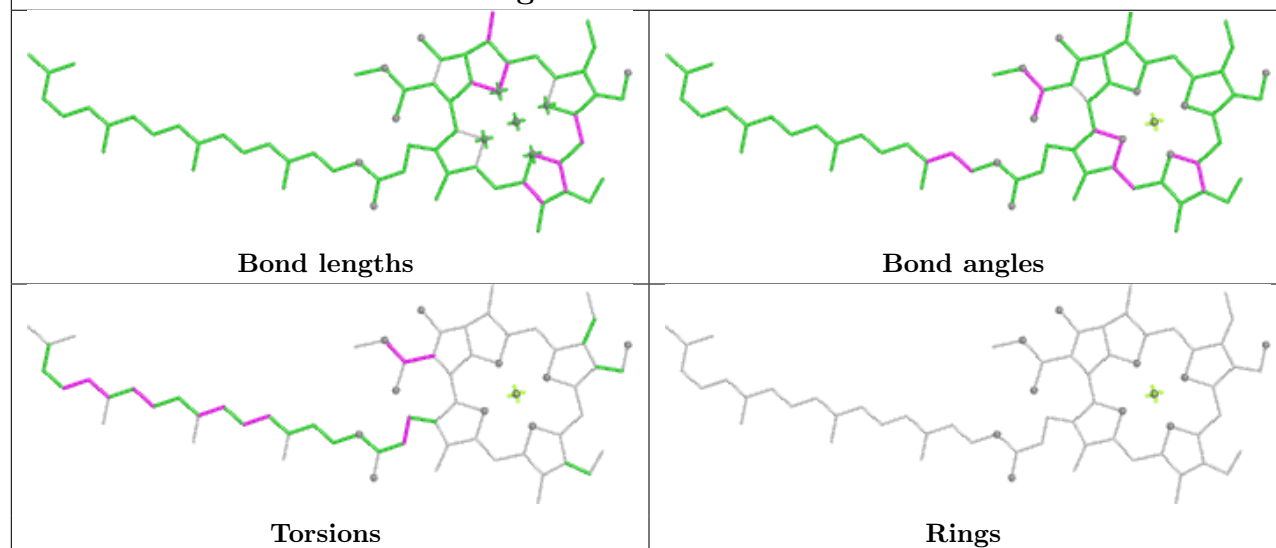


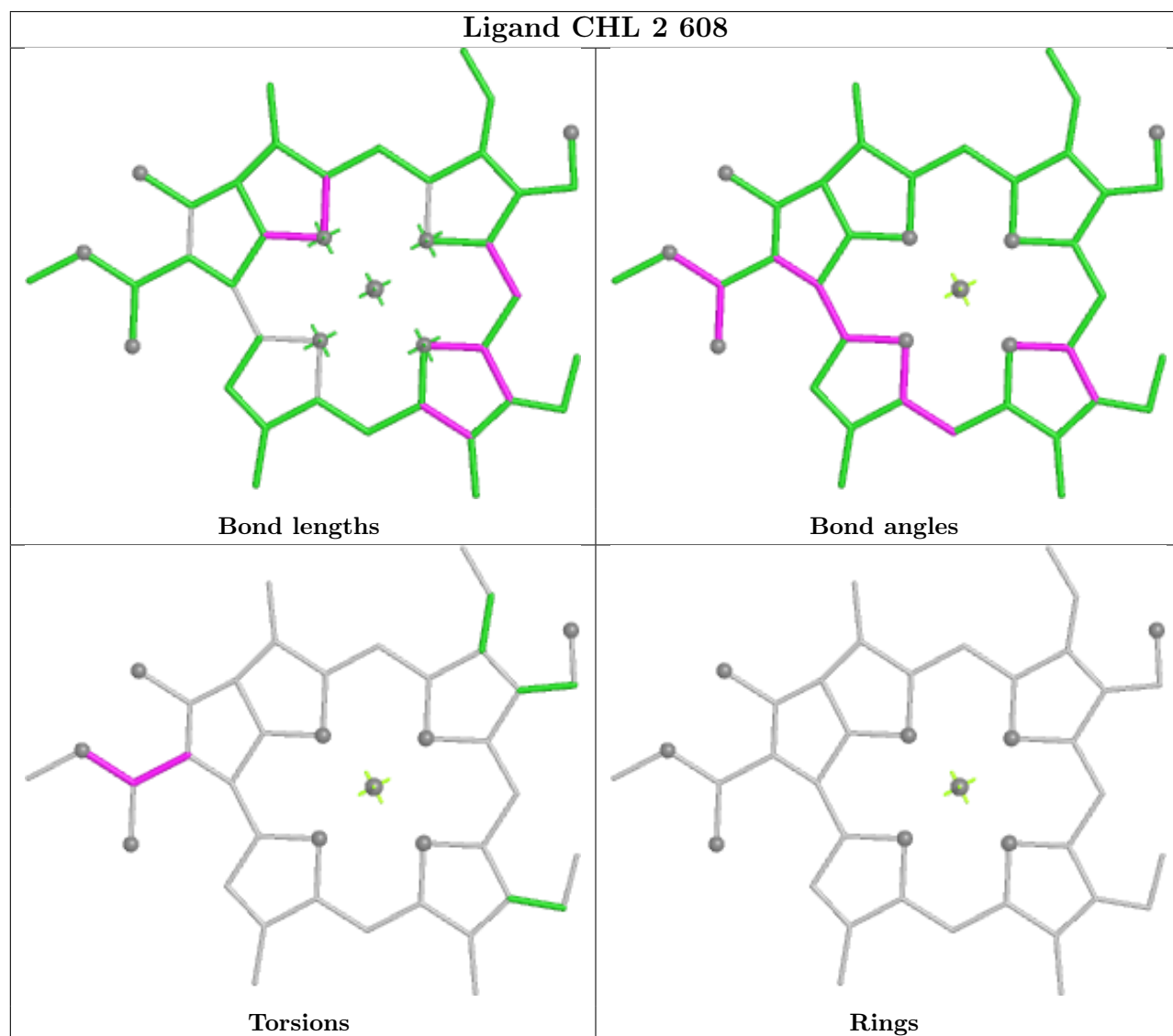
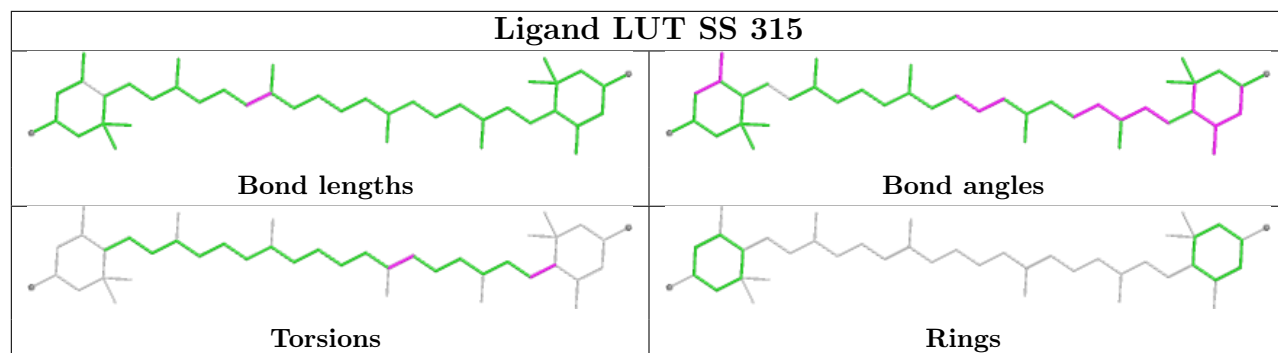
Rings

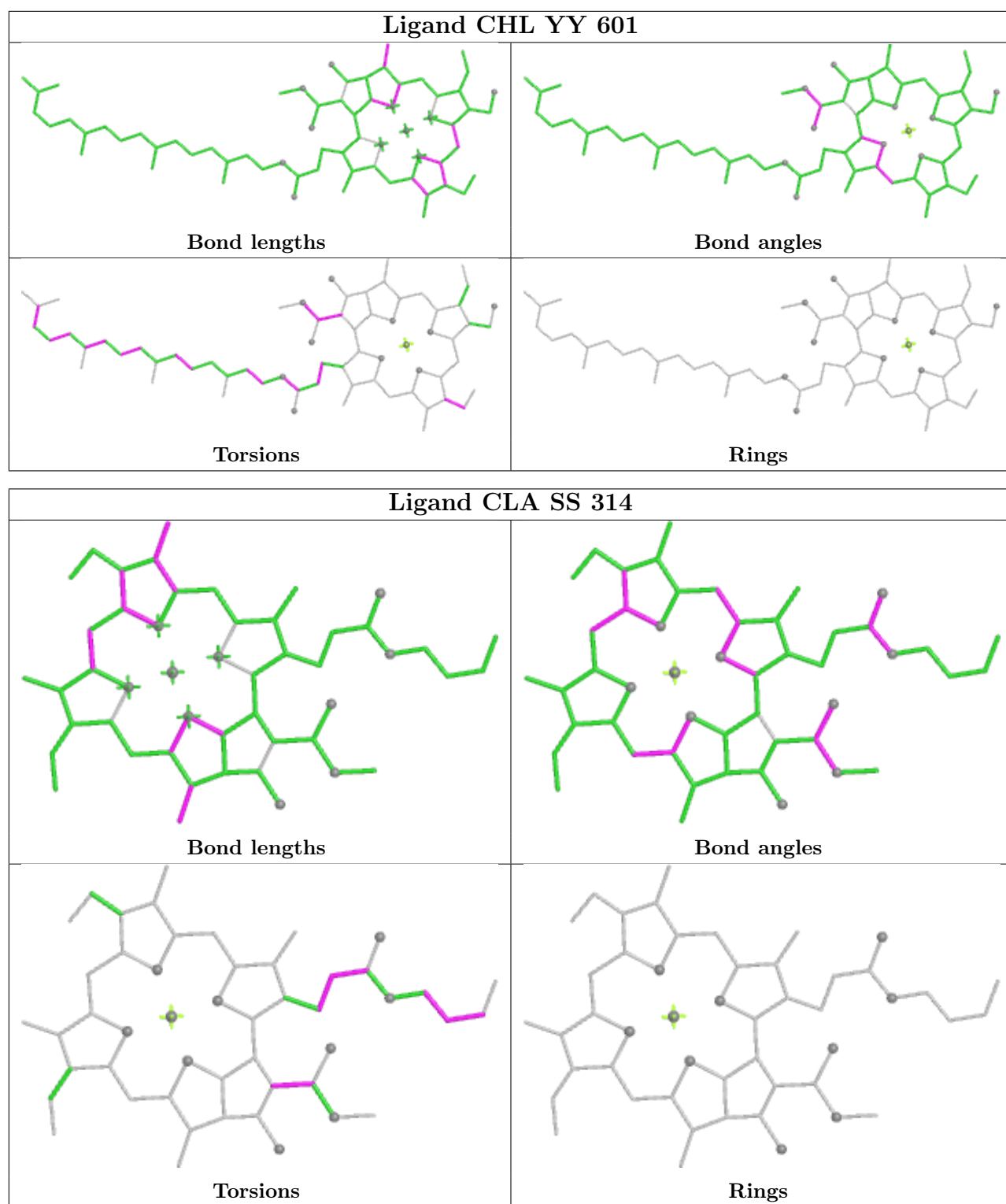
Ligand CHL 4 307

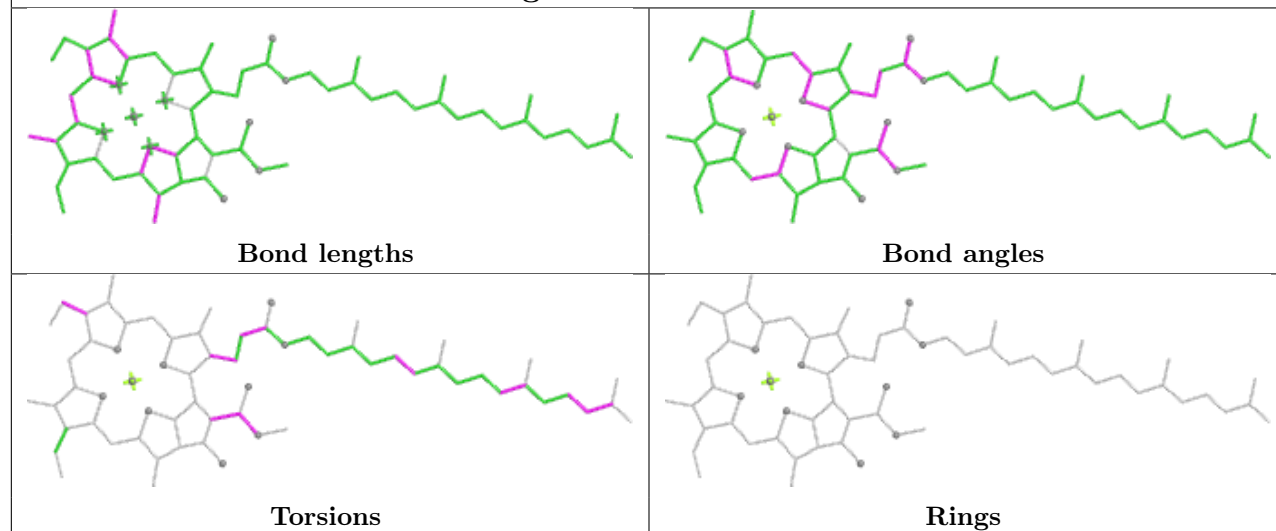
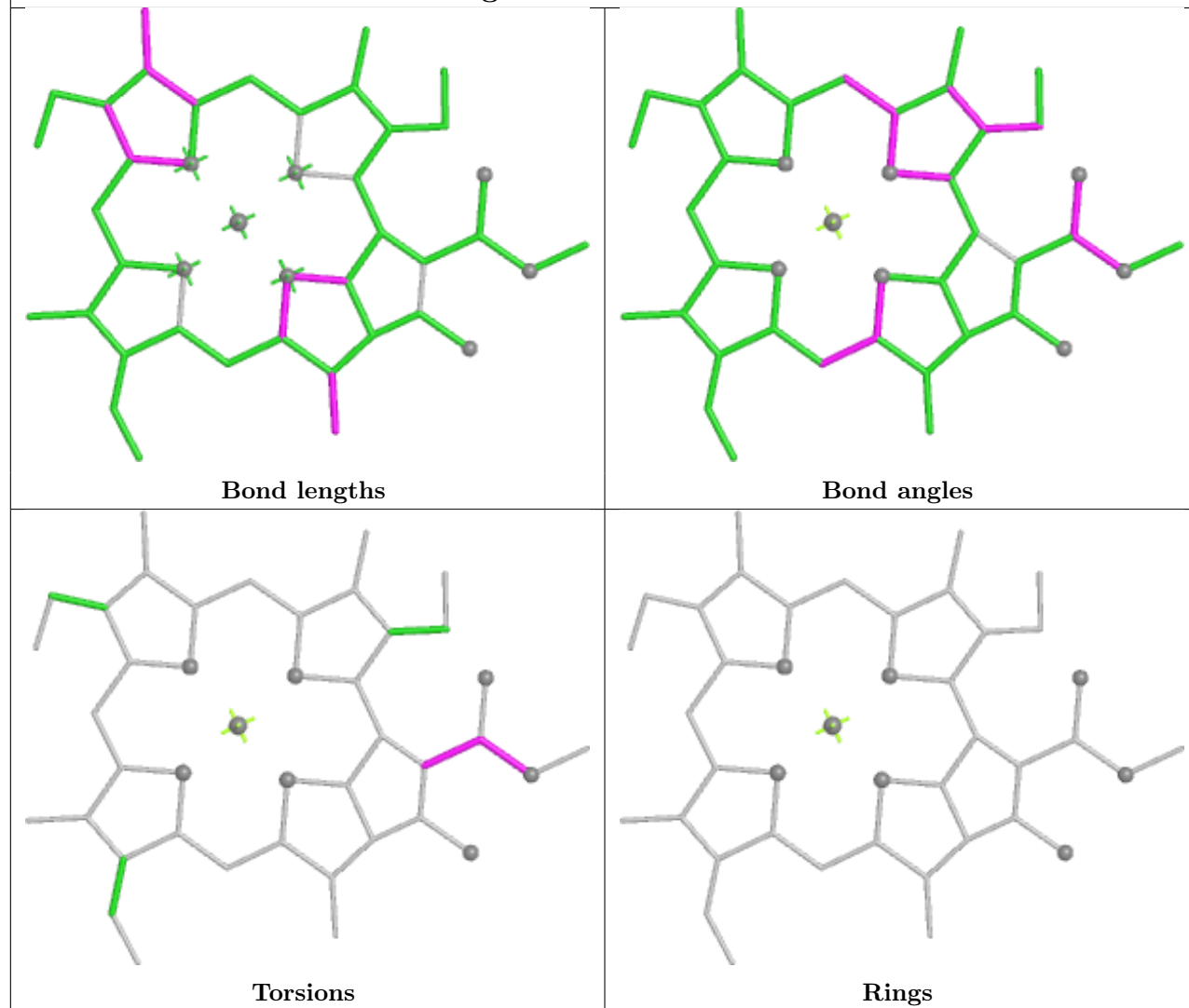


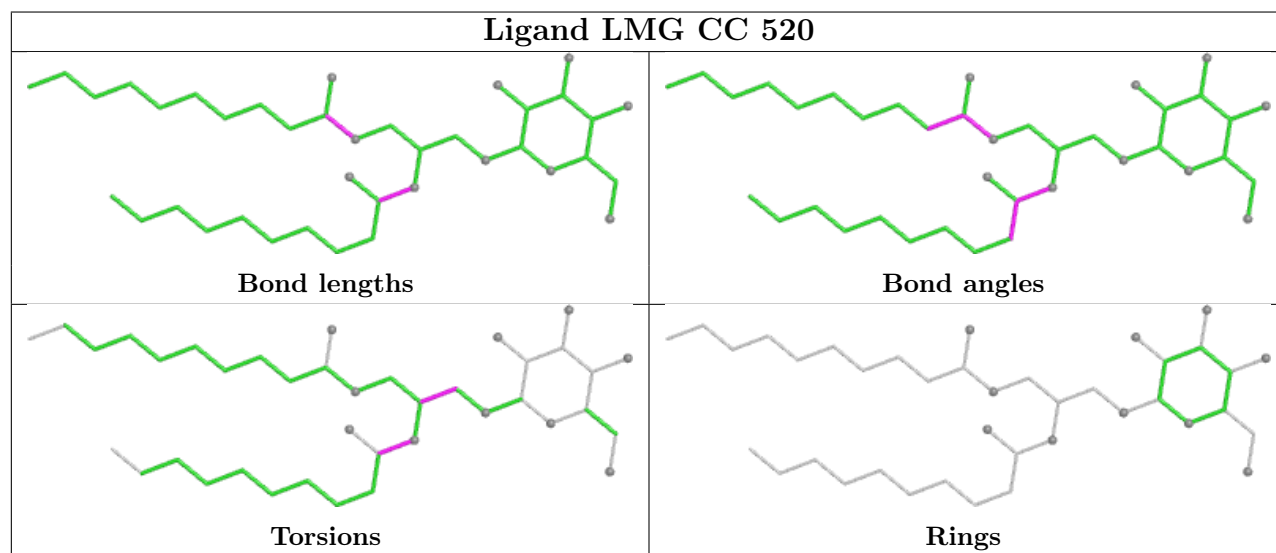
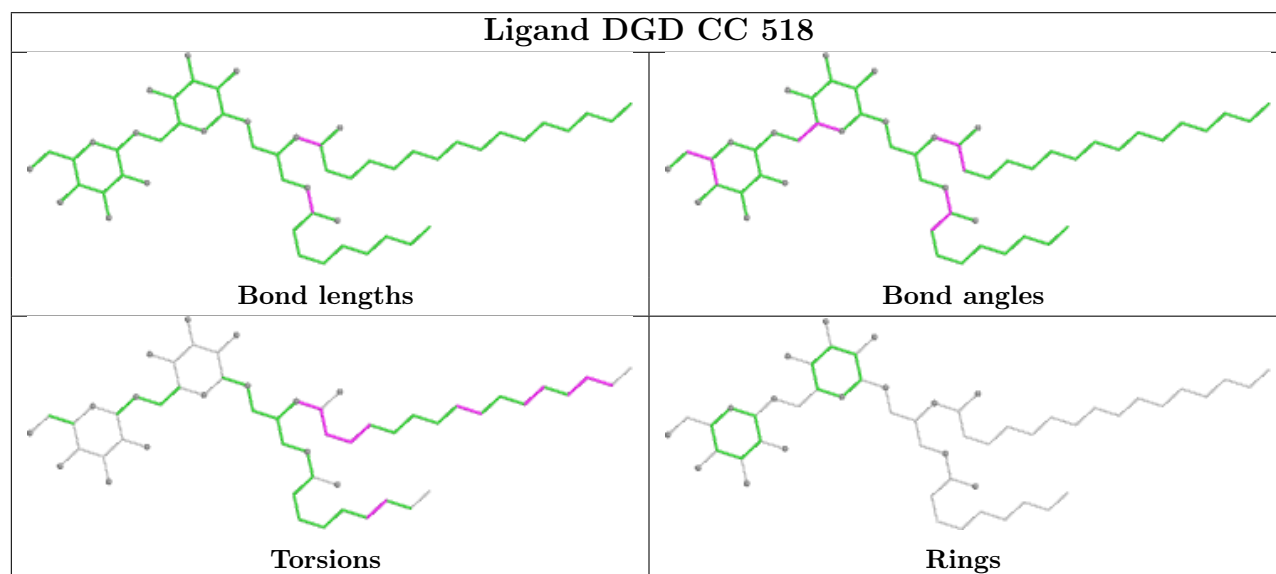
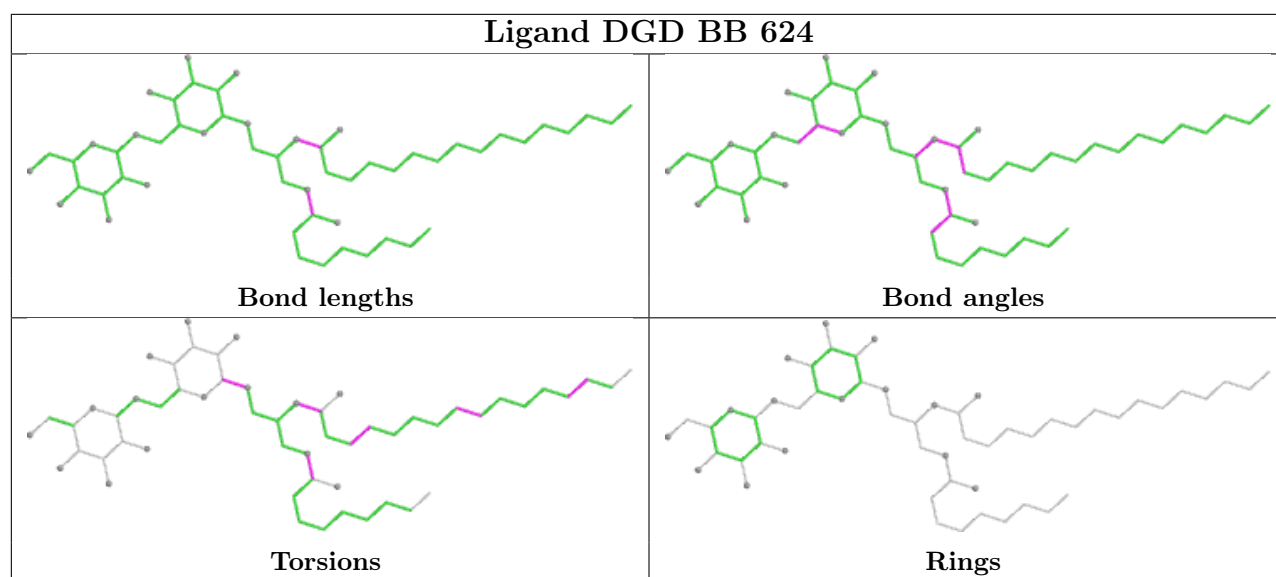
Ligand CHL NN 607



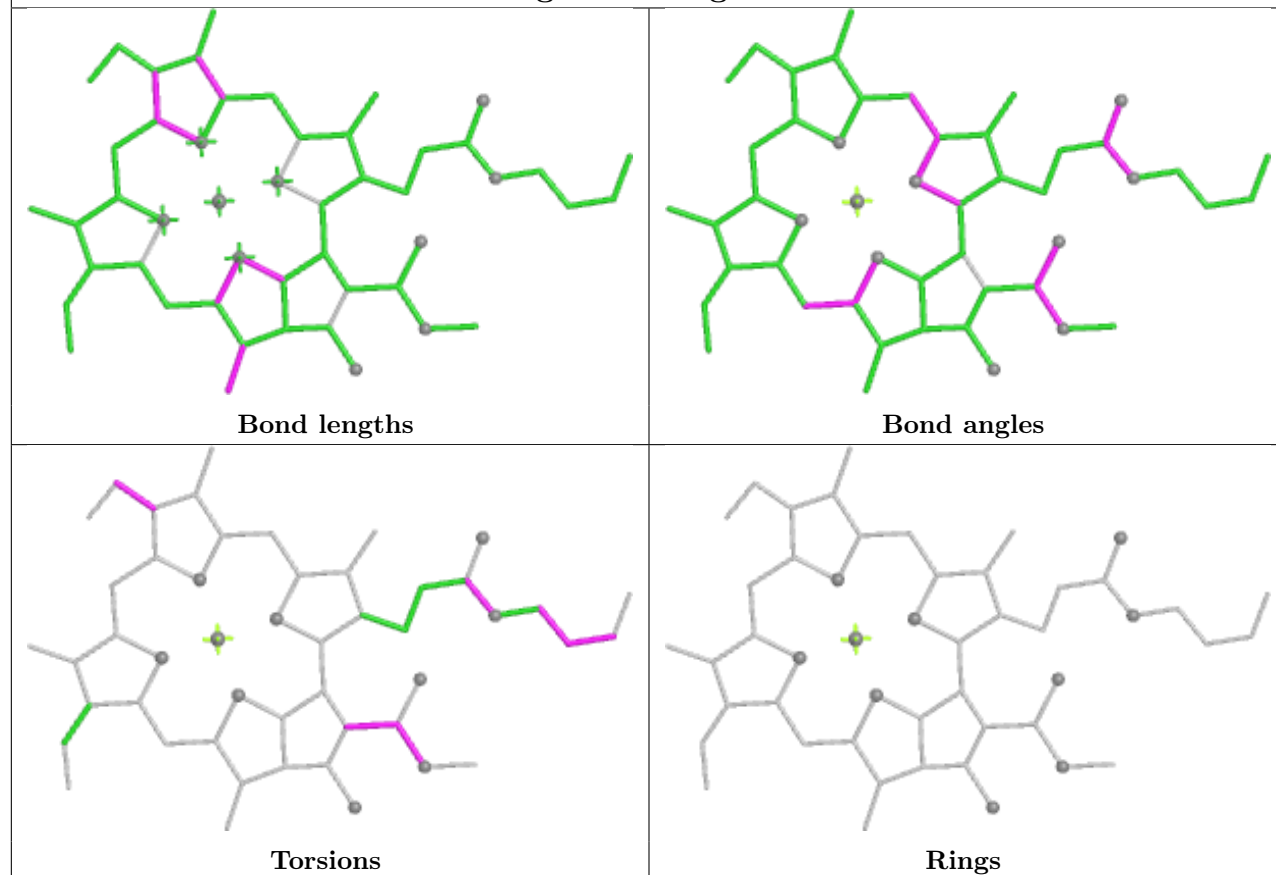




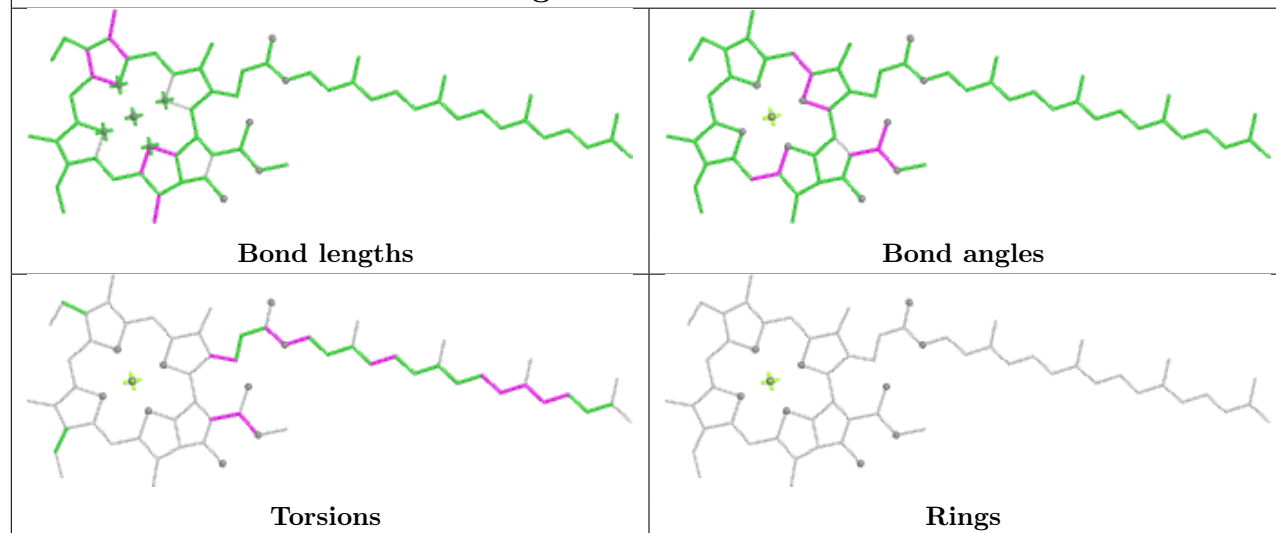
Ligand CLA Bb 601**Ligand CLA NN 603**

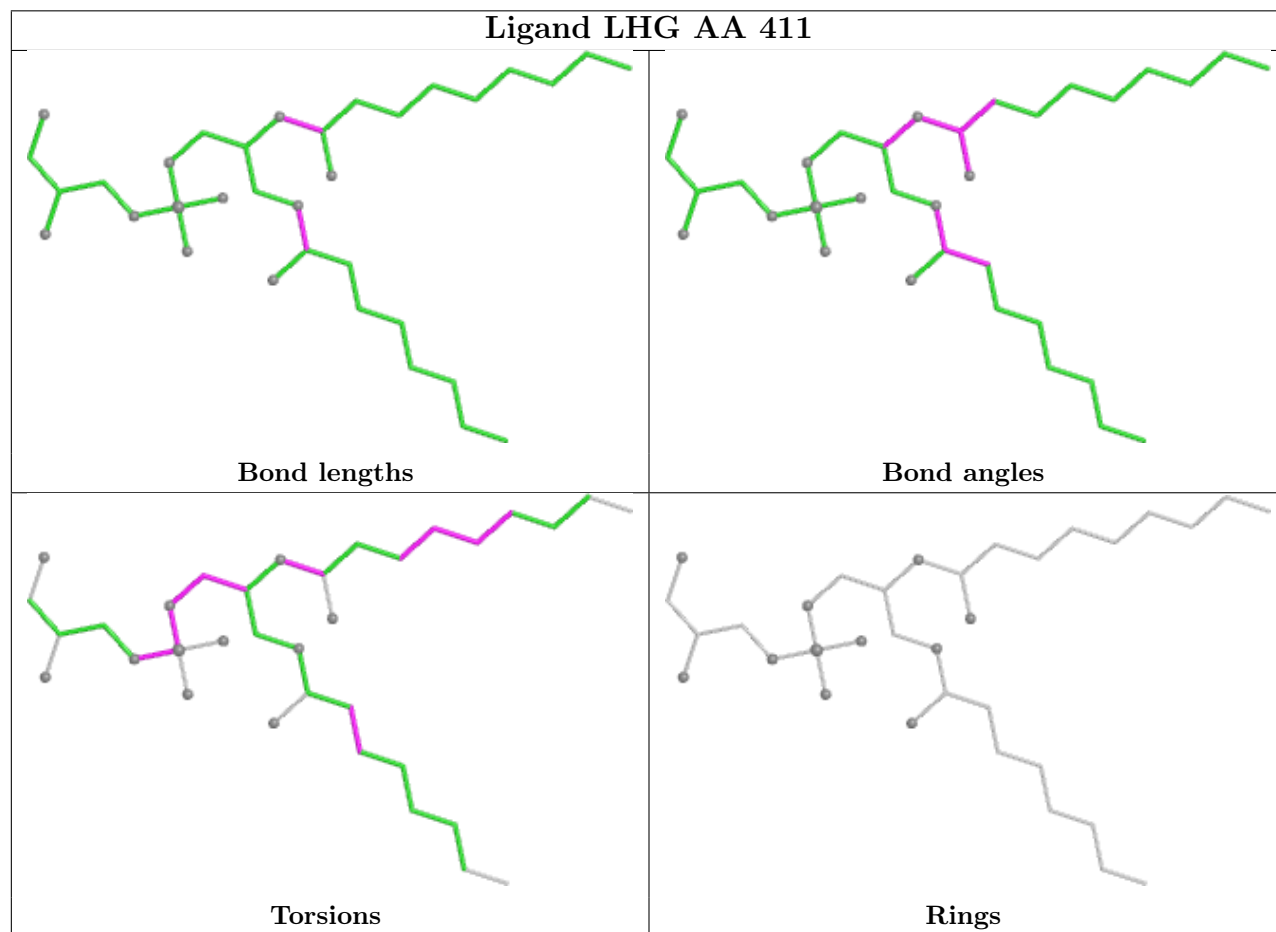
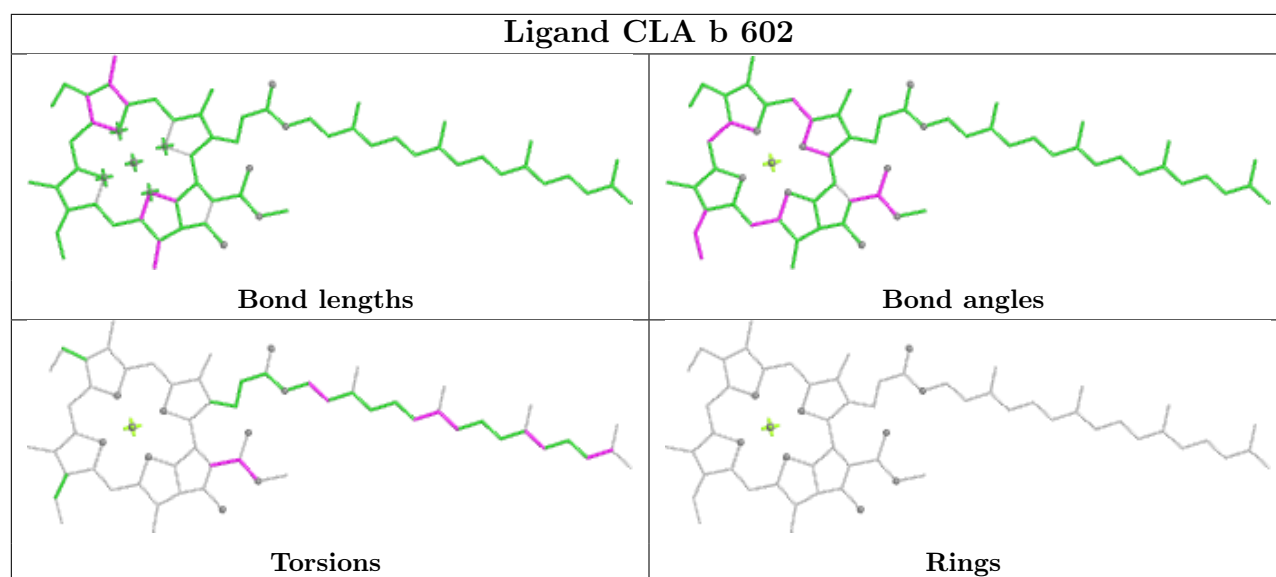


Ligand CLA g 614

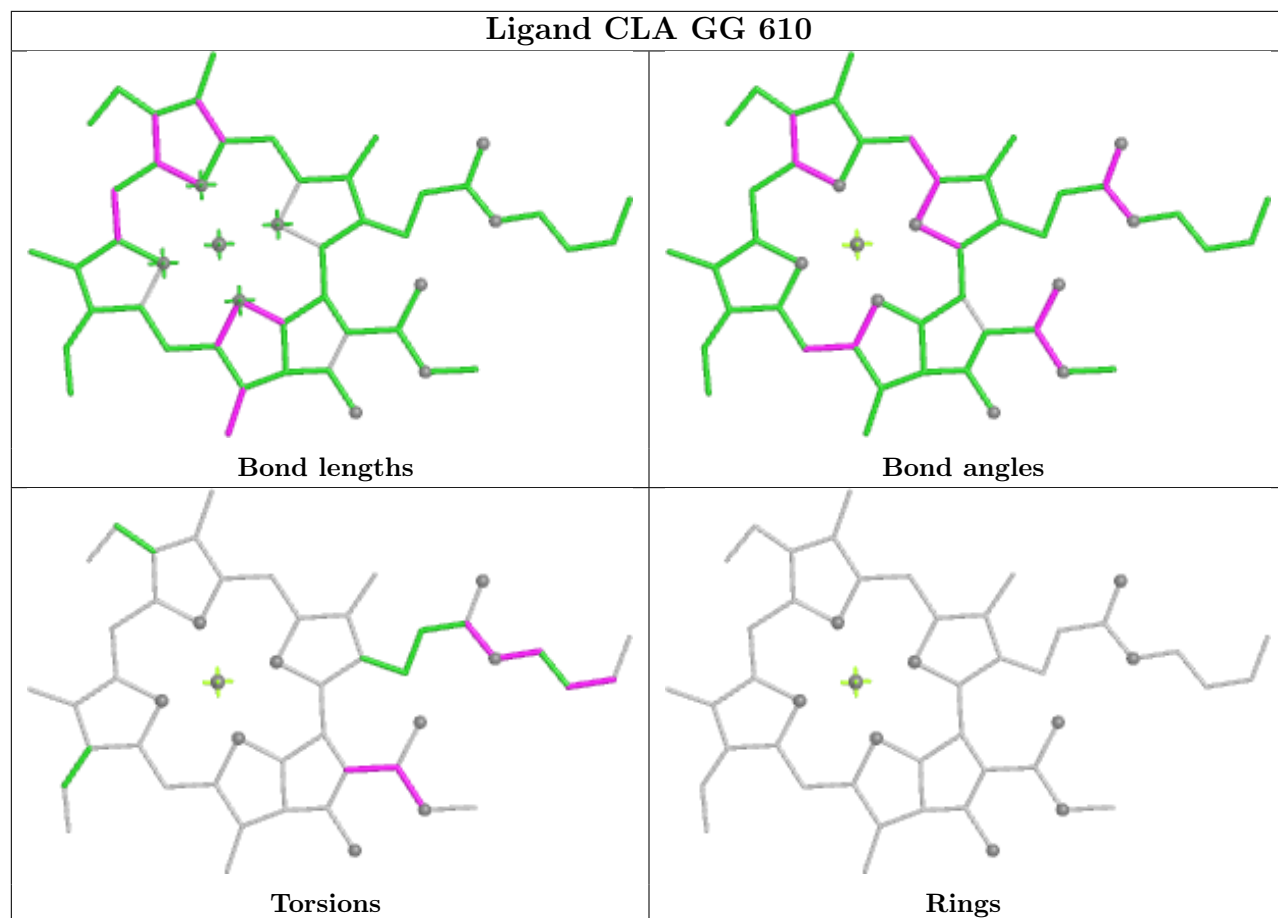


Ligand CLA C 510

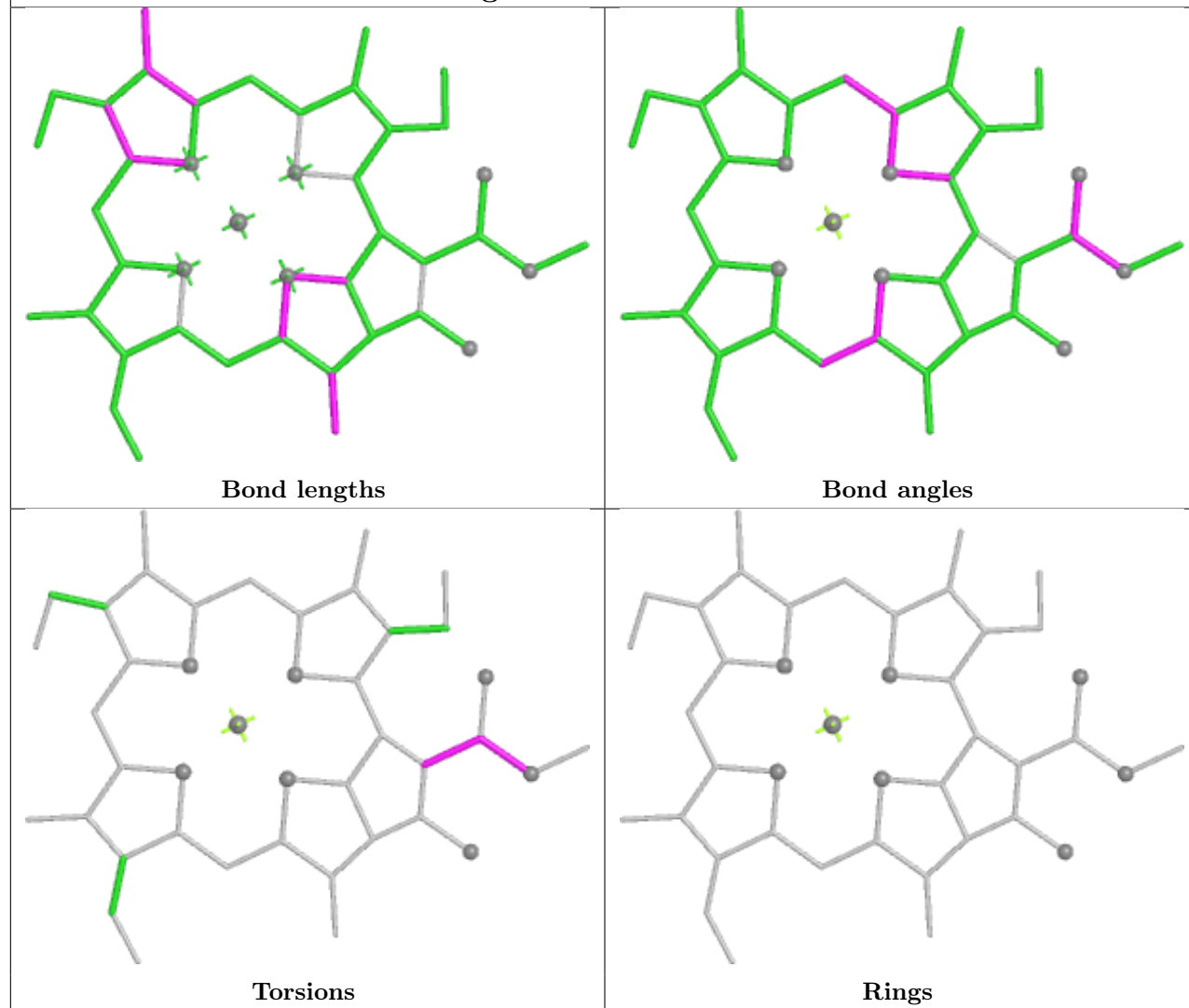




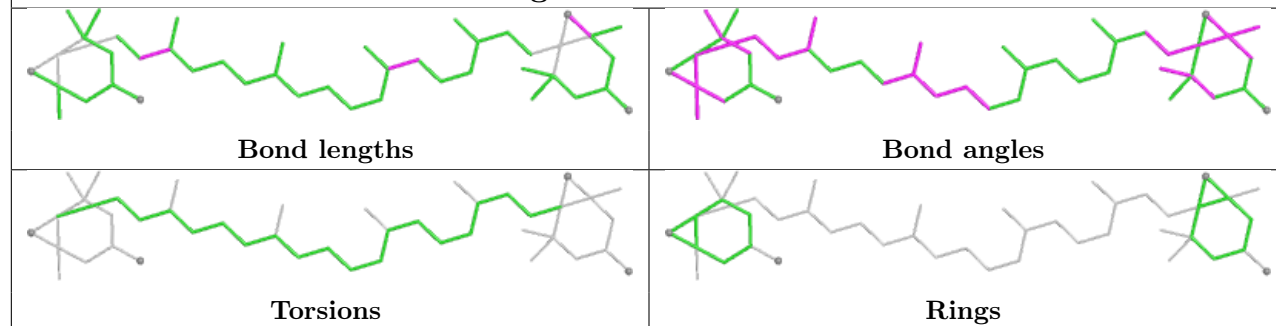
Ligand CLA GG 610

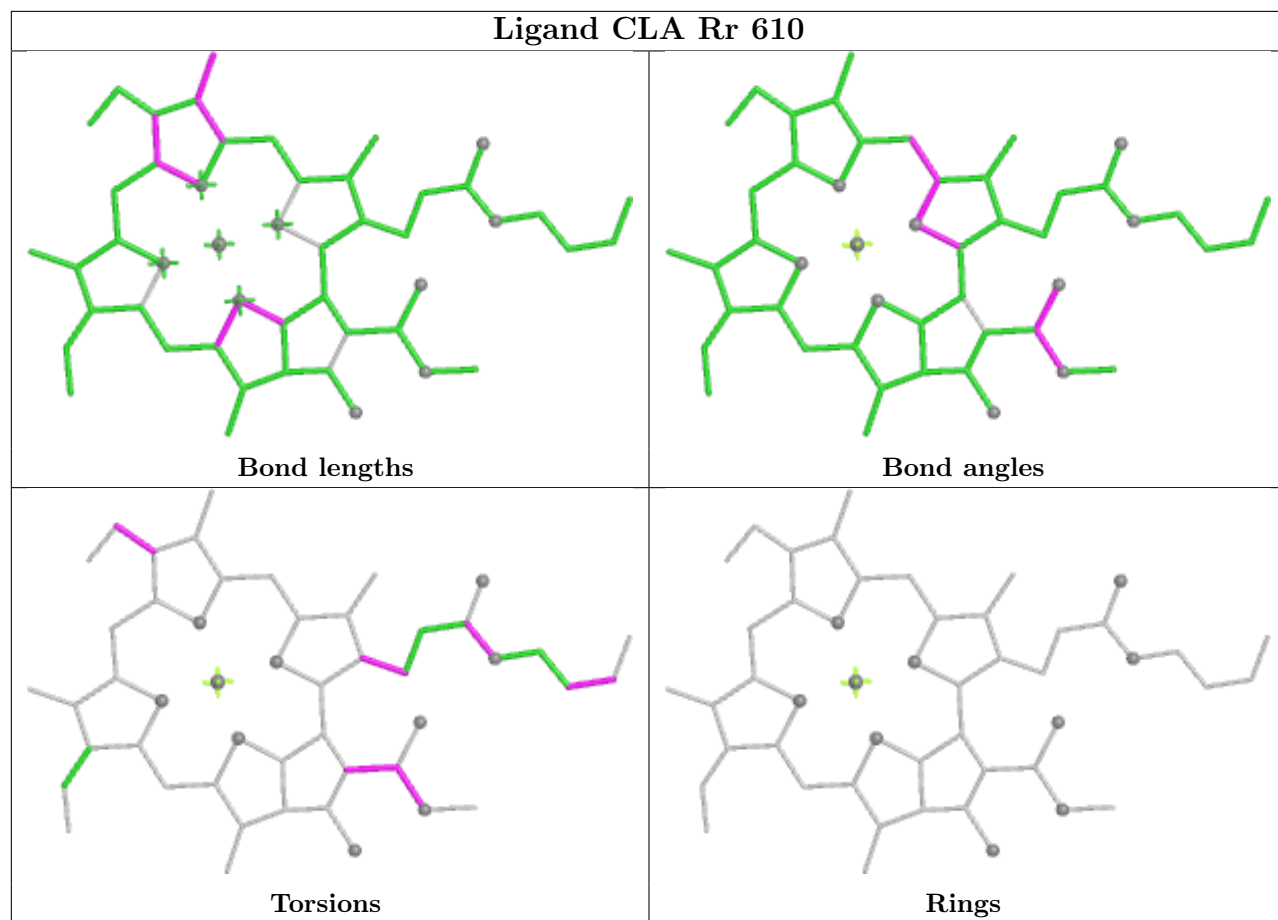


Ligand CLA GG 604

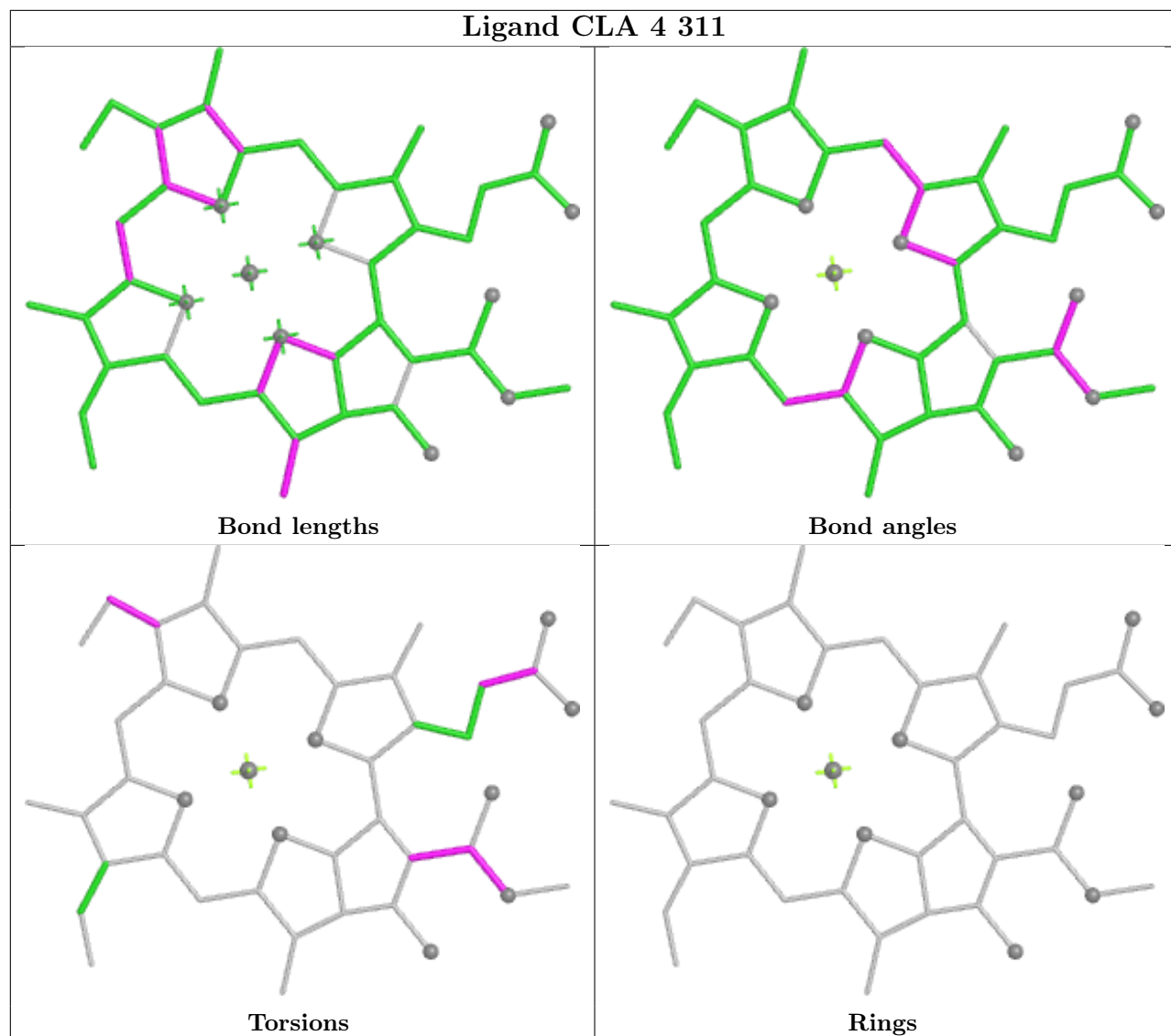


Ligand XAT N 617

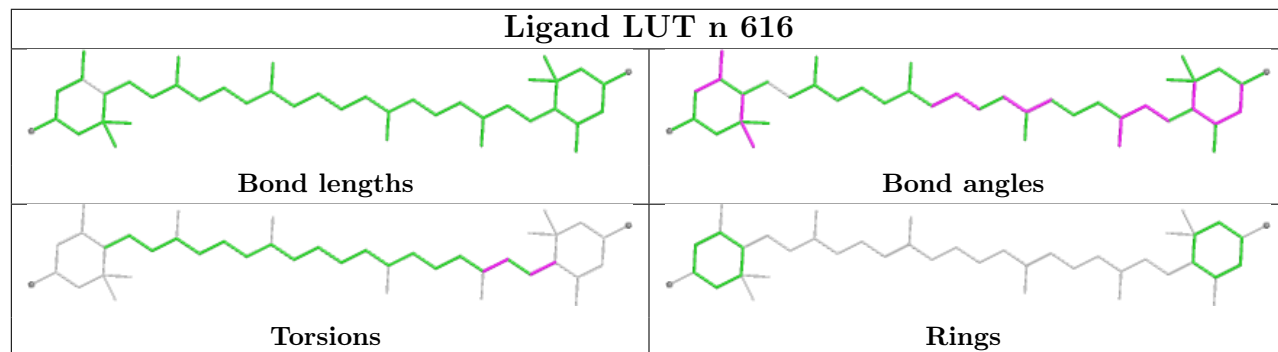




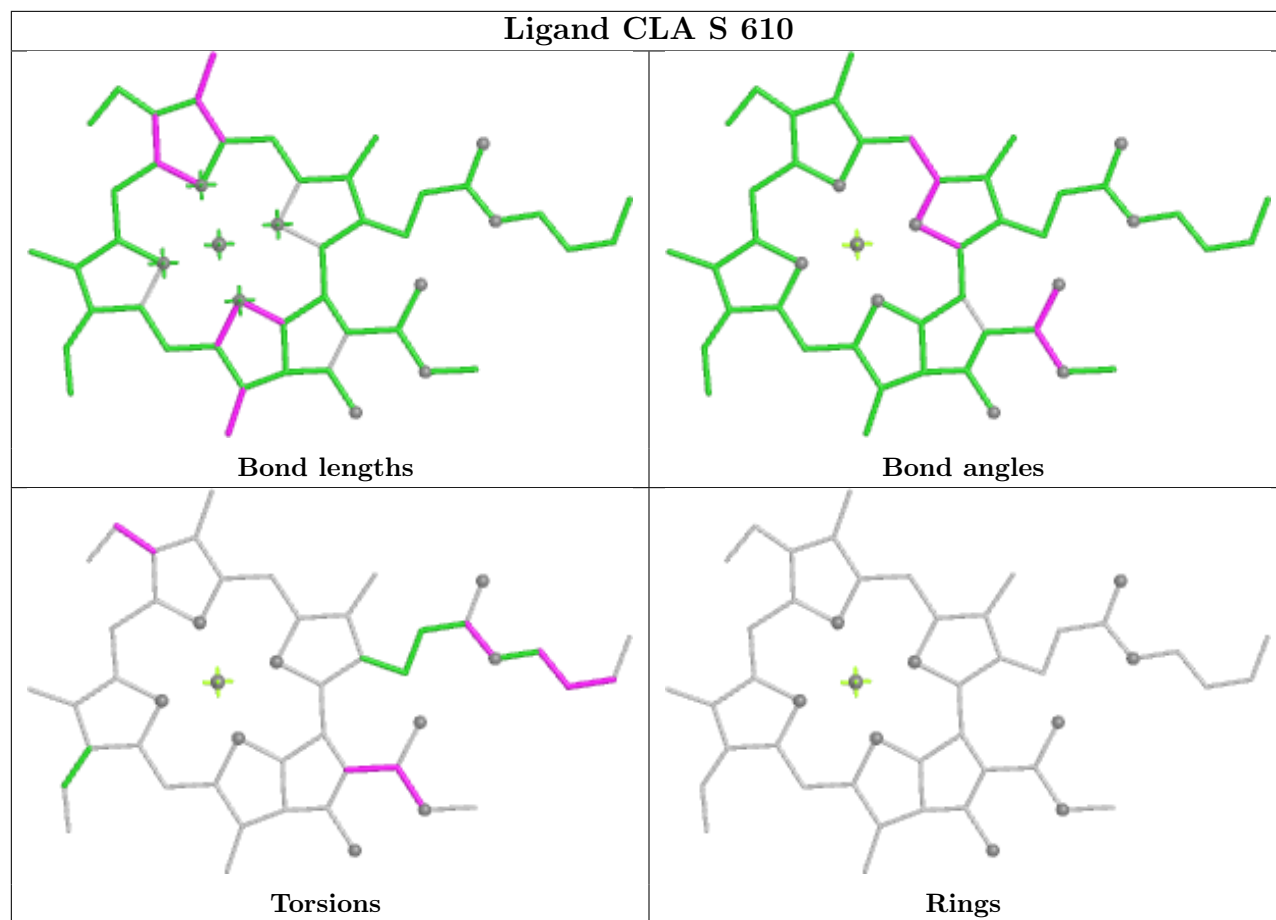
Ligand CLA 4 311



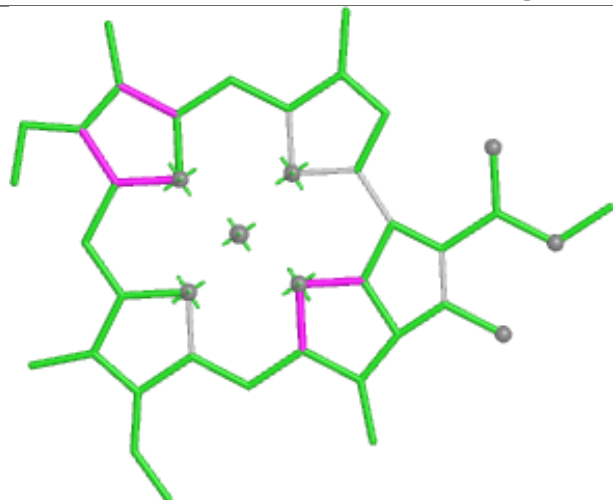
Ligand LUT n 616



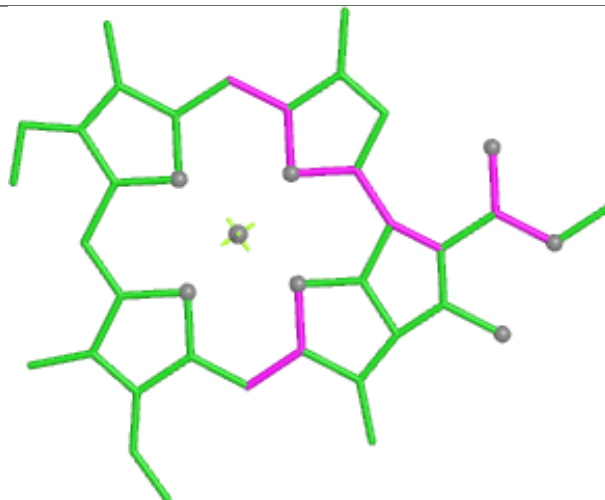
Ligand CLA S 610



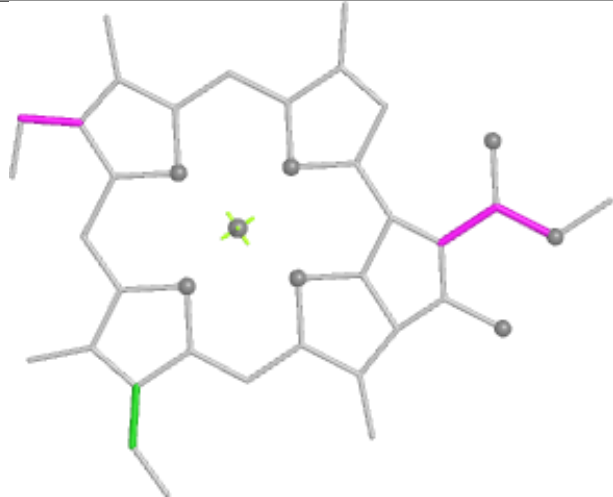
Ligand CLA 3 603



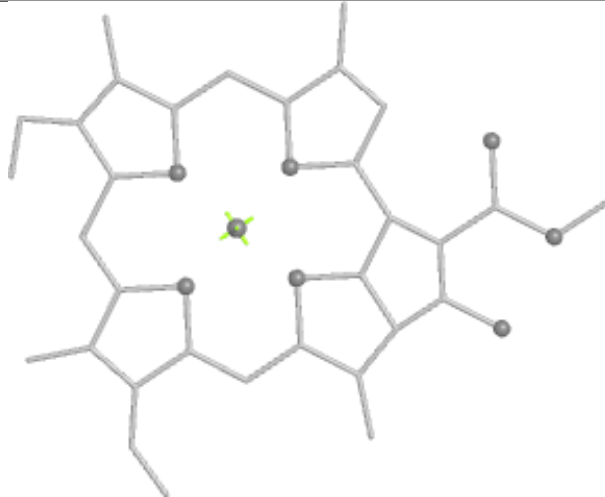
Bond lengths



Bond angles

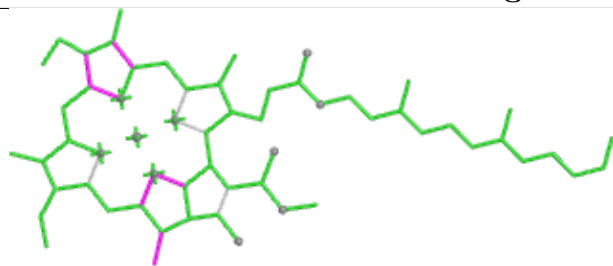


Torsions

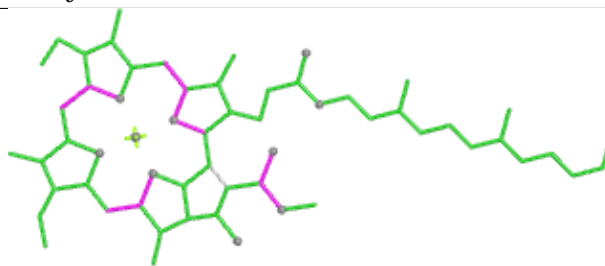


Rings

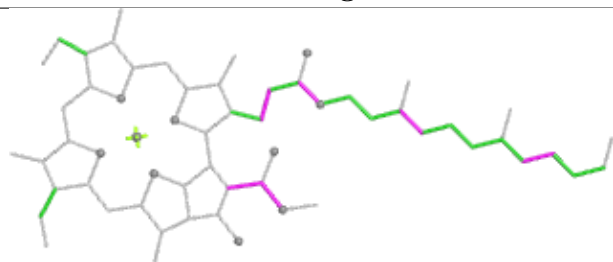
Ligand CLA Yy 613



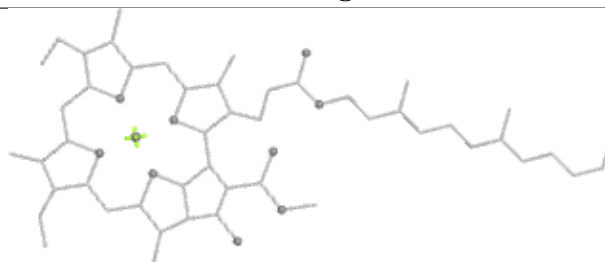
Bond lengths



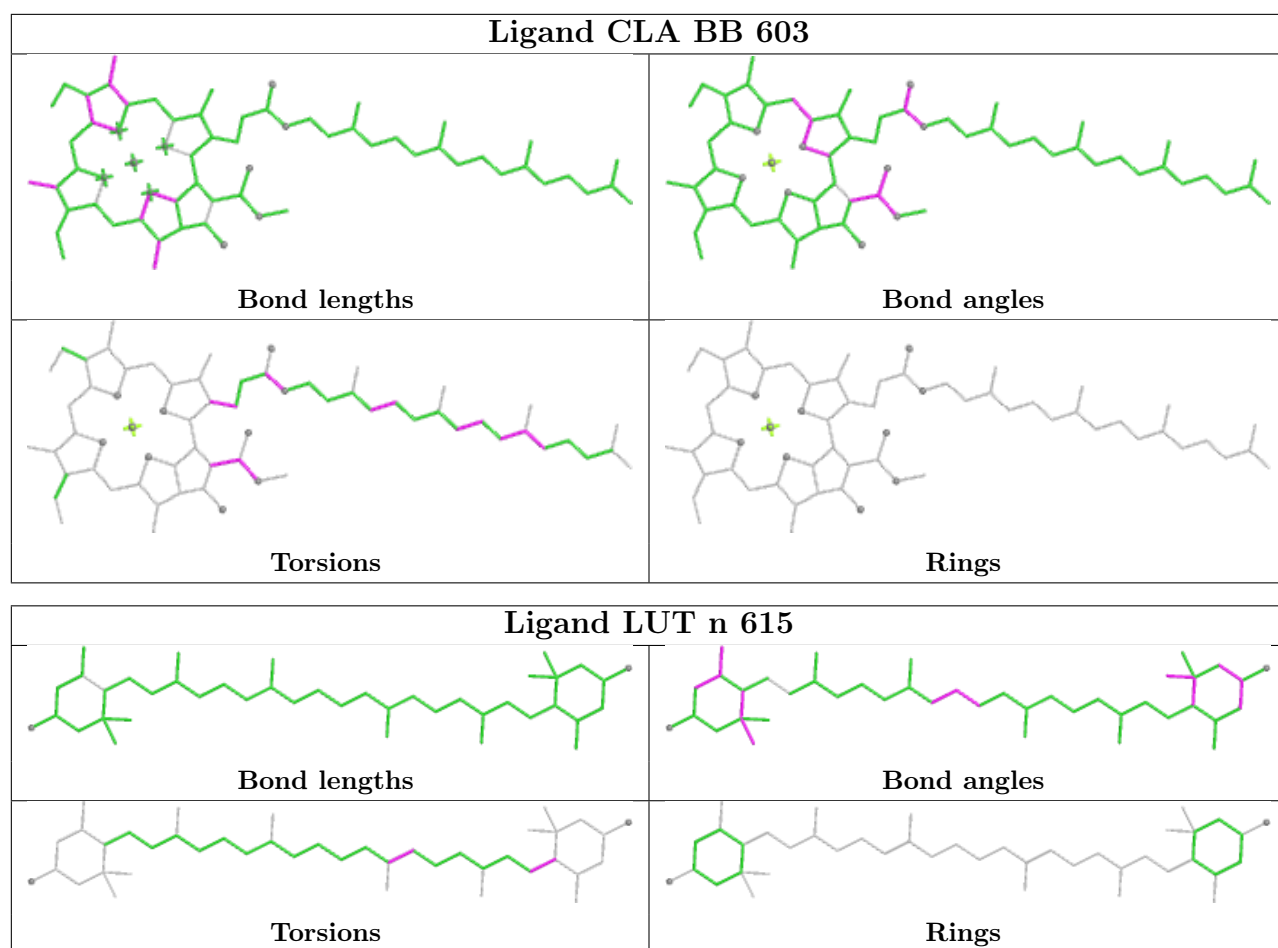
Bond angles

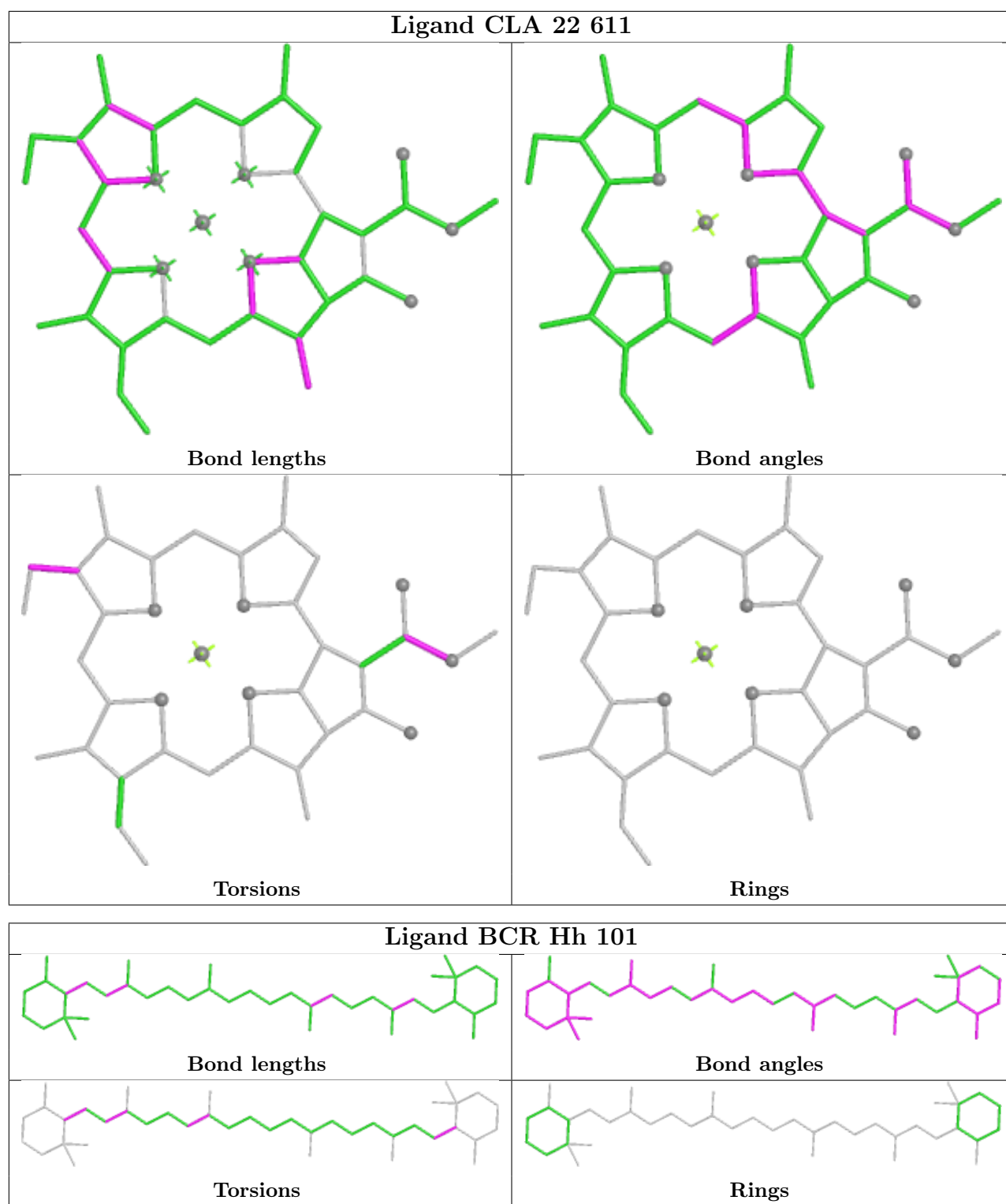


Torsions

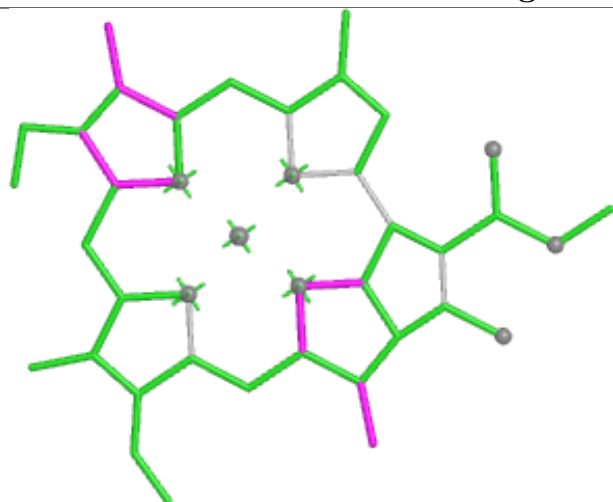


Rings





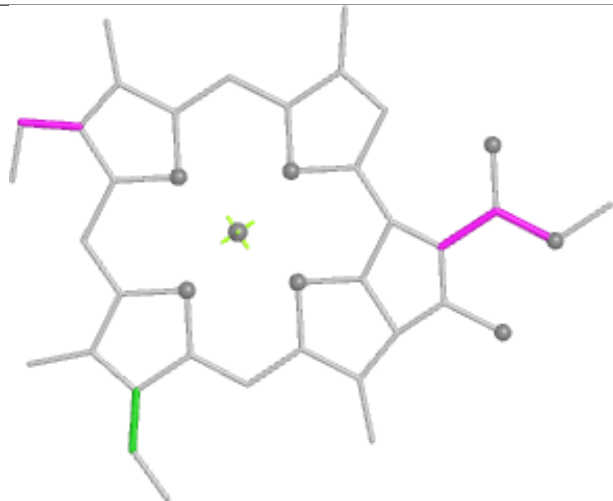
Ligand CLA 2 604



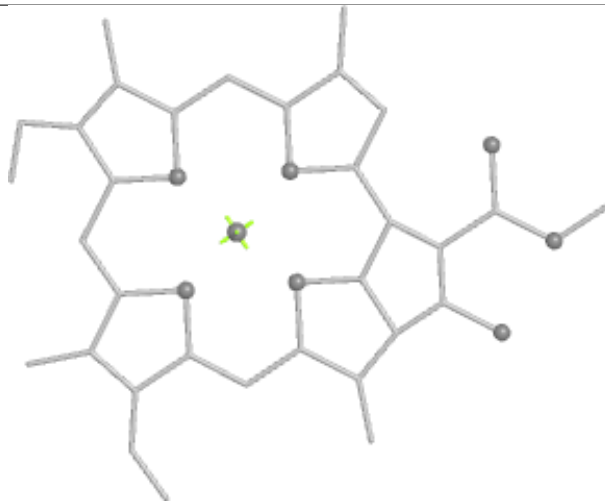
Bond lengths



Bond angles

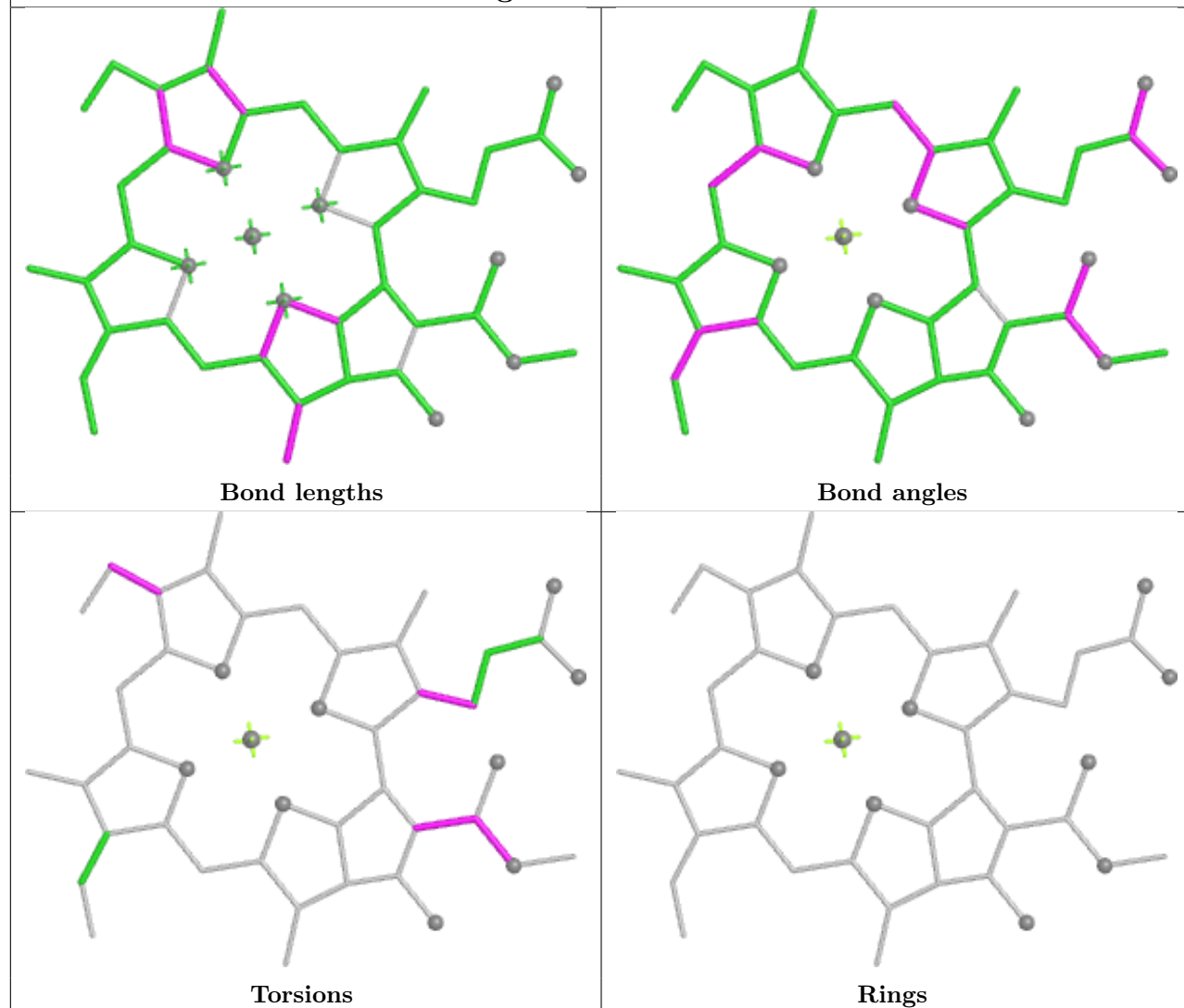


Torsions

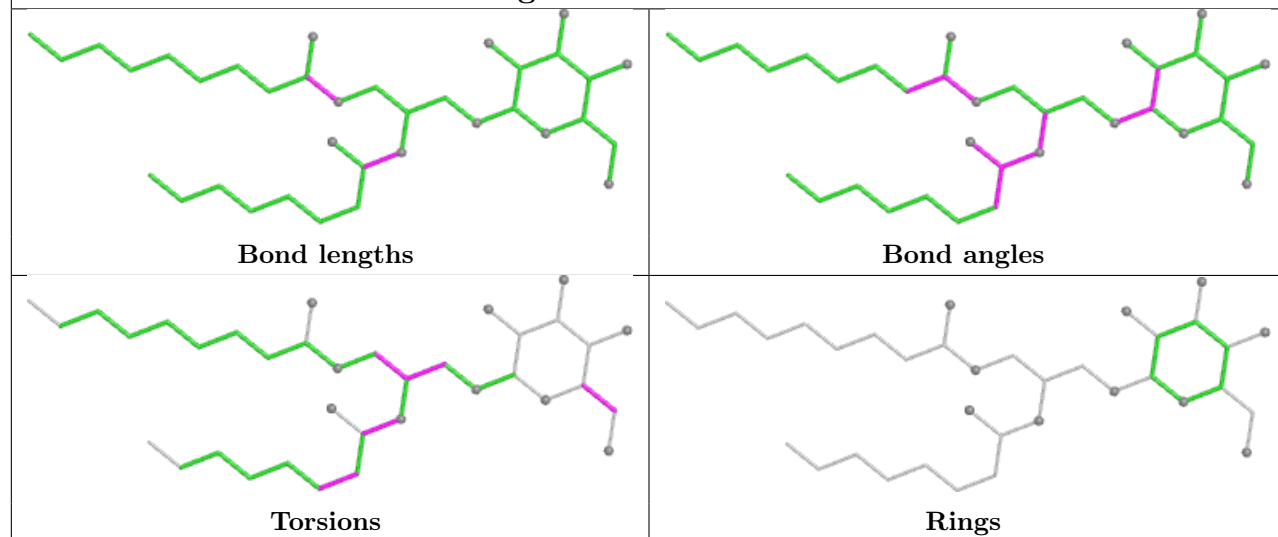


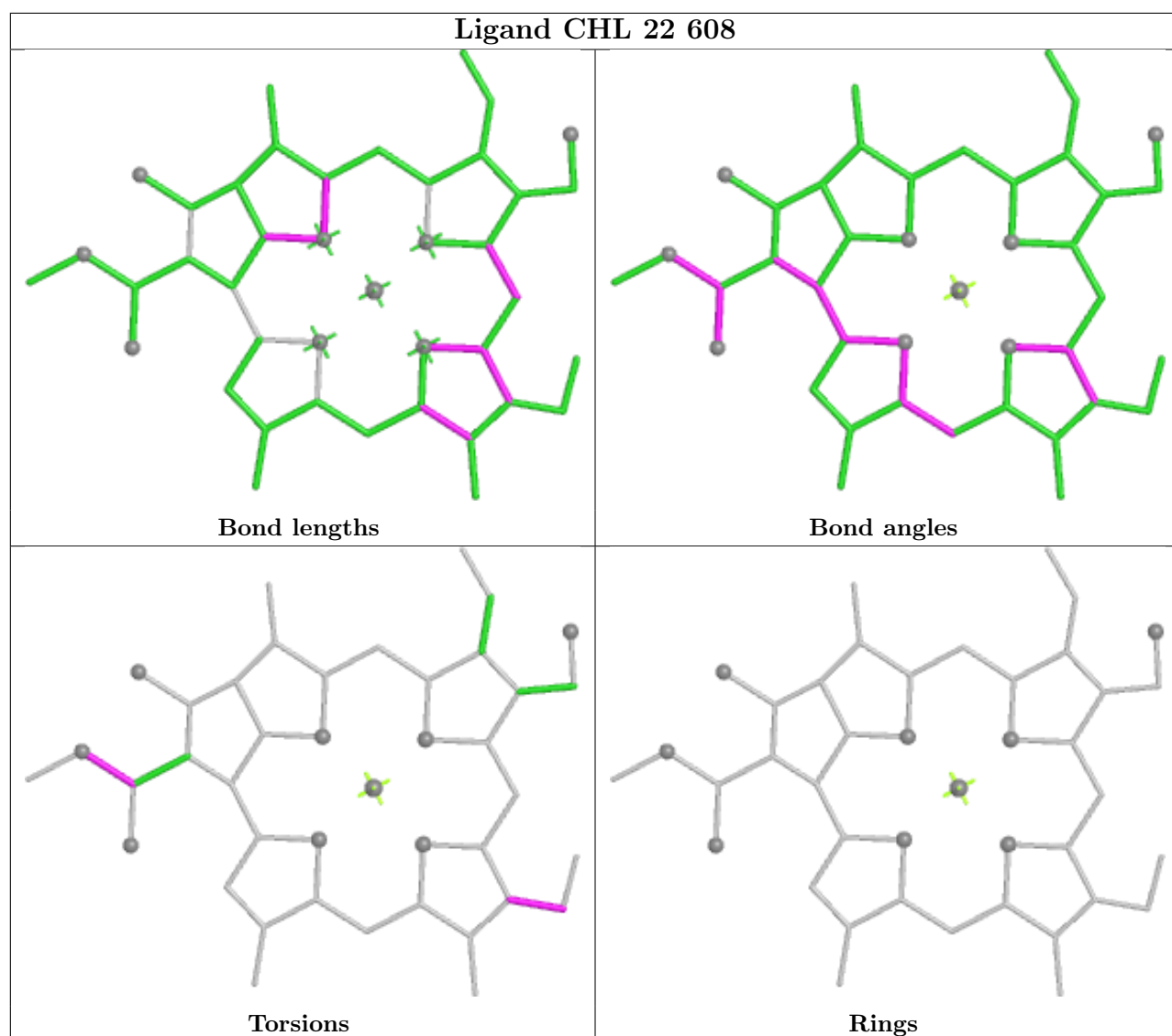
Rings

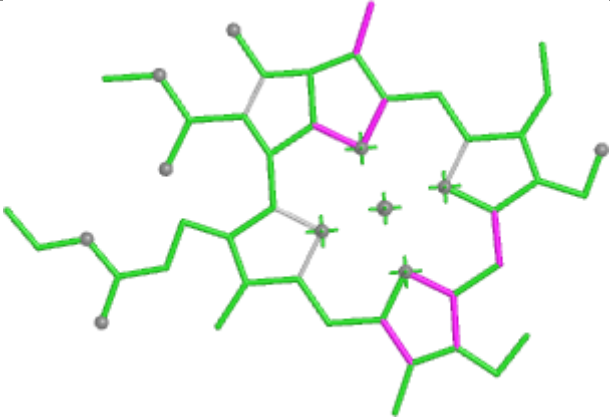
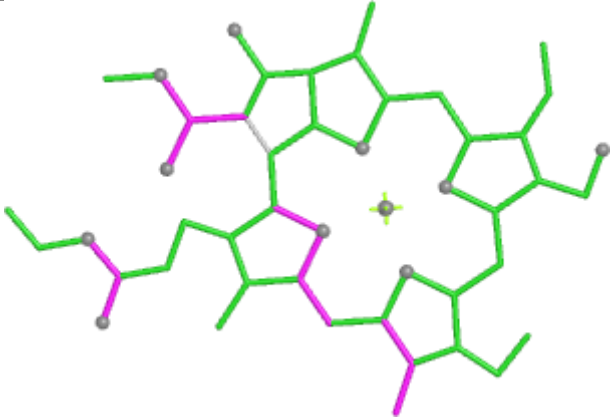
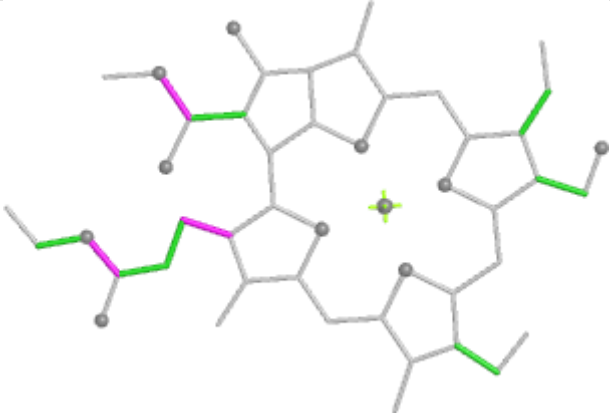
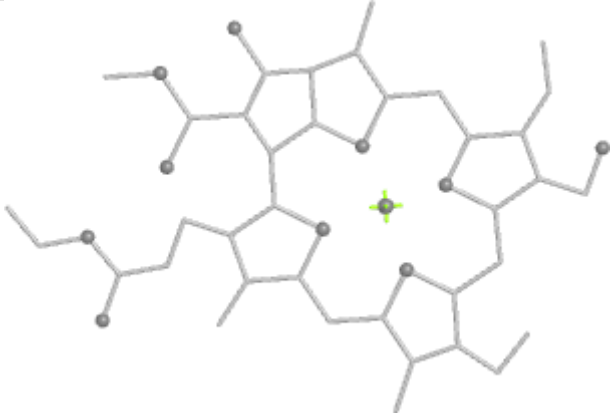
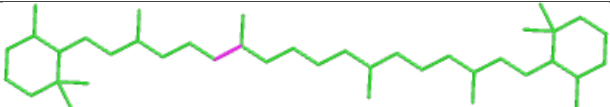
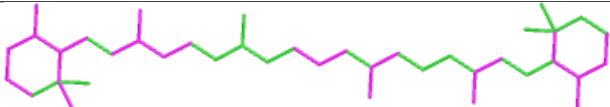
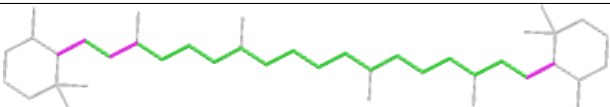
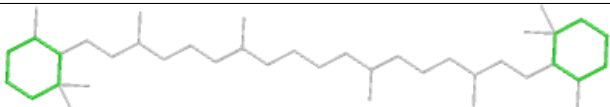
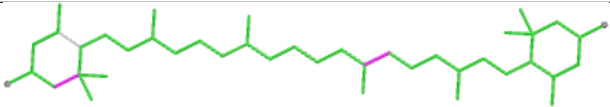
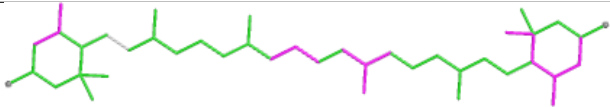
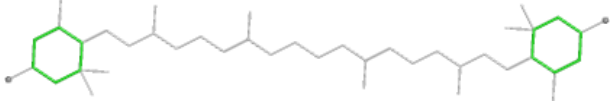
Ligand CLA 4 304

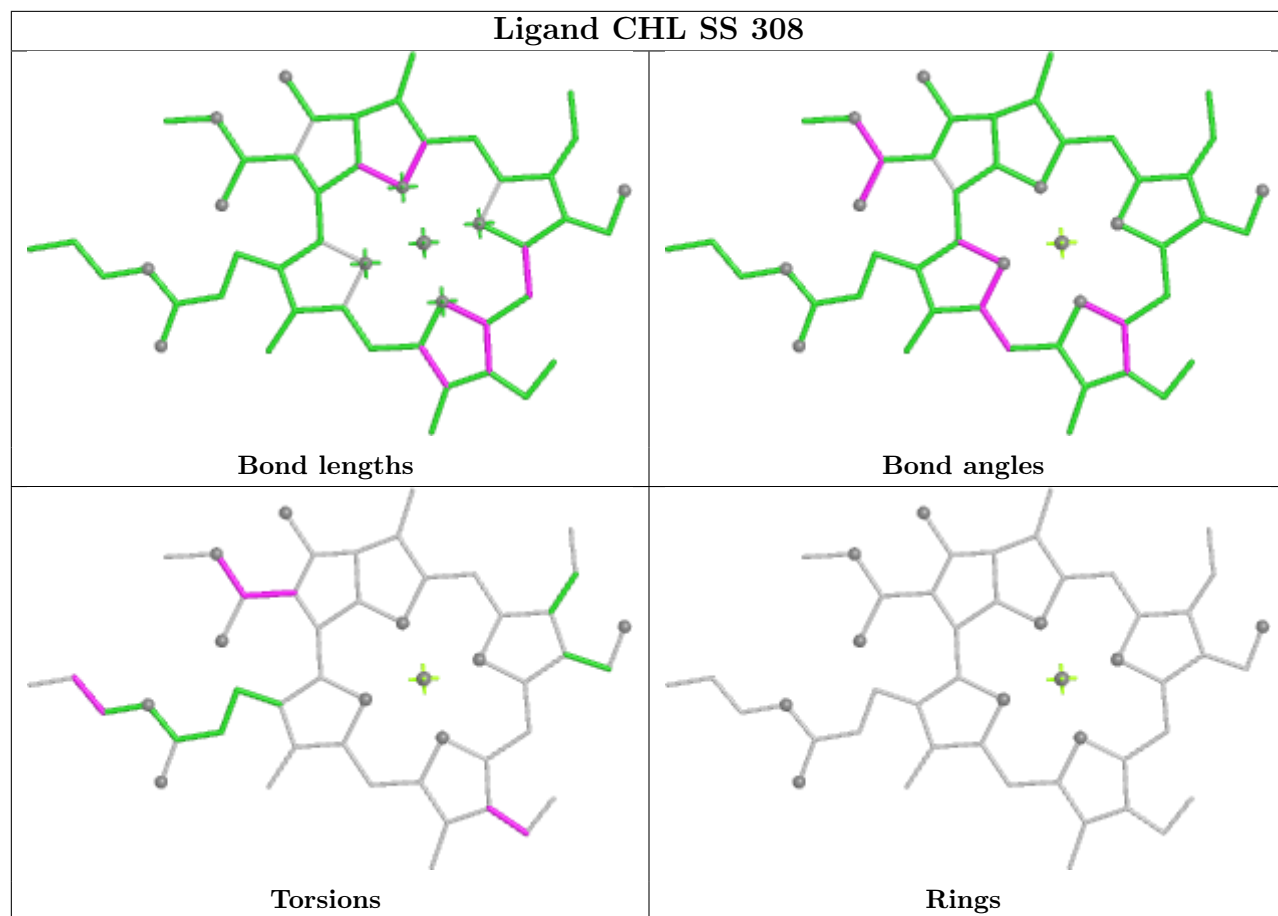


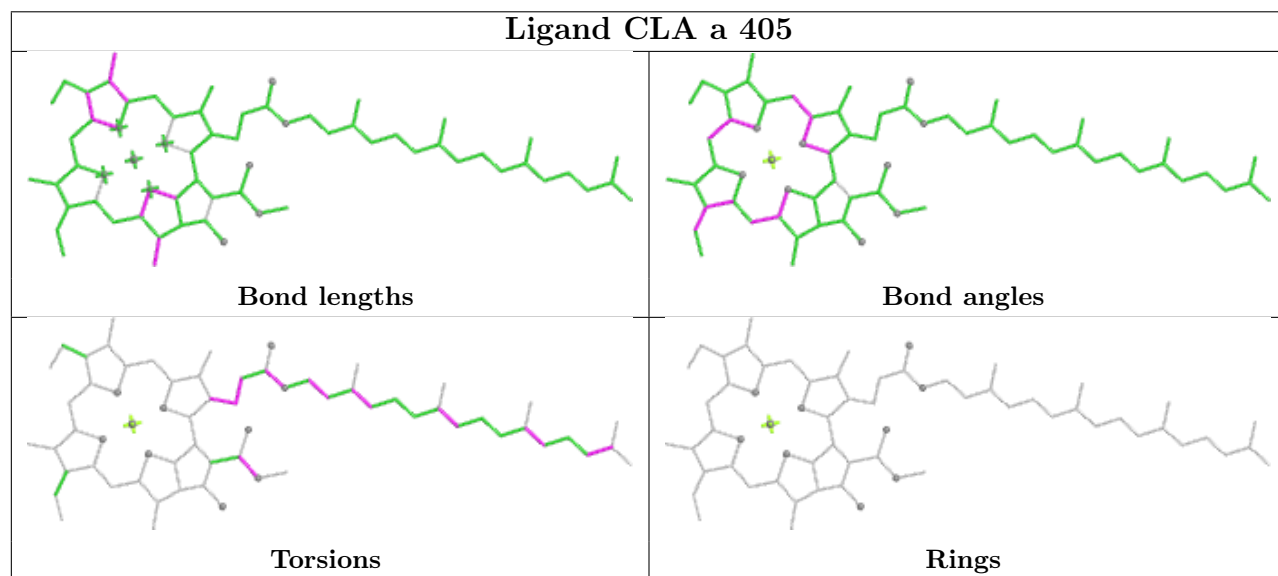
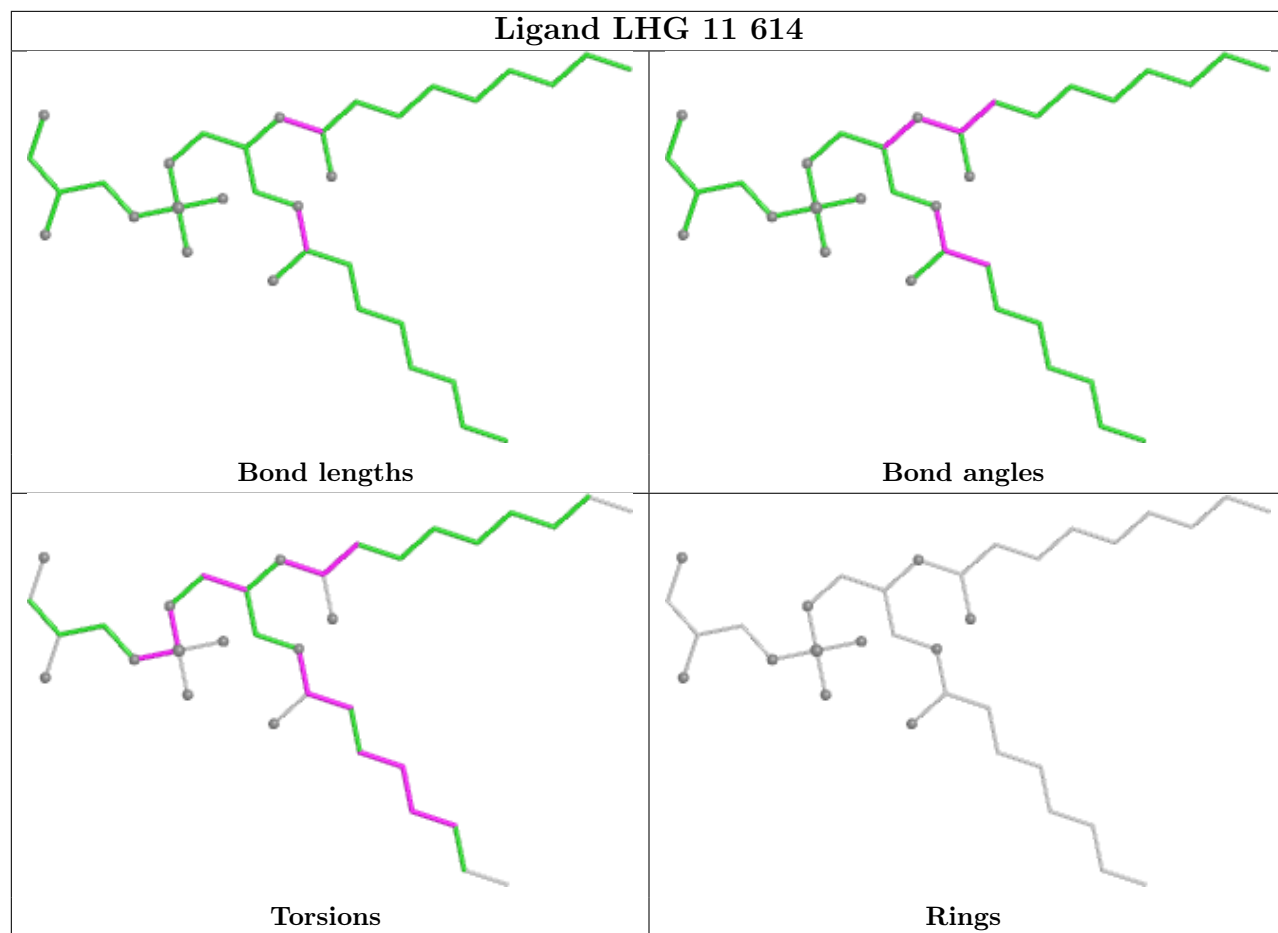
Ligand LMG Bb 621



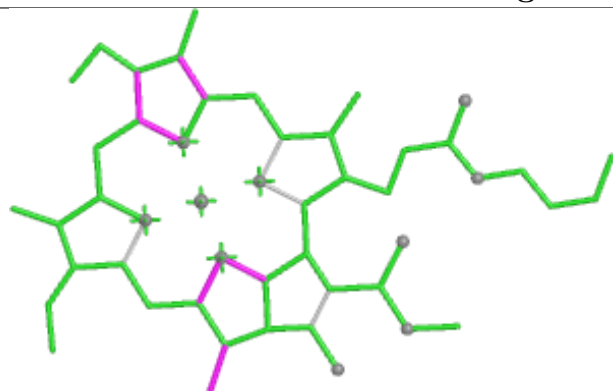


Ligand CHL Nn 315	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR CC 515	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LUT N 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

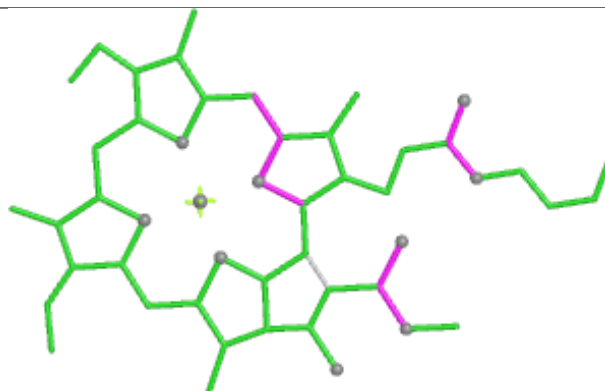




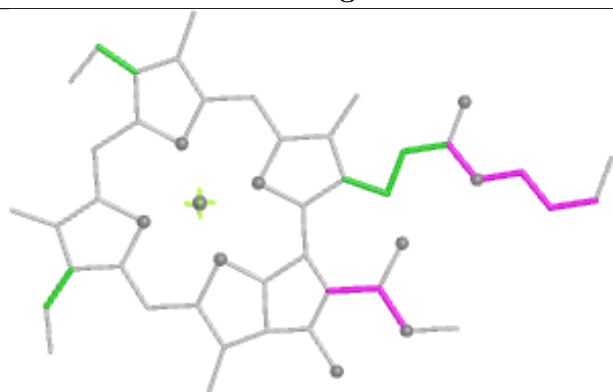
Ligand CLA S 611



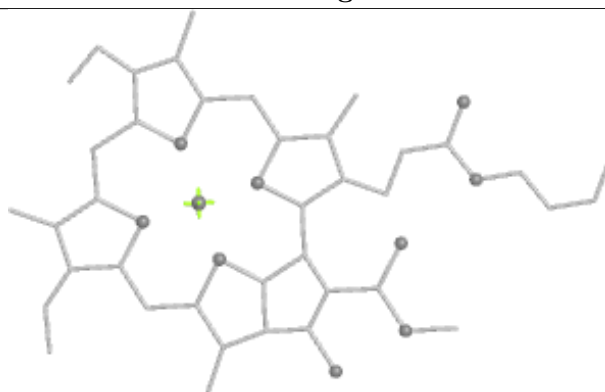
Bond lengths



Bond angles

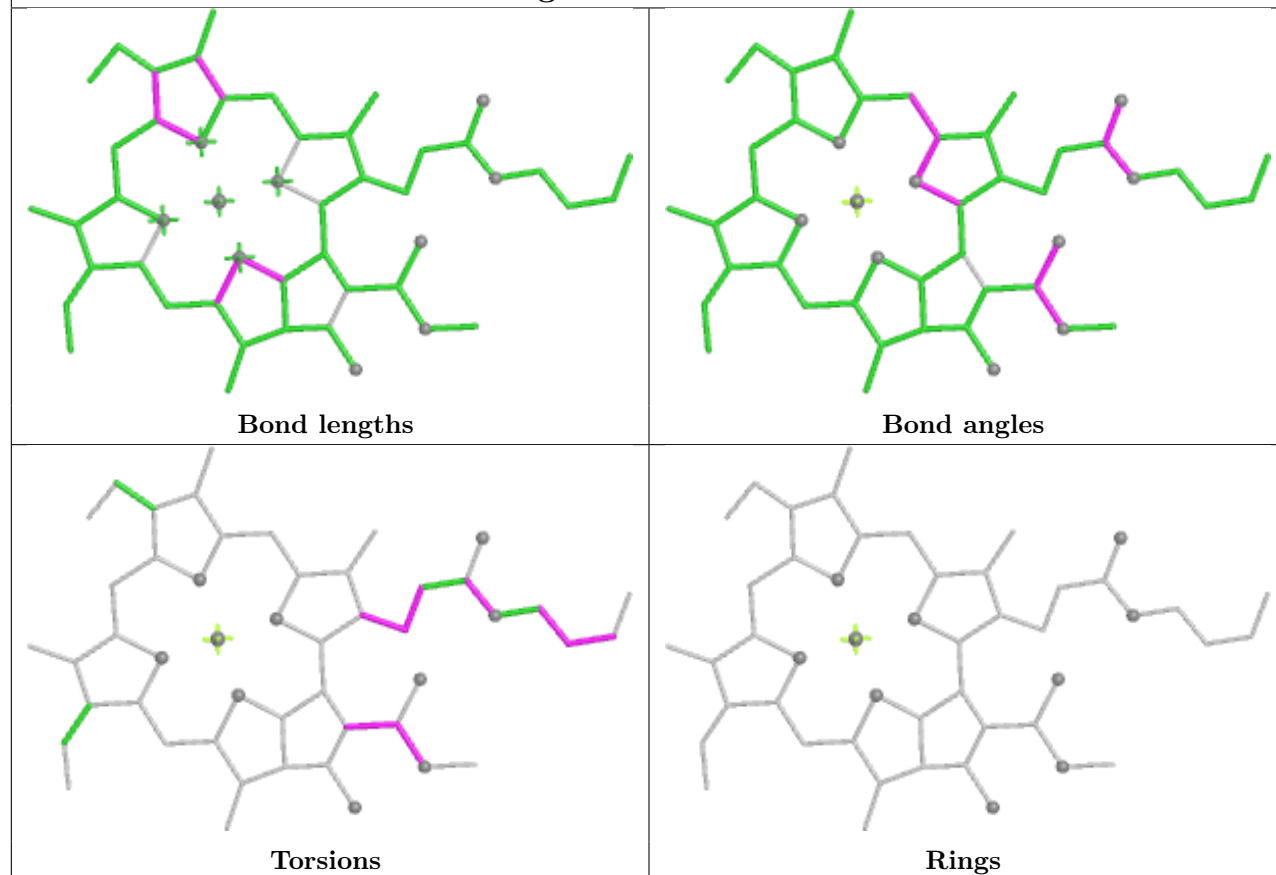


Torsions

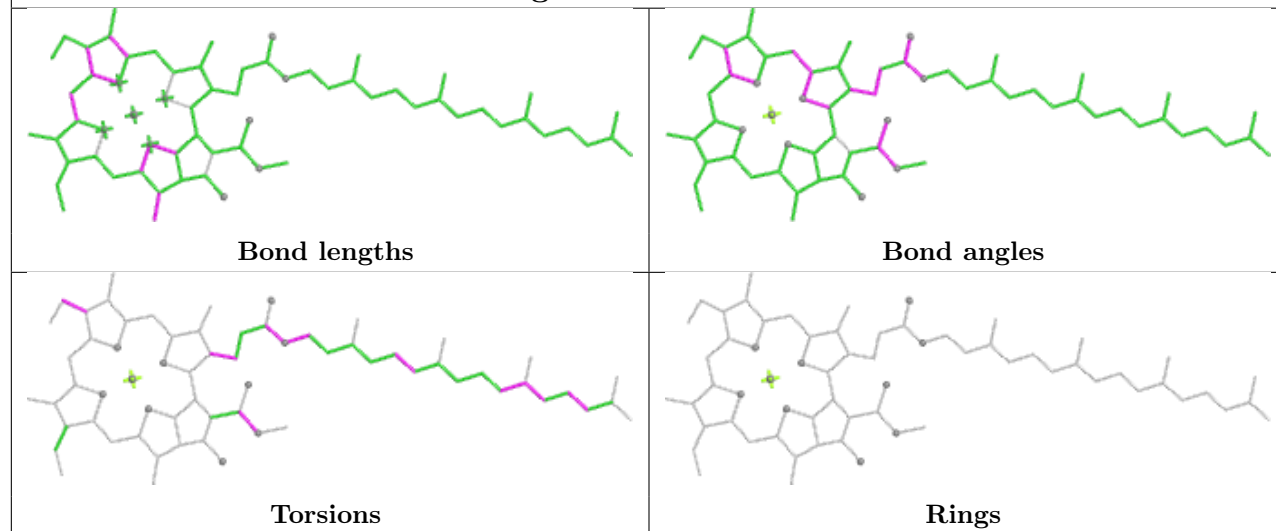


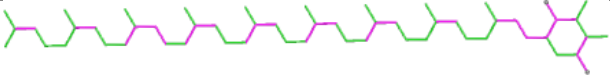
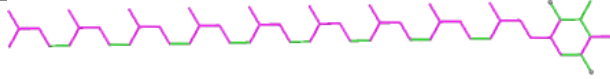
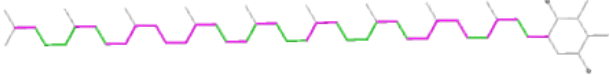
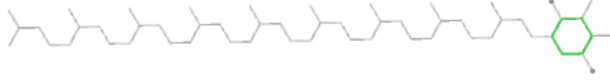
Rings

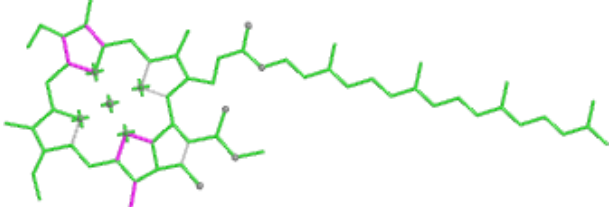
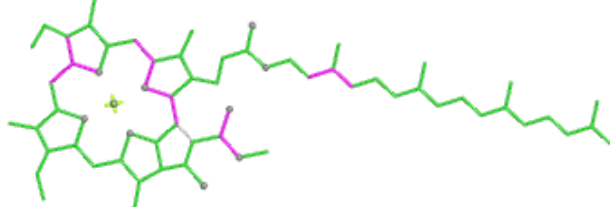
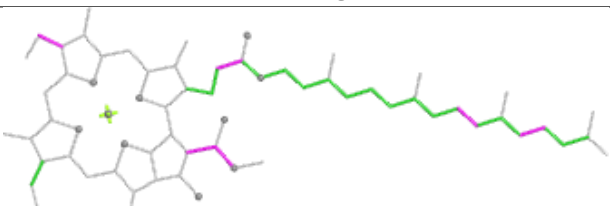
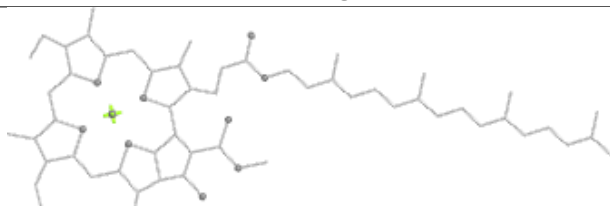
Ligand CLA r 610

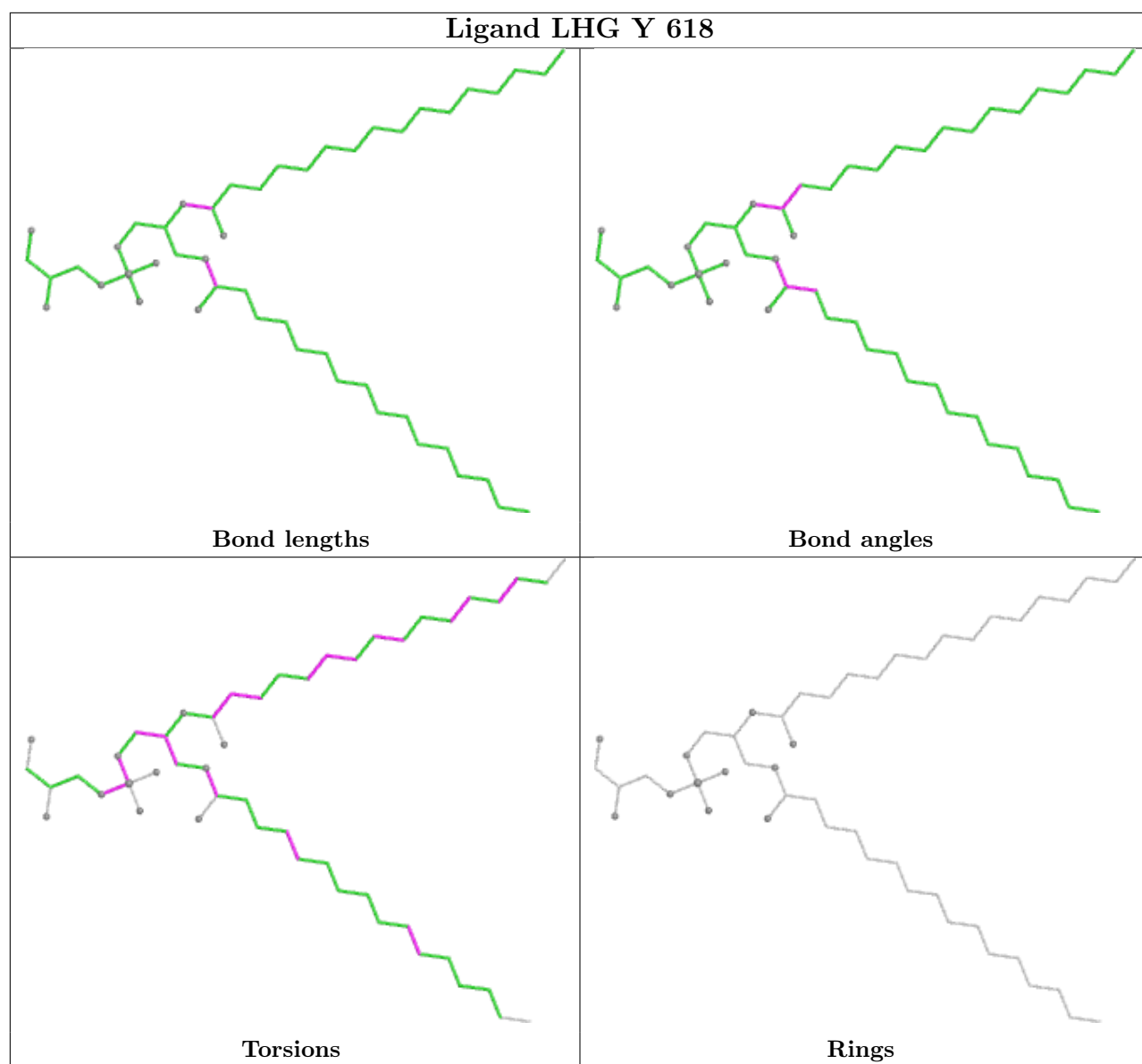


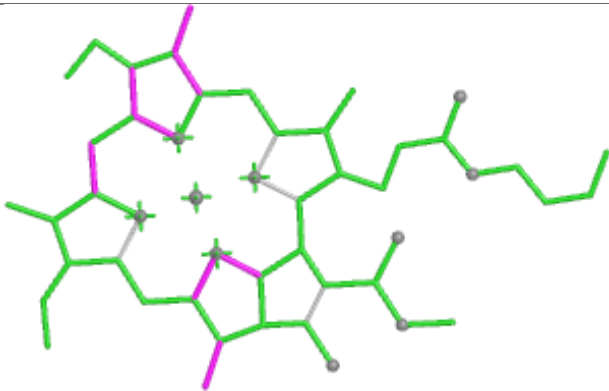
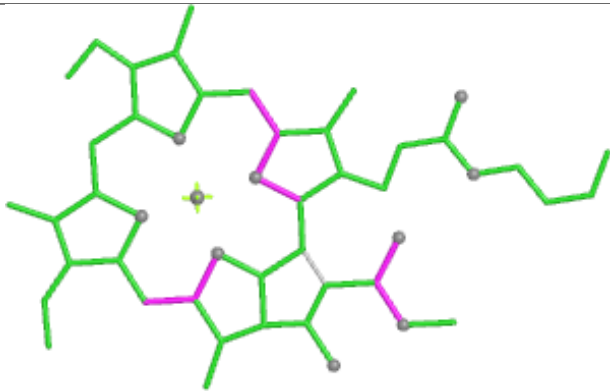
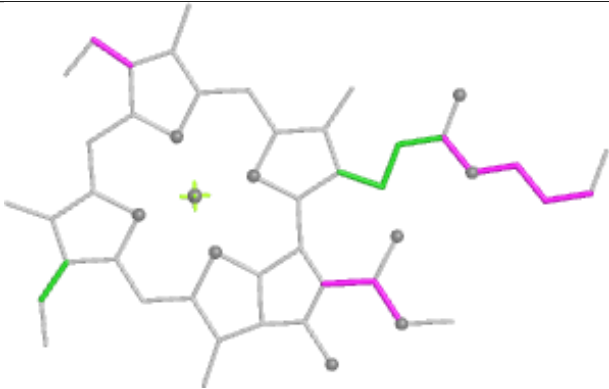
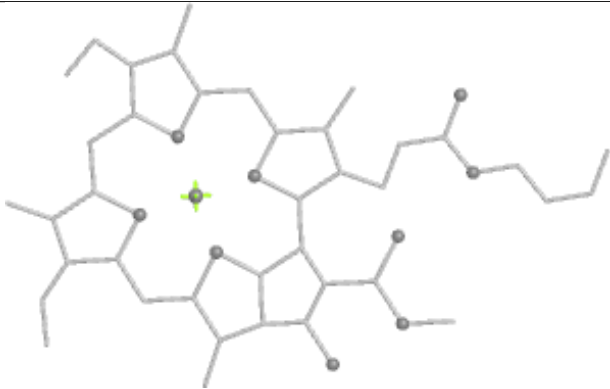
Ligand CLA N 610

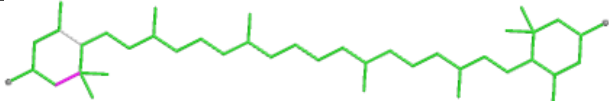
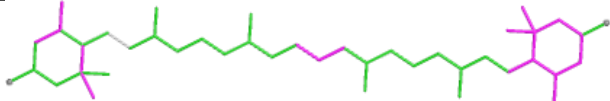
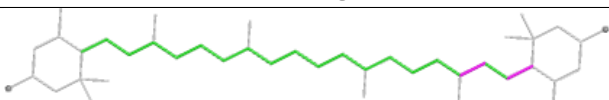


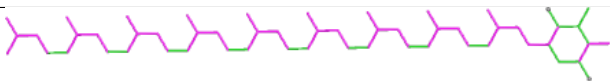
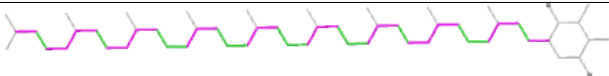
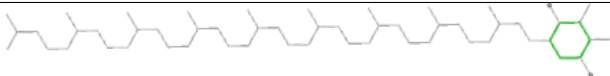
Ligand PL9 A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

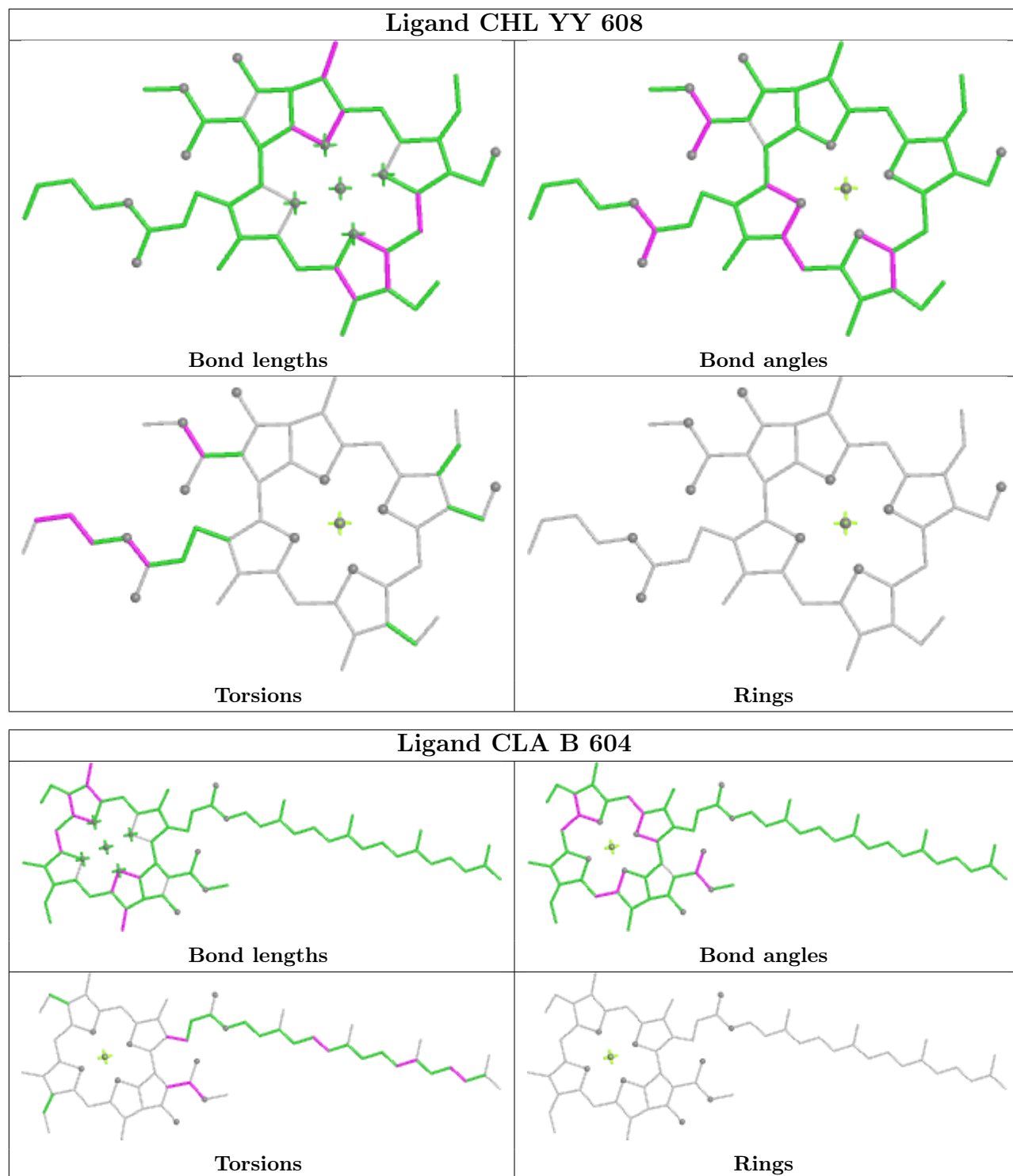
Ligand CLA c 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

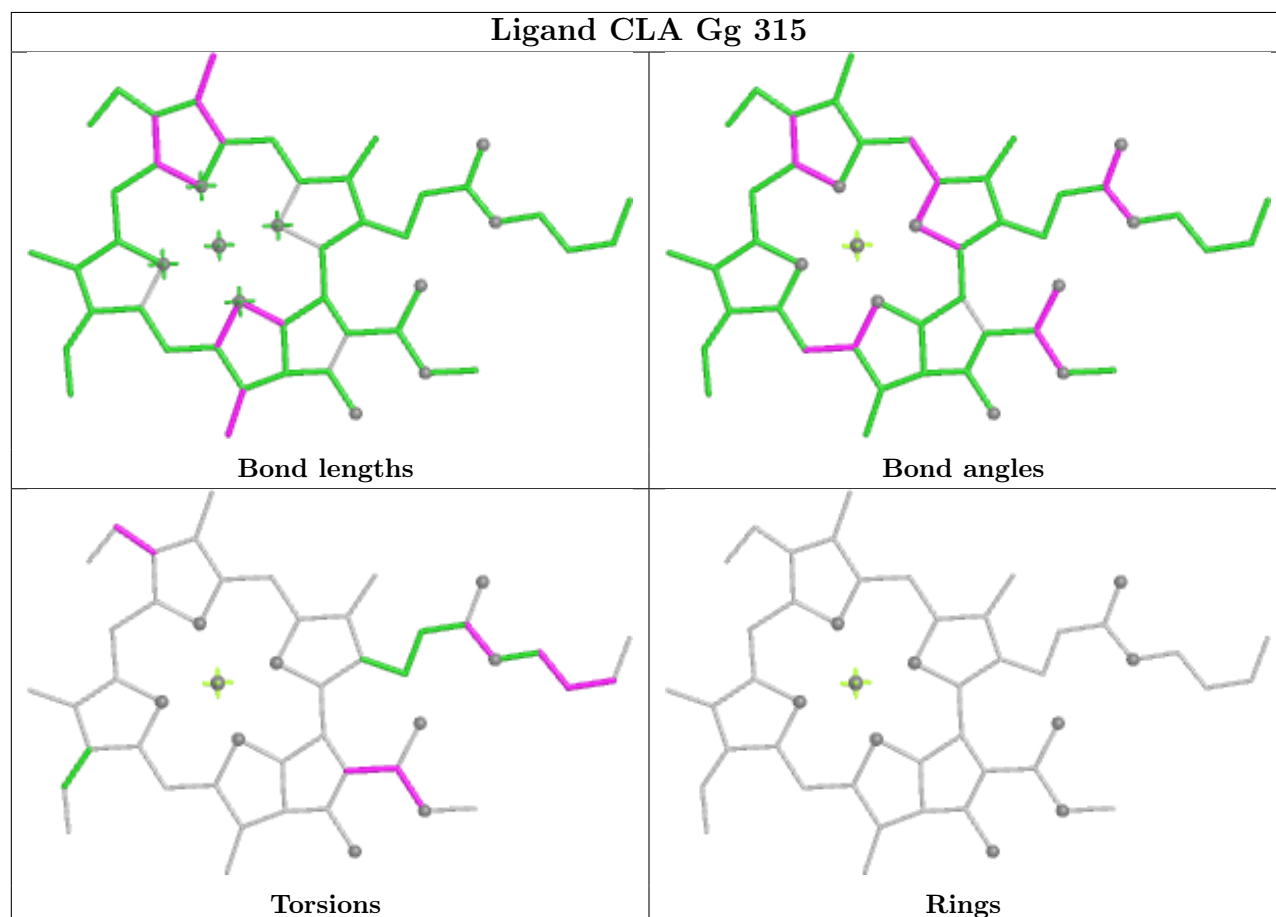
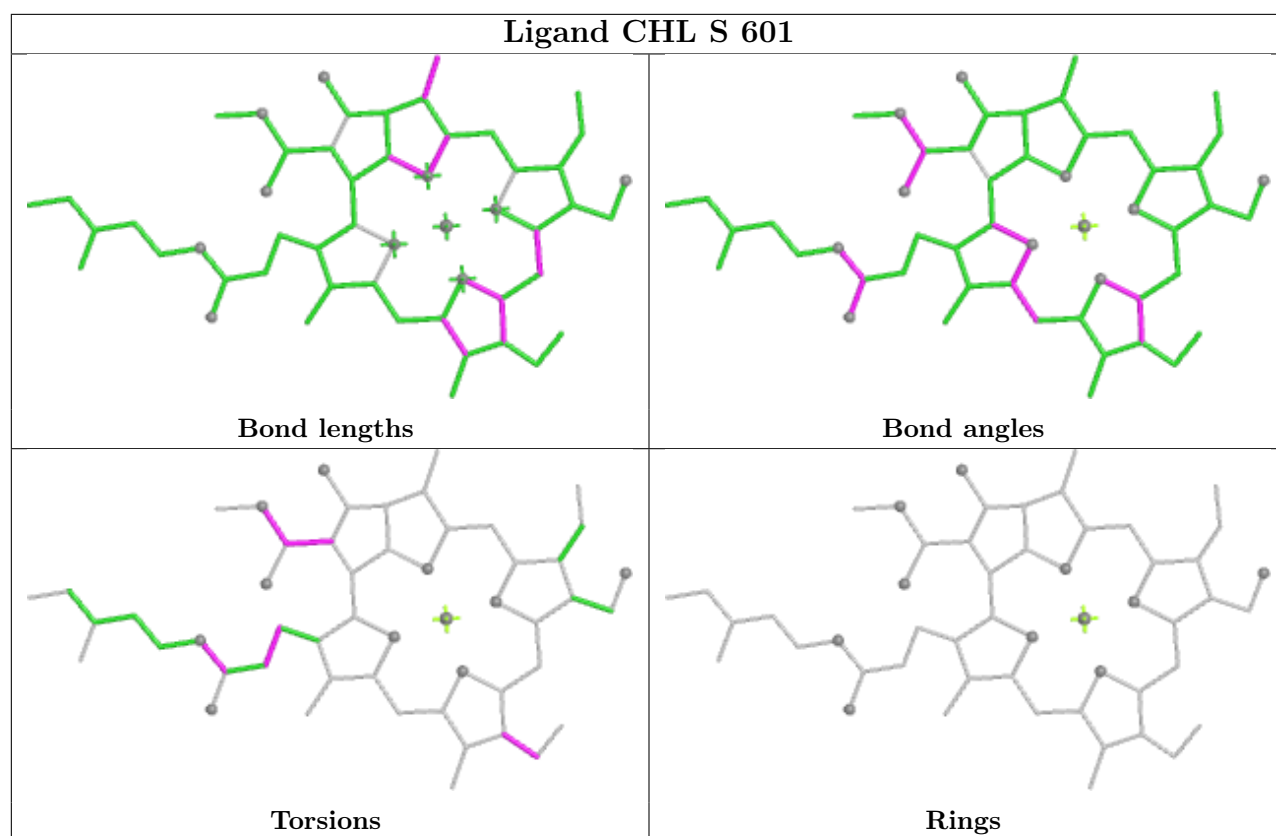


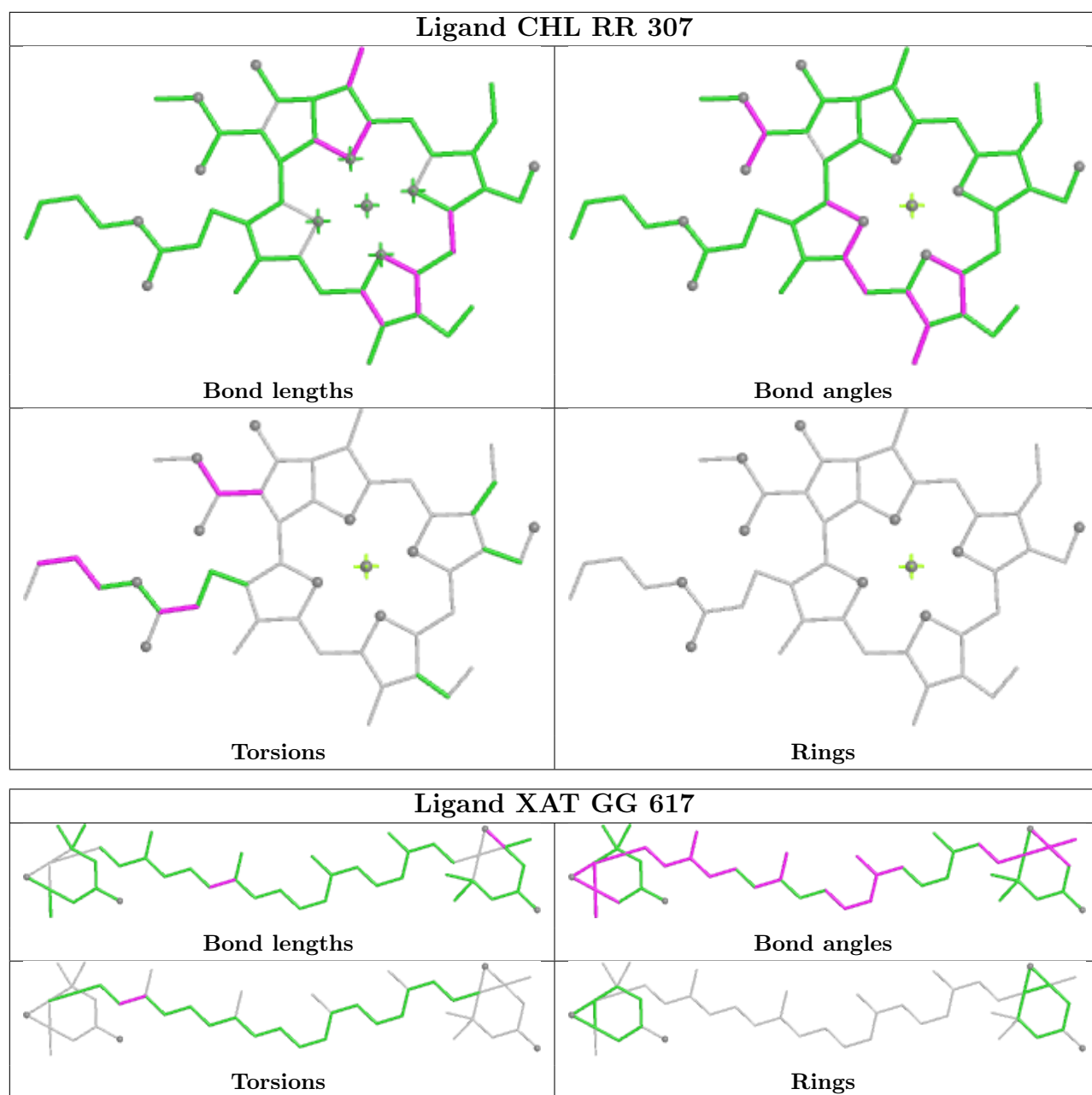
Ligand CLA R 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

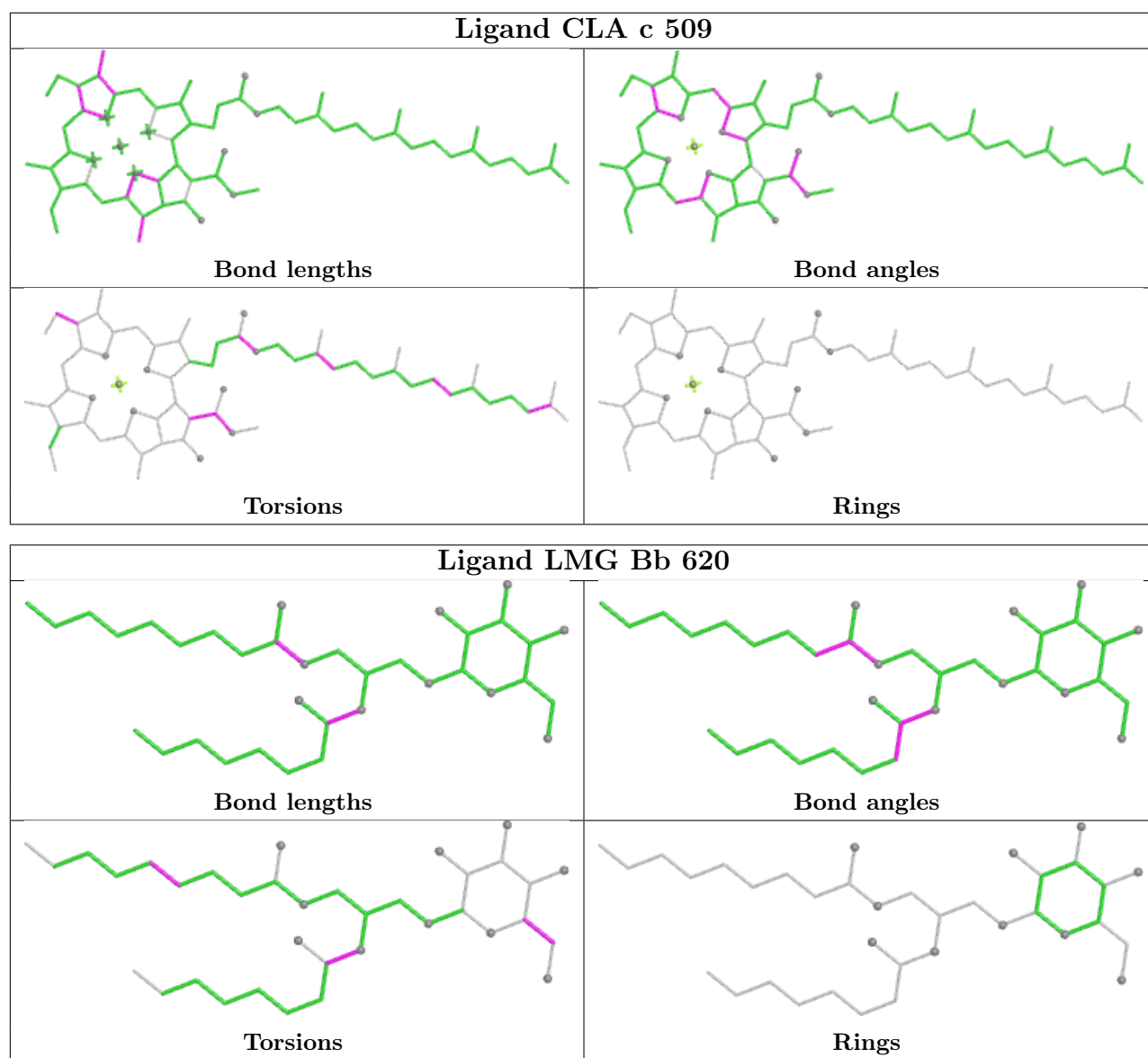
Ligand LUT y 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

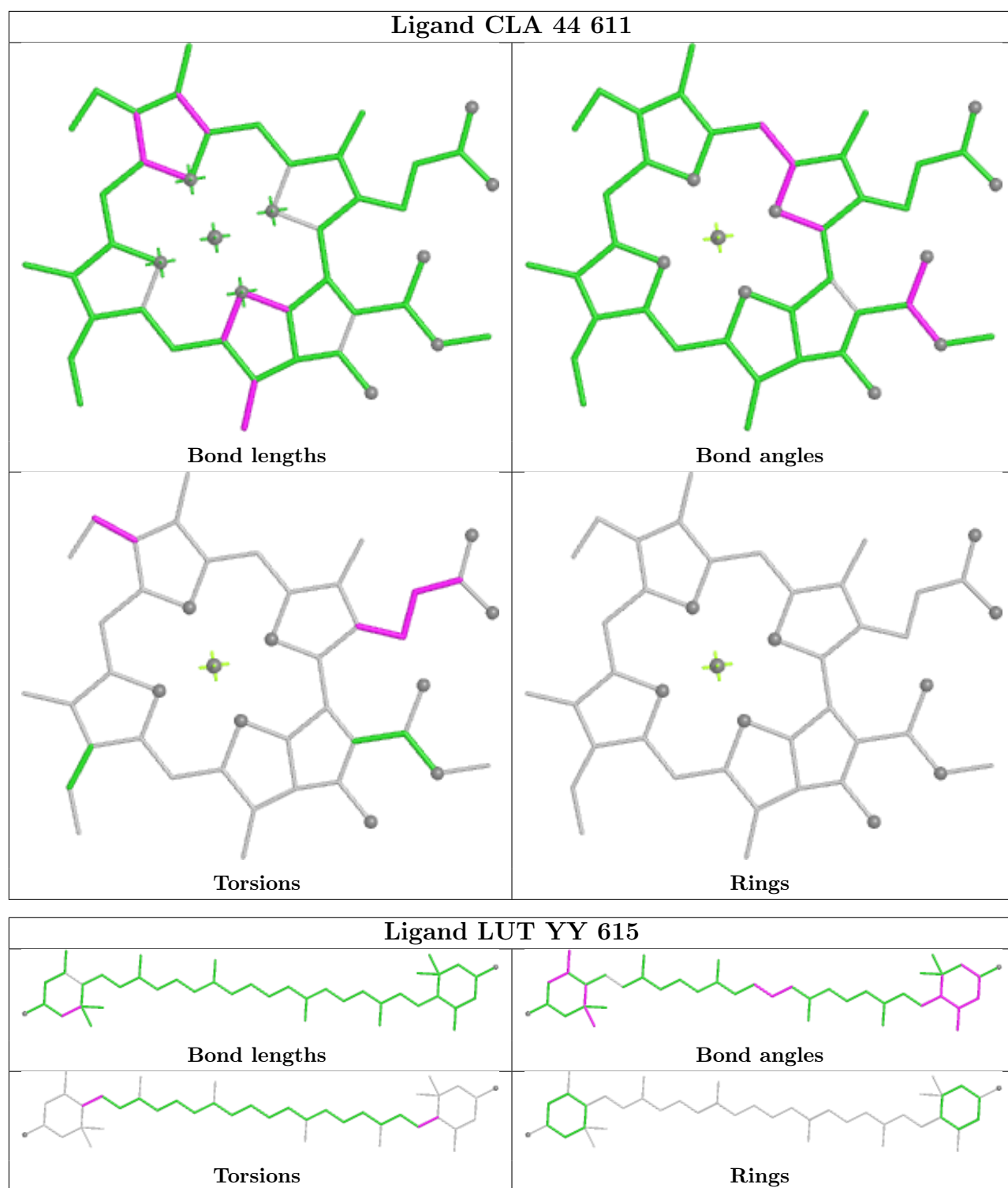
Ligand PL9 DD 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

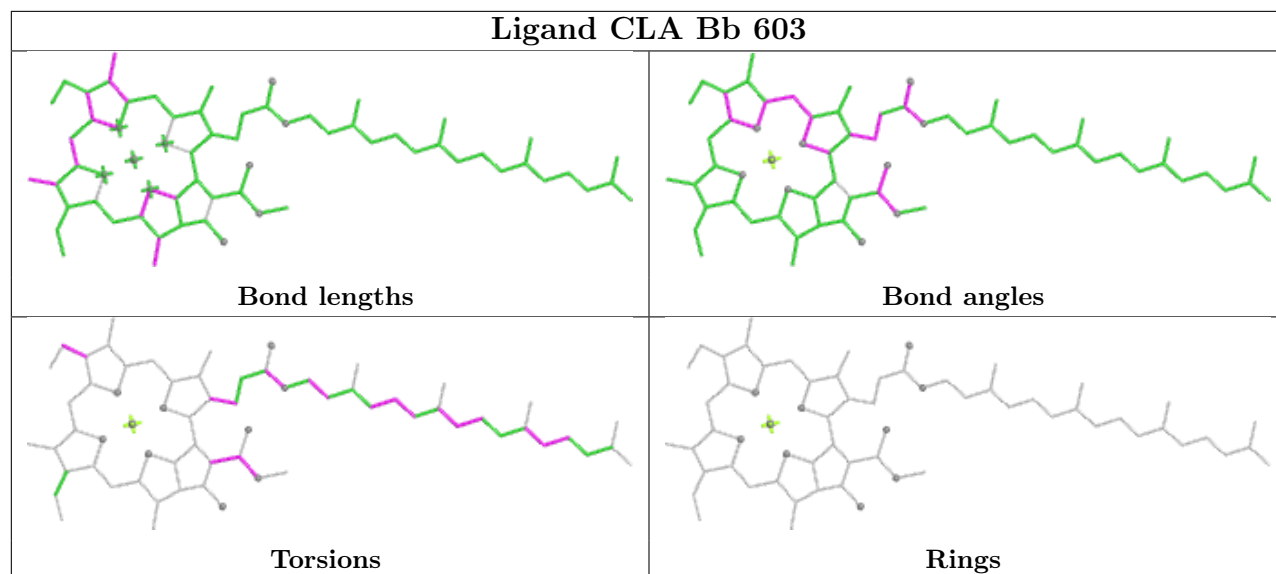
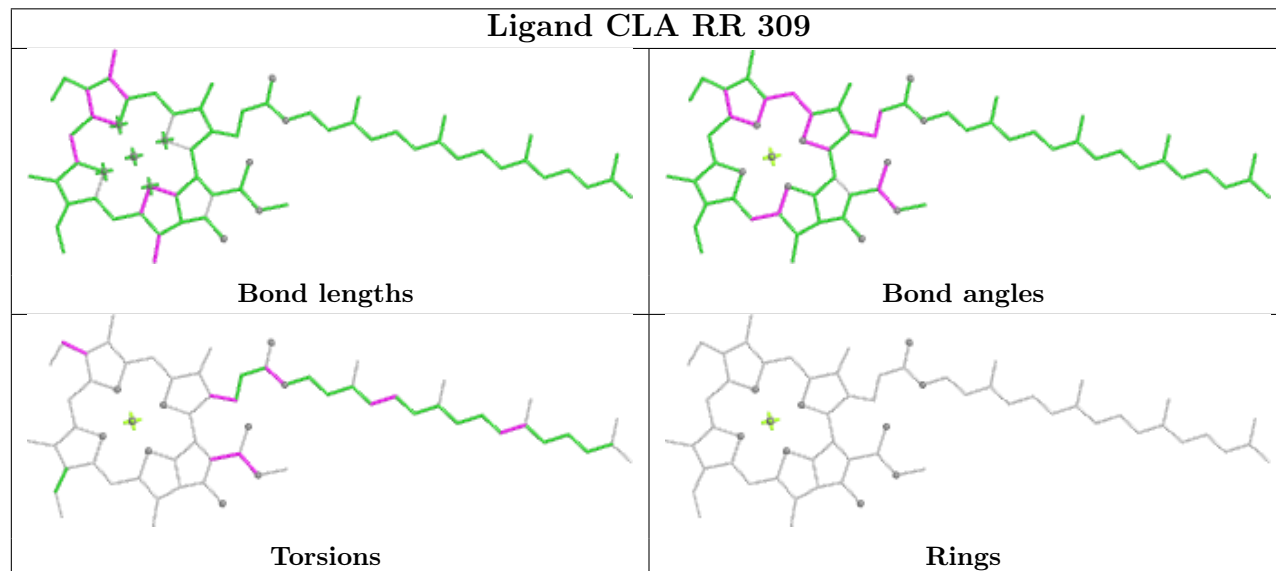


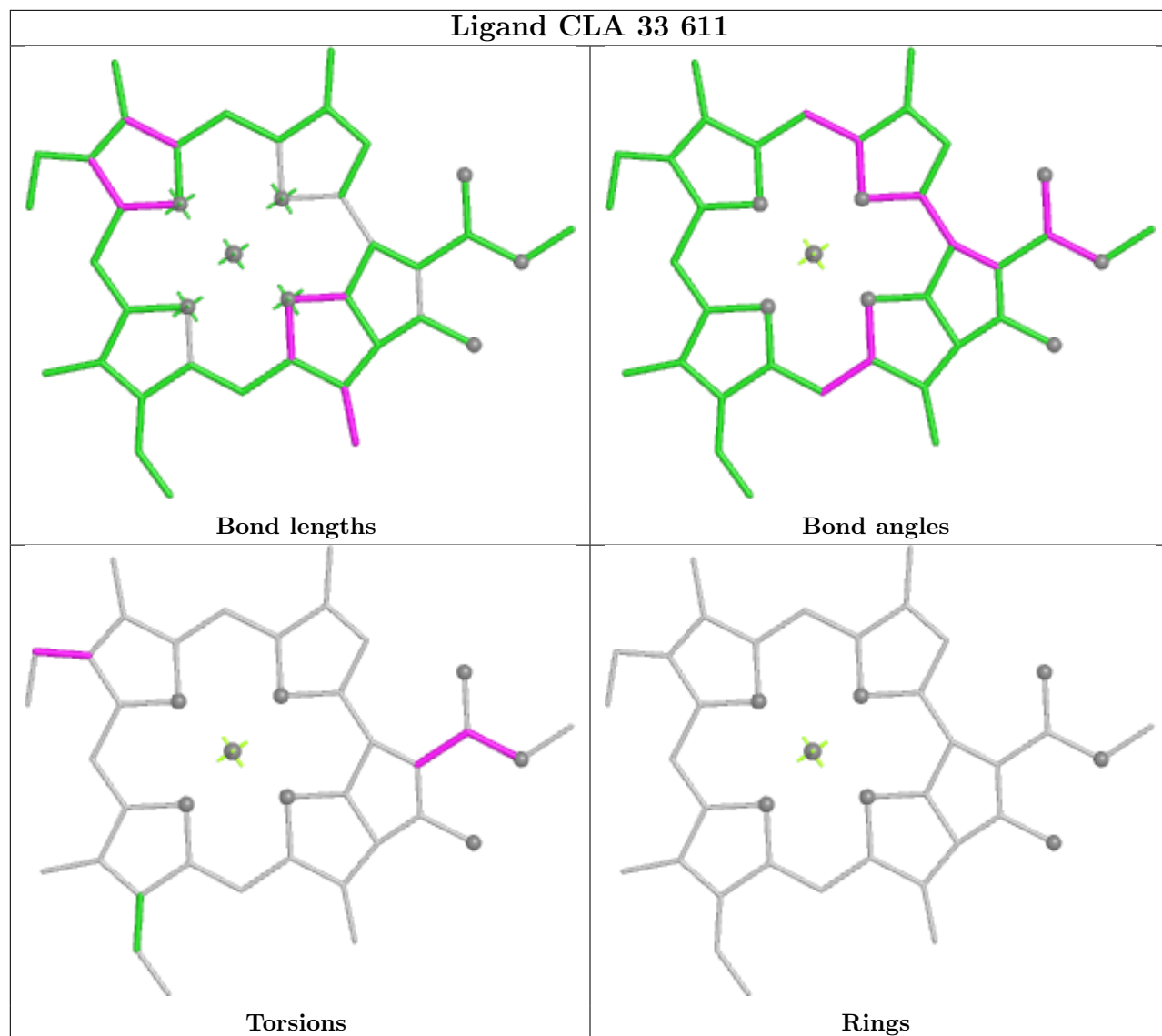


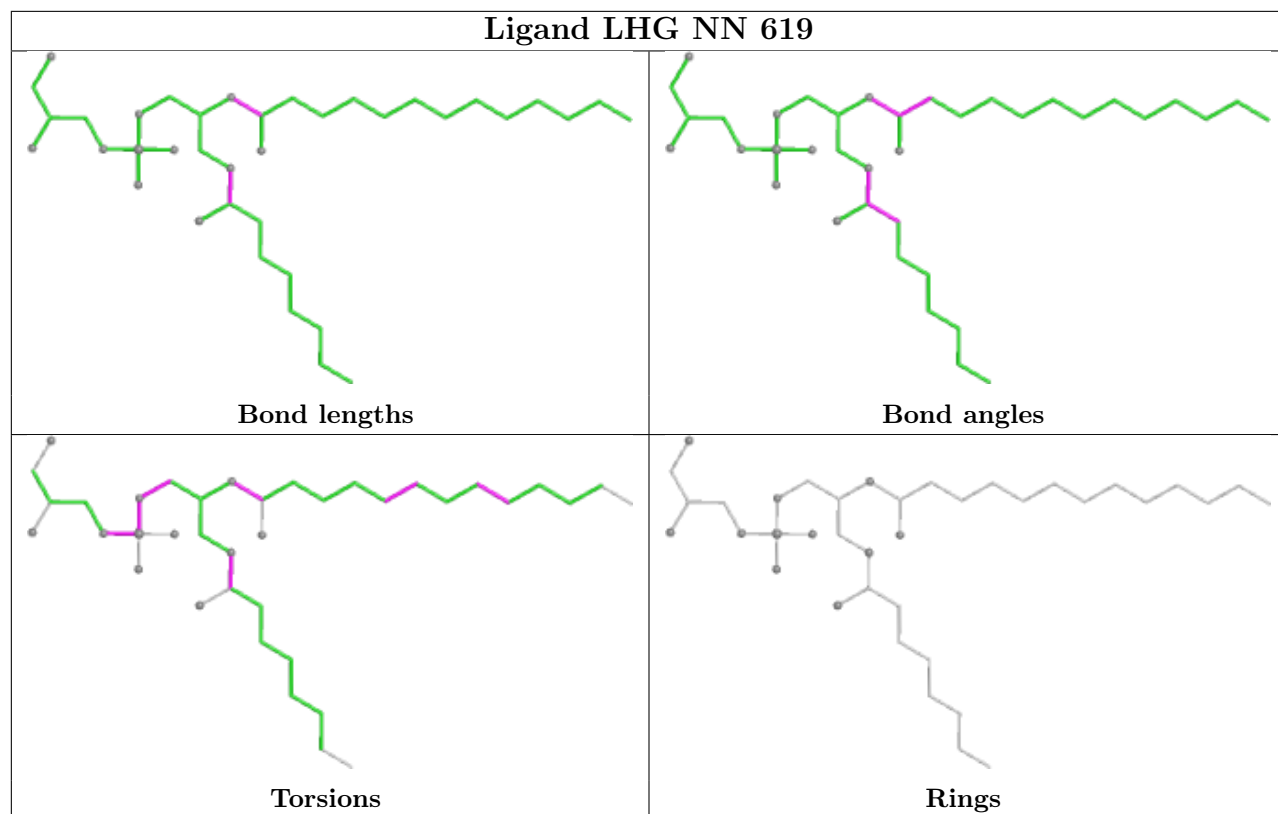




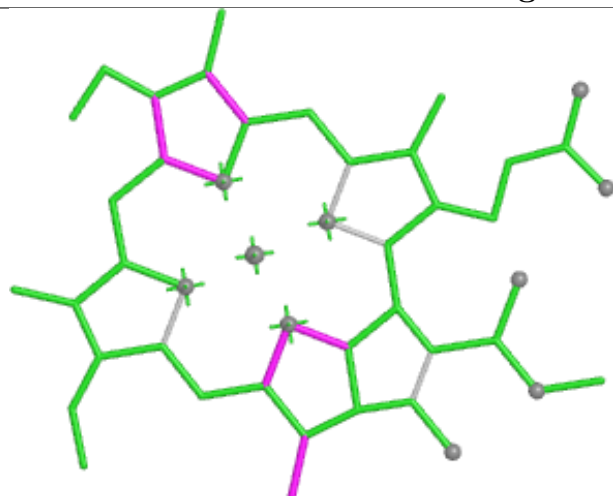


Ligand CLA Bb 603**Ligand CLA RR 309**

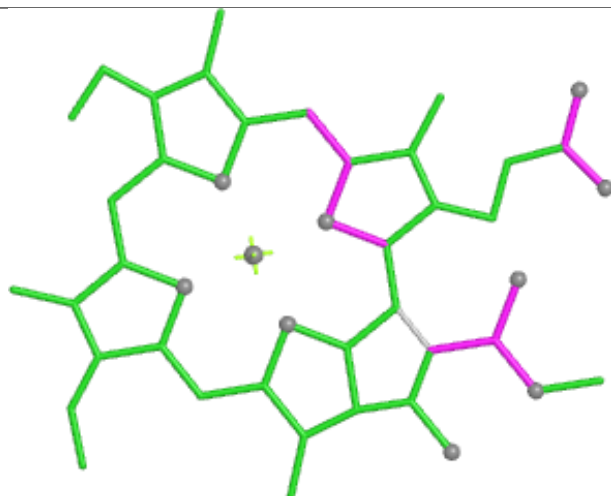




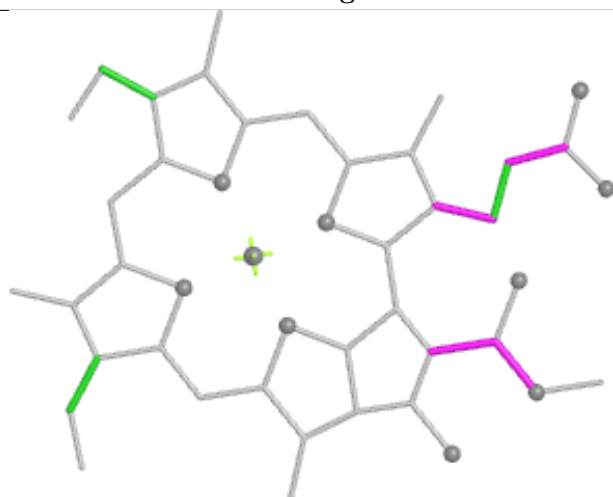
Ligand CLA 4 303



Bond lengths



Bond angles

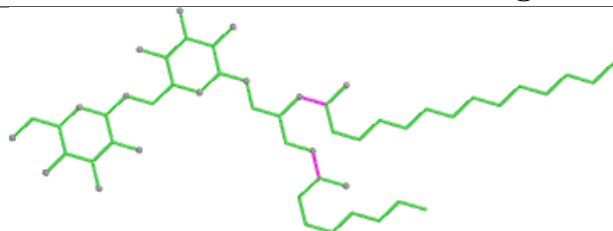


Torsions

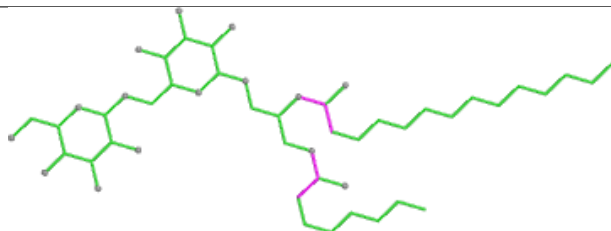


Rings

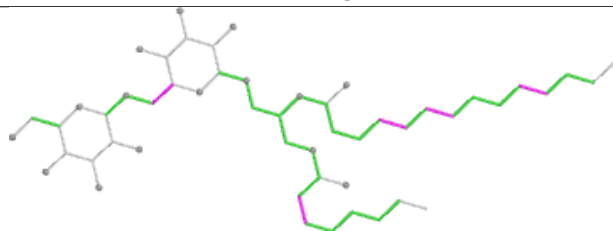
Ligand DGD c 518



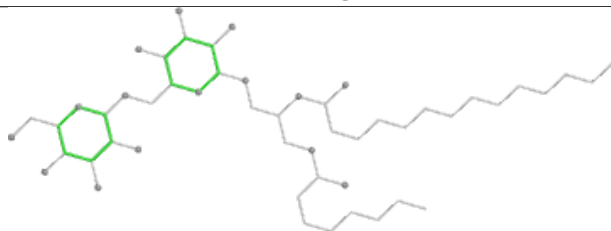
Bond lengths



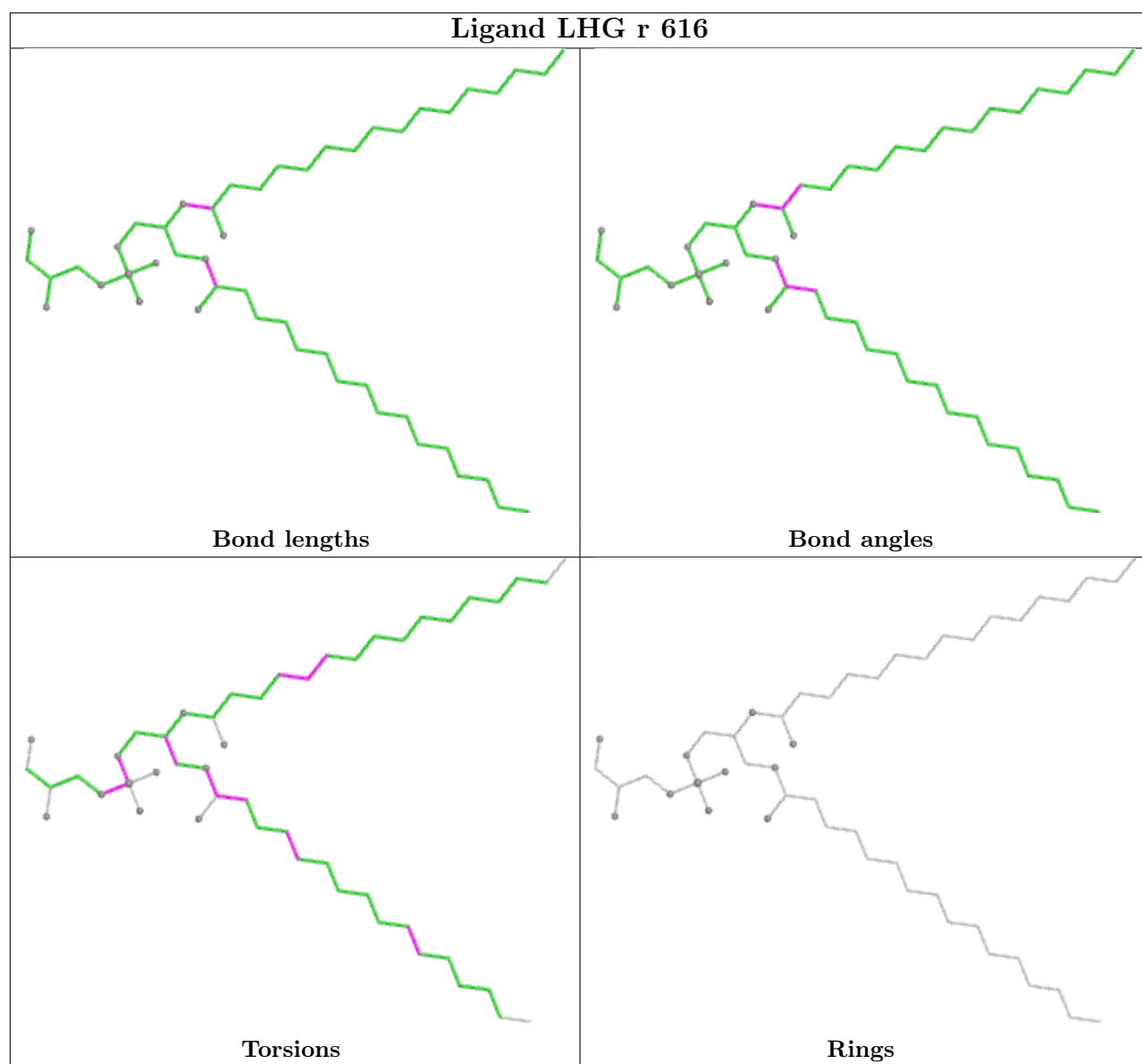
Bond angles

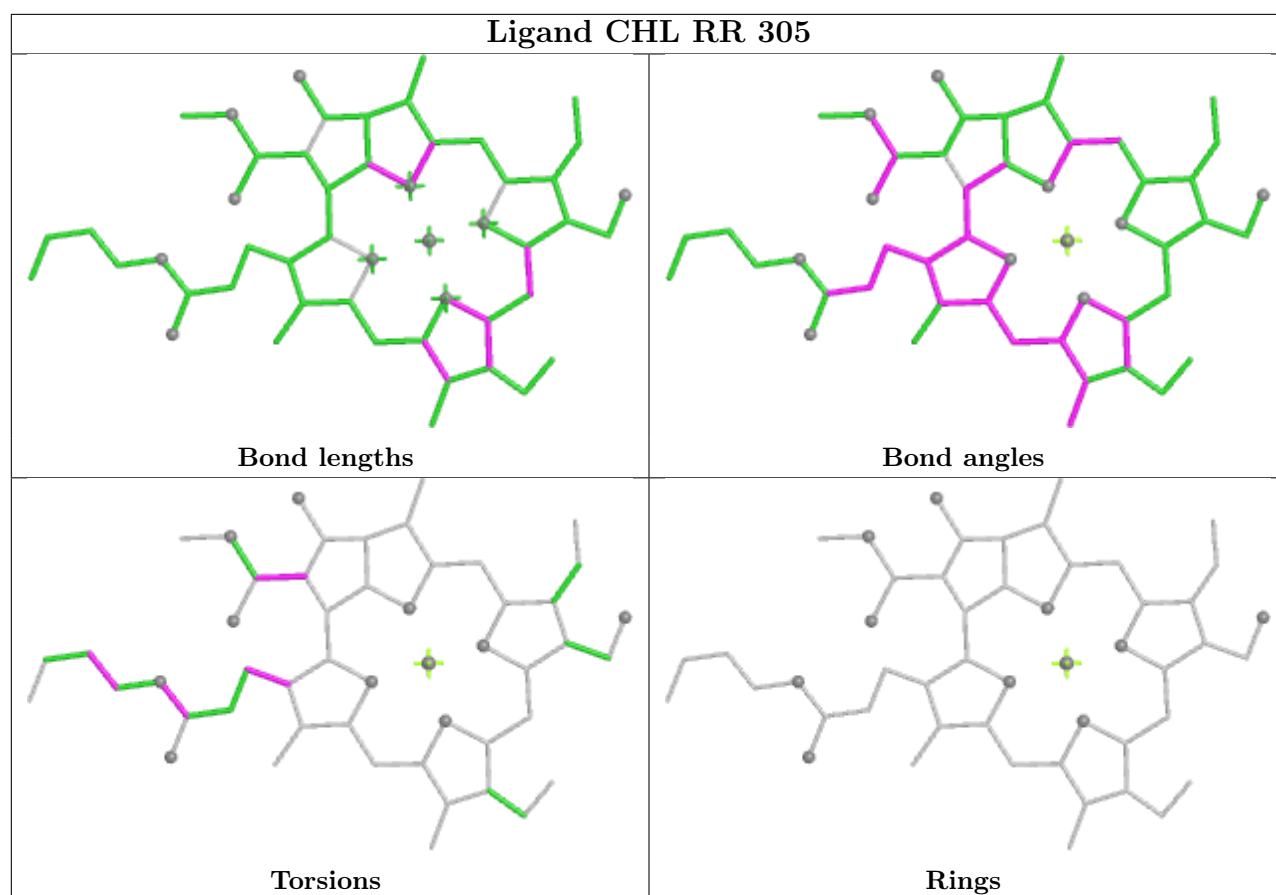


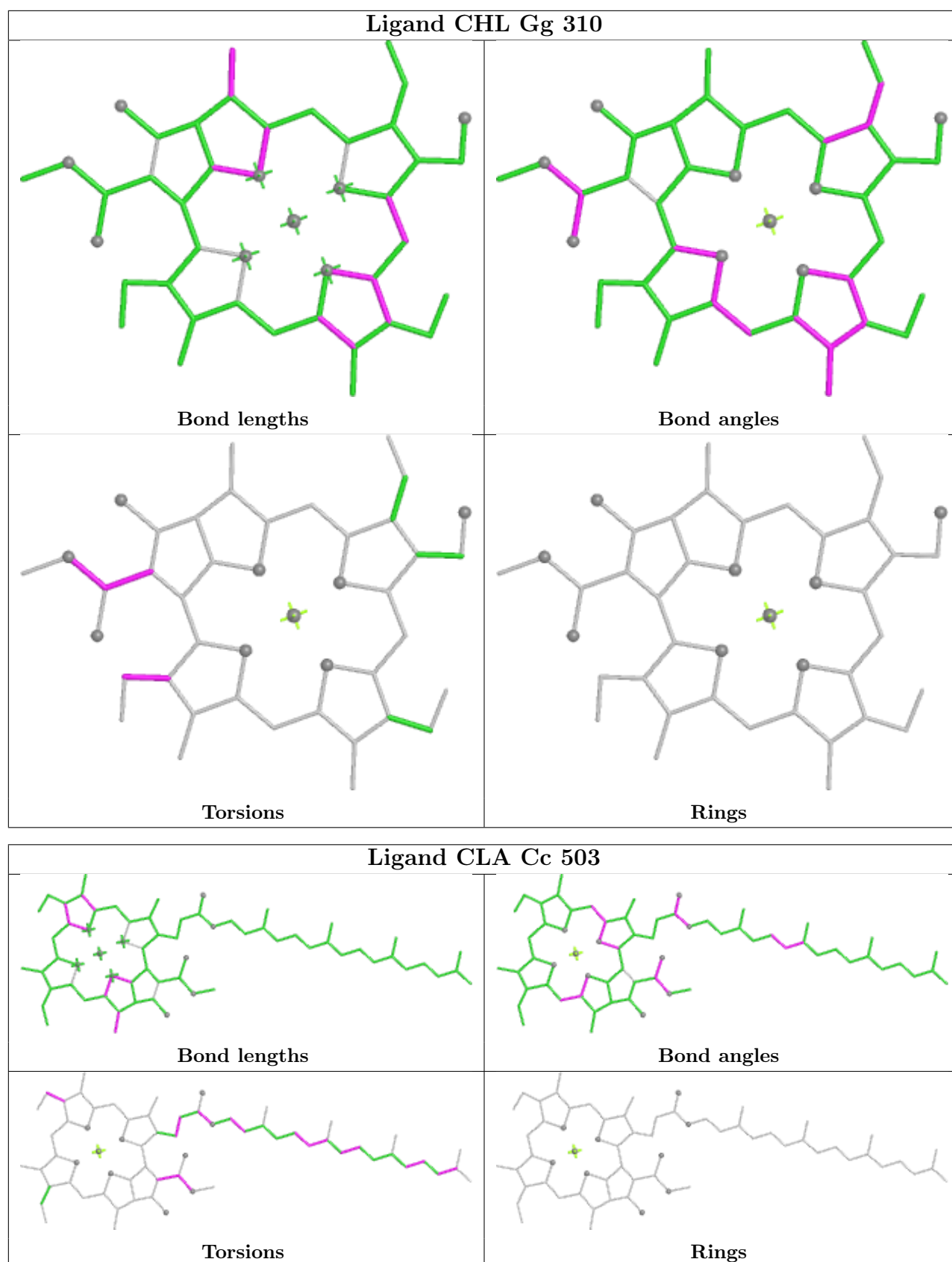
Torsions



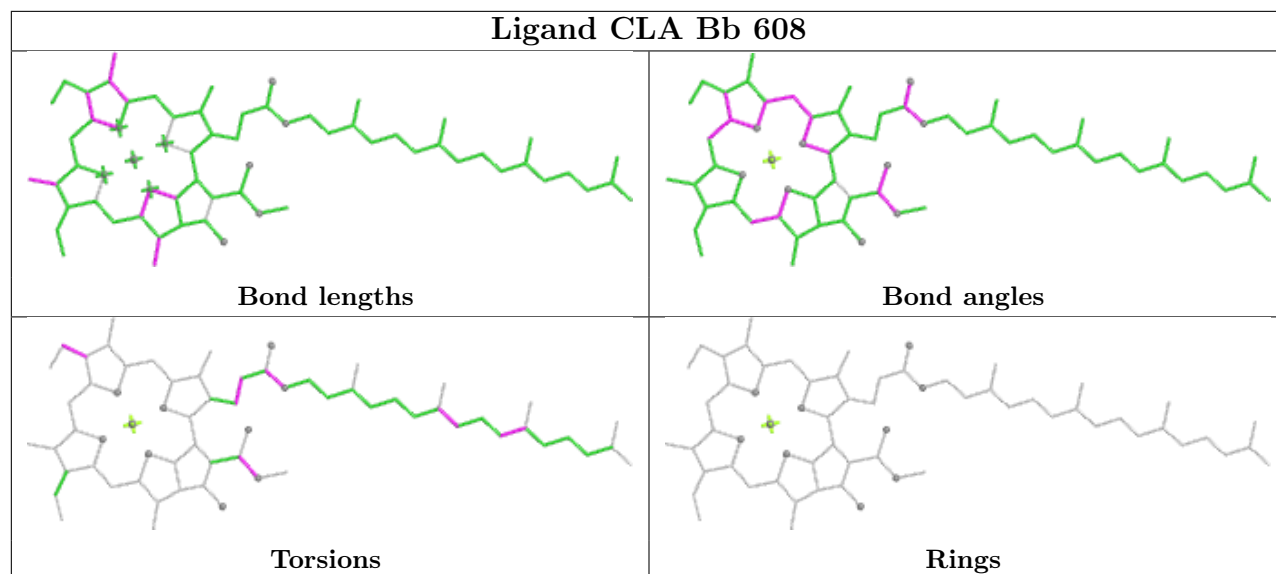
Rings



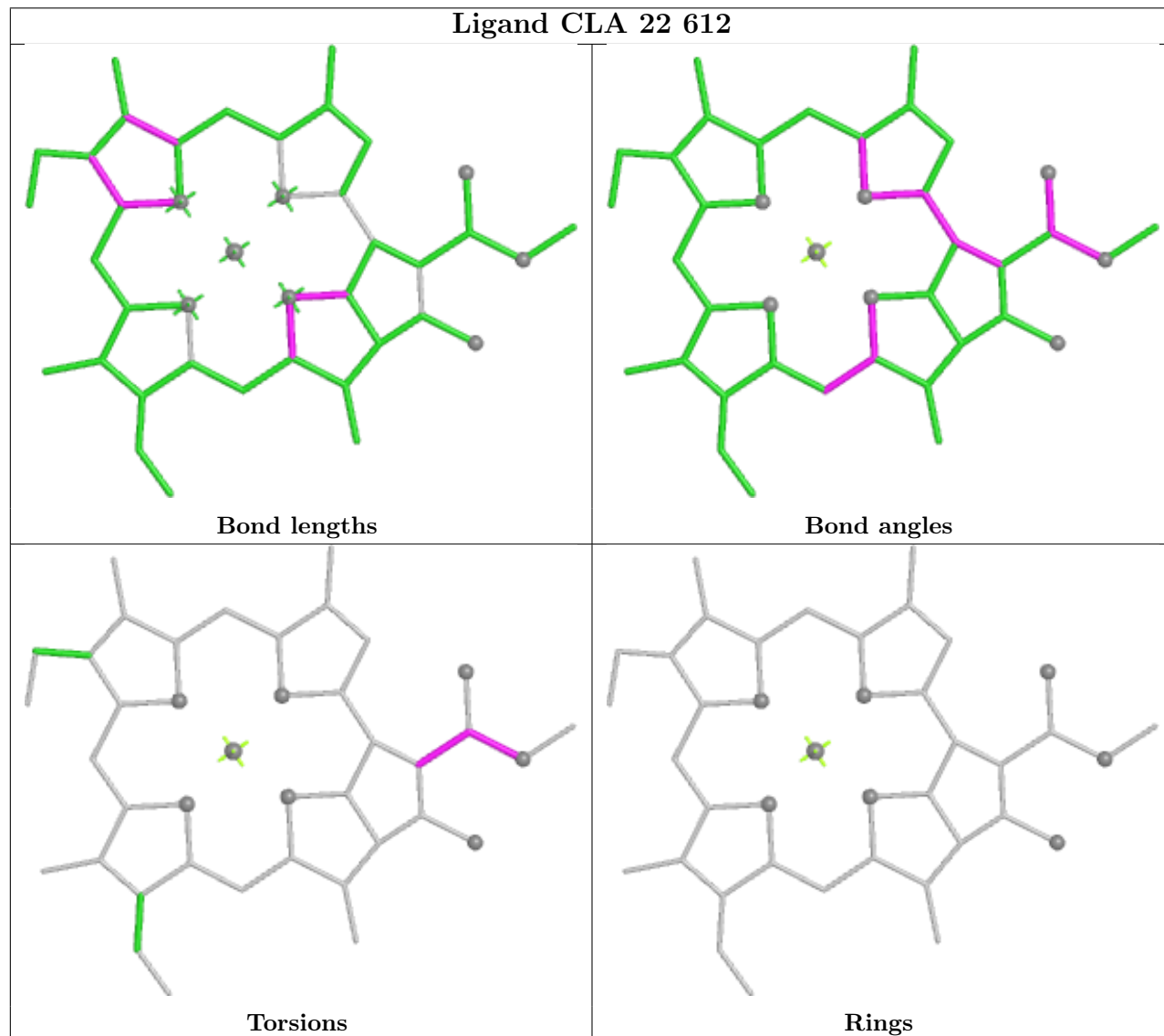


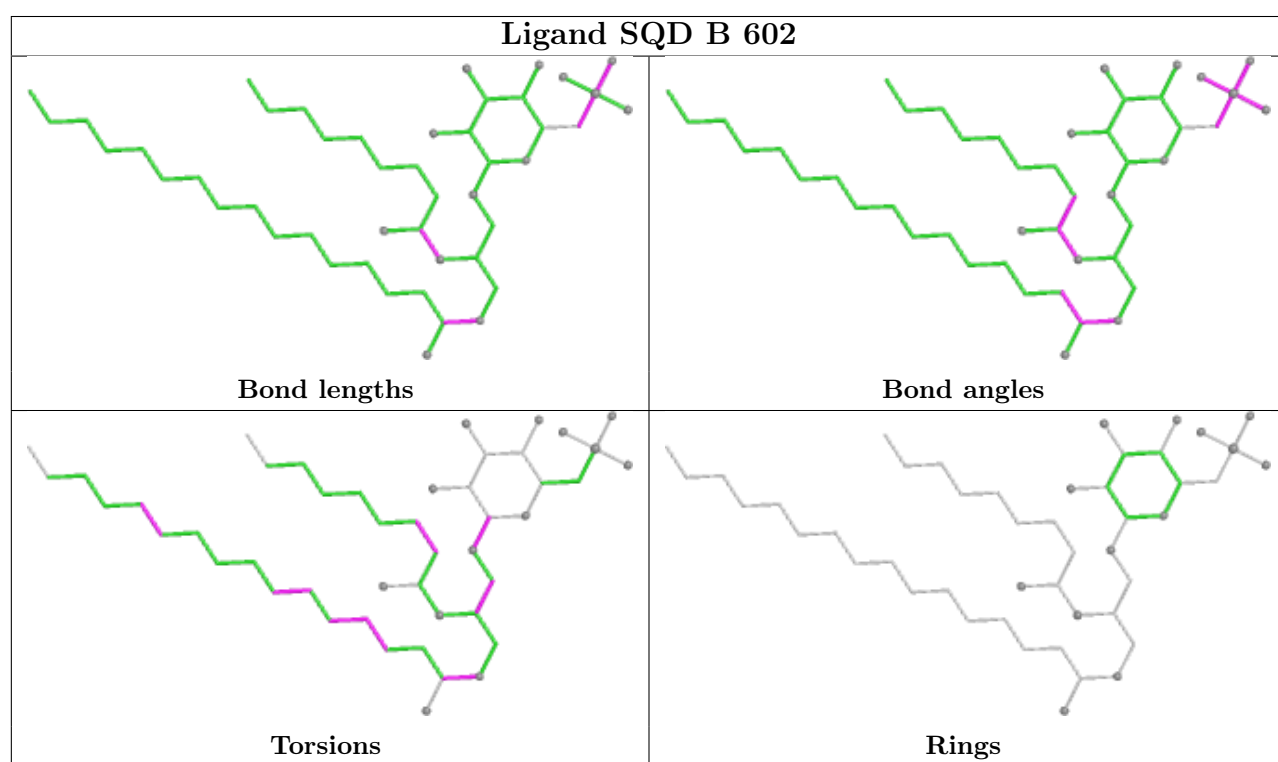
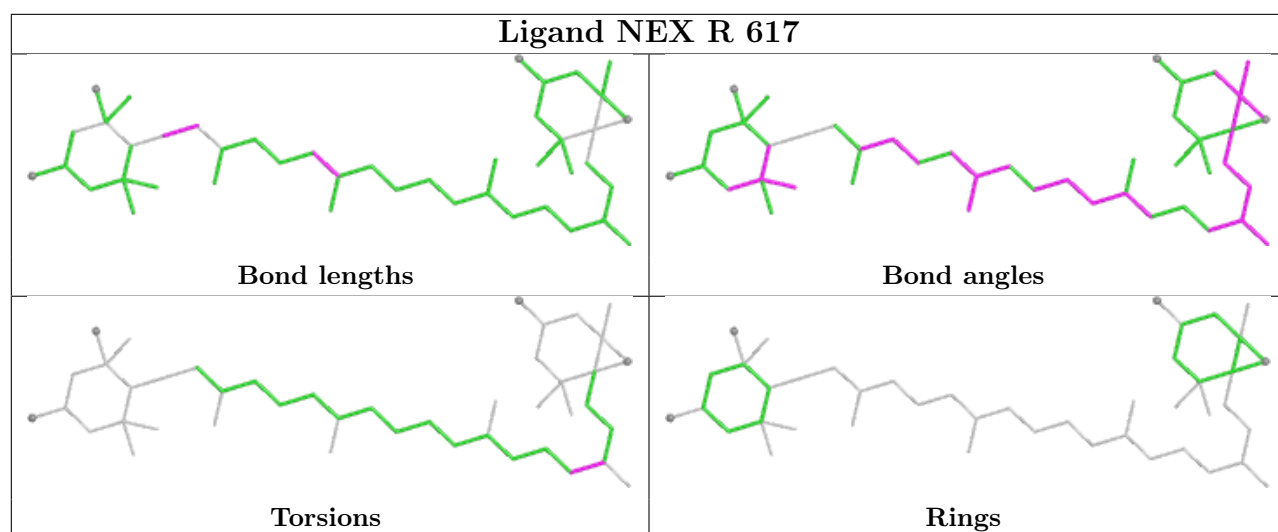


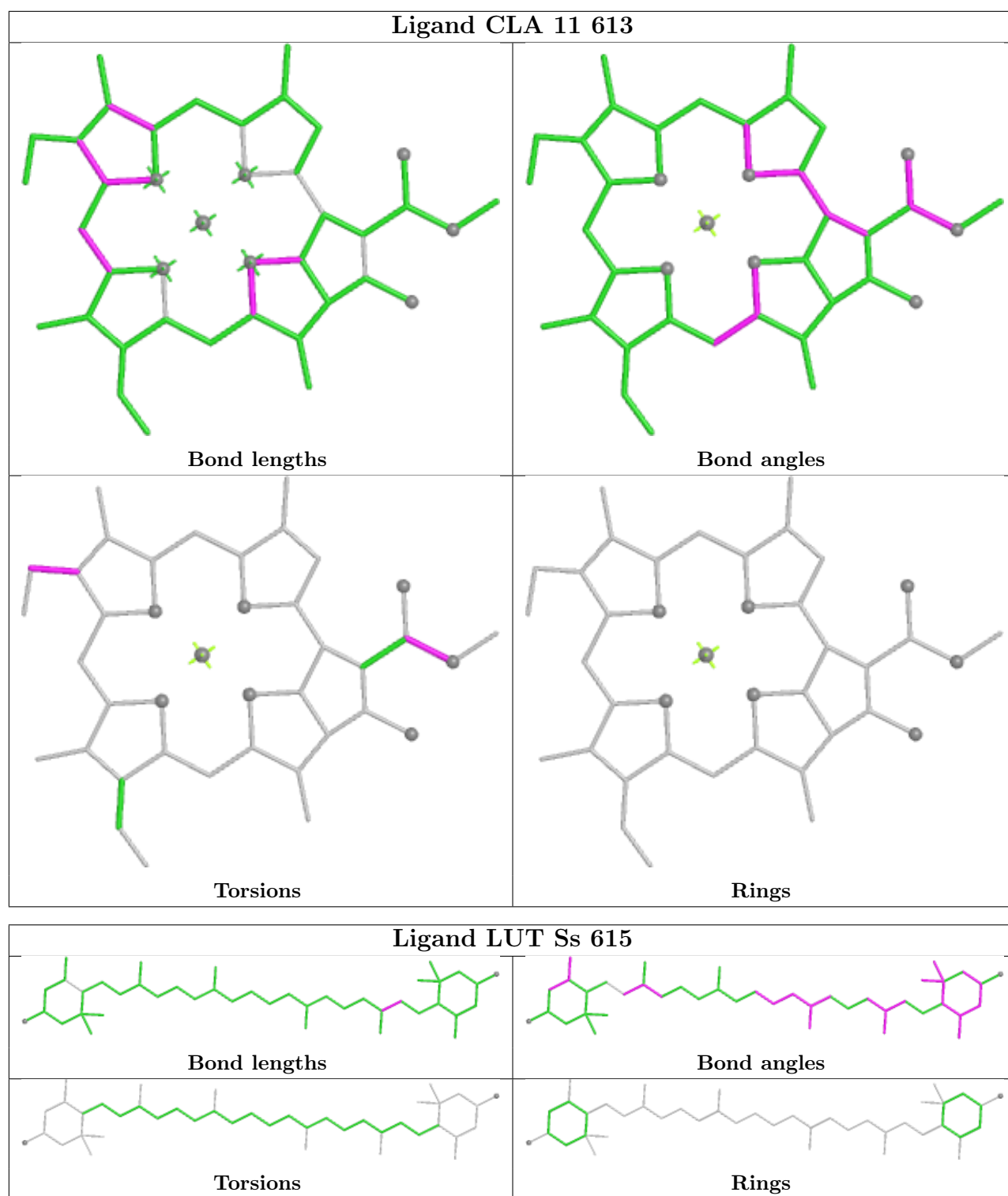
Ligand CLA Bb 608

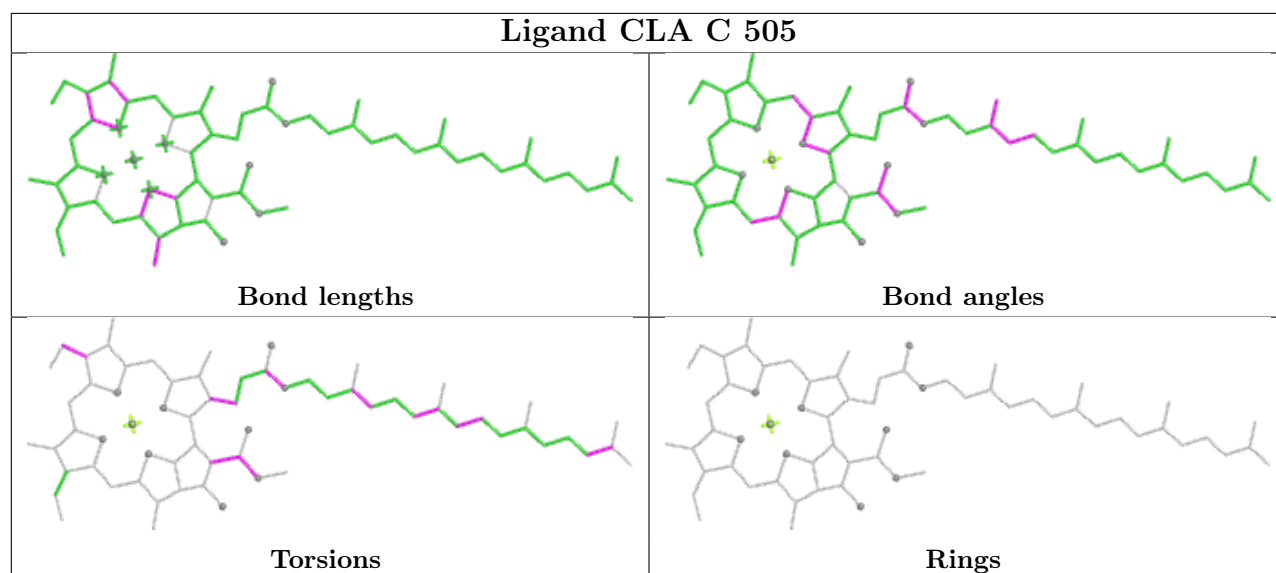
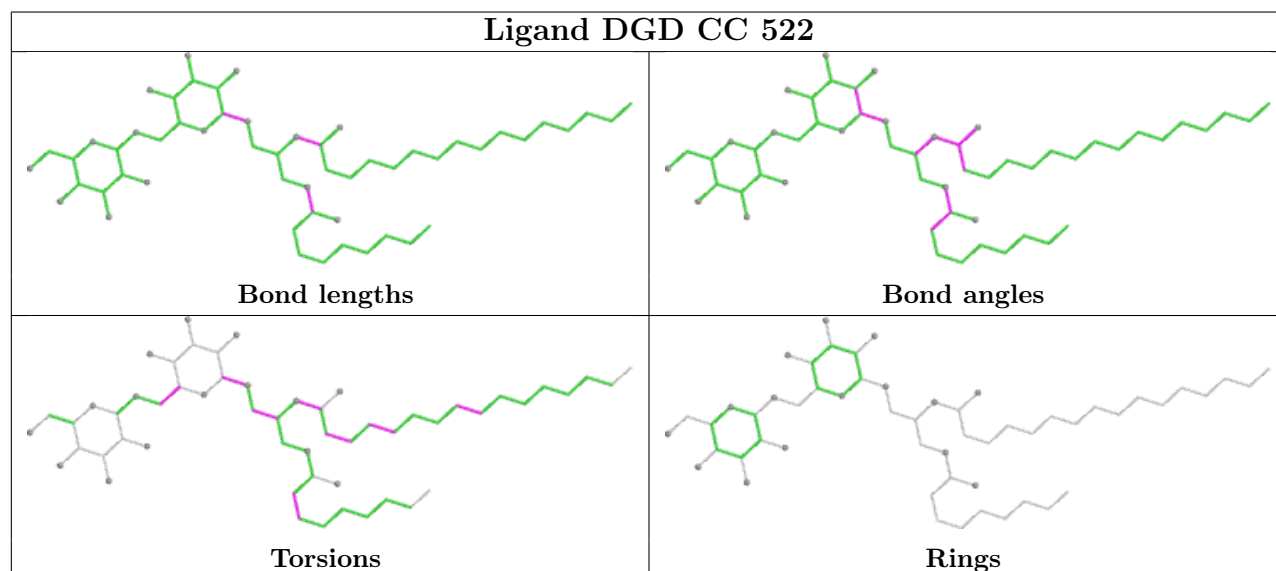
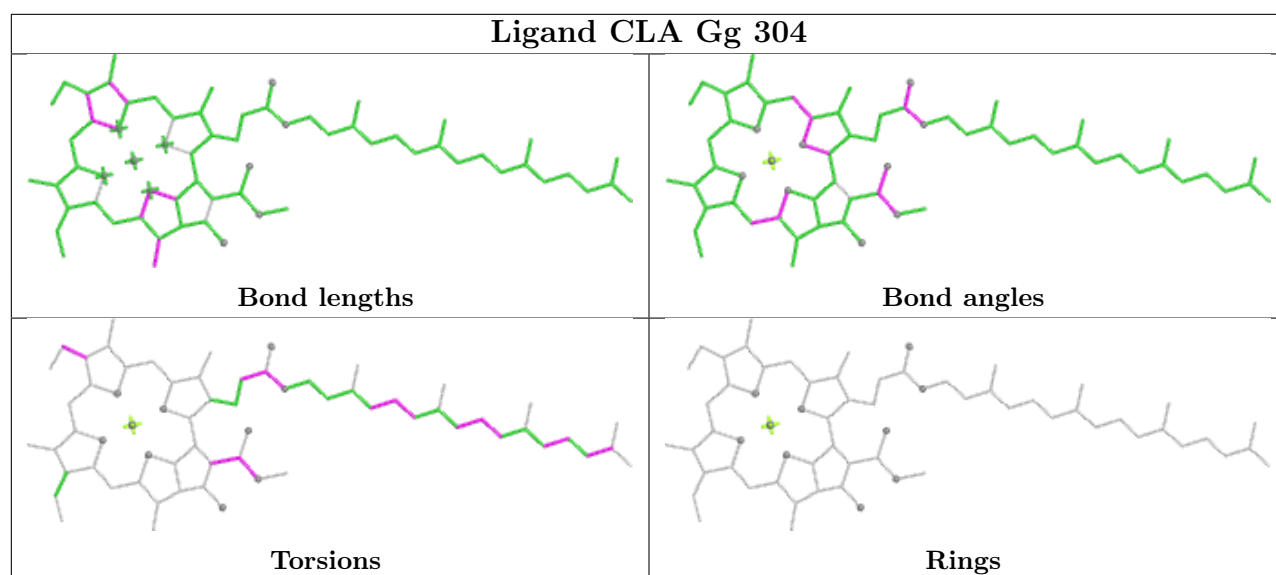


Ligand CLA 22 612

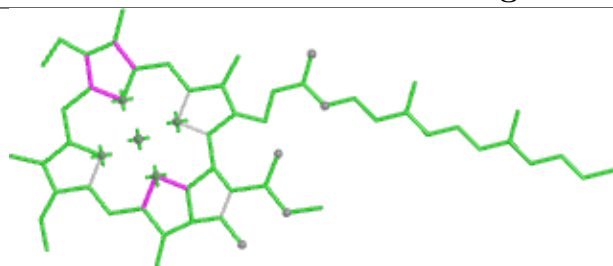




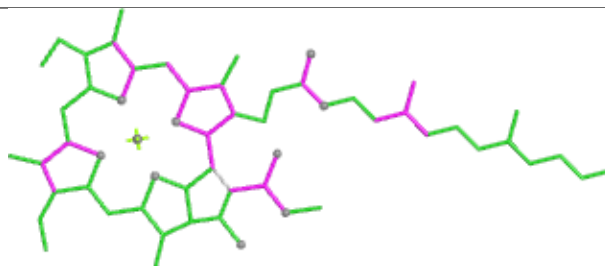




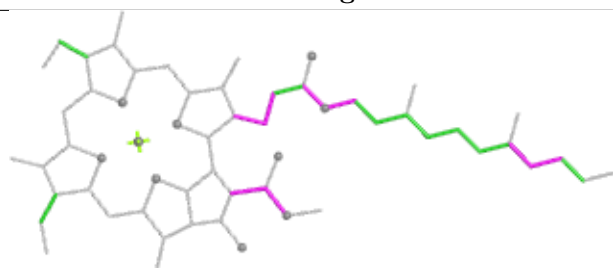
Ligand CLA YY 612



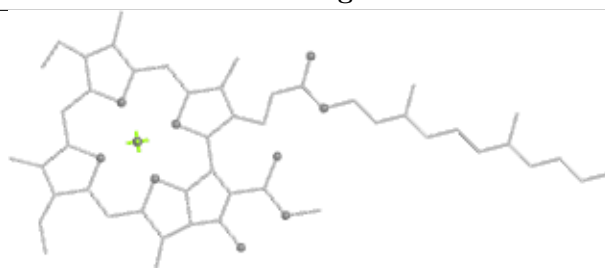
Bond lengths



Bond angles

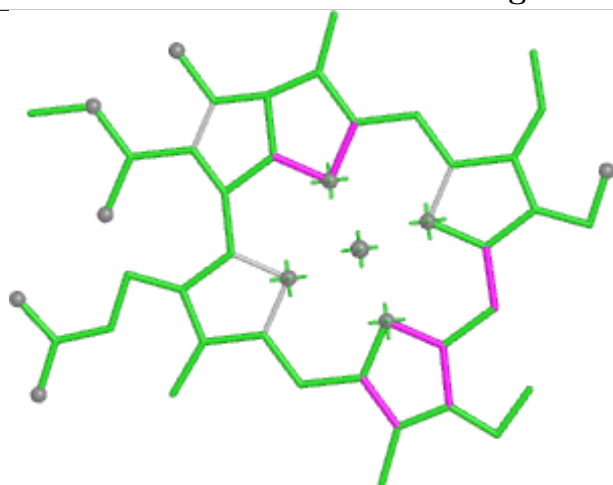


Torsions

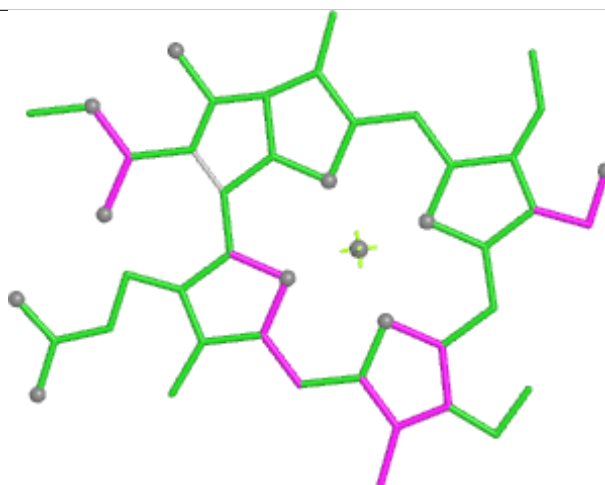


Rings

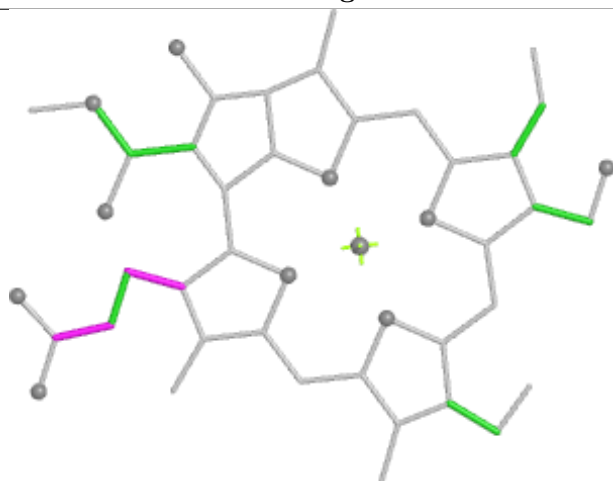
Ligand CHL 44 608



Bond lengths



Bond angles

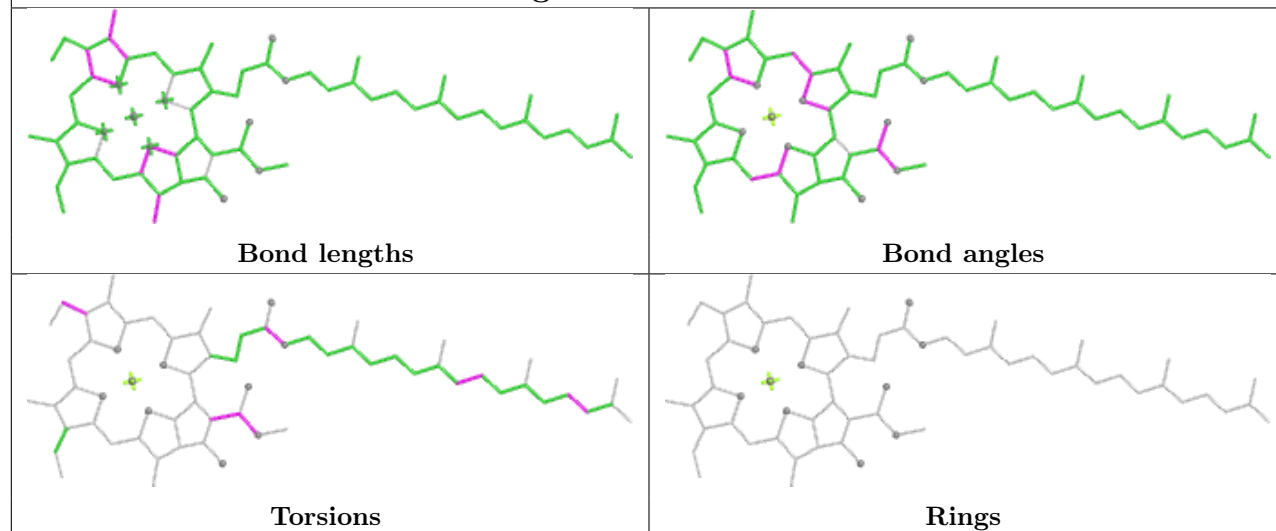


Torsions

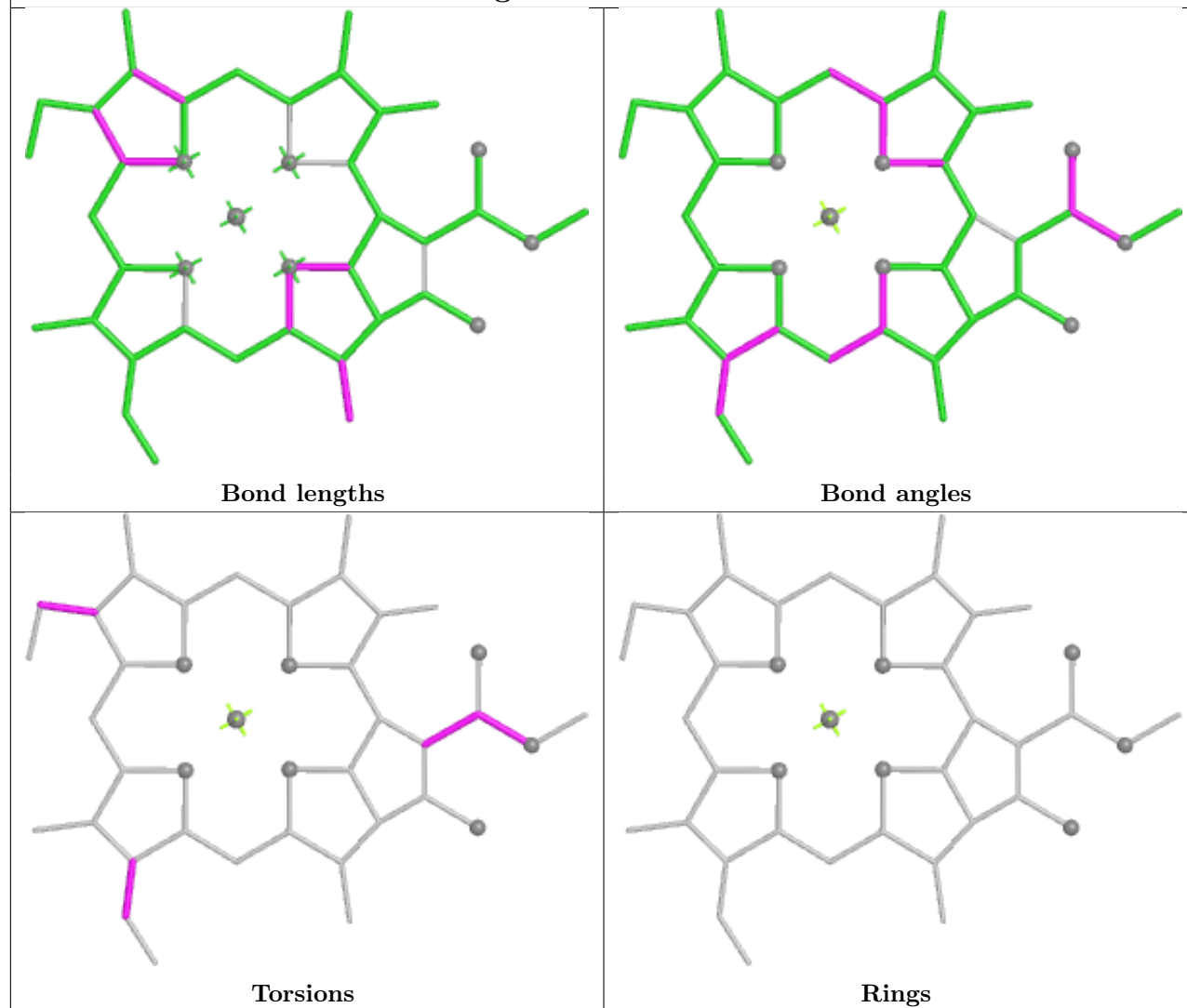


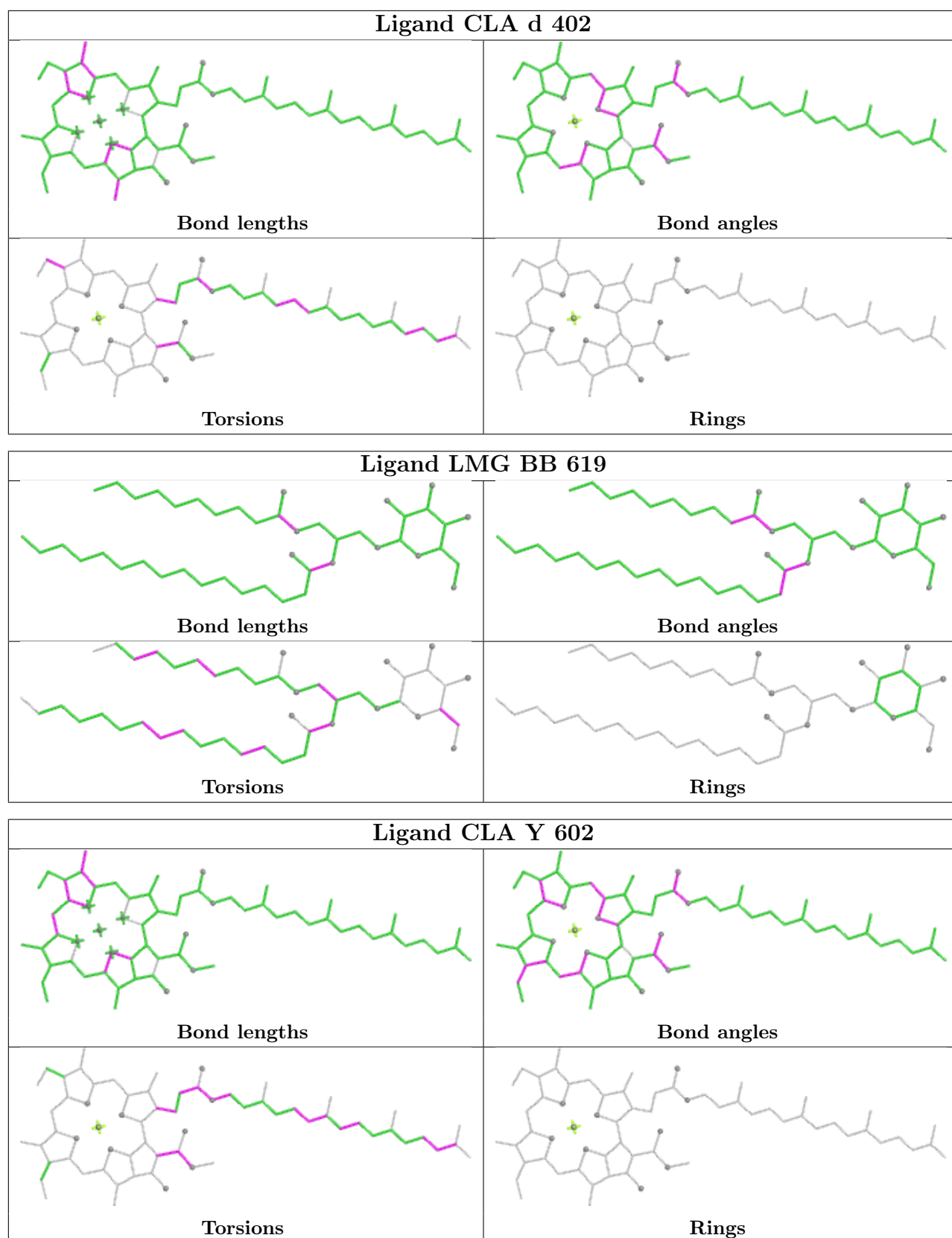
Rings

Ligand CLA C 506

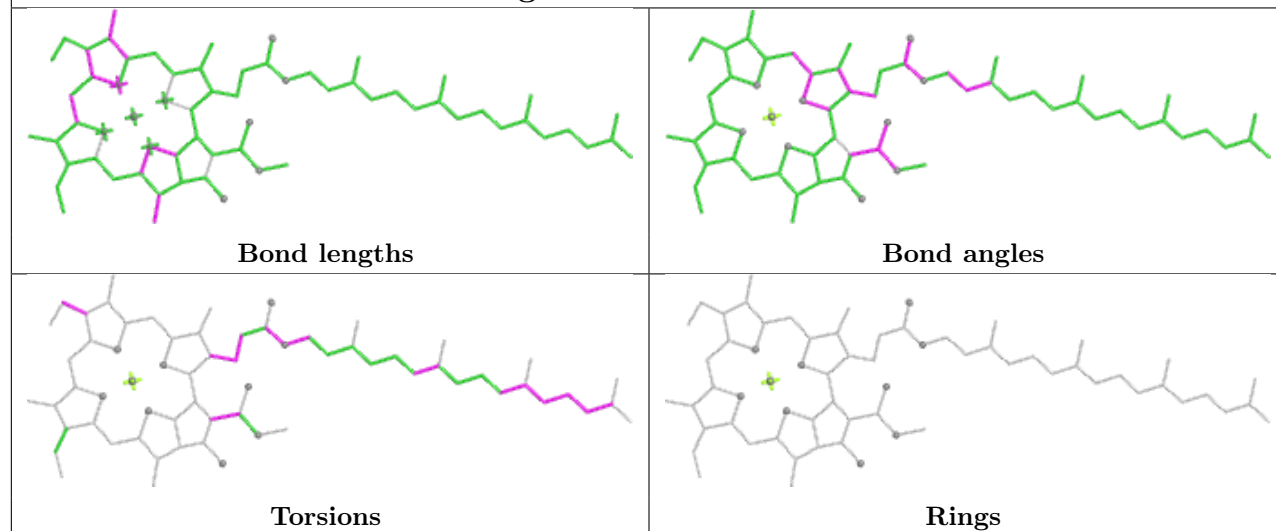


Ligand CLA R 613

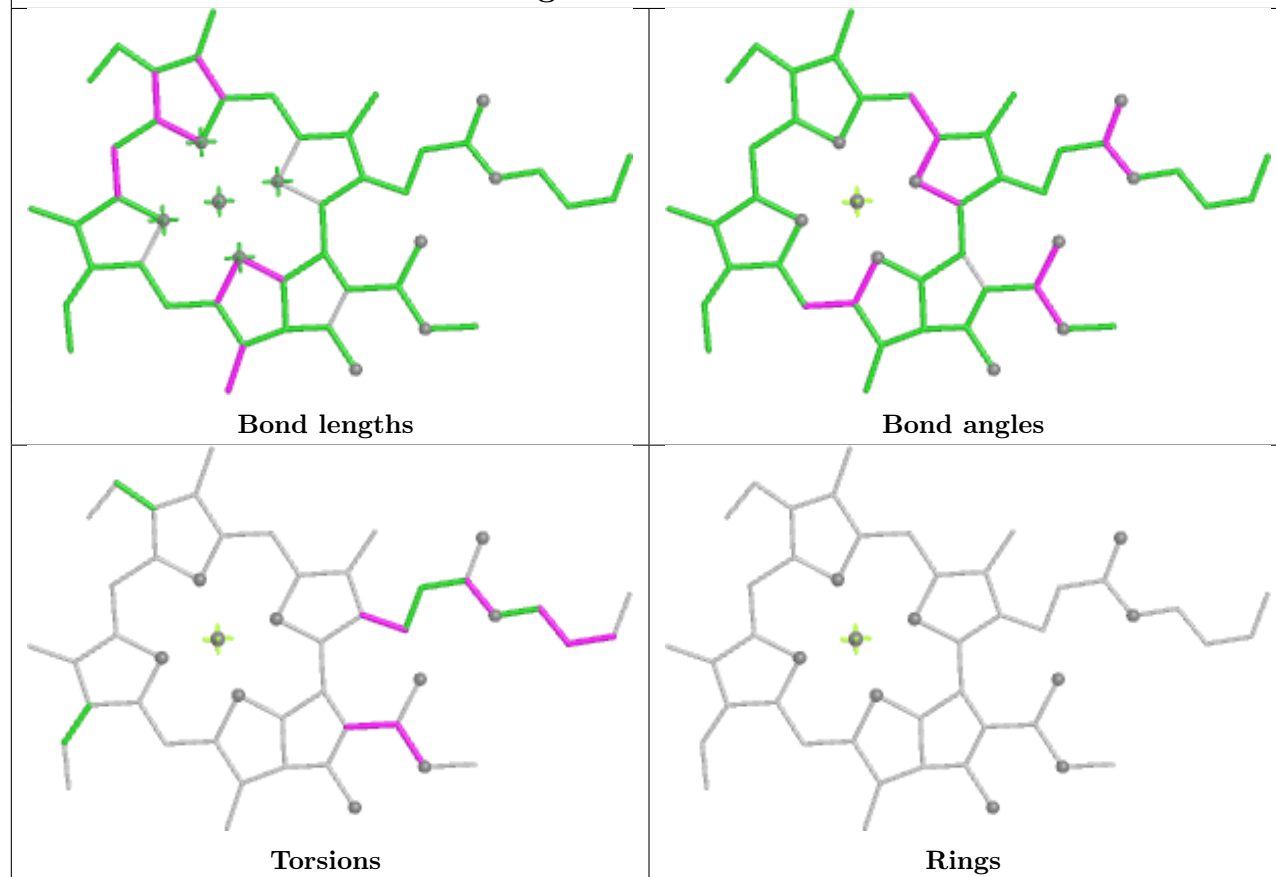


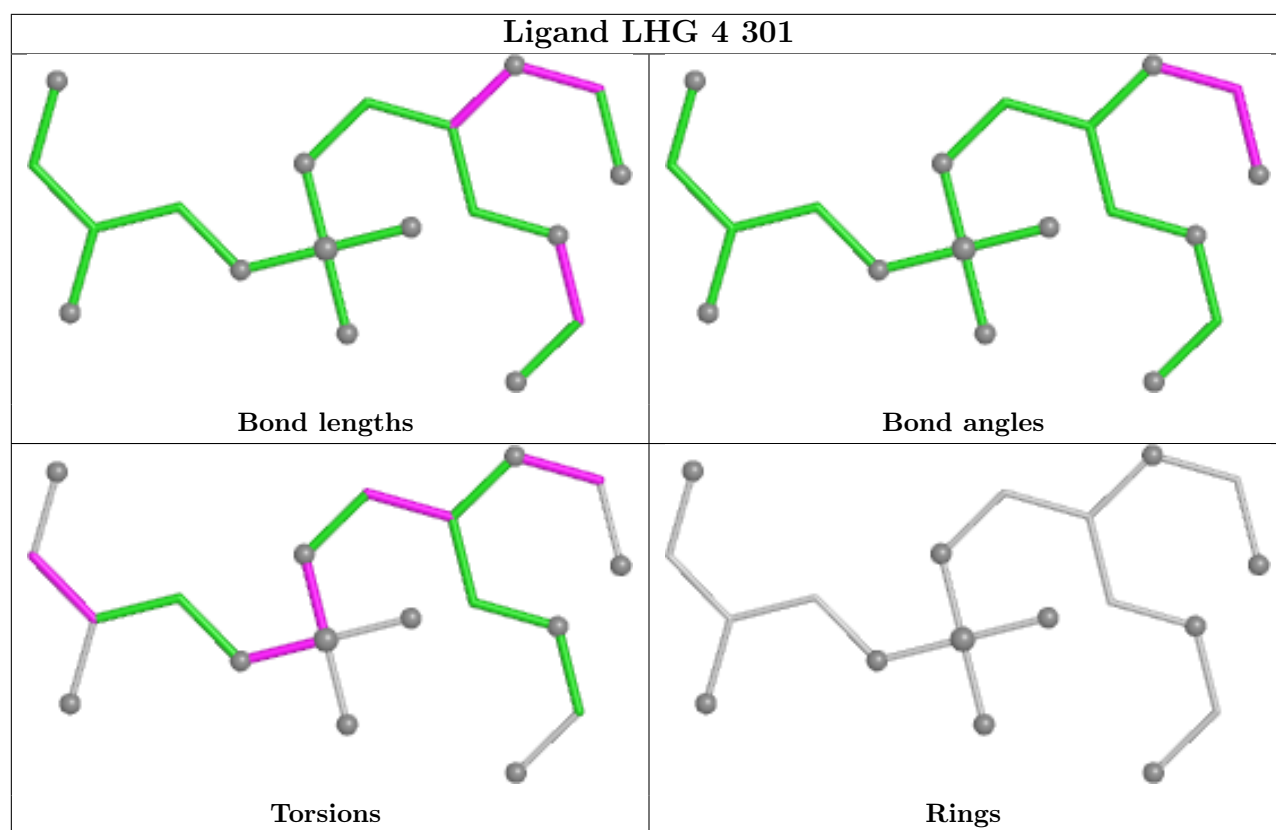


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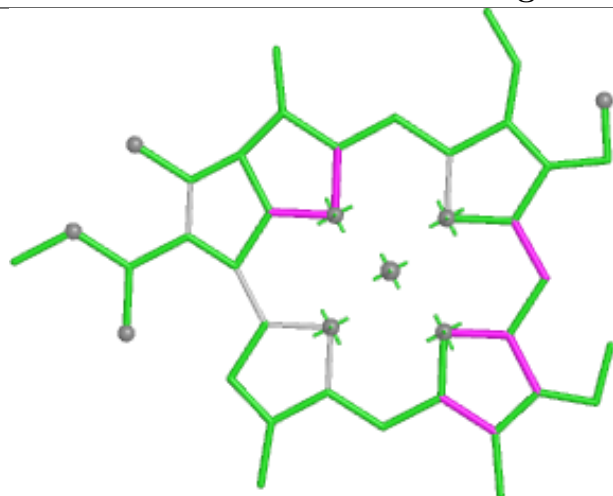


Ligand CLA s 608

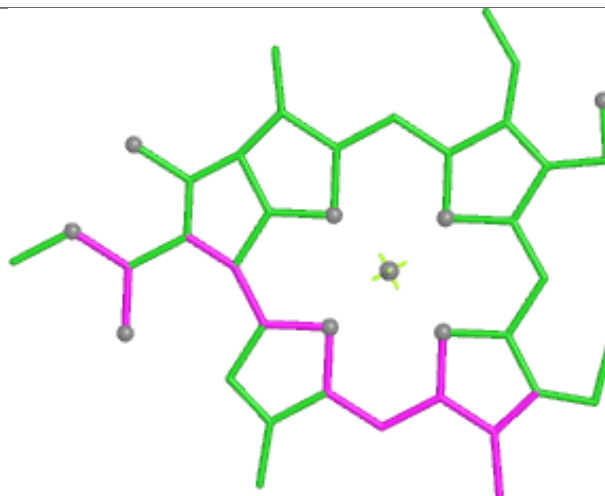




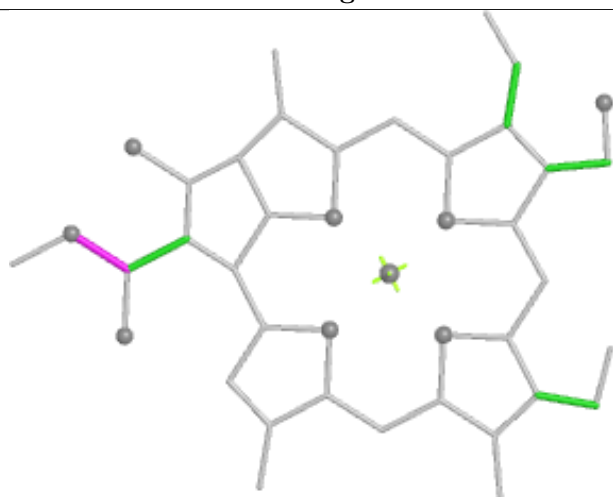
Ligand CHL 2 606



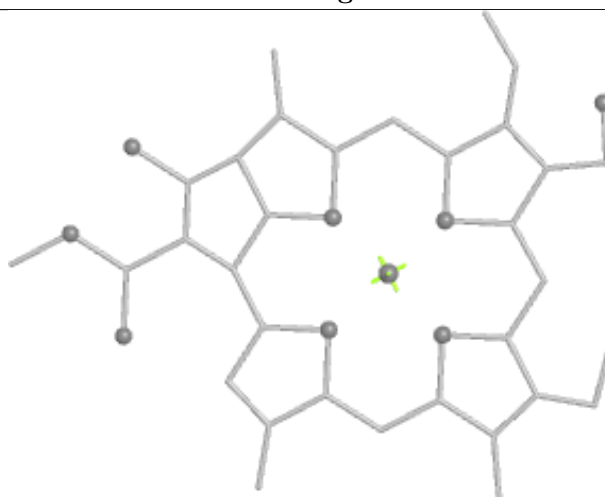
Bond lengths



Bond angles

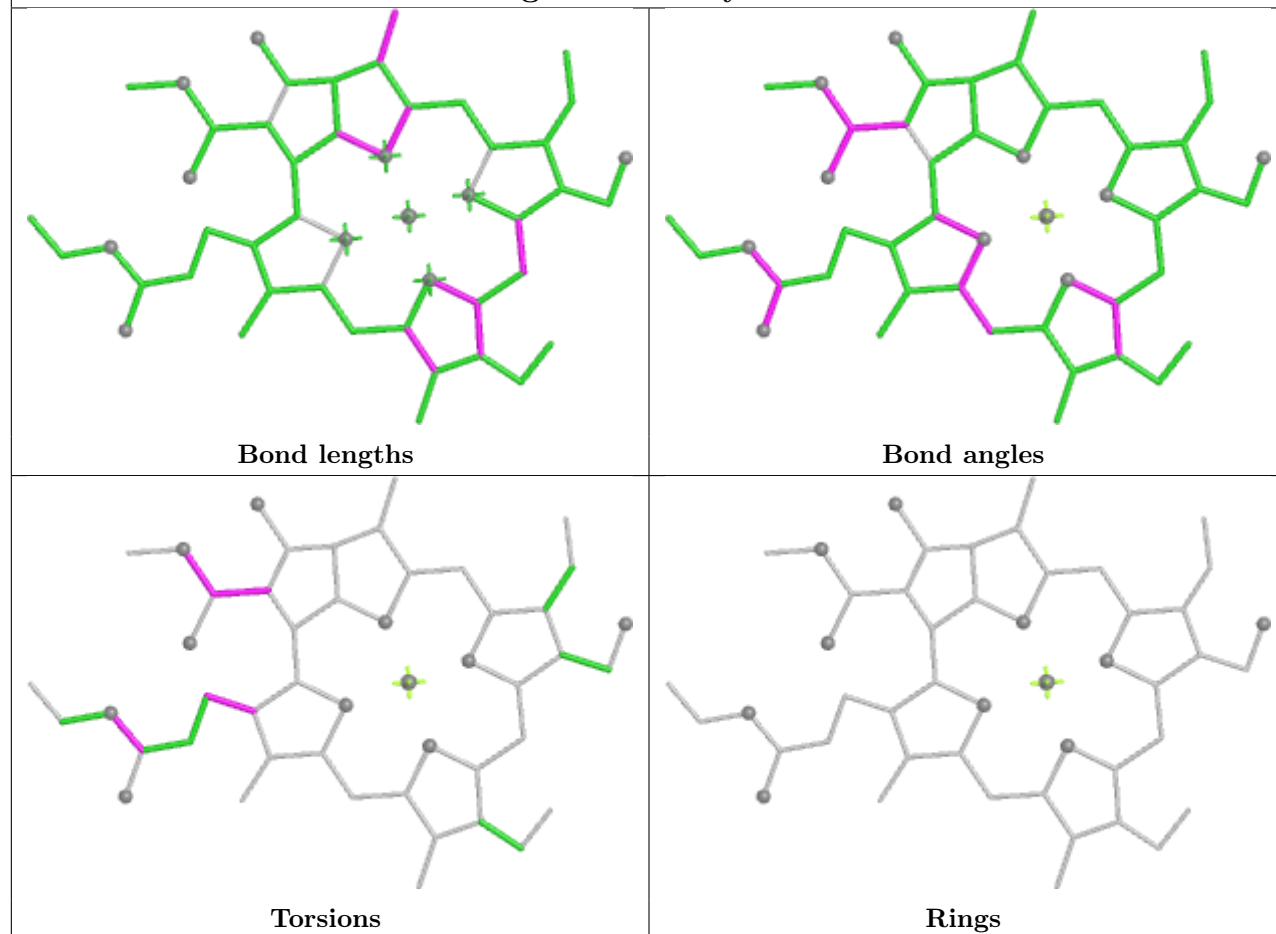


Torsions

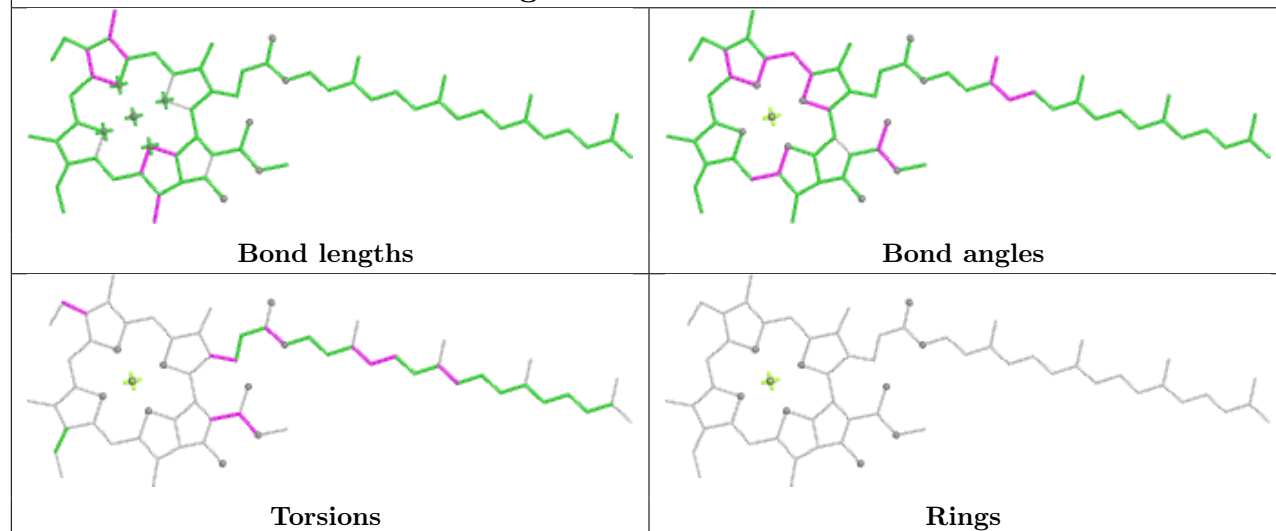


Rings

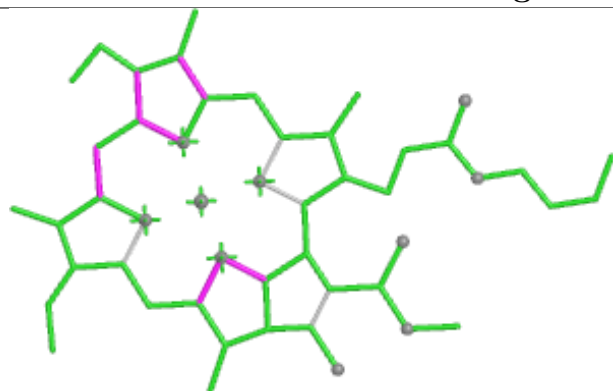
Ligand CHL Yy 605



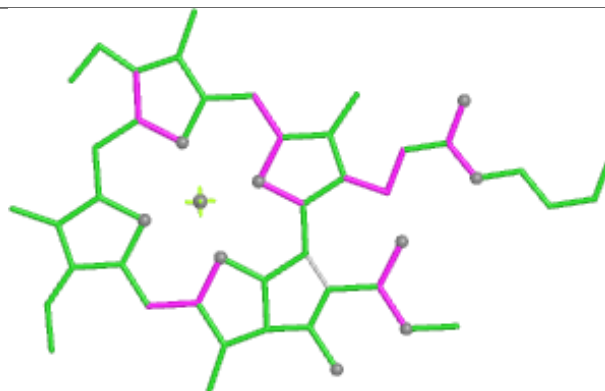
Ligand CLA BB 604



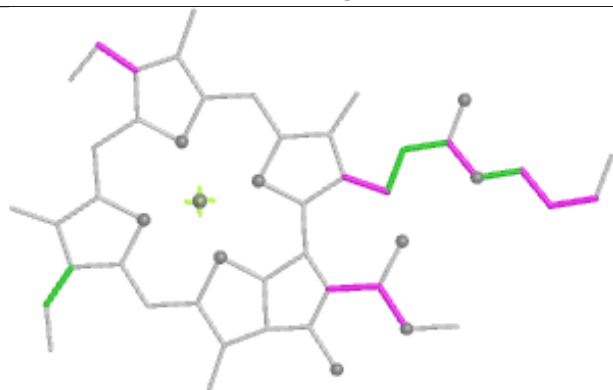
Ligand CLA N 611



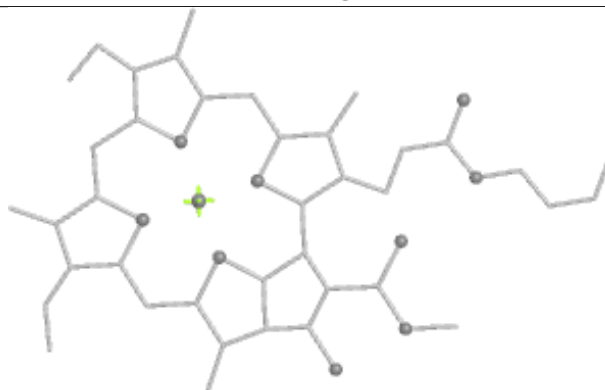
Bond lengths



Bond angles

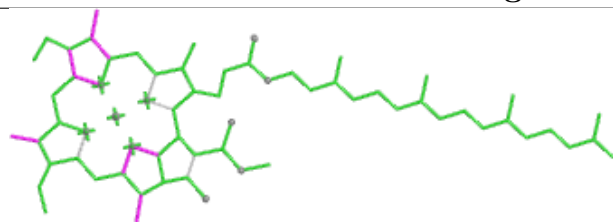


Torsions

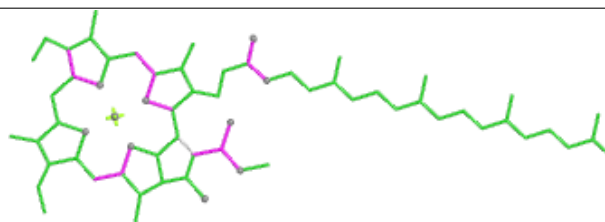


Rings

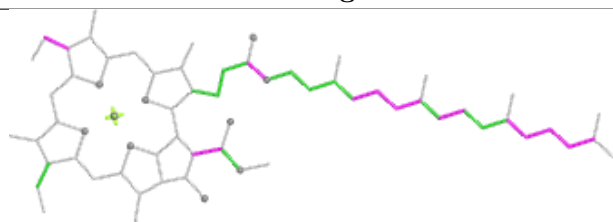
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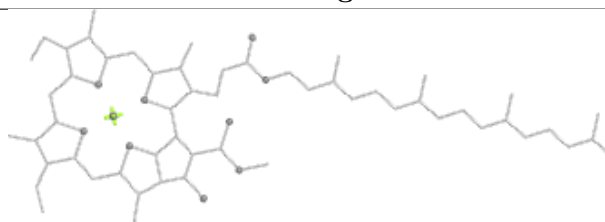
Bond lengths



