



wwPDB EM Validation Summary Report ⓘ

Aug 10, 2022 – 05:18 am BST

PDB ID : 7PIN
EMDB ID : EMD-13444
Title : Stacked compact Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-08-22
Resolution : 3.60 Å (reported)
Based on initial model : 6KAC

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.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

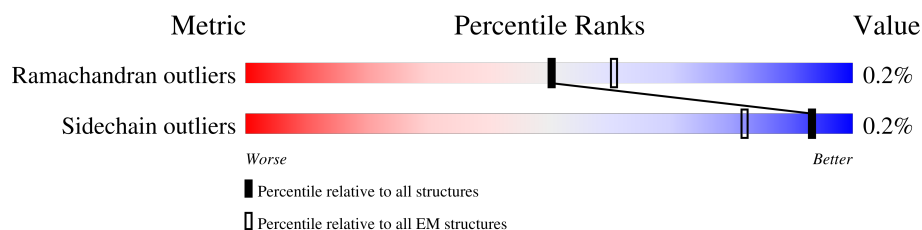
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

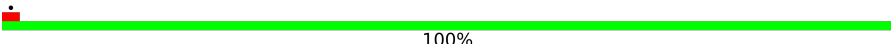
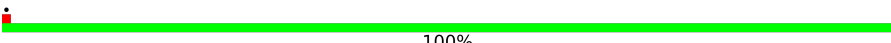
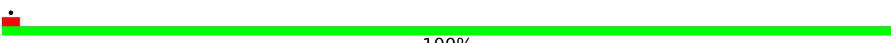
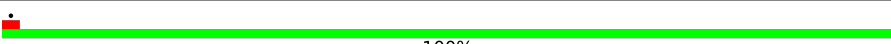




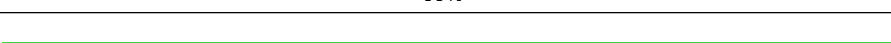
The reported resolution of this entry is 3.60 Å.

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




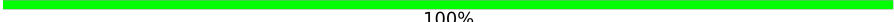
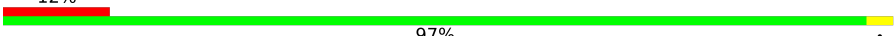



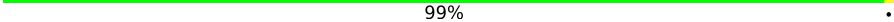
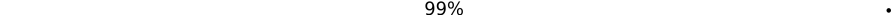
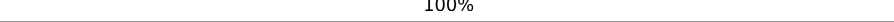
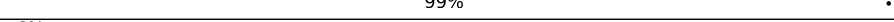
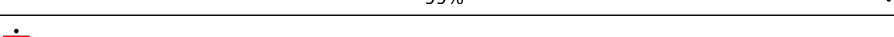




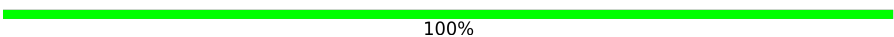

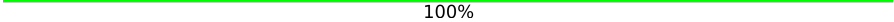
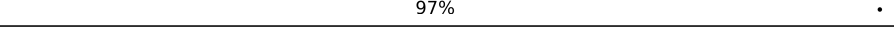
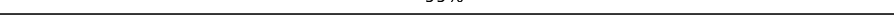





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	336	 100%
1	A1	336	 100%
1	a	336	 100%
1	a1	336	 100%
2	B	484	 100%
2	B1	484	 99%
2	b	484	 100%
2	b1	484	 99%
3	V	32	 100%

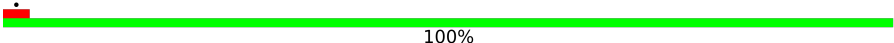
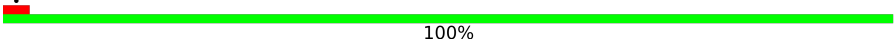
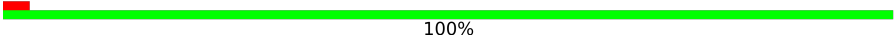
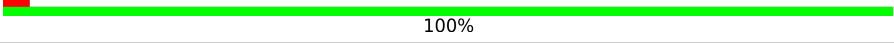
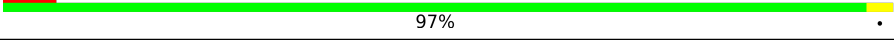
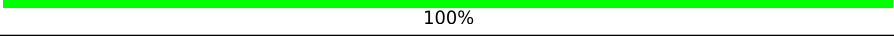
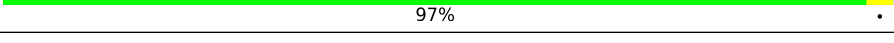
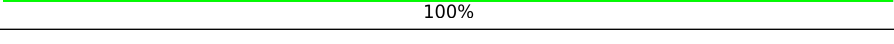
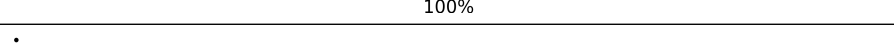
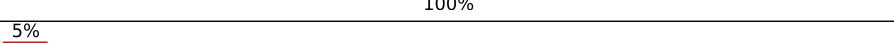
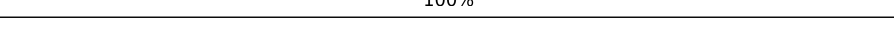
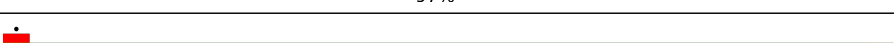






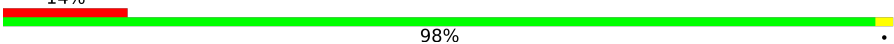
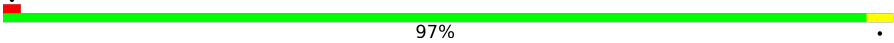
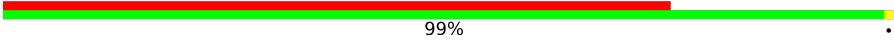
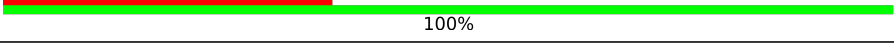
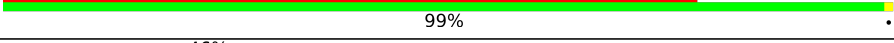
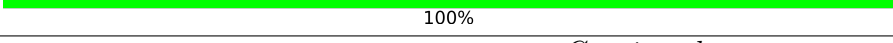

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Mol	Chain	Length	Quality of chain
3	V1	32	 100%
3	v	32	 100%
3	v1	32	 12% 97%
4	C	449	 100%
4	C1	449	 100%
4	c	449	 100%
4	c1	449	 99%
5	D	348	 99%
5	D1	348	 100%
5	d	348	 99%
5	d1	348	 6% 99%
6	E	76	 100%
6	E1	76	 100%
6	e	76	 5% 99%
6	e1	76	 100%
7	F	31	 6% 100%
7	F1	31	 100%
7	f	31	 100%
7	f1	31	 10% 100%
8	H	67	 97%
8	H1	67	 99%
8	h	67	 99%
8	h1	67	 100%
9	I	35	 100%
9	I1	35	 100%

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Mol	Chain	Length	Quality of chain
9	i	35	 100%
9	i1	35	 100%
10	J	36	 100%
10	J1	36	 100%
10	j	36	 6% 97%
10	j1	36	 100%
11	K	37	 97%
11	K1	37	 100%
11	k	37	 100%
11	k1	37	 100%
12	L	38	 5% 100%
12	L1	38	 97%
12	l	38	 97%
13	M	31	 100%
13	M1	31	 100%
13	m	31	 13% 100%
13	m1	31	 6% 100%
14	O	238	 12% 98%
14	O1	238	 98%
14	o	238	 14% 98%
14	o1	238	 97%
15	P	187	 75% 99%
15	P1	187	 37% 100%
15	p	187	 78% 99%
15	p1	187	 46% 100%

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Mol	Chain	Length	Quality of chain
16	T	30	 7% 97%
16	T1	30	 93% 7%
16	t	30	 100%
16	t1	30	 7% 100%
17	W	44	 11% 100%
17	W1	44	 100%
17	w	44	 9% 100%
17	w1	44	 7% 100%
18	X	30	 23% 100%
18	X1	30	 100%
18	x	30	 17% 100%
18	x1	30	 10% 100%
19	Z	61	 100%
19	Z1	61	 98%
19	z	61	 100%
19	z1	61	 10% 100%
20	N	222	 5% 98%
20	N1	222	 99%
20	n	222	 8% 99%
20	n1	222	 98%
21	G	221	 9% 100%
21	G1	221	 99%
21	g	221	 15% 100%
21	g1	221	 100%
22	R	196	 16% 99%

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Mol	Chain	Length	Quality of chain
22	R1	196	 99%
22	r	196	 99%
22	r1	196	 99%
23	S	243	 99%
23	S1	243	 99%
23	s	243	 98%
23	s1	243	 98%
24	Y	222	 99%
24	Y1	222	 99%
24	y	222	 99%
24	y1	222	 100%
25	U	27	 96%
25	U1	27	 100%
25	u	27	 96%
25	u1	27	 100%

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
29	CLA	A	405	X	-	-	-
29	CLA	A	406	X	-	-	-
29	CLA	A	407	X	-	-	-
29	CLA	A	410	X	-	-	-
29	CLA	A1	405	X	-	-	-
29	CLA	A1	406	X	-	-	-
29	CLA	A1	407	X	-	-	-
29	CLA	A1	410	X	-	-	-
29	CLA	B	602	X	-	-	-
29	CLA	B	603	X	-	-	-
29	CLA	B	604	X	-	-	-
29	CLA	B	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	B	606	X	-	-	-
29	CLA	B	607	X	-	-	-
29	CLA	B	608	X	-	-	-
29	CLA	B	609	X	-	-	-
29	CLA	B	610	X	-	-	-
29	CLA	B	611	X	-	-	-
29	CLA	B	612	X	-	-	-
29	CLA	B	613	X	-	-	-
29	CLA	B	614	X	-	-	-
29	CLA	B	615	X	-	-	-
29	CLA	B	616	X	-	-	-
29	CLA	B	617	X	-	-	-
29	CLA	B1	602	X	-	-	-
29	CLA	B1	603	X	-	-	-
29	CLA	B1	604	X	-	-	-
29	CLA	B1	605	X	-	-	-
29	CLA	B1	606	X	-	-	-
29	CLA	B1	607	X	-	-	-
29	CLA	B1	608	X	-	-	-
29	CLA	B1	609	X	-	-	-
29	CLA	B1	610	X	-	-	-
29	CLA	B1	611	X	-	-	-
29	CLA	B1	612	X	-	-	-
29	CLA	B1	613	X	-	-	-
29	CLA	B1	614	X	-	-	-
29	CLA	B1	615	X	-	-	-
29	CLA	B1	616	X	-	-	-
29	CLA	B1	617	X	-	-	-
29	CLA	C	501	X	-	-	-
29	CLA	C	502	X	-	-	-
29	CLA	C	503	X	-	-	-
29	CLA	C	504	X	-	-	-
29	CLA	C	505	X	-	-	-
29	CLA	C	506	X	-	-	-
29	CLA	C	507	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	C	513	X	-	-	-
29	CLA	C1	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	C1	502	X	-	-	-
29	CLA	C1	503	X	-	-	-
29	CLA	C1	504	X	-	-	-
29	CLA	C1	505	X	-	-	-
29	CLA	C1	506	X	-	-	-
29	CLA	C1	507	X	-	-	-
29	CLA	C1	508	X	-	-	-
29	CLA	C1	509	X	-	-	-
29	CLA	C1	510	X	-	-	-
29	CLA	C1	511	X	-	-	-
29	CLA	C1	512	X	-	-	-
29	CLA	C1	513	X	-	-	-
29	CLA	D	402	X	-	-	-
29	CLA	D	403	X	-	-	-
29	CLA	D1	402	X	-	-	-
29	CLA	D1	403	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	G1	602	X	-	-	-
29	CLA	G1	603	X	-	-	-
29	CLA	G1	604	X	-	-	-
29	CLA	G1	610	X	-	-	-
29	CLA	G1	611	X	-	-	-
29	CLA	G1	612	X	-	-	-
29	CLA	G1	613	X	-	-	-
29	CLA	G1	614	X	-	-	-
29	CLA	N	602	X	-	-	-
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-
29	CLA	N	614	X	-	-	-
29	CLA	N1	602	X	-	-	-
29	CLA	N1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	N1	604	X	-	-	-
29	CLA	N1	610	X	-	-	-
29	CLA	N1	611	X	-	-	-
29	CLA	N1	612	X	-	-	-
29	CLA	N1	613	X	-	-	-
29	CLA	N1	614	X	-	-	-
29	CLA	R	602	X	-	-	-
29	CLA	R	603	X	-	-	-
29	CLA	R	604	X	-	-	-
29	CLA	R	608	X	-	-	-
29	CLA	R	609	X	-	-	-
29	CLA	R	610	X	-	-	-
29	CLA	R	612	X	-	-	-
29	CLA	R1	602	X	-	-	-
29	CLA	R1	603	X	-	-	-
29	CLA	R1	604	X	-	-	-
29	CLA	R1	608	X	-	-	-
29	CLA	R1	609	X	-	-	-
29	CLA	R1	610	X	-	-	-
29	CLA	R1	612	X	-	-	-
29	CLA	S	602	X	-	-	-
29	CLA	S	603	X	-	-	-
29	CLA	S	604	X	-	-	-
29	CLA	S	605	X	-	-	-
29	CLA	S	609	X	-	-	-
29	CLA	S	610	X	-	-	-
29	CLA	S	611	X	-	-	-
29	CLA	S	612	X	-	-	-
29	CLA	S	613	X	-	-	-
29	CLA	S	614	X	-	-	-
29	CLA	S	617	X	-	-	-
29	CLA	S1	602	X	-	-	-
29	CLA	S1	603	X	-	-	-
29	CLA	S1	604	X	-	-	-
29	CLA	S1	605	X	-	-	-
29	CLA	S1	609	X	-	-	-
29	CLA	S1	610	X	-	-	-
29	CLA	S1	611	X	-	-	-
29	CLA	S1	612	X	-	-	-
29	CLA	S1	613	X	-	-	-
29	CLA	S1	614	X	-	-	-
29	CLA	S1	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	Y	602	X	-	-	-
29	CLA	Y	603	X	-	-	-
29	CLA	Y	604	X	-	-	-
29	CLA	Y	608	X	-	-	-
29	CLA	Y	610	X	-	-	-
29	CLA	Y	611	X	-	-	-
29	CLA	Y	612	X	-	-	-
29	CLA	Y	613	X	-	-	-
29	CLA	Y	614	X	-	-	-
29	CLA	Y1	602	X	-	-	-
29	CLA	Y1	603	X	-	-	-
29	CLA	Y1	604	X	-	-	-
29	CLA	Y1	608	X	-	-	-
29	CLA	Y1	610	X	-	-	-
29	CLA	Y1	611	X	-	-	-
29	CLA	Y1	612	X	-	-	-
29	CLA	Y1	613	X	-	-	-
29	CLA	Y1	614	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	a	406	X	-	-	-
29	CLA	a	407	X	-	-	-
29	CLA	a	410	X	-	-	-
29	CLA	a1	405	X	-	-	-
29	CLA	a1	406	X	-	-	-
29	CLA	a1	407	X	-	-	-
29	CLA	a1	410	X	-	-	-
29	CLA	b	602	X	-	-	-
29	CLA	b	603	X	-	-	-
29	CLA	b	604	X	-	-	-
29	CLA	b	605	X	-	-	-
29	CLA	b	606	X	-	-	-
29	CLA	b	607	X	-	-	-
29	CLA	b	608	X	-	-	-
29	CLA	b	609	X	-	-	-
29	CLA	b	610	X	-	-	-
29	CLA	b	611	X	-	-	-
29	CLA	b	612	X	-	-	-
29	CLA	b	613	X	-	-	-
29	CLA	b	614	X	-	-	-
29	CLA	b	615	X	-	-	-
29	CLA	b	616	X	-	-	-
29	CLA	b	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	b1	602	X	-	-	-
29	CLA	b1	603	X	-	-	-
29	CLA	b1	604	X	-	-	-
29	CLA	b1	605	X	-	-	-
29	CLA	b1	606	X	-	-	-
29	CLA	b1	607	X	-	-	-
29	CLA	b1	608	X	-	-	-
29	CLA	b1	609	X	-	-	-
29	CLA	b1	610	X	-	-	-
29	CLA	b1	611	X	-	-	-
29	CLA	b1	612	X	-	-	-
29	CLA	b1	613	X	-	-	-
29	CLA	b1	614	X	-	-	-
29	CLA	b1	615	X	-	-	-
29	CLA	b1	616	X	-	-	-
29	CLA	b1	617	X	-	-	-
29	CLA	c	501	X	-	-	-
29	CLA	c	502	X	-	-	-
29	CLA	c	503	X	-	-	-
29	CLA	c	504	X	-	-	-
29	CLA	c	505	X	-	-	-
29	CLA	c	506	X	-	-	-
29	CLA	c	507	X	-	-	-
29	CLA	c	508	X	-	-	-
29	CLA	c	509	X	-	-	-
29	CLA	c	510	X	-	-	-
29	CLA	c	511	X	-	-	-
29	CLA	c	512	X	-	-	-
29	CLA	c	513	X	-	-	-
29	CLA	c1	501	X	-	-	-
29	CLA	c1	502	X	-	-	-
29	CLA	c1	503	X	-	-	-
29	CLA	c1	504	X	-	-	-
29	CLA	c1	505	X	-	-	-
29	CLA	c1	506	X	-	-	-
29	CLA	c1	507	X	-	-	-
29	CLA	c1	508	X	-	-	-
29	CLA	c1	509	X	-	-	-
29	CLA	c1	510	X	-	-	-
29	CLA	c1	511	X	-	-	-
29	CLA	c1	512	X	-	-	-
29	CLA	c1	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	d	402	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	d1	402	X	-	-	-
29	CLA	d1	403	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	612	X	-	-	-
29	CLA	g	613	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	g1	602	X	-	-	-
29	CLA	g1	603	X	-	-	-
29	CLA	g1	604	X	-	-	-
29	CLA	g1	610	X	-	-	-
29	CLA	g1	611	X	-	-	-
29	CLA	g1	612	X	-	-	-
29	CLA	g1	613	X	-	-	-
29	CLA	g1	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-
29	CLA	n	612	X	-	-	-
29	CLA	n	613	X	-	-	-
29	CLA	n	614	X	-	-	-
29	CLA	n1	602	X	-	-	-
29	CLA	n1	603	X	-	-	-
29	CLA	n1	604	X	-	-	-
29	CLA	n1	610	X	-	-	-
29	CLA	n1	611	X	-	-	-
29	CLA	n1	612	X	-	-	-
29	CLA	n1	613	X	-	-	-
29	CLA	n1	614	X	-	-	-
29	CLA	r	602	X	-	-	-
29	CLA	r	603	X	-	-	-
29	CLA	r	604	X	-	-	-
29	CLA	r	608	X	-	-	-
29	CLA	r	609	X	-	-	-
29	CLA	r	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	r	612	X	-	-	-
29	CLA	r1	602	X	-	-	-
29	CLA	r1	603	X	-	-	-
29	CLA	r1	604	X	-	-	-
29	CLA	r1	608	X	-	-	-
29	CLA	r1	609	X	-	-	-
29	CLA	r1	610	X	-	-	-
29	CLA	r1	612	X	-	-	-
29	CLA	s	602	X	-	-	-
29	CLA	s	603	X	-	-	-
29	CLA	s	604	X	-	-	-
29	CLA	s	605	X	-	-	-
29	CLA	s	609	X	-	-	-
29	CLA	s	610	X	-	-	-
29	CLA	s	611	X	-	-	-
29	CLA	s	612	X	-	-	-
29	CLA	s	613	X	-	-	-
29	CLA	s	614	X	-	-	-
29	CLA	s	617	X	-	-	-
29	CLA	s1	602	X	-	-	-
29	CLA	s1	603	X	-	-	-
29	CLA	s1	604	X	-	-	-
29	CLA	s1	605	X	-	-	-
29	CLA	s1	609	X	-	-	-
29	CLA	s1	610	X	-	-	-
29	CLA	s1	611	X	-	-	-
29	CLA	s1	612	X	-	-	-
29	CLA	s1	613	X	-	-	-
29	CLA	s1	614	X	-	-	-
29	CLA	s1	617	X	-	-	-
29	CLA	y	602	X	-	-	-
29	CLA	y	603	X	-	-	-
29	CLA	y	604	X	-	-	-
29	CLA	y	608	X	-	-	-
29	CLA	y	610	X	-	-	-
29	CLA	y	611	X	-	-	-
29	CLA	y	612	X	-	-	-
29	CLA	y	613	X	-	-	-
29	CLA	y	614	X	-	-	-
29	CLA	y1	602	X	-	-	-
29	CLA	y1	603	X	-	-	-
29	CLA	y1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	y1	608	X	-	-	-
29	CLA	y1	610	X	-	-	-
29	CLA	y1	611	X	-	-	-
29	CLA	y1	612	X	-	-	-
29	CLA	y1	613	X	-	-	-
29	CLA	y1	614	X	-	-	-
36	C7Z	B	620	X	-	-	-
36	C7Z	B1	620	X	-	-	-
36	C7Z	b	620	X	-	-	-
36	C7Z	b1	620	X	-	-	-
41	LMK	C	527	X	-	-	-
41	LMK	C1	527	X	-	-	-
41	LMK	c	527	X	-	-	-
41	LMK	c1	527	X	-	-	-
45	RRX	H	101	X	-	-	-
45	RRX	H1	101	X	-	-	-
45	RRX	h	101	X	-	-	-
45	RRX	h1	101	X	-	-	-
48	CHL	G	601	X	-	-	-
48	CHL	G	605	X	-	-	-
48	CHL	G	606	X	-	-	-
48	CHL	G	607	X	-	-	-
48	CHL	G	608	X	-	-	-
48	CHL	G	609	X	-	-	-
48	CHL	G1	601	X	-	-	-
48	CHL	G1	605	X	-	-	-
48	CHL	G1	606	X	-	-	-
48	CHL	G1	607	X	-	-	-
48	CHL	G1	608	X	-	-	-
48	CHL	G1	609	X	-	-	-
48	CHL	N	601	X	-	-	-
48	CHL	N	605	X	-	-	-
48	CHL	N	606	X	-	-	-
48	CHL	N	607	X	-	-	-
48	CHL	N	608	X	-	-	-
48	CHL	N	609	X	-	-	-
48	CHL	N1	601	X	-	-	-
48	CHL	N1	605	X	-	-	-
48	CHL	N1	606	X	-	-	-
48	CHL	N1	607	X	-	-	-
48	CHL	N1	608	X	-	-	-
48	CHL	N1	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	R	606	X	-	-	-
48	CHL	R	607	X	-	-	-
48	CHL	R1	606	X	-	-	-
48	CHL	R1	607	X	-	-	-
48	CHL	S	601	X	-	-	-
48	CHL	S	606	X	-	-	-
48	CHL	S	607	X	-	-	-
48	CHL	S	608	X	-	-	-
48	CHL	S1	601	X	-	-	-
48	CHL	S1	606	X	-	-	-
48	CHL	S1	607	X	-	-	-
48	CHL	S1	608	X	-	-	-
48	CHL	Y	601	X	-	-	-
48	CHL	Y	605	X	-	-	-
48	CHL	Y	606	X	-	-	-
48	CHL	Y	607	X	-	-	-
48	CHL	Y	609	X	-	-	-
48	CHL	Y1	601	X	-	-	-
48	CHL	Y1	605	X	-	-	-
48	CHL	Y1	606	X	-	-	-
48	CHL	Y1	607	X	-	-	-
48	CHL	Y1	609	X	-	-	-
48	CHL	g	601	X	-	-	-
48	CHL	g	605	X	-	-	-
48	CHL	g	606	X	-	-	-
48	CHL	g	607	X	-	-	-
48	CHL	g	608	X	-	-	-
48	CHL	g	609	X	-	-	-
48	CHL	g1	601	X	-	-	-
48	CHL	g1	605	X	-	-	-
48	CHL	g1	606	X	-	-	-
48	CHL	g1	607	X	-	-	-
48	CHL	g1	608	X	-	-	-
48	CHL	g1	609	X	-	-	-
48	CHL	n	601	X	-	-	-
48	CHL	n	605	X	-	-	-
48	CHL	n	606	X	-	-	-
48	CHL	n	607	X	-	-	-
48	CHL	n	608	X	-	-	-
48	CHL	n	609	X	-	-	-
48	CHL	n1	601	X	-	-	-
48	CHL	n1	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	n1	606	X	-	-	-
48	CHL	n1	607	X	-	-	-
48	CHL	n1	608	X	-	-	-
48	CHL	n1	609	X	-	-	-
48	CHL	r	606	X	-	-	-
48	CHL	r	607	X	-	-	-
48	CHL	r1	606	X	-	-	-
48	CHL	r1	607	X	-	-	-
48	CHL	s	601	X	-	-	-
48	CHL	s	606	X	-	-	-
48	CHL	s	607	X	-	-	-
48	CHL	s	608	X	-	-	-
48	CHL	s1	601	X	-	-	-
48	CHL	s1	606	X	-	-	-
48	CHL	s1	607	X	-	-	-
48	CHL	s1	608	X	-	-	-
48	CHL	y	601	X	-	-	-
48	CHL	y	605	X	-	-	-
48	CHL	y	606	X	-	-	-
48	CHL	y	607	X	-	-	-
48	CHL	y	609	X	-	-	-
48	CHL	y1	601	X	-	-	-
48	CHL	y1	605	X	-	-	-
48	CHL	y1	606	X	-	-	-
48	CHL	y1	607	X	-	-	-
48	CHL	y1	609	X	-	-	-
49	LUT	G	621	X	-	-	-
49	LUT	R	620	X	-	-	-
49	LUT	n1	621	X	-	-	-
50	XAT	G	622	X	-	-	-
50	XAT	G1	622	X	-	-	-
50	XAT	N	622	X	-	-	-
50	XAT	N1	622	X	-	-	-
50	XAT	Y1	622	X	-	-	-
50	XAT	g	622	X	-	-	-
50	XAT	g1	622	X	-	-	-
50	XAT	n	622	X	-	-	-
50	XAT	r	621	X	-	-	-
50	XAT	r1	621	X	-	-	-
51	NEX	g	623	X	-	-	-
51	NEX	g1	623	X	-	-	-
53	ERG	R	626	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	ERG	R1	626	X	-	-	-
53	ERG	r	626	X	-	-	-
53	ERG	r1	626	X	-	-	-

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 152240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	A1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	B1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		
3	V1	32	Total	C	N	O	0	0
			227	152	37	38		
3	v1	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	C1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	D1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		
6	e	76	Total	C	N	O	0	0
			621	404	102	115		
6	E1	76	Total	C	N	O	0	0
			621	404	102	115		
6	e1	76	Total	C	N	O	0	0
			621	404	102	115		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	F1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	f1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	H1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	I1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

- Molecule 10 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		
10	j	36	Total	C	N	O	0	0
			266	183	40	43		
10	J1	36	Total	C	N	O	0	0
			266	183	40	43		
10	j1	36	Total	C	N	O	0	0
			266	183	40	43		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		
11	K1	37	Total	C	N	O	0	0
			297	207	43	47		
11	k1	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	L1	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

- Molecule 13 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		
13	M1	31	Total	C	N	O	0	0
			234	159	33	42		
13	m1	31	Total	C	N	O	0	0
			234	159	33	42		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	O1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	P1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	T1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	W1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total	C	N	O	0	0
			201	132	32	37		
18	x	30	Total	C	N	O	0	0
			201	132	32	37		
18	X1	30	Total	C	N	O	0	0
			201	132	32	37		

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Mol	Chain	Residues	Atoms				AltConf	Trace
18	x1	30	Total	C	N	O	0	0
			201	132	32	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	Z1	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z1	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	N1	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n1	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	G1	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g1	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7
g	180	ALA	PRO	conflict	UNP A1XKU7
G1	180	ALA	PRO	conflict	UNP A1XKU7
g1	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	R	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	R1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	S1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

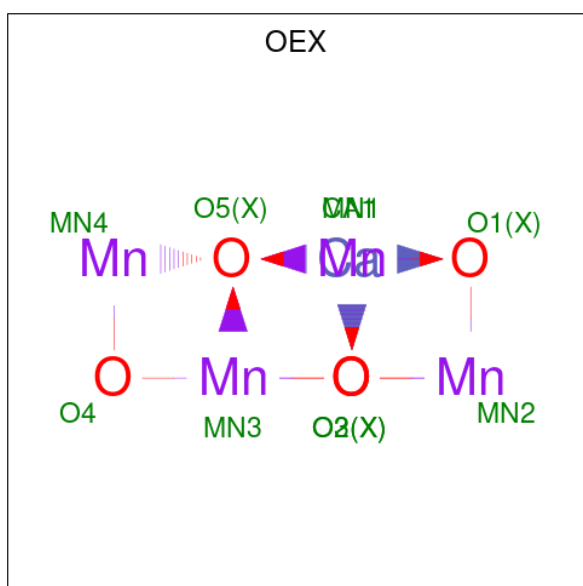
- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	Y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	U1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	a	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	A1	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	a1	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 27 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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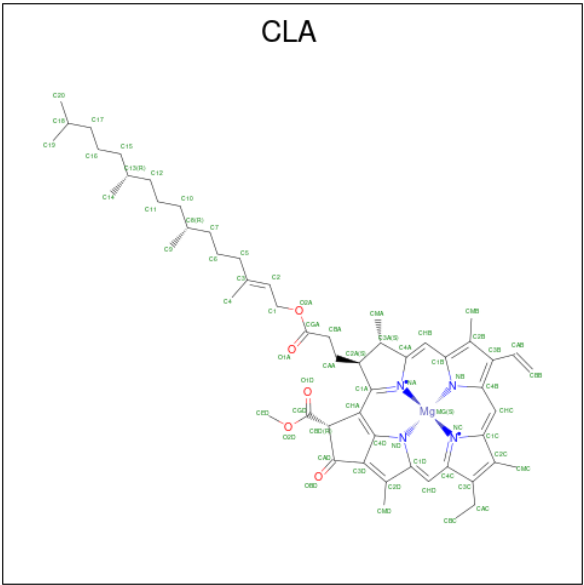
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Mol	Chain	Residues	Atoms		AltConf
27	A1	1	Total	Fe	0
			1	1	
27	a1	1	Total	Fe	0
			1	1	

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
28	A	2	Total	Cl	0
			2	2	
28	a	2	Total	Cl	0
			2	2	
28	A1	2	Total	Cl	0
			2	2	
28	a1	2	Total	Cl	0
			2	2	

- Molecule 29 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	G	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	G	1	Total	C	Mg	N	O	0
			466	388	8	32	38	

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Mol	Chain	Residues	Atoms					AltConf
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0

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Mol	Chain	Residues	Atoms					AltConf
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	

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Mol	Chain	Residues	Atoms					AltConf
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	A1	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A1	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A1	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A1	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	D1	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	D1	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	N1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0

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Mol	Chain	Residues	Atoms					AltConf
29	R1	1	Total	C	Mg	N	O	0
			409	339	7	28	35	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	Y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	

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Mol	Chain	Residues	Atoms					AltConf
29	a1	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a1	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a1	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a1	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	d1	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	d1	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	

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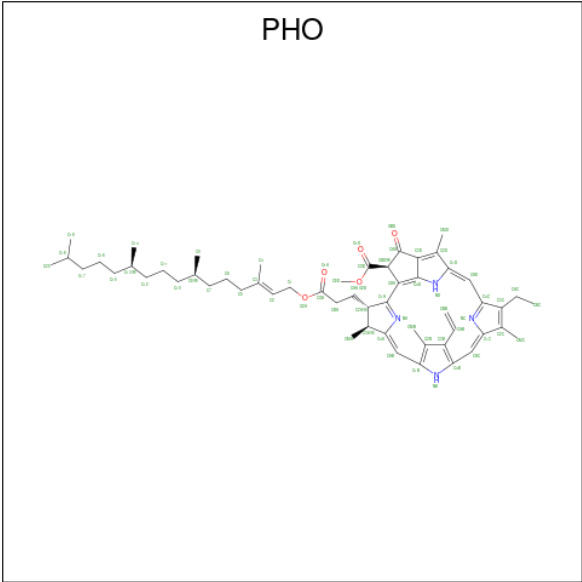
Mol	Chain	Residues	Atoms					AltConf
29	n1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0

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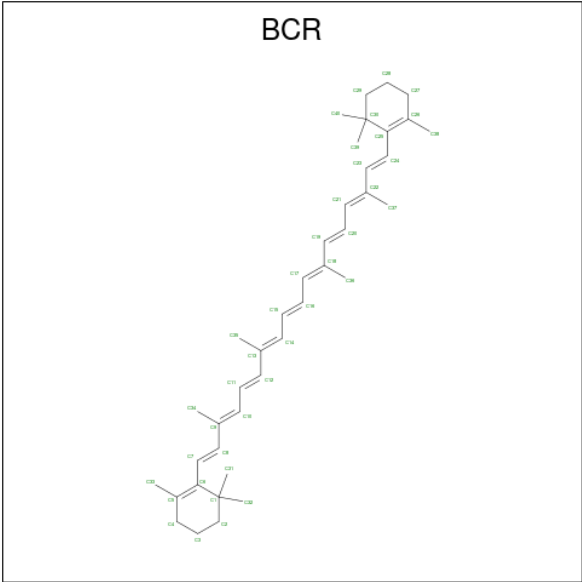
Mol	Chain	Residues	Atoms					AltConf
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	

- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	N	O	0
			128	110	8	10	
30	A	1	Total	C	N	O	0
			128	110	8	10	
30	a	1	Total	C	N	O	0
			128	110	8	10	
30	a	1	Total	C	N	O	0
			128	110	8	10	
30	A1	1	Total	C	N	O	0
			128	110	8	10	
30	A1	1	Total	C	N	O	0
			128	110	8	10	
30	a1	1	Total	C	N	O	0
			128	110	8	10	
30	a1	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



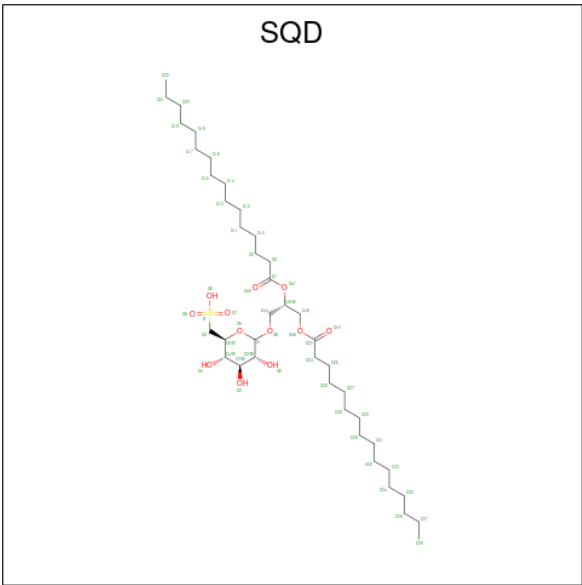
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			80	80	
31	B	1	Total	C	0
			80	80	
31	C	1	Total	C	0
			160	160	
31	C	1	Total	C	0
			160	160	
31	C	1	Total	C	0
			160	160	
31	C	1	Total	C	0
			160	160	
31	D	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			80	80	
31	b	1	Total	C	0
			80	80	
31	c	1	Total	C	0
			160	160	
31	c	1	Total	C	0
			160	160	
31	c	1	Total	C	0
			160	160	

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Mol	Chain	Residues	Atoms	AltConf
31	c	1	Total C 160 160	0
31	d	1	Total C 40 40	0
31	A1	1	Total C 40 40	0
31	B1	1	Total C 80 80	0
31	B1	1	Total C 80 80	0
31	C1	1	Total C 160 160	0
31	C1	1	Total C 160 160	0
31	C1	1	Total C 160 160	0
31	C1	1	Total C 160 160	0
31	D1	1	Total C 40 40	0
31	a1	1	Total C 40 40	0
31	b1	1	Total C 80 80	0
31	b1	1	Total C 80 80	0
31	c1	1	Total C 160 160	0
31	c1	1	Total C 160 160	0
31	c1	1	Total C 160 160	0
31	c1	1	Total C 160 160	0
31	d1	1	Total C 40 40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



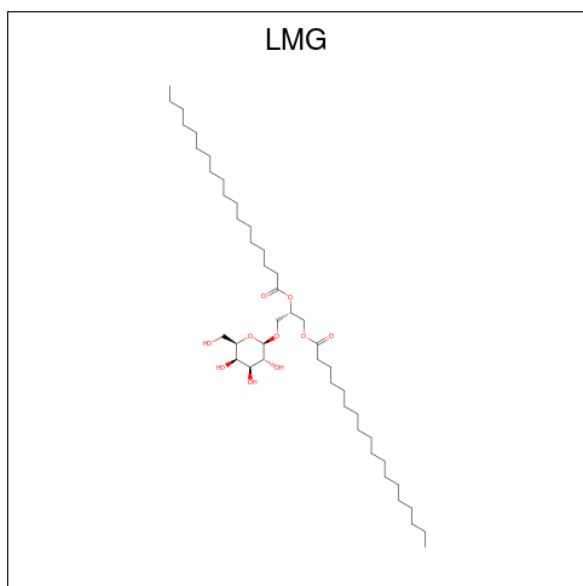
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			51	38	12	1	
32	B	1	Total	C	O	S	0
			96	70	24	2	
32	B	1	Total	C	O	S	0
			96	70	24	2	
32	C	1	Total	C	O	S	0
			54	41	12	1	
32	M	1	Total	C	O	S	0
			42	29	12	1	
32	a	1	Total	C	O	S	0
			51	38	12	1	
32	b	1	Total	C	O	S	0
			96	70	24	2	
32	b	1	Total	C	O	S	0
			96	70	24	2	
32	c	1	Total	C	O	S	0
			54	41	12	1	
32	m	1	Total	C	O	S	0
			42	29	12	1	
32	A1	1	Total	C	O	S	0
			51	38	12	1	
32	B1	1	Total	C	O	S	0
			96	70	24	2	
32	B1	1	Total	C	O	S	0
			96	70	24	2	
32	C1	1	Total	C	O	S	0
			54	41	12	1	

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Mol	Chain	Residues	Atoms				AltConf
32	M1	1	Total	C	O	S	0
			42	29	12	1	
32	a1	1	Total	C	O	S	0
			51	38	12	1	
32	b1	1	Total	C	O	S	0
			96	70	24	2	
32	b1	1	Total	C	O	S	0
			96	70	24	2	
32	c1	1	Total	C	O	S	0
			54	41	12	1	
32	m1	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O		0
			48	38	10		
33	B	1	Total	C	O		0
			44	34	10		
33	C	1	Total	C	O		0
			106	86	20		
33	C	1	Total	C	O		0
			106	86	20		
33	D	1	Total	C	O		0
			46	36	10		

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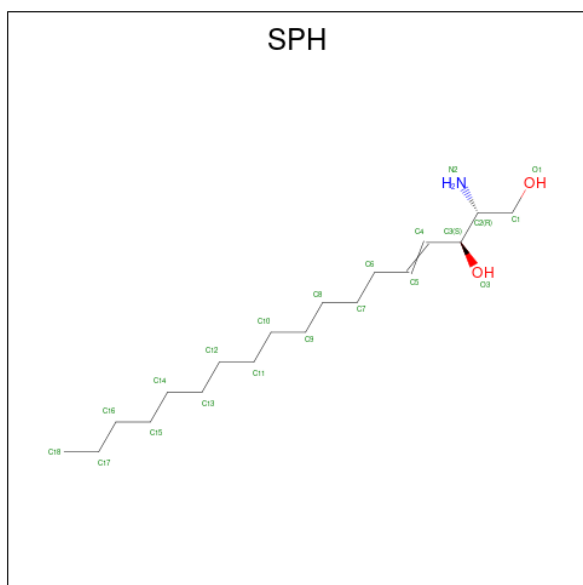
Mol	Chain	Residues	Atoms			AltConf
33	H	1	Total 48	C 38	O 10	0
33	W	1	Total 39	C 29	O 10	0
33	a	1	Total 48	C 38	O 10	0
33	b	1	Total 44	C 34	O 10	0
33	c	1	Total 106	C 86	O 20	0
33	c	1	Total 106	C 86	O 20	0
33	d	1	Total 46	C 36	O 10	0
33	h	1	Total 48	C 38	O 10	0
33	w	1	Total 39	C 29	O 10	0
33	A1	1	Total 48	C 38	O 10	0
33	B1	1	Total 44	C 34	O 10	0
33	C1	1	Total 106	C 86	O 20	0
33	C1	1	Total 106	C 86	O 20	0
33	D1	1	Total 46	C 36	O 10	0
33	H1	1	Total 48	C 38	O 10	0
33	W1	1	Total 39	C 29	O 10	0
33	a1	1	Total 48	C 38	O 10	0
33	b1	1	Total 44	C 34	O 10	0
33	c1	1	Total 106	C 86	O 20	0
33	c1	1	Total 106	C 86	O 20	0
33	d1	1	Total 46	C 36	O 10	0

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Mol	Chain	Residues	Atoms			AltConf
33	h1	1	Total	C	O	0
			48	38	10	
33	w1	1	Total	C	O	0
			39	29	10	

- Molecule 34 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).

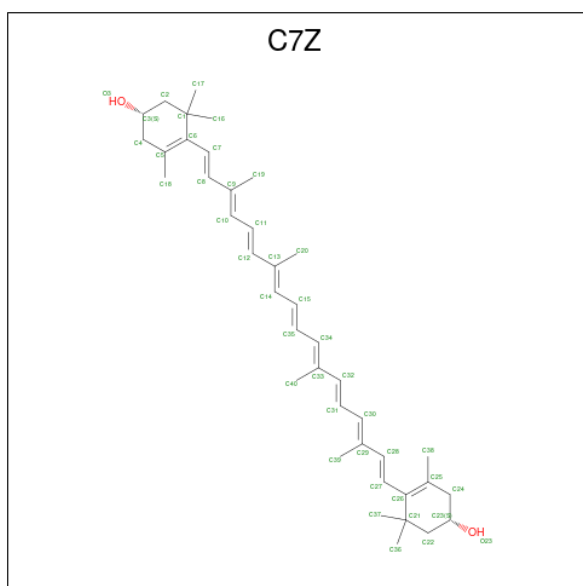


Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	N	O	0
			21	18	1	2	
34	Y	1	Total	C	N	O	0
			21	18	1	2	
34	a	1	Total	C	N	O	0
			21	18	1	2	
34	y	1	Total	C	N	O	0
			21	18	1	2	
34	A1	1	Total	C	N	O	0
			21	18	1	2	
34	Y1	1	Total	C	N	O	0
			21	18	1	2	
34	a1	1	Total	C	N	O	0
			21	18	1	2	
34	y1	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

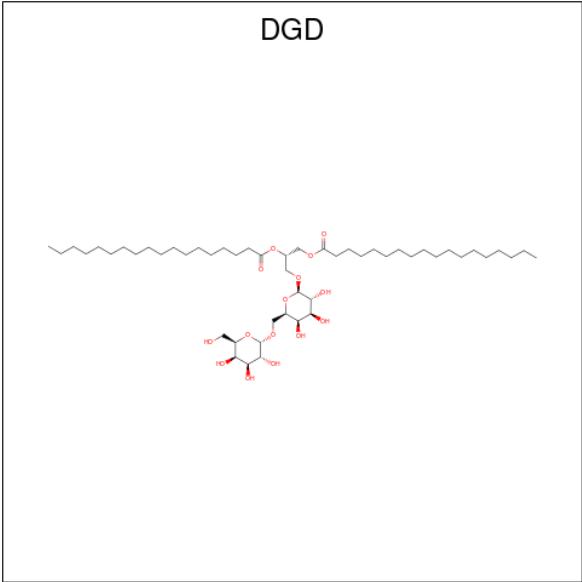
Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Na	0
			1	1	
35	a	1	Total	Na	0
			1	1	
35	A1	1	Total	Na	0
			1	1	
35	a1	1	Total	Na	0
			1	1	

- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	
36	B1	1	Total	C	O	0
			42	40	2	
36	b1	1	Total	C	O	0
			42	40	2	

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



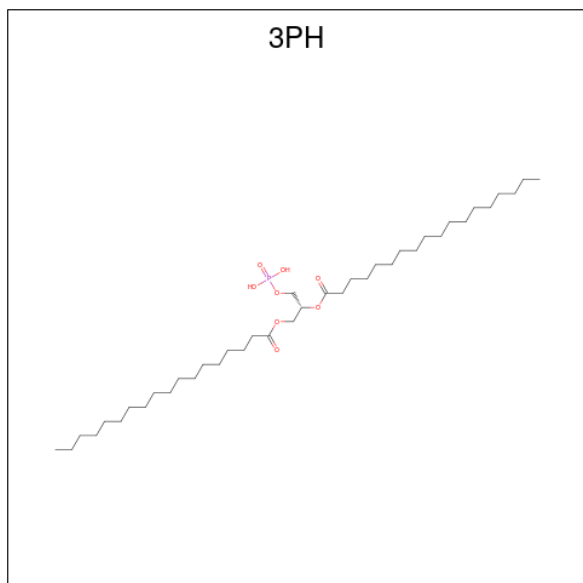
Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			43	28	15	
37	C	1	Total	C	O	0
			176	131	45	
37	C	1	Total	C	O	0
			176	131	45	
37	C	1	Total	C	O	0
			176	131	45	
37	b	1	Total	C	O	0
			43	28	15	
37	c	1	Total	C	O	0
			176	131	45	
37	c	1	Total	C	O	0
			176	131	45	
37	c	1	Total	C	O	0
			176	131	45	
37	B1	1	Total	C	O	0
			43	28	15	
37	C1	1	Total	C	O	0
			176	131	45	
37	C1	1	Total	C	O	0
			176	131	45	
37	C1	1	Total	C	O	0
			176	131	45	
37	b1	1	Total	C	O	0
			43	28	15	
37	c1	1	Total	C	O	0
			176	131	45	

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Mol	Chain	Residues	Atoms			AltConf
37	c1	1	Total	C	O	0
			176	131	45	
37	c1	1	Total	C	O	0
			176	131	45	

- Molecule 38 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



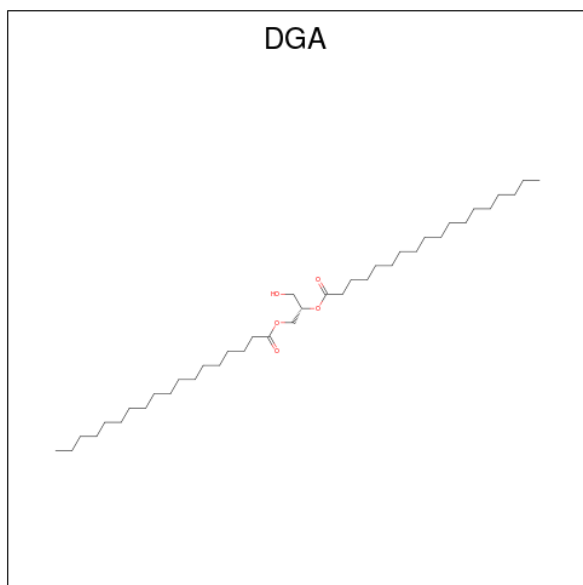
Mol	Chain	Residues	Atoms				AltConf
38	B	1	Total	C	O	P	0
			48	39	8	1	
38	T	1	Total	C	O	P	0
			48	39	8	1	
38	S	1	Total	C	O	P	0
			48	39	8	1	
38	b	1	Total	C	O	P	0
			48	39	8	1	
38	t	1	Total	C	O	P	0
			48	39	8	1	
38	s	1	Total	C	O	P	0
			48	39	8	1	
38	B1	1	Total	C	O	P	0
			48	39	8	1	
38	T1	1	Total	C	O	P	0
			48	39	8	1	
38	S1	1	Total	C	O	P	0
			48	39	8	1	

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Mol	Chain	Residues	Atoms				AltConf
38	b1	1	Total	C	O	P	0
			48	39	8	1	
38	t1	1	Total	C	O	P	0
			48	39	8	1	
38	s1	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 39 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



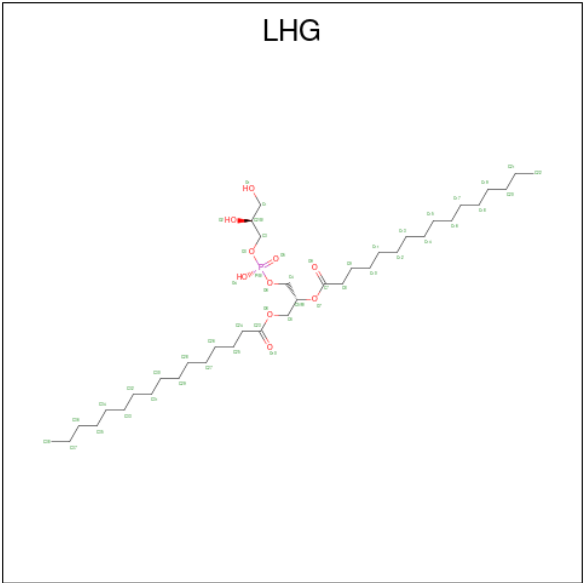
Mol	Chain	Residues	Atoms				AltConf
39	B	1	Total	C	O		0
			44	39	5		
39	C	1	Total	C	O		0
			44	39	5		
39	J	1	Total	C	O		0
			29	24	5		
39	b	1	Total	C	O		0
			44	39	5		
39	c	1	Total	C	O		0
			44	39	5		
39	j	1	Total	C	O		0
			29	24	5		
39	B1	1	Total	C	O		0
			44	39	5		
39	C1	1	Total	C	O		0
			44	39	5		

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Mol	Chain	Residues	Atoms			AltConf
39	J1	1	Total	C	O	0
			29	24	5	
39	b1	1	Total	C	O	0
			44	39	5	
39	c1	1	Total	C	O	0
			44	39	5	
39	j1	1	Total	C	O	0
			29	24	5	

- Molecule 40 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	O	P	0
			47	36	10	1	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	L	1	Total	C	O	P	0
			49	38	10	1	
40	N	1	Total	C	O	P	0
			49	38	10	1	
40	G	1	Total	C	O	P	0
			49	38	10	1	

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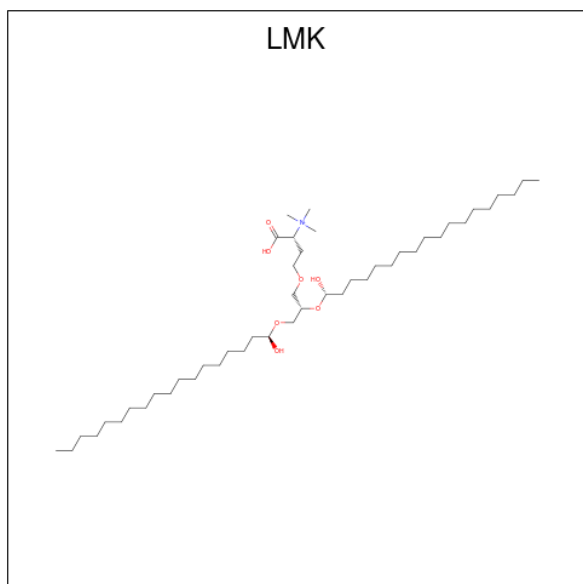
Mol	Chain	Residues	Atoms				AltConf
40	S	1	Total 45	C 34	O 10	P 1	0
40	Y	1	Total 49	C 38	O 10	P 1	0
40	c	1	Total 47	C 36	O 10	P 1	0
40	d	1	Total 132	C 99	O 30	P 3	0
40	d	1	Total 132	C 99	O 30	P 3	0
40	d	1	Total 132	C 99	O 30	P 3	0
40	l	1	Total 49	C 38	O 10	P 1	0
40	n	1	Total 49	C 38	O 10	P 1	0
40	g	1	Total 49	C 38	O 10	P 1	0
40	s	1	Total 45	C 34	O 10	P 1	0
40	y	1	Total 49	C 38	O 10	P 1	0
40	C1	1	Total 47	C 36	O 10	P 1	0
40	D1	1	Total 132	C 99	O 30	P 3	0
40	D1	1	Total 132	C 99	O 30	P 3	0
40	D1	1	Total 132	C 99	O 30	P 3	0
40	L1	1	Total 49	C 38	O 10	P 1	0
40	N1	1	Total 49	C 38	O 10	P 1	0
40	G1	1	Total 49	C 38	O 10	P 1	0
40	S1	1	Total 45	C 34	O 10	P 1	0
40	Y1	1	Total 49	C 38	O 10	P 1	0
40	c1	1	Total 47	C 36	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
40	d1	1	Total	C	O	P	0
			132	99	30	3	
40	d1	1	Total	C	O	P	0
			132	99	30	3	
40	d1	1	Total	C	O	P	0
			132	99	30	3	
40	n1	1	Total	C	O	P	0
			49	38	10	1	
40	g1	1	Total	C	O	P	0
			49	38	10	1	
40	s1	1	Total	C	O	P	0
			45	34	10	1	
40	y1	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 41 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxido-nyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanum (three-letter code: LMK) (formula: C₄₆H₉₄NO₇).



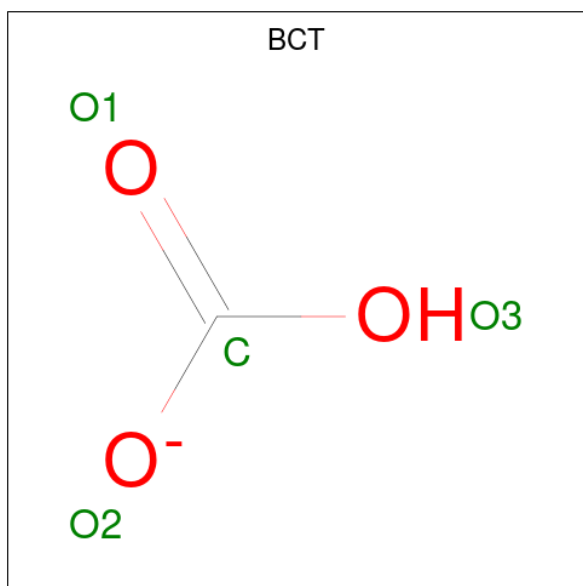
Mol	Chain	Residues	Atoms				AltConf
41	C	1	Total	C	N	O	0
			40	32	1	7	
41	c	1	Total	C	N	O	0
			40	32	1	7	
41	C1	1	Total	C	N	O	0
			40	32	1	7	

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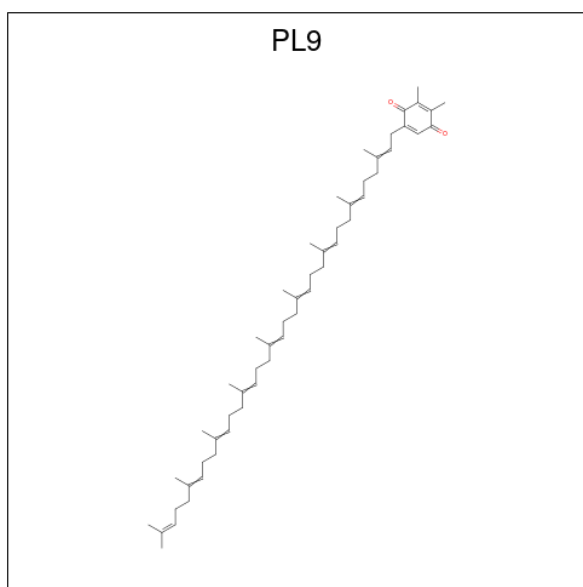
Mol	Chain	Residues	Atoms				AltConf
41	c1	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 42 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



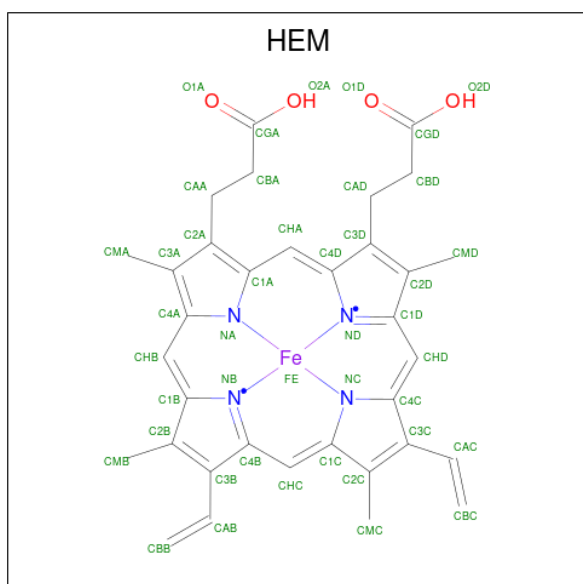
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			4	1	3	
42	d	1	Total	C	O	0
			4	1	3	
42	D1	1	Total	C	O	0
			4	1	3	
42	d1	1	Total	C	O	0
			4	1	3	

- Molecule 43 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 (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



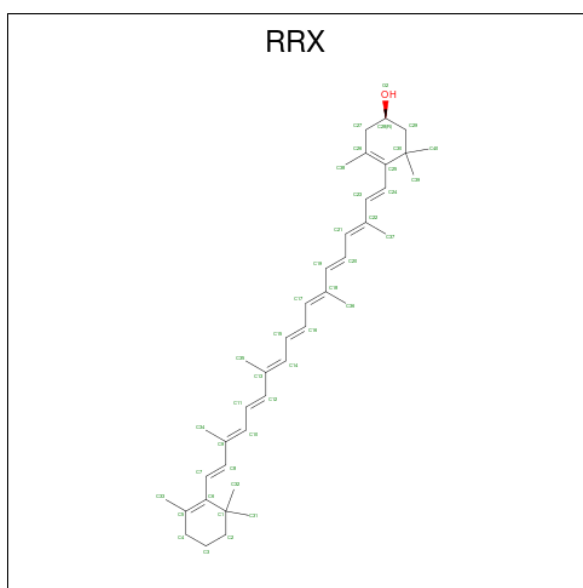
Mol	Chain	Residues	Atoms			AltConf
43	D	1	Total	C	O	0
			55	53	2	
43	d	1	Total	C	O	0
			55	53	2	
43	D1	1	Total	C	O	0
			55	53	2	
43	d1	1	Total	C	O	0
			55	53	2	

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



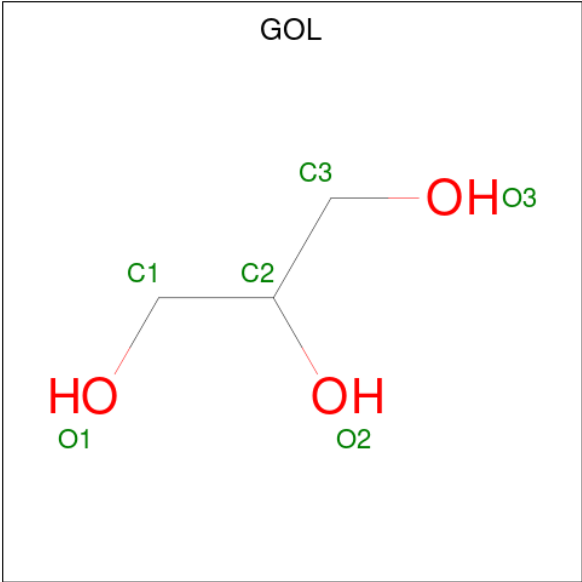
Mol	Chain	Residues	Atoms					AltConf
44	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	F1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 45 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



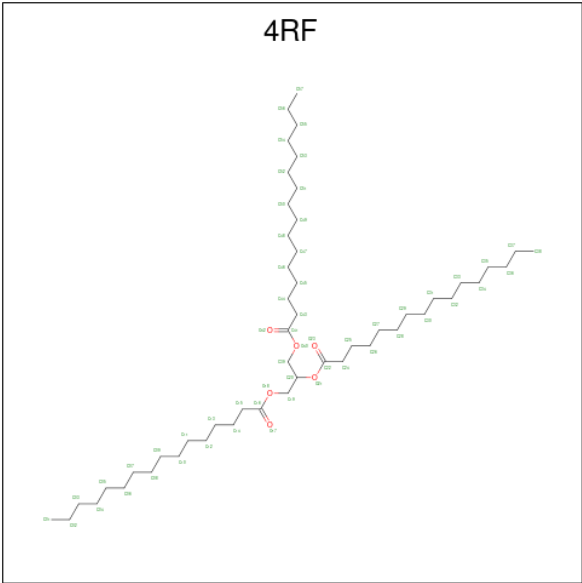
Mol	Chain	Residues	Atoms			AltConf
45	H	1	Total	C	O	0
			41	40	1	
45	h	1	Total	C	O	0
			41	40	1	
45	H1	1	Total	C	O	0
			41	40	1	
45	h1	1	Total	C	O	0
			41	40	1	

- Molecule 46 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
46	I	1	Total	C	O	0
			6	3	3	
46	I1	1	Total	C	O	0
			6	3	3	

- Molecule 47 is Tripalmitoylglycerol (three-letter code: 4RF) (formula: C₅₁H₉₈O₆).



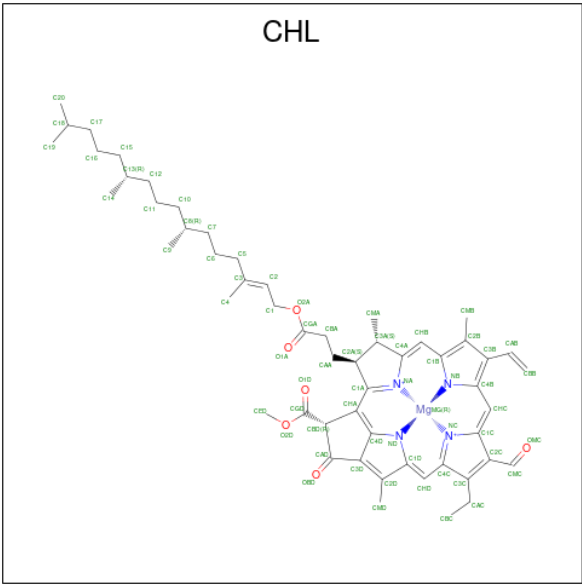
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	C	O	0
			57	51	6	
47	K	1	Total	C	O	0
			57	51	6	

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Mol	Chain	Residues	Atoms			AltConf
47	i	1	Total	C	O	0
			57	51	6	
47	k	1	Total	C	O	0
			57	51	6	
47	I1	1	Total	C	O	0
			57	51	6	
47	K1	1	Total	C	O	0
			57	51	6	
47	i1	1	Total	C	O	0
			57	51	6	
47	k1	1	Total	C	O	0
			57	51	6	

- Molecule 48 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
48	N	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	R	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	R	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	r	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	r	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	N1	1	Total 380	C 314	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
48	N1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	N1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	N1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	N1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	N1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	G1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	R1	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	R1	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	S1	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	S1	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	S1	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	S1	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	Y1	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y1	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y1	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y1	1	Total 310	C 255	Mg 5	N 20	O 30	0

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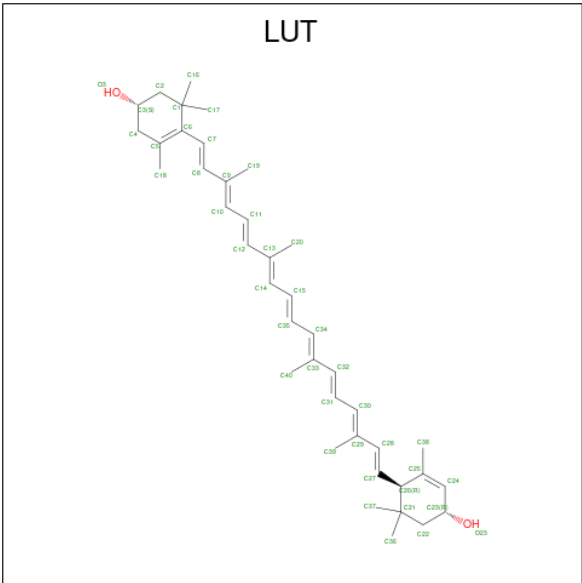
Mol	Chain	Residues	Atoms					AltConf
48	Y1	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	n1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n1	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	g1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g1	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	r1	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	r1	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	s1	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	s1	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	s1	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	s1	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	y1	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	y1	1	Total 310	C 255	Mg 5	N 20	O 30	0

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Mol	Chain	Residues	Atoms					AltConf
48	y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
48	y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
48	y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	

- Molecule 49 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			84	80	4	
49	N	1	Total	C	O	0
			84	80	4	
49	G	1	Total	C	O	0
			84	80	4	
49	G	1	Total	C	O	0
			84	80	4	
49	R	1	Total	C	O	0
			42	40	2	
49	S	1	Total	C	O	0
			84	80	4	
49	S	1	Total	C	O	0
			84	80	4	
49	Y	1	Total	C	O	0
			84	80	4	

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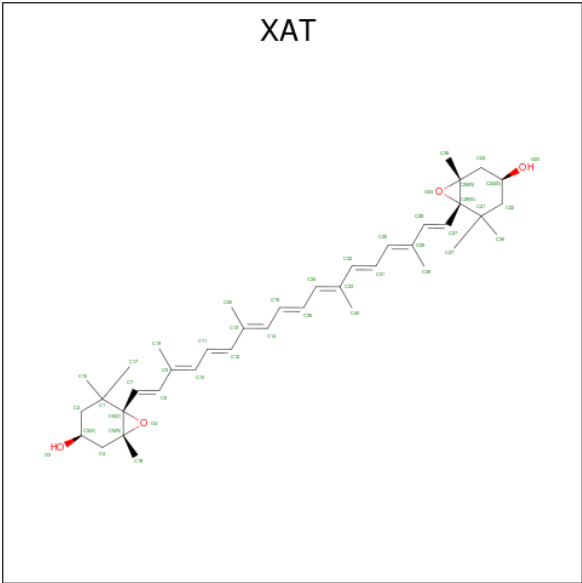
Mol	Chain	Residues	Atoms			AltConf
49	Y	1	Total	C	O	0
			84	80	4	
49	n	1	Total	C	O	0
			84	80	4	
49	n	1	Total	C	O	0
			84	80	4	
49	g	1	Total	C	O	0
			84	80	4	
49	g	1	Total	C	O	0
			84	80	4	
49	r	1	Total	C	O	0
			42	40	2	
49	s	1	Total	C	O	0
			84	80	4	
49	s	1	Total	C	O	0
			84	80	4	
49	y	1	Total	C	O	0
			84	80	4	
49	y	1	Total	C	O	0
			84	80	4	
49	N1	1	Total	C	O	0
			84	80	4	
49	N1	1	Total	C	O	0
			84	80	4	
49	G1	1	Total	C	O	0
			84	80	4	
49	G1	1	Total	C	O	0
			84	80	4	
49	R1	1	Total	C	O	0
			42	40	2	
49	S1	1	Total	C	O	0
			84	80	4	
49	S1	1	Total	C	O	0
			84	80	4	
49	Y1	1	Total	C	O	0
			84	80	4	
49	Y1	1	Total	C	O	0
			84	80	4	
49	n1	1	Total	C	O	0
			84	80	4	
49	n1	1	Total	C	O	0
			84	80	4	

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Mol	Chain	Residues	Atoms			AltConf
49	g1	1	Total	C	O	0
			84	80	4	
49	g1	1	Total	C	O	0
			84	80	4	
49	r1	1	Total	C	O	0
			42	40	2	
49	s1	1	Total	C	O	0
			84	80	4	
49	s1	1	Total	C	O	0
			84	80	4	
49	y1	1	Total	C	O	0
			84	80	4	
49	y1	1	Total	C	O	0
			84	80	4	

- Molecule 50 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



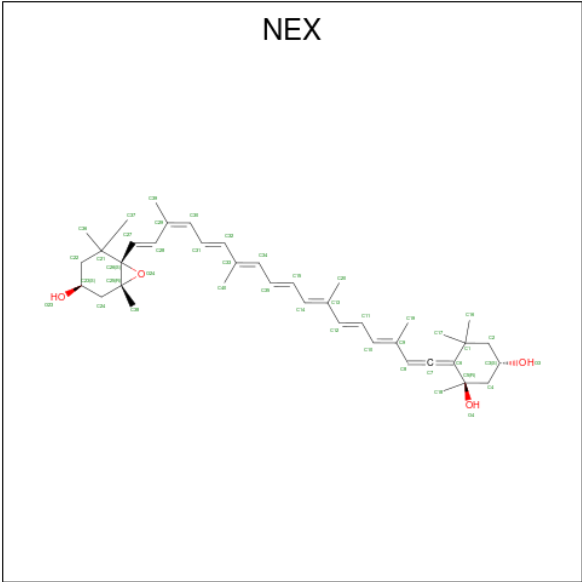
Mol	Chain	Residues	Atoms			AltConf
50	N	1	Total	C	O	0
			44	40	4	
50	G	1	Total	C	O	0
			44	40	4	
50	R	1	Total	C	O	0
			44	40	4	
50	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
50	n	1	Total	C	O	0
			44	40	4	
50	g	1	Total	C	O	0
			44	40	4	
50	r	1	Total	C	O	0
			44	40	4	
50	y	1	Total	C	O	0
			44	40	4	
50	N1	1	Total	C	O	0
			44	40	4	
50	G1	1	Total	C	O	0
			44	40	4	
50	R1	1	Total	C	O	0
			44	40	4	
50	Y1	1	Total	C	O	0
			44	40	4	
50	n1	1	Total	C	O	0
			44	40	4	
50	g1	1	Total	C	O	0
			44	40	4	
50	r1	1	Total	C	O	0
			44	40	4	
50	y1	1	Total	C	O	0
			44	40	4	

- Molecule 51 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 (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



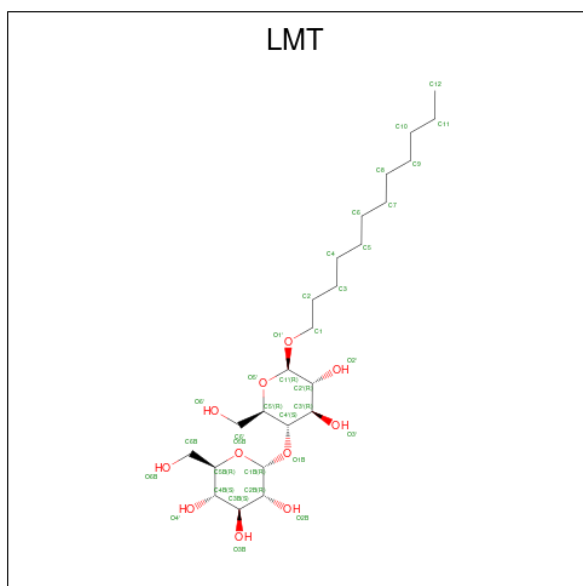
Mol	Chain	Residues	Atoms			AltConf
51	N	1	Total	C	O	0
			44	40	4	
51	G	1	Total	C	O	0
			44	40	4	
51	R	1	Total	C	O	0
			44	40	4	
51	S	1	Total	C	O	0
			44	40	4	
51	Y	1	Total	C	O	0
			44	40	4	
51	n	1	Total	C	O	0
			44	40	4	
51	g	1	Total	C	O	0
			44	40	4	
51	r	1	Total	C	O	0
			44	40	4	
51	s	1	Total	C	O	0
			44	40	4	
51	y	1	Total	C	O	0
			44	40	4	
51	N1	1	Total	C	O	0
			44	40	4	
51	G1	1	Total	C	O	0
			44	40	4	
51	R1	1	Total	C	O	0
			44	40	4	
51	S1	1	Total	C	O	0
			44	40	4	

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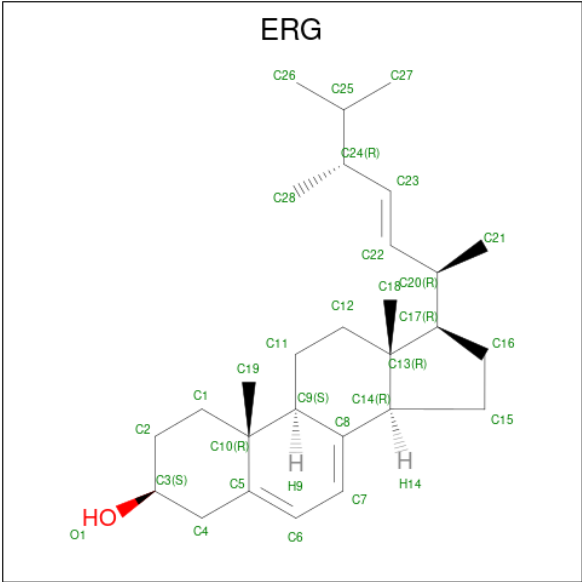
Mol	Chain	Residues	Atoms			AltConf
51	Y1	1	Total	C	O	0
			44	40	4	
51	n1	1	Total	C	O	0
			44	40	4	
51	g1	1	Total	C	O	0
			44	40	4	
51	r1	1	Total	C	O	0
			44	40	4	
51	s1	1	Total	C	O	0
			44	40	4	
51	y1	1	Total	C	O	0
			44	40	4	

- Molecule 52 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



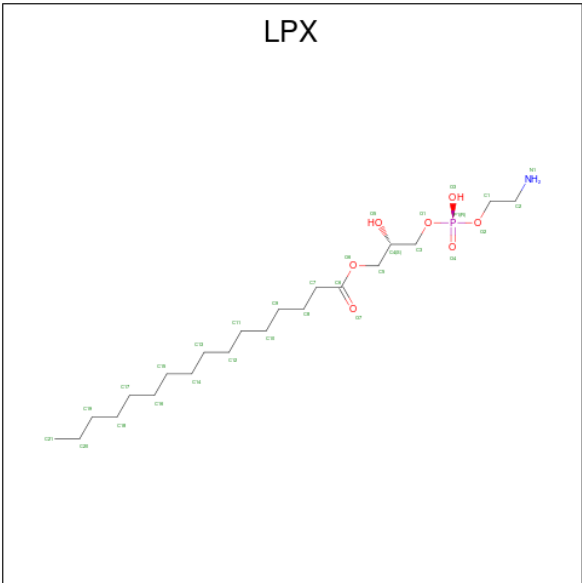
Mol	Chain	Residues	Atoms			AltConf
52	R	1	Total	C	O	0
			35	24	11	
52	r	1	Total	C	O	0
			35	24	11	
52	R1	1	Total	C	O	0
			35	24	11	
52	r1	1	Total	C	O	0
			35	24	11	

- Molecule 53 is ERGOSTEROL (three-letter code: ERG) (formula: $C_{28}H_{44}O$).



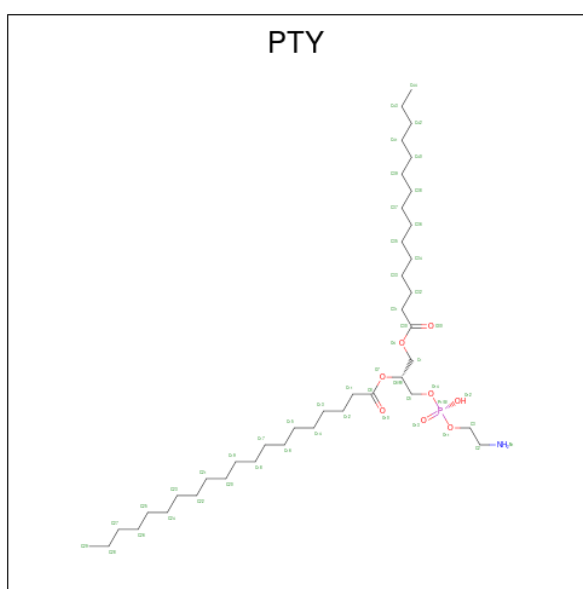
Mol	Chain	Residues	Atoms			AltConf
53	R	1	Total	C	O	0
			29	28	1	
53	r	1	Total	C	O	0
			29	28	1	
53	R1	1	Total	C	O	0
			29	28	1	
53	r1	1	Total	C	O	0
			29	28	1	

- Molecule 54 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
54	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	s	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	S1	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	s1	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 55 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
55	Y	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	Y	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	y	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	y	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	Y1	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	Y1	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	y1	1	Total	C	N	O	P	0
			69	49	2	16	2	

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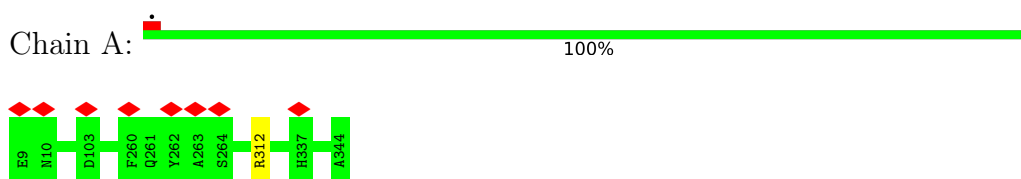
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	y1	1	69	49	2	16	2	0

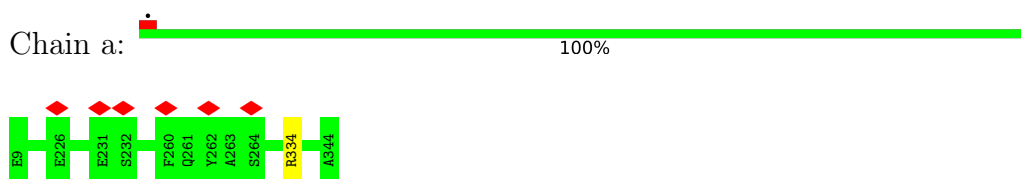
3 Residue-property plots [i](#)

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

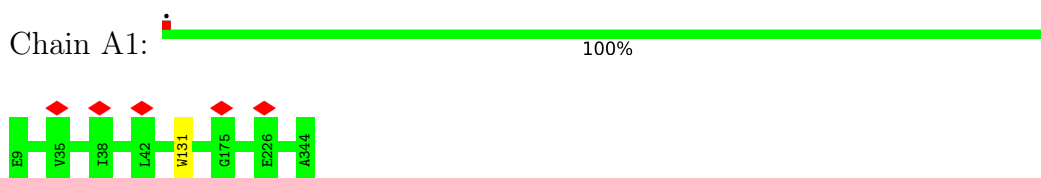
- Molecule 1: Photosystem II protein D1



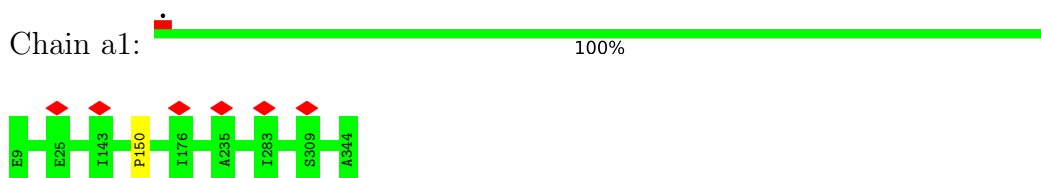
- Molecule 1: Photosystem II protein D1



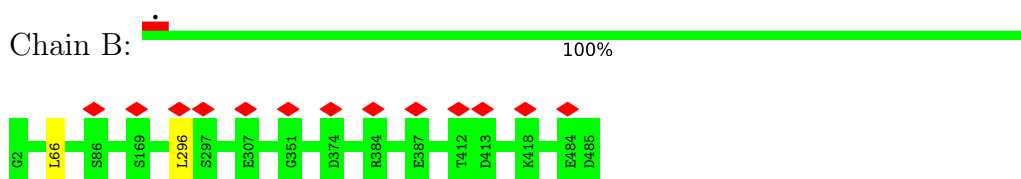
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

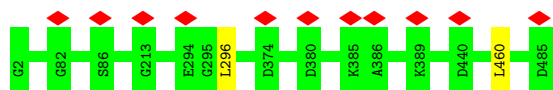


- Molecule 2: Photosystem II CP47 reaction center protein



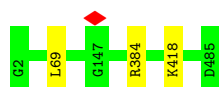
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  100%



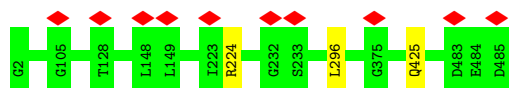
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B1:  99%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b1:  99%



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:  100%

There are no outlier residues recorded for this chain.

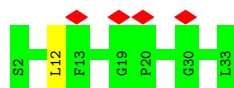
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V1:  100%

There are no outlier residues recorded for this chain.

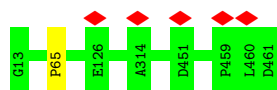
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v1:  12% 97%

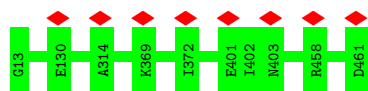


- Molecule 4: Photosystem II CP43 reaction center protein

Chain C:  100%



- Molecule 4: Photosystem II CP43 reaction center protein

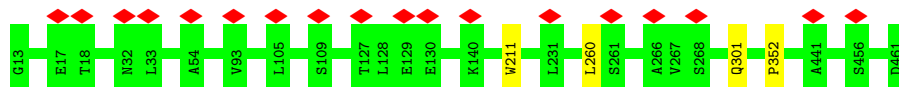


- Molecule 4: Photosystem II CP43 reaction center protein

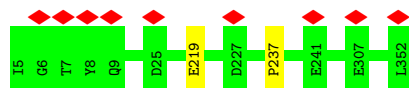


There are no outlier residues recorded for this chain.

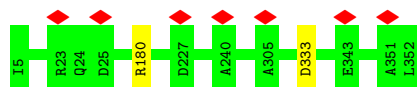
- Molecule 4: Photosystem II CP43 reaction center protein



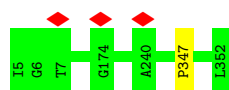
- Molecule 5: Photosystem II D2 protein



- Molecule 5: Photosystem II D2 protein

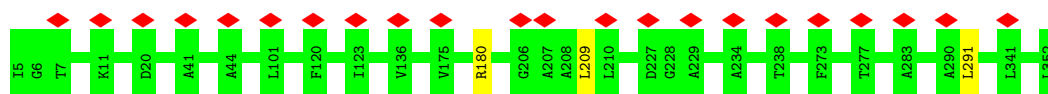


- Molecule 5: Photosystem II D2 protein



- Molecule 5: Photosystem II D2 protein





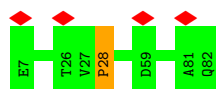
- Molecule 6: Cytochrome b559 subunit alpha

Chain E: 100%



- Molecule 6: Cytochrome b559 subunit alpha

Chain e: 99%



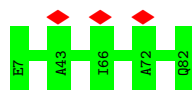
- Molecule 6: Cytochrome b559 subunit alpha

Chain E1: 100%

There are no outlier residues recorded for this chain.

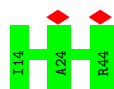
- Molecule 6: Cytochrome b559 subunit alpha

Chain e1: 100%



- Molecule 7: Cytochrome b559 subunit beta

Chain F: 100%



- Molecule 7: Cytochrome b559 subunit beta

Chain f: 100%

There are no outlier residues recorded for this chain.

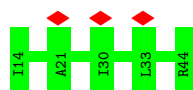
- Molecule 7: Cytochrome b559 subunit beta

Chain F1: 100%

There are no outlier residues recorded for this chain.

- Molecule 7: Cytochrome b559 subunit beta

Chain f1:  10% 100%



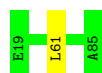
- Molecule 8: Photosystem II reaction center protein H

Chain H:  97%



- Molecule 8: Photosystem II reaction center protein H

Chain h:  99%



- Molecule 8: Photosystem II reaction center protein H

Chain H1:  99%



- Molecule 8: Photosystem II reaction center protein H

Chain h1:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein I

Chain I:  100%



- Molecule 9: Photosystem II reaction center protein I

Chain i:  100%



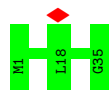
- Molecule 9: Photosystem II reaction center protein I

Chain I1:  100%

There are no outlier residues recorded for this chain.

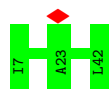
- Molecule 9: Photosystem II reaction center protein I

Chain i1:  100%



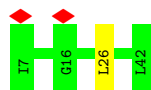
- Molecule 10: PsbJ

Chain J:  100%



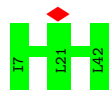
- Molecule 10: PsbJ

Chain j:  97%



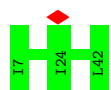
- Molecule 10: PsbJ

Chain J1:  100%



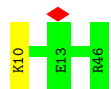
- Molecule 10: PsbJ

Chain j1:  100%



- Molecule 11: Photosystem II reaction center protein K

Chain K:  97%



- Molecule 11: Photosystem II reaction center protein K

Chain k:  100%

There are no outlier residues recorded for this chain.

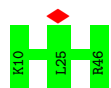
- Molecule 11: Photosystem II reaction center protein K

Chain K1:  100%

There are no outlier residues recorded for this chain.

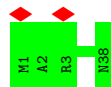
- Molecule 11: Photosystem II reaction center protein K

Chain k1:  100%



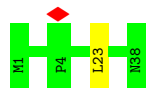
- Molecule 12: Photosystem II reaction center protein L

Chain L:  100%



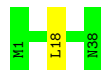
- Molecule 12: Photosystem II reaction center protein L

Chain l:  97%



- Molecule 12: Photosystem II reaction center protein L

Chain L1:  97%



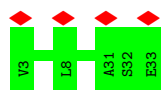
- Molecule 13: PsbM

Chain M:  100%

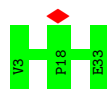


- Molecule 13: PsbM

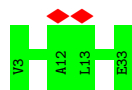
Chain m:  100%



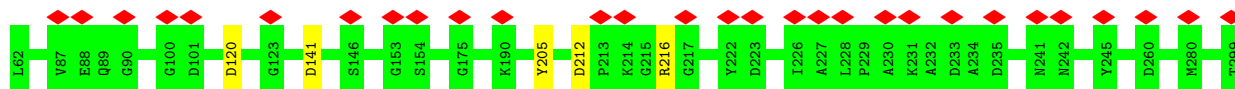
- Molecule 13: PsbM



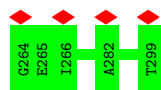
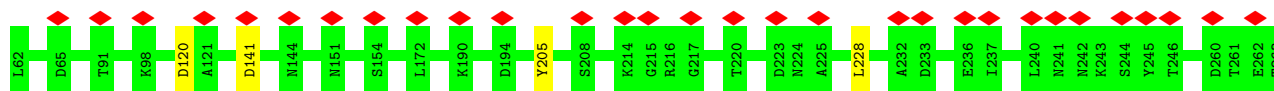
- Molecule 13: PsbM



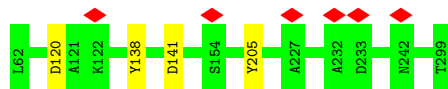
- Molecule 14: PsbO



- Molecule 14: PsbO

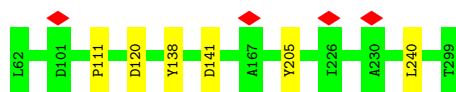


- Molecule 14: PsbO

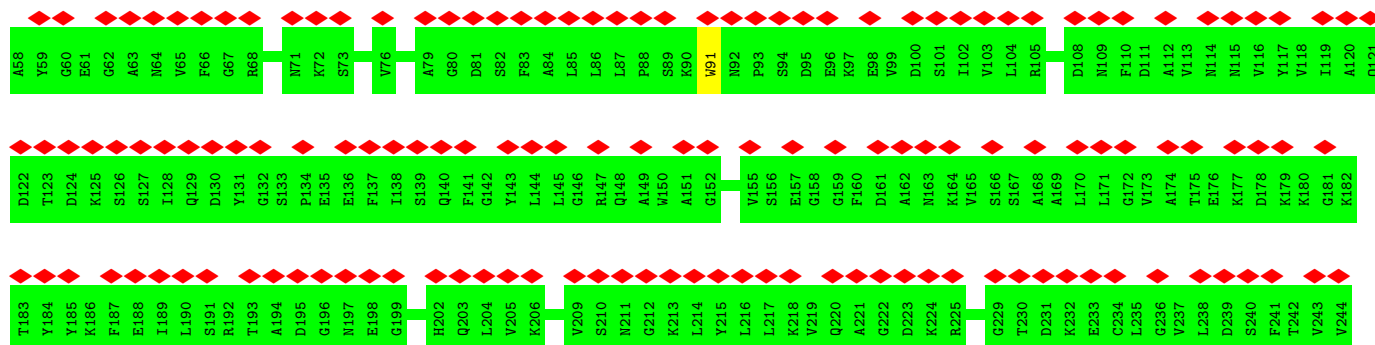
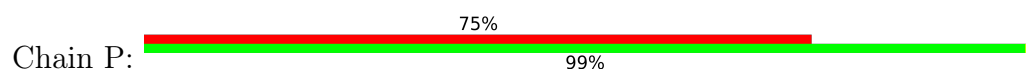


- Molecule 14: PsbO

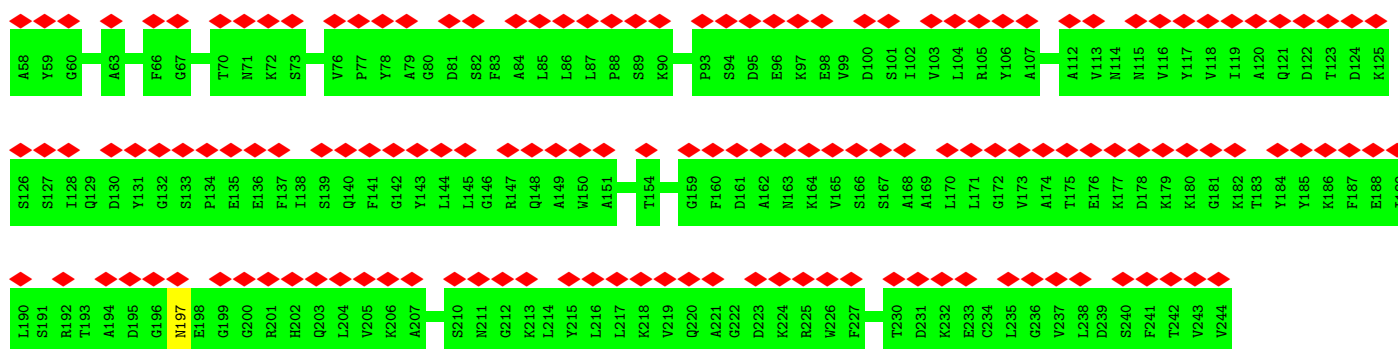
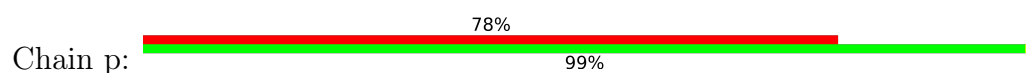




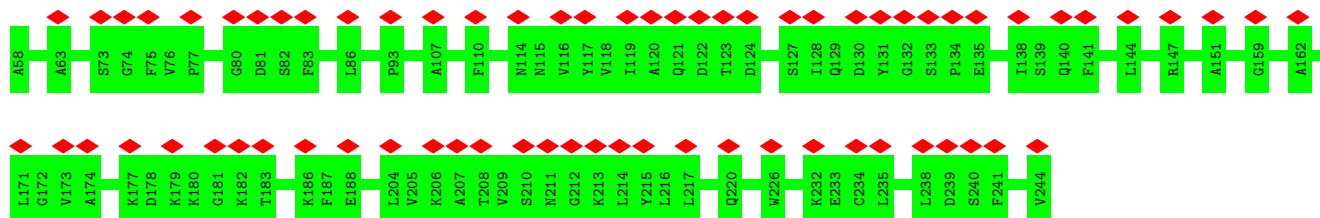
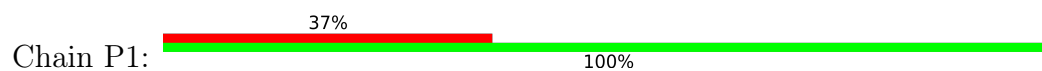
• Molecule 15: PsbP



• Molecule 15: PsbP

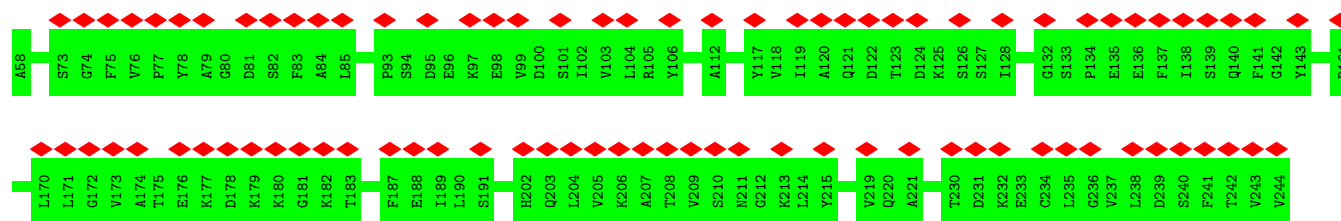


• Molecule 15: PsbP

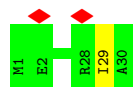


• Molecule 15: PsbP





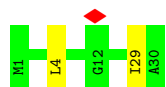
- Molecule 16: Photosystem II reaction center protein T



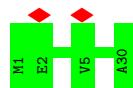
- Molecule 16: Photosystem II reaction center protein T



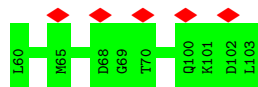
- Molecule 16: Photosystem II reaction center protein T



- Molecule 16: Photosystem II reaction center protein T

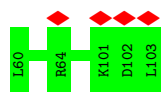


- Molecule 17: PsbW



- Molecule 17: PsbW





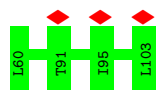
- Molecule 17: PsbW

Chain W1:  100%

There are no outlier residues recorded for this chain.

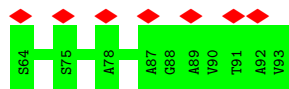
- Molecule 17: PsbW

Chain w1:  7%  100%



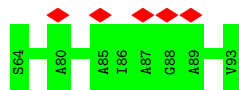
- Molecule 18: PsbX

Chain X:  23%  100%



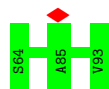
- Molecule 18: PsbX

Chain x:  17%  100%



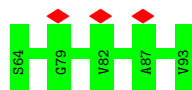
- Molecule 18: PsbX

Chain X1:  0%  100%



- Molecule 18: PsbX

Chain x1:  10%  100%



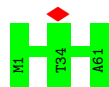
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  100%

There are no outlier residues recorded for this chain.

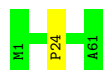
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  100%



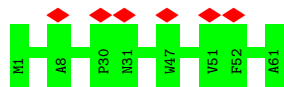
- Molecule 19: Photosystem II reaction center protein Z

Chain Z1:  98%



- Molecule 19: Photosystem II reaction center protein Z

Chain z1:  10% 100%



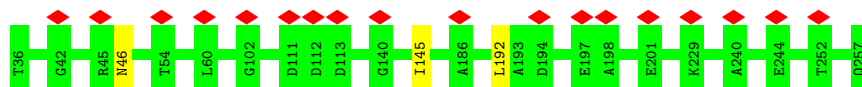
- Molecule 20: LHCII M3

Chain N:  5% 98%



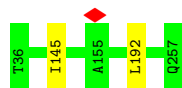
- Molecule 20: LHCII M3

Chain n:  8% 99%



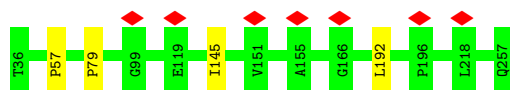
- Molecule 20: LHCII M3

Chain N1:  99%

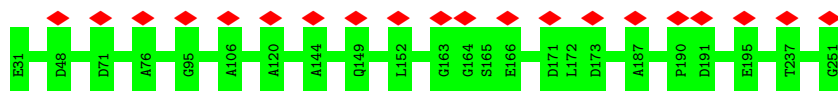


- Molecule 20: LHCII M3

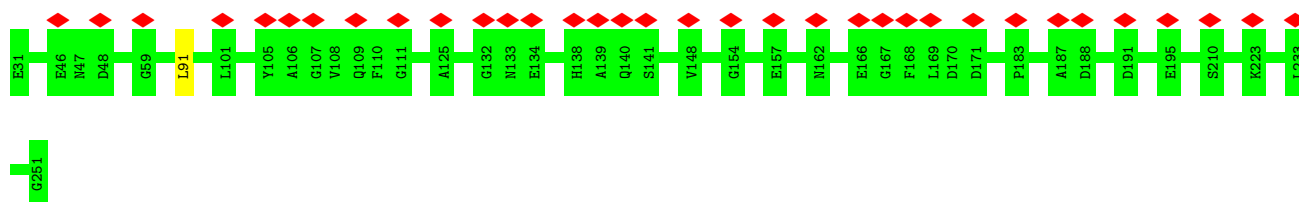
Chain n1:  98%



- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



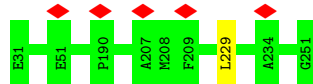
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



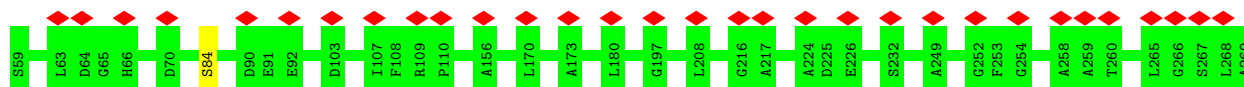
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

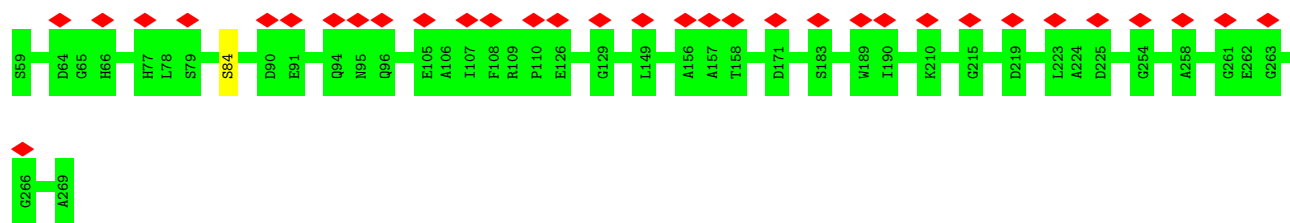


- Molecule 22: CP29

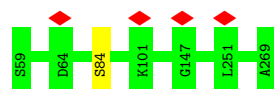


- Molecule 22: CP29

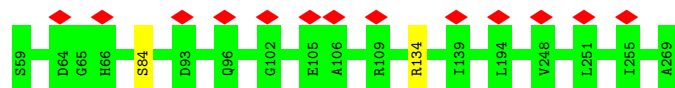




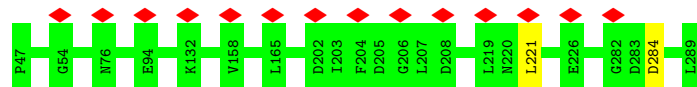
• Molecule 22: CP29



• Molecule 22: CP29



• Molecule 23: CP26



• Molecule 23: CP26



• Molecule 23: CP26

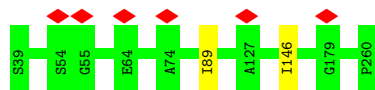


• Molecule 23: CP26



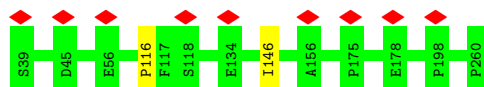
- Molecule 24: LHCII M1

Chain Y:  99%



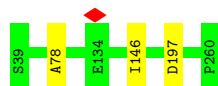
- Molecule 24: LHCII M1

Chain y:  99%



- Molecule 24: LHCII M1

Chain Y1:  99%



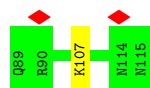
- Molecule 24: LHCII M1

Chain y1:  100%



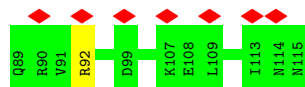
- Molecule 25: PsbU

Chain U:  7% 96%



- Molecule 25: PsbU

Chain u:  26% 96%



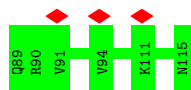
- Molecule 25: PsbU

Chain U1:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: PsbU

Chain u1:  11% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.013	Depositor
Map size (\AA)	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.96, 0.96, 0.96	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, LMT, SPH, C7Z, GOL, 4RF, PL9, LPX, FE2, DGD, LHG, ERG, LMG, CHL, OEX, LMK, NA, HEM, NEX, DGA, BCT, XAT, PTY, PHO, CLA, SEP, RRX, LUT, CL, 3PH, SQD

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	0.41	0/2723	0.60	0/3715
1	A1	0.36	0/2723	0.61	0/3715
1	a	0.41	0/2723	0.61	0/3715
1	a1	0.36	0/2723	0.65	2/3715 (0.1%)
2	B	0.40	0/3912	0.63	2/5327 (0.0%)
2	B1	0.35	0/3912	0.61	1/5327 (0.0%)
2	b	0.39	0/3912	0.61	2/5327 (0.0%)
2	b1	0.33	0/3912	0.60	1/5327 (0.0%)
3	V	0.34	0/228	0.67	0/311
3	V1	0.26	0/228	0.54	0/311
3	v	0.30	0/228	0.66	0/311
3	v1	0.29	0/228	0.76	1/311 (0.3%)
4	C	0.46	2/3602 (0.1%)	0.70	4/4913 (0.1%)
4	C1	0.34	0/3602	0.59	0/4913
4	c	0.39	0/3602	0.59	0/4913
4	c1	0.40	2/3602 (0.1%)	0.67	4/4913 (0.1%)
5	D	0.45	1/2860 (0.0%)	0.64	2/3899 (0.1%)
5	D1	0.36	0/2860	0.62	2/3899 (0.1%)
5	d	0.41	0/2860	0.61	1/3899 (0.0%)
5	d1	0.36	0/2860	0.65	2/3899 (0.1%)
6	E	0.34	0/639	0.59	0/870
6	E1	0.33	0/639	0.63	0/870
6	e	0.55	1/639 (0.2%)	0.85	3/870 (0.3%)
6	e1	0.30	0/639	0.59	0/870
7	F	0.33	0/259	0.56	0/351
7	F1	0.31	0/259	0.58	0/351
7	f	0.38	0/259	0.68	0/351
7	f1	0.33	0/259	0.64	0/351
8	H	0.37	0/513	0.77	2/703 (0.3%)
8	H1	0.31	0/513	0.65	1/703 (0.1%)
8	h	0.36	0/513	0.68	1/703 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	h1	0.31	0/513	0.62	0/703
9	I	0.44	0/287	0.57	0/386
9	I1	0.34	0/287	0.60	0/386
9	i	0.38	0/287	0.55	0/386
9	i1	0.36	0/287	0.59	0/386
10	J	0.29	0/272	0.54	0/369
10	J1	0.31	0/272	0.58	0/369
10	j	0.35	0/272	0.69	1/369 (0.3%)
10	j1	0.29	0/272	0.61	0/369
11	K	0.40	0/308	0.64	0/423
11	K1	0.33	0/308	0.63	0/423
11	k	0.43	0/308	0.61	0/423
11	k1	0.36	0/308	0.66	0/423
12	L	0.37	0/321	0.53	0/435
12	L1	0.37	0/321	0.74	1/435 (0.2%)
12	l	0.43	0/321	0.71	1/435 (0.2%)
13	M	0.33	0/237	0.54	0/323
13	M1	0.29	0/237	0.54	0/323
13	m	0.36	0/237	0.66	0/323
13	m1	0.35	0/237	0.60	0/323
14	O	0.36	0/1855	0.70	3/2505 (0.1%)
14	O1	0.34	0/1855	0.68	2/2505 (0.1%)
14	o	0.36	0/1855	0.68	3/2505 (0.1%)
14	o1	0.48	1/1855 (0.1%)	0.82	7/2505 (0.3%)
15	P	0.28	0/1473	0.57	1/1988 (0.1%)
15	P1	0.30	0/1473	0.57	0/1988
15	p	0.31	0/1473	0.57	0/1988
15	p1	0.32	0/1473	0.58	0/1988
16	T	0.33	0/254	0.62	0/342
16	T1	0.39	0/254	0.72	1/342 (0.3%)
16	t	0.36	0/254	0.55	0/342
16	t1	0.32	0/254	0.60	0/342
17	W	0.32	0/339	0.63	0/460
17	W1	0.31	0/339	0.59	0/460
17	w	0.32	0/339	0.57	0/460
17	w1	0.29	0/339	0.60	0/460
18	X	0.32	0/202	0.55	0/276
18	X1	0.31	0/202	0.53	0/276
18	x	0.35	0/202	0.69	0/276
18	x1	0.27	0/202	0.58	0/276
19	Z	0.31	0/469	0.52	0/641
19	Z1	0.31	0/469	0.59	1/641 (0.2%)
19	z	0.33	0/469	0.53	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	z1	0.28	0/469	0.52	0/641
20	N	0.36	0/1751	0.59	1/2386 (0.0%)
20	N1	0.35	0/1751	0.58	0/2386
20	n	0.37	0/1750	0.58	0/2382
20	n1	0.44	2/1750 (0.1%)	0.71	5/2382 (0.2%)
21	G	0.34	0/1725	0.59	0/2348
21	G1	0.38	1/1725 (0.1%)	0.64	2/2348 (0.1%)
21	g	0.34	0/1725	0.60	1/2348 (0.0%)
21	g1	0.33	0/1725	0.58	1/2348 (0.0%)
22	R	0.34	0/1506	0.61	0/2035
22	R1	0.30	0/1506	0.55	0/2035
22	r	0.31	0/1506	0.60	0/2035
22	r1	0.33	0/1506	0.62	0/2035
23	S	0.35	0/1903	0.64	1/2590 (0.0%)
23	S1	0.32	0/1903	0.63	2/2590 (0.1%)
23	s	0.34	0/1903	0.68	1/2590 (0.0%)
23	s1	0.37	1/1903 (0.1%)	0.73	4/2590 (0.2%)
24	Y	0.35	0/1715	0.58	1/2338 (0.0%)
24	Y1	0.35	0/1715	0.65	2/2338 (0.1%)
24	y	0.37	0/1715	0.55	1/2338 (0.0%)
24	y1	0.32	0/1715	0.57	0/2338
25	U	0.37	0/224	0.69	0/298
25	U1	0.36	0/224	0.67	0/298
25	u	0.38	0/224	0.76	0/298
25	u1	0.36	0/224	0.67	0/298
All	All	0.37	11/117985 (0.0%)	0.63	74/160485 (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
1	A	0	1
1	A1	0	1
2	B1	0	1
All	All	0	3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	o1	111	PRO	CG-CD	-14.28	1.03	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	65	PRO	CG-CD	-13.03	1.07	1.50
6	e	28	PRO	CG-CD	-10.62	1.15	1.50
4	c1	352	PRO	CG-CD	-9.09	1.20	1.50
20	n1	57	PRO	CG-CD	-8.65	1.22	1.50

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	65	PRO	N-CD-CG	-18.59	75.32	103.20
14	o1	111	PRO	N-CD-CG	-18.29	75.77	103.20
6	e	28	PRO	N-CD-CG	-12.50	84.44	103.20
20	n1	57	PRO	N-CD-CG	-12.30	84.74	103.20
4	C	65	PRO	CA-CB-CG	-11.58	82.00	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	ARG	Sidechain
1	A1	131	TRP	Peptide
2	B1	384	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

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	335/336 (100%)	321 (96%)	14 (4%)	0	100	100
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	335/336 (100%)	318 (95%)	17 (5%)	0	100	100
1	a1	335/336 (100%)	314 (94%)	21 (6%)	0	100	100
2	B	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	B1	482/484 (100%)	447 (93%)	35 (7%)	0	100	100
2	b	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	b1	482/484 (100%)	454 (94%)	28 (6%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	V1	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	30 (100%)	0	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	430 (96%)	17 (4%)	0	100	100
4	C1	447/449 (100%)	421 (94%)	26 (6%)	0	100	100
4	c	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
4	c1	447/449 (100%)	421 (94%)	25 (6%)	1 (0%)	47	79
5	D	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
5	D1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
5	d	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
5	d1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
6	E	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	E1	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	e	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
6	e1	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	F1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
7	f1	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	H1	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	h1	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
9	i	33/35 (94%)	29 (88%)	4 (12%)	0	100	100
9	i1	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	J1	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
10	j1	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	K1	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k1	35/37 (95%)	35 (100%)	0	0	100	100
12	L	36/38 (95%)	36 (100%)	0	0	100	100
12	L1	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	29 (100%)	0	0	100	100
13	M1	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	215 (91%)	19 (8%)	2 (1%)	19	59
14	O1	236/238 (99%)	212 (90%)	23 (10%)	1 (0%)	34	71
14	o	236/238 (99%)	218 (92%)	17 (7%)	1 (0%)	34	71
14	o1	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	34	71
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	170 (92%)	15 (8%)	0	100	100
15	p1	185/187 (99%)	169 (91%)	16 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	3	29
16	T1	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	3	29
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	t1	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
17	W	42/44 (96%)	38 (90%)	4 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	W1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	X1	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100
18	x1	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	Z1	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
19	z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
20	N	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	17	57
20	N1	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	17	57
20	n	218/222 (98%)	199 (91%)	17 (8%)	2 (1%)	17	57
20	n1	218/222 (98%)	202 (93%)	14 (6%)	2 (1%)	17	57
21	G	219/221 (99%)	196 (90%)	23 (10%)	0	100	100
21	G1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
21	g	219/221 (99%)	197 (90%)	22 (10%)	0	100	100
21	g1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
22	R	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	R1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
22	r	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	r1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
23	S	241/243 (99%)	219 (91%)	21 (9%)	1 (0%)	34	71
23	S1	241/243 (99%)	208 (86%)	32 (13%)	1 (0%)	34	71
23	s	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	19	59
23	s1	241/243 (99%)	214 (89%)	26 (11%)	1 (0%)	34	71
24	Y	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	29	68
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	29	68
24	y	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	29	68
24	y1	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
25	U1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u1	25/27 (93%)	25 (100%)	0	0	100	100
All	All	14636/14846 (99%)	13696 (94%)	915 (6%)	25 (0%)	50	79

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
20	n	192	LEU
23	s	284	ASP

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	276/275 (100%)	276 (100%)	0	100	100
1	A1	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	275 (100%)	1 (0%)	91	97
1	a1	276/275 (100%)	276 (100%)	0	100	100
2	B	388/388 (100%)	388 (100%)	0	100	100
2	B1	388/388 (100%)	387 (100%)	1 (0%)	92	97
2	b	388/388 (100%)	388 (100%)	0	100	100
2	b1	388/388 (100%)	386 (100%)	2 (0%)	88	95
3	V	25/25 (100%)	25 (100%)	0	100	100
3	V1	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
3	v1	25/25 (100%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	350/350 (100%)	350 (100%)	0	100	100
4	C1	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
4	c1	350/350 (100%)	349 (100%)	1 (0%)	92	97
5	D	279/279 (100%)	279 (100%)	0	100	100
5	D1	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	278 (100%)	1 (0%)	91	97
5	d1	279/279 (100%)	278 (100%)	1 (0%)	91	97
6	E	68/68 (100%)	68 (100%)	0	100	100
6	E1	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	67 (98%)	1 (2%)	65	84
6	e1	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	F1	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
7	f1	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	H1	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
8	h1	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	I1	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
9	i1	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	J1	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
10	j1	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	32 (97%)	1 (3%)	41	71
11	K1	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	k1	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	L1	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	M1	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
13	m1	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	O1	195/195 (100%)	194 (100%)	1 (0%)	88	95
14	o	195/195 (100%)	195 (100%)	0	100	100
14	o1	195/195 (100%)	194 (100%)	1 (0%)	88	95
15	P	151/151 (100%)	151 (100%)	0	100	100
15	P1	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	150 (99%)	1 (1%)	84	93
15	p1	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	T1	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
16	t1	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	W1	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
17	w1	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	X1	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
18	x1	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	Z1	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	z1	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	170 (99%)	1 (1%)	86	94
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	170 (99%)	1 (1%)	86	94
20	n1	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	G1	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
21	g1	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	R1	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
22	r1	151/151 (100%)	150 (99%)	1 (1%)	84	93
23	S	190/190 (100%)	190 (100%)	0	100	100
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	189 (100%)	1 (0%)	88	95
23	s1	190/190 (100%)	188 (99%)	2 (1%)	73	88
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	Y1	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
24	y1	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	25 (96%)	1 (4%)	33	66
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	25 (96%)	1 (4%)	33	66
25	u1	26/26 (100%)	26 (100%)	0	100	100
All	All	11841/11837 (100%)	11821 (100%)	20 (0%)	93	98

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	c1	301	GLN
22	r1	134	ARG
23	s1	132	LYS

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Mol	Chain	Res	Type
23	s1	99	LYS
15	p	197	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
5	D1	117	HIS
22	R1	174	GLN
24	y1	236	ASN
5	D1	230	ASN
14	O1	82	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	SEP	R1	84	22	8,9,10	1.52	1 (12%)	8,12,14	1.71	2 (25%)
22	SEP	r	84	22	8,9,10	1.51	1 (12%)	8,12,14	1.39	2 (25%)
22	SEP	R	84	22	8,9,10	1.58	1 (12%)	8,12,14	1.40	2 (25%)
22	SEP	r1	84	22	8,9,10	1.53	1 (12%)	8,12,14	1.69	2 (25%)

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
22	SEP	R1	84	22	-	4/5/8/10	-
22	SEP	r	84	22	-	2/5/8/10	-
22	SEP	R	84	22	-	2/5/8/10	-
22	SEP	r1	84	22	-	5/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.37	1.61	1.50
22	r1	84	SEP	P-O1P	3.30	1.61	1.50
22	R1	84	SEP	P-O1P	3.29	1.61	1.50
22	r	84	SEP	P-O1P	3.22	1.60	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r1	84	SEP	P-OG-CB	-3.36	109.03	118.30
22	R1	84	SEP	OG-CB-CA	3.23	111.29	108.14
22	R1	84	SEP	P-OG-CB	-3.07	109.85	118.30
22	r1	84	SEP	OG-CB-CA	2.79	110.86	108.14
22	r	84	SEP	P-OG-CB	-2.56	111.25	118.30

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	R1	84	SEP	N-CA-CB-OG
22	R1	84	SEP	CB-OG-P-O2P
22	R1	84	SEP	CB-OG-P-O3P
22	r1	84	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 721 ligands modelled in this entry, 16 are monoatomic - leaving 705 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
48	CHL	N1	606	-	66,74,74	0.94	4 (6%)	73,114,114	1.11	8 (10%)
50	XAT	R1	621	-	39,47,47	0.68	1 (2%)	54,74,74	1.91	18 (33%)
29	CLA	B	609	-	65,73,73	1.34	8 (12%)	76,113,113	2.24	18 (23%)
49	LUT	N1	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.99	14 (27%)
29	CLA	N	603	-	65,73,73	1.33	8 (12%)	76,113,113	2.07	18 (23%)
33	LMG	W	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.21	4 (8%)
29	CLA	y1	611	40	65,73,73	1.34	8 (12%)	76,113,113	2.05	17 (22%)
29	CLA	B	603	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	17 (22%)
29	CLA	c	512	-	65,73,73	1.39	9 (13%)	76,113,113	2.00	19 (25%)
33	LMG	B	622	-	44,44,55	0.86	3 (6%)	52,52,63	1.24	2 (3%)
29	CLA	Y	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
37	DGD	B1	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.21	6 (10%)
49	LUT	G1	621	-	42,43,43	2.23	1 (2%)	51,60,60	2.08	10 (19%)
49	LUT	s1	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.02	16 (31%)
49	LUT	S	620	-	42,43,43	2.29	1 (2%)	51,60,60	2.12	18 (35%)
37	DGD	b	623	-	44,44,67	0.89	2 (4%)	58,58,81	1.26	6 (10%)
29	CLA	Y	613	24	65,73,73	1.38	8 (12%)	76,113,113	2.14	21 (27%)
29	CLA	r	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.37	13 (23%)
40	LHG	S1	624	29	44,44,48	0.44	0	47,50,54	1.12	4 (8%)
29	CLA	n1	614	-	49,57,73	1.56	8 (16%)	55,93,113	2.40	15 (27%)
29	CLA	g1	612	21	43,51,73	1.67	10 (23%)	49,86,113	2.28	13 (26%)
30	PHO	a1	408	-	51,69,69	1.04	4 (7%)	47,99,99	1.17	6 (12%)
49	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.92	15 (29%)
29	CLA	c1	513	-	65,73,73	1.39	9 (13%)	76,113,113	2.04	18 (23%)
29	CLA	A1	406	-	65,73,73	1.38	9 (13%)	76,113,113	2.04	20 (26%)
29	CLA	C1	513	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	a1	410	-	60,68,73	1.43	9 (15%)	70,107,113	2.17	19 (27%)
43	PL9	d	405	-	55,55,55	1.75	10 (18%)	68,69,69	1.54	11 (16%)
40	LHG	s	624	29	44,44,48	0.43	0	47,50,54	1.13	3 (6%)
29	CLA	b	605	-	65,73,73	1.40	7 (10%)	76,113,113	2.17	21 (27%)
33	LMG	d	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.19	4 (7%)
50	XAT	r1	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.16	18 (33%)
48	CHL	y	606	-	66,74,74	0.91	4 (6%)	73,114,114	1.21	10 (13%)
29	CLA	R1	612	-	60,68,73	1.44	7 (11%)	70,107,113	2.07	17 (24%)
29	CLA	d	403	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	17 (22%)
31	BCR	b	619	-	41,41,41	1.83	5 (12%)	56,56,56	4.15	16 (28%)
31	BCR	c1	515	-	41,41,41	1.91	4 (9%)	56,56,56	4.38	13 (23%)
44	HEM	F	101	7,6	41,50,50	1.44	4 (9%)	45,82,82	1.30	3 (6%)
29	CLA	r1	604	-	49,57,73	1.56	7 (14%)	55,93,113	2.28	16 (29%)
29	CLA	b1	614	-	65,73,73	1.38	10 (15%)	76,113,113	1.89	17 (22%)
31	BCR	C	515	-	41,41,41	1.83	6 (14%)	56,56,56	4.20	16 (28%)
49	LUT	S1	620	-	42,43,43	2.32	1 (2%)	51,60,60	1.76	9 (17%)
29	CLA	S	609	-	60,68,73	1.43	8 (13%)	70,107,113	1.98	16 (22%)
29	CLA	C1	502	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	17 (22%)
40	LHG	Y1	624	-	48,48,48	0.40	0	51,54,54	1.11	4 (7%)
45	RRX	h1	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.65	25 (43%)
31	BCR	B1	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.43	19 (33%)
39	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.27	2 (6%)
51	NEX	y1	623	-	38,46,46	3.26	10 (26%)	50,70,70	2.03	18 (36%)
40	LHG	d	408	-	43,43,48	0.40	0	46,49,54	1.04	3 (6%)
29	CLA	b	615	-	65,73,73	1.34	7 (10%)	76,113,113	2.08	18 (23%)
29	CLA	g1	604	-	49,57,73	1.52	7 (14%)	55,93,113	2.31	18 (32%)
37	DGD	B	623	-	44,44,67	0.89	1 (2%)	58,58,81	1.36	6 (10%)
51	NEX	R1	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.93	14 (28%)
29	CLA	y	602	24	65,73,73	1.40	8 (12%)	76,113,113	1.90	14 (18%)
36	C7Z	B	620	-	43,43,43	5.27	26 (60%)	58,60,60	2.44	22 (37%)
42	BCT	D	401	27	2,3,3	1.26	0	2,3,3	2.71	2 (100%)
29	CLA	C	512	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
29	CLA	s	604	-	55,63,73	1.48	7 (12%)	64,101,113	2.10	16 (25%)
29	CLA	Y1	614	-	65,73,73	1.37	7 (10%)	76,113,113	2.02	17 (22%)
37	DGD	c1	518	-	56,56,67	1.02	5 (8%)	70,70,81	1.11	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	LUT	G	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	12 (23%)
29	CLA	n	612	-	45,53,73	1.63	7 (15%)	52,89,113	2.07	13 (25%)
29	CLA	b	609	-	65,73,73	1.39	10 (15%)	76,113,113	2.04	19 (25%)
29	CLA	N1	603	-	65,73,73	1.37	7 (10%)	76,113,113	2.10	22 (28%)
29	CLA	Y1	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.05	19 (25%)
48	CHL	s	608	-	61,69,74	0.91	3 (4%)	67,108,114	1.30	11 (16%)
48	CHL	g1	609	-	66,74,74	0.88	3 (4%)	73,114,114	1.25	9 (12%)
29	CLA	G	610	21	65,73,73	1.35	8 (12%)	76,113,113	2.04	18 (23%)
29	CLA	c1	501	-	65,73,73	1.38	8 (12%)	76,113,113	2.05	18 (23%)
33	LMG	b	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.15	2 (3%)
40	LHG	g1	624	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
32	SQD	M	101	-	41,42,54	0.90	0	50,53,65	0.98	3 (6%)
29	CLA	b	604	-	65,73,73	1.39	8 (12%)	76,113,113	1.87	15 (19%)
38	3PH	B1	624	-	47,47,47	0.86	3 (6%)	51,52,52	1.11	2 (3%)
29	CLA	c	509	-	65,73,73	1.35	6 (9%)	76,113,113	1.94	16 (21%)
51	NEX	N1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.68	10 (20%)
55	PTY	Y	627	-	18,18,49	1.31	3 (16%)	21,23,54	1.40	2 (9%)
29	CLA	S	611	40	65,73,73	1.38	7 (10%)	76,113,113	1.94	16 (21%)
49	LUT	N1	621	-	42,43,43	2.33	2 (4%)	51,60,60	2.10	13 (25%)
29	CLA	g	612	-	43,51,73	1.70	7 (16%)	49,86,113	2.18	13 (26%)
32	SQD	b	626	-	53,54,54	0.82	0	62,65,65	0.91	3 (4%)
29	CLA	b1	615	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	16 (21%)
39	DGA	b1	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.50	3 (6%)
40	LHG	c1	525	-	46,46,48	0.39	0	49,52,54	1.01	2 (4%)
48	CHL	y1	606	-	66,74,74	0.83	2 (3%)	73,114,114	1.16	10 (13%)
29	CLA	N	610	-	65,73,73	1.36	7 (10%)	76,113,113	2.07	18 (23%)
40	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
32	SQD	c1	526	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
32	SQD	C1	526	-	53,54,54	0.81	0	62,65,65	0.88	2 (3%)
51	NEX	G	623	-	38,46,46	3.37	11 (28%)	50,70,70	1.92	12 (24%)
33	LMG	a1	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.31	4 (7%)
29	CLA	c	504	-	65,73,73	1.33	8 (12%)	76,113,113	2.05	16 (21%)
48	CHL	S	608	-	61,69,74	0.89	3 (4%)	67,108,114	1.27	11 (16%)
48	CHL	G	605	21	48,56,74	0.96	3 (6%)	51,92,114	1.32	8 (15%)
31	BCR	c1	516	-	41,41,41	1.91	4 (9%)	56,56,56	4.43	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	CHL	N1	608	-	50,58,74	0.96	2 (4%)	52,94,114	1.51	8 (15%)
29	CLA	y1	613	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	17 (22%)
26	OEX	A1	401	1,4	0,15,15	-	-	-		
37	DGD	c1	520	-	60,60,67	1.09	6 (10%)	74,74,81	1.00	3 (4%)
38	3PH	b	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.18	3 (5%)
29	CLA	y1	612	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	20 (26%)
29	CLA	G1	602	-	65,73,73	1.40	8 (12%)	76,113,113	2.08	21 (27%)
29	CLA	a1	405	-	65,73,73	1.30	6 (9%)	76,113,113	2.12	19 (25%)
29	CLA	s1	609	-	60,68,73	1.40	9 (15%)	70,107,113	2.18	15 (21%)
29	CLA	B	616	-	65,73,73	1.36	9 (13%)	76,113,113	1.95	19 (25%)
29	CLA	b	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.11	17 (22%)
29	CLA	B	608	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	16 (21%)
29	CLA	g1	613	-	65,73,73	1.38	8 (12%)	76,113,113	2.03	16 (21%)
48	CHL	N	605	20	66,74,74	0.92	4 (6%)	73,114,114	1.24	11 (15%)
29	CLA	Y	611	-	65,73,73	1.34	9 (13%)	76,113,113	1.91	13 (17%)
29	CLA	S1	617	23	50,58,73	1.54	8 (16%)	58,95,113	2.32	19 (32%)
29	CLA	b	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.04	18 (23%)
42	BCT	D1	401	27	2,3,3	1.29	0	2,3,3	3.02	2 (100%)
47	4RF	I	102	-	56,56,56	1.05	4 (7%)	59,59,59	0.97	3 (5%)
49	LUT	Y1	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.87	14 (27%)
29	CLA	c	506	-	65,73,73	1.38	9 (13%)	76,113,113	2.07	19 (25%)
29	CLA	R1	608	-	60,68,73	1.42	8 (13%)	70,107,113	2.08	16 (22%)
29	CLA	c	508	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	17 (22%)
48	CHL	Y1	609	-	66,74,74	0.84	2 (3%)	73,114,114	1.28	10 (13%)
33	LMG	w	201	-	39,39,55	0.89	2 (5%)	47,47,63	1.29	4 (8%)
52	LMT	r1	625	-	36,36,36	1.18	4 (11%)	47,47,47	1.08	4 (8%)
31	BCR	D	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	16 (28%)
37	DGD	b1	623	-	44,44,67	0.92	2 (4%)	58,58,81	1.32	5 (8%)
48	CHL	G	609	21	66,74,74	0.90	3 (4%)	73,114,114	1.18	12 (16%)
29	CLA	C	507	-	65,73,73	1.38	8 (12%)	76,113,113	2.04	17 (22%)
49	LUT	S1	621	-	42,43,43	2.39	2 (4%)	51,60,60	1.99	19 (37%)
29	CLA	C	504	-	65,73,73	1.34	8 (12%)	76,113,113	1.96	13 (17%)
33	LMG	C1	523	-	55,55,55	1.12	6 (10%)	63,63,63	1.15	6 (9%)
29	CLA	N1	602	-	65,73,73	1.36	7 (10%)	76,113,113	1.98	18 (23%)
29	CLA	R	612	-	60,68,73	1.44	10 (16%)	70,107,113	2.14	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	b1	609	-	65,73,73	1.36	8 (12%)	76,113,113	2.05	15 (19%)
33	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.12	3 (4%)
29	CLA	G	614	-	49,57,73	1.55	7 (14%)	55,93,113	2.35	20 (36%)
29	CLA	n1	612	-	45,53,73	1.67	9 (20%)	52,89,113	2.05	13 (25%)
53	ERG	r1	626	-	31,32,32	7.77	19 (61%)	47,50,50	2.72	18 (38%)
29	CLA	y1	608	-	50,58,73	1.55	10 (20%)	58,95,113	2.21	17 (29%)
48	CHL	S	607	-	43,51,74	1.07	3 (6%)	45,86,114	1.46	7 (15%)
49	LUT	N	620	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	15 (29%)
33	LMG	A	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.20	4 (7%)
39	DGA	B1	625	-	43,43,43	1.14	3 (6%)	45,45,45	1.46	3 (6%)
40	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
33	LMG	c1	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	3 (4%)
45	RRX	H	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.85	22 (38%)
29	CLA	Y	608	-	50,58,73	1.54	9 (18%)	58,95,113	2.29	17 (29%)
29	CLA	s	614	-	55,63,73	1.48	7 (12%)	64,101,113	2.12	15 (23%)
31	BCR	c	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.24	12 (21%)
29	CLA	A1	407	-	50,58,73	1.56	8 (16%)	58,95,113	2.22	18 (31%)
40	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.16	4 (9%)
37	DGD	c	520	-	60,60,67	1.05	4 (6%)	74,74,81	1.03	3 (4%)
37	DGD	C	518	-	56,56,67	0.98	4 (7%)	70,70,81	0.95	2 (2%)
39	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.50	3 (6%)
29	CLA	n	610	-	65,73,73	1.38	9 (13%)	76,113,113	2.12	20 (26%)
51	NEX	R	622	-	38,46,46	3.42	11 (28%)	50,70,70	1.98	12 (24%)
49	LUT	g	620	-	42,43,43	2.32	1 (2%)	51,60,60	2.16	16 (31%)
50	XAT	g	622	-	39,47,47	0.80	1 (2%)	54,74,74	2.22	16 (29%)
29	CLA	N1	612	-	45,53,73	1.64	8 (17%)	52,89,113	2.16	12 (23%)
29	CLA	C1	508	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	14 (18%)
51	NEX	G1	623	-	38,46,46	3.38	10 (26%)	50,70,70	1.77	11 (22%)
29	CLA	C1	505	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	17 (22%)
29	CLA	S1	611	40	65,73,73	1.41	9 (13%)	76,113,113	1.94	14 (18%)
48	CHL	n1	605	-	66,74,74	0.90	3 (4%)	73,114,114	1.29	11 (15%)
29	CLA	c1	512	-	65,73,73	1.38	7 (10%)	76,113,113	2.03	19 (25%)
48	CHL	S	606	-	44,52,74	1.10	3 (6%)	46,87,114	1.48	10 (21%)
29	CLA	R	603	-	60,68,73	1.48	9 (15%)	70,107,113	2.00	17 (24%)
43	PL9	d1	405	-	55,55,55	1.13	3 (5%)	68,69,69	1.57	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B1	604	-	65,73,73	1.37	7 (10%)	76,113,113	1.86	16 (21%)
29	CLA	B	611	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	19 (25%)
29	CLA	C1	503	-	65,73,73	1.38	9 (13%)	76,113,113	2.01	21 (27%)
32	SQD	b1	626	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
29	CLA	y	611	40	65,73,73	1.35	7 (10%)	76,113,113	1.88	15 (19%)
29	CLA	Y1	608	-	50,58,73	1.57	8 (16%)	58,95,113	2.24	16 (27%)
29	CLA	g1	603	-	65,73,73	1.38	8 (12%)	76,113,113	1.88	16 (21%)
29	CLA	y	613	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	18 (23%)
48	CHL	s1	601	23	46,54,74	1.07	3 (6%)	49,90,114	1.46	12 (24%)
29	CLA	s1	610	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	19 (25%)
29	CLA	c	511	4	65,73,73	1.36	8 (12%)	76,113,113	2.01	19 (25%)
29	CLA	R1	610	-	60,68,73	1.43	9 (15%)	70,107,113	2.28	18 (25%)
47	4RF	i1	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.92	3 (5%)
29	CLA	s	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.02	17 (22%)
29	CLA	S	604	-	55,63,73	1.45	8 (14%)	64,101,113	2.22	17 (26%)
50	XAT	r	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	13 (24%)
48	CHL	n1	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.32	12 (16%)
29	CLA	S	602	-	60,68,73	1.45	8 (13%)	70,107,113	2.17	18 (25%)
48	CHL	Y1	607	-	66,74,74	0.86	3 (4%)	73,114,114	1.19	9 (12%)
29	CLA	g	614	-	49,57,73	1.57	9 (18%)	55,93,113	2.23	15 (27%)
29	CLA	C1	512	-	65,73,73	1.35	7 (10%)	76,113,113	2.09	21 (27%)
51	NEX	n1	623	-	38,46,46	3.26	9 (23%)	50,70,70	1.71	11 (22%)
29	CLA	C	506	-	65,73,73	1.43	8 (12%)	76,113,113	2.05	18 (23%)
31	BCR	B	619	-	41,41,41	1.85	4 (9%)	56,56,56	3.81	21 (37%)
48	CHL	Y	605	24	46,54,74	1.07	3 (6%)	49,90,114	1.51	10 (20%)
48	CHL	G1	608	-	44,52,74	1.10	3 (6%)	46,87,114	1.43	7 (15%)
38	3PH	S	626	-	47,47,47	0.87	2 (4%)	51,52,52	4.41	4 (7%)
48	CHL	g1	606	-	50,58,74	1.06	4 (8%)	52,94,114	1.28	9 (17%)
55	PTY	Y1	627	-	18,18,49	1.28	2 (11%)	21,23,54	1.41	2 (9%)
37	DGD	C	520	-	60,60,67	1.06	6 (10%)	74,74,81	1.07	3 (4%)
29	CLA	S1	613	-	55,63,73	1.45	7 (12%)	64,101,113	2.15	15 (23%)
33	LMG	w1	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.17	3 (6%)
49	LUT	R1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	10 (19%)
40	LHG	G	624	29	48,48,48	0.37	0	51,54,54	1.06	3 (5%)
49	LUT	s	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.91	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	Y	610	-	65,73,73	1.36	9 (13%)	76,113,113	2.14	18 (23%)
29	CLA	c1	506	-	65,73,73	1.30	6 (9%)	76,113,113	2.09	20 (26%)
48	CHL	n	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.27	12 (16%)
29	CLA	n	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.01	17 (22%)
48	CHL	R1	606	-	44,52,74	1.07	3 (6%)	46,87,114	1.30	8 (17%)
29	CLA	C	503	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	17 (22%)
48	CHL	s	606	-	44,52,74	1.04	3 (6%)	46,87,114	1.46	7 (15%)
29	CLA	S1	609	-	60,68,73	1.39	8 (13%)	70,107,113	2.09	17 (24%)
42	BCT	d	401	-	2,3,3	1.27	0	2,3,3	2.80	2 (100%)
37	DGD	C1	519	-	63,63,67	1.10	7 (11%)	77,77,81	1.05	3 (3%)
29	CLA	S1	602	23	60,68,73	1.39	9 (15%)	70,107,113	2.13	17 (24%)
33	LMG	h1	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.23	4 (7%)
29	CLA	A1	410	-	60,68,73	1.40	7 (11%)	70,107,113	2.13	20 (28%)
29	CLA	N1	604	-	65,73,73	1.36	8 (12%)	76,113,113	2.15	17 (22%)
51	NEX	r	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.78	11 (22%)
33	LMG	C1	521	-	51,51,55	1.07	5 (9%)	59,59,63	1.14	2 (3%)
29	CLA	c	502	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	16 (21%)
29	CLA	B1	602	-	65,73,73	1.39	9 (13%)	76,113,113	2.02	17 (22%)
29	CLA	S1	604	-	55,63,73	1.49	9 (16%)	64,101,113	2.20	18 (28%)
48	CHL	Y	609	-	66,74,74	0.91	4 (6%)	73,114,114	1.43	14 (19%)
48	CHL	g	607	-	66,74,74	0.85	2 (3%)	73,114,114	1.27	11 (15%)
48	CHL	Y1	606	-	66,74,74	0.90	4 (6%)	73,114,114	1.25	10 (13%)
50	XAT	G	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.11	15 (27%)
48	CHL	s	601	-	46,54,74	1.15	4 (8%)	49,90,114	1.43	8 (16%)
29	CLA	C	511	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	18 (23%)
32	SQD	B	626	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
55	PTY	y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.50	2 (9%)
37	DGD	c	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.14	4 (5%)
33	LMG	H1	102	-	48,48,55	1.02	5 (10%)	56,56,63	1.16	3 (5%)
55	PTY	y1	626	-	49,49,49	0.87	4 (8%)	52,54,54	1.08	2 (3%)
34	SPH	A1	414	-	19,20,20	0.67	1 (5%)	18,21,21	1.17	1 (5%)
48	CHL	R	606	-	44,52,74	1.20	4 (9%)	46,87,114	1.30	7 (15%)
48	CHL	n	601	20	66,74,74	0.91	3 (4%)	73,114,114	1.26	9 (12%)
52	LMT	R	625	-	36,36,36	1.22	6 (16%)	47,47,47	1.14	3 (6%)
52	LMT	R1	625	-	36,36,36	1.27	8 (22%)	47,47,47	1.15	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	s	609	-	60,68,73	1.42	9 (15%)	70,107,113	2.03	15 (21%)
31	BCR	b1	618	-	41,41,41	2.03	4 (9%)	56,56,56	4.25	19 (33%)
49	LUT	S	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.10	19 (37%)
48	CHL	g1	605	-	48,56,74	0.95	2 (4%)	51,92,114	1.50	10 (19%)
29	CLA	C	510	-	65,73,73	1.37	7 (10%)	76,113,113	1.97	18 (23%)
29	CLA	S1	612	-	45,53,73	1.59	6 (13%)	52,89,113	2.18	15 (28%)
48	CHL	Y1	601	-	66,74,74	0.91	3 (4%)	73,114,114	1.23	10 (13%)
31	BCR	C	516	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
29	CLA	S	605	23	50,58,73	1.59	9 (18%)	58,95,113	2.42	16 (27%)
29	CLA	y1	603	-	65,73,73	1.36	8 (12%)	76,113,113	1.93	16 (21%)
41	LMK	C1	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.47	2 (4%)
49	LUT	N	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.97	12 (23%)
50	XAT	R	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	18 (33%)
29	CLA	n1	602	20	65,73,73	1.31	8 (12%)	76,113,113	2.04	20 (26%)
38	3PH	S1	626	-	47,47,47	0.87	4 (8%)	51,52,52	4.40	4 (7%)
29	CLA	A	405	-	65,73,73	1.35	6 (9%)	76,113,113	2.09	17 (22%)
42	BCT	d1	401	-	2,3,3	1.18	0	2,3,3	4.36	2 (100%)
49	LUT	y1	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.97	10 (19%)
29	CLA	y1	614	-	65,73,73	1.40	9 (13%)	76,113,113	1.90	19 (25%)
48	CHL	g	601	21	66,74,74	0.88	4 (6%)	73,114,114	1.25	10 (13%)
49	LUT	y	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.98	14 (27%)
29	CLA	n	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	20 (26%)
38	3PH	T1	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.09	2 (3%)
29	CLA	N1	614	-	49,57,73	1.54	7 (14%)	55,93,113	2.33	17 (30%)
49	LUT	Y1	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.33	13 (25%)
29	CLA	B1	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	19 (25%)
48	CHL	N	607	-	66,74,74	0.82	2 (3%)	73,114,114	1.23	12 (16%)
29	CLA	G1	611	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	15 (19%)
29	CLA	G	603	-	65,73,73	1.33	8 (12%)	76,113,113	2.03	20 (26%)
29	CLA	y	610	24	65,73,73	1.33	7 (10%)	76,113,113	2.03	17 (22%)
40	LHG	s1	624	29	44,44,48	0.43	0	47,50,54	1.08	4 (8%)
29	CLA	g	610	-	65,73,73	1.33	8 (12%)	76,113,113	2.12	20 (26%)
29	CLA	B1	617	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	16 (21%)
29	CLA	c	507	-	65,73,73	1.39	9 (13%)	76,113,113	2.02	16 (21%)
49	LUT	g1	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.93	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	c	515	-	41,41,41	1.88	5 (12%)	56,56,56	4.18	16 (28%)
29	CLA	g	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.03	17 (22%)
26	OEX	A	401	1,4	0,15,15	-	-	-	-	-
29	CLA	D1	403	-	65,73,73	1.36	9 (13%)	76,113,113	2.05	22 (28%)
29	CLA	b1	604	-	65,73,73	1.38	9 (13%)	76,113,113	2.03	17 (22%)
34	SPH	a	414	-	19,20,20	0.70	1 (5%)	18,21,21	1.10	1 (5%)
32	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.92	2 (3%)
33	LMG	A1	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.20	5 (8%)
45	RRX	H1	101	-	42,42,42	4.95	24 (57%)	57,58,58	2.34	19 (33%)
48	CHL	s	607	-	43,51,74	1.09	3 (6%)	45,86,114	1.49	8 (17%)
31	BCR	b1	619	-	41,41,41	1.91	4 (9%)	56,56,56	4.36	15 (26%)
47	4RF	K	101	-	56,56,56	1.08	3 (5%)	59,59,59	0.91	3 (5%)
29	CLA	n1	603	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	16 (21%)
31	BCR	C	514	-	41,41,41	1.87	5 (12%)	56,56,56	4.28	14 (25%)
48	CHL	n	606	-	66,74,74	0.92	4 (6%)	73,114,114	1.25	12 (16%)
29	CLA	a	407	-	49,57,73	1.55	7 (14%)	55,93,113	2.52	18 (32%)
33	LMG	W1	201	-	39,39,55	0.87	2 (5%)	47,47,63	1.37	6 (12%)
40	LHG	d	409	-	48,48,48	0.41	0	51,54,54	1.06	3 (5%)
39	DGA	C1	524	-	43,43,43	1.17	3 (6%)	45,45,45	1.54	4 (8%)
48	CHL	y1	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.29	10 (13%)
30	PHO	A1	408	-	51,69,69	1.06	4 (7%)	47,99,99	1.15	4 (8%)
29	CLA	R	610	-	60,68,73	1.49	10 (16%)	70,107,113	2.14	21 (30%)
29	CLA	G1	604	-	49,57,73	1.57	7 (14%)	55,93,113	2.34	18 (32%)
29	CLA	s1	602	-	60,68,73	1.40	7 (11%)	70,107,113	2.30	21 (30%)
29	CLA	B1	606	-	65,73,73	1.38	9 (13%)	76,113,113	2.03	18 (23%)
48	CHL	Y	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.28	9 (12%)
50	XAT	n1	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.04	14 (25%)
29	CLA	A	406	-	65,73,73	1.32	7 (10%)	76,113,113	2.12	17 (22%)
29	CLA	c1	503	-	65,73,73	1.37	9 (13%)	76,113,113	2.06	19 (25%)
48	CHL	g	606	-	50,58,74	0.99	2 (4%)	52,94,114	1.55	9 (17%)
29	CLA	y	608	-	50,58,73	1.57	9 (18%)	58,95,113	2.25	17 (29%)
31	BCR	b	618	-	41,41,41	1.89	5 (12%)	56,56,56	4.48	20 (35%)
48	CHL	N	606	-	66,74,74	0.96	3 (4%)	73,114,114	1.21	13 (17%)
29	CLA	B1	603	-	65,73,73	1.39	9 (13%)	76,113,113	2.13	20 (26%)
49	LUT	Y	620	-	42,43,43	2.31	1 (2%)	51,60,60	1.81	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LHG	n1	624	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)
36	C7Z	b	620	-	43,43,43	5.32	27 (62%)	58,60,60	2.48	19 (32%)
31	BCR	A1	411	-	41,41,41	1.88	4 (9%)	56,56,56	4.17	15 (26%)
26	OEX	a	401	1,4	0,15,15	-	-	-	-	-
29	CLA	G1	613	-	65,73,73	1.32	7 (10%)	76,113,113	2.19	21 (27%)
37	DGD	c	519	-	63,63,67	1.12	5 (7%)	77,77,81	1.01	2 (2%)
49	LUT	n	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.78	12 (23%)
29	CLA	B	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.14	17 (22%)
48	CHL	y1	601	24	66,74,74	0.79	2 (3%)	73,114,114	1.28	9 (12%)
29	CLA	y1	610	24	65,73,73	1.39	9 (13%)	76,113,113	2.02	21 (27%)
32	SQD	C	526	-	53,54,54	0.81	1 (1%)	62,65,65	0.94	3 (4%)
29	CLA	N	613	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	13 (17%)
29	CLA	G1	612	-	43,51,73	1.71	9 (20%)	49,86,113	2.15	12 (24%)
33	LMG	c	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.16	4 (6%)
48	CHL	n1	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.29	10 (13%)
29	CLA	R1	609	-	60,68,73	1.40	9 (15%)	70,107,113	4.53	19 (27%)
48	CHL	s1	607	-	43,51,74	1.02	3 (6%)	45,86,114	1.45	8 (17%)
33	LMG	H	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.10	2 (3%)
40	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.03	2 (4%)
40	LHG	D1	410	-	38,38,48	0.43	0	41,44,54	1.09	3 (7%)
46	GOL	I	101	-	5,5,5	0.54	0	5,5,5	0.39	0
29	CLA	B1	611	-	65,73,73	1.37	7 (10%)	76,113,113	2.09	16 (21%)
39	DGA	j1	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.26	2 (6%)
49	LUT	s1	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.37	13 (25%)
29	CLA	B1	613	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	14 (18%)
29	CLA	b1	611	-	65,73,73	1.42	6 (9%)	76,113,113	2.02	18 (23%)
29	CLA	c1	510	-	65,73,73	1.39	8 (12%)	76,113,113	1.92	16 (21%)
53	ERG	R	626	-	31,32,32	7.79	18 (58%)	47,50,50	3.10	19 (40%)
29	CLA	S1	614	-	55,63,73	1.49	7 (12%)	64,101,113	2.12	17 (26%)
38	3PH	t	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.19	2 (3%)
29	CLA	r	610	-	60,68,73	1.41	9 (15%)	70,107,113	2.20	20 (28%)
29	CLA	D	403	-	65,73,73	1.35	9 (13%)	76,113,113	2.08	19 (25%)
29	CLA	Y1	602	-	65,73,73	1.38	9 (13%)	76,113,113	2.07	17 (22%)
48	CHL	n1	601	-	66,74,74	0.82	2 (3%)	73,114,114	1.29	9 (12%)
34	SPH	Y1	625	-	19,20,20	0.64	0	18,21,21	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LHG	y	624	29	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
49	LUT	n	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.09	17 (33%)
50	XAT	n	622	-	39,47,47	0.78	1 (2%)	54,74,74	2.09	13 (24%)
40	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.45	4 (7%)
29	CLA	r1	608	-	60,68,73	1.45	7 (11%)	70,107,113	2.03	16 (22%)
29	CLA	s	611	40	65,73,73	1.37	8 (12%)	76,113,113	1.91	13 (17%)
31	BCR	c1	517	-	41,41,41	1.91	5 (12%)	56,56,56	4.37	19 (33%)
29	CLA	d1	403	-	65,73,73	1.34	7 (10%)	76,113,113	2.04	19 (25%)
29	CLA	B1	608	-	65,73,73	1.38	8 (12%)	76,113,113	1.97	16 (21%)
40	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.12	3 (6%)
36	C7Z	b1	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.51	22 (37%)
29	CLA	b1	616	-	65,73,73	1.38	7 (10%)	76,113,113	1.94	14 (18%)
29	CLA	r1	602	-	60,68,73	1.40	7 (11%)	70,107,113	2.09	19 (27%)
33	LMG	b1	622	-	44,44,55	0.86	2 (4%)	52,52,63	1.17	3 (5%)
31	BCR	d	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
33	LMG	d1	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.11	3 (5%)
29	CLA	c	505	-	65,73,73	1.40	8 (12%)	76,113,113	2.00	16 (21%)
51	NEX	s1	623	-	38,46,46	3.40	12 (31%)	50,70,70	2.71	15 (30%)
51	NEX	S	623	-	38,46,46	3.42	10 (26%)	50,70,70	1.71	12 (24%)
29	CLA	b1	608	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	19 (25%)
32	SQD	m1	101	-	41,42,54	0.88	0	50,53,65	0.99	3 (6%)
29	CLA	N1	611	-	49,57,73	1.59	8 (16%)	55,93,113	2.29	16 (29%)
50	XAT	y	622	-	39,47,47	0.73	1 (2%)	54,74,74	3.68	19 (35%)
29	CLA	N1	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	17 (22%)
49	LUT	g1	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.33	14 (27%)
29	CLA	C1	506	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	17 (22%)
29	CLA	R1	603	-	60,68,73	1.45	8 (13%)	70,107,113	1.89	14 (20%)
50	XAT	N	622	-	39,47,47	0.70	1 (2%)	54,74,74	2.21	13 (24%)
29	CLA	d1	402	-	65,73,73	1.39	9 (13%)	76,113,113	1.95	17 (22%)
41	LMK	c1	527	-	38,39,53	1.51	3 (7%)	41,46,60	1.24	2 (4%)
39	DGA	c	524	-	43,43,43	1.10	3 (6%)	45,45,45	1.55	3 (6%)
29	CLA	R1	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.34	15 (27%)
29	CLA	Y1	603	-	65,73,73	1.39	10 (15%)	76,113,113	1.95	16 (21%)
29	CLA	b	613	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	11 (14%)
29	CLA	n	613	-	65,73,73	1.36	6 (9%)	76,113,113	2.12	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	G	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	20 (26%)
29	CLA	r	608	-	60,68,73	1.40	9 (15%)	70,107,113	2.00	18 (25%)
47	4RF	i	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.93	3 (5%)
29	CLA	a	406	-	65,73,73	1.34	8 (12%)	76,113,113	2.25	20 (26%)
44	HEM	f	101	7,6	41,50,50	1.45	4 (9%)	45,82,82	1.35	6 (13%)
48	CHL	Y	601	24	66,74,74	0.91	3 (4%)	73,114,114	1.21	9 (12%)
48	CHL	s1	608	-	61,69,74	1.04	5 (8%)	67,108,114	1.38	11 (16%)
45	RRX	h	101	-	42,42,42	4.74	24 (57%)	57,58,58	3.10	25 (43%)
40	LHG	d1	408	-	43,43,48	0.40	0	46,49,54	1.05	2 (4%)
40	LHG	L	101	-	48,48,48	0.38	0	51,54,54	4.46	5 (9%)
29	CLA	G	612	-	43,51,73	1.66	6 (13%)	49,86,113	2.20	14 (28%)
29	CLA	a	410	-	60,68,73	1.39	9 (15%)	70,107,113	2.17	18 (25%)
29	CLA	r1	612	-	60,68,73	1.42	7 (11%)	70,107,113	2.05	19 (27%)
29	CLA	n	614	-	49,57,73	1.56	9 (18%)	55,93,113	2.36	20 (36%)
40	LHG	N	624	-	48,48,48	0.40	0	51,54,54	1.08	3 (5%)
48	CHL	g1	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.23	9 (12%)
50	XAT	y1	622	-	39,47,47	0.74	1 (2%)	54,74,74	3.88	20 (37%)
49	LUT	s	621	-	42,43,43	2.30	1 (2%)	51,60,60	1.98	16 (31%)
33	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.19	4 (7%)
29	CLA	b	602	-	65,73,73	1.38	8 (12%)	76,113,113	1.98	18 (23%)
29	CLA	s1	605	-	50,58,73	1.60	11 (22%)	58,95,113	2.28	18 (31%)
51	NEX	Y	623	-	38,46,46	3.34	9 (23%)	50,70,70	1.85	12 (24%)
49	LUT	Y	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.00	15 (29%)
29	CLA	r1	603	-	60,68,73	1.41	8 (13%)	70,107,113	2.11	17 (24%)
29	CLA	g	613	-	65,73,73	1.33	7 (10%)	76,113,113	2.04	18 (23%)
39	DGA	j	101	-	28,28,43	1.28	3 (10%)	30,30,45	1.28	2 (6%)
51	NEX	S1	623	-	38,46,46	3.20	9 (23%)	50,70,70	1.79	10 (20%)
40	LHG	C	525	-	46,46,48	0.42	0	49,52,54	1.04	2 (4%)
44	HEM	f1	101	7	41,50,50	1.52	7 (17%)	45,82,82	1.19	4 (8%)
40	LHG	y1	624	29	48,48,48	0.41	0	51,54,54	0.98	2 (3%)
40	LHG	L1	101	-	48,48,48	0.37	0	51,54,54	1.11	3 (5%)
48	CHL	N1	605	20	66,74,74	0.90	3 (4%)	73,114,114	1.31	13 (17%)
43	PL9	D1	405	-	55,55,55	1.18	5 (9%)	68,69,69	1.72	15 (22%)
47	4RF	k	101	-	56,56,56	1.06	5 (8%)	59,59,59	0.83	3 (5%)
29	CLA	n	611	-	49,57,73	1.58	7 (14%)	55,93,113	2.30	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	y	604	-	65,73,73	1.33	7 (10%)	76,113,113	2.09	19 (25%)
29	CLA	r	612	-	60,68,73	1.43	8 (13%)	70,107,113	2.03	16 (22%)
48	CHL	R	607	-	50,58,74	1.00	3 (6%)	52,94,114	1.44	9 (17%)
48	CHL	S1	608	-	61,69,74	0.84	2 (3%)	67,108,114	1.33	13 (19%)
29	CLA	C	505	-	65,73,73	1.40	8 (12%)	76,113,113	2.00	16 (21%)
29	CLA	C1	501	-	65,73,73	1.35	8 (12%)	76,113,113	2.15	19 (25%)
51	NEX	Y1	623	-	38,46,46	3.15	10 (26%)	50,70,70	1.99	13 (26%)
29	CLA	r	603	-	60,68,73	1.45	8 (13%)	70,107,113	1.95	16 (22%)
30	PHO	a	408	-	51,69,69	1.08	6 (11%)	47,99,99	1.23	5 (10%)
29	CLA	g	611	-	65,73,73	1.34	7 (10%)	76,113,113	2.10	17 (22%)
29	CLA	B1	610	-	65,73,73	1.36	8 (12%)	76,113,113	1.91	14 (18%)
34	SPH	y1	625	-	19,20,20	0.62	0	18,21,21	1.27	2 (11%)
29	CLA	s	602	-	60,68,73	1.41	8 (13%)	70,107,113	2.10	21 (30%)
29	CLA	B	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	17 (22%)
48	CHL	N1	609	-	66,74,74	0.77	2 (3%)	73,114,114	1.44	13 (17%)
31	BCR	C1	517	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	16 (28%)
54	LPX	S1	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.93	1 (3%)
44	HEM	F1	101	7	41,50,50	1.48	3 (7%)	45,82,82	1.47	9 (20%)
29	CLA	B	615	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	19 (25%)
29	CLA	b	617	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	16 (21%)
32	SQD	B1	626	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
37	DGD	c1	519	-	63,63,67	1.14	6 (9%)	77,77,81	1.04	3 (3%)
48	CHL	N	609	-	66,74,74	0.79	3 (4%)	73,114,114	1.22	11 (15%)
29	CLA	C1	507	-	65,73,73	1.38	8 (12%)	76,113,113	1.92	17 (22%)
29	CLA	b1	606	-	65,73,73	1.35	7 (10%)	76,113,113	2.05	18 (23%)
33	LMG	D	411	-	46,46,55	0.91	4 (8%)	54,54,63	0.99	2 (3%)
37	DGD	C	519	-	63,63,67	1.13	7 (11%)	77,77,81	1.01	2 (2%)
51	NEX	n	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.66	11 (22%)
51	NEX	N	623	-	38,46,46	3.40	9 (23%)	50,70,70	1.64	11 (22%)
48	CHL	n	605	20	66,74,74	0.93	5 (7%)	73,114,114	1.24	8 (10%)
29	CLA	y	614	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	18 (23%)
47	4RF	I1	102	-	56,56,56	1.06	4 (7%)	59,59,59	0.98	3 (5%)
48	CHL	G1	606	-	50,58,74	0.99	2 (4%)	52,94,114	1.39	11 (21%)
49	LUT	R	620	-	42,43,43	2.33	1 (2%)	51,60,60	2.03	17 (33%)
29	CLA	Y1	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.95	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	c1	511	-	65,73,73	1.36	7 (10%)	76,113,113	2.06	17 (22%)
48	CHL	y	607	-	66,74,74	0.82	3 (4%)	73,114,114	1.31	12 (16%)
29	CLA	C1	511	-	65,73,73	1.37	8 (12%)	76,113,113	2.13	19 (25%)
29	CLA	B	617	-	65,73,73	1.37	8 (12%)	76,113,113	2.04	15 (19%)
31	BCR	c1	514	-	41,41,41	1.85	4 (9%)	56,56,56	4.49	17 (30%)
29	CLA	Y	602	-	65,73,73	1.38	9 (13%)	76,113,113	2.06	19 (25%)
32	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.94	3 (5%)
38	3PH	s	626	-	47,47,47	0.87	3 (6%)	51,52,52	4.40	4 (7%)
31	BCR	C1	514	-	41,41,41	1.84	5 (12%)	56,56,56	4.05	13 (23%)
38	3PH	s1	626	-	47,47,47	0.86	3 (6%)	51,52,52	4.37	4 (7%)
29	CLA	D	402	-	65,73,73	1.38	8 (12%)	76,113,113	1.90	13 (17%)
40	LHG	d1	410	-	38,38,48	0.44	0	41,44,54	1.04	2 (4%)
36	C7Z	B1	620	-	43,43,43	5.38	26 (60%)	58,60,60	2.39	22 (37%)
29	CLA	y	603	-	65,73,73	1.39	10 (15%)	76,113,113	2.10	16 (21%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	14 (25%)
32	SQD	B	621	-	41,42,54	0.88	0	50,53,65	1.01	3 (6%)
29	CLA	A	407	-	50,58,73	1.54	9 (18%)	58,95,113	2.32	18 (31%)
51	NEX	g	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.86	15 (30%)
29	CLA	R1	602	-	60,68,73	1.45	9 (15%)	70,107,113	2.05	17 (24%)
29	CLA	N1	610	-	65,73,73	1.31	7 (10%)	76,113,113	1.99	18 (23%)
34	SPH	A	414	-	19,20,20	0.66	0	18,21,21	1.13	2 (11%)
51	NEX	y	623	-	38,46,46	3.41	9 (23%)	50,70,70	1.96	15 (30%)
29	CLA	S1	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	18 (23%)
39	DGA	c1	524	-	43,43,43	1.14	3 (6%)	45,45,45	1.51	3 (6%)
29	CLA	G1	614	-	49,57,73	1.53	7 (14%)	55,93,113	2.37	17 (30%)
30	PHO	a1	409	-	51,69,69	1.03	3 (5%)	47,99,99	1.21	6 (12%)
48	CHL	Y	606	-	66,74,74	0.90	4 (6%)	73,114,114	1.14	8 (10%)
29	CLA	c	503	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	21 (27%)
48	CHL	n	609	-	66,74,74	0.77	2 (3%)	73,114,114	1.40	12 (16%)
29	CLA	S	610	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	21 (27%)
29	CLA	G	611	40	65,73,73	1.37	7 (10%)	76,113,113	2.01	17 (22%)
49	LUT	y1	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.41	16 (31%)
48	CHL	y	601	24	66,74,74	0.86	3 (4%)	73,114,114	1.32	12 (16%)
49	LUT	g	621	-	42,43,43	2.37	2 (4%)	51,60,60	1.91	12 (23%)
29	CLA	R	609	-	60,68,73	1.45	8 (13%)	70,107,113	4.48	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	CHL	g1	601	-	66,74,74	0.82	2 (3%)	73,114,114	1.29	11 (15%)
29	CLA	c	513	-	65,73,73	1.37	8 (12%)	76,113,113	2.12	18 (23%)
29	CLA	B	604	-	65,73,73	1.38	7 (10%)	76,113,113	1.94	14 (18%)
29	CLA	b	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	20 (26%)
32	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
29	CLA	s1	604	-	55,63,73	1.46	5 (9%)	64,101,113	2.22	18 (28%)
33	LMG	C	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.19	3 (5%)
40	LHG	S	624	29	44,44,48	0.43	0	47,50,54	1.05	3 (6%)
48	CHL	n	608	-	50,58,74	1.01	3 (6%)	52,94,114	1.28	10 (19%)
29	CLA	Y	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.01	18 (23%)
48	CHL	G	601	21	66,74,74	0.87	3 (4%)	73,114,114	1.24	11 (15%)
29	CLA	A	410	-	60,68,73	1.43	9 (15%)	70,107,113	2.17	18 (25%)
48	CHL	y1	605	24	46,54,74	1.03	3 (6%)	49,90,114	1.31	8 (16%)
29	CLA	S1	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.01	16 (21%)
40	LHG	C1	525	-	46,46,48	0.39	0	49,52,54	1.04	3 (6%)
29	CLA	C	502	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	15 (19%)
48	CHL	G1	605	21	48,56,74	0.96	3 (6%)	51,92,114	1.38	9 (17%)
33	LMG	h	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.22	4 (7%)
32	SQD	B1	621	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
48	CHL	g	609	-	66,74,74	0.91	3 (4%)	73,114,114	1.25	8 (10%)
29	CLA	S	613	-	55,63,73	1.47	7 (12%)	64,101,113	2.18	16 (25%)
29	CLA	b1	617	-	65,73,73	1.36	6 (9%)	76,113,113	1.97	18 (23%)
29	CLA	n1	613	-	65,73,73	1.36	9 (13%)	76,113,113	2.16	17 (22%)
31	BCR	a1	411	-	41,41,41	1.92	5 (12%)	56,56,56	4.06	15 (26%)
32	SQD	b	621	-	41,42,54	0.87	0	50,53,65	1.02	3 (6%)
29	CLA	B1	614	-	65,73,73	1.38	9 (13%)	76,113,113	1.98	14 (18%)
48	CHL	r	606	-	44,52,74	1.05	3 (6%)	46,87,114	1.34	7 (15%)
48	CHL	g	608	-	44,52,74	1.07	3 (6%)	46,87,114	1.47	12 (26%)
32	SQD	b1	621	-	41,42,54	0.89	0	50,53,65	0.98	3 (6%)
52	LMT	r	625	-	36,36,36	1.22	5 (13%)	47,47,47	1.16	3 (6%)
29	CLA	c1	505	-	65,73,73	1.35	10 (15%)	76,113,113	2.07	17 (22%)
31	BCR	A	411	-	41,41,41	1.86	4 (9%)	56,56,56	4.22	14 (25%)
29	CLA	a	405	-	65,73,73	1.34	6 (9%)	76,113,113	2.08	18 (23%)
29	CLA	B1	616	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	15 (19%)
31	BCR	B	618	-	41,41,41	1.88	5 (12%)	56,56,56	4.32	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	b	611	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
51	NEX	s	623	-	38,46,46	3.52	11 (28%)	50,70,70	2.12	14 (28%)
29	CLA	r	609	-	60,68,73	1.42	7 (11%)	70,107,113	2.05	17 (24%)
48	CHL	N	608	-	50,58,74	0.97	3 (6%)	52,94,114	1.35	9 (17%)
48	CHL	n1	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.38	10 (19%)
40	LHG	d1	409	-	48,48,48	0.40	0	51,54,54	1.03	2 (3%)
53	ERG	R1	626	-	31,32,32	7.67	19 (61%)	47,50,50	2.83	19 (40%)
29	CLA	g1	610	-	65,73,73	1.30	6 (9%)	76,113,113	2.29	20 (26%)
29	CLA	r	602	22	60,68,73	1.44	8 (13%)	70,107,113	2.03	19 (27%)
29	CLA	c	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	16 (21%)
48	CHL	y1	609	-	66,74,74	0.82	2 (3%)	73,114,114	1.29	10 (13%)
29	CLA	d	402	-	65,73,73	1.38	8 (12%)	76,113,113	1.94	16 (21%)
33	LMG	D1	411	-	46,46,55	0.91	4 (8%)	54,54,63	1.12	3 (5%)
40	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
29	CLA	B	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	17 (22%)
29	CLA	s1	614	-	55,63,73	1.49	10 (18%)	64,101,113	2.16	16 (25%)
29	CLA	c1	508	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	19 (25%)
48	CHL	G1	609	-	66,74,74	0.90	3 (4%)	73,114,114	1.20	11 (15%)
40	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
29	CLA	C	508	-	65,73,73	1.42	7 (10%)	76,113,113	2.06	19 (25%)
29	CLA	b	614	-	65,73,73	1.34	8 (12%)	76,113,113	2.14	16 (21%)
39	DGA	B	625	-	43,43,43	1.09	2 (4%)	45,45,45	1.52	3 (6%)
55	PTY	Y1	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.04	2 (3%)
49	LUT	n1	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.13	18 (35%)
29	CLA	b1	610	-	65,73,73	1.36	9 (13%)	76,113,113	1.93	17 (22%)
48	CHL	S1	607	-	43,51,74	1.01	2 (4%)	45,86,114	1.53	9 (20%)
29	CLA	D1	402	-	65,73,73	1.37	7 (10%)	76,113,113	2.04	18 (23%)
29	CLA	r1	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.05	18 (25%)
41	LMK	C	527	-	38,39,53	1.47	2 (5%)	41,46,60	1.56	4 (9%)
29	CLA	G1	610	-	65,73,73	1.36	9 (13%)	76,113,113	2.06	20 (26%)
31	BCR	c	517	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	17 (30%)
29	CLA	n	602	-	65,73,73	1.43	8 (12%)	76,113,113	1.92	19 (25%)
29	CLA	R	604	-	49,57,73	1.54	8 (16%)	55,93,113	2.35	17 (30%)
48	CHL	N	601	20	66,74,74	0.87	3 (4%)	73,114,114	1.34	9 (12%)
39	DGA	J1	101	-	28,28,43	1.27	2 (7%)	30,30,45	1.34	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	613	-	65,73,73	1.37	8 (12%)	76,113,113	2.04	16 (21%)
51	NEX	r1	622	-	38,46,46	3.37	9 (23%)	50,70,70	1.83	12 (24%)
29	CLA	Y1	604	-	65,73,73	1.39	6 (9%)	76,113,113	1.95	15 (19%)
34	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.00	0
29	CLA	G	604	-	49,57,73	1.58	8 (16%)	55,93,113	2.28	18 (32%)
29	CLA	N	612	-	45,53,73	1.66	9 (20%)	52,89,113	2.05	12 (23%)
32	SQD	a1	412	-	50,51,54	0.82	0	59,62,65	0.95	2 (3%)
29	CLA	B	612	-	65,73,73	1.38	7 (10%)	76,113,113	1.98	16 (21%)
30	PHO	a	409	-	51,69,69	0.97	3 (5%)	47,99,99	1.38	8 (17%)
50	XAT	N1	622	-	39,47,47	0.72	1 (2%)	54,74,74	2.10	15 (27%)
46	GOL	I1	101	-	5,5,5	0.56	0	5,5,5	0.31	0
29	CLA	S	603	-	65,73,73	1.38	9 (13%)	76,113,113	1.85	17 (22%)
29	CLA	B1	605	-	65,73,73	1.34	8 (12%)	76,113,113	2.06	18 (23%)
29	CLA	n1	611	-	49,57,73	1.57	7 (14%)	55,93,113	2.29	15 (27%)
29	CLA	C1	509	-	65,73,73	1.34	8 (12%)	76,113,113	2.07	17 (22%)
54	LPX	s1	625	-	29,29,29	1.01	2 (6%)	31,33,33	1.05	2 (6%)
54	LPX	S	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
50	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.77	16 (29%)
47	4RF	k1	101	-	56,56,56	1.04	3 (5%)	59,59,59	0.88	3 (5%)
29	CLA	N	602	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	21 (27%)
29	CLA	y	612	-	65,73,73	1.37	8 (12%)	76,113,113	1.99	16 (21%)
47	4RF	K1	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.84	3 (5%)
48	CHL	R1	607	-	50,58,74	0.94	2 (4%)	52,94,114	1.37	9 (17%)
29	CLA	s1	611	40	65,73,73	1.40	8 (12%)	76,113,113	2.00	18 (23%)
29	CLA	g	602	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	22 (28%)
49	LUT	r1	620	-	42,43,43	2.36	2 (4%)	51,60,60	2.32	15 (29%)
29	CLA	s1	617	-	50,58,73	1.51	8 (16%)	58,95,113	2.27	19 (32%)
49	LUT	G1	620	-	42,43,43	2.26	1 (2%)	51,60,60	1.86	13 (25%)
34	SPH	a1	414	-	19,20,20	0.73	1 (5%)	18,21,21	0.98	1 (5%)
29	CLA	S	617	23	50,58,73	1.52	8 (16%)	58,95,113	2.29	17 (29%)
48	CHL	N1	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.28	11 (15%)
40	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.08	2 (3%)
29	CLA	Y1	613	-	65,73,73	1.33	8 (12%)	76,113,113	2.12	17 (22%)
29	CLA	s1	603	-	65,73,73	1.37	8 (12%)	76,113,113	2.05	17 (22%)
29	CLA	y1	602	-	65,73,73	1.33	9 (13%)	76,113,113	2.03	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	CHL	G	606	-	50,58,74	1.08	3 (6%)	52,94,114	1.45	11 (21%)
48	CHL	r1	606	-	44,52,74	1.10	3 (6%)	46,87,114	1.12	4 (8%)
53	ERG	r	626	-	31,32,32	7.80	18 (58%)	47,50,50	3.01	16 (34%)
49	LUT	G	620	-	42,43,43	2.25	1 (2%)	51,60,60	1.99	17 (33%)
29	CLA	R	608	-	60,68,73	1.46	10 (16%)	70,107,113	2.07	16 (22%)
31	BCR	a	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	14 (25%)
48	CHL	g	605	21	48,56,74	0.98	3 (6%)	51,92,114	1.62	12 (23%)
29	CLA	g1	611	-	65,73,73	1.37	8 (12%)	76,113,113	1.88	16 (21%)
29	CLA	y1	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.07	17 (22%)
29	CLA	B1	609	-	65,73,73	1.38	8 (12%)	76,113,113	1.99	17 (22%)
40	LHG	g	624	-	48,48,48	0.39	0	51,54,54	0.97	2 (3%)
29	CLA	R	602	-	60,68,73	1.44	9 (15%)	70,107,113	1.99	19 (27%)
29	CLA	c1	502	-	65,73,73	1.43	8 (12%)	76,113,113	1.84	13 (17%)
29	CLA	C	509	-	65,73,73	1.36	8 (12%)	76,113,113	2.07	19 (25%)
33	LMG	B1	622	-	44,44,55	0.88	3 (6%)	52,52,63	1.08	4 (7%)
41	LMK	c	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.25	2 (4%)
29	CLA	C	513	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	17 (22%)
29	CLA	Y	614	-	65,73,73	1.38	10 (15%)	76,113,113	2.01	18 (23%)
29	CLA	b1	613	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	16 (21%)
48	CHL	n1	606	-	66,74,74	0.86	4 (6%)	73,114,114	1.23	11 (15%)
38	3PH	T	101	-	47,47,47	0.85	3 (6%)	51,52,52	1.19	2 (3%)
43	PL9	D	405	-	55,55,55	1.56	5 (9%)	68,69,69	1.47	12 (17%)
38	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
29	CLA	c1	504	-	65,73,73	1.38	8 (12%)	76,113,113	2.10	14 (18%)
29	CLA	g1	602	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	19 (25%)
29	CLA	C1	504	-	65,73,73	1.37	7 (10%)	76,113,113	2.02	17 (22%)
29	CLA	Y1	612	-	65,73,73	1.38	8 (12%)	76,113,113	1.96	18 (23%)
33	LMG	c1	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.10	3 (5%)
48	CHL	Y1	605	-	46,54,74	0.97	2 (4%)	49,90,114	1.40	7 (14%)
29	CLA	G	602	-	65,73,73	1.34	7 (10%)	76,113,113	2.10	21 (27%)
26	OEX	a1	401	1	0,15,15	-	-	-	-	-
50	XAT	g1	622	-	39,47,47	0.75	1 (2%)	54,74,74	1.88	16 (29%)
29	CLA	s	617	-	50,58,73	1.54	7 (14%)	58,95,113	2.35	18 (31%)
31	BCR	D1	404	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	16 (28%)
34	SPH	y	625	-	19,20,20	0.61	0	18,21,21	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	CHL	N1	601	-	66,74,74	0.87	3 (4%)	73,114,114	1.42	12 (16%)
29	CLA	g	604	-	49,57,73	1.57	9 (18%)	55,93,113	2.21	17 (30%)
29	CLA	b1	602	-	65,73,73	1.39	10 (15%)	76,113,113	1.93	18 (23%)
48	CHL	r	607	-	50,58,74	1.02	3 (6%)	52,94,114	1.45	9 (17%)
54	LPX	s	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
31	BCR	d1	404	-	41,41,41	1.88	4 (9%)	56,56,56	4.27	22 (39%)
29	CLA	B1	615	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	19 (25%)
29	CLA	b	610	-	65,73,73	1.32	7 (10%)	76,113,113	2.03	17 (22%)
40	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.10	2 (4%)
29	CLA	b	612	-	65,73,73	1.37	8 (12%)	76,113,113	2.10	17 (22%)
32	SQD	M1	101	-	41,42,54	0.90	0	50,53,65	0.97	2 (4%)
49	LUT	r	620	-	42,43,43	2.34	1 (2%)	51,60,60	2.12	14 (27%)
55	PTY	y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.12	3 (5%)
37	DGD	C1	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.07	6 (8%)
29	CLA	N	604	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	19 (25%)
29	CLA	n1	604	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	16 (21%)
29	CLA	B1	612	-	65,73,73	1.35	6 (9%)	76,113,113	2.12	21 (27%)
38	3PH	b1	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.15	2 (3%)
31	BCR	C1	516	-	41,41,41	1.89	4 (9%)	56,56,56	4.66	17 (30%)
29	CLA	A1	405	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	17 (22%)
30	PHO	A	408	-	51,69,69	1.01	4 (7%)	47,99,99	1.20	5 (10%)
30	PHO	A	409	-	51,69,69	1.02	4 (7%)	47,99,99	1.33	6 (12%)
48	CHL	S1	606	-	44,52,74	1.05	3 (6%)	46,87,114	1.46	8 (17%)
32	SQD	m	101	-	41,42,54	0.91	0	50,53,65	0.99	3 (6%)
29	CLA	b1	612	-	65,73,73	1.35	8 (12%)	76,113,113	2.17	19 (25%)
31	BCR	C1	515	-	41,41,41	1.93	4 (9%)	56,56,56	3.77	16 (28%)
48	CHL	s1	606	-	44,52,74	0.95	2 (4%)	46,87,114	1.40	8 (17%)
29	CLA	a1	406	-	65,73,73	1.36	8 (12%)	76,113,113	2.09	21 (27%)
55	PTY	Y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.02	2 (3%)
33	LMG	C	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	2 (3%)
29	CLA	s	610	-	65,73,73	1.42	9 (13%)	76,113,113	1.96	17 (22%)
32	SQD	A1	412	-	50,51,54	0.81	0	59,62,65	0.98	4 (6%)
29	CLA	s1	612	-	45,53,73	1.66	10 (22%)	52,89,113	2.01	11 (21%)
29	CLA	b1	603	-	65,73,73	1.38	7 (10%)	76,113,113	2.00	19 (25%)
48	CHL	S	601	23	46,54,74	1.21	5 (10%)	49,90,114	1.37	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PTY	y1	627	-	18,18,49	1.27	2 (11%)	21,23,54	1.45	2 (9%)
29	CLA	b	616	-	65,73,73	1.35	8 (12%)	76,113,113	1.87	15 (19%)
39	DGA	b	625	-	43,43,43	1.11	2 (4%)	45,45,45	1.45	3 (6%)
29	CLA	b1	607	-	65,73,73	1.38	8 (12%)	76,113,113	1.97	17 (22%)
31	BCR	B1	619	-	41,41,41	1.82	4 (9%)	56,56,56	4.44	18 (32%)
40	LHG	d	410	-	38,38,48	0.43	0	41,44,54	1.11	3 (7%)
29	CLA	S	614	-	55,63,73	1.48	7 (12%)	64,101,113	2.14	16 (25%)
48	CHL	G	607	-	66,74,74	0.88	2 (3%)	73,114,114	1.21	10 (13%)
29	CLA	s1	613	-	55,63,73	1.51	10 (18%)	64,101,113	2.12	17 (26%)
29	CLA	b	608	-	65,73,73	1.32	7 (10%)	76,113,113	2.02	17 (22%)
48	CHL	G	608	-	44,52,74	1.08	3 (6%)	46,87,114	1.41	7 (15%)
29	CLA	a1	407	-	49,57,73	1.55	7 (14%)	55,93,113	2.44	18 (32%)
48	CHL	g1	608	-	44,52,74	1.01	3 (6%)	46,87,114	1.40	6 (13%)
29	CLA	Y	604	-	65,73,73	1.33	6 (9%)	76,113,113	2.02	18 (23%)
29	CLA	N	614	-	49,57,73	1.57	7 (14%)	55,93,113	2.34	15 (27%)
29	CLA	C	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	18 (23%)
50	XAT	G1	622	-	39,47,47	0.76	1 (2%)	54,74,74	1.88	17 (31%)
48	CHL	S1	601	23	46,54,74	1.08	5 (10%)	49,90,114	1.41	9 (18%)
29	CLA	G1	603	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	17 (22%)
29	CLA	C1	510	-	65,73,73	1.35	9 (13%)	76,113,113	1.94	15 (19%)
48	CHL	y	605	24	46,54,74	0.99	2 (4%)	49,90,114	1.48	10 (20%)
29	CLA	B	602	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	15 (19%)
29	CLA	S1	605	-	50,58,73	1.57	9 (18%)	58,95,113	2.22	17 (29%)
48	CHL	G1	607	-	66,74,74	0.87	2 (3%)	73,114,114	1.16	8 (10%)
29	CLA	b1	605	-	65,73,73	1.30	7 (10%)	76,113,113	2.11	19 (25%)
29	CLA	c	510	-	65,73,73	1.37	7 (10%)	76,113,113	2.05	17 (22%)
29	CLA	B	605	-	65,73,73	1.40	8 (12%)	76,113,113	2.06	18 (23%)
37	DGD	C1	520	-	60,60,67	1.08	5 (8%)	74,74,81	0.95	2 (2%)
29	CLA	s	605	-	50,58,73	1.57	8 (16%)	58,95,113	2.30	16 (27%)
50	XAT	Y1	622	-	39,47,47	0.69	1 (2%)	54,74,74	3.83	20 (37%)
30	PHO	A1	409	-	51,69,69	0.99	3 (5%)	47,99,99	1.31	6 (12%)
29	CLA	B	614	-	65,73,73	1.32	8 (12%)	76,113,113	2.06	18 (23%)
51	NEX	g1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.91	15 (30%)
40	LHG	D1	409	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)
31	BCR	C	517	-	41,41,41	1.87	5 (12%)	56,56,56	4.32	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	r1	610	-	60,68,73	1.44	8 (13%)	70,107,113	1.96	16 (22%)
49	LUT	n1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.77	10 (19%)
29	CLA	c1	507	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	20 (26%)
29	CLA	S	612	-	45,53,73	1.62	8 (17%)	52,89,113	2.23	14 (26%)
29	CLA	s	612	-	45,53,73	1.60	8 (17%)	52,89,113	2.21	15 (28%)
38	3PH	t1	101	-	47,47,47	0.87	3 (6%)	51,52,52	1.05	2 (3%)
29	CLA	N	611	-	49,57,73	1.57	7 (14%)	55,93,113	2.24	15 (27%)
29	CLA	g1	614	-	49,57,73	1.61	10 (20%)	55,93,113	2.31	17 (30%)
48	CHL	r1	607	-	50,58,74	0.99	3 (6%)	52,94,114	1.64	12 (23%)
48	CHL	y	609	-	66,74,74	0.87	4 (6%)	73,114,114	1.24	10 (13%)
29	CLA	c1	509	-	65,73,73	1.37	8 (12%)	76,113,113	1.82	16 (21%)
48	CHL	G1	601	21	66,74,74	0.89	3 (4%)	73,114,114	1.33	13 (17%)
29	CLA	s	613	-	55,63,73	1.45	7 (12%)	64,101,113	2.25	18 (28%)
29	CLA	n1	610	-	65,73,73	1.35	6 (9%)	76,113,113	1.98	16 (21%)