Bond angles

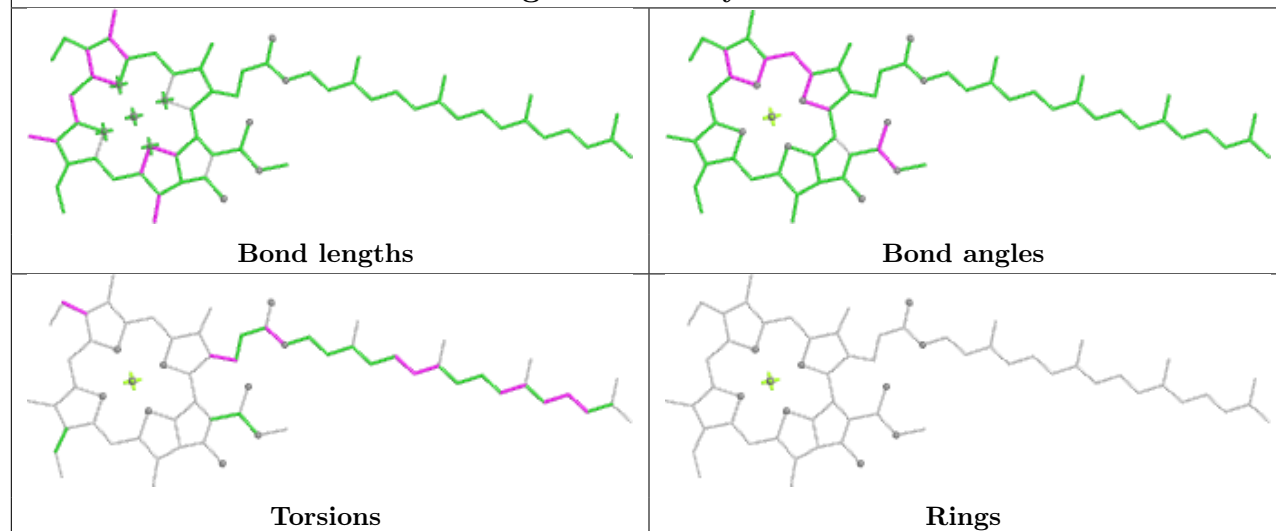


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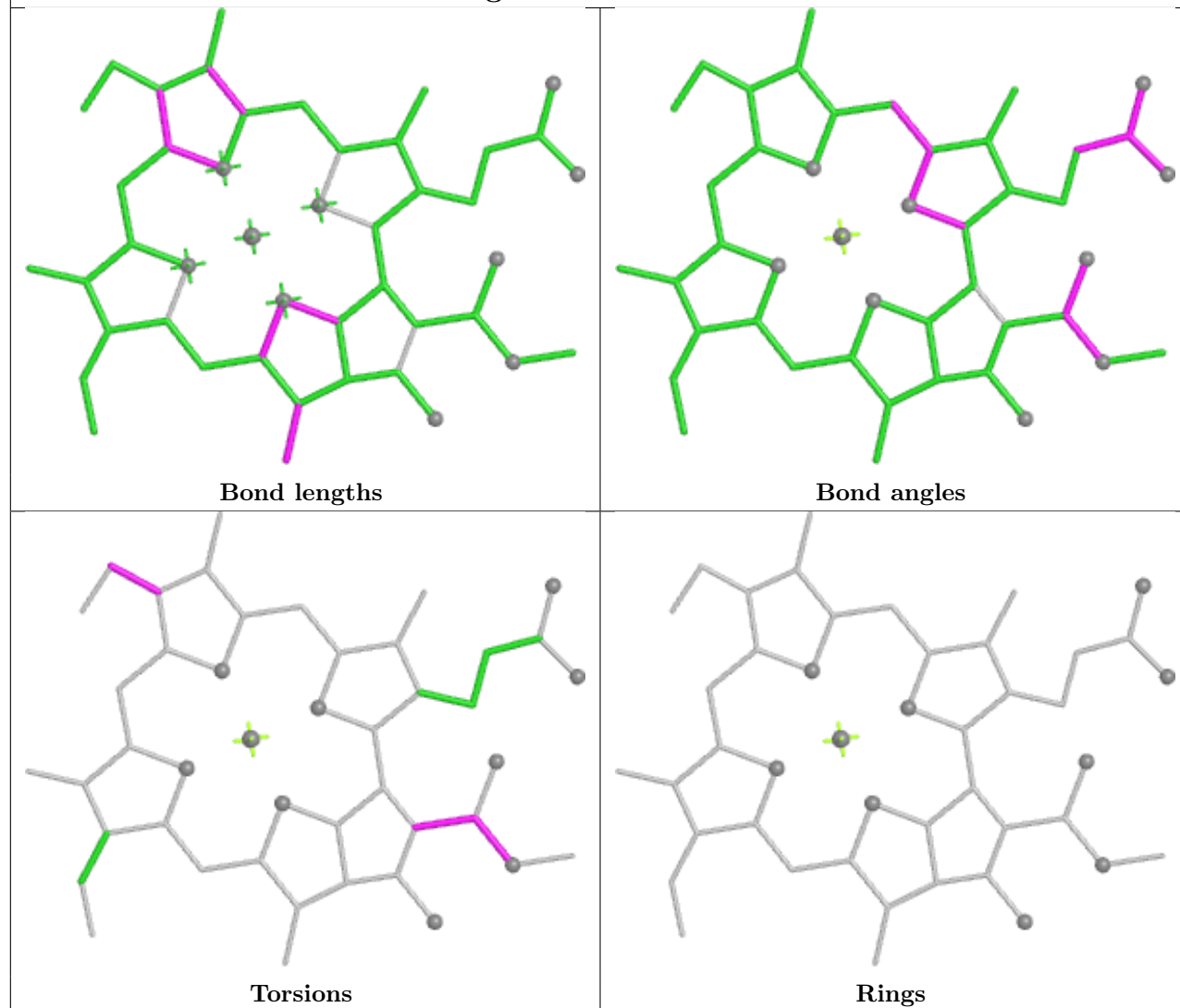


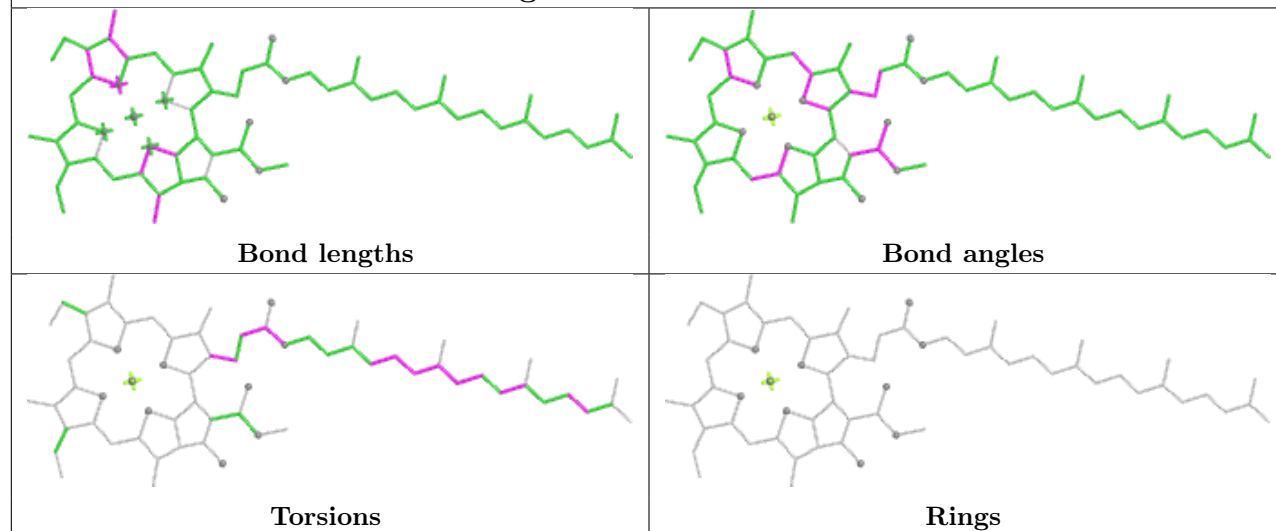
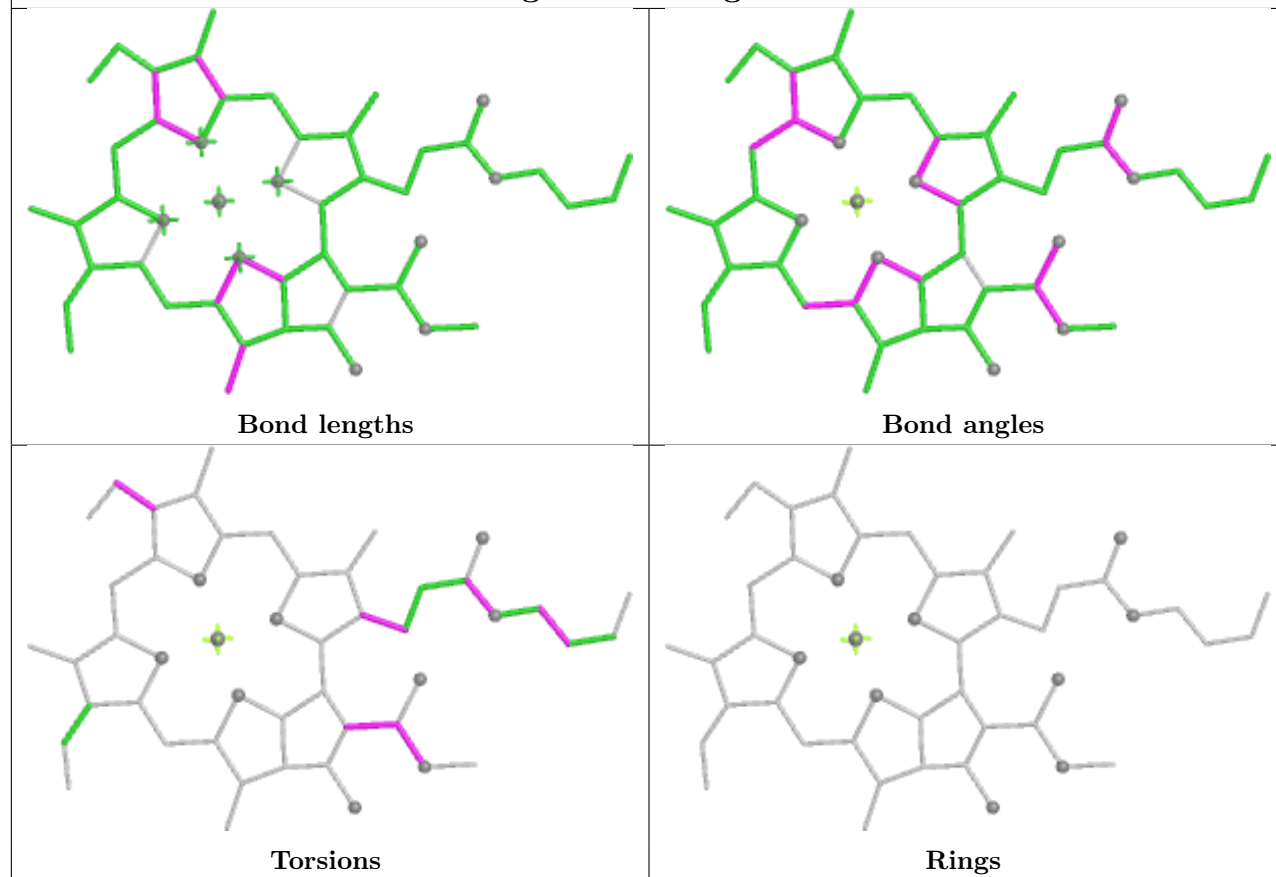
Rings

Ligand CLA Yy 610

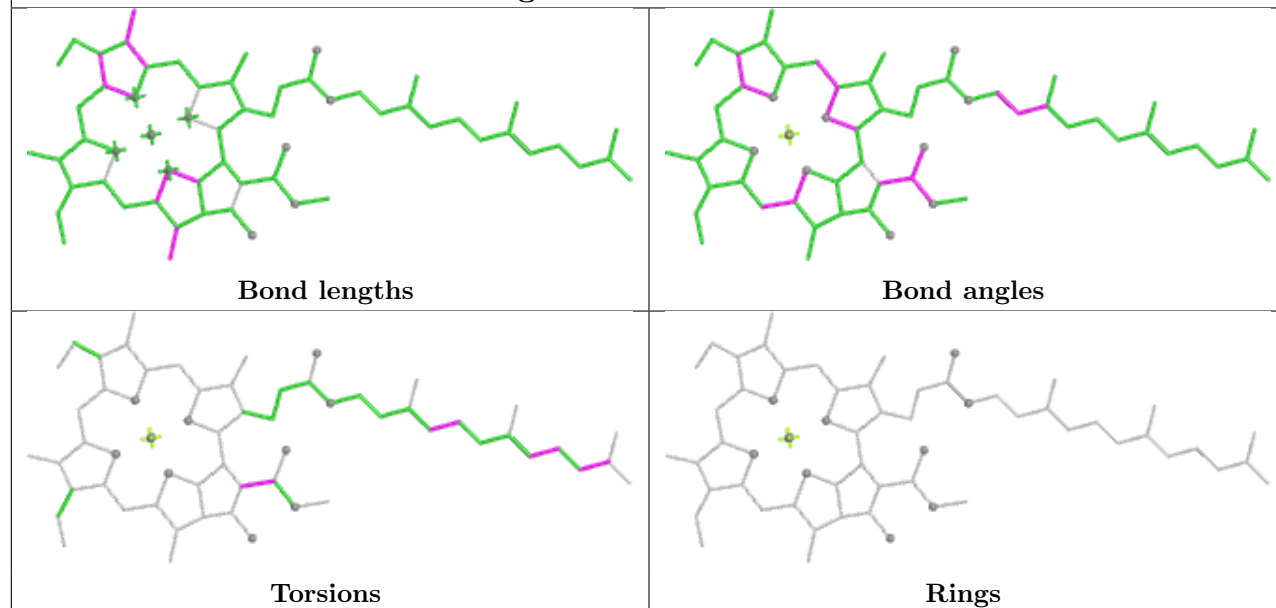


Ligand CLA SS 304

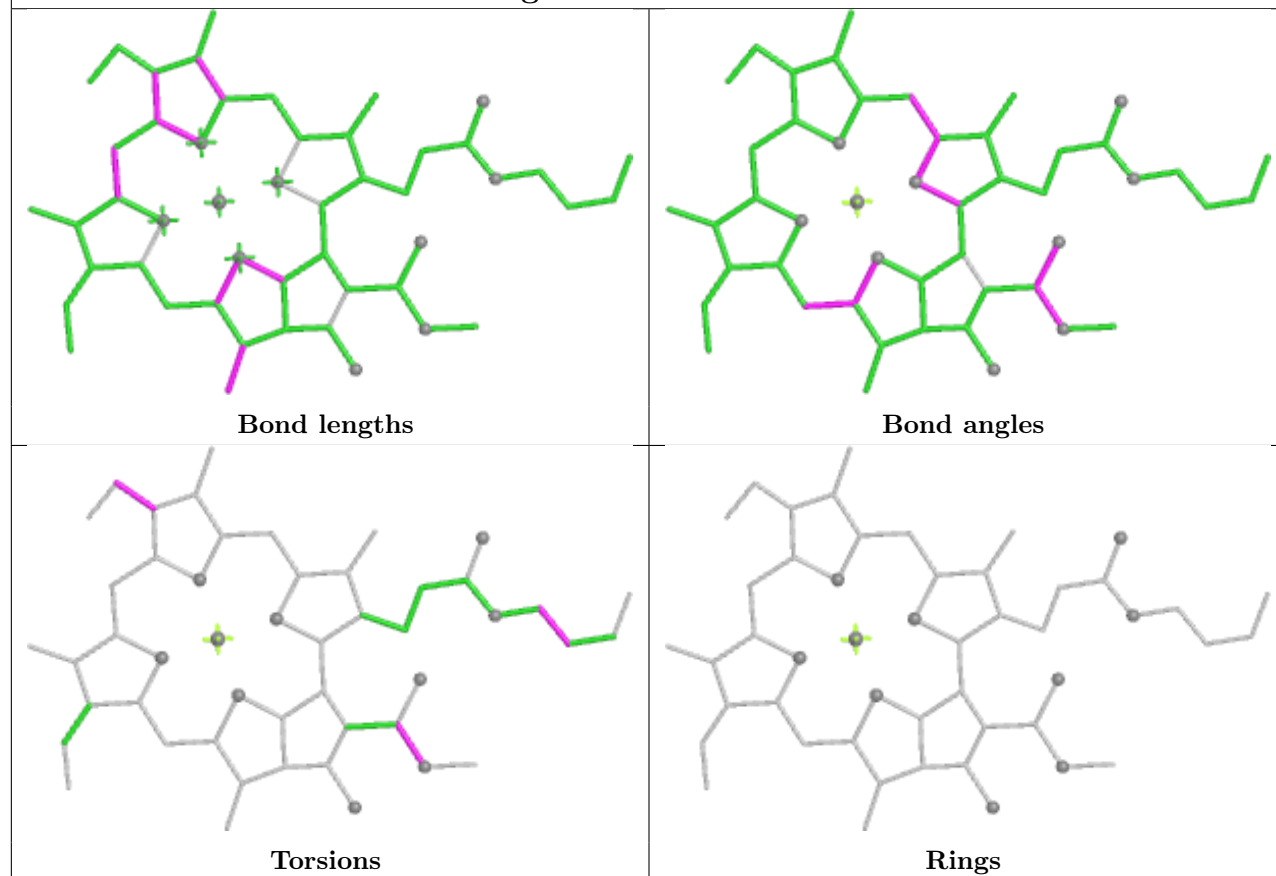


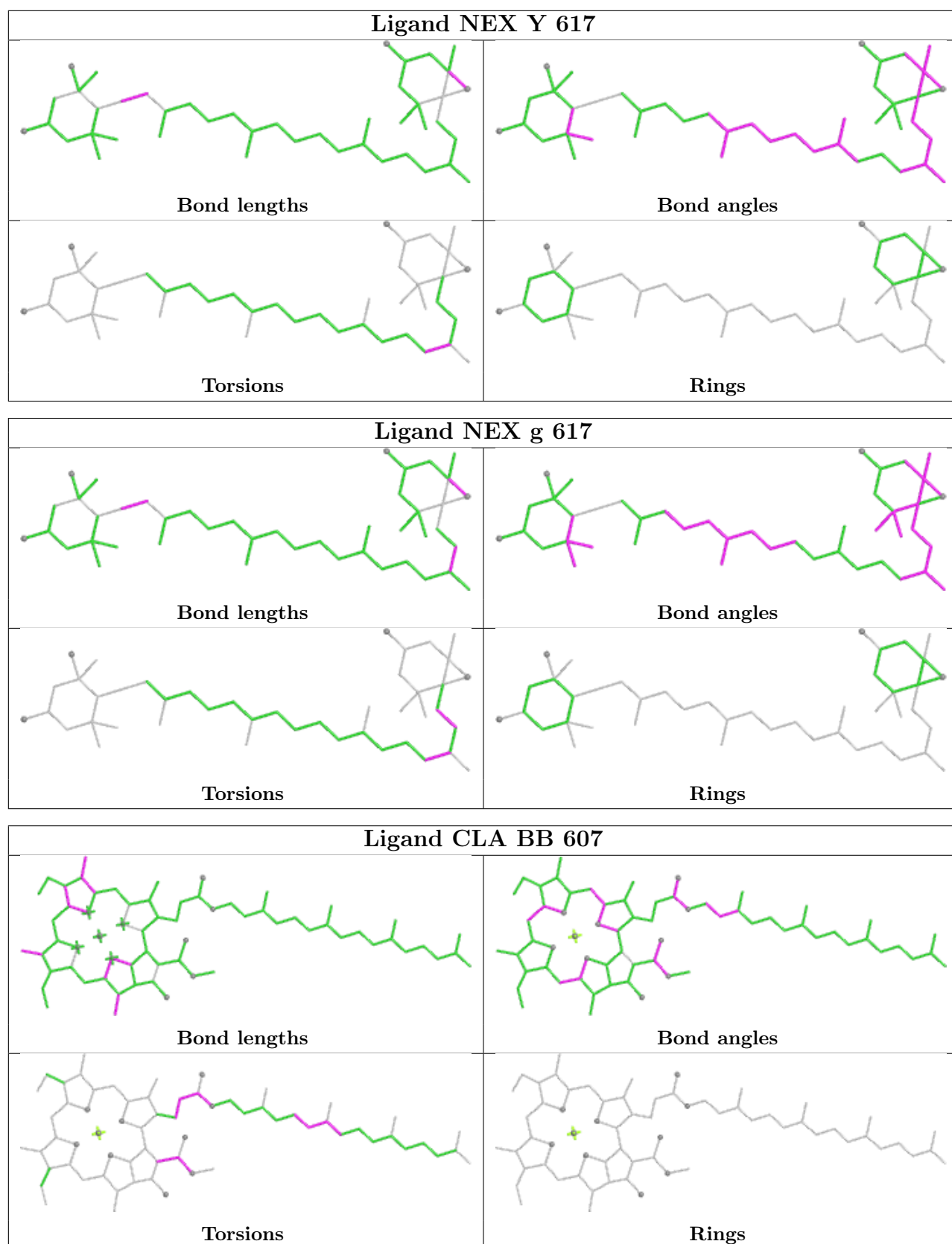
Ligand CLA CC 502**Ligand CLA Gg 303**

Ligand CLA AA 408

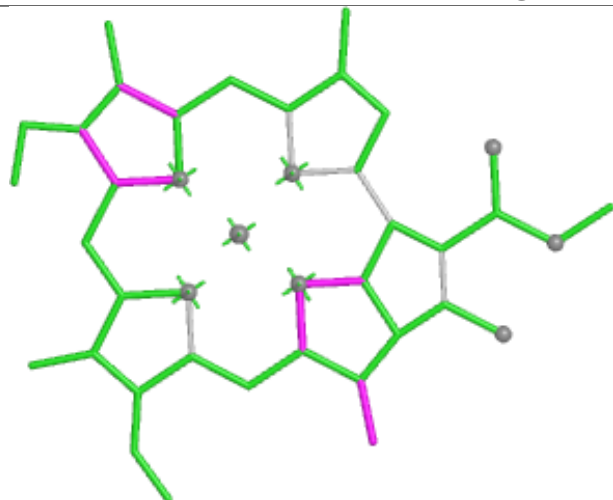


Ligand CLA Nn 302

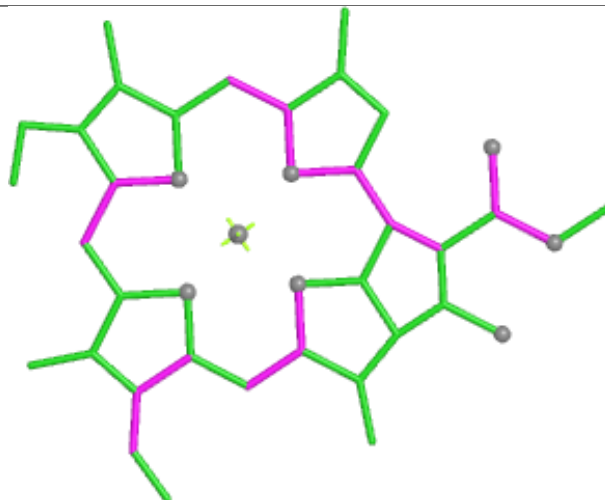




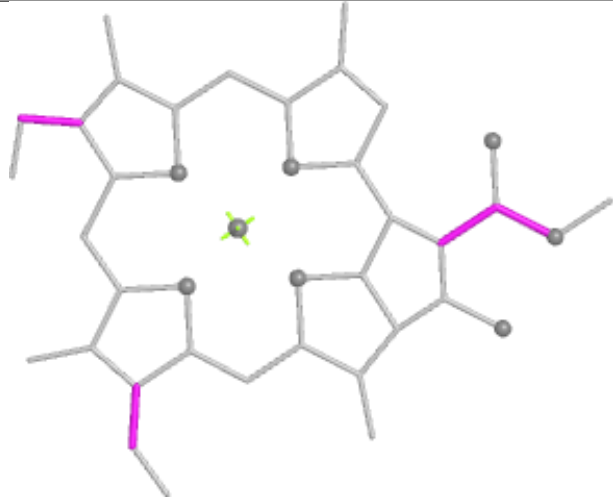
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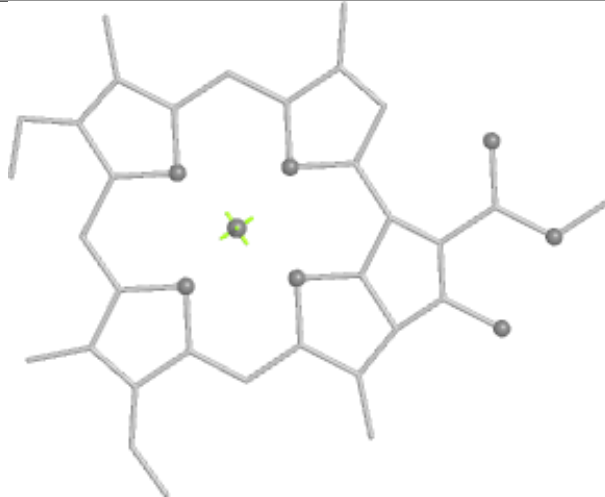
Bond lengths



Bond angles

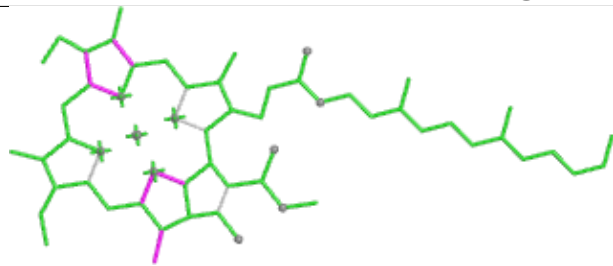


Torsions

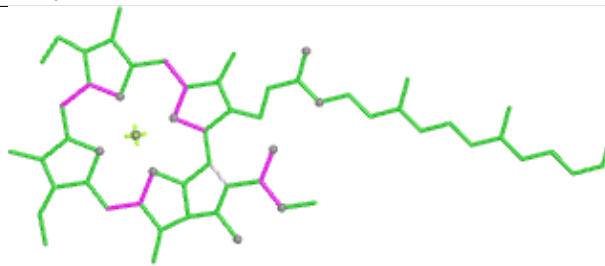


Rings

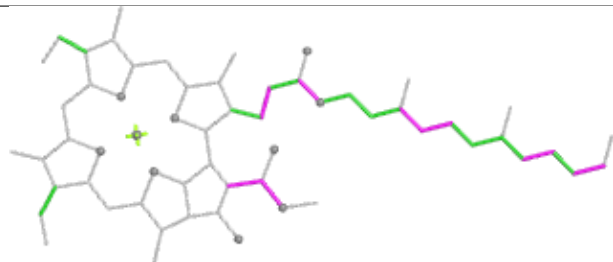
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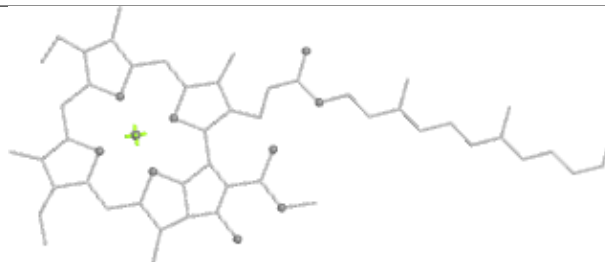
Bond lengths



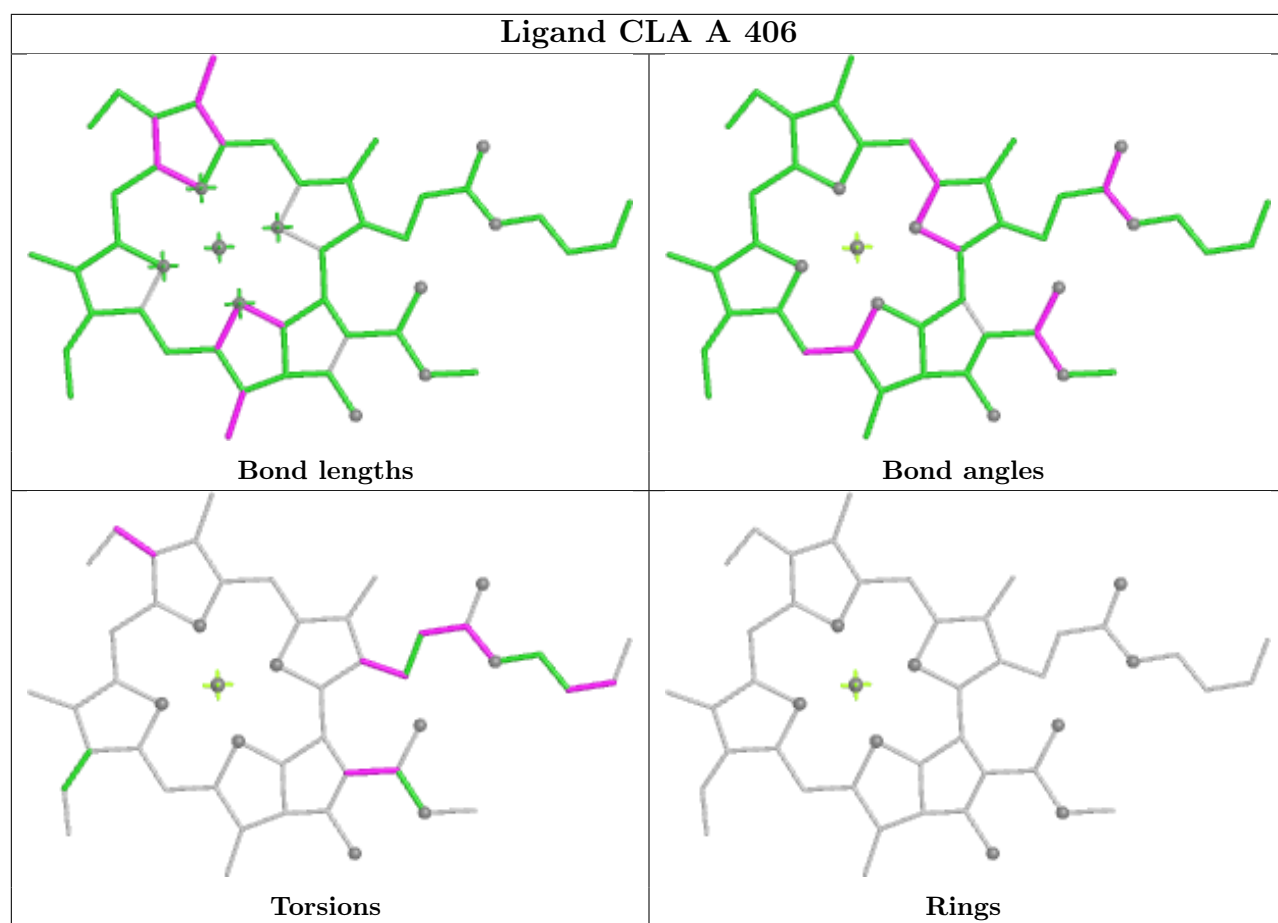
Bond angles



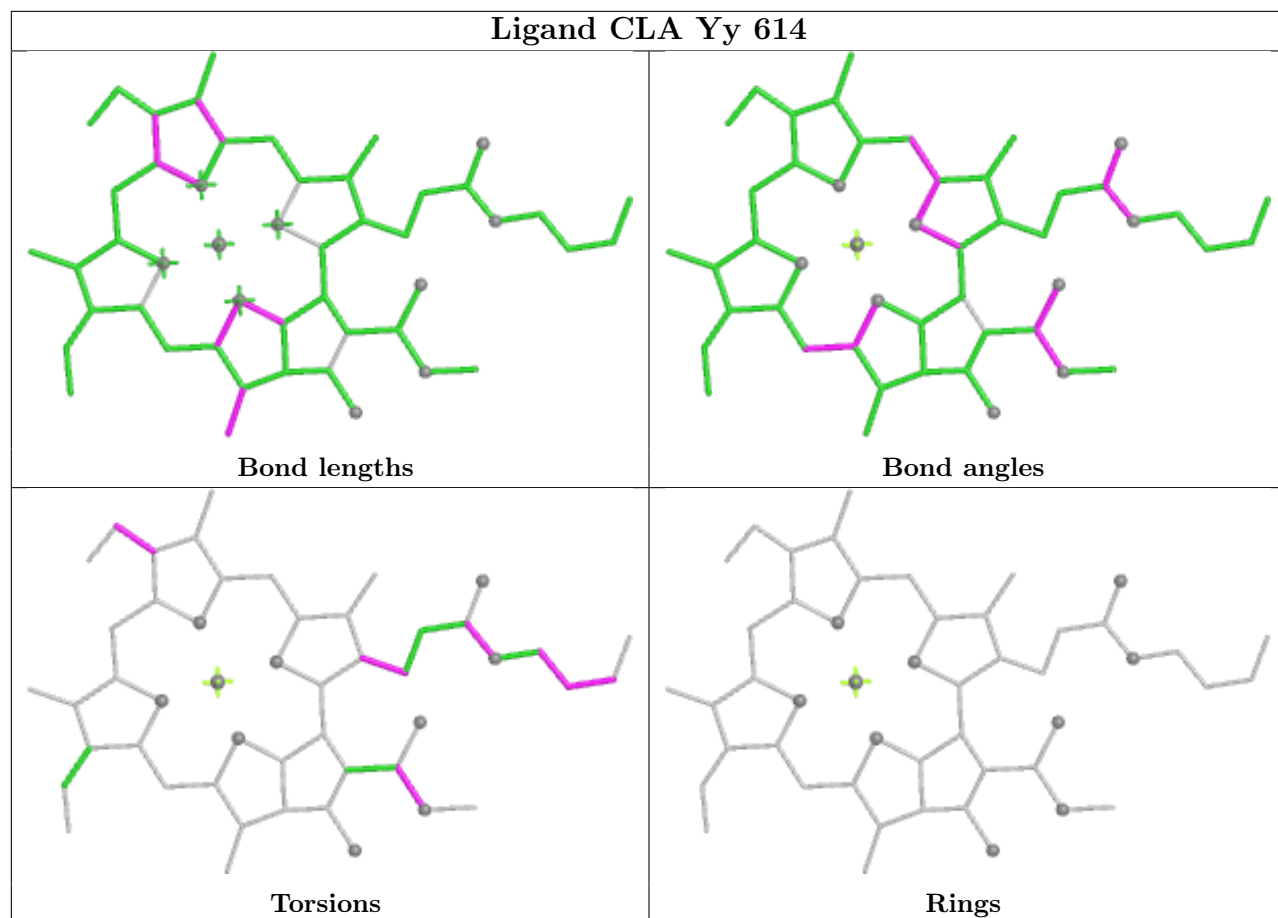
Torsions



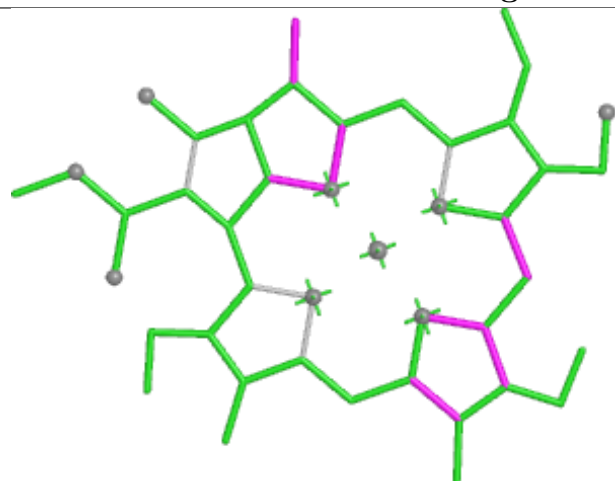
Rings



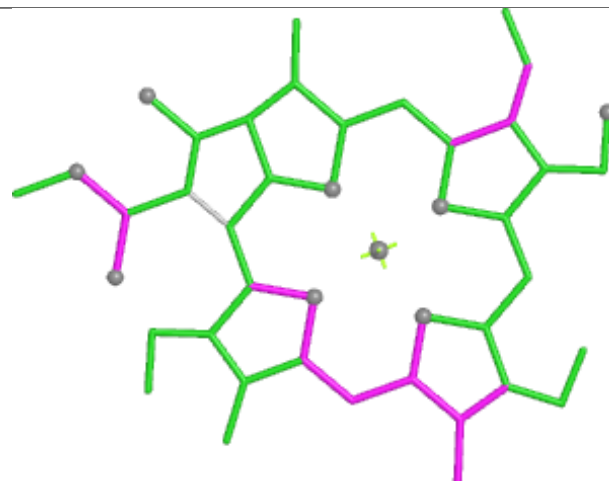
Ligand CLA Yy 614



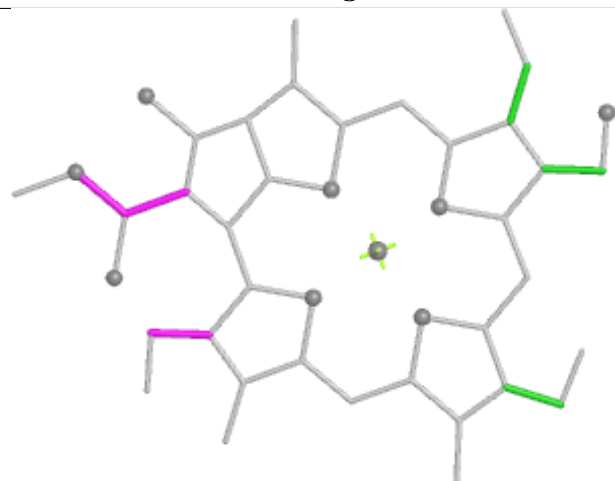
Ligand CHL GG 609



Bond lengths



Bond angles

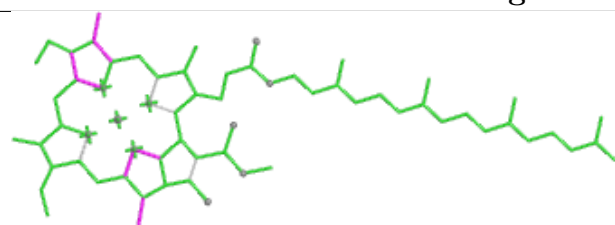


Torsions

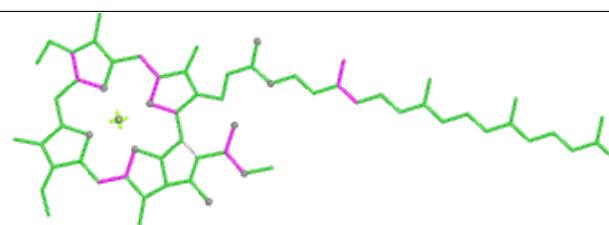


Rings

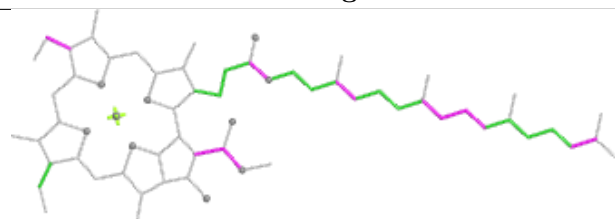
Ligand CLA Cc 511



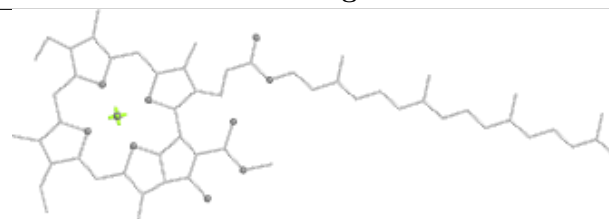
Bond lengths



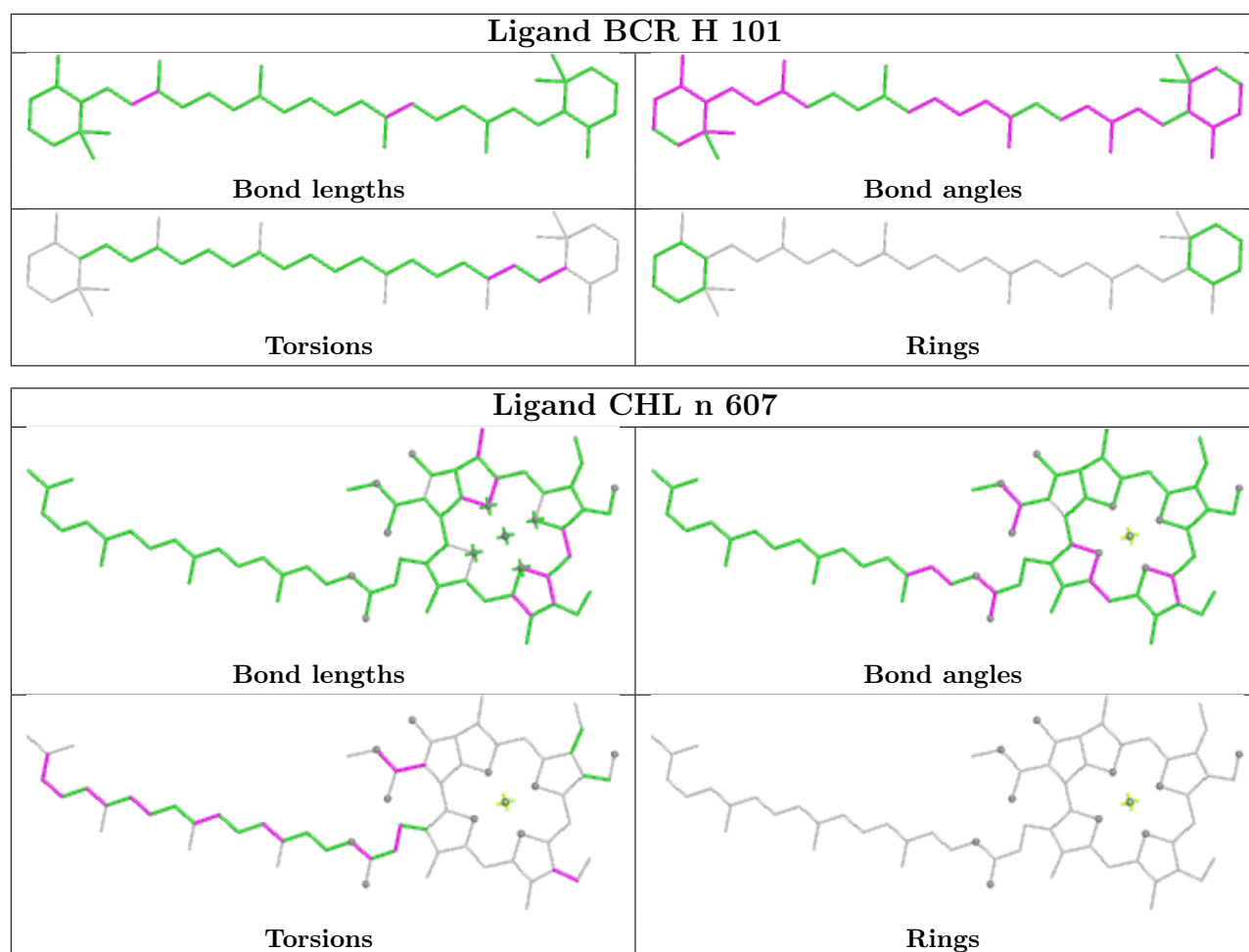
Bond angles

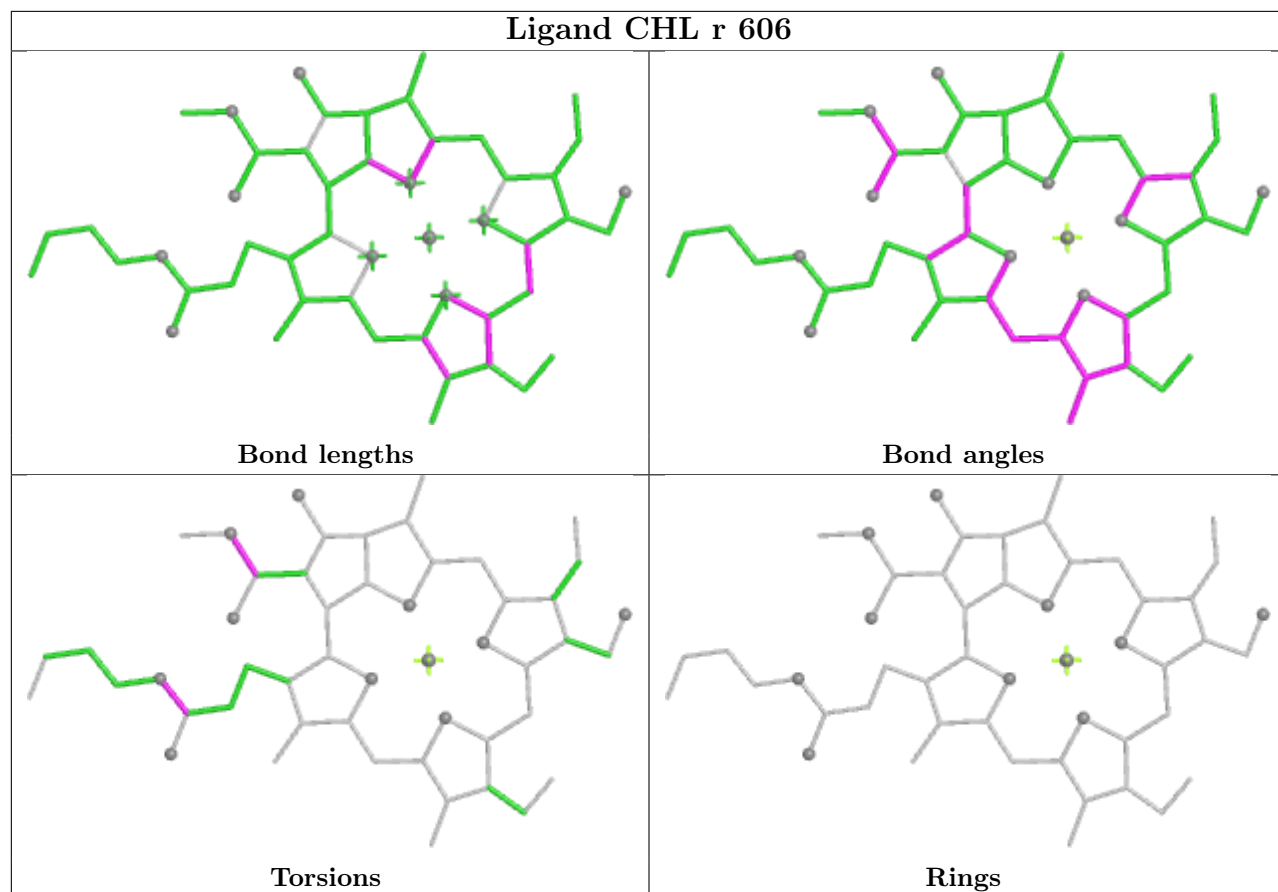


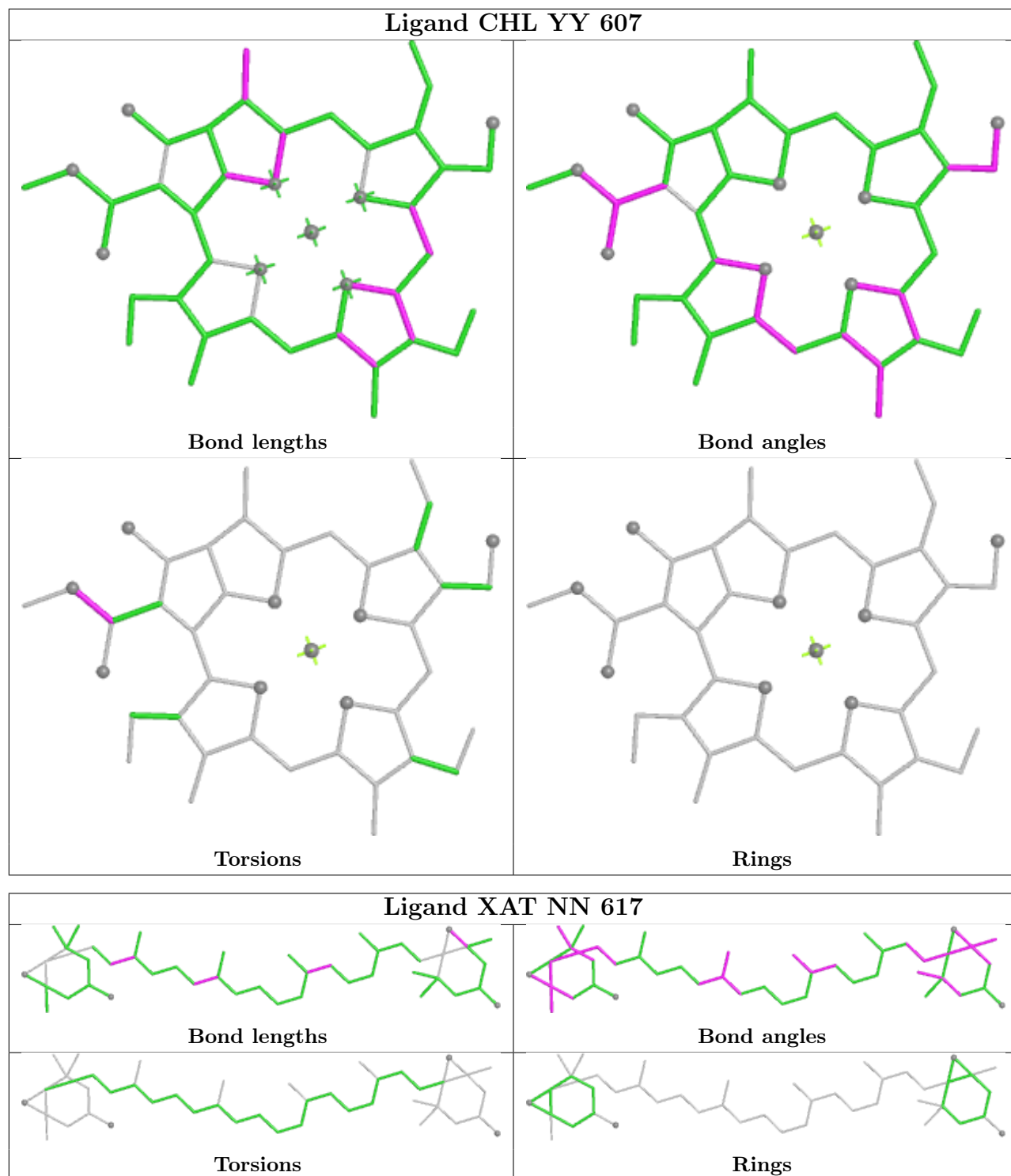
Torsions

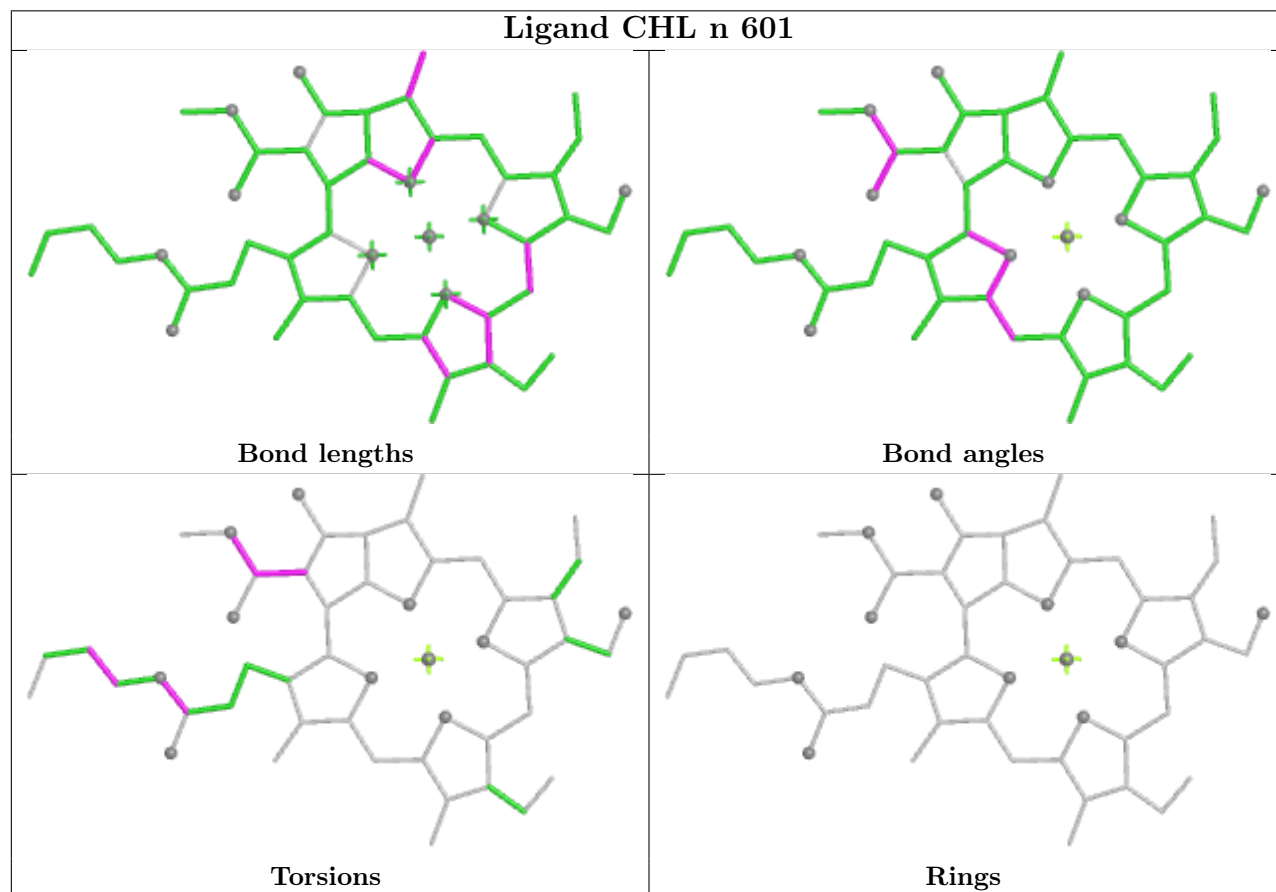
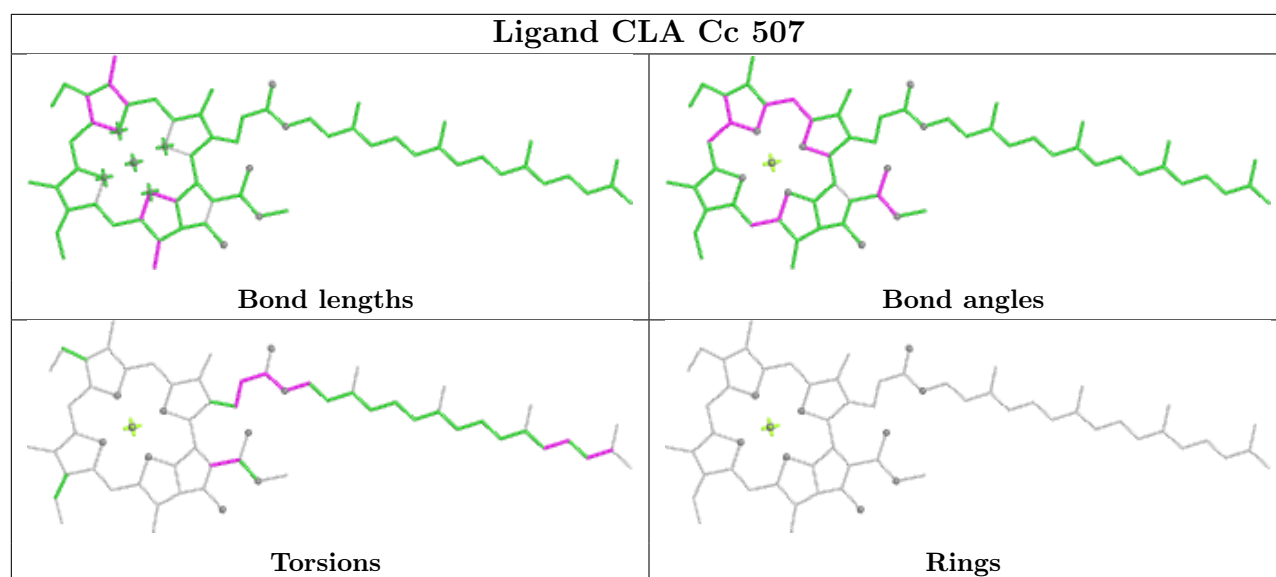


Rings

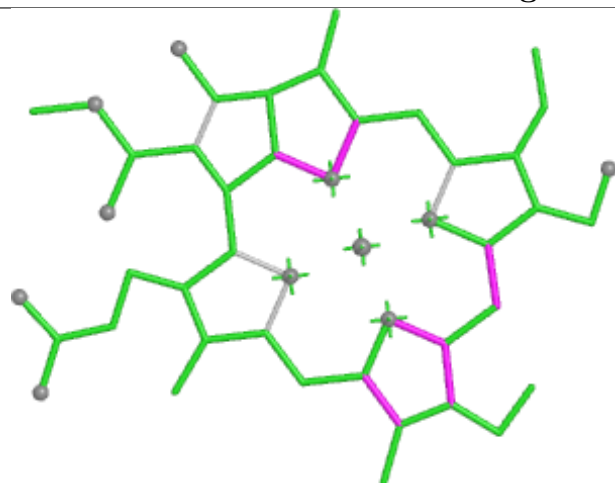




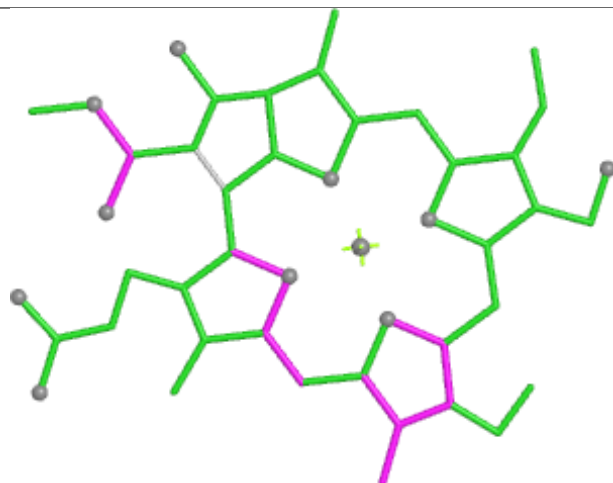




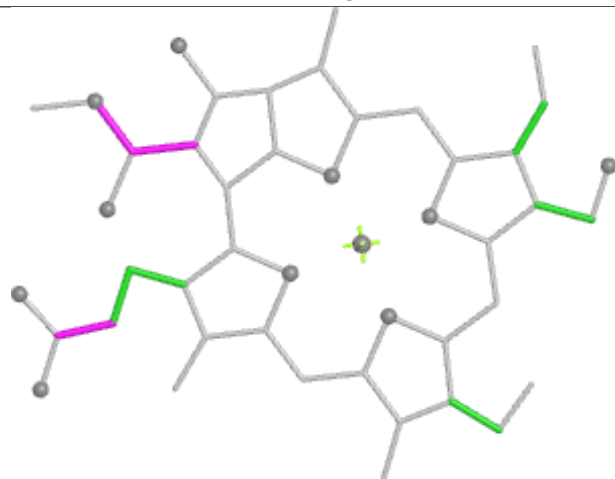
Ligand CHL 4 306



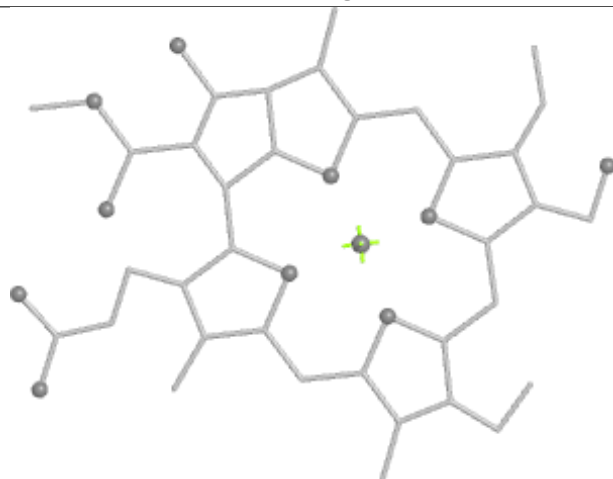
Bond lengths



Bond angles

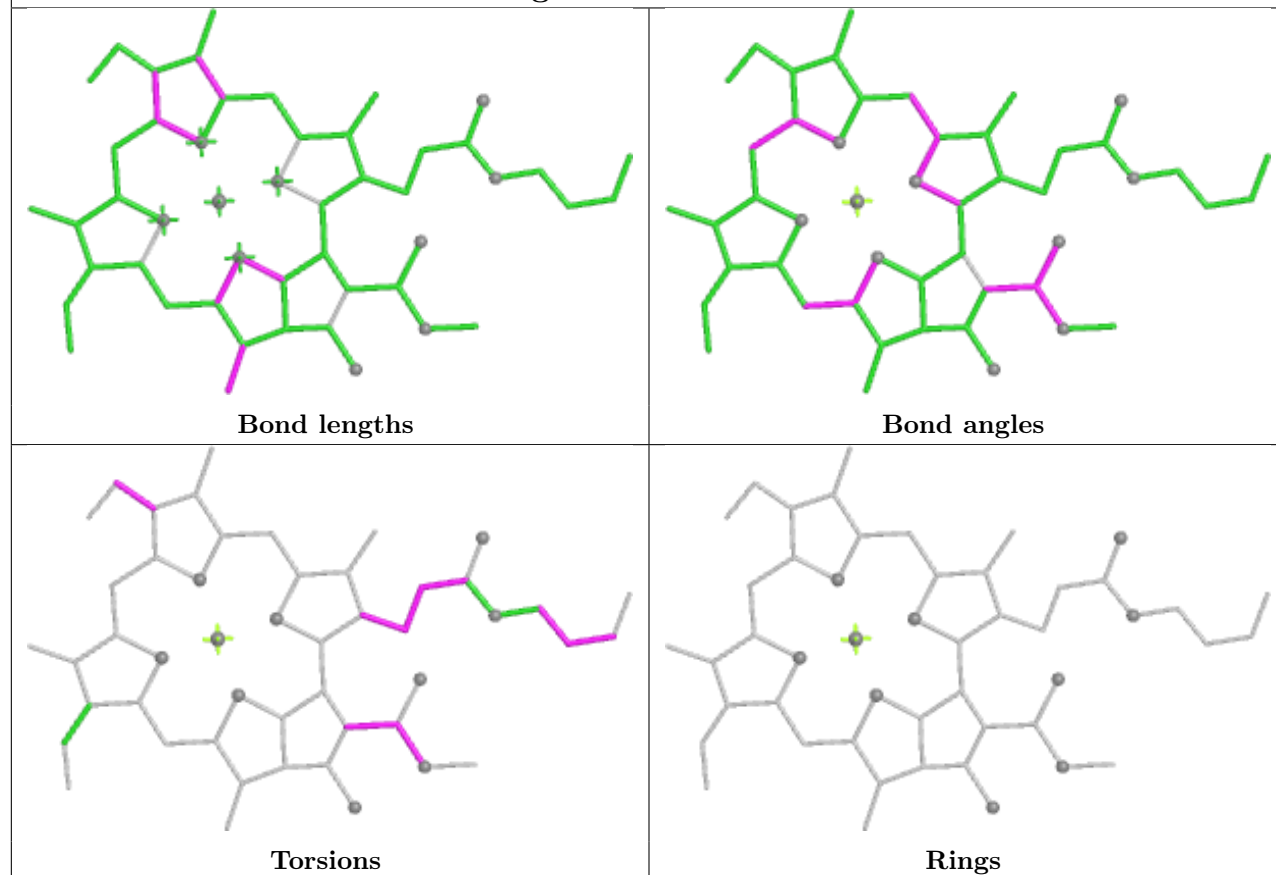


Torsions

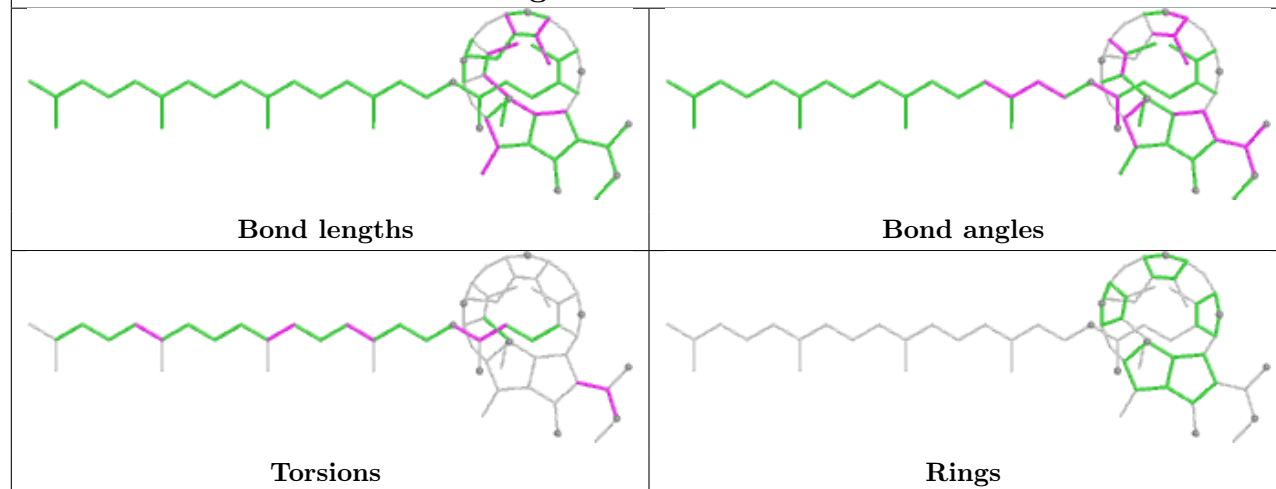


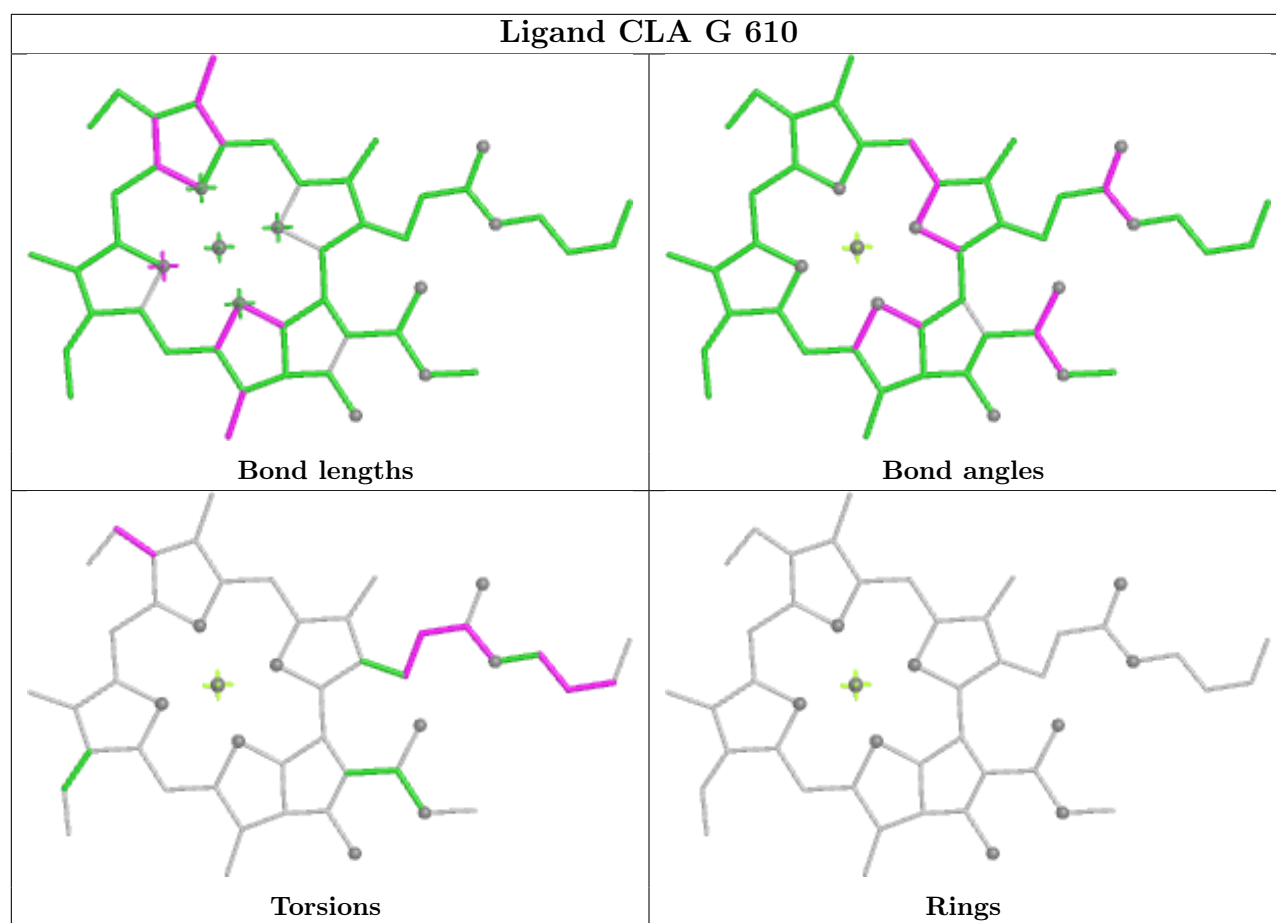
Rings

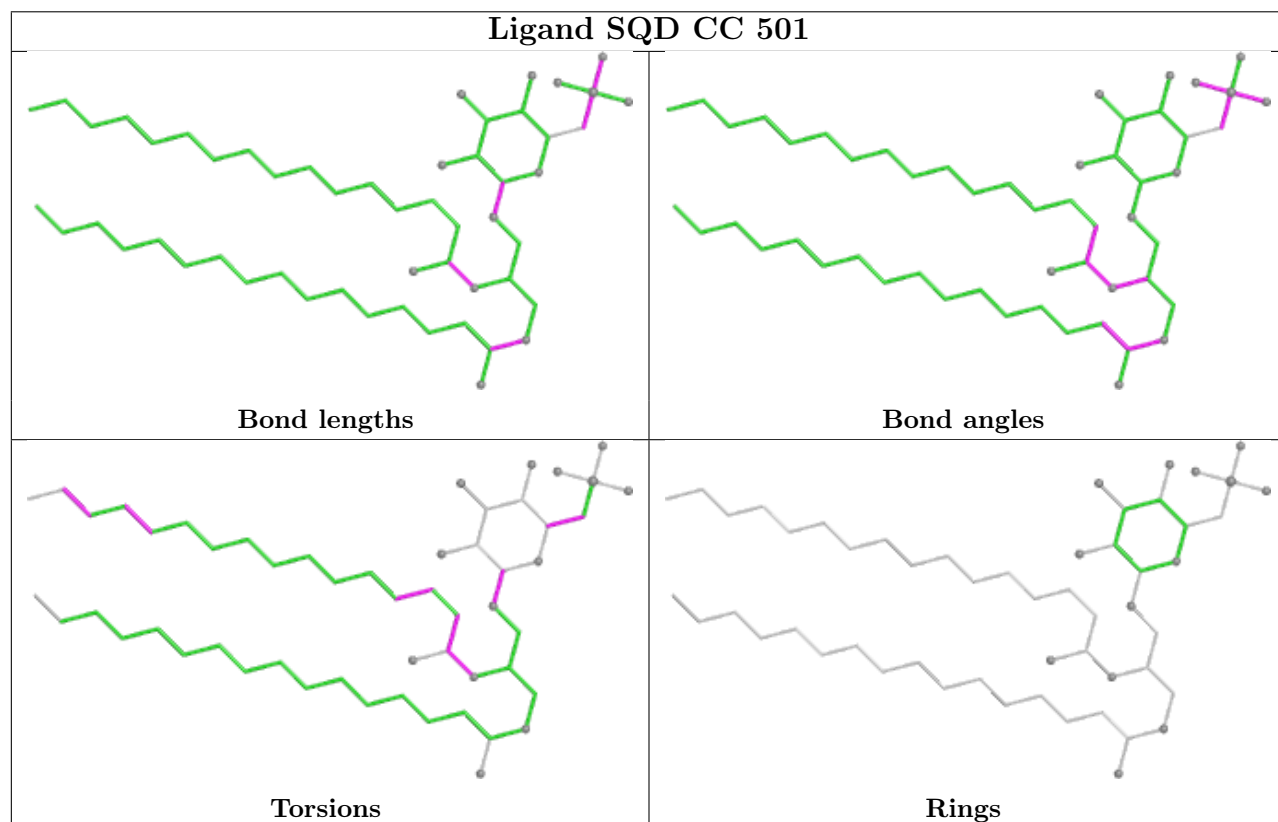
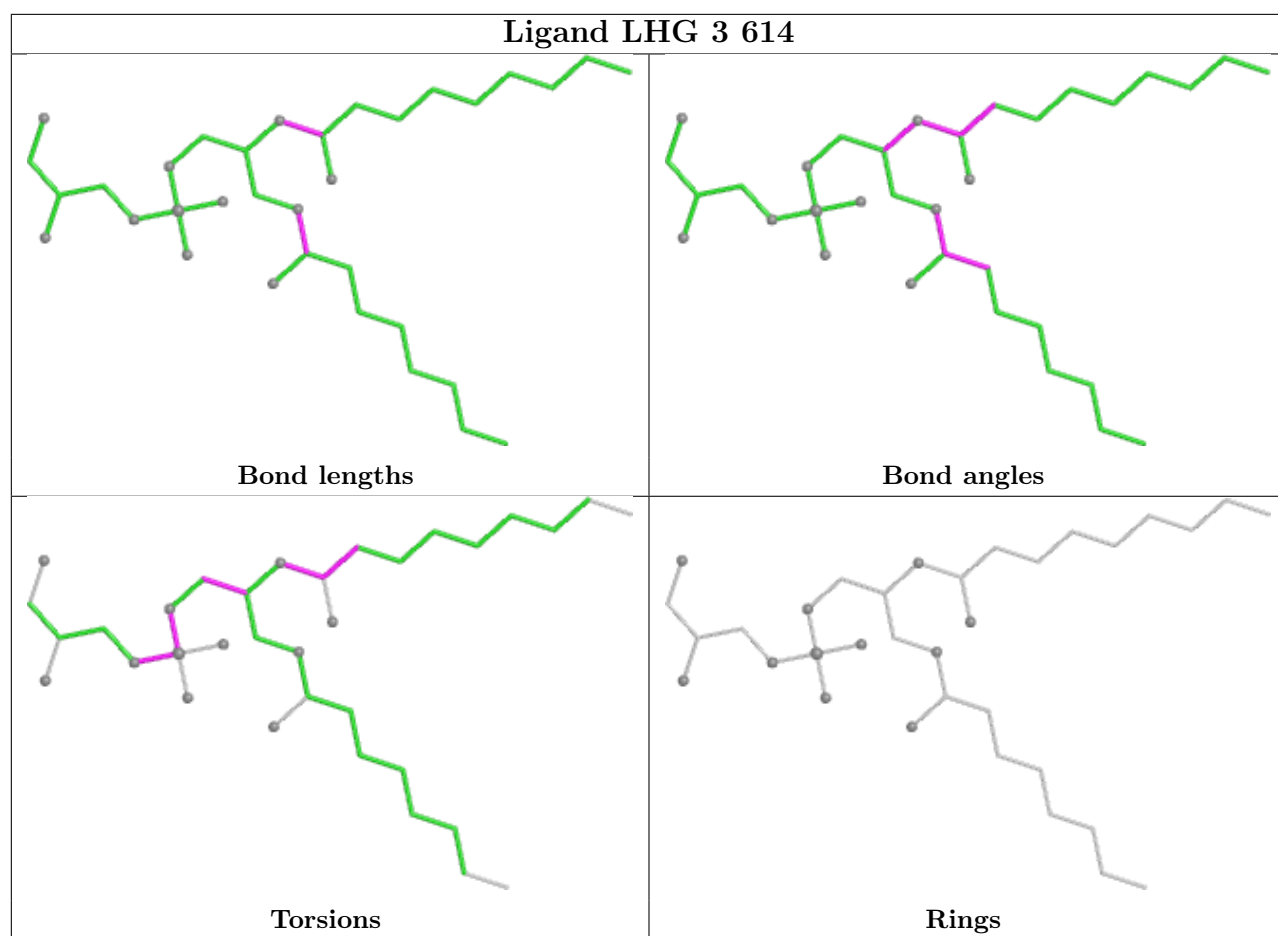
Ligand CLA Y 604

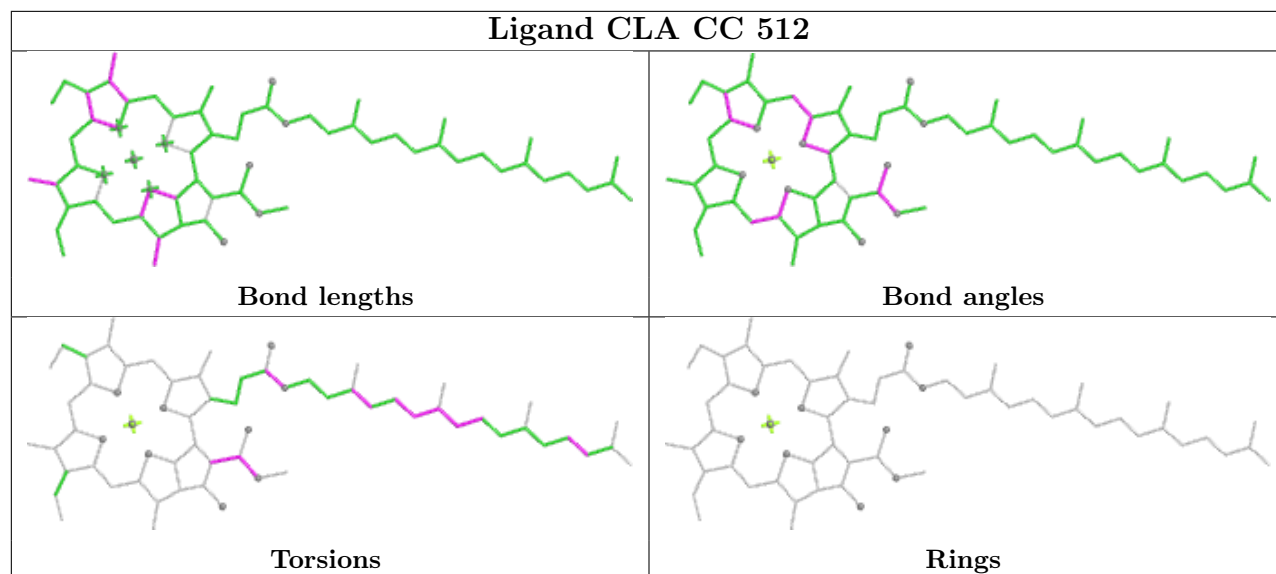
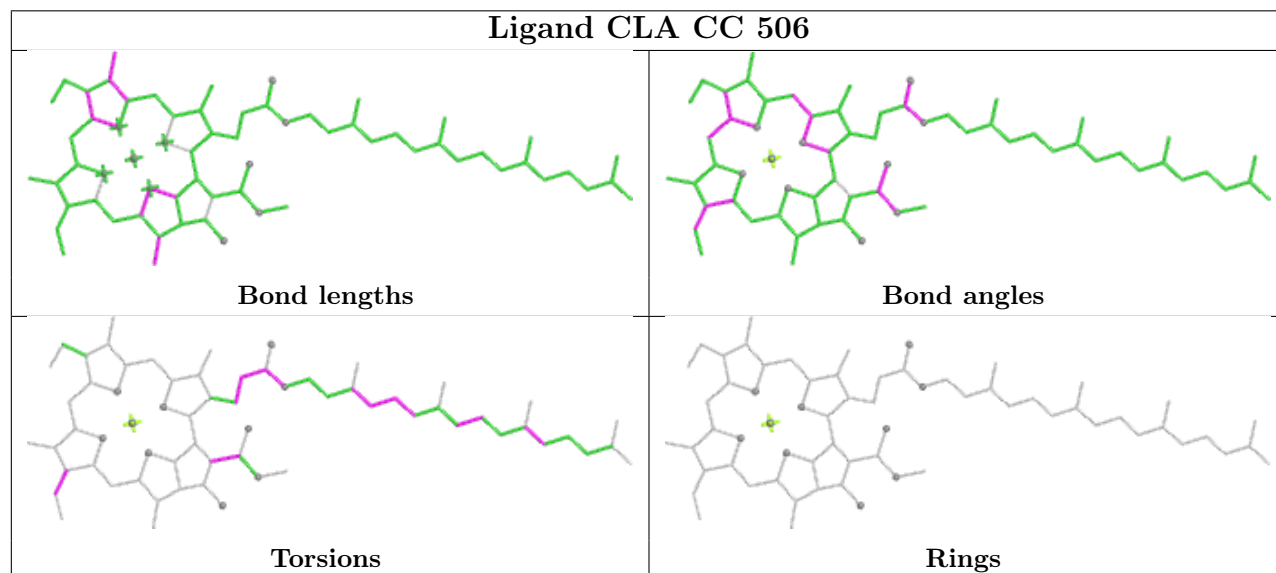


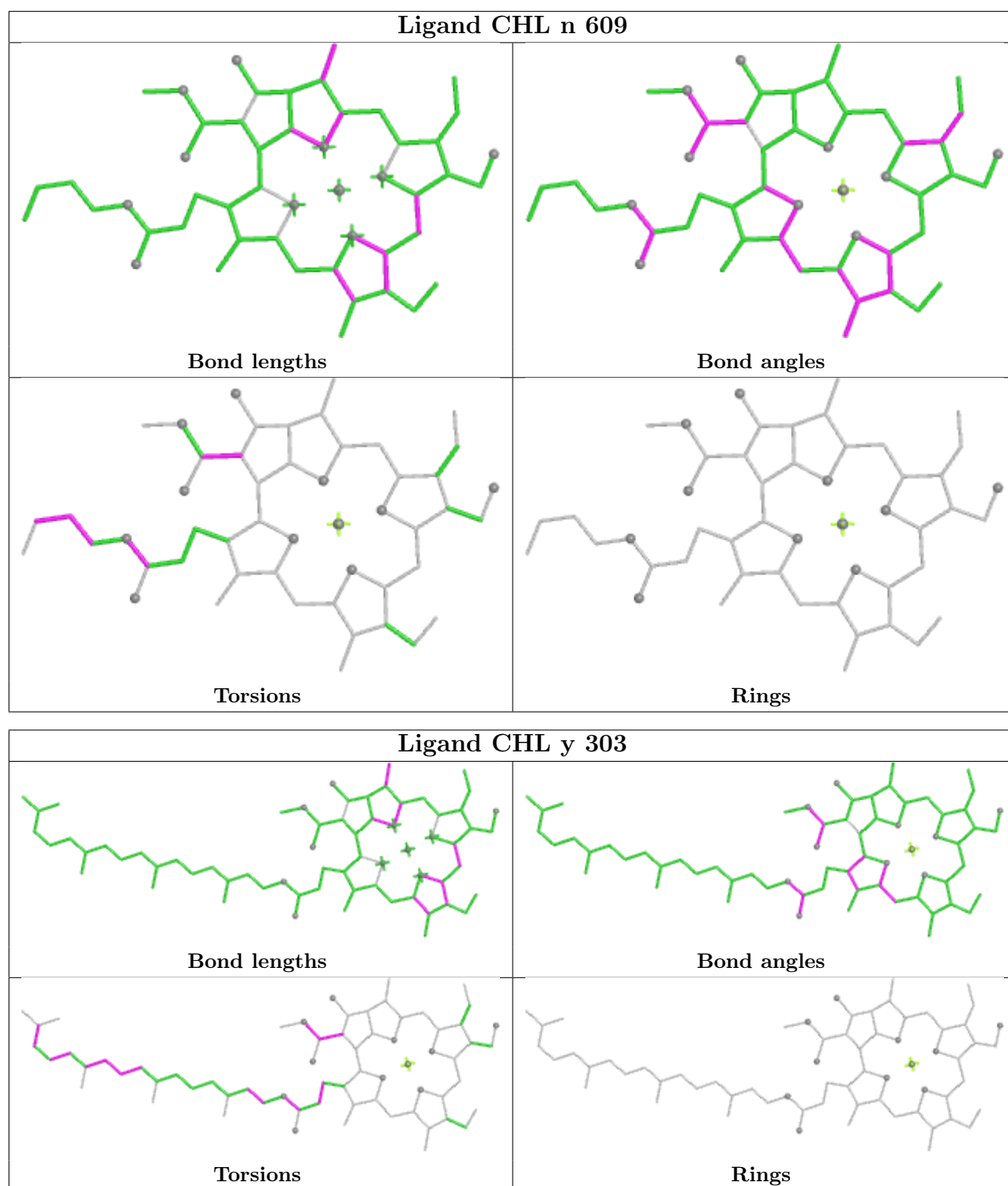
Ligand PHO A 407

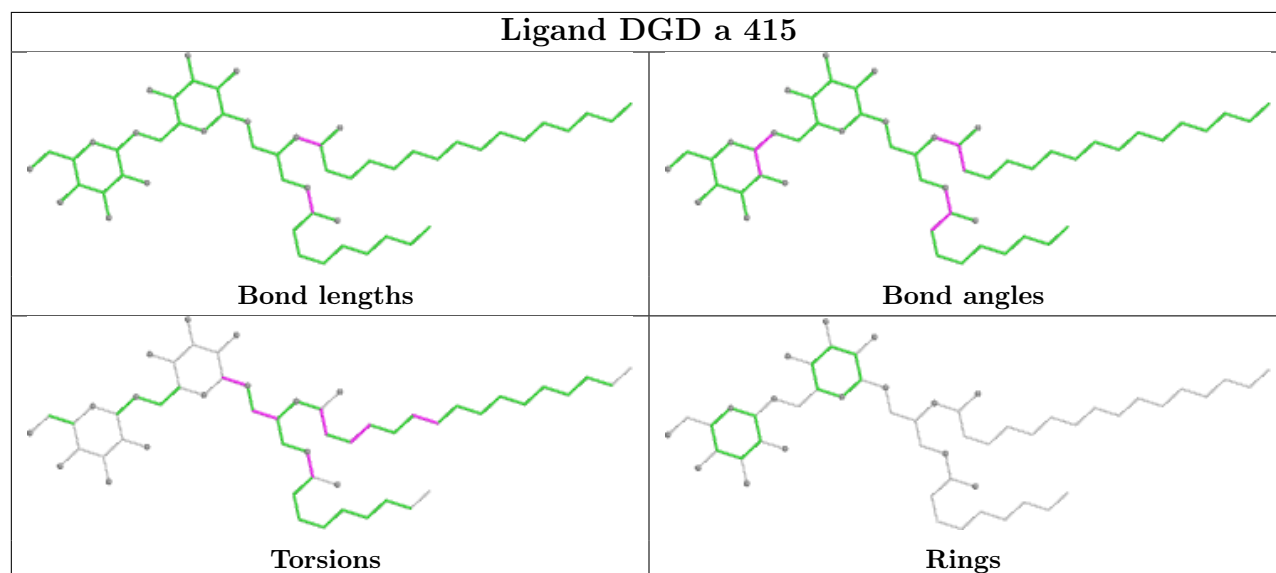
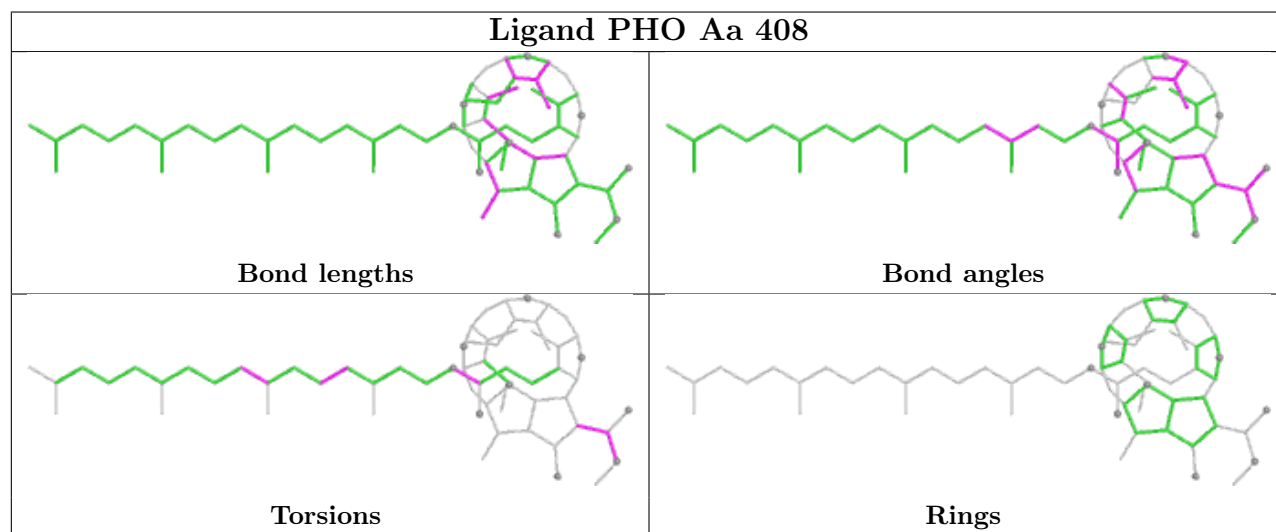
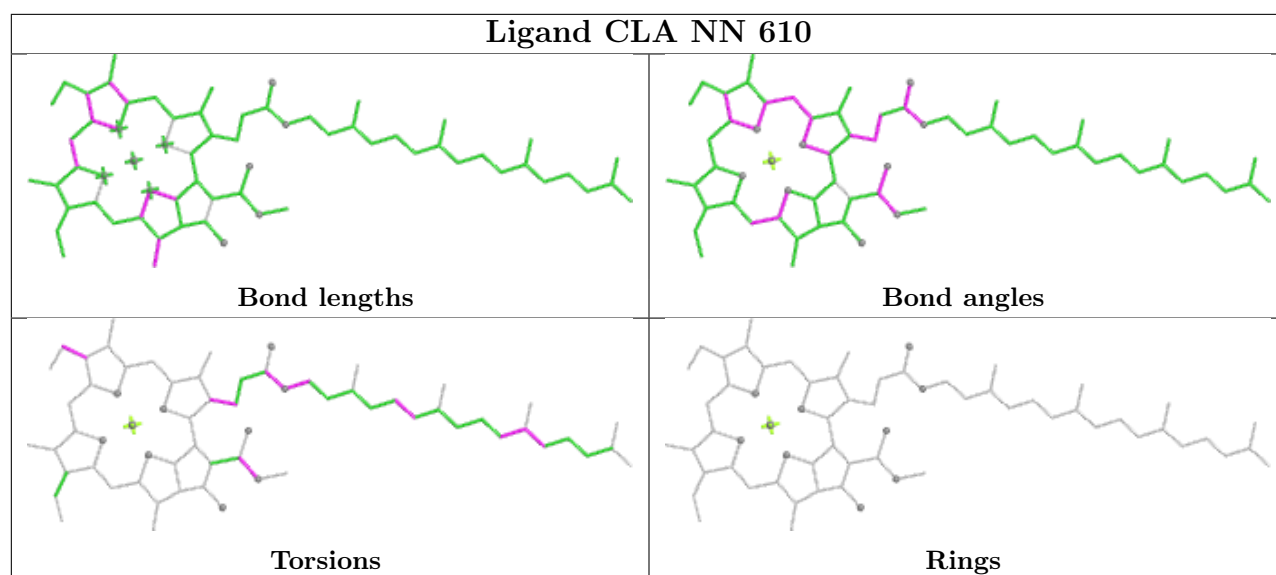




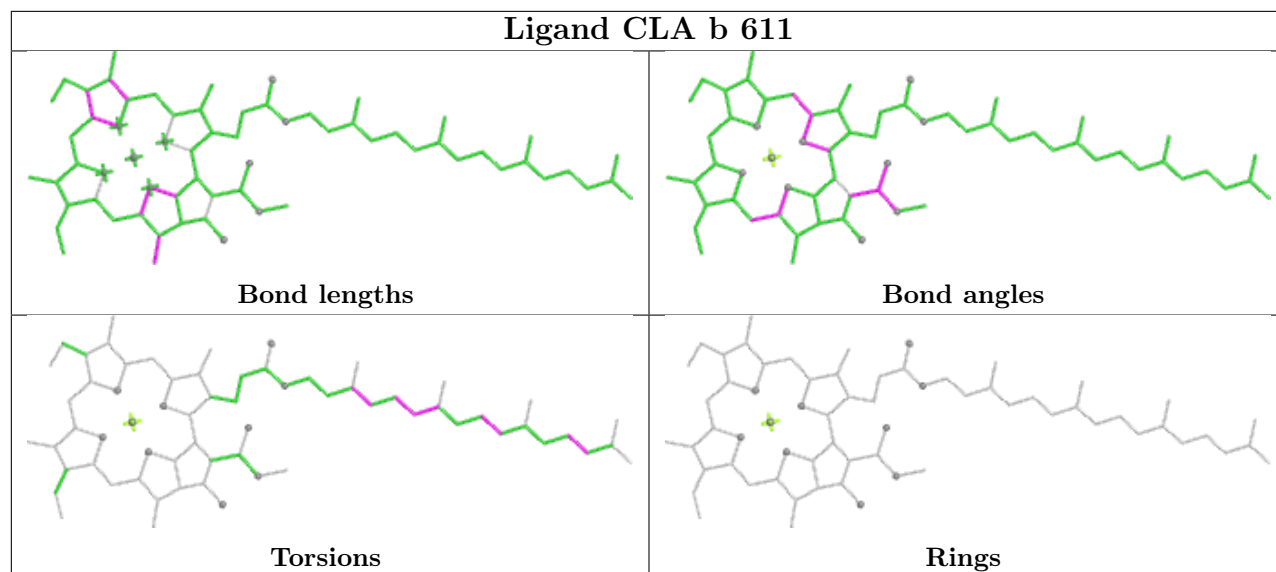


Ligand CLA CC 512**Ligand CLA CC 506**

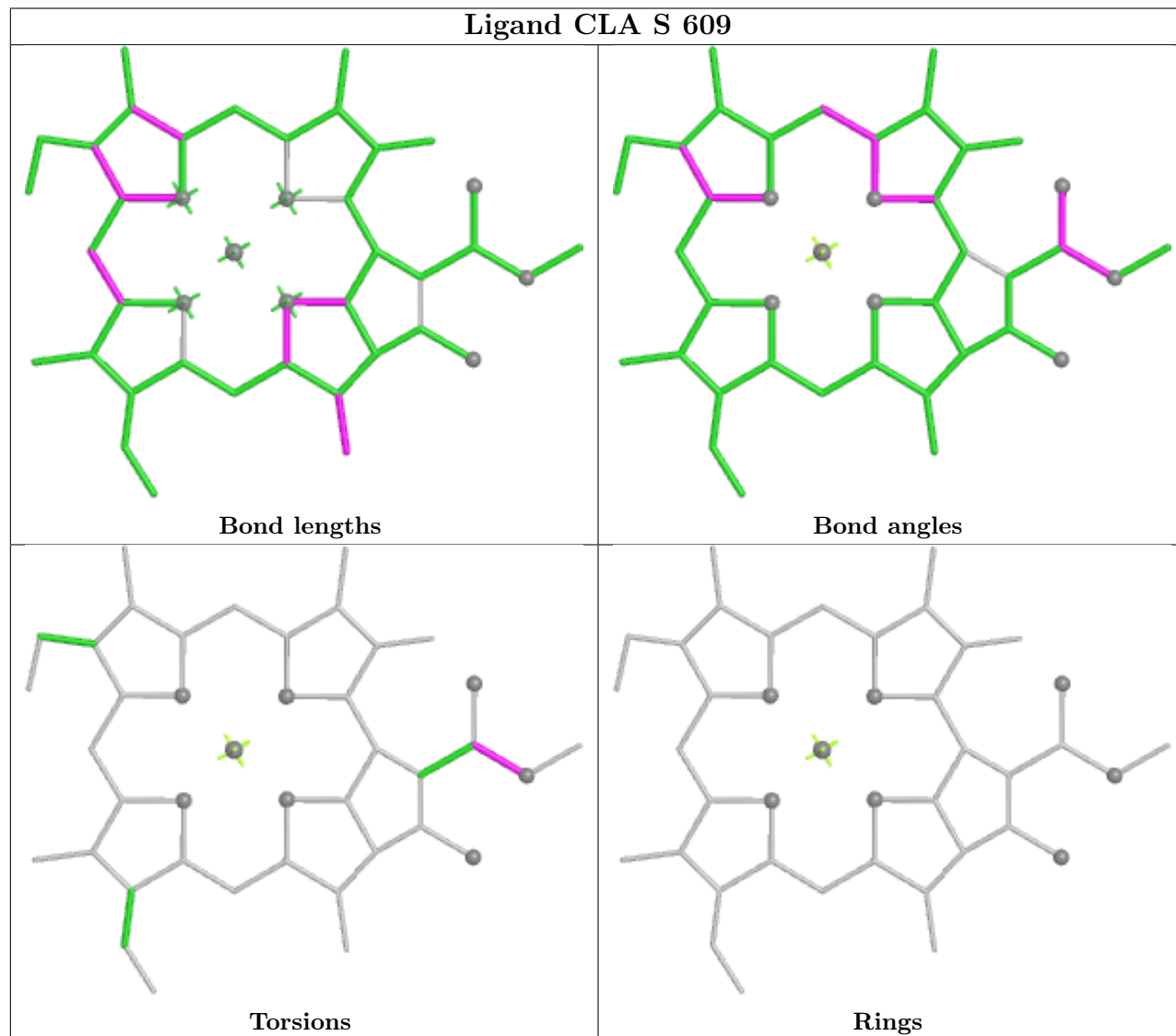


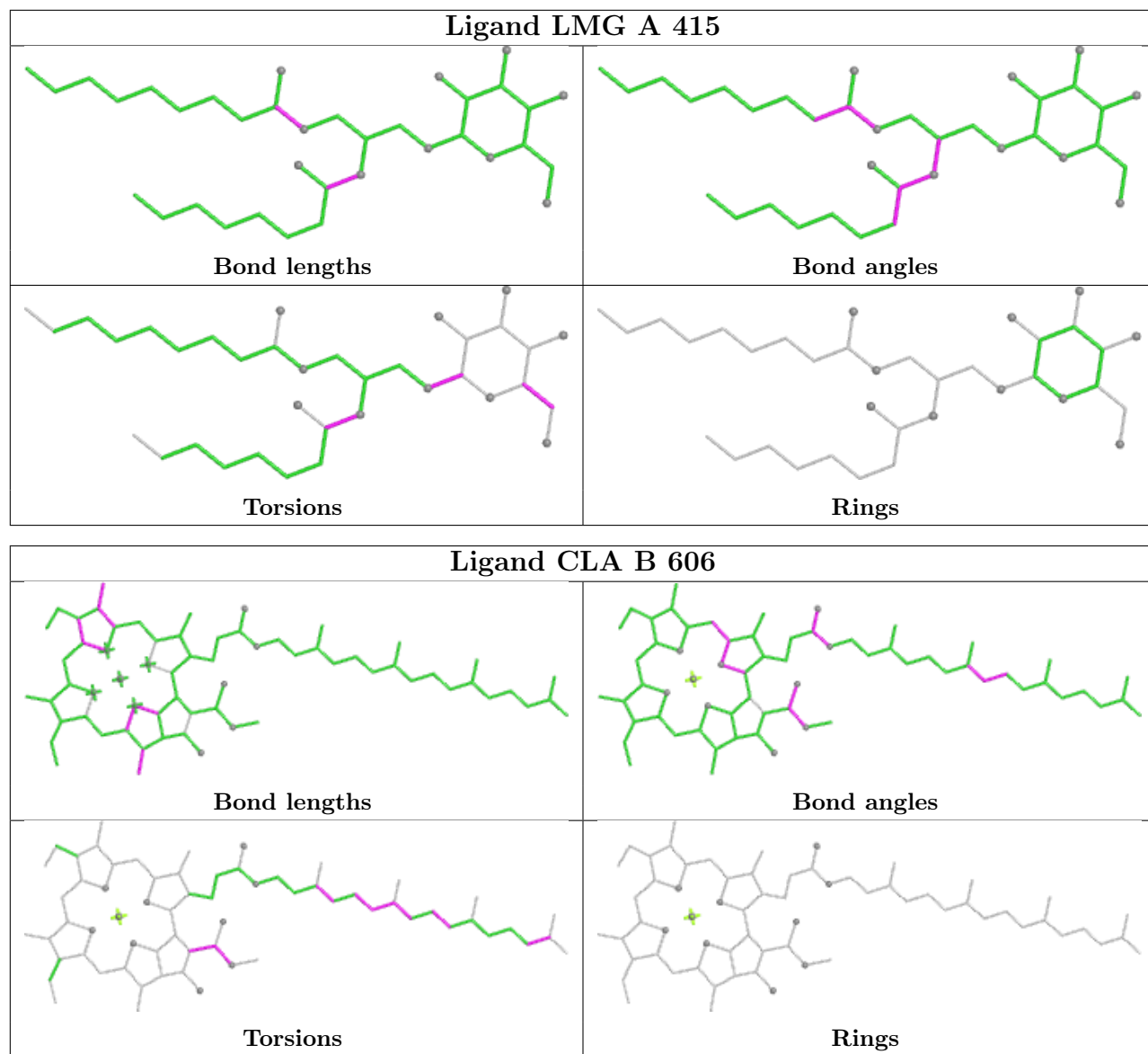


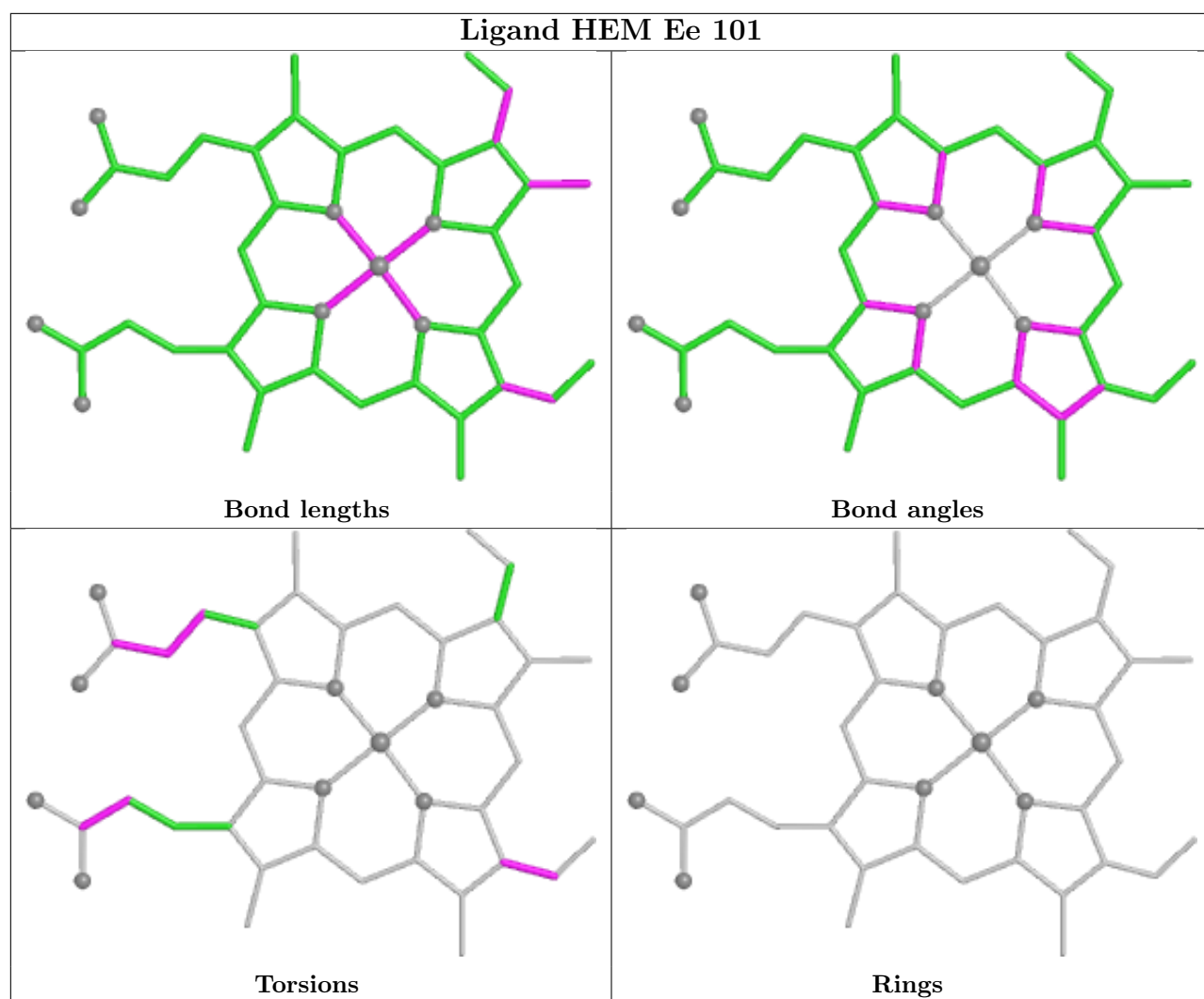
Ligand CLA b 611



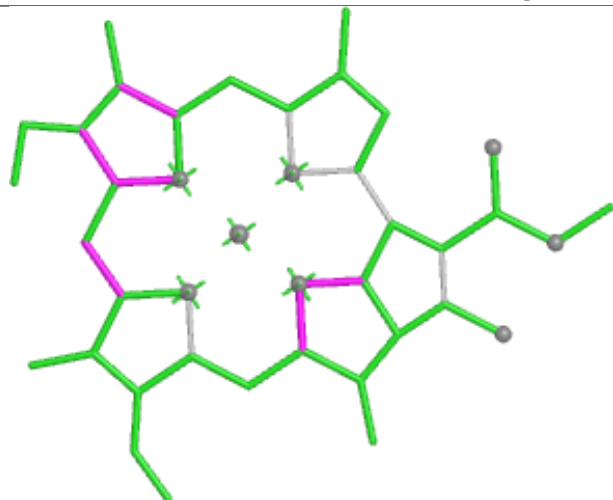
Ligand CLA S 609



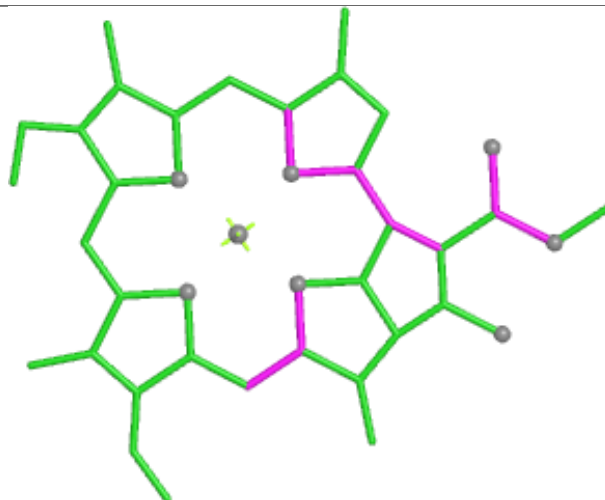




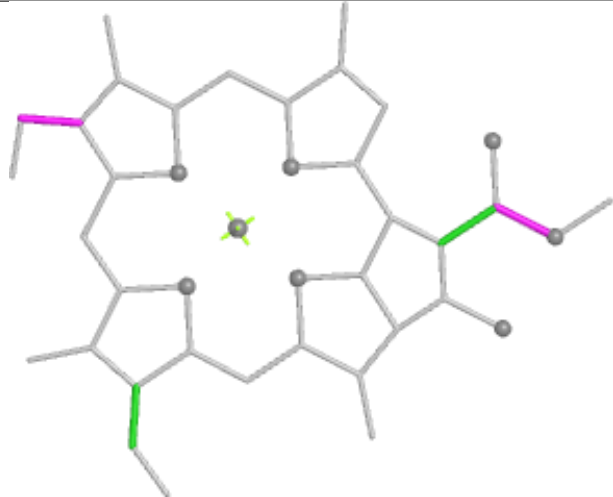
Ligand CLA 1 613



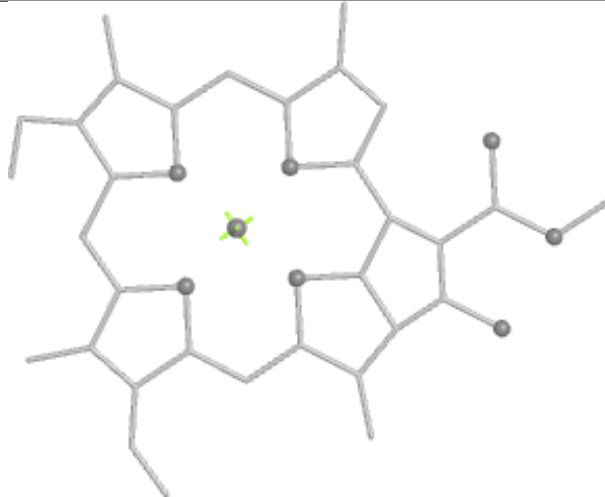
Bond lengths



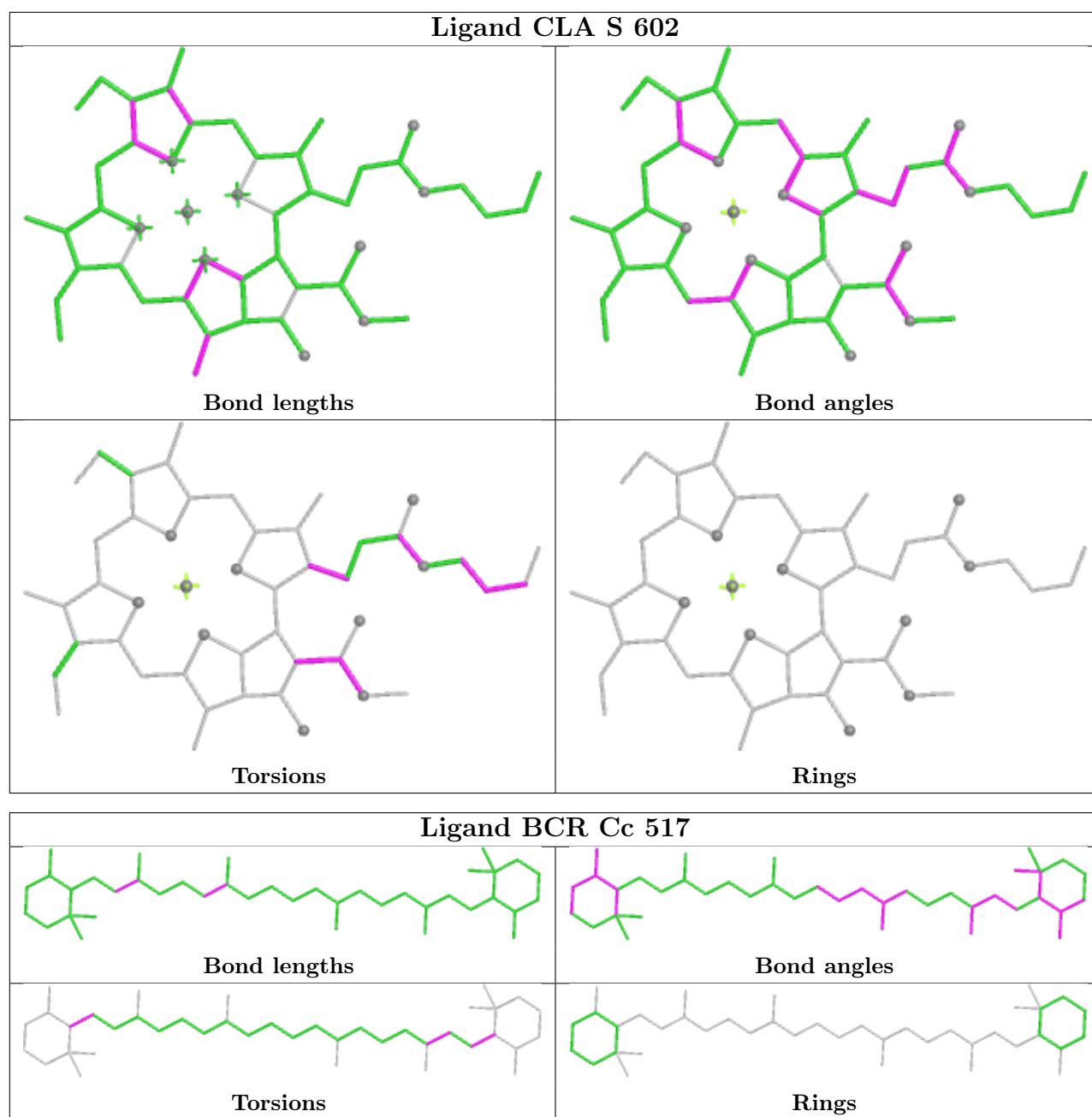
Bond angles

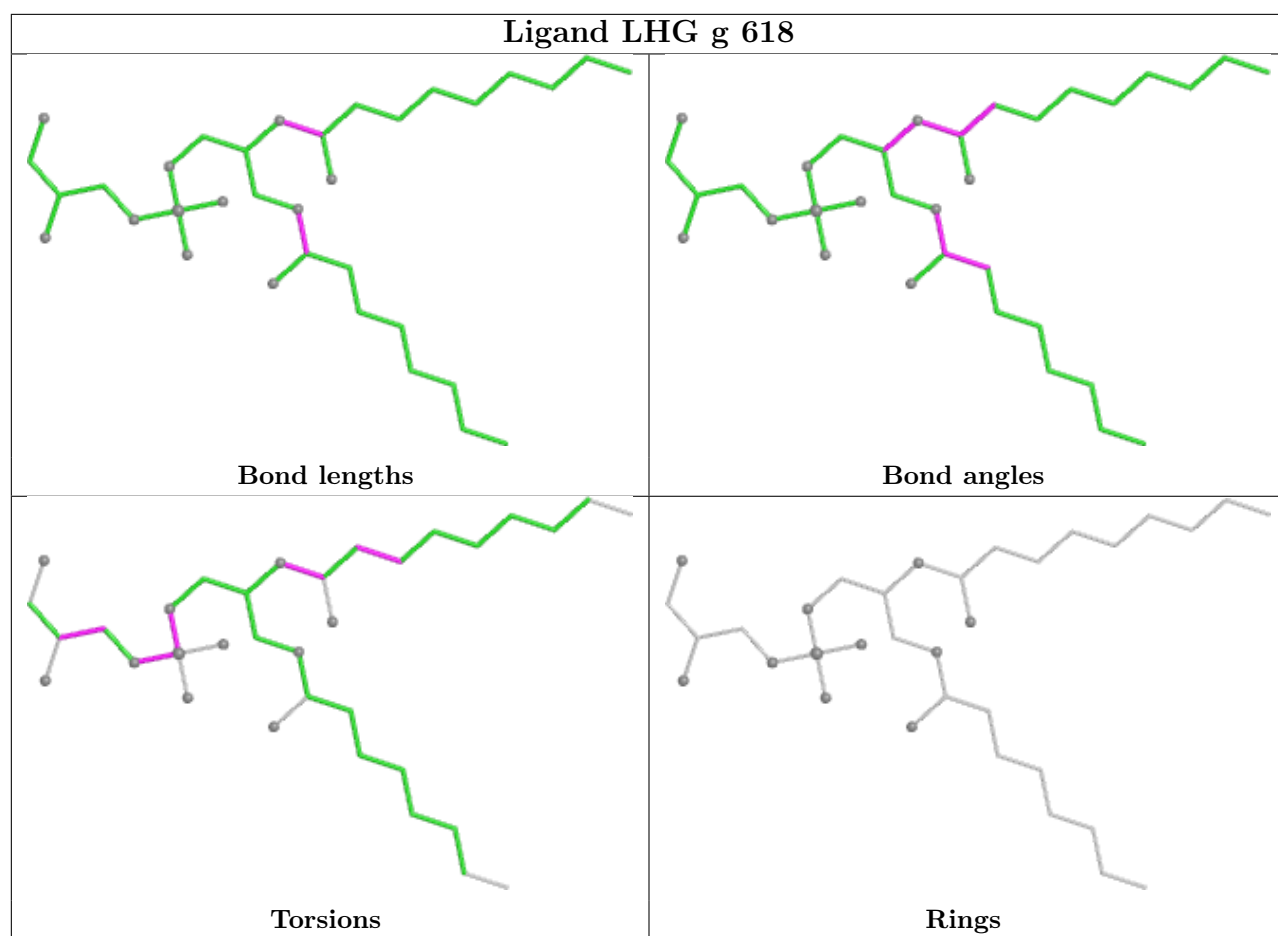


Torsions

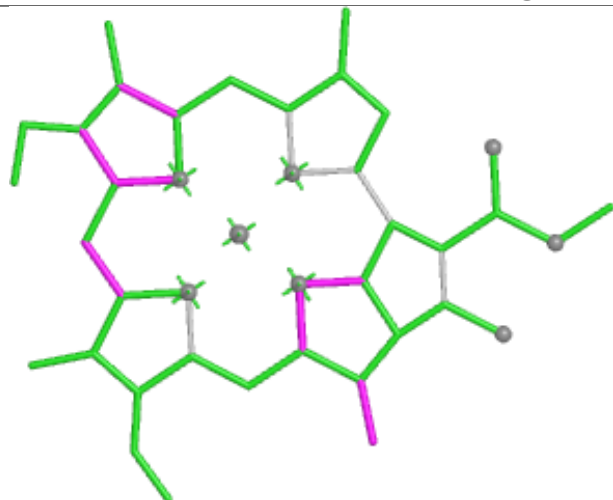


Rings

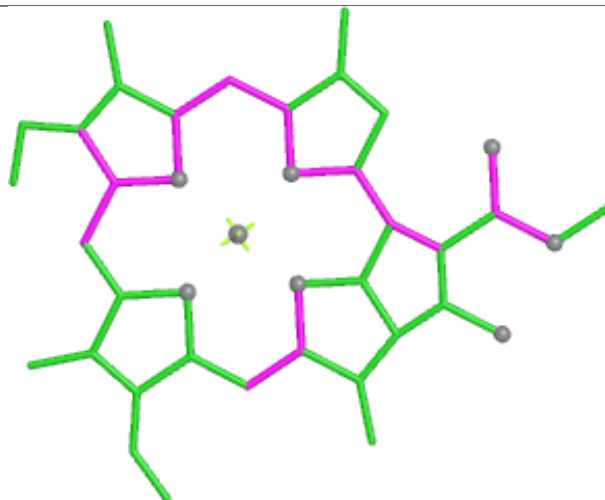




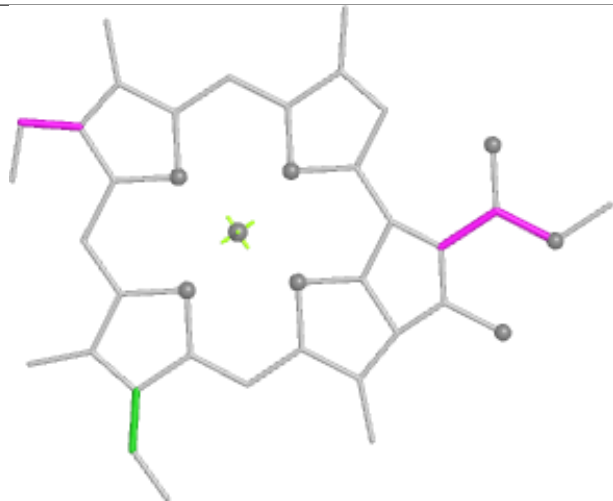
Ligand CLA 1 604



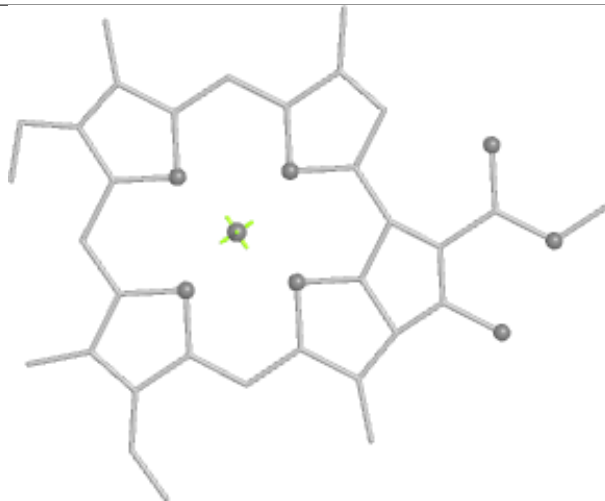
Bond lengths



Bond angles

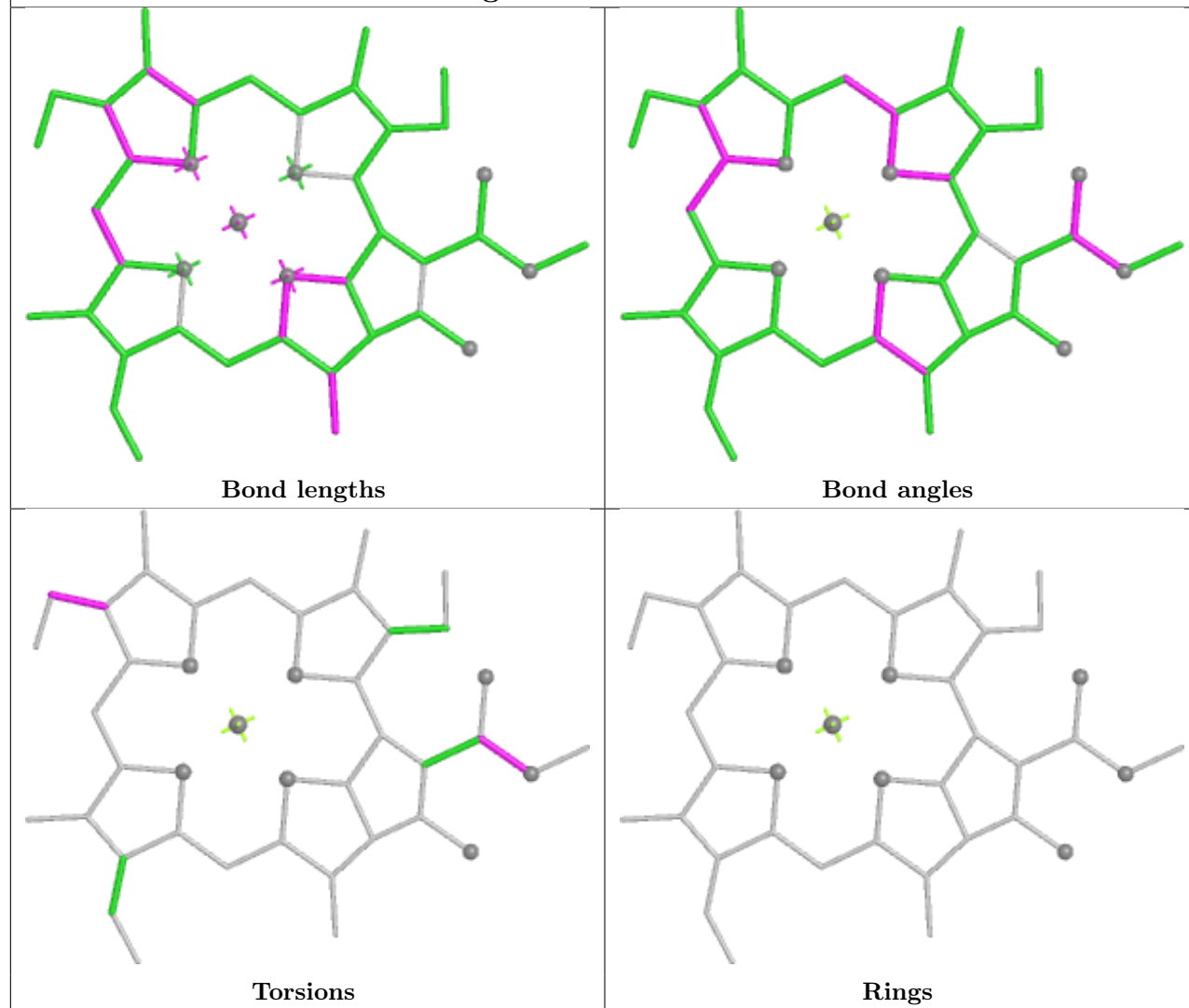


Torsions

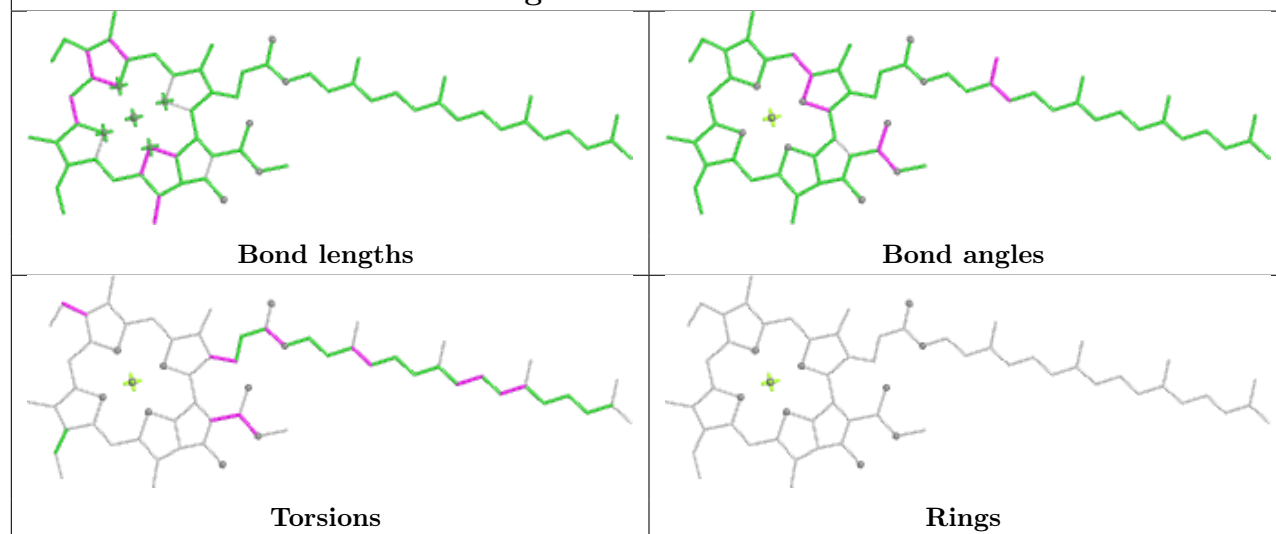


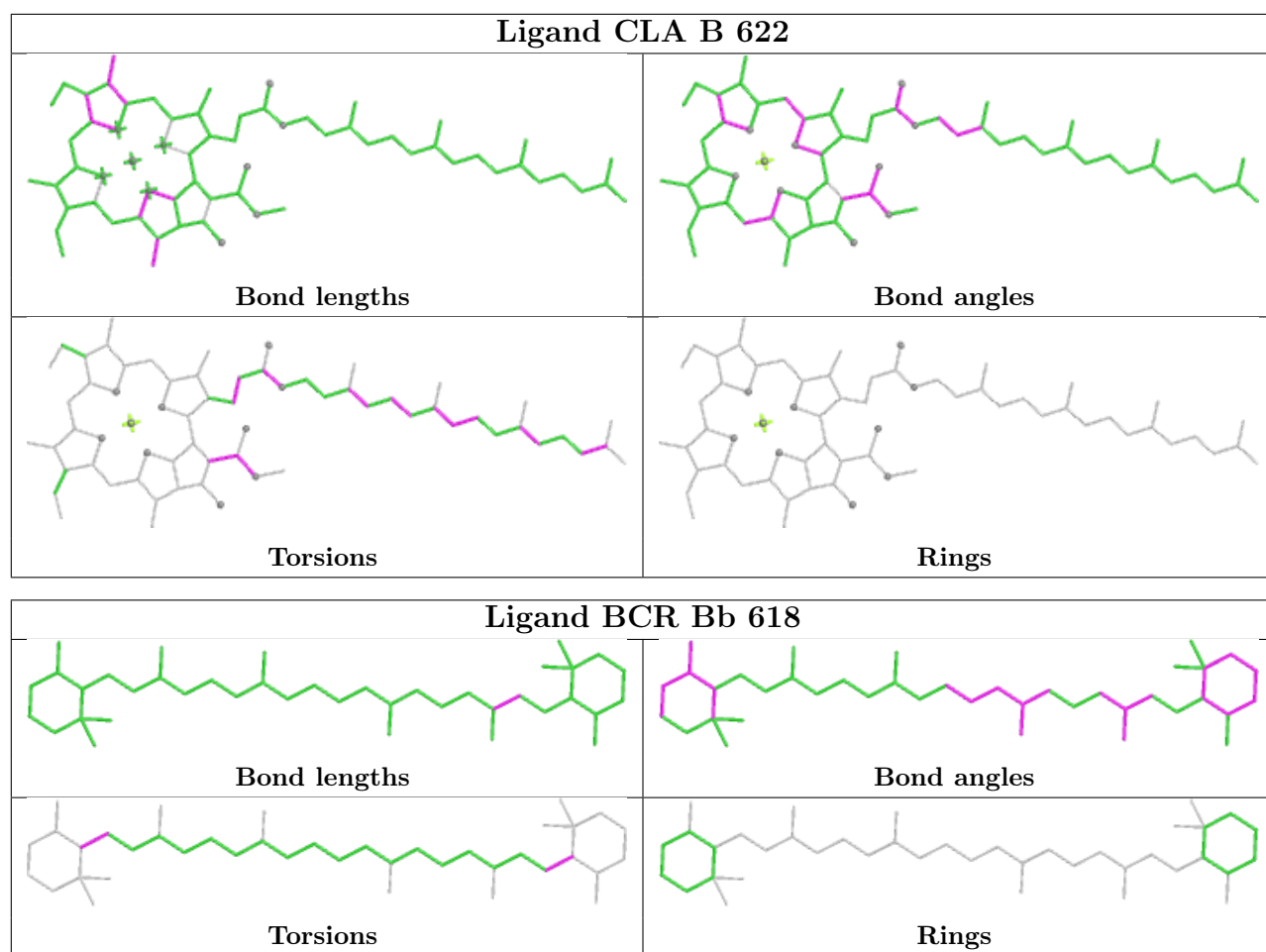
Rings

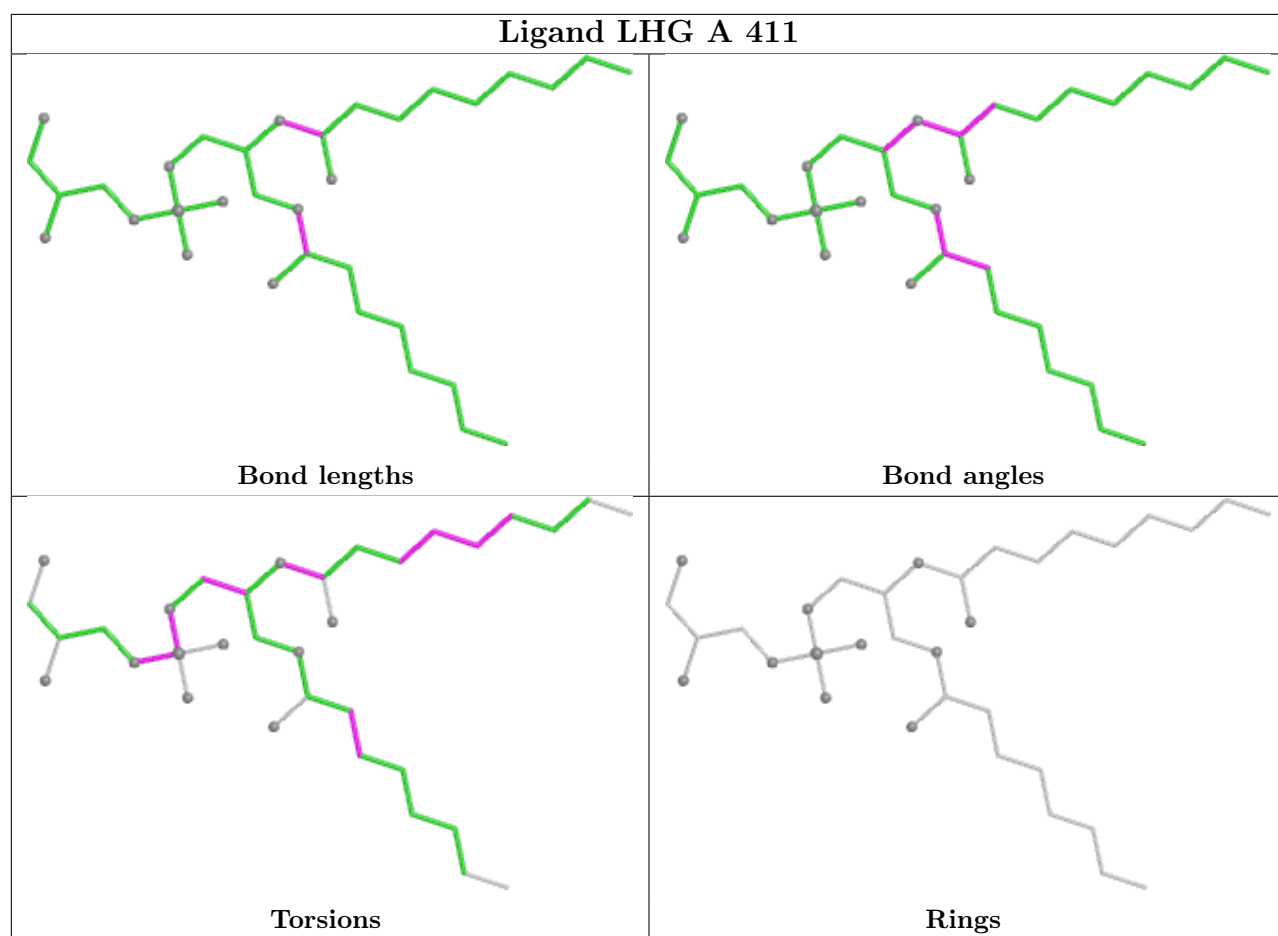
Ligand CLA YY 611

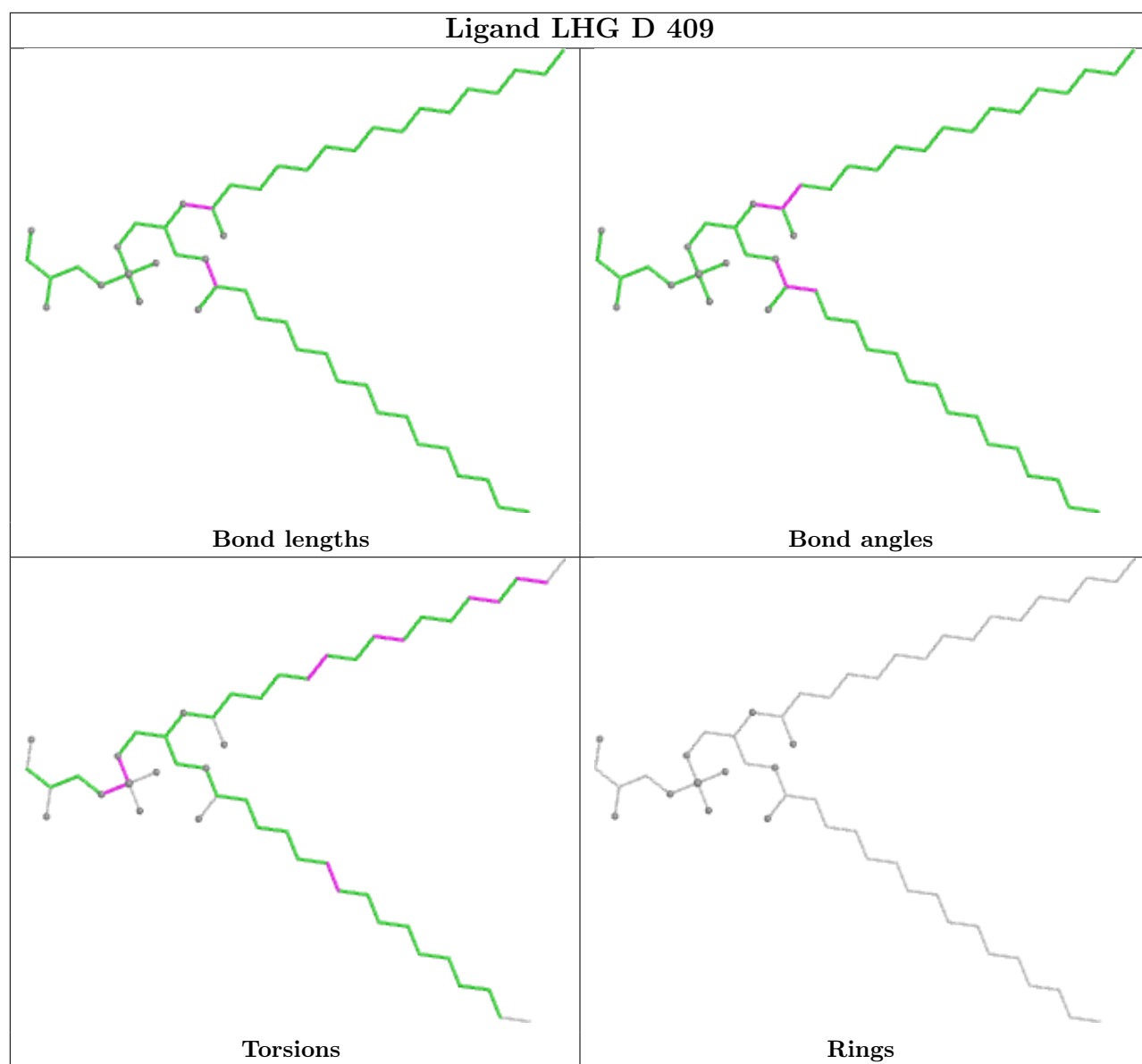


Ligand CLA Rr 609

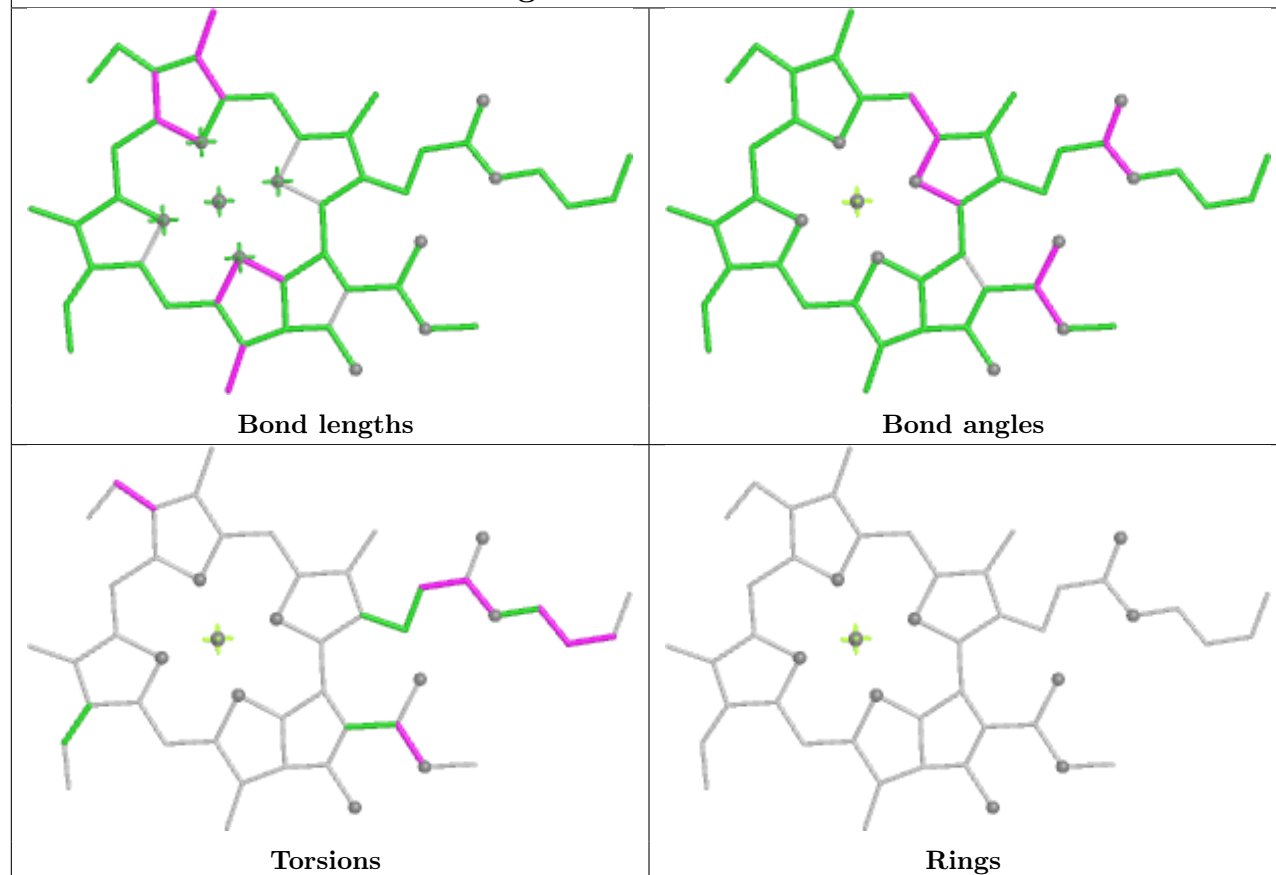




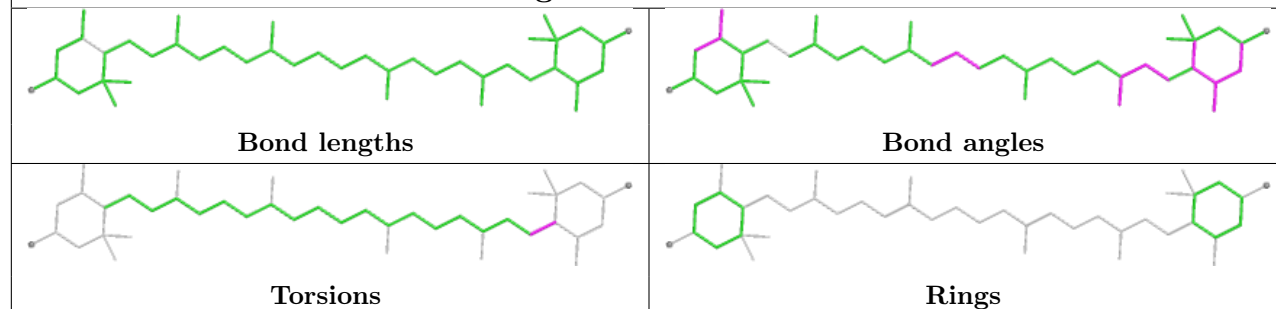


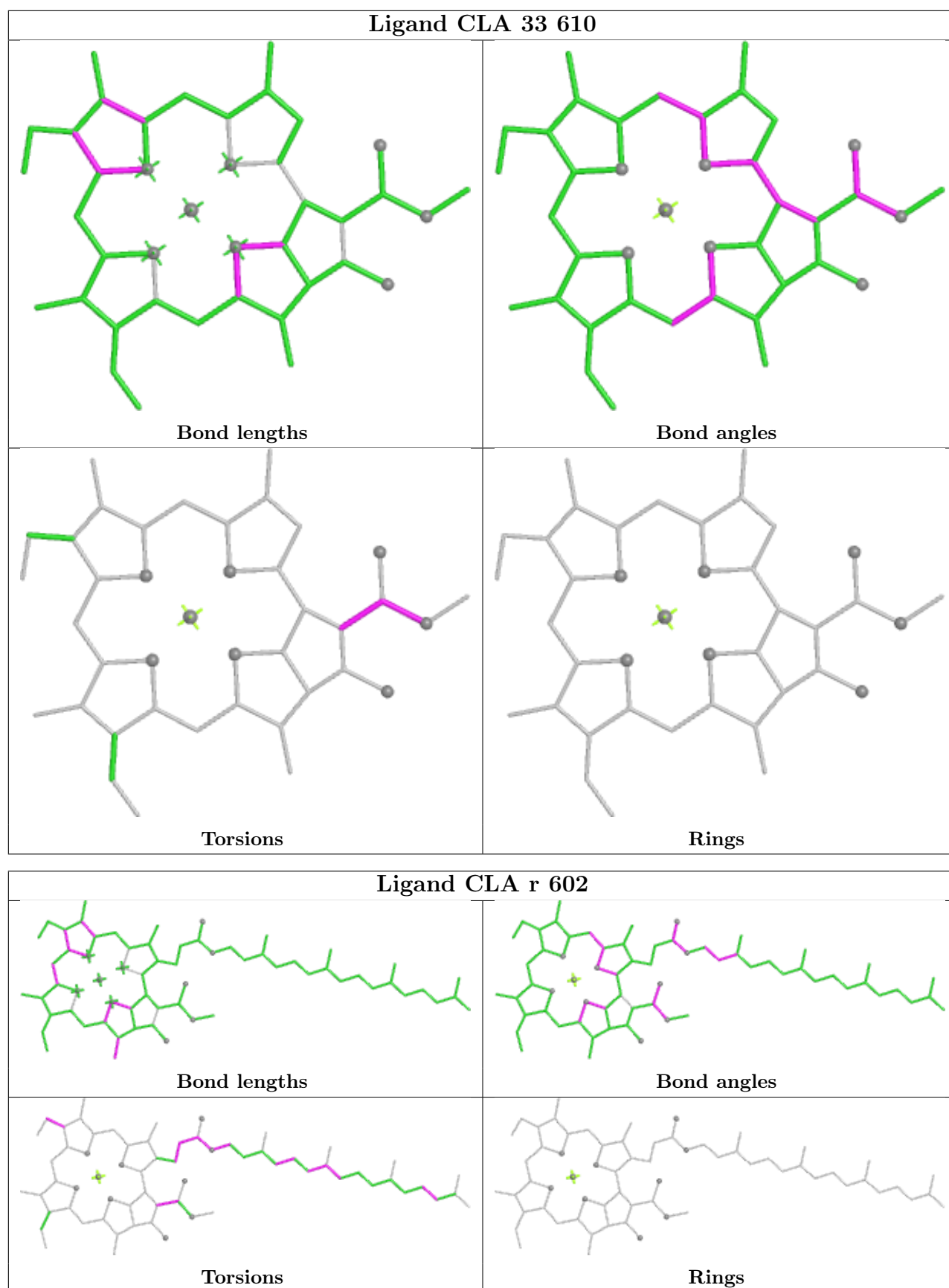


Ligand CLA YY 603

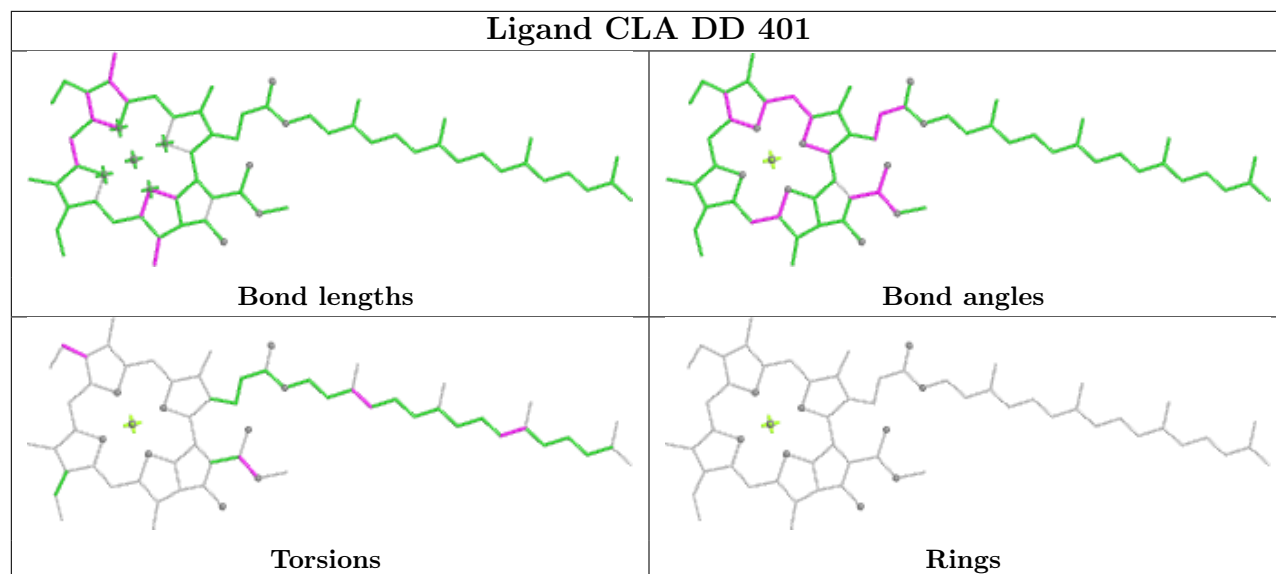


Ligand LUT S 614

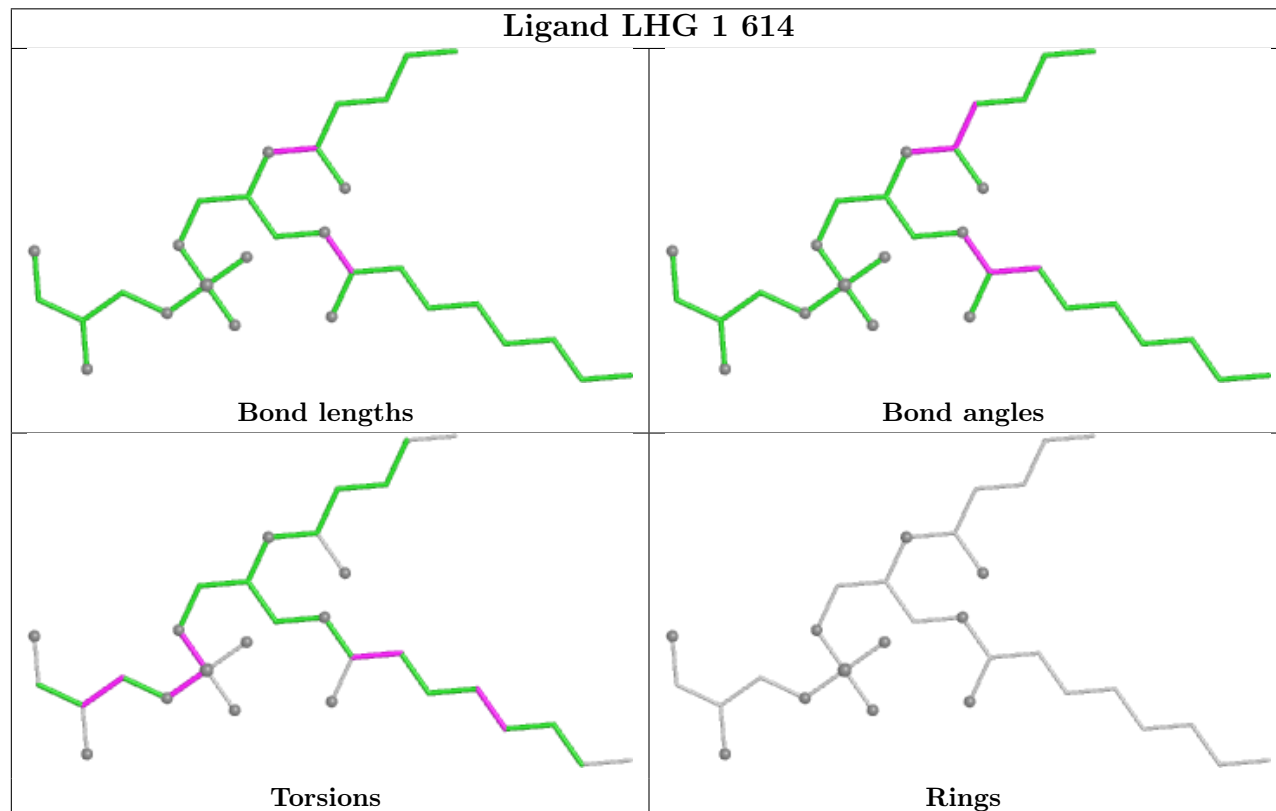


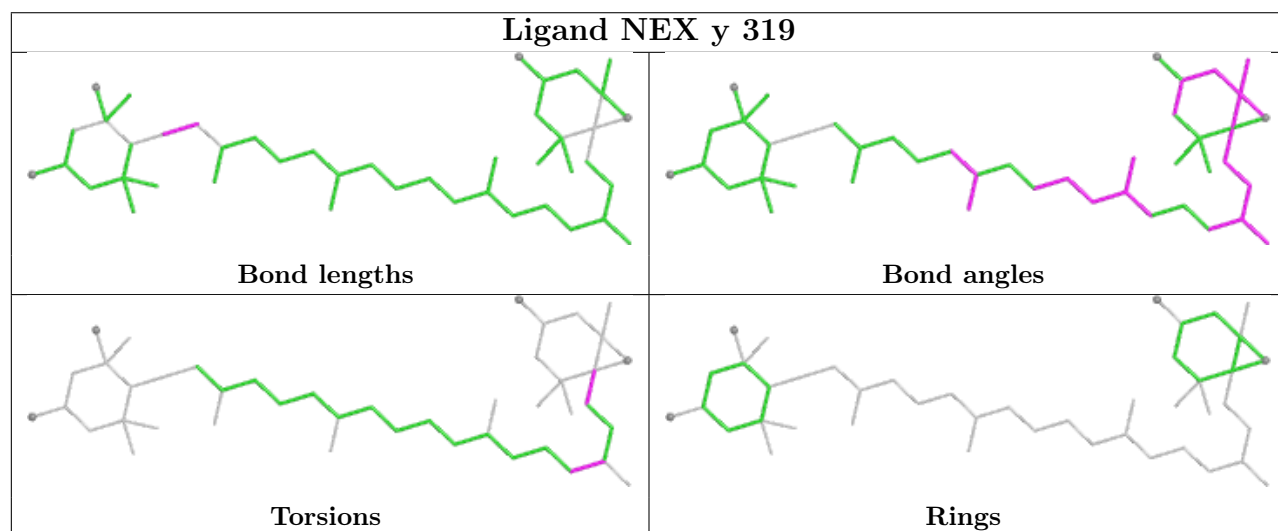
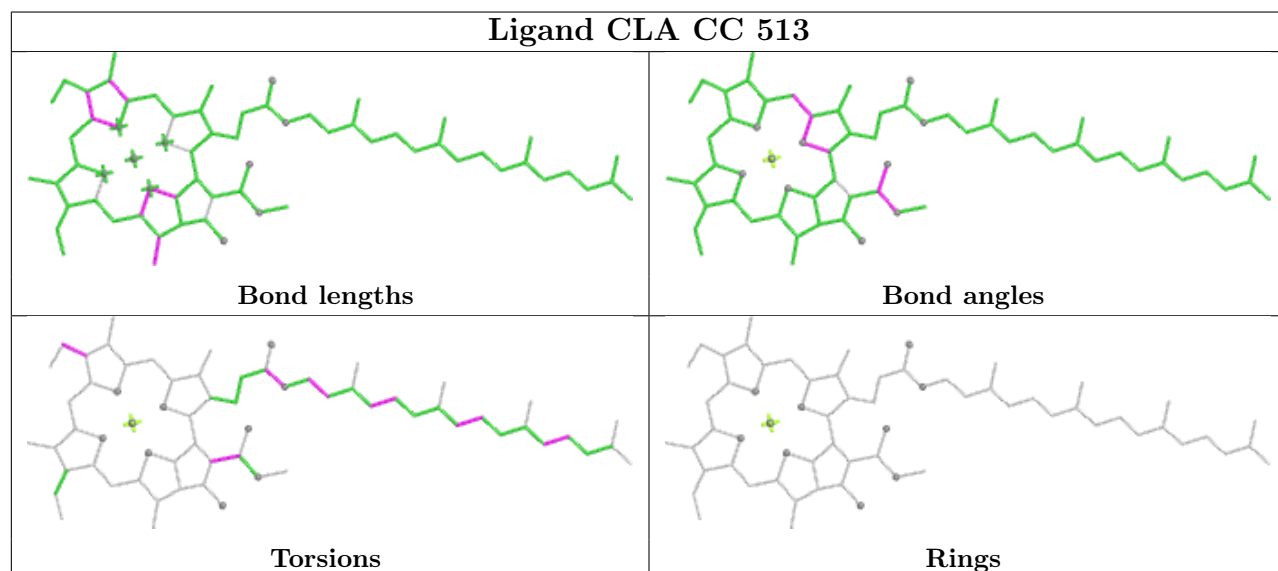
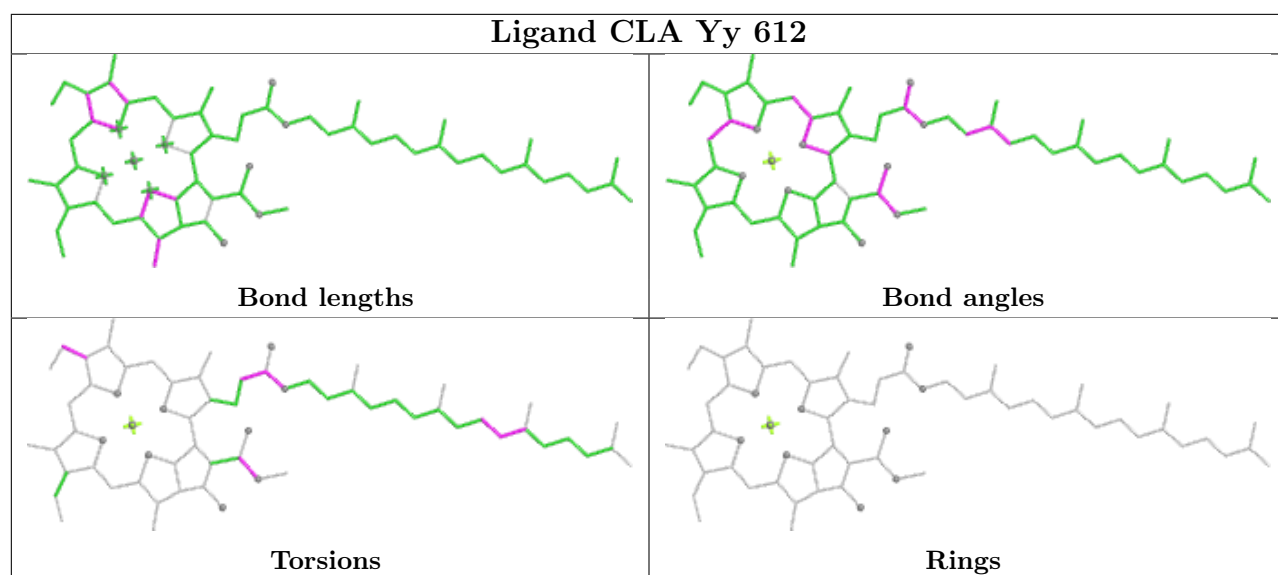


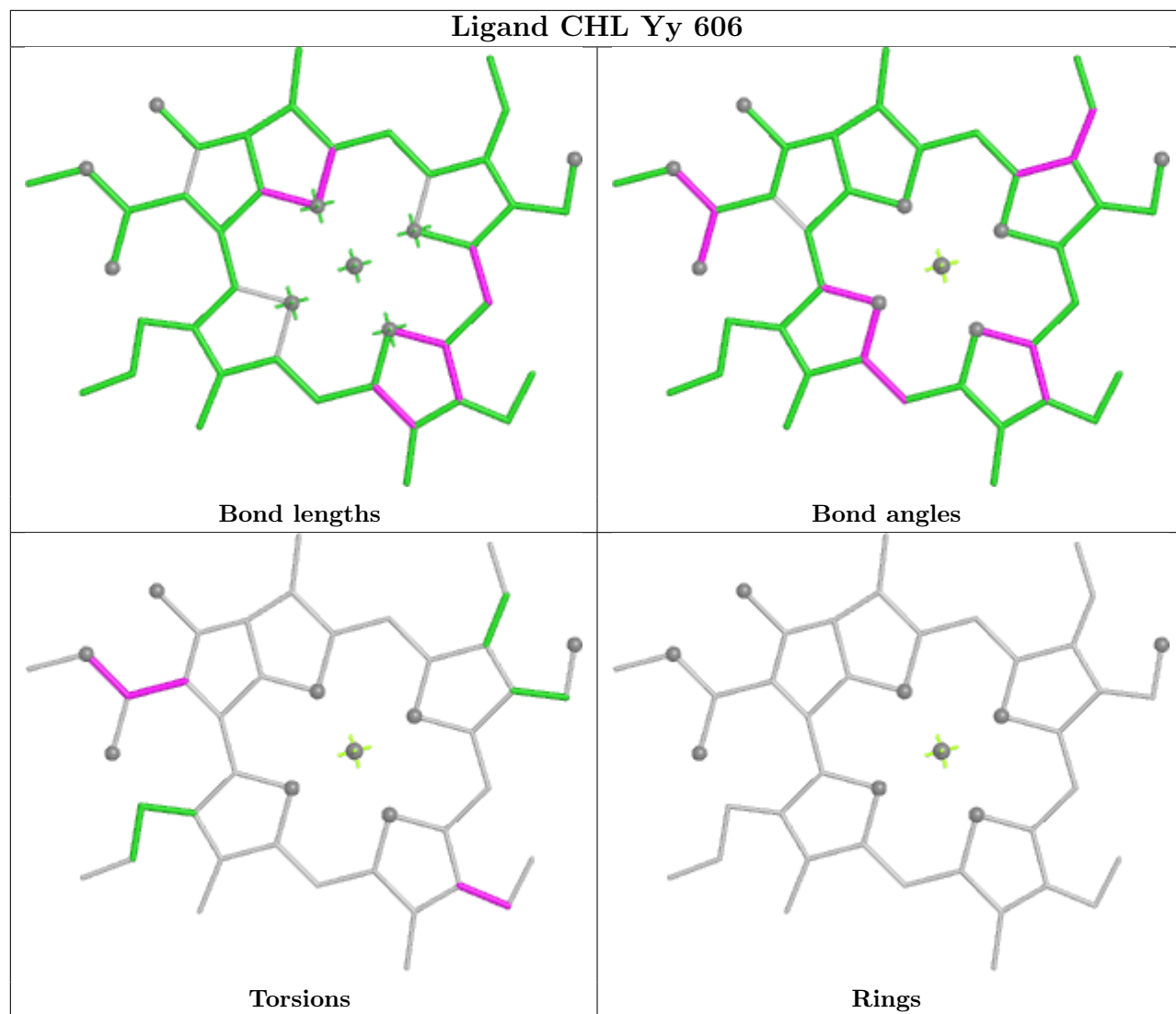
Ligand CLA DD 401

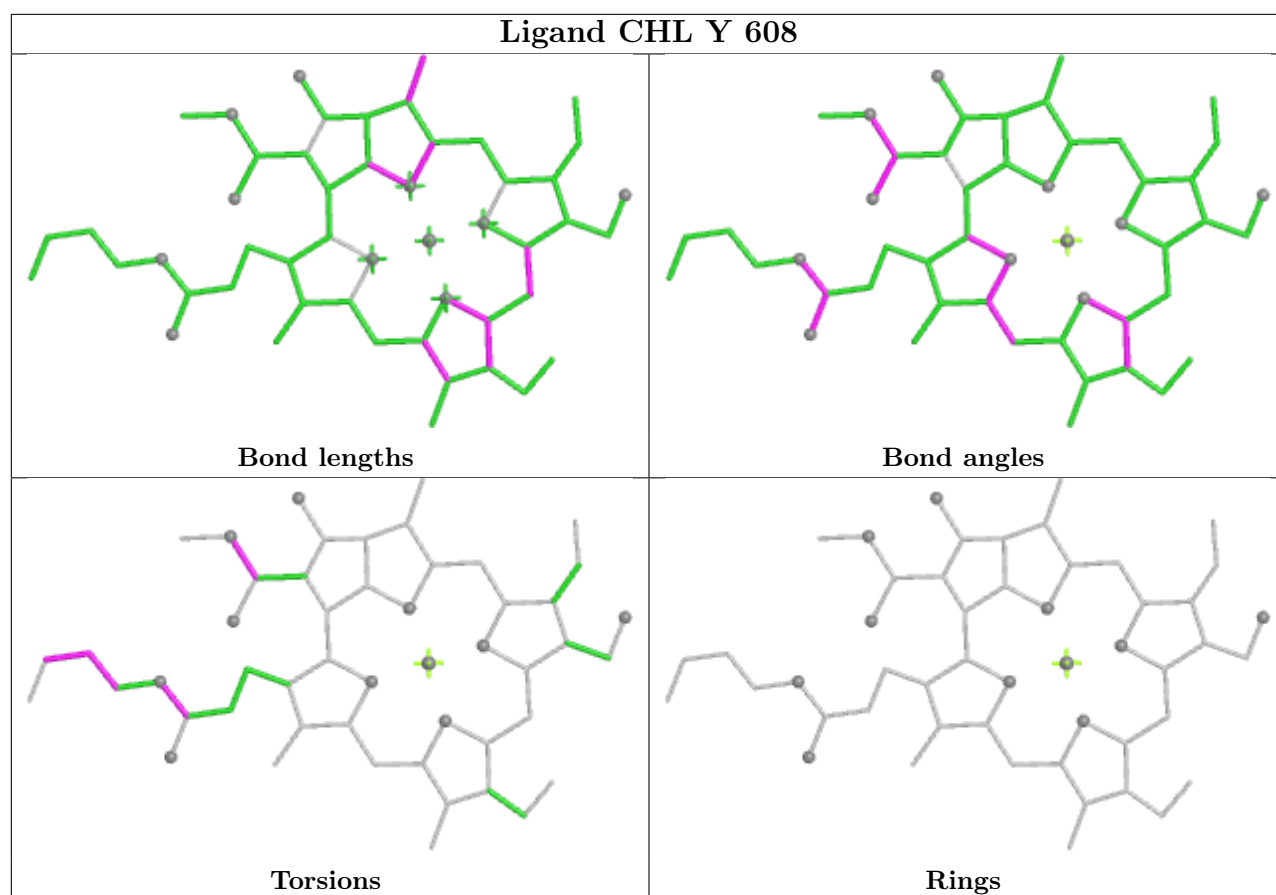


Ligand LHG 1 614

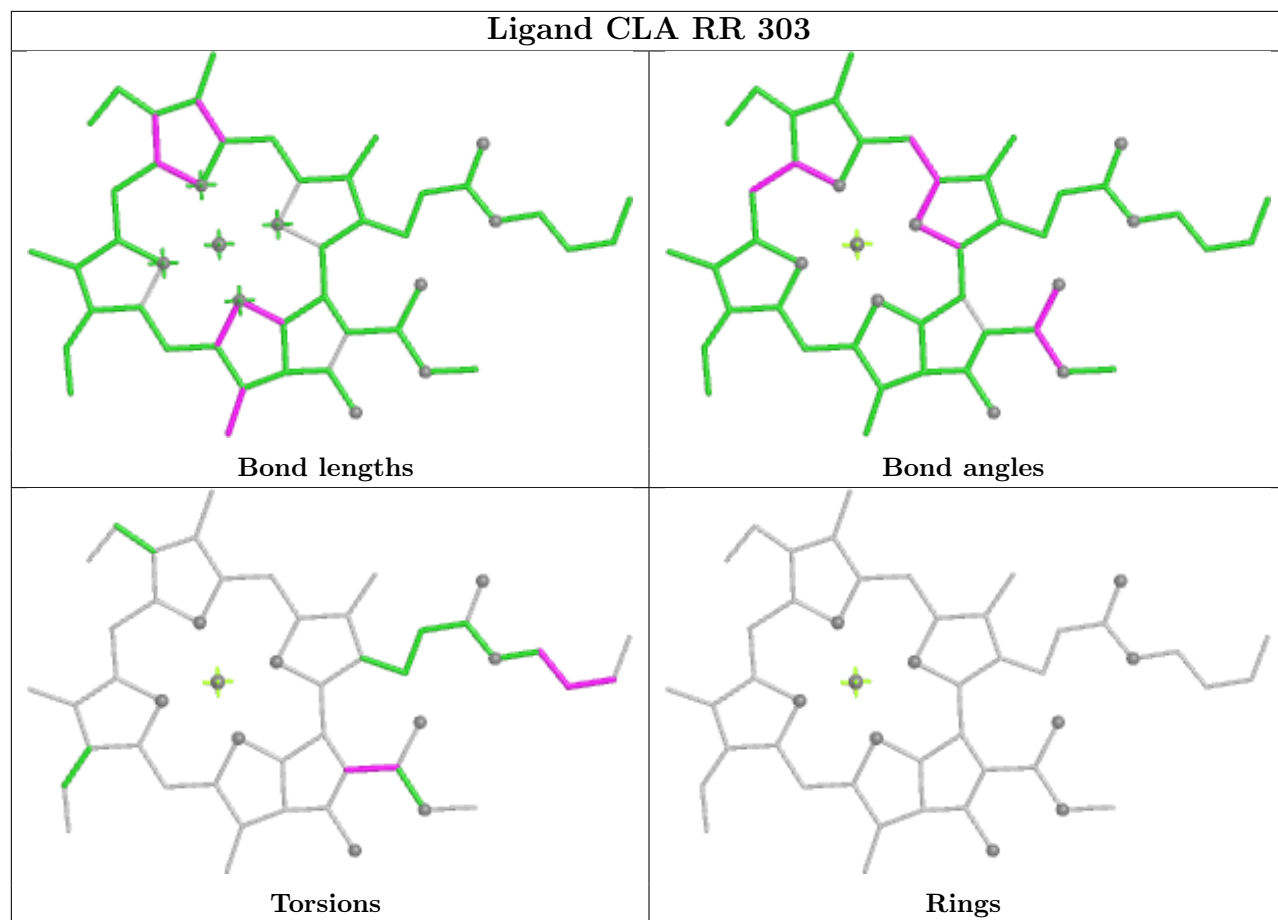




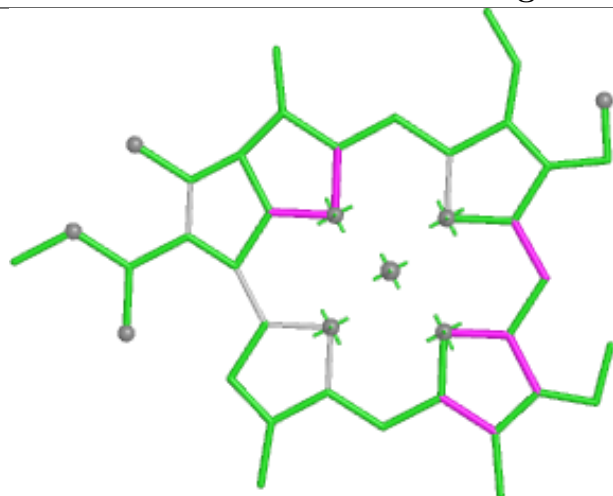




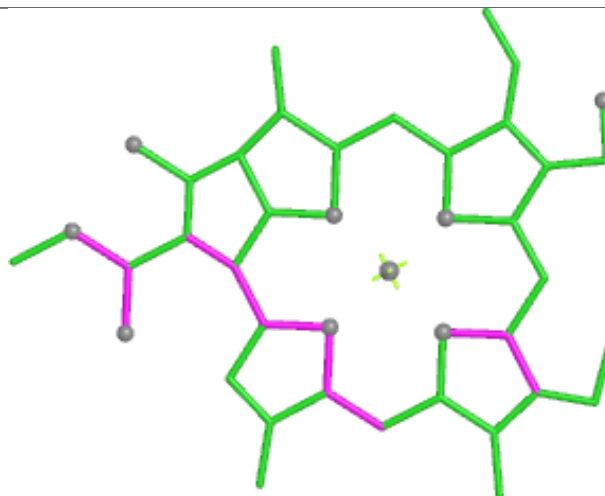
Ligand CLA RR 303



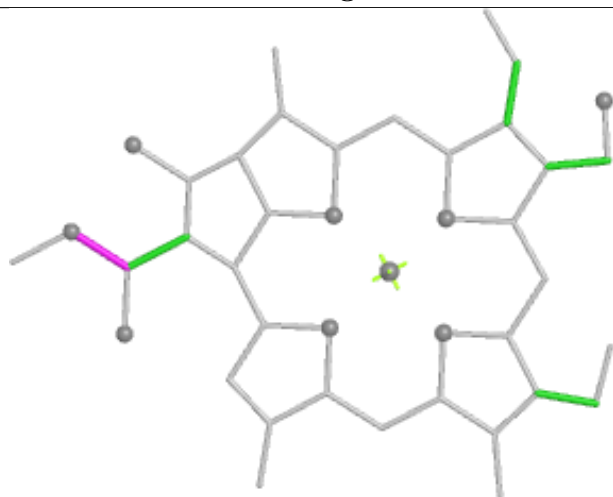
Ligand CHL 2 601



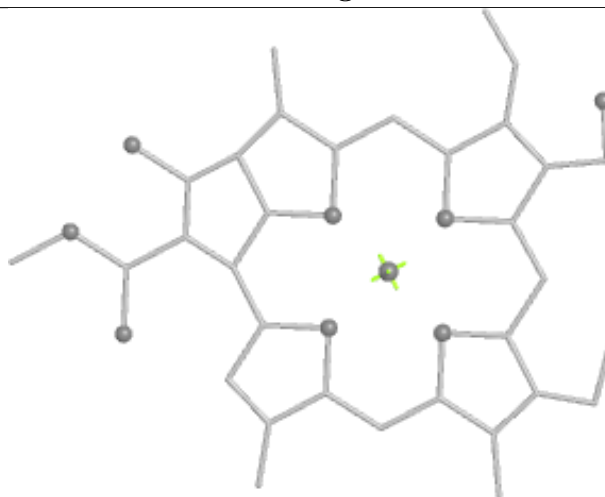
Bond lengths



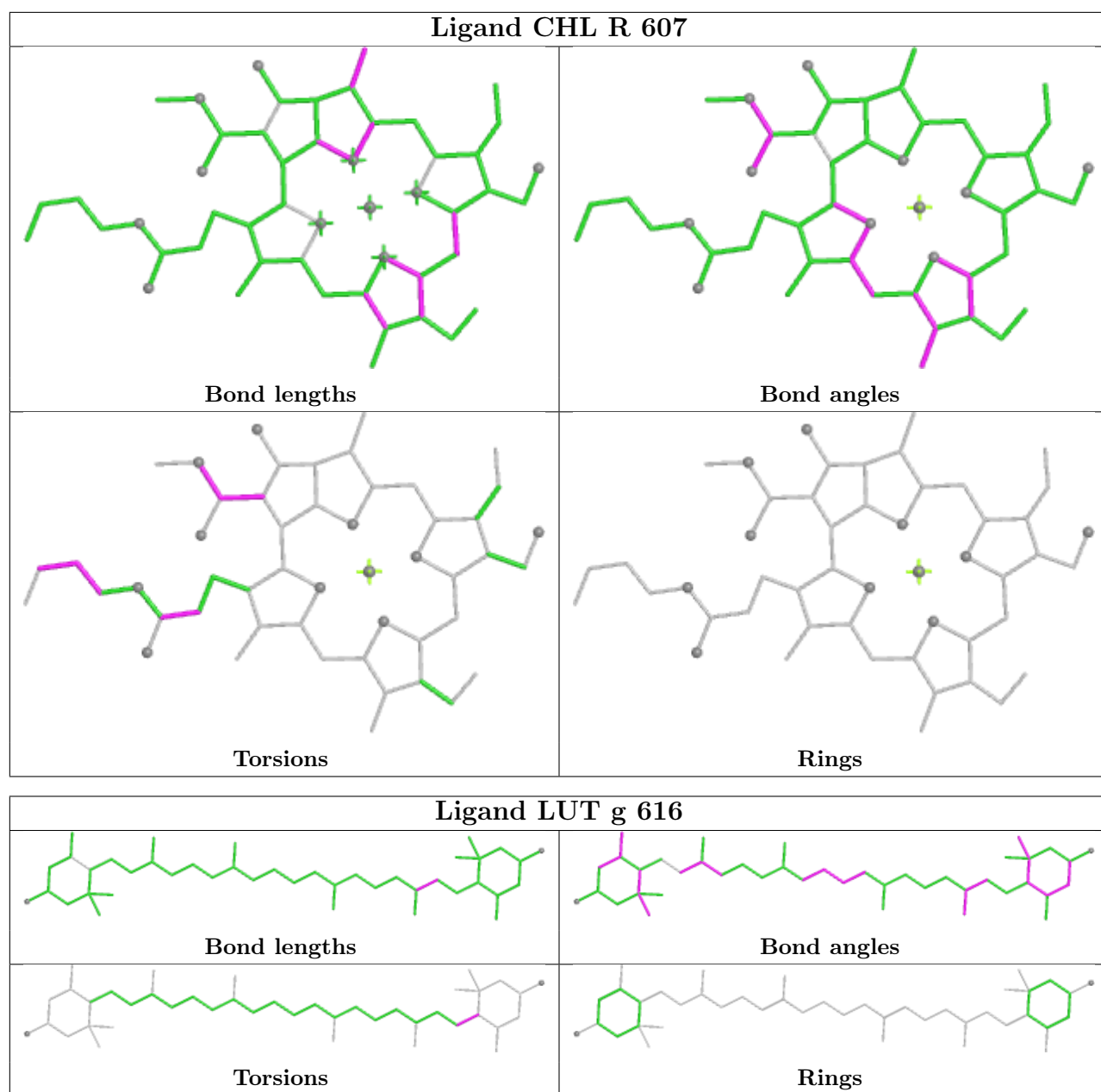
Bond angles

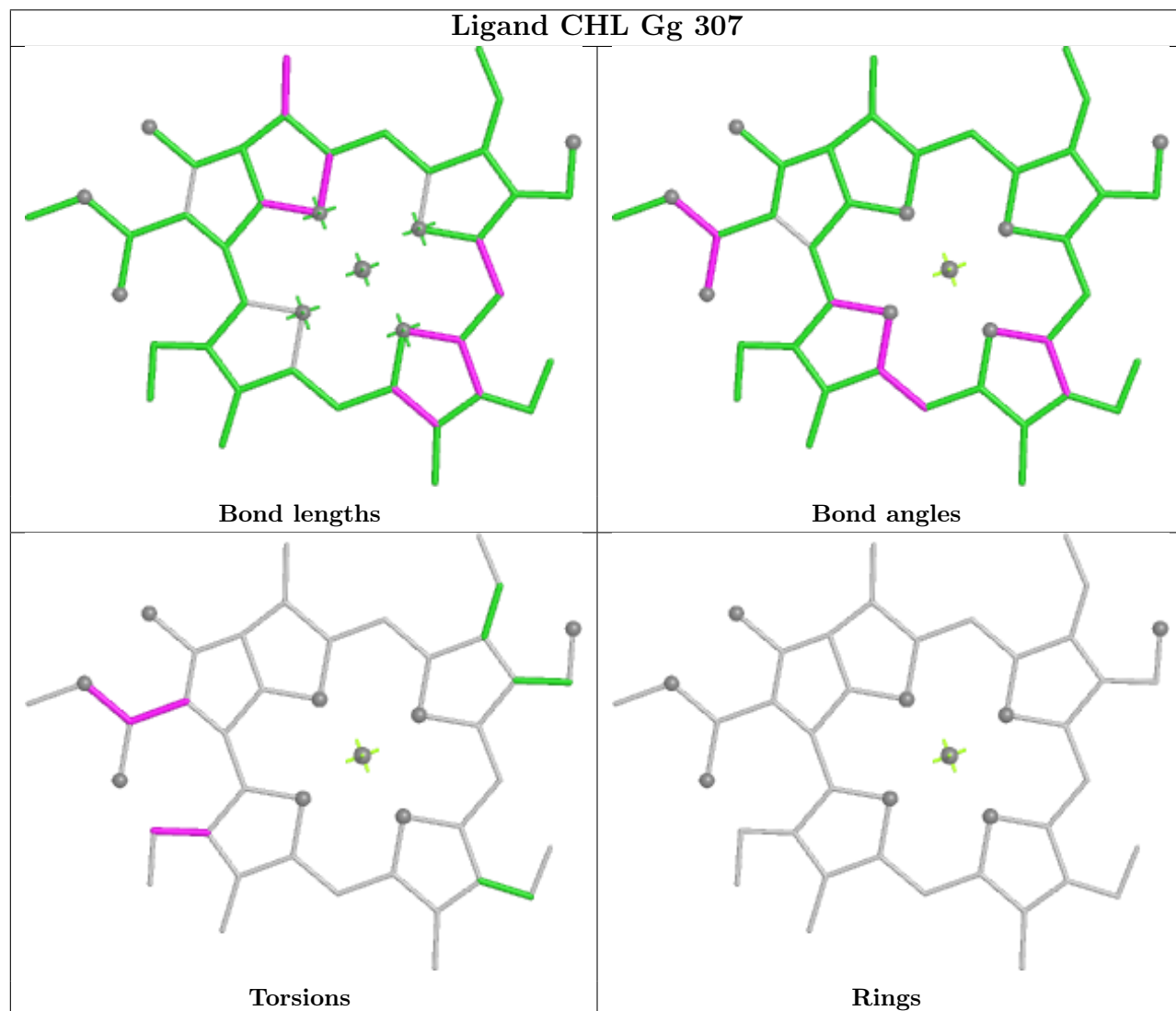
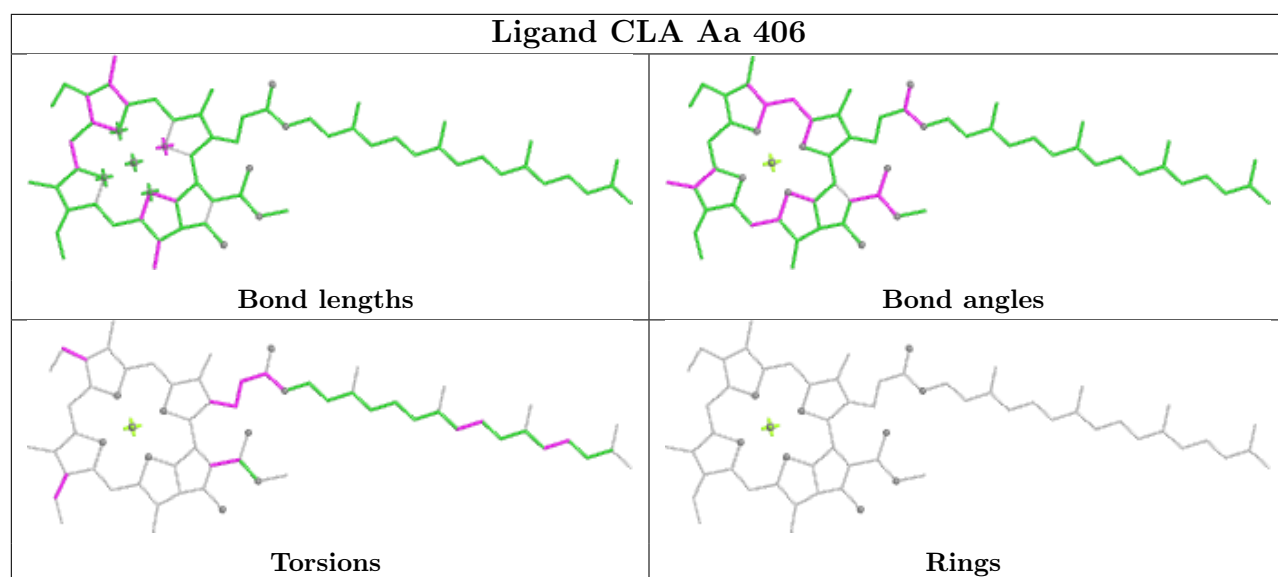


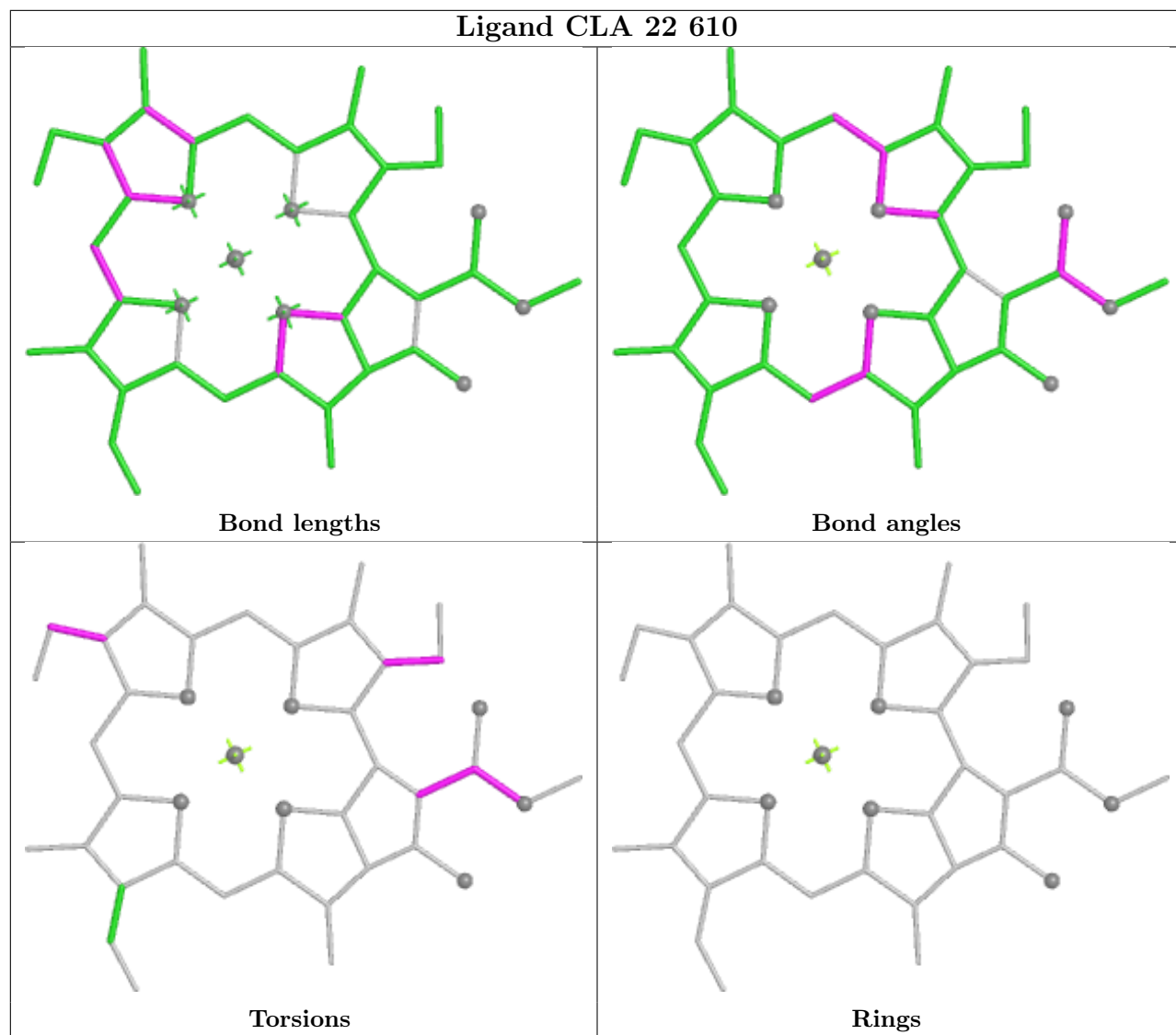
Torsions

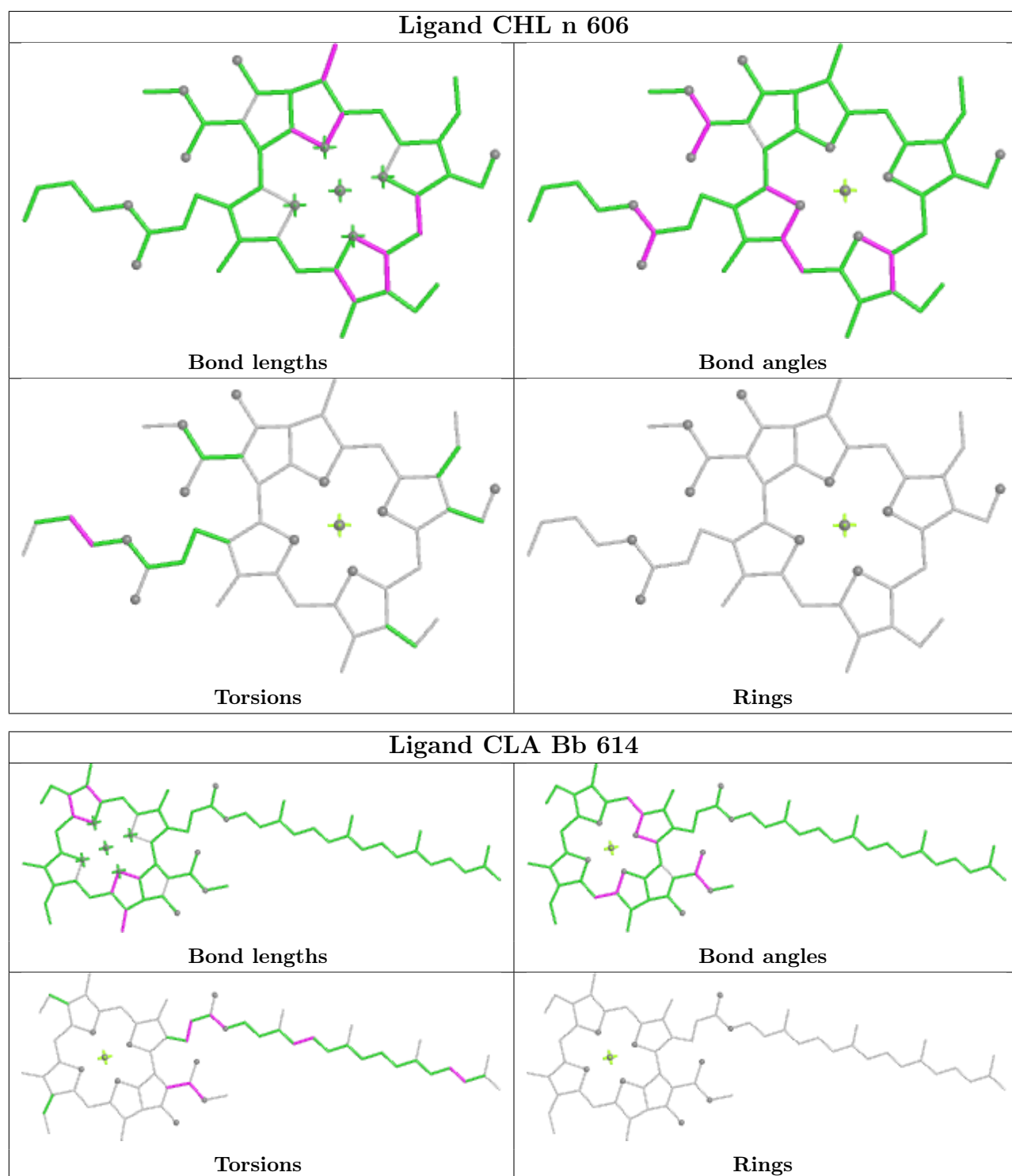


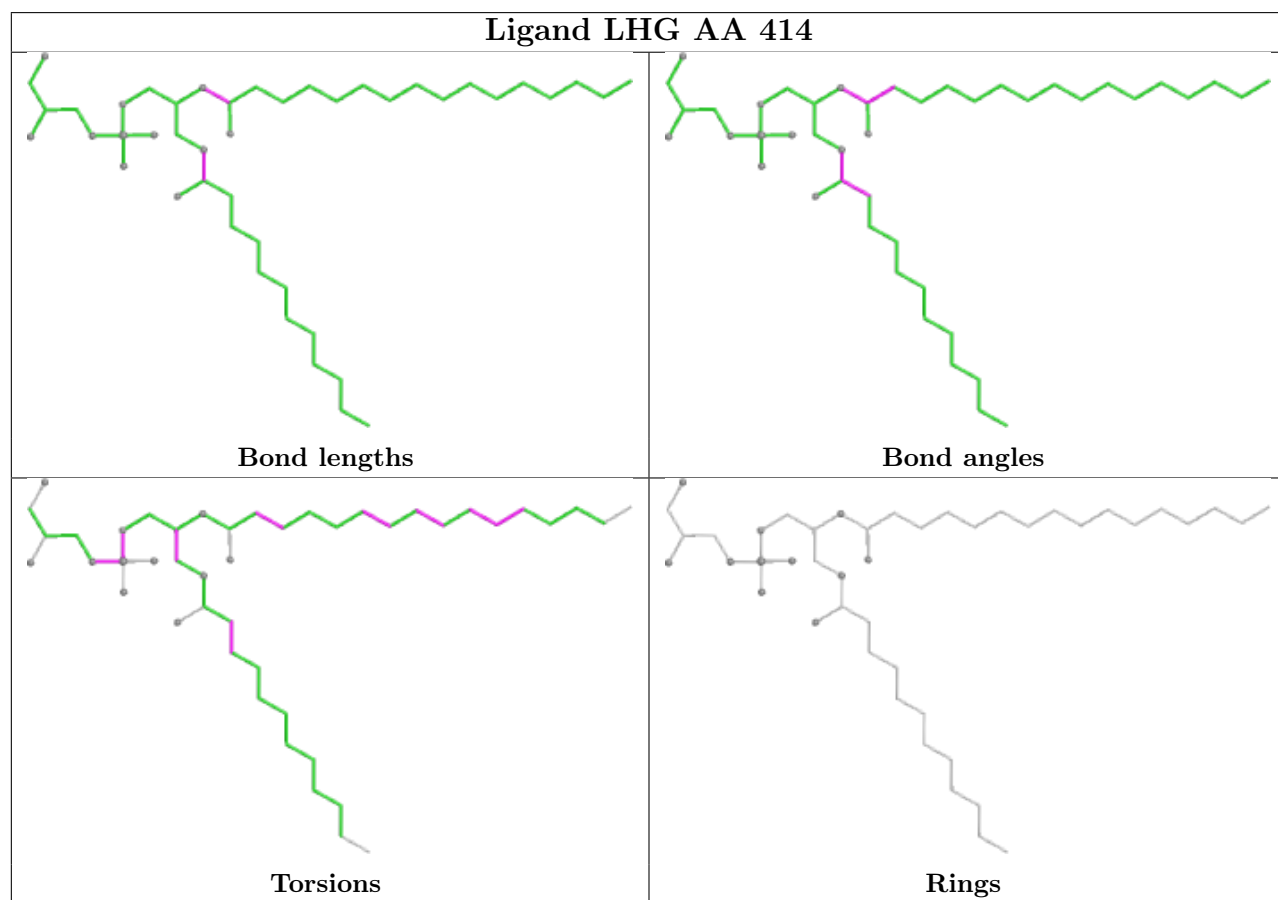
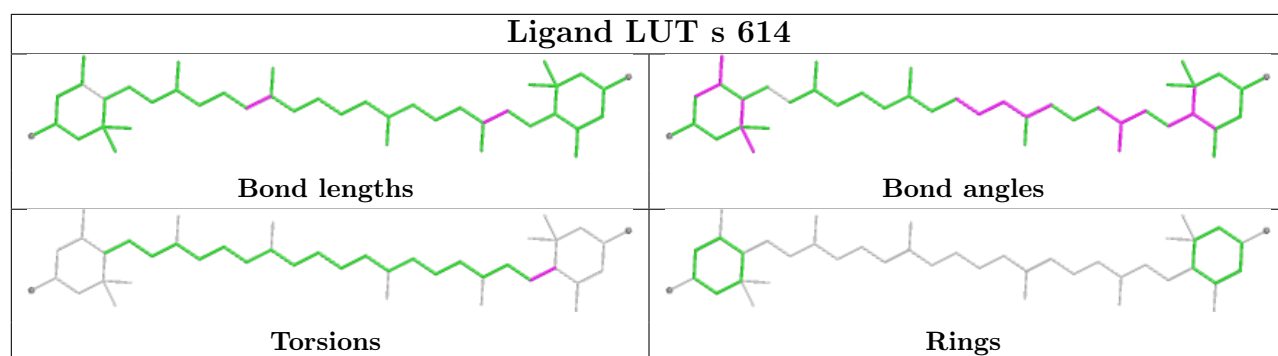
Rings

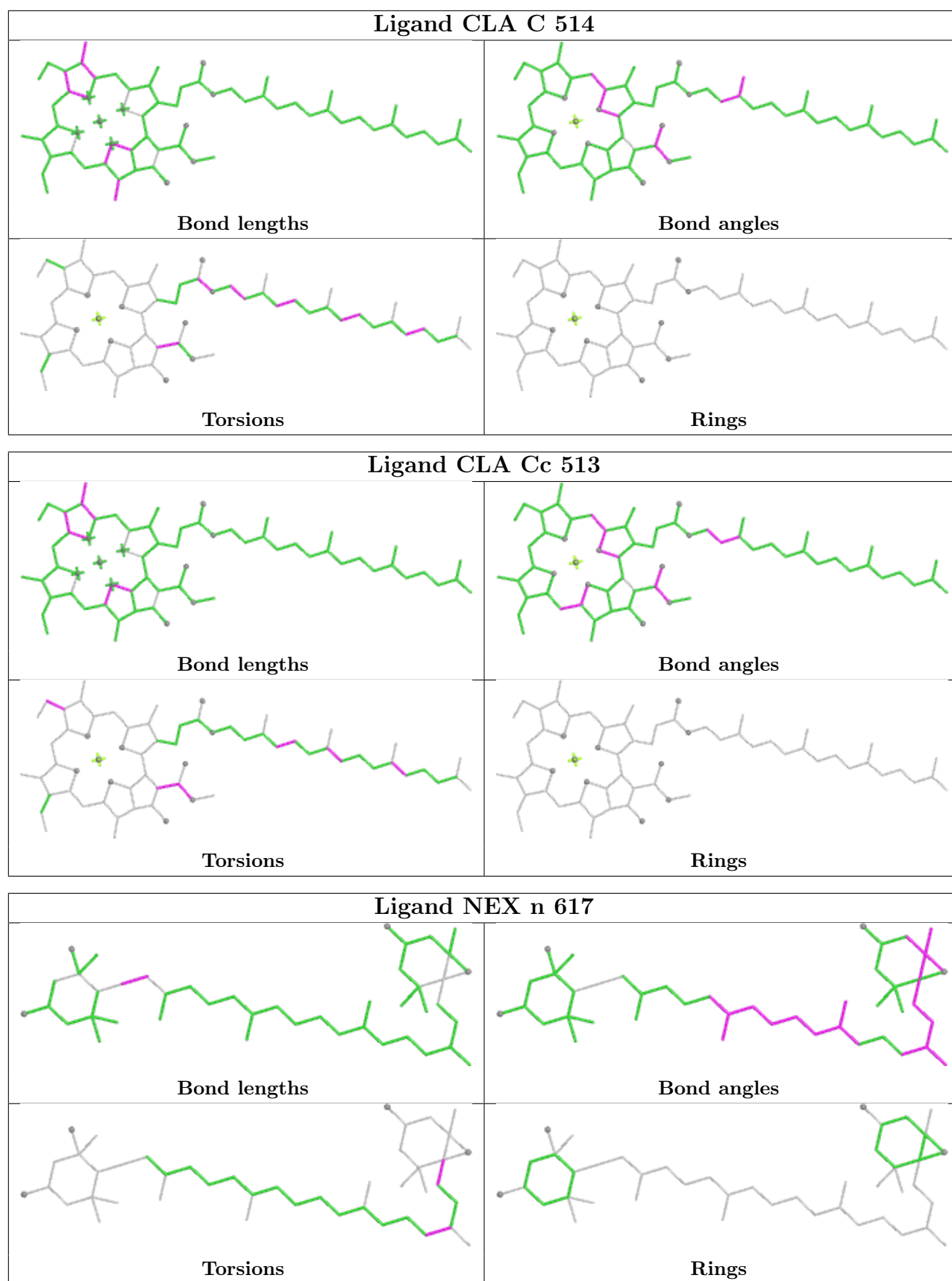




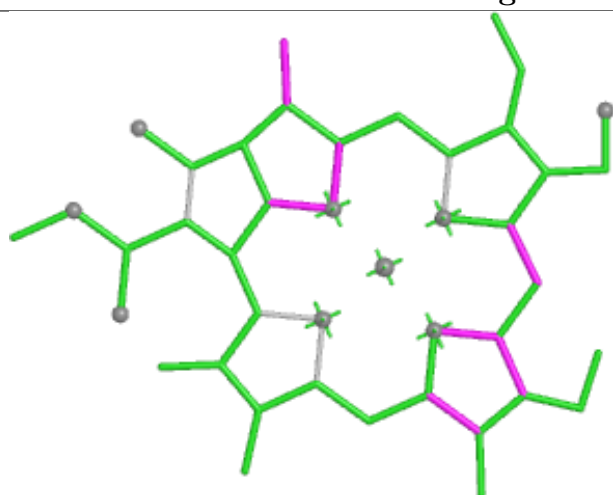




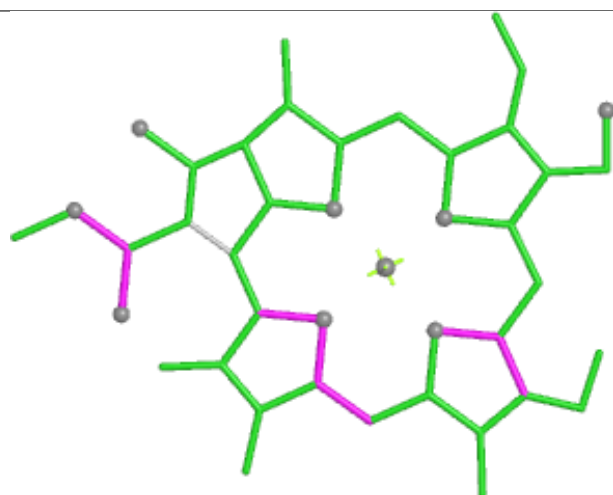




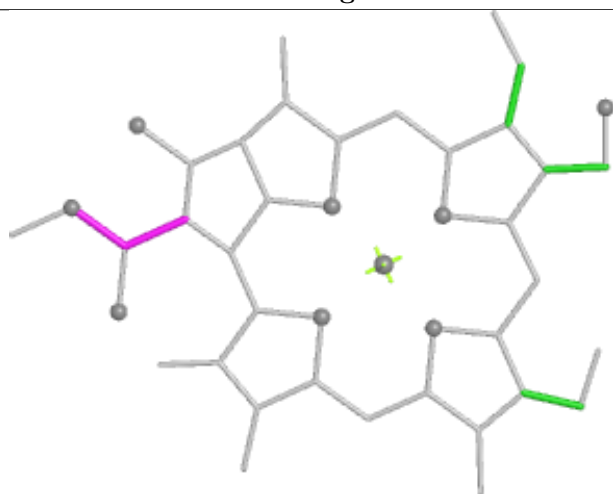
Ligand CHL NN 606



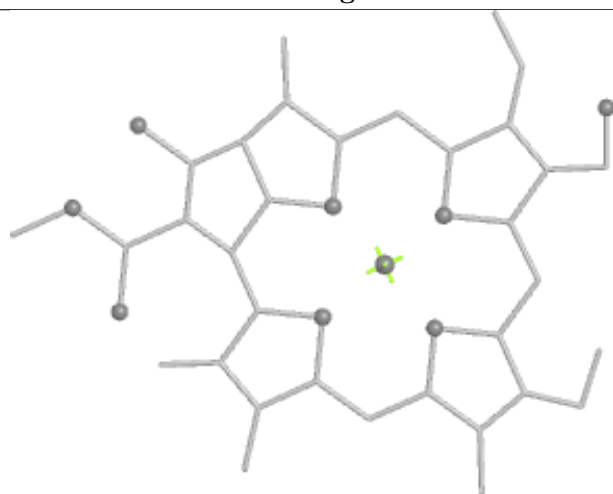
Bond lengths



Bond angles

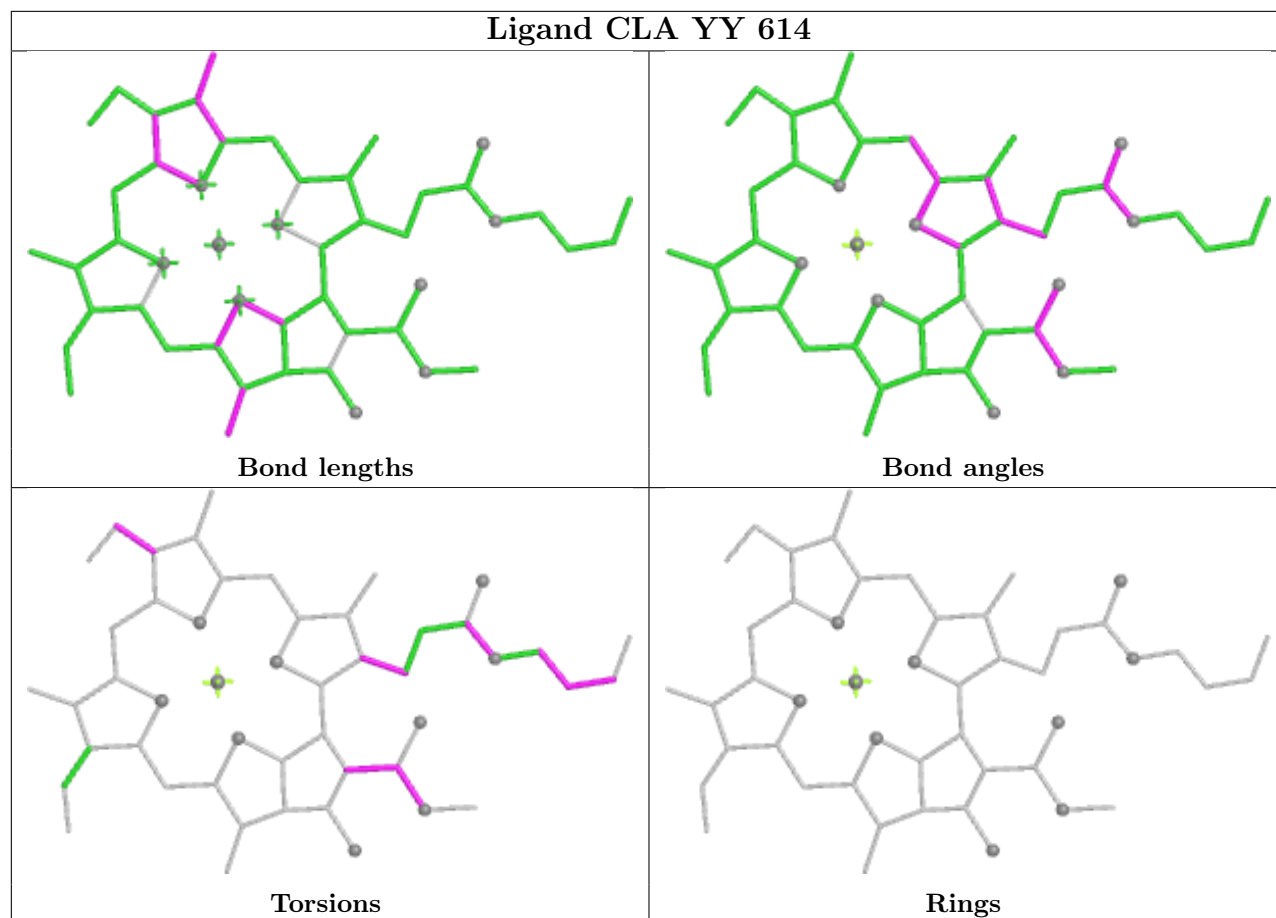


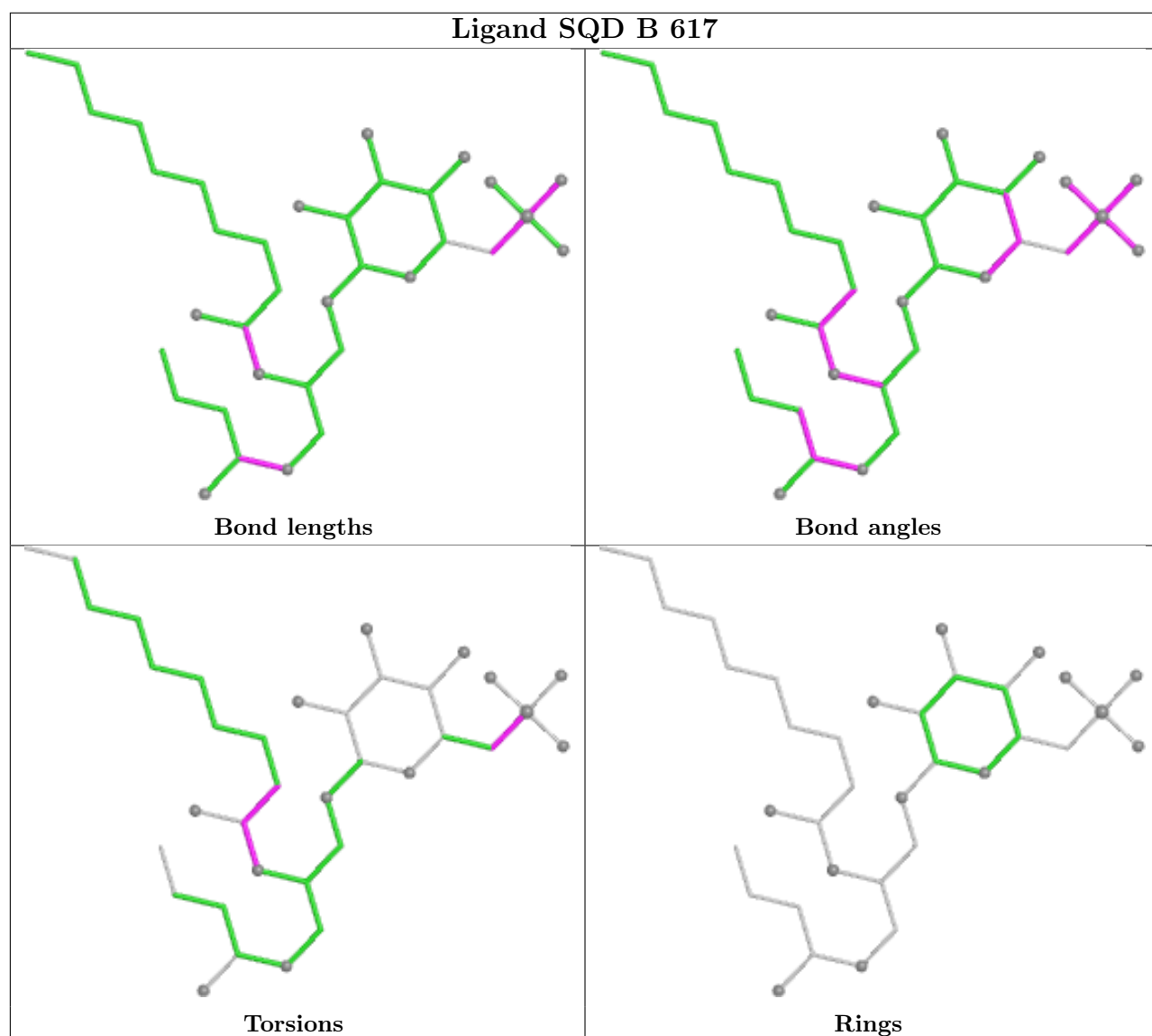
Torsions



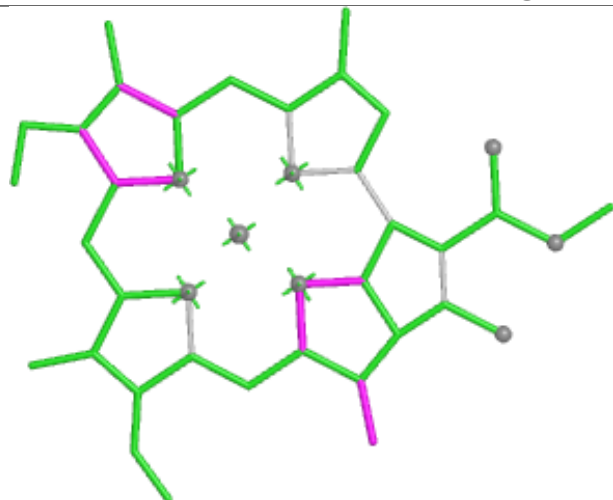
Rings

Ligand CLA YY 614

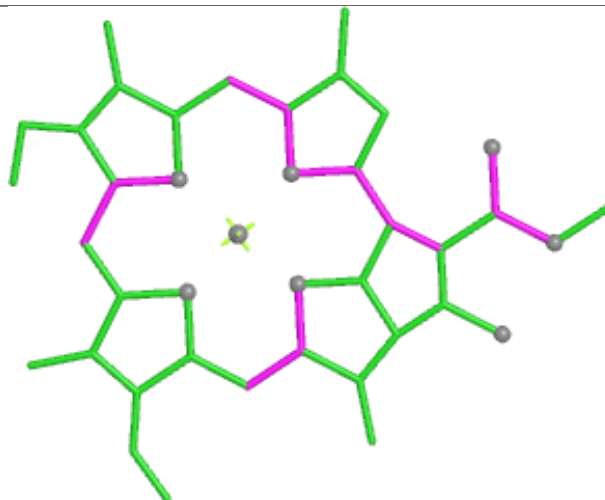




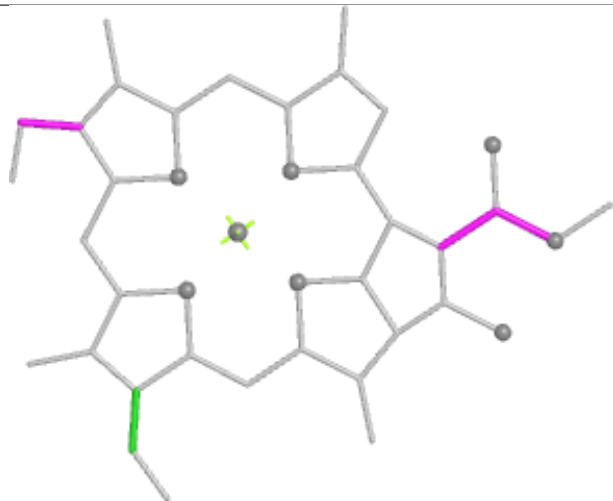
Ligand CLA 3 613



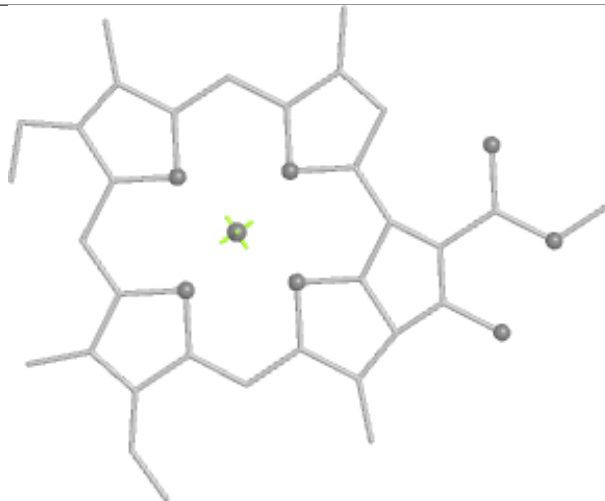
Bond lengths



Bond angles

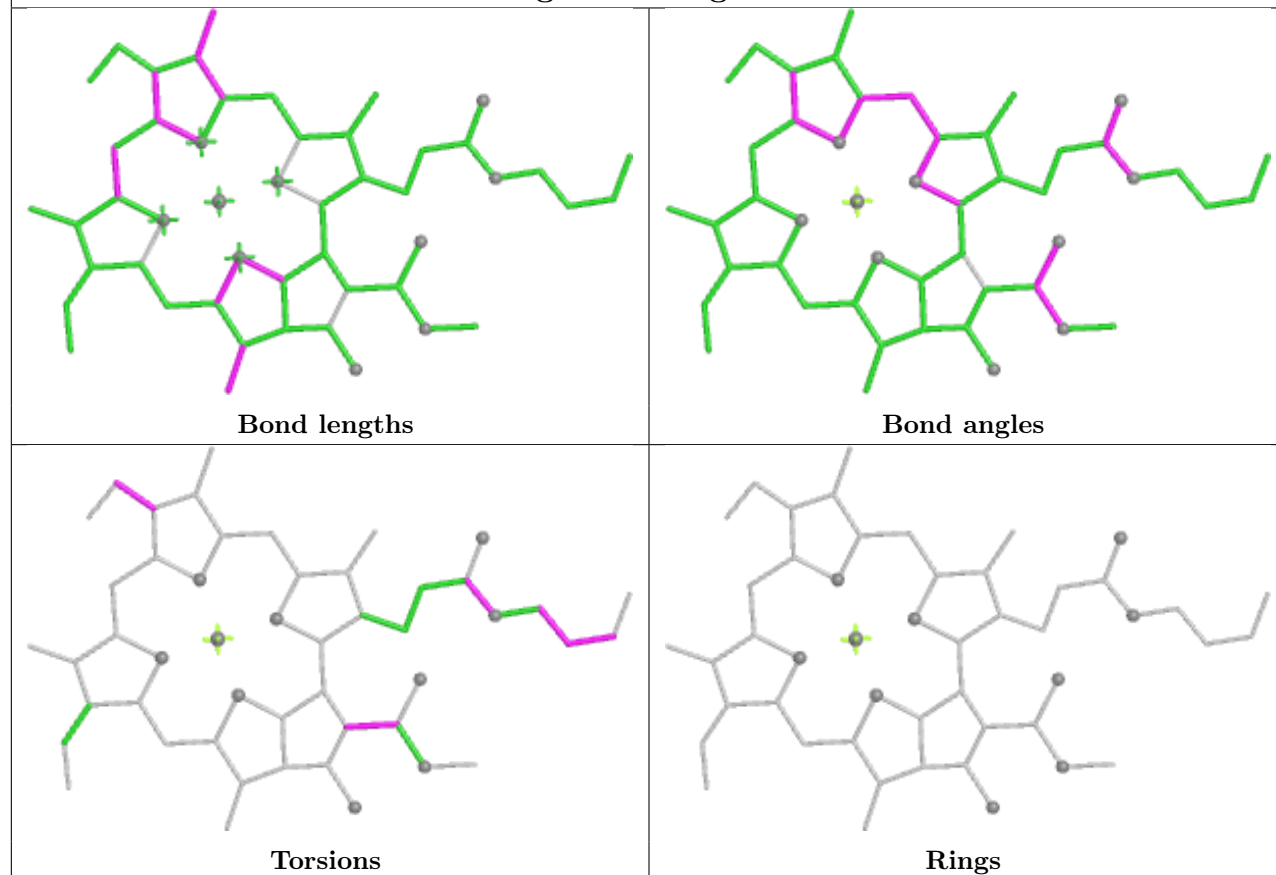


Torsions

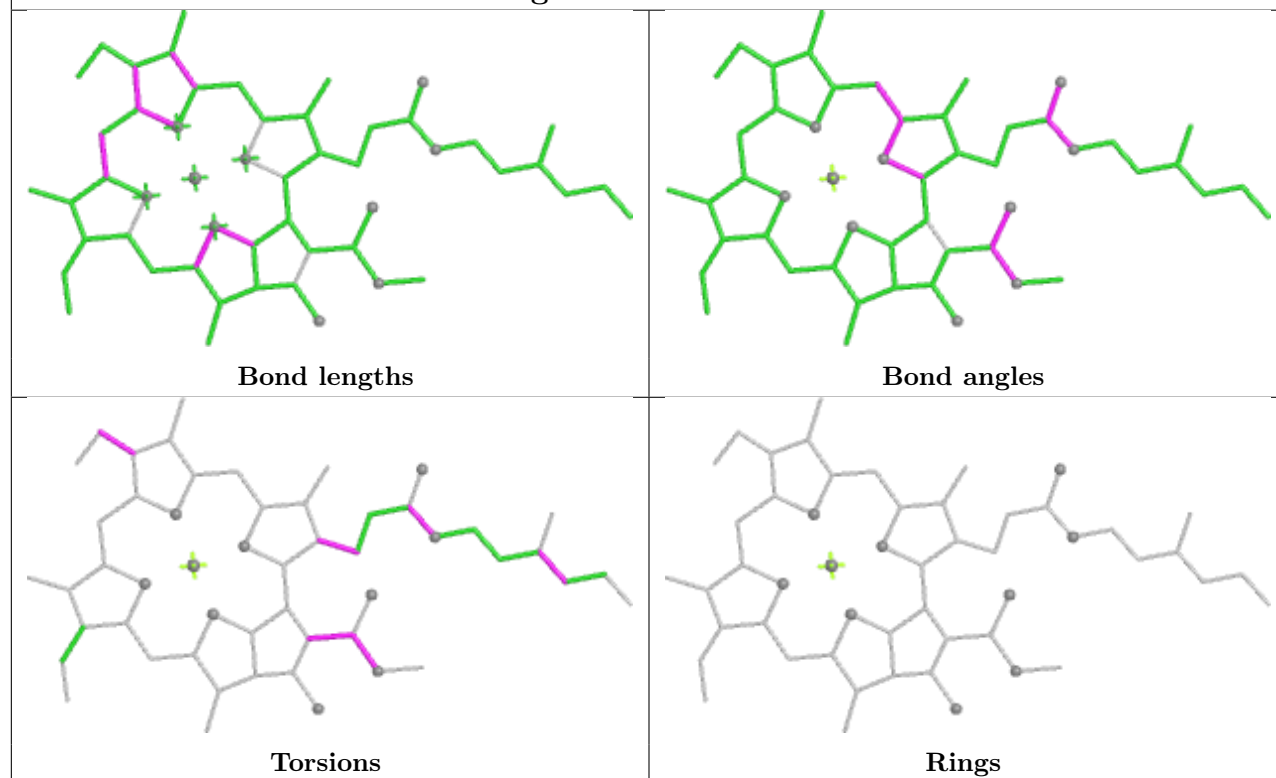


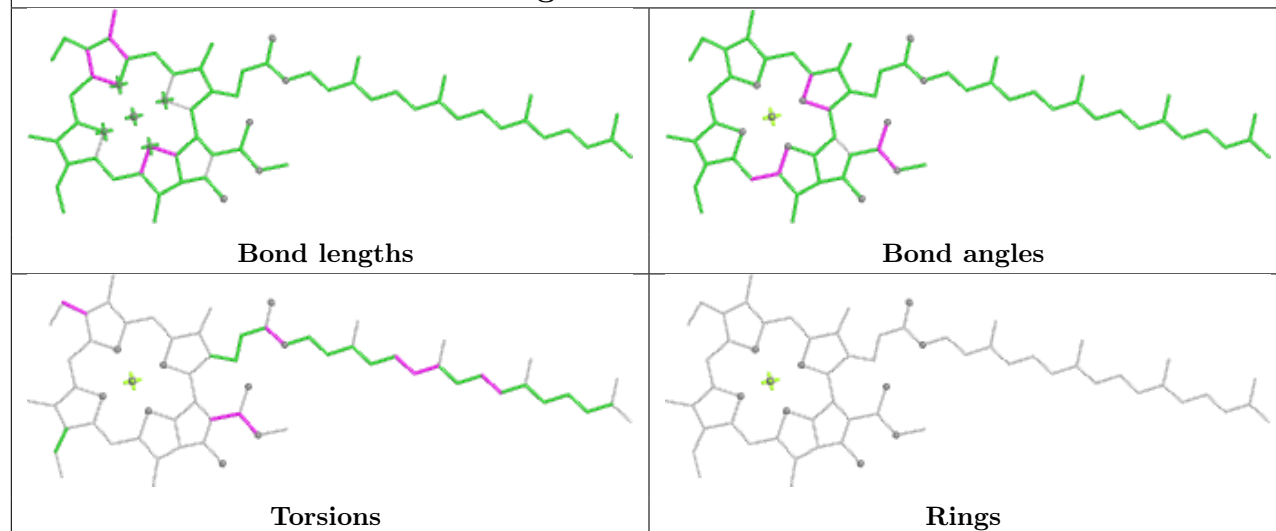
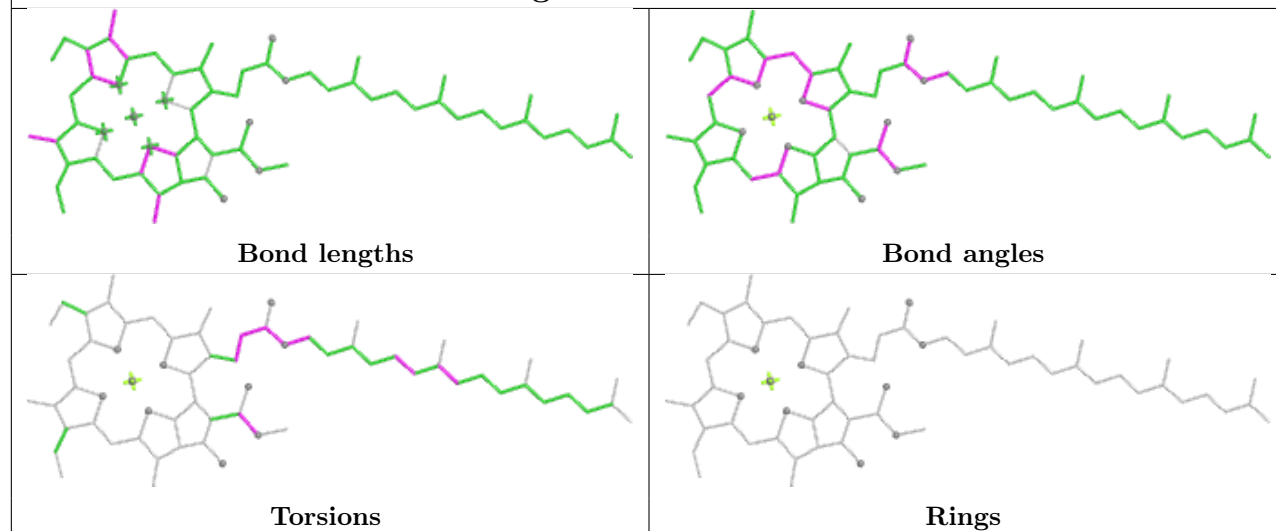
Rings

Ligand CLA g 610

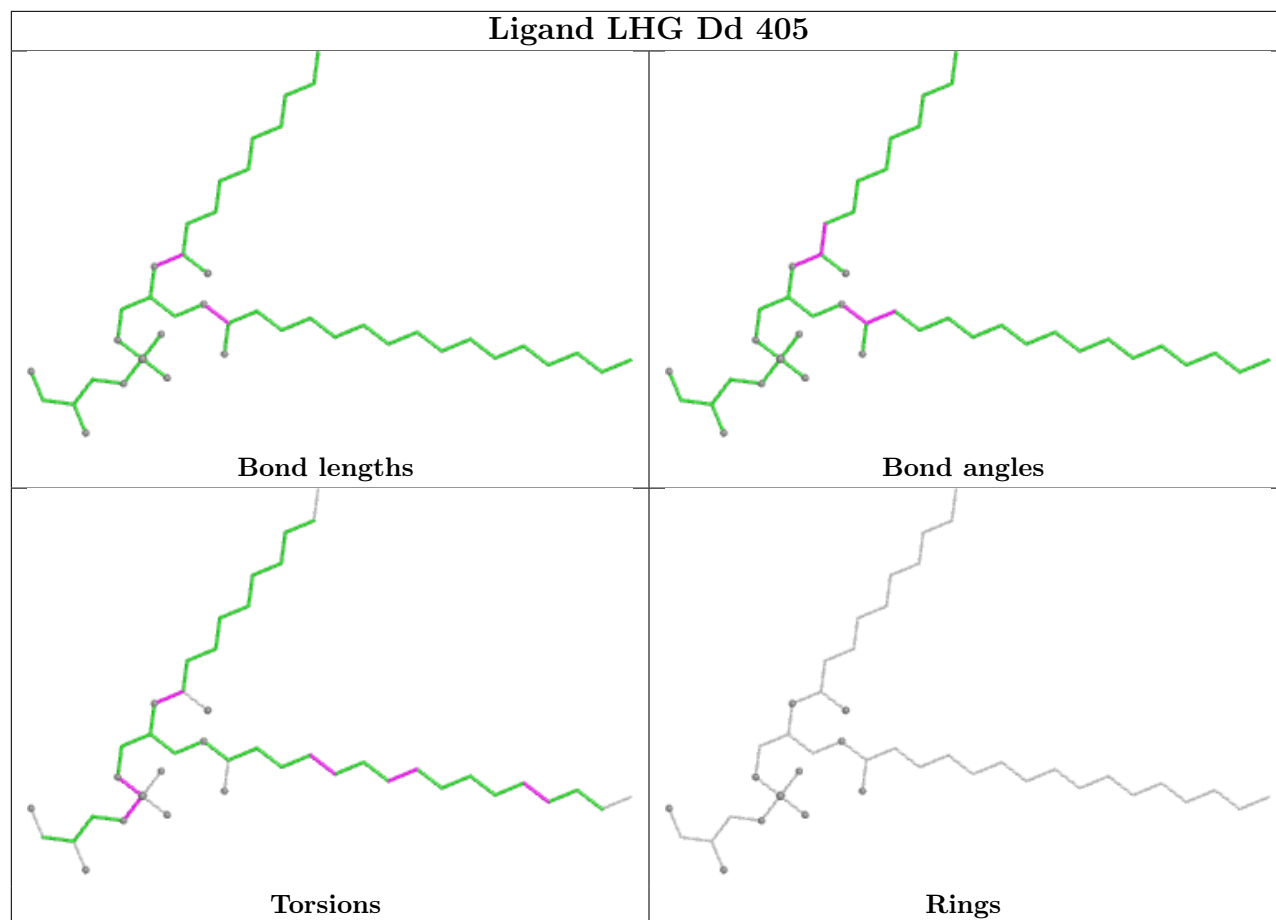


Ligand CLA G 611

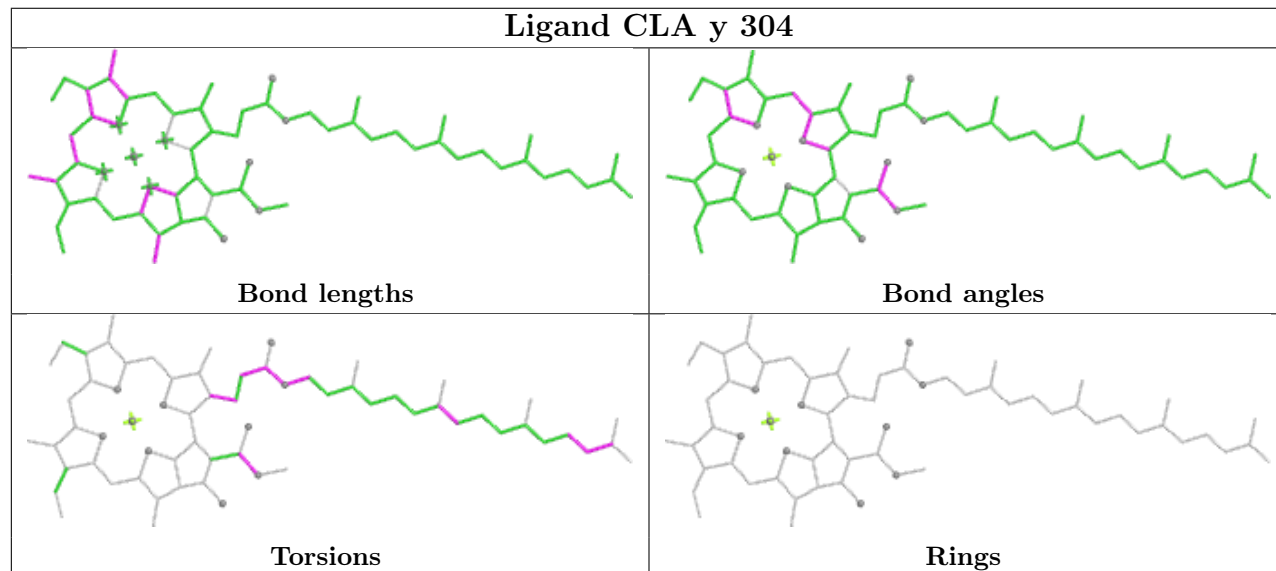


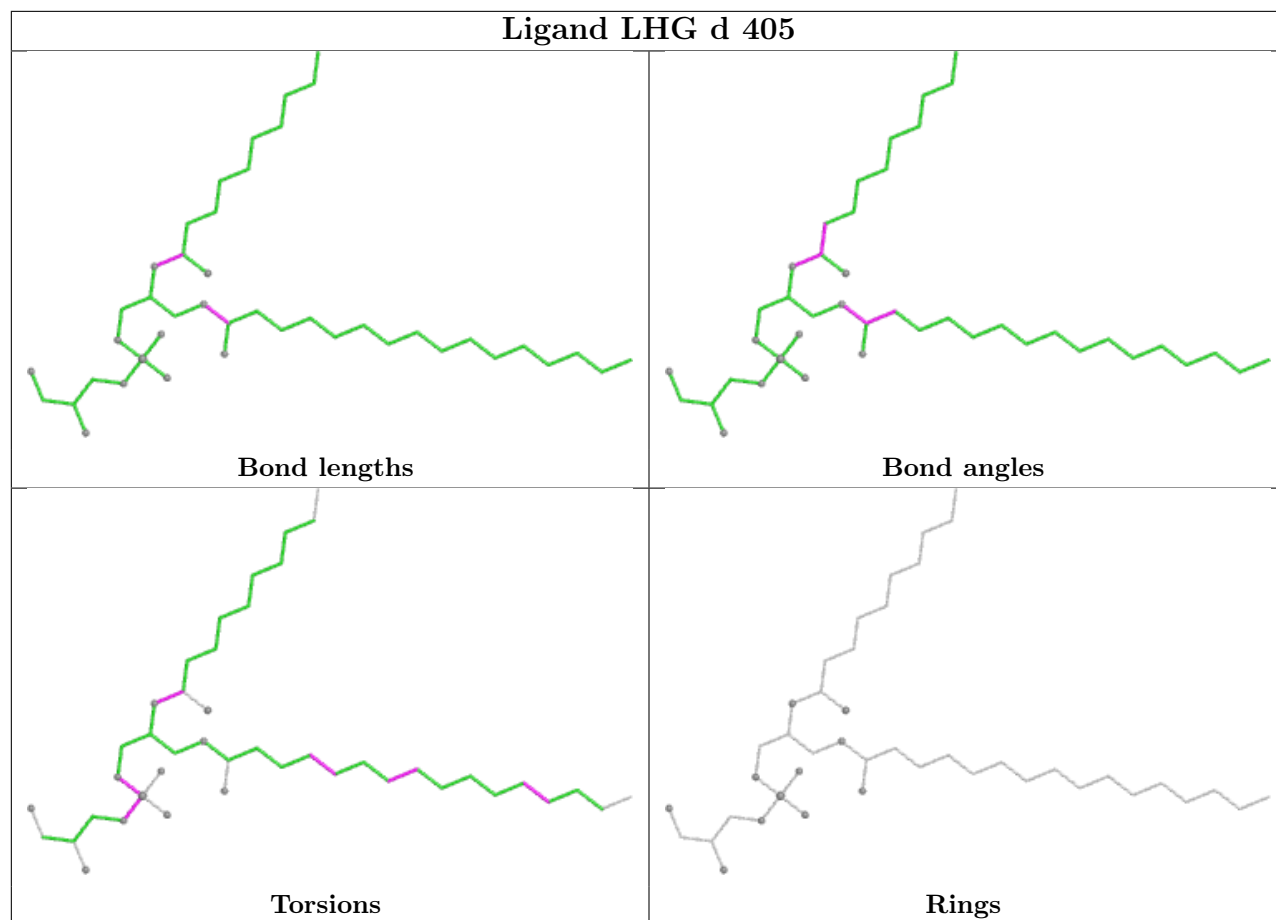
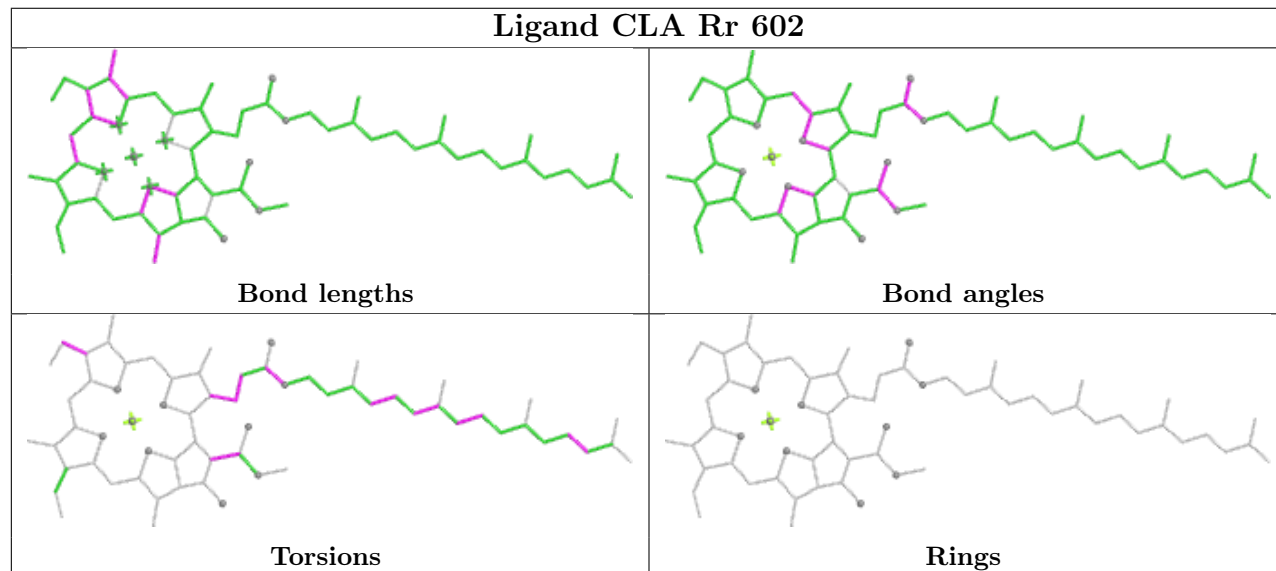
Ligand CLA c 511**Ligand CLA B 624**

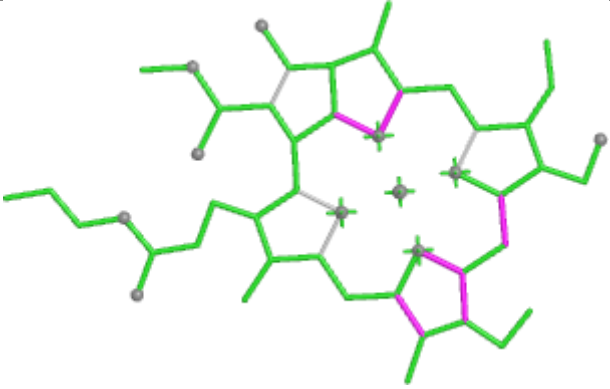
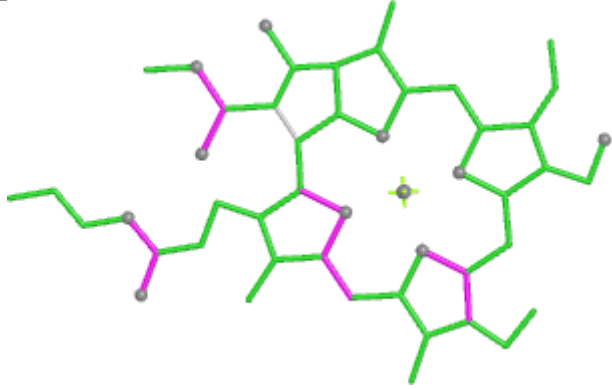
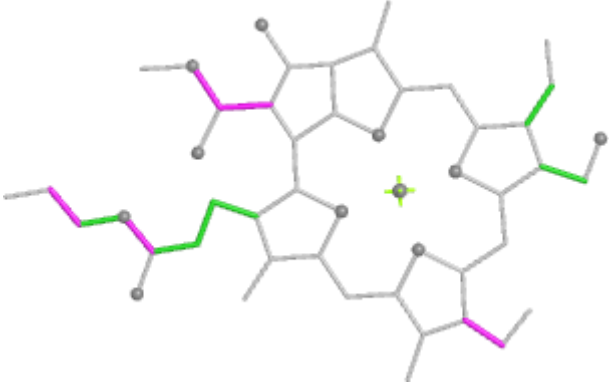
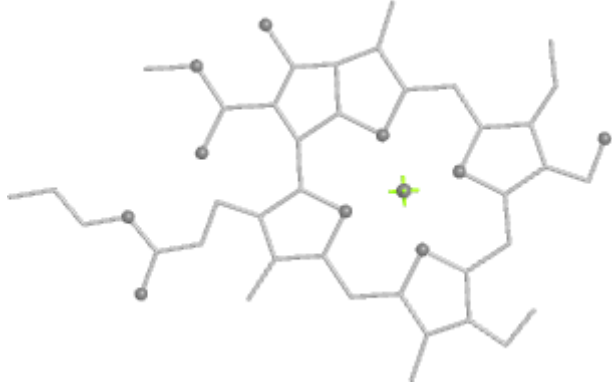
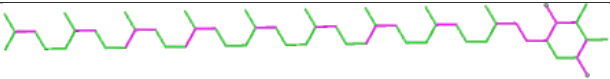
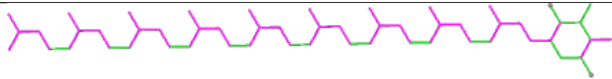
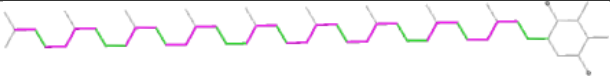
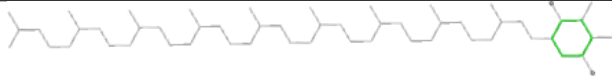
Ligand LHG Dd 405

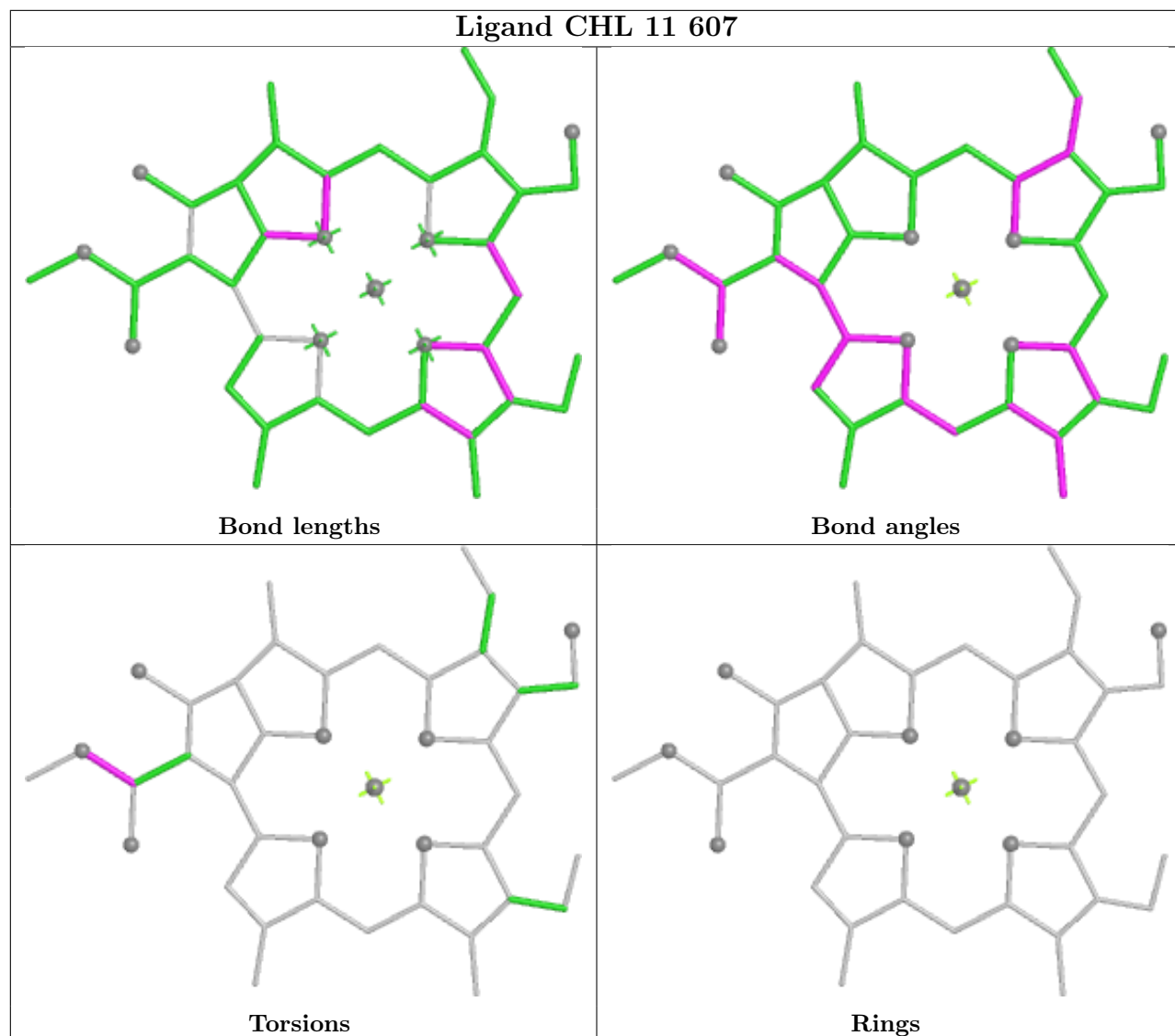


Ligand CLA y 304

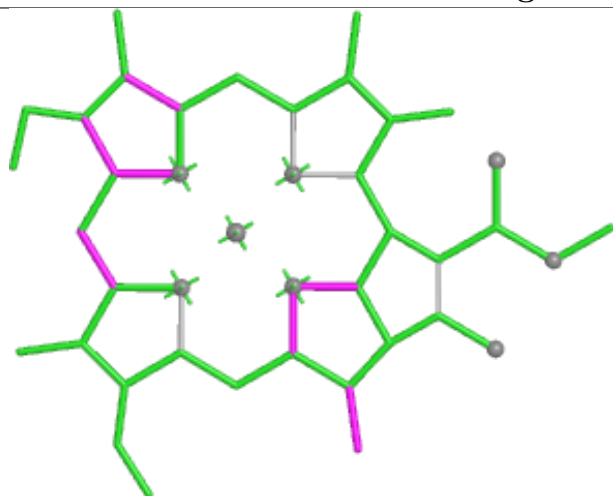


Ligand LHG d 405**Ligand CLA Rr 602**

Ligand CHL Ss 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings



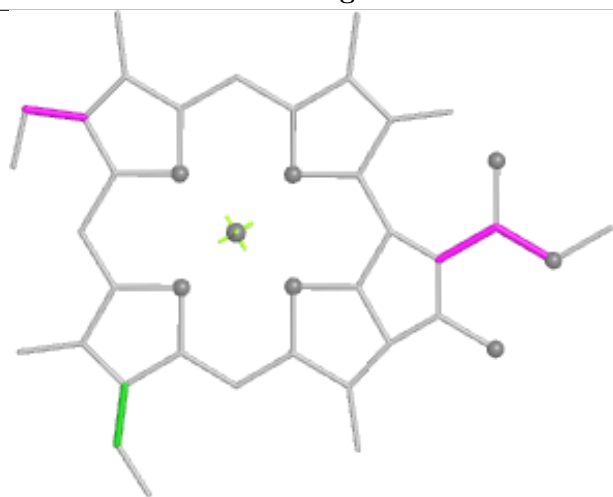
Ligand CLA S 608



Bond lengths



Bond angles

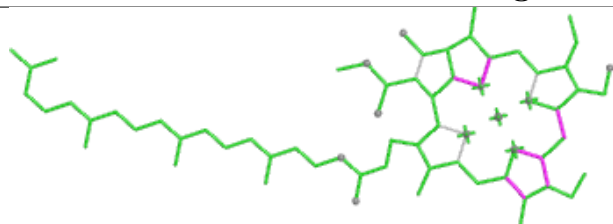


Torsions

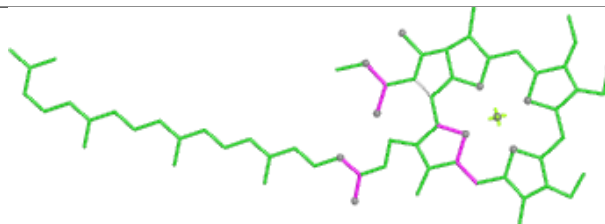


Rings

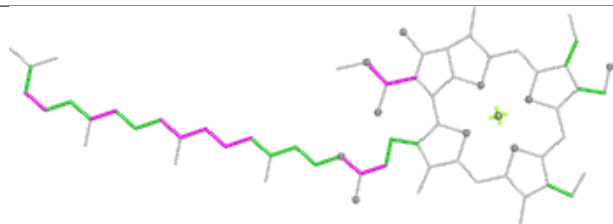
Ligand CHL G 601



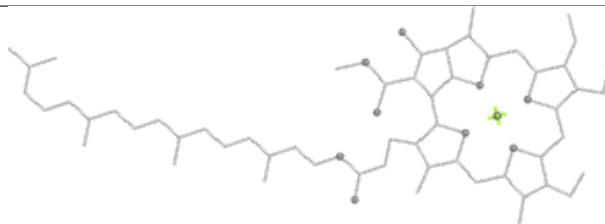
Bond lengths



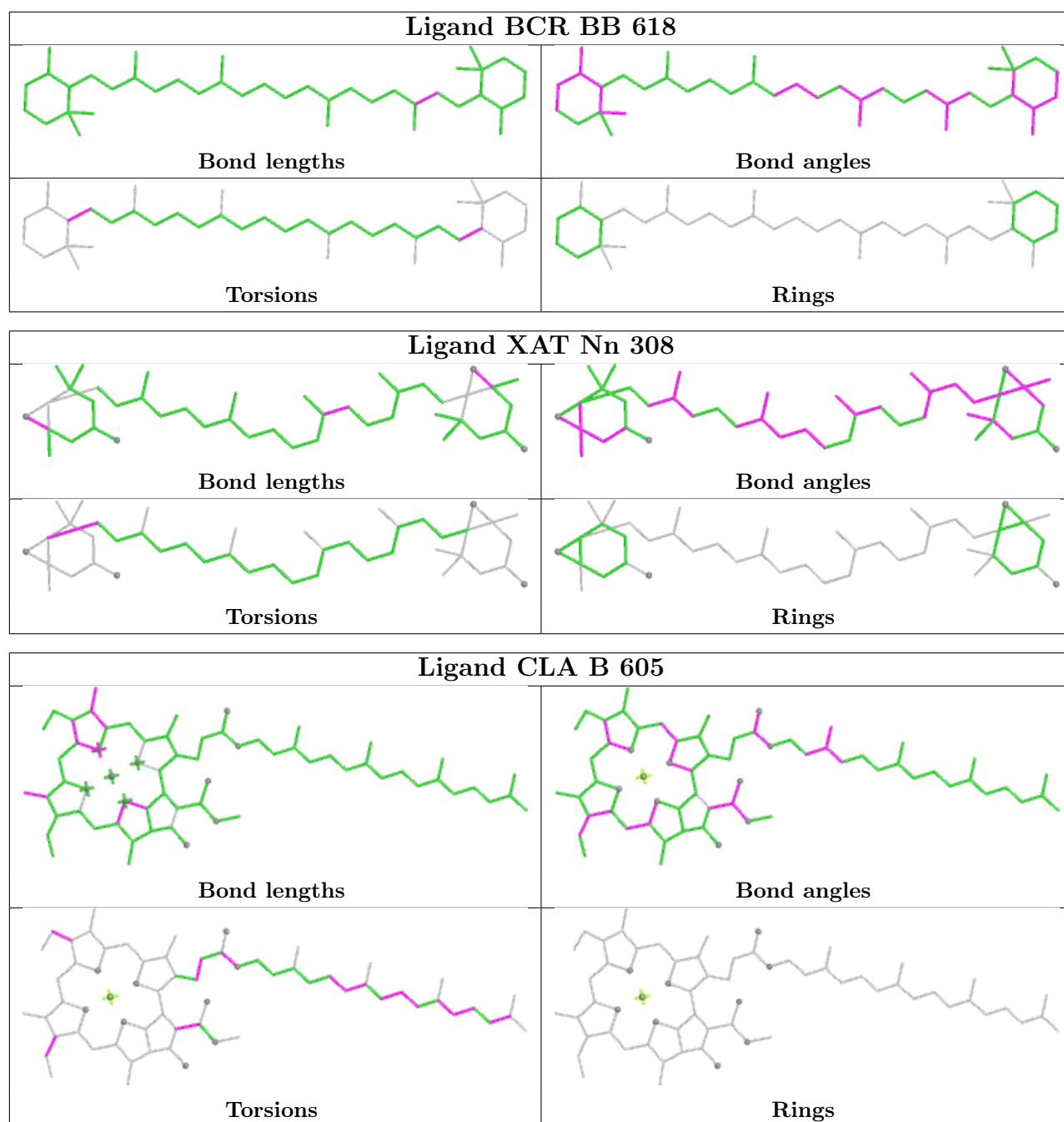
Bond angles

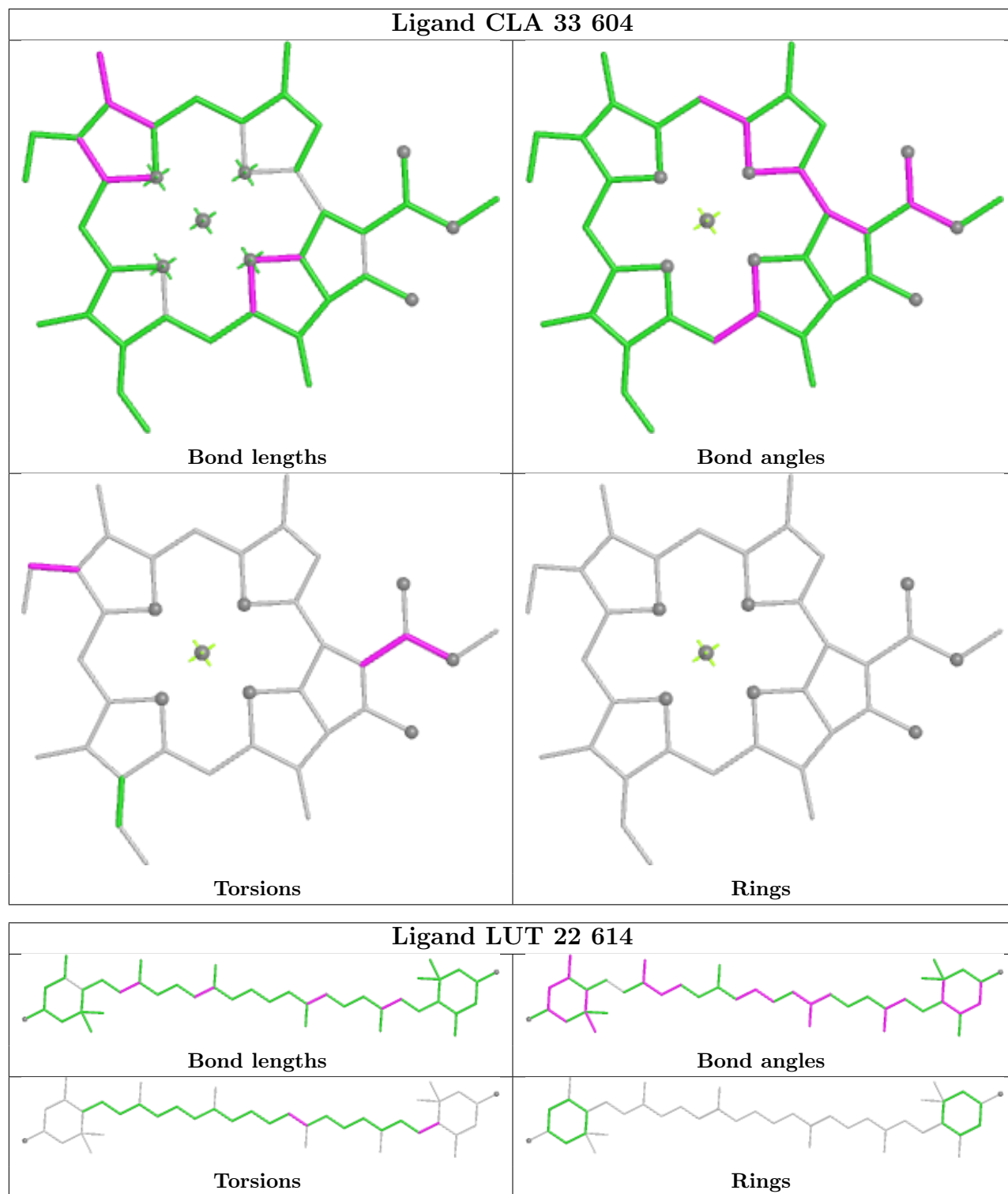


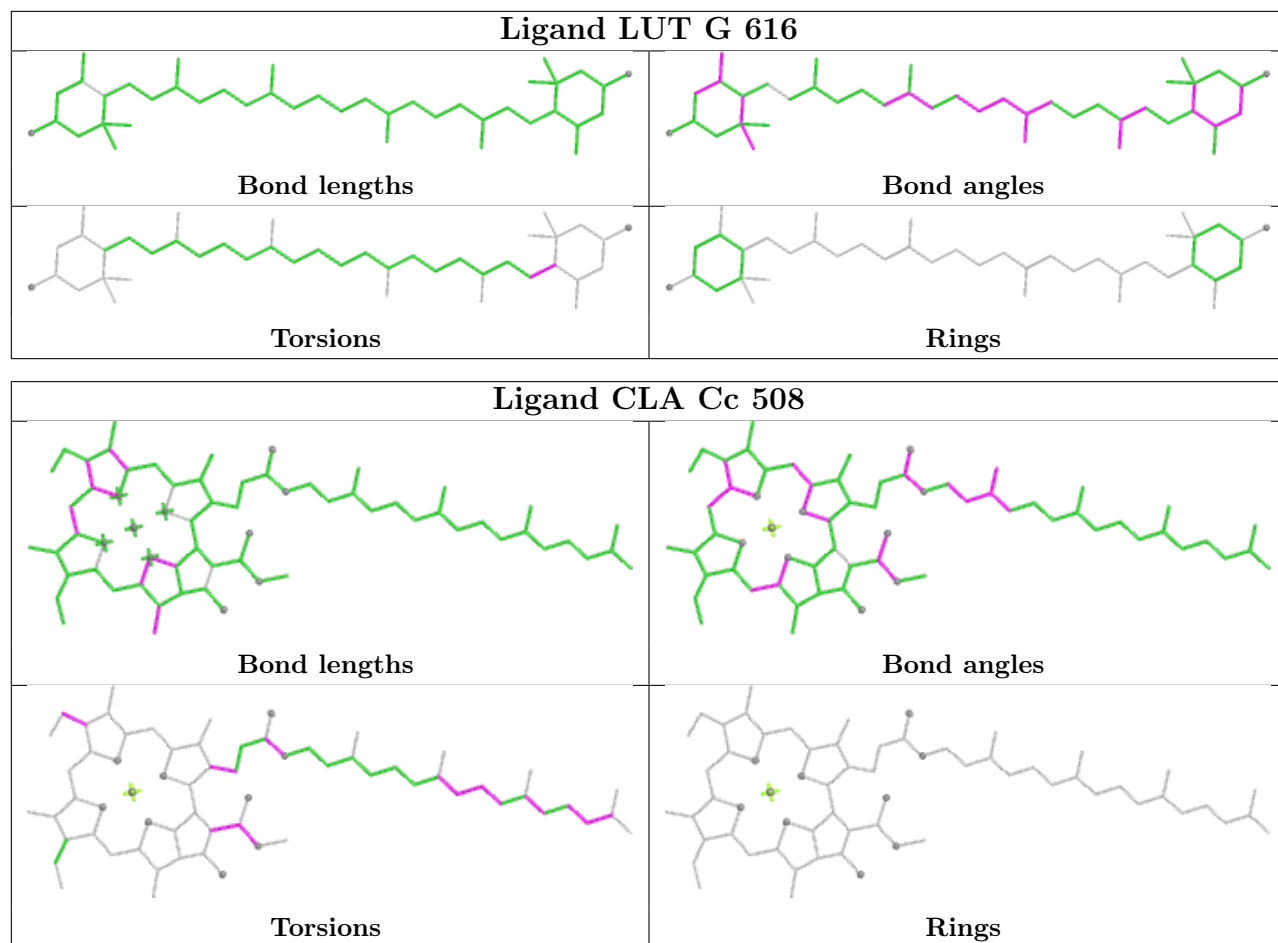
Torsions

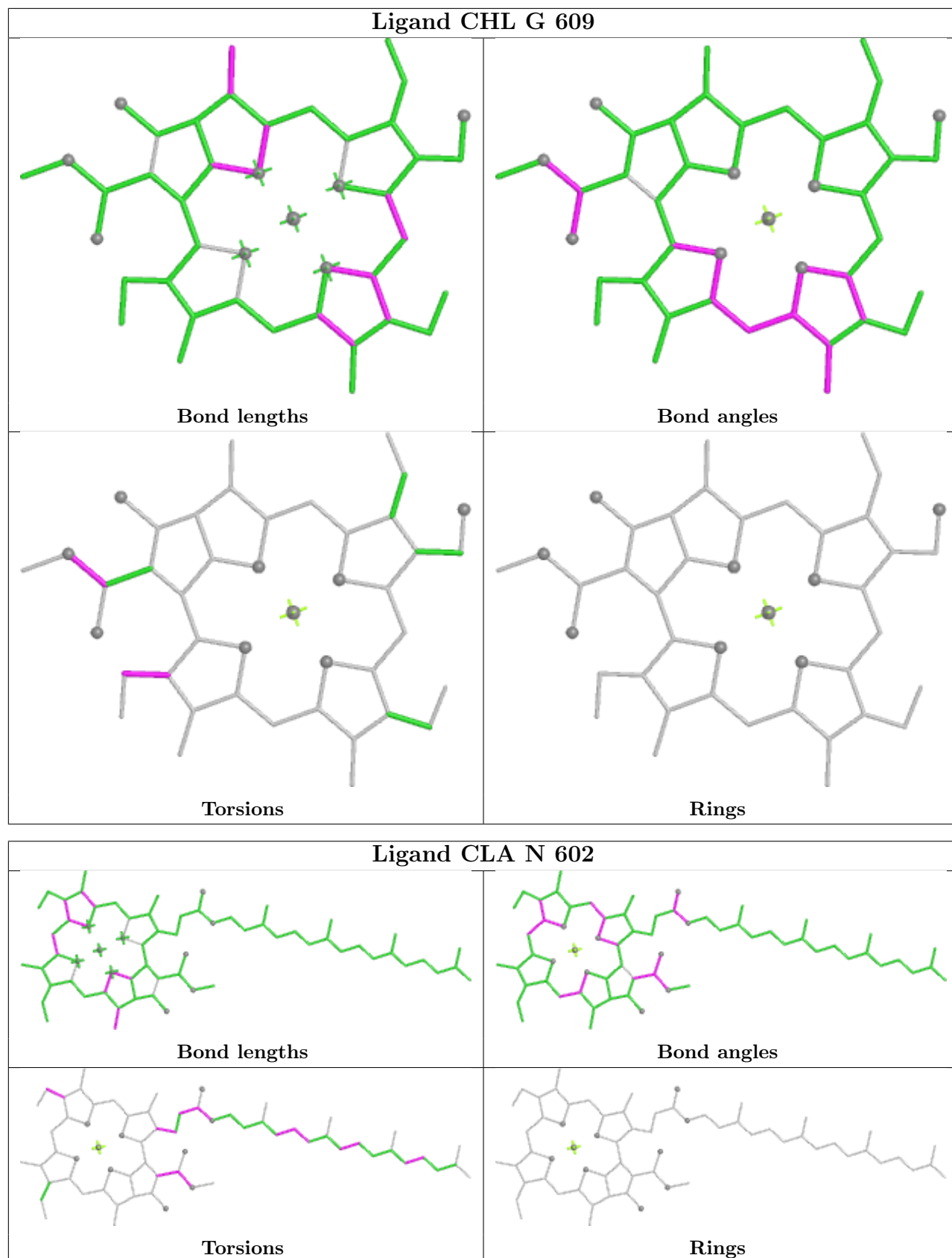


Rings

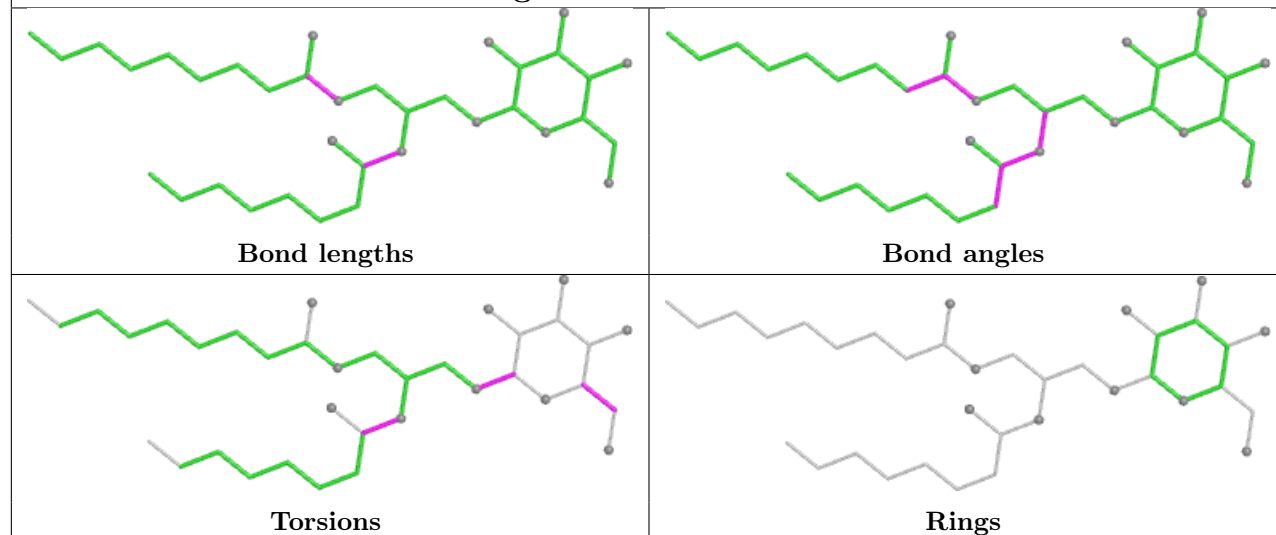




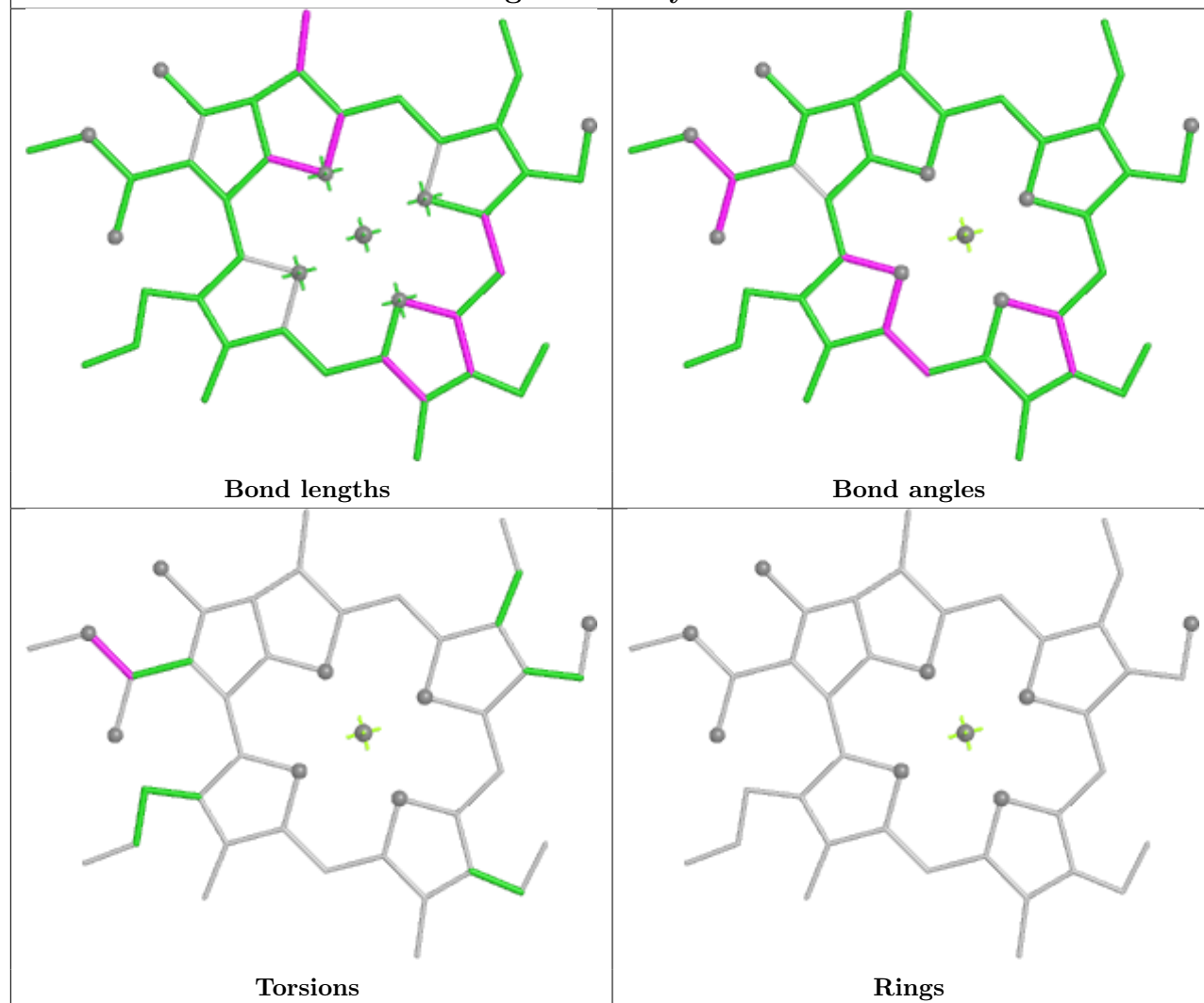


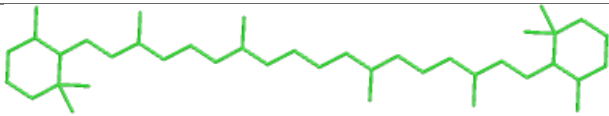
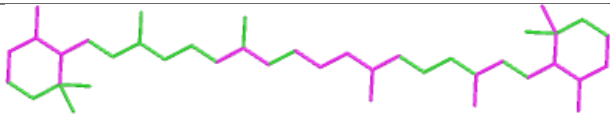
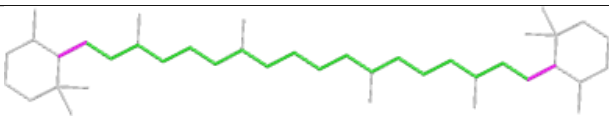
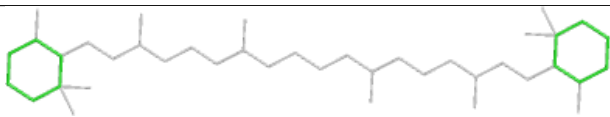


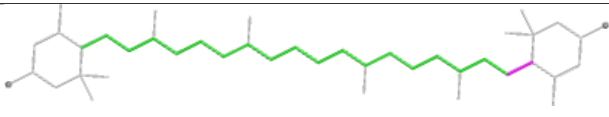
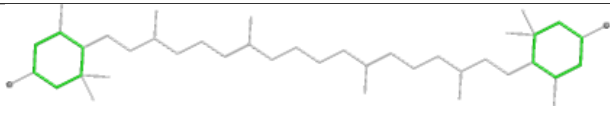
Ligand LMG AA 415



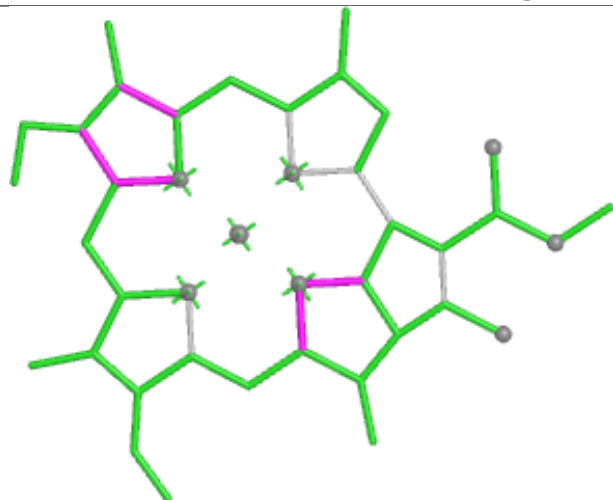
Ligand CHL y 308



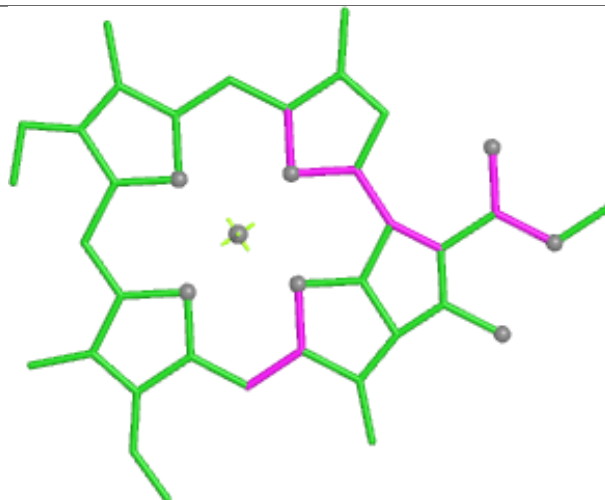
Ligand BCR d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT G 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

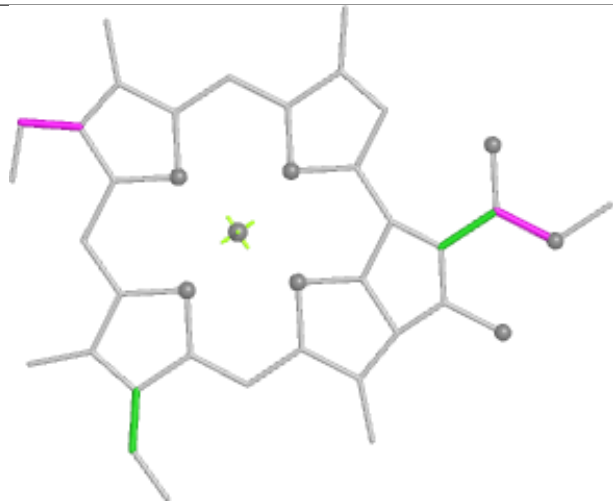
Ligand CLA 2 609



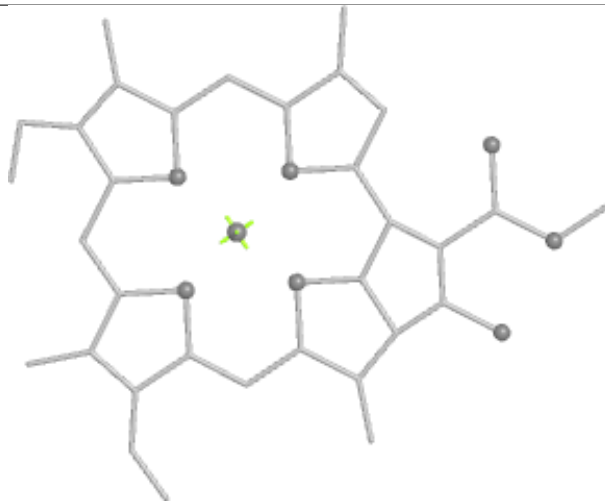
Bond lengths



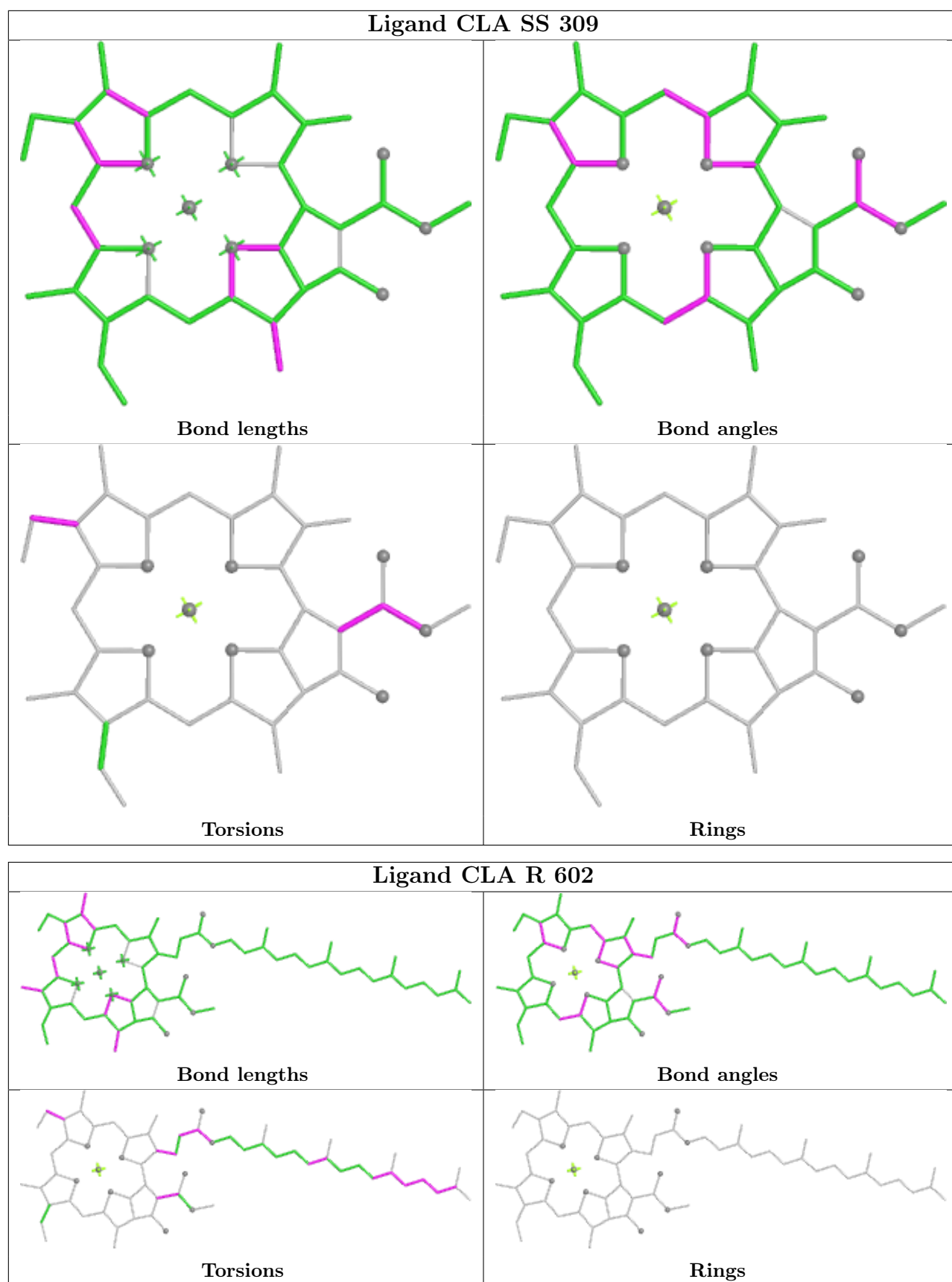
Bond angles

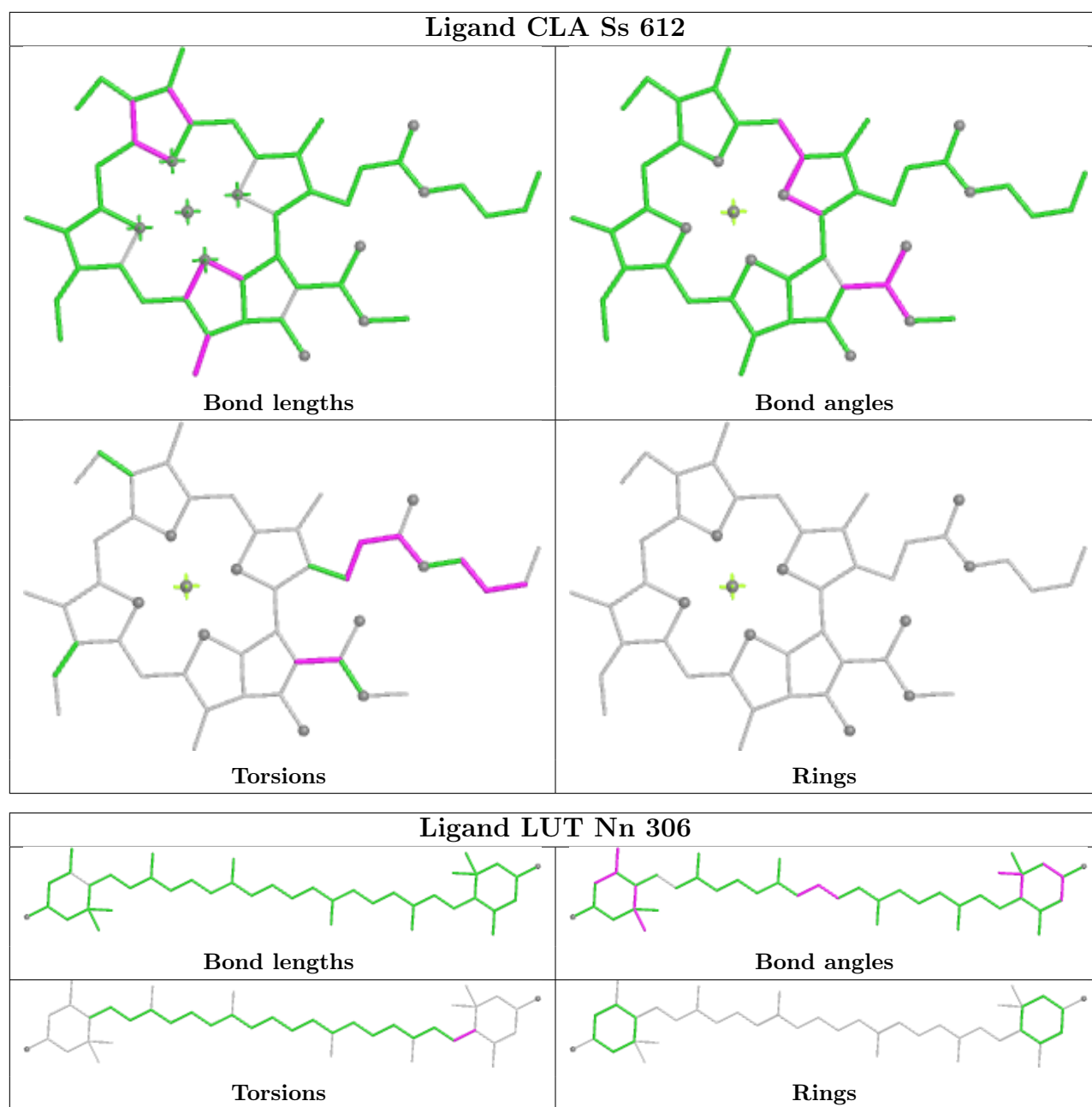


Torsions

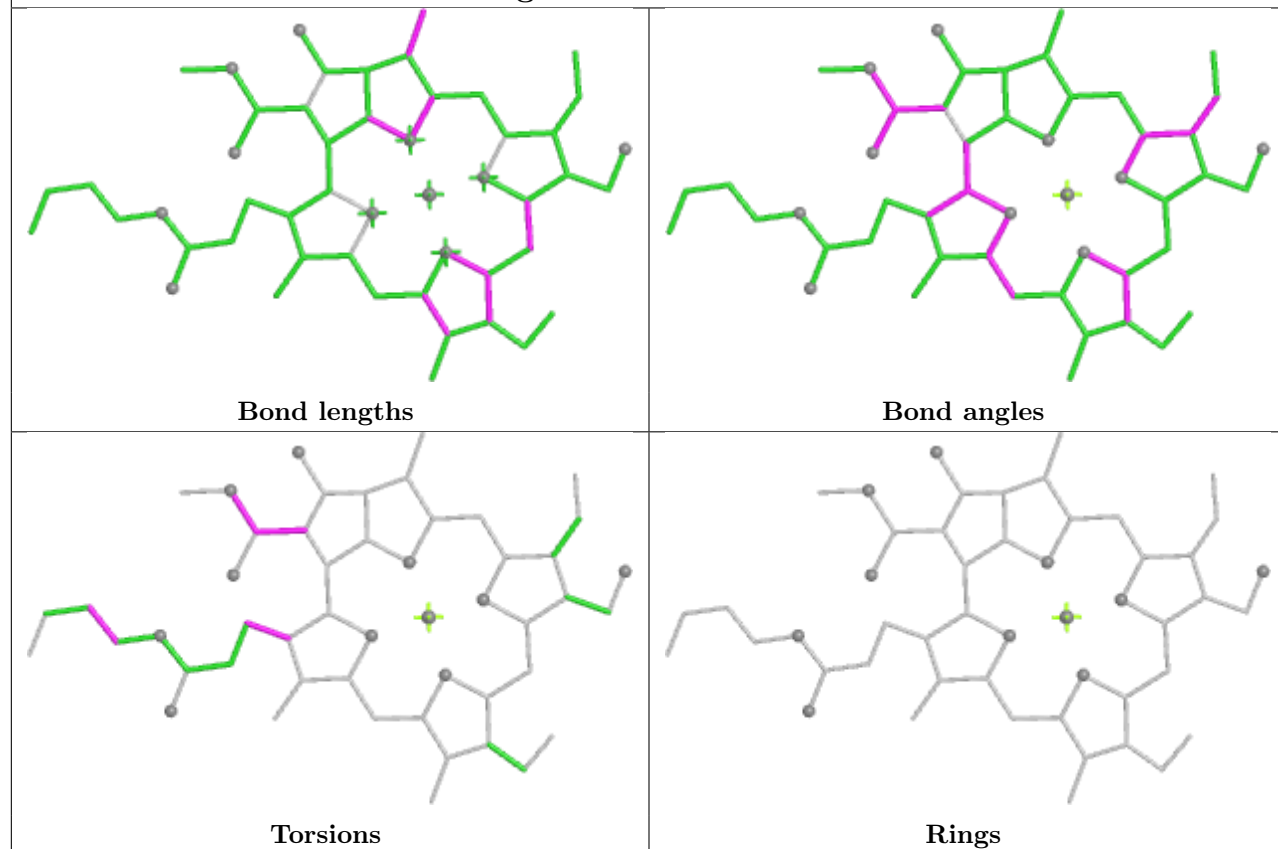


Rings

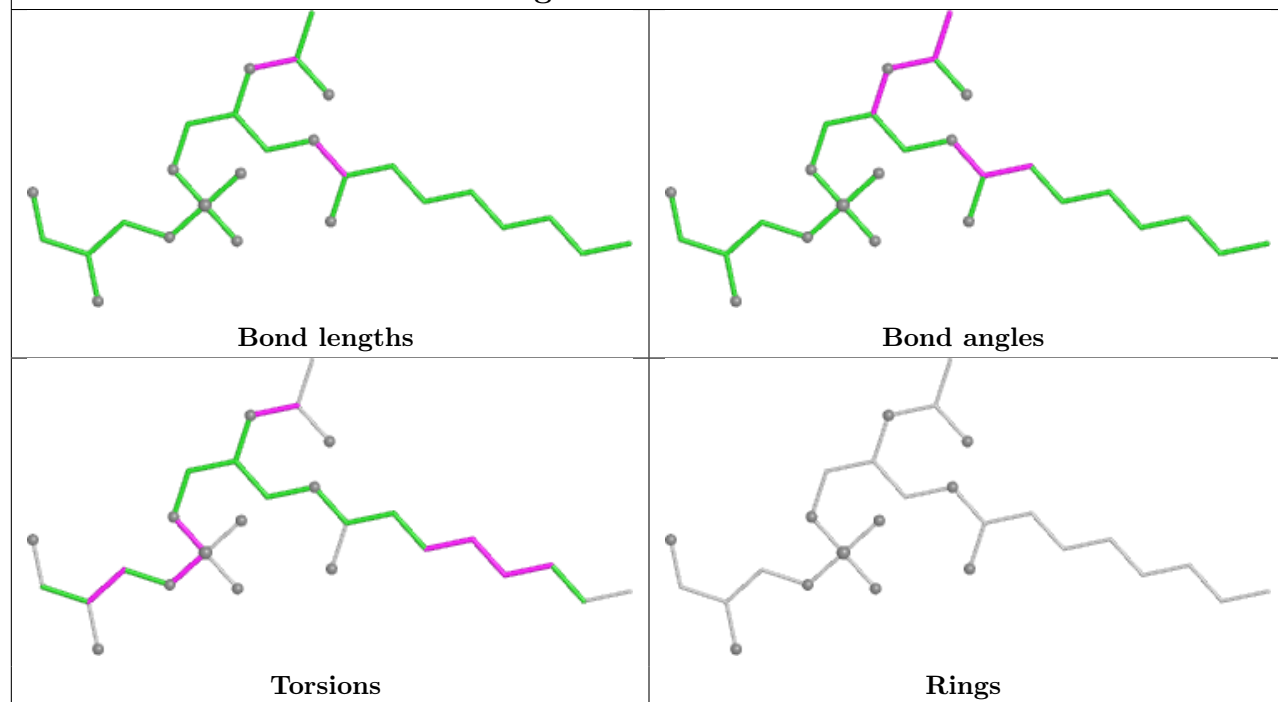


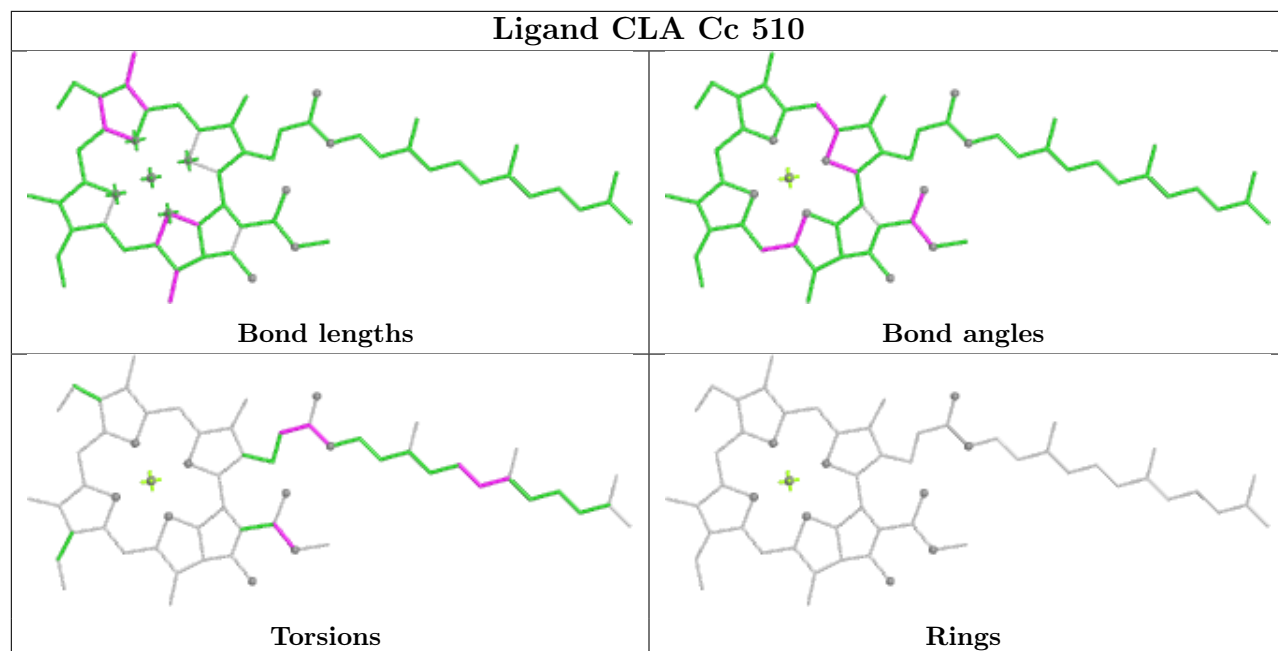


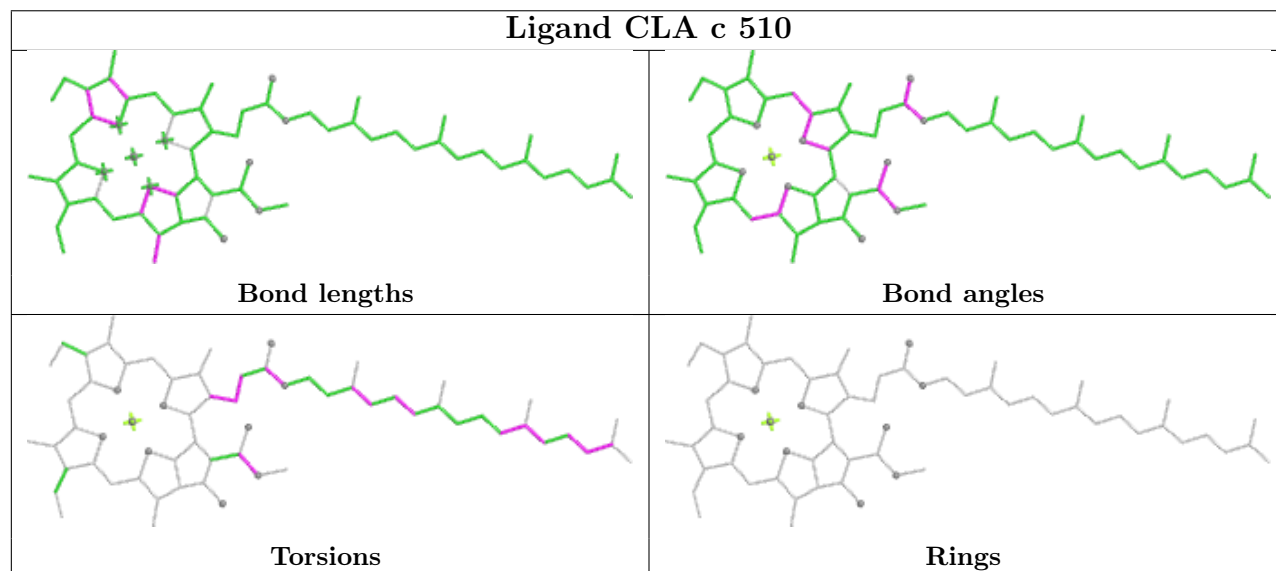
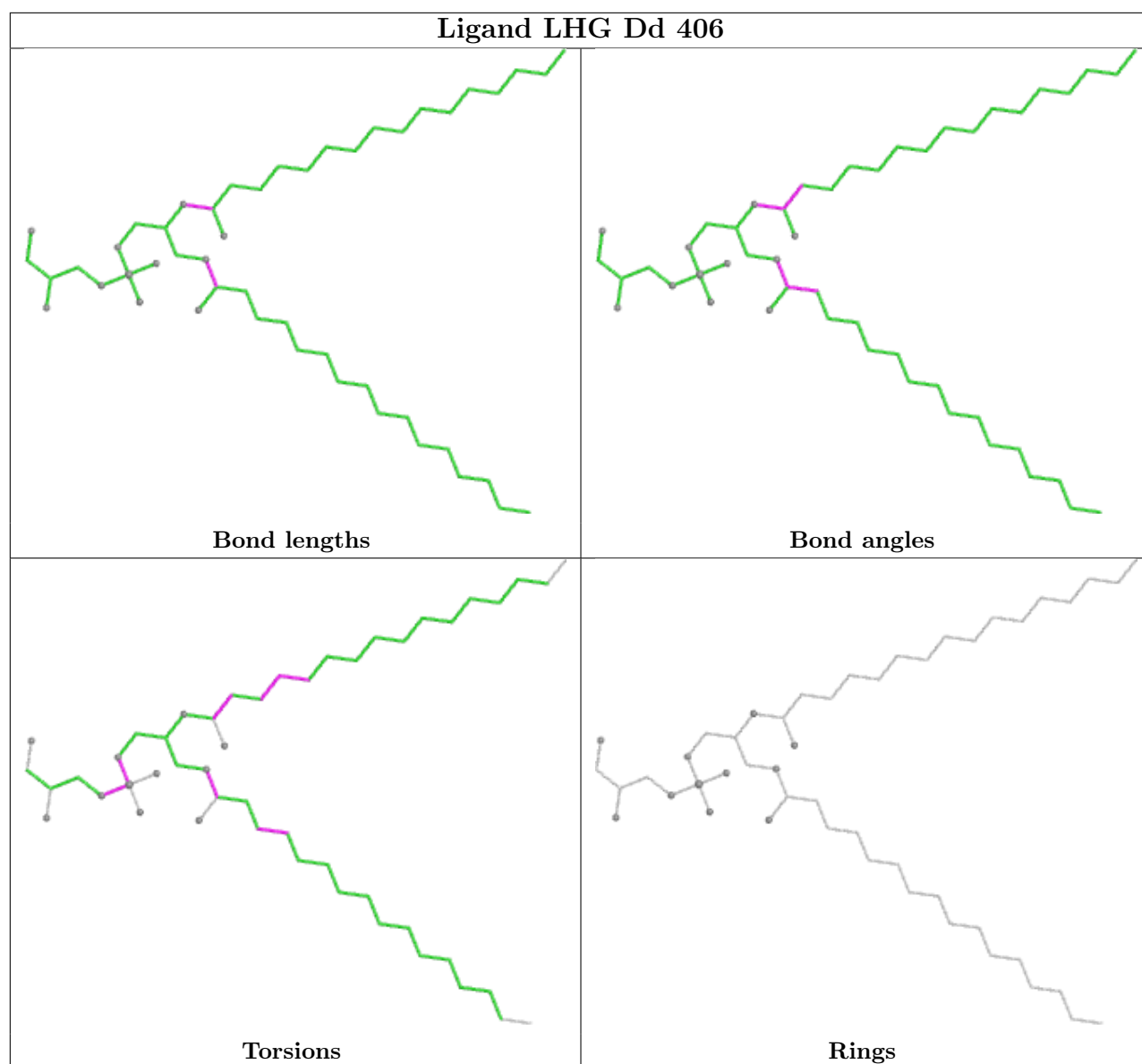
Ligand CHL NN 609

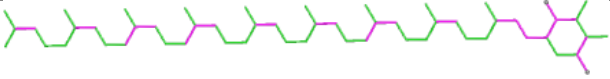
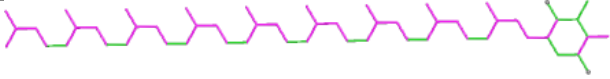
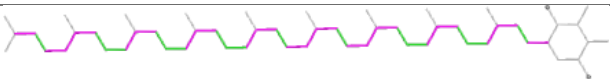
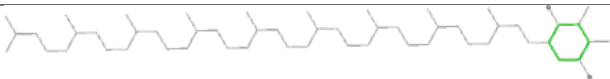
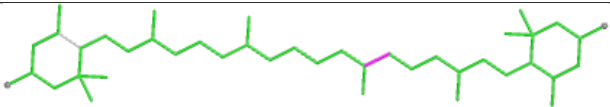
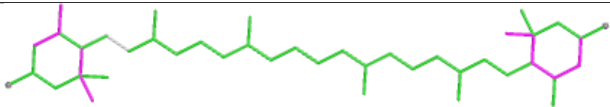
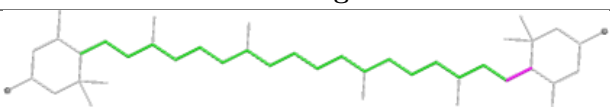
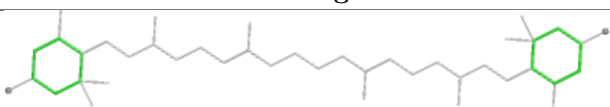
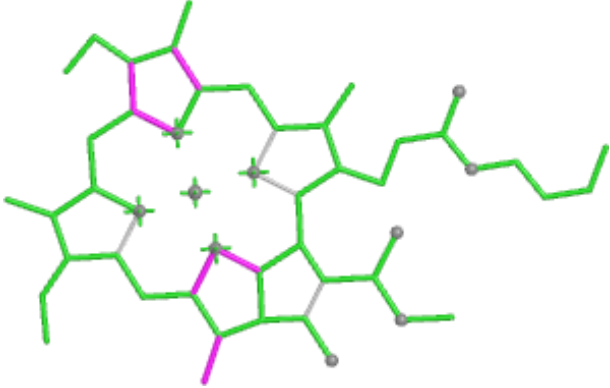
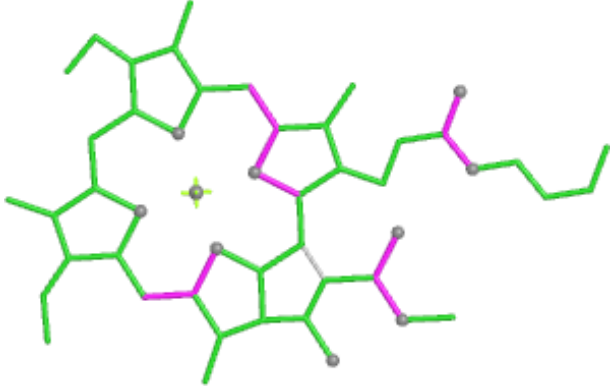
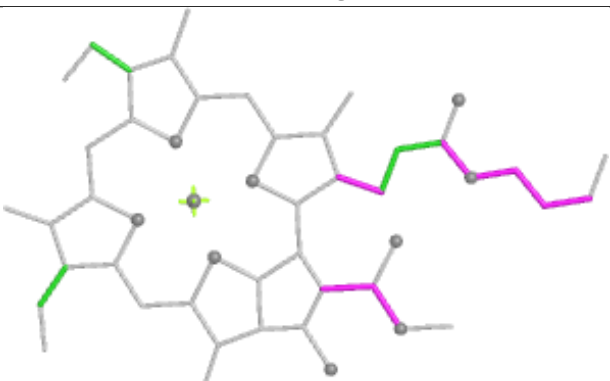
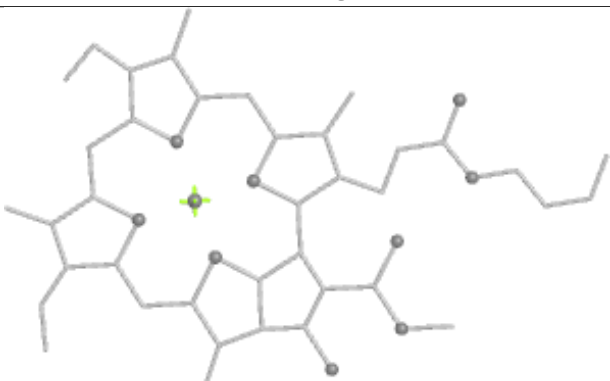


Ligand LHG J 101

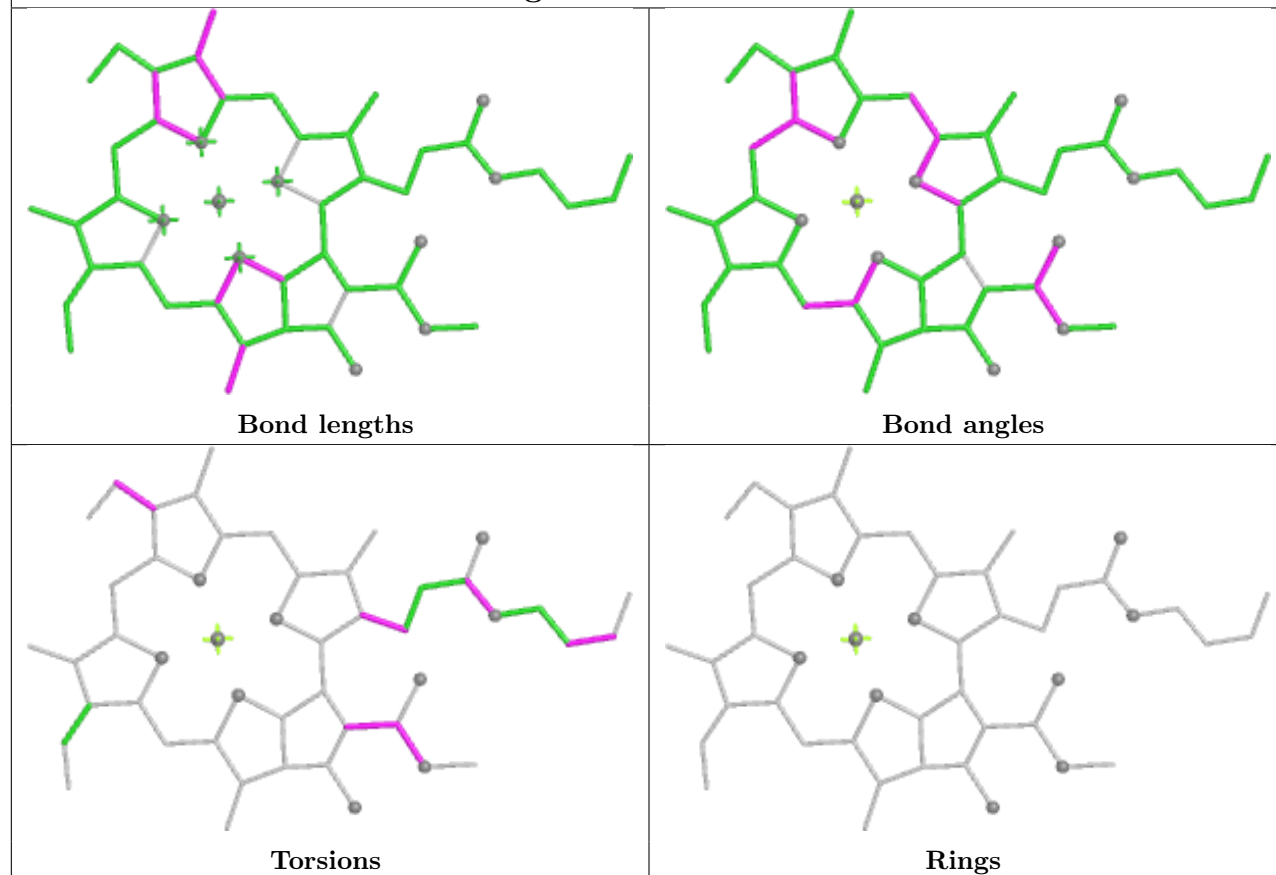




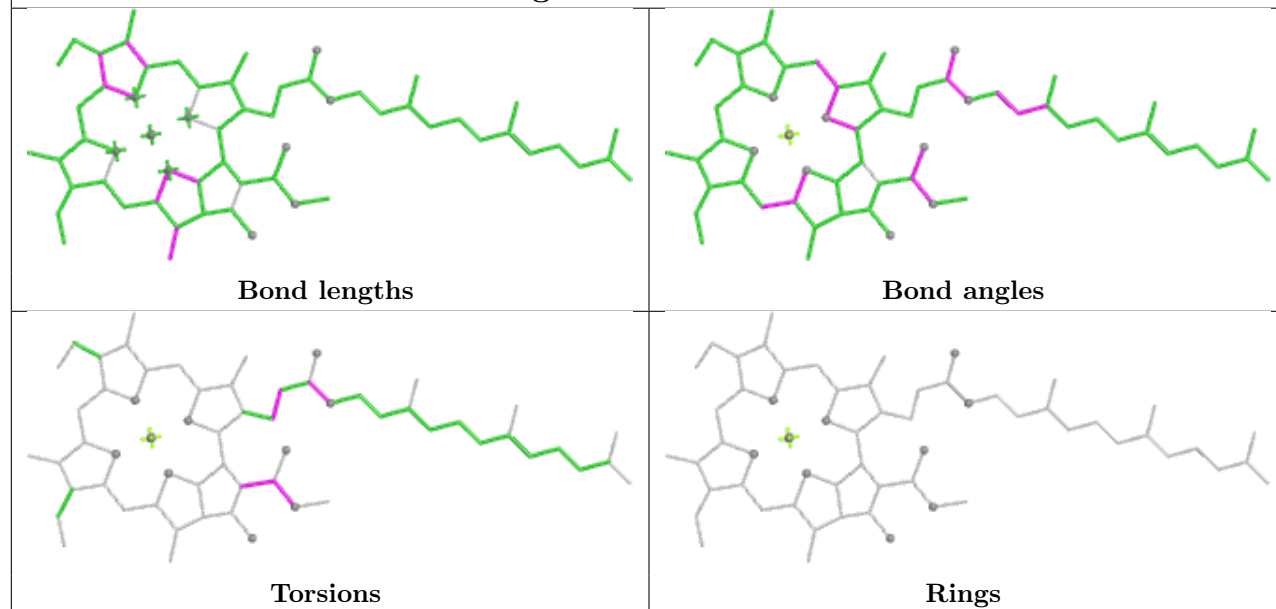


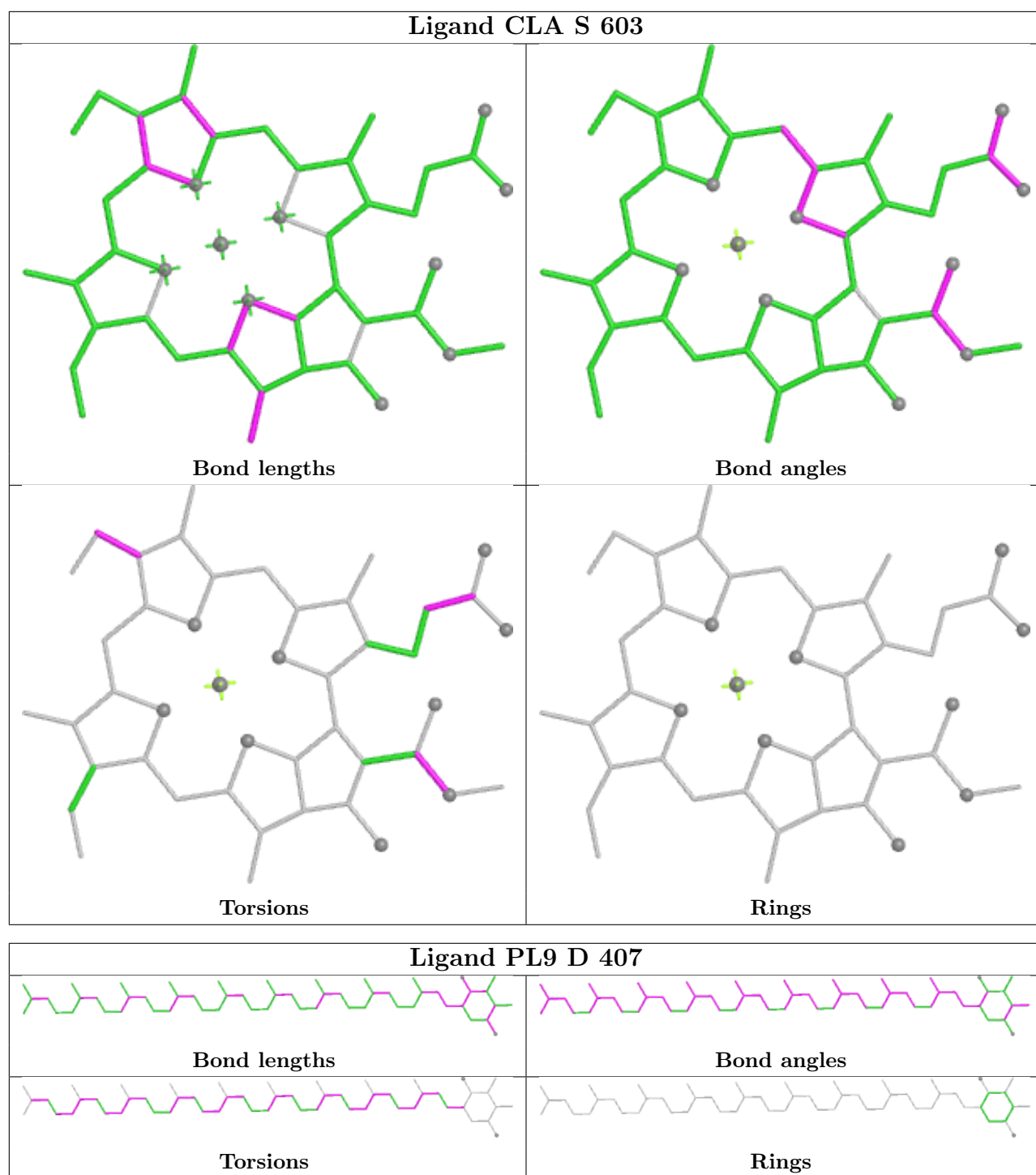
Ligand PL9 Dd 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT g 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA Nn 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Rr 613

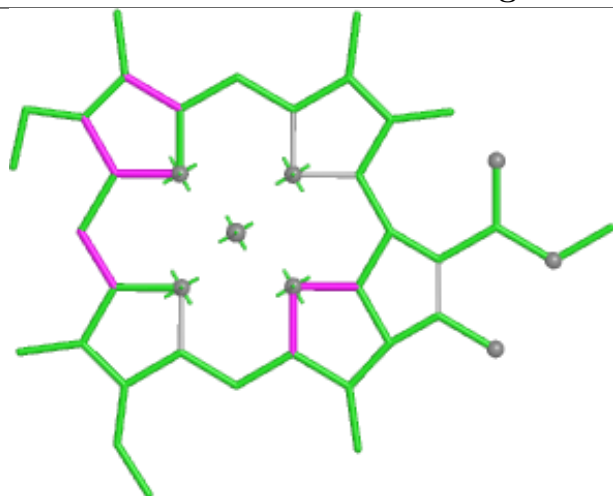


Ligand CLA B 609





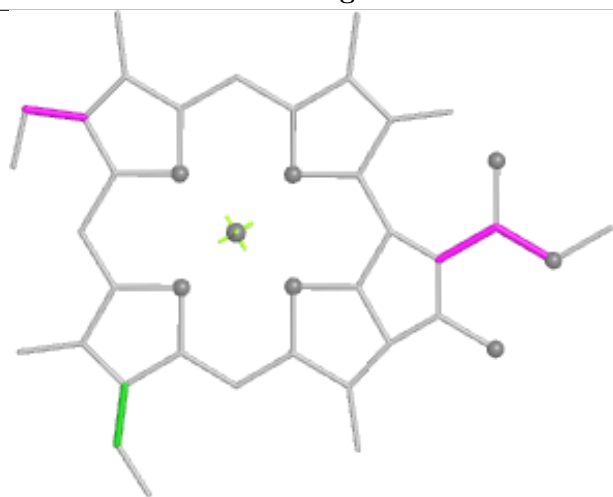
Ligand CLA NN 614



Bond lengths



Bond angles

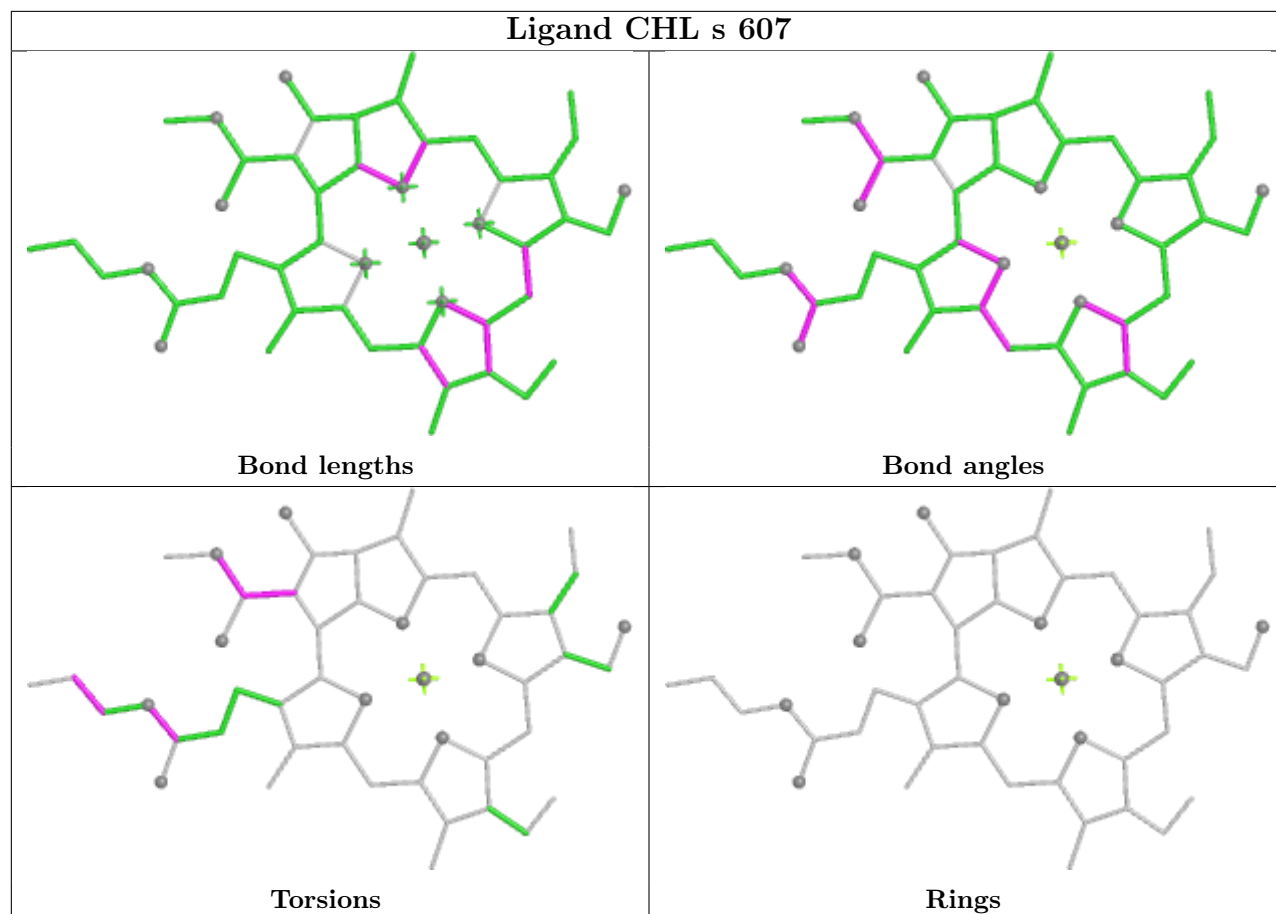


Torsions

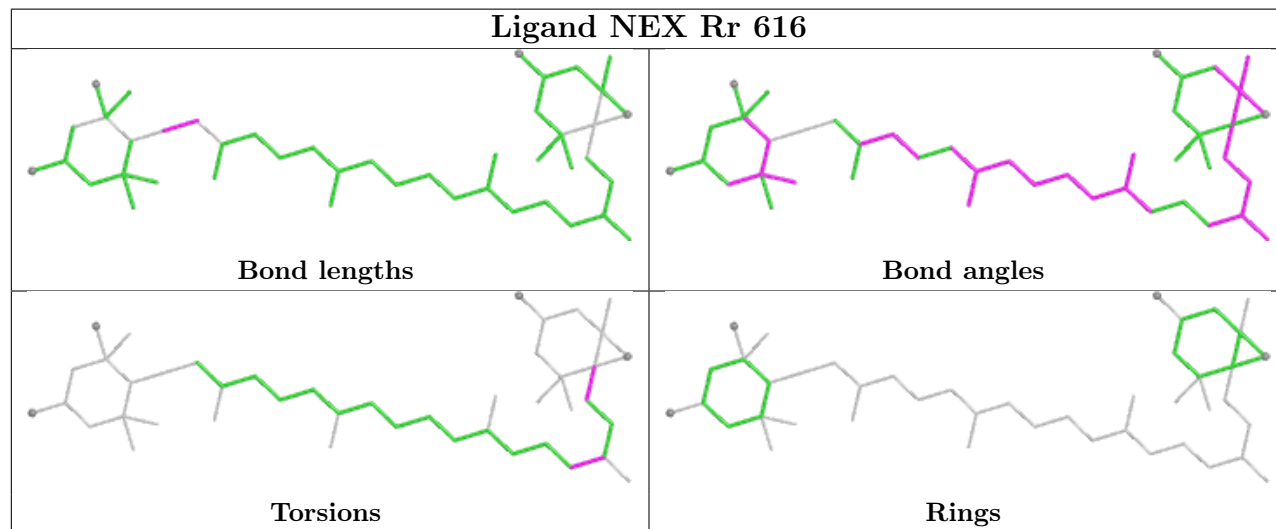


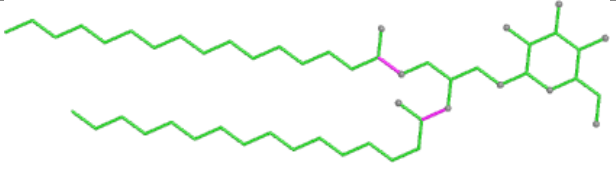
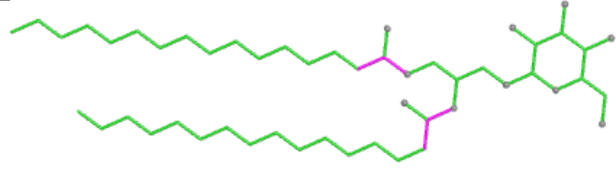
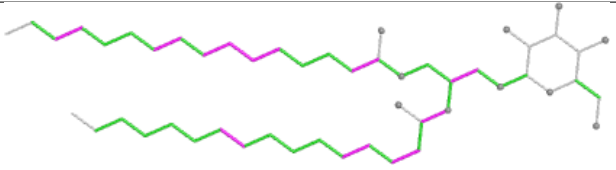
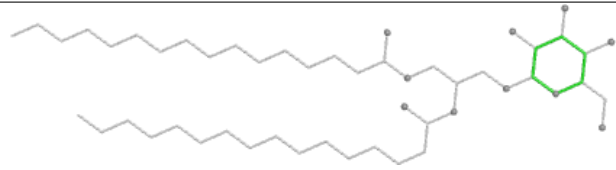
Rings

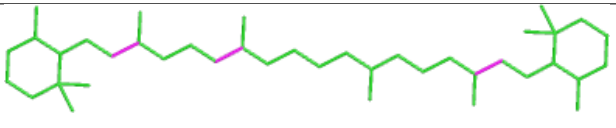
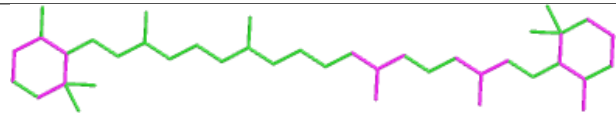
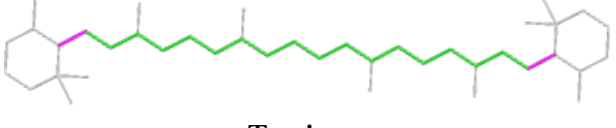
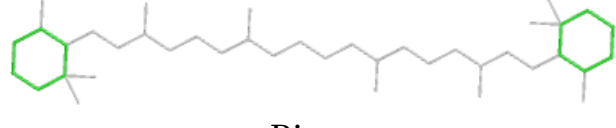
Ligand CHL s 607

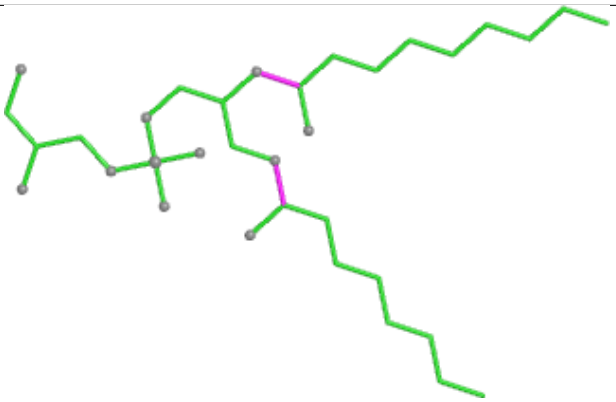
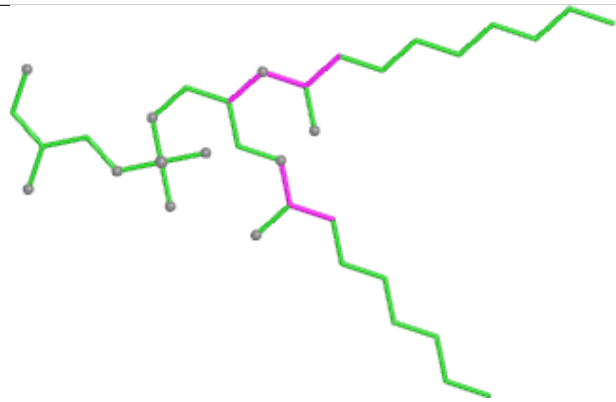
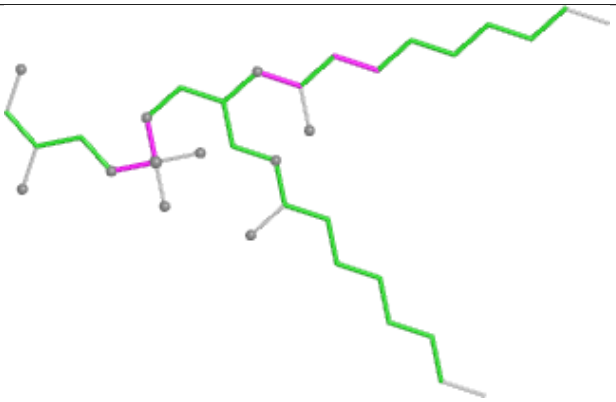
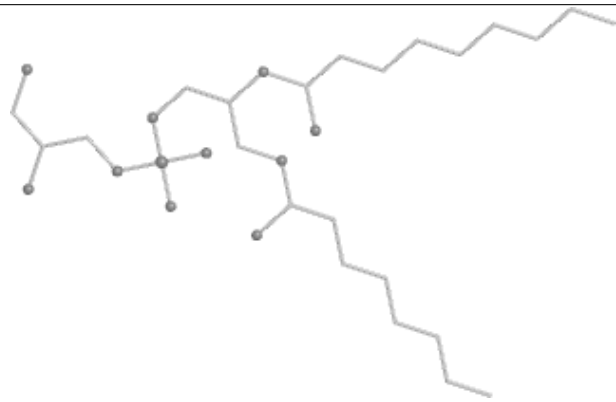


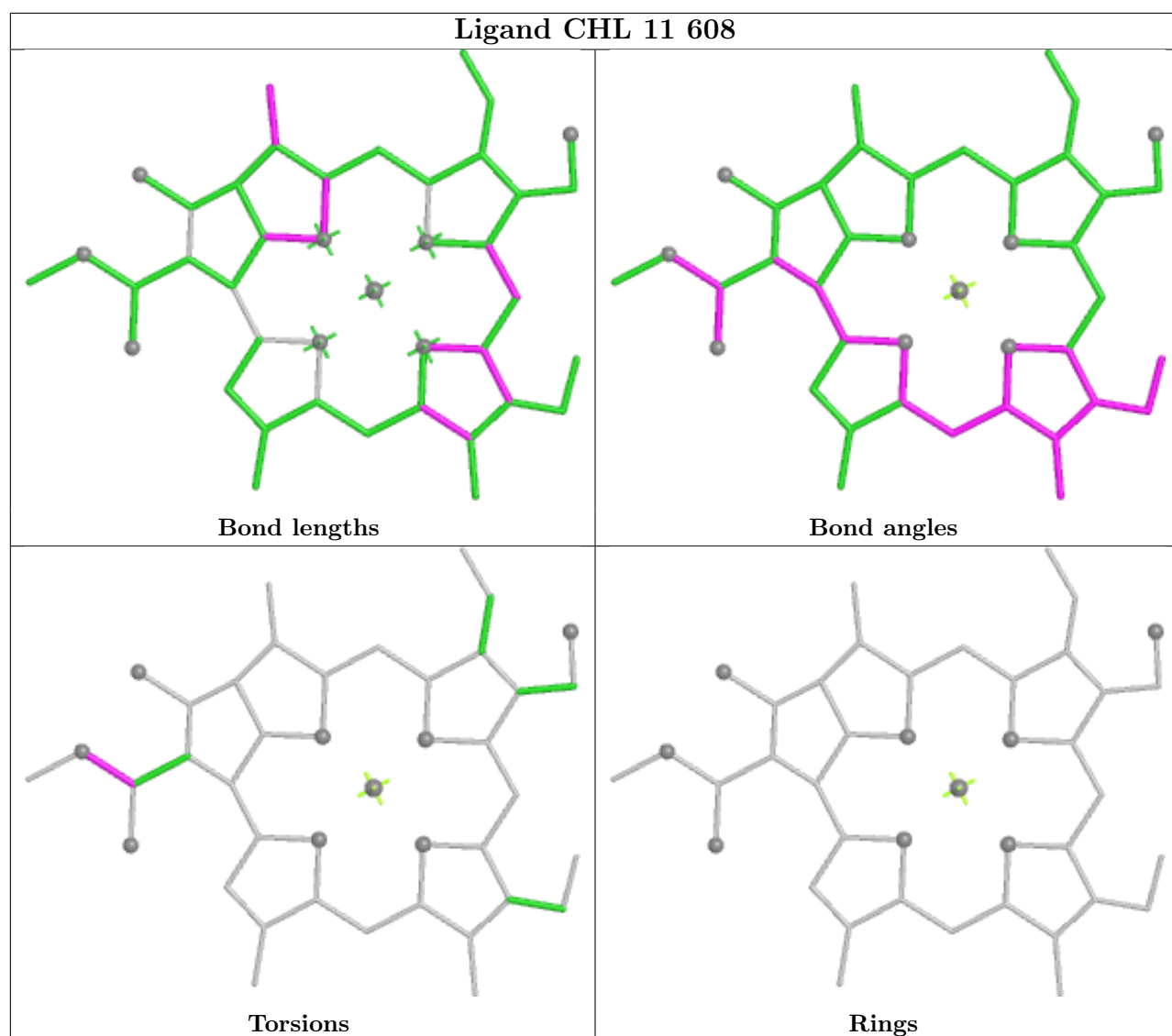
Ligand NEX Rr 616



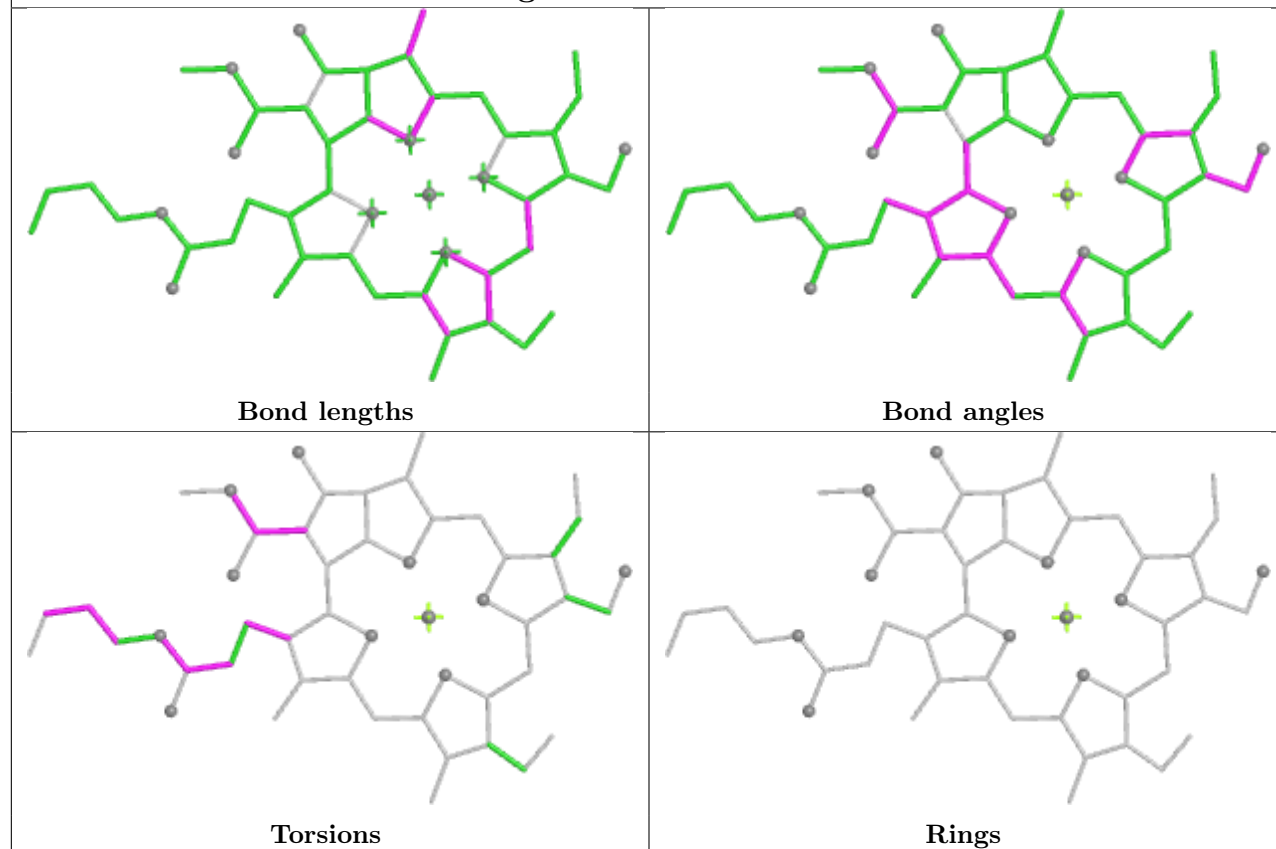
Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Aa 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

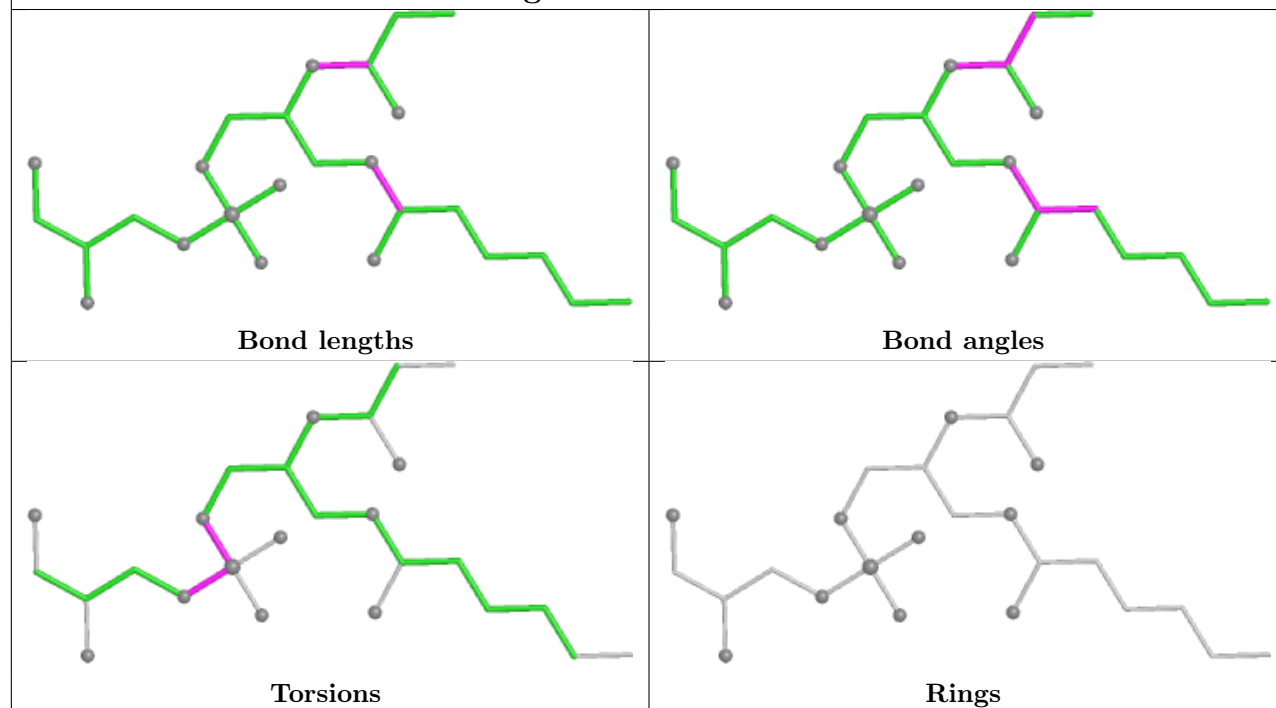
Ligand LHG Gg 319	
	
Bond lengths	Bond angles
	
Torsions	Rings



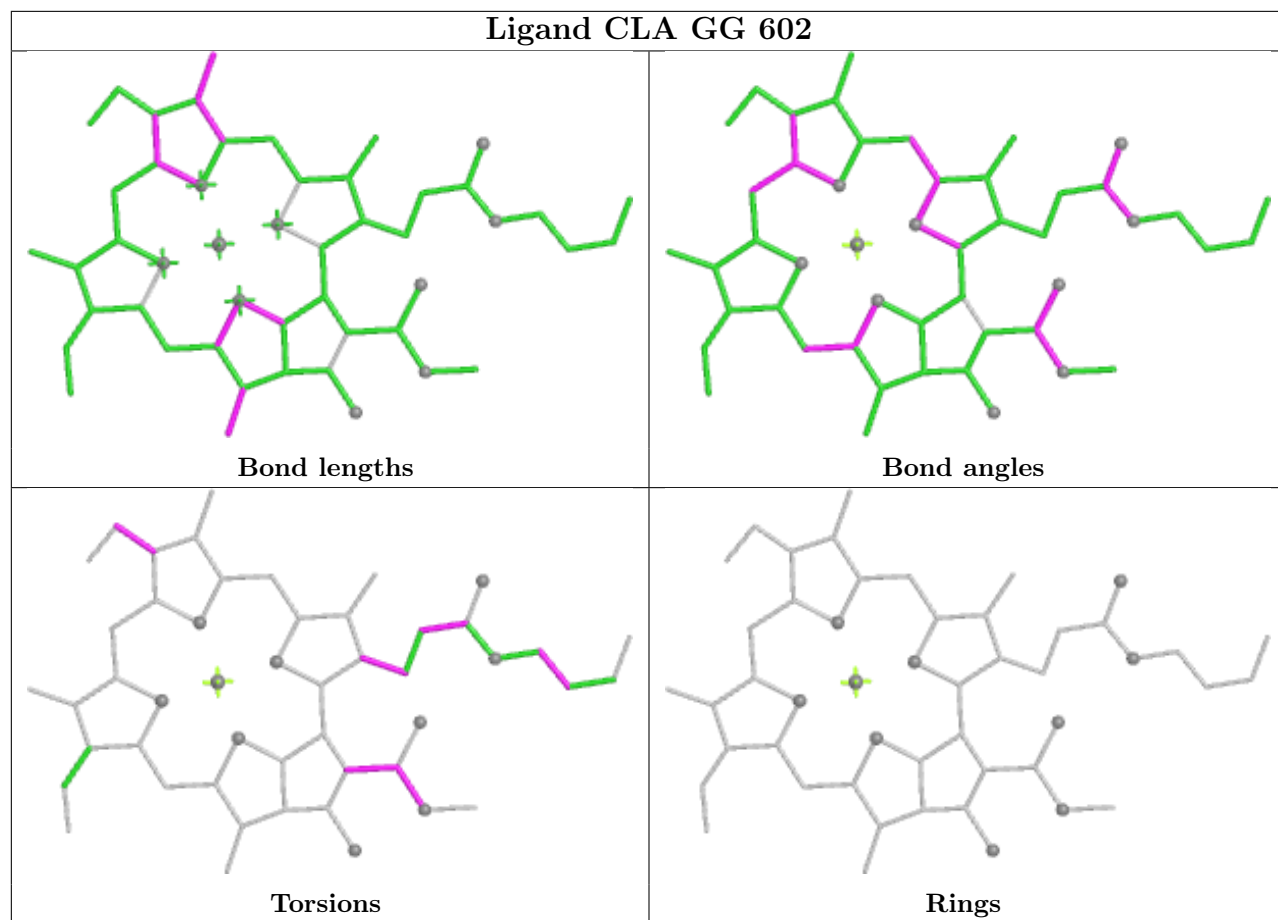
Ligand CHL RR 306



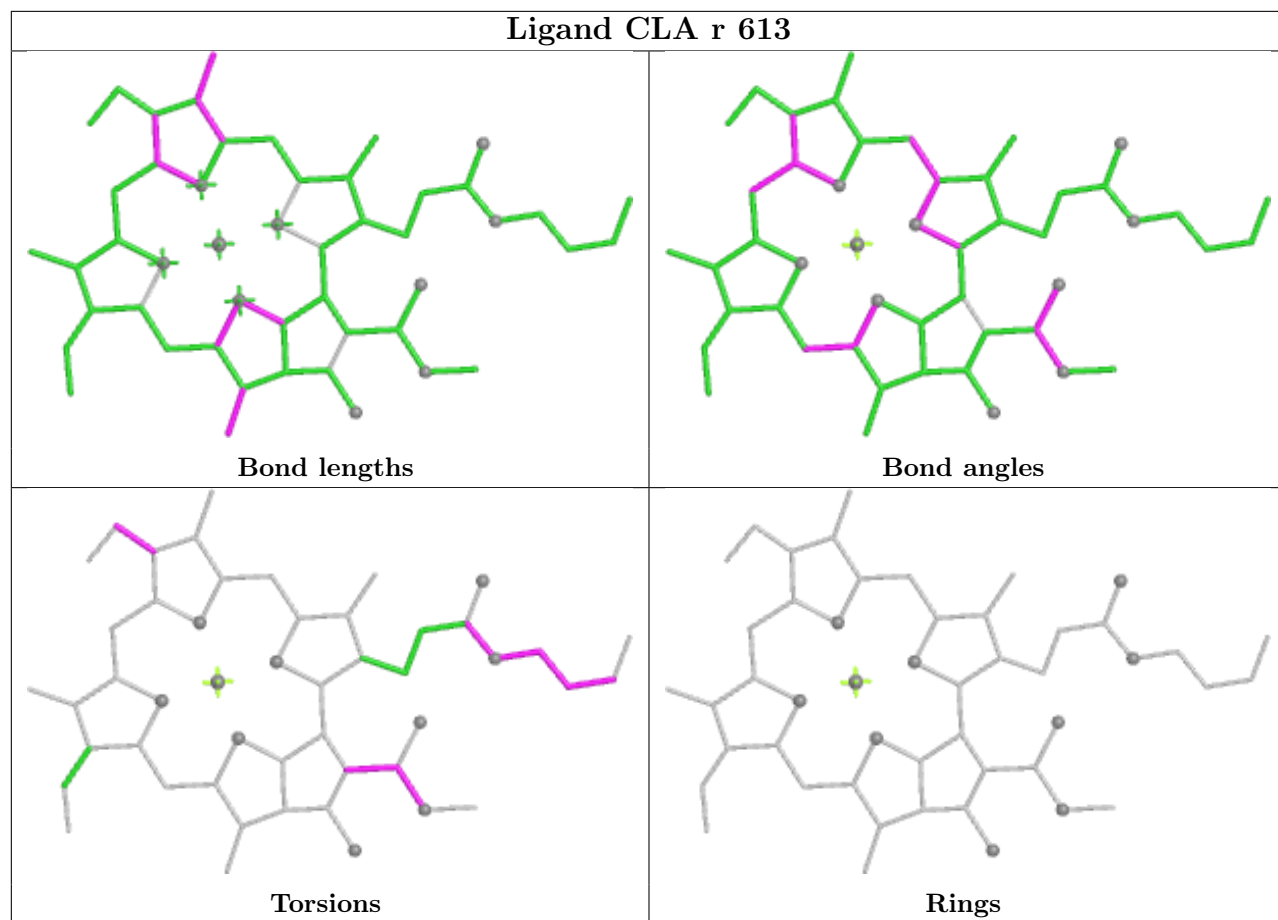
Ligand LHG SS 301



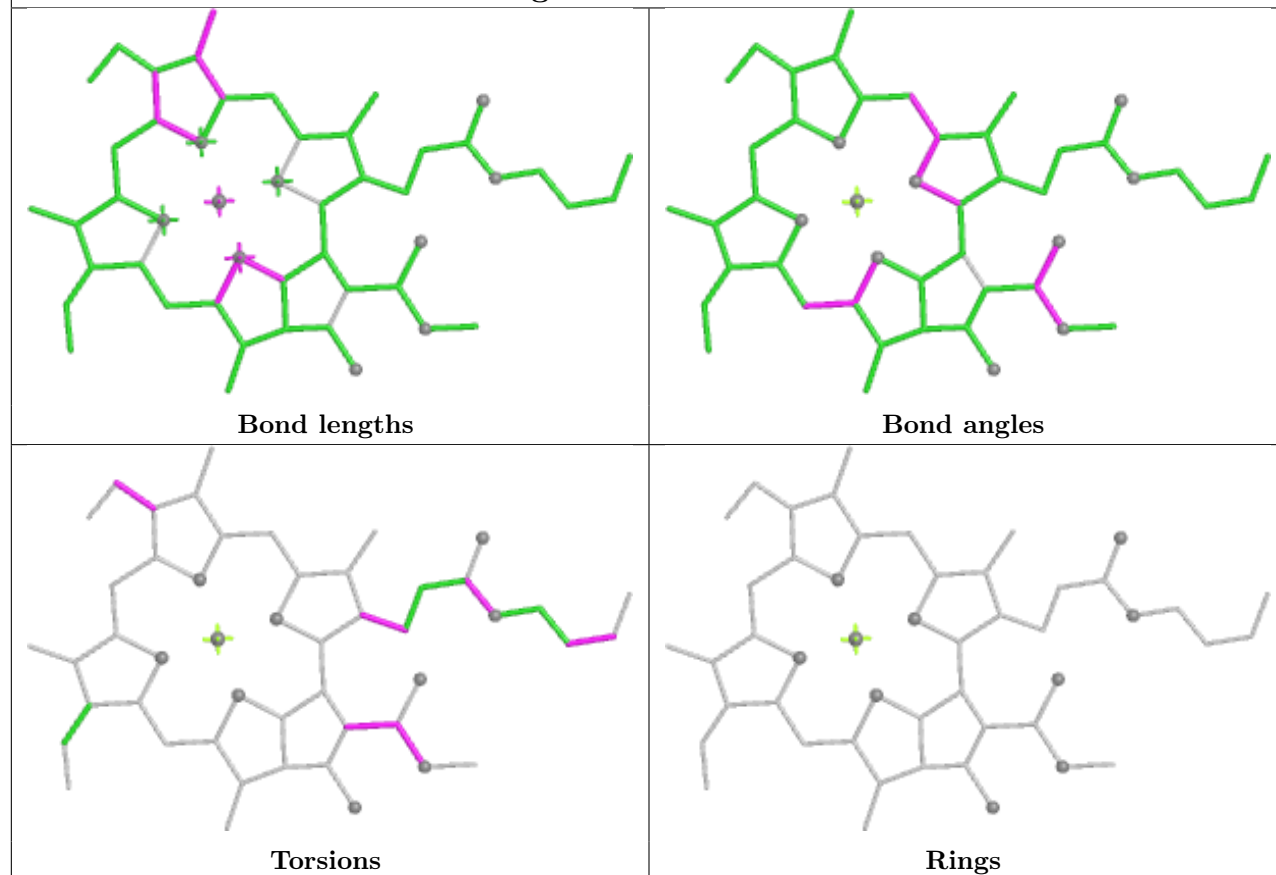
Ligand CLA GG 602



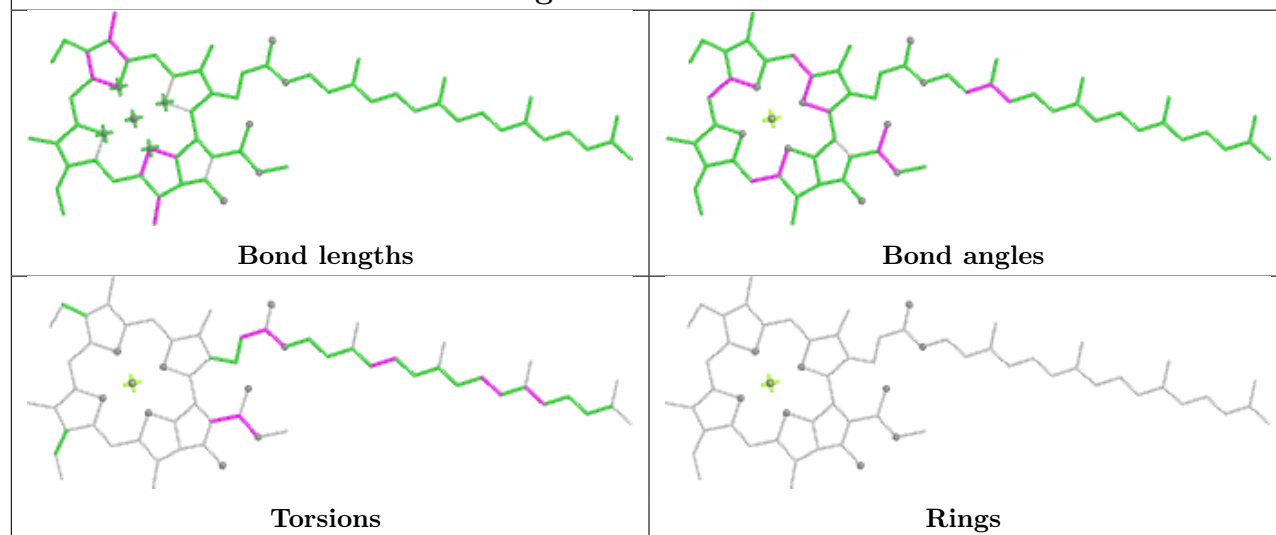
Ligand CLA r 613



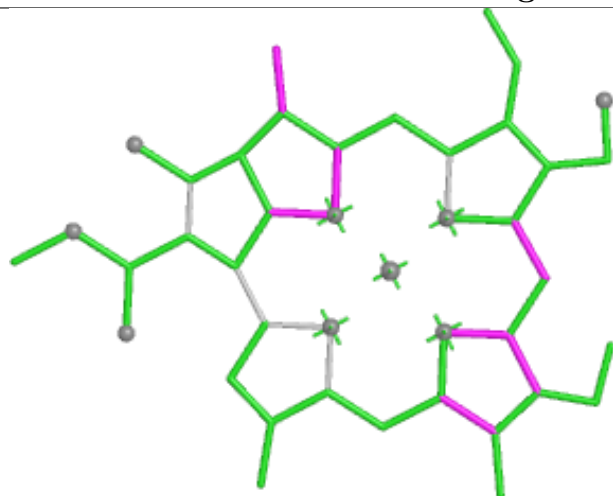
Ligand CLA N 613



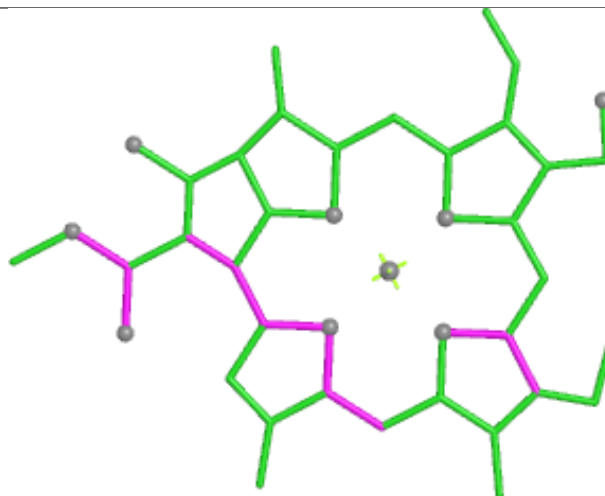
Ligand CLA b 605



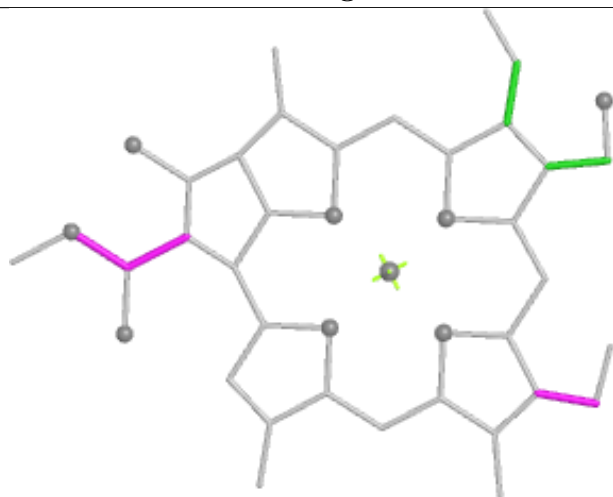
Ligand CHL 1 601



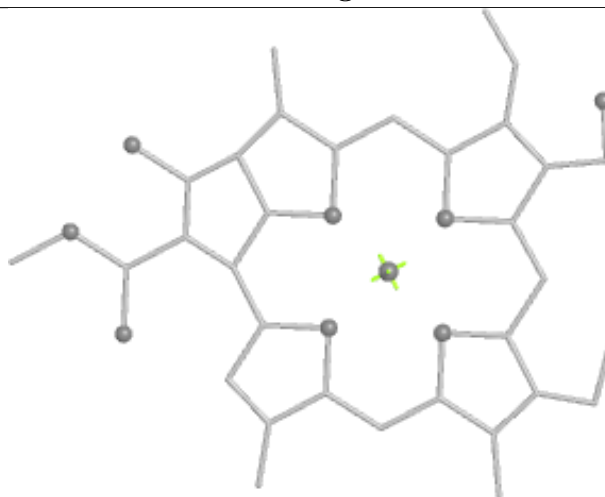
Bond lengths



Bond angles

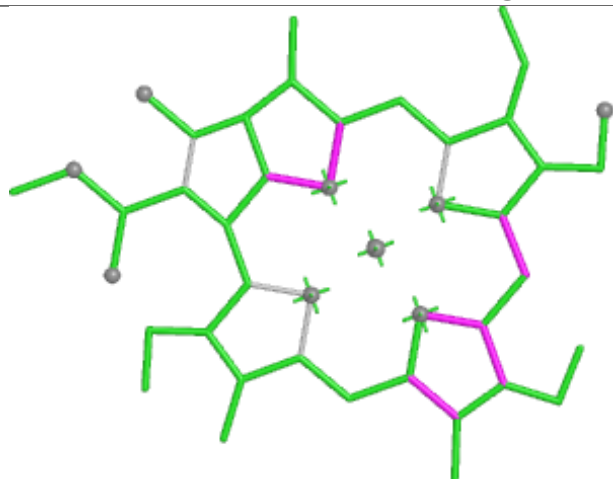


Torsions

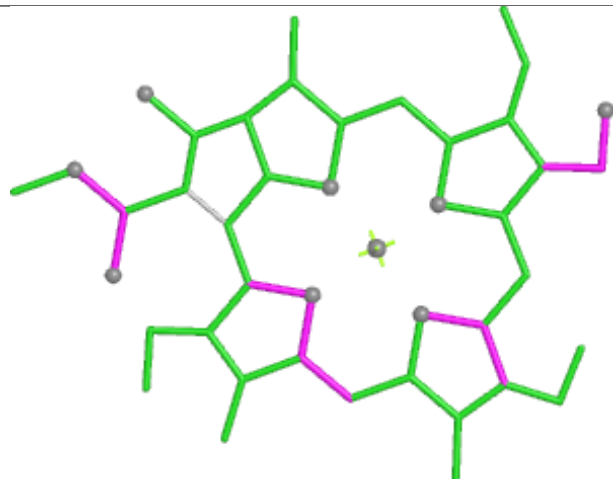


Rings

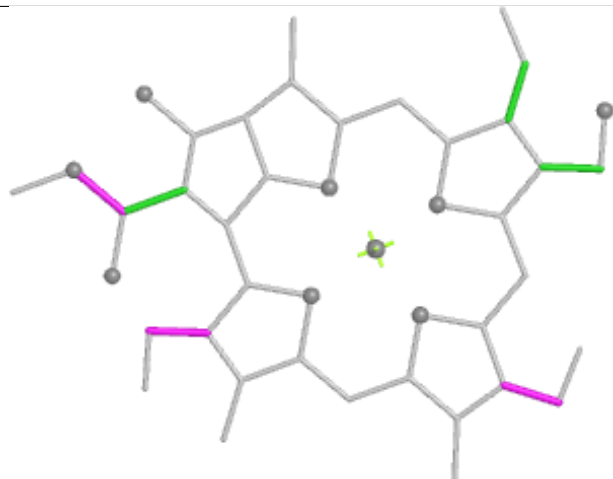
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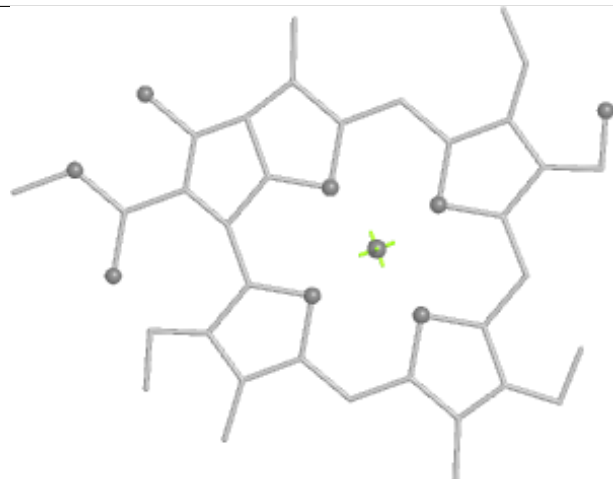
Bond lengths



Bond angles



Torsions

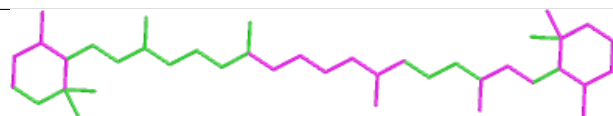


Rings

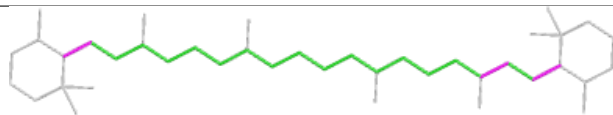
Ligand BCR TT 101



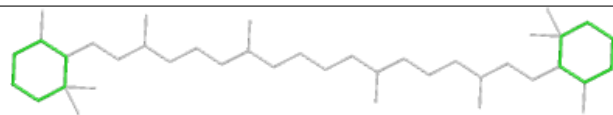
Bond lengths



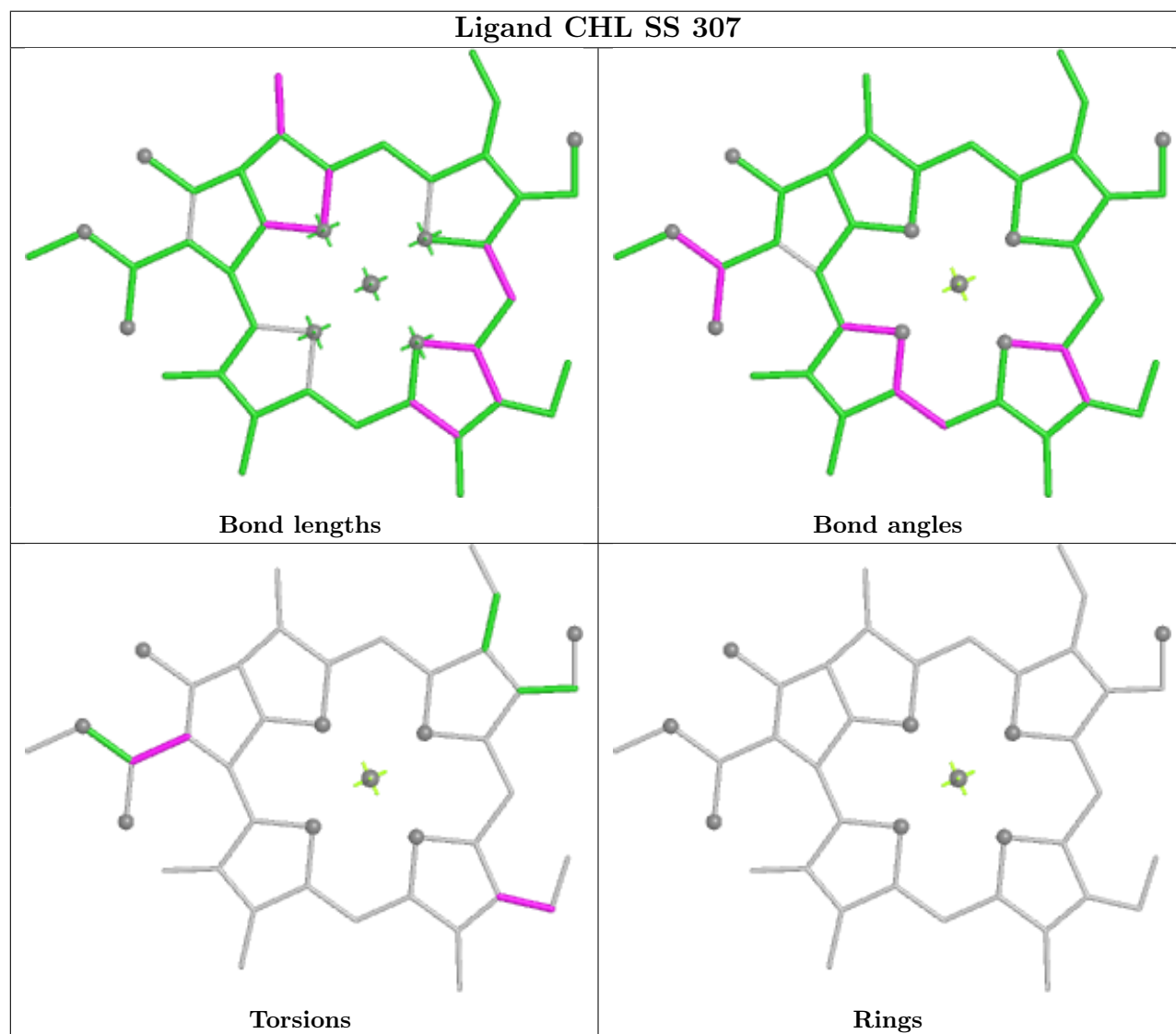
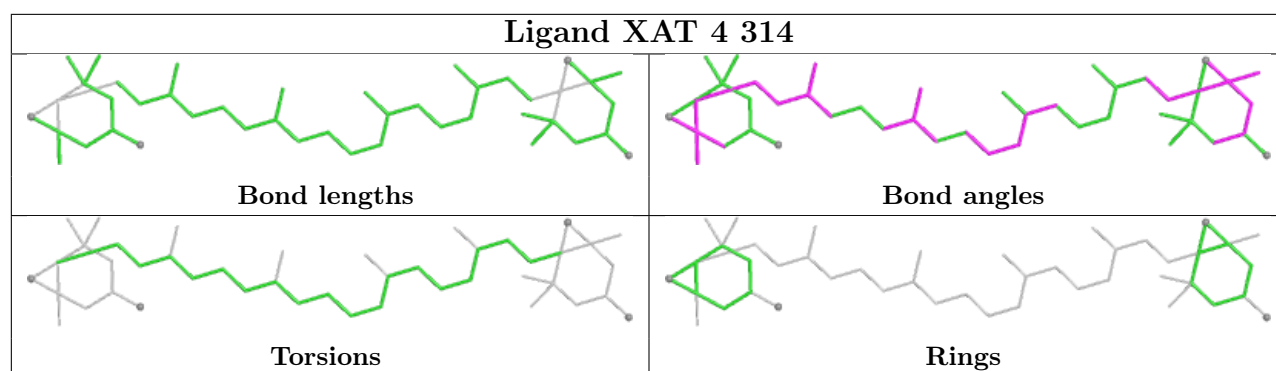
Bond angles

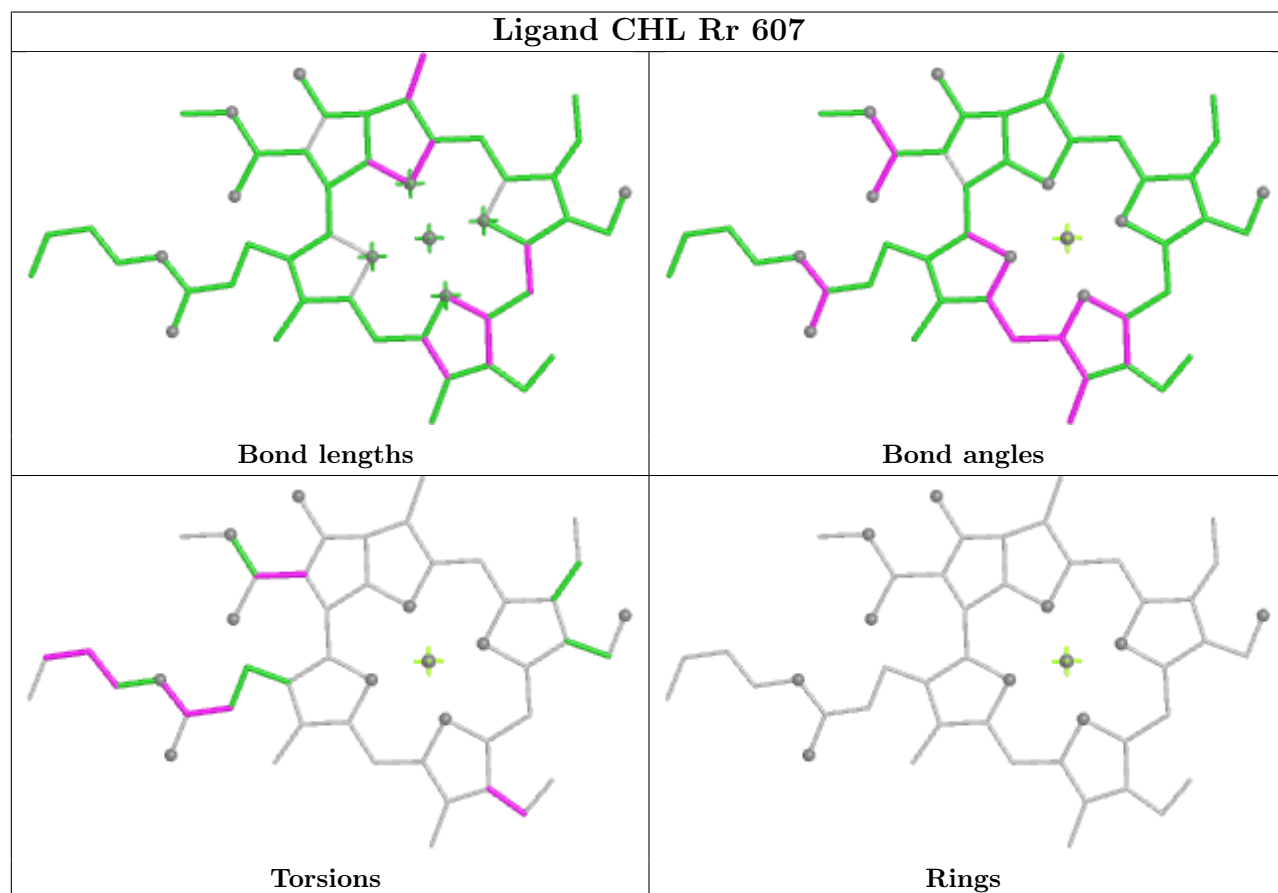
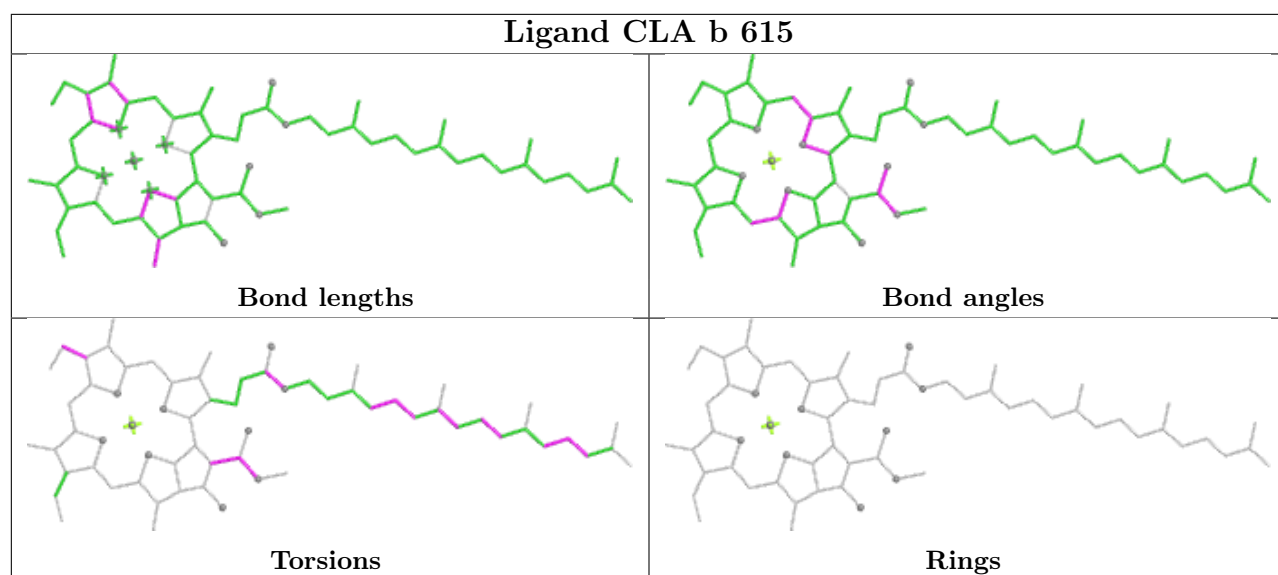


Torsions

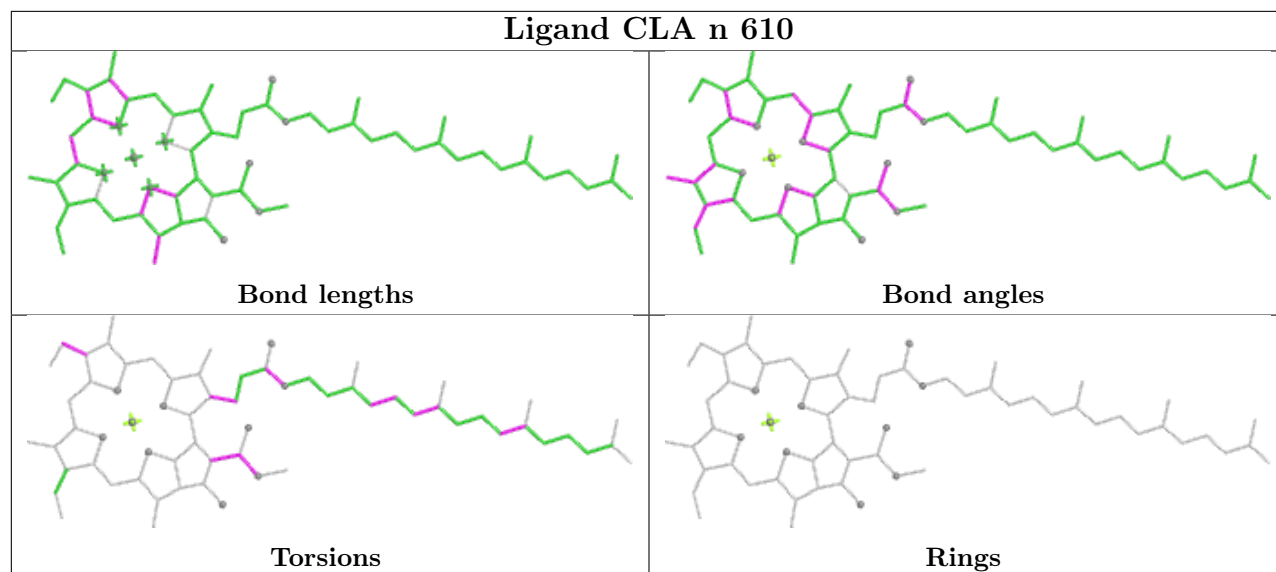


Rings

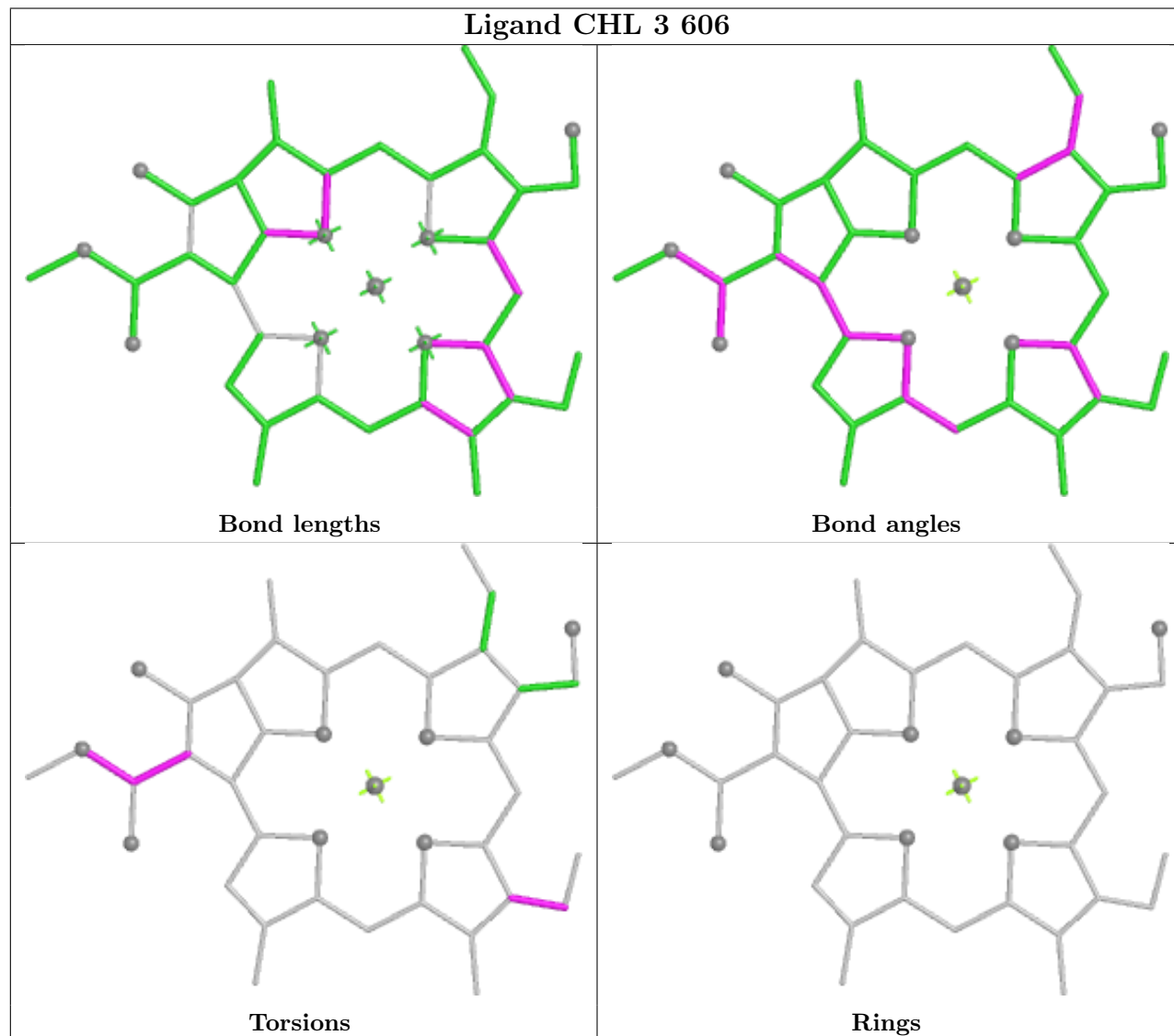


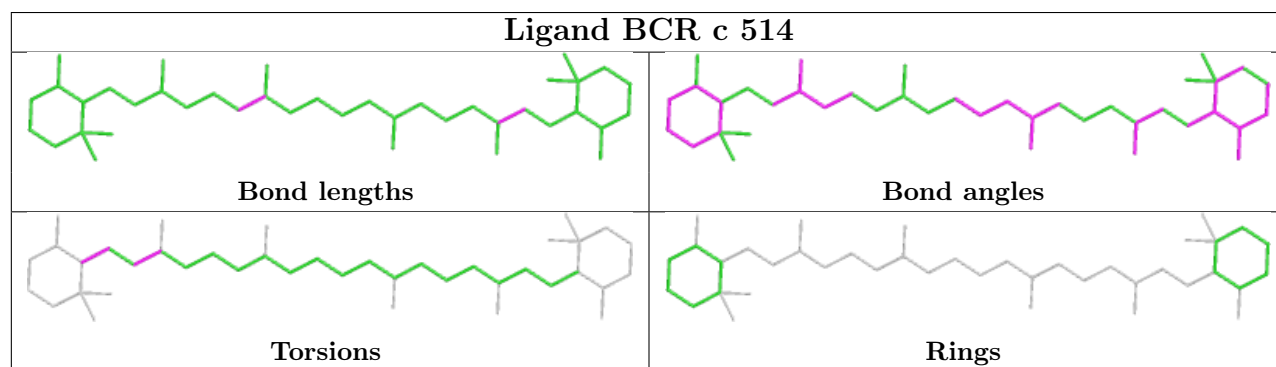
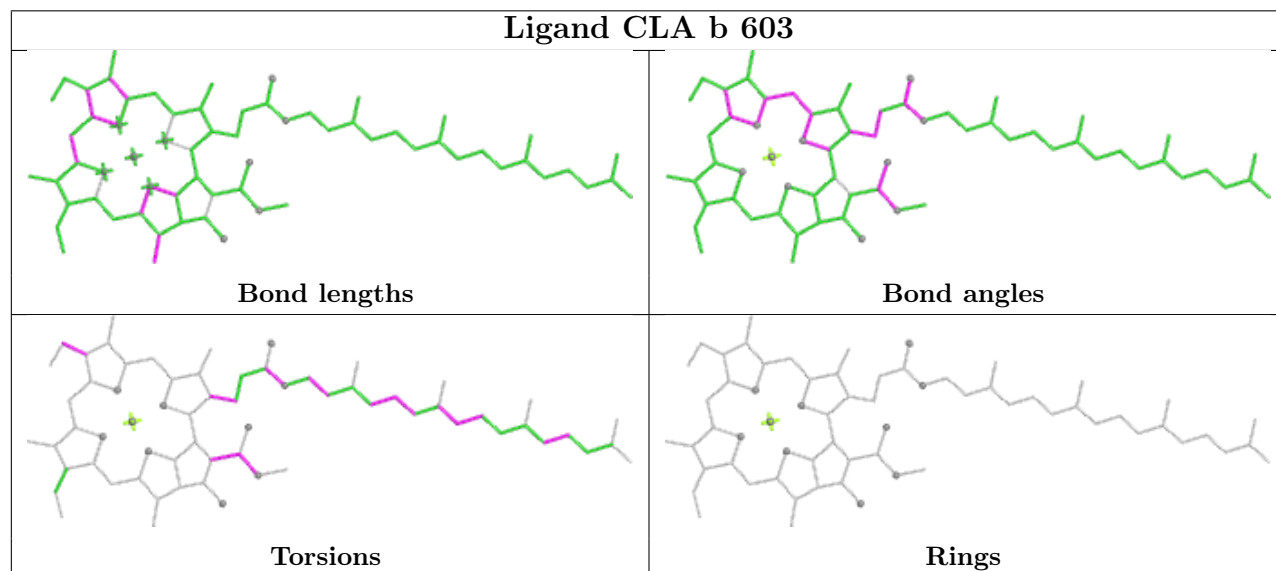
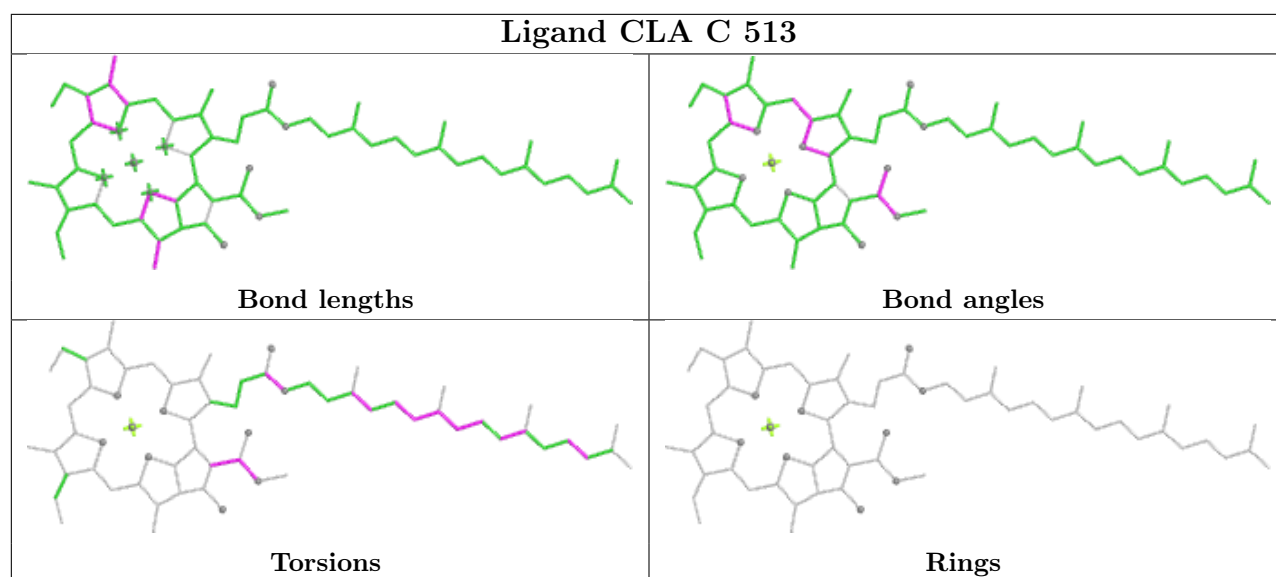


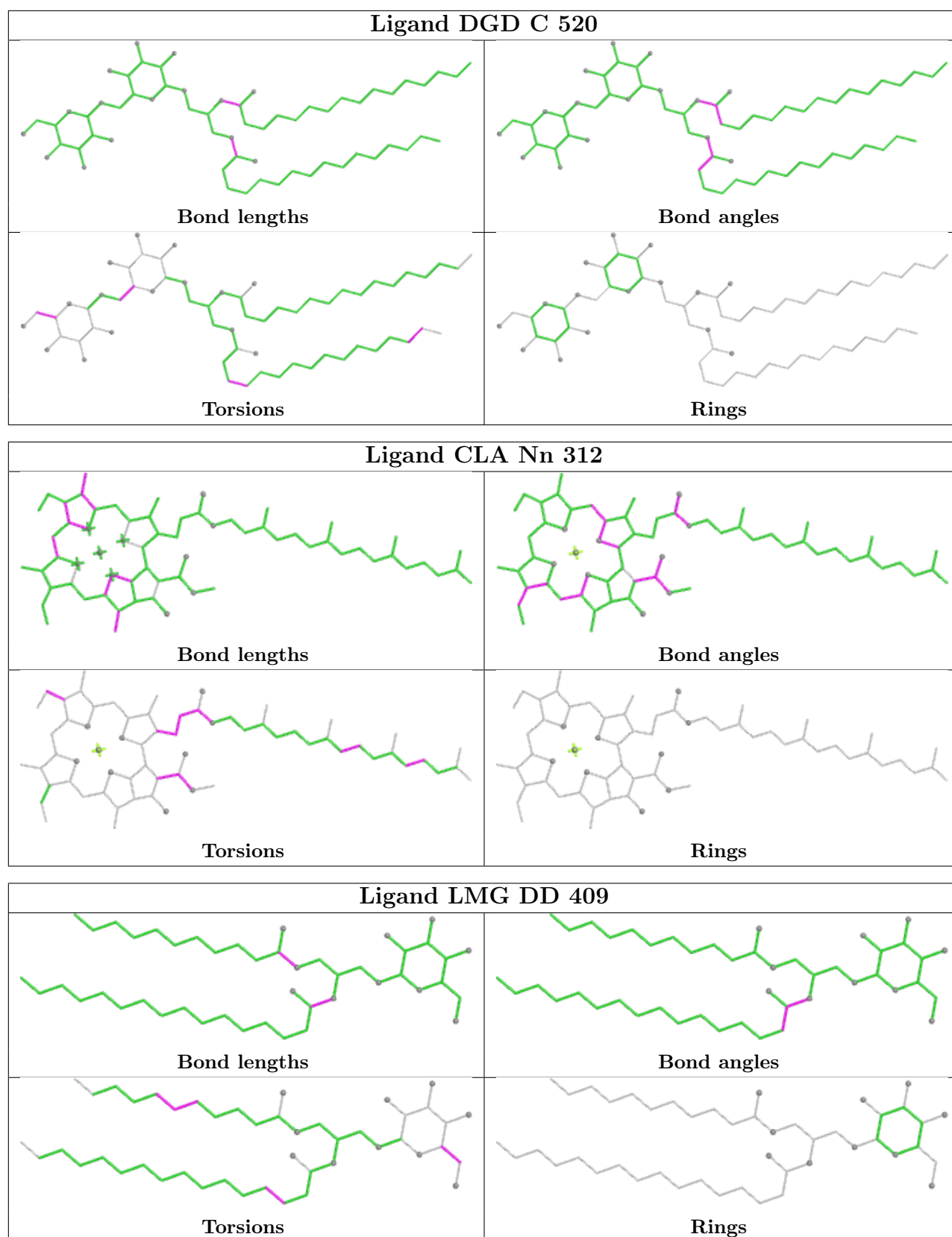
Ligand CLA n 610



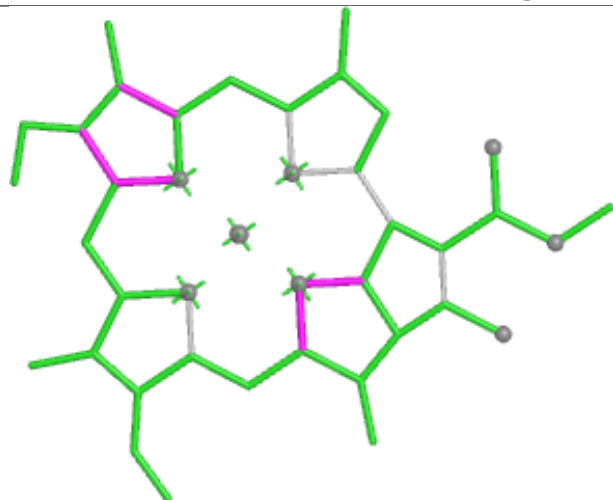
Ligand CHL 3 606



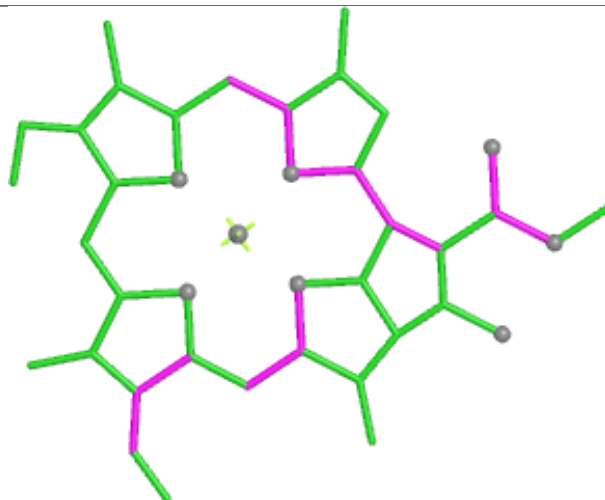




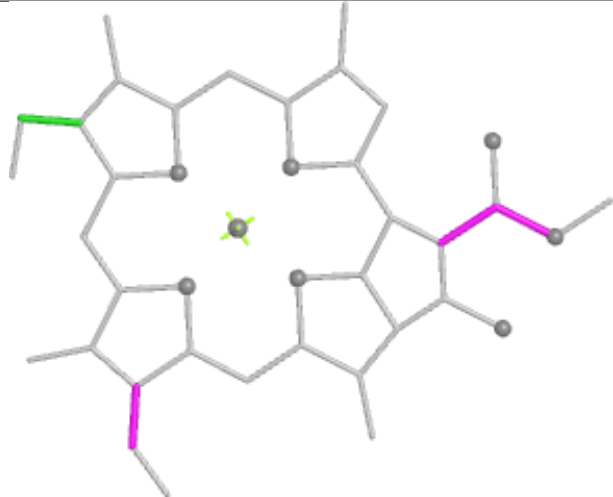
Ligand CLA 3 610



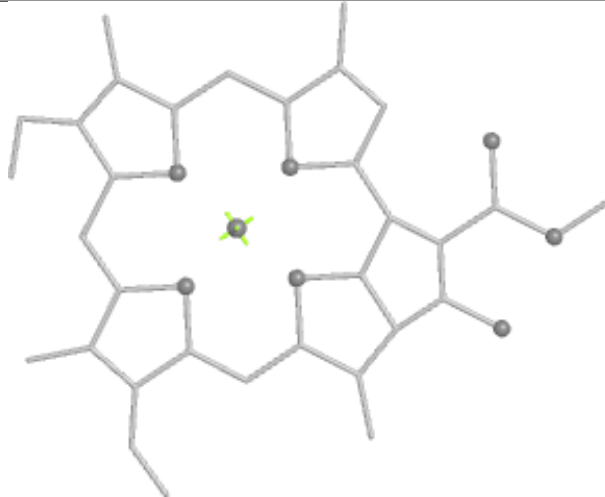
Bond lengths



Bond angles

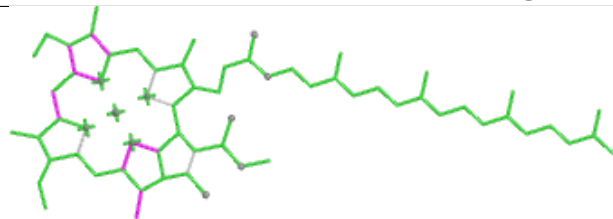


Torsions

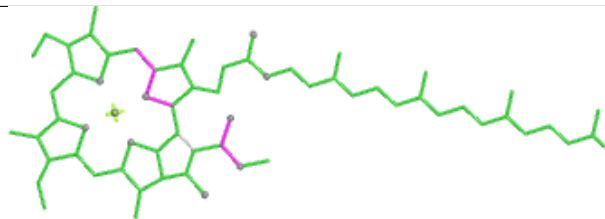


Rings

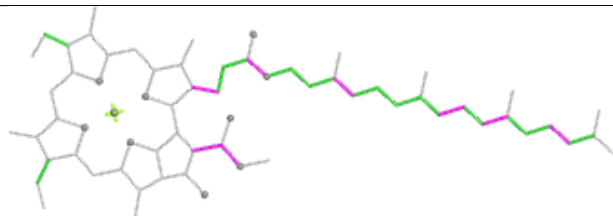
Ligand CLA r 609



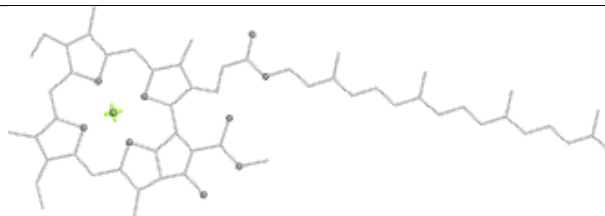
Bond lengths



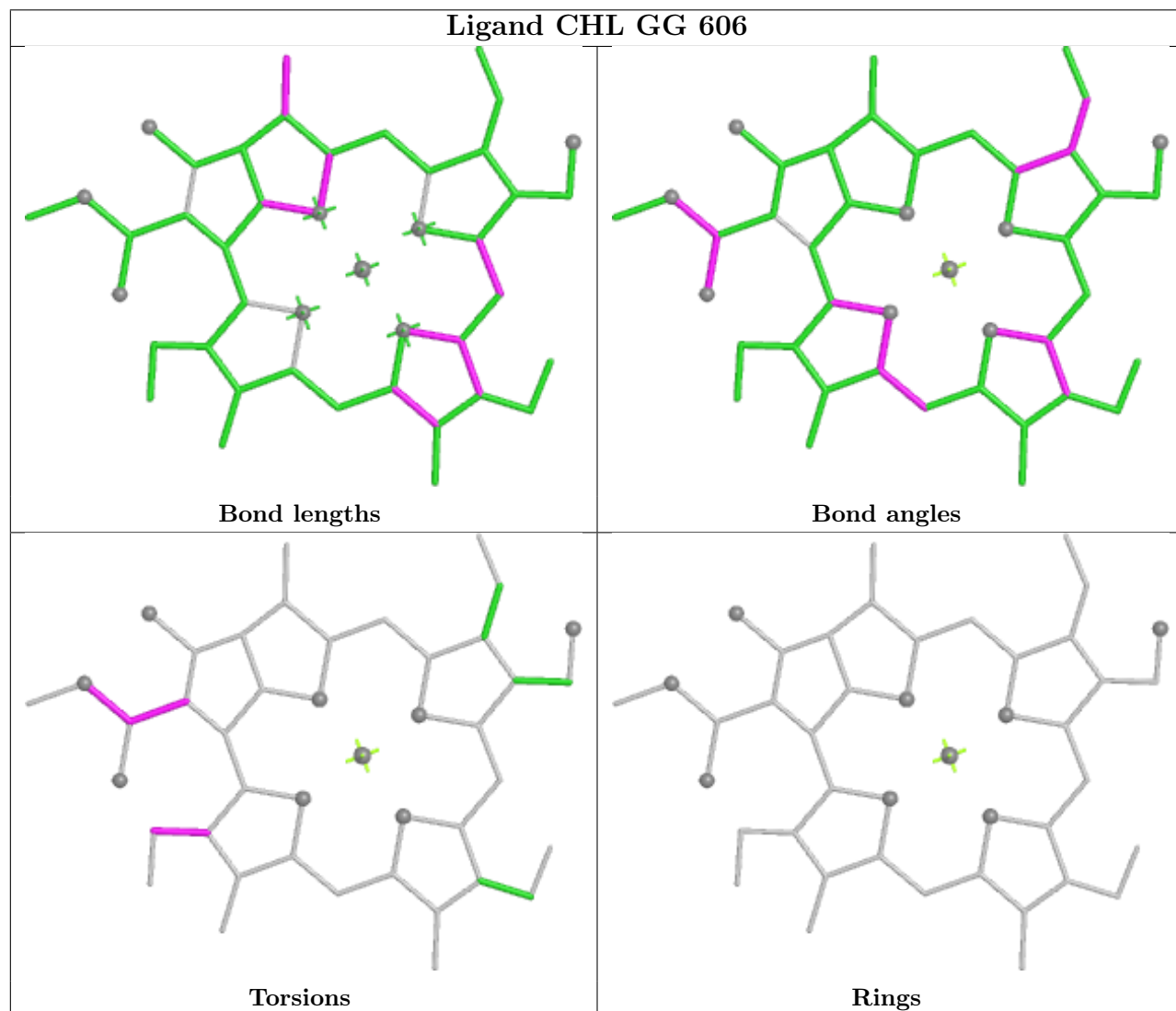
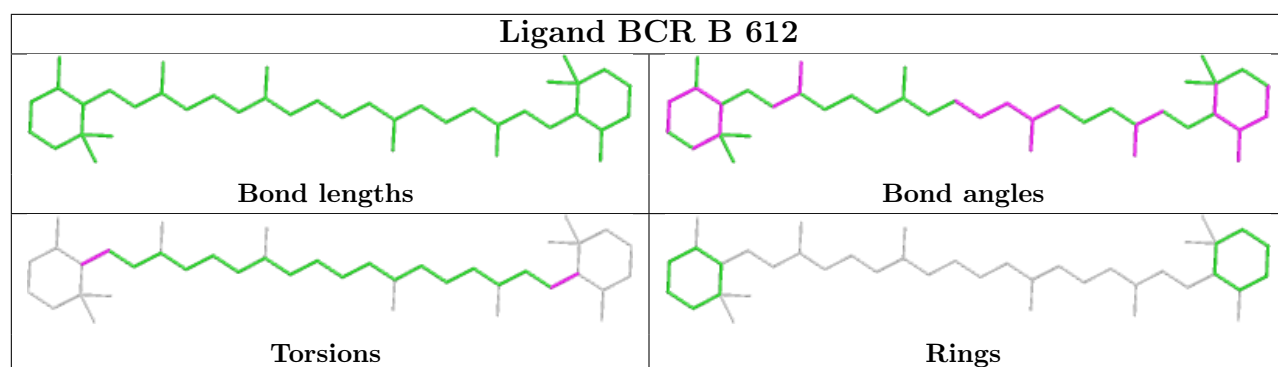
Bond angles



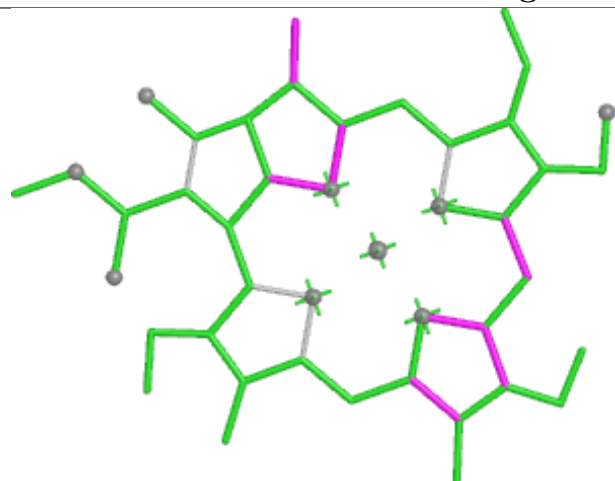
Torsions



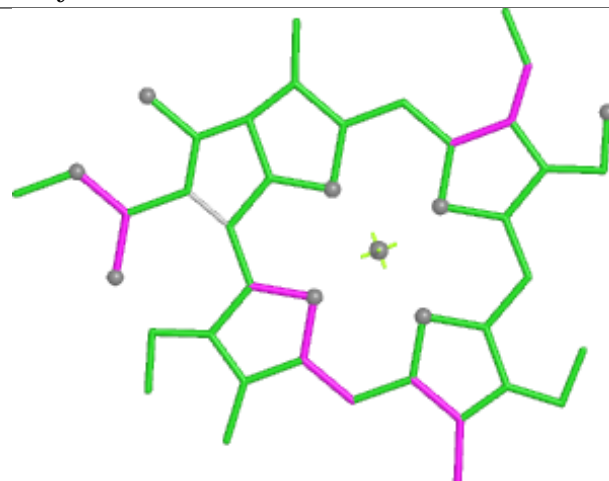
Rings



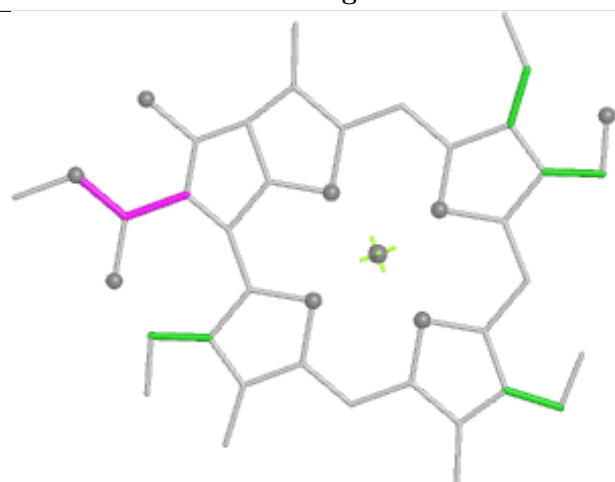
Ligand CHL y 309



Bond lengths



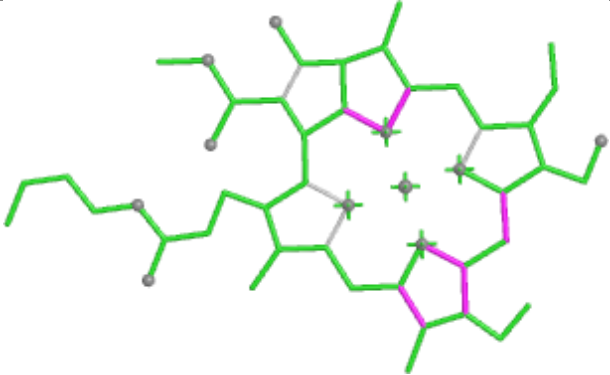
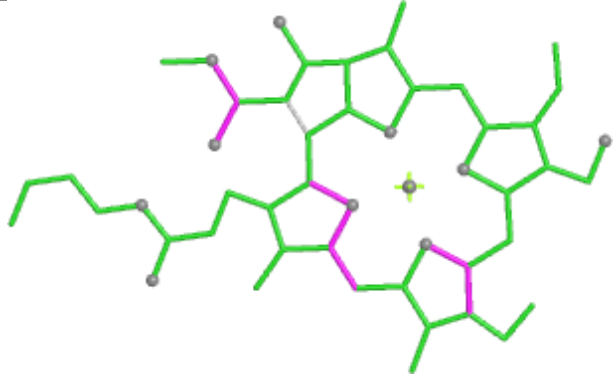
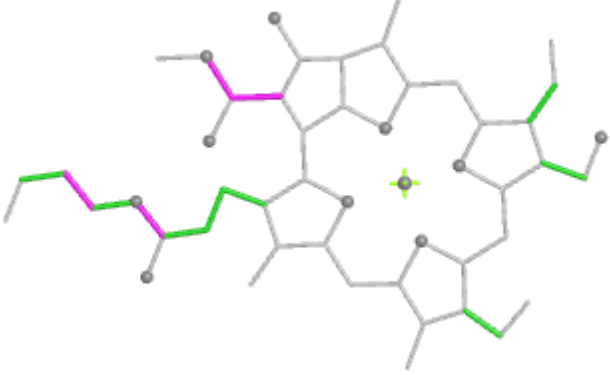
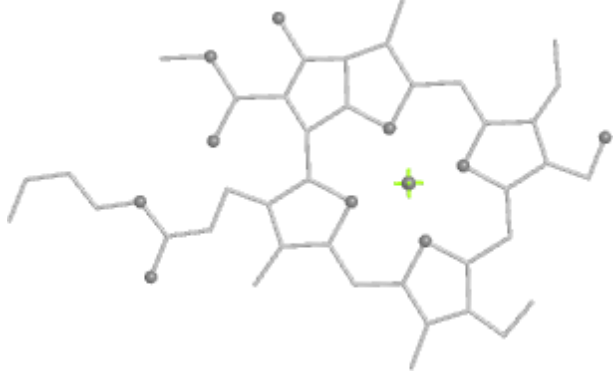
Bond angles

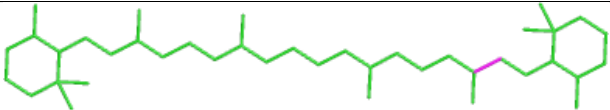
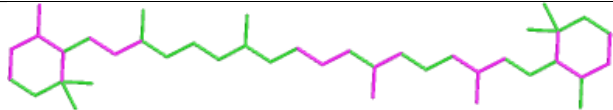
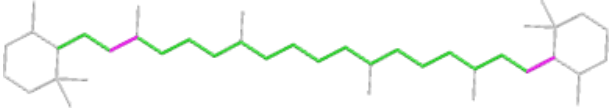
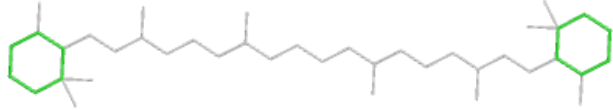


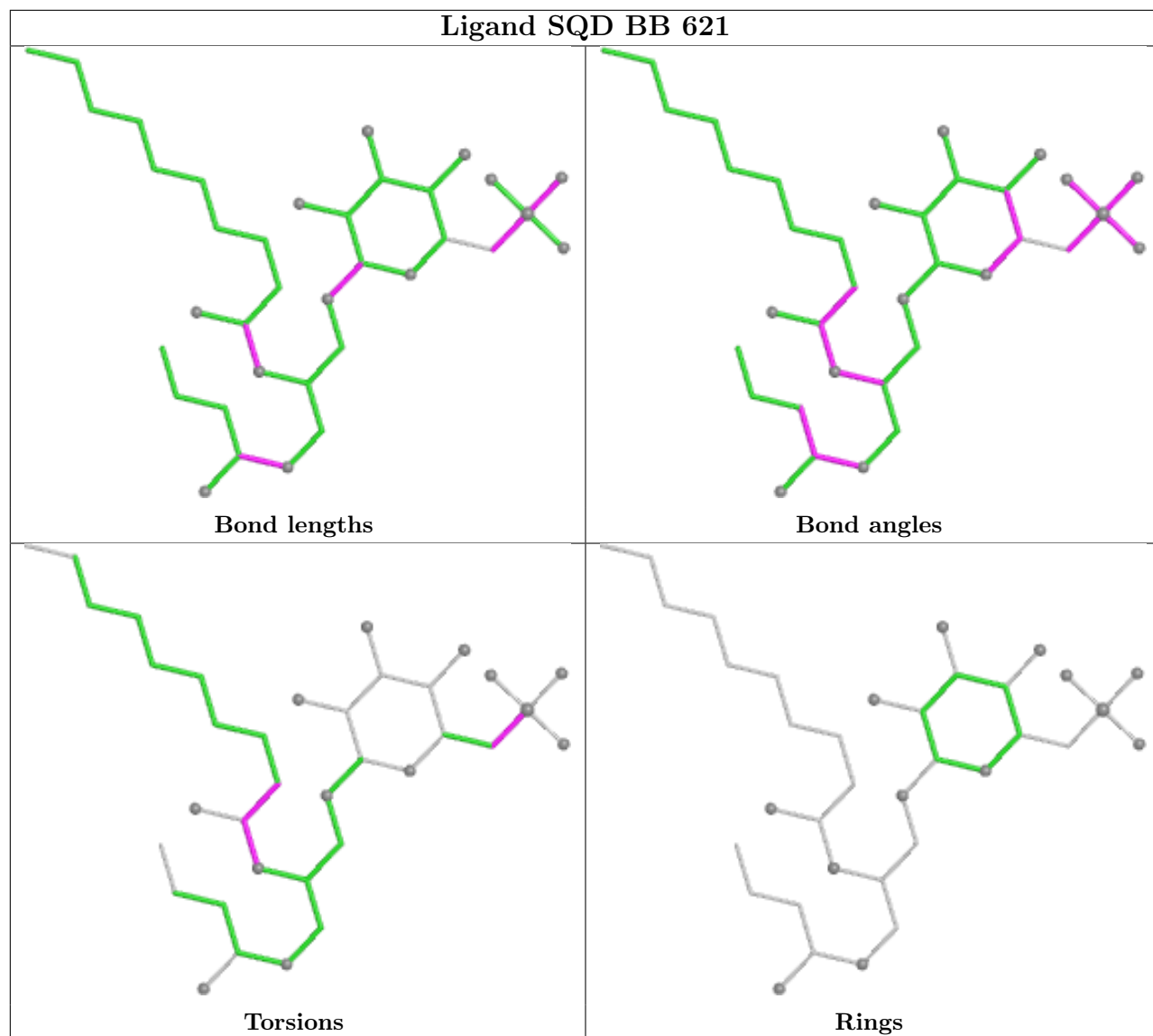
Torsions

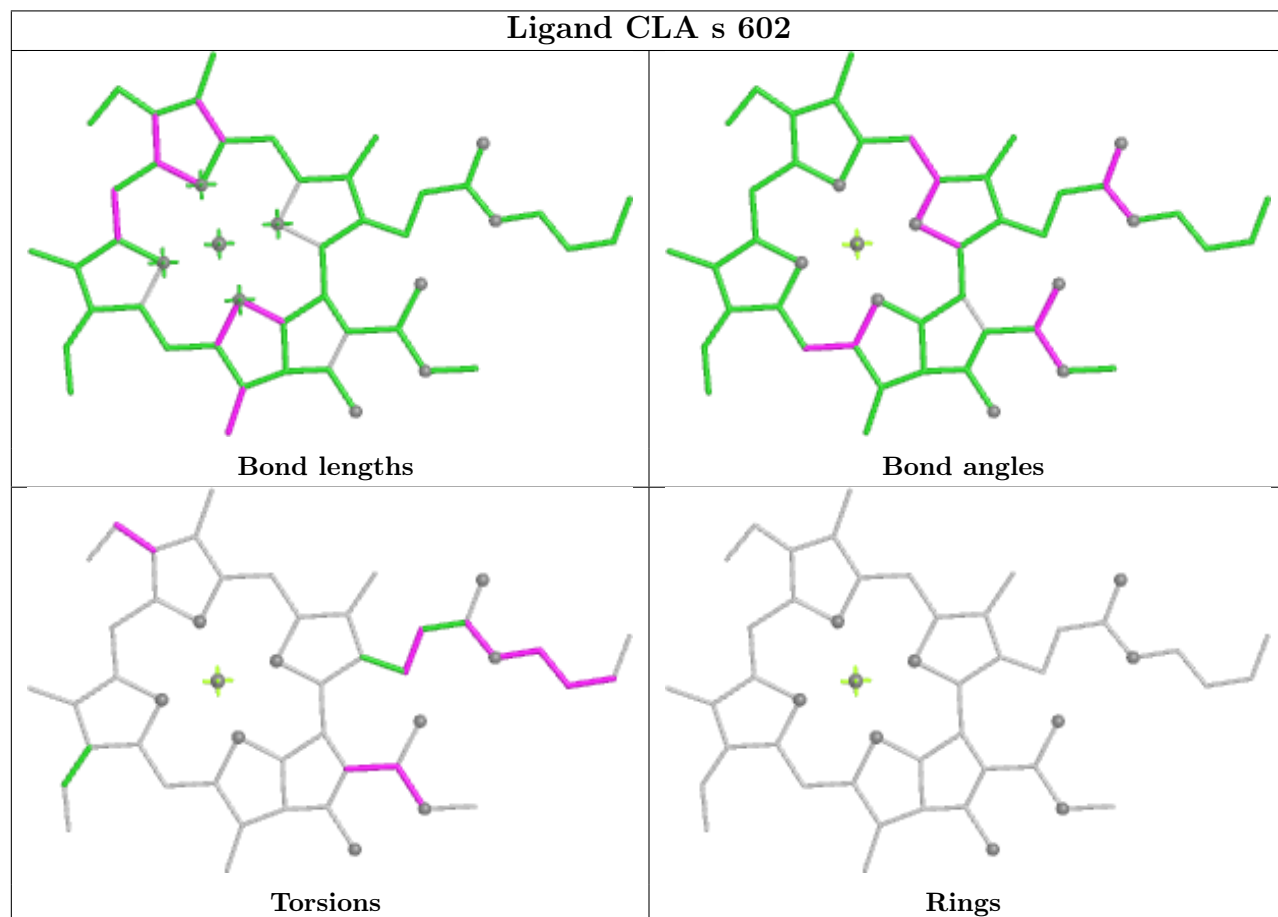
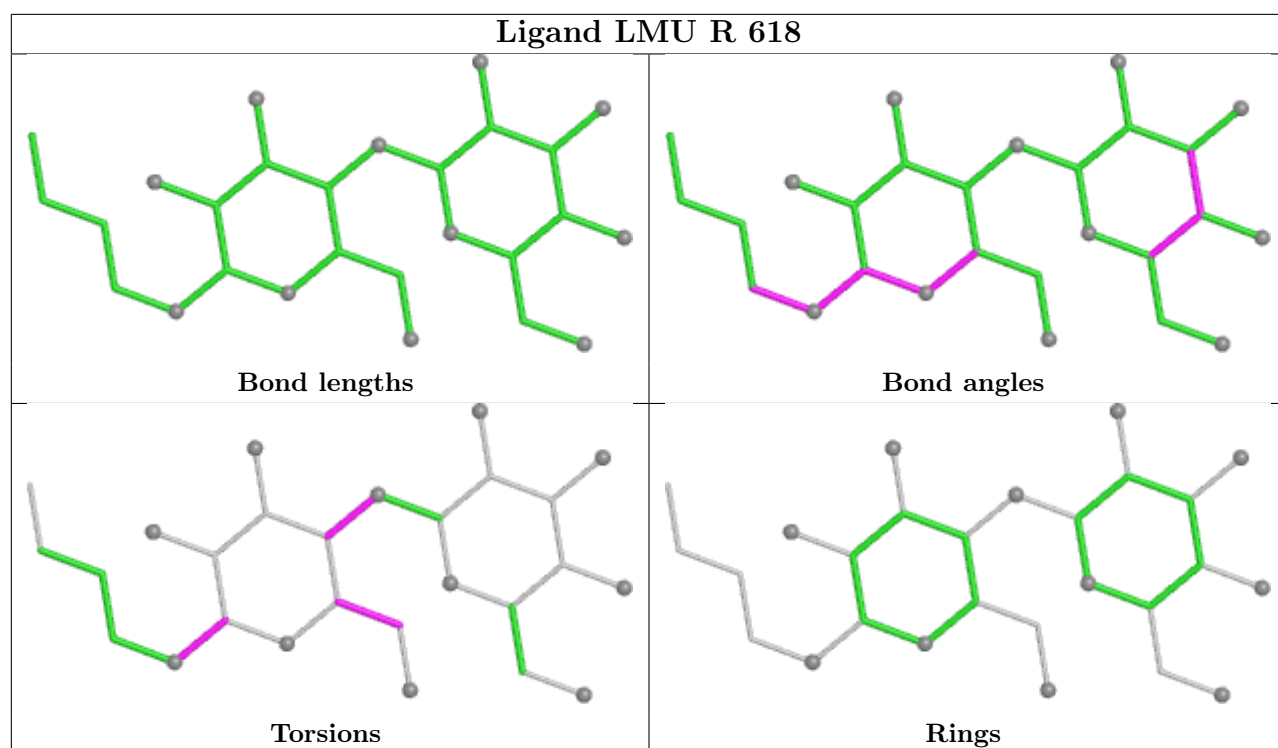