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
48	CHL	N1	606	-	4/4/20/26	12/39/137/137	-
50	XAT	R1	621	-	-	4/31/93/93	0/4/4/4
29	CLA	B	609	-	1/1/15/20	12/37/115/115	-
49	LUT	N1	620	-	-	8/29/67/67	0/2/2/2
29	CLA	N	603	-	1/1/15/20	17/37/115/115	-
33	LMG	W	201	-	-	14/34/54/70	0/1/1/1
29	CLA	y1	611	40	1/1/15/20	19/37/115/115	-
29	CLA	B	603	-	1/1/15/20	21/37/115/115	-
29	CLA	c	512	-	1/1/15/20	18/37/115/115	-
33	LMG	B	622	-	-	20/39/59/70	0/1/1/1
29	CLA	Y	612	-	1/1/15/20	13/37/115/115	-
37	DGD	B1	623	-	-	11/32/72/95	0/2/2/2
49	LUT	G1	621	-	-	3/29/67/67	0/2/2/2
49	LUT	s1	620	-	-	6/29/67/67	0/2/2/2
49	LUT	S	620	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	b	623	-	-	13/32/72/95	0/2/2/2
29	CLA	Y	613	24	1/1/15/20	22/37/115/115	-
29	CLA	r	604	-	1/1/11/20	9/18/96/115	-
40	LHG	S1	624	29	-	32/49/49/53	-
29	CLA	n1	614	-	1/1/11/20	9/18/96/115	-
29	CLA	g1	612	21	1/1/10/20	4/11/89/115	-
30	PHO	a1	408	-	-	17/37/103/103	0/5/6/6
49	LUT	y	620	-	-	4/29/67/67	0/2/2/2
29	CLA	c1	513	-	1/1/15/20	23/37/115/115	-
29	CLA	A1	406	-	1/1/15/20	21/37/115/115	-
29	CLA	C1	513	-	1/1/15/20	16/37/115/115	-
29	CLA	a1	410	-	1/1/14/20	13/31/109/115	-
43	PL9	d	405	-	-	9/53/73/73	0/1/1/1
40	LHG	s	624	29	-	26/49/49/53	-
29	CLA	b	605	-	1/1/15/20	19/37/115/115	-
33	LMG	d	411	-	-	19/41/61/70	0/1/1/1
50	XAT	r1	621	-	1/1/12/26	2/31/93/93	0/4/4/4
48	CHL	y	606	-	4/4/20/26	12/39/137/137	-
29	CLA	R1	612	-	1/1/14/20	19/31/109/115	-
29	CLA	d	403	-	1/1/15/20	16/37/115/115	-
31	BCR	b	619	-	-	6/29/63/63	0/2/2/2
31	BCR	c1	515	-	-	11/29/63/63	0/2/2/2
44	HEM	F	101	7,6	-	1/12/54/54	-
29	CLA	r1	604	-	1/1/11/20	10/18/96/115	-
29	CLA	b1	614	-	1/1/15/20	10/37/115/115	-
31	BCR	C	515	-	-	9/29/63/63	0/2/2/2
49	LUT	S1	620	-	-	4/29/67/67	0/2/2/2
29	CLA	S	609	-	1/1/14/20	10/31/109/115	-
29	CLA	C1	502	-	1/1/15/20	12/37/115/115	-
45	RRX	h1	101	-	1/1/11/25	10/29/65/65	0/2/2/2
40	LHG	Y1	624	-	-	18/53/53/53	-
31	BCR	B1	618	-	-	15/29/63/63	0/2/2/2
39	DGA	J	101	-	-	12/30/30/45	-
51	NEX	y1	623	-	-	10/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LHG	d	408	-	-	26/48/48/53	-
29	CLA	b	615	-	1/1/15/20	19/37/115/115	-
29	CLA	g1	604	-	1/1/11/20	9/18/96/115	-
37	DGD	B	623	-	-	15/32/72/95	0/2/2/2
51	NEX	R1	622	-	-	14/27/83/83	0/3/3/3
29	CLA	y	602	24	1/1/15/20	15/37/115/115	-
36	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
29	CLA	C	512	-	1/1/15/20	15/37/115/115	-
29	CLA	s	604	-	1/1/13/20	11/25/103/115	-
29	CLA	Y1	614	-	1/1/15/20	14/37/115/115	-
49	LUT	G	621	-	1/1/12/27	4/29/67/67	0/2/2/2
37	DGD	c1	518	-	-	14/44/84/95	0/2/2/2
29	CLA	n	612	-	1/1/11/20	5/13/91/115	-
29	CLA	b	609	-	1/1/15/20	13/37/115/115	-
29	CLA	N1	603	-	1/1/15/20	15/37/115/115	-
29	CLA	Y1	610	-	1/1/15/20	12/37/115/115	-
48	CHL	s	608	-	4/4/19/26	5/33/131/137	-
48	CHL	g1	609	-	4/4/20/26	7/39/137/137	-
29	CLA	G	610	21	1/1/15/20	16/37/115/115	-
29	CLA	c1	501	-	1/1/15/20	17/37/115/115	-
33	LMG	b	622	-	-	17/39/59/70	0/1/1/1
40	LHG	g1	624	-	-	35/53/53/53	-
32	SQD	M	101	-	-	24/37/57/69	0/1/1/1
29	CLA	b	604	-	1/1/15/20	14/37/115/115	-
38	3PH	B1	624	-	-	27/49/49/49	-
29	CLA	c	509	-	1/1/15/20	16/37/115/115	-
51	NEX	N1	623	-	-	6/27/83/83	0/3/3/3
55	PTY	Y	627	-	-	15/20/20/53	-
29	CLA	S	611	40	1/1/15/20	16/37/115/115	-
49	LUT	N1	621	-	-	4/29/67/67	0/2/2/2
29	CLA	g	612	-	1/1/10/20	6/11/89/115	-
32	SQD	b	626	-	-	17/49/69/69	0/1/1/1
29	CLA	b1	615	-	1/1/15/20	17/37/115/115	-
39	DGA	b1	625	-	-	22/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LHG	c1	525	-	-	33/51/51/53	-
48	CHL	y1	606	-	4/4/20/26	6/39/137/137	-
29	CLA	N	610	-	1/1/15/20	19/37/115/115	-
40	LHG	G1	624	-	-	29/53/53/53	-
32	SQD	c1	526	-	-	22/49/69/69	0/1/1/1
32	SQD	C1	526	-	-	25/49/69/69	0/1/1/1
51	NEX	G	623	-	-	5/27/83/83	0/3/3/3
33	LMG	a1	413	-	-	20/43/63/70	0/1/1/1
29	CLA	c	504	-	1/1/15/20	18/37/115/115	-
48	CHL	S	608	-	4/4/19/26	7/33/131/137	-
48	CHL	G	605	21	4/4/16/26	6/18/116/137	-
48	CHL	N1	608	-	3/3/16/26	5/20/118/137	-
31	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
29	CLA	y1	613	-	1/1/15/20	18/37/115/115	-
37	DGD	c1	520	-	-	11/48/88/95	0/2/2/2
38	3PH	b	624	-	-	23/49/49/49	-
29	CLA	y1	612	-	1/1/15/20	17/37/115/115	-
29	CLA	G1	602	-	1/1/15/20	21/37/115/115	-
29	CLA	a1	405	-	1/1/15/20	17/37/115/115	-
29	CLA	s1	609	-	1/1/14/20	17/31/109/115	-
29	CLA	B	616	-	1/1/15/20	7/37/115/115	-
29	CLA	b	606	-	1/1/15/20	15/37/115/115	-
29	CLA	B	608	-	1/1/15/20	27/37/115/115	-
29	CLA	g1	613	-	1/1/15/20	22/37/115/115	-
48	CHL	N	605	20	4/4/20/26	9/39/137/137	-
29	CLA	Y	611	-	1/1/15/20	12/37/115/115	-
29	CLA	S1	617	23	1/1/12/20	7/19/97/115	-
29	CLA	b	603	-	1/1/15/20	21/37/115/115	-
47	4RF	I	102	-	-	30/59/59/59	-
49	LUT	Y1	620	-	-	8/29/67/67	0/2/2/2
29	CLA	c	506	-	1/1/15/20	17/37/115/115	-
29	CLA	R1	608	-	1/1/14/20	11/31/109/115	-
29	CLA	c	508	-	1/1/15/20	12/37/115/115	-
48	CHL	Y1	609	-	4/4/20/26	8/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	w	201	-	-	17/34/54/70	0/1/1/1
52	LMT	r1	625	-	-	10/21/61/61	0/2/2/2
31	BCR	D	404	-	-	13/29/63/63	0/2/2/2
48	CHL	G	609	21	4/4/20/26	10/39/137/137	-
37	DGD	b1	623	-	-	14/32/72/95	0/2/2/2
29	CLA	C	507	-	1/1/15/20	14/37/115/115	-
49	LUT	S1	621	-	-	7/29/67/67	0/2/2/2
29	CLA	C	504	-	1/1/15/20	16/37/115/115	-
33	LMG	C1	523	-	-	19/50/70/70	0/1/1/1
29	CLA	N1	602	-	1/1/15/20	17/37/115/115	-
29	CLA	R	612	-	1/1/14/20	10/31/109/115	-
29	CLA	b1	609	-	1/1/15/20	16/37/115/115	-
33	LMG	c	523	-	-	21/50/70/70	0/1/1/1
29	CLA	G	614	-	1/1/11/20	10/18/96/115	-
29	CLA	n1	612	-	1/1/11/20	5/13/91/115	-
53	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
29	CLA	y1	608	-	1/1/12/20	9/19/97/115	-
48	CHL	S	607	-	3/3/15/26	1/12/110/137	-
49	LUT	N	620	-	-	2/29/67/67	0/2/2/2
33	LMG	A	413	-	-	15/43/63/70	0/1/1/1
39	DGA	B1	625	-	-	26/45/45/45	-
40	LHG	D	409	-	-	25/53/53/53	-
33	LMG	c1	523	-	-	18/50/70/70	0/1/1/1
45	RRX	H	101	-	1/1/11/25	7/29/65/65	0/2/2/2
29	CLA	Y	608	-	1/1/12/20	7/19/97/115	-
29	CLA	s	614	-	1/1/13/20	4/25/103/115	-
31	BCR	c	516	-	-	15/29/63/63	0/2/2/2
29	CLA	A1	407	-	1/1/12/20	9/19/97/115	-
40	LHG	D	410	-	-	26/43/43/53	-
37	DGD	c	520	-	-	9/48/88/95	0/2/2/2
37	DGD	C	518	-	-	18/44/84/95	0/2/2/2
39	DGA	C	524	-	-	18/45/45/45	-
29	CLA	n	610	-	1/1/15/20	18/37/115/115	-
51	NEX	R	622	-	-	8/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	LUT	g	620	-	-	4/29/67/67	0/2/2/2
50	XAT	g	622	-	2/2/12/26	3/31/93/93	0/4/4/4
29	CLA	N1	612	-	1/1/11/20	4/13/91/115	-
29	CLA	C1	508	-	1/1/15/20	13/37/115/115	-
51	NEX	G1	623	-	-	12/27/83/83	0/3/3/3
29	CLA	C1	505	-	1/1/15/20	19/37/115/115	-
29	CLA	S1	611	40	1/1/15/20	16/37/115/115	-
48	CHL	n1	605	-	4/4/20/26	7/39/137/137	-
29	CLA	c1	512	-	1/1/15/20	17/37/115/115	-
48	CHL	S	606	-	3/3/15/26	2/13/111/137	-
29	CLA	R	603	-	1/1/14/20	16/31/109/115	-
43	PL9	d1	405	-	-	20/53/73/73	0/1/1/1
29	CLA	B1	604	-	1/1/15/20	14/37/115/115	-
29	CLA	B	611	-	1/1/15/20	13/37/115/115	-
29	CLA	C1	503	-	1/1/15/20	19/37/115/115	-
32	SQD	b1	626	-	-	26/49/69/69	0/1/1/1
29	CLA	y	611	40	1/1/15/20	16/37/115/115	-
29	CLA	Y1	608	-	1/1/12/20	7/19/97/115	-
29	CLA	g1	603	-	1/1/15/20	18/37/115/115	-
29	CLA	y	613	-	1/1/15/20	24/37/115/115	-
48	CHL	s1	601	23	3/3/16/26	4/15/113/137	-
29	CLA	s1	610	-	1/1/15/20	18/37/115/115	-
29	CLA	c	511	4	1/1/15/20	9/37/115/115	-
29	CLA	R1	610	-	1/1/14/20	17/31/109/115	-
47	4RF	i1	101	-	-	30/59/59/59	-
29	CLA	s	603	-	1/1/15/20	15/37/115/115	-
29	CLA	S	604	-	1/1/13/20	9/25/103/115	-
50	XAT	r	621	-	2/2/12/26	2/31/93/93	0/4/4/4
48	CHL	n1	609	-	4/4/20/26	5/39/137/137	-
29	CLA	S	602	-	1/1/14/20	16/31/109/115	-
48	CHL	Y1	607	-	4/4/20/26	11/39/137/137	-
29	CLA	g	614	-	1/1/11/20	11/18/96/115	-
29	CLA	C1	512	-	1/1/15/20	16/37/115/115	-
51	NEX	n1	623	-	-	5/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C	506	-	1/1/15/20	13/37/115/115	-
31	BCR	B	619	-	-	8/29/63/63	0/2/2/2
48	CHL	Y	605	24	3/3/16/26	3/15/113/137	-
48	CHL	G1	608	-	2/2/15/26	1/13/111/137	-
38	3PH	S	626	-	-	24/49/49/49	-
48	CHL	g1	606	-	3/3/16/26	3/20/118/137	-
55	PTY	Y1	627	-	-	12/20/20/53	-
37	DGD	C	520	-	-	14/48/88/95	0/2/2/2
29	CLA	S1	613	-	1/1/13/20	9/25/103/115	-
33	LMG	w1	201	-	-	17/34/54/70	0/1/1/1
49	LUT	R1	620	-	-	9/29/67/67	0/2/2/2
40	LHG	G	624	29	-	33/53/53/53	-
49	LUT	s	620	-	-	1/29/67/67	0/2/2/2
29	CLA	Y	610	-	1/1/15/20	12/37/115/115	-
29	CLA	c1	506	-	1/1/15/20	16/37/115/115	-
48	CHL	n	607	-	4/4/20/26	8/39/137/137	-
29	CLA	n	604	-	1/1/15/20	13/37/115/115	-
48	CHL	R1	606	-	3/3/15/26	4/13/111/137	-
29	CLA	C	503	-	1/1/15/20	18/37/115/115	-
48	CHL	s	606	-	3/3/15/26	2/13/111/137	-
29	CLA	S1	609	-	1/1/14/20	10/31/109/115	-
37	DGD	C1	519	-	-	22/51/91/95	0/2/2/2
29	CLA	S1	602	23	1/1/14/20	17/31/109/115	-
33	LMG	h1	102	-	-	22/43/63/70	0/1/1/1
29	CLA	A1	410	-	1/1/14/20	12/31/109/115	-
29	CLA	N1	604	-	1/1/15/20	18/37/115/115	-
51	NEX	r	622	-	-	9/27/83/83	0/3/3/3
33	LMG	C1	521	-	-	12/46/66/70	0/1/1/1
29	CLA	c	502	-	1/1/15/20	12/37/115/115	-
29	CLA	B1	602	-	1/1/15/20	24/37/115/115	-
29	CLA	S1	604	-	1/1/13/20	10/25/103/115	-
48	CHL	Y	609	-	4/4/20/26	6/39/137/137	-
48	CHL	g	607	-	4/4/20/26	10/39/137/137	-
48	CHL	Y1	606	-	4/4/20/26	7/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	XAT	G	622	-	1/1/12/26	2/31/93/93	0/4/4/4
48	CHL	s	601	-	3/3/16/26	4/15/113/137	-
29	CLA	C	511	-	1/1/15/20	14/37/115/115	-
32	SQD	B	626	-	-	23/49/69/69	0/1/1/1
55	PTY	y	627	-	-	15/20/20/53	-
37	DGD	c	518	-	-	9/44/84/95	0/2/2/2
33	LMG	H1	102	-	-	17/43/63/70	0/1/1/1
55	PTY	y1	626	-	-	33/53/53/53	-
48	CHL	R	606	-	3/3/15/26	1/13/111/137	-
48	CHL	n	601	20	4/4/20/26	4/39/137/137	-
34	SPH	A1	414	-	-	16/21/21/21	-
52	LMT	R	625	-	-	9/21/61/61	0/2/2/2
52	LMT	R1	625	-	-	10/21/61/61	0/2/2/2
29	CLA	s	609	-	1/1/14/20	16/31/109/115	-
31	BCR	b1	618	-	-	11/29/63/63	0/2/2/2
49	LUT	S	621	-	-	4/29/67/67	0/2/2/2
48	CHL	g1	605	-	4/4/16/26	7/18/116/137	-
29	CLA	C	510	-	1/1/15/20	13/37/115/115	-
29	CLA	S1	612	-	1/1/11/20	6/13/91/115	-
48	CHL	Y1	601	-	4/4/20/26	7/39/137/137	-
31	BCR	C	516	-	-	13/29/63/63	0/2/2/2
29	CLA	S	605	23	1/1/12/20	9/19/97/115	-
29	CLA	y1	603	-	1/1/15/20	18/37/115/115	-
41	LMK	C1	527	-	2/2/6/6	19/46/46/60	-
49	LUT	N	621	-	-	4/29/67/67	0/2/2/2
50	XAT	R	621	-	-	2/31/93/93	0/4/4/4
29	CLA	n1	602	20	1/1/15/20	17/37/115/115	-
38	3PH	S1	626	-	-	30/49/49/49	-
29	CLA	A	405	-	1/1/15/20	14/37/115/115	-
49	LUT	y1	620	-	-	3/29/67/67	0/2/2/2
29	CLA	y1	614	-	1/1/15/20	16/37/115/115	-
48	CHL	g	601	21	4/4/20/26	16/39/137/137	-
49	LUT	y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	n	603	-	1/1/15/20	23/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	3PH	T1	101	-	-	29/49/49/49	-
29	CLA	N1	614	-	1/1/11/20	7/18/96/115	-
49	LUT	Y1	621	-	-	6/29/67/67	0/2/2/2
29	CLA	B1	607	-	1/1/15/20	14/37/115/115	-
48	CHL	N	607	-	4/4/20/26	7/39/137/137	-
29	CLA	G1	611	-	1/1/15/20	19/37/115/115	-
29	CLA	G	603	-	1/1/15/20	14/37/115/115	-
29	CLA	y	610	24	1/1/15/20	13/37/115/115	-
40	LHG	s1	624	29	-	27/49/49/53	-
29	CLA	g	610	-	1/1/15/20	19/37/115/115	-
29	CLA	B1	617	-	1/1/15/20	16/37/115/115	-
29	CLA	c	507	-	1/1/15/20	15/37/115/115	-
49	LUT	g1	620	-	-	6/29/67/67	0/2/2/2
31	BCR	c	515	-	-	10/29/63/63	0/2/2/2
29	CLA	g	603	-	1/1/15/20	21/37/115/115	-
29	CLA	D1	403	-	1/1/15/20	17/37/115/115	-
29	CLA	b1	604	-	1/1/15/20	18/37/115/115	-
34	SPH	a	414	-	-	11/21/21/21	-
45	RRX	H1	101	-	1/1/11/25	9/29/65/65	0/2/2/2
32	SQD	c	526	-	-	20/49/69/69	0/1/1/1
48	CHL	s	607	-	3/3/15/26	0/12/110/137	-
33	LMG	A1	413	-	-	18/43/63/70	0/1/1/1
31	BCR	b1	619	-	-	9/29/63/63	0/2/2/2
47	4RF	K	101	-	-	32/59/59/59	-
29	CLA	n1	603	-	1/1/15/20	14/37/115/115	-
31	BCR	C	514	-	-	17/29/63/63	0/2/2/2
48	CHL	n	606	-	4/4/20/26	7/39/137/137	-
29	CLA	a	407	-	1/1/11/20	7/18/96/115	-
33	LMG	W1	201	-	-	16/34/54/70	0/1/1/1
40	LHG	d	409	-	-	26/53/53/53	-
39	DGA	C1	524	-	-	23/45/45/45	-
48	CHL	y1	607	-	4/4/20/26	4/39/137/137	-
30	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
29	CLA	R	610	-	1/1/14/20	14/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G1	604	-	1/1/11/20	8/18/96/115	-
29	CLA	s1	602	-	1/1/14/20	13/31/109/115	-
29	CLA	B1	606	-	1/1/15/20	18/37/115/115	-
48	CHL	Y	607	-	4/4/20/26	6/39/137/137	-
50	XAT	n1	622	-	-	4/31/93/93	0/4/4/4
29	CLA	A	406	-	1/1/15/20	14/37/115/115	-
29	CLA	c1	503	-	1/1/15/20	18/37/115/115	-
48	CHL	g	606	-	3/3/16/26	4/20/118/137	-
29	CLA	y	608	-	1/1/12/20	10/19/97/115	-
31	BCR	b	618	-	-	9/29/63/63	0/2/2/2
48	CHL	N	606	-	4/4/20/26	10/39/137/137	-
29	CLA	B1	603	-	1/1/15/20	21/37/115/115	-
49	LUT	Y	620	-	-	5/29/67/67	0/2/2/2
40	LHG	n1	624	-	-	29/53/53/53	-
36	C7Z	b	620	-	1/1/12/26	13/29/67/67	0/2/2/2
31	BCR	A1	411	-	-	9/29/63/63	0/2/2/2
29	CLA	G1	613	-	1/1/15/20	15/37/115/115	-
37	DGD	c	519	-	-	23/51/91/95	0/2/2/2
49	LUT	n	621	-	-	2/29/67/67	0/2/2/2
29	CLA	B	606	-	1/1/15/20	20/37/115/115	-
48	CHL	y1	601	24	4/4/20/26	5/39/137/137	-
29	CLA	y1	610	24	1/1/15/20	13/37/115/115	-
32	SQD	C	526	-	-	23/49/69/69	0/1/1/1
29	CLA	N	613	-	1/1/15/20	17/37/115/115	-
29	CLA	G1	612	-	1/1/10/20	7/11/89/115	-
33	LMG	c	521	-	-	14/46/66/70	0/1/1/1
48	CHL	n1	607	-	4/4/20/26	7/39/137/137	-
29	CLA	R1	609	-	1/1/14/20	14/31/109/115	-
48	CHL	s1	607	-	3/3/15/26	0/12/110/137	-
33	LMG	H	102	-	-	14/43/63/70	0/1/1/1
40	LHG	D1	408	-	-	26/48/48/53	-
40	LHG	D1	410	-	-	25/43/43/53	-
46	GOL	I	101	-	-	2/4/4/4	-
29	CLA	B1	611	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DGA	j1	101	-	-	20/30/30/45	-
49	LUT	s1	621	-	-	5/29/67/67	0/2/2/2
29	CLA	B1	613	-	1/1/15/20	19/37/115/115	-
29	CLA	b1	611	-	1/1/15/20	10/37/115/115	-
29	CLA	c1	510	-	1/1/15/20	12/37/115/115	-
53	ERG	R	626	-	5/5/11/15	6/13/71/71	0/4/4/4
29	CLA	S1	614	-	1/1/13/20	8/25/103/115	-
38	3PH	t	101	-	-	27/49/49/49	-
29	CLA	r	610	-	1/1/14/20	11/31/109/115	-
29	CLA	D	403	-	1/1/15/20	16/37/115/115	-
29	CLA	Y1	602	-	1/1/15/20	20/37/115/115	-
48	CHL	n1	601	-	4/4/20/26	11/39/137/137	-
34	SPH	Y1	625	-	-	9/21/21/21	-
40	LHG	y	624	29	-	30/53/53/53	-
49	LUT	n	620	-	-	3/29/67/67	0/2/2/2
50	XAT	n	622	-	1/1/12/26	4/31/93/93	0/4/4/4
40	LHG	l	101	-	-	38/53/53/53	-
29	CLA	r1	608	-	1/1/14/20	16/31/109/115	-
29	CLA	s	611	40	1/1/15/20	15/37/115/115	-
31	BCR	c1	517	-	-	9/29/63/63	0/2/2/2
29	CLA	d1	403	-	1/1/15/20	12/37/115/115	-
29	CLA	B1	608	-	1/1/15/20	26/37/115/115	-
40	LHG	c	525	-	-	30/51/51/53	-
36	C7Z	b1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
29	CLA	b1	616	-	1/1/15/20	9/37/115/115	-
29	CLA	r1	602	-	1/1/14/20	11/31/109/115	-
33	LMG	b1	622	-	-	19/39/59/70	0/1/1/1
31	BCR	d	404	-	-	13/29/63/63	0/2/2/2
33	LMG	d1	411	-	-	19/41/61/70	0/1/1/1
29	CLA	c	505	-	1/1/15/20	19/37/115/115	-
51	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
51	NEX	S	623	-	-	8/27/83/83	0/3/3/3
29	CLA	b1	608	-	1/1/15/20	25/37/115/115	-
32	SQD	m1	101	-	-	22/37/57/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	N1	611	-	1/1/11/20	10/18/96/115	-
50	XAT	y	622	-	-	8/31/93/93	0/4/4/4
29	CLA	N1	613	-	1/1/15/20	14/37/115/115	-
49	LUT	g1	621	-	-	6/29/67/67	0/2/2/2
29	CLA	C1	506	-	1/1/15/20	19/37/115/115	-
29	CLA	R1	603	-	1/1/14/20	17/31/109/115	-
50	XAT	N	622	-	1/1/12/26	2/31/93/93	0/4/4/4
29	CLA	d1	402	-	1/1/15/20	10/37/115/115	-
41	LMK	c1	527	-	2/2/6/6	14/46/46/60	-
39	DGA	c	524	-	-	31/45/45/45	-
29	CLA	R1	604	-	1/1/11/20	10/18/96/115	-
29	CLA	Y1	603	-	1/1/15/20	14/37/115/115	-
29	CLA	b	613	-	1/1/15/20	19/37/115/115	-
29	CLA	n	613	-	1/1/15/20	18/37/115/115	-
29	CLA	G	613	-	1/1/15/20	19/37/115/115	-
29	CLA	r	608	-	1/1/14/20	17/31/109/115	-
48	CHL	Y	601	24	4/4/20/26	7/39/137/137	-
29	CLA	a	406	-	1/1/15/20	17/37/115/115	-
44	HEM	f	101	7,6	-	1/12/54/54	-
47	4RF	i	101	-	-	31/59/59/59	-
48	CHL	s1	608	-	4/4/19/26	5/33/131/137	-
45	RRX	h	101	-	1/1/11/25	4/29/65/65	0/2/2/2
40	LHG	d1	408	-	-	30/48/48/53	-
40	LHG	L	101	-	-	38/53/53/53	-
29	CLA	G	612	-	1/1/10/20	5/11/89/115	-
29	CLA	a	410	-	1/1/14/20	15/31/109/115	-
29	CLA	r1	612	-	1/1/14/20	16/31/109/115	-
29	CLA	n	614	-	1/1/11/20	4/18/96/115	-
48	CHL	g1	607	-	4/4/20/26	7/39/137/137	-
40	LHG	N	624	-	-	31/53/53/53	-
50	XAT	y1	622	-	-	7/31/93/93	0/4/4/4
49	LUT	s	621	-	-	3/29/67/67	0/2/2/2
33	LMG	a	413	-	-	20/43/63/70	0/1/1/1
29	CLA	b	602	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s1	605	-	1/1/12/20	9/19/97/115	-
51	NEX	Y	623	-	-	7/27/83/83	0/3/3/3
49	LUT	Y	621	-	-	4/29/67/67	0/2/2/2
29	CLA	r1	603	-	1/1/14/20	20/31/109/115	-
29	CLA	g	613	-	1/1/15/20	19/37/115/115	-
39	DGA	j	101	-	-	20/30/30/45	-
51	NEX	S1	623	-	-	4/27/83/83	0/3/3/3
40	LHG	C	525	-	-	32/51/51/53	-
44	HEM	f1	101	7	-	2/12/54/54	-
40	LHG	y1	624	29	-	25/53/53/53	-
40	LHG	L1	101	-	-	36/53/53/53	-
48	CHL	N1	605	20	4/4/20/26	9/39/137/137	-
43	PL9	D1	405	-	-	18/53/73/73	0/1/1/1
47	4RF	k	101	-	-	31/59/59/59	-
29	CLA	n	611	-	1/1/11/20	8/18/96/115	-
29	CLA	y	604	-	1/1/15/20	15/37/115/115	-
29	CLA	r	612	-	1/1/14/20	14/31/109/115	-
48	CHL	R	607	-	3/3/16/26	7/20/118/137	-
48	CHL	S1	608	-	4/4/19/26	10/33/131/137	-
29	CLA	C	505	-	1/1/15/20	16/37/115/115	-
29	CLA	C1	501	-	1/1/15/20	15/37/115/115	-
51	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3
29	CLA	r	603	-	1/1/14/20	17/31/109/115	-
30	PHO	a	408	-	-	12/37/103/103	0/5/6/6
29	CLA	g	611	-	1/1/15/20	15/37/115/115	-
29	CLA	B1	610	-	1/1/15/20	23/37/115/115	-
34	SPH	y1	625	-	-	12/21/21/21	-
29	CLA	s	602	-	1/1/14/20	16/31/109/115	-
29	CLA	B	610	-	1/1/15/20	21/37/115/115	-
48	CHL	N1	609	-	4/4/20/26	10/39/137/137	-
31	BCR	C1	517	-	-	11/29/63/63	0/2/2/2
54	LPX	S1	625	-	-	15/31/31/31	-
44	HEM	F1	101	7	-	1/12/54/54	-
29	CLA	B	615	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	617	-	1/1/15/20	13/37/115/115	-
48	CHL	N	609	-	4/4/20/26	11/39/137/137	-
32	SQD	B1	626	-	-	17/49/69/69	0/1/1/1
37	DGD	c1	519	-	-	24/51/91/95	0/2/2/2
29	CLA	C1	507	-	1/1/15/20	14/37/115/115	-
29	CLA	b1	606	-	1/1/15/20	13/37/115/115	-
33	LMG	D	411	-	-	11/41/61/70	0/1/1/1
37	DGD	C	519	-	-	26/51/91/95	0/2/2/2
51	NEX	n	623	-	-	5/27/83/83	1/3/3/3
51	NEX	N	623	-	-	4/27/83/83	1/3/3/3
48	CHL	n	605	20	4/4/20/26	8/39/137/137	-
29	CLA	y	614	-	1/1/15/20	15/37/115/115	-
48	CHL	G1	606	-	3/3/16/26	4/20/118/137	-
47	4RF	I1	102	-	-	24/59/59/59	-
49	LUT	R	620	-	1/1/12/27	2/29/67/67	0/2/2/2
29	CLA	Y1	611	-	1/1/15/20	16/37/115/115	-
29	CLA	c1	511	-	1/1/15/20	18/37/115/115	-
48	CHL	y	607	-	4/4/20/26	9/39/137/137	-
29	CLA	C1	511	-	1/1/15/20	10/37/115/115	-
29	CLA	B	617	-	1/1/15/20	17/37/115/115	-
31	BCR	c1	514	-	-	12/29/63/63	0/2/2/2
29	CLA	Y	602	-	1/1/15/20	18/37/115/115	-
32	SQD	A	412	-	-	24/46/66/69	0/1/1/1
38	3PH	s	626	-	-	22/49/49/49	-
31	BCR	C1	514	-	-	12/29/63/63	0/2/2/2
38	3PH	s1	626	-	-	27/49/49/49	-
29	CLA	D	402	-	1/1/15/20	19/37/115/115	-
40	LHG	d1	410	-	-	33/43/43/53	-
36	C7Z	B1	620	-	1/1/12/26	7/29/67/67	0/2/2/2
29	CLA	y	603	-	1/1/15/20	18/37/115/115	-
51	NEX	g	623	-	1/1/12/25	9/27/83/83	0/3/3/3
31	BCR	c	514	-	-	14/29/63/63	0/2/2/2
29	CLA	A	407	-	1/1/12/20	9/19/97/115	-
32	SQD	B	621	-	-	20/37/57/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	R1	602	-	1/1/14/20	12/31/109/115	-
29	CLA	N1	610	-	1/1/15/20	21/37/115/115	-
34	SPH	A	414	-	-	12/21/21/21	-
51	NEX	y	623	-	-	6/27/83/83	0/3/3/3
29	CLA	S1	610	-	1/1/15/20	22/37/115/115	-
39	DGA	c1	524	-	-	28/45/45/45	-
29	CLA	G1	614	-	1/1/11/20	8/18/96/115	-
30	PHO	a1	409	-	-	12/37/103/103	0/5/6/6
48	CHL	Y	606	-	4/4/20/26	7/39/137/137	-
29	CLA	c	503	-	1/1/15/20	20/37/115/115	-
48	CHL	n	609	-	4/4/20/26	5/39/137/137	-
29	CLA	S	610	-	1/1/15/20	20/37/115/115	-
29	CLA	G	611	40	1/1/15/20	17/37/115/115	-
49	LUT	y1	621	-	-	4/29/67/67	0/2/2/2
48	CHL	y	601	24	4/4/20/26	9/39/137/137	-
49	LUT	g	621	-	-	4/29/67/67	0/2/2/2
29	CLA	R	609	-	1/1/14/20	13/31/109/115	-
48	CHL	g1	601	-	4/4/20/26	12/39/137/137	-
29	CLA	c	513	-	1/1/15/20	23/37/115/115	-
29	CLA	B	604	-	1/1/15/20	16/37/115/115	-
29	CLA	b	607	-	1/1/15/20	16/37/115/115	-
32	SQD	a	412	-	-	14/46/66/69	0/1/1/1
29	CLA	s1	604	-	1/1/13/20	8/25/103/115	-
33	LMG	C	521	-	-	16/46/66/70	0/1/1/1
40	LHG	S	624	29	-	27/49/49/53	-
48	CHL	n	608	-	3/3/16/26	6/20/118/137	-
29	CLA	Y	603	-	1/1/15/20	17/37/115/115	-
48	CHL	G	601	21	4/4/20/26	11/39/137/137	-
29	CLA	A	410	-	1/1/14/20	14/31/109/115	-
48	CHL	y1	605	24	3/3/16/26	4/15/113/137	-
29	CLA	S1	603	-	1/1/15/20	12/37/115/115	-
40	LHG	C1	525	-	-	30/51/51/53	-
29	CLA	C	502	-	1/1/15/20	13/37/115/115	-
48	CHL	G1	605	21	4/4/16/26	4/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	h	102	-	-	11/43/63/70	0/1/1/1
32	SQD	B1	621	-	-	11/37/57/69	0/1/1/1
48	CHL	g	609	-	4/4/20/26	10/39/137/137	-
29	CLA	S	613	-	1/1/13/20	12/25/103/115	-
29	CLA	b1	617	-	1/1/15/20	14/37/115/115	-
29	CLA	n1	613	-	1/1/15/20	20/37/115/115	-
31	BCR	a1	411	-	-	6/29/63/63	0/2/2/2
32	SQD	b	621	-	-	19/37/57/69	0/1/1/1
29	CLA	B1	614	-	1/1/15/20	14/37/115/115	-
48	CHL	r	606	-	3/3/15/26	3/13/111/137	-
48	CHL	g	608	-	3/3/15/26	3/13/111/137	-
32	SQD	b1	621	-	-	17/37/57/69	0/1/1/1
52	LMT	r	625	-	-	13/21/61/61	0/2/2/2
29	CLA	c1	505	-	1/1/15/20	16/37/115/115	-
31	BCR	A	411	-	-	12/29/63/63	0/2/2/2
29	CLA	a	405	-	1/1/15/20	15/37/115/115	-
29	CLA	B1	616	-	1/1/15/20	18/37/115/115	-
31	BCR	B	618	-	-	11/29/63/63	0/2/2/2
29	CLA	b	611	-	1/1/15/20	7/37/115/115	-
51	NEX	s	623	-	-	4/27/83/83	0/3/3/3
29	CLA	r	609	-	1/1/14/20	12/31/109/115	-
48	CHL	N	608	-	3/3/16/26	3/20/118/137	-
48	CHL	n1	608	-	3/3/16/26	8/20/118/137	-
53	ERG	R1	626	-	5/5/11/15	9/13/71/71	0/4/4/4
40	LHG	d1	409	-	-	30/53/53/53	-
29	CLA	g1	610	-	1/1/15/20	18/37/115/115	-
29	CLA	r	602	22	1/1/14/20	14/31/109/115	-
29	CLA	c	501	-	1/1/15/20	19/37/115/115	-
48	CHL	y1	609	-	4/4/20/26	8/39/137/137	-
29	CLA	d	402	-	1/1/15/20	13/37/115/115	-
33	LMG	D1	411	-	-	10/41/61/70	0/1/1/1
40	LHG	N1	624	-	-	34/53/53/53	-
29	CLA	B	607	-	1/1/15/20	18/37/115/115	-
29	CLA	s1	614	-	1/1/13/20	15/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c1	508	-	1/1/15/20	12/37/115/115	-
48	CHL	G1	609	-	4/4/20/26	10/39/137/137	-
40	LHG	Y	624	-	-	29/53/53/53	-
29	CLA	C	508	-	1/1/15/20	12/37/115/115	-
29	CLA	b	614	-	1/1/15/20	13/37/115/115	-
39	DGA	B	625	-	-	23/45/45/45	-
55	PTY	Y1	626	-	-	26/53/53/53	-
49	LUT	n1	621	-	1/1/12/27	5/29/67/67	0/2/2/2
29	CLA	b1	610	-	1/1/15/20	19/37/115/115	-
48	CHL	S1	607	-	3/3/15/26	1/12/110/137	-
29	CLA	D1	402	-	1/1/15/20	13/37/115/115	-
29	CLA	r1	609	-	1/1/14/20	17/31/109/115	-
41	LMK	C	527	-	2/2/6/6	21/46/46/60	-
29	CLA	G1	610	-	1/1/15/20	15/37/115/115	-
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
29	CLA	n	602	-	1/1/15/20	14/37/115/115	-
29	CLA	R	604	-	1/1/11/20	10/18/96/115	-
48	CHL	N	601	20	4/4/20/26	5/39/137/137	-
39	DGA	J1	101	-	-	15/30/30/45	-
29	CLA	B	613	-	1/1/15/20	18/37/115/115	-
51	NEX	r1	622	-	-	8/27/83/83	0/3/3/3
29	CLA	Y1	604	-	1/1/15/20	13/37/115/115	-
34	SPH	Y	625	-	-	10/21/21/21	-
29	CLA	G	604	-	1/1/11/20	8/18/96/115	-
29	CLA	N	612	-	1/1/11/20	4/13/91/115	-
32	SQD	a1	412	-	-	19/46/66/69	0/1/1/1
29	CLA	B	612	-	1/1/15/20	16/37/115/115	-
30	PHO	a	409	-	-	11/37/103/103	0/5/6/6
50	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
46	GOL	I1	101	-	-	2/4/4/4	-
29	CLA	S	603	-	1/1/15/20	17/37/115/115	-
29	CLA	B1	605	-	1/1/15/20	15/37/115/115	-
29	CLA	n1	611	-	1/1/11/20	9/18/96/115	-
29	CLA	C1	509	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	LPX	s1	625	-	-	18/31/31/31	-
54	LPX	S	625	-	-	14/31/31/31	-
50	XAT	Y	622	-	-	7/31/93/93	0/4/4/4
47	4RF	k1	101	-	-	37/59/59/59	-
29	CLA	N	602	-	1/1/15/20	15/37/115/115	-
29	CLA	y	612	-	1/1/15/20	17/37/115/115	-
48	CHL	R1	607	-	3/3/16/26	4/20/118/137	-
47	4RF	K1	101	-	-	32/59/59/59	-
29	CLA	s1	611	40	1/1/15/20	20/37/115/115	-
29	CLA	g	602	-	1/1/15/20	22/37/115/115	-
49	LUT	r1	620	-	-	4/29/67/67	0/2/2/2
29	CLA	s1	617	-	1/1/12/20	11/19/97/115	-
49	LUT	G1	620	-	-	5/29/67/67	0/2/2/2
34	SPH	a1	414	-	-	10/21/21/21	-
29	CLA	S	617	23	1/1/12/20	7/19/97/115	-
48	CHL	N1	607	-	4/4/20/26	10/39/137/137	-
40	LHG	n	624	-	-	35/53/53/53	-
29	CLA	Y1	613	-	1/1/15/20	19/37/115/115	-
29	CLA	s1	603	-	1/1/15/20	15/37/115/115	-
29	CLA	y1	602	-	1/1/15/20	15/37/115/115	-
48	CHL	G	606	-	3/3/16/26	5/20/118/137	-
48	CHL	r1	606	-	3/3/15/26	4/13/111/137	-
53	ERG	r	626	-	5/5/11/15	8/13/71/71	0/4/4/4
49	LUT	G	620	-	-	3/29/67/67	0/2/2/2
29	CLA	R	608	-	1/1/14/20	19/31/109/115	-
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
48	CHL	g	605	21	4/4/16/26	5/18/116/137	-
29	CLA	g1	611	-	1/1/15/20	18/37/115/115	-
29	CLA	y1	604	-	1/1/15/20	13/37/115/115	-
29	CLA	B1	609	-	1/1/15/20	15/37/115/115	-
40	LHG	g	624	-	-	27/53/53/53	-
29	CLA	R	602	-	1/1/14/20	11/31/109/115	-
29	CLA	c1	502	-	1/1/15/20	16/37/115/115	-
29	CLA	C	509	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	B1	622	-	-	19/39/59/70	0/1/1/1
41	LMK	c	527	-	2/2/6/6	13/46/46/60	-
29	CLA	C	513	-	1/1/15/20	20/37/115/115	-
29	CLA	Y	614	-	1/1/15/20	17/37/115/115	-
29	CLA	b1	613	-	1/1/15/20	16/37/115/115	-
48	CHL	n1	606	-	4/4/20/26	7/39/137/137	-
38	3PH	T	101	-	-	26/49/49/49	-
43	PL9	D	405	-	-	9/53/73/73	0/1/1/1
38	3PH	B	624	-	-	34/49/49/49	-
29	CLA	c1	504	-	1/1/15/20	19/37/115/115	-
29	CLA	g1	602	-	1/1/15/20	19/37/115/115	-
29	CLA	C1	504	-	1/1/15/20	18/37/115/115	-
29	CLA	Y1	612	-	1/1/15/20	18/37/115/115	-
33	LMG	c1	521	-	-	14/46/66/70	0/1/1/1
48	CHL	Y1	605	-	3/3/16/26	3/15/113/137	-
29	CLA	G	602	-	1/1/15/20	17/37/115/115	-
50	XAT	g1	622	-	1/1/12/26	7/31/93/93	0/4/4/4
29	CLA	s	617	-	1/1/12/20	8/19/97/115	-
48	CHL	N1	601	-	4/4/20/26	9/39/137/137	-
31	BCR	D1	404	-	-	14/29/63/63	0/2/2/2
34	SPH	y	625	-	-	8/21/21/21	-
29	CLA	g	604	-	1/1/11/20	7/18/96/115	-
29	CLA	b1	602	-	1/1/15/20	22/37/115/115	-
48	CHL	r	607	-	3/3/16/26	4/20/118/137	-
54	LPX	s	625	-	-	15/31/31/31	-
31	BCR	d1	404	-	-	12/29/63/63	0/2/2/2
29	CLA	B1	615	-	1/1/15/20	14/37/115/115	-
29	CLA	b	610	-	1/1/15/20	15/37/115/115	-
40	LHG	D	408	-	-	23/48/48/53	-
29	CLA	b	612	-	1/1/15/20	16/37/115/115	-
32	SQD	M1	101	-	-	17/37/57/69	0/1/1/1
49	LUT	r	620	-	-	6/29/67/67	0/2/2/2
55	PTY	y	626	-	-	27/53/53/53	-
37	DGD	C1	518	-	-	12/44/84/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	N	604	-	1/1/15/20	19/37/115/115	-
29	CLA	n1	604	-	1/1/15/20	14/37/115/115	-
29	CLA	B1	612	-	1/1/15/20	15/37/115/115	-
38	3PH	b1	624	-	-	24/49/49/49	-
31	BCR	C1	516	-	-	15/29/63/63	0/2/2/2
29	CLA	A1	405	-	1/1/15/20	12/37/115/115	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
30	PHO	A	409	-	-	14/37/103/103	0/5/6/6
48	CHL	S1	606	-	3/3/15/26	2/13/111/137	-
32	SQD	m	101	-	-	20/37/57/69	0/1/1/1
29	CLA	b1	612	-	1/1/15/20	18/37/115/115	-
48	CHL	s1	606	-	3/3/15/26	0/13/111/137	-
31	BCR	C1	515	-	-	12/29/63/63	0/2/2/2
29	CLA	a1	406	-	1/1/15/20	16/37/115/115	-
55	PTY	Y	626	-	-	31/53/53/53	-
33	LMG	C	523	-	-	21/50/70/70	0/1/1/1
29	CLA	s	610	-	1/1/15/20	18/37/115/115	-
32	SQD	A1	412	-	-	15/46/66/69	0/1/1/1
29	CLA	s1	612	-	1/1/11/20	6/13/91/115	-
29	CLA	b1	603	-	1/1/15/20	19/37/115/115	-
48	CHL	S	601	23	3/3/16/26	3/15/113/137	-
55	PTY	y1	627	-	-	11/20/20/53	-
29	CLA	b	616	-	1/1/15/20	15/37/115/115	-
39	DGA	b	625	-	-	26/45/45/45	-
29	CLA	b1	607	-	1/1/15/20	12/37/115/115	-
31	BCR	B1	619	-	-	6/29/63/63	0/2/2/2
40	LHG	d	410	-	-	20/43/43/53	-
29	CLA	S	614	-	1/1/13/20	8/25/103/115	-
48	CHL	G	607	-	4/4/20/26	11/39/137/137	-
29	CLA	s1	613	-	1/1/13/20	11/25/103/115	-
29	CLA	b	608	-	1/1/15/20	28/37/115/115	-
48	CHL	G	608	-	3/3/15/26	1/13/111/137	-
29	CLA	a1	407	-	1/1/11/20	7/18/96/115	-
48	CHL	g1	608	-	3/3/15/26	1/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	Y	604	-	1/1/15/20	17/37/115/115	-
29	CLA	N	614	-	1/1/11/20	5/18/96/115	-
29	CLA	C	501	-	1/1/15/20	18/37/115/115	-
50	XAT	G1	622	-	1/1/12/26	2/31/93/93	0/4/4/4
48	CHL	S1	601	23	3/3/16/26	3/15/113/137	-
29	CLA	G1	603	-	1/1/15/20	23/37/115/115	-
29	CLA	C1	510	-	1/1/15/20	17/37/115/115	-
48	CHL	y	605	24	3/3/16/26	3/15/113/137	-
29	CLA	B	602	-	1/1/15/20	20/37/115/115	-
29	CLA	S1	605	-	1/1/12/20	8/19/97/115	-
48	CHL	G1	607	-	4/4/20/26	11/39/137/137	-
29	CLA	b1	605	-	1/1/15/20	18/37/115/115	-
29	CLA	c	510	-	1/1/15/20	14/37/115/115	-
29	CLA	B	605	-	1/1/15/20	19/37/115/115	-
50	XAT	Y1	622	-	1/1/12/26	4/31/93/93	0/4/4/4
29	CLA	s	605	-	1/1/12/20	11/19/97/115	-
37	DGD	C1	520	-	-	16/48/88/95	0/2/2/2
30	PHO	A1	409	-	-	11/37/103/103	0/5/6/6
29	CLA	B	614	-	1/1/15/20	14/37/115/115	-
51	NEX	g1	623	-	1/1/12/25	7/27/83/83	0/3/3/3
40	LHG	D1	409	-	-	31/53/53/53	-
31	BCR	C	517	-	-	13/29/63/63	0/2/2/2
29	CLA	r1	610	-	1/1/14/20	13/31/109/115	-
49	LUT	n1	620	-	-	5/29/67/67	0/2/2/2
29	CLA	c1	507	-	1/1/15/20	16/37/115/115	-
29	CLA	S	612	-	1/1/11/20	6/13/91/115	-
29	CLA	s	612	-	1/1/11/20	5/13/91/115	-
38	3PH	t1	101	-	-	30/49/49/49	-
29	CLA	N	611	-	1/1/11/20	7/18/96/115	-
29	CLA	g1	614	-	1/1/11/20	11/18/96/115	-
48	CHL	r1	607	-	3/3/16/26	4/20/118/137	-
48	CHL	y	609	-	4/4/20/26	6/39/137/137	-
29	CLA	c1	509	-	1/1/15/20	20/37/115/115	-
48	CHL	G1	601	21	4/4/20/26	13/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s	613	-	1/1/13/20	9/25/103/115	-
29	CLA	n1	610	-	1/1/15/20	20/37/115/115	-

The worst 5 of 3829 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	R	626	ERG	C1-C10	-23.16	1.10	1.54
53	r	626	ERG	C1-C10	-22.96	1.10	1.54
53	R1	626	ERG	C1-C10	-22.89	1.10	1.54
53	r1	626	ERG	C1-C10	-22.73	1.11	1.54
53	r	626	ERG	C10-C9	-20.15	1.28	1.55

The worst 5 of 8657 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L	101	LHG	O7-C7-C8	22.97	161.00	111.50
40	l	101	LHG	O7-C7-C8	22.96	160.99	111.50
29	R	609	CLA	C4-C3-C5	-22.39	77.60	115.27
38	S	626	3PH	O21-C21-C22	22.18	159.31	111.50
38	S1	626	3PH	O21-C21-C22	22.13	159.19	111.50

5 of 696 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	405	CLA	ND
29	A	406	CLA	ND
29	A	407	CLA	ND
29	A	410	CLA	ND
29	B	602	CLA	ND

5 of 9527 torsion outliers are listed below:

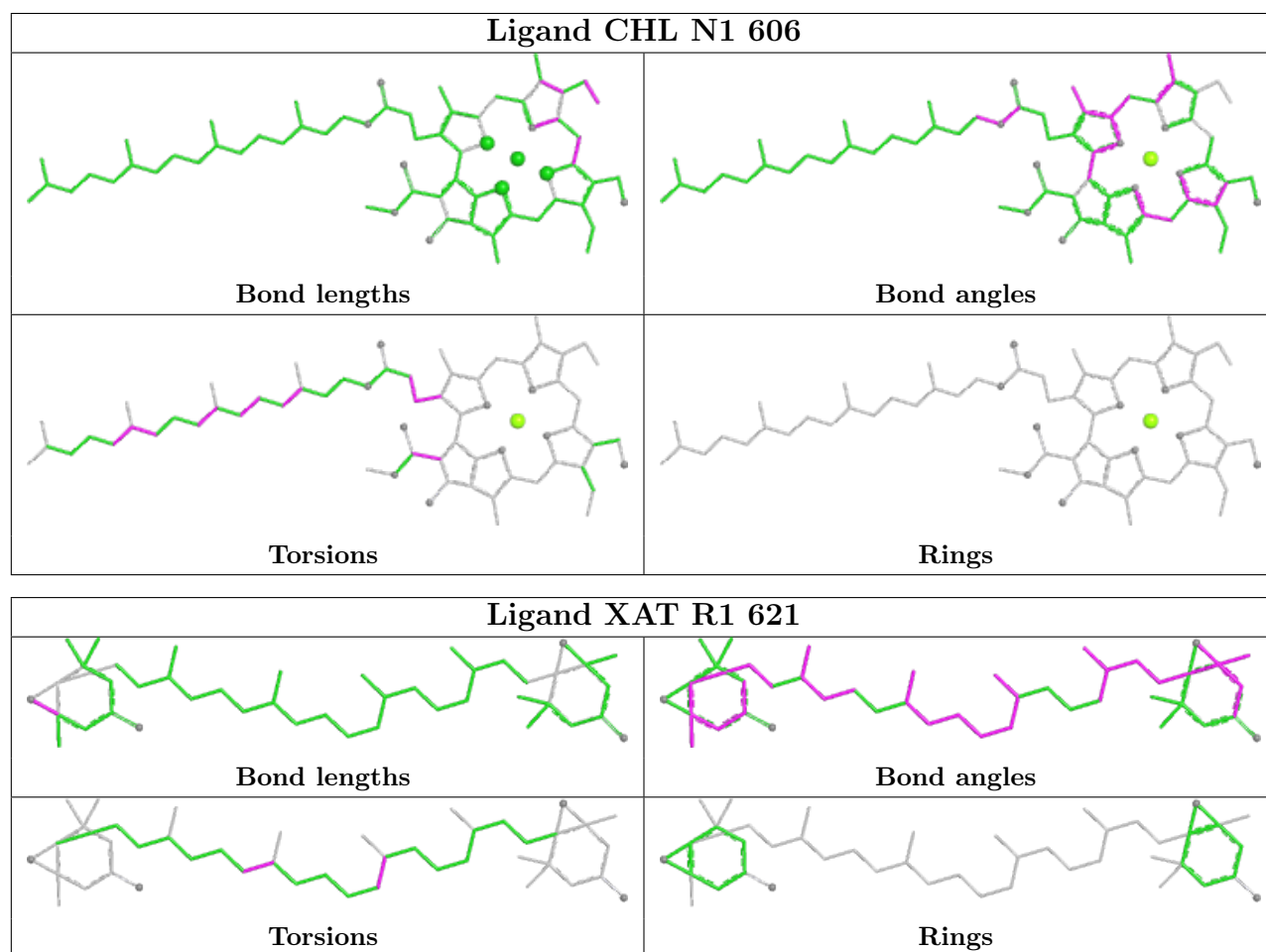
Mol	Chain	Res	Type	Atoms
29	A	405	CLA	O2A-C1-C2-C3
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA
29	A	407	CLA	C2-C1-O2A-CGA

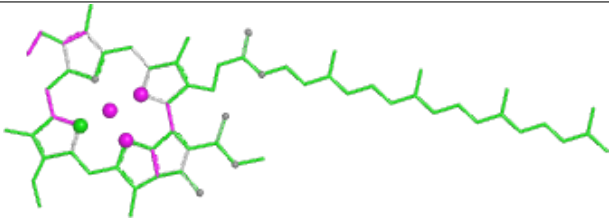
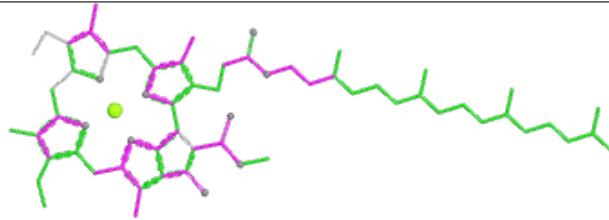
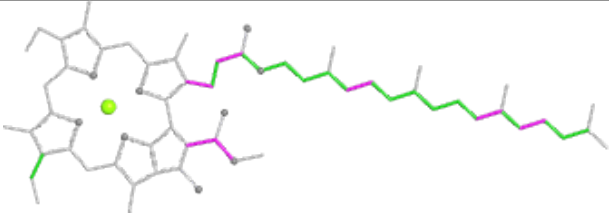
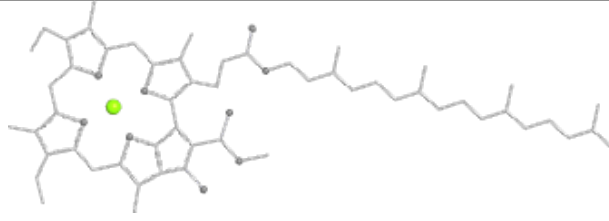
All (2) ring outliers are listed below:

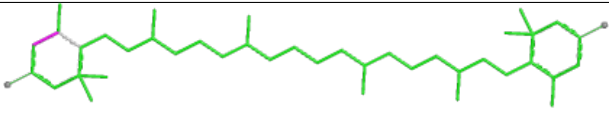
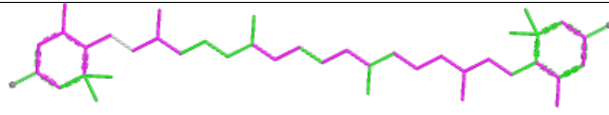
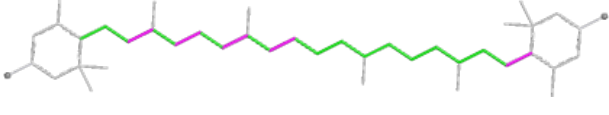
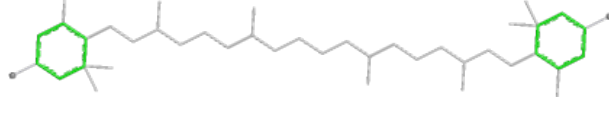
Mol	Chain	Res	Type	Atoms
51	N	623	NEX	C1-C2-C3-C4-C5-C6
51	n	623	NEX	C1-C2-C3-C4-C5-C6

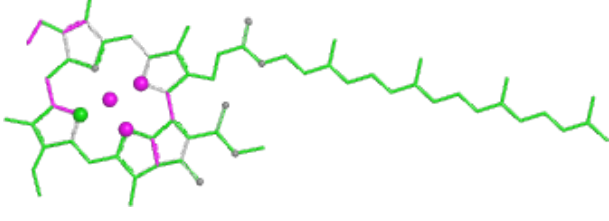
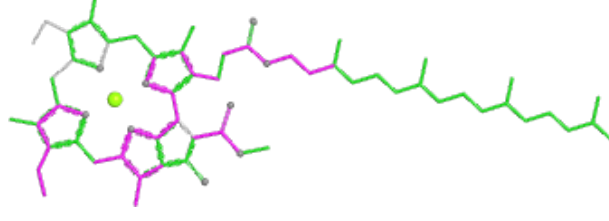
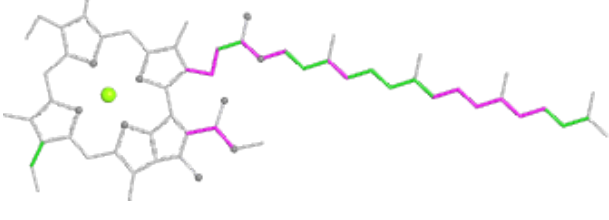
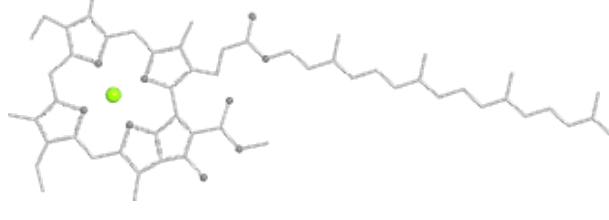
No monomer is involved in short contacts.

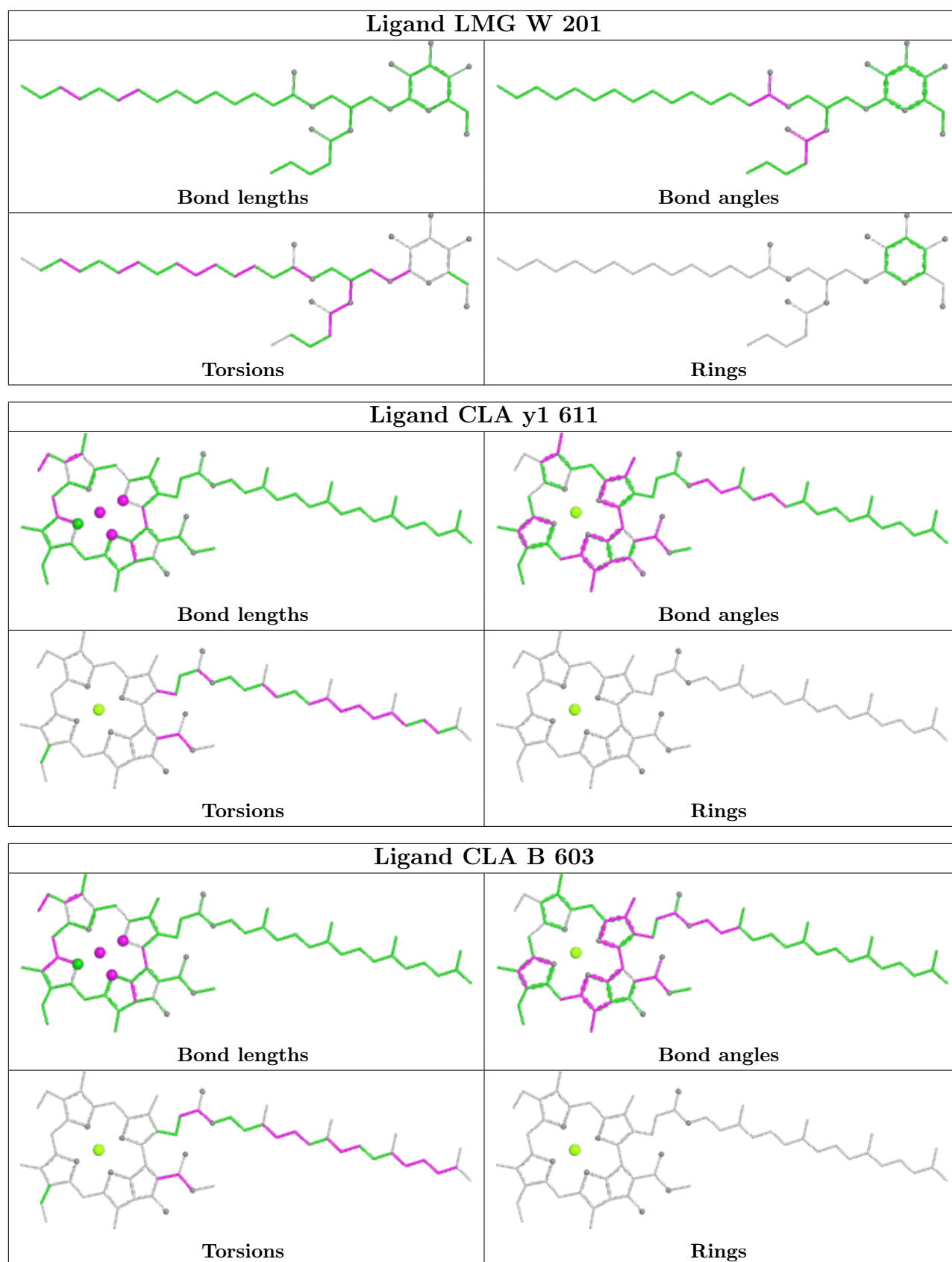
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

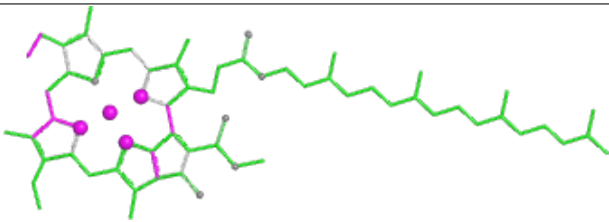
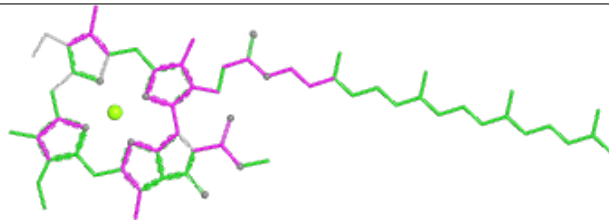
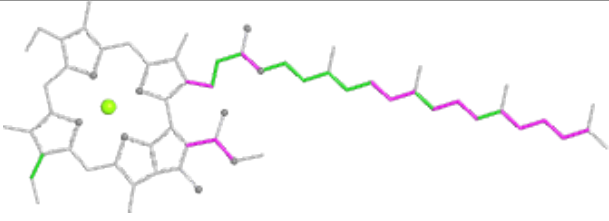
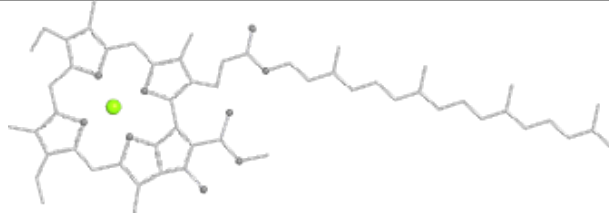


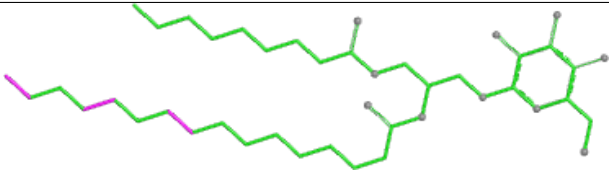
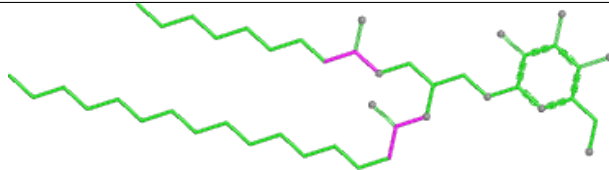
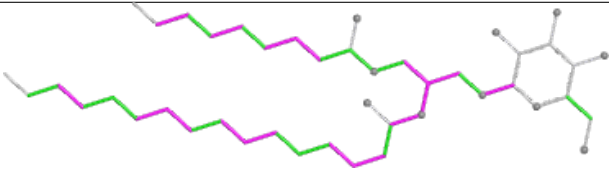
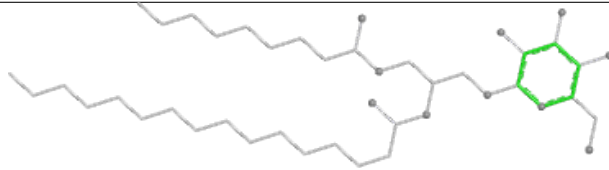
Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

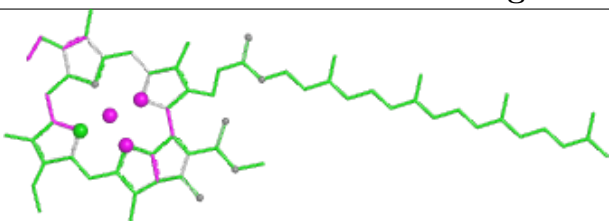
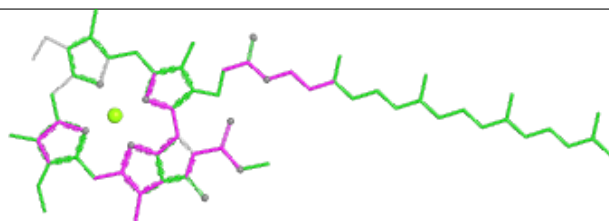
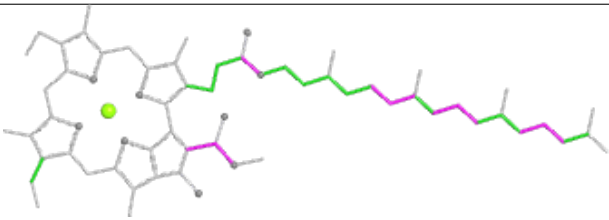
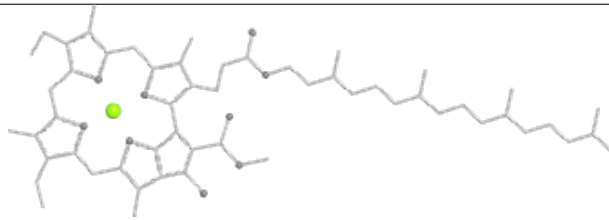
Ligand LUT N1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

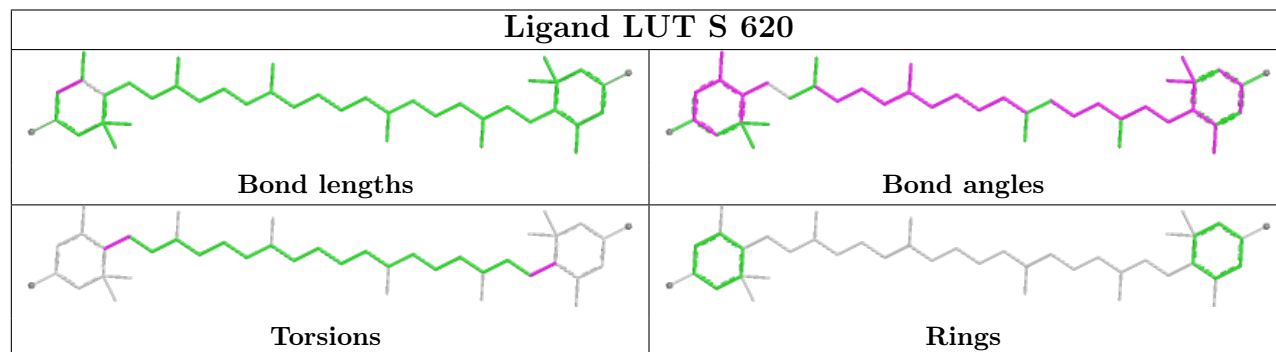
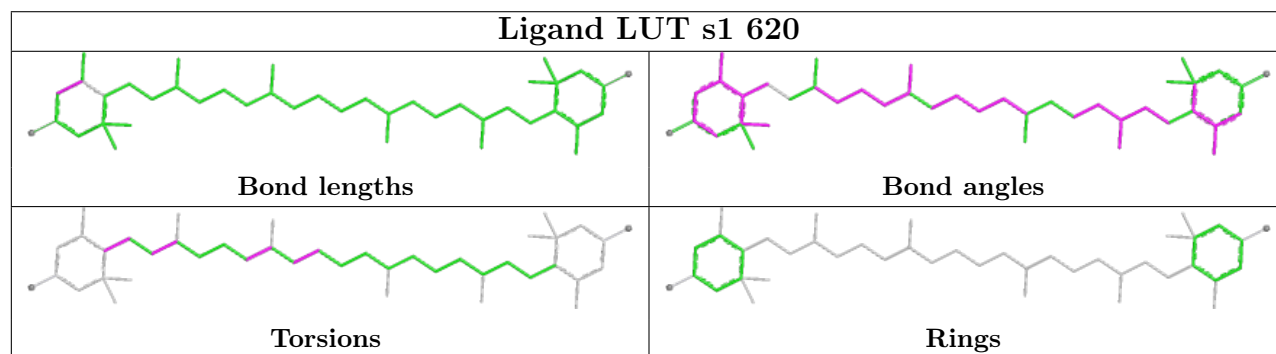
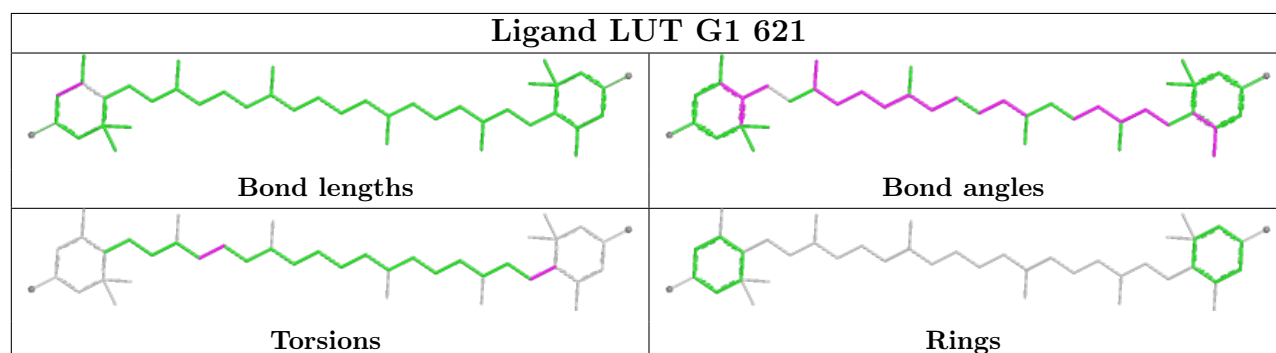
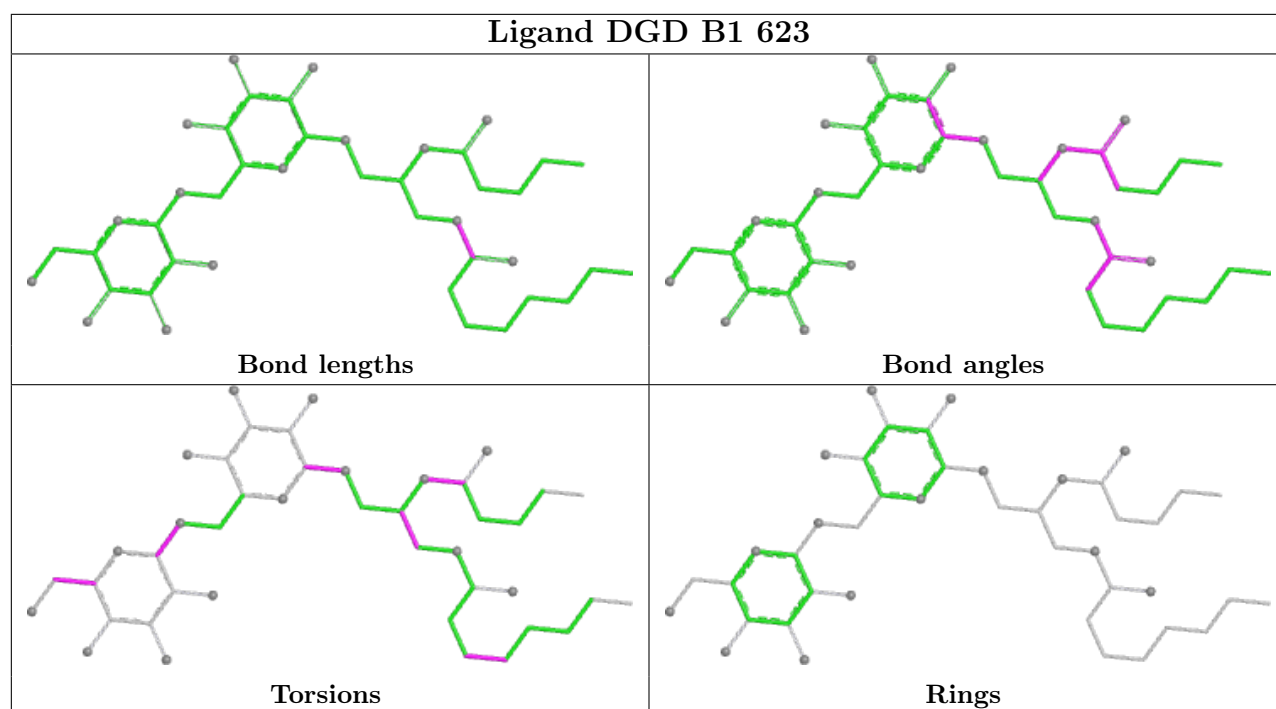
Ligand CLA N 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

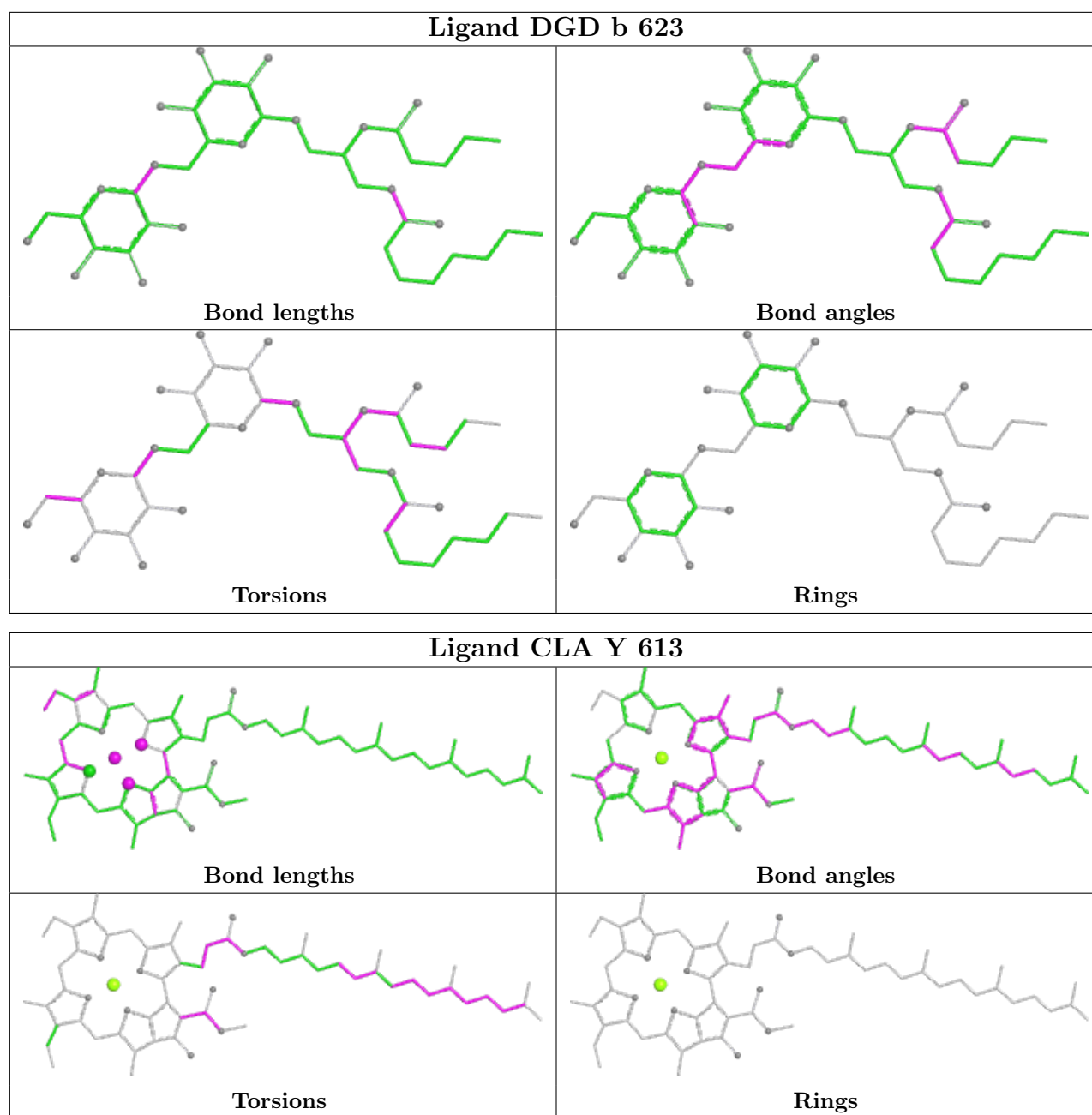


Ligand CLA c 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

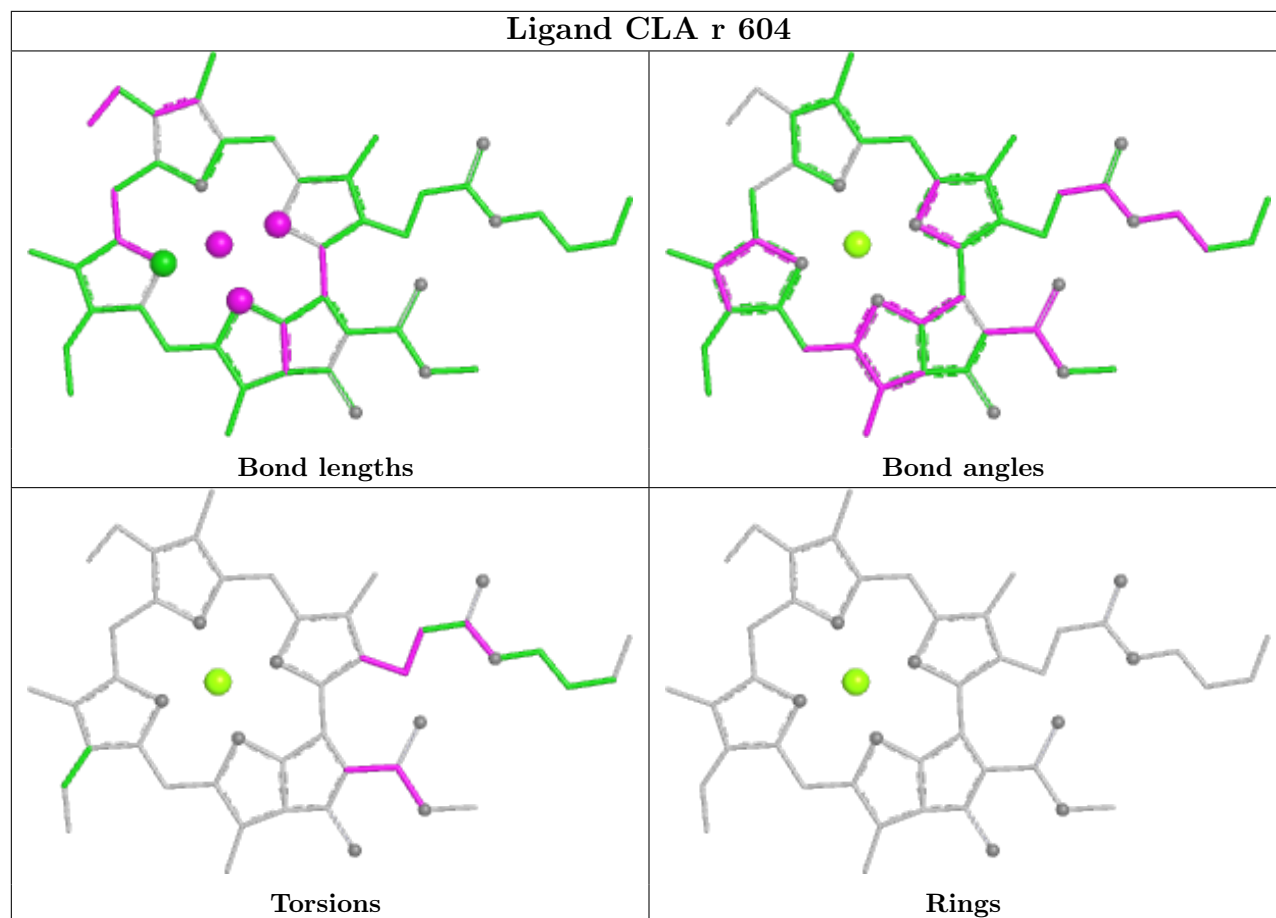
Ligand LMG B 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

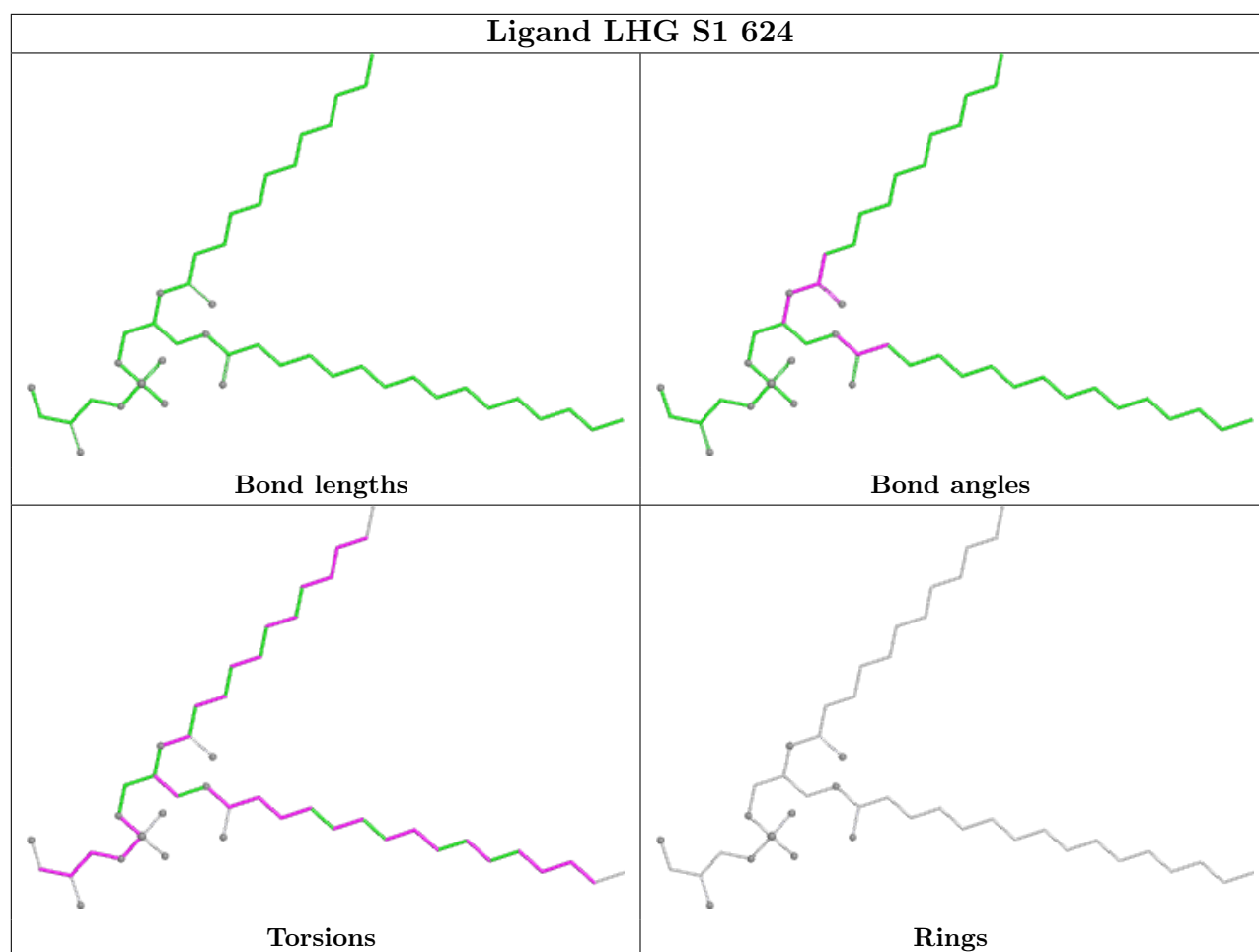
Ligand CLA Y 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

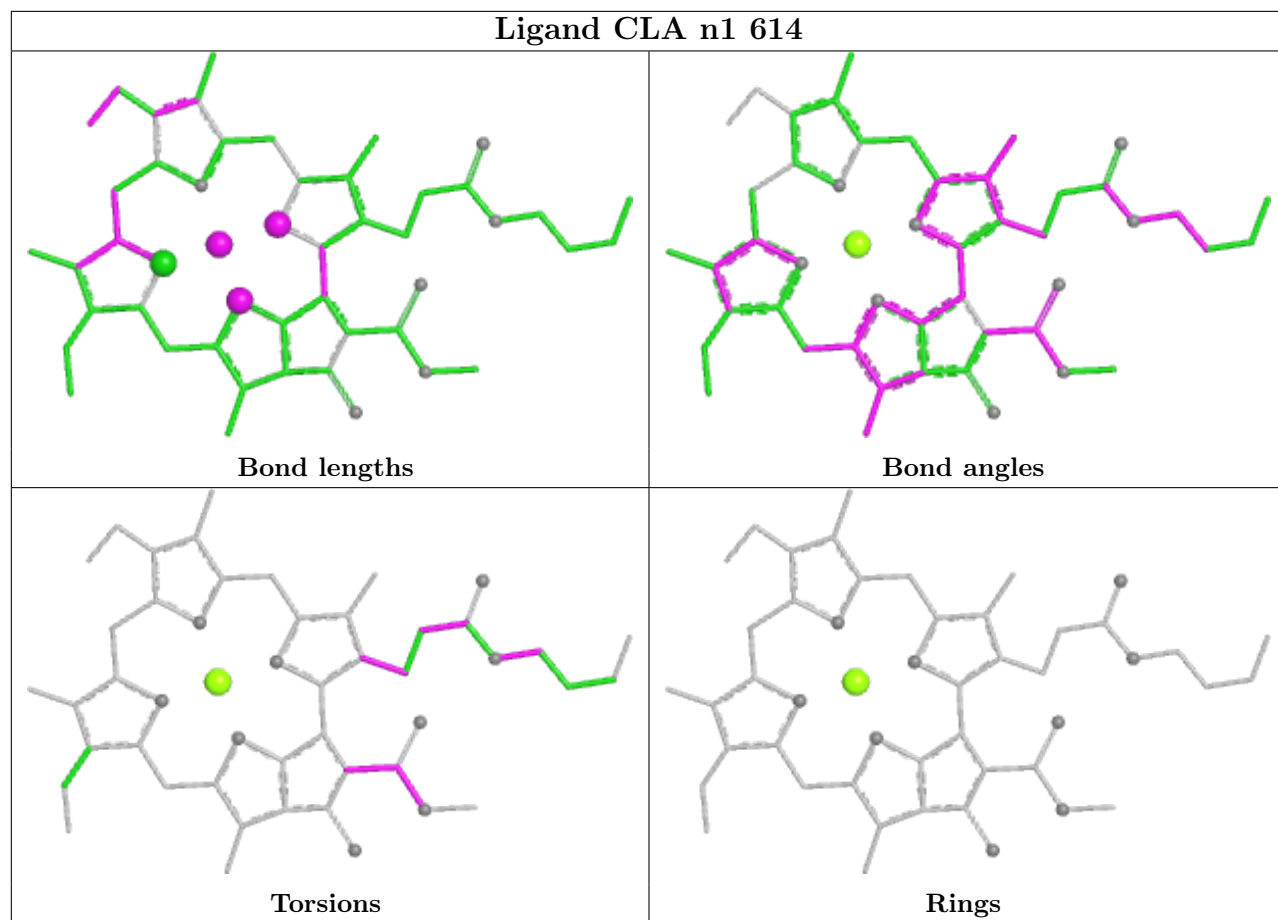


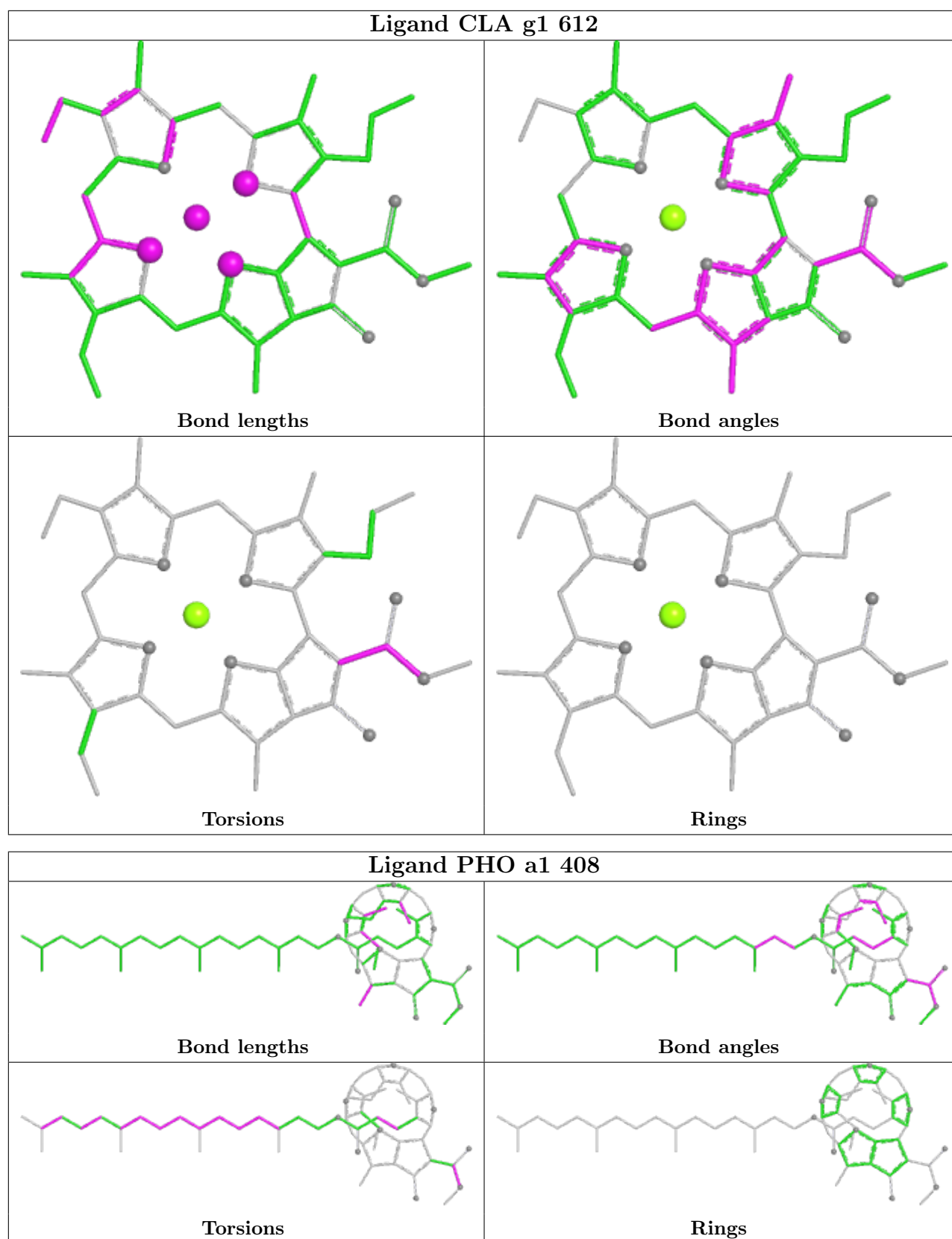


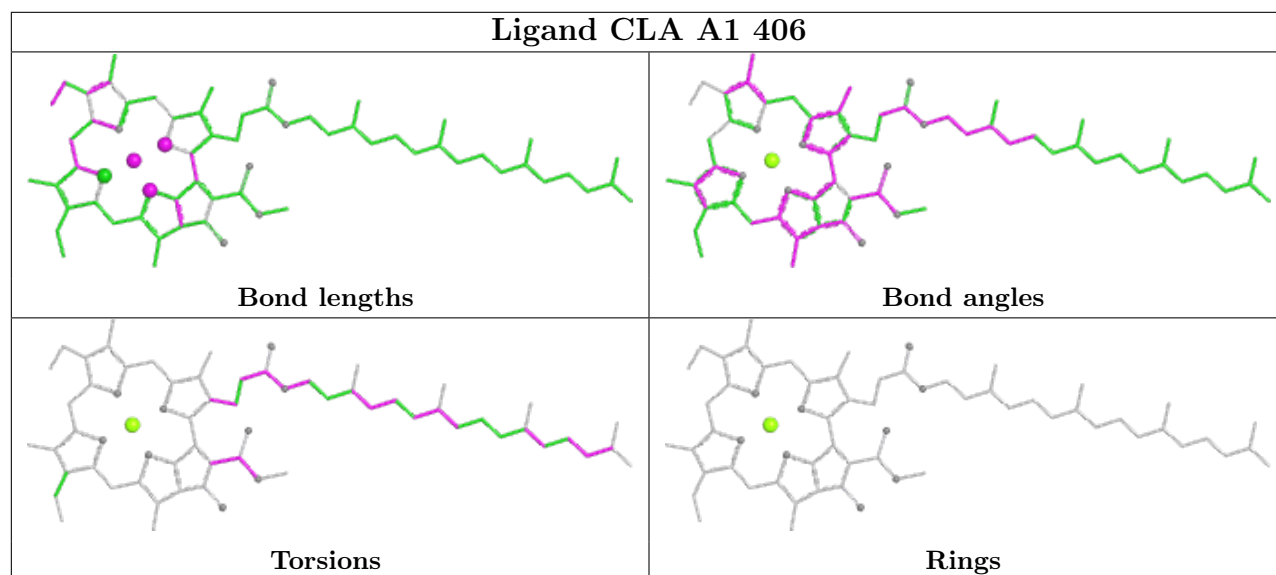
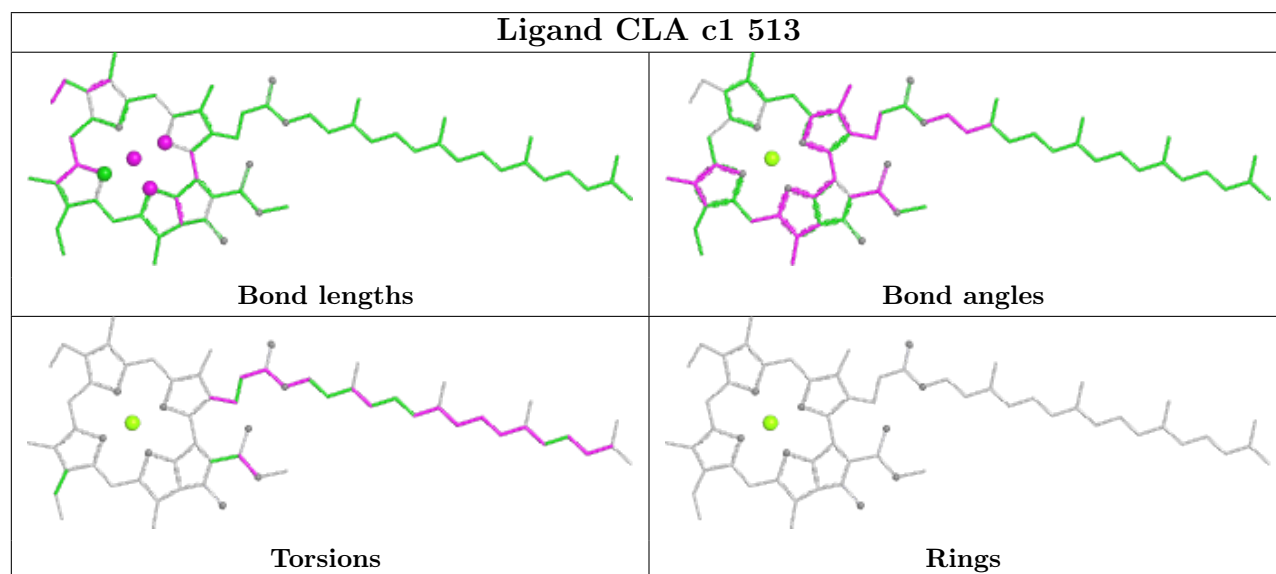
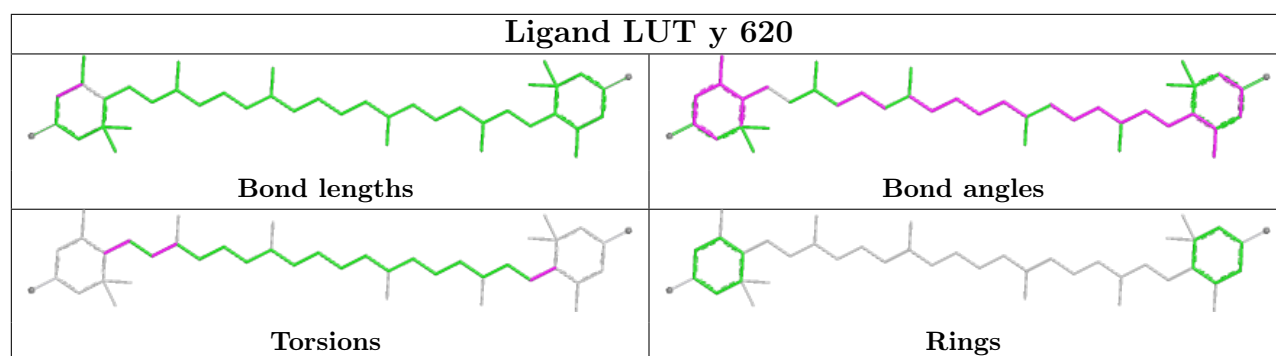
Ligand CLA r 604

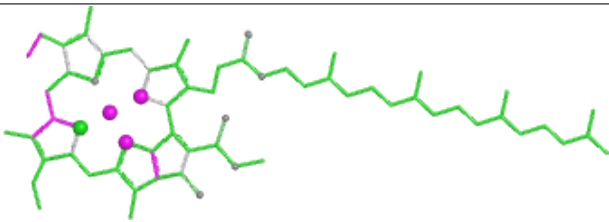
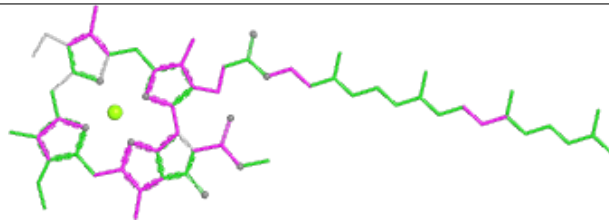
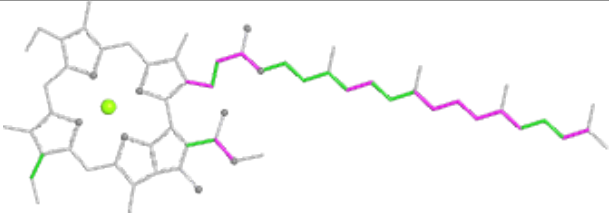
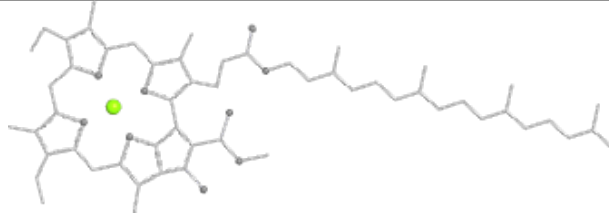


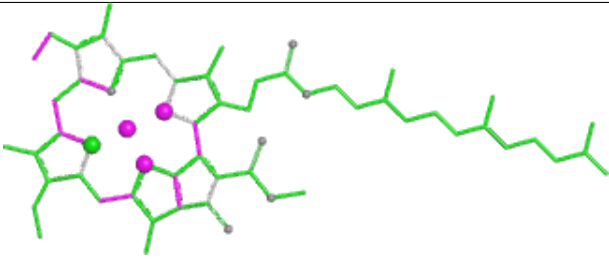
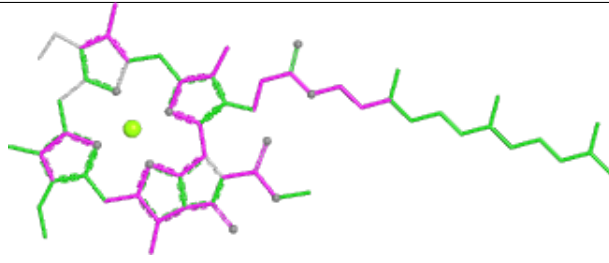
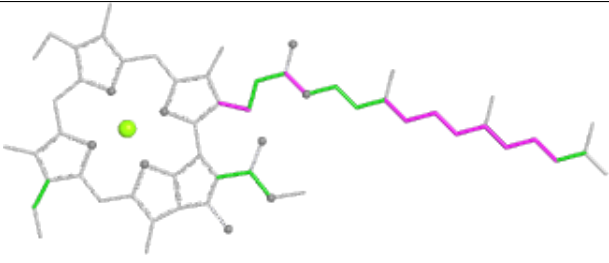
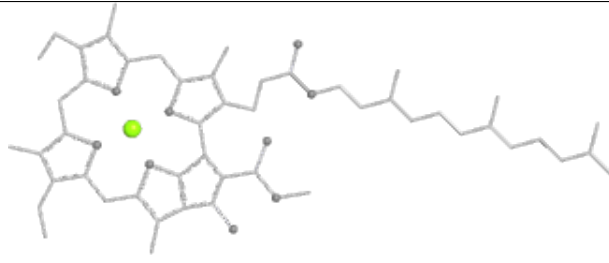


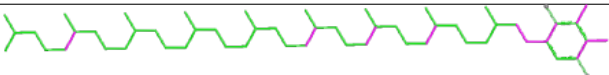
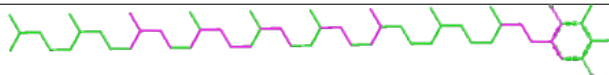
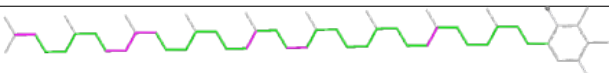
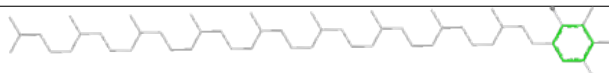


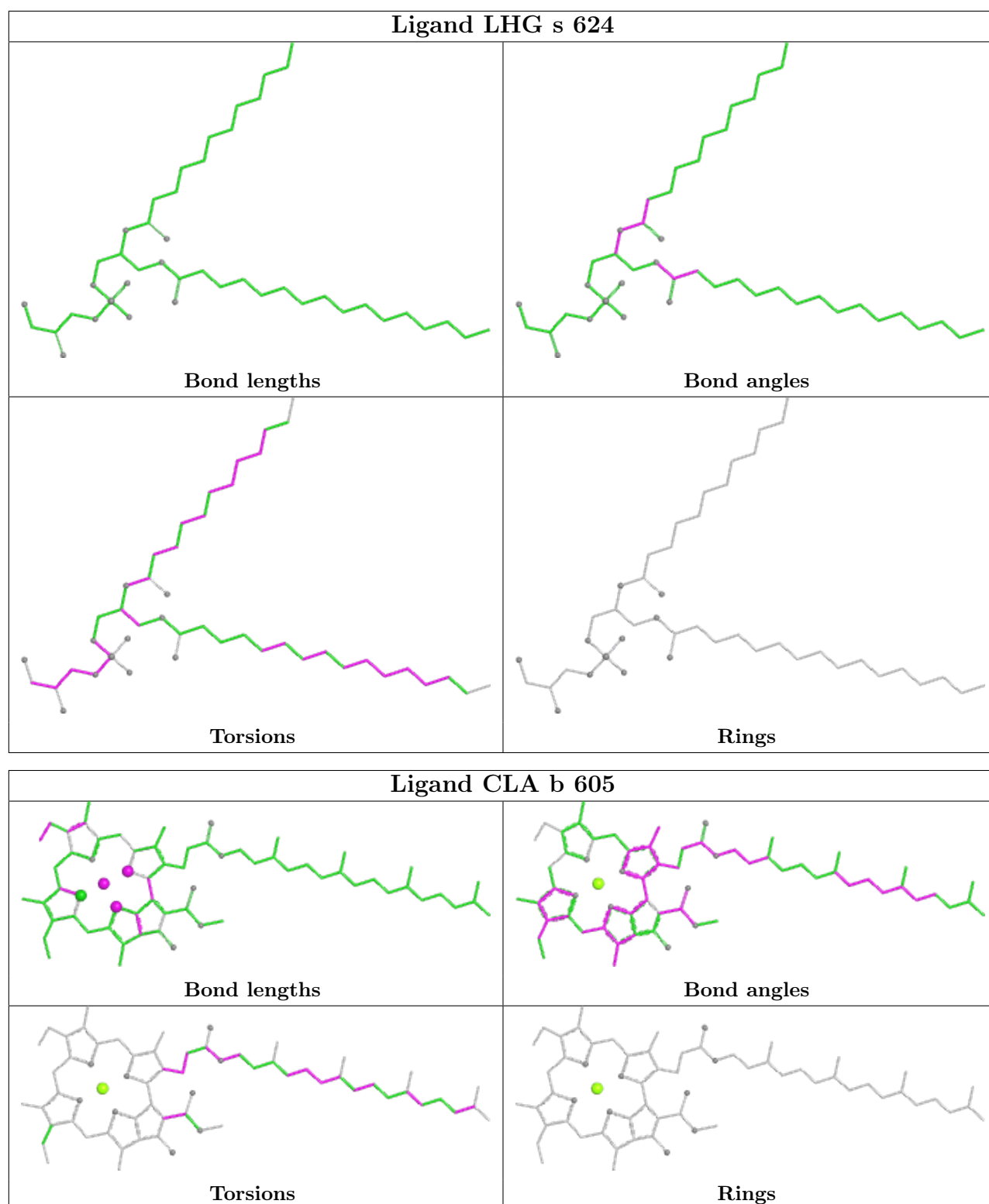


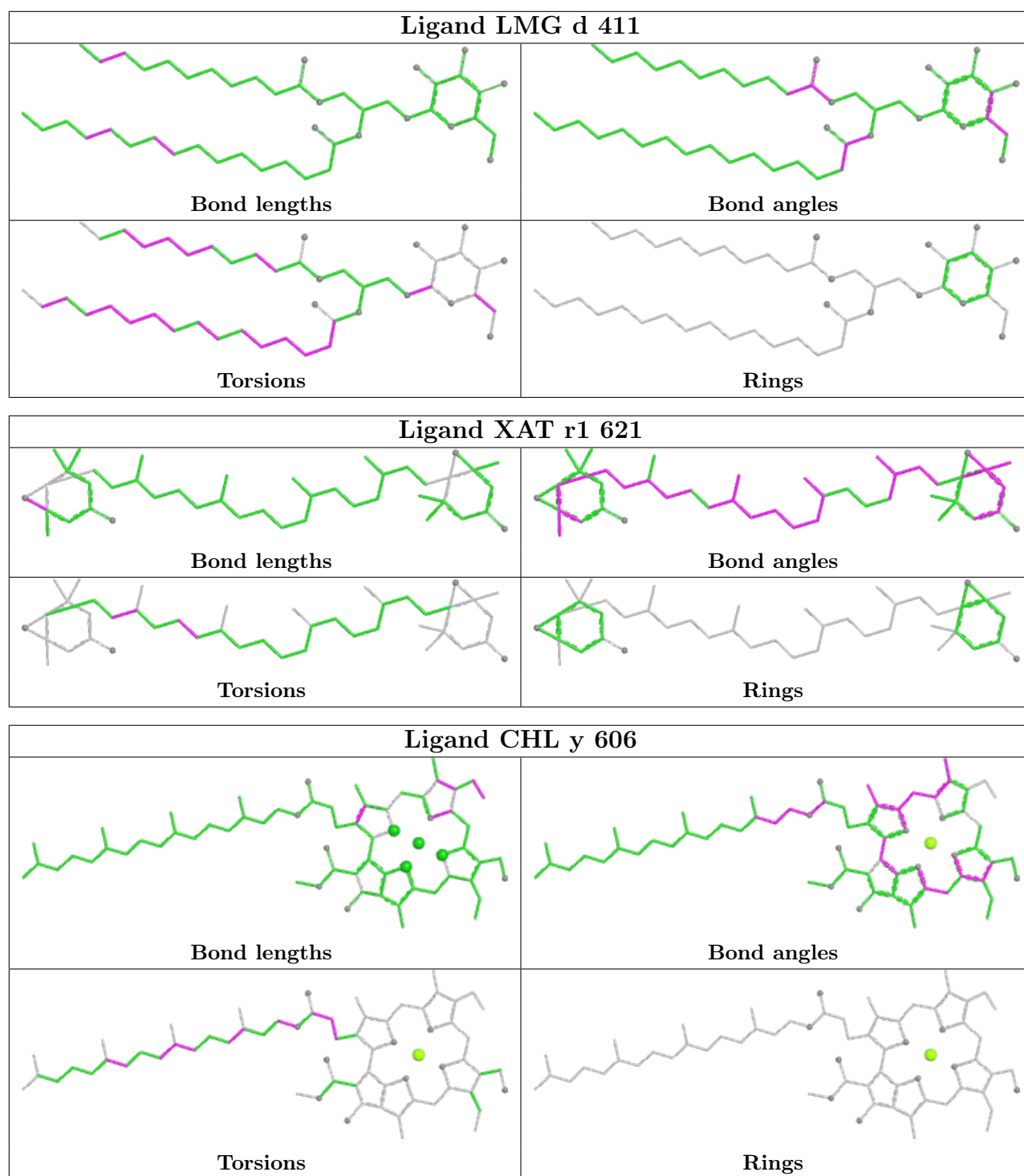


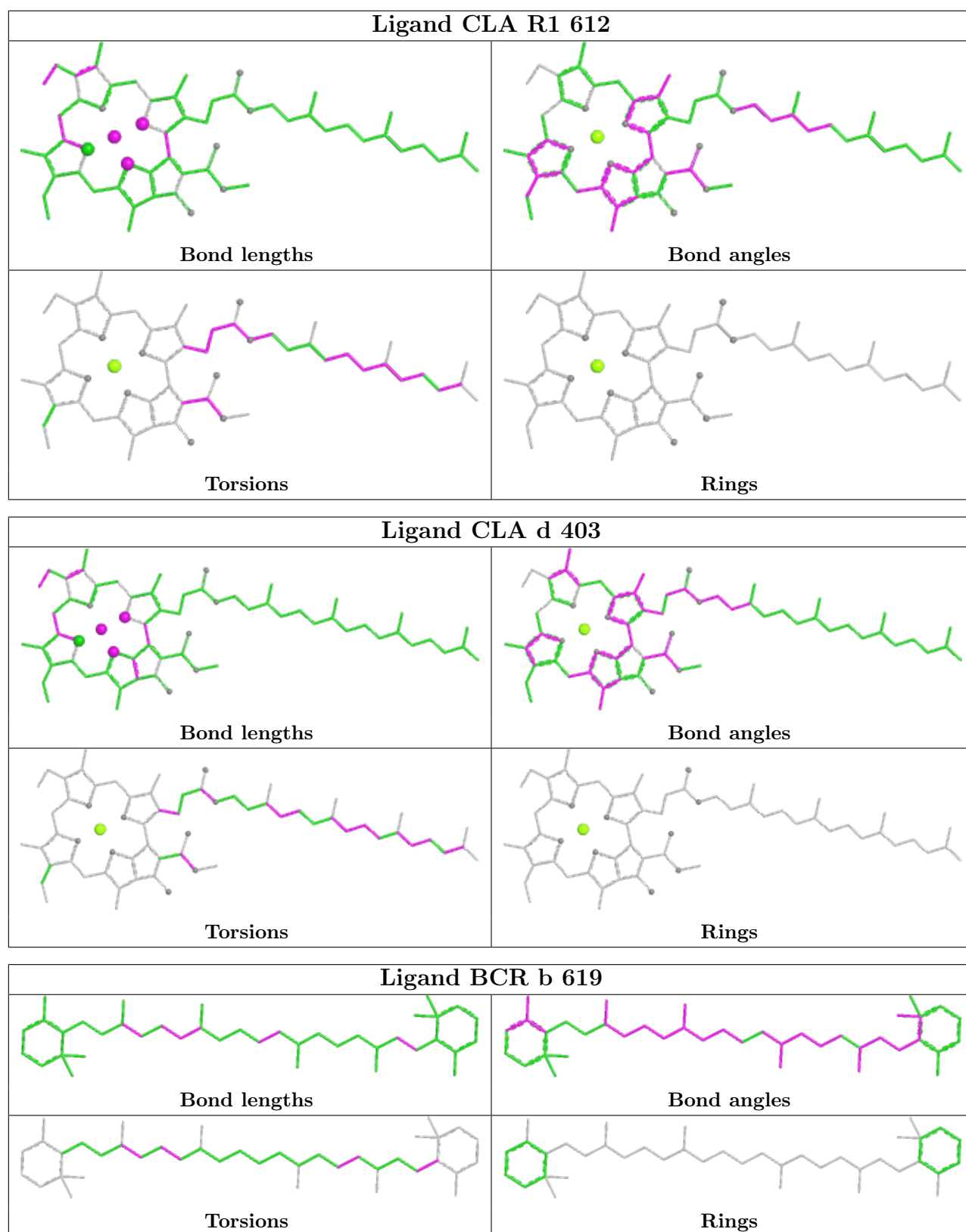
Ligand CLA C1 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

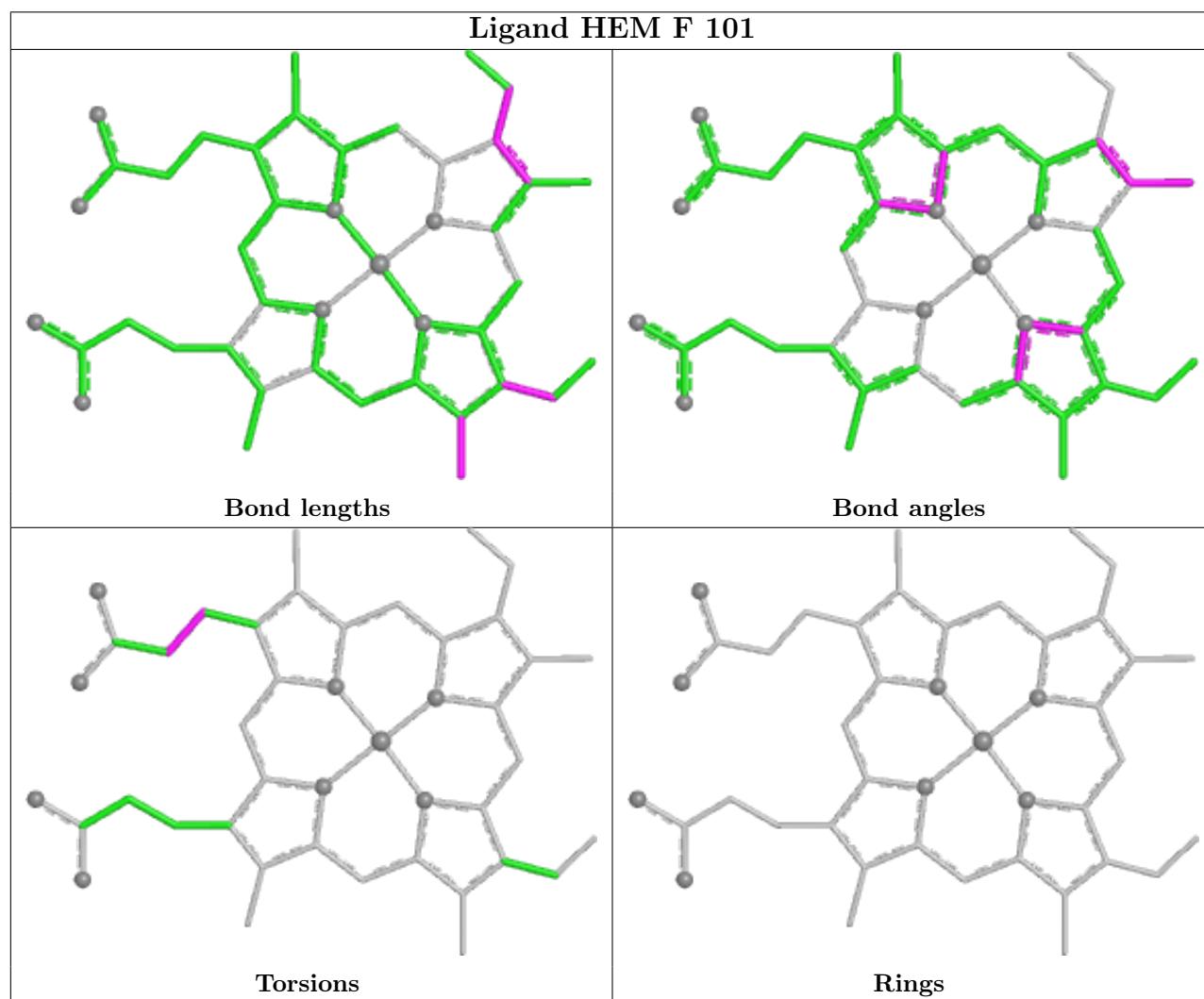
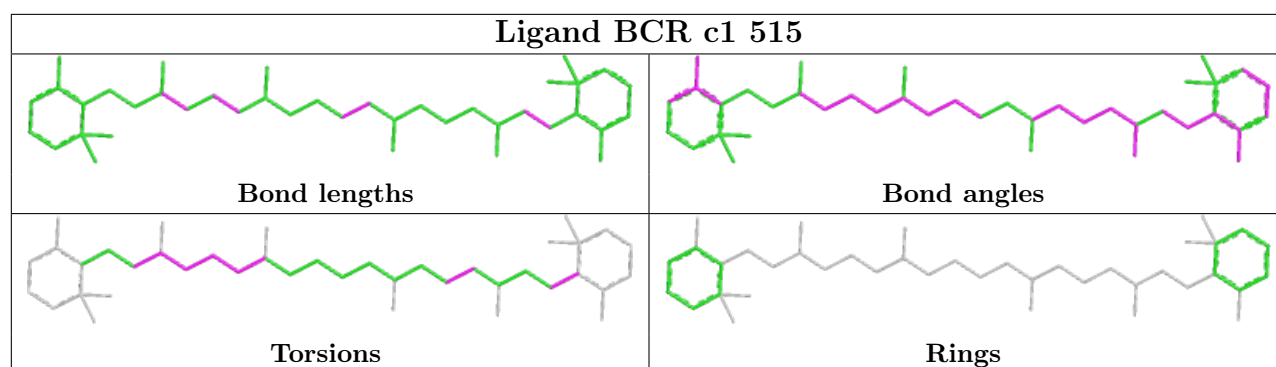
Ligand CLA a1 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

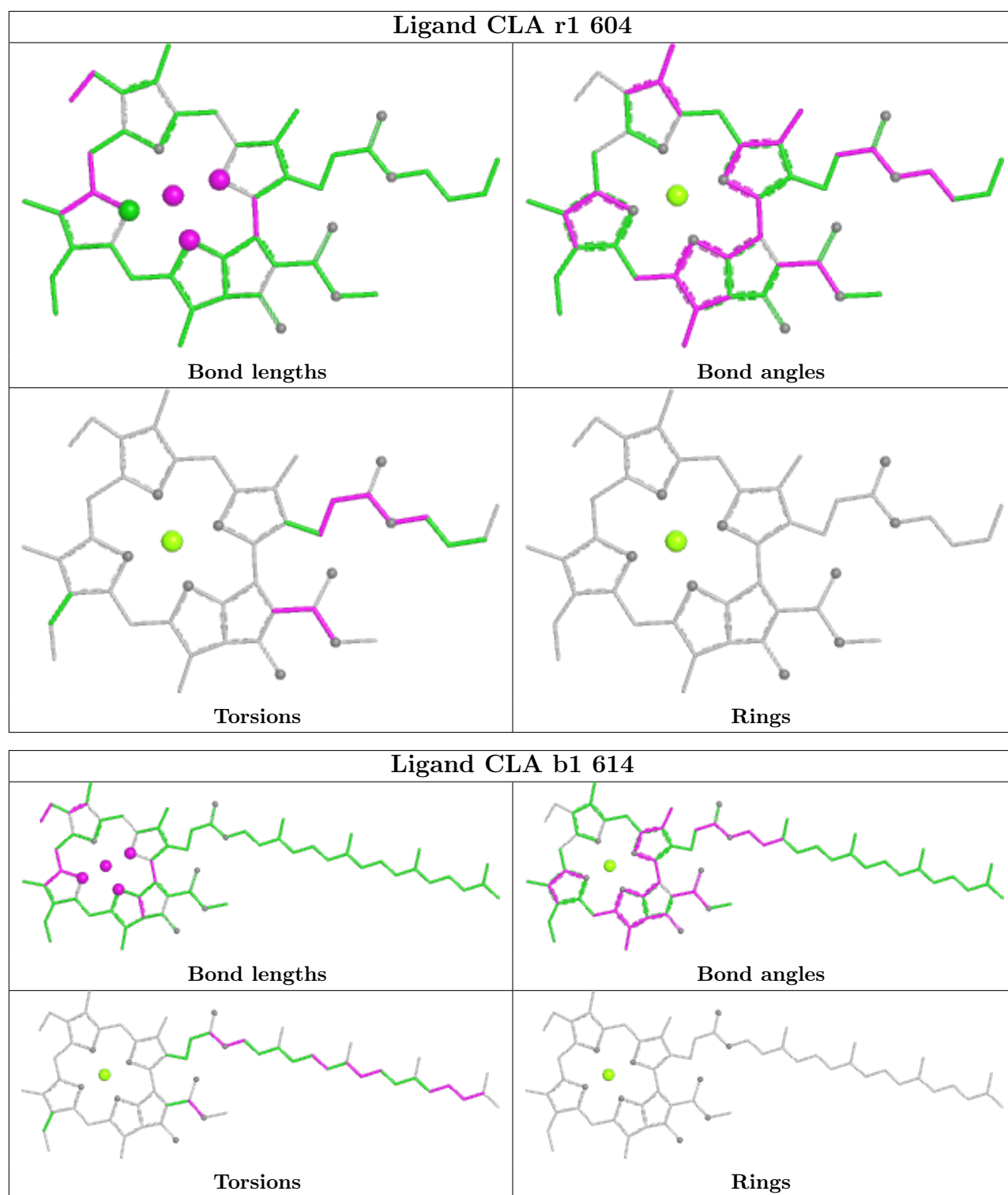
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

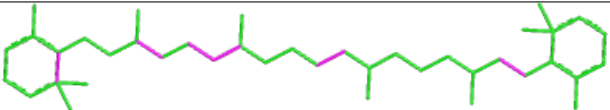
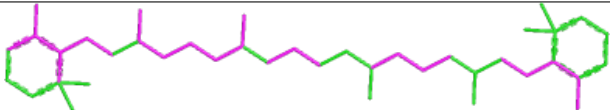
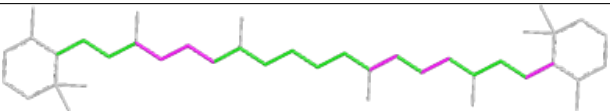
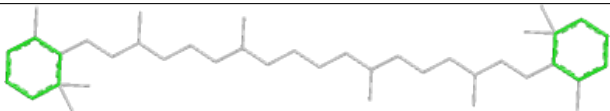
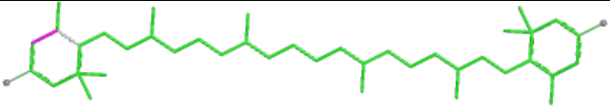
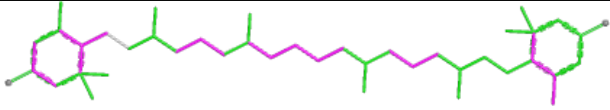
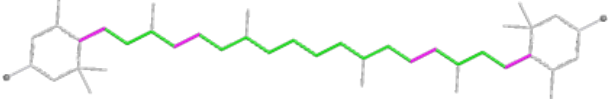
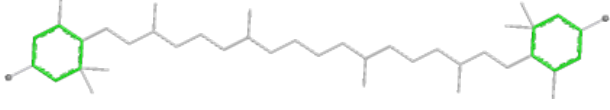
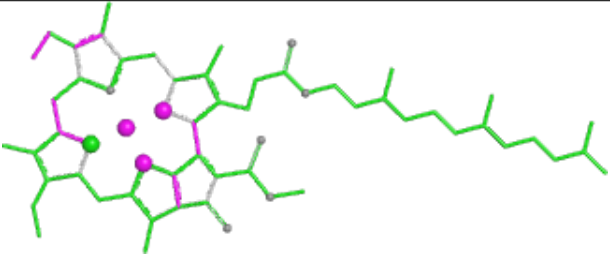
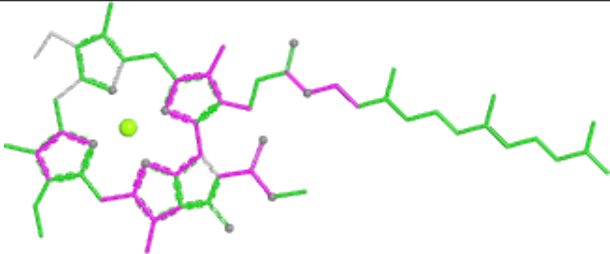
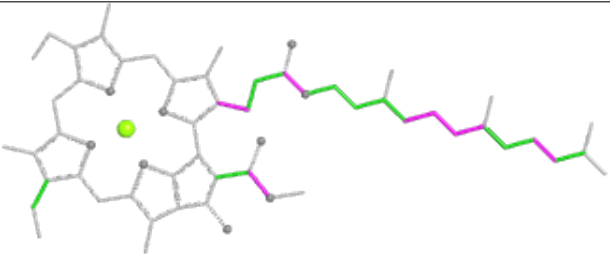
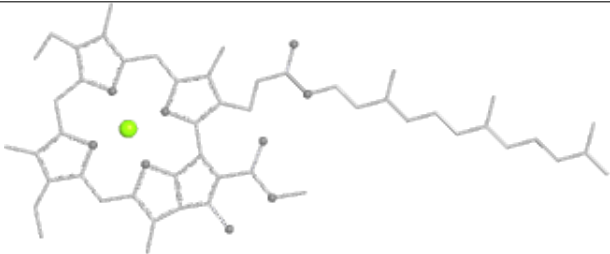


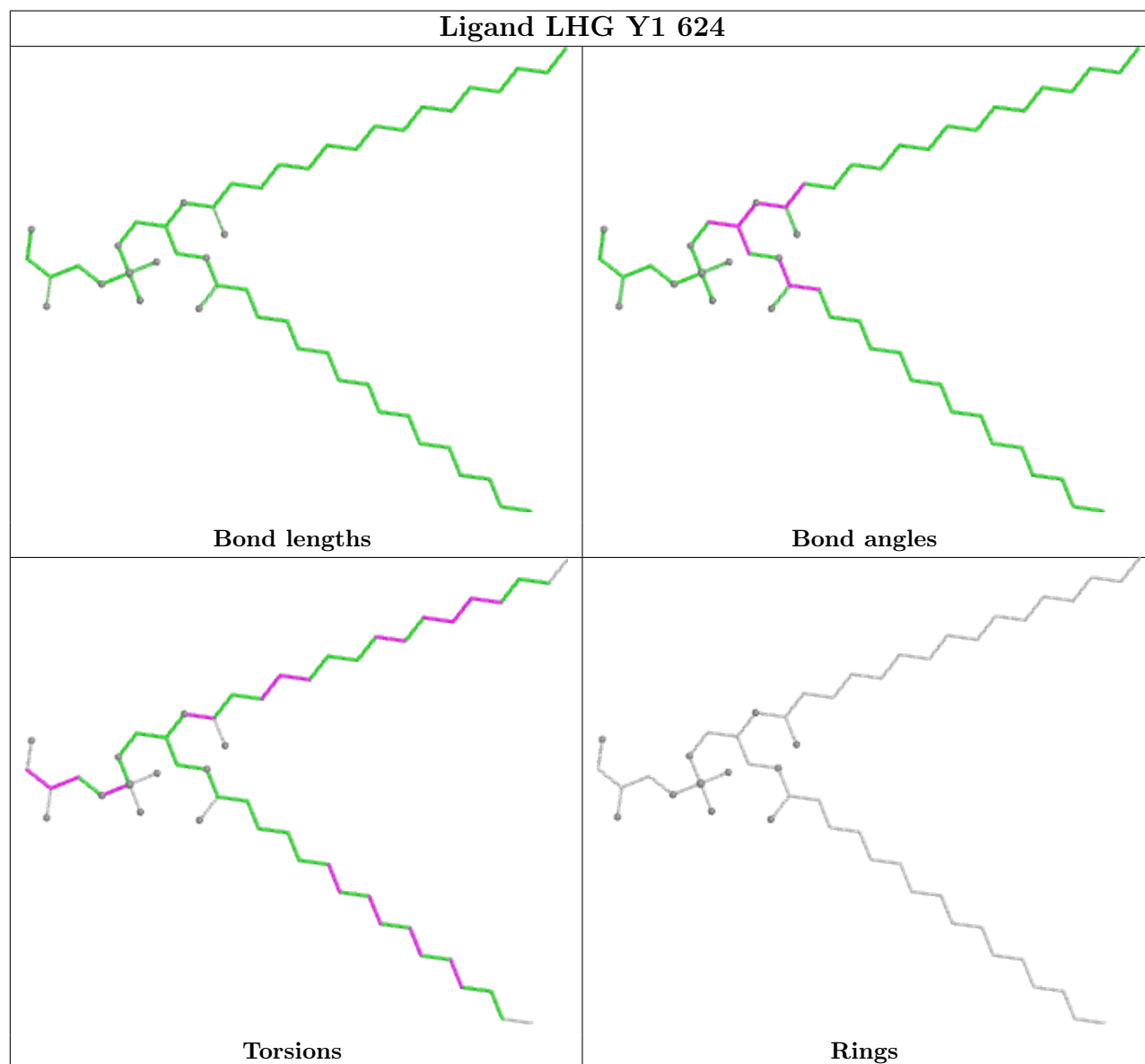
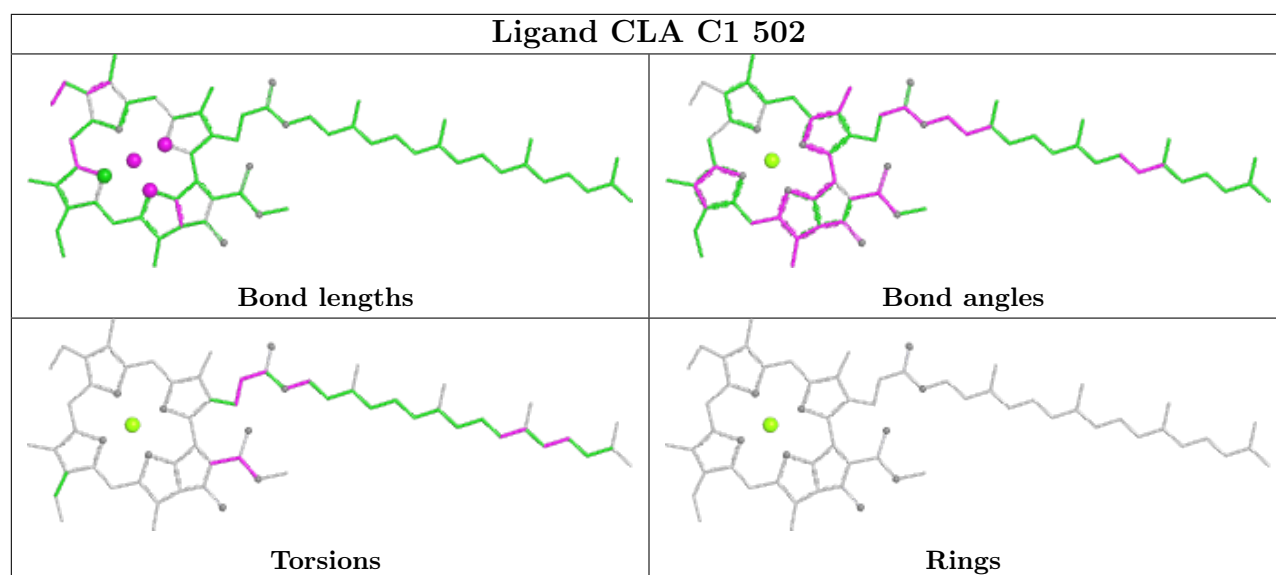


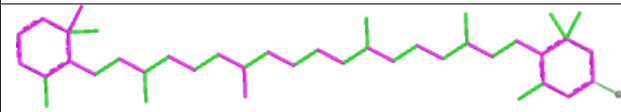
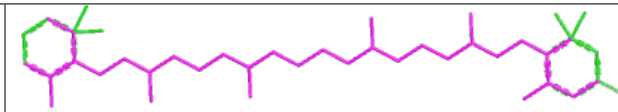
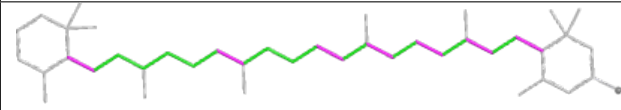
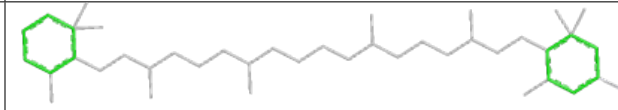


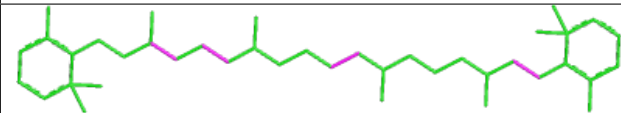
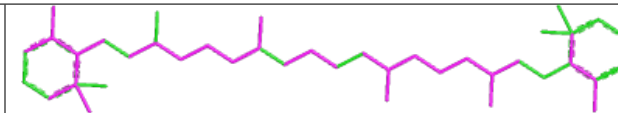
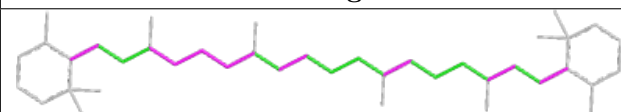
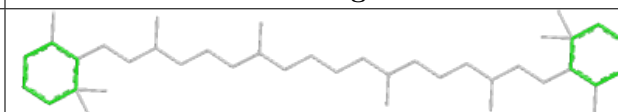


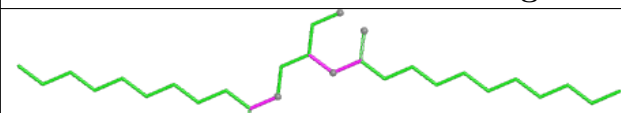
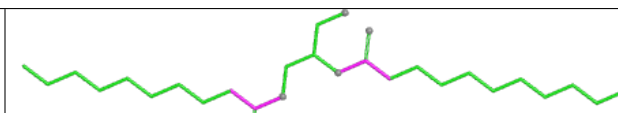
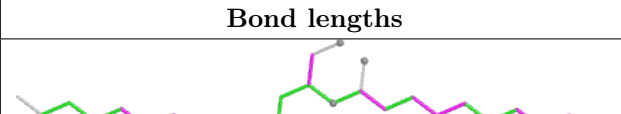
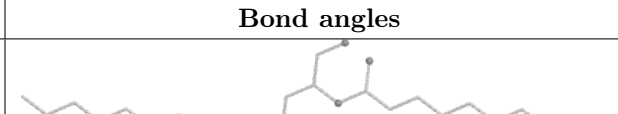


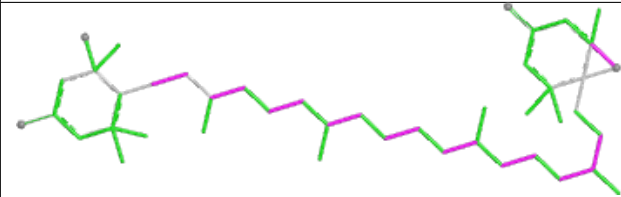
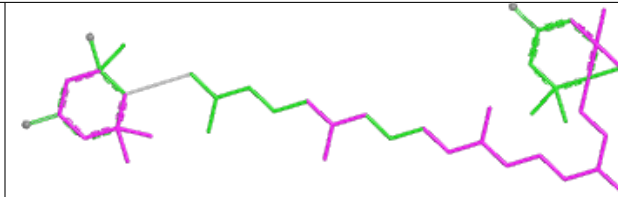
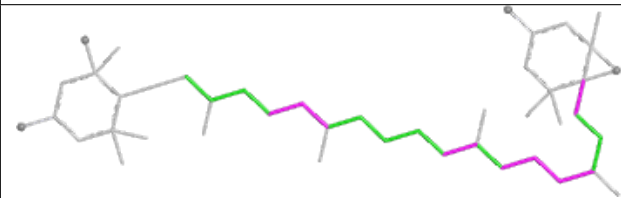
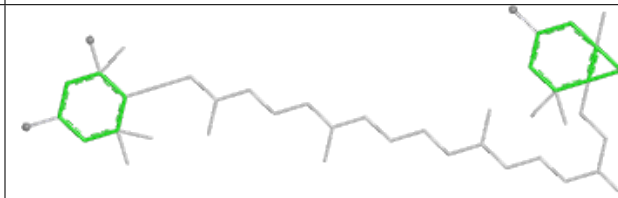
Ligand BCR C 515	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT S1 620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA S 609	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

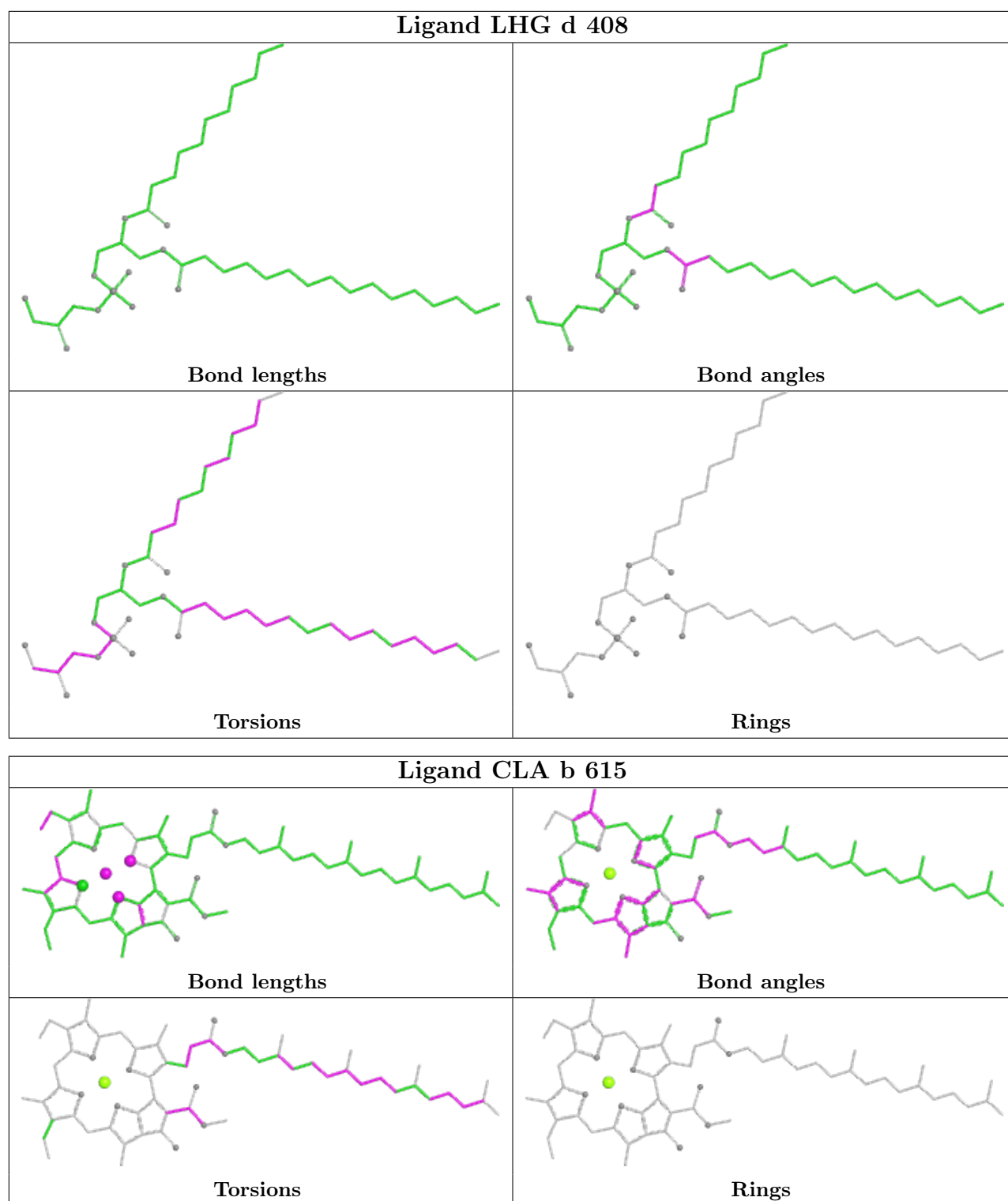


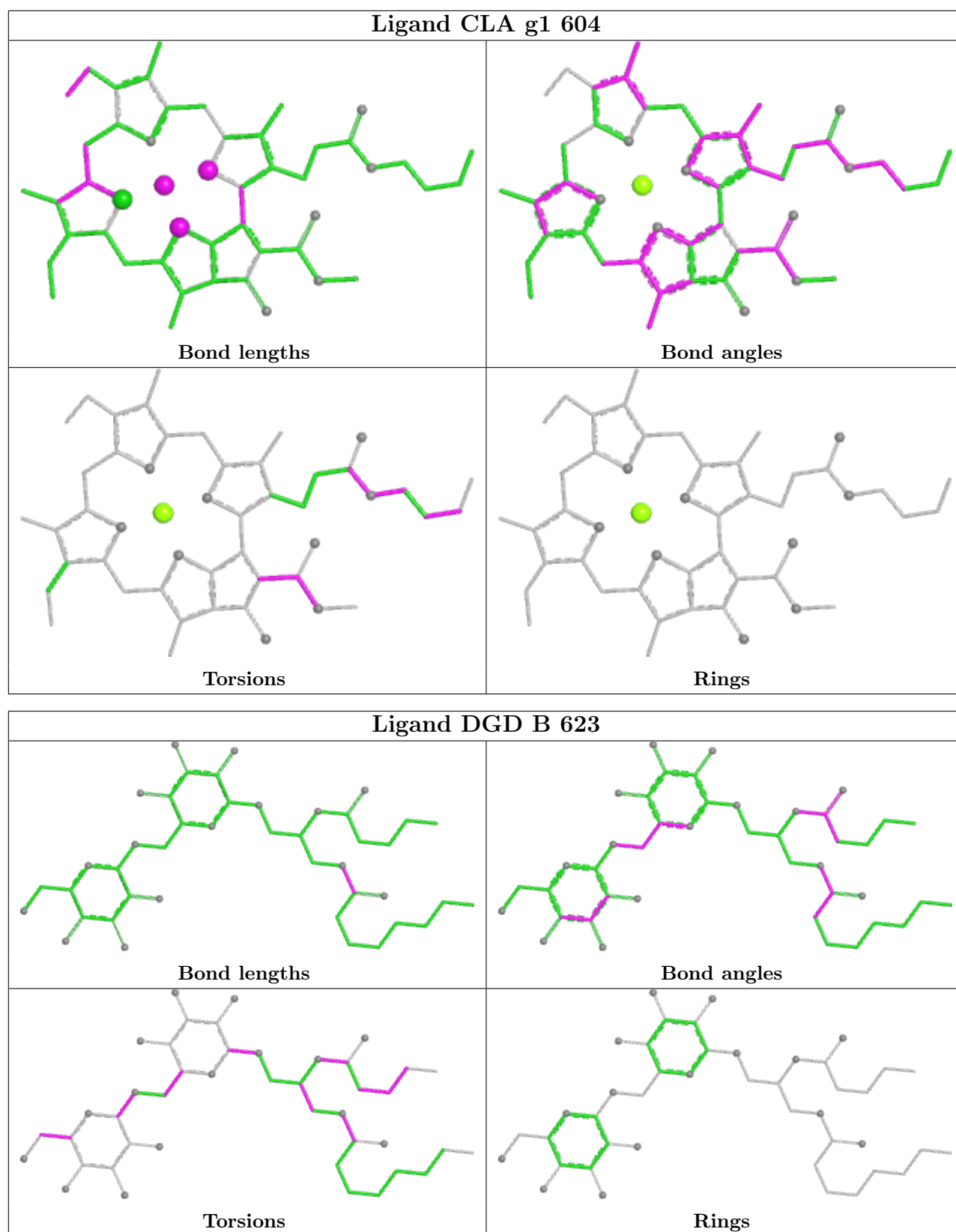
Ligand RRX h1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

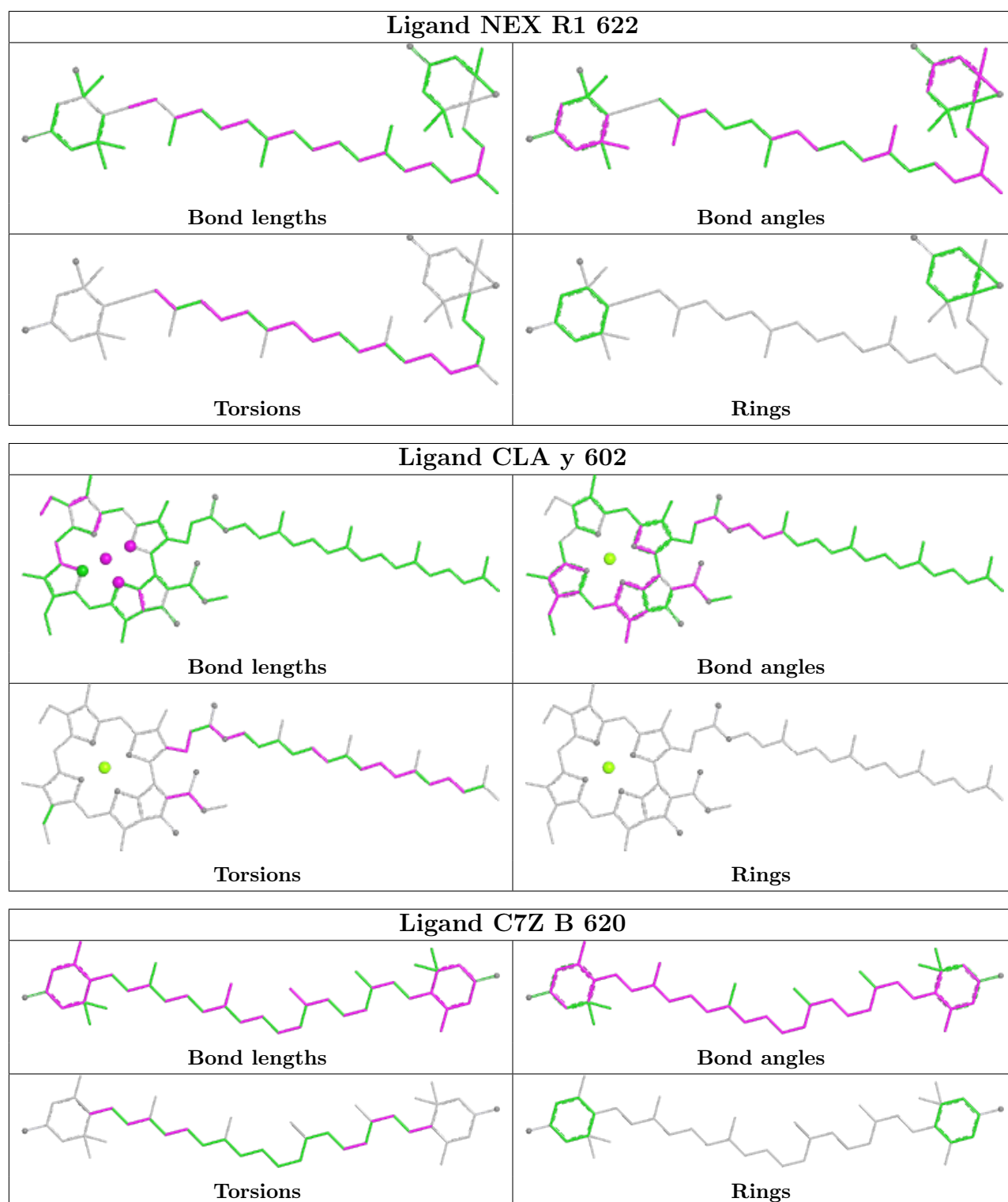
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Bond lengths	Bond angles
	
Torsions	Rings

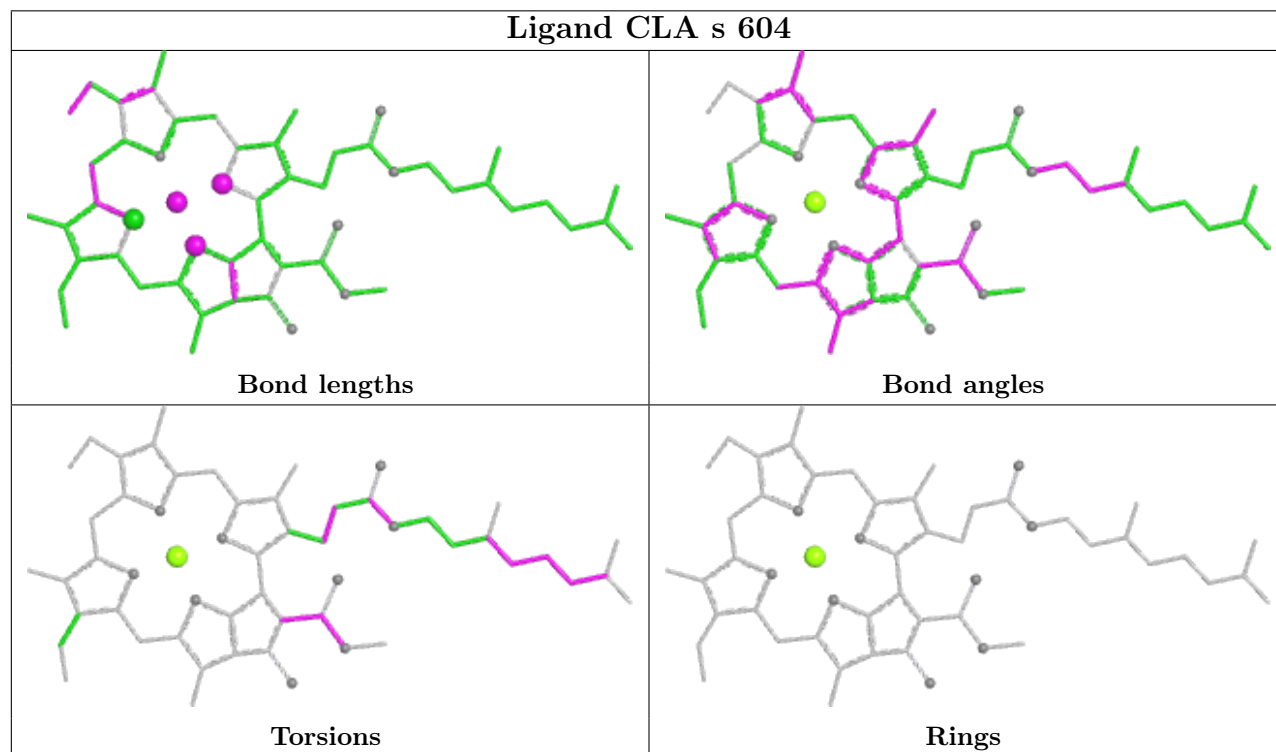
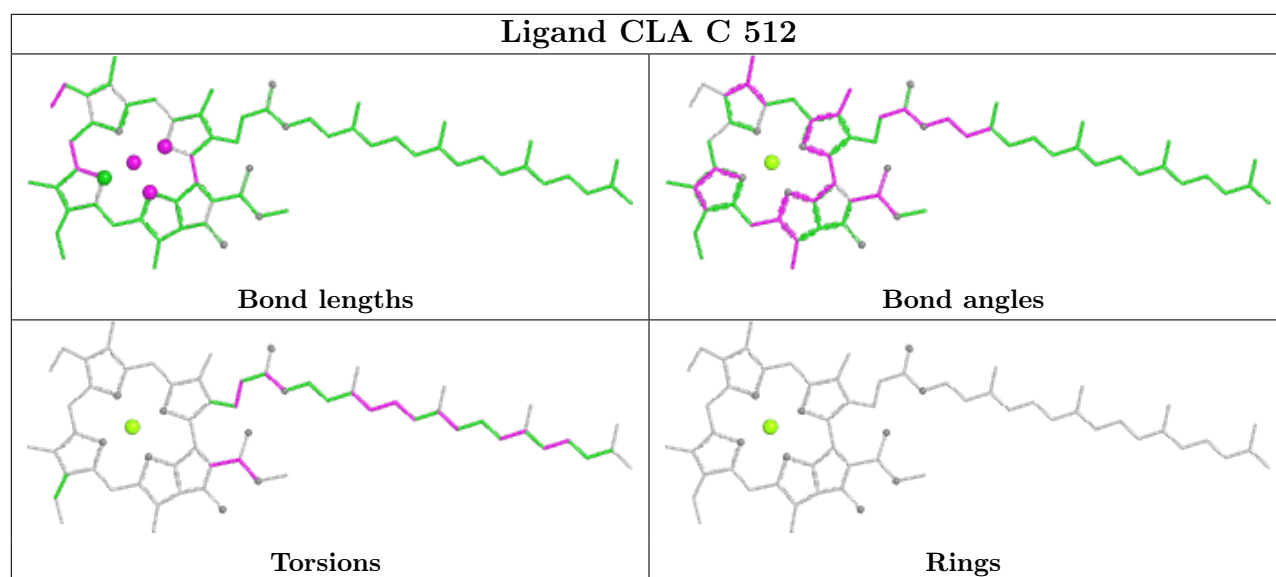
Ligand DGA J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

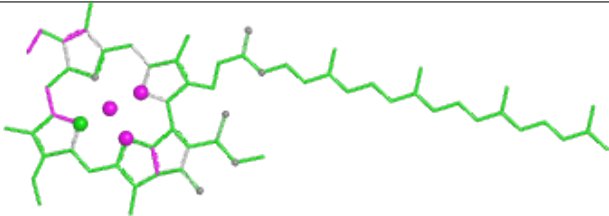
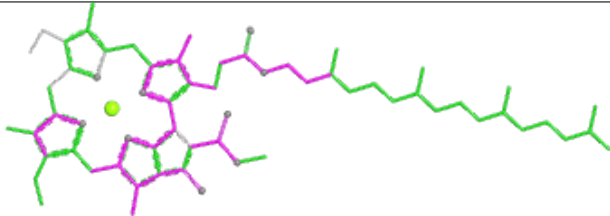
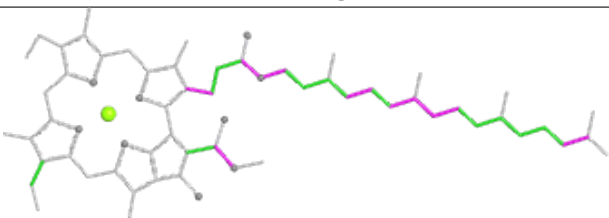
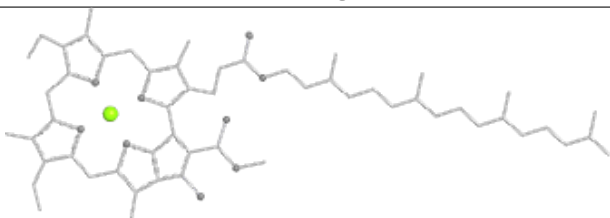
Ligand NEX y1 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

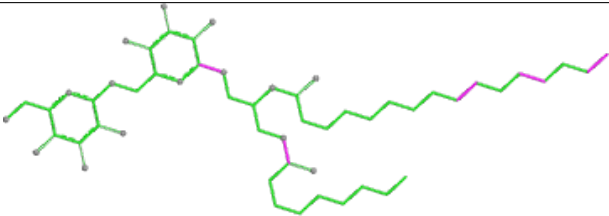
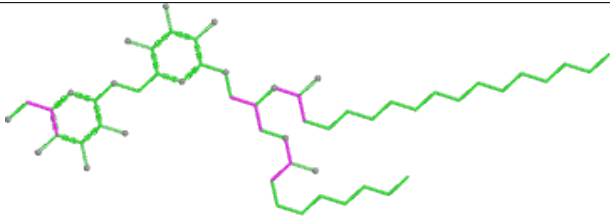
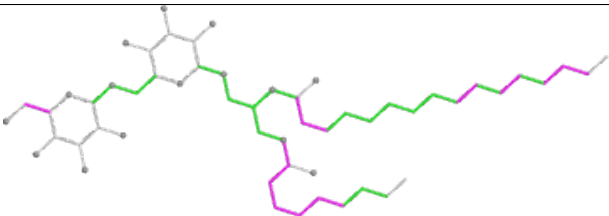
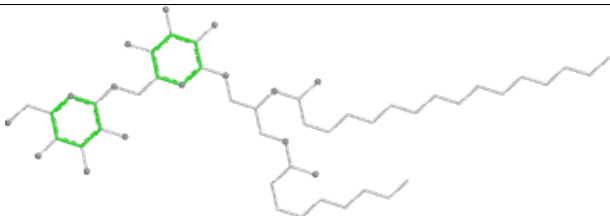


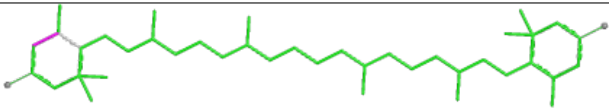
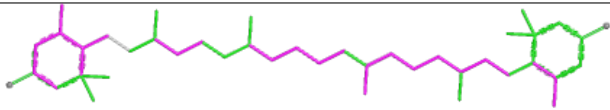
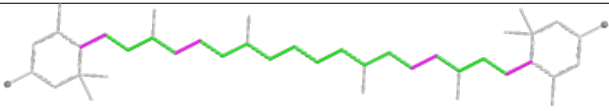
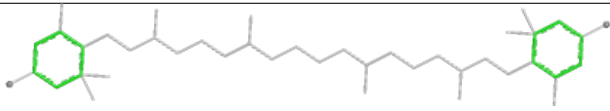




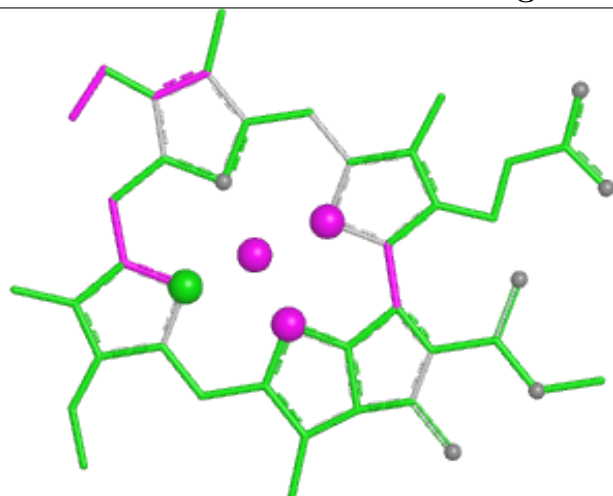


Ligand CLA Y1 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

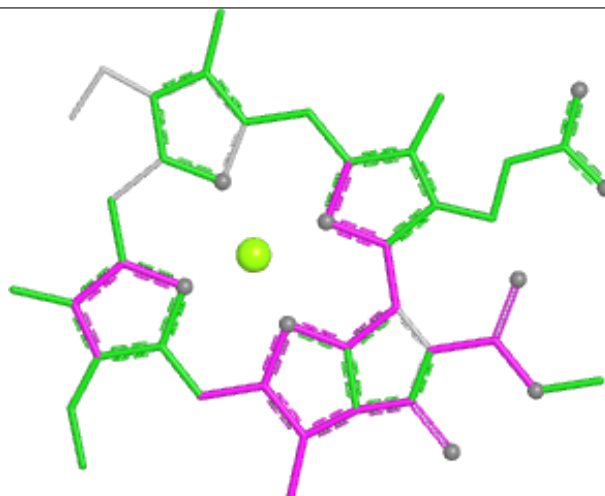
Ligand DGD c1 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT G 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

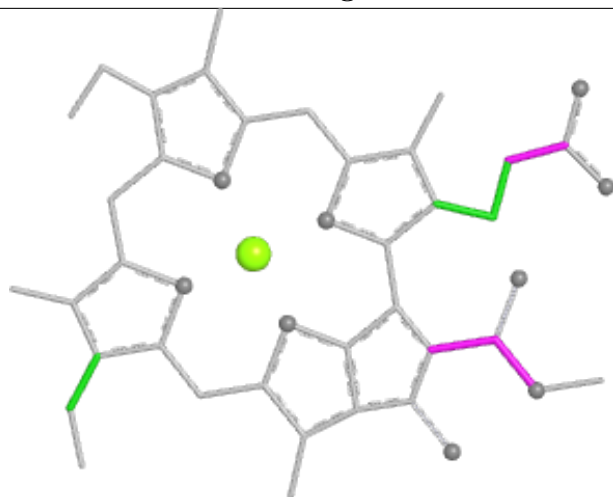
Ligand CLA n 612



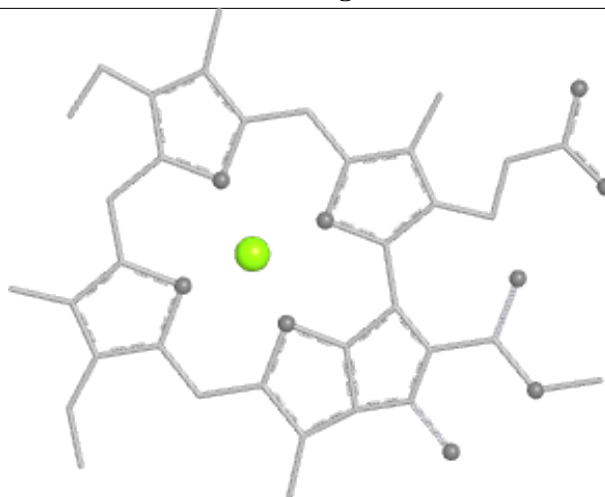
Bond lengths



Bond angles

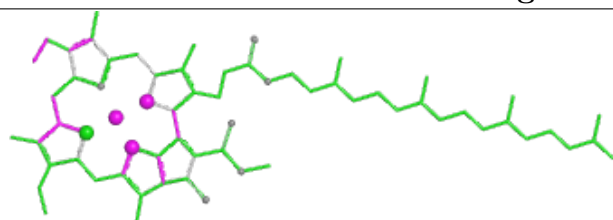


Torsions

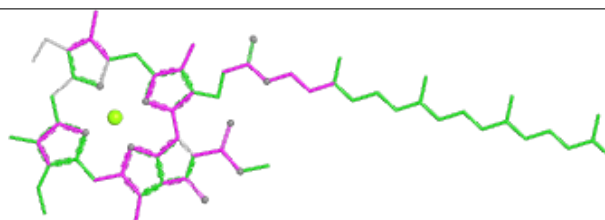


Rings

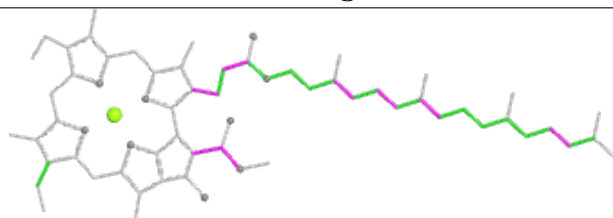
Ligand CLA b 609



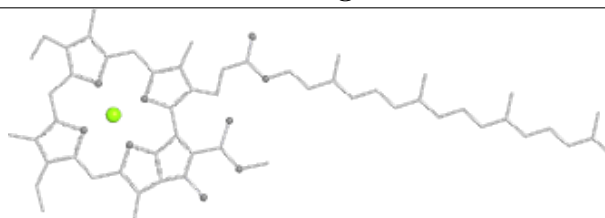
Bond lengths



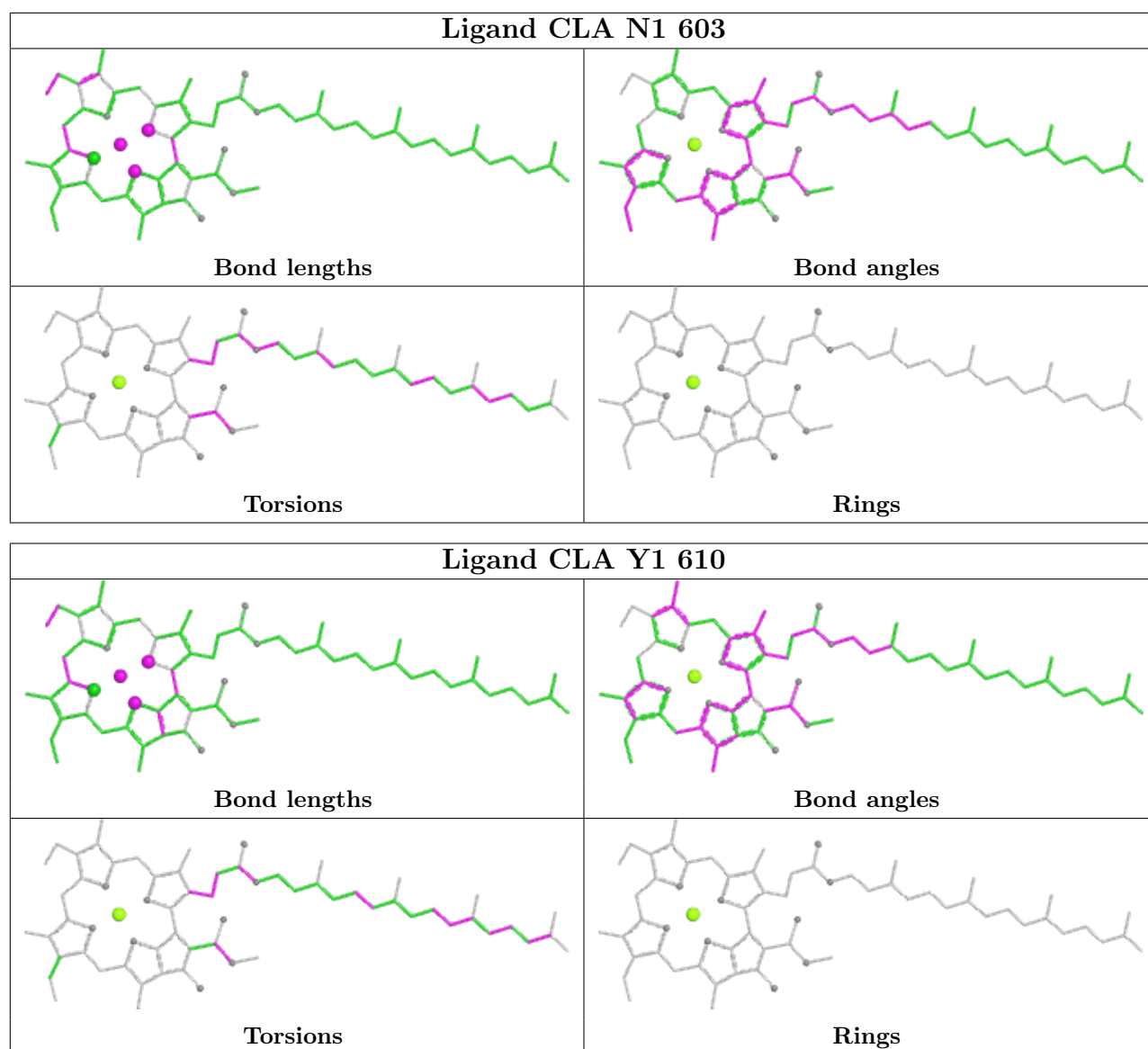
Bond angles

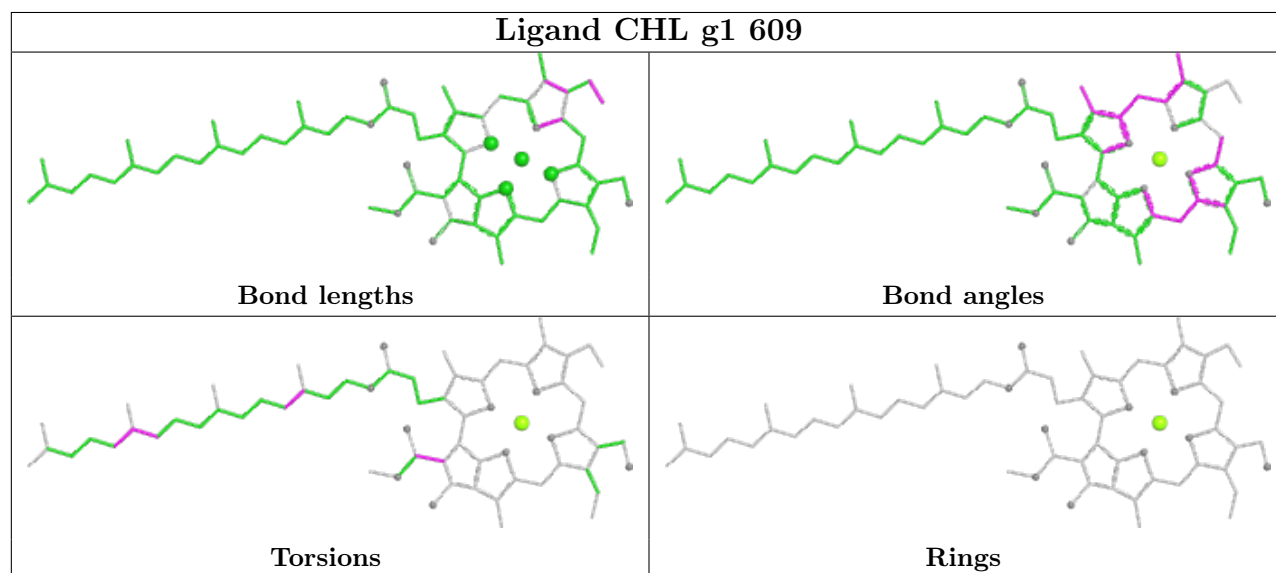
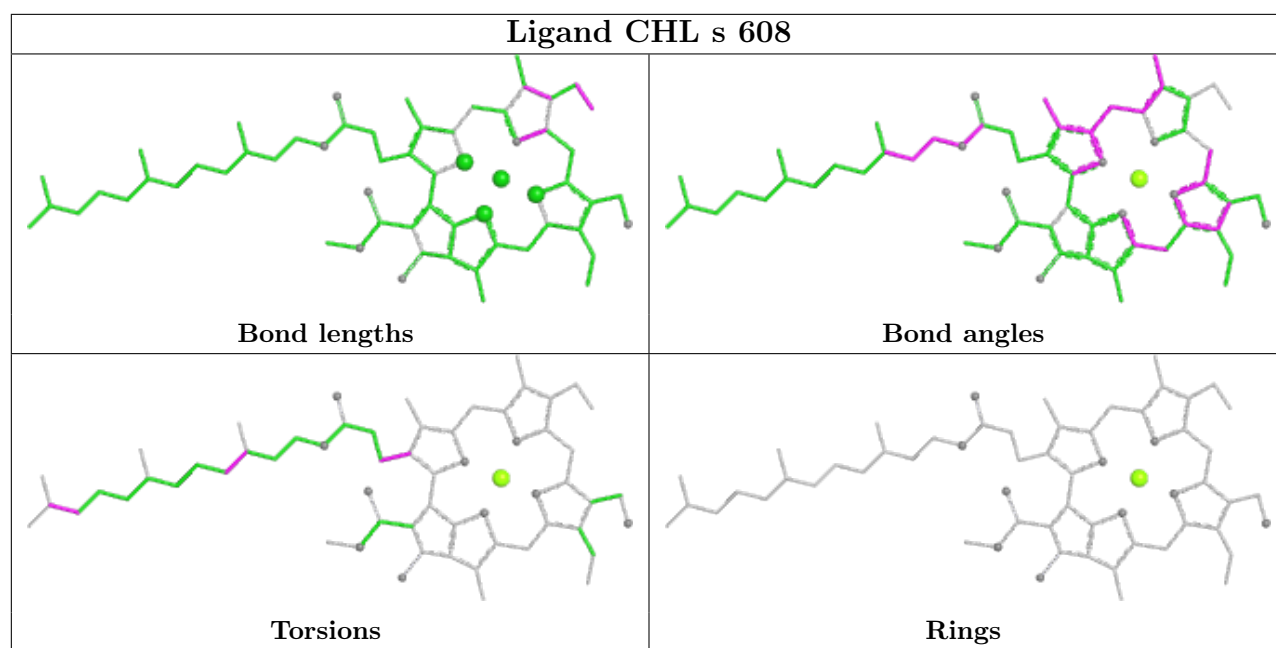


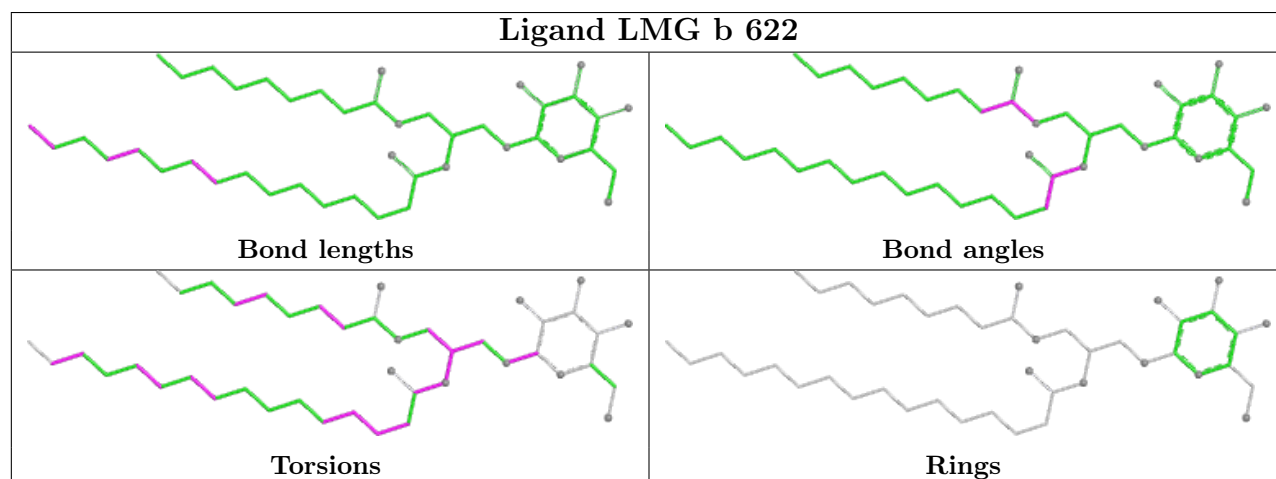
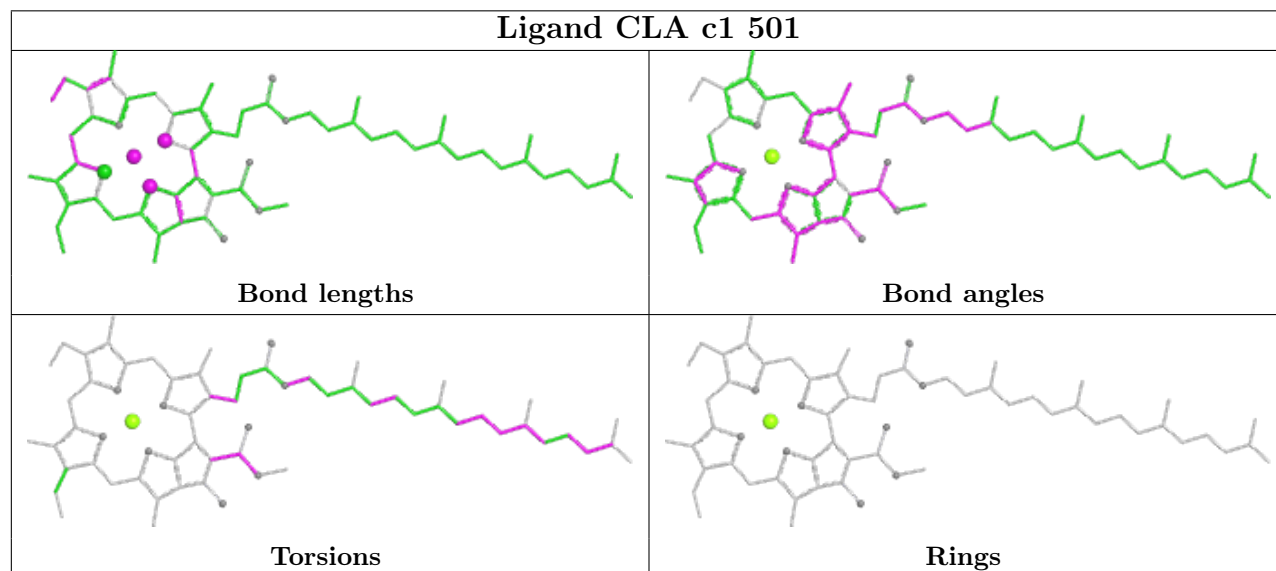
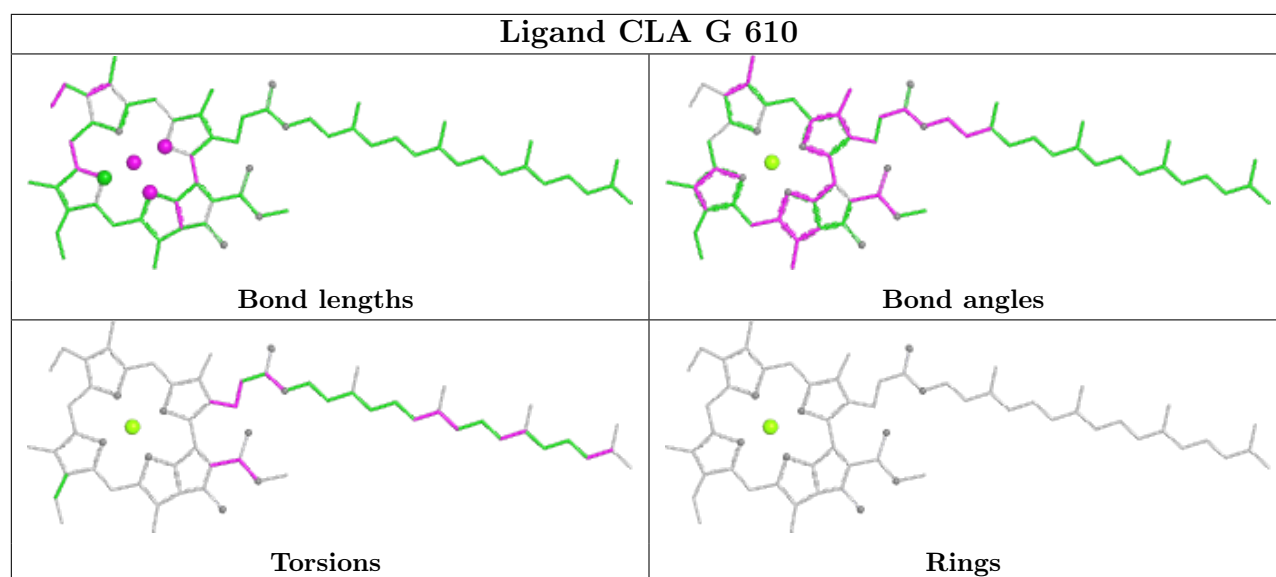
Torsions

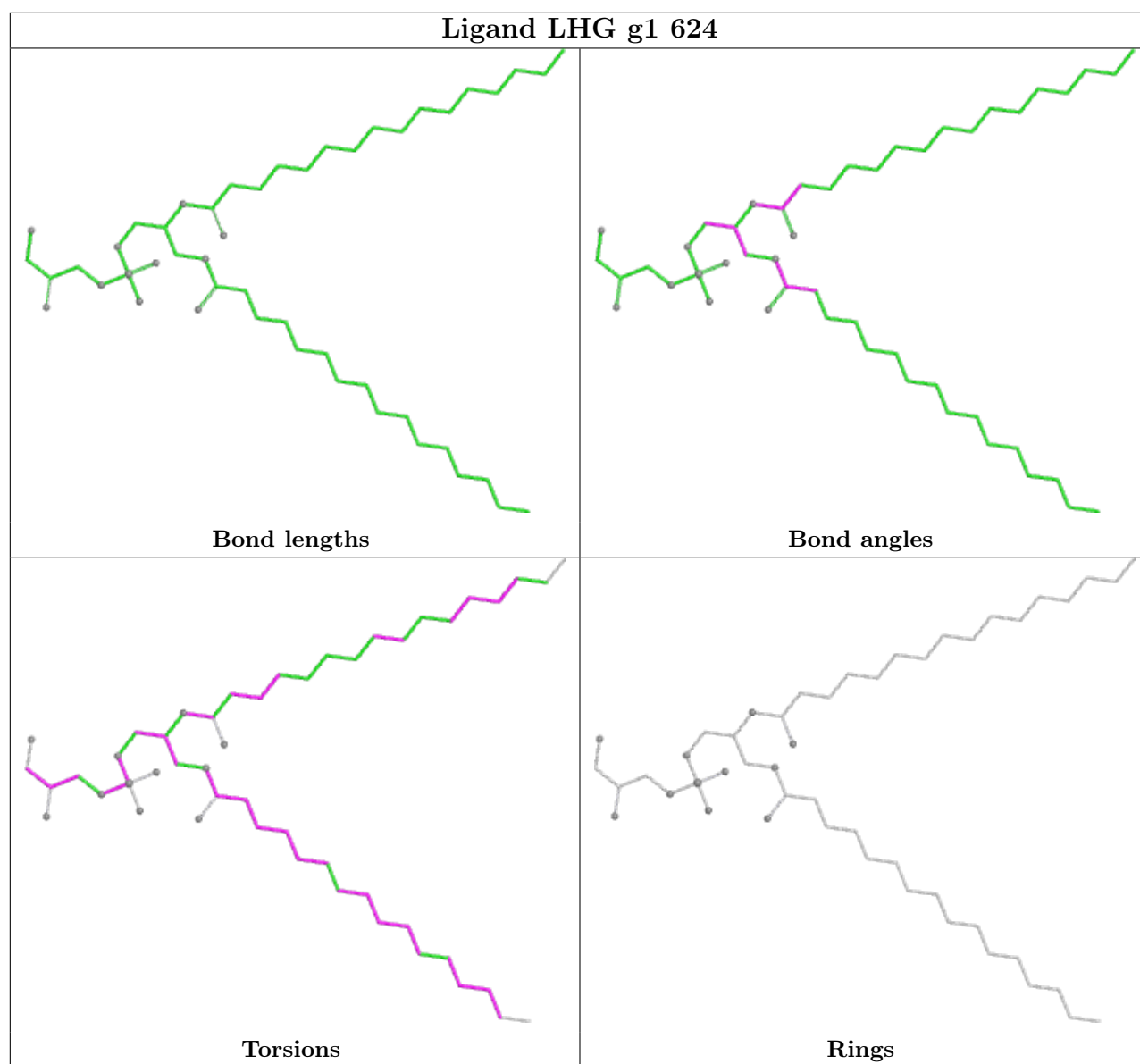


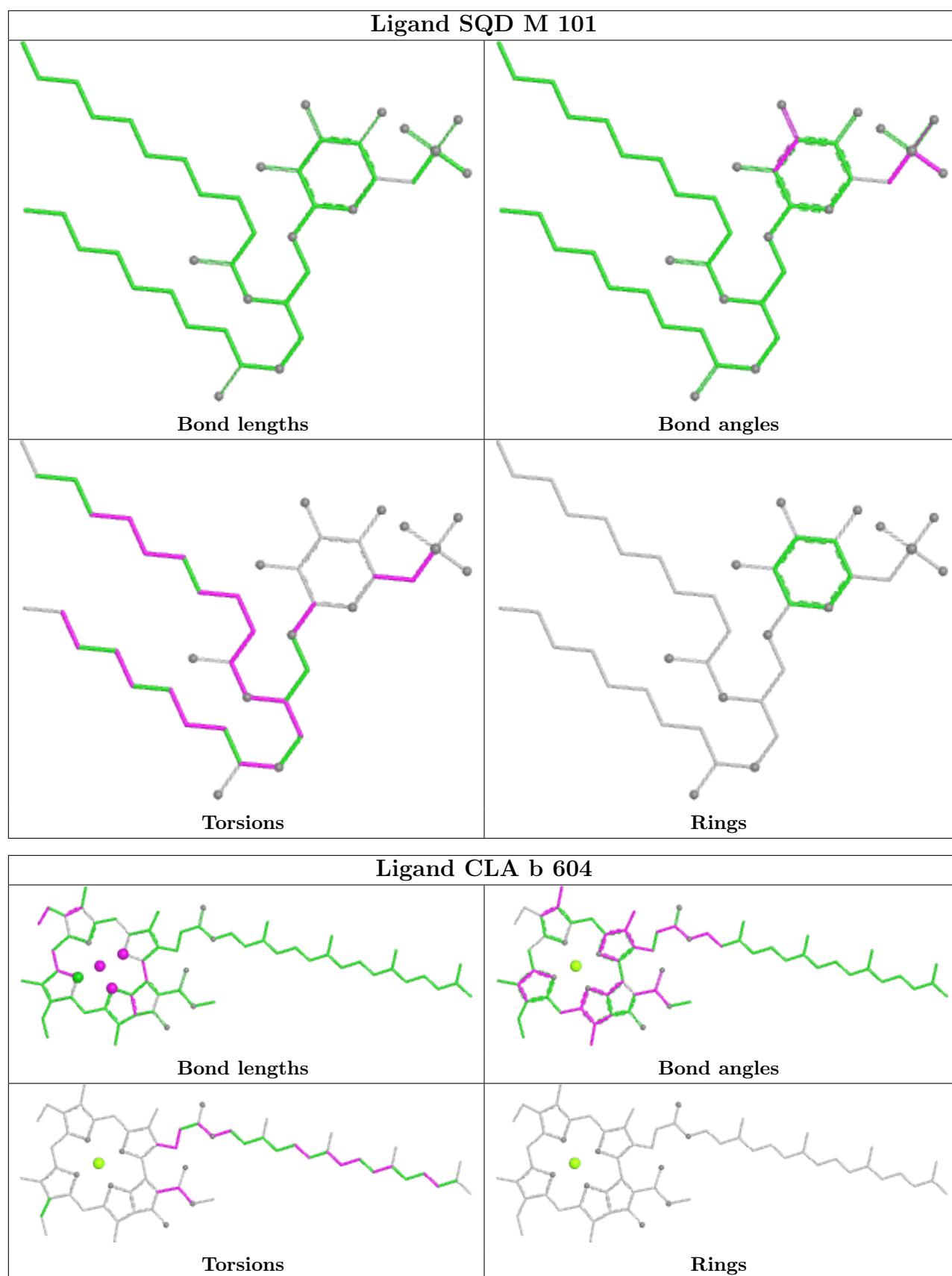
Rings

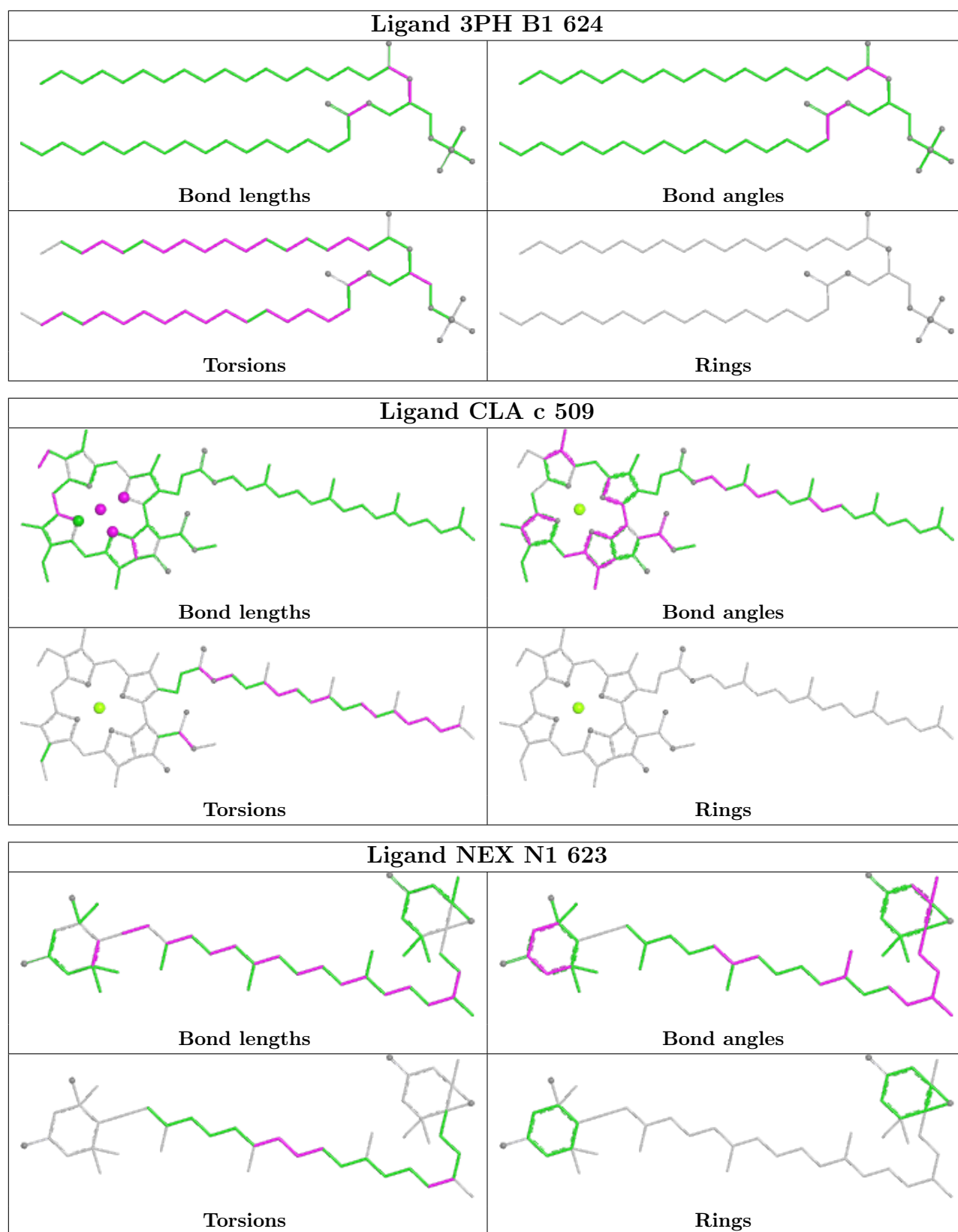




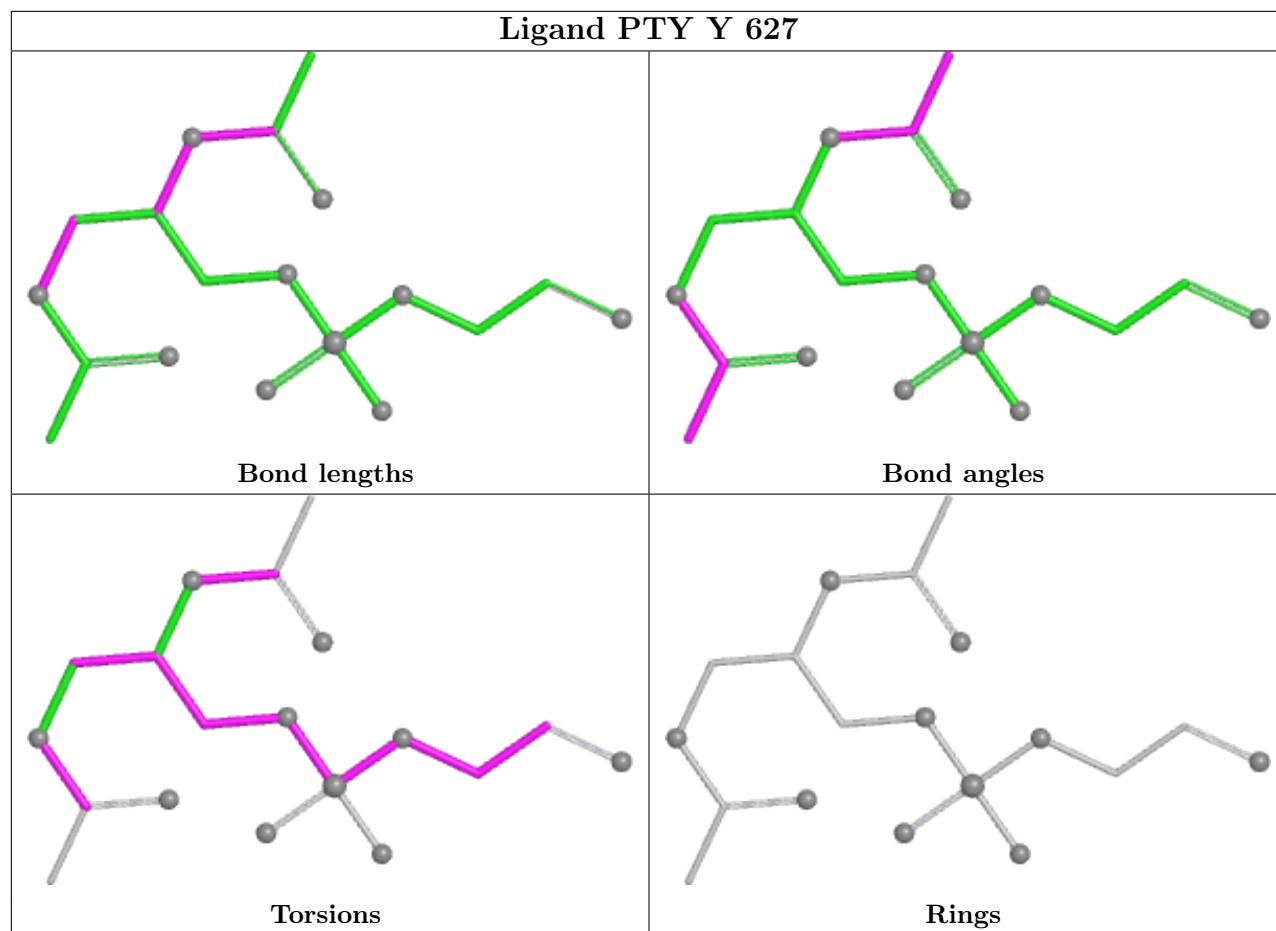




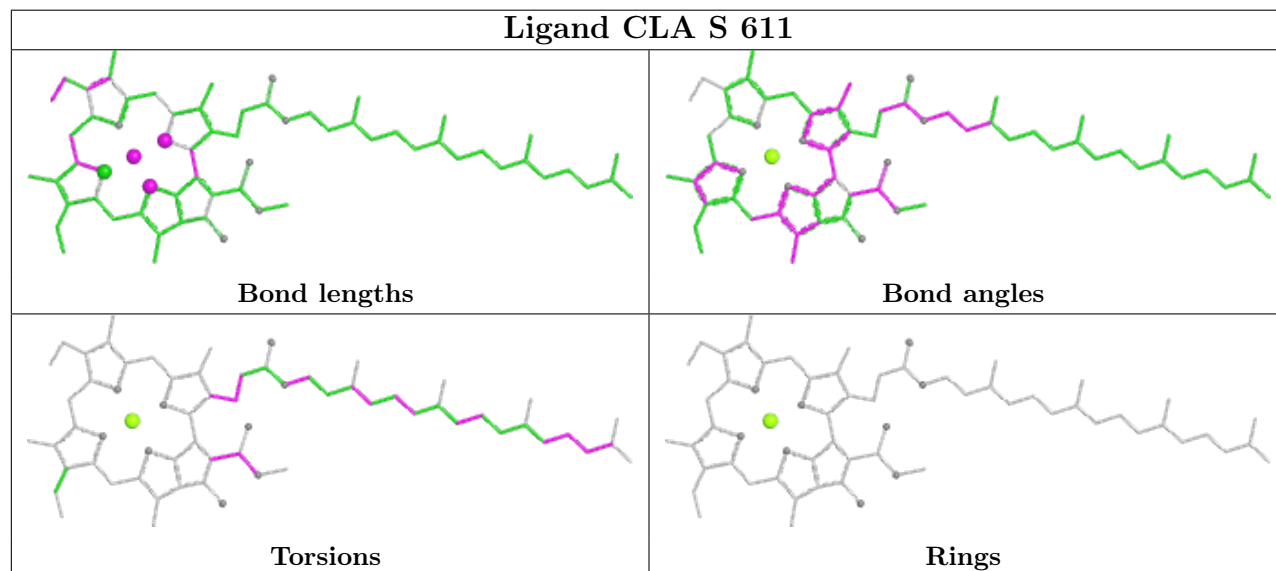




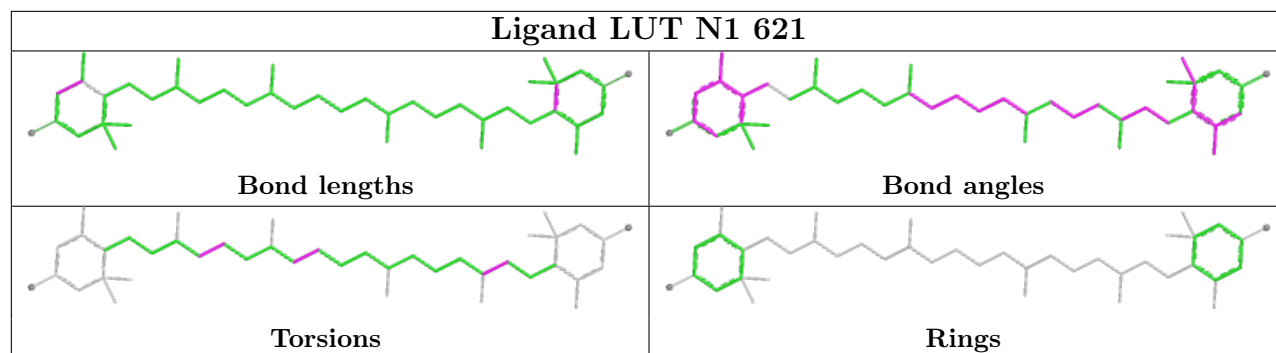
Ligand PTY Y 627



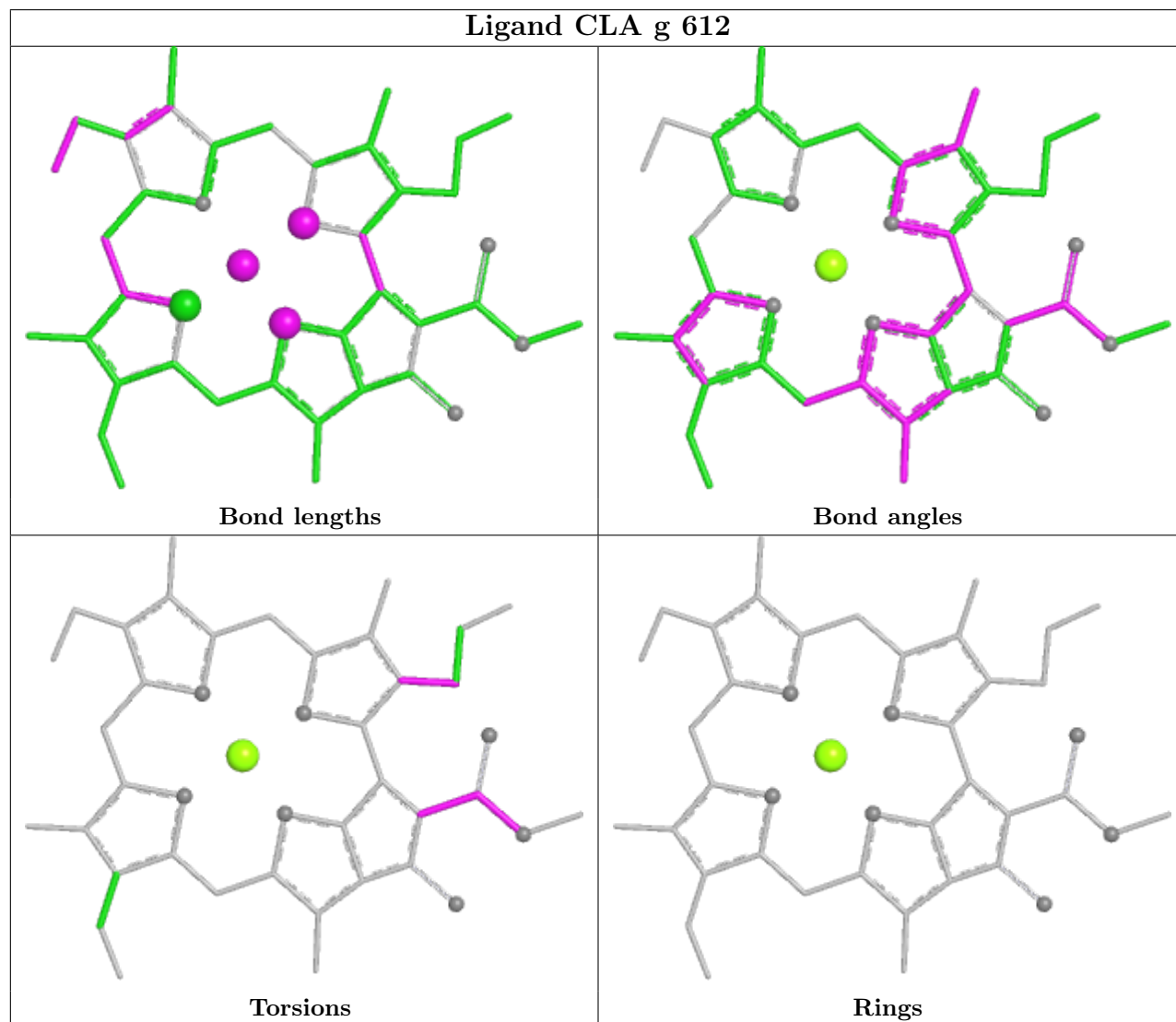
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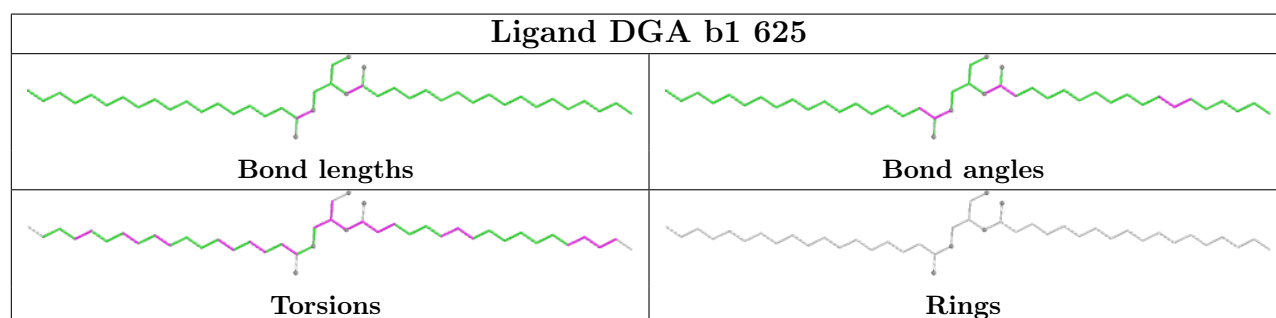
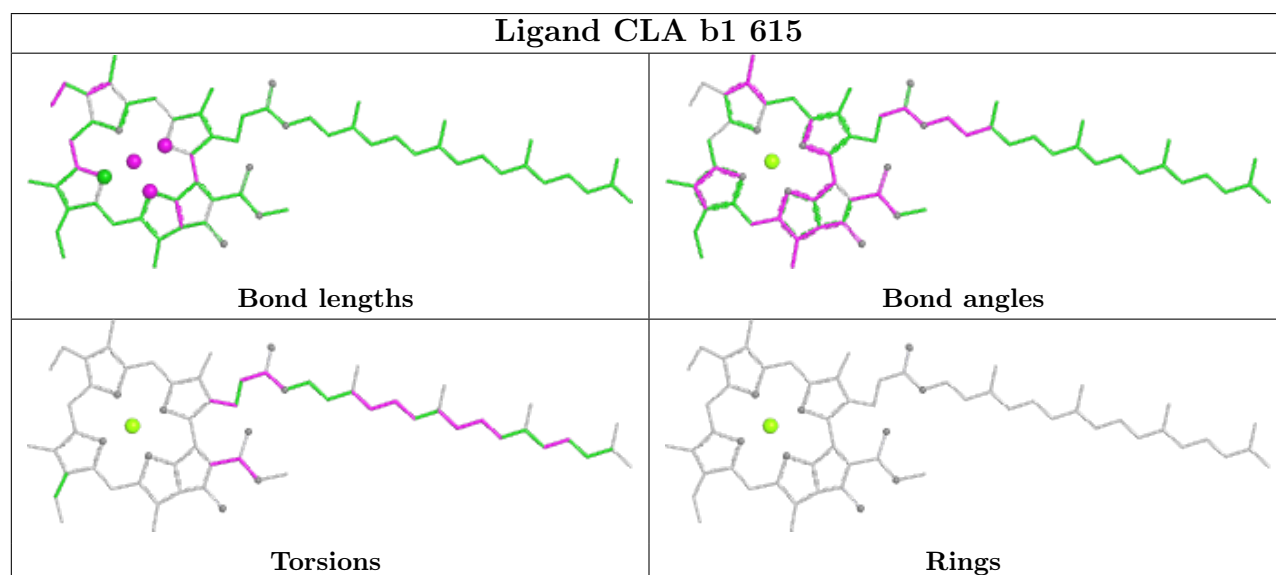
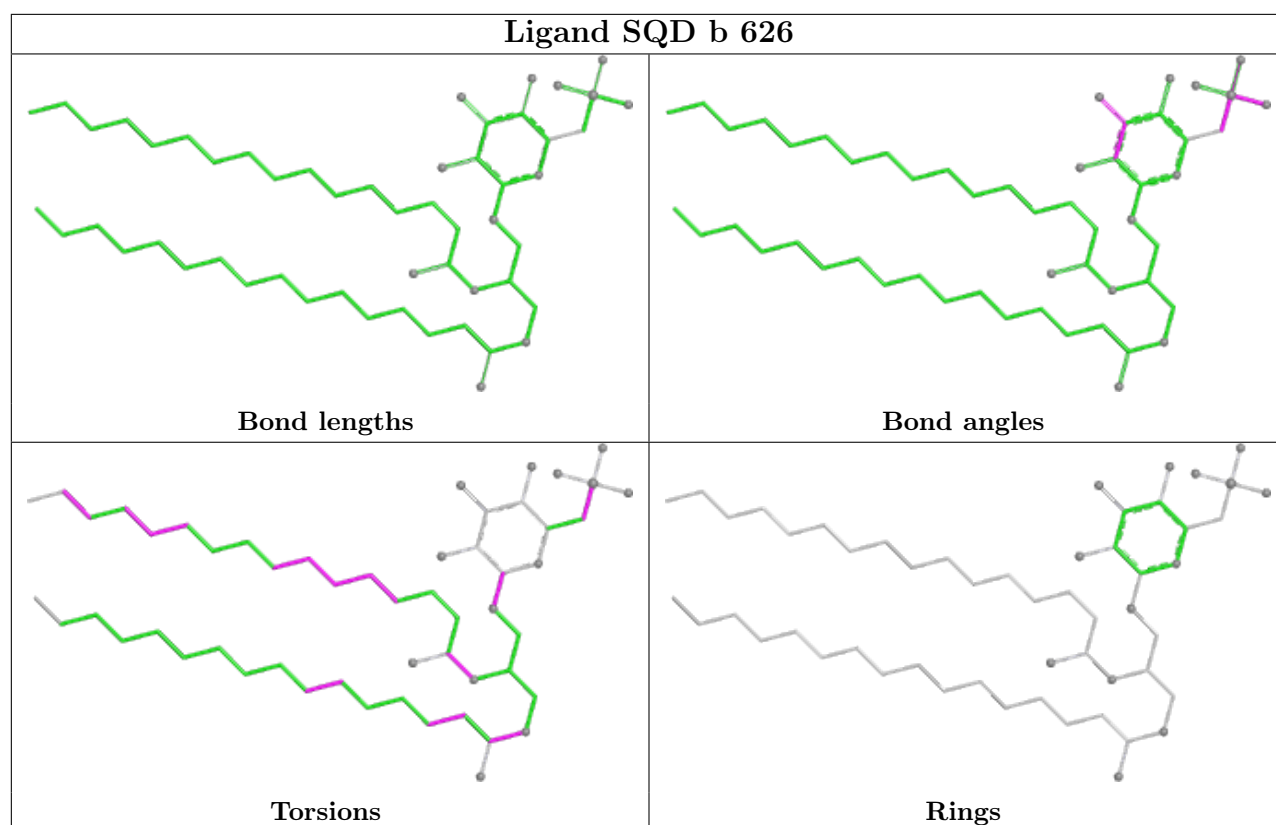