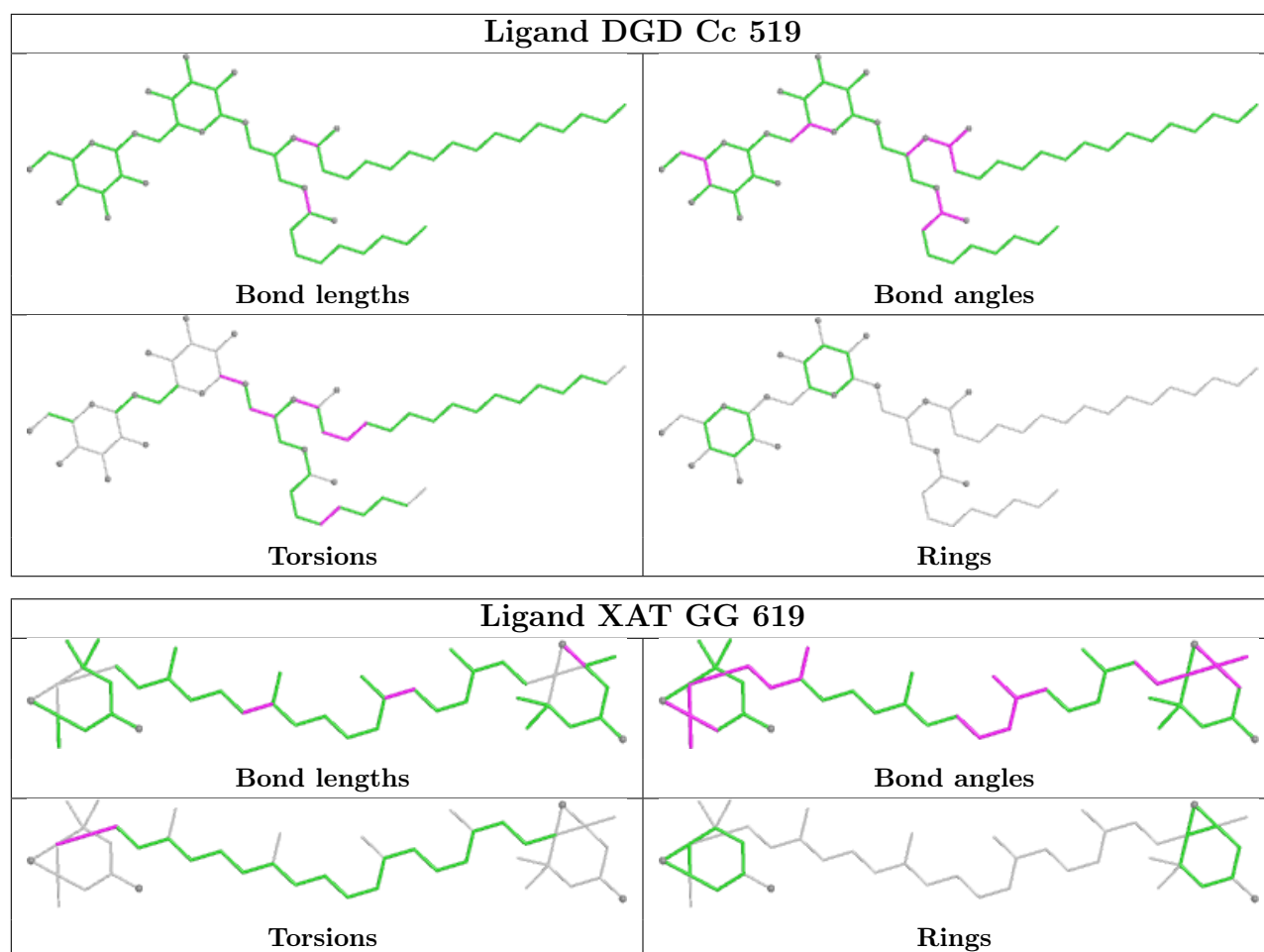
Rings

Ligand CHL Rr 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

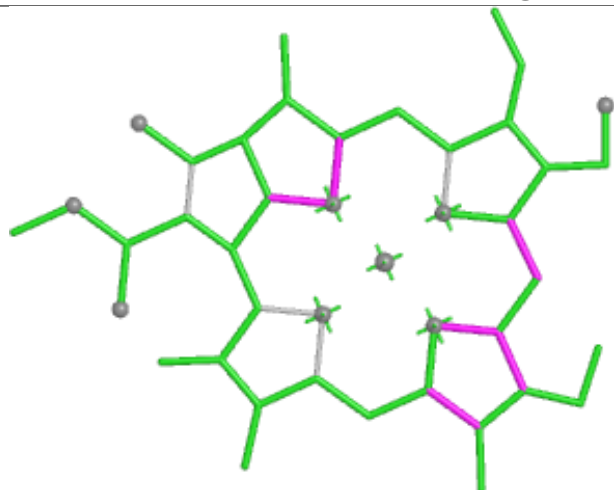
Ligand BCR Cc 518	
	
Bond lengths	Bond angles
	
Torsions	Rings



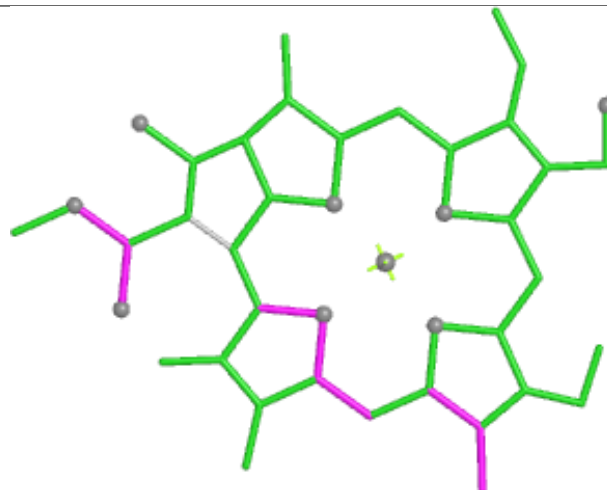




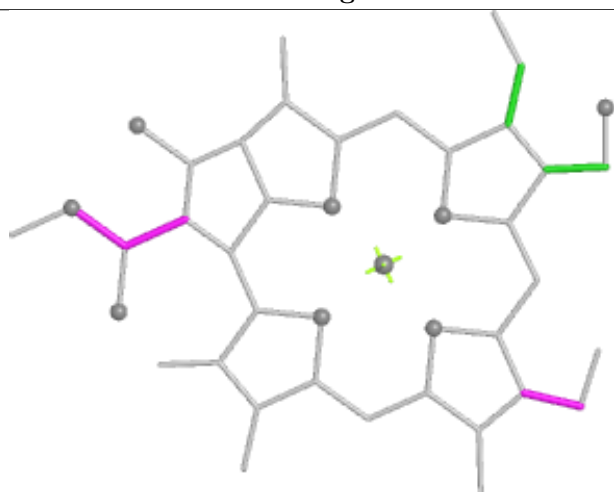
Ligand CHL S 605



Bond lengths



Bond angles

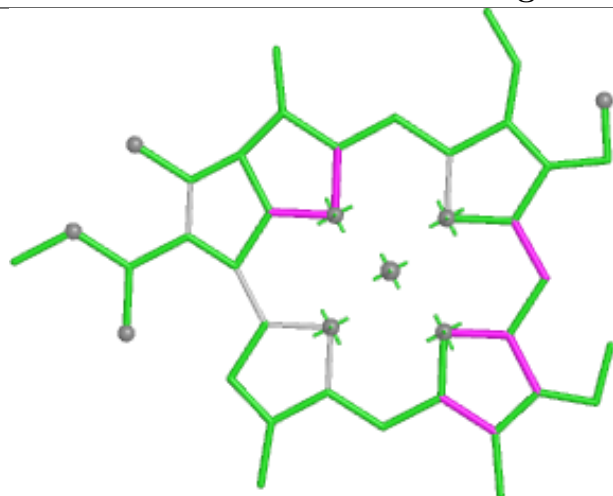


Torsions

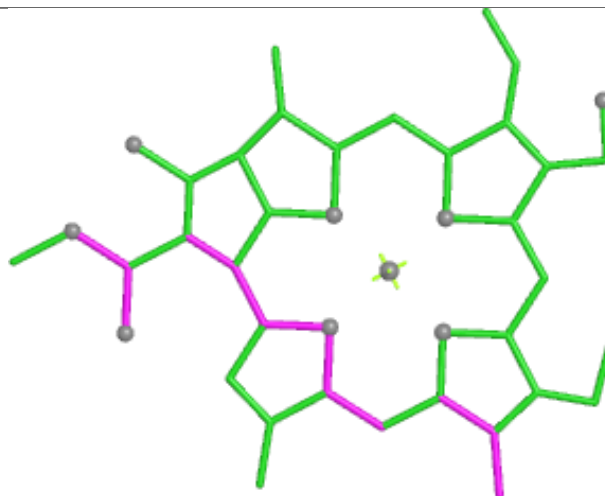


Rings

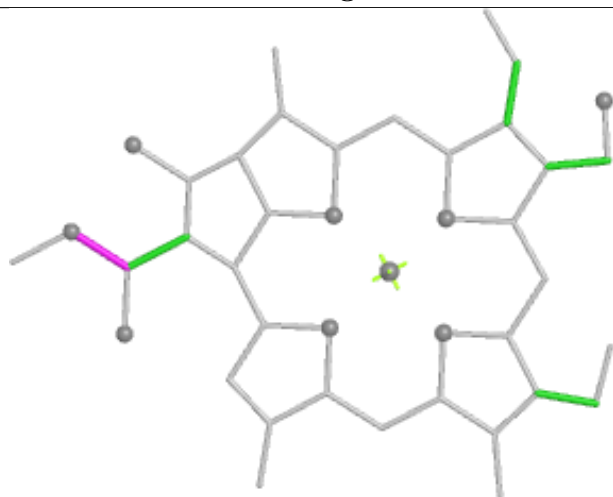
Ligand CHL 3 607



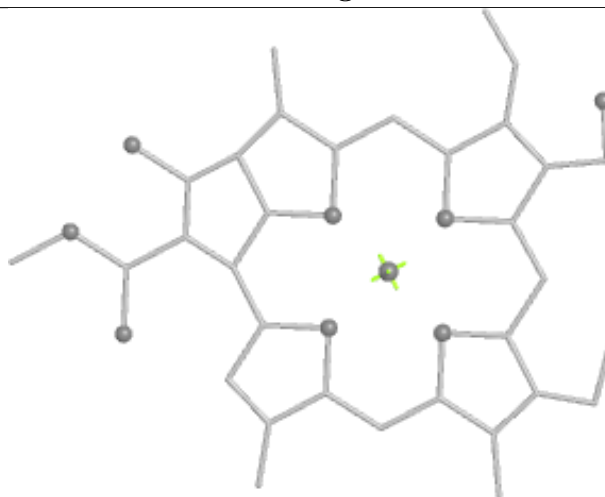
Bond lengths



Bond angles

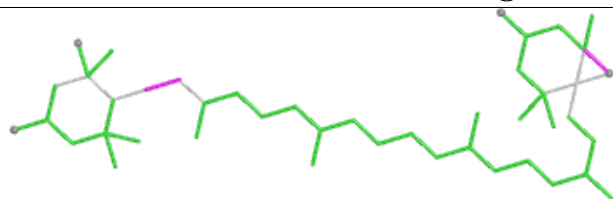


Torsions

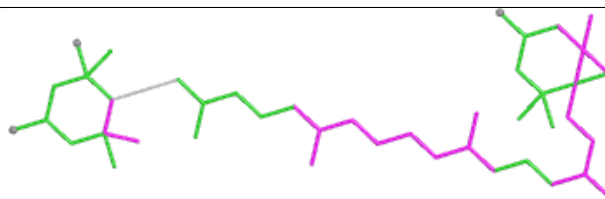


Rings

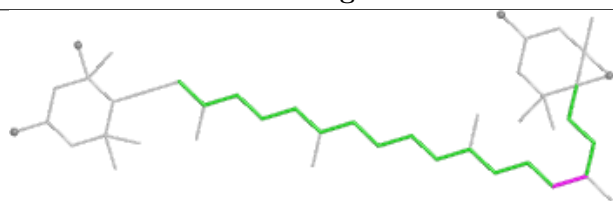
Ligand NEX YY 617



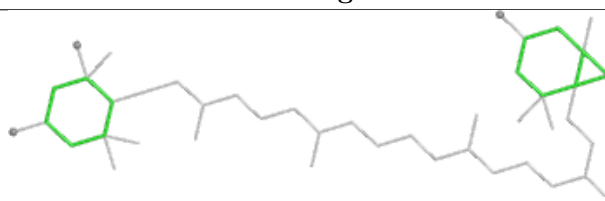
Bond lengths



Bond angles

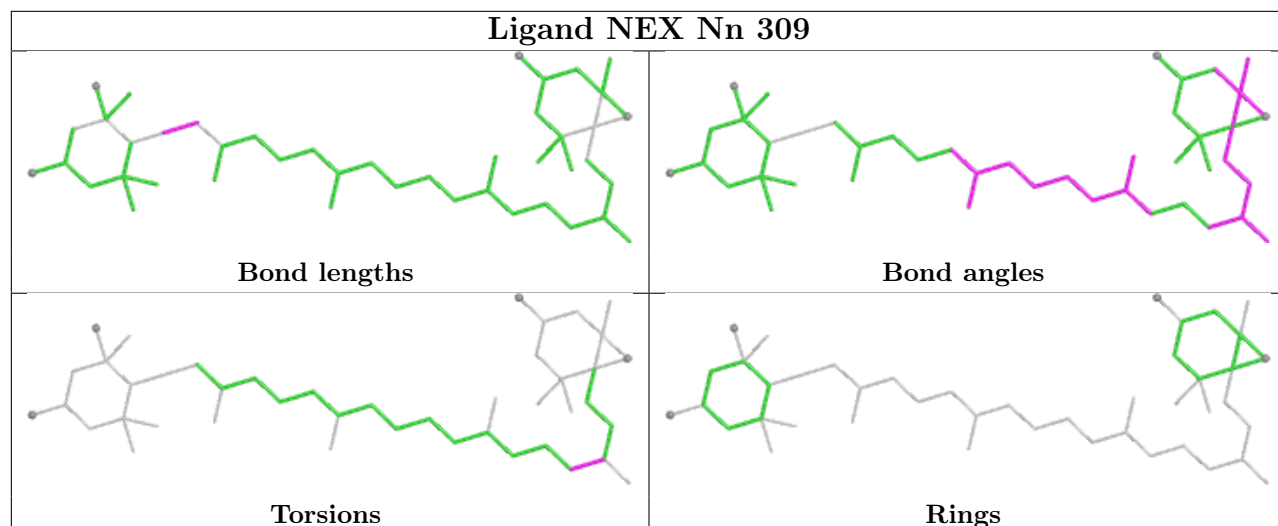


Torsions

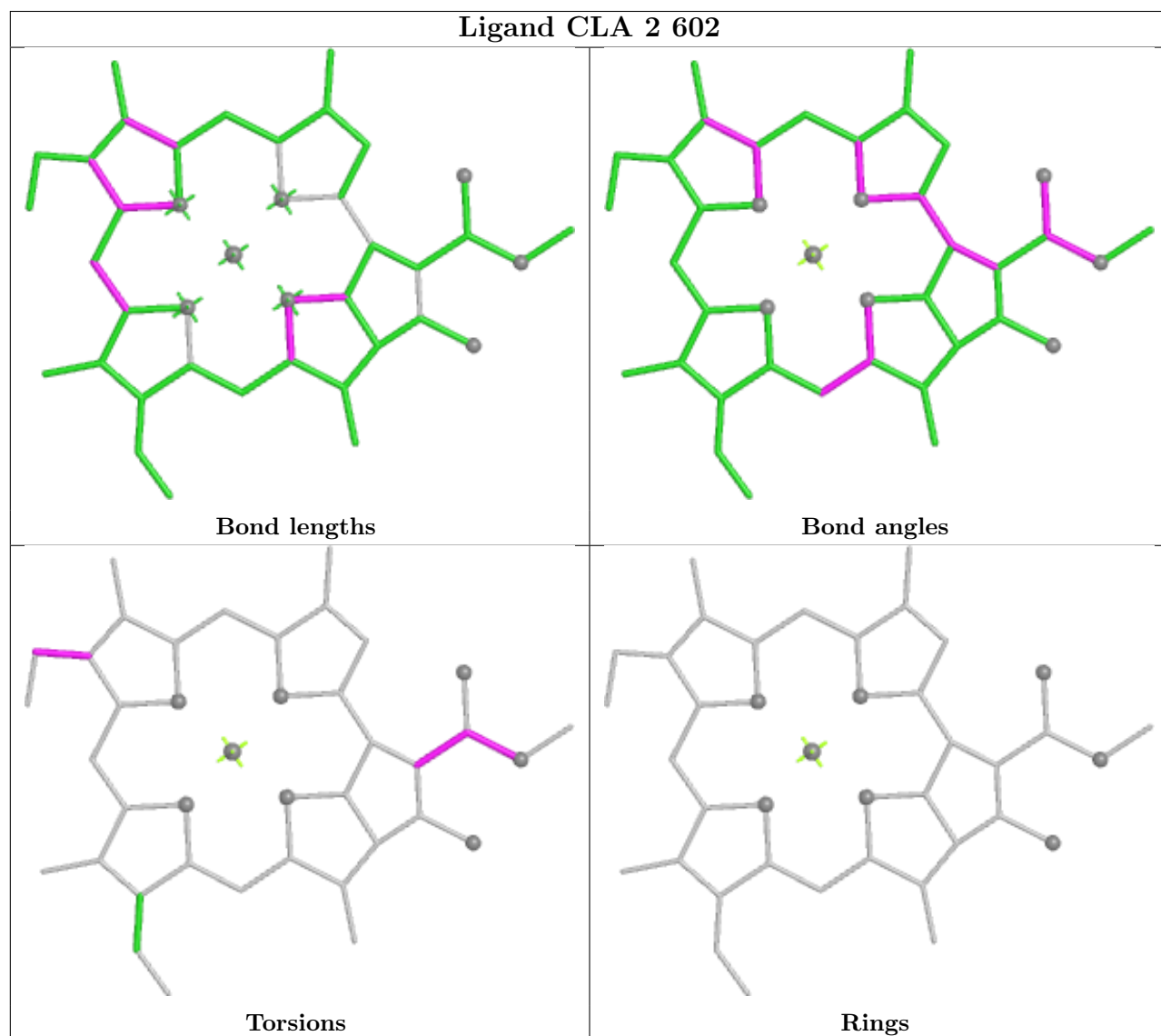


Rings

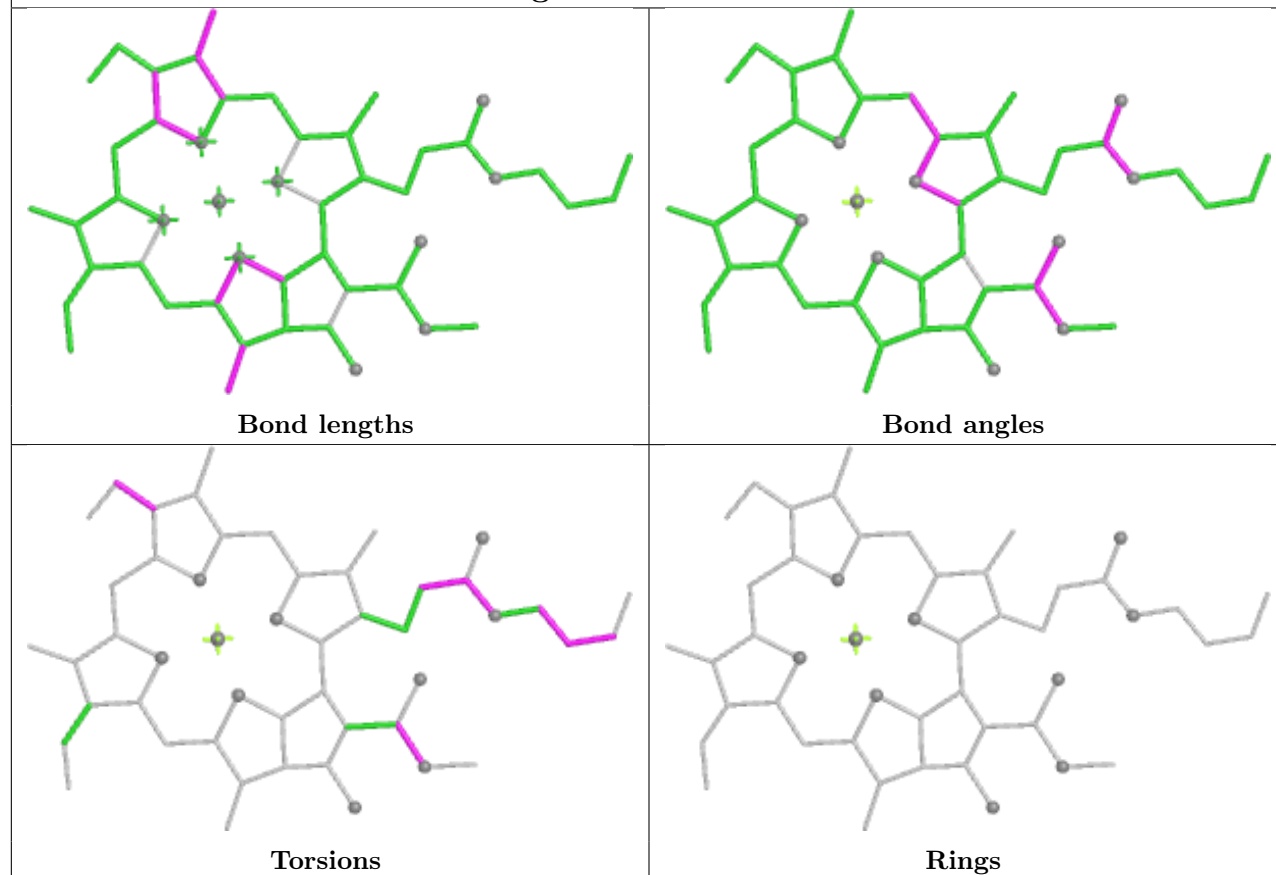
Ligand NEX Nn 309



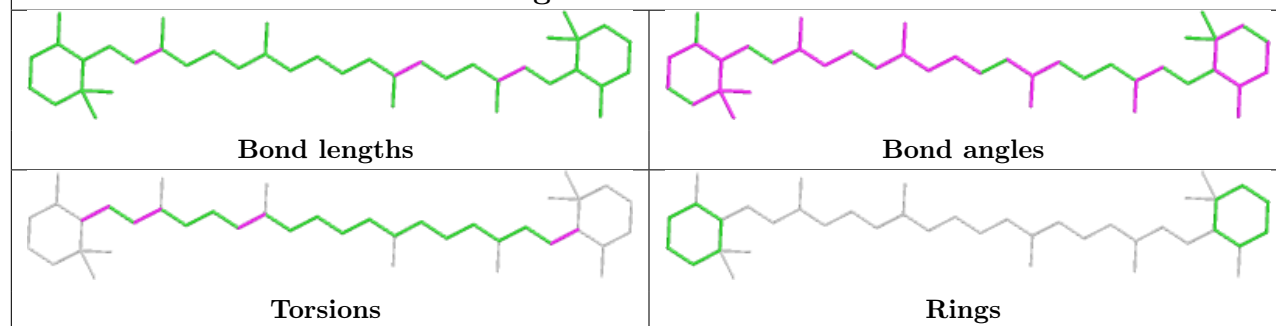
Ligand CLA 2 602

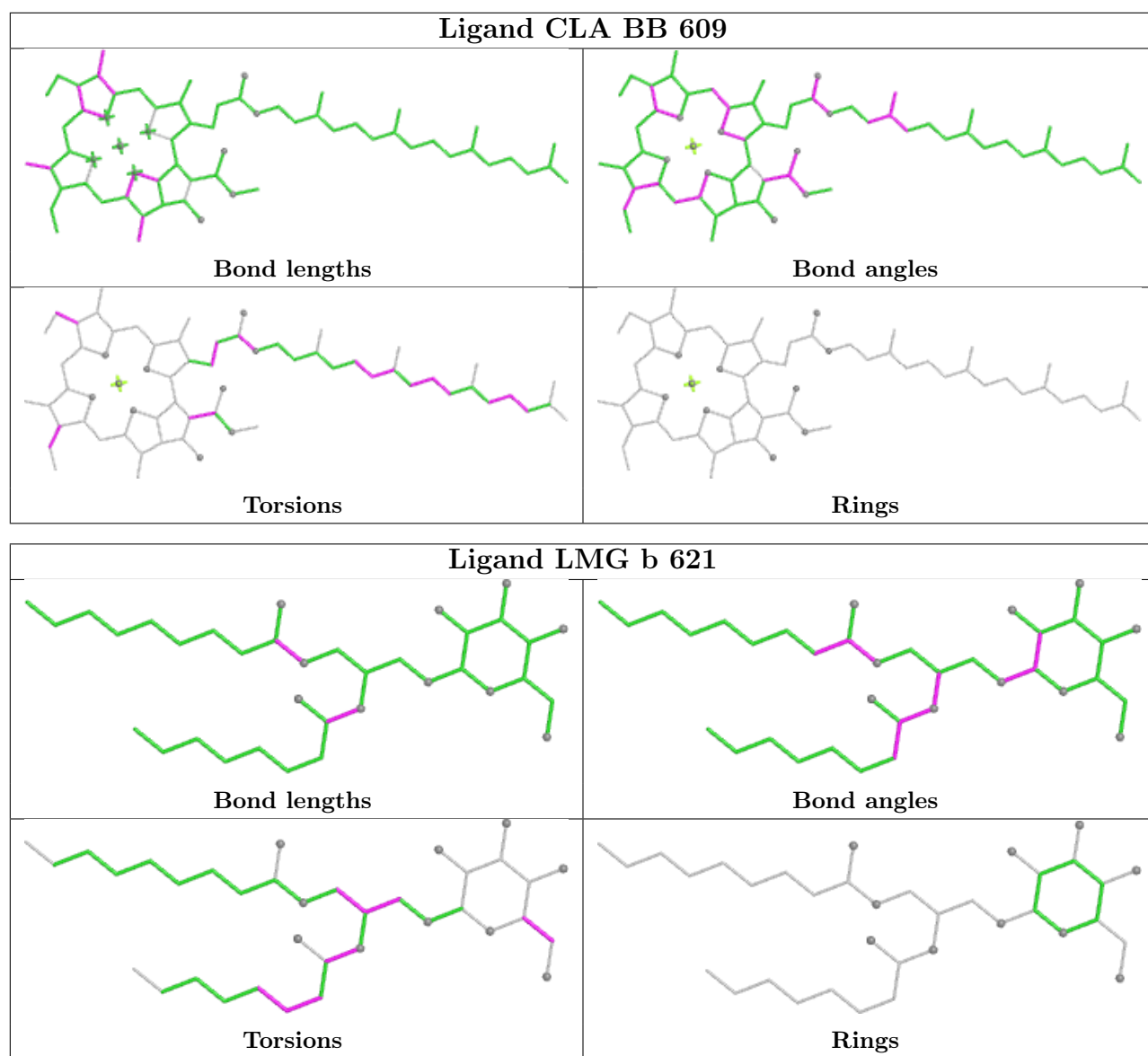


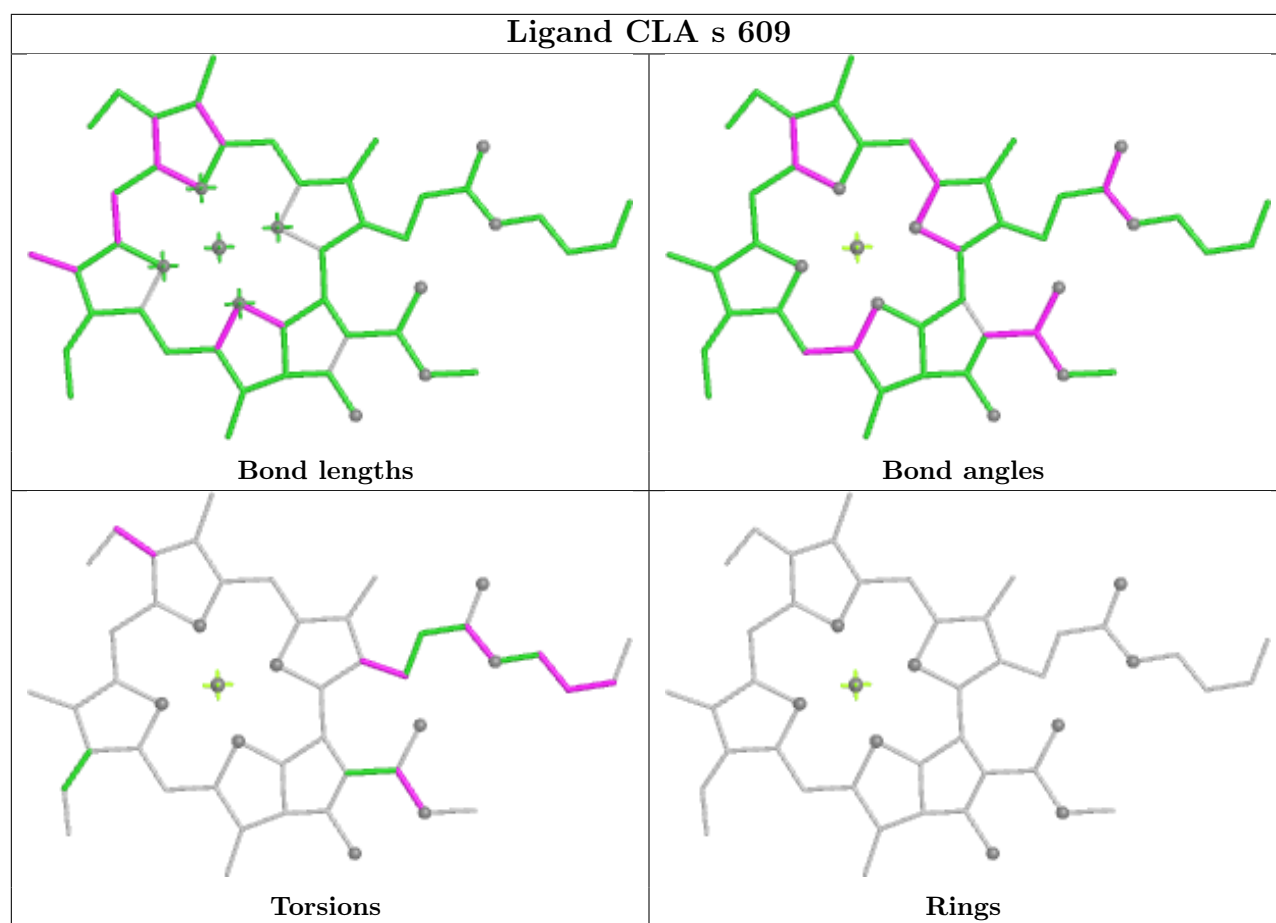
Ligand CLA Y 603

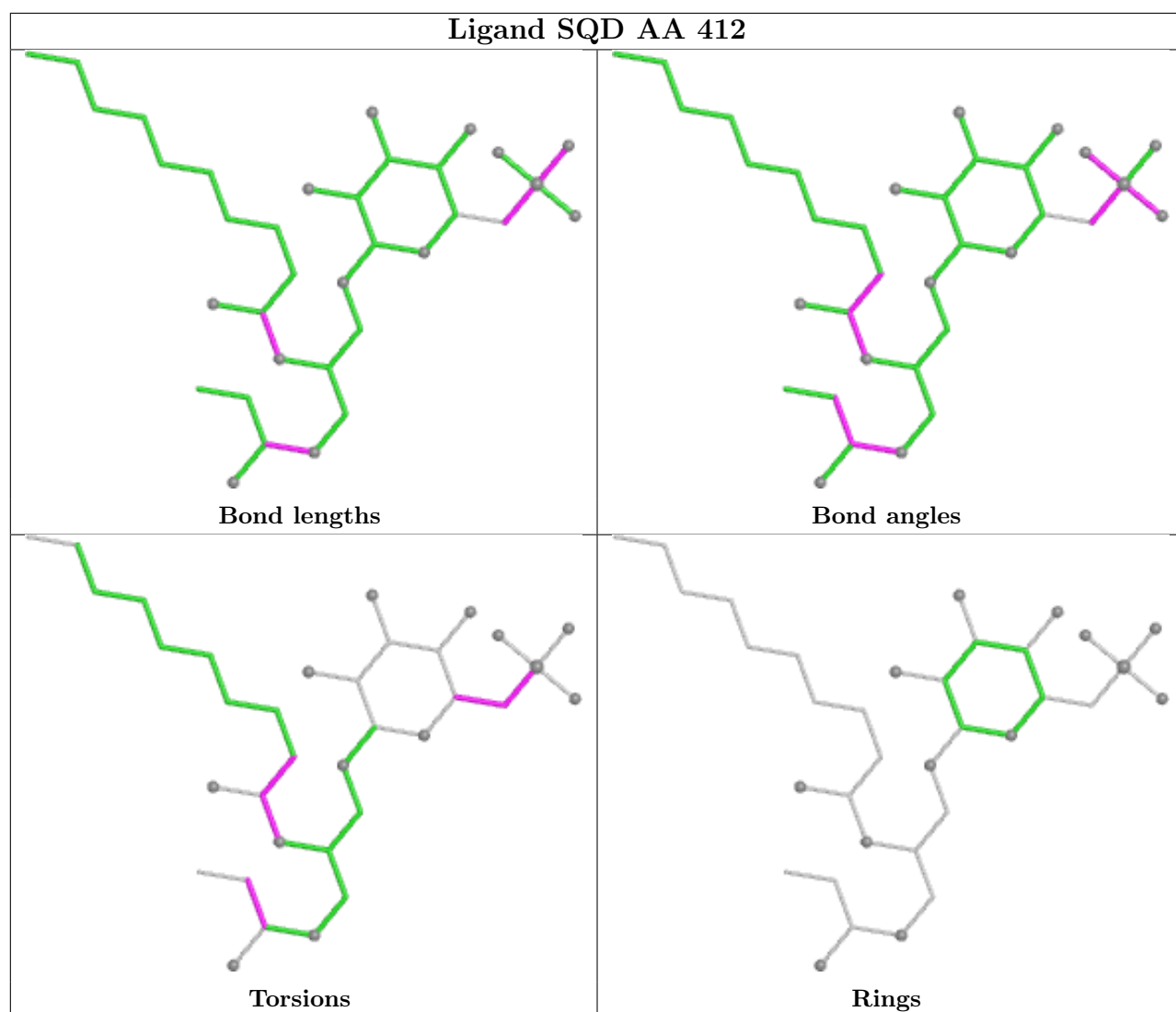


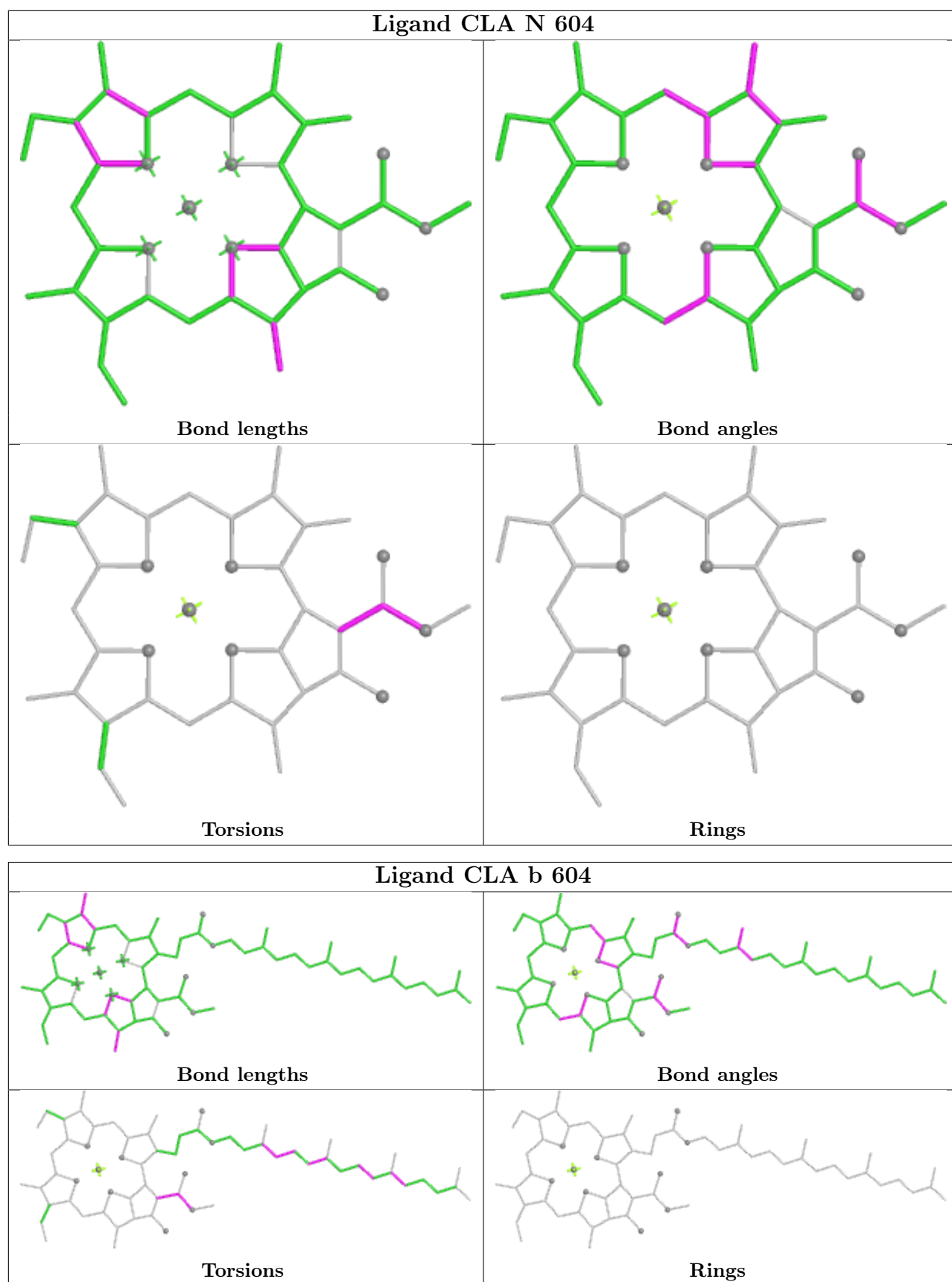
Ligand BCR h 101

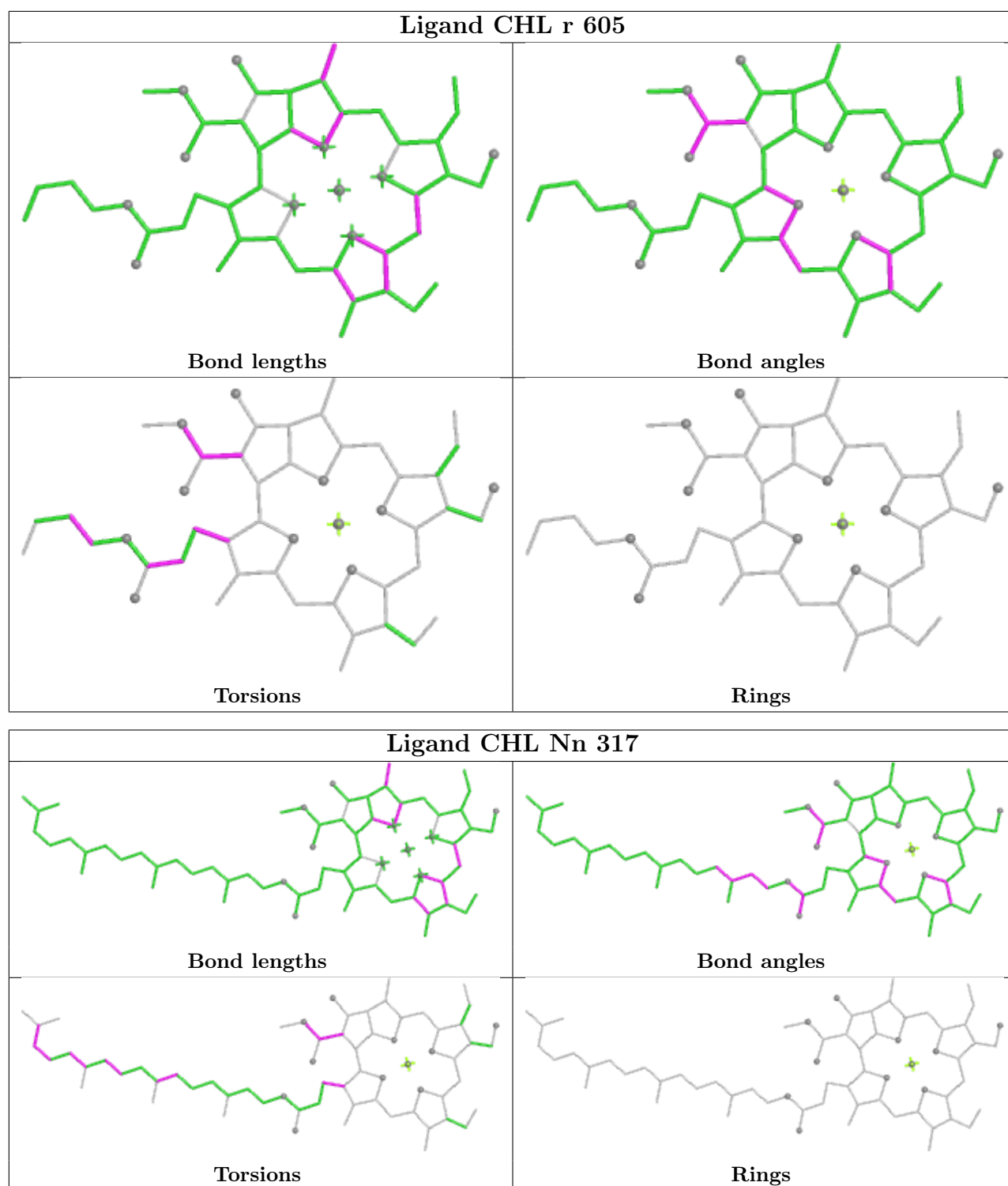


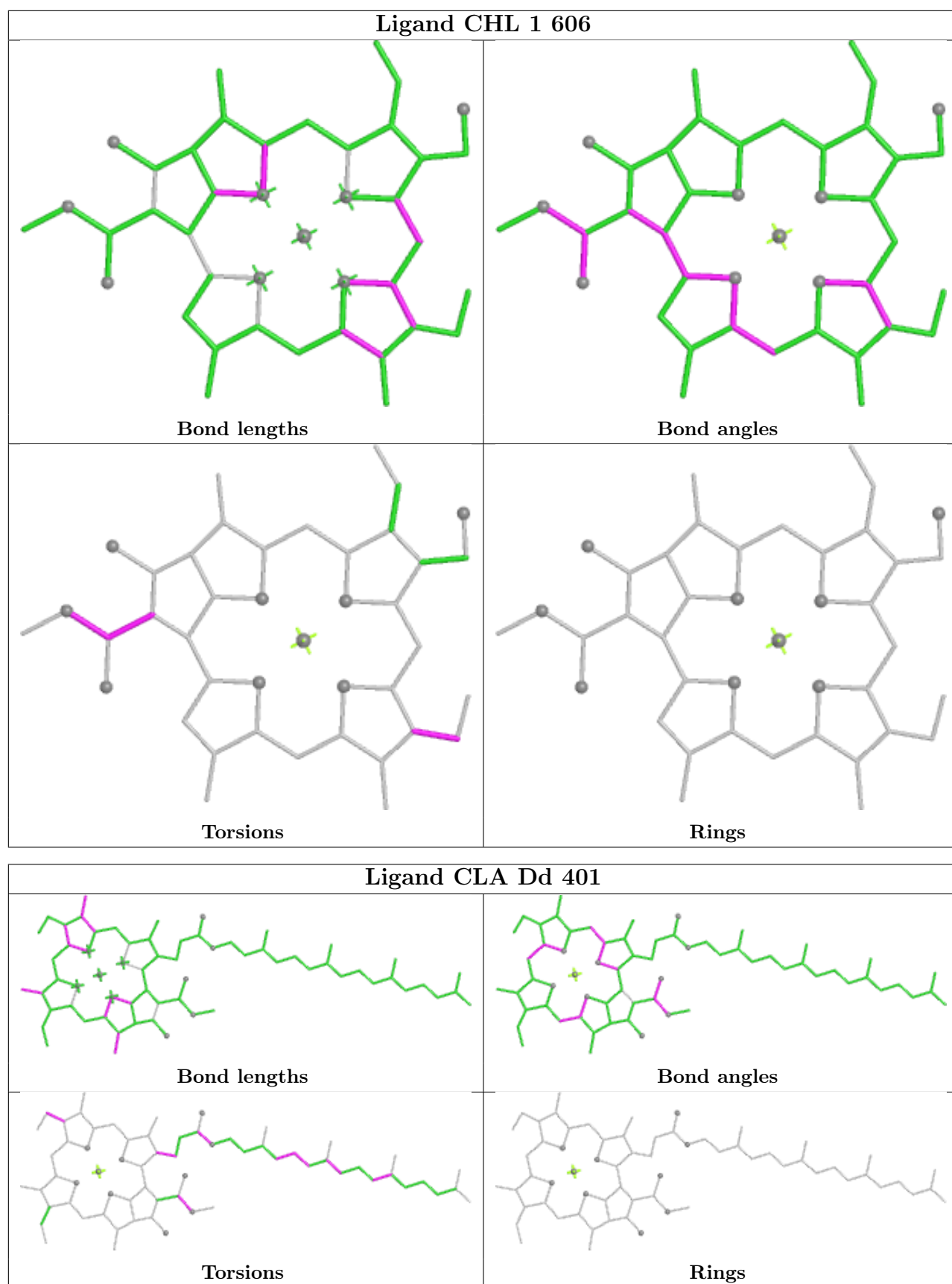


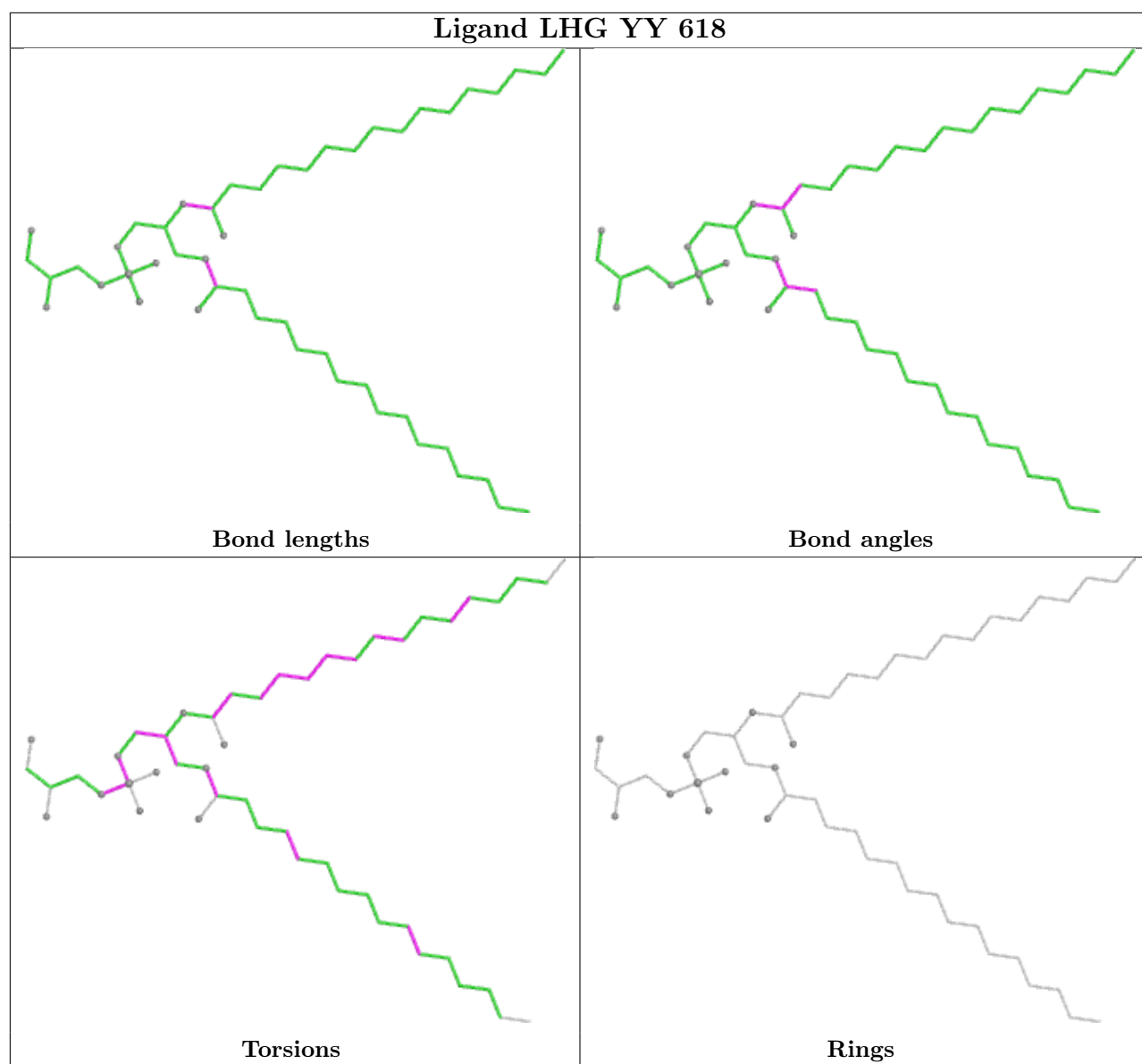




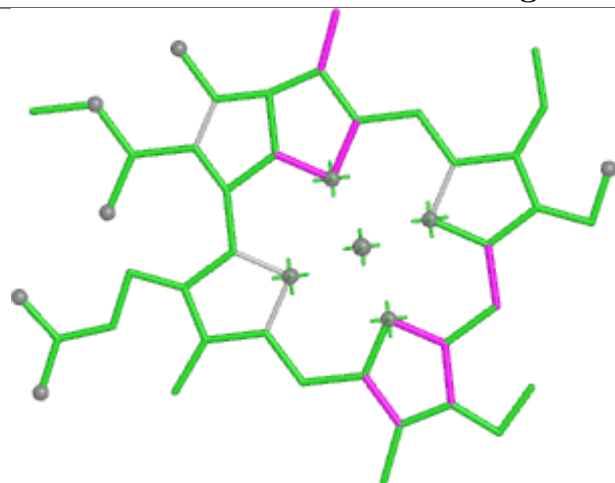




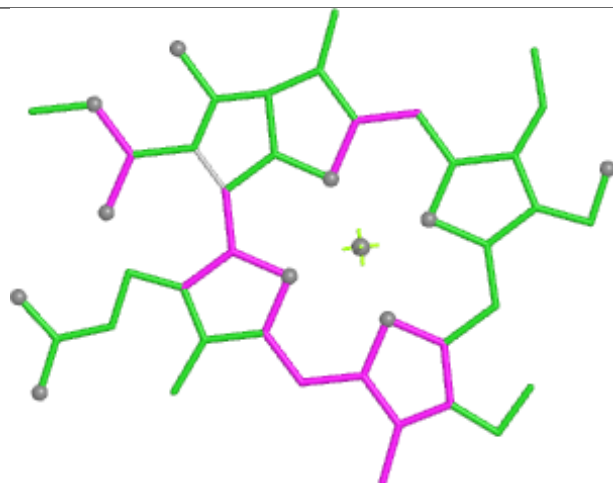




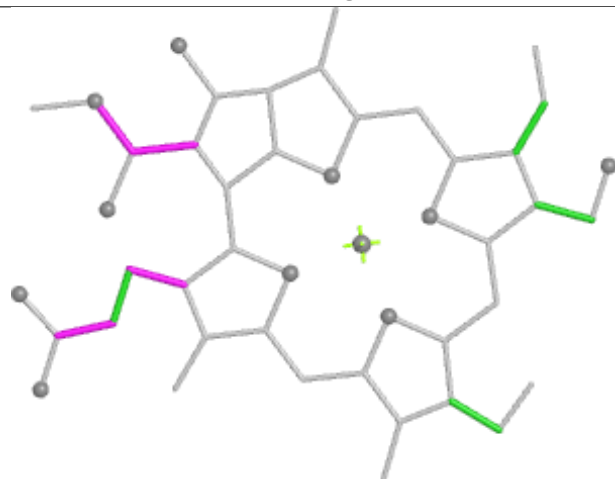
Ligand CHL 4 309



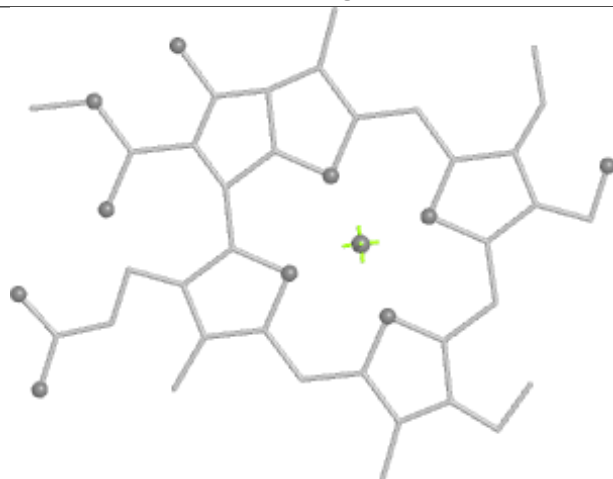
Bond lengths



Bond angles

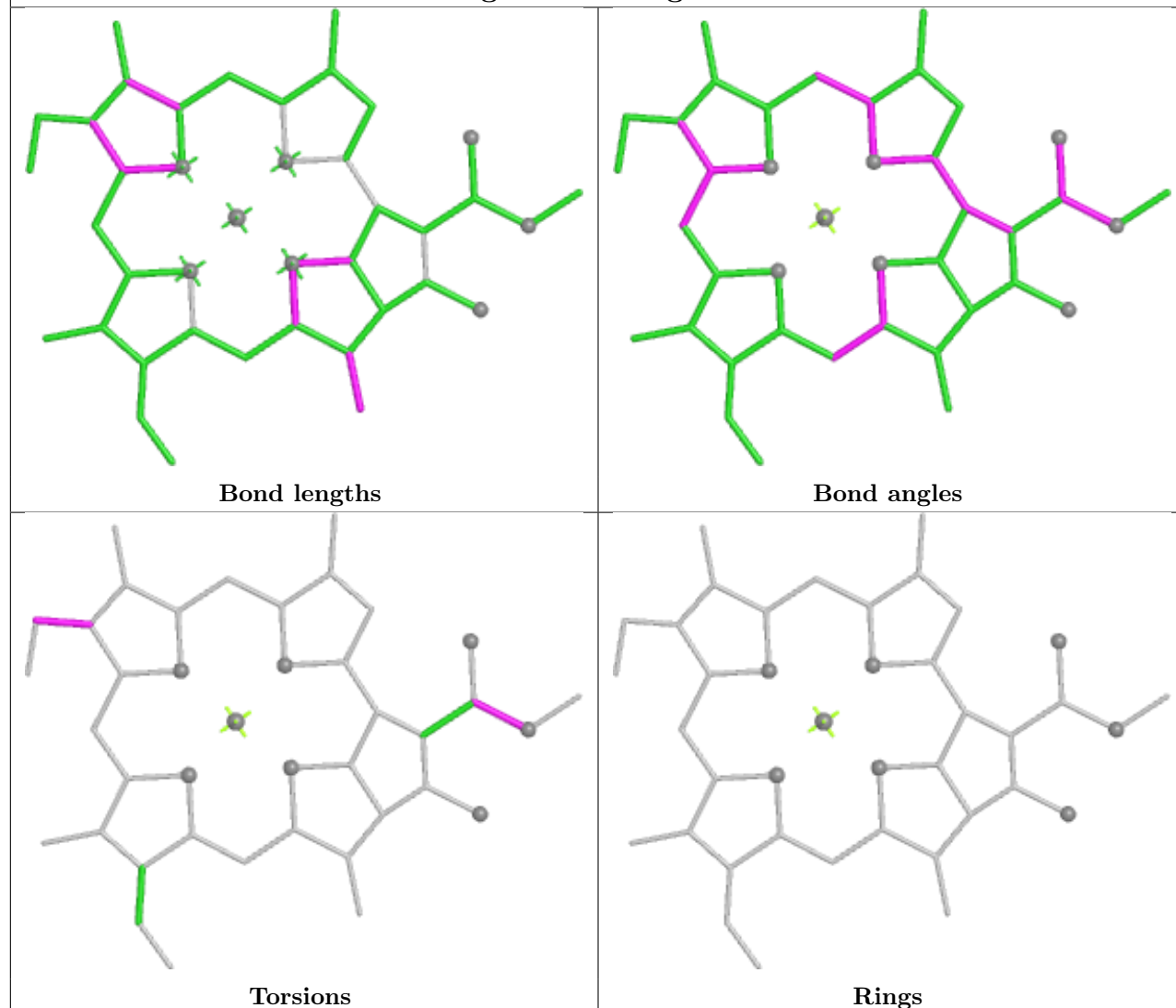


Torsions

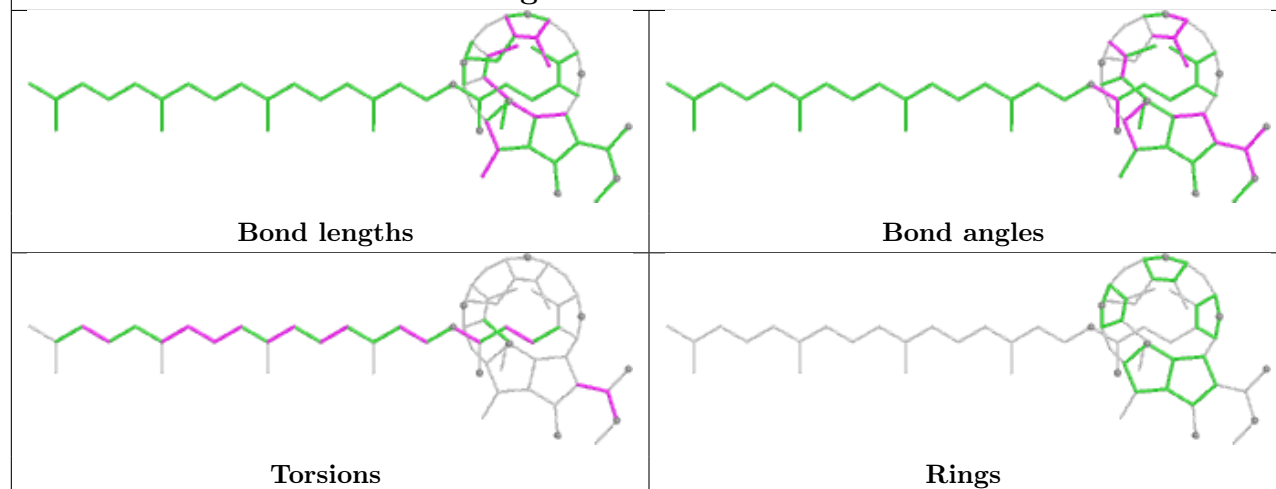


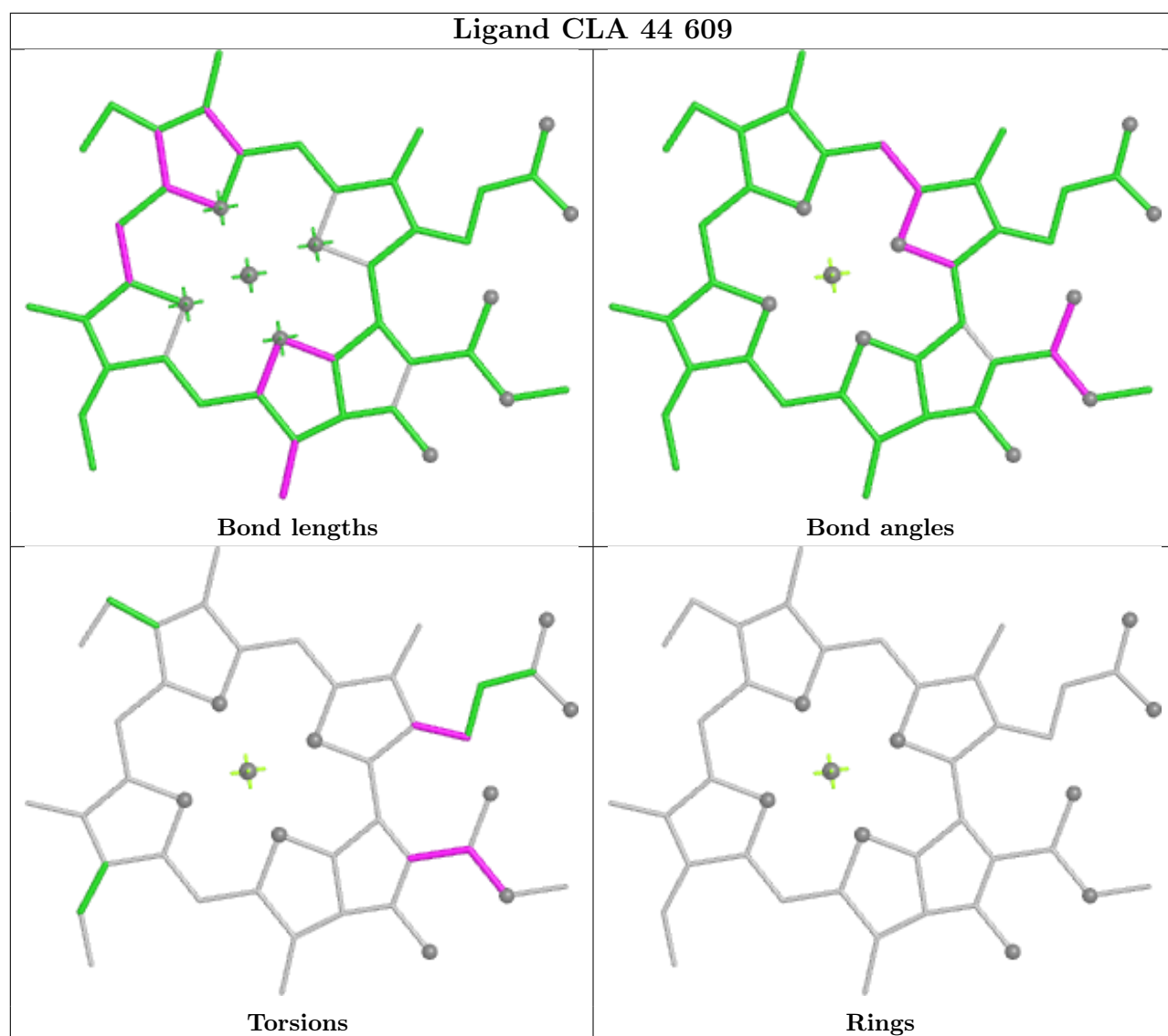
Rings

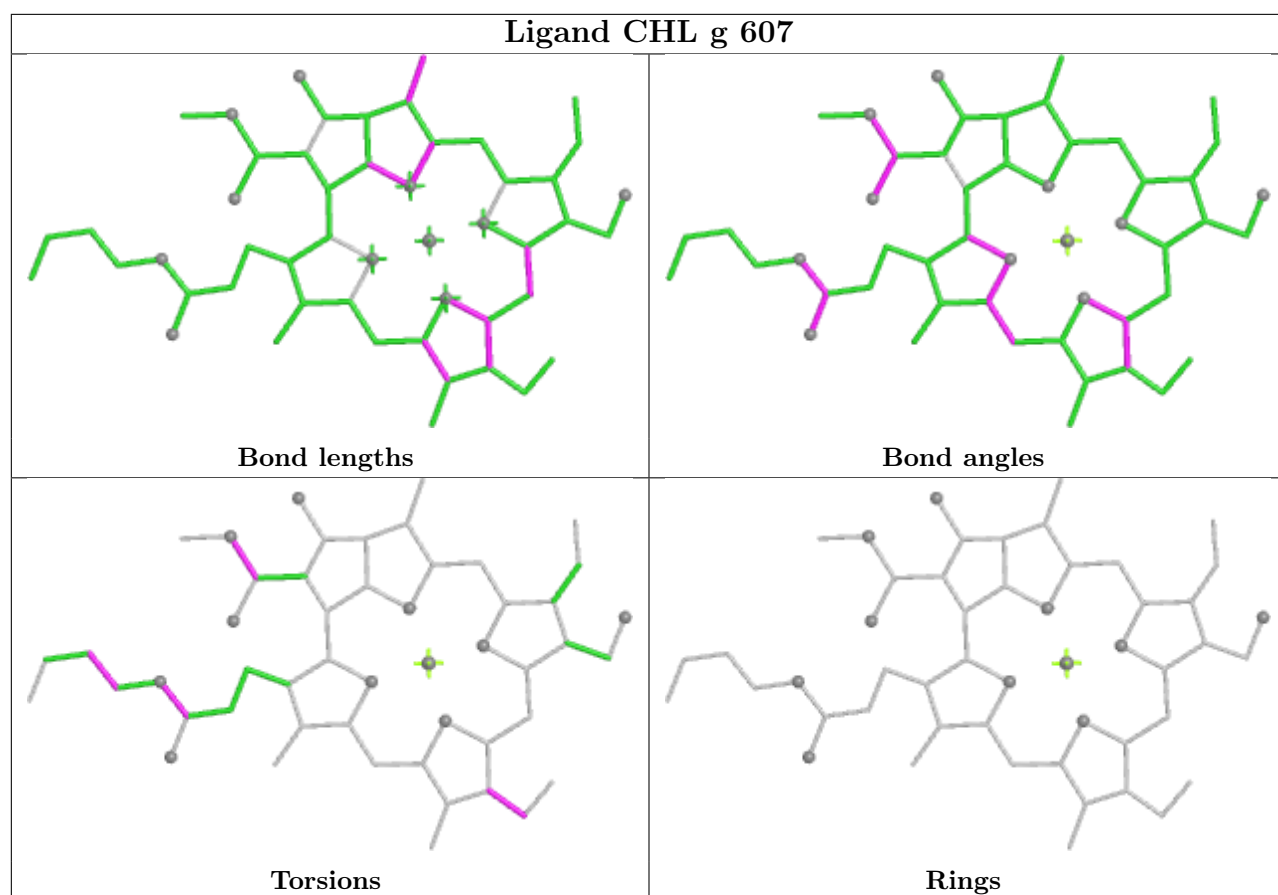
Ligand CLA Gg 314

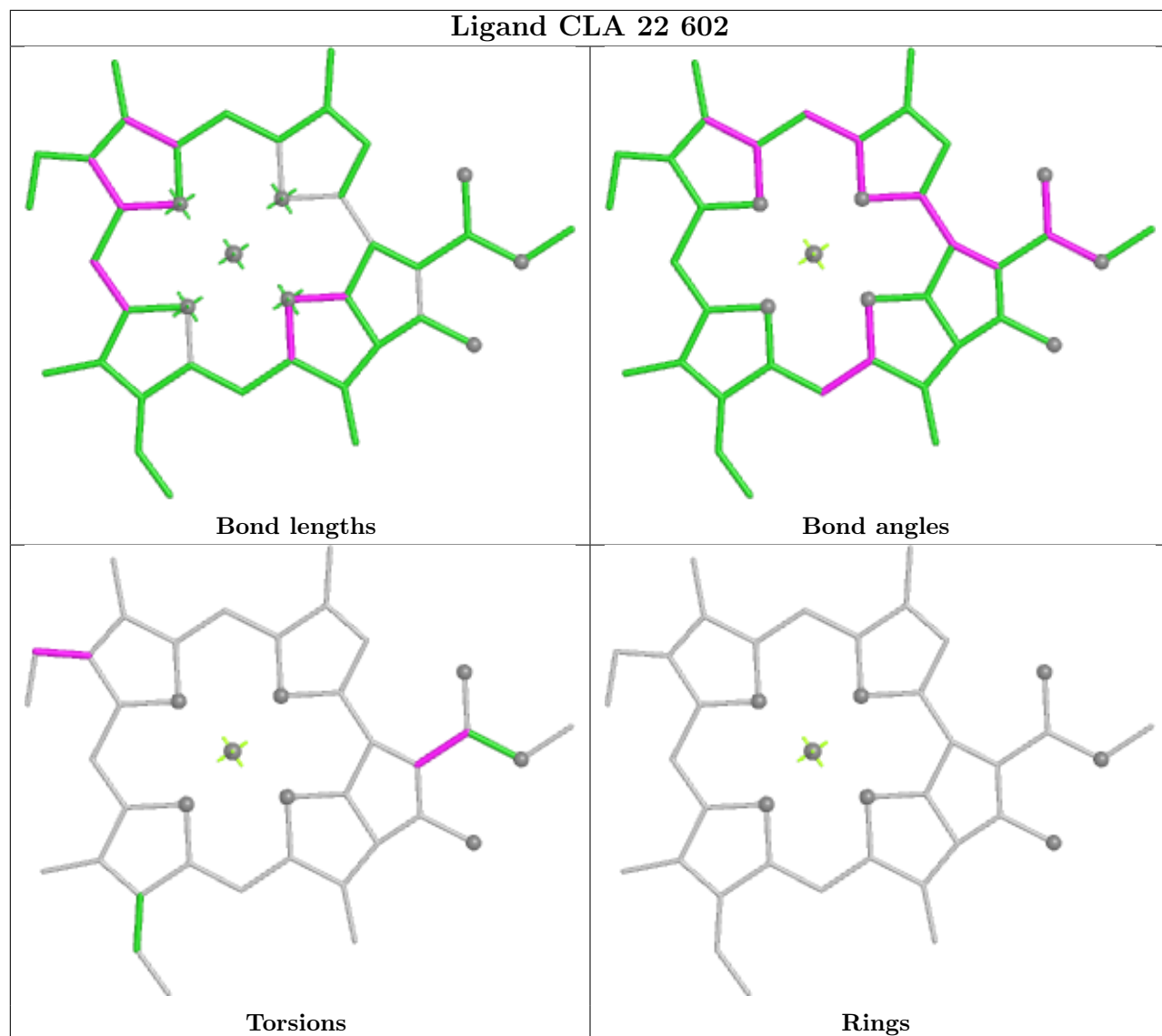


Ligand PHO Aa 409

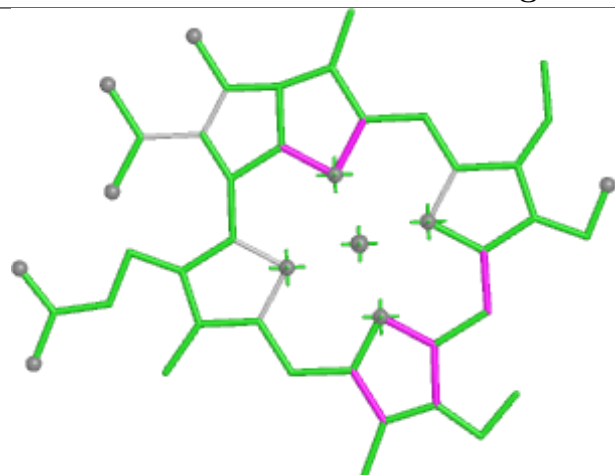




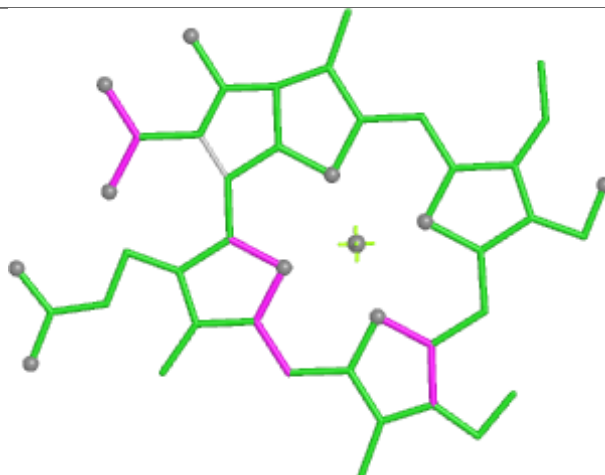




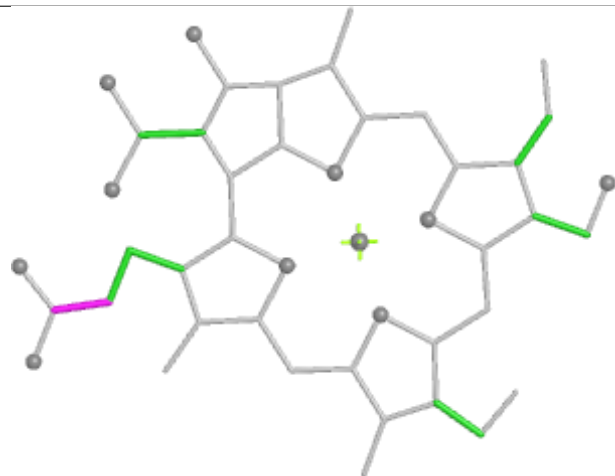
Ligand CHL 4 302



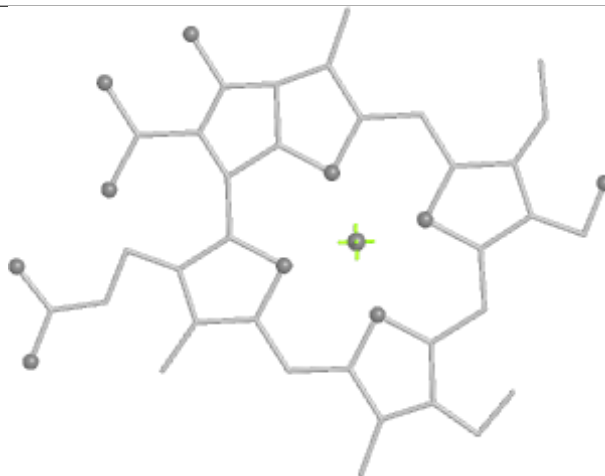
Bond lengths



Bond angles

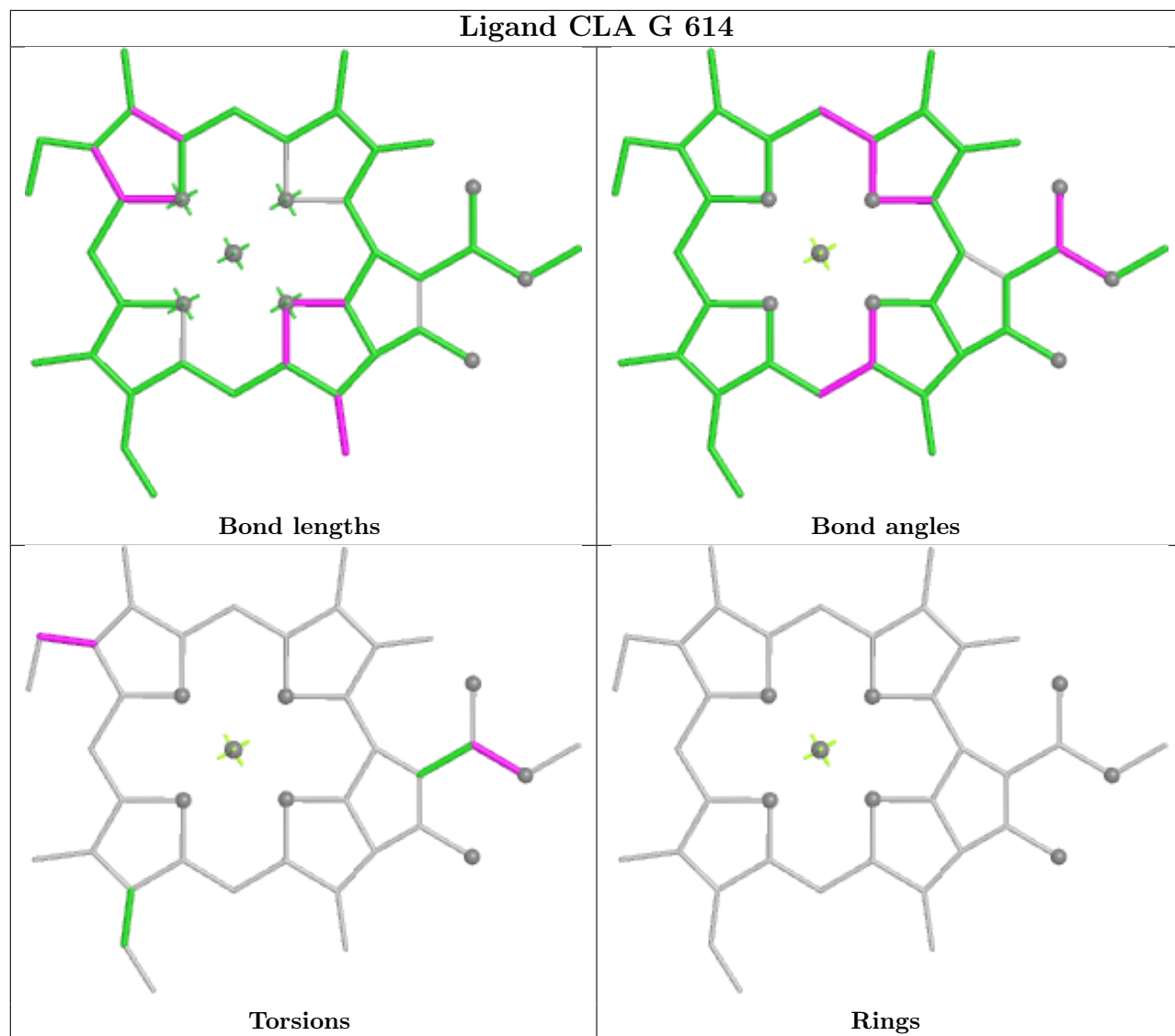


Torsions

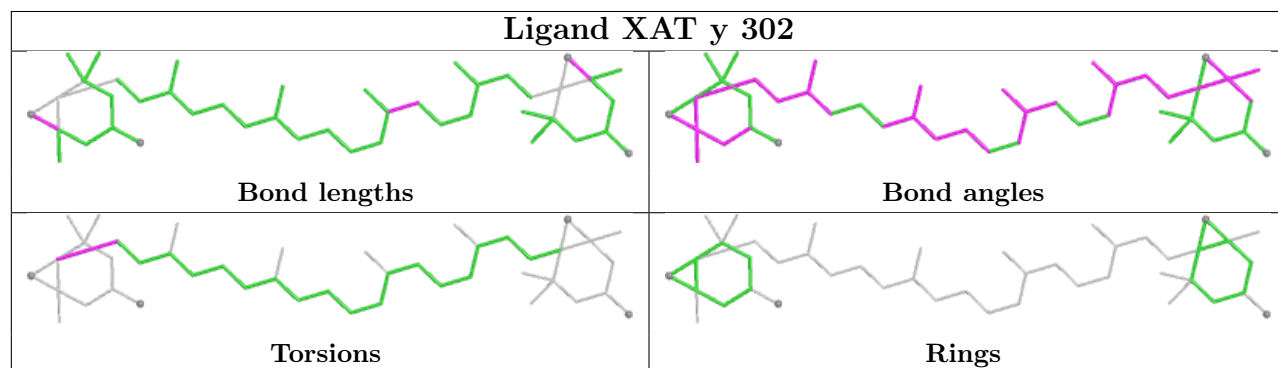


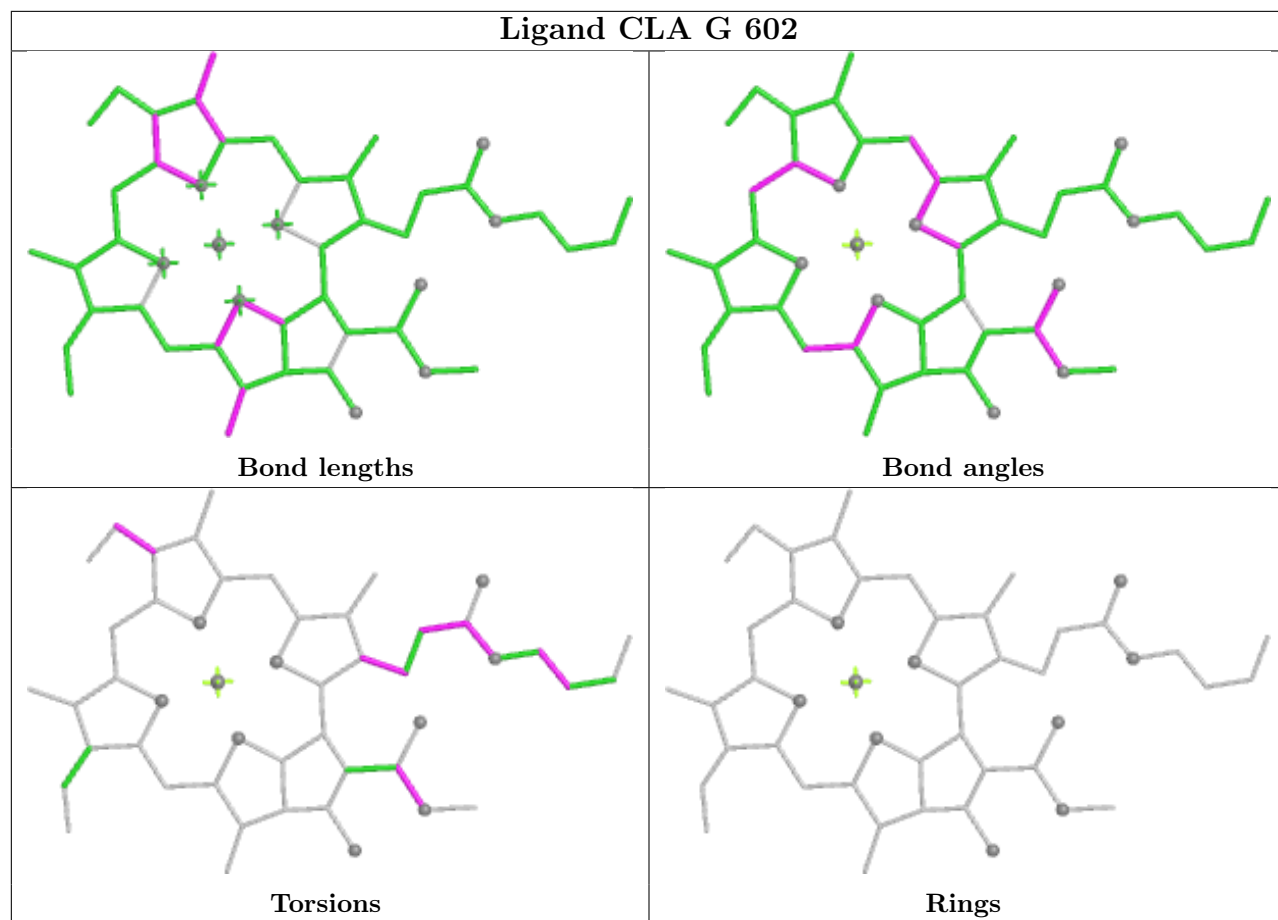
Rings

Ligand CLA G 614

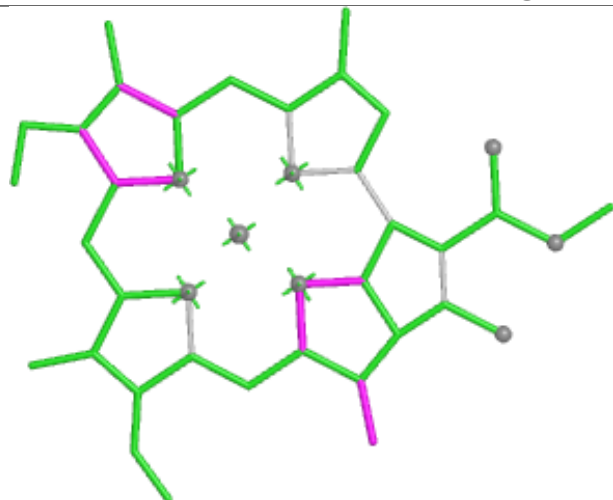


Ligand XAT y 302

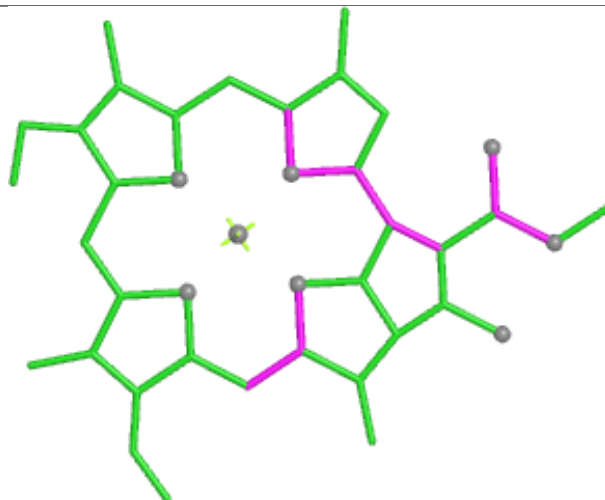




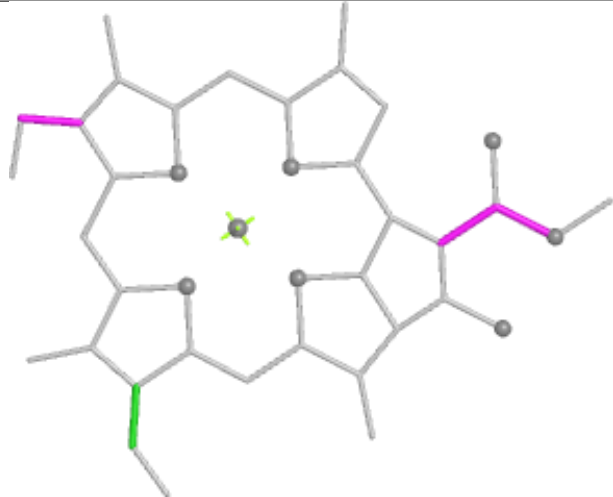
Ligand CLA 1 603



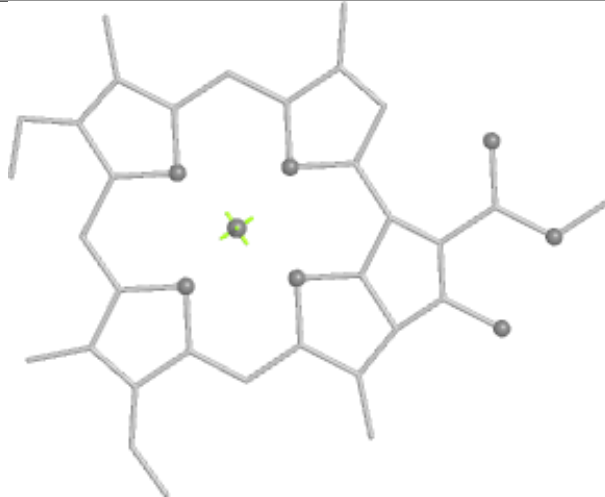
Bond lengths



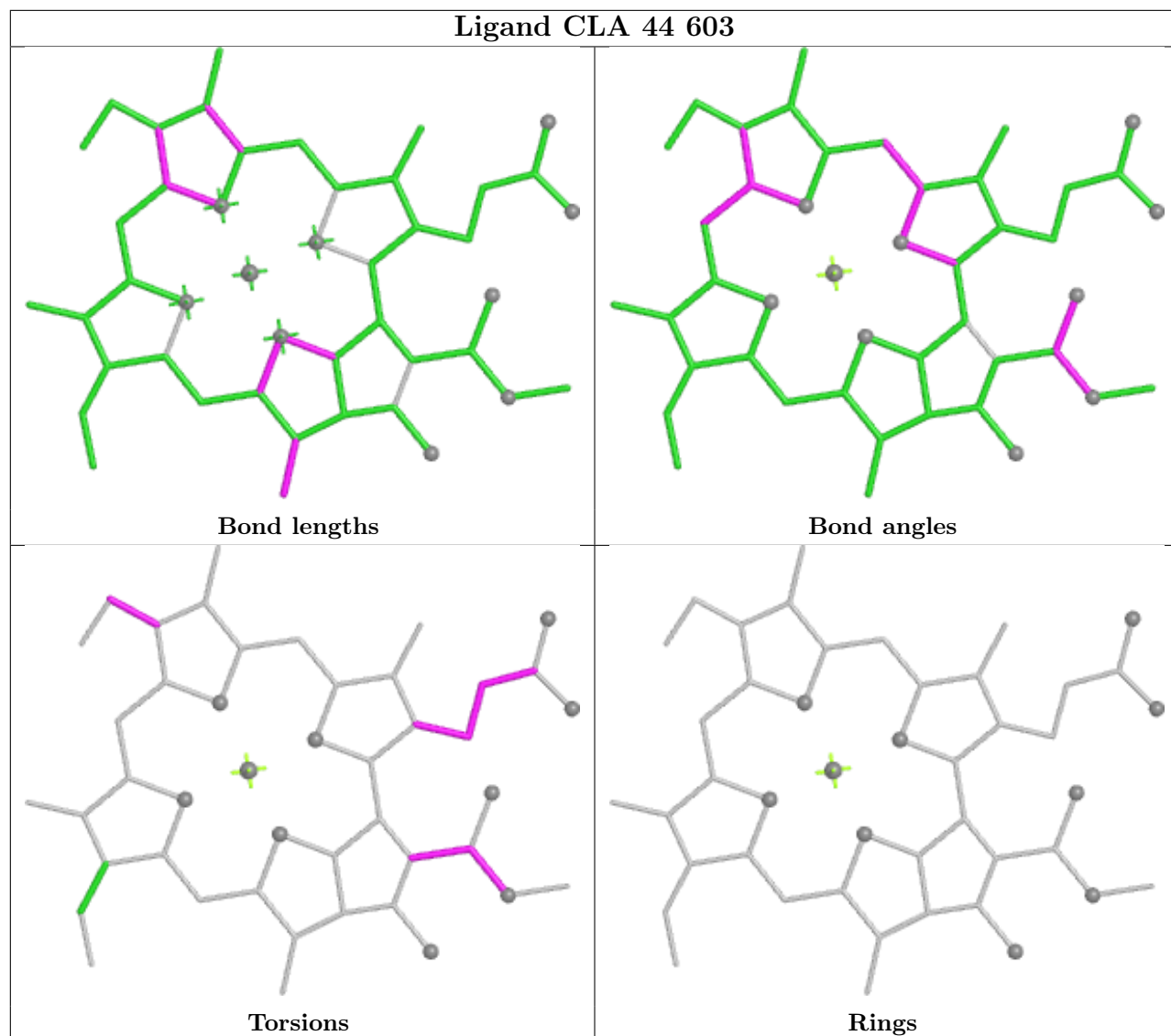
Bond angles



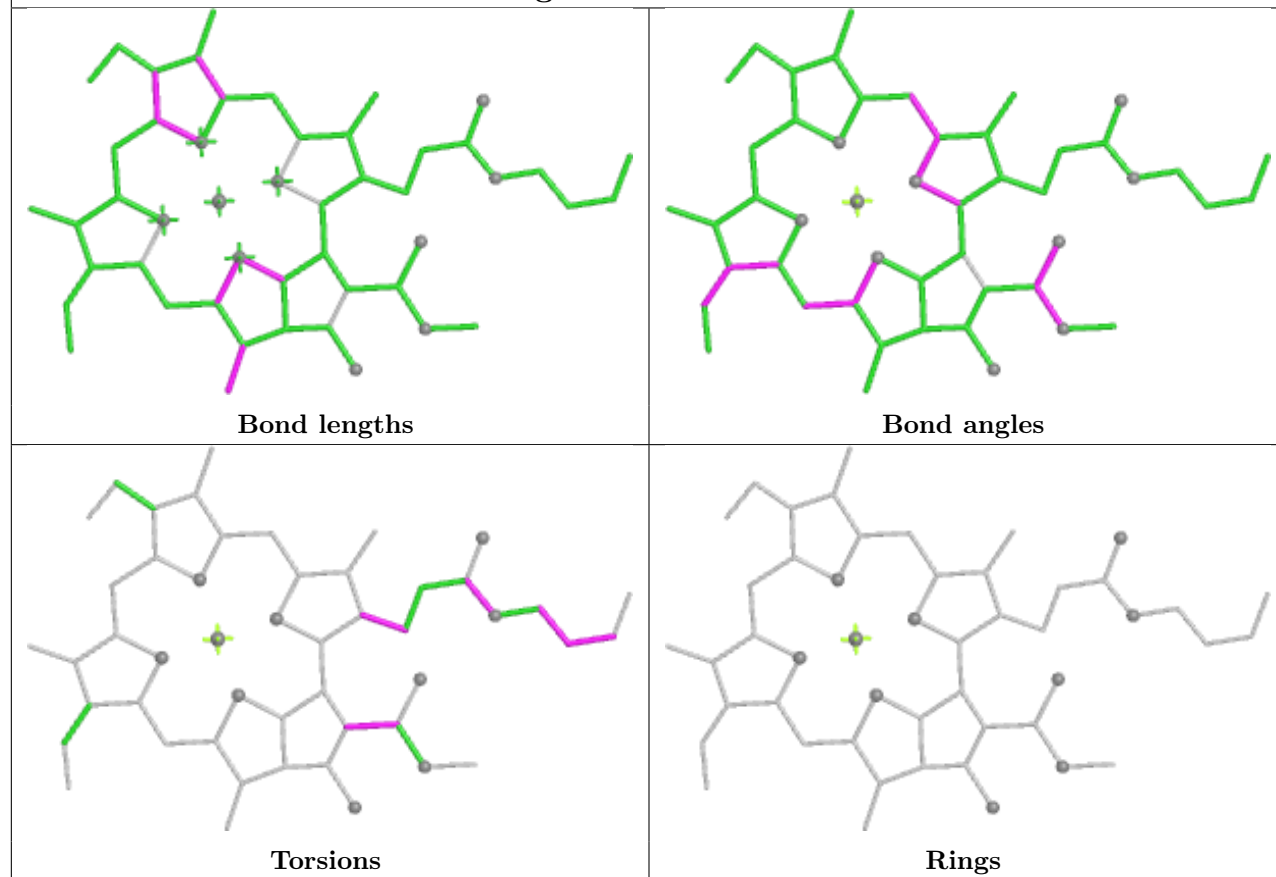
Torsions



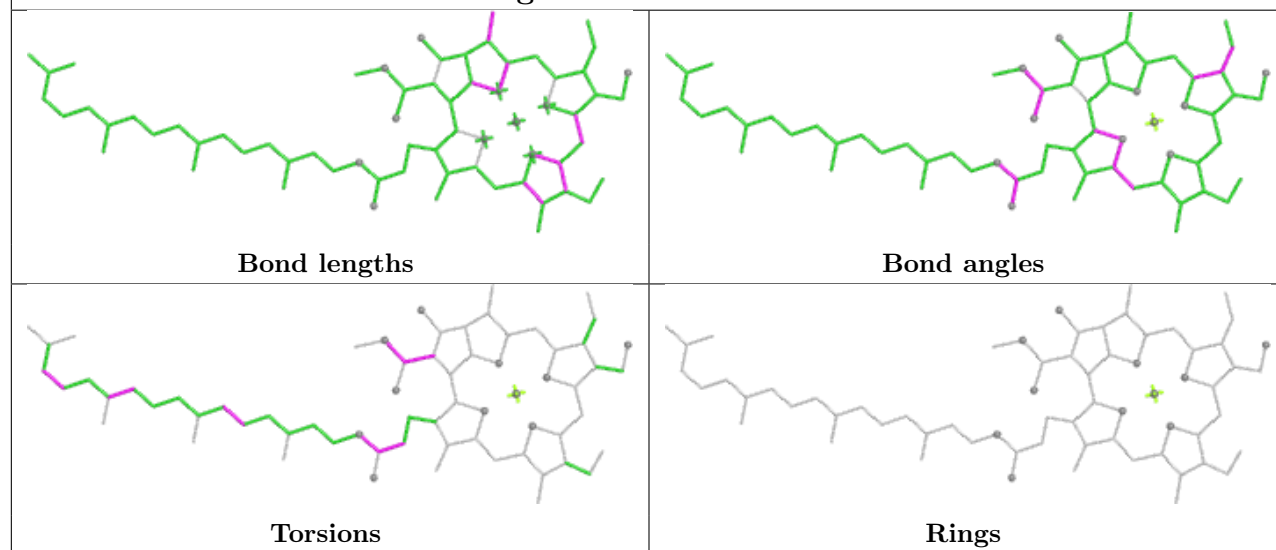
Rings



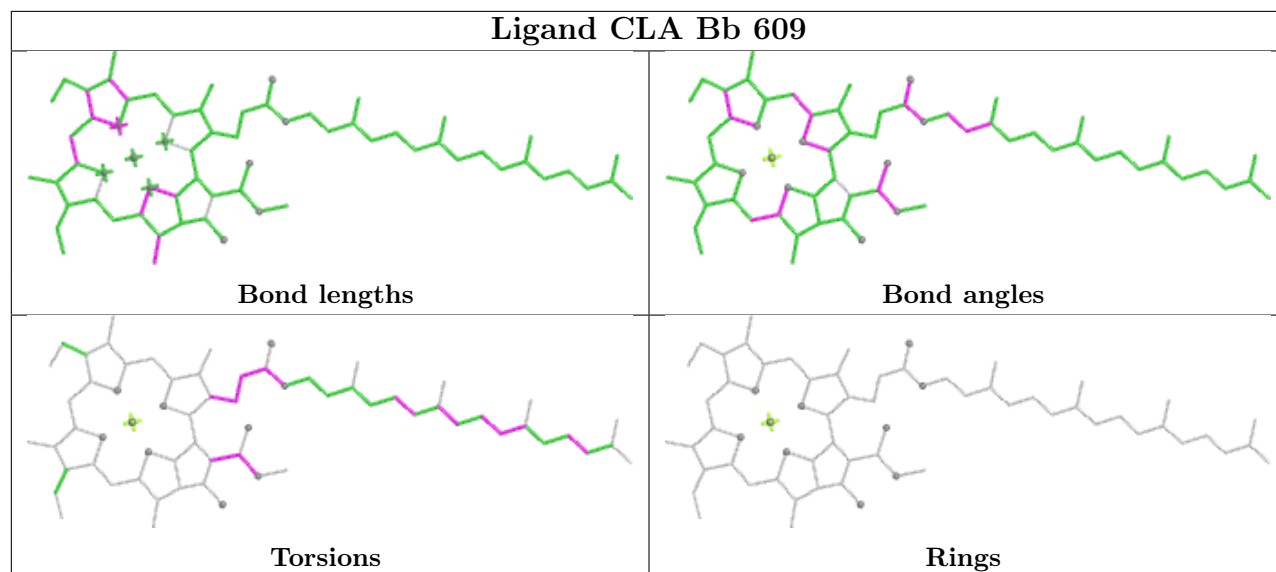
Ligand CLA S 604



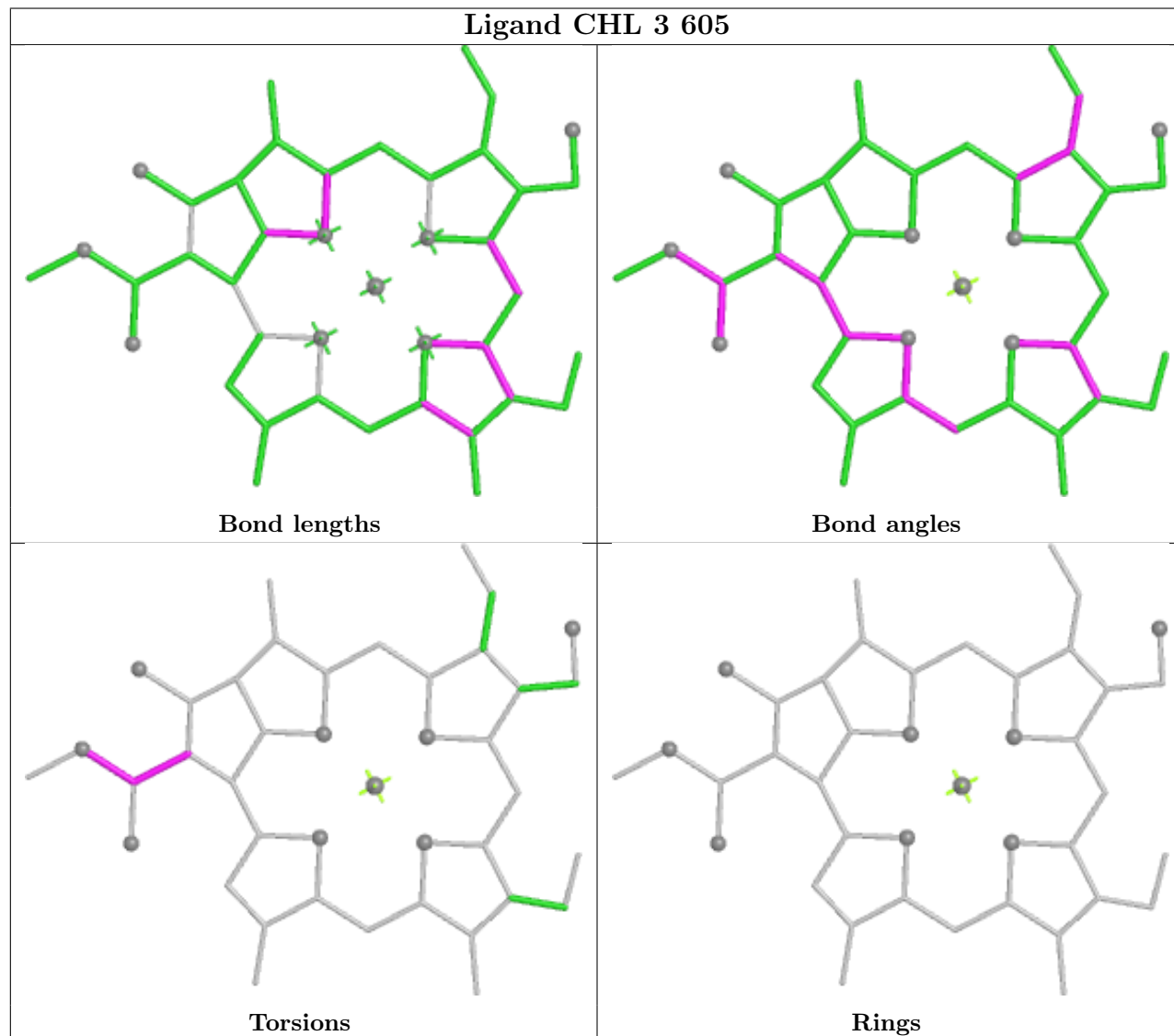
Ligand CHL GG 601



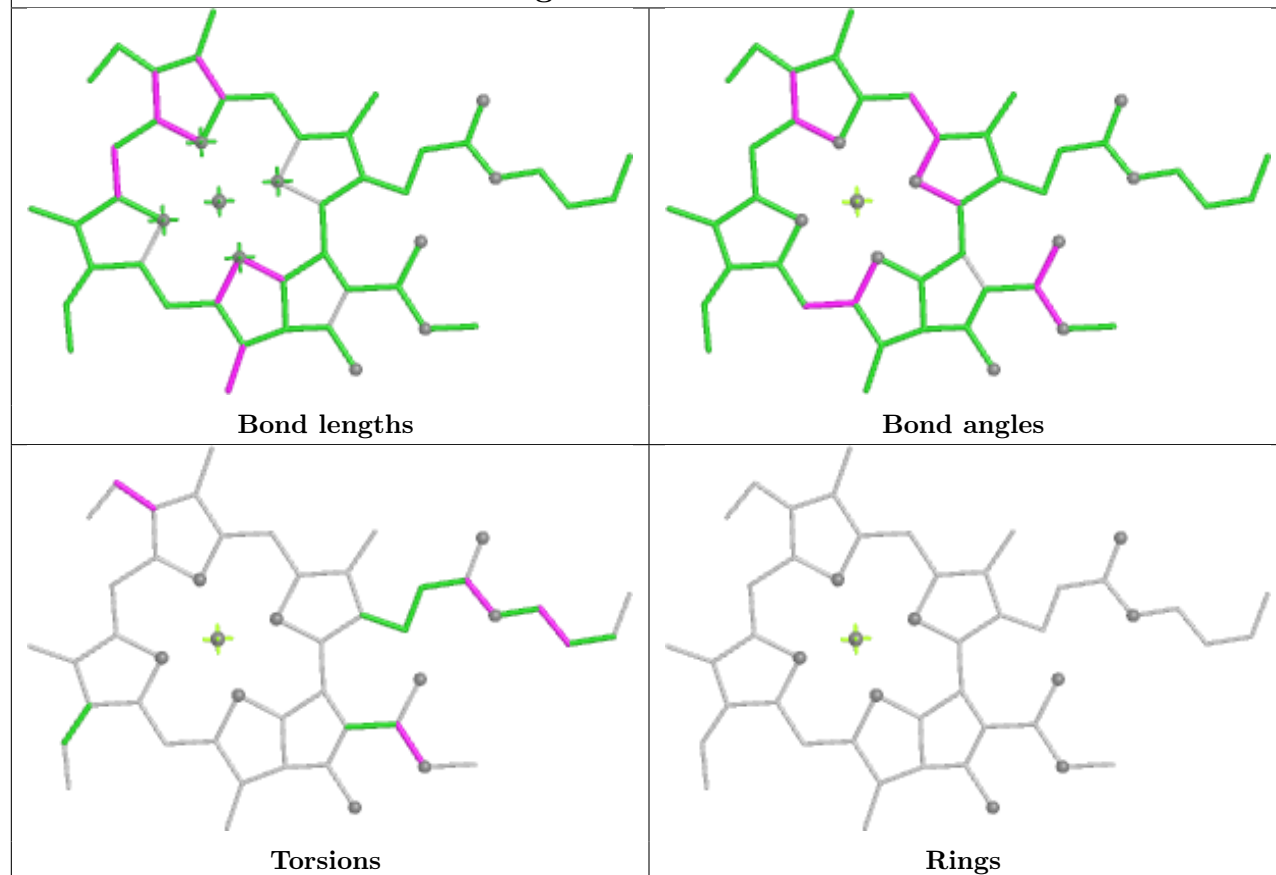
Ligand CLA Bb 609



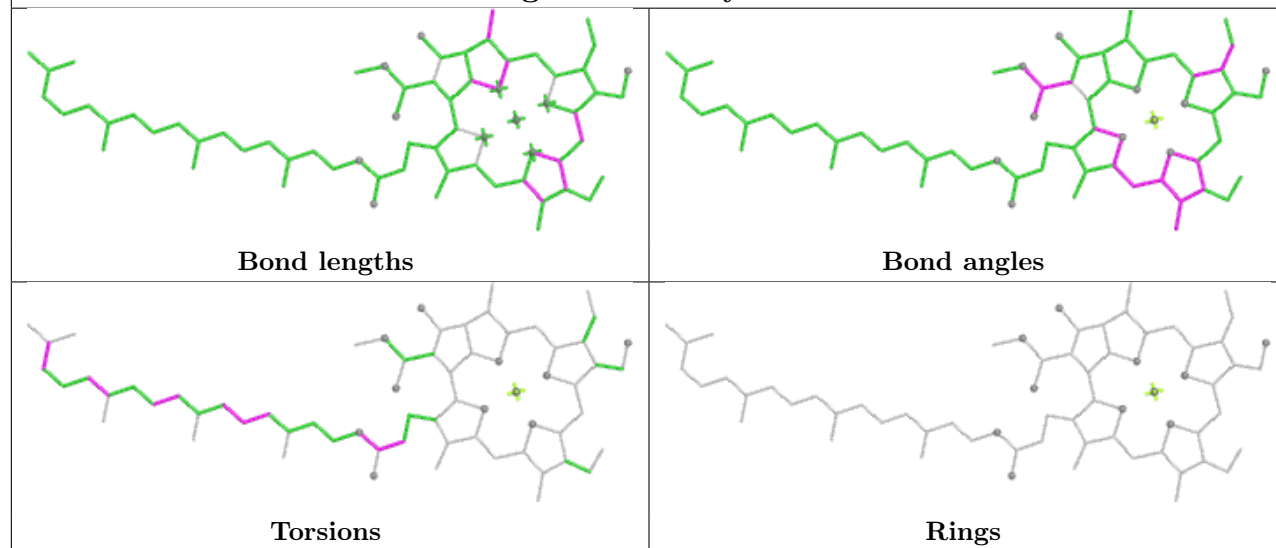
Ligand CHL 3 605



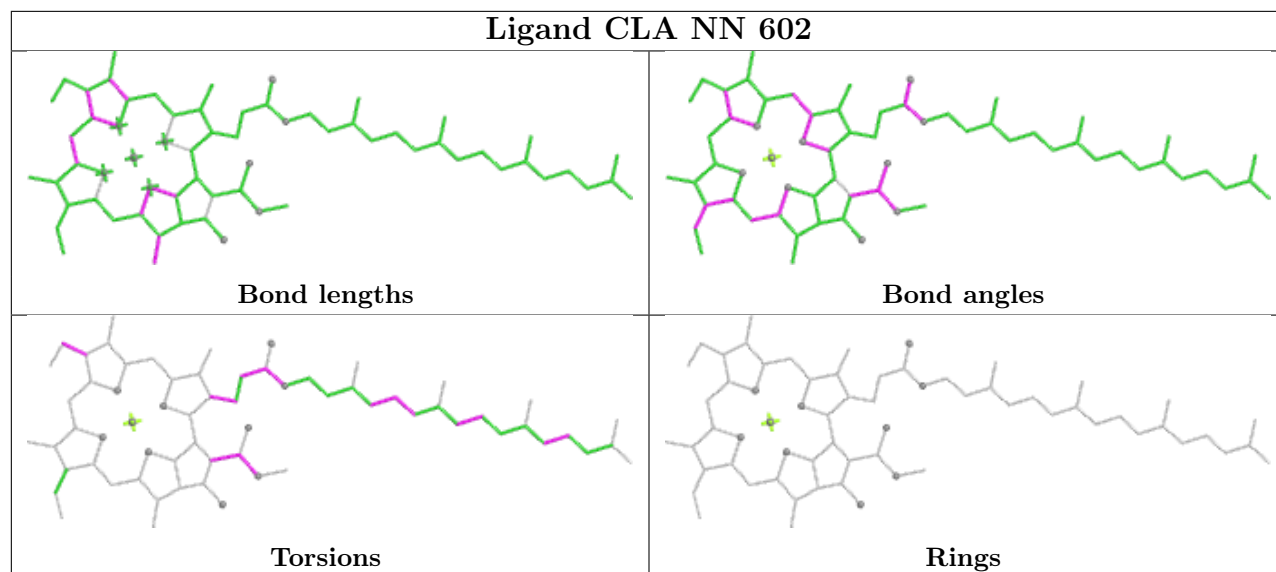
Ligand CLA n 611



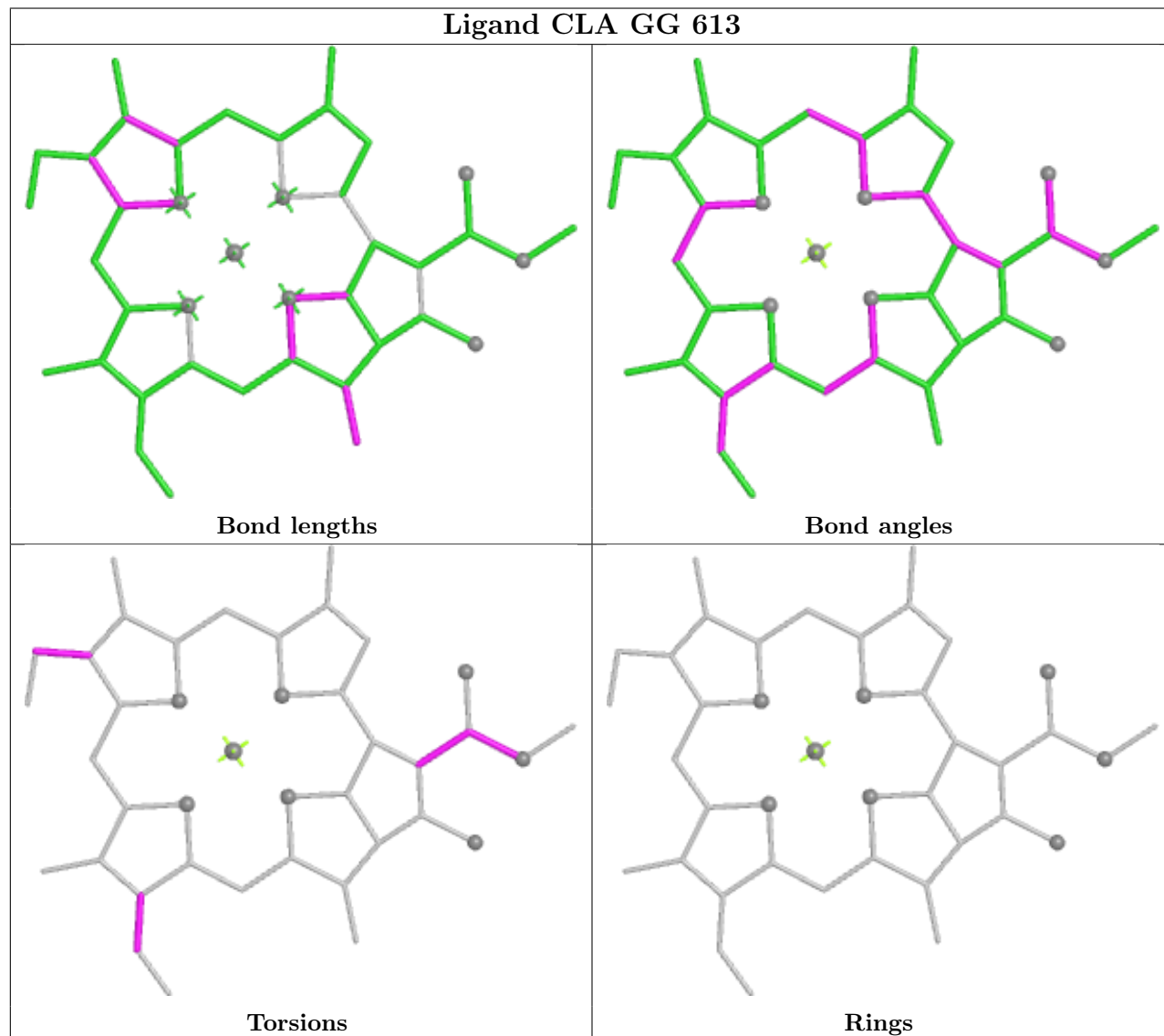
Ligand CHL Yy 609

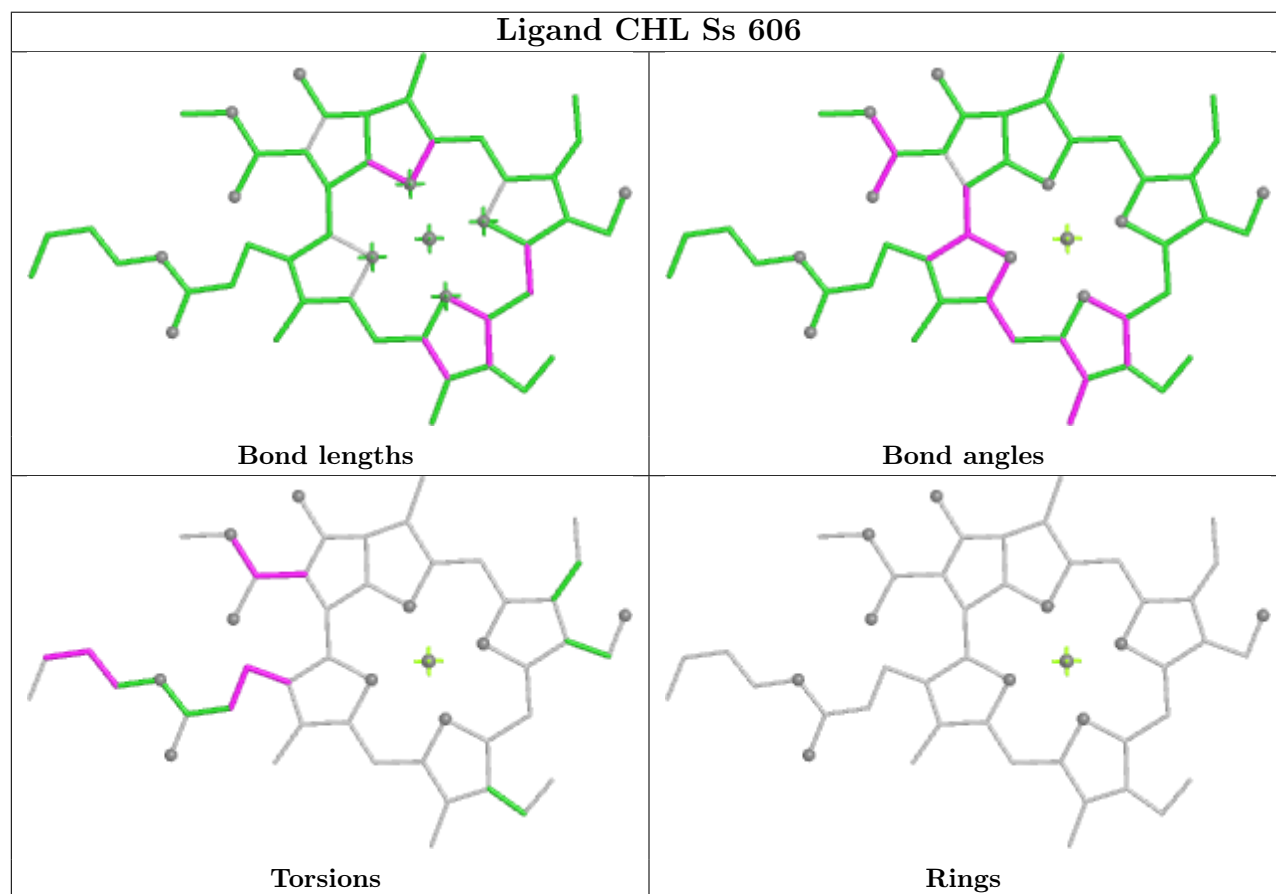
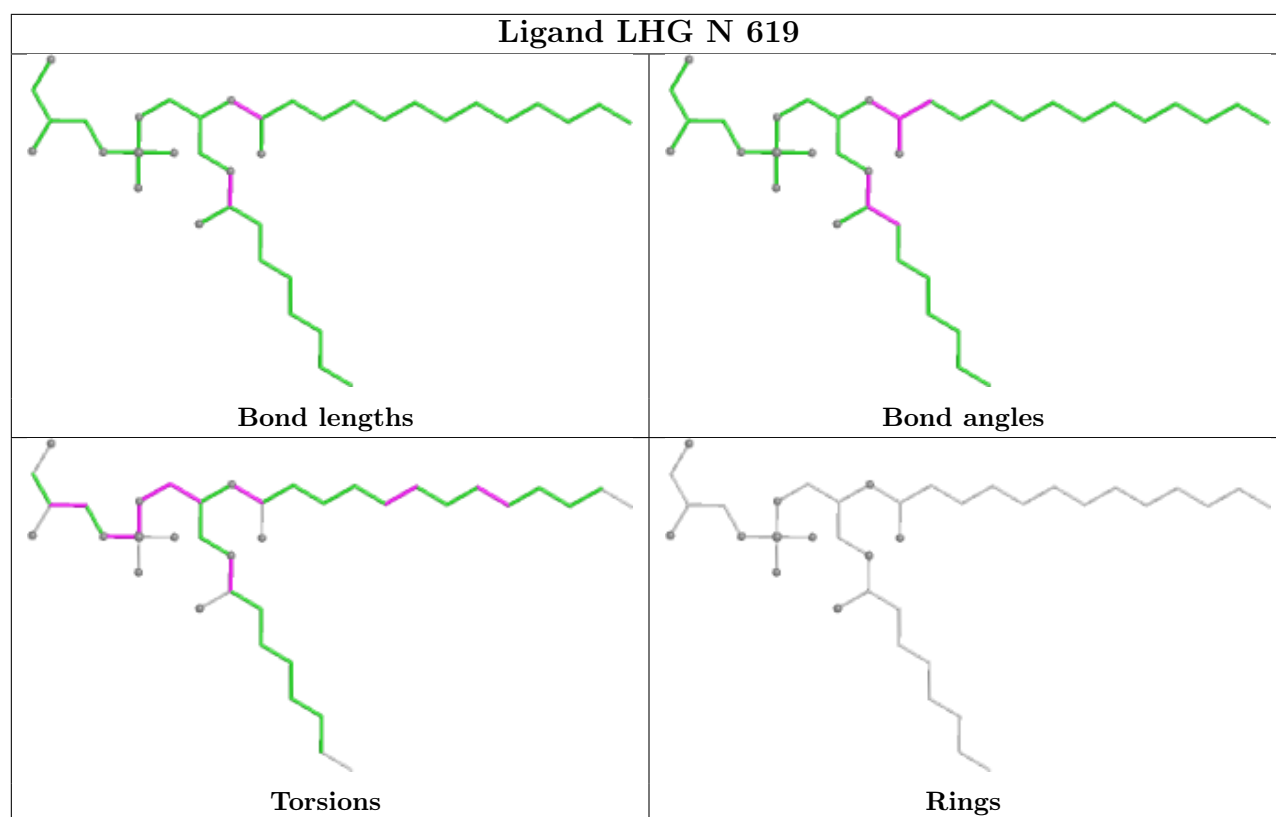


Ligand CLA NN 602

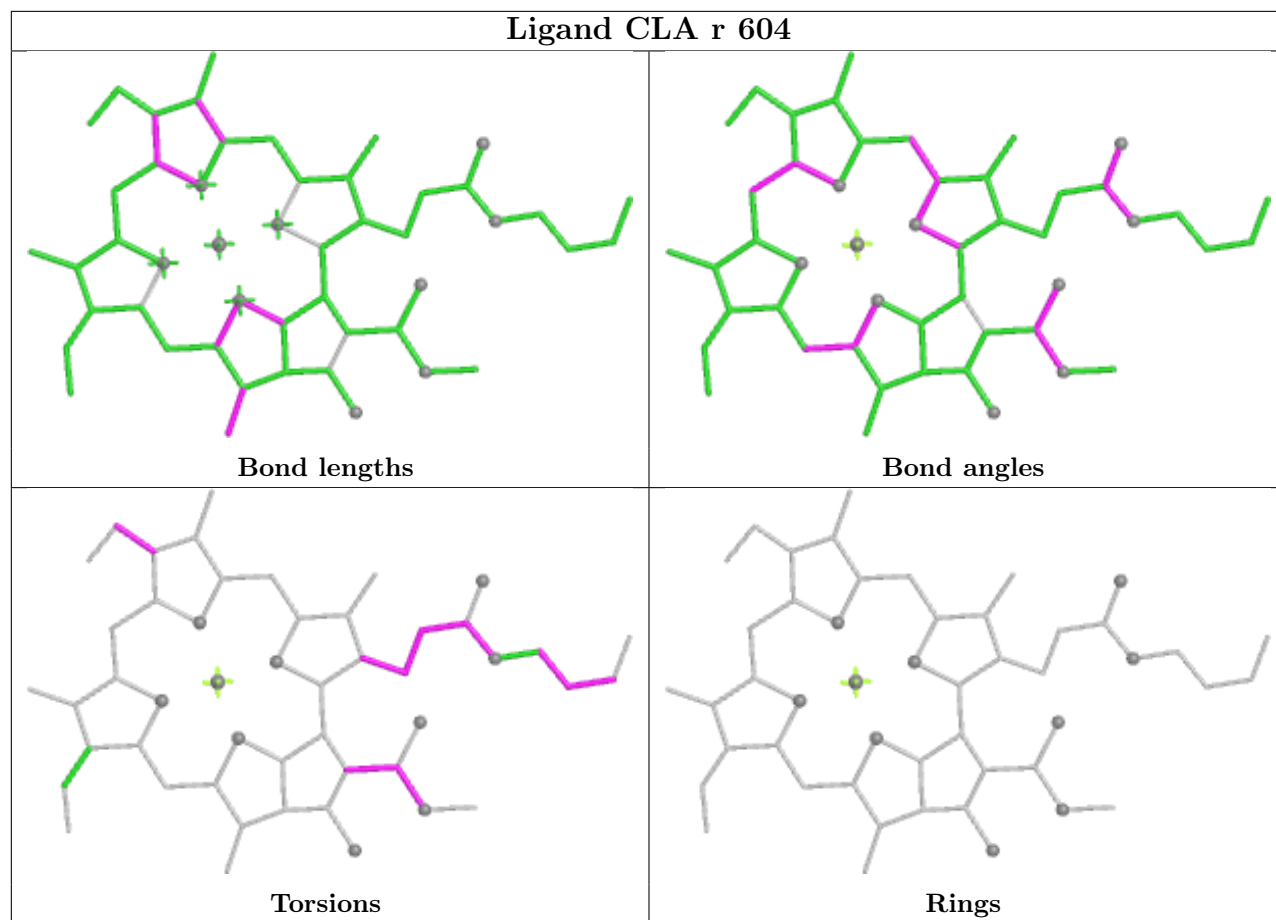


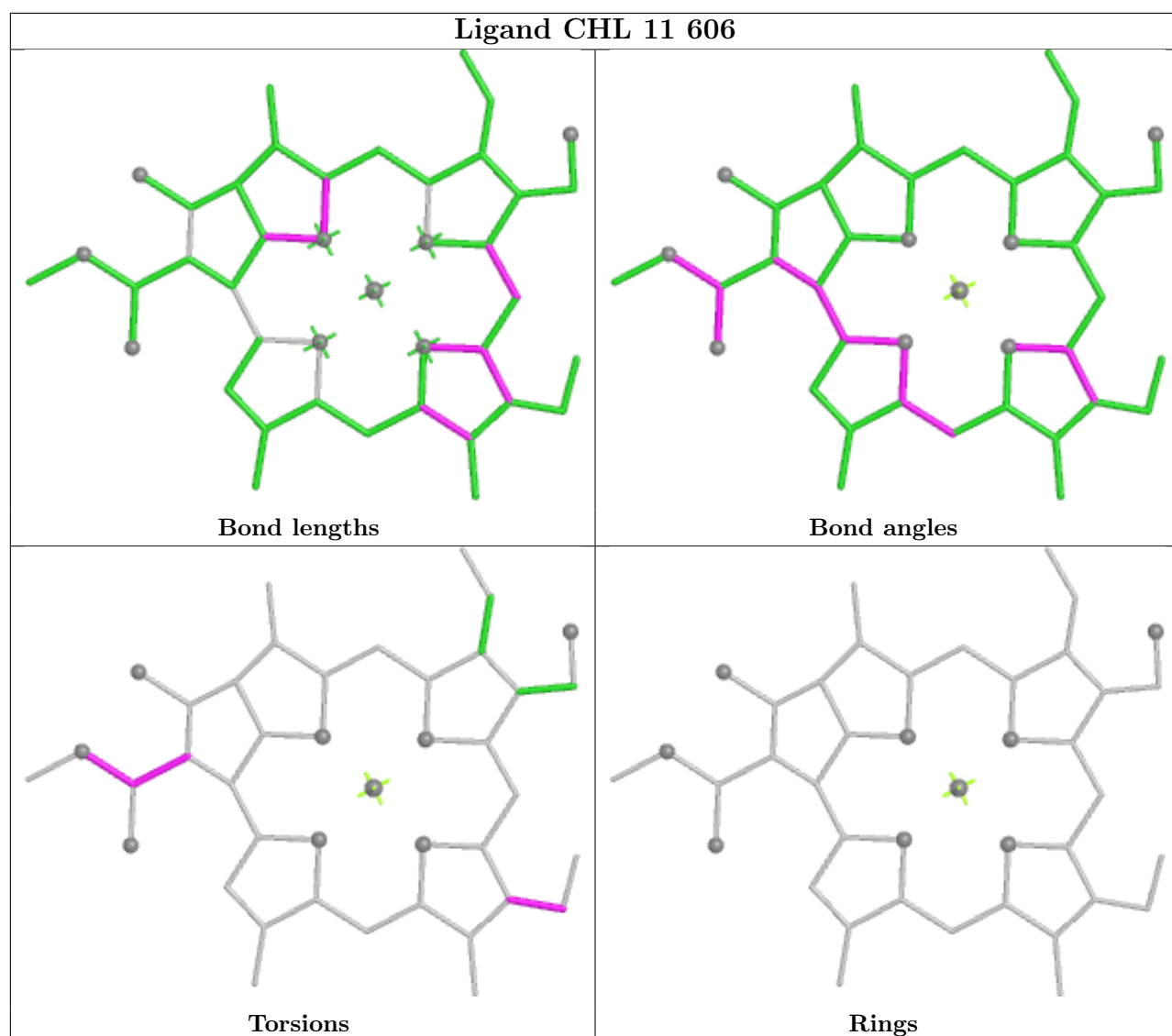
Ligand CLA GG 613

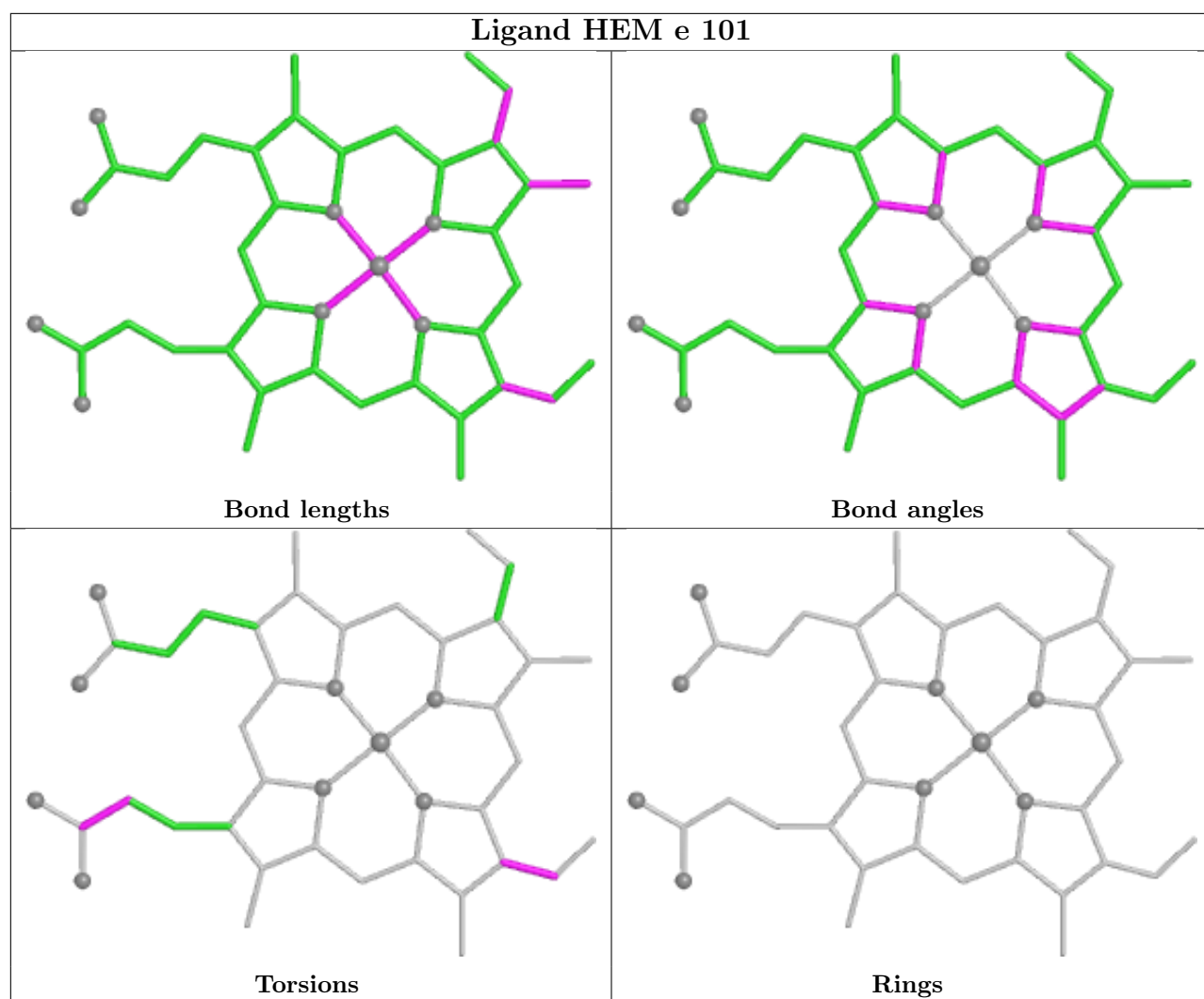




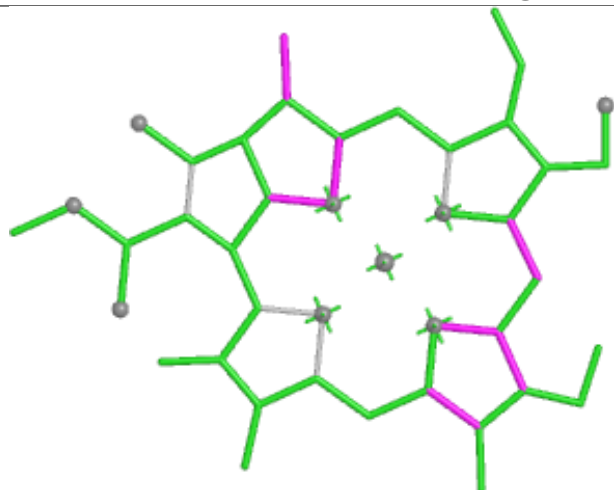
Ligand CLA r 604



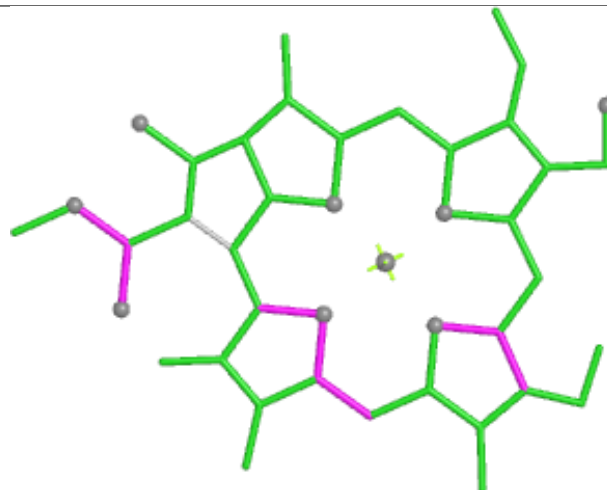




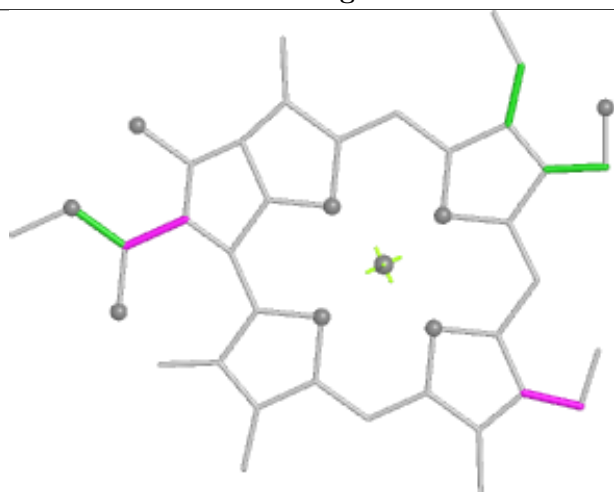
Ligand CHL S 606



Bond lengths



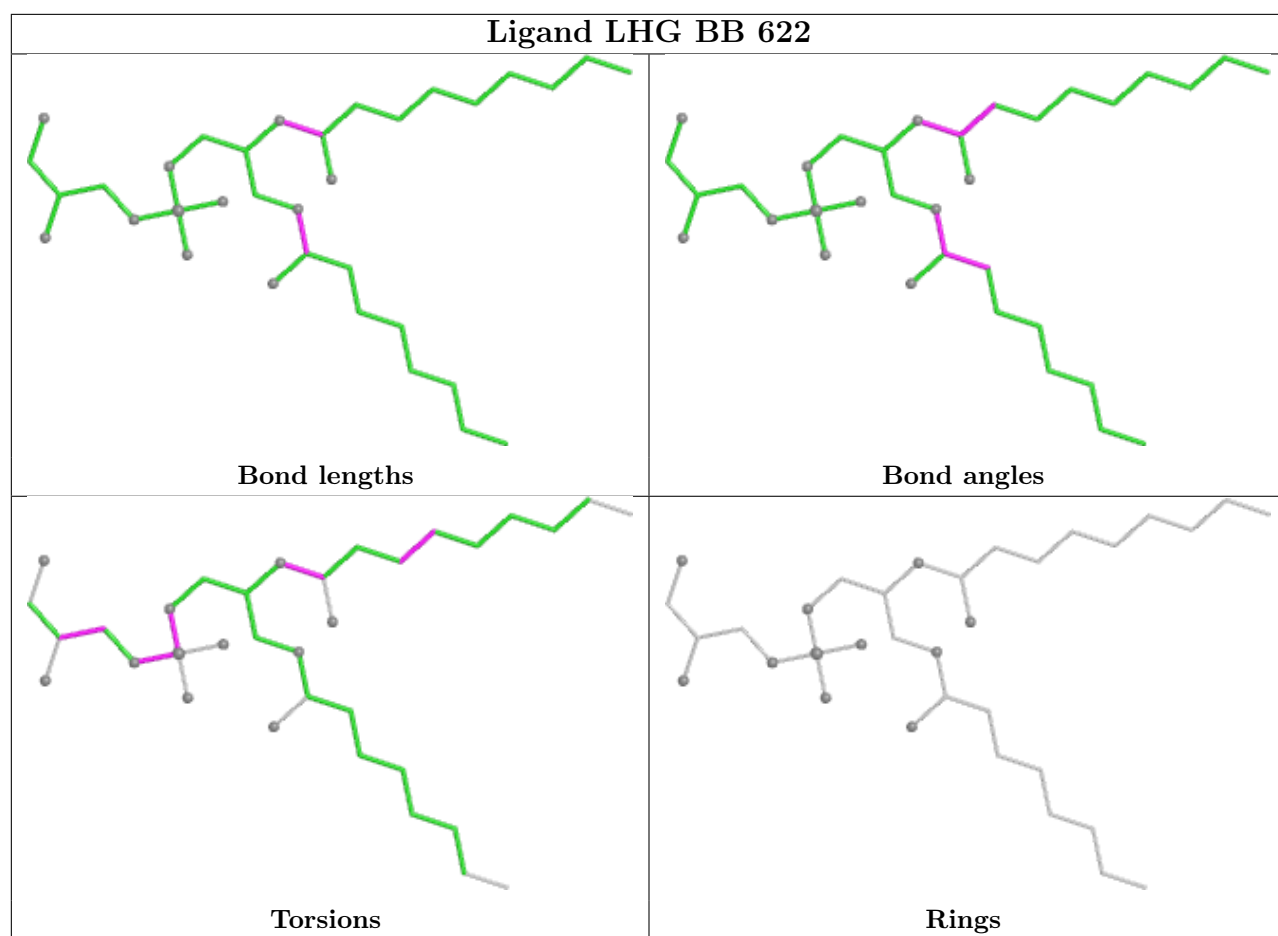
Bond angles



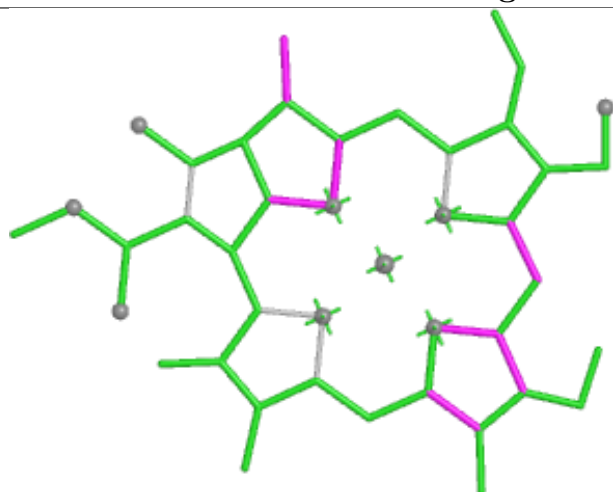
Torsions



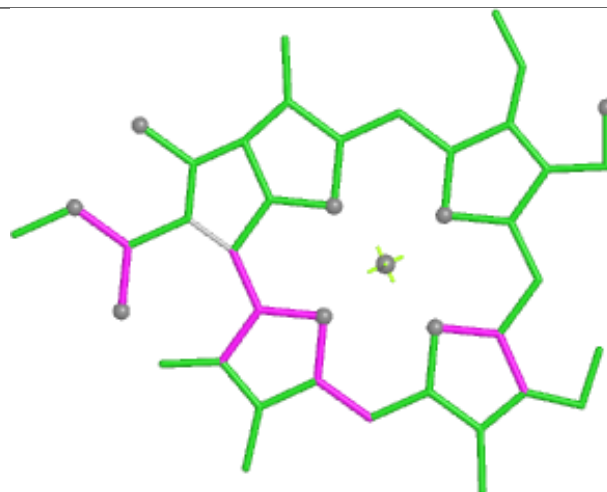
Rings



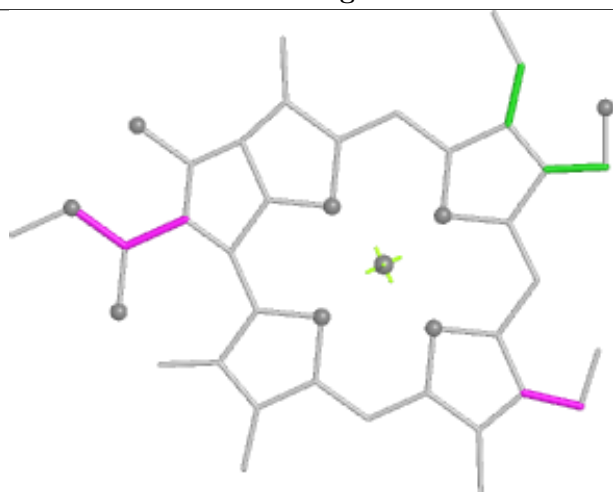
Ligand CHL GG 608



Bond lengths



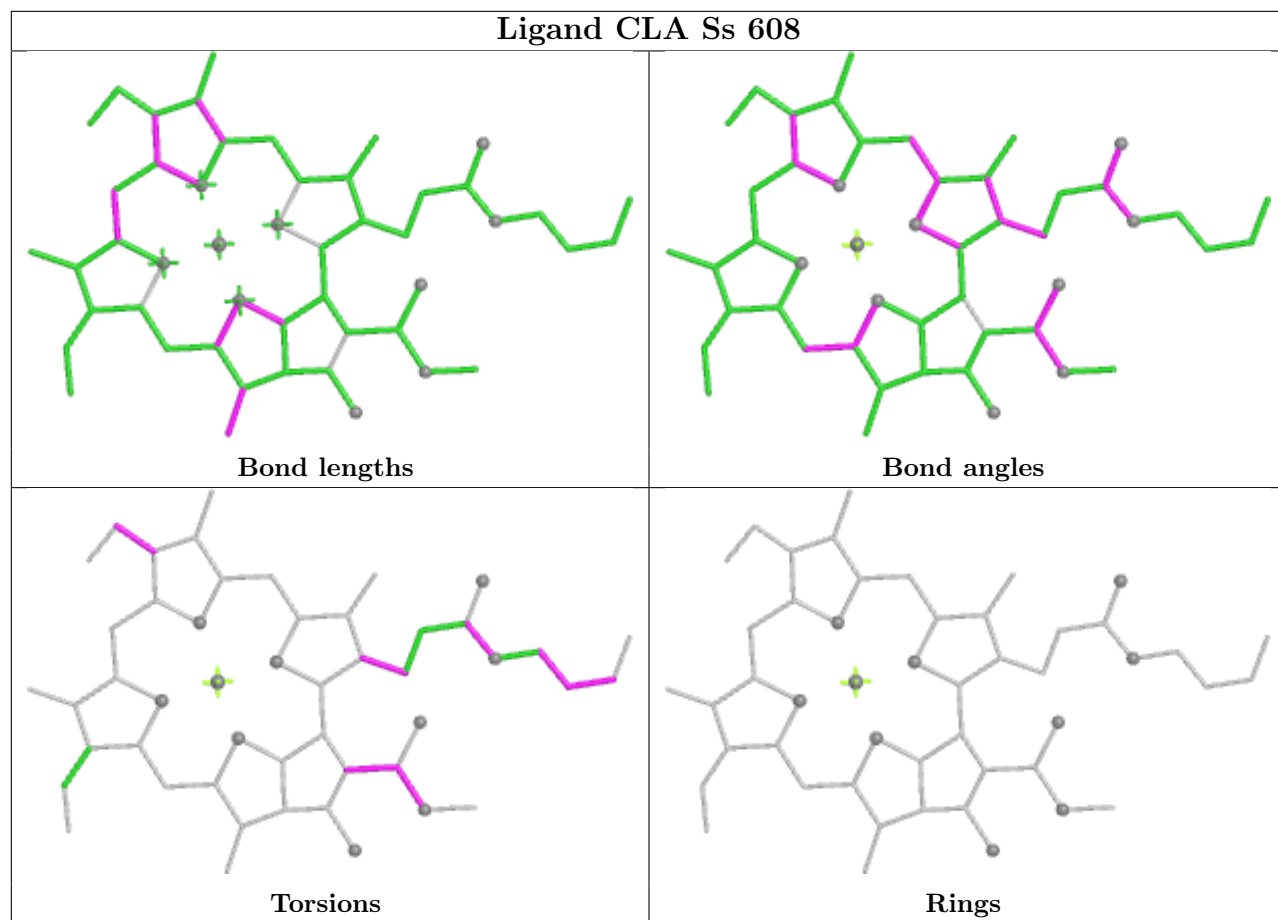
Bond angles

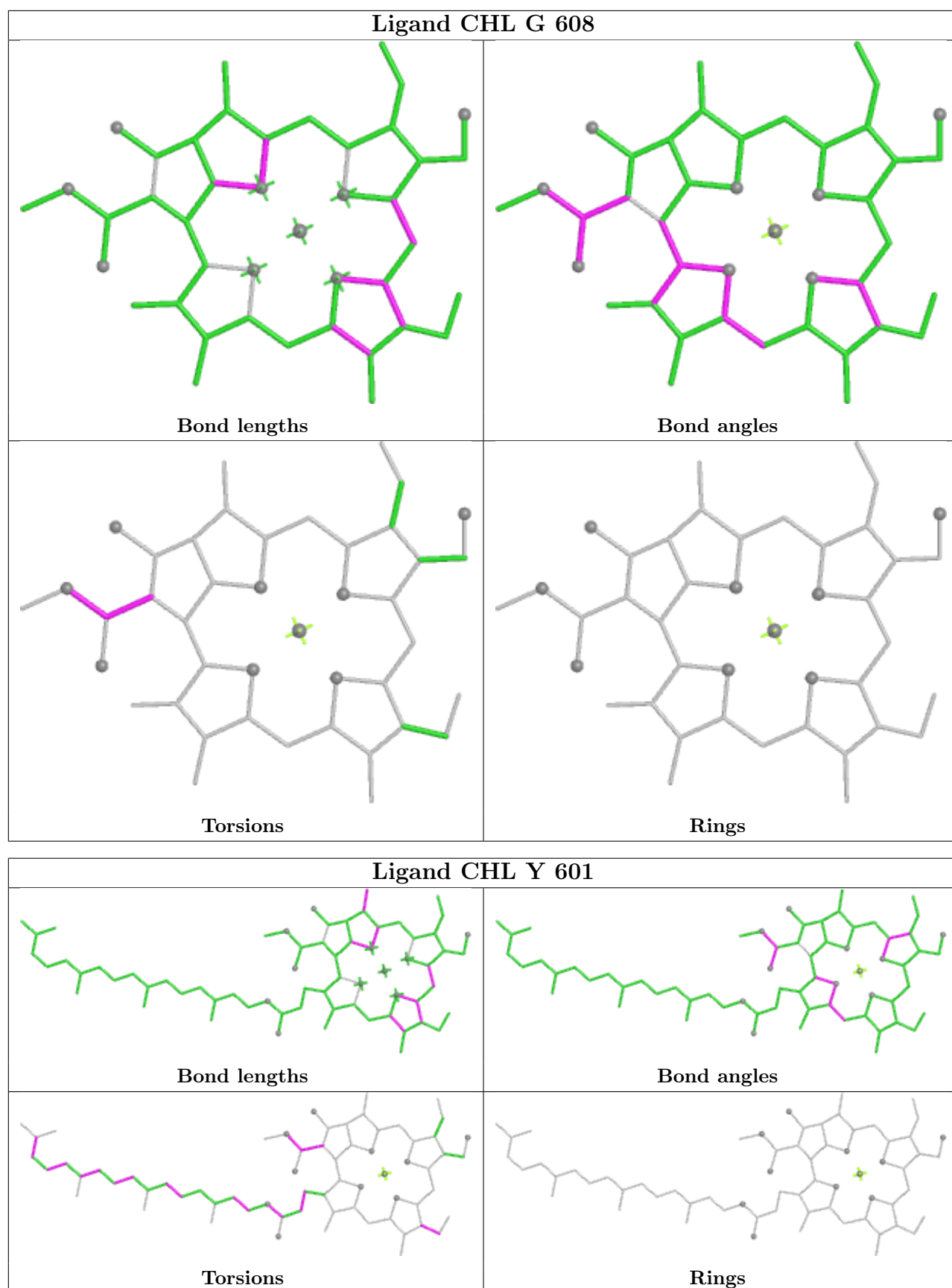


Torsions

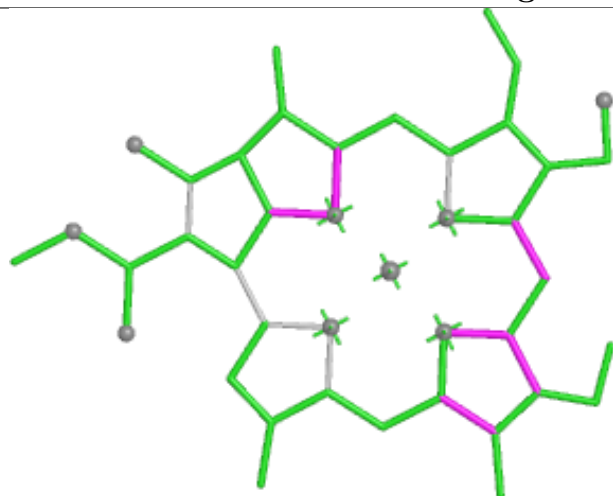


Rings

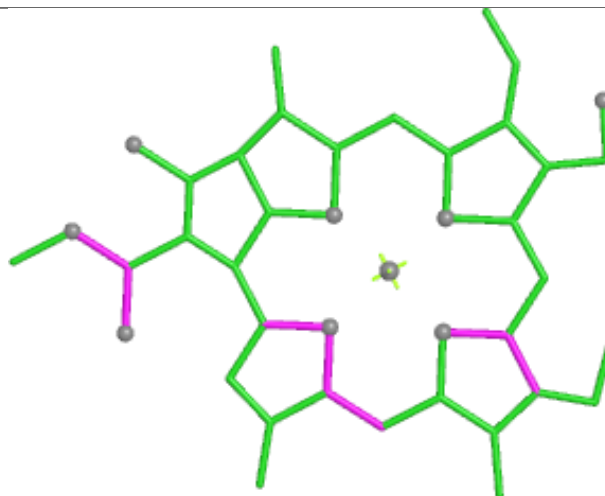




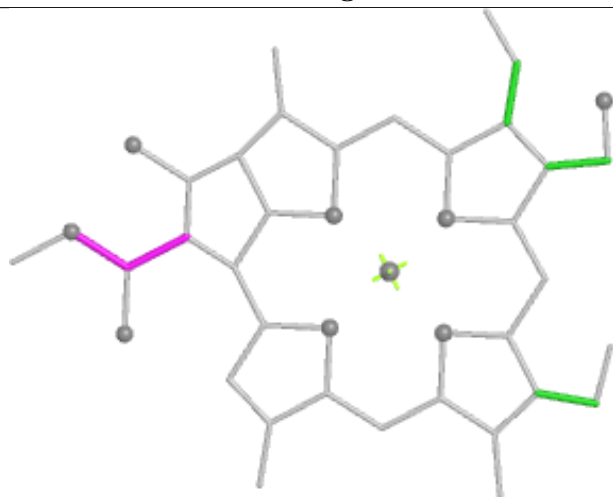
Ligand CHL 3 601



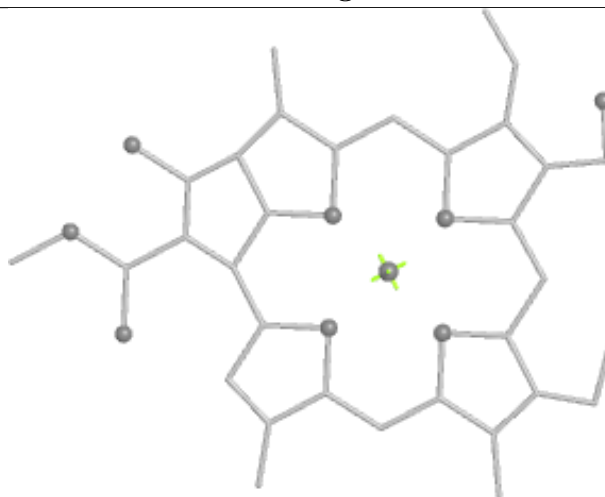
Bond lengths



Bond angles

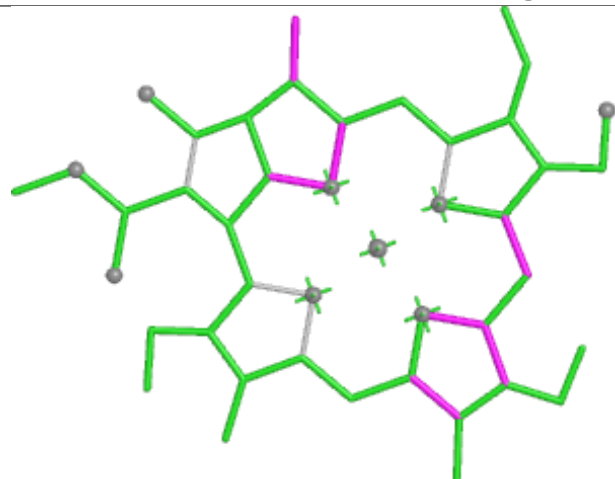


Torsions

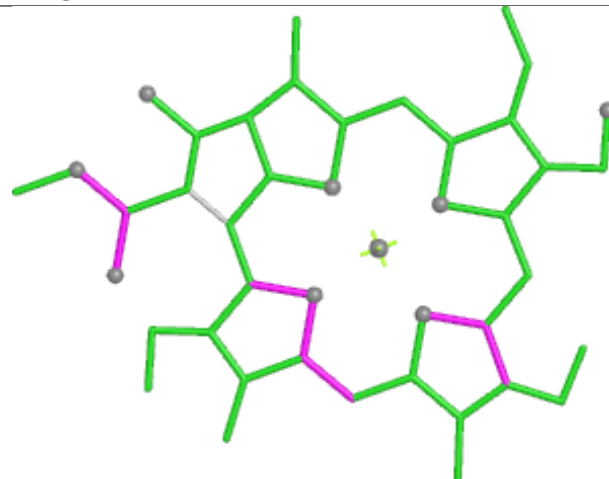


Rings

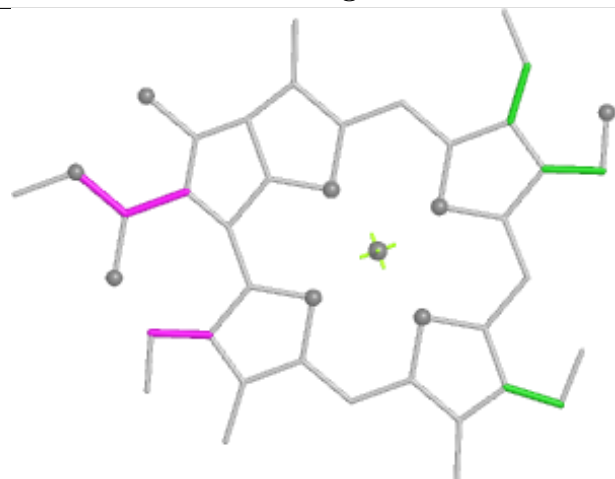
Ligand CHL g 606



Bond lengths



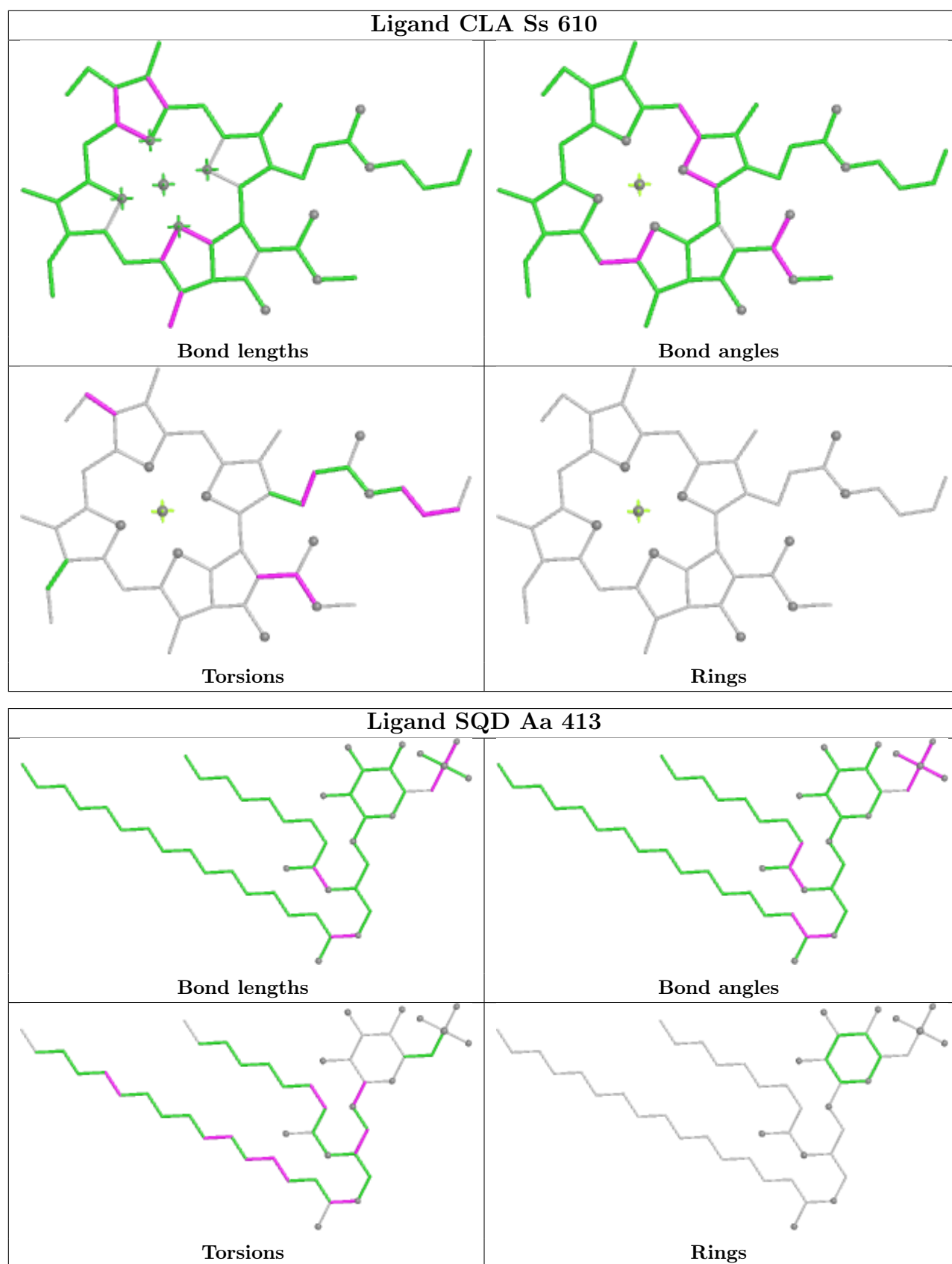
Bond angles



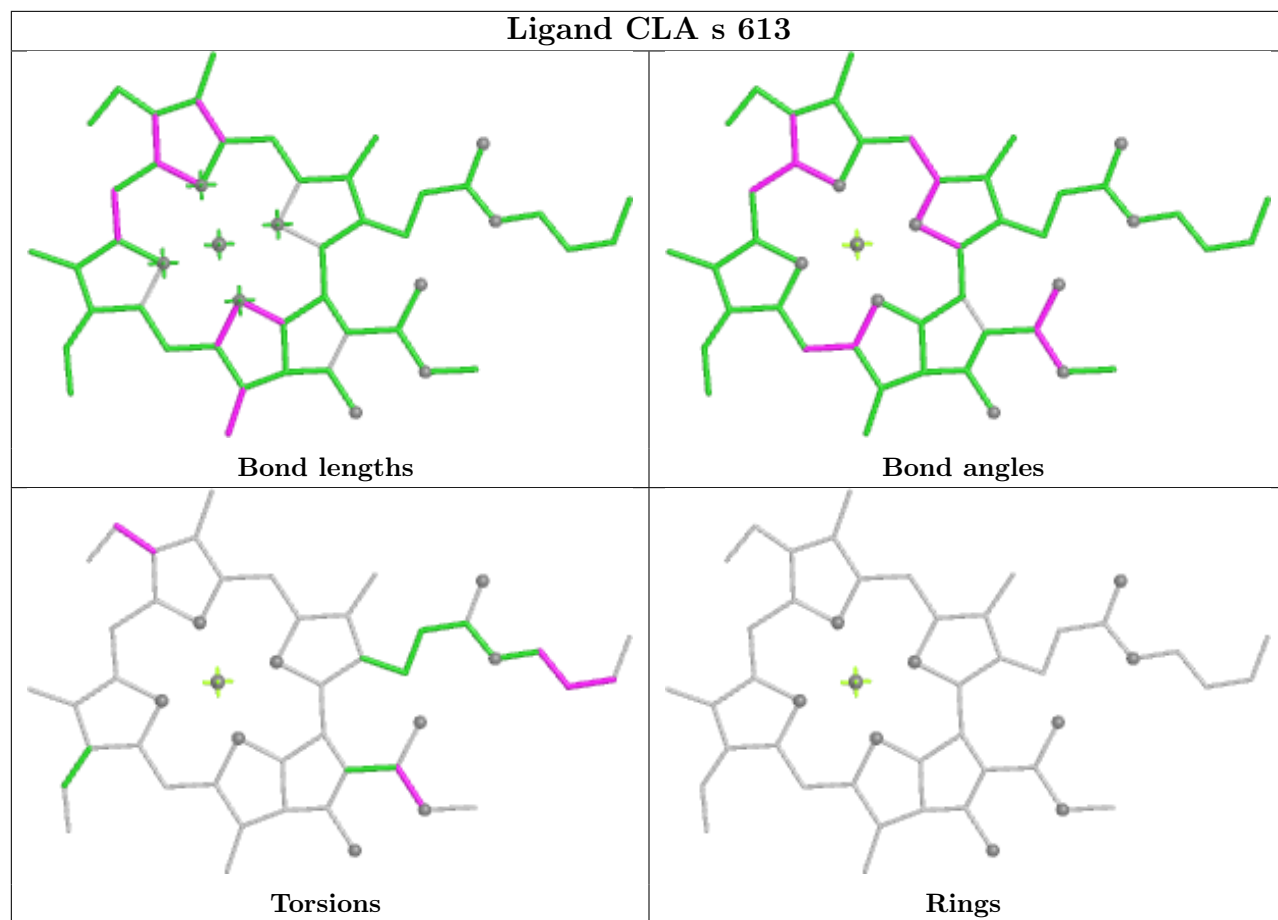
Torsions

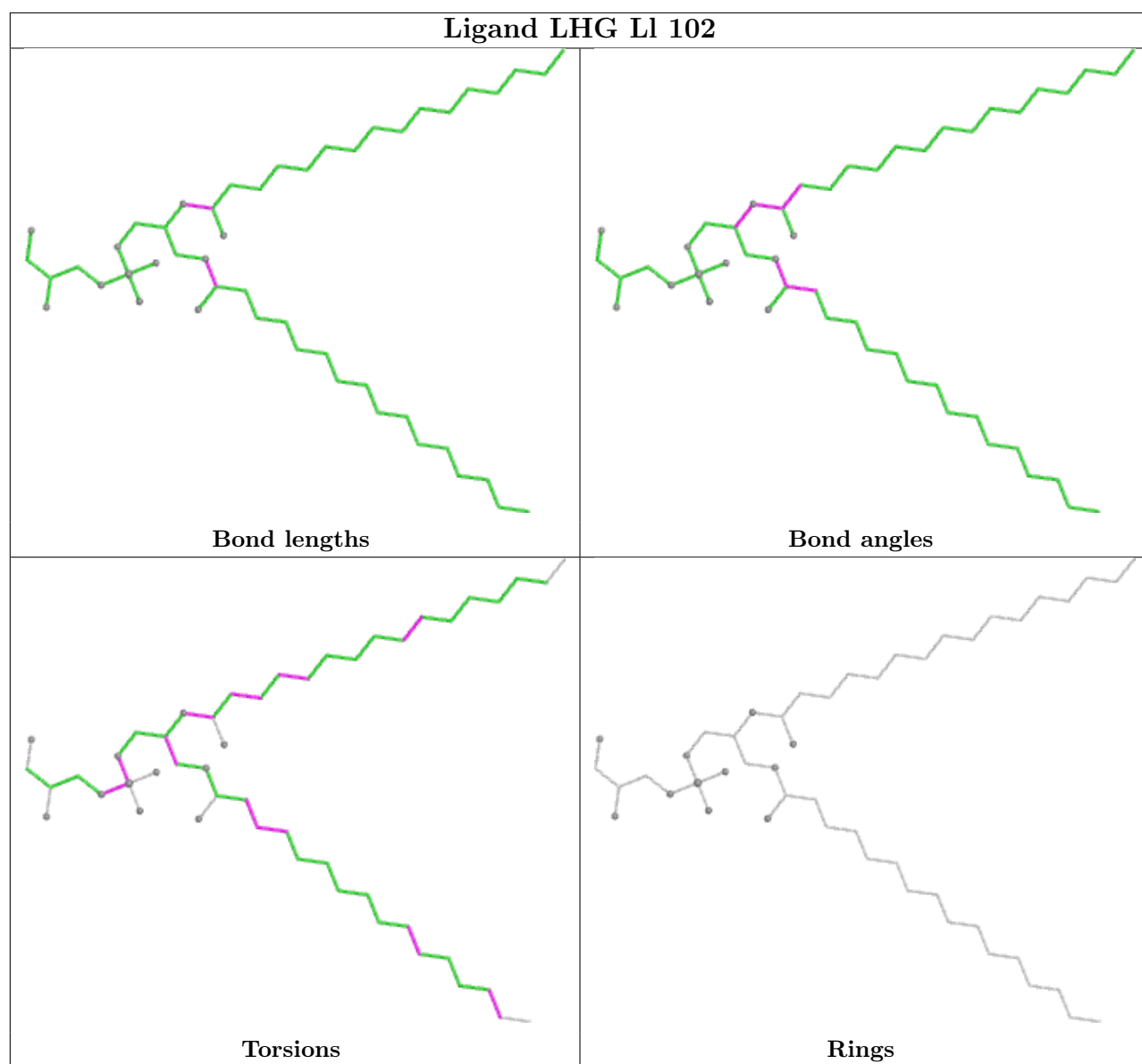


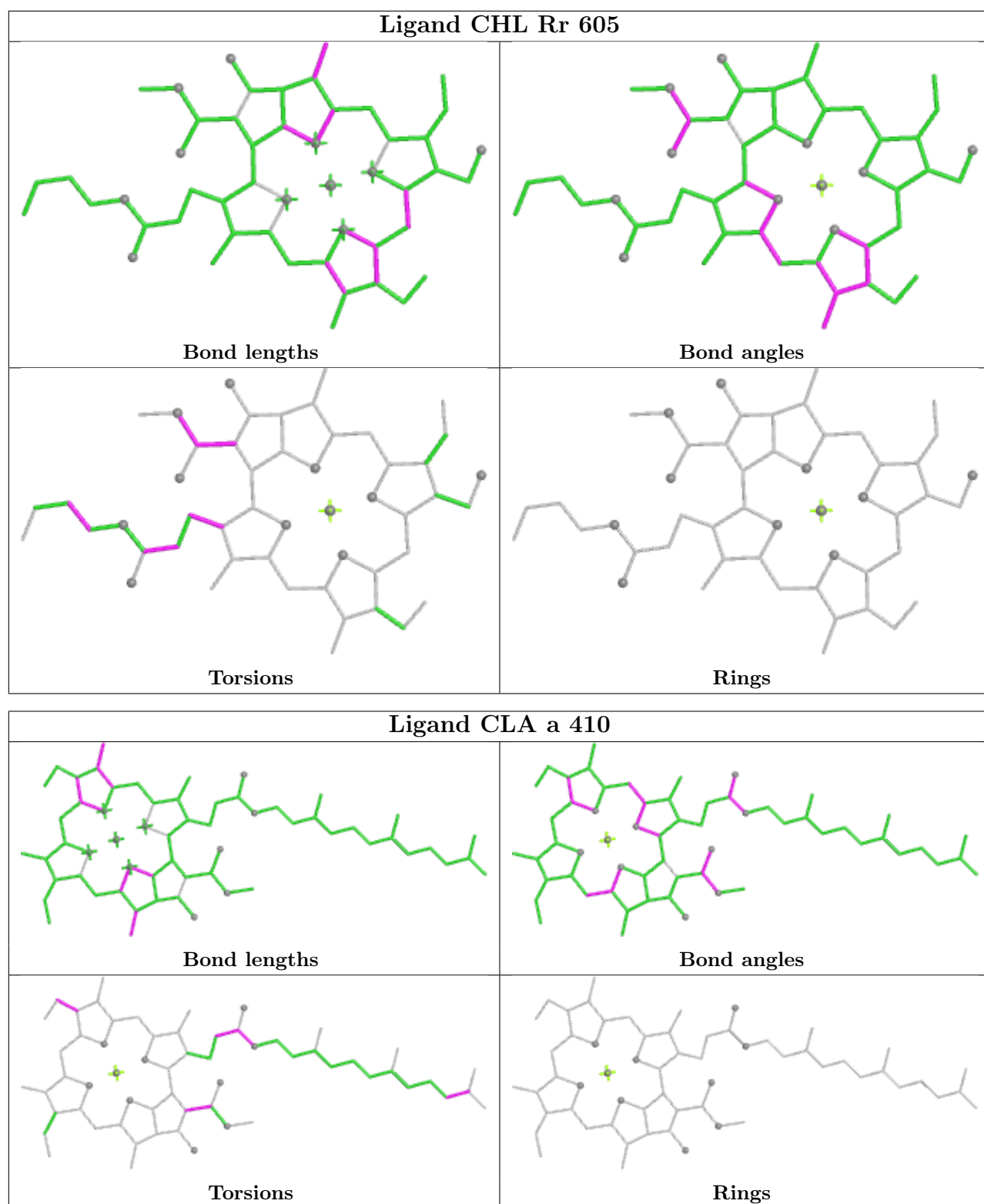
Rings



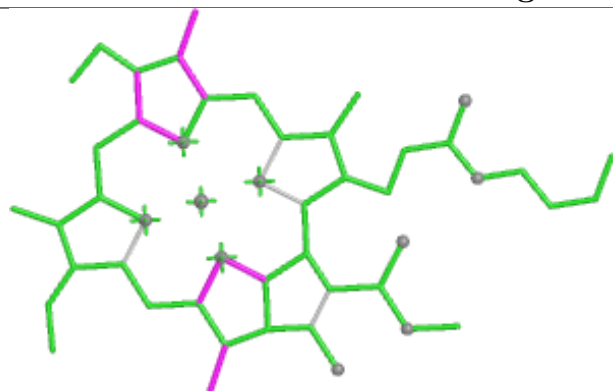
Ligand CLA s 613



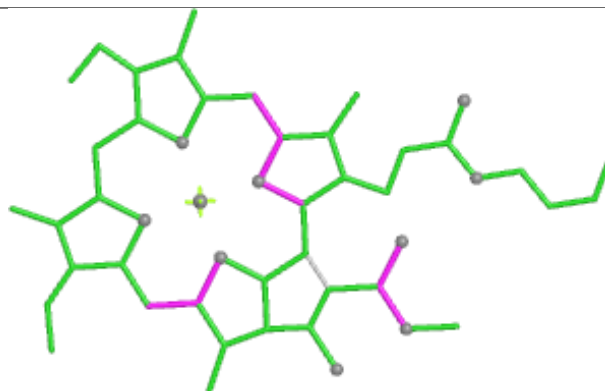




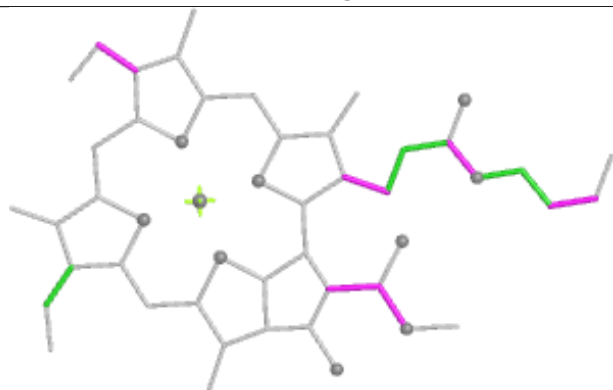
Ligand CLA n 613



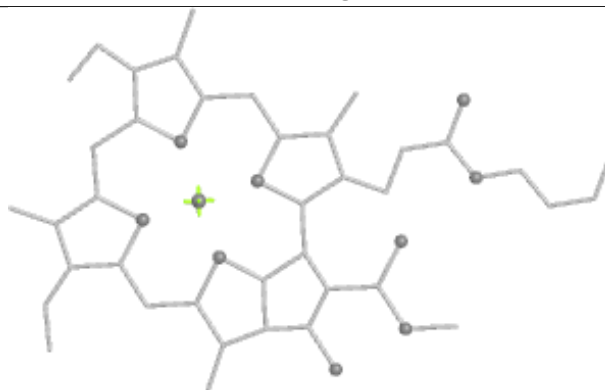
Bond lengths



Bond angles

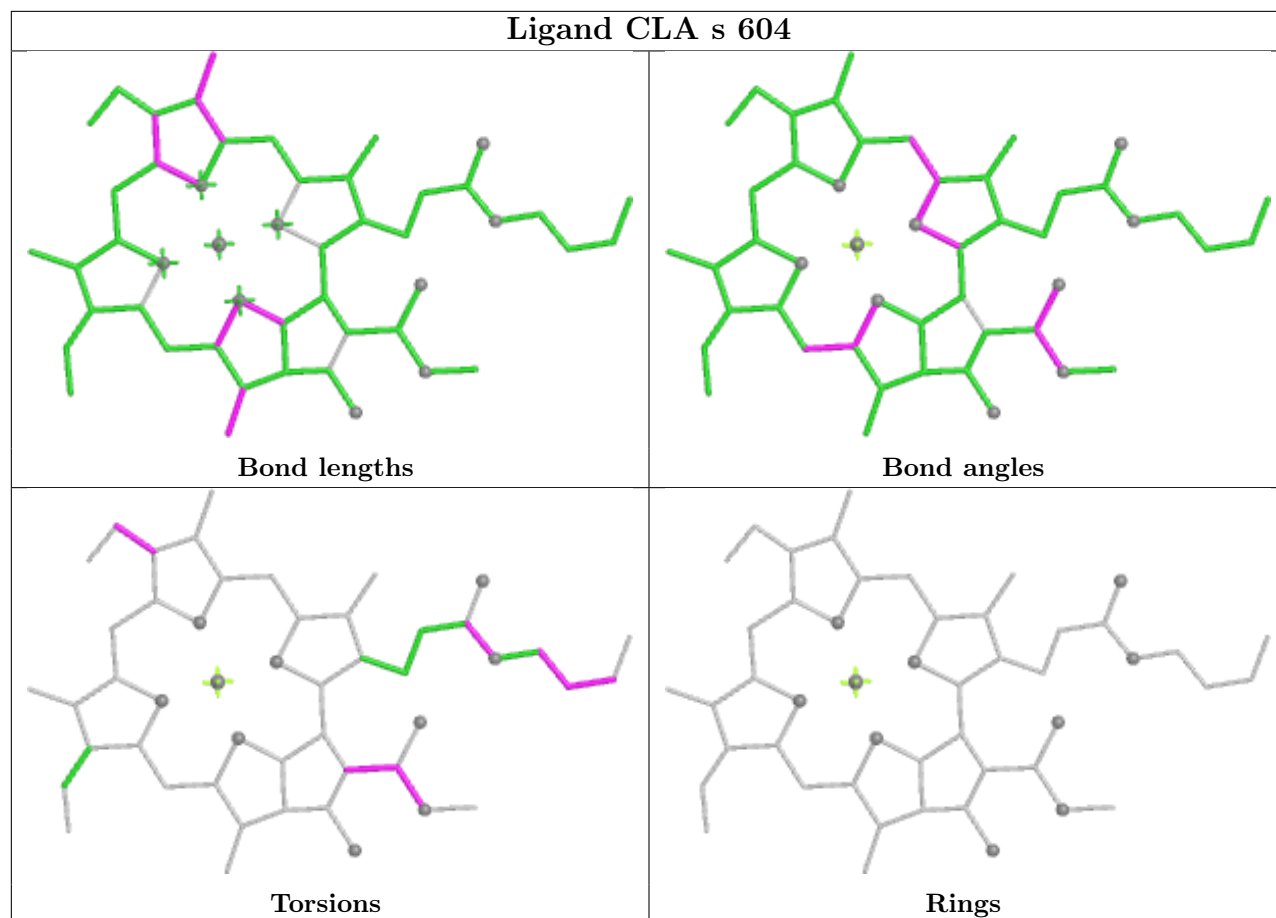


Torsions

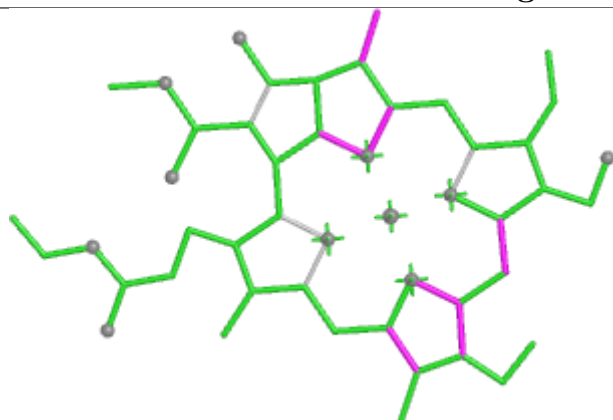


Rings

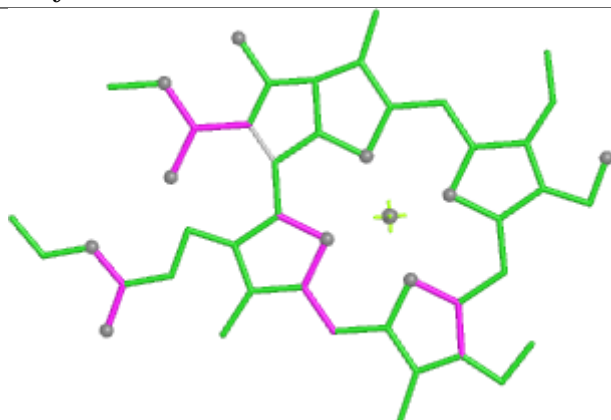
Ligand CLA s 604



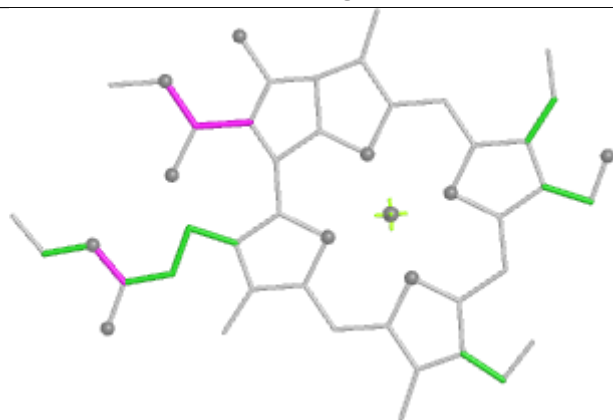
Ligand CHL y 307



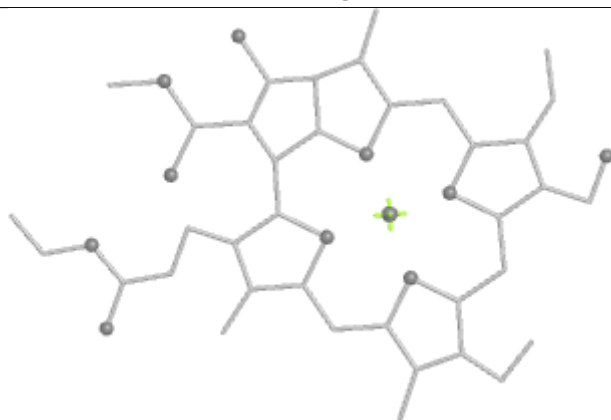
Bond lengths



Bond angles

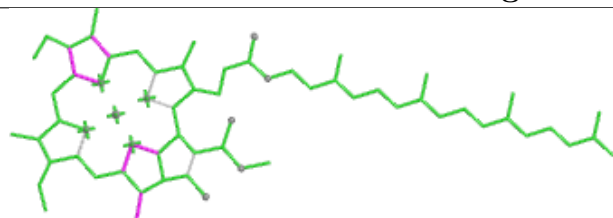


Torsions

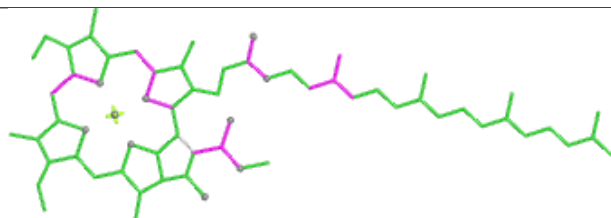


Rings

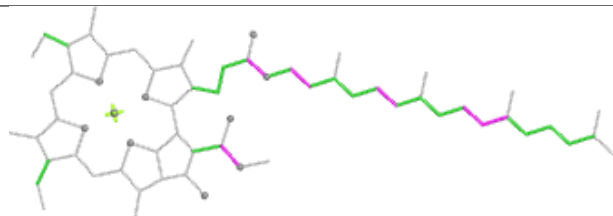
Ligand CLA BB 614



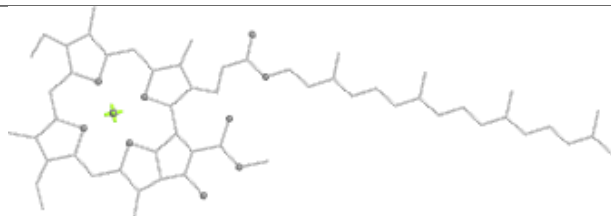
Bond lengths



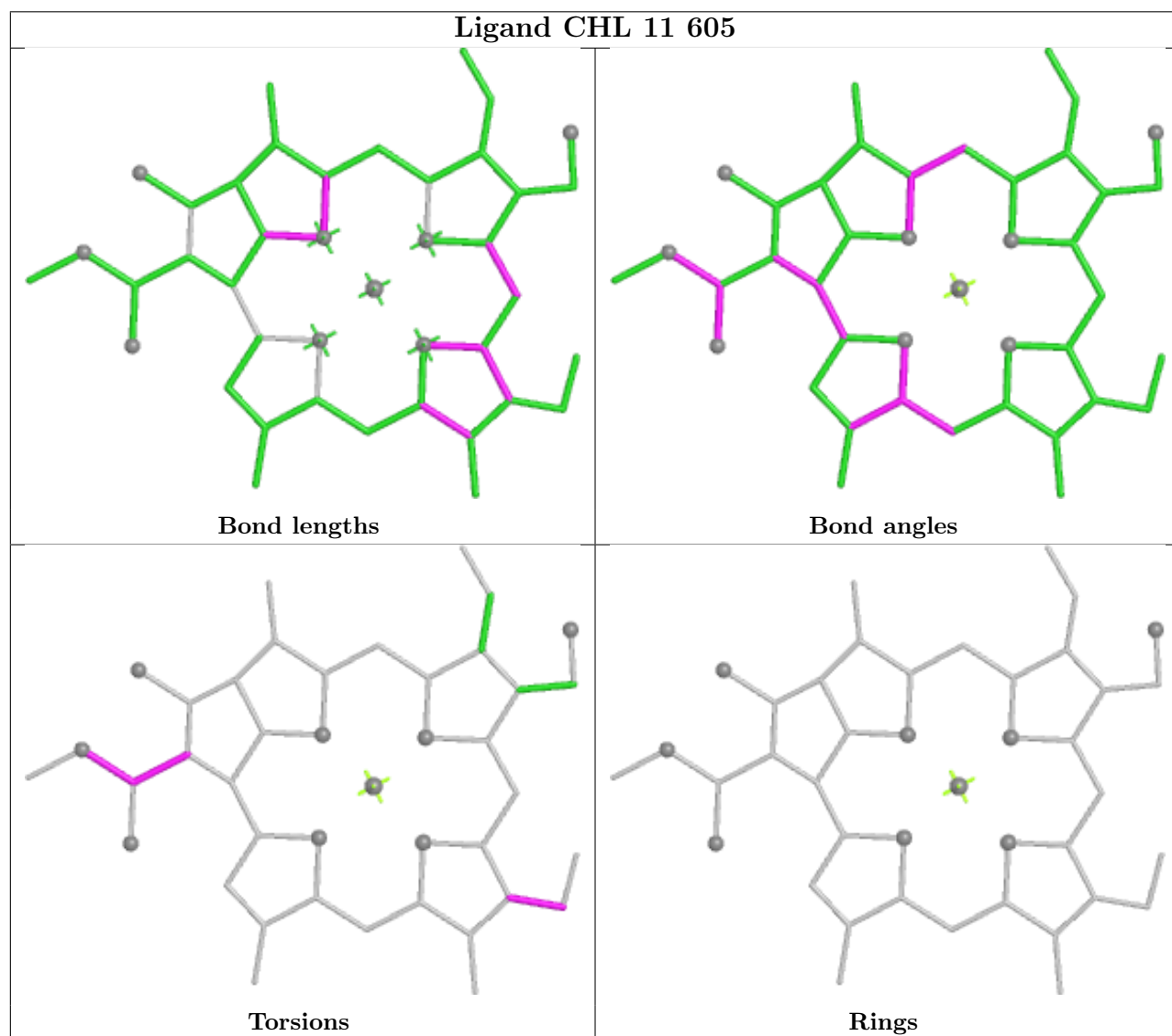
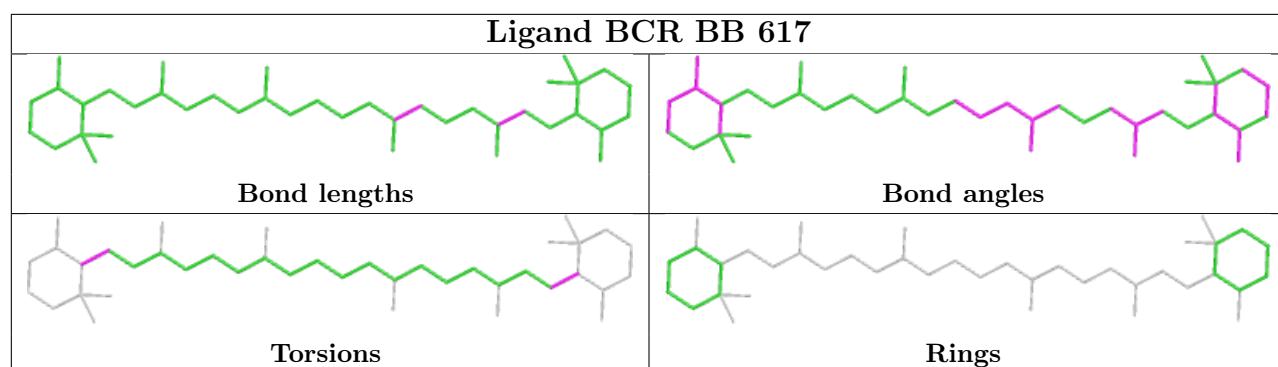
Bond angles



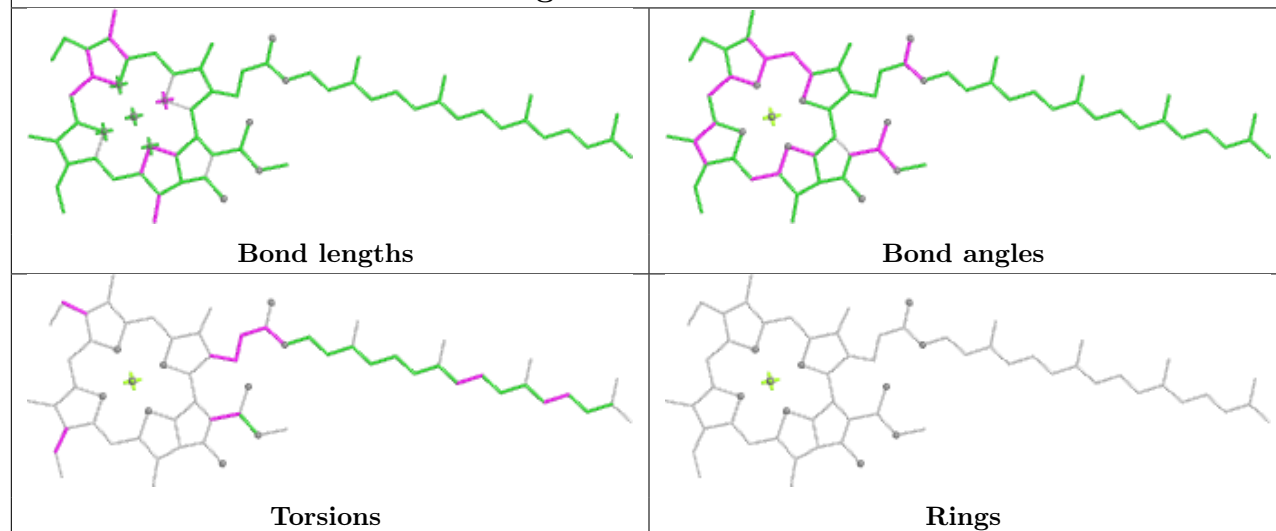
Torsions



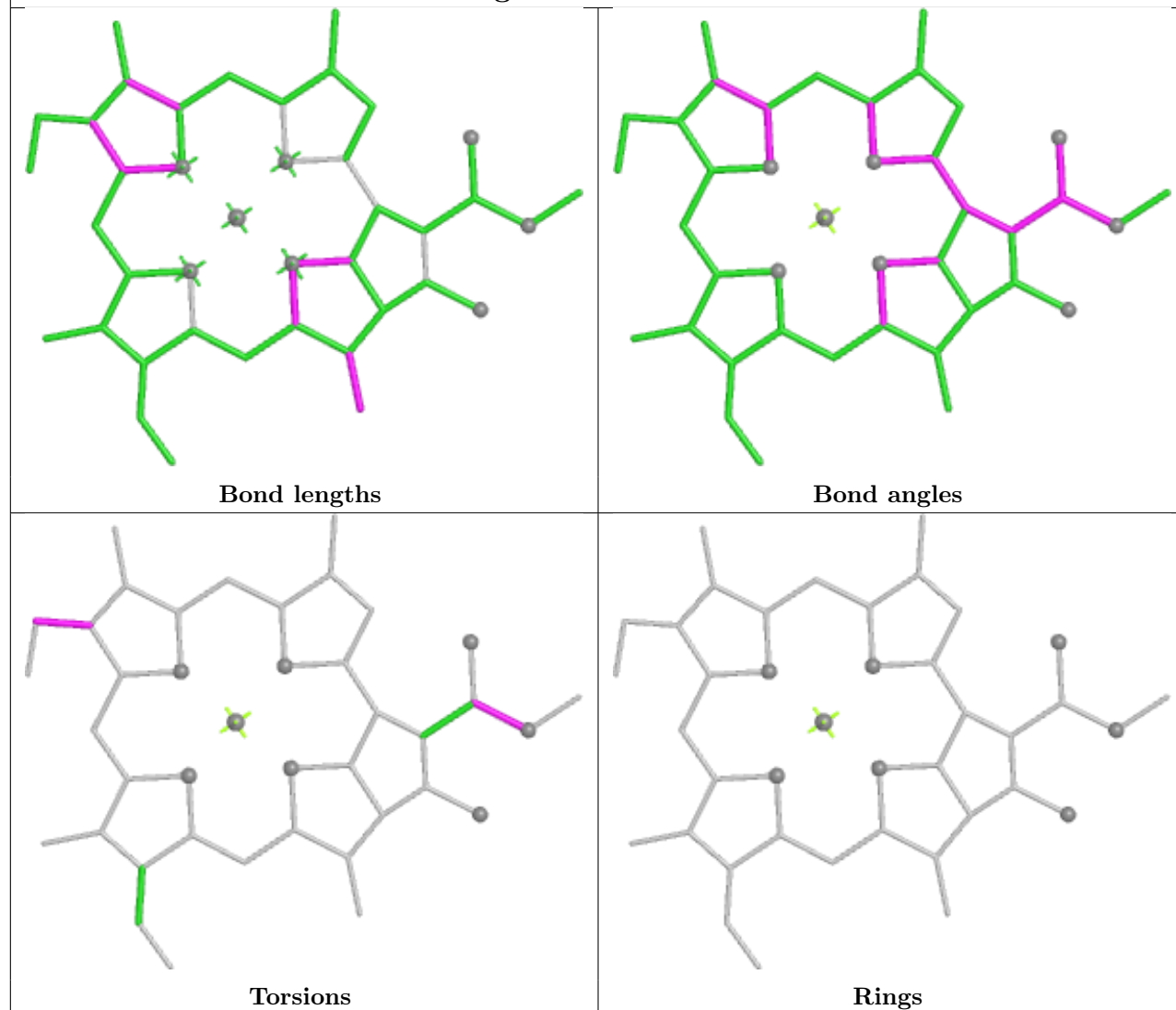
Rings

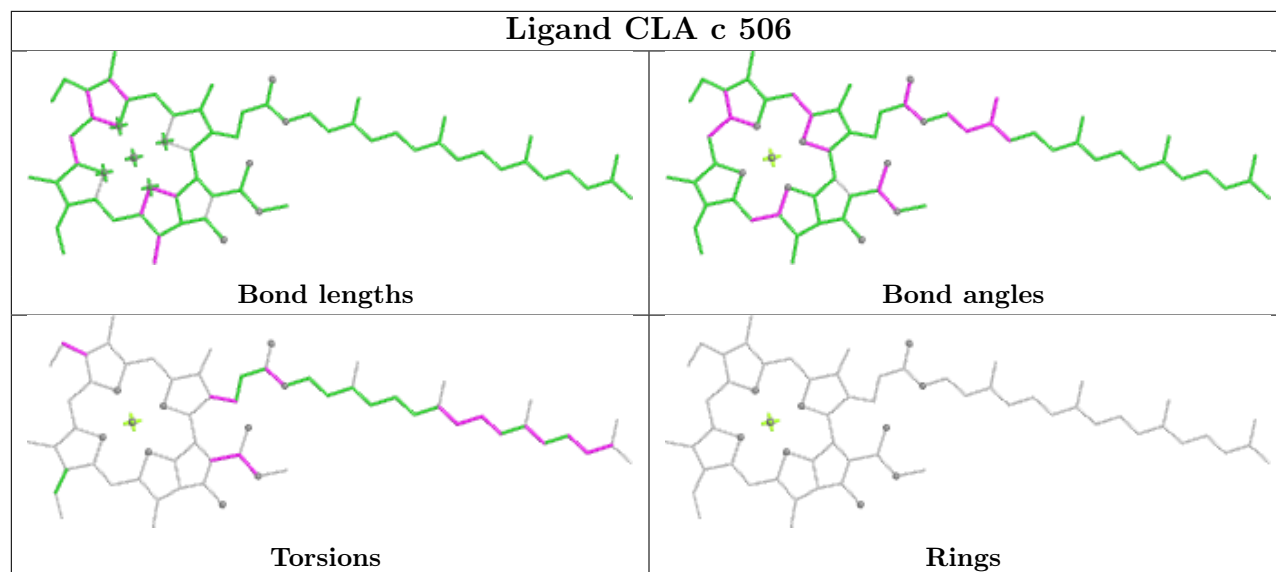
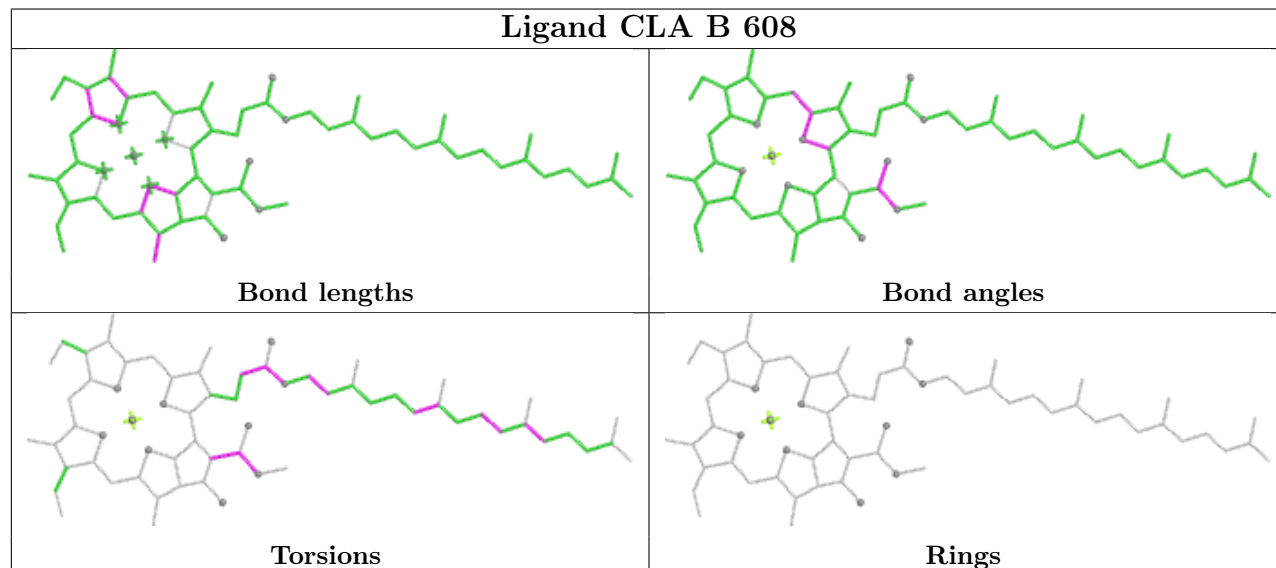


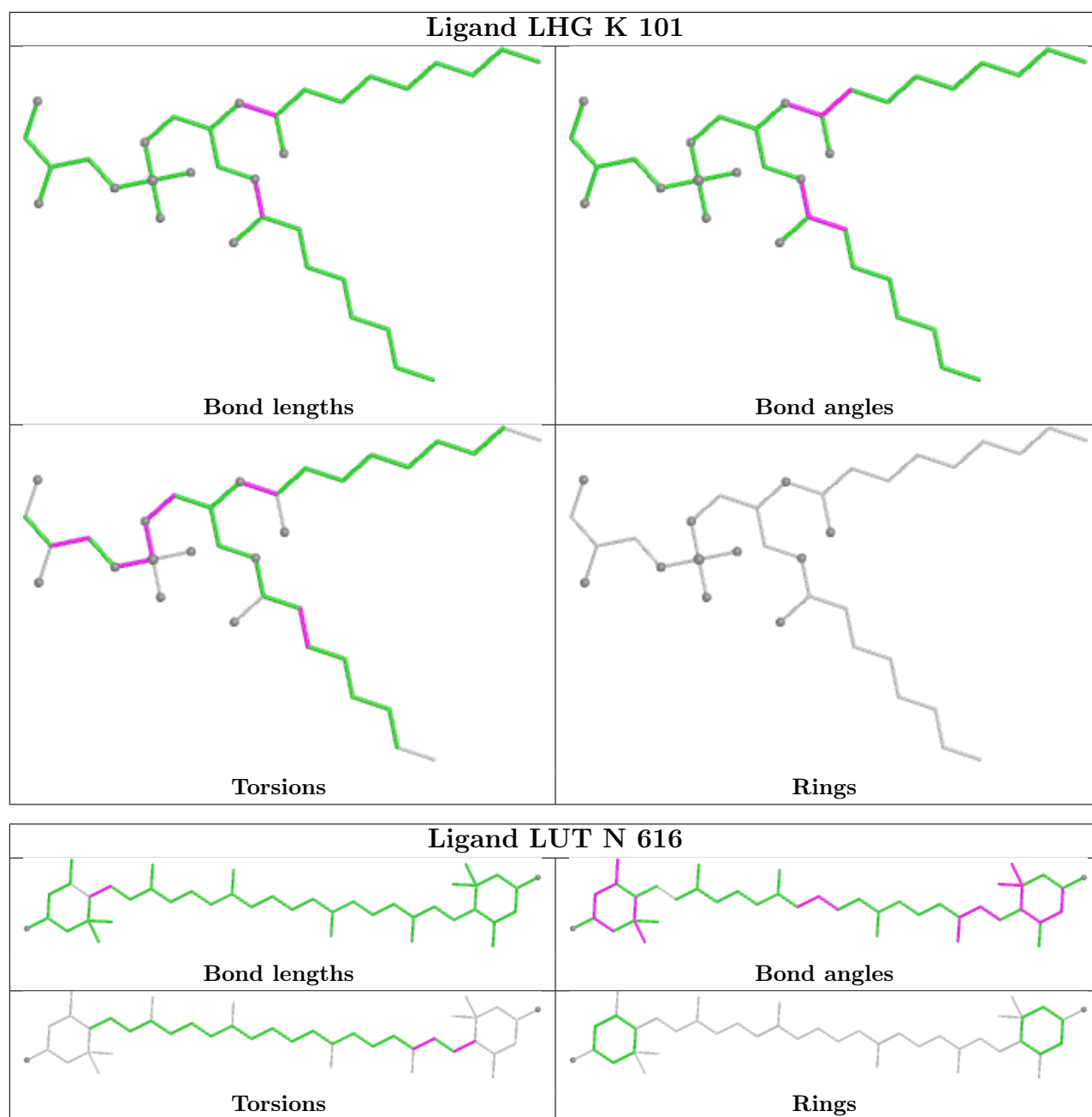
Ligand CLA a 406

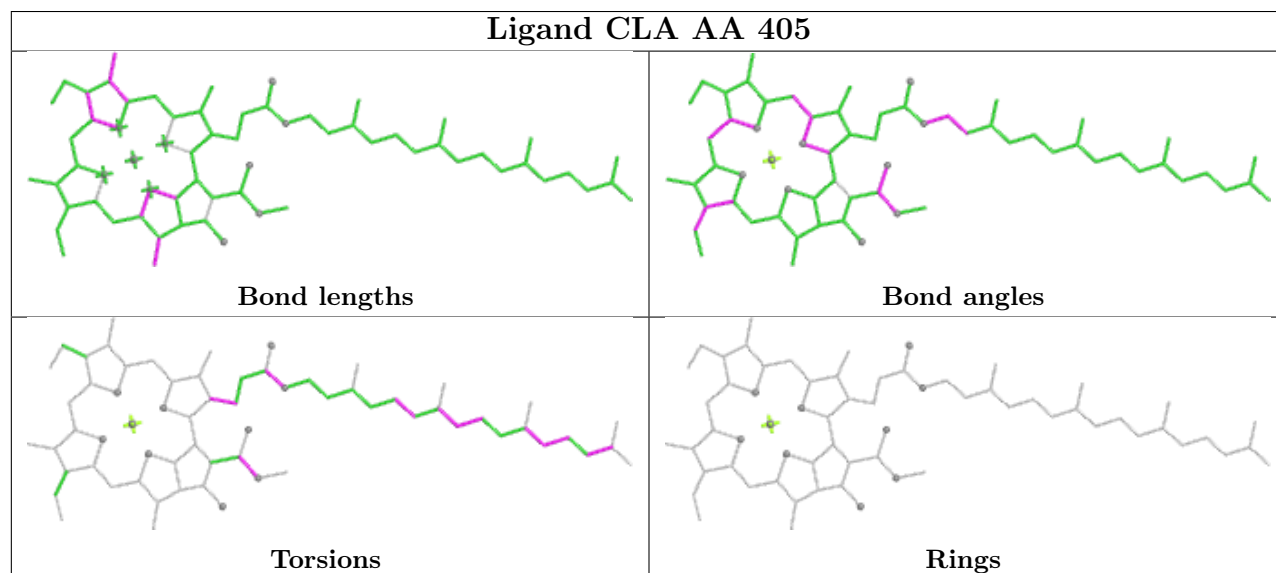
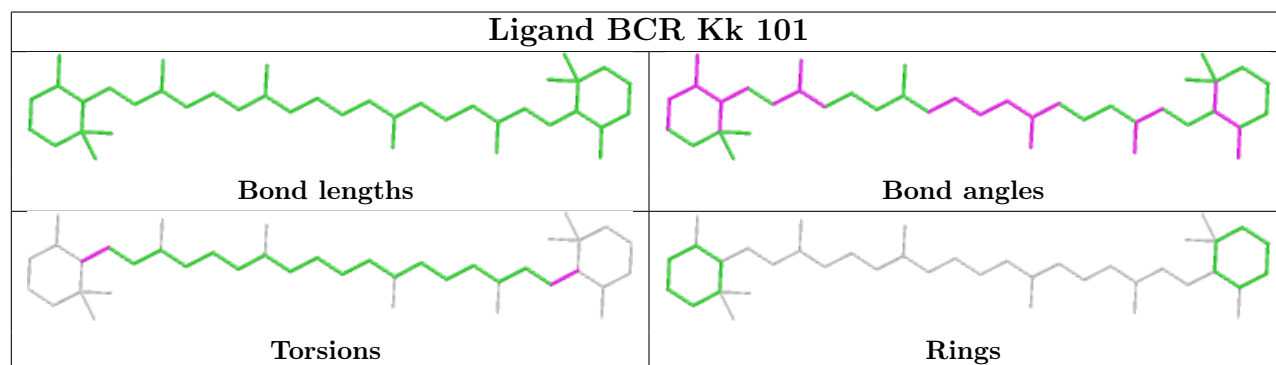
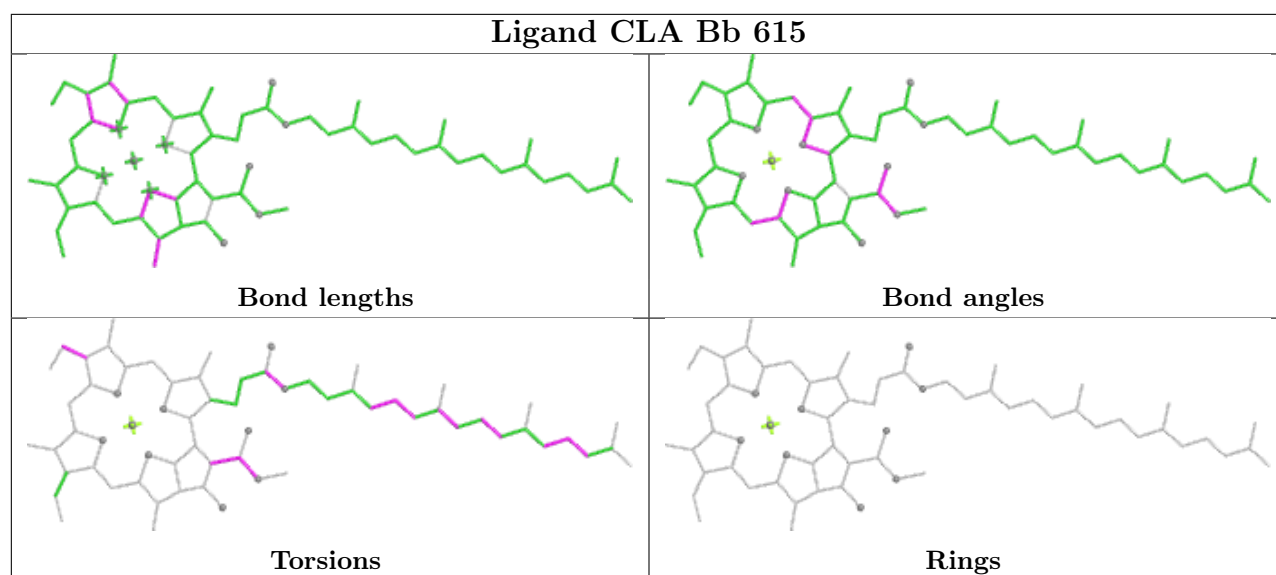


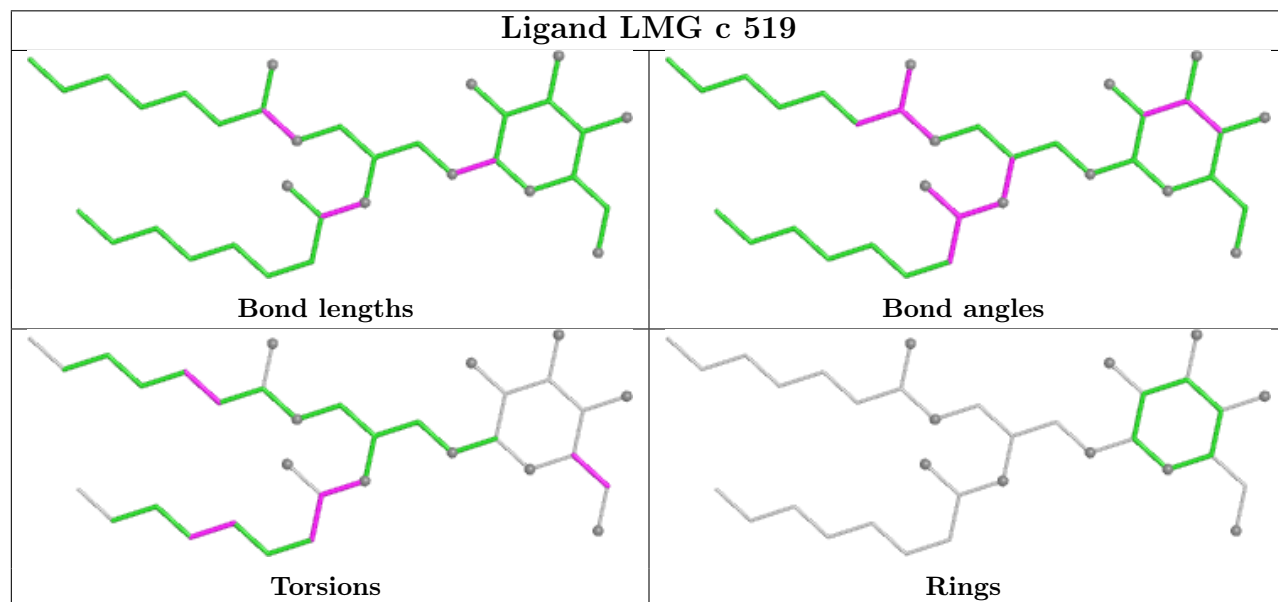
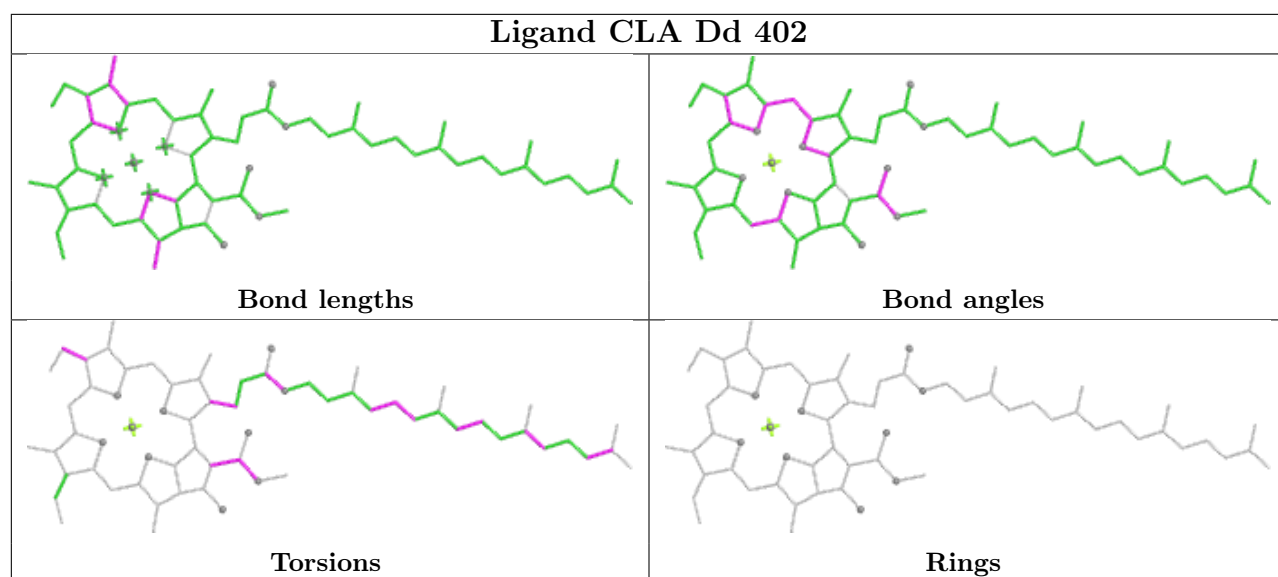
Ligand CLA 1 609

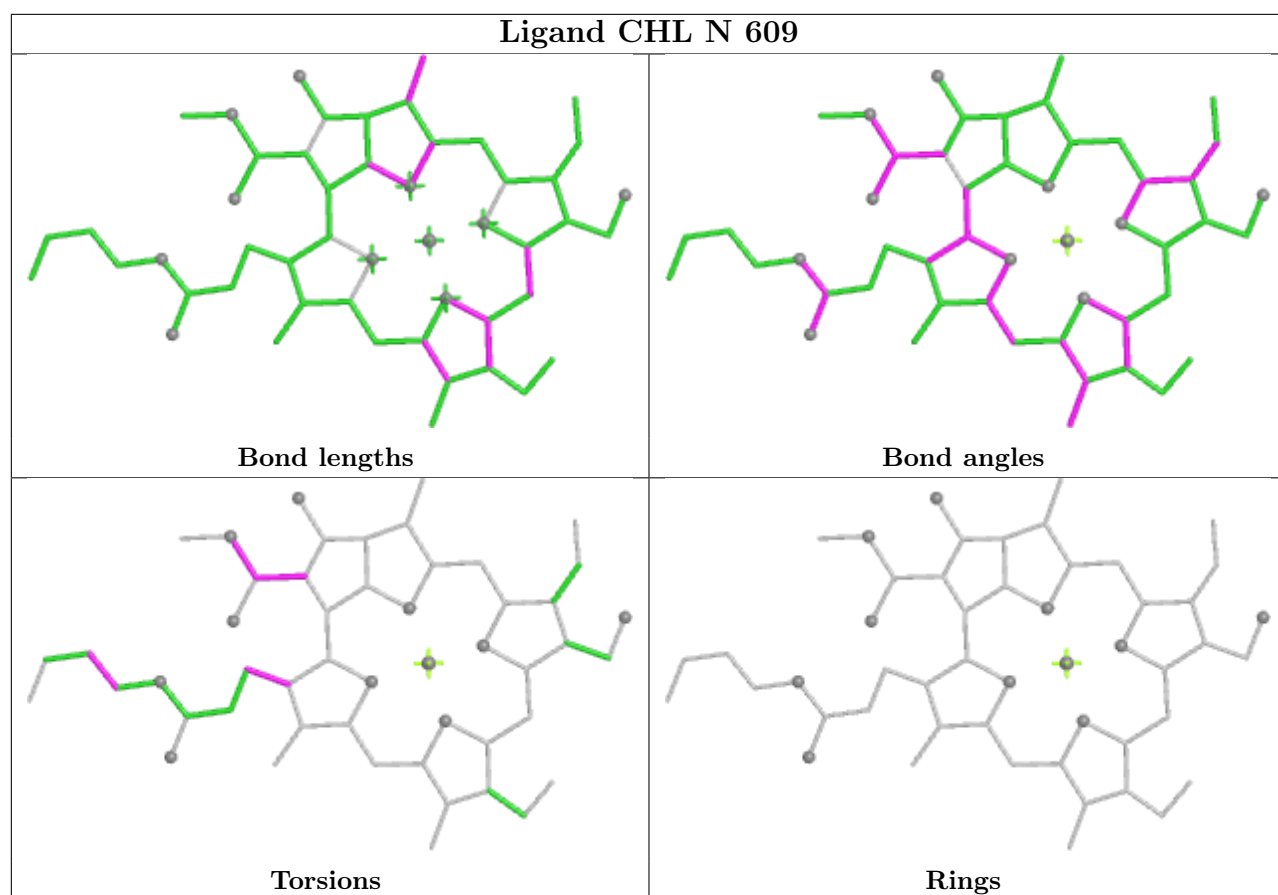


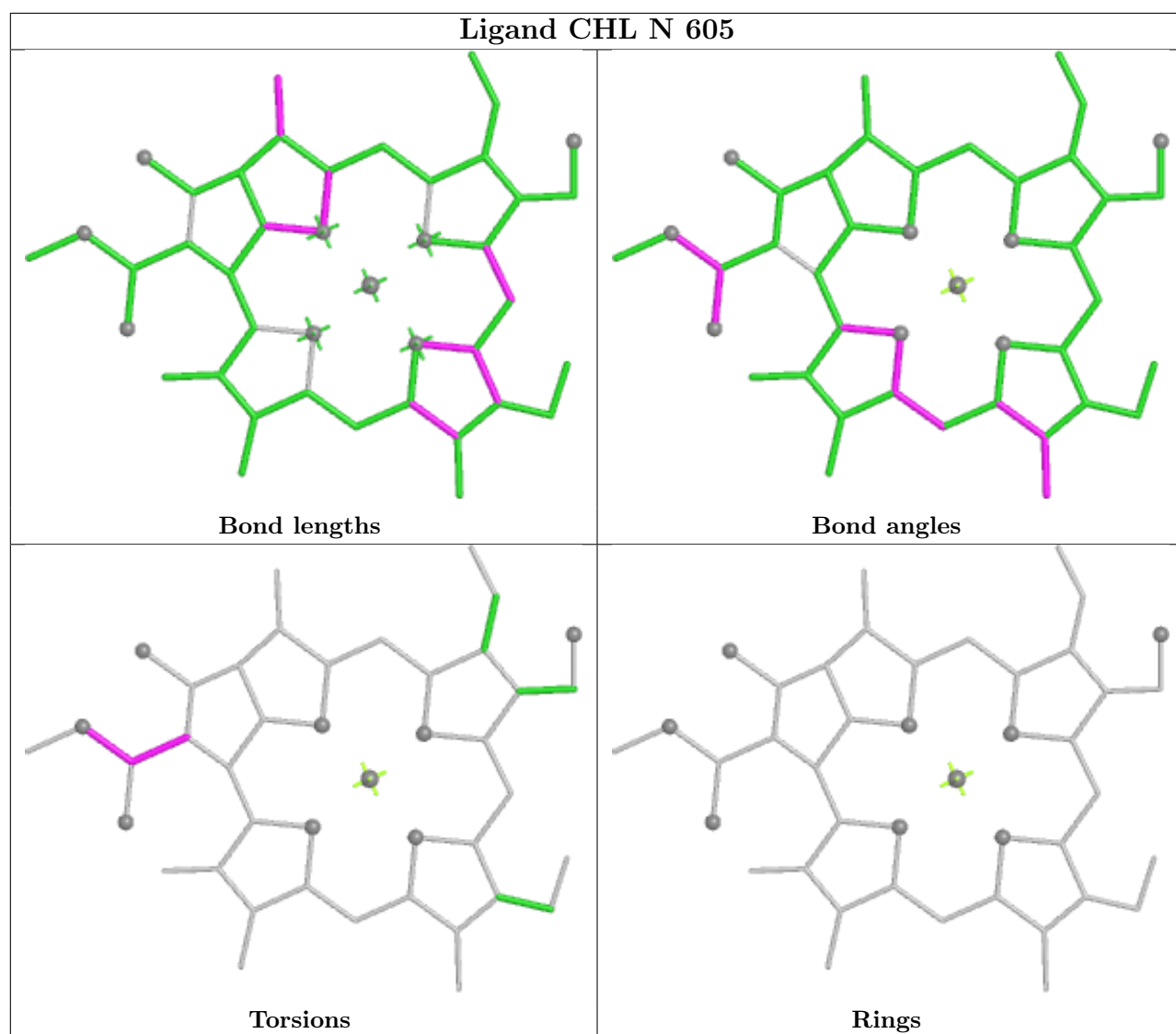
Ligand CLA c 506**Ligand CLA B 608**



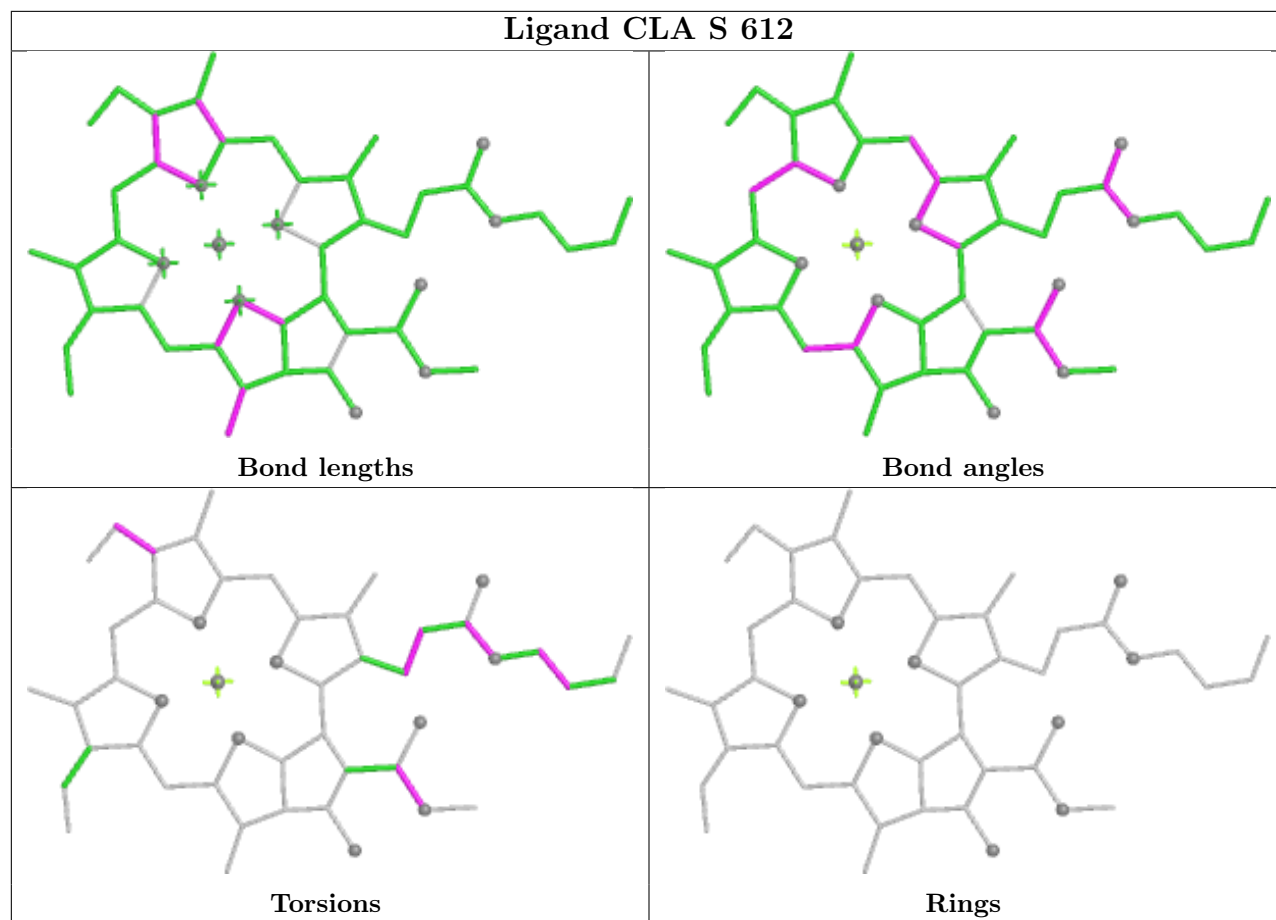


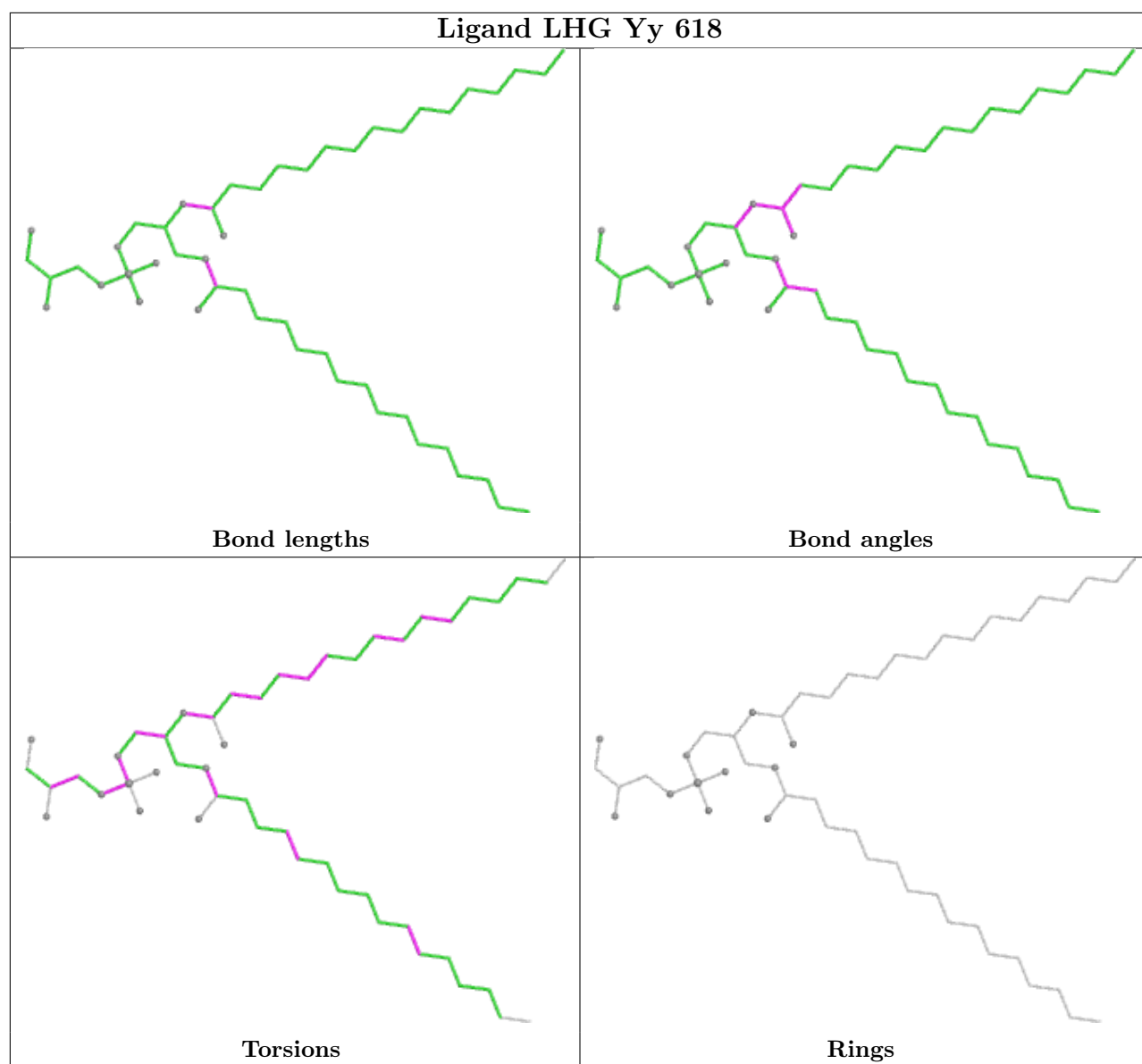




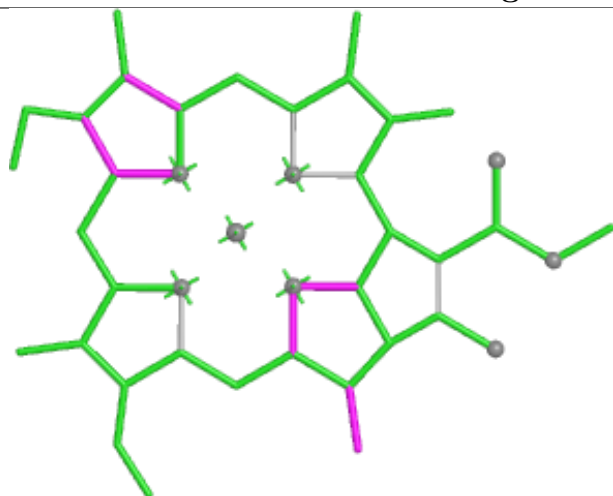


Ligand CLA S 612





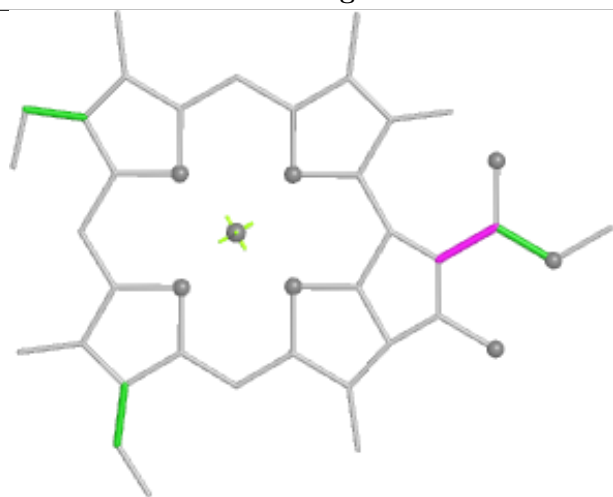
Ligand CLA BB 615



Bond lengths



Bond angles

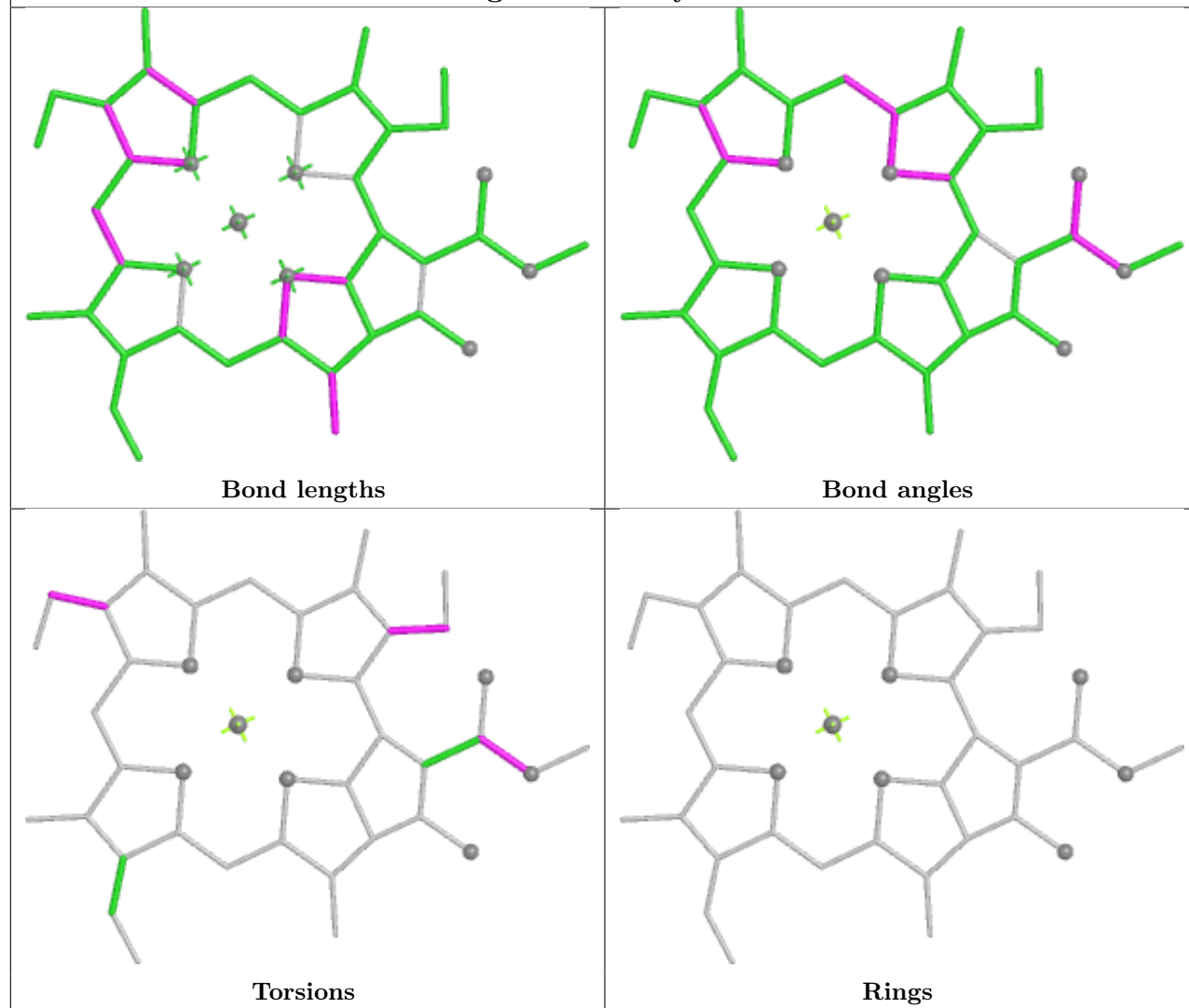


Torsions

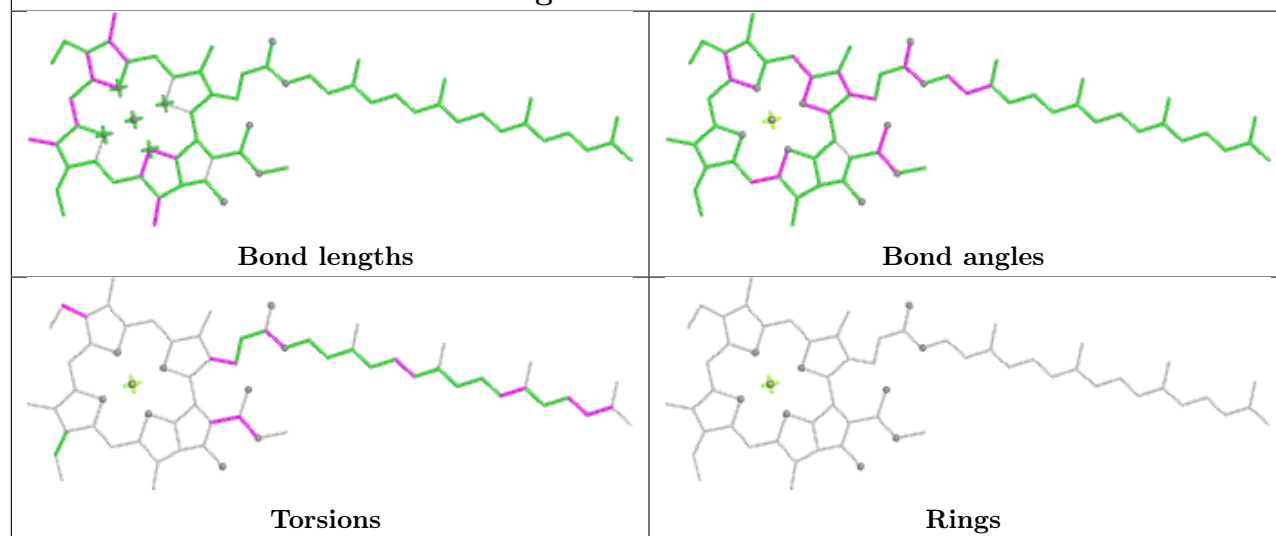


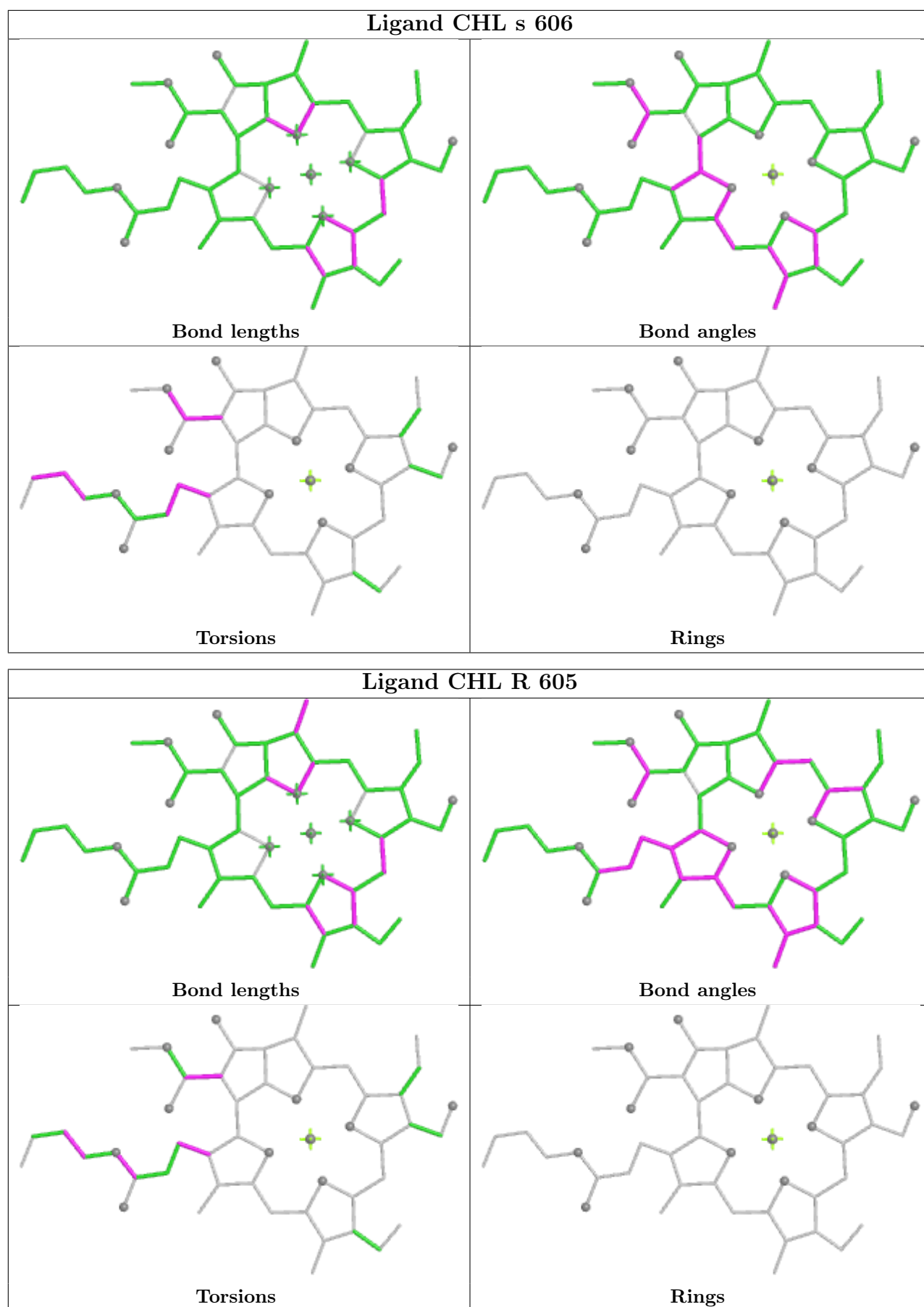
Rings

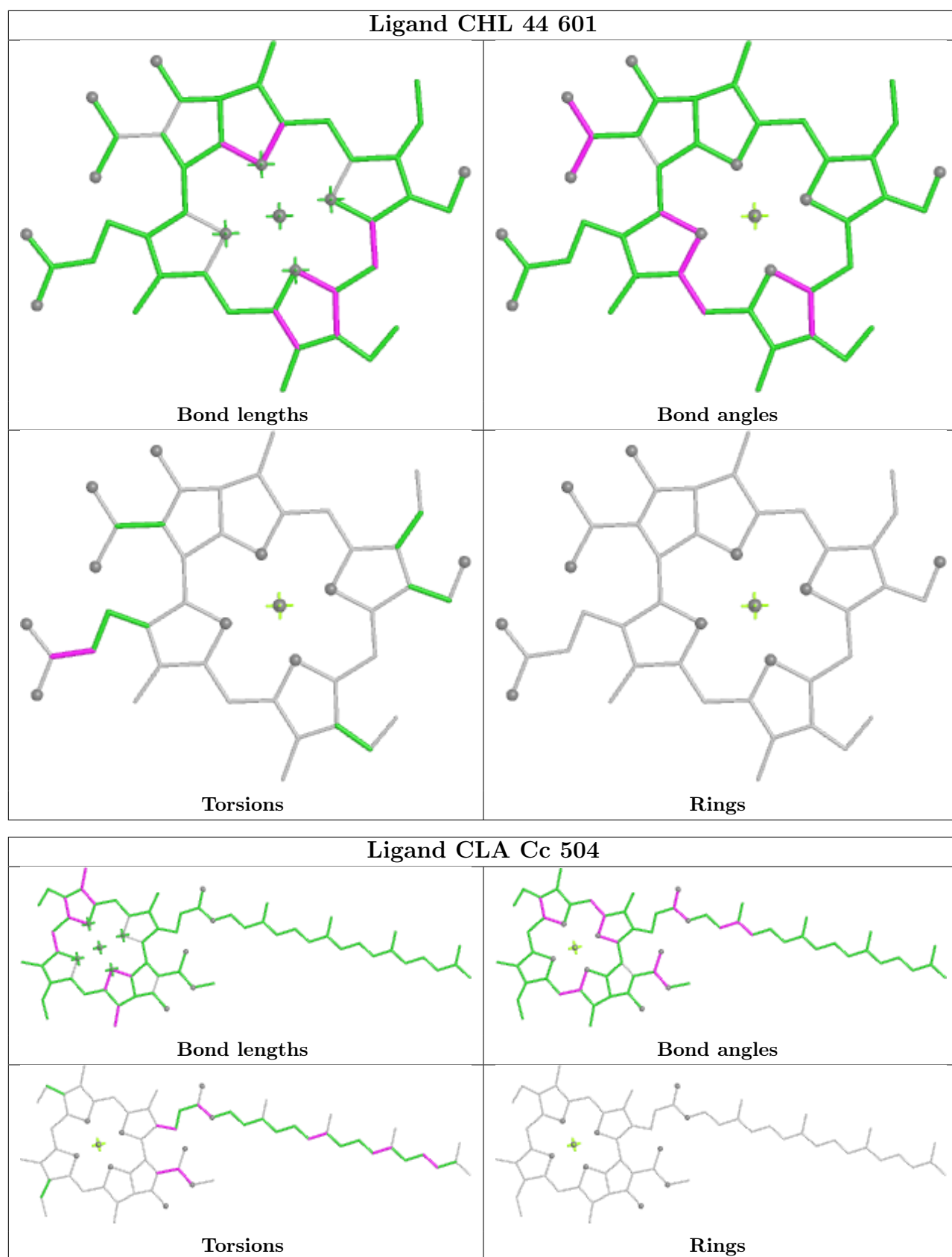
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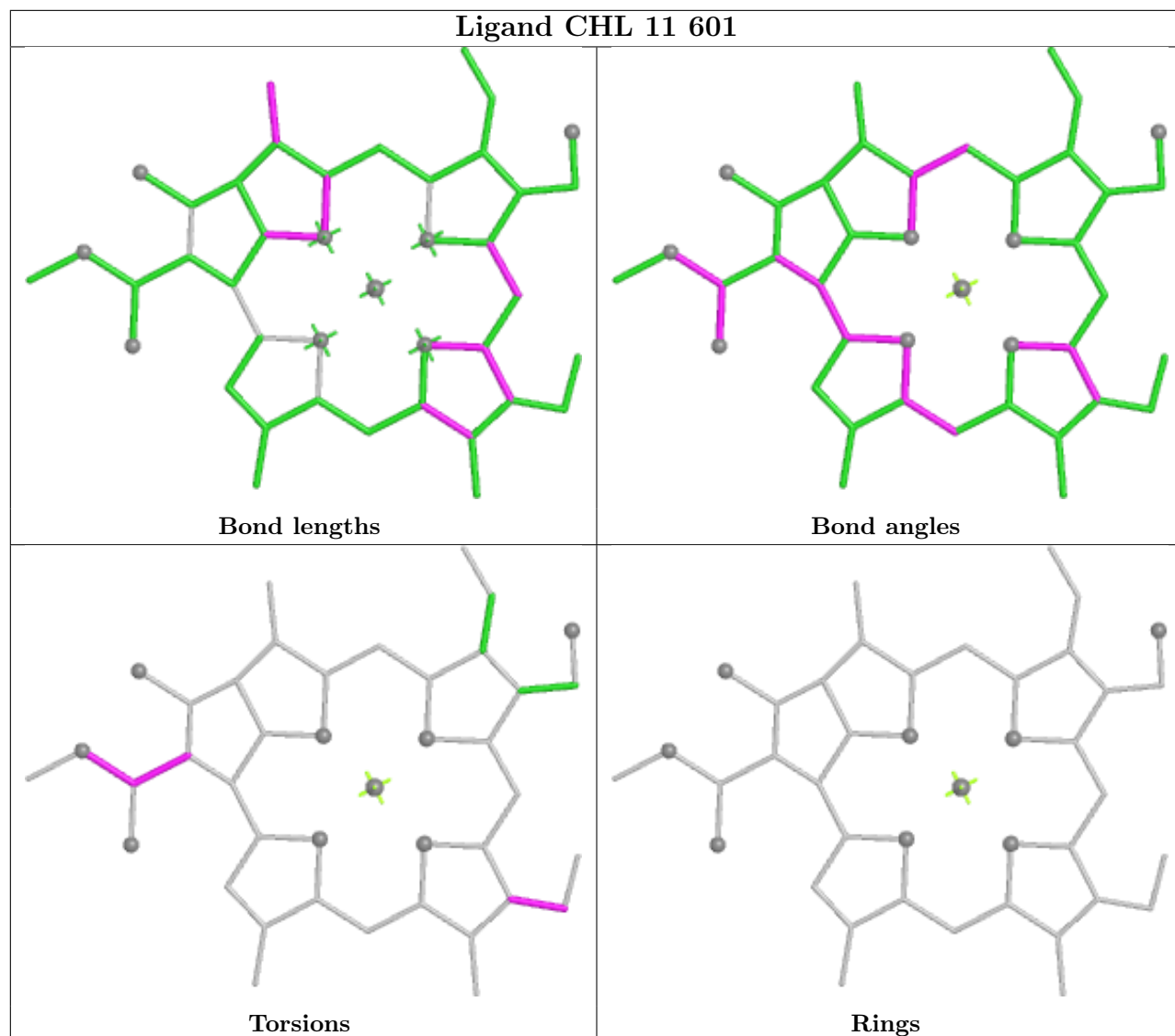


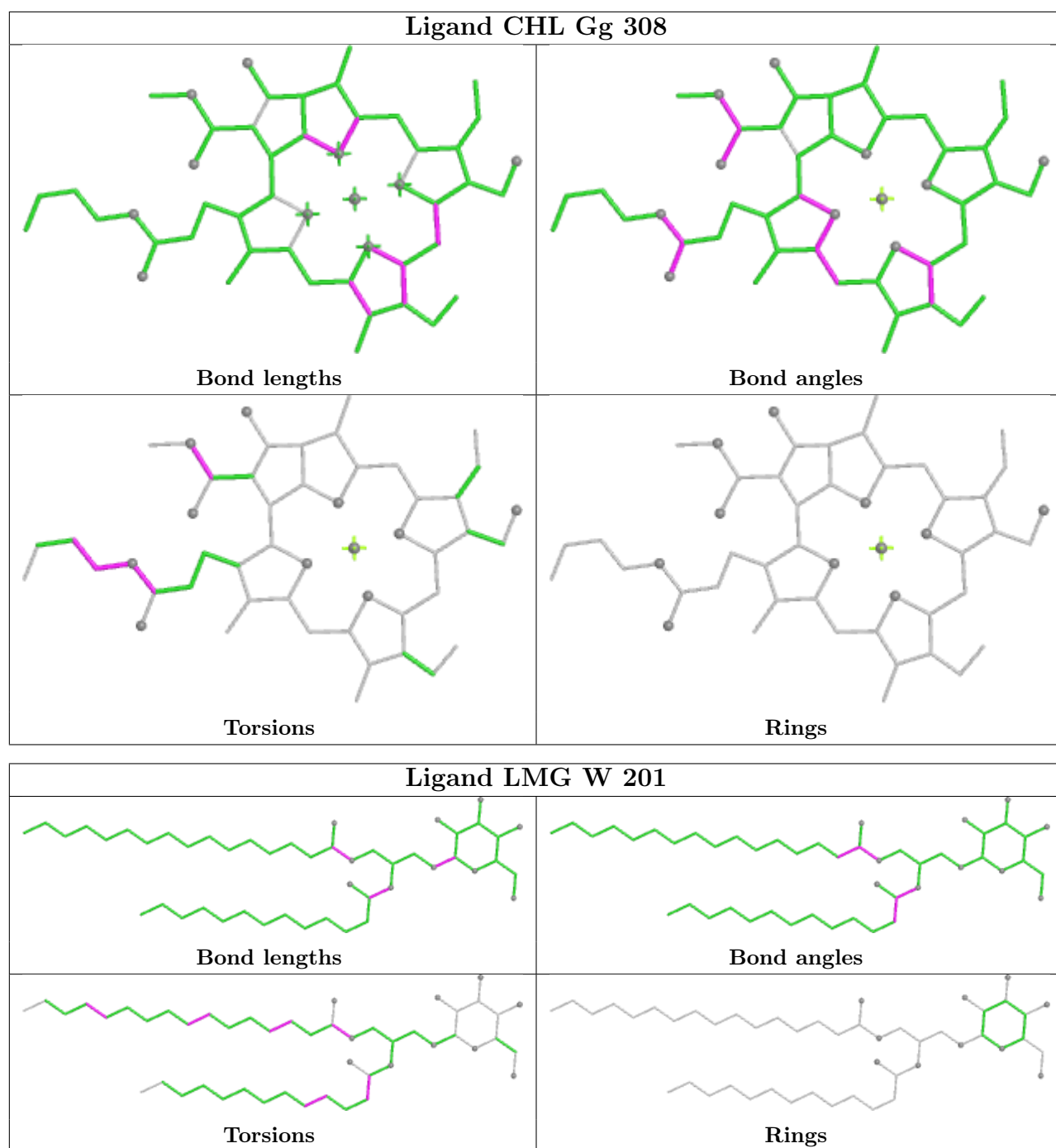
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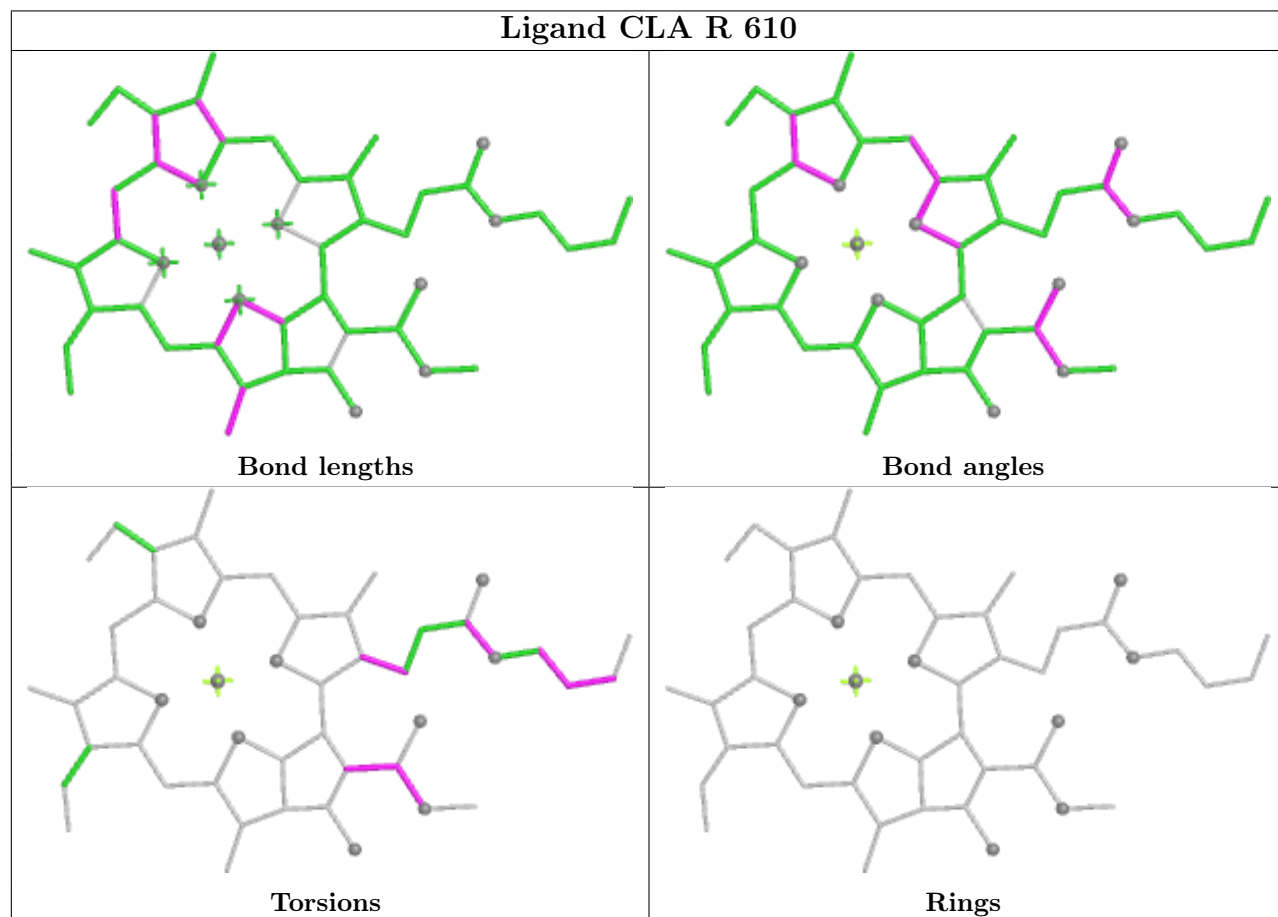
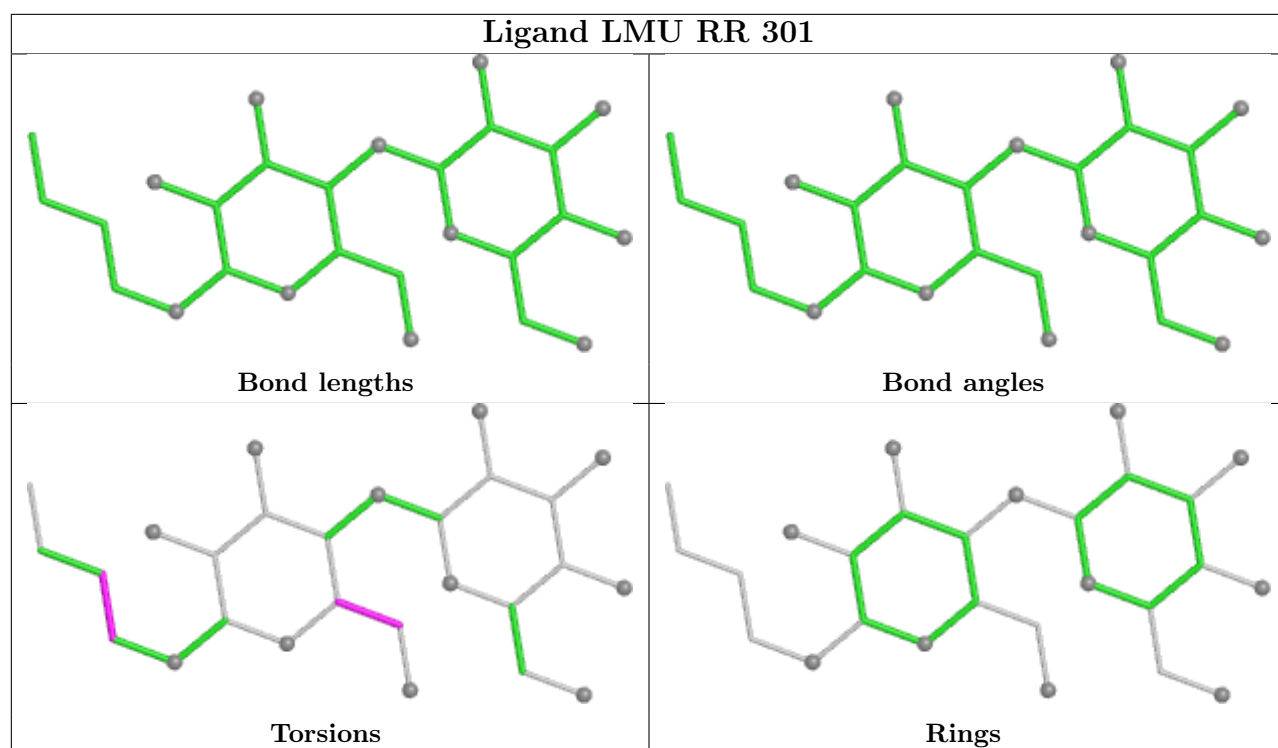


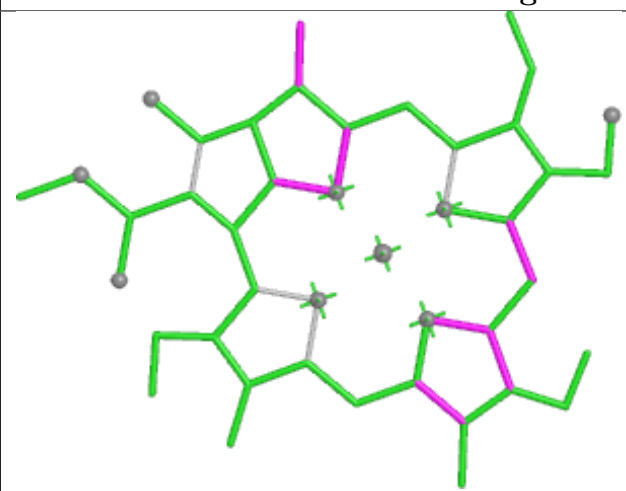
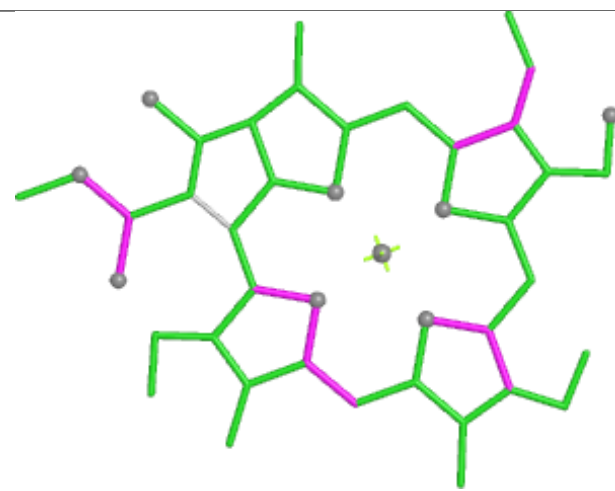
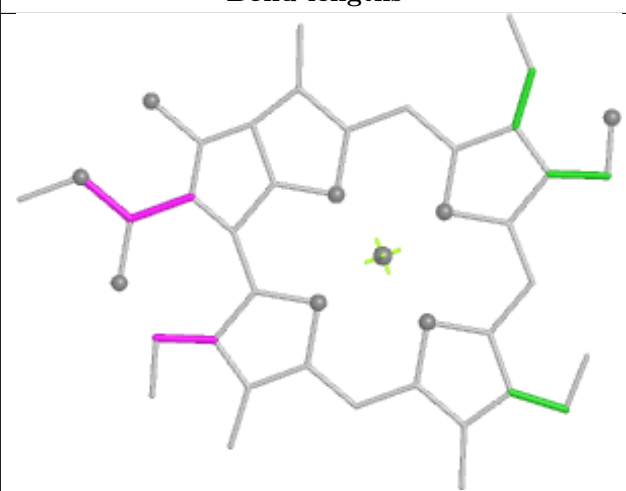


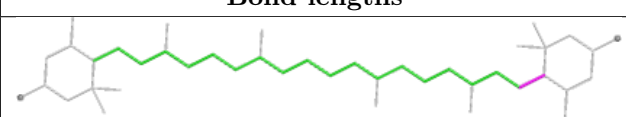
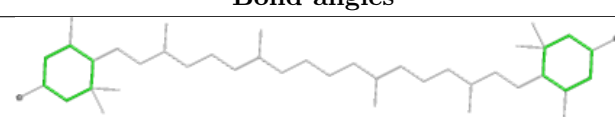


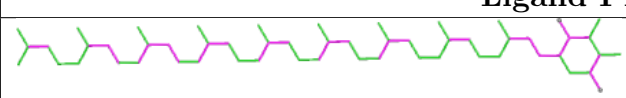
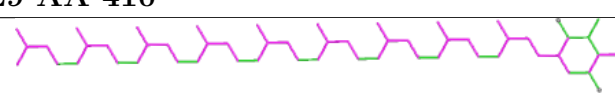
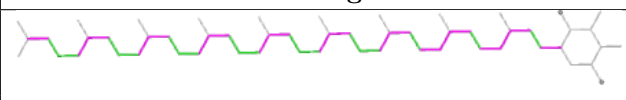
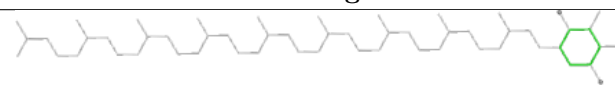


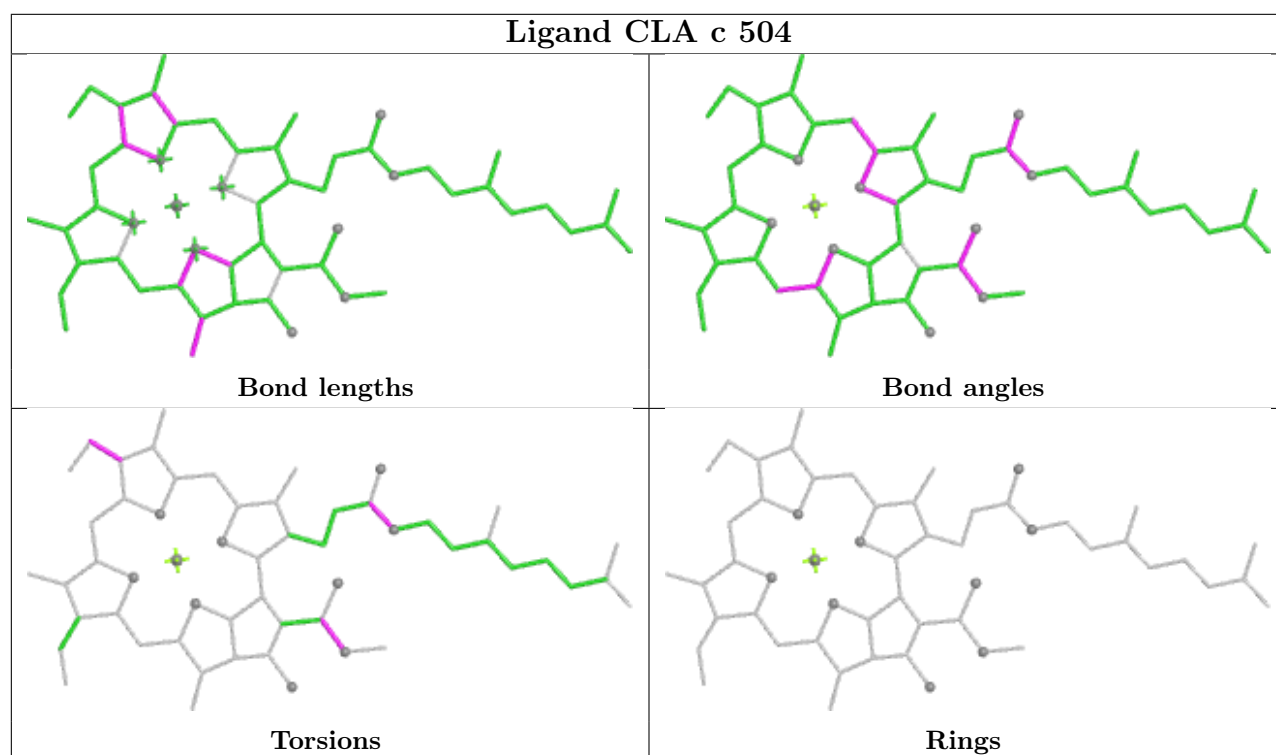
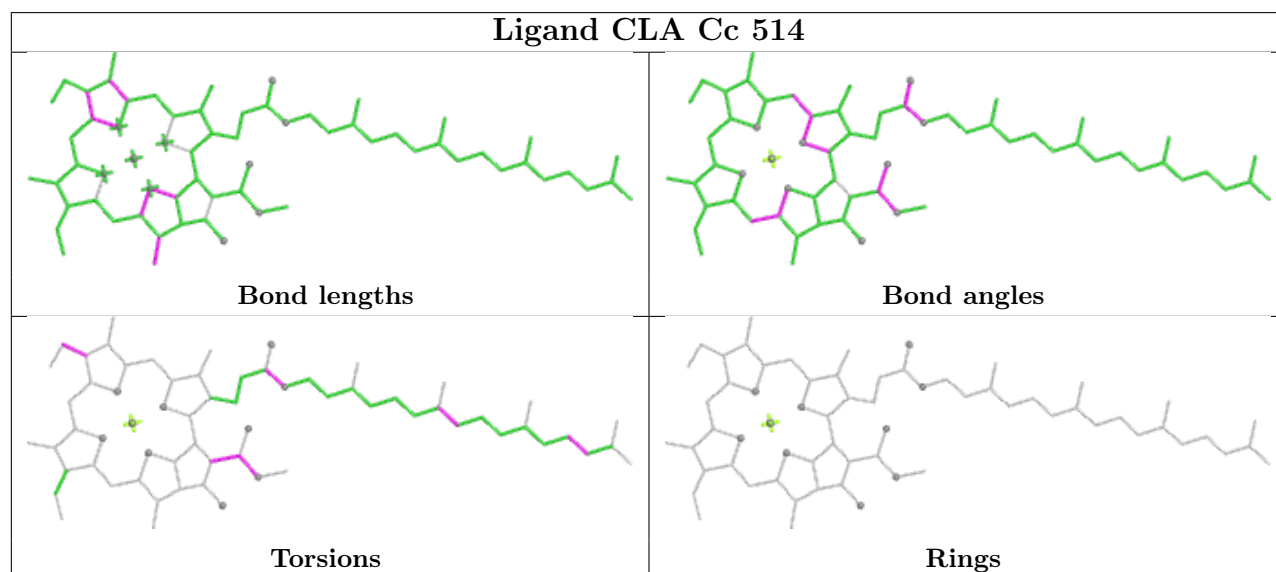
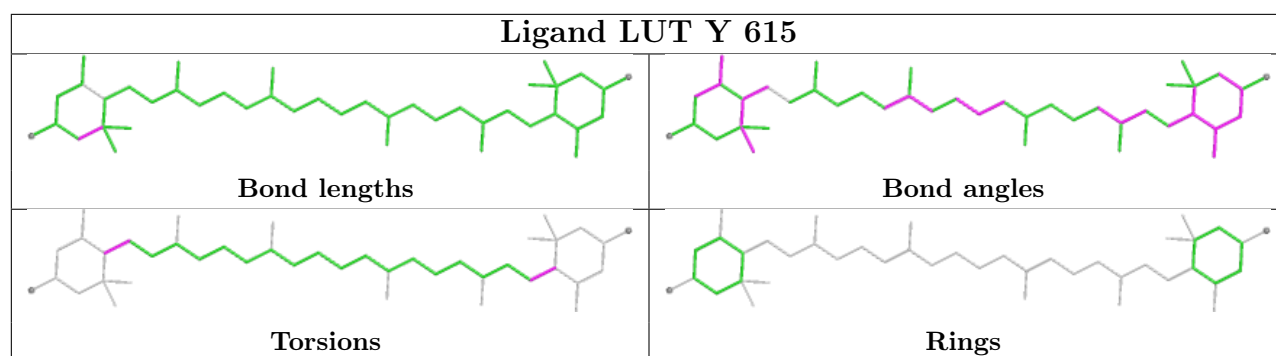




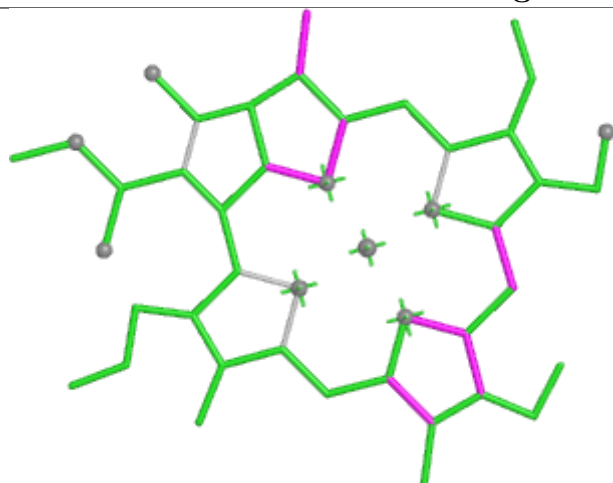
Ligand CHL G 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT Y 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

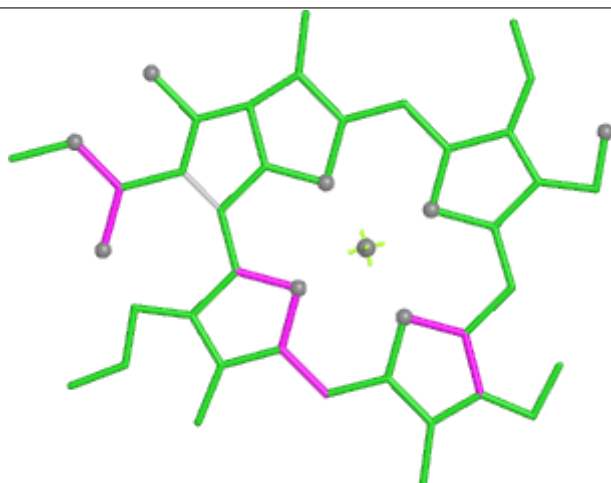
Ligand PL9 AA 410	
	
Bond lengths	Bond angles
	
Torsions	Rings



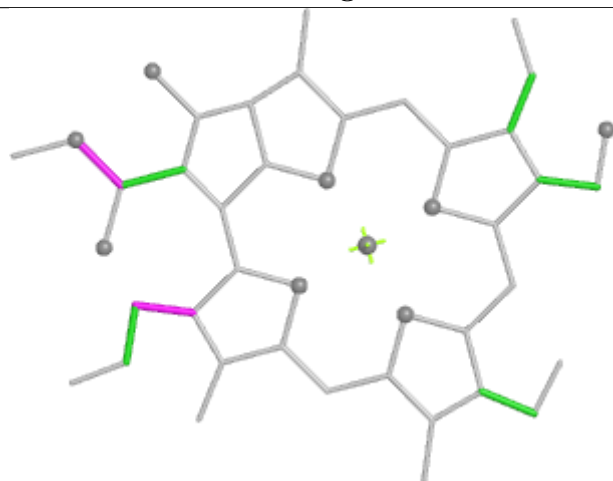
Ligand CHL Y 606



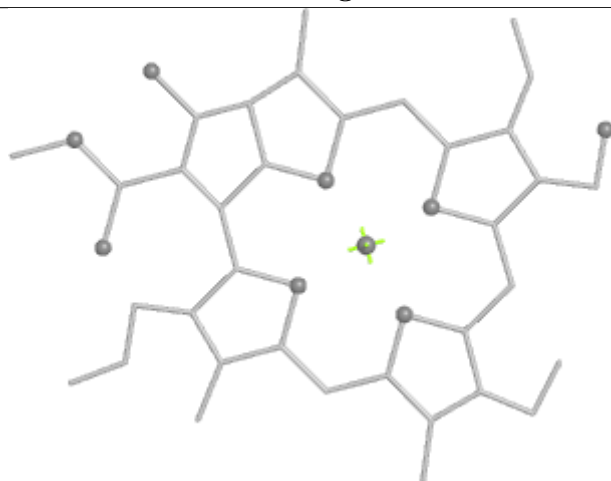
Bond lengths



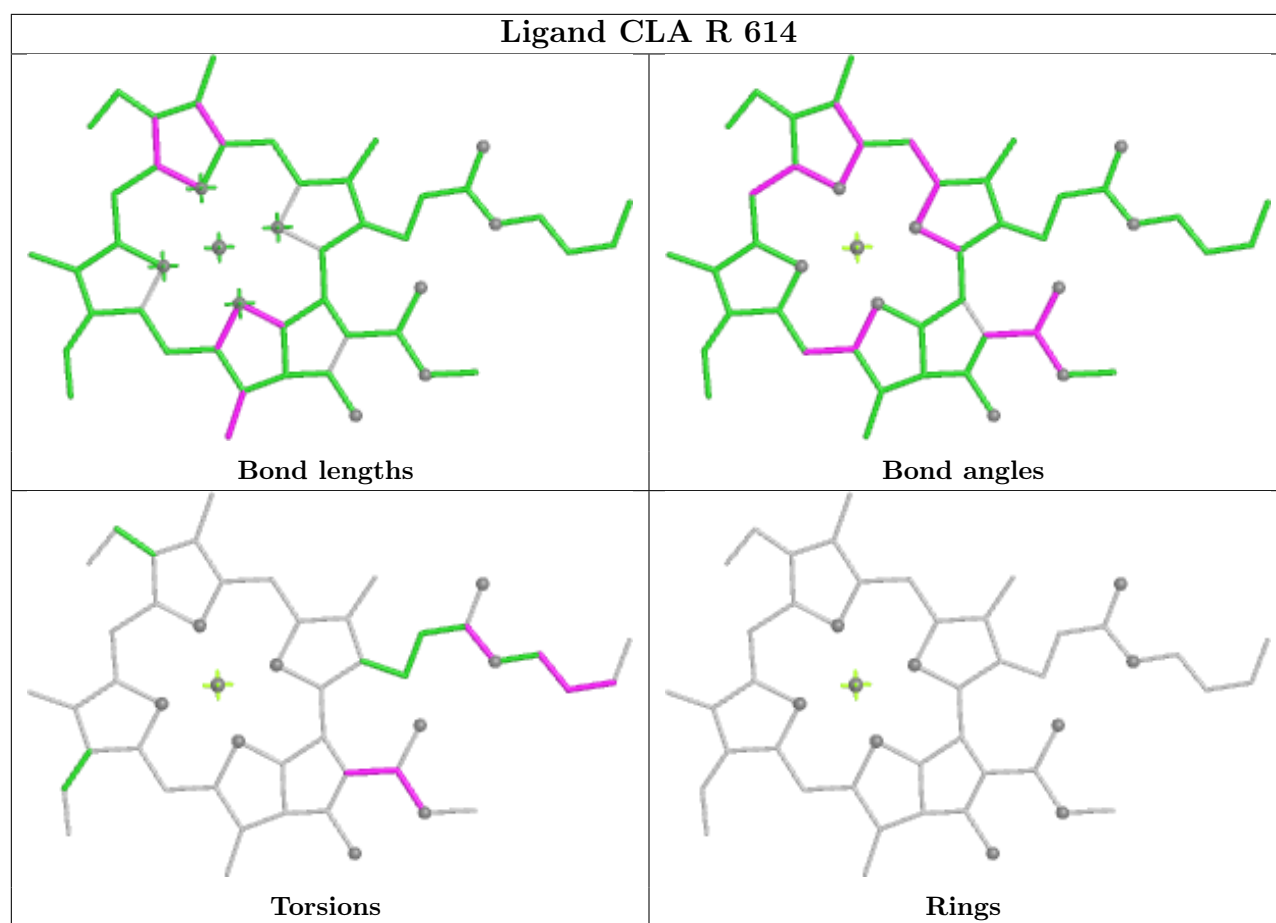
Bond angles



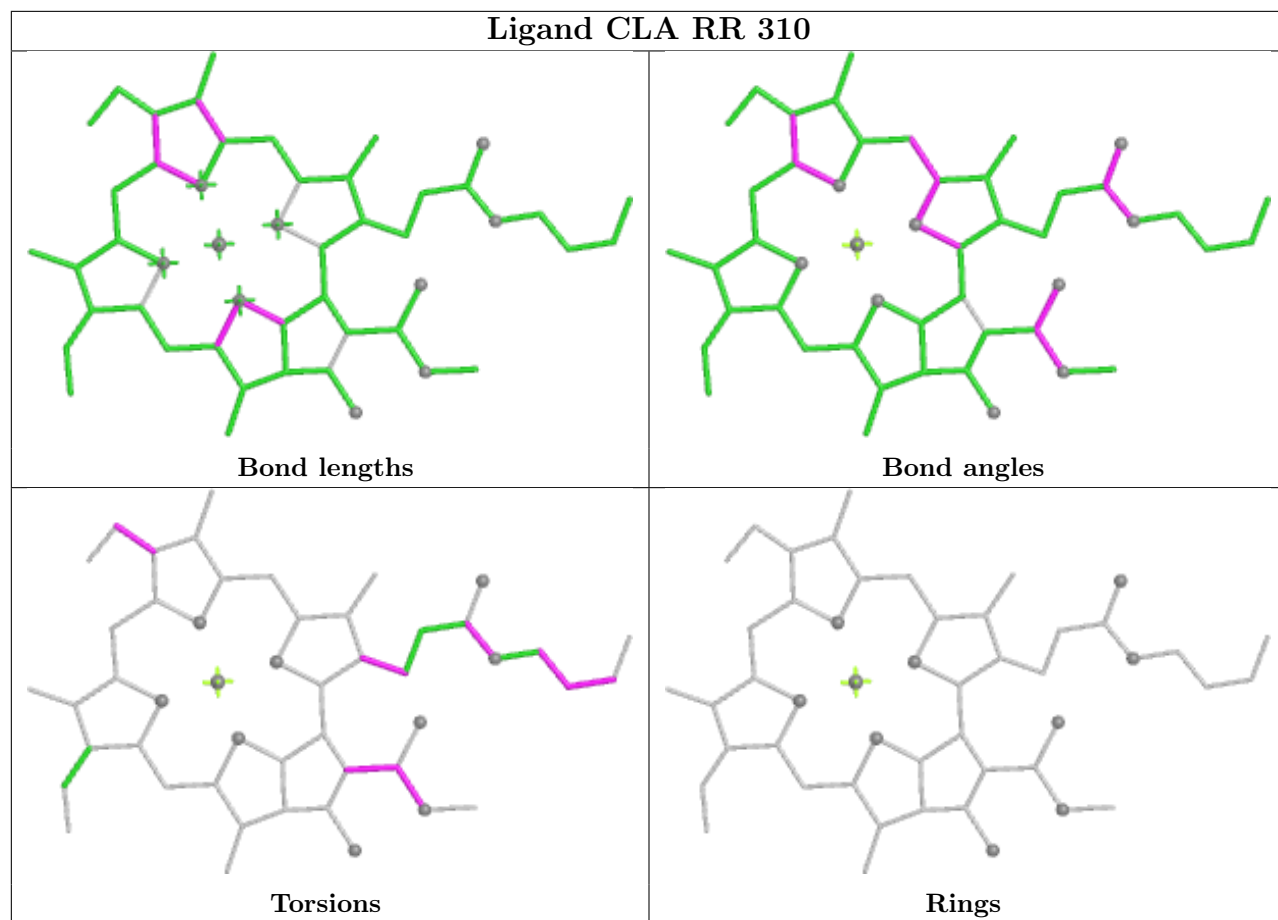
Torsions

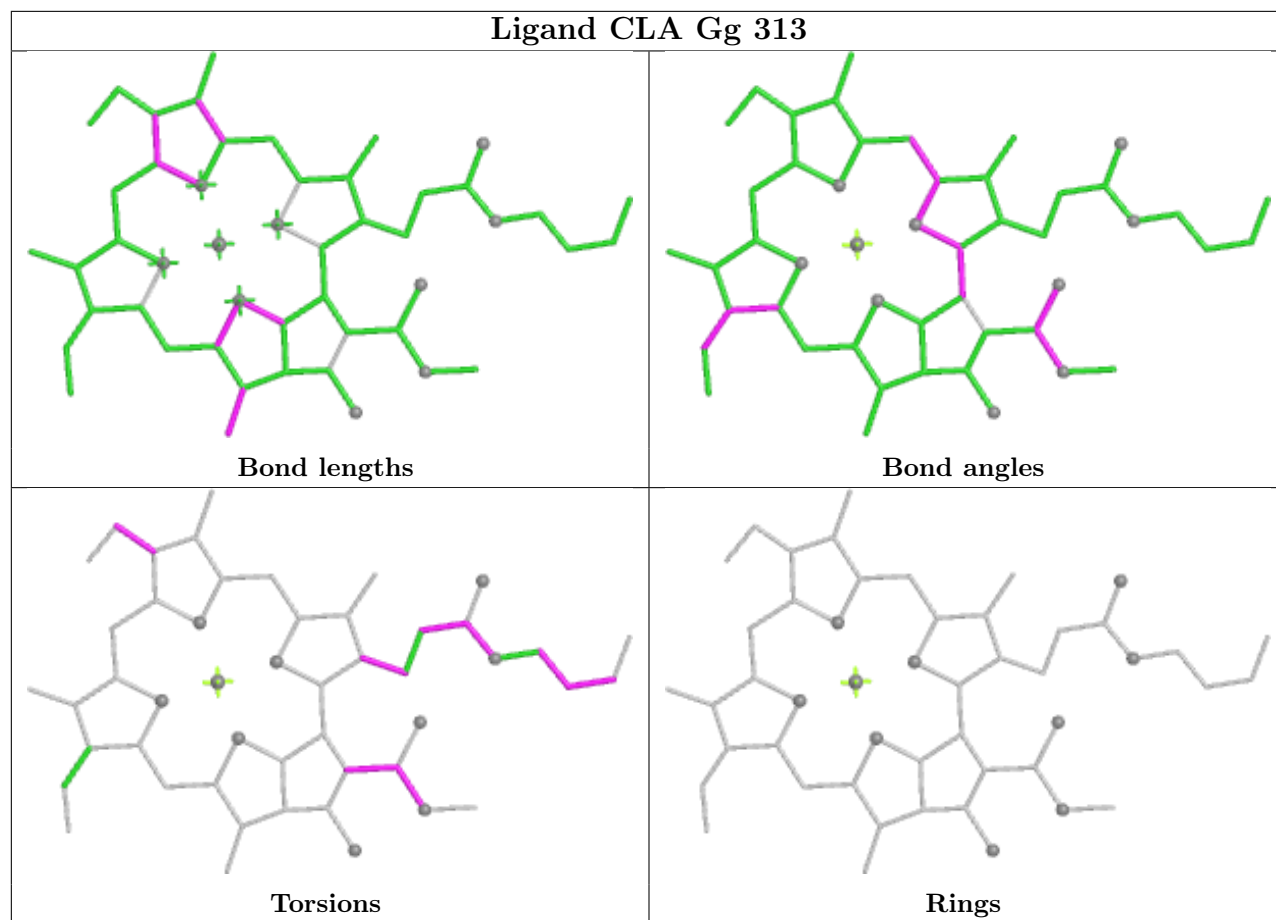


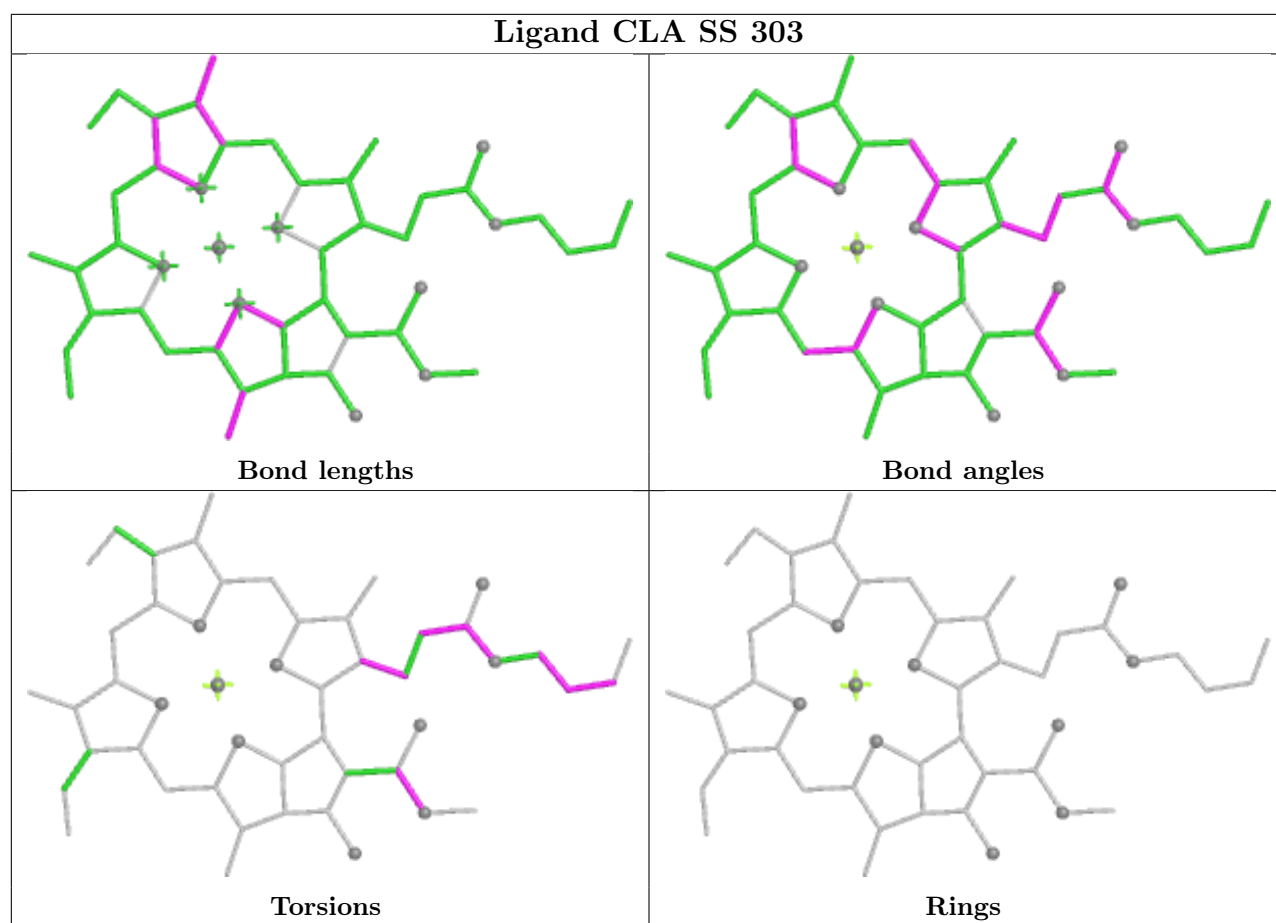
Rings



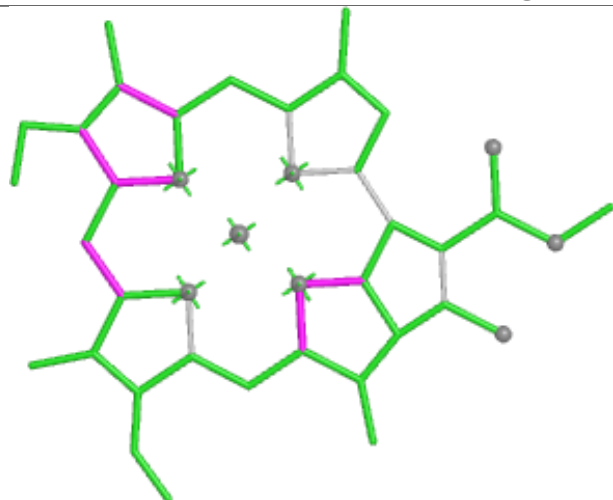
Ligand CLA RR 310



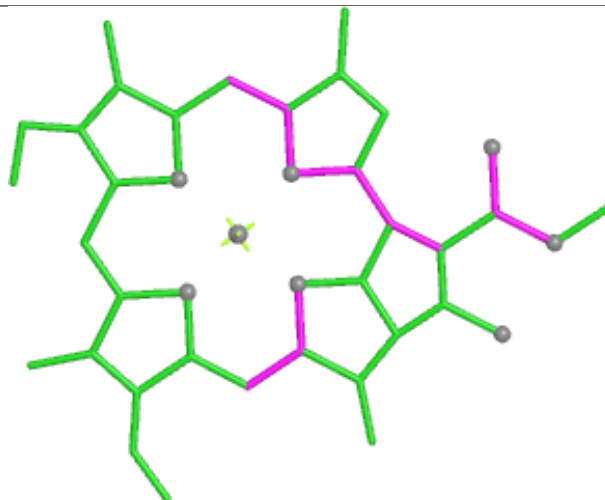




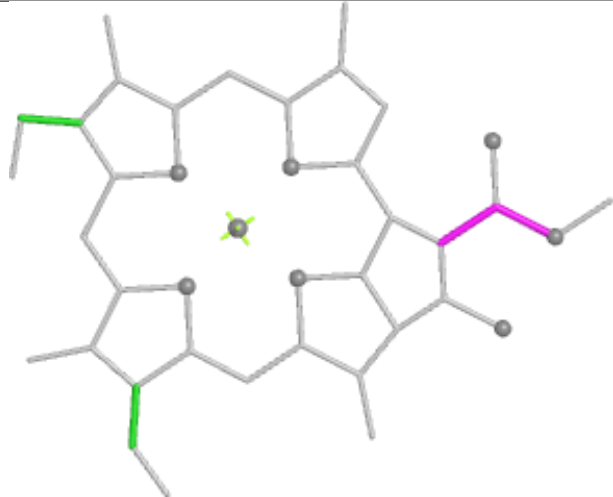
Ligand CLA 1 602



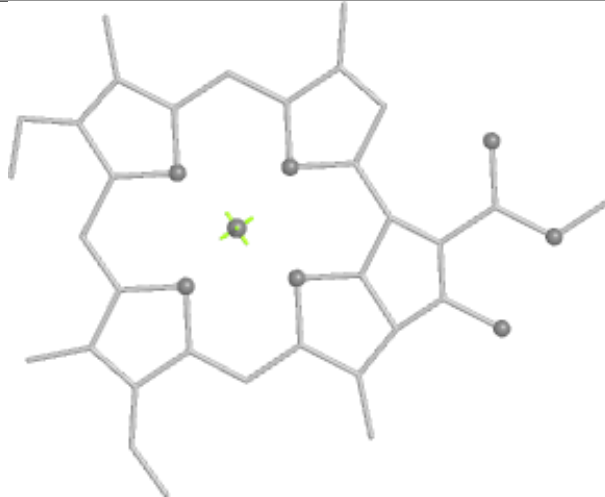
Bond lengths



Bond angles

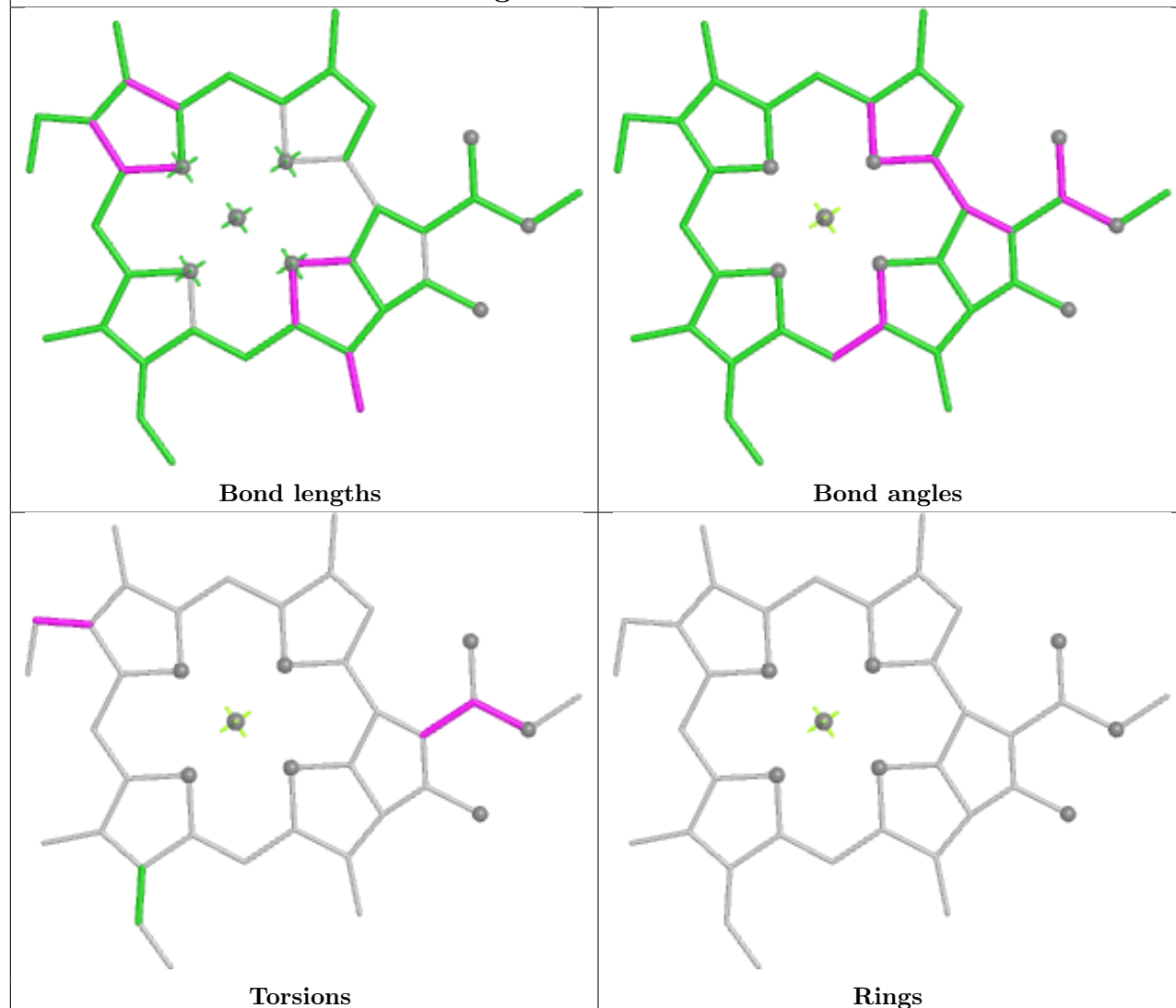


Torsions

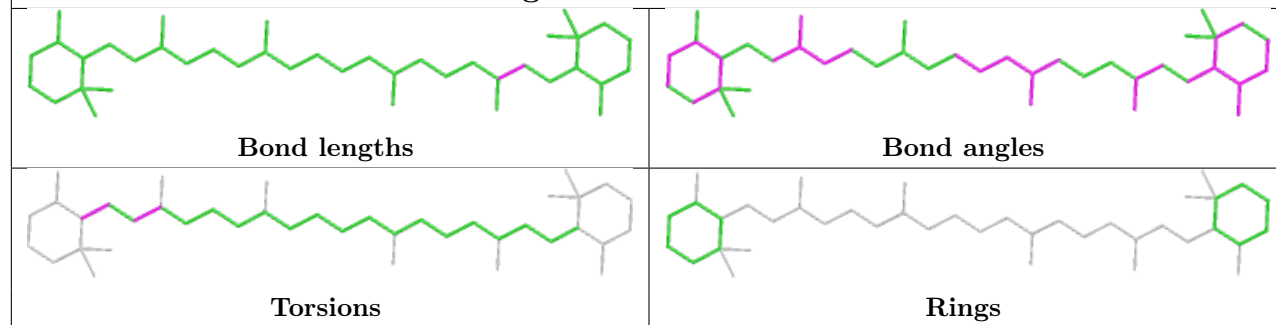


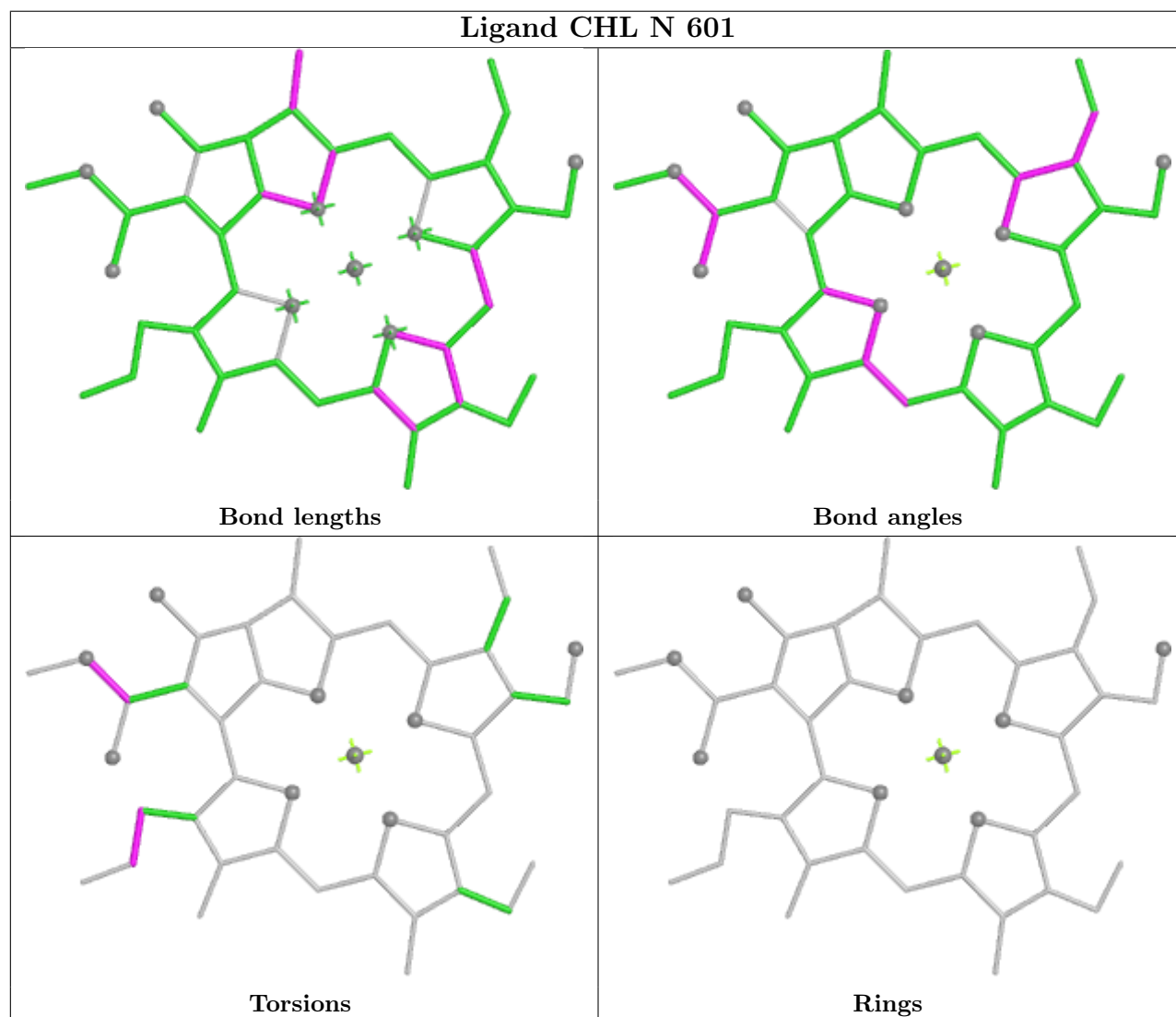
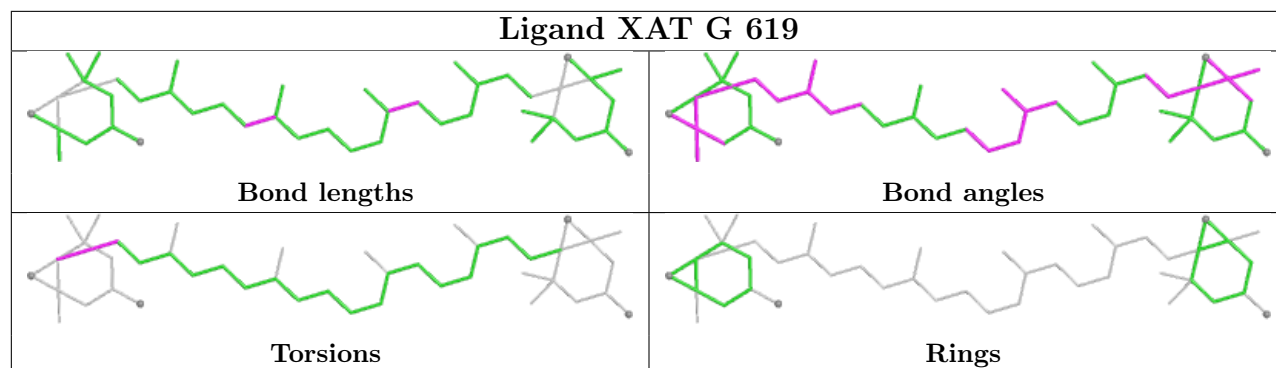
Rings

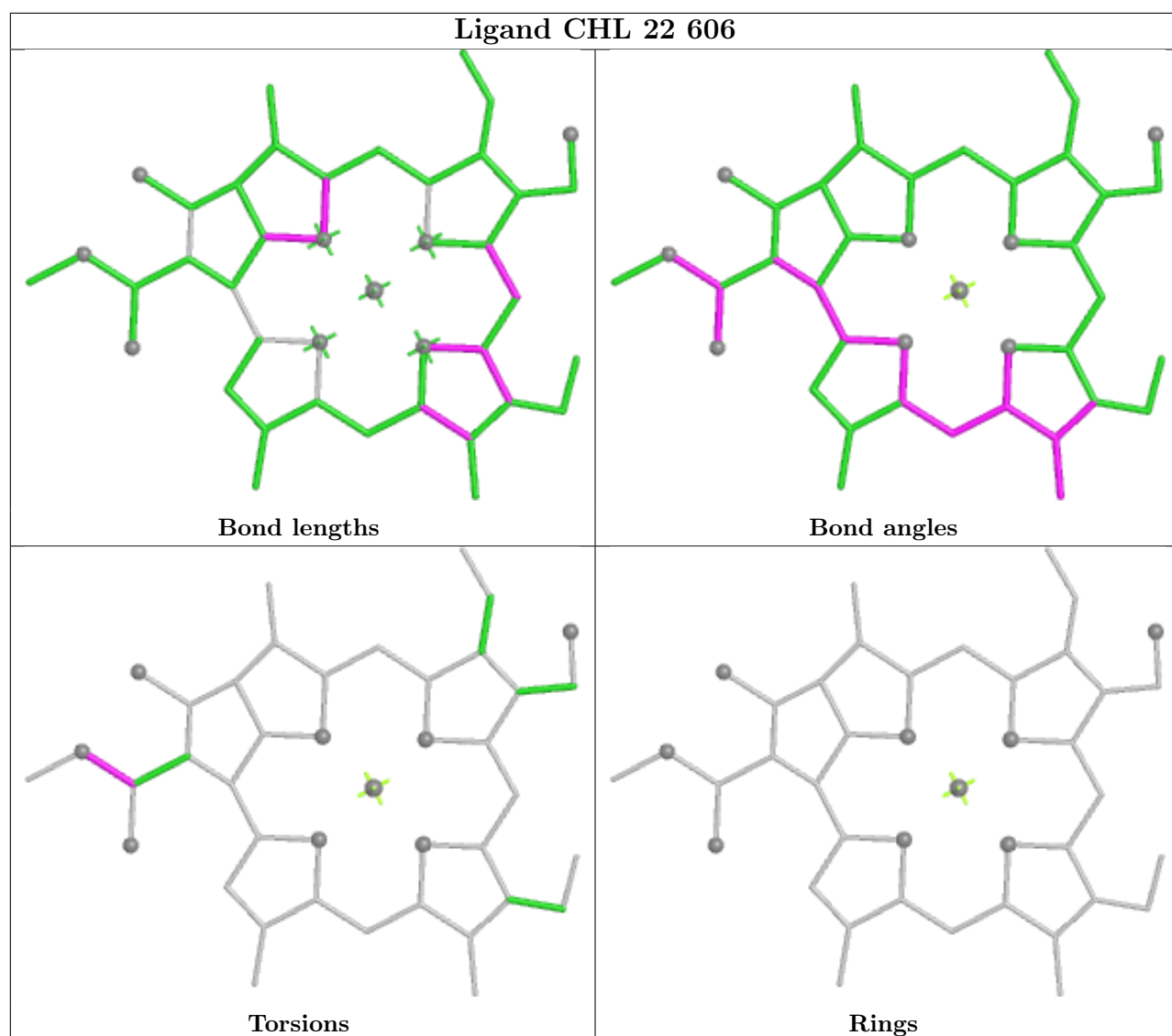
Ligand CLA 3 612

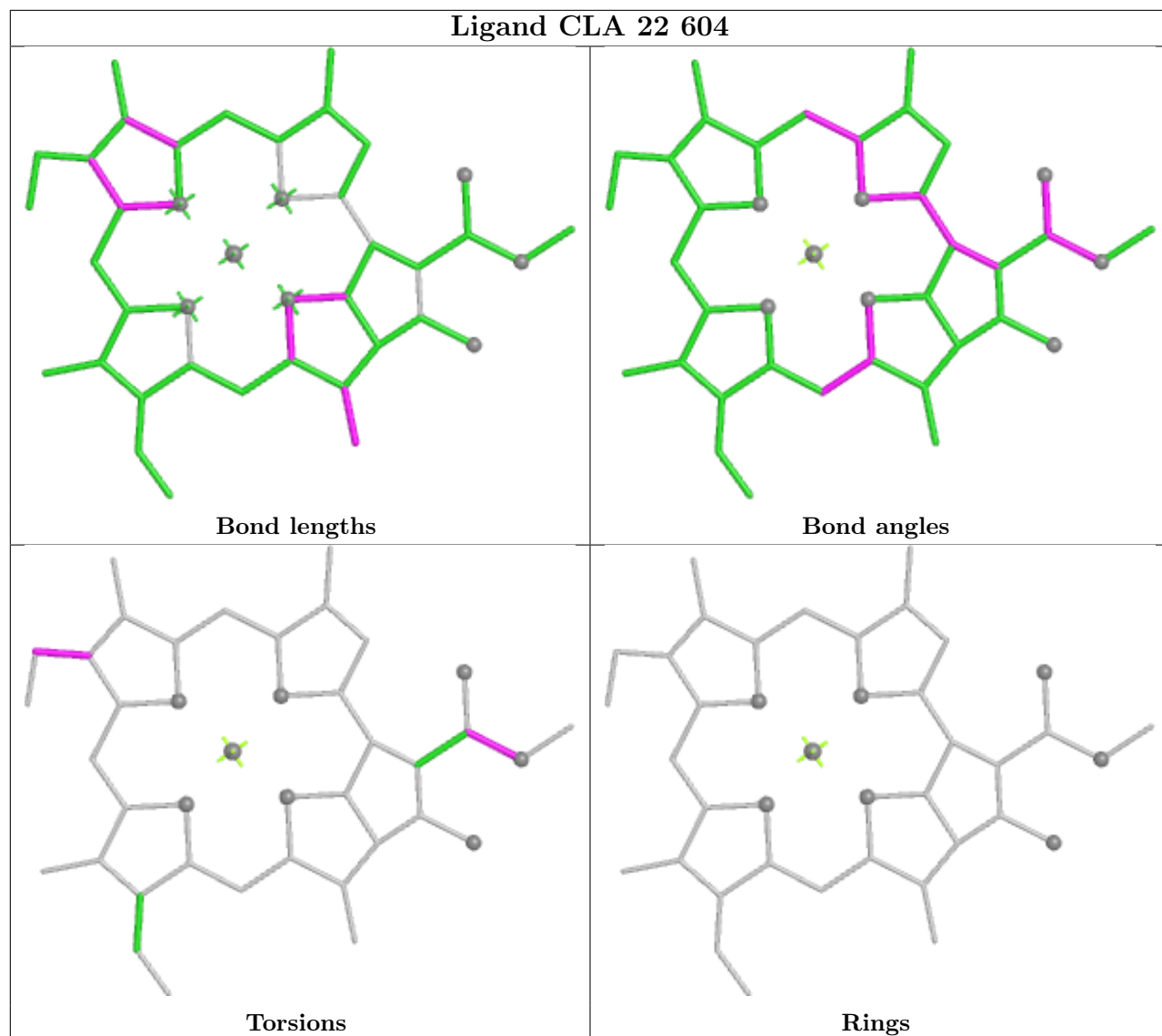


Ligand BCR Cc 516

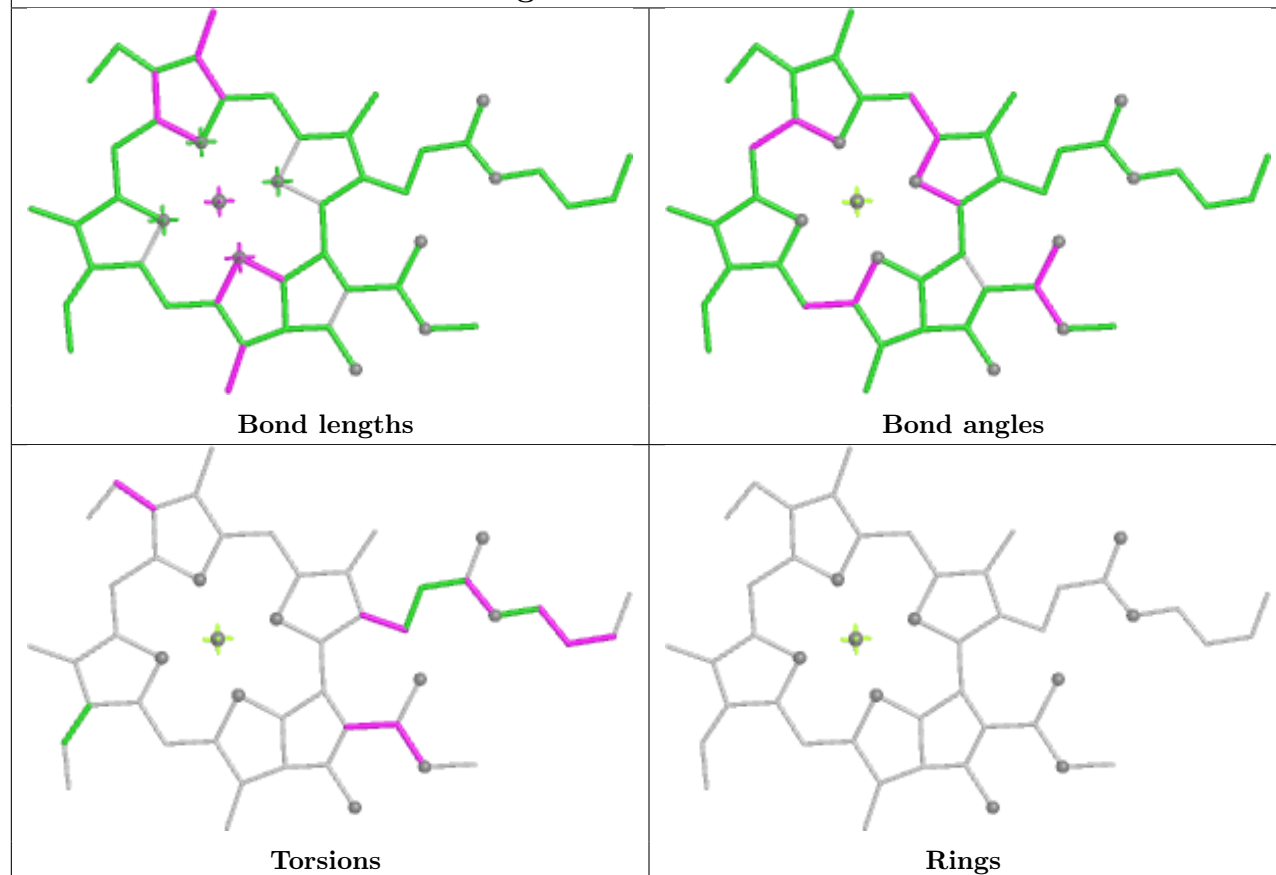




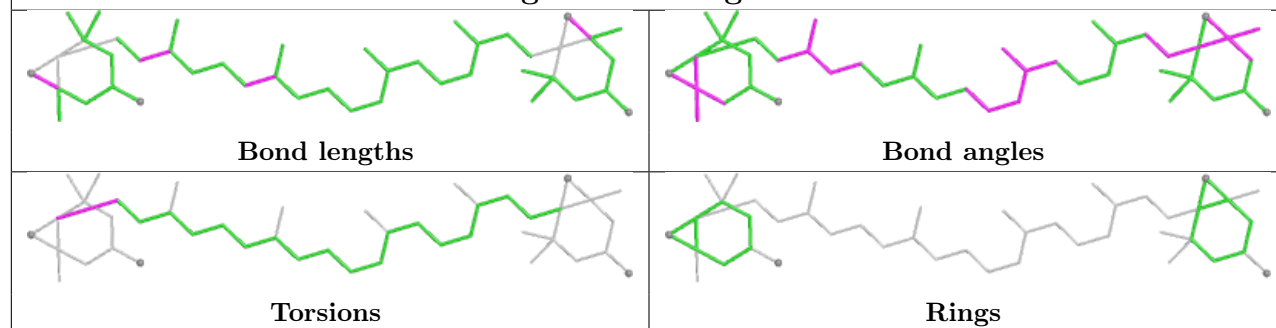


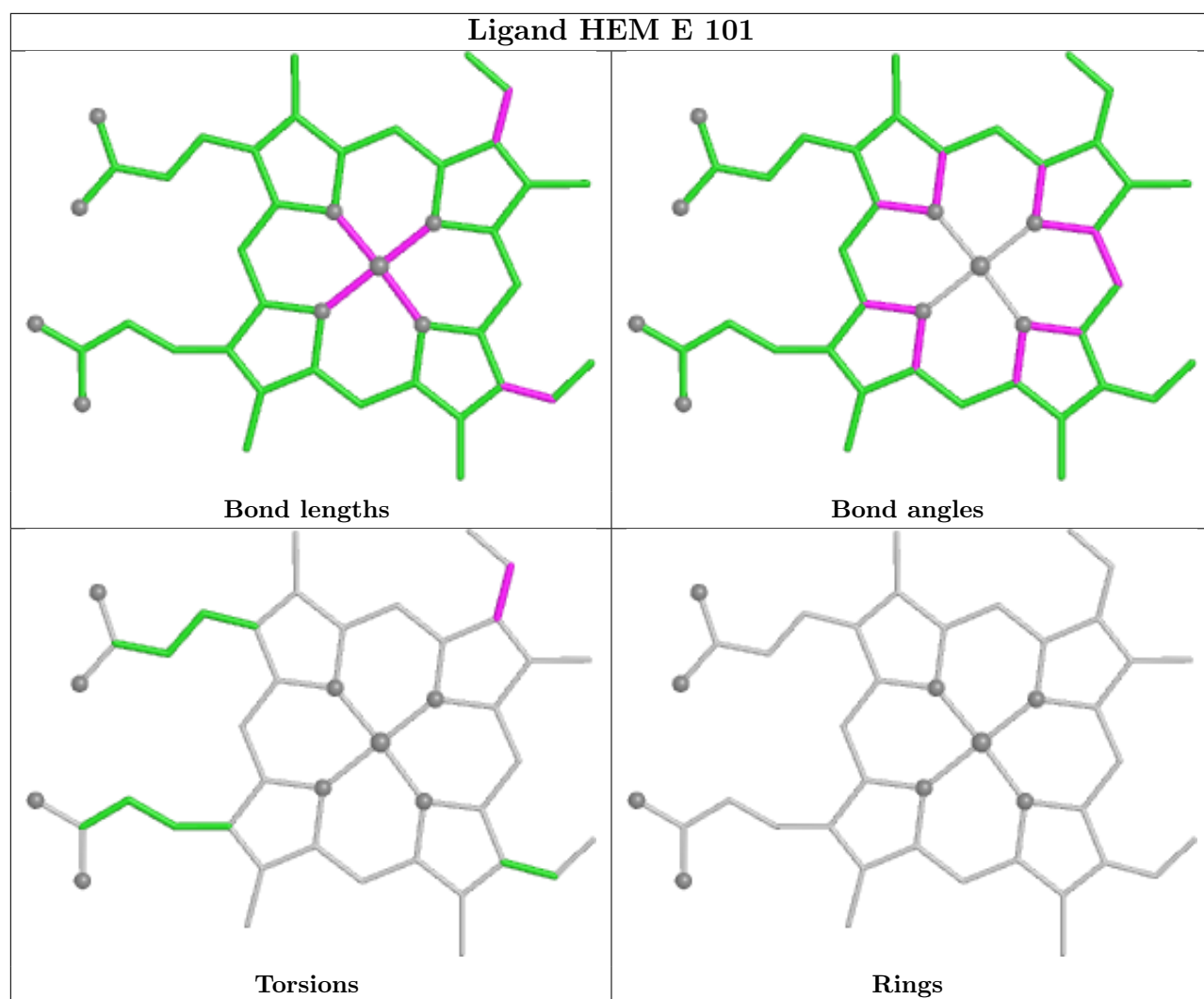


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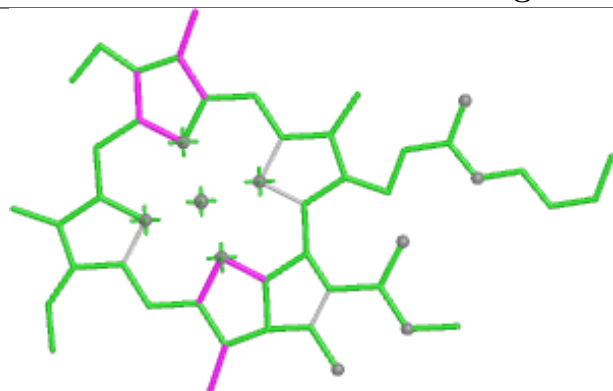


Ligand XAT Gg 301

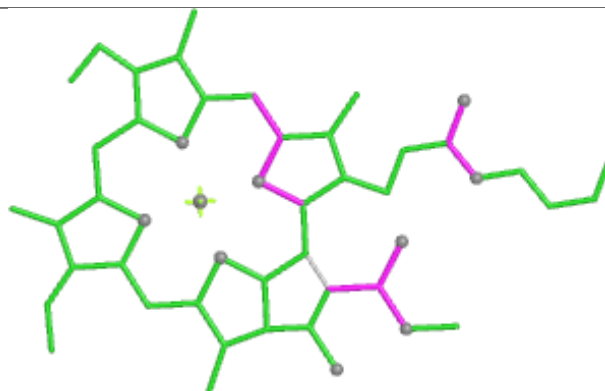




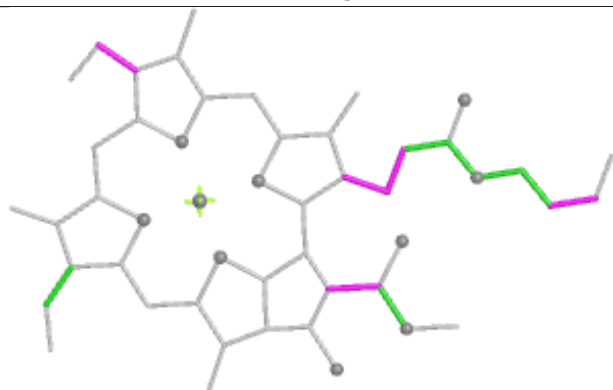
Ligand CLA R 604



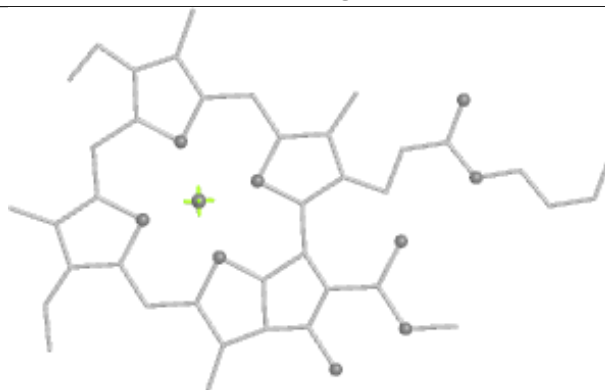
Bond lengths



Bond angles

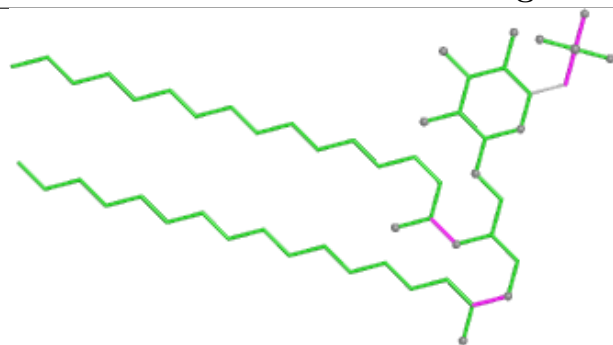


Torsions

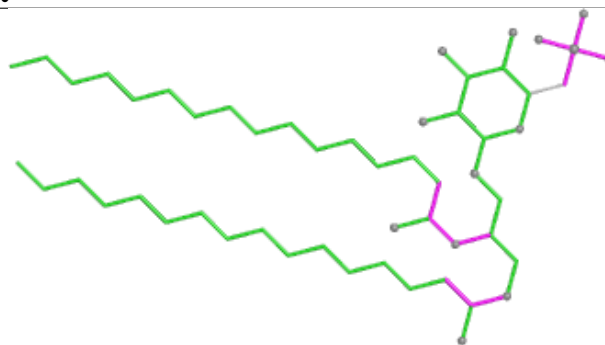


Rings

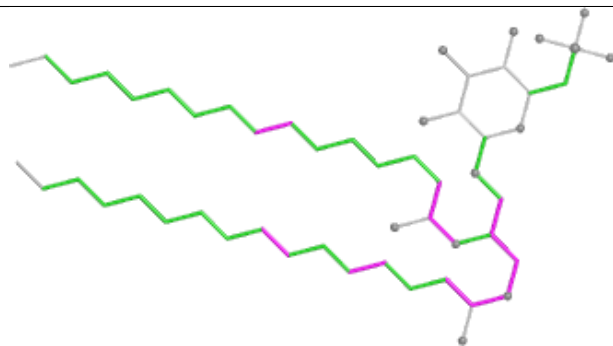
Ligand SQD L 101



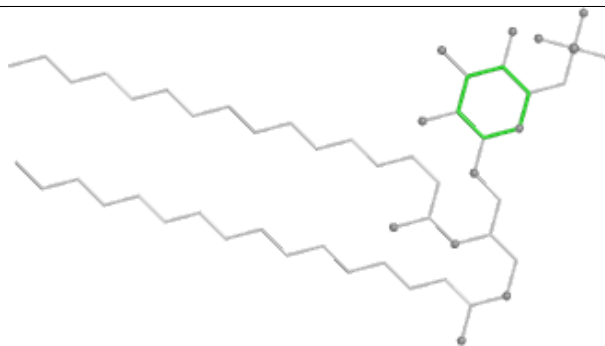
Bond lengths



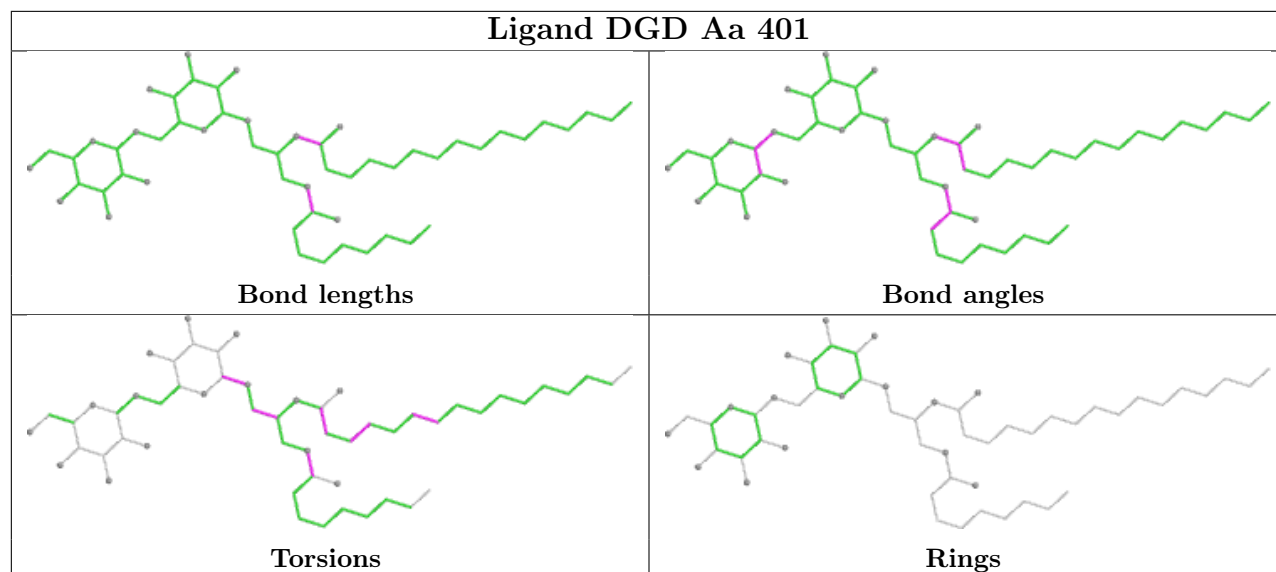
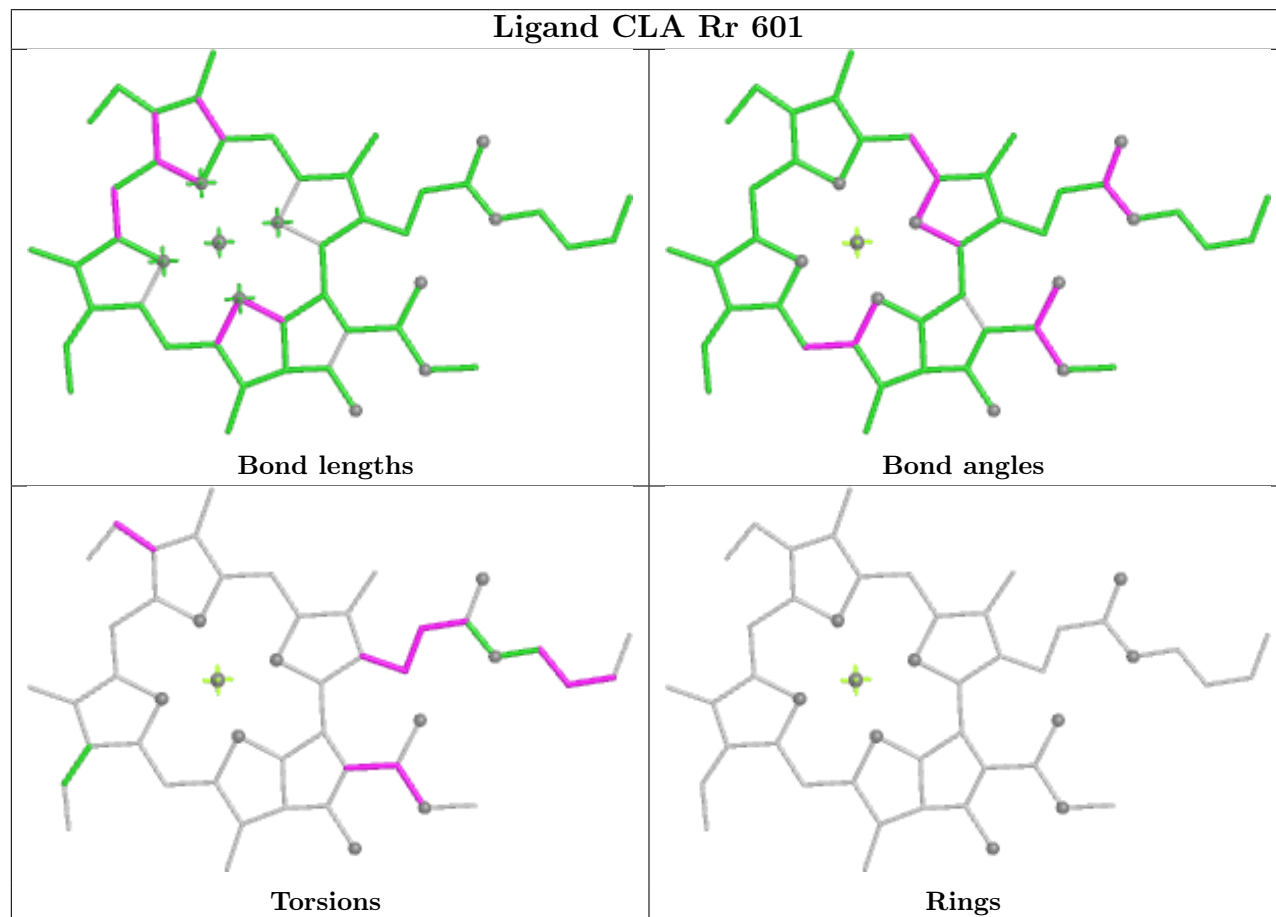
Bond angles

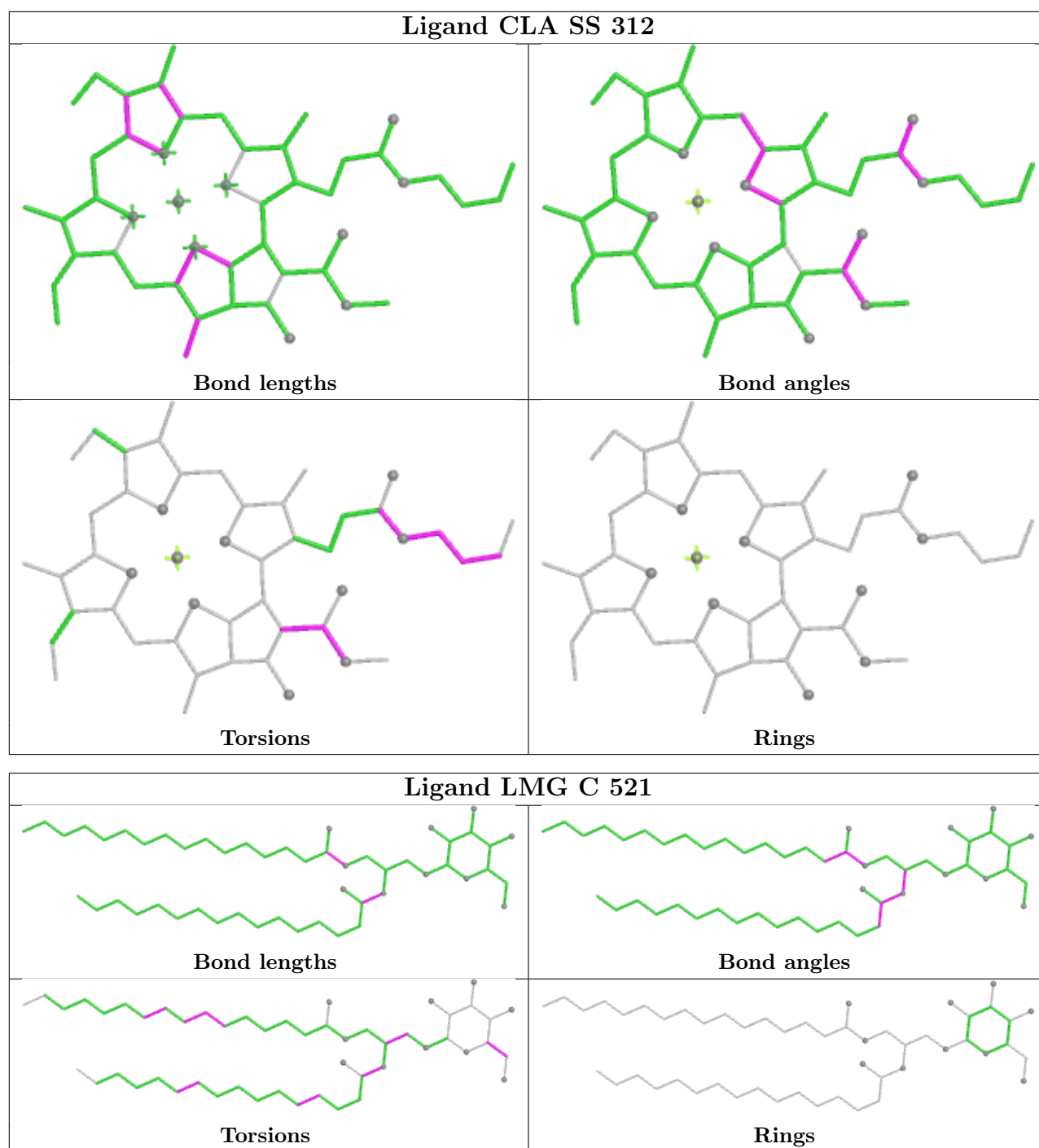


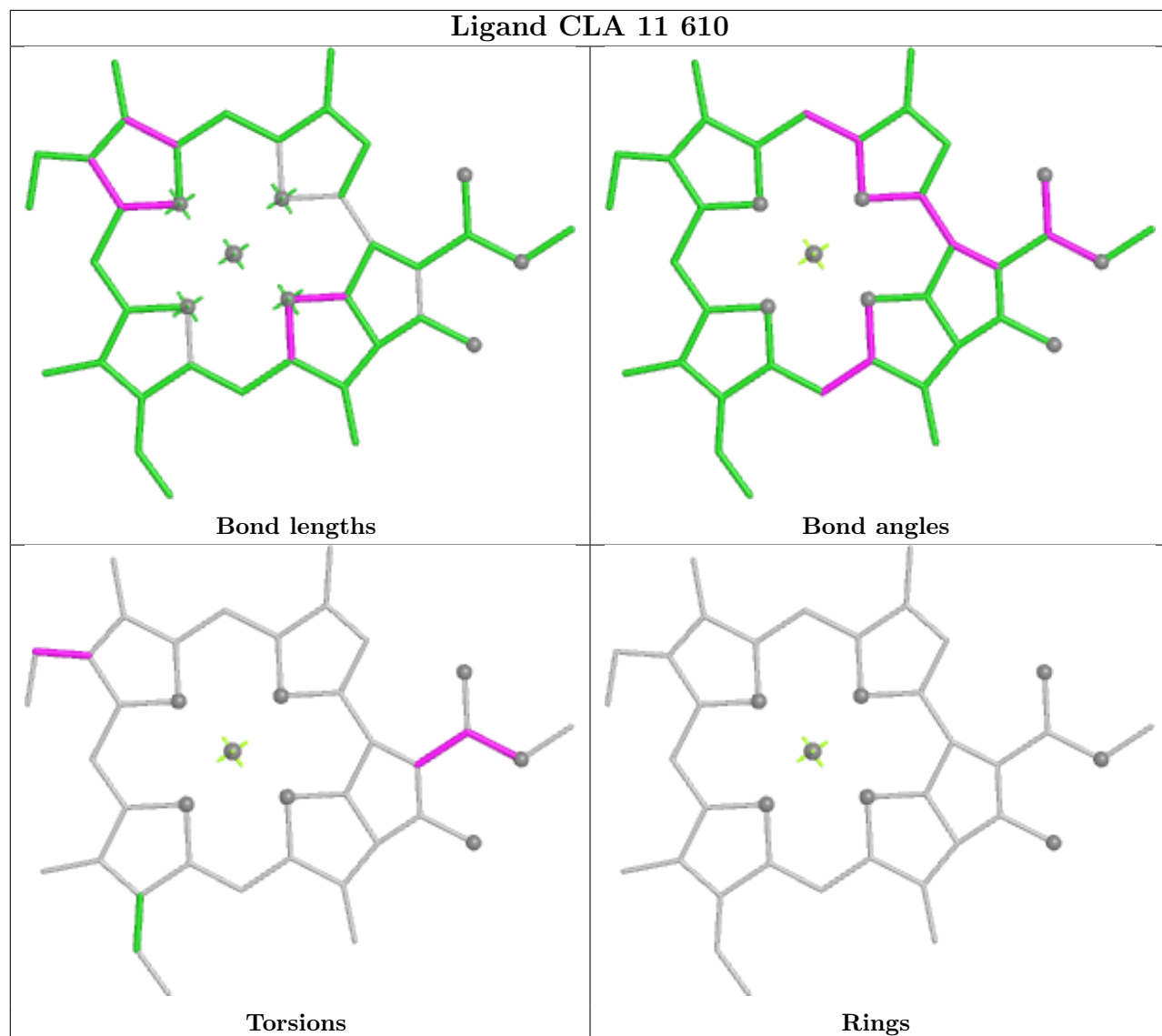
Torsions

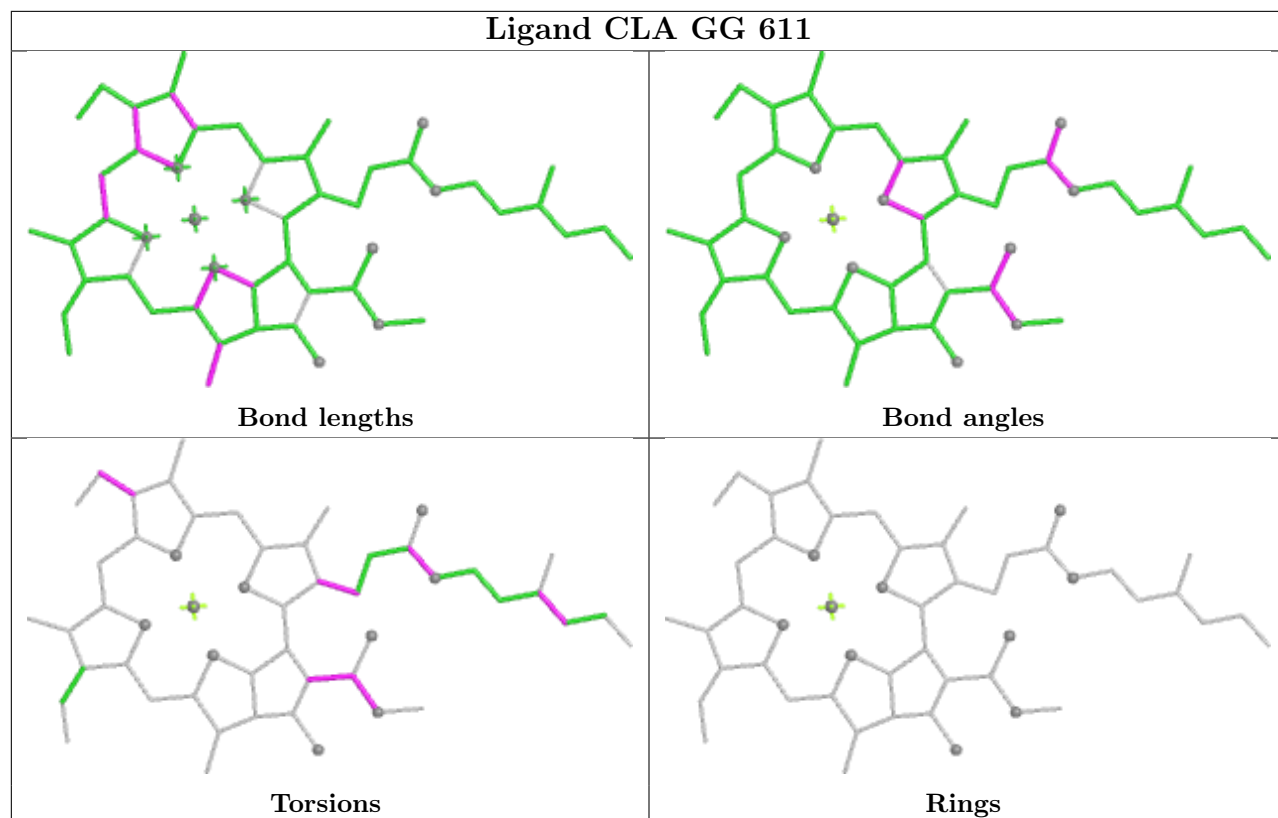


Rings

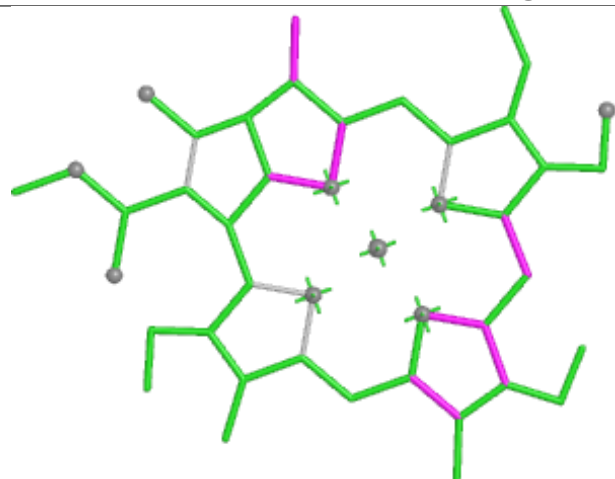
Ligand DGD Aa 401**Ligand CLA Rr 601**







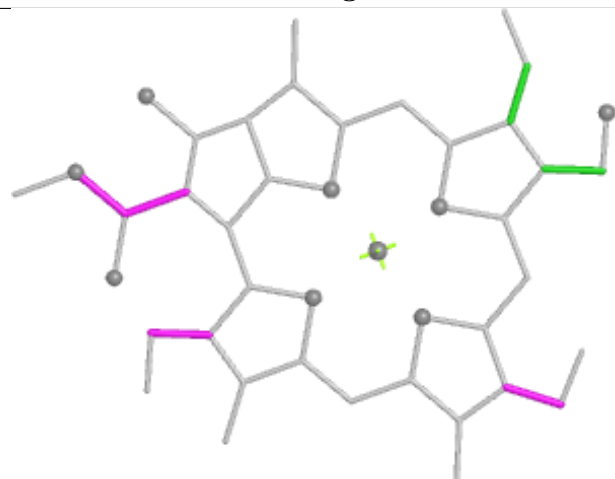
Ligand CHL g 609



Bond lengths



Bond angles

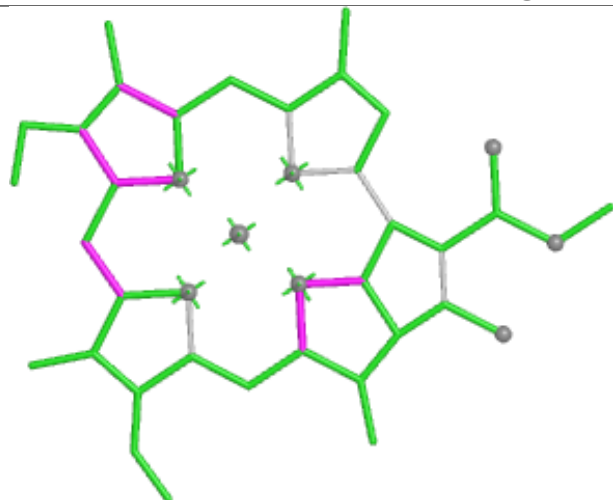


Torsions

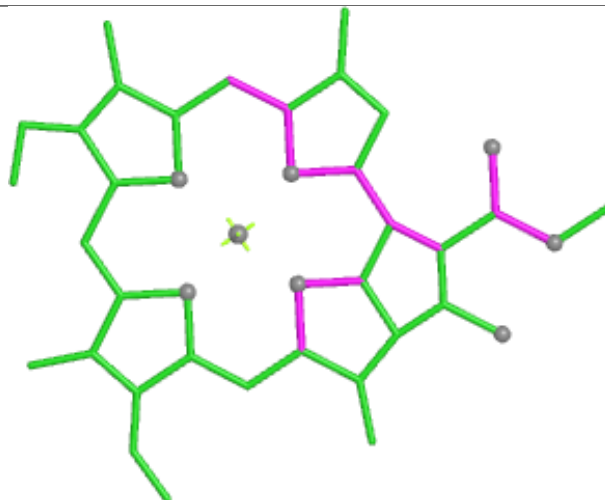


Rings

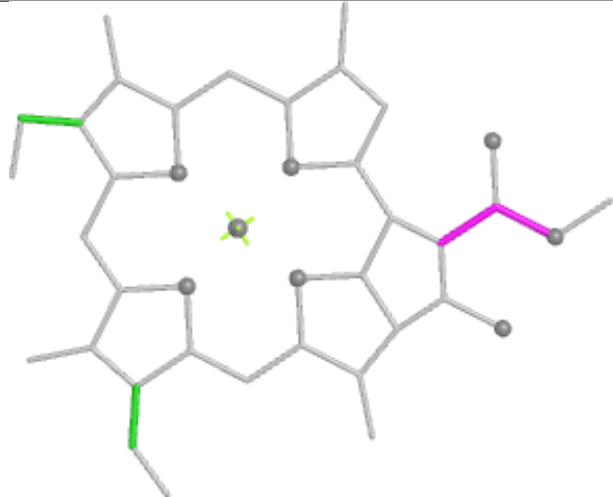
Ligand CLA 3 609



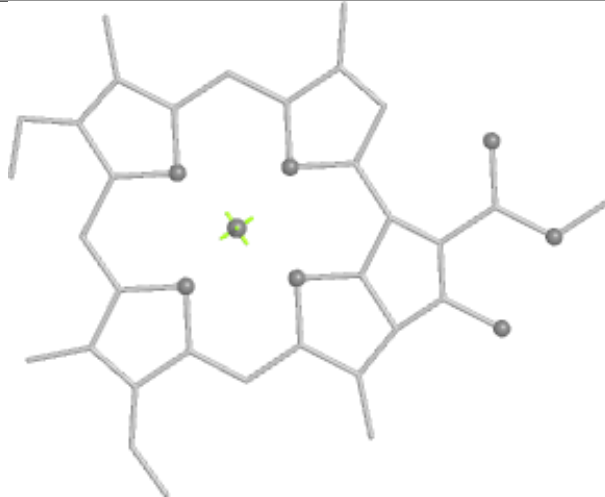
Bond lengths



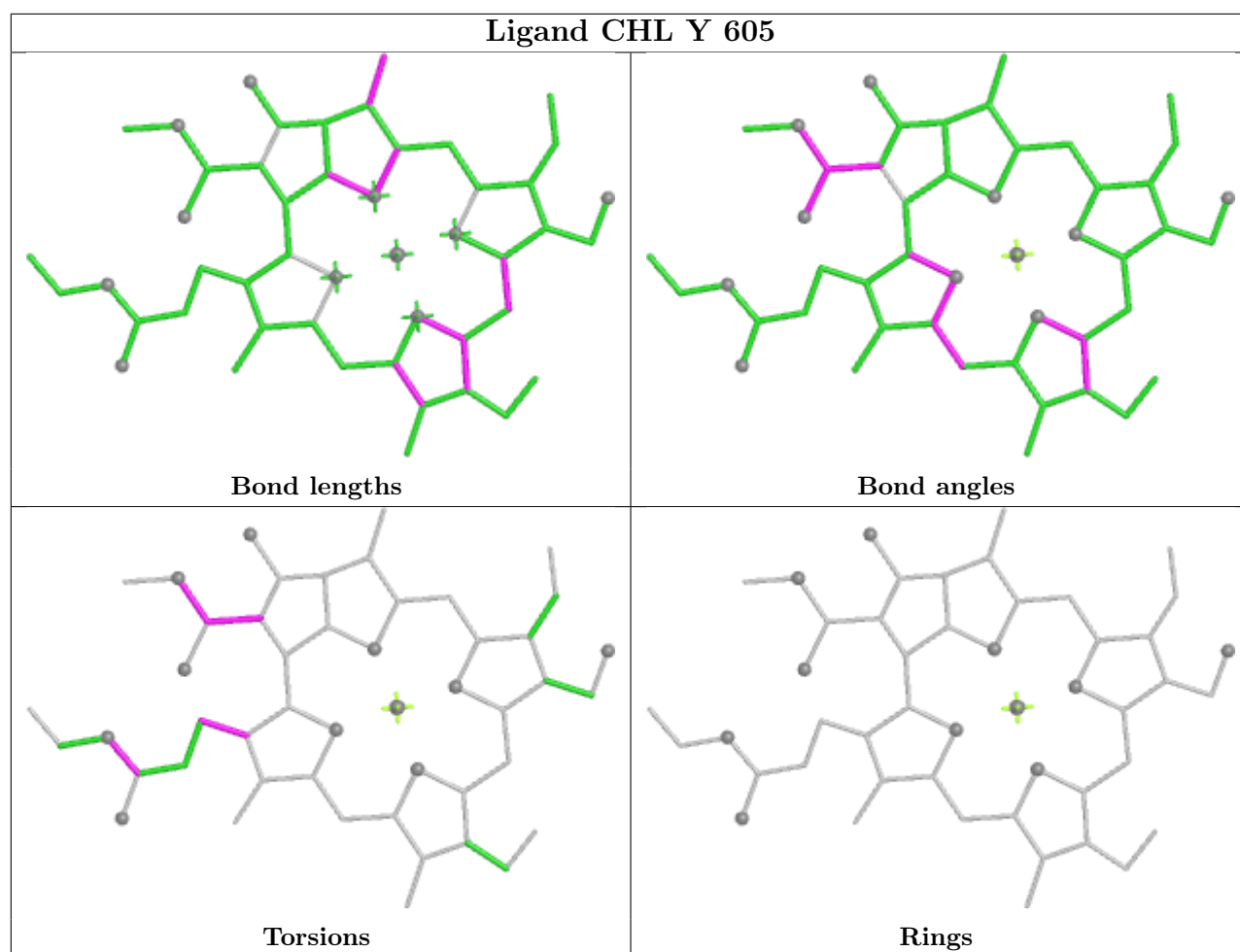
Bond angles



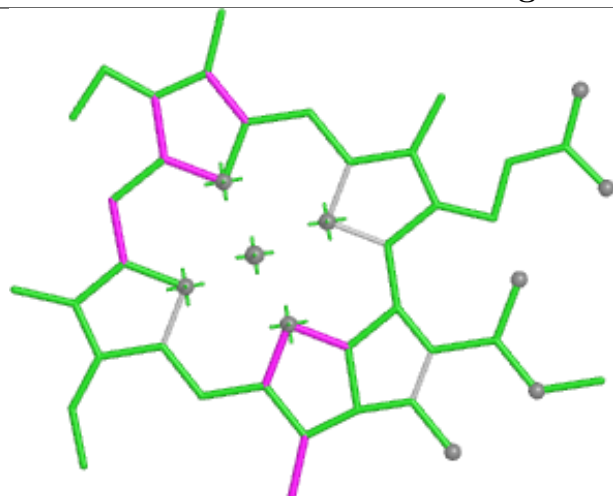
Torsions



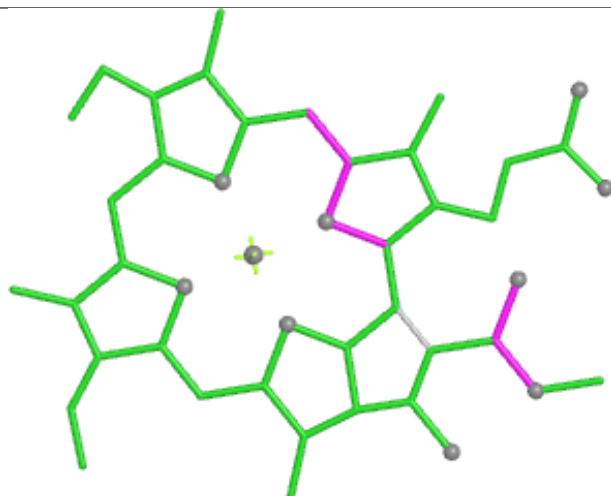
Rings



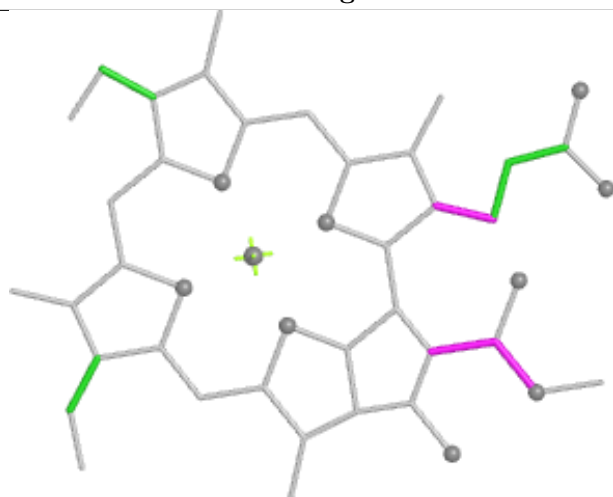
Ligand CLA 4 310



Bond lengths



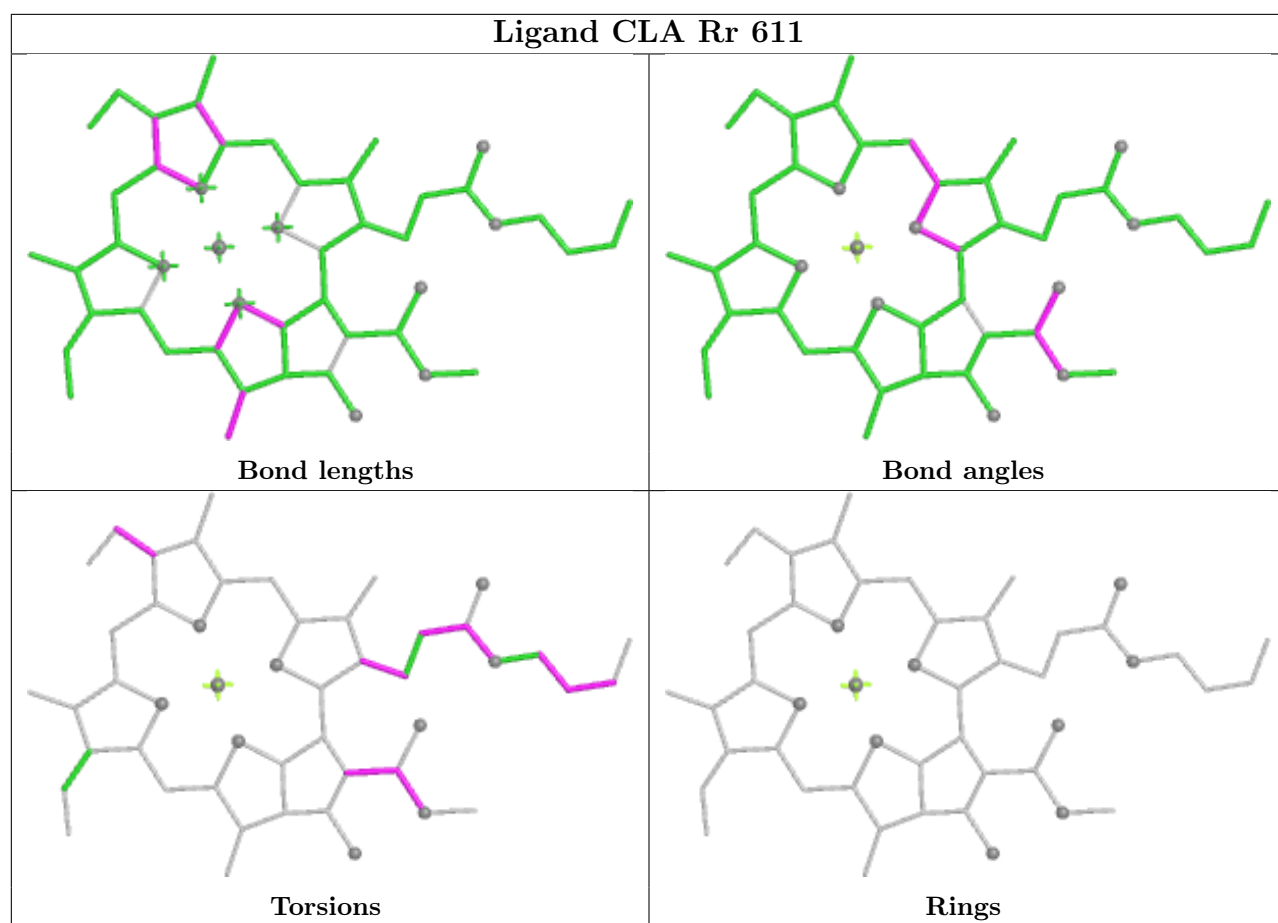
Bond angles



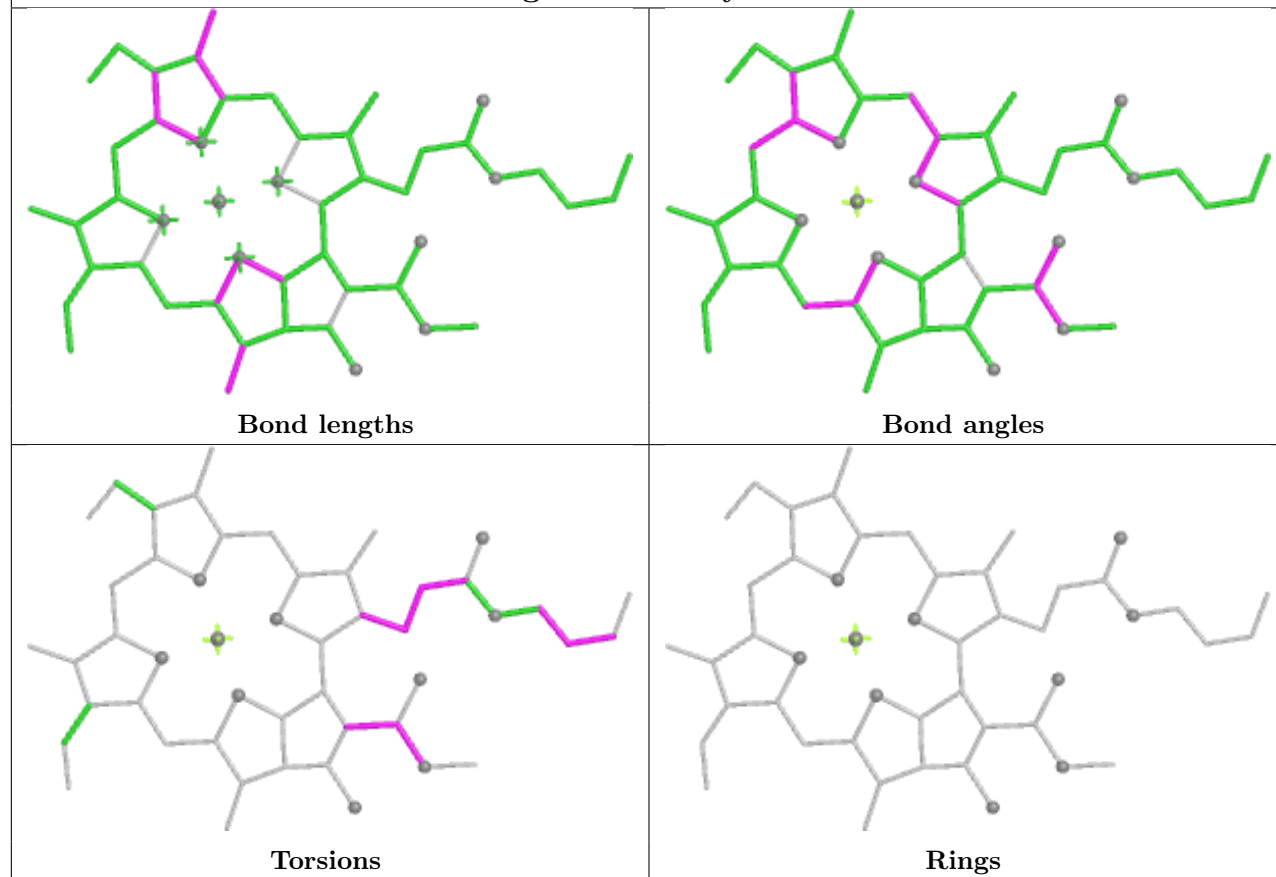
Torsions



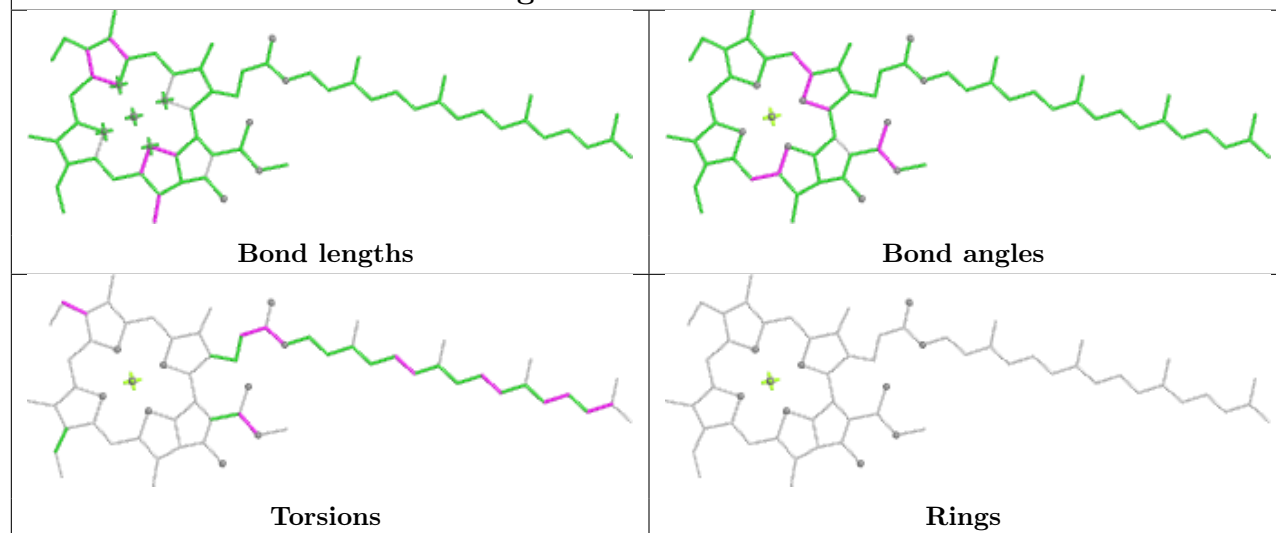
Rings

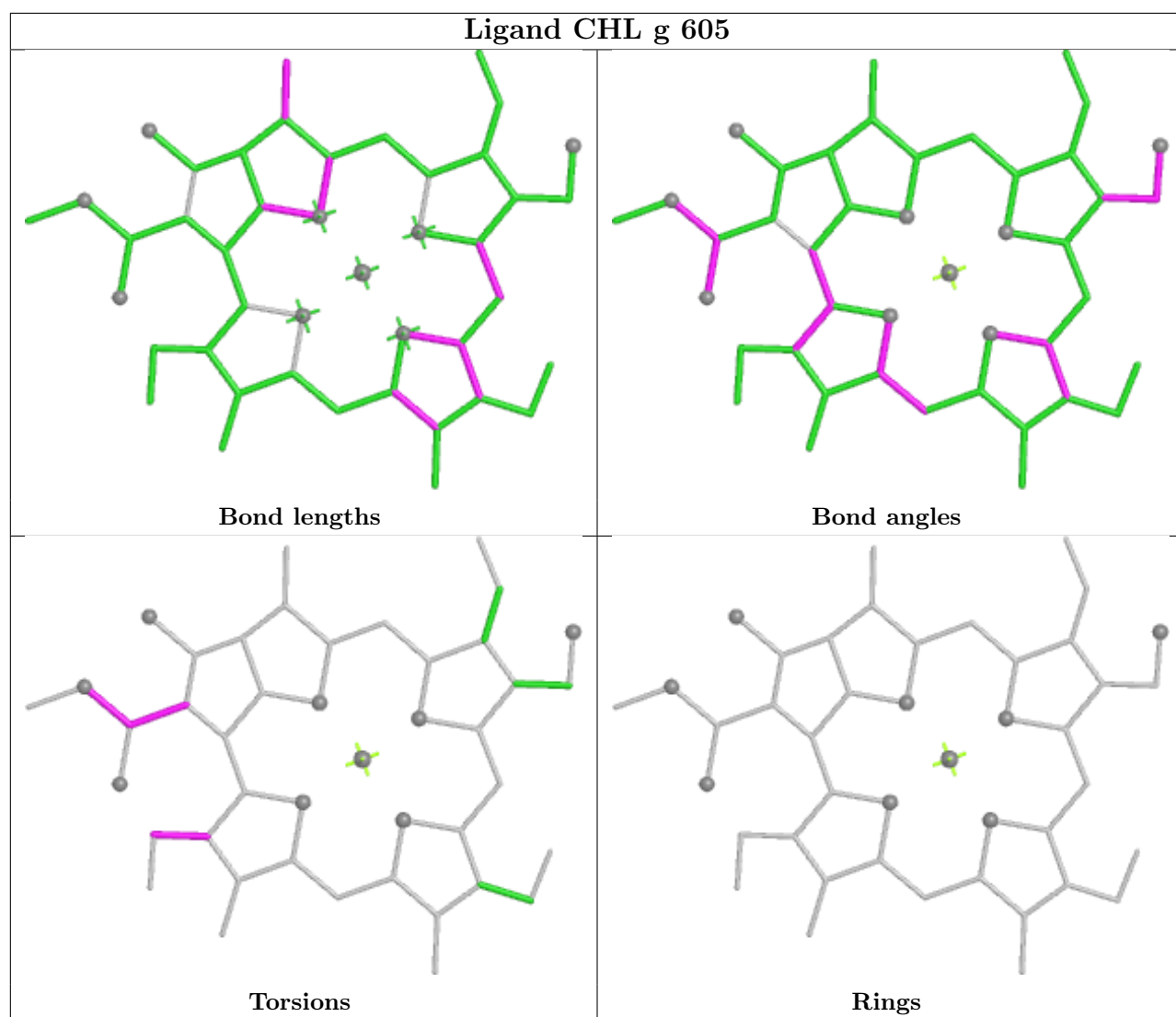


Ligand CLA Yy 604

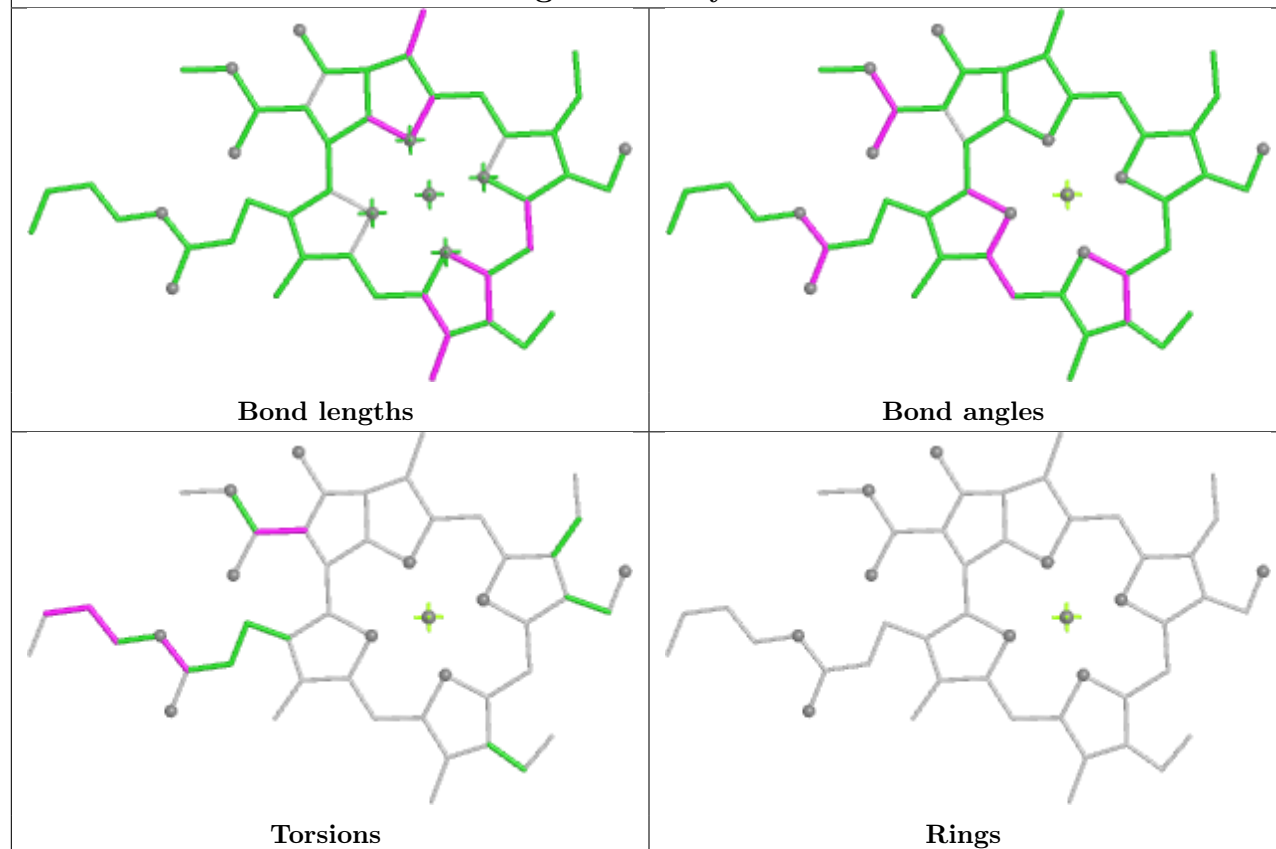


Ligand CLA GG 603

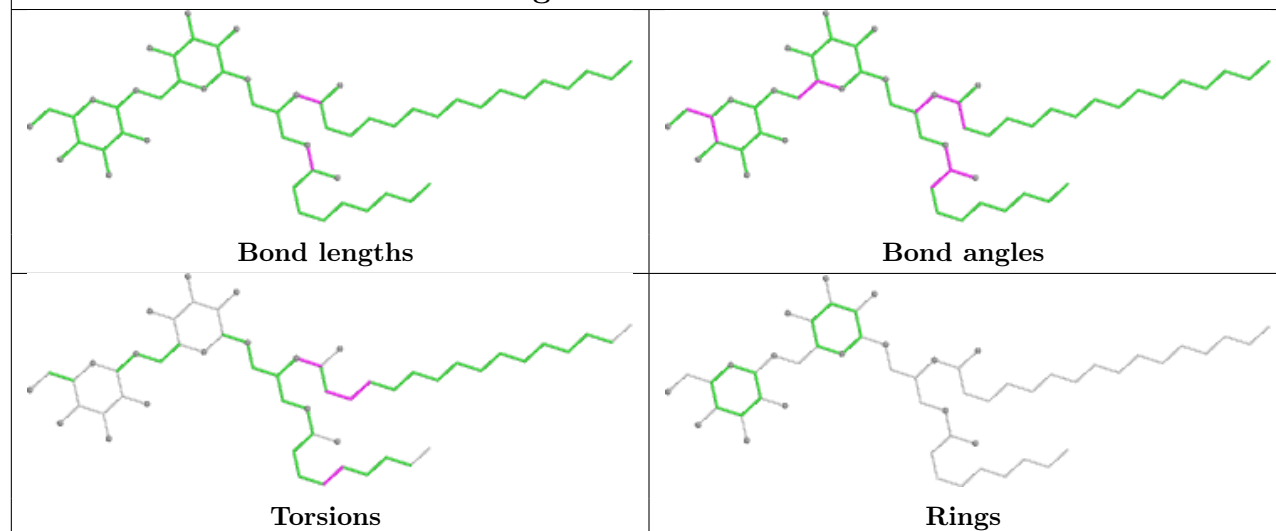


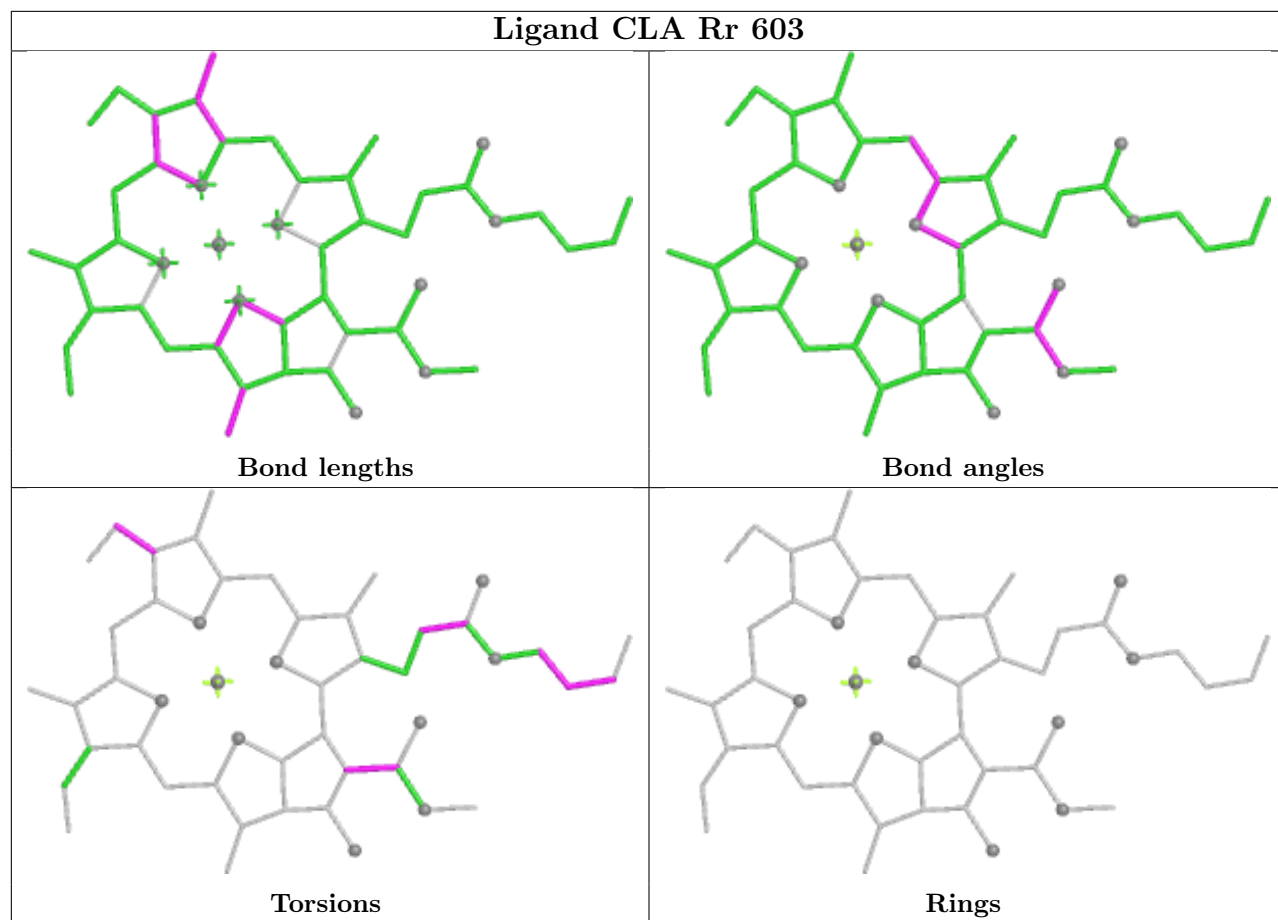


Ligand CHL y 310

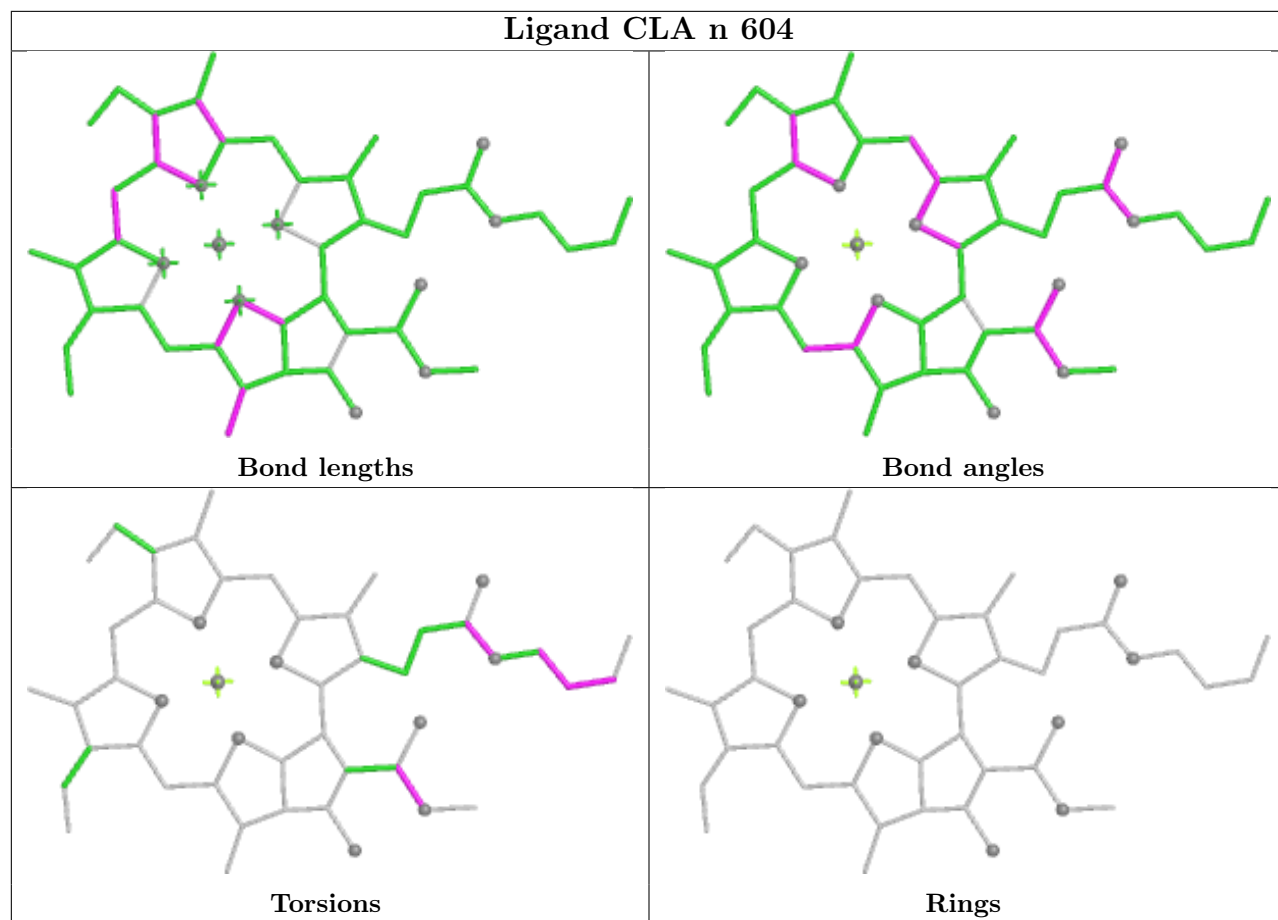


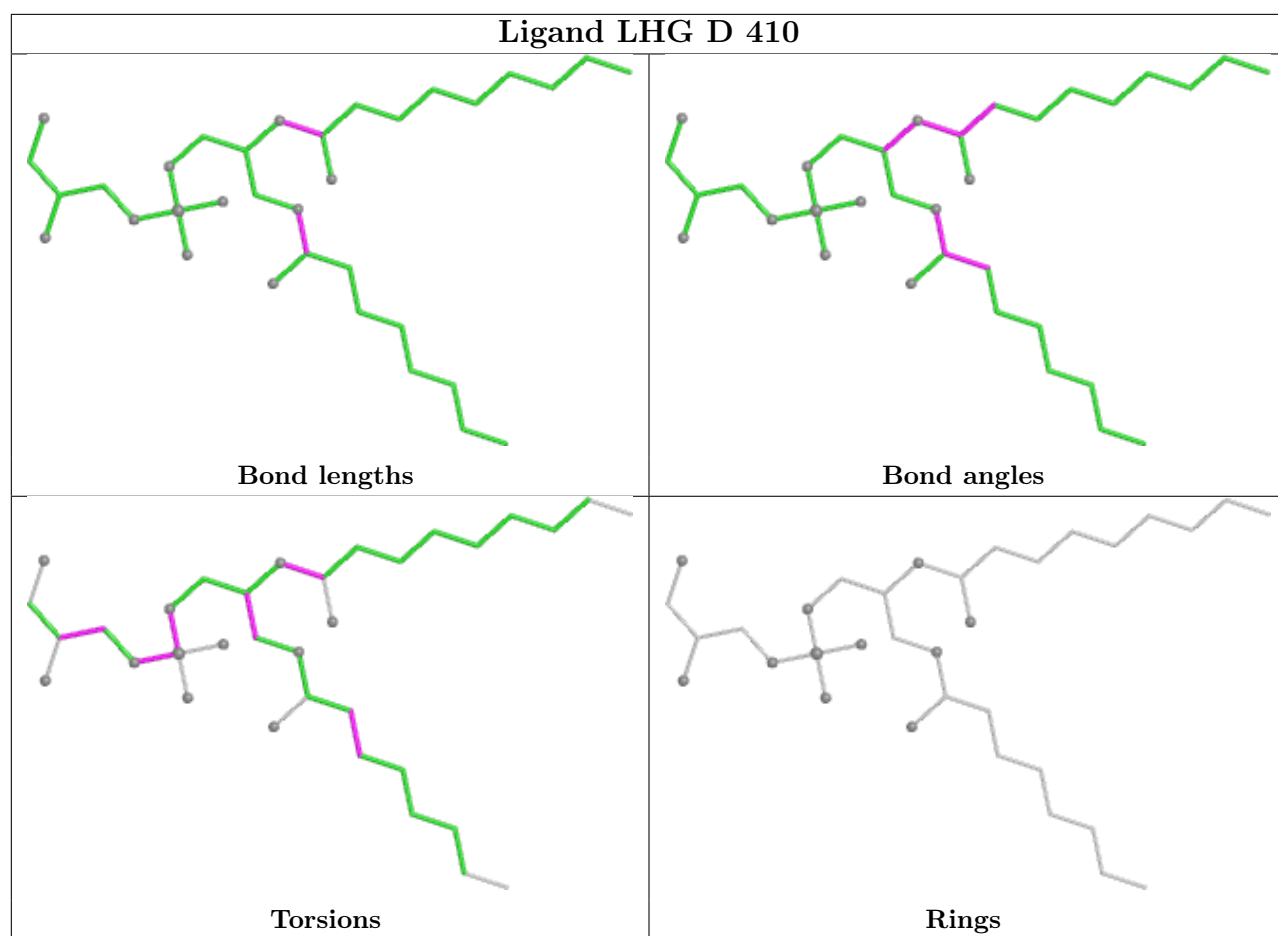
Ligand DGD c 517



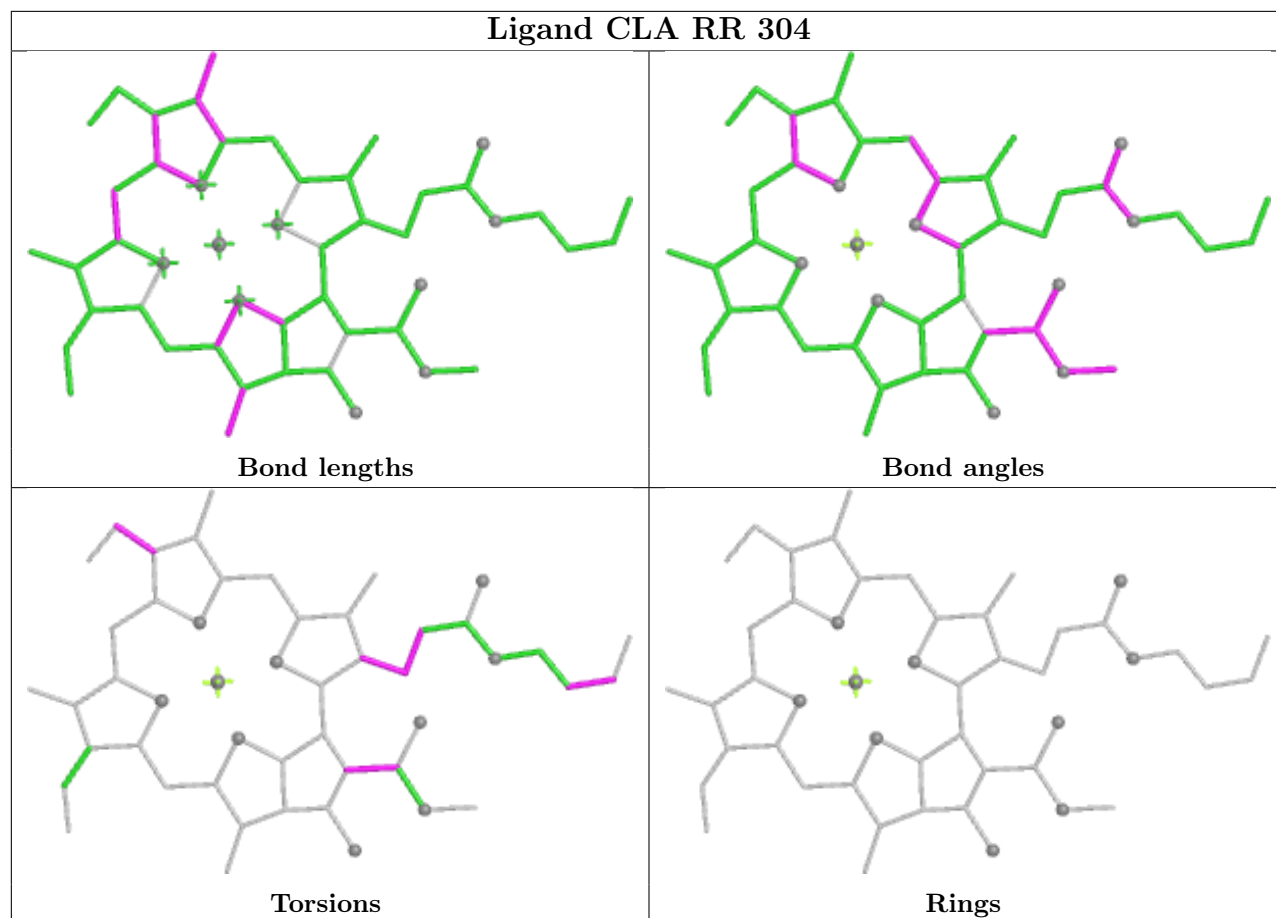


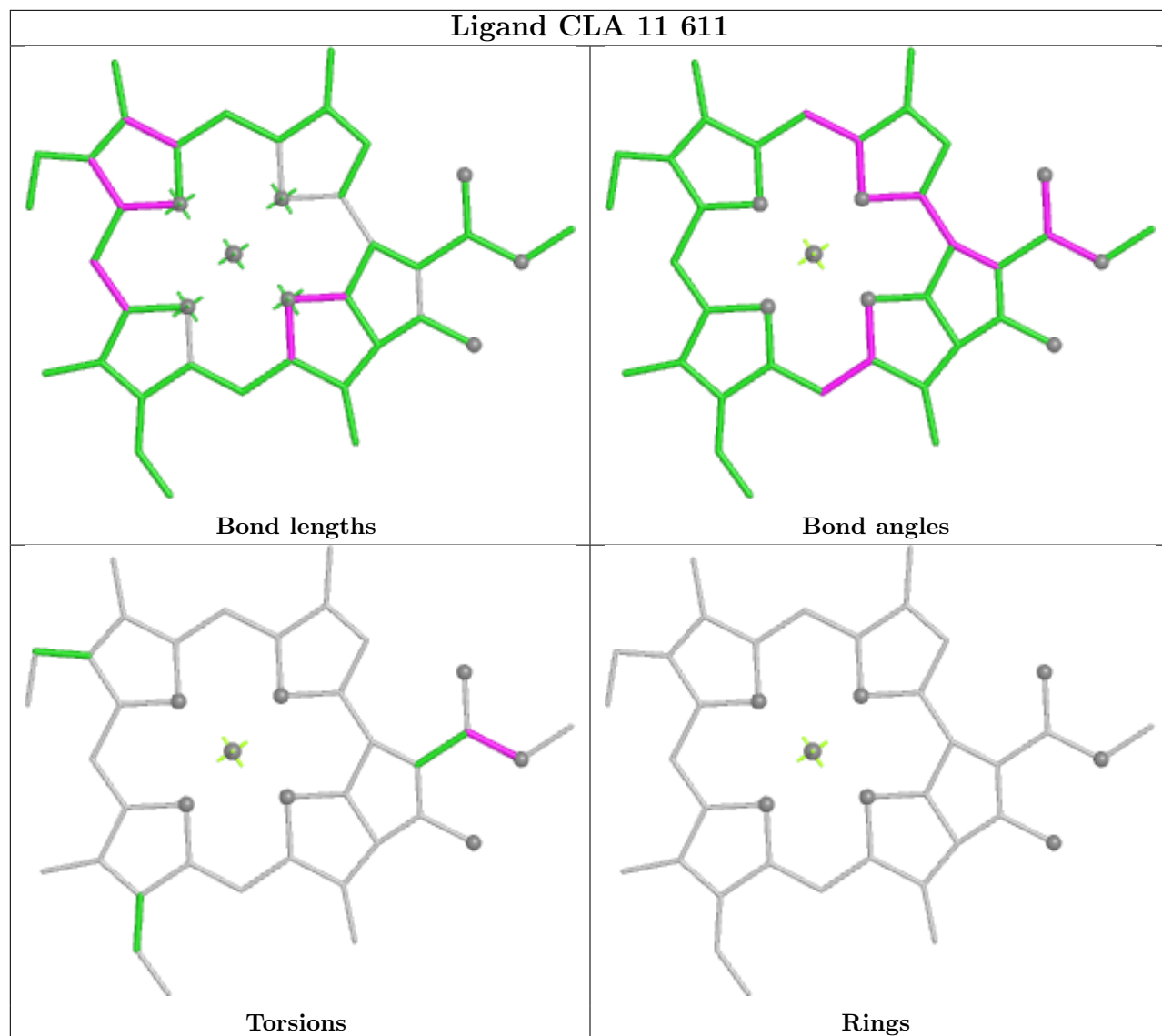
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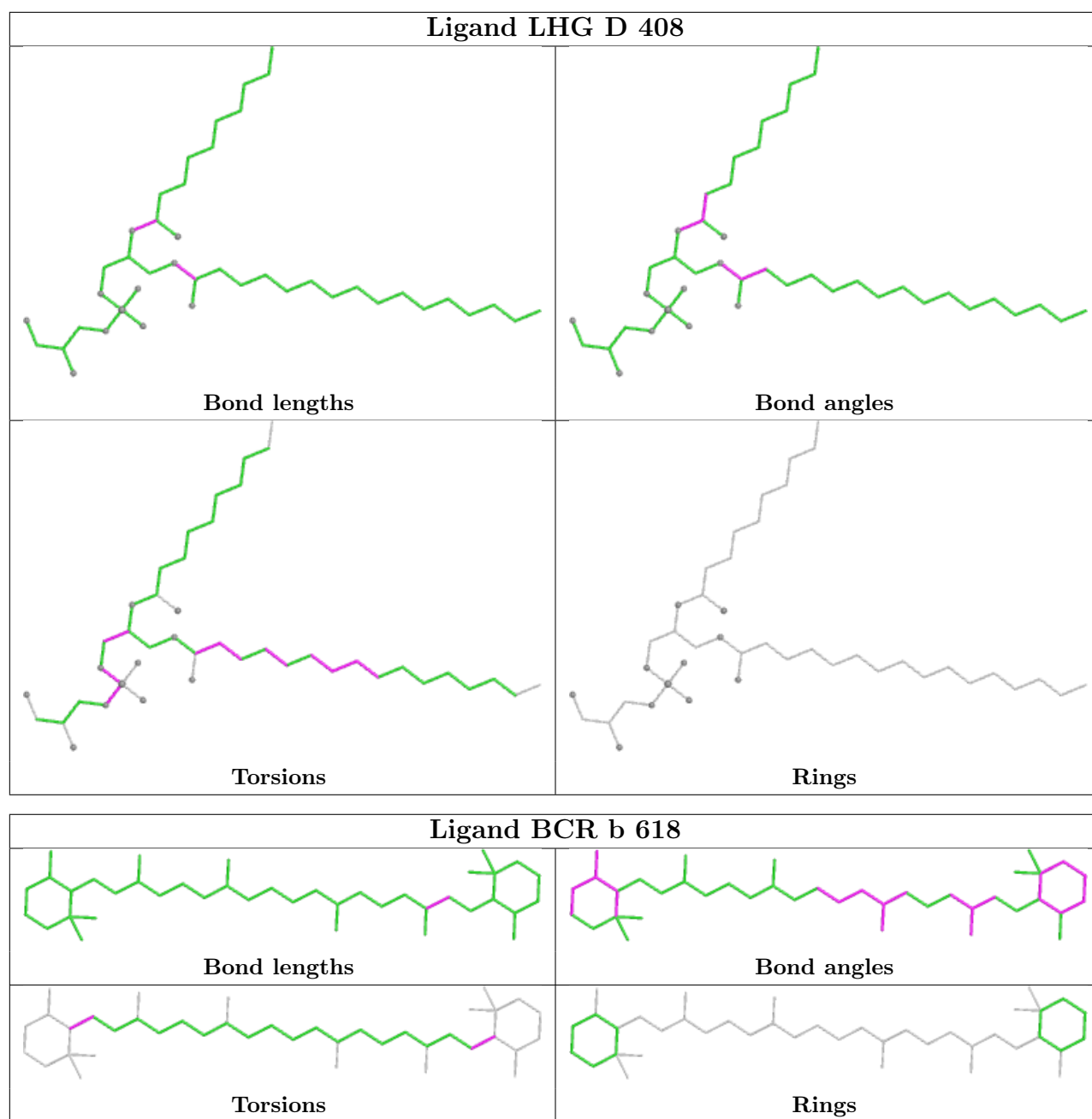




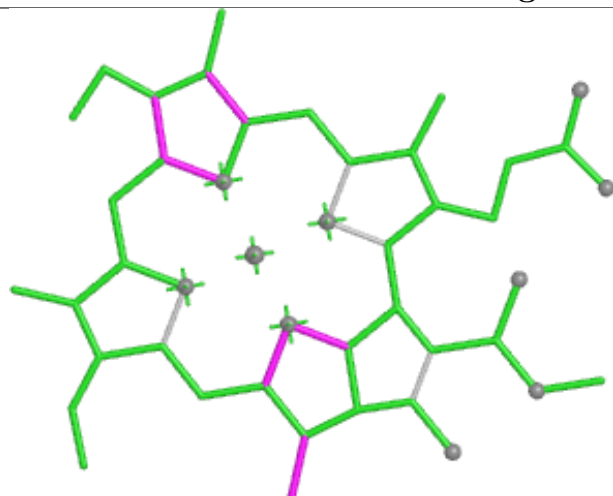
Ligand CLA RR 304



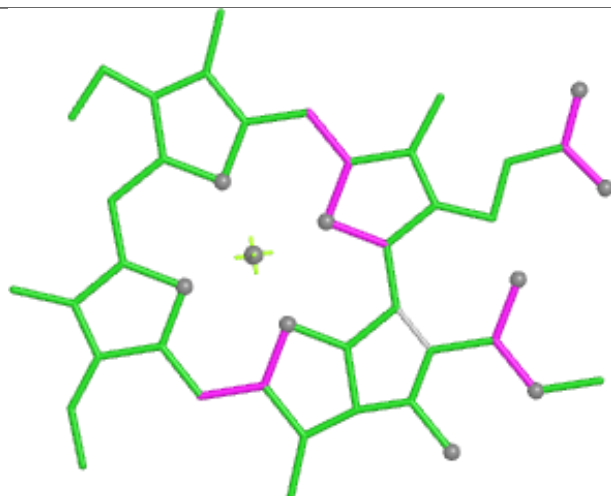




Ligand CLA 4 305



Bond lengths



Bond angles

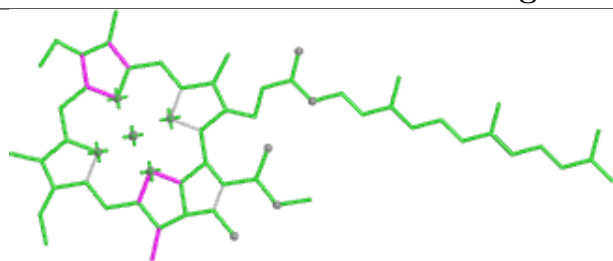


Torsions

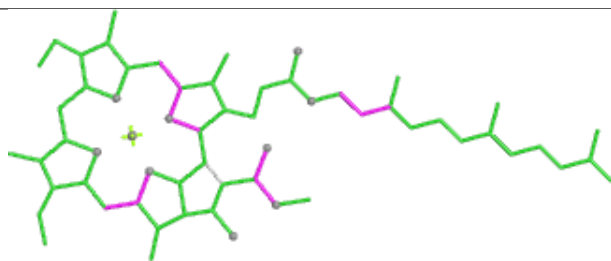


Rings

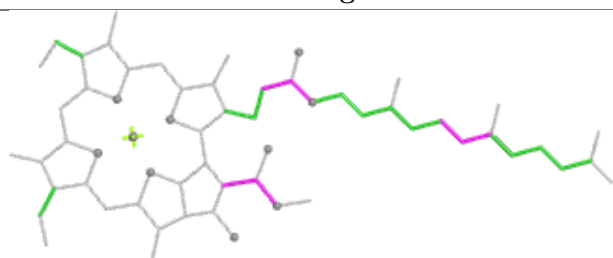
Ligand CLA c 508



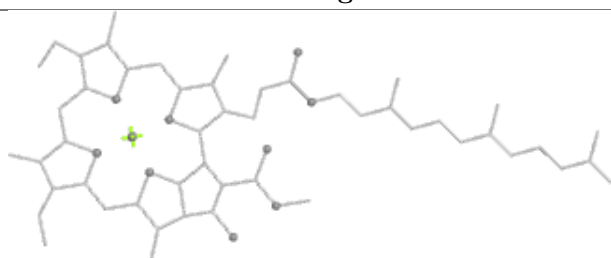
Bond lengths



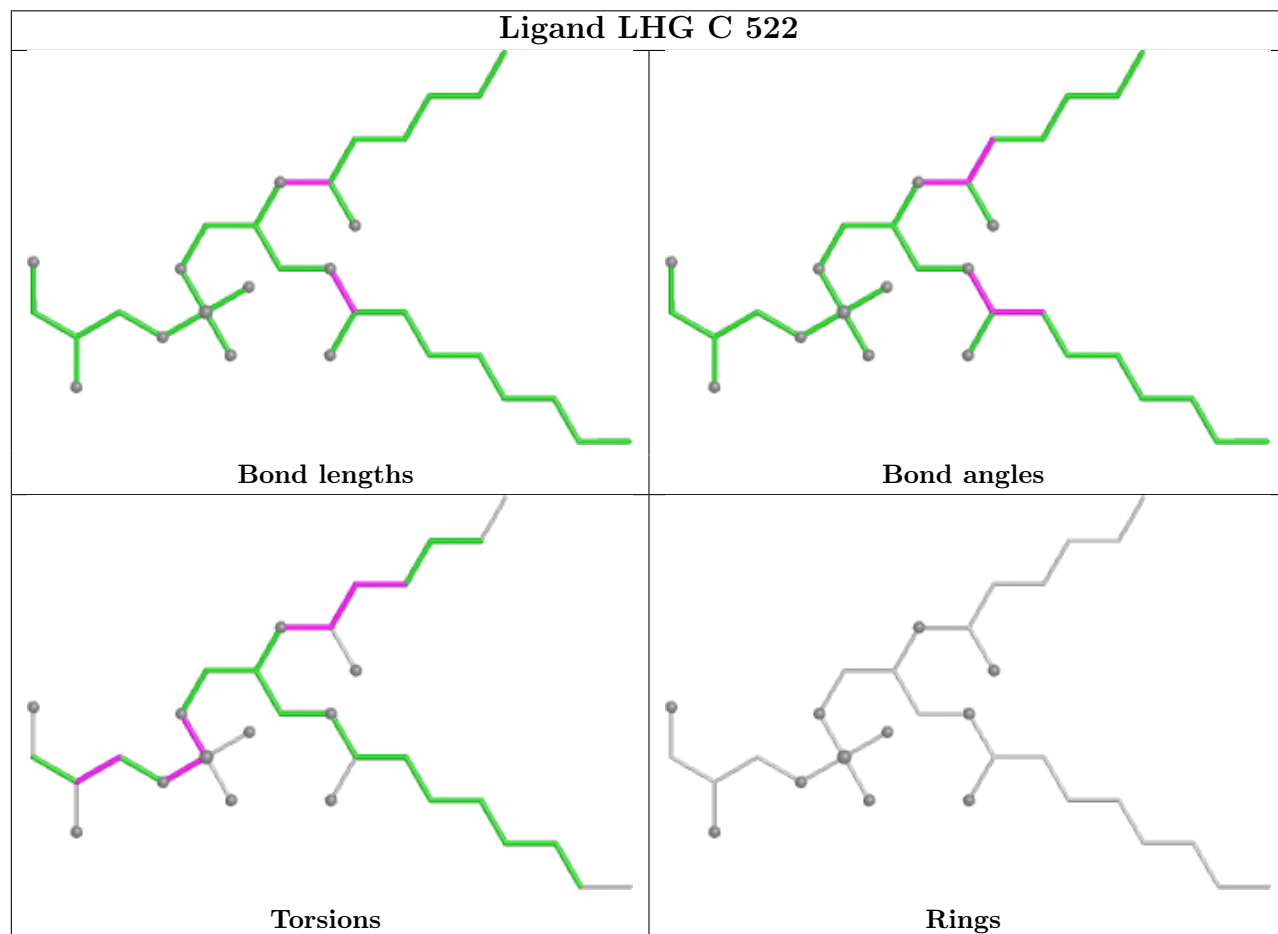
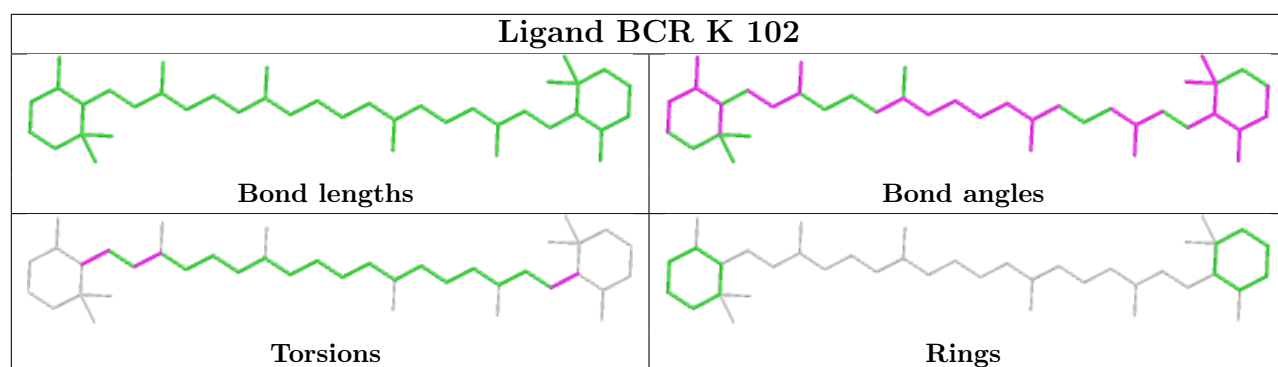
Bond angles

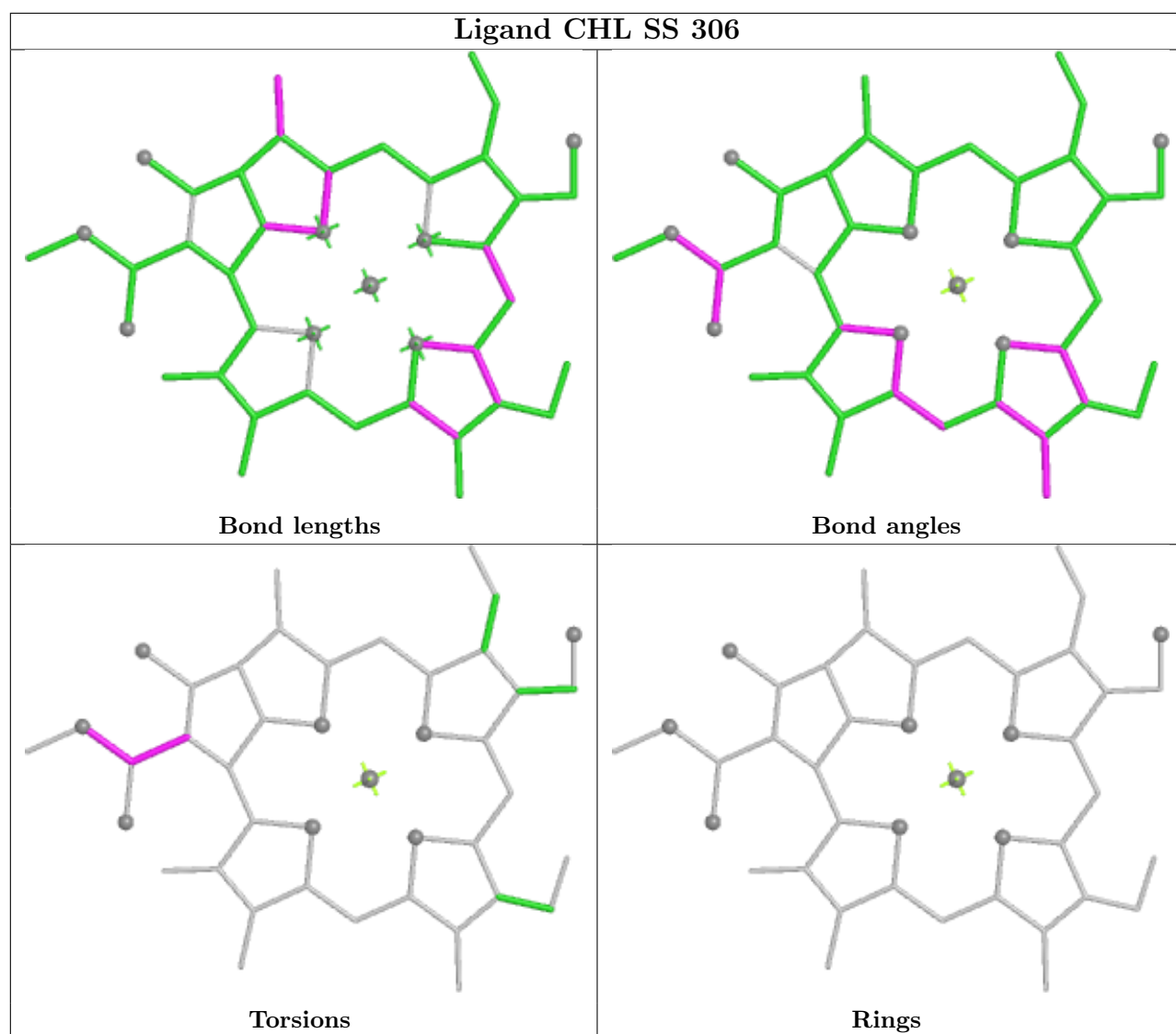


Torsions

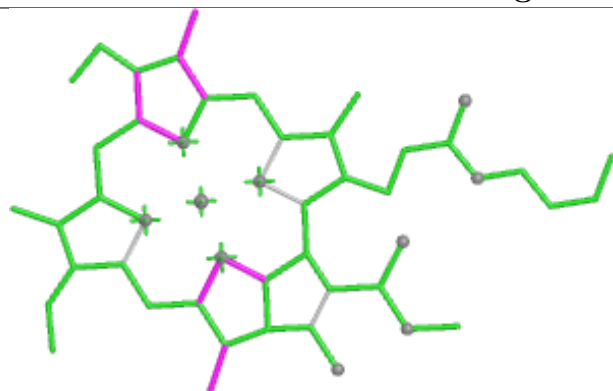


Rings

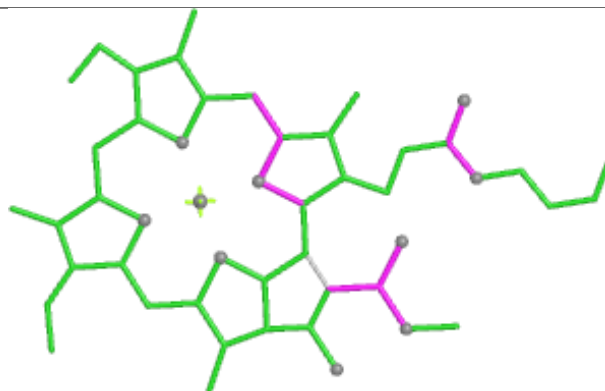




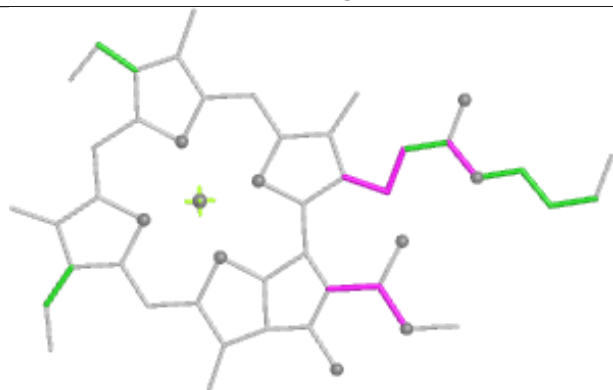
Ligand CLA C 515



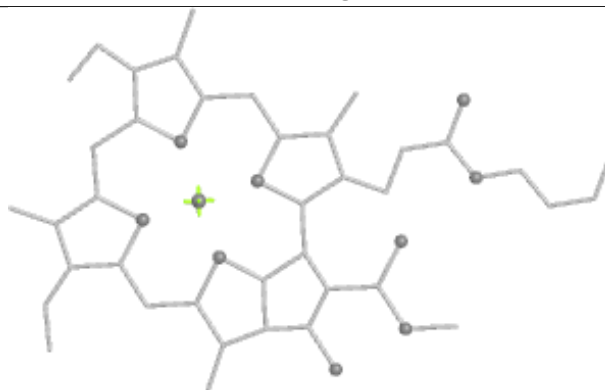
Bond lengths



Bond angles

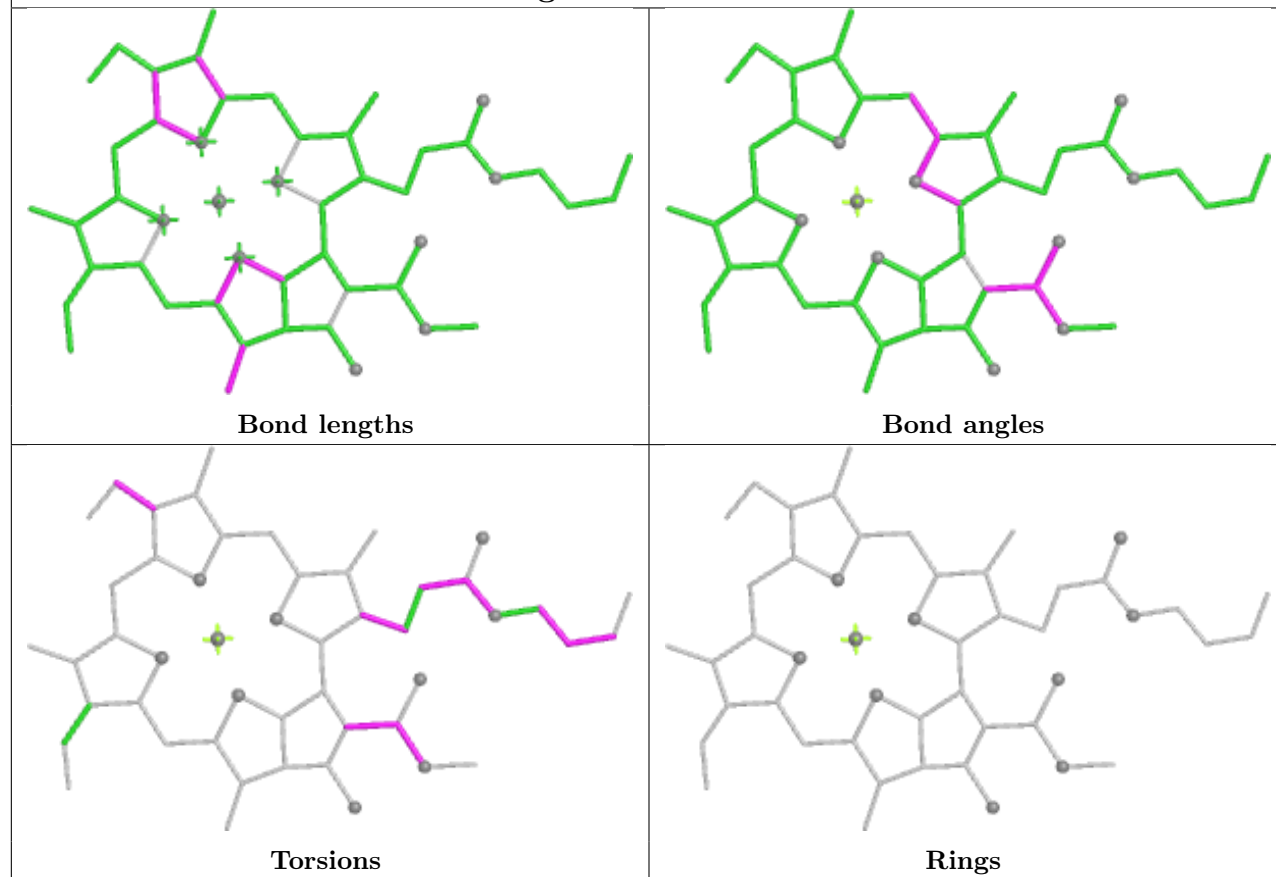


Torsions

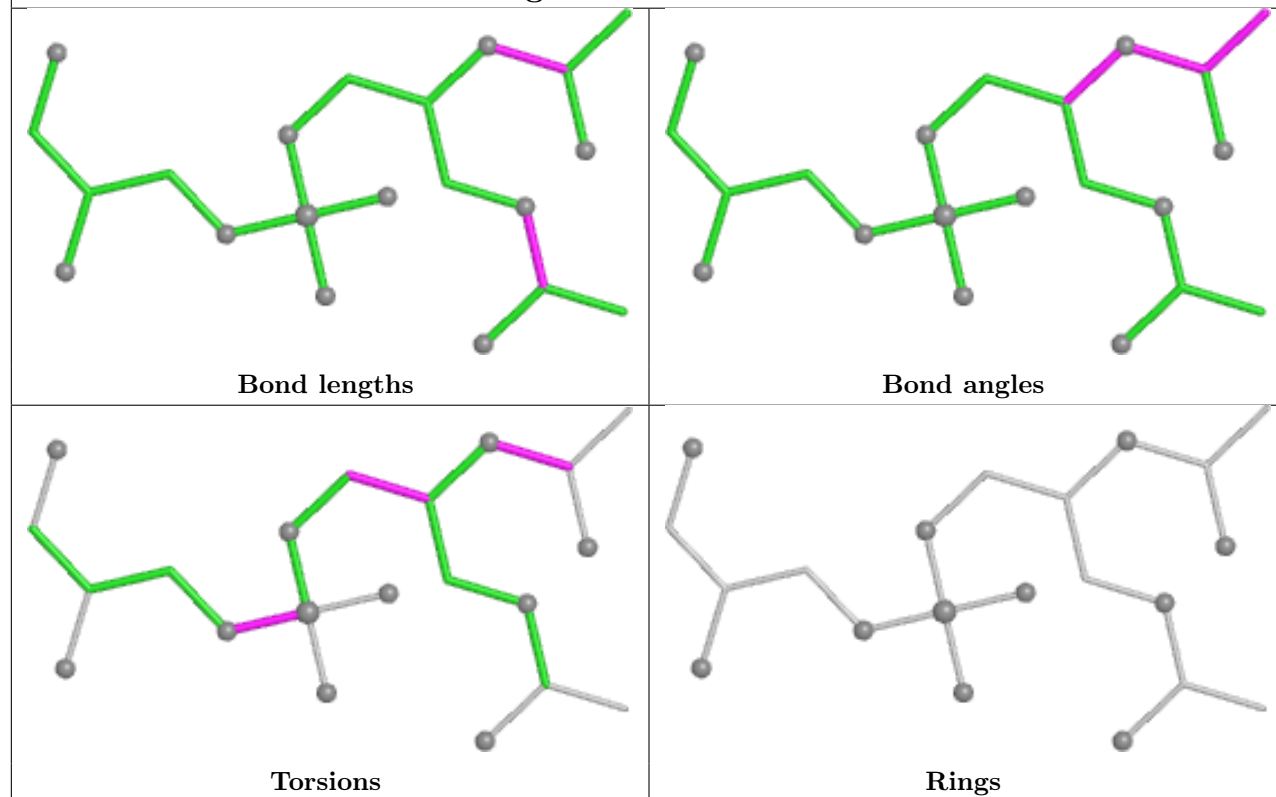


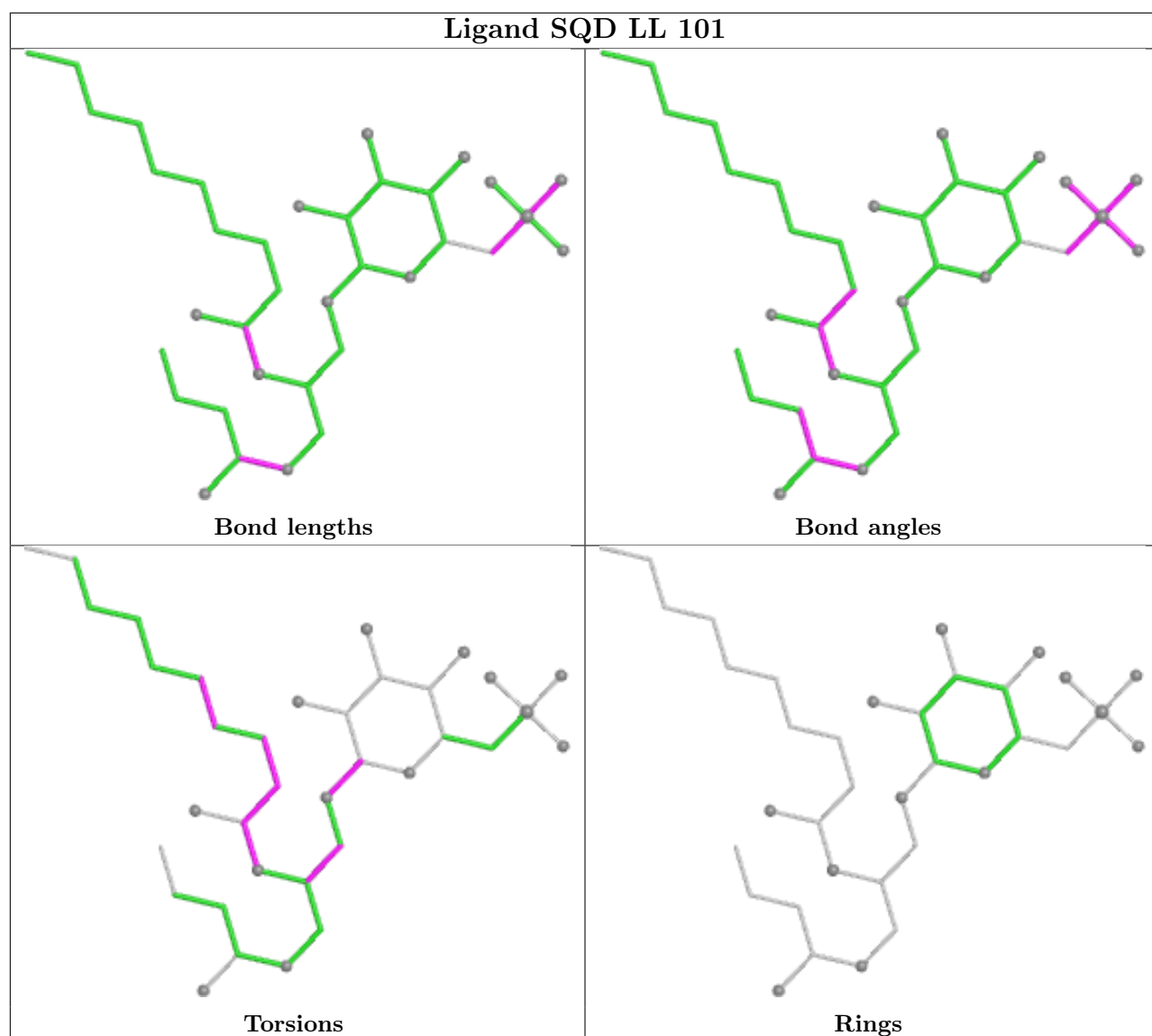
Rings

Ligand CLA r 611

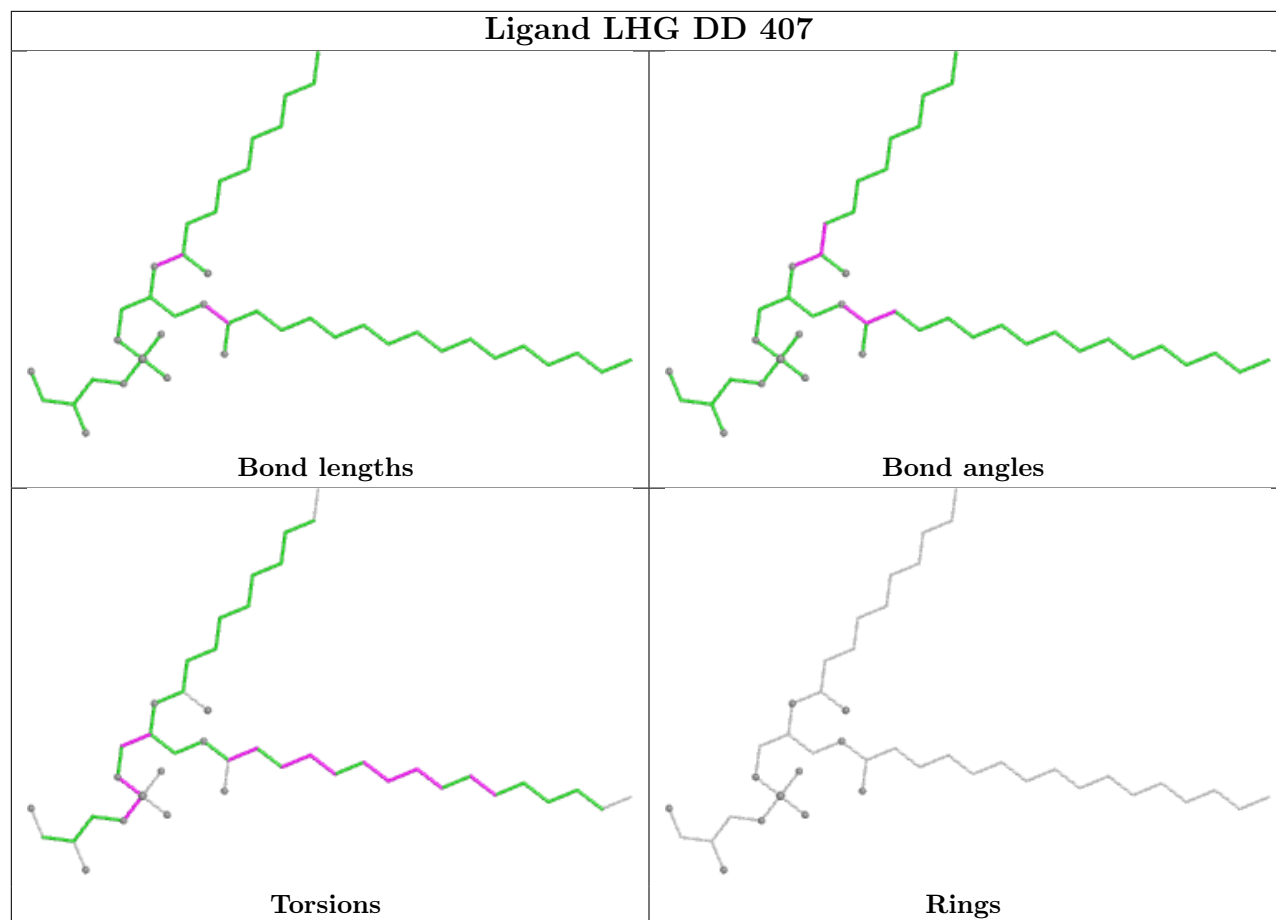


Ligand LHG 44 614

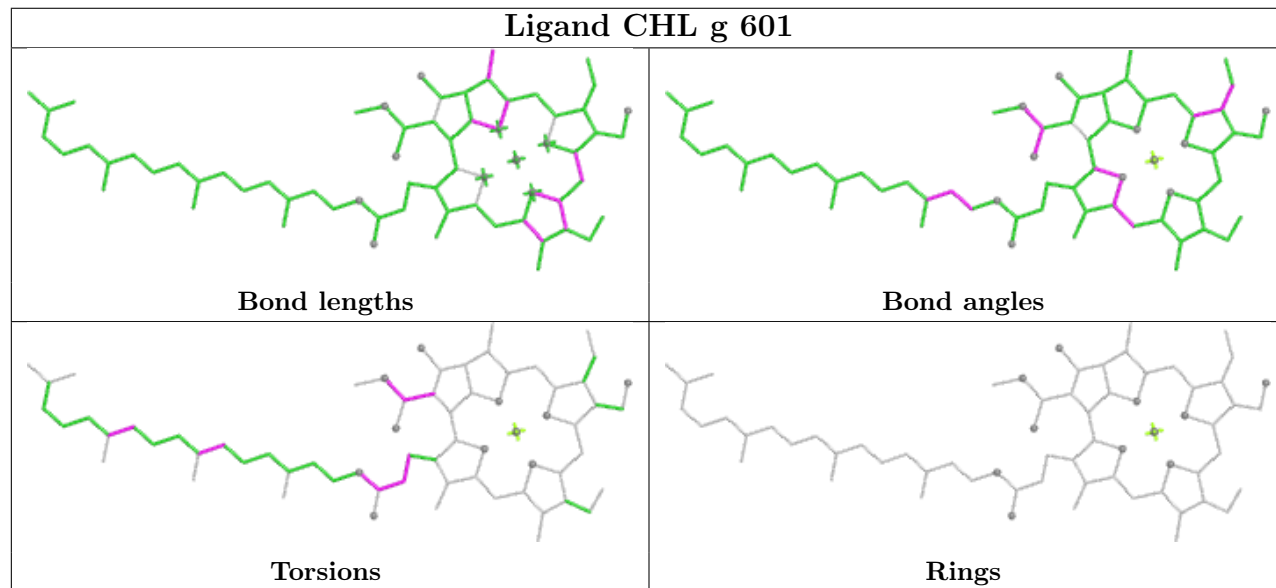


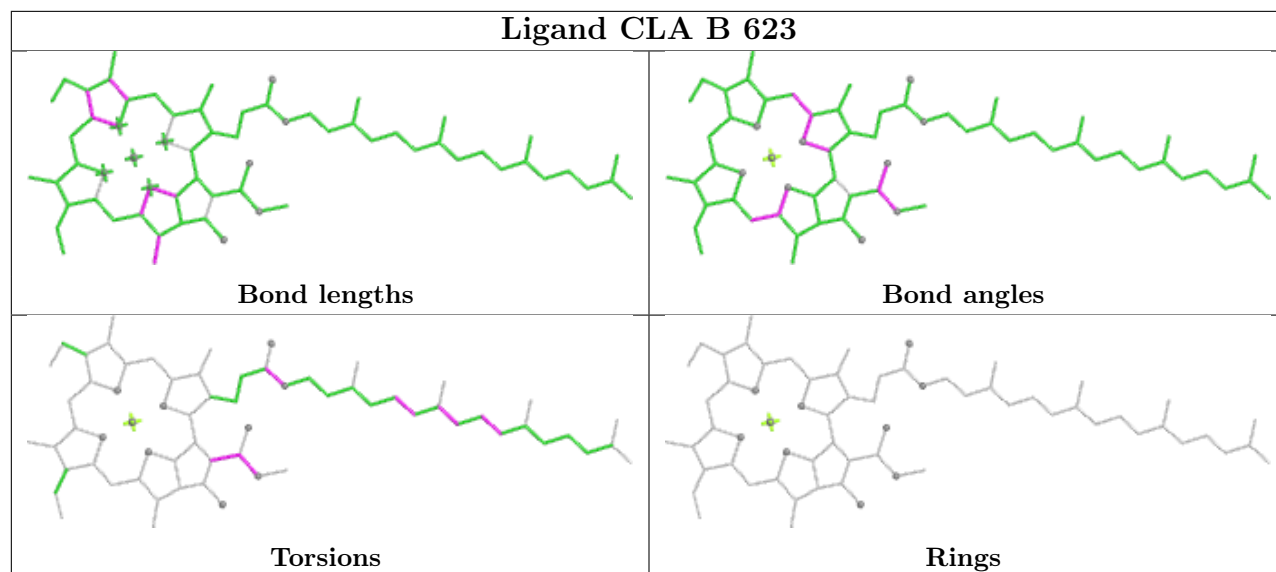
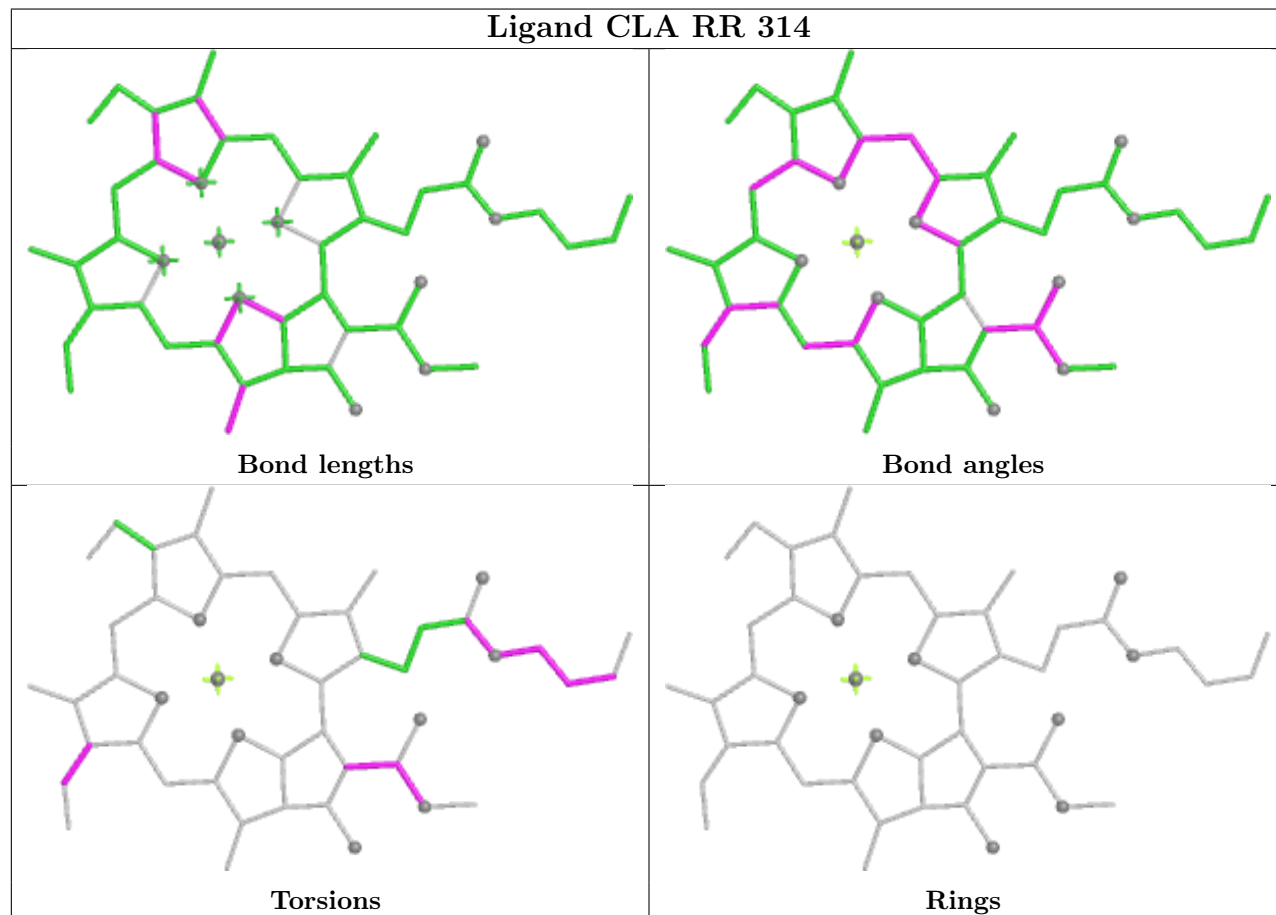


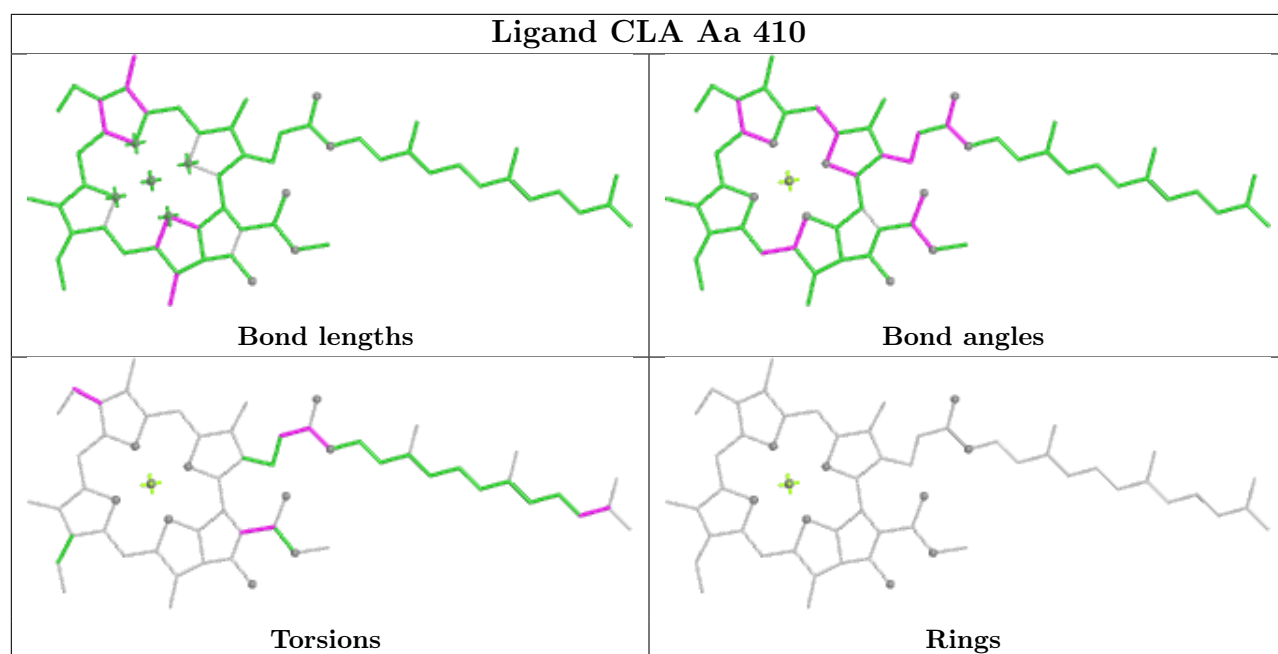
Ligand LHG DD 407

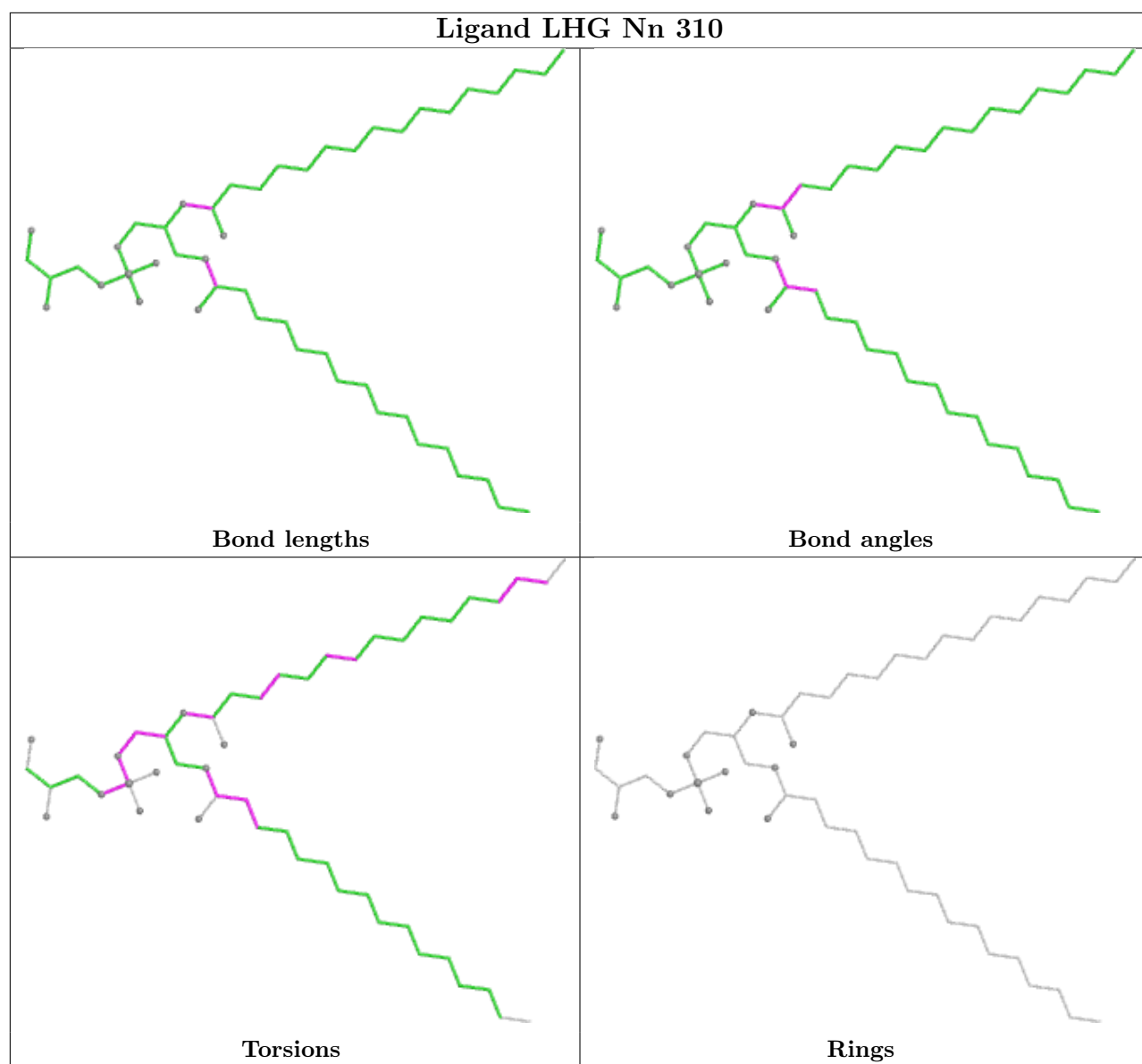


Ligand CHL g 601

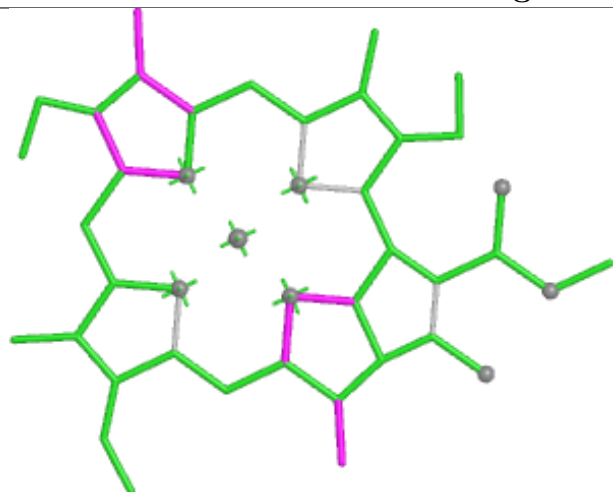


Ligand CLA B 623**Ligand CLA RR 314**

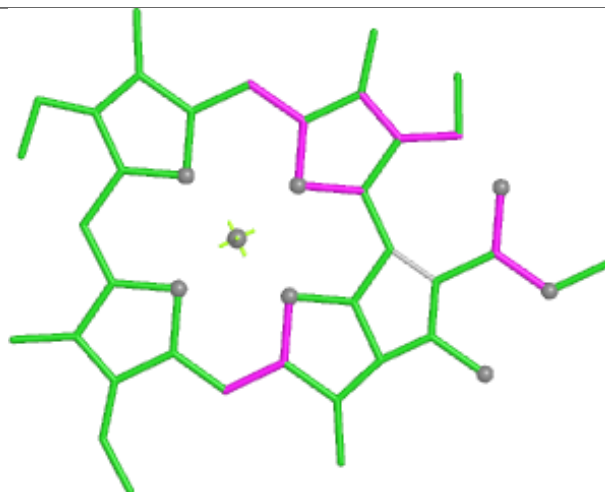




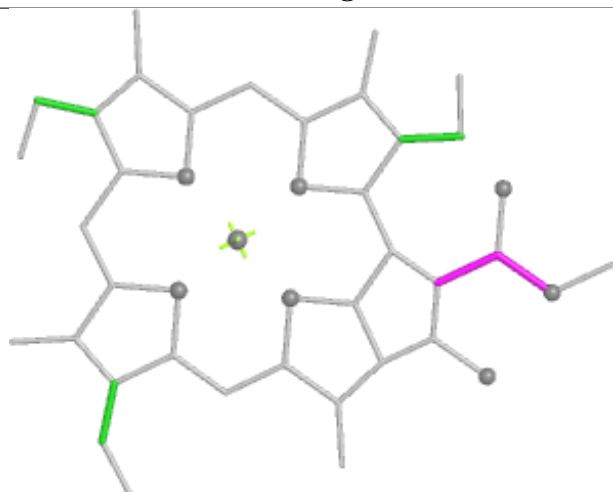
Ligand CLA N 603



Bond lengths



Bond angles

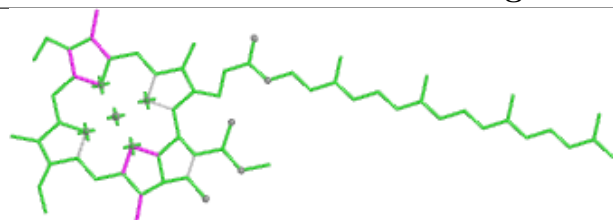


Torsions

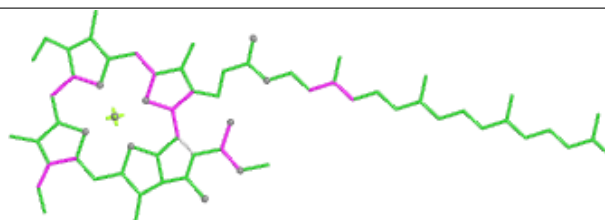


Rings

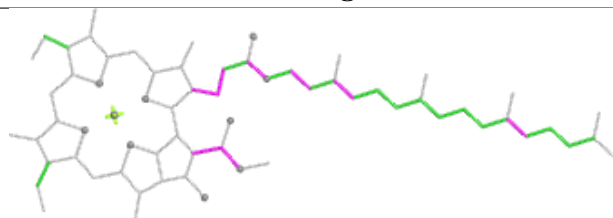
Ligand CLA Aa 405



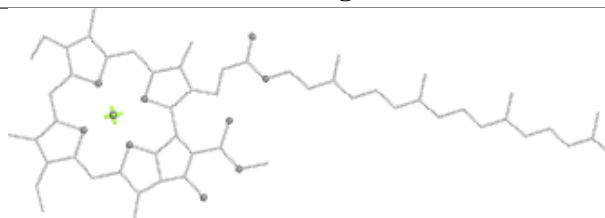
Bond lengths



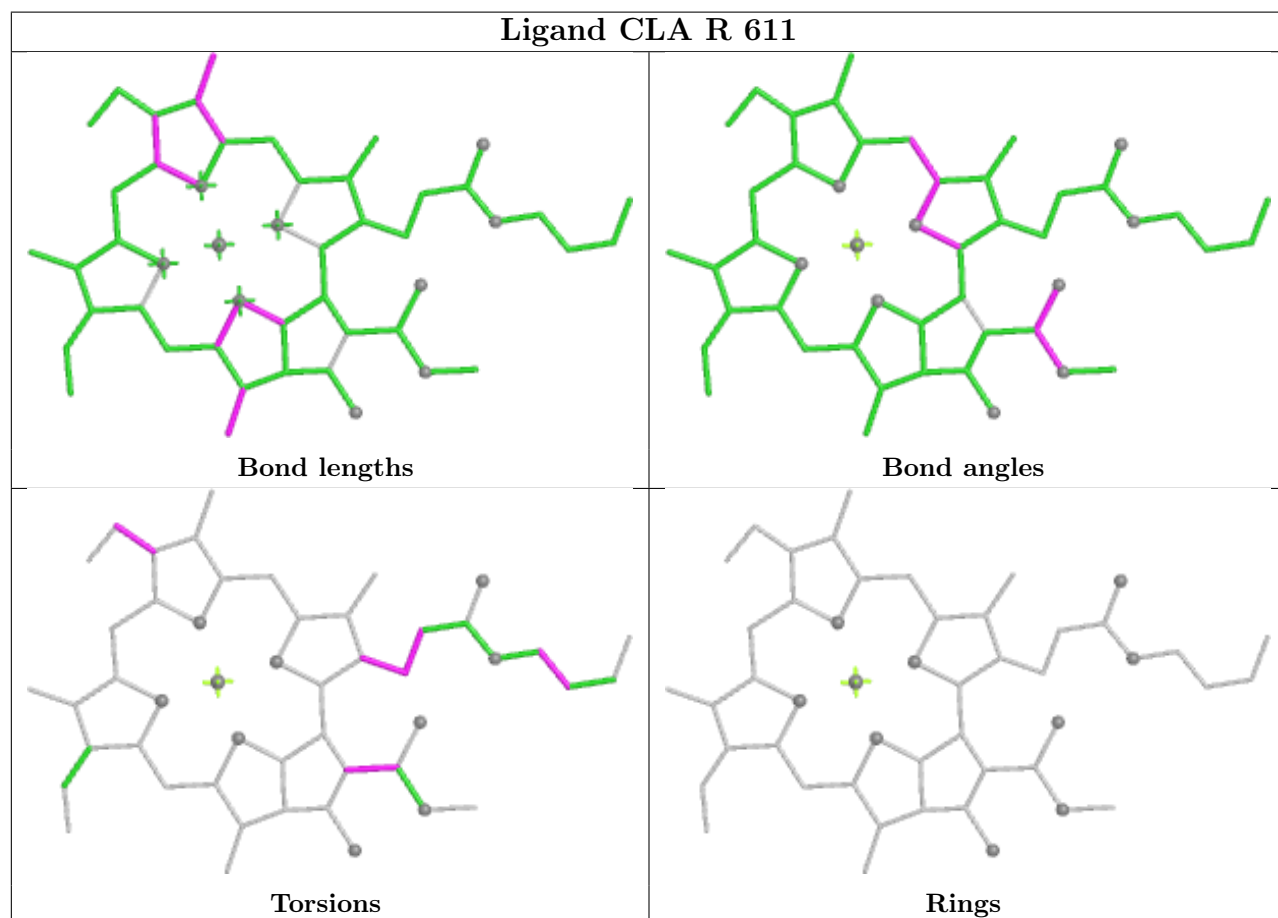
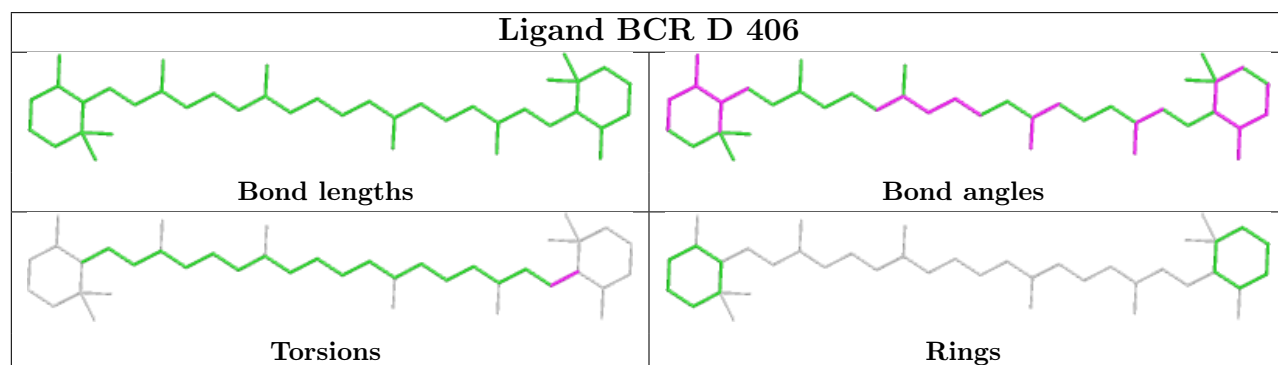
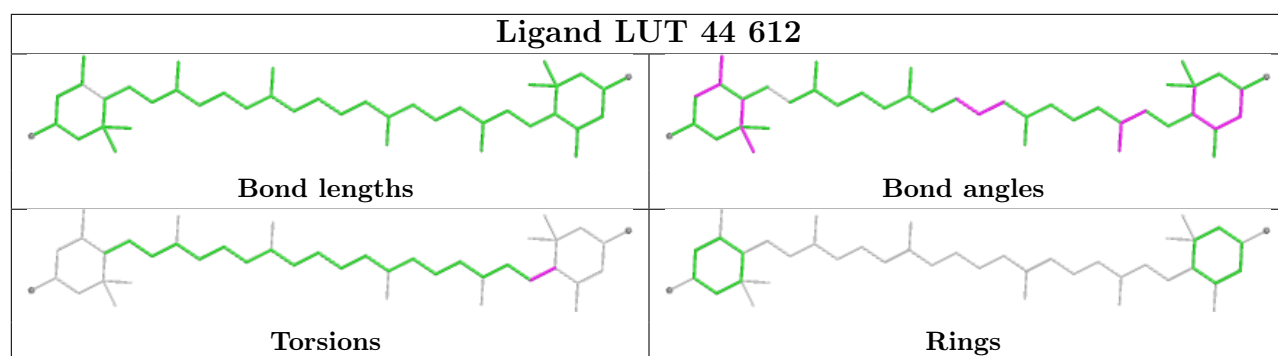
Bond angles

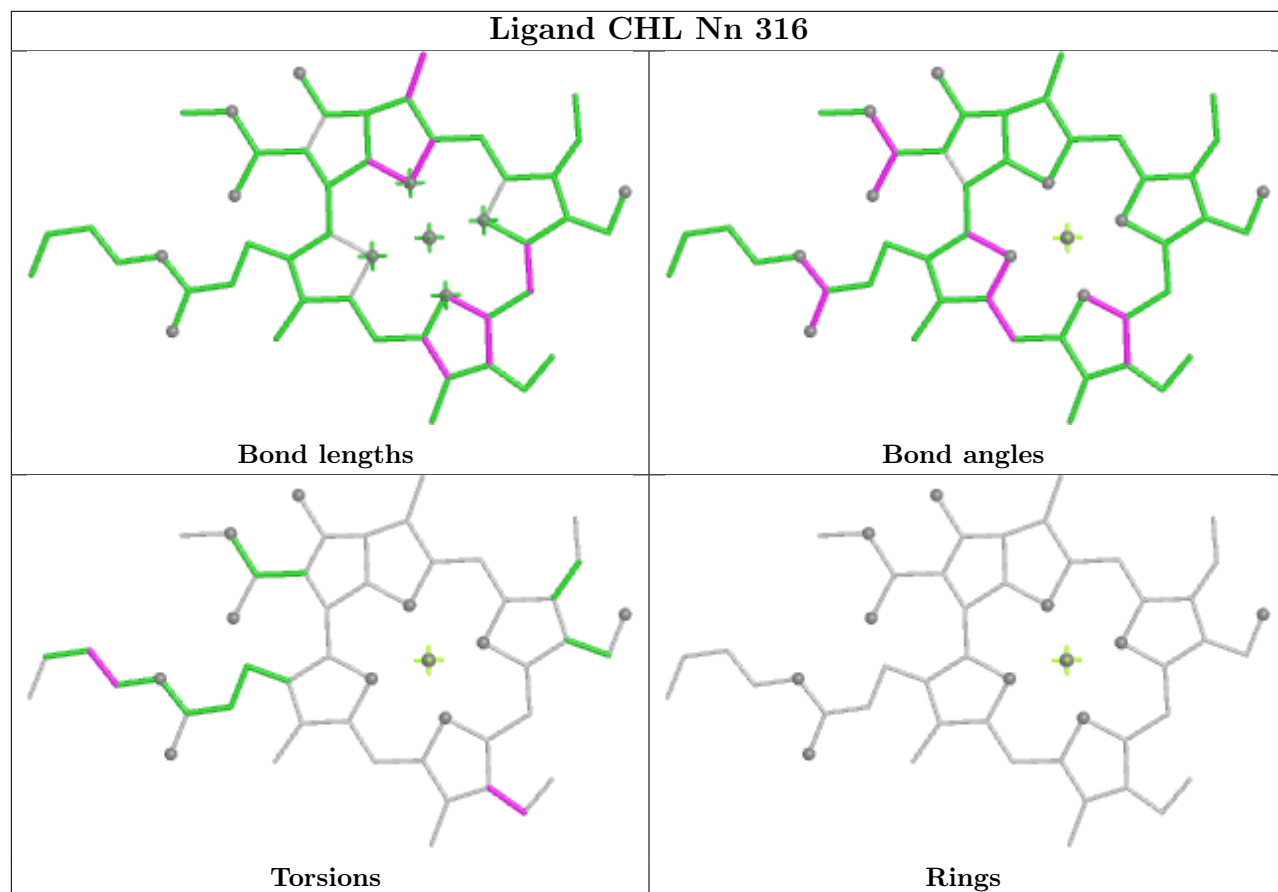


Torsions

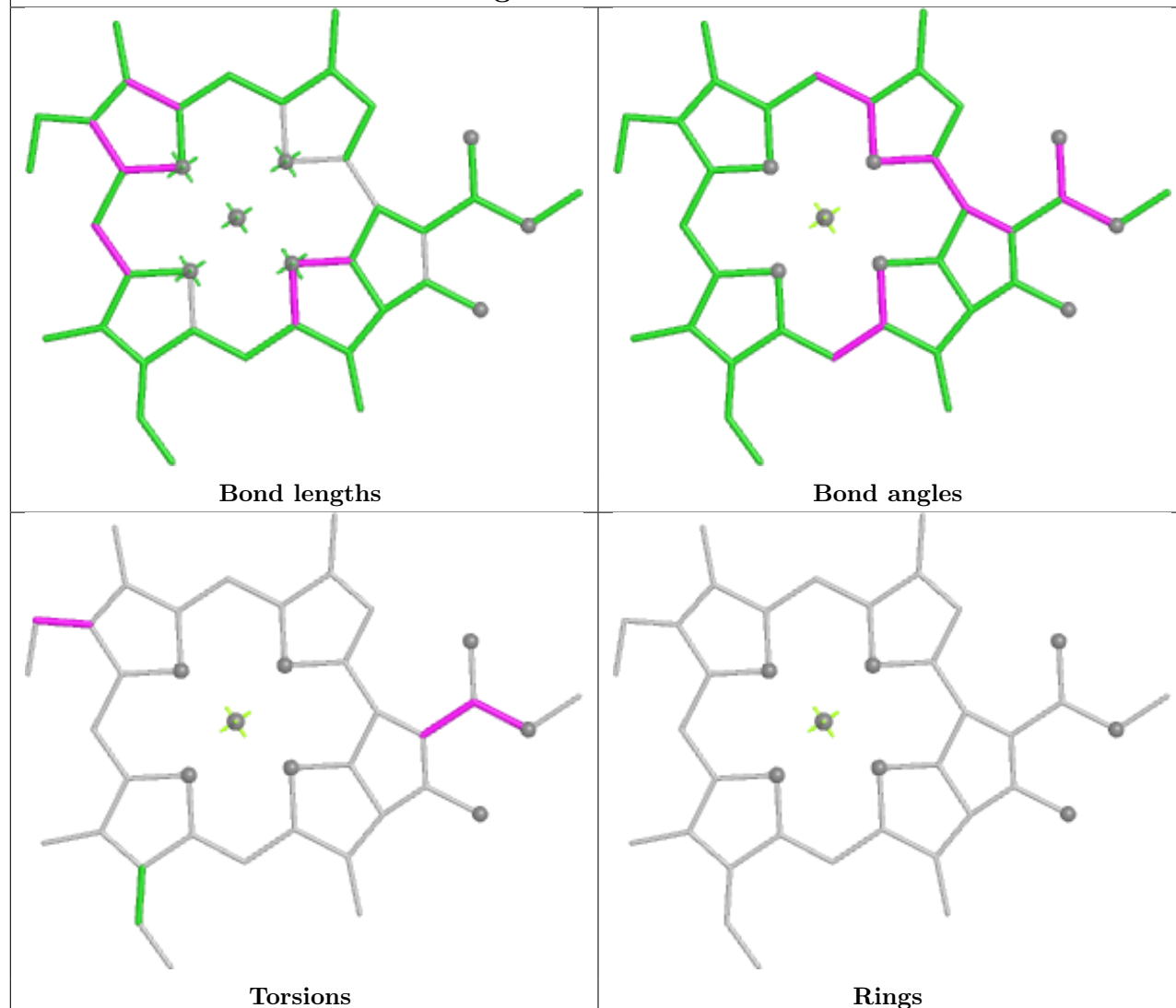


Rings

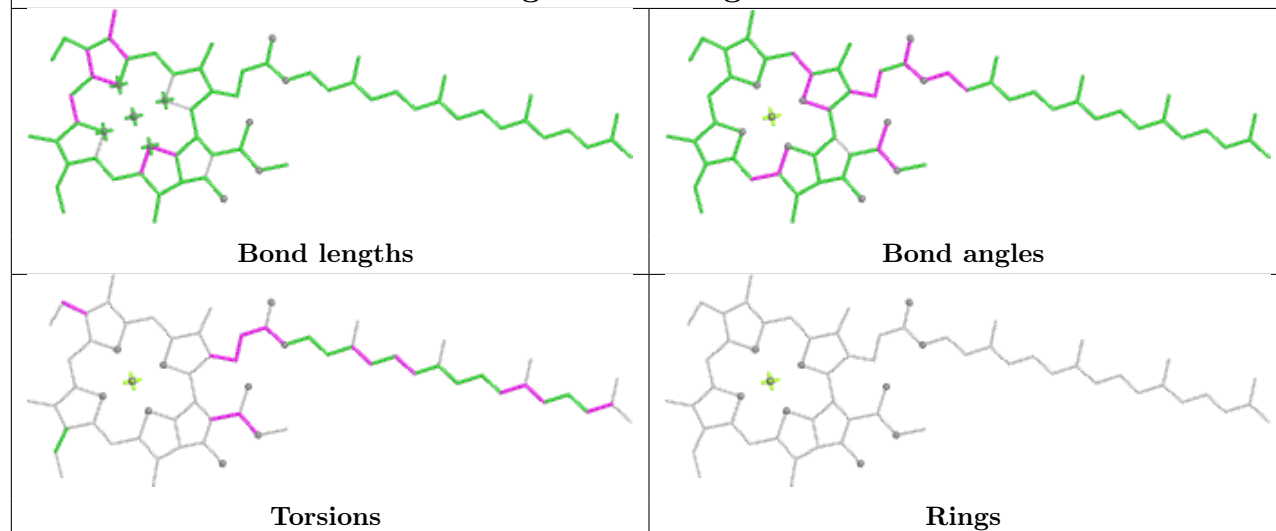




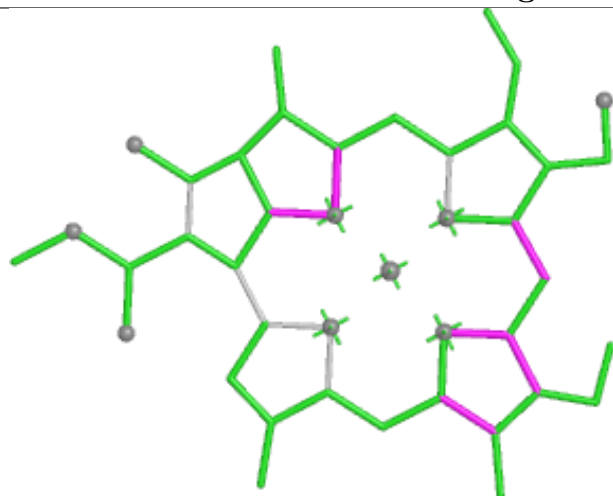
Ligand CLA 2 611



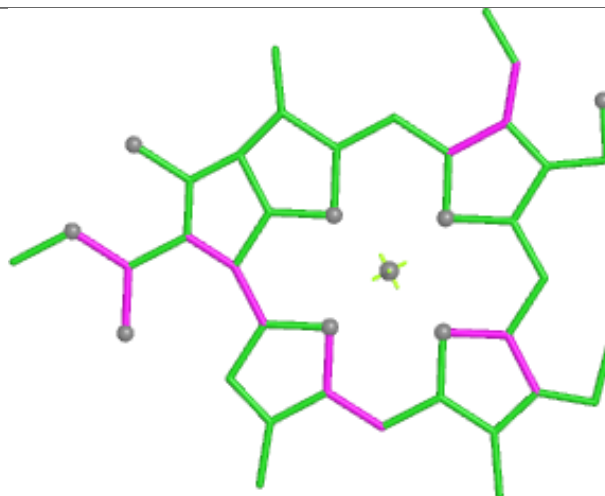
Ligand CLA Gg 312



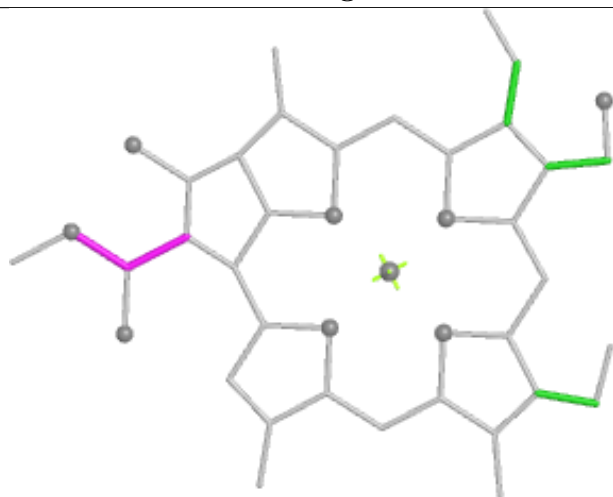
Ligand CHL 3 608



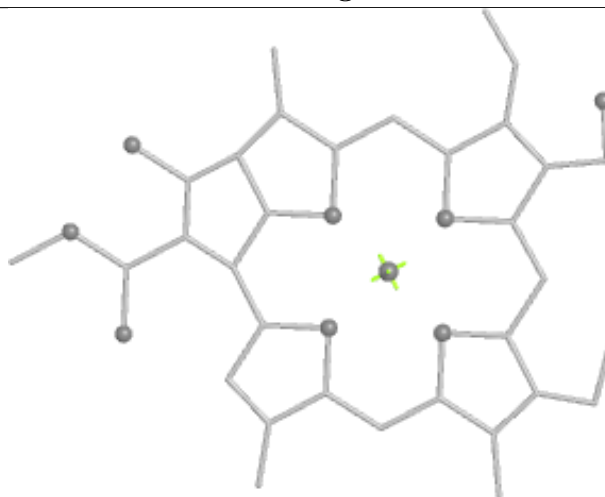
Bond lengths



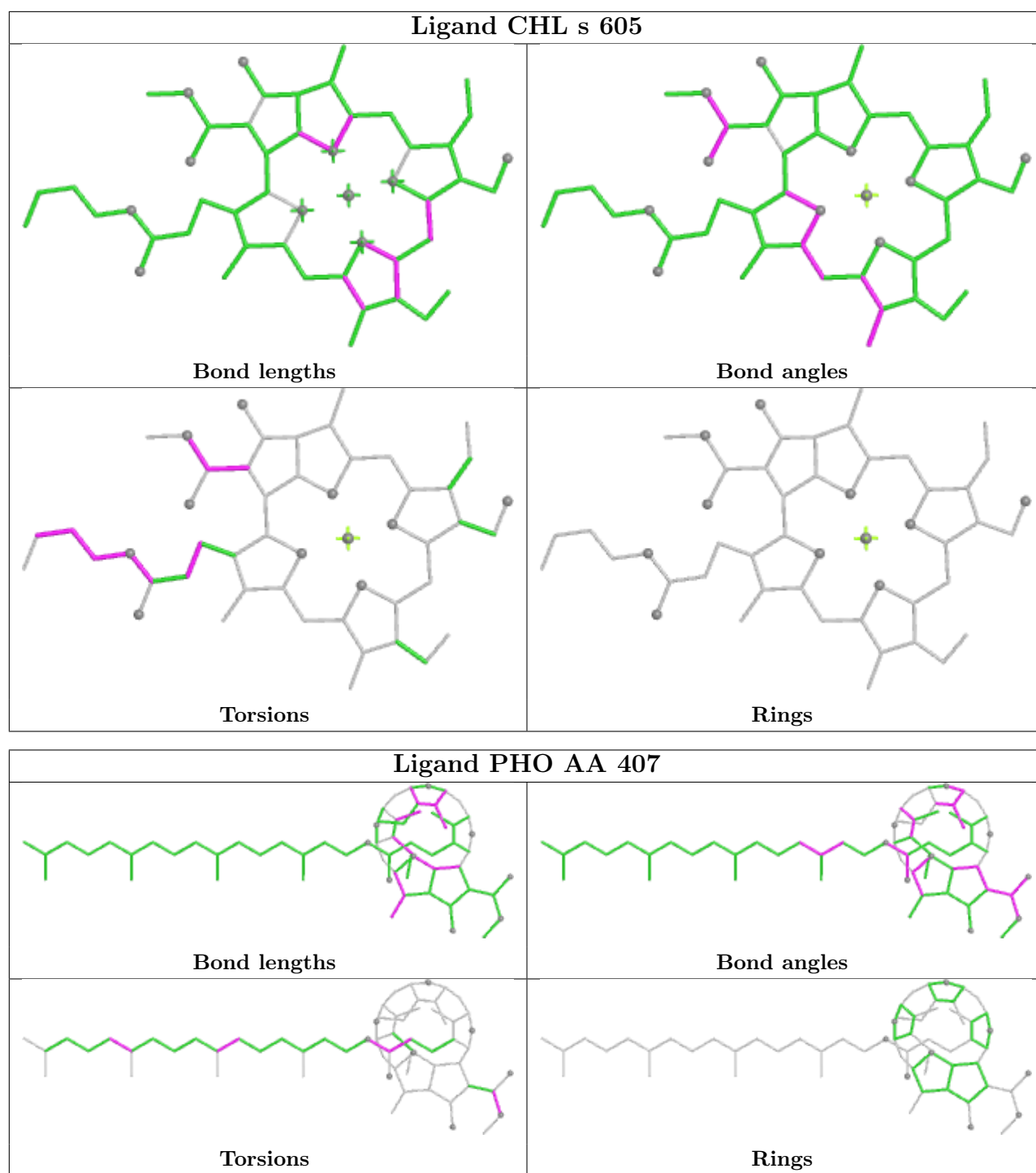
Bond angles

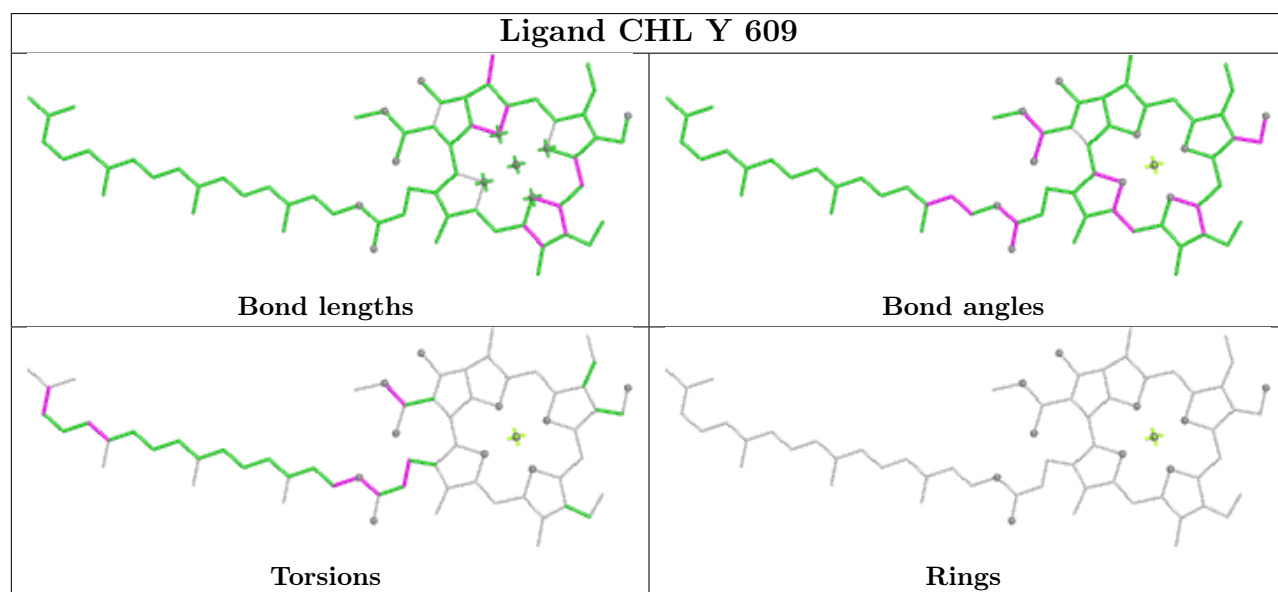
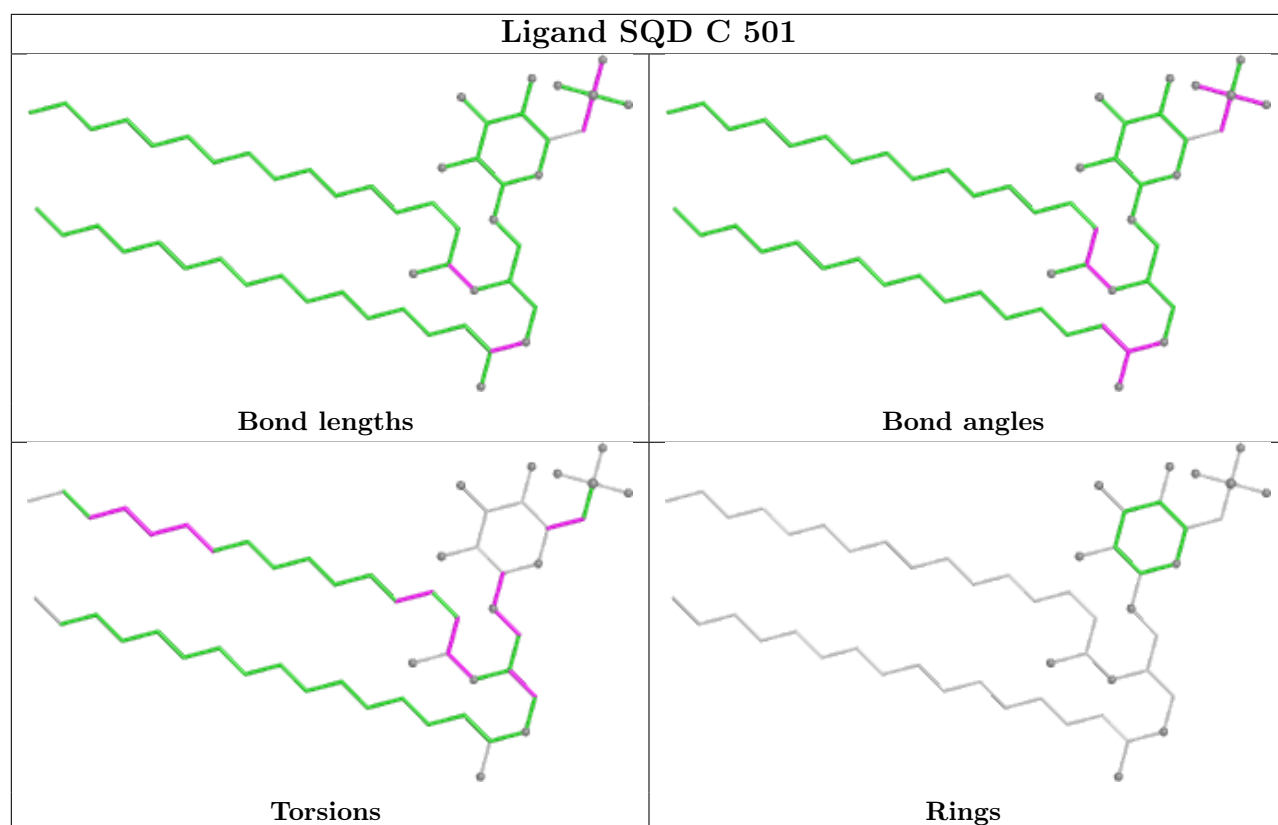


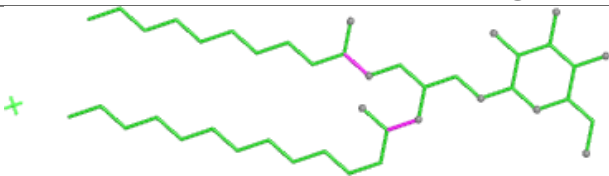
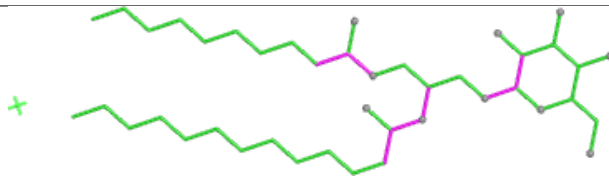
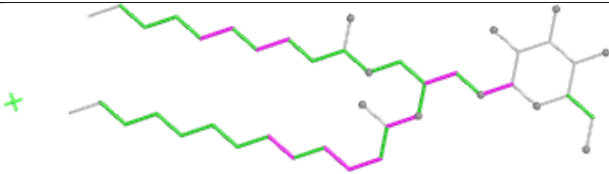
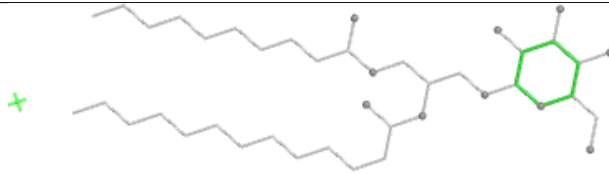
Torsions

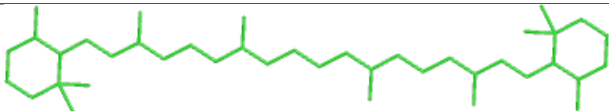
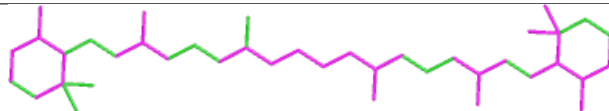
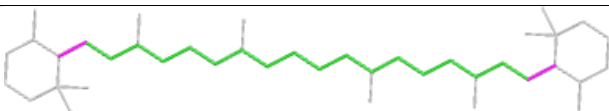
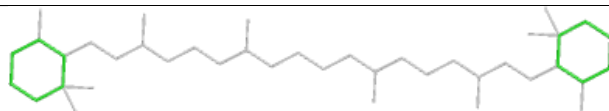


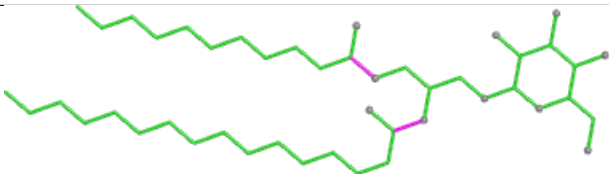
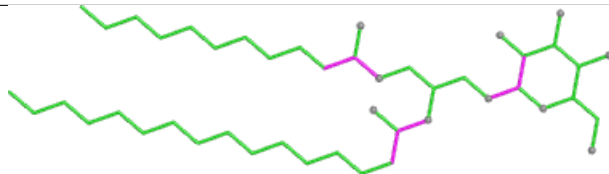
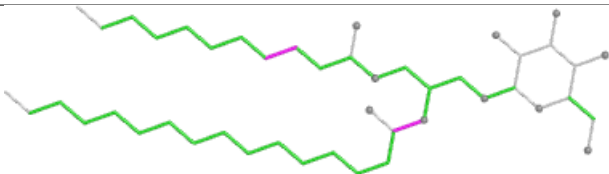
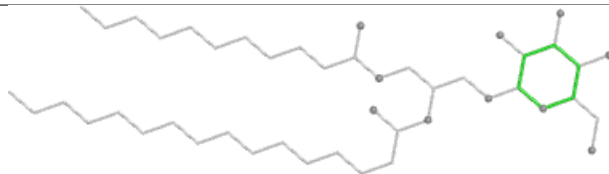
Rings



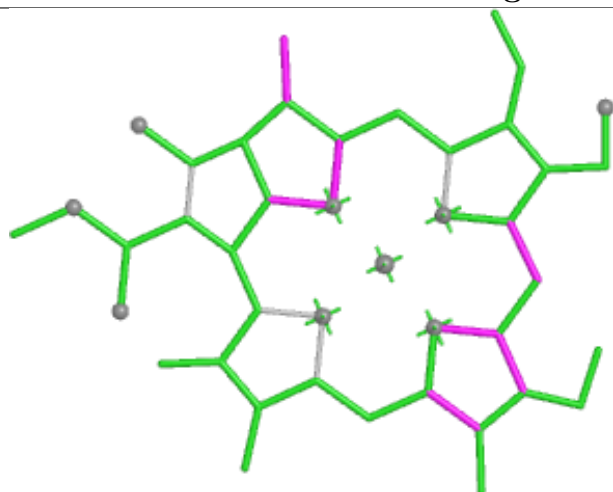


Ligand LMG a 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

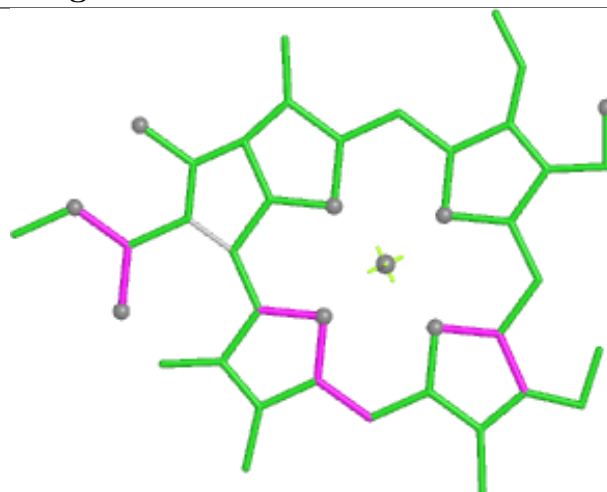
Ligand BCR KK 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

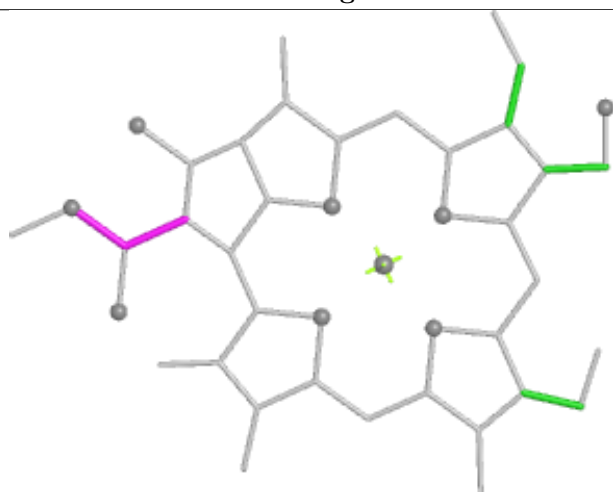
Ligand CHL Gg 309



Bond lengths



Bond angles

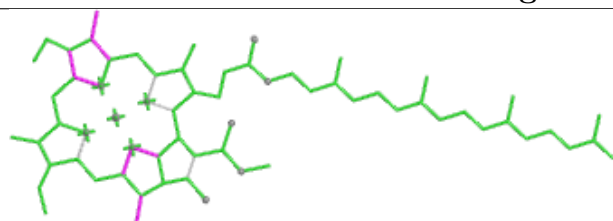


Torsions

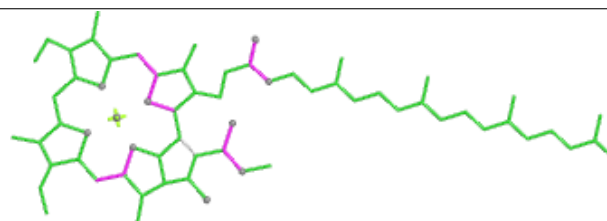


Rings

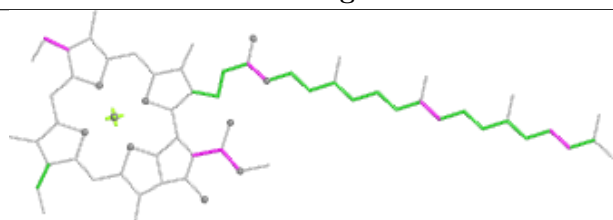
Ligand CLA c 512



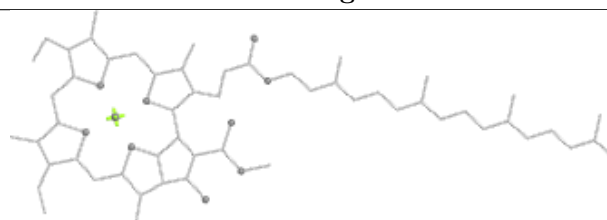
Bond lengths



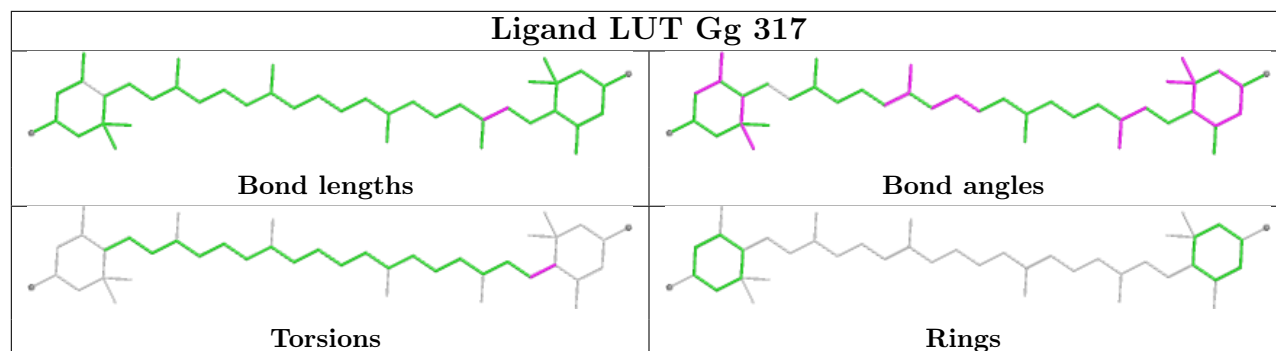
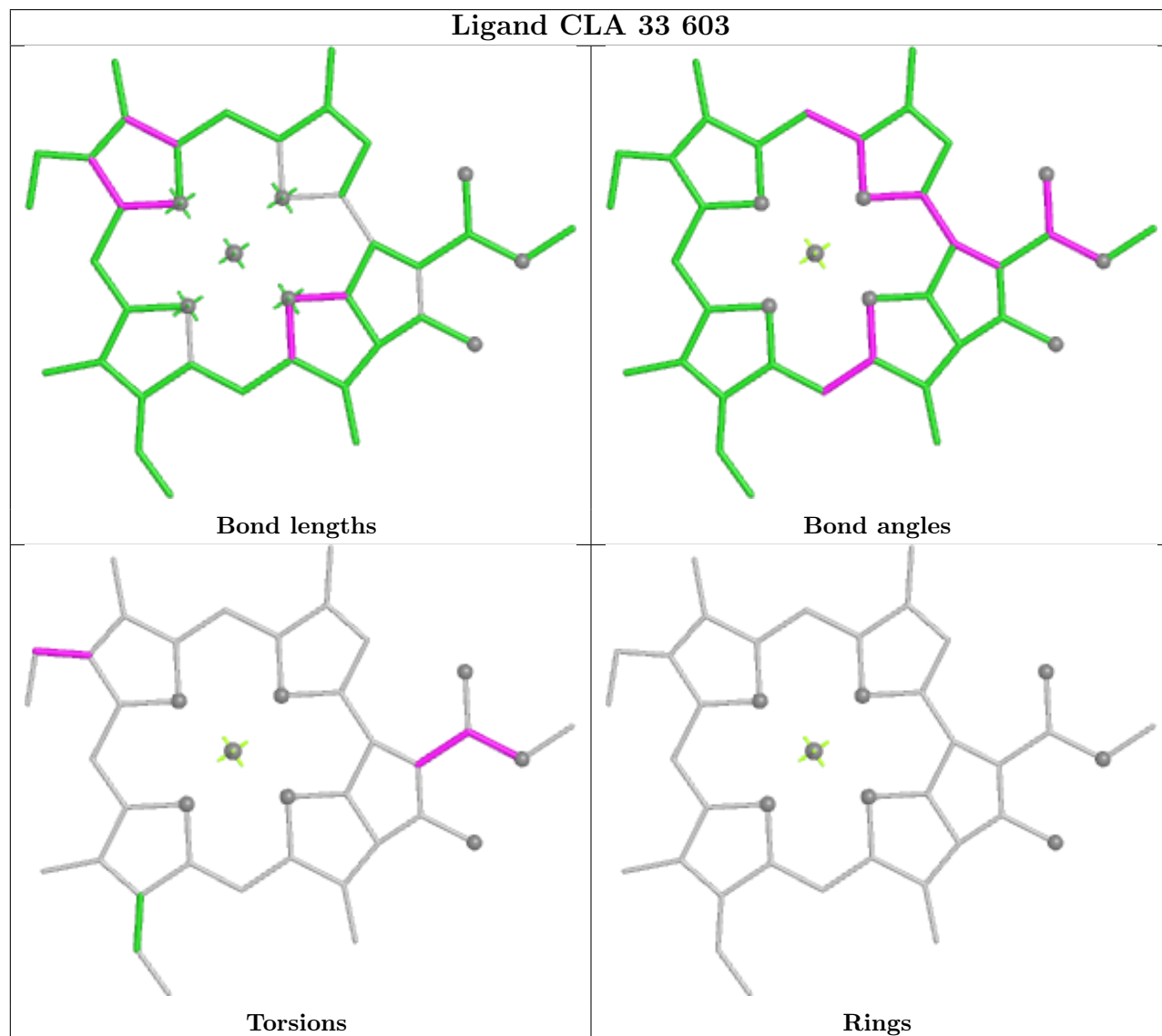
Bond angles

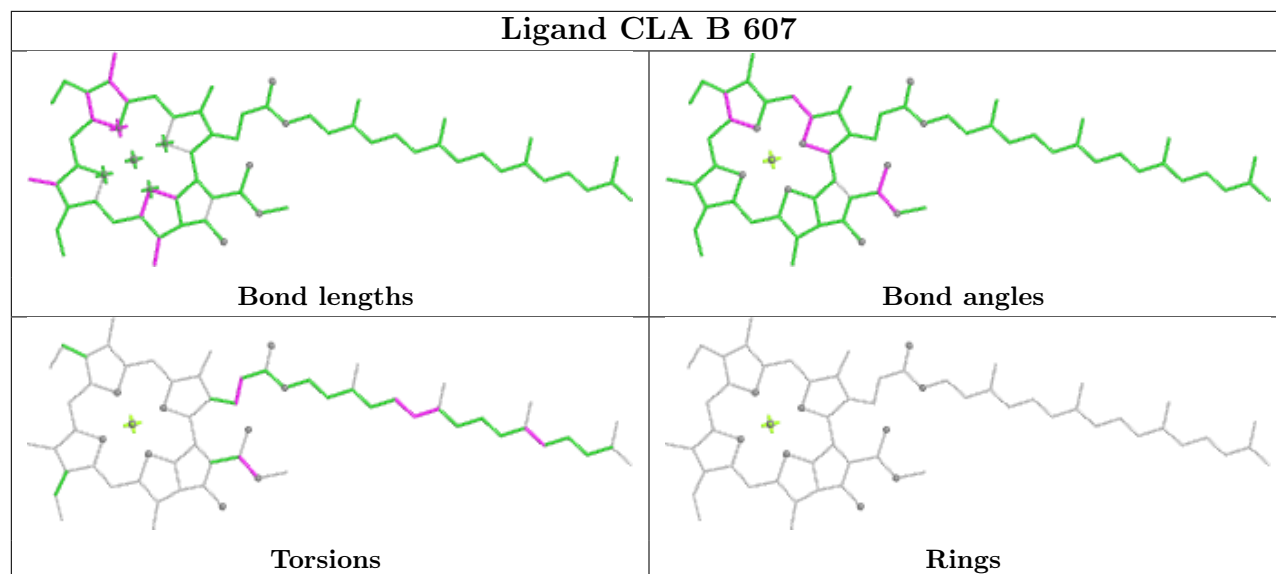
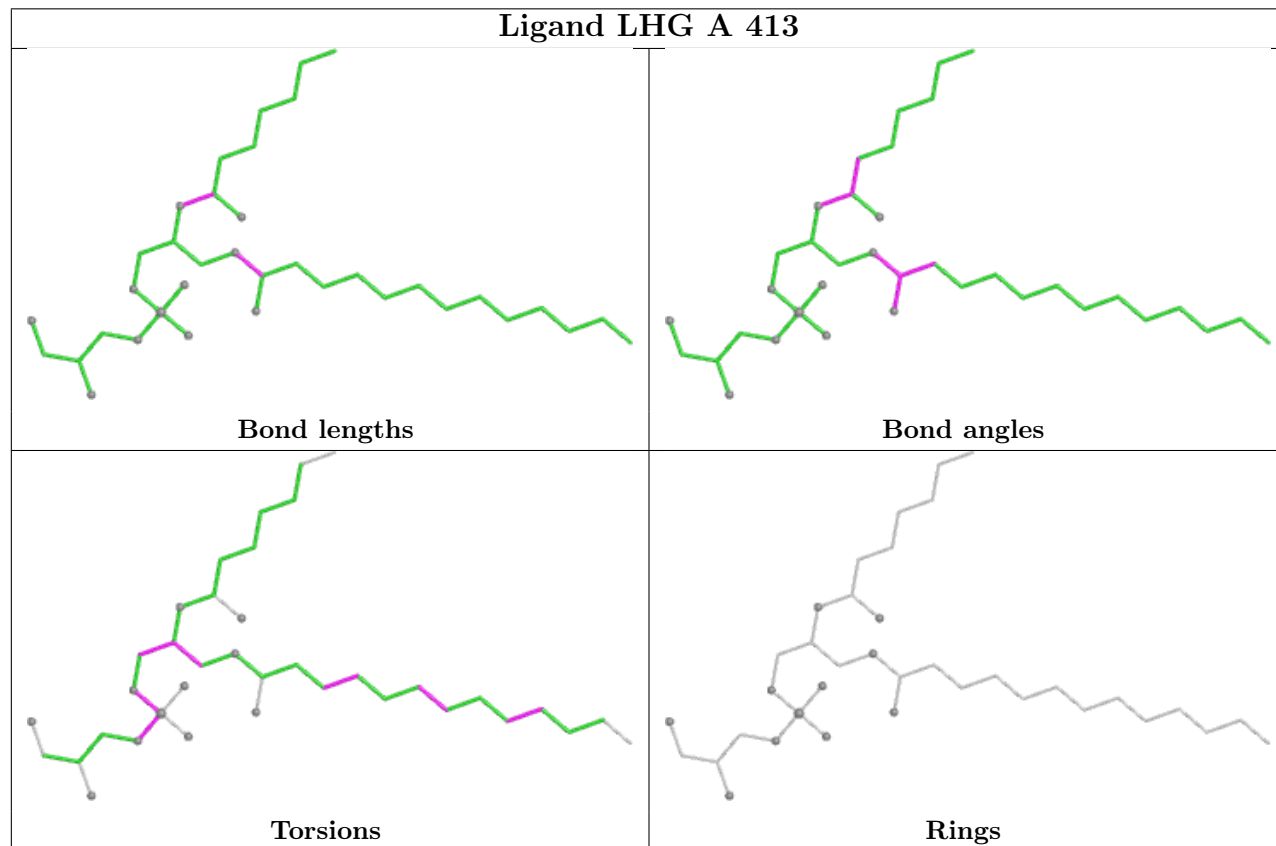


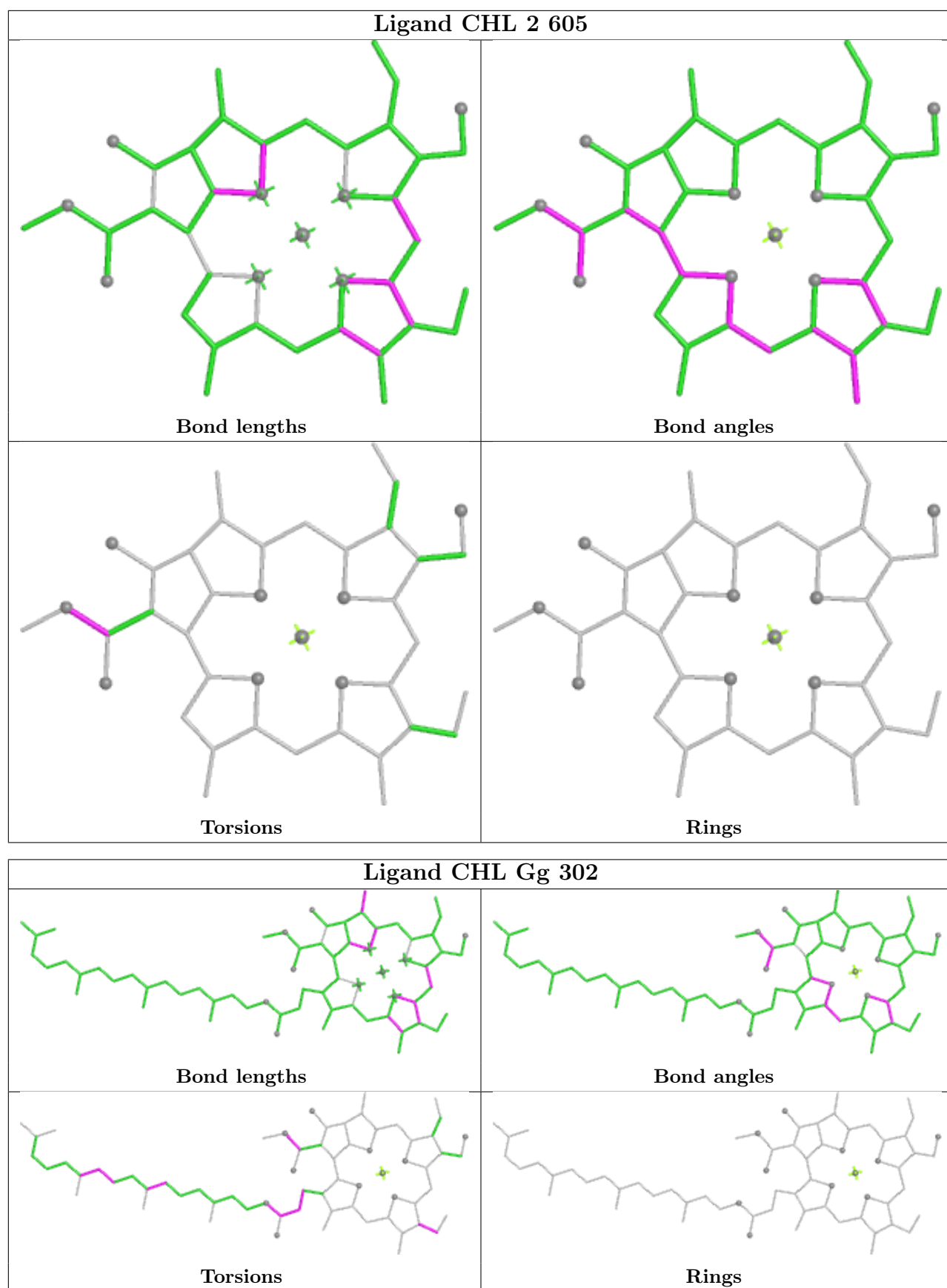
Torsions

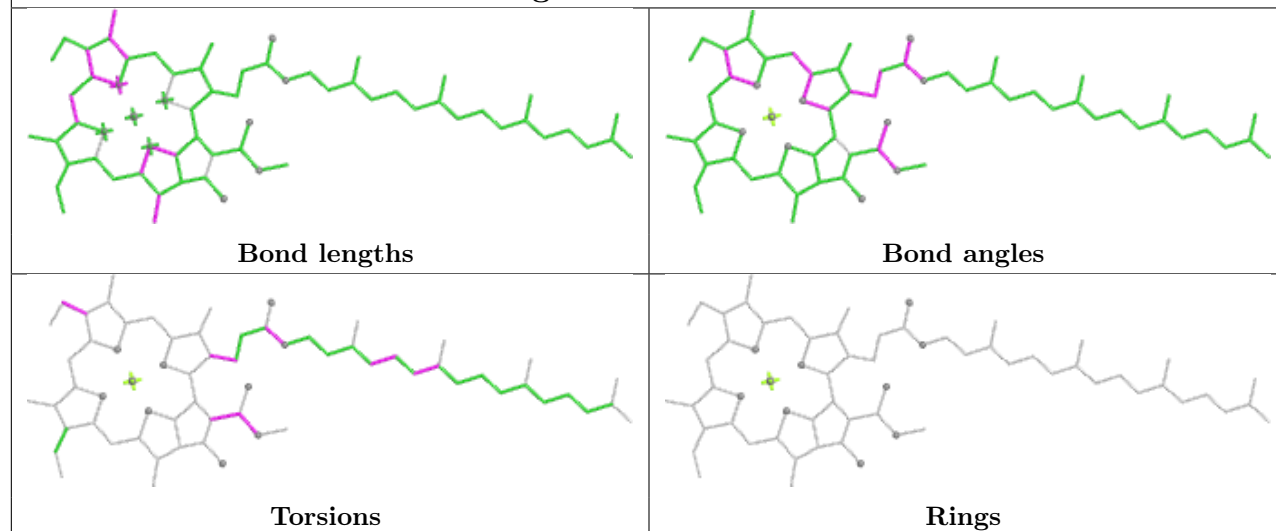
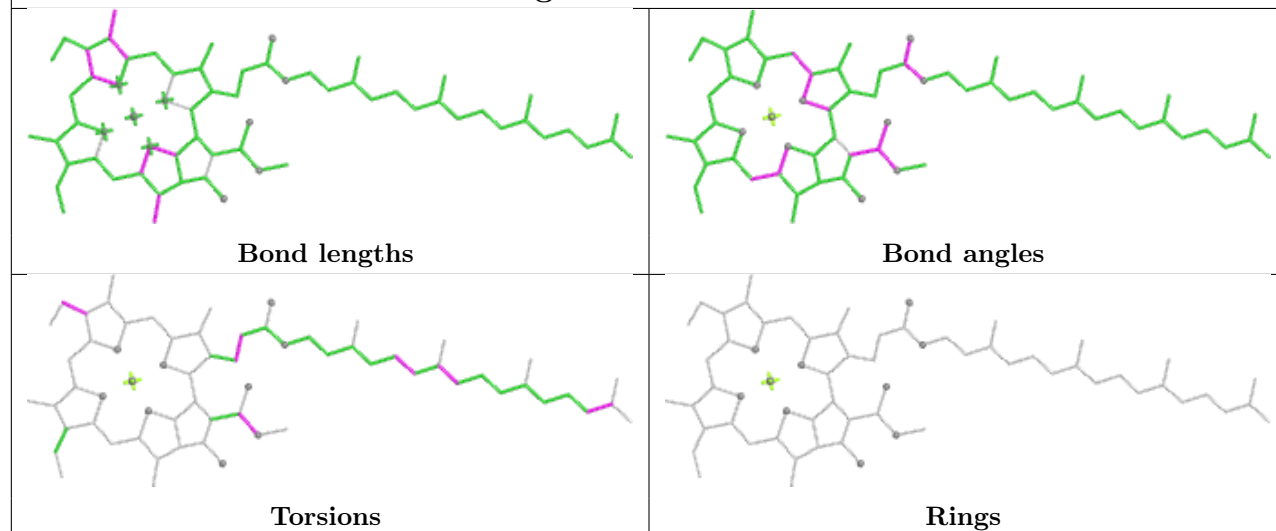


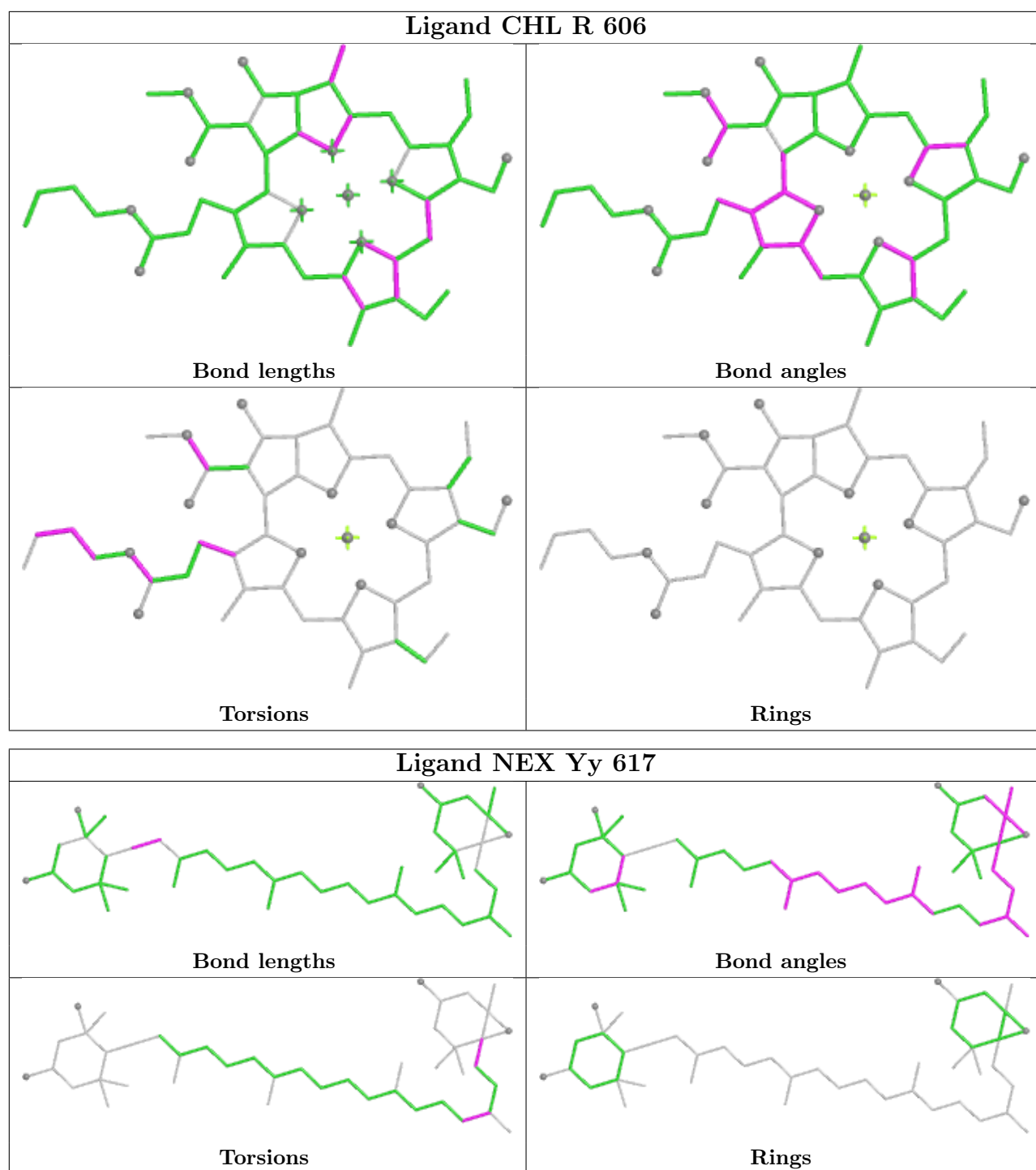
Rings

Ligand LUT Gg 317**Ligand CLA 33 603**

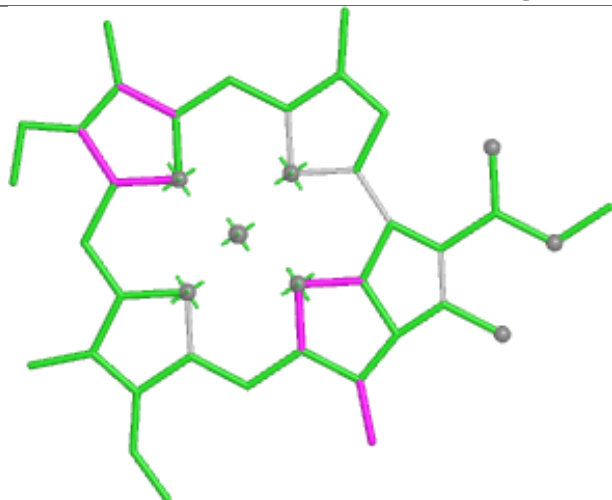
Ligand CLA B 607**Ligand LHG A 413**



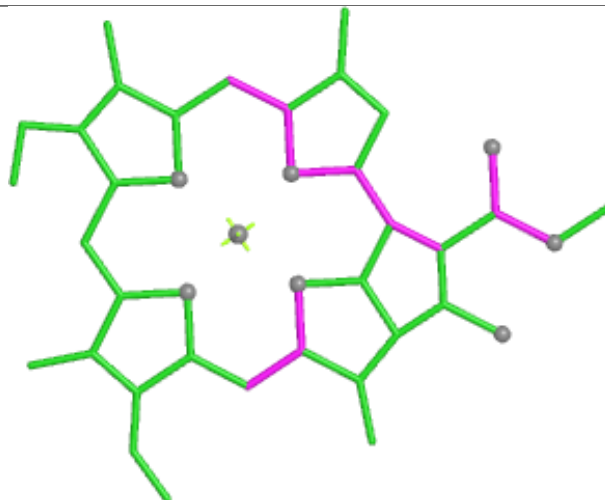
Ligand CLA C 508**Ligand CLA b 606**



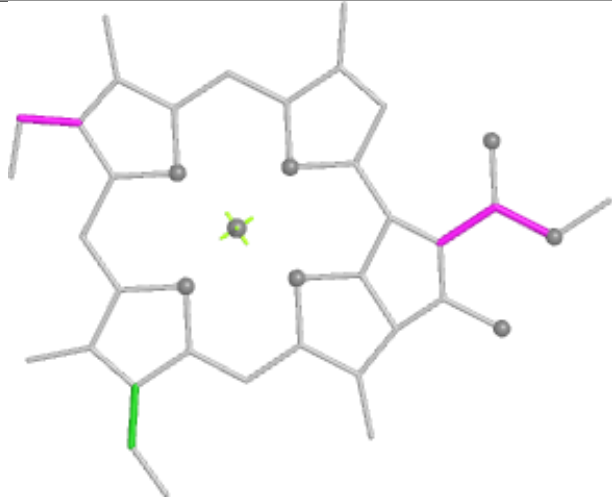
Ligand CLA 3 611



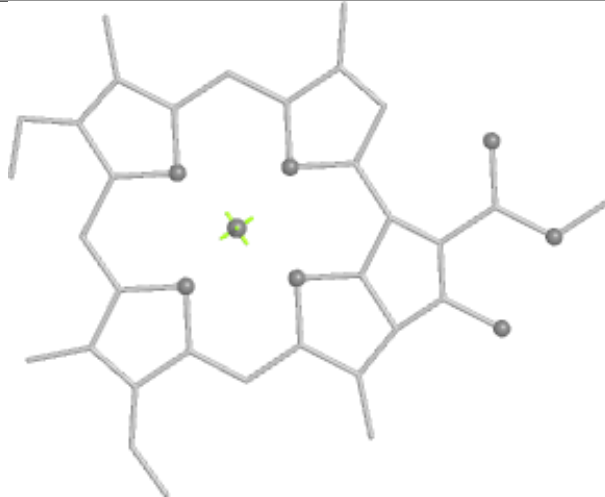
Bond lengths



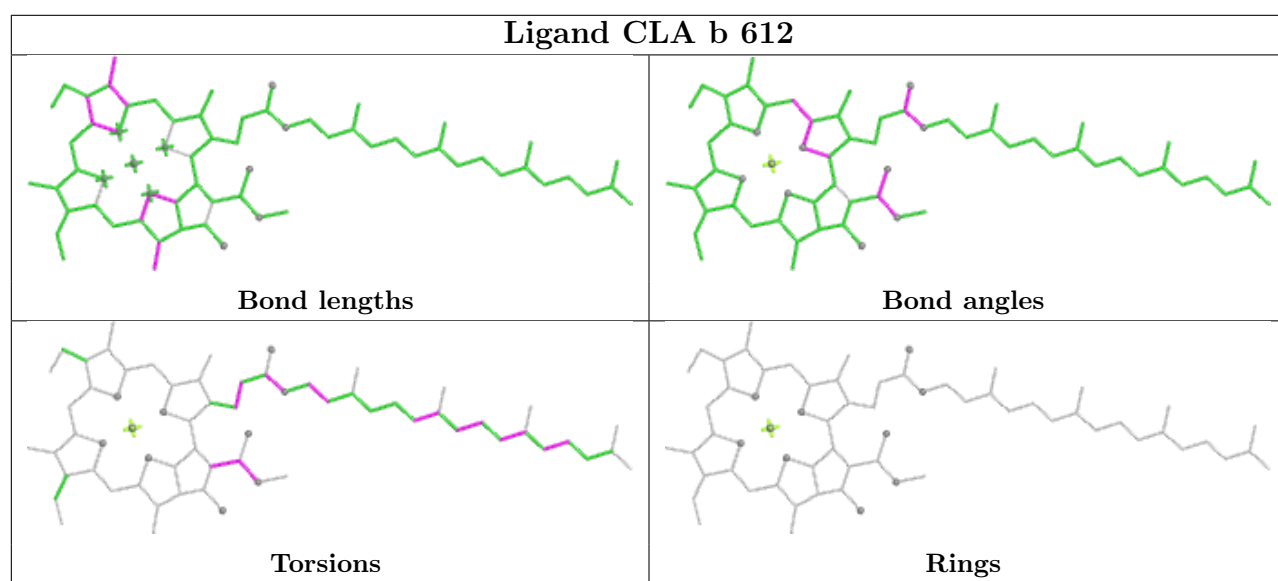
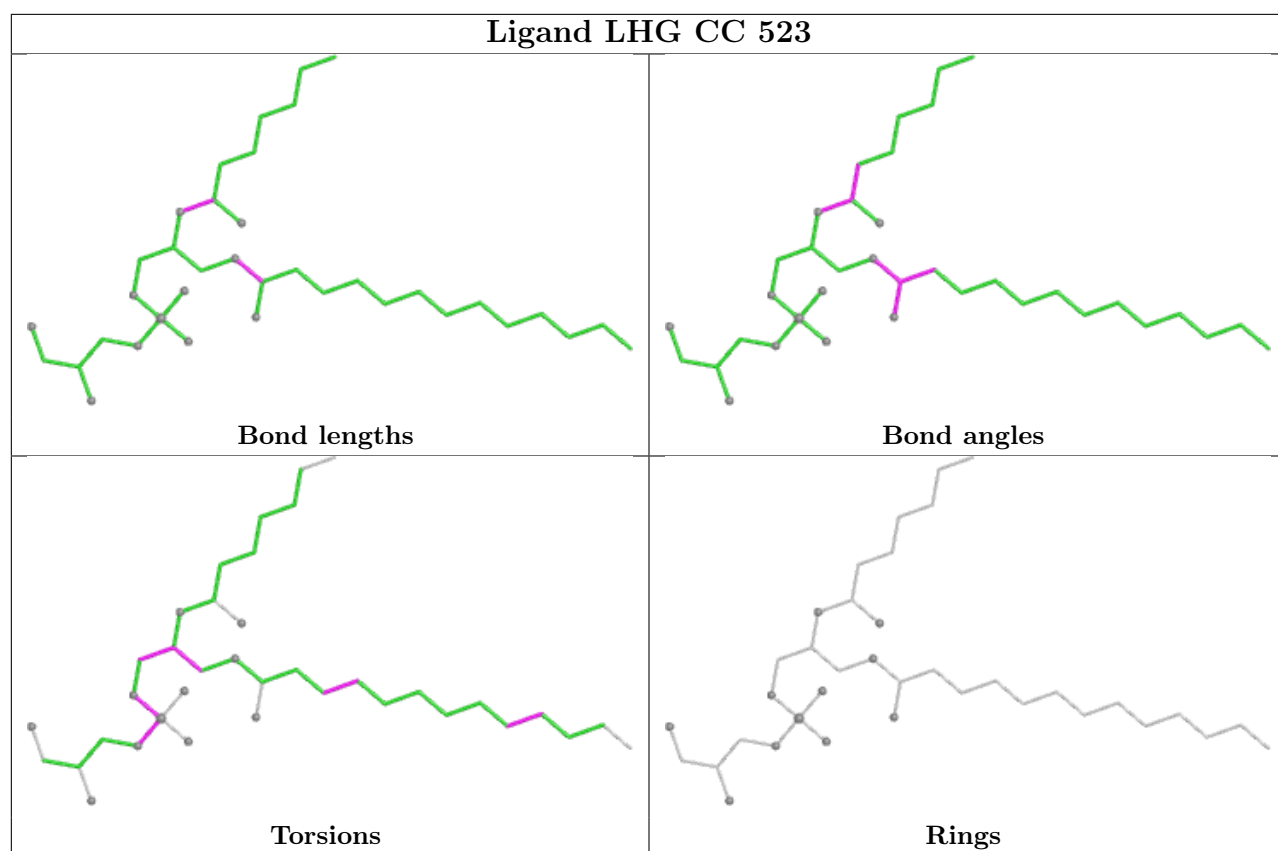
Bond angles