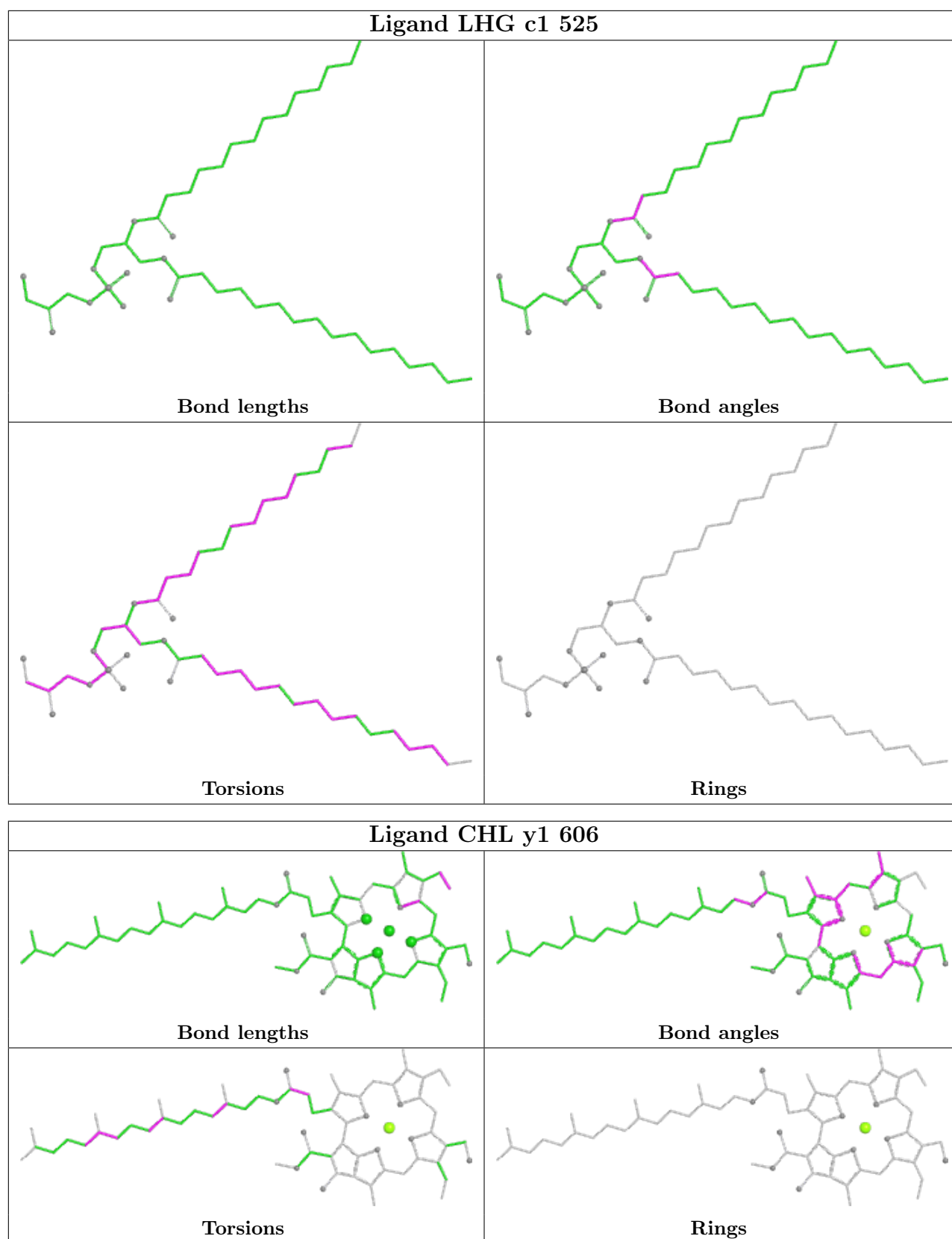
Ligand LUT N1 621

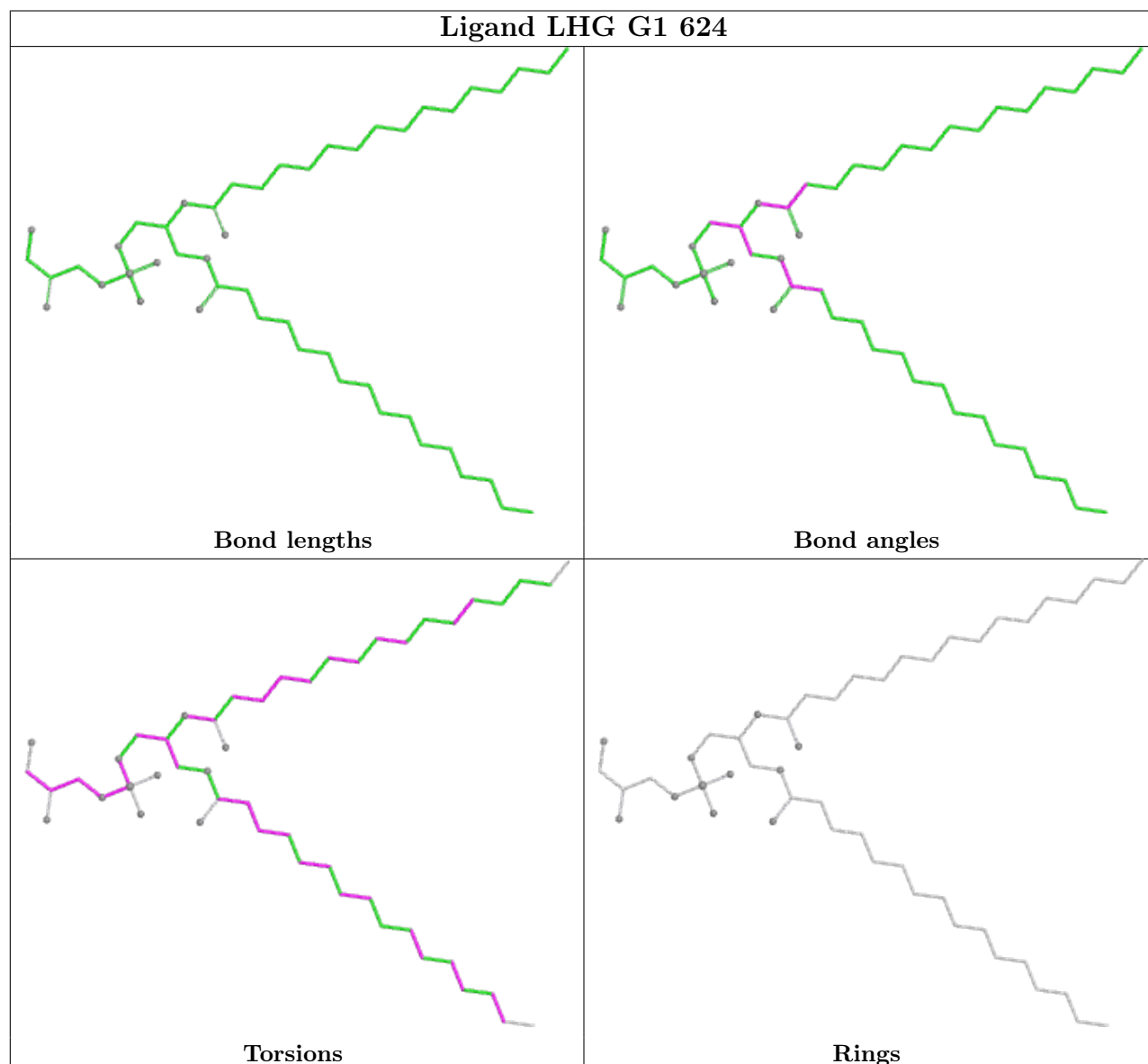
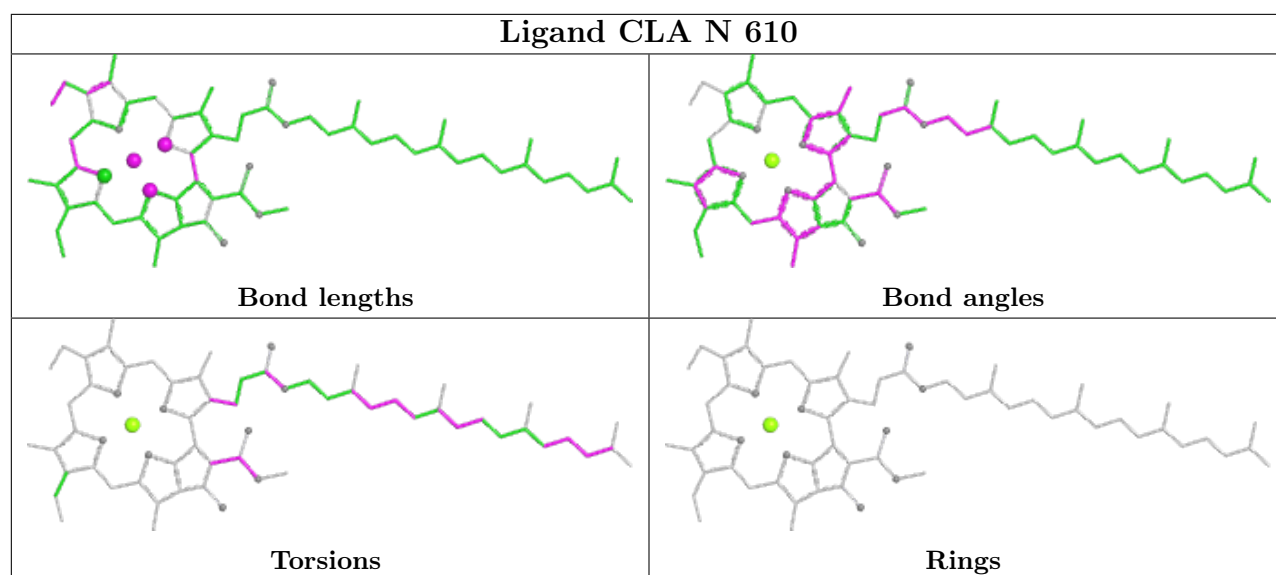


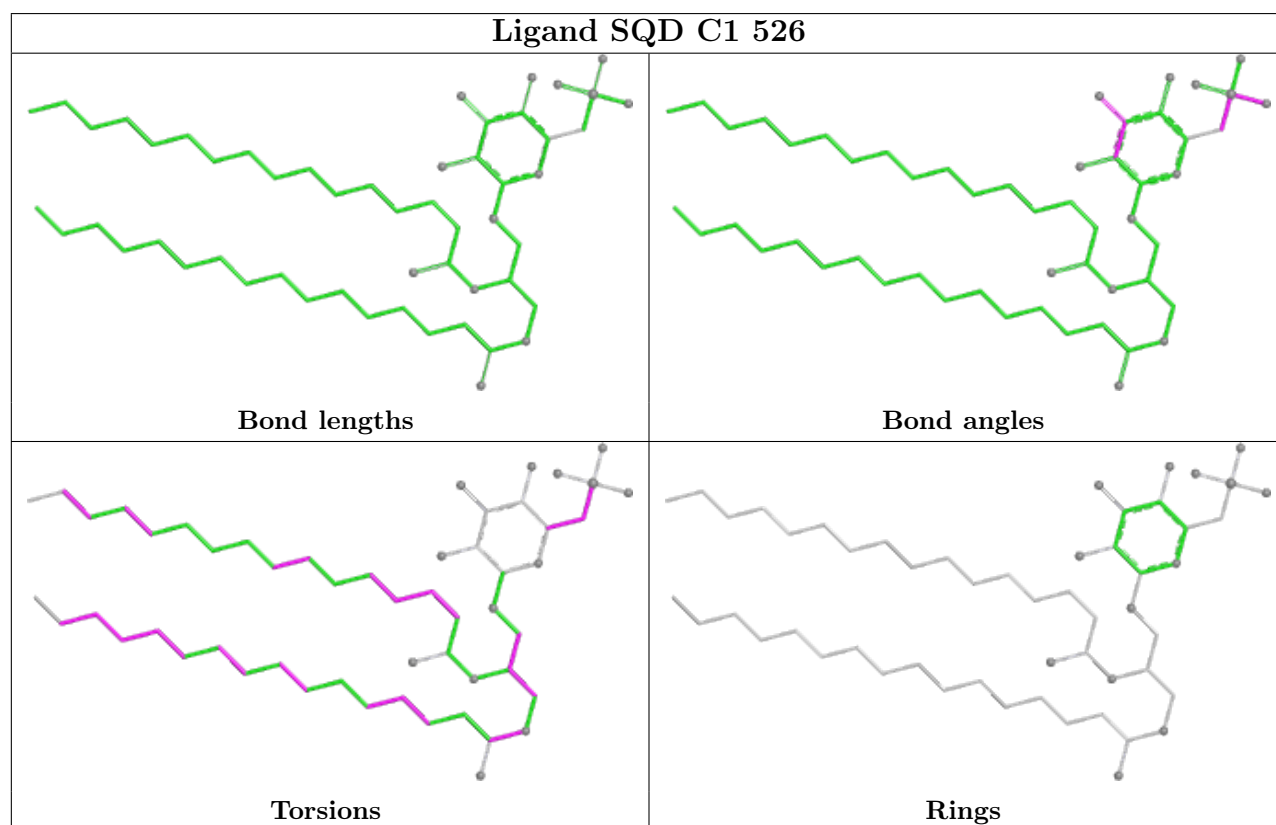
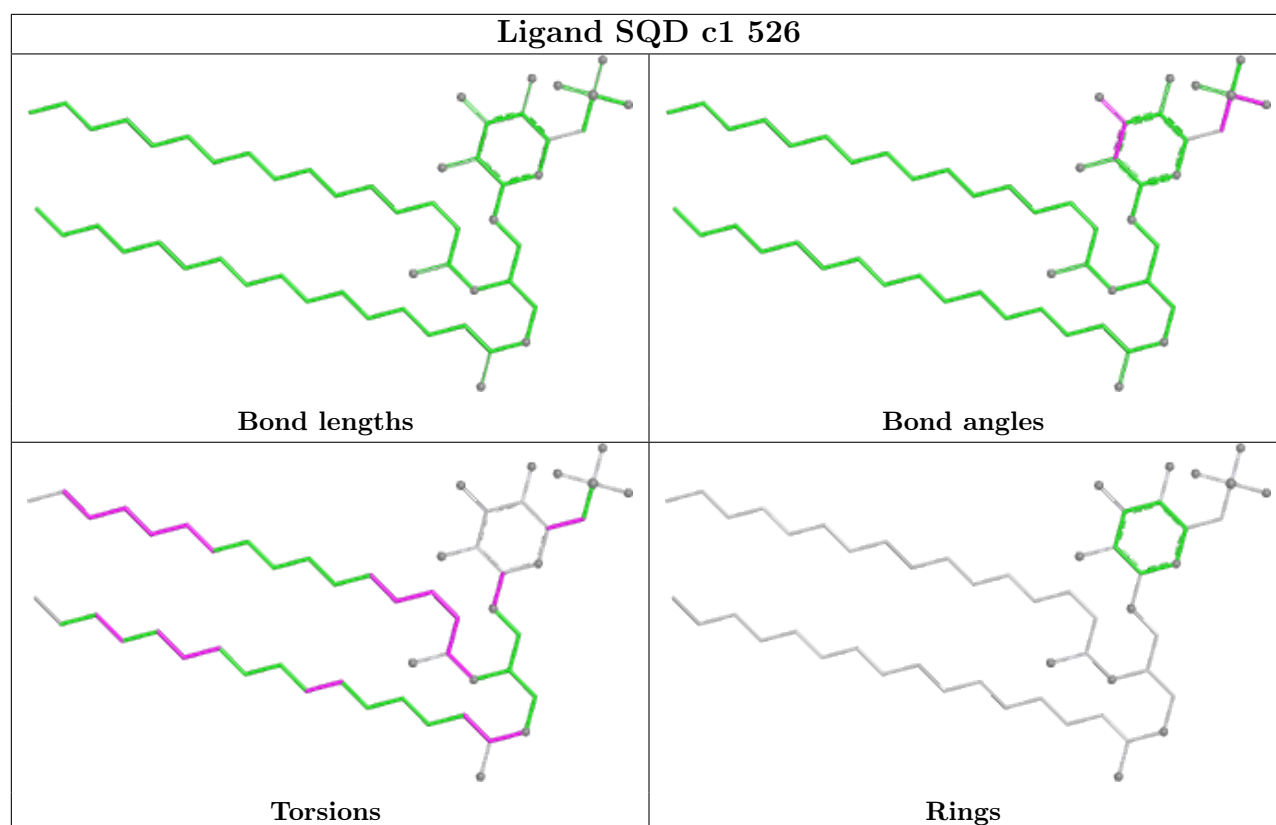
Ligand CLA g 612

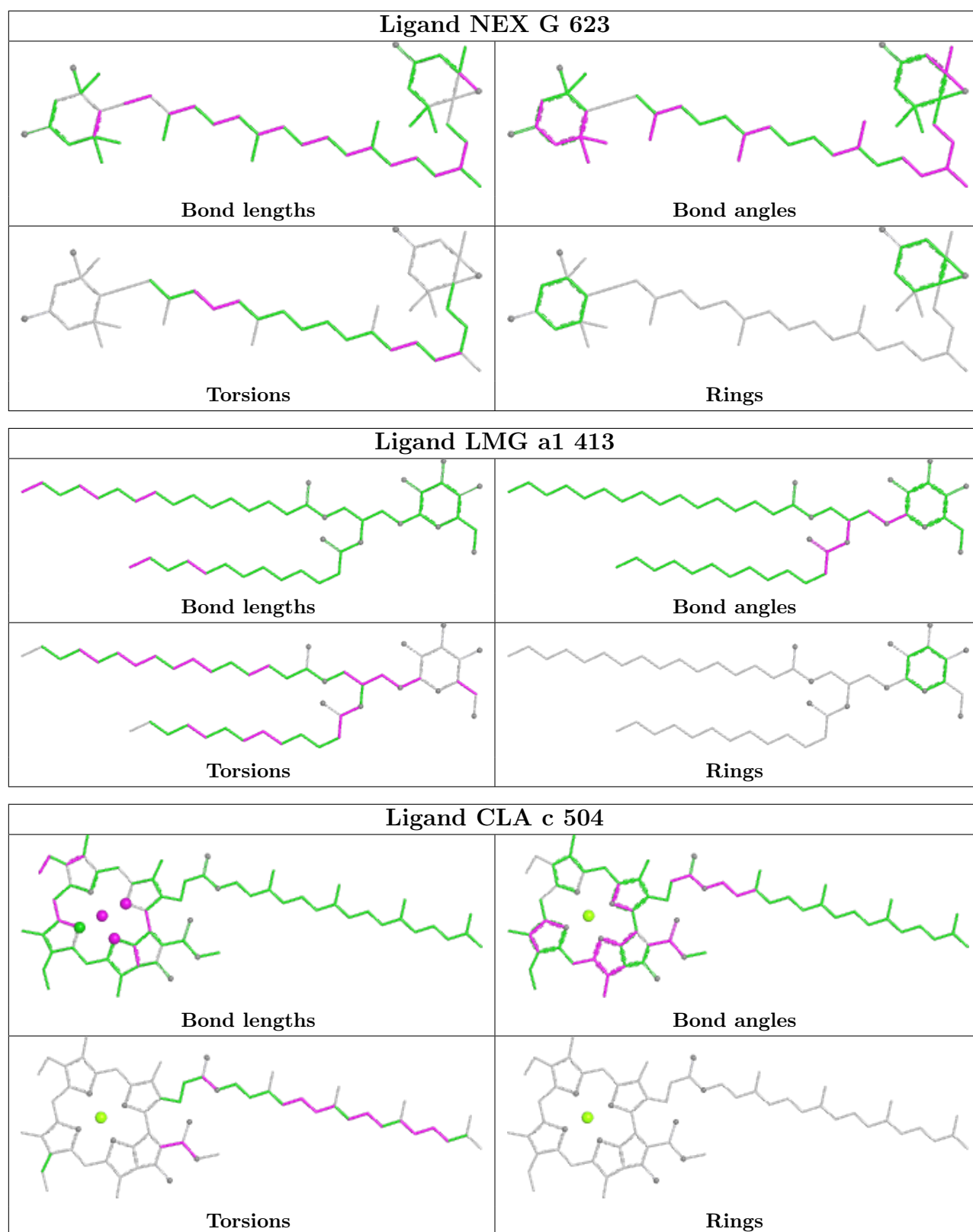


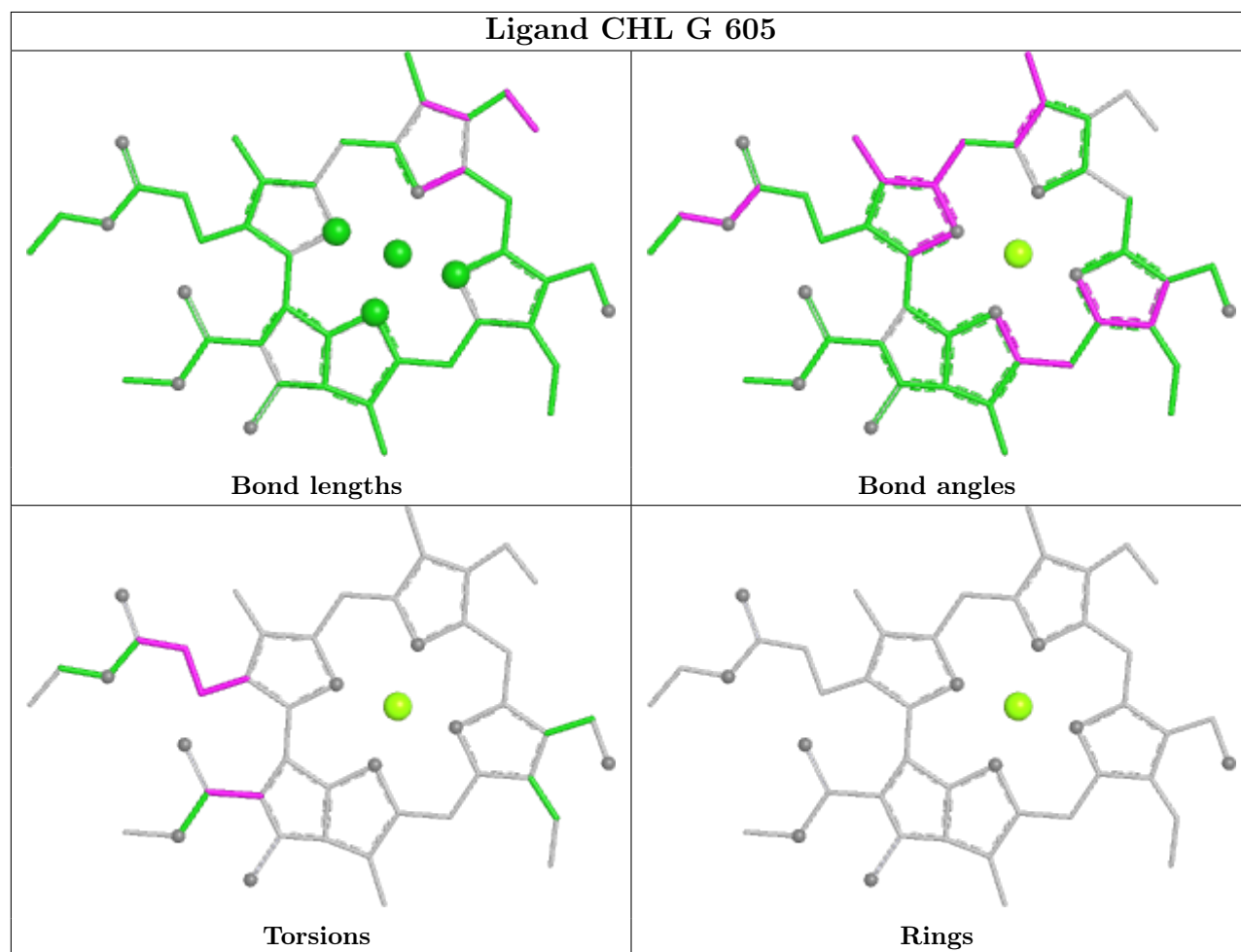
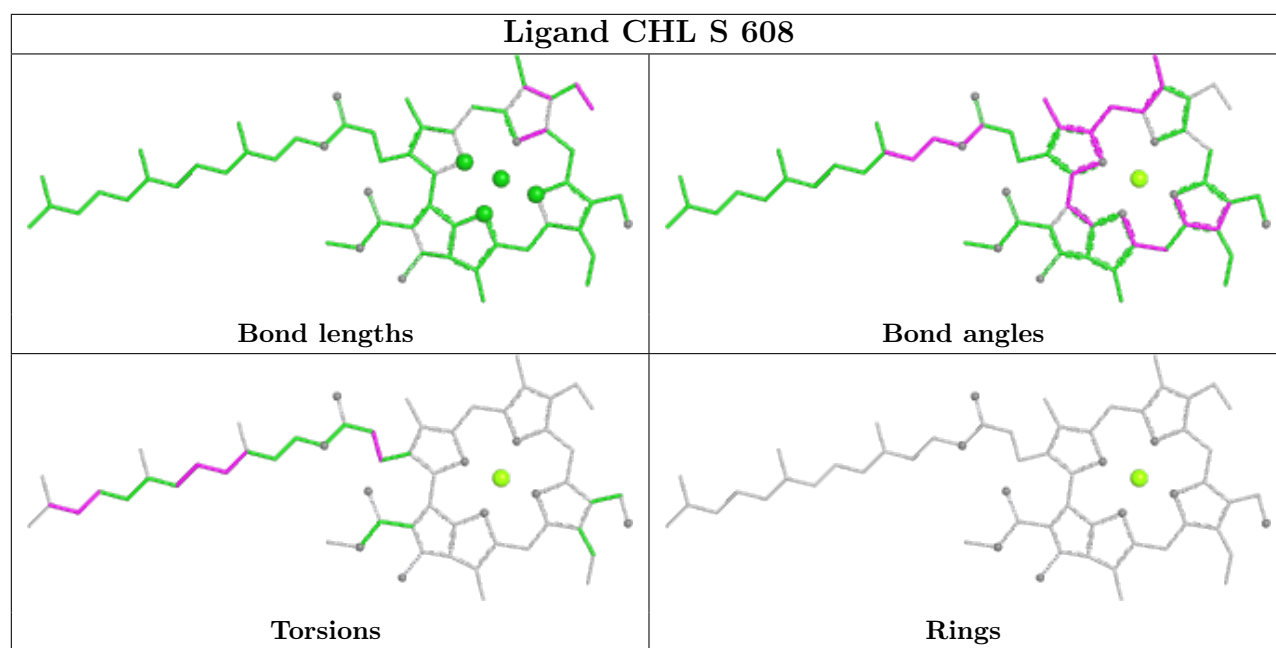


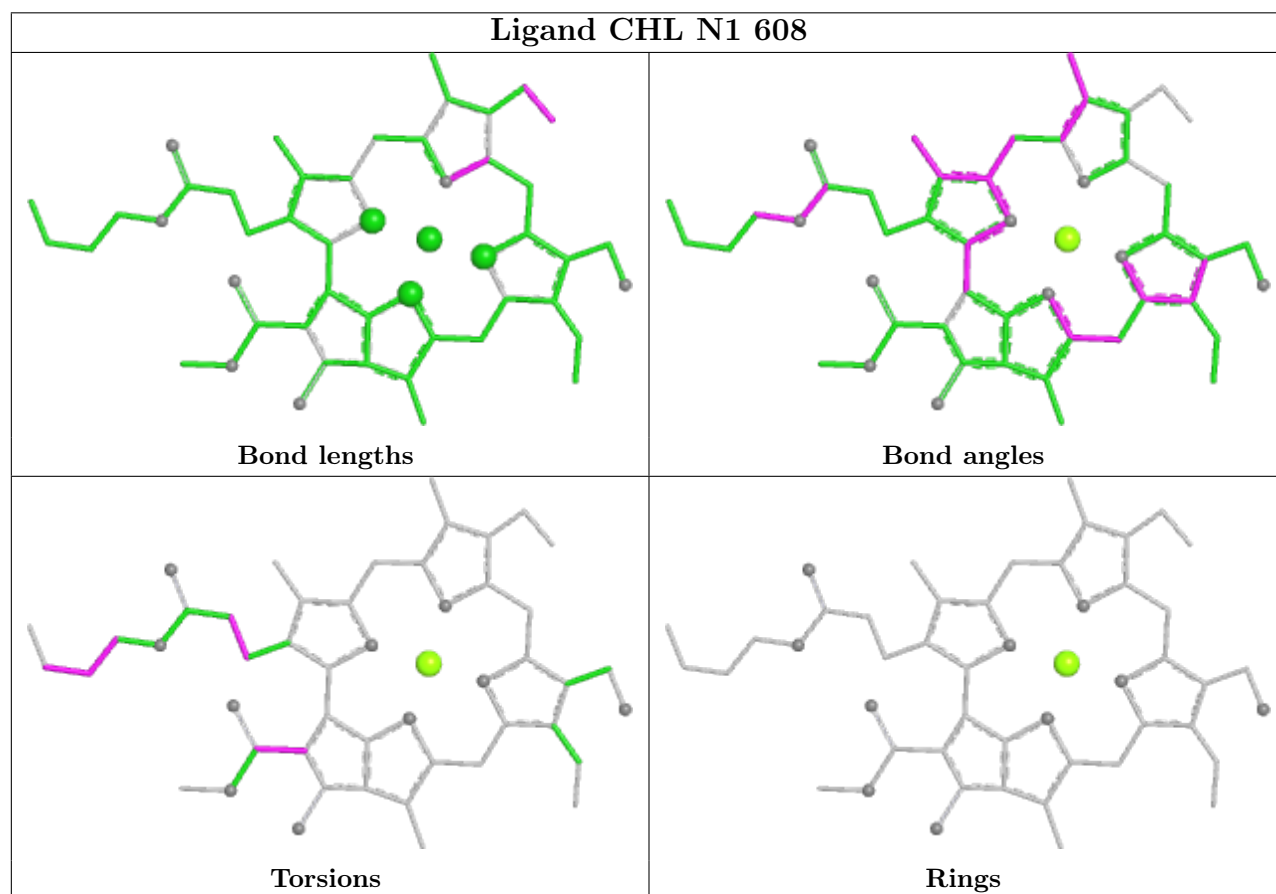
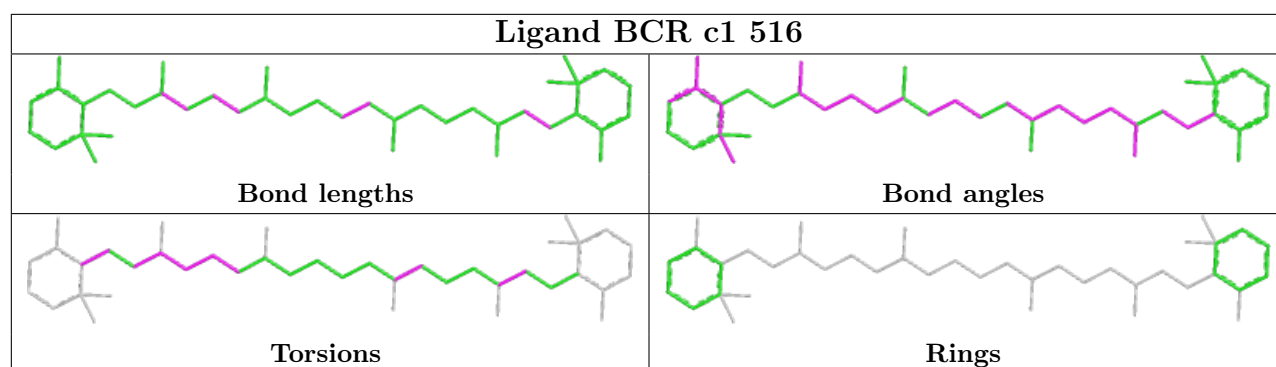


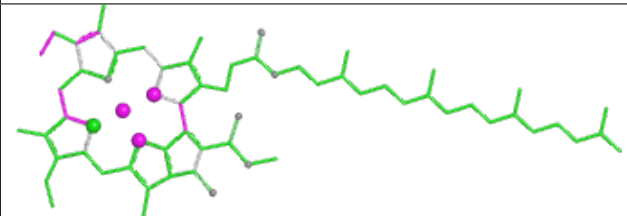
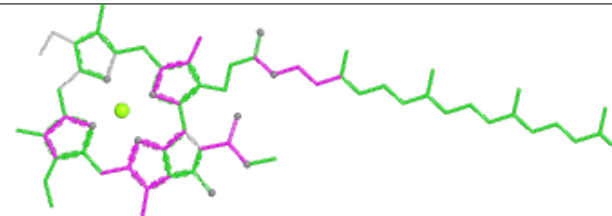
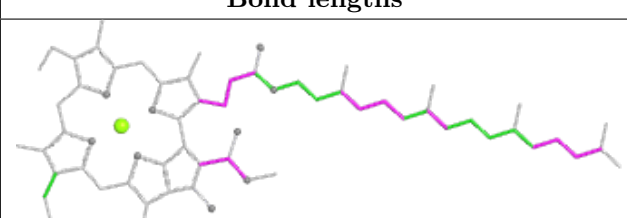
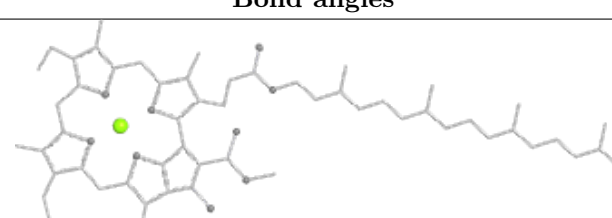


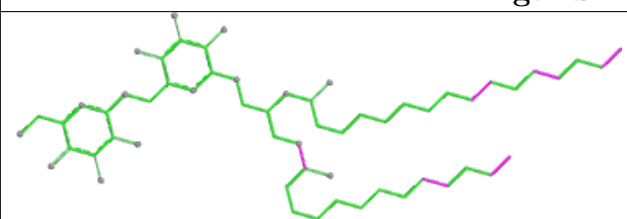
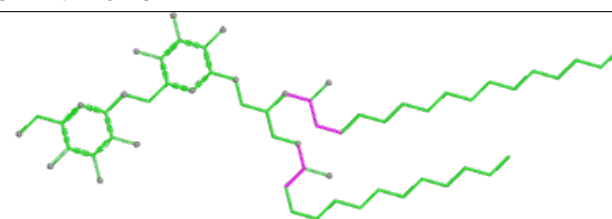
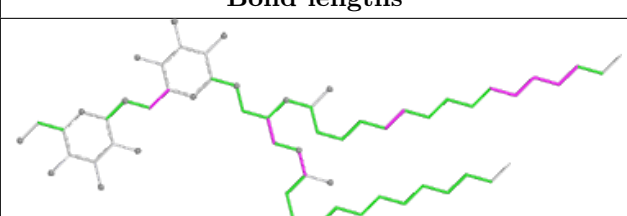
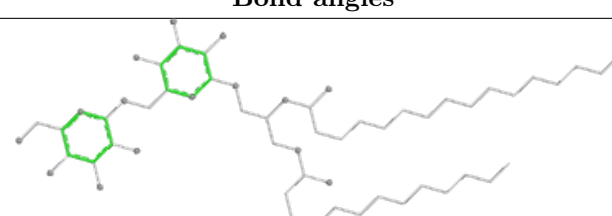


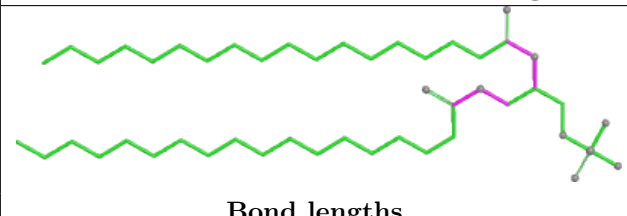
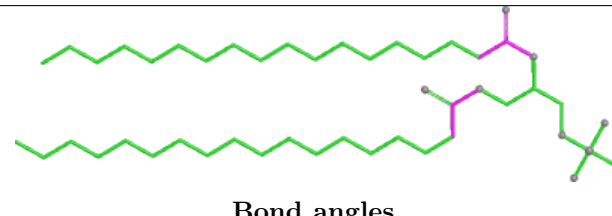
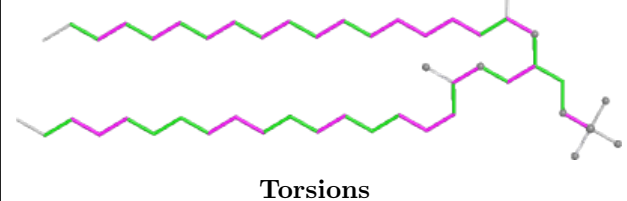
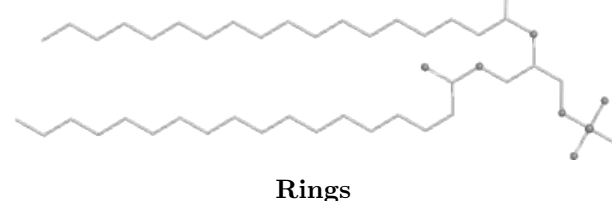


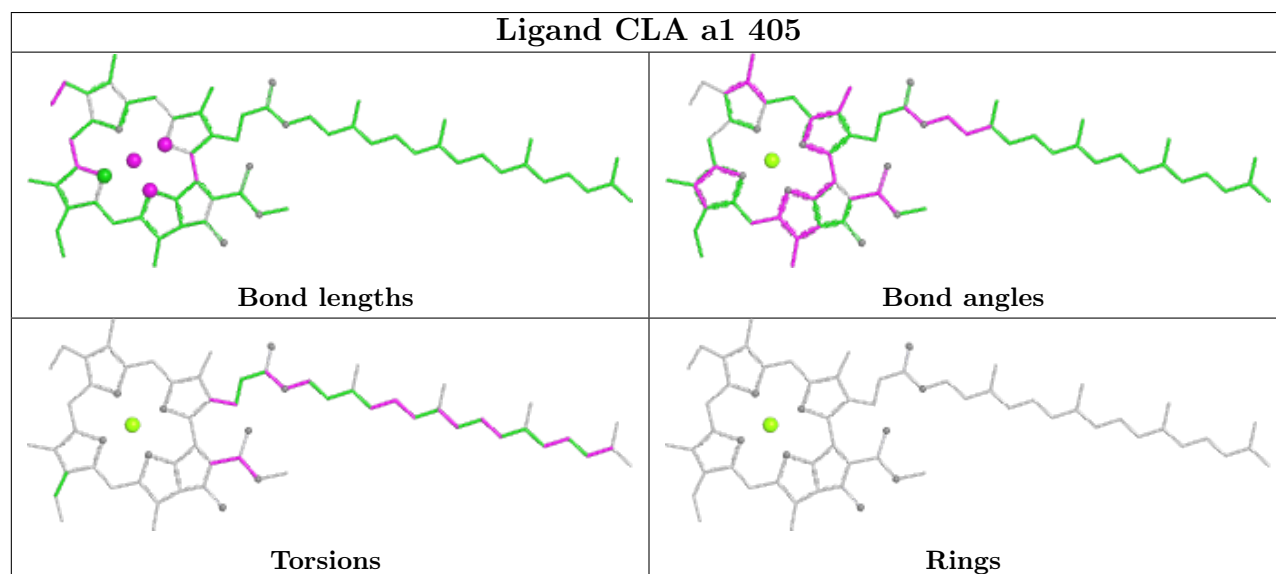
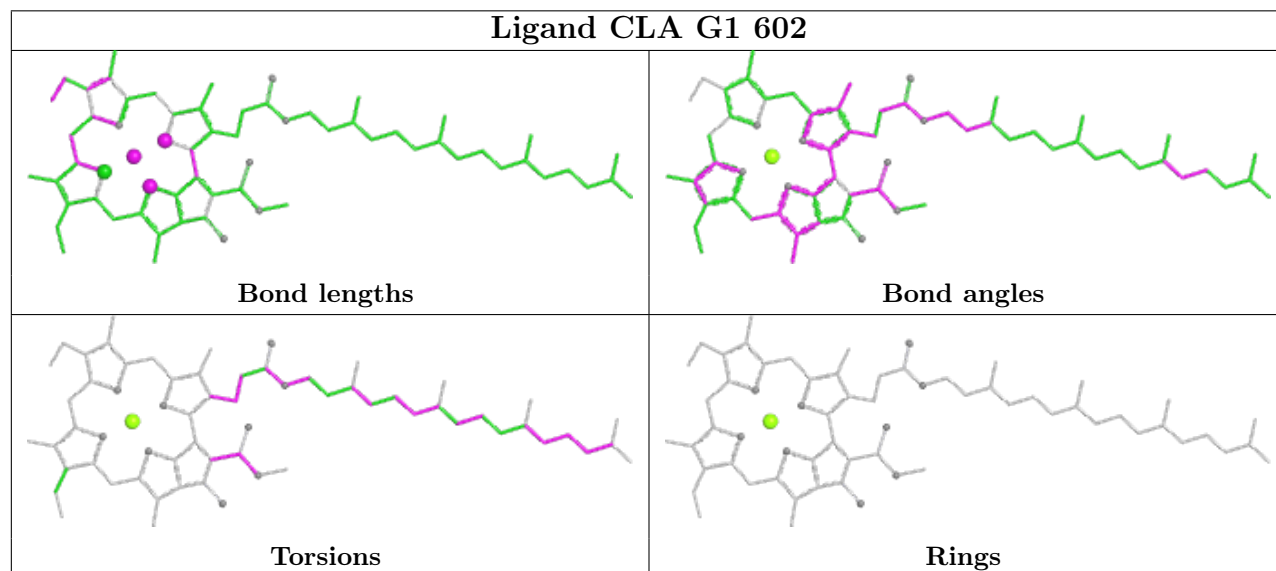
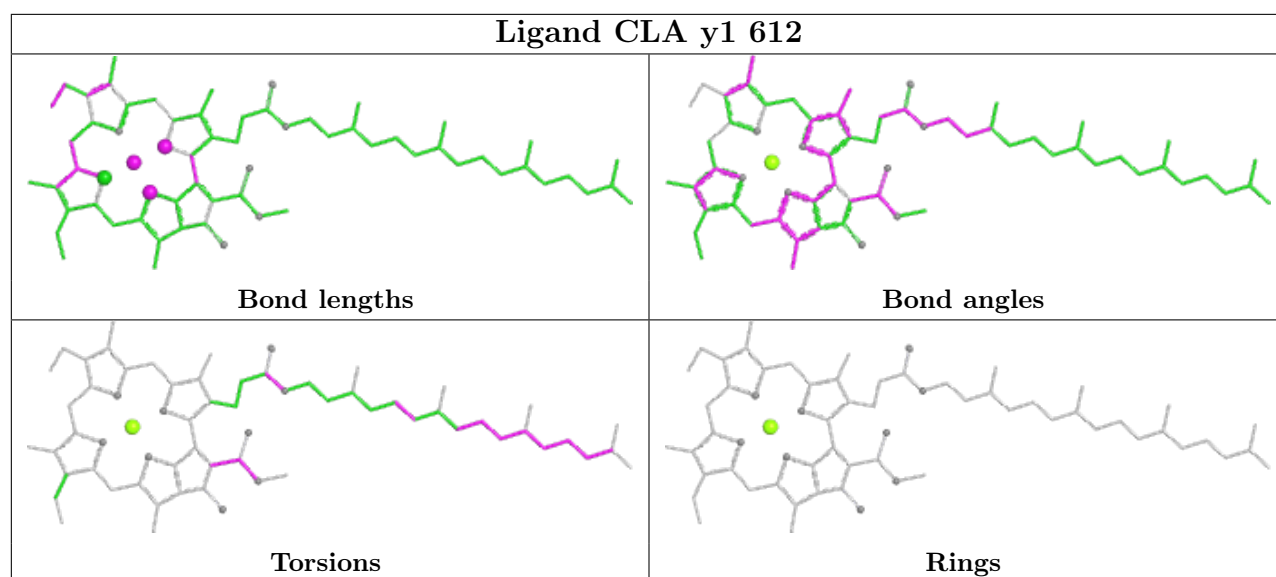


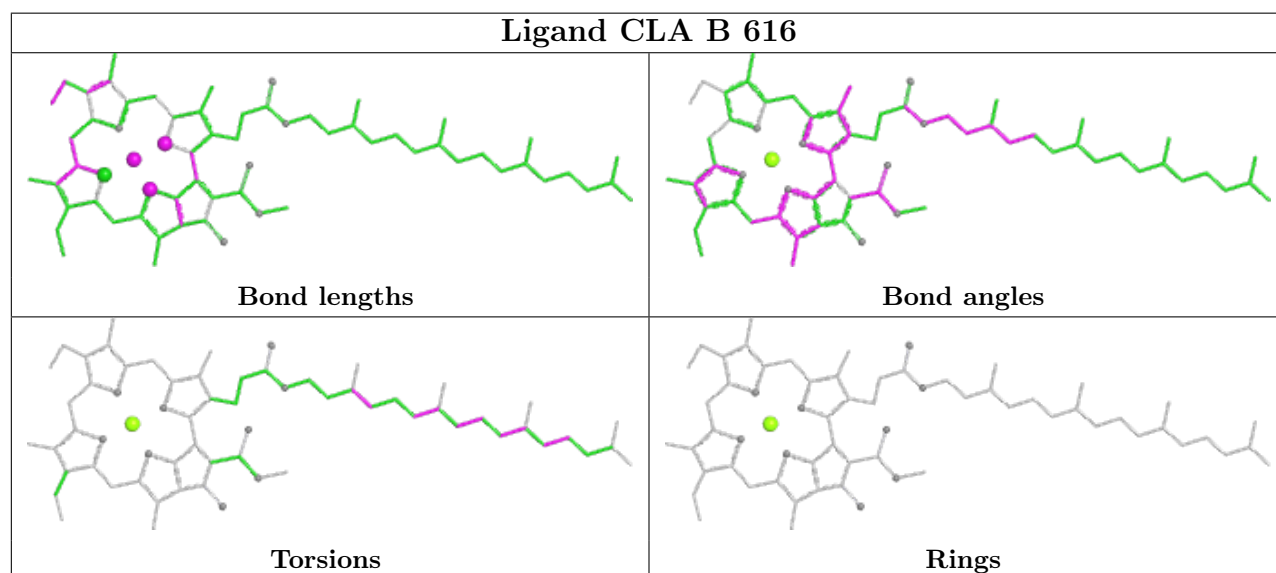
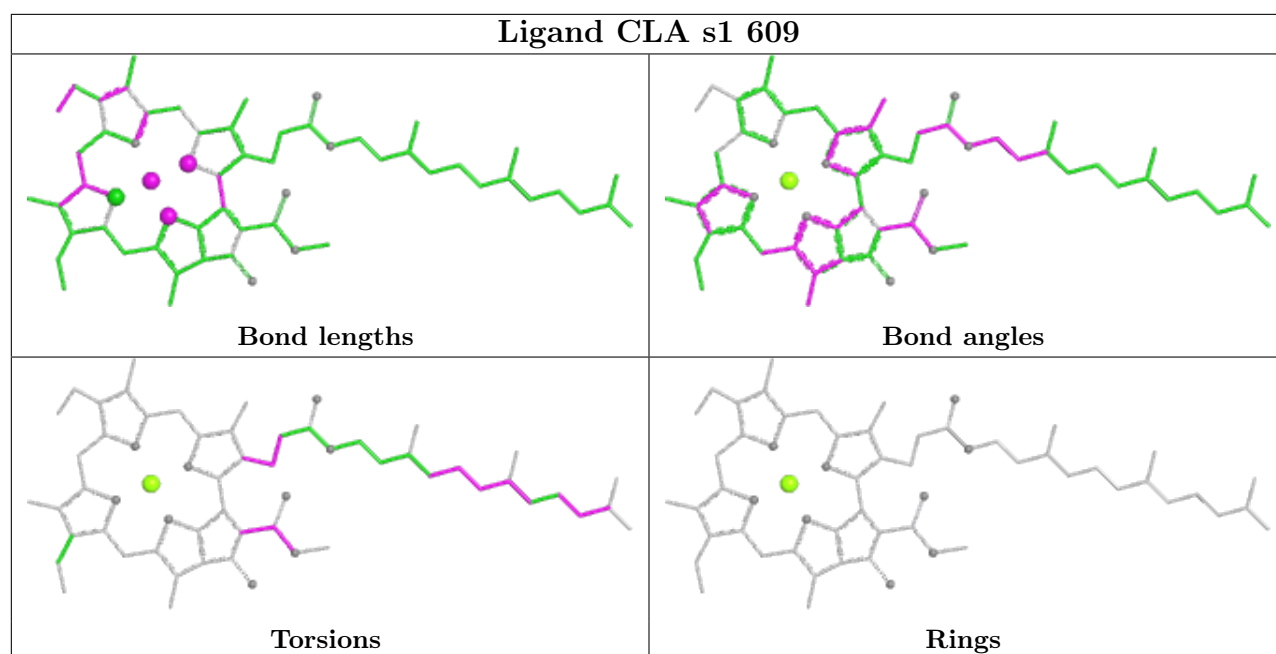


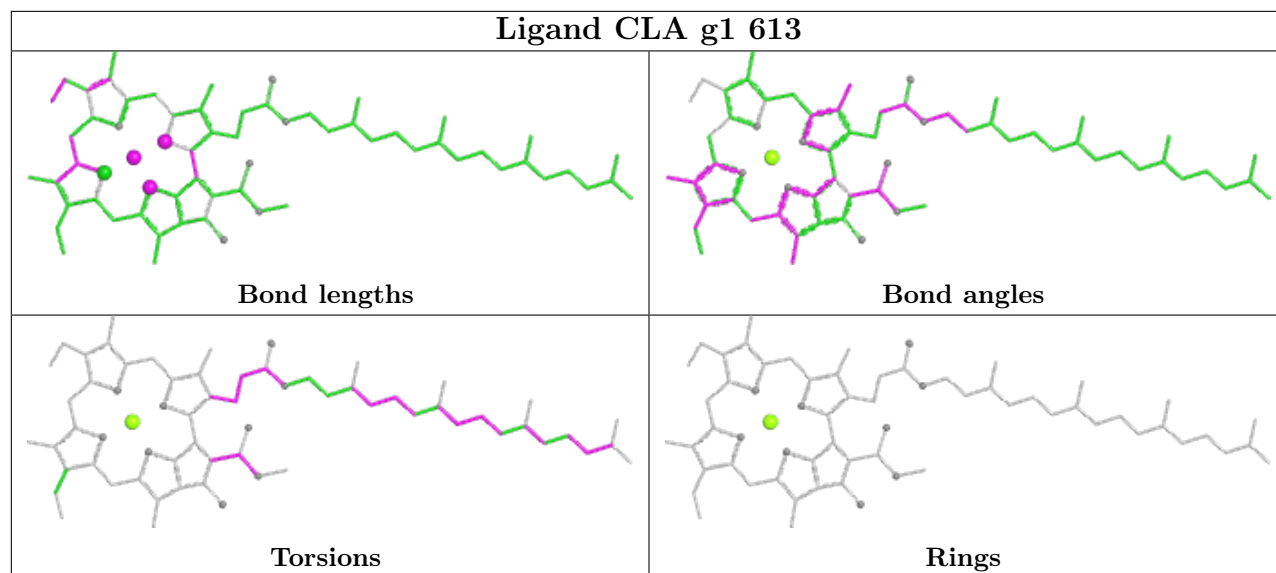
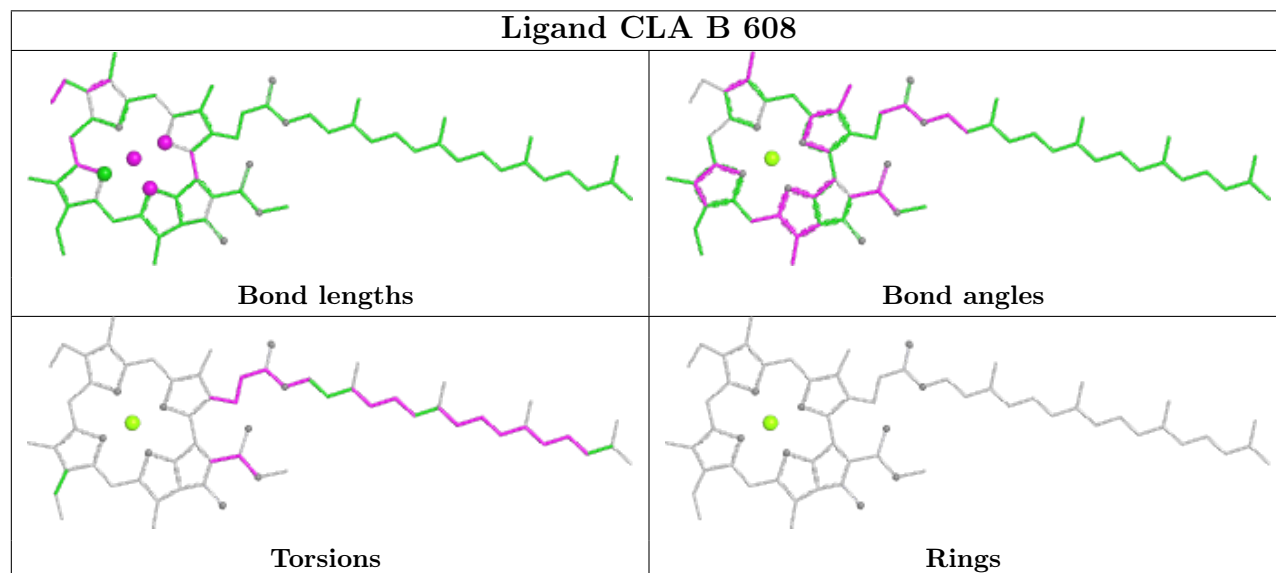
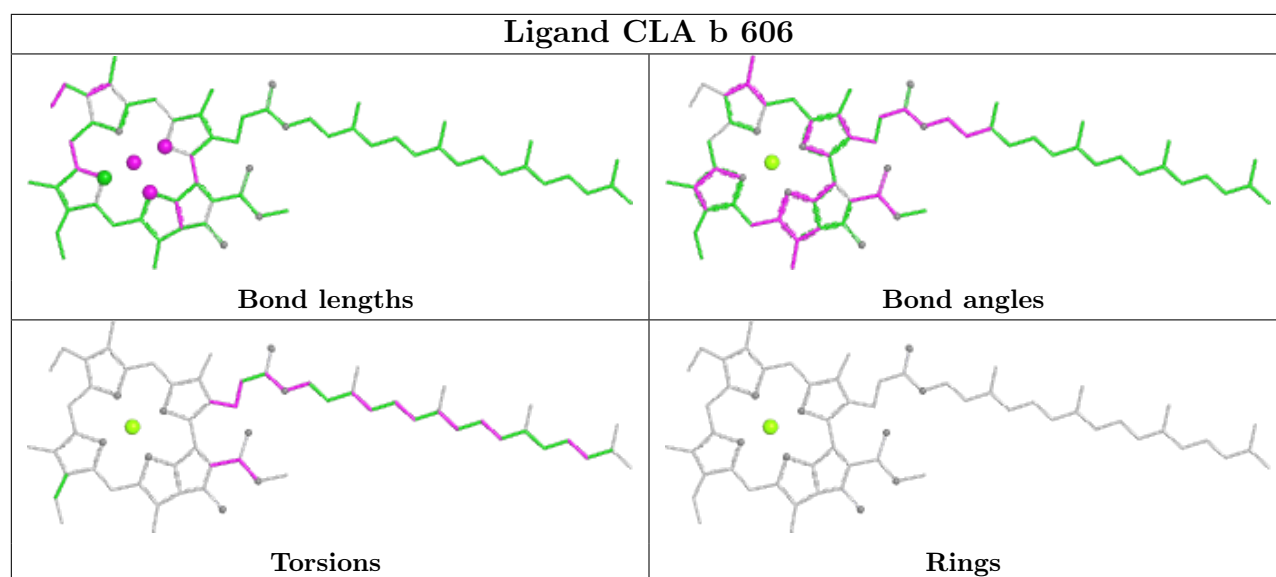
Ligand CLA y1 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

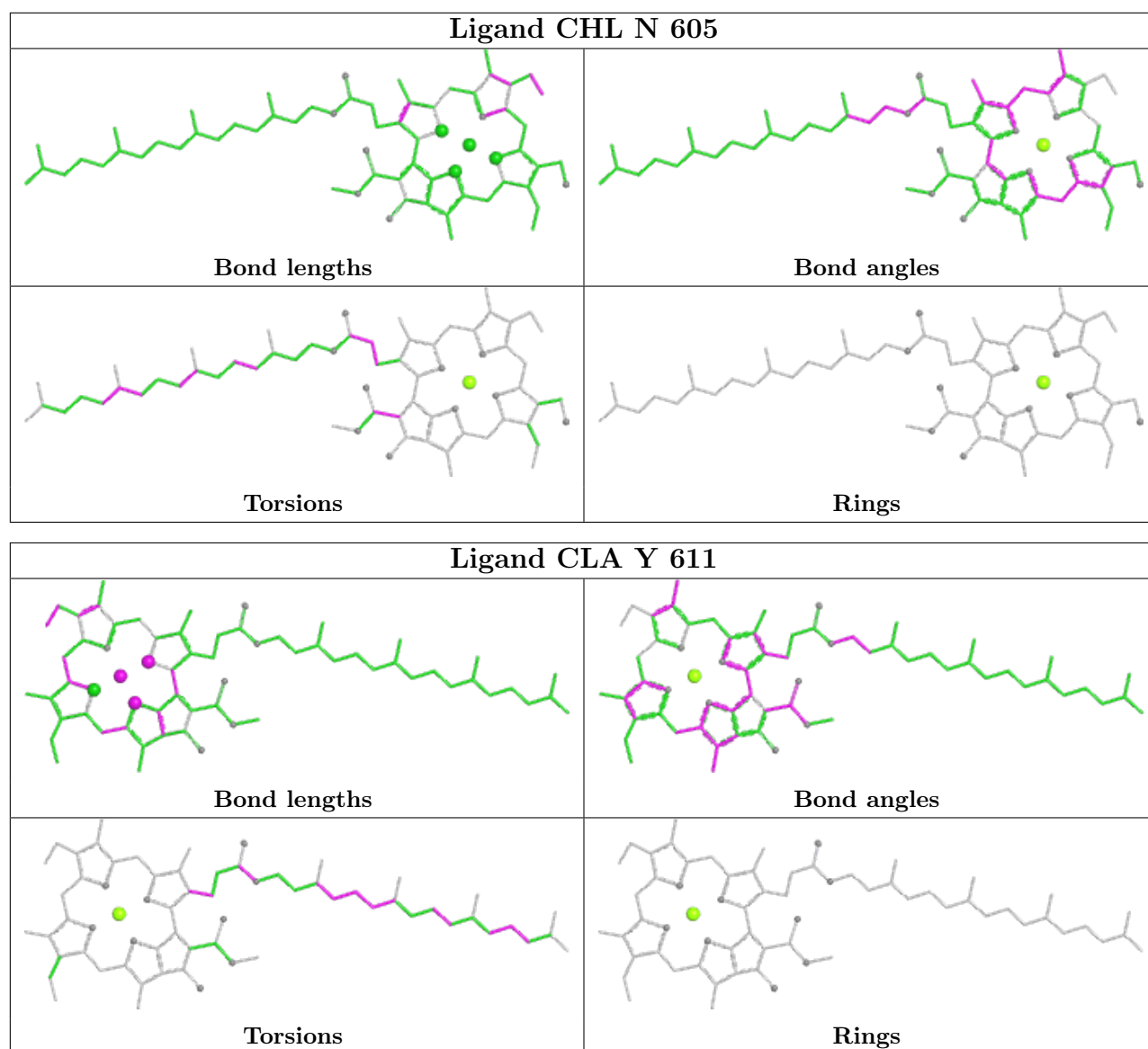
Ligand DGD c1 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

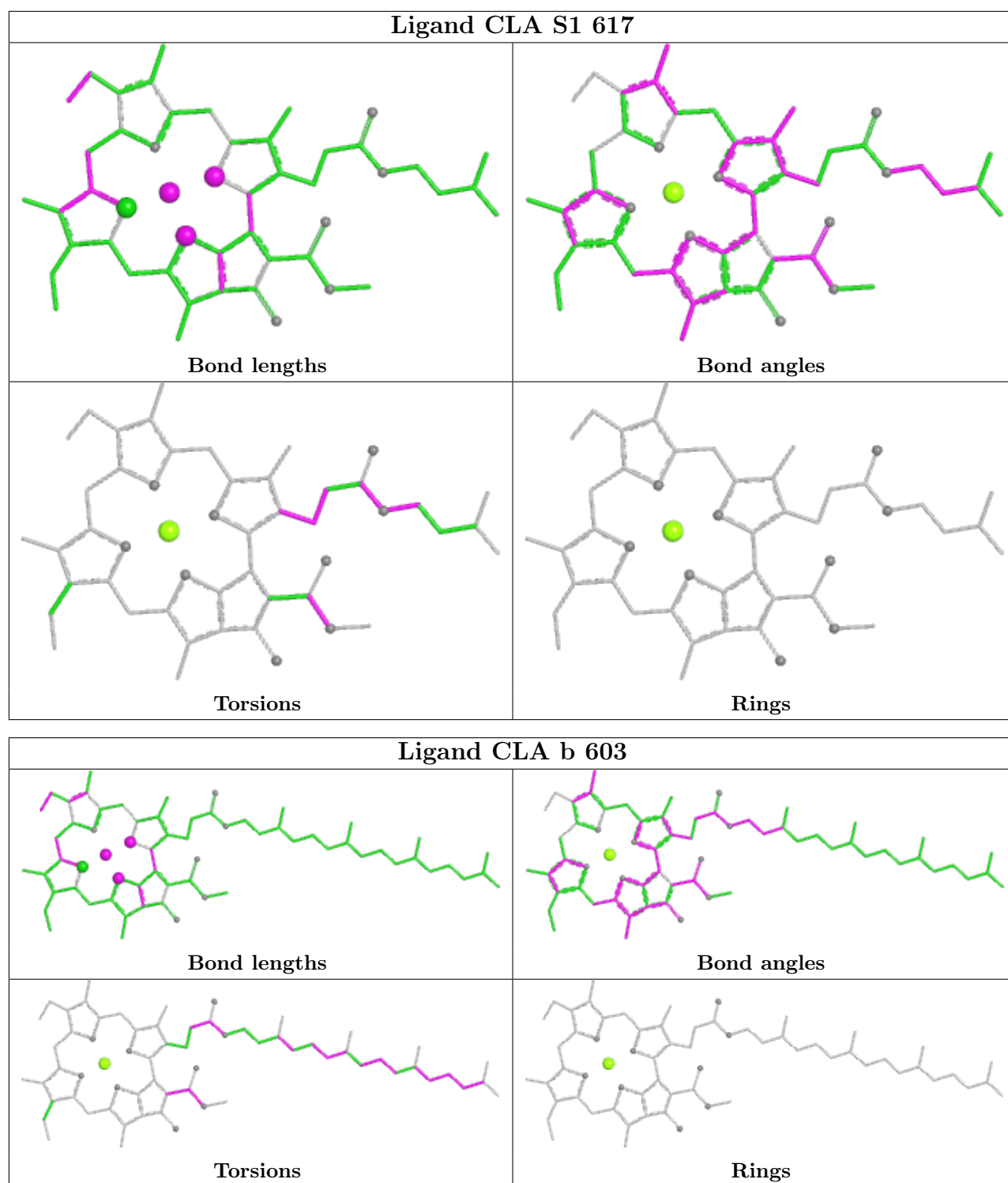
Ligand 3PH b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

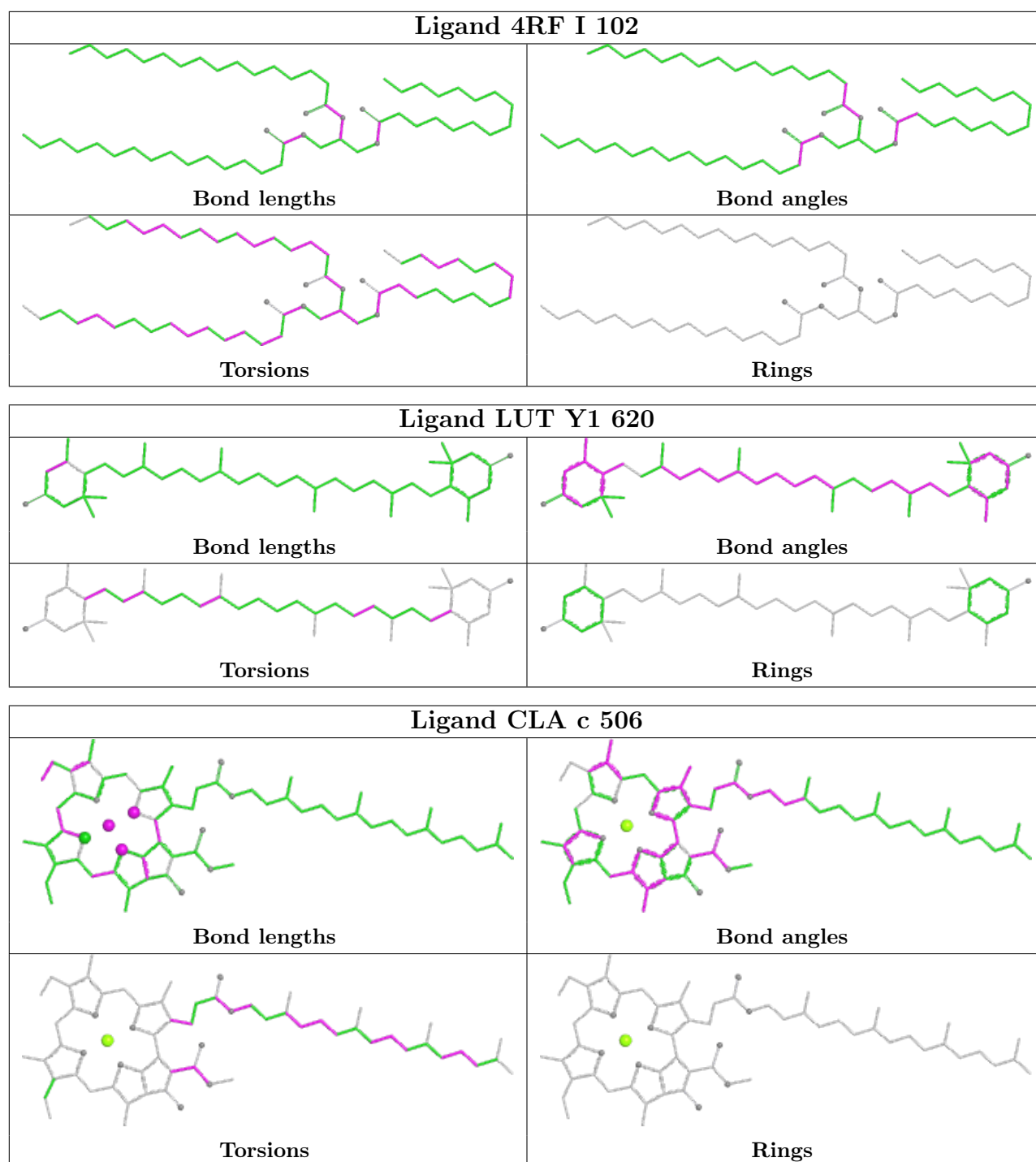


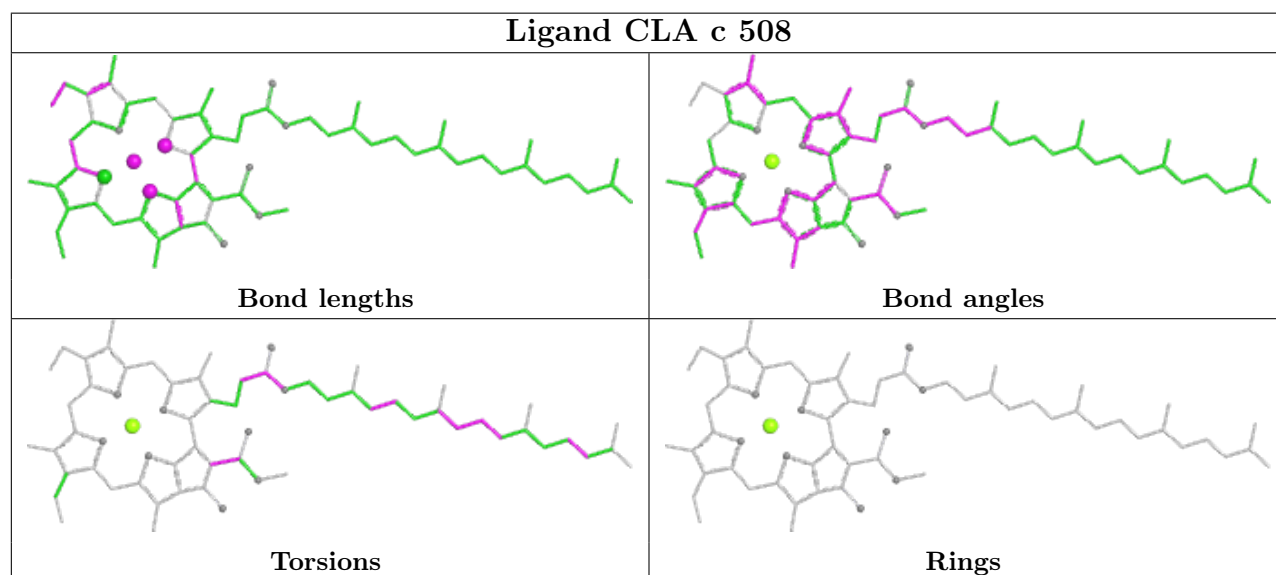
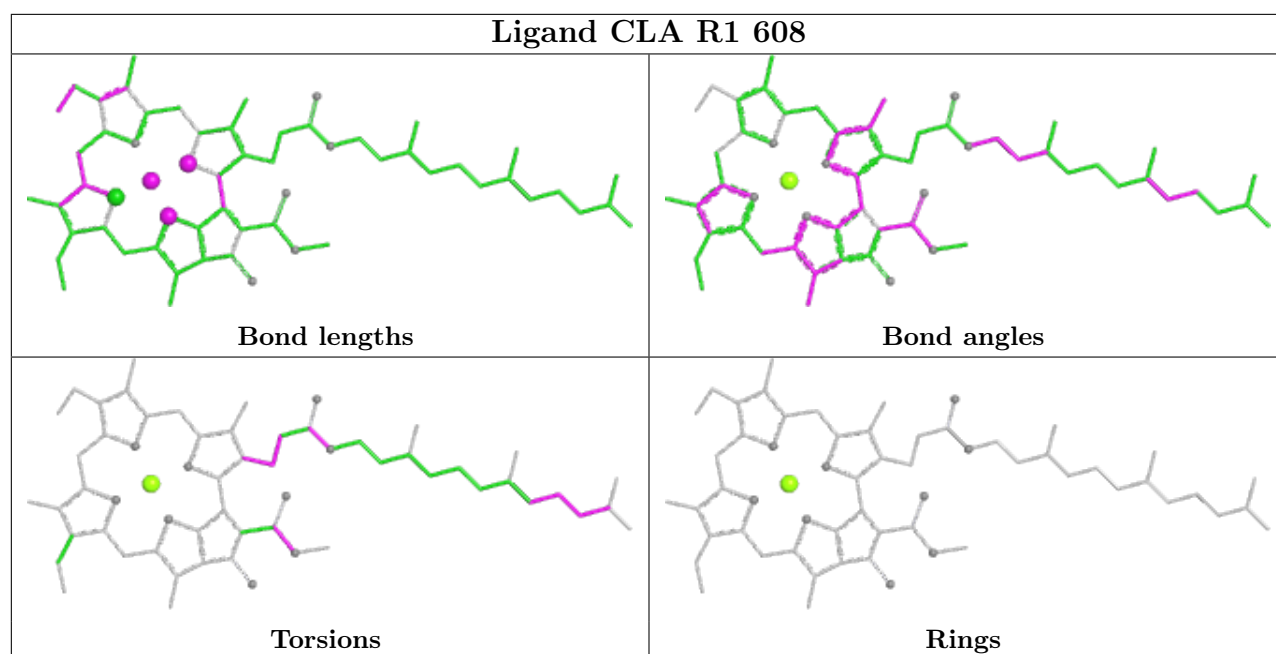


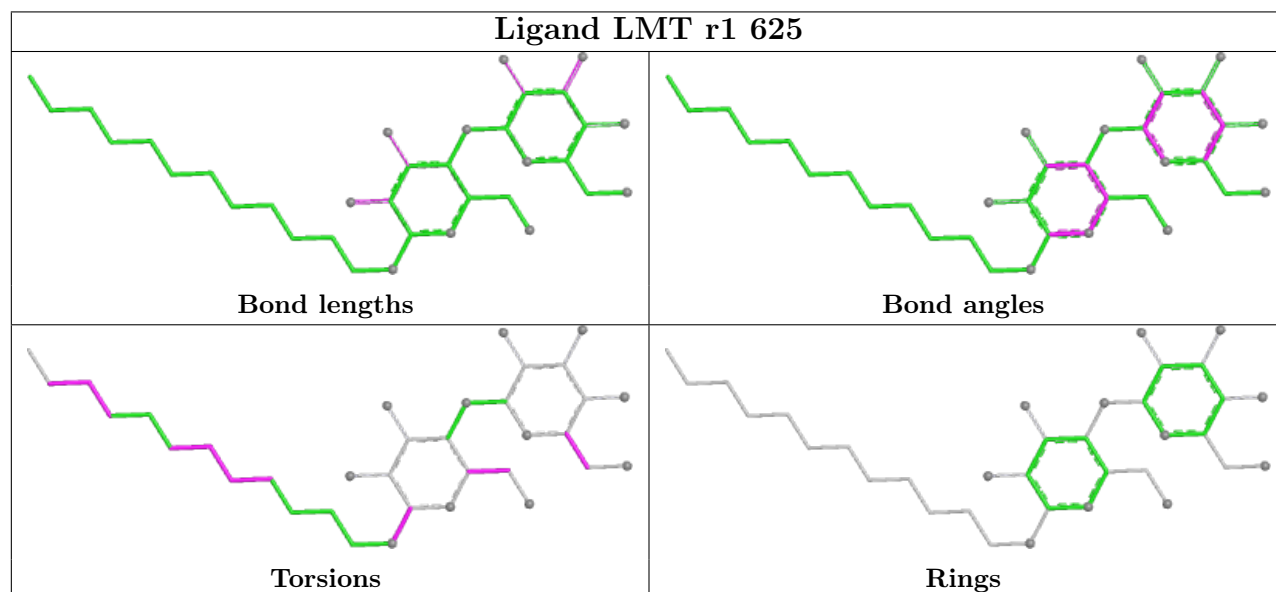
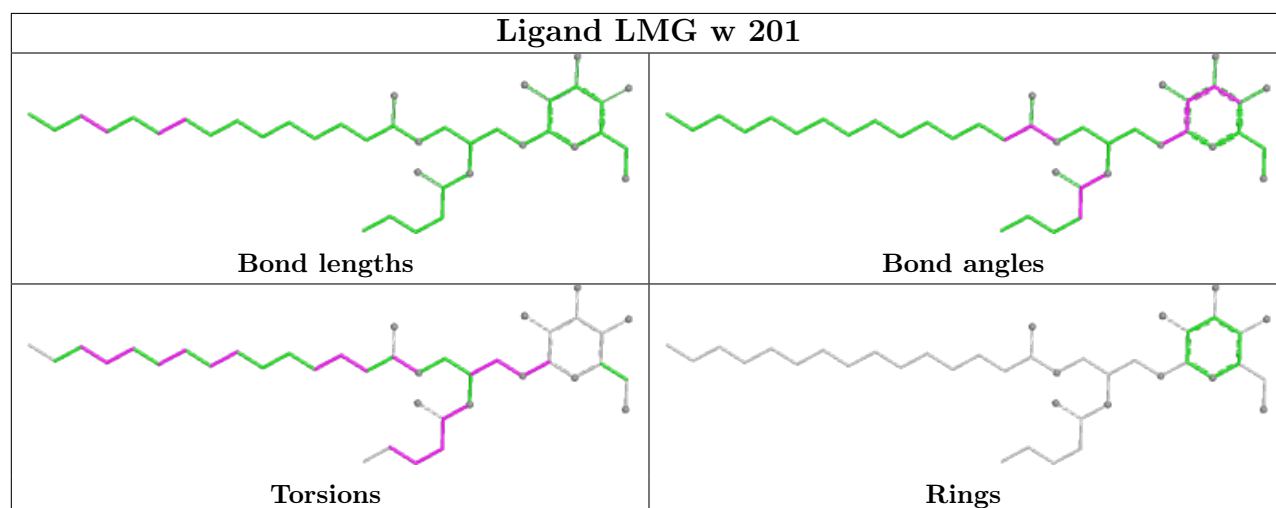
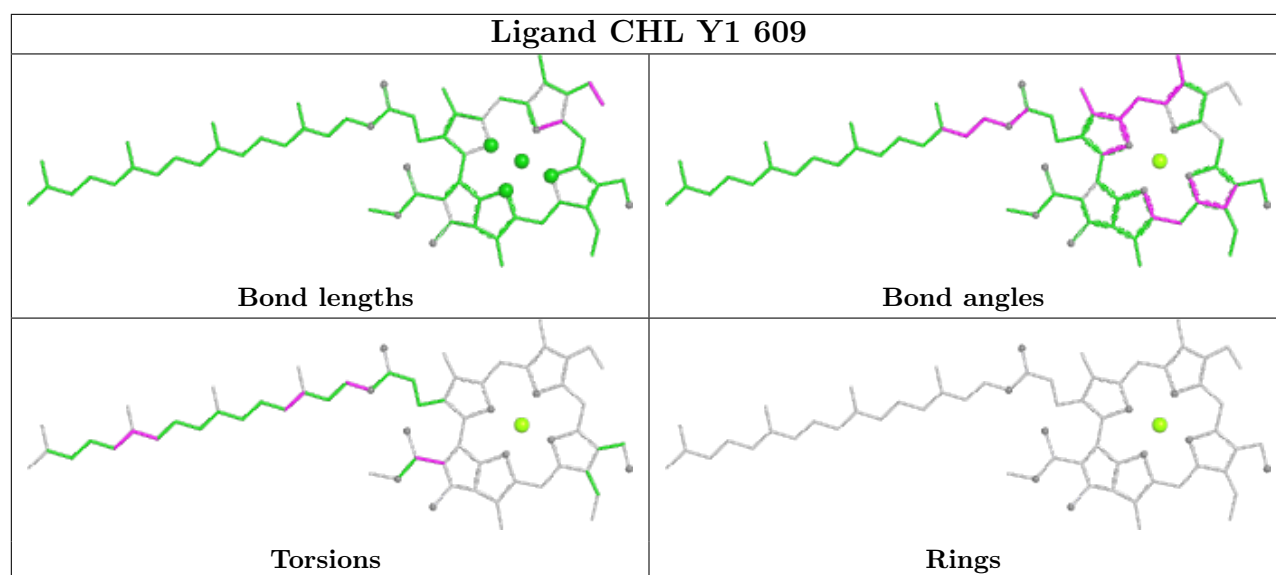


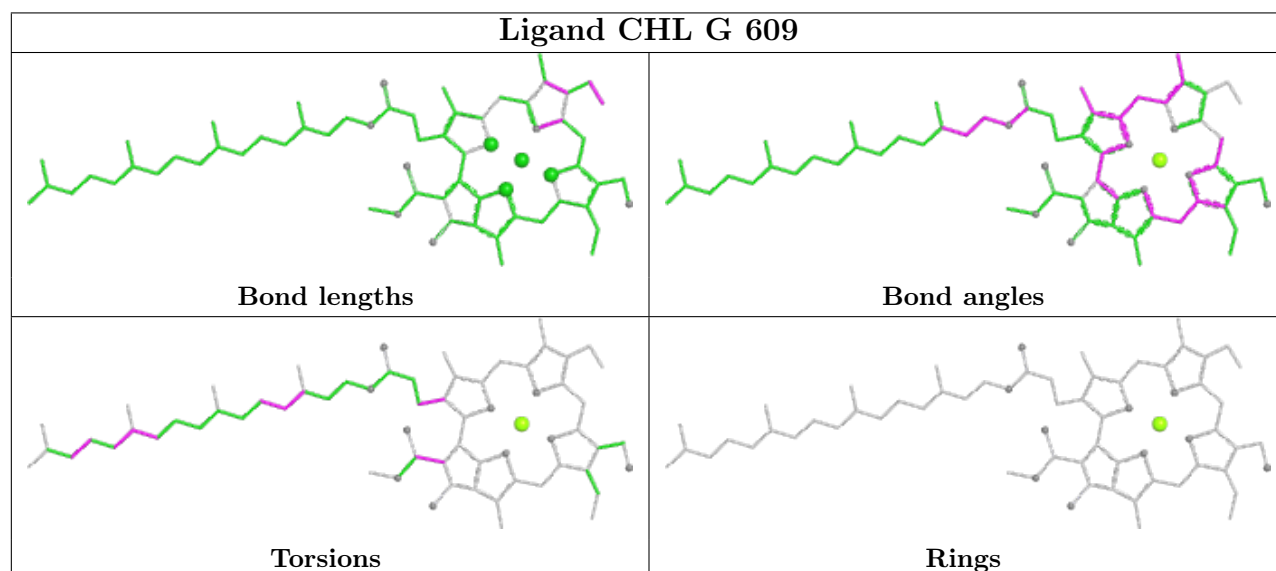
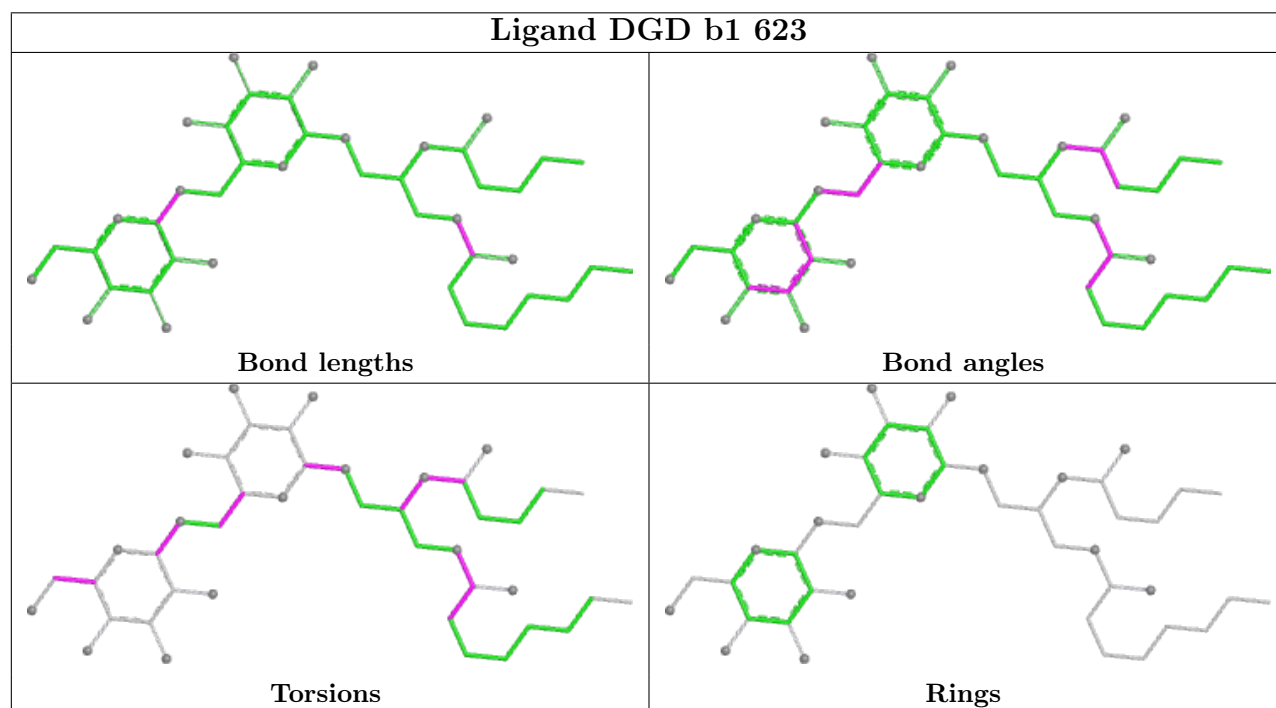
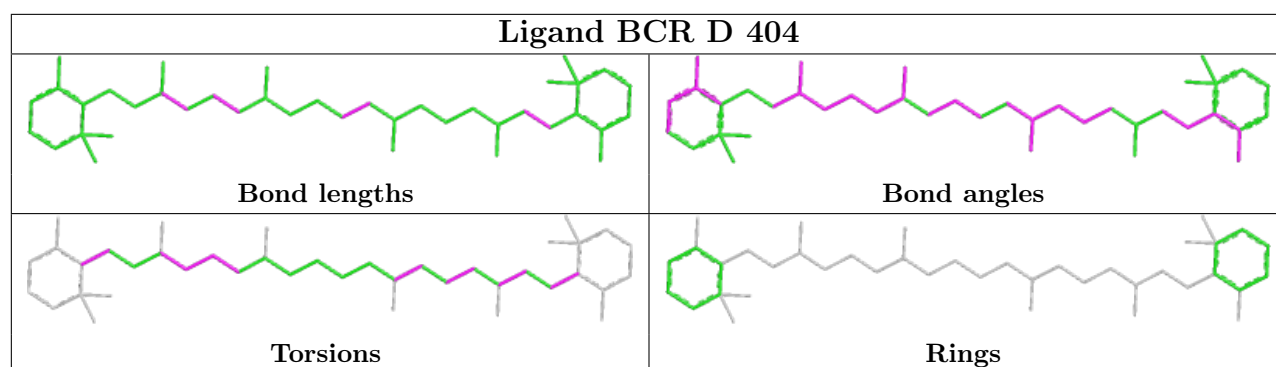


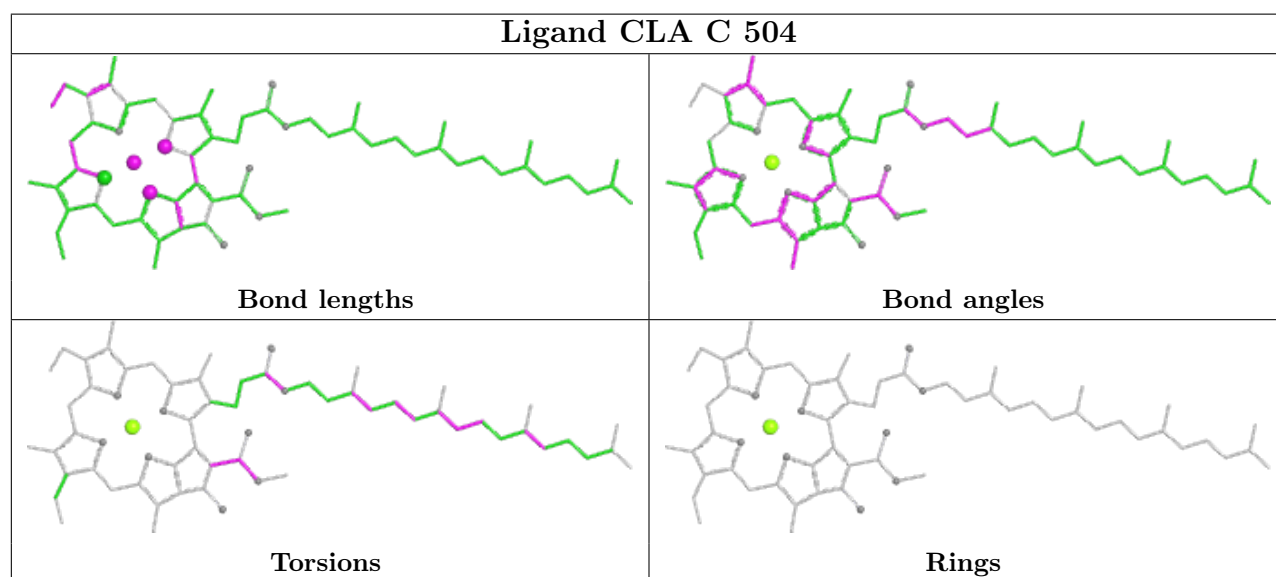
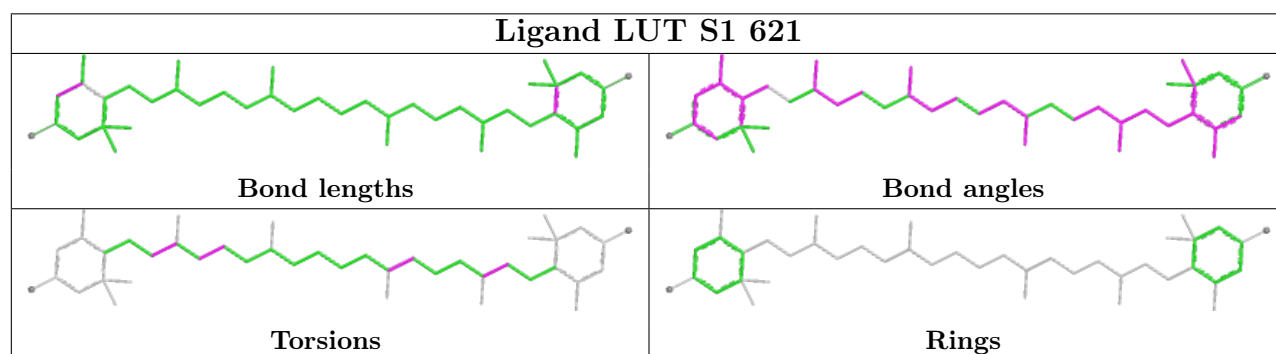
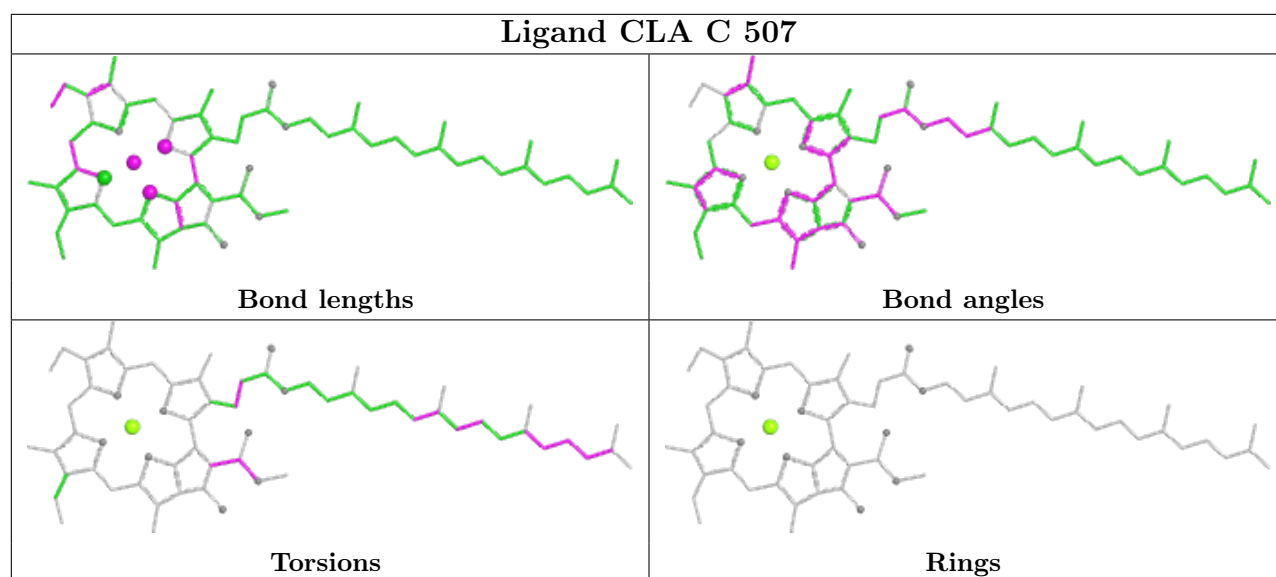


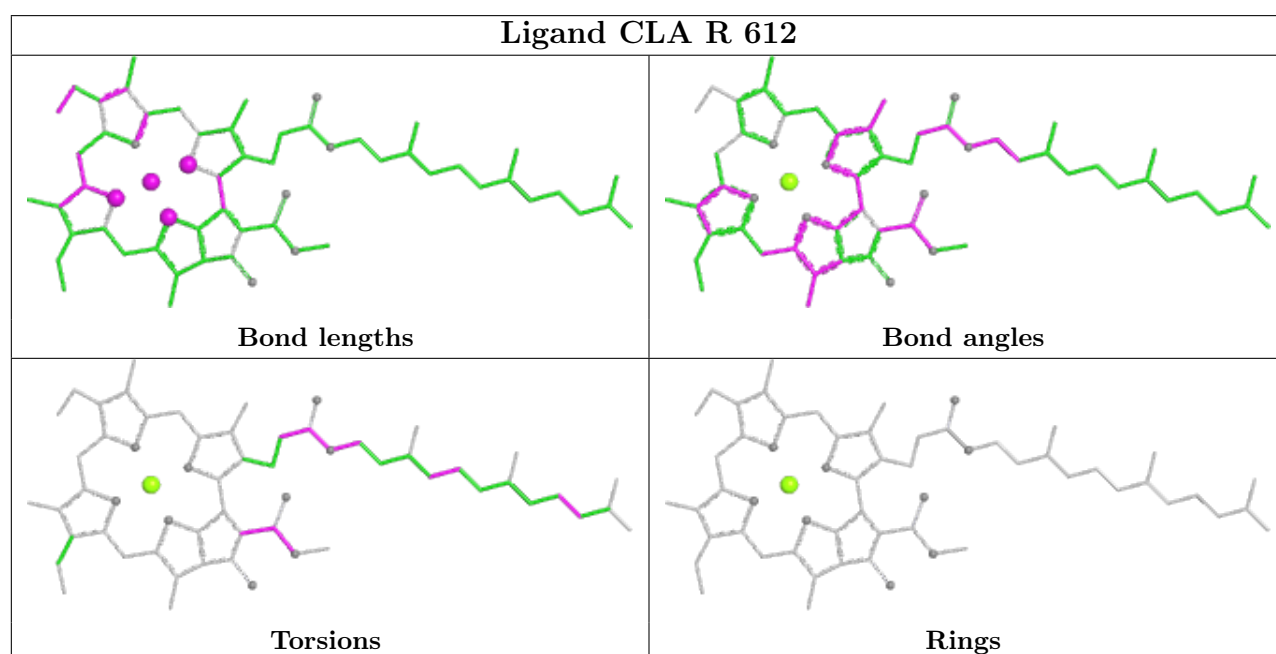
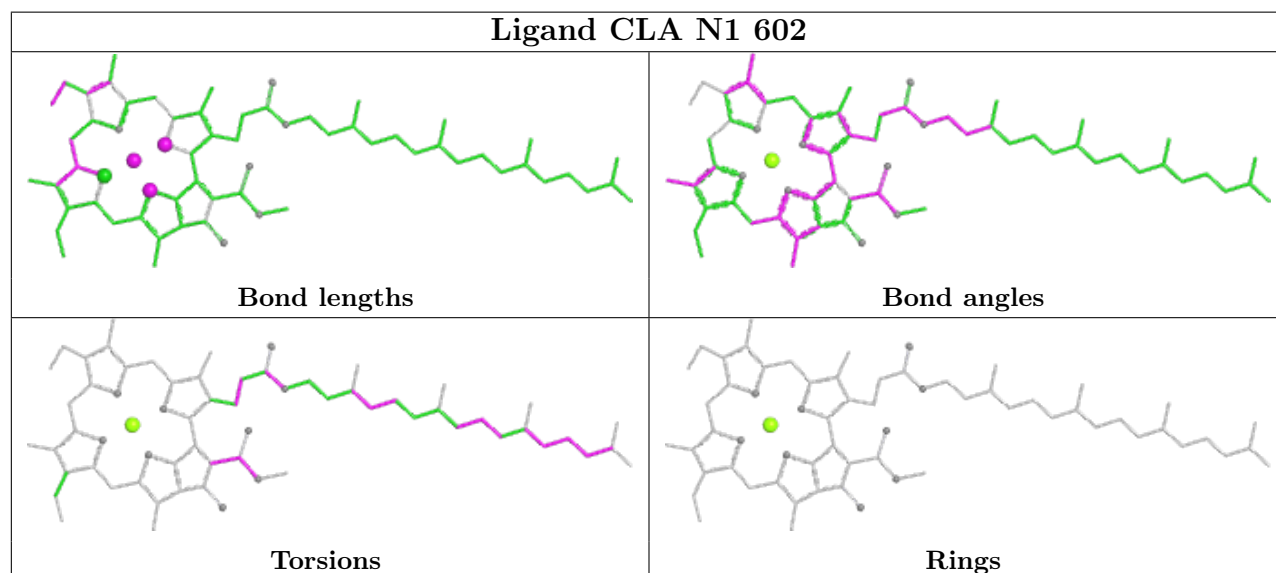
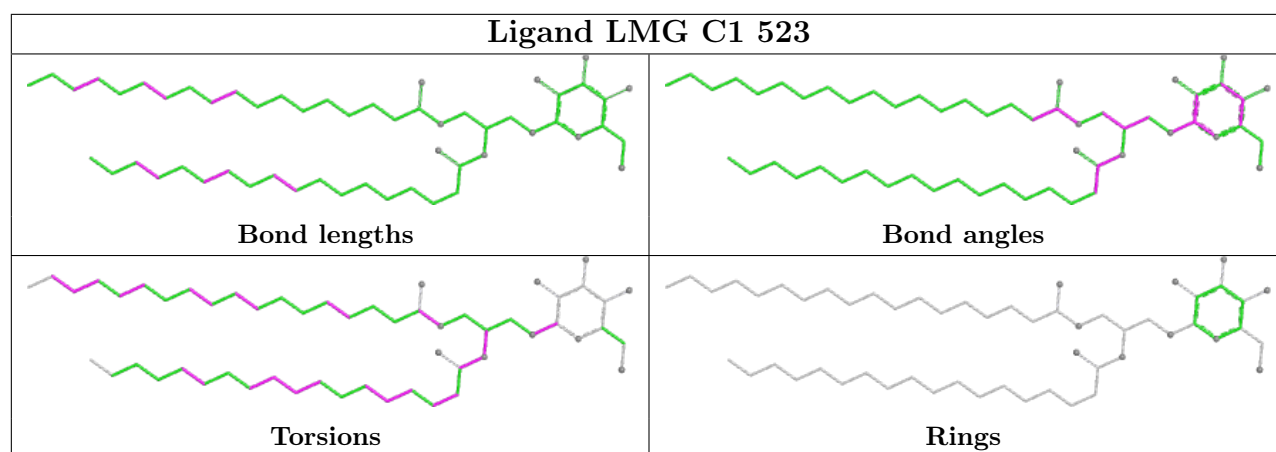


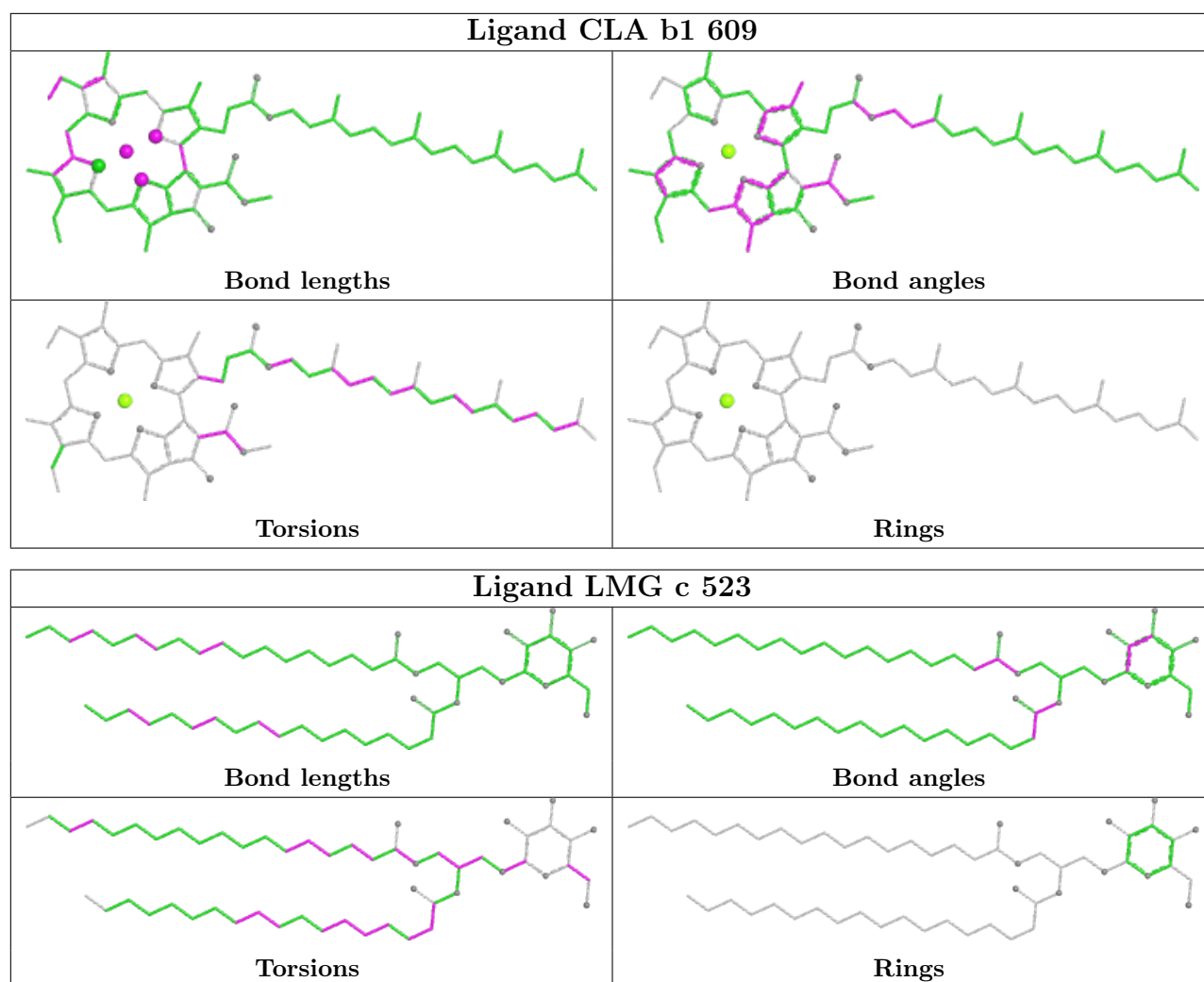


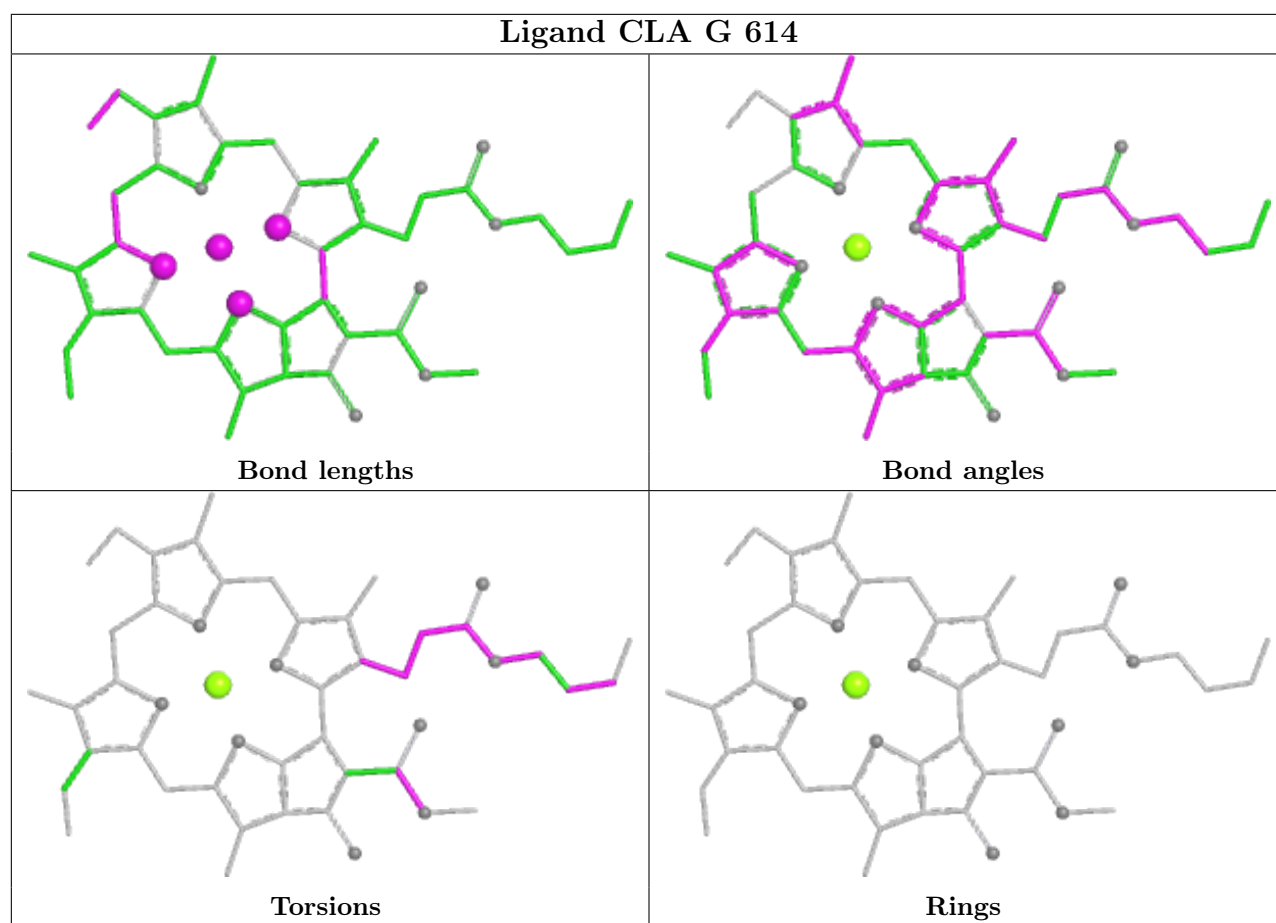


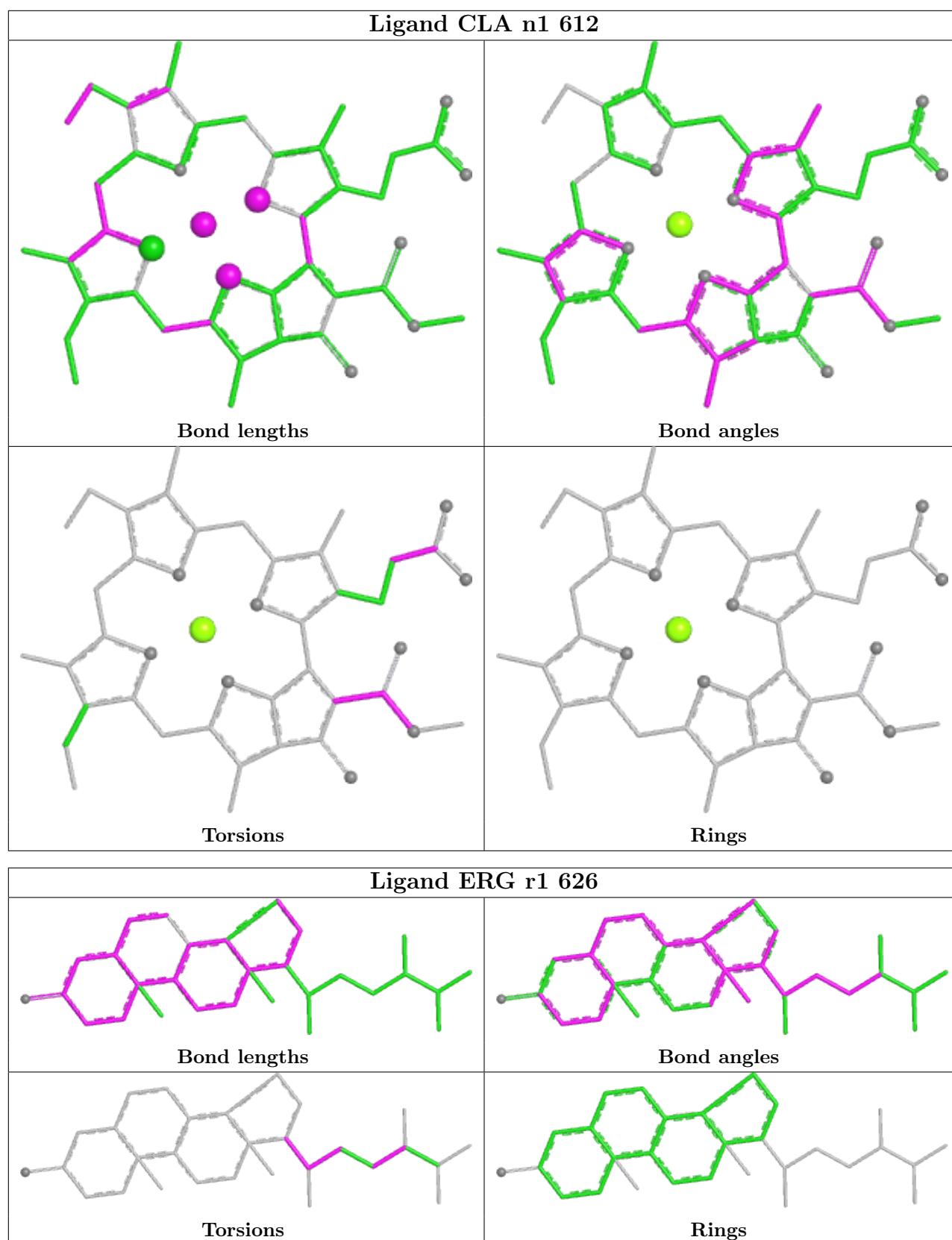


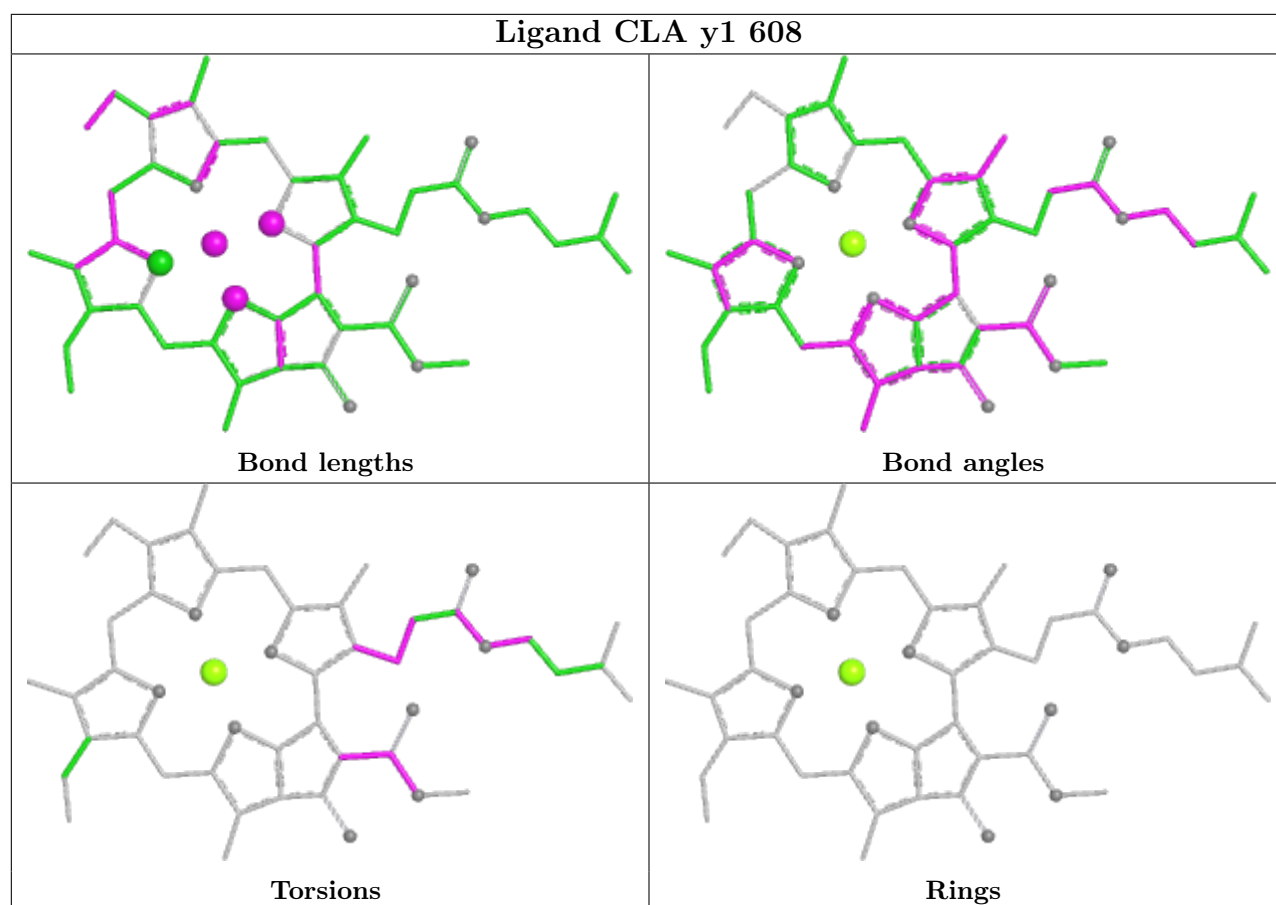




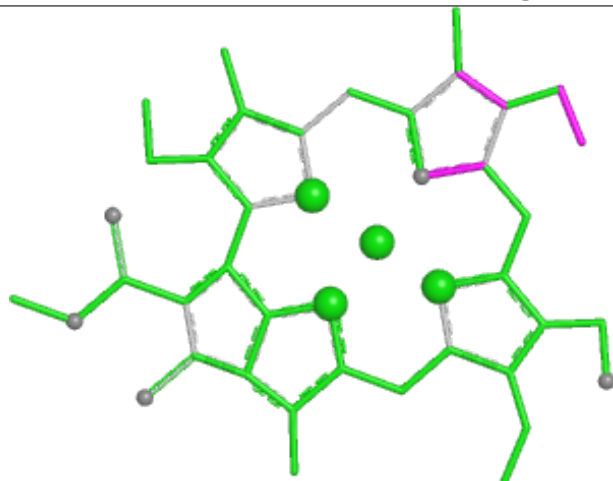




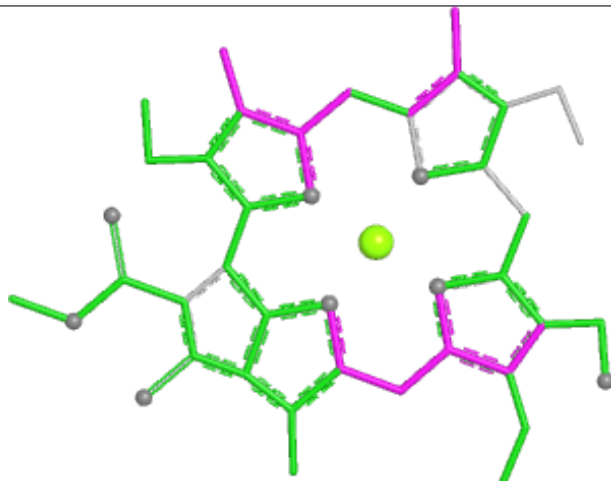




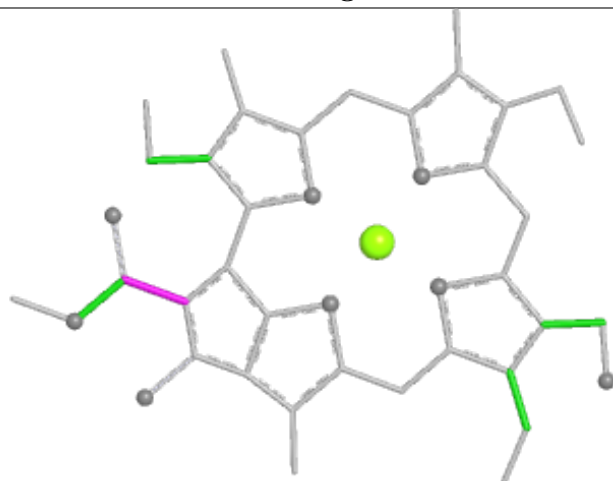
Ligand CHL S 607



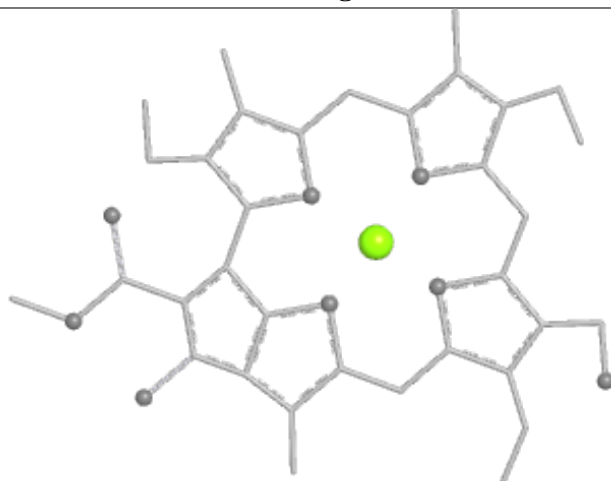
Bond lengths



Bond angles

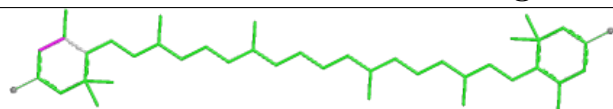


Torsions

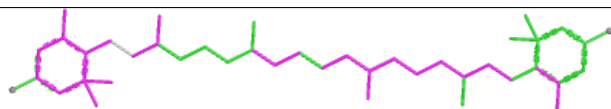


Rings

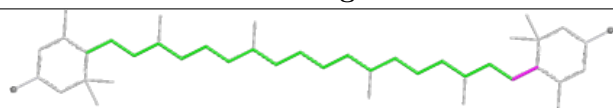
Ligand LUT N 620



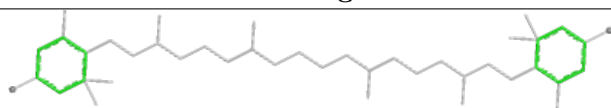
Bond lengths



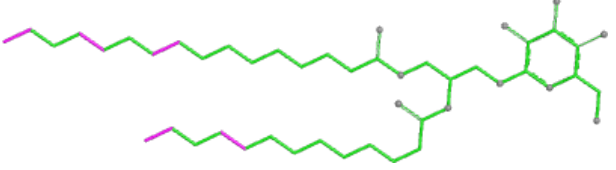
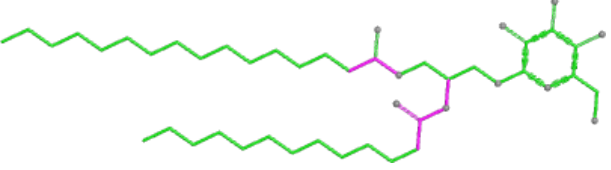
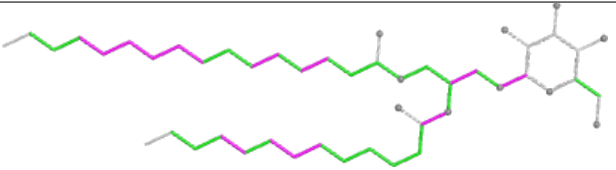
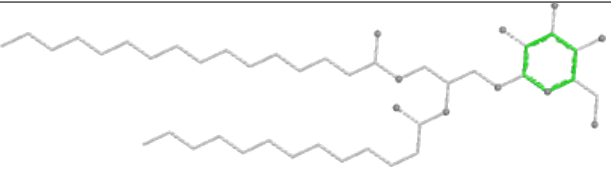
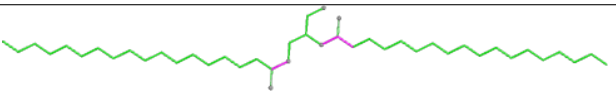
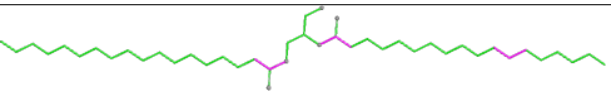
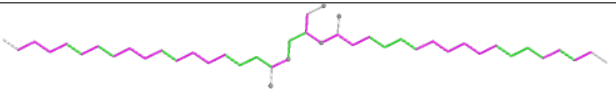
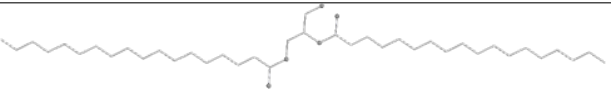
Bond angles

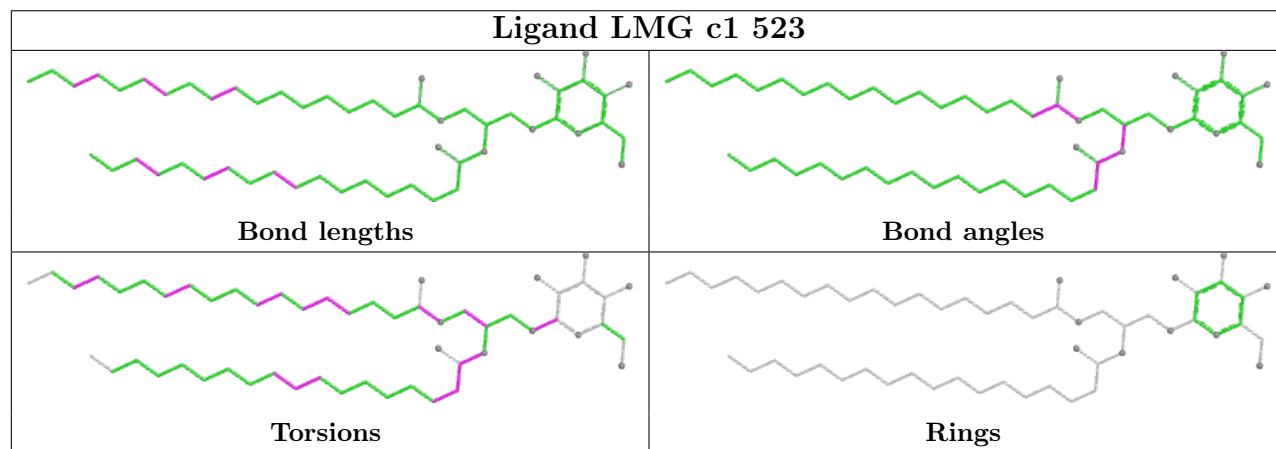
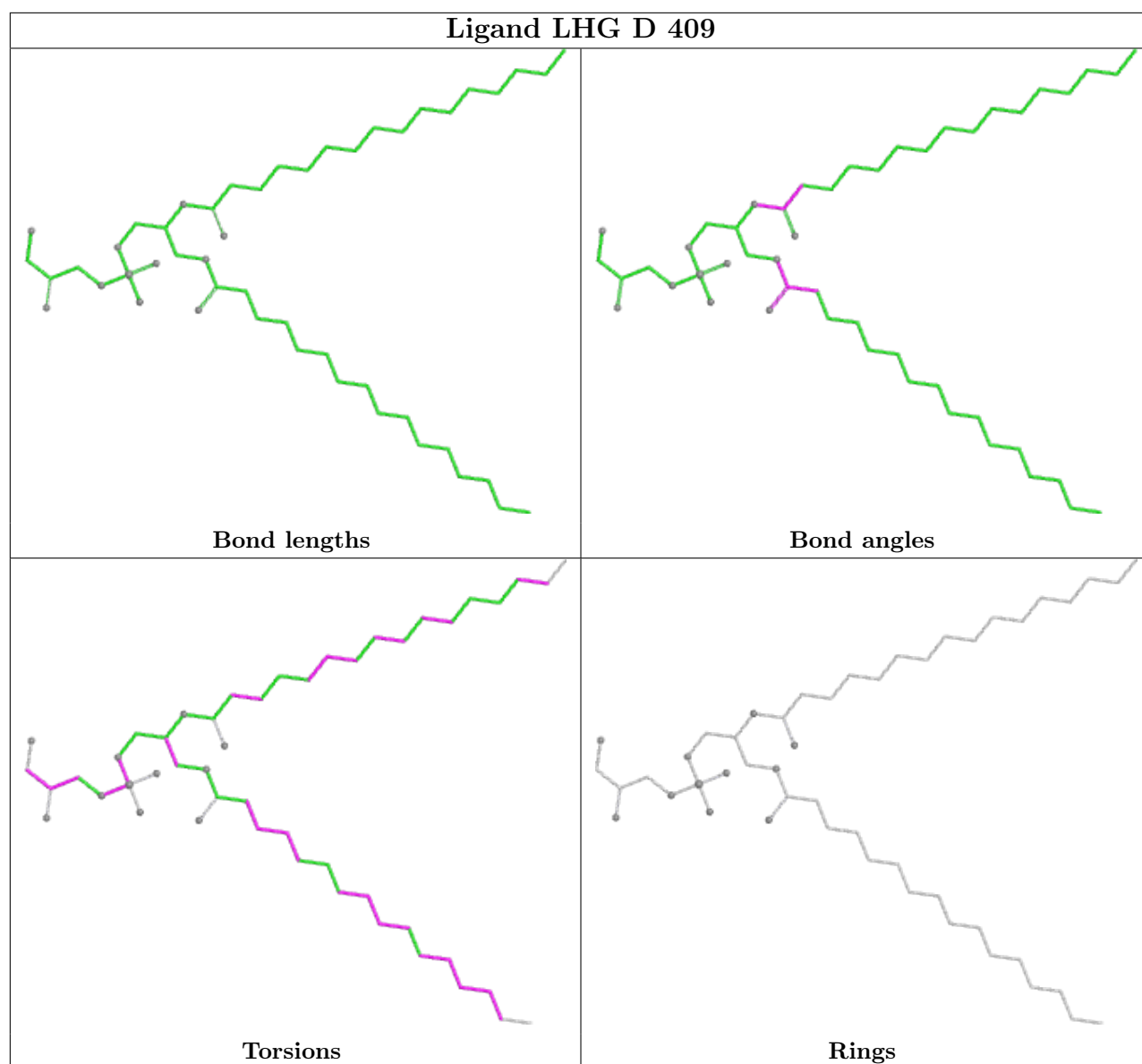


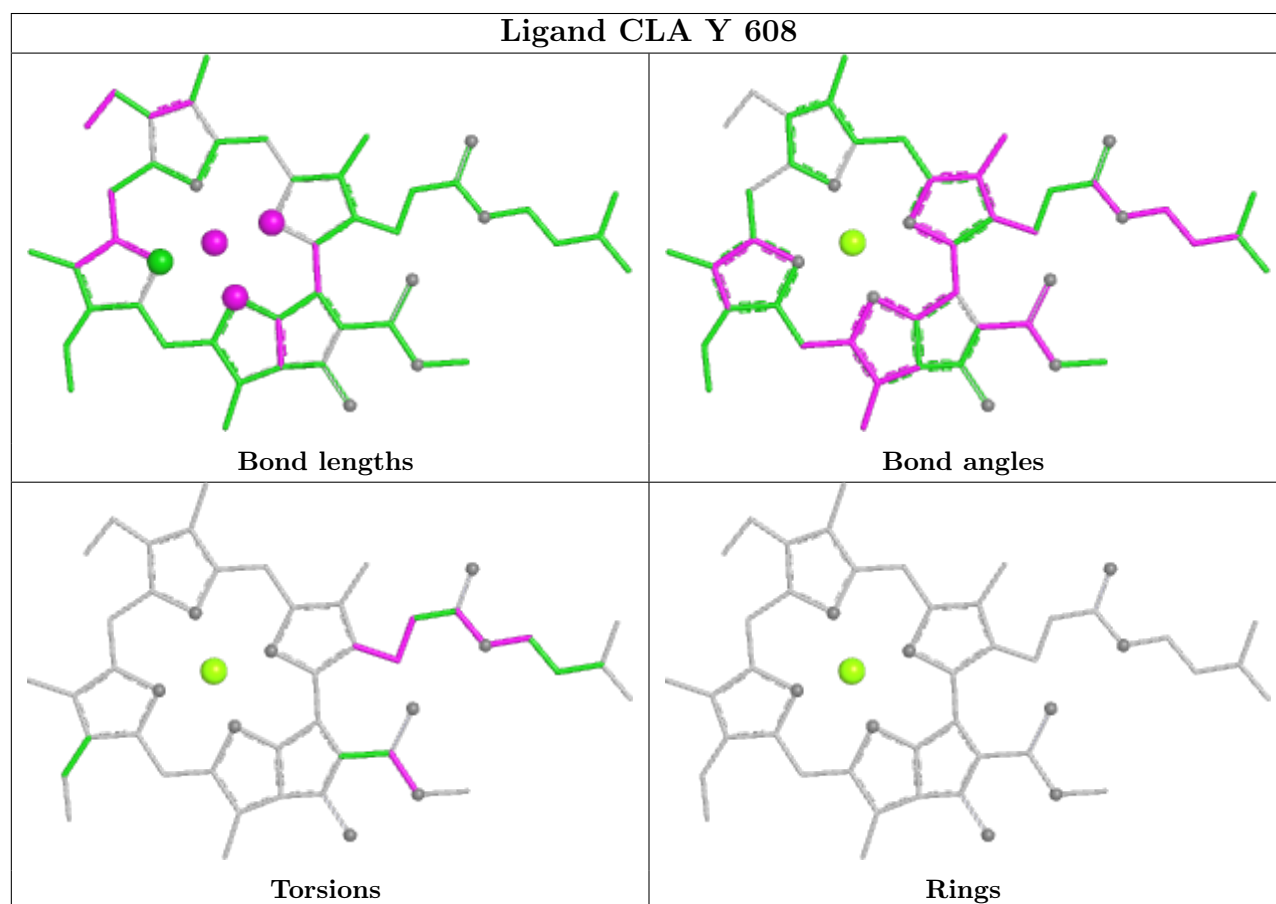
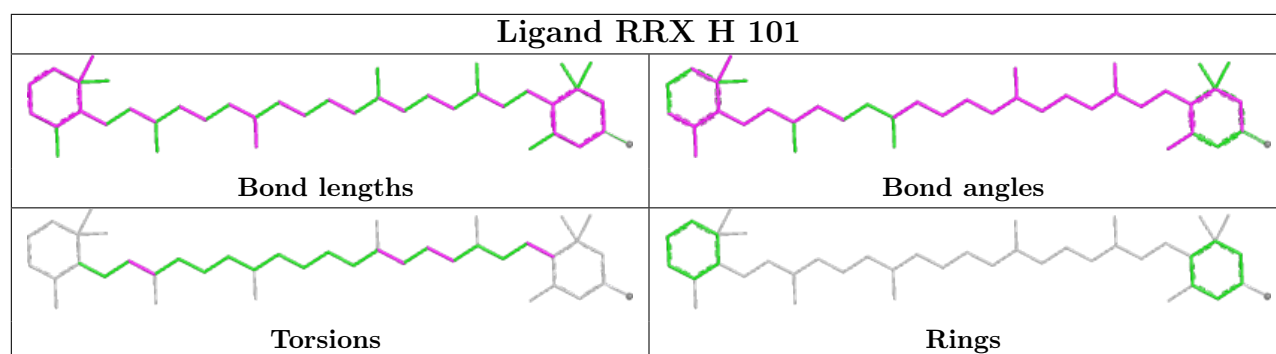
Torsions

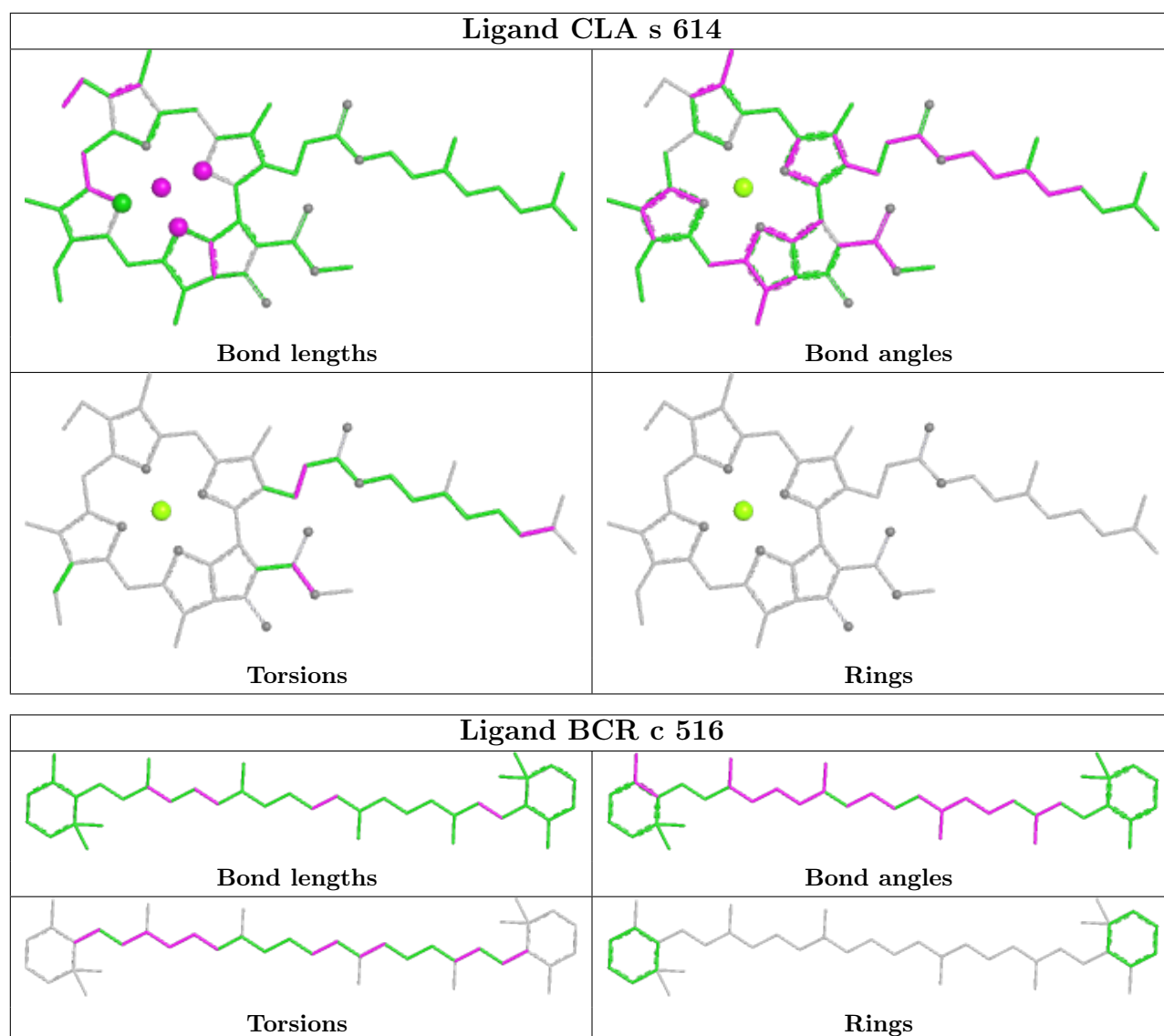


Rings

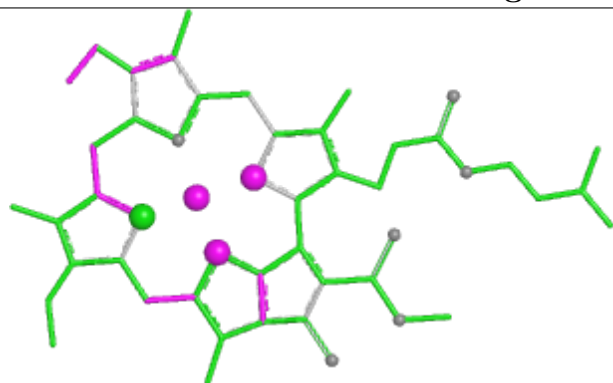
Ligand LMG A 413	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGA B1 625	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



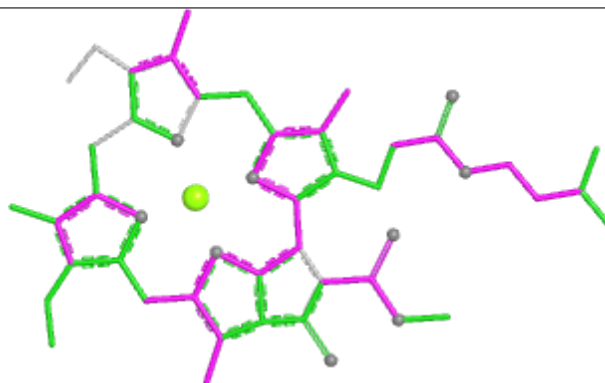




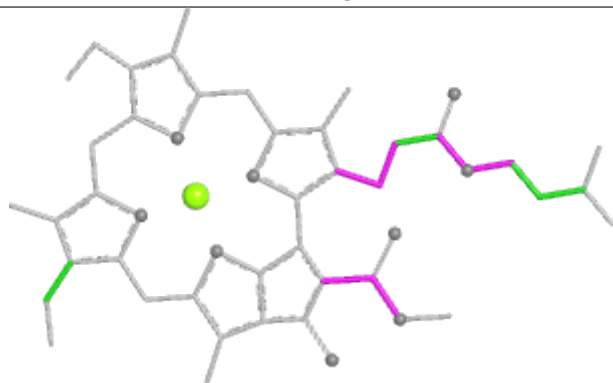
Ligand CLA A1 407



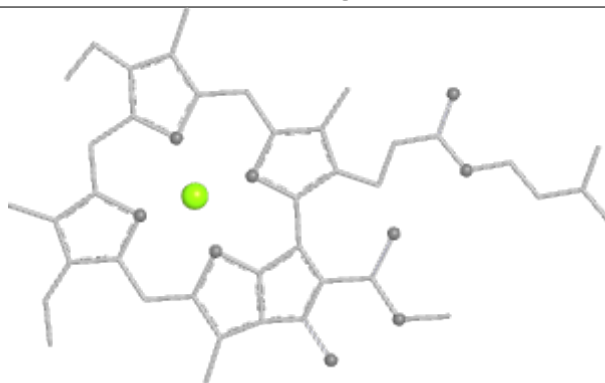
Bond lengths



Bond angles

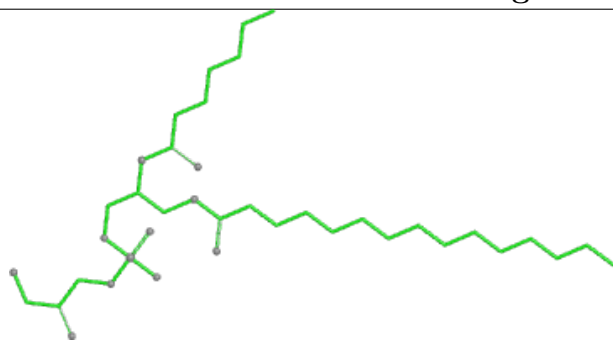


Torsions

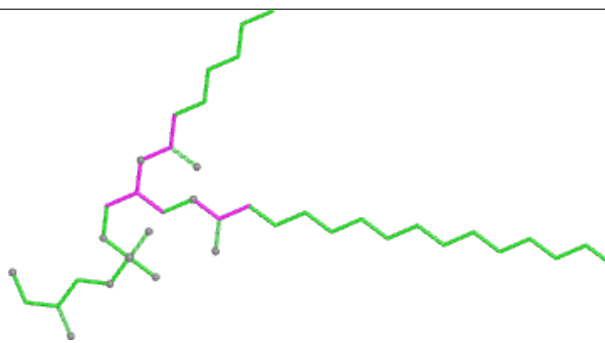


Rings

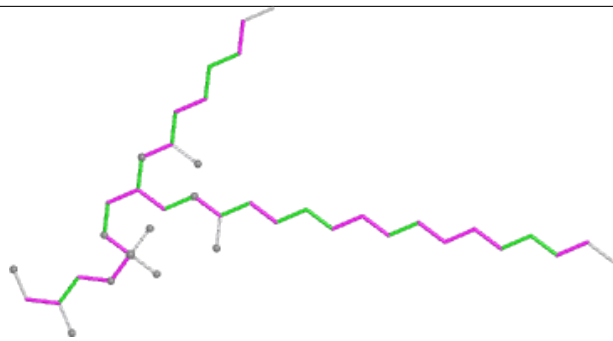
Ligand LHG D 410



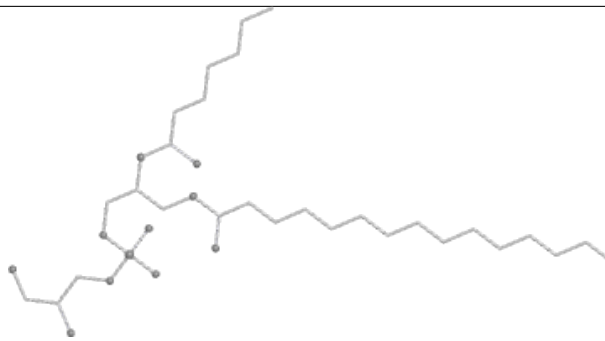
Bond lengths



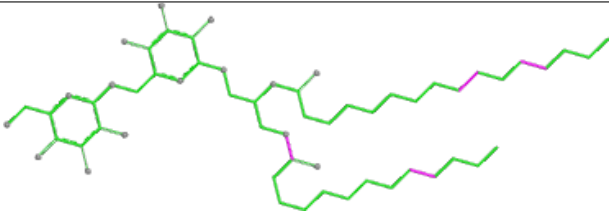
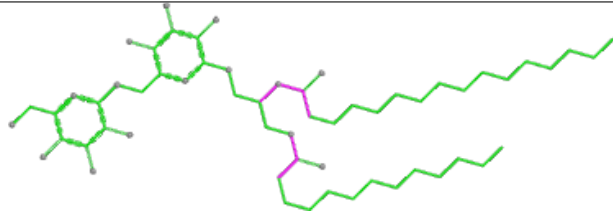
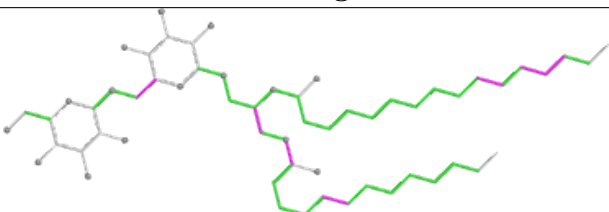
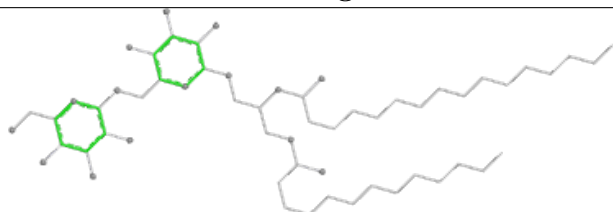
Bond angles

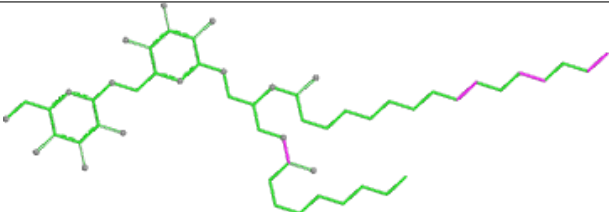
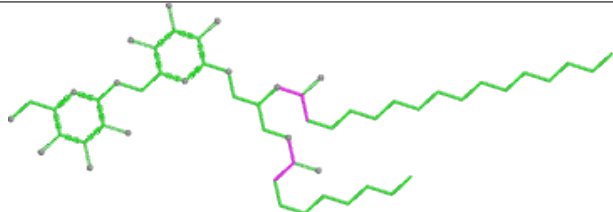
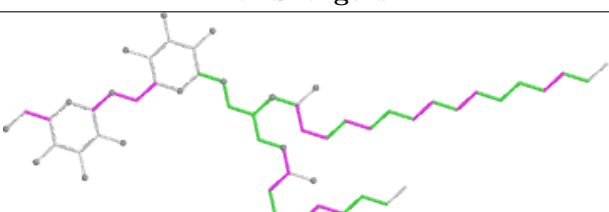
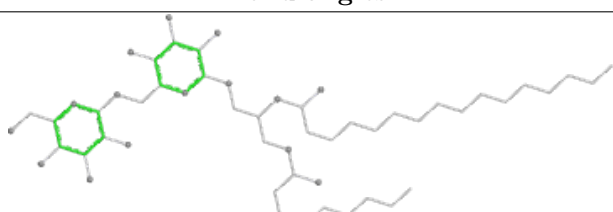


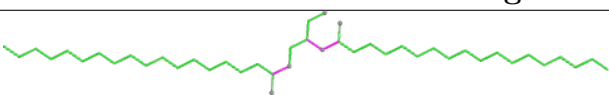
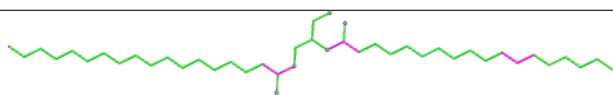
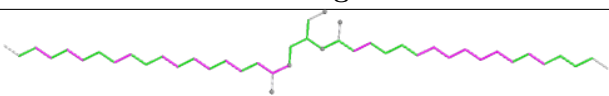
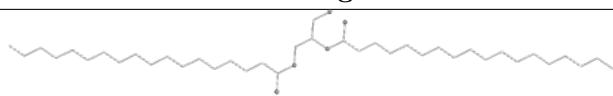
Torsions

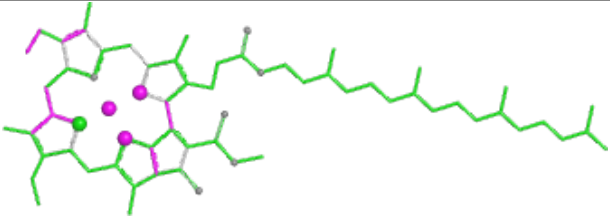
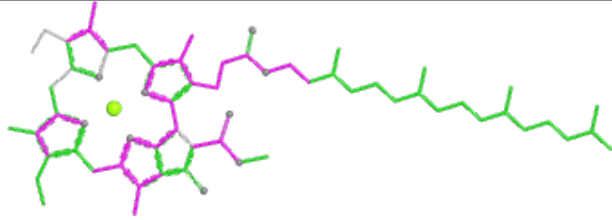
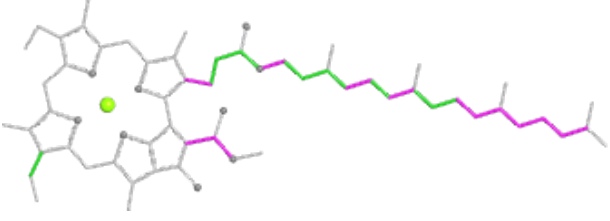
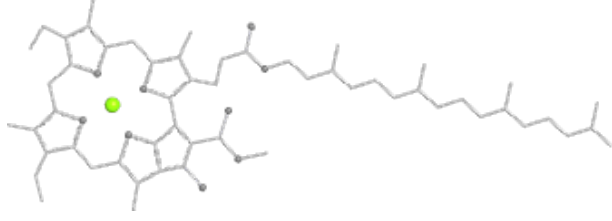

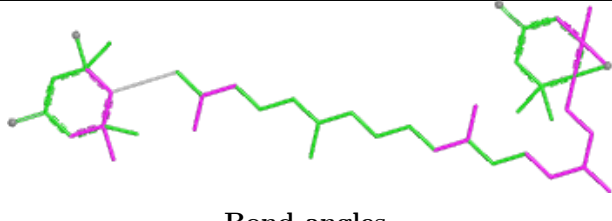
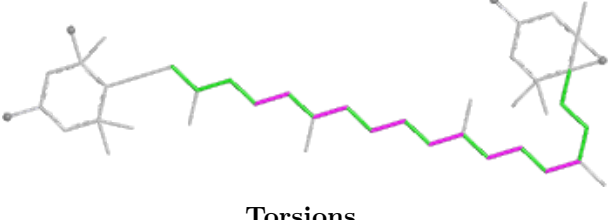

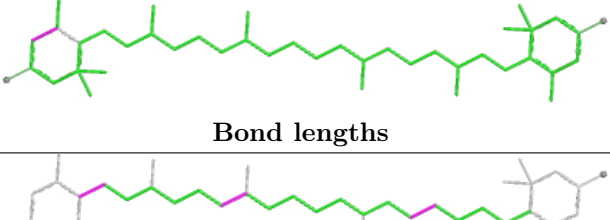
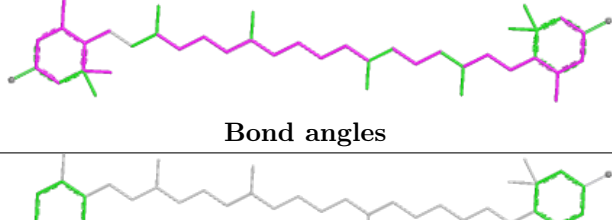
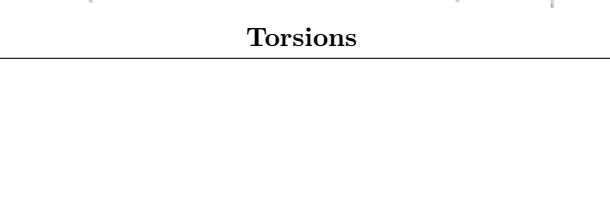
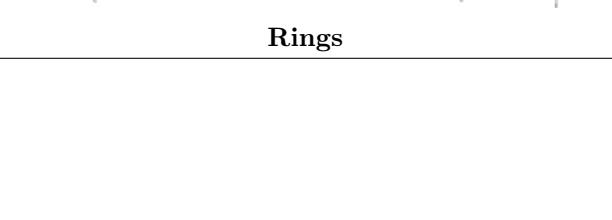


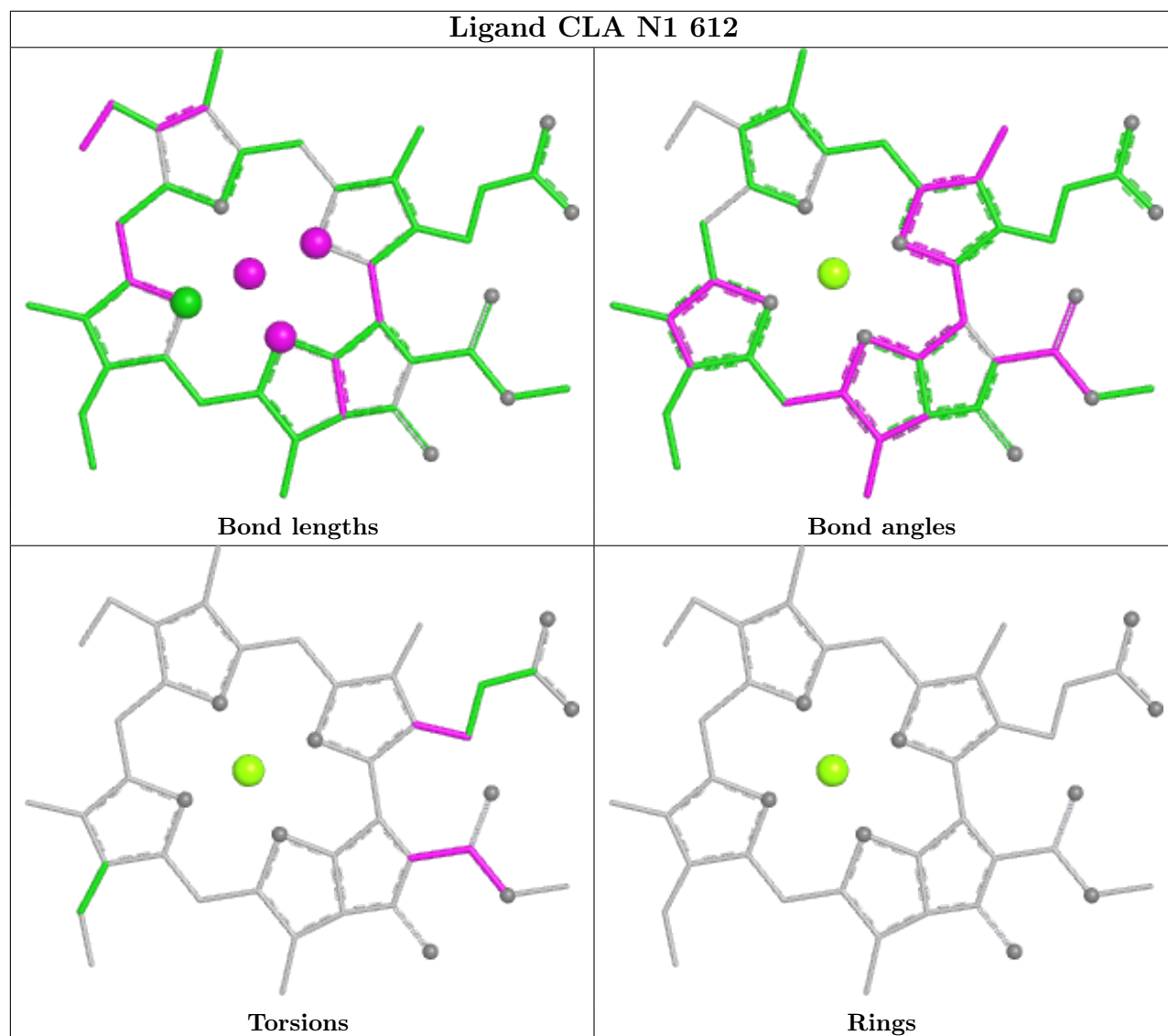
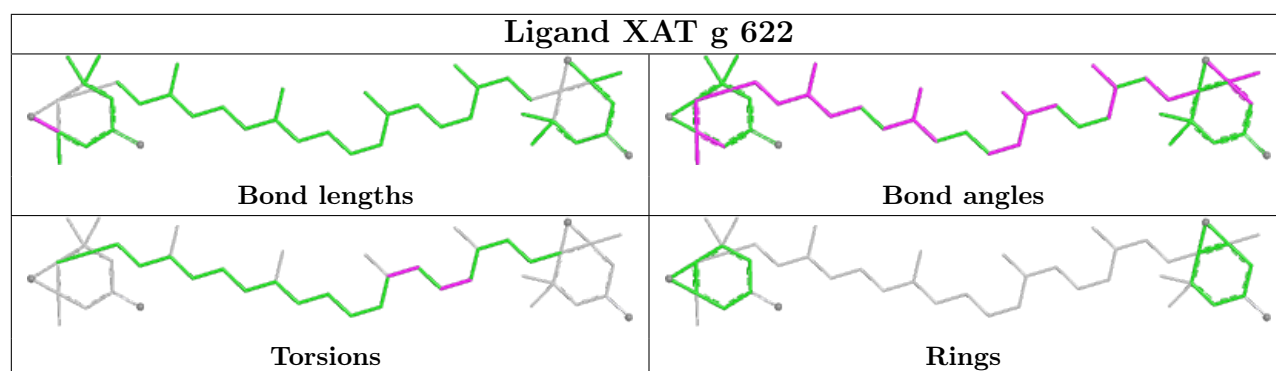
Rings

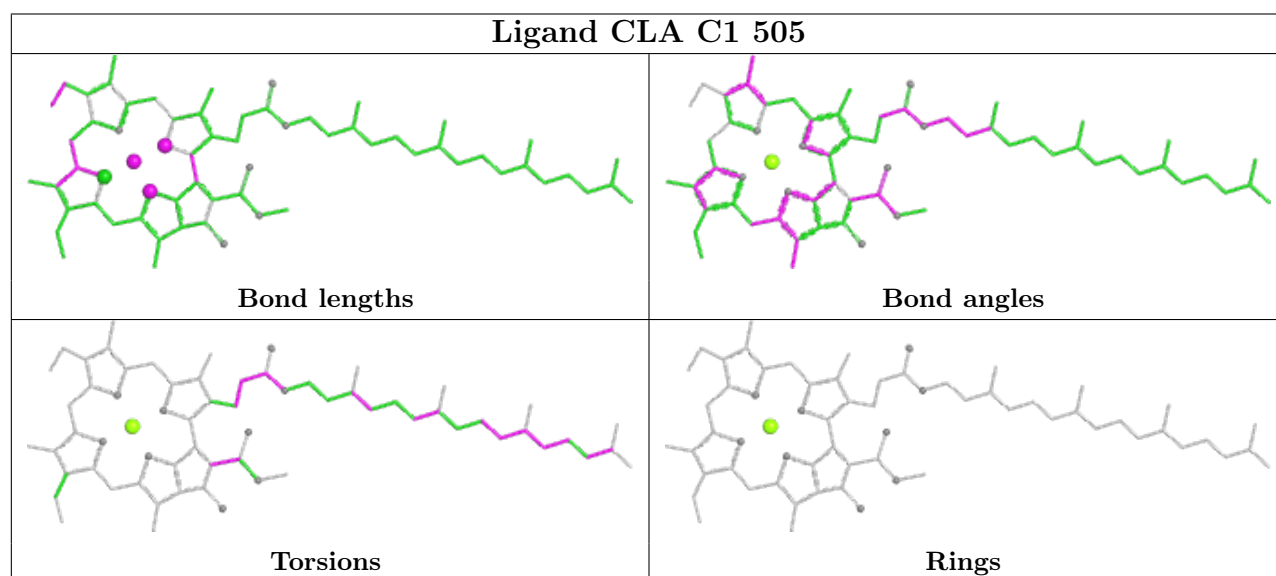
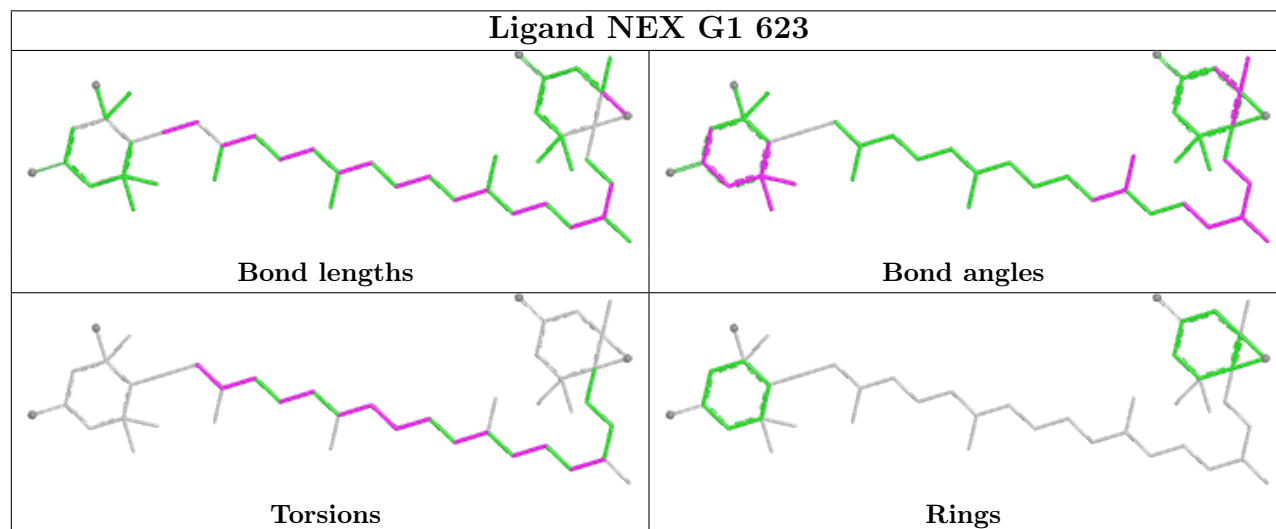
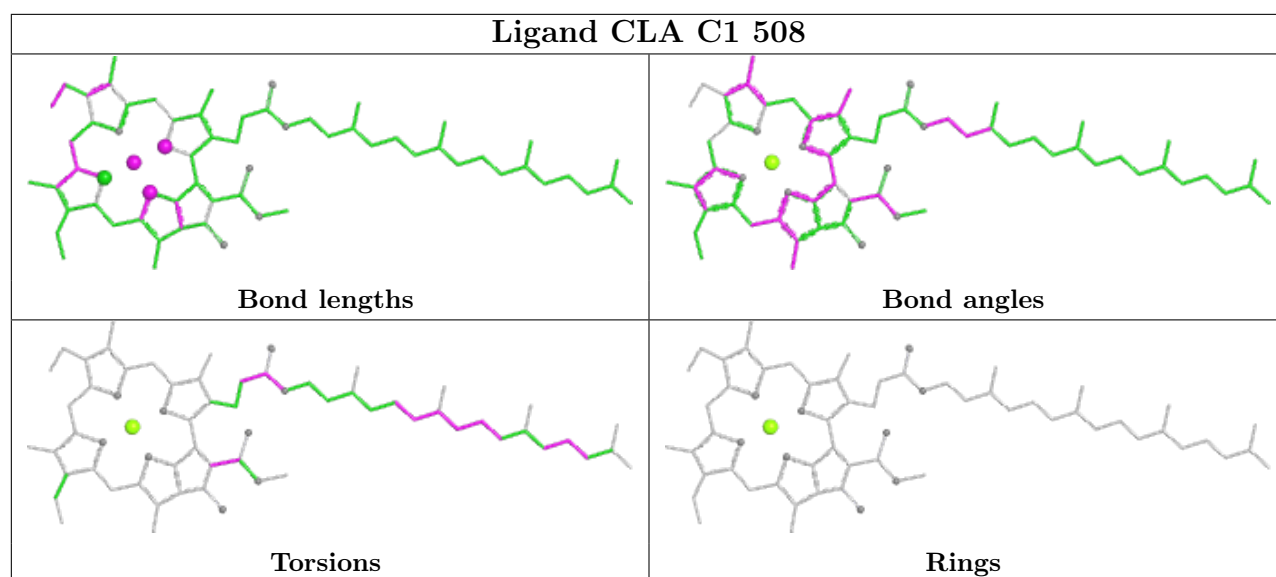
Ligand DGD c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

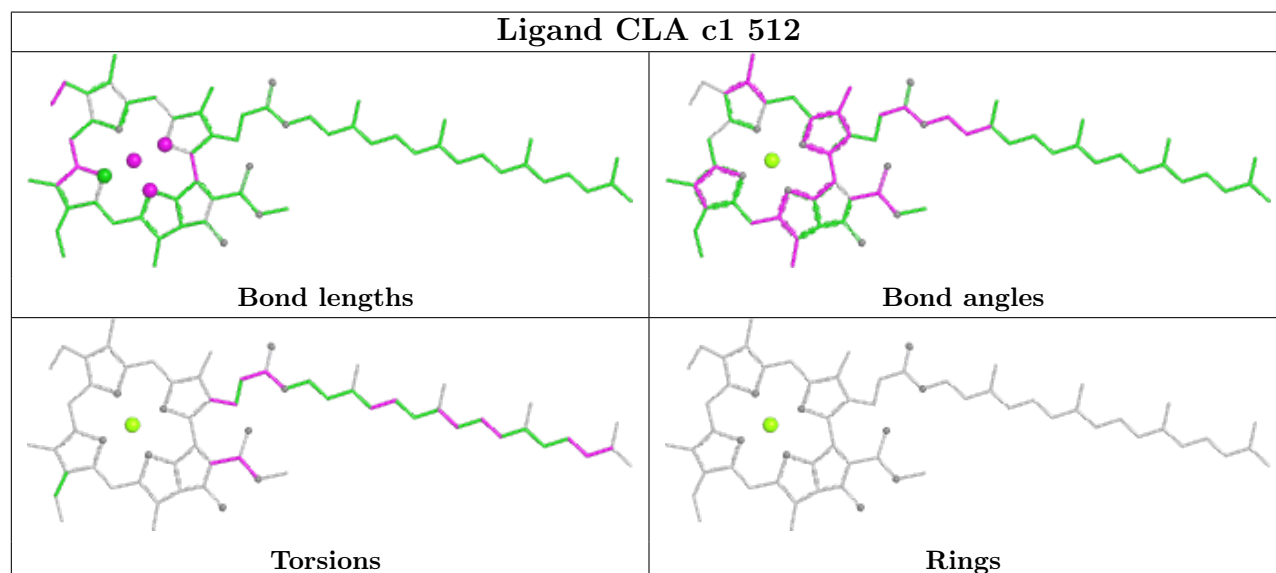
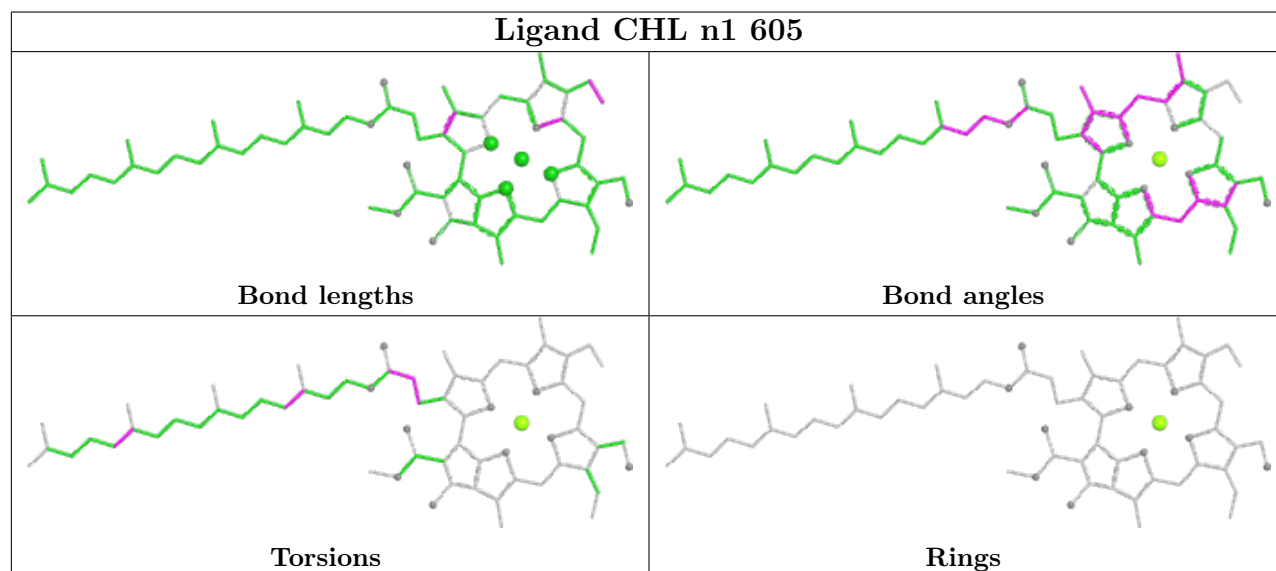
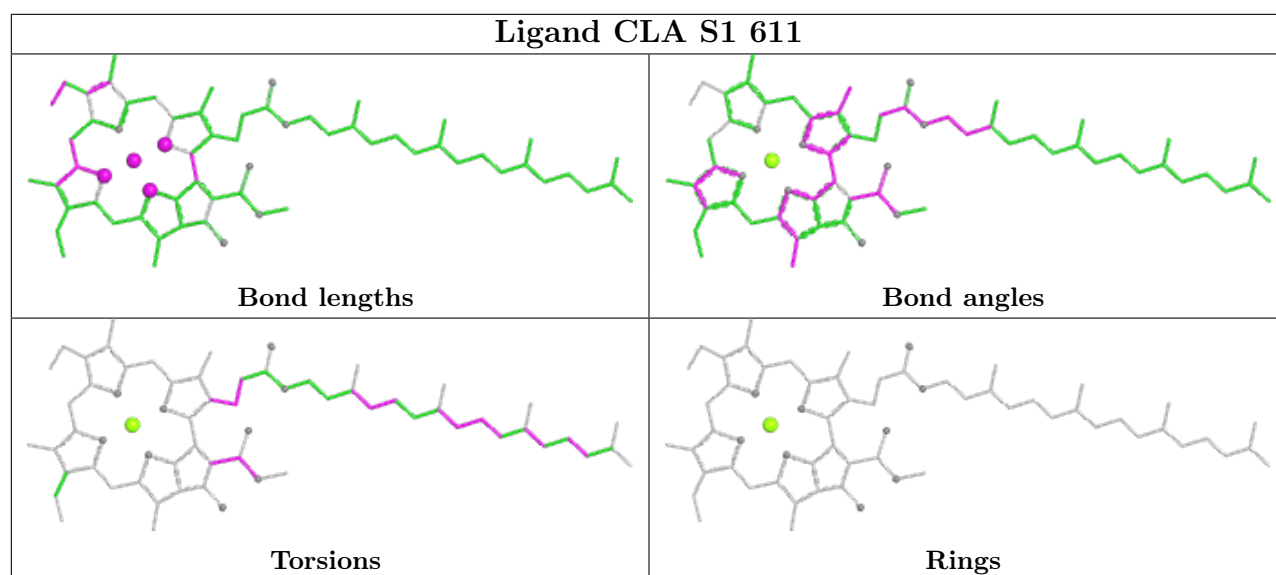
Ligand DGD C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGA C 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

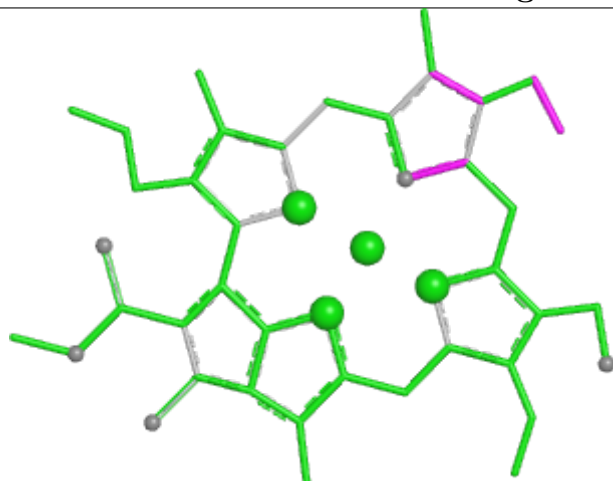
Ligand CLA n 610	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand NEX R 622	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT g 620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



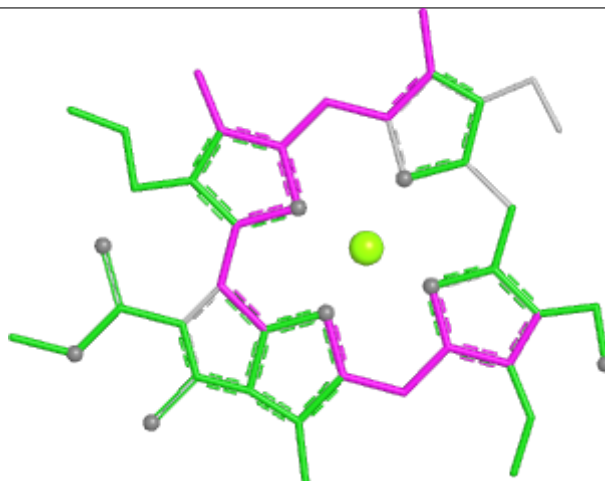




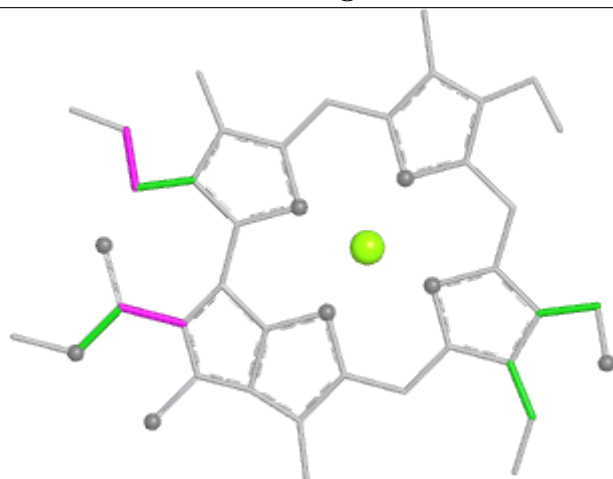
Ligand CHL S 606



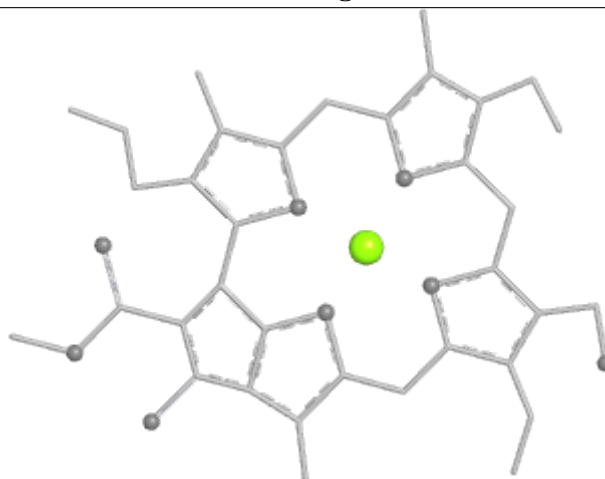
Bond lengths



Bond angles

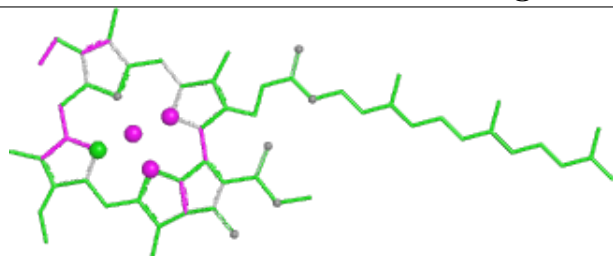


Torsions

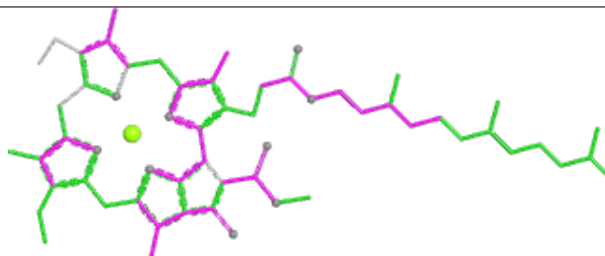


Rings

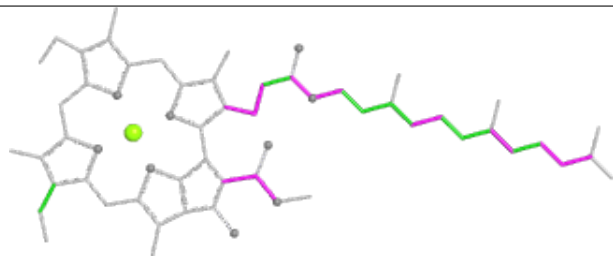
Ligand CLA R 603



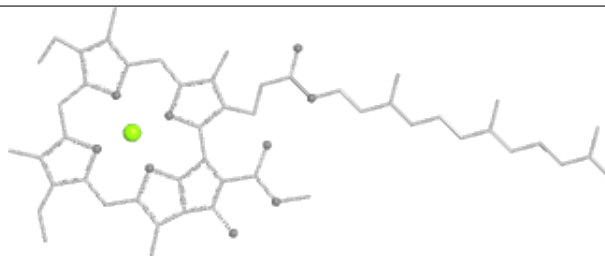
Bond lengths



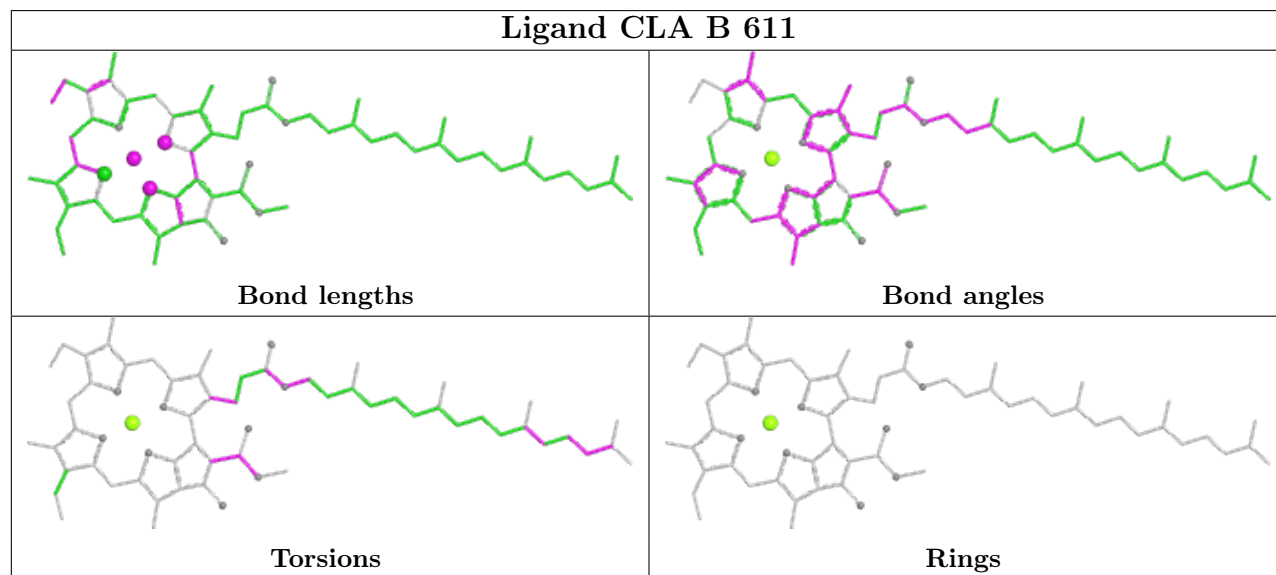
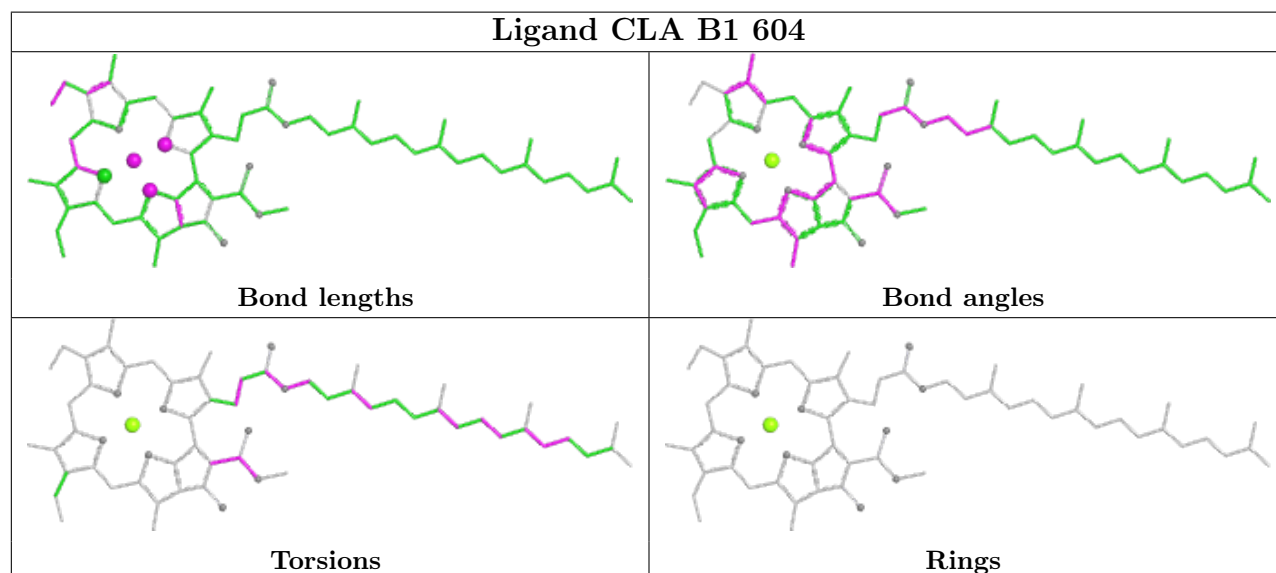
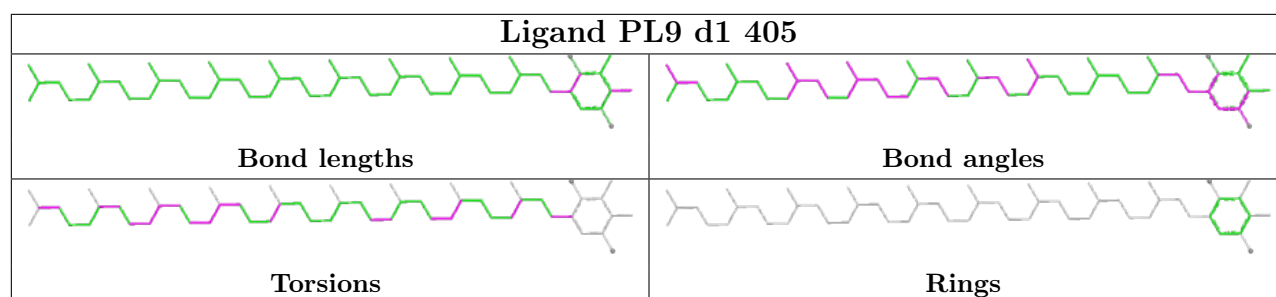
Bond angles

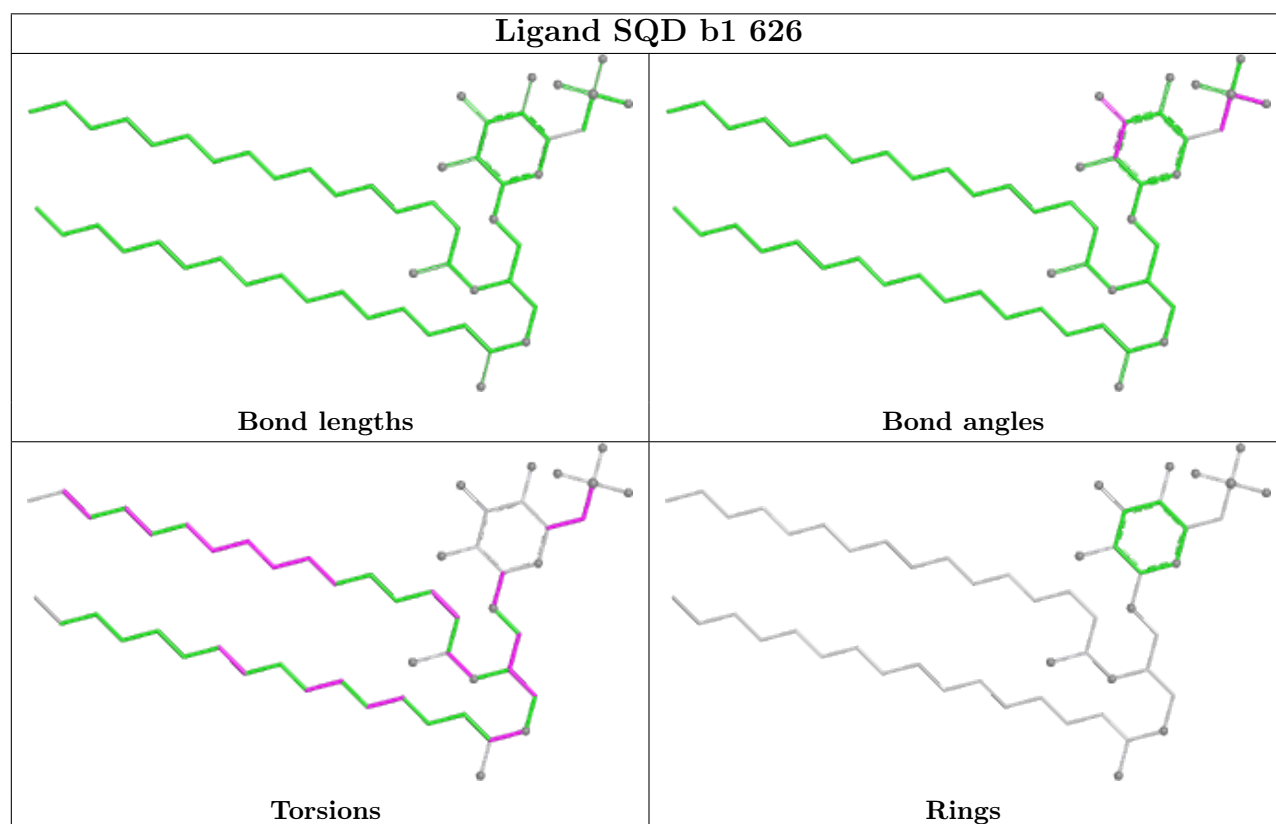
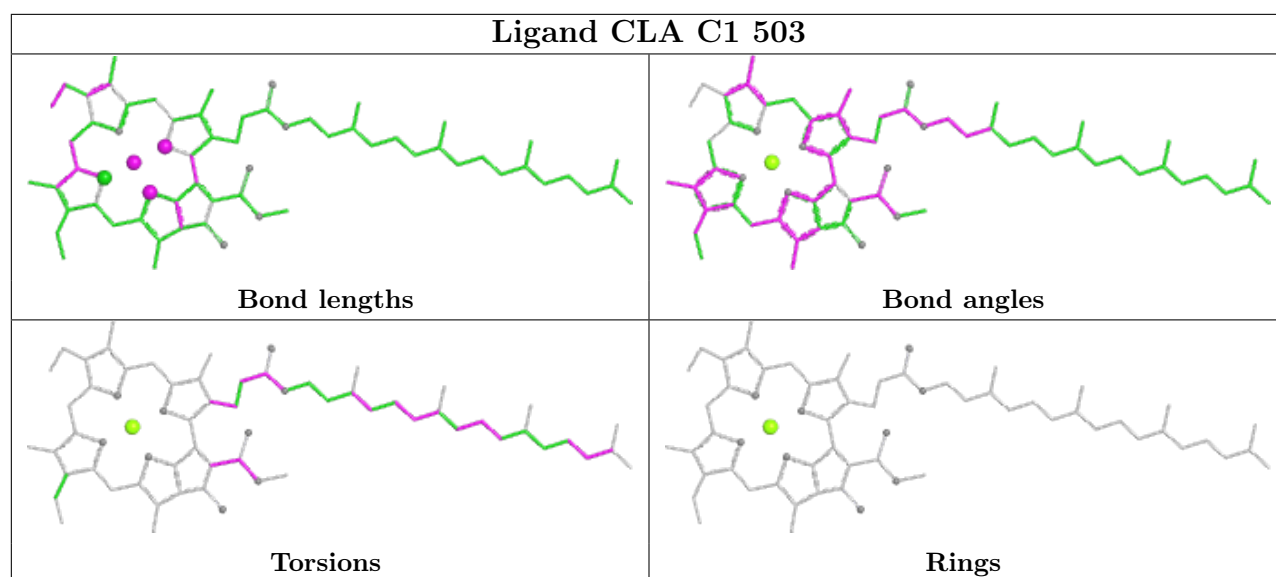