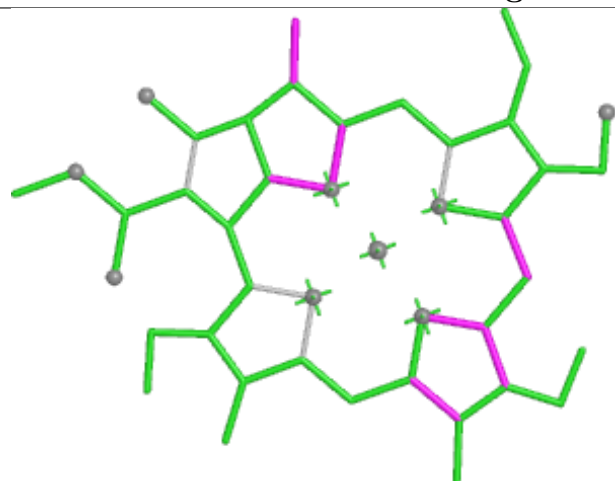
Torsions



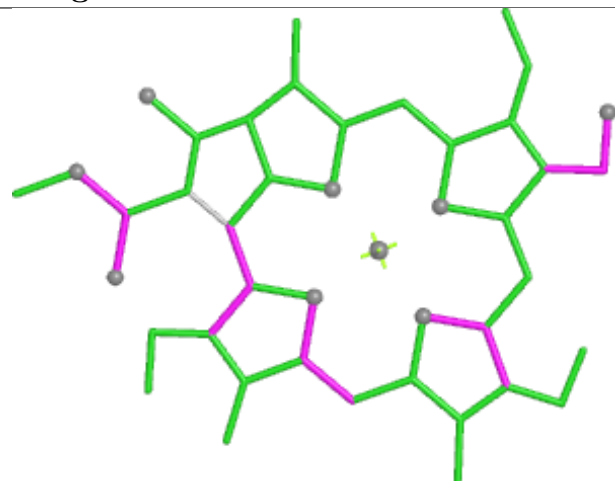
Rings



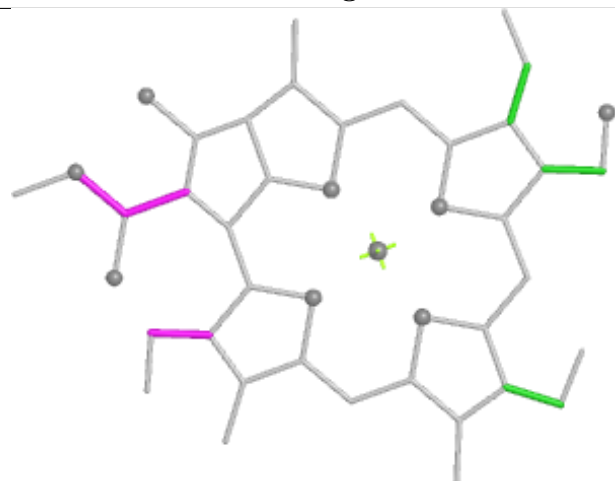
Ligand CHL Gg 306



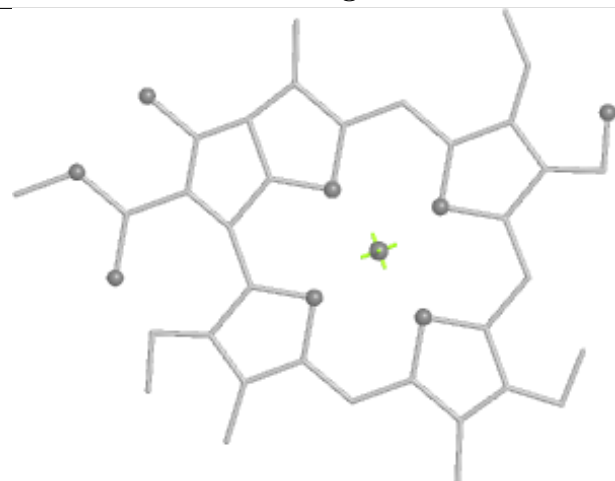
Bond lengths



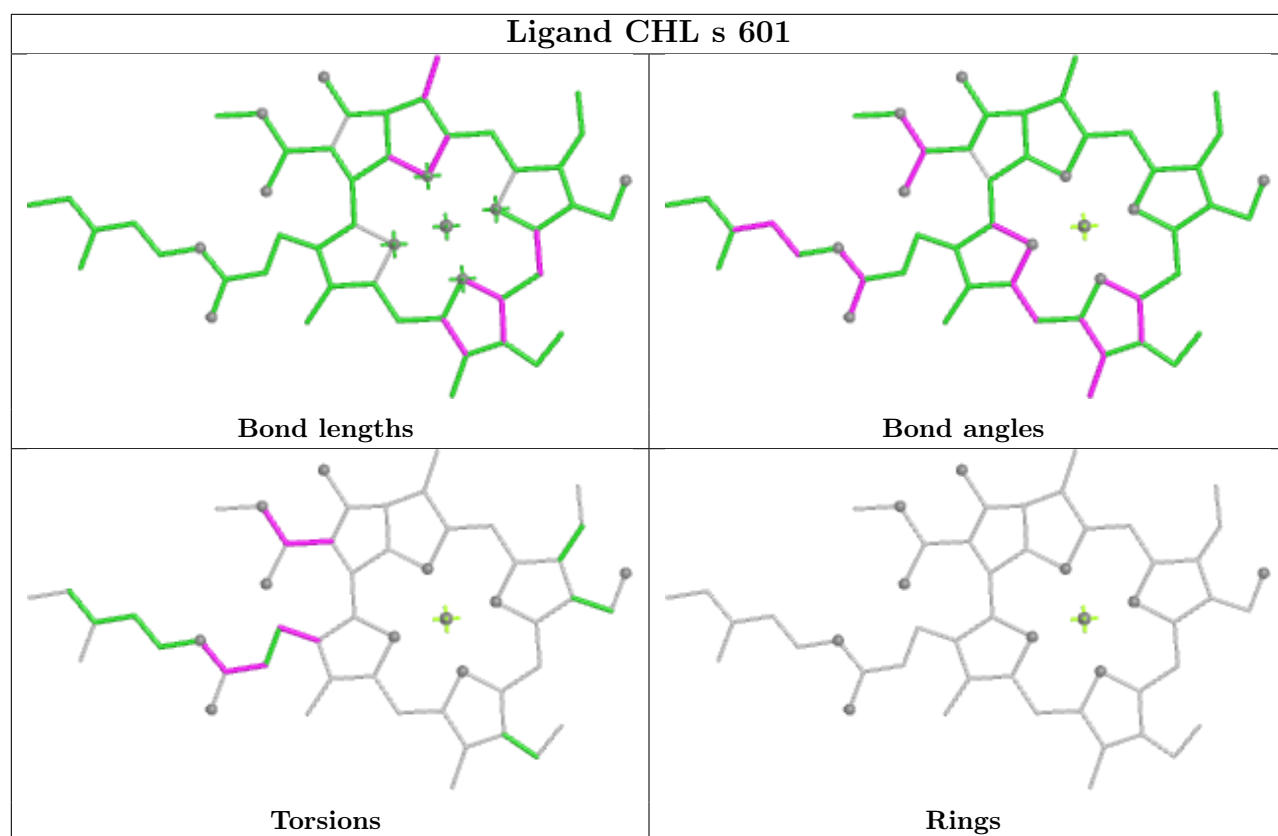
Bond angles

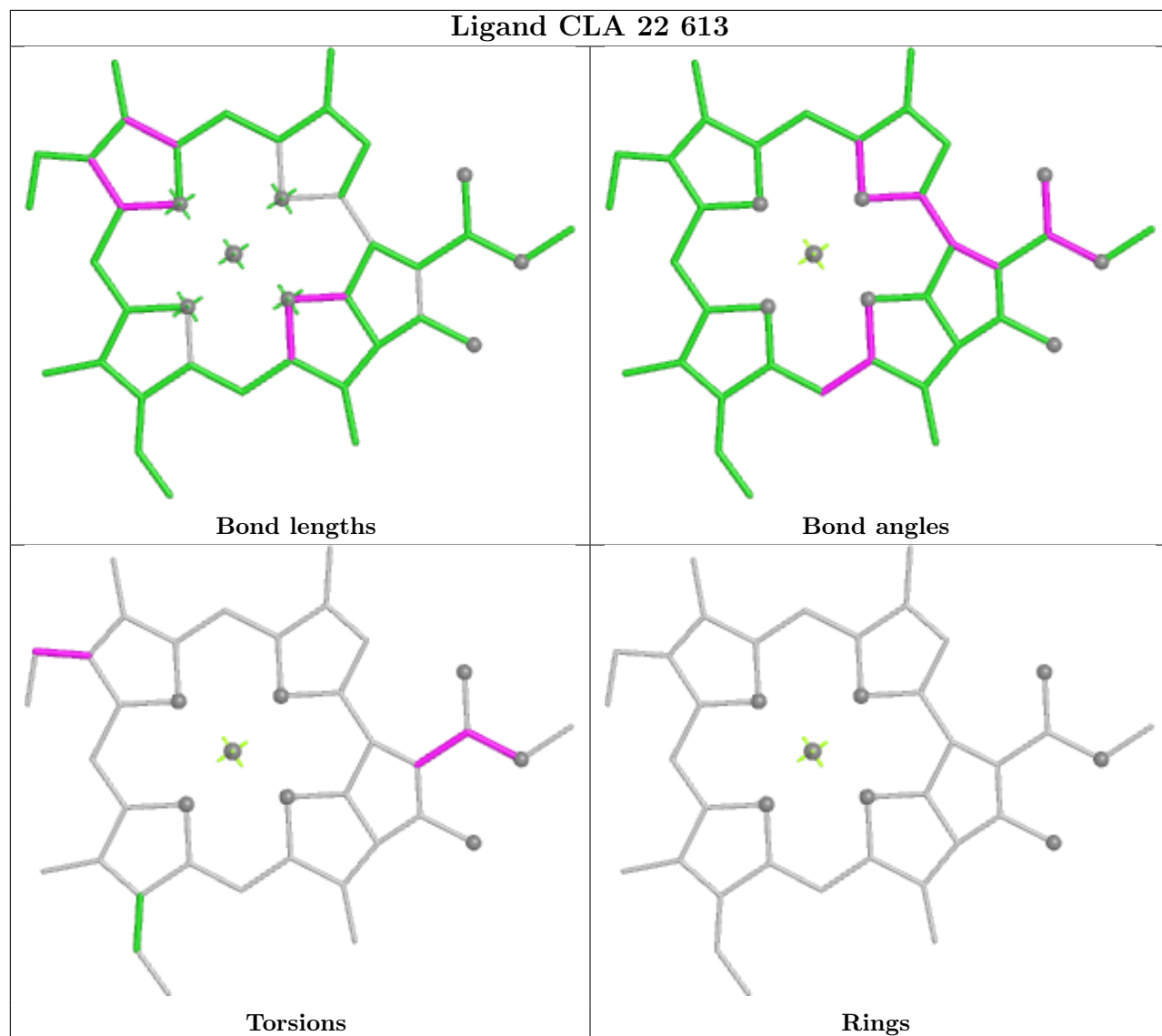


Torsions

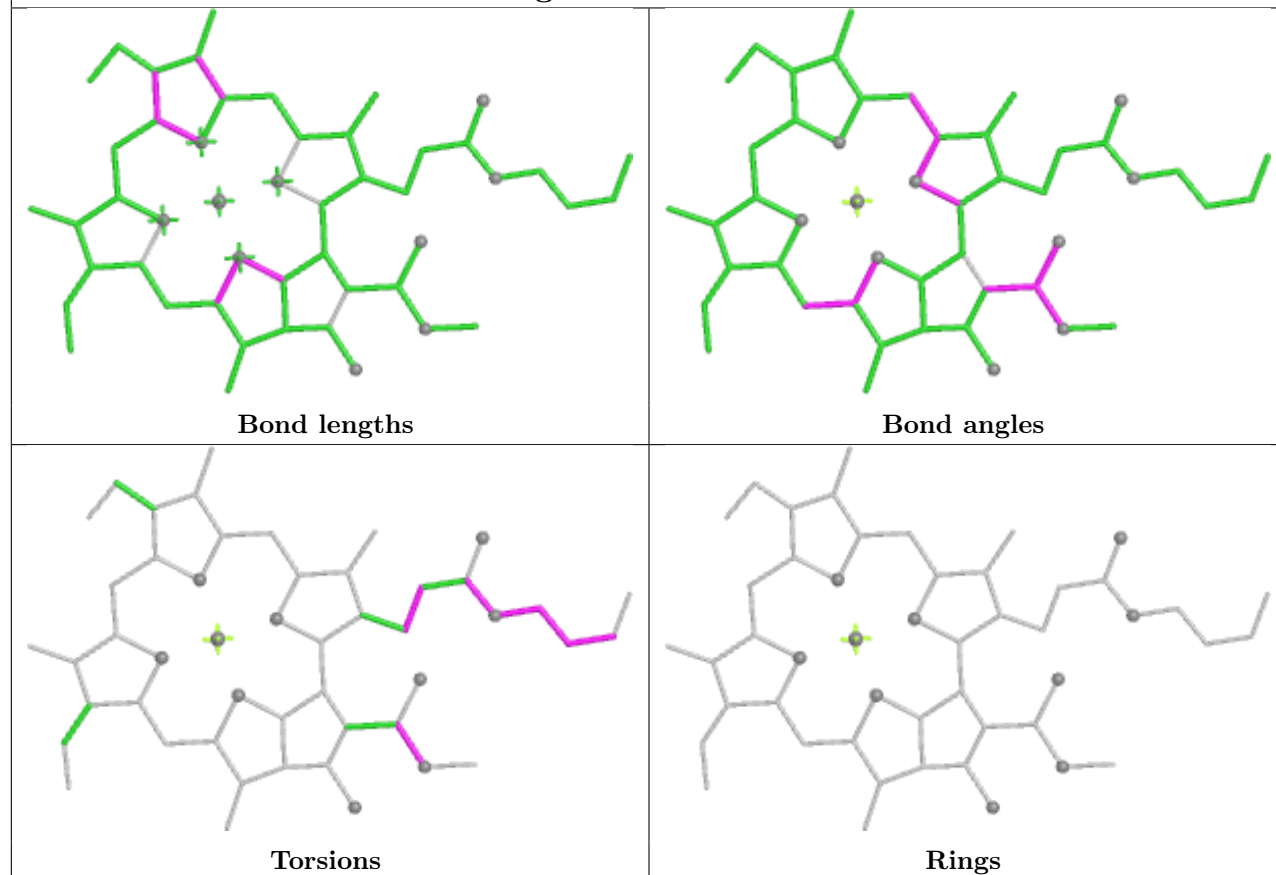


Rings

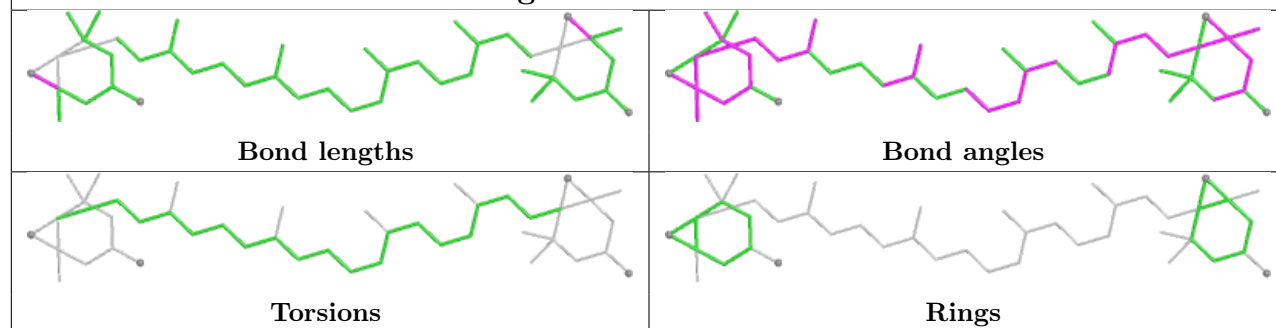


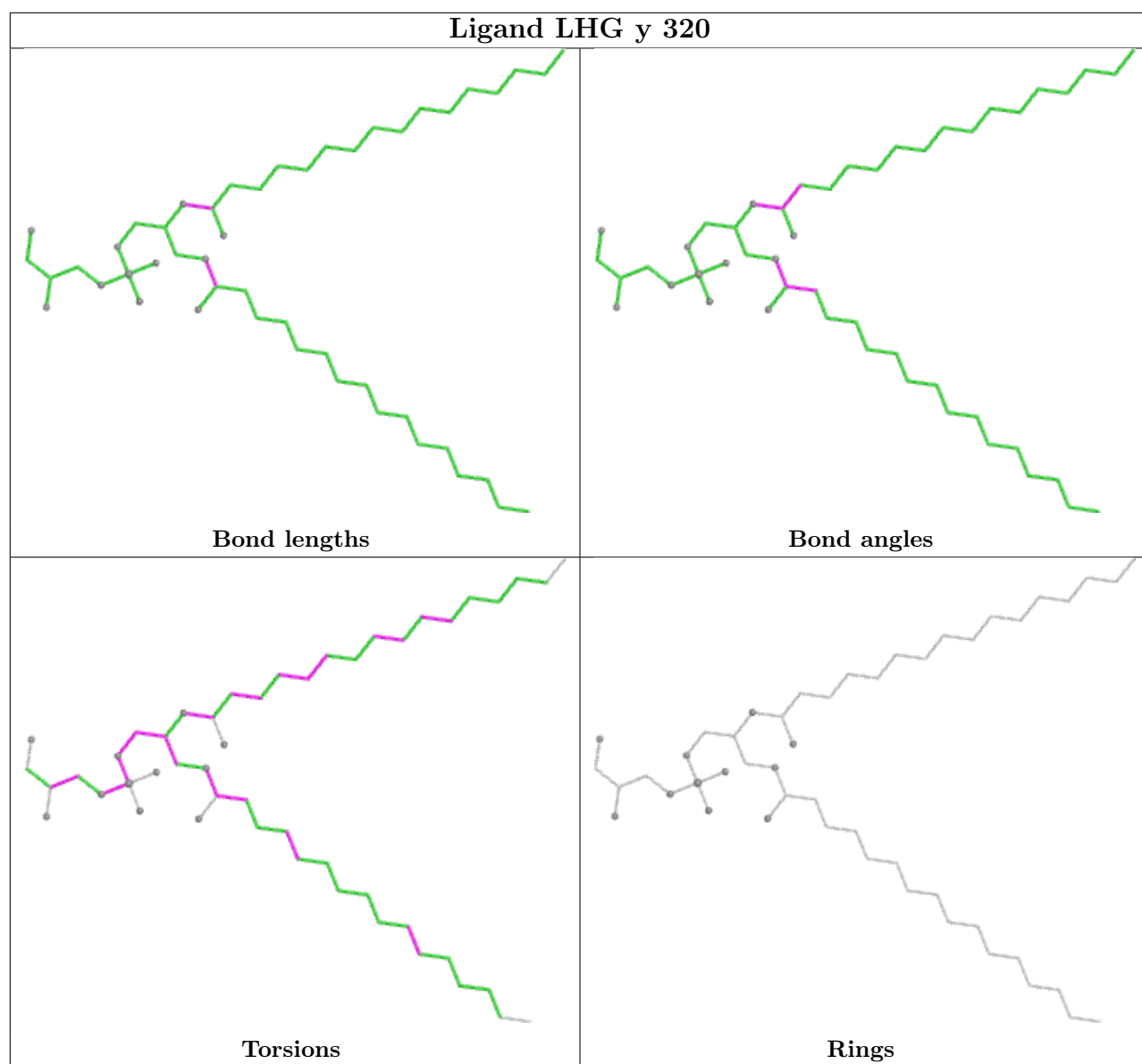


Ligand CLA n 614

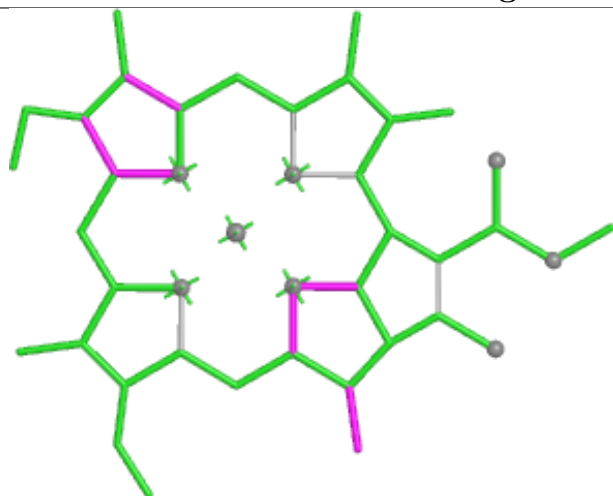


Ligand XAT RR 316





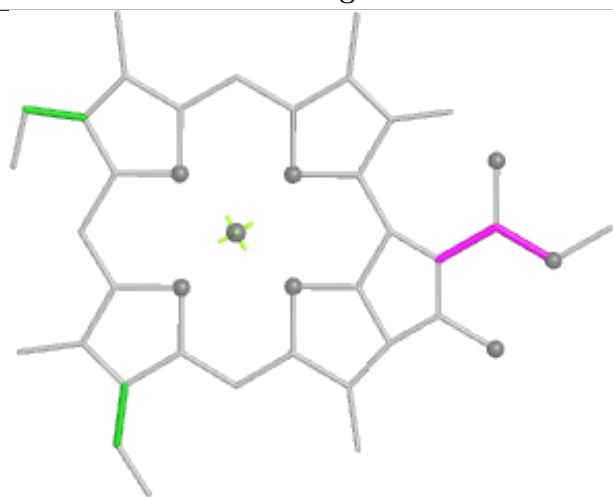
Ligand CLA NN 604



Bond lengths



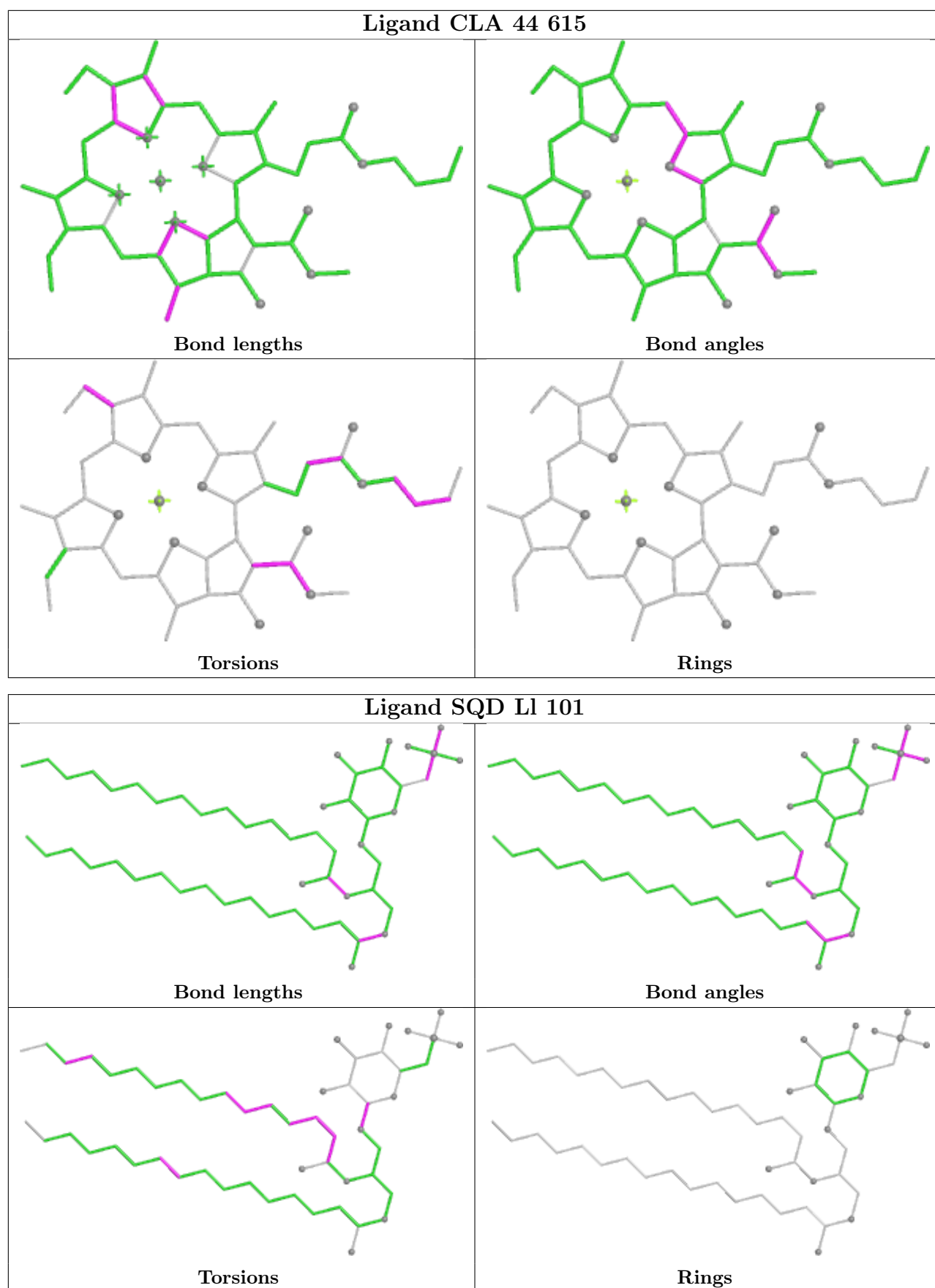
Bond angles

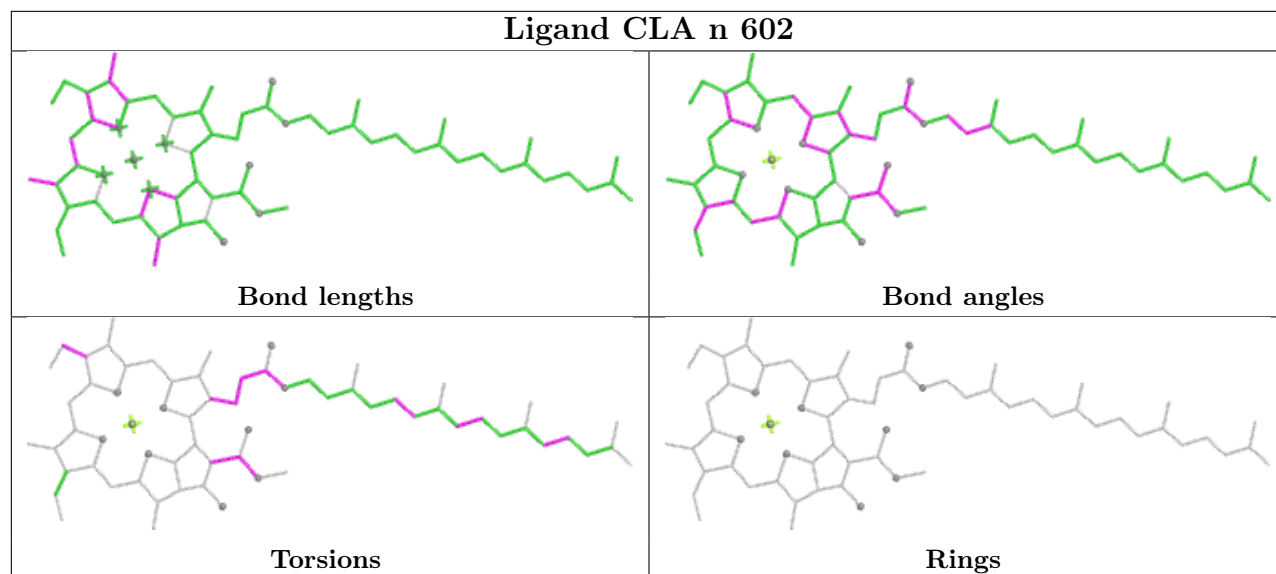
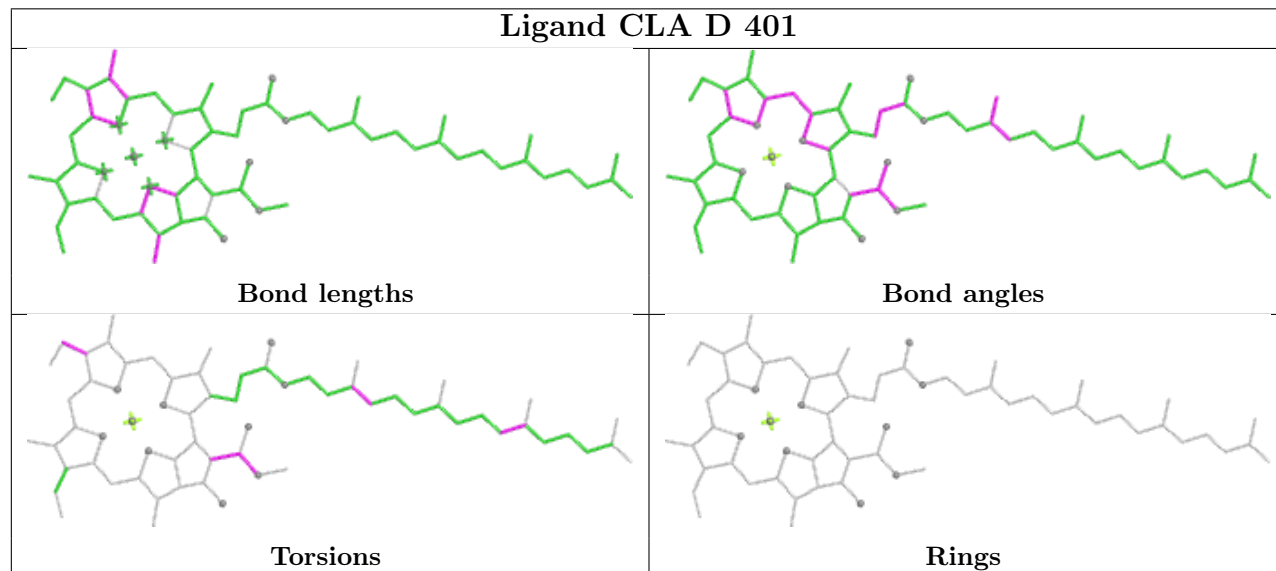


Torsions

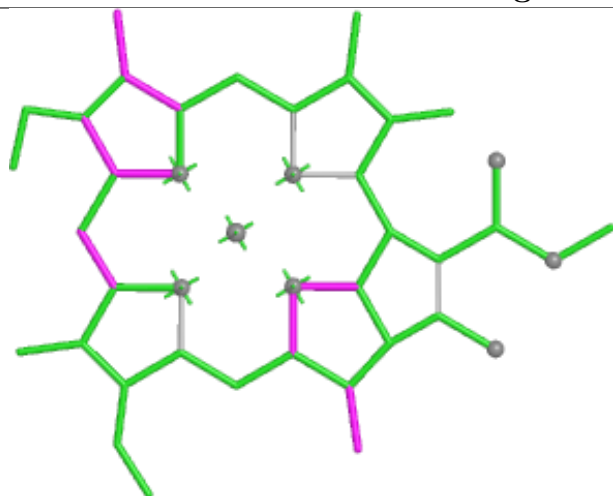


Rings



Ligand CLA n 602**Ligand CLA D 401**

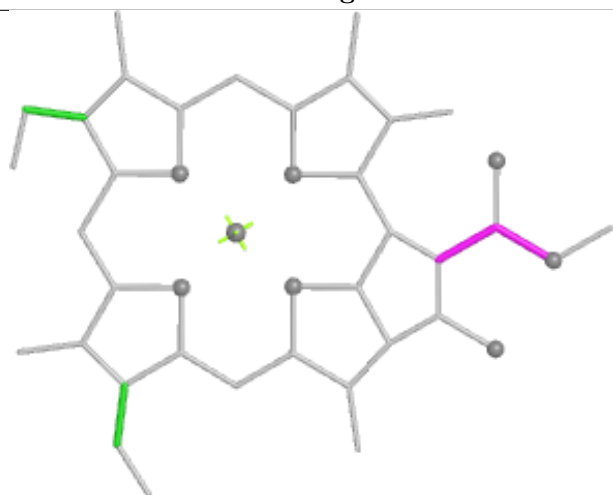
Ligand CLA X 201



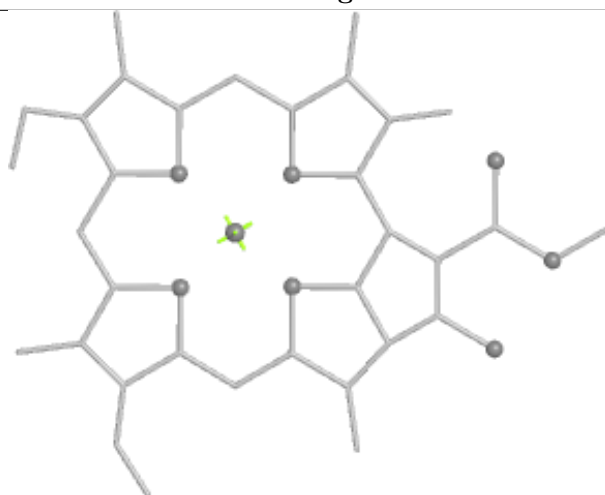
Bond lengths



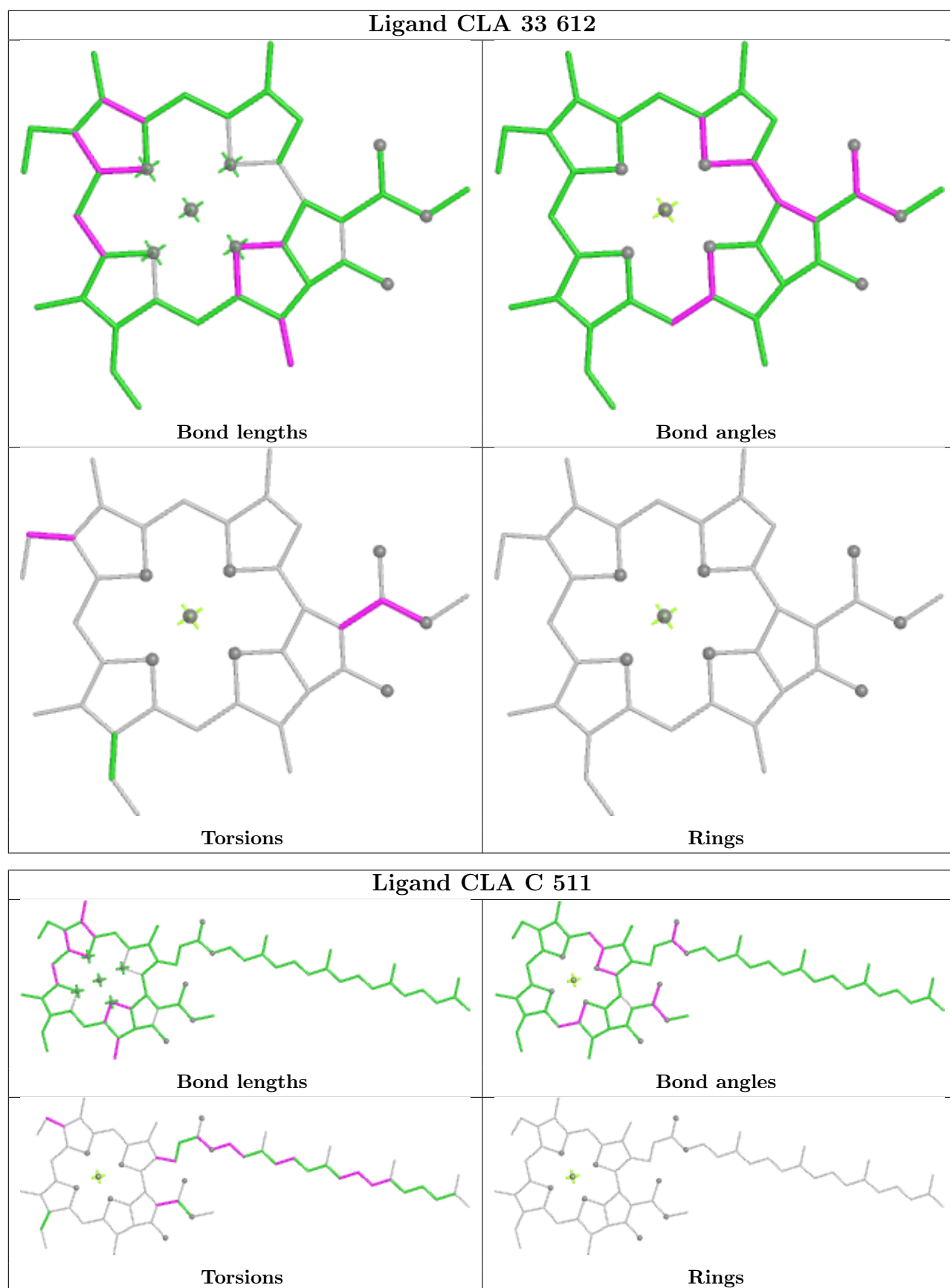
Bond angles

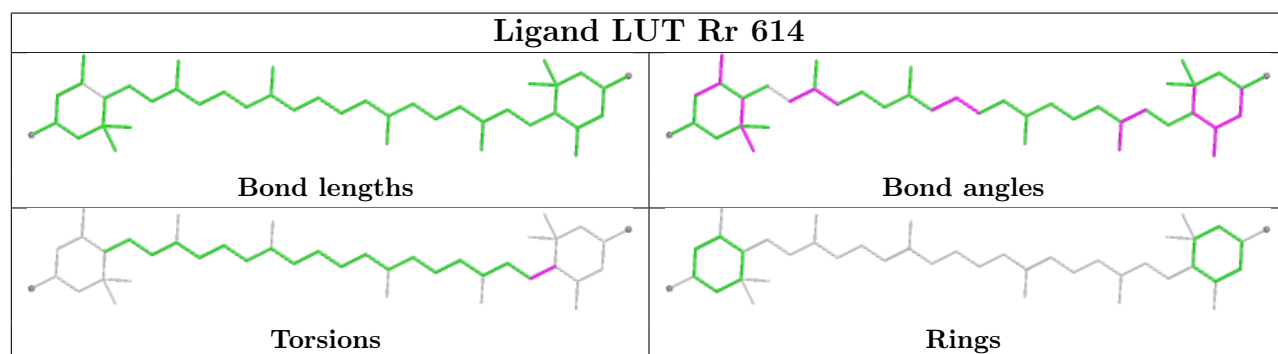
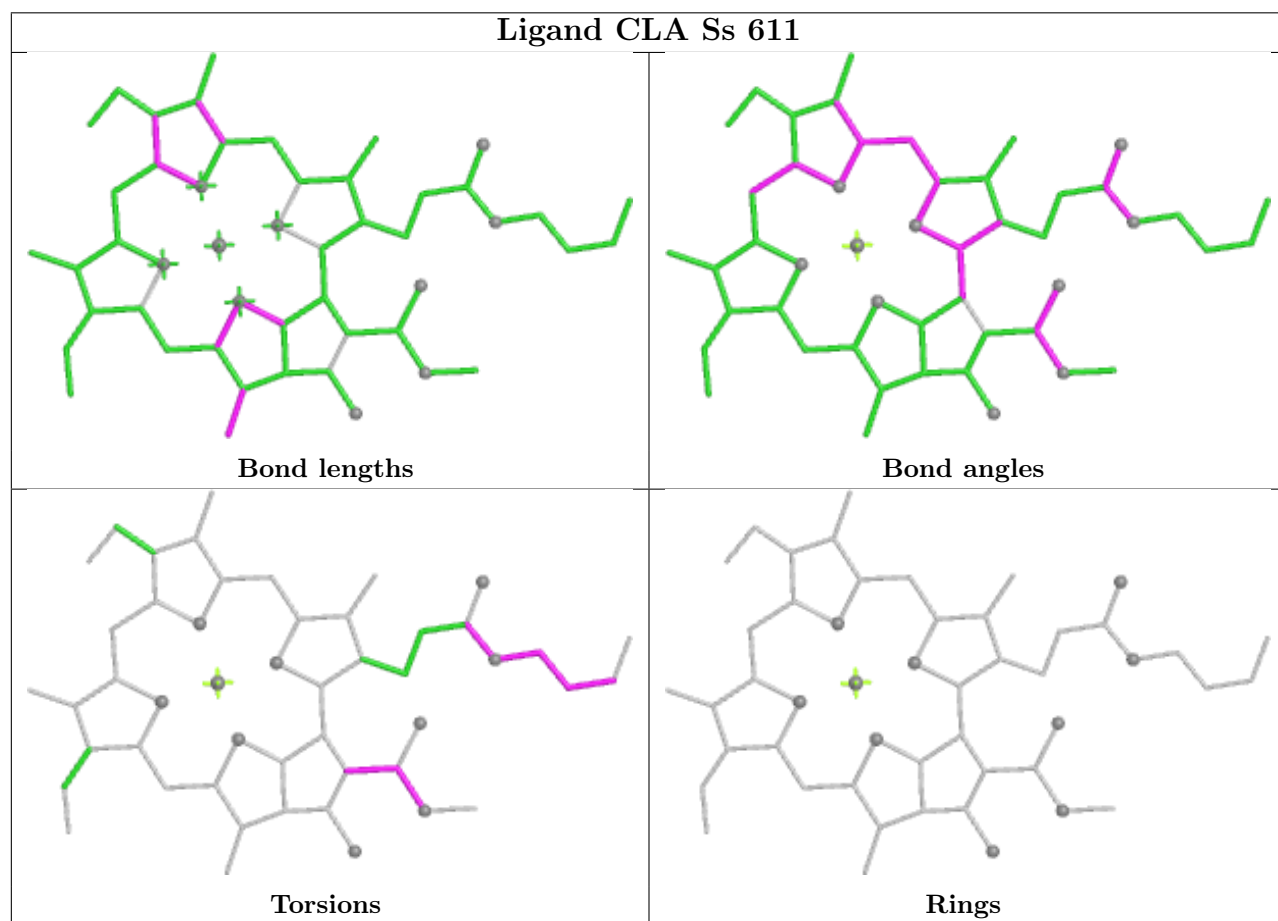
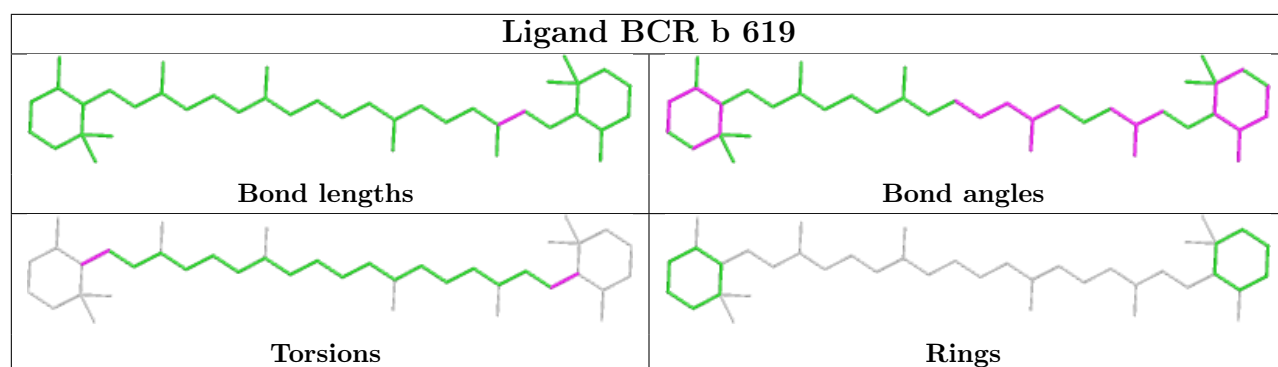


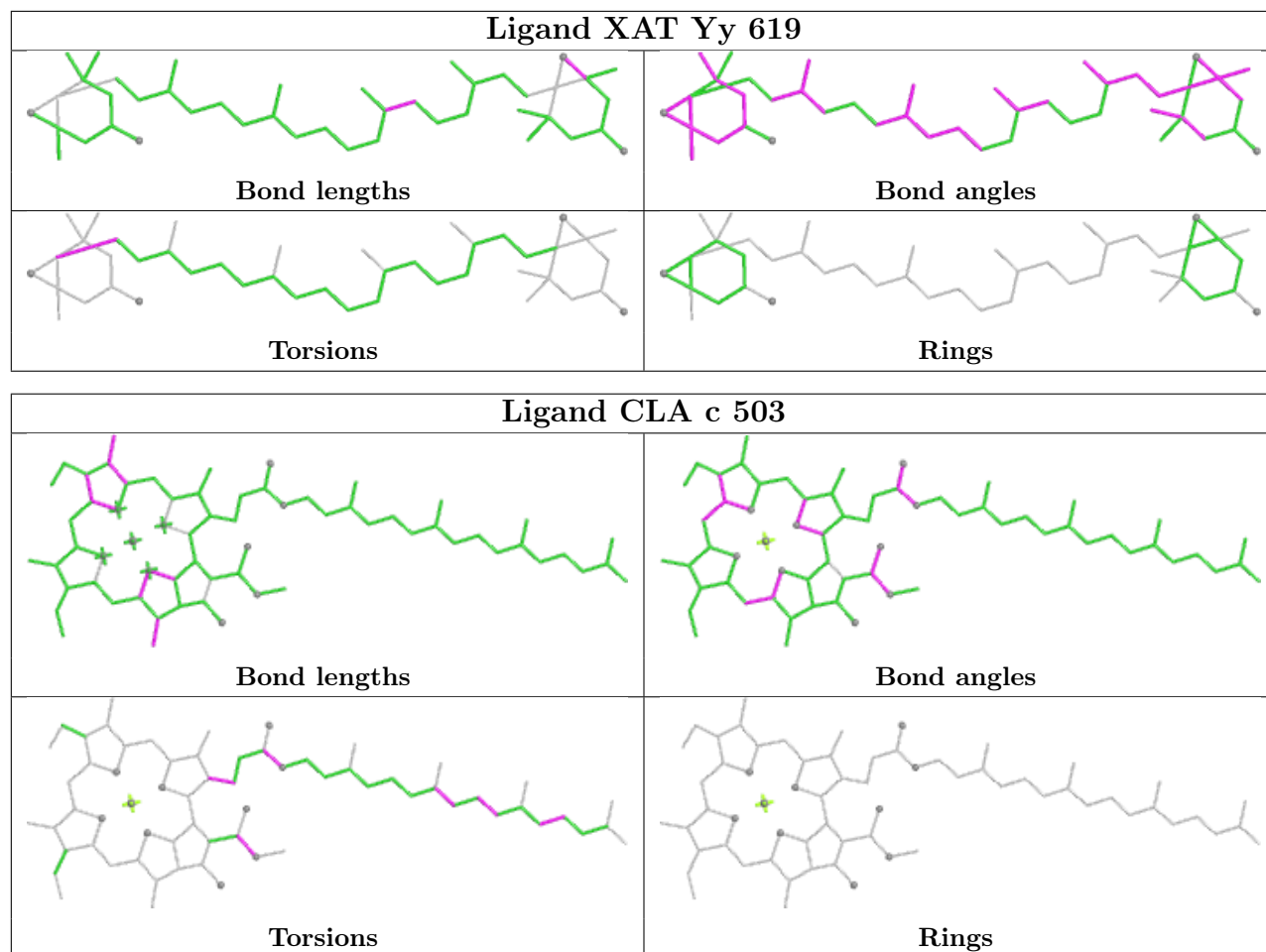
Torsions

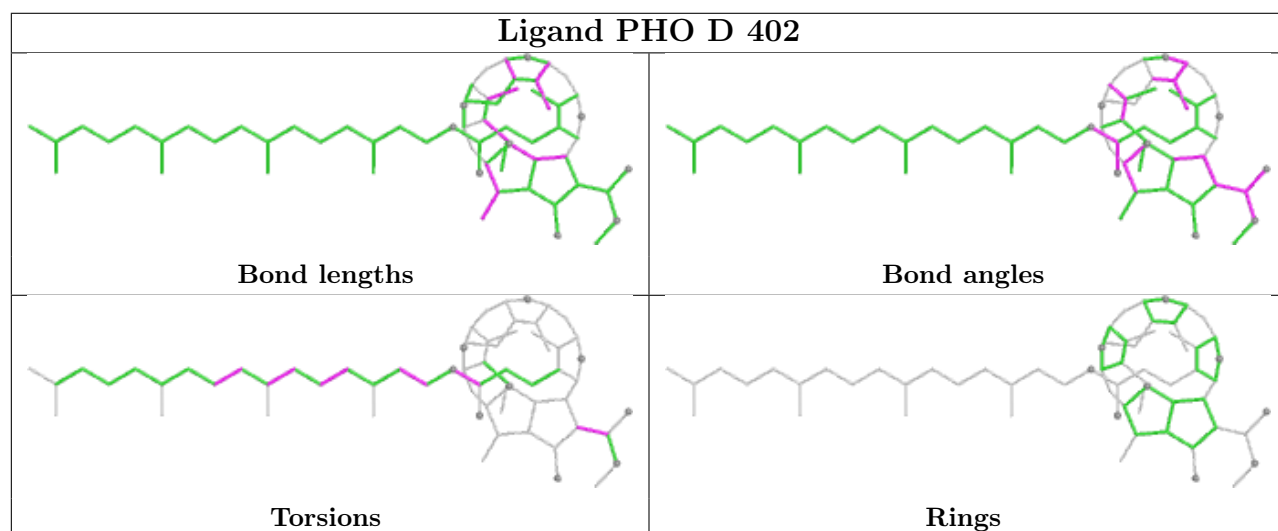
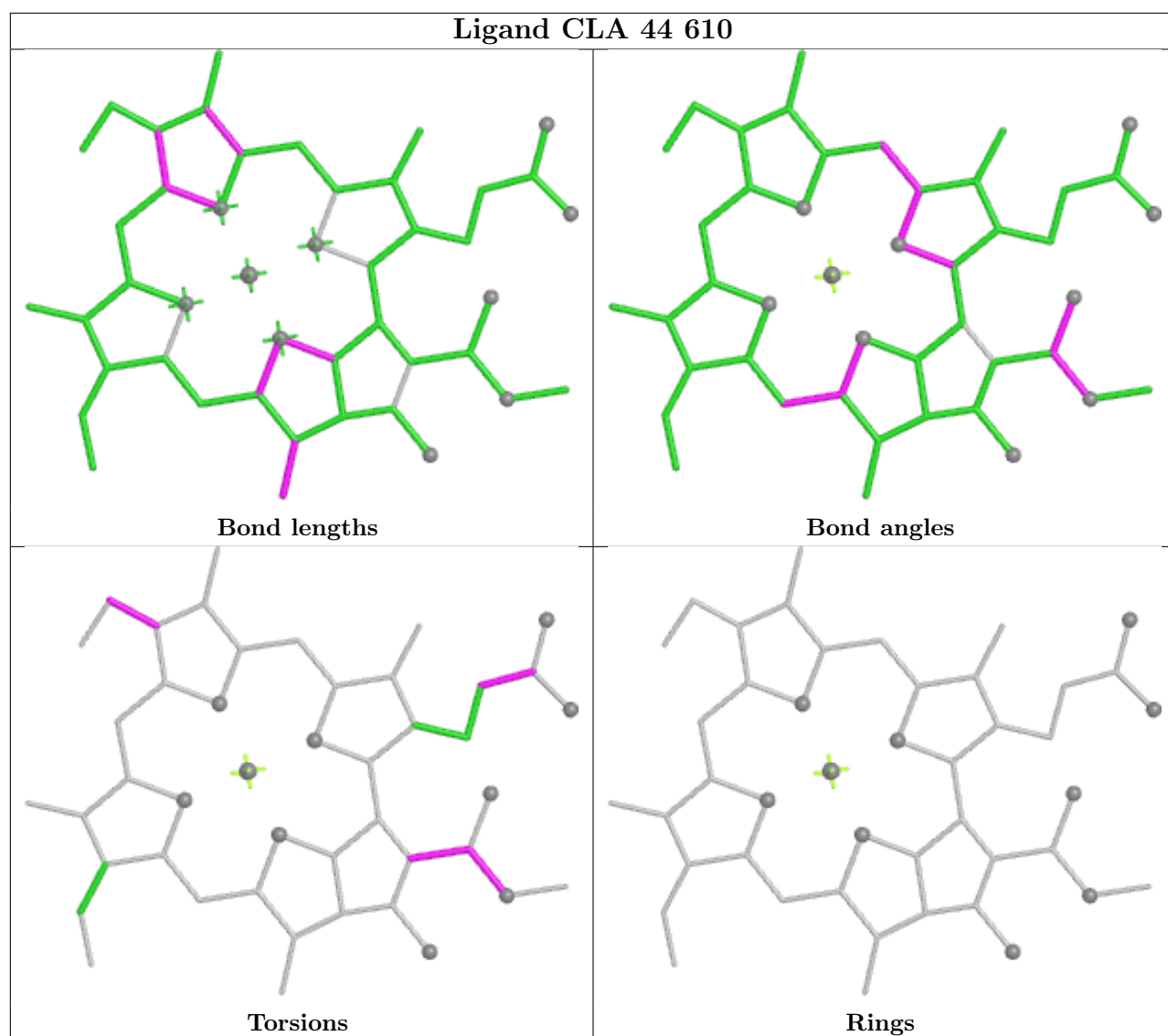


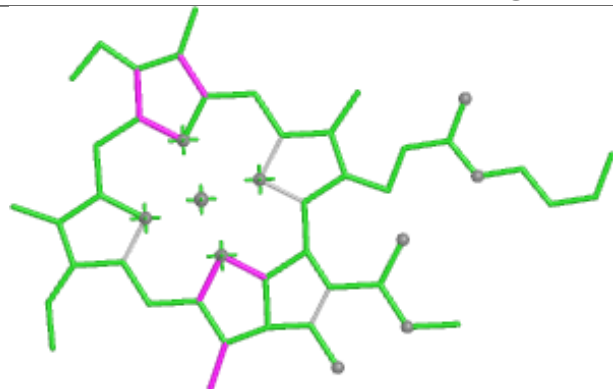
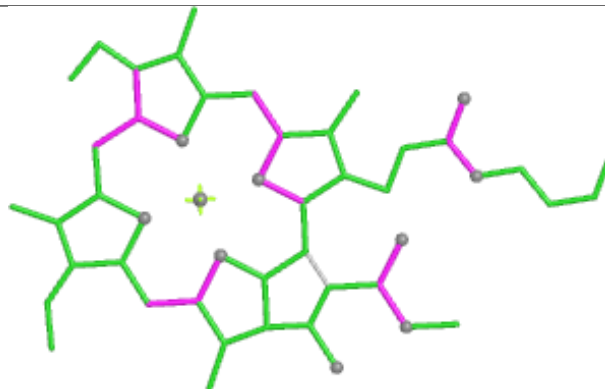
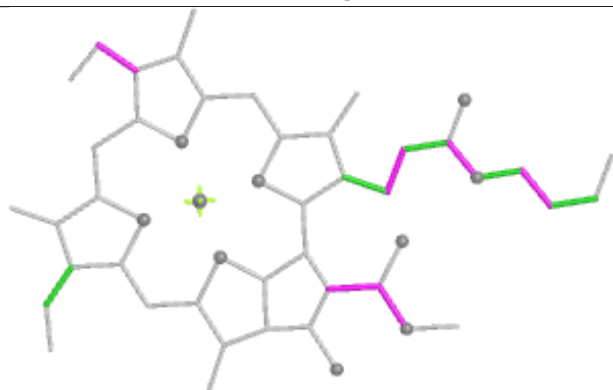
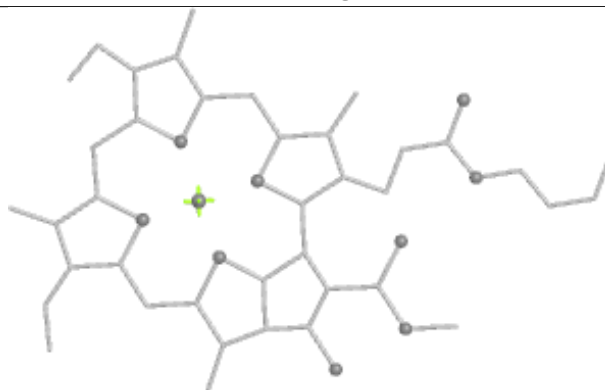
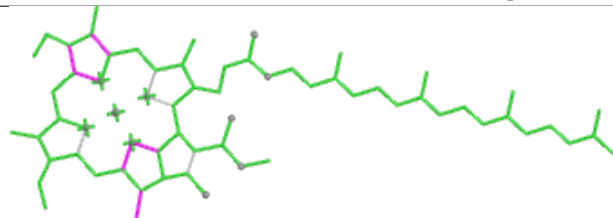
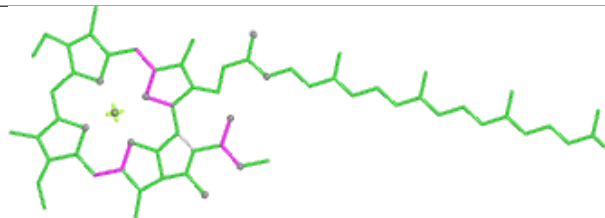
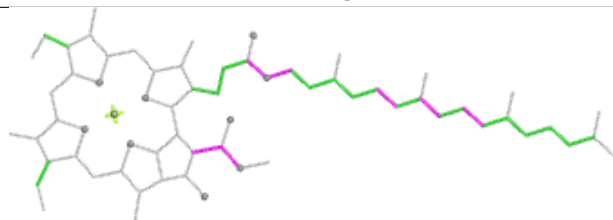
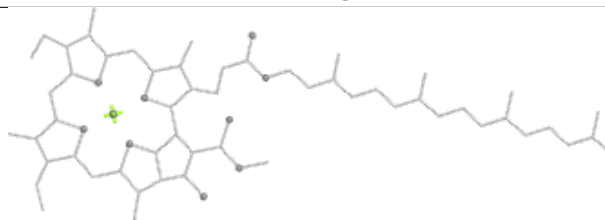
Rings

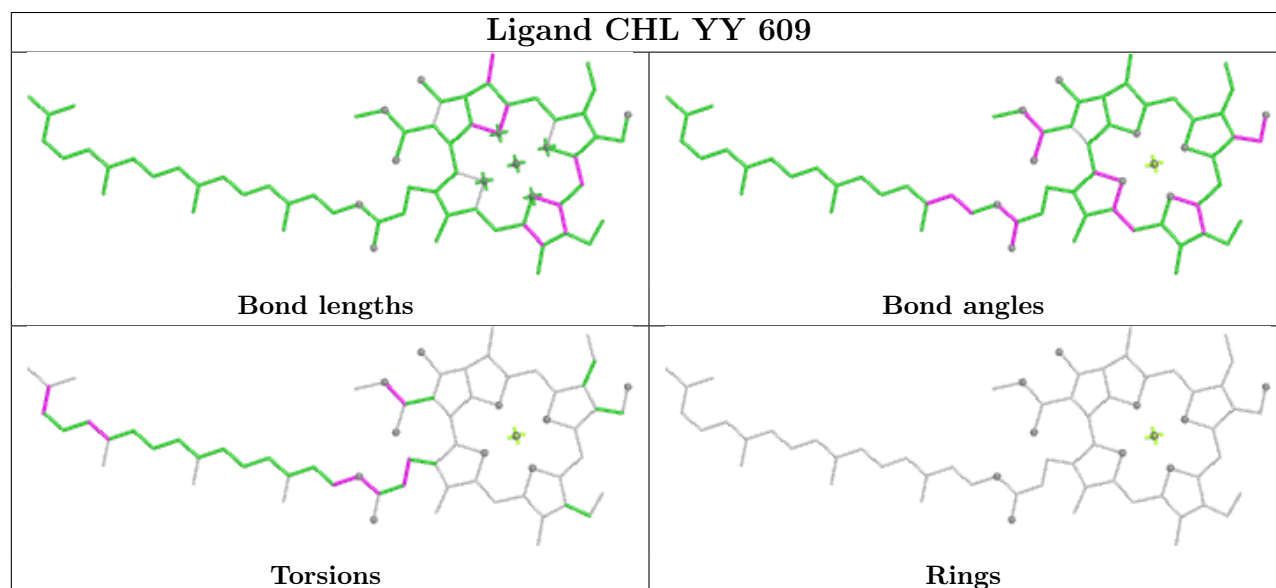
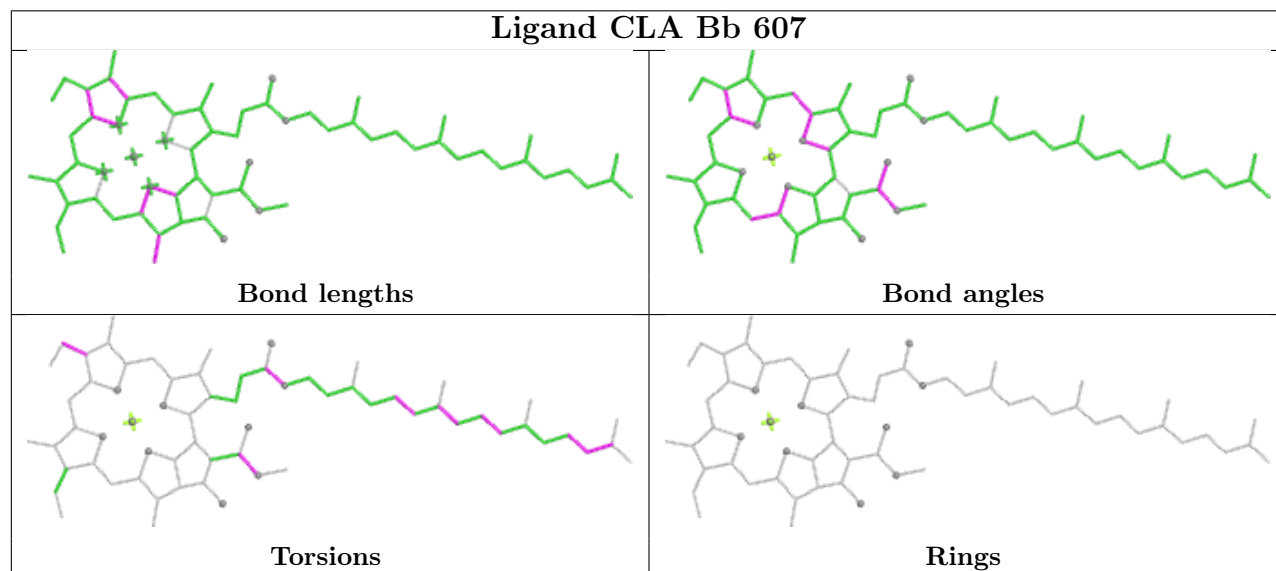
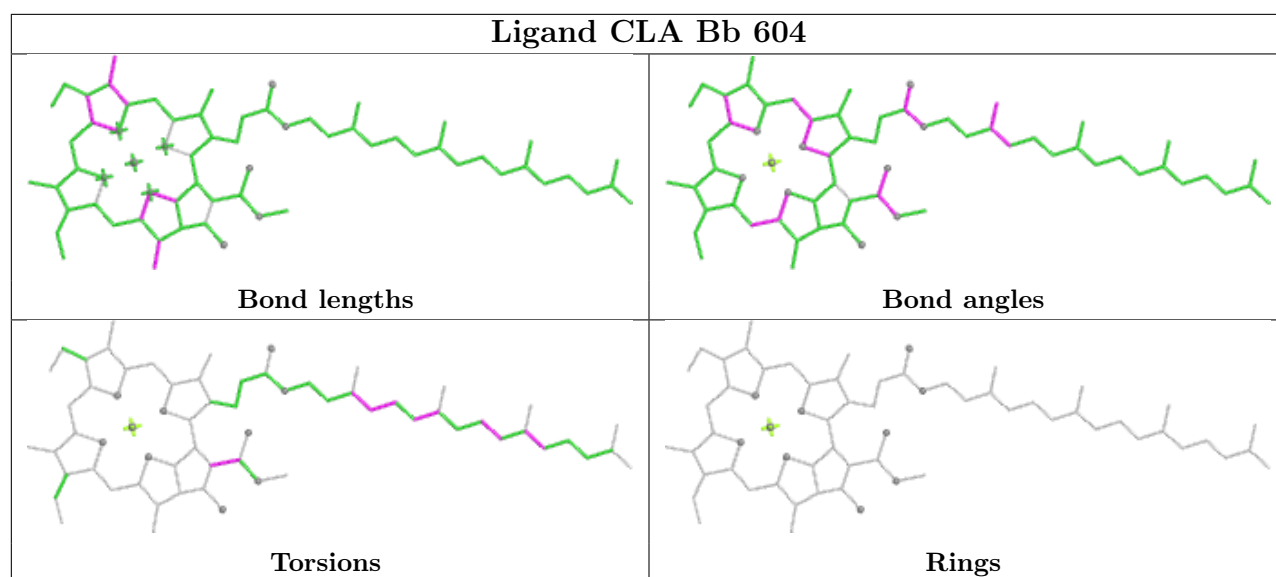


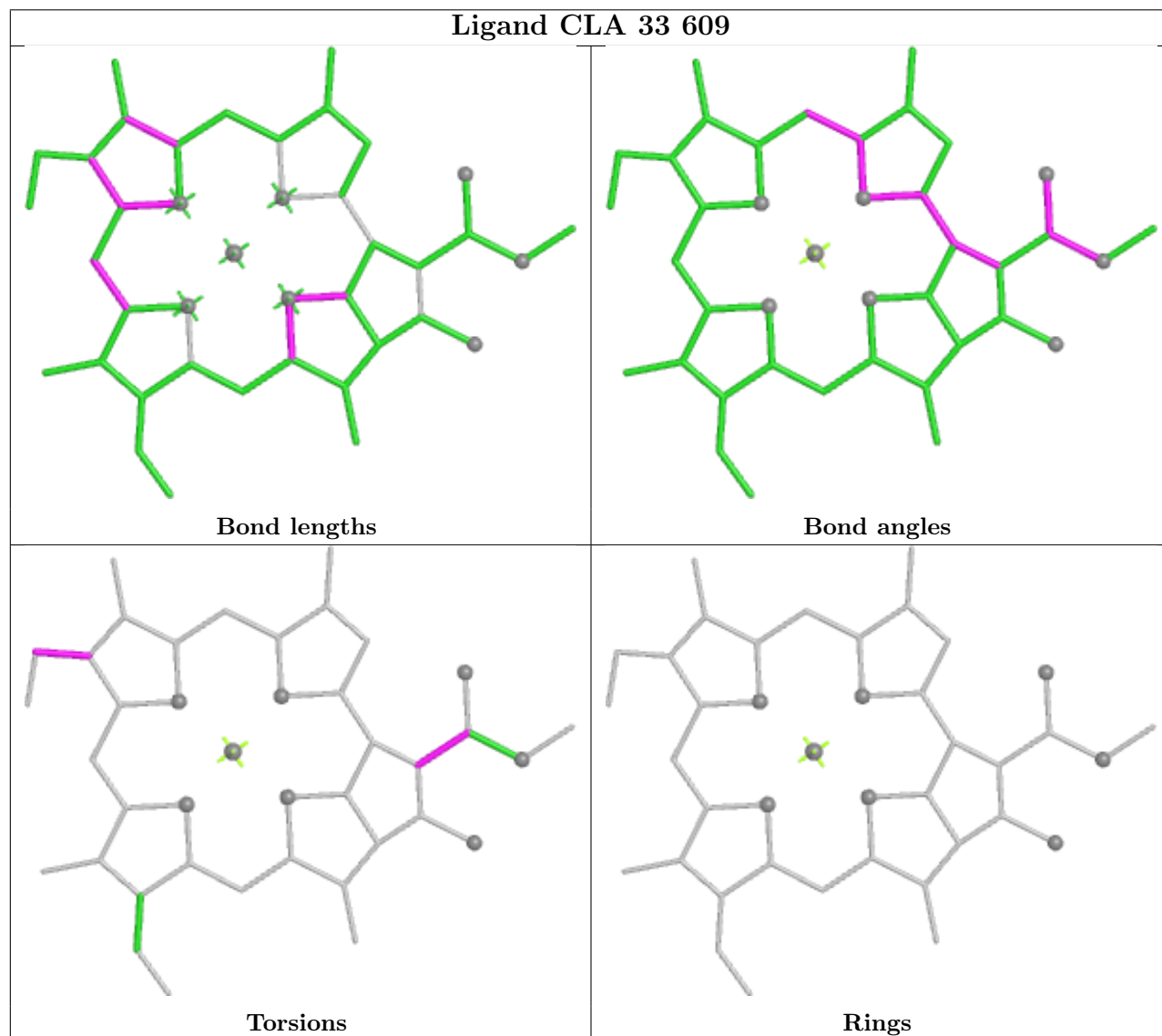
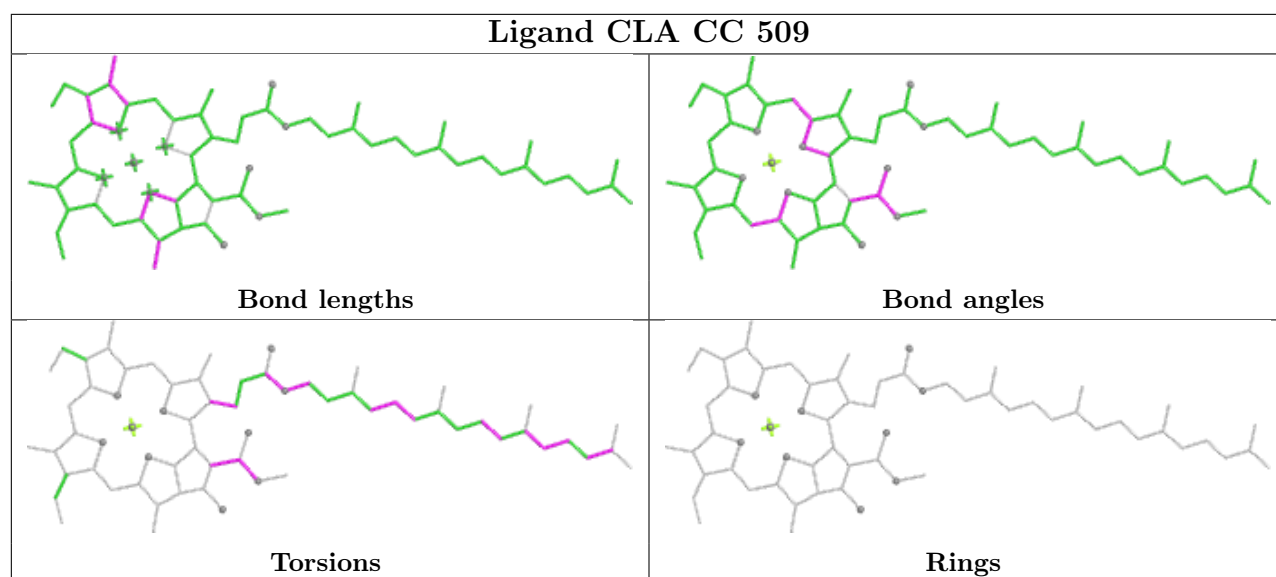




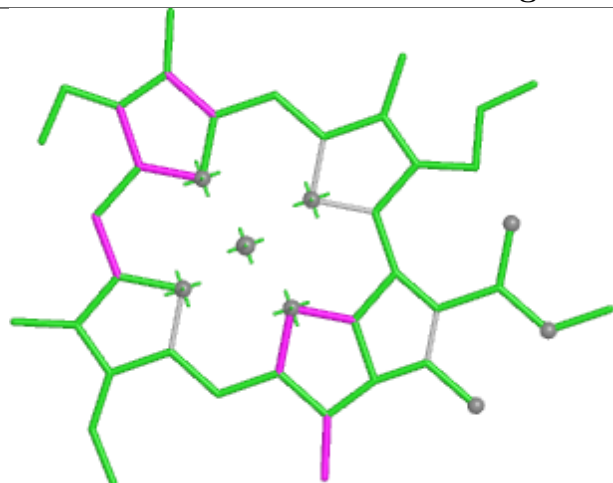


Ligand CLA SS 313**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA BB 606****Bond lengths****Bond angles****Torsions****Rings**

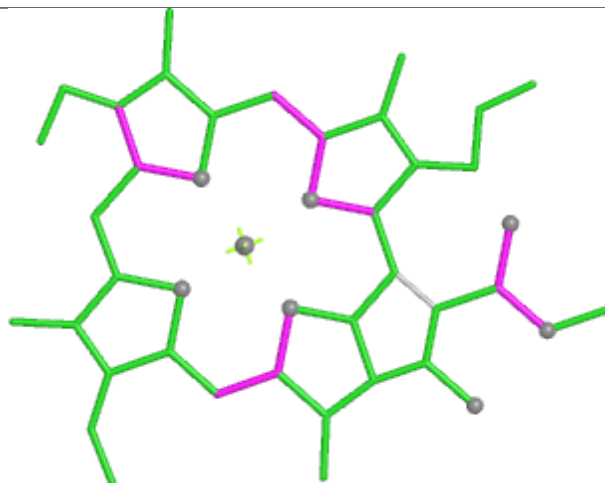




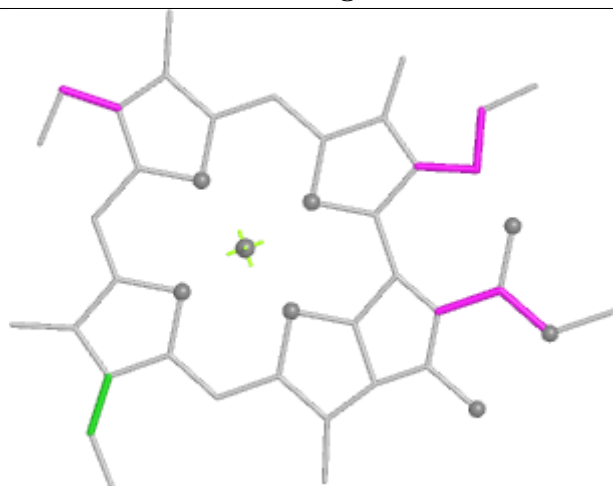
Ligand CLA c 513



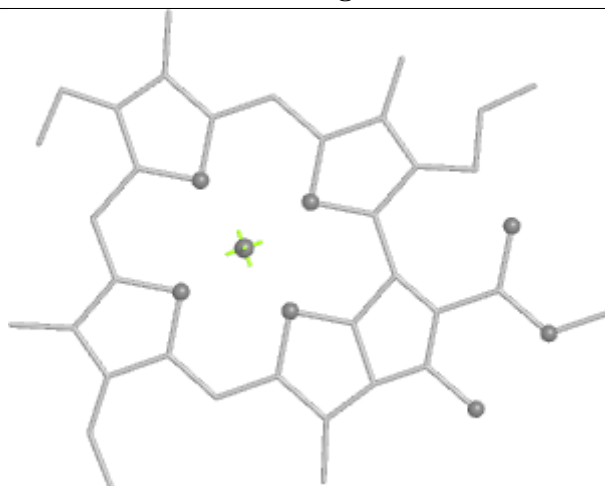
Bond lengths



Bond angles

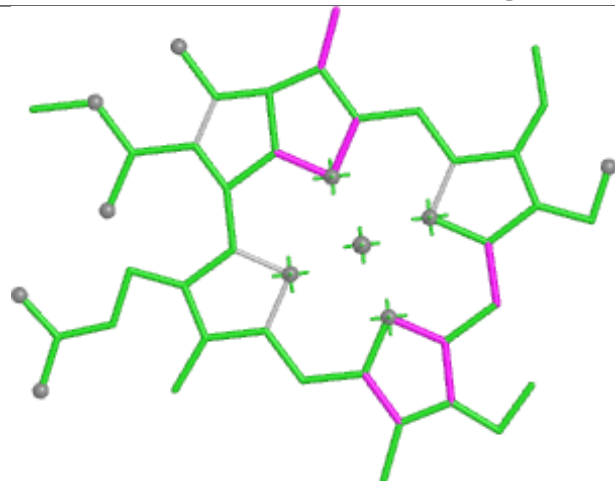


Torsions

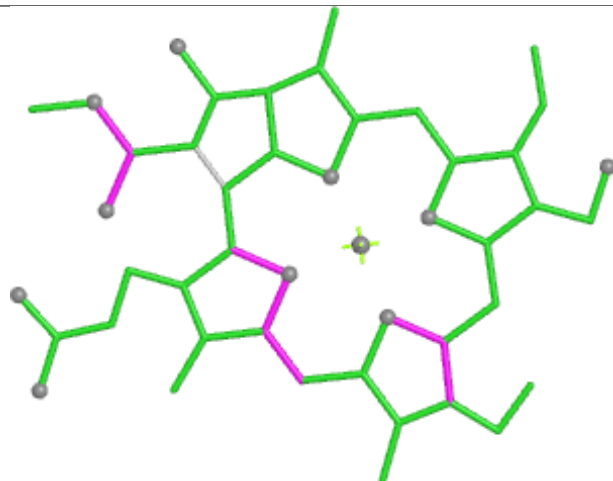


Rings

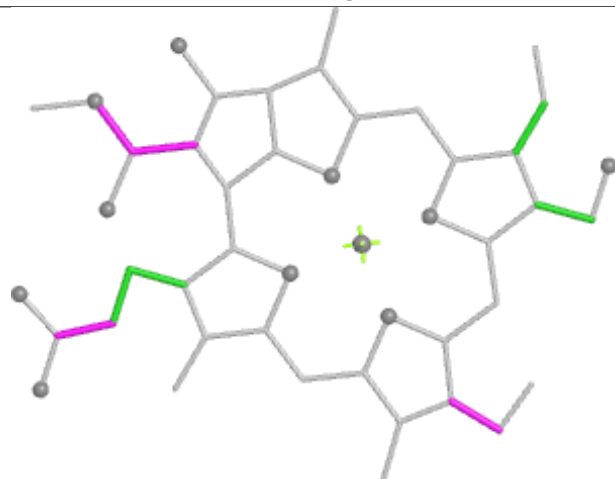
Ligand CHL GG 607



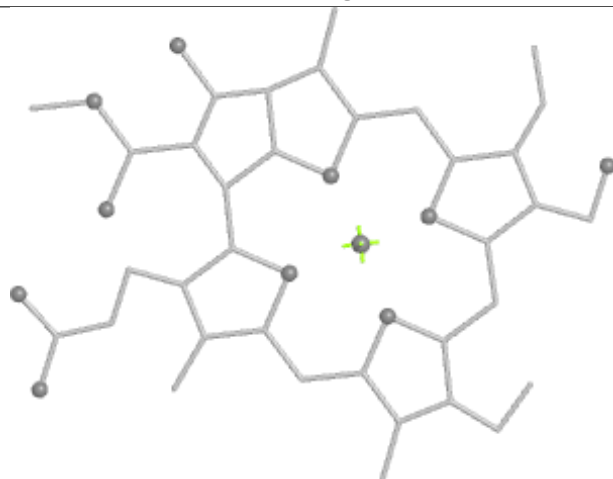
Bond lengths



Bond angles

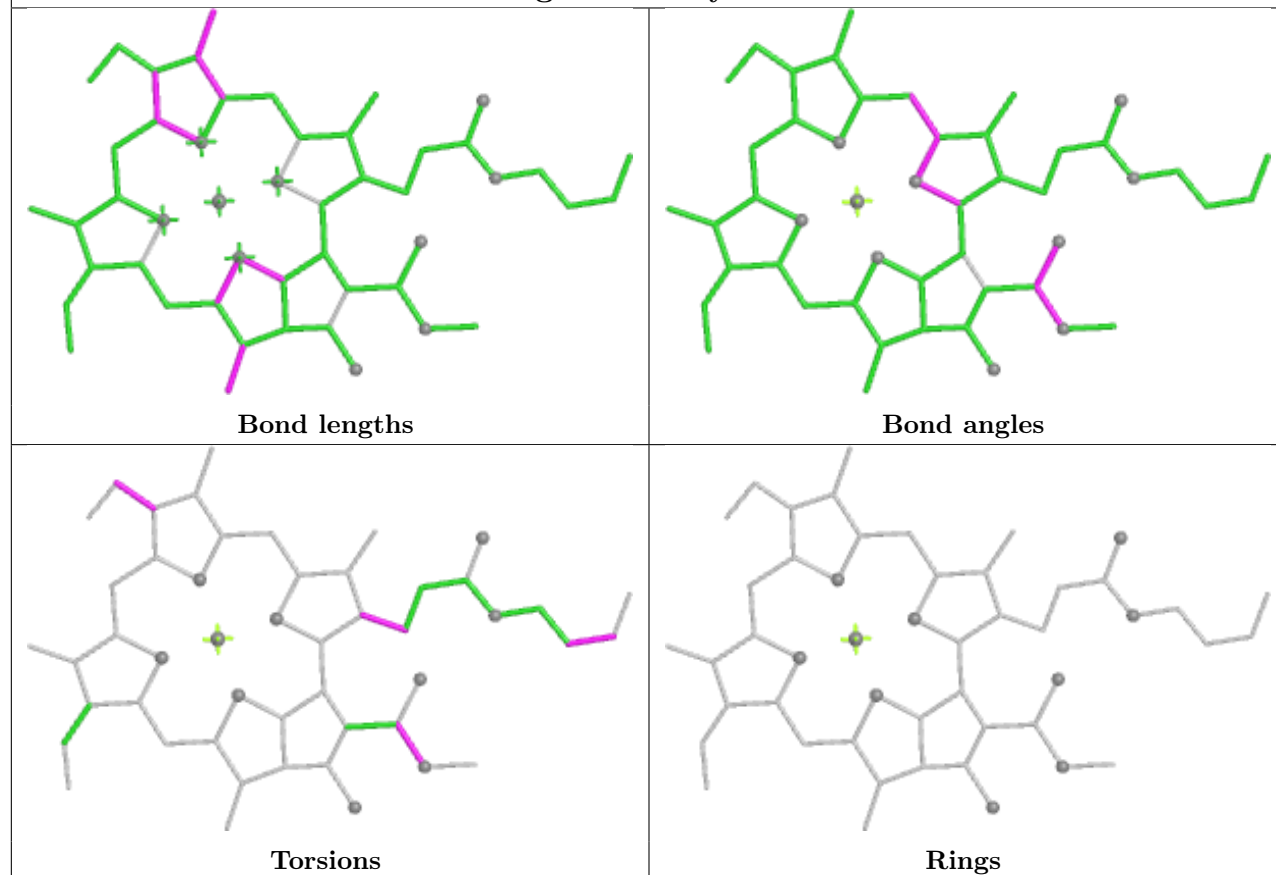


Torsions

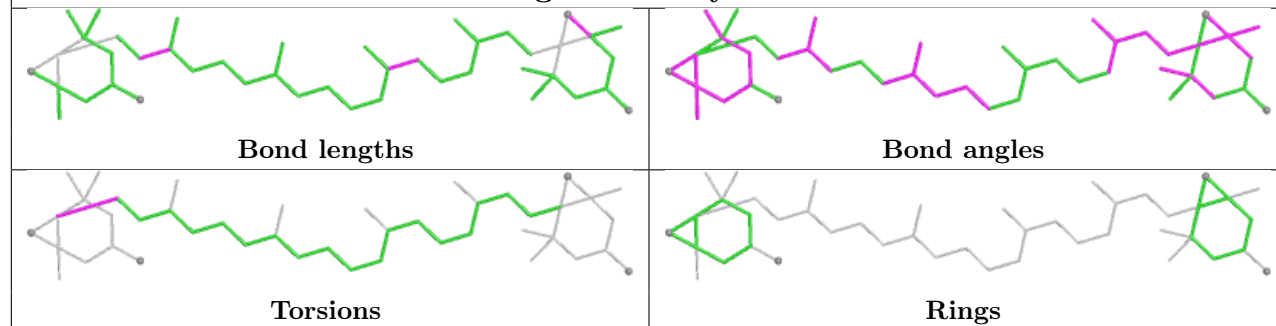


Rings

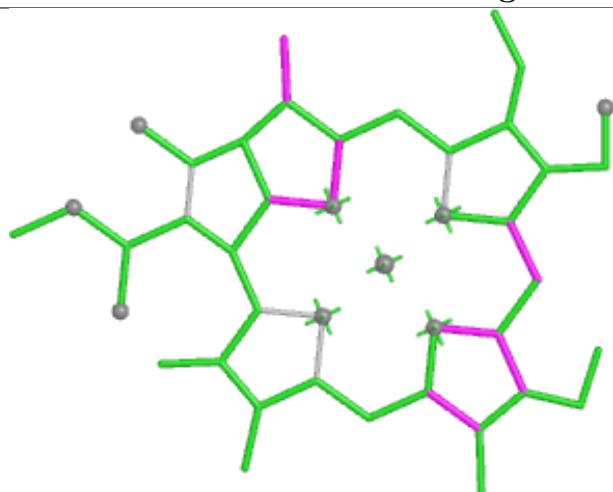
Ligand CLA y 305



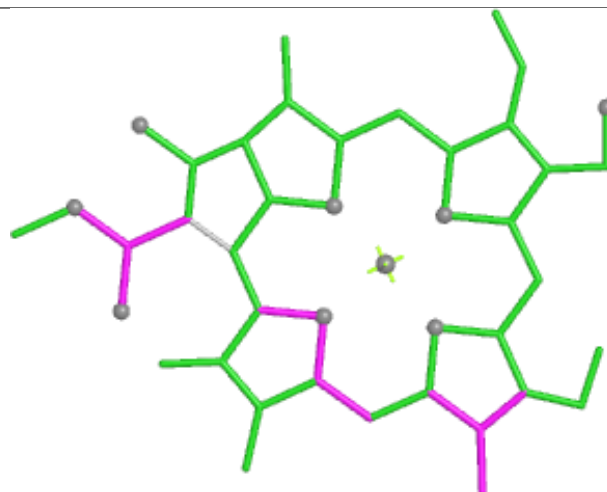
Ligand XAT y 301



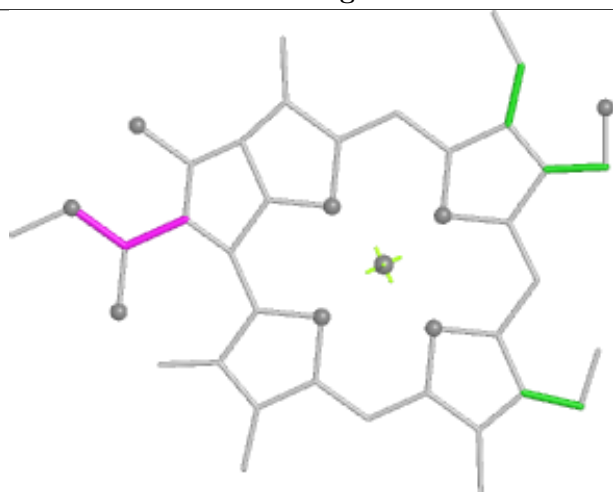
Ligand CHL NN 605



Bond lengths



Bond angles

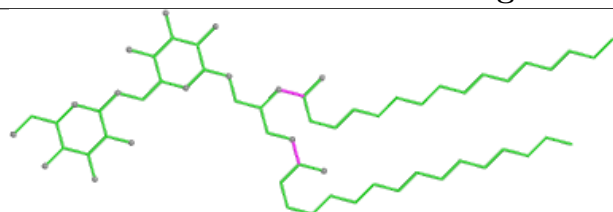


Torsions

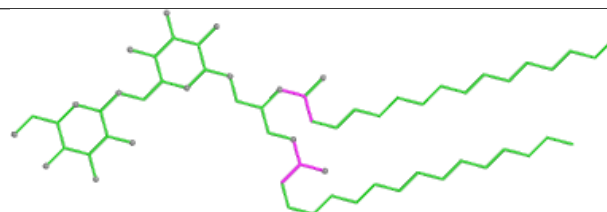


Rings

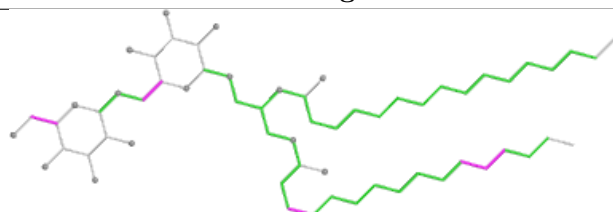
Ligand DGD CC 519



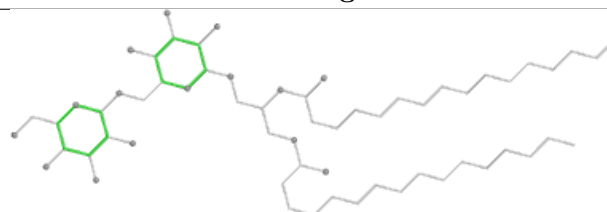
Bond lengths



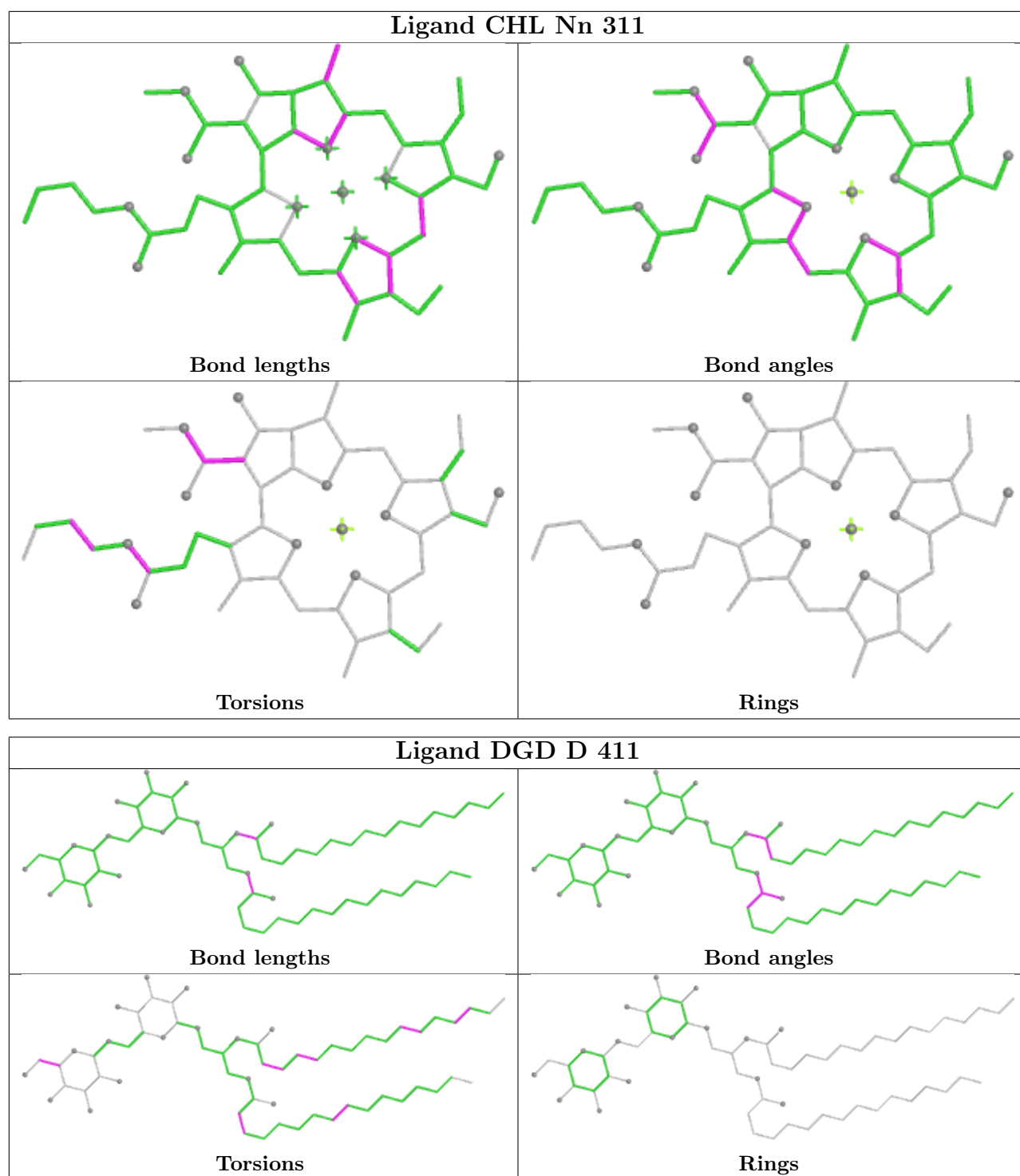
Bond angles

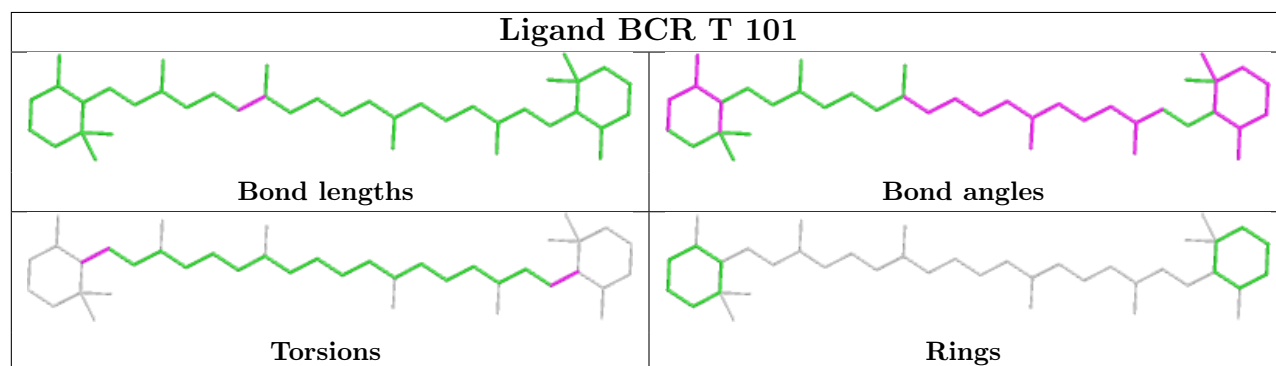
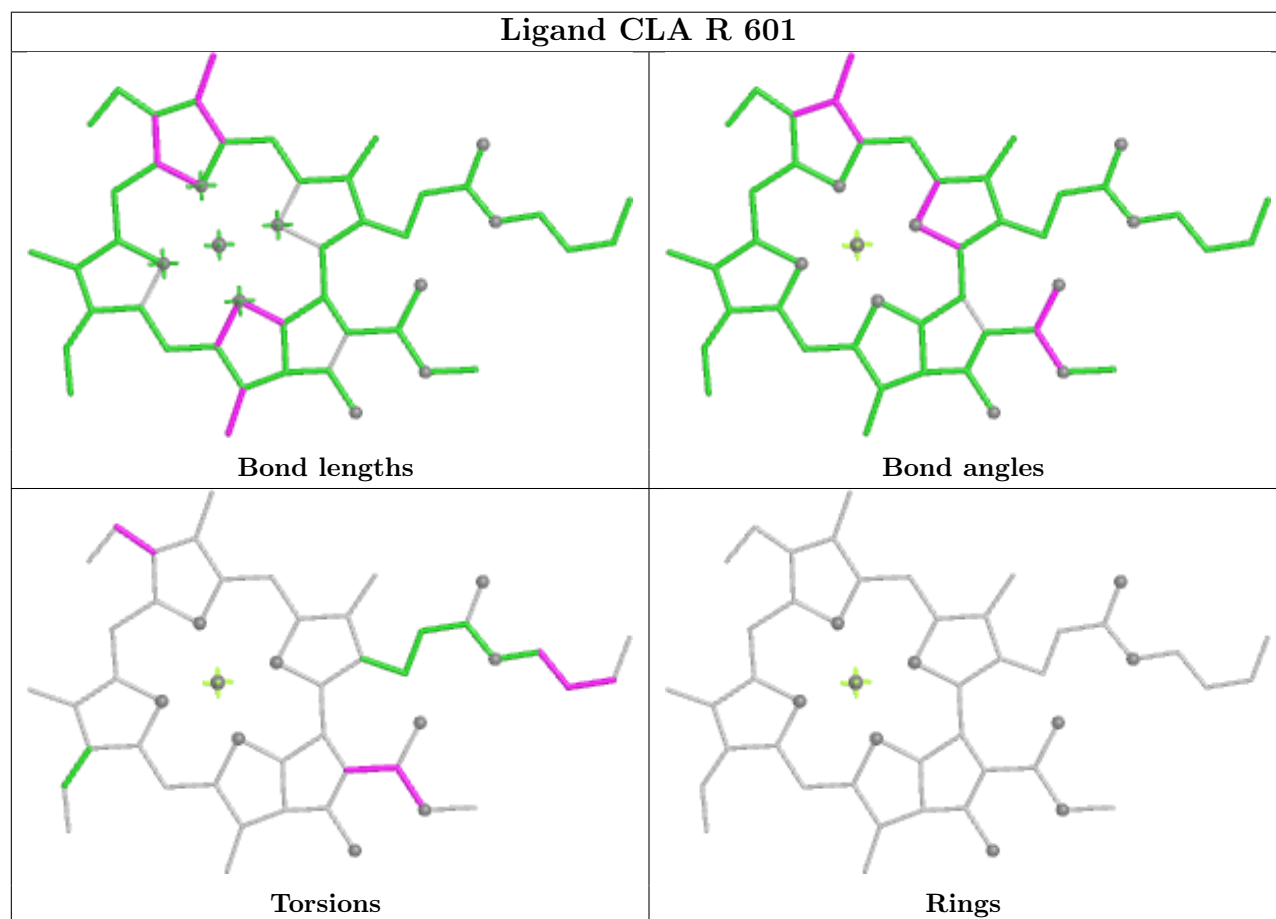
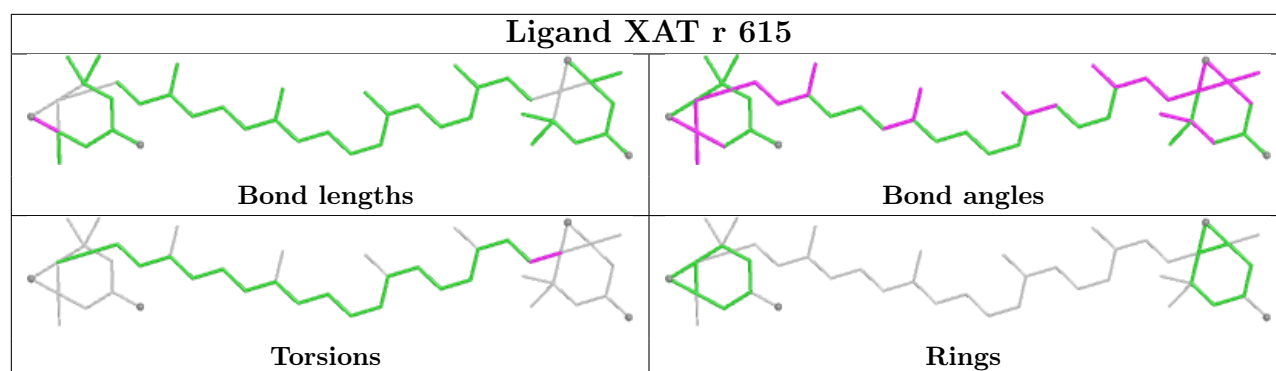


Torsions

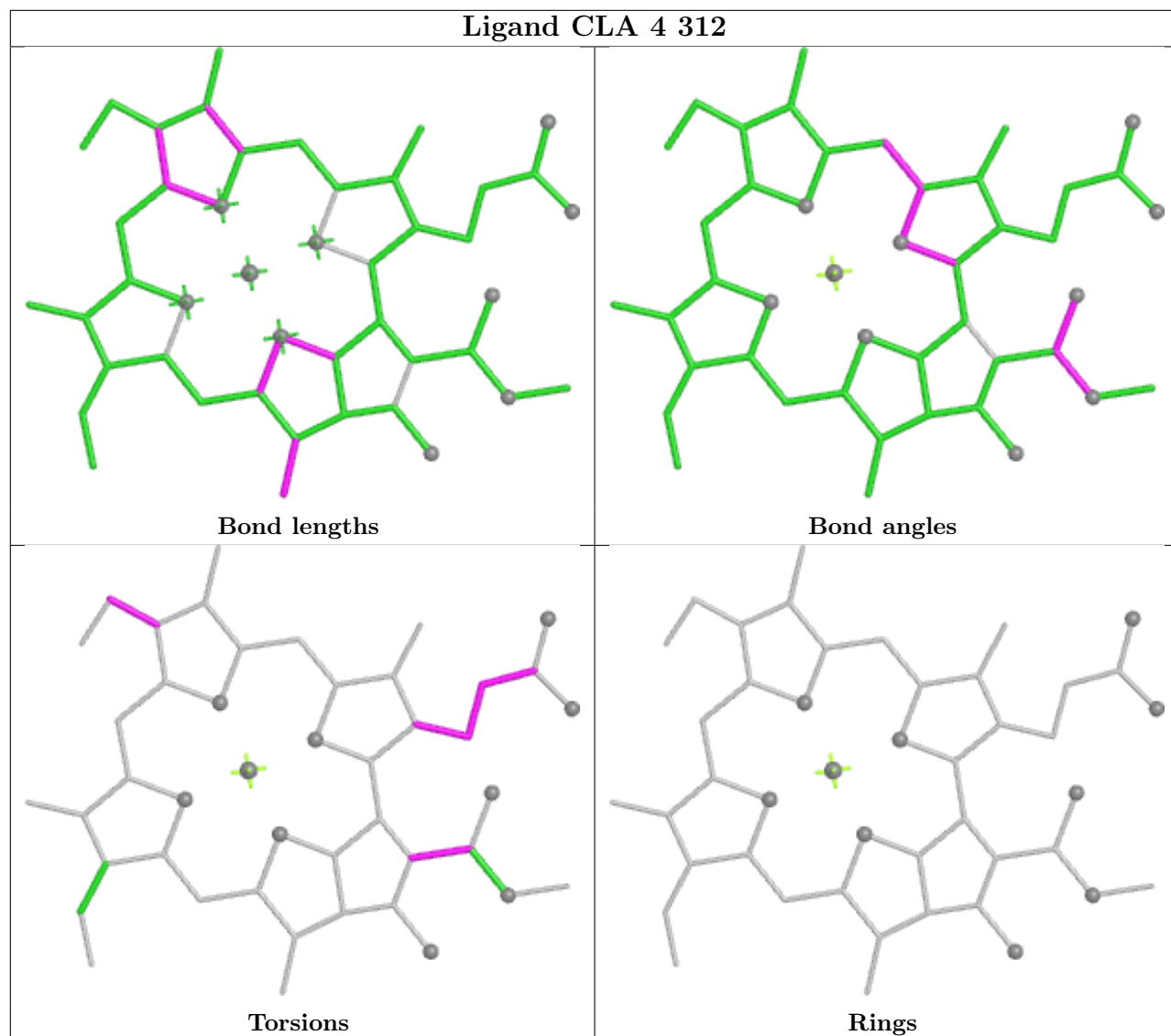


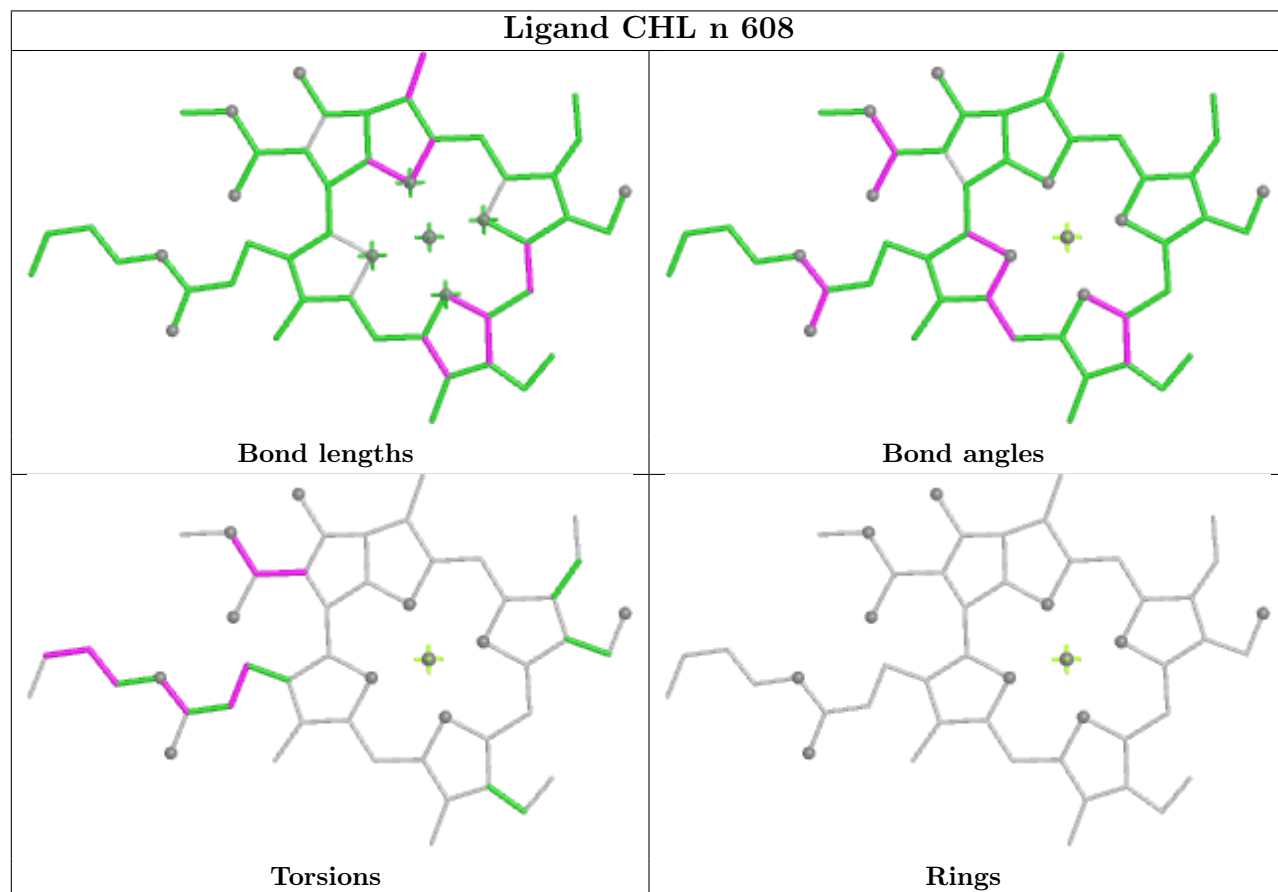
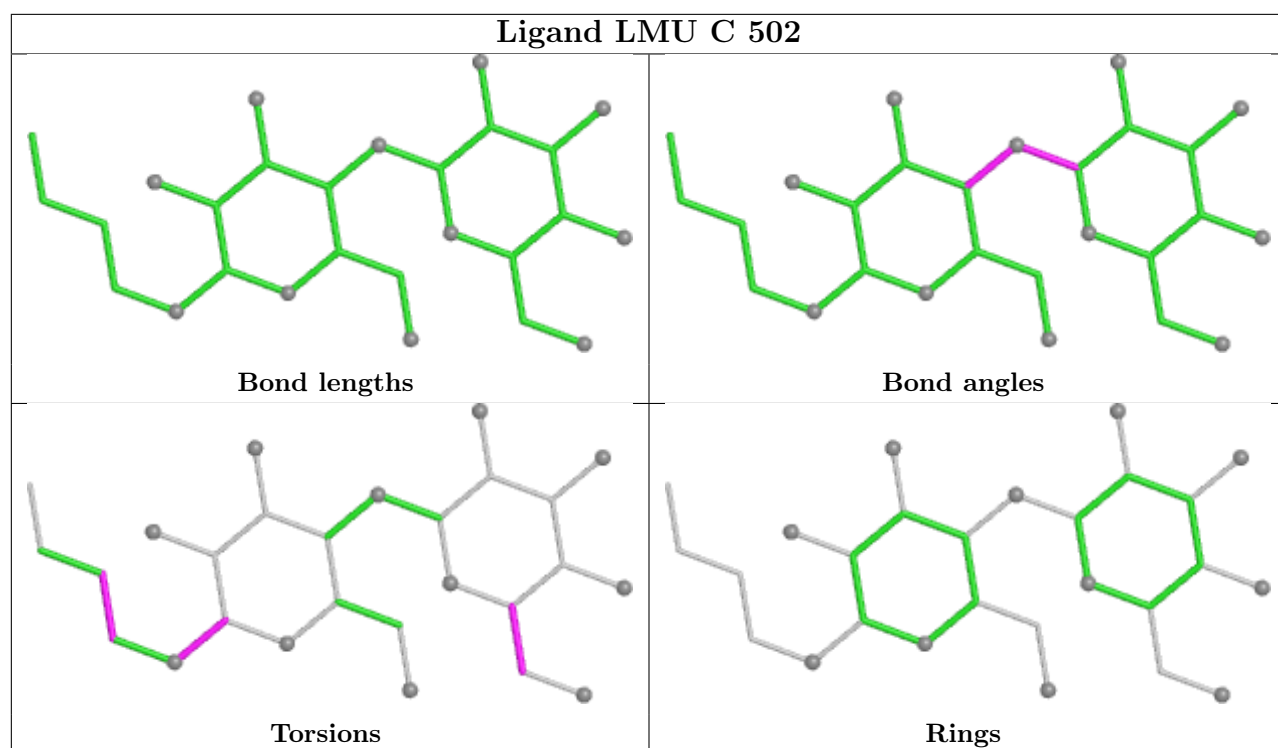
Rings



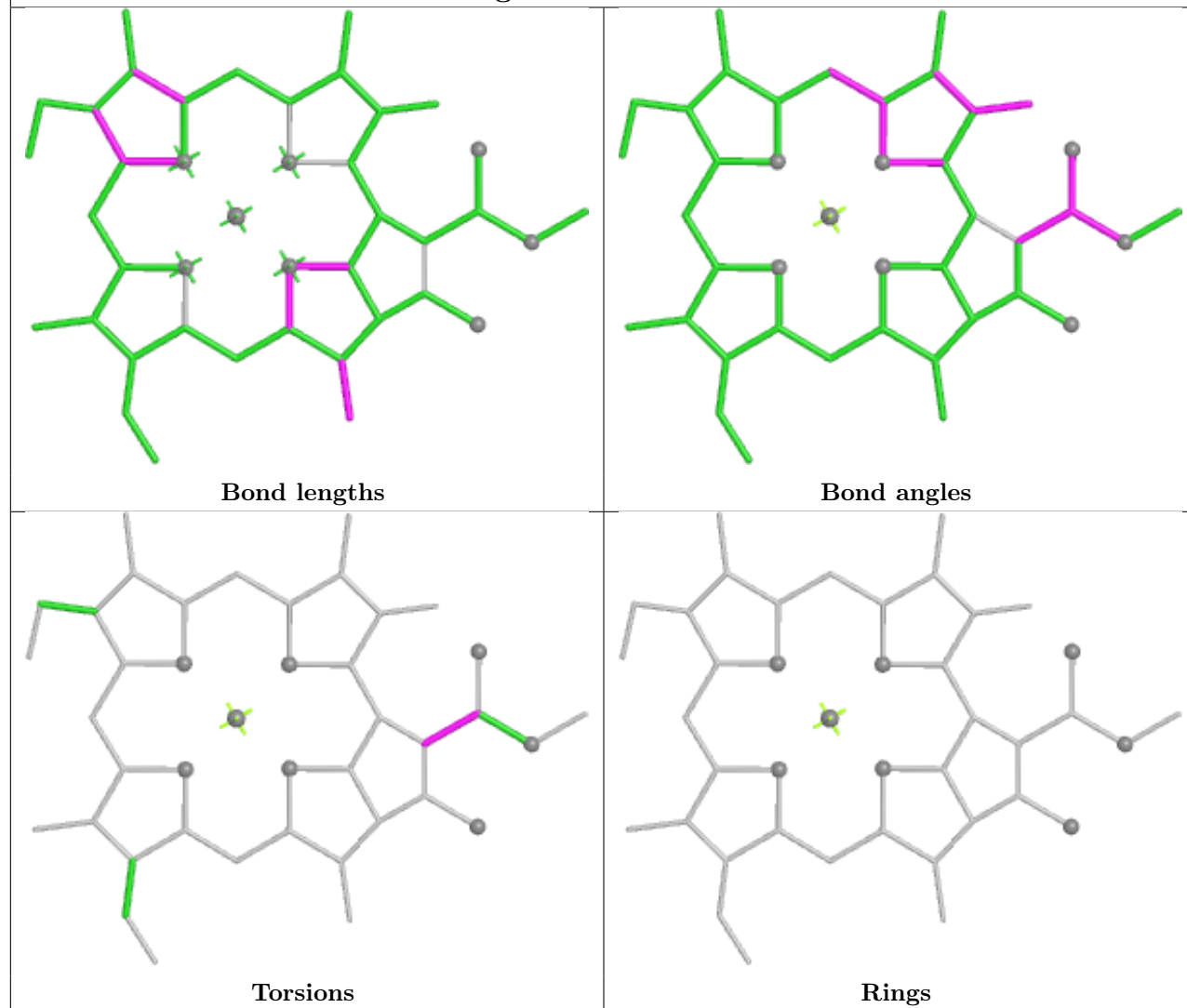


Ligand CLA 4 312

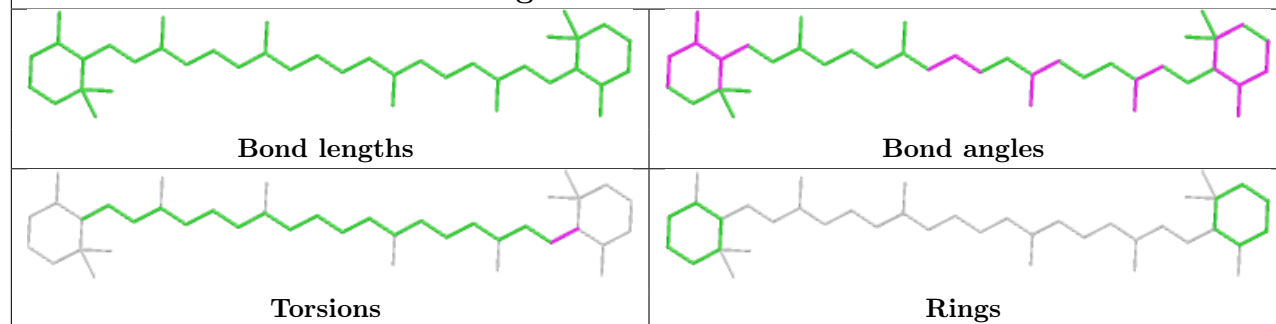




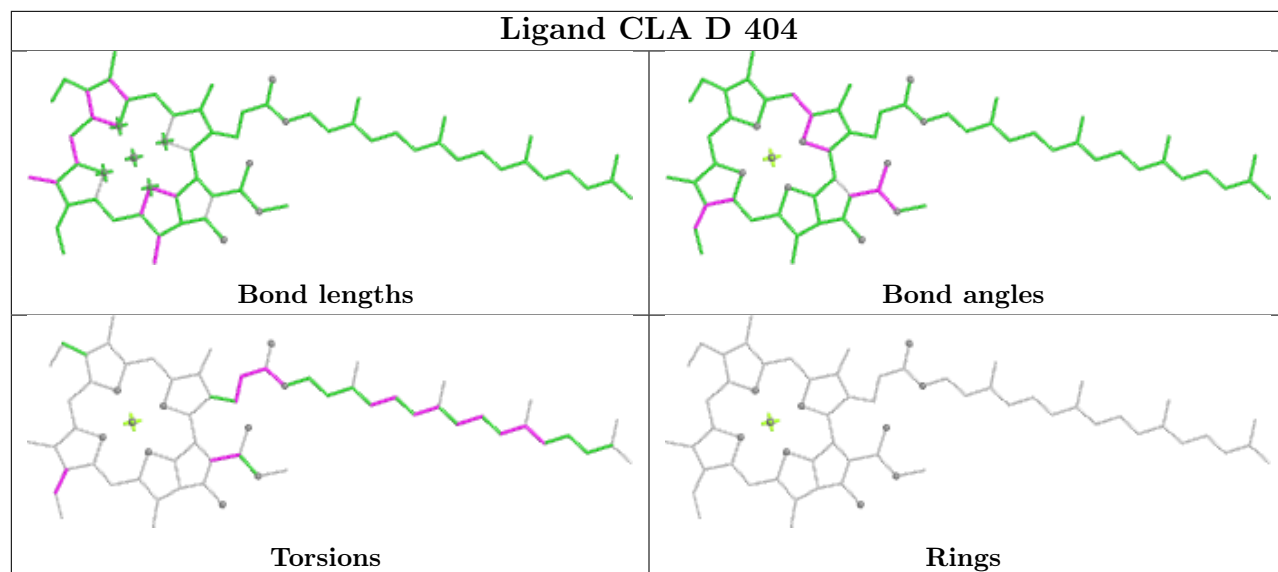
Ligand CLA B 611



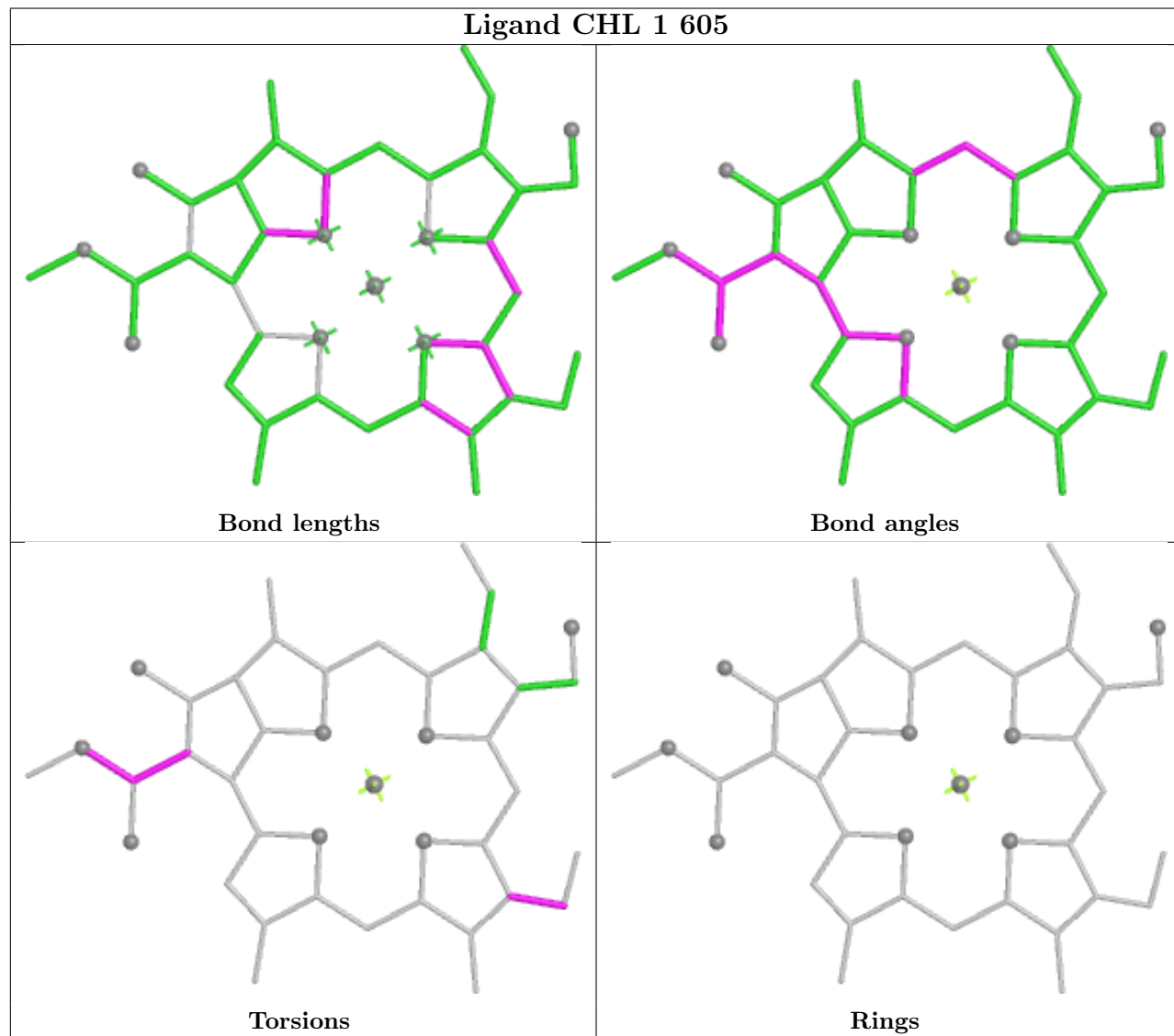
Ligand BCR DD 405

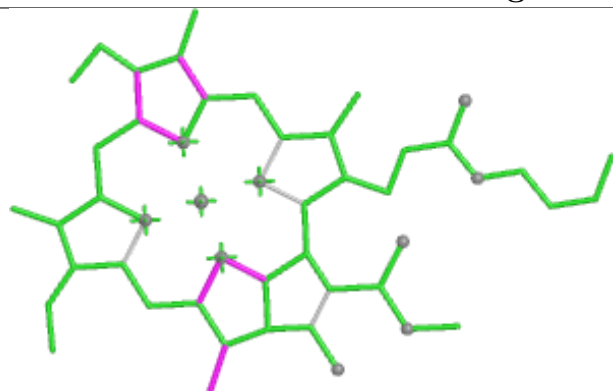


Ligand CLA D 404

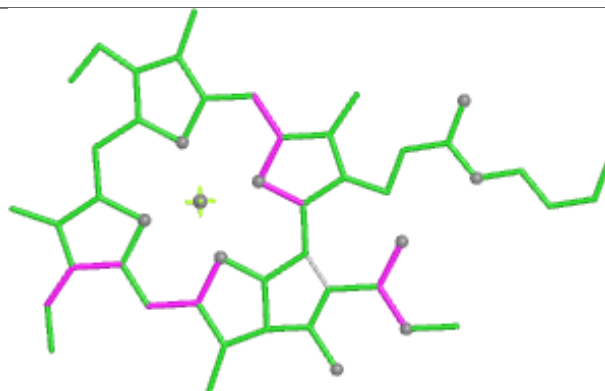


Ligand CHL 1 605

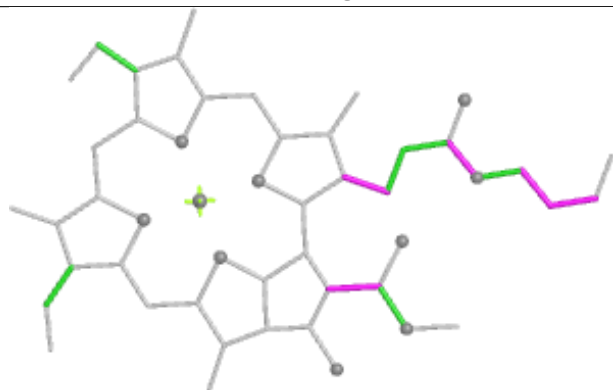


Ligand CLA SS 305

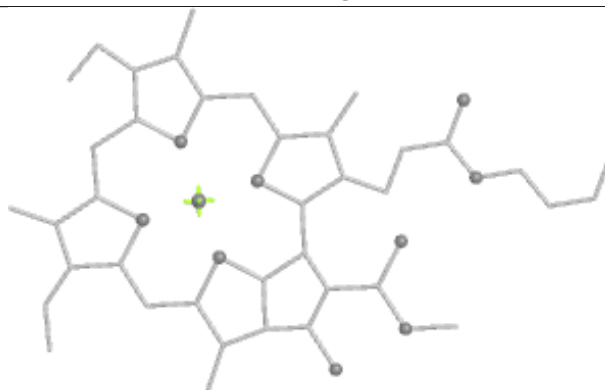
Bond lengths



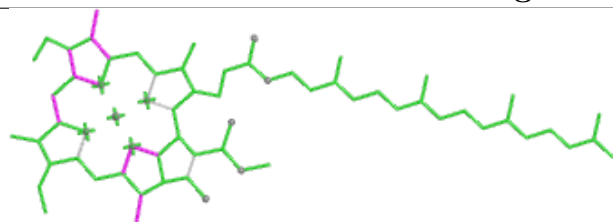
Bond angles



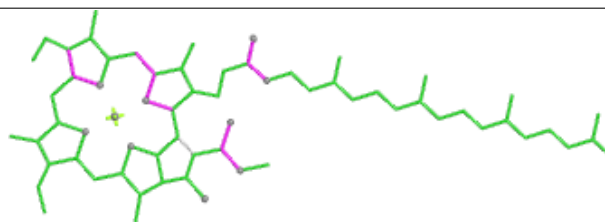
Torsions



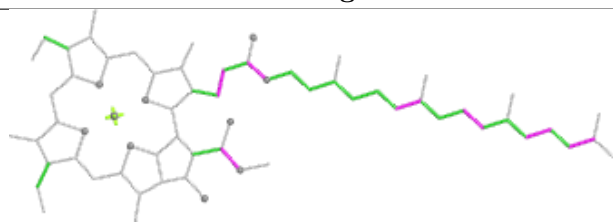
Rings

Ligand CLA C 512

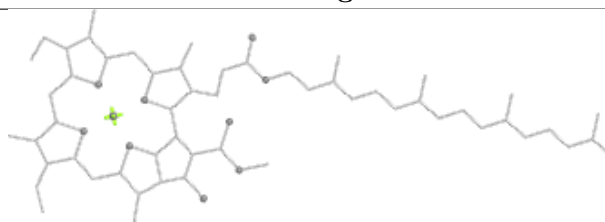
Bond lengths



Bond angles

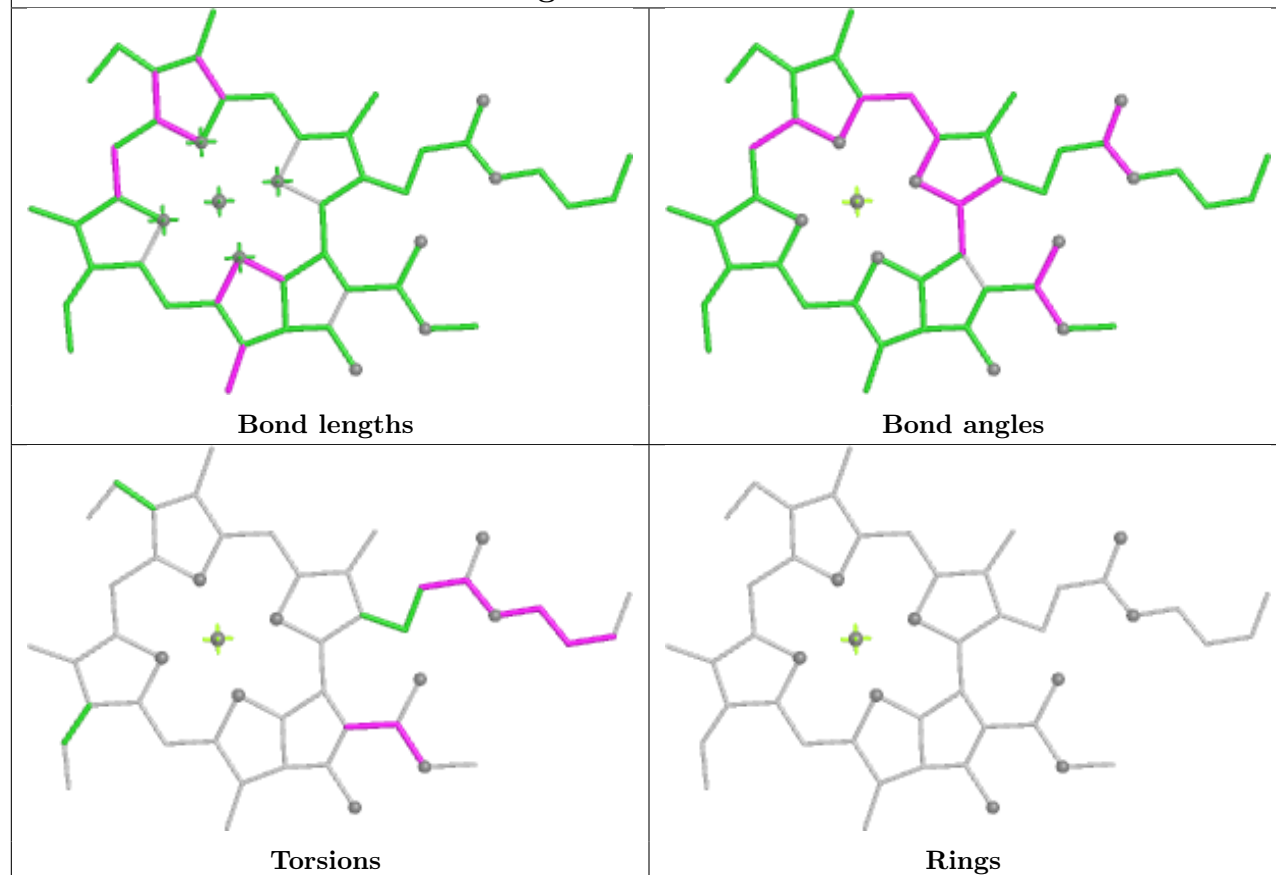


Torsions

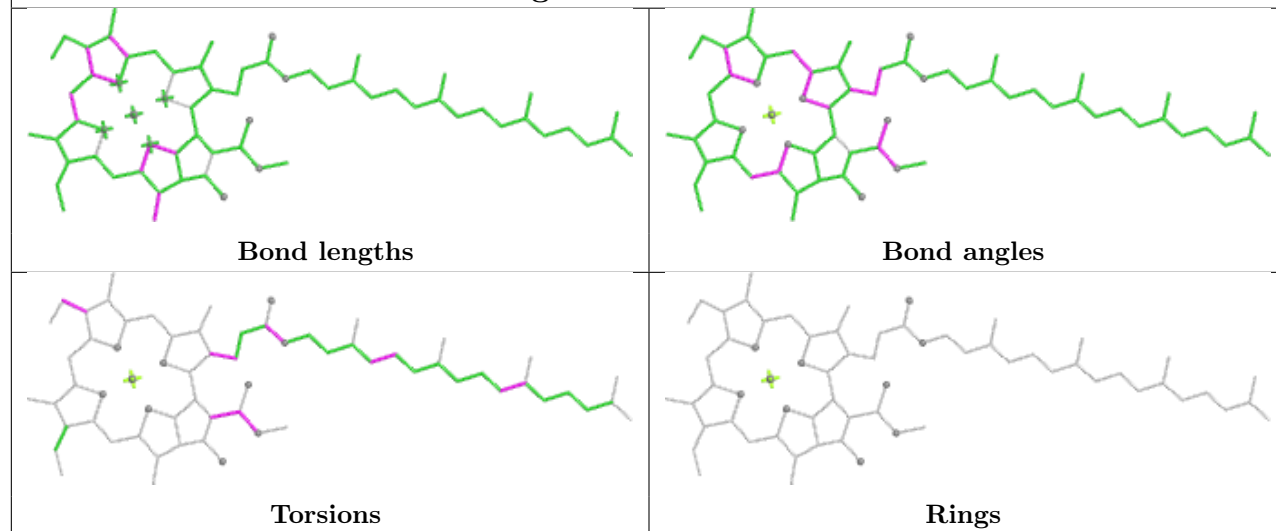


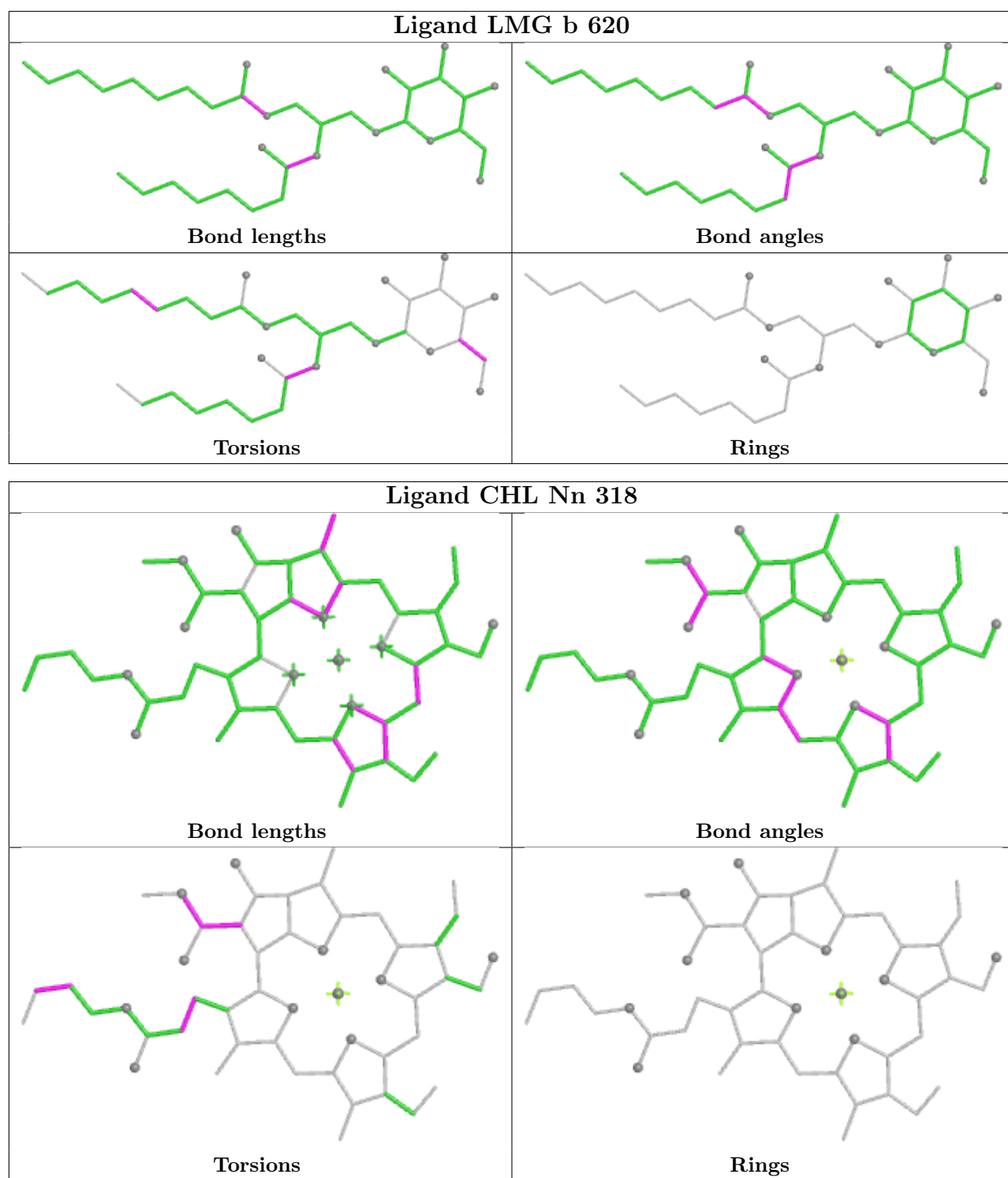
Rings

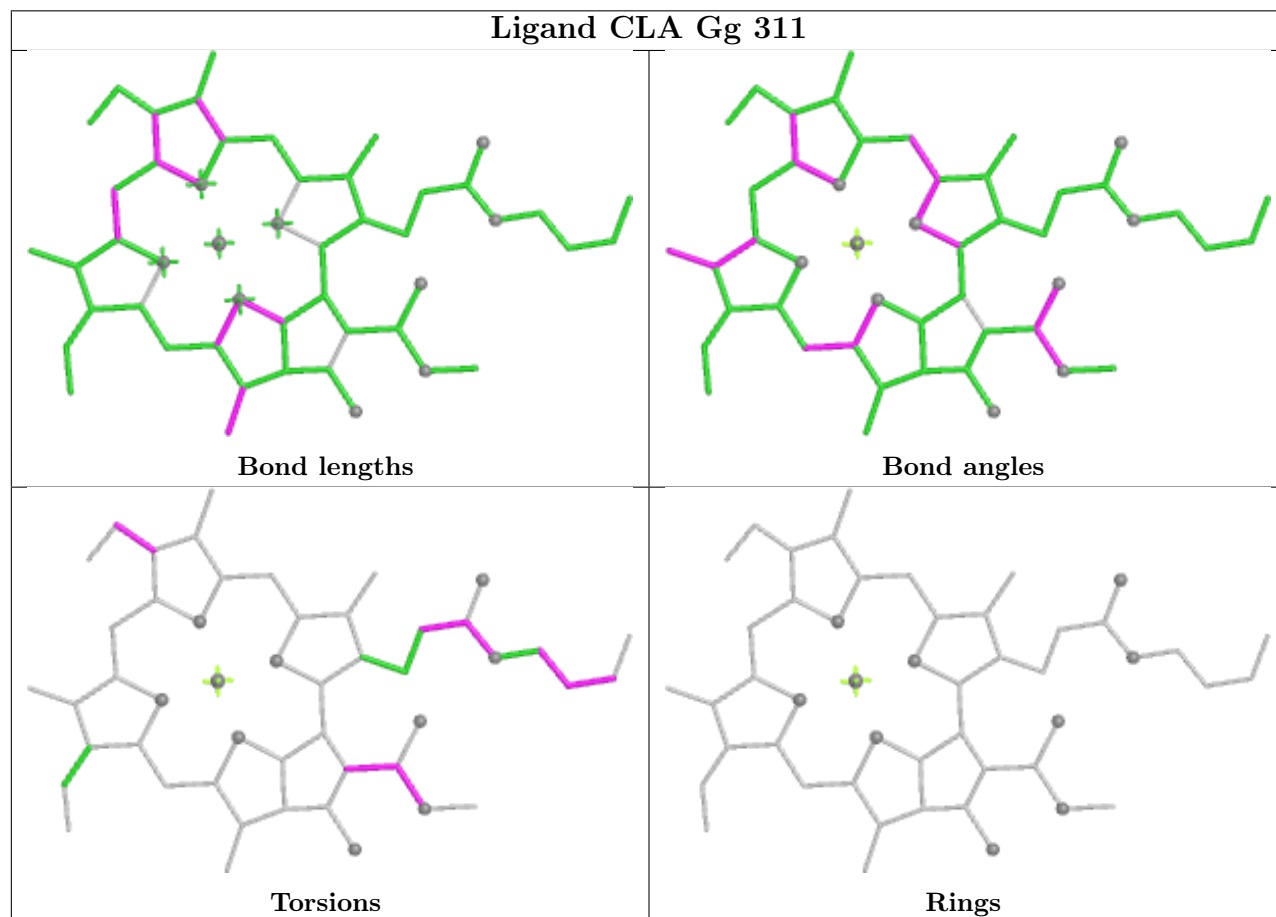
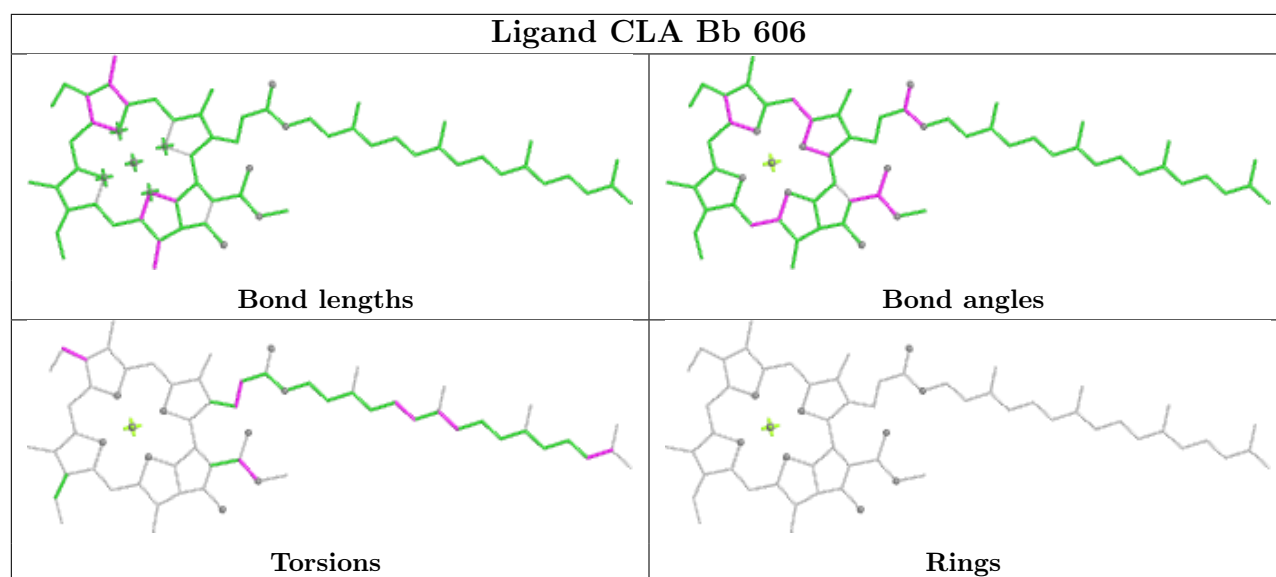
Ligand CLA s 611

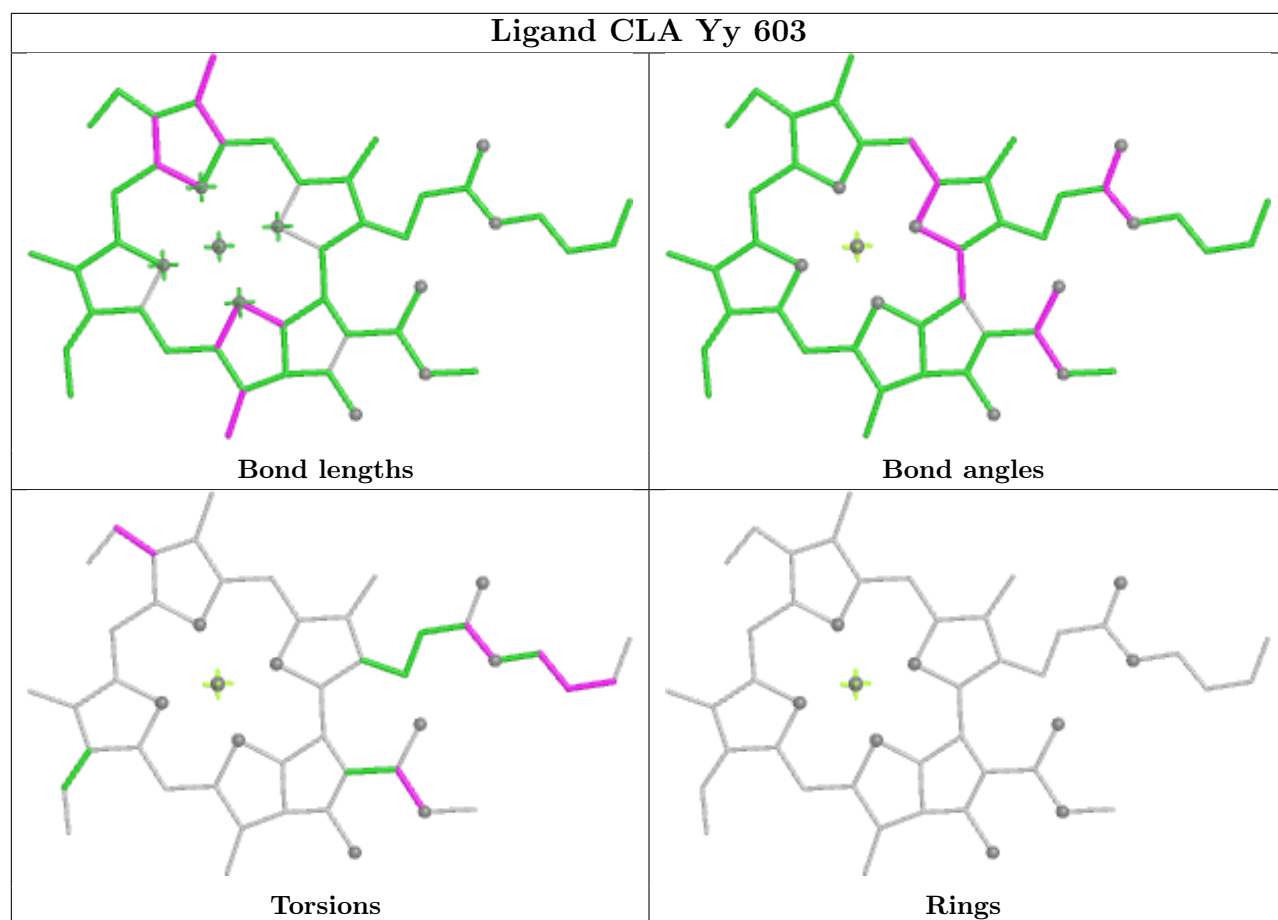
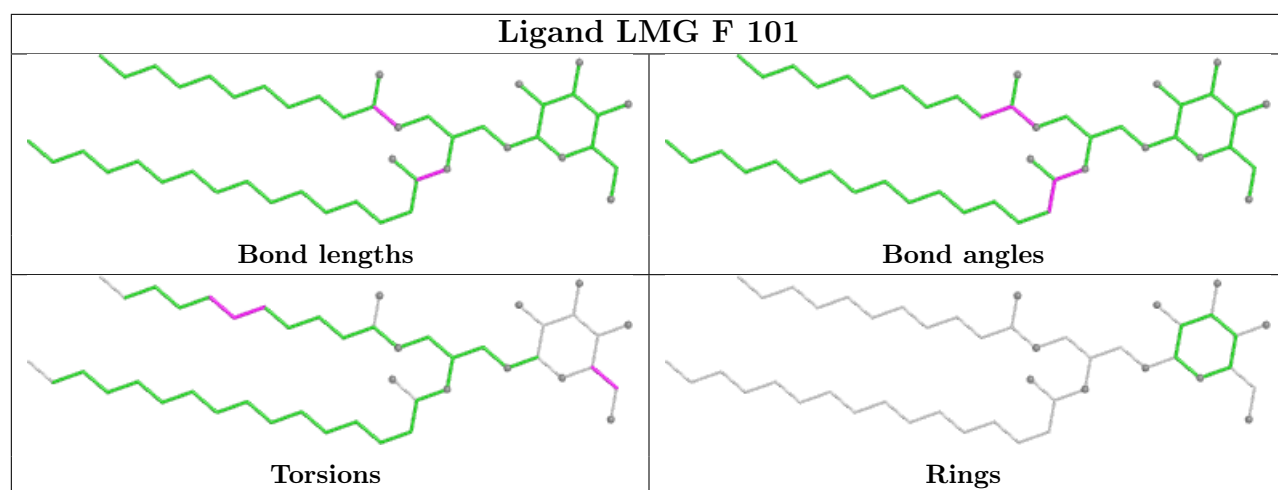


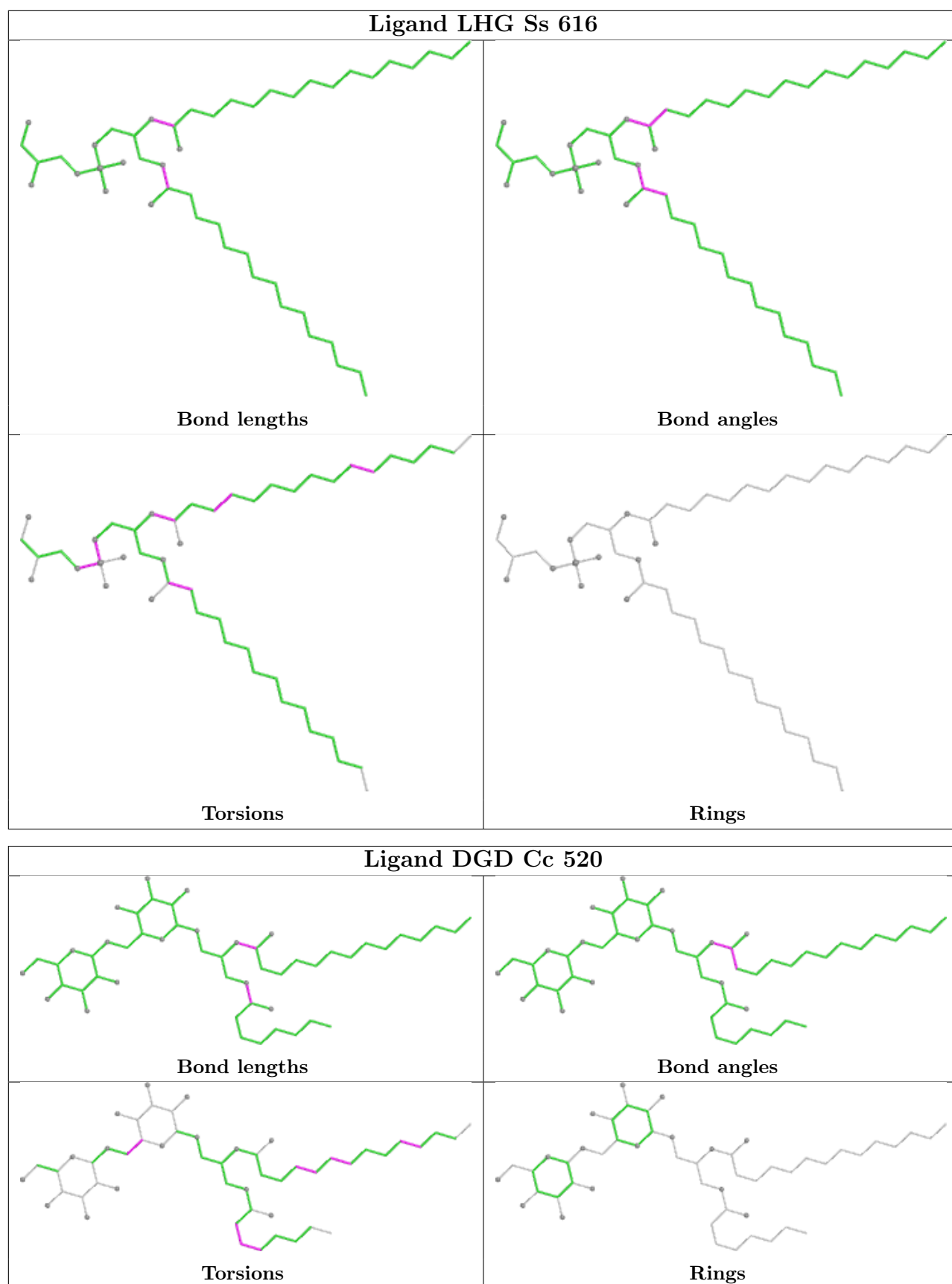
Ligand CLA R 609



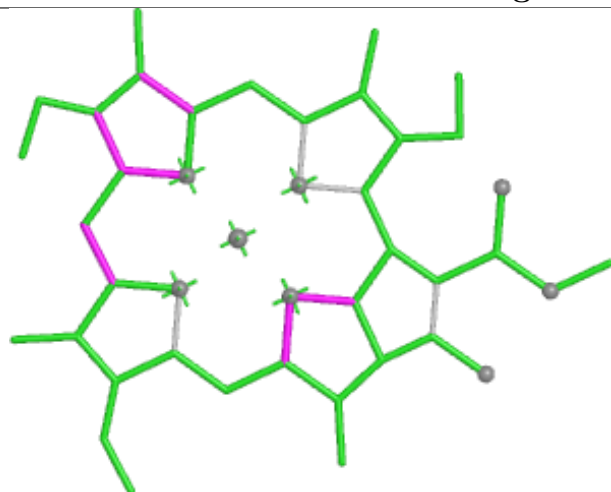




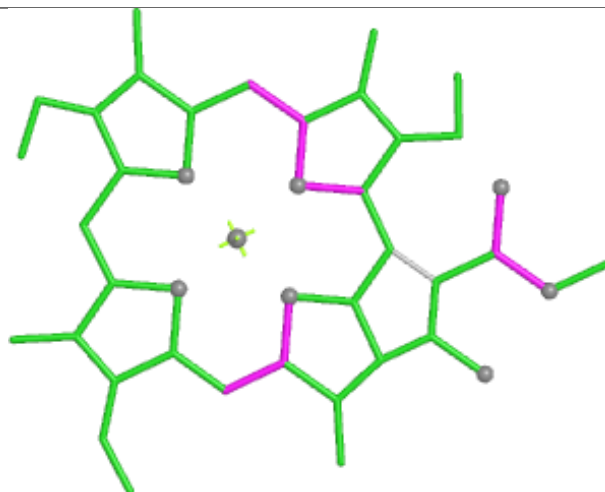




Ligand CLA G 604



Bond lengths



Bond angles

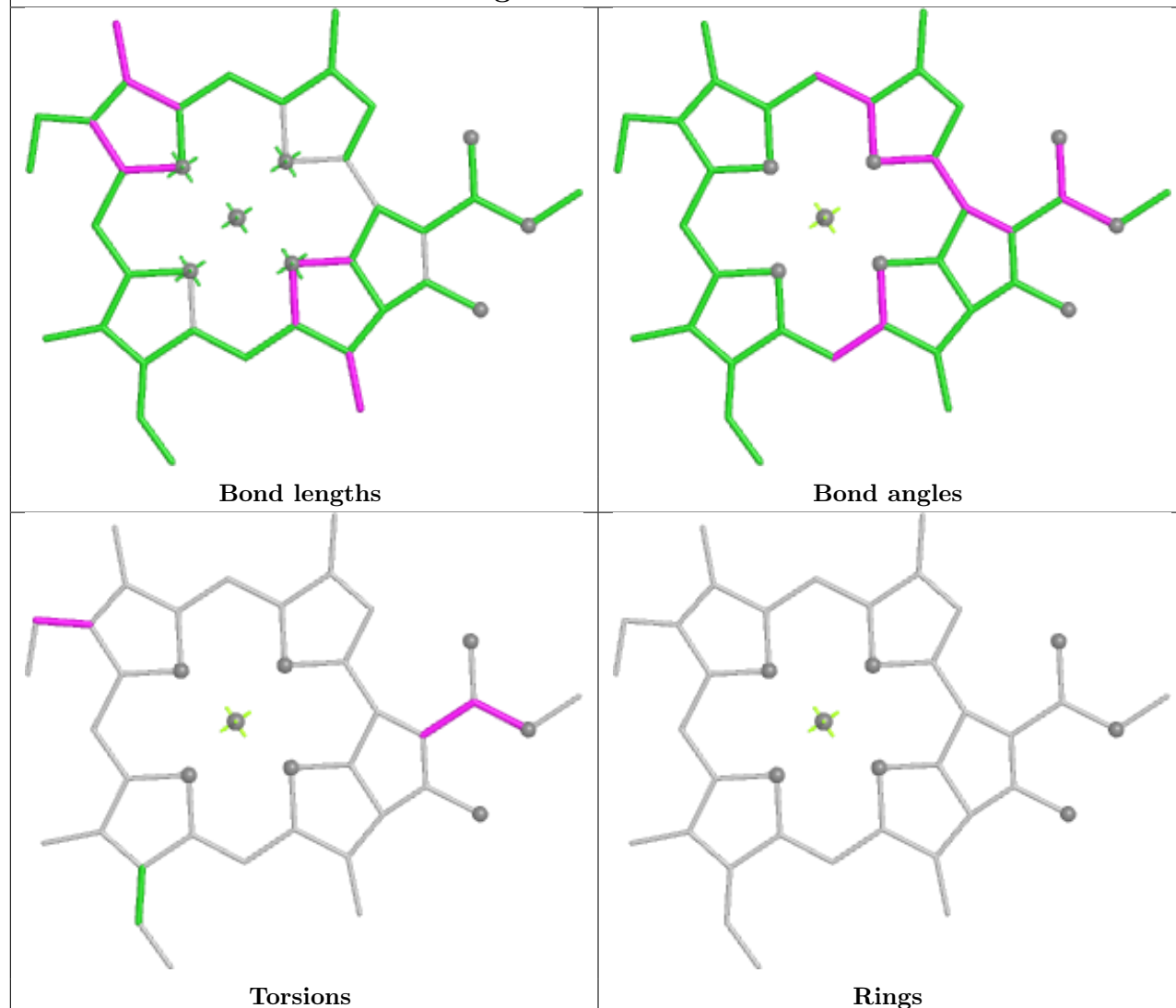


Torsions

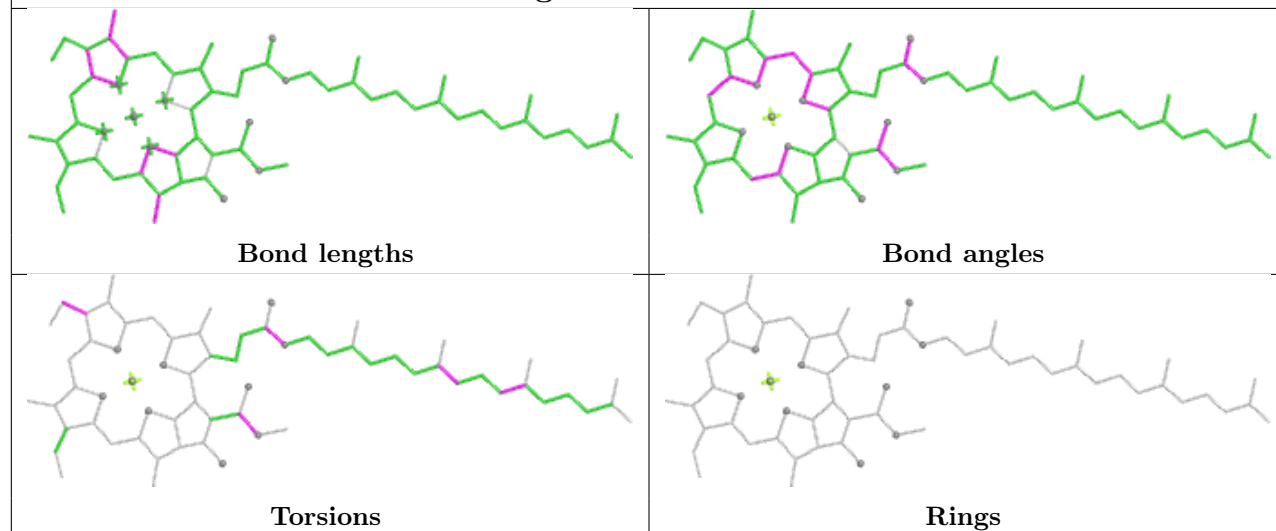


Rings

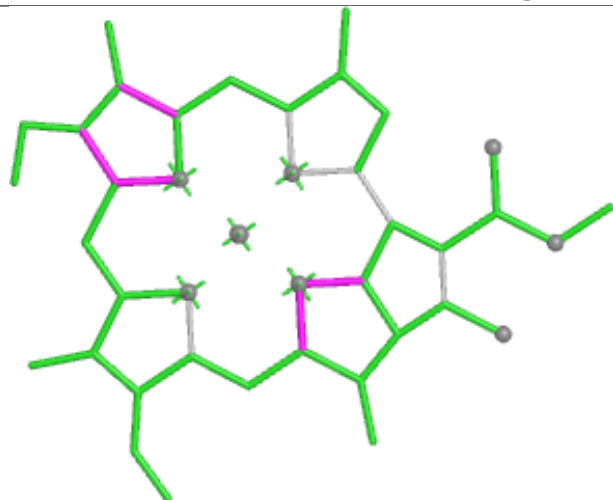
Ligand CLA 2 603



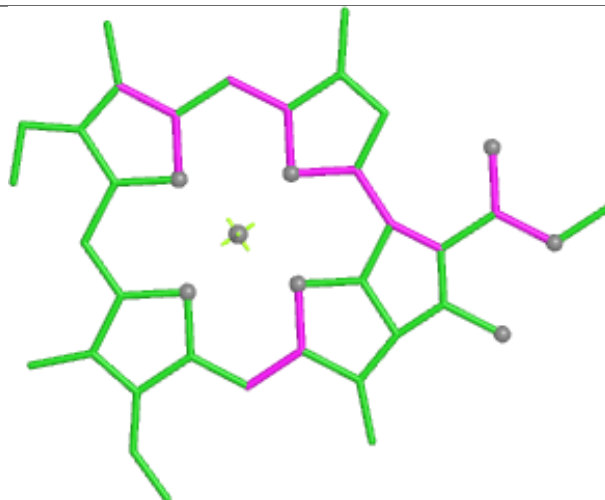
Ligand CLA b 608



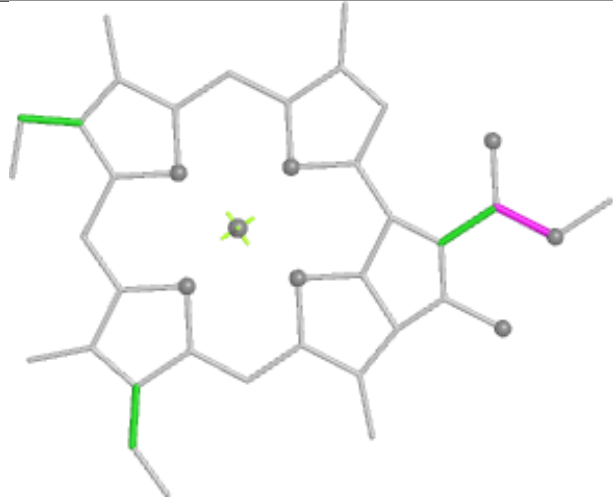
Ligand CLA 2 612



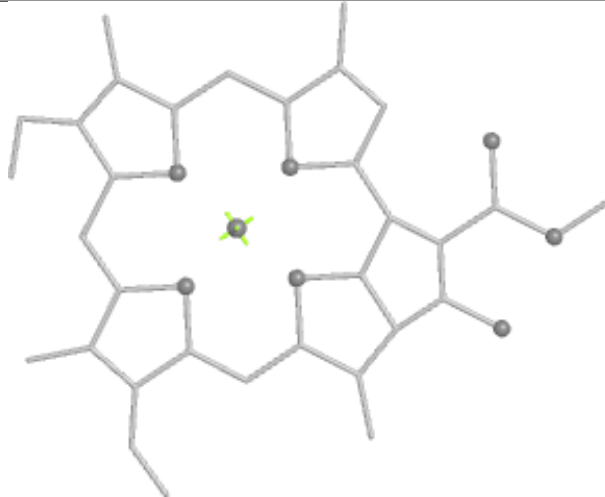
Bond lengths



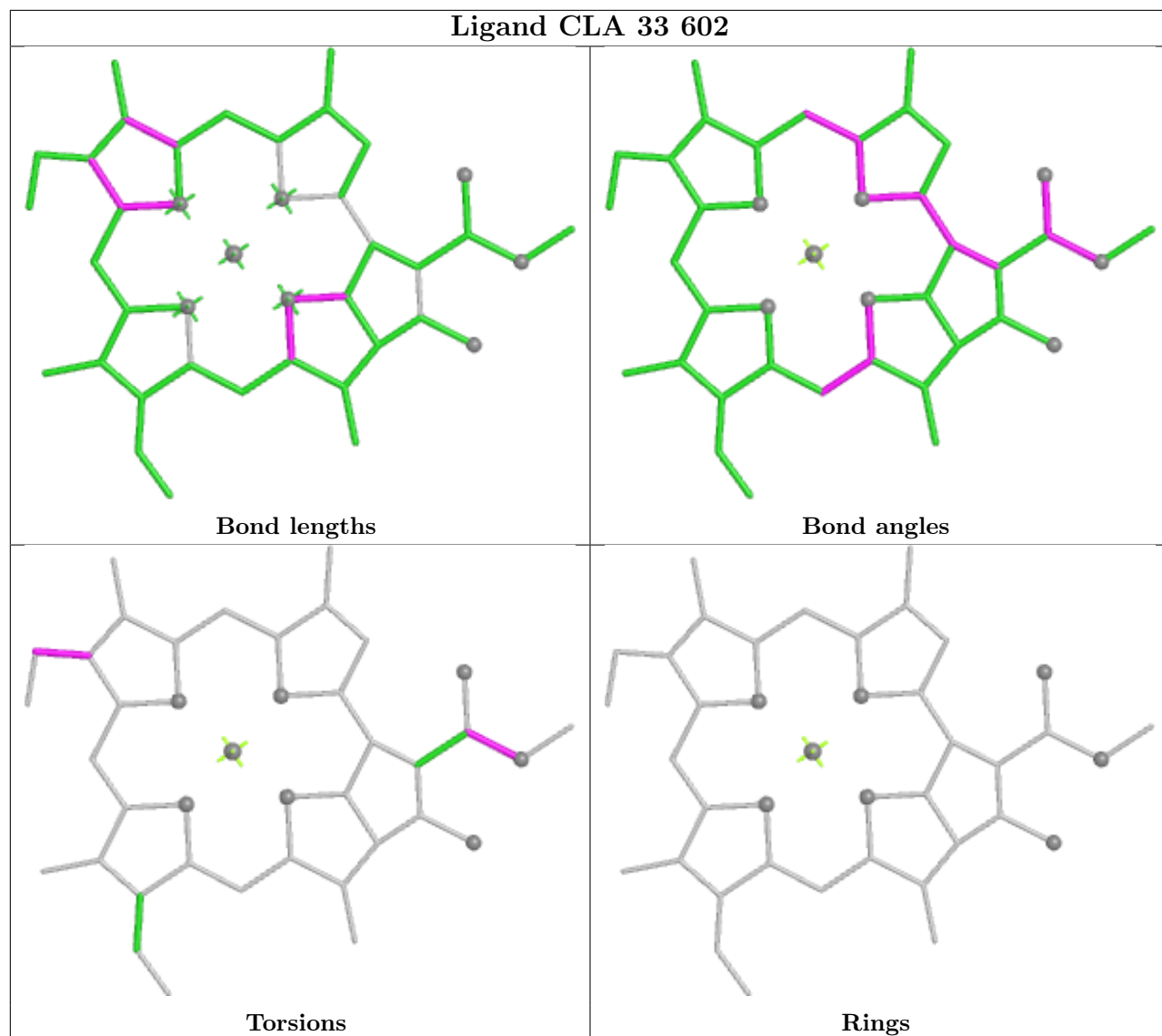
Bond angles



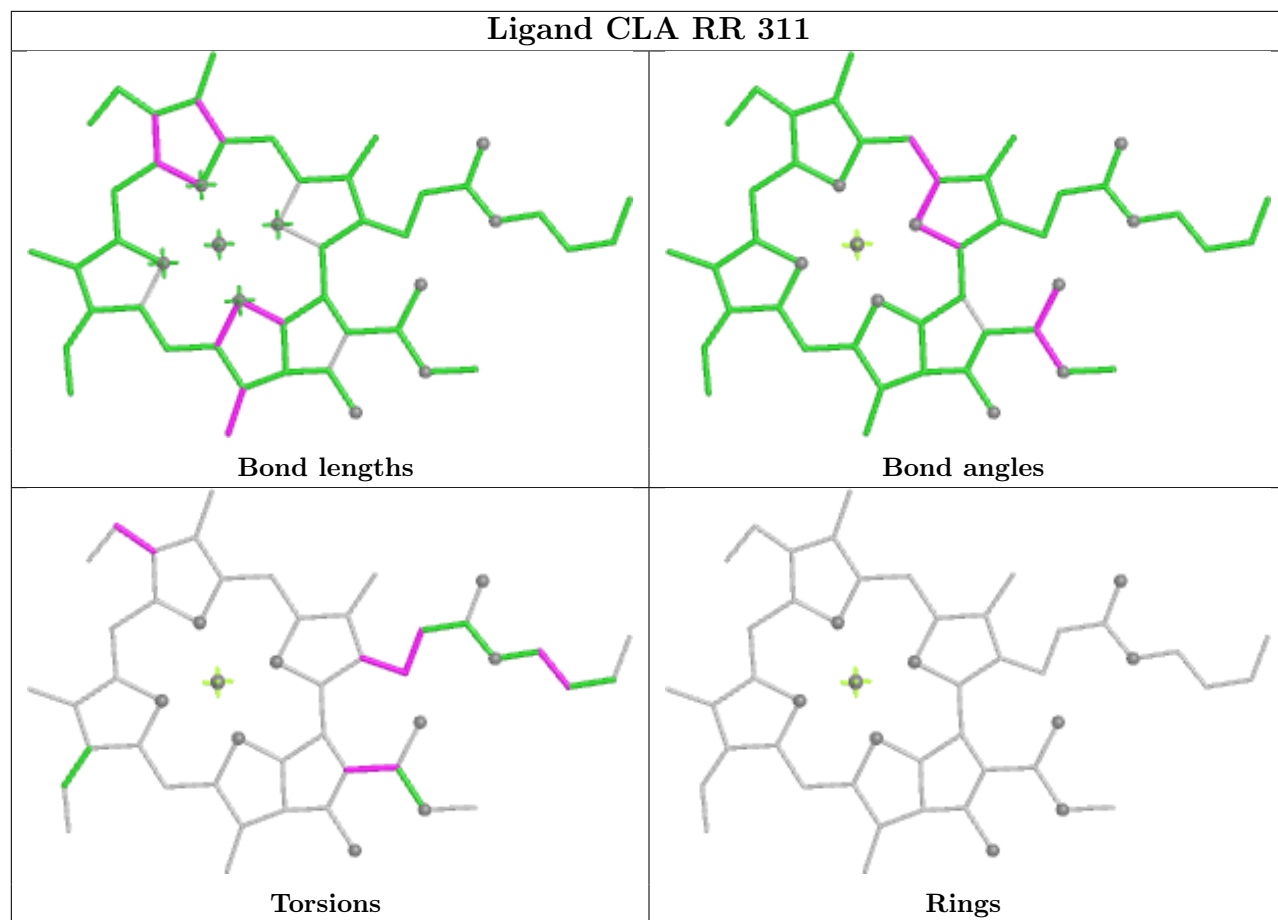
Torsions

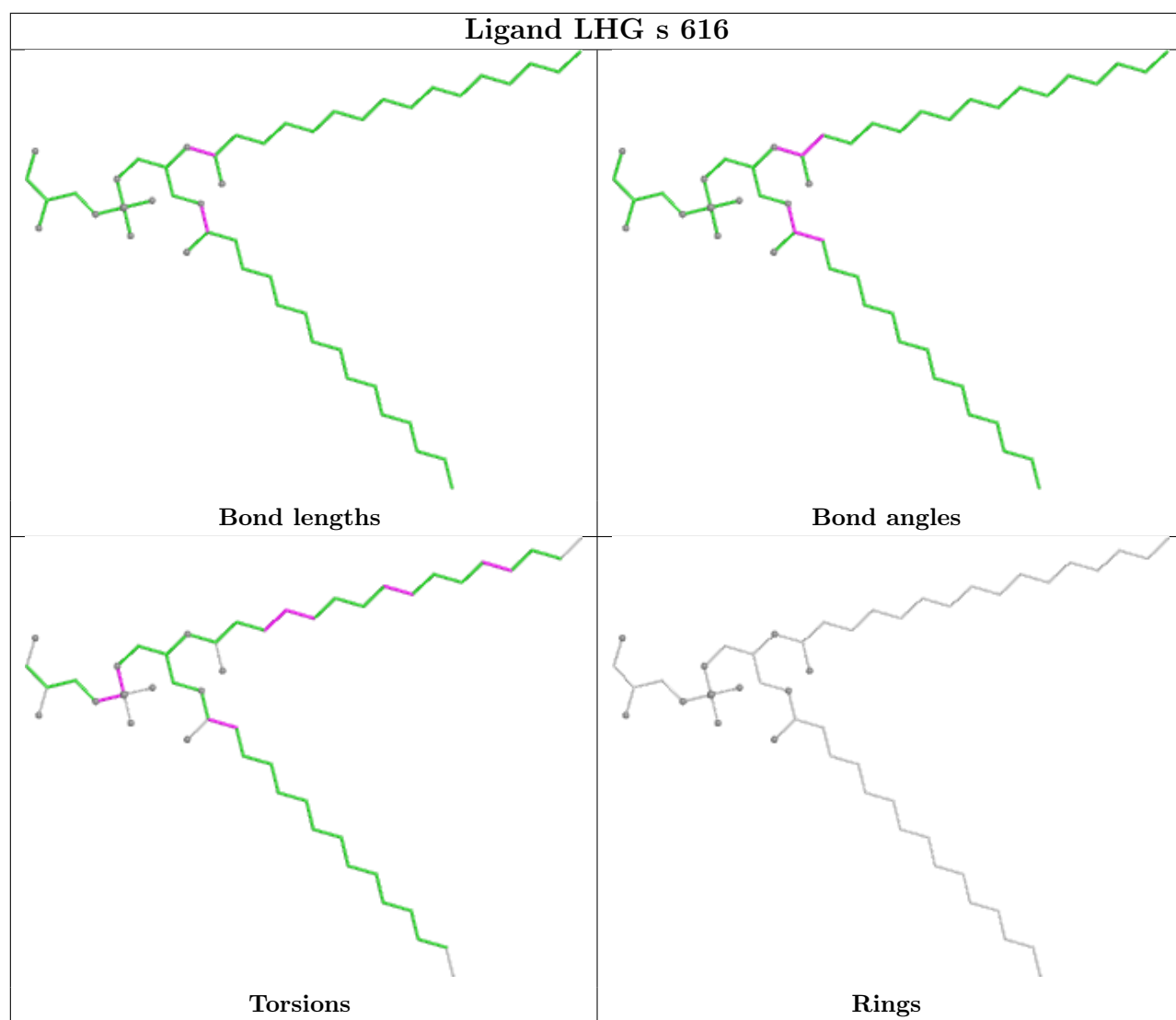


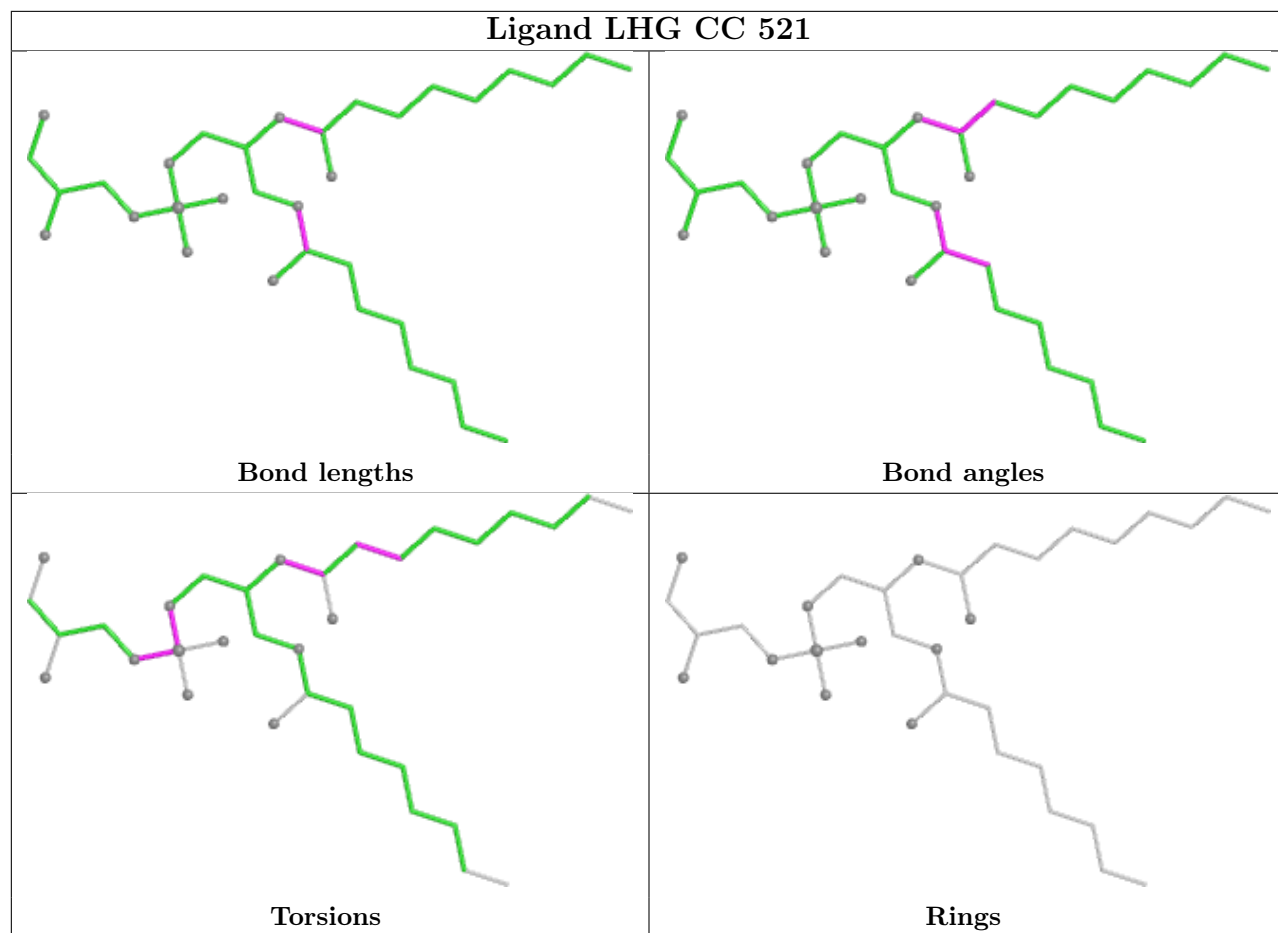
Rings



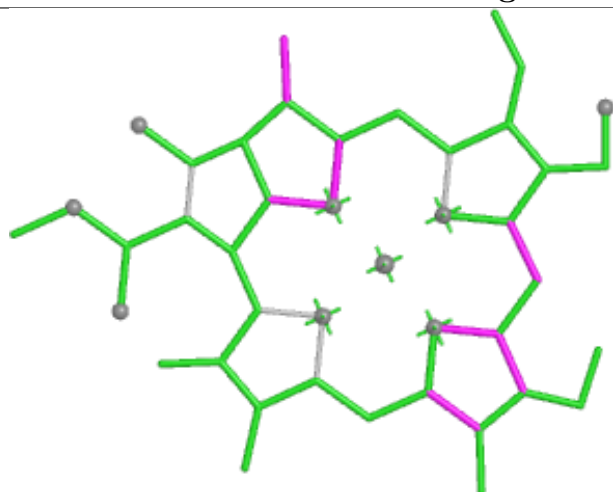
Ligand CLA RR 311



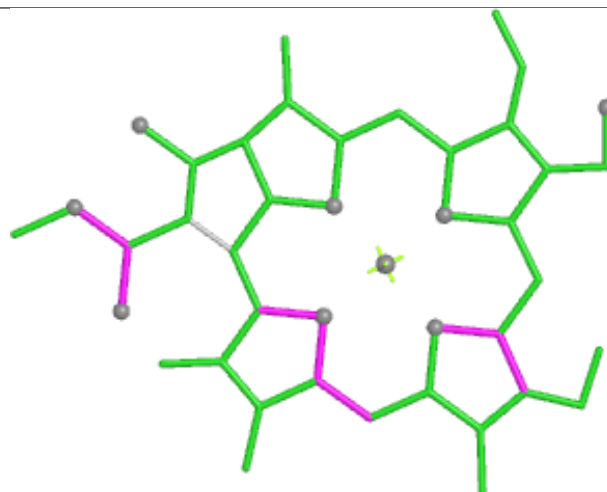




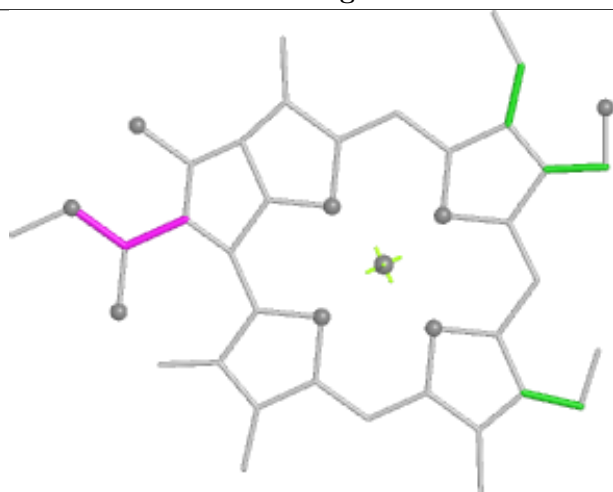
Ligand CHL NN 608



Bond lengths



Bond angles

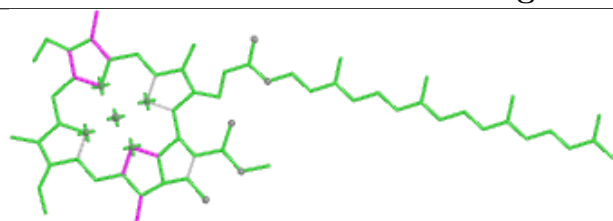


Torsions

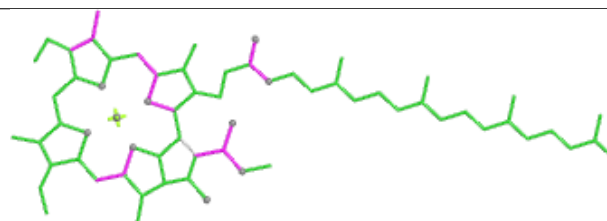


Rings

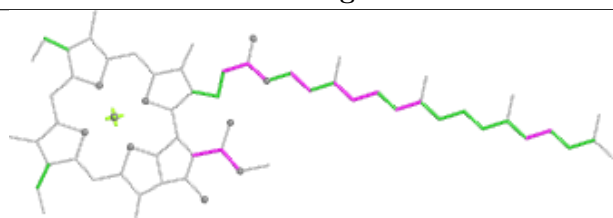
Ligand CLA b 613



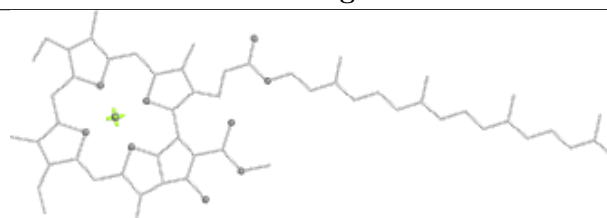
Bond lengths



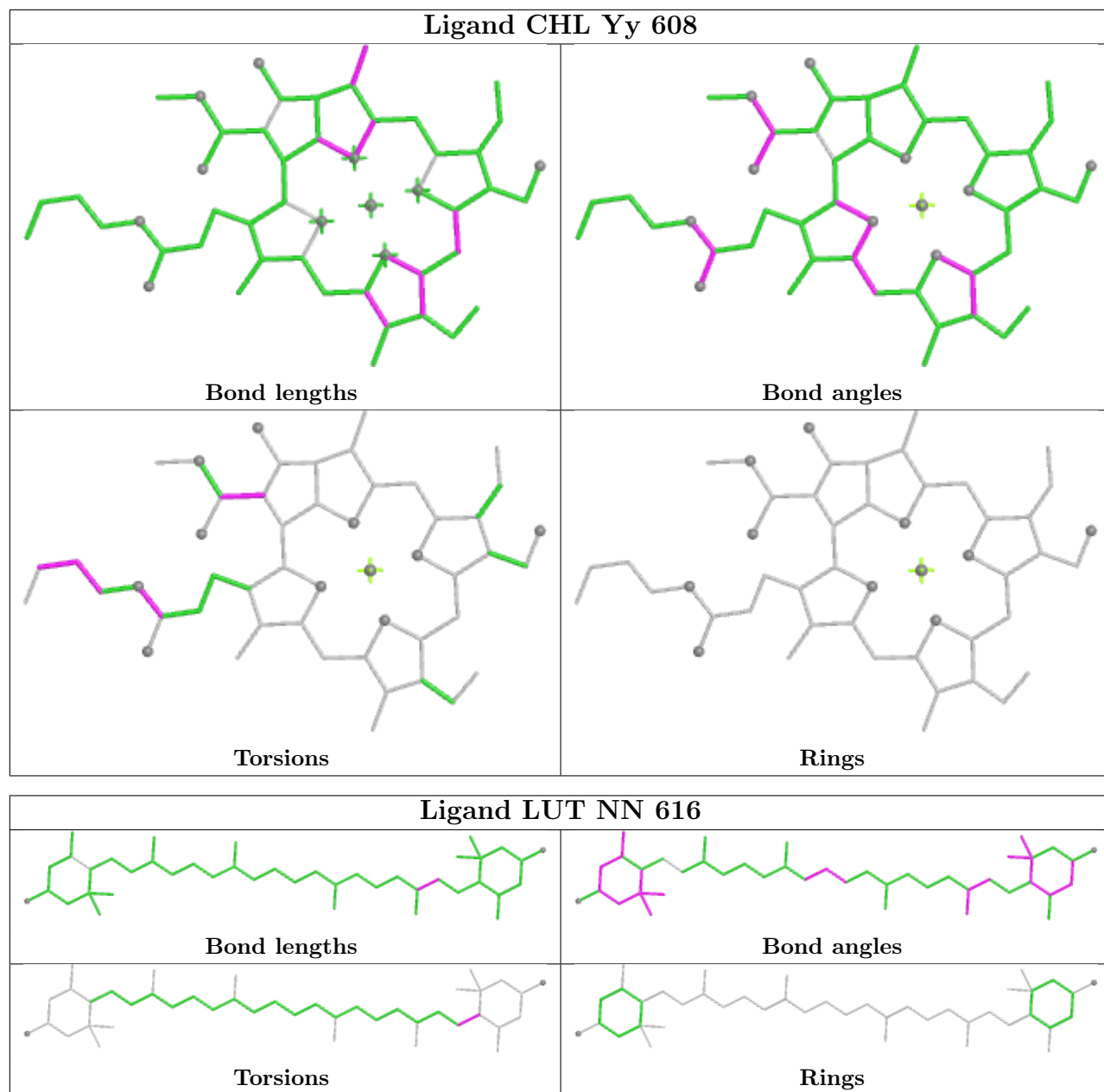
Bond angles

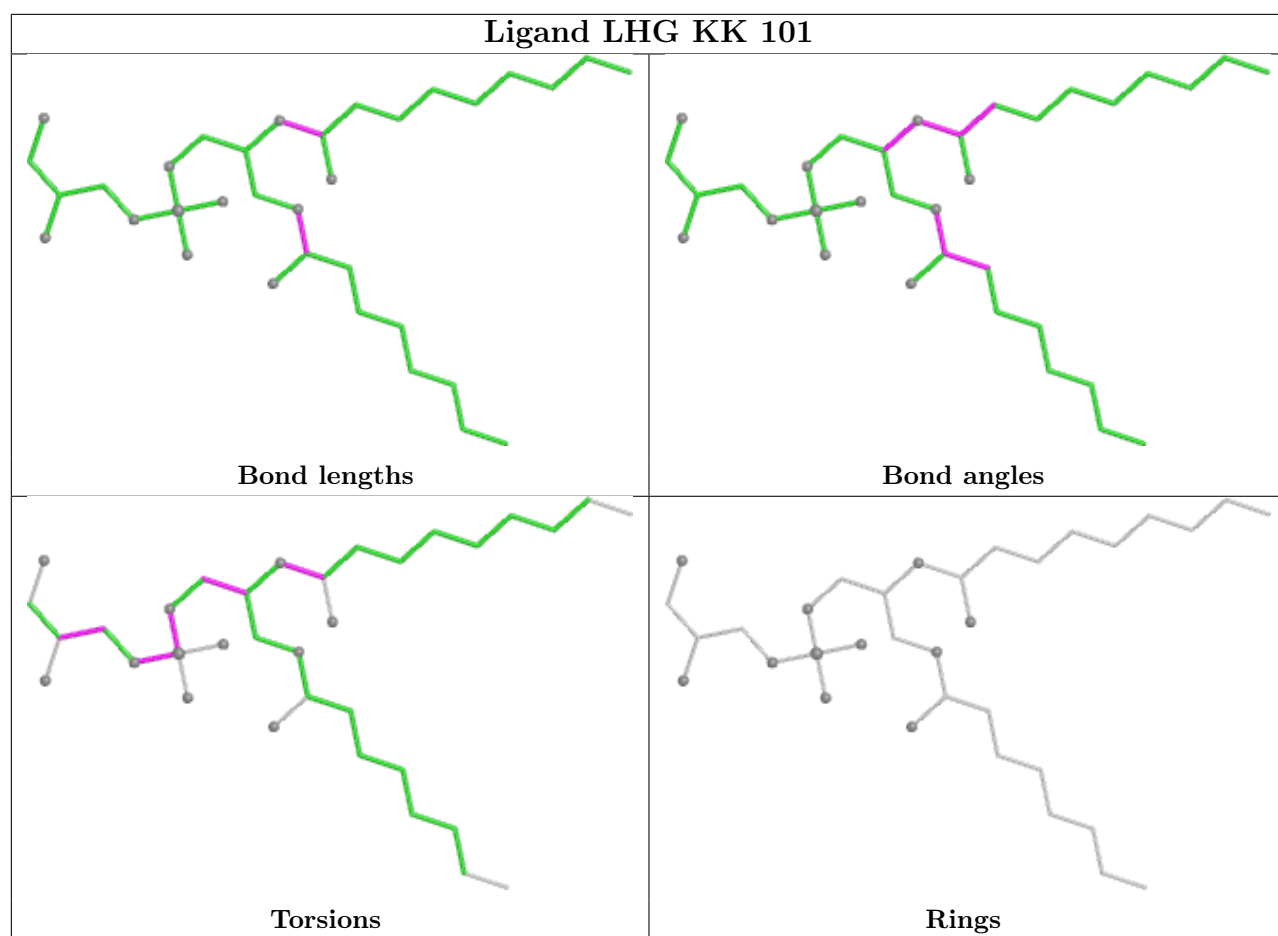


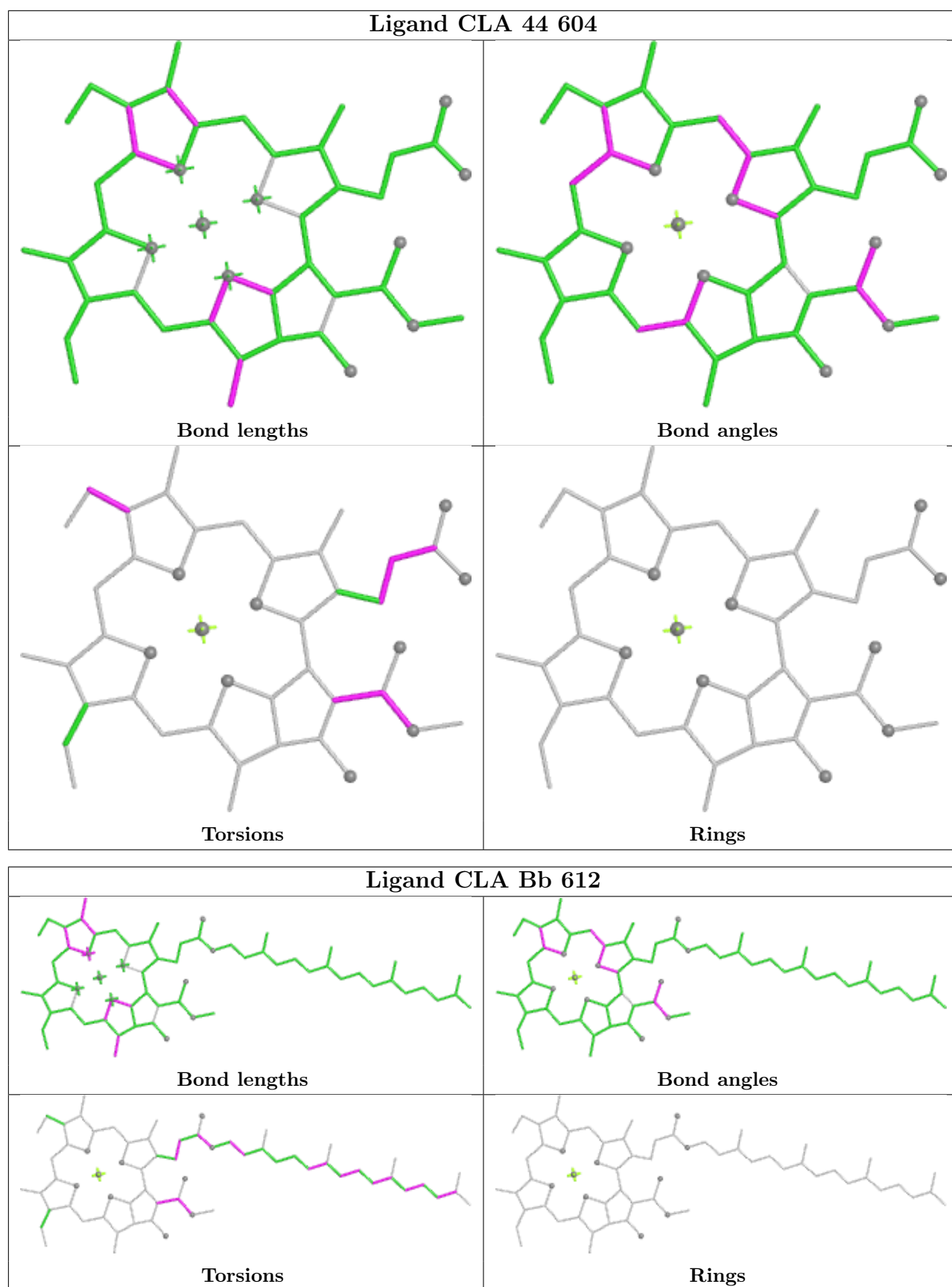
Torsions

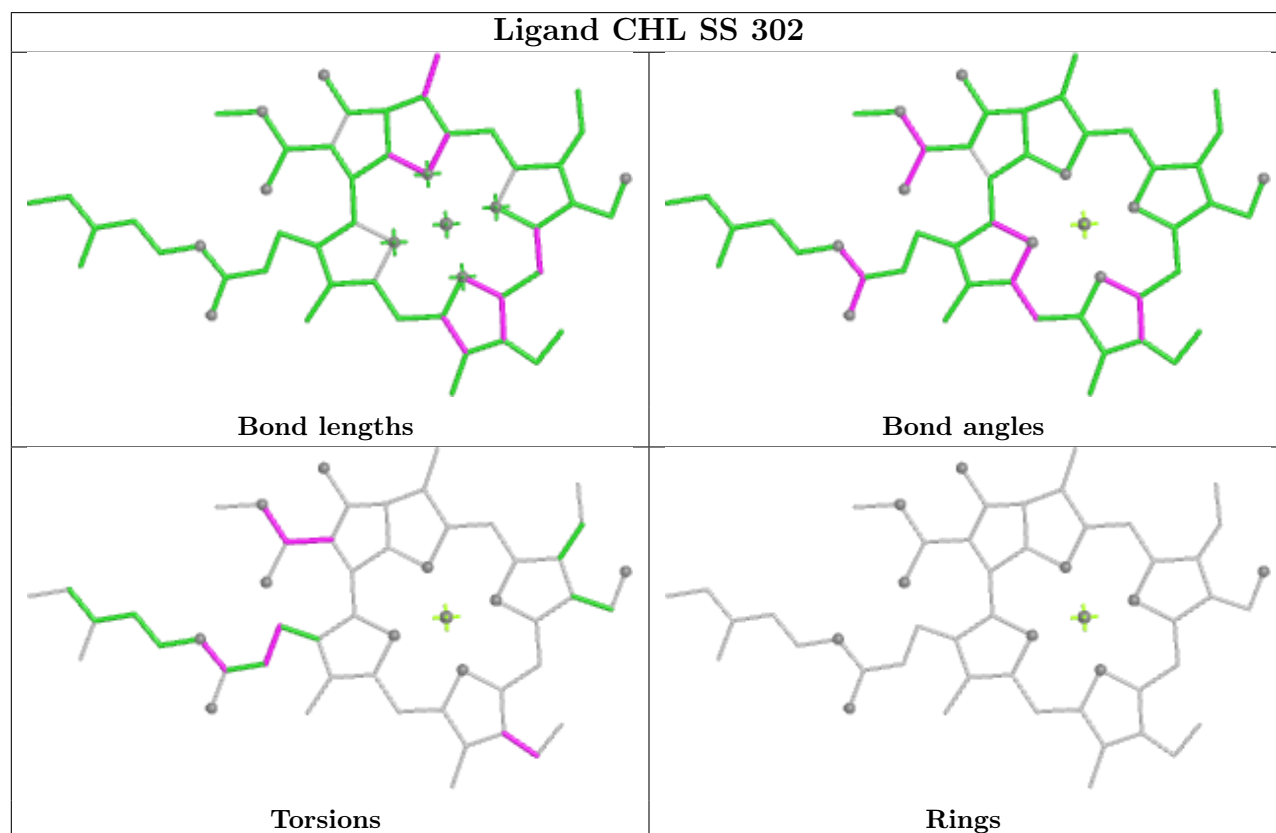
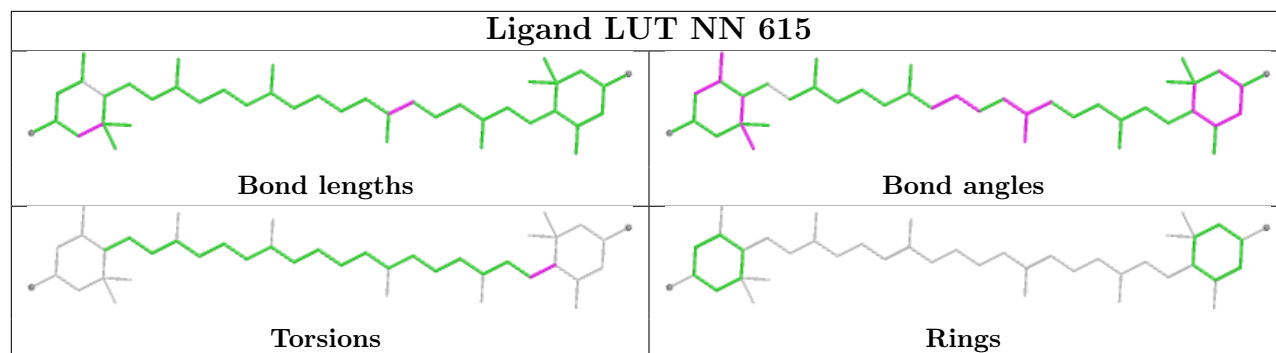


Rings

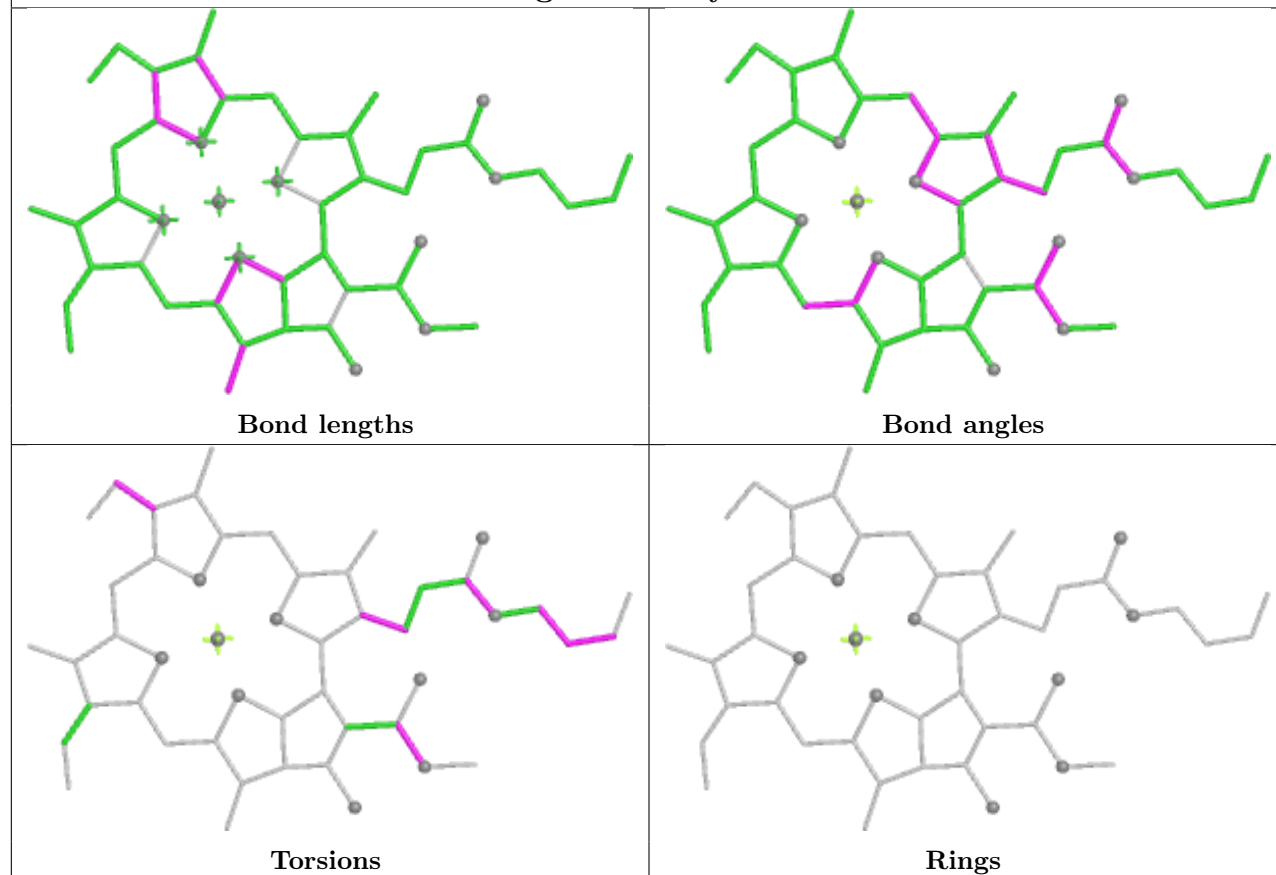




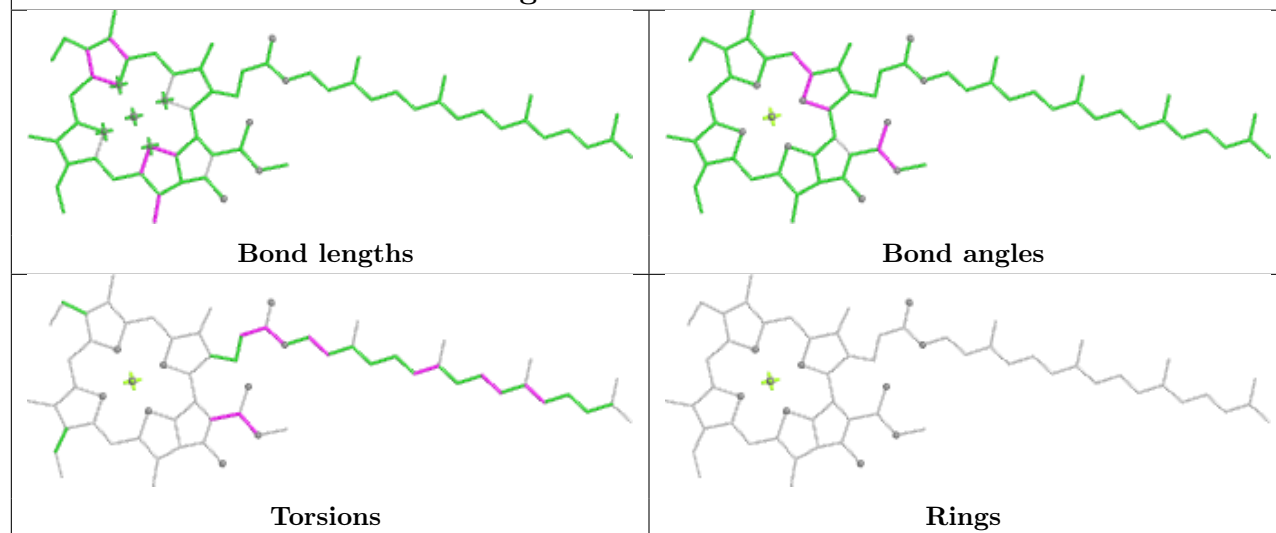


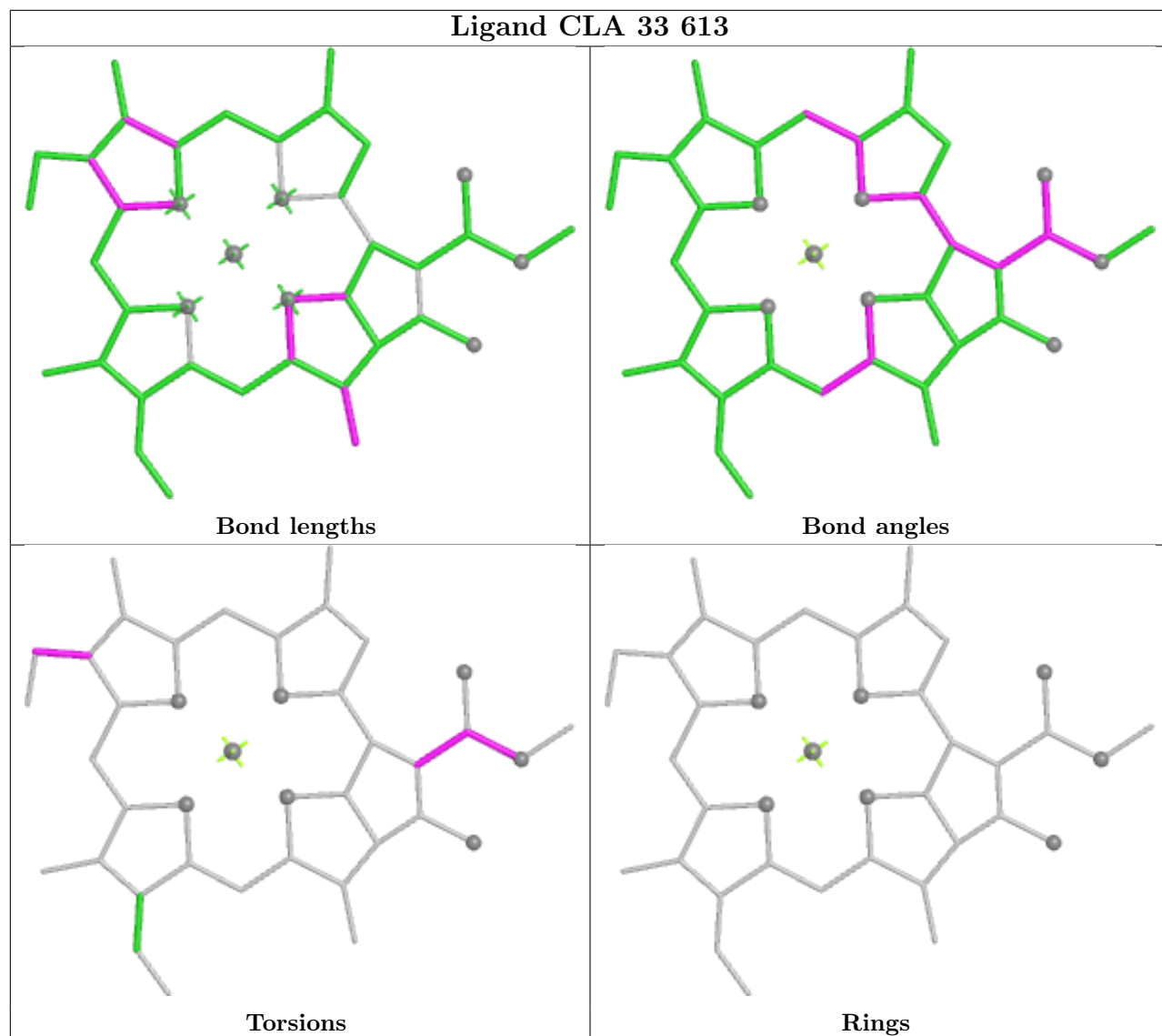


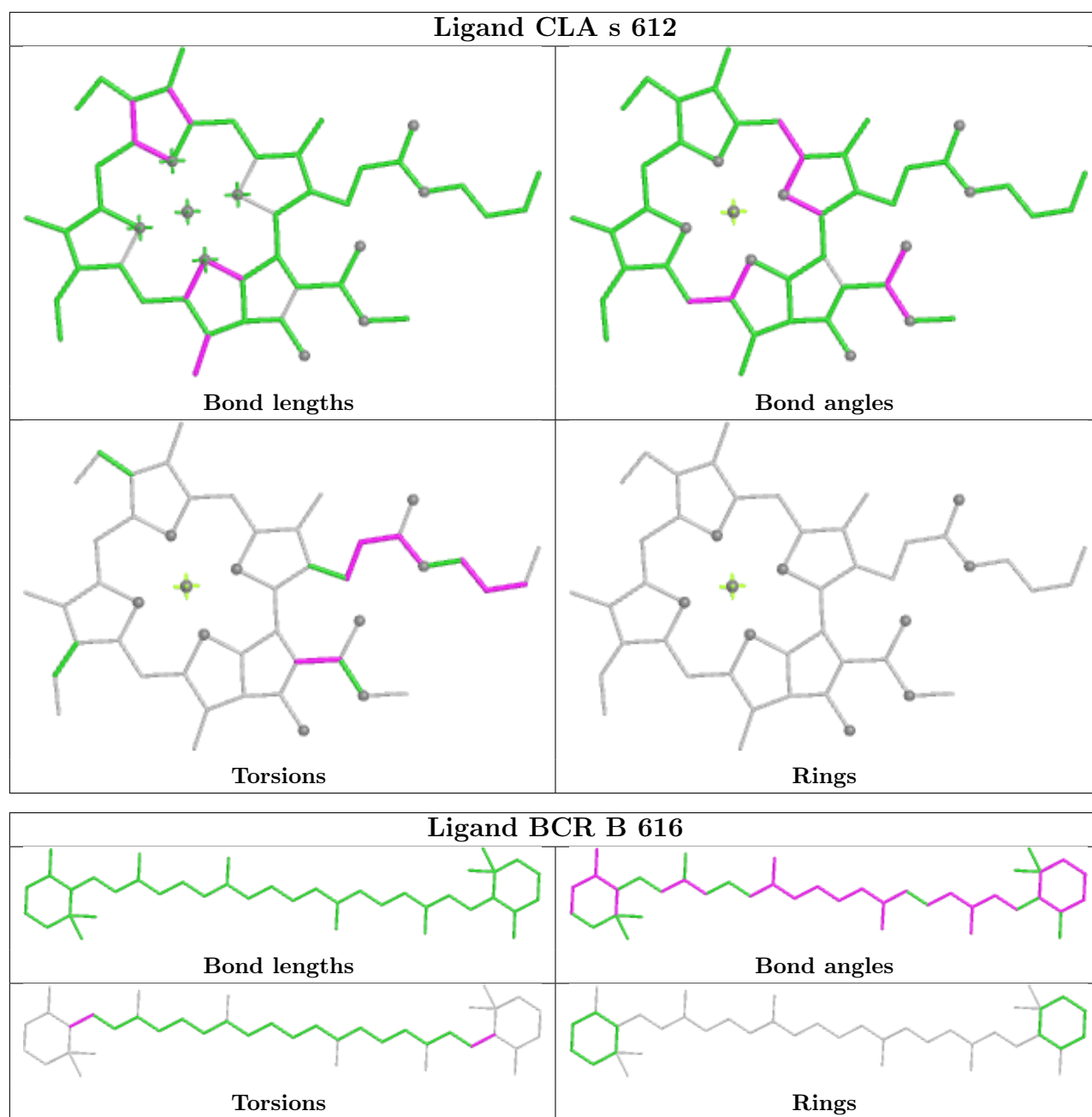
Ligand CLA y 316

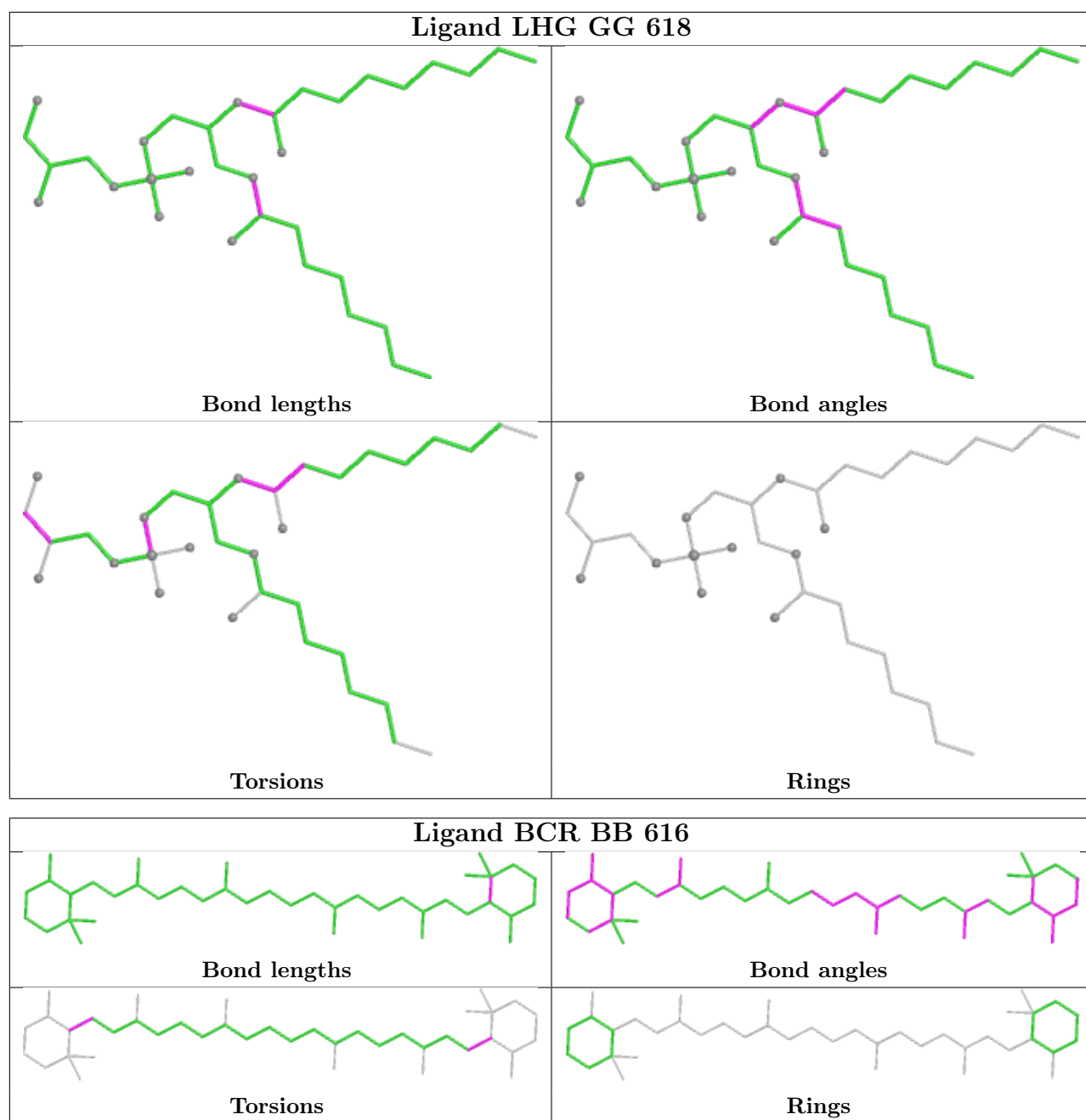


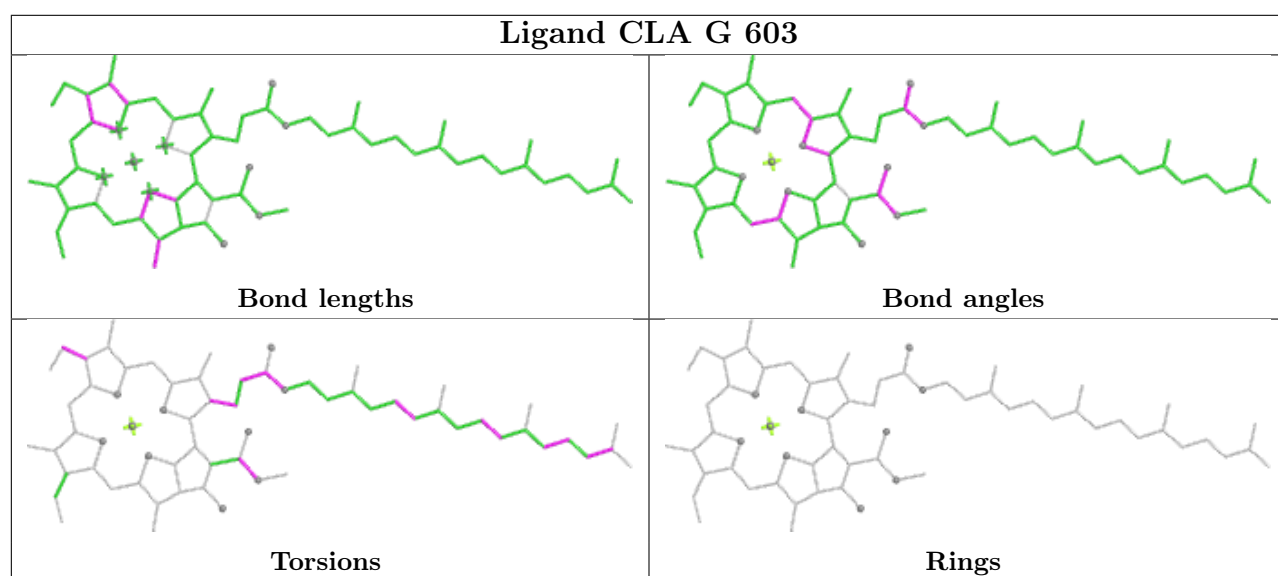
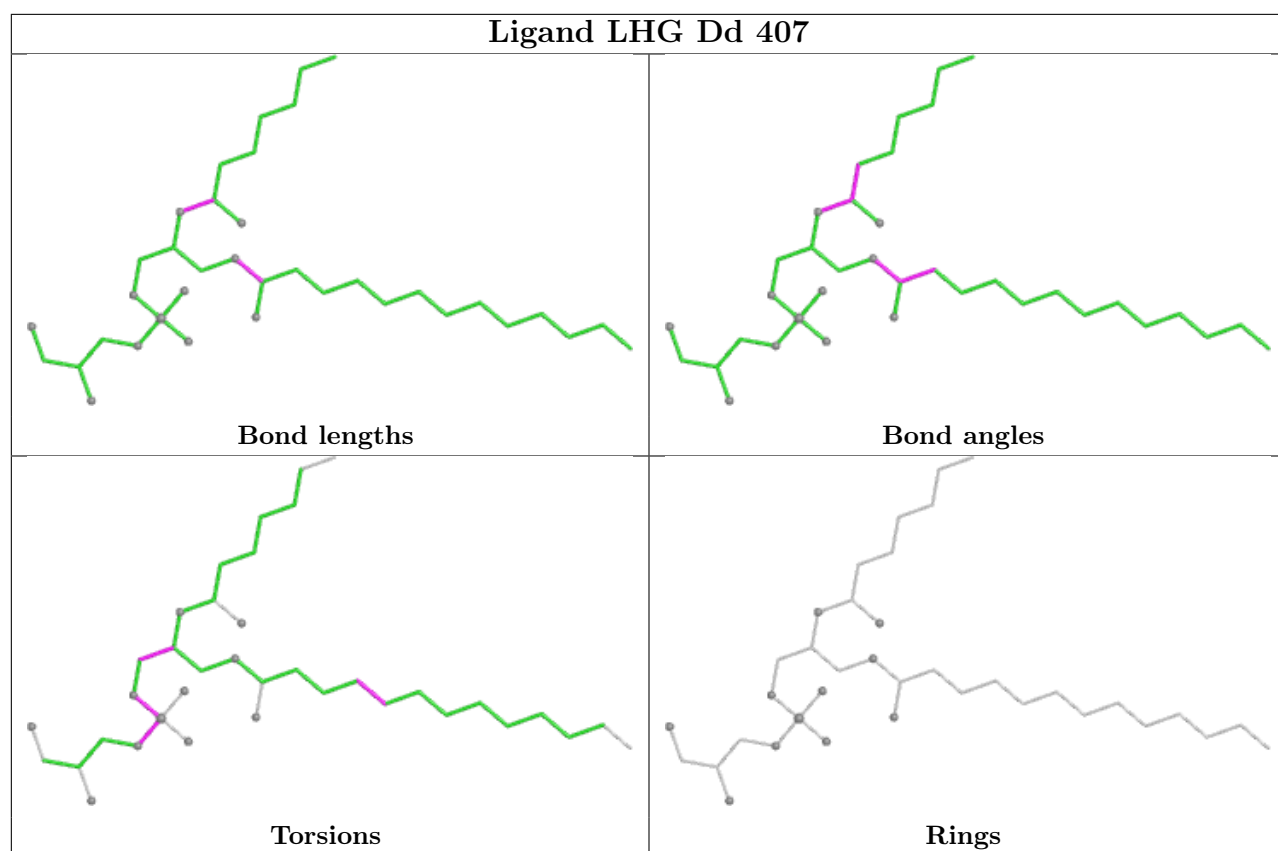
Ligand CLA BB 612

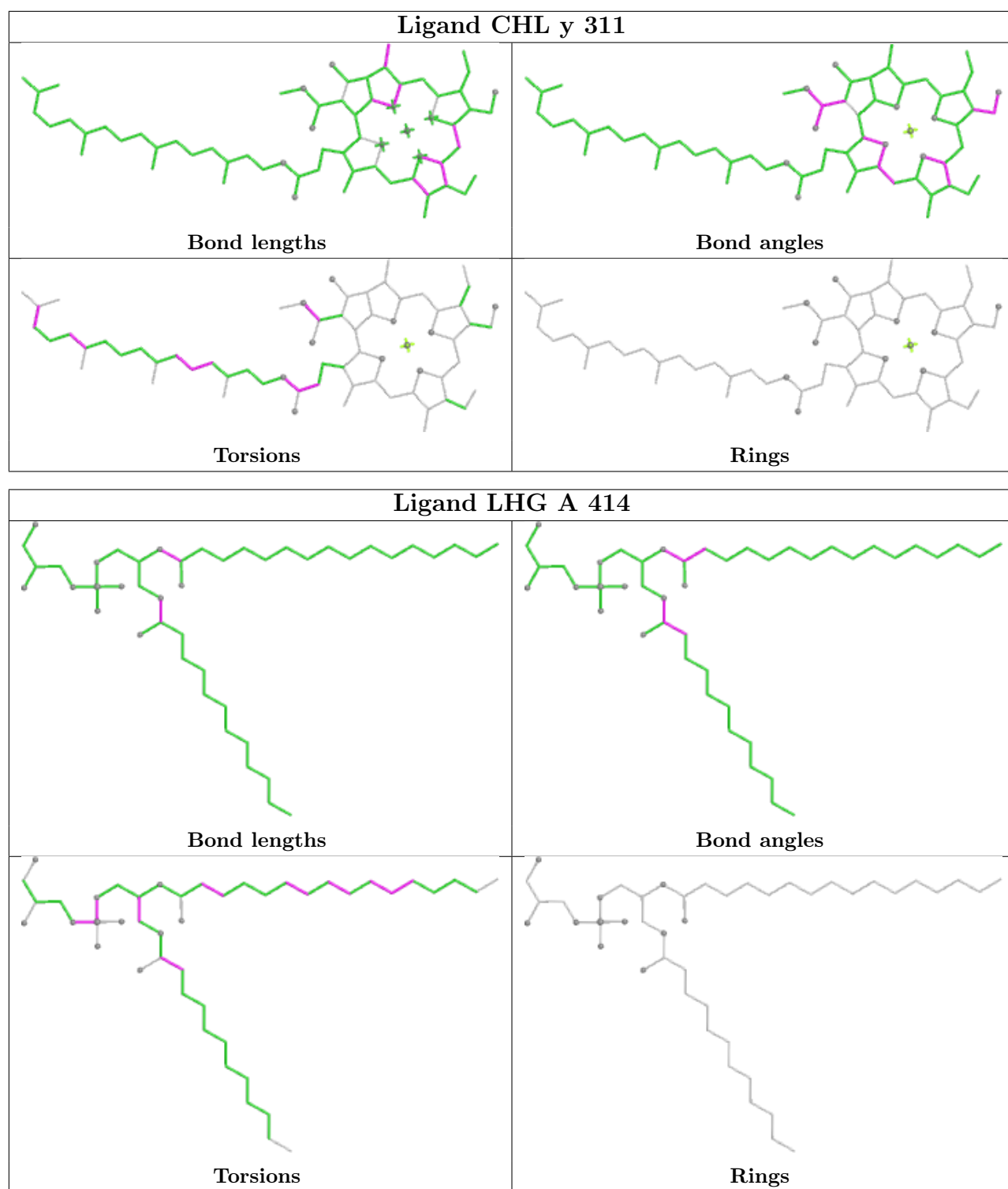


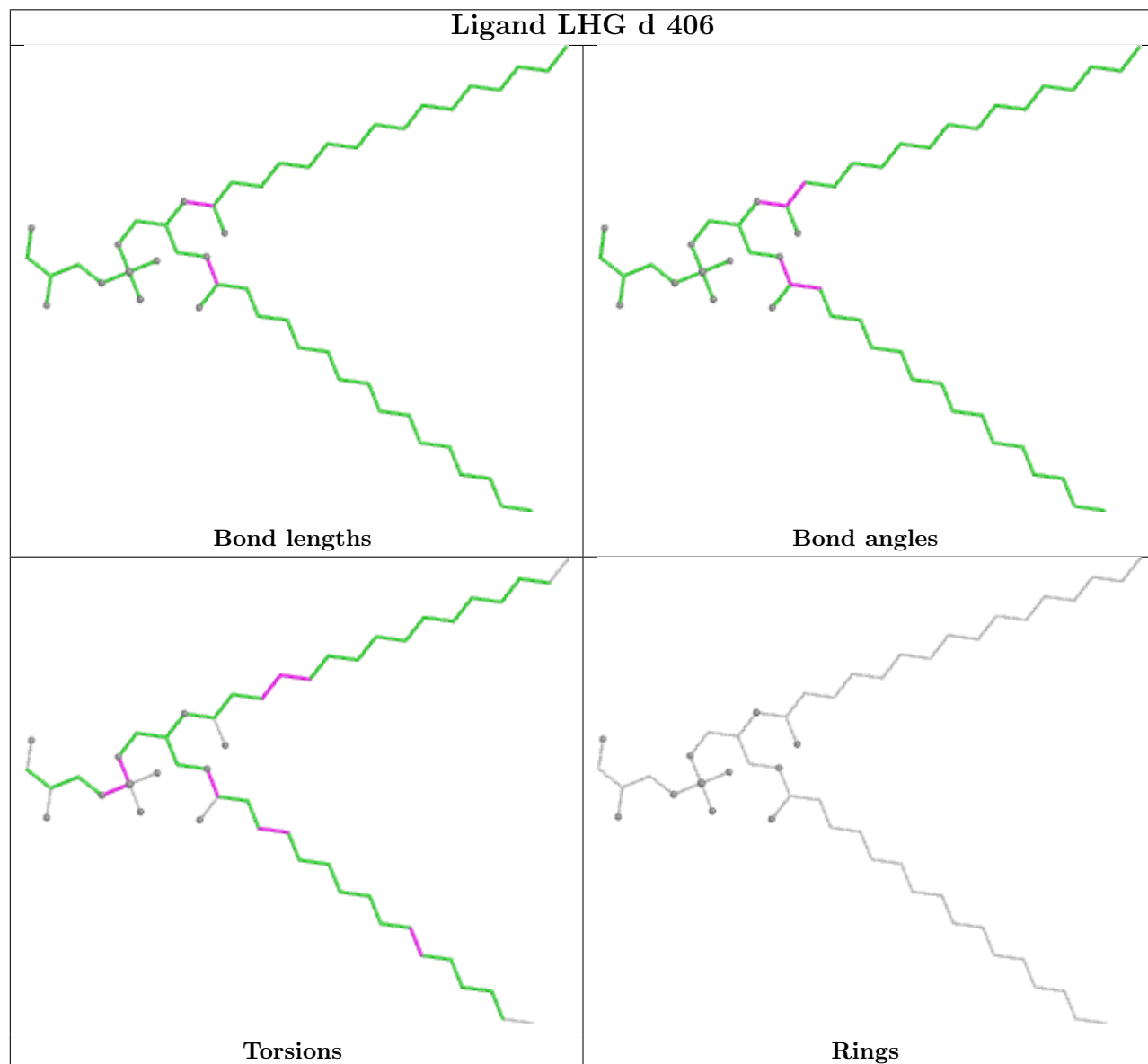
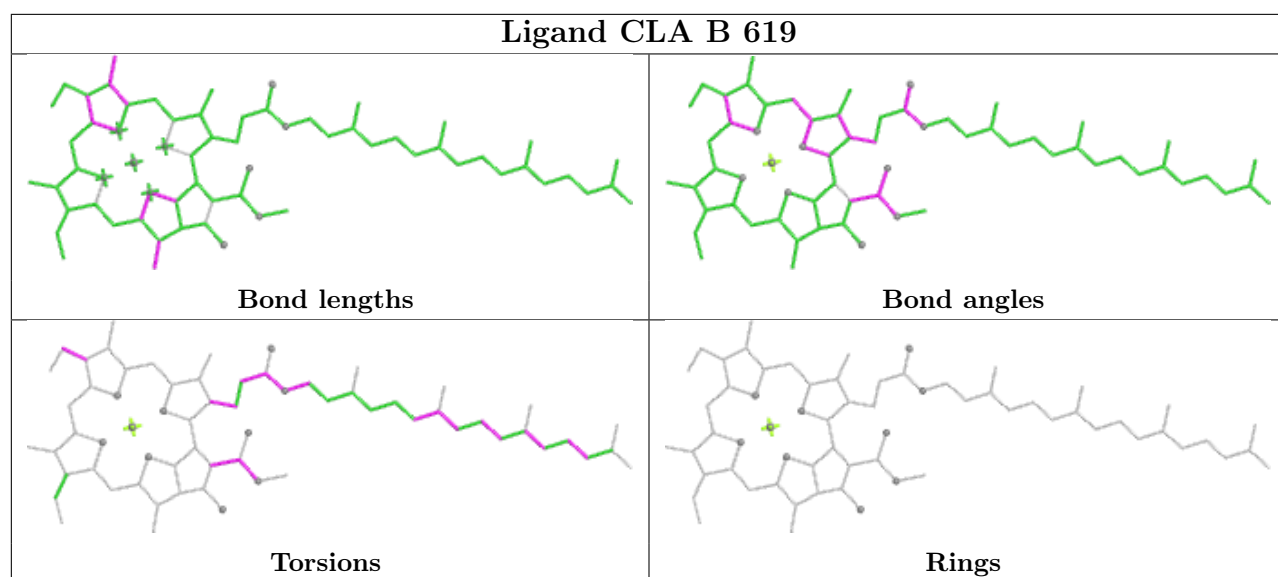


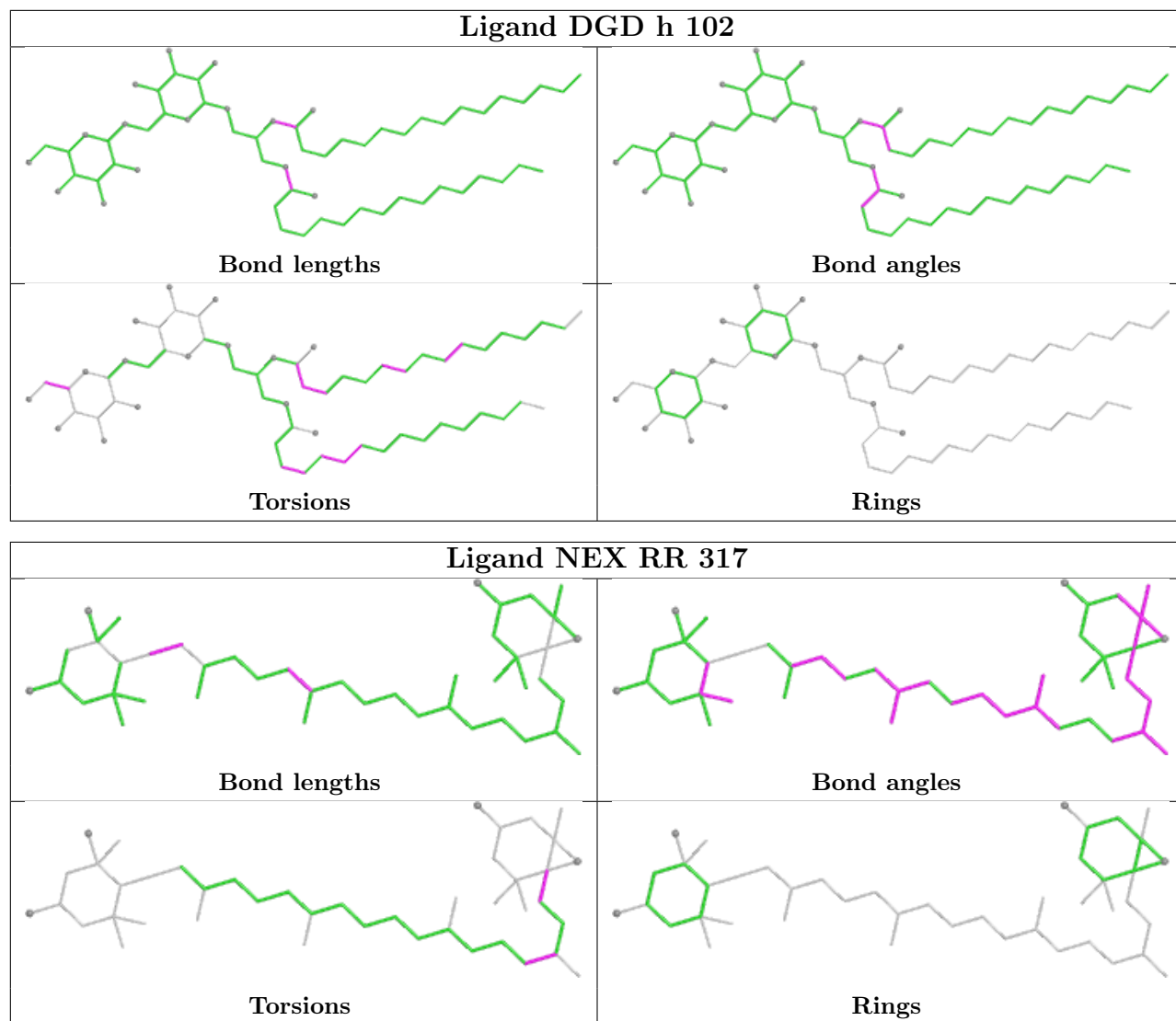


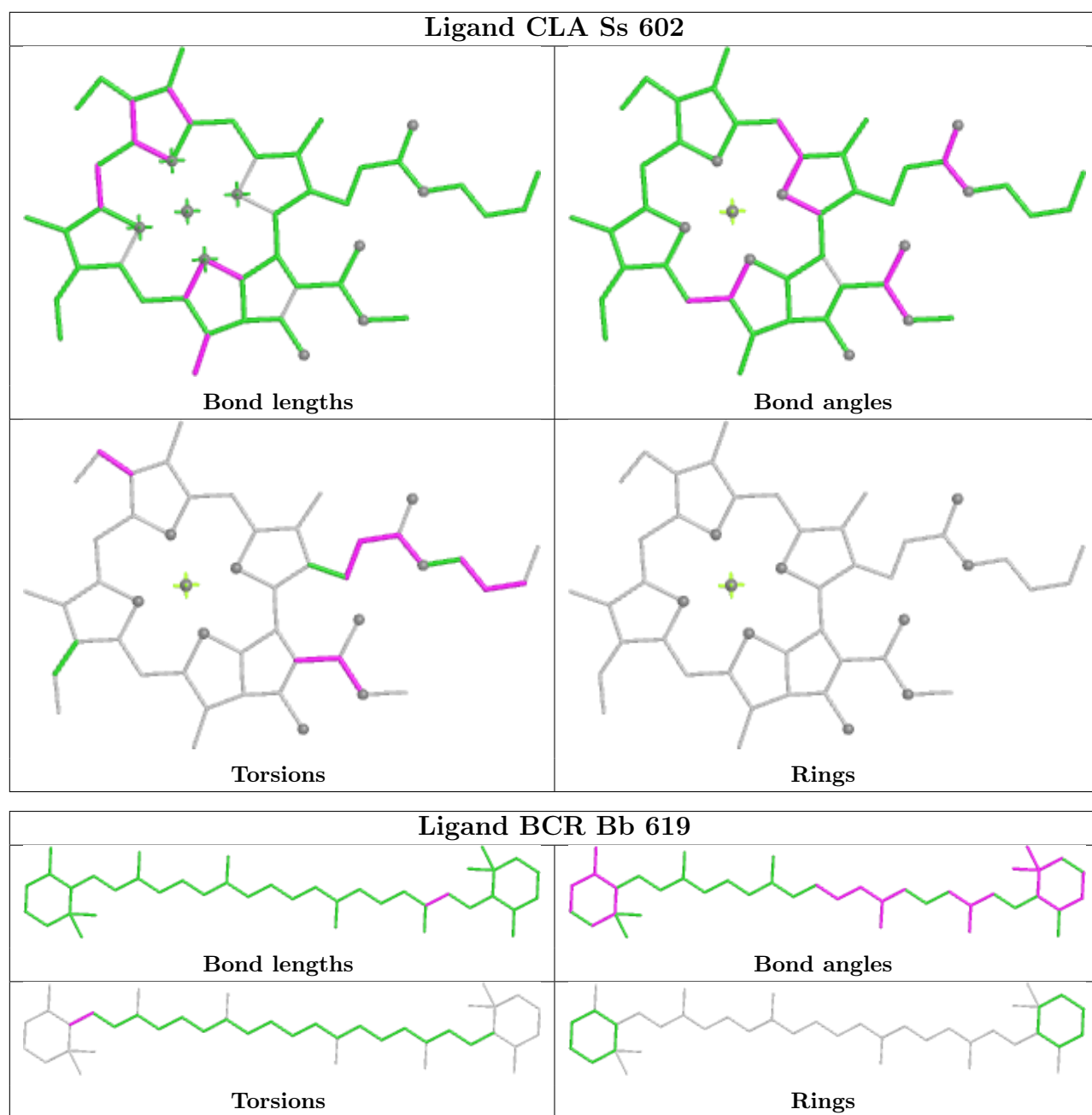


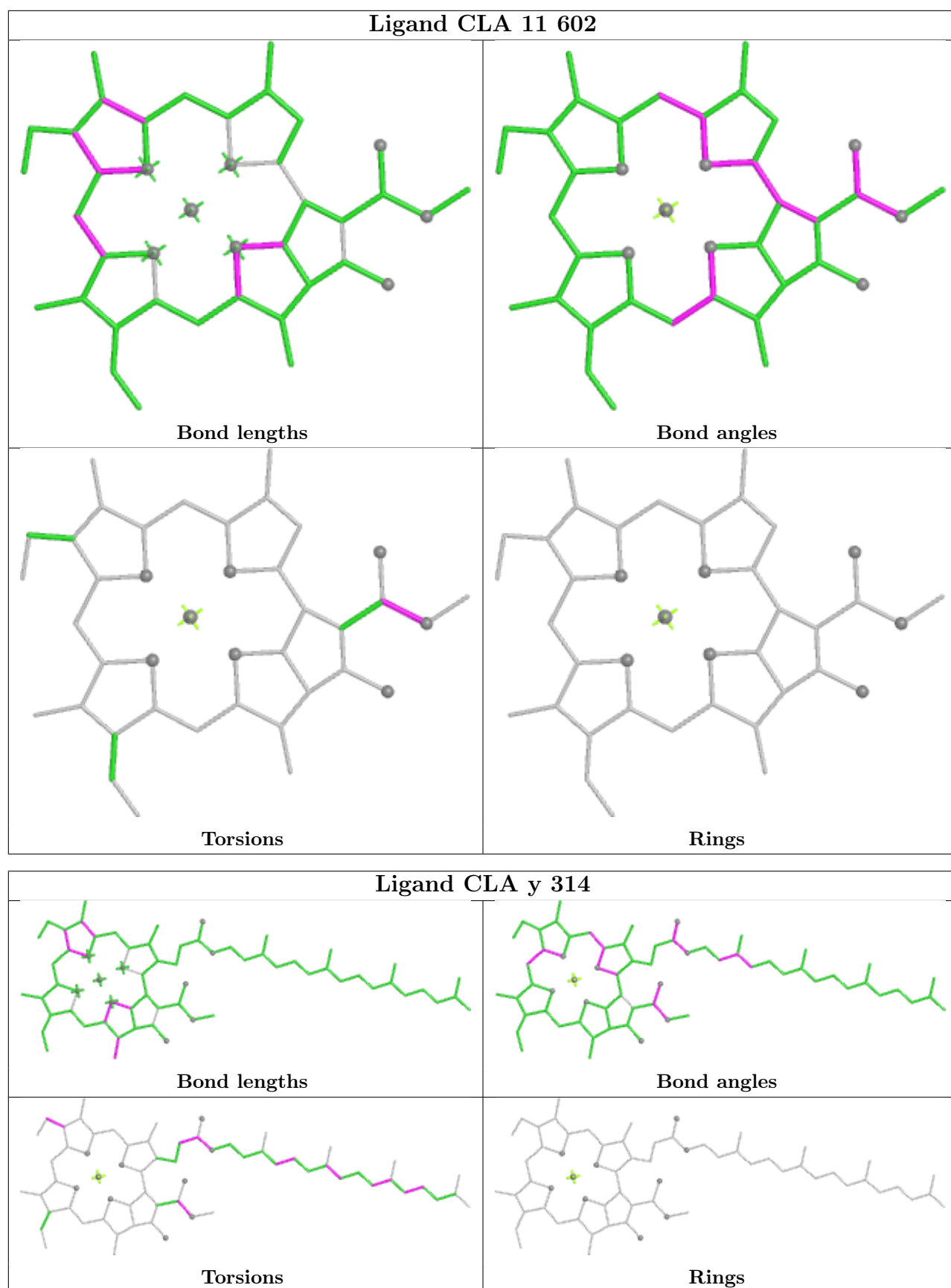


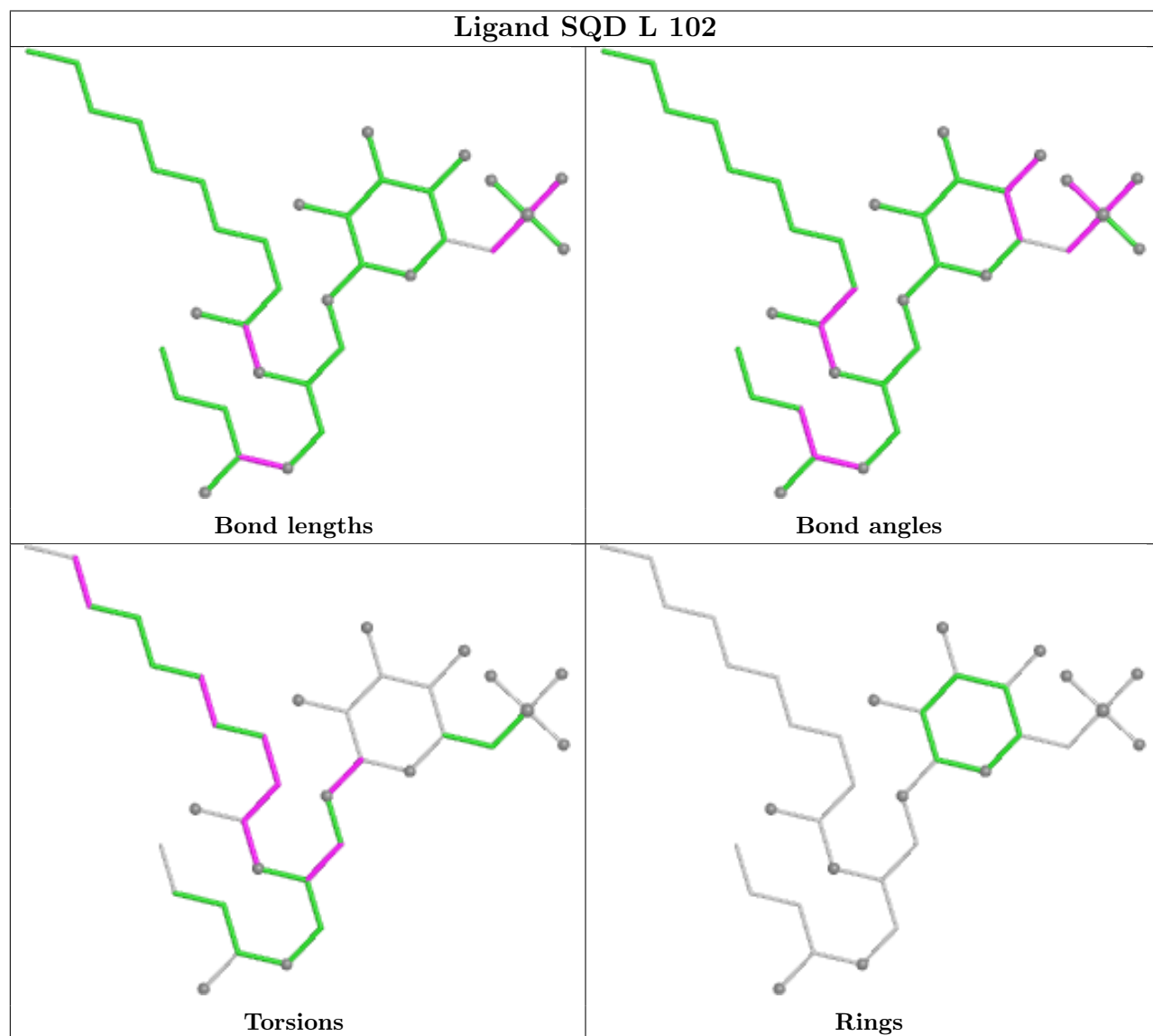
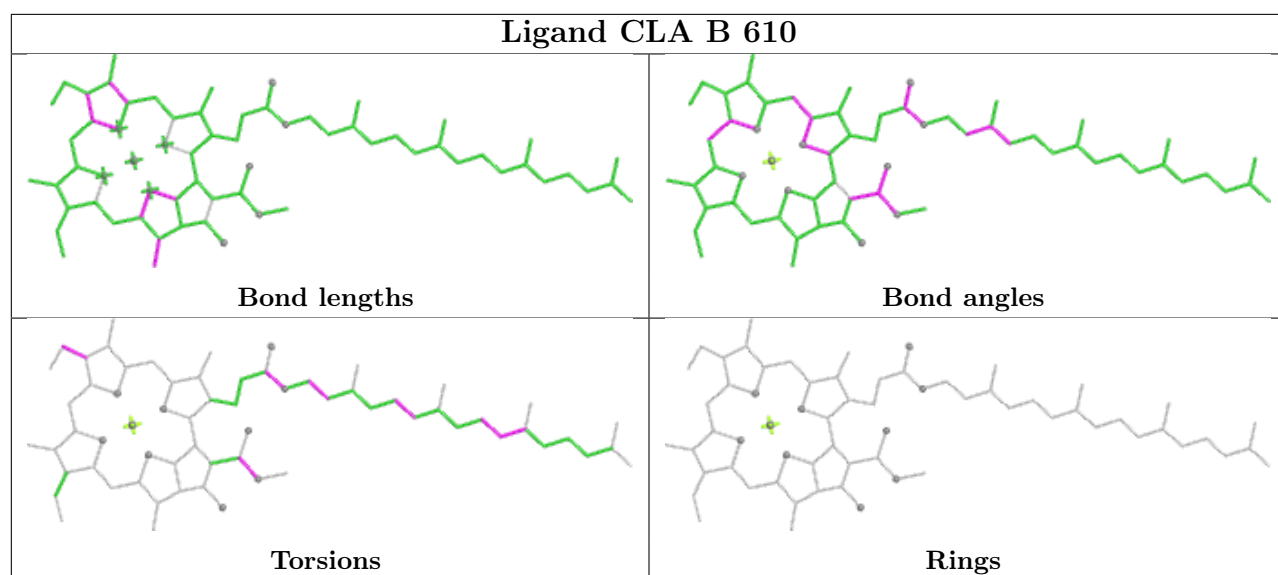


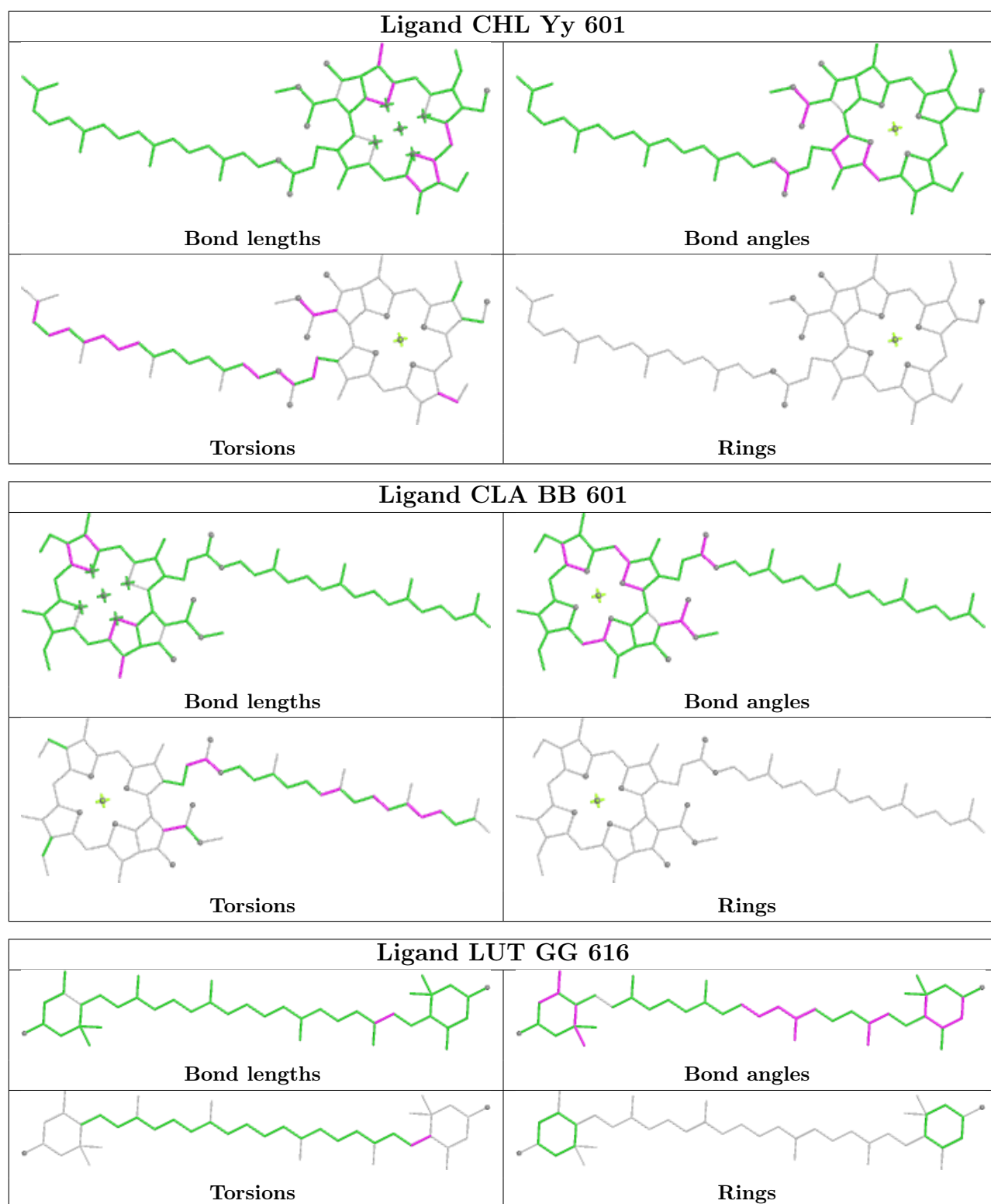




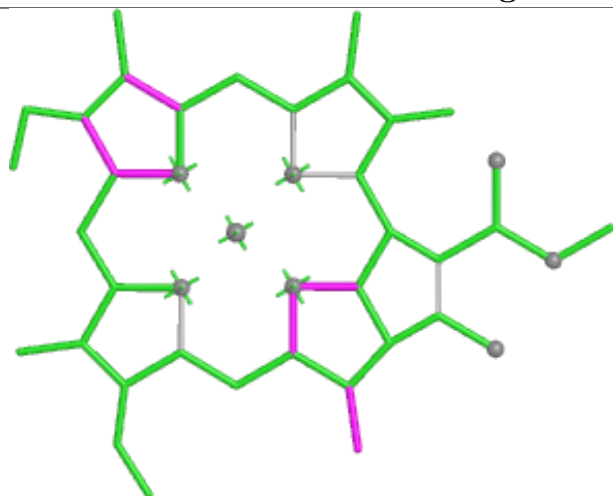








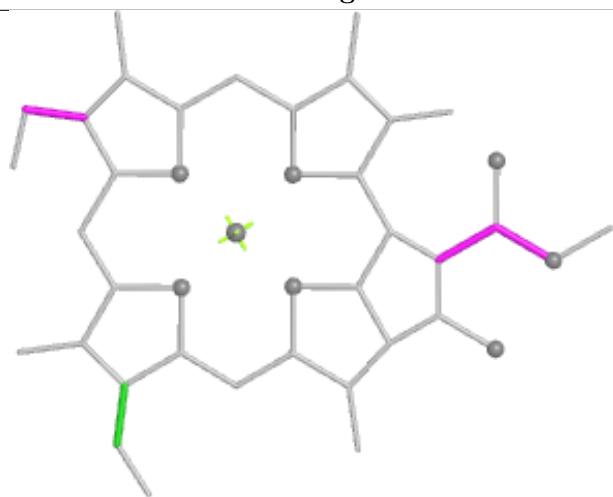
Ligand CLA GG 614



Bond lengths



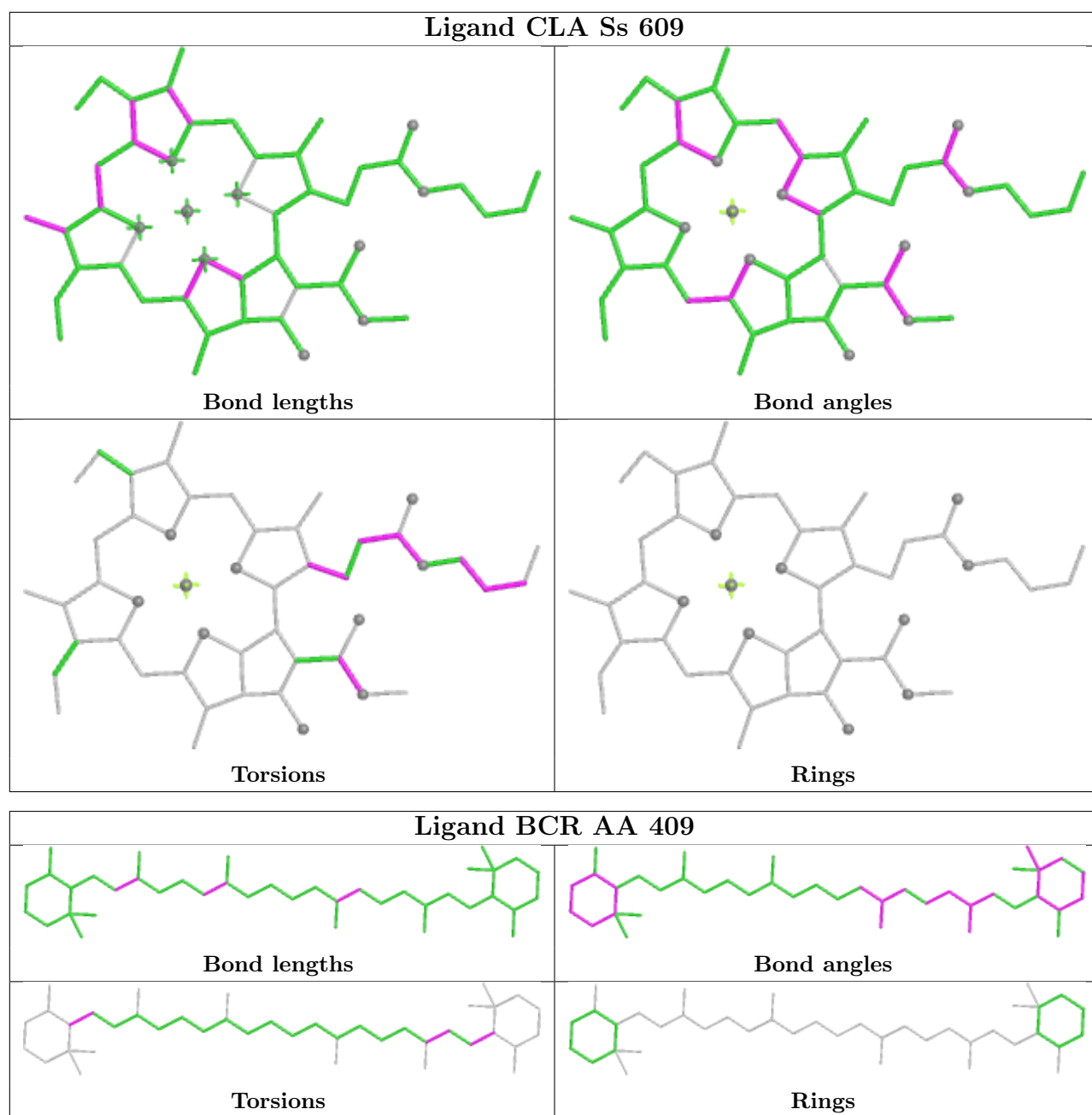
Bond angles

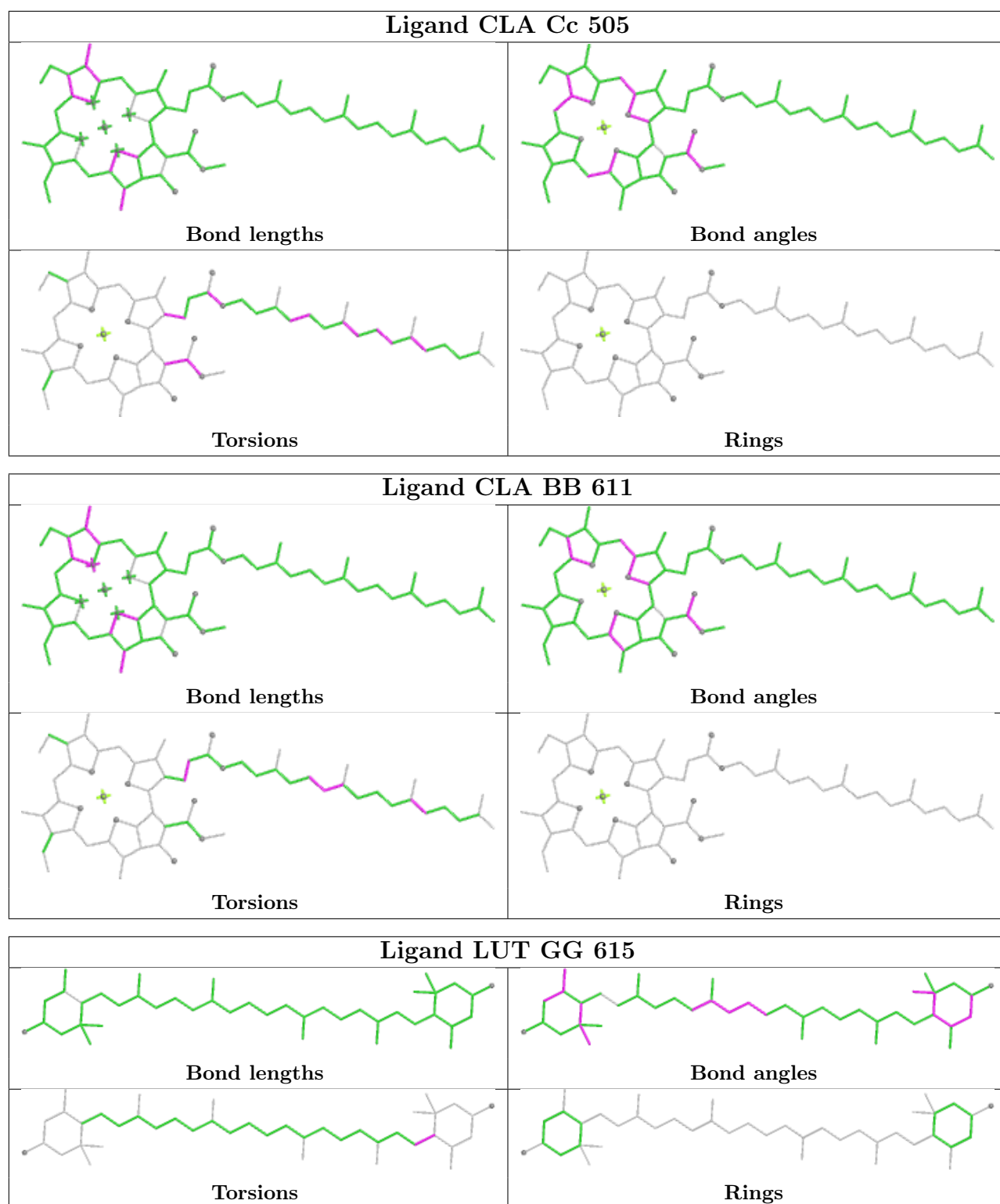


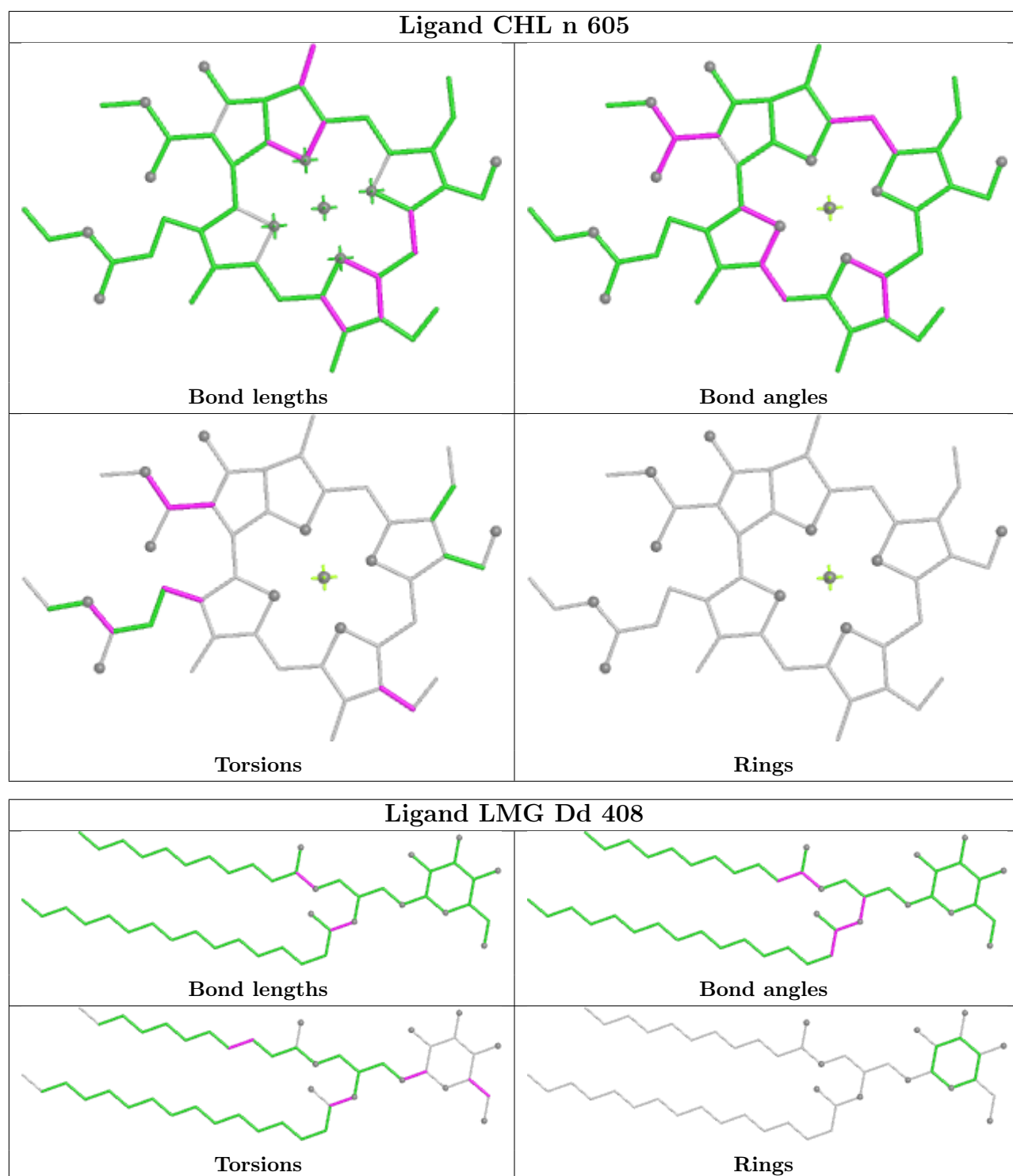
Torsions

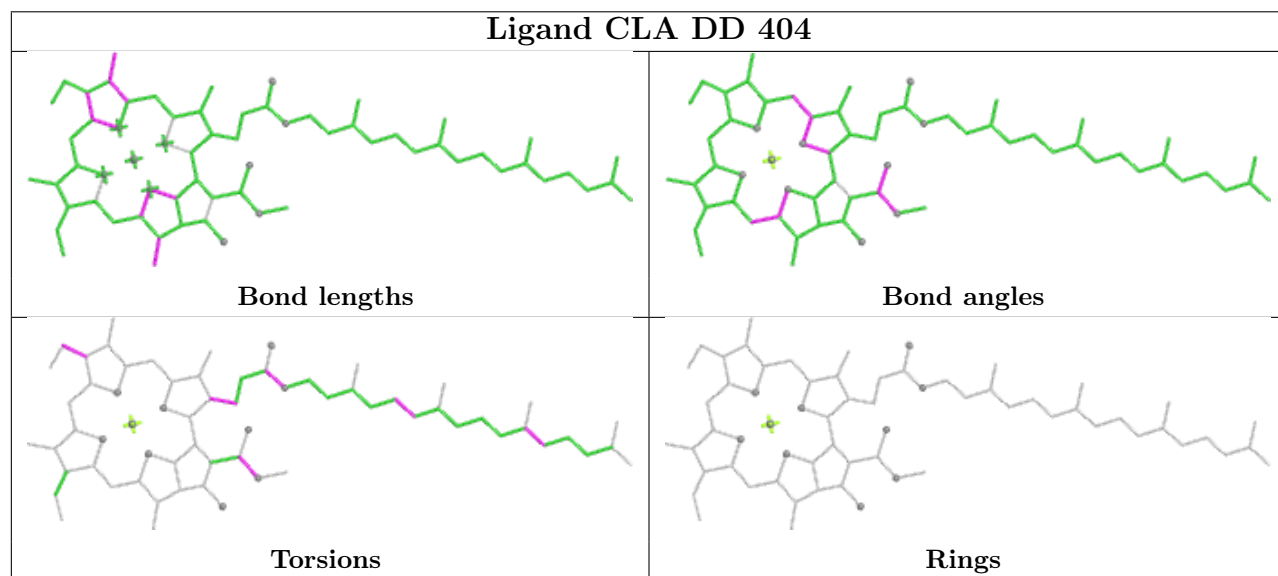
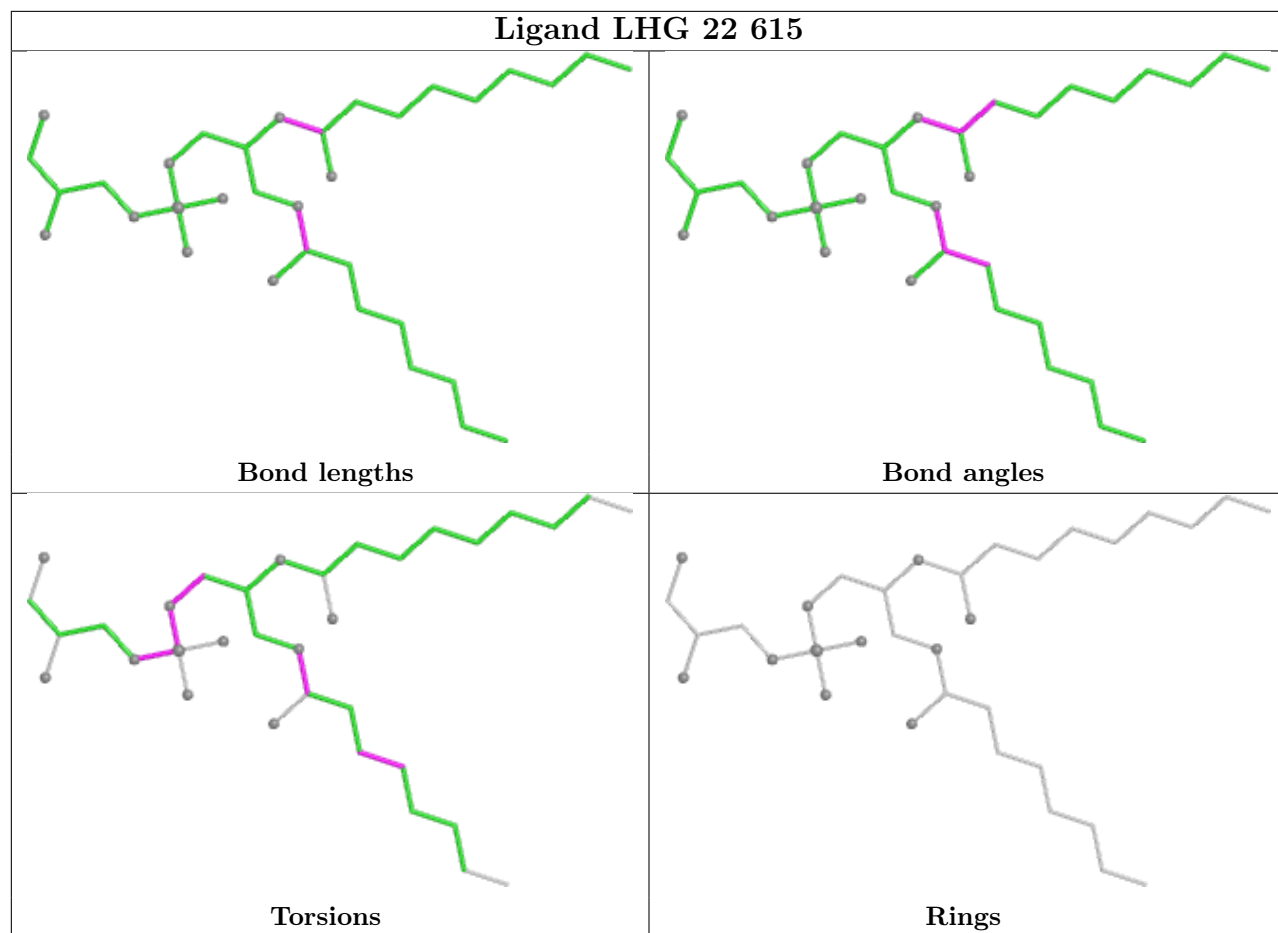


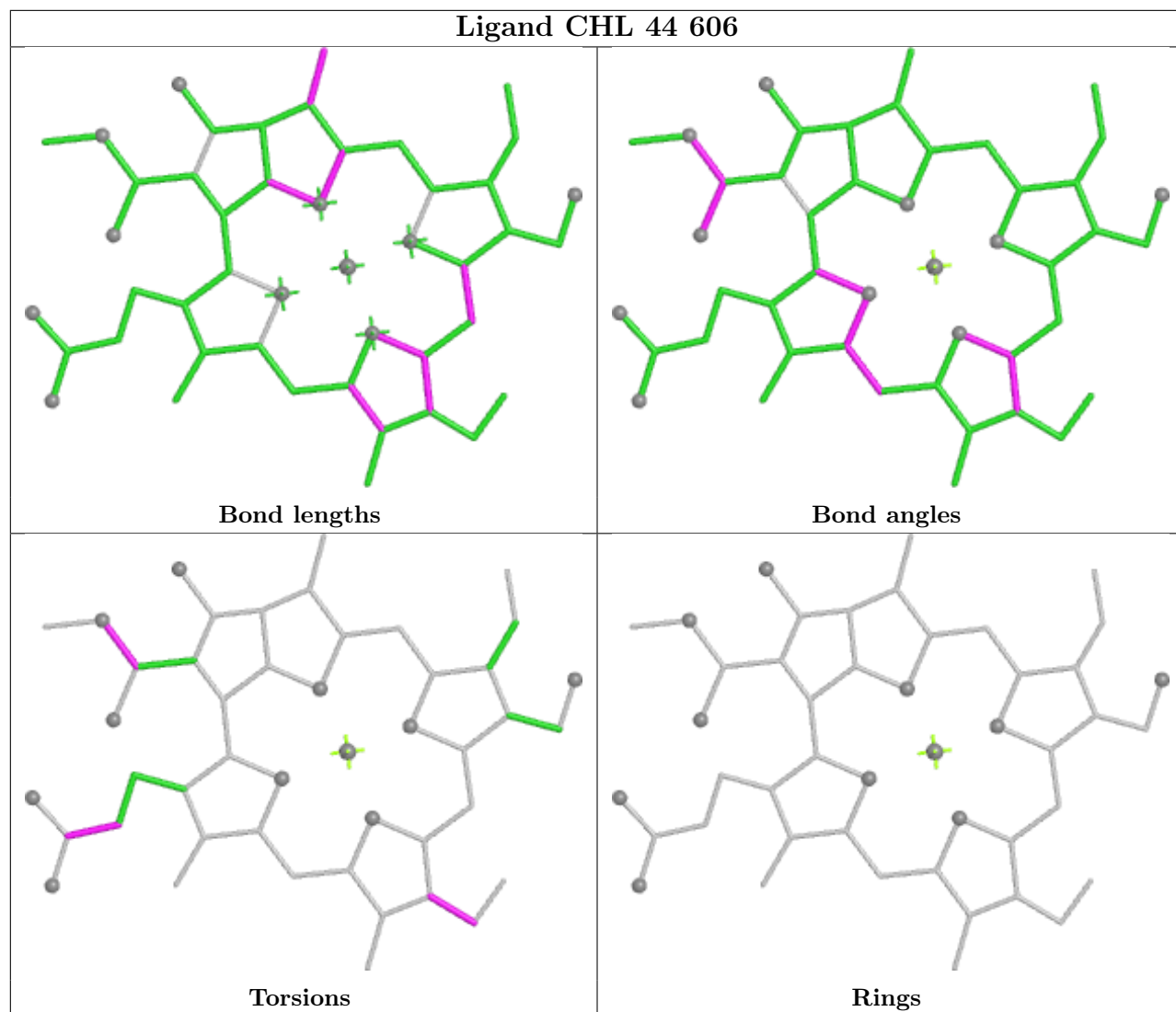
Rings

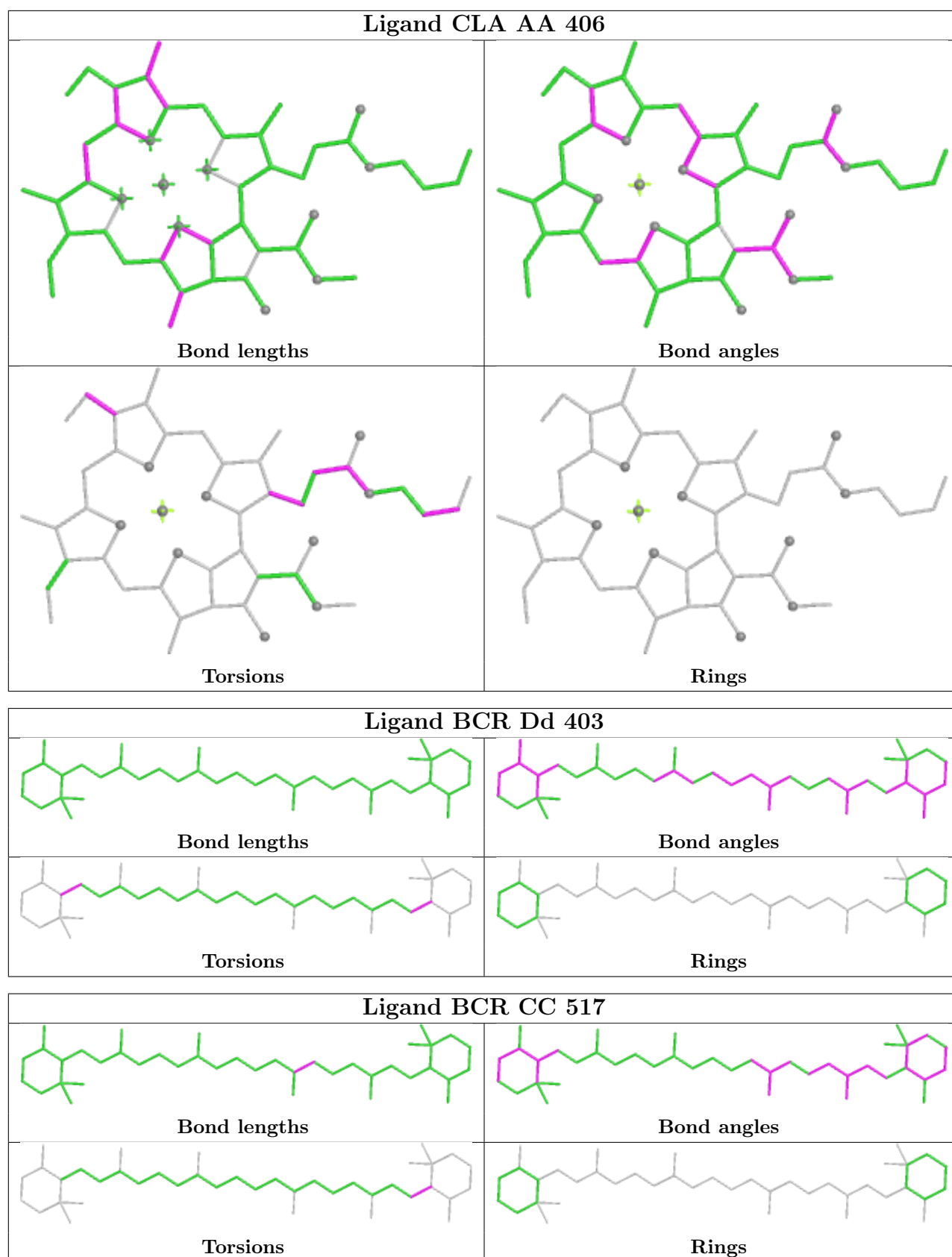


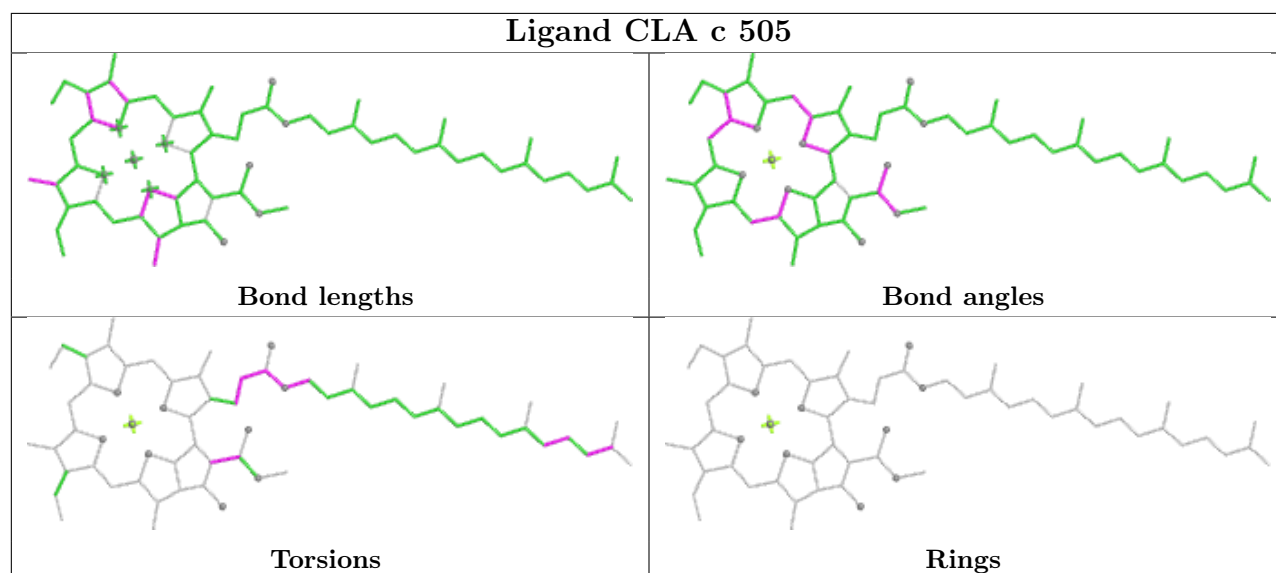
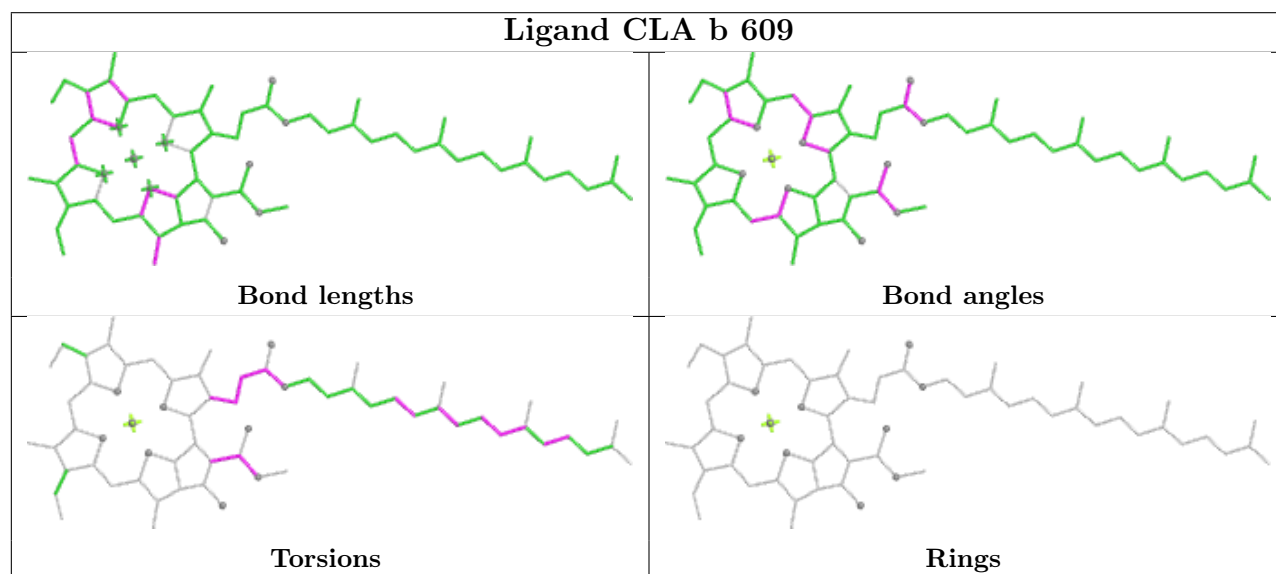
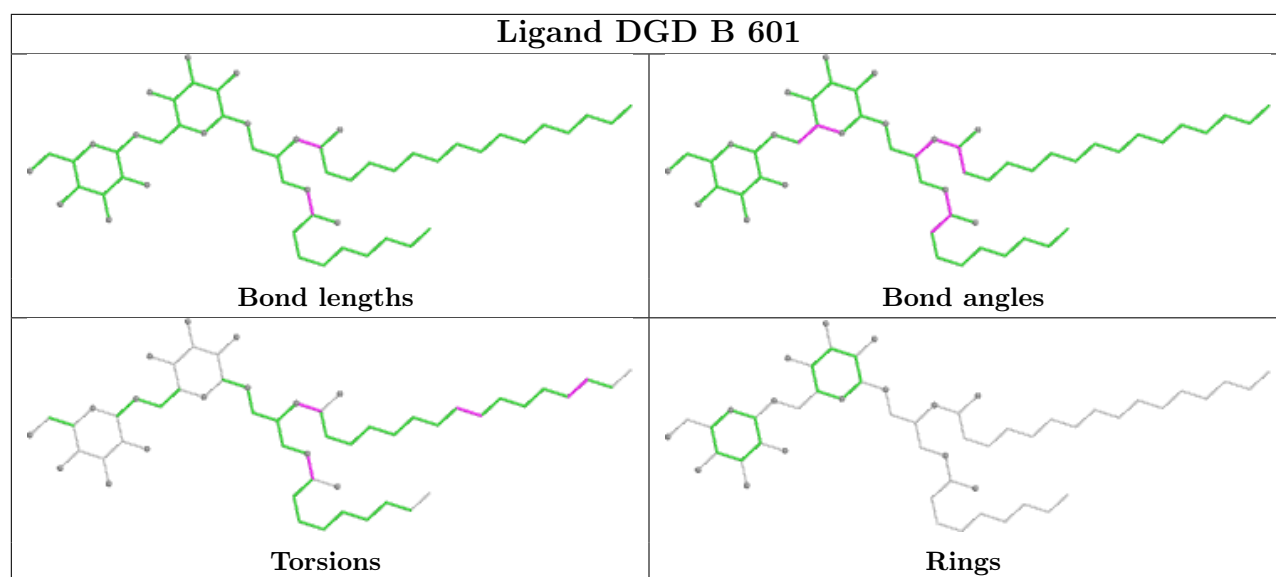


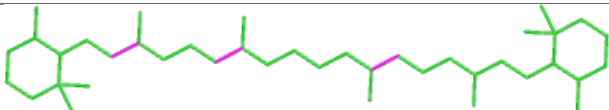
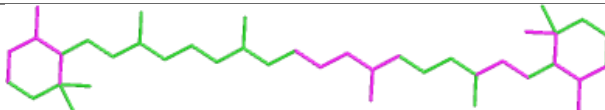
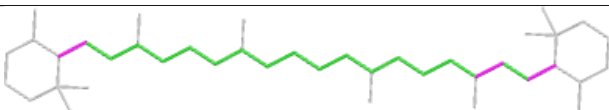
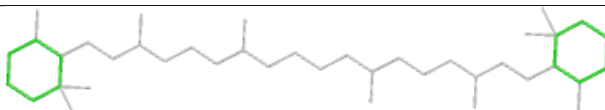


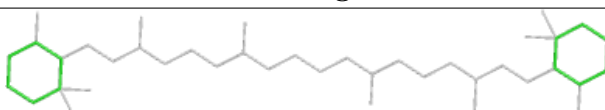


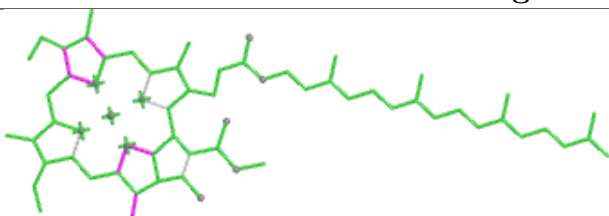
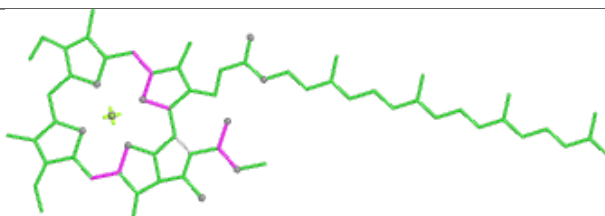
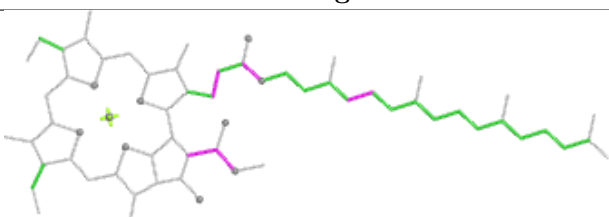
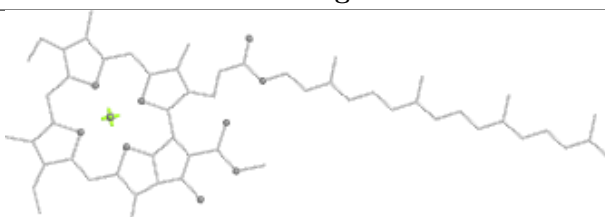


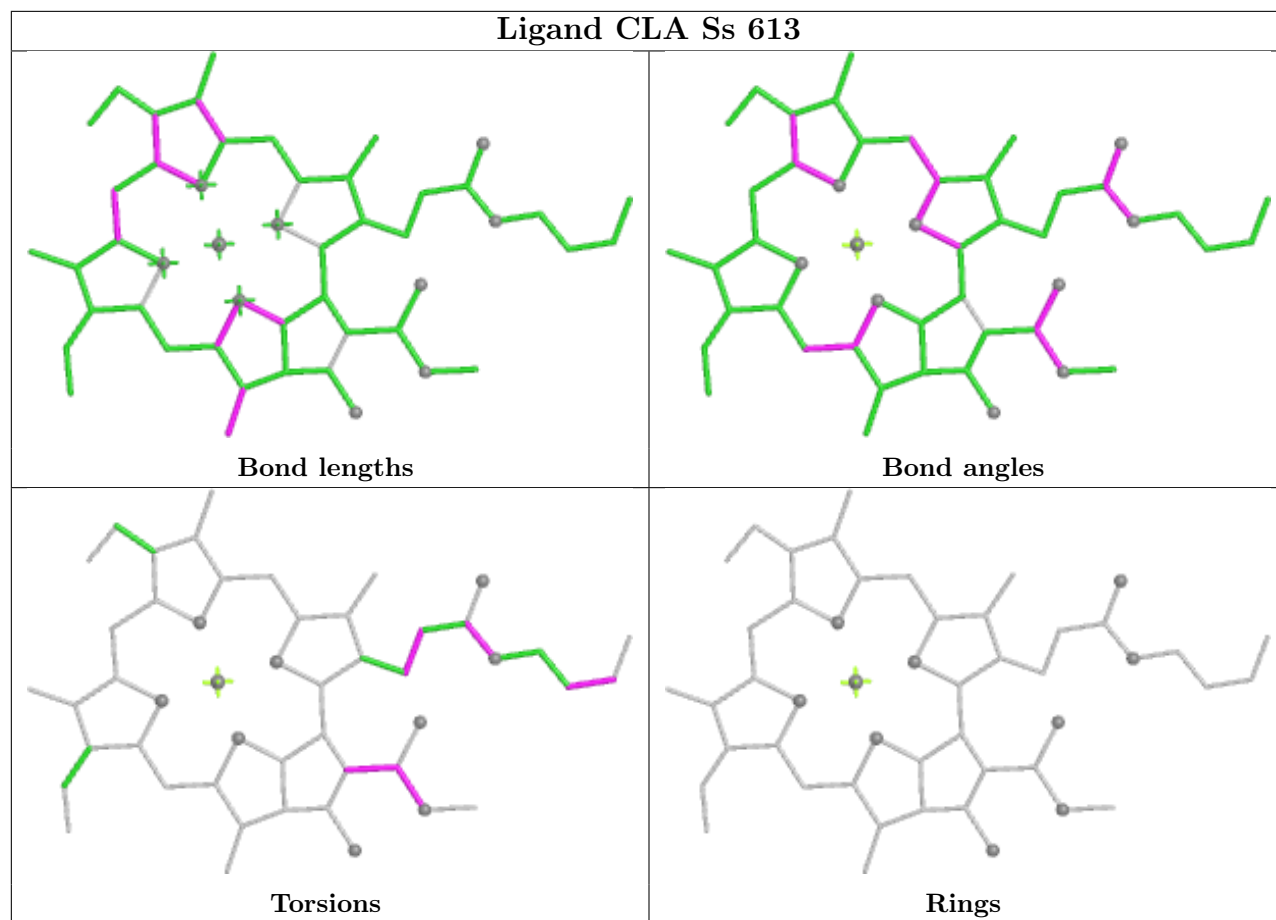




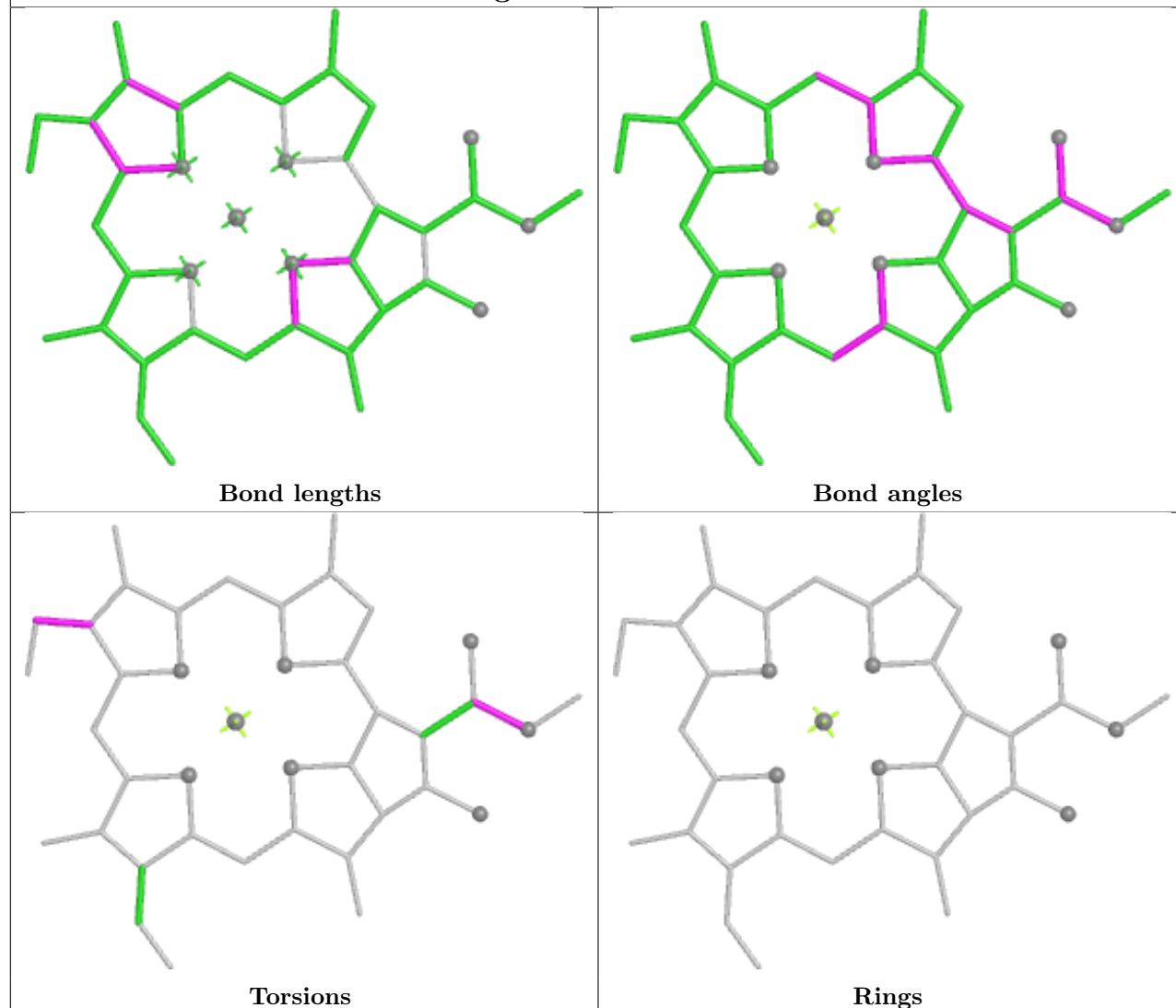
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Bb 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

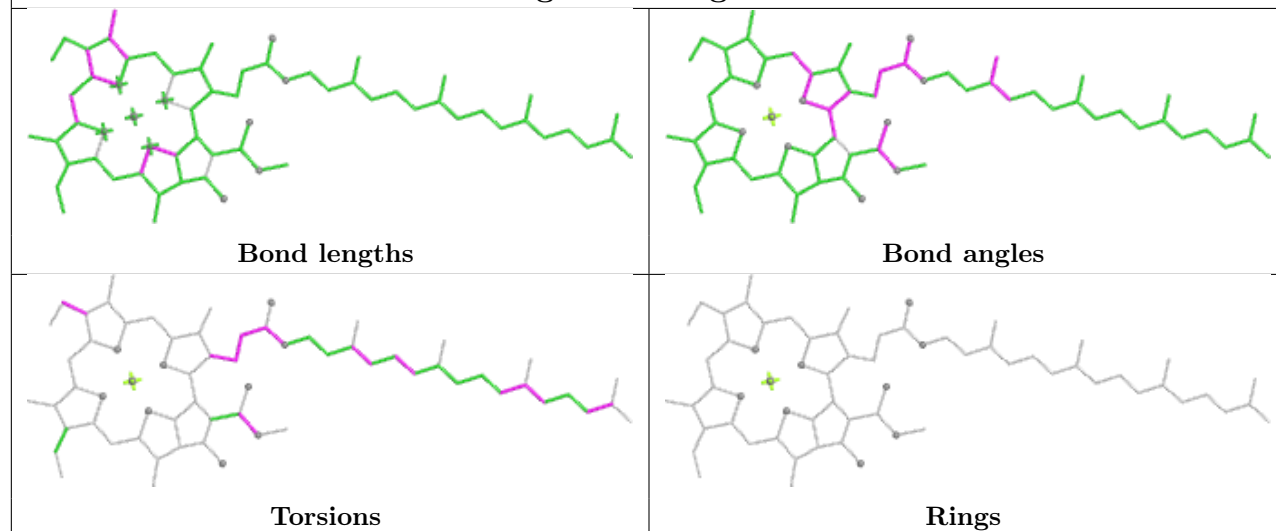
Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

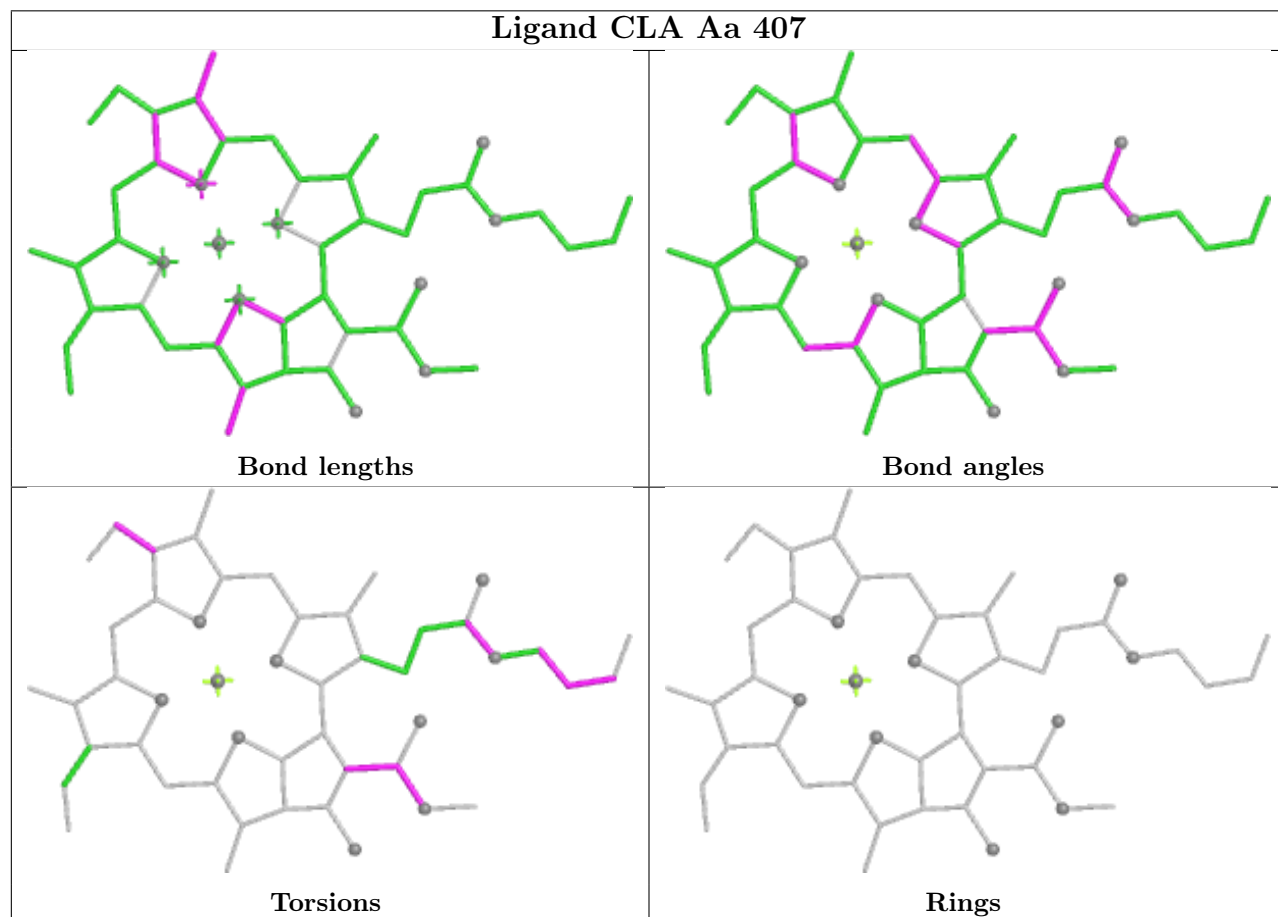
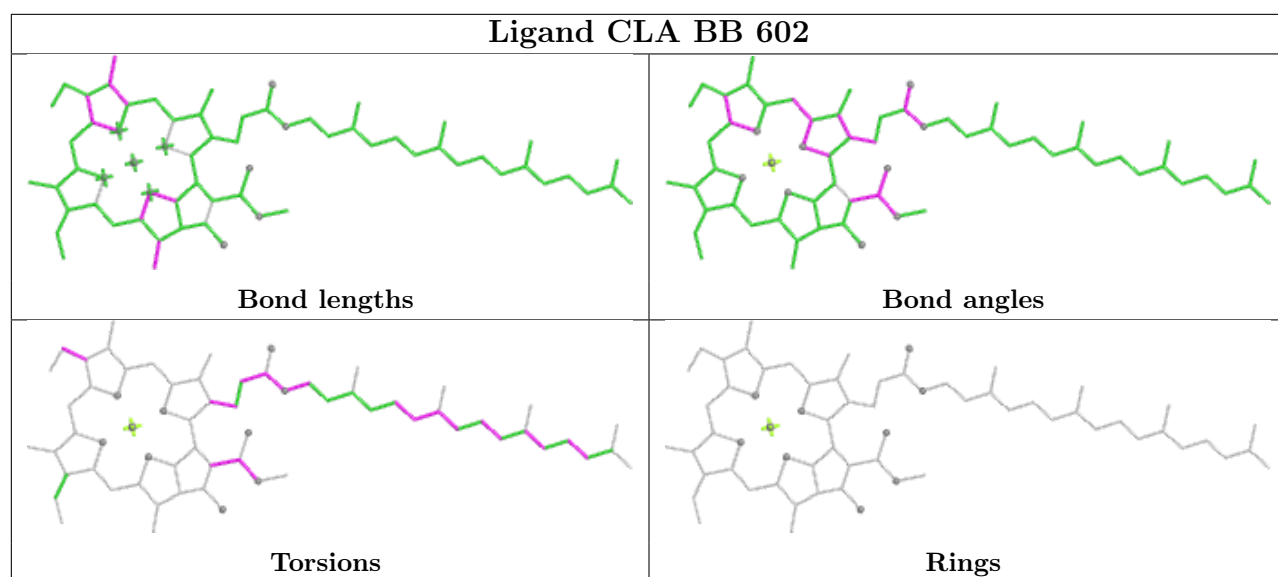


Ligand CLA 3 602

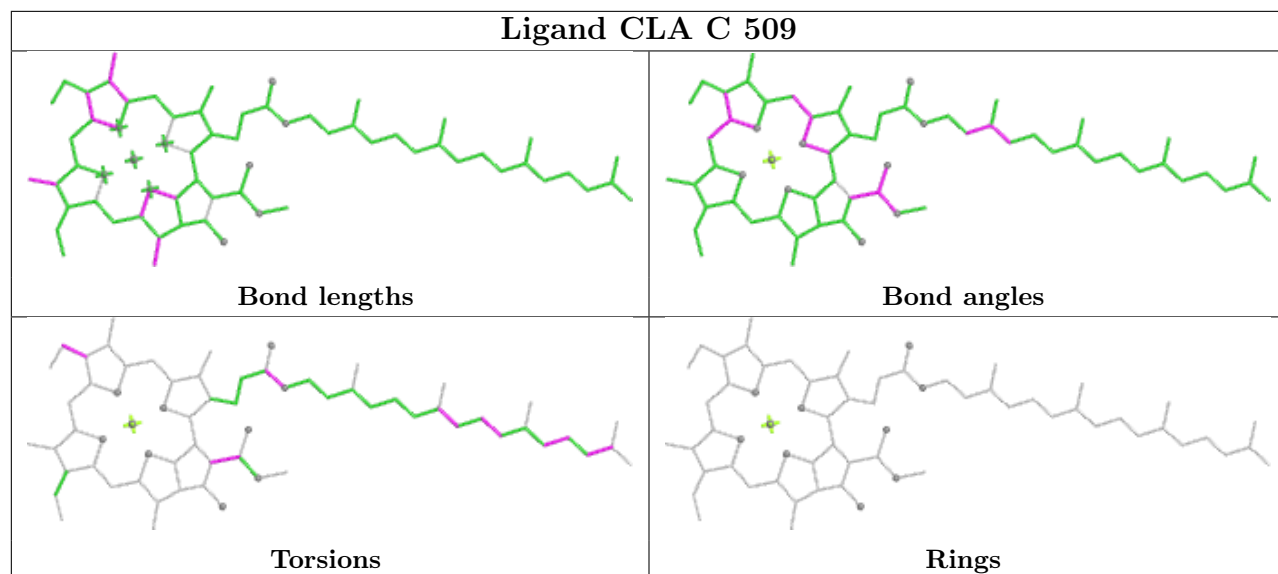


Ligand CLA g 611

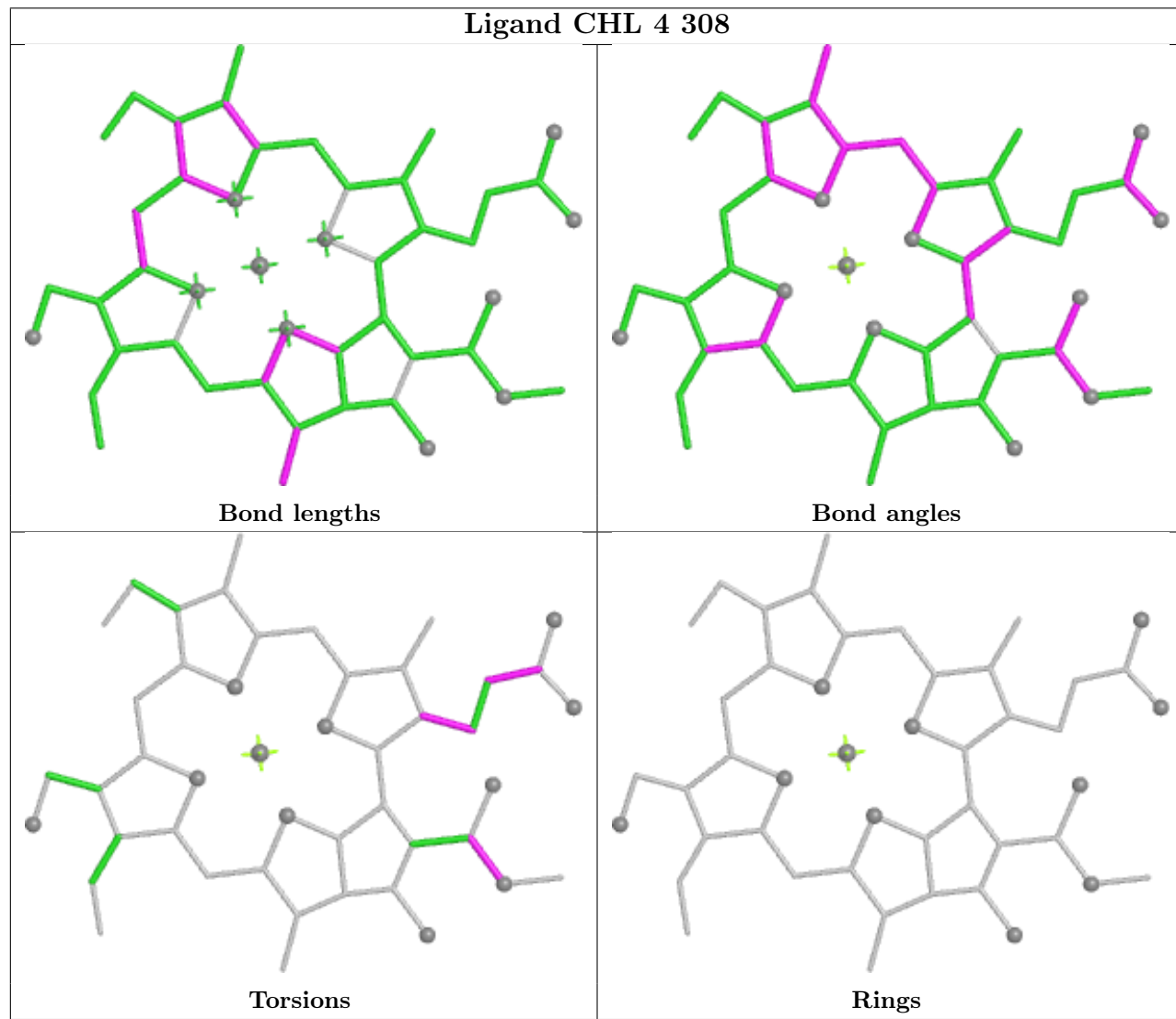


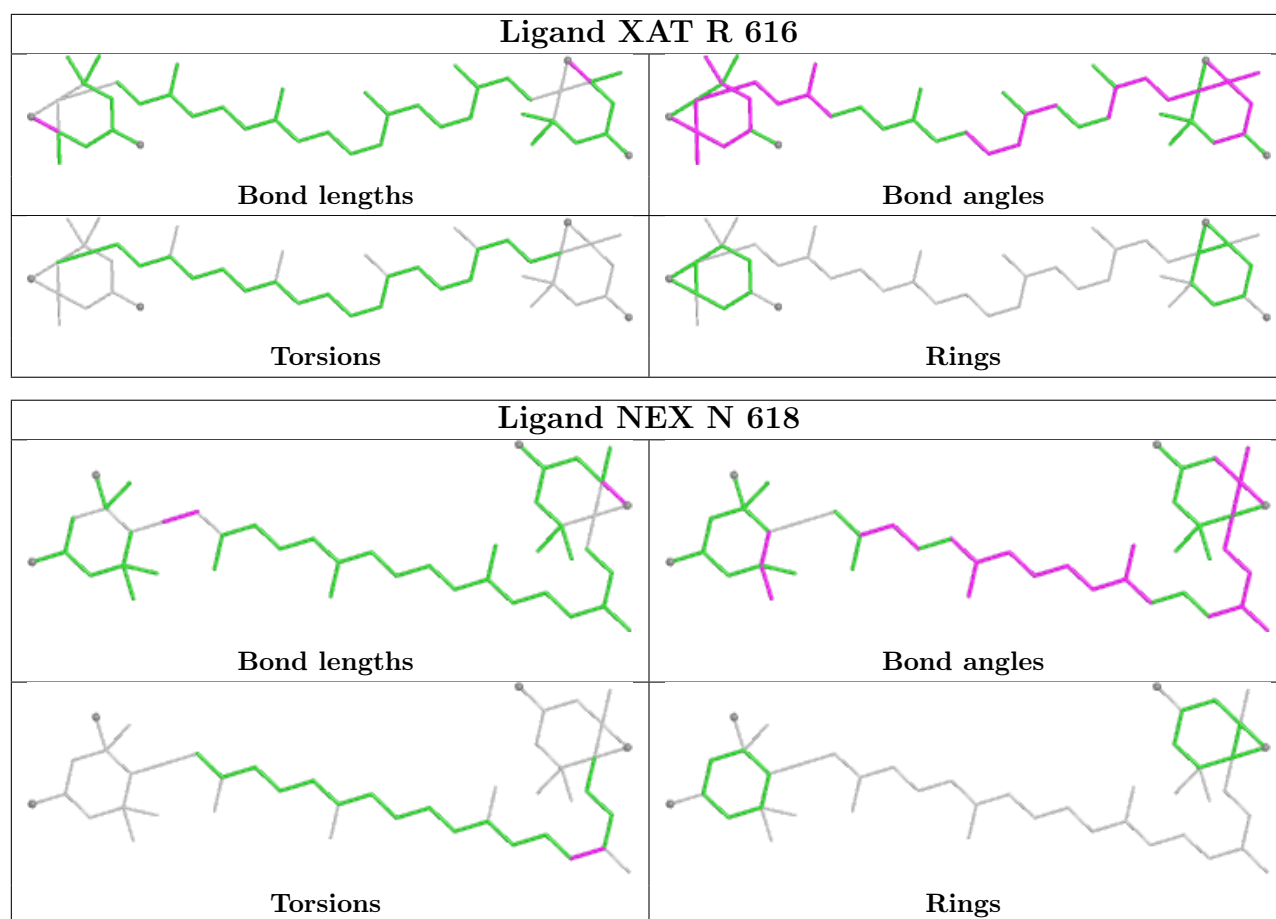


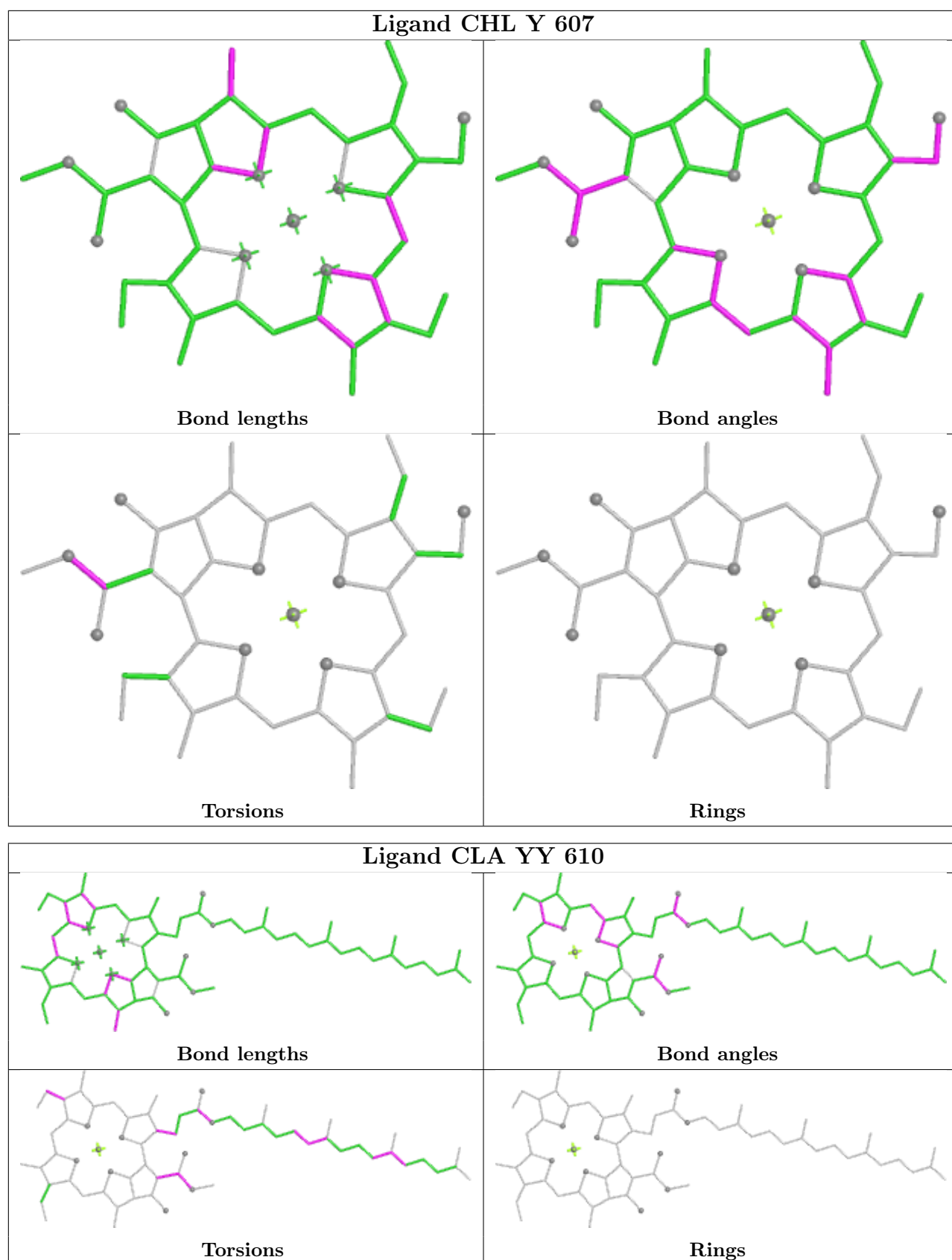
Ligand CLA C 509

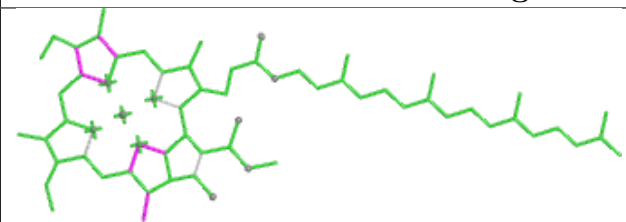
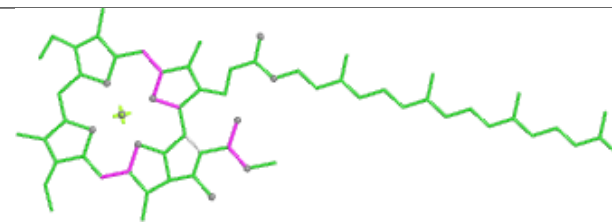
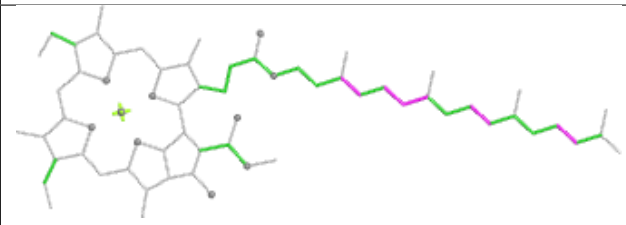
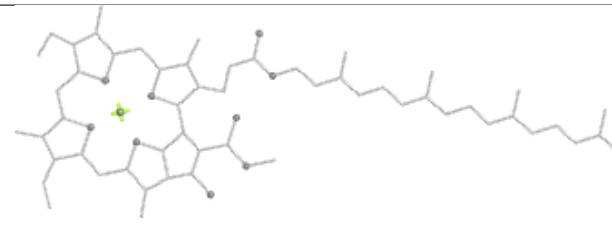


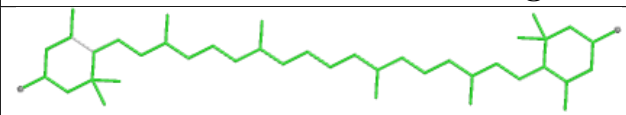
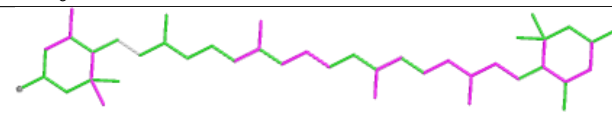
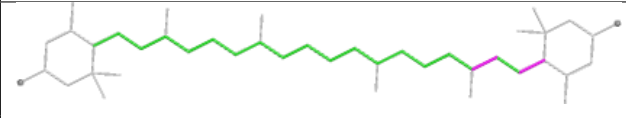
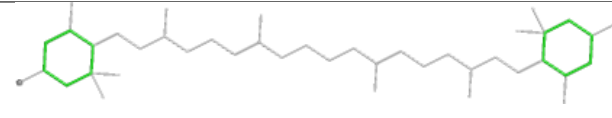
Ligand CHL 4 308

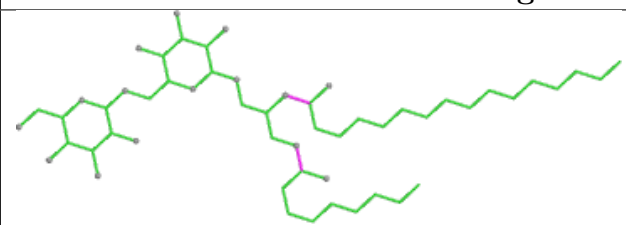
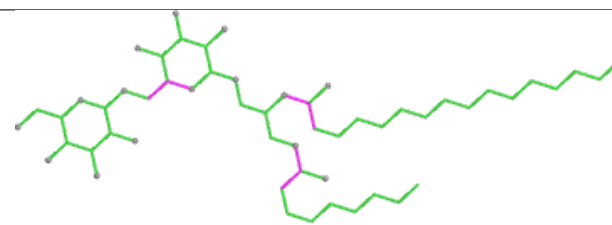
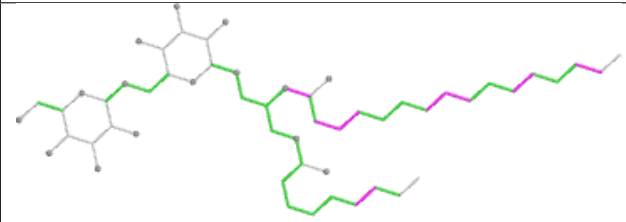
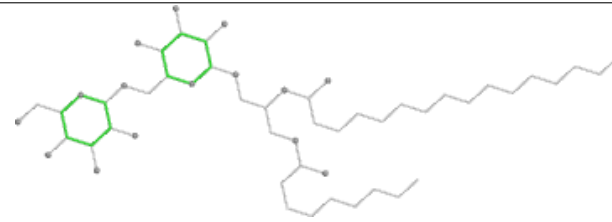


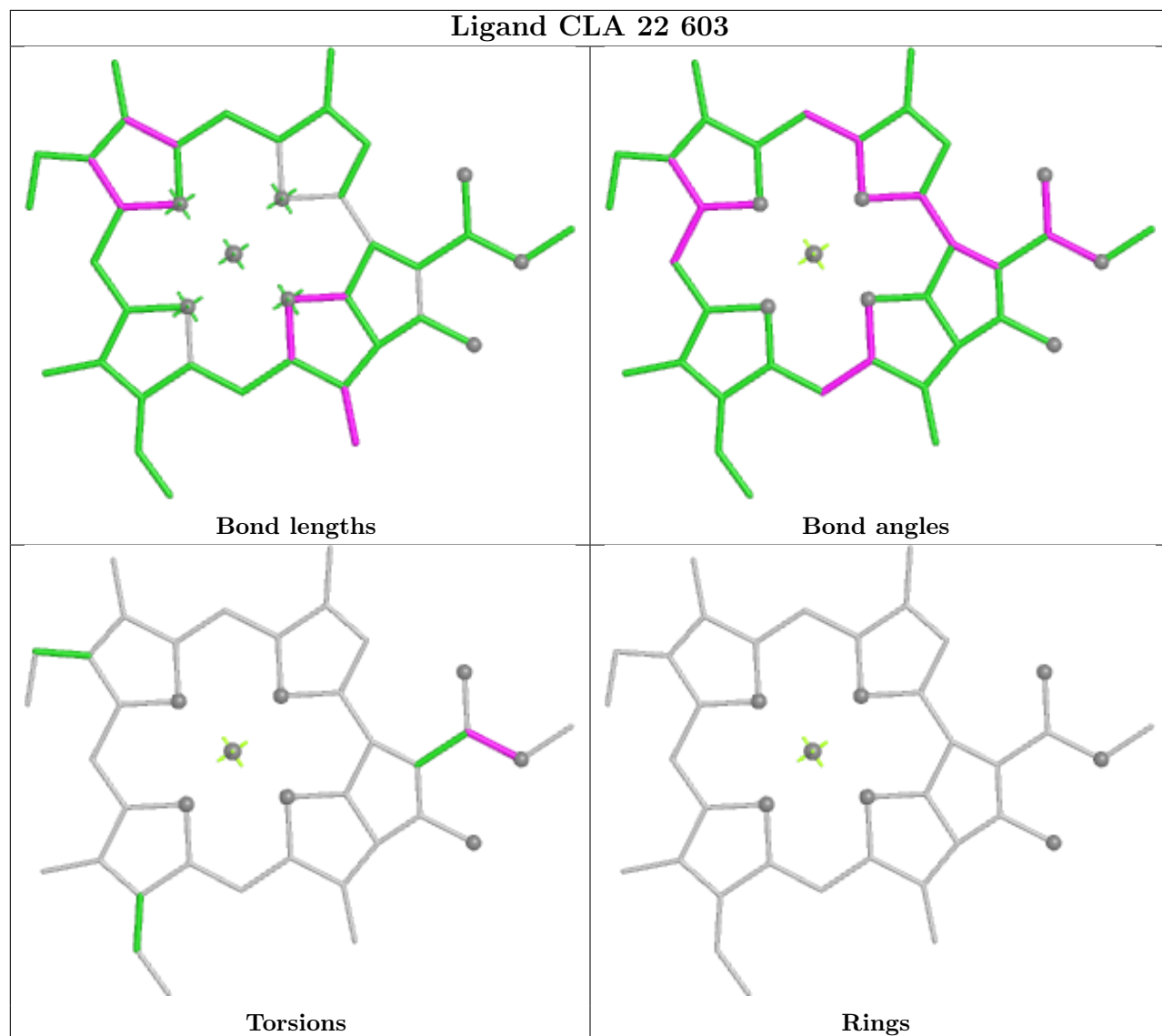


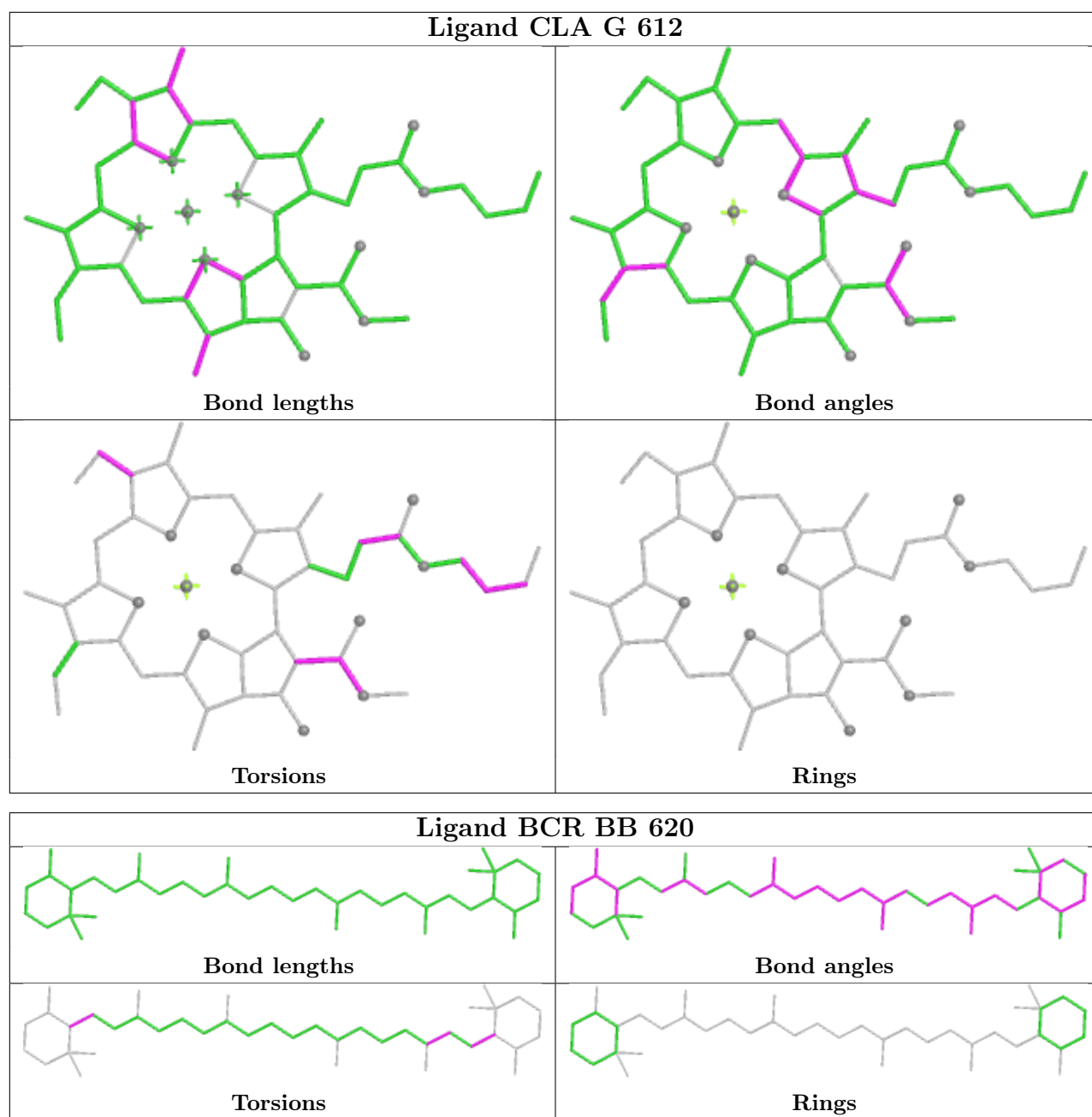


Ligand CLA Bb 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

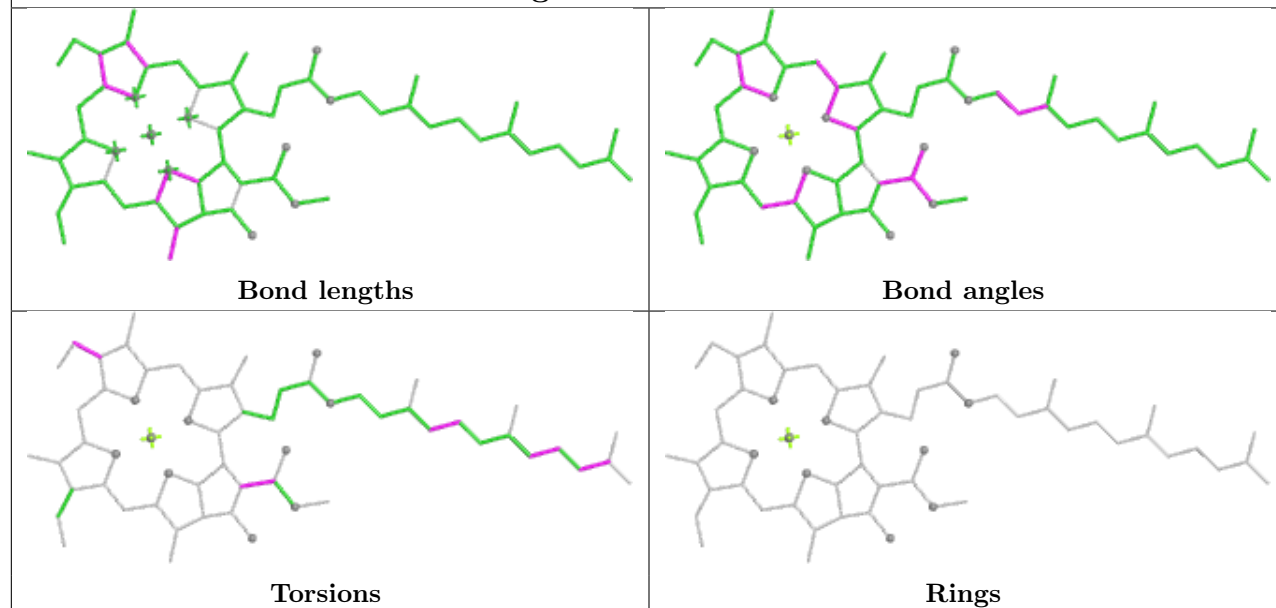
Ligand LUT y 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

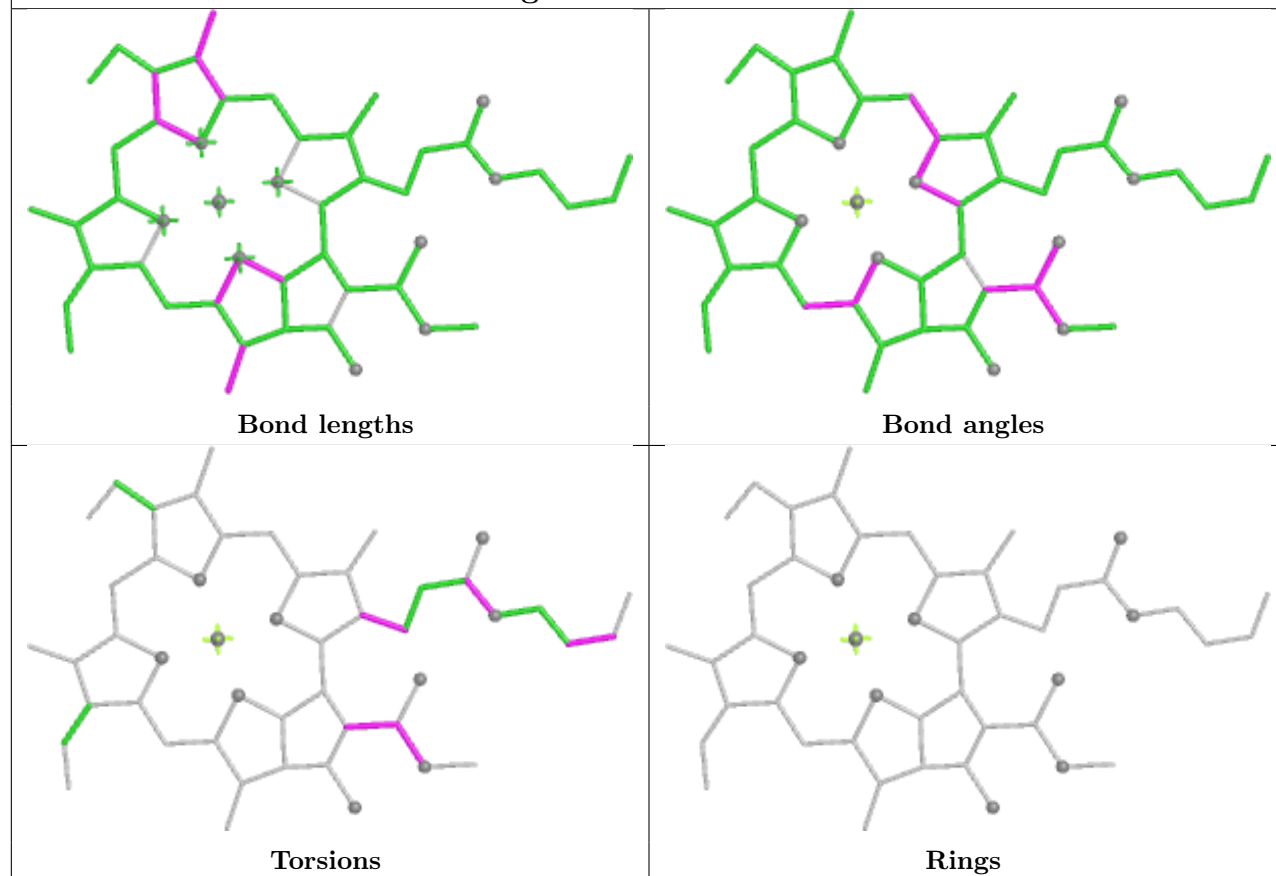


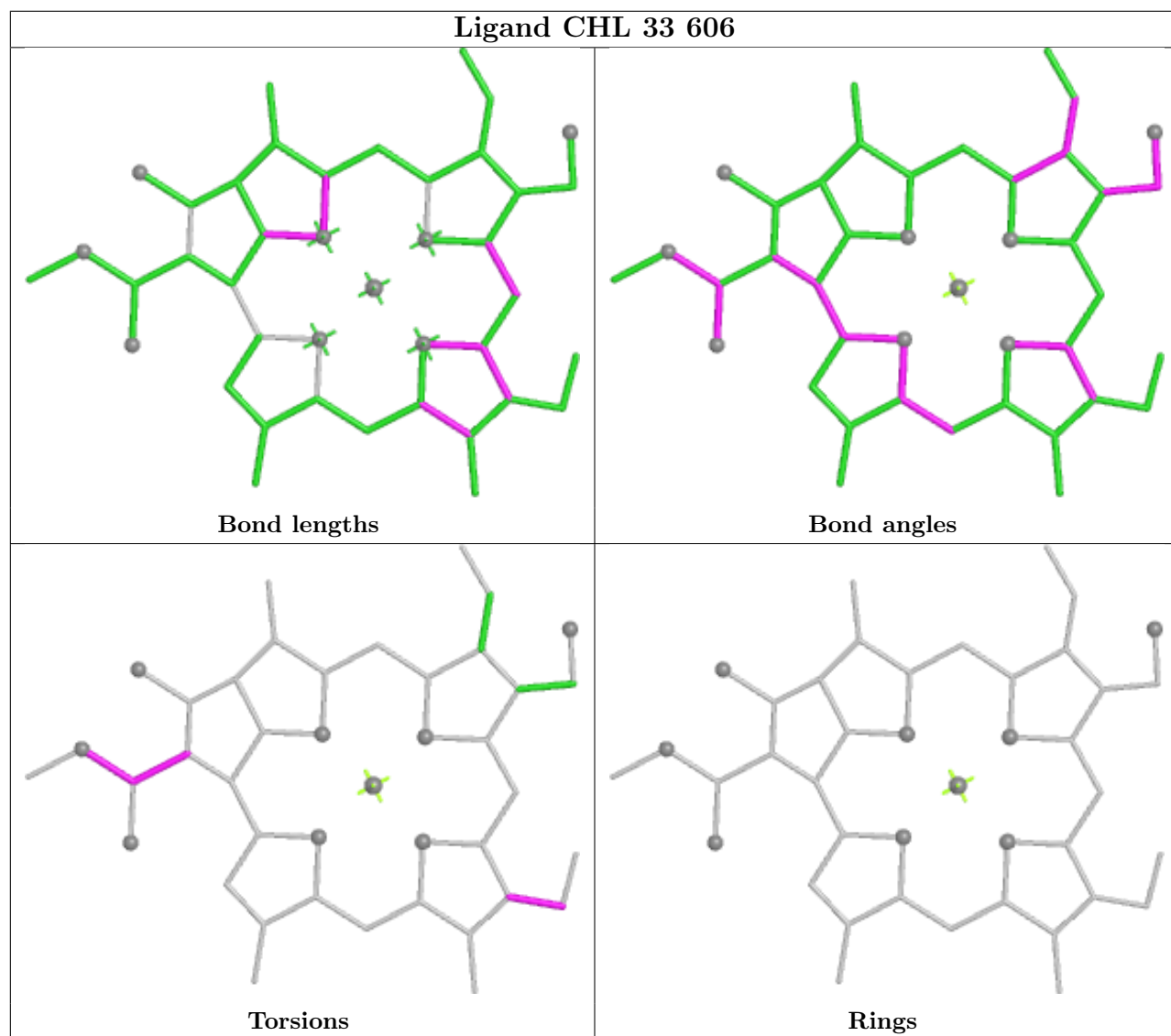
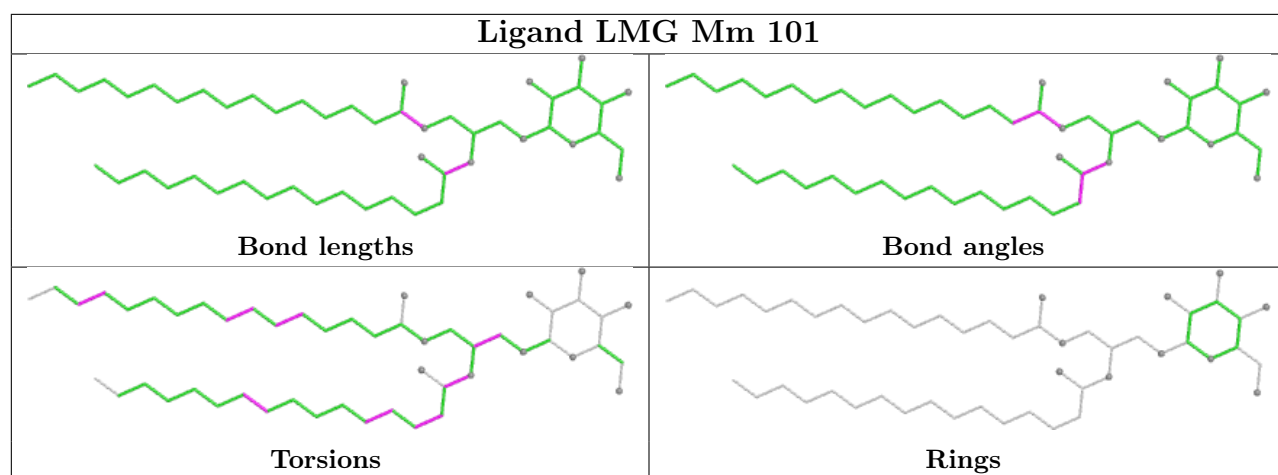


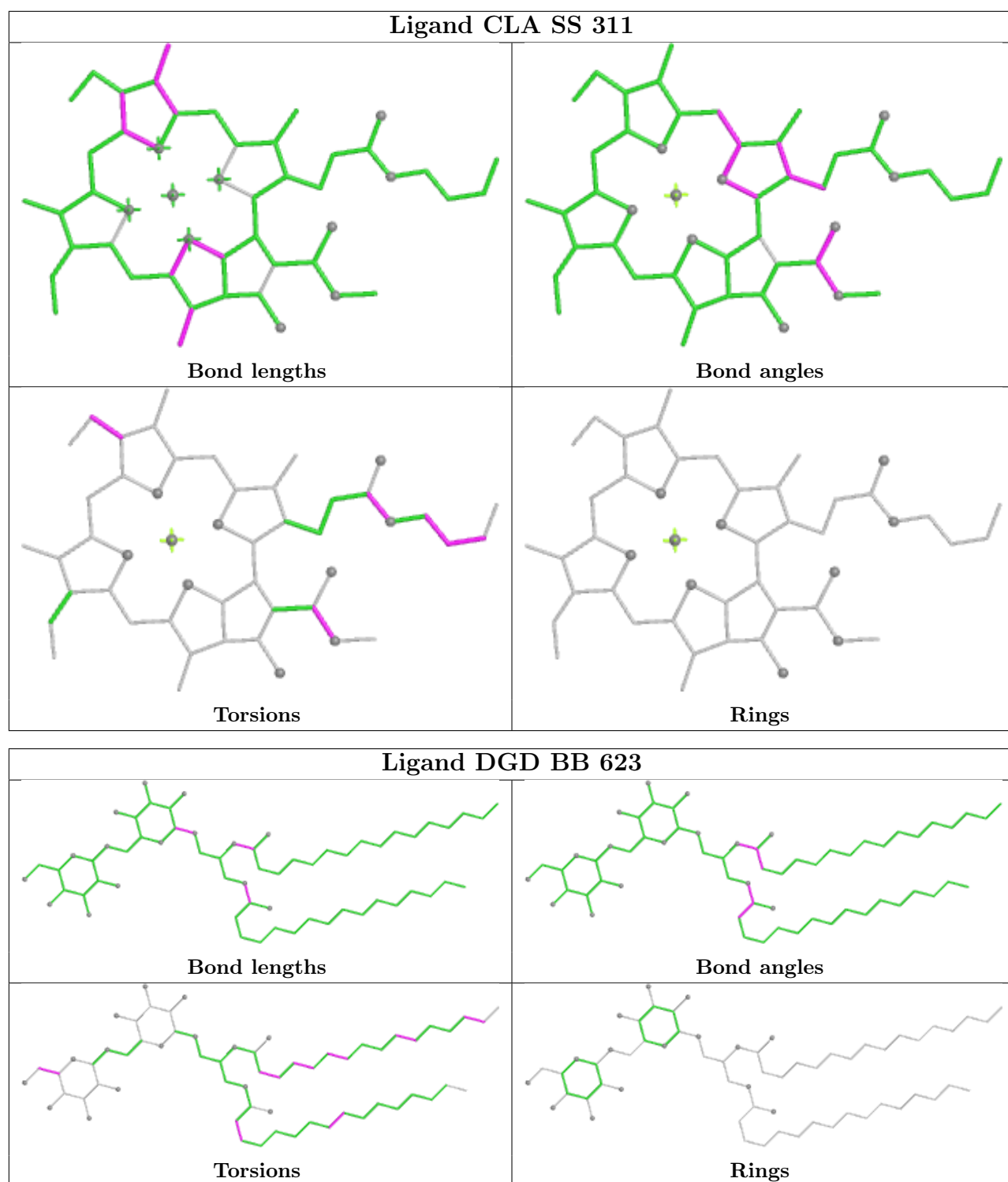
Ligand CLA A 408

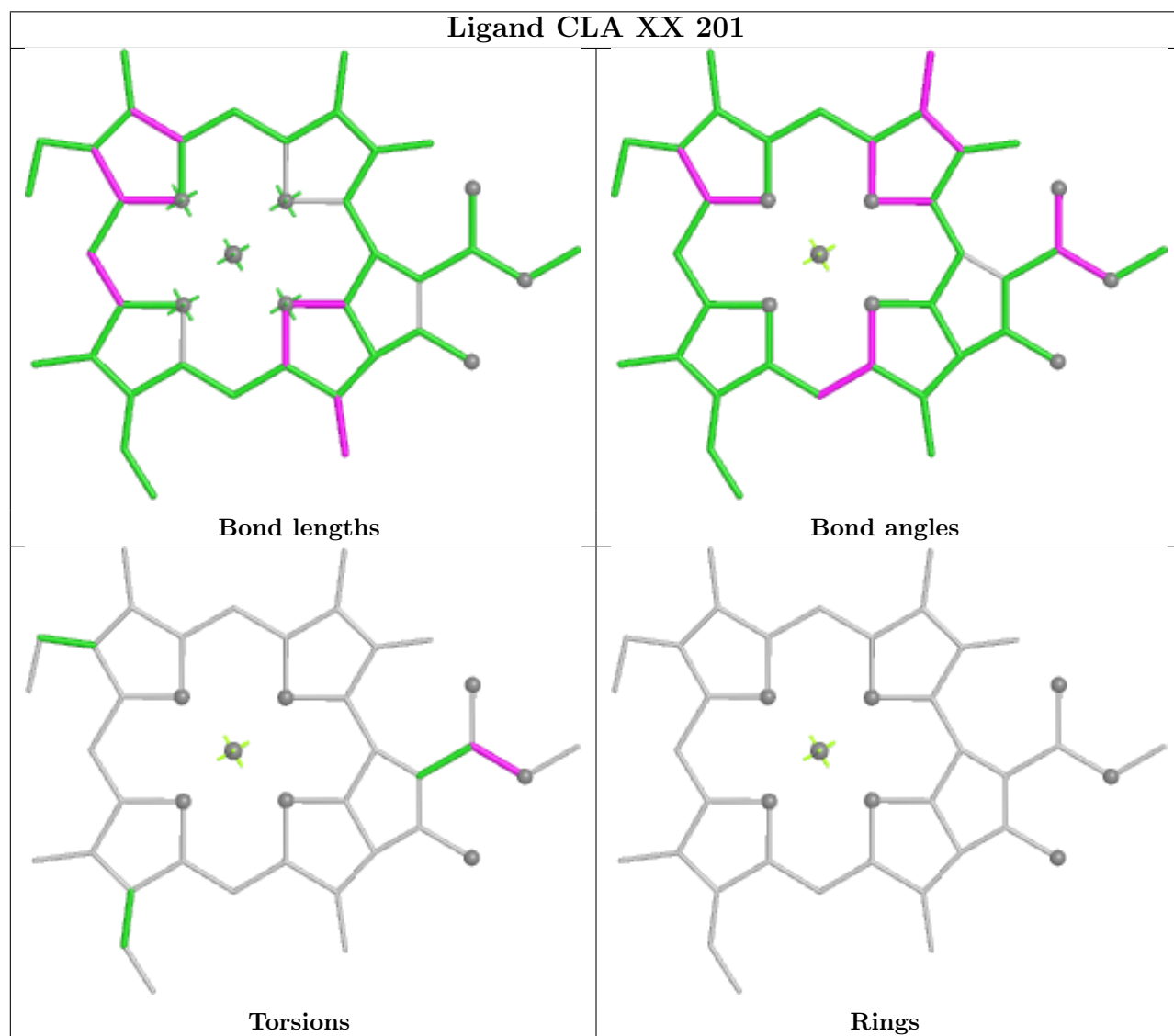
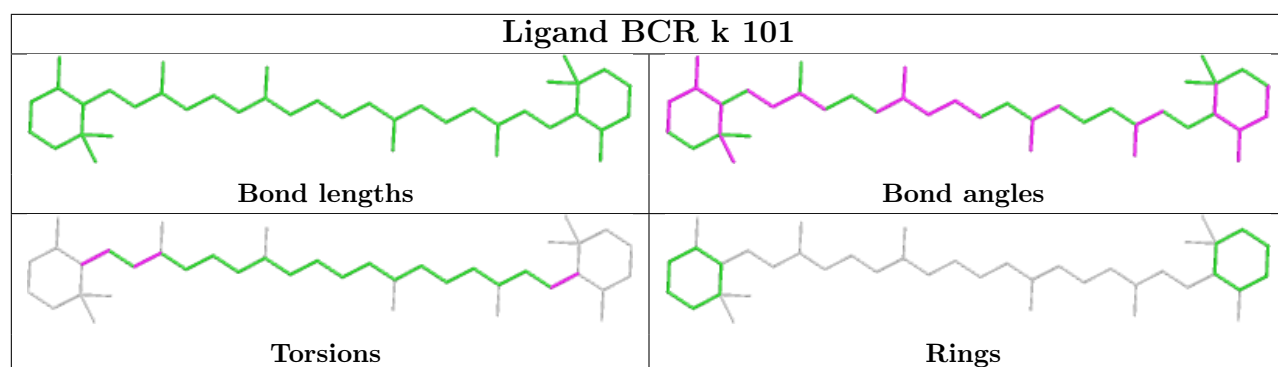


Ligand CLA Nn 304

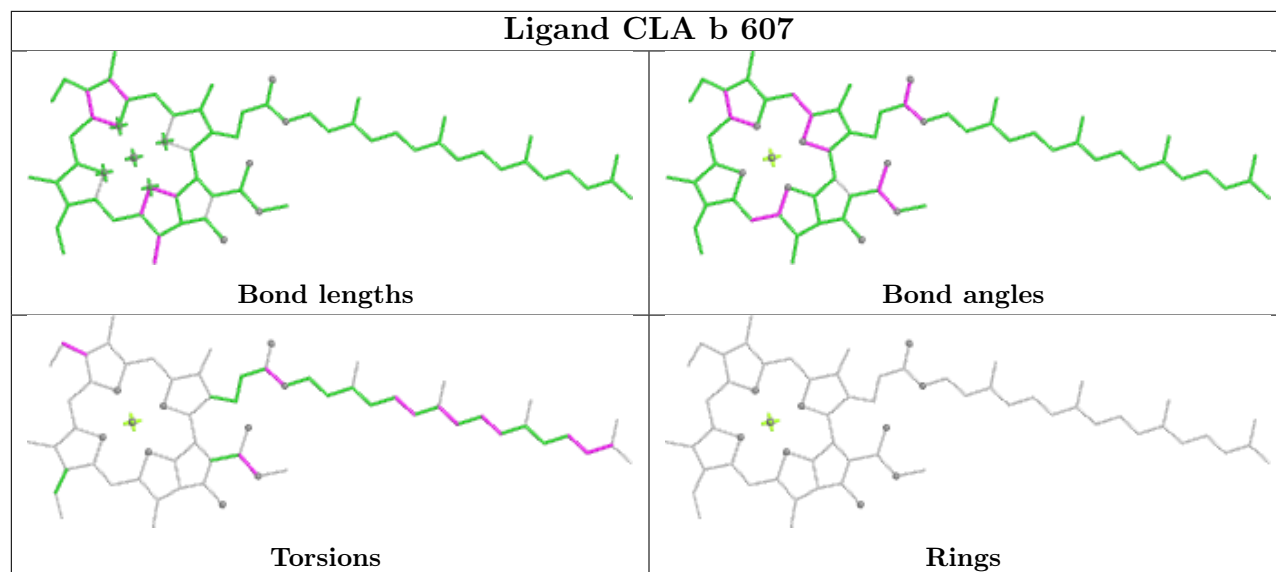




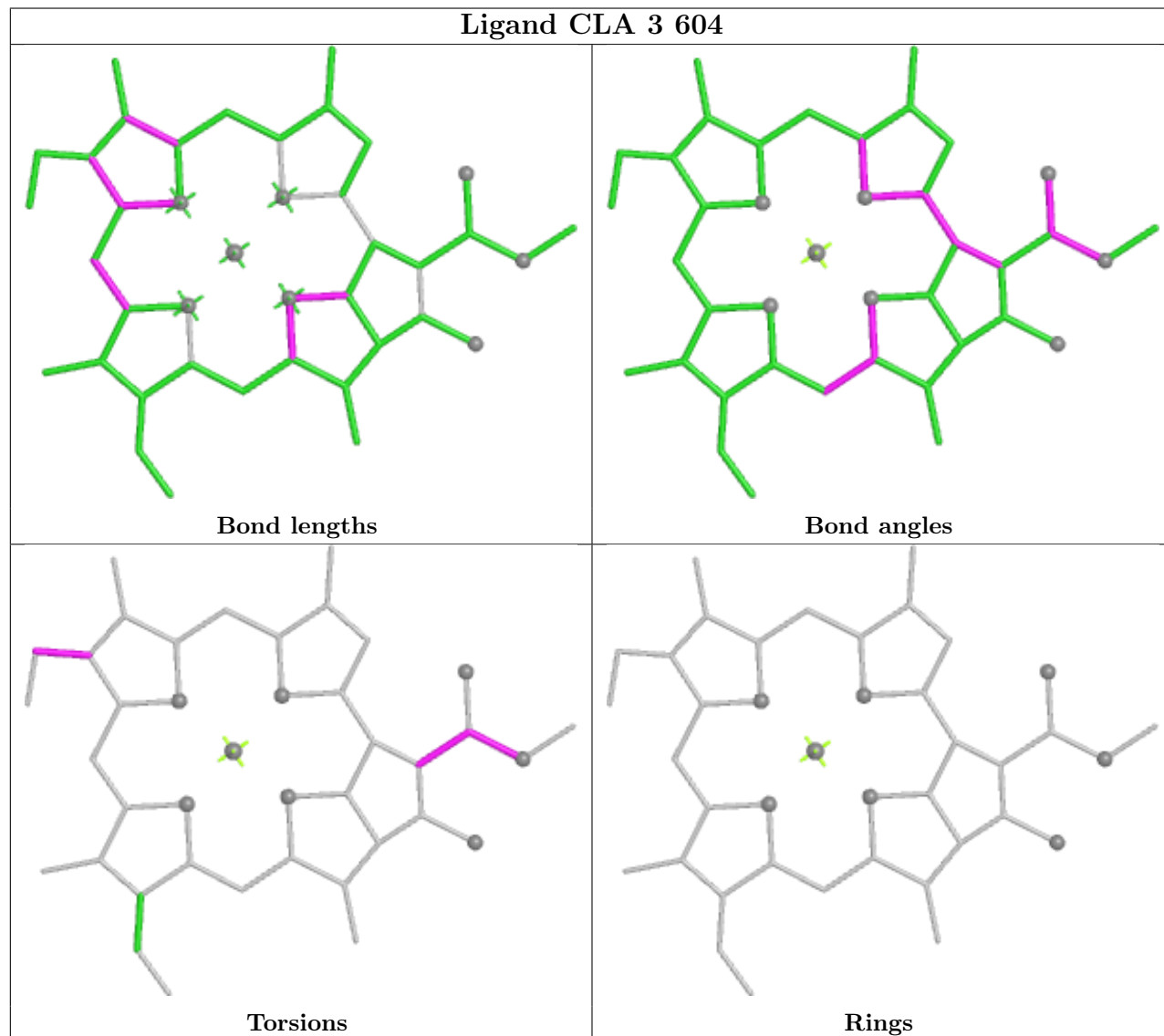


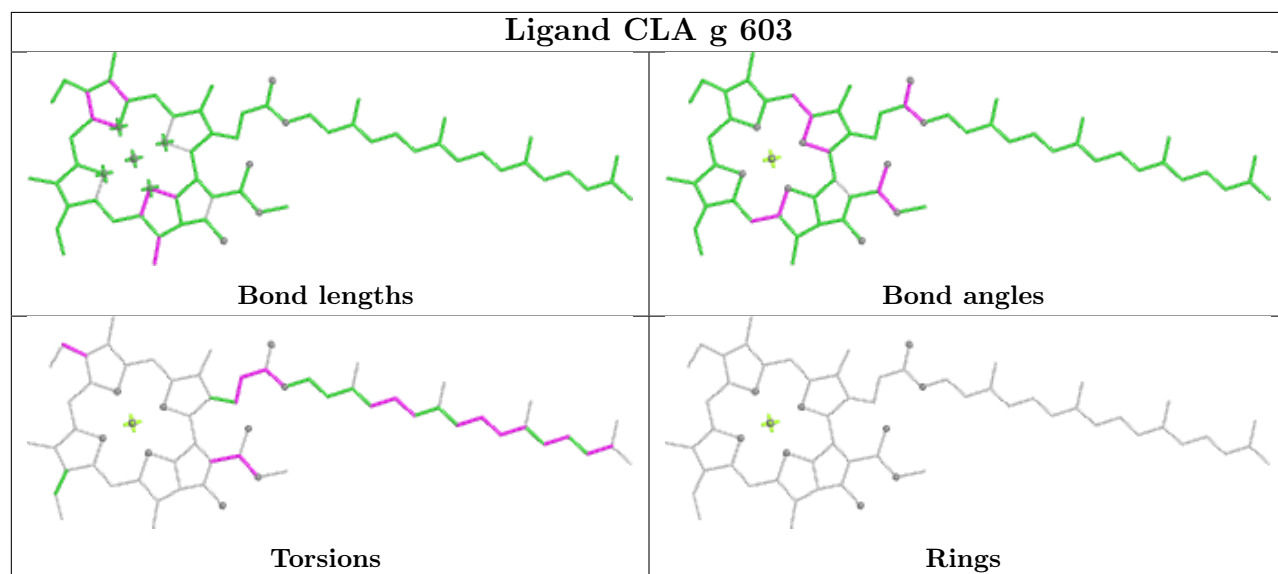
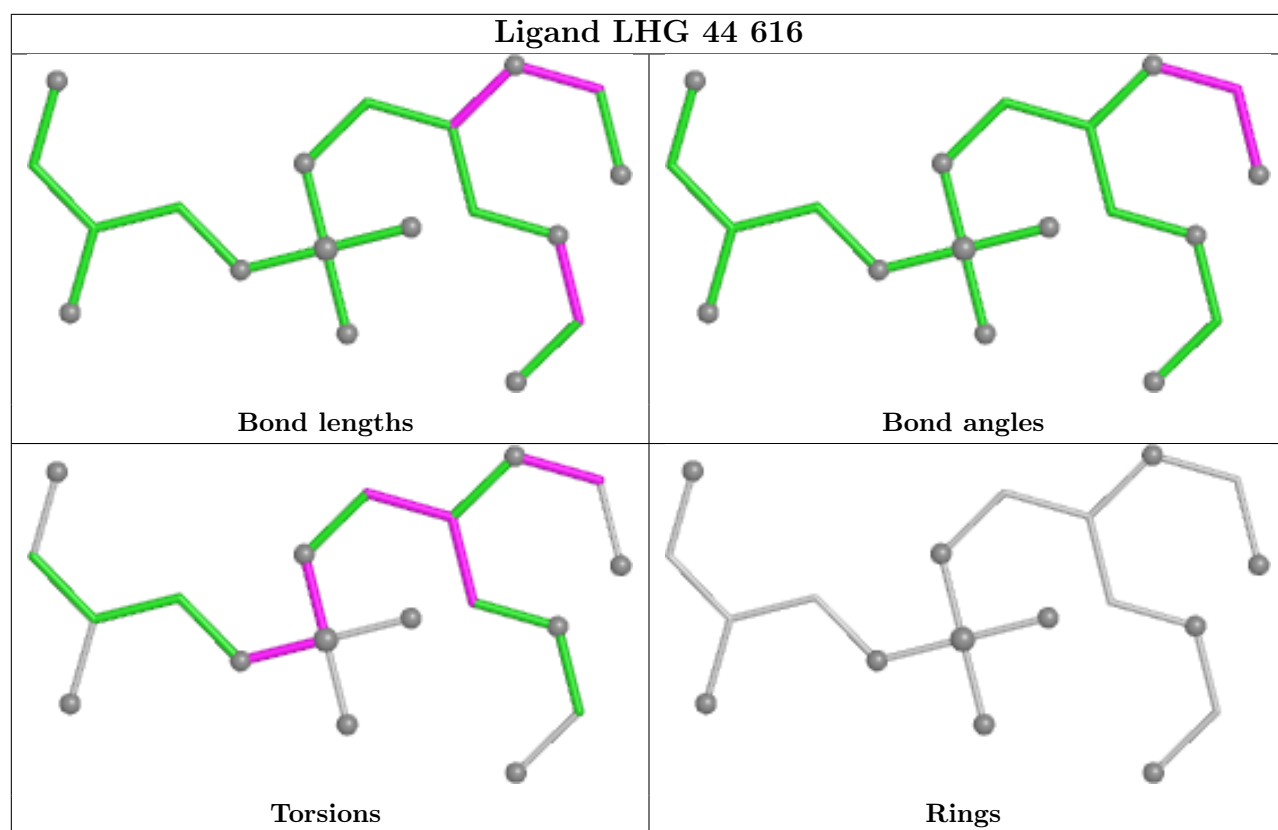


Ligand CLA b 607

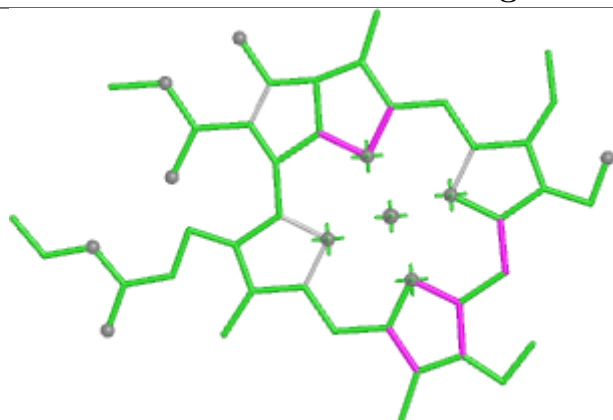


Ligand CLA 3 604

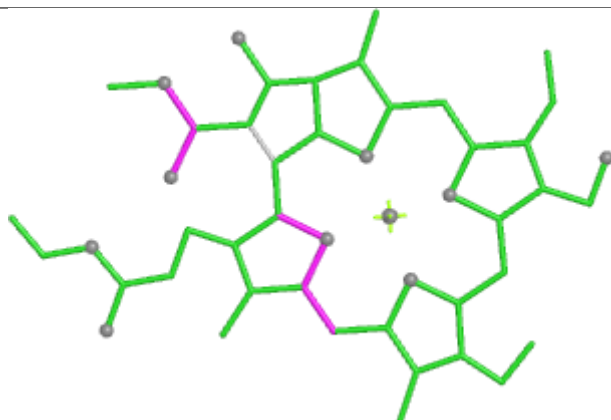




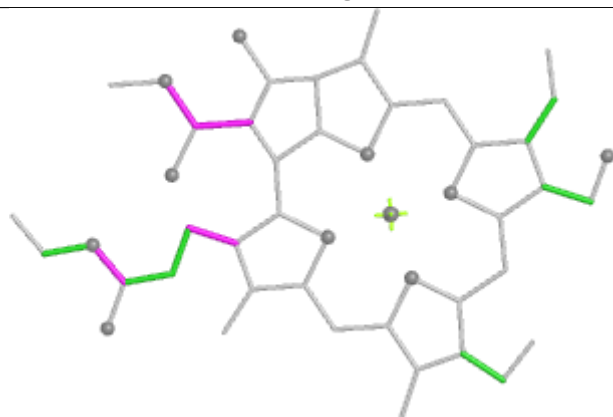
Ligand CHL YY 605



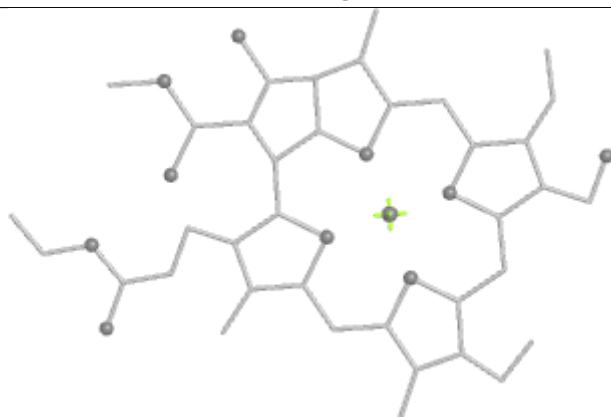
Bond lengths



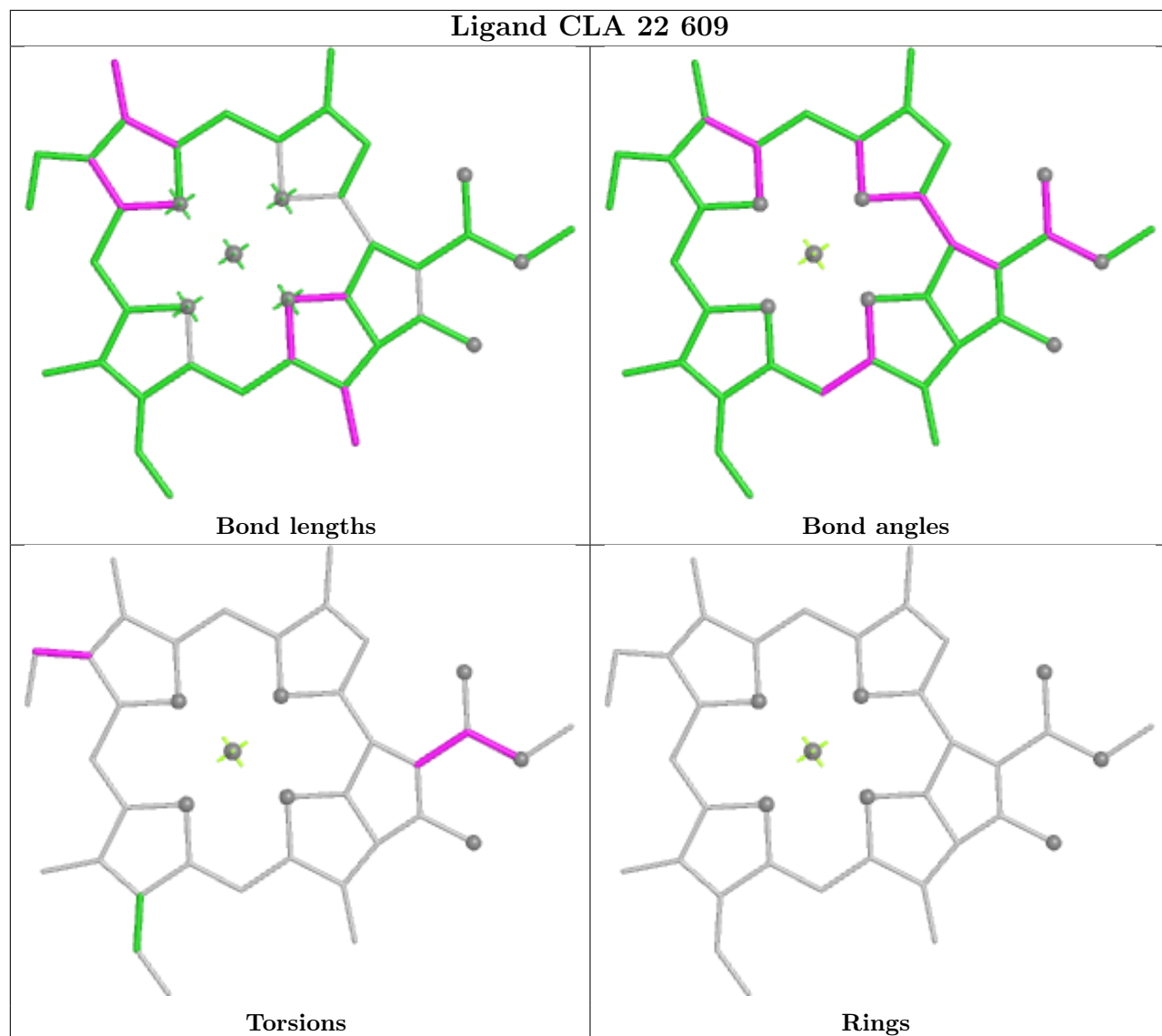
Bond angles

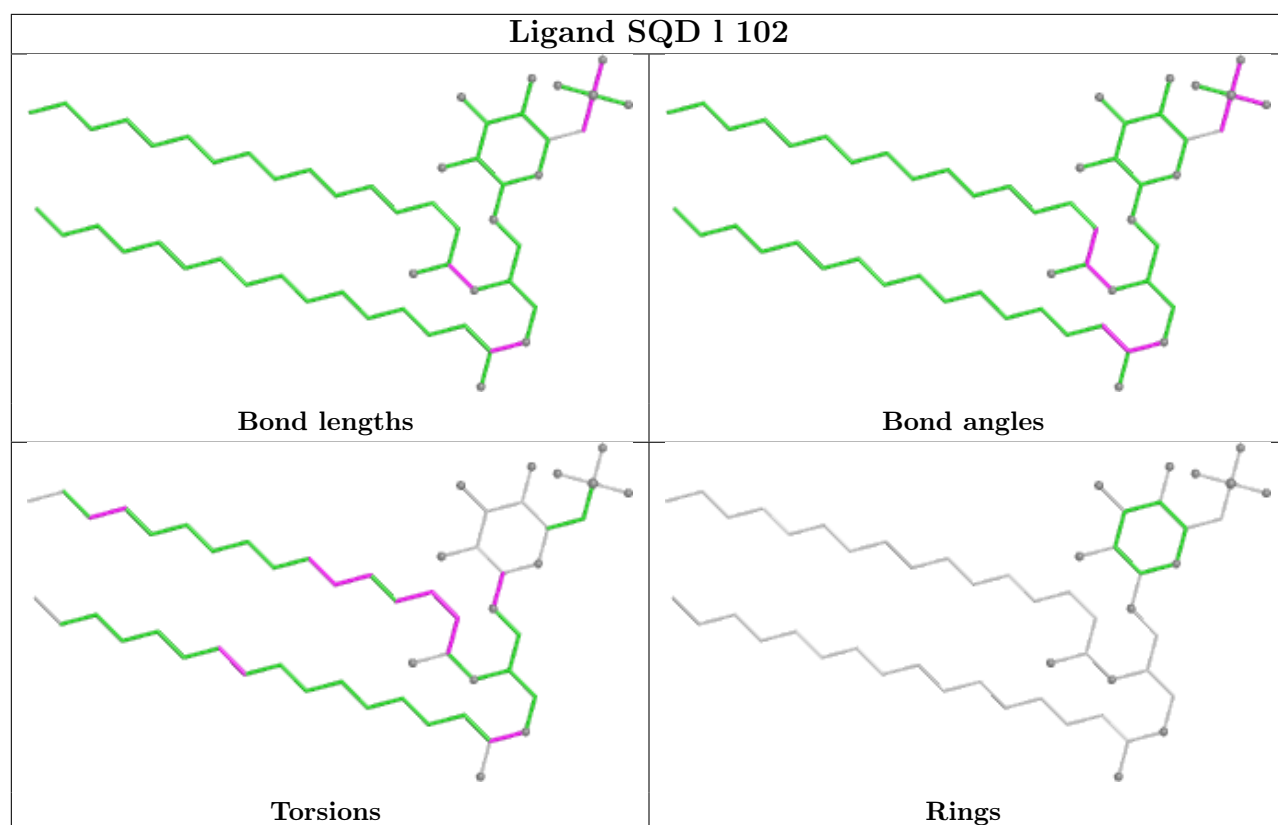


Torsions

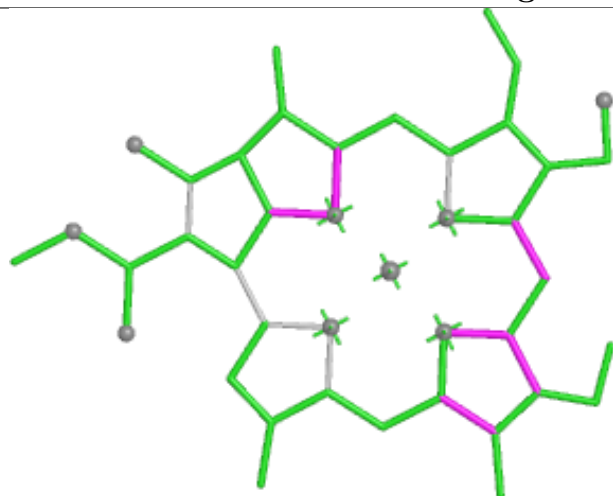


Rings

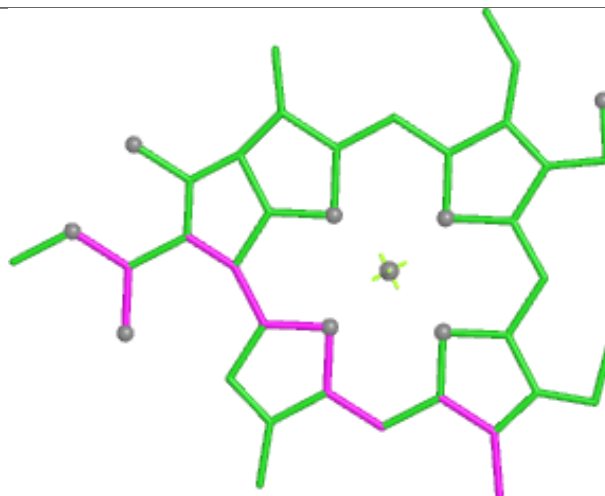




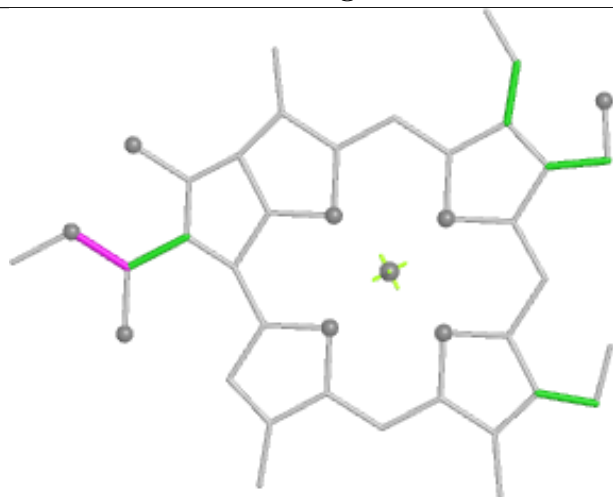
Ligand CHL 1 607



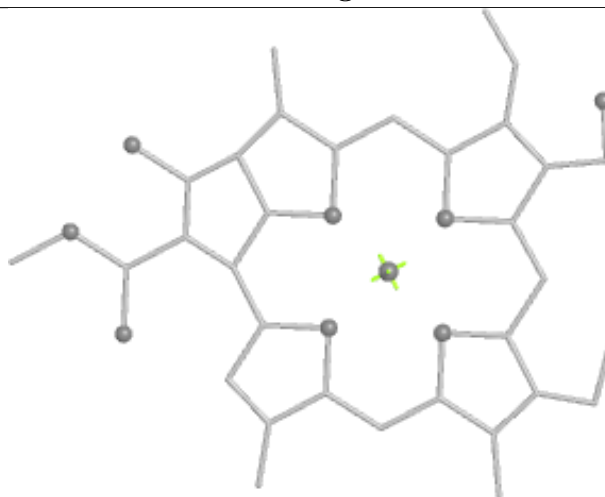
Bond lengths



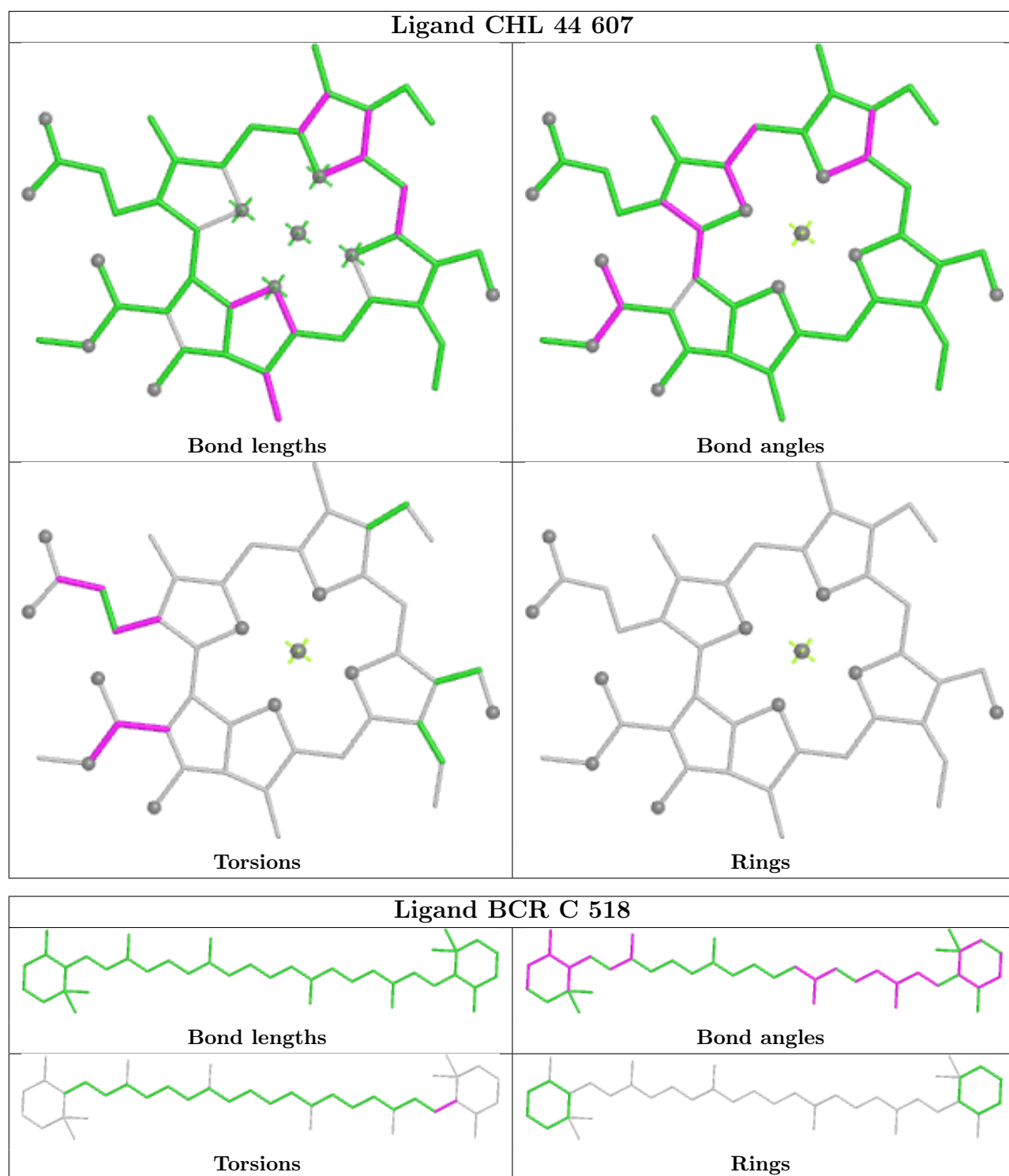
Bond angles

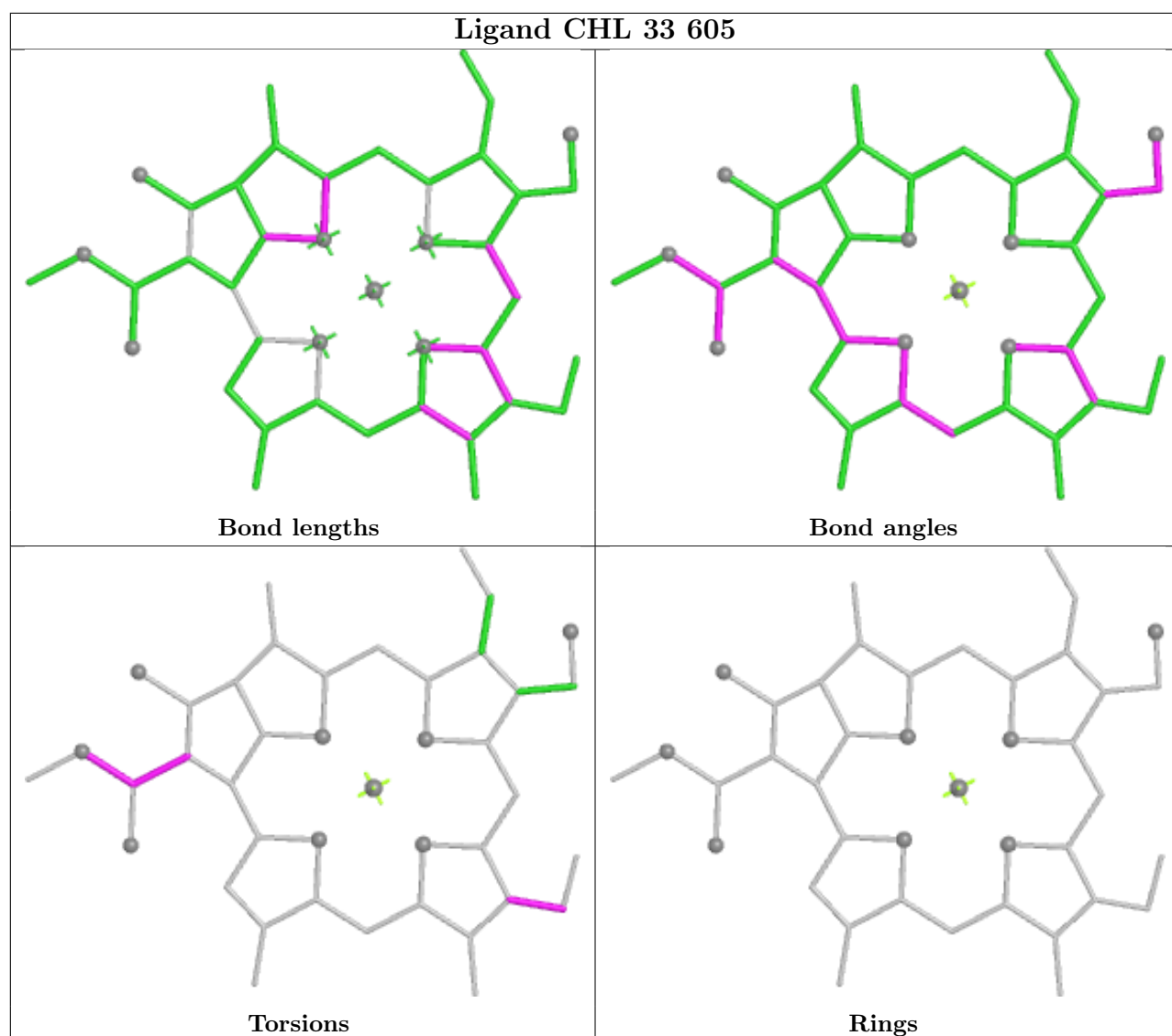


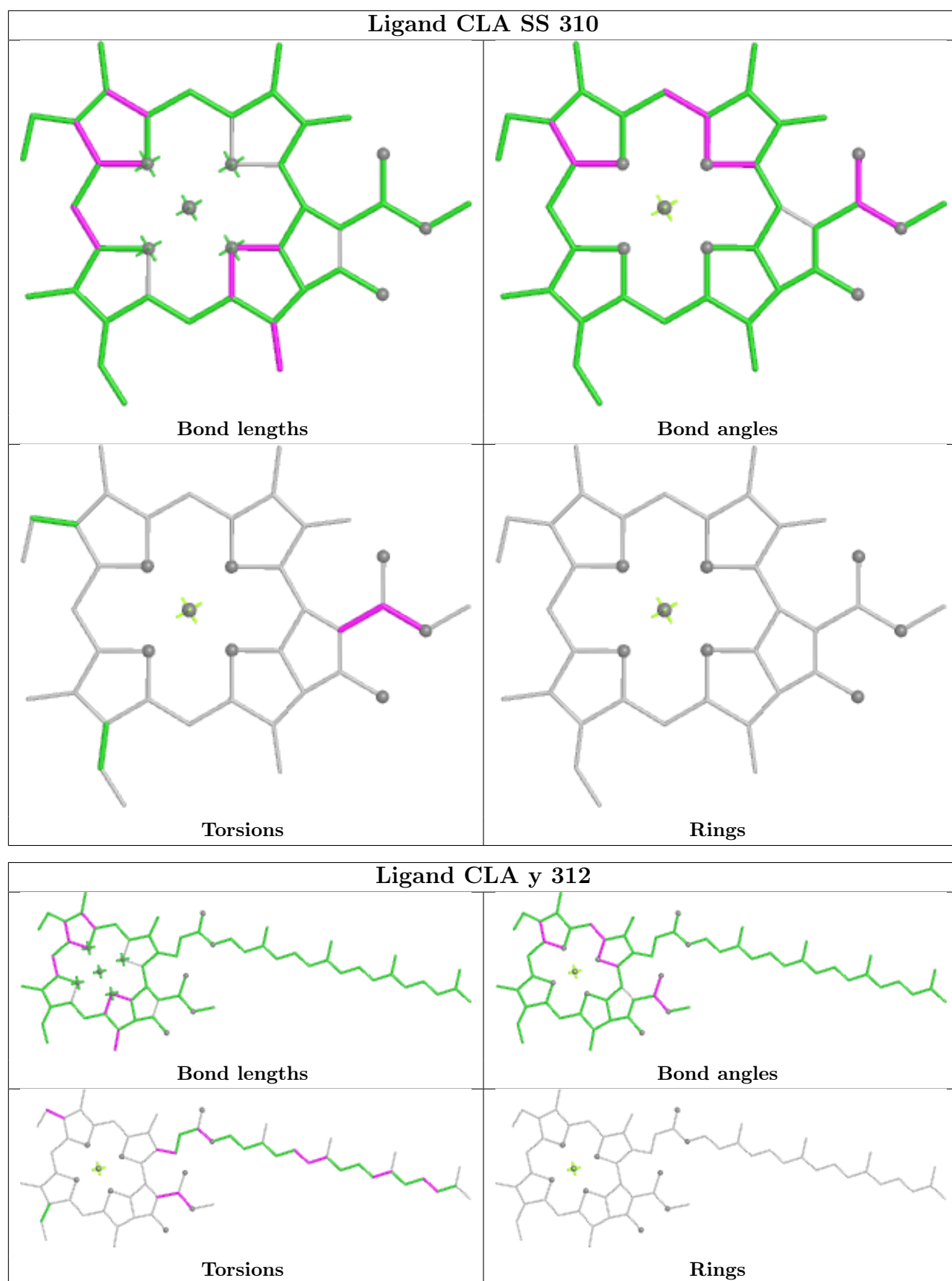
Torsions



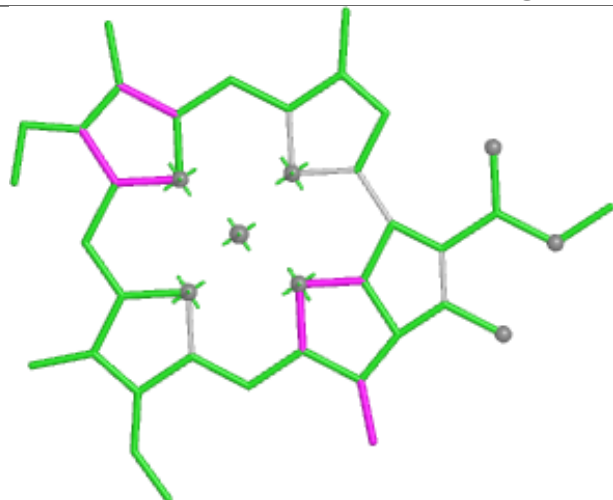
Rings



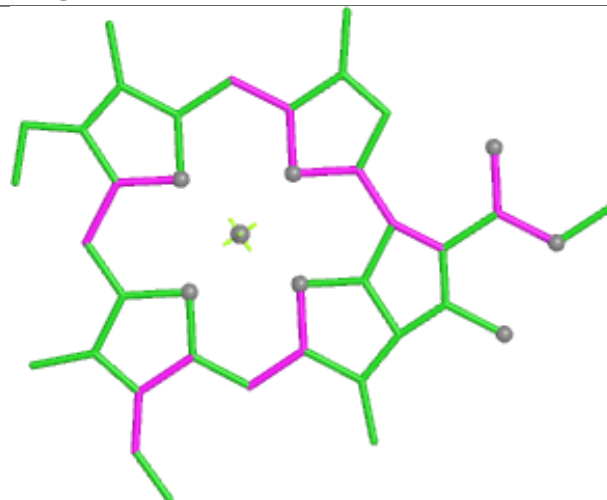




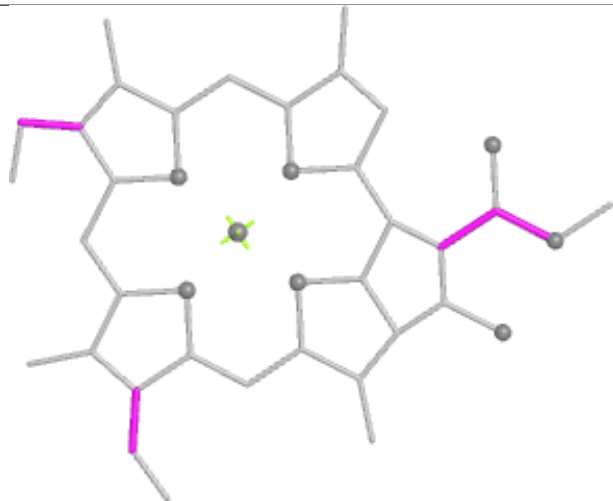
Ligand CLA g 613



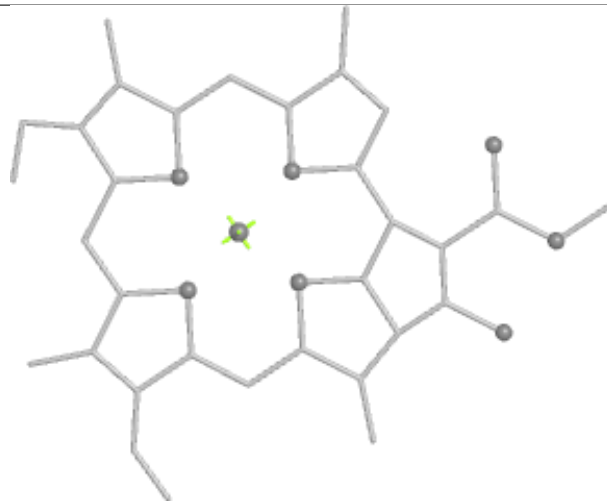
Bond lengths



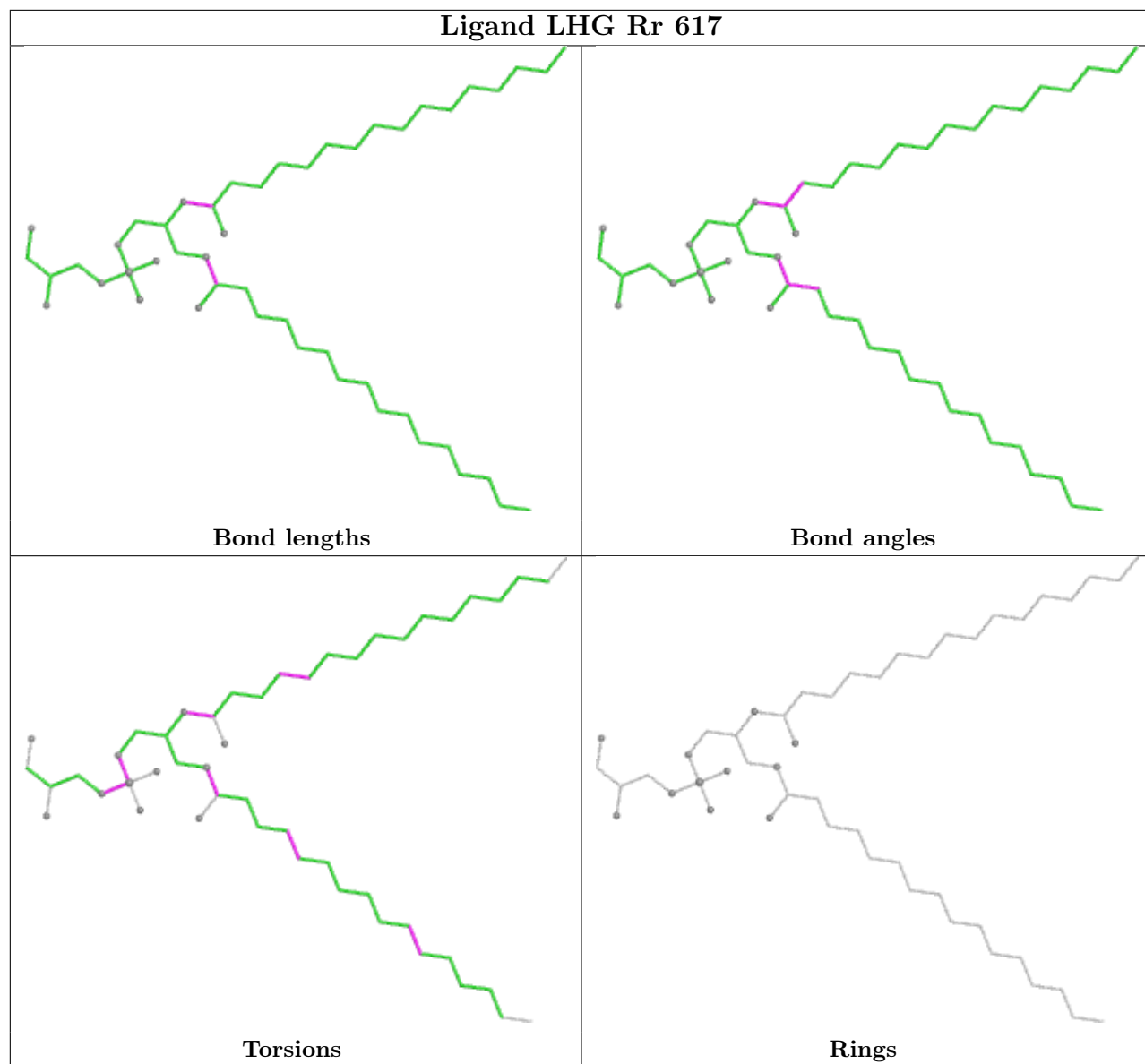
Bond angles

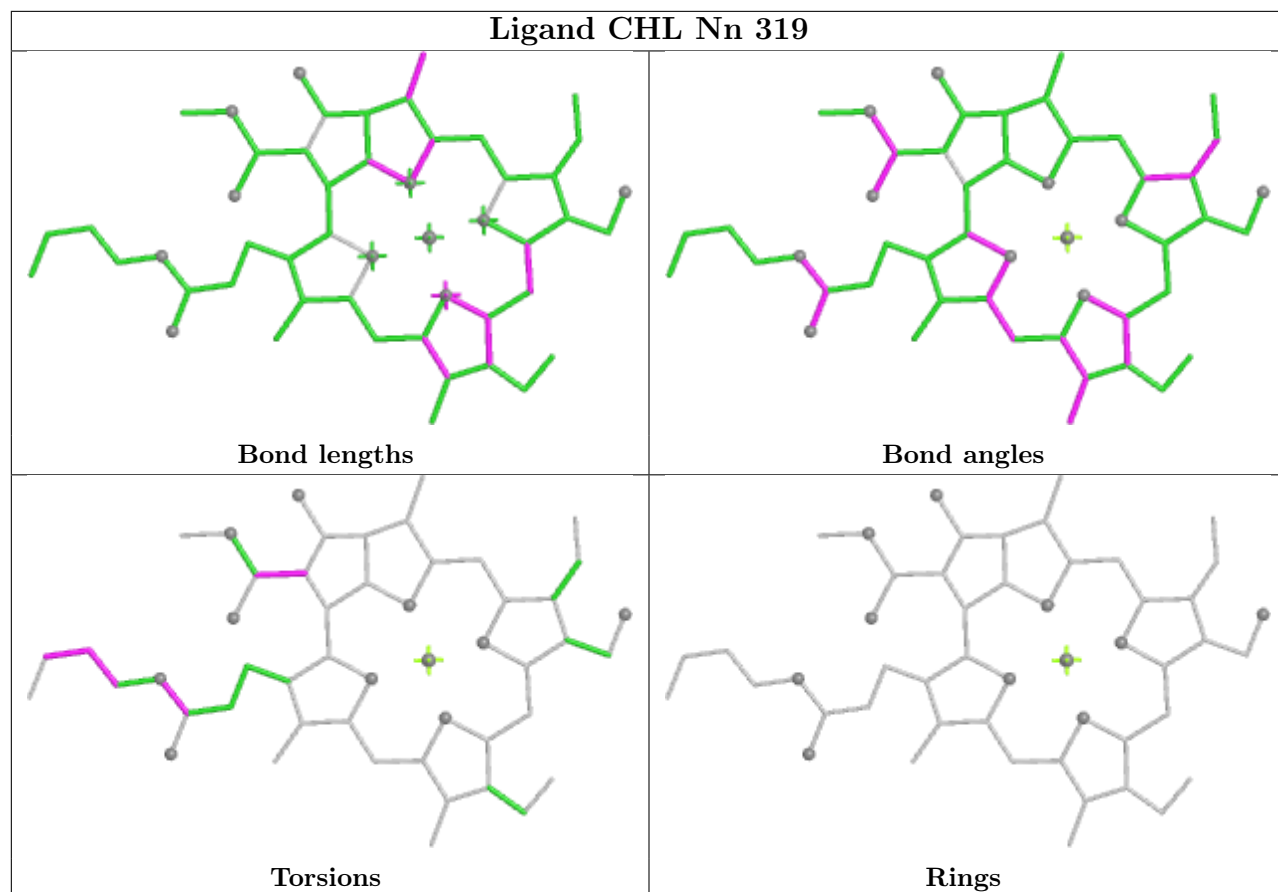


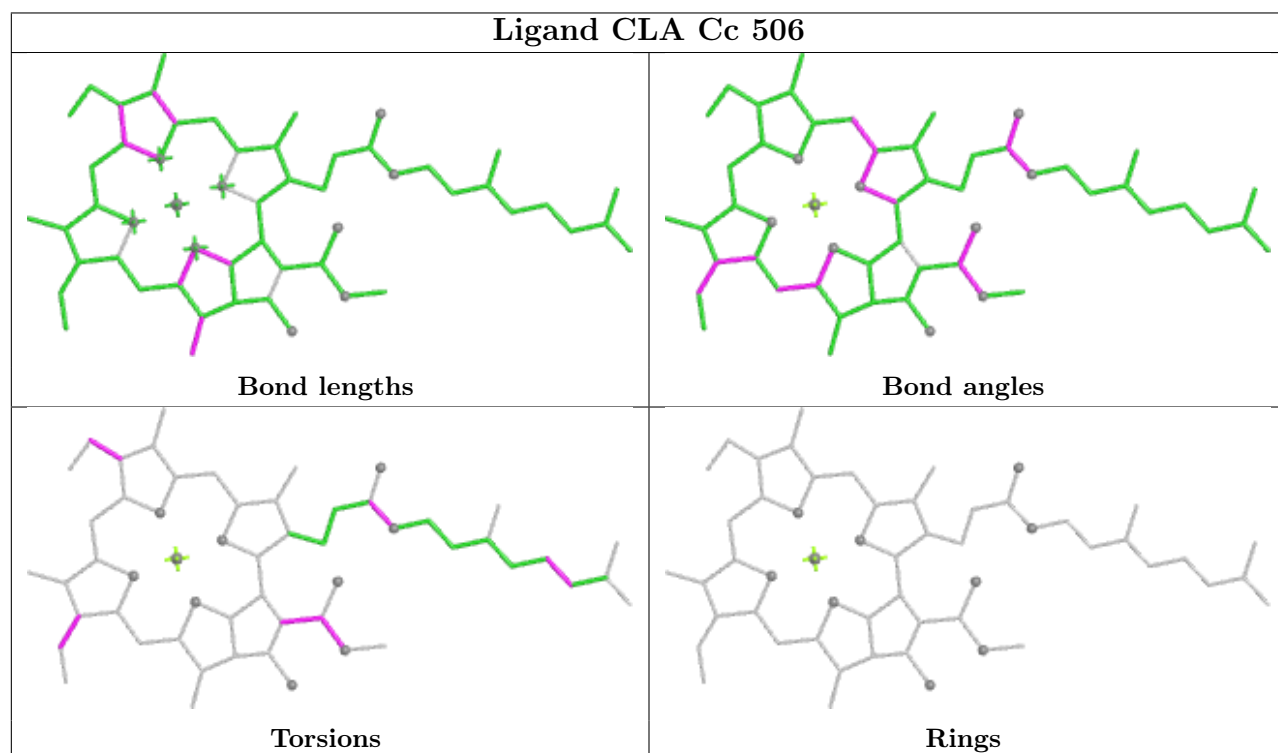
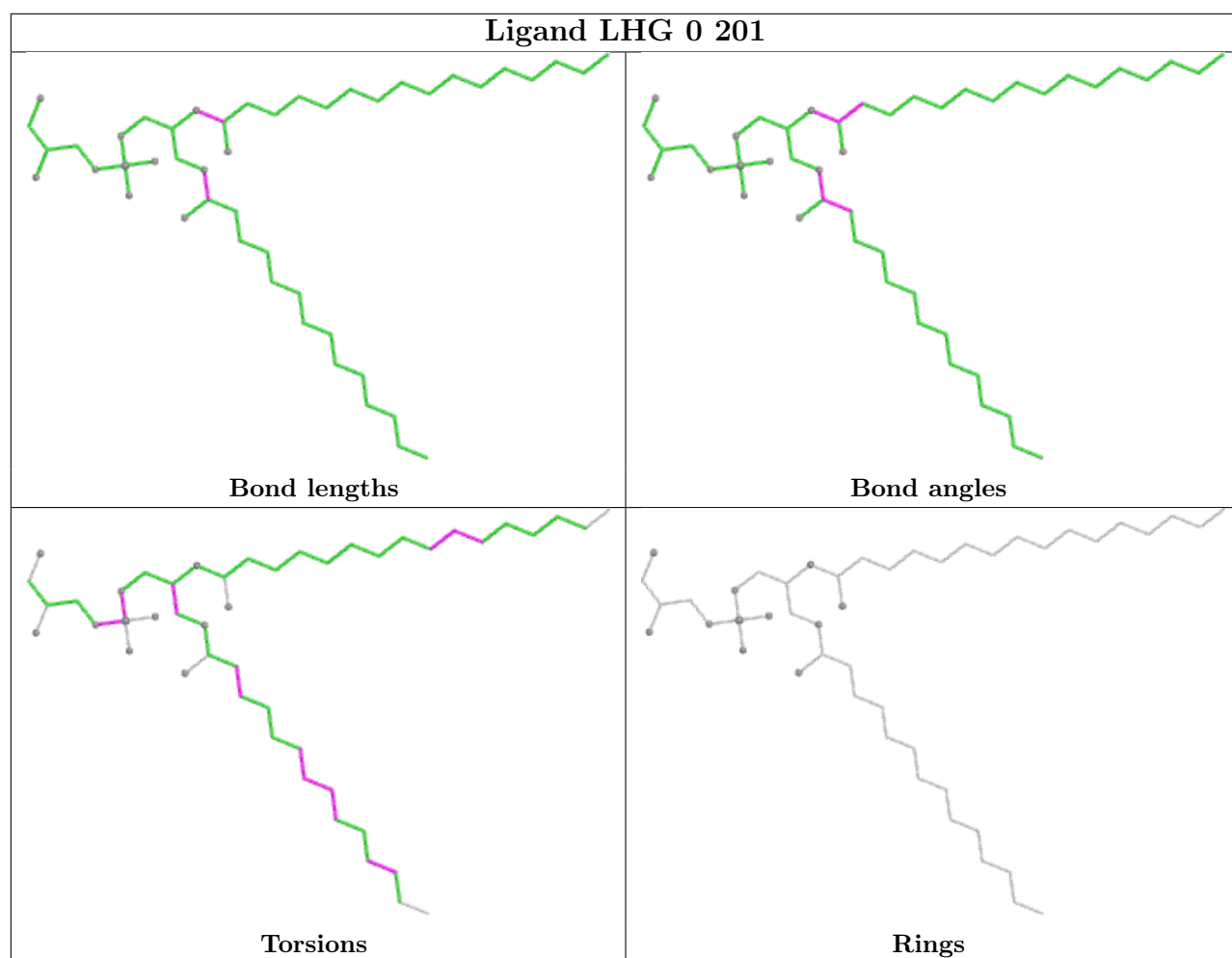
Torsions

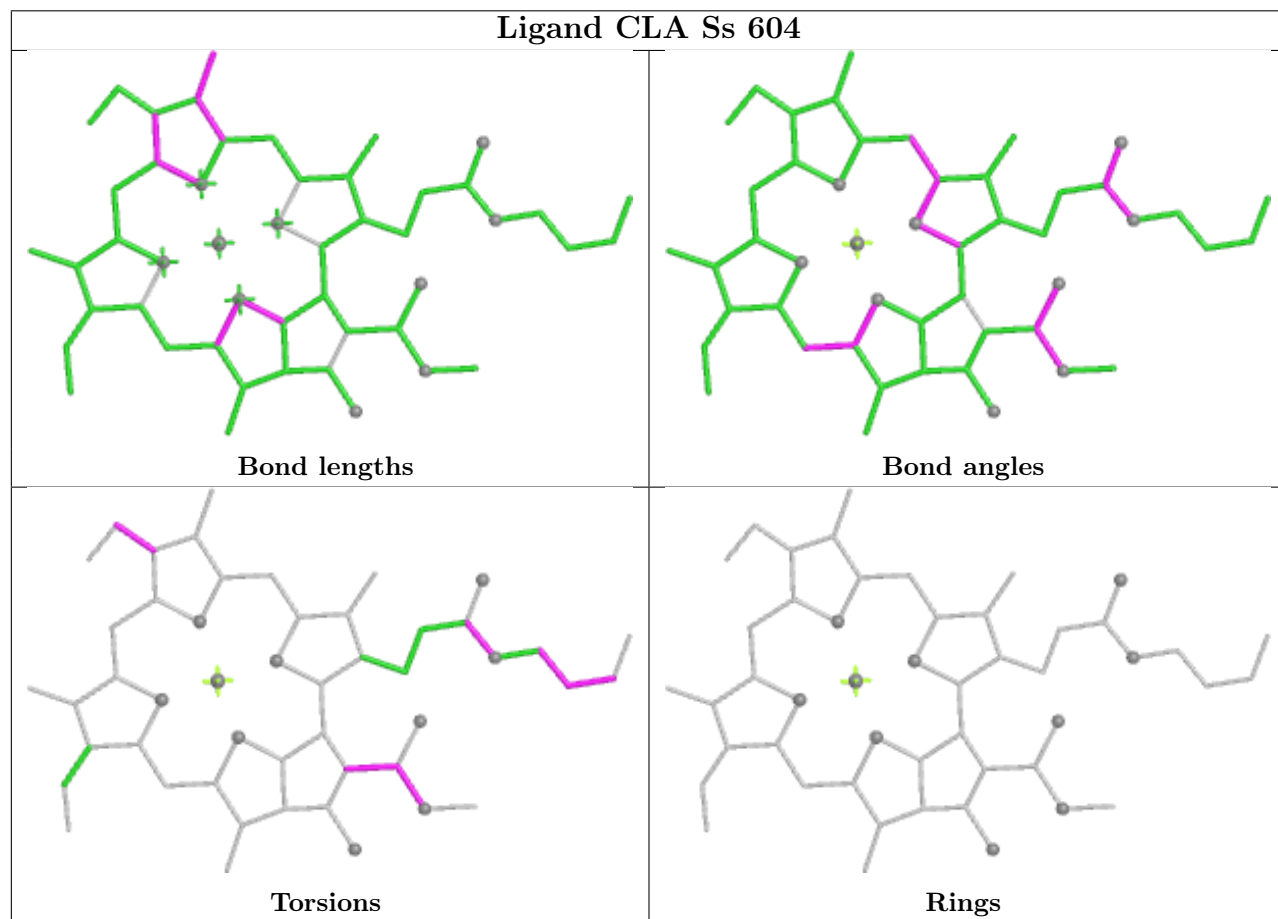
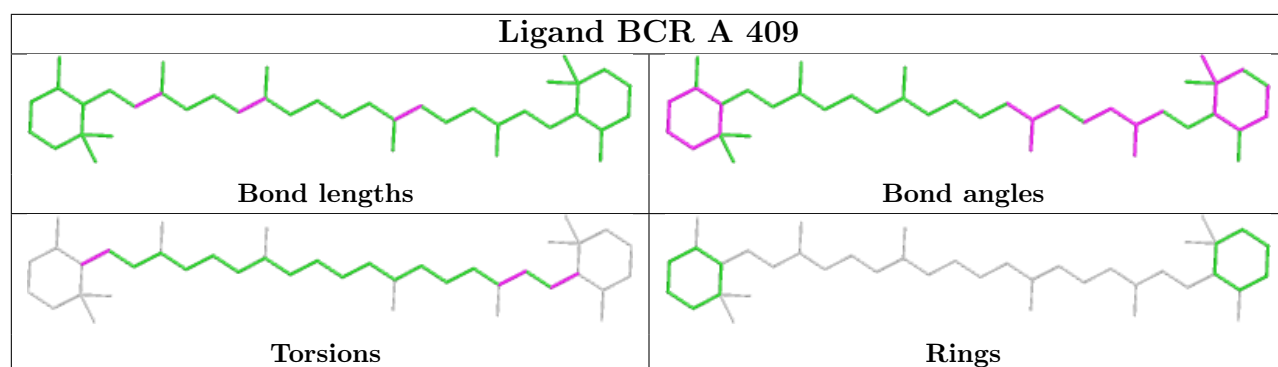


Rings

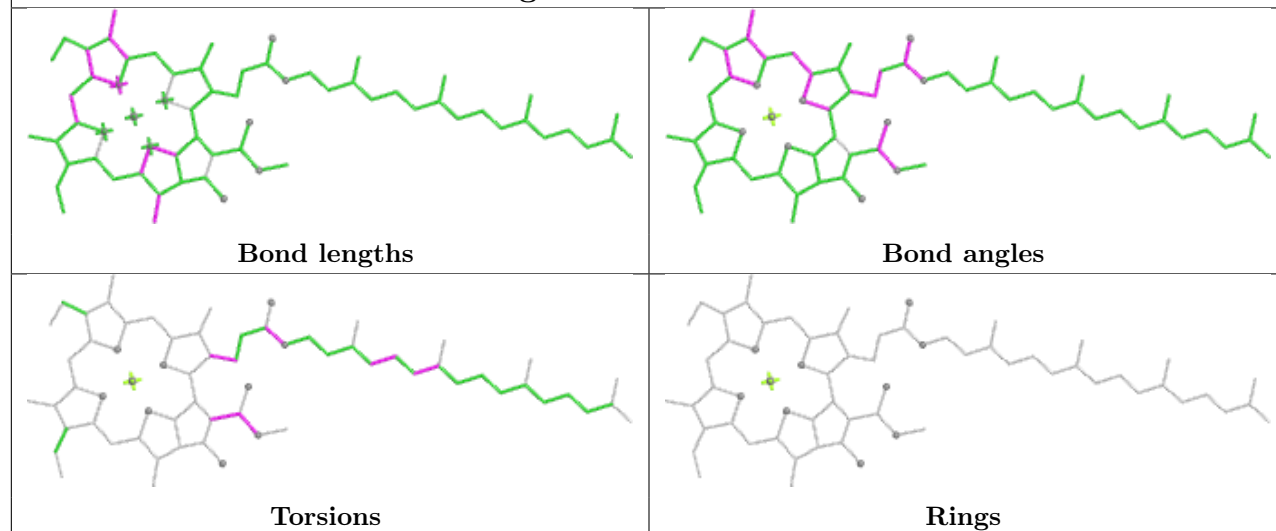




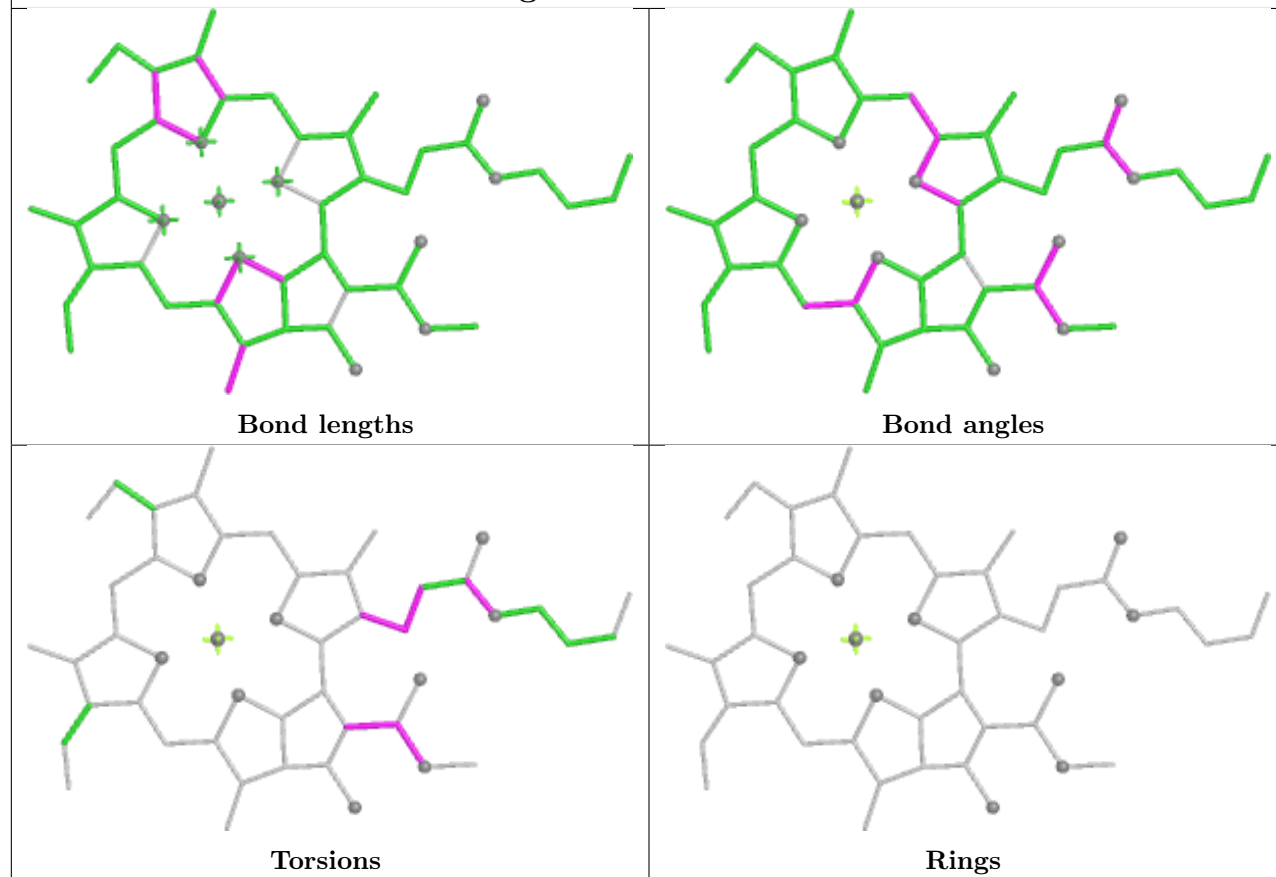




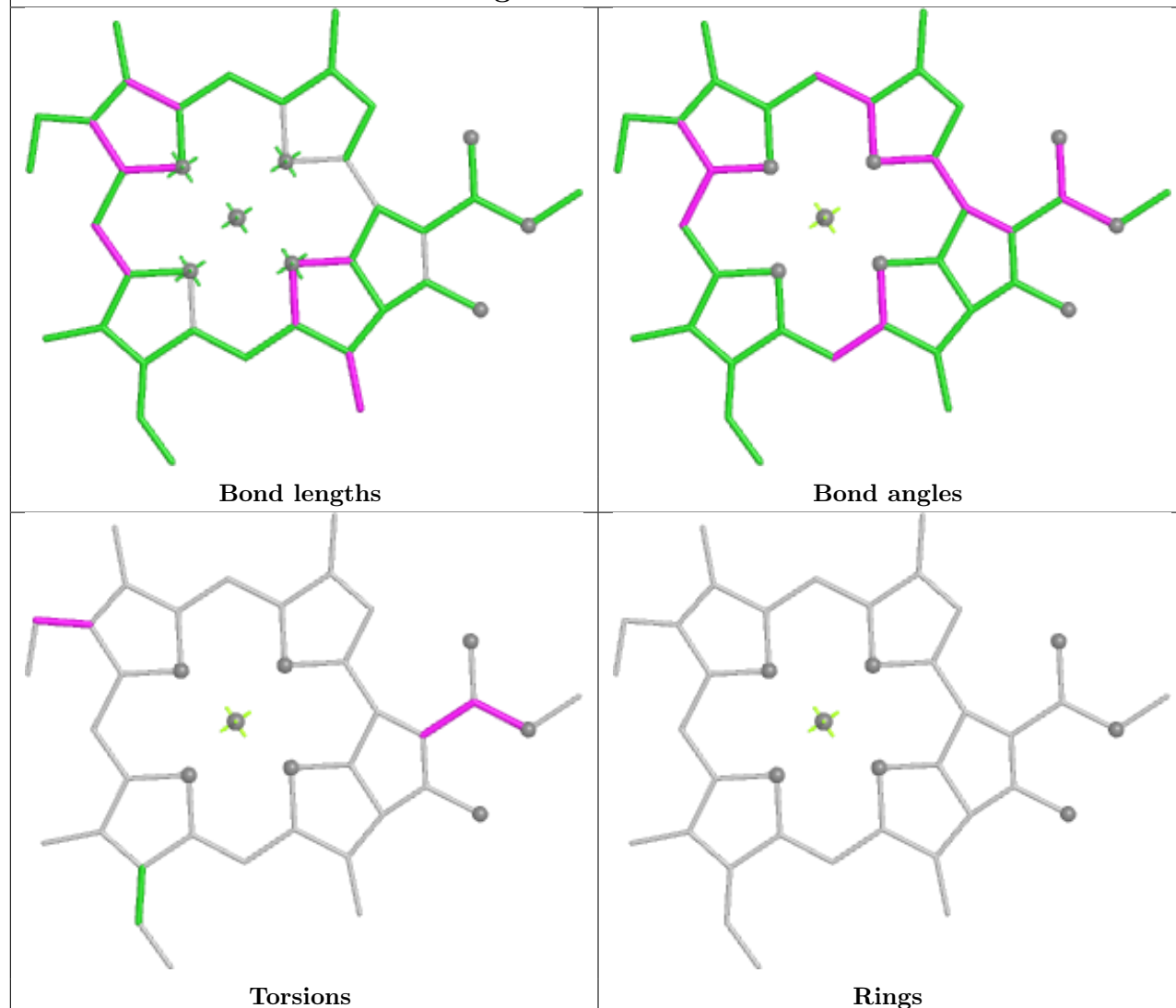
Ligand CLA CC 507



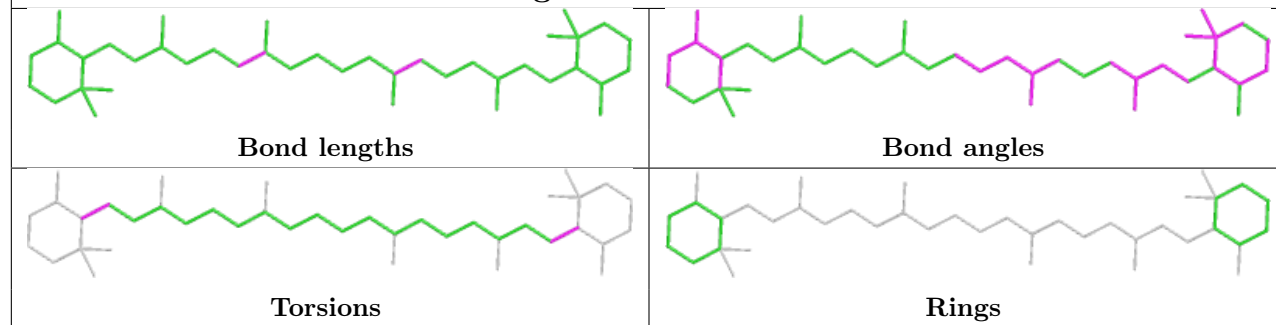
Ligand CLA CC 514

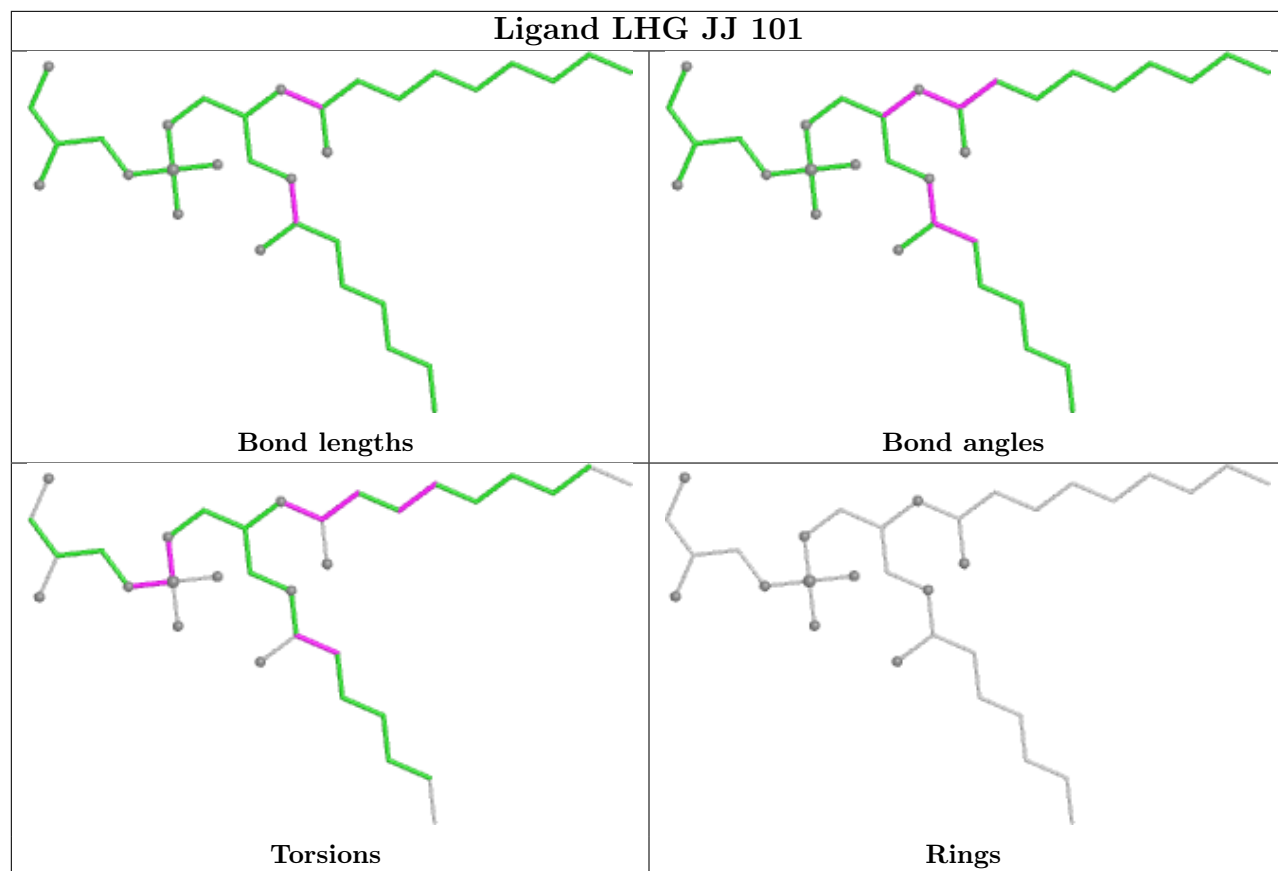


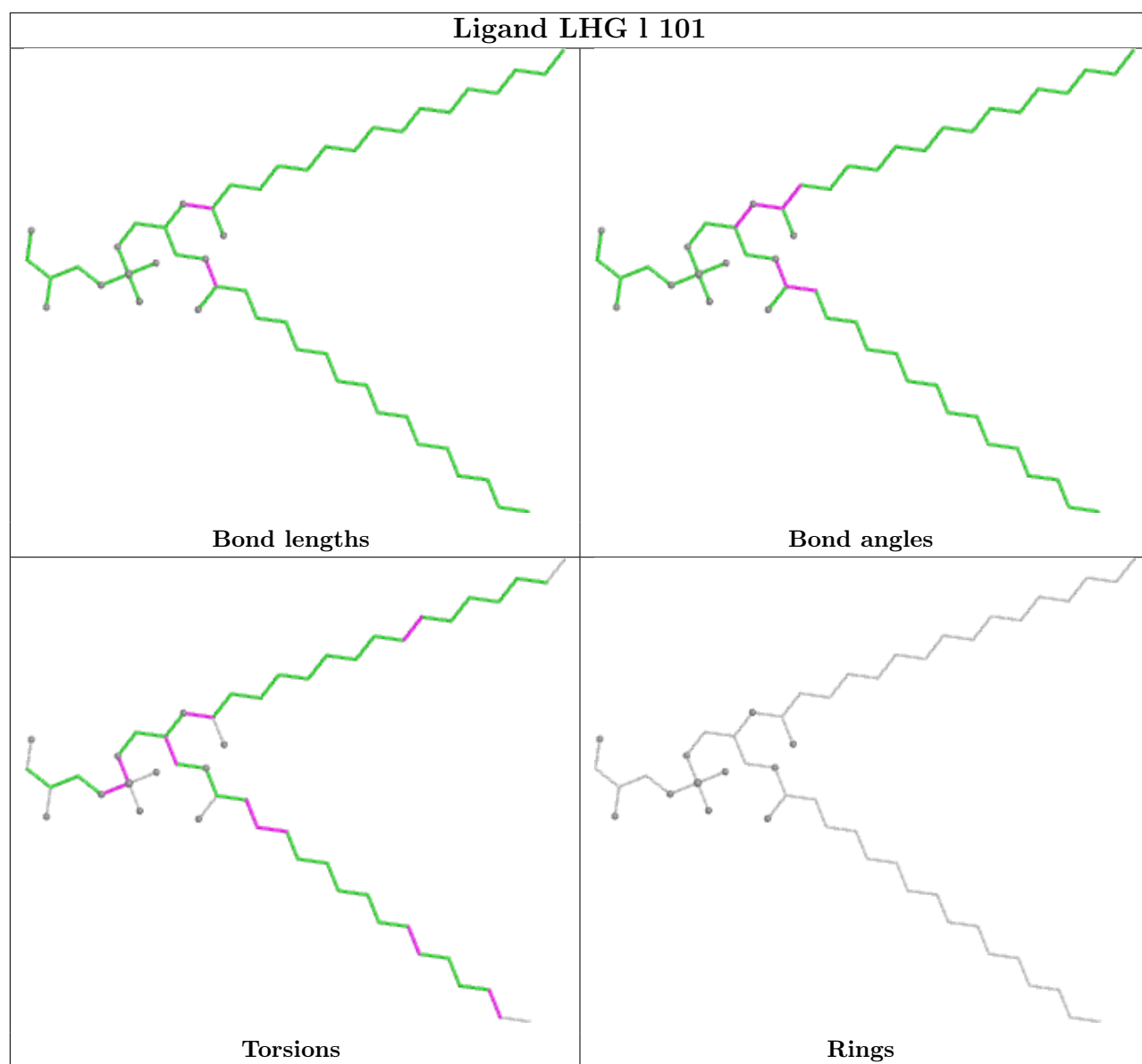
Ligand CLA 2 610

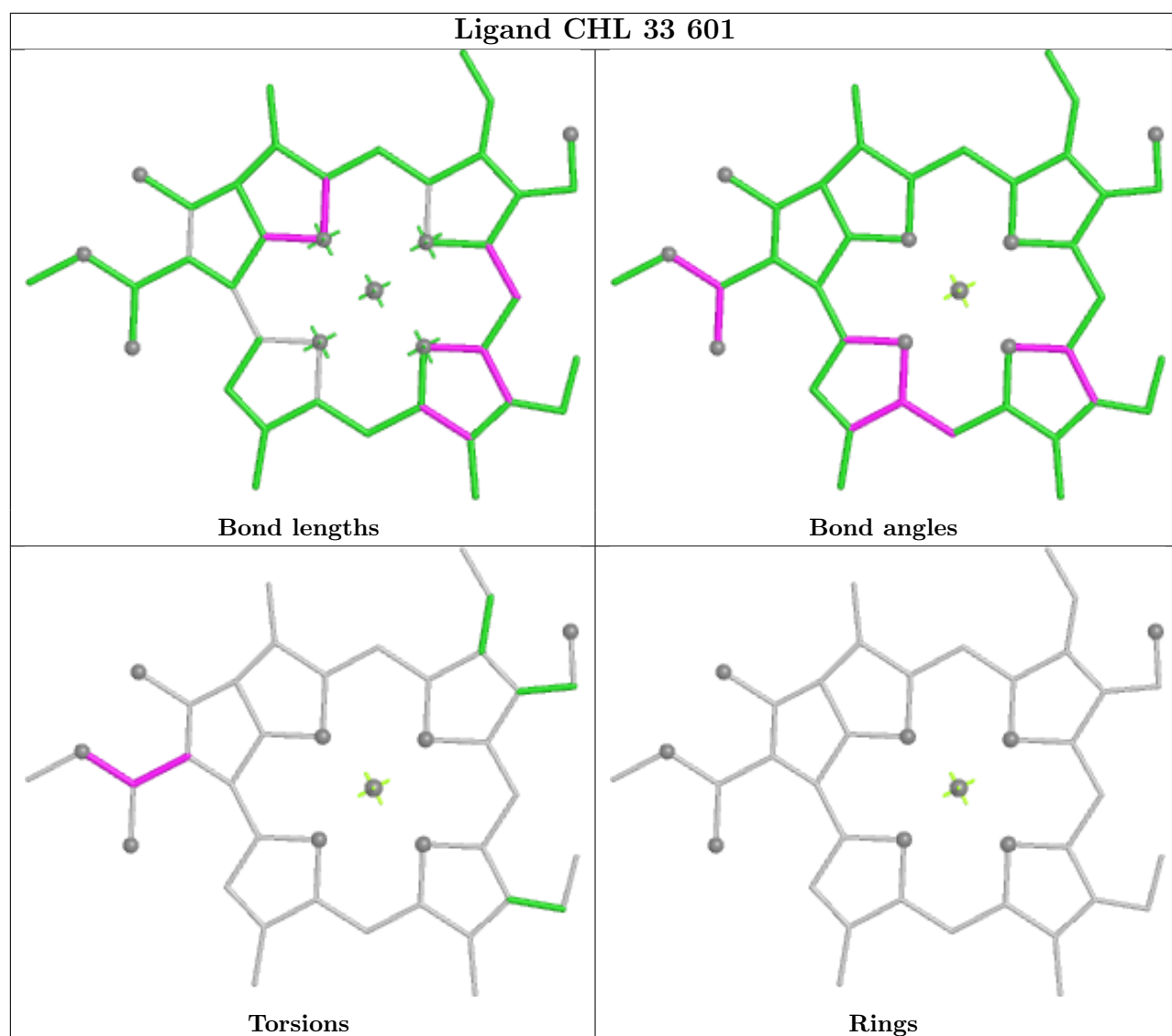


Ligand BCR b 617

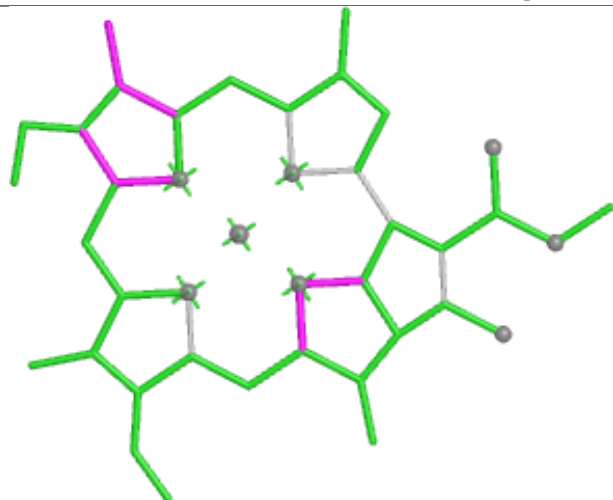




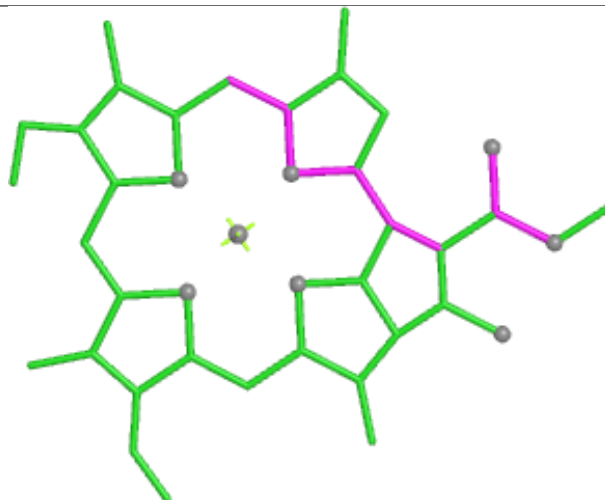




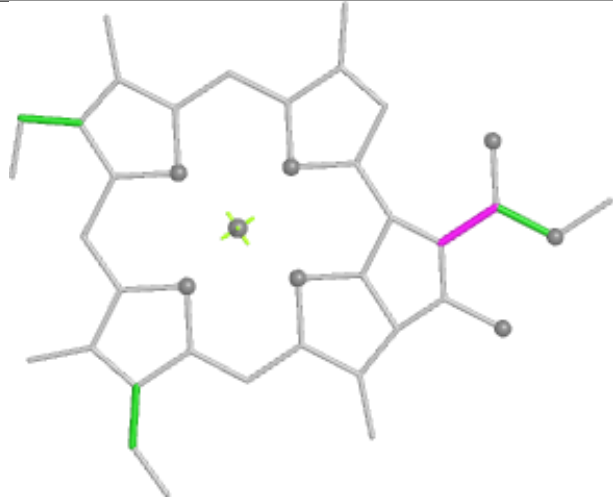
Ligand CLA 1 612



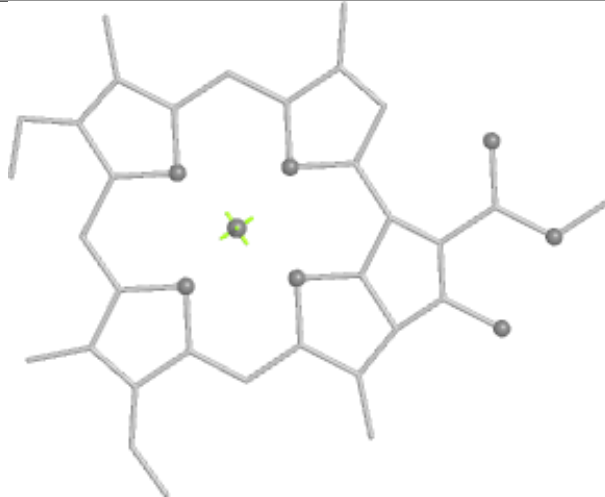
Bond lengths



Bond angles

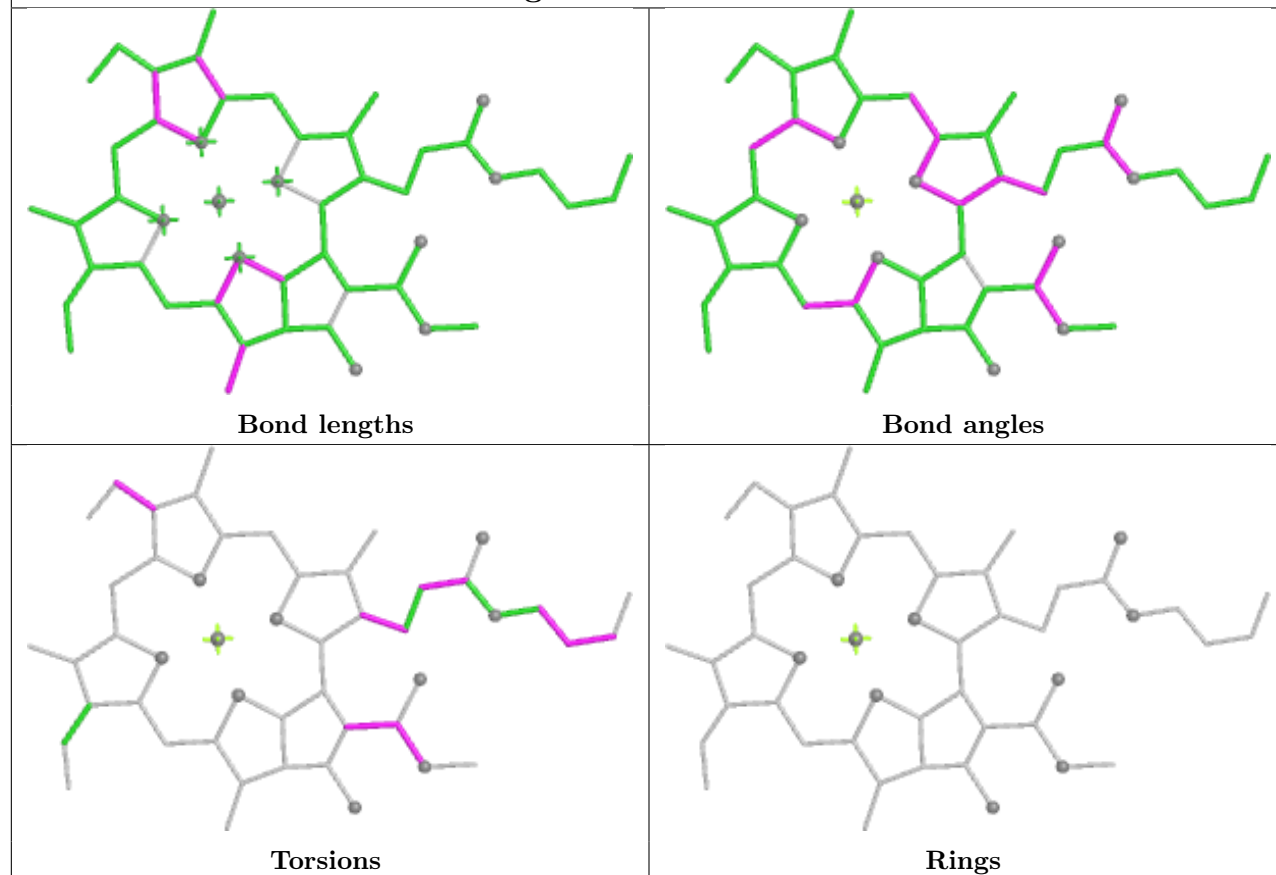


Torsions

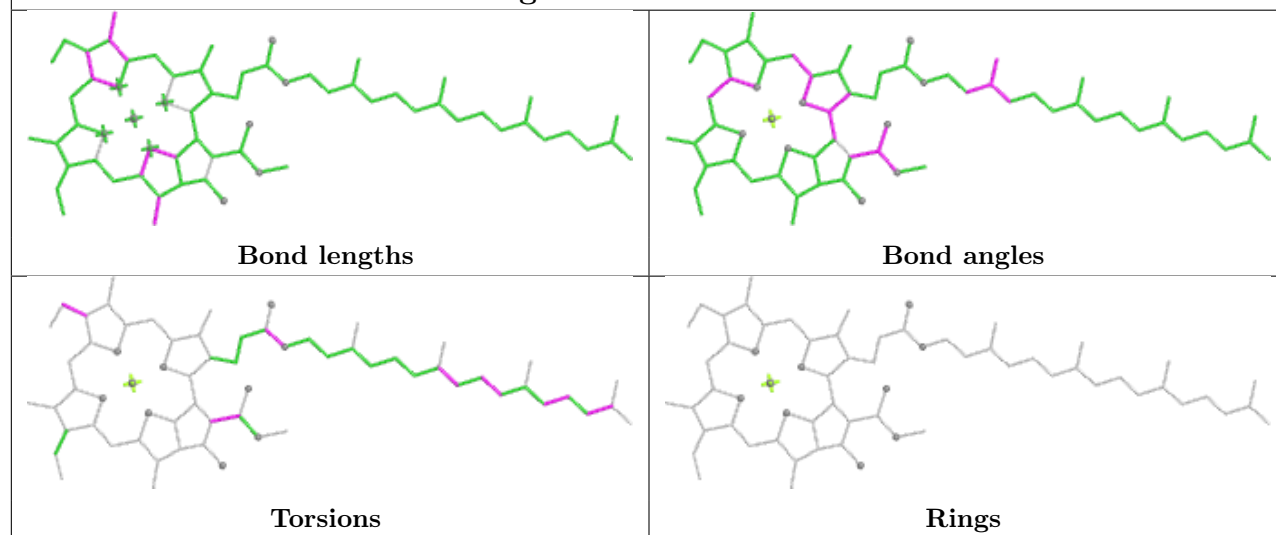


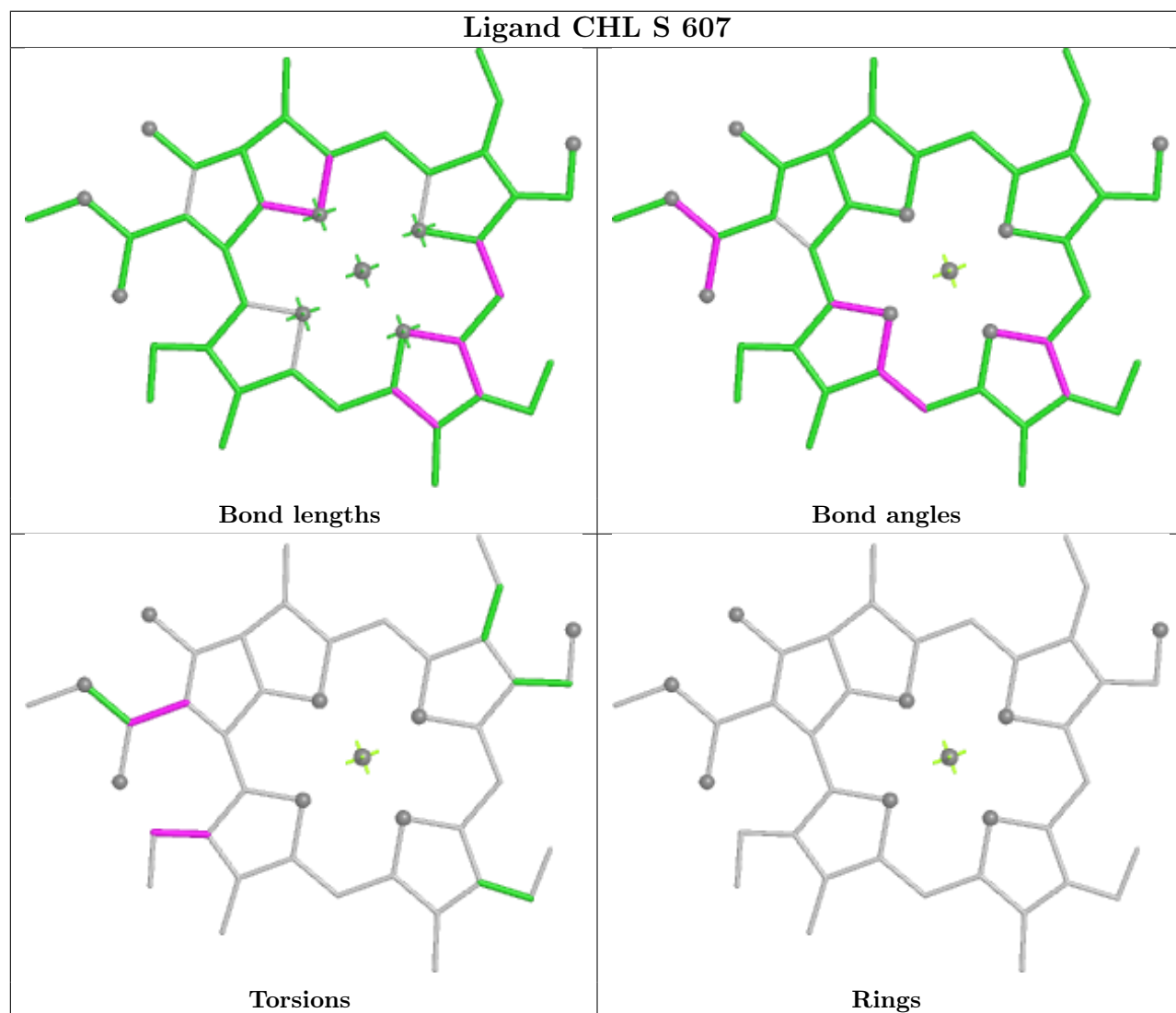
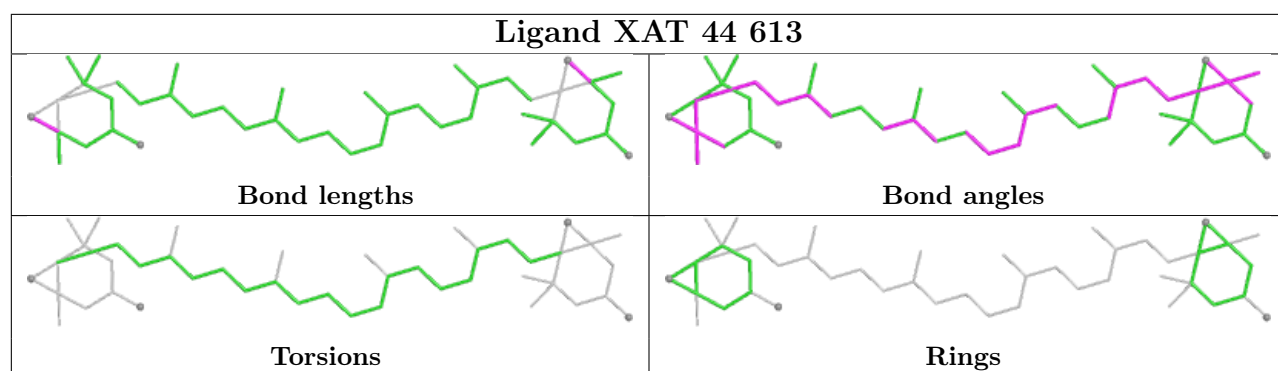
Rings

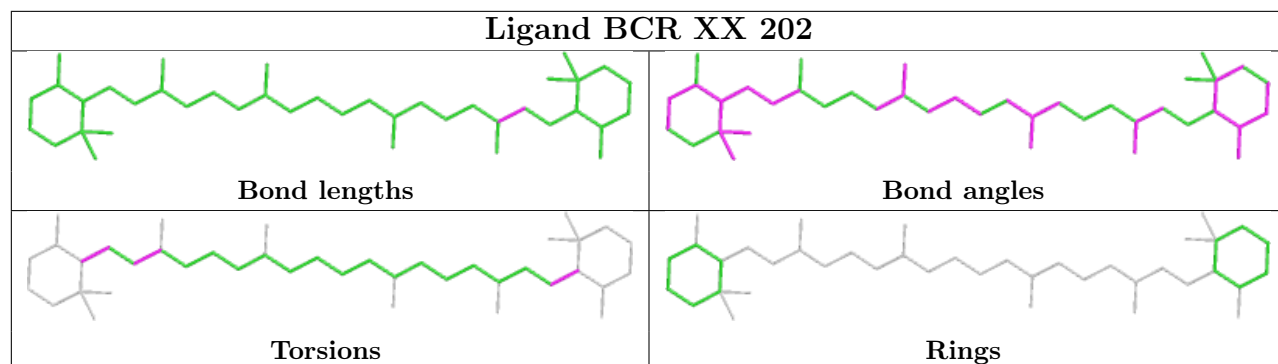
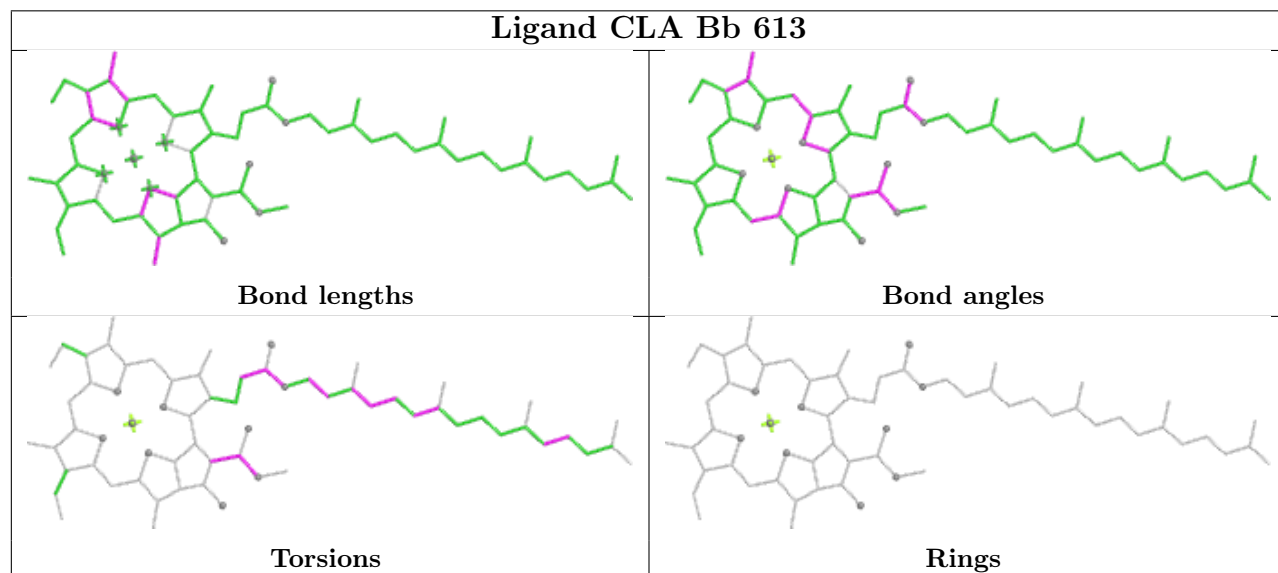
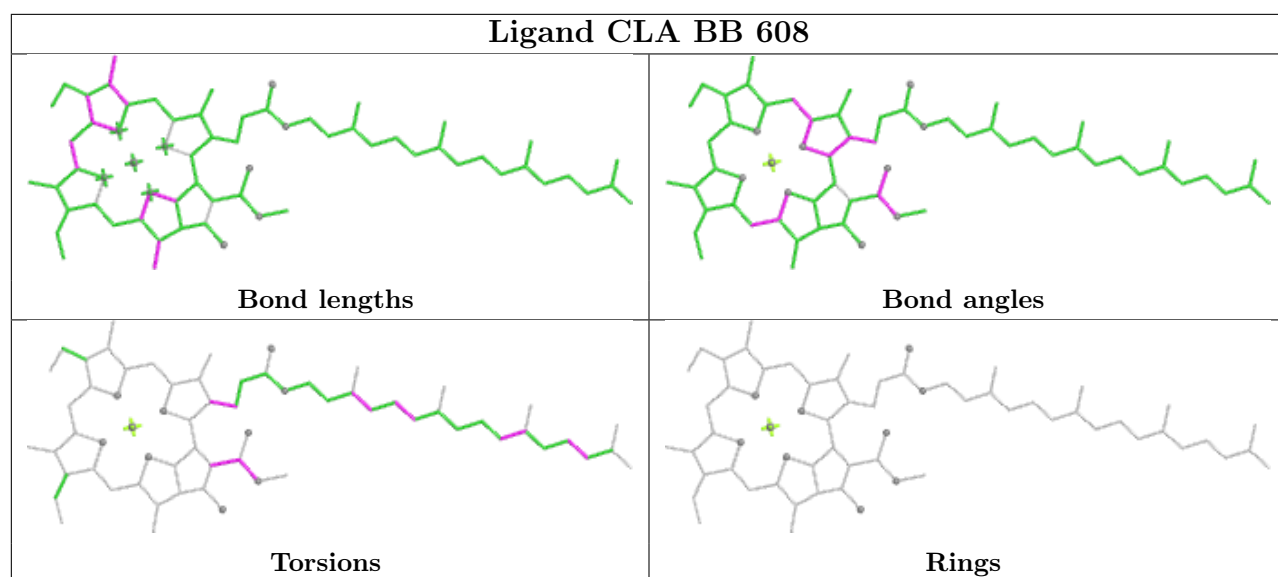
Ligand CLA Rr 604