Torsions

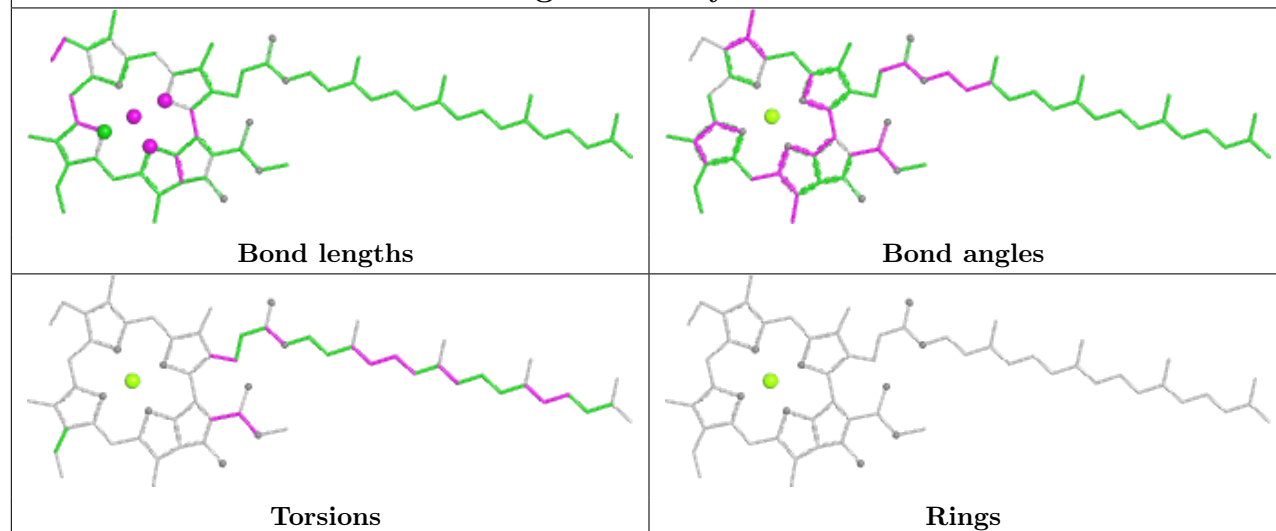


Rings

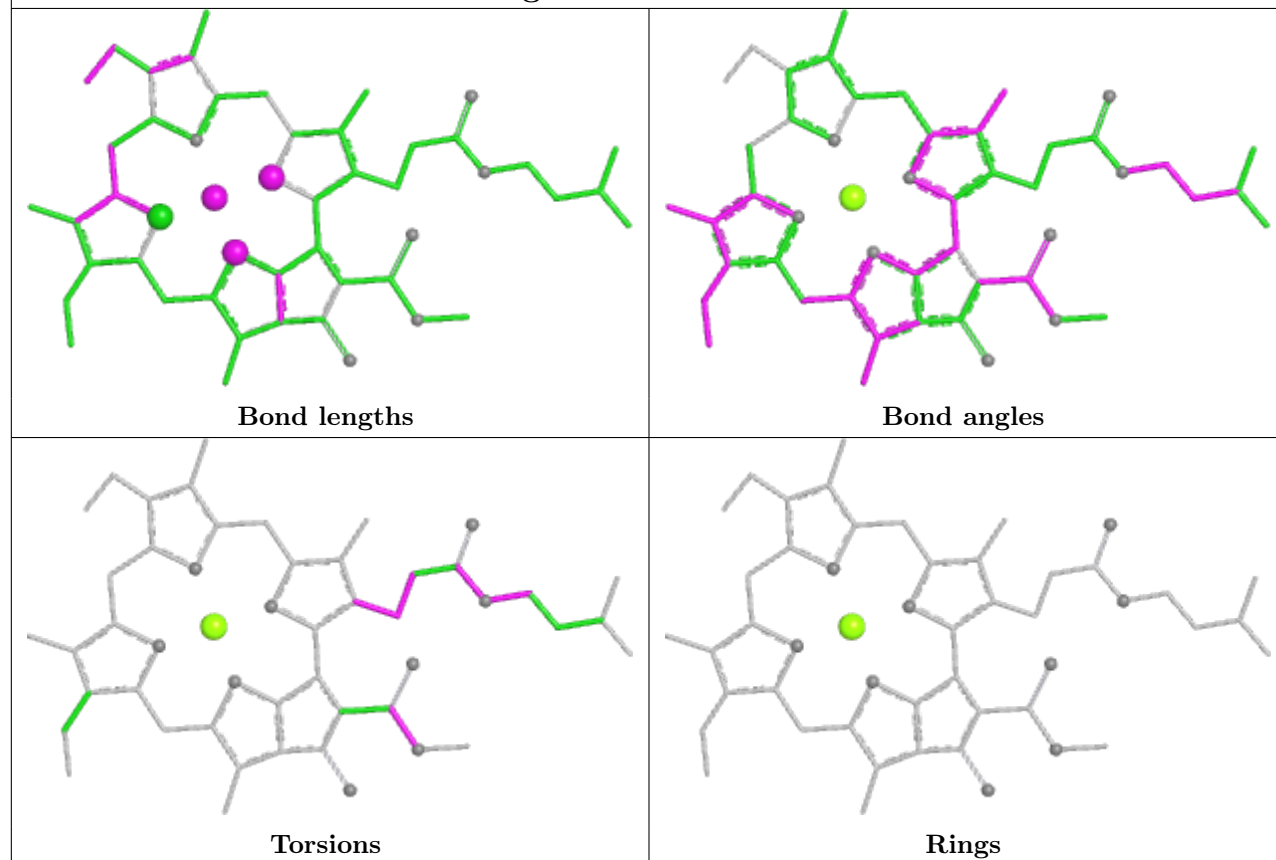


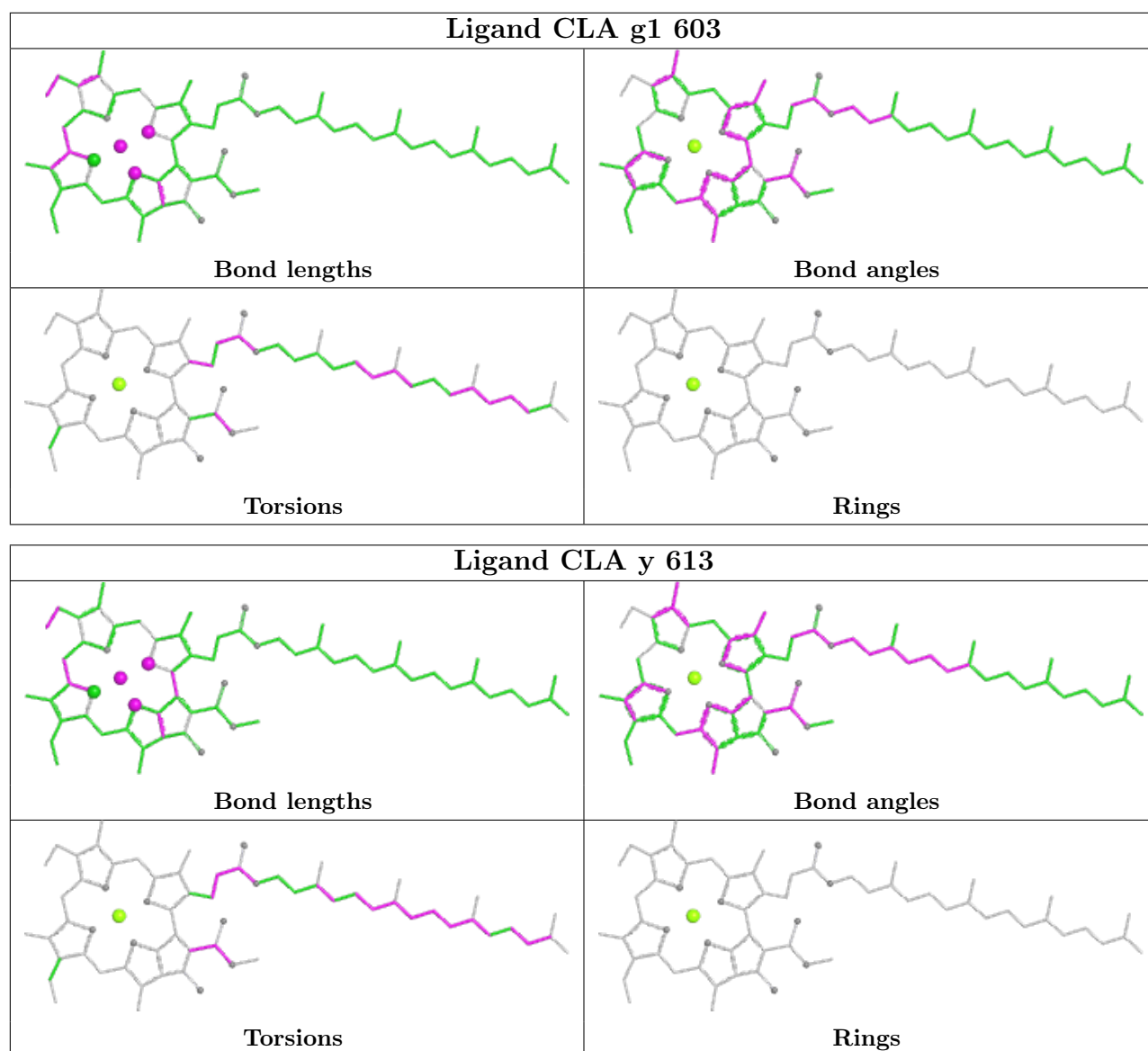


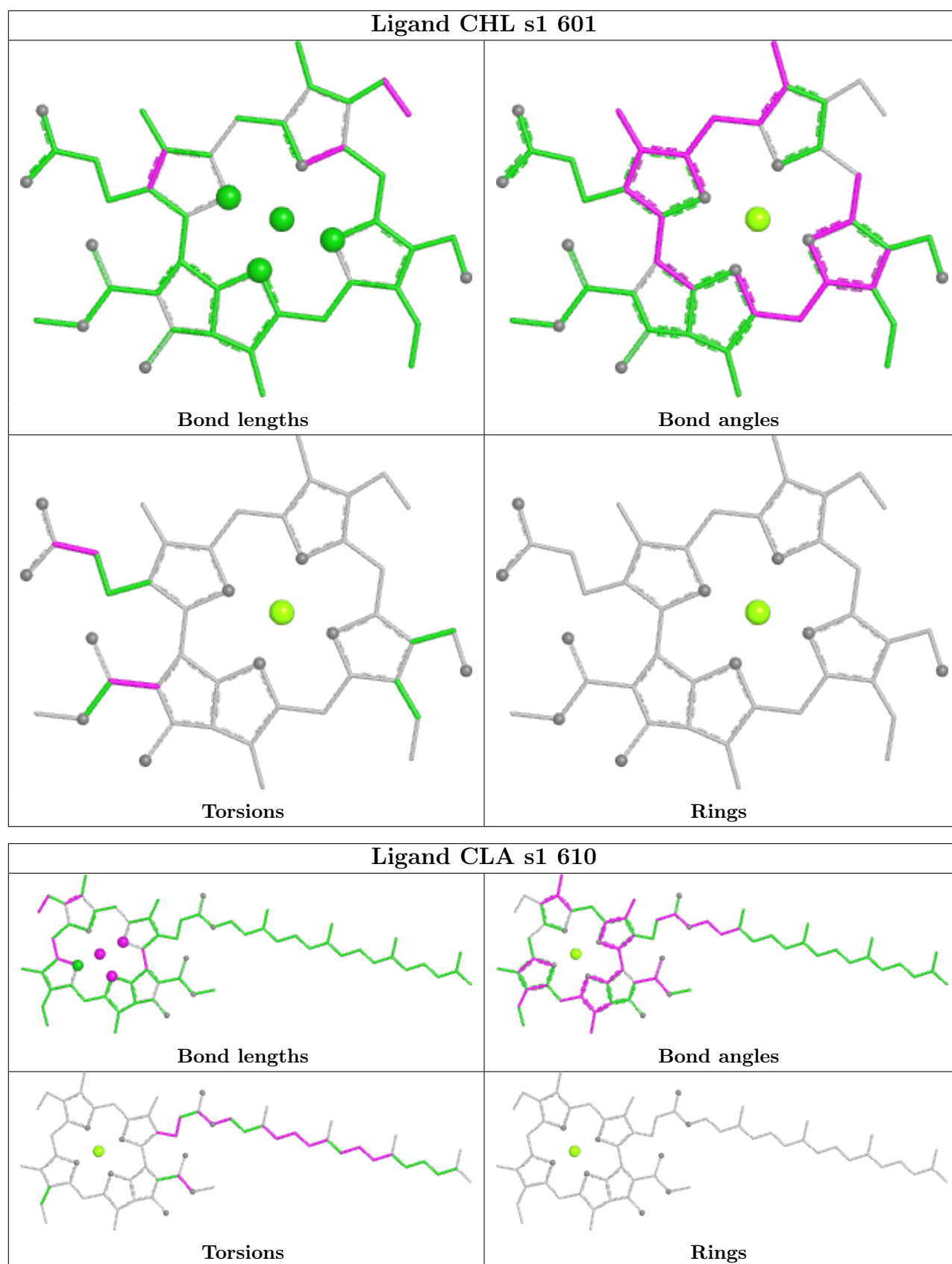
Ligand CLA y 611

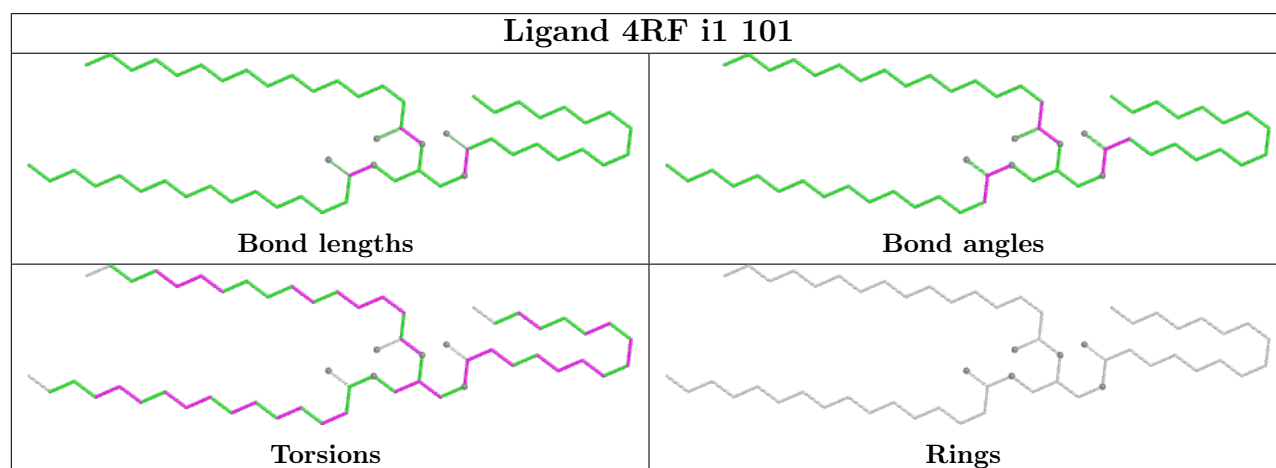
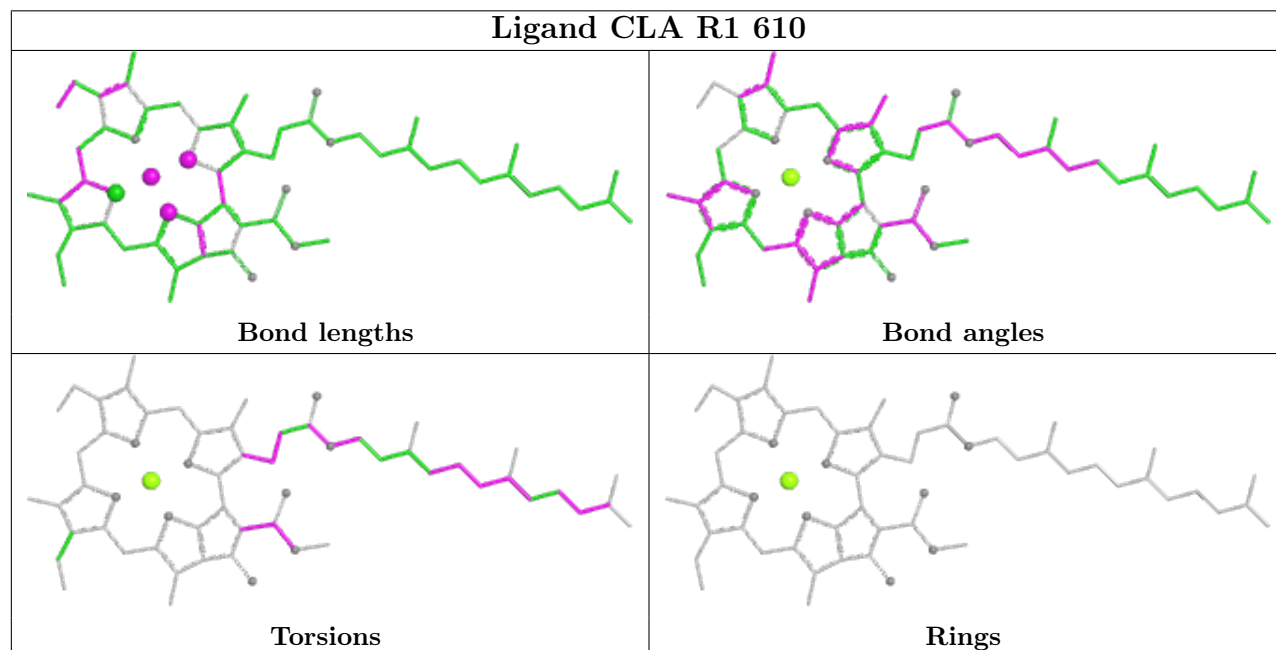
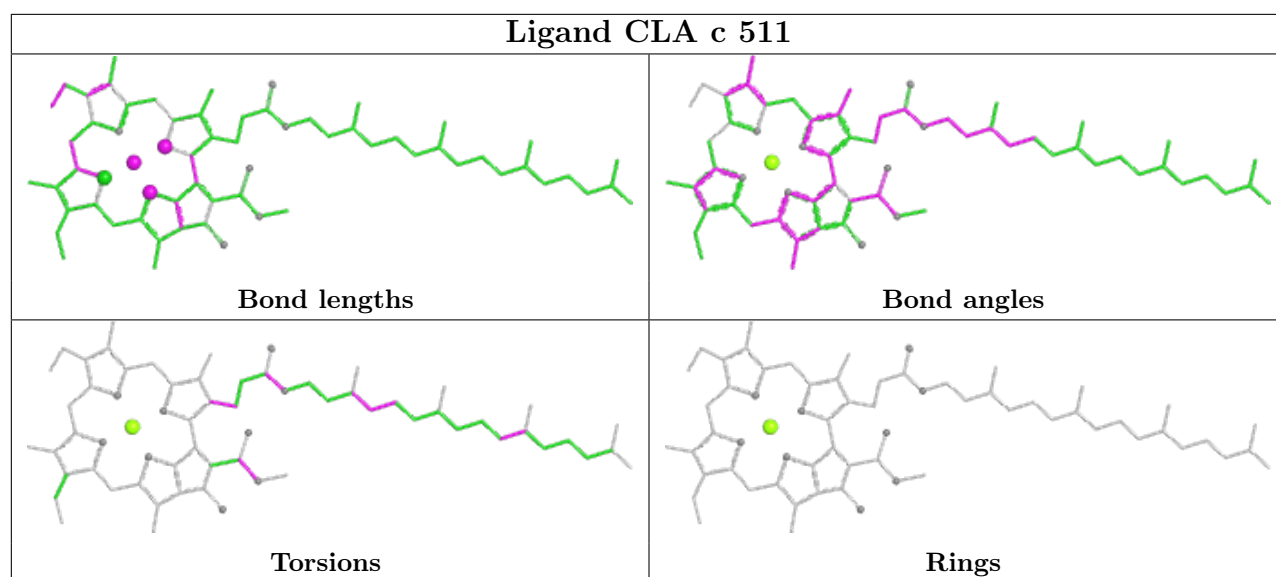


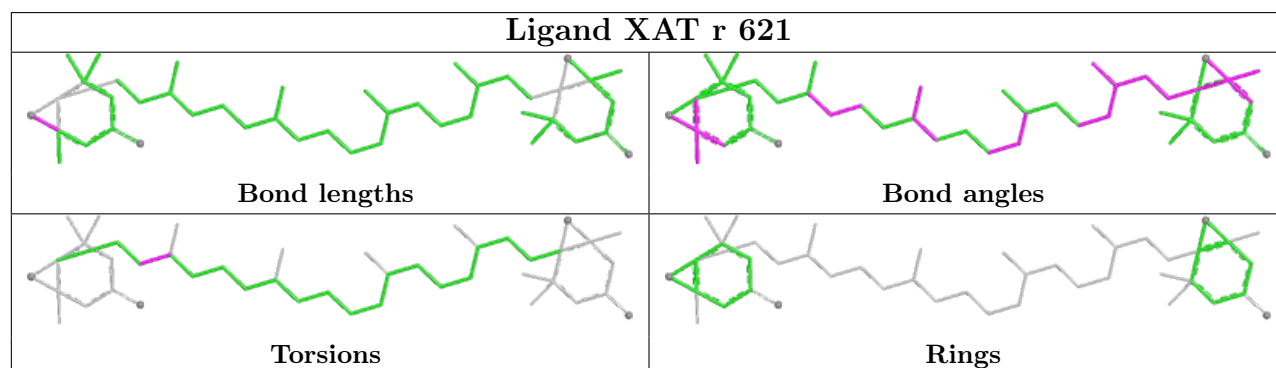
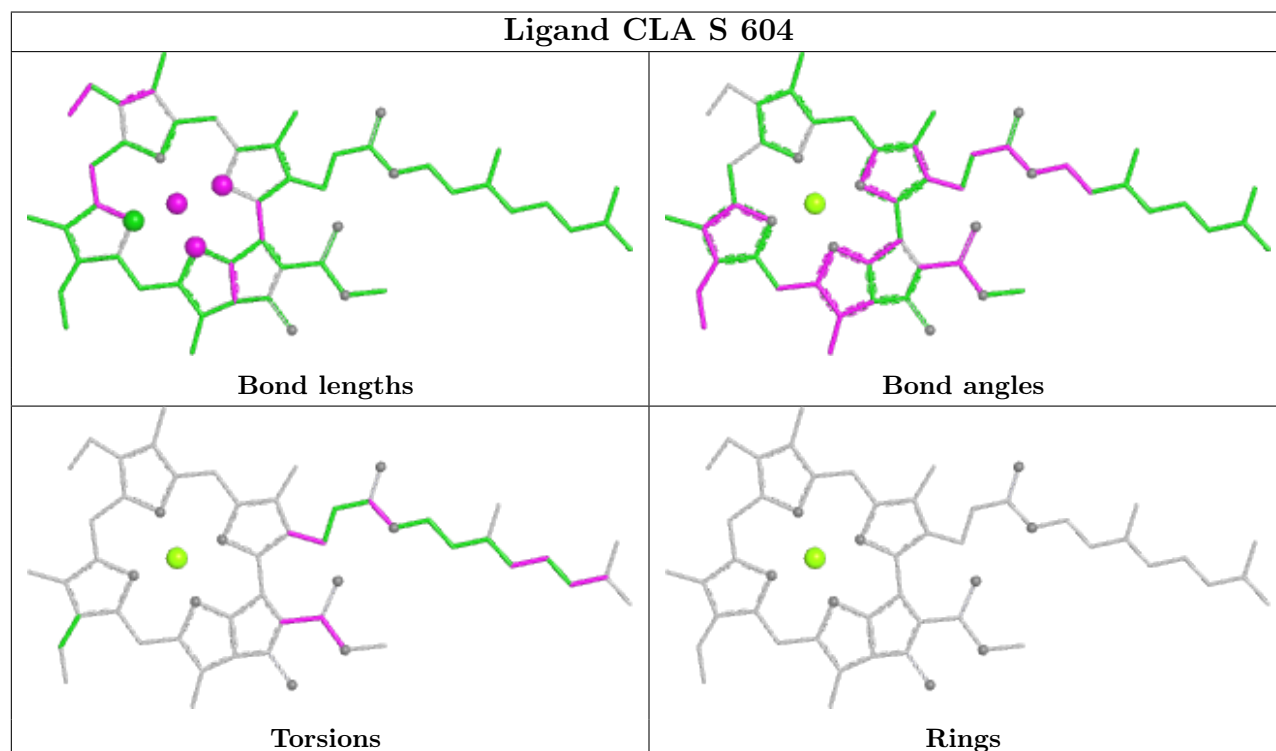
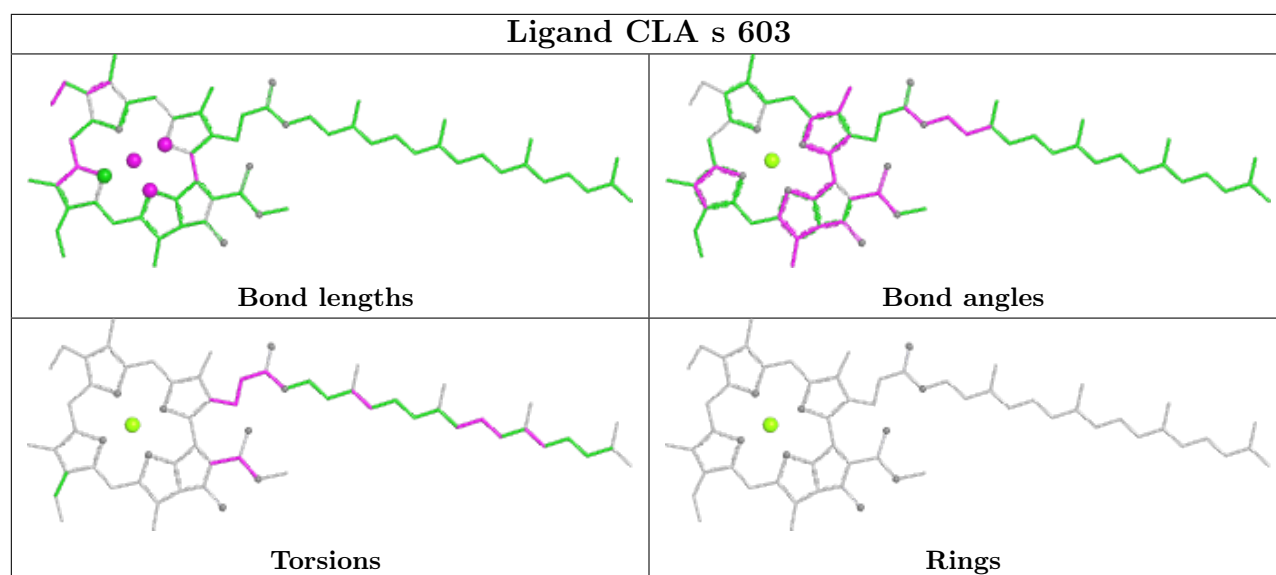
Ligand CLA Y1 608

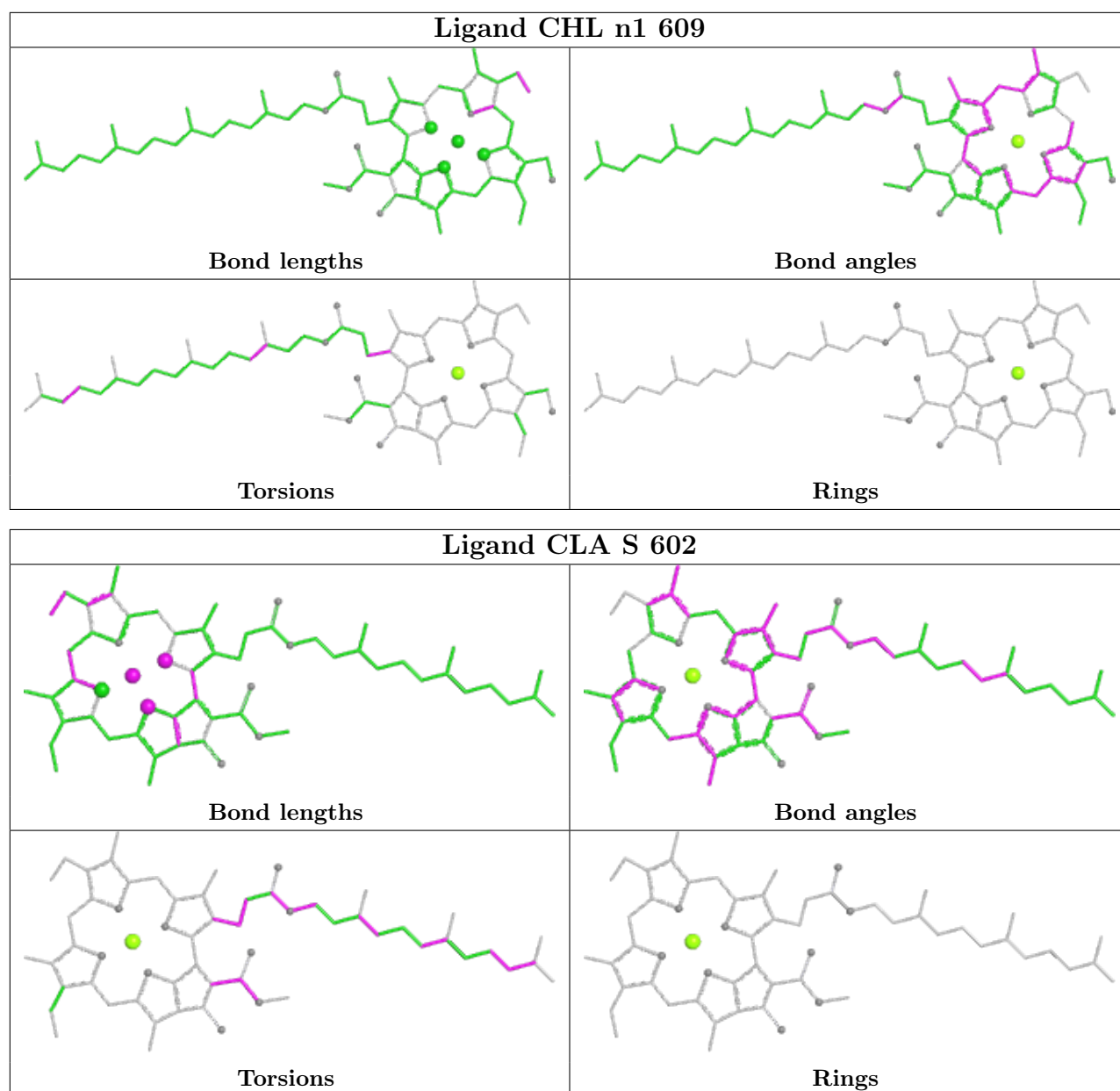


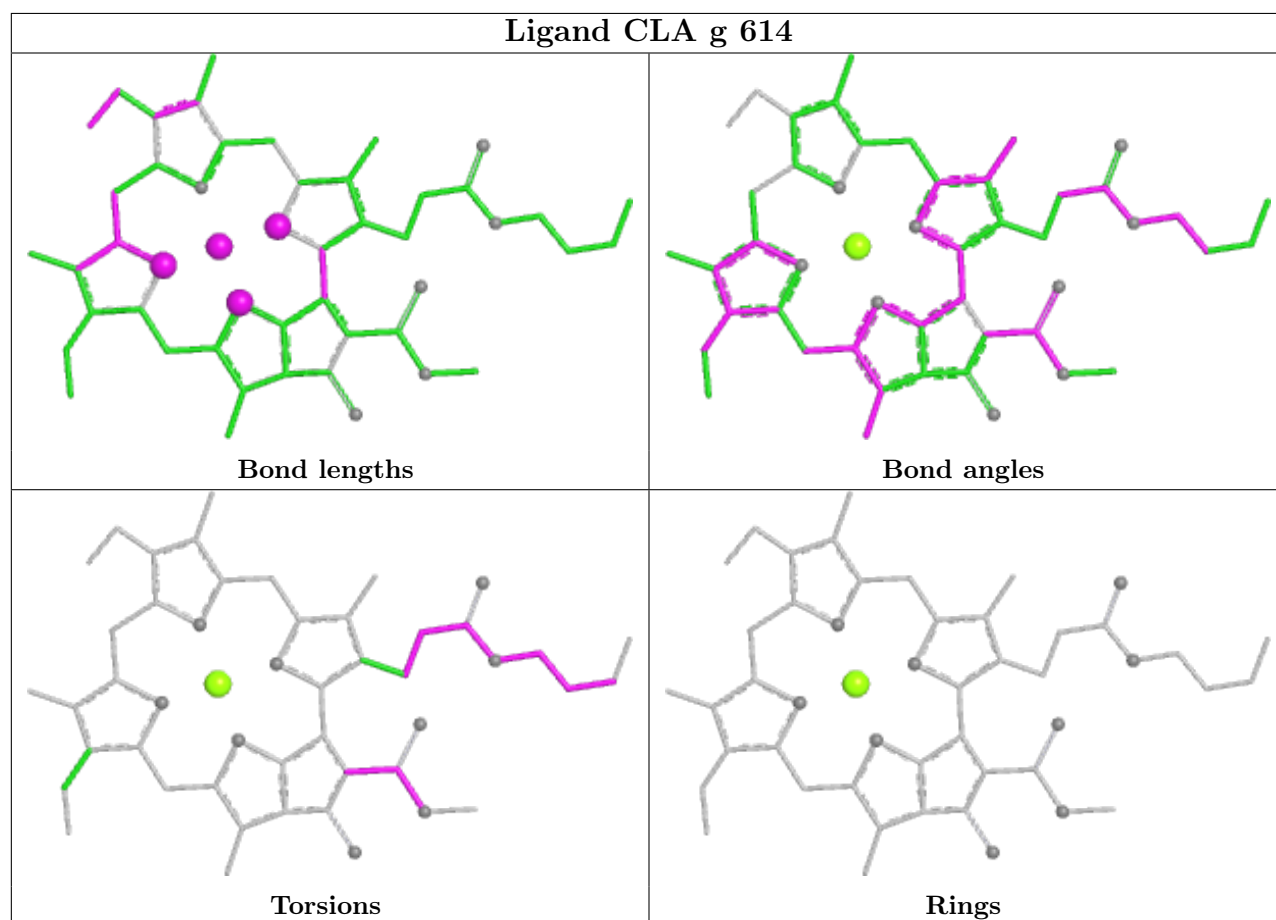
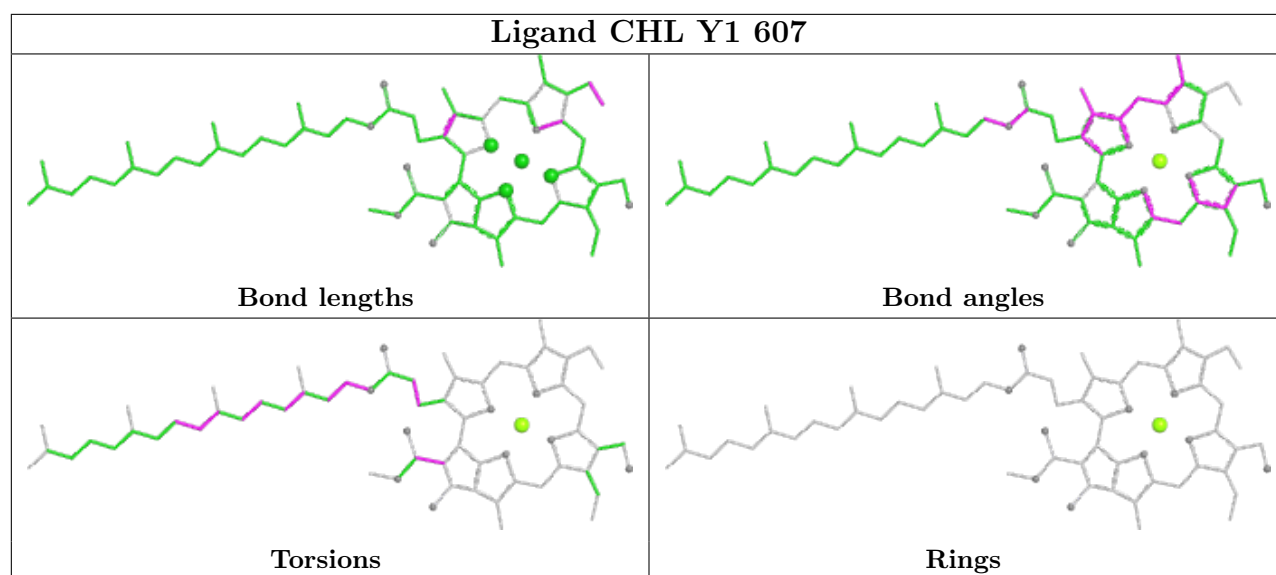


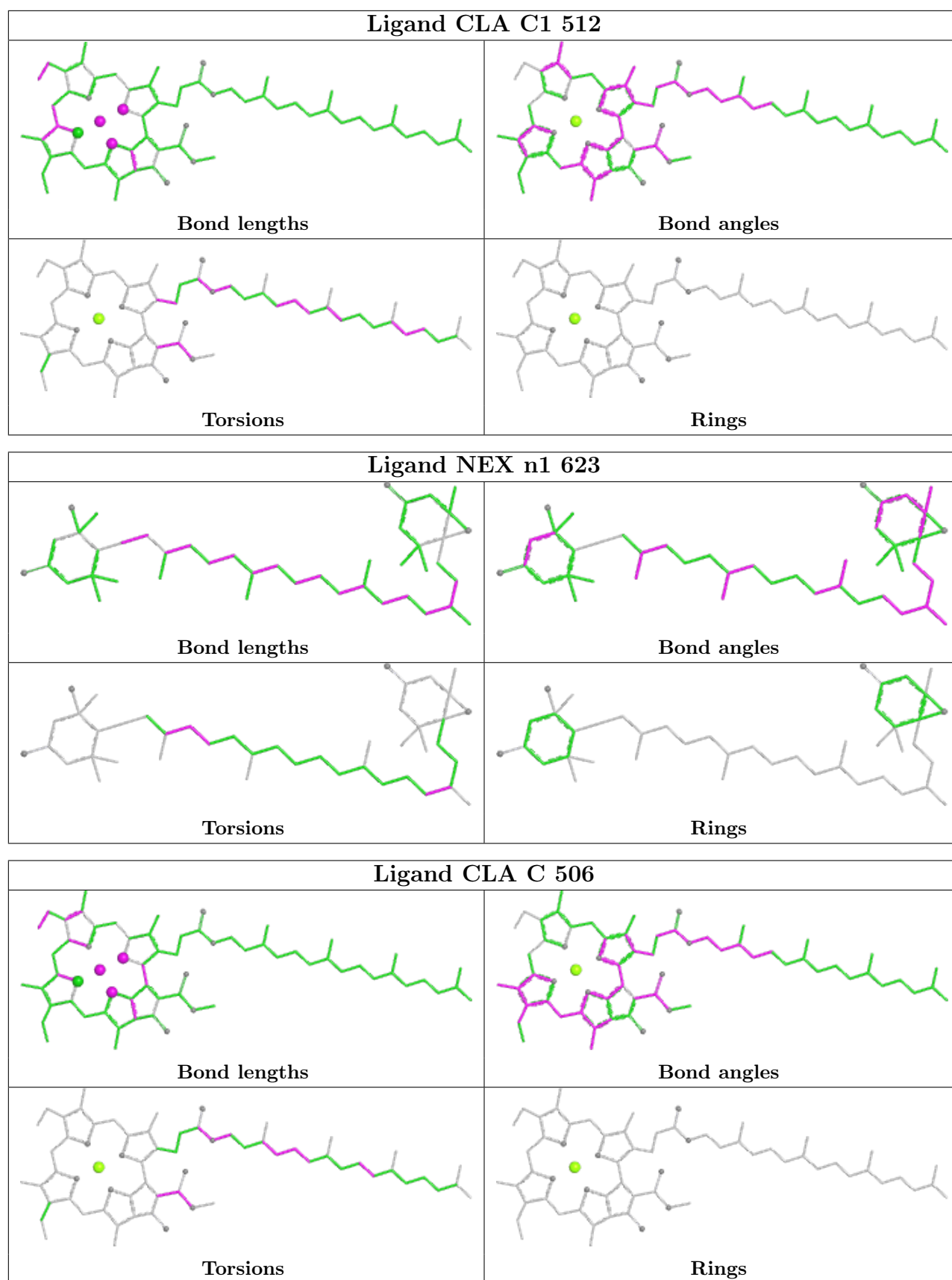


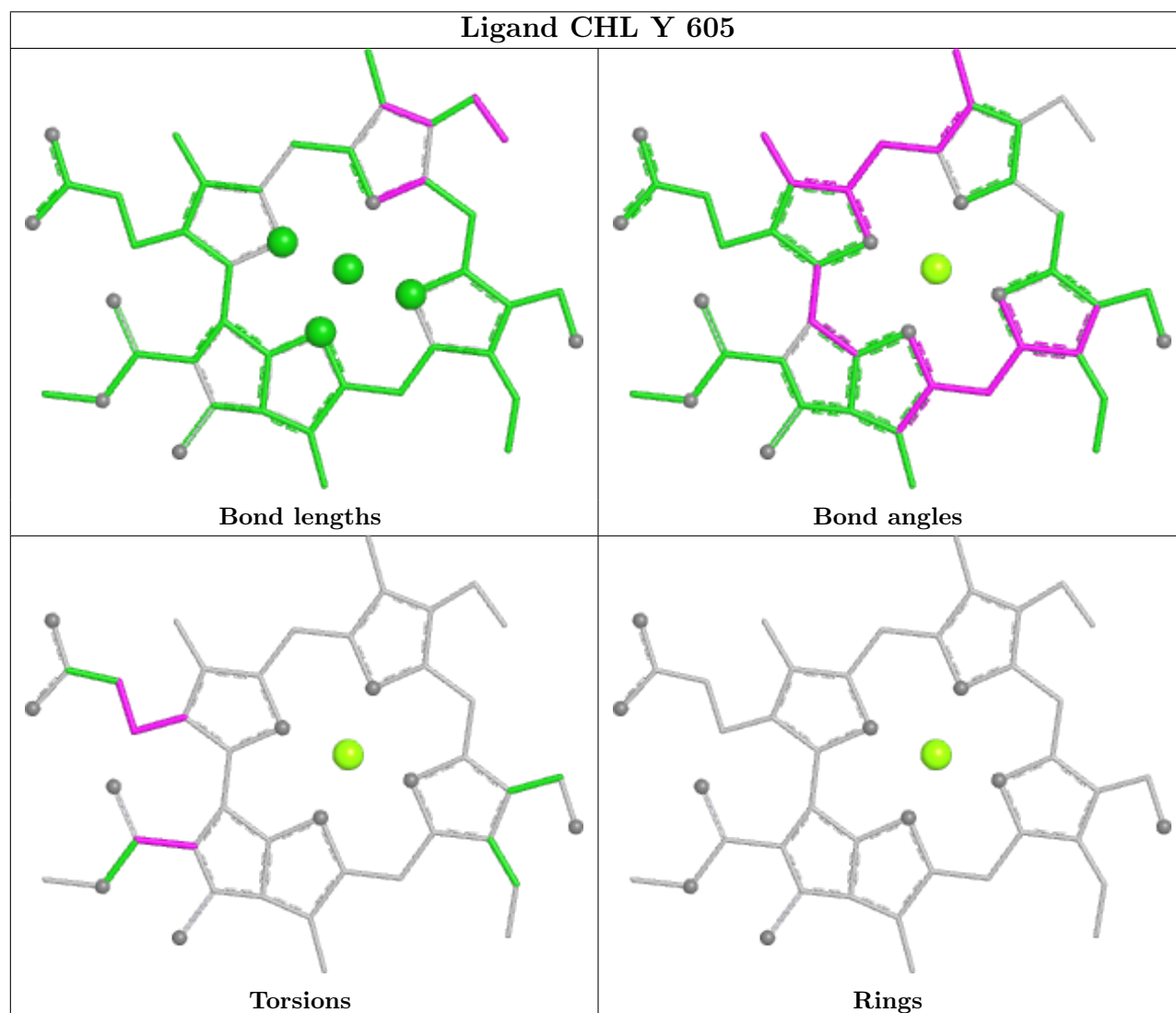
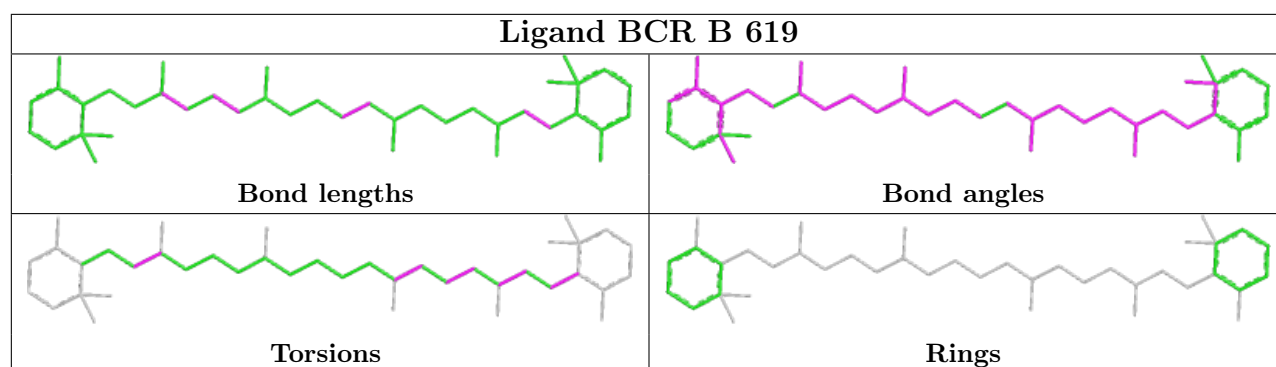


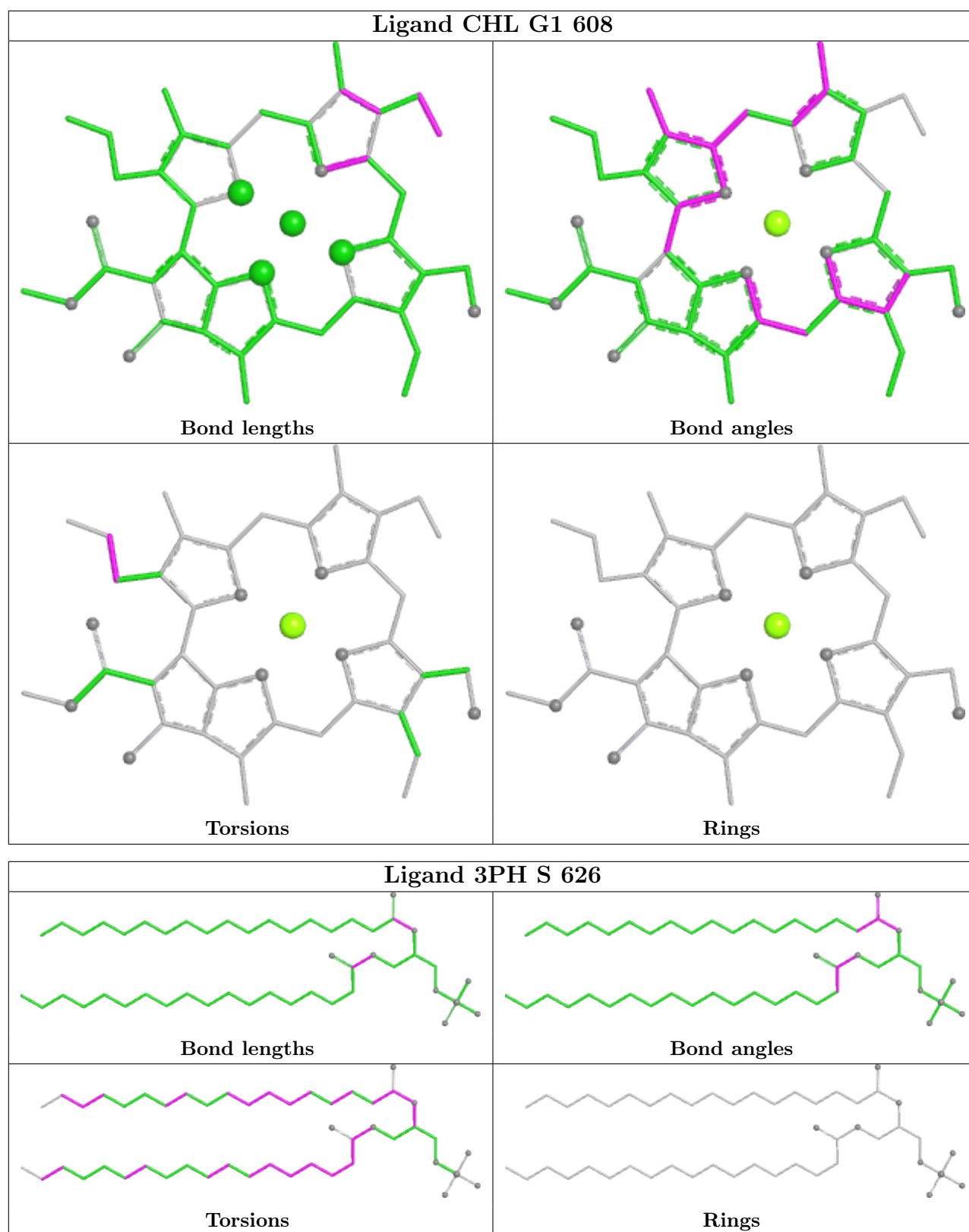


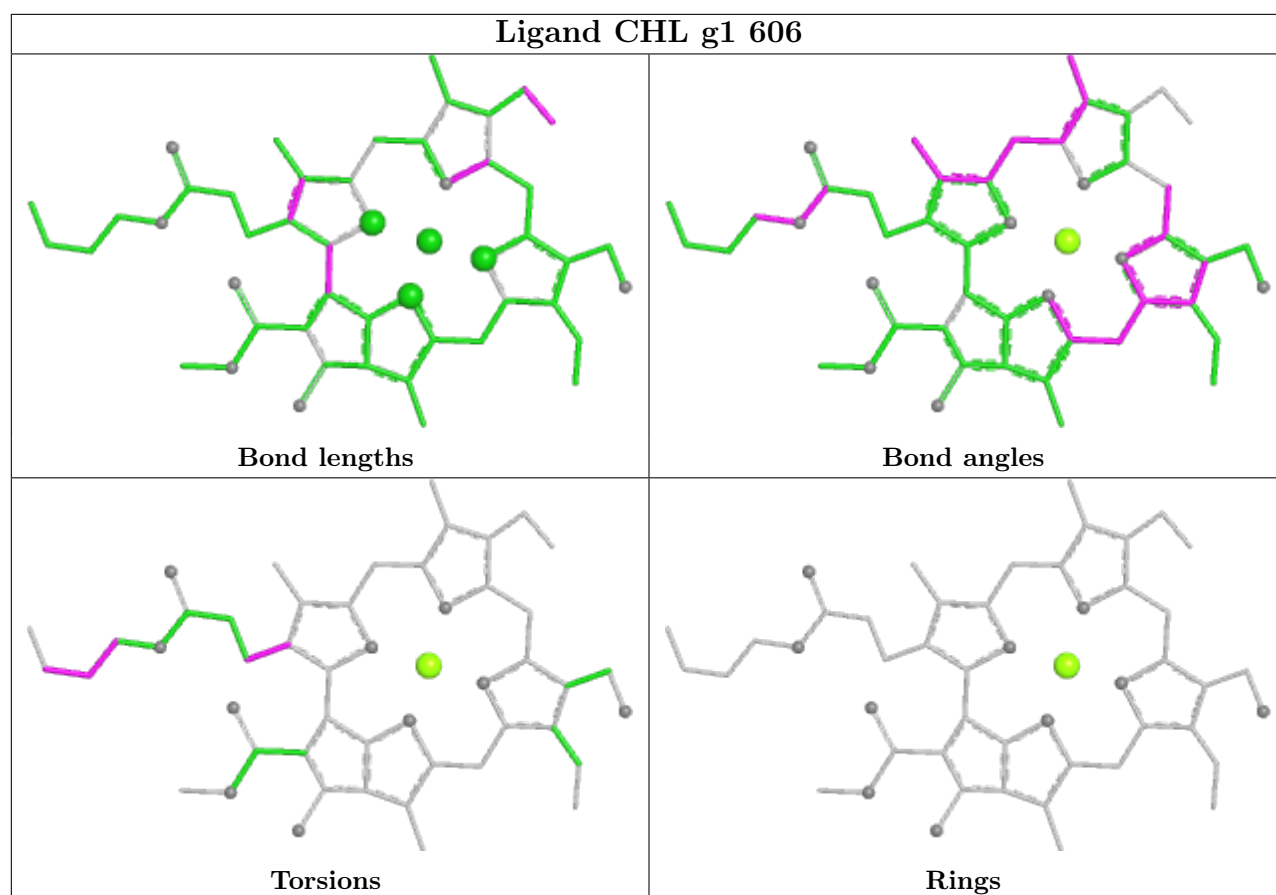




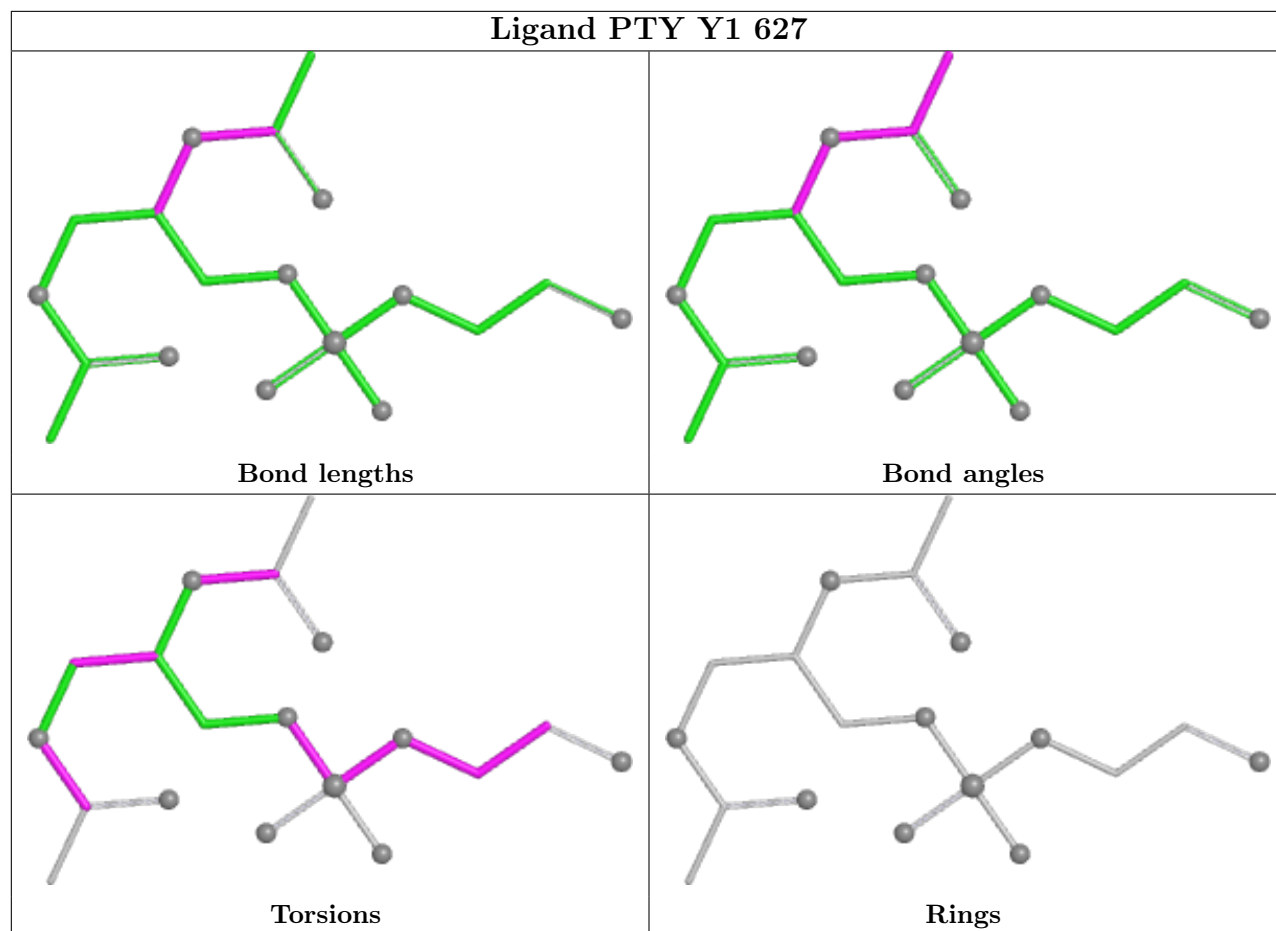




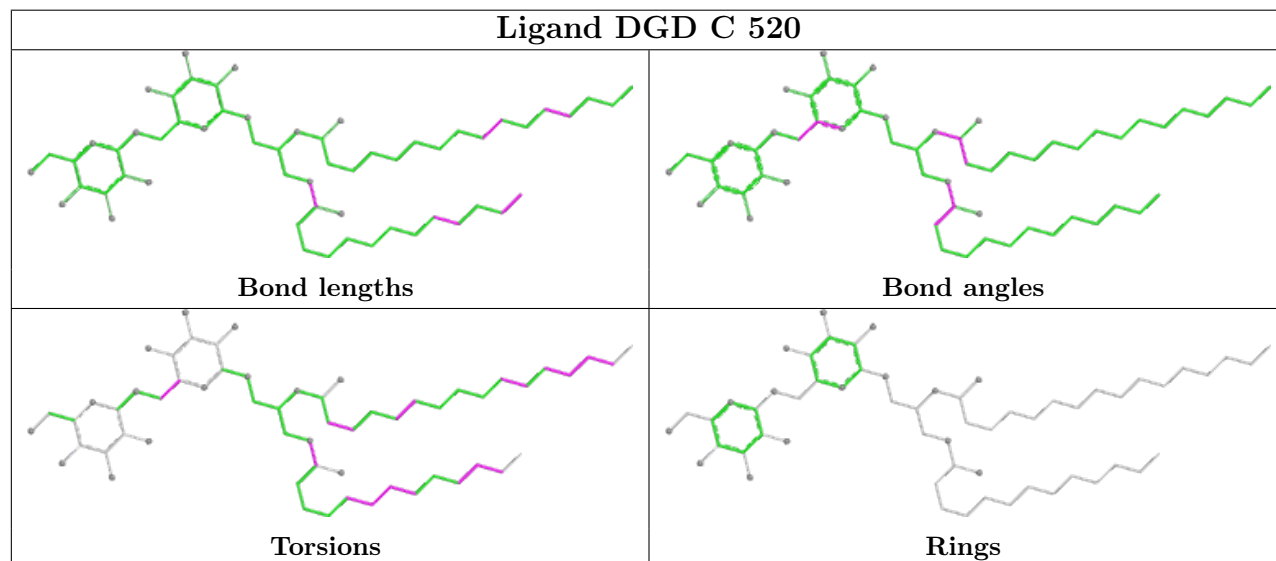


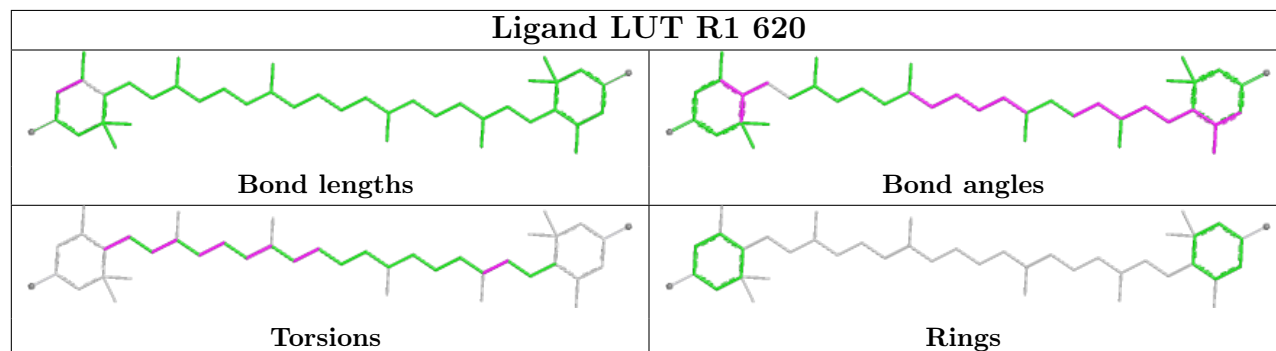
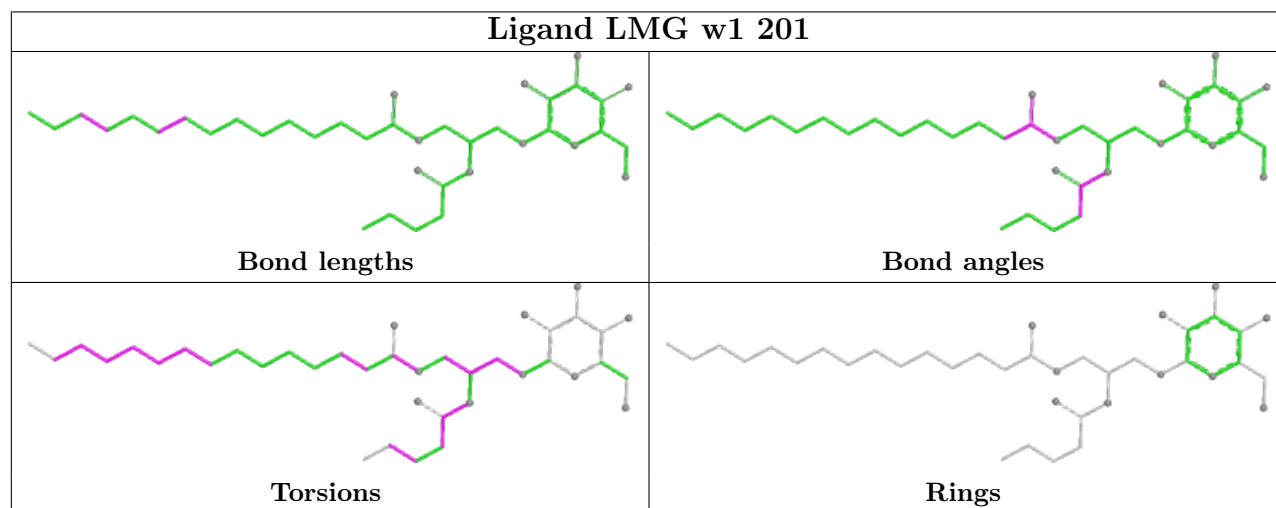
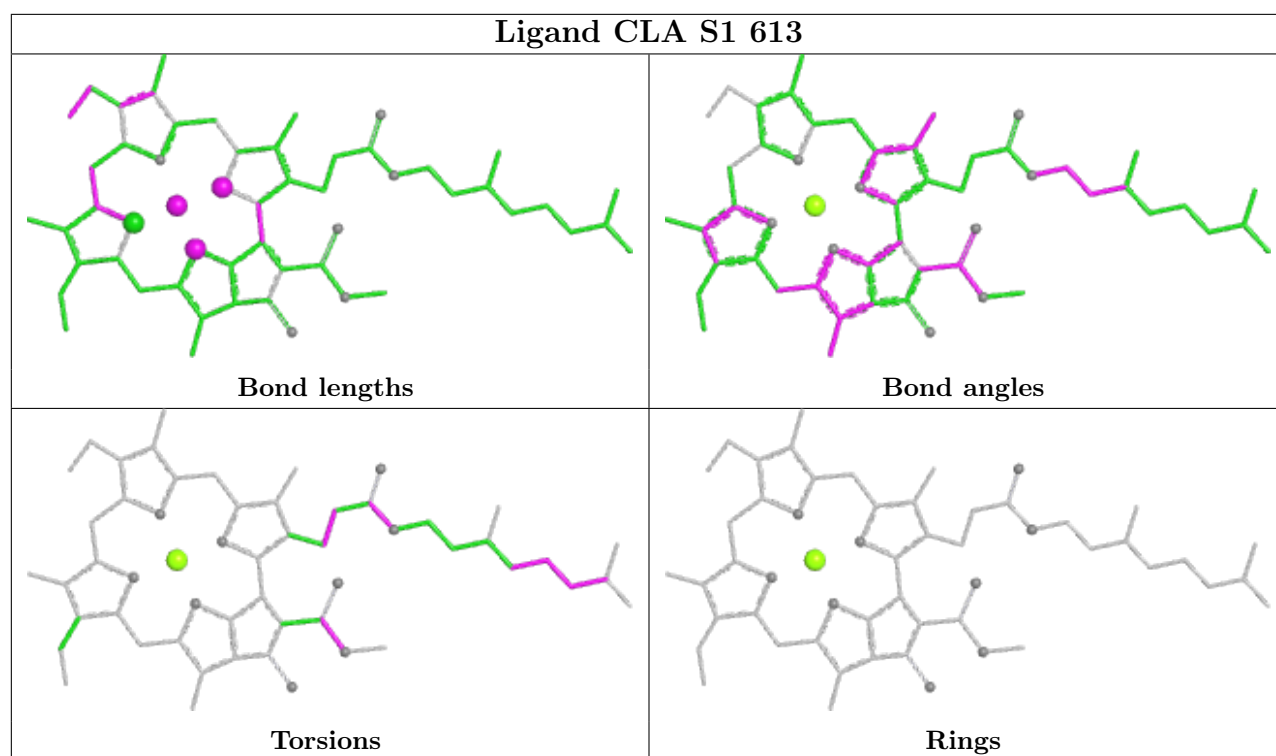


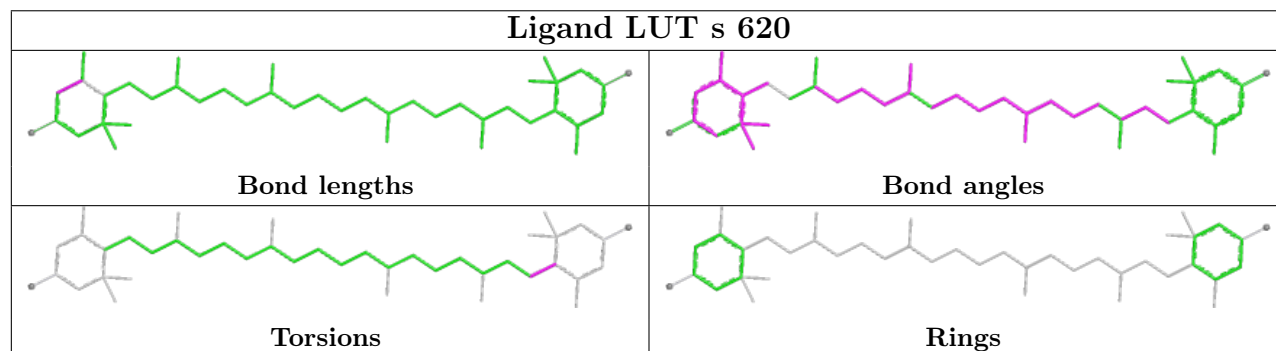
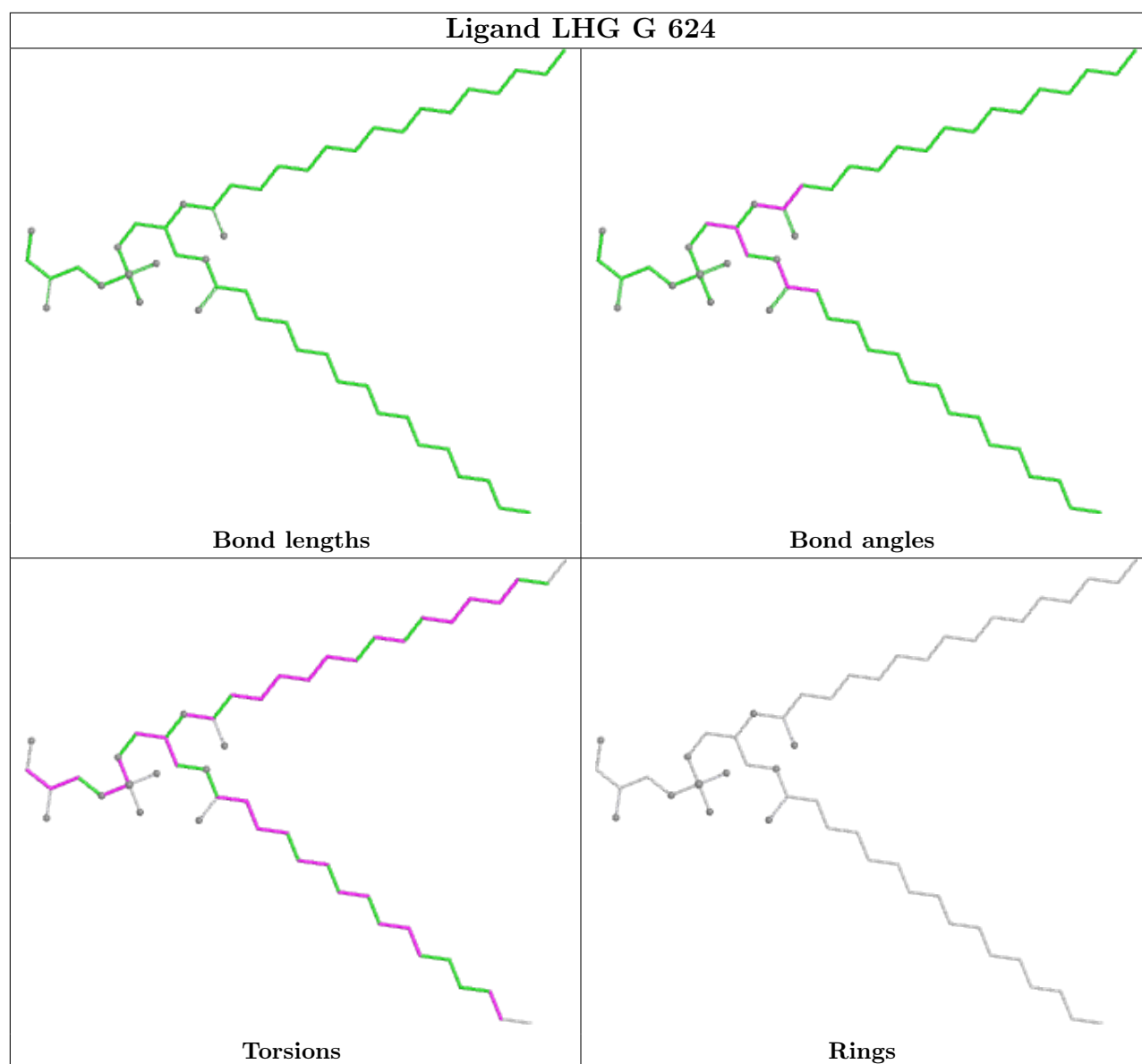
Ligand PTY Y1 627

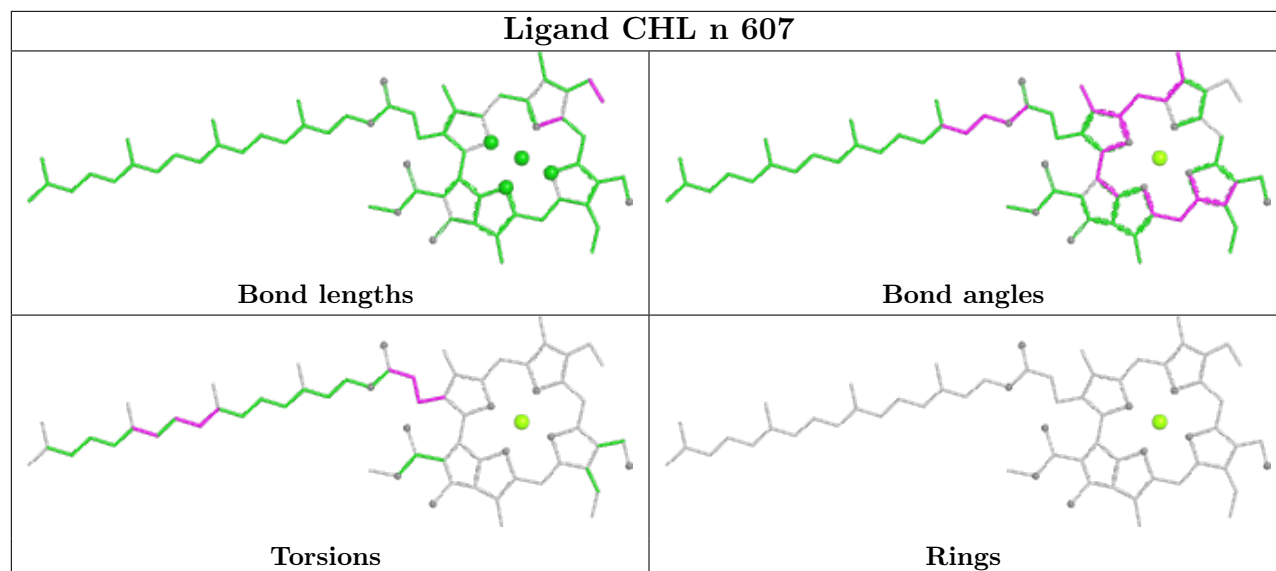
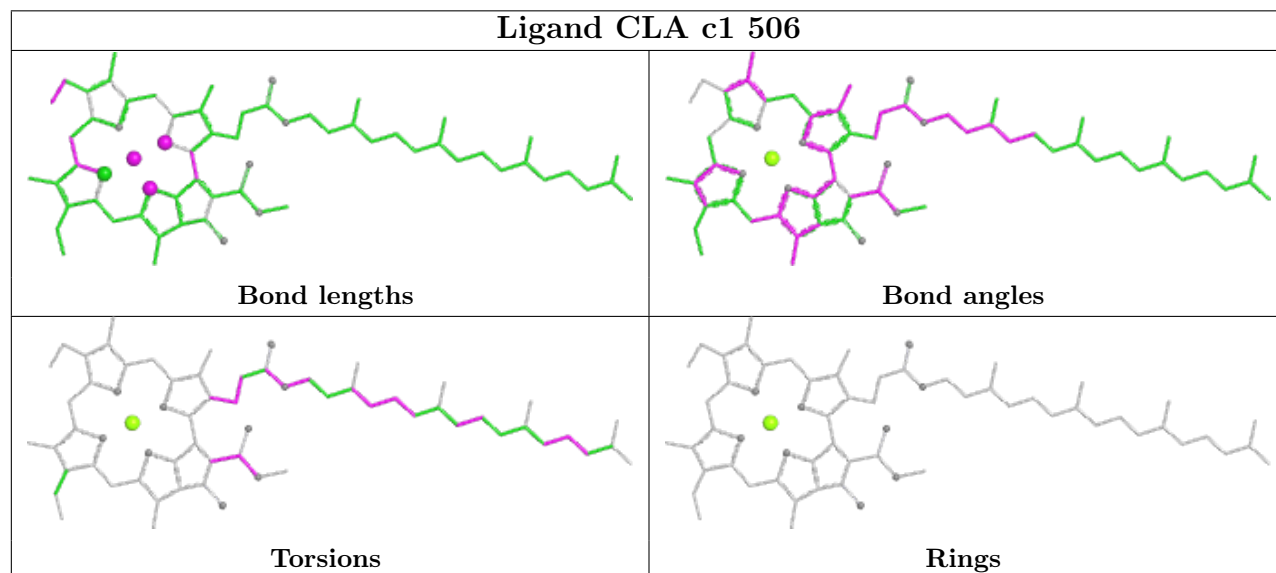
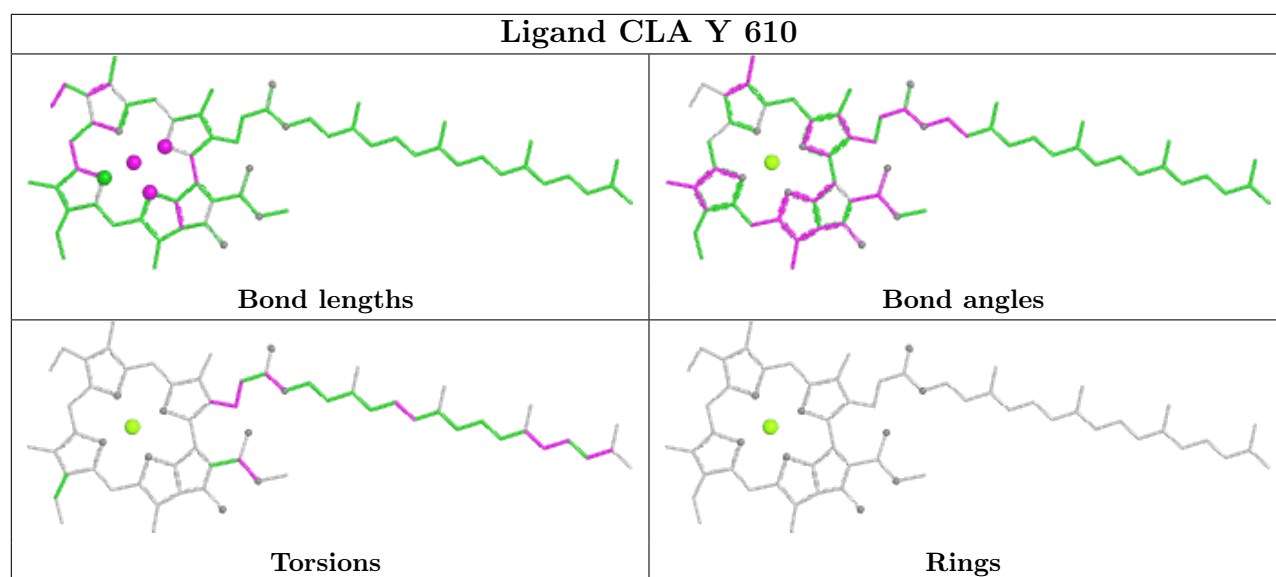


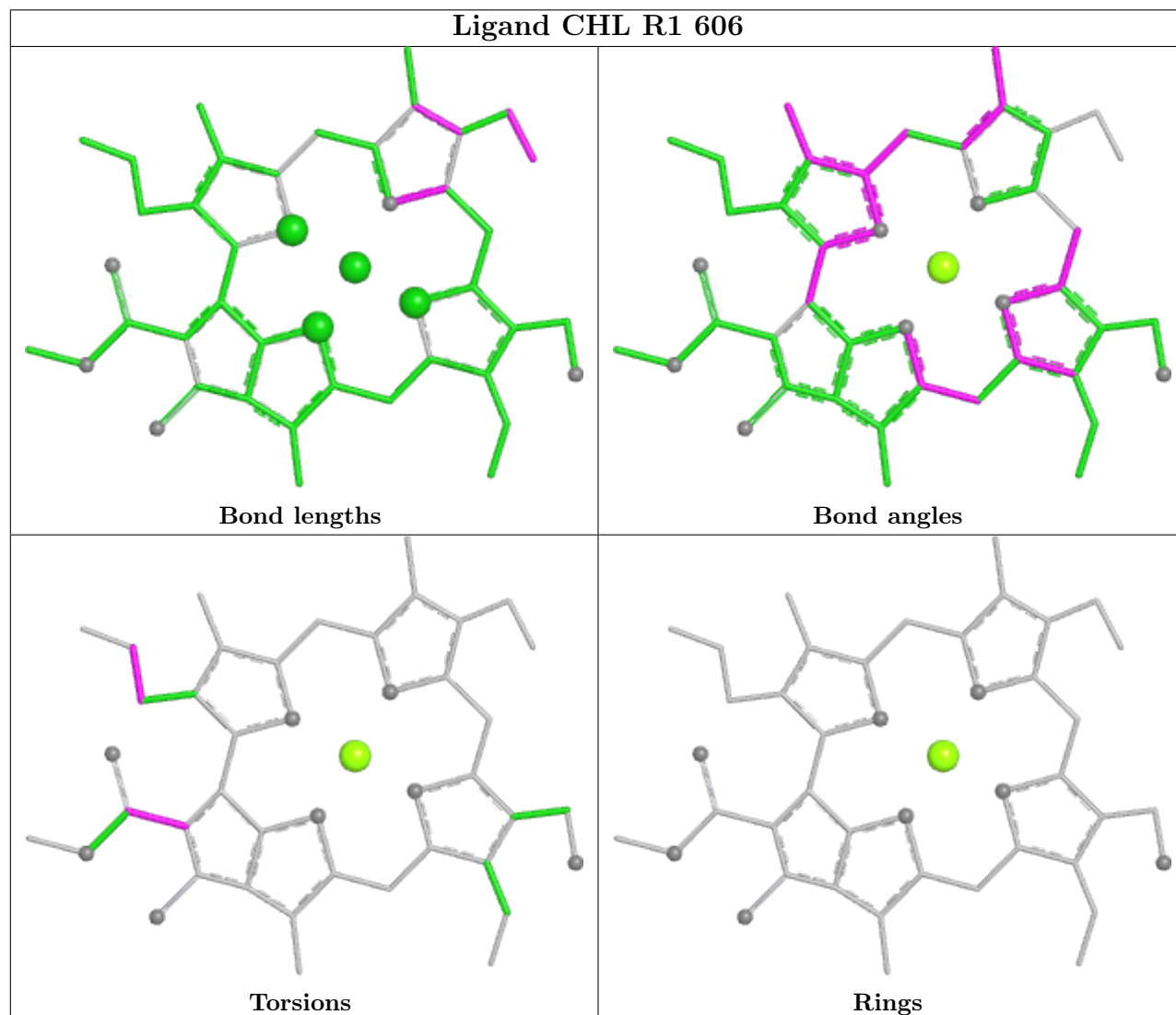
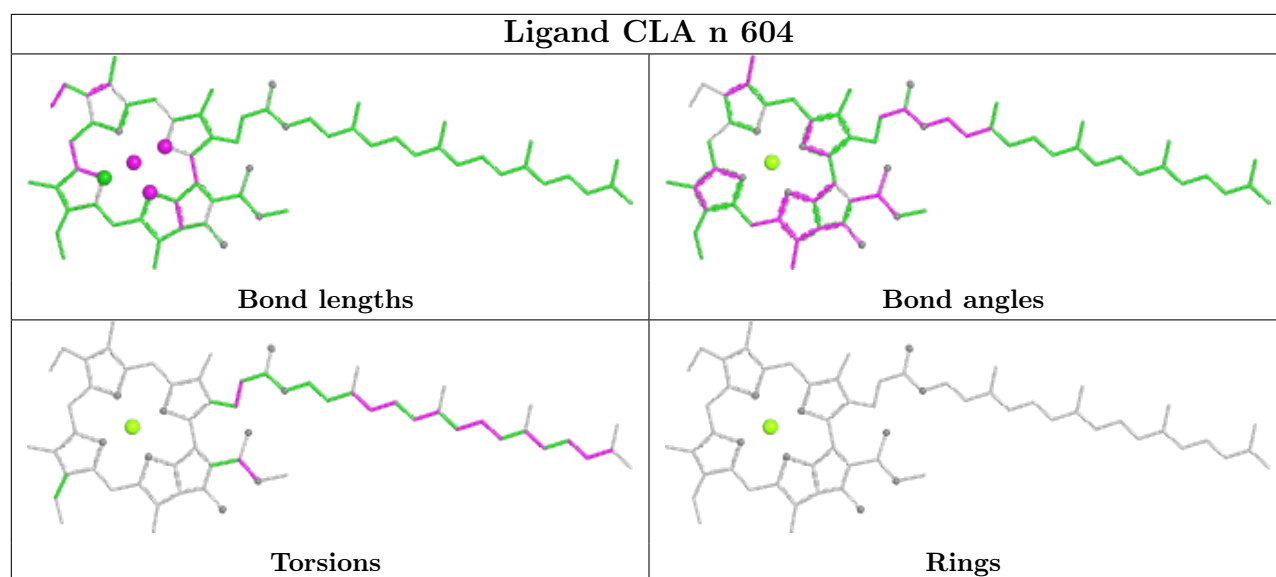
Ligand DGD C 520

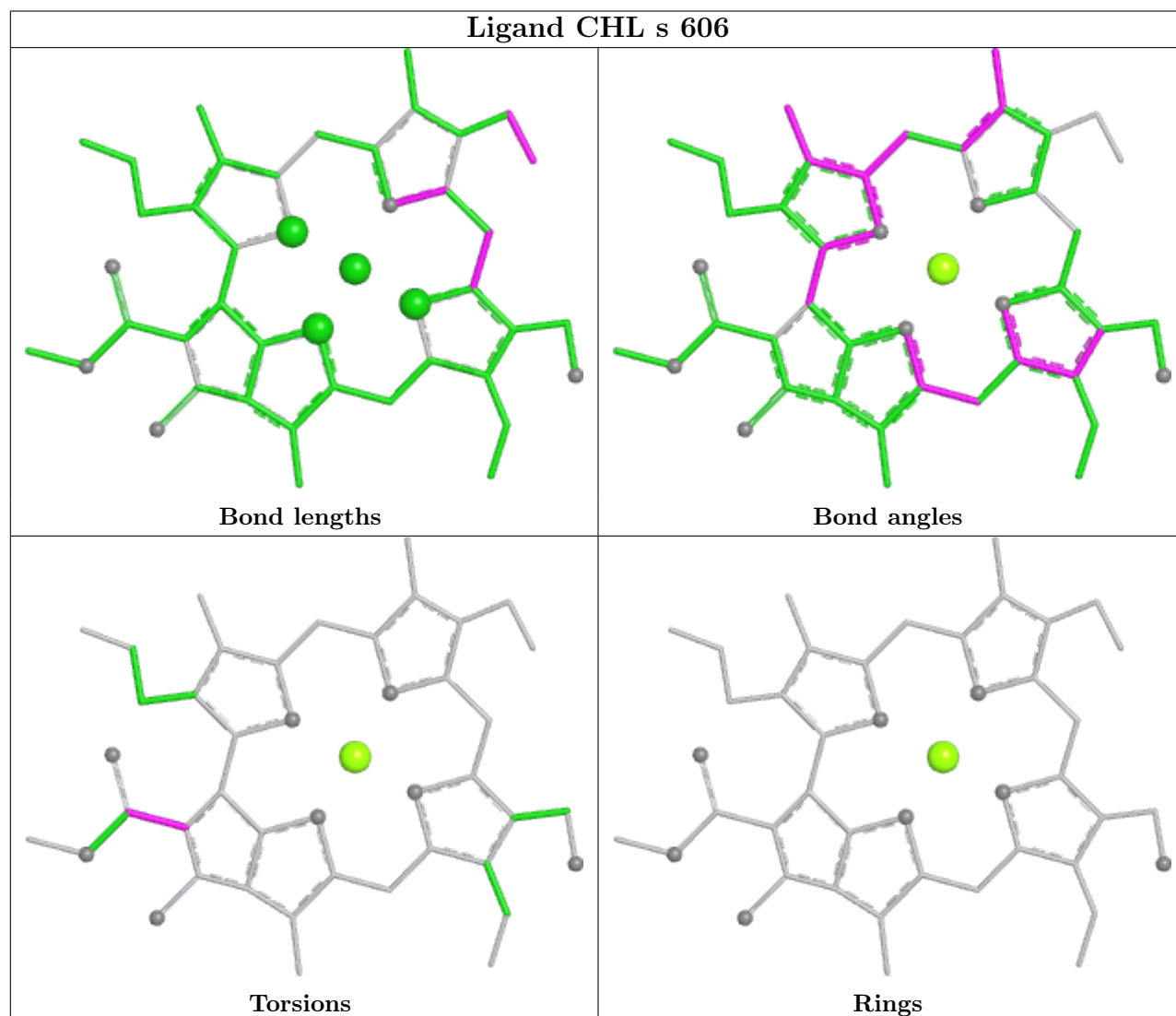
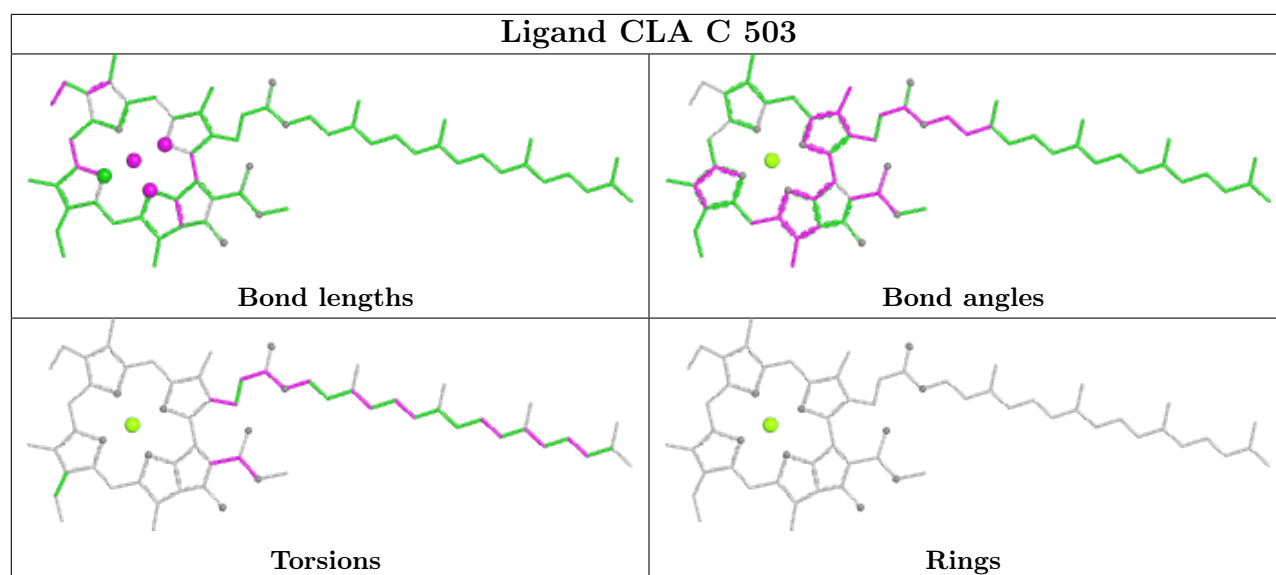


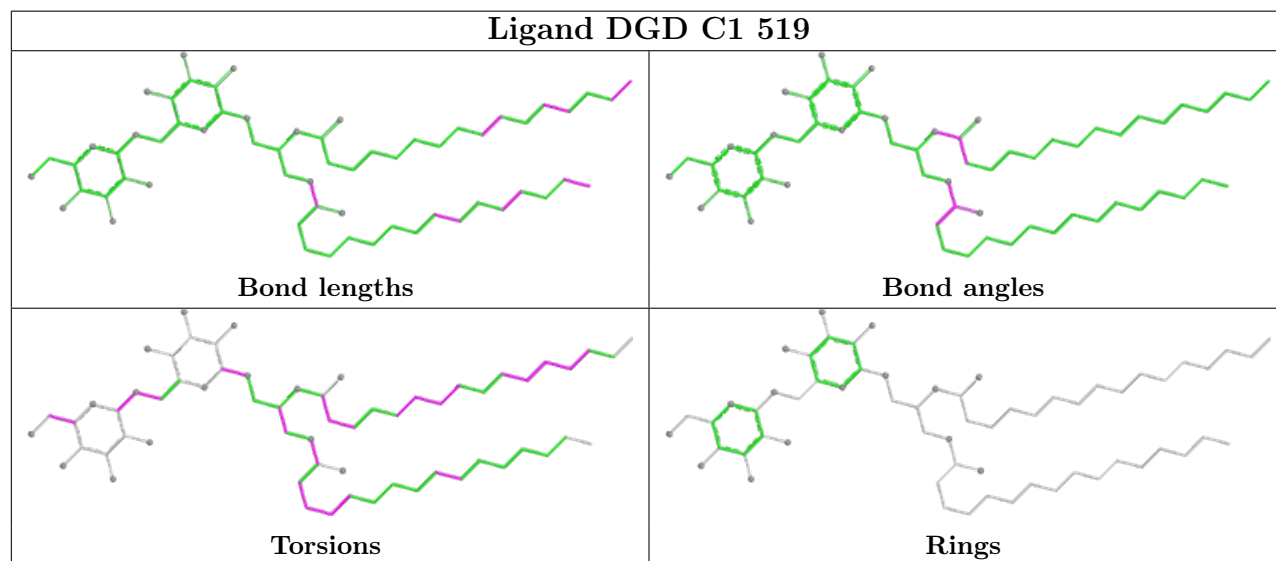
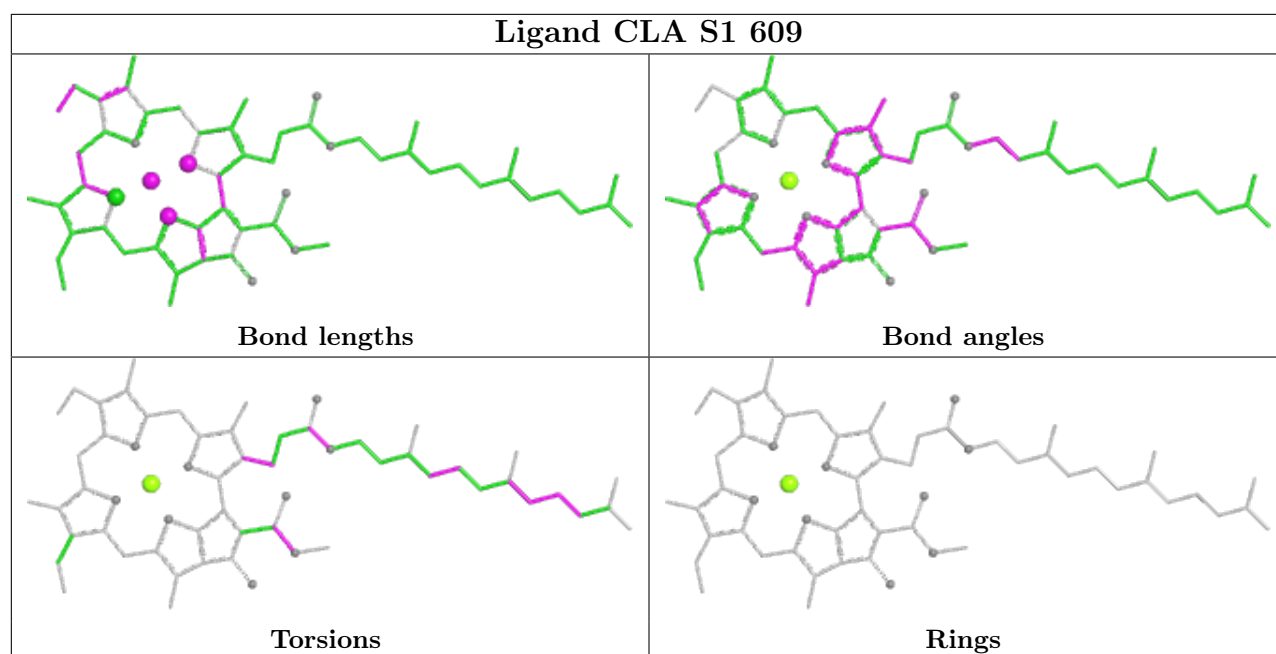


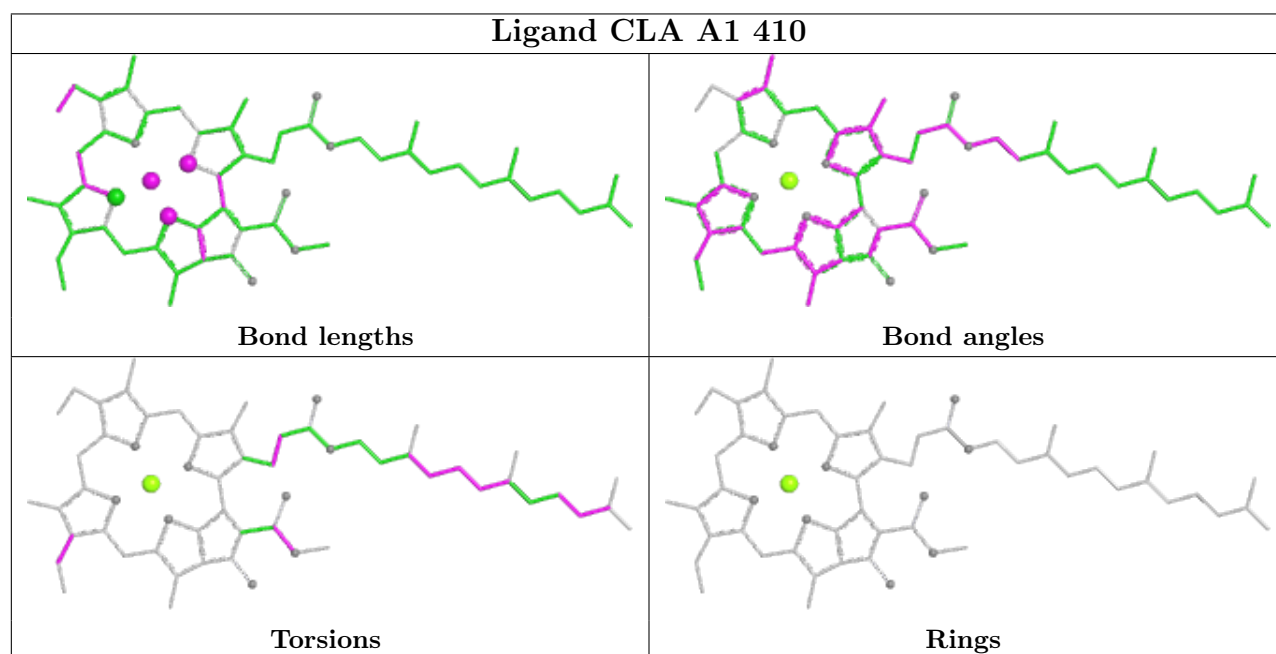
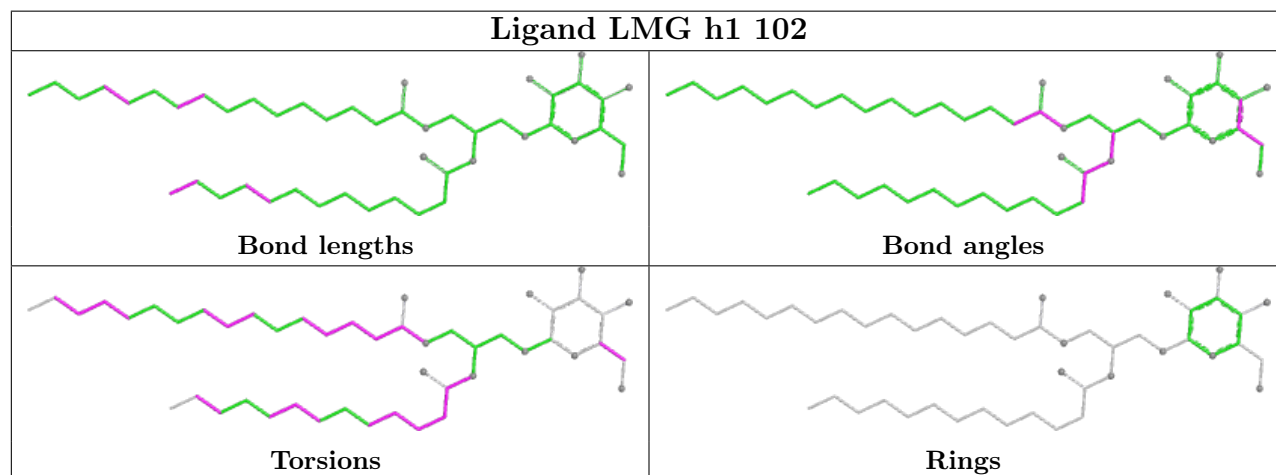
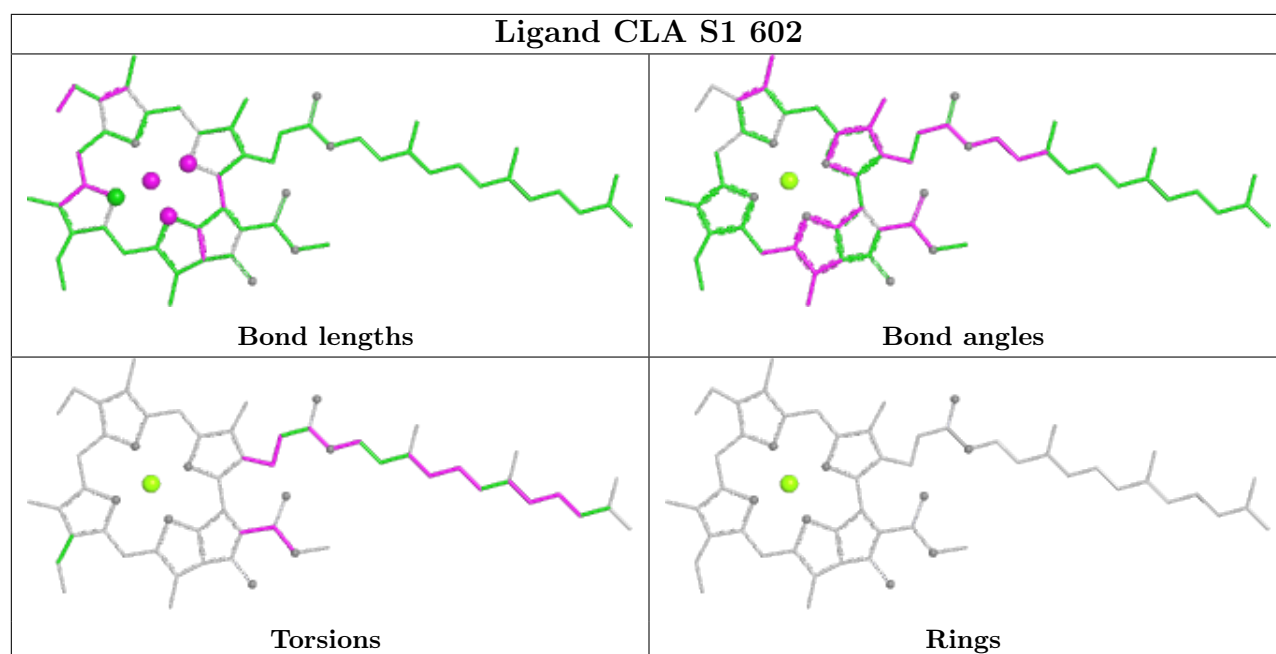


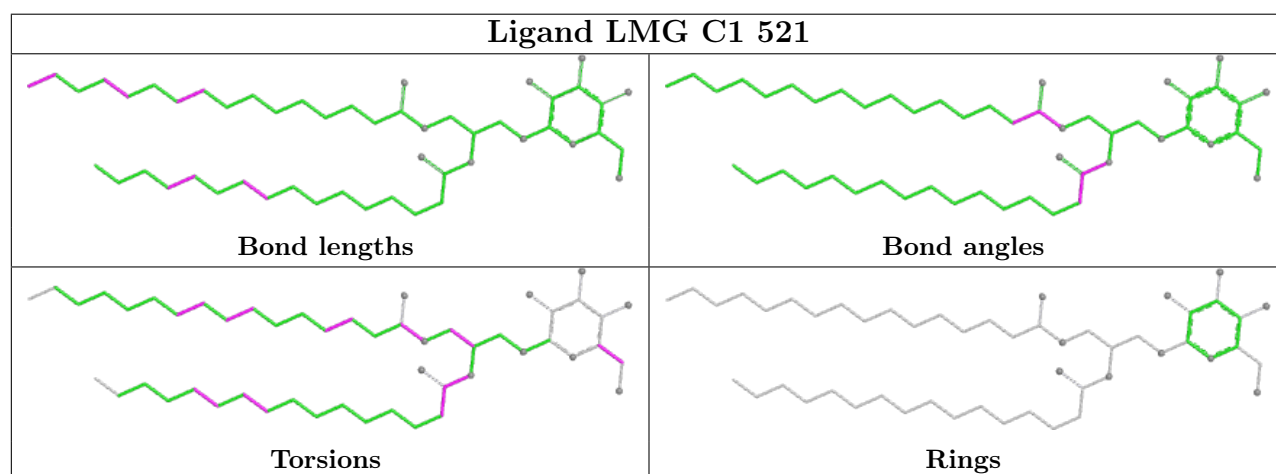
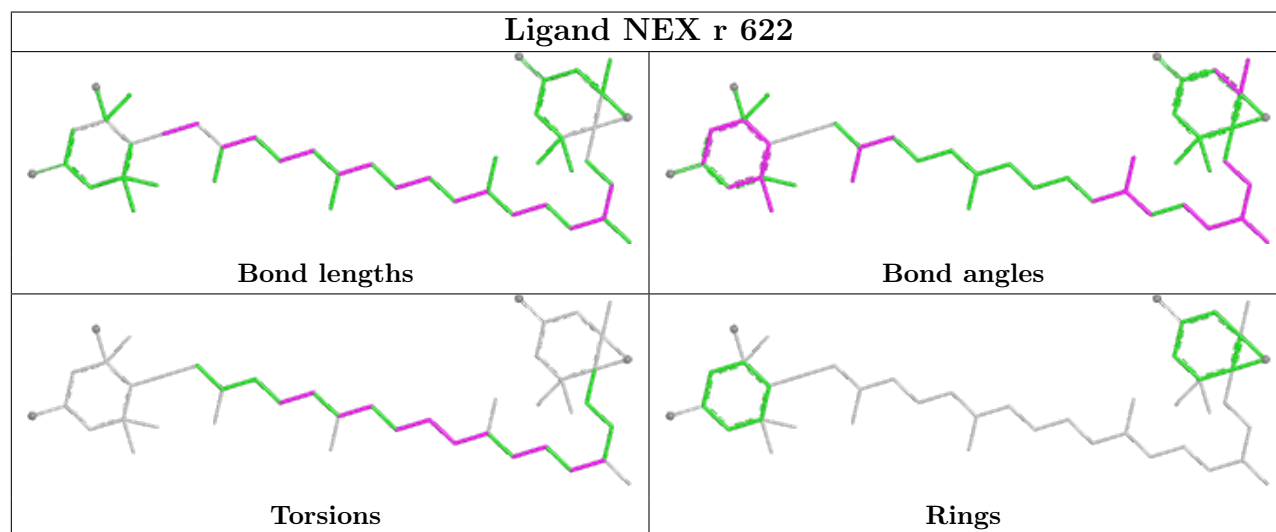
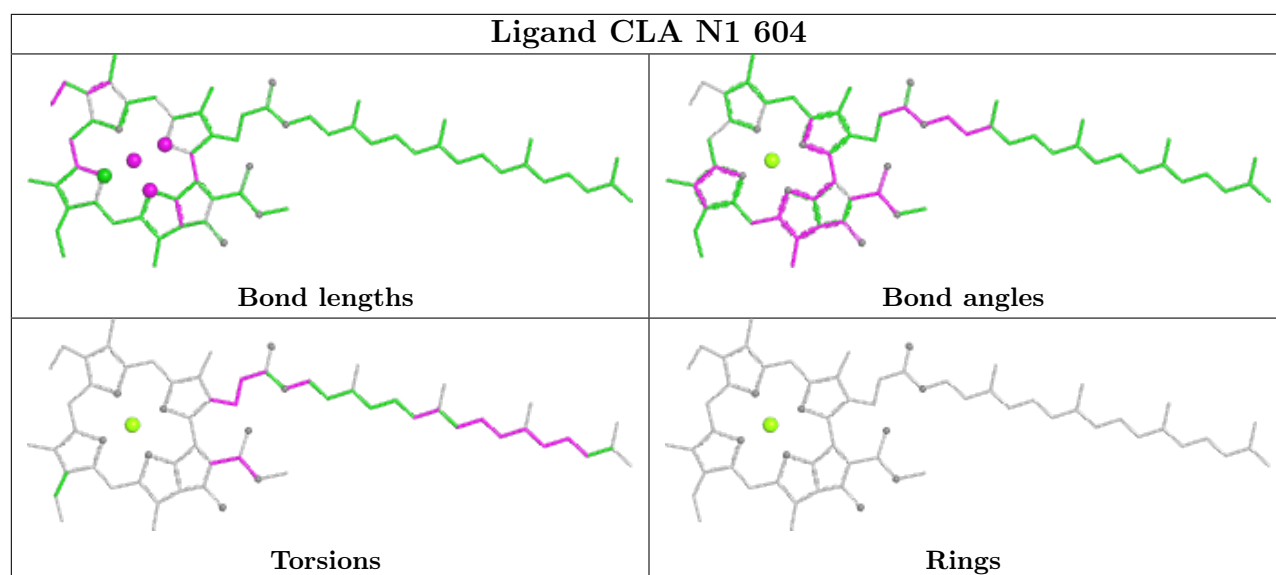


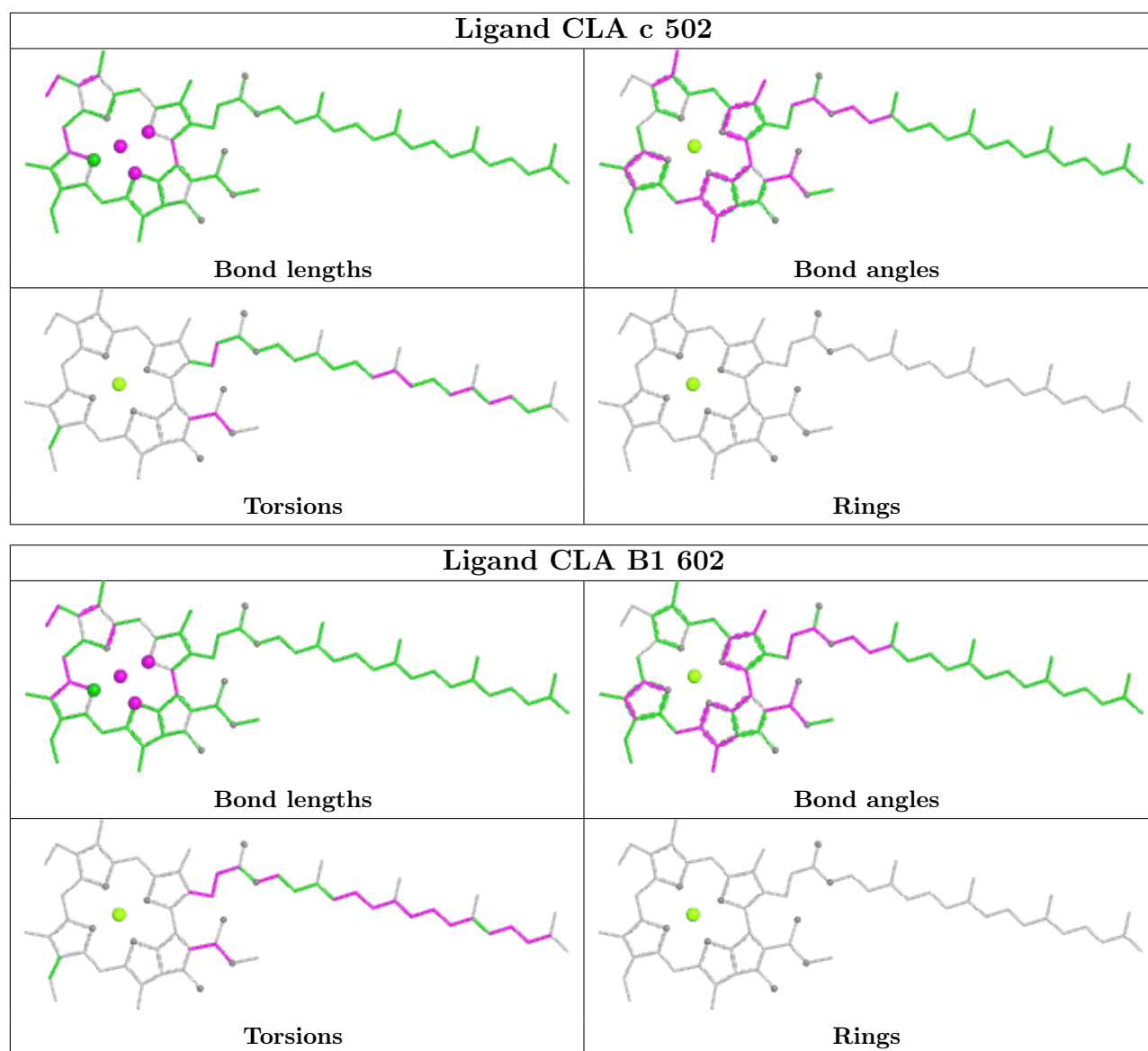


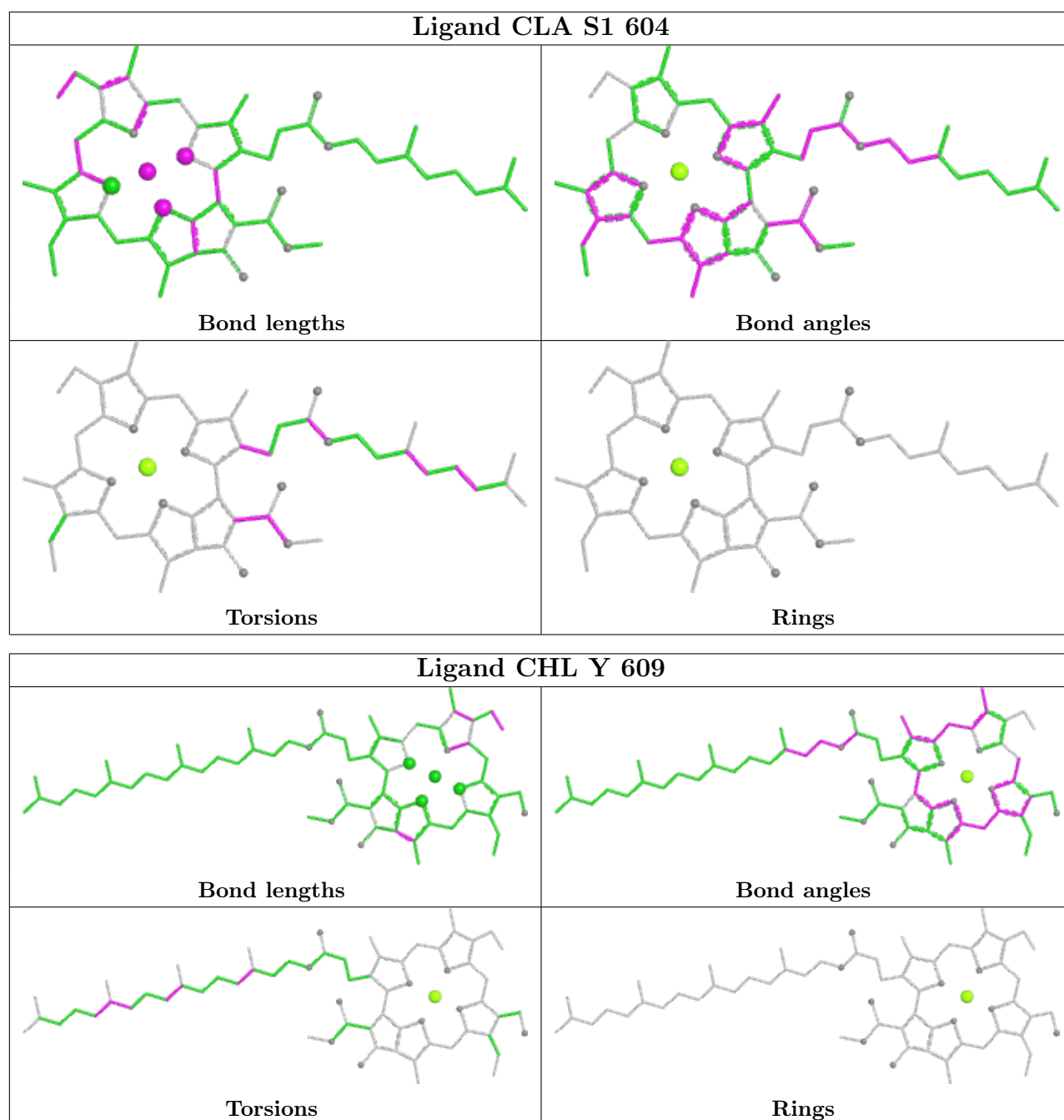


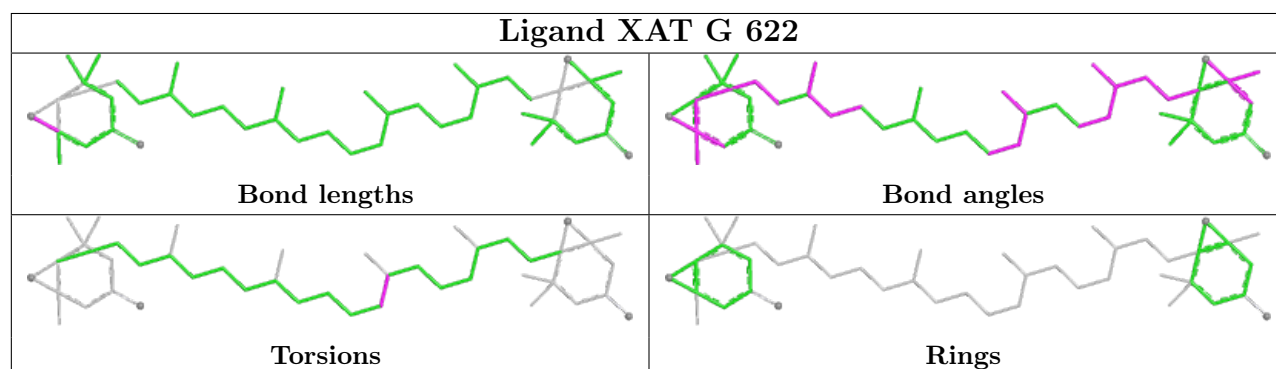
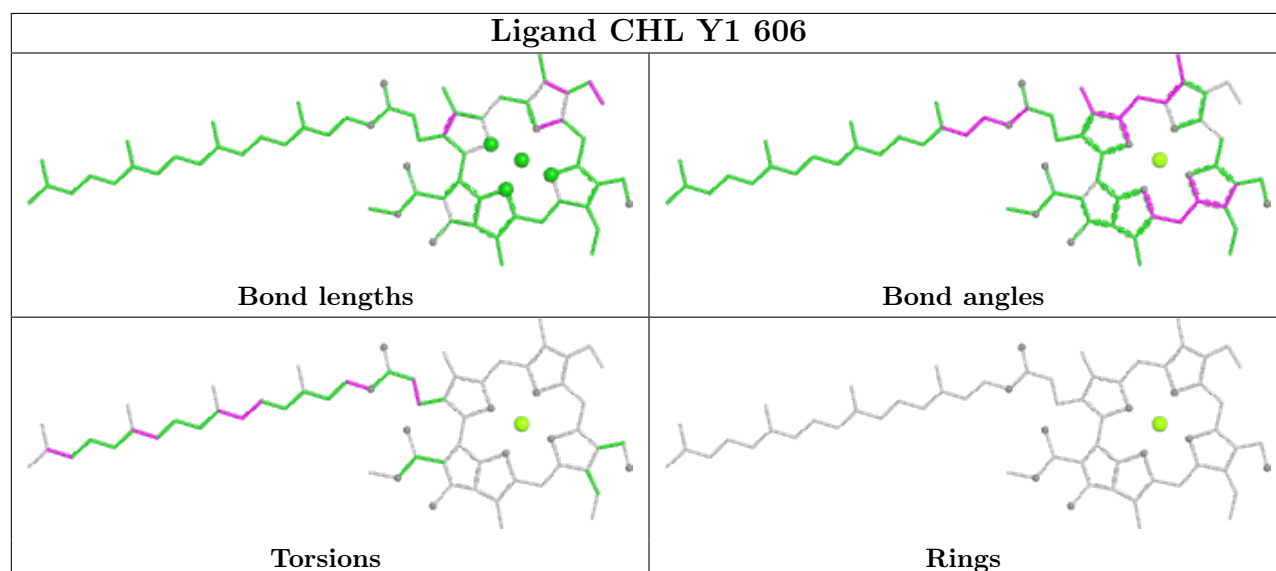
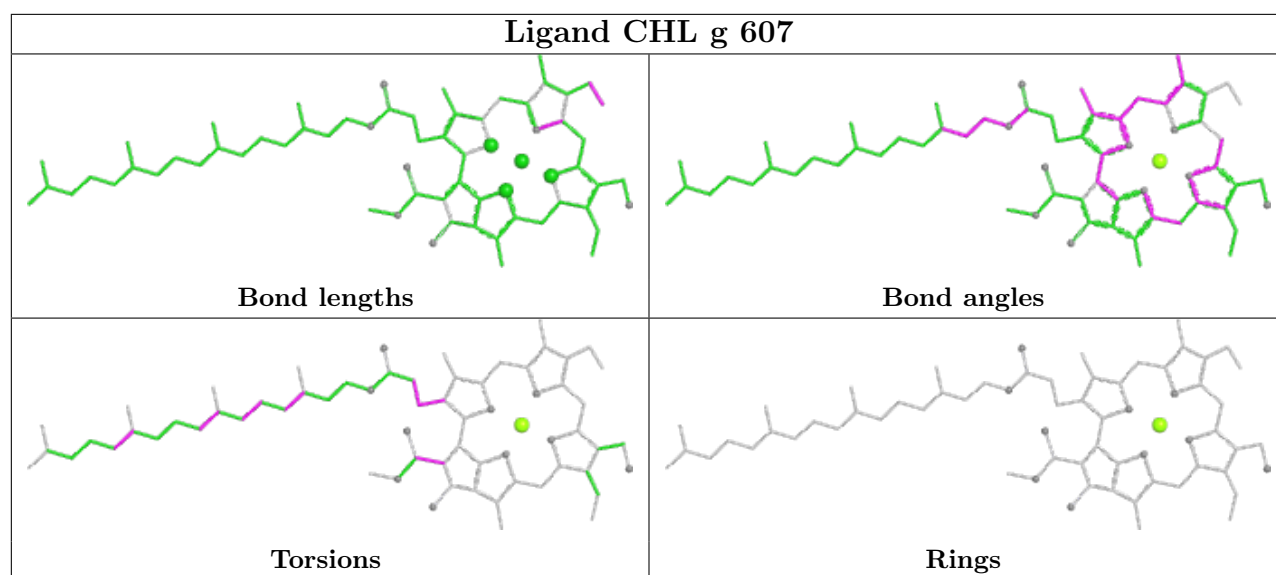


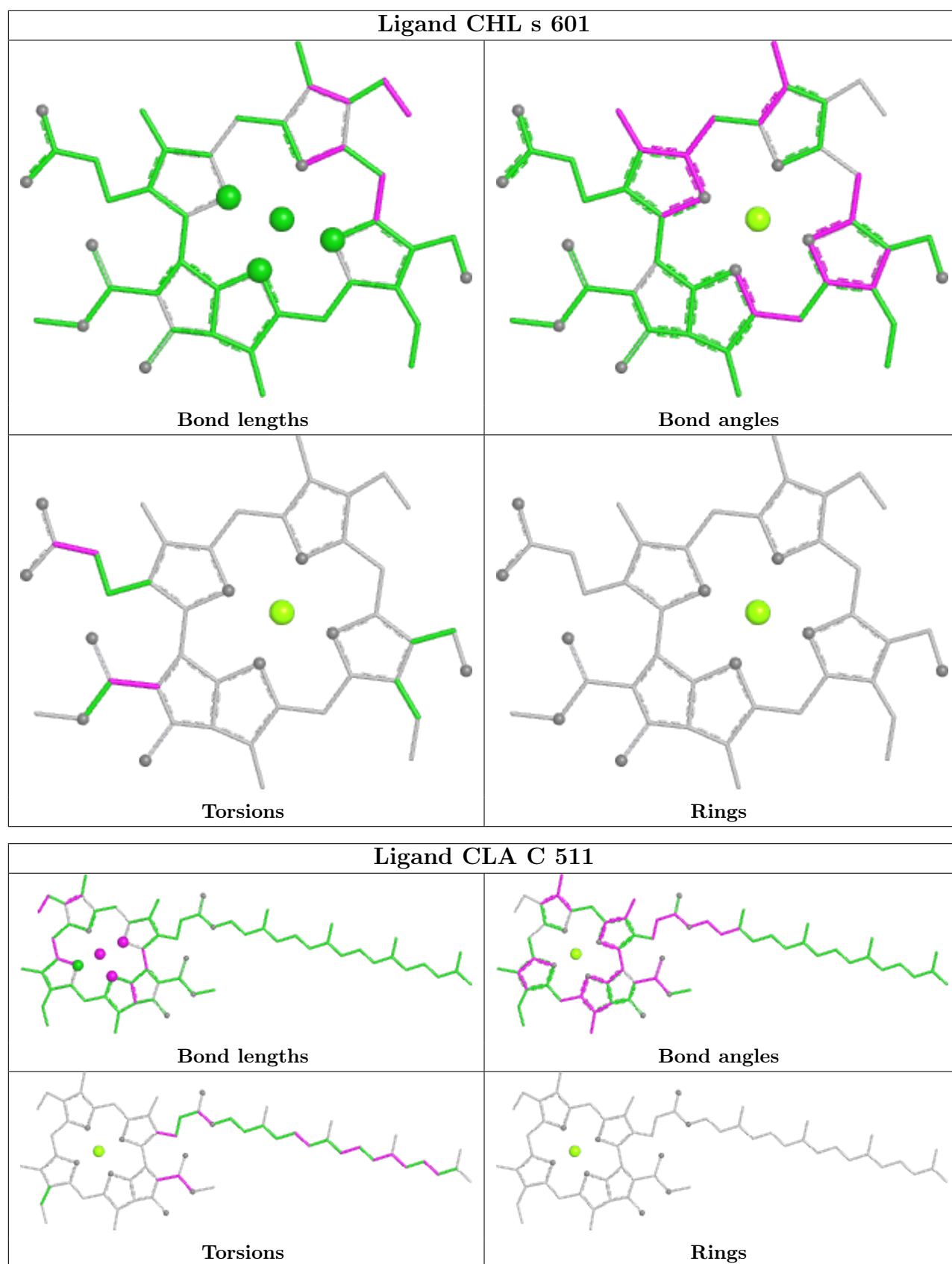


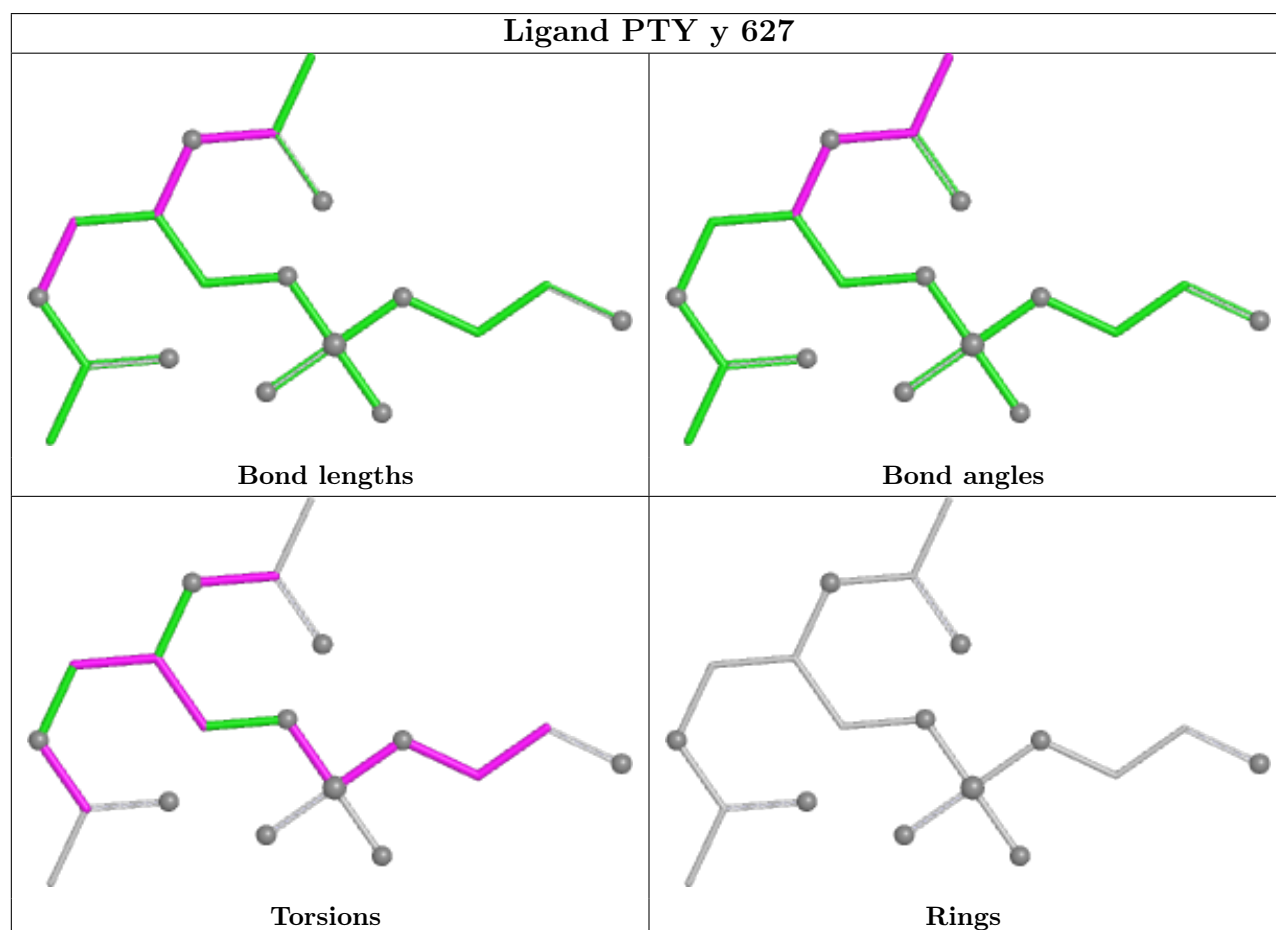
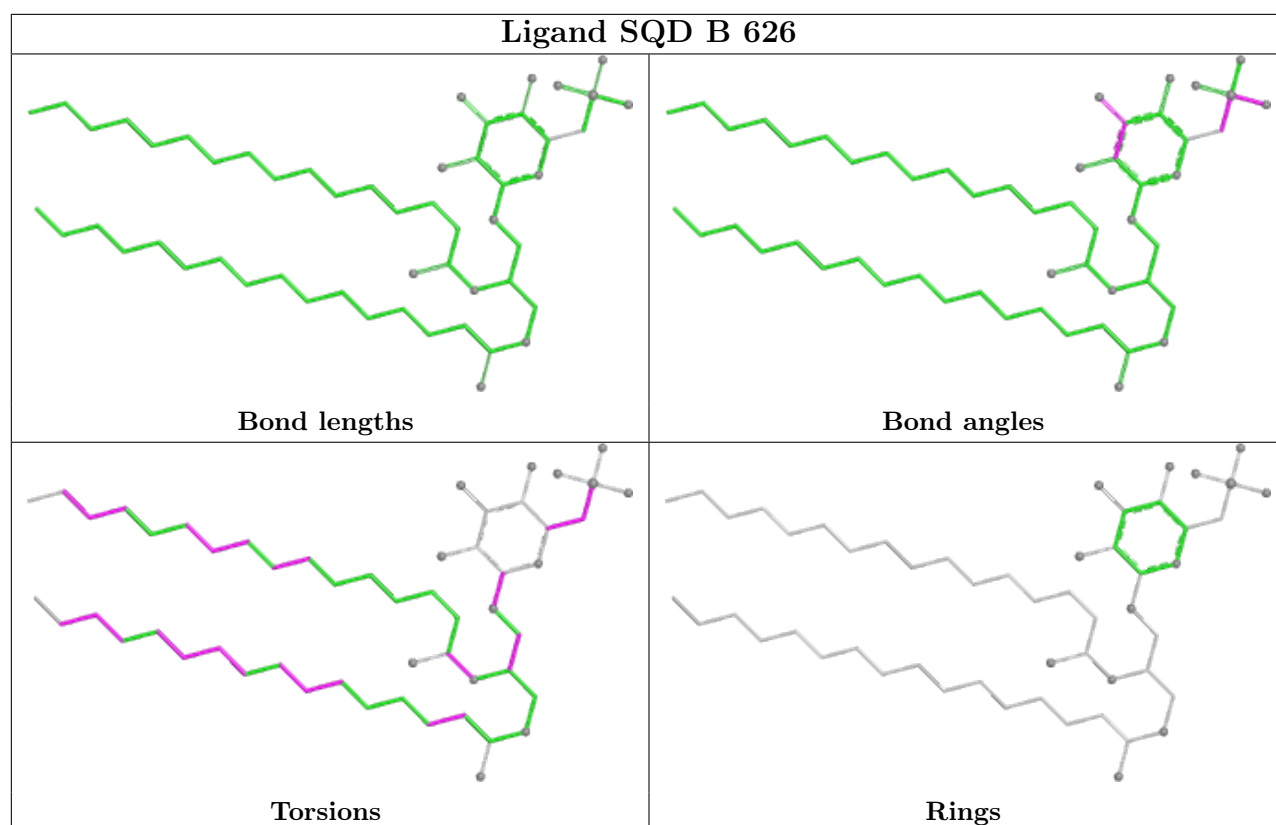


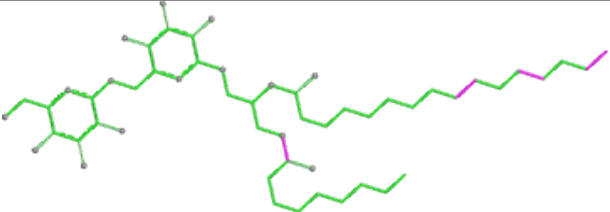
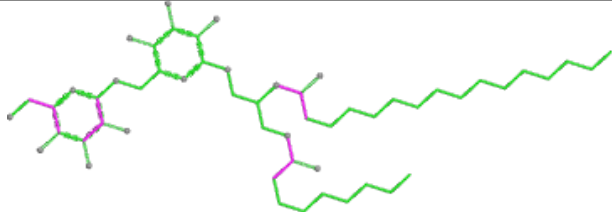
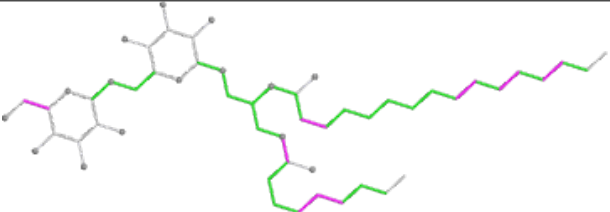
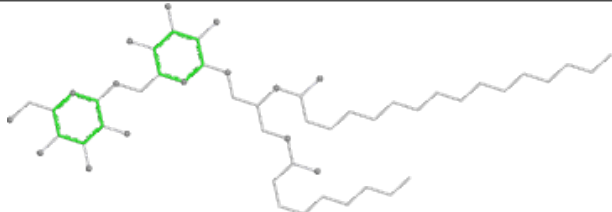


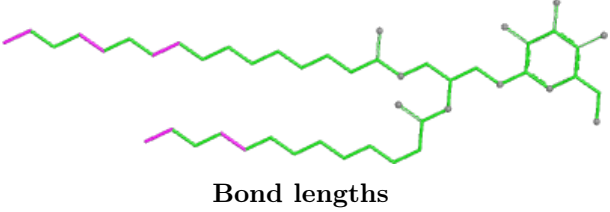
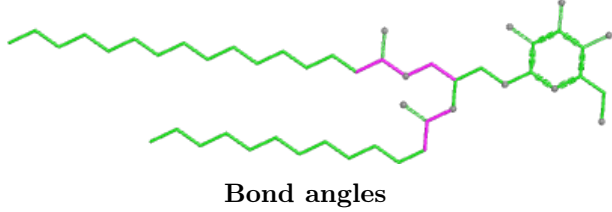
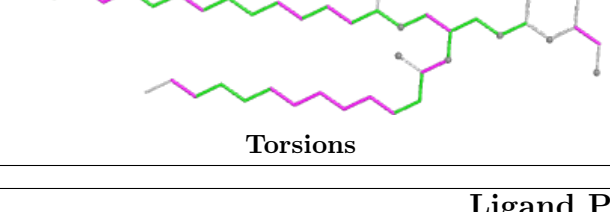
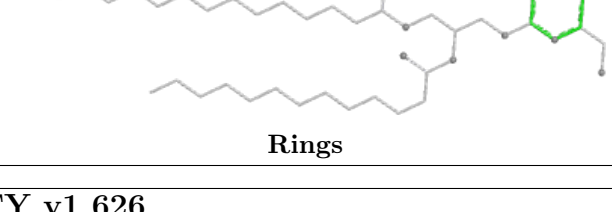


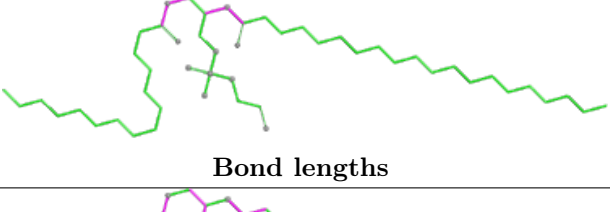
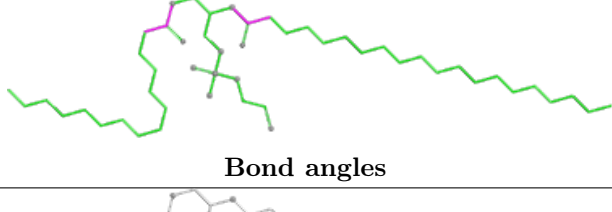
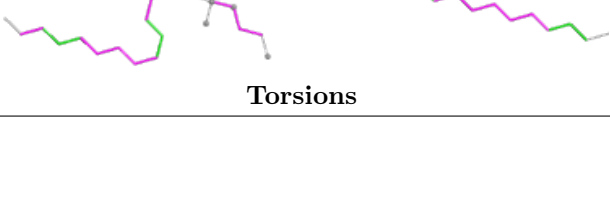



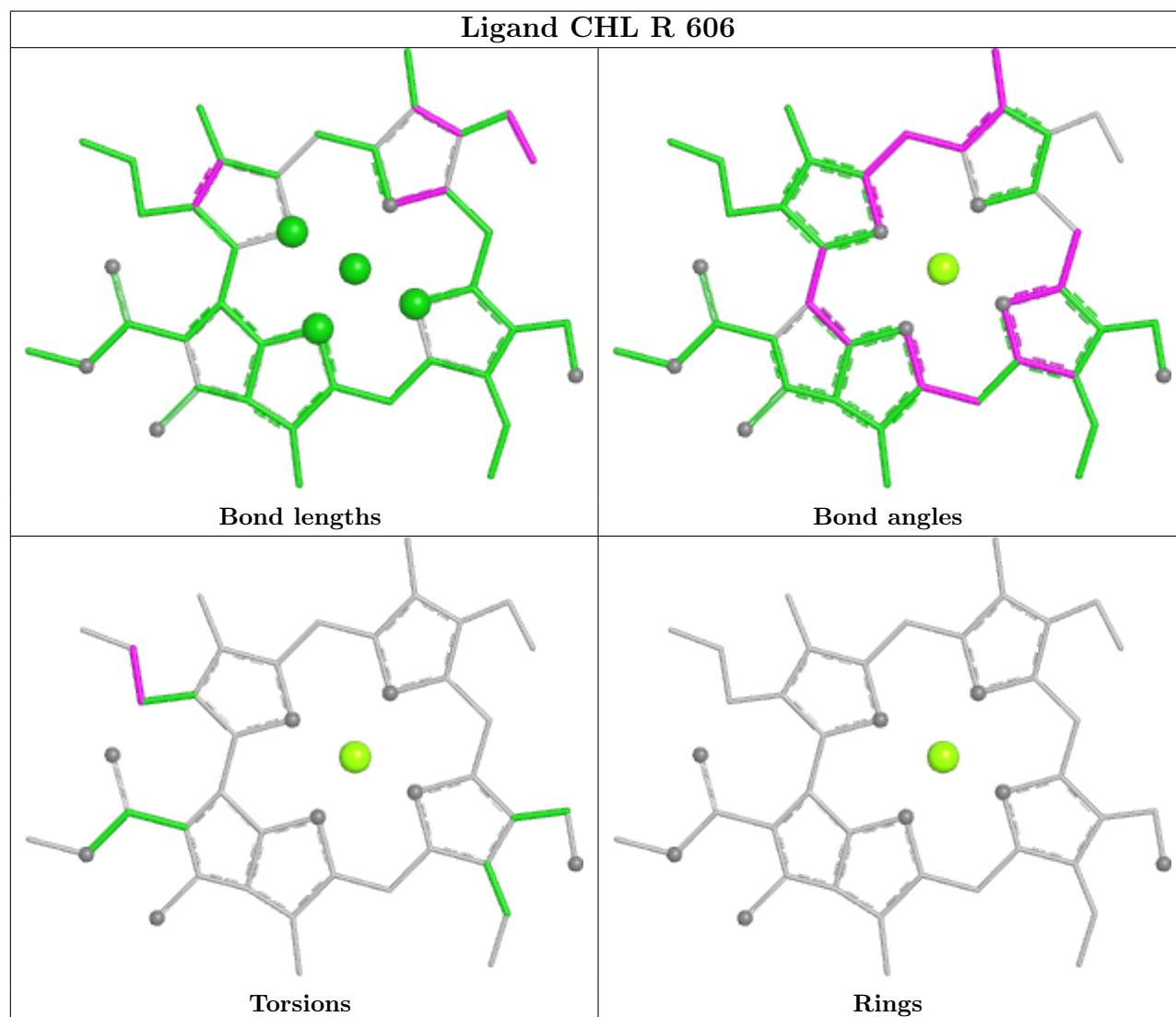
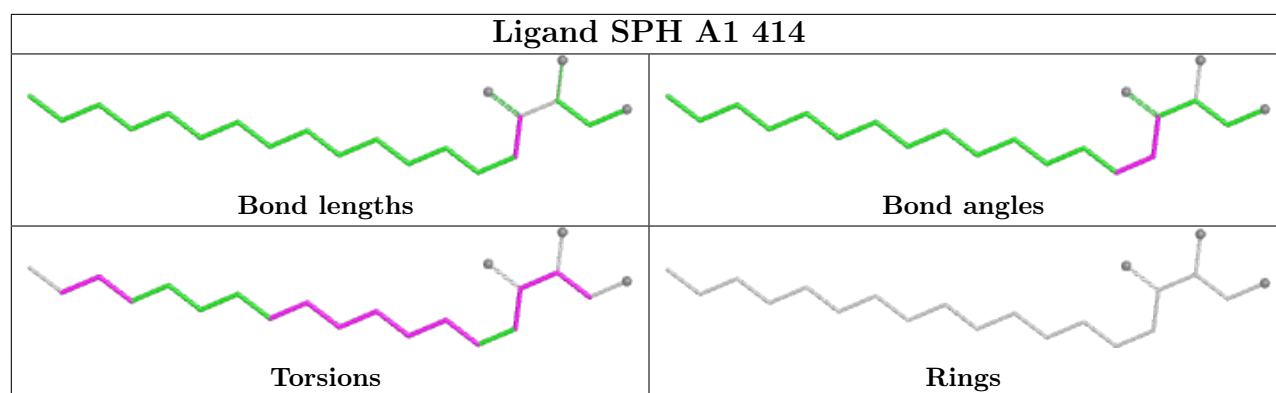


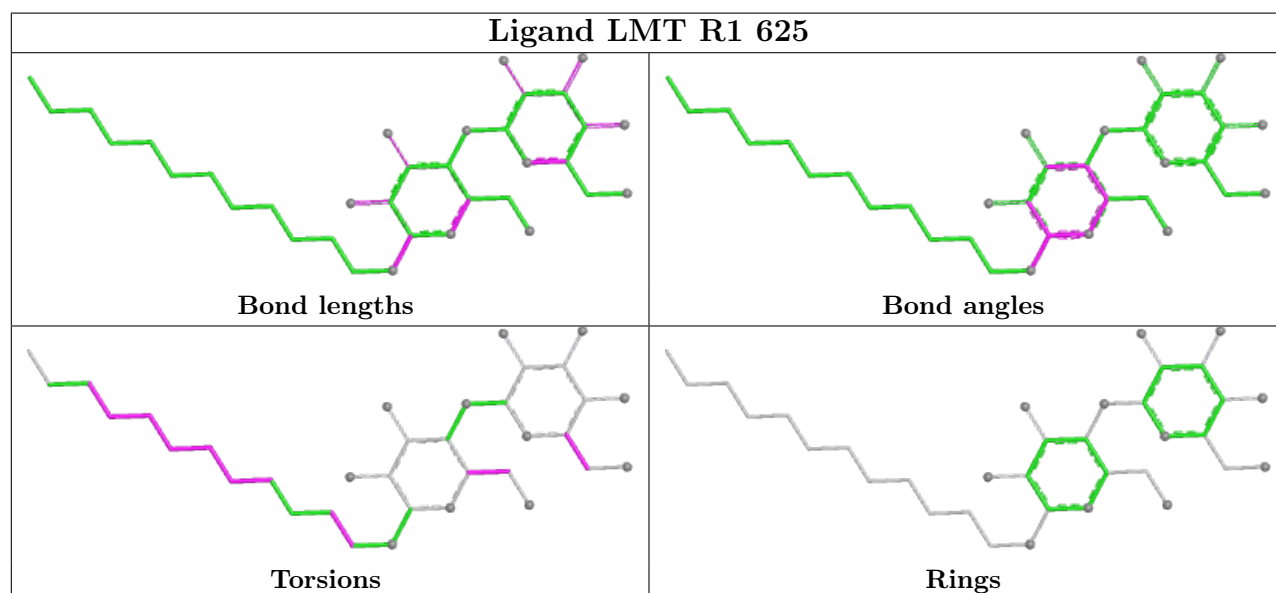
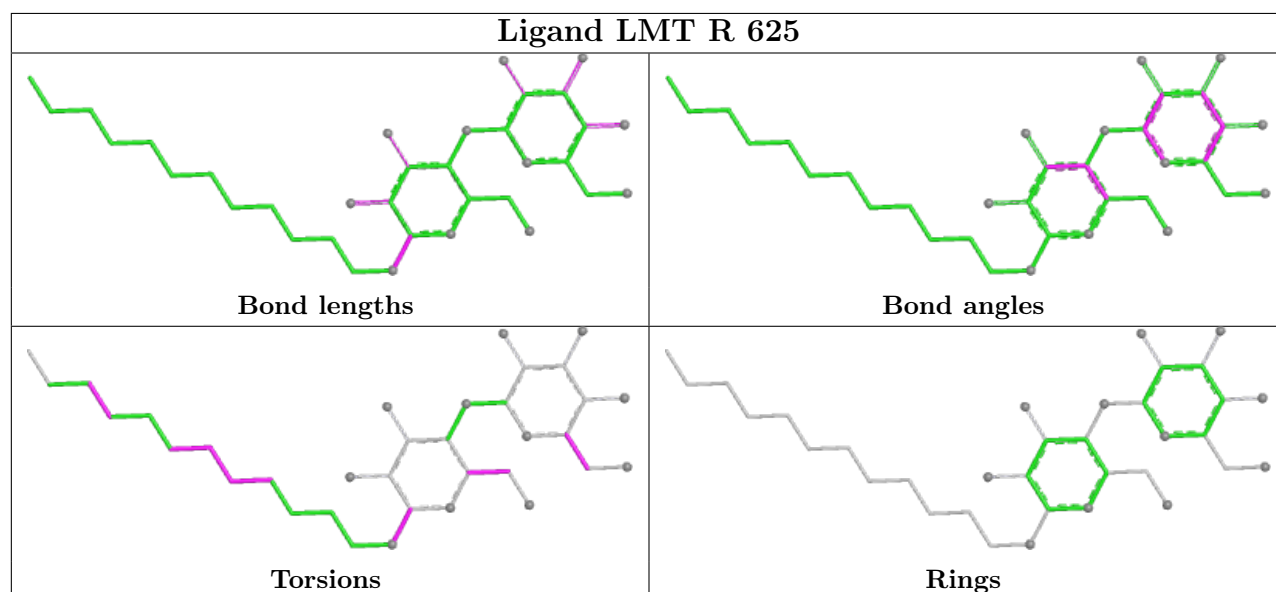
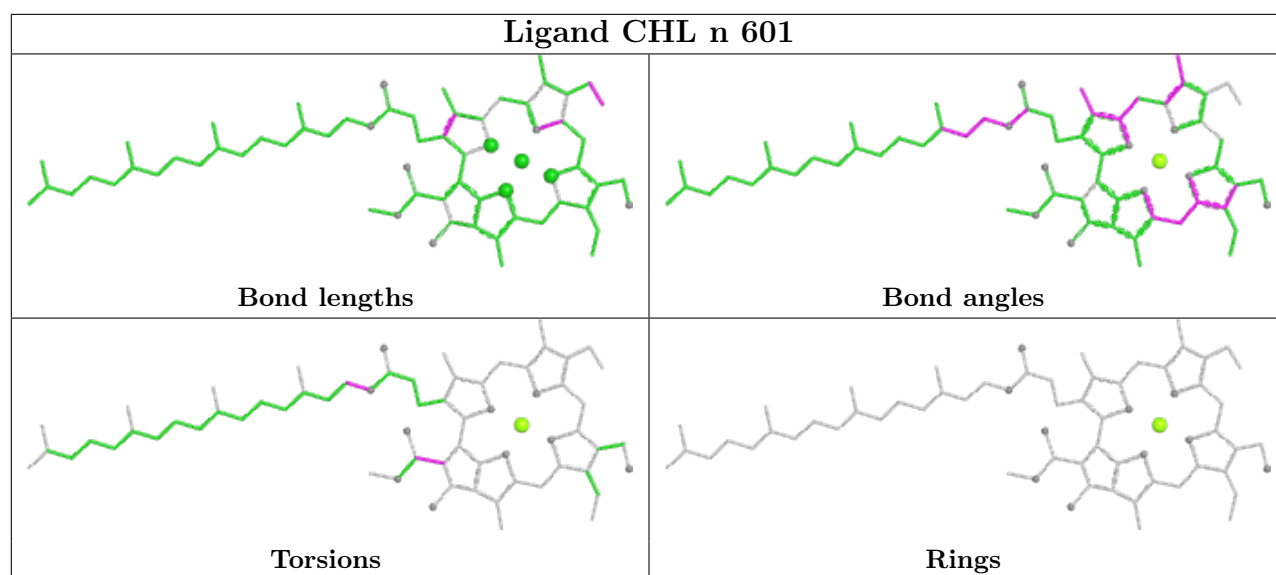


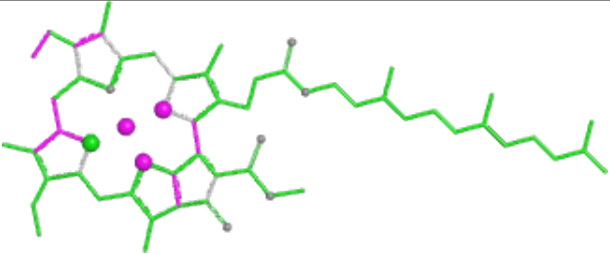
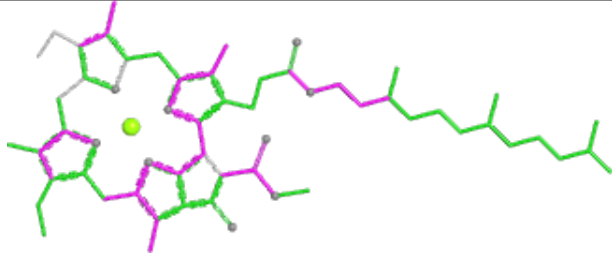
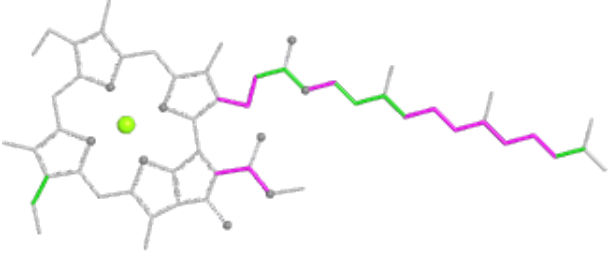
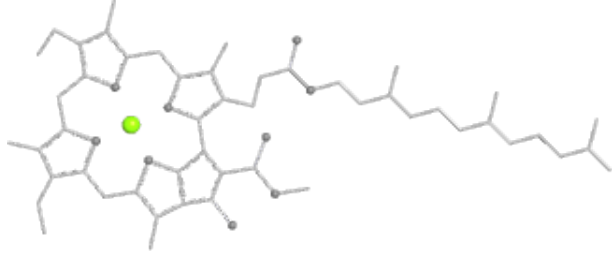
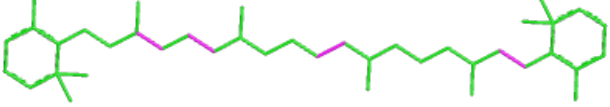
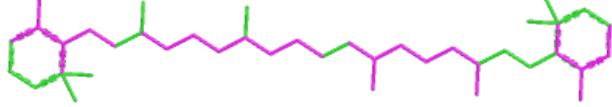
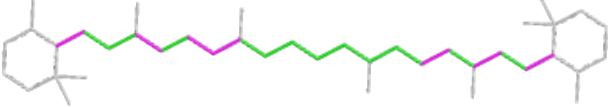
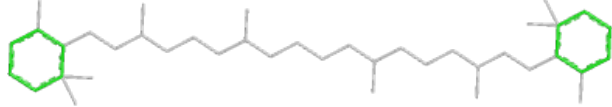
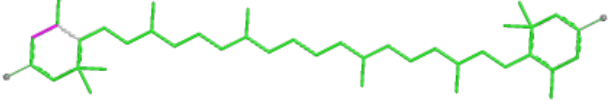
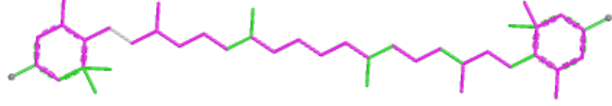
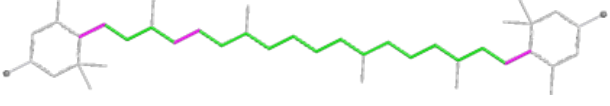
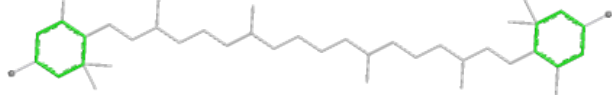
Ligand DGD c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

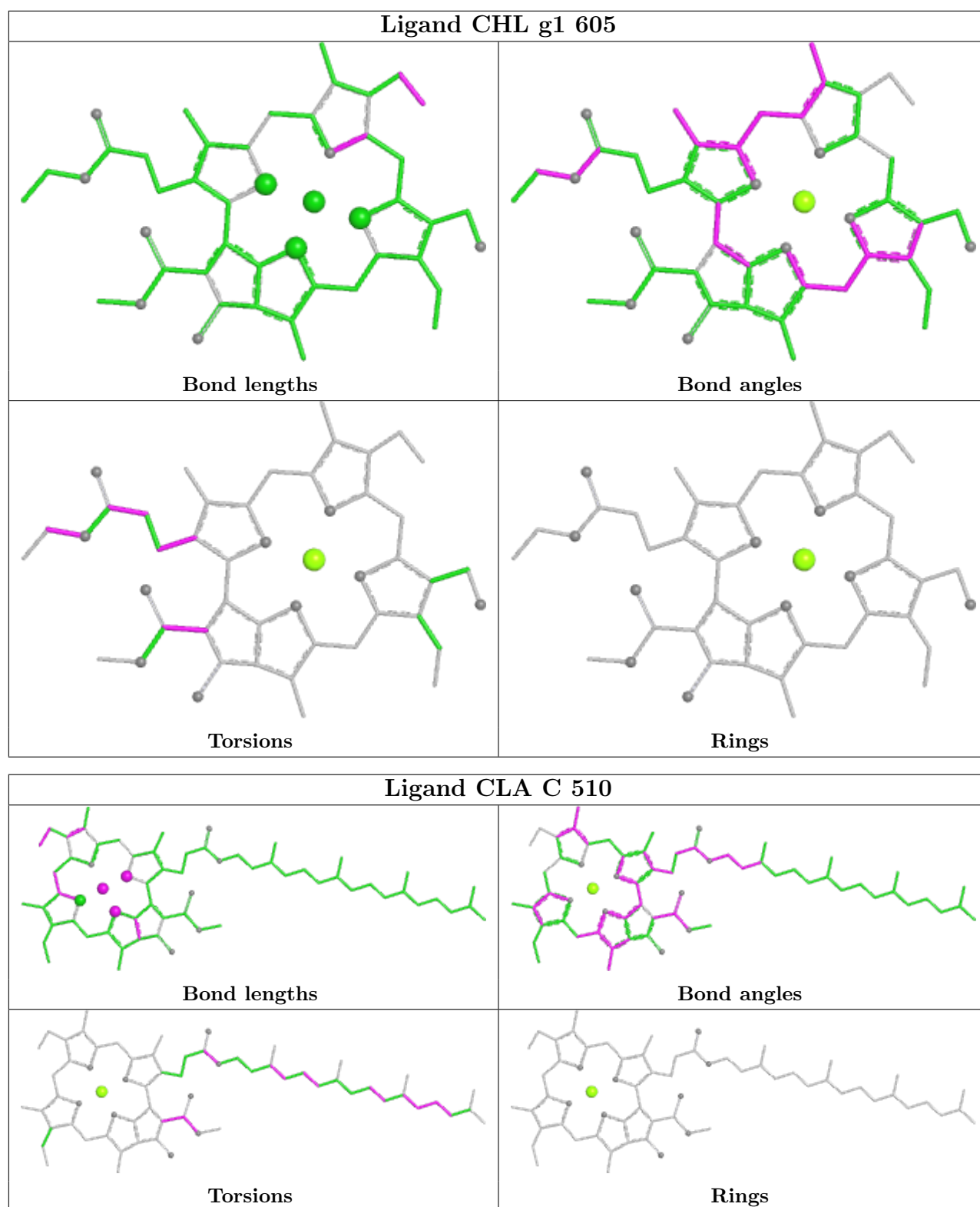
Ligand LMG H1 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

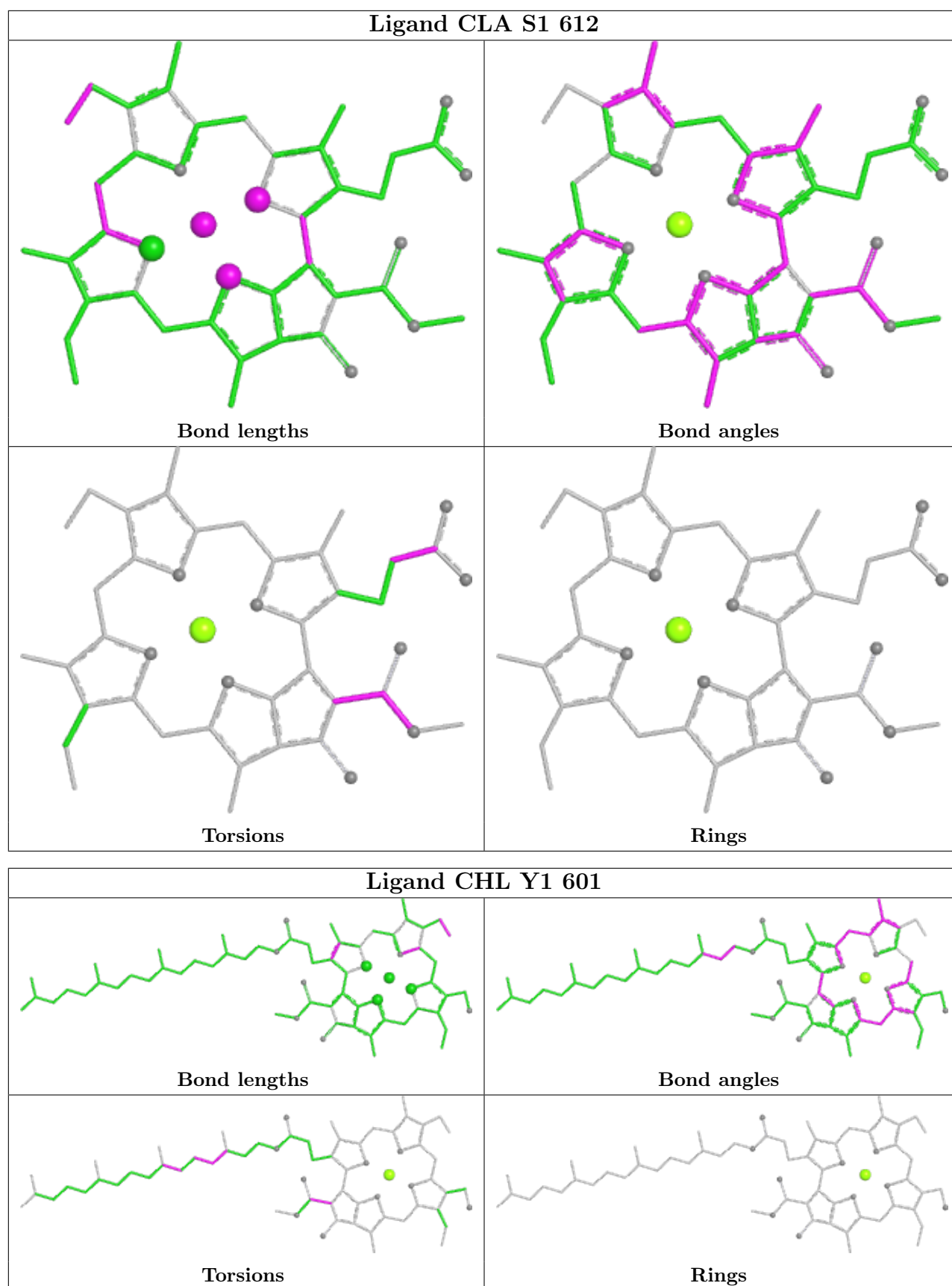
Ligand PTY y1 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

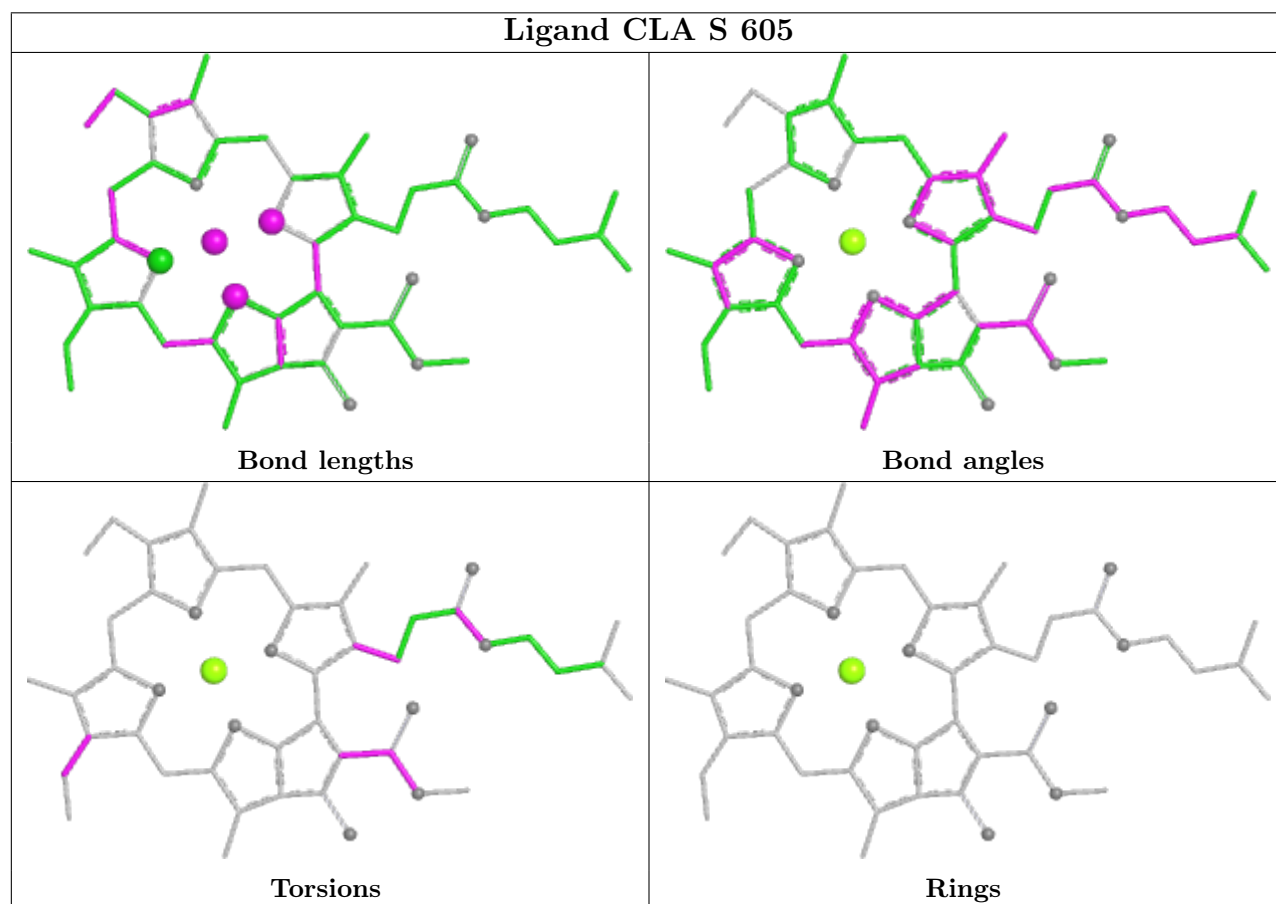
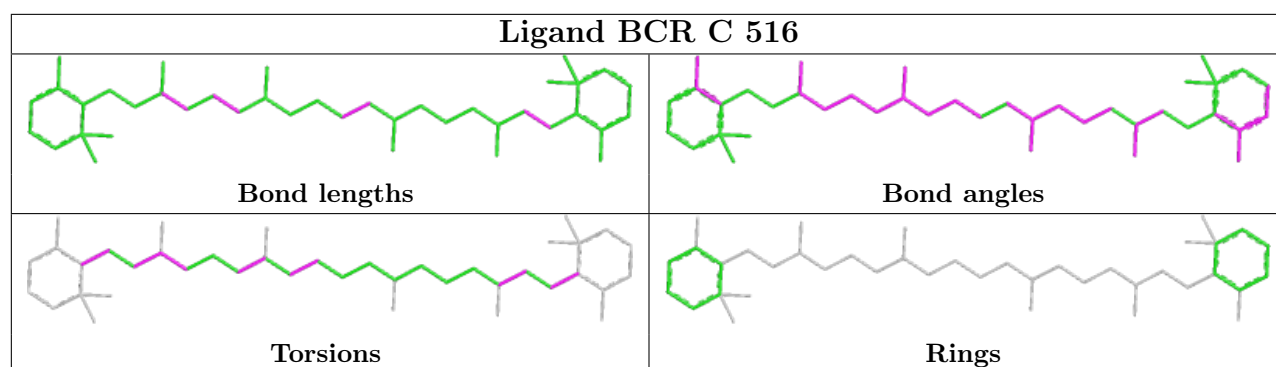


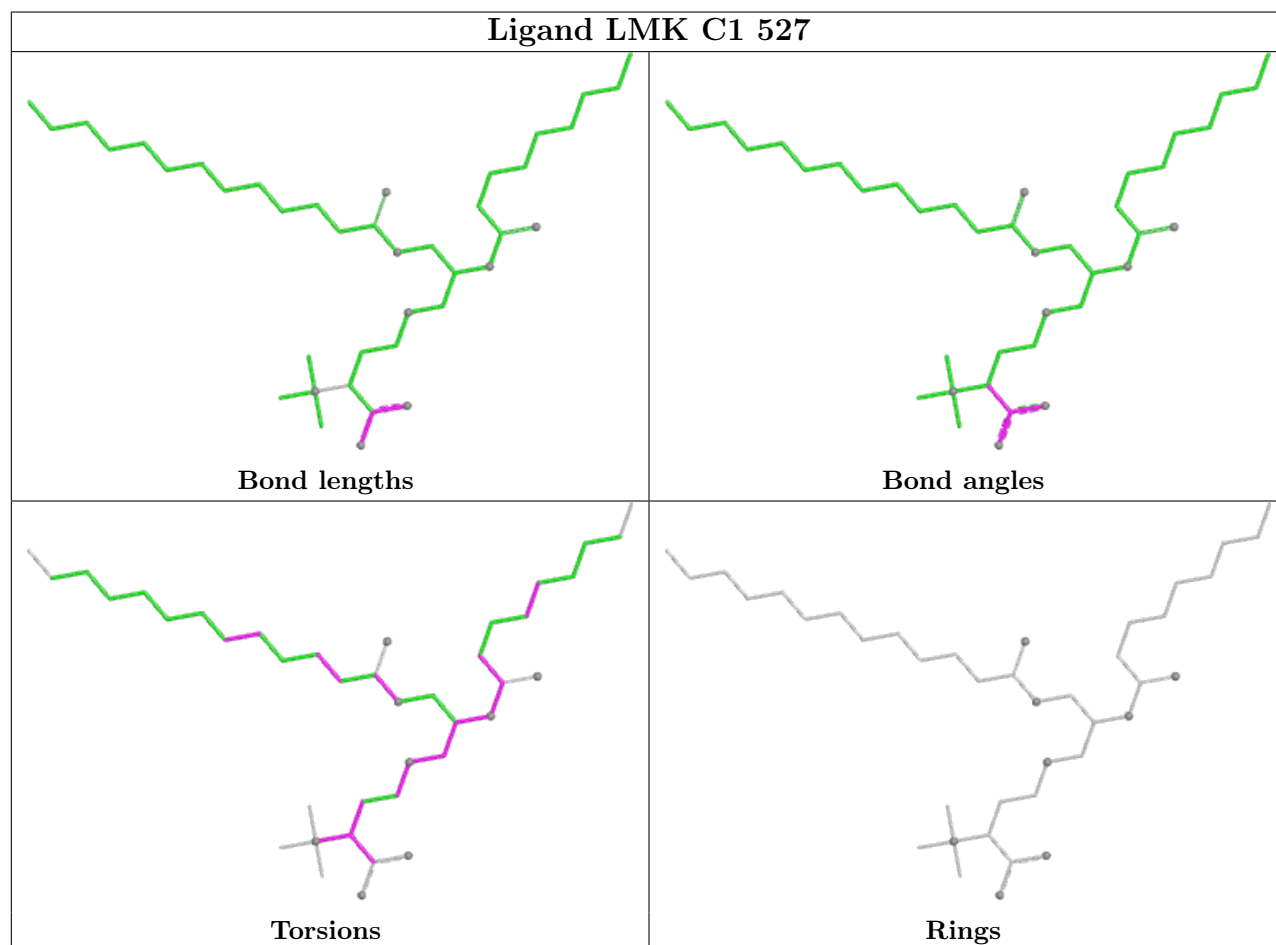
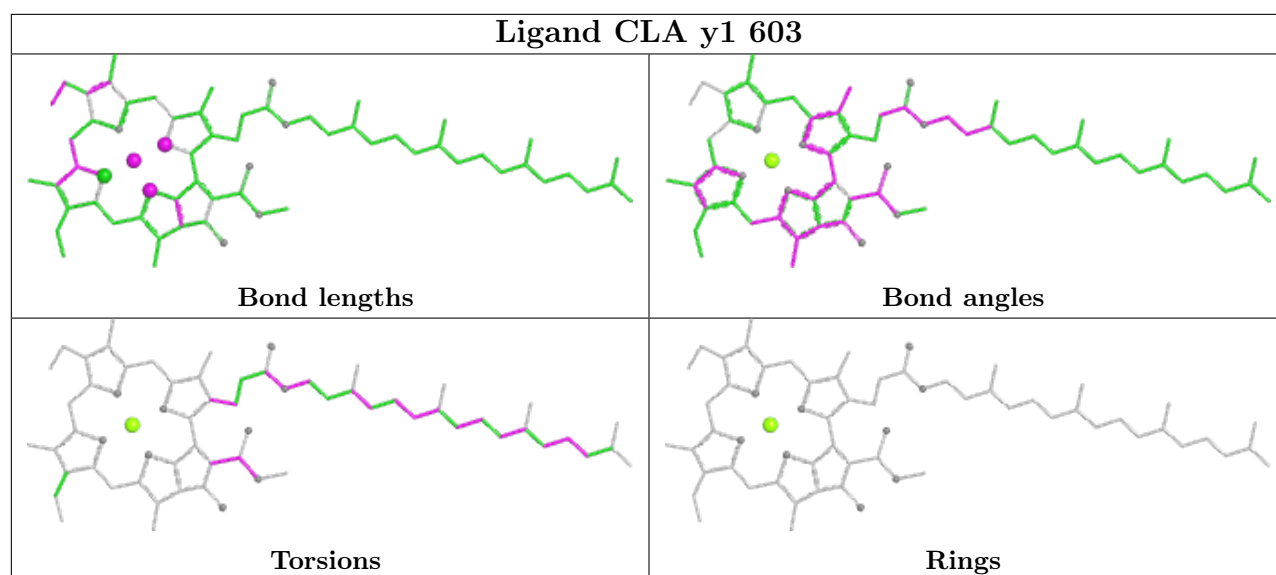


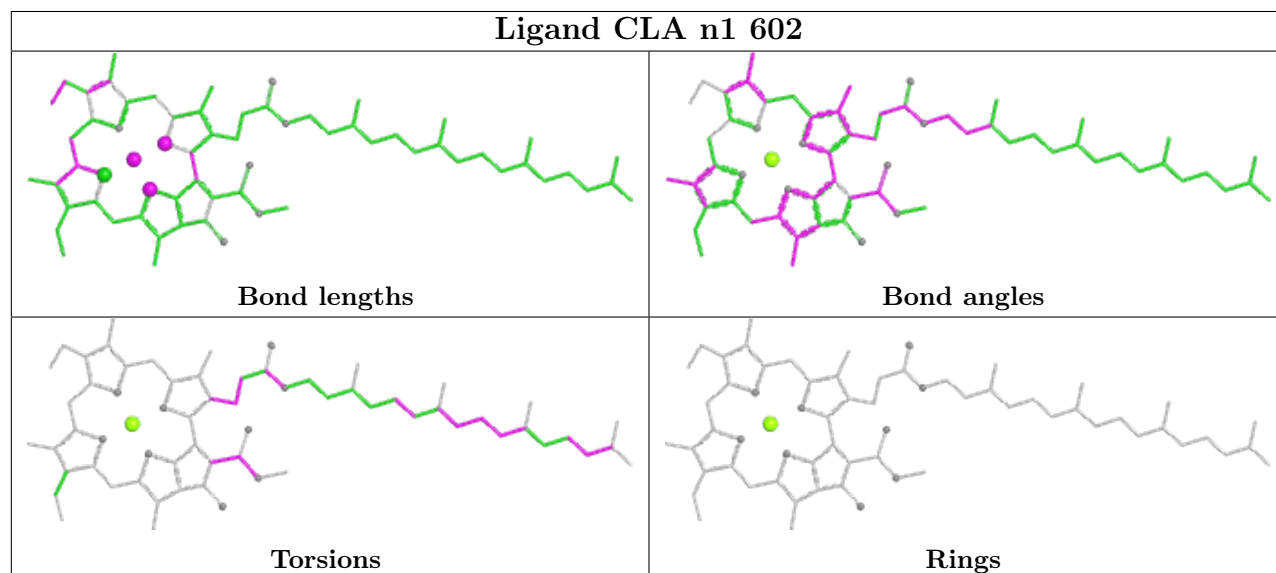
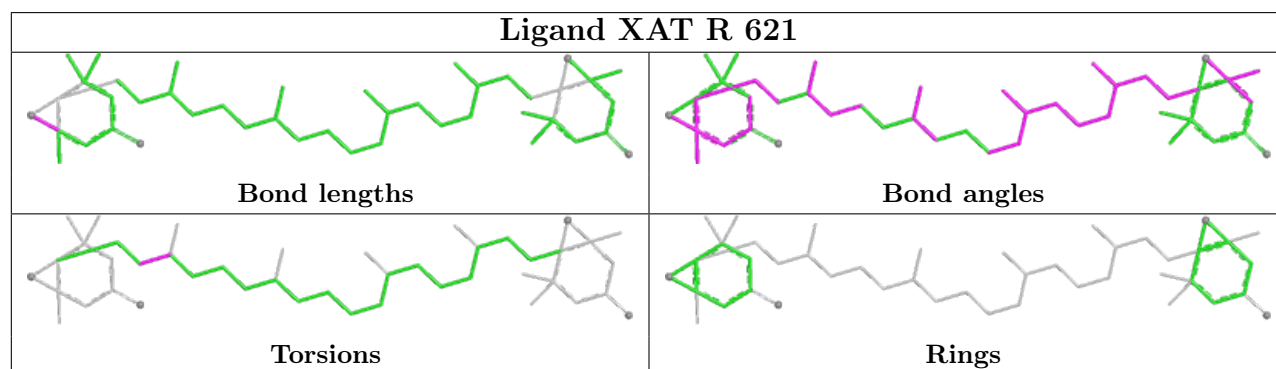
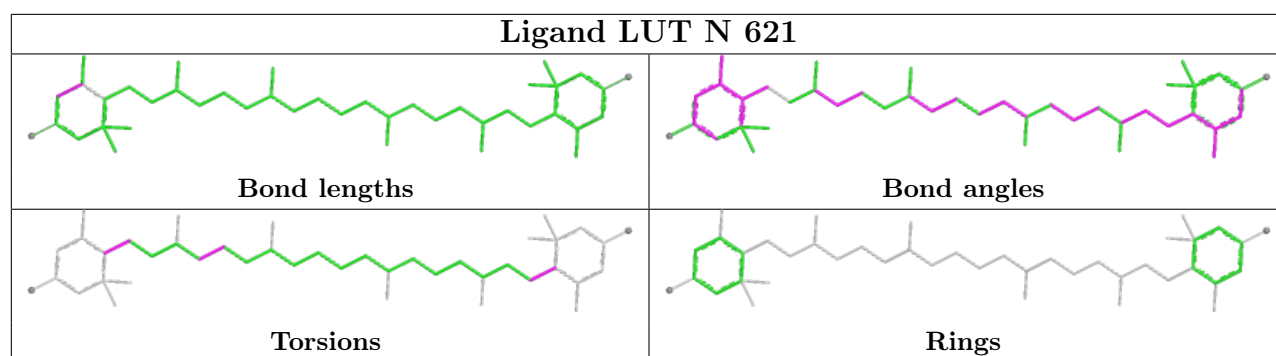
Ligand CLA s 609	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b1 618	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT S 621	
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 <p>Torsions</p>	 <p>Rings</p>

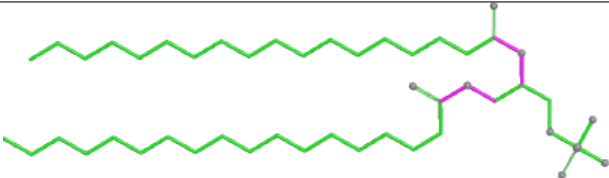
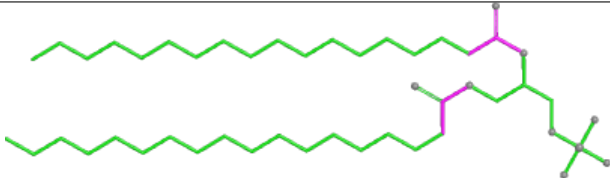
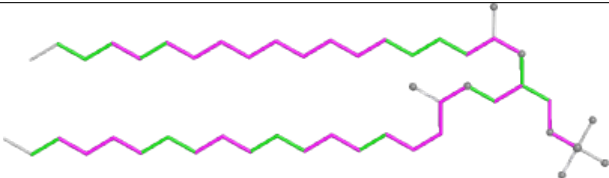
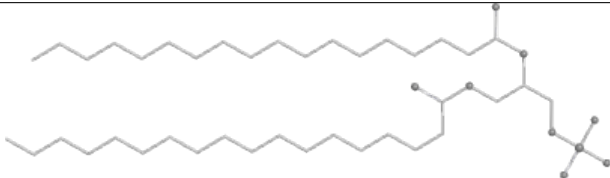


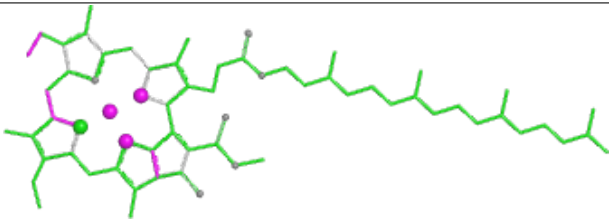
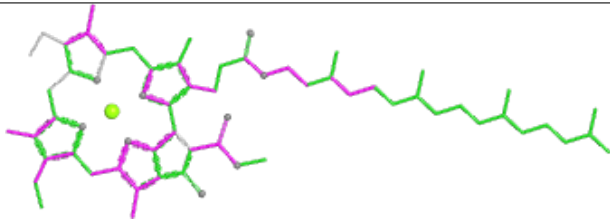
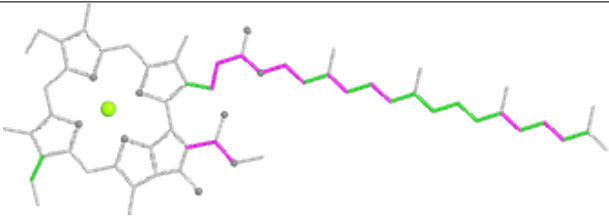
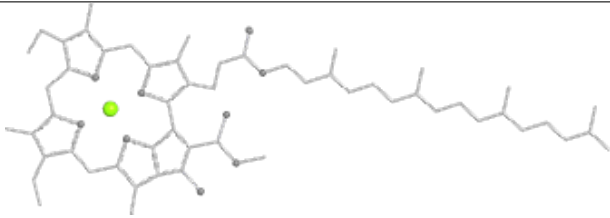


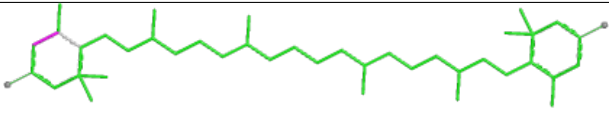
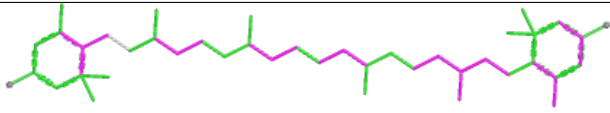
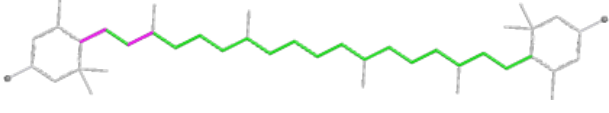
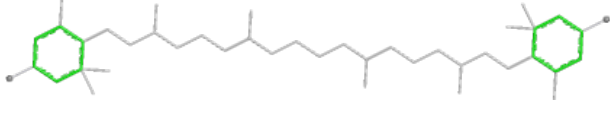


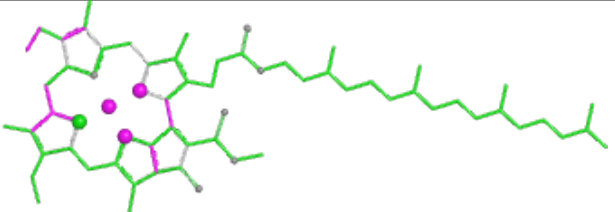
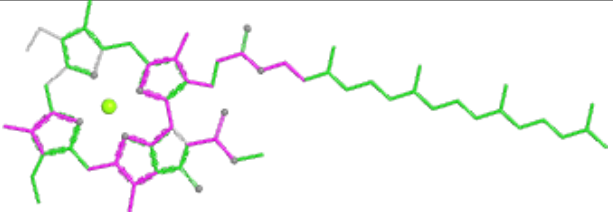
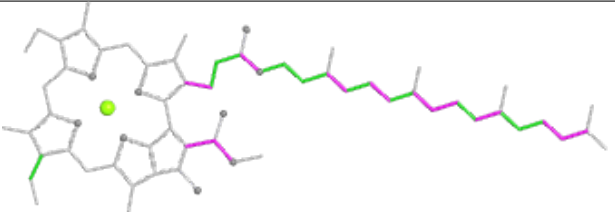
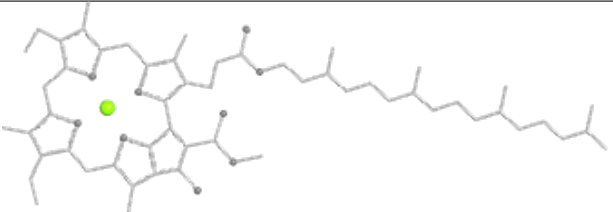
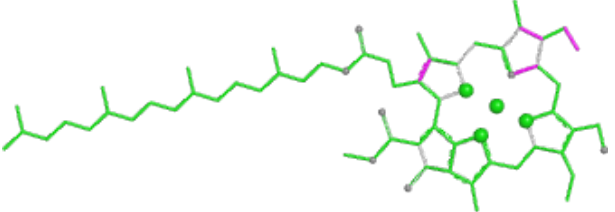
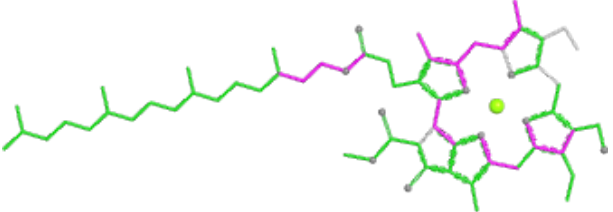
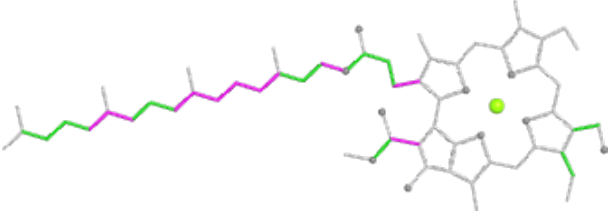
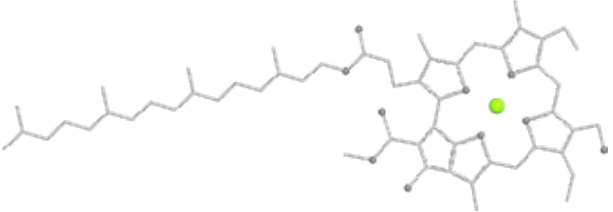
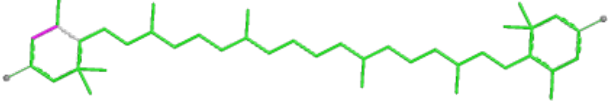
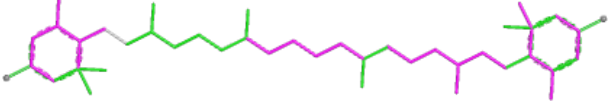
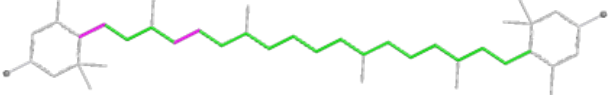
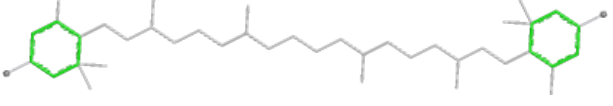


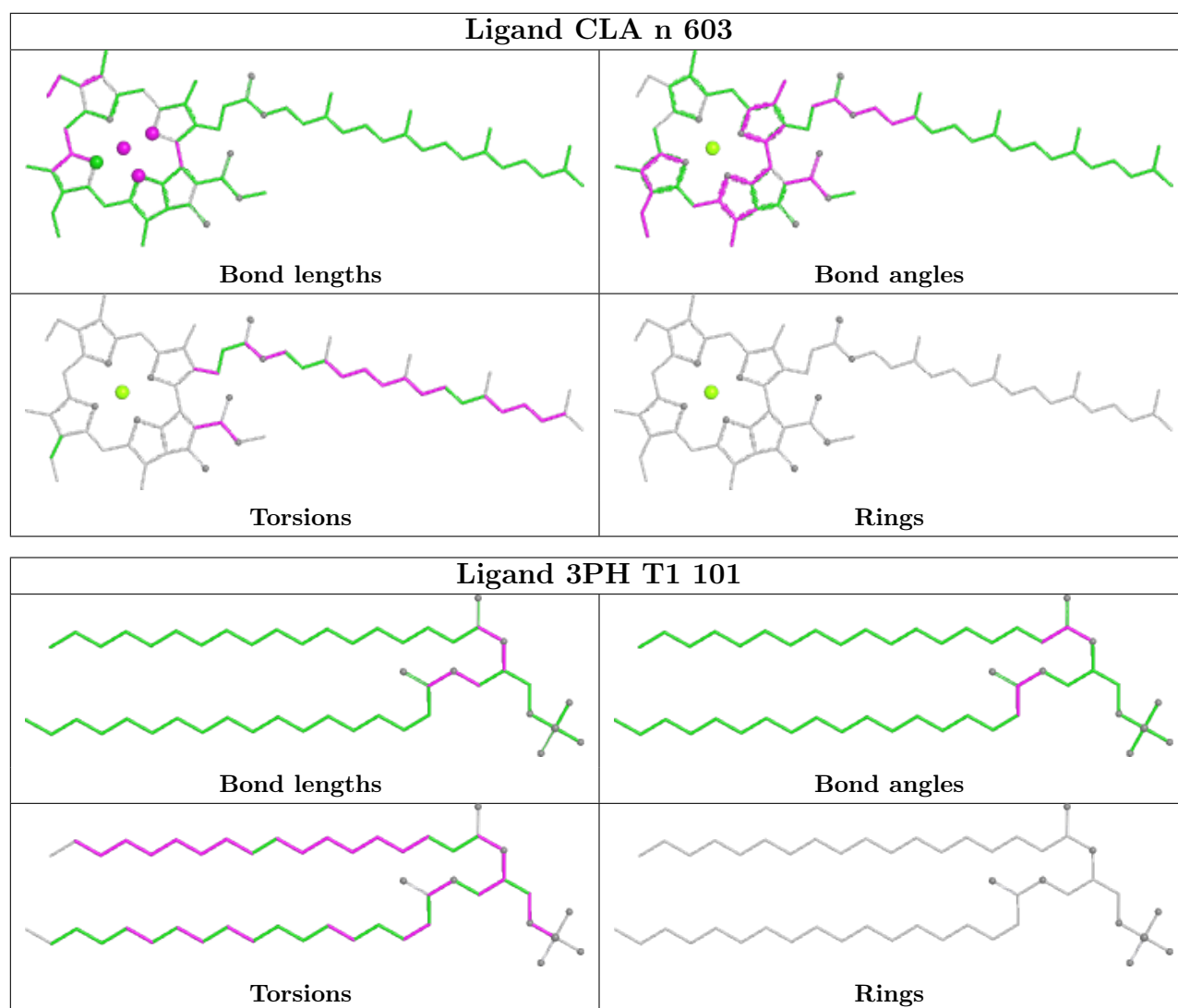


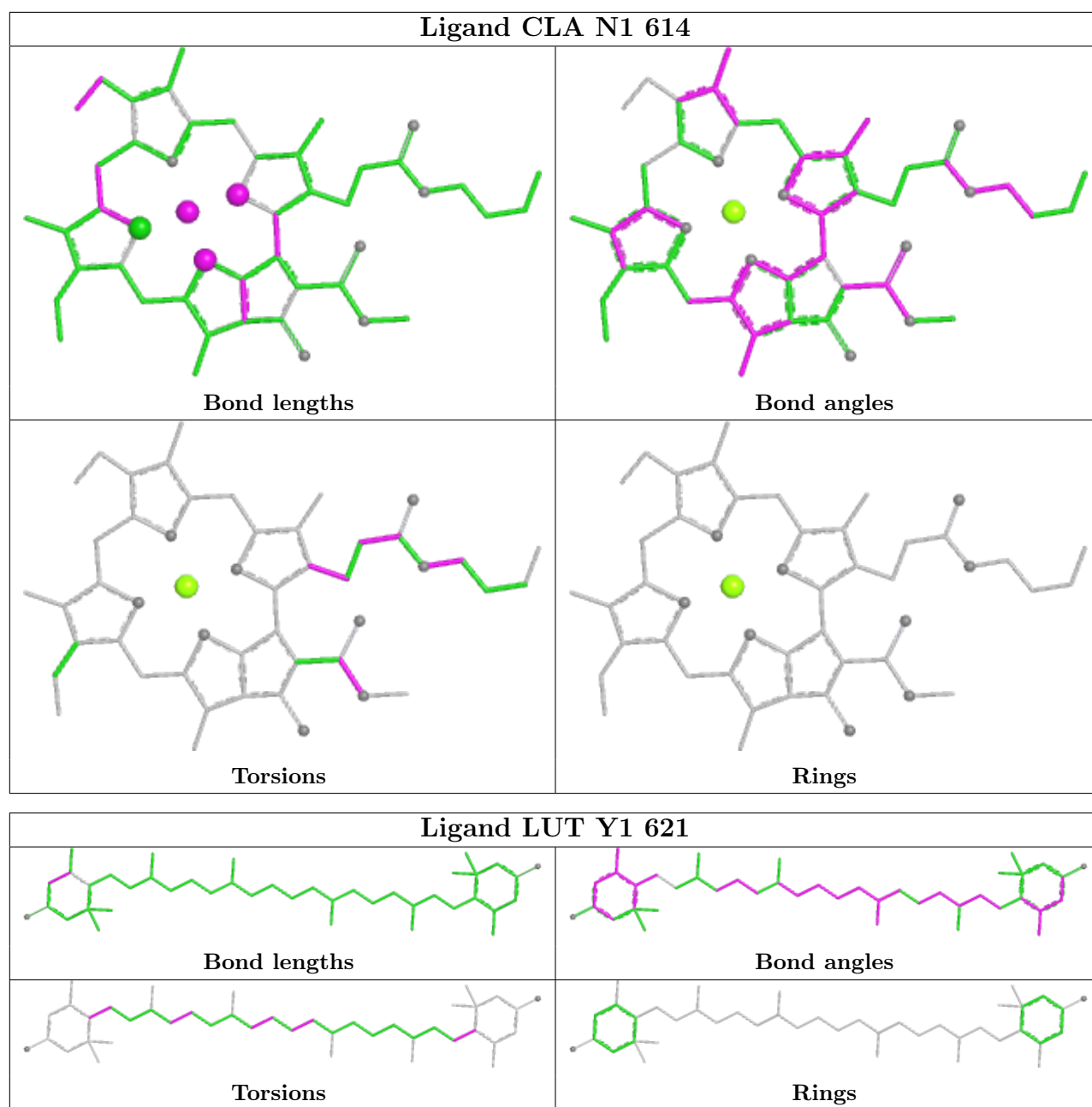
Ligand 3PH S1 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

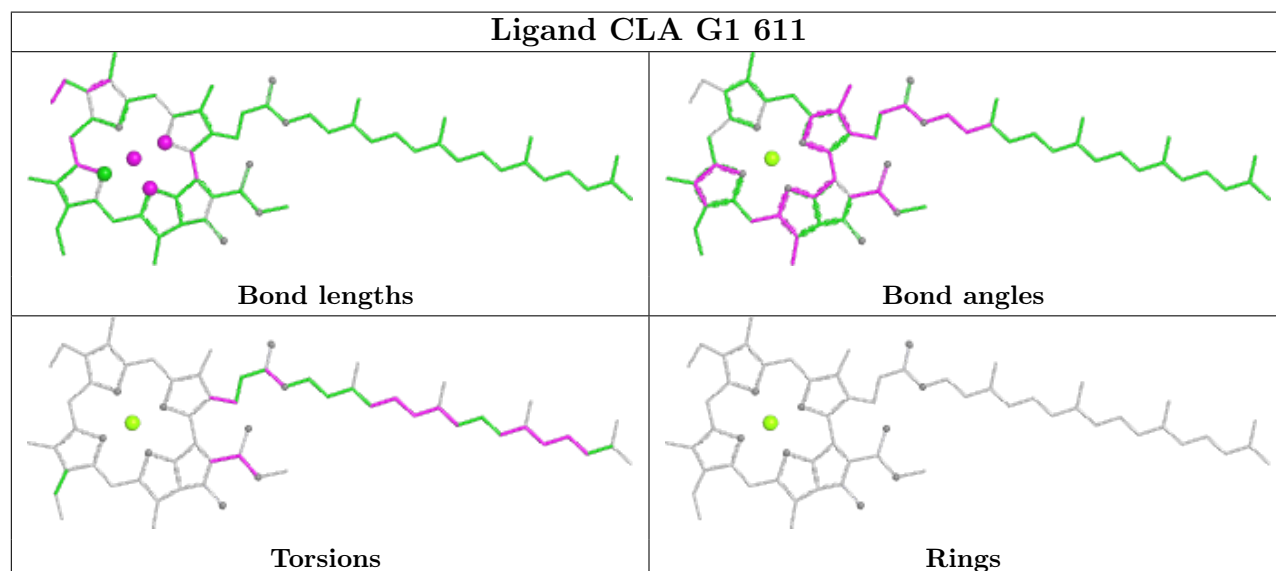
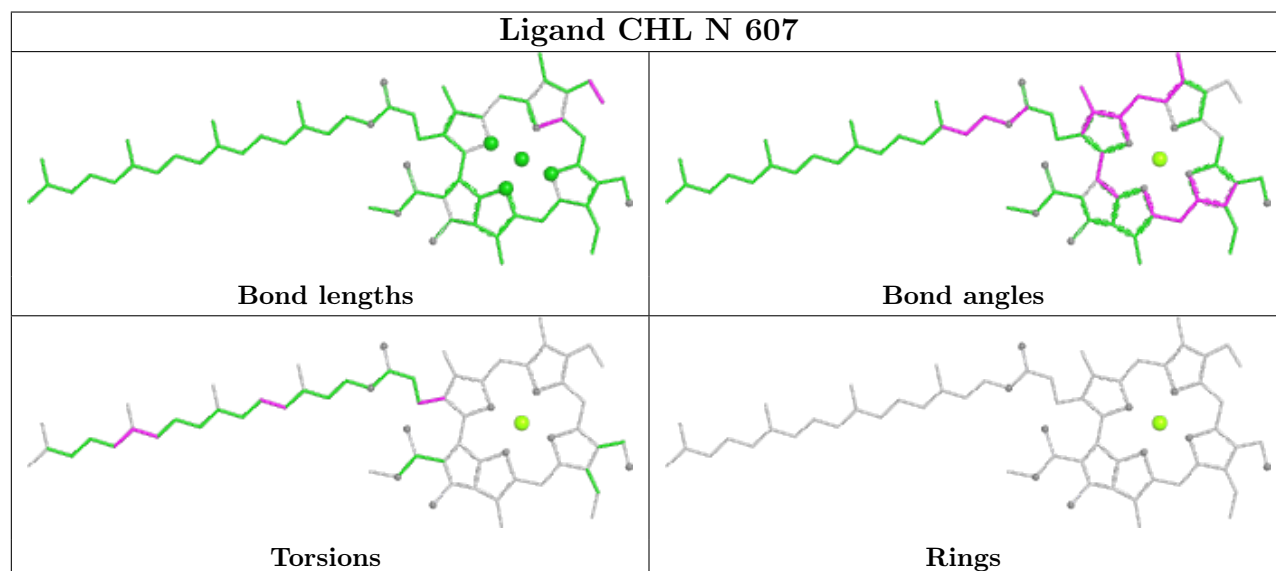
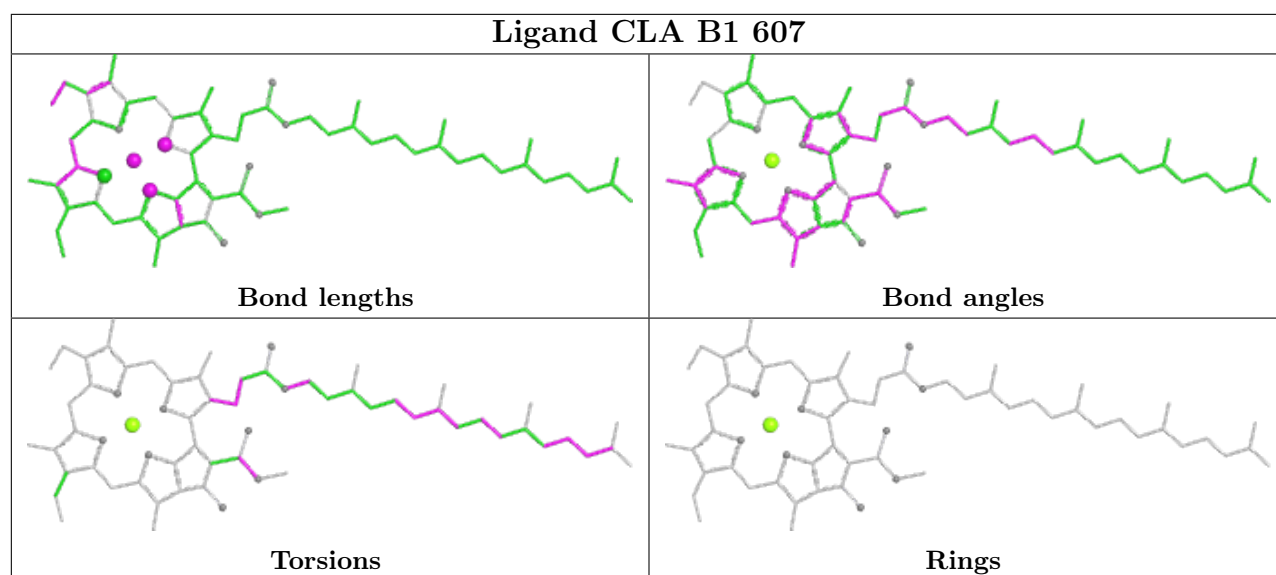
Ligand CLA A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

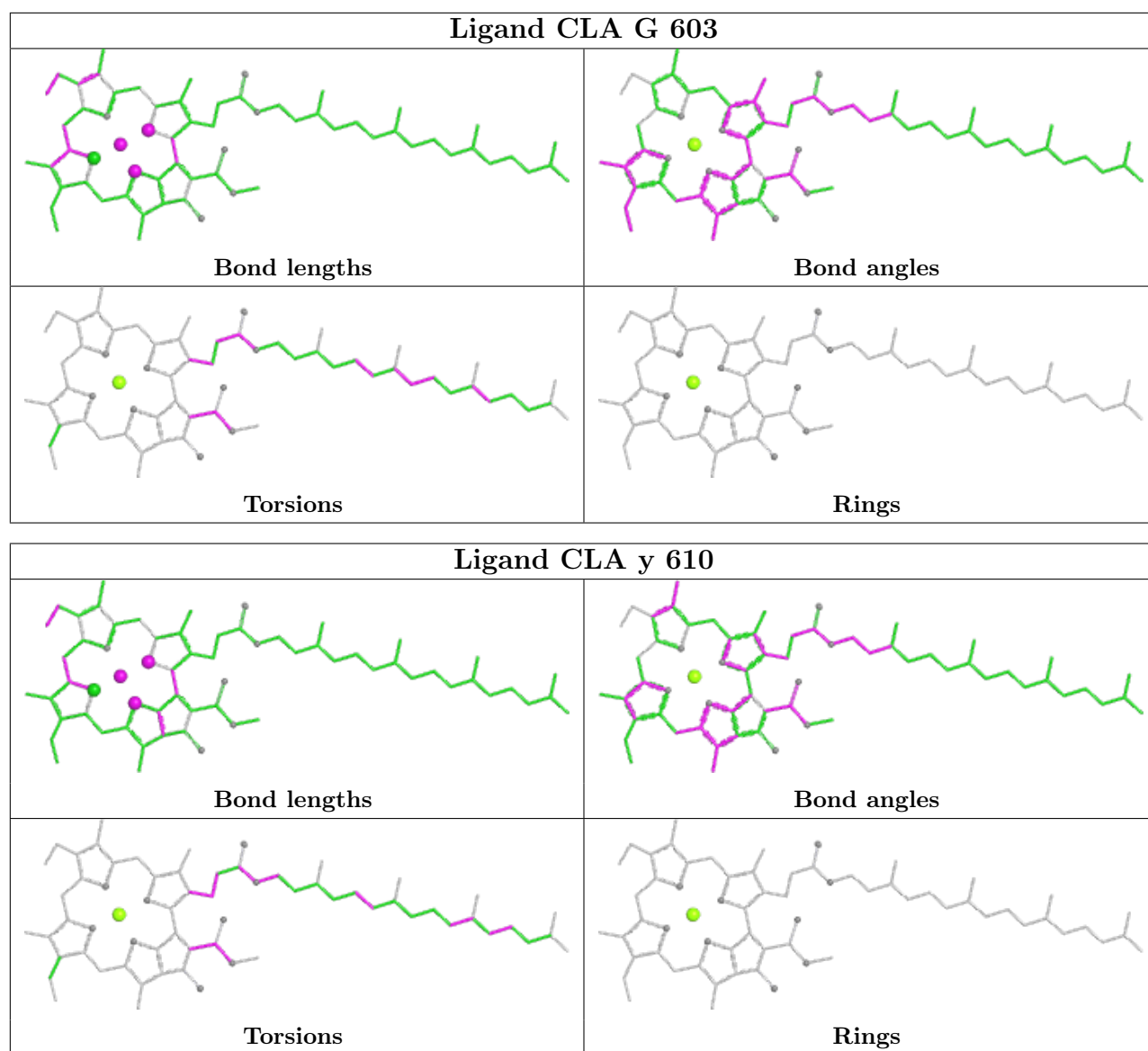
Ligand LUT y1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

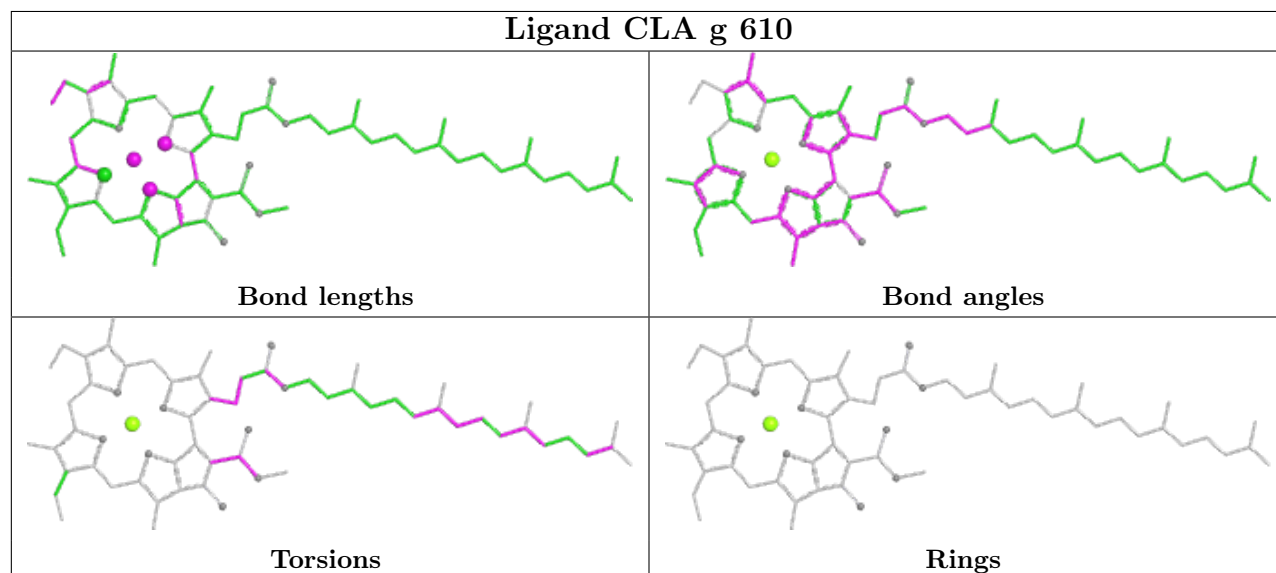
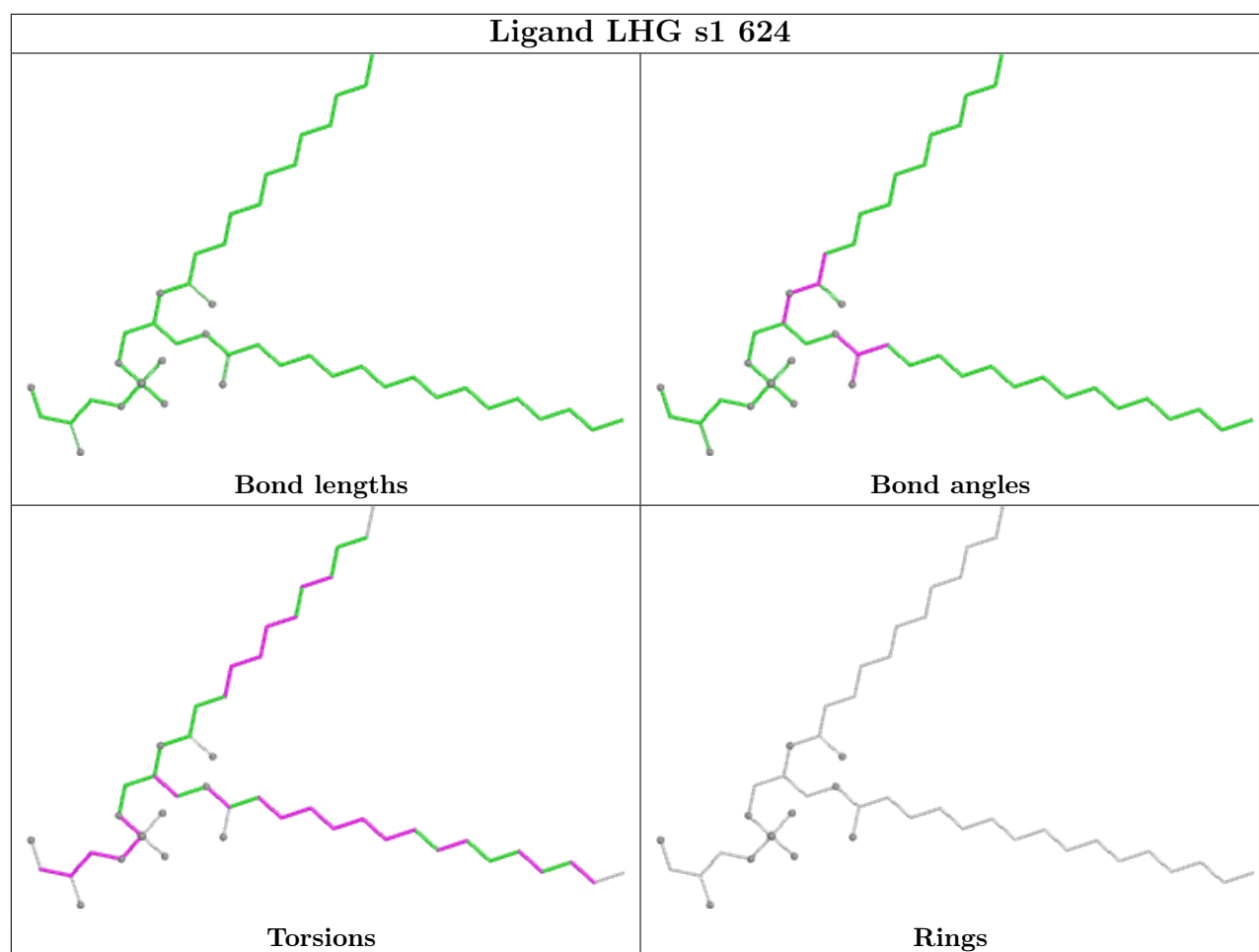
Ligand CLA y1 614	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CHL g 601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT y 621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

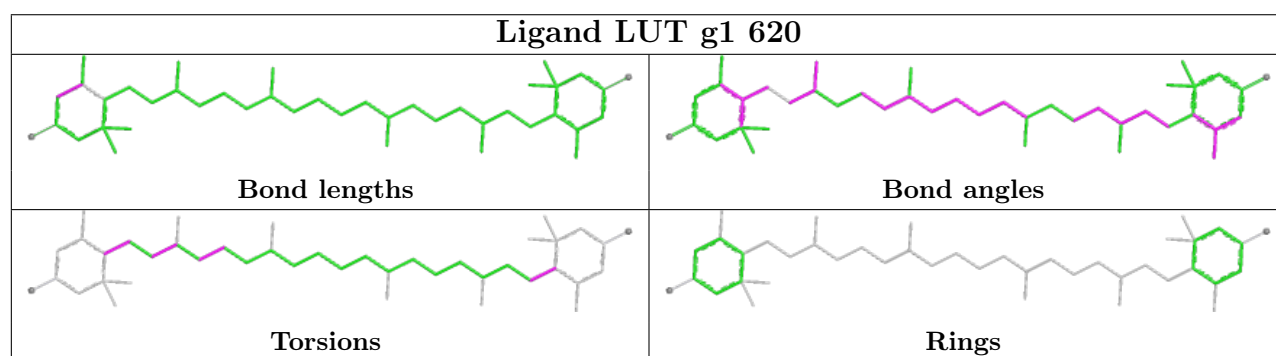
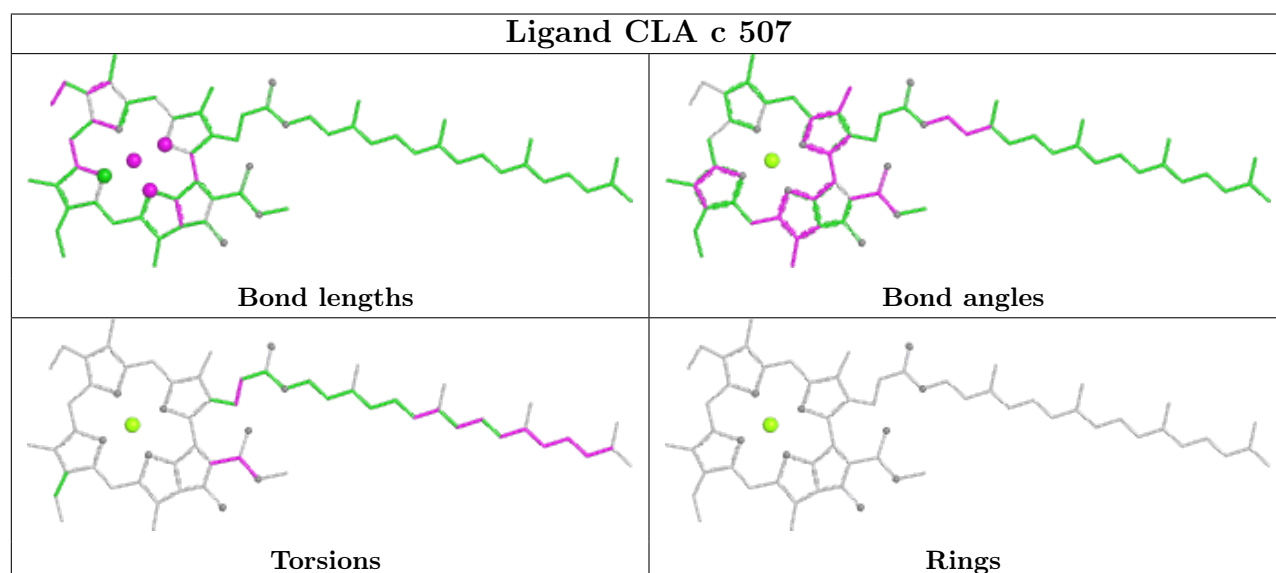
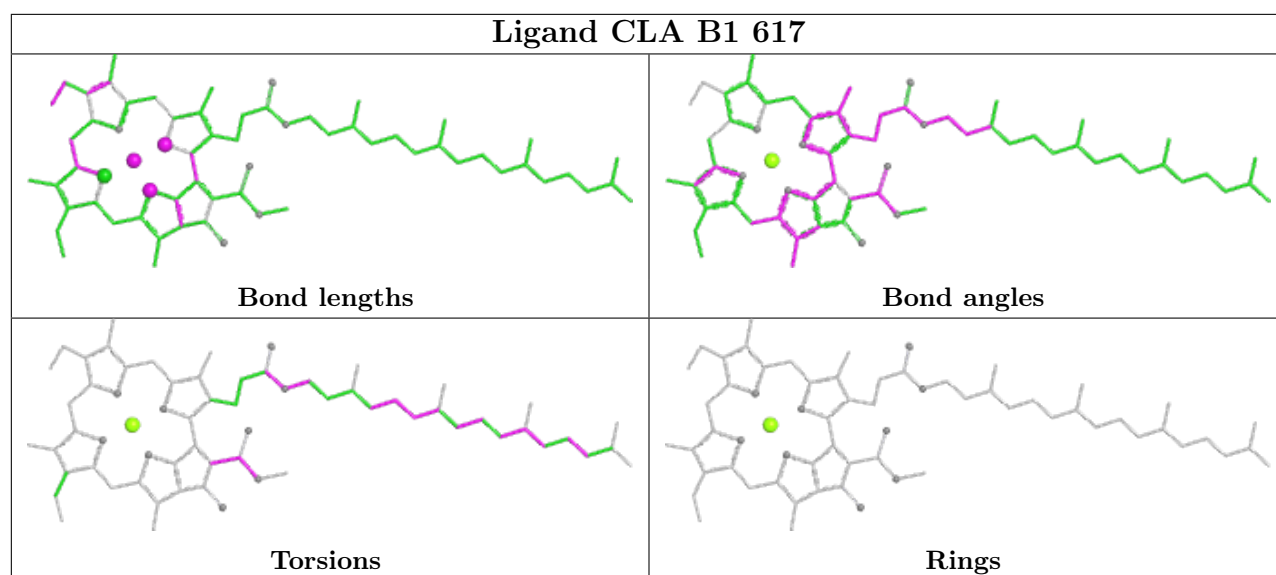


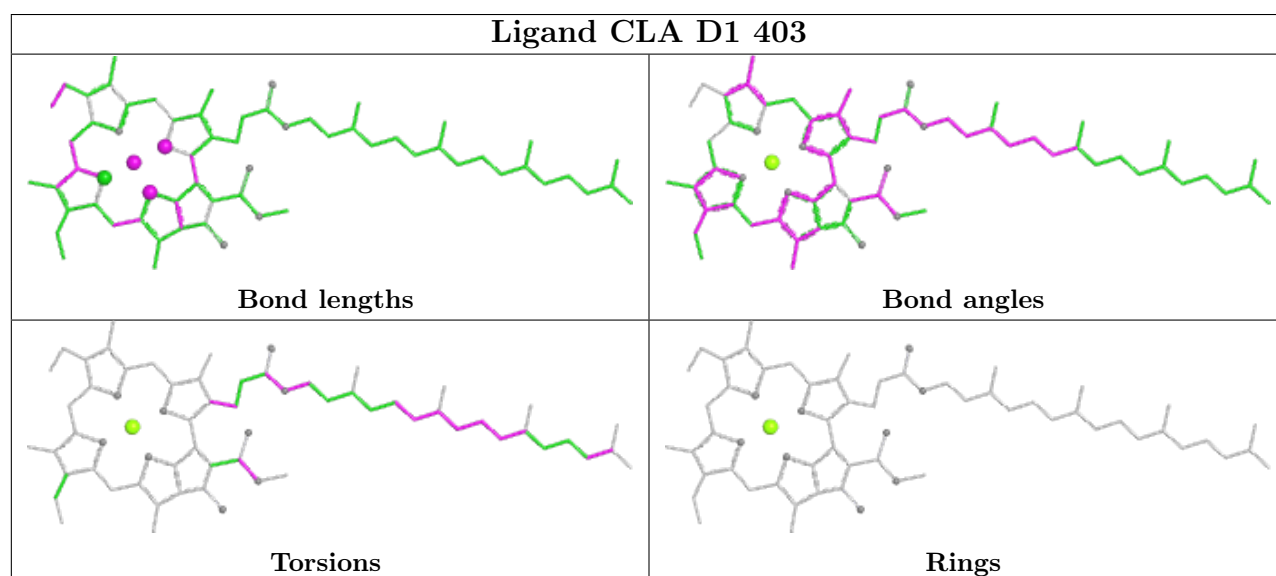
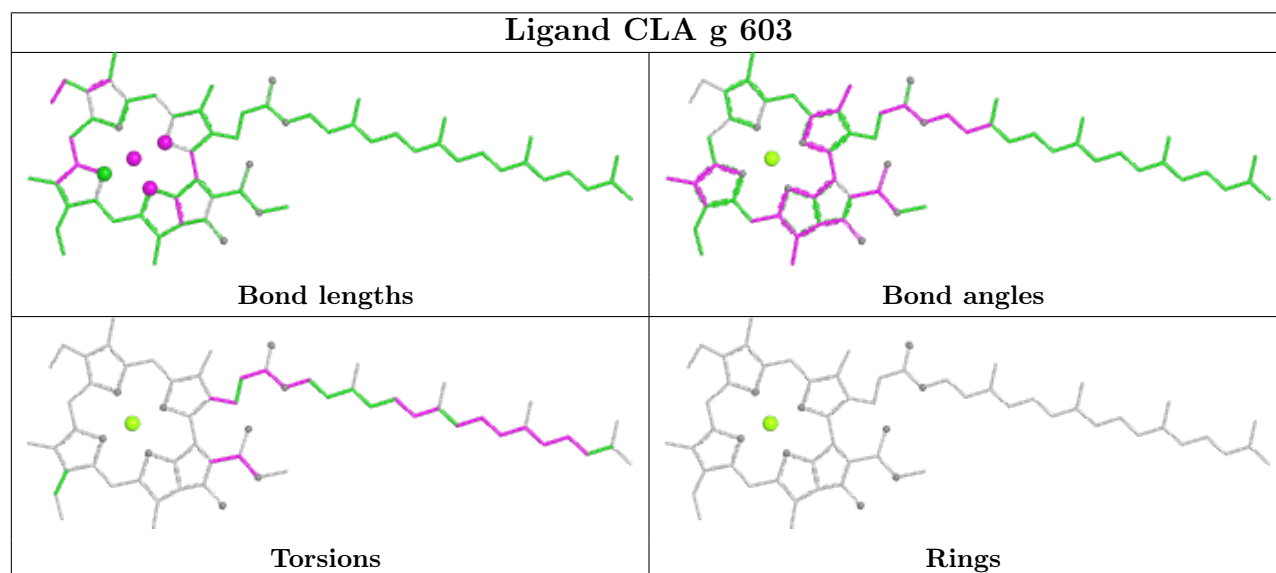
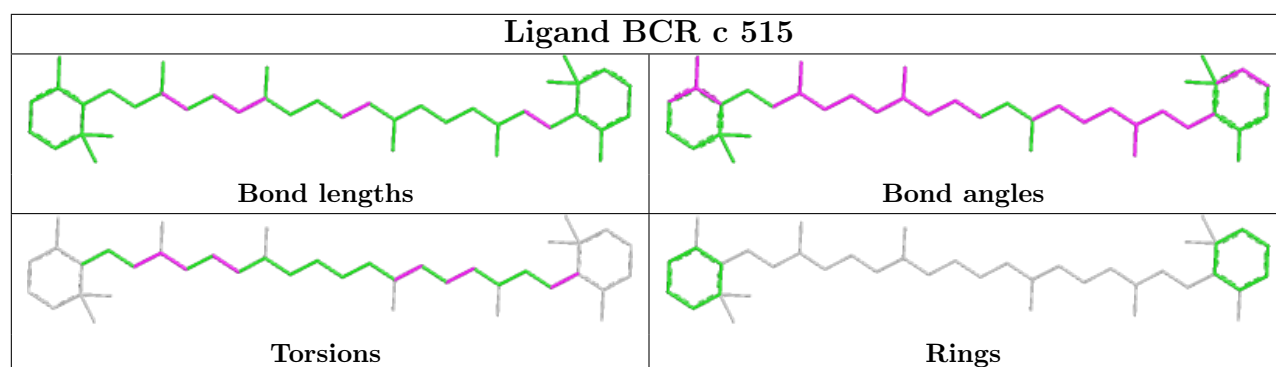


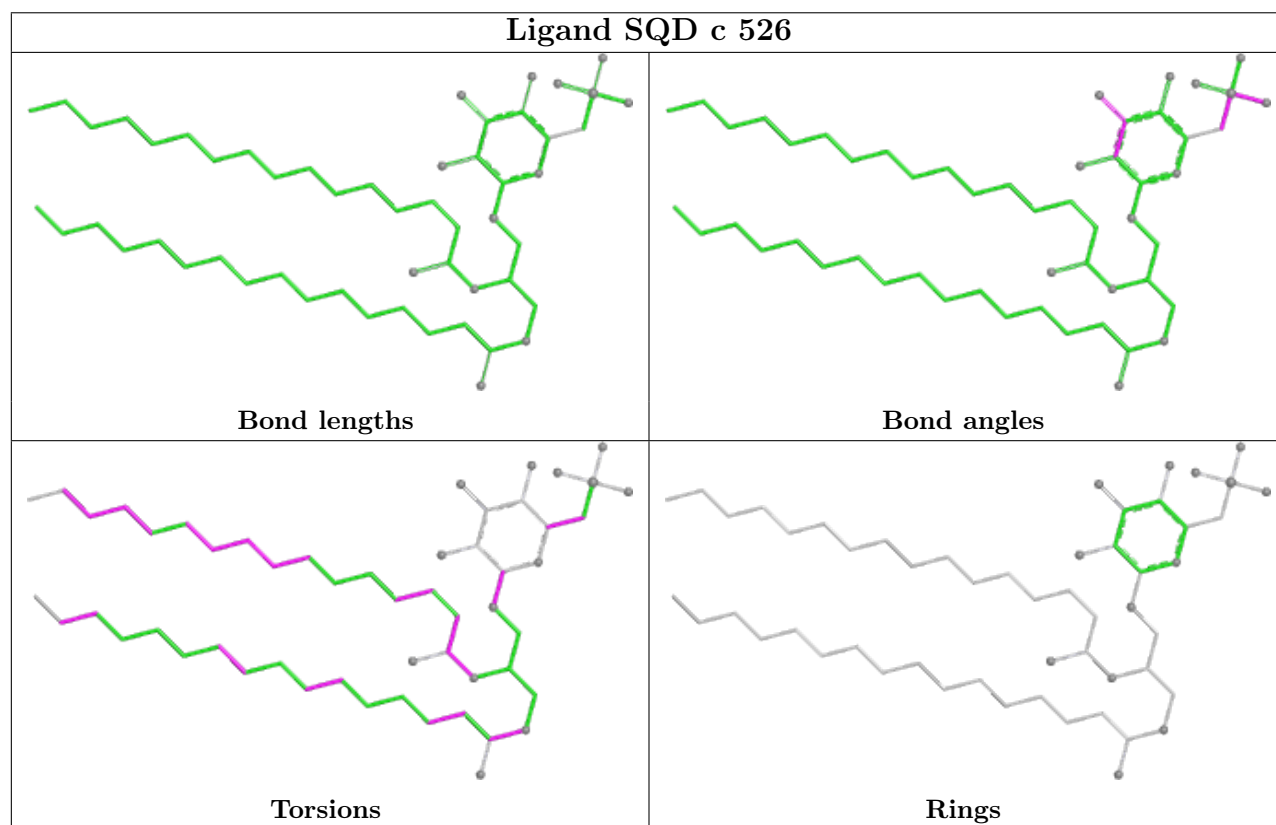
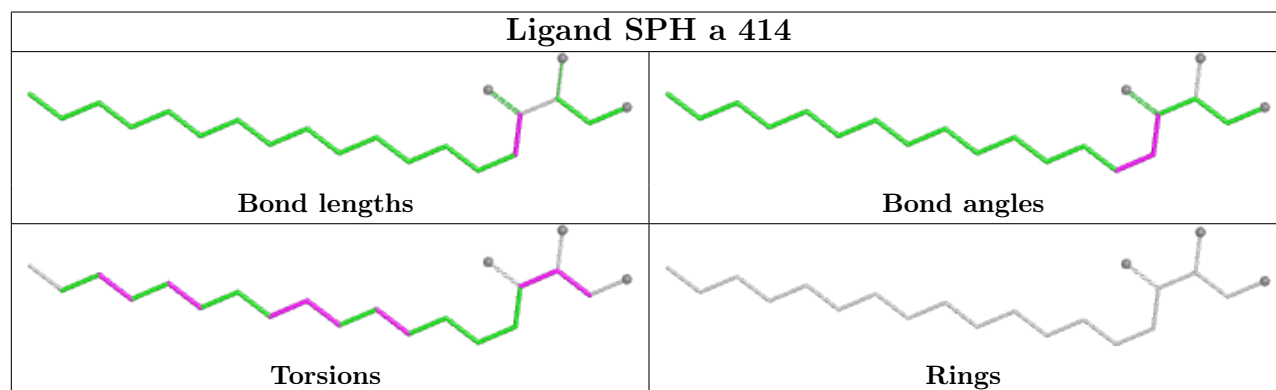
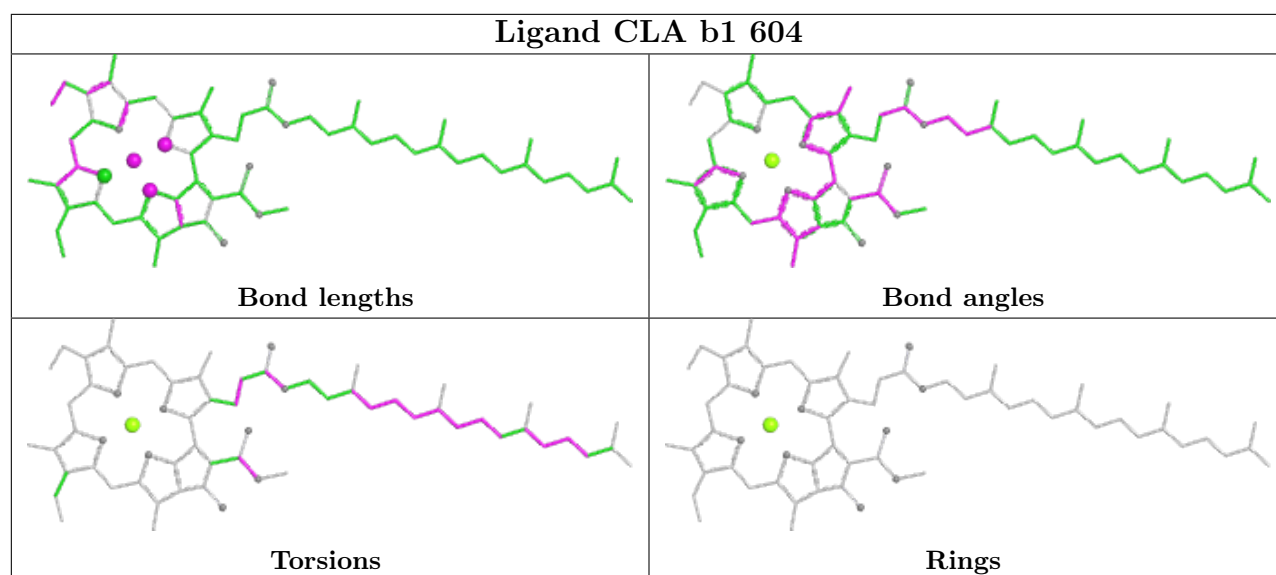


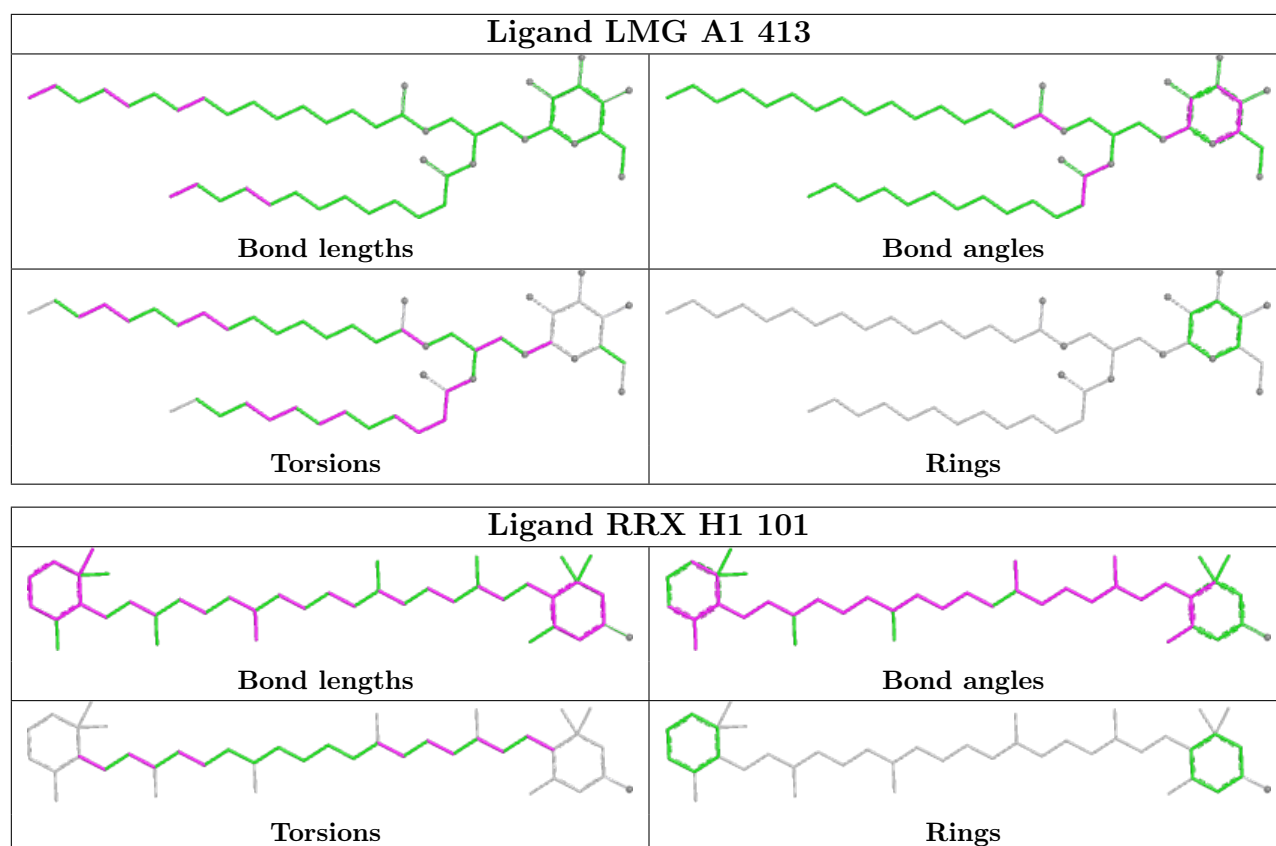


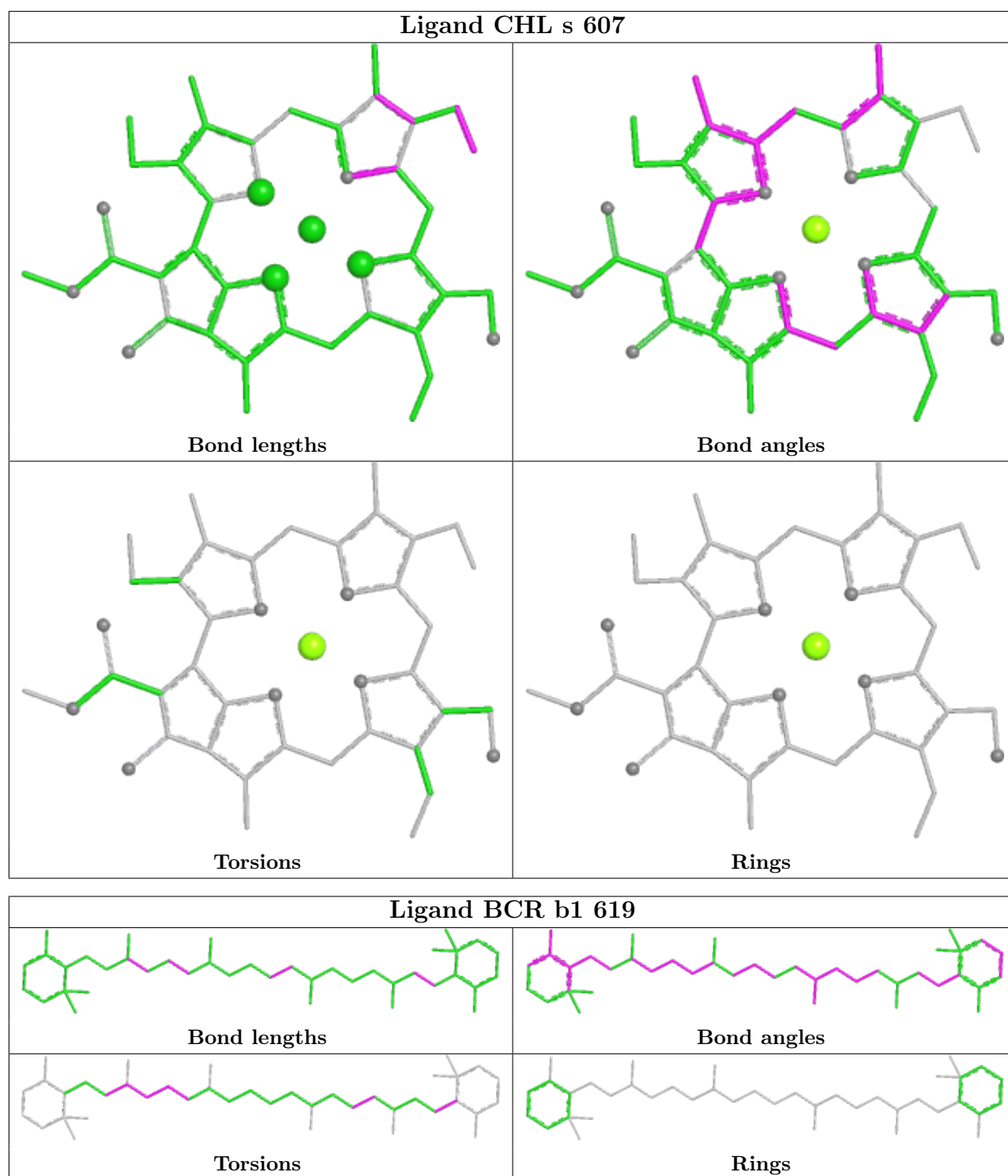


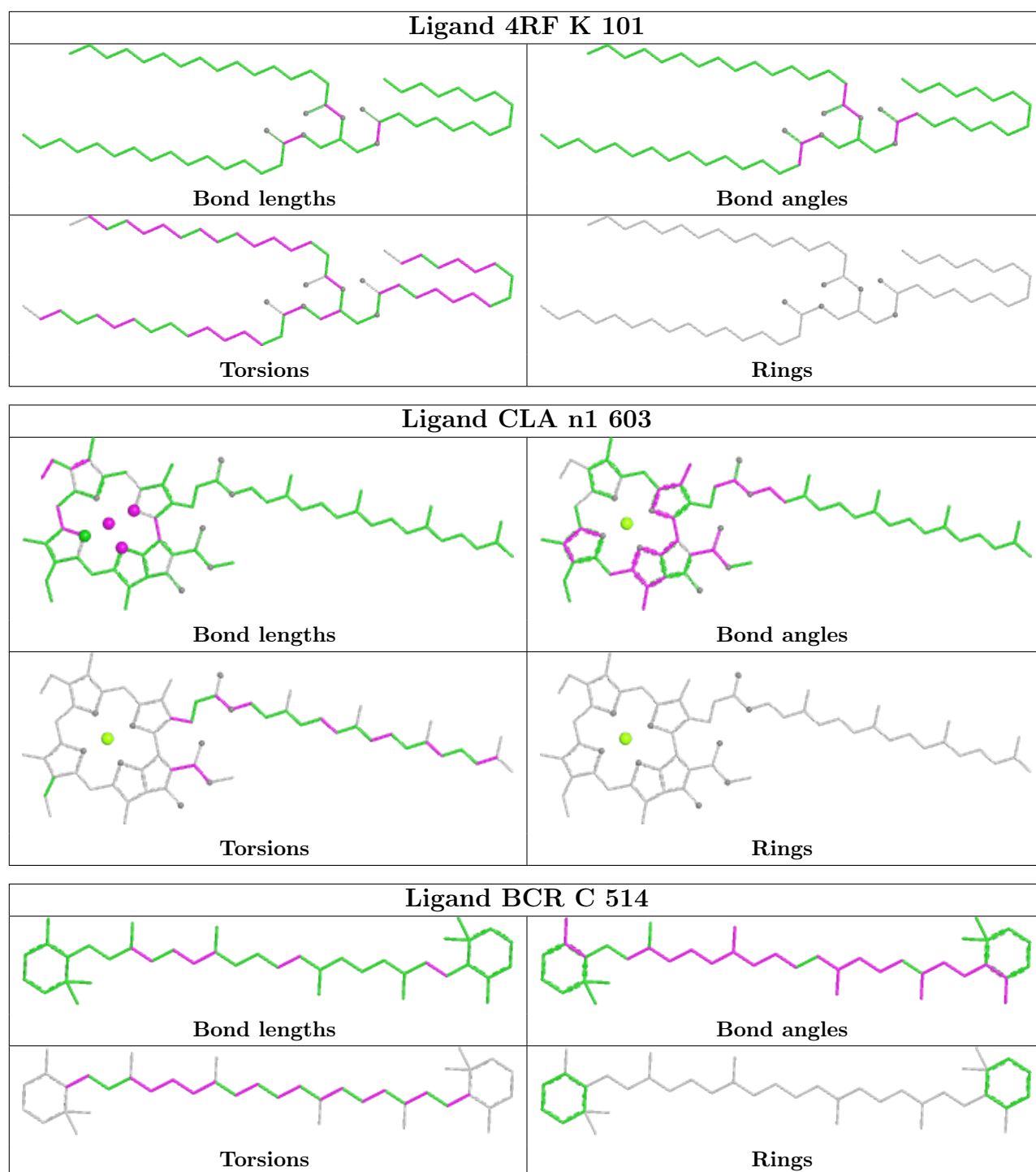


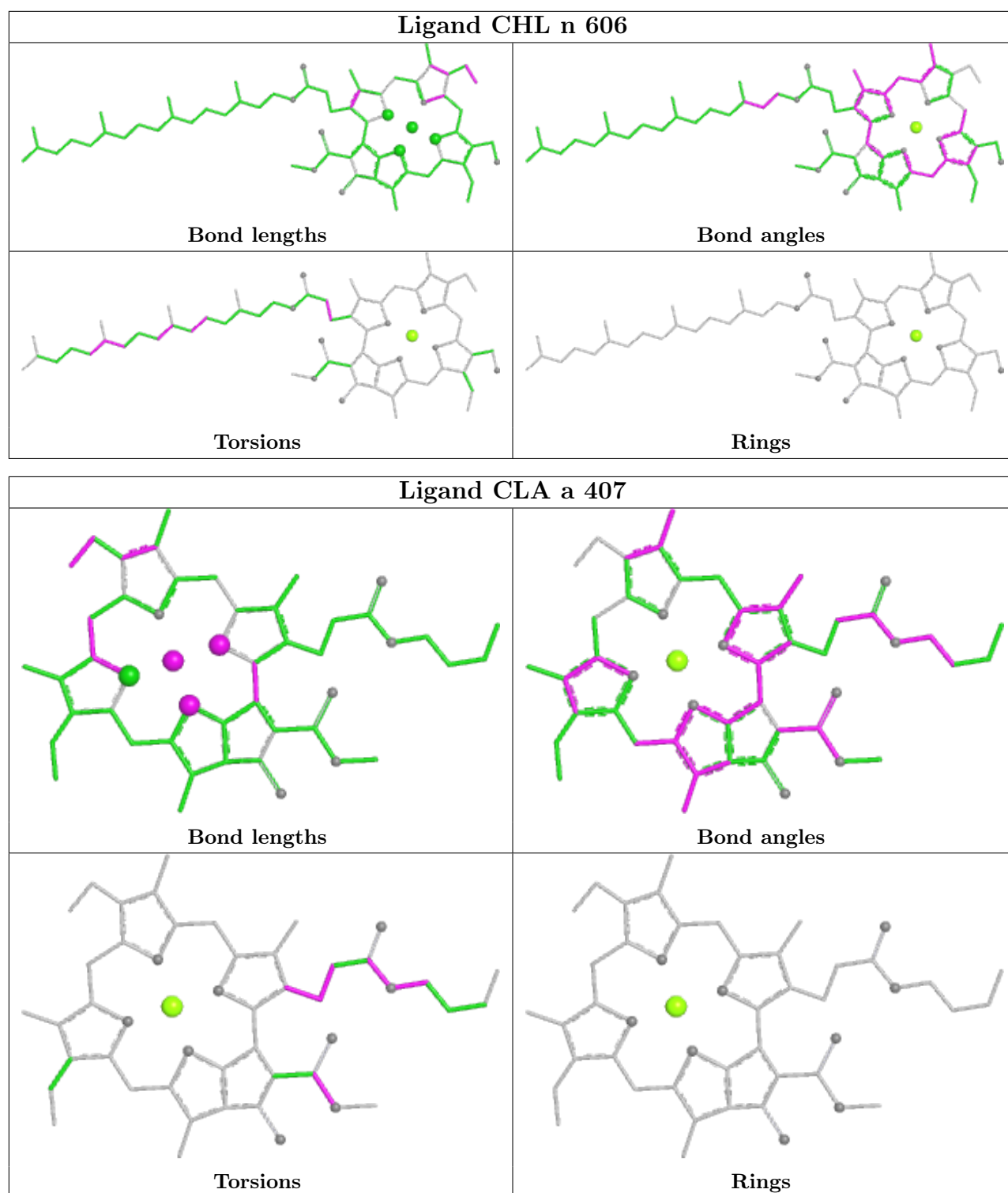


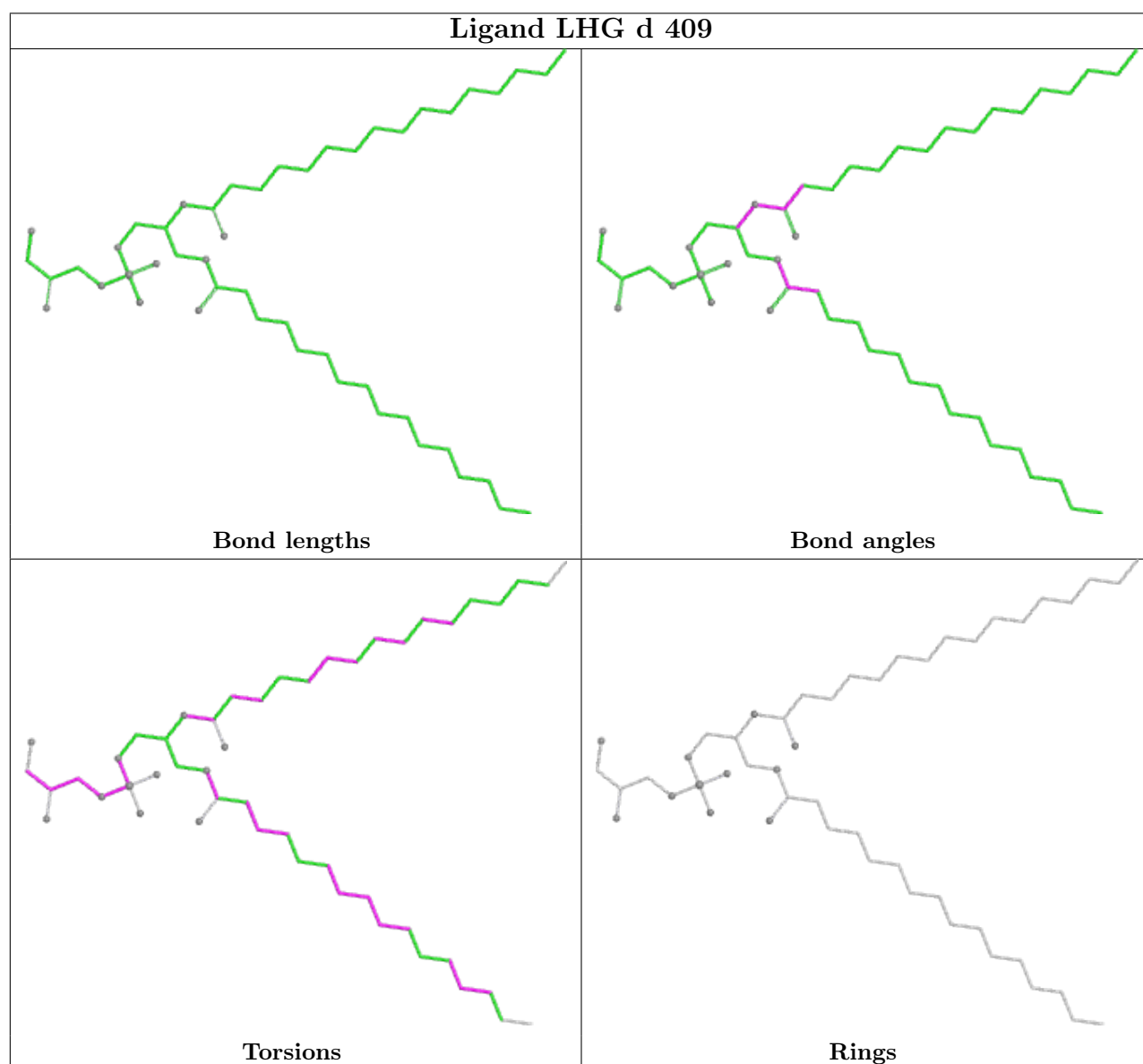
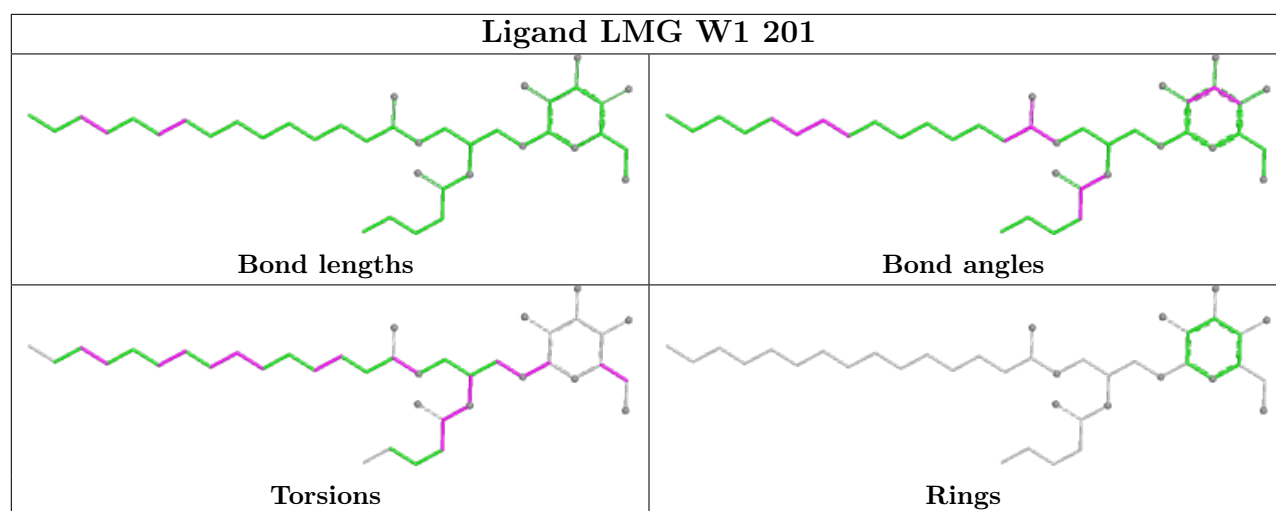


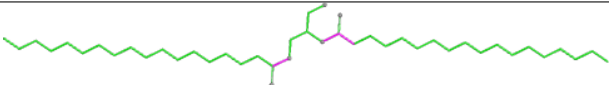
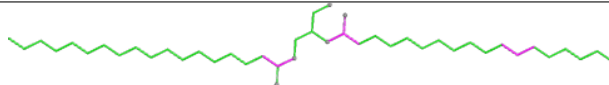
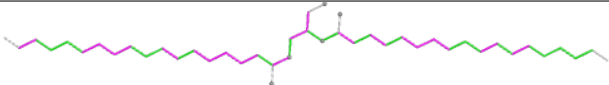
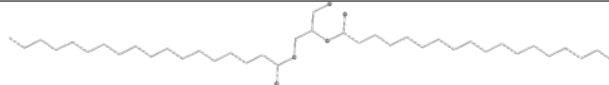


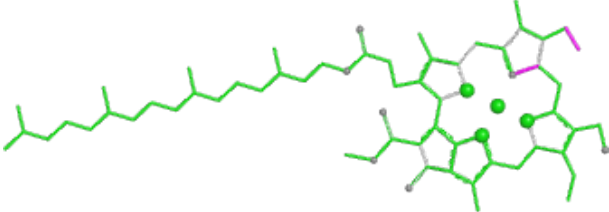
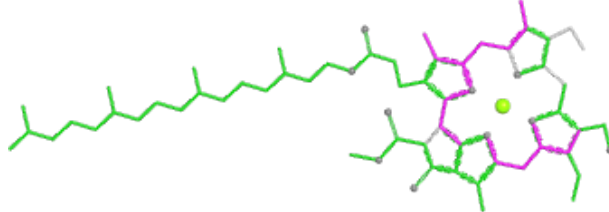
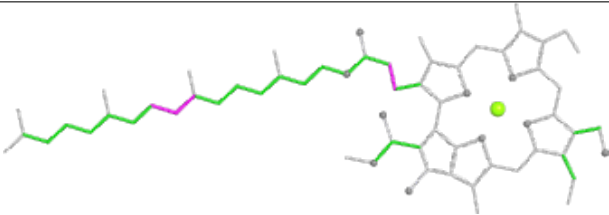
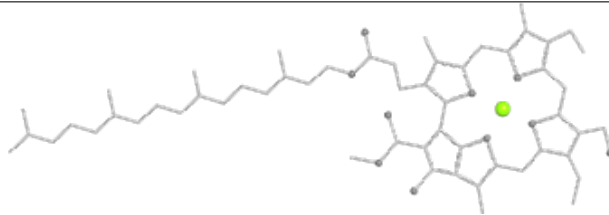


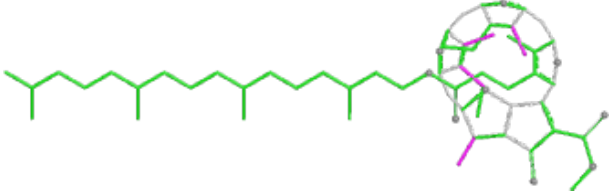
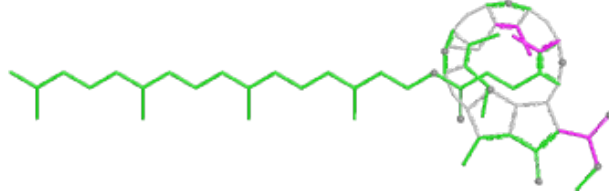
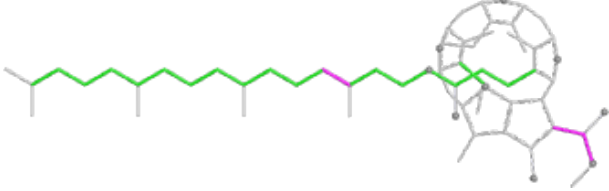
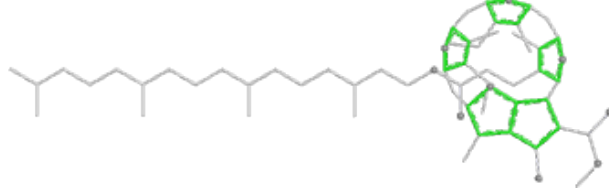




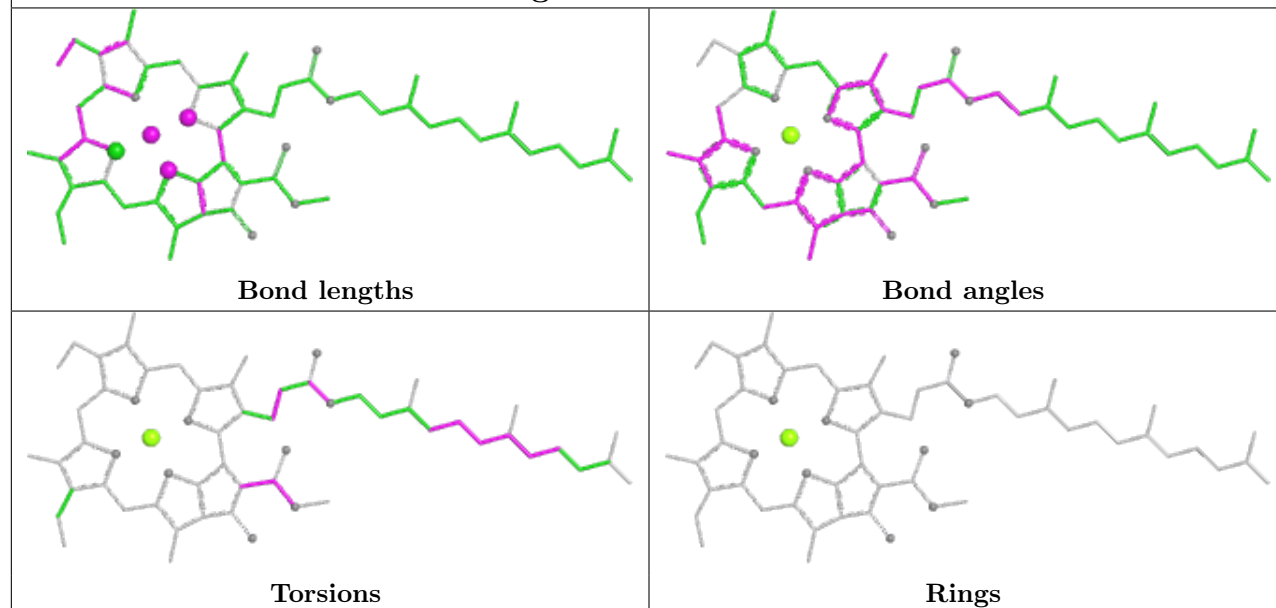


Ligand DGA C1 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

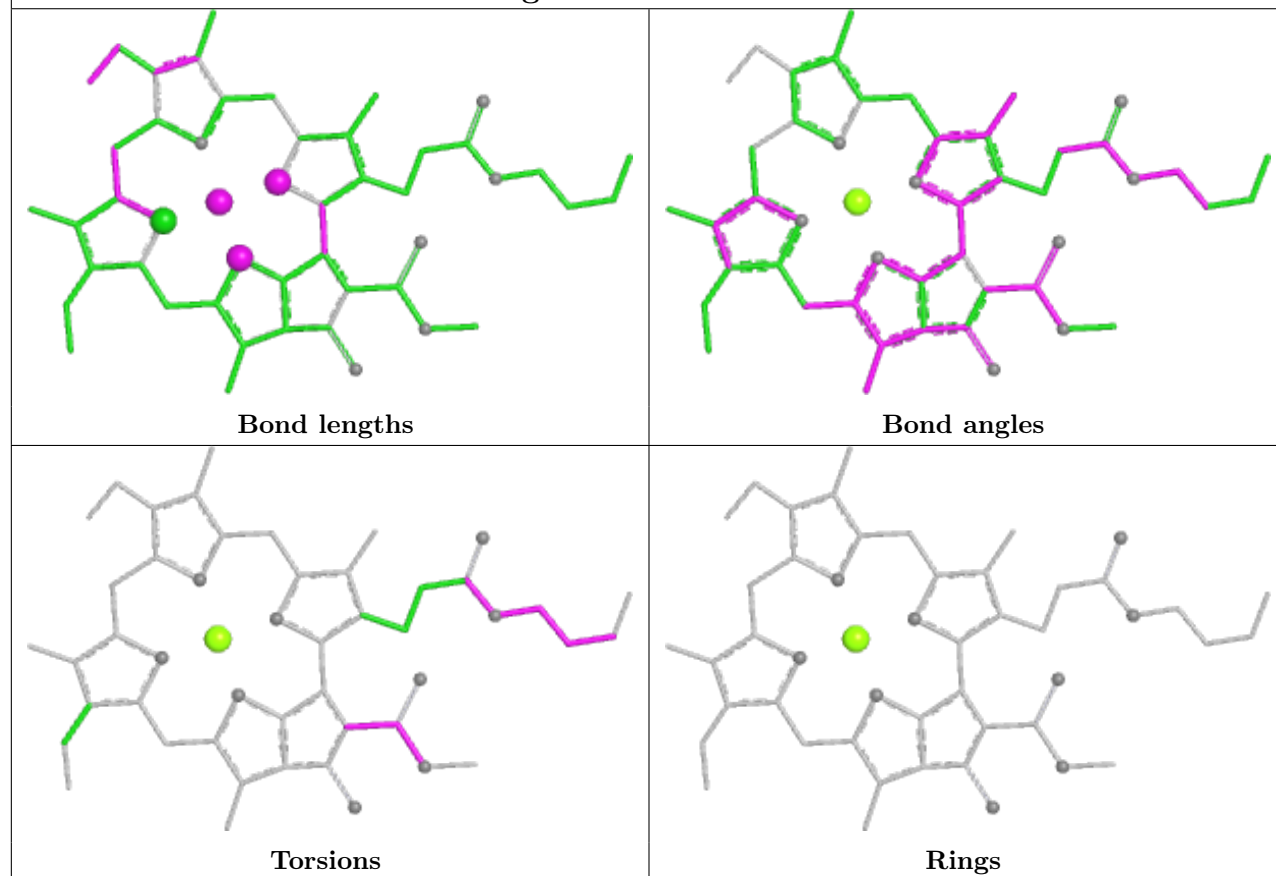
Ligand CHL y1 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

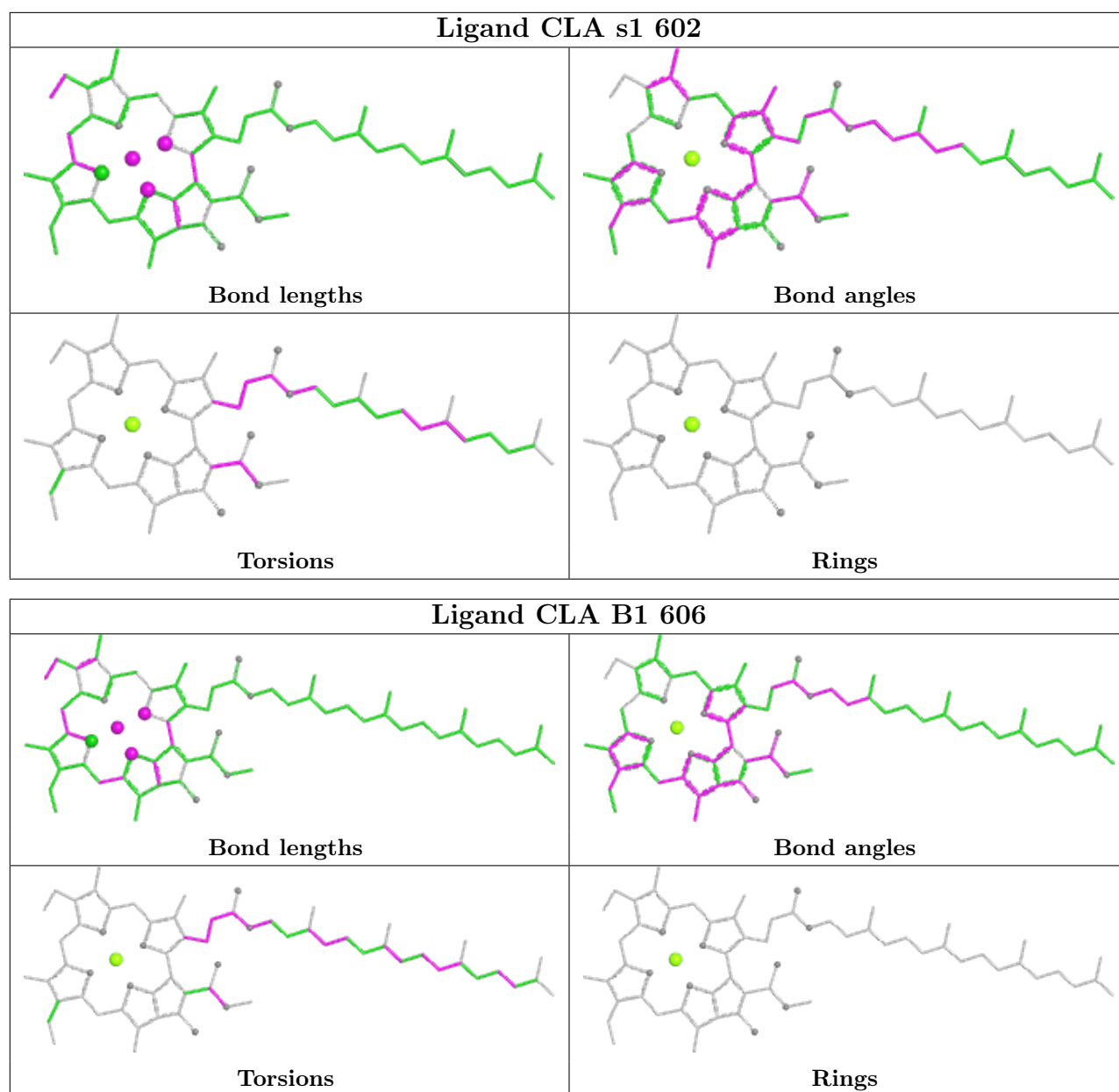
Ligand PHO A1 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

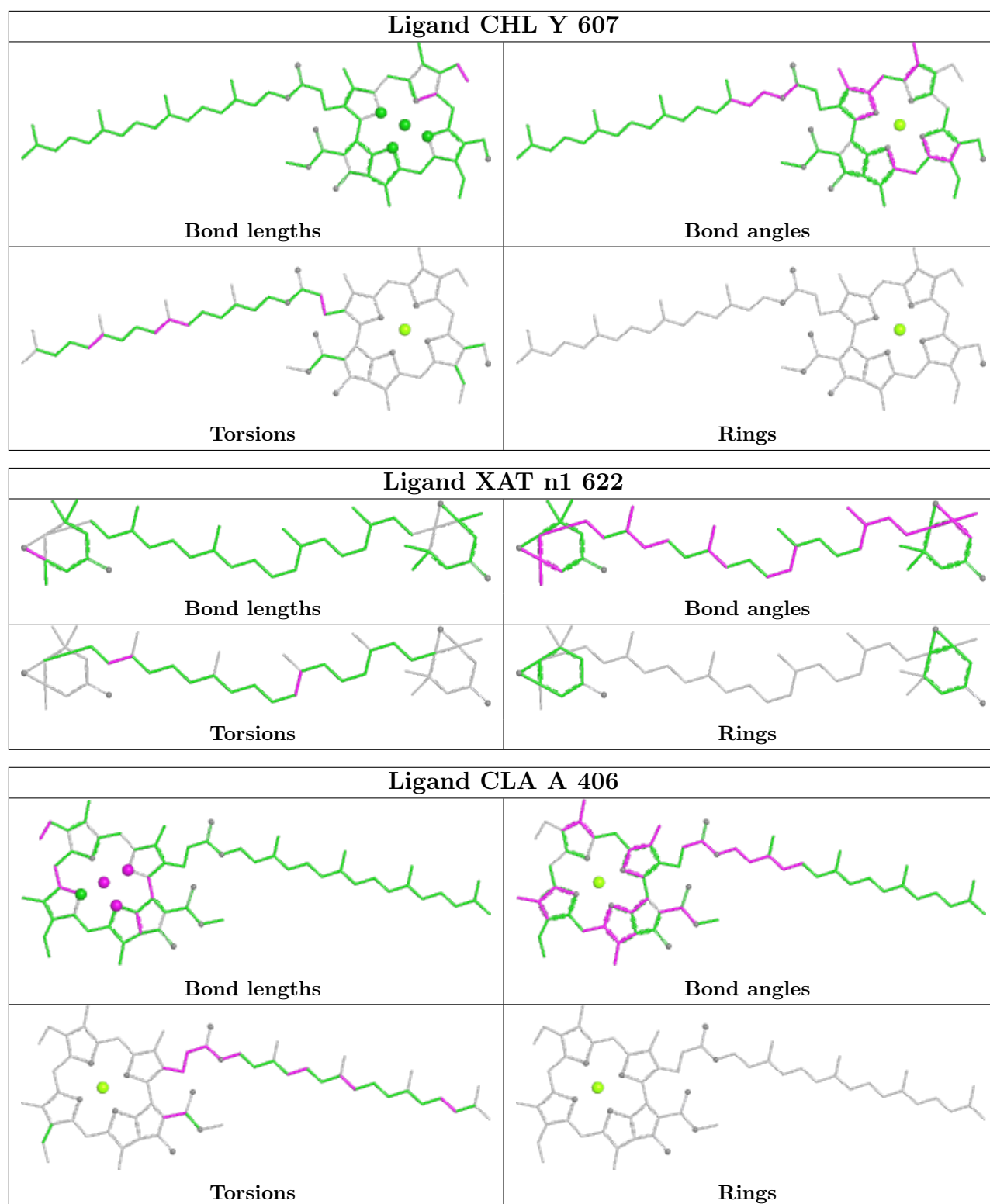
Ligand CLA R 610

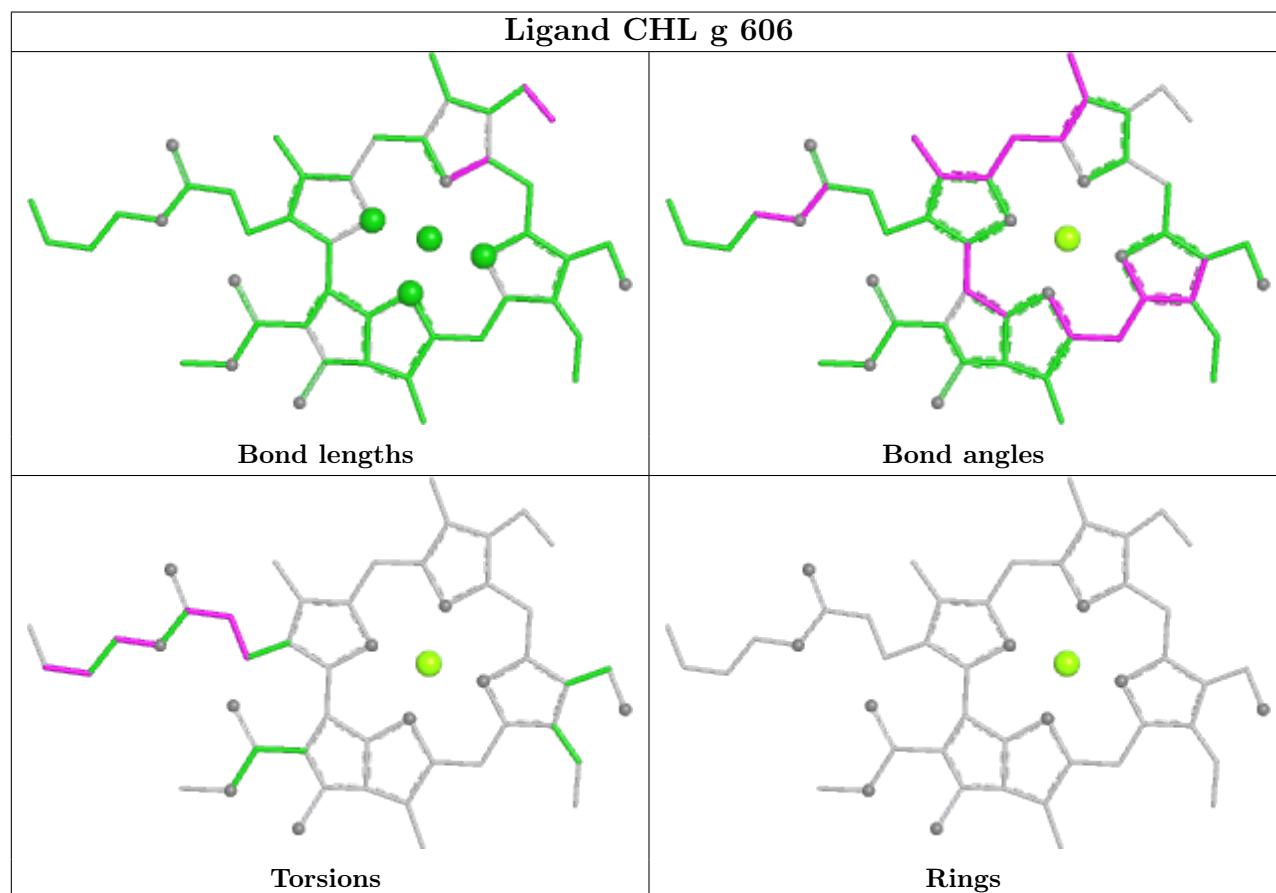
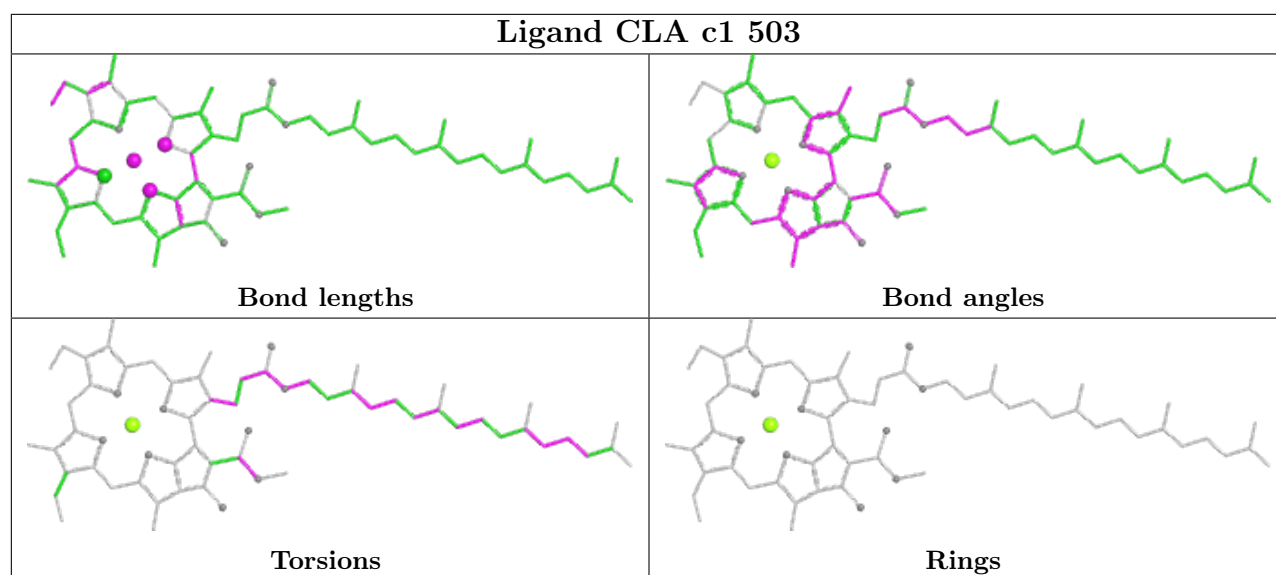


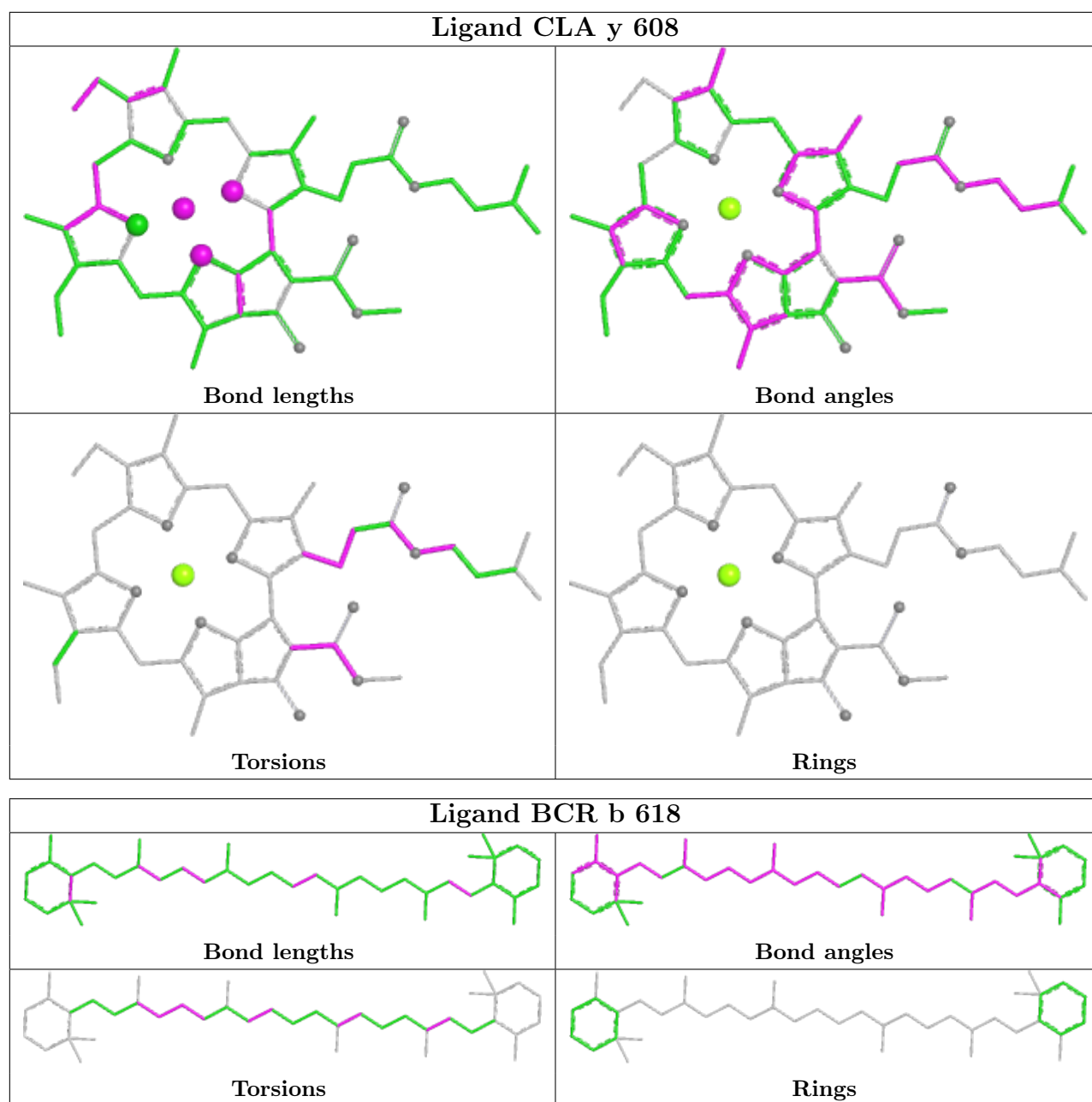
Ligand CLA G1 604

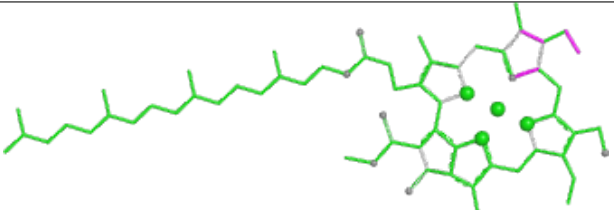
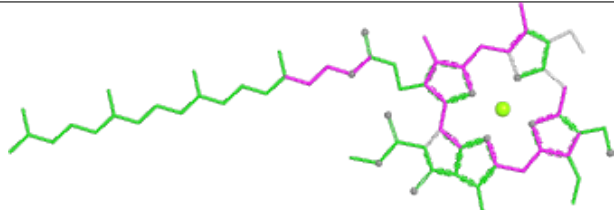
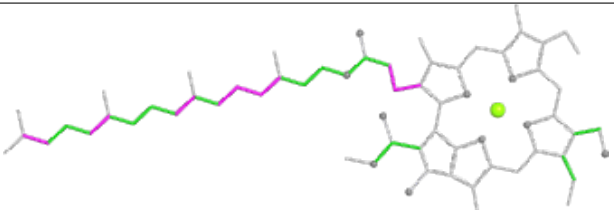
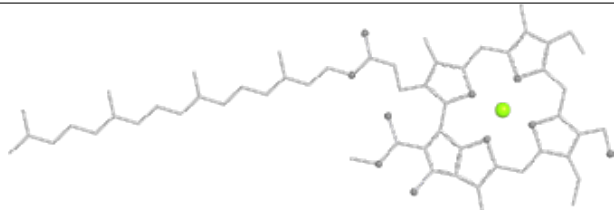


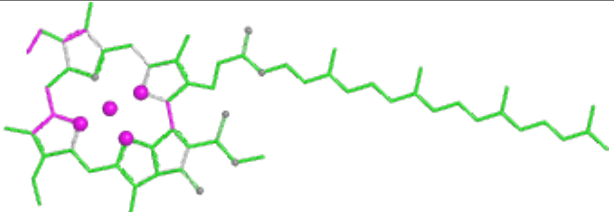
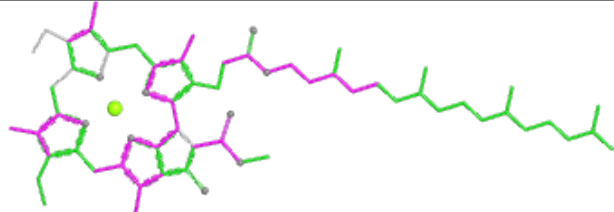
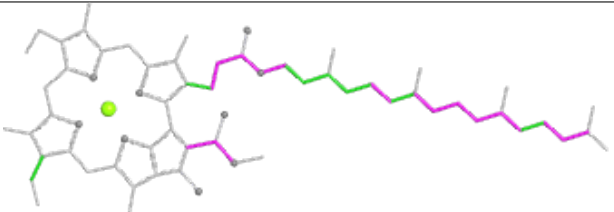
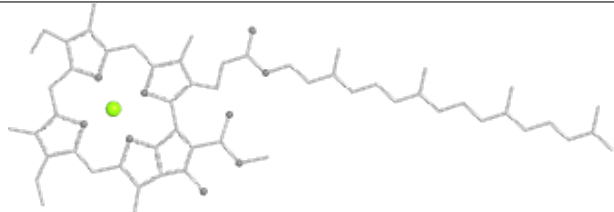


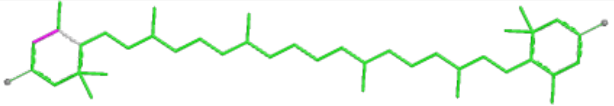
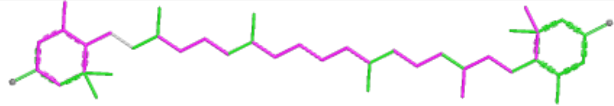
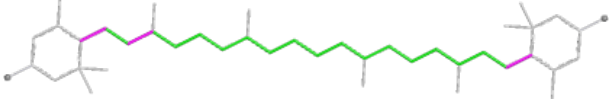
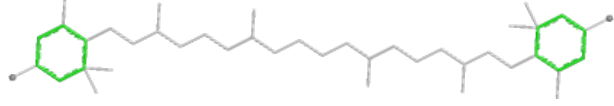


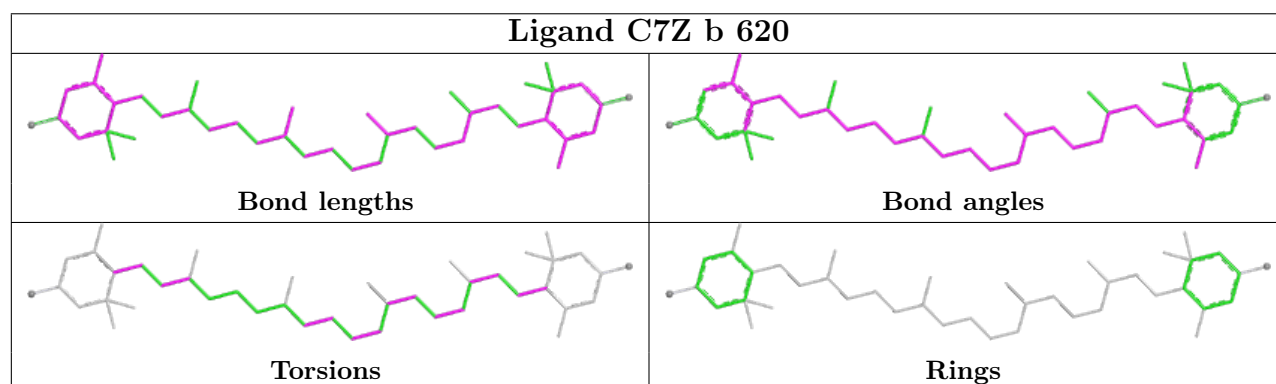
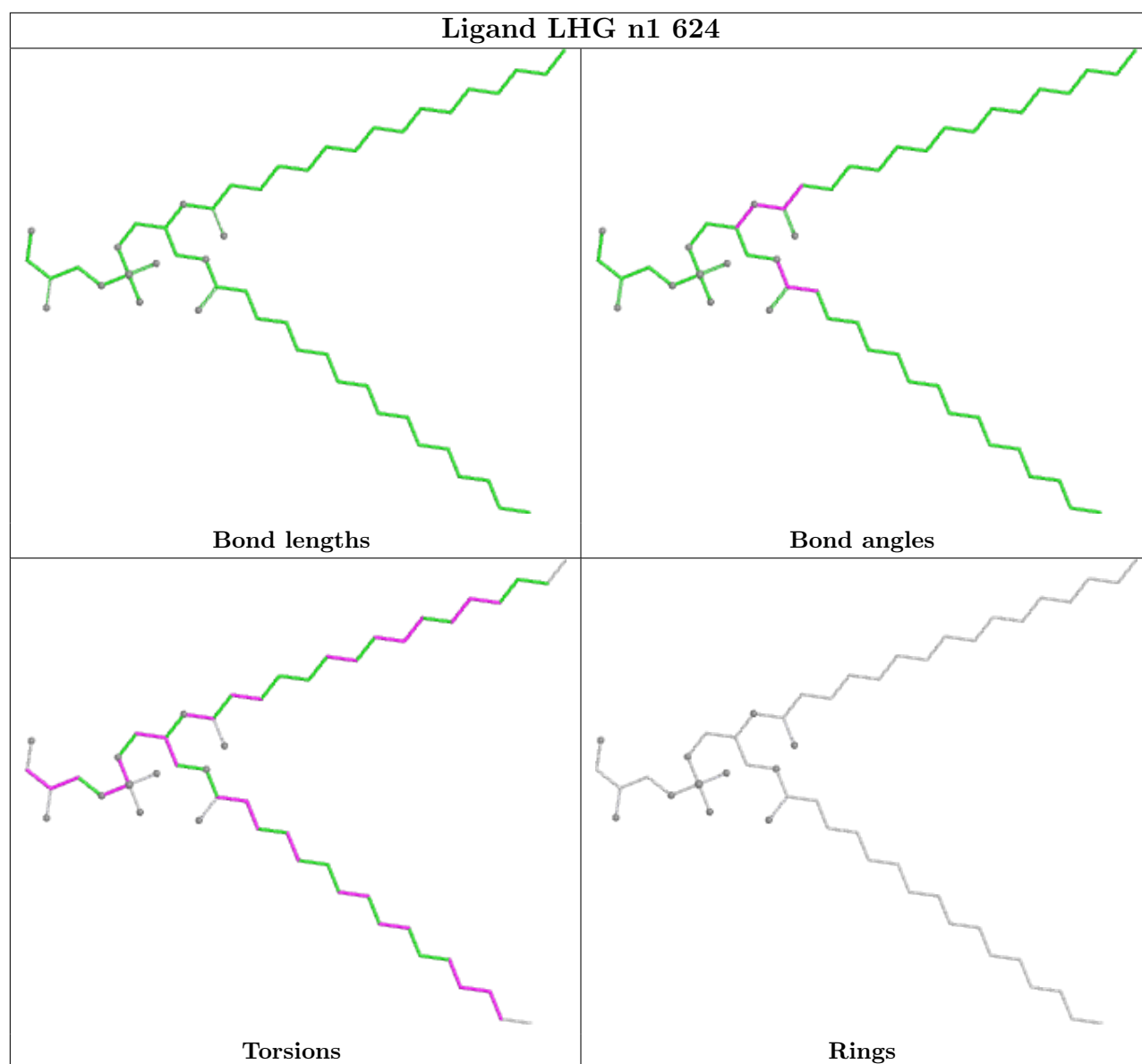


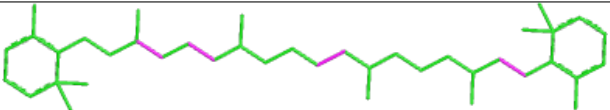
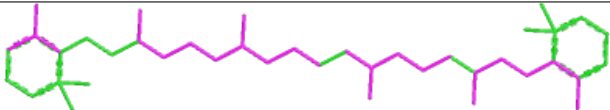
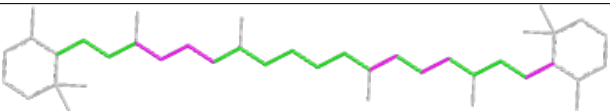
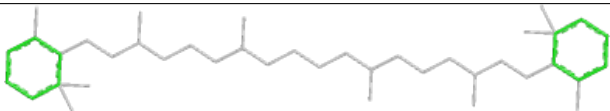
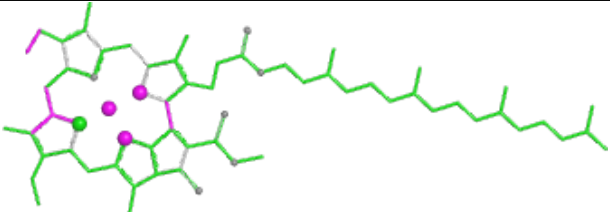
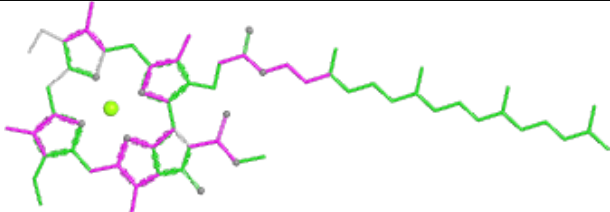
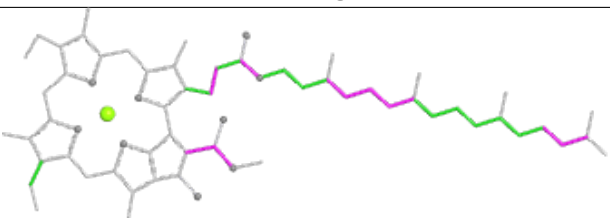
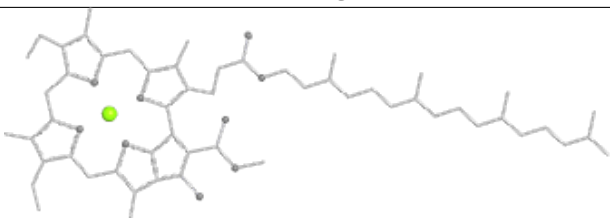
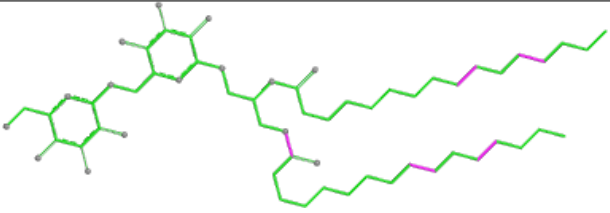
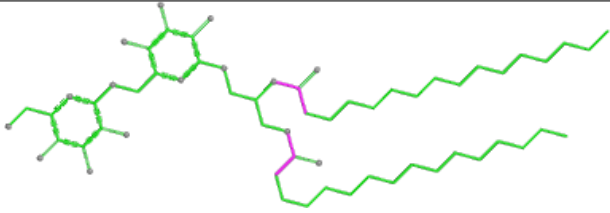
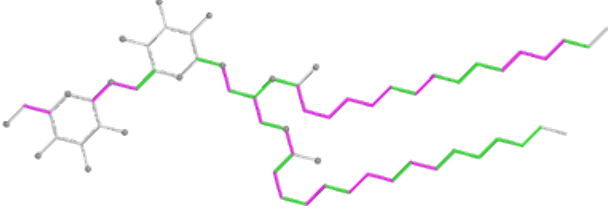
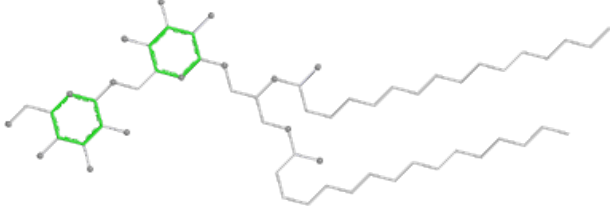


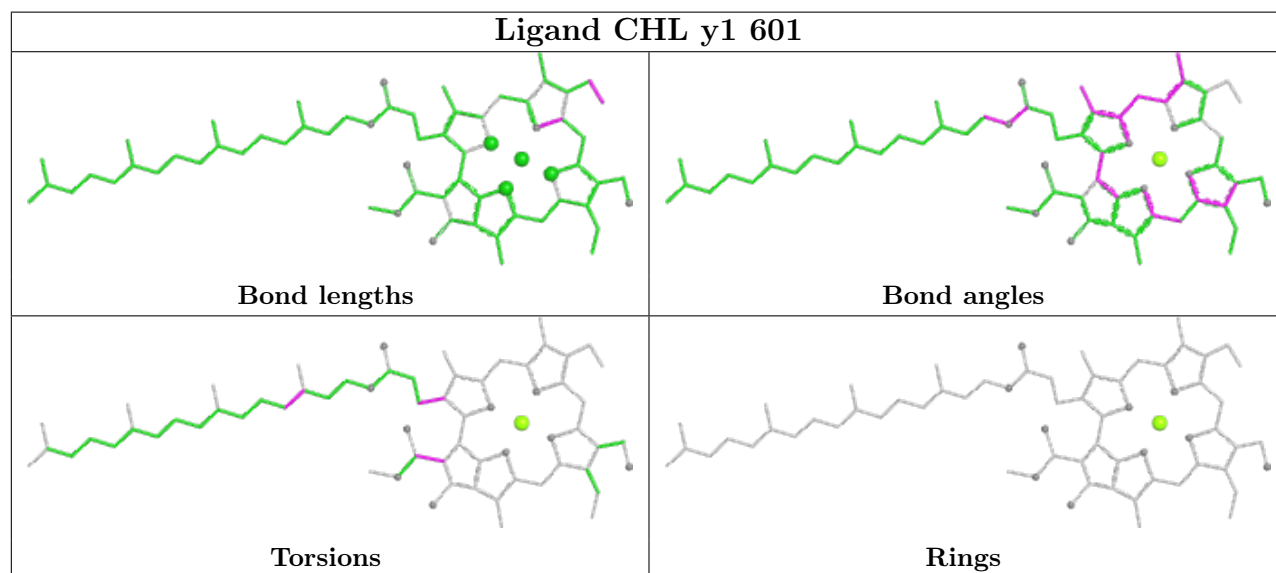
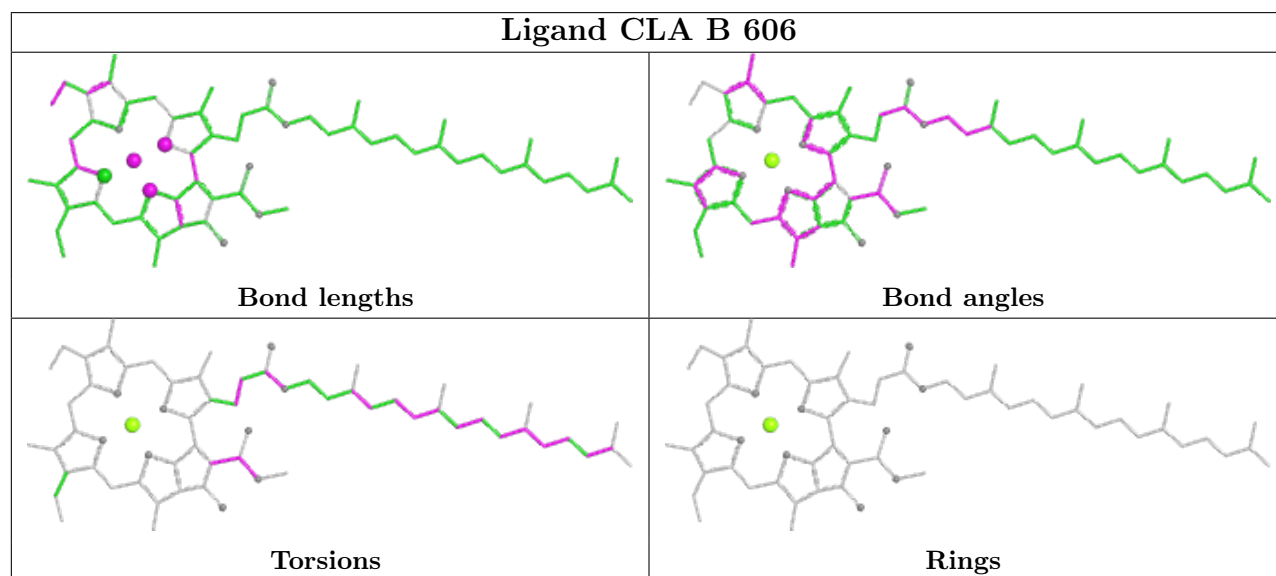
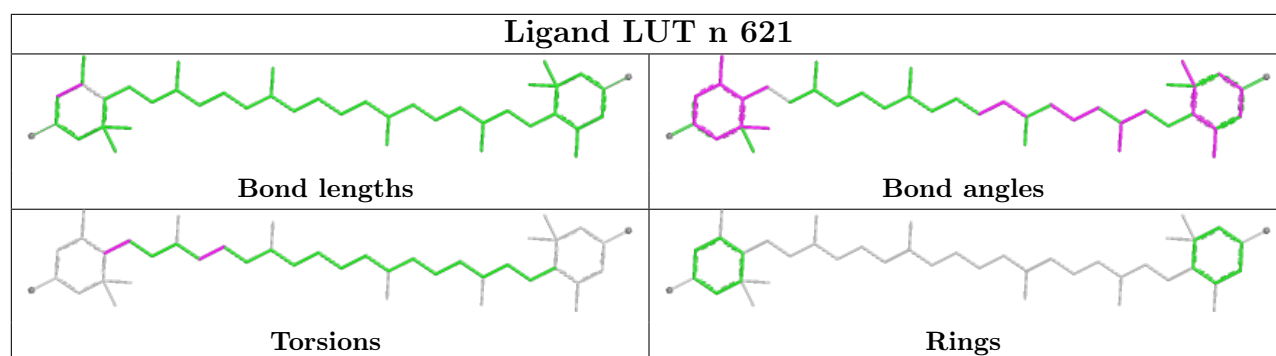
Ligand CHL N 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

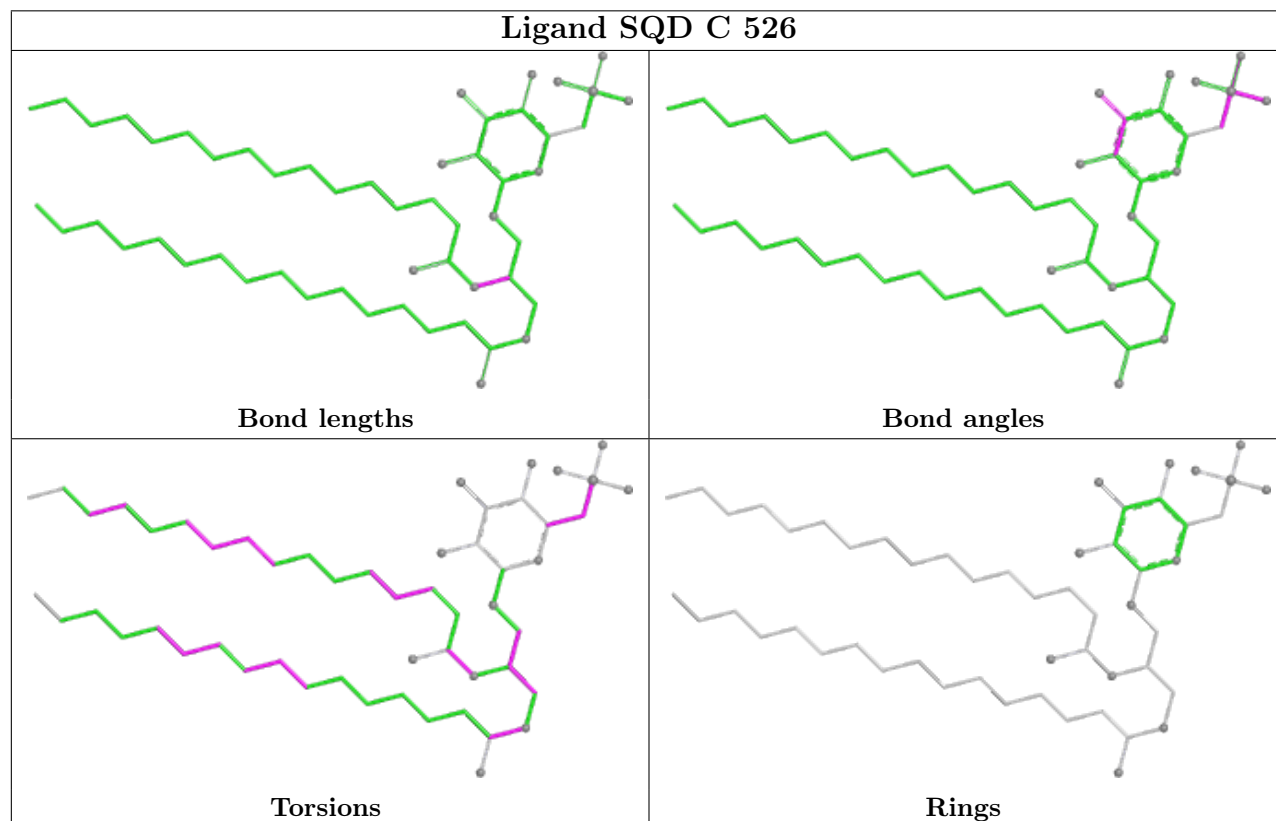
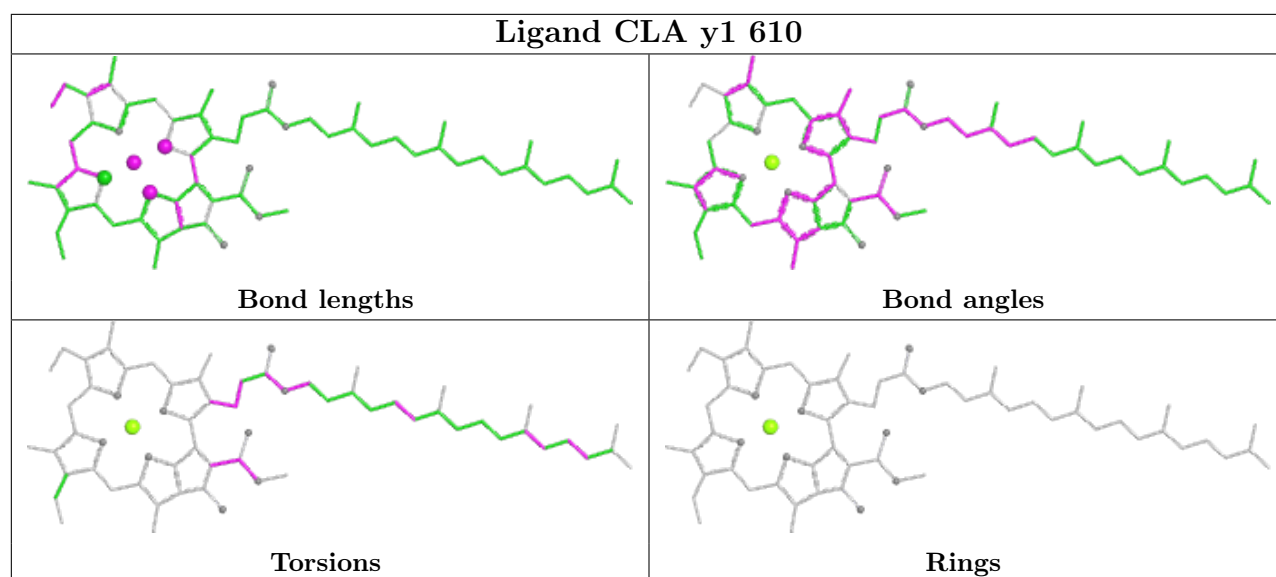
Ligand CLA B1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

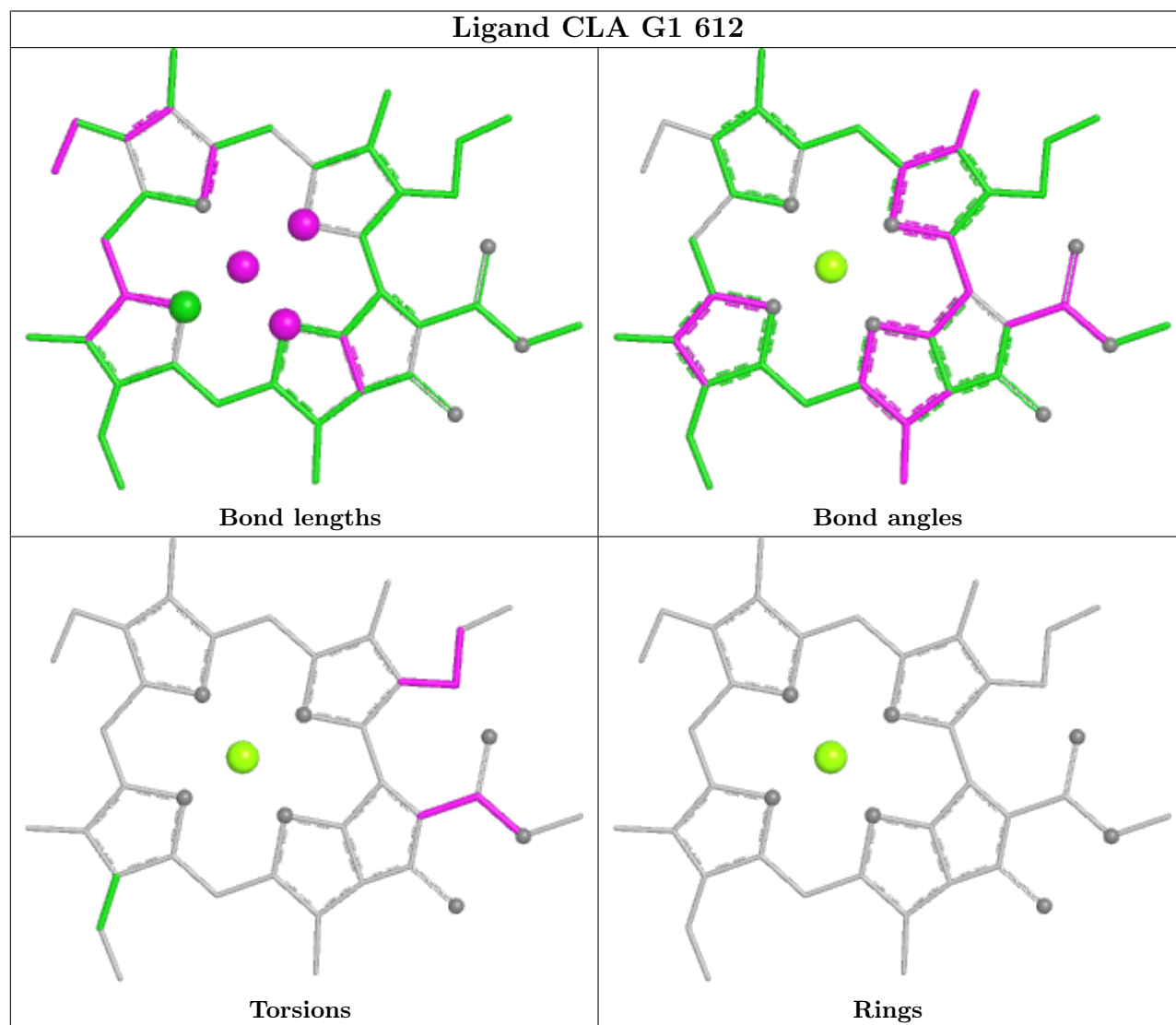
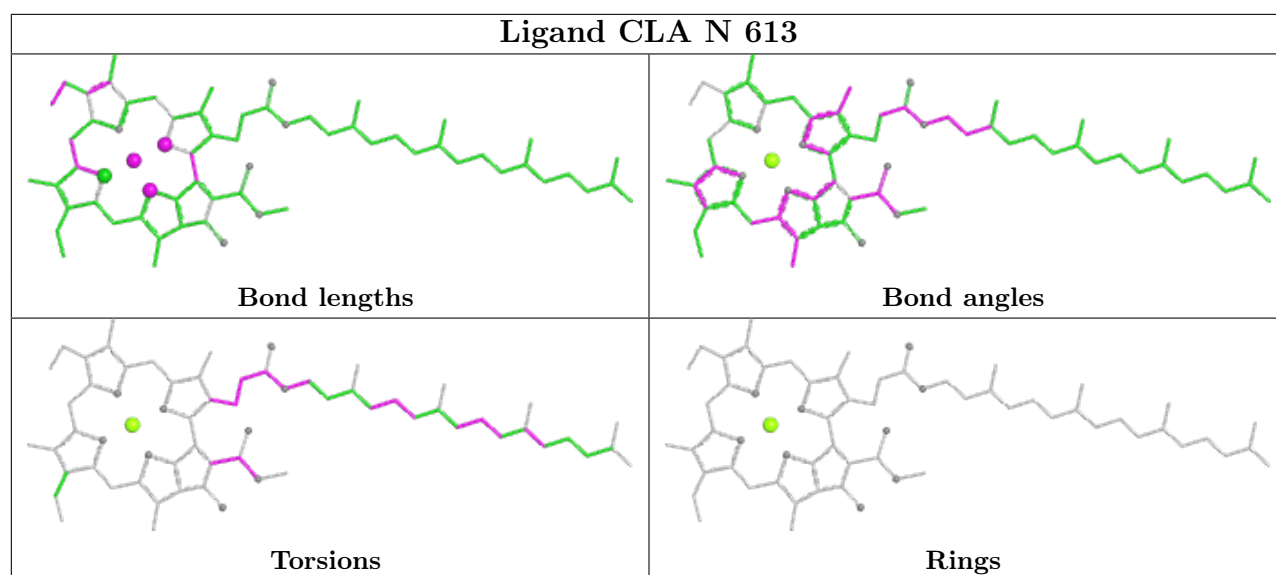
Ligand LUT Y 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

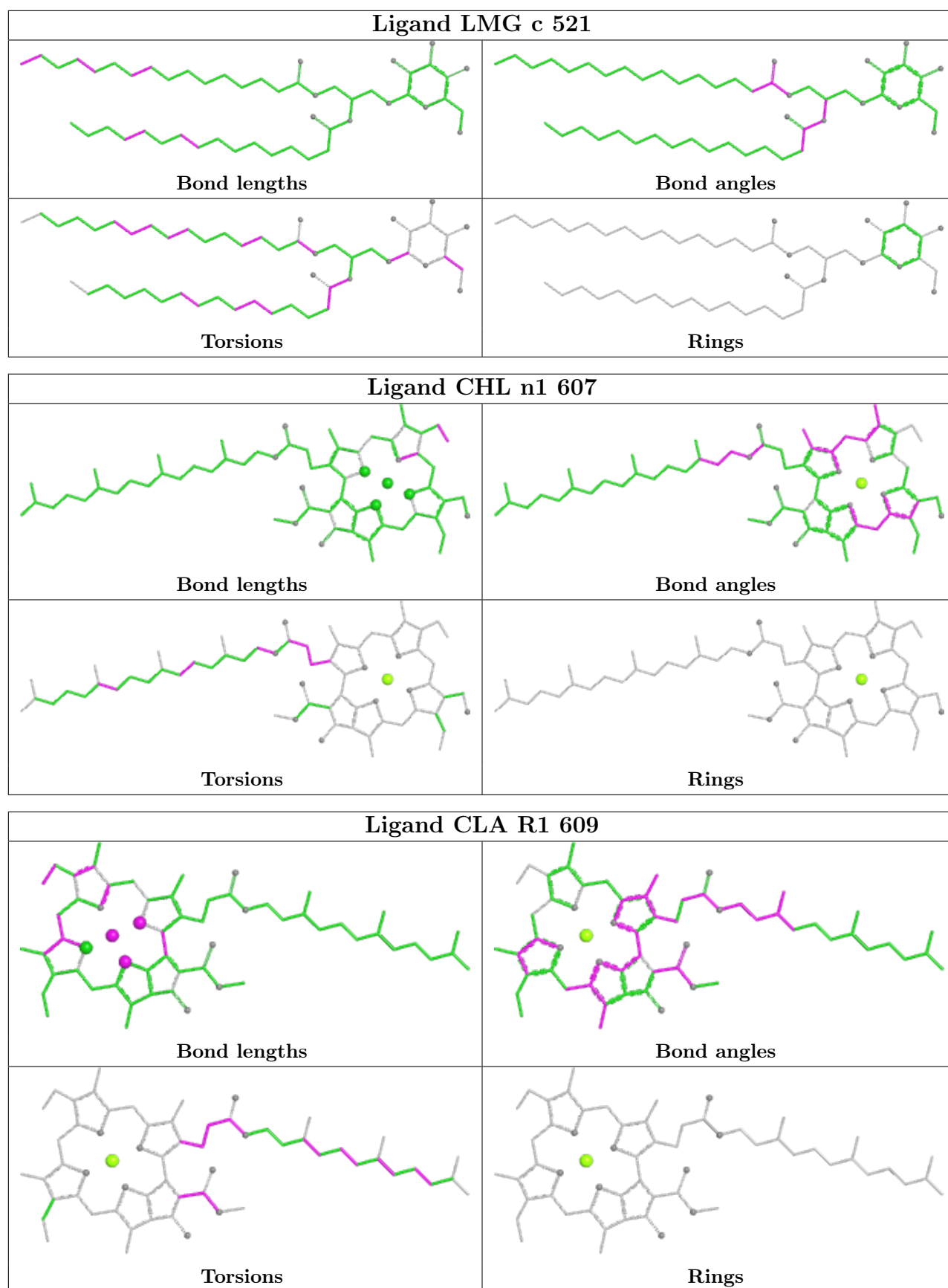


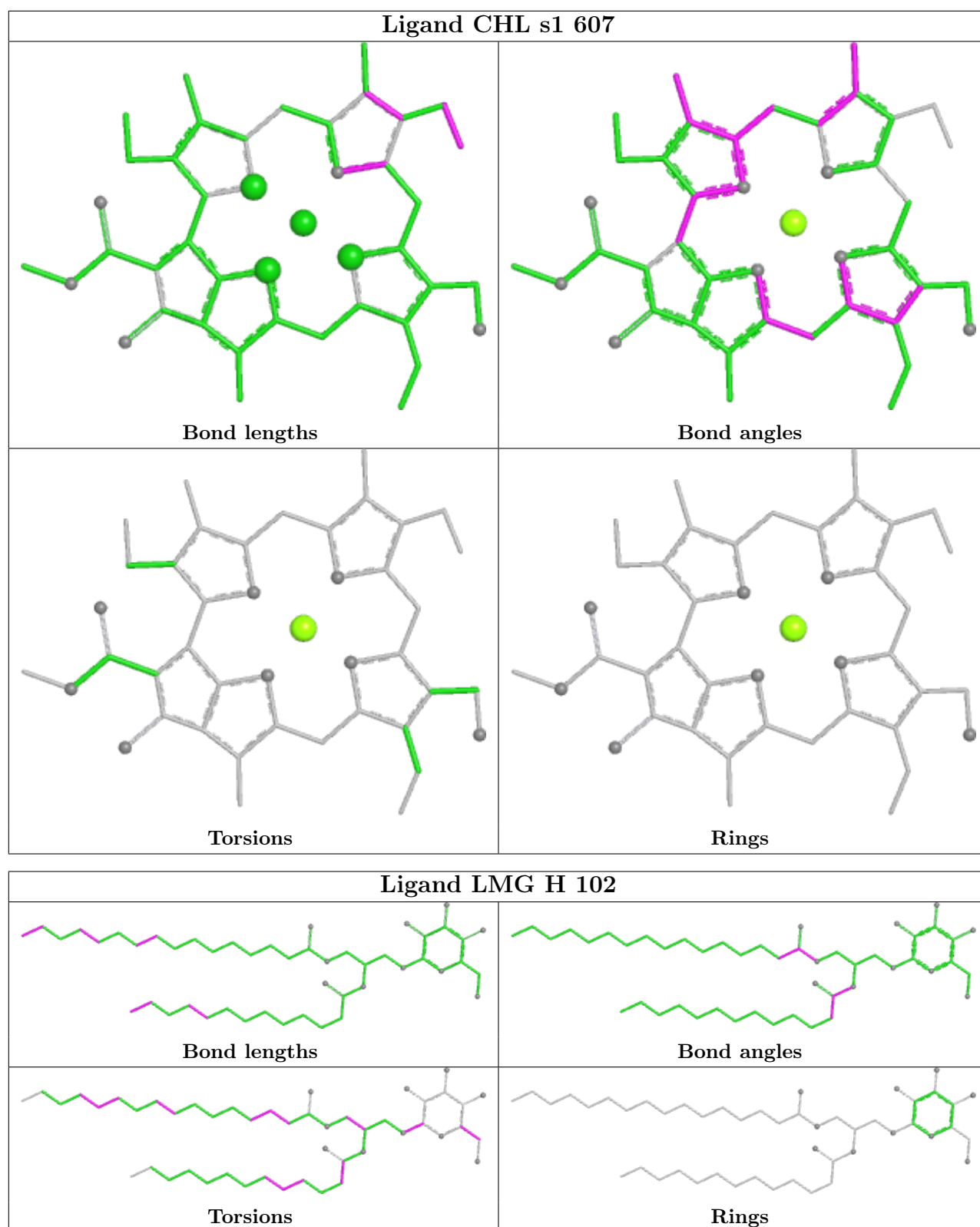
Ligand BCR A1 411	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA G1 613	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGD c 519	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

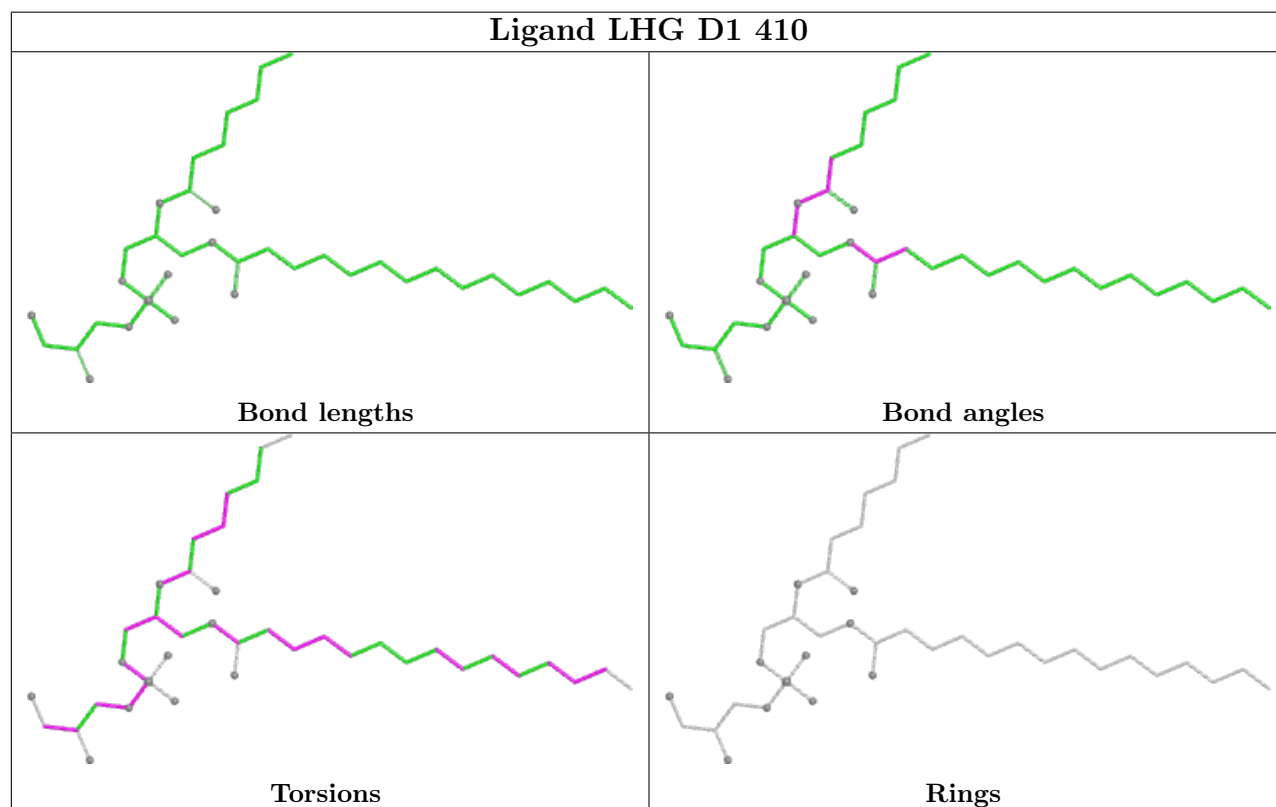
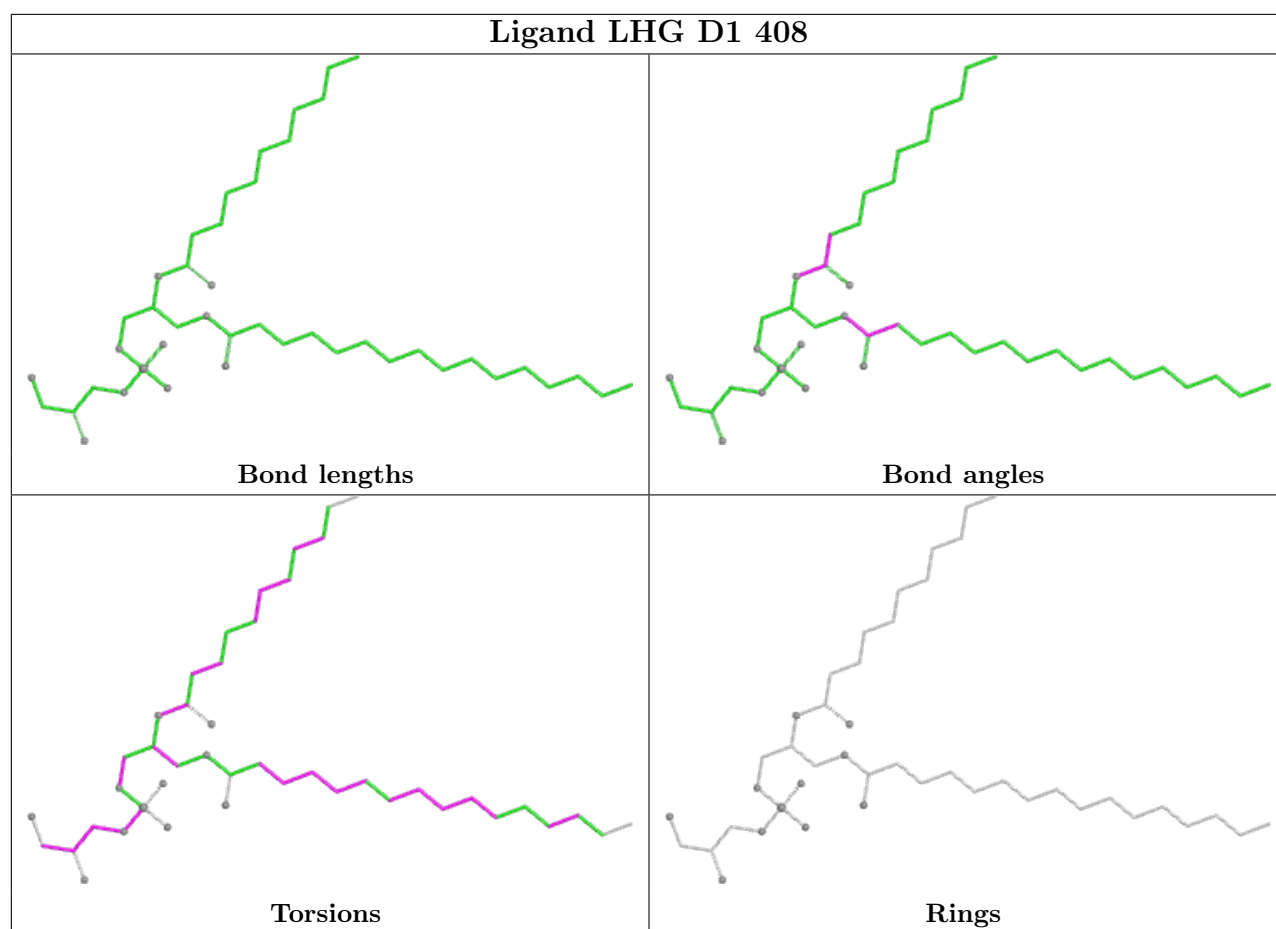


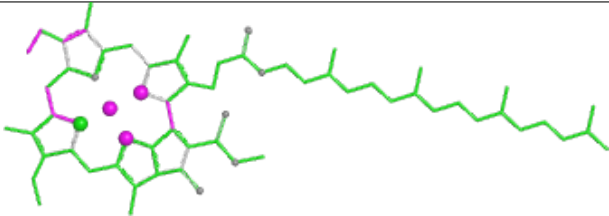
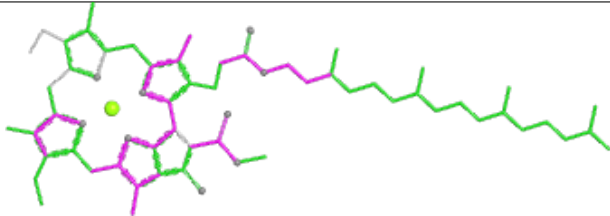
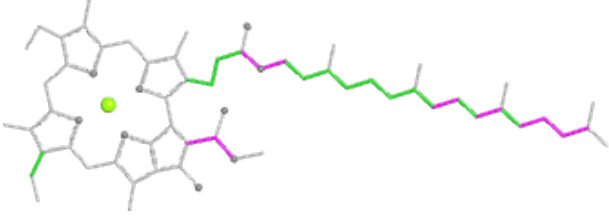
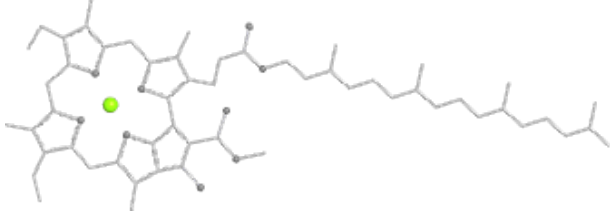


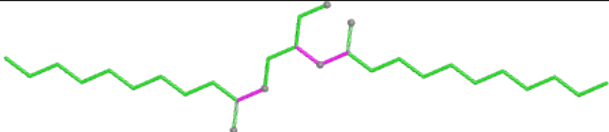
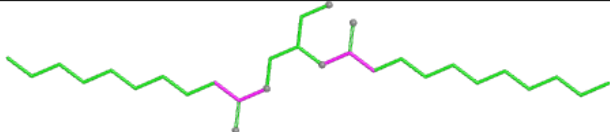
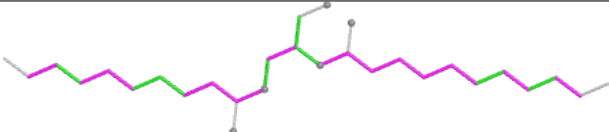
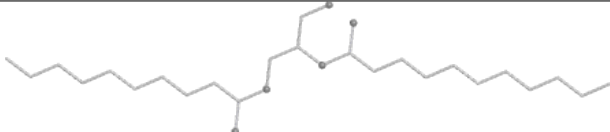


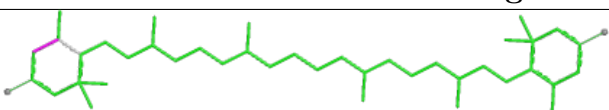
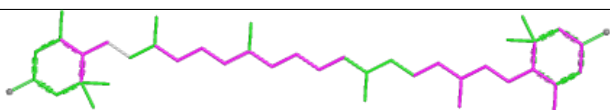
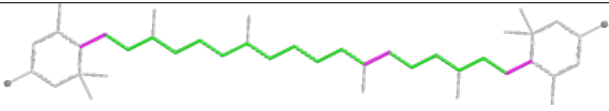
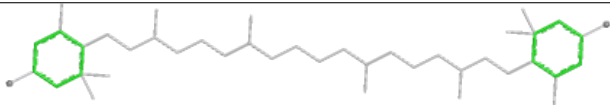


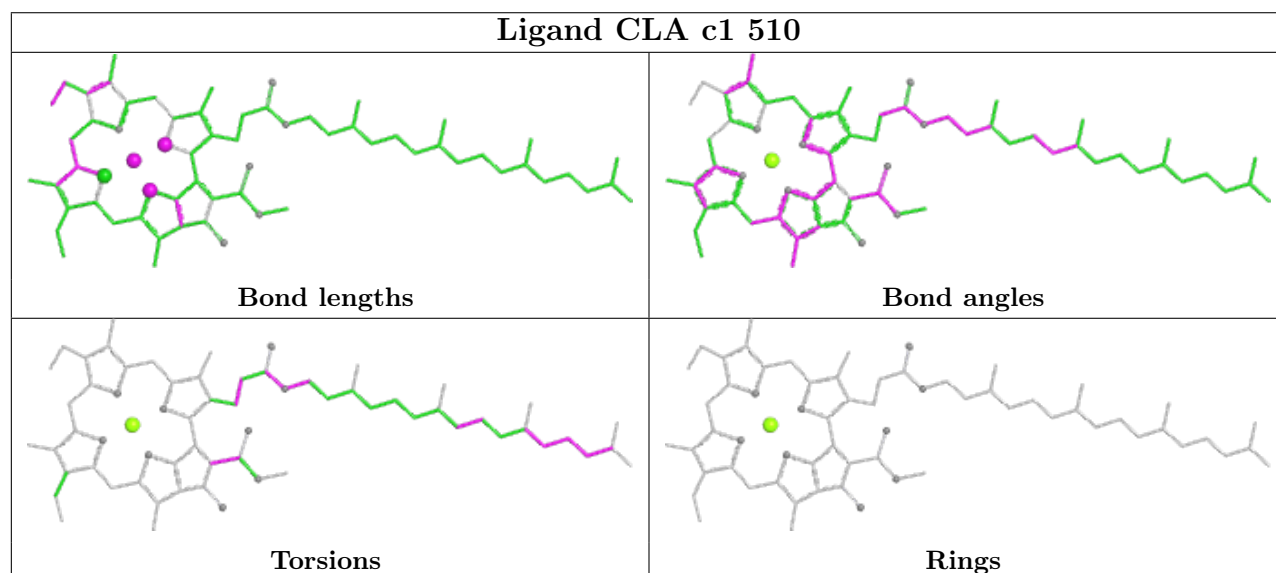
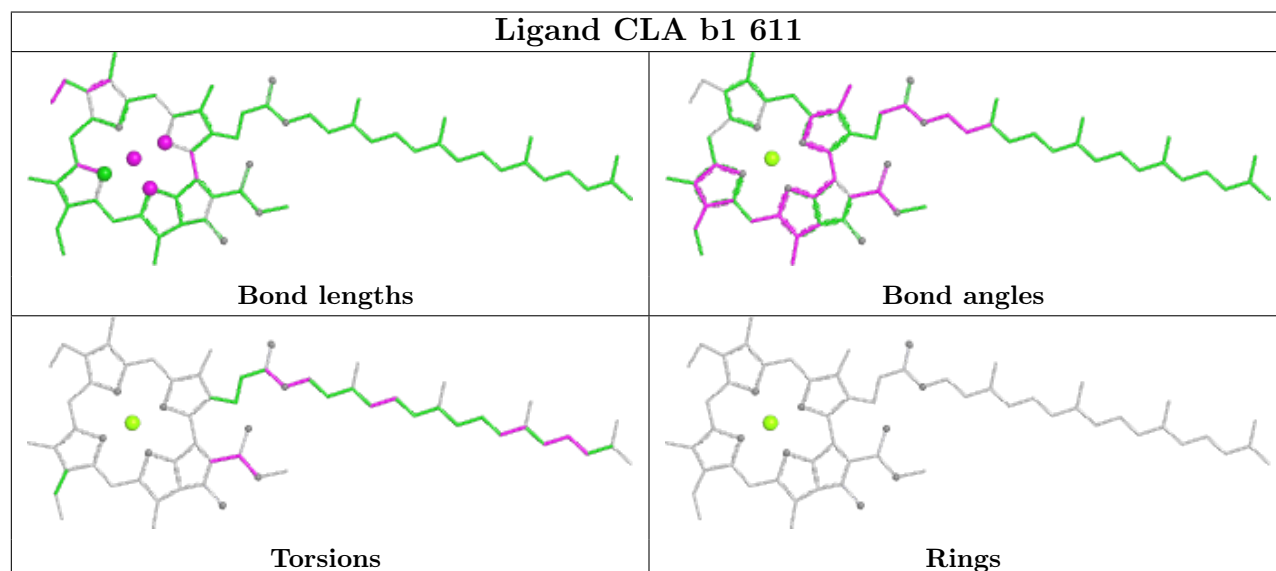
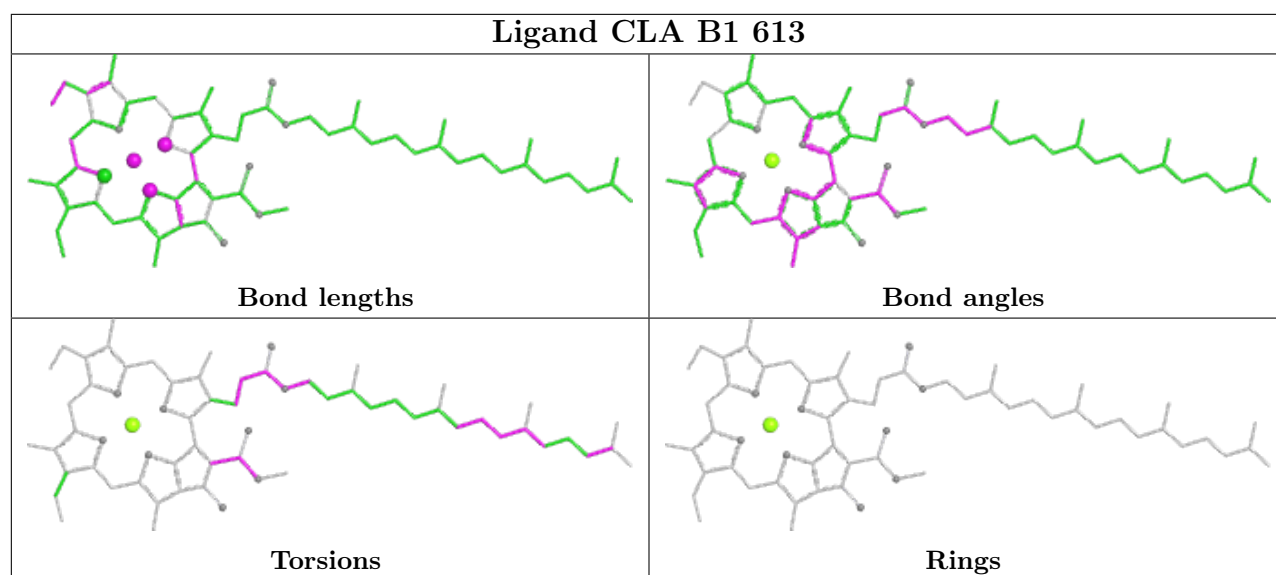


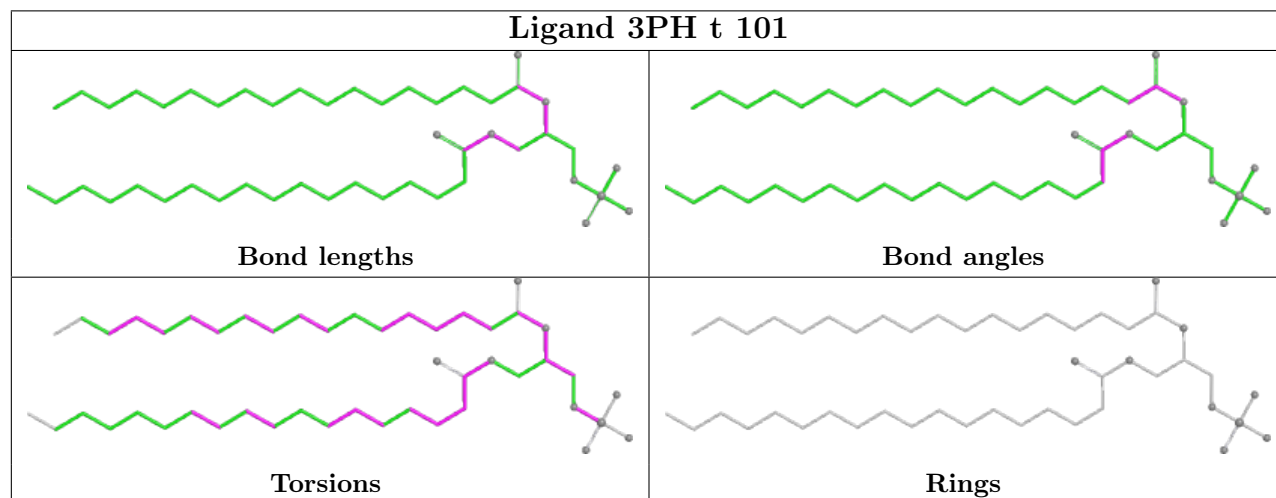
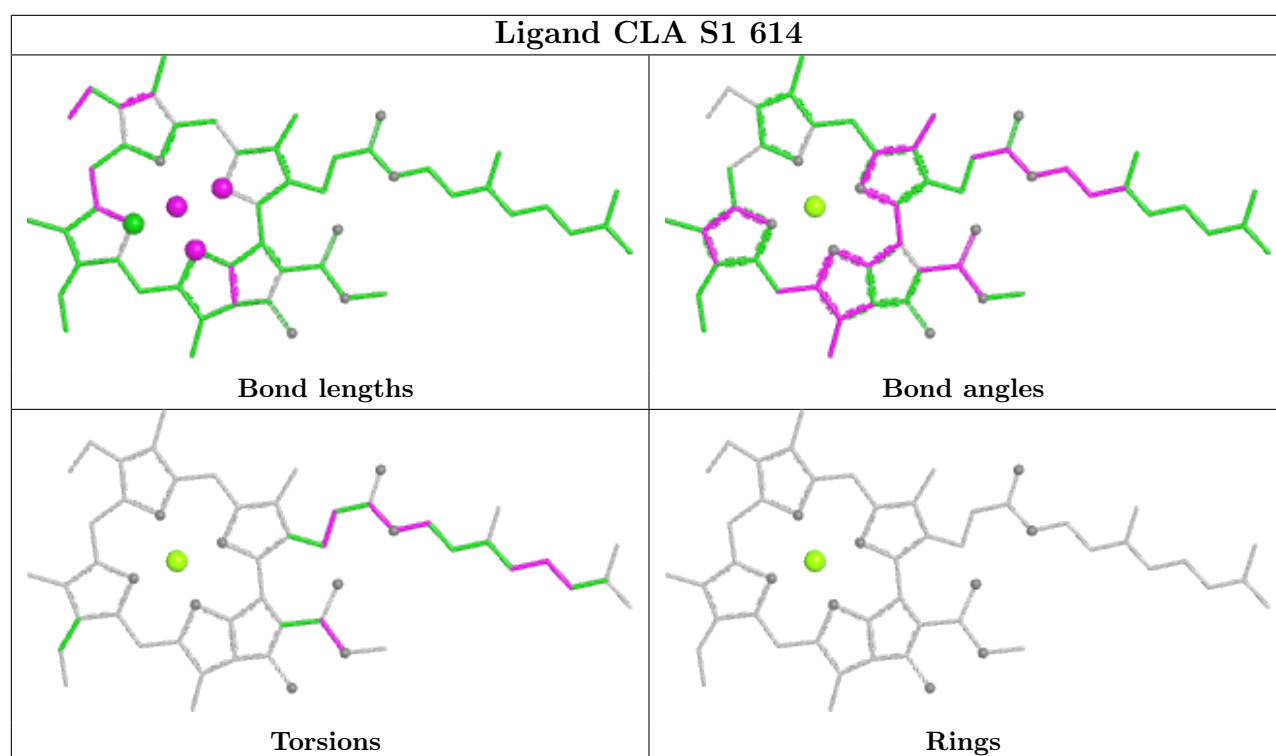
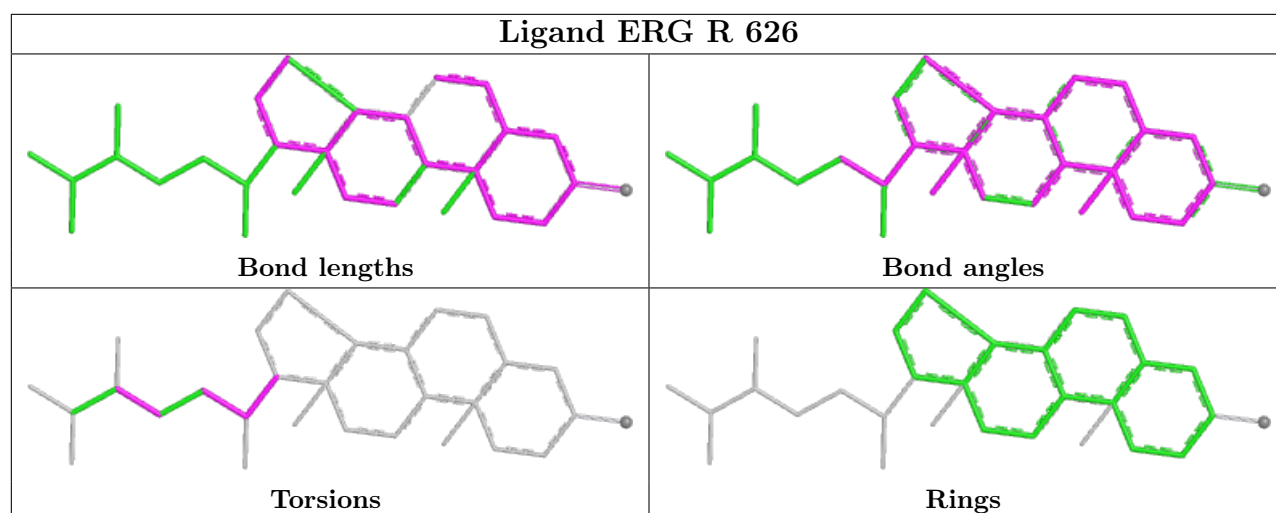


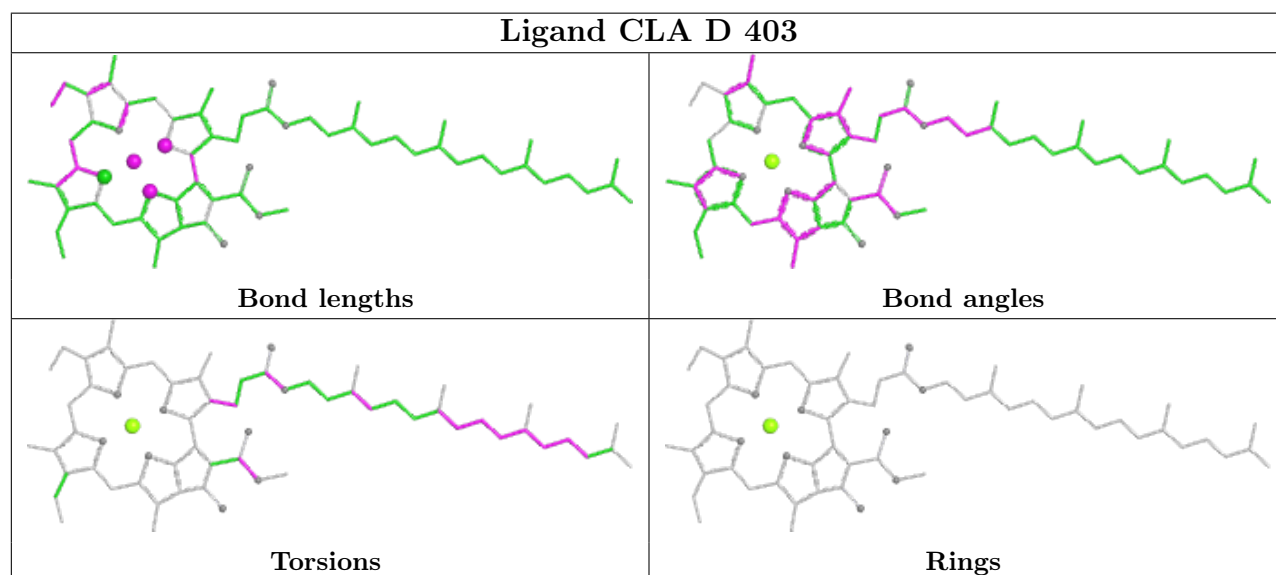
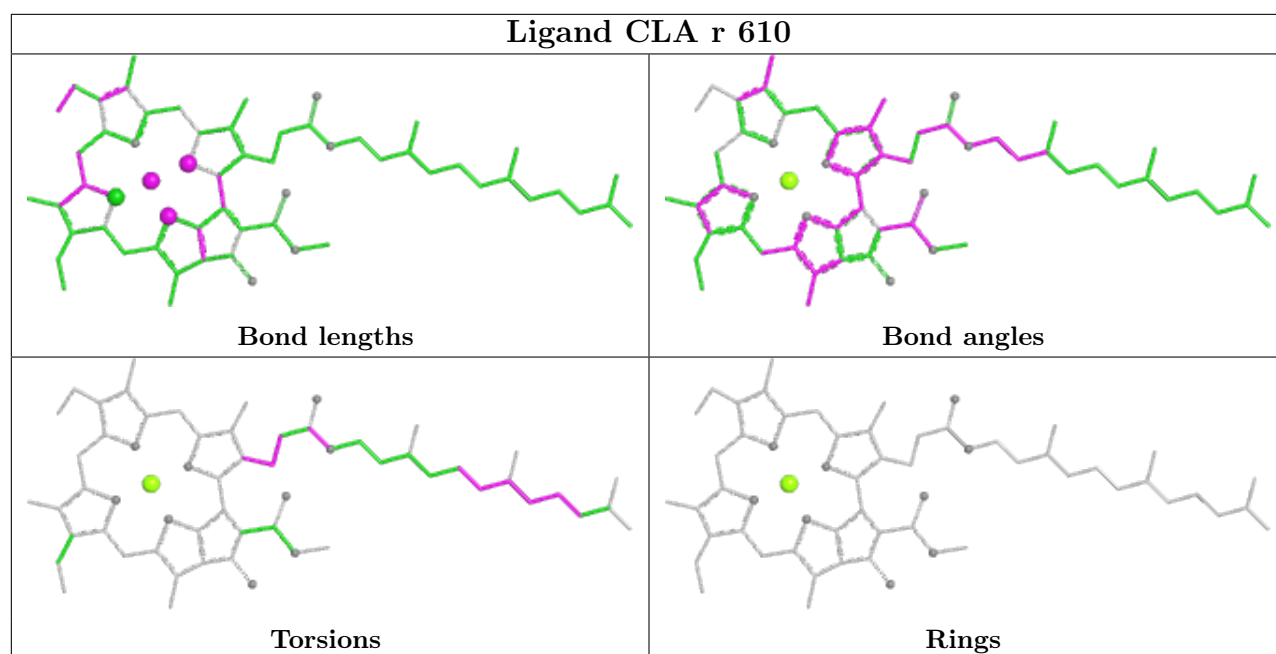
Ligand CLA B1 611	
	Bond lengths
	Bond angles
	Torsions
	Rings

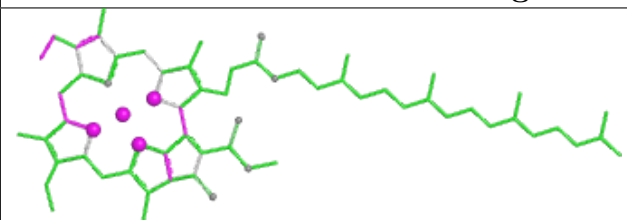
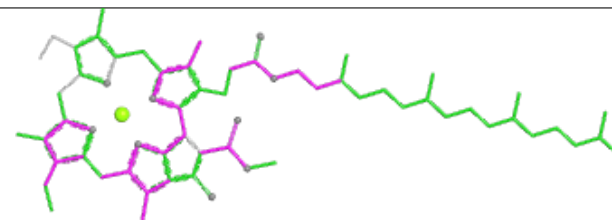
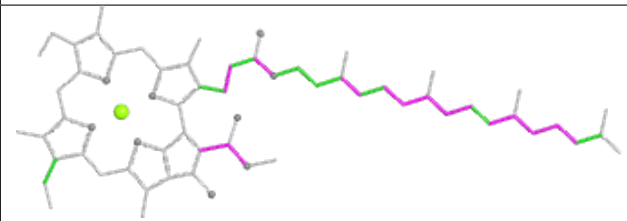
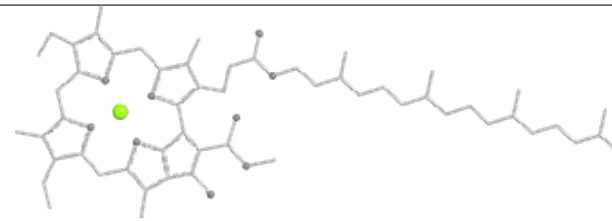
Ligand DGA j1 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

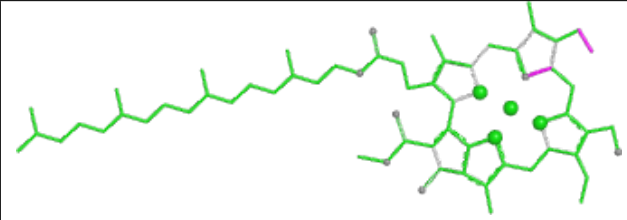
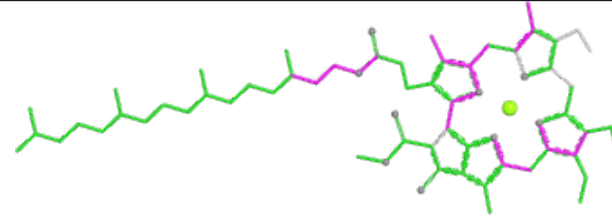
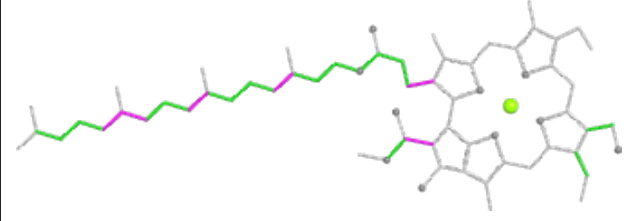
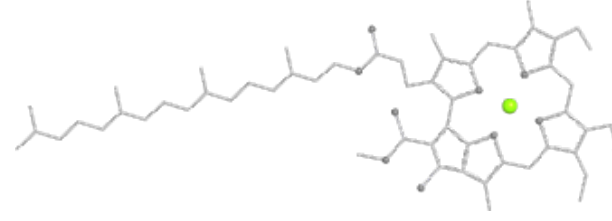
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	Bond lengths
	Bond angles
	Torsions
	Rings

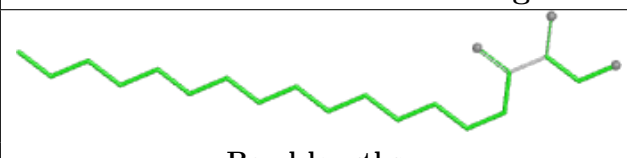
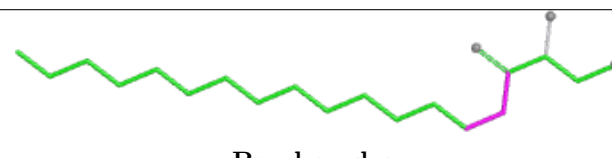
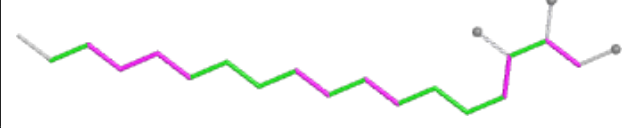
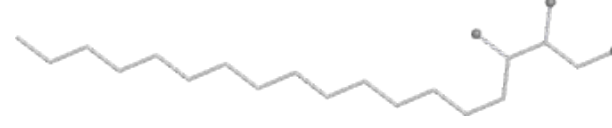


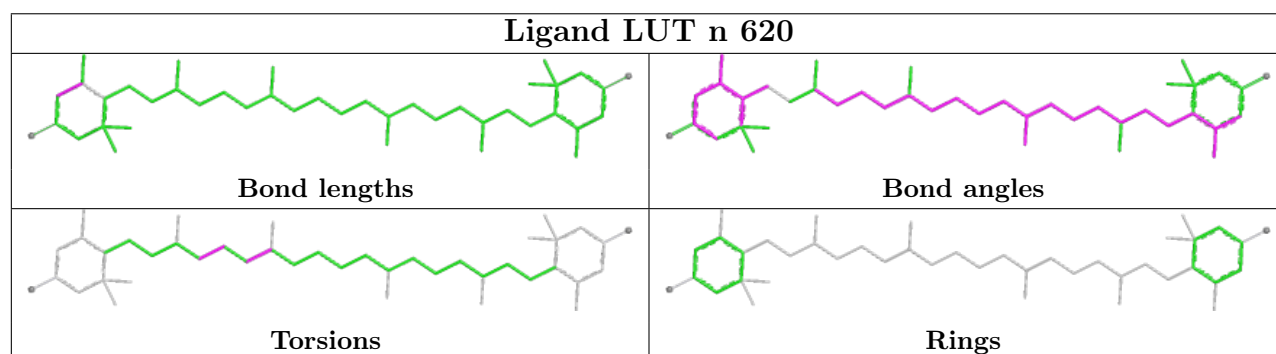
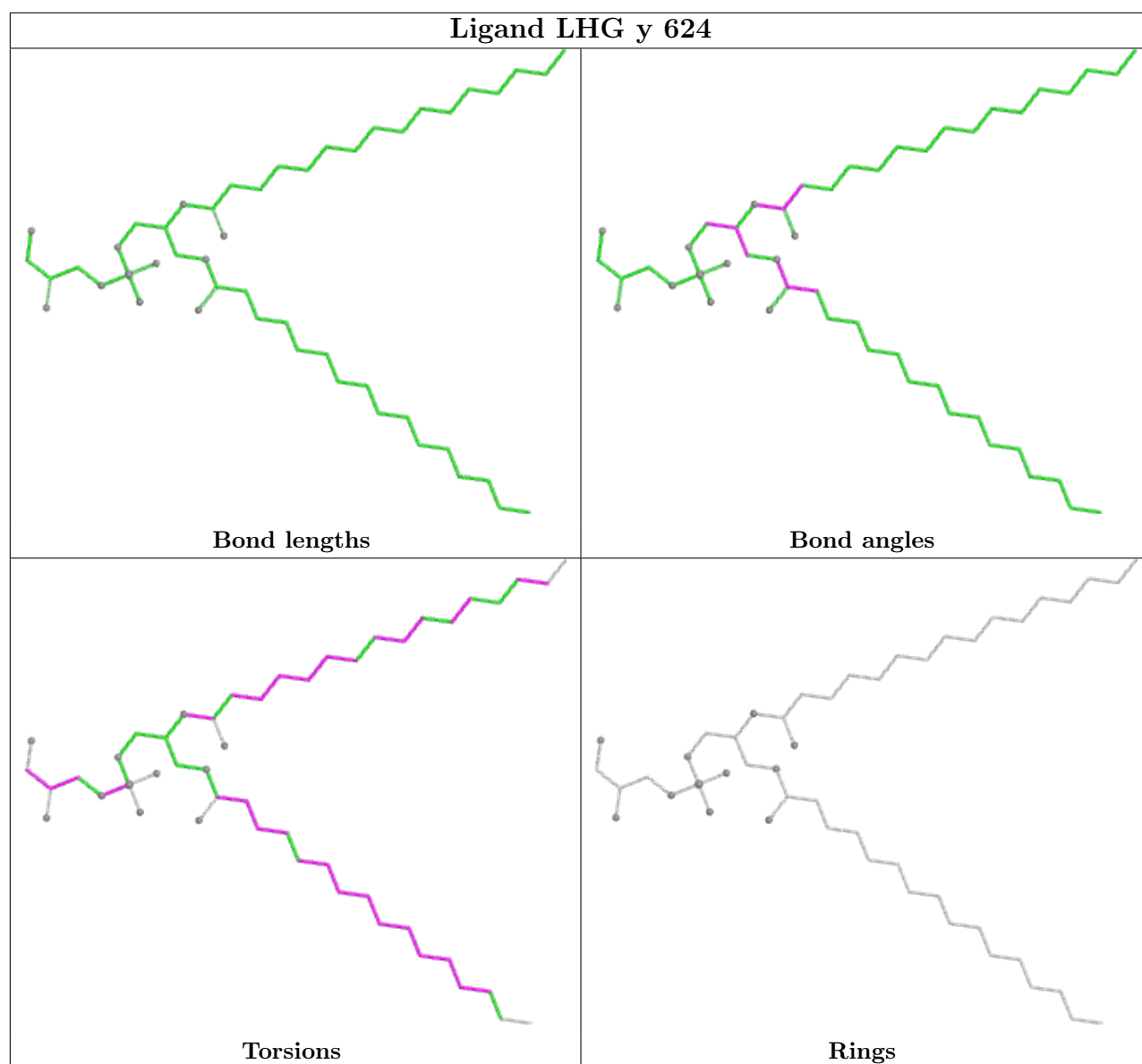


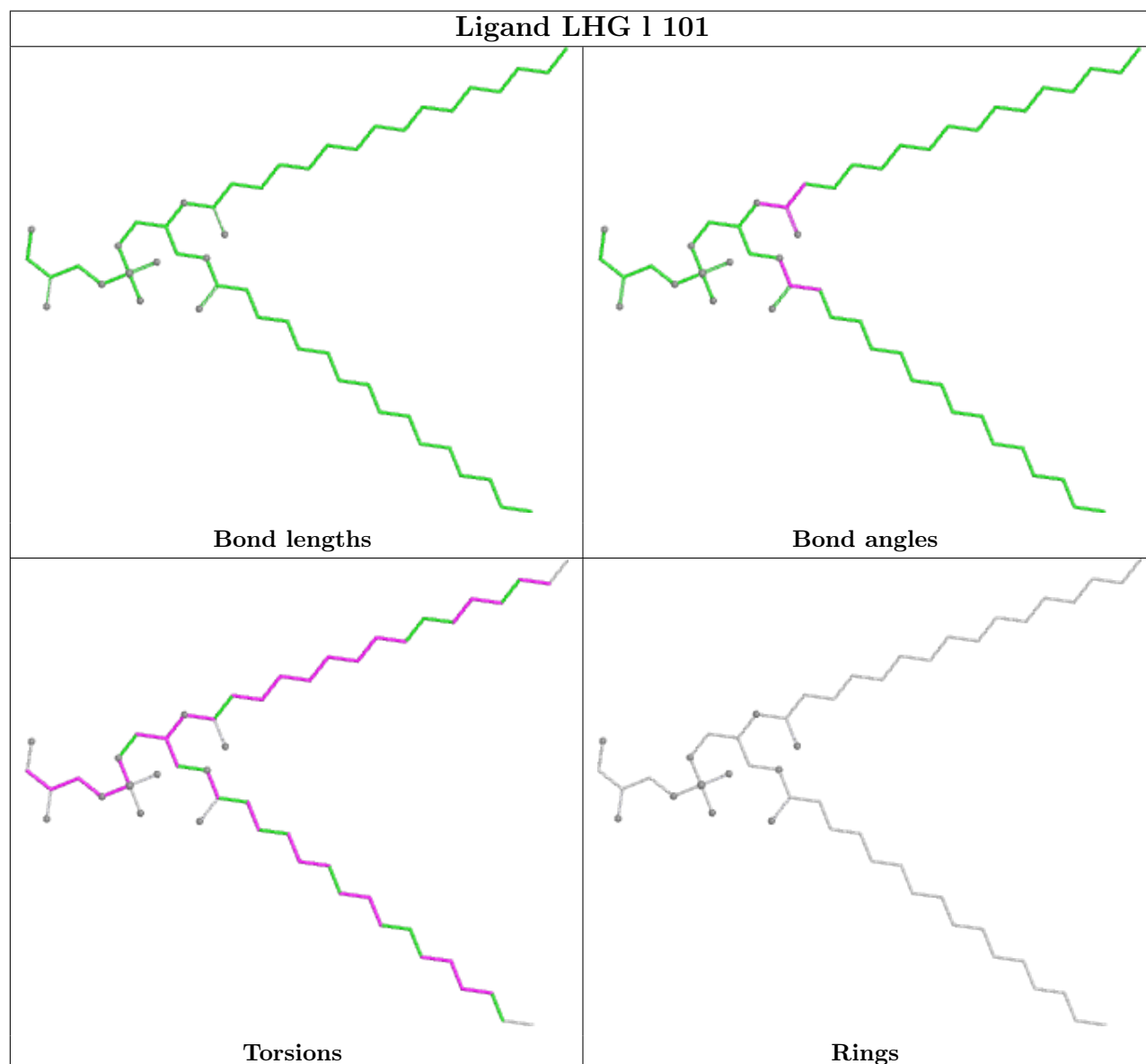
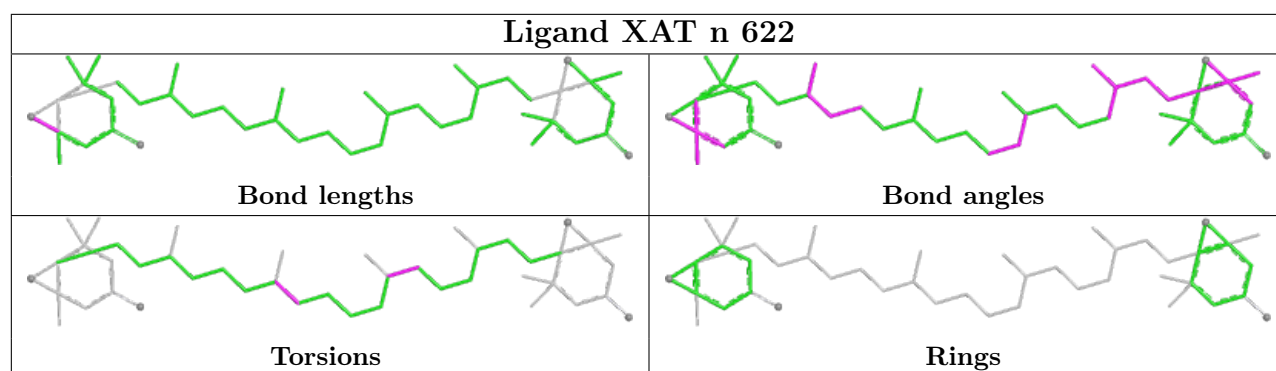


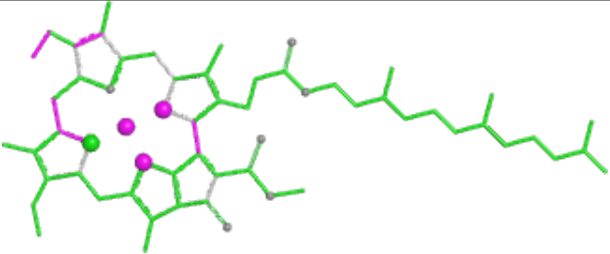
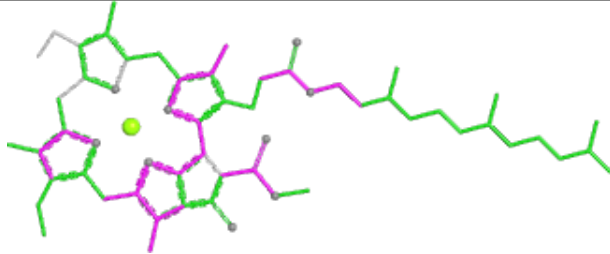
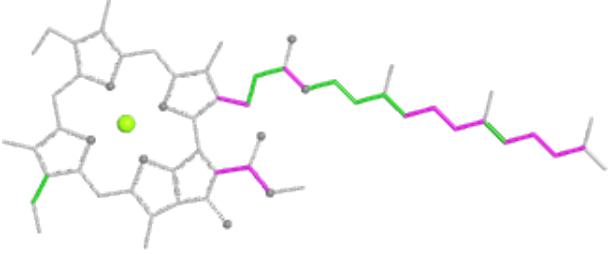
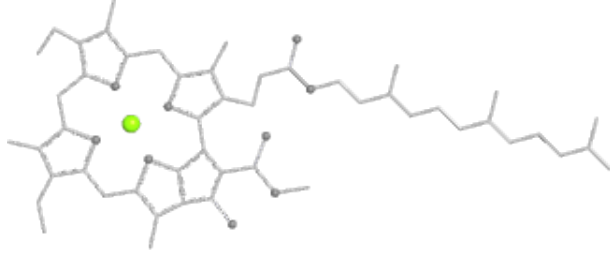
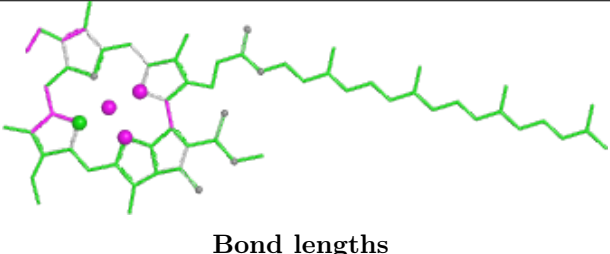
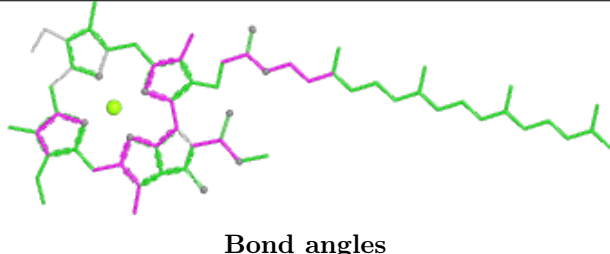
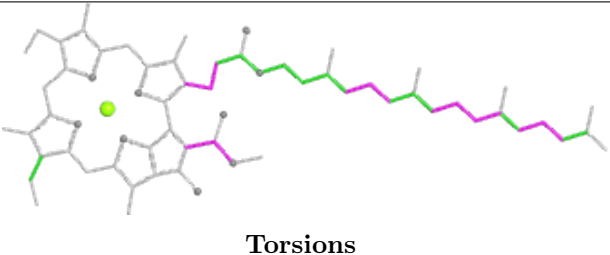
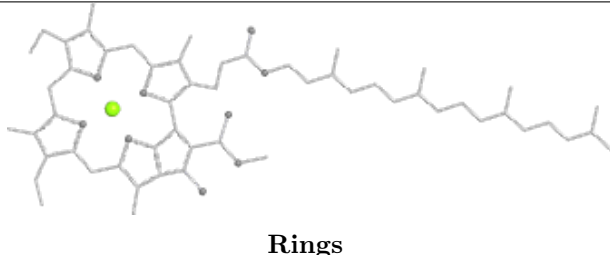
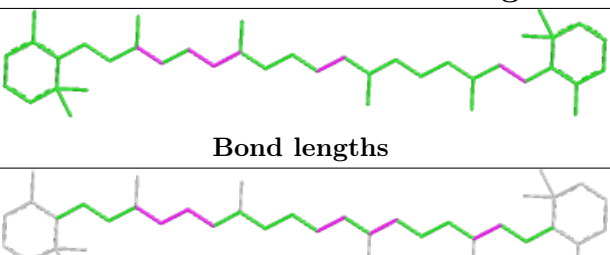
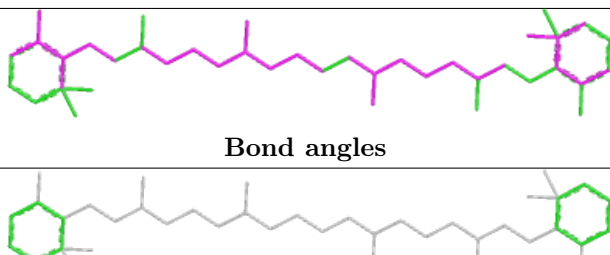
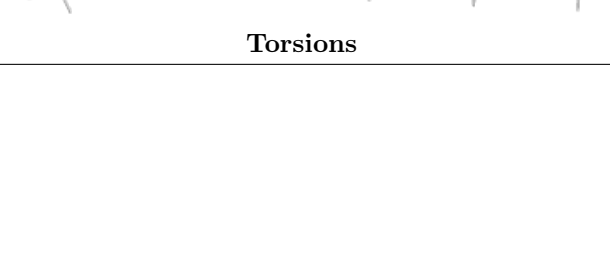
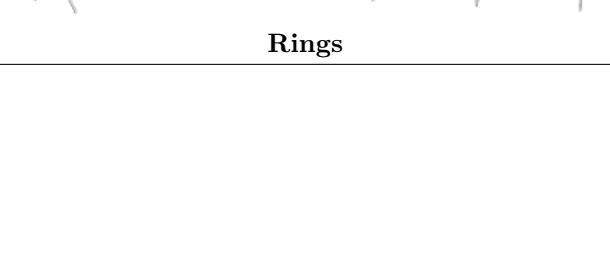
Ligand CLA Y1 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

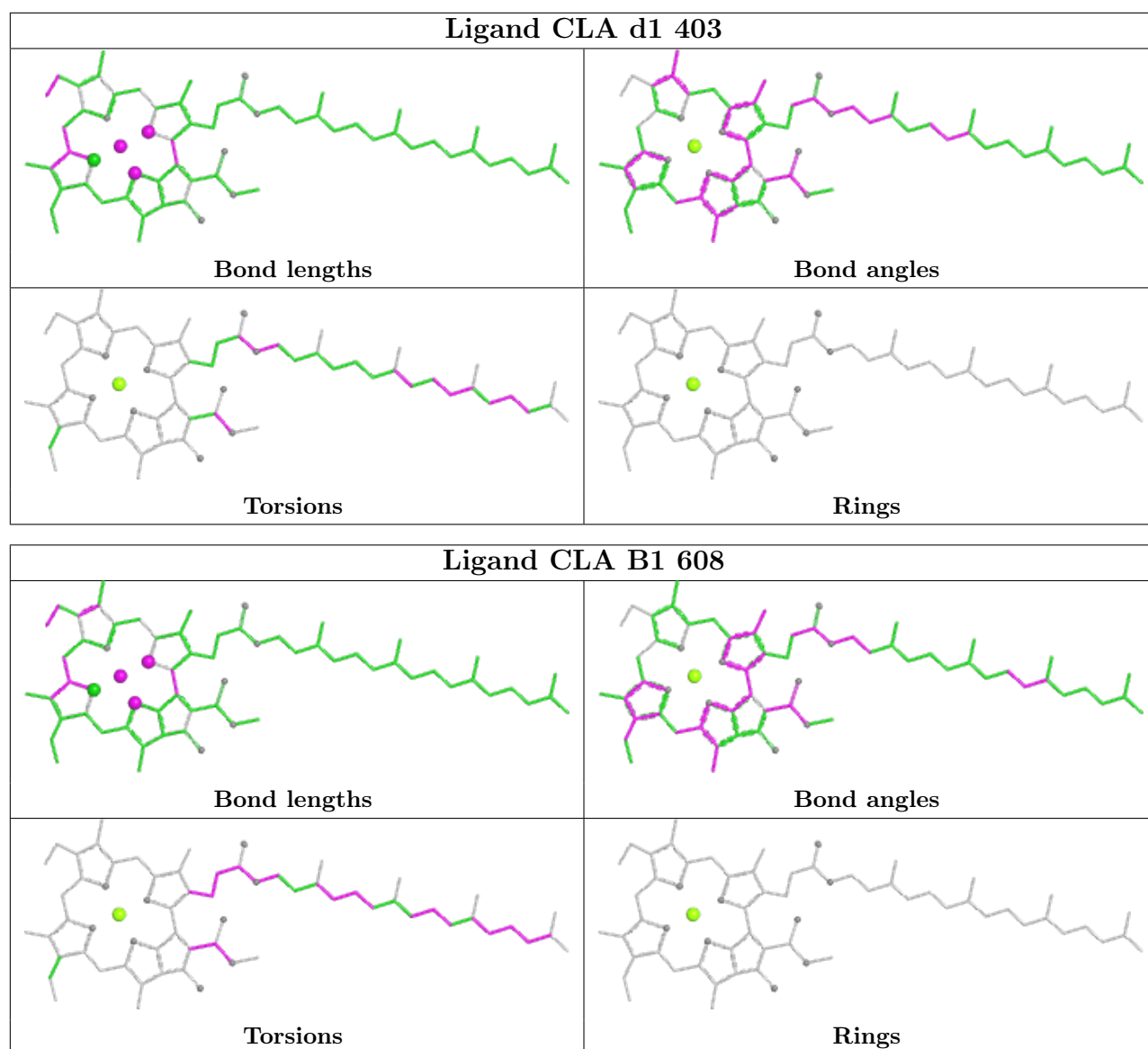
Ligand CHL n1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

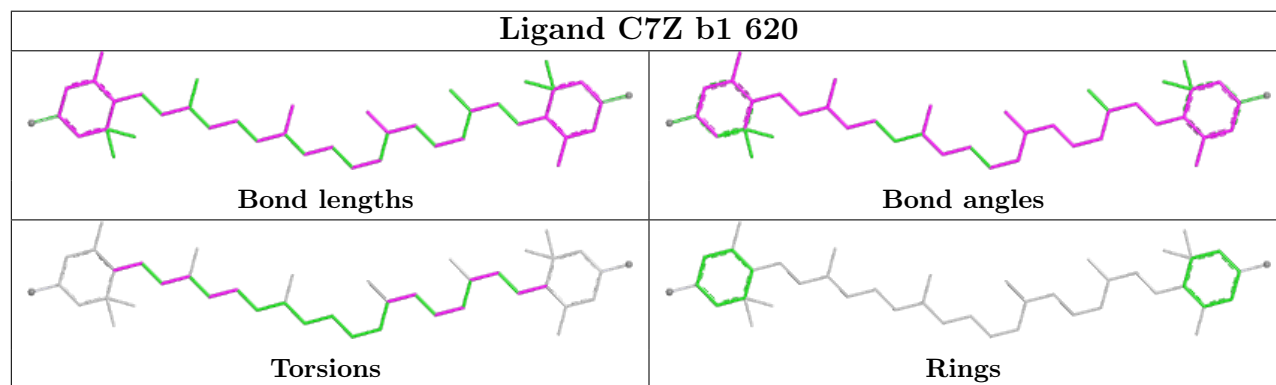
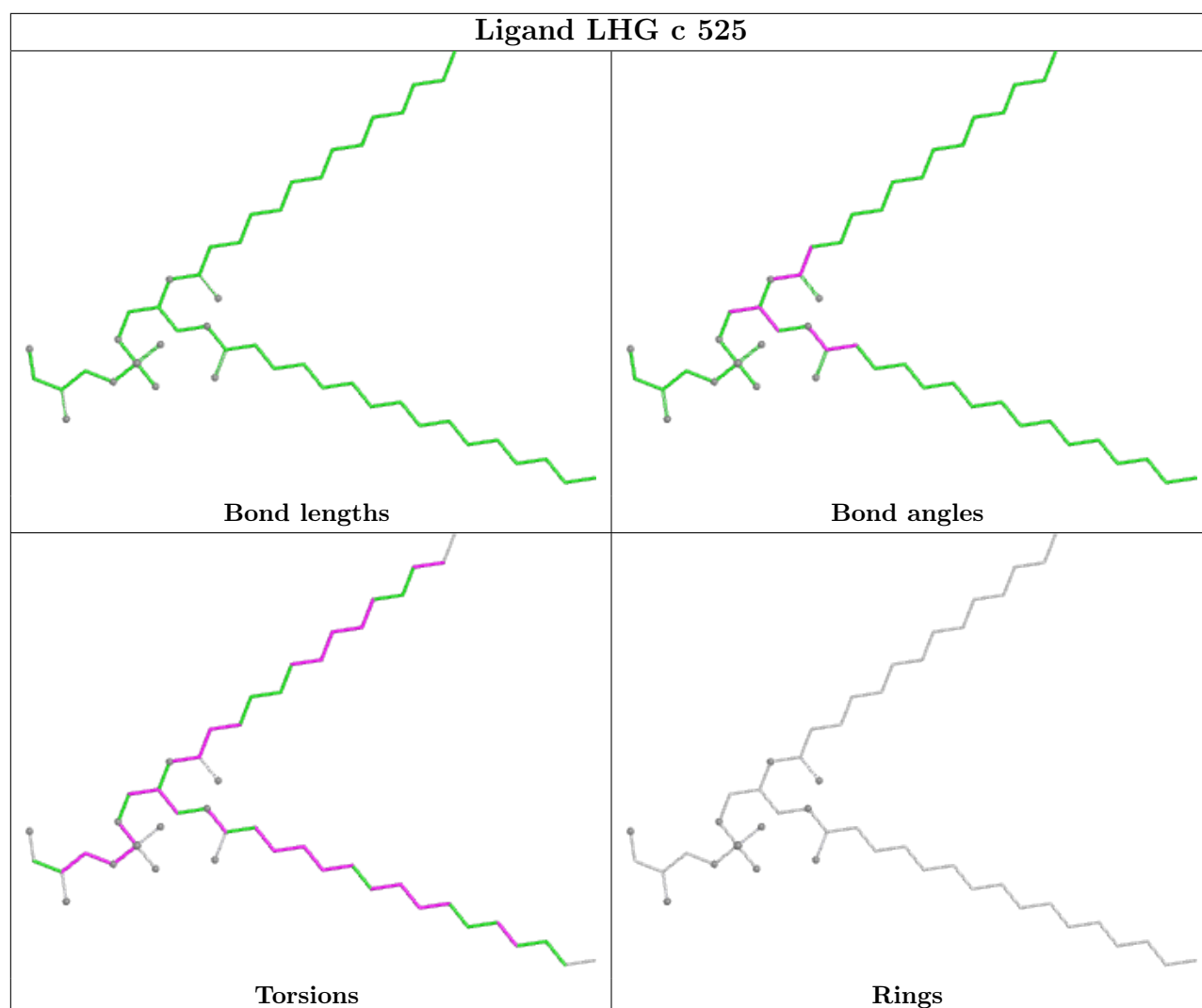
Ligand SPH Y1 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

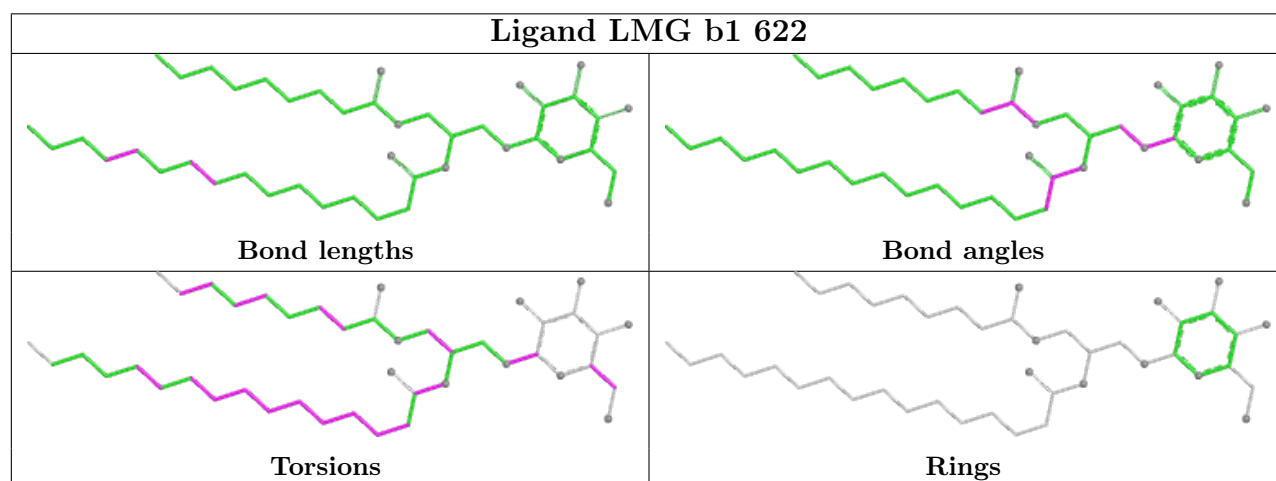
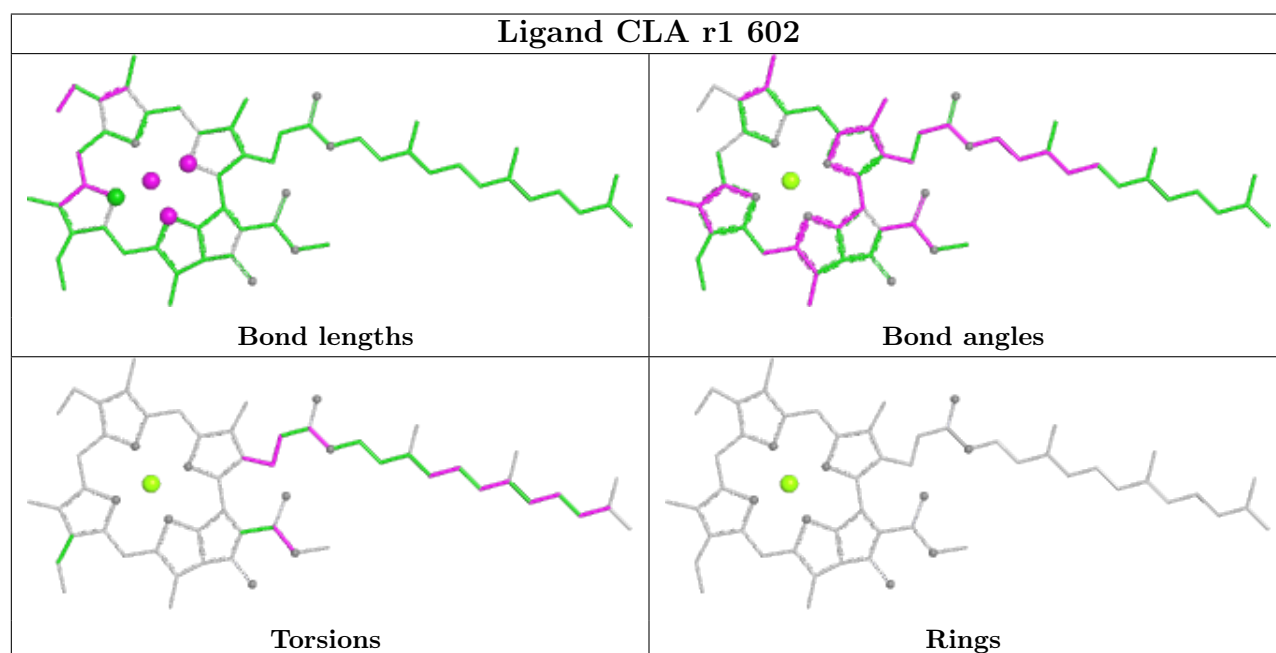
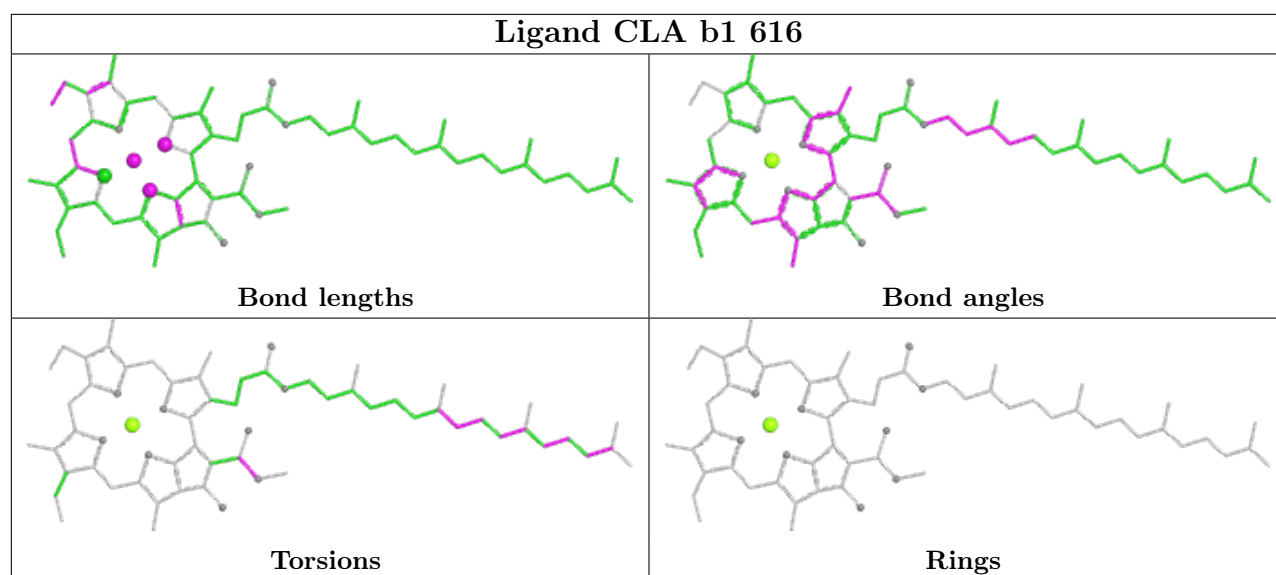


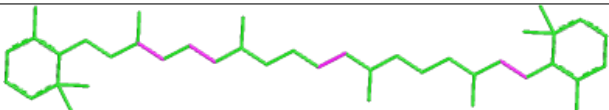
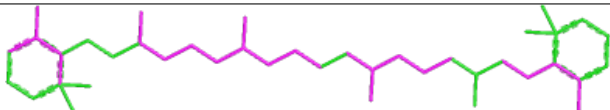
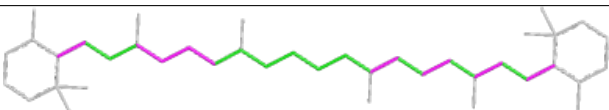
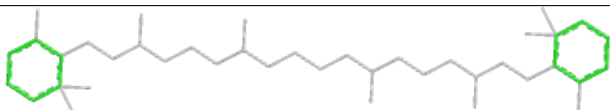


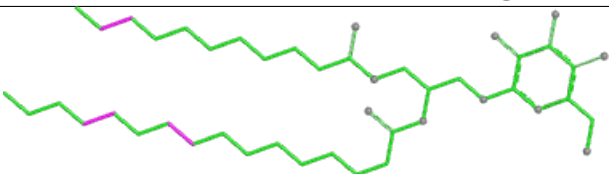
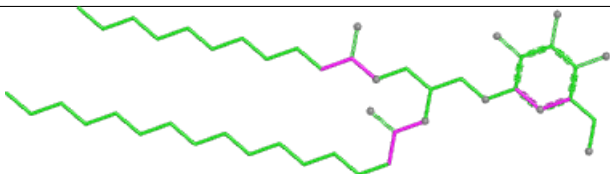
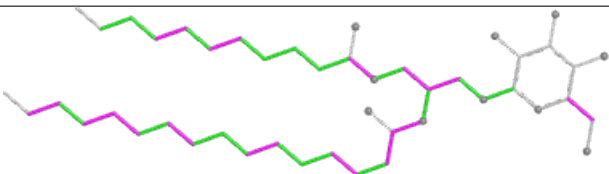
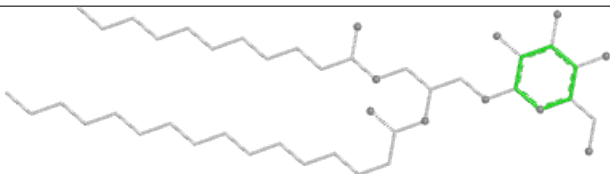
Ligand CLA r1 608	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA s 611	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c1 517	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

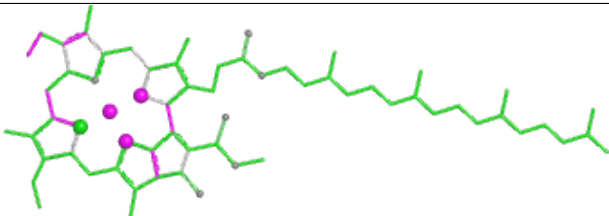
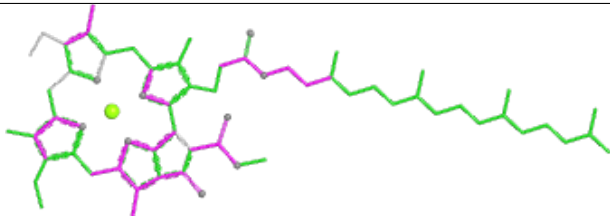
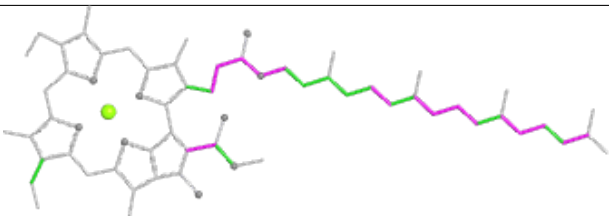
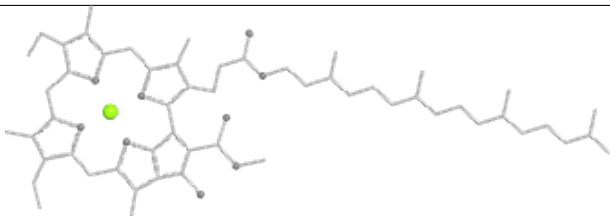


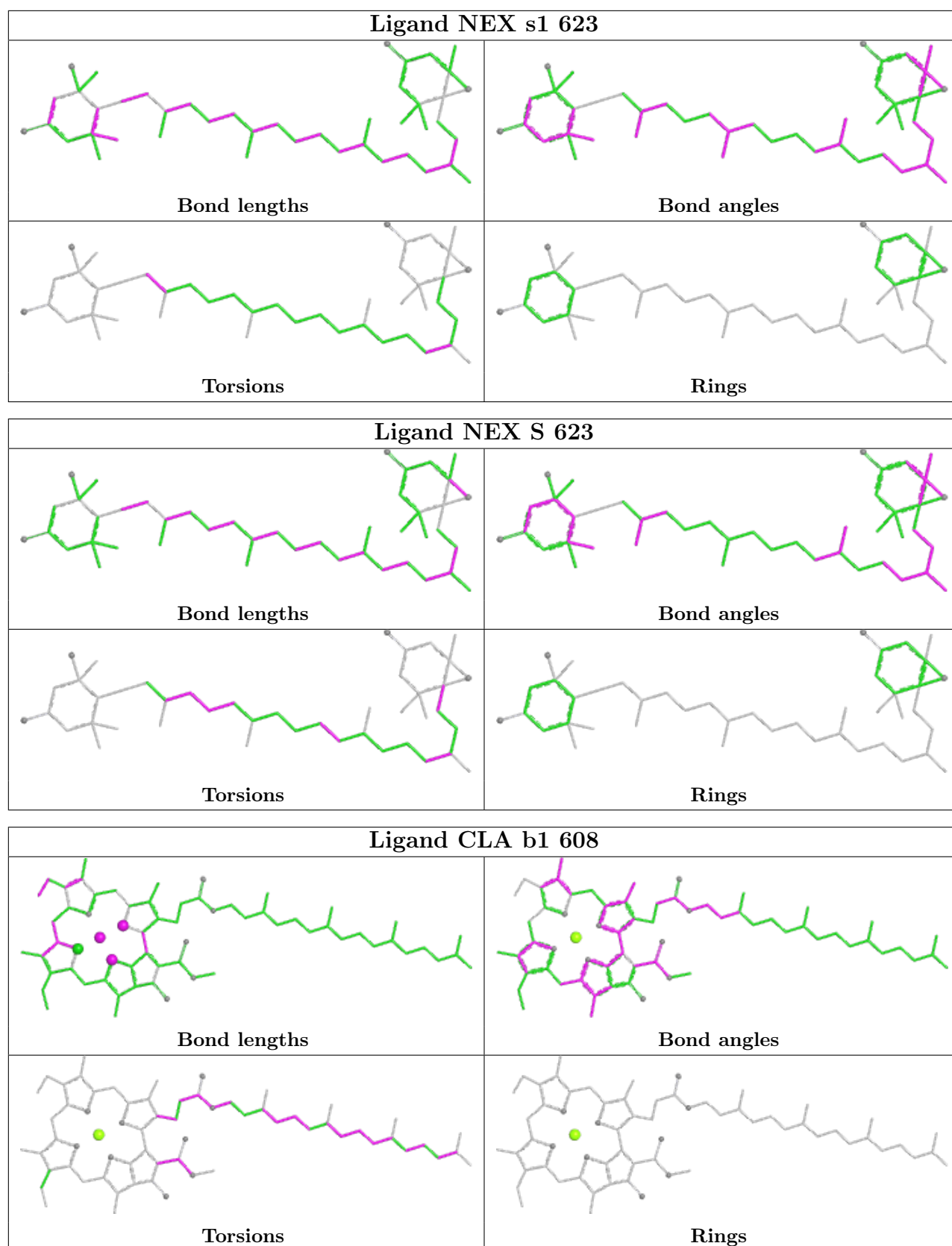


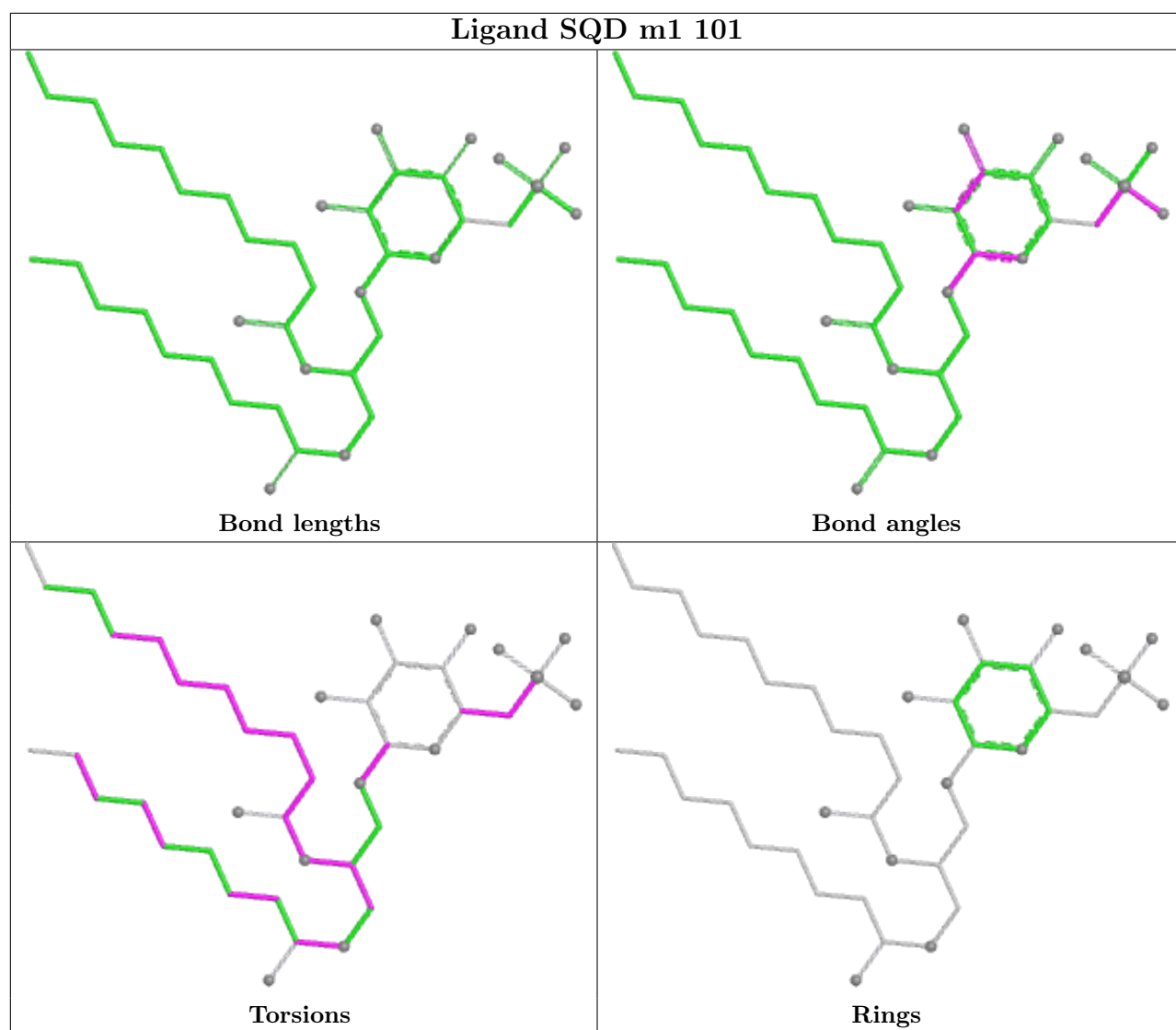


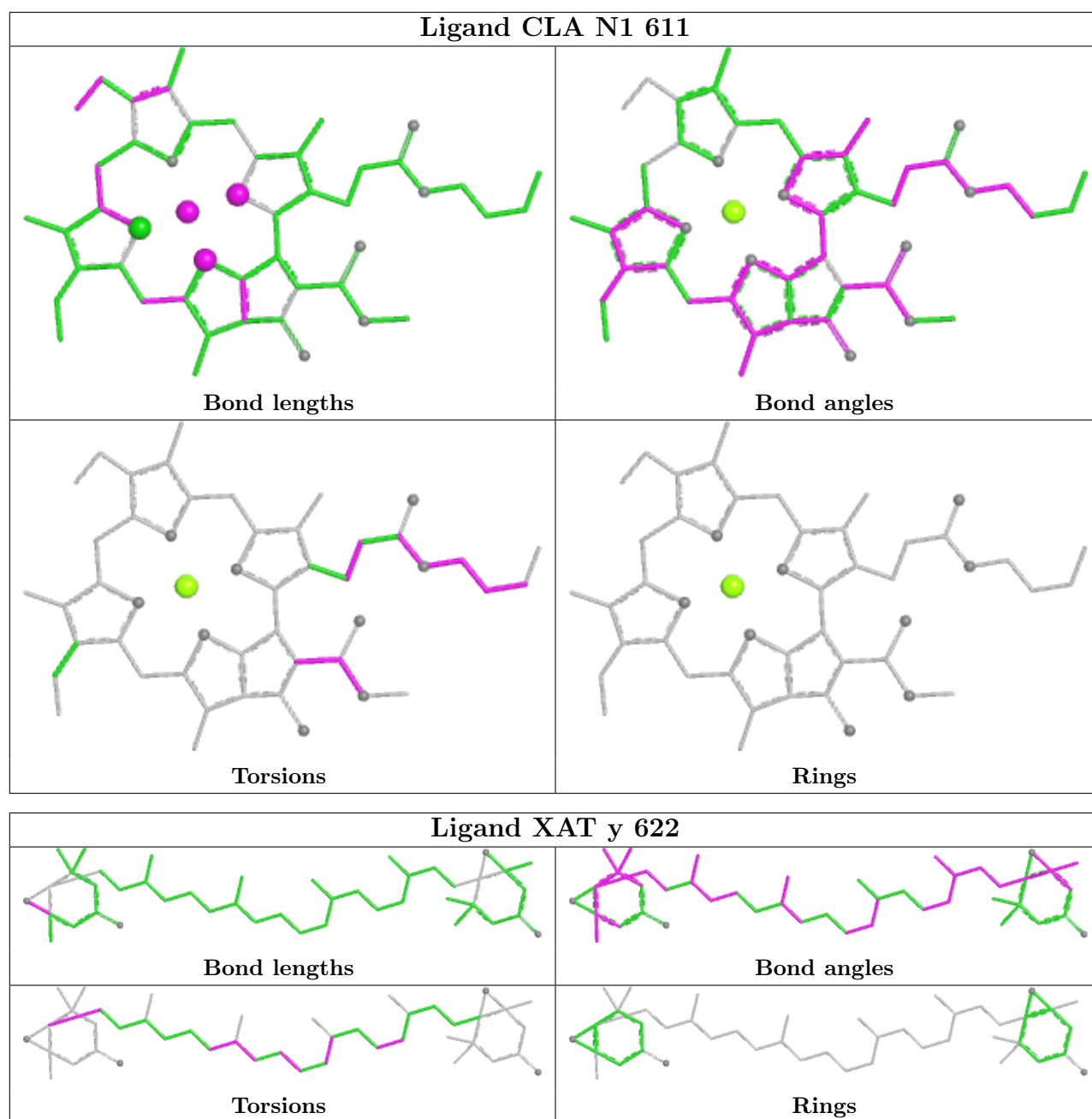
Ligand BCR d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

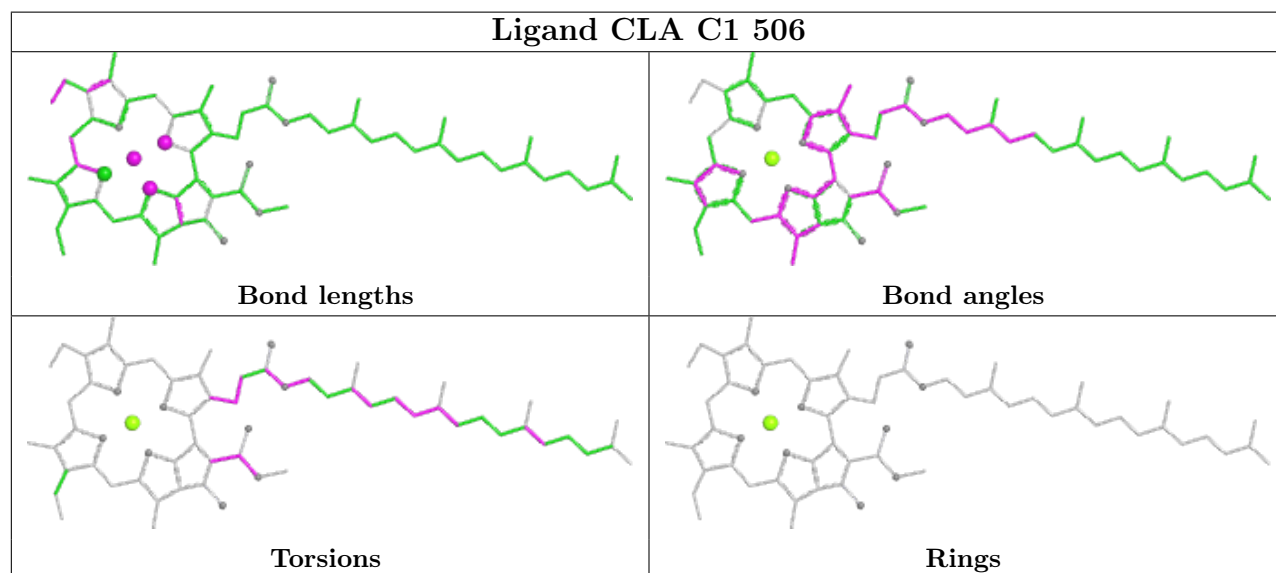
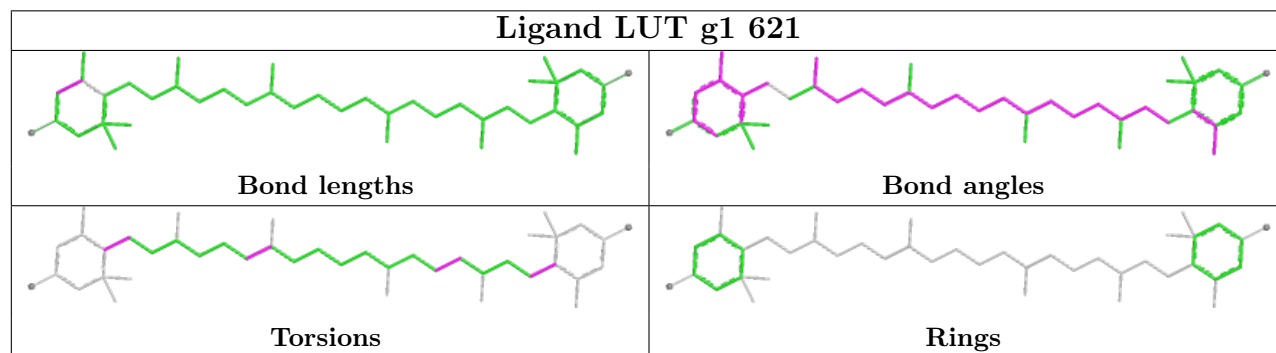
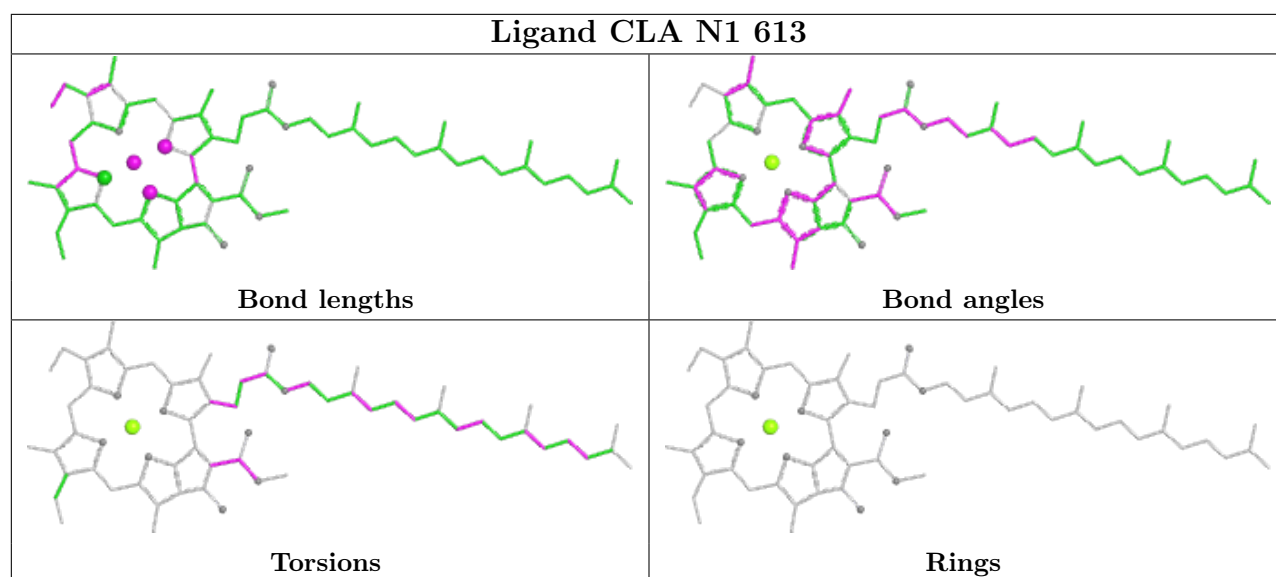
Ligand LMG d1 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

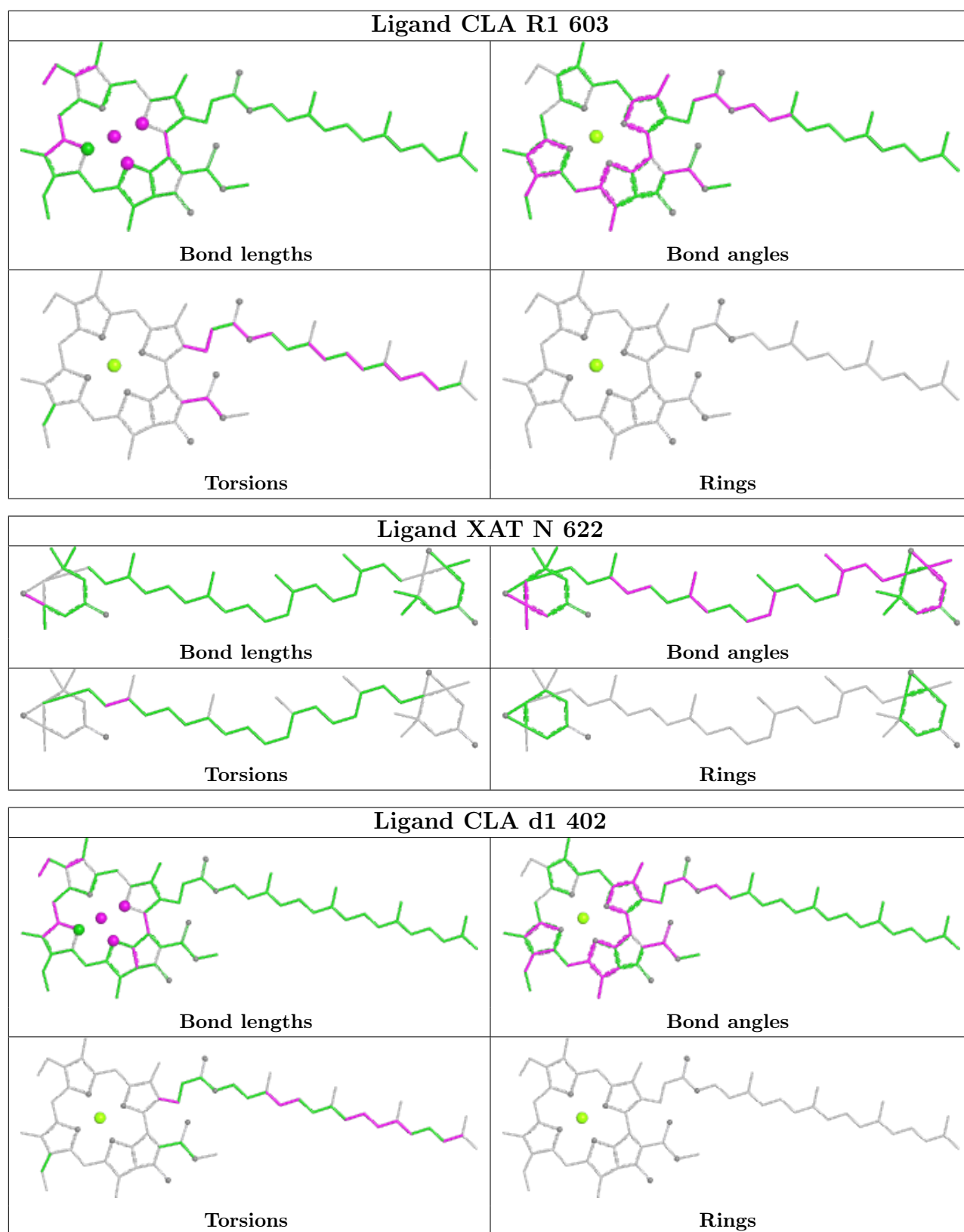
Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

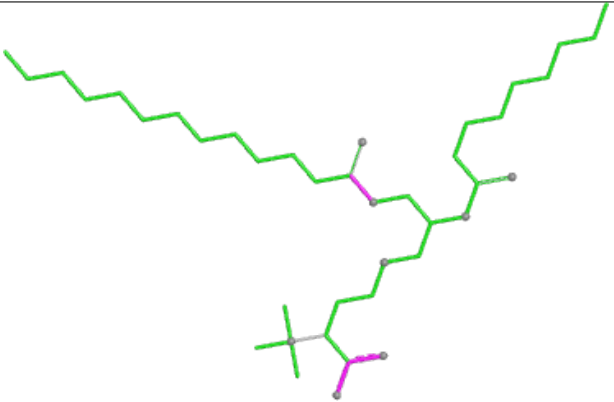
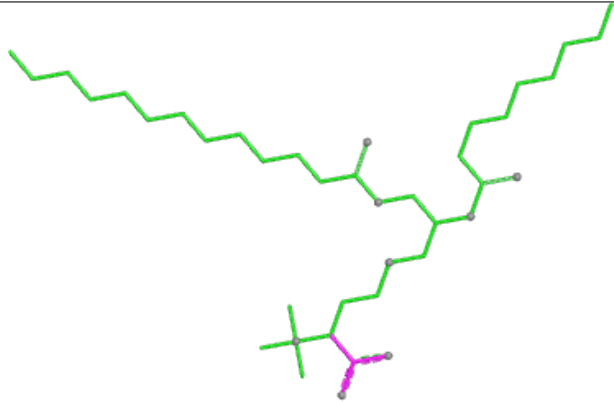
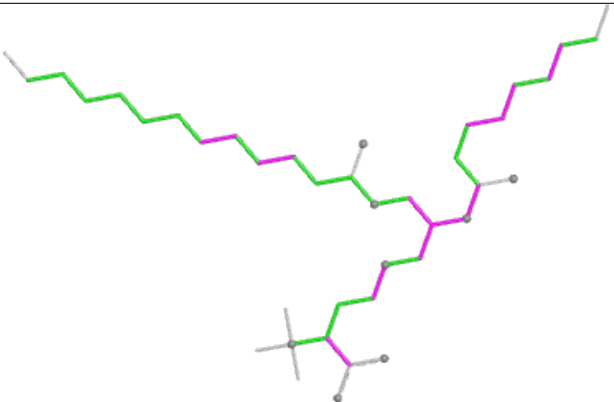
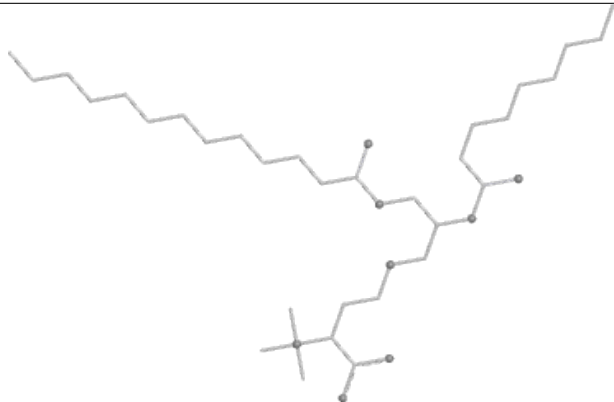


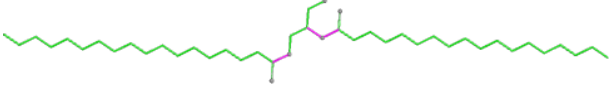
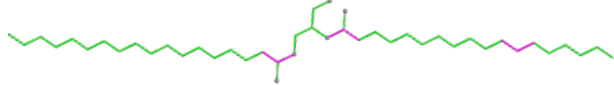
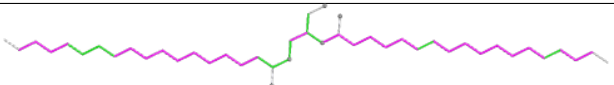
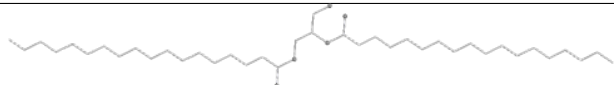




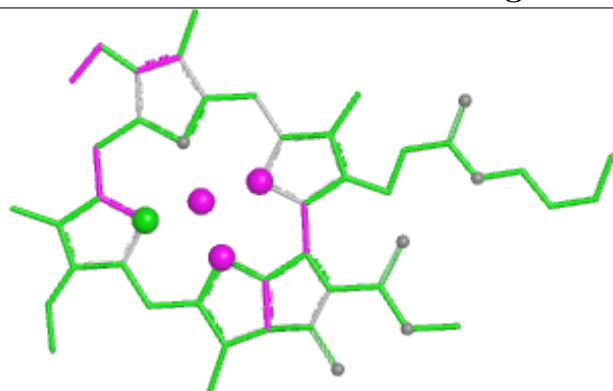




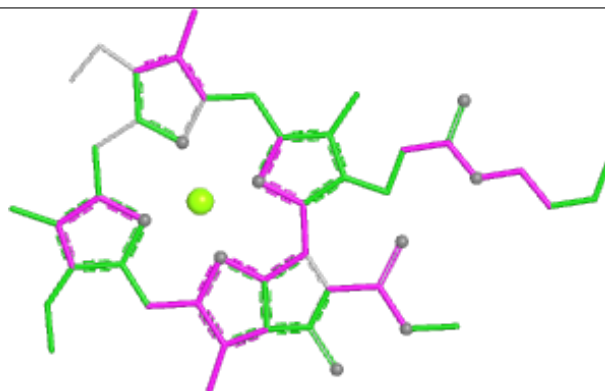
Ligand LMK c1 527	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGA c 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

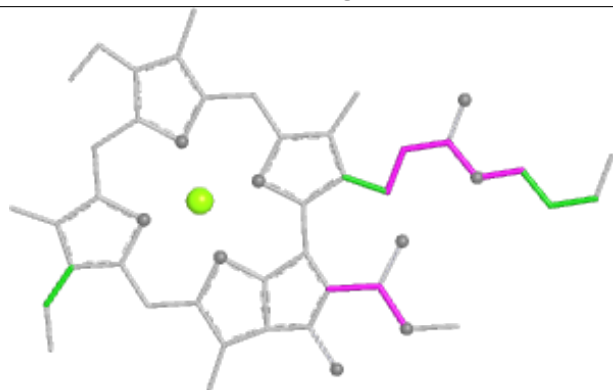
Ligand CLA R1 604



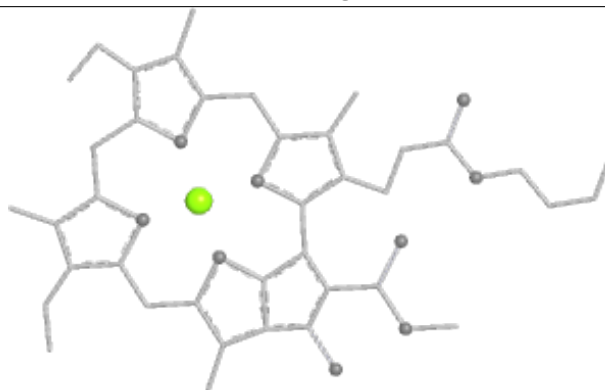
Bond lengths



Bond angles

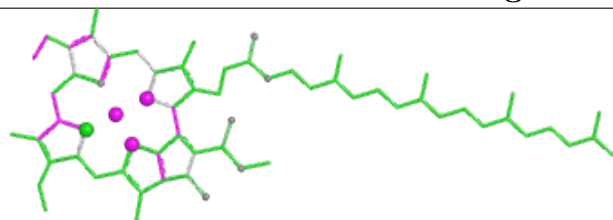


Torsions

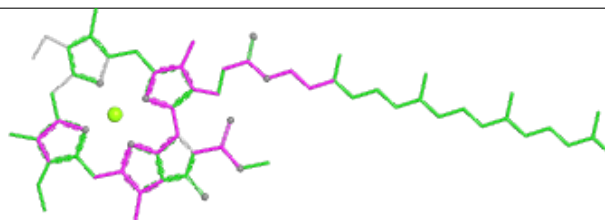


Rings

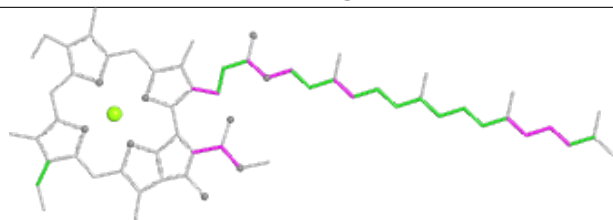
Ligand CLA Y1 603



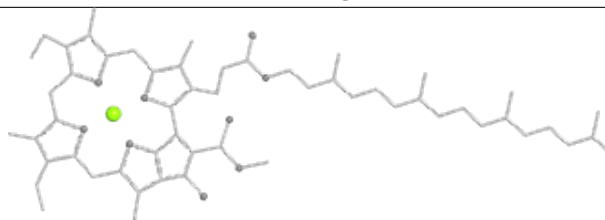
Bond lengths



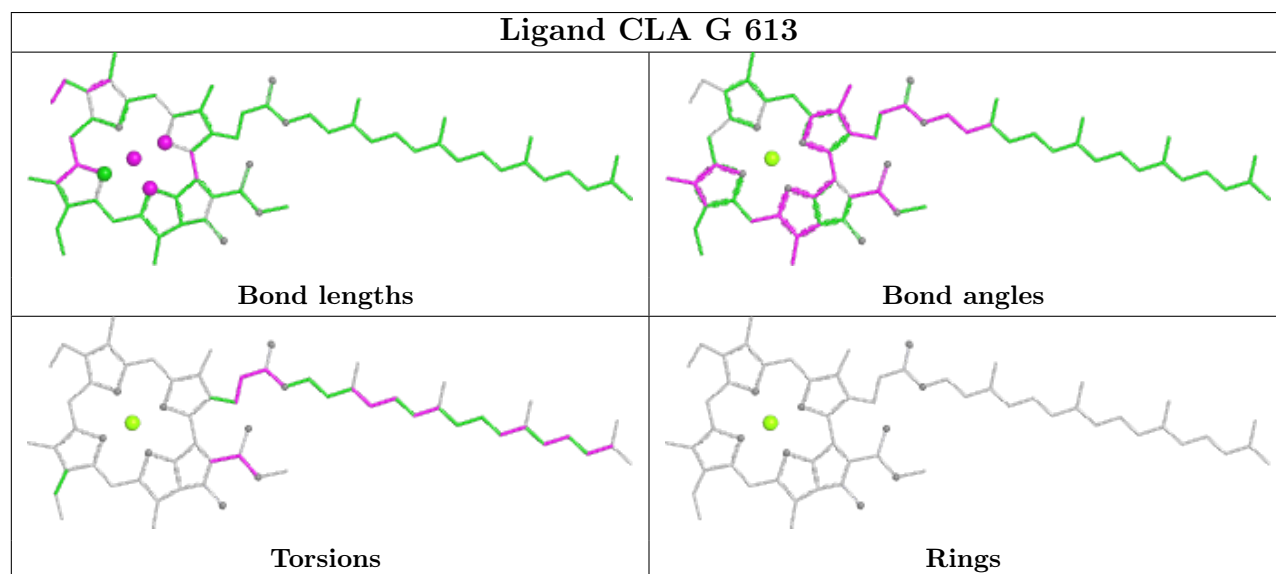
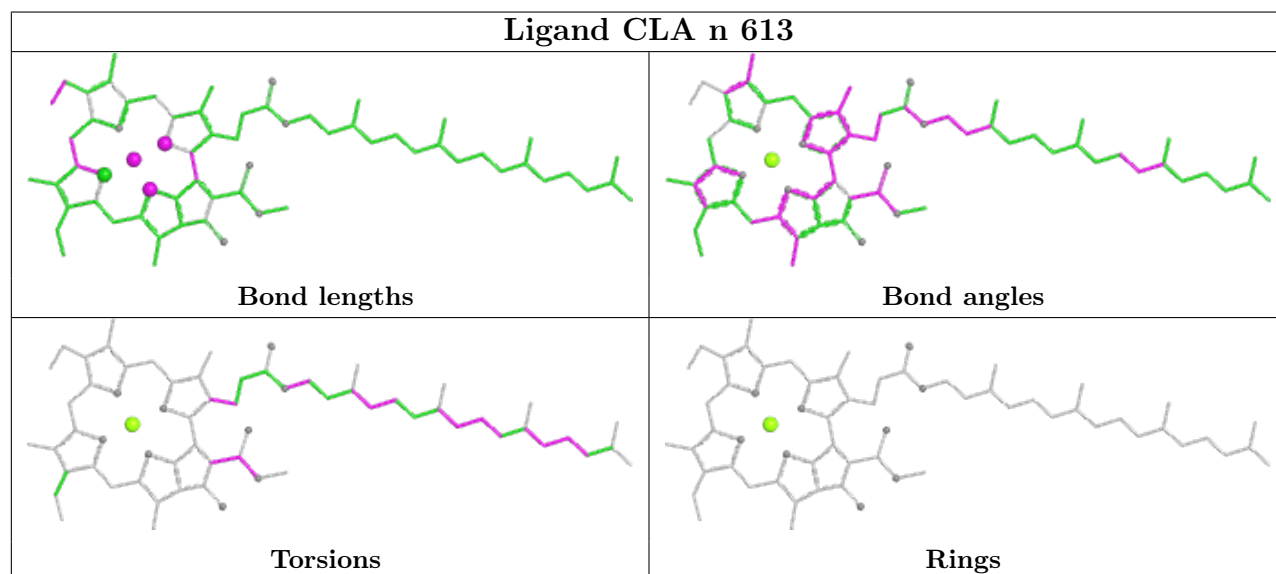
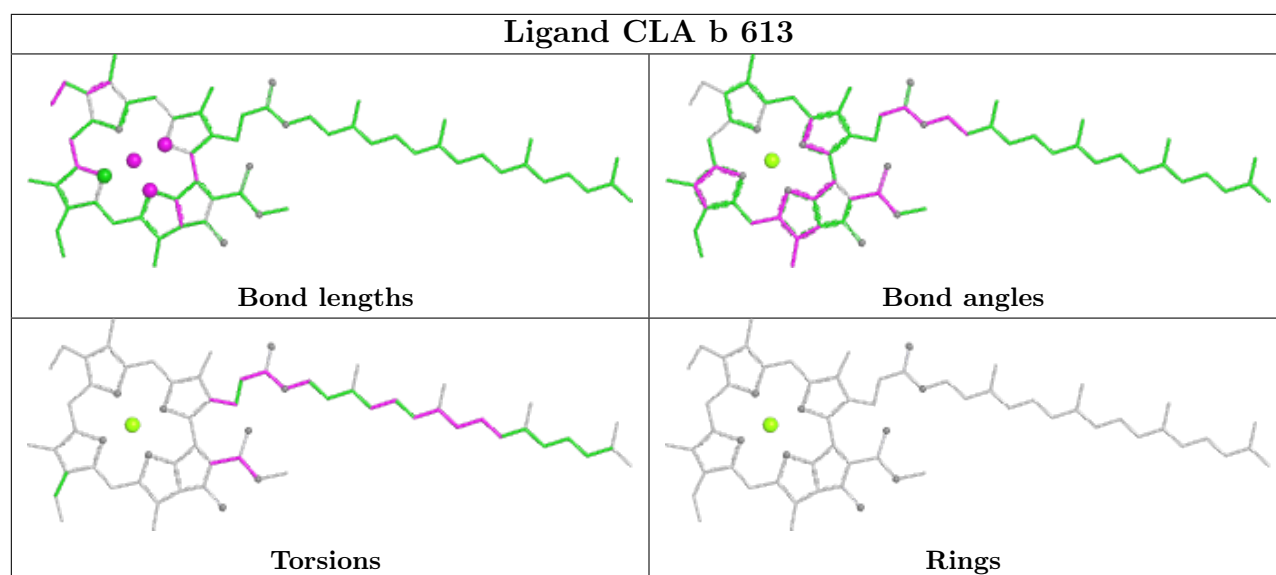
Bond angles

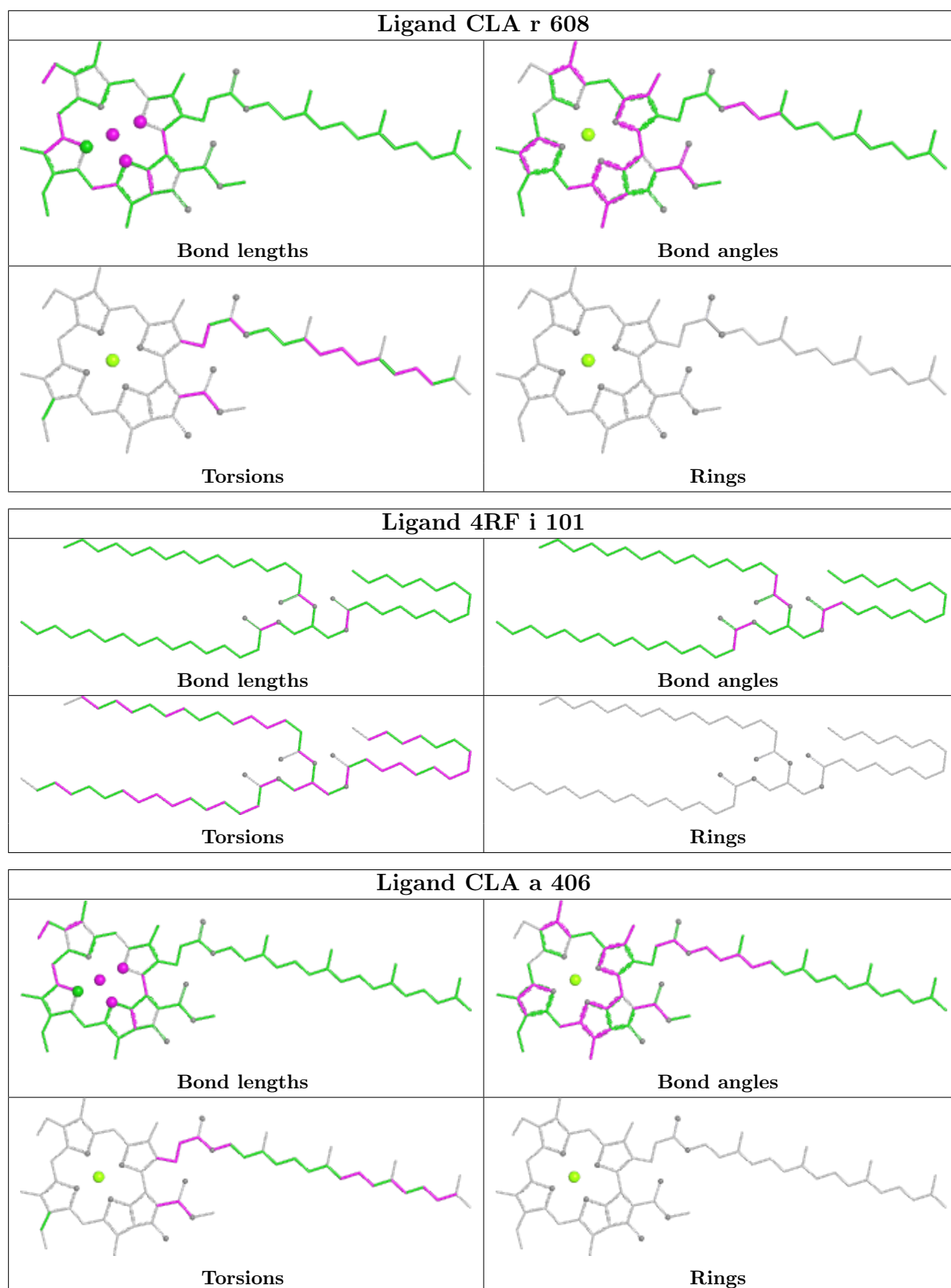


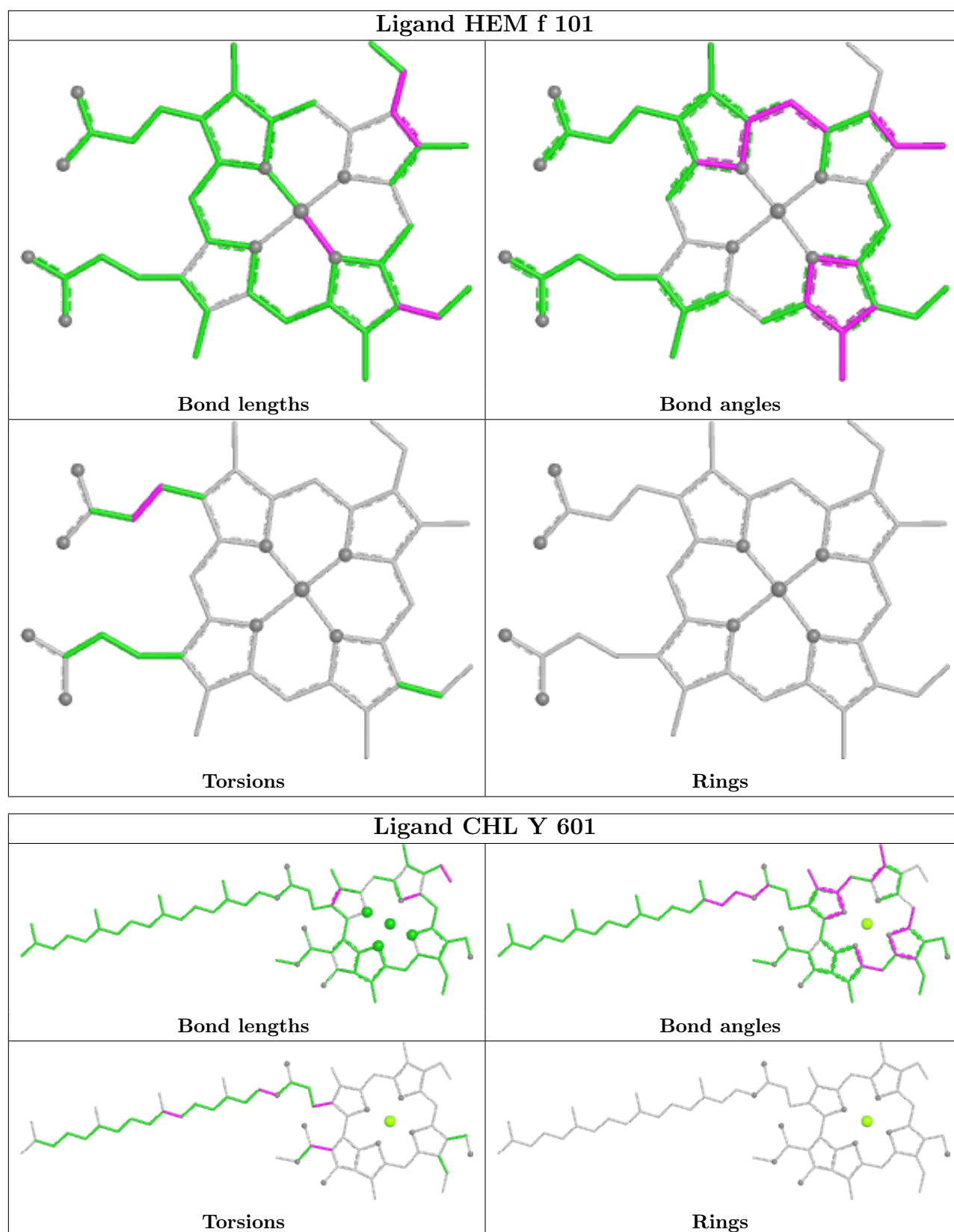
Torsions

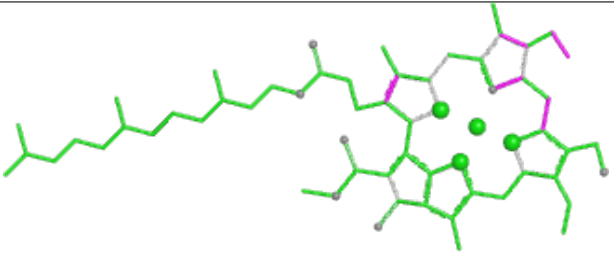
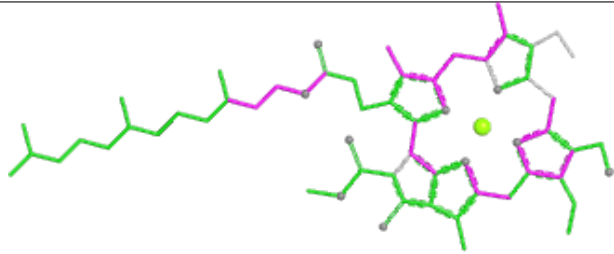
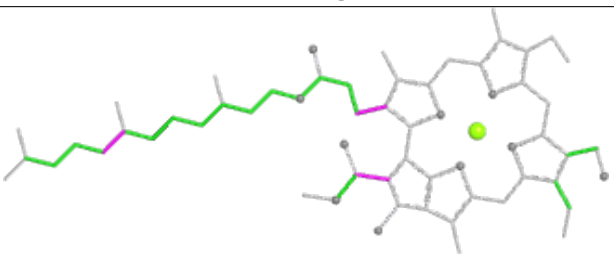
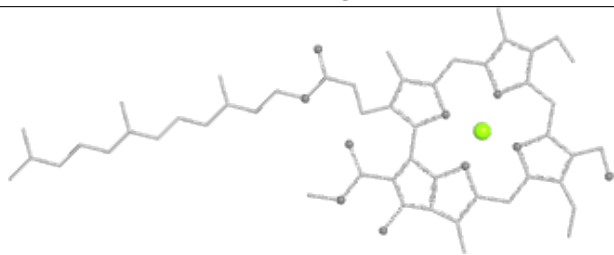


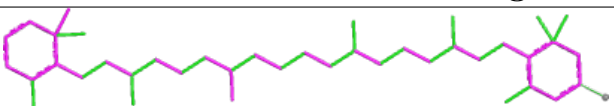
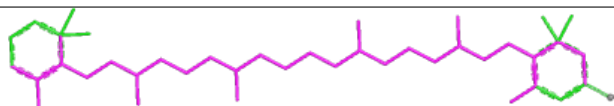
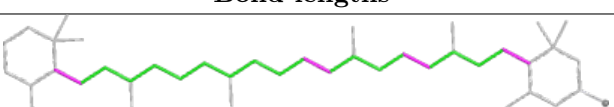
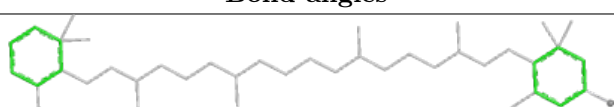
Rings

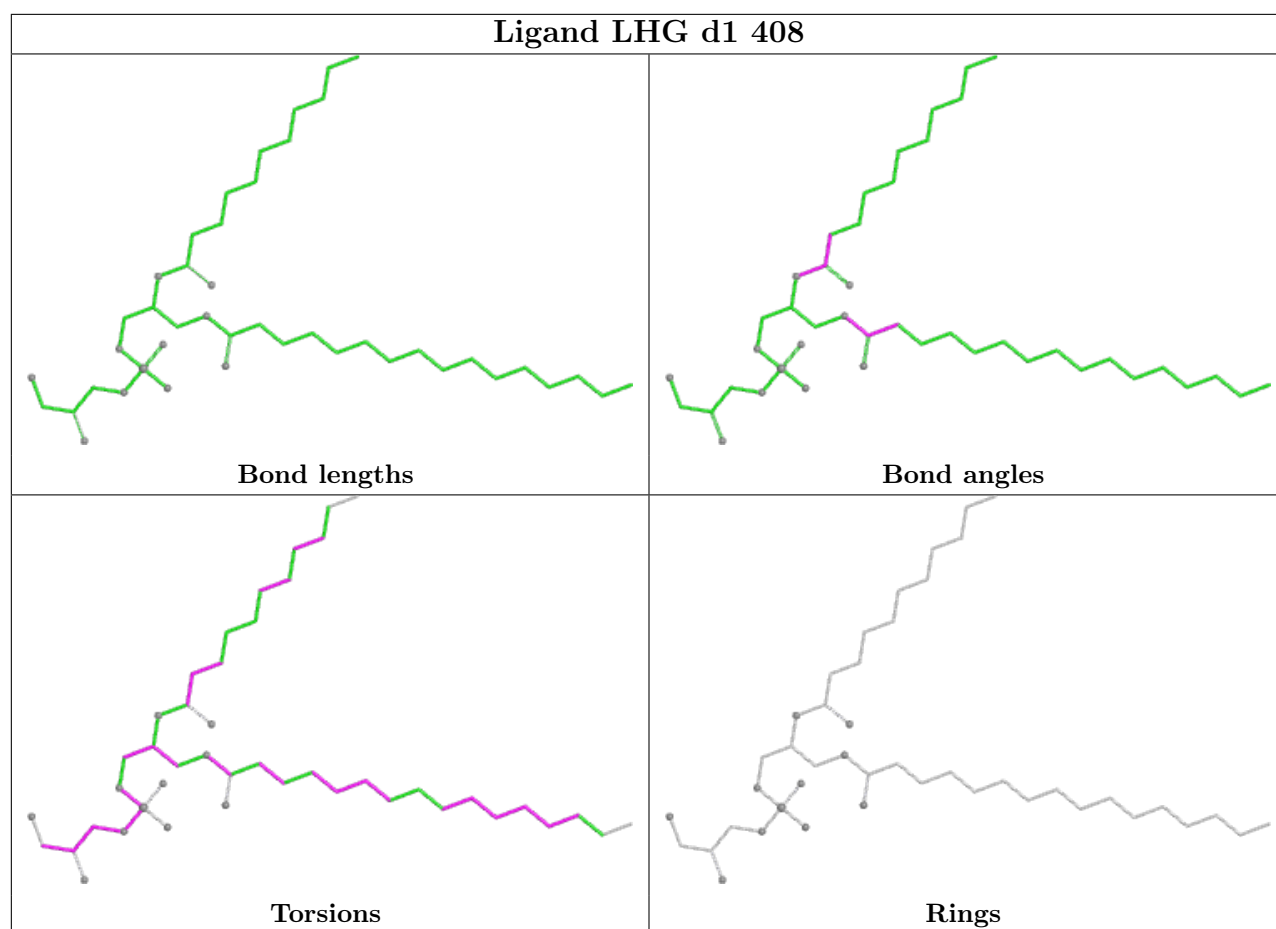


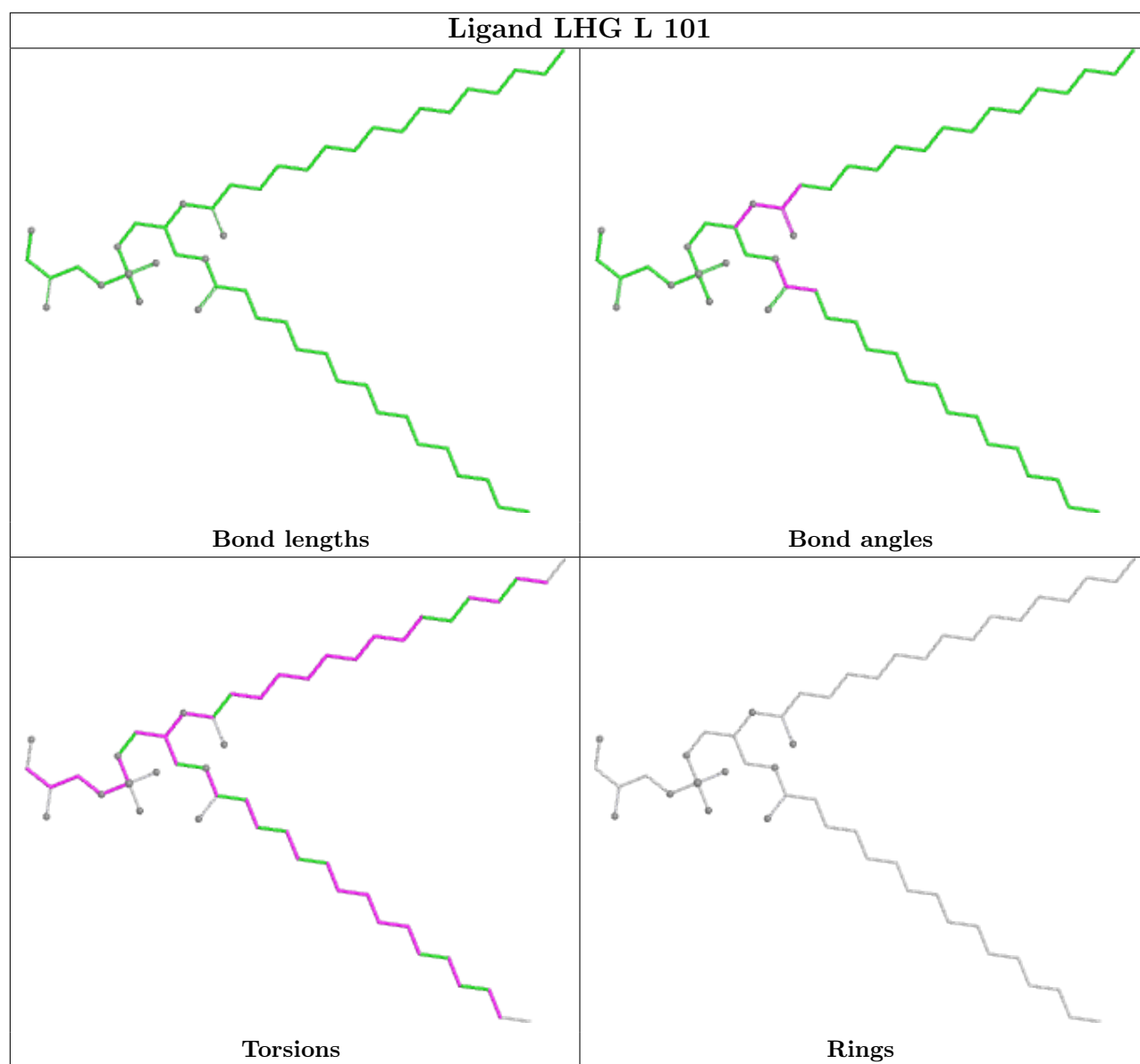




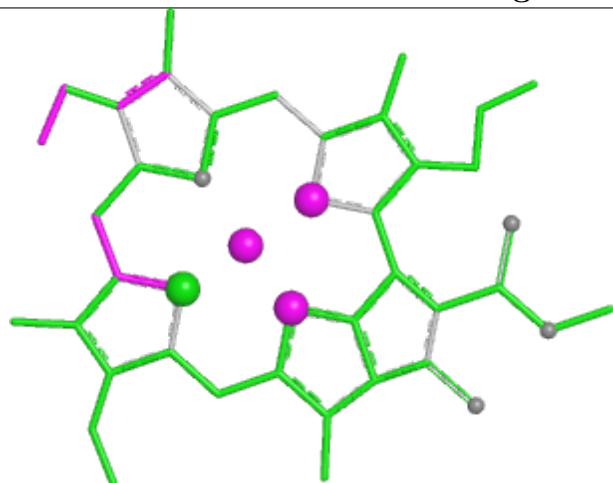
Ligand CHL s1 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand RRX h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

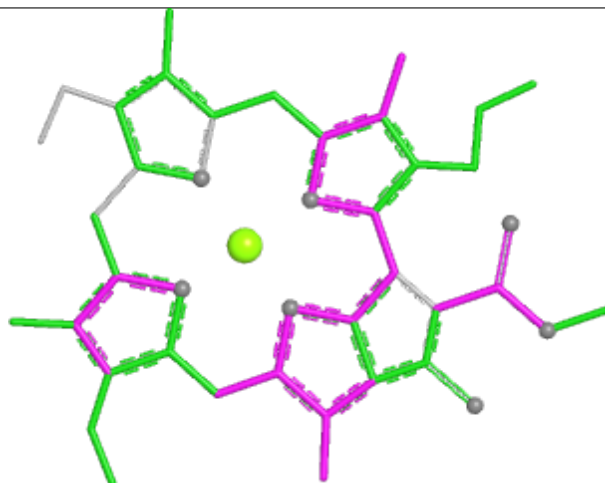




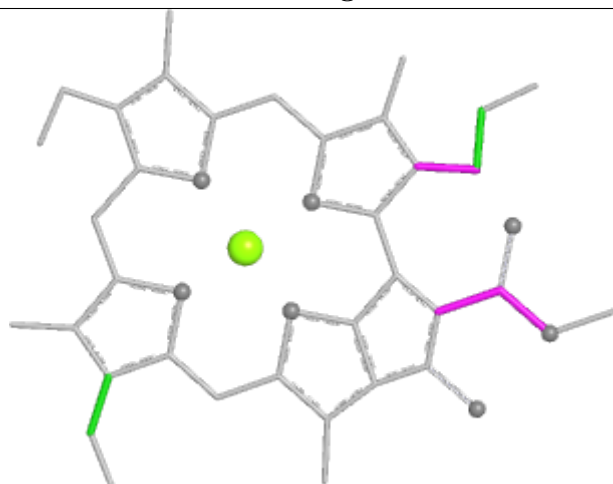
Ligand CLA G 612



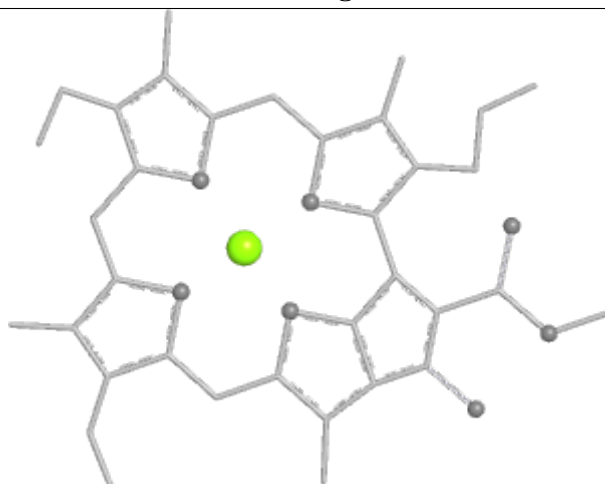
Bond lengths



Bond angles

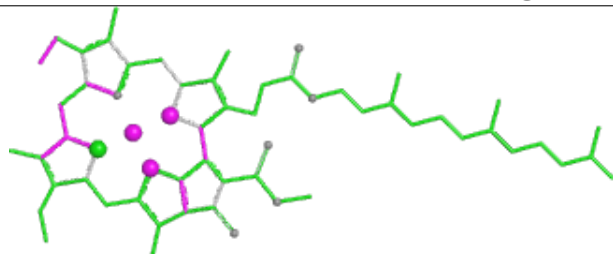


Torsions

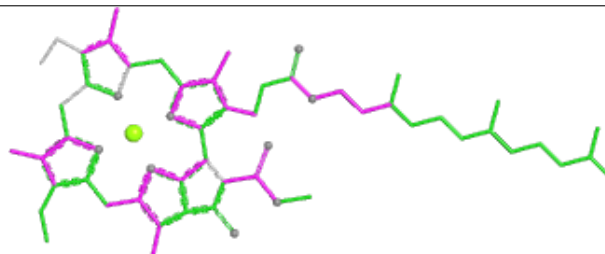


Rings

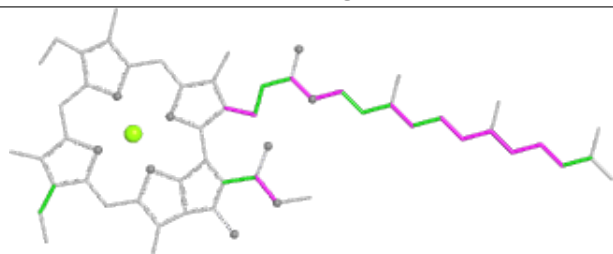
Ligand CLA a 410



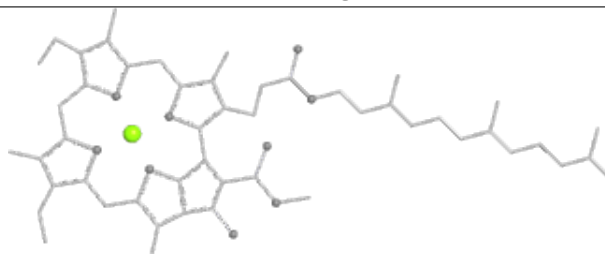
Bond lengths



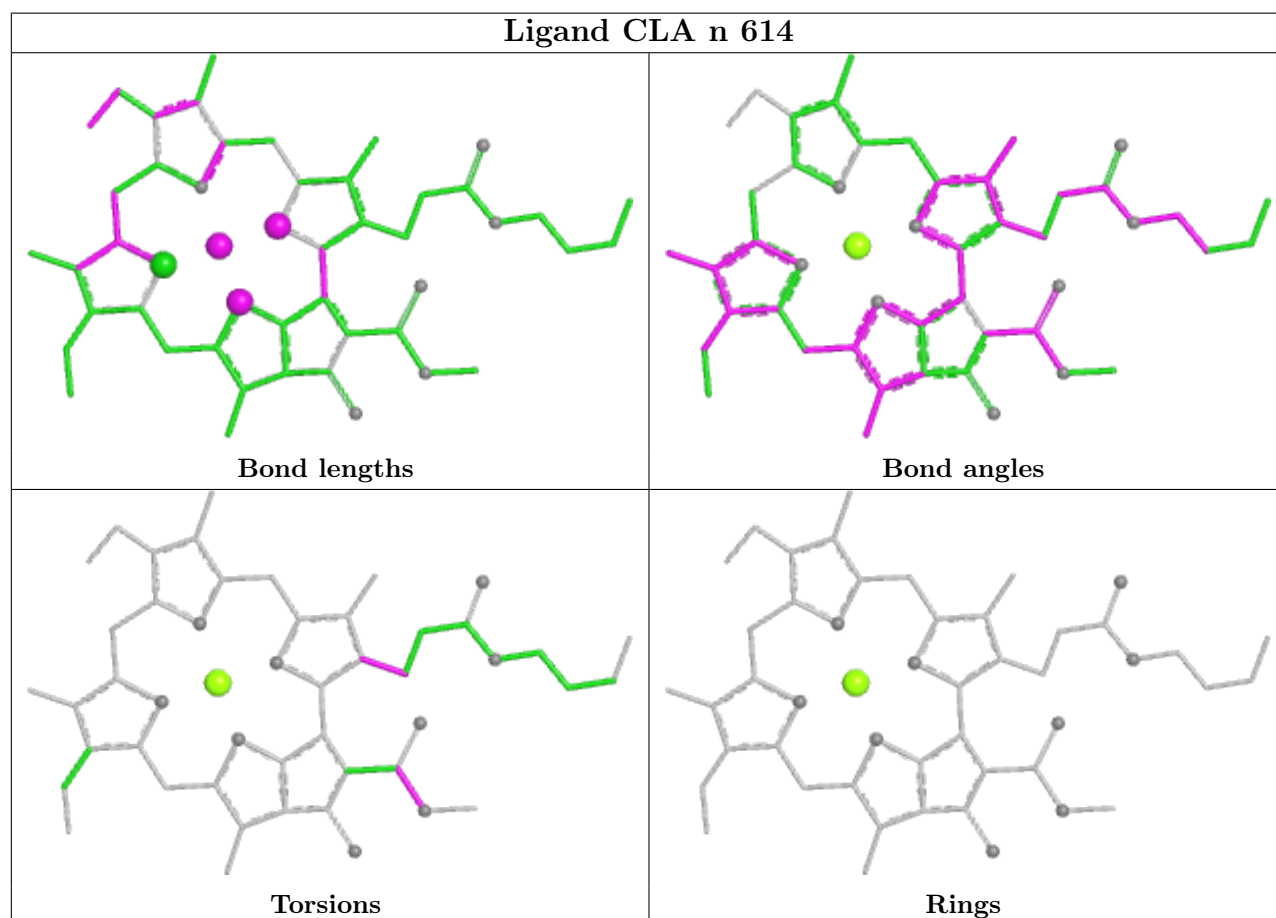
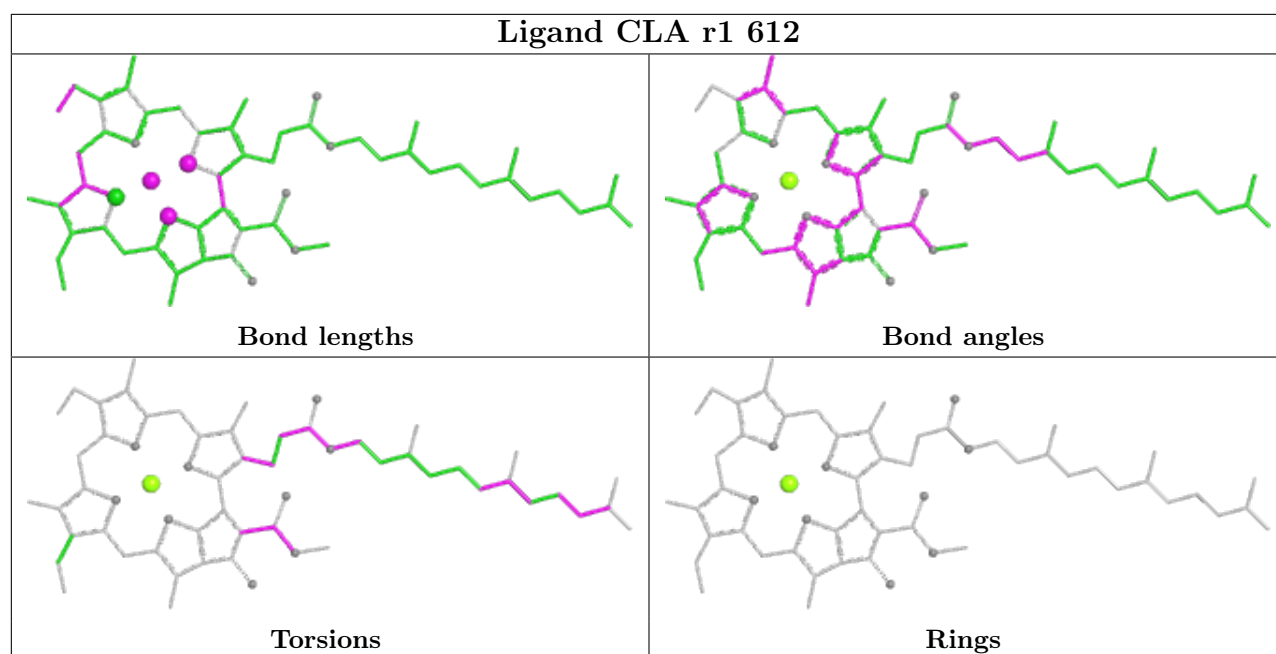
Bond angles

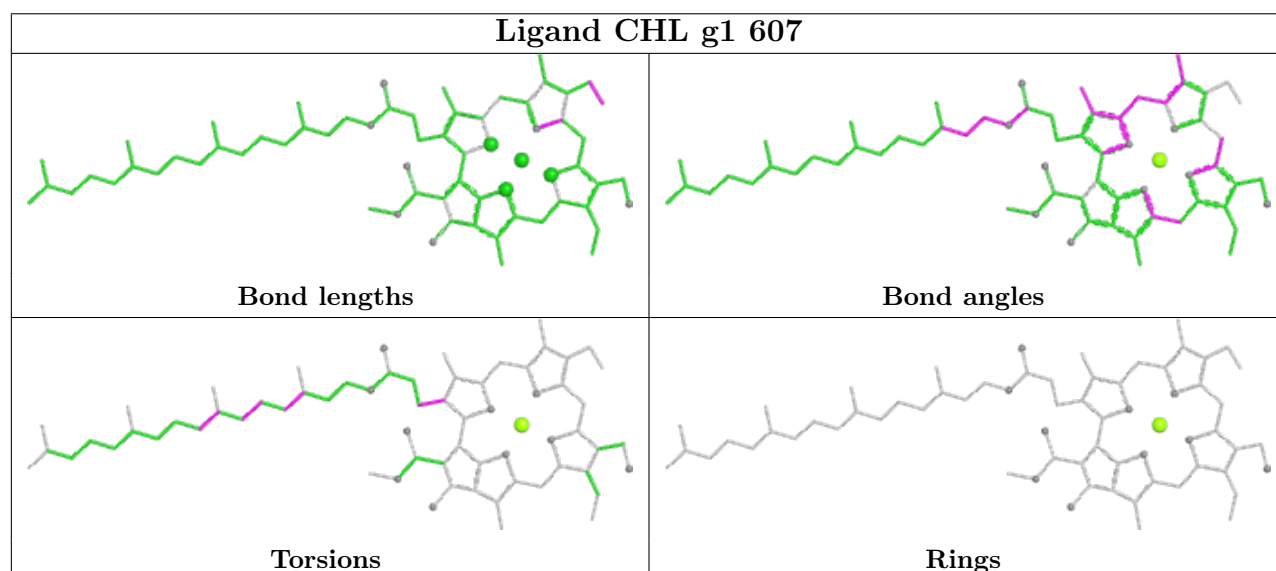
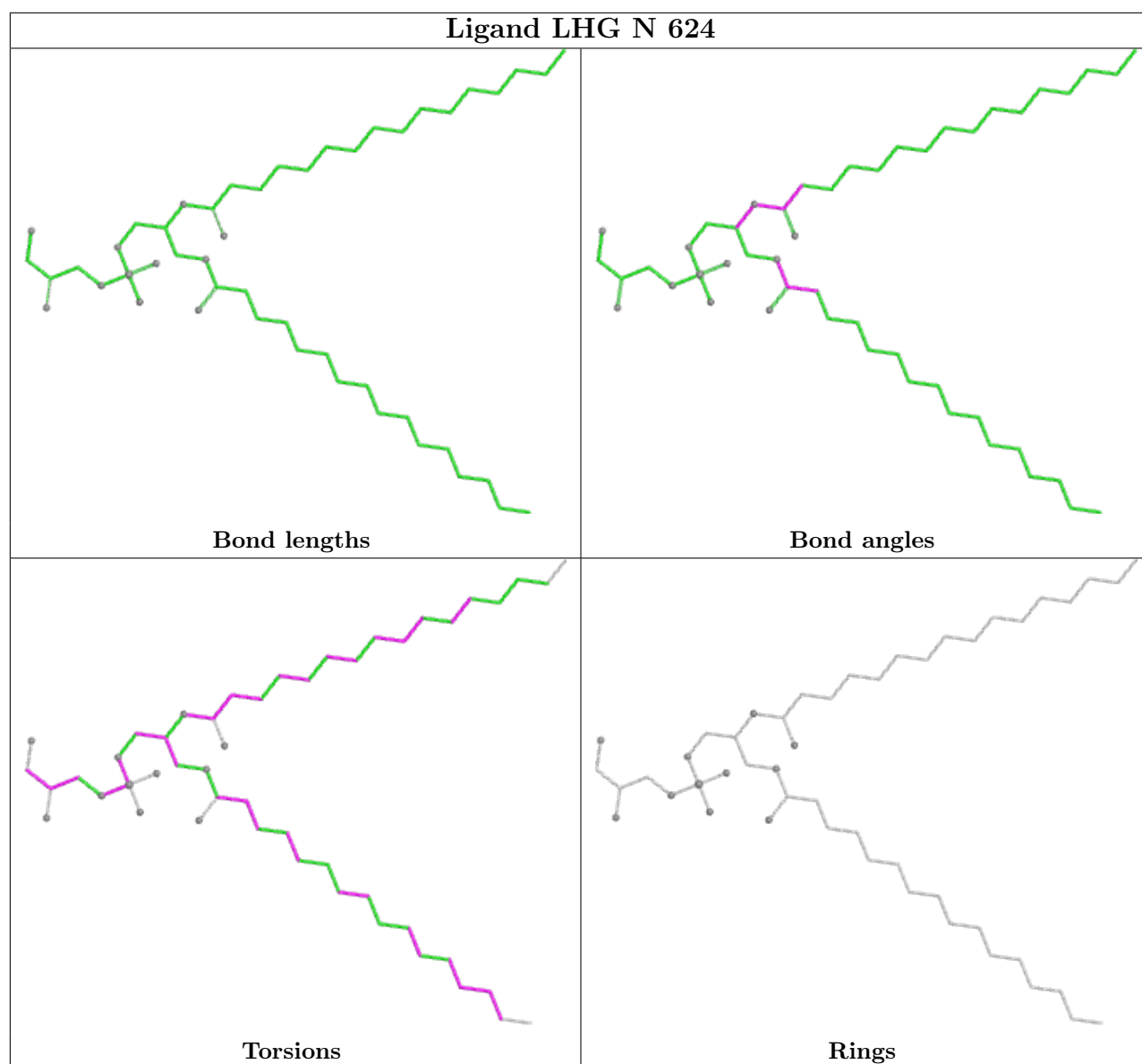


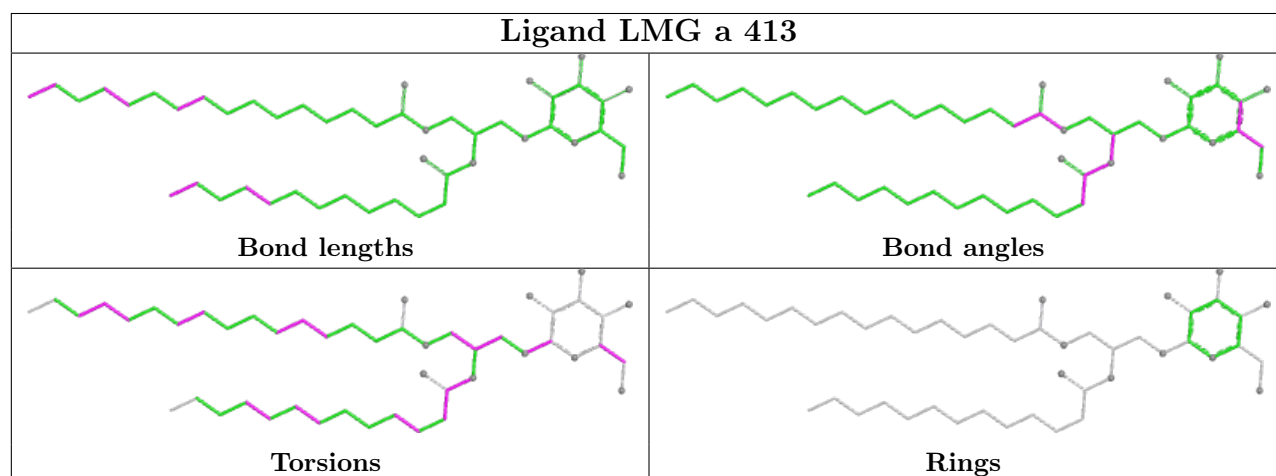
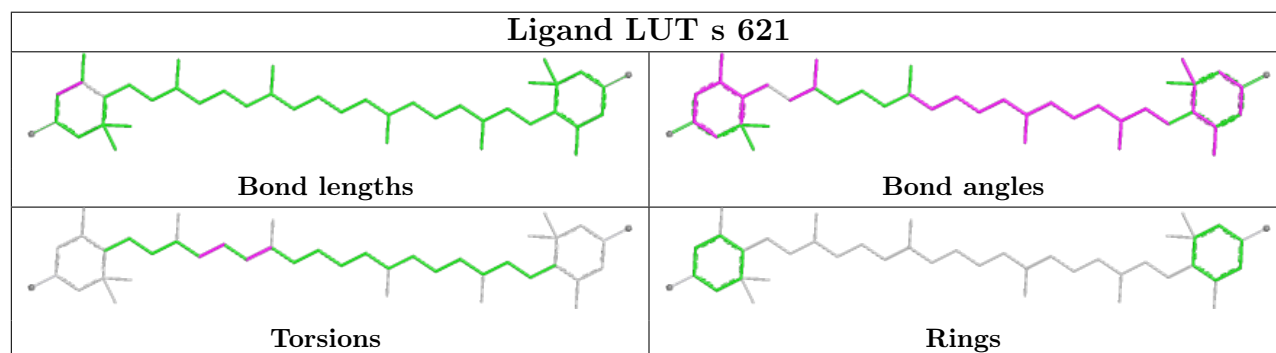
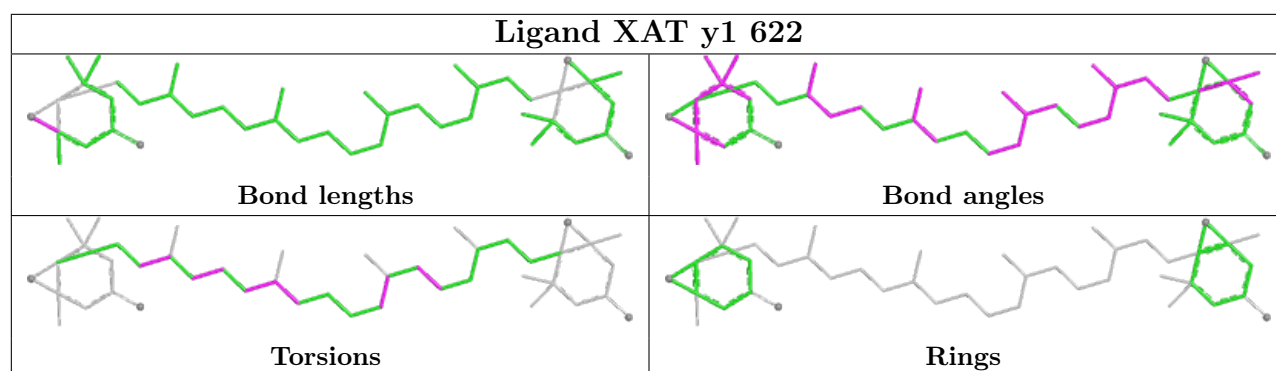
Torsions

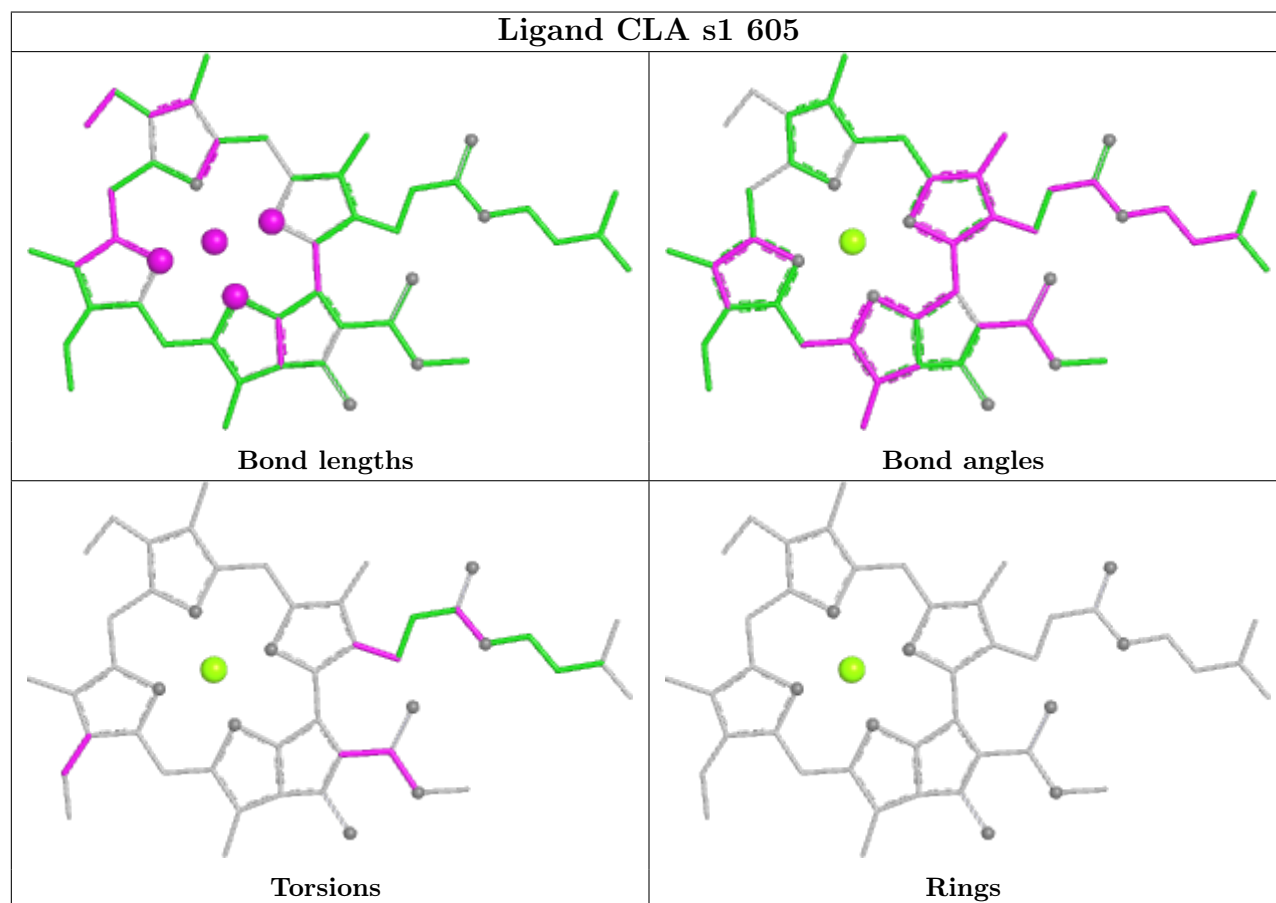
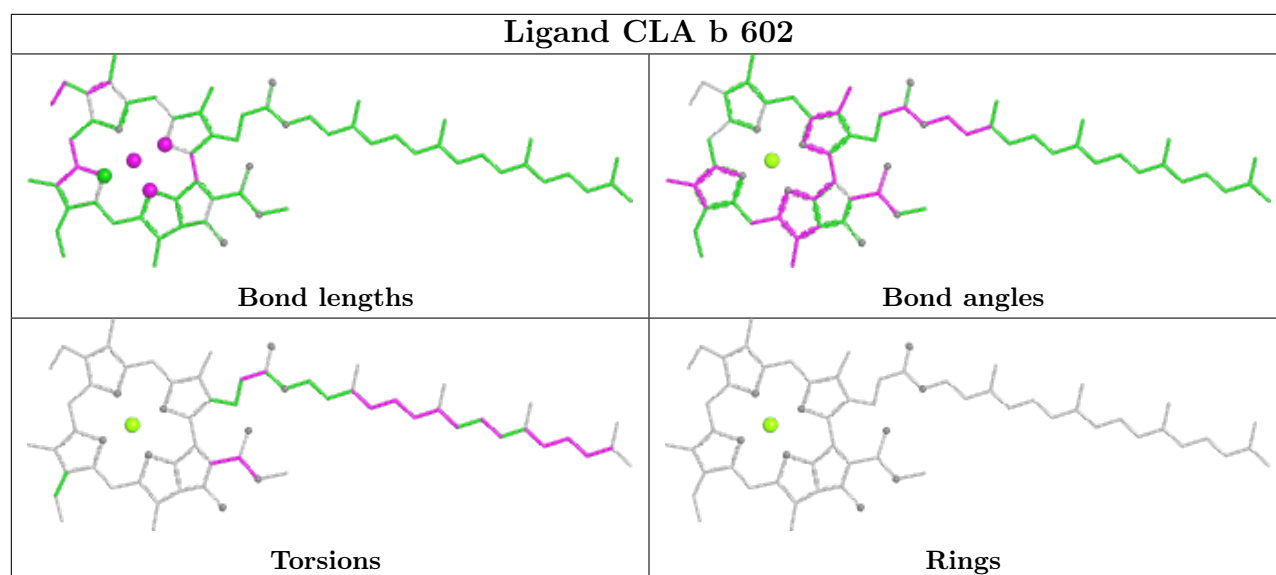


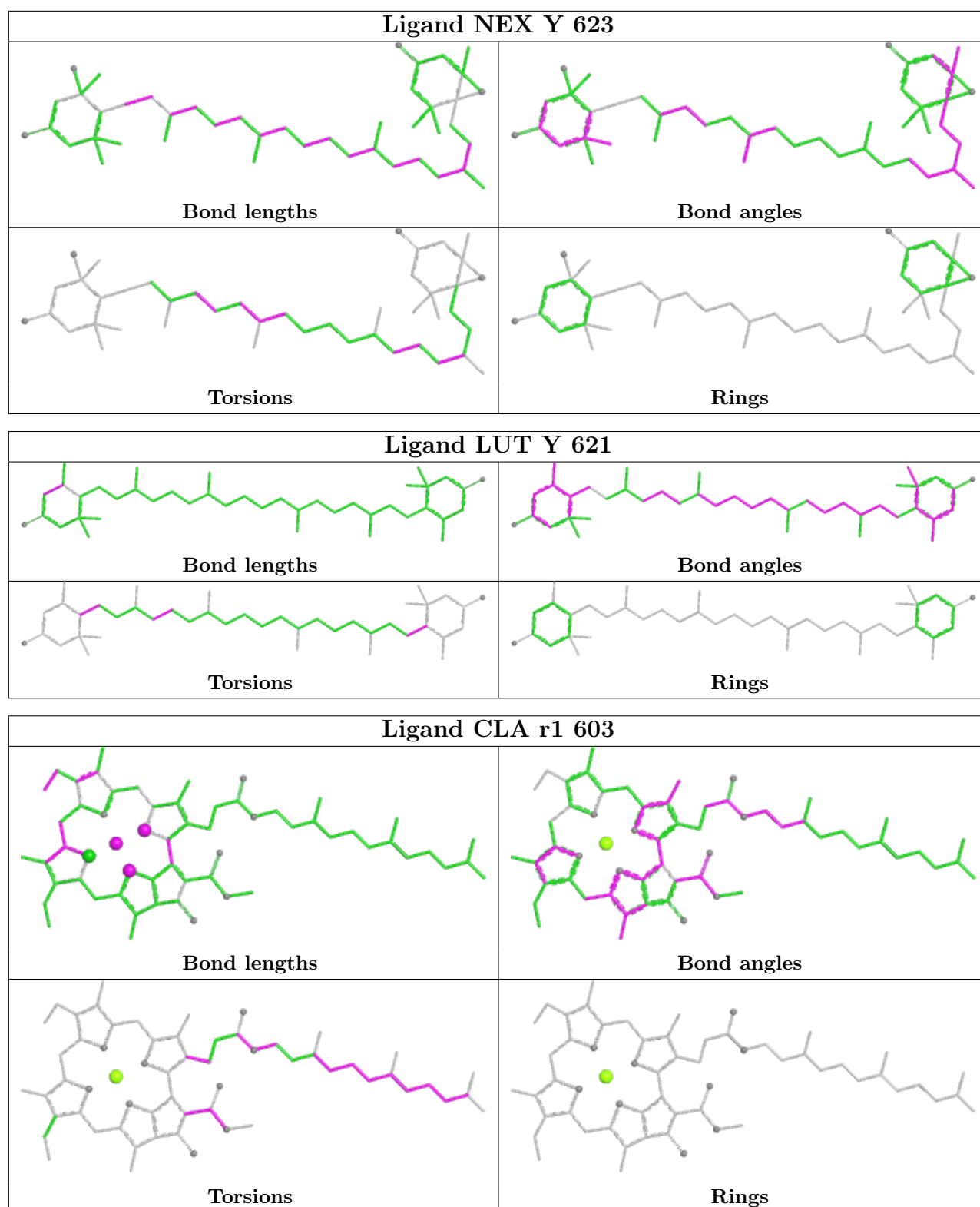
Rings

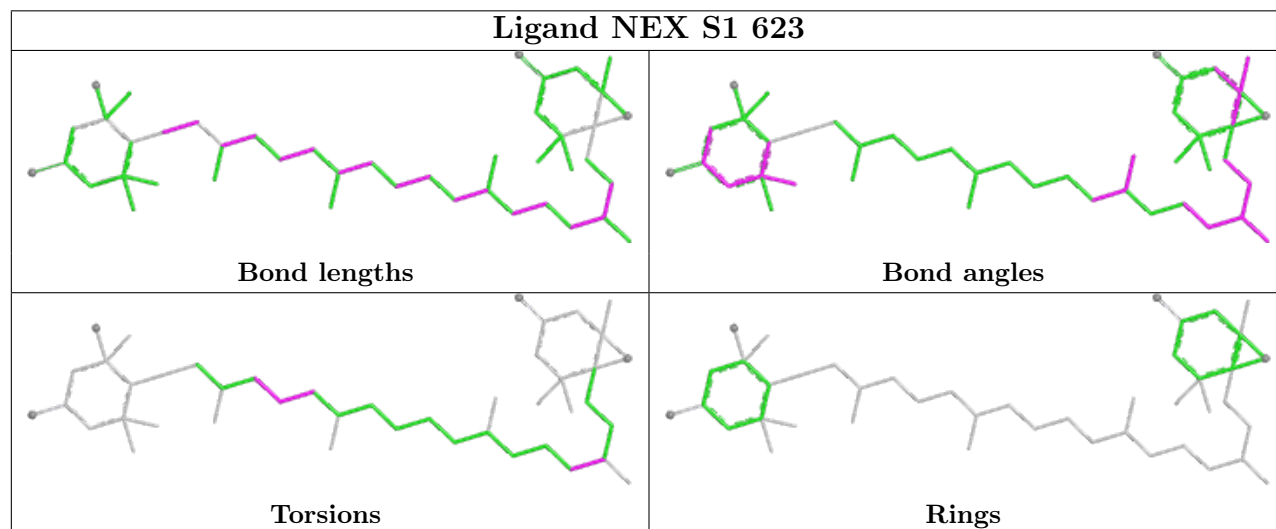
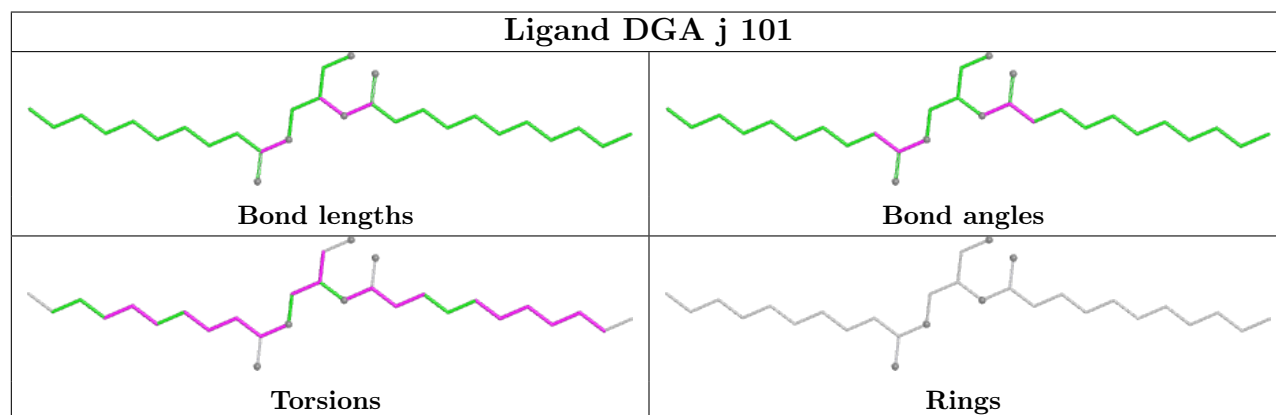
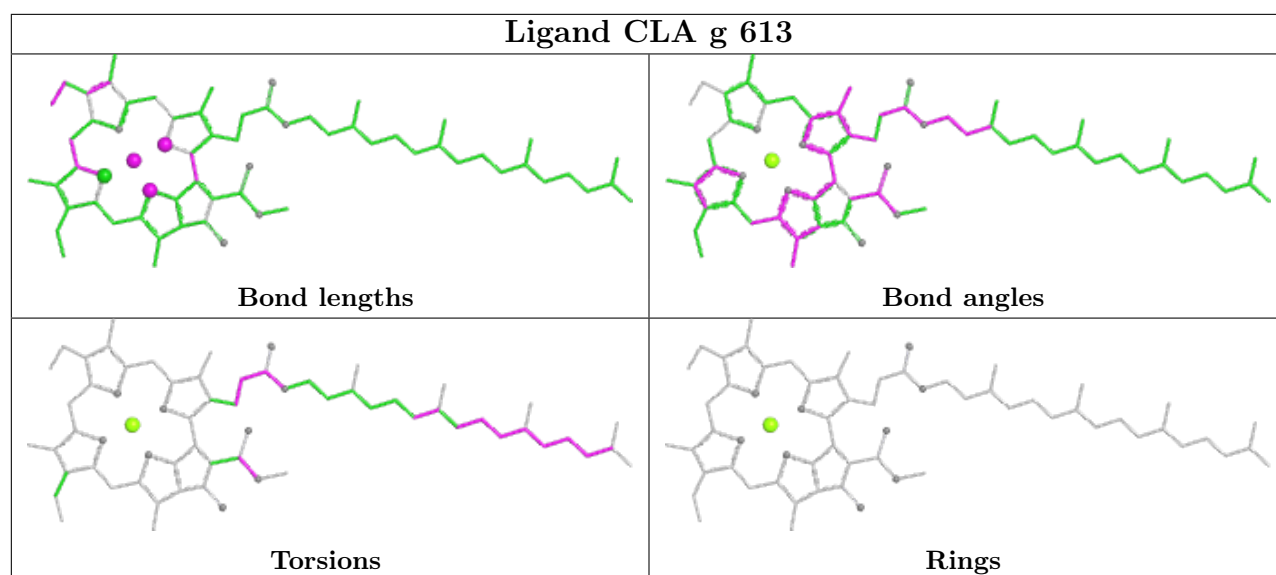


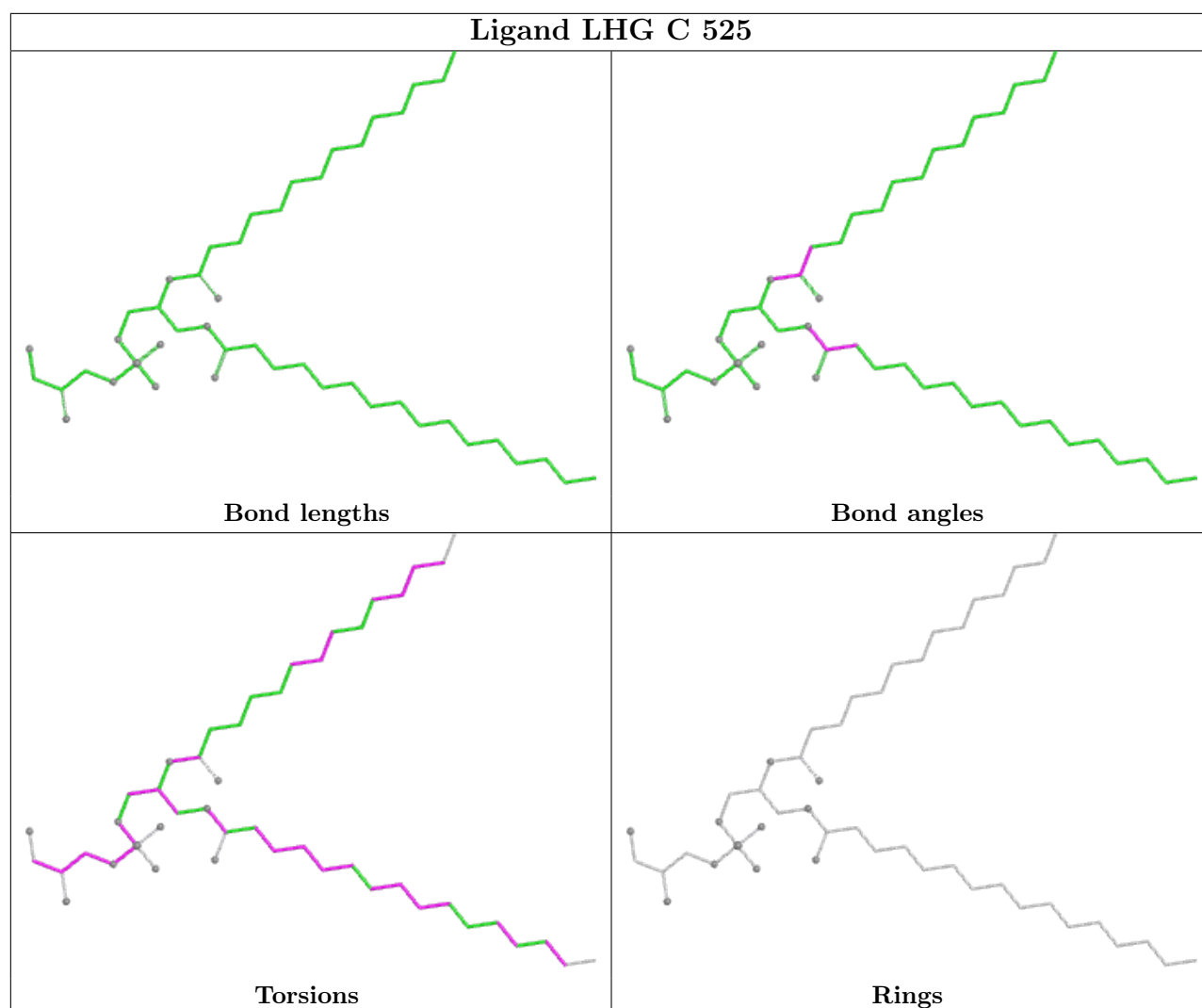


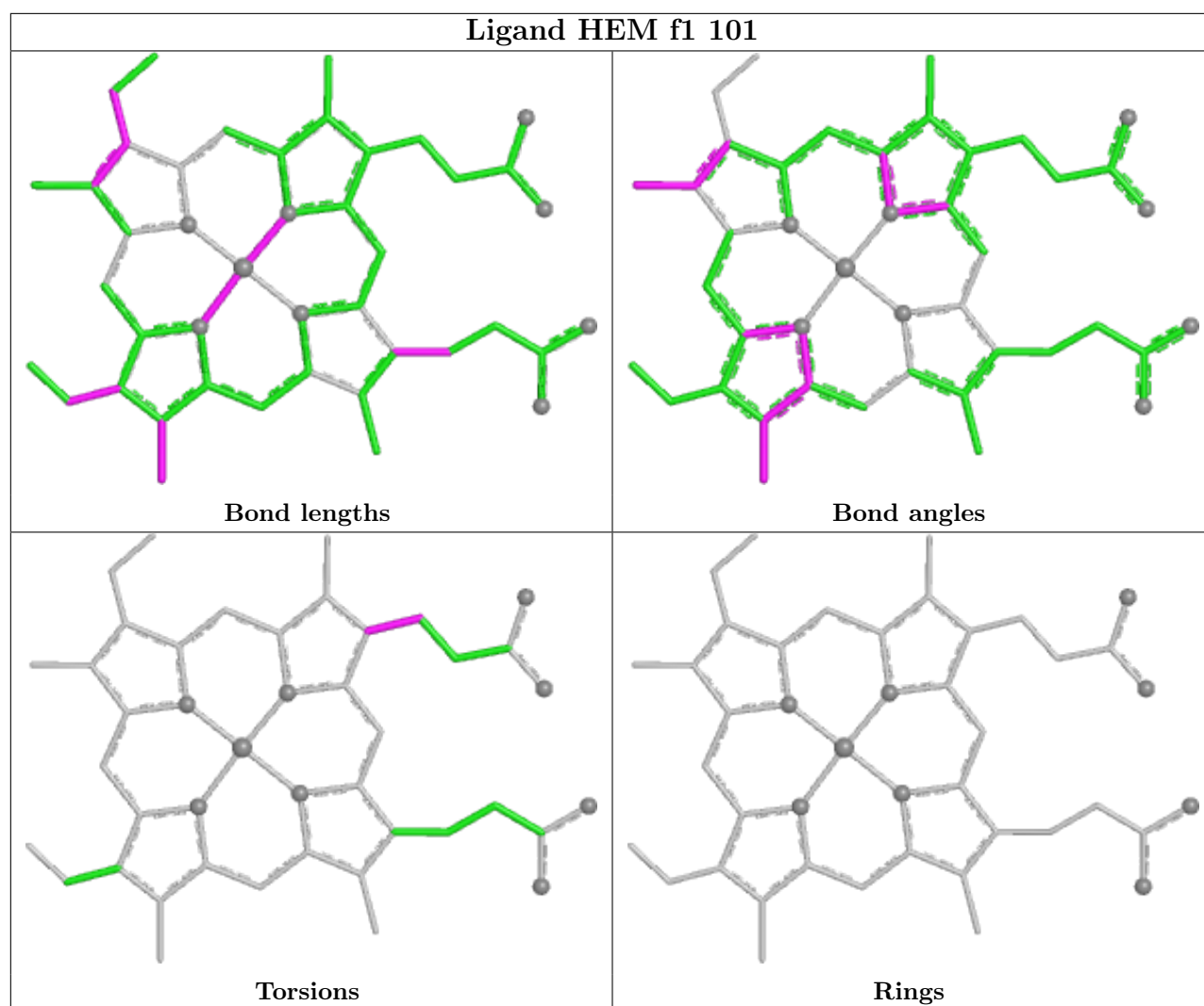


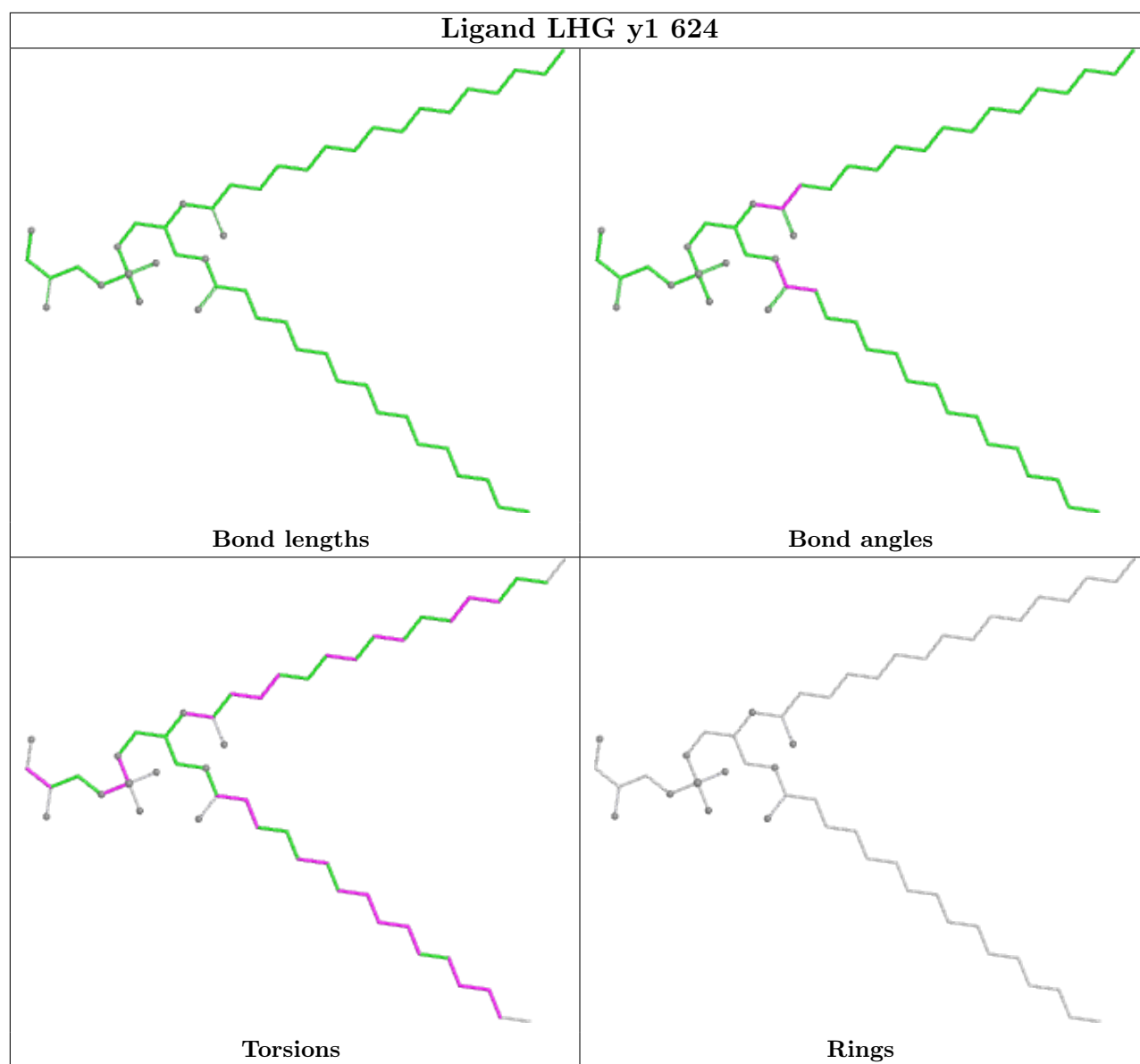


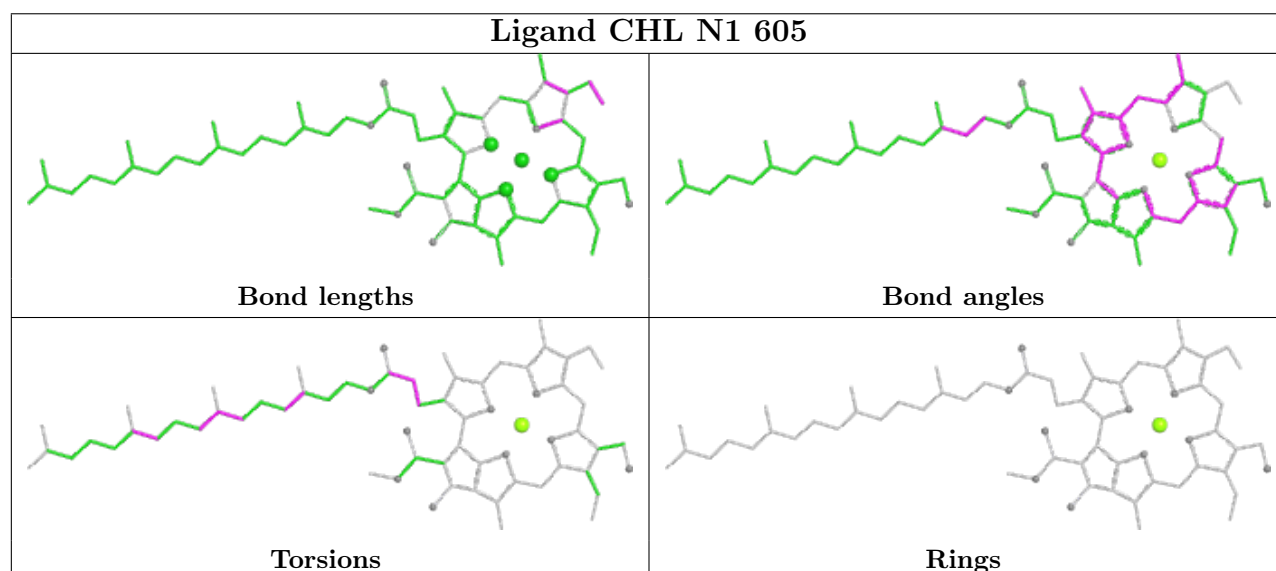
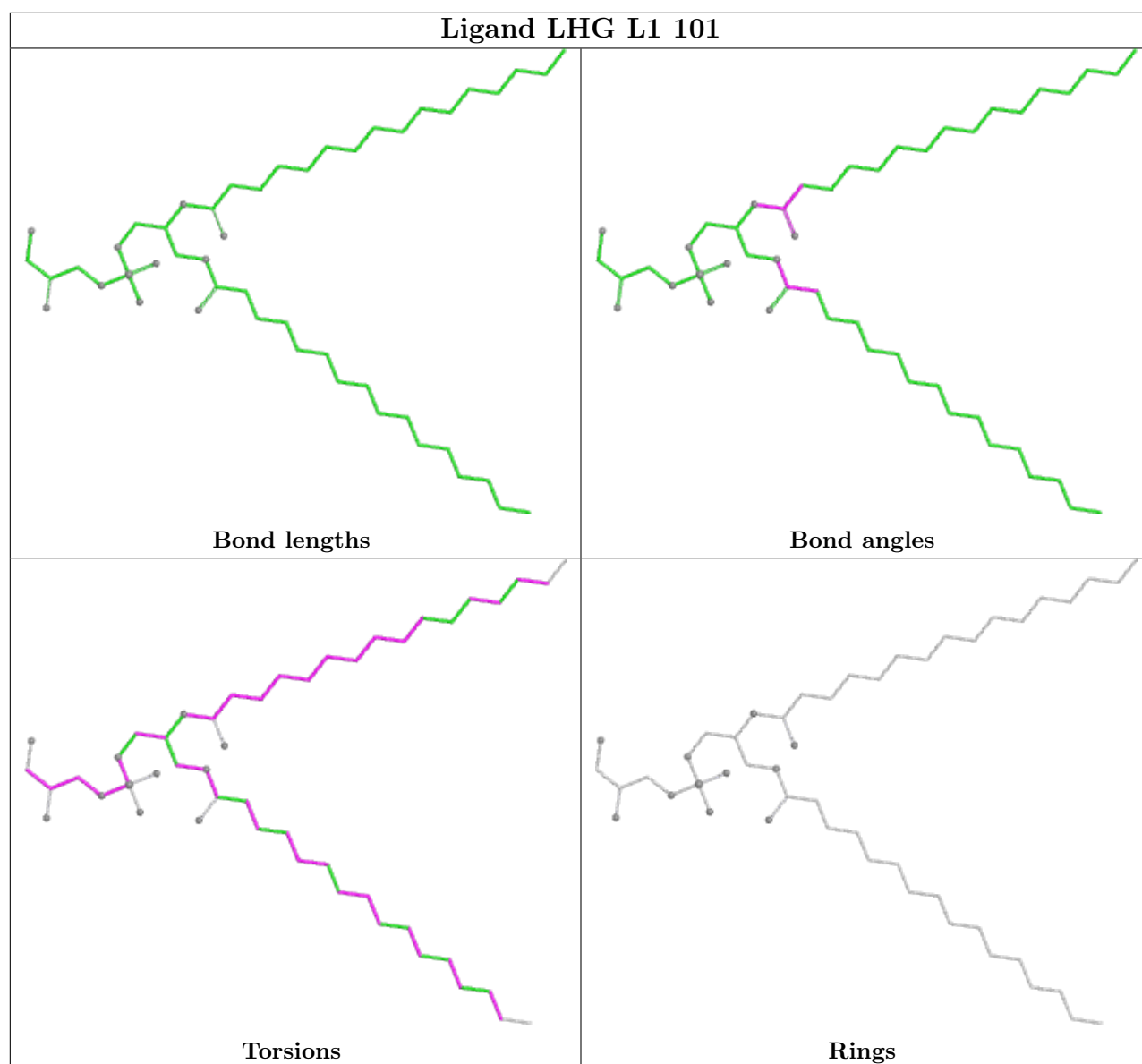


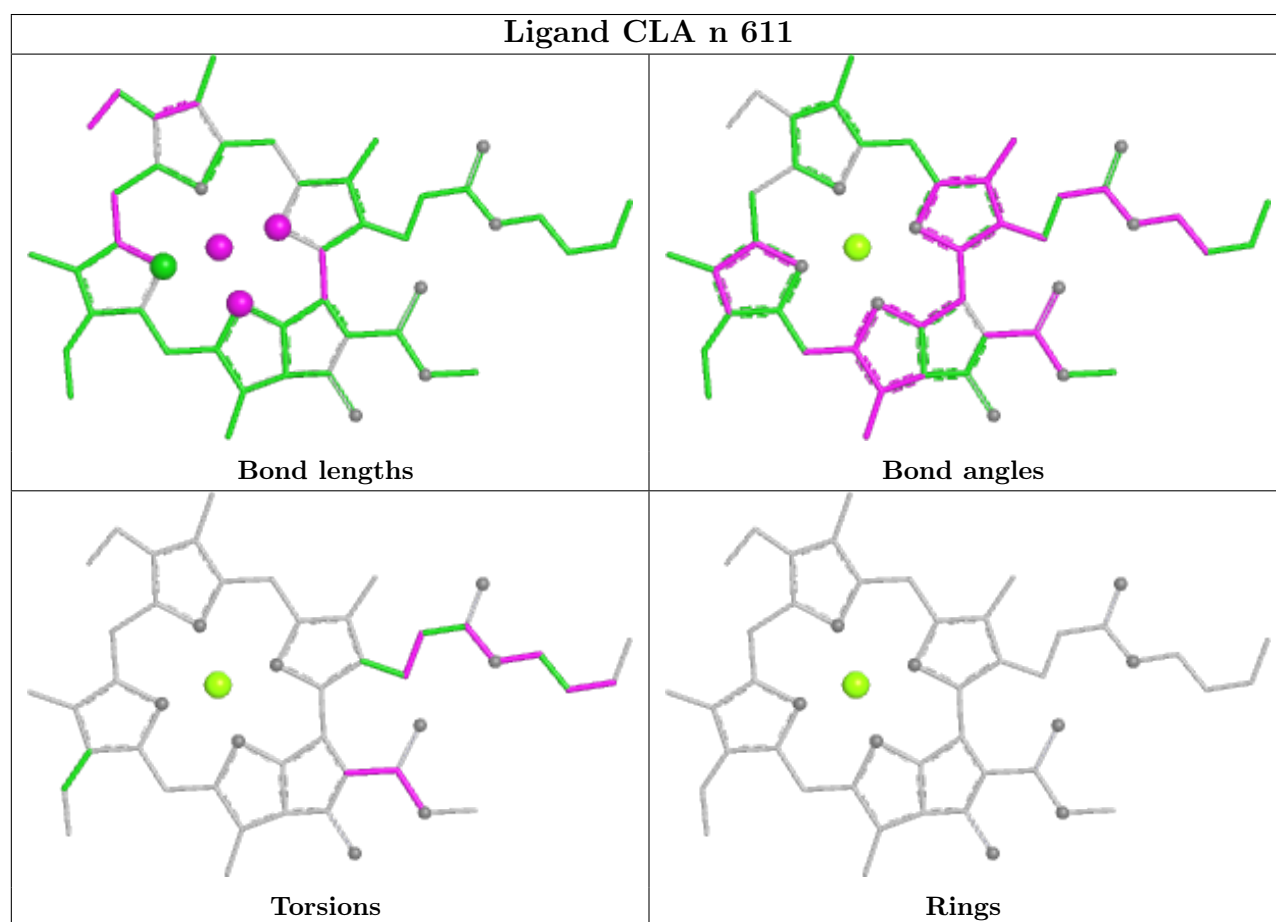
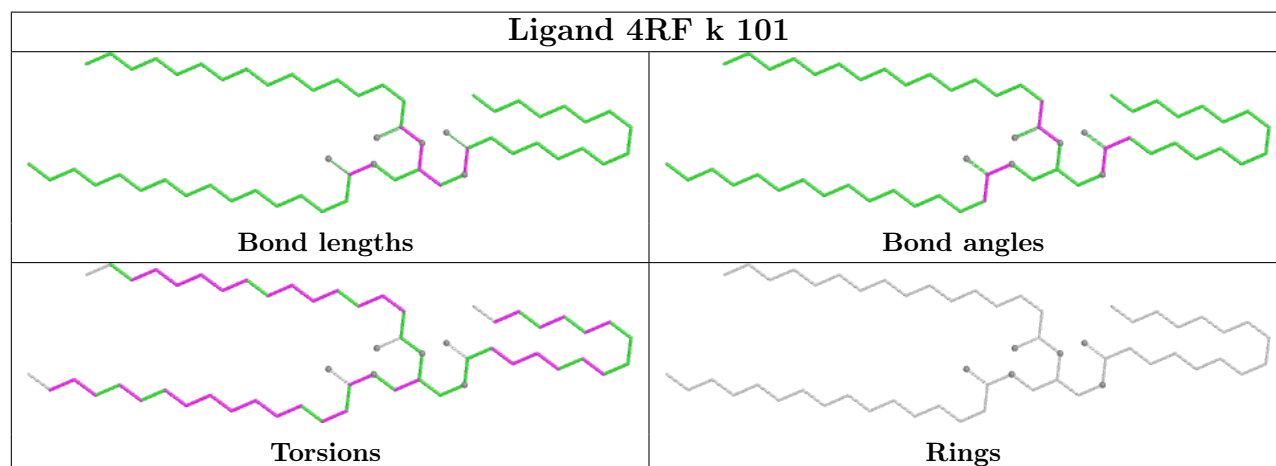
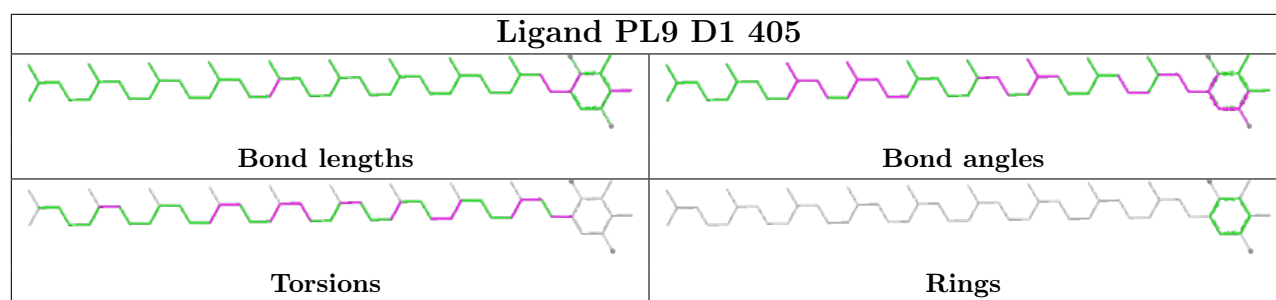


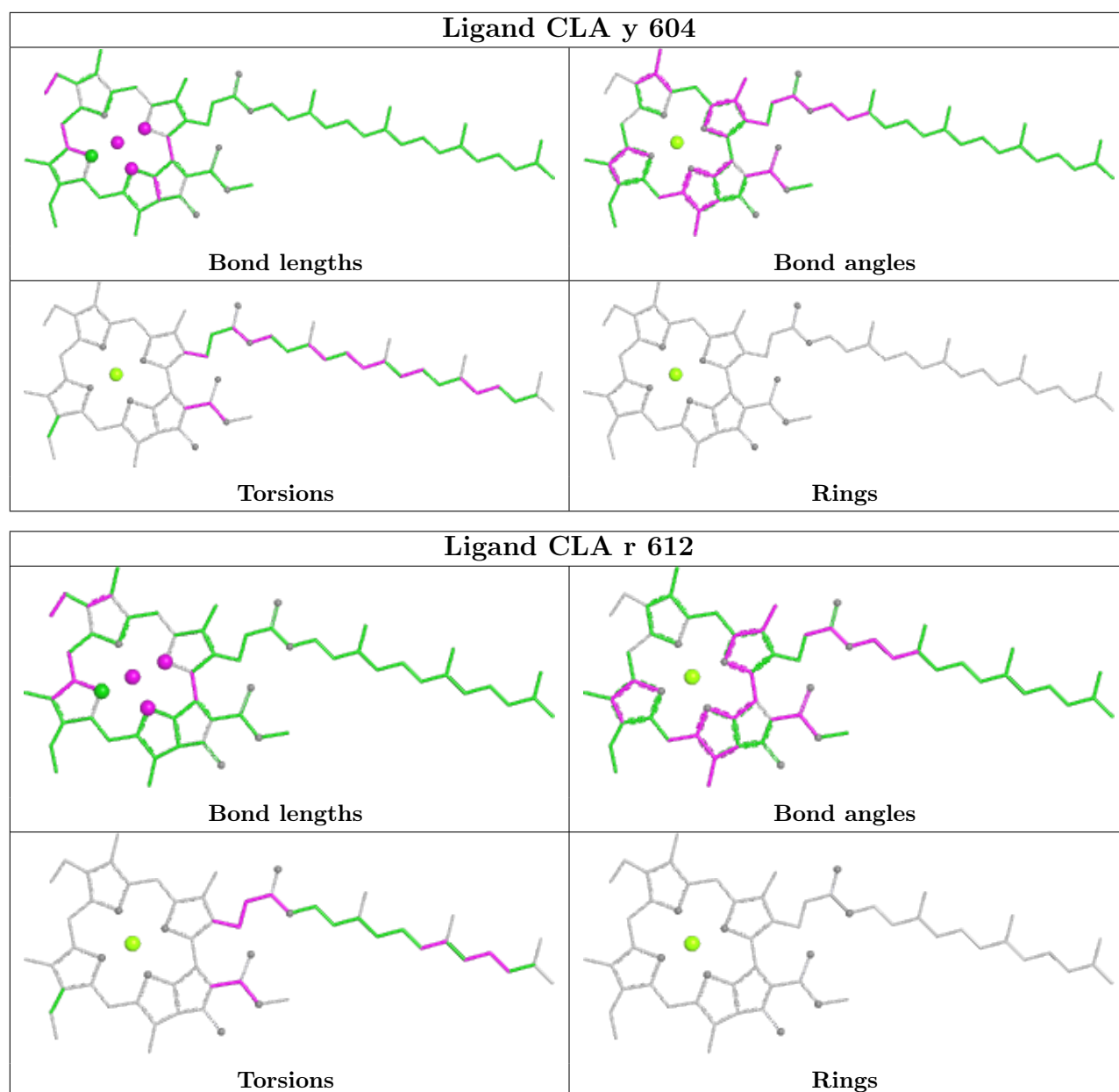


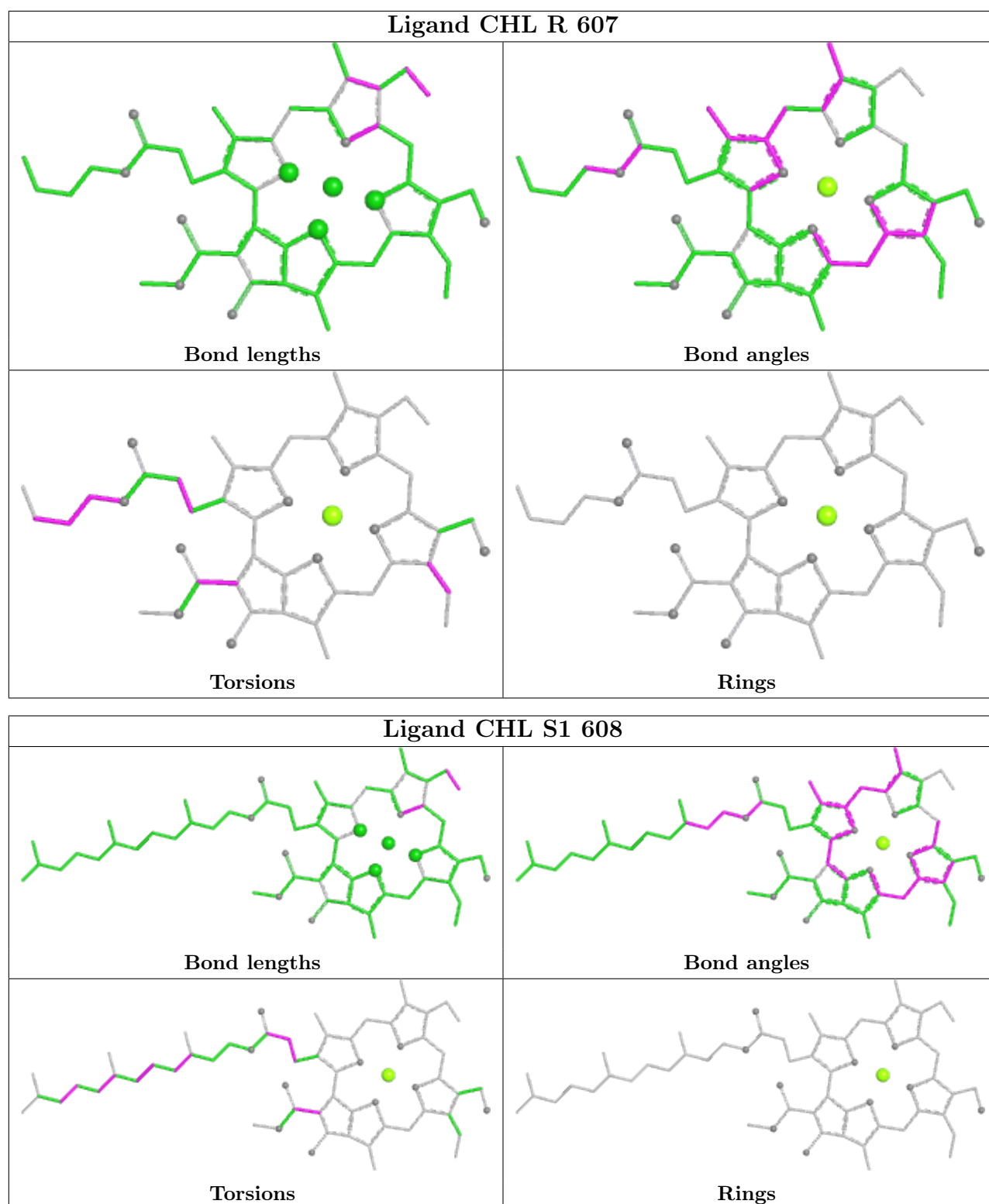


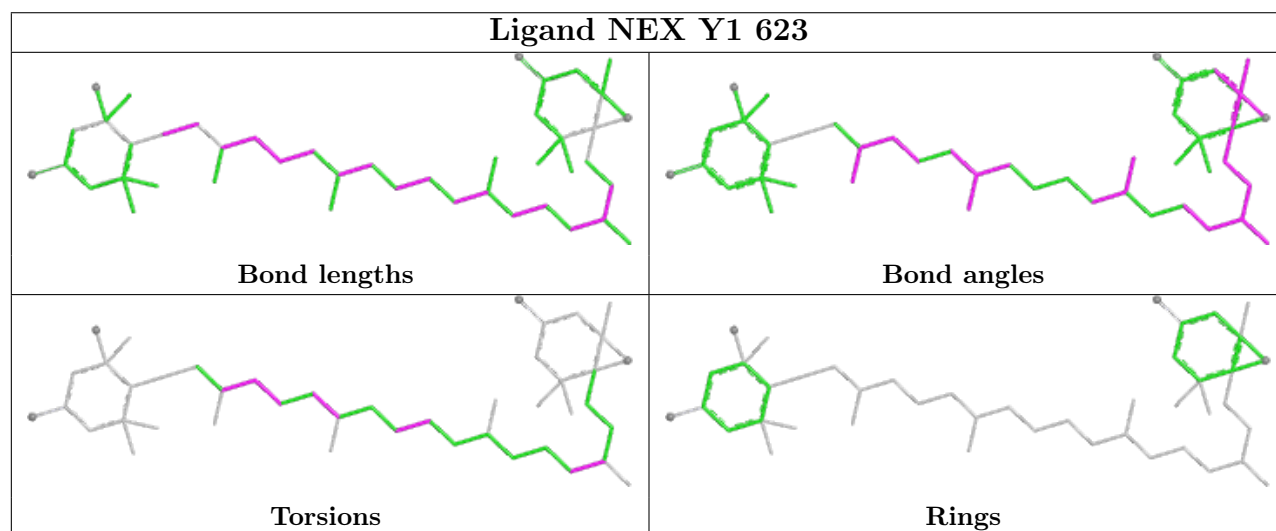
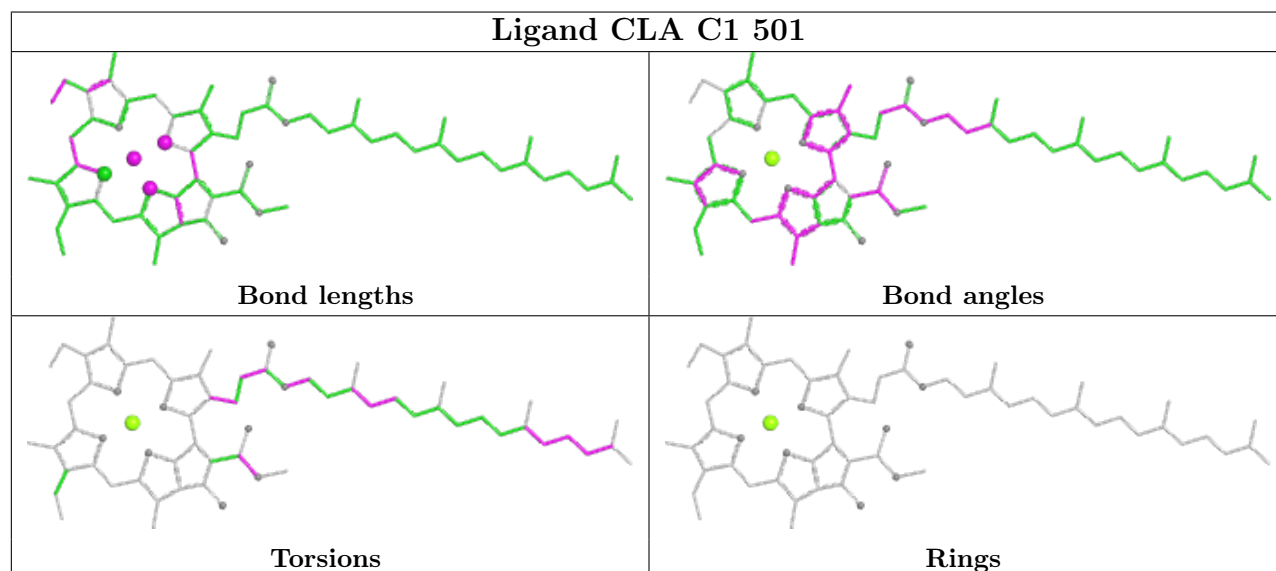
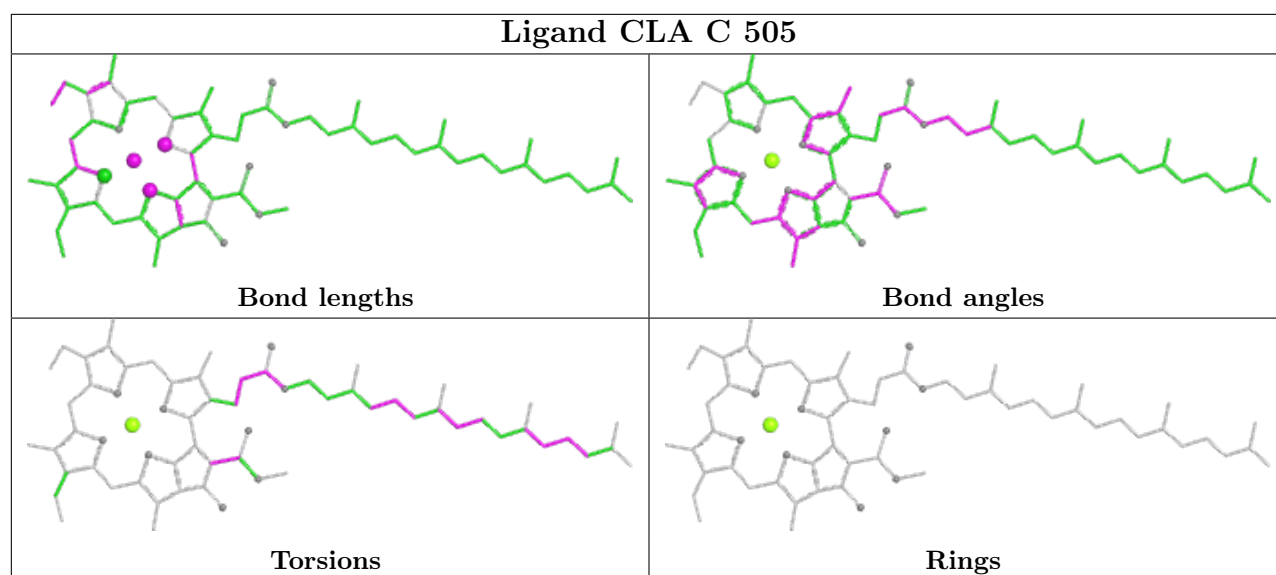




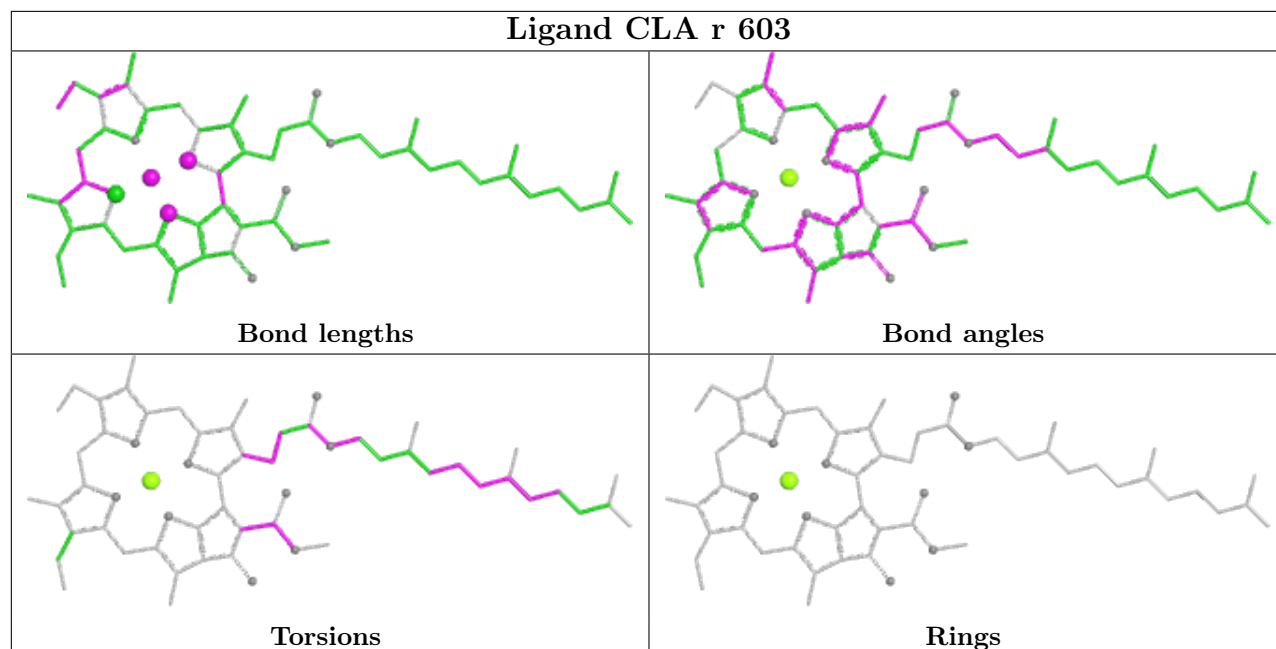




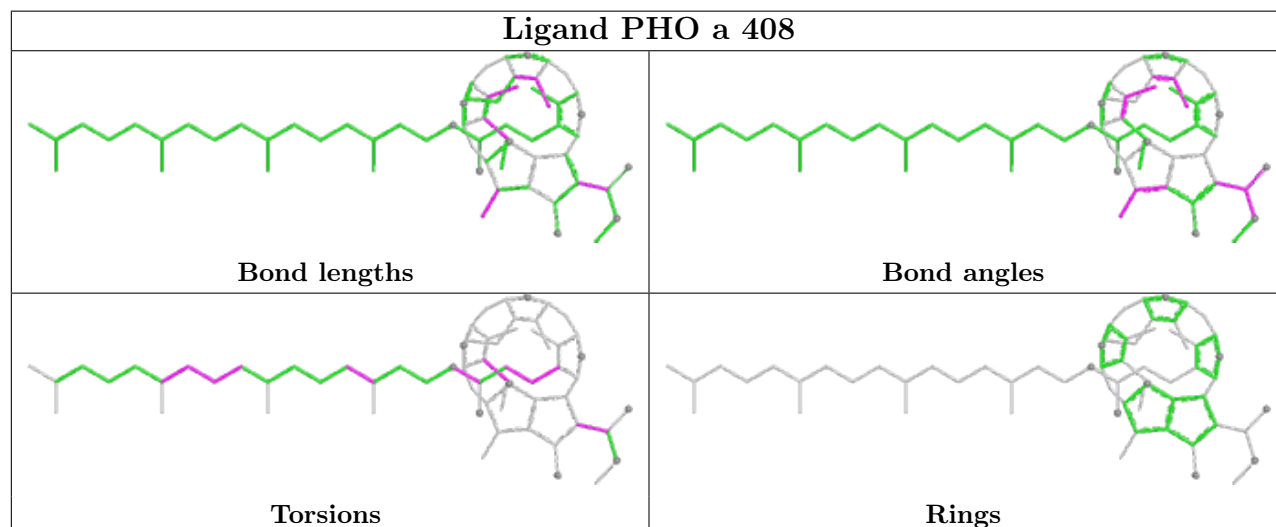




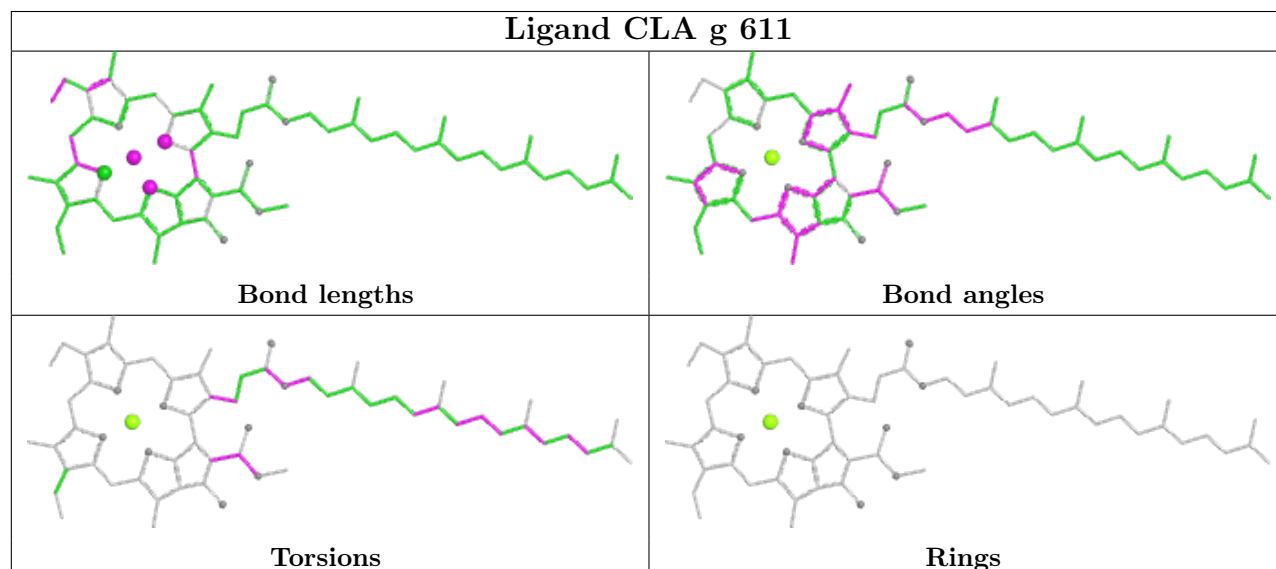
Ligand CLA r 603

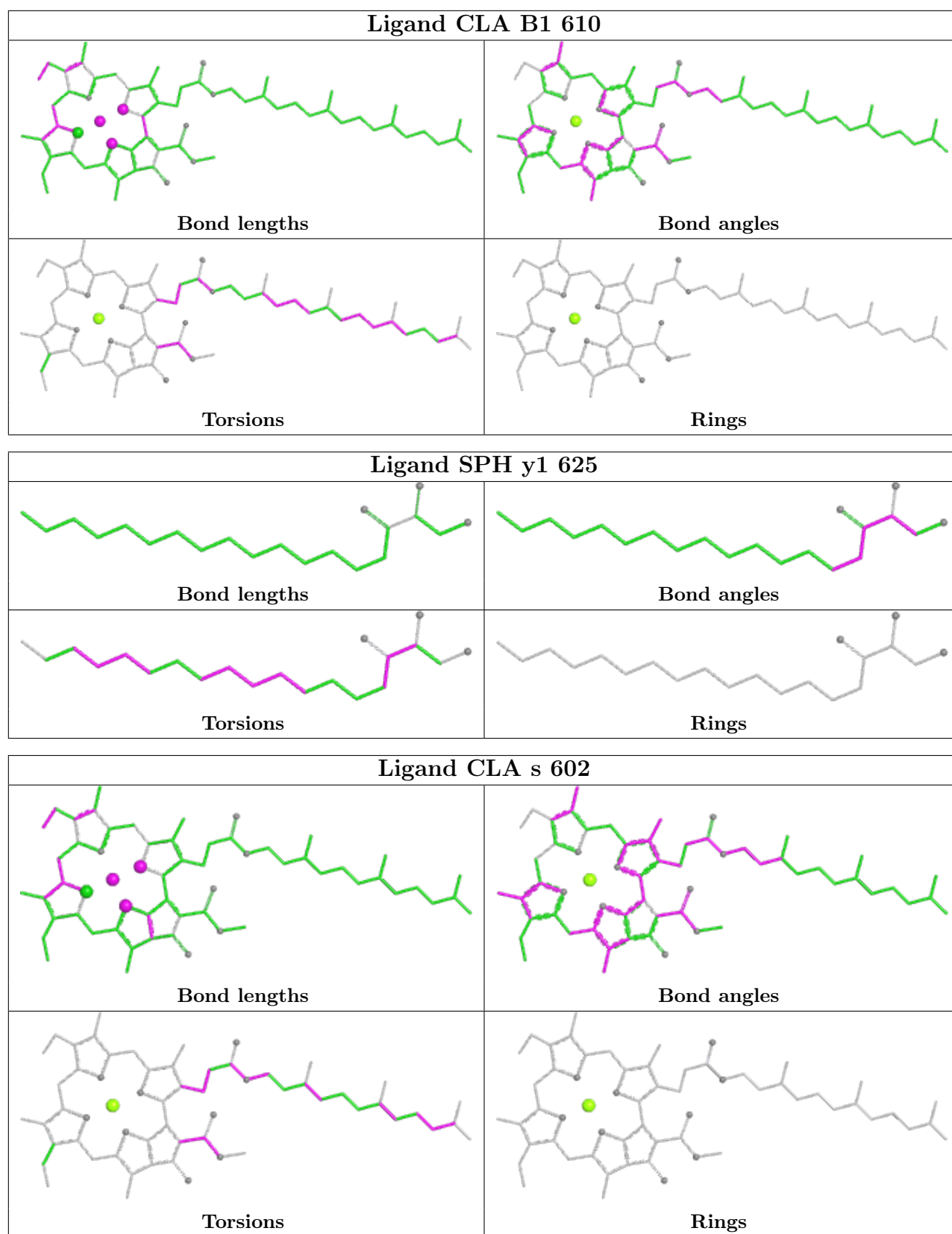


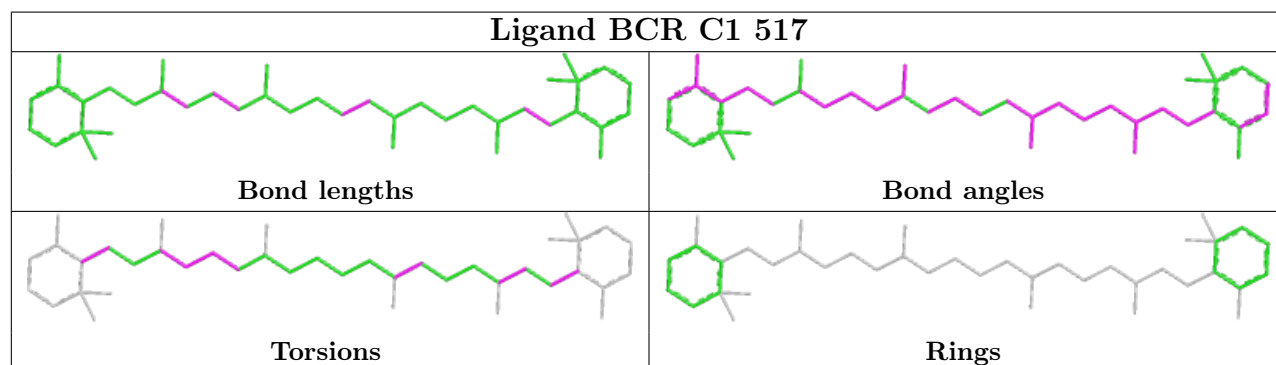
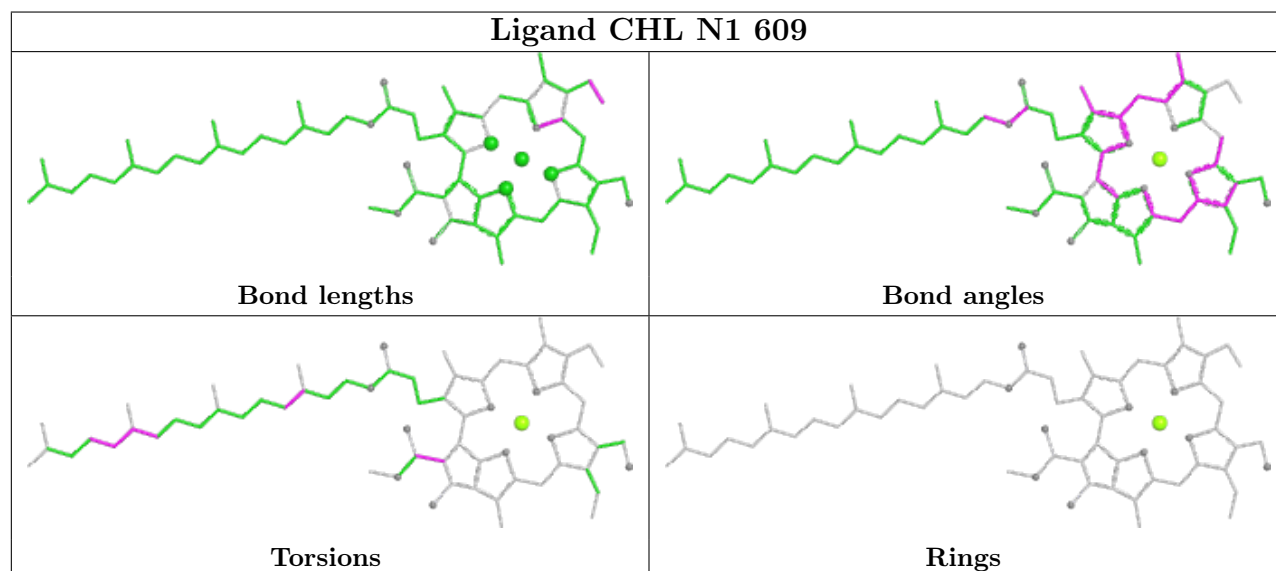
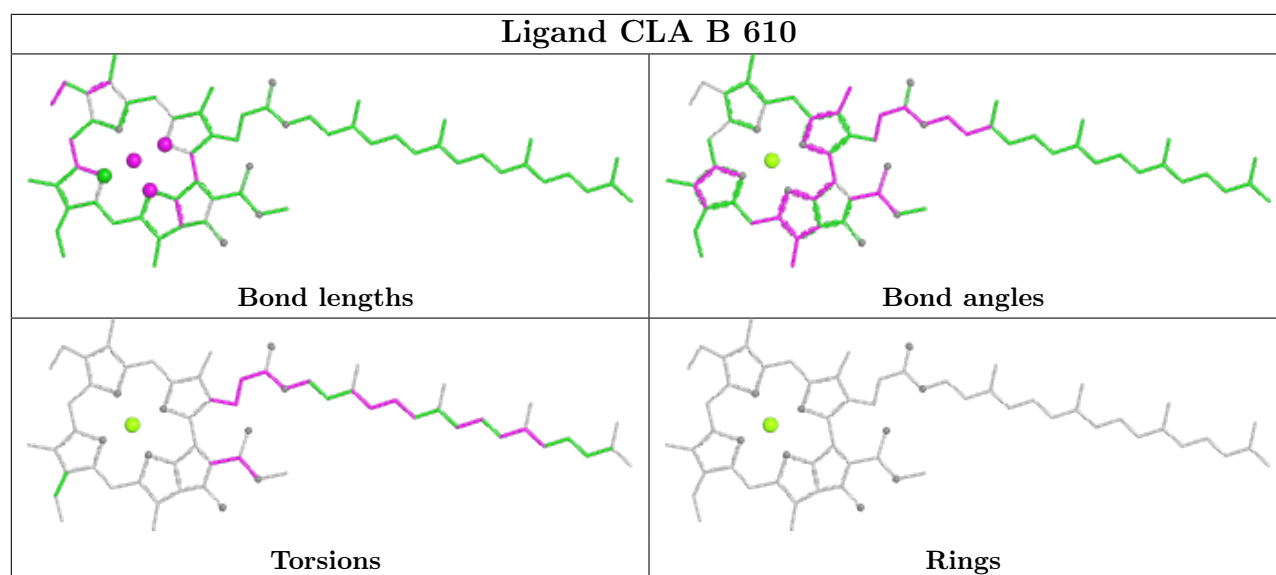
Ligand PHO a 408

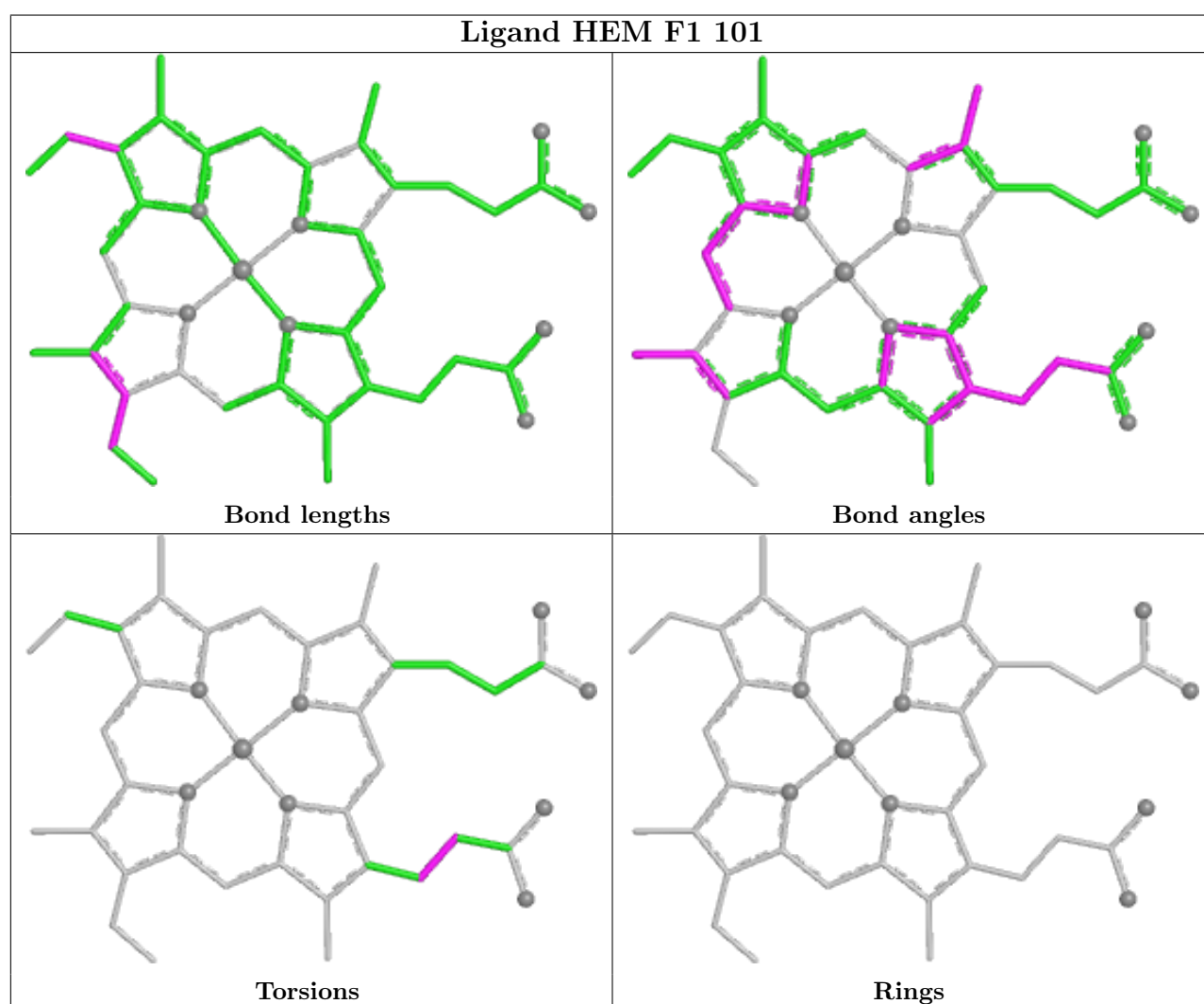
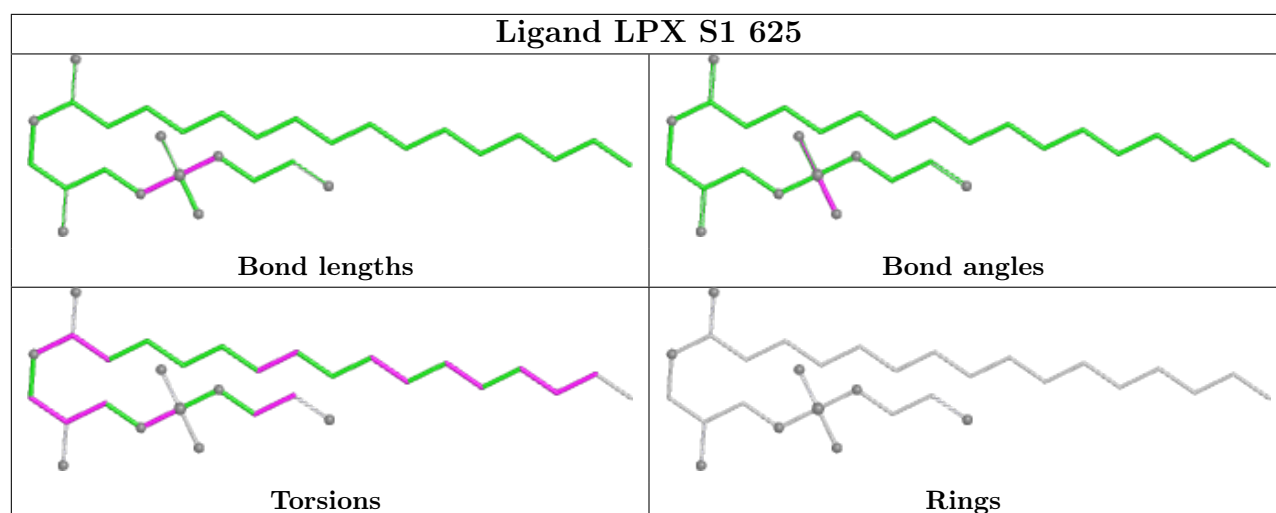


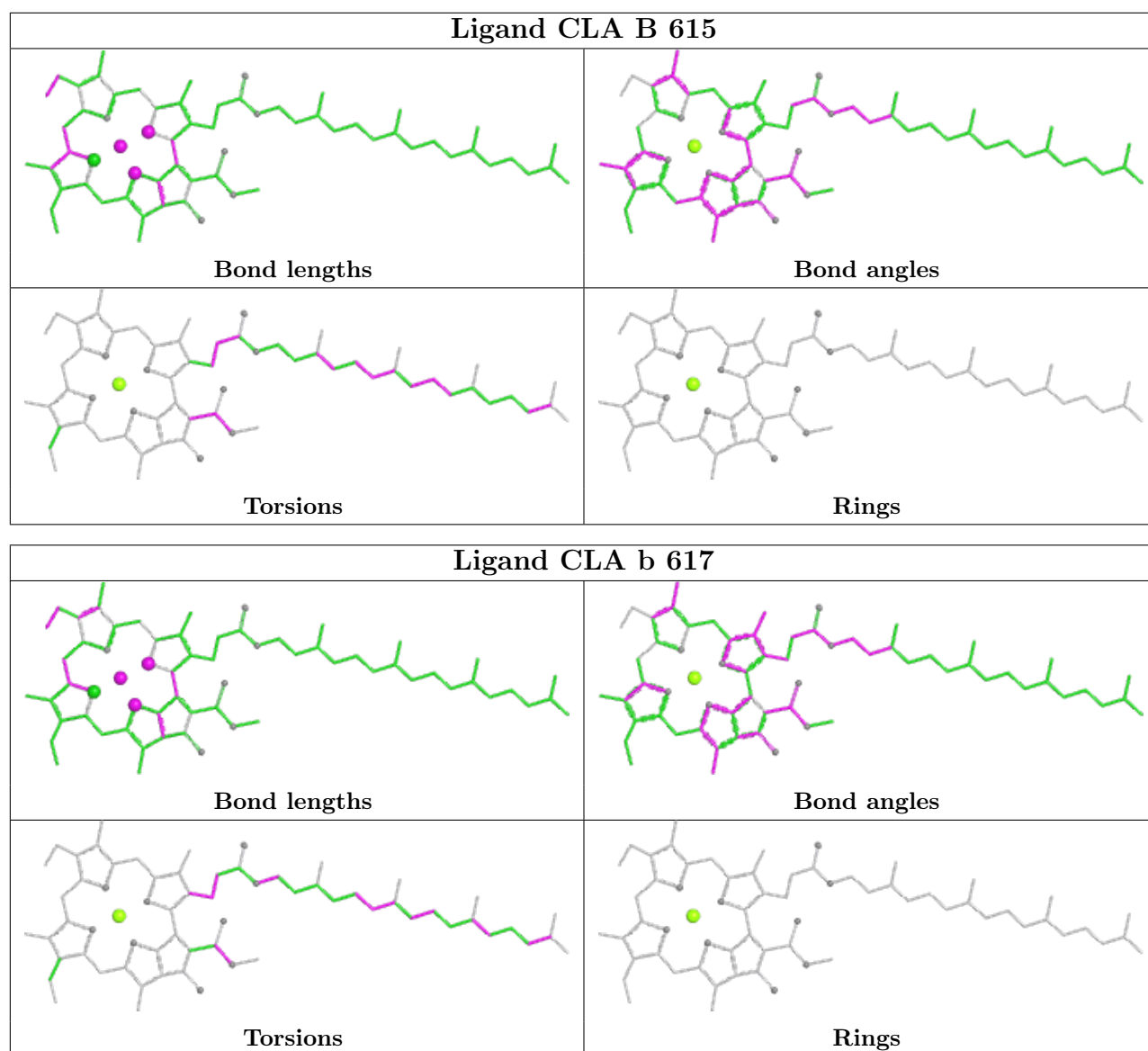
Ligand CLA g 611

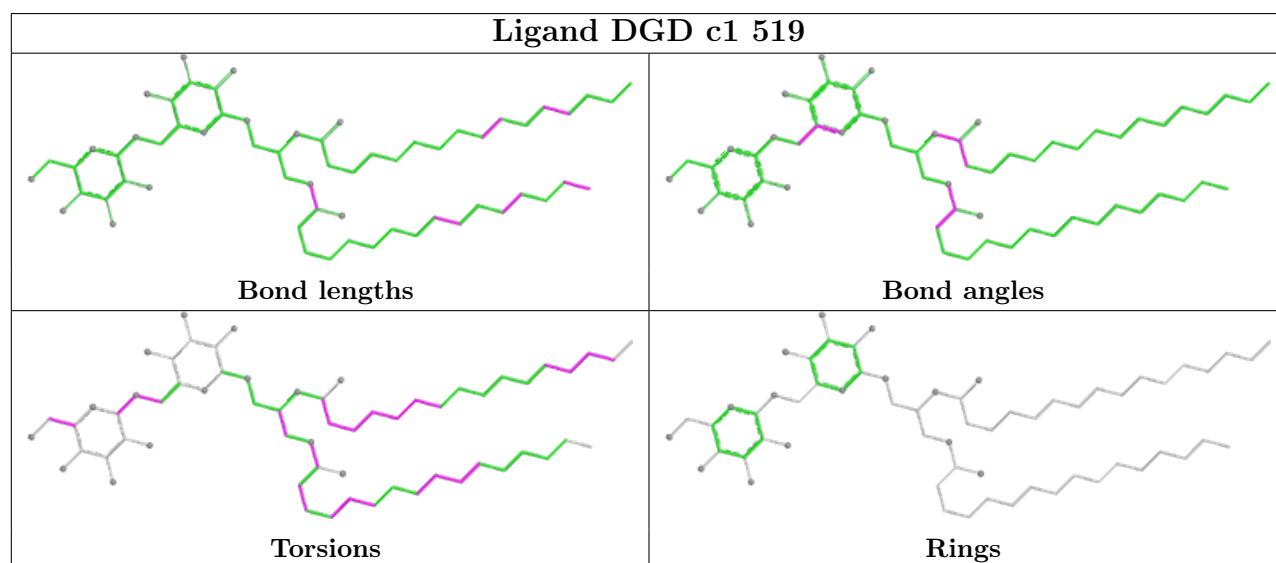
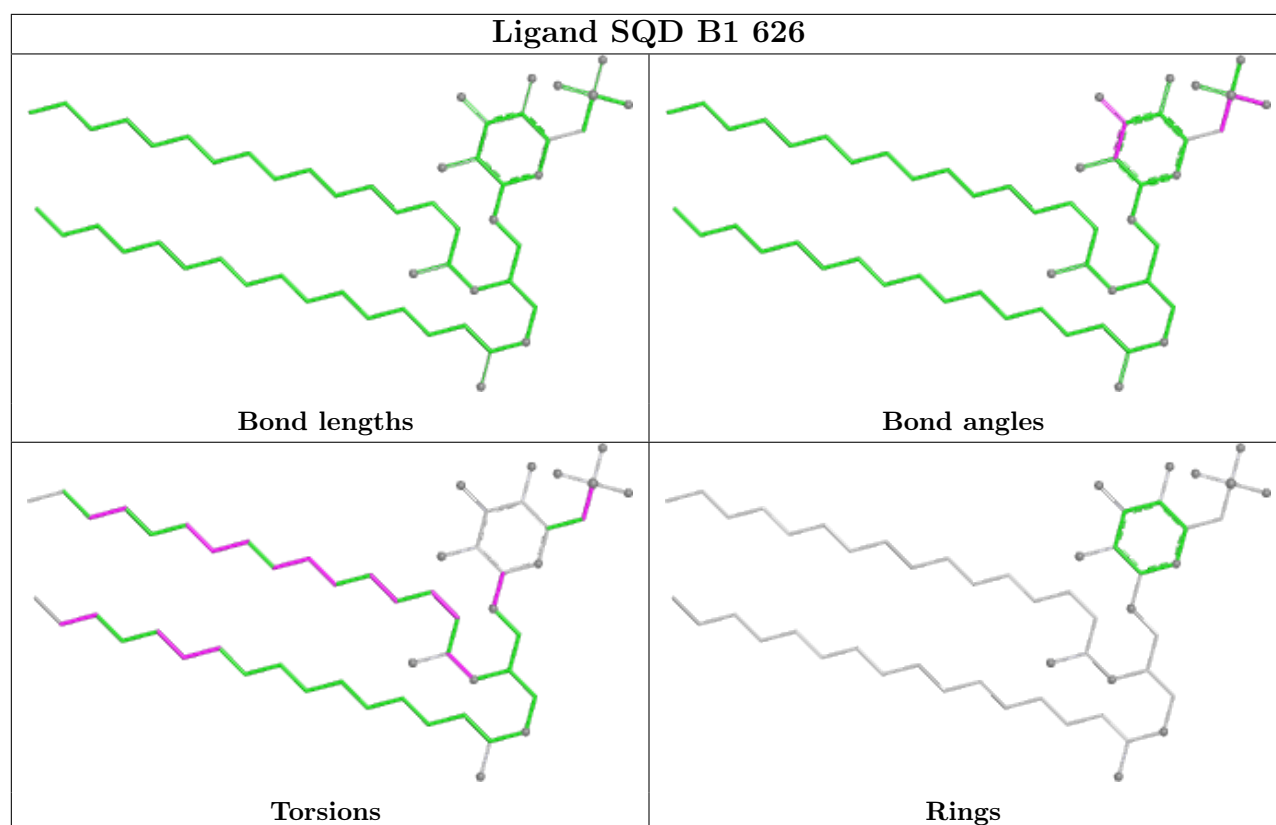


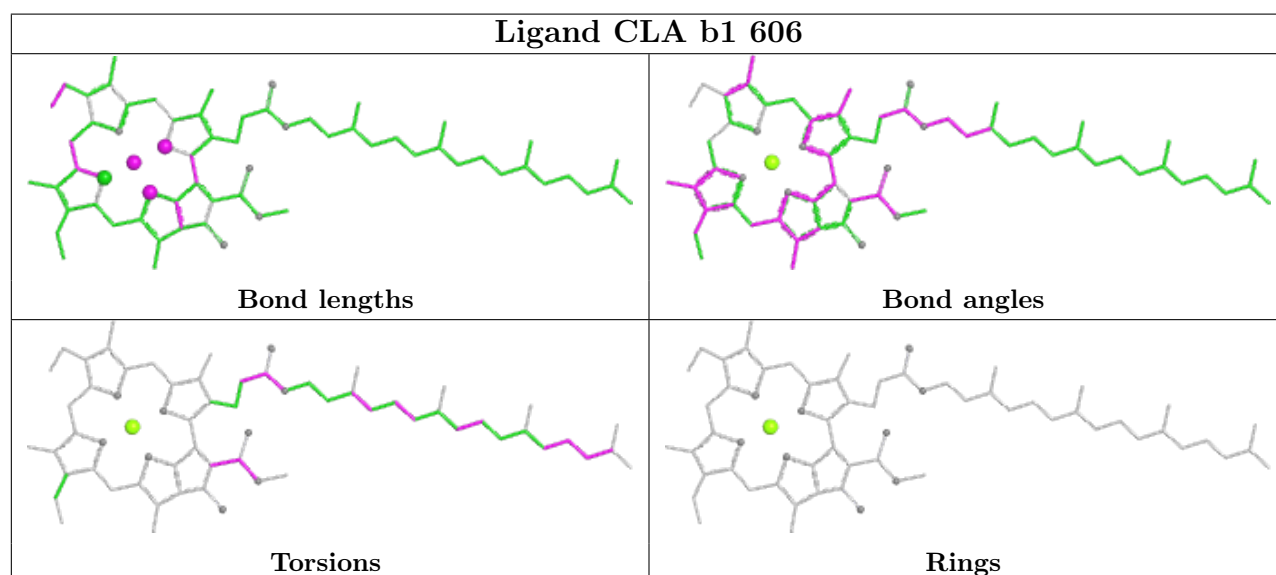
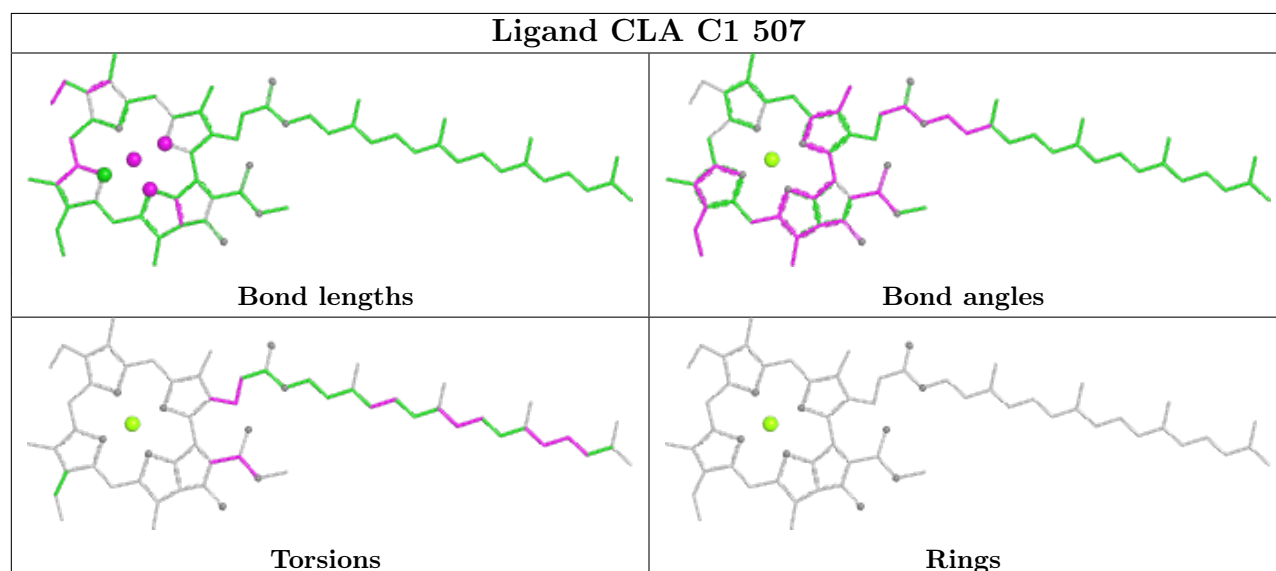
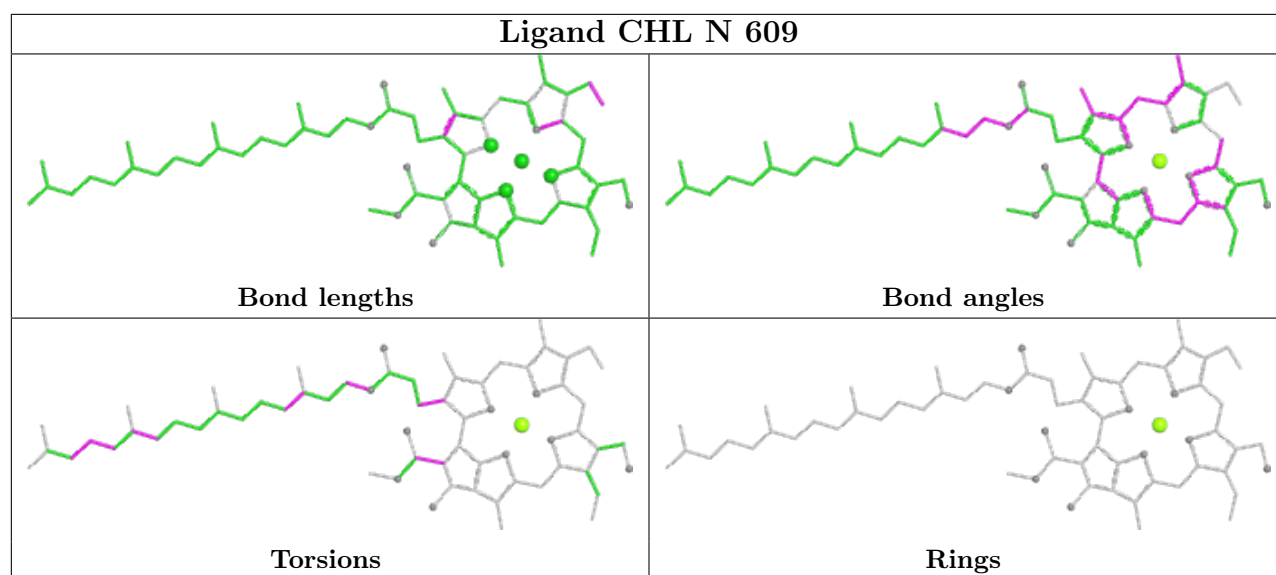


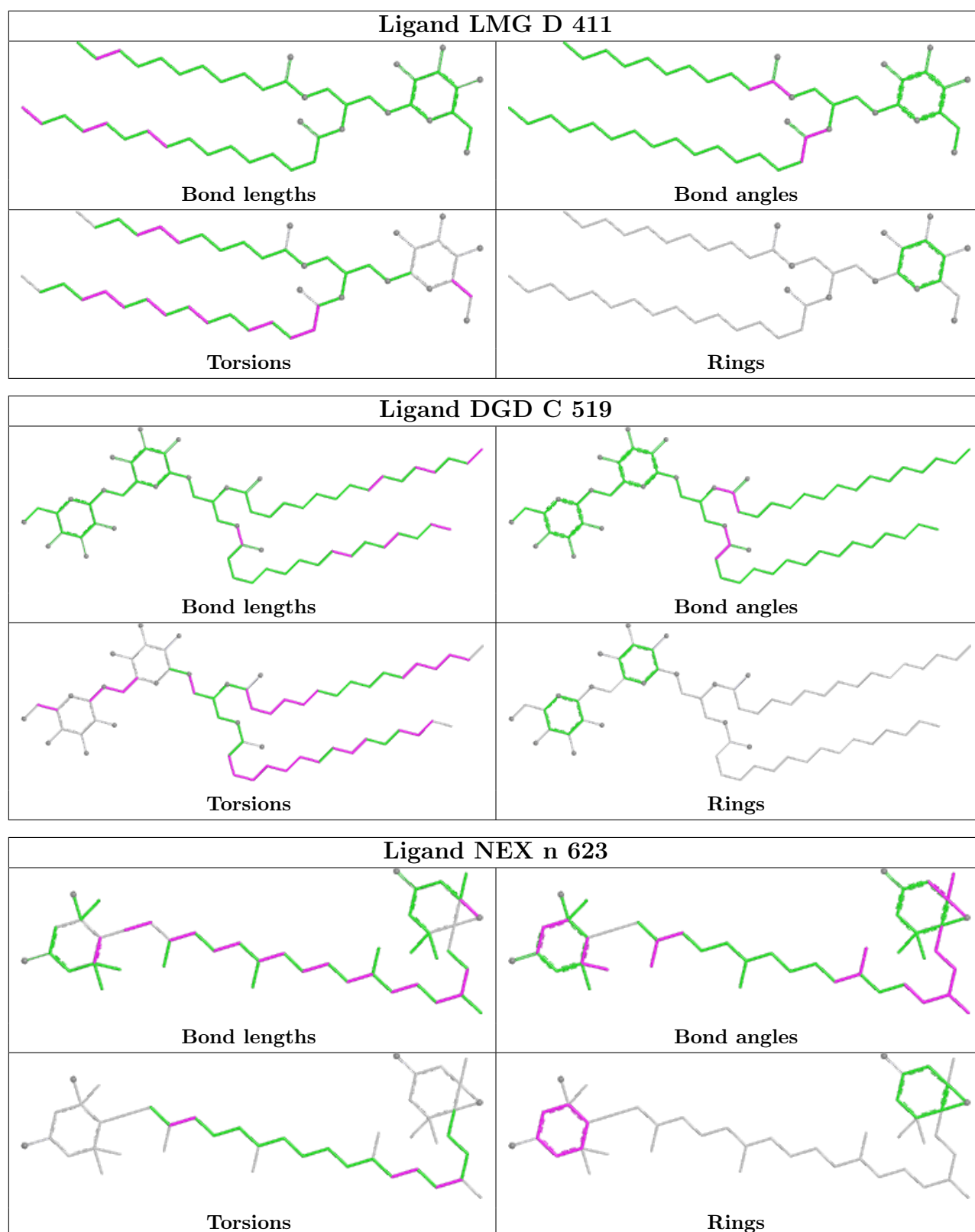


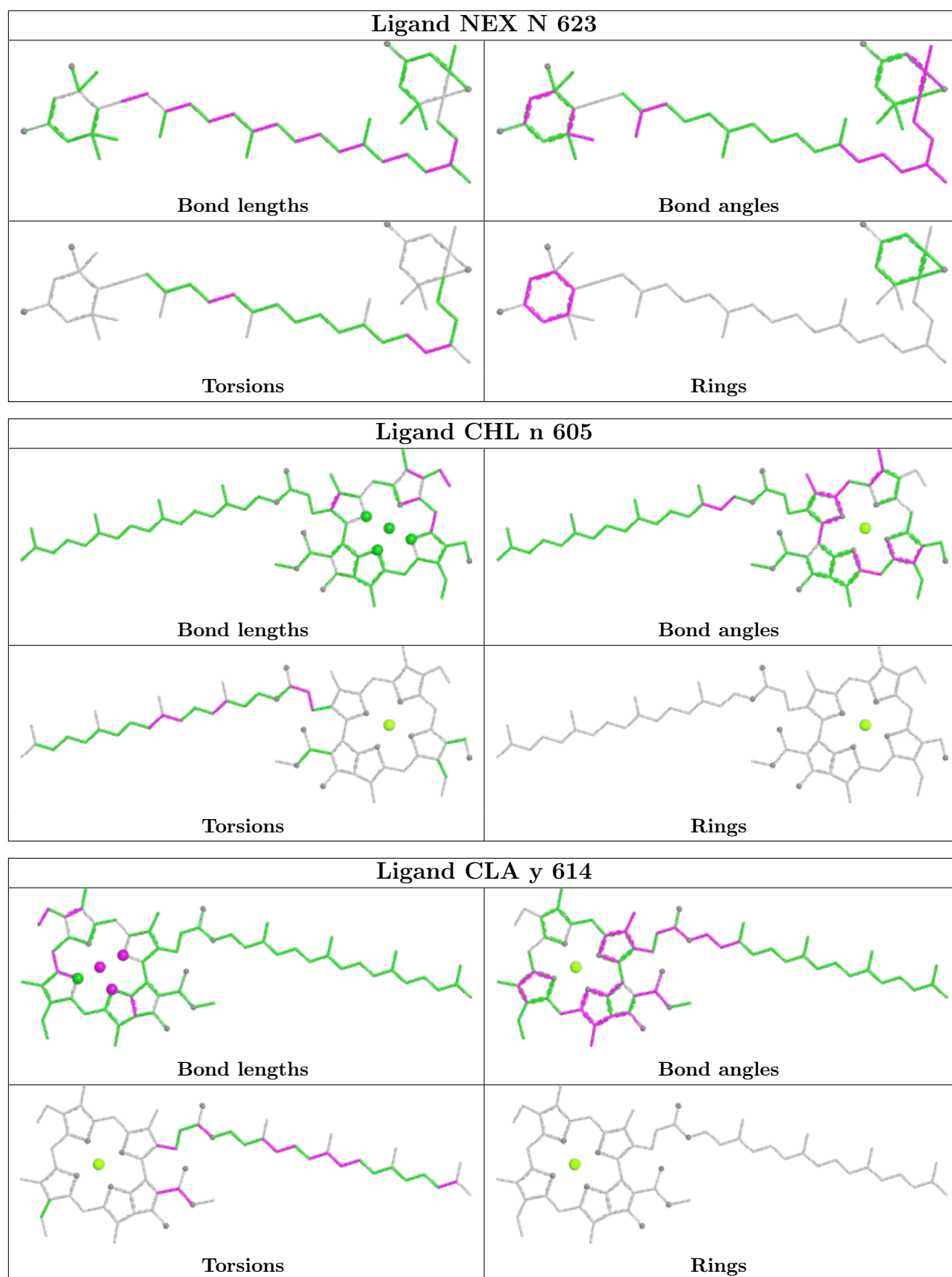


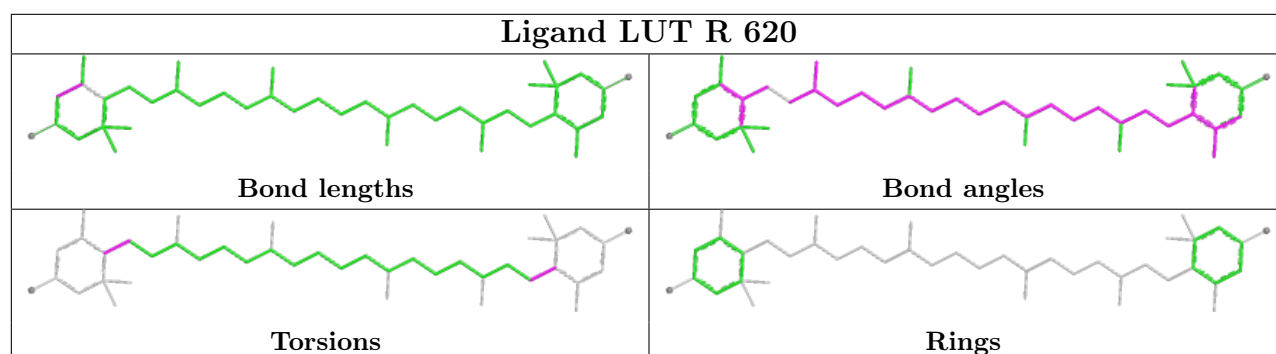
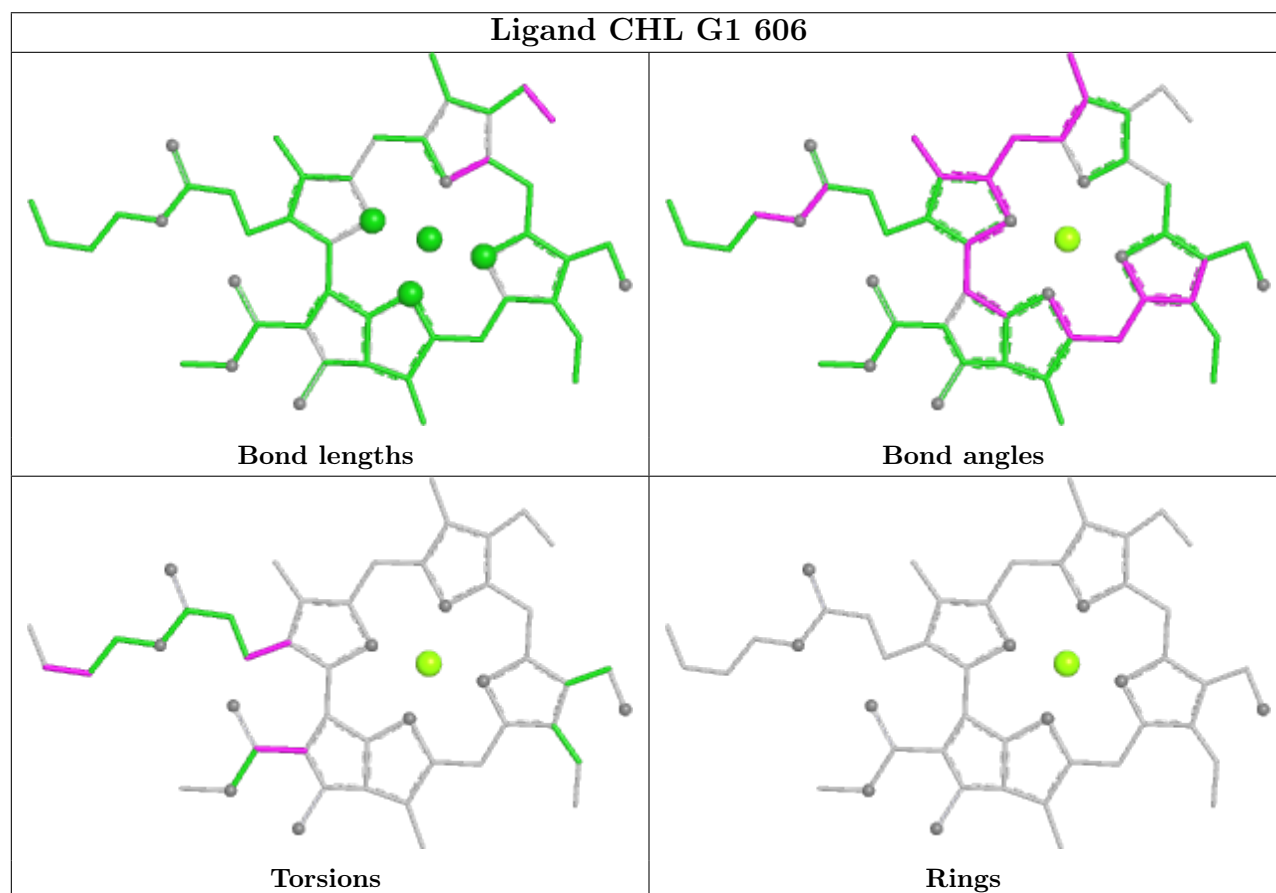
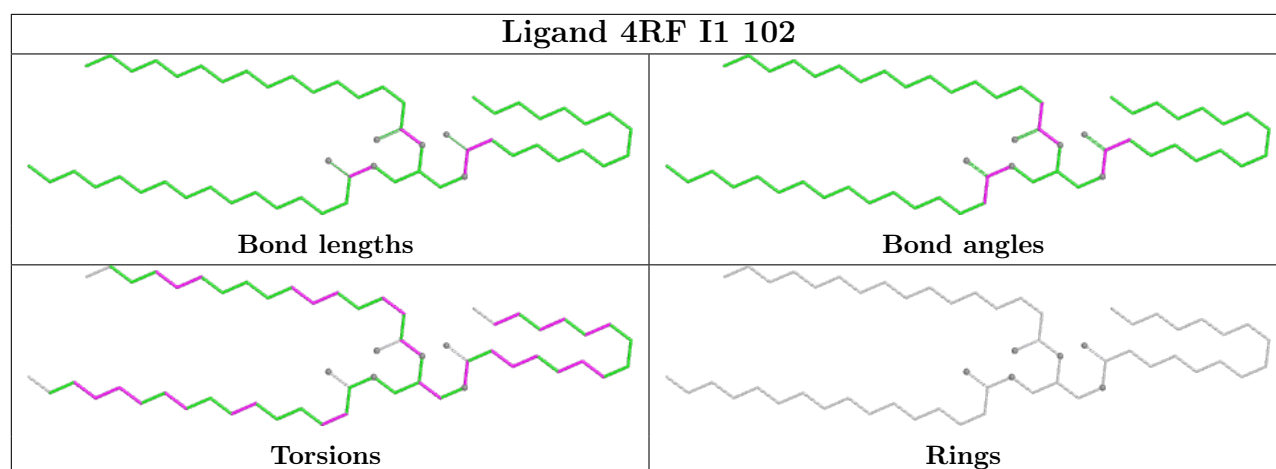


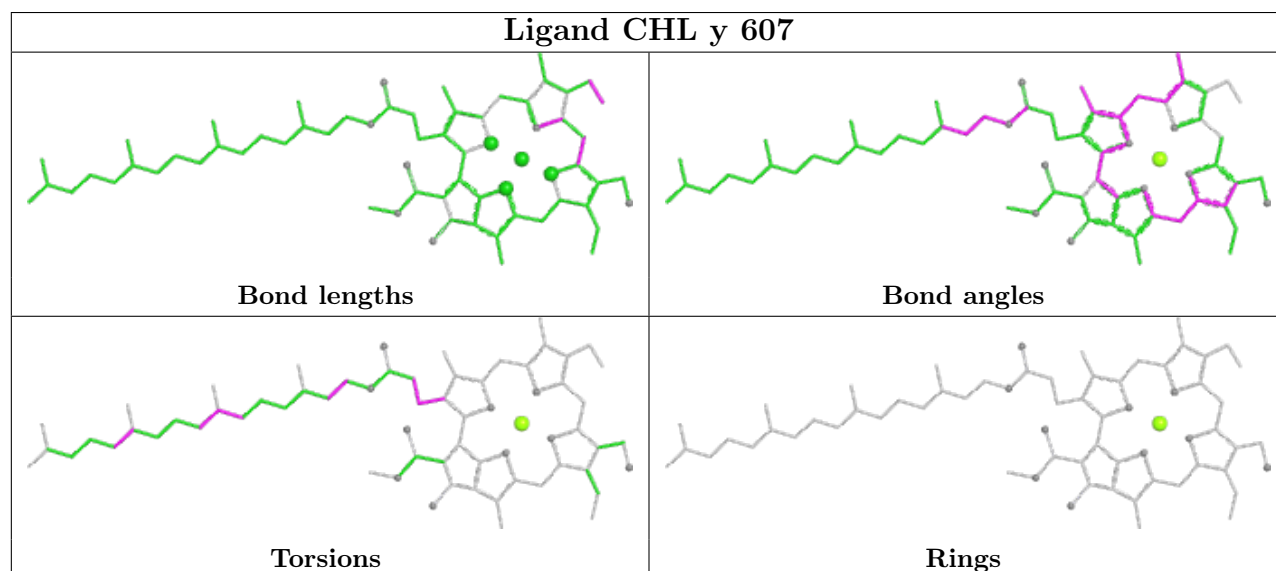
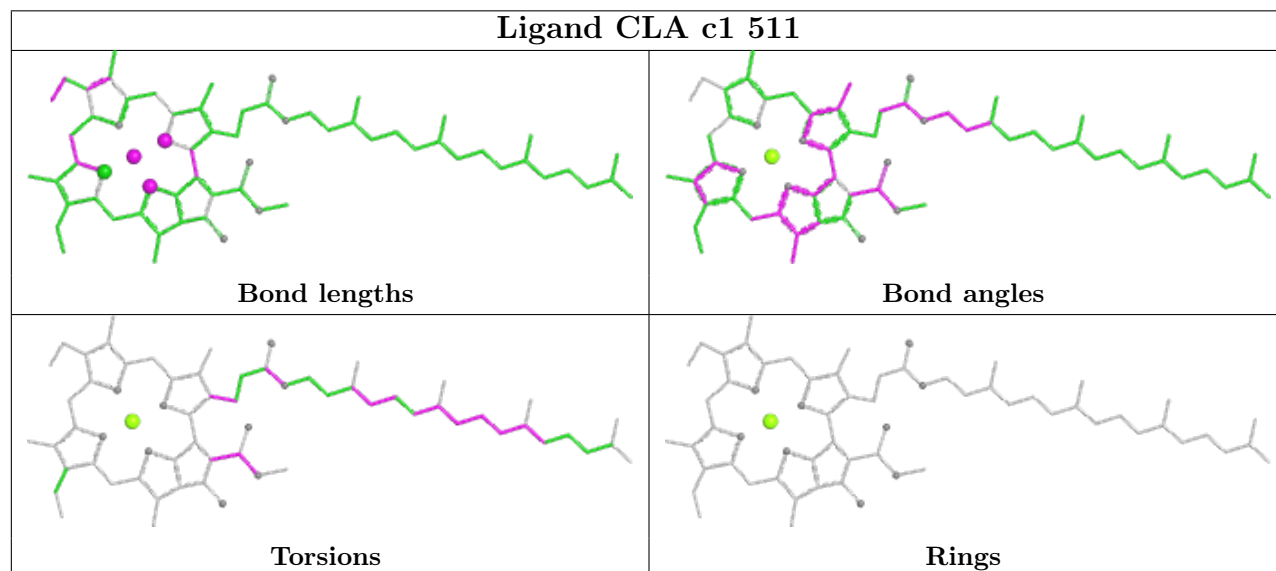
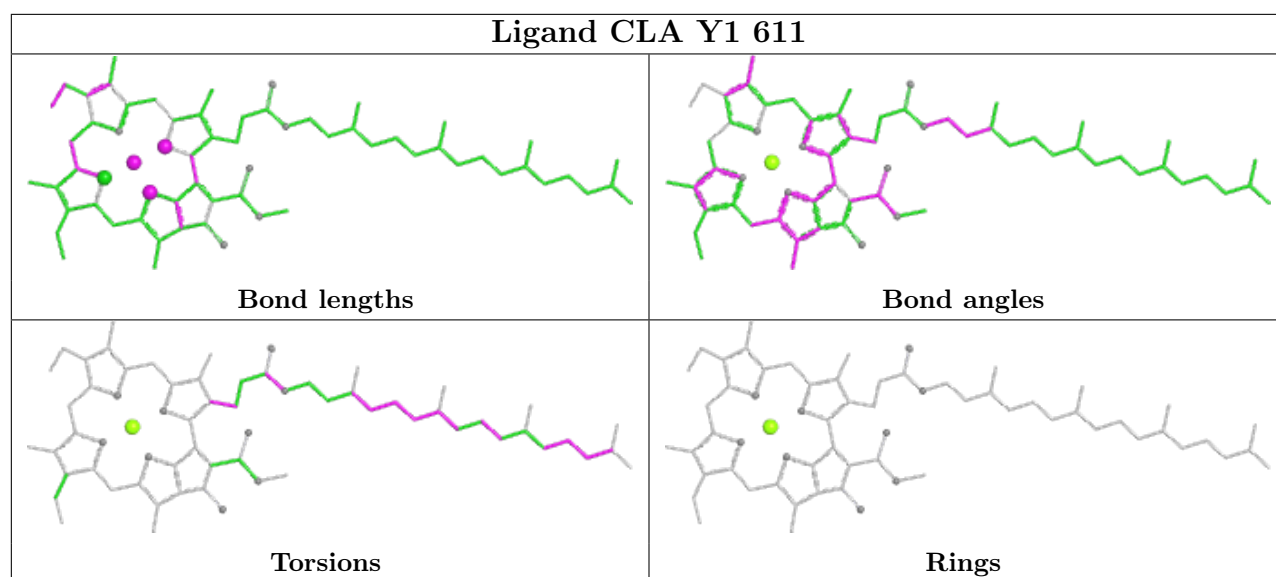


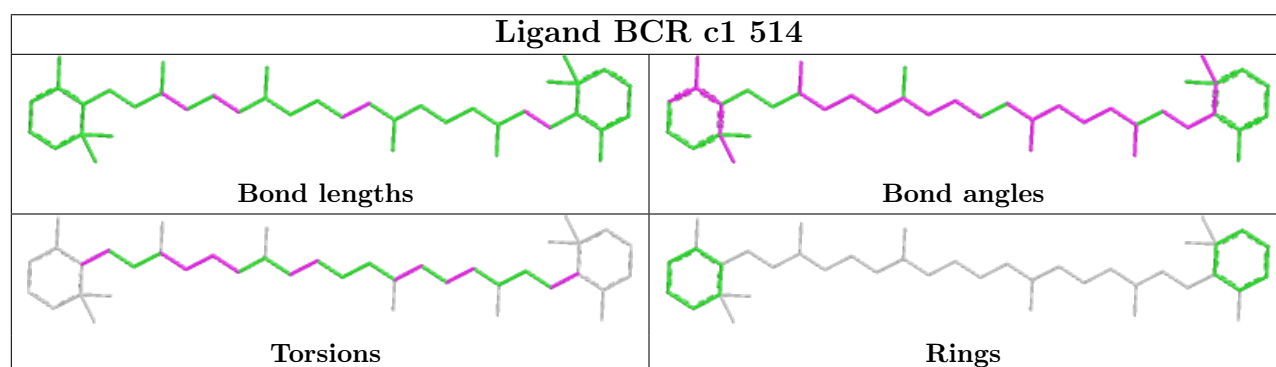
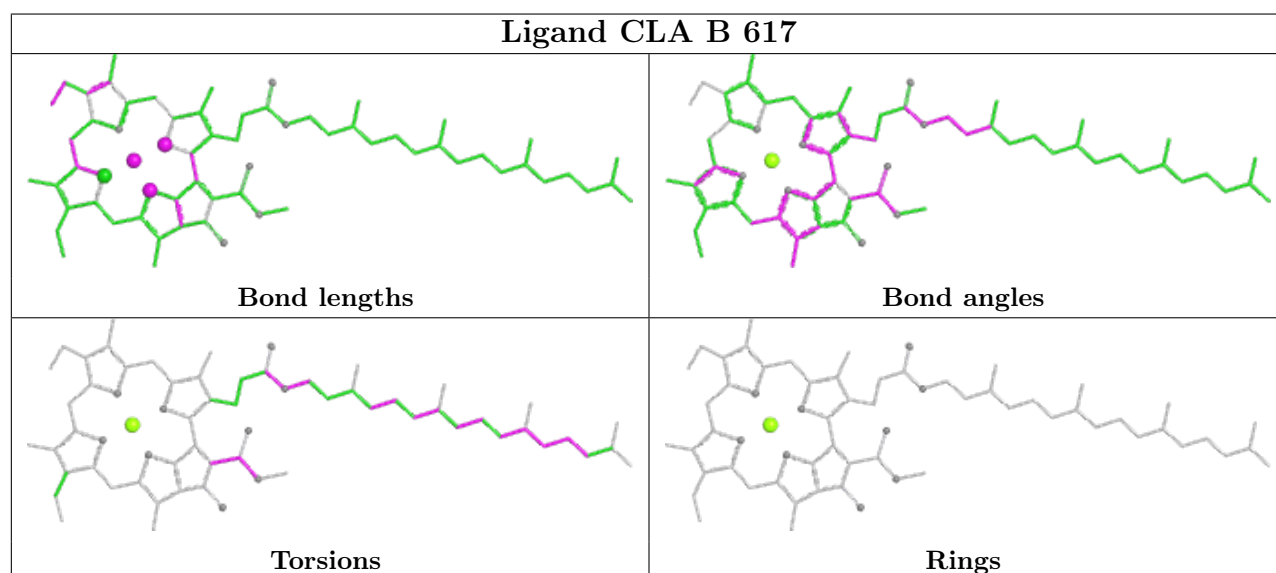
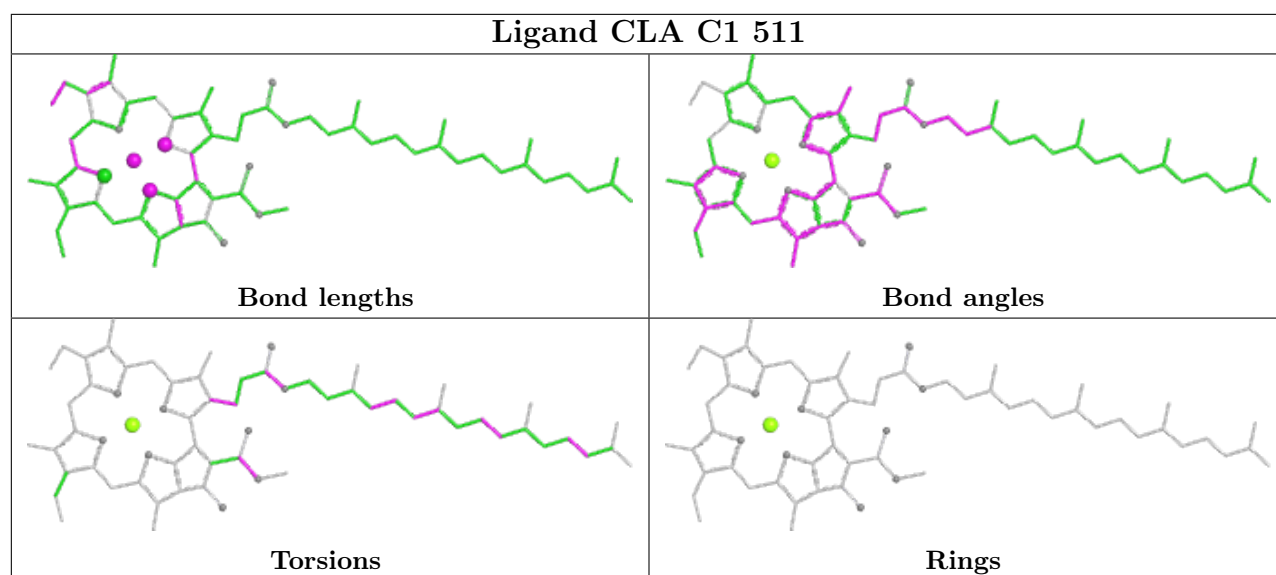


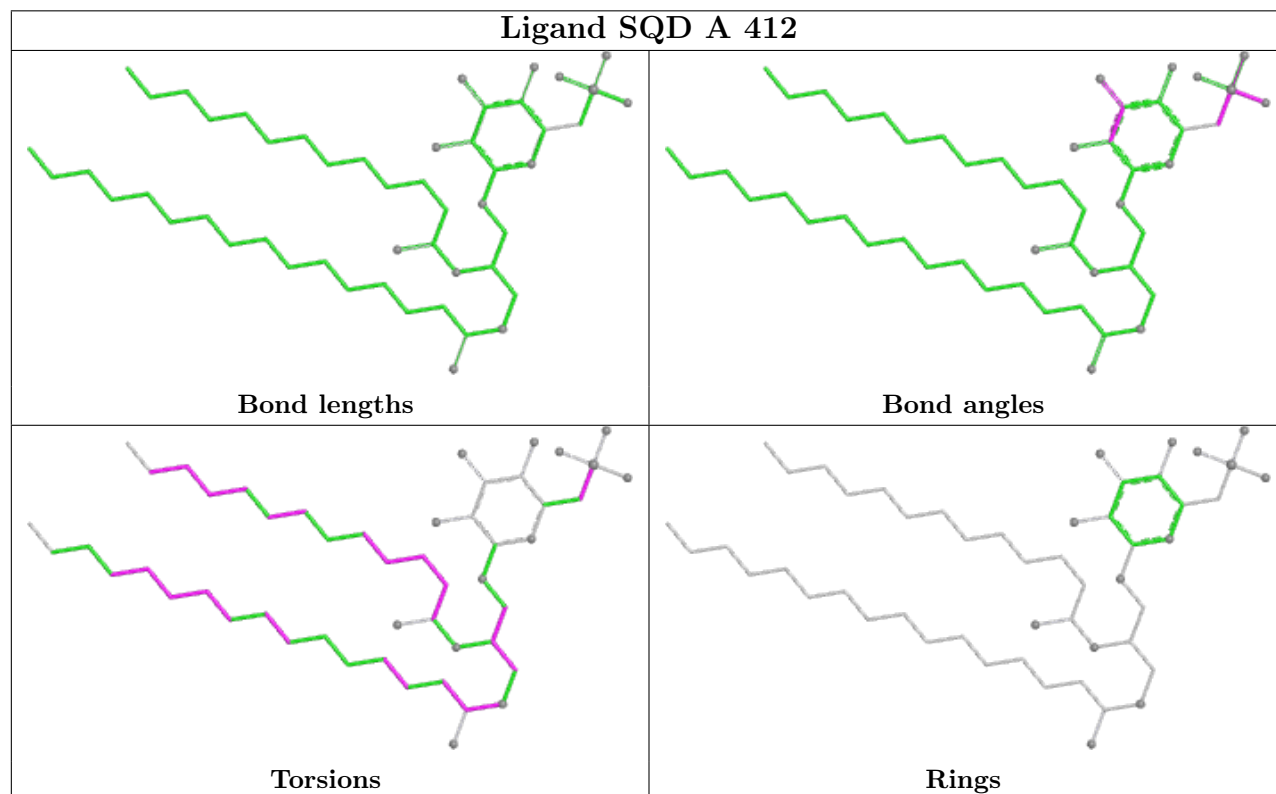
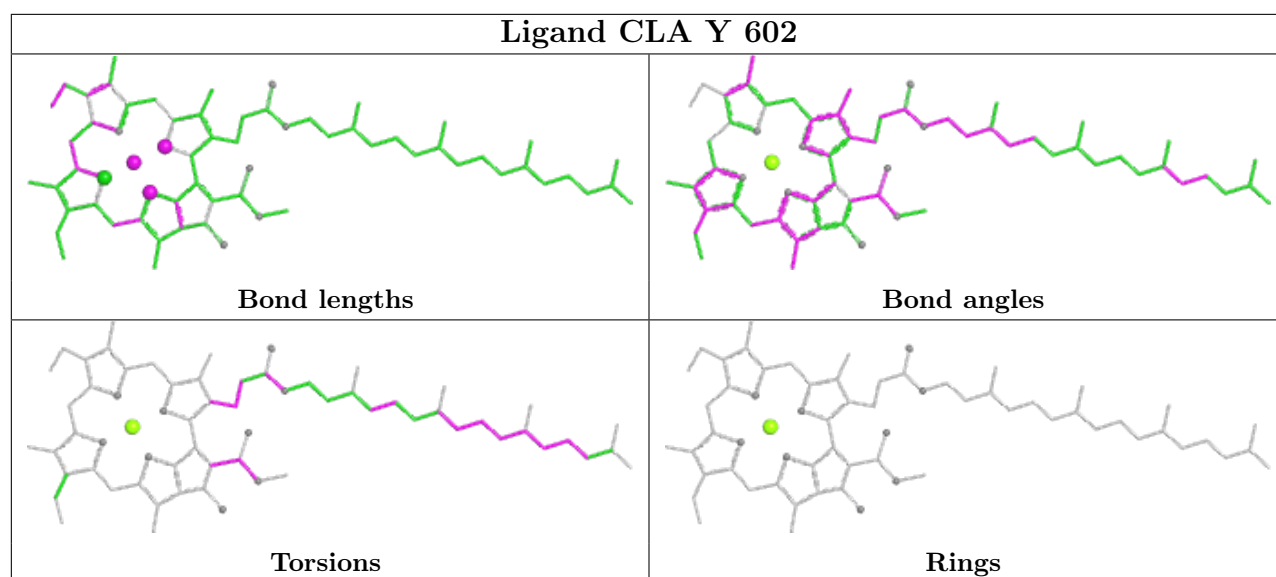


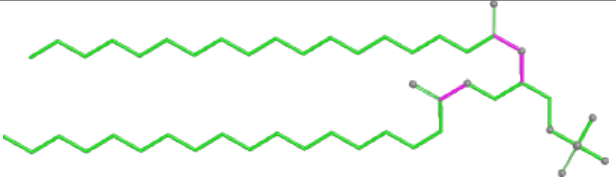
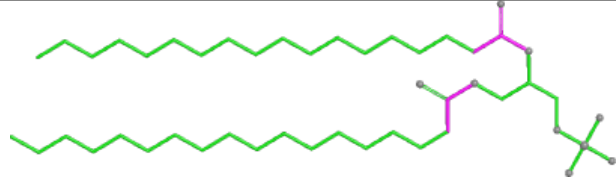
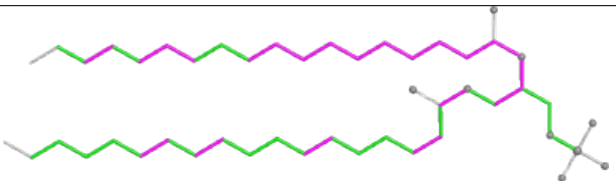
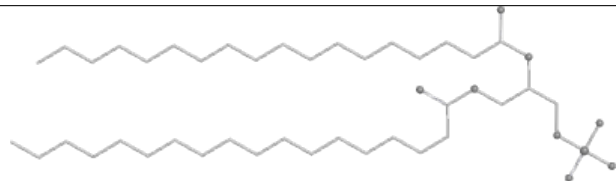


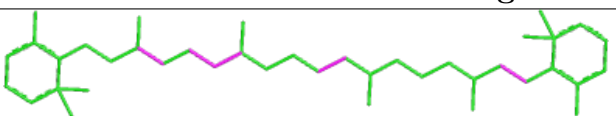
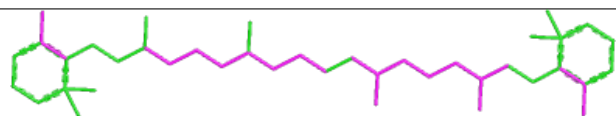
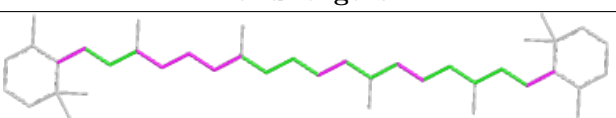
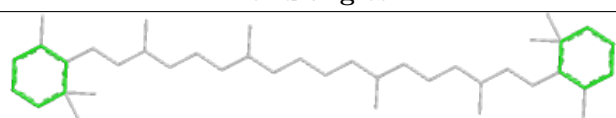


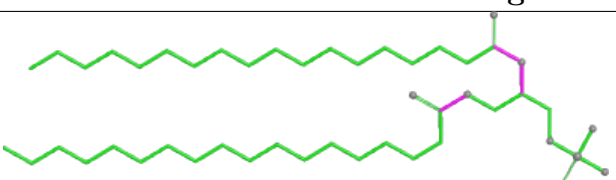
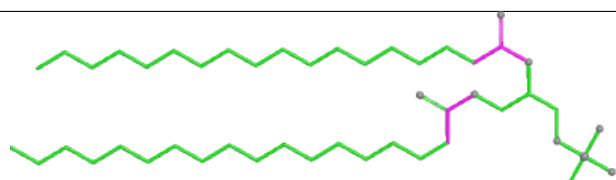
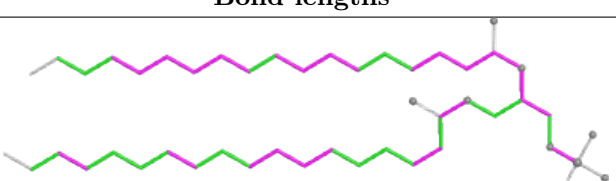
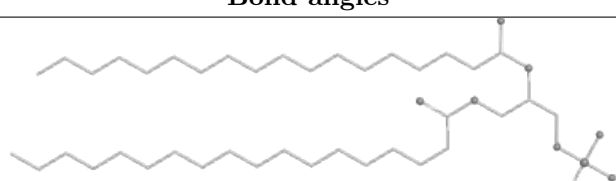


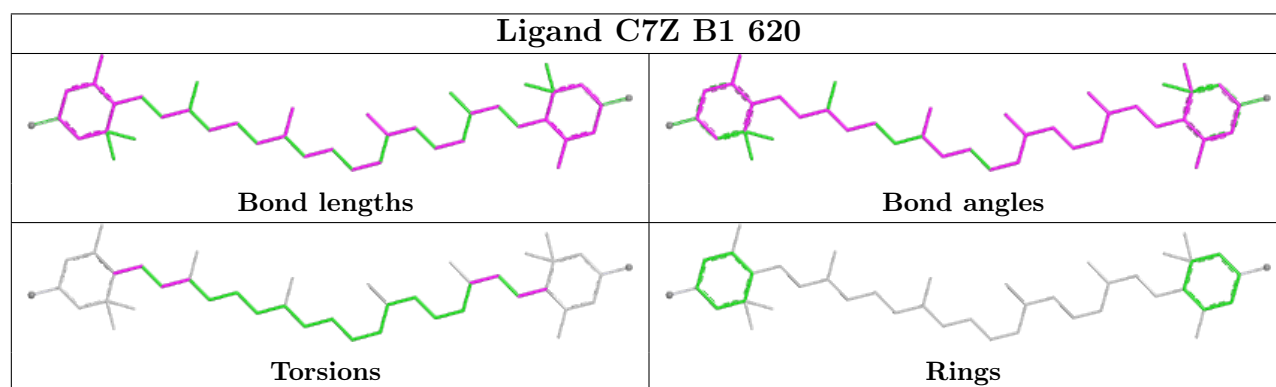
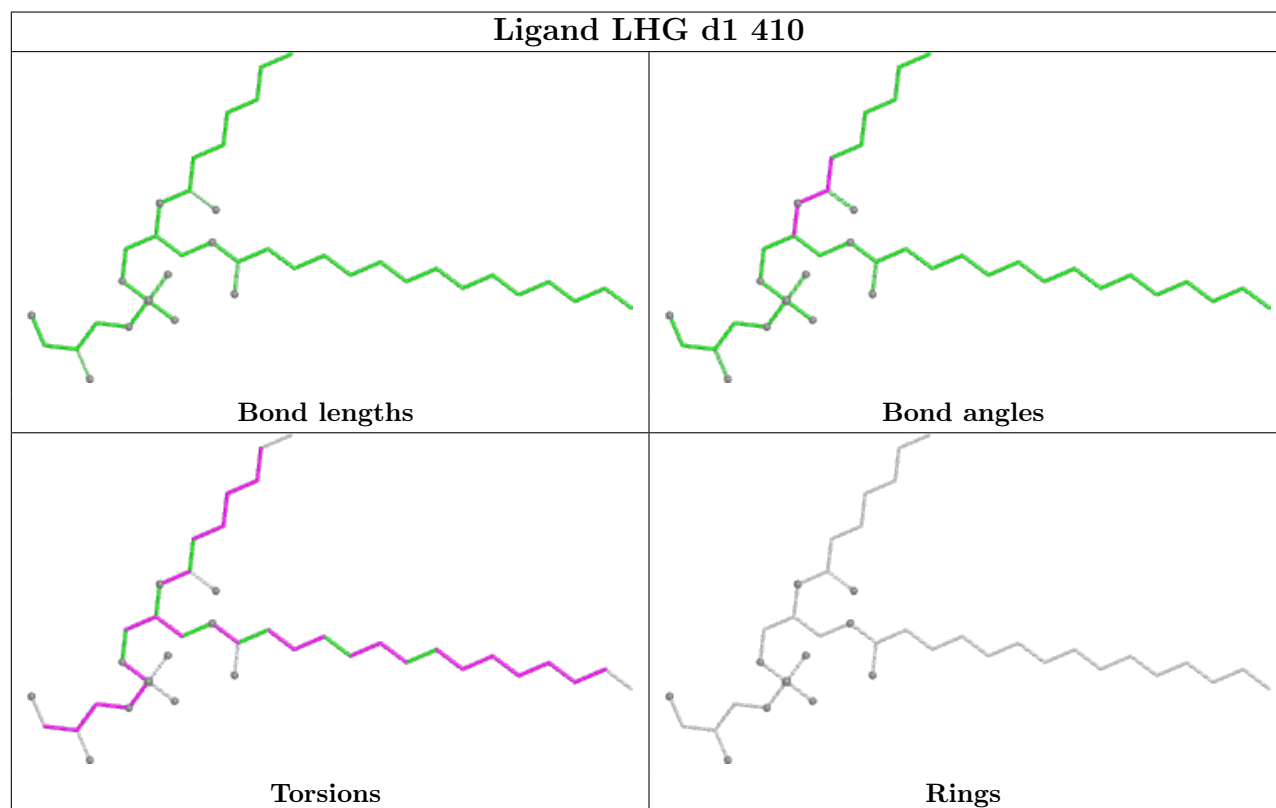
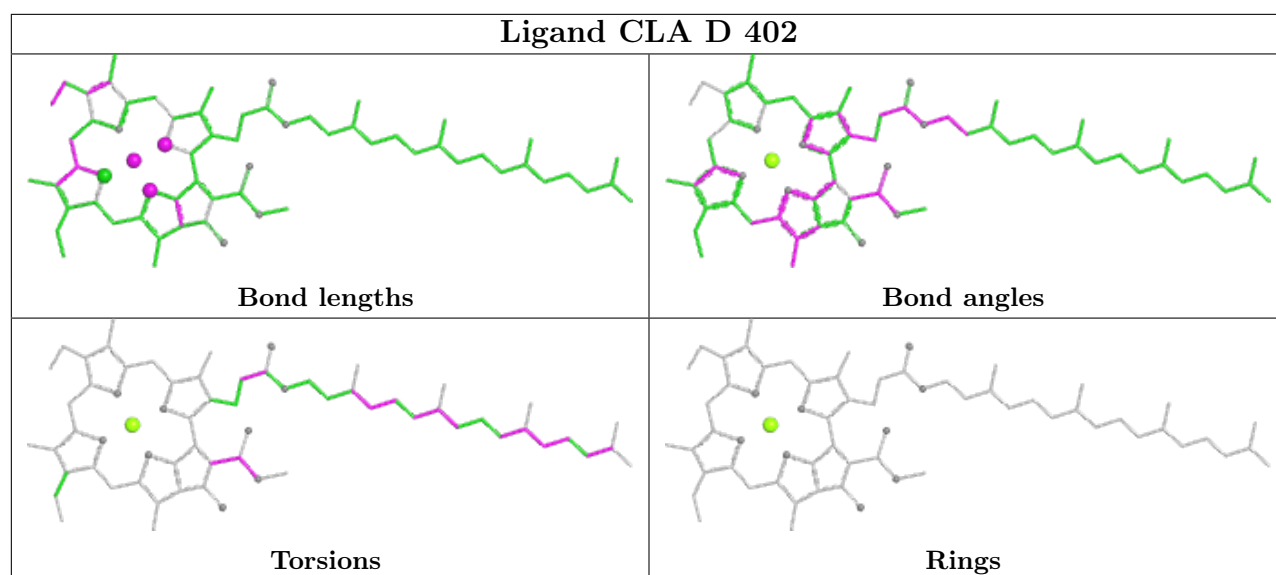


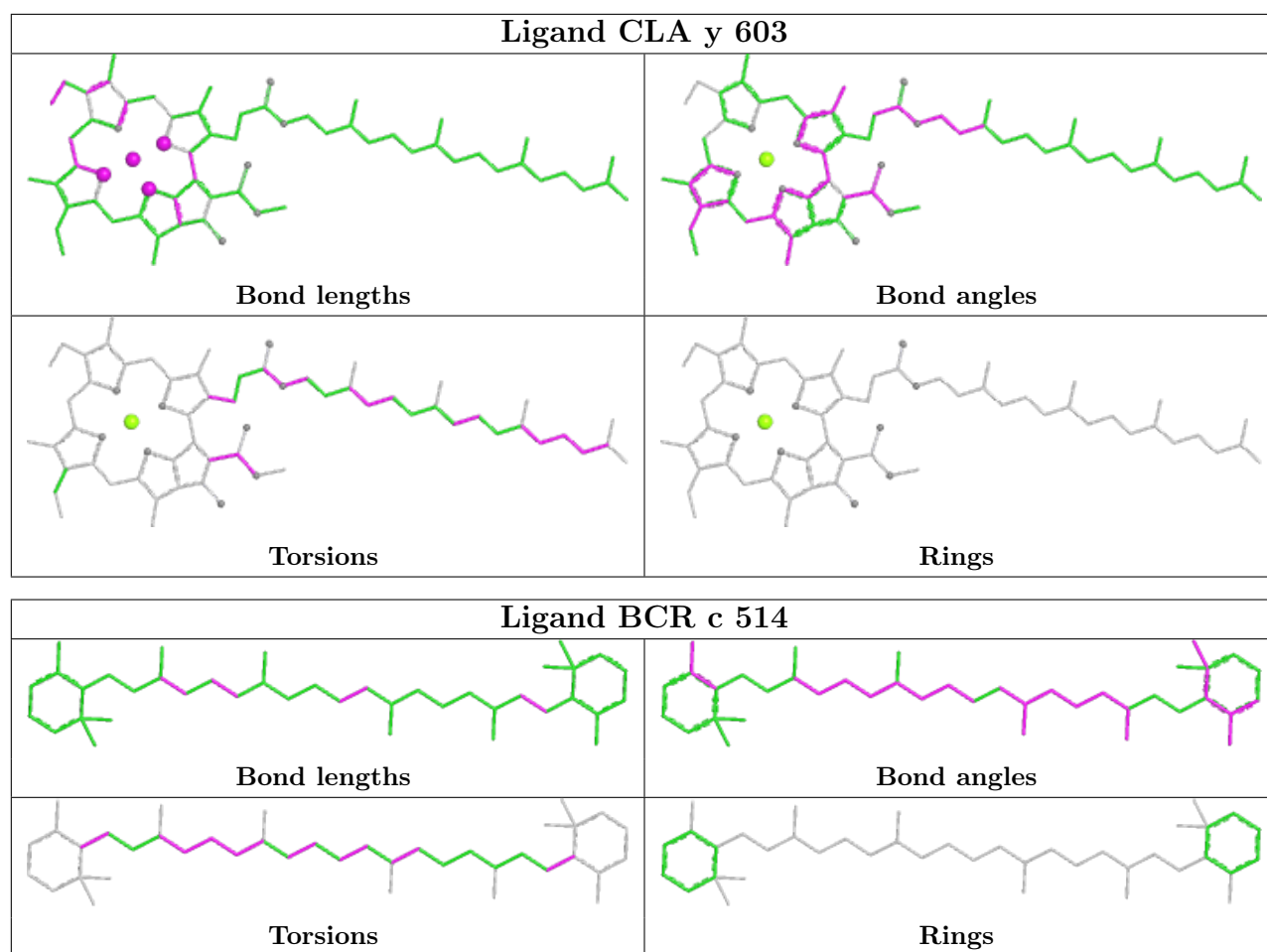


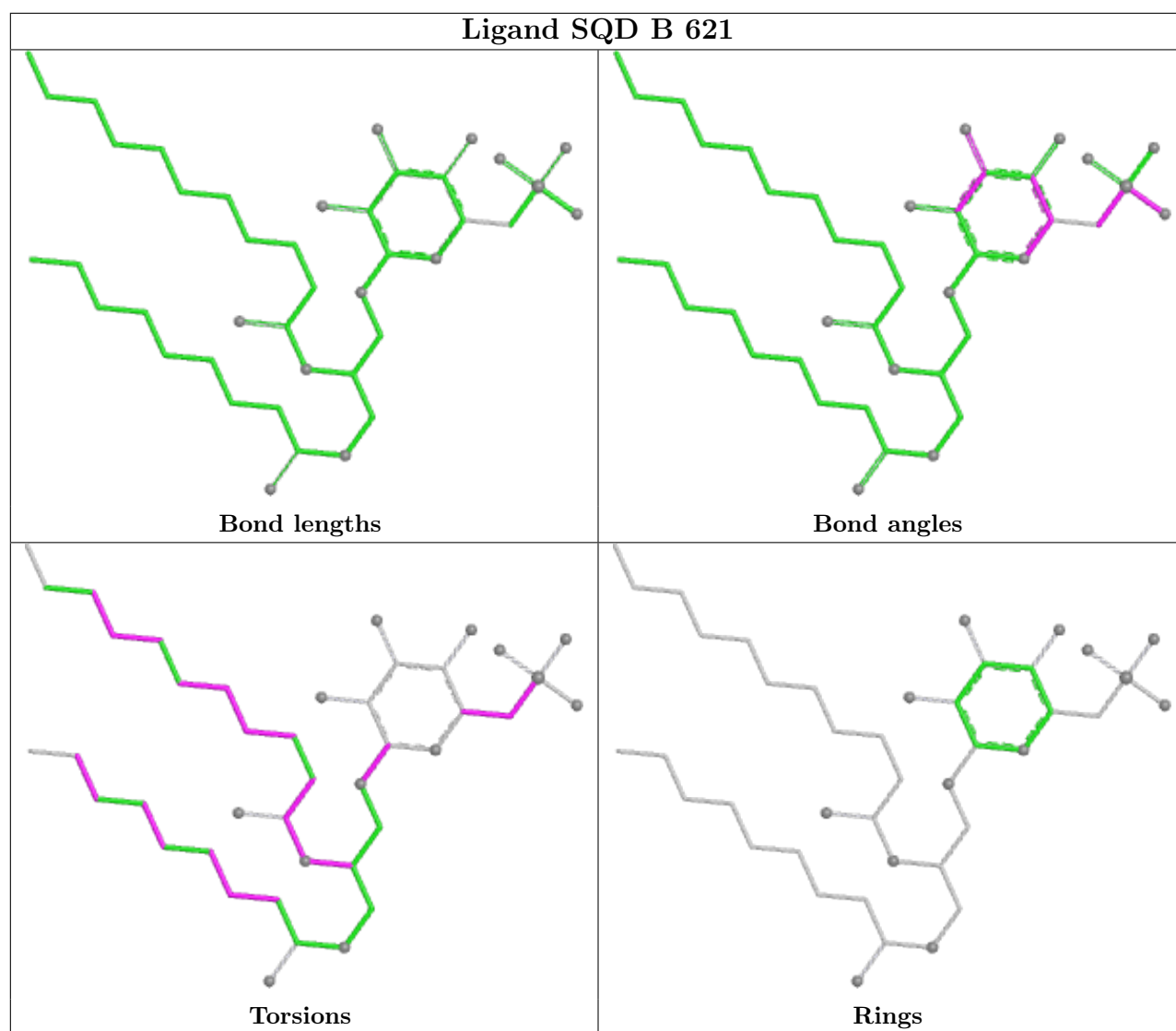
Ligand 3PH s 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

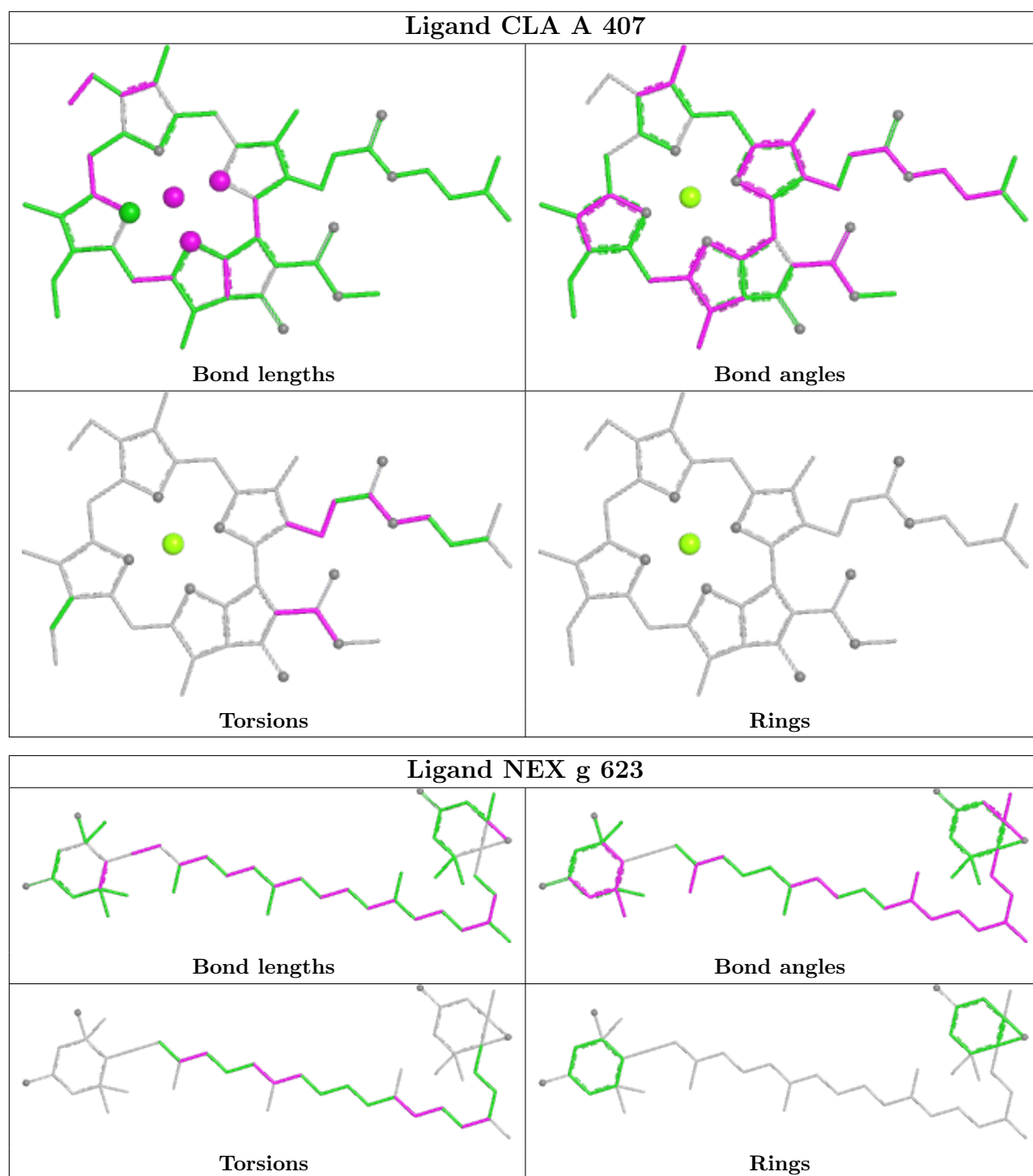
Ligand BCR C1 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

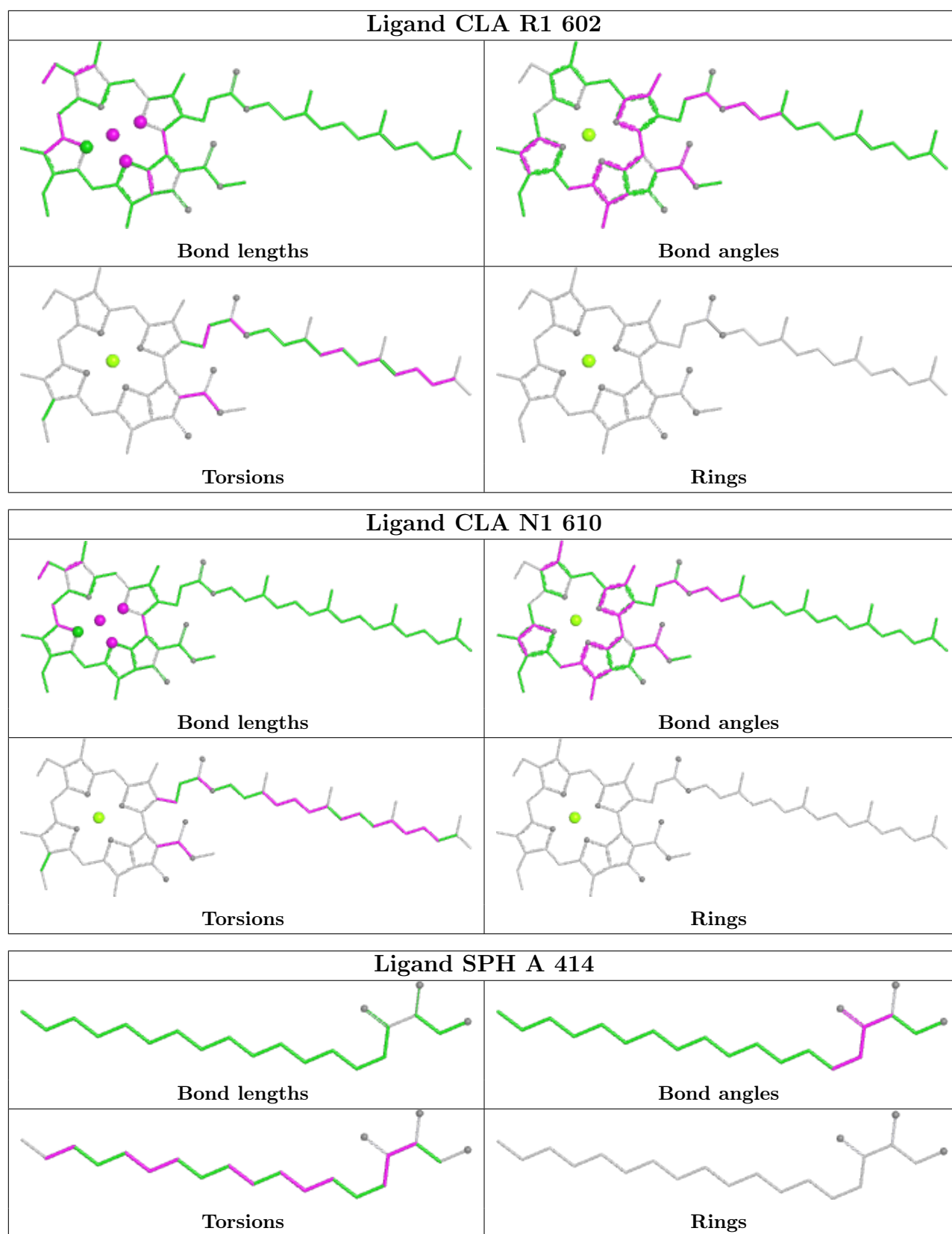
Ligand 3PH s1 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

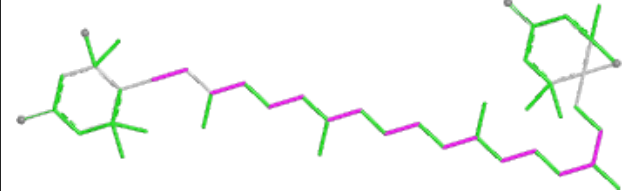
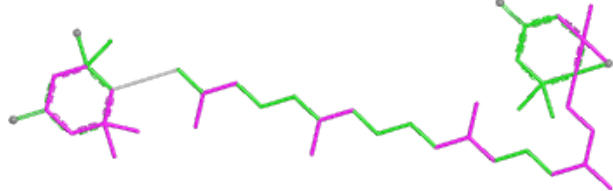
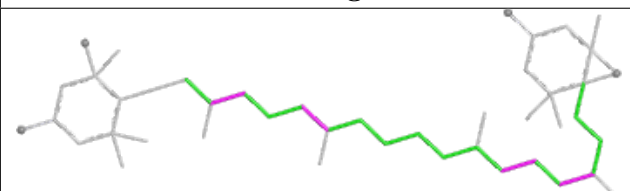
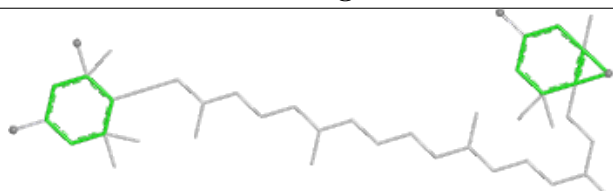
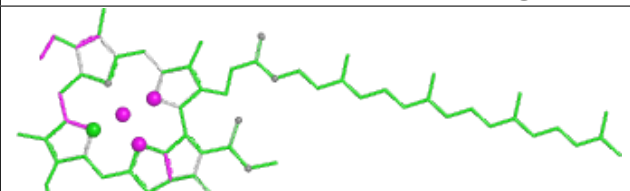
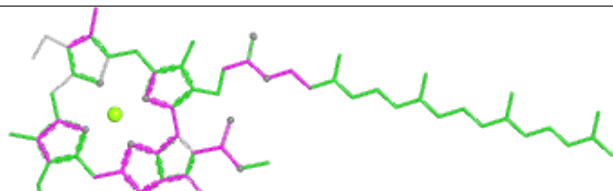
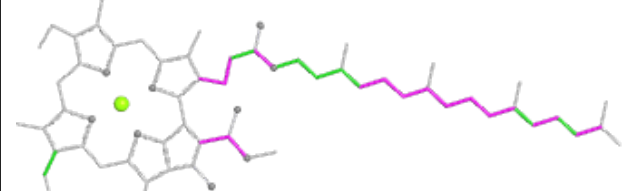
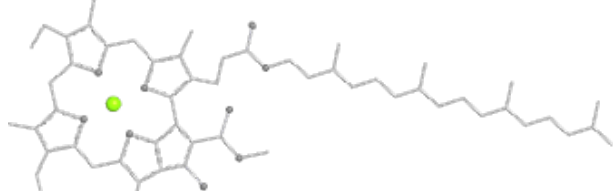
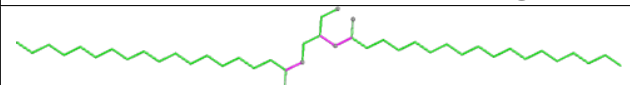
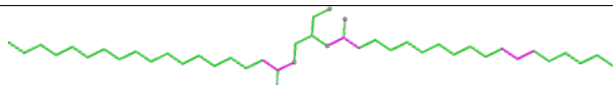
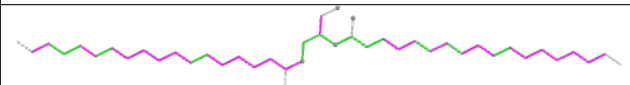
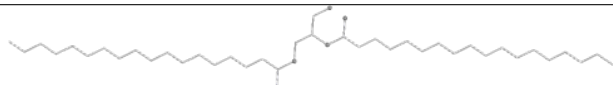




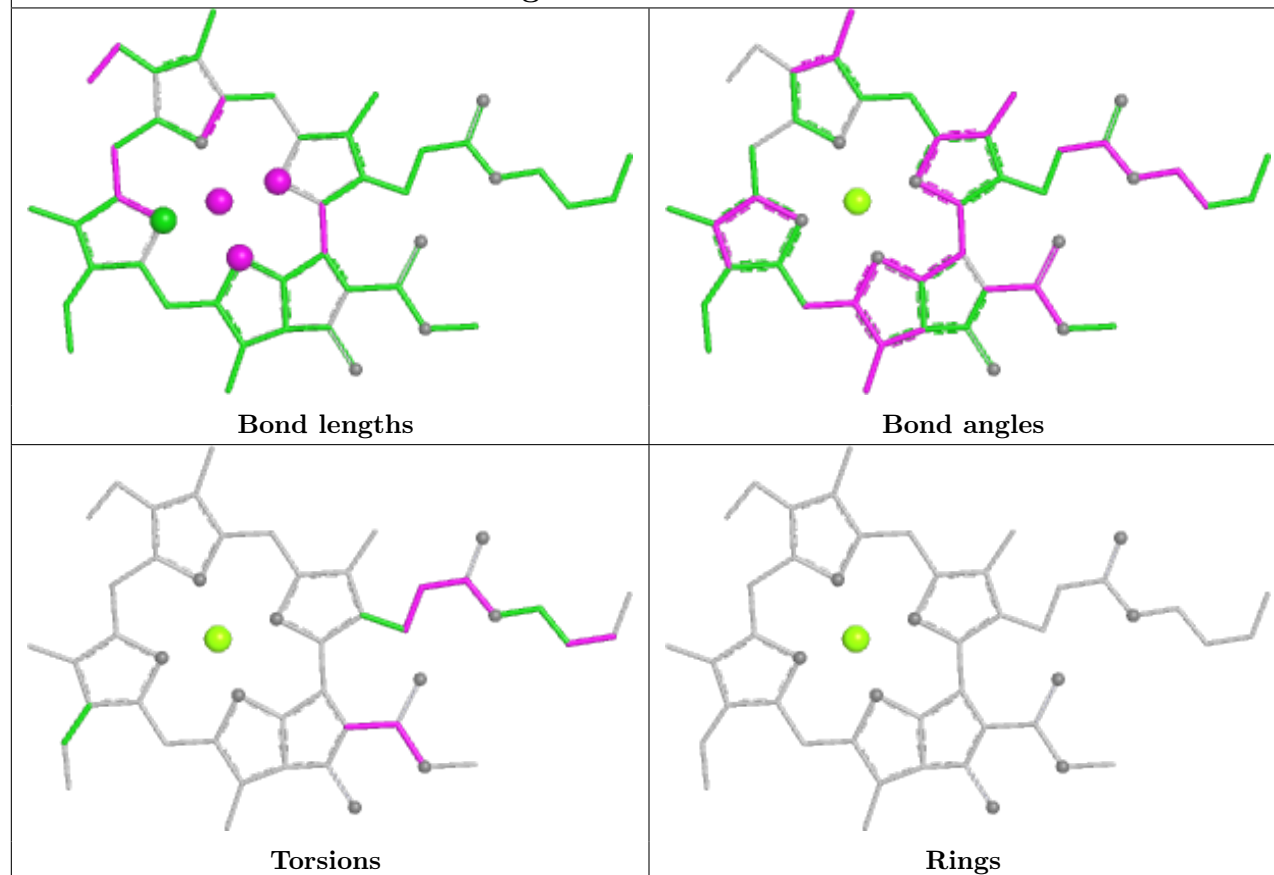




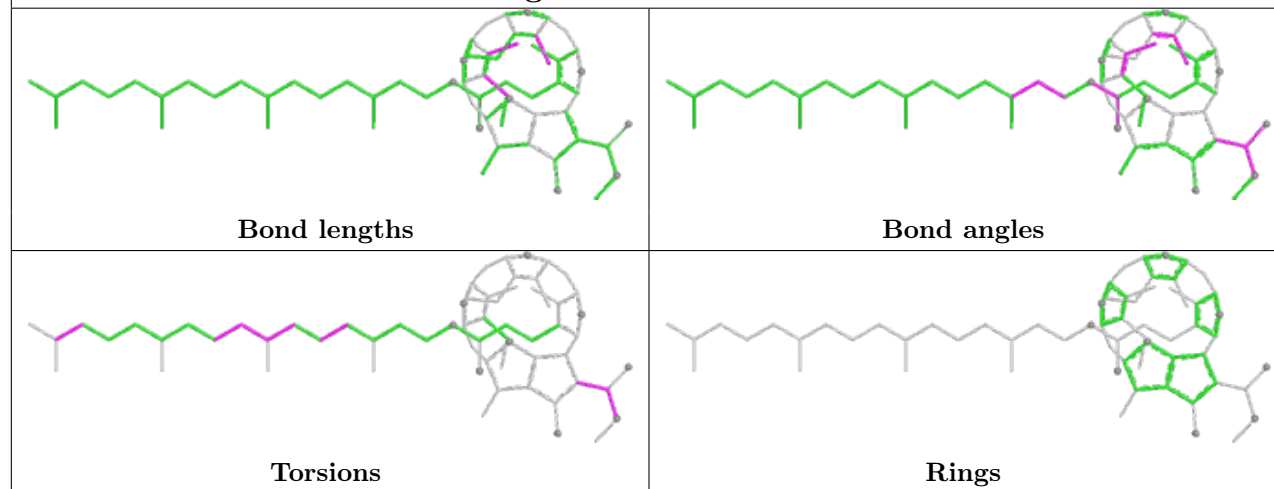


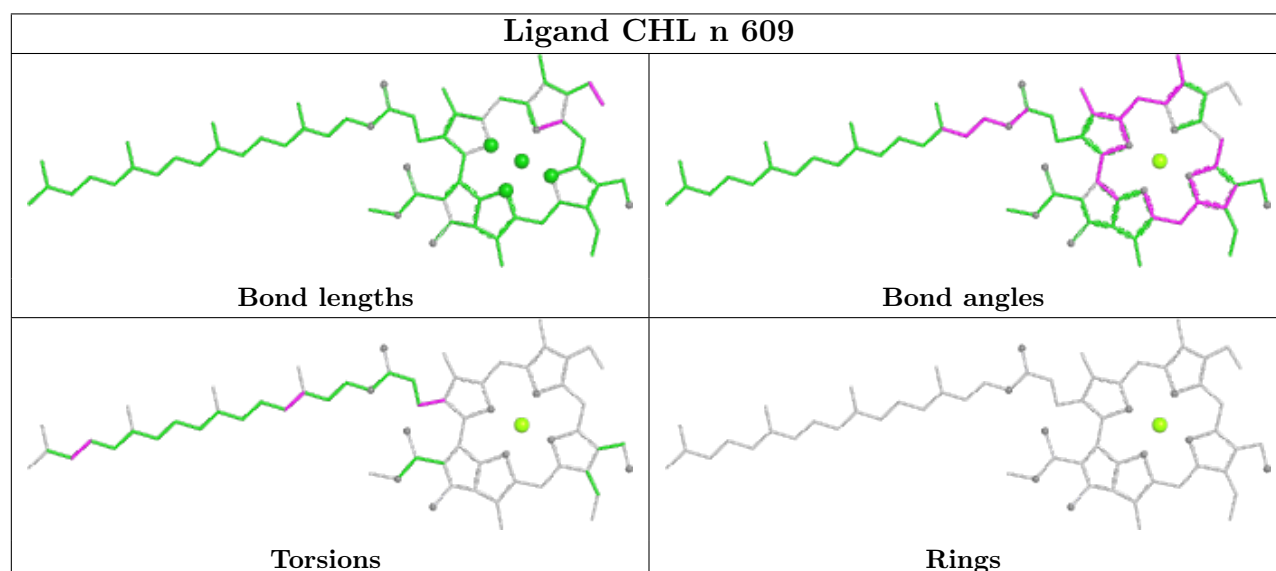
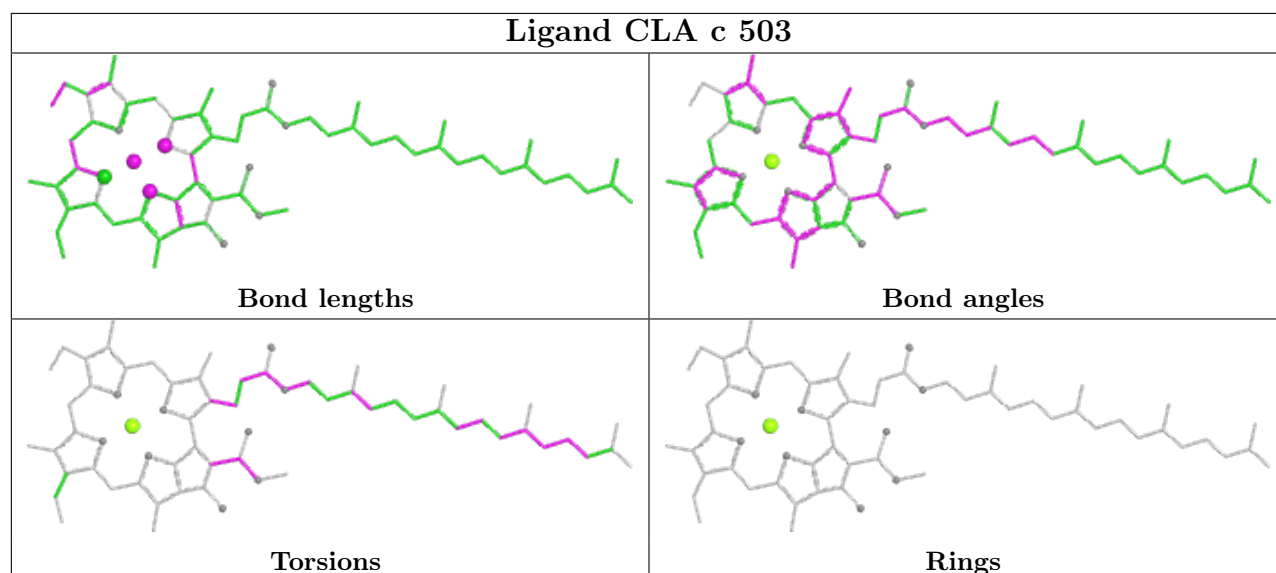
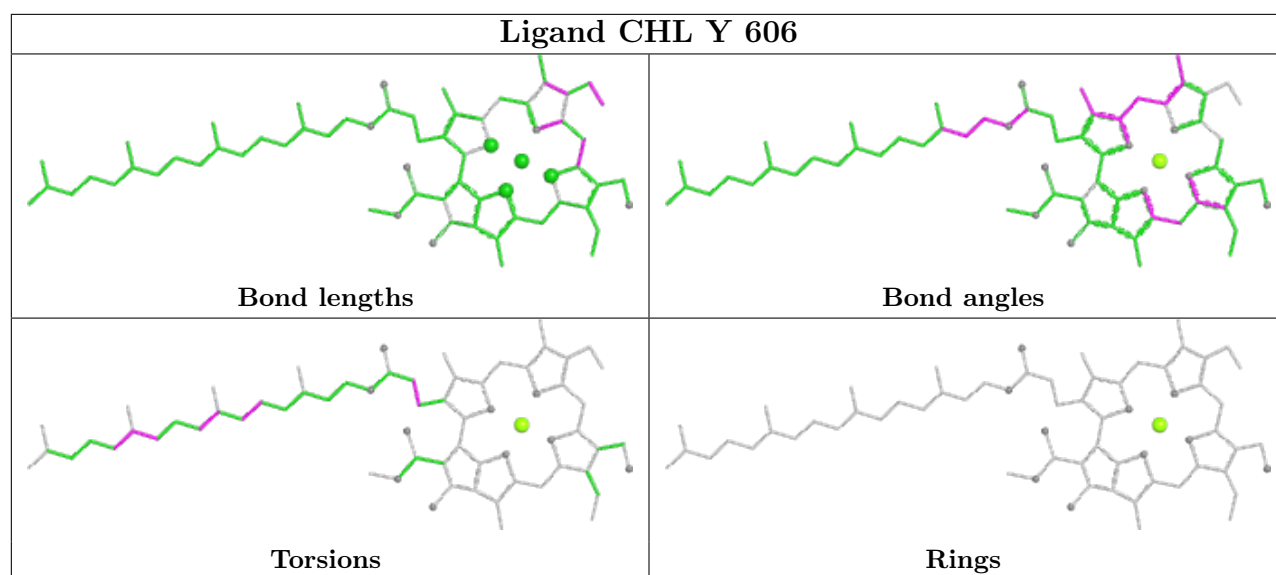
Ligand NEX y 623	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA S1 610	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGA c1 524	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

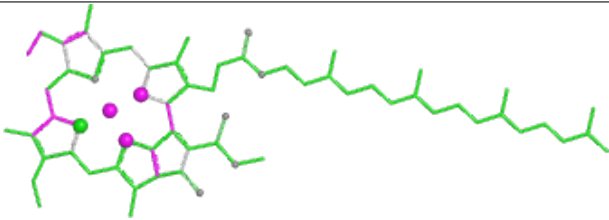
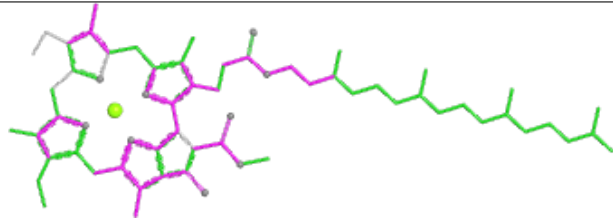
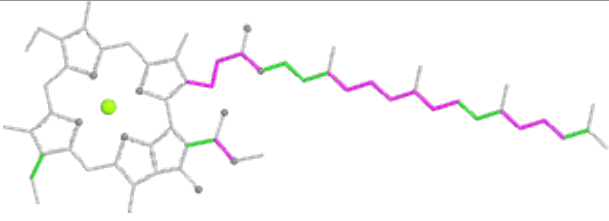
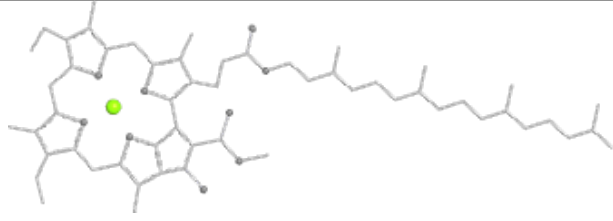
Ligand CLA G1 614

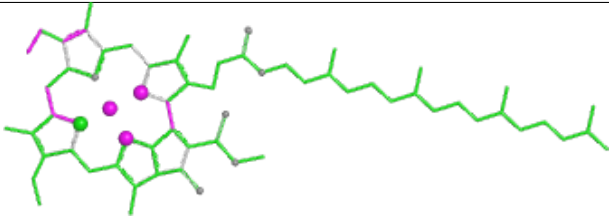
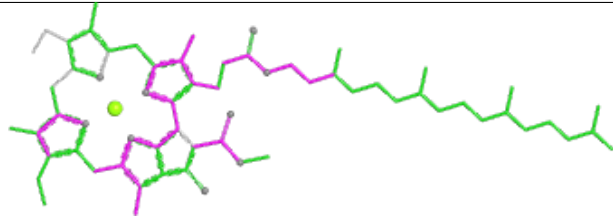
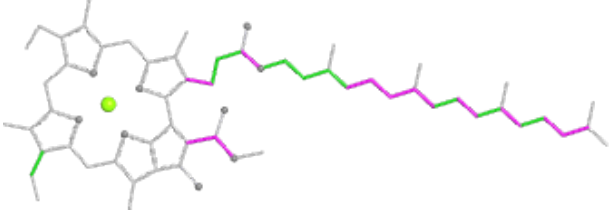
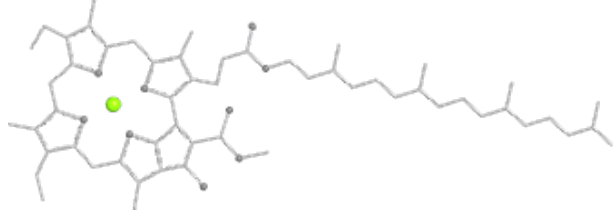


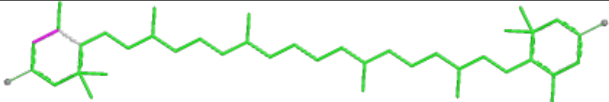
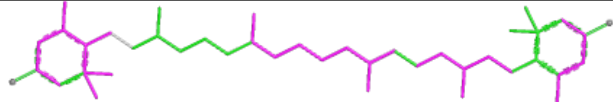
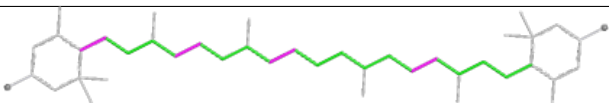
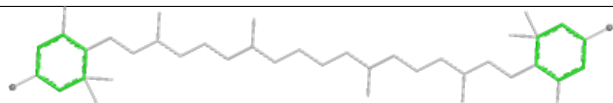
Ligand PHO a1 409

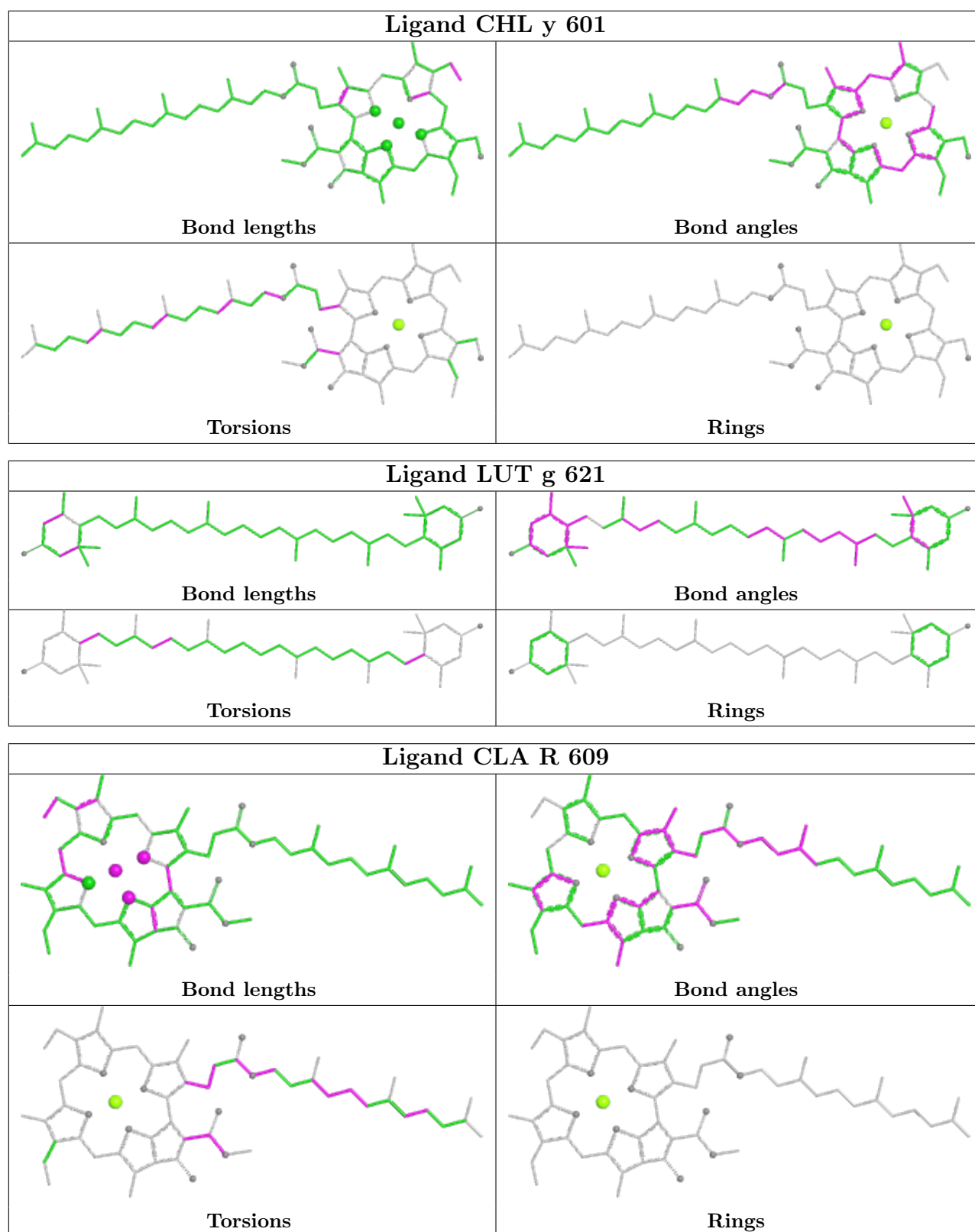


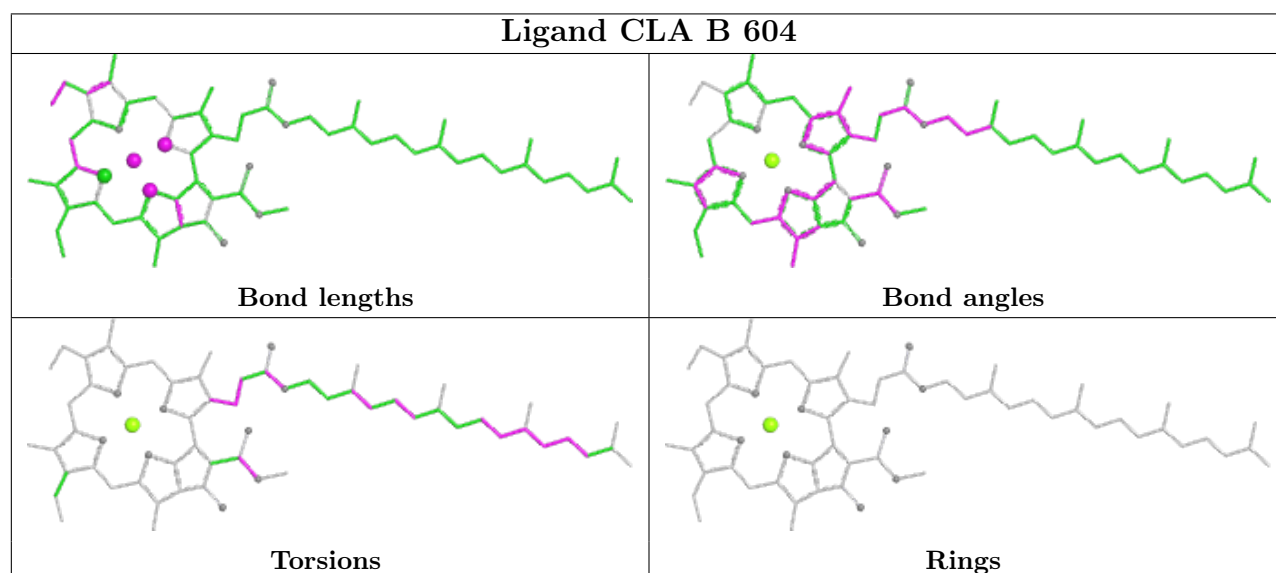
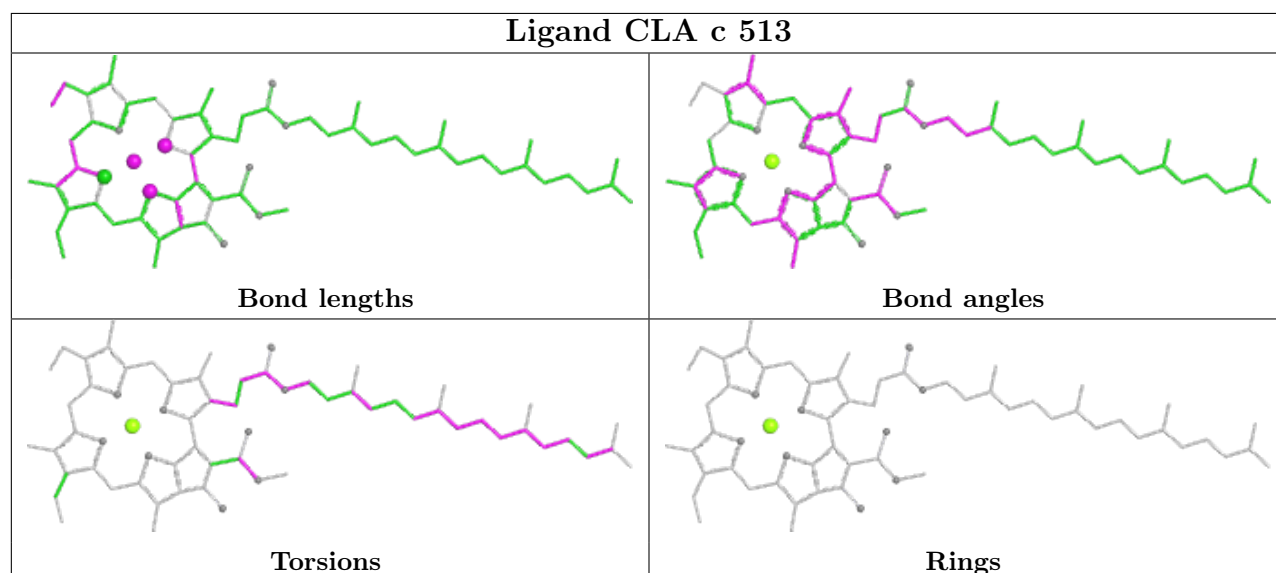
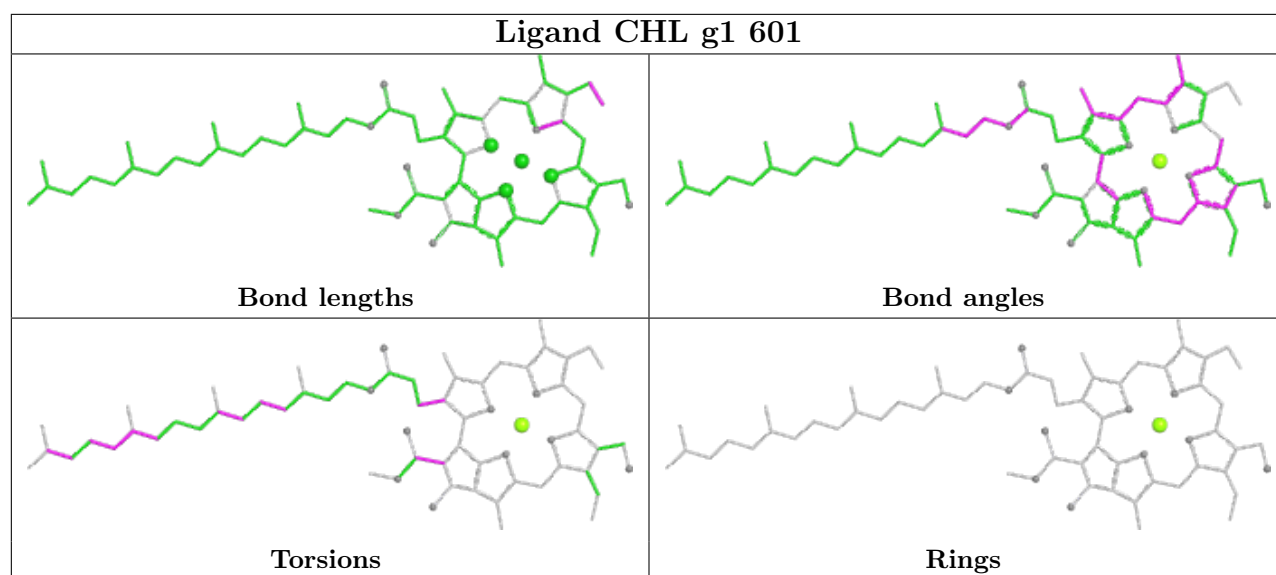


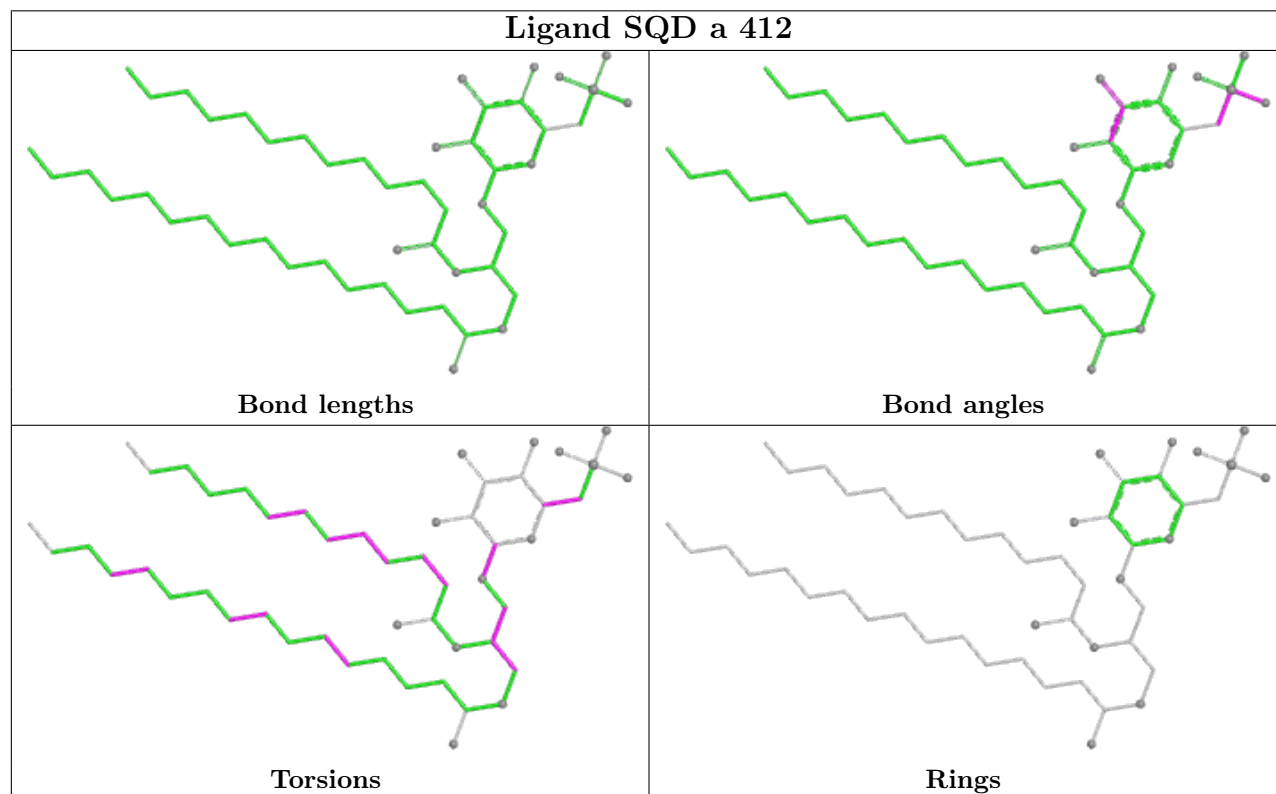
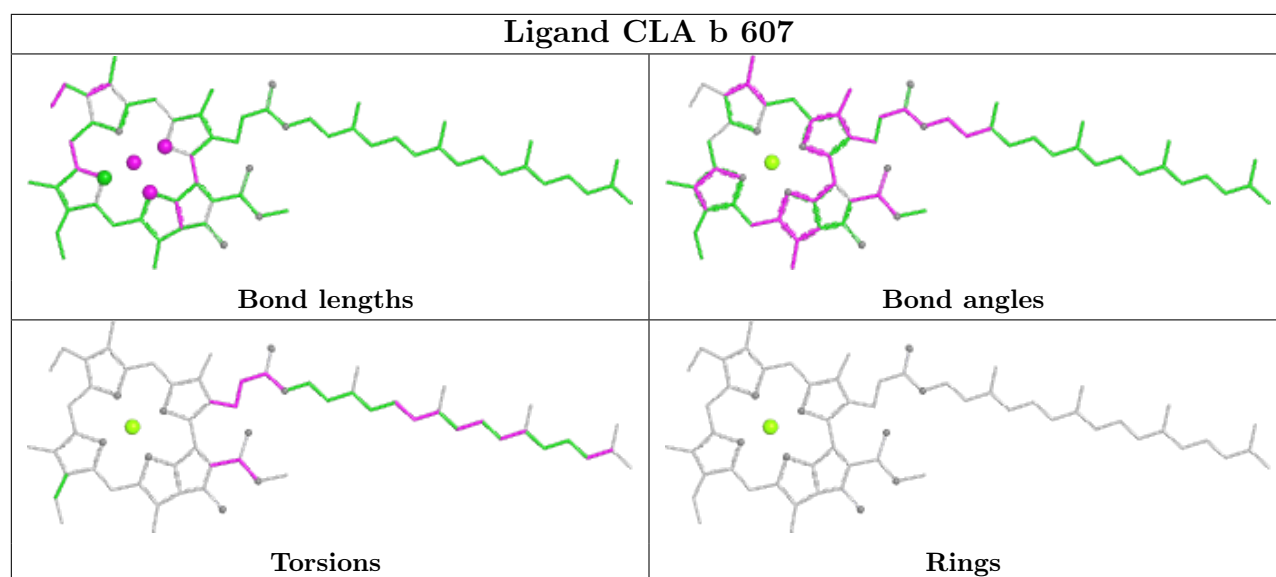
Ligand CLA S 610	
	Bond lengths
	Bond angles
	Torsions
	Rings

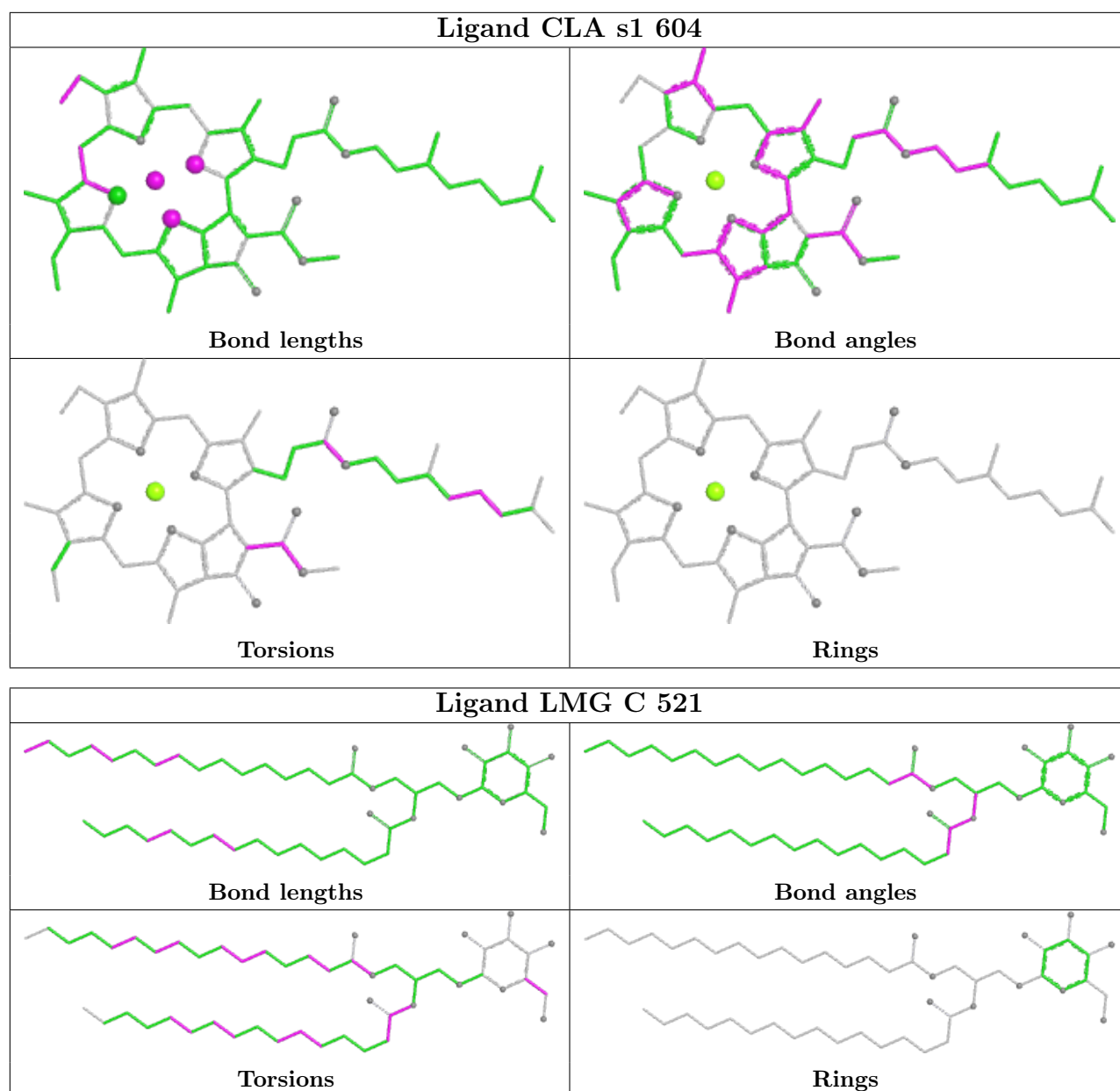
Ligand CLA G 611	
	Bond lengths
	Bond angles
	Torsions
	Rings

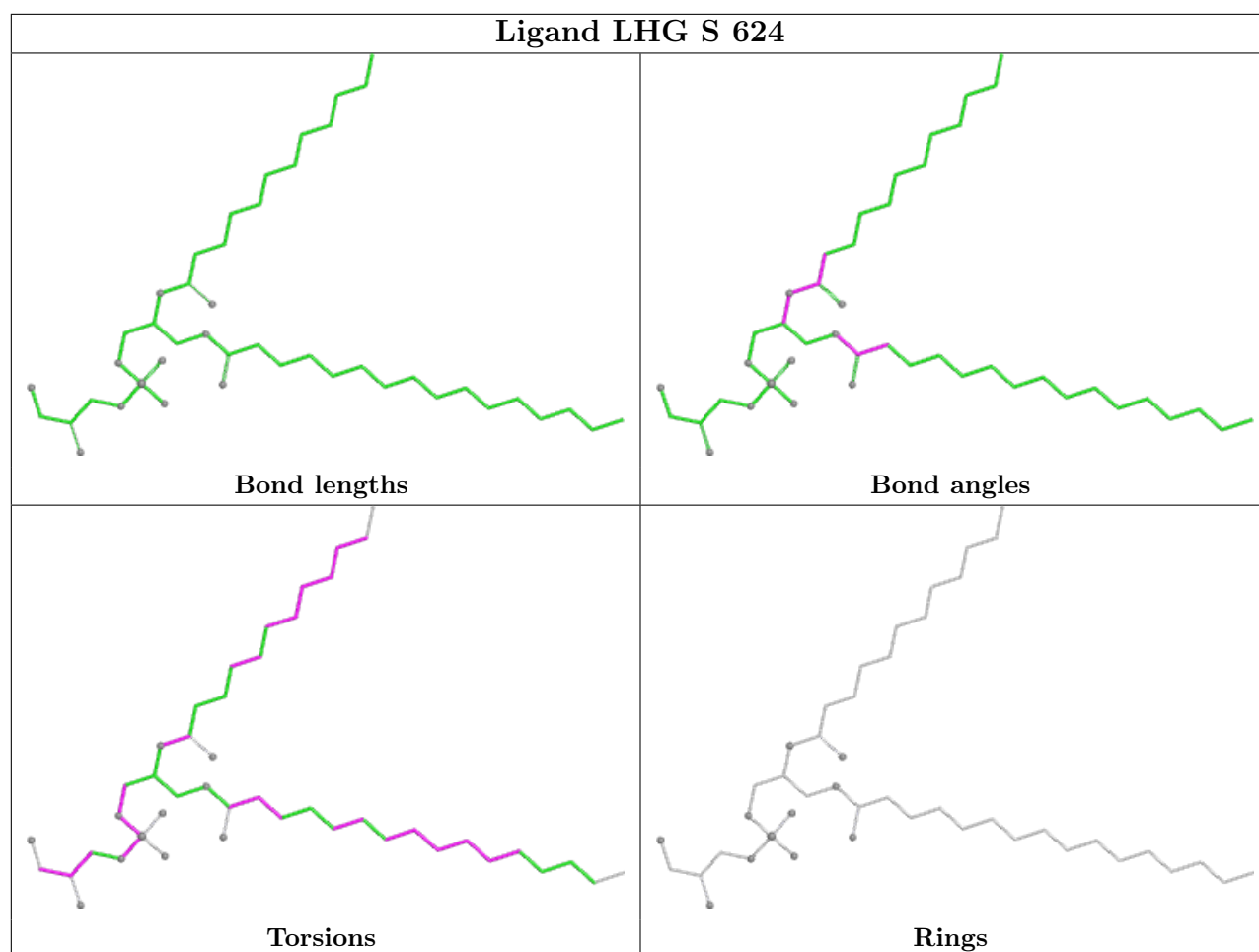
Ligand LUT y1 621	
	Bond lengths
	Bond angles
	Torsions
	Rings

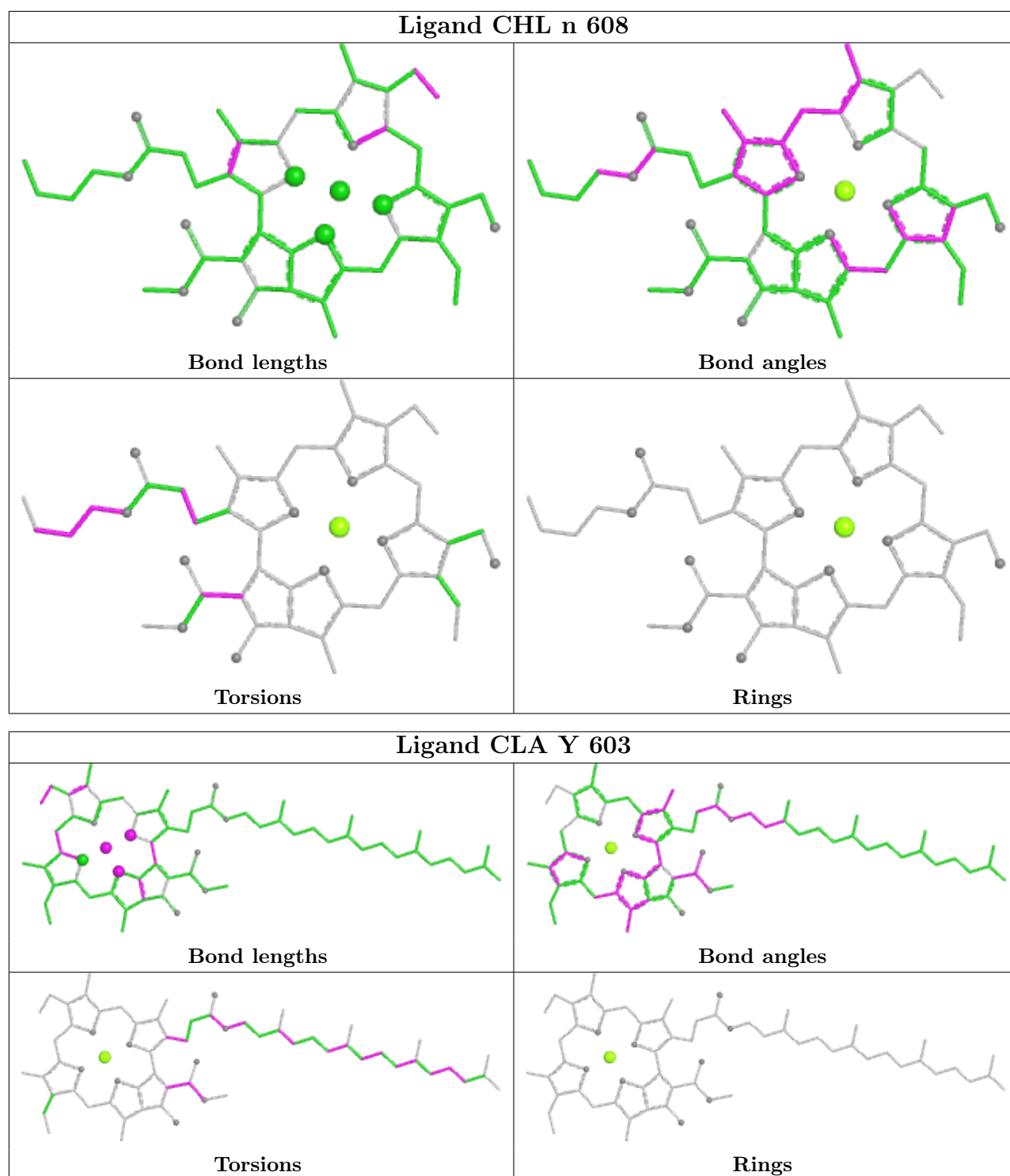


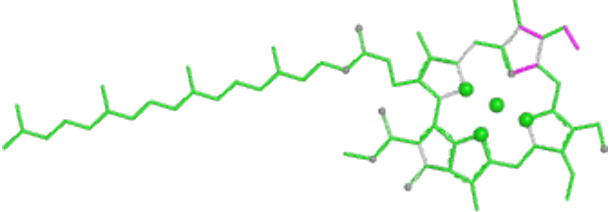
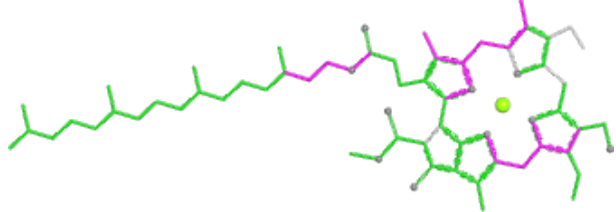
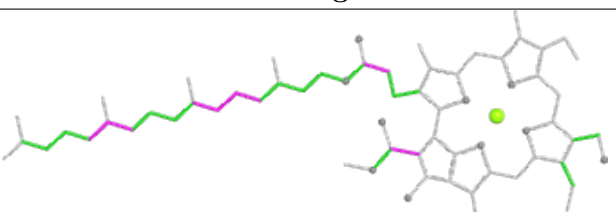
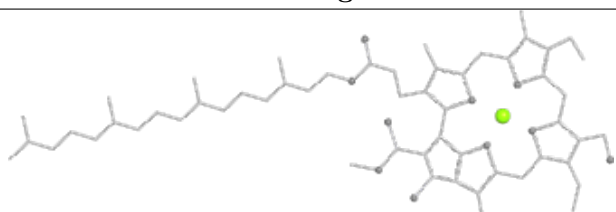
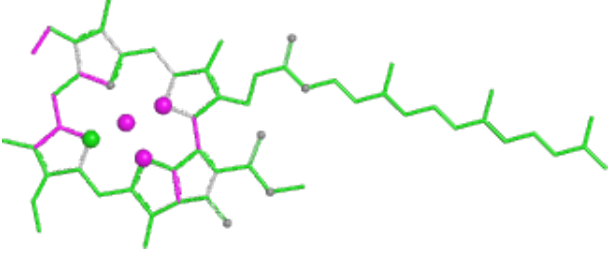
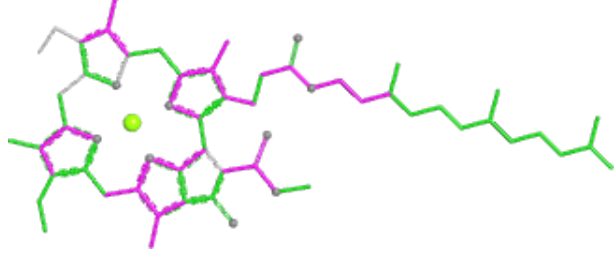
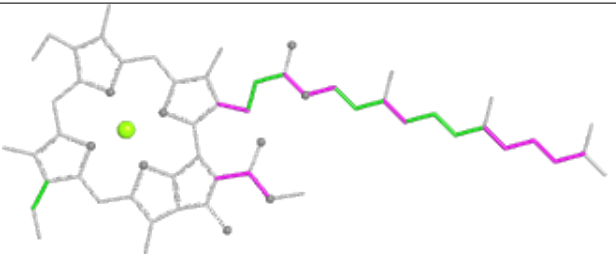
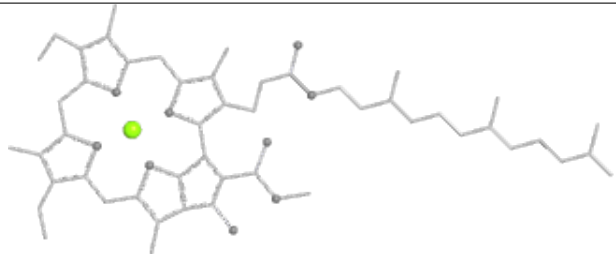


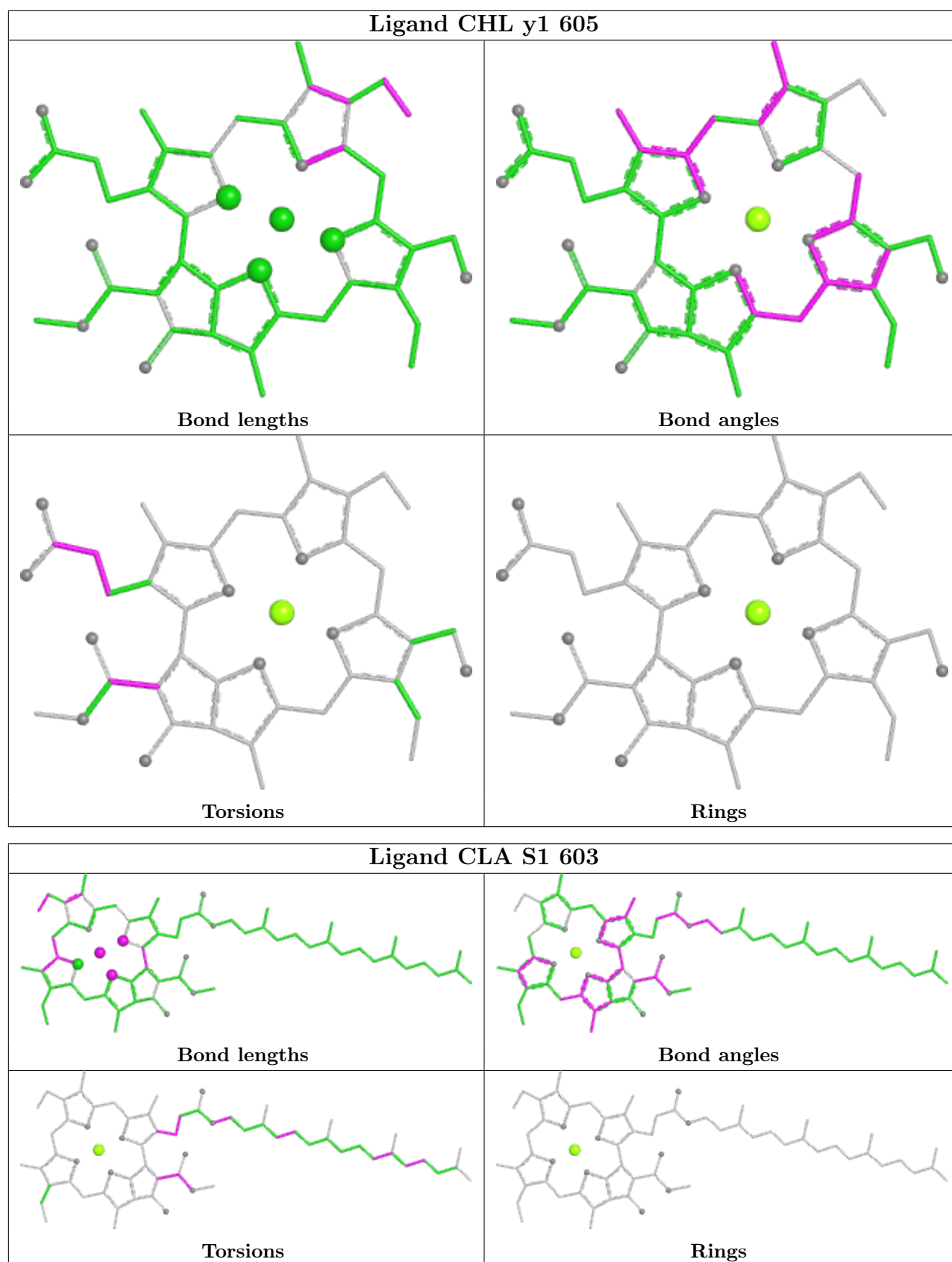


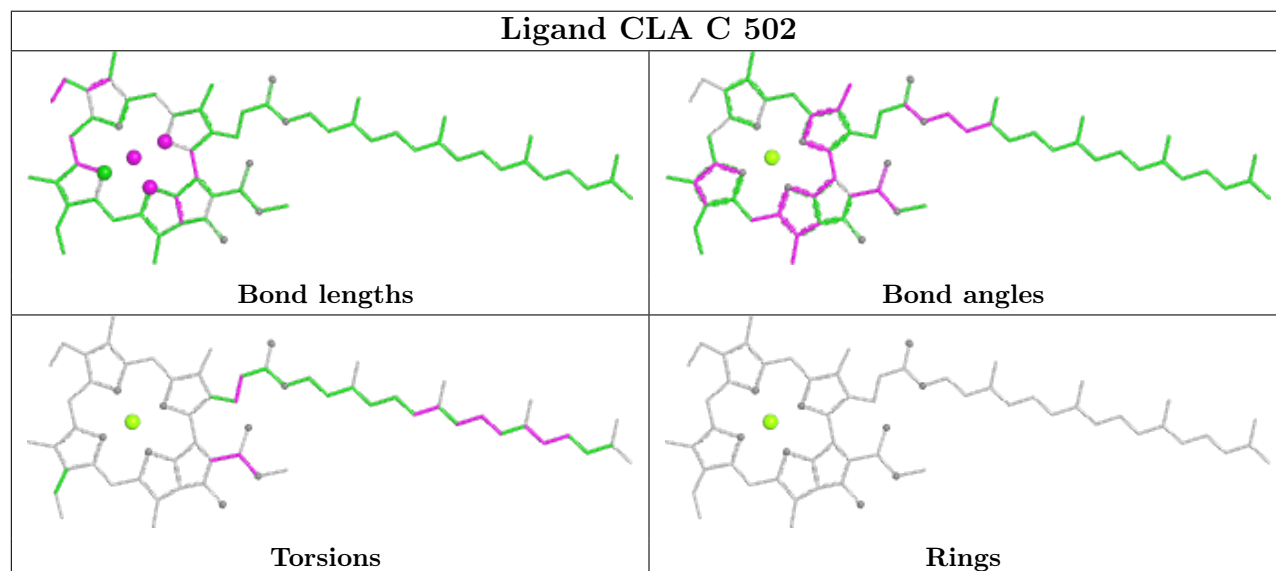
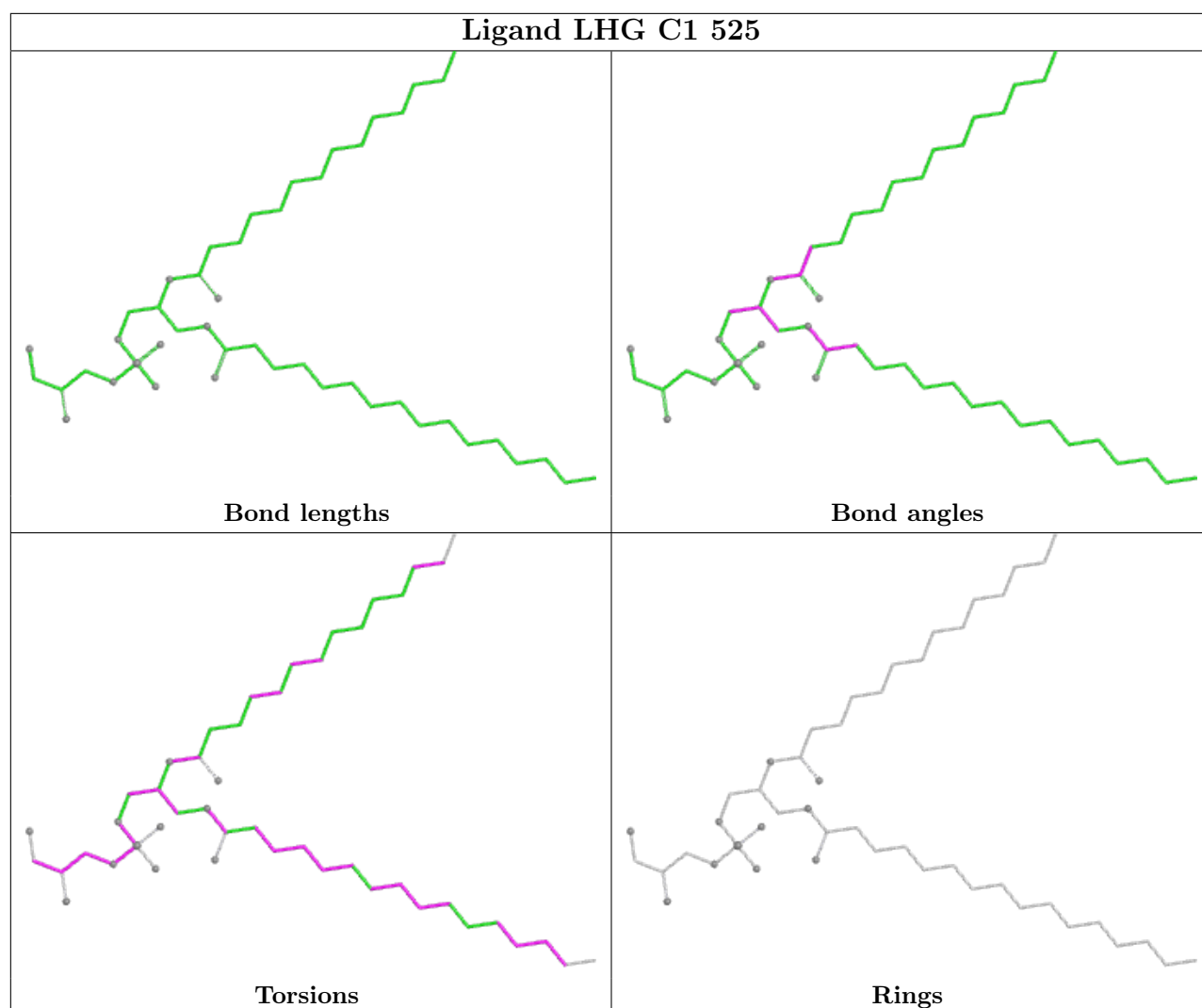


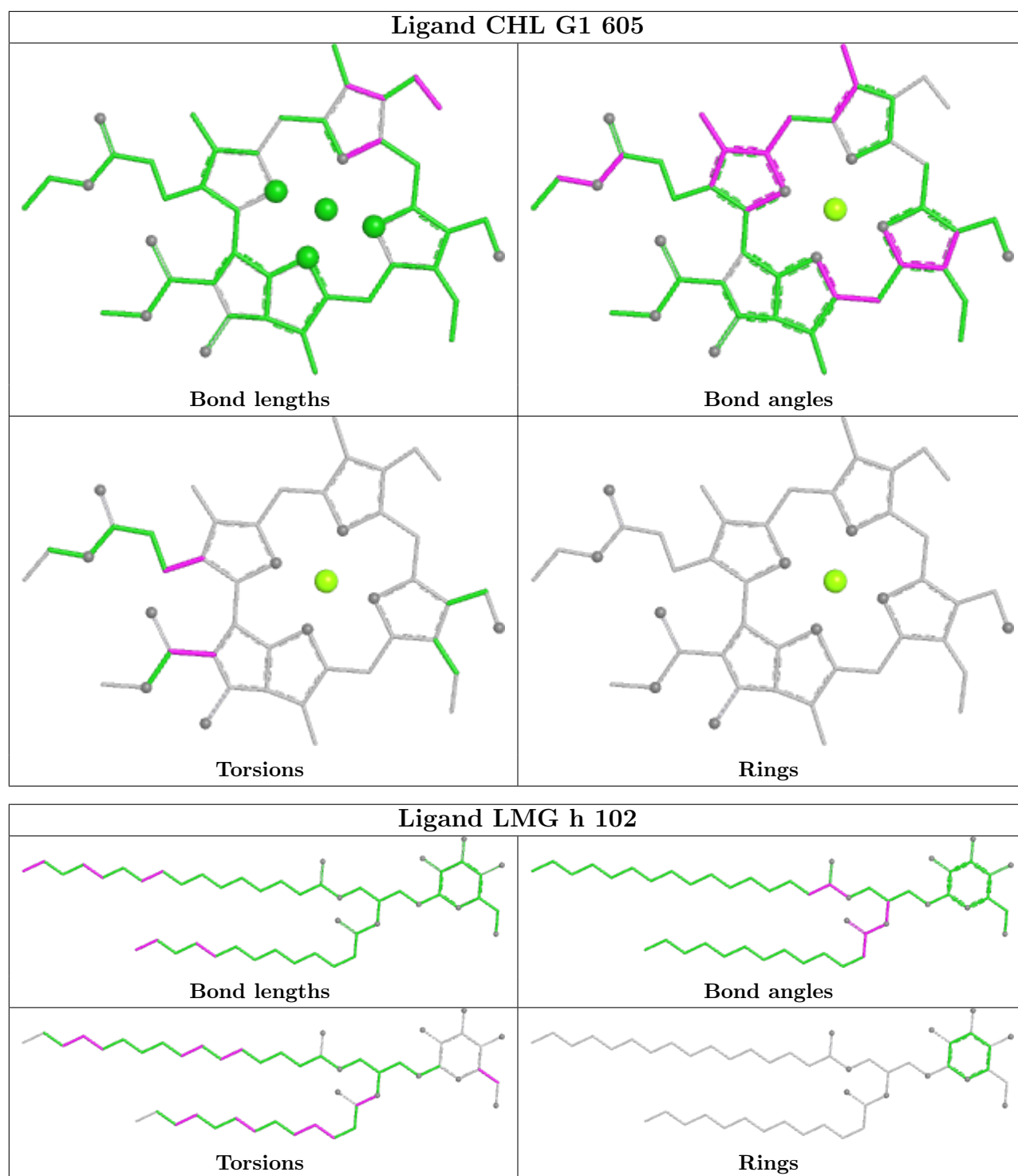


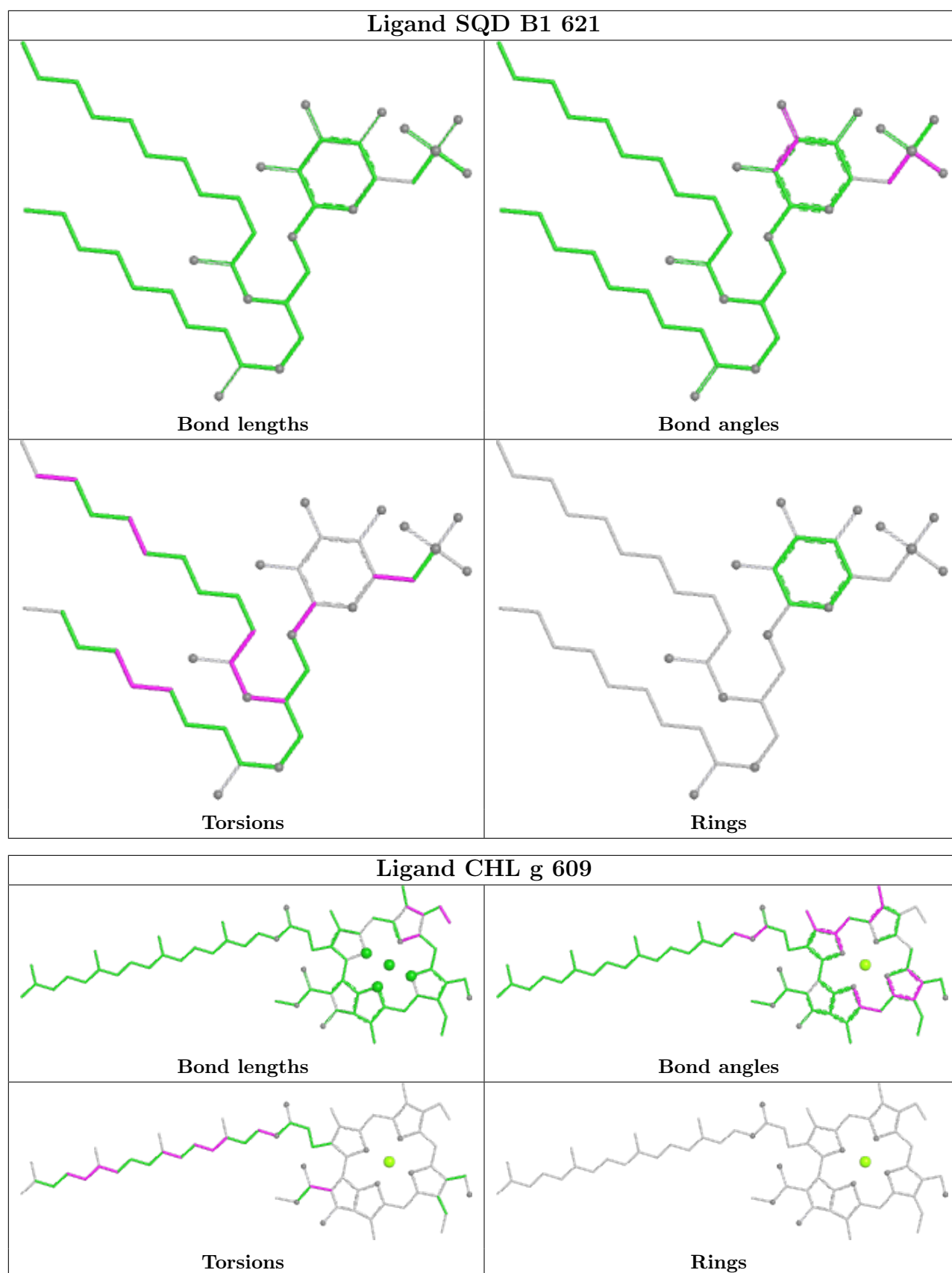


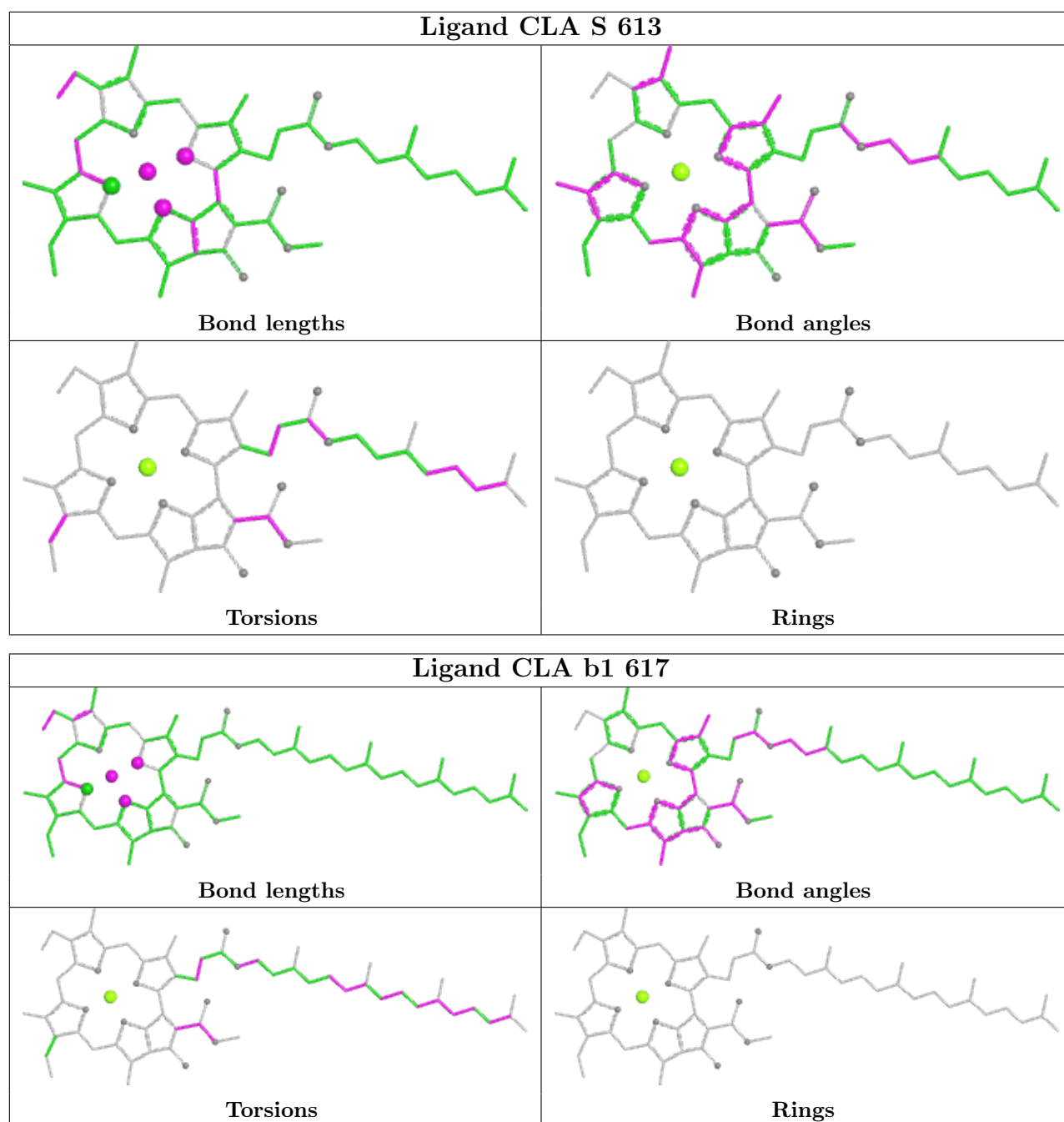
Ligand CHL G 601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA A 410	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

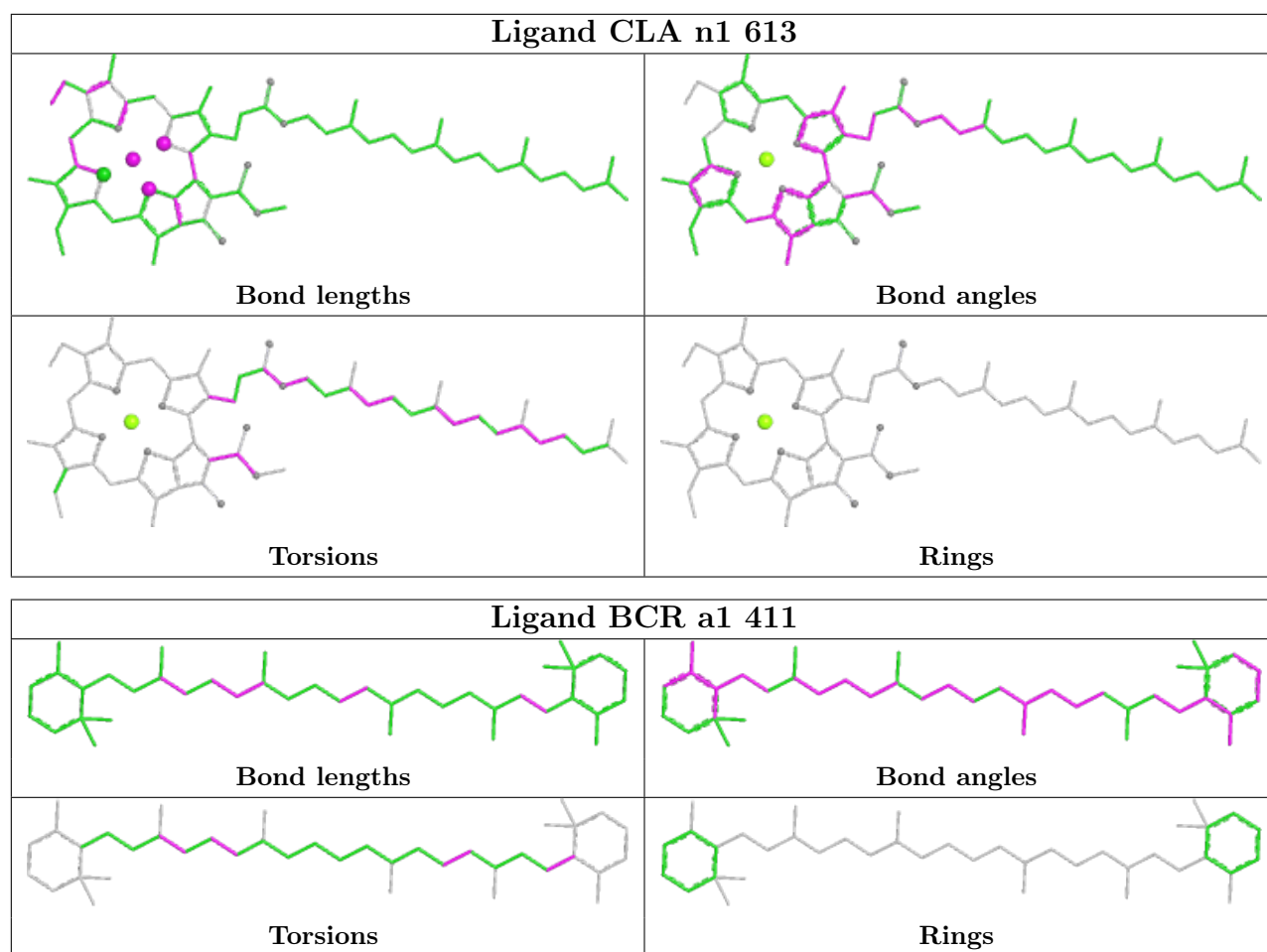


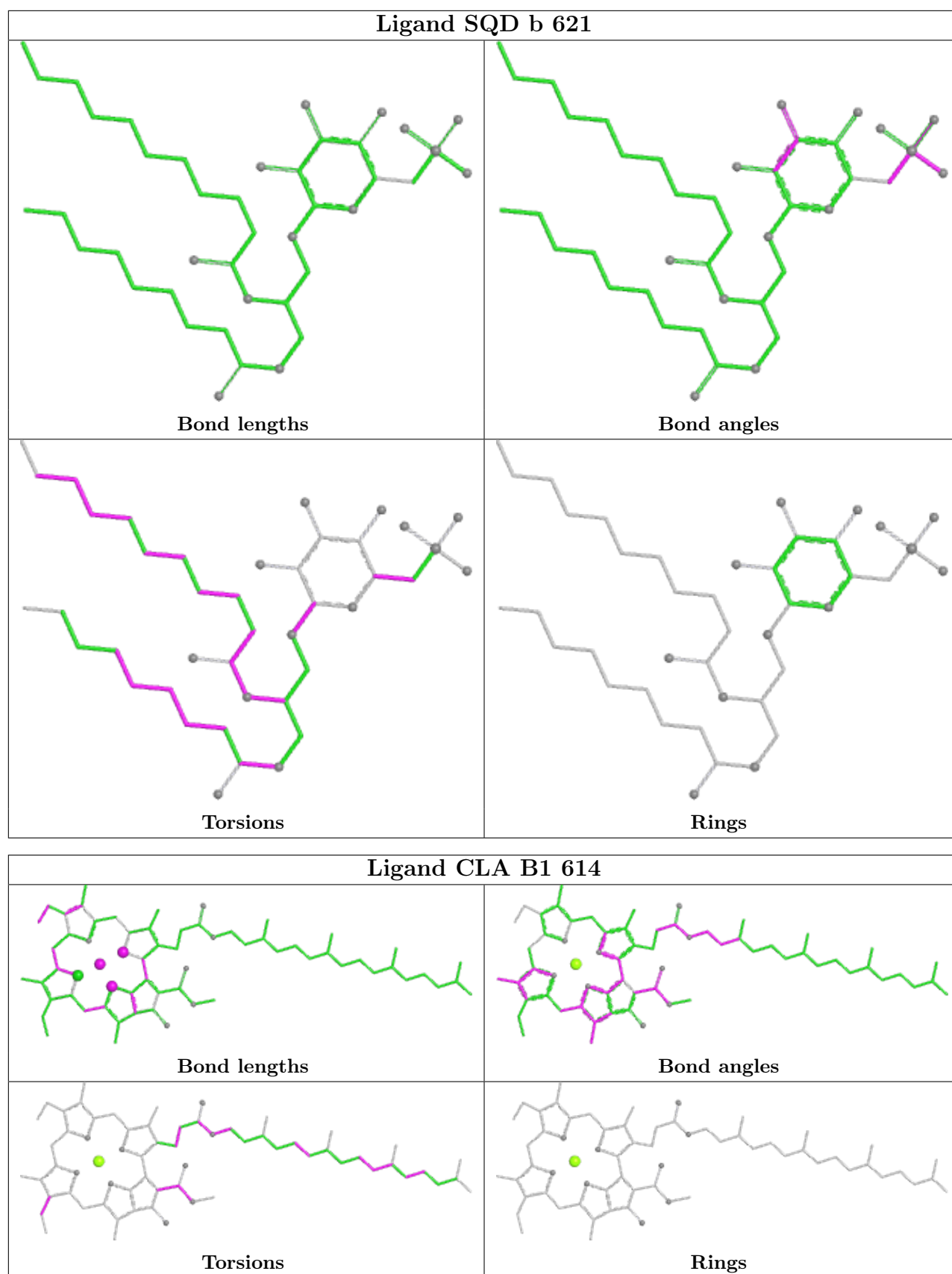




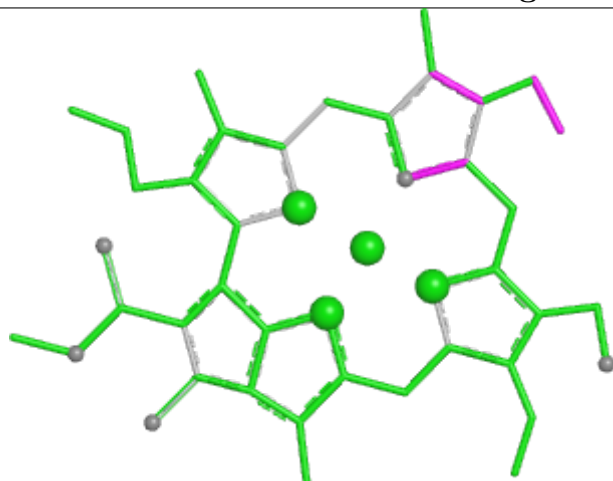




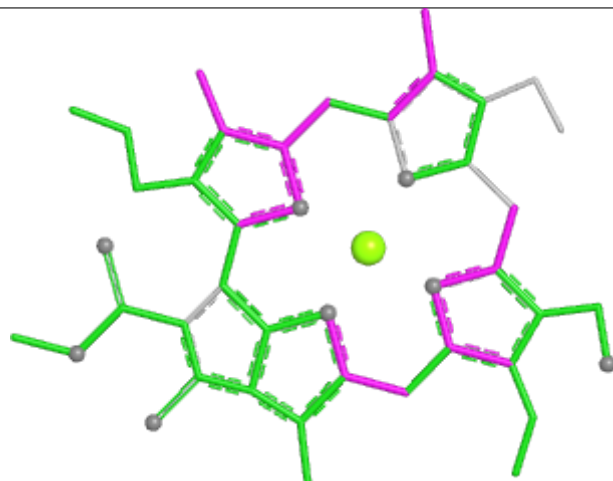




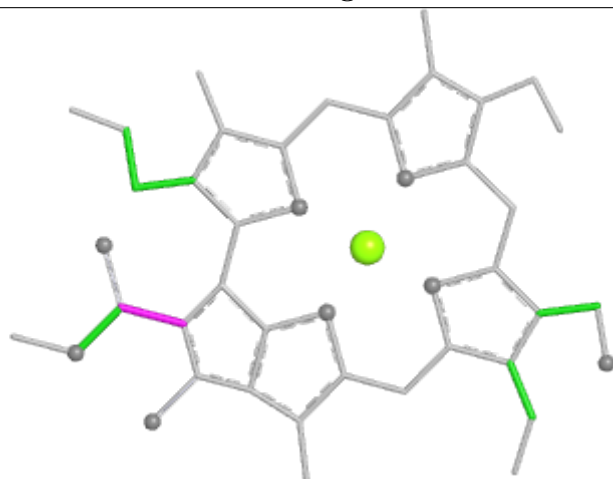
Ligand CHL r 606



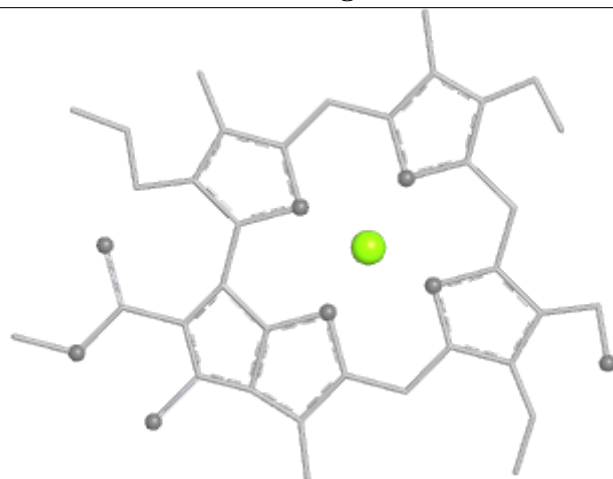
Bond lengths



Bond angles

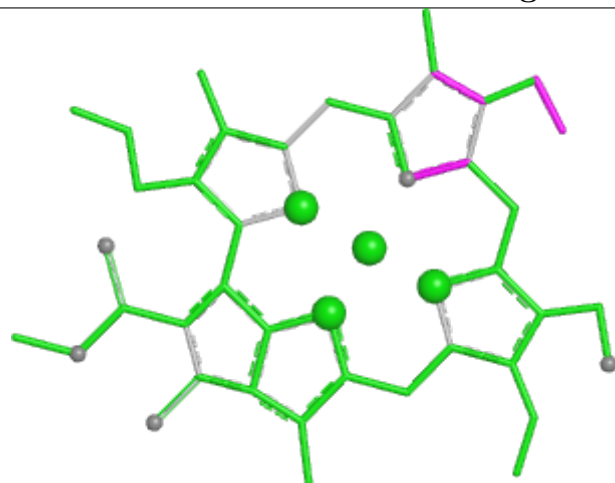


Torsions

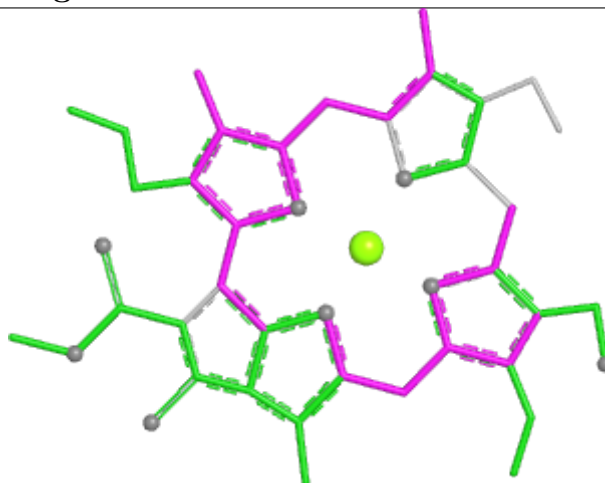


Rings

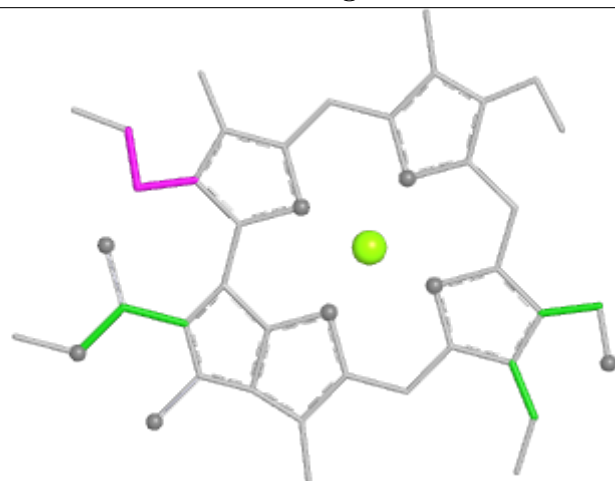
Ligand CHL g 608



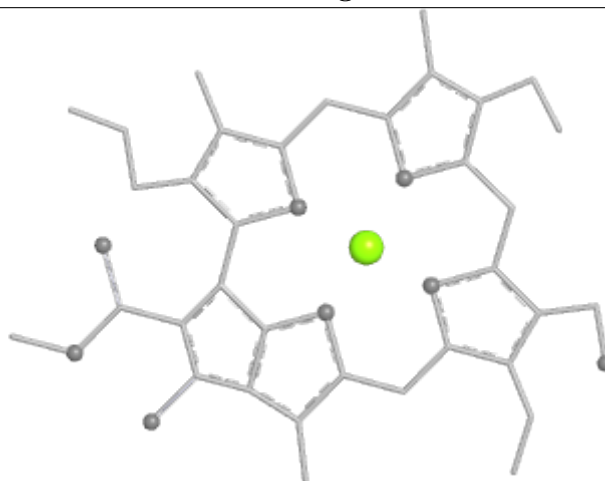
Bond lengths



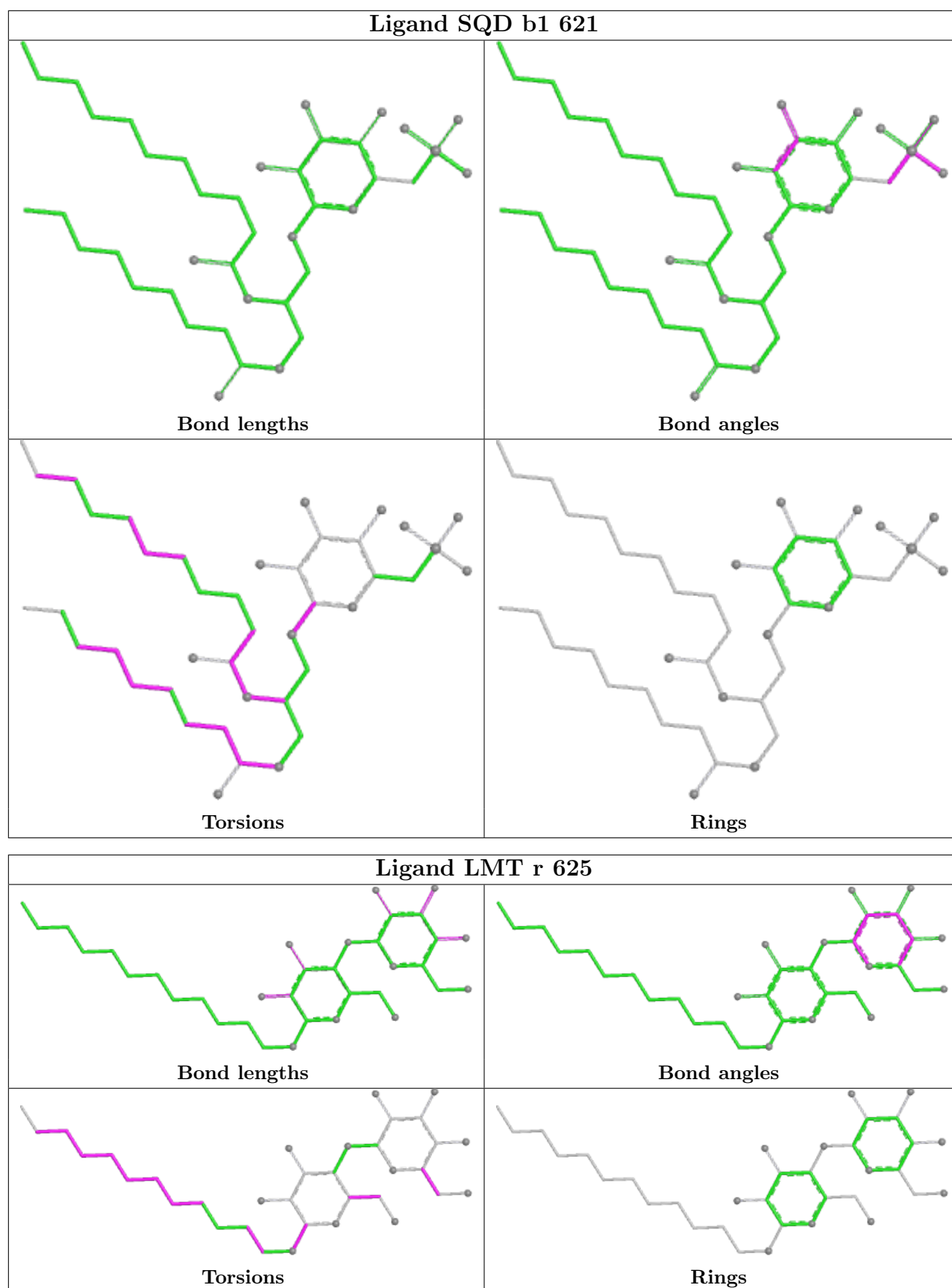
Bond angles

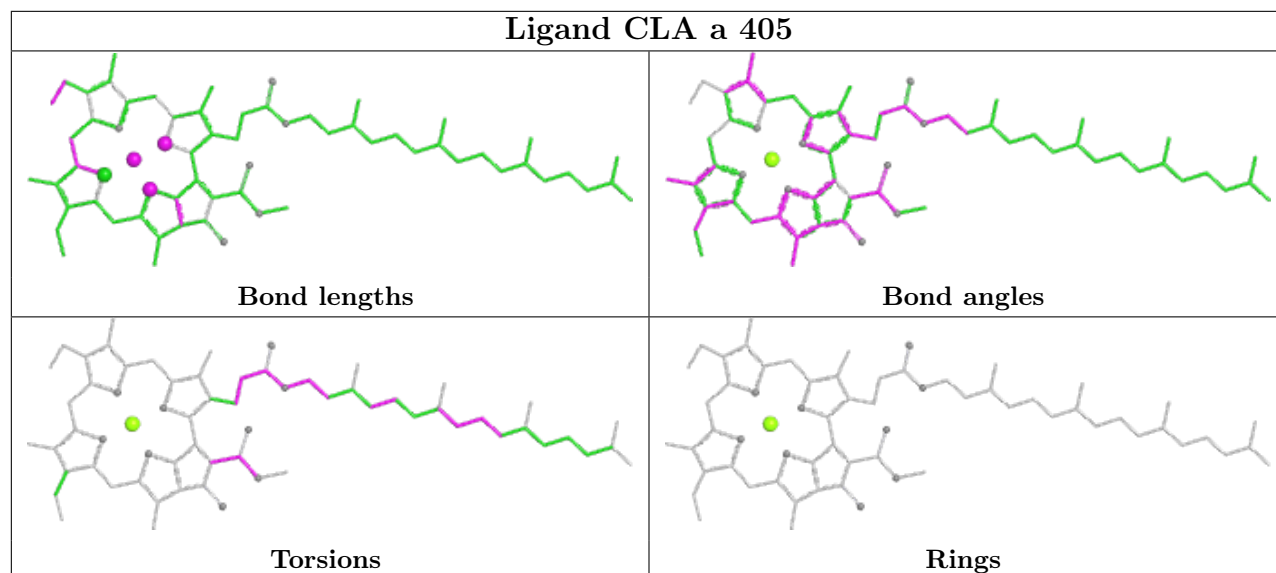
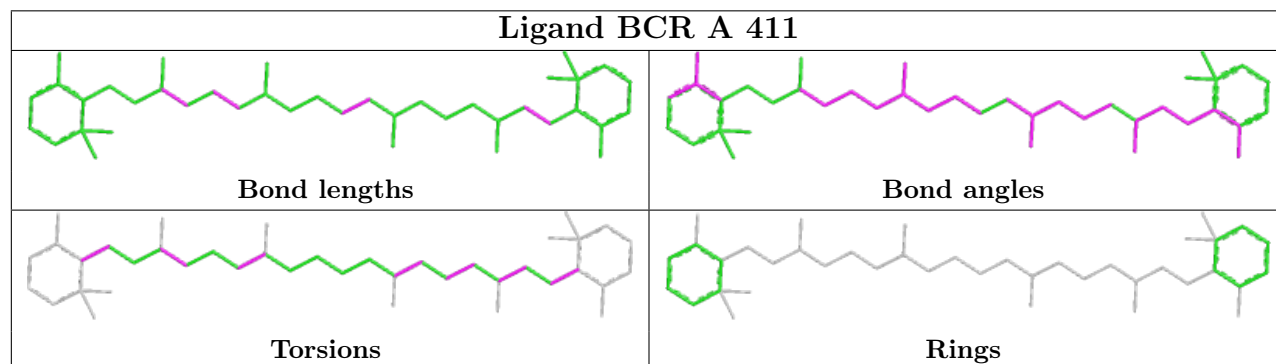
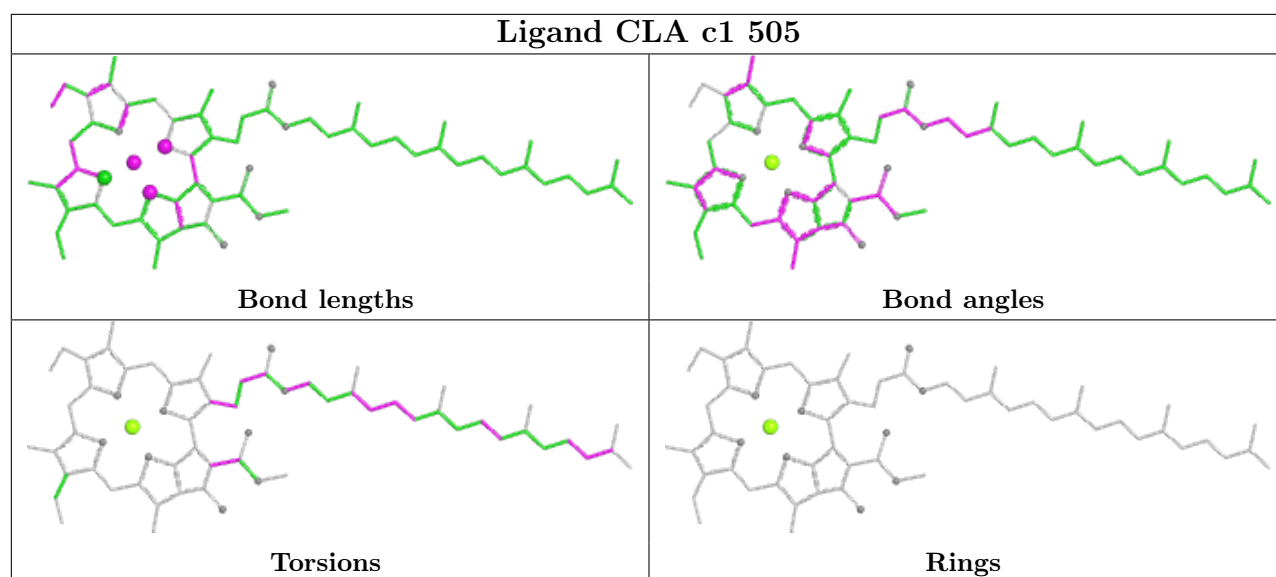


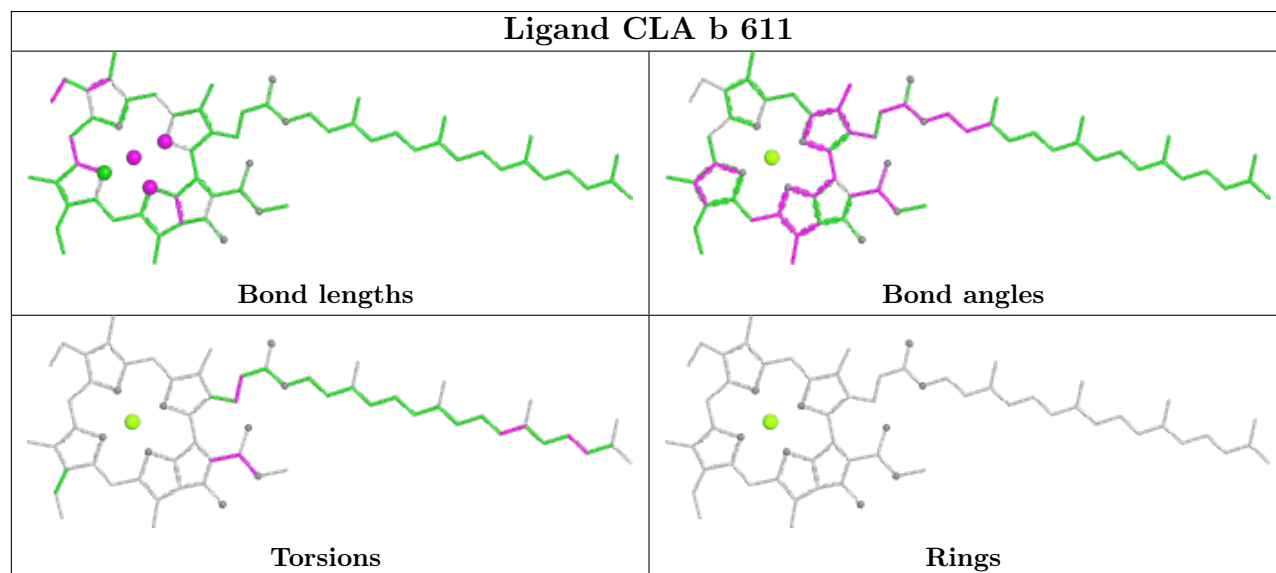
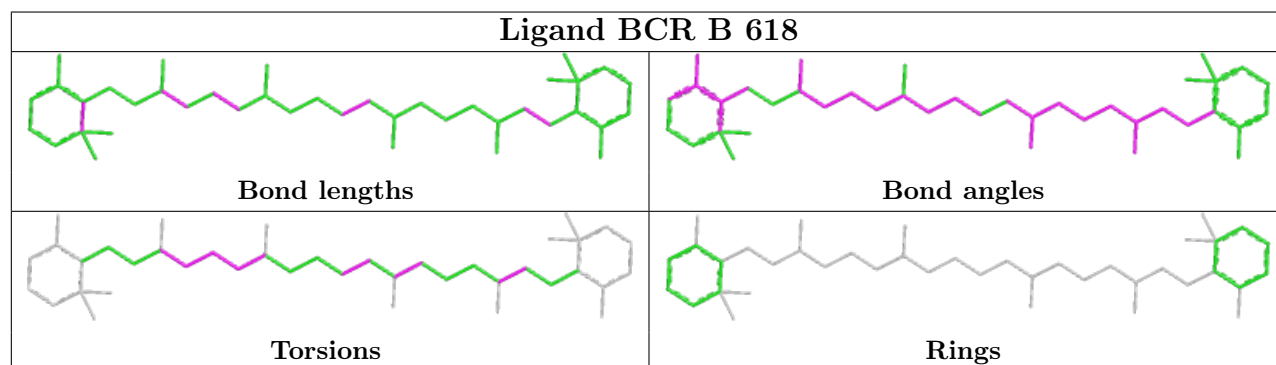
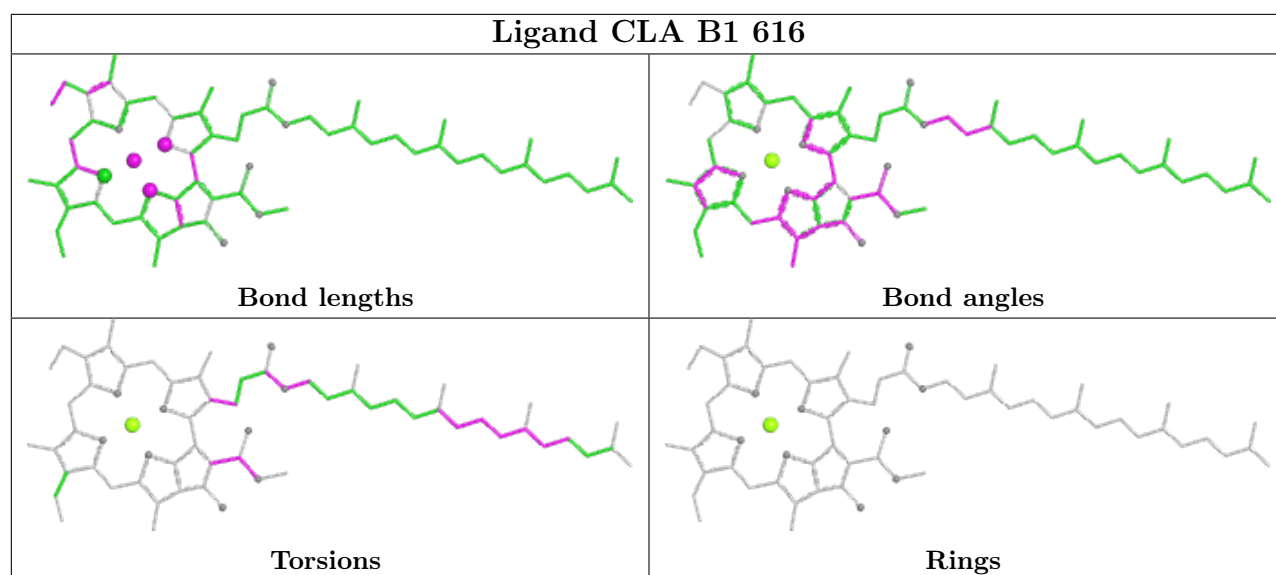
Torsions

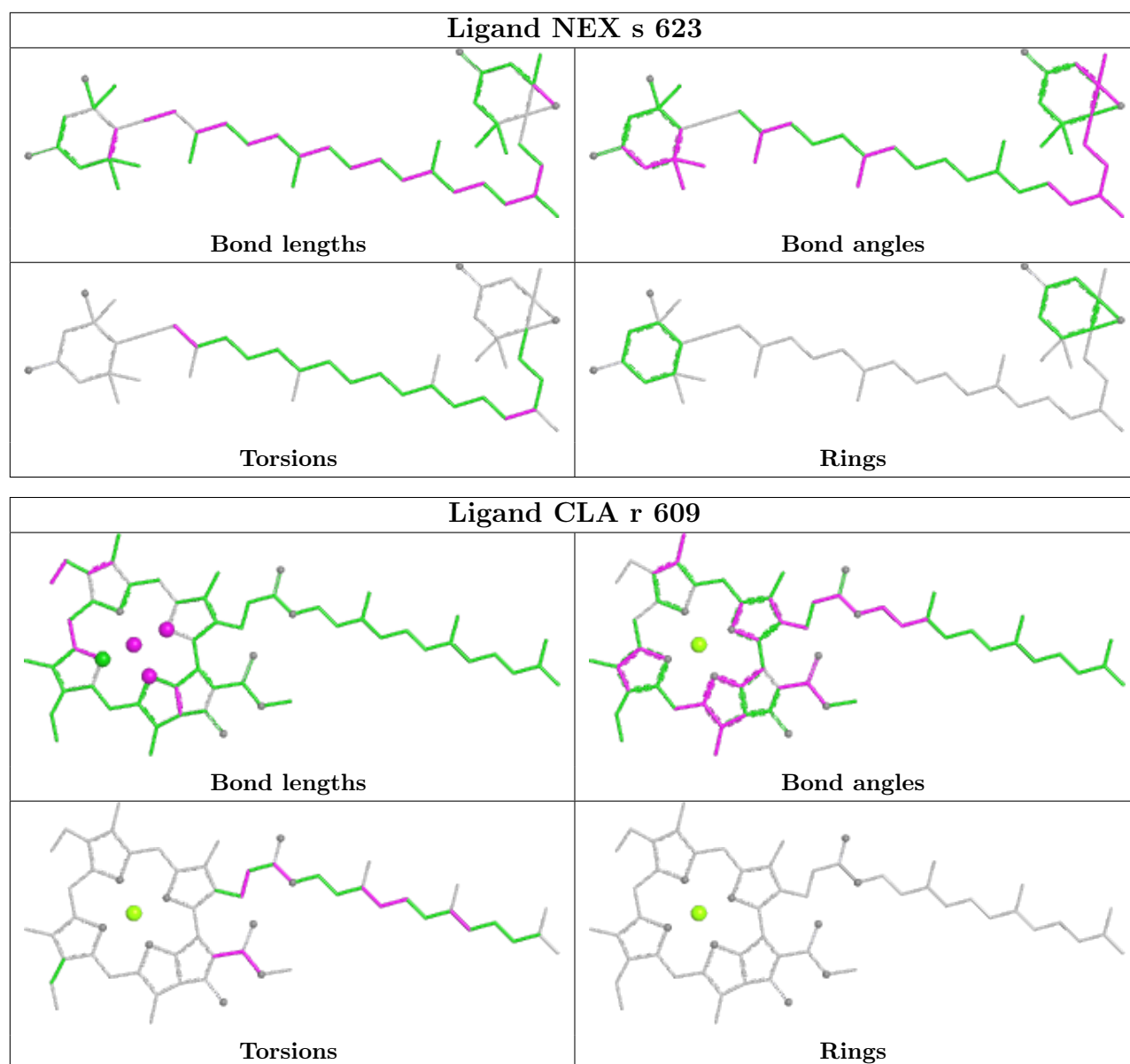


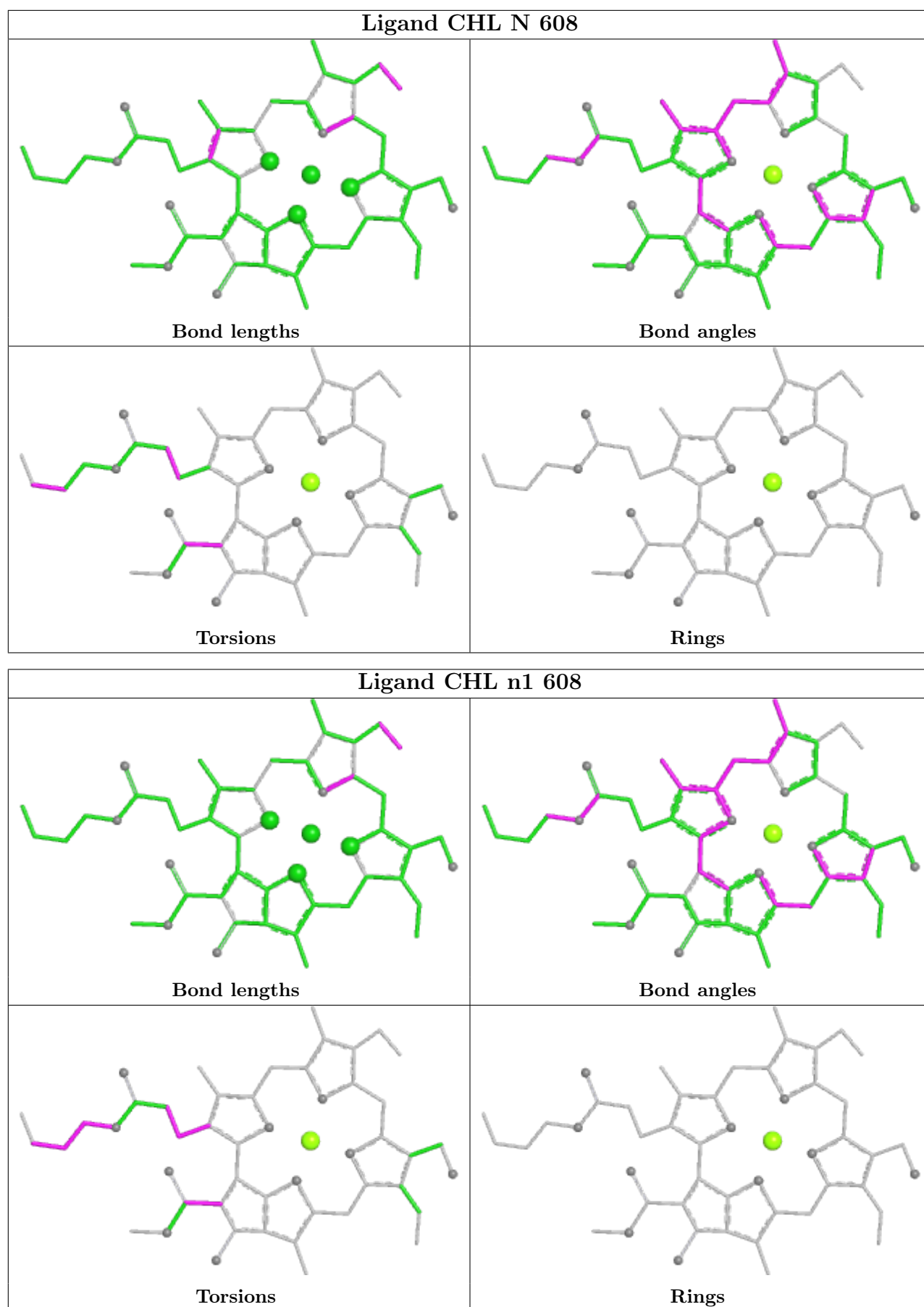
Rings

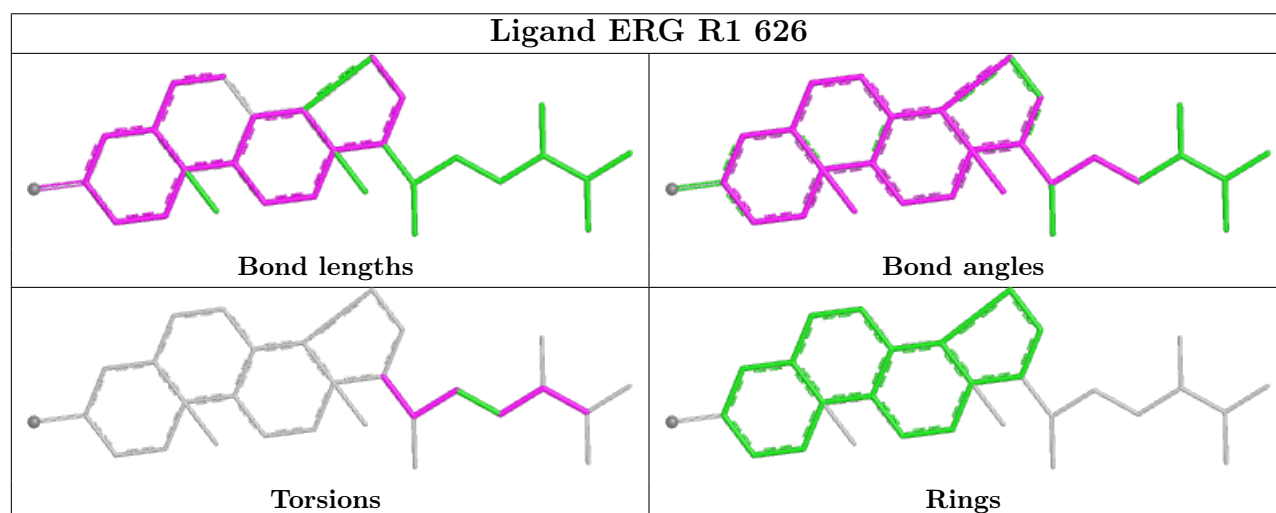
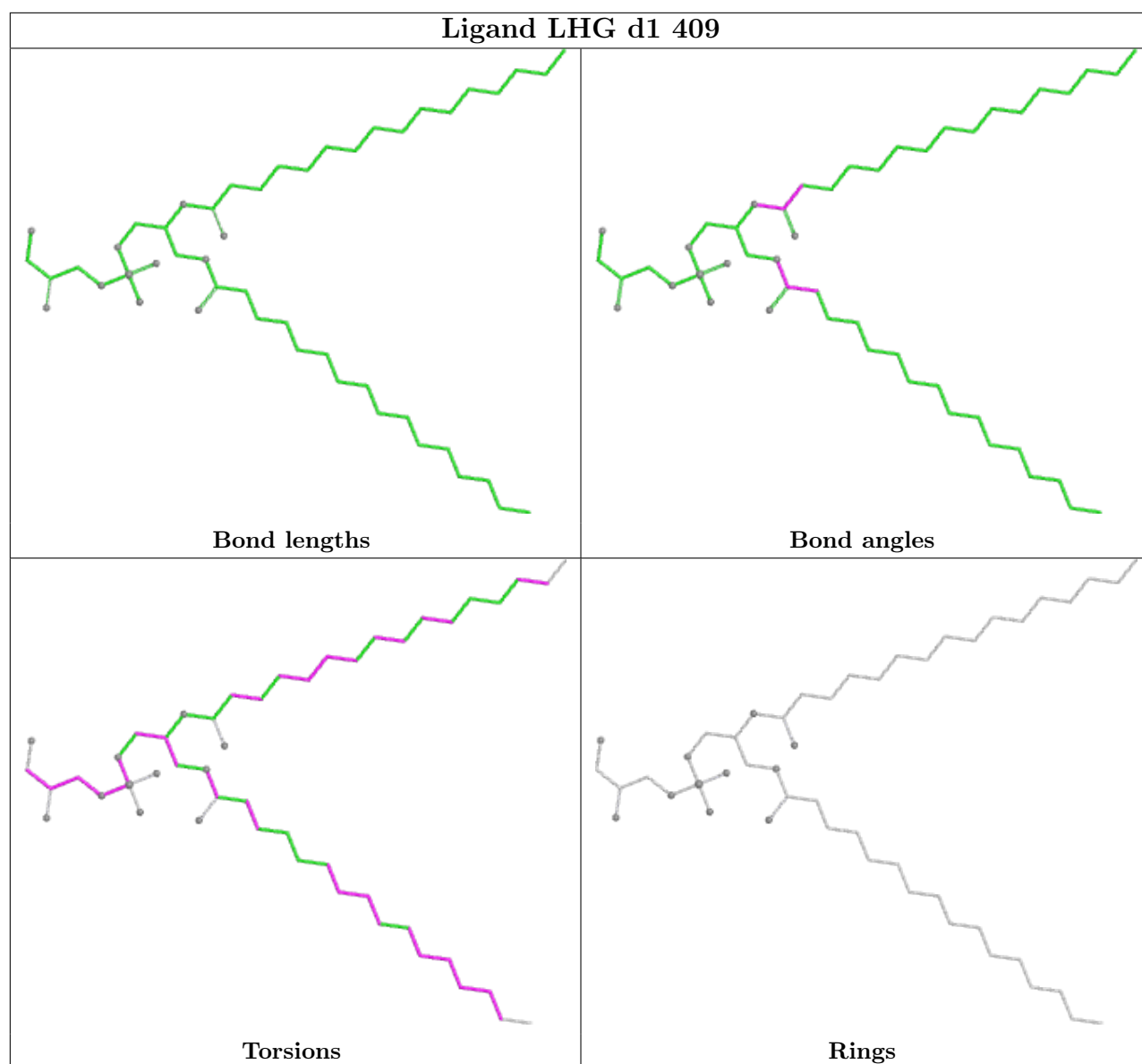


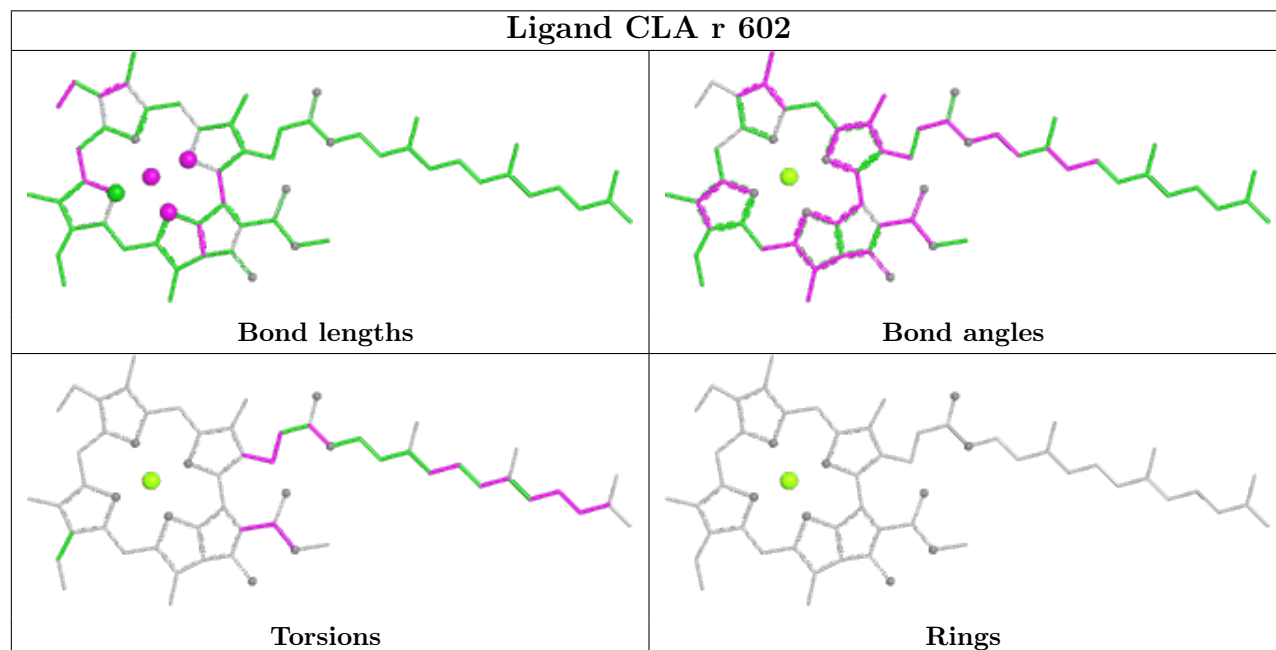
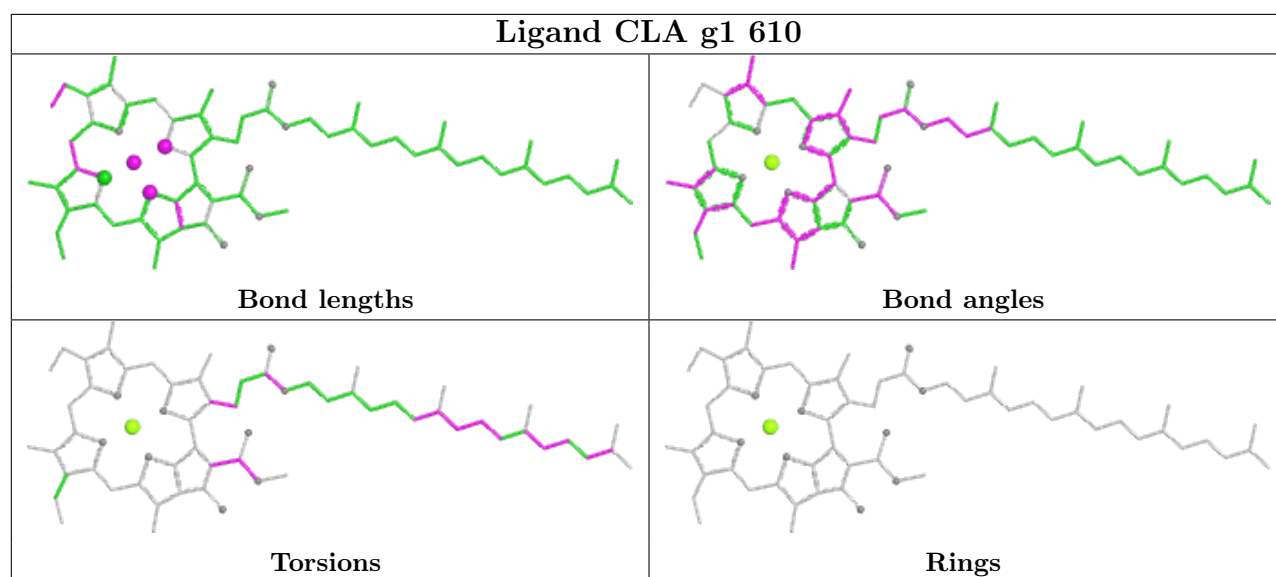


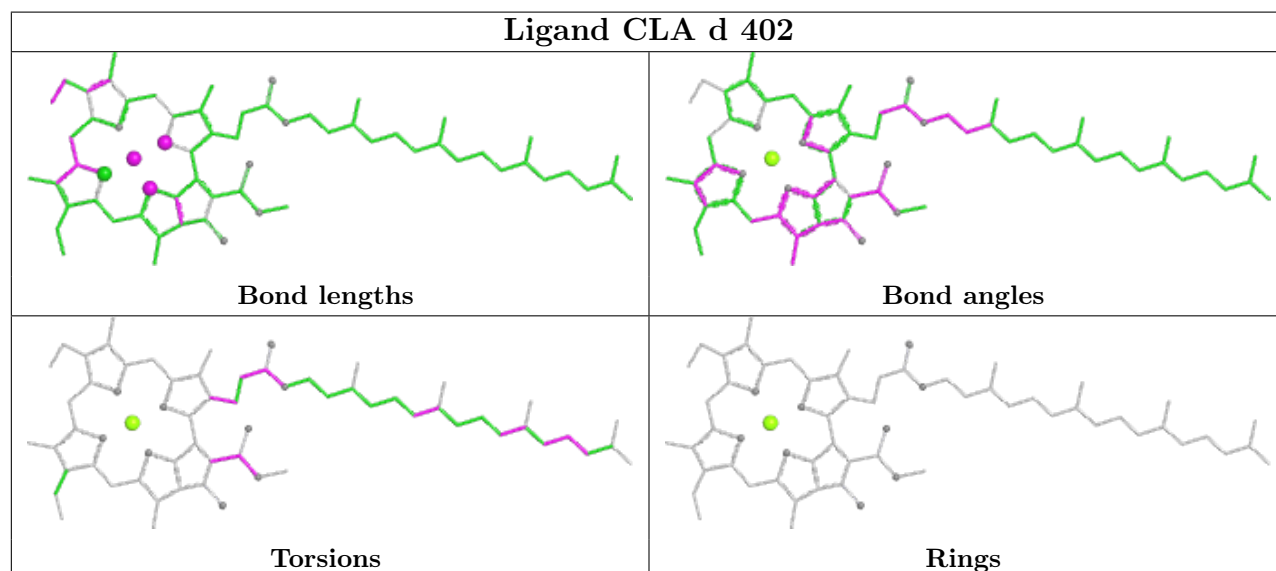
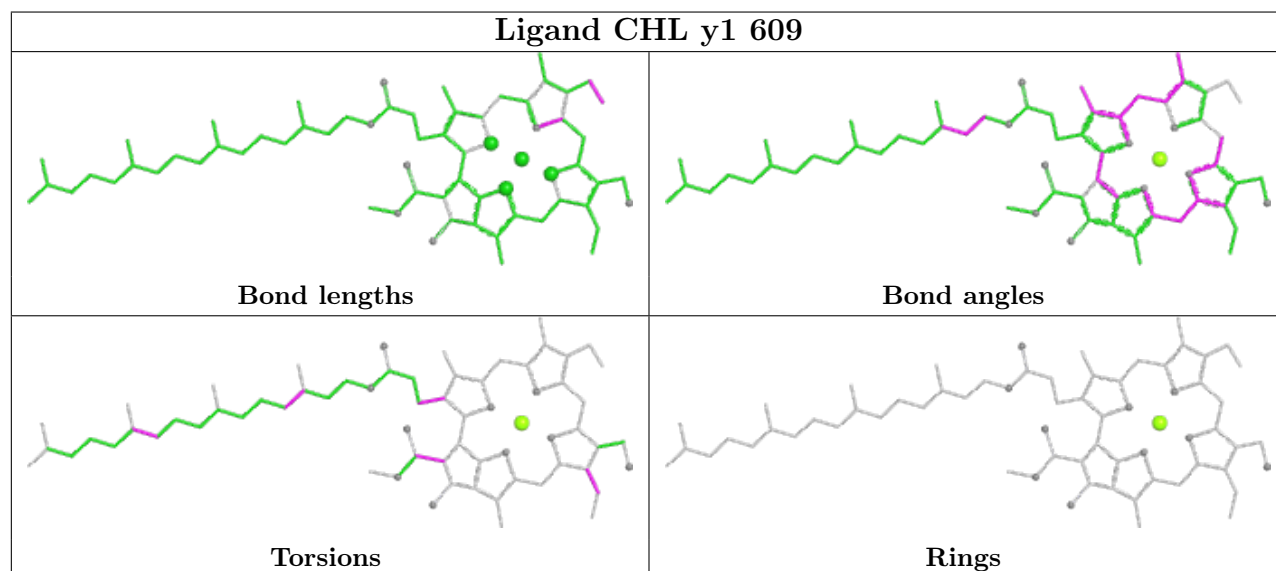
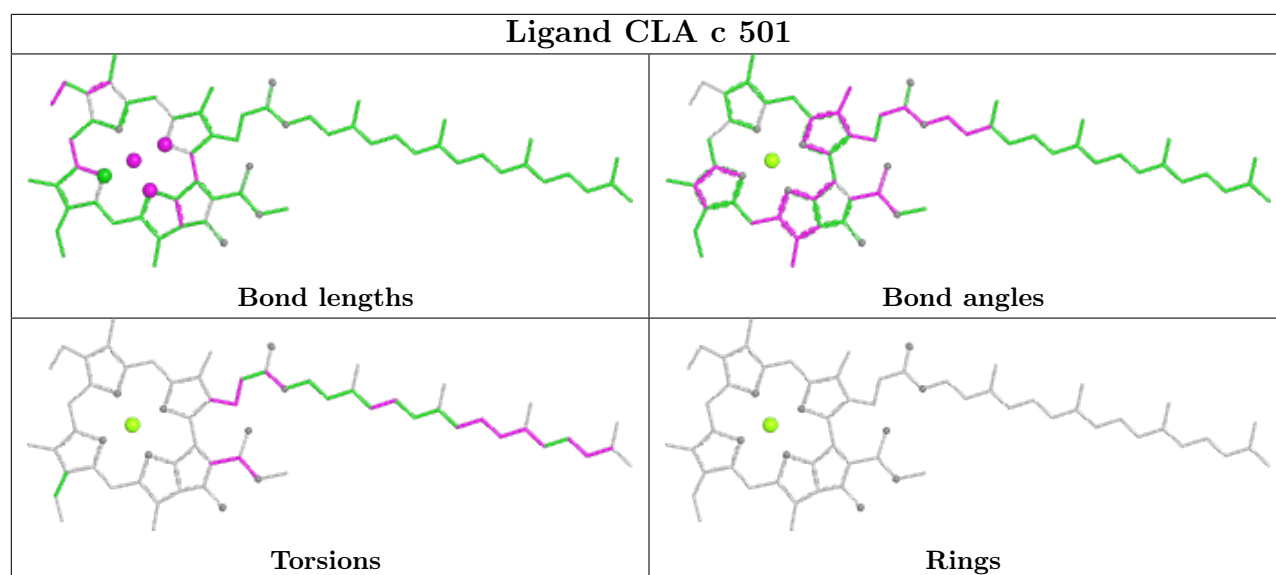


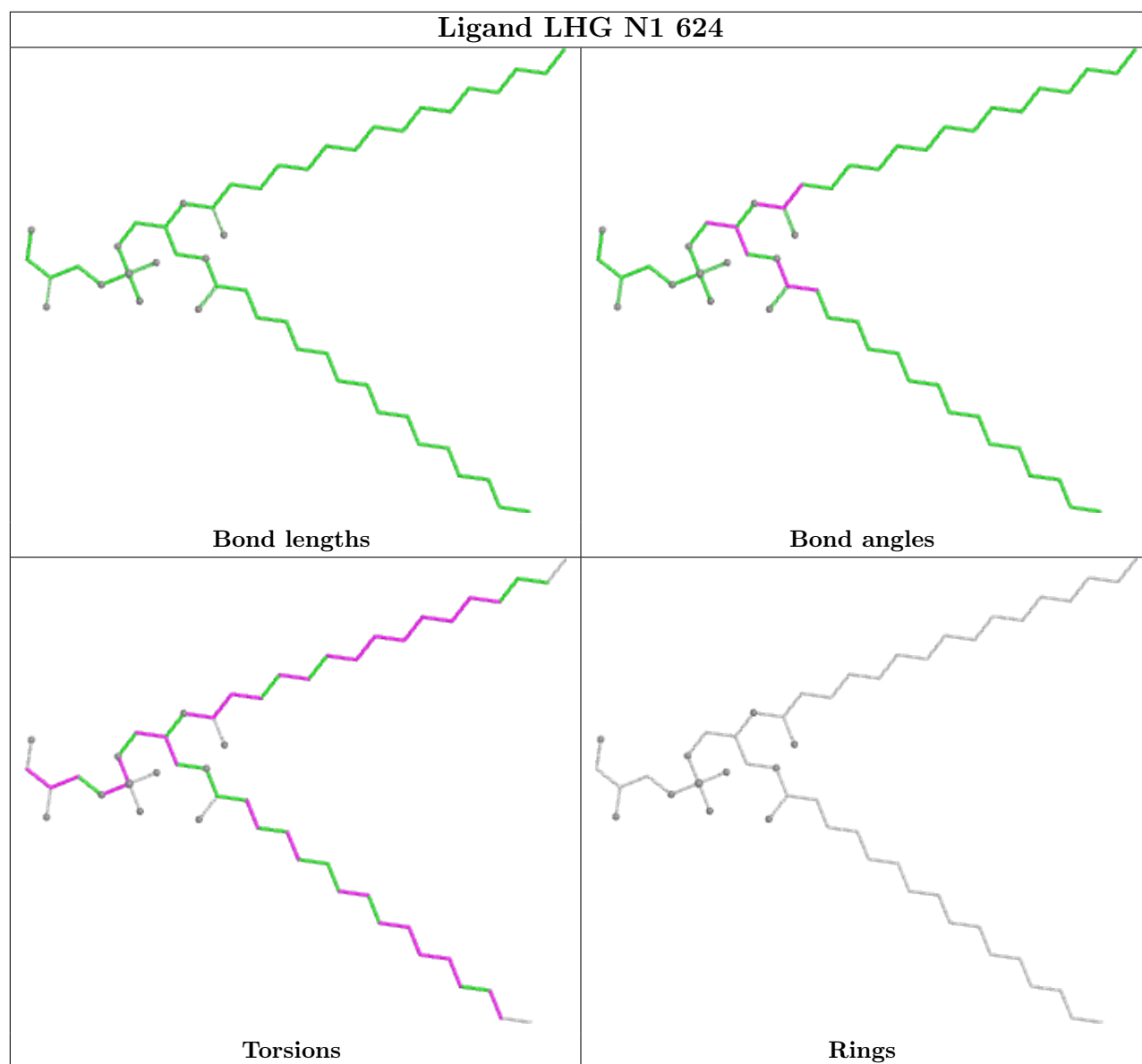
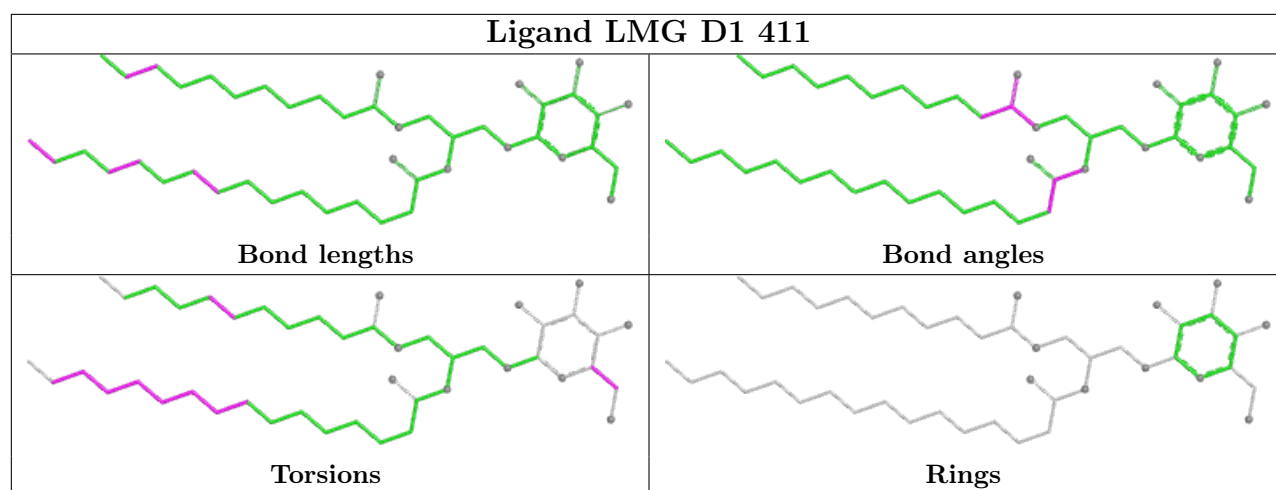


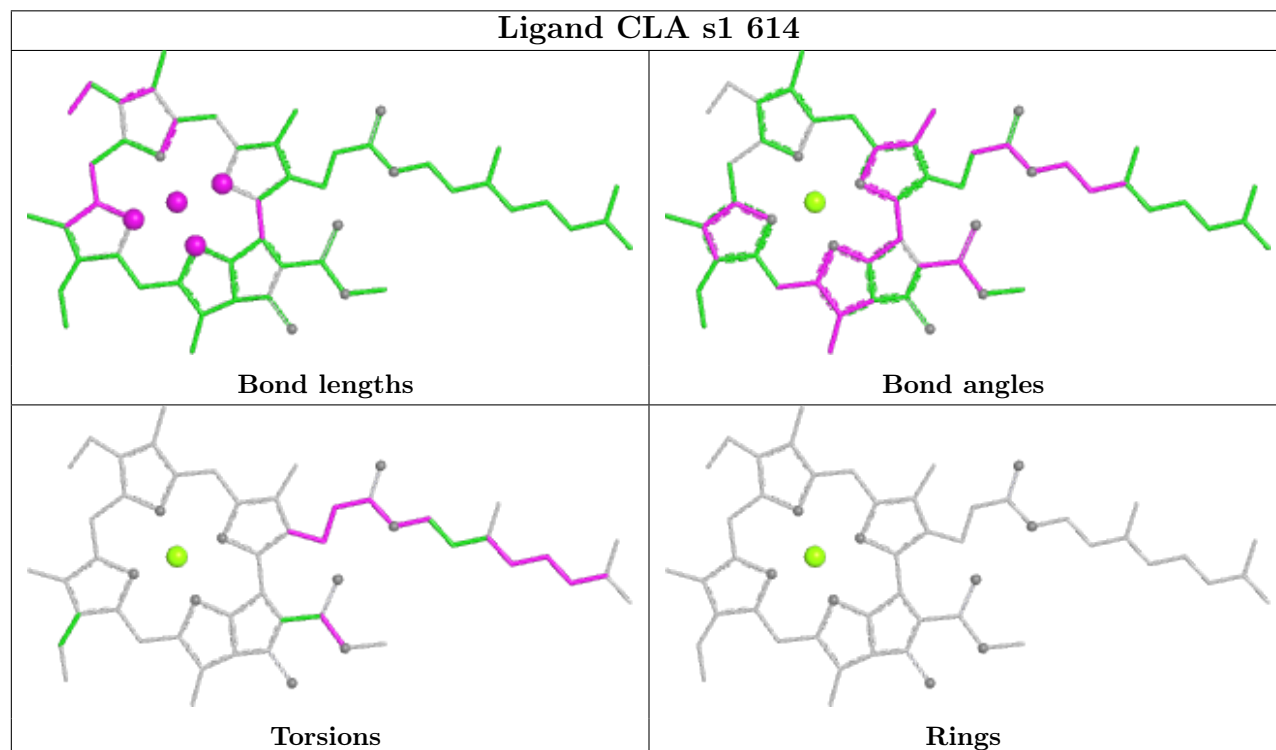
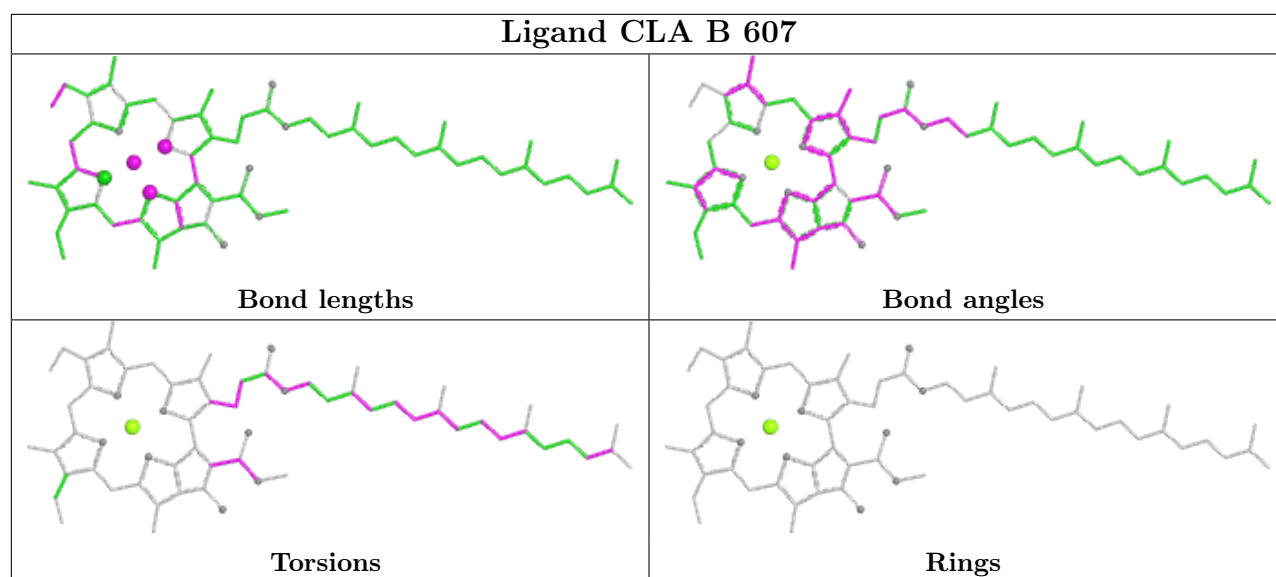


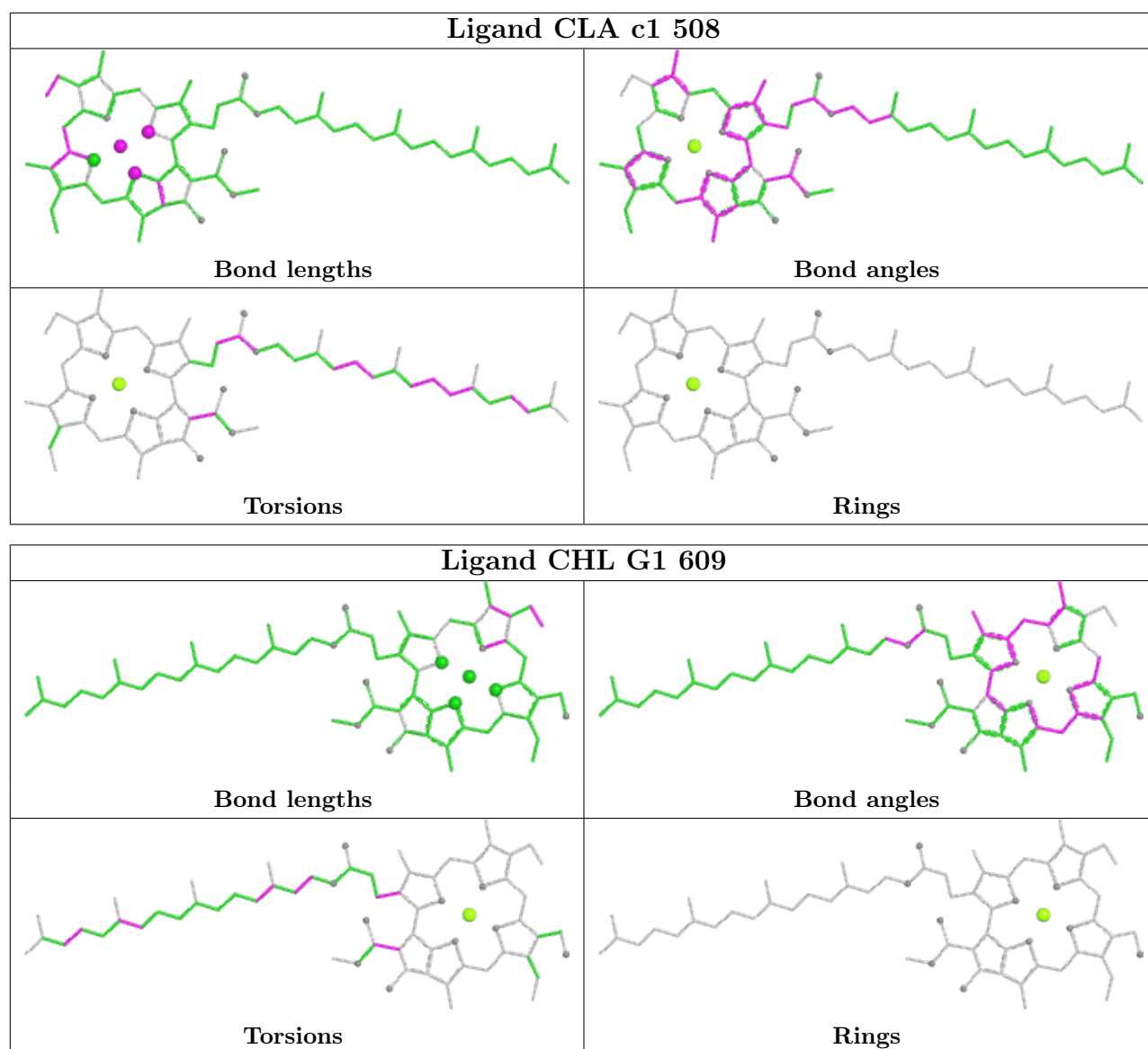


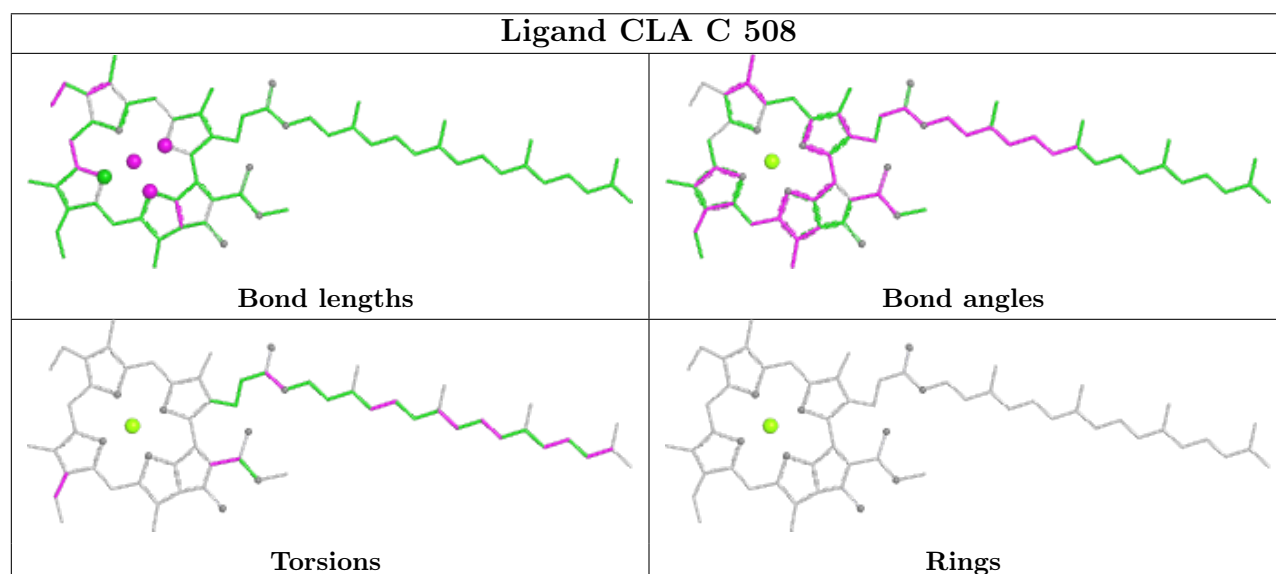
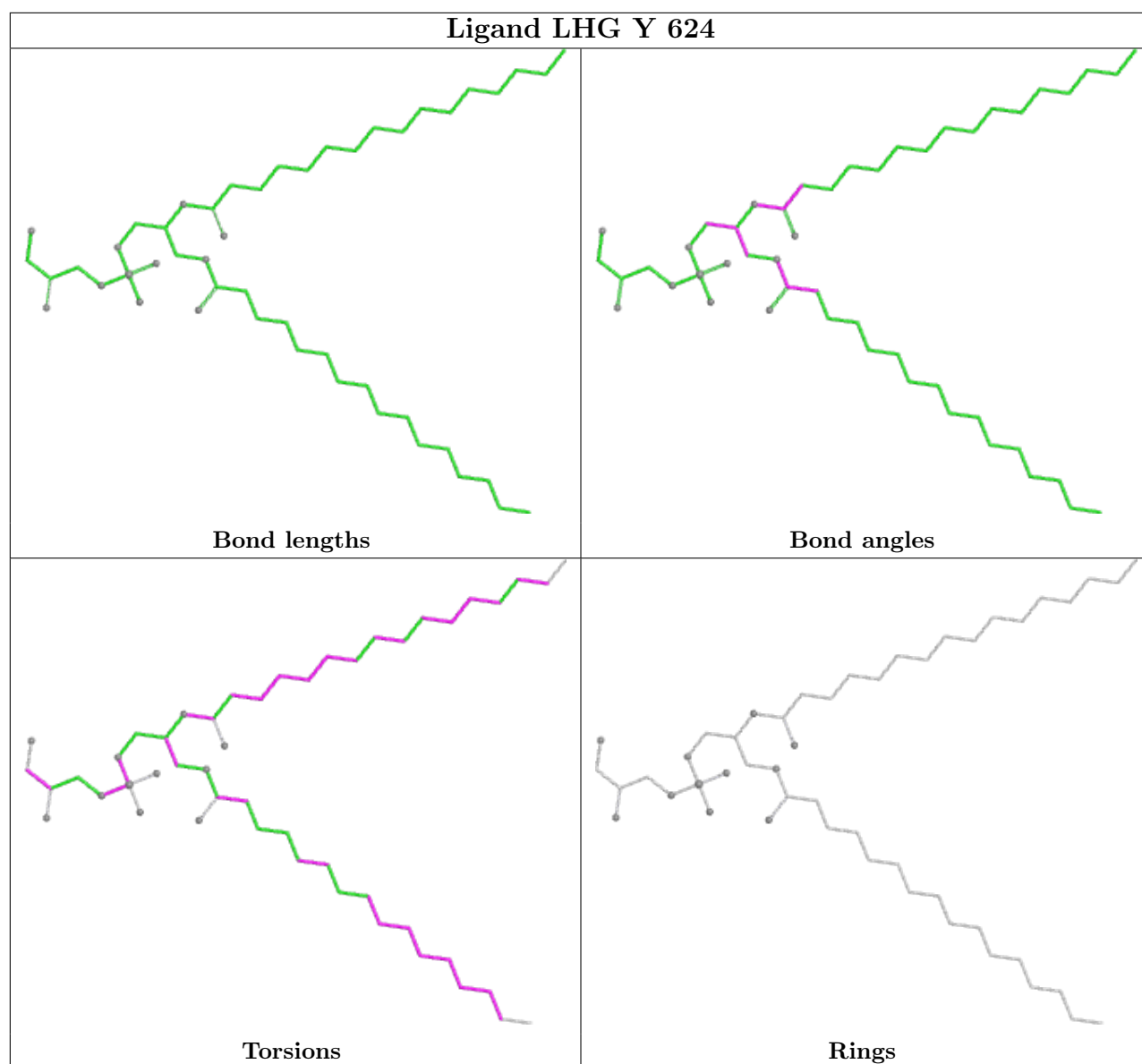


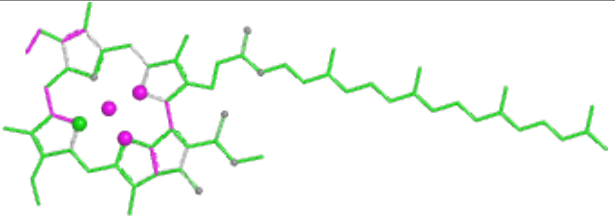
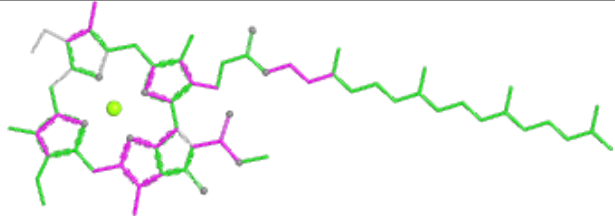
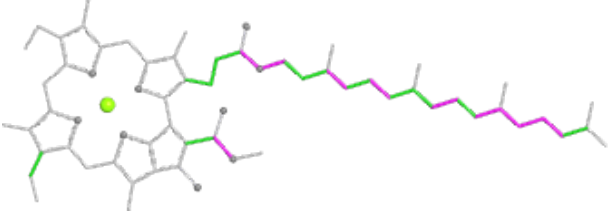
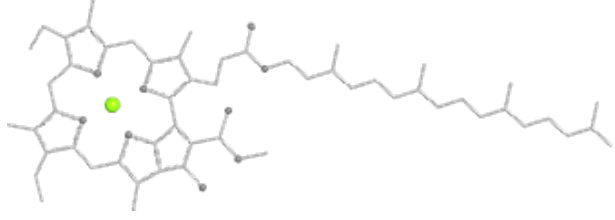
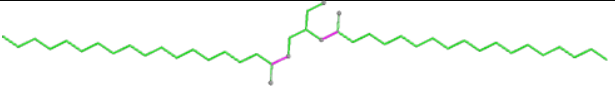
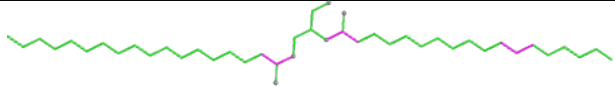
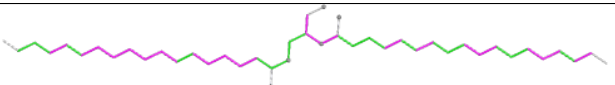
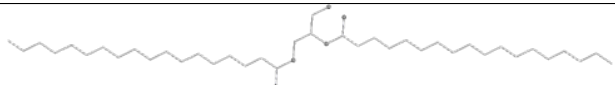
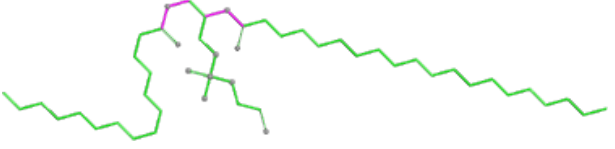
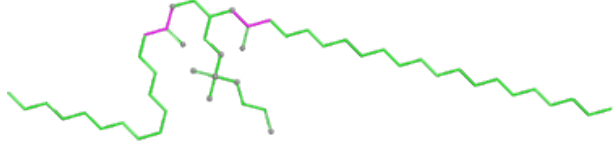
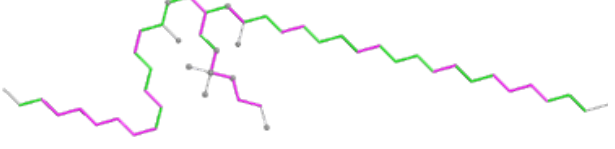
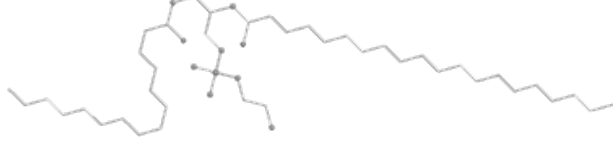
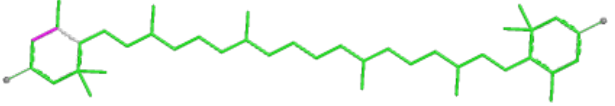
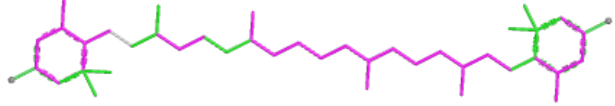
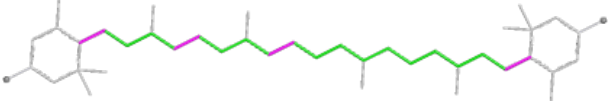
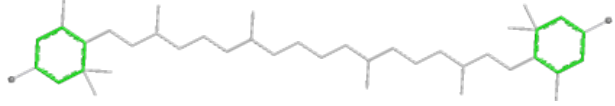


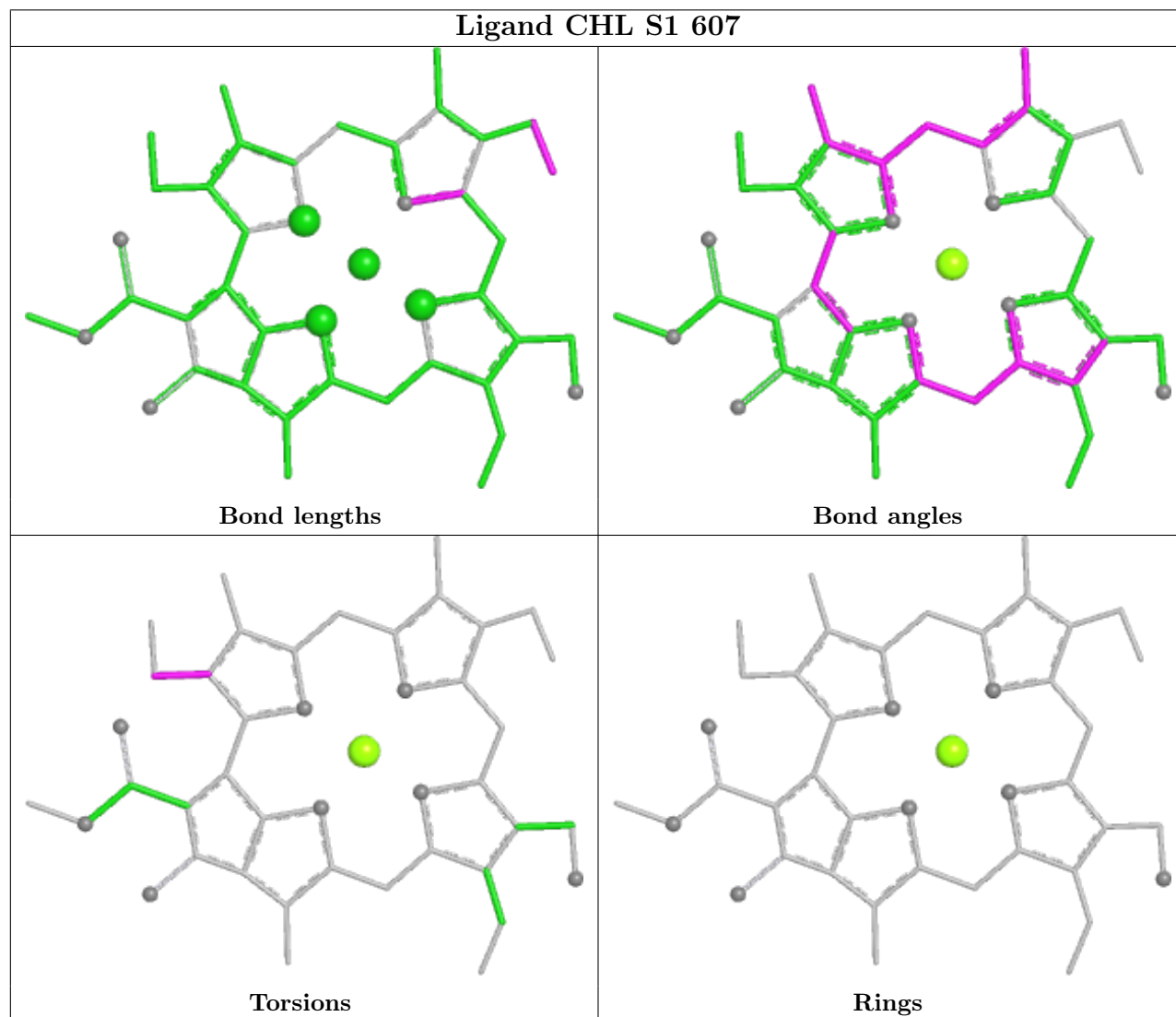
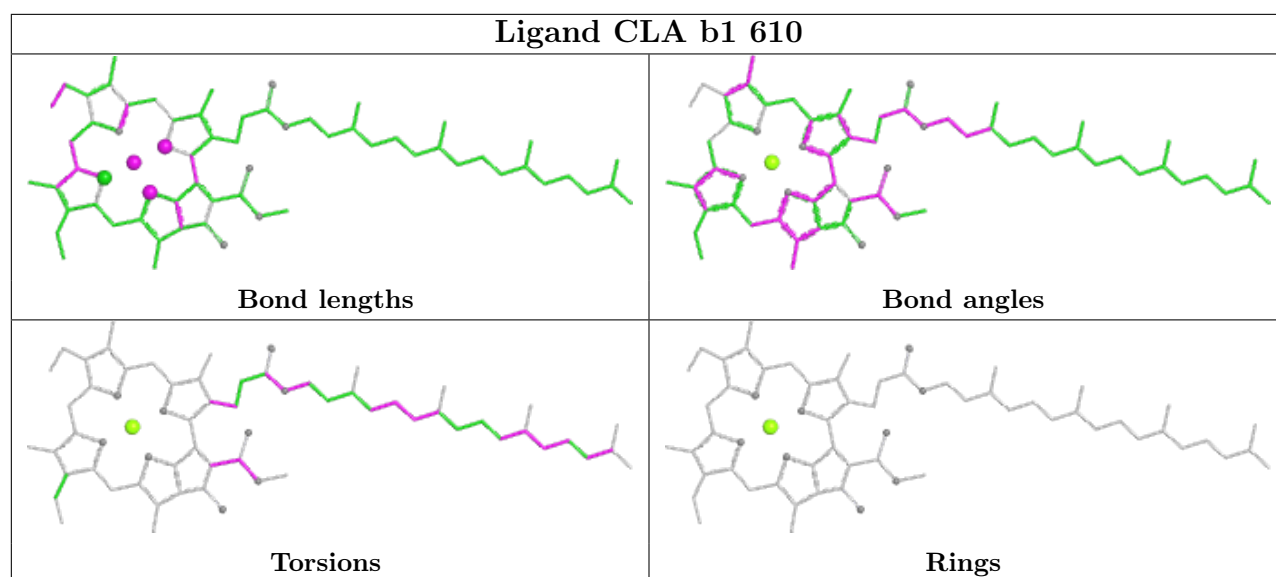


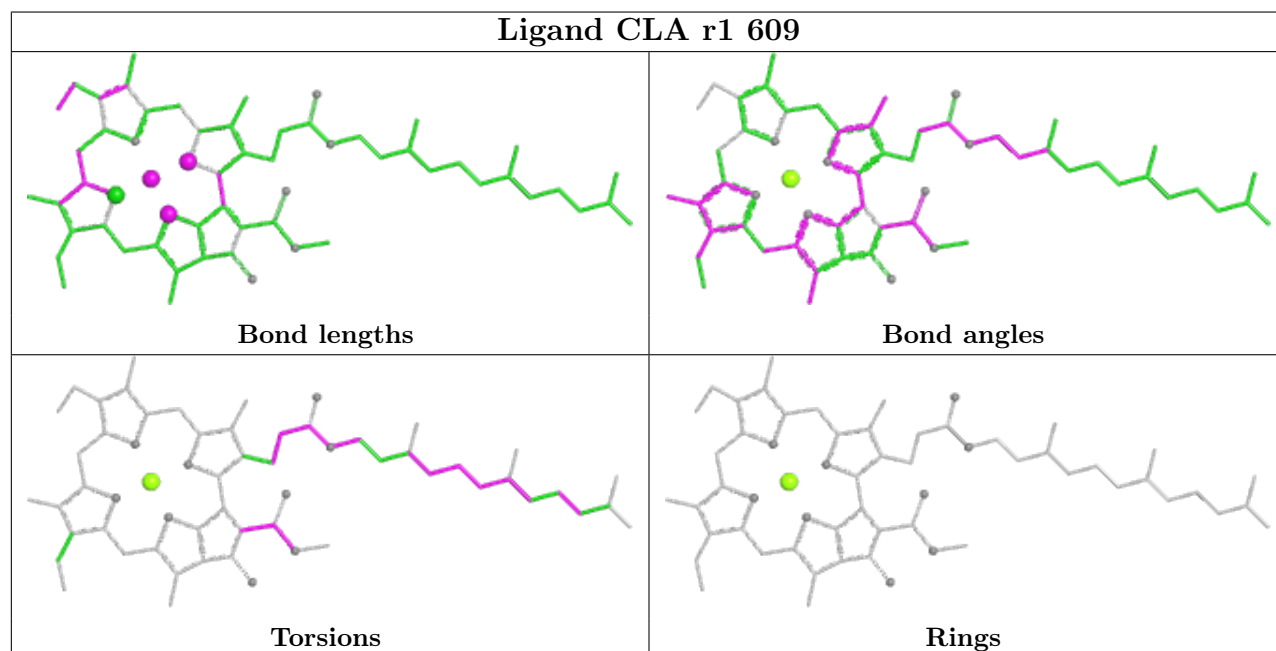
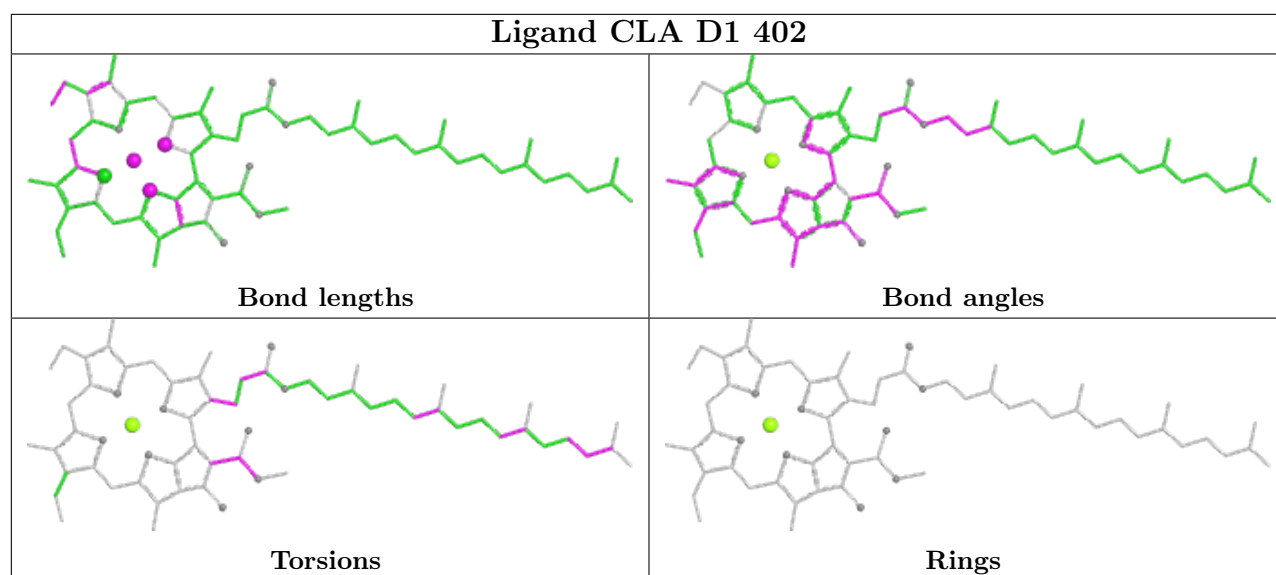


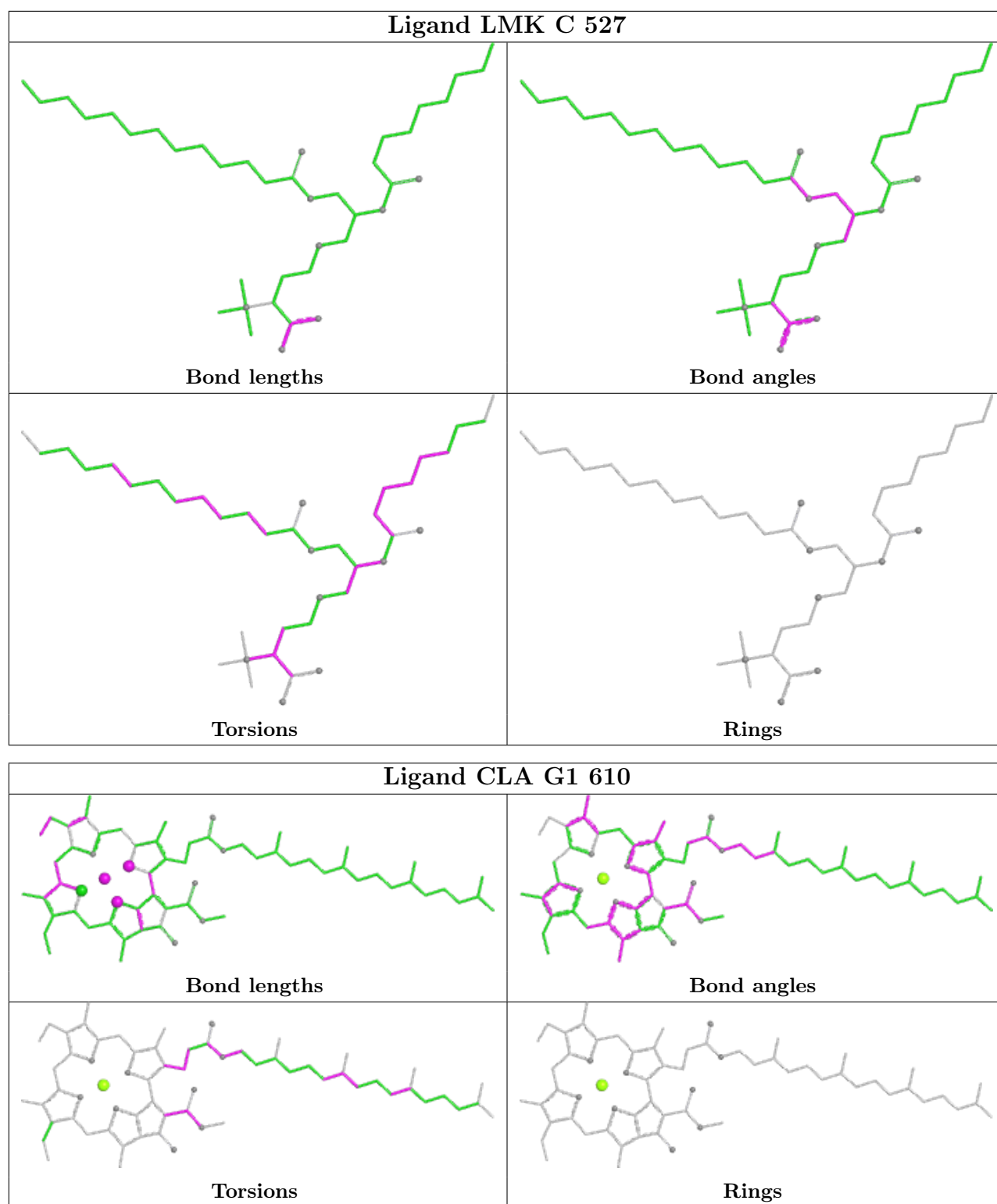


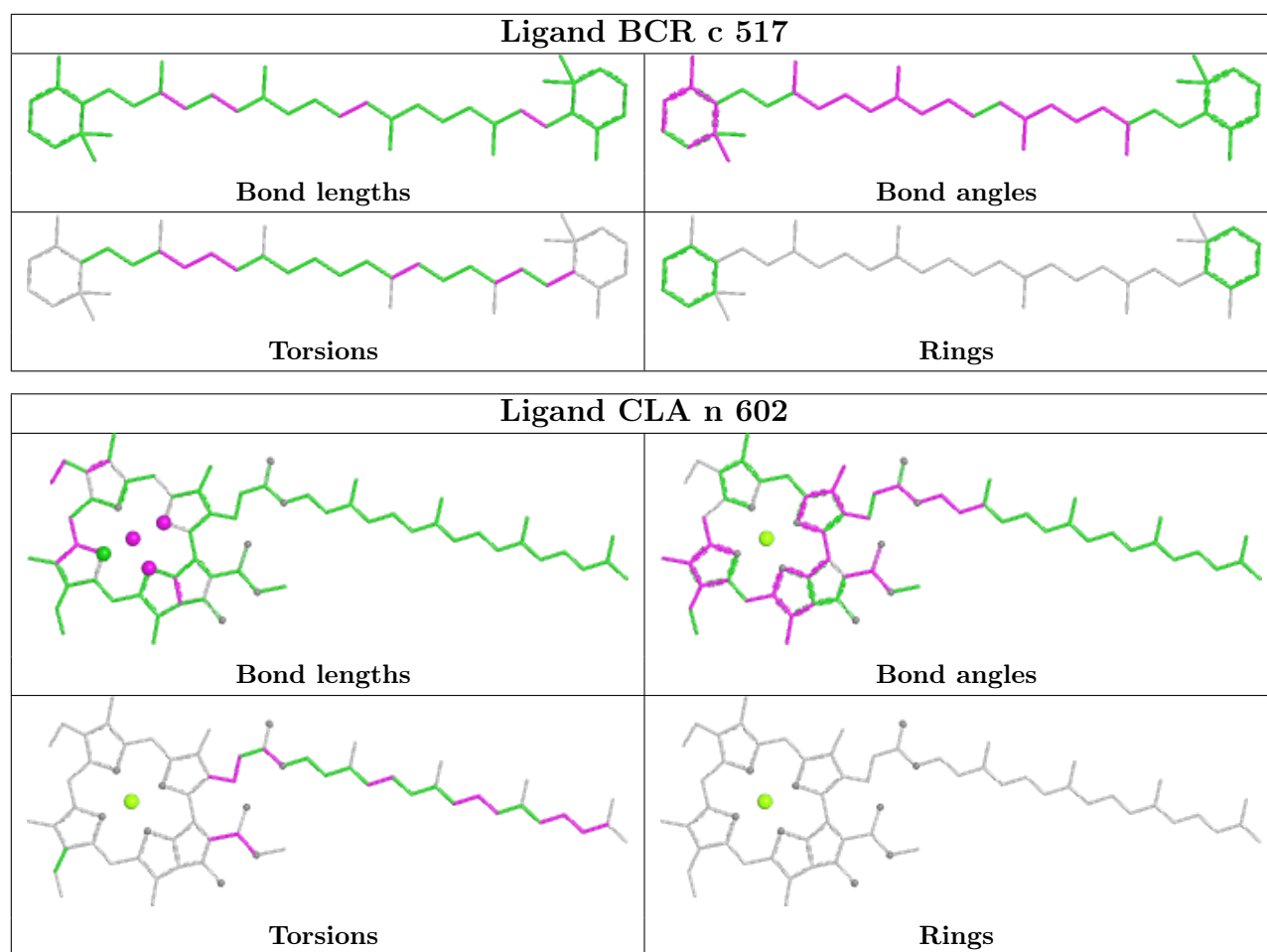


Ligand CLA b 614	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGA B 625	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PTY Y1 626	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT n1 621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

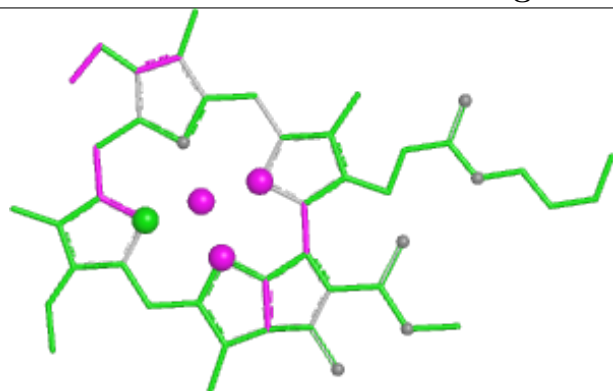




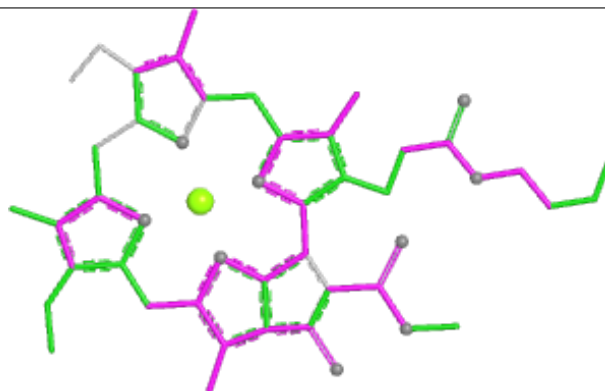




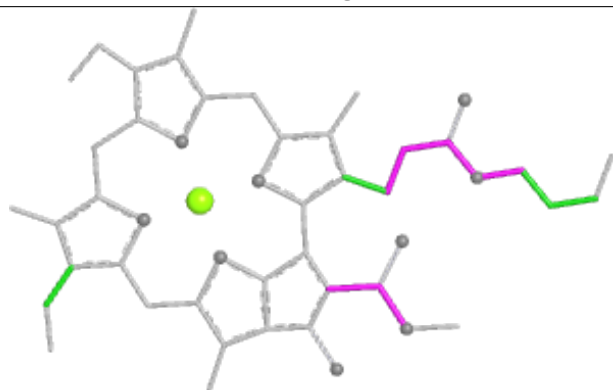
Ligand CLA R 604



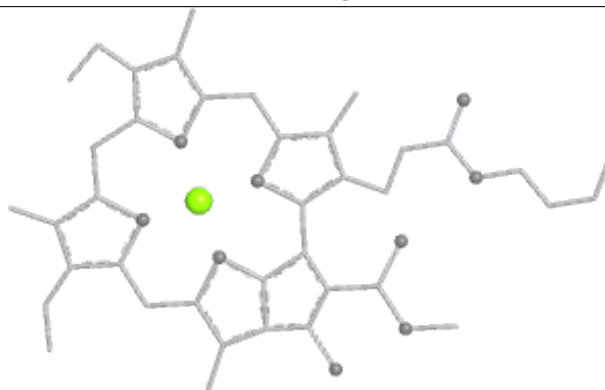
Bond lengths



Bond angles

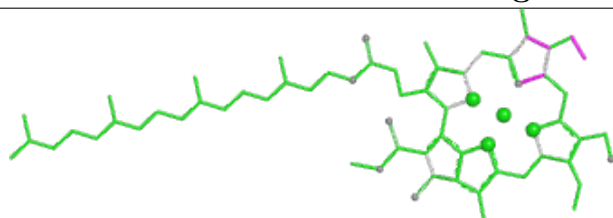


Torsions

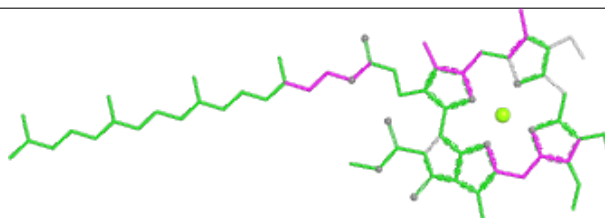


Rings

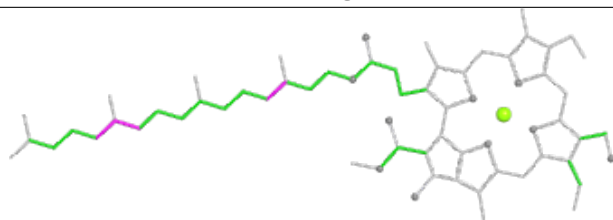
Ligand CHL N 601



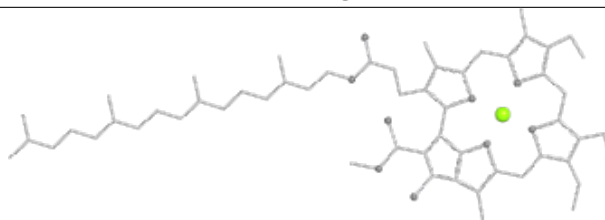
Bond lengths



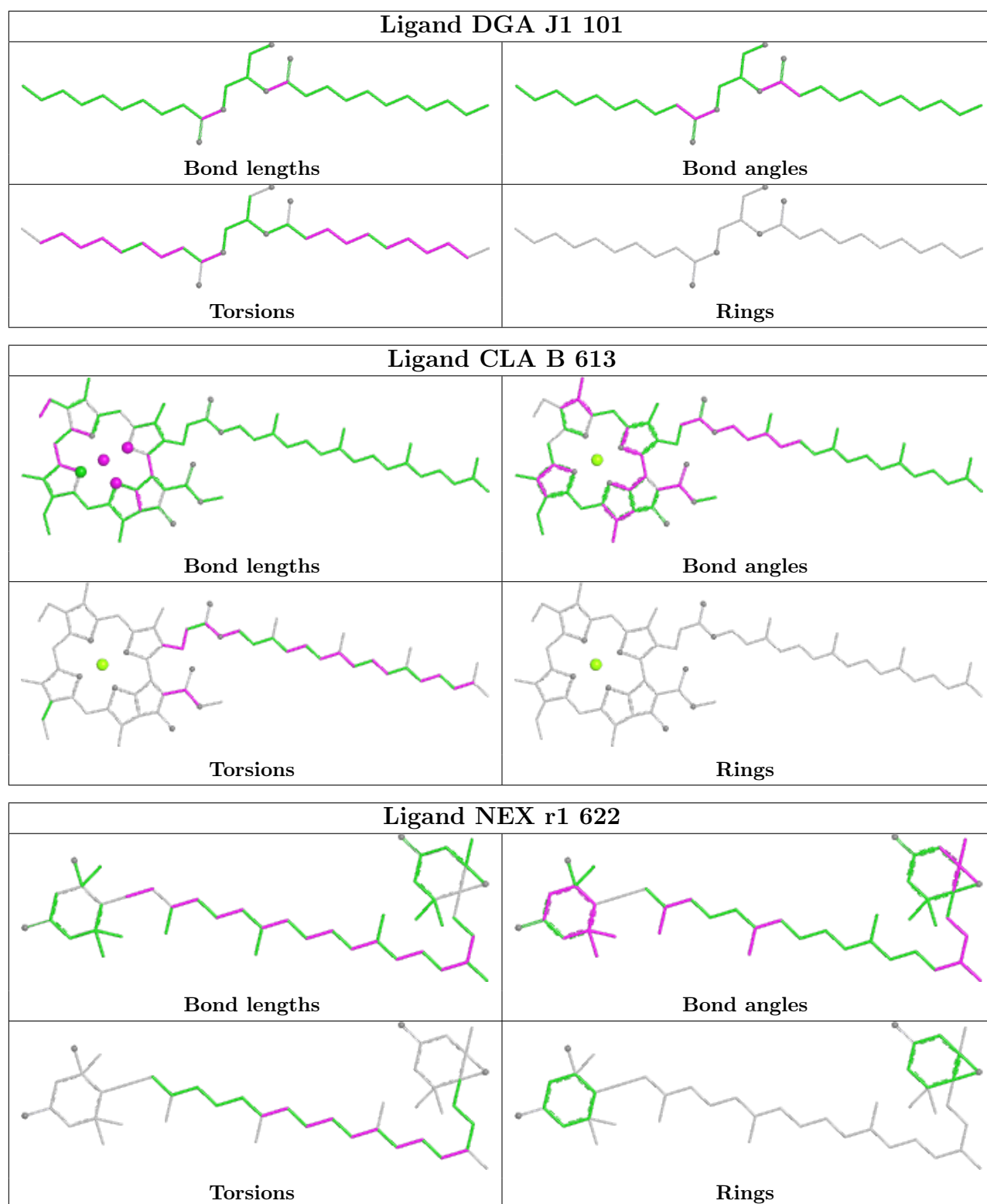
Bond angles

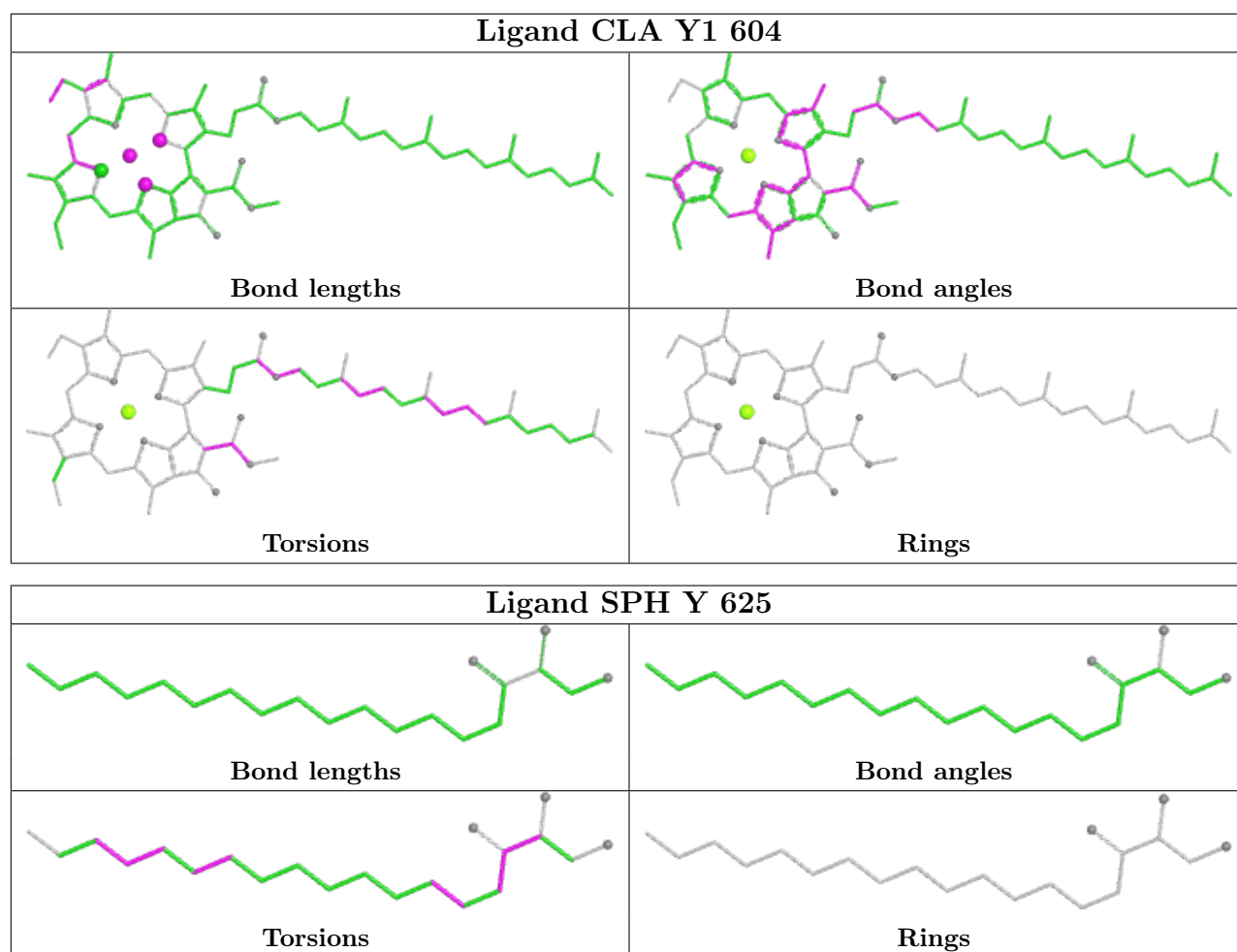


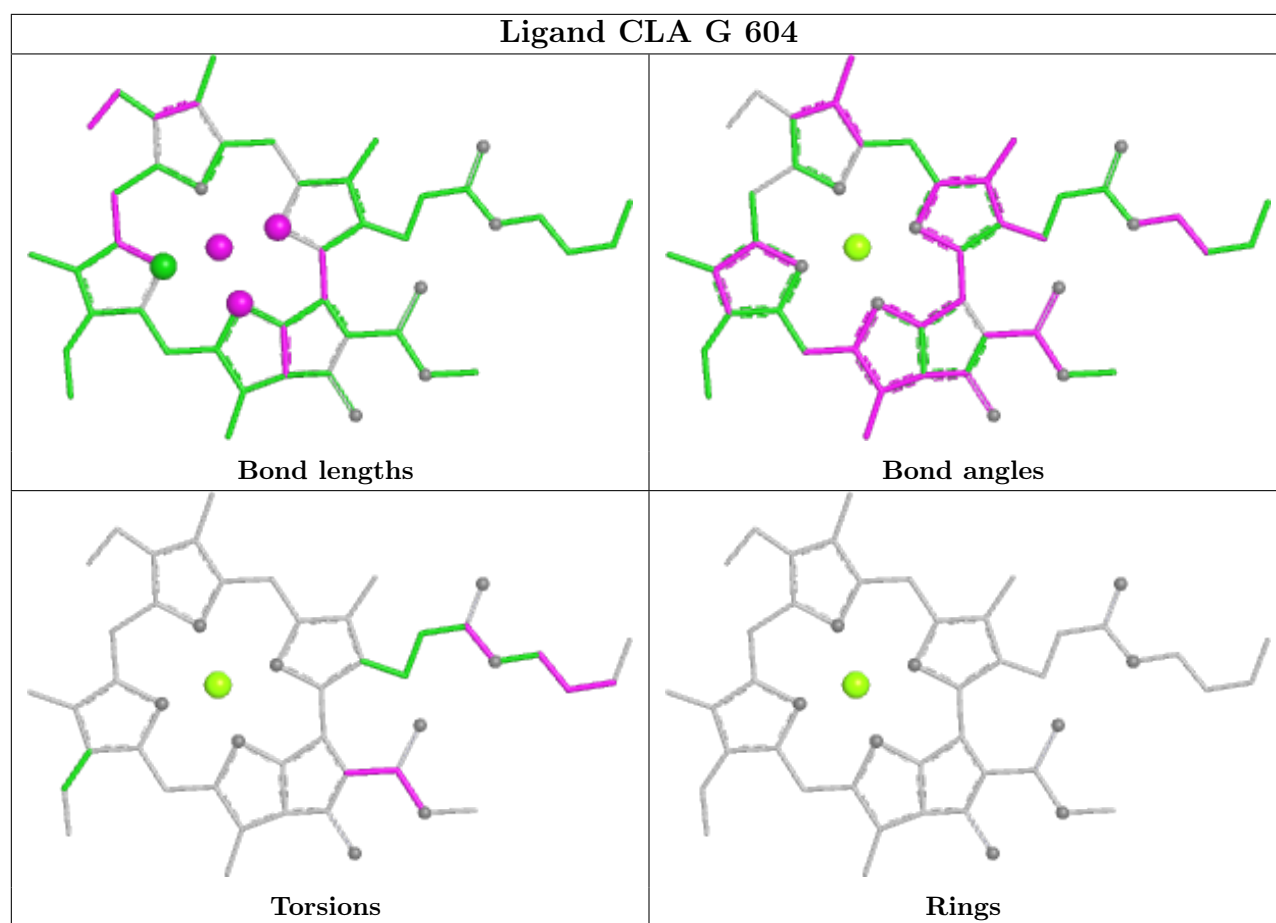
Torsions

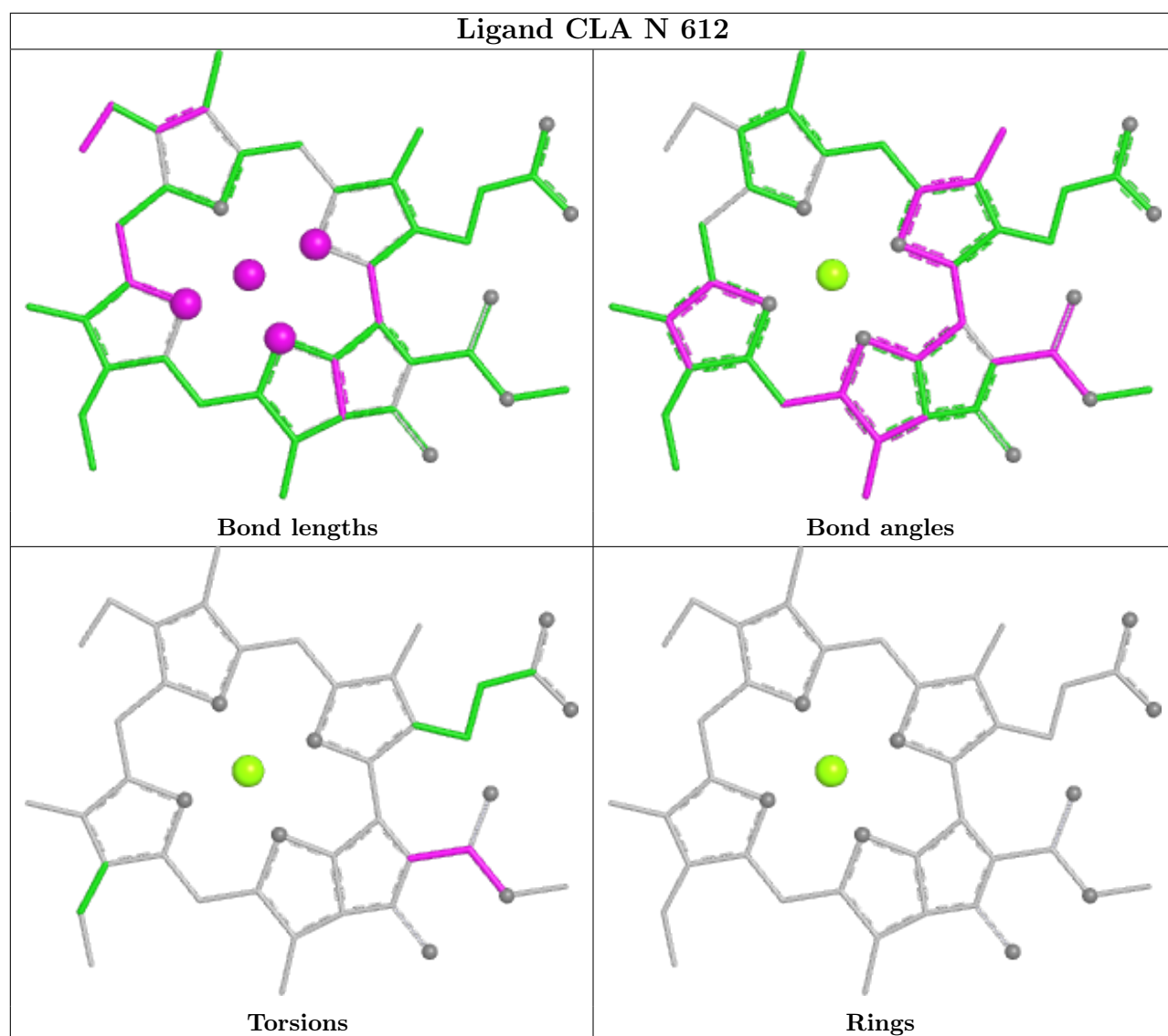


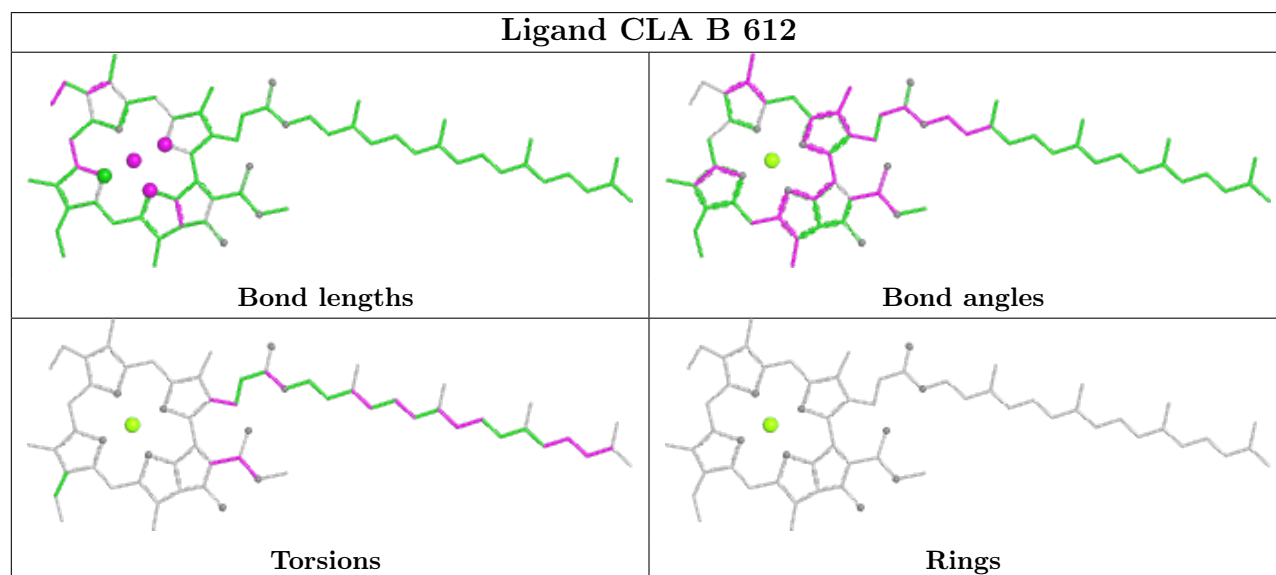
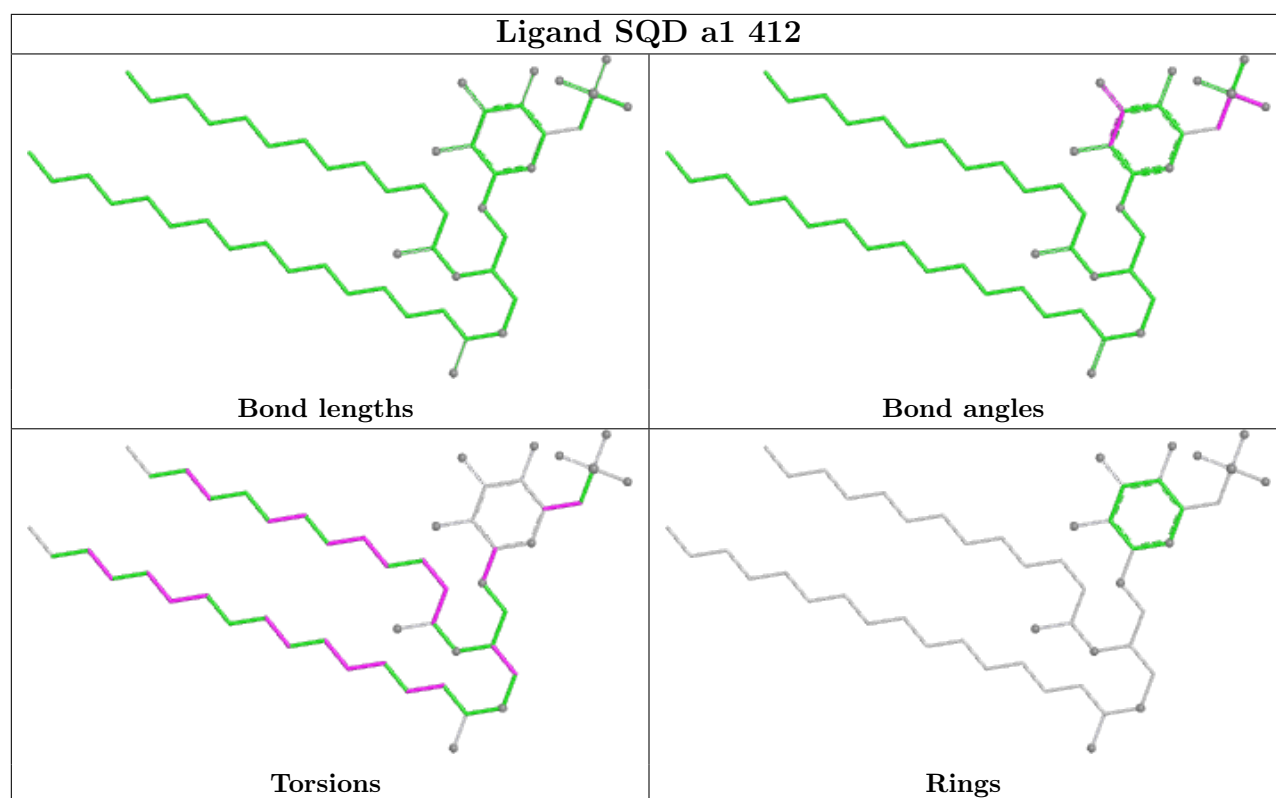
Rings

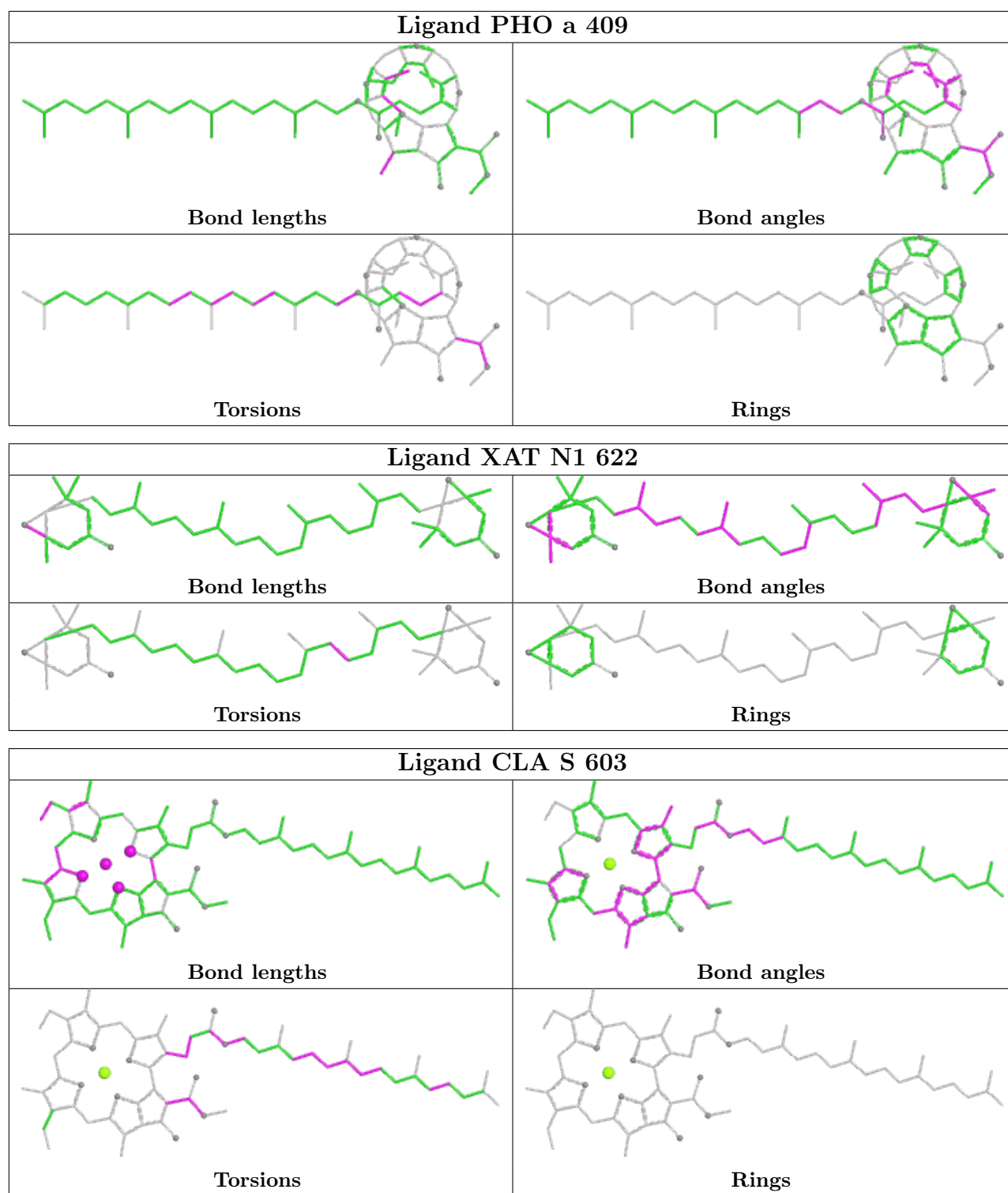


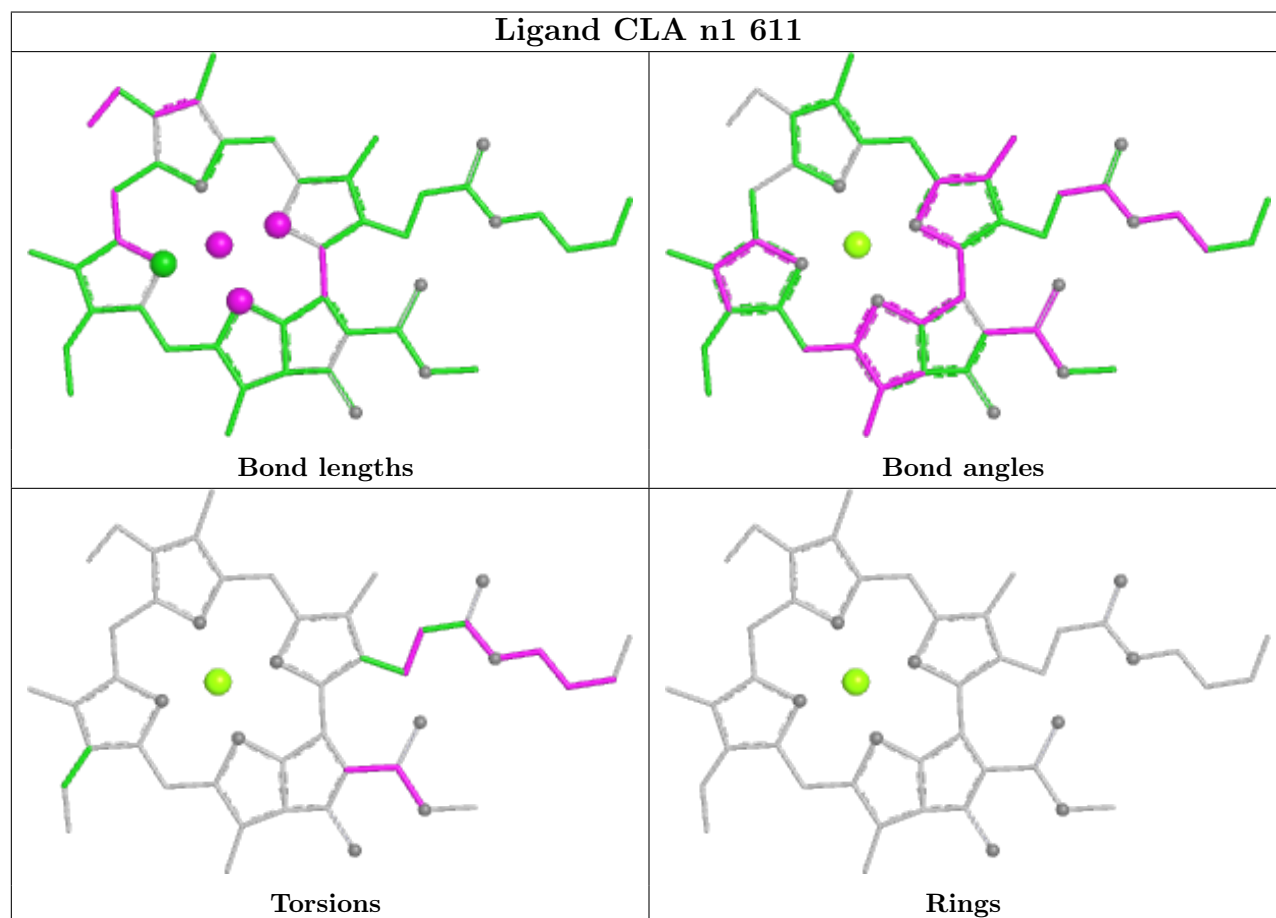
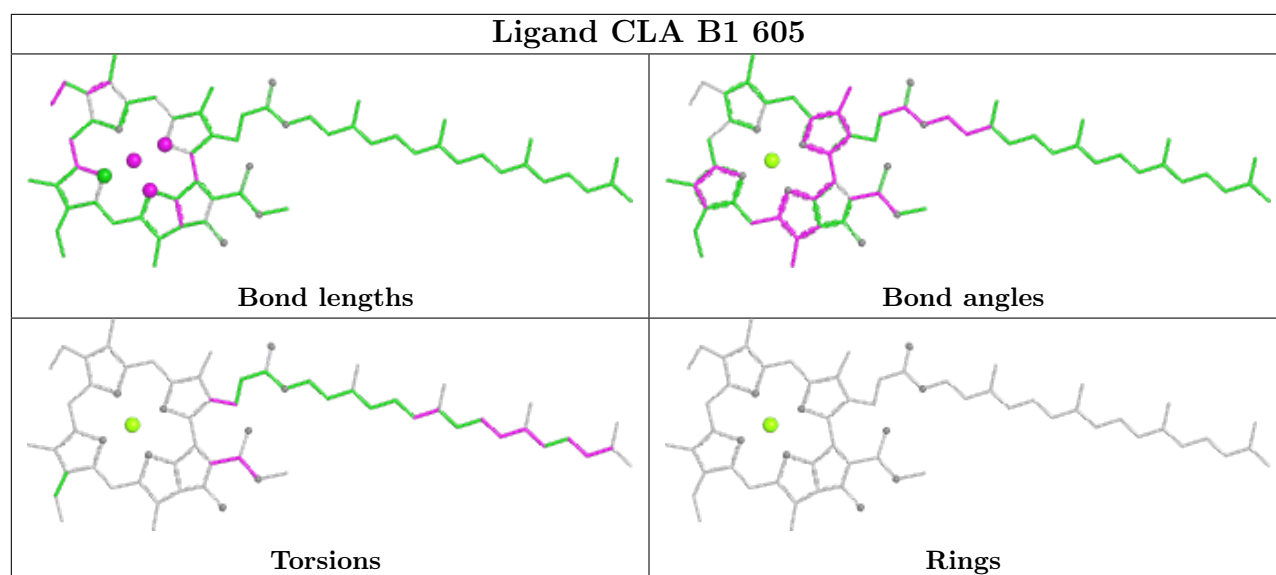


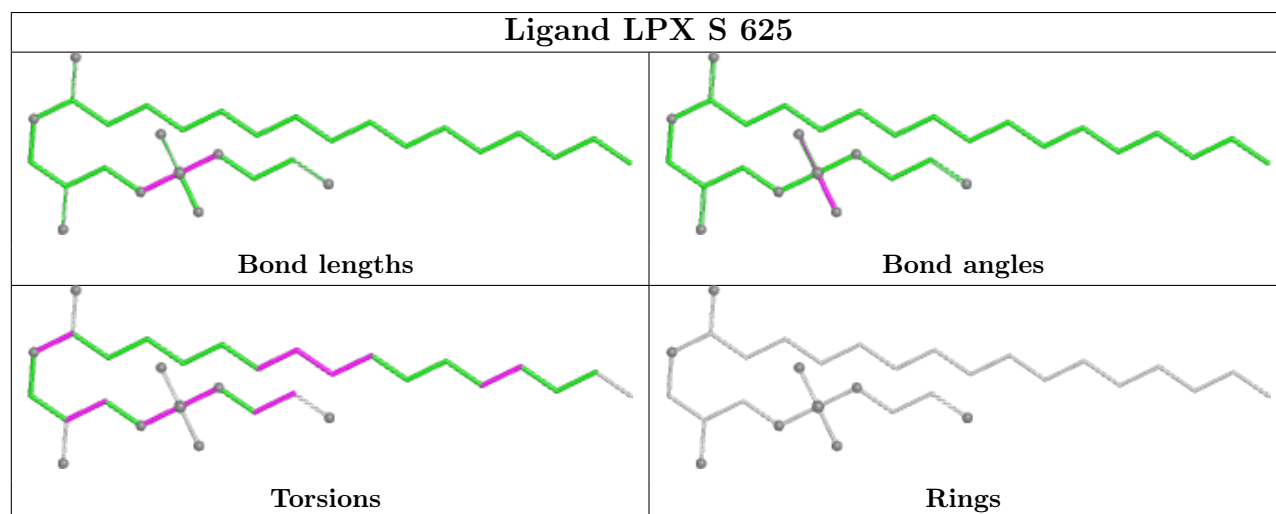
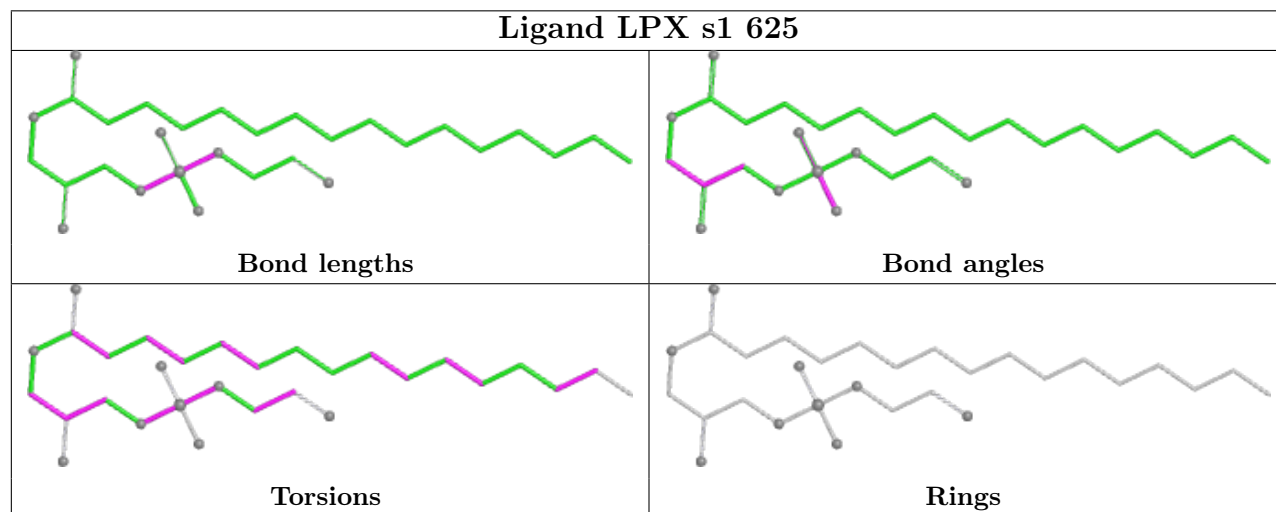
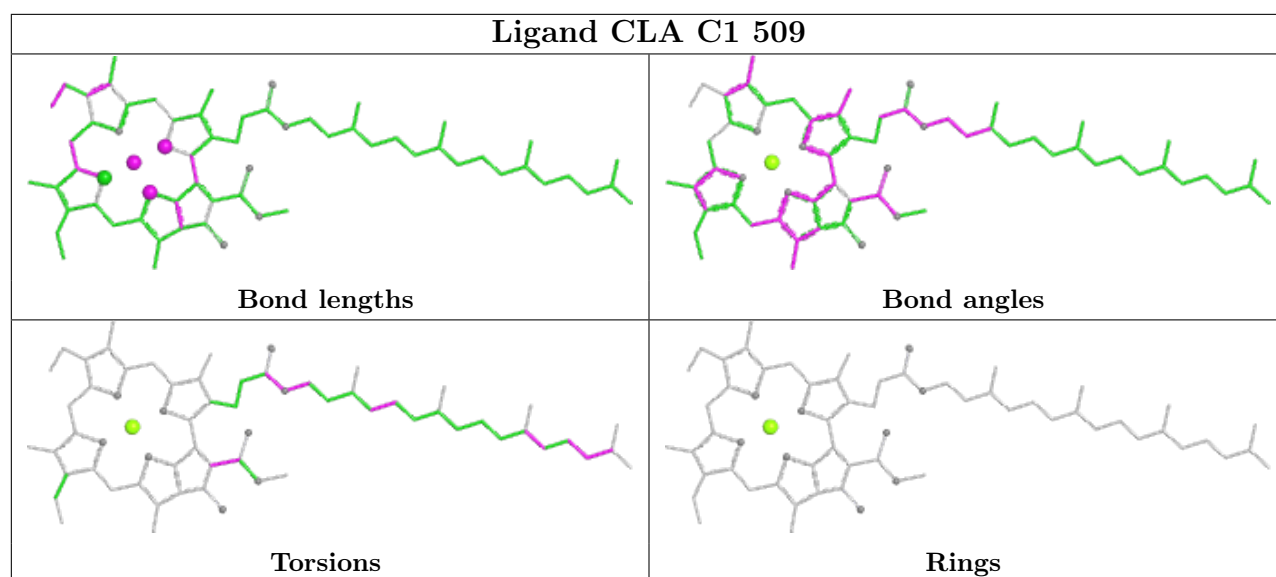


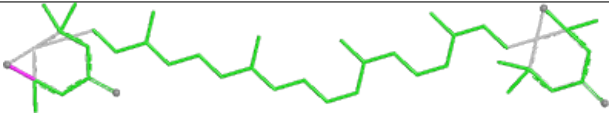
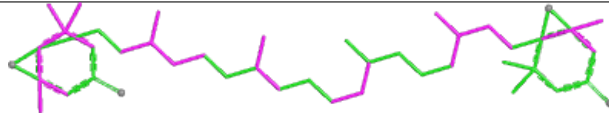
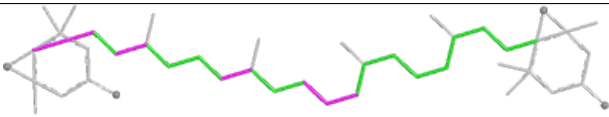
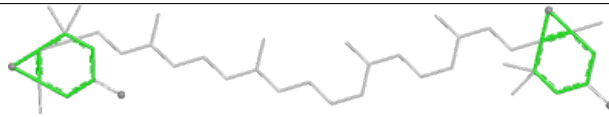


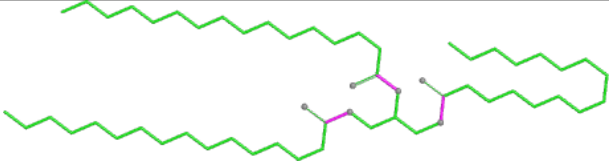
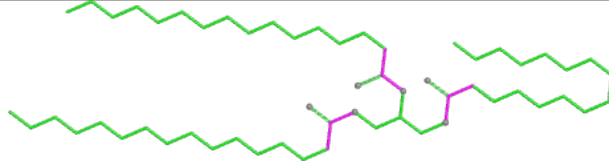
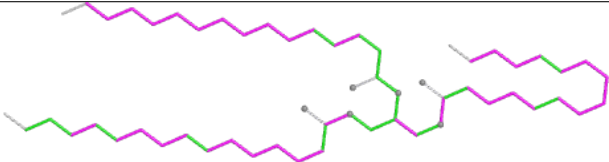
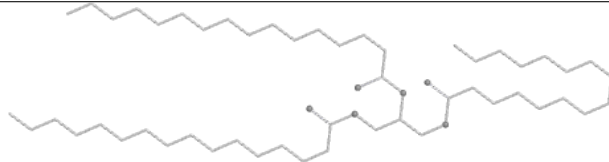


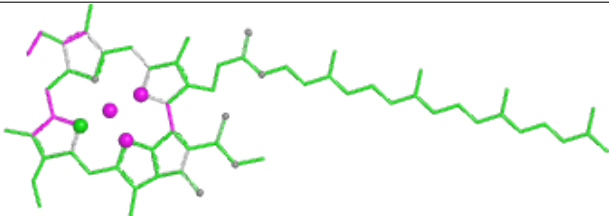
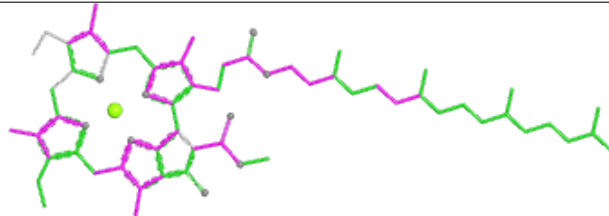
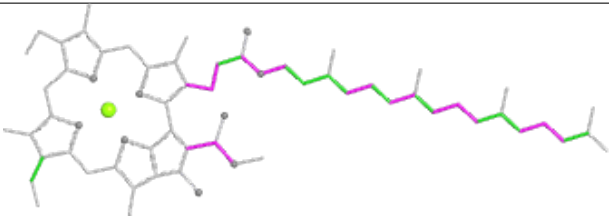
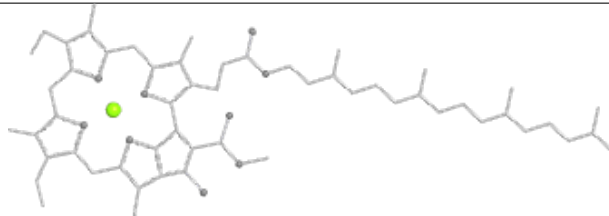


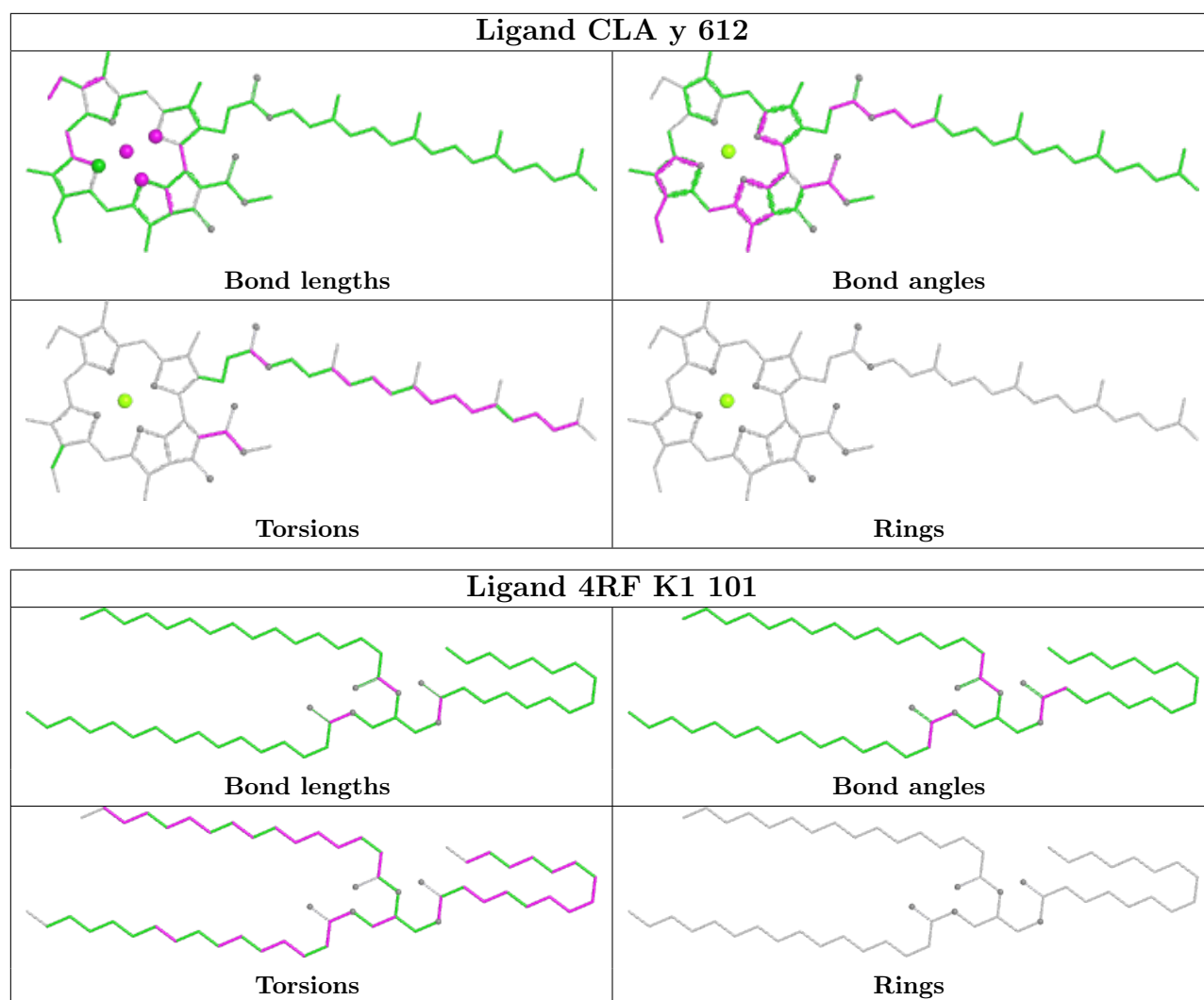


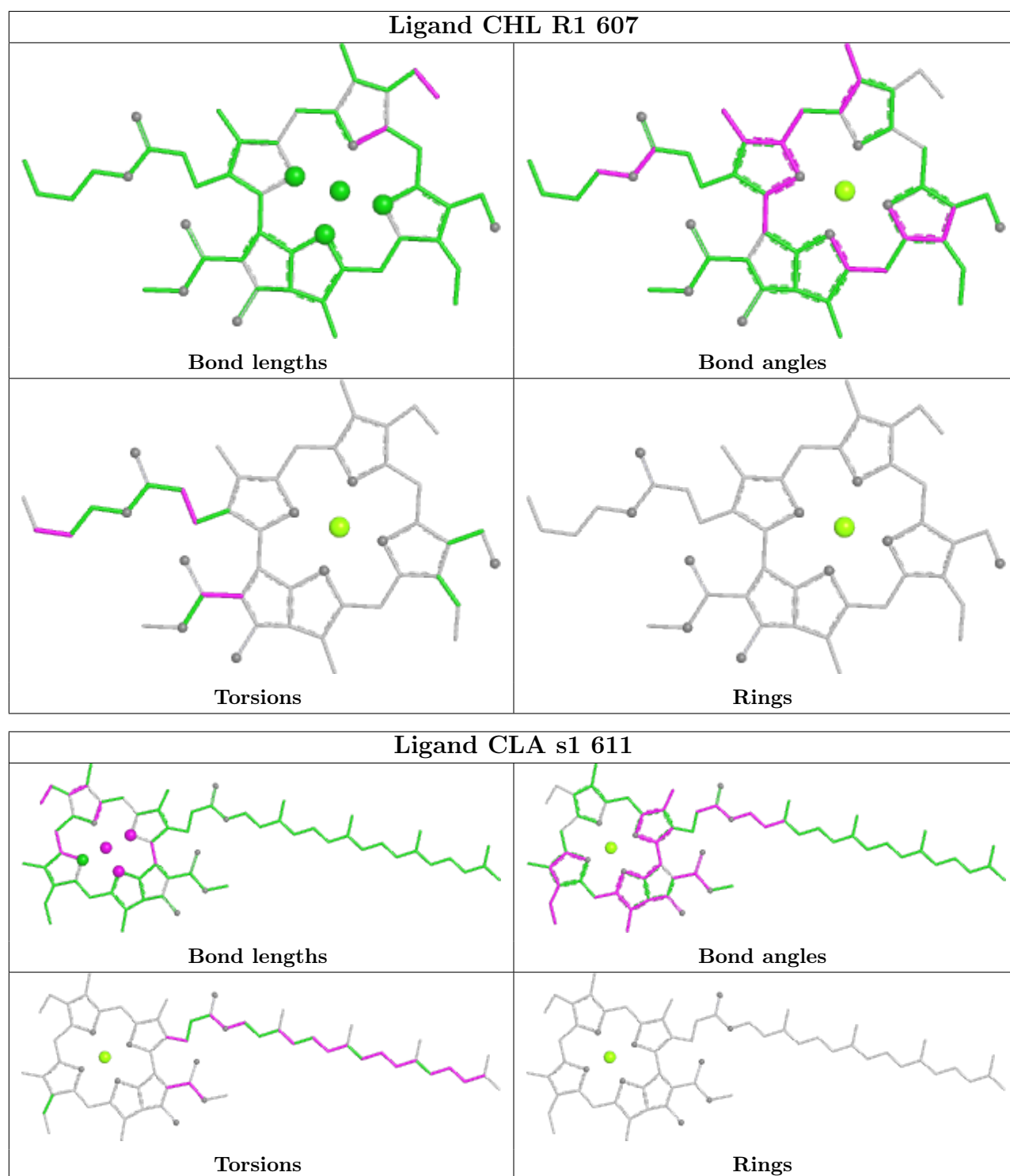


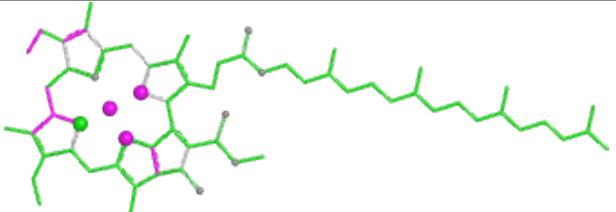
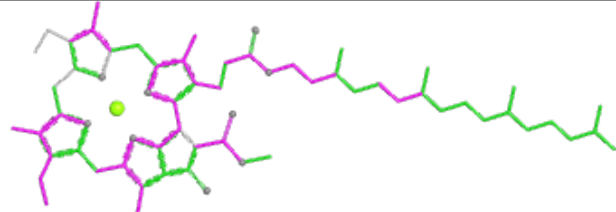
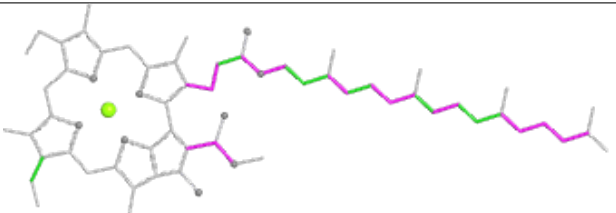
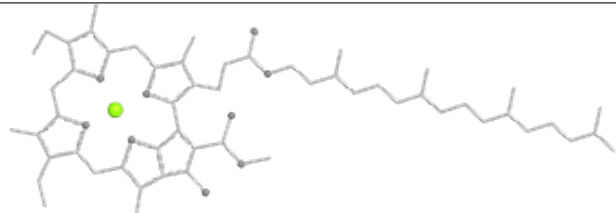
Ligand XAT Y 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

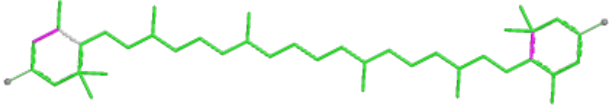
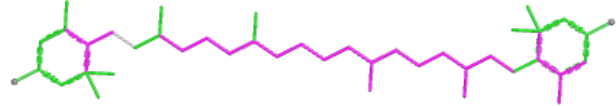
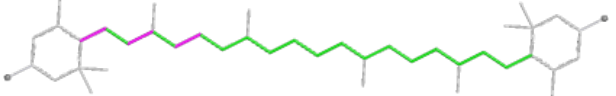

Ligand 4RF k1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

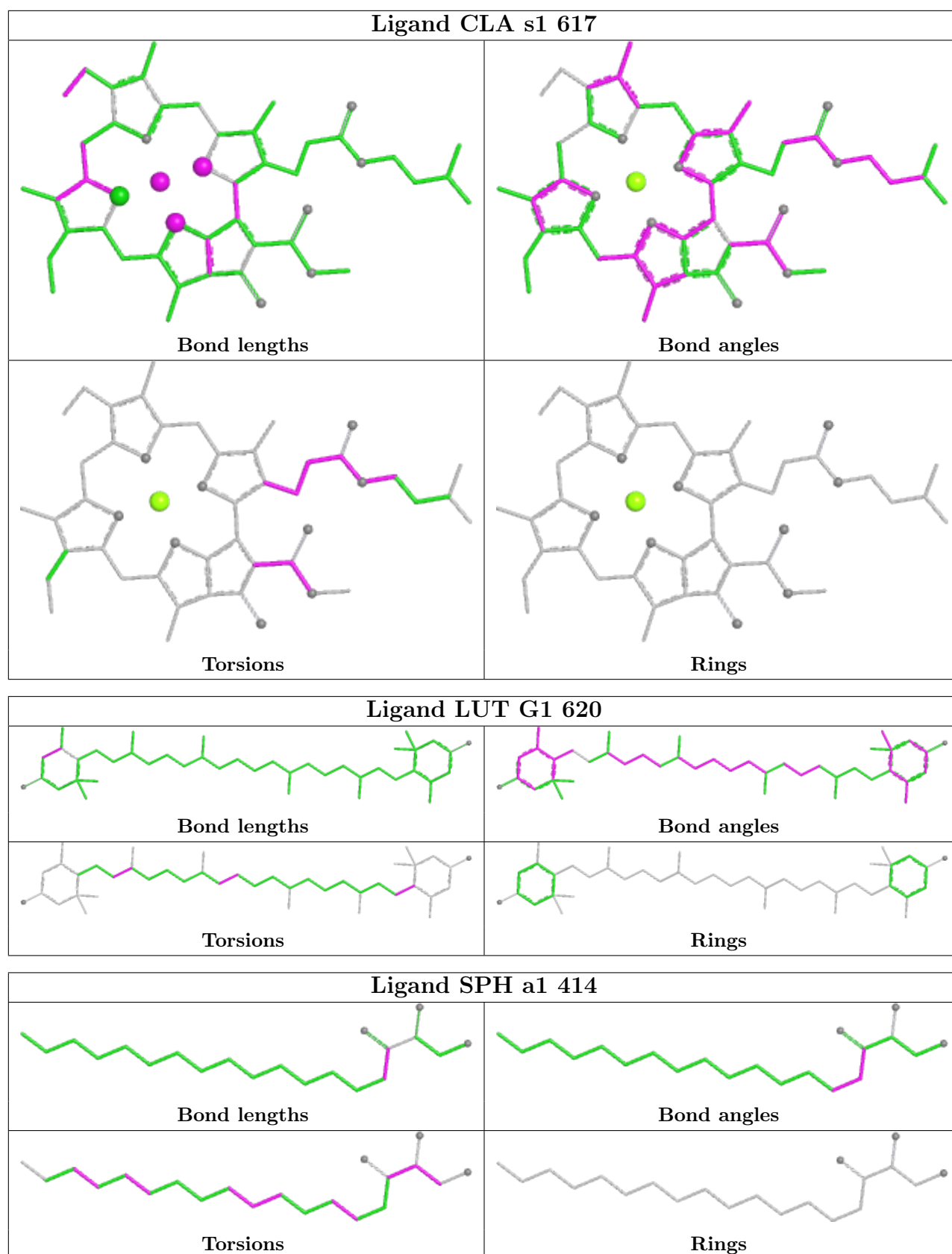
Ligand CLA N 602	
	
Bond lengths	Bond angles
	
Torsions	Rings



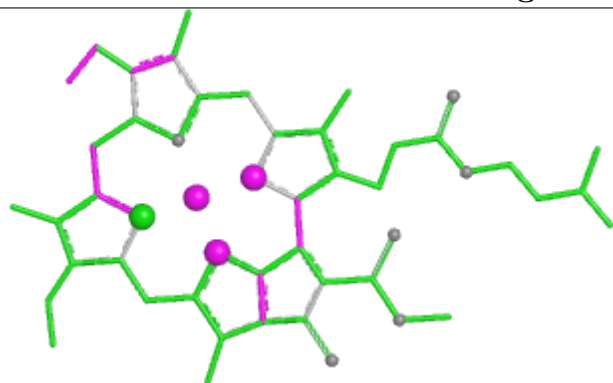


Ligand CLA g 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

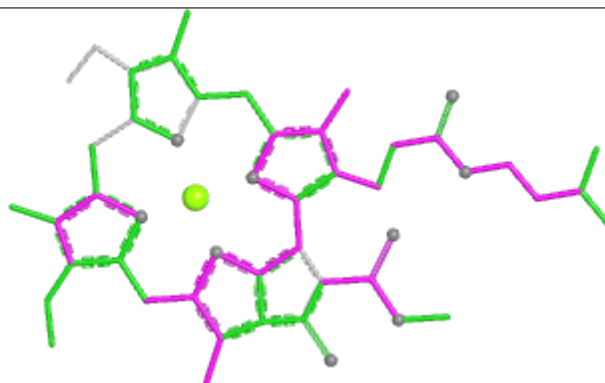
Ligand LUT r1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



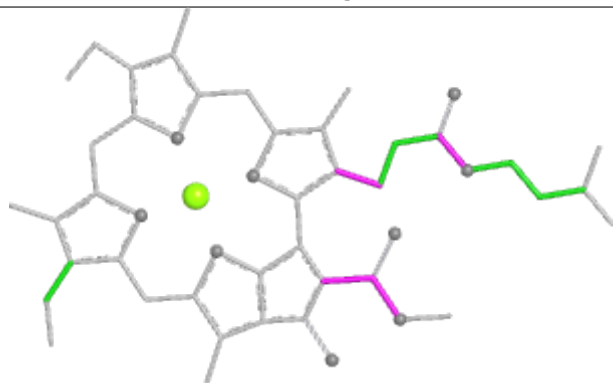
Ligand CLA S 617



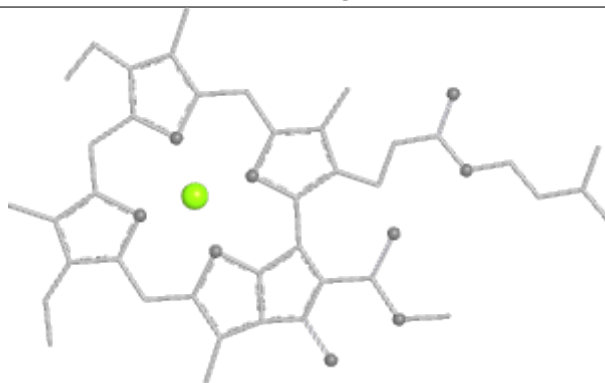
Bond lengths



Bond angles

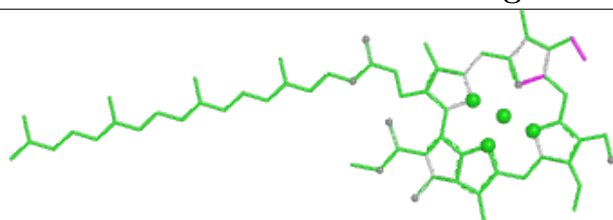


Torsions

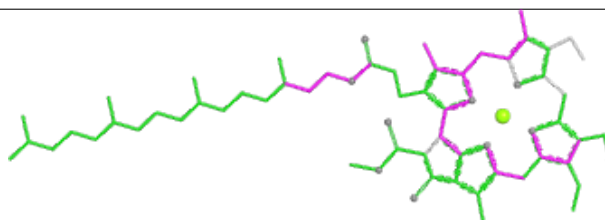


Rings

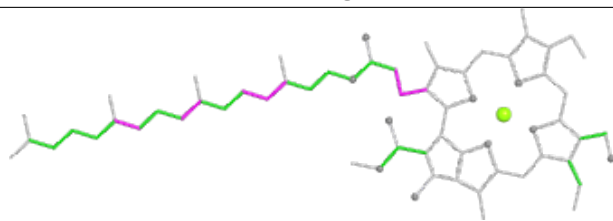
Ligand CHL N1 607



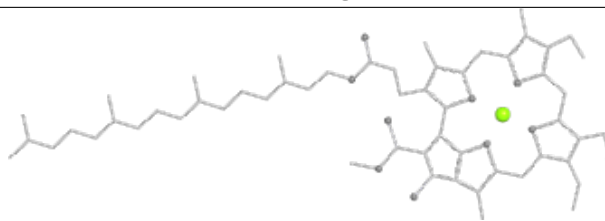
Bond lengths



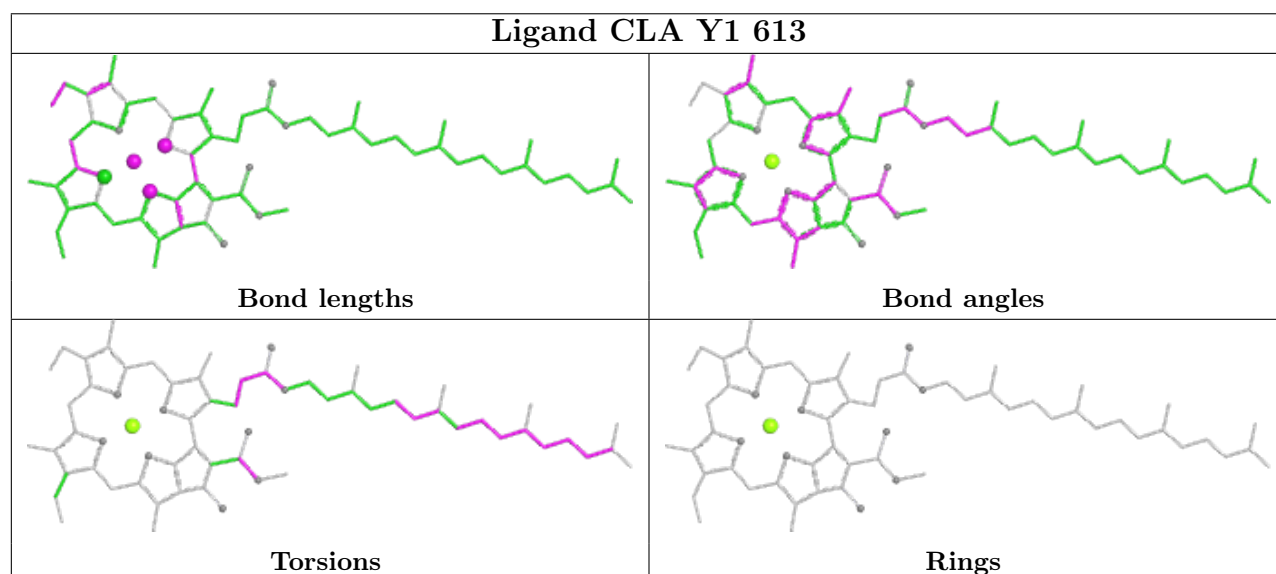
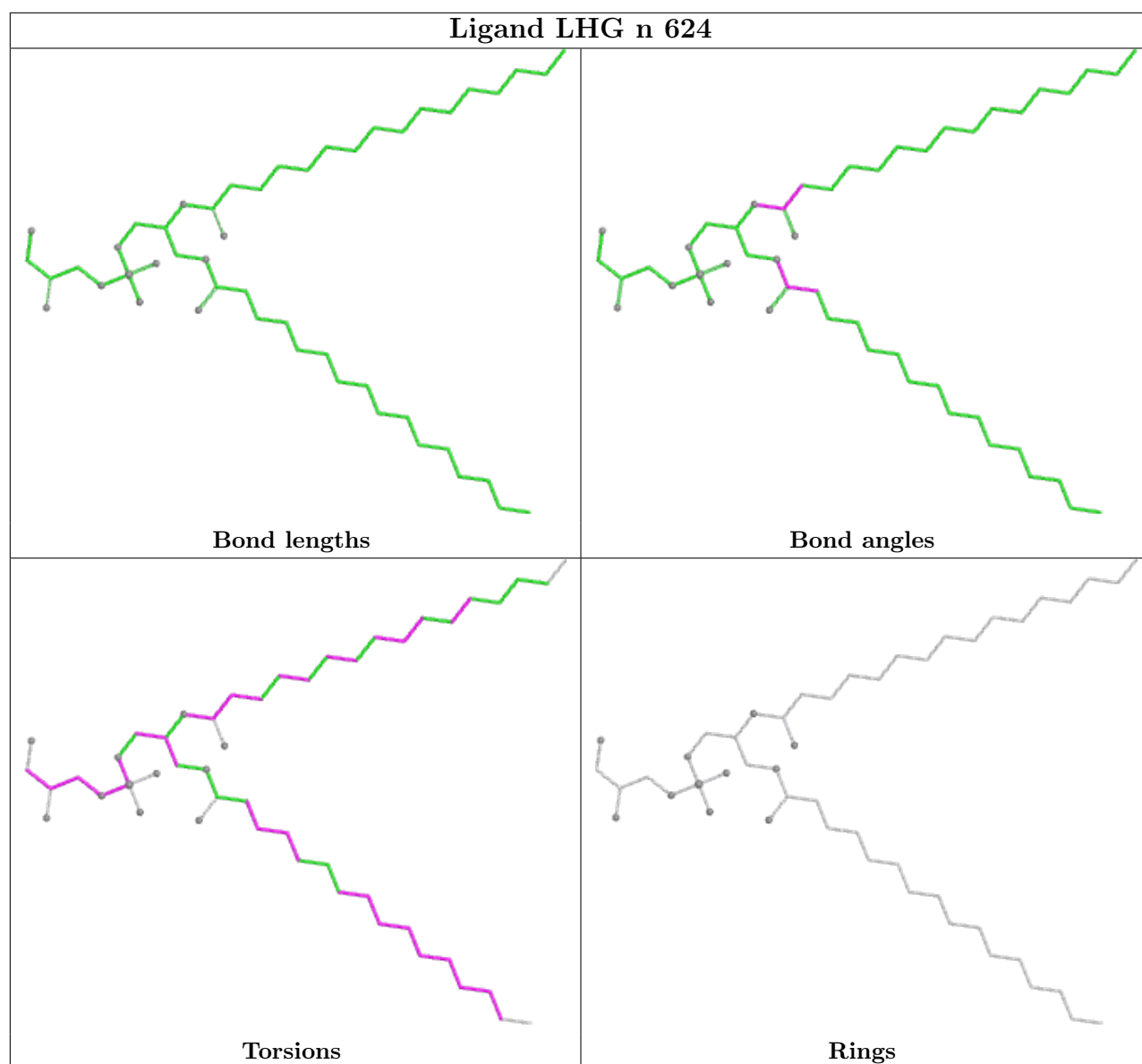
Bond angles

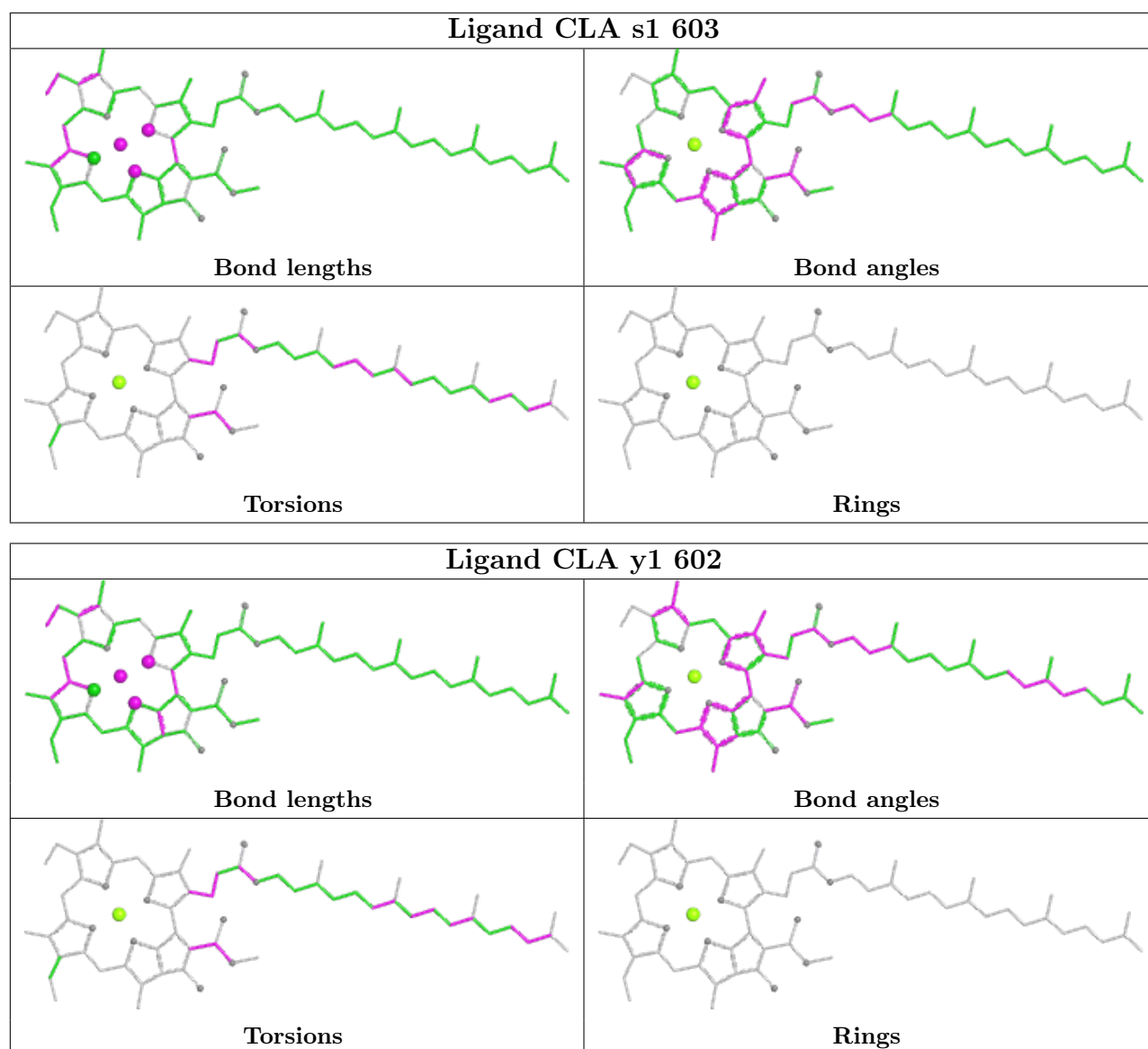


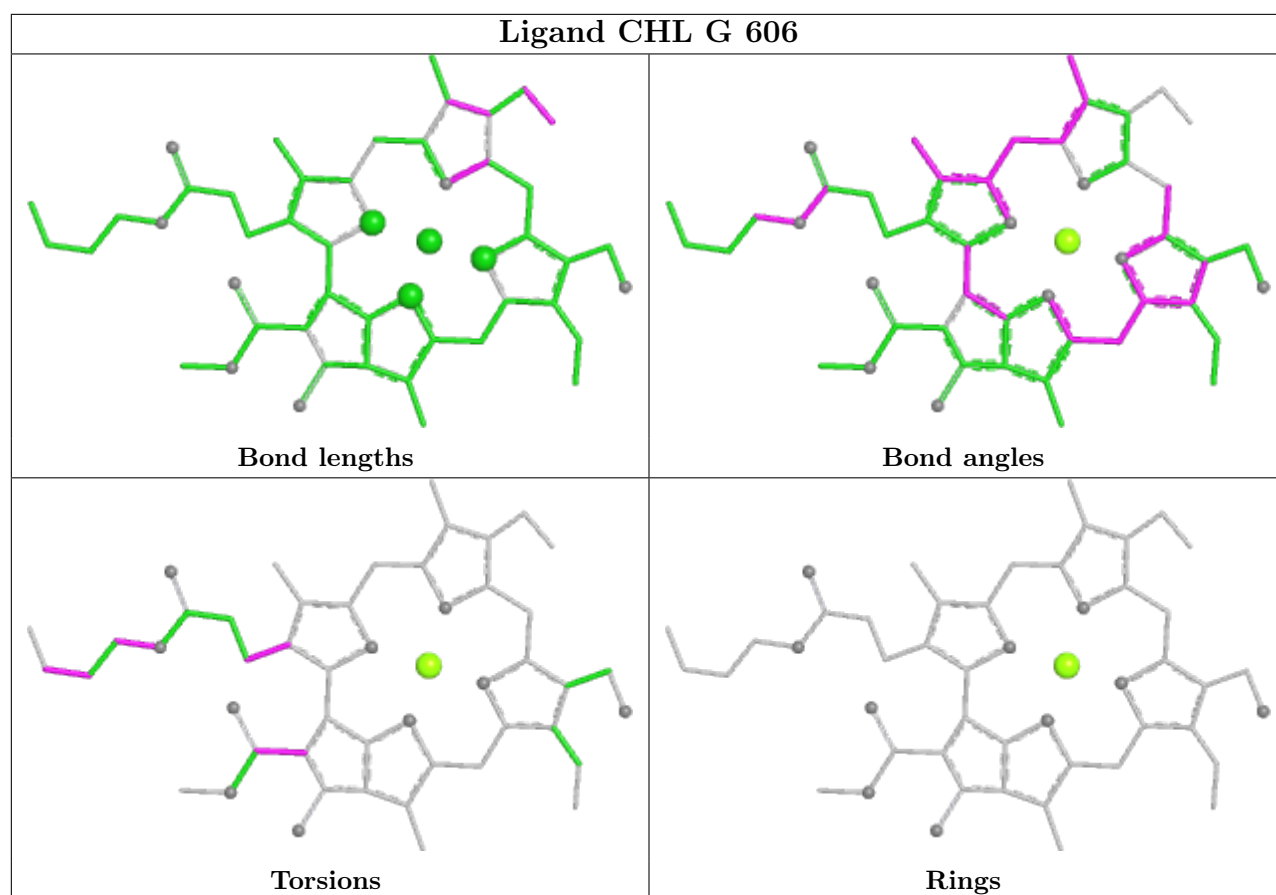
Torsions

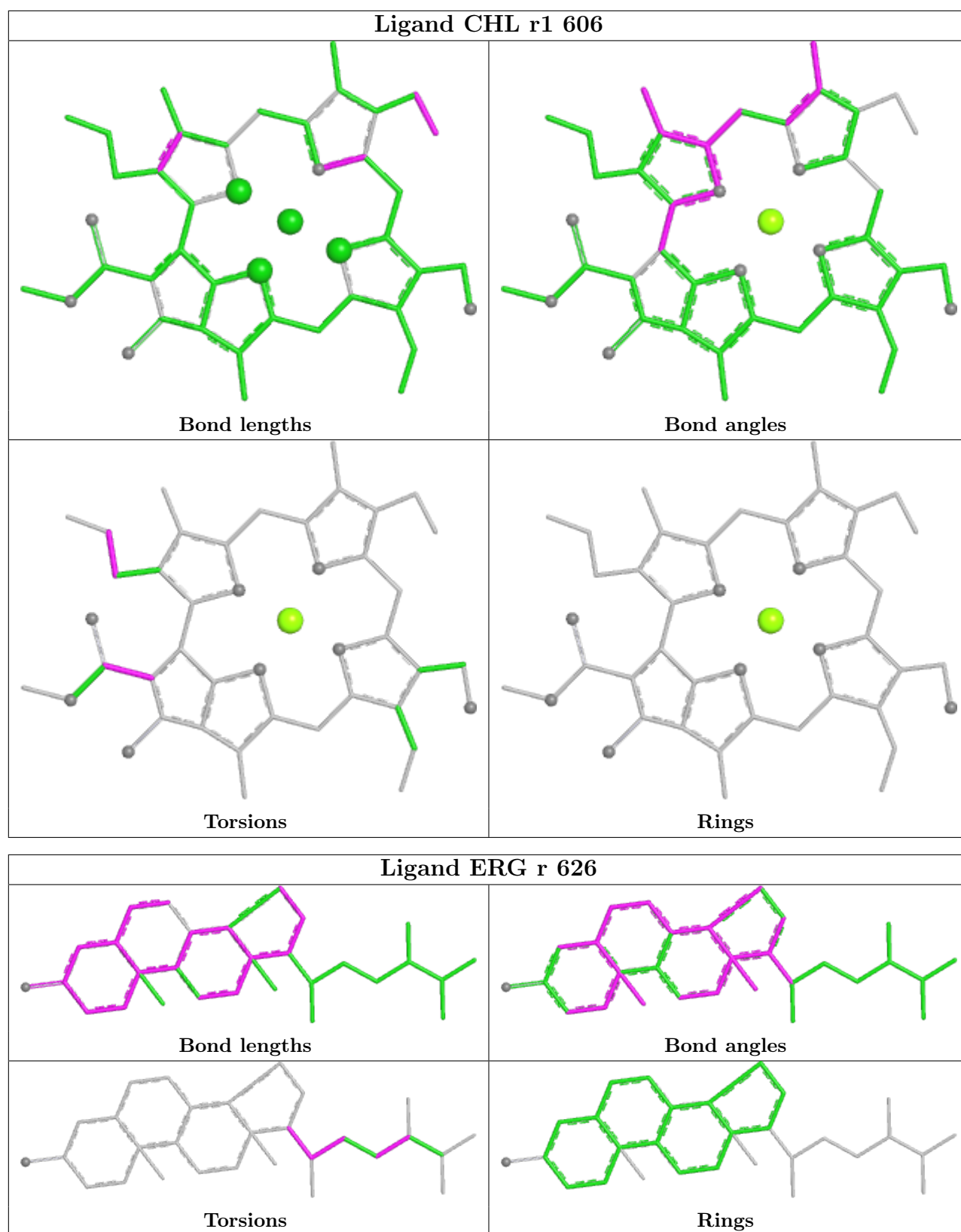


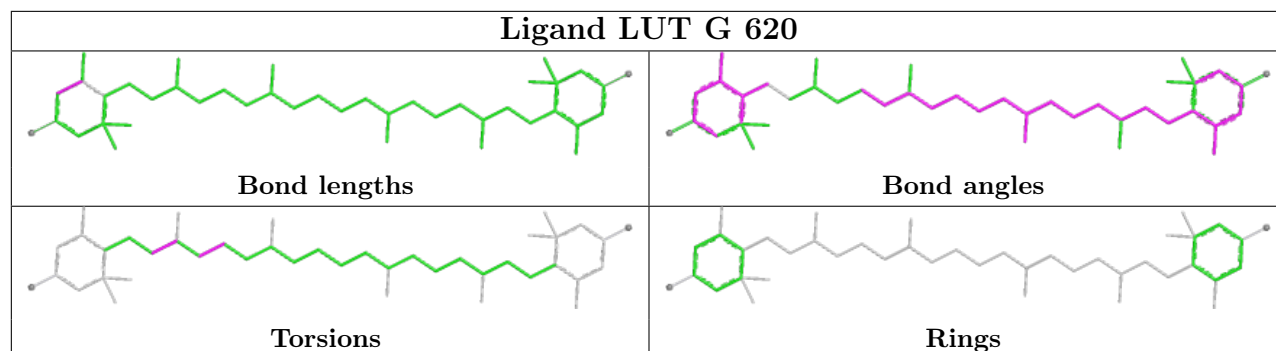
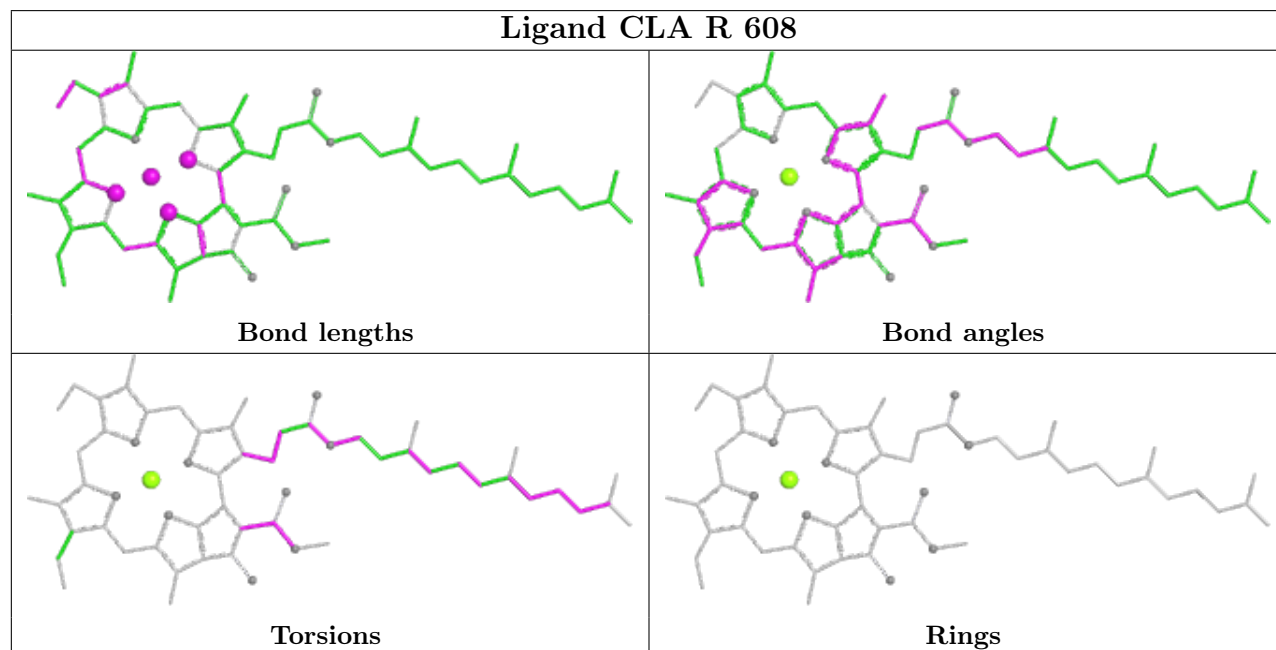
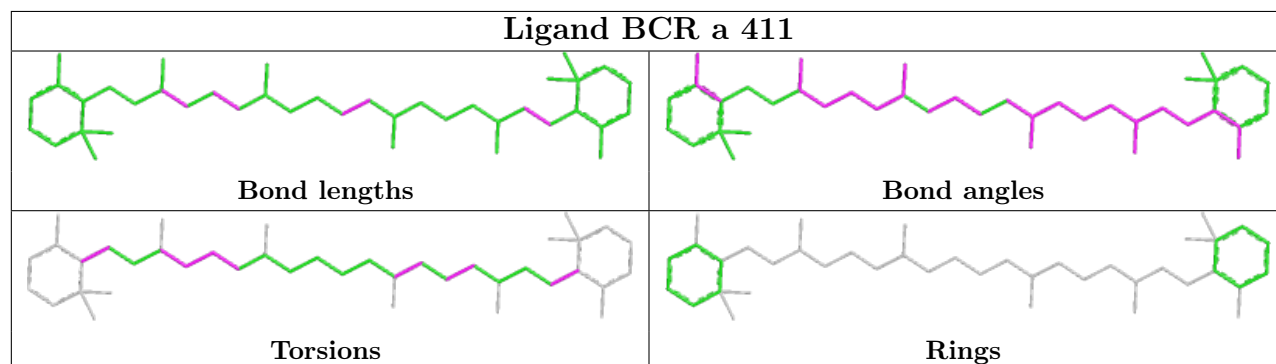
Rings

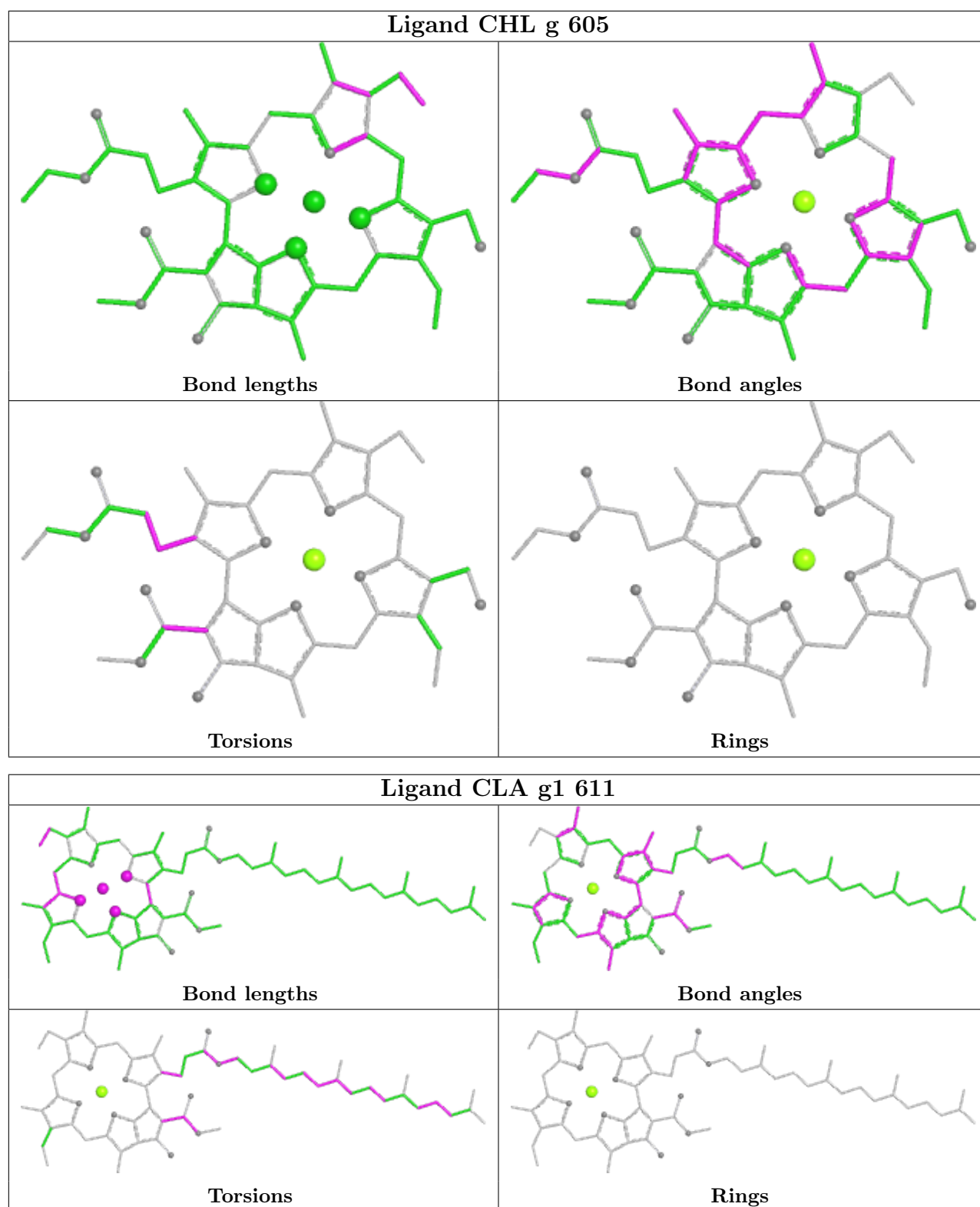


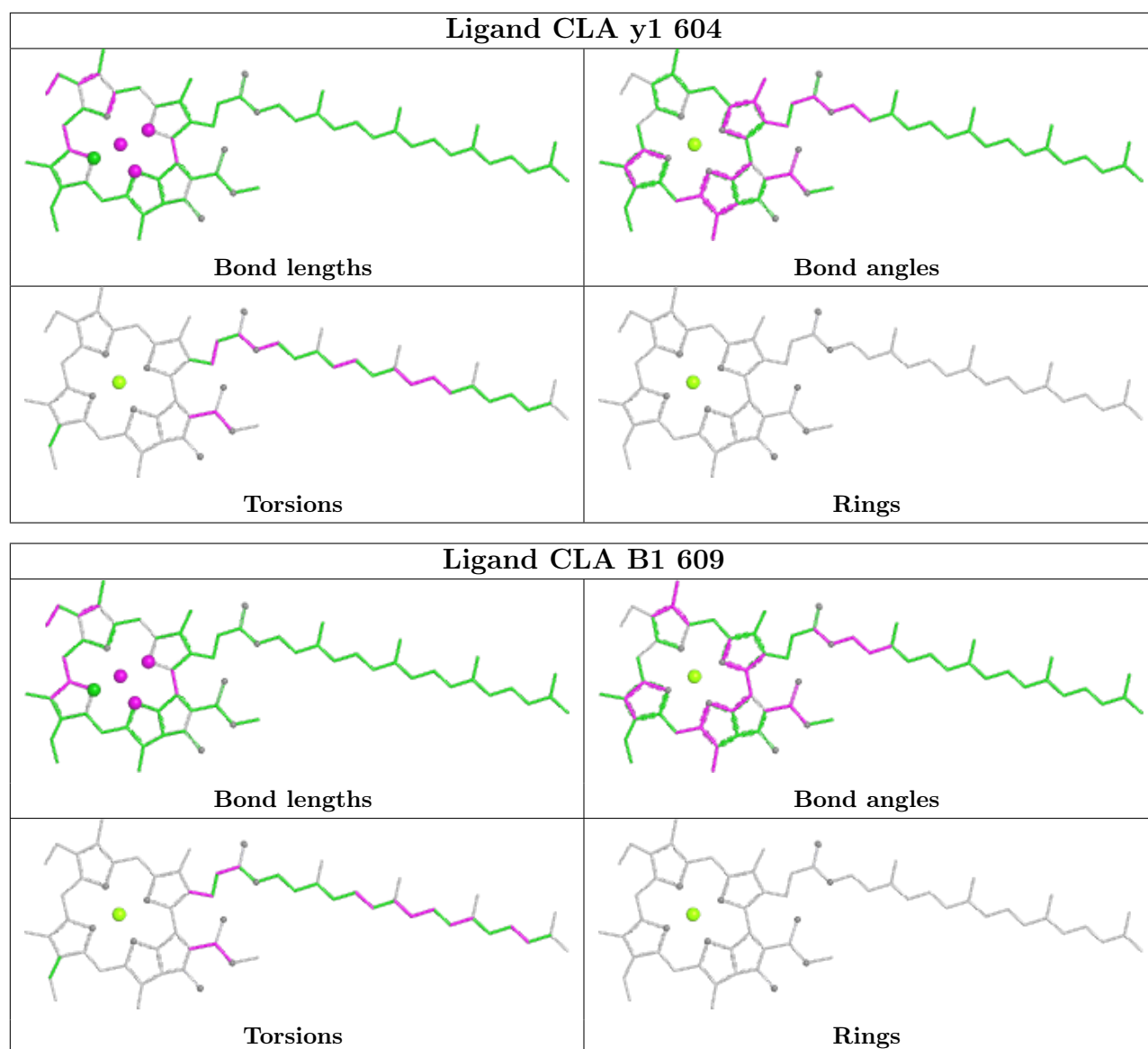


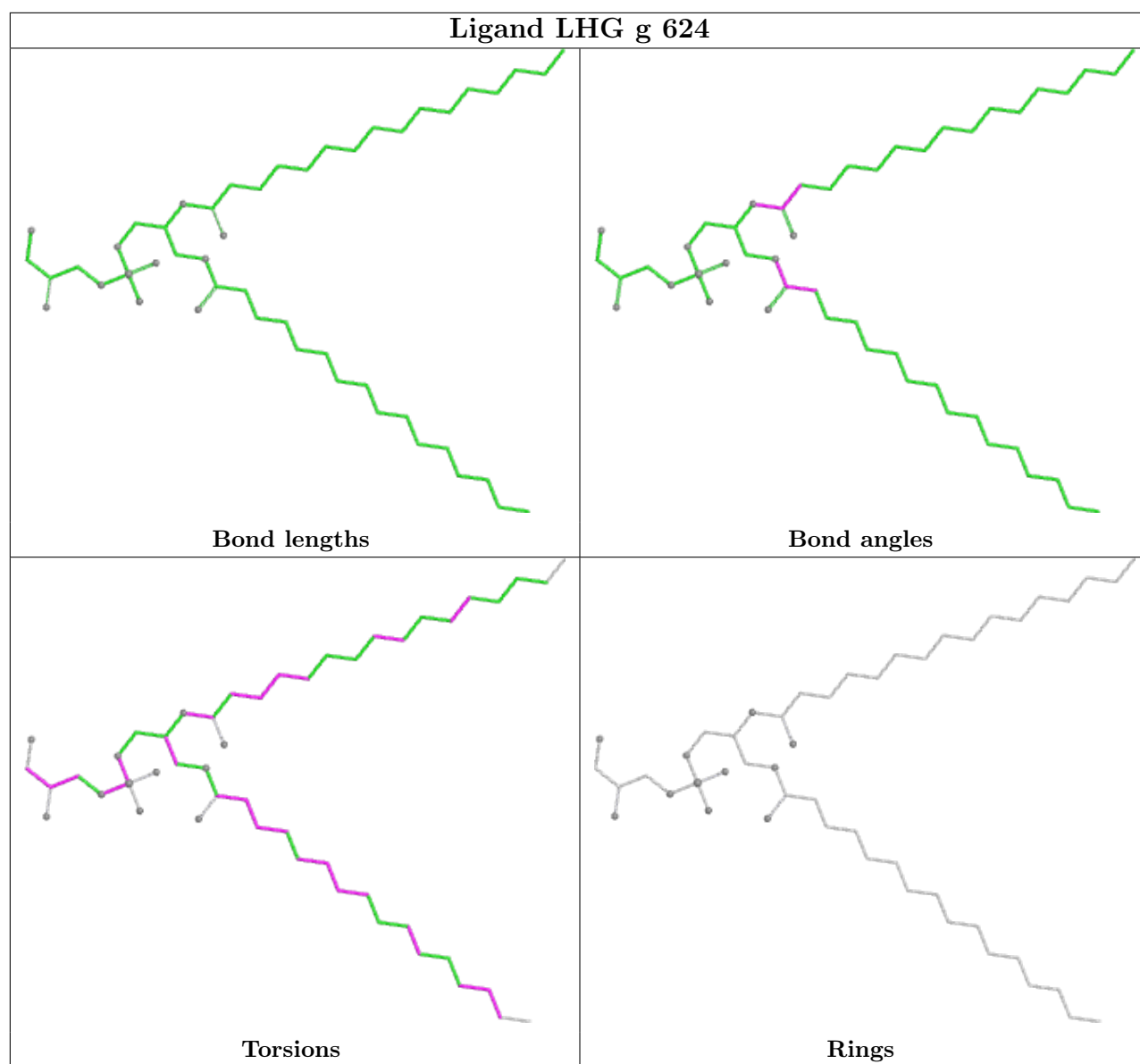




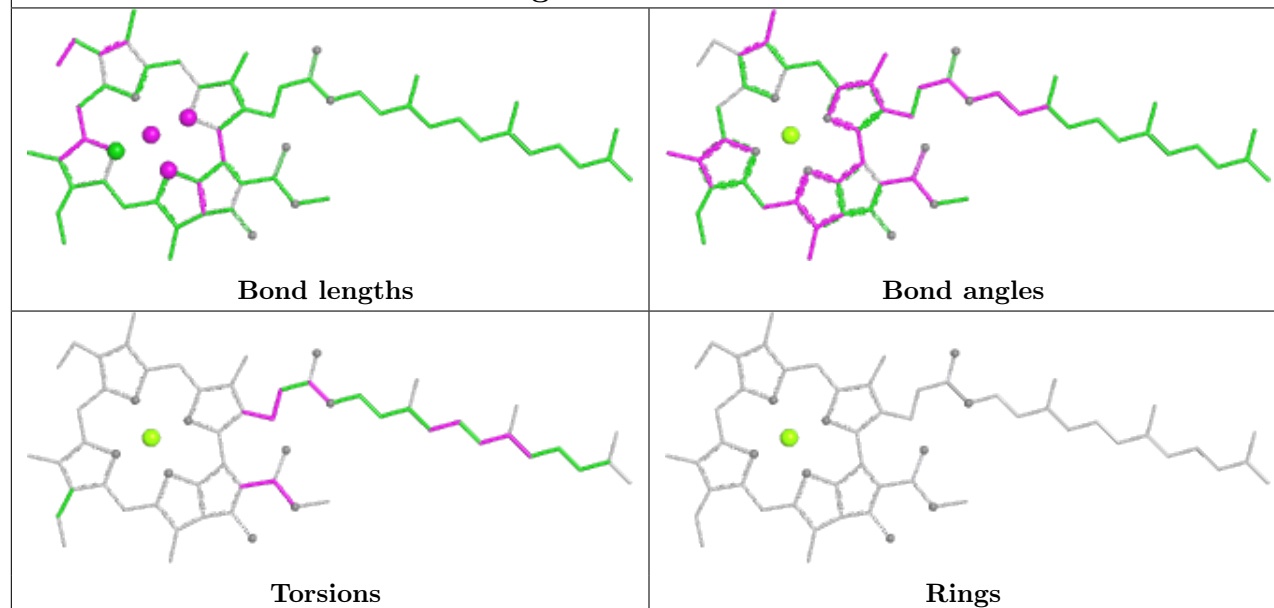
Ligand LUT G 620**Ligand CLA R 608****Ligand BCR a 411**



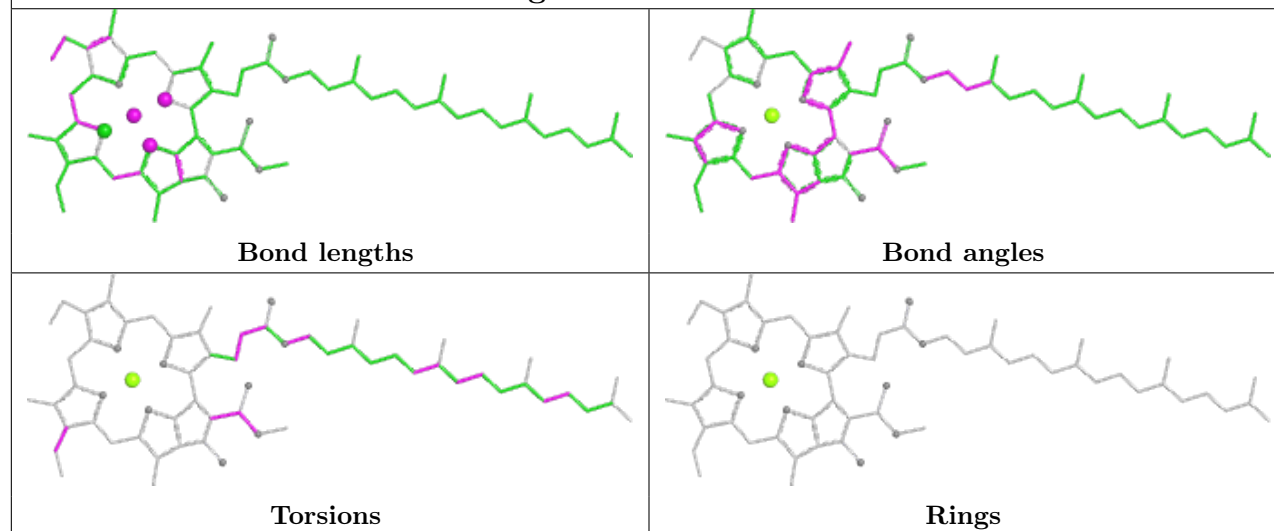


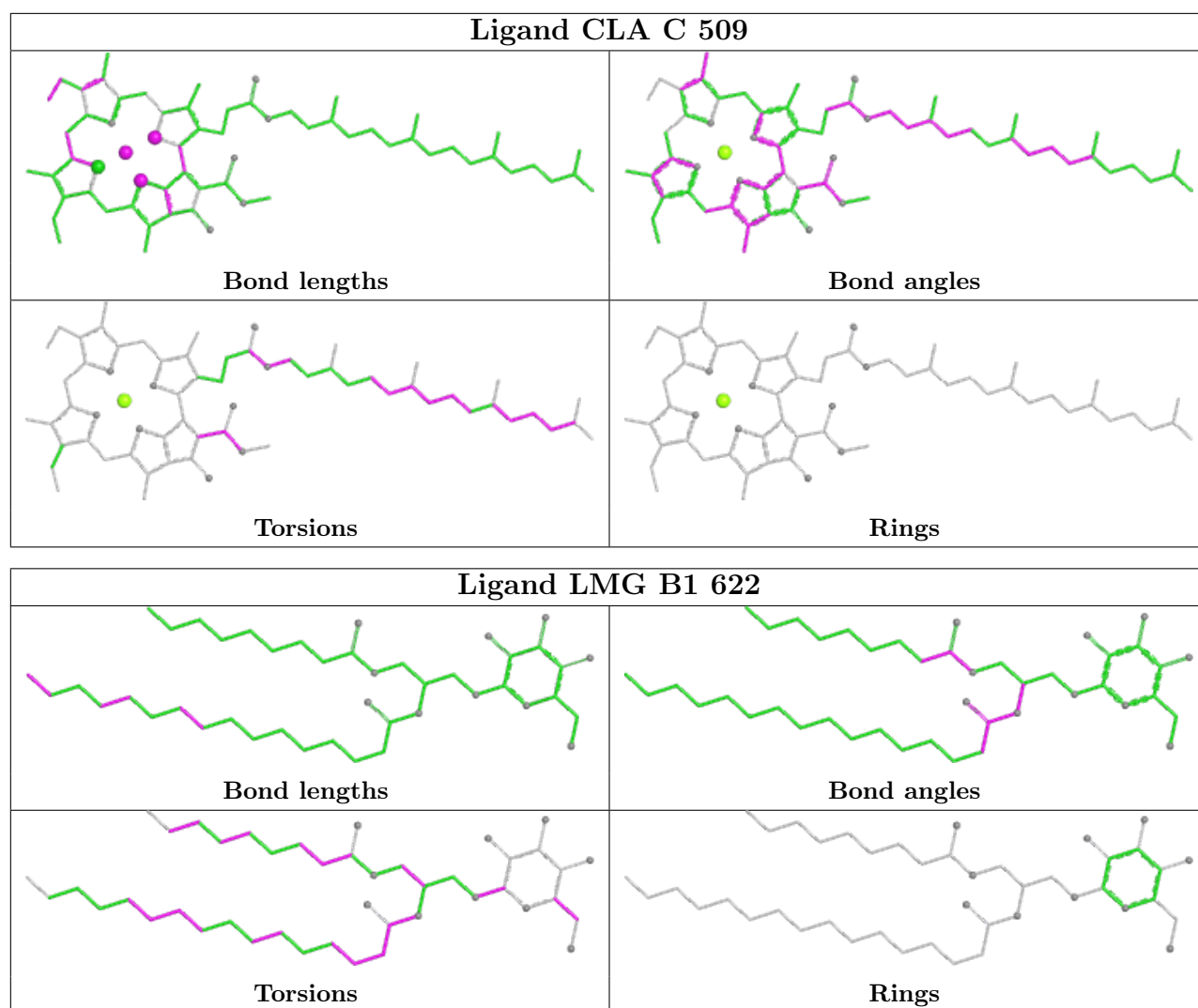


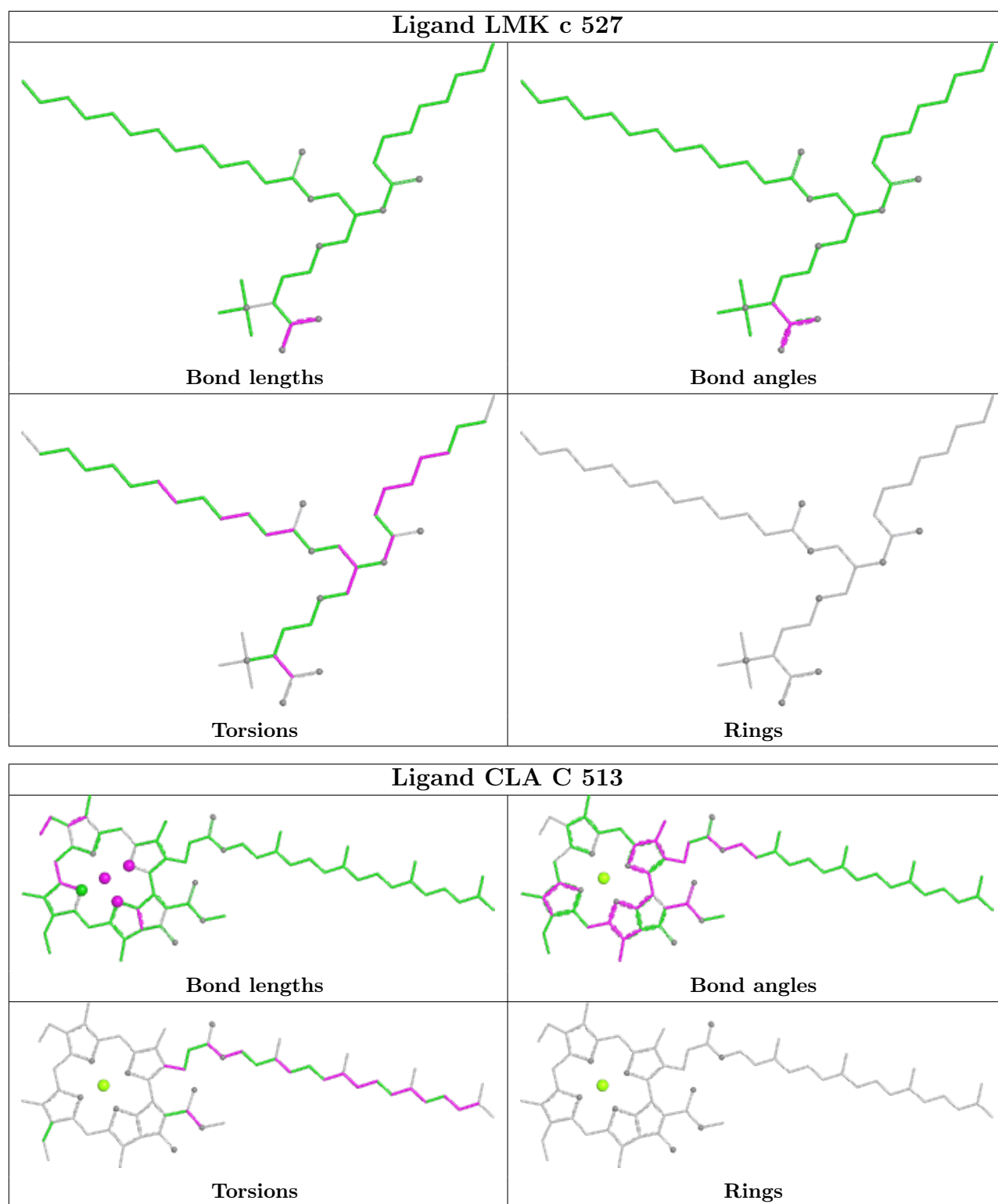
Ligand CLA R 602

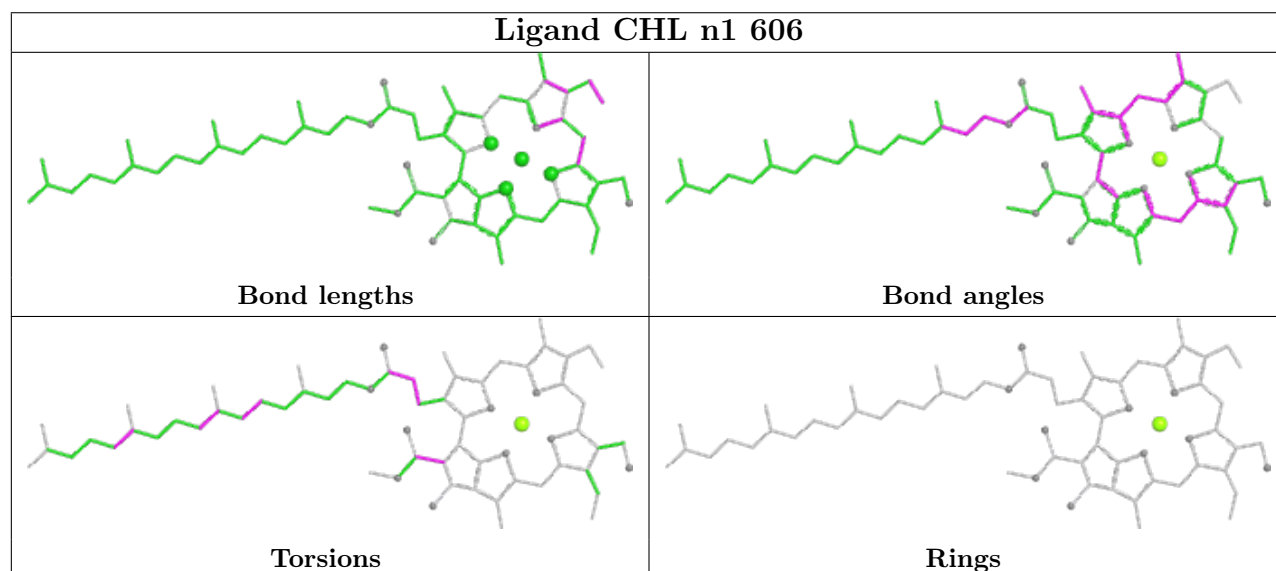
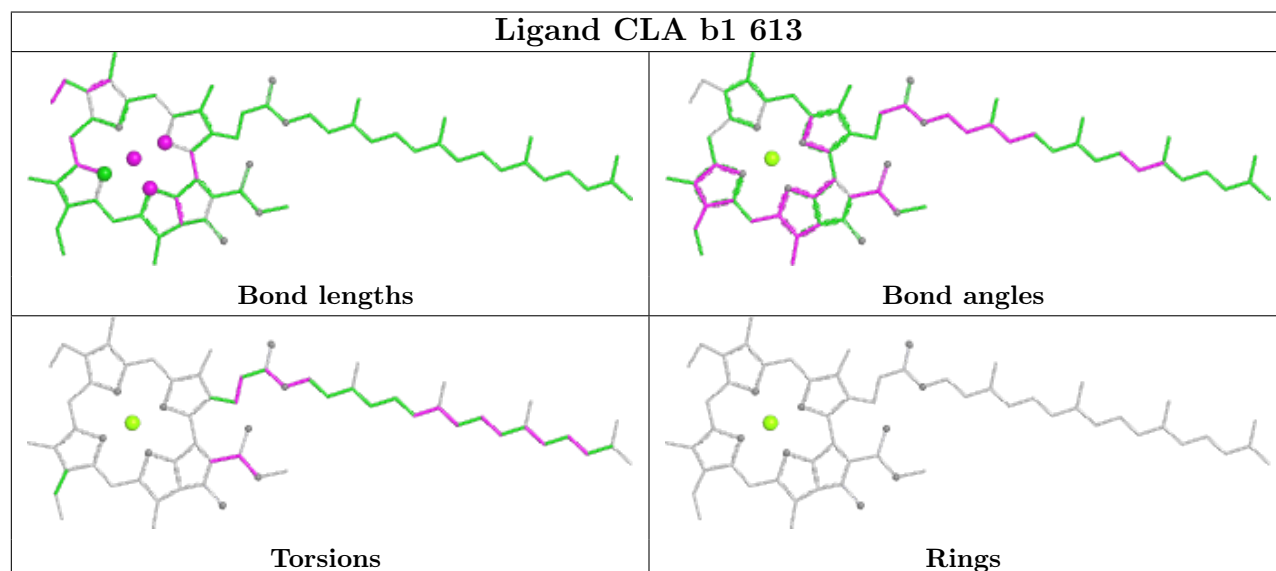
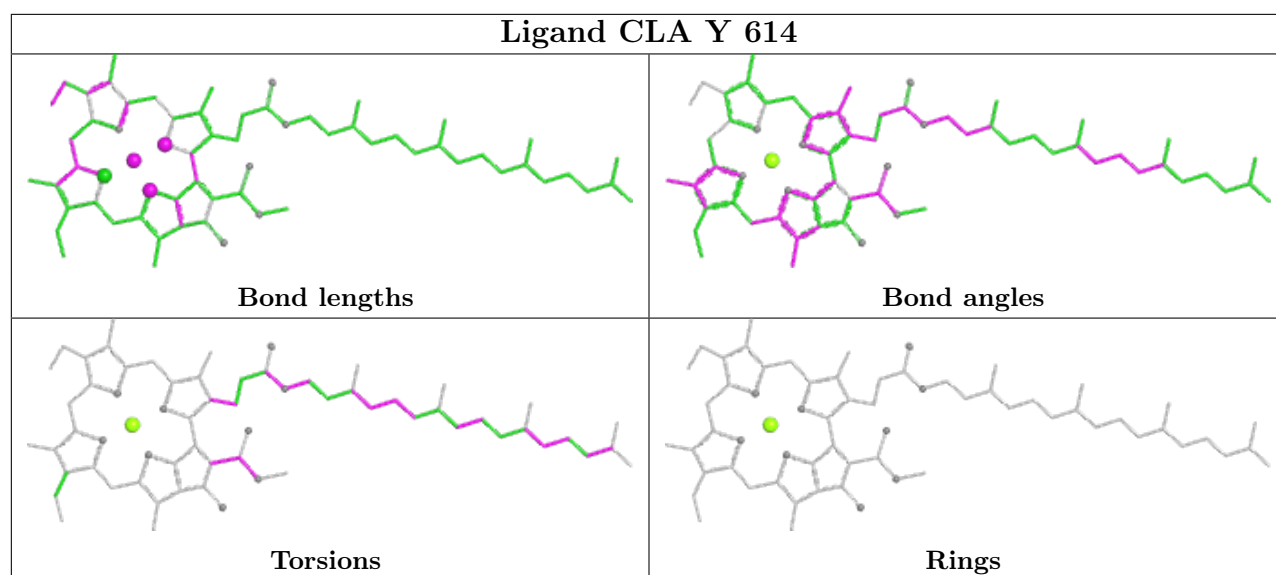


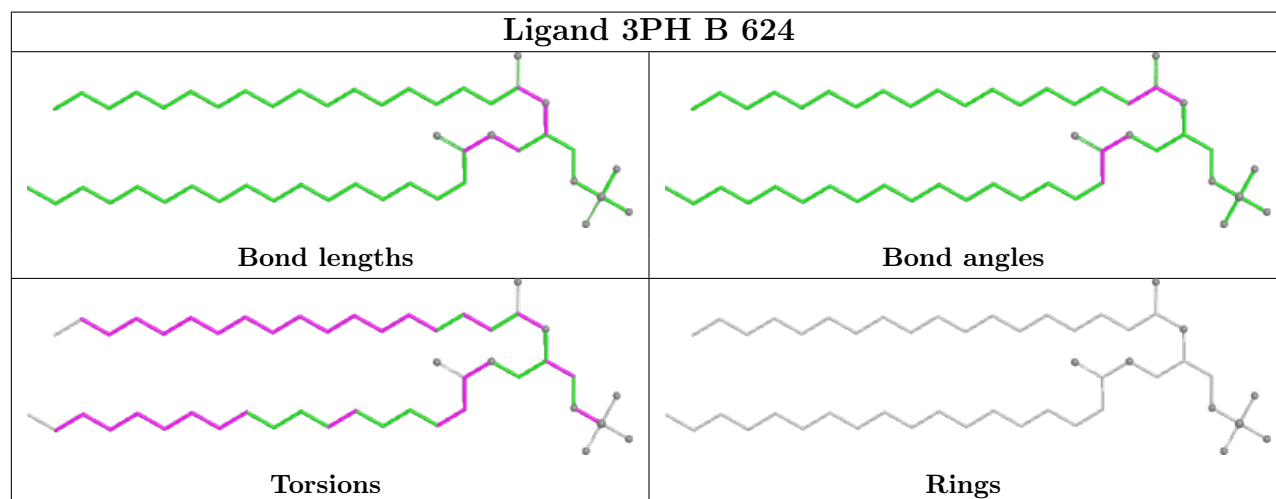
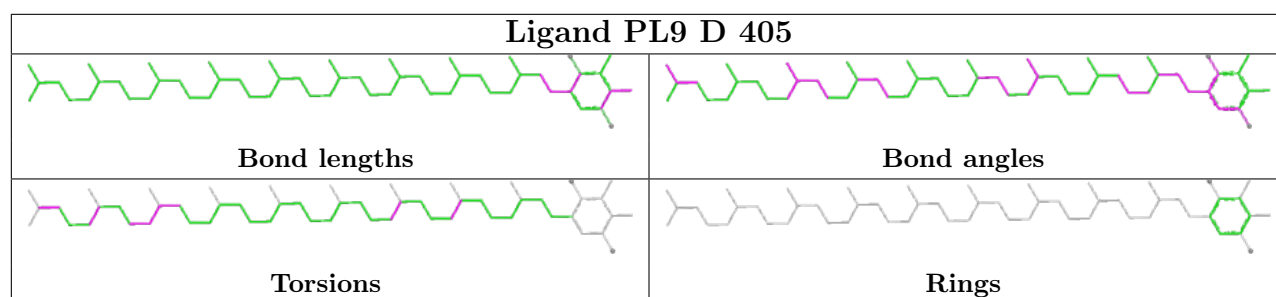
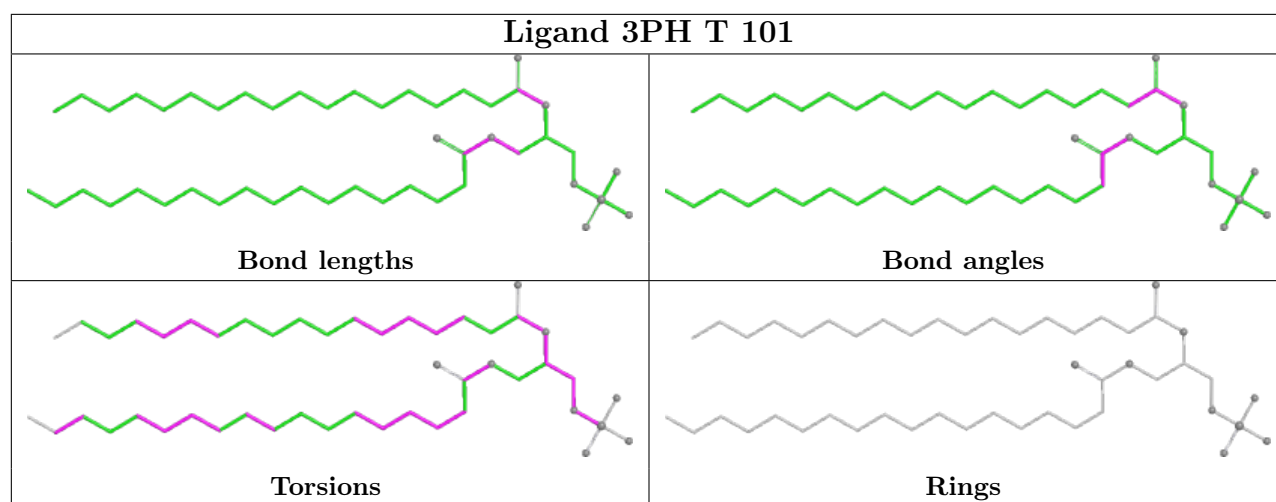
Ligand CLA c1 502

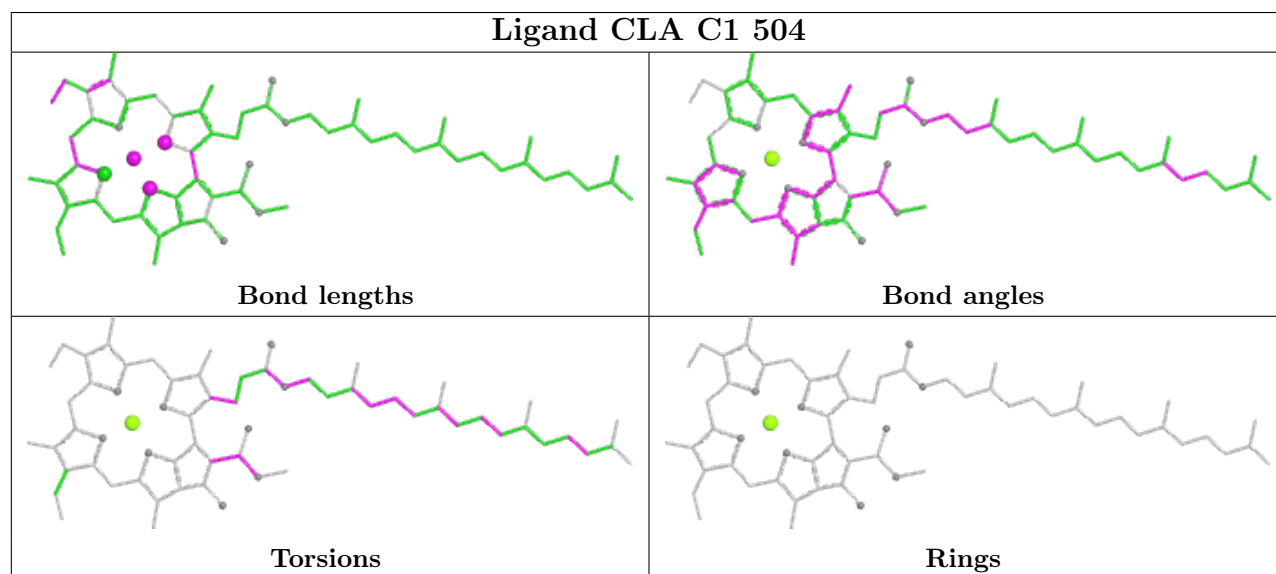
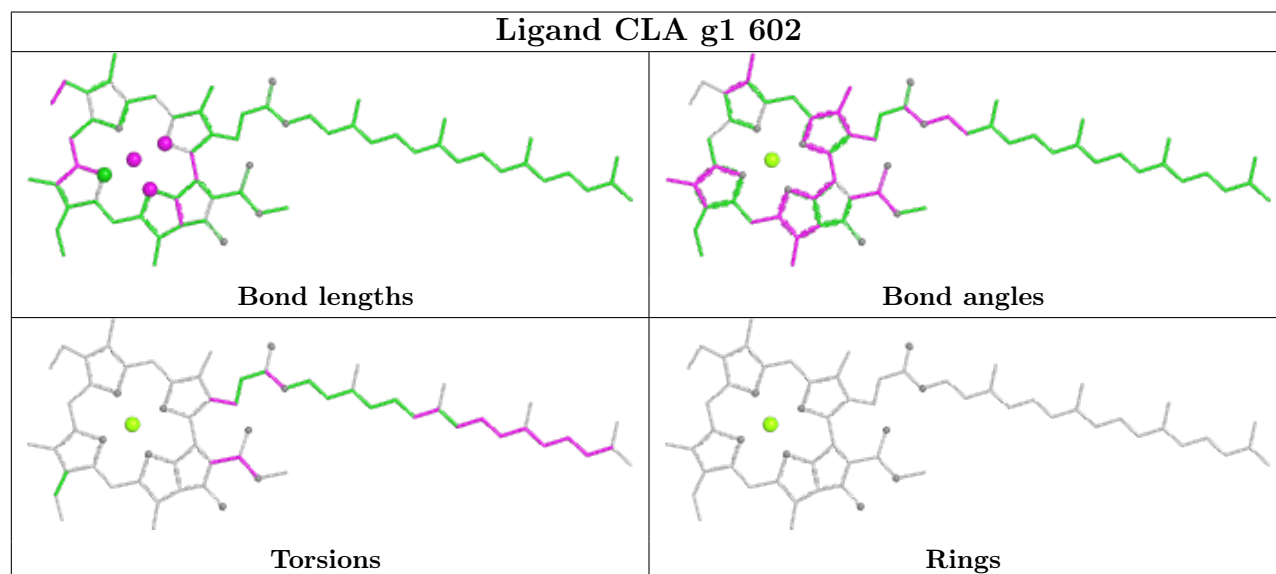
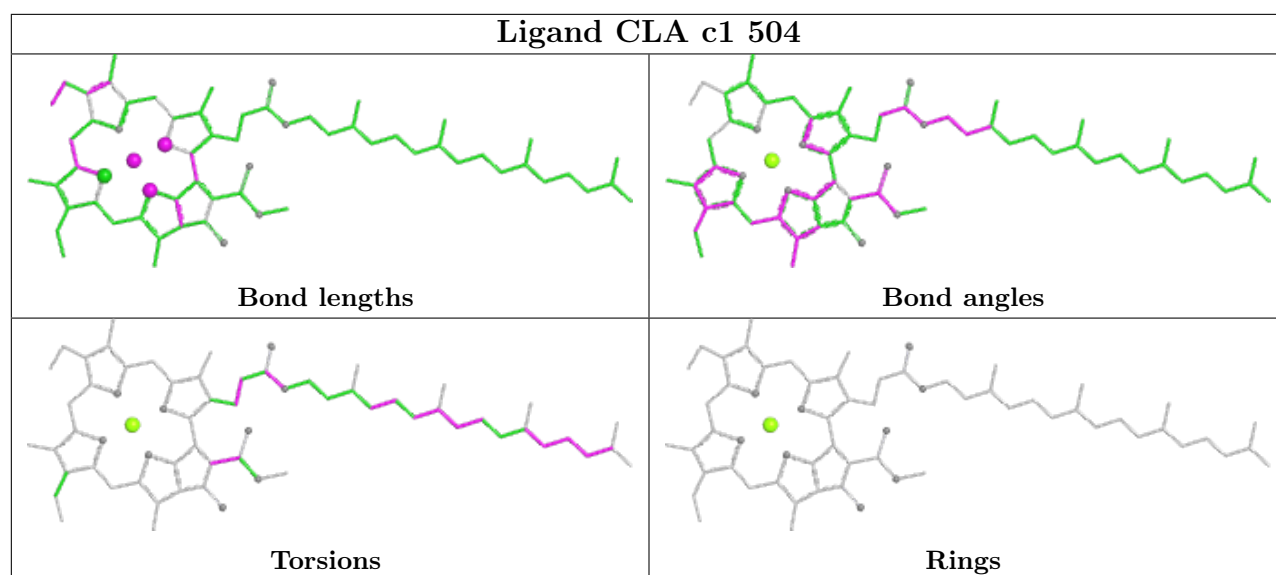


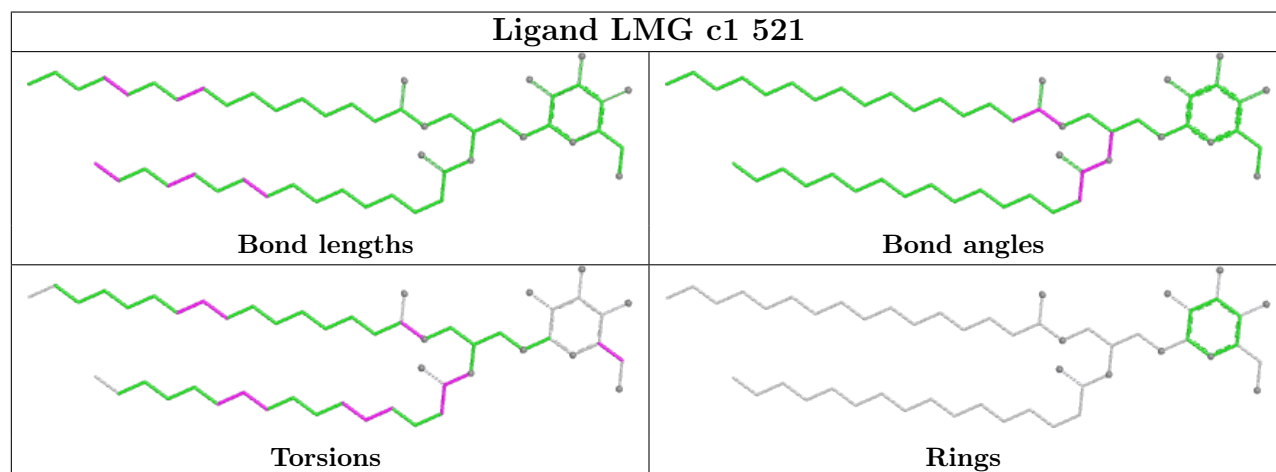
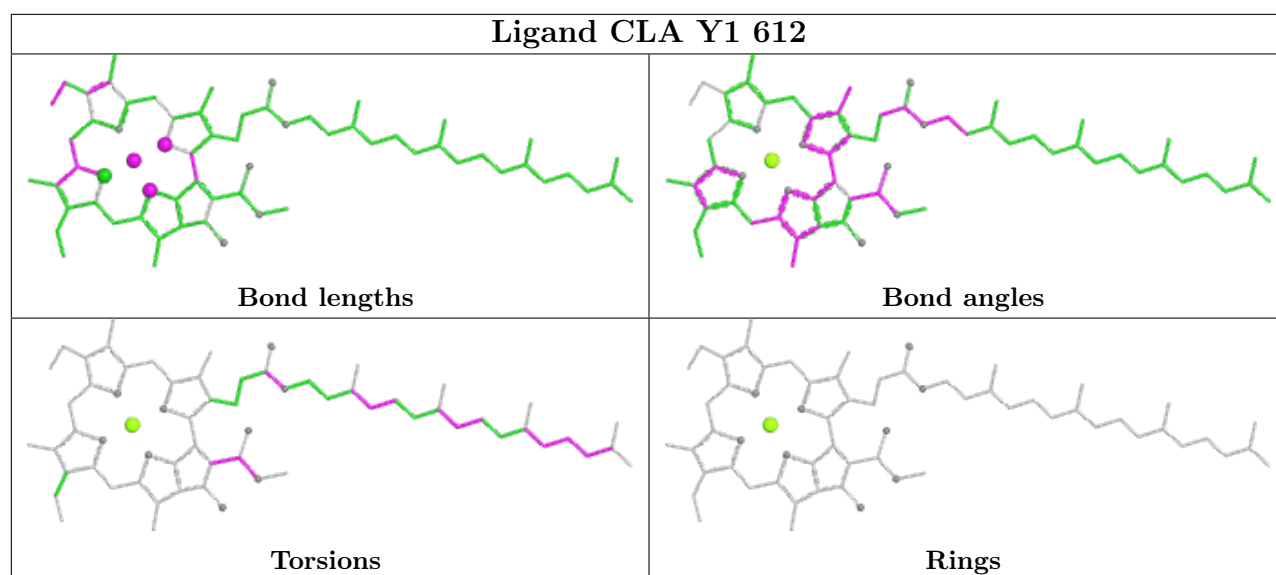


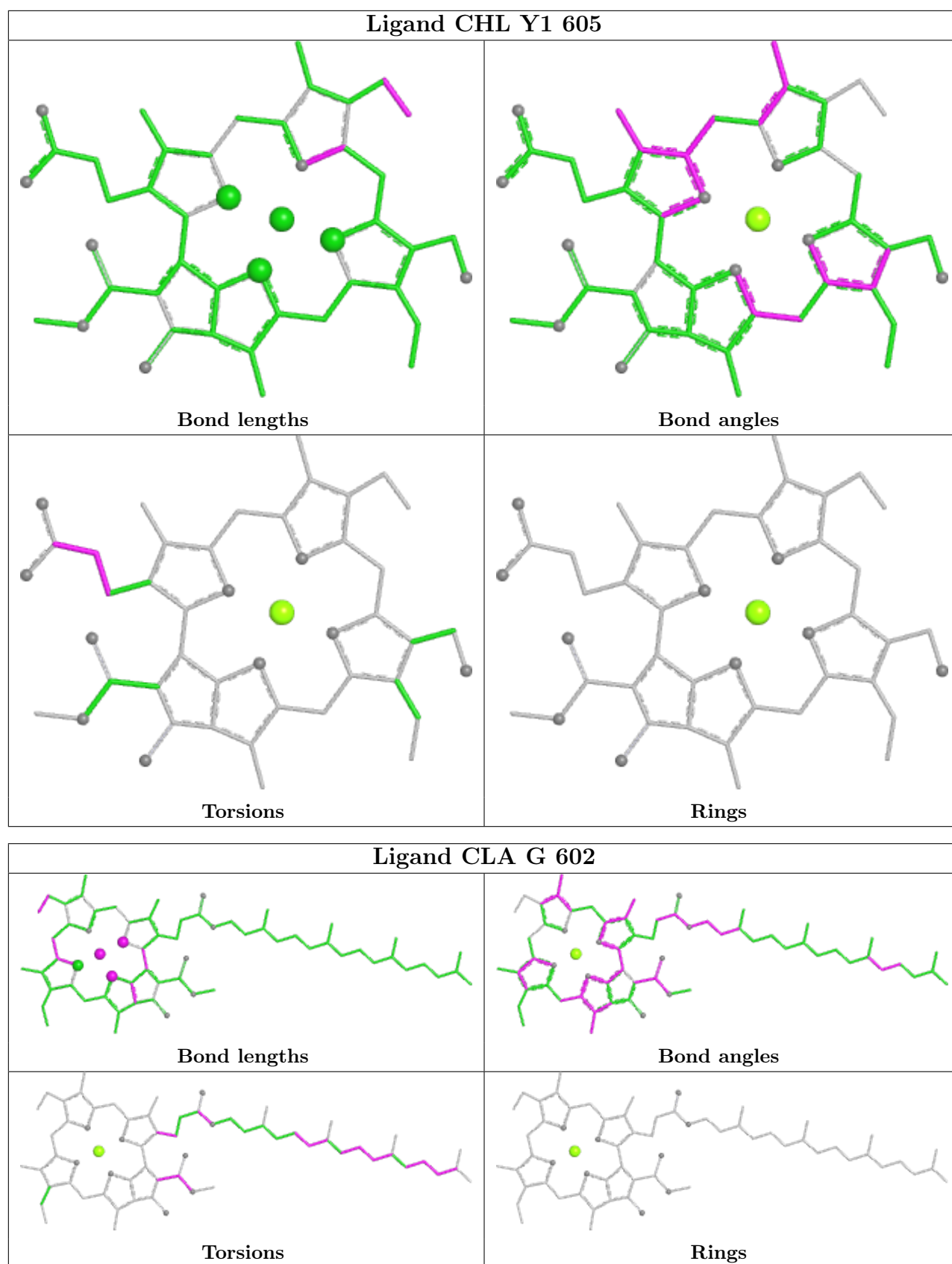


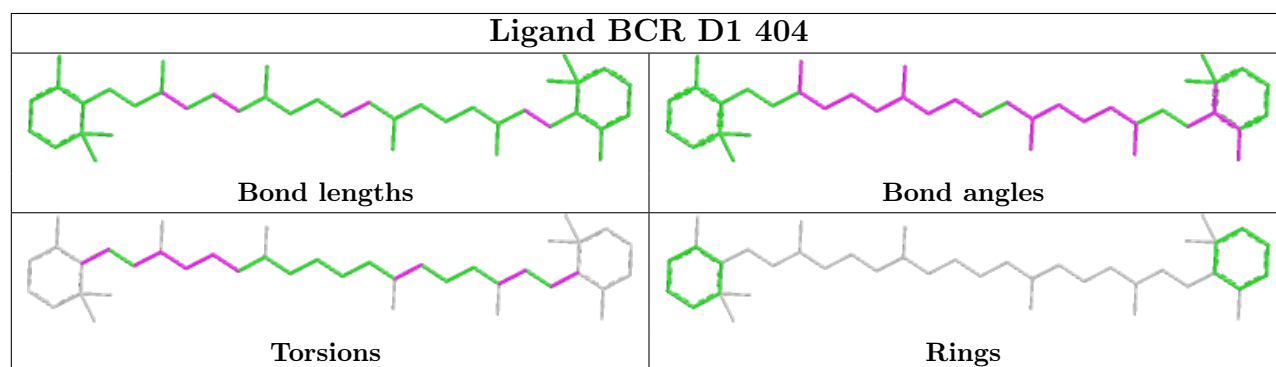
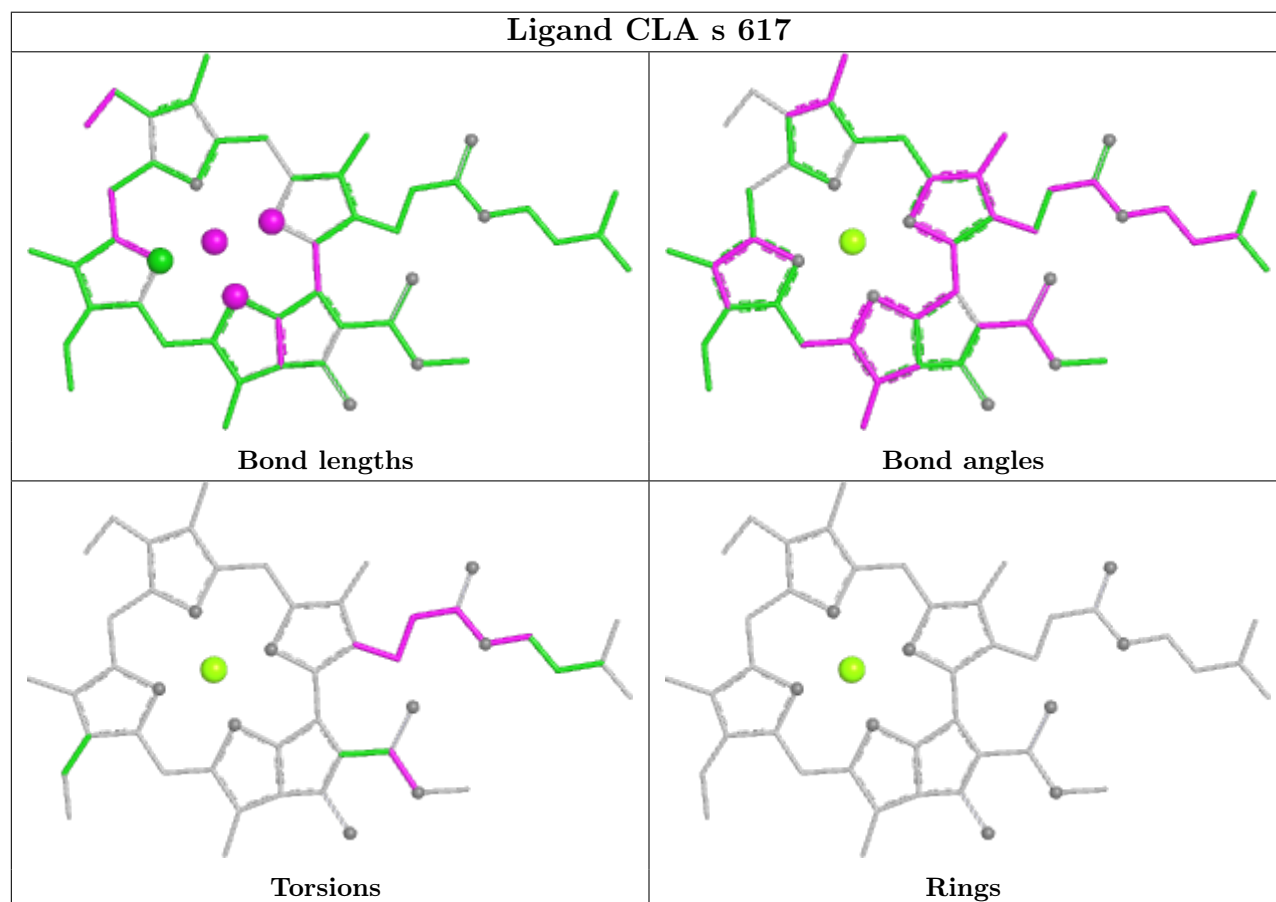
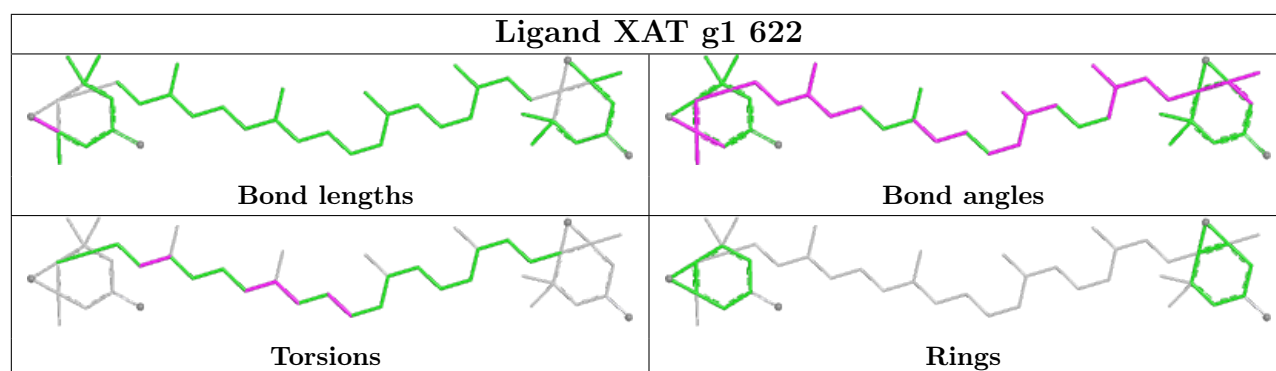


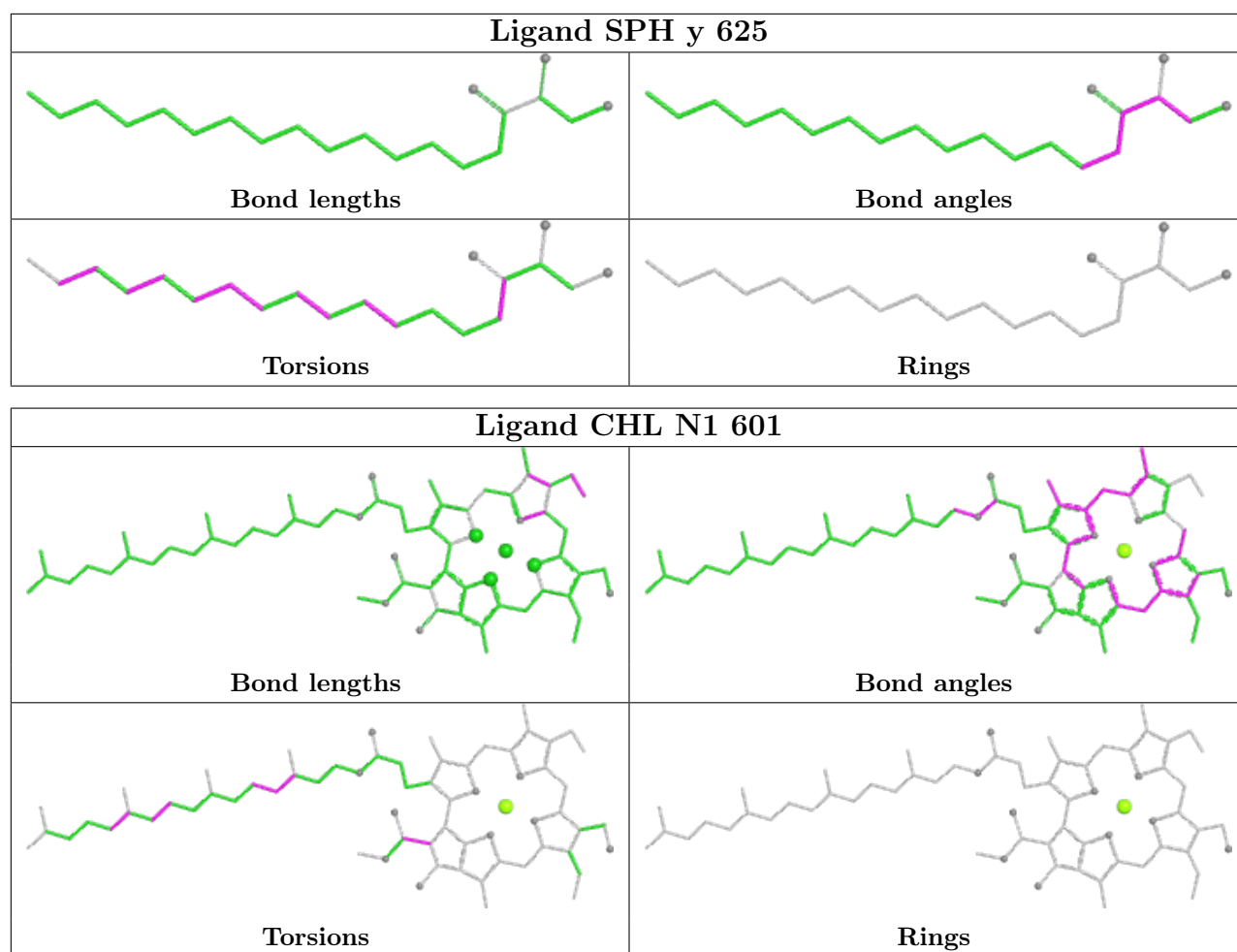




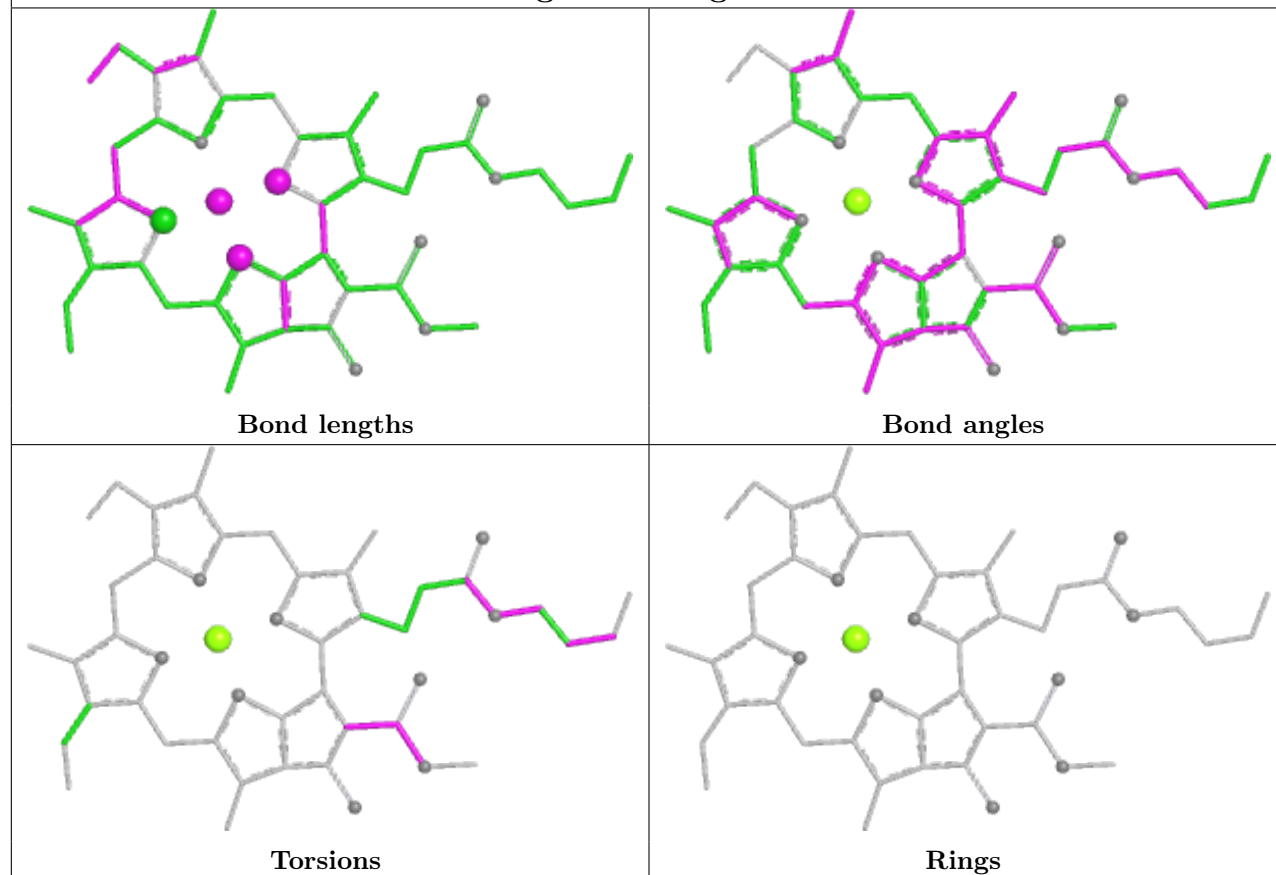




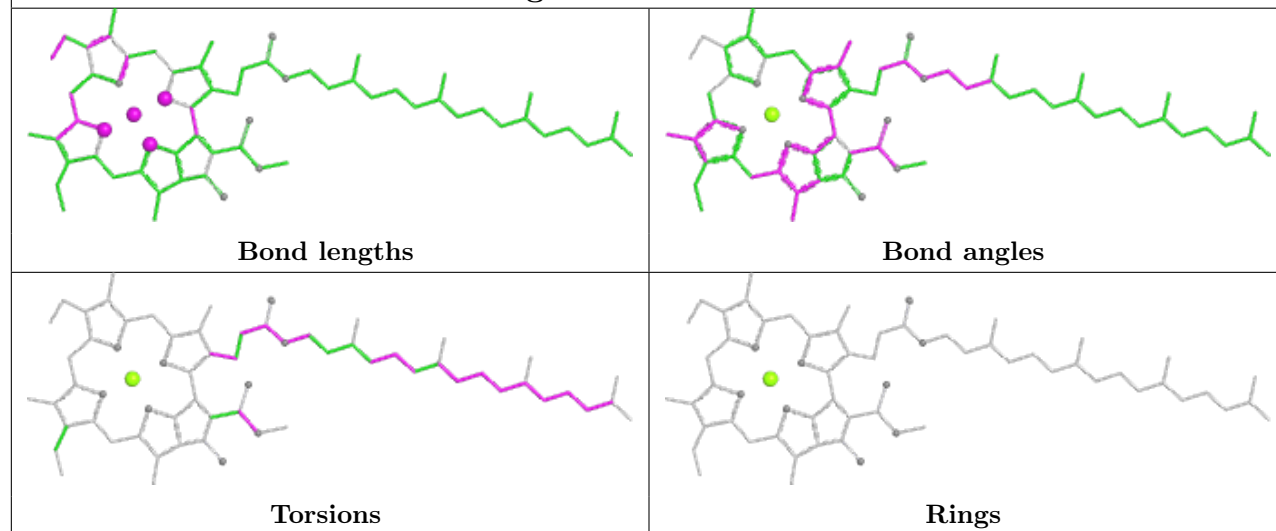


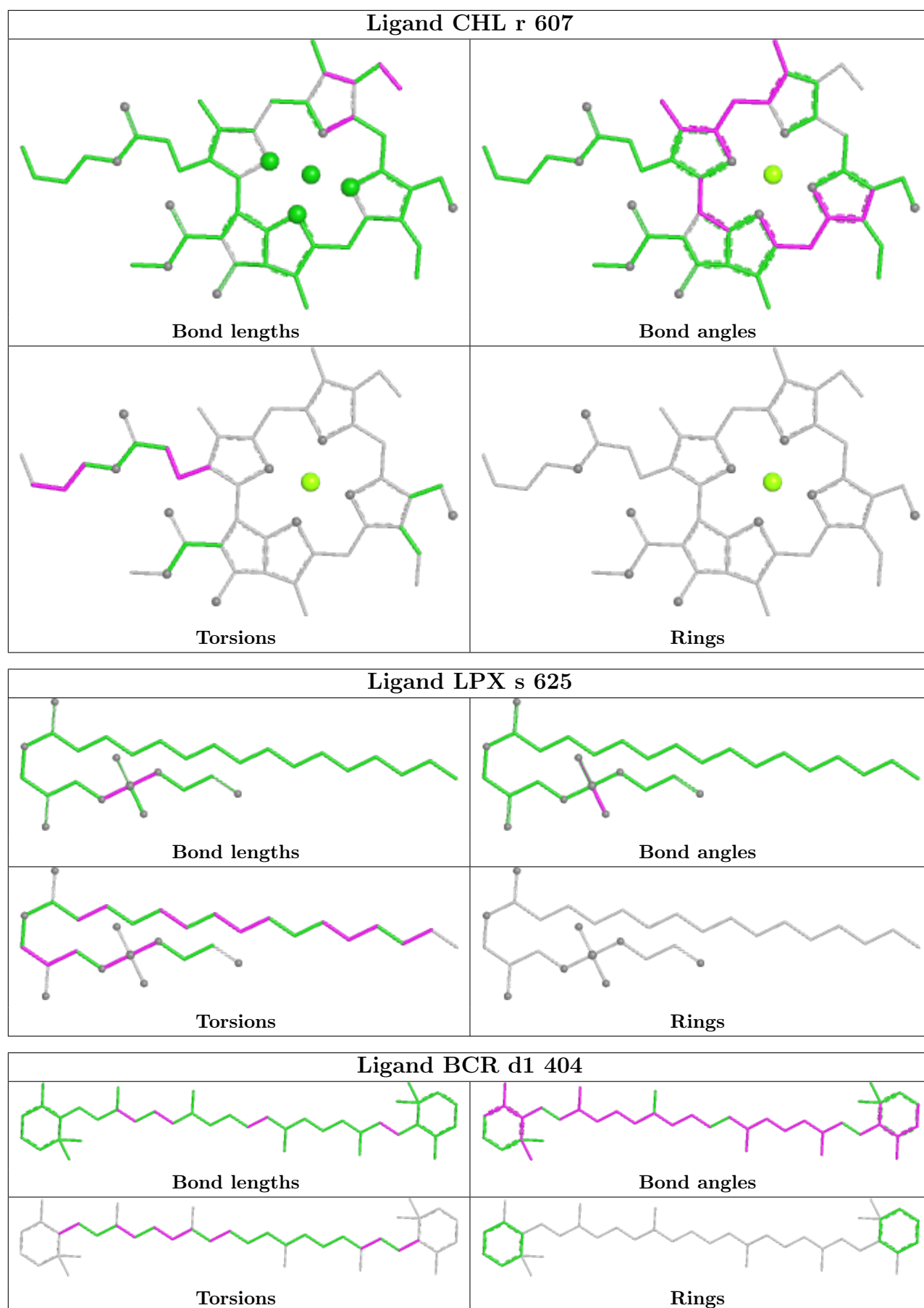


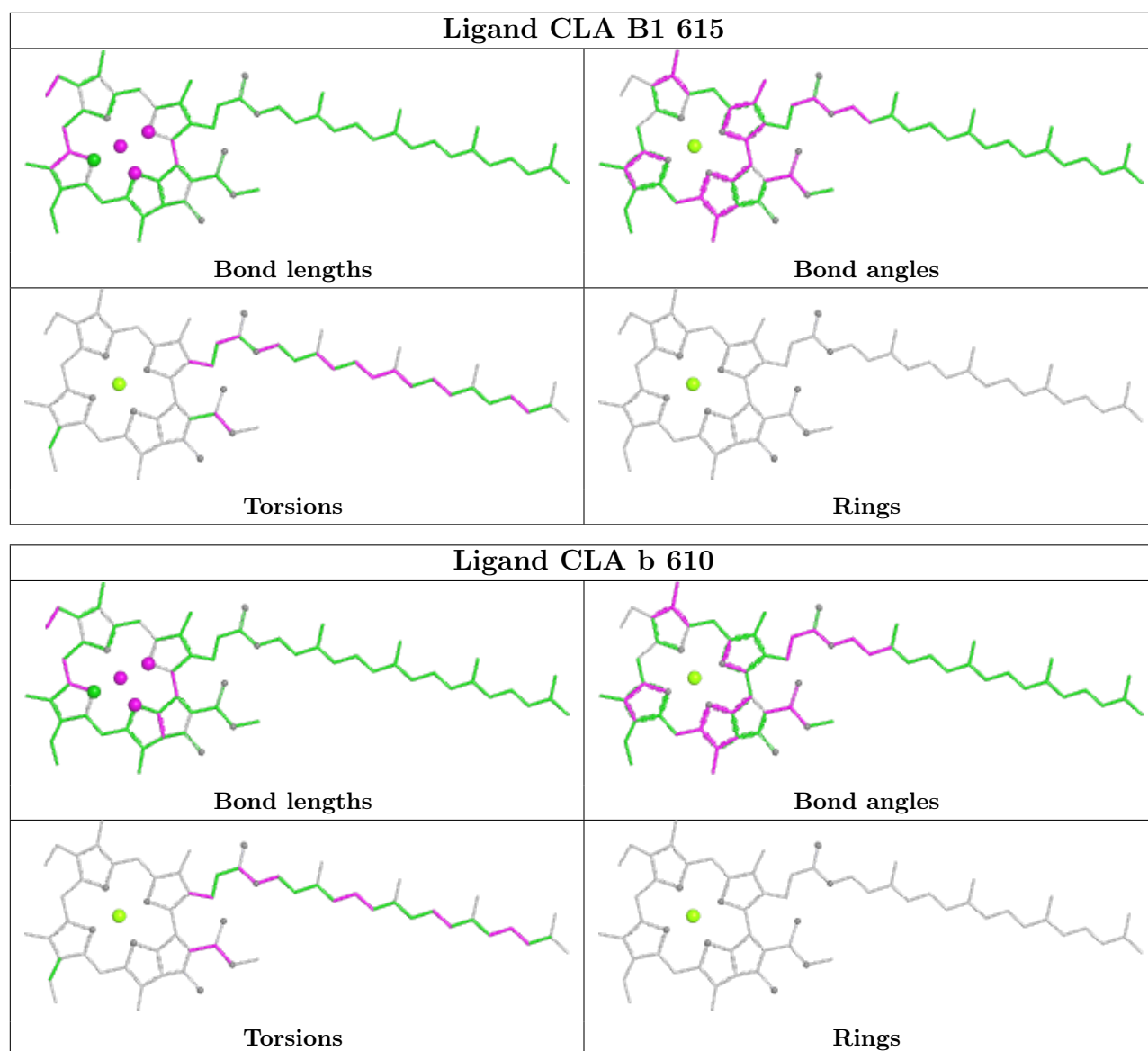
Ligand CLA g 604

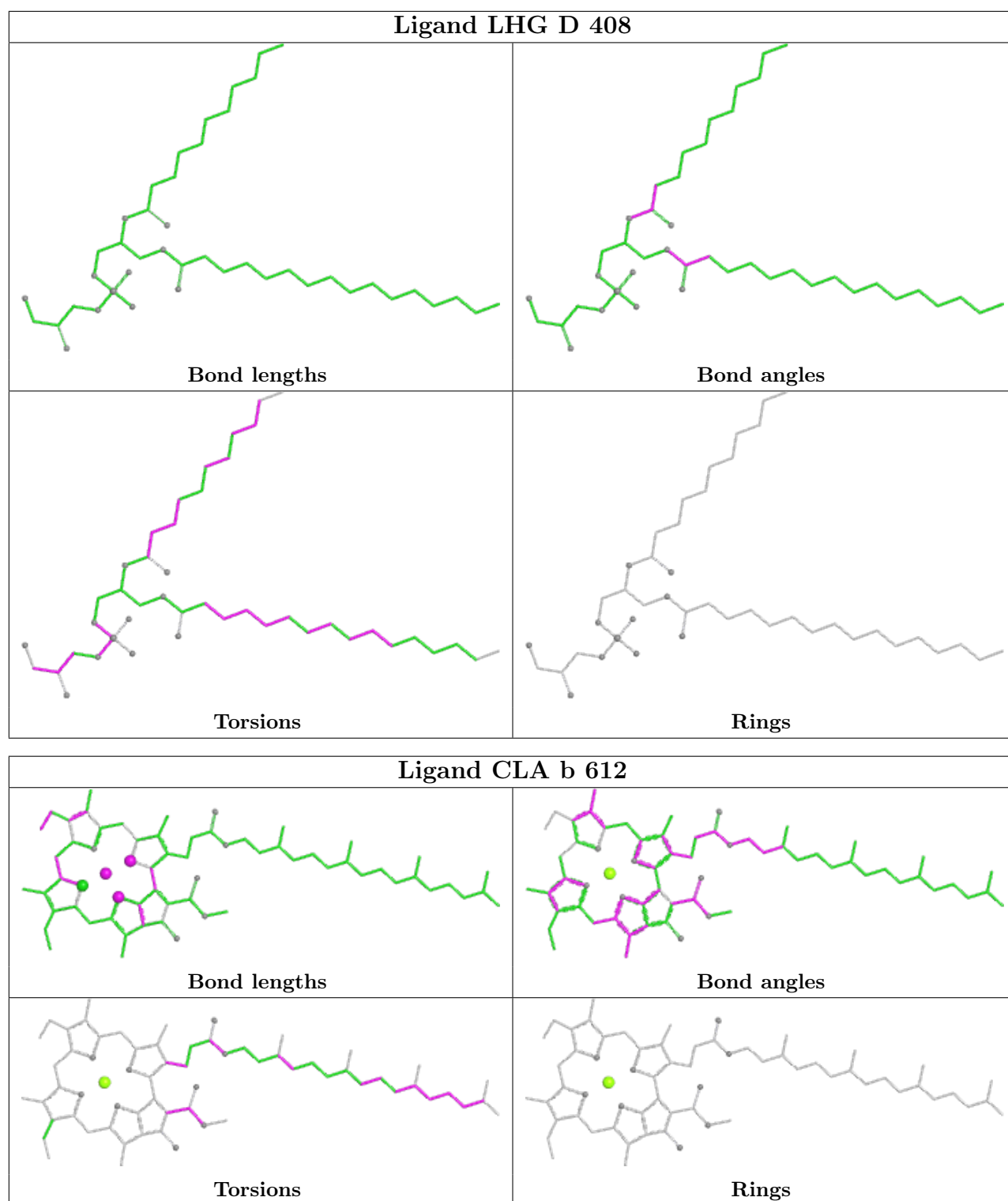


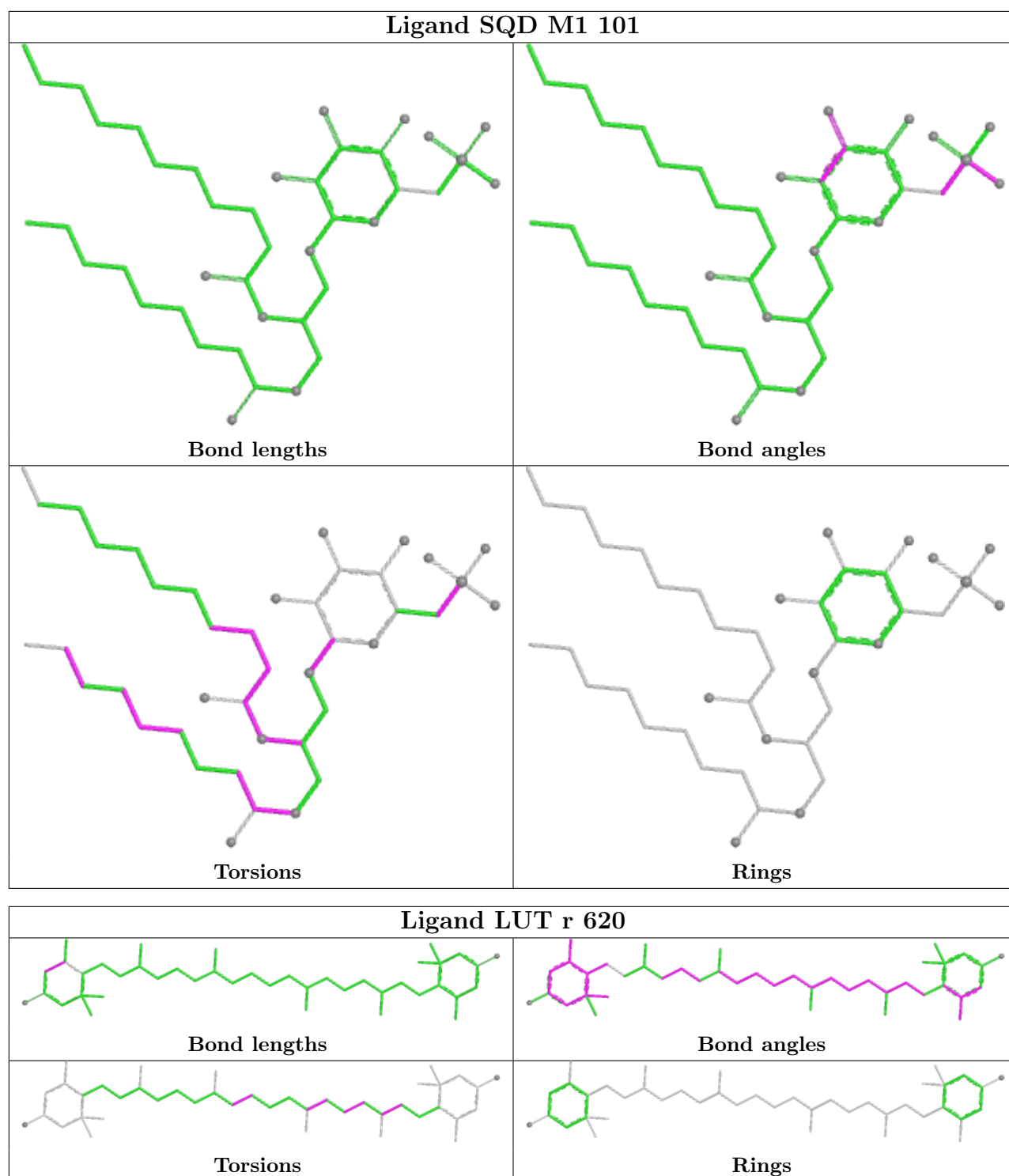
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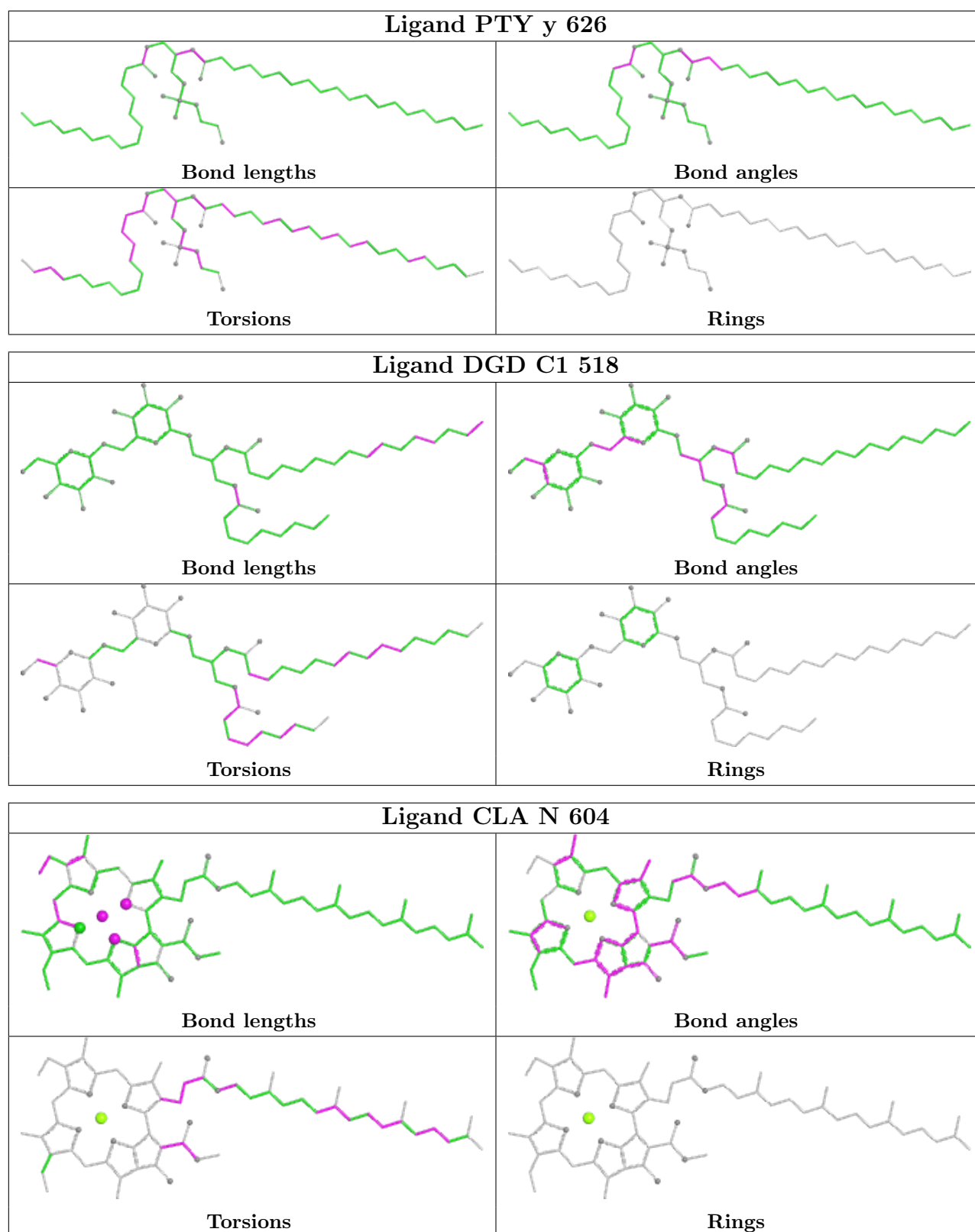


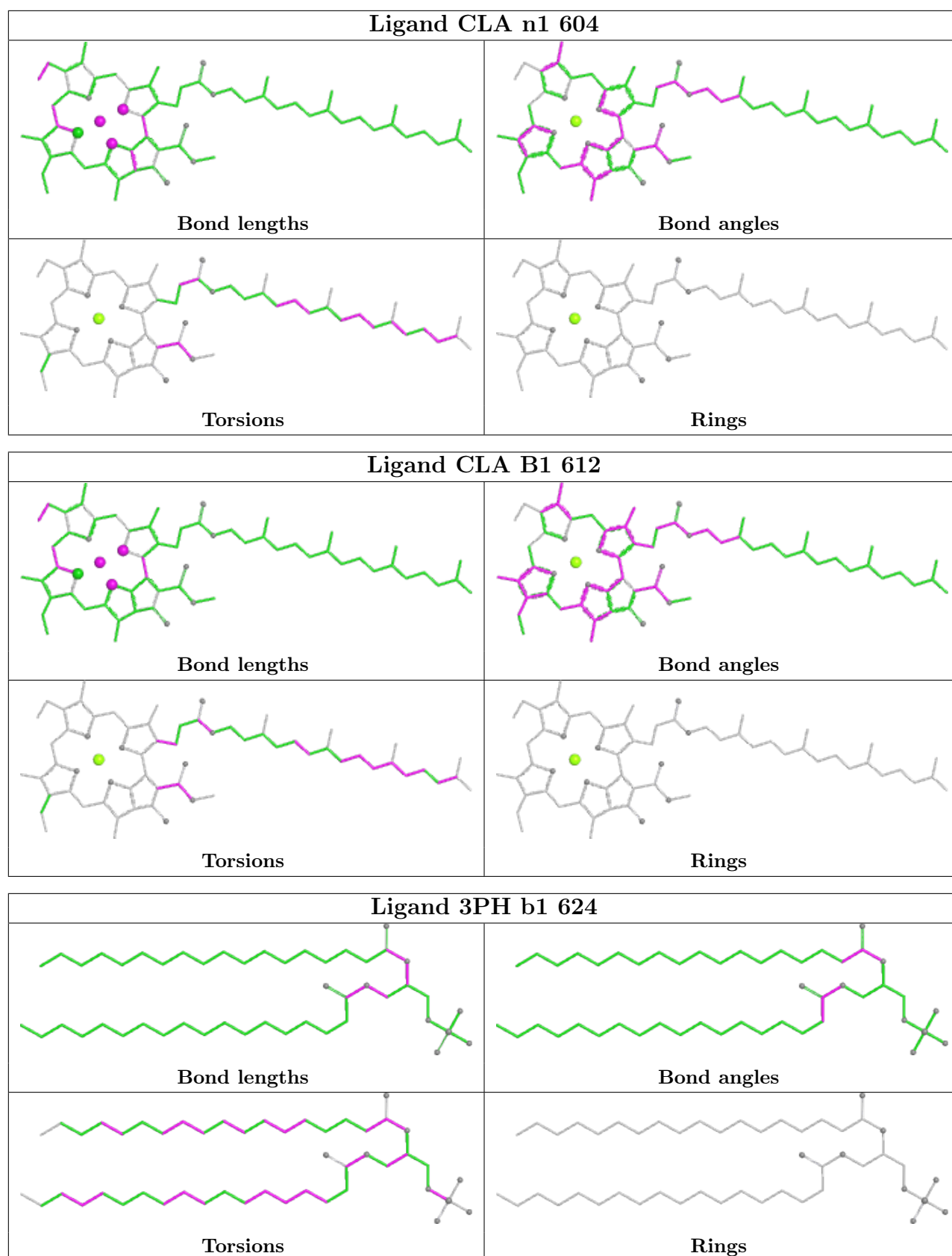


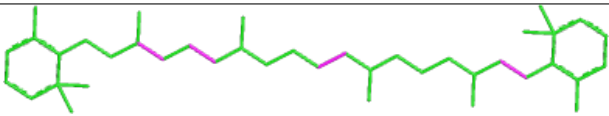
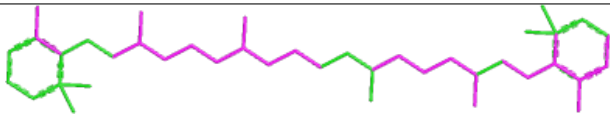
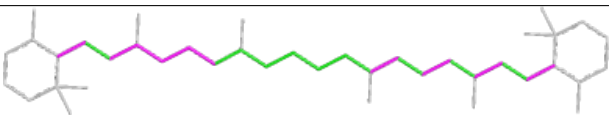
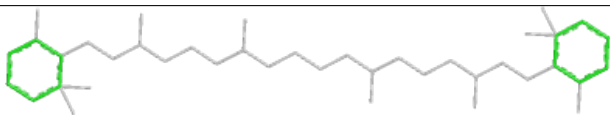


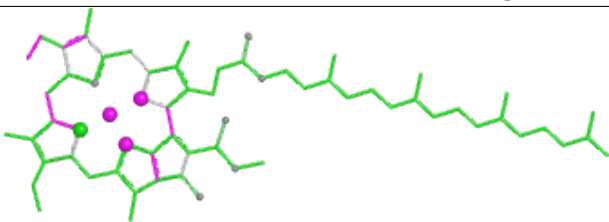
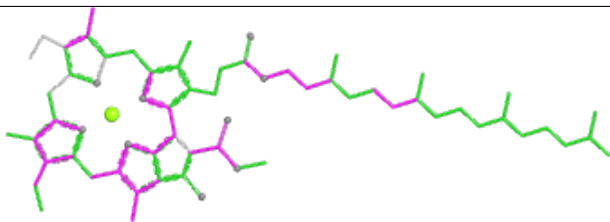
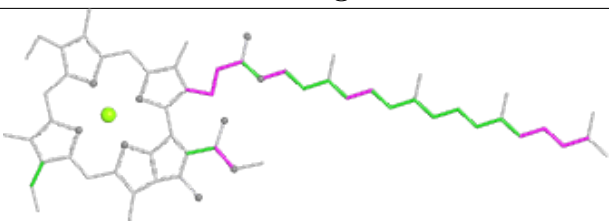
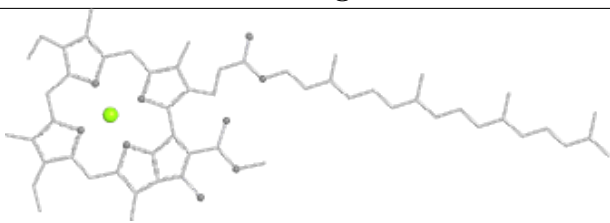


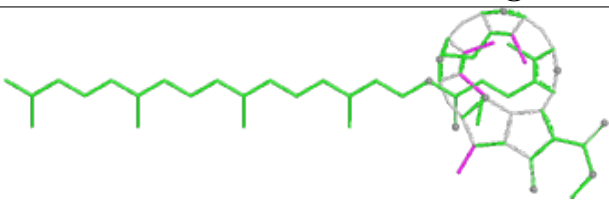
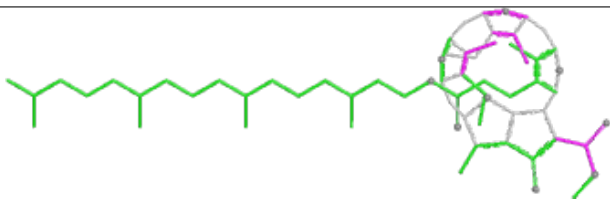
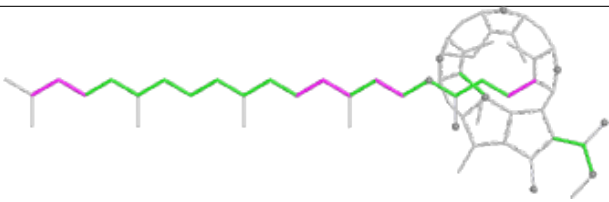
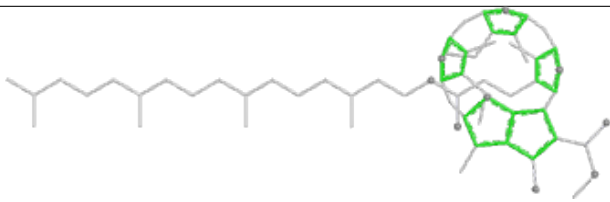