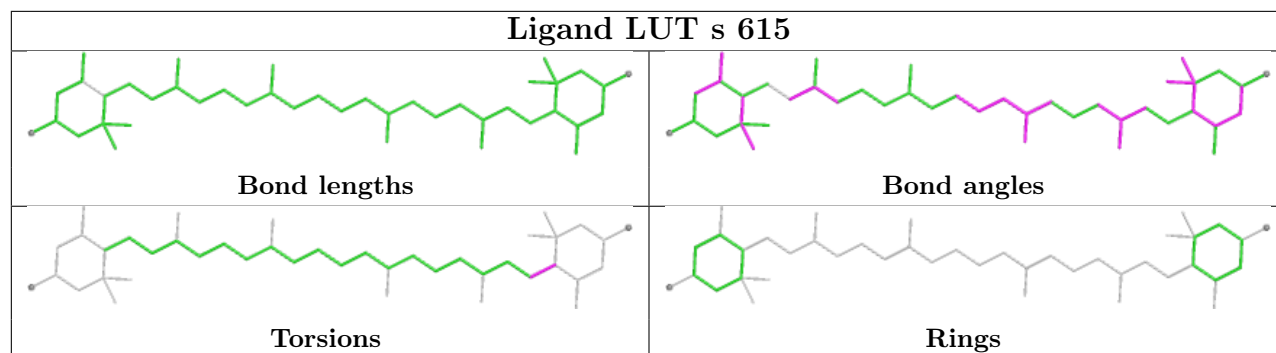
Ligand CLA CC 508



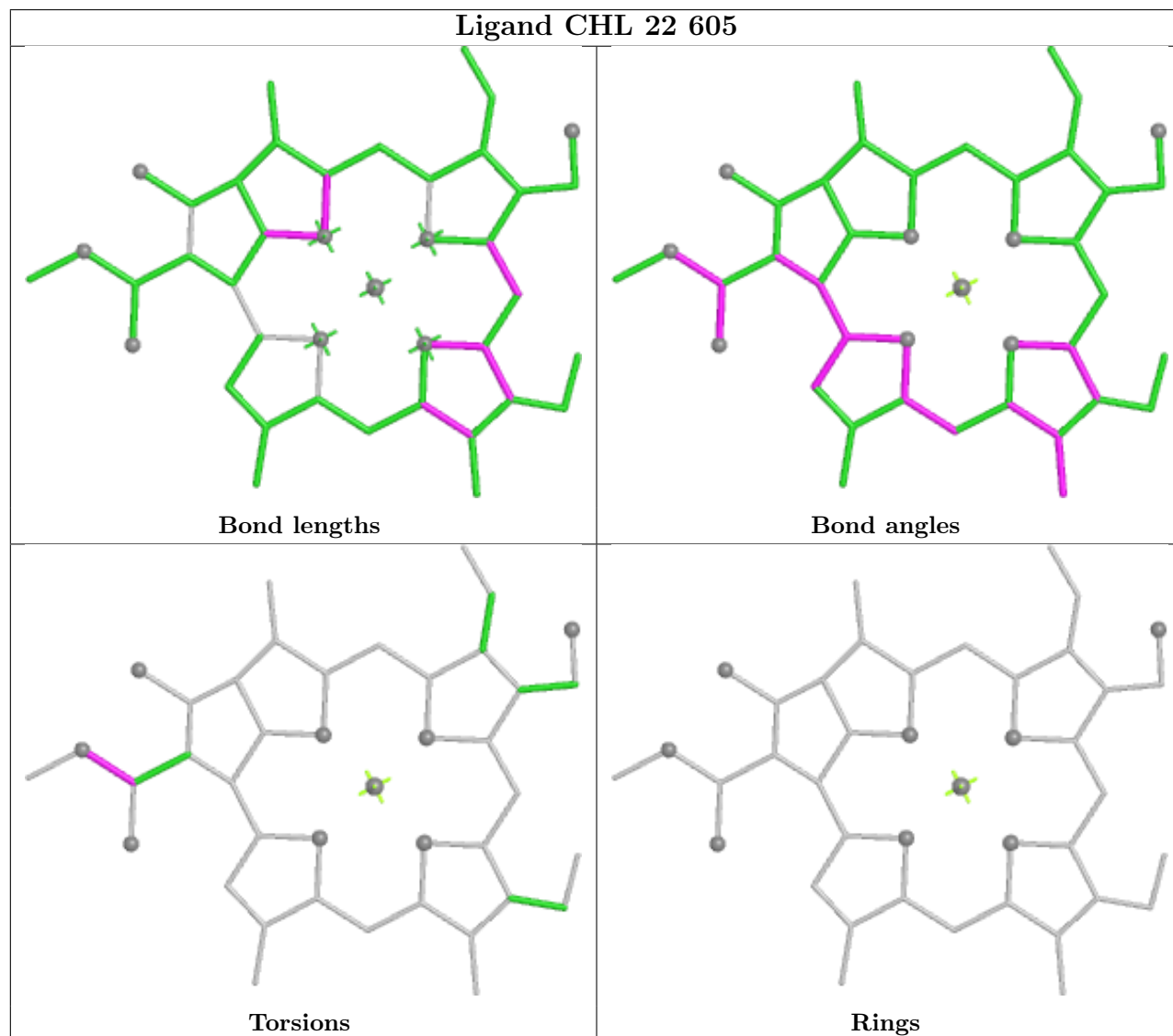




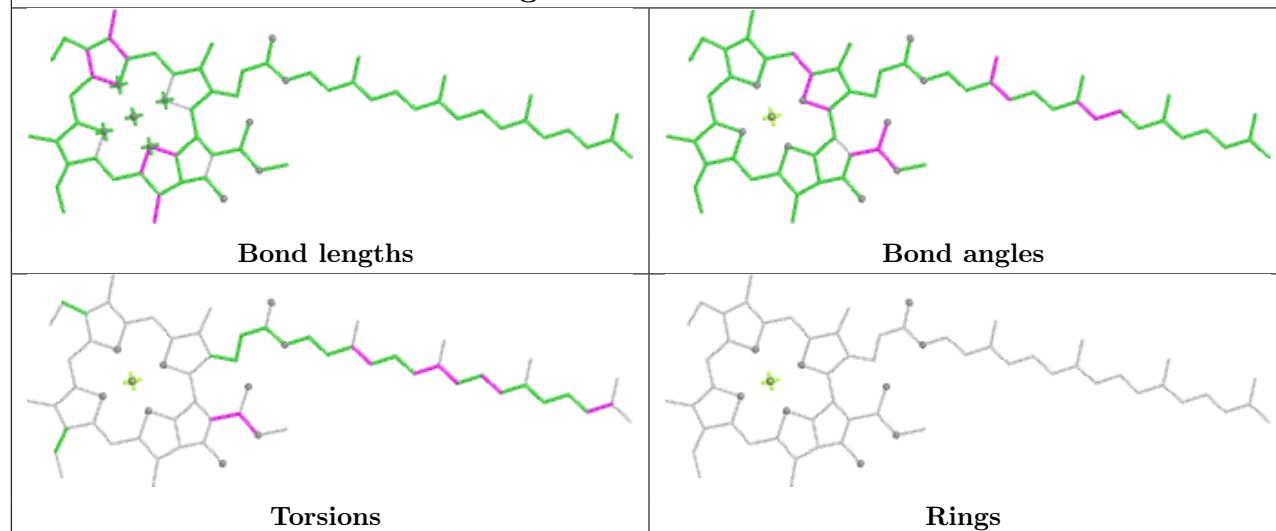
Ligand LUT s 615



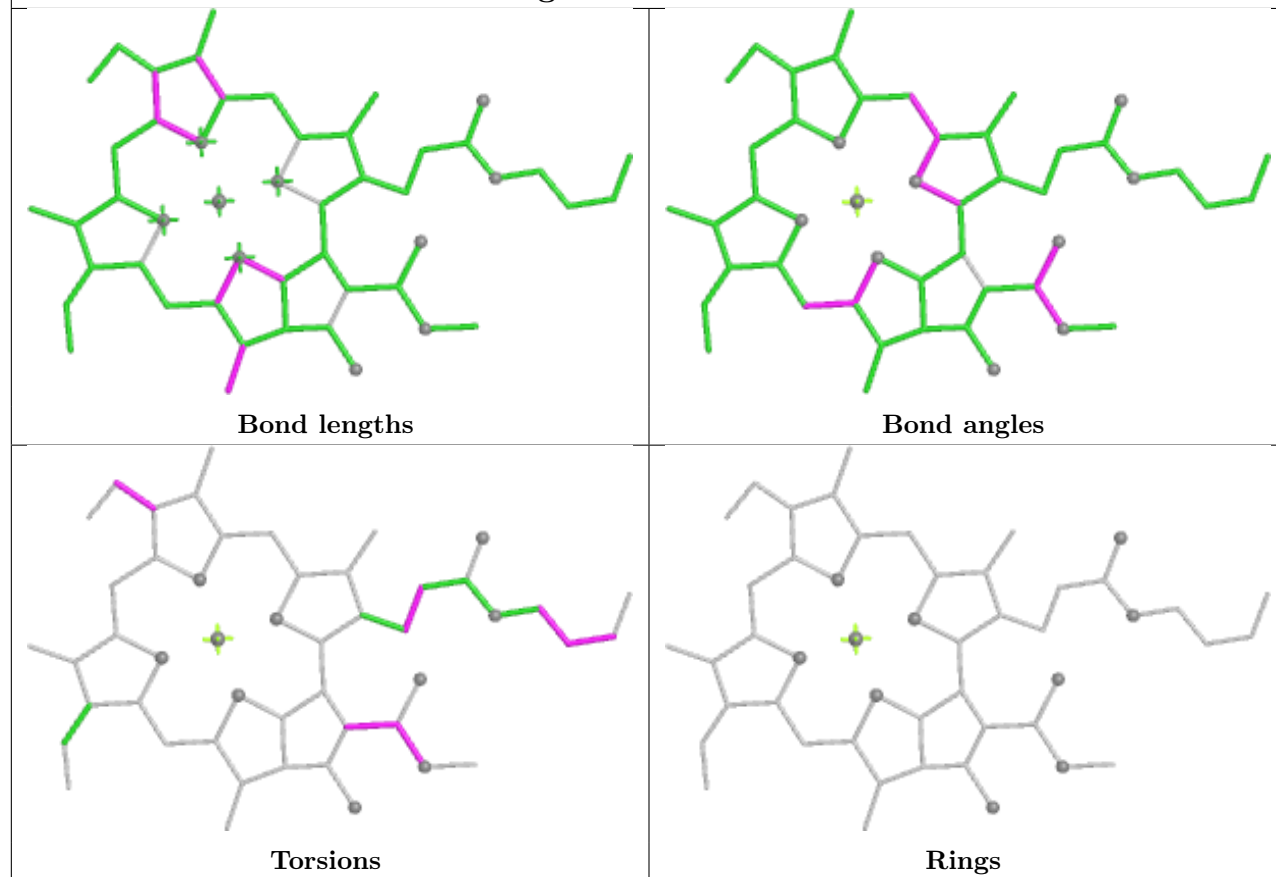
Ligand CHL 22 605



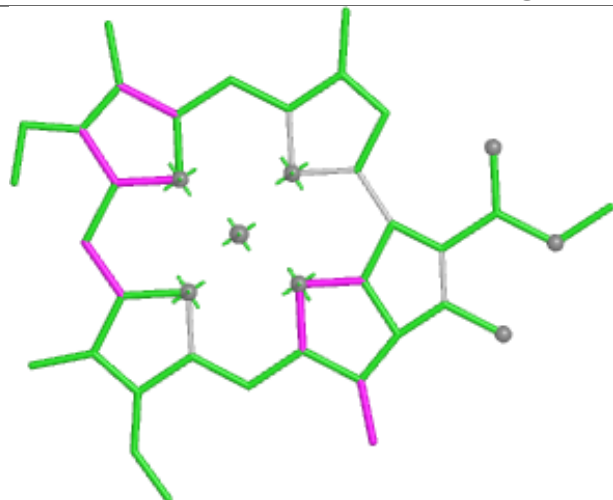
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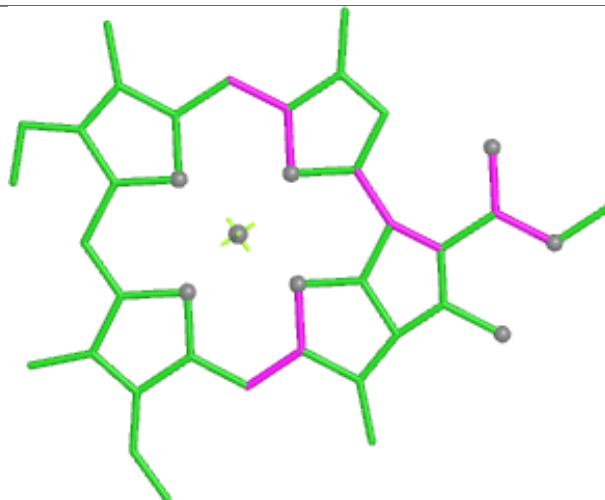
Ligand CLA s 610



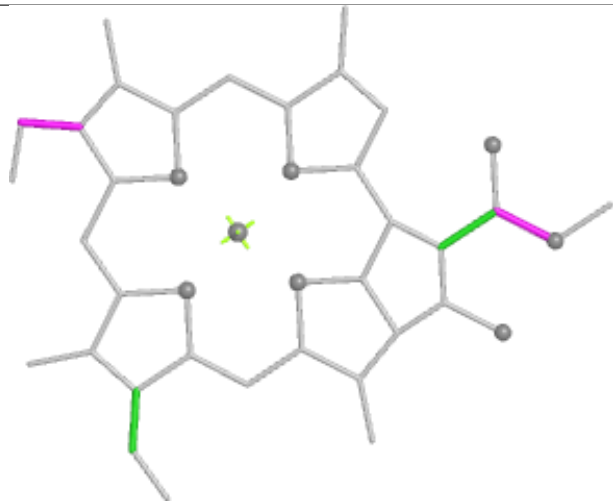
Ligand CLA 2 613



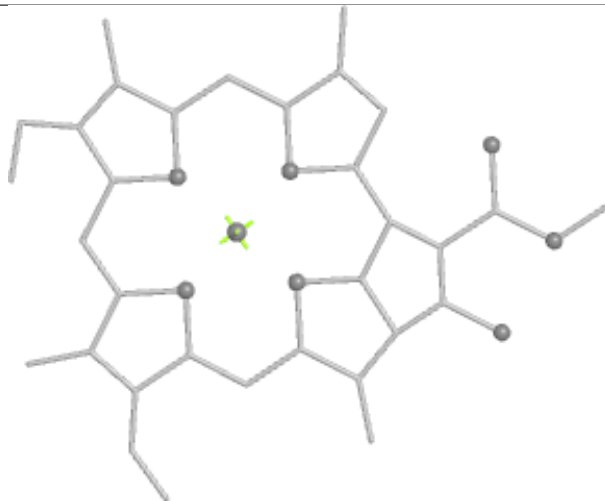
Bond lengths



Bond angles

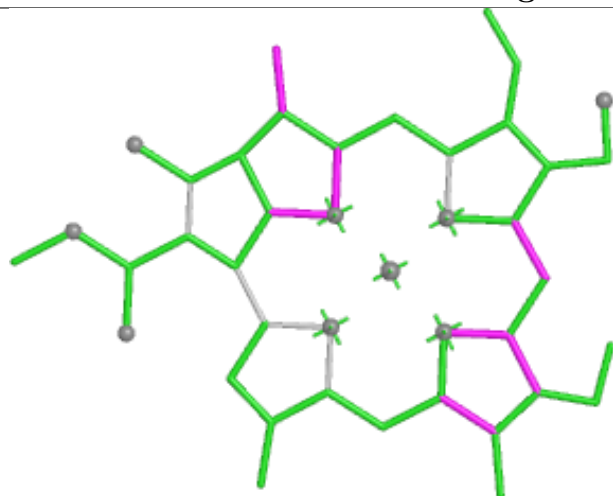


Torsions

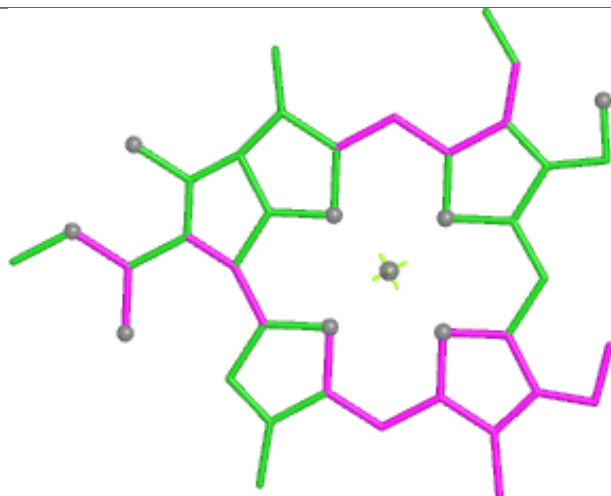


Rings

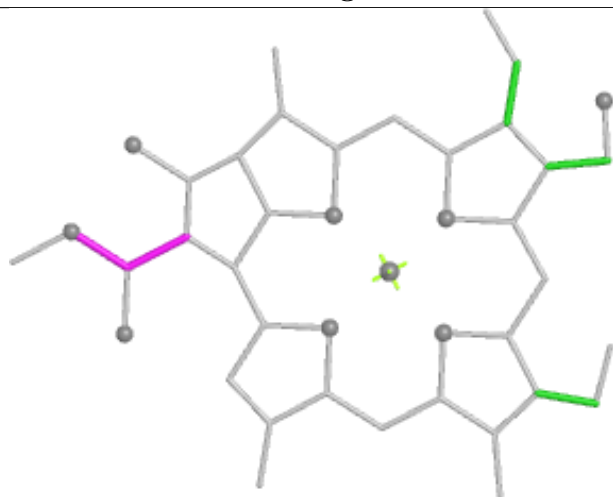
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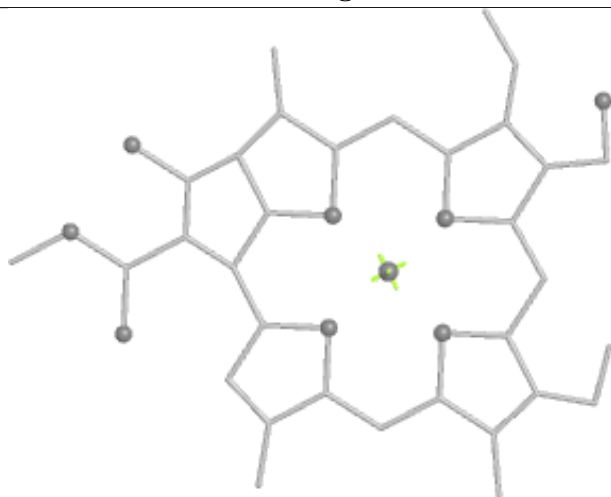
Bond lengths



Bond angles

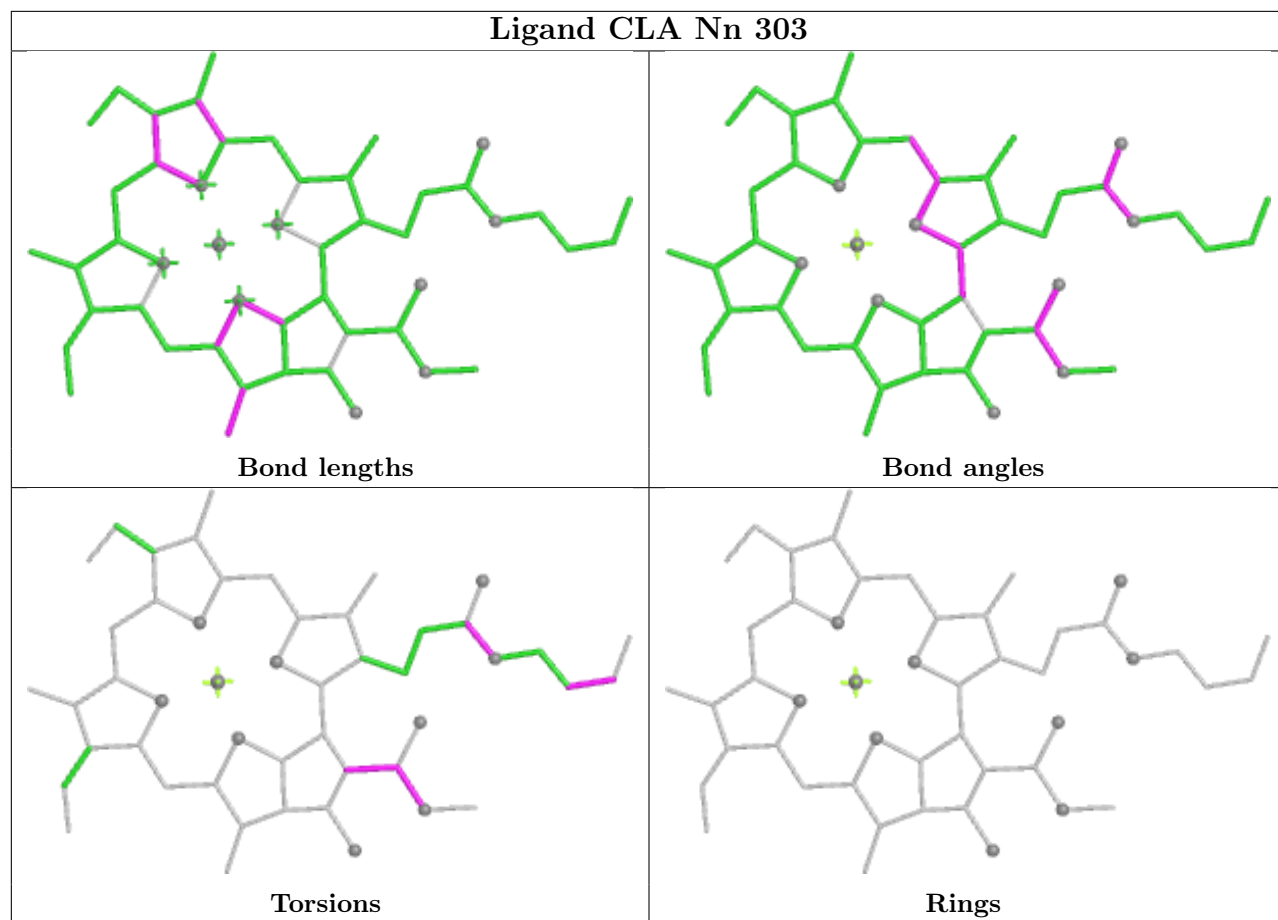


Torsions

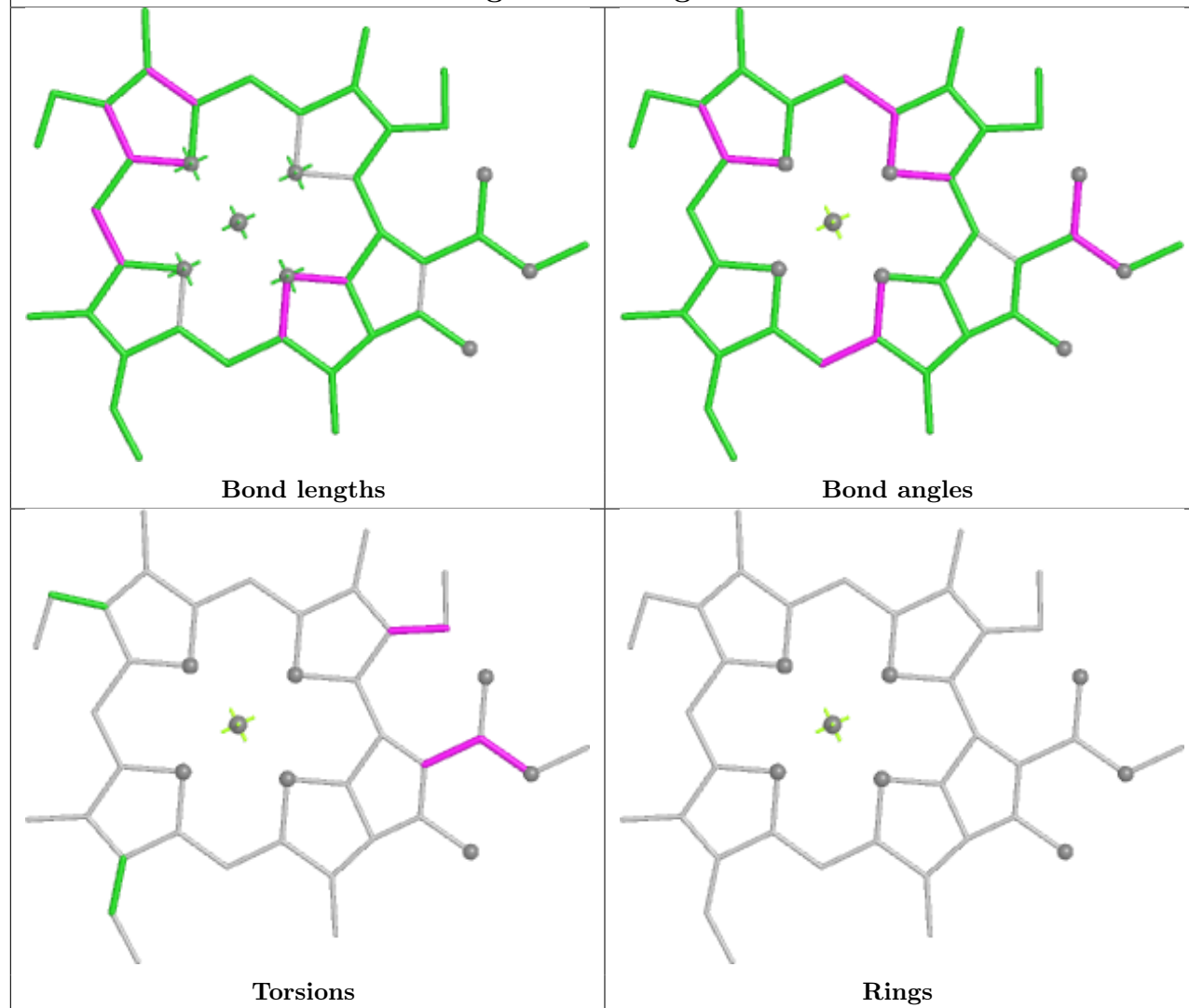


Rings

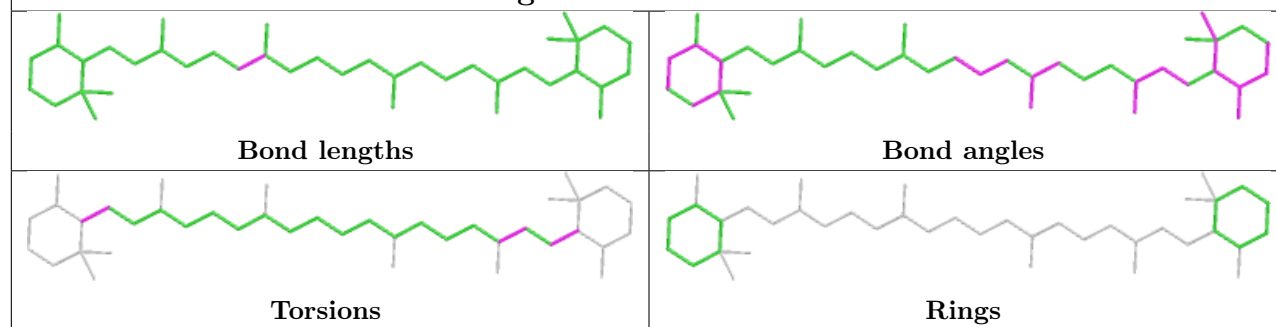
Ligand CLA Nn 303

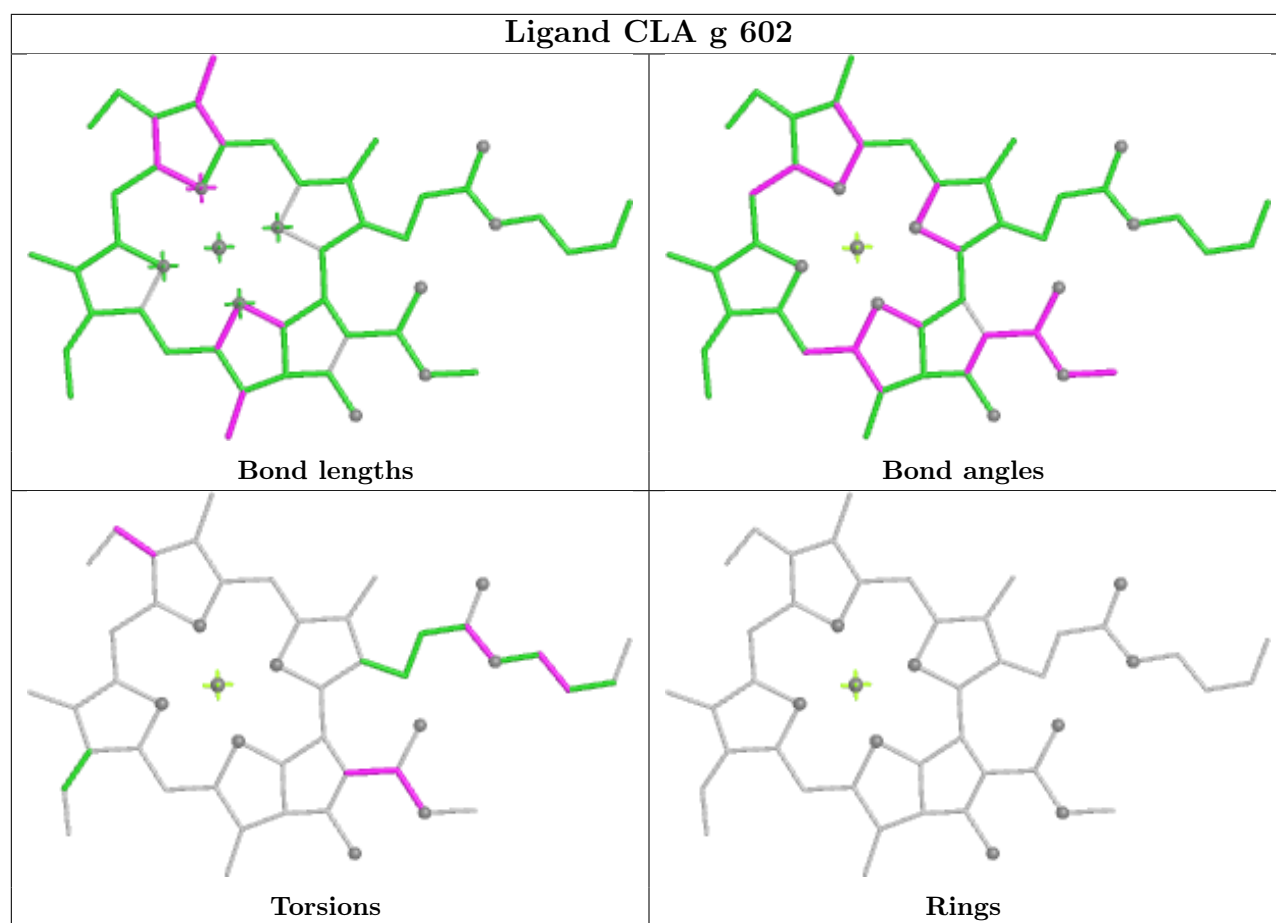


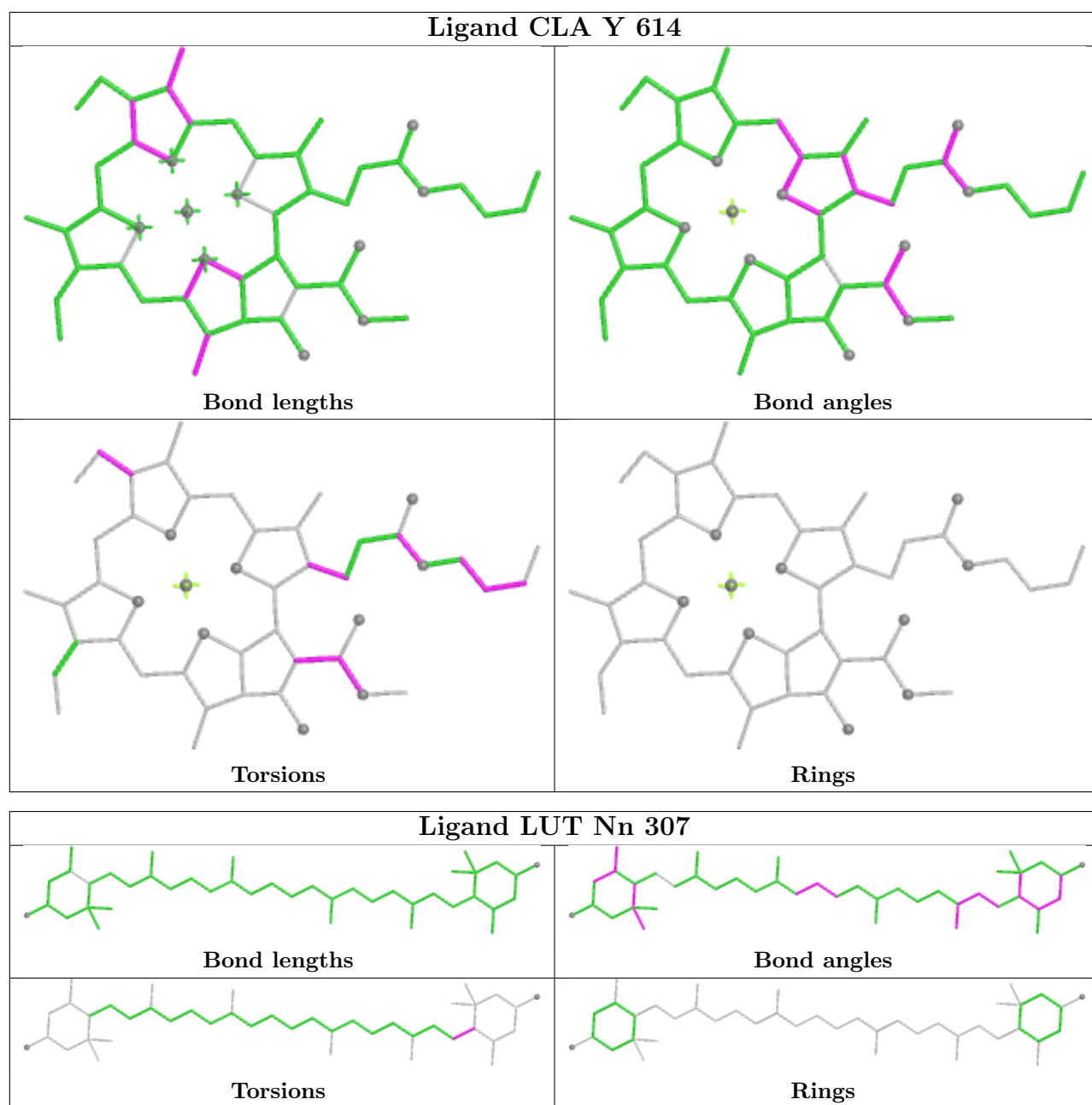
Ligand CLA Gg 305



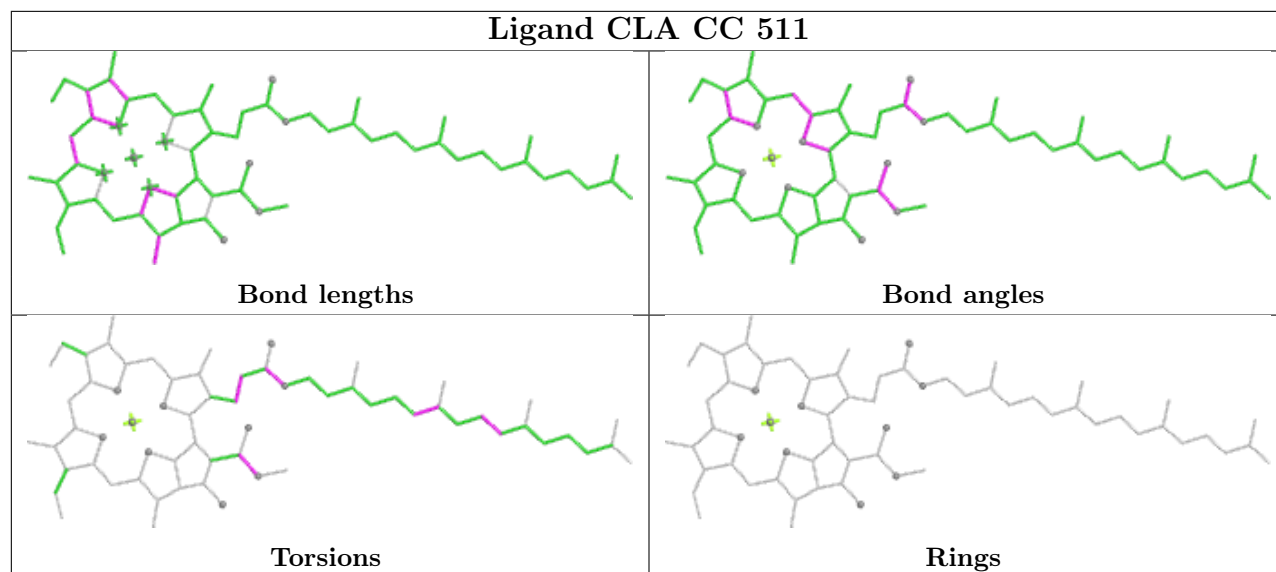
Ligand BCR CC 516



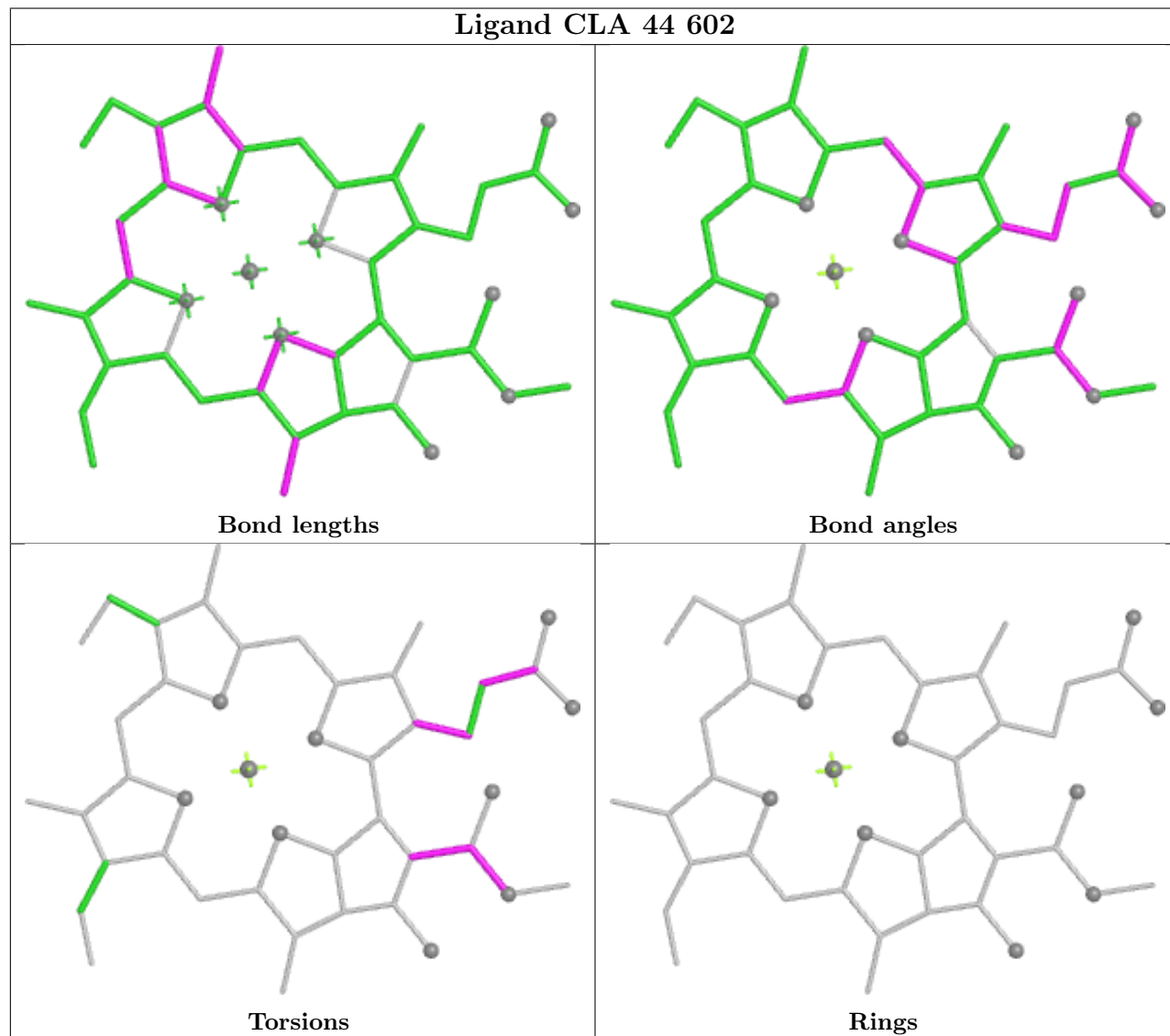




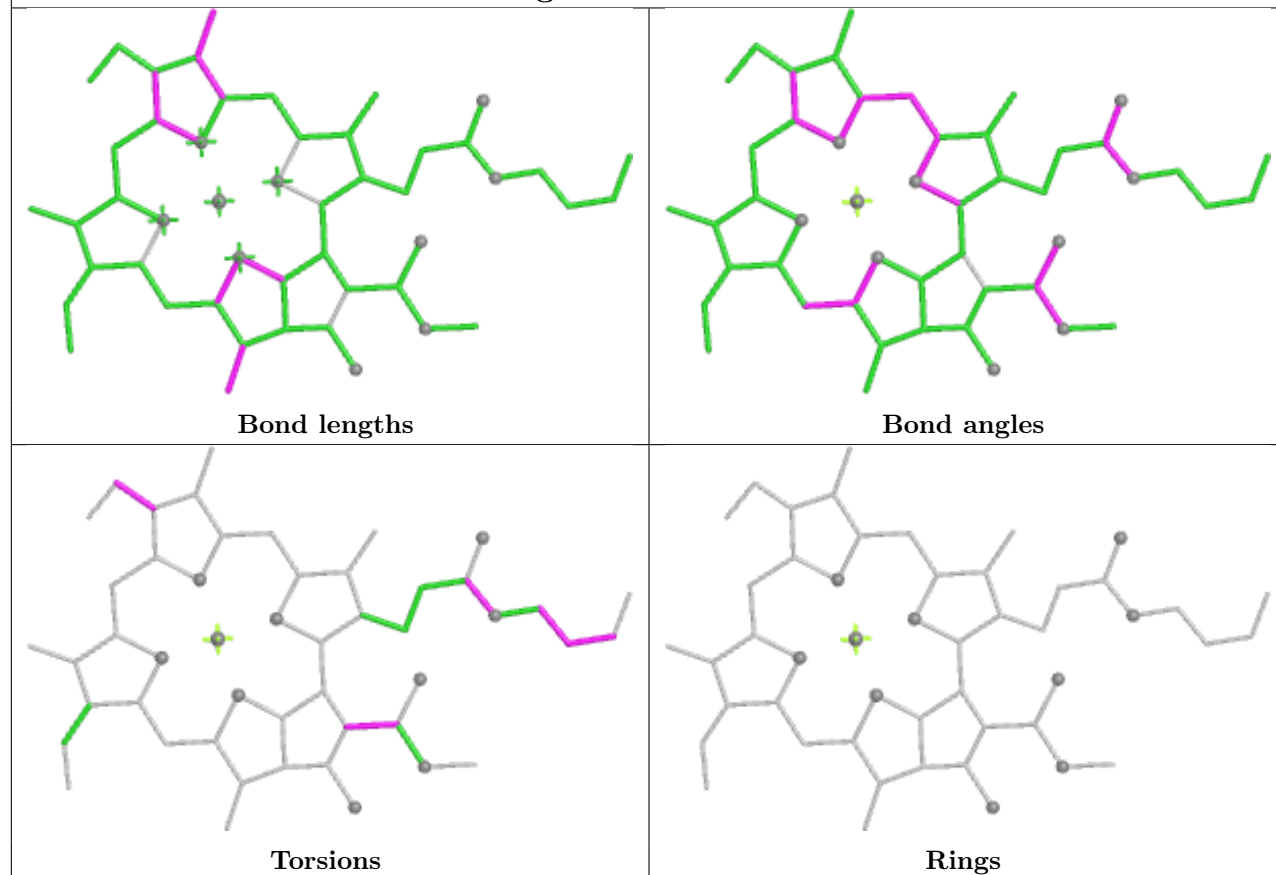
Ligand CLA CC 511



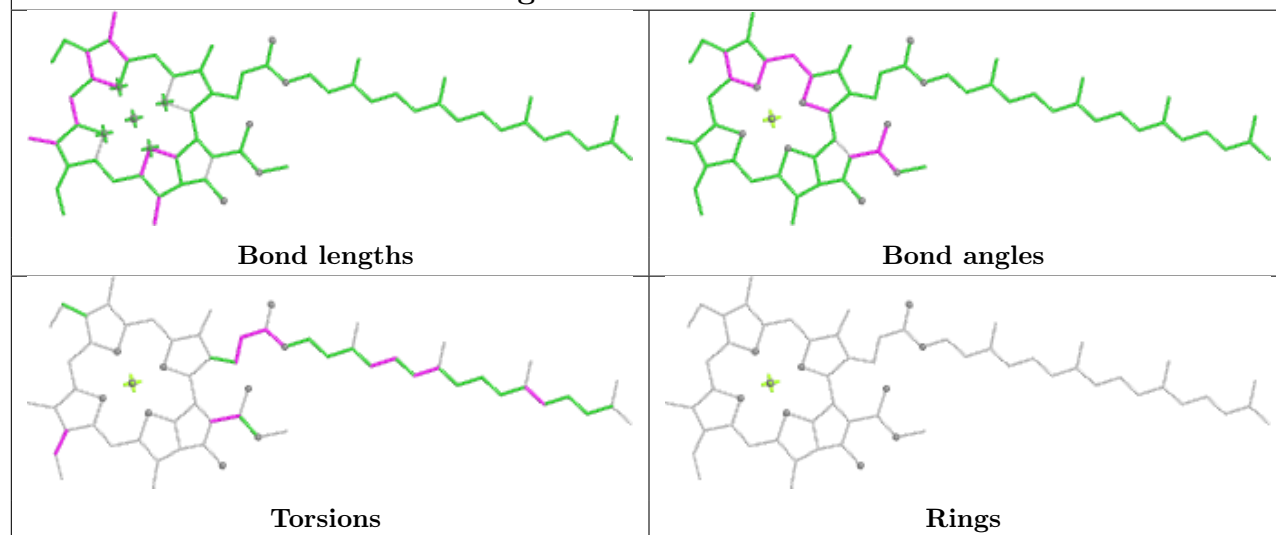
Ligand CLA 44 602

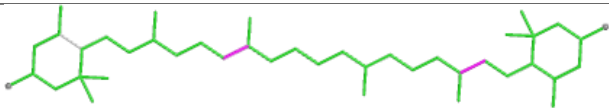
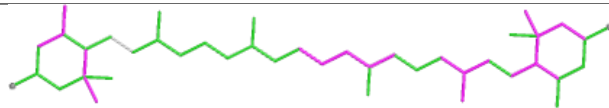
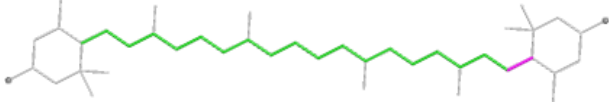
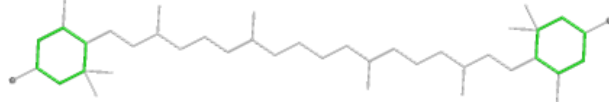


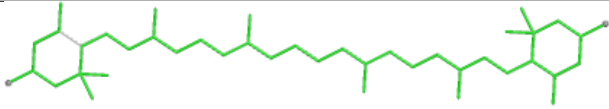
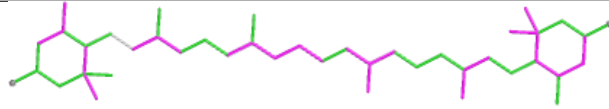
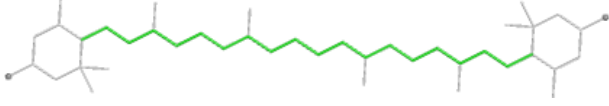
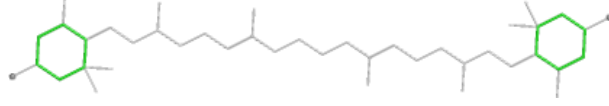
Ligand CLA a 407

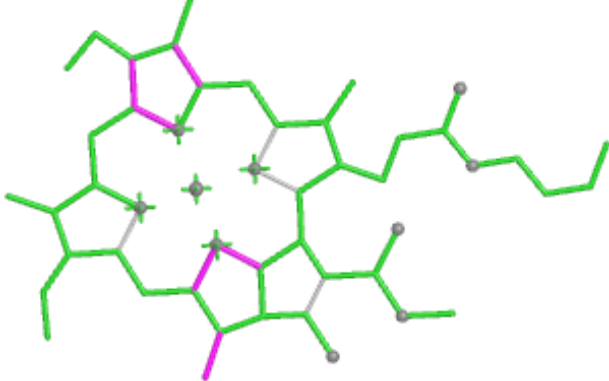
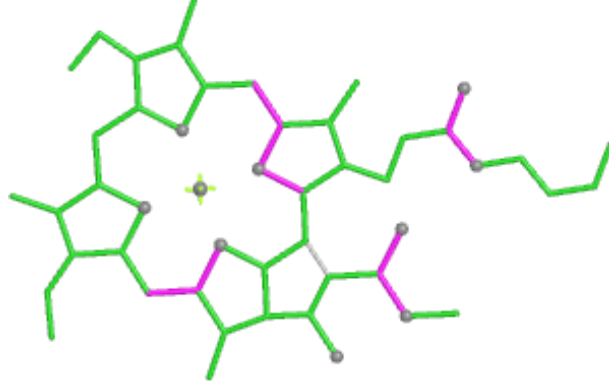
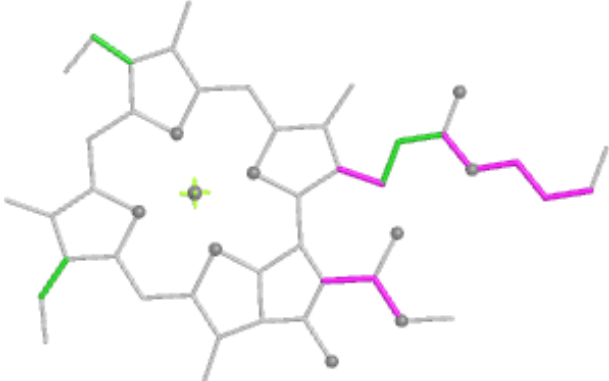
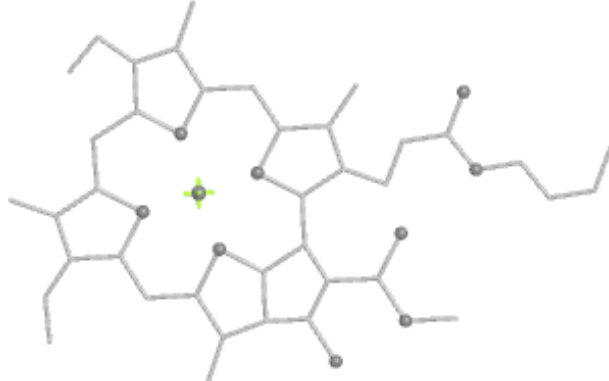


Ligand CLA DD 403

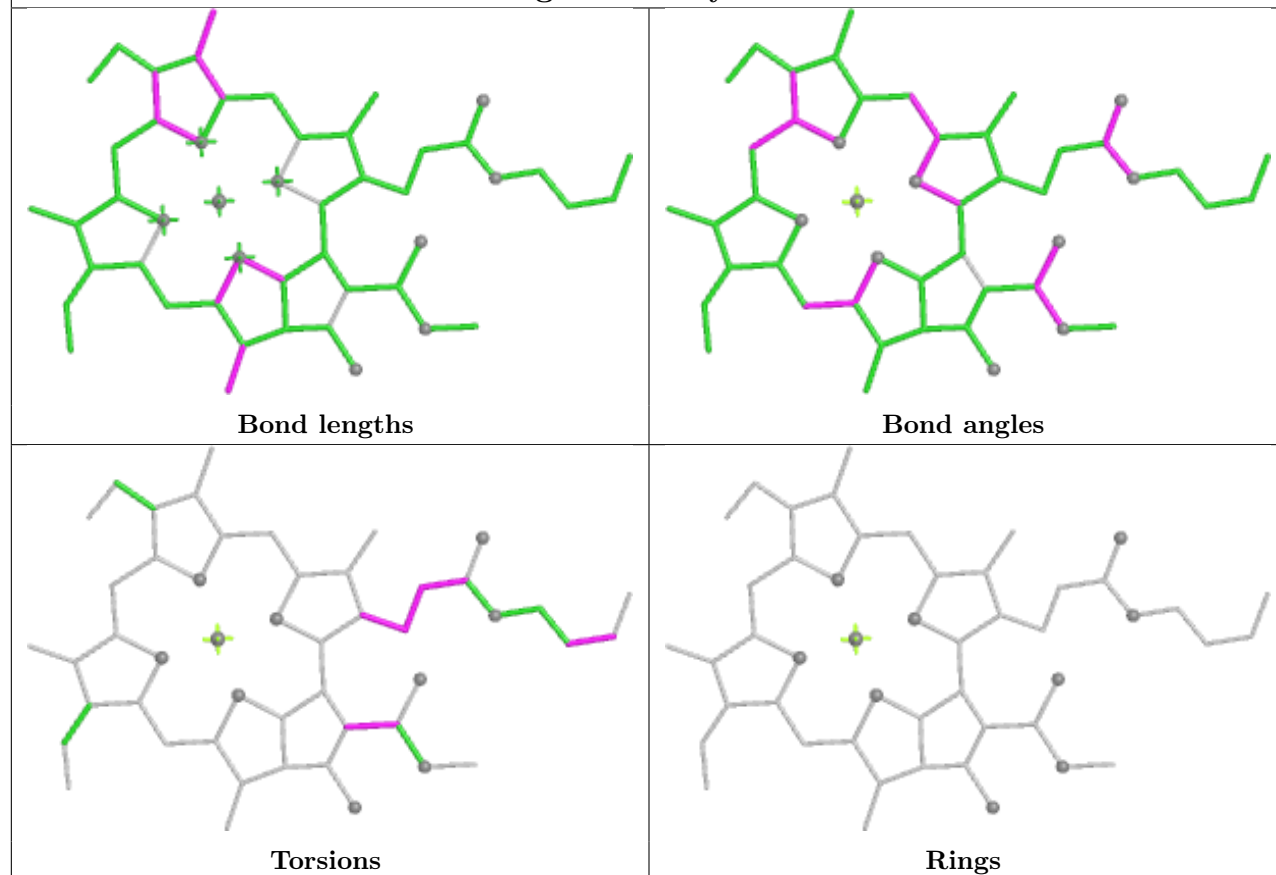


Ligand LUT Ss 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

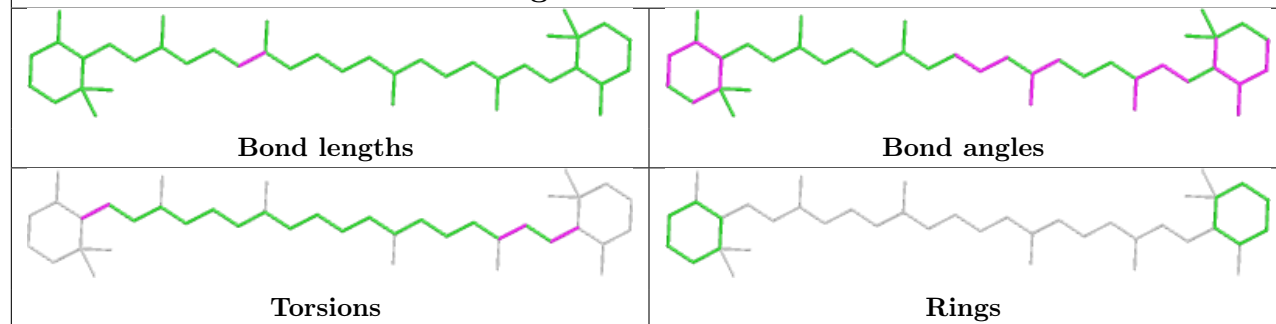
Ligand LUT R 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

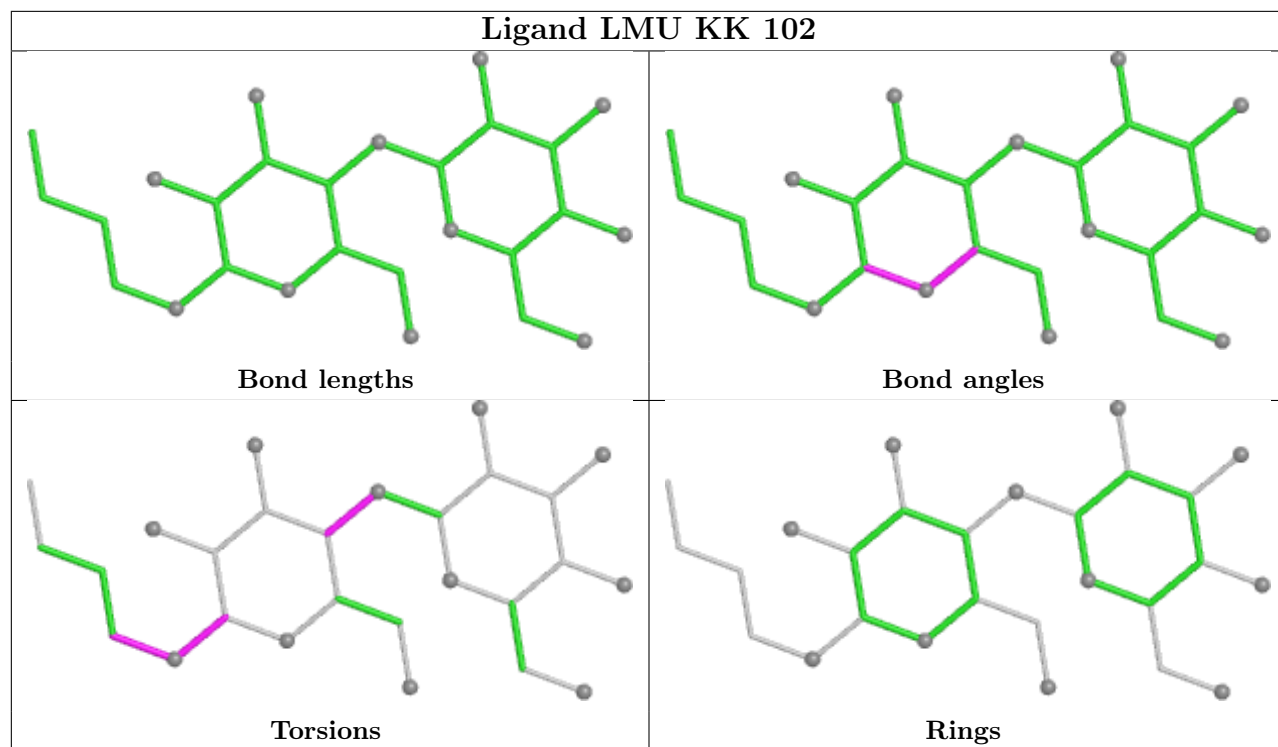
Ligand CLA n 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA y 306

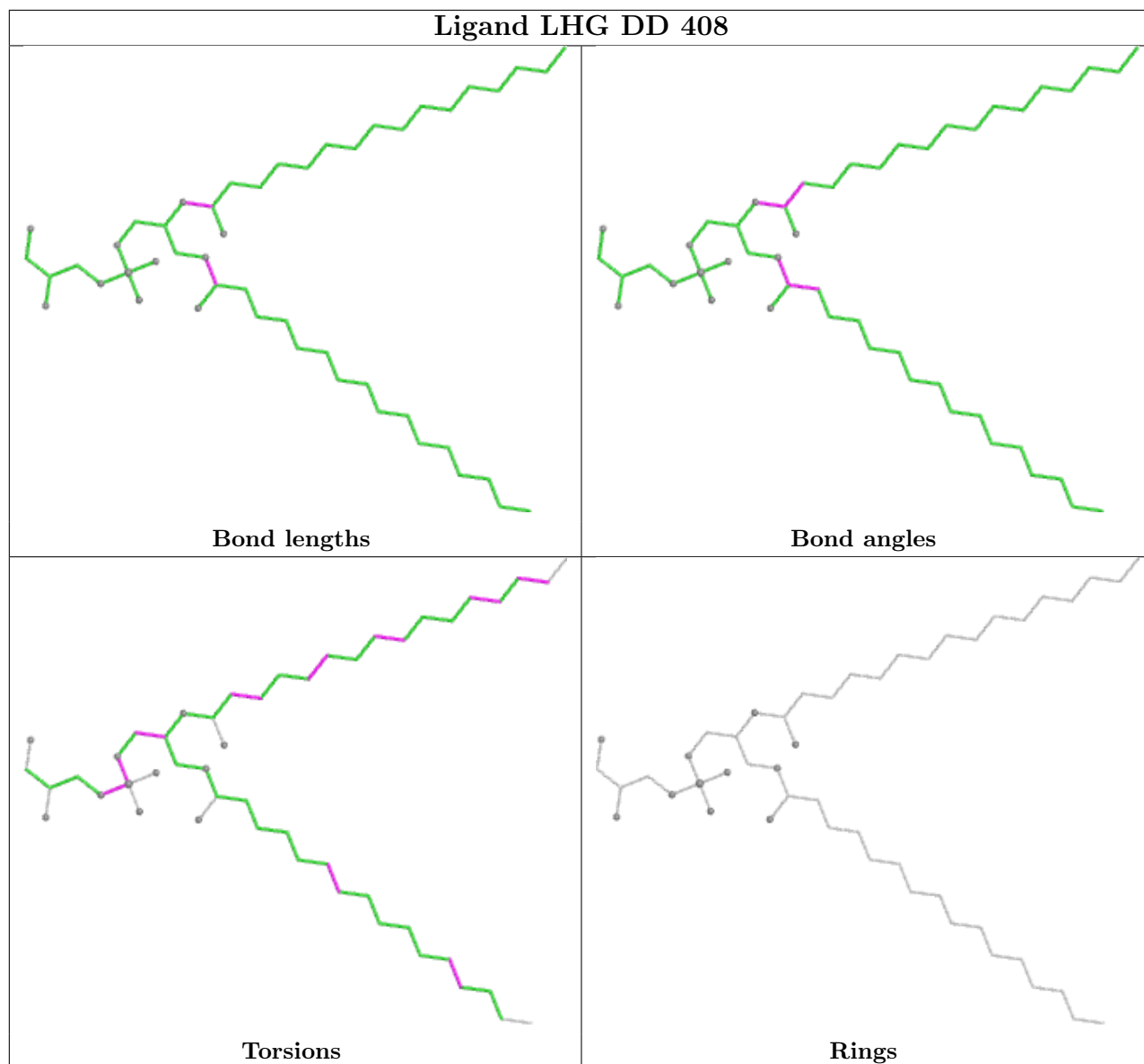


Ligand BCR C 517

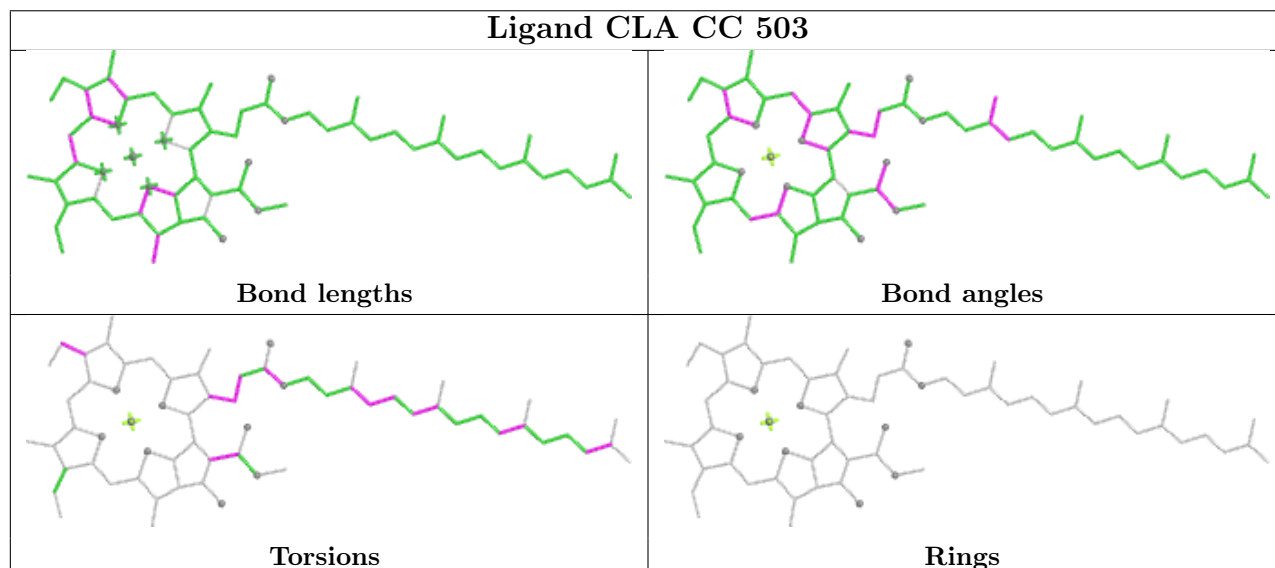


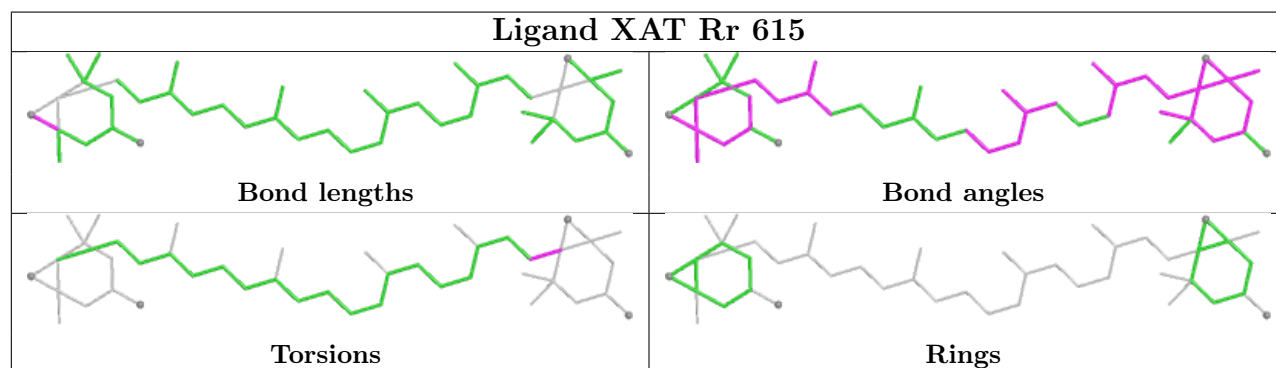
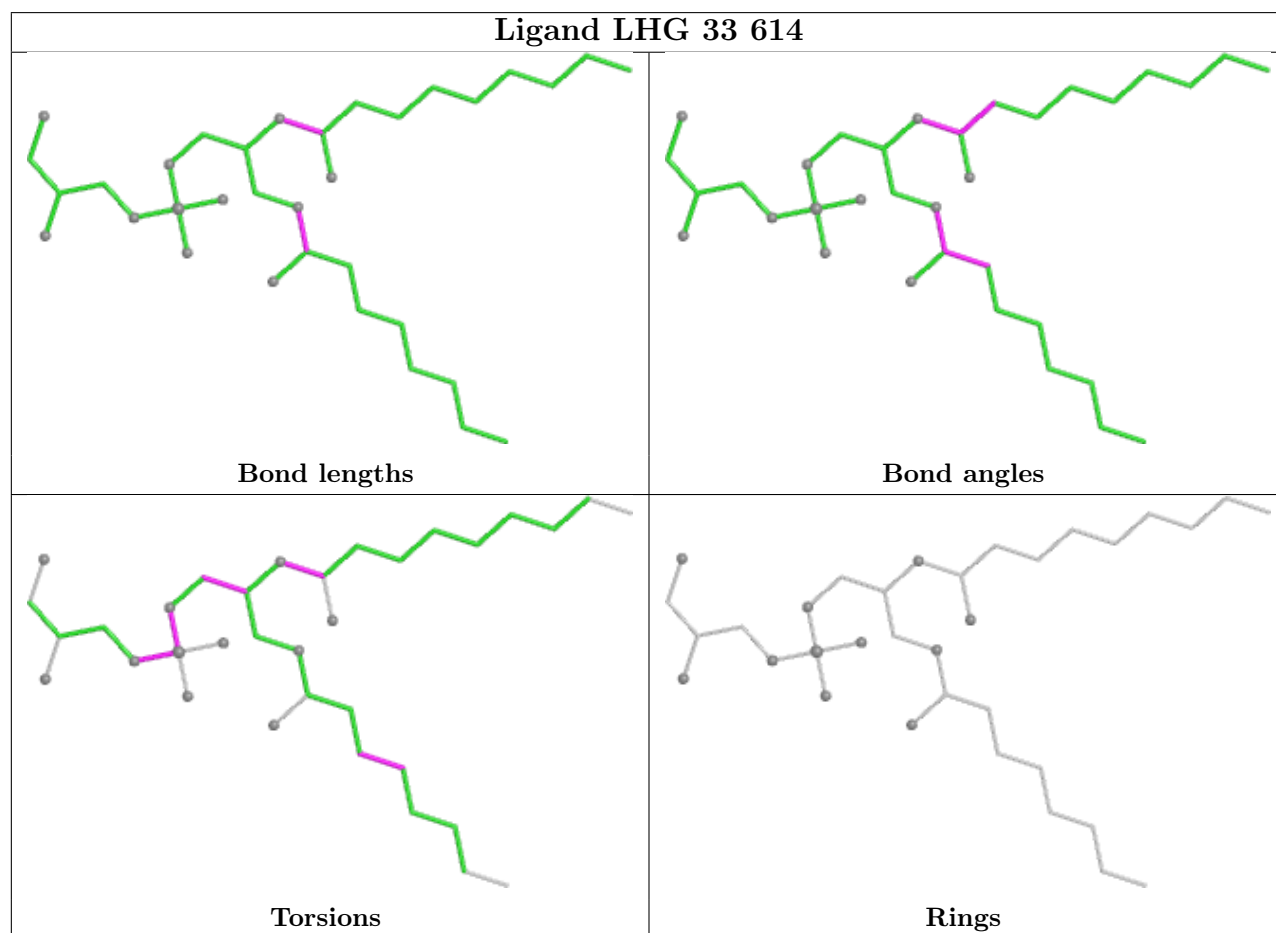
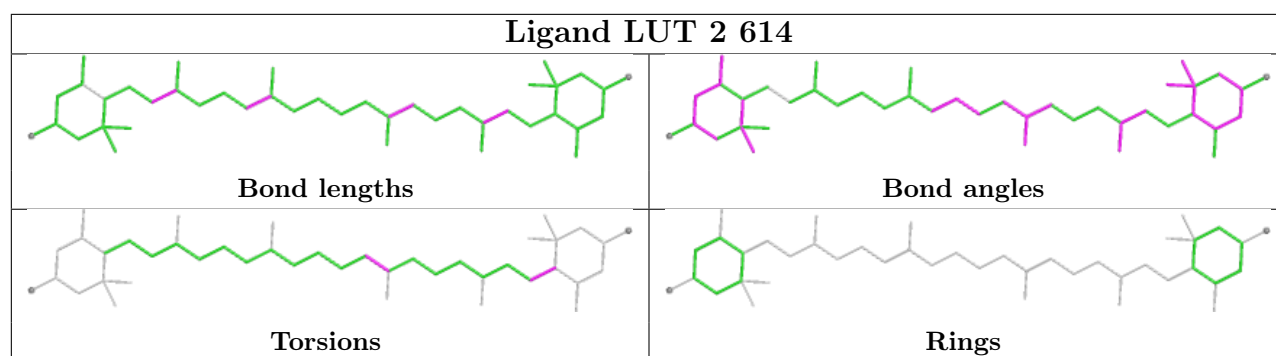


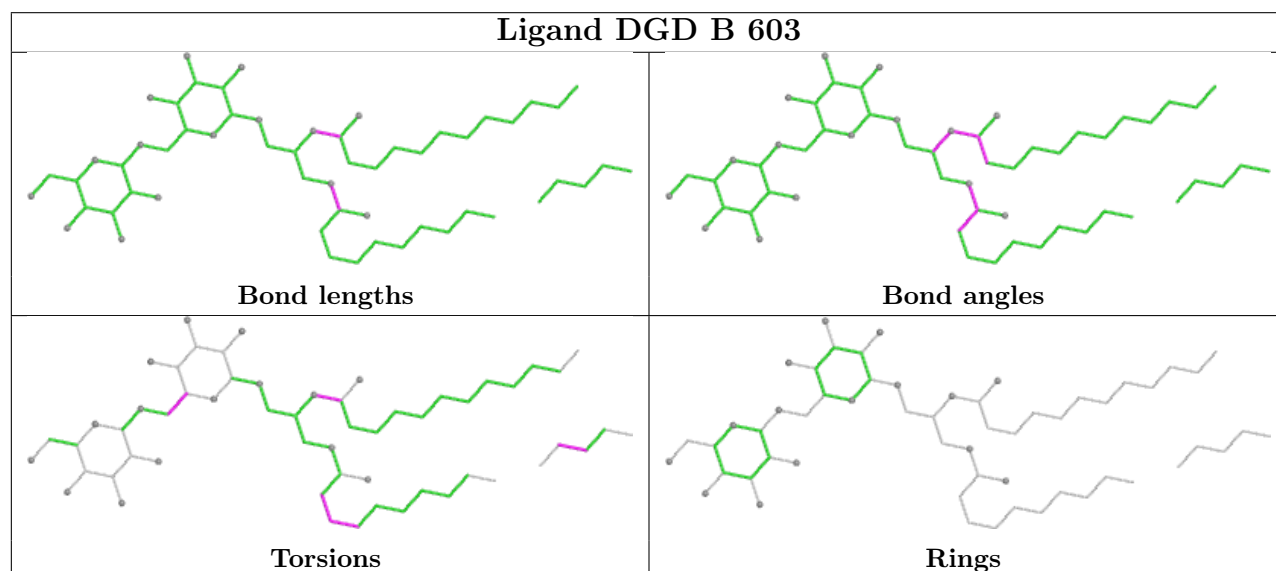
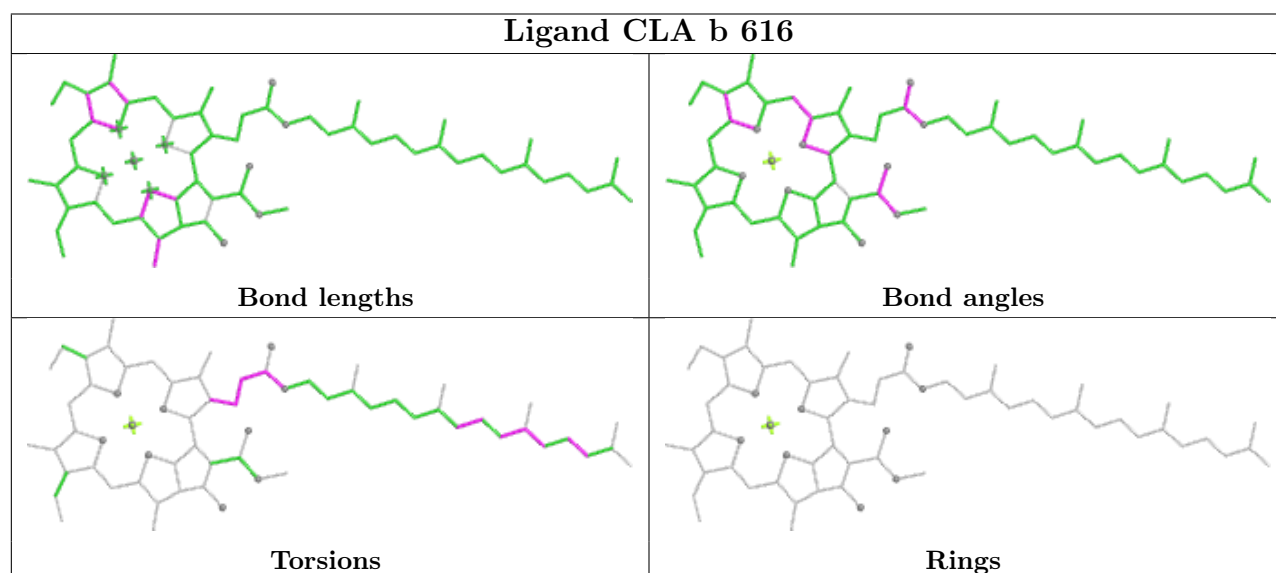
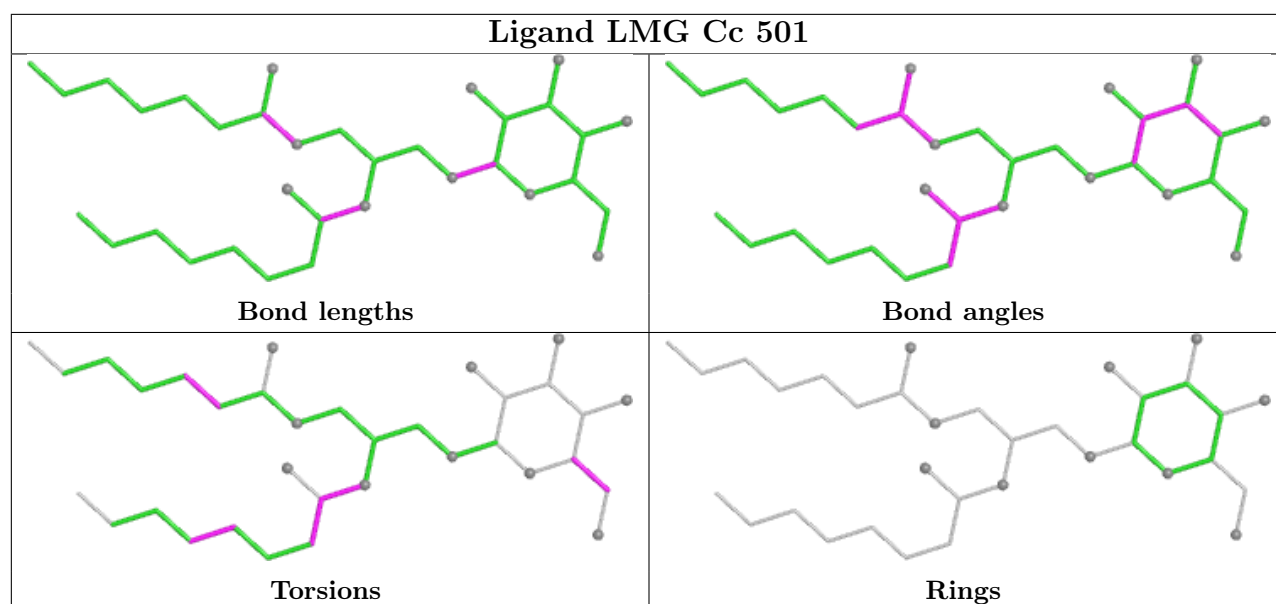
Ligand LHG DD 408



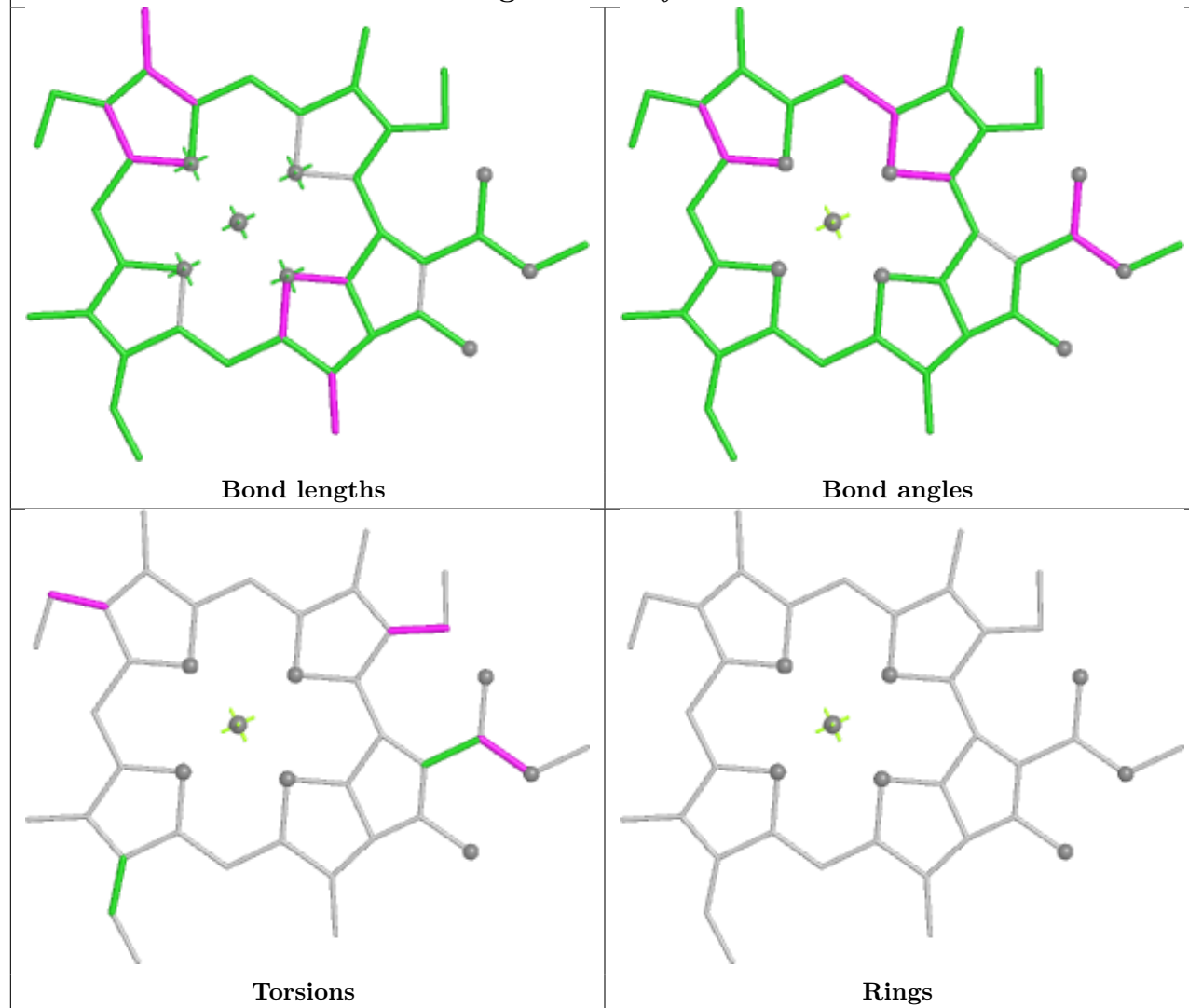
Ligand CLA CC 503



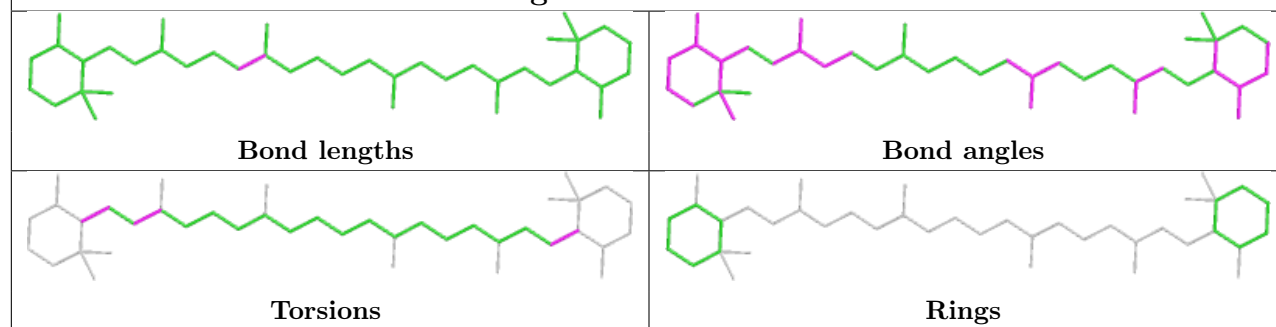


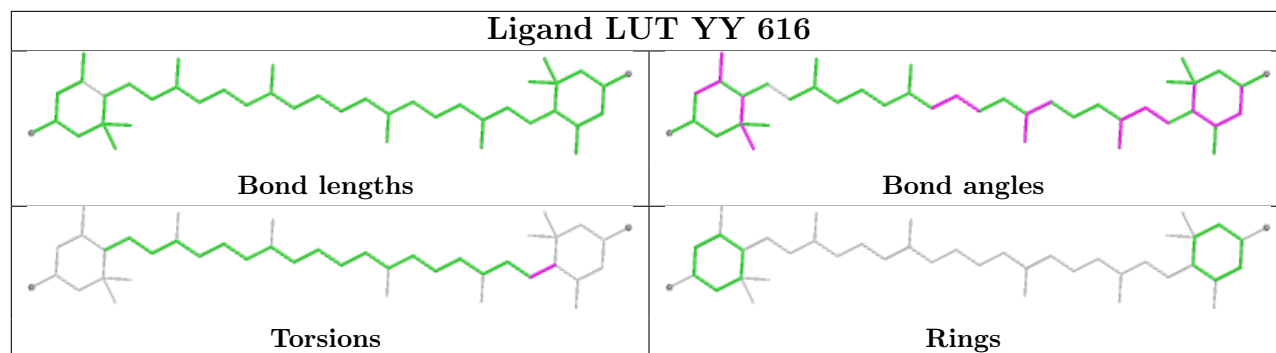
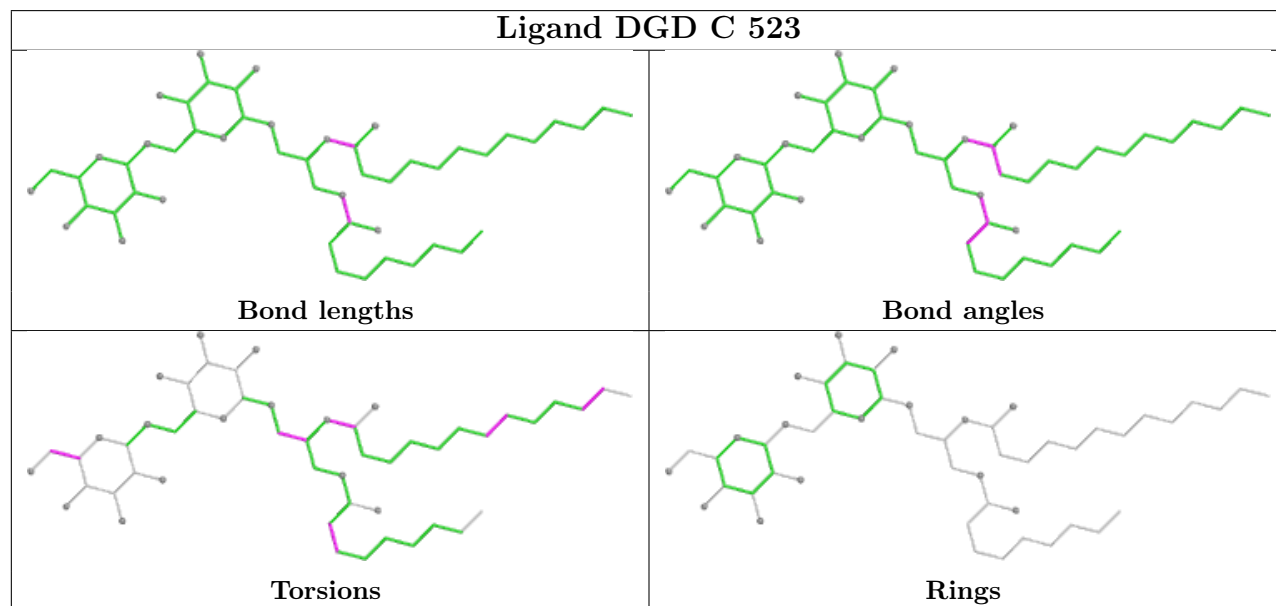


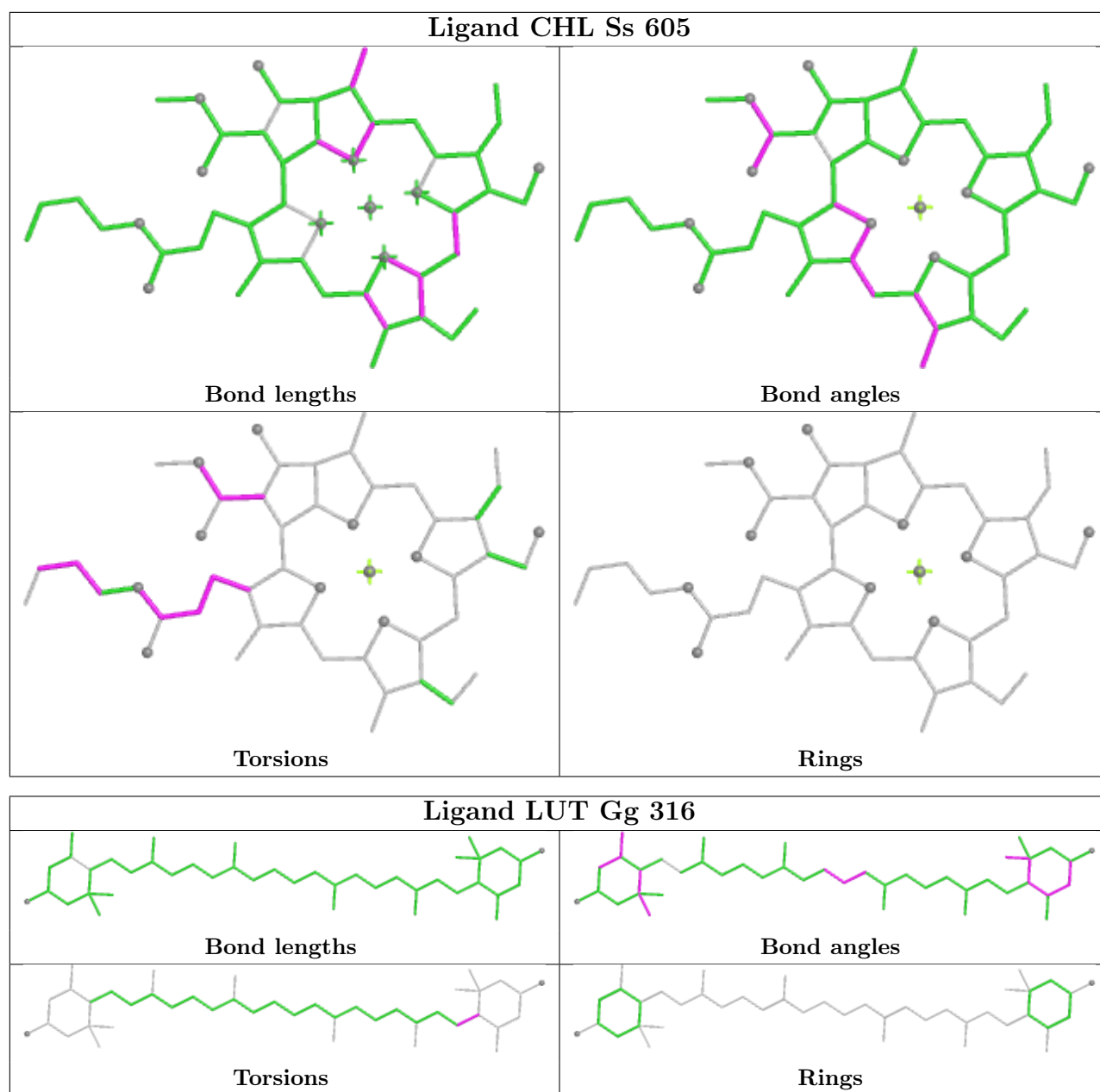
Ligand CLA y 313

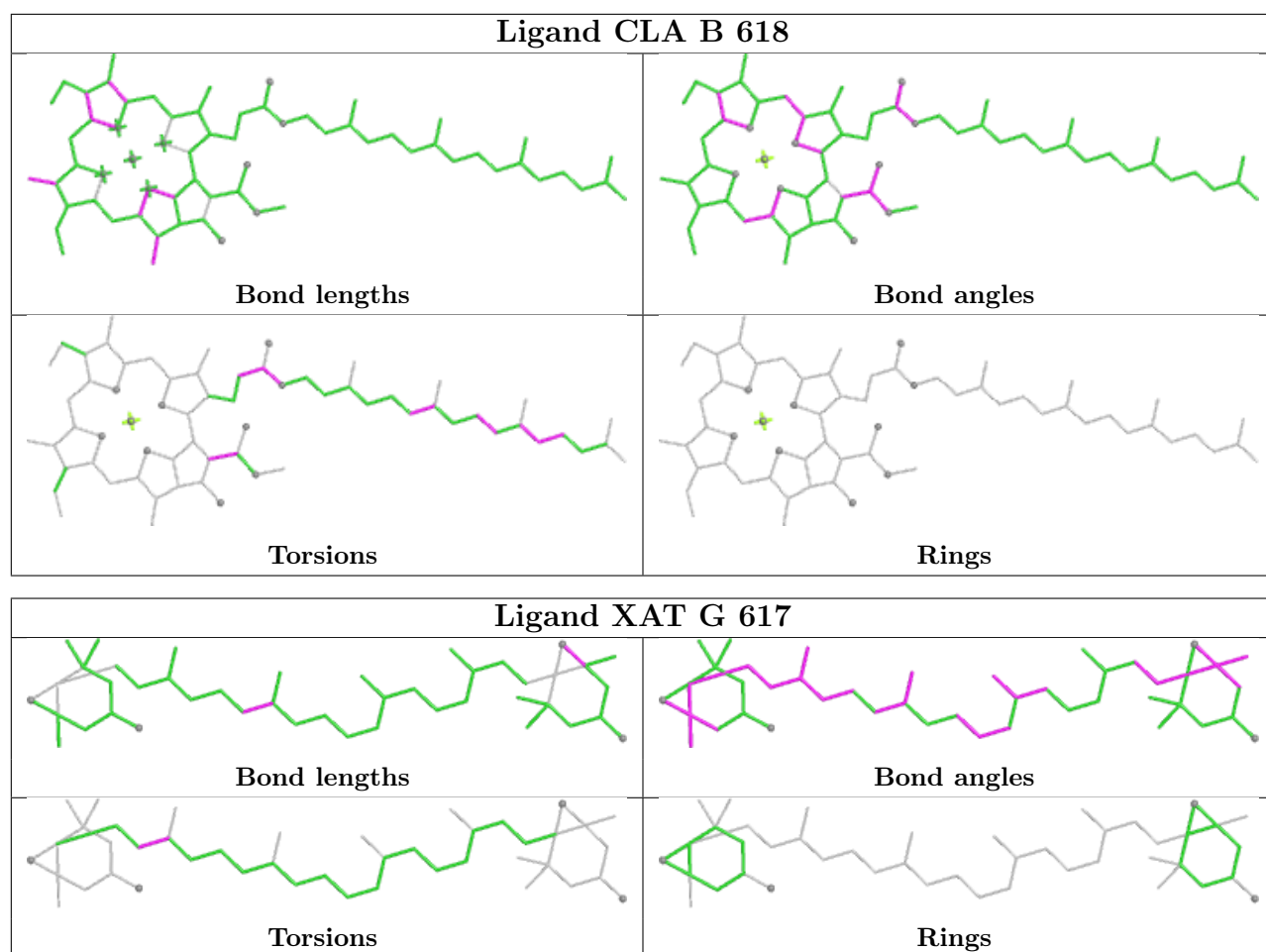


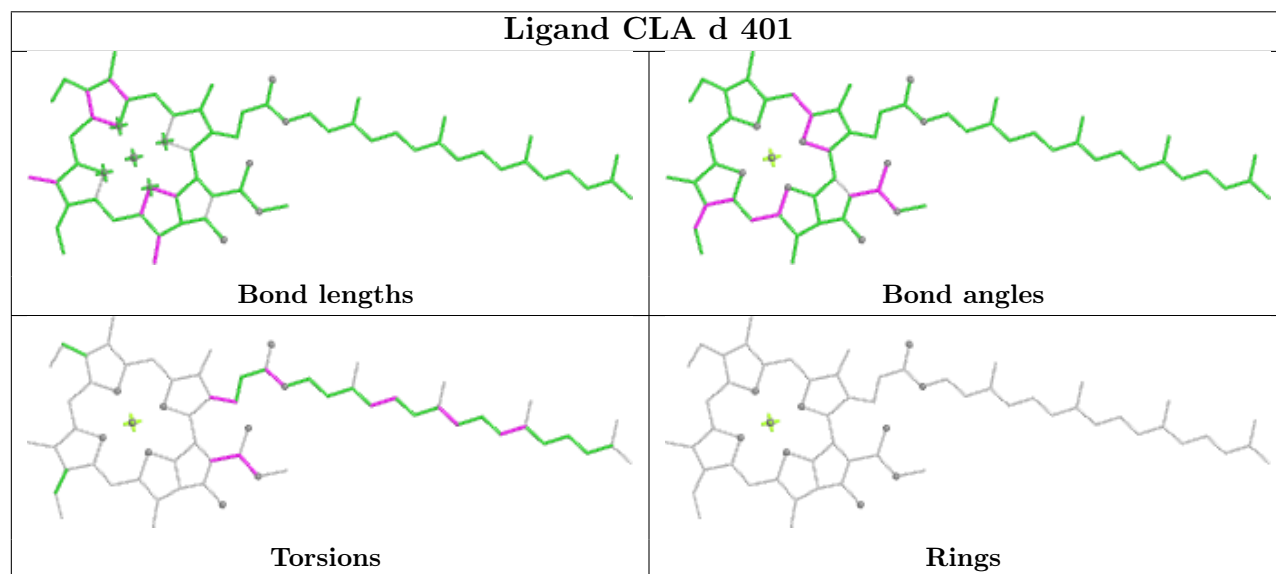
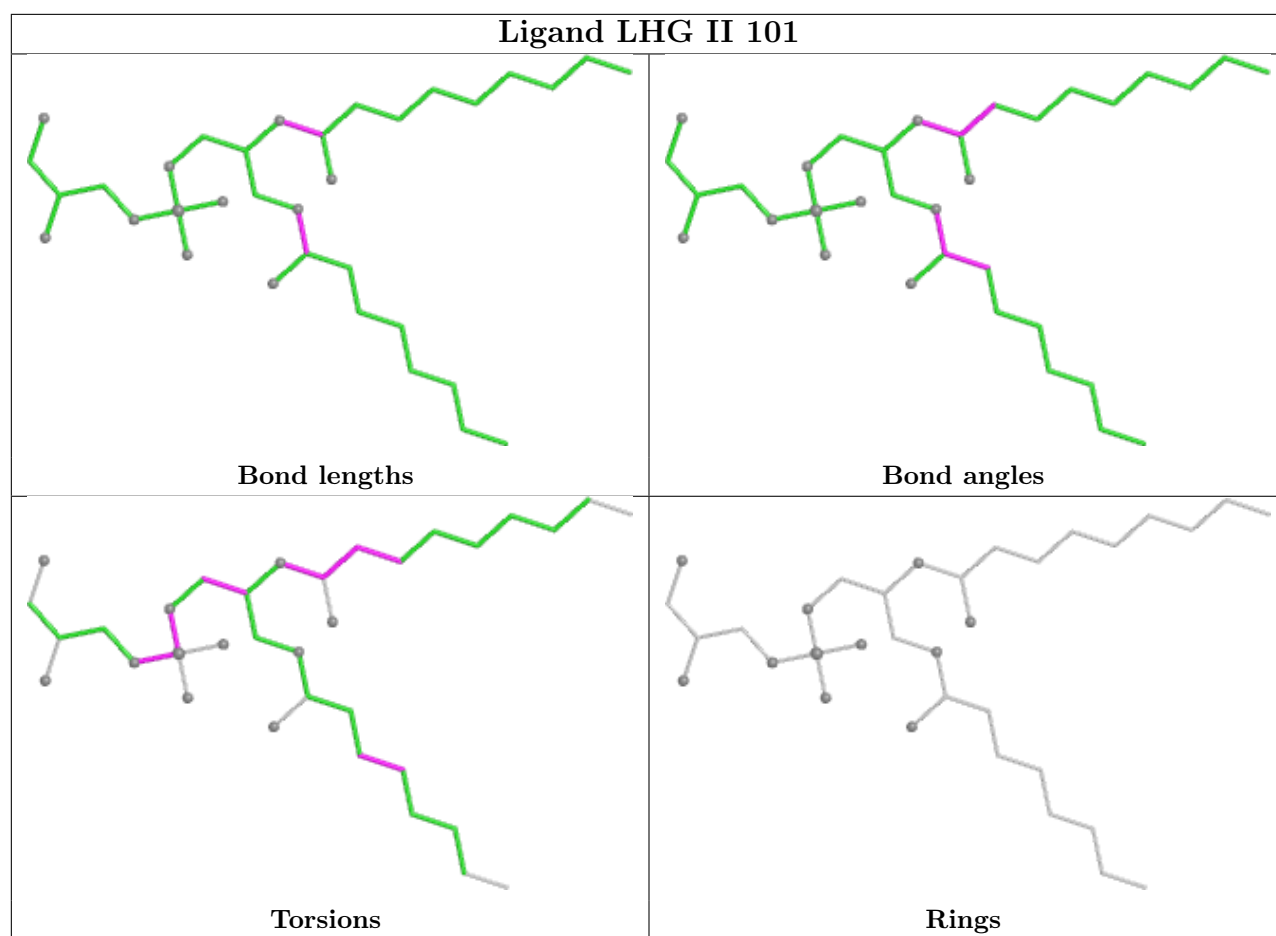
Ligand BCR C 516



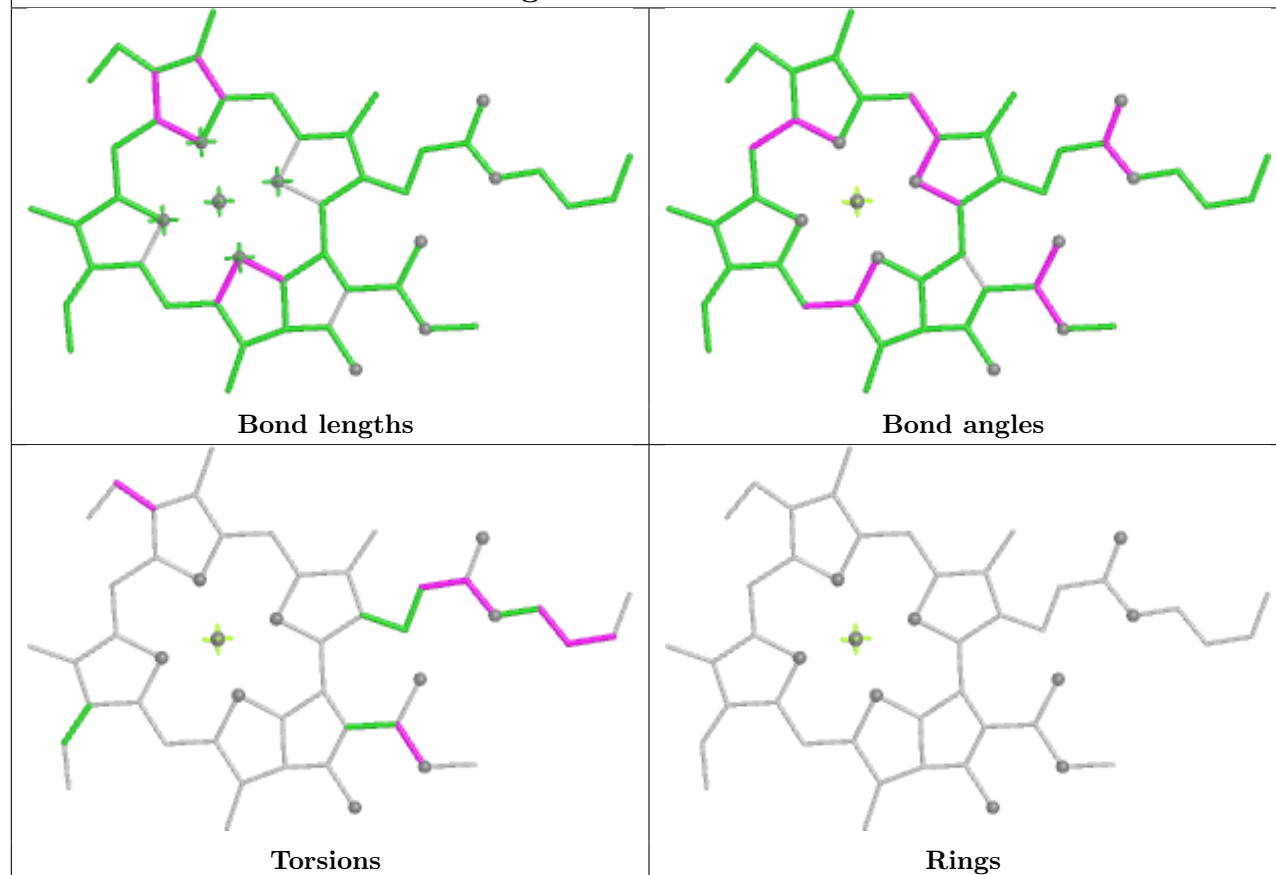
Ligand LUT YY 616**Ligand DGD C 523**



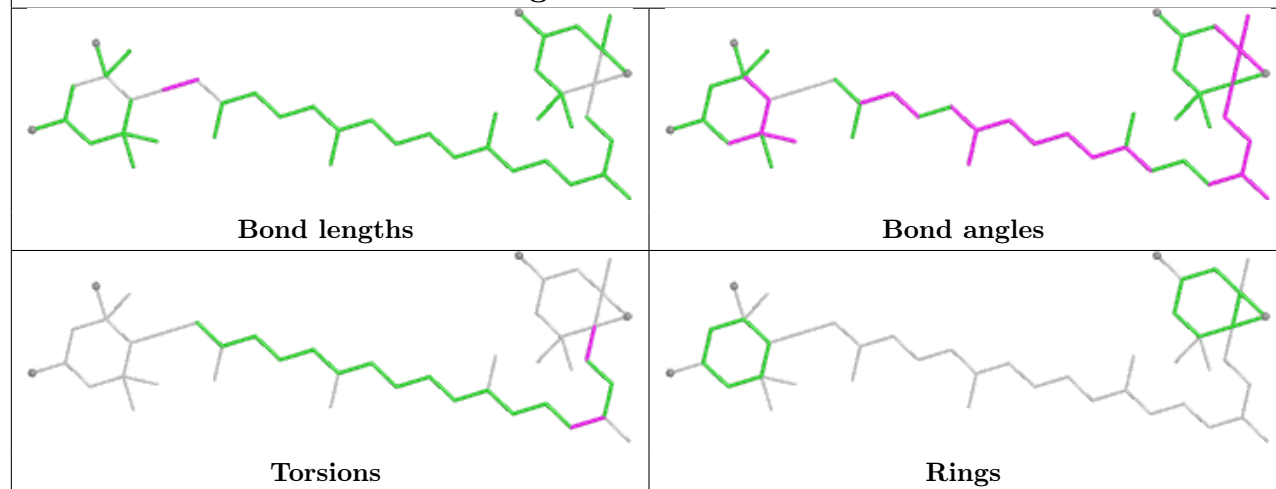


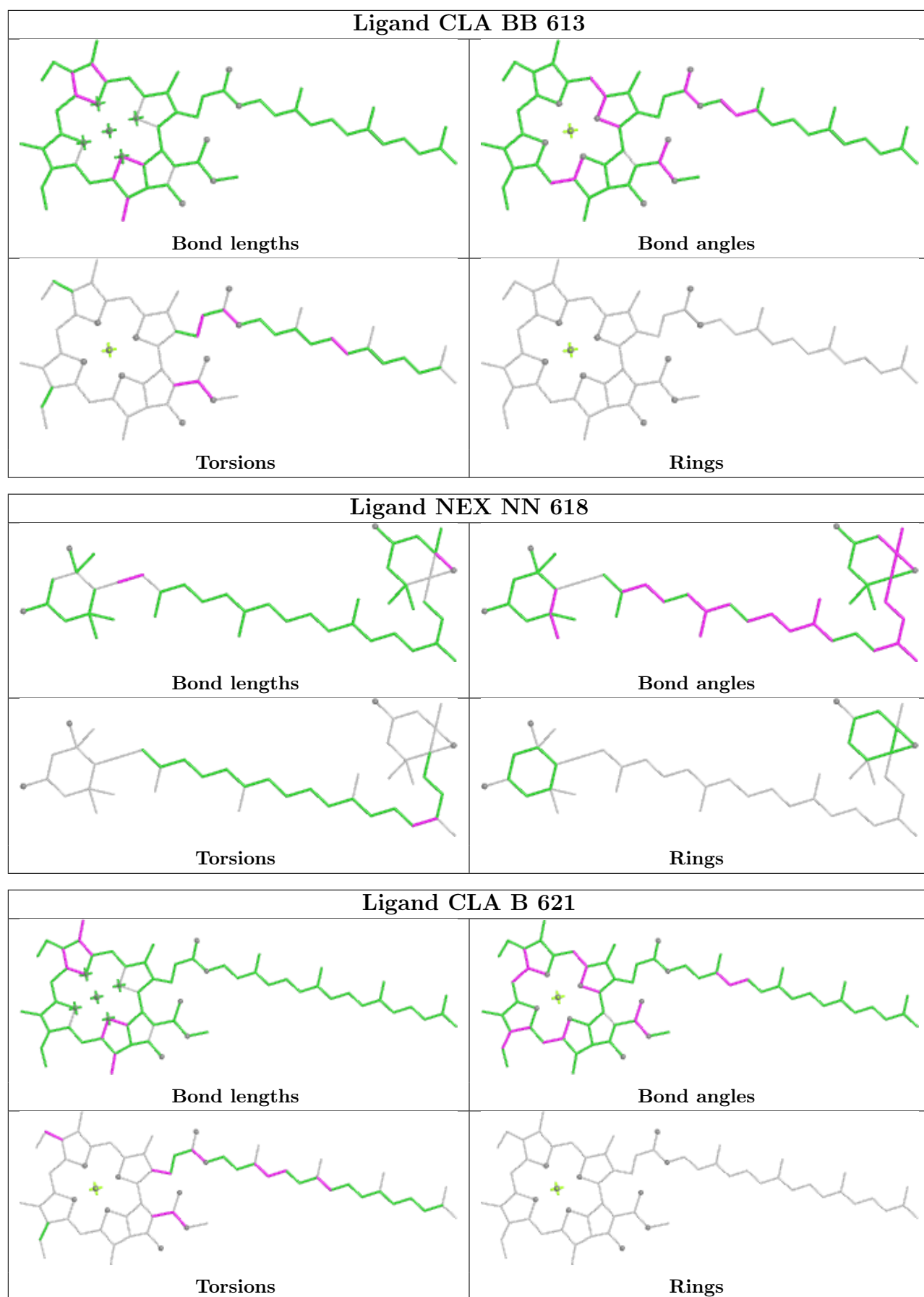


Ligand CLA Nn 305

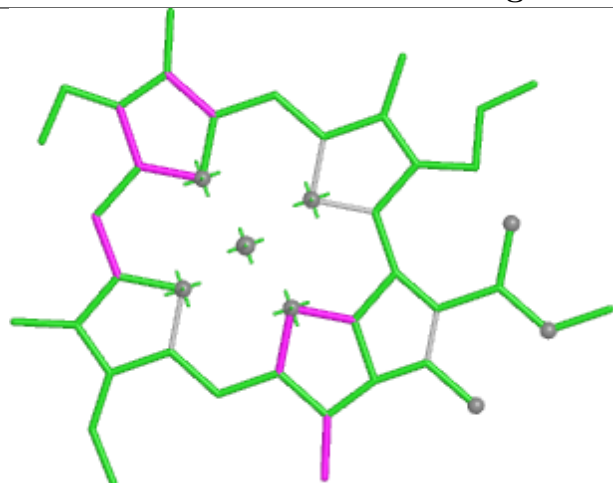


Ligand NEX Y 619

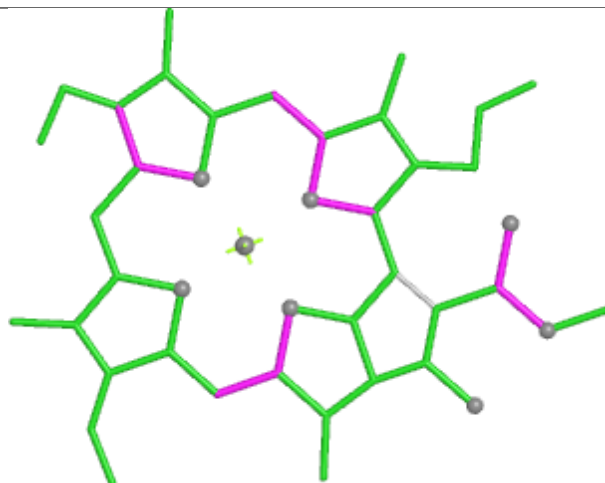




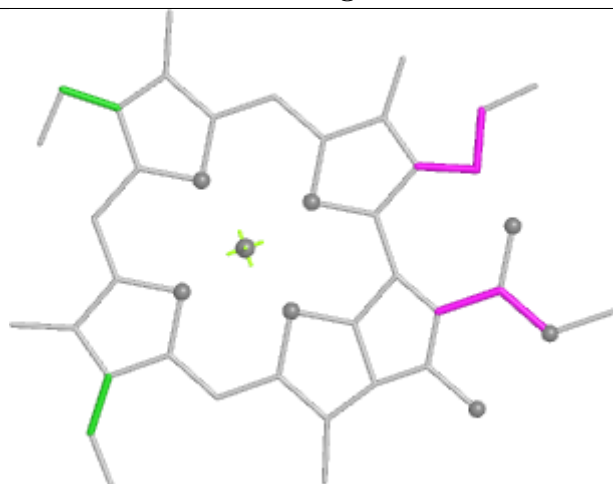
Ligand CLA Cc 515



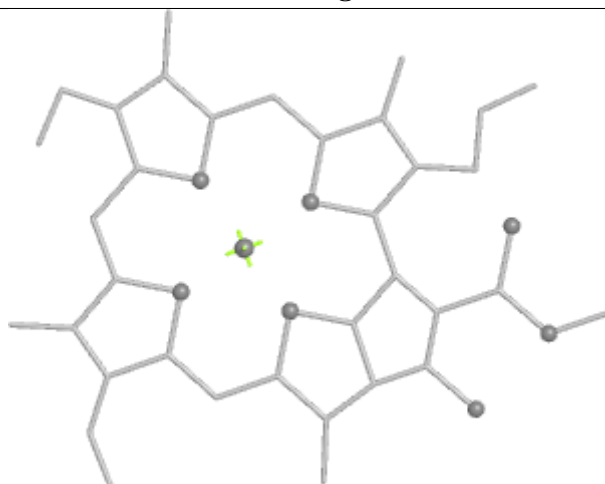
Bond lengths



Bond angles

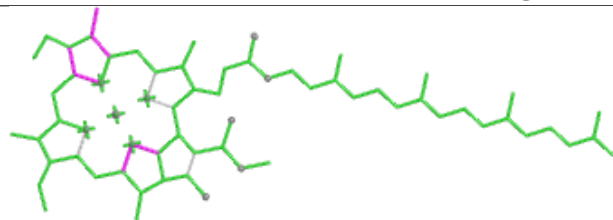


Torsions

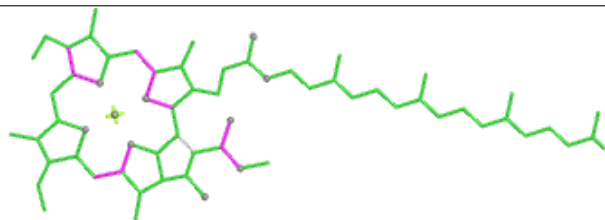


Rings

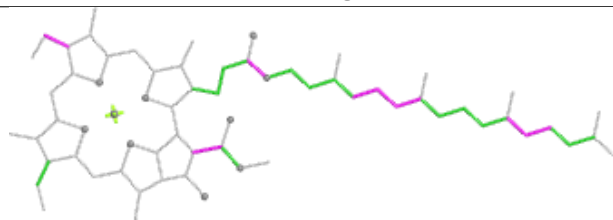
Ligand CLA b 610



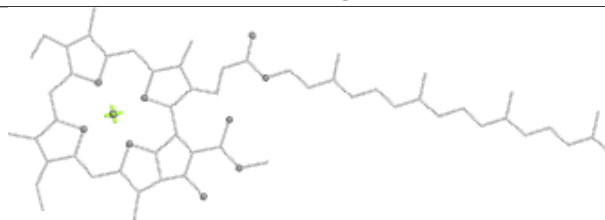
Bond lengths



Bond angles

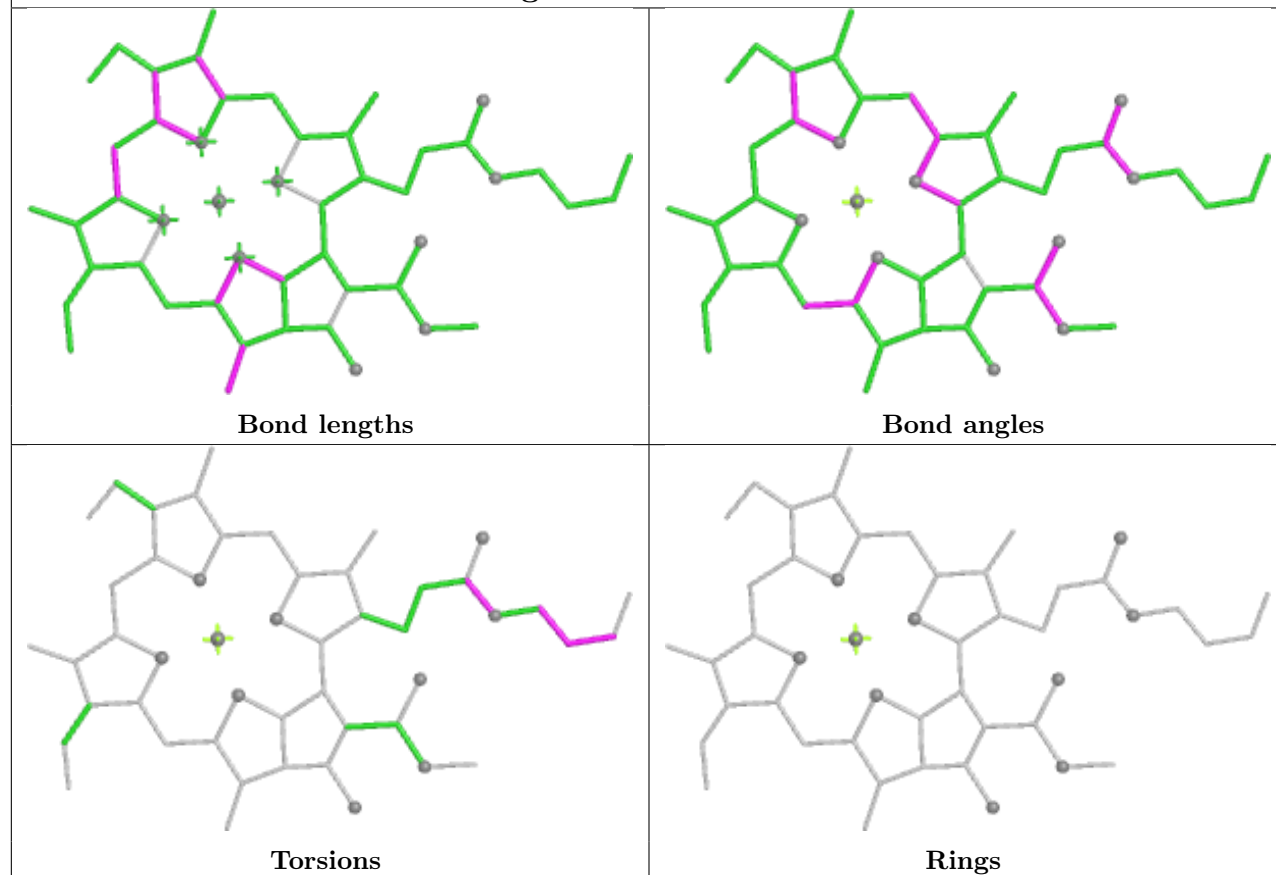


Torsions

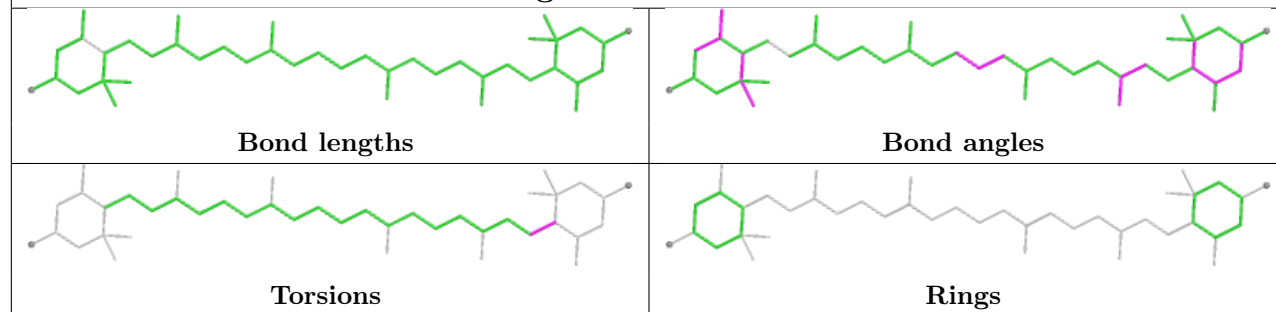


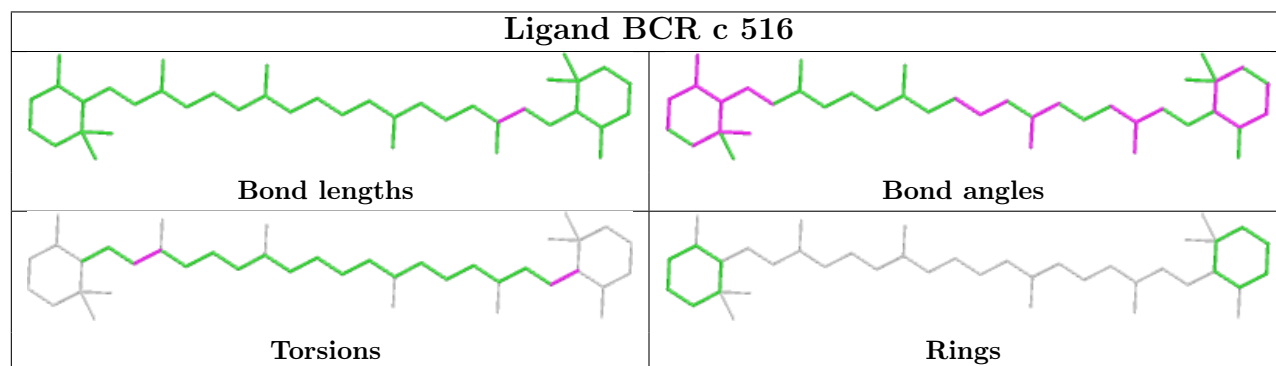
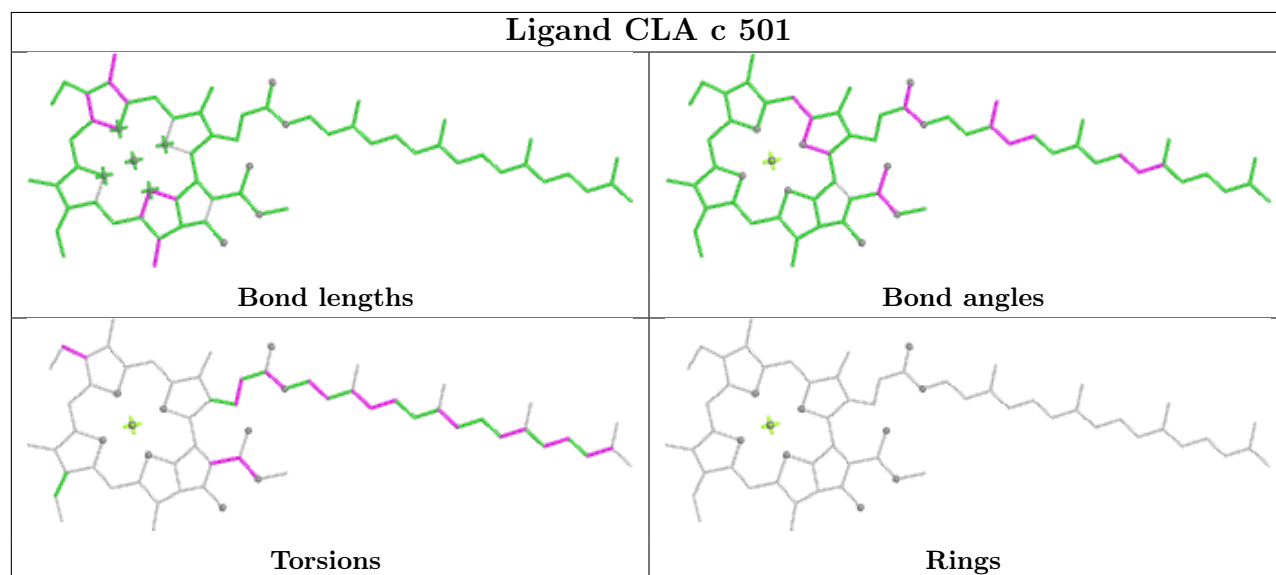
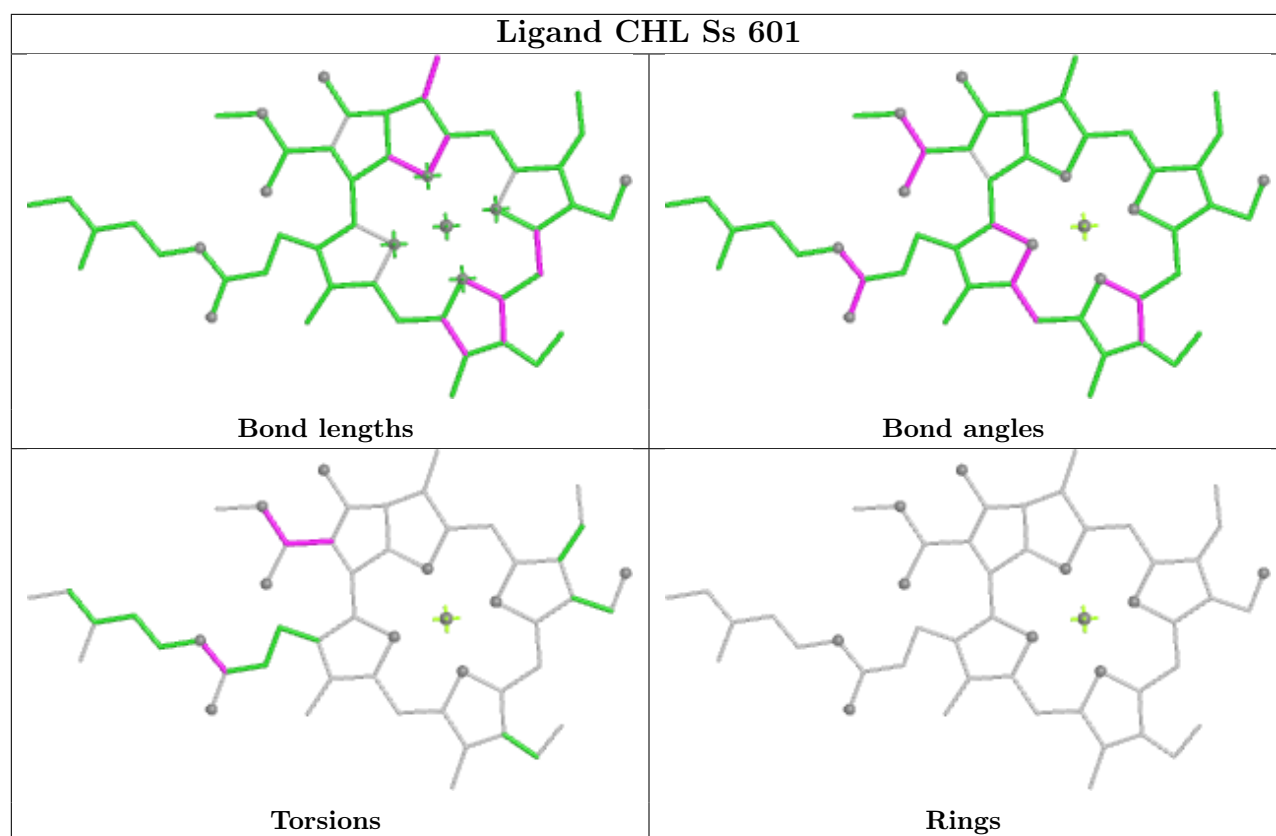
Rings

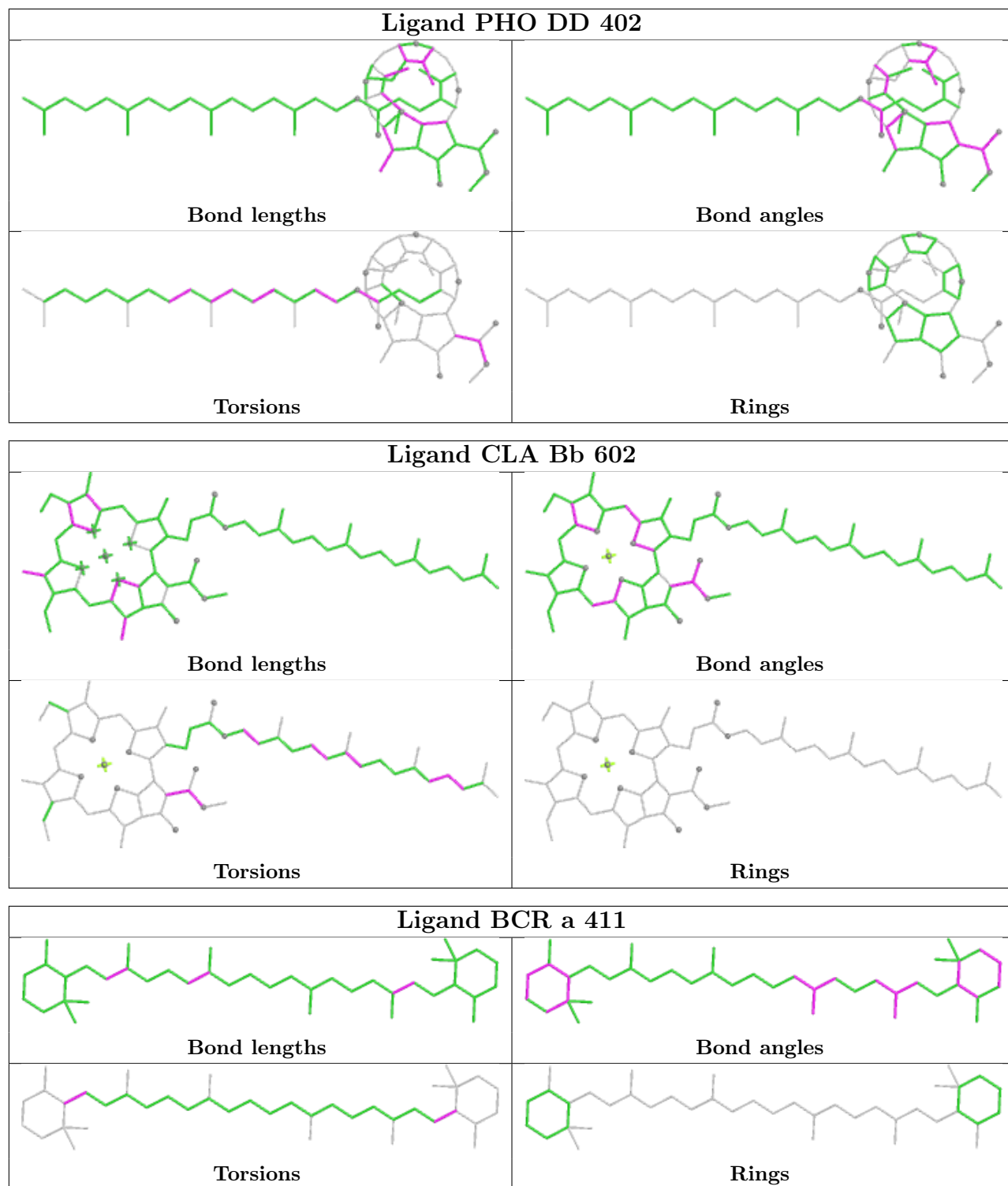
Ligand CLA Nn 314

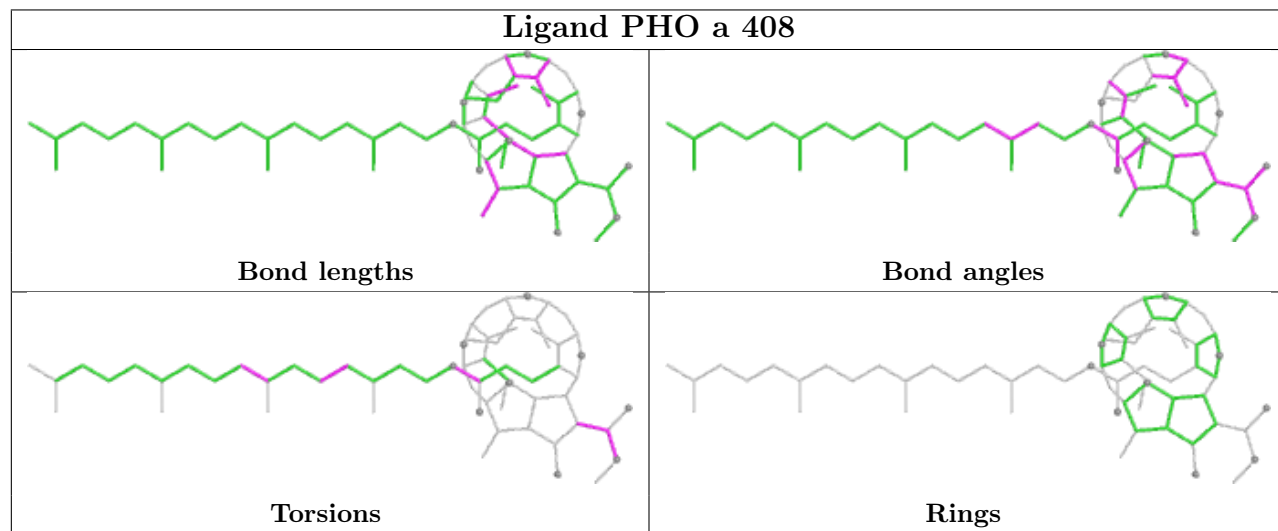
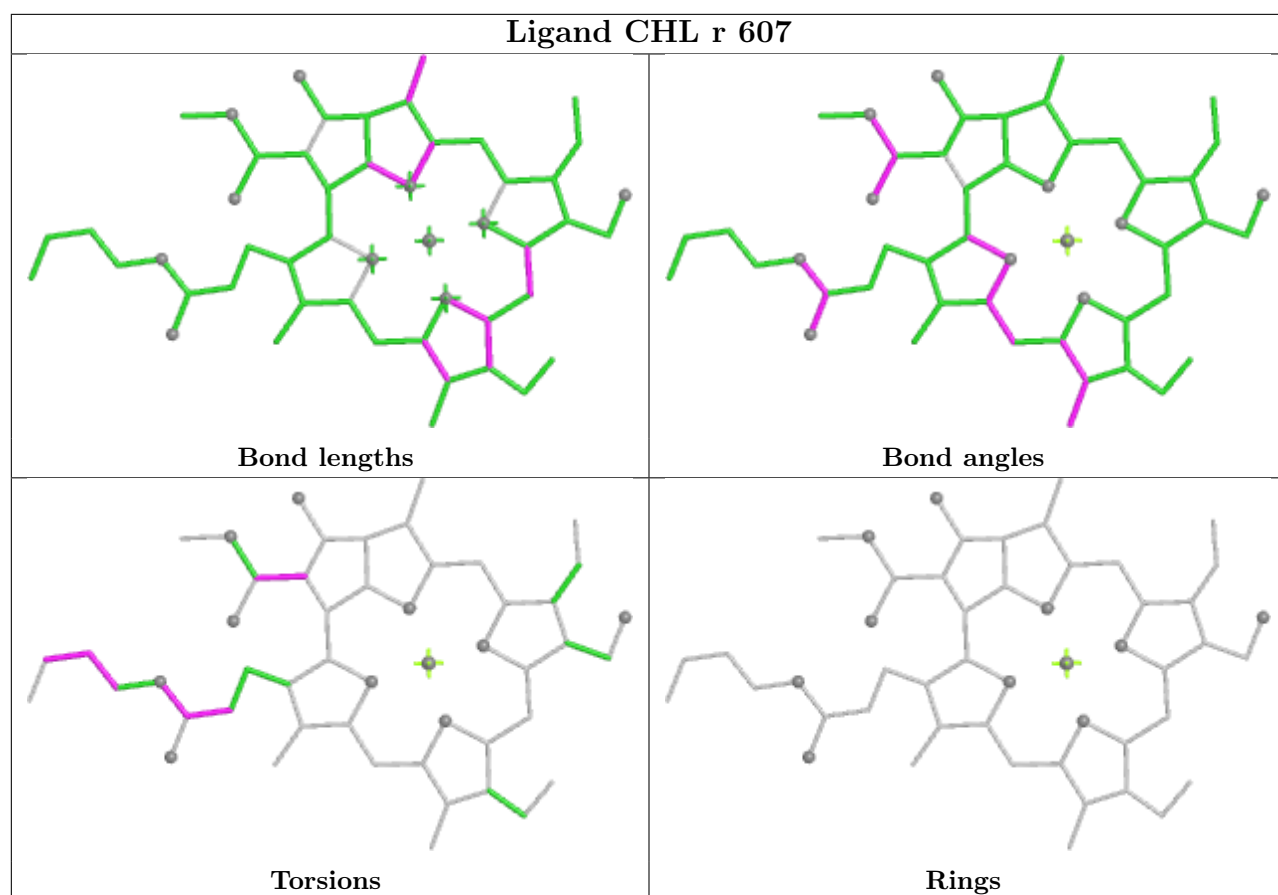


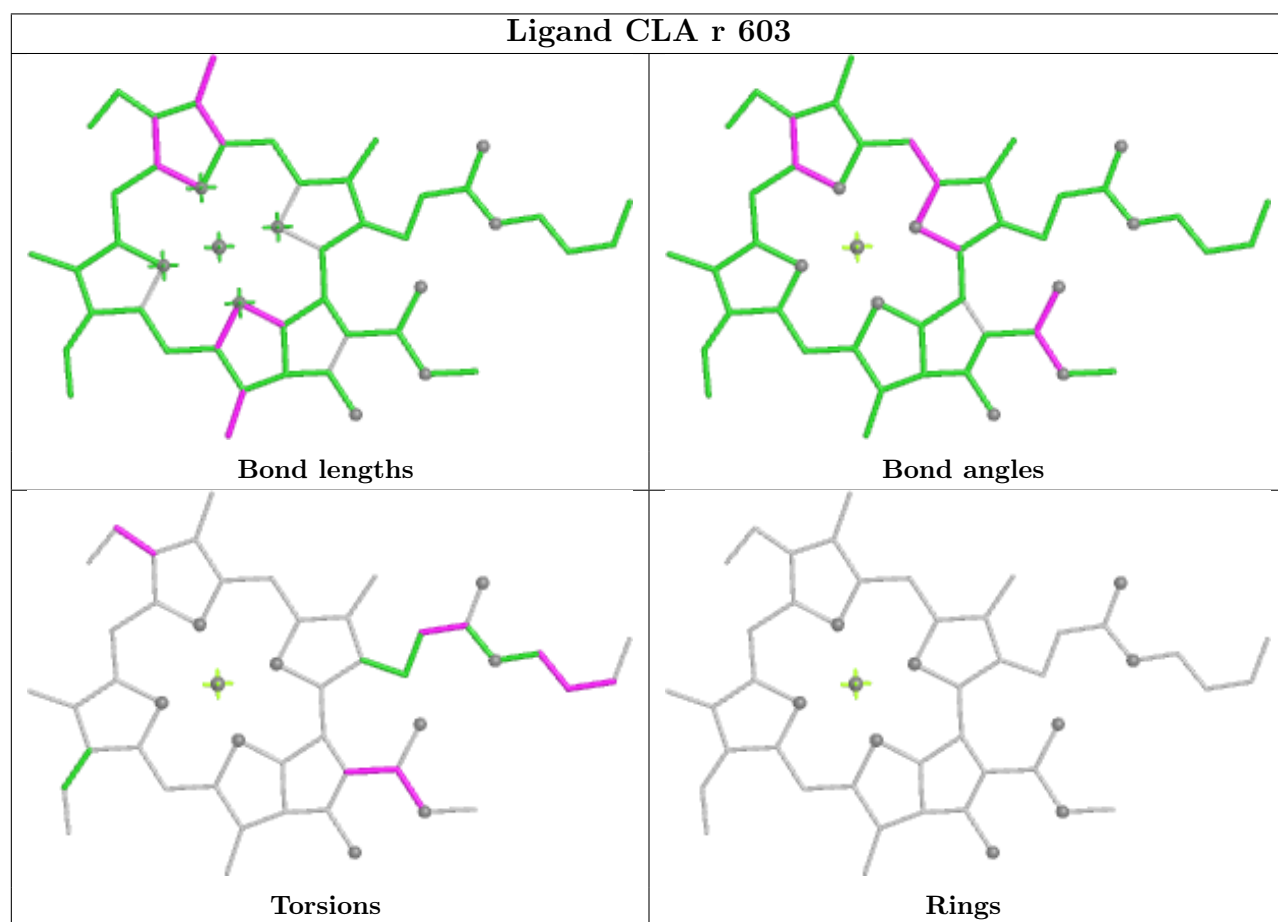
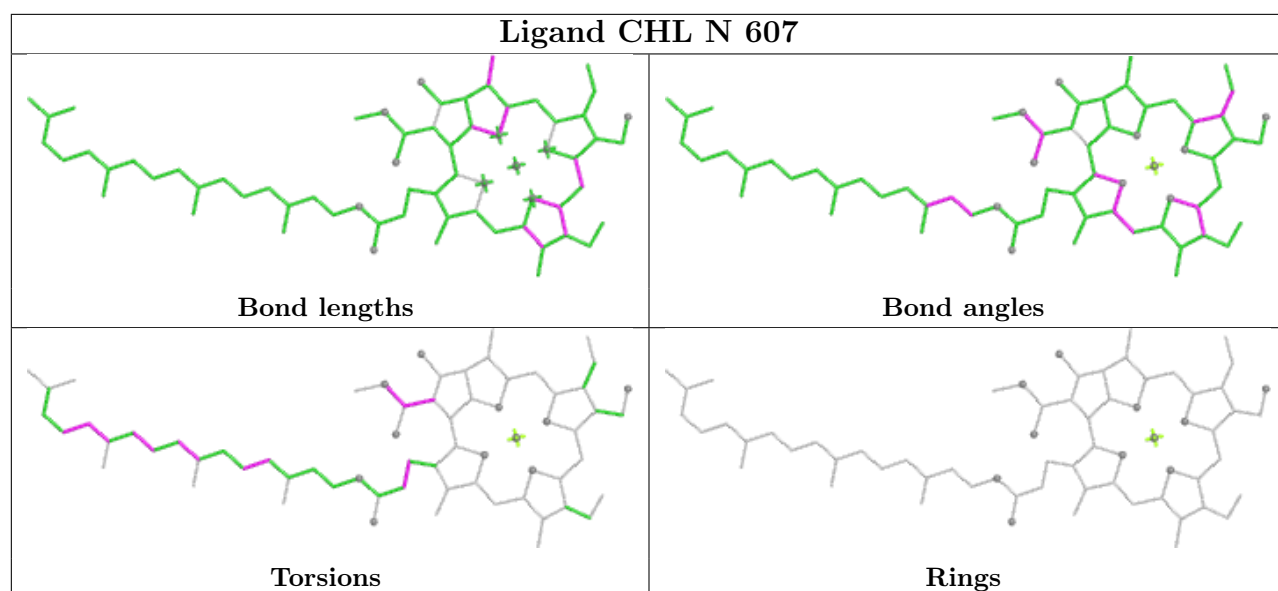
Ligand LUT 4 313

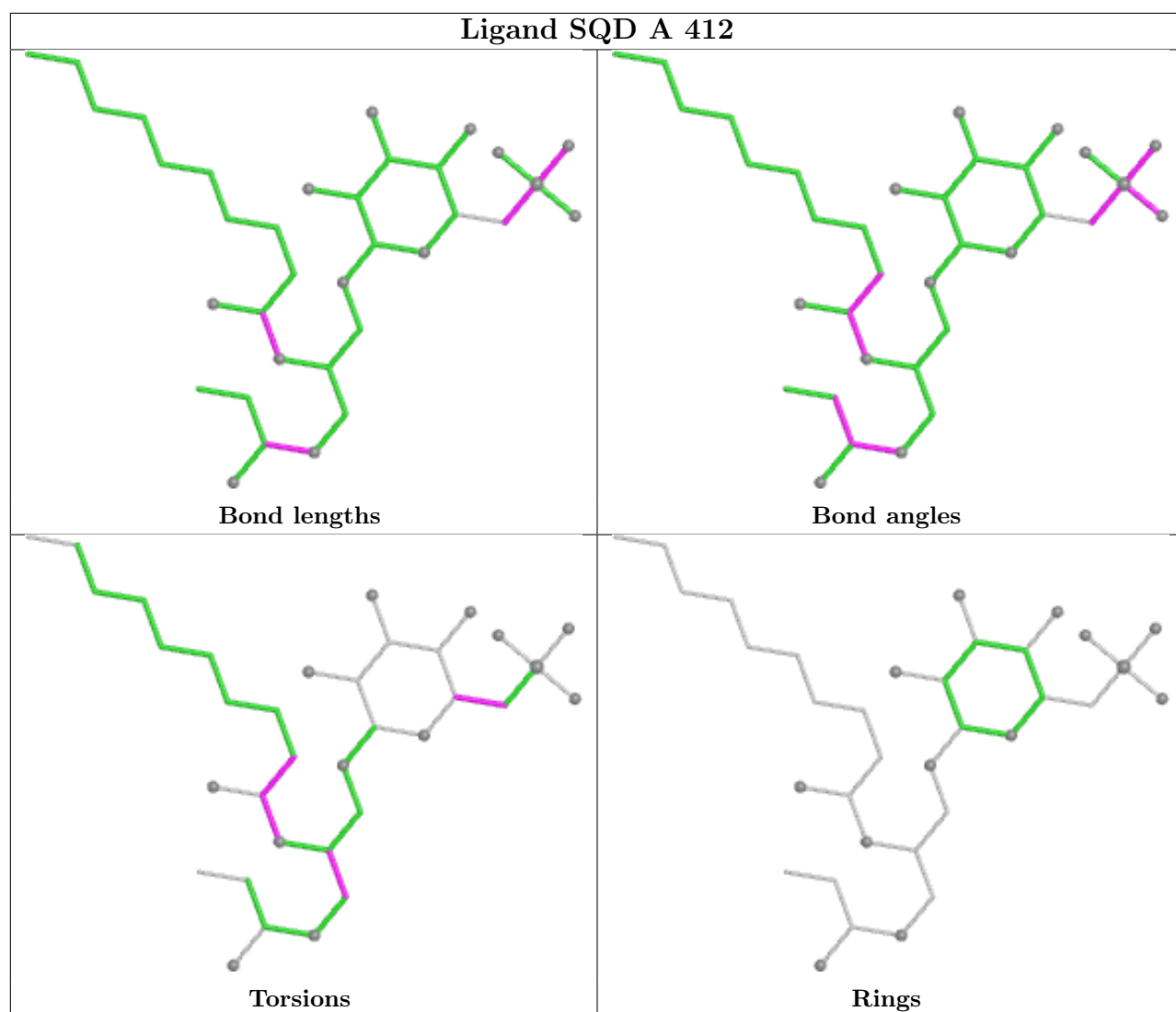




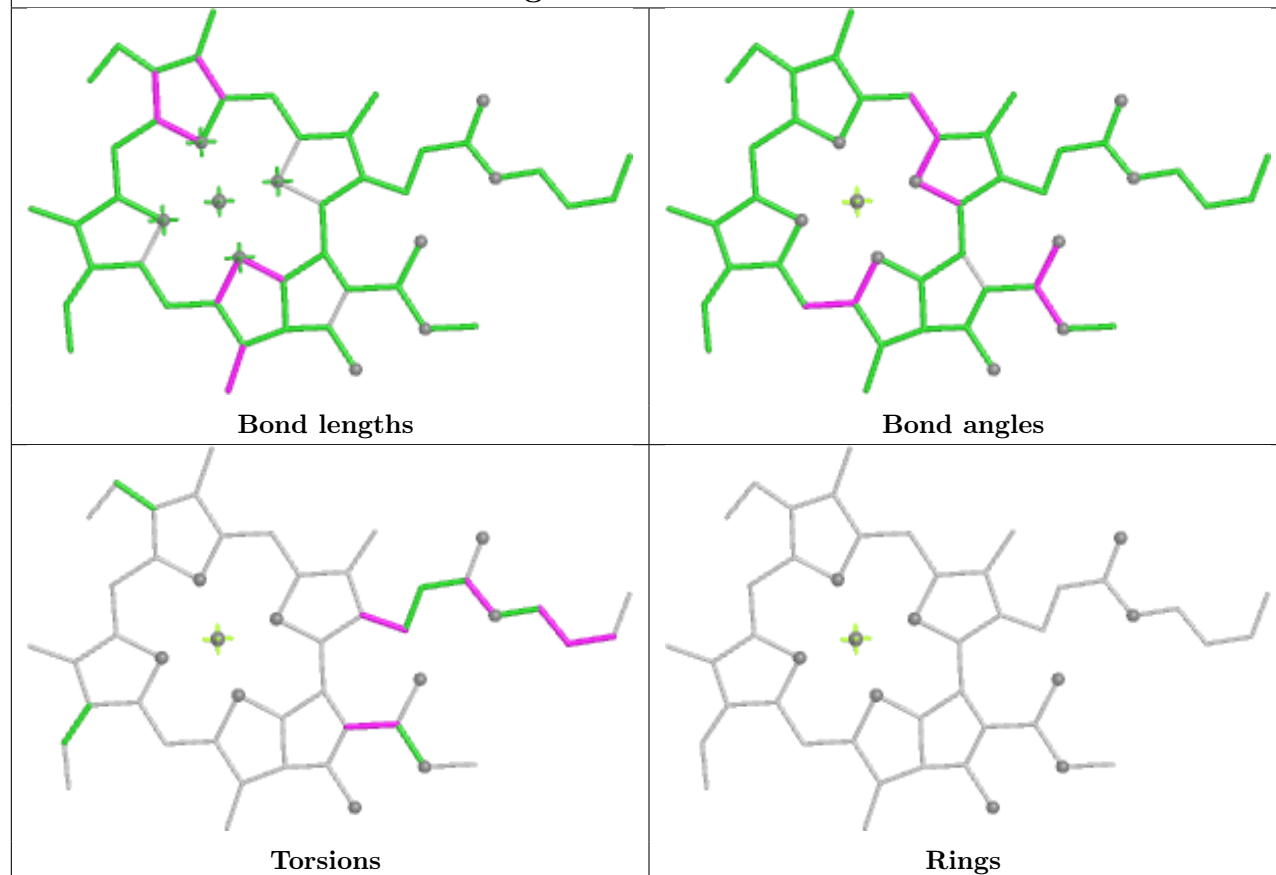




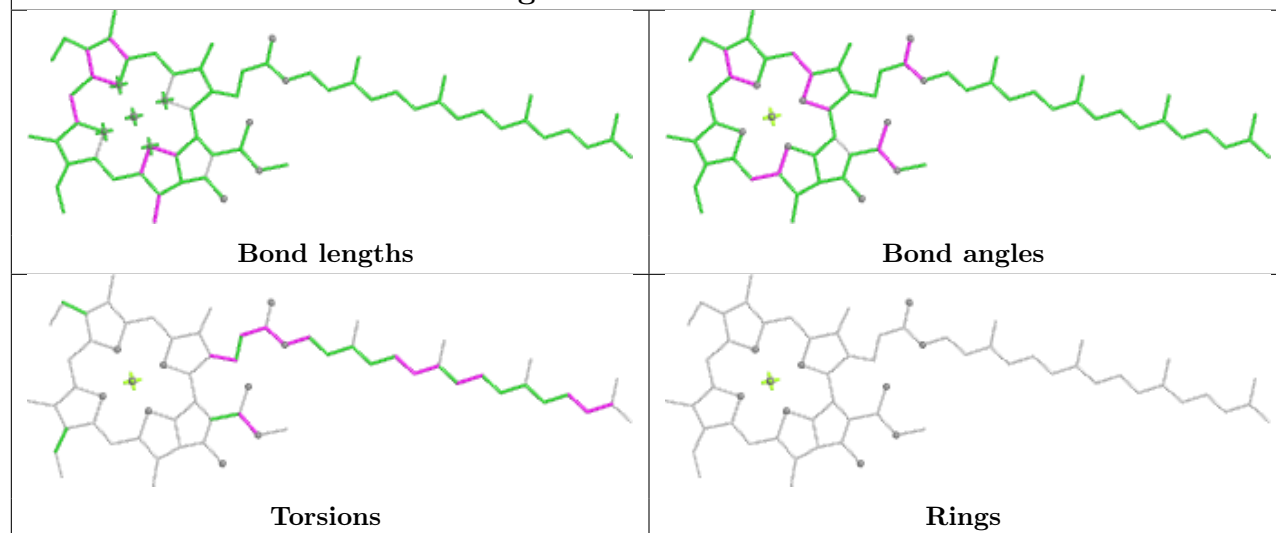


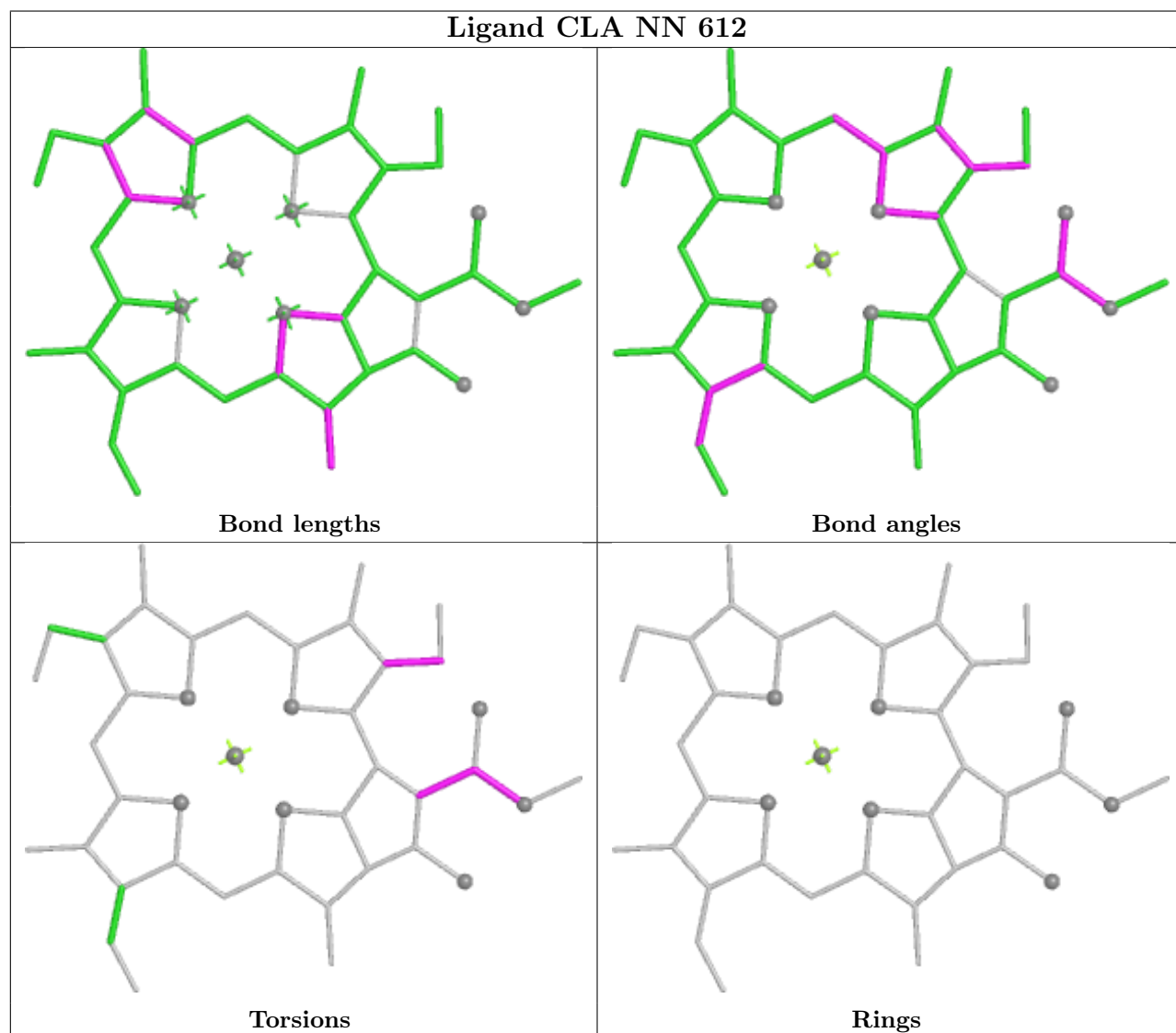
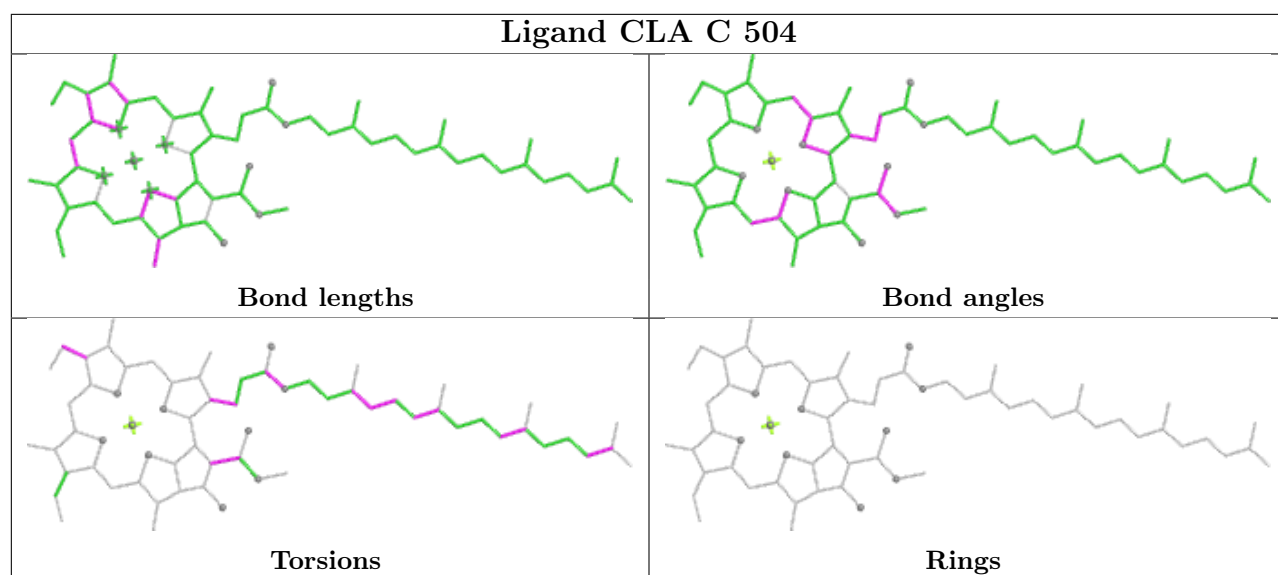


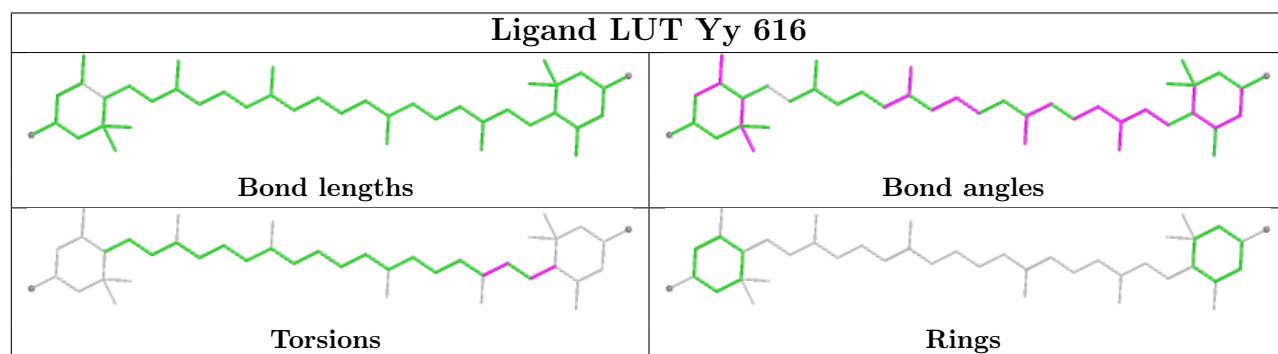
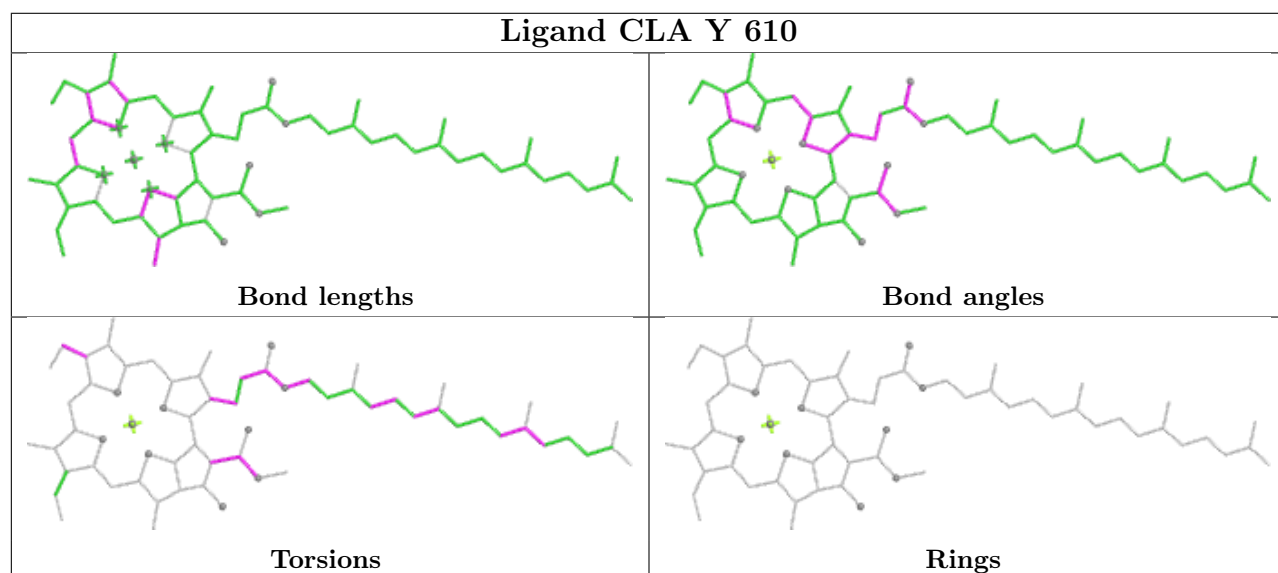
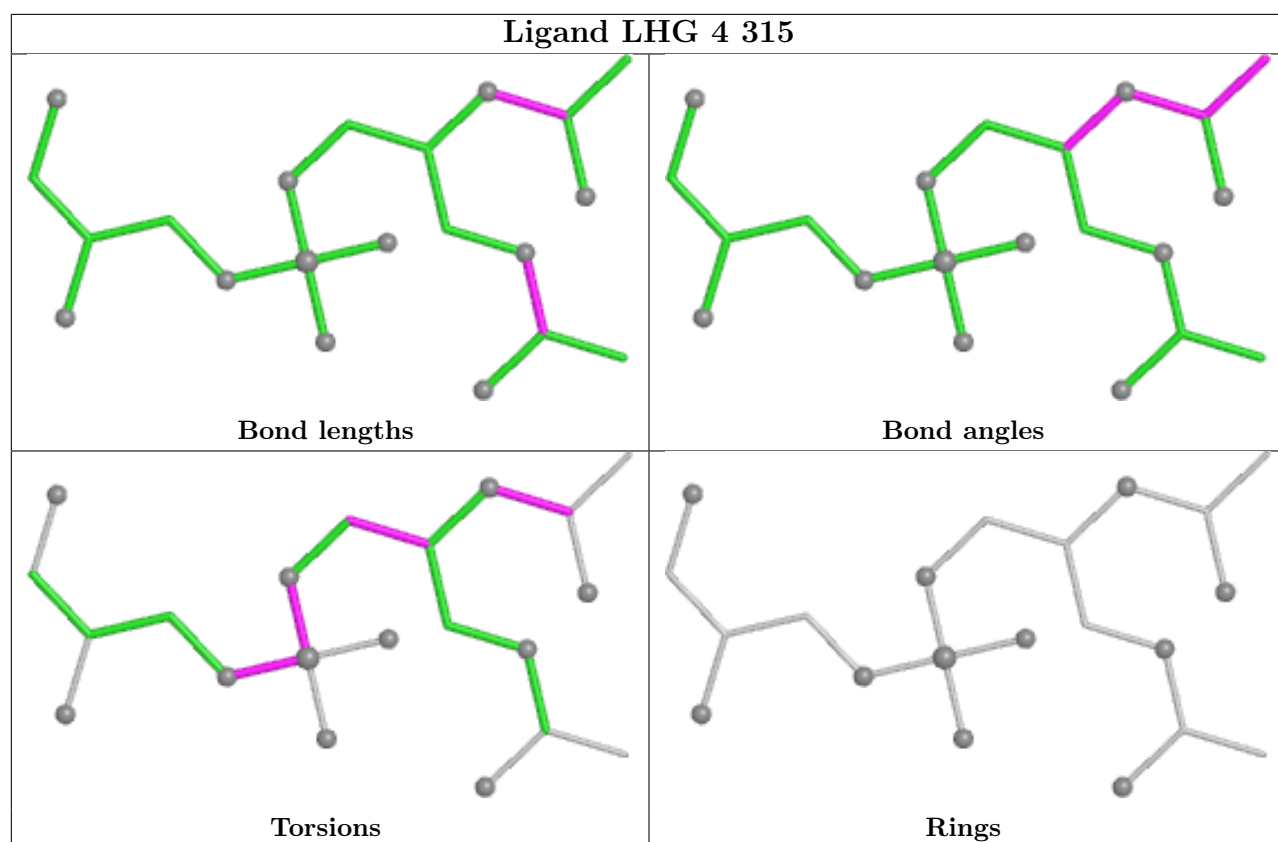
Ligand CLA Rr 612

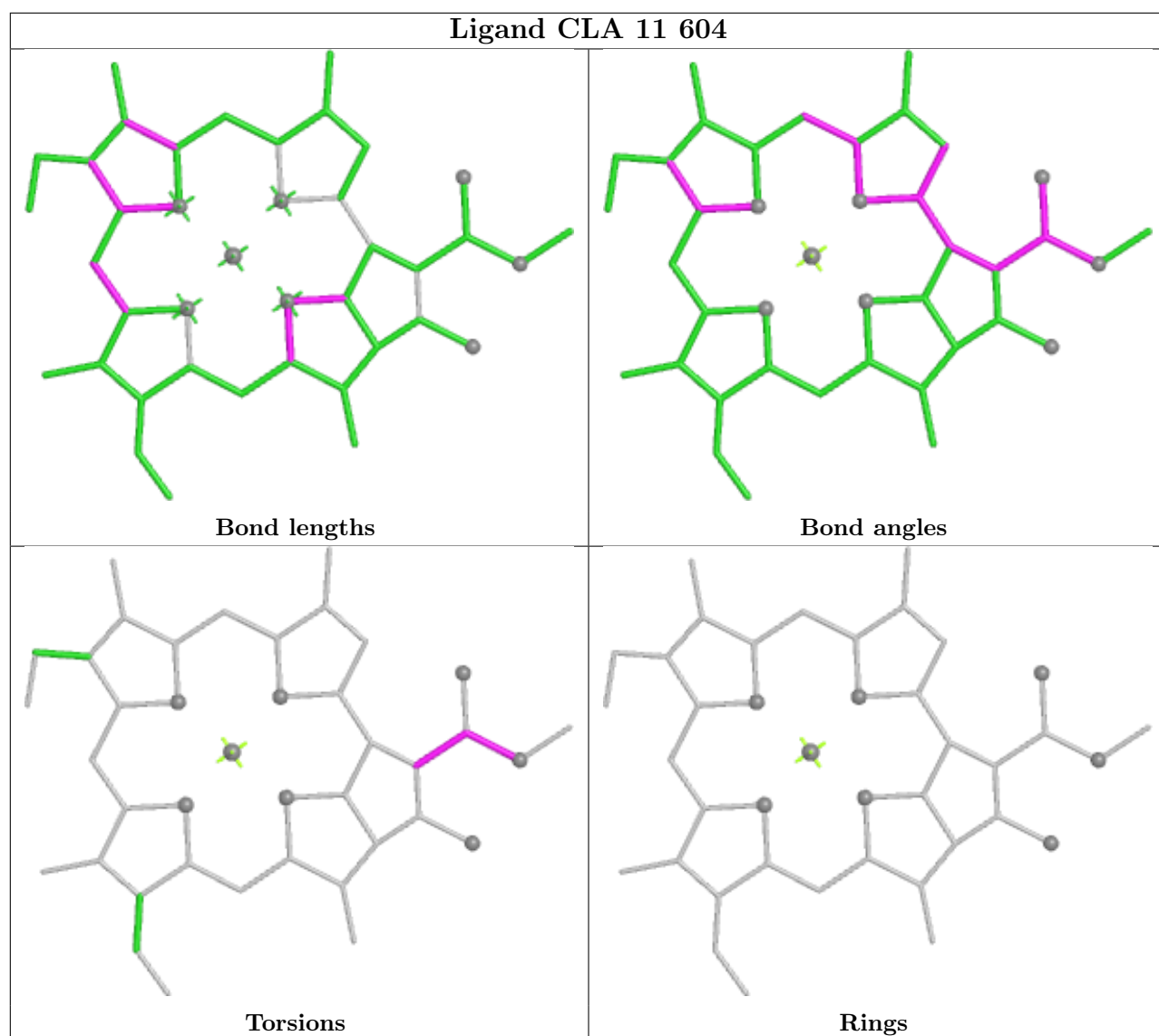


Ligand CLA YY 602

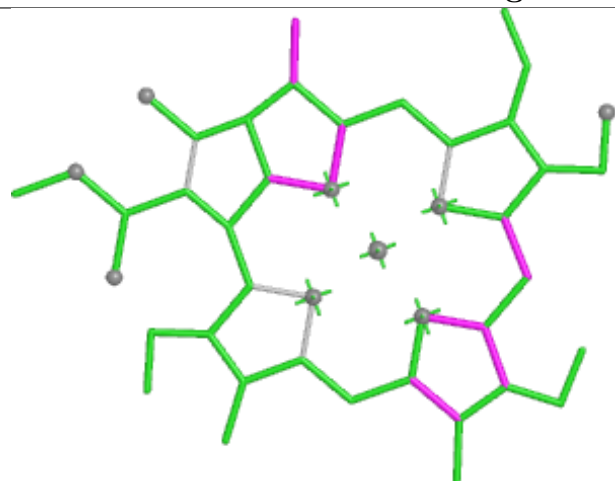




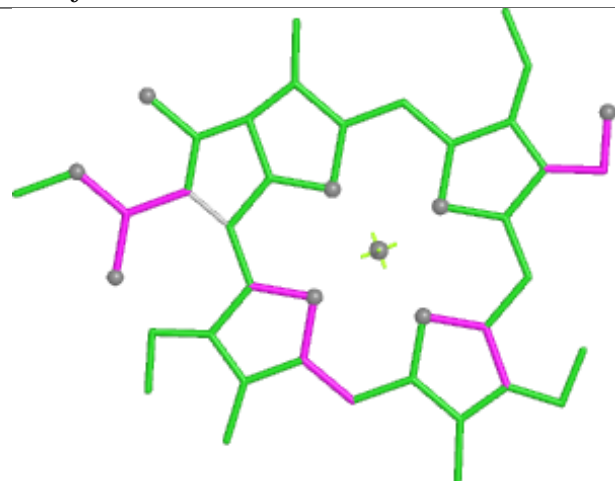




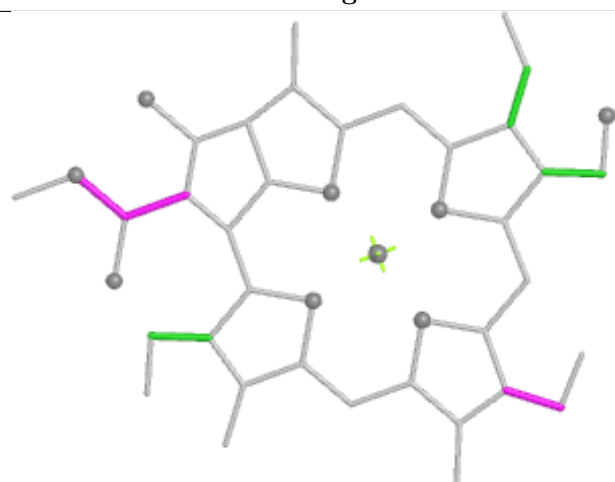
Ligand CHL Yy 607



Bond lengths



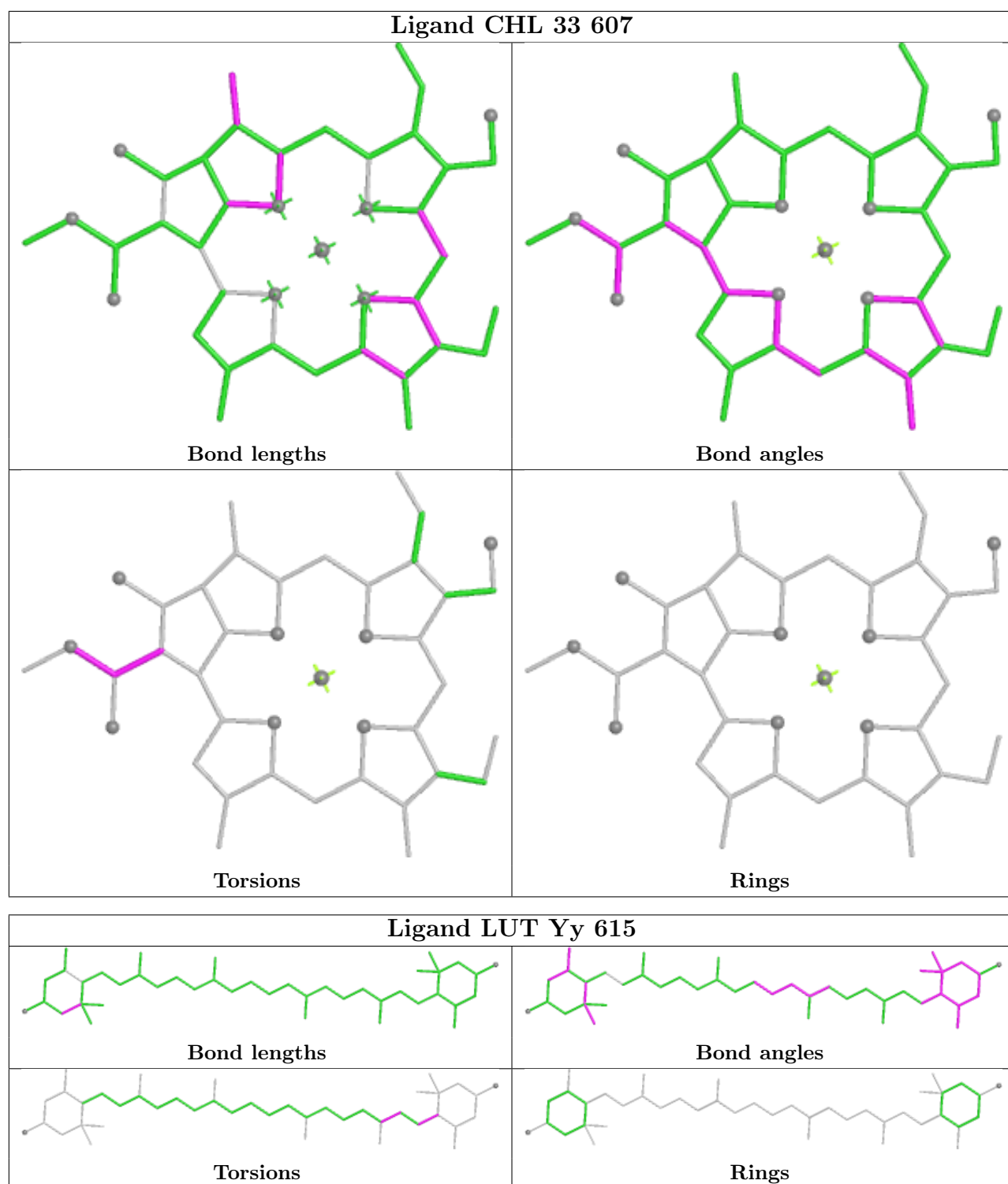
Bond angles



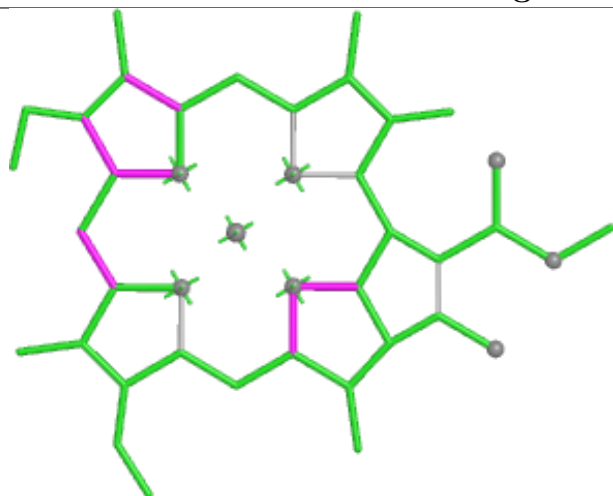
Torsions



Rings



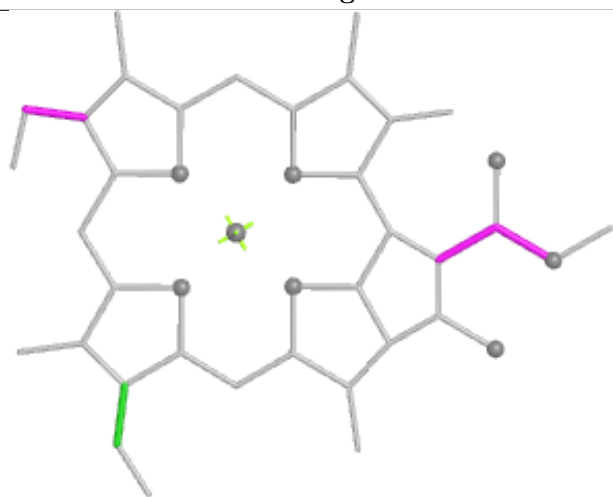
Ligand CLA N 614



Bond lengths



Bond angles

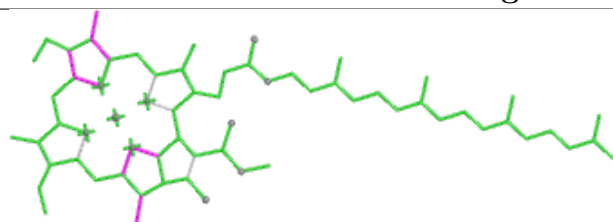


Torsions

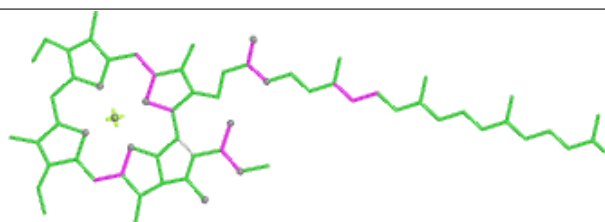


Rings

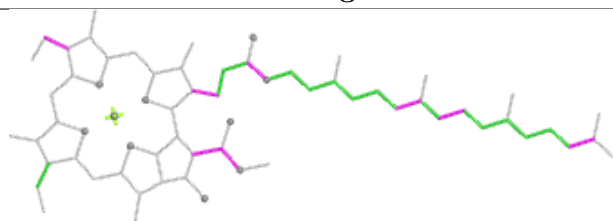
Ligand CLA CC 504



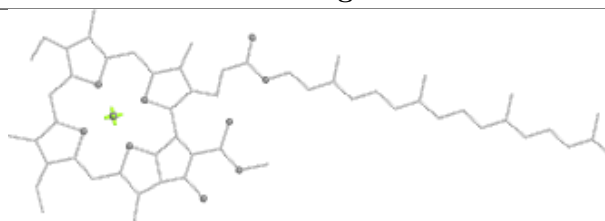
Bond lengths



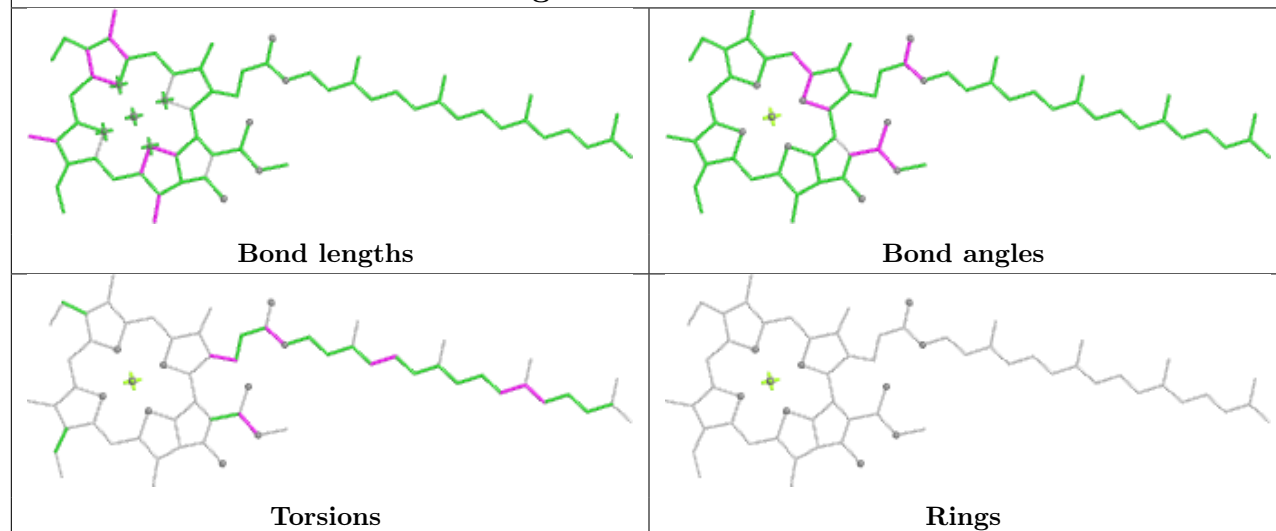
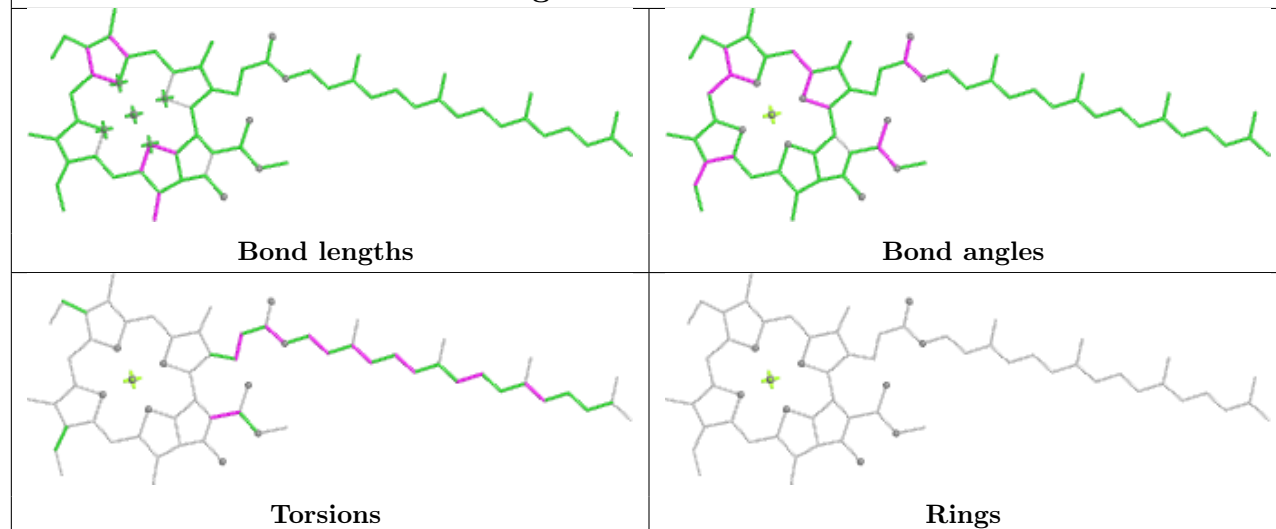
Bond angles

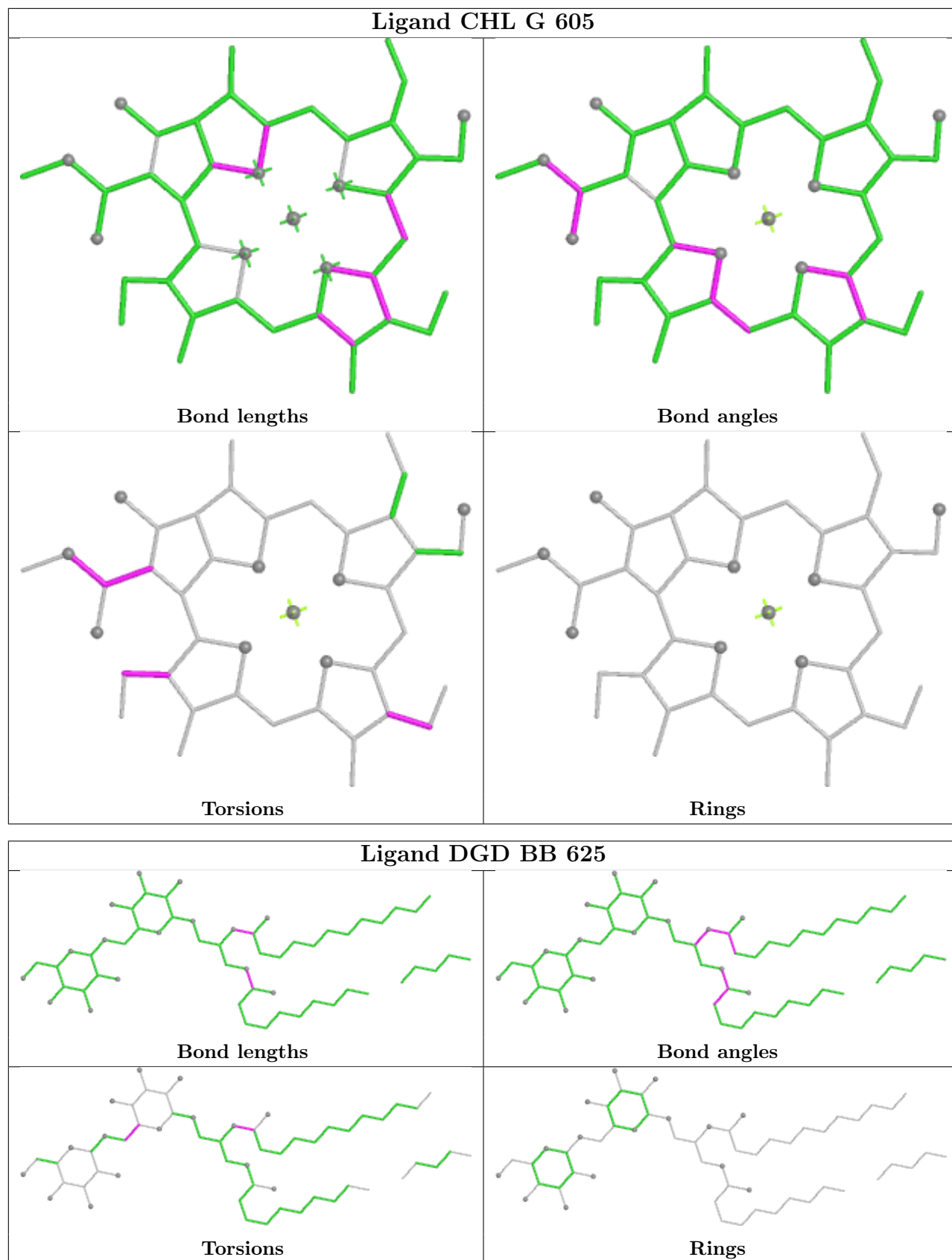


Torsions

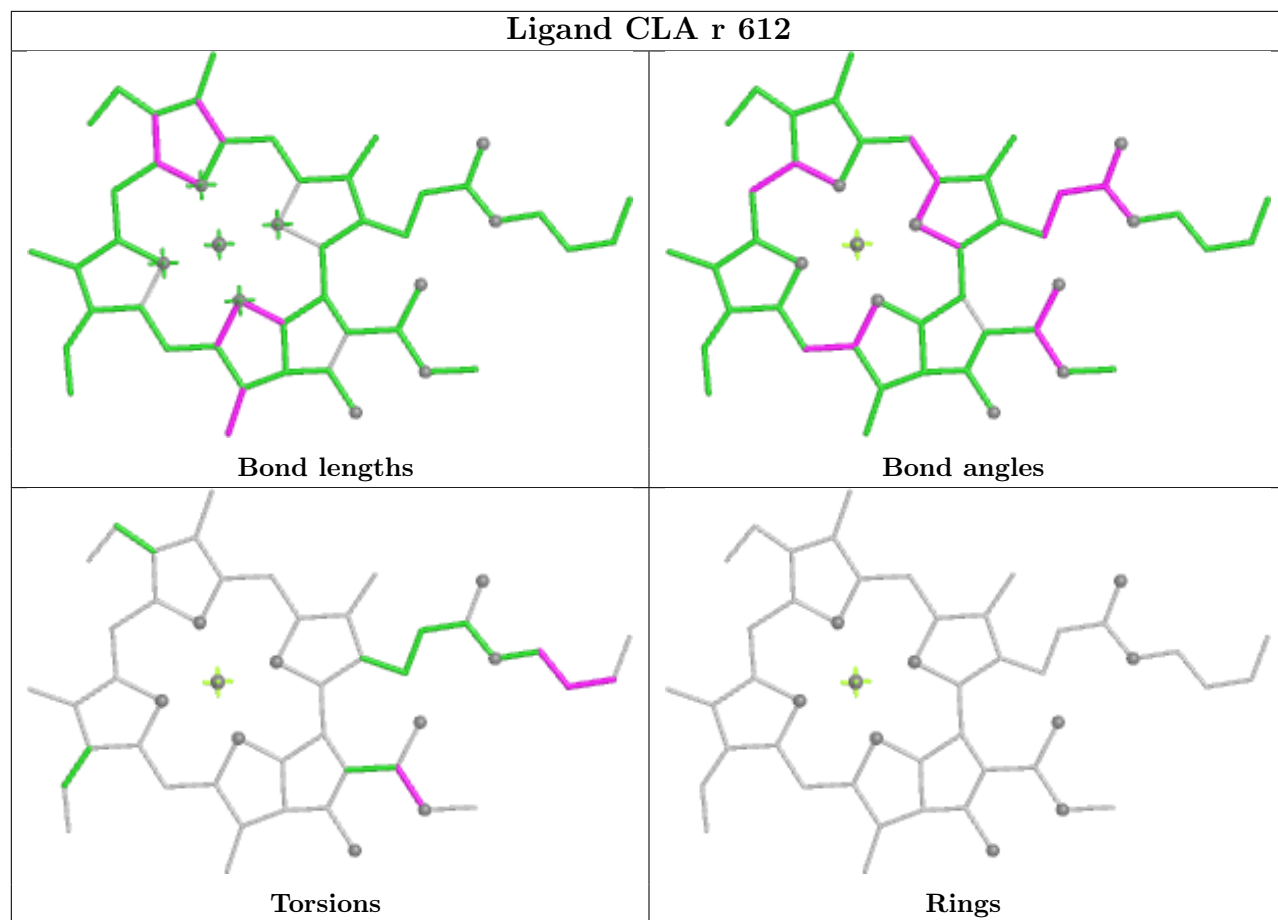


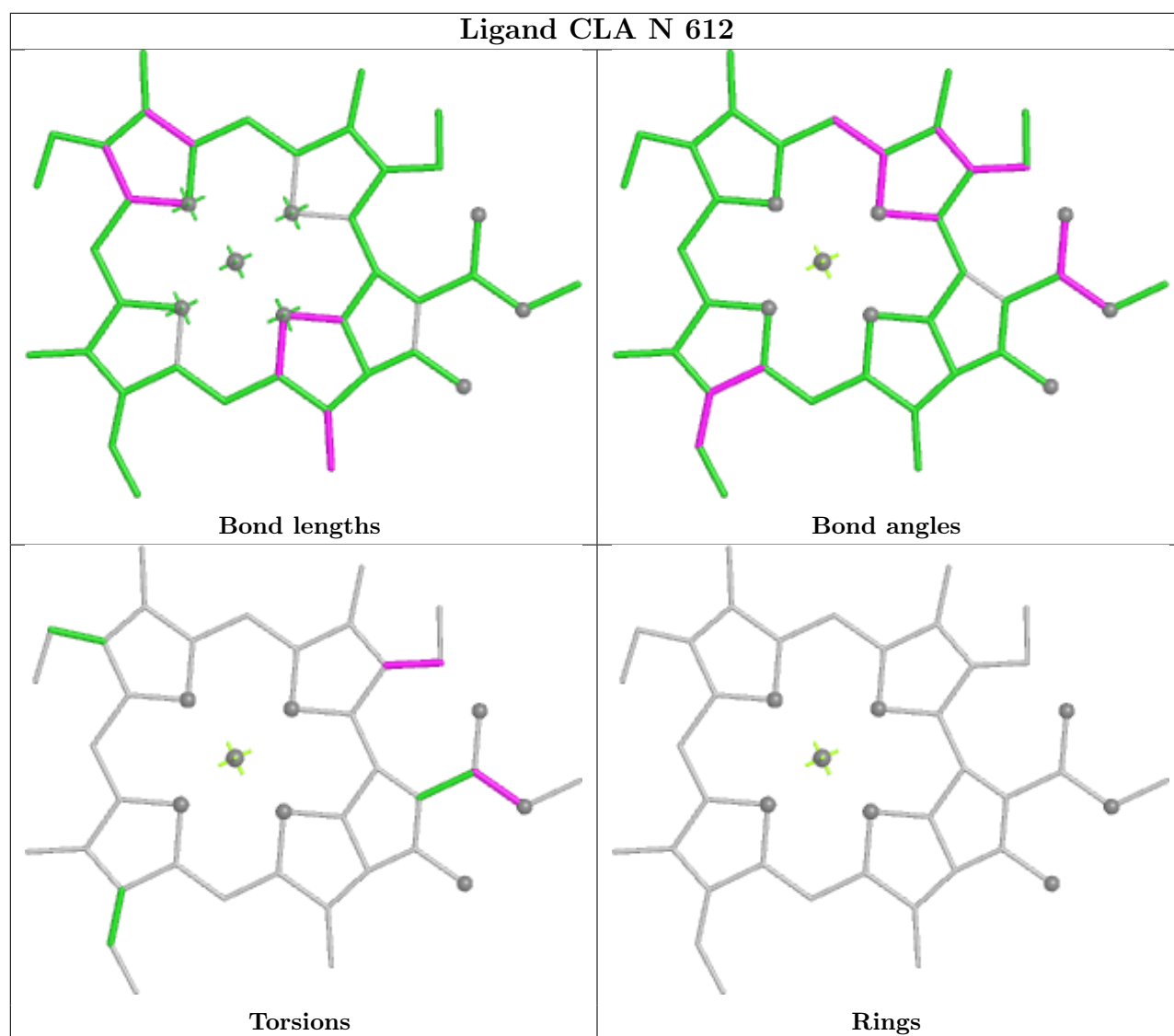
Rings

Ligand CLA B 620**Ligand CLA C 507**



Ligand CLA r 612





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.

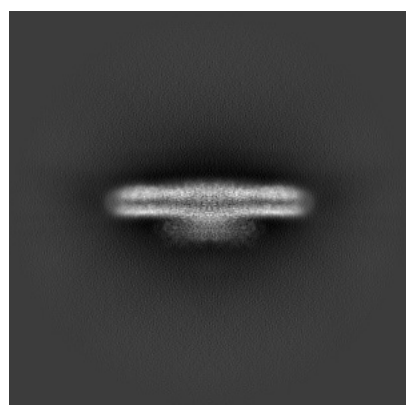
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39860. These allow visual inspection of the internal detail of the map and identification of artifacts.

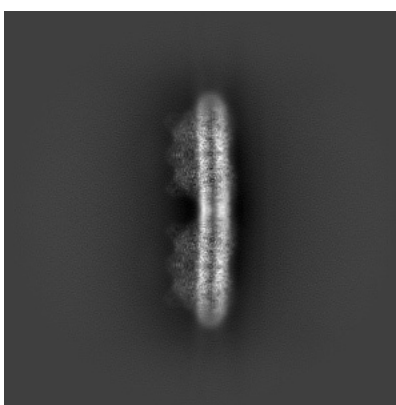
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

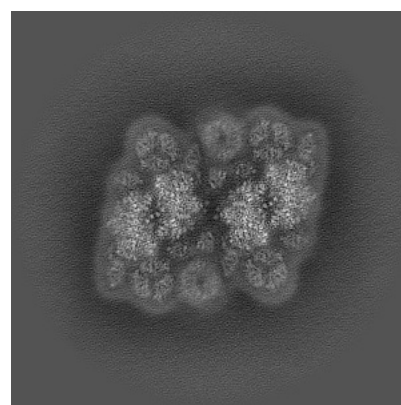
6.1.1 Primary map



X



Y

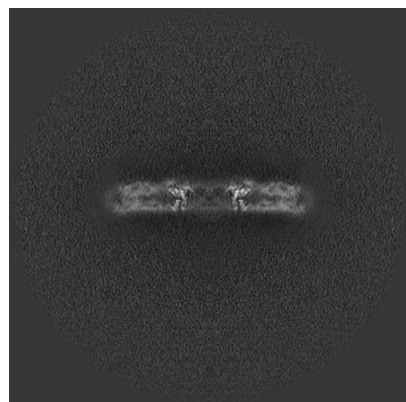


Z

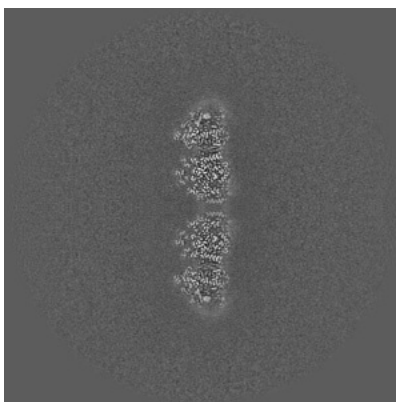
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

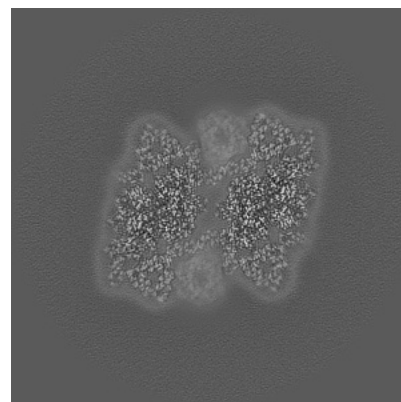
6.2.1 Primary map



X Index: 240



Y Index: 240

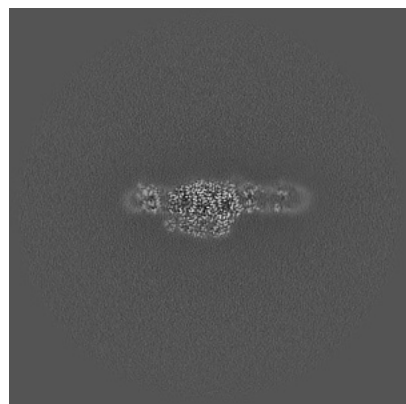


Z Index: 240

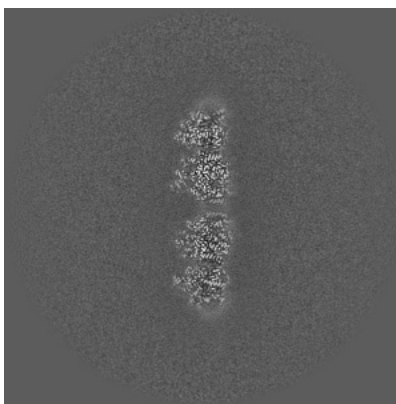
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

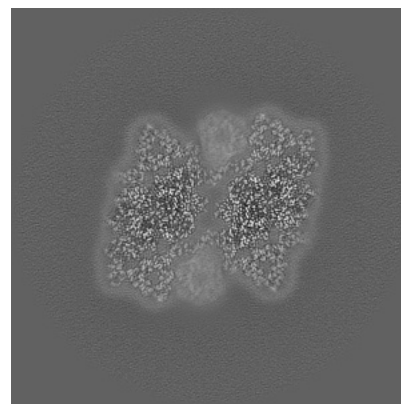
6.3.1 Primary map



X Index: 286



Y Index: 239

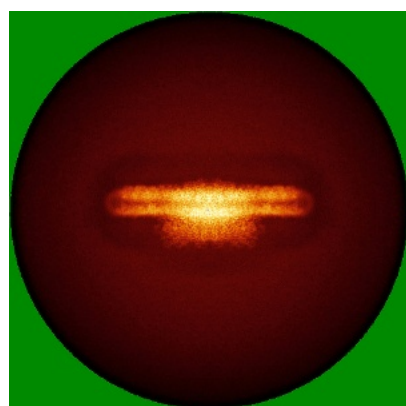


Z Index: 239

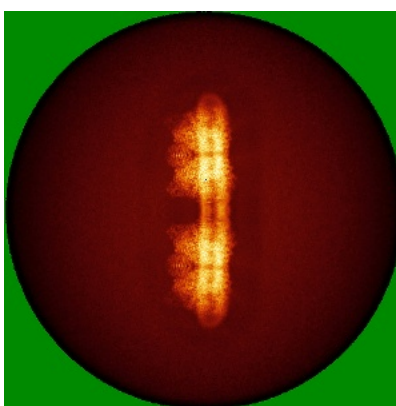
The images above show the largest variance slices of the map in three orthogonal directions.

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

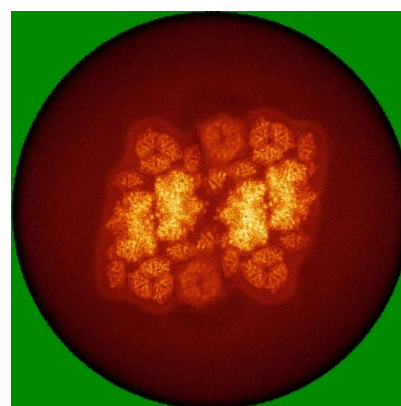
6.4.1 Primary map



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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

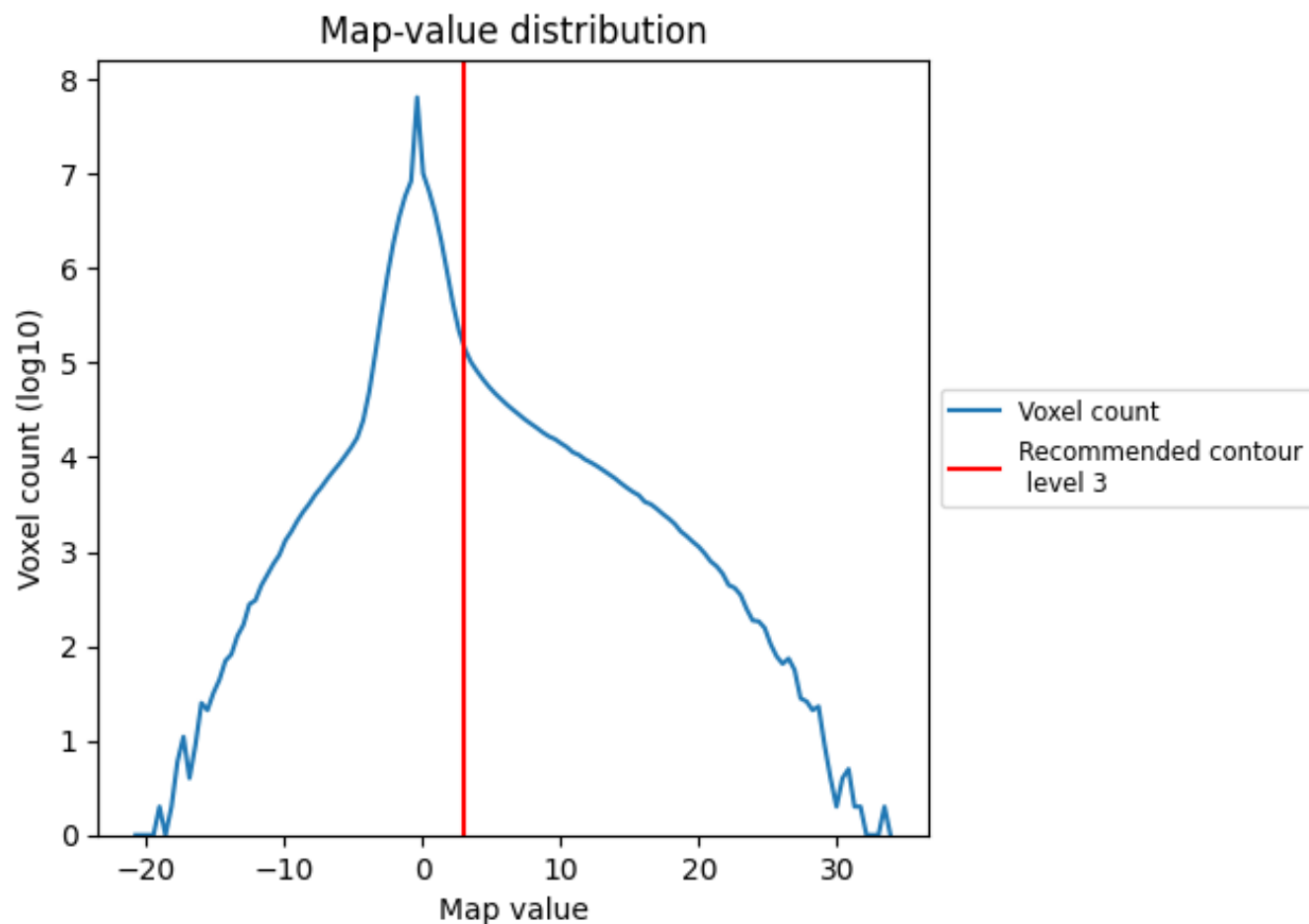
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

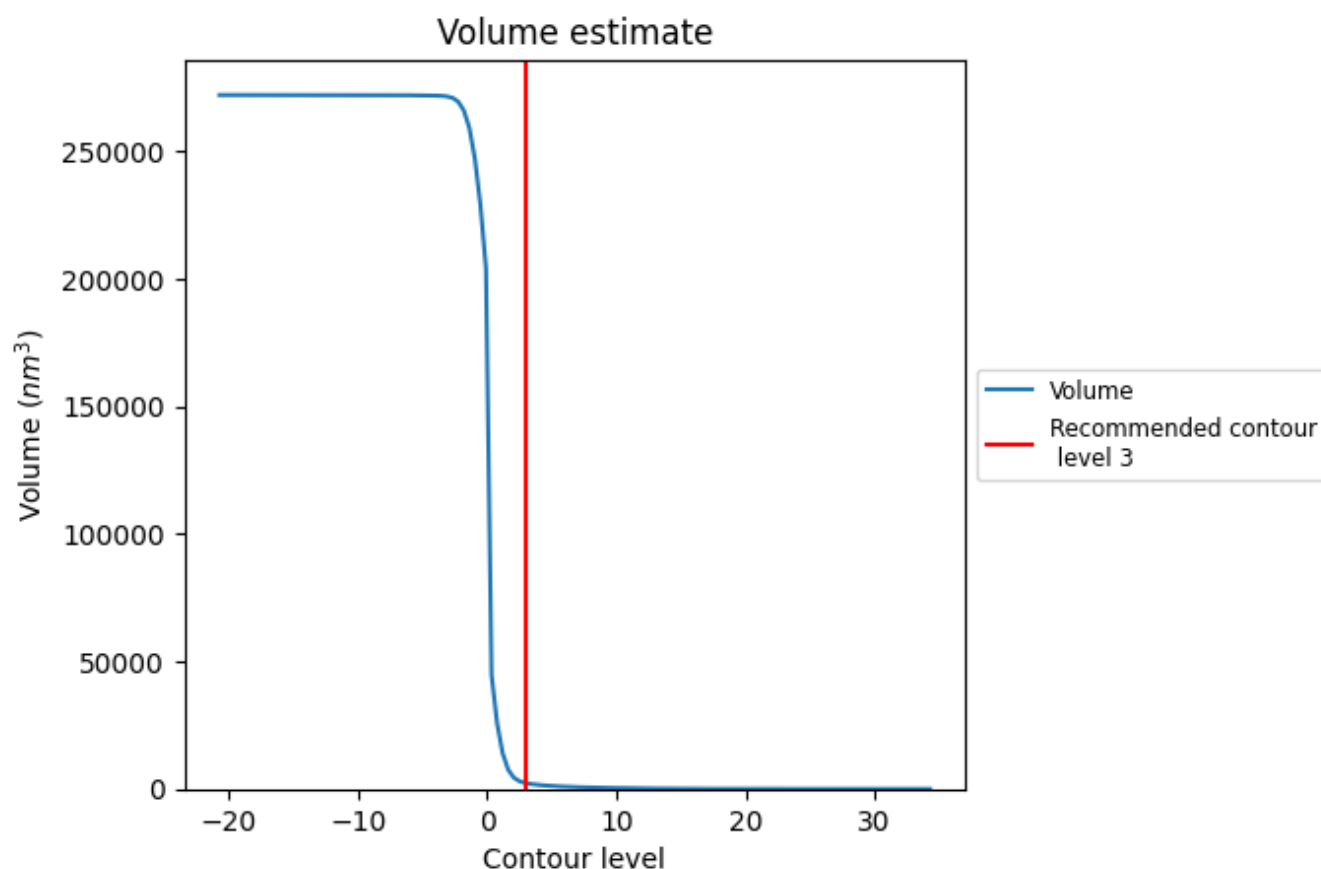
This section contains the results of statistical analysis of the map.

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.

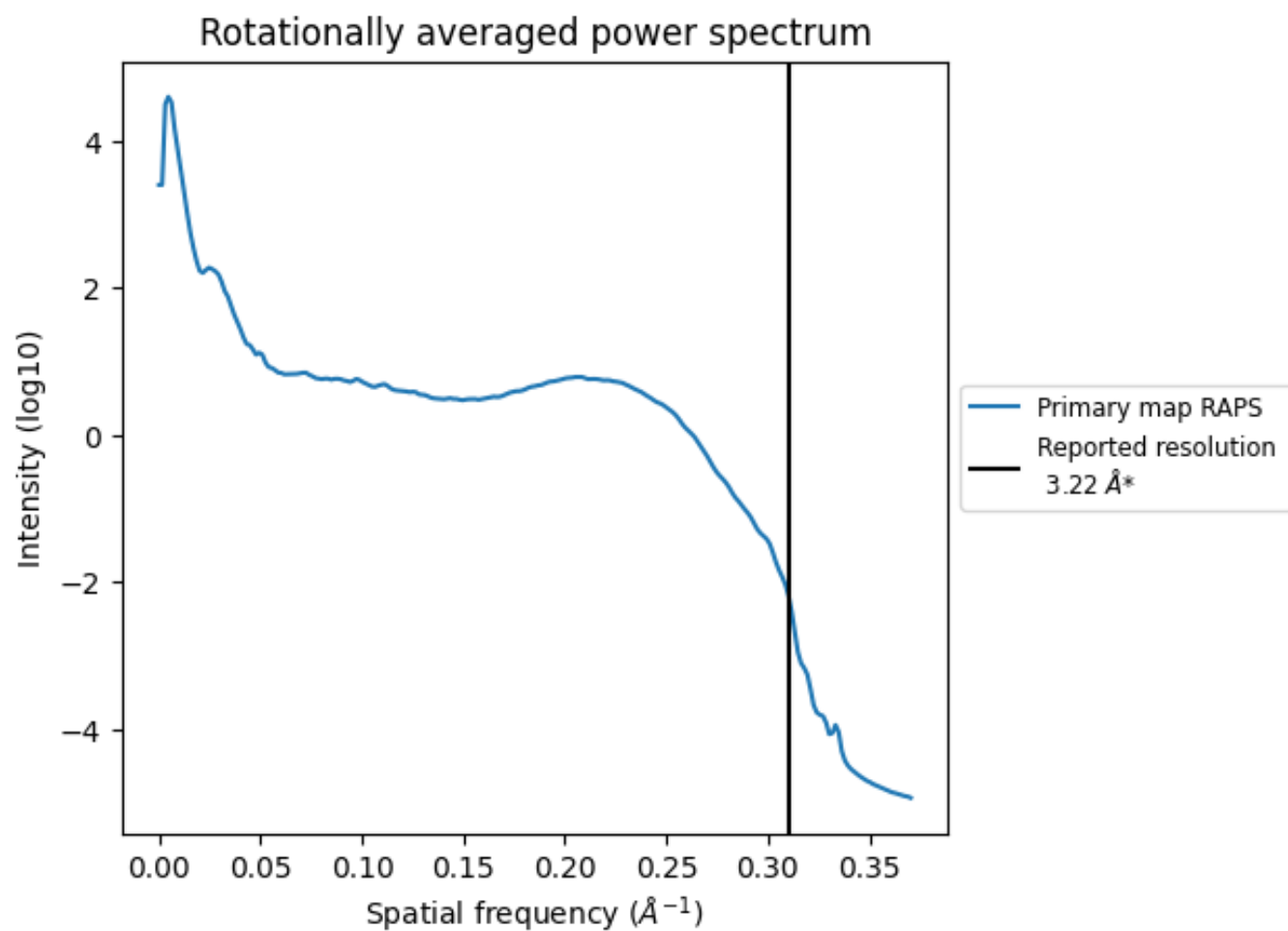
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2290 nm^3 ; this corresponds to an approximate mass of 2069 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 ⓘ

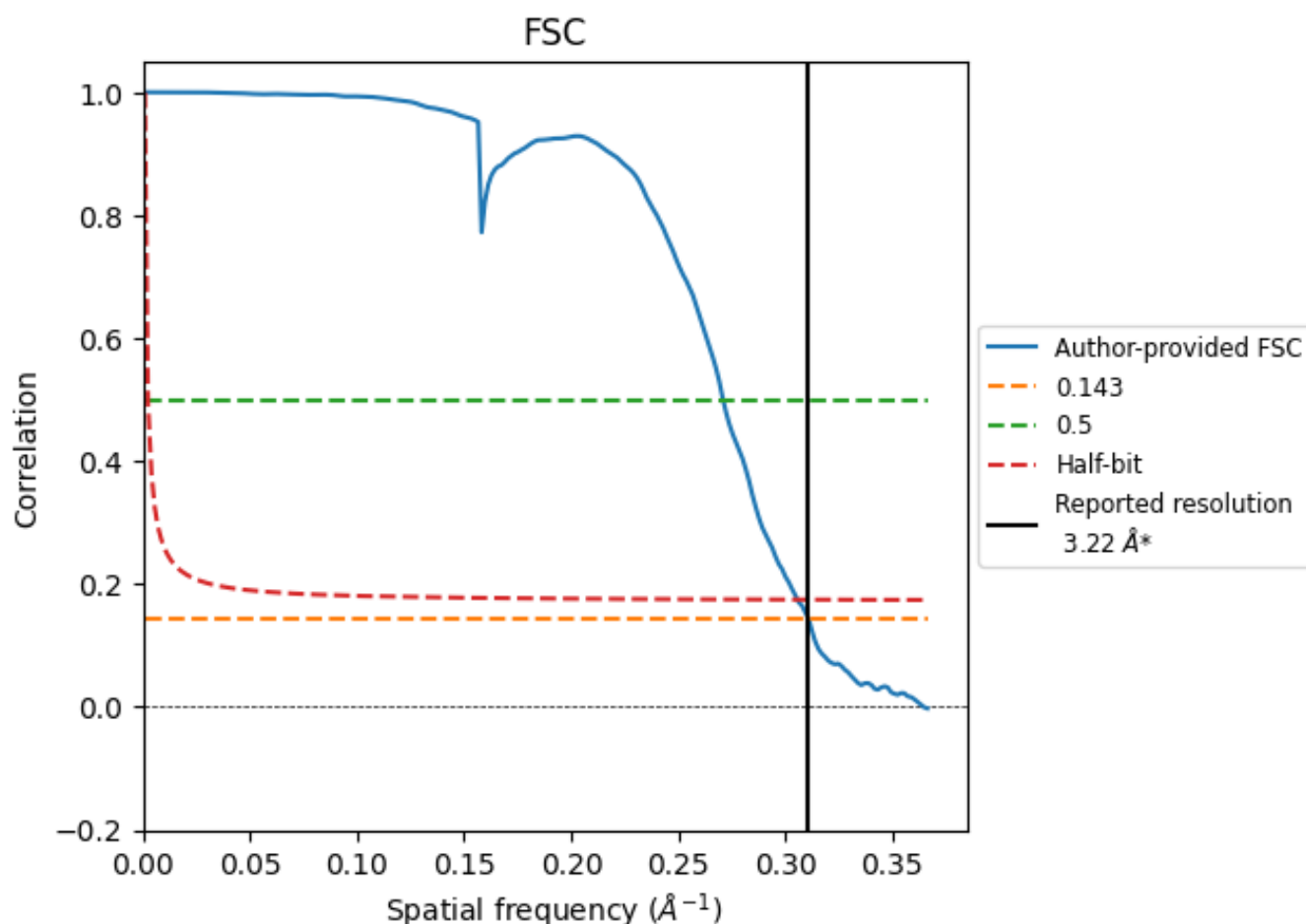


*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

8.2 Resolution estimates [i](#)

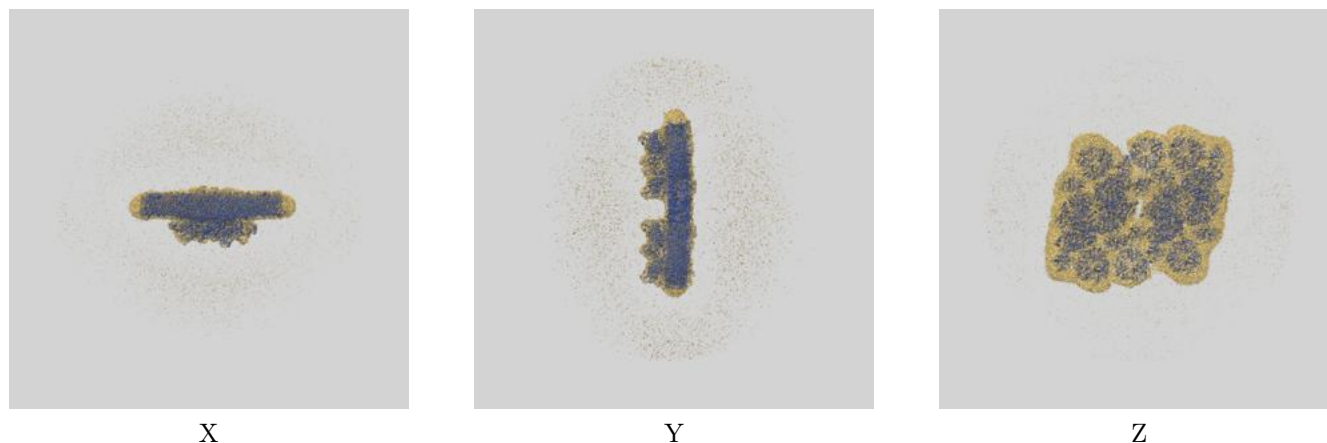
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.22	3.69	3.27
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

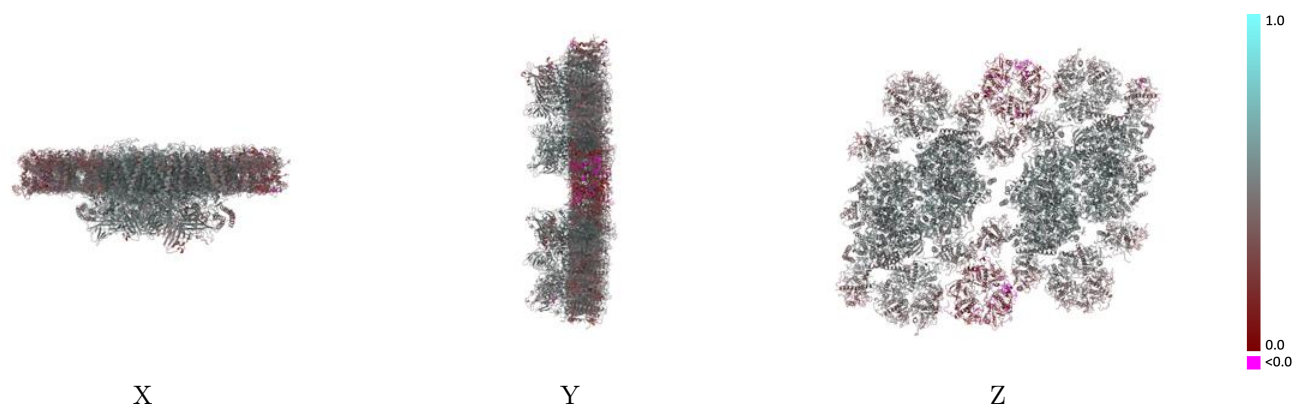
This section contains information regarding the fit between EMDB map EMD-39860 and PDB model 8Z9D. Per-residue inclusion information can be found in section [3](#) on page [62](#).

9.1 Map-model overlay [i](#)



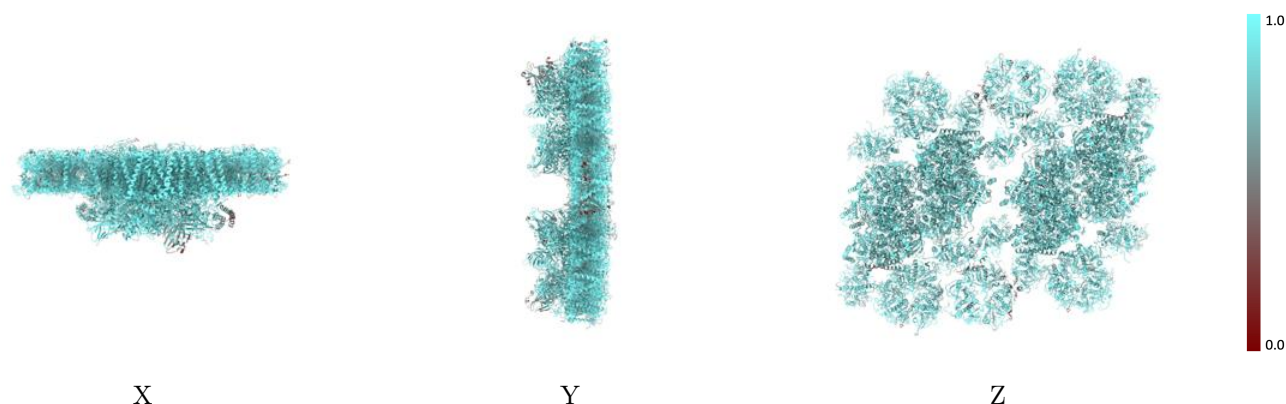
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



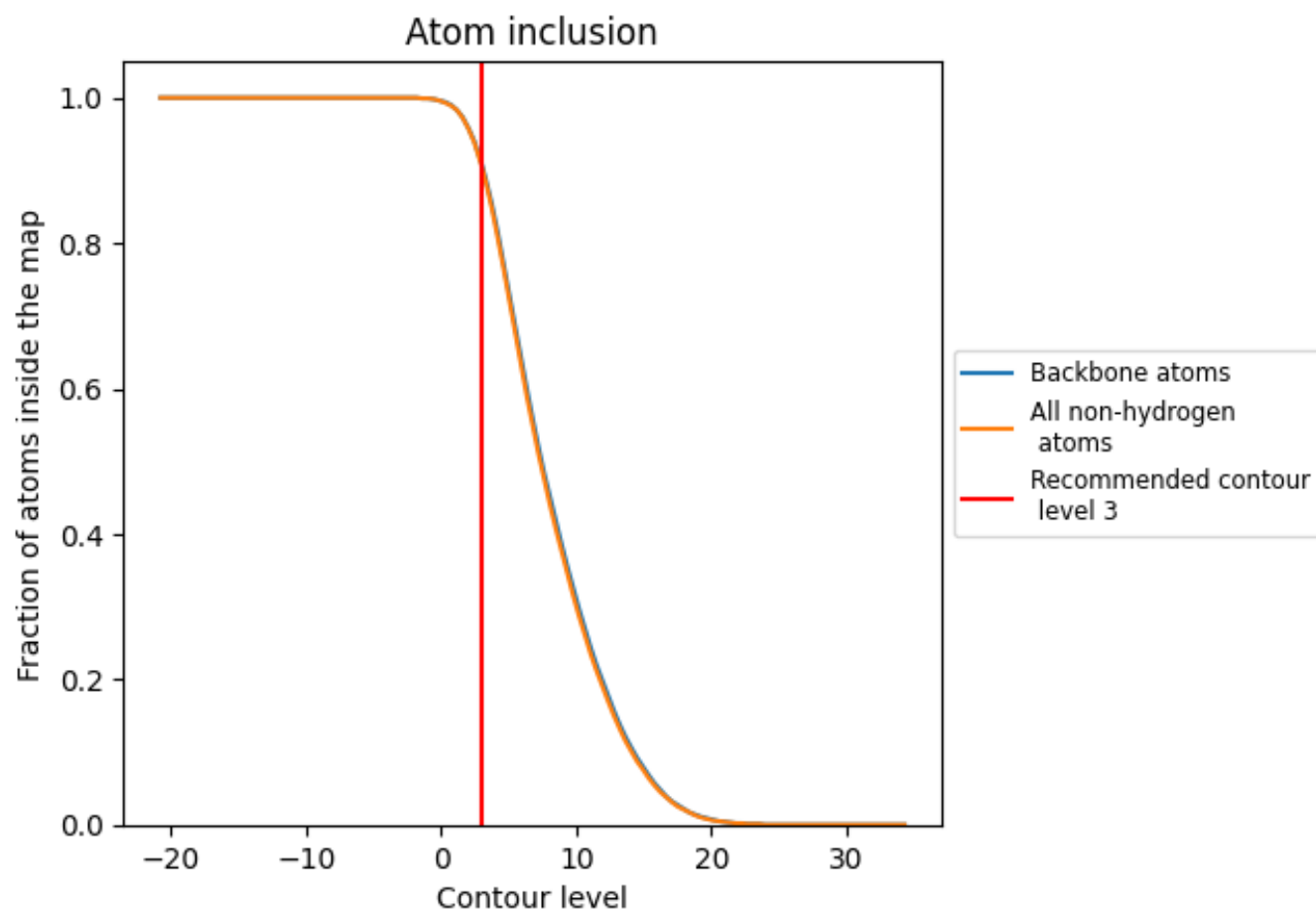
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.4520
0	 0.7820	 0.4470
00	 0.8280	 0.4610
1	 0.9110	 0.2140
11	 0.9050	 0.2020
2	 0.8440	 0.1600
22	 0.8610	 0.1580
3	 0.8500	 0.2130
33	 0.8750	 0.2150
4	 0.8810	 0.3570
44	 0.8990	 0.3600
5	 0.7560	 0.4260
55	 0.7820	 0.4450
A	 0.9570	 0.5300
AA	 0.9670	 0.5400
Aa	 0.9620	 0.5300
B	 0.9400	 0.5240
BB	 0.9600	 0.5340
Bb	 0.9510	 0.5250
C	 0.9370	 0.5200
CC	 0.9590	 0.5350
Cc	 0.9490	 0.5110
D	 0.9610	 0.5370
DD	 0.9730	 0.5490
Dd	 0.9620	 0.5260
E	 0.9460	 0.5120
EE	 0.9570	 0.5310
Ee	 0.9620	 0.4650
F	 0.9400	 0.5180
FF	 0.9630	 0.5240
Ff	 0.9590	 0.4630
G	 0.8850	 0.3760
GG	 0.8850	 0.3780
Gg	 0.8880	 0.4220
H	 0.9450	 0.5020



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Chain	Atom inclusion	Q-score
HH	 0.9680	 0.5110
Hh	 0.9590	 0.5020
I	 0.9610	 0.5120
II	 0.9360	 0.5160
Ii	 0.9810	 0.5360
J	 0.9140	 0.5180
JJ	 0.9390	 0.5160
Jj	 0.9170	 0.4780
K	 0.9280	 0.5180
KK	 0.9460	 0.5210
Kk	 0.9330	 0.4940
L	 0.9450	 0.5110
LL	 0.9660	 0.5290
Ll	 0.9600	 0.5350
M	 0.9070	 0.4980
MM	 0.9530	 0.5190
Mm	 0.9300	 0.5070
N	 0.9150	 0.4240
NN	 0.9210	 0.4310
Nn	 0.9130	 0.4370
O	 0.9310	 0.4960
OO	 0.9490	 0.5030
Oo	 0.9220	 0.4880
P	 0.8840	 0.4920
PP	 0.9000	 0.4970
Pp	 0.6740	 0.4290
Q	 0.7830	 0.4040
QQ	 0.8270	 0.4370
Qq	 0.6200	 0.3860
R	 0.8940	 0.4400
RR	 0.8960	 0.4460
Rr	 0.8500	 0.4130
S	 0.7940	 0.3810
SS	 0.8480	 0.3780
Ss	 0.8570	 0.3590
T	 0.8830	 0.5030
TT	 0.9150	 0.5170
Tt	 0.9550	 0.5320
U	 0.8820	 0.4630
UU	 0.9210	 0.4980
Uu	 0.9390	 0.4600
W	 0.9390	 0.4990

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Chain	Atom inclusion	Q-score
WW	 0.9440	 0.5110
Ww	 0.9320	 0.4960
X	 0.8750	 0.4520
XX	 0.8870	 0.4570
Xx	 0.9750	 0.4450
Y	 0.9120	 0.4590
YY	 0.9200	 0.4640
Yy	 0.9240	 0.4790
Z	 0.8960	 0.4590
ZZ	 0.9490	 0.4830
Zz	 0.9030	 0.4090
a	 0.9510	 0.5180
b	 0.9400	 0.5140
c	 0.9320	 0.4970
d	 0.9470	 0.5150
e	 0.9380	 0.4520
f	 0.9430	 0.4510
g	 0.8810	 0.4140
h	 0.9510	 0.4950
i	 0.9510	 0.4960
j	 0.8720	 0.4540
k	 0.9070	 0.4750
l	 0.9480	 0.5210
m	 0.9000	 0.4900
n	 0.9050	 0.4240
o	 0.8960	 0.4860
p	 0.6280	 0.4170
q	 0.5550	 0.3560
r	 0.8720	 0.4080
s	 0.8580	 0.3630
t	 0.9260	 0.5160
u	 0.9130	 0.4260
w	 0.9130	 0.4860
x	 0.9370	 0.4280
y	 0.9190	 0.4750
z	 0.8800	 0.3990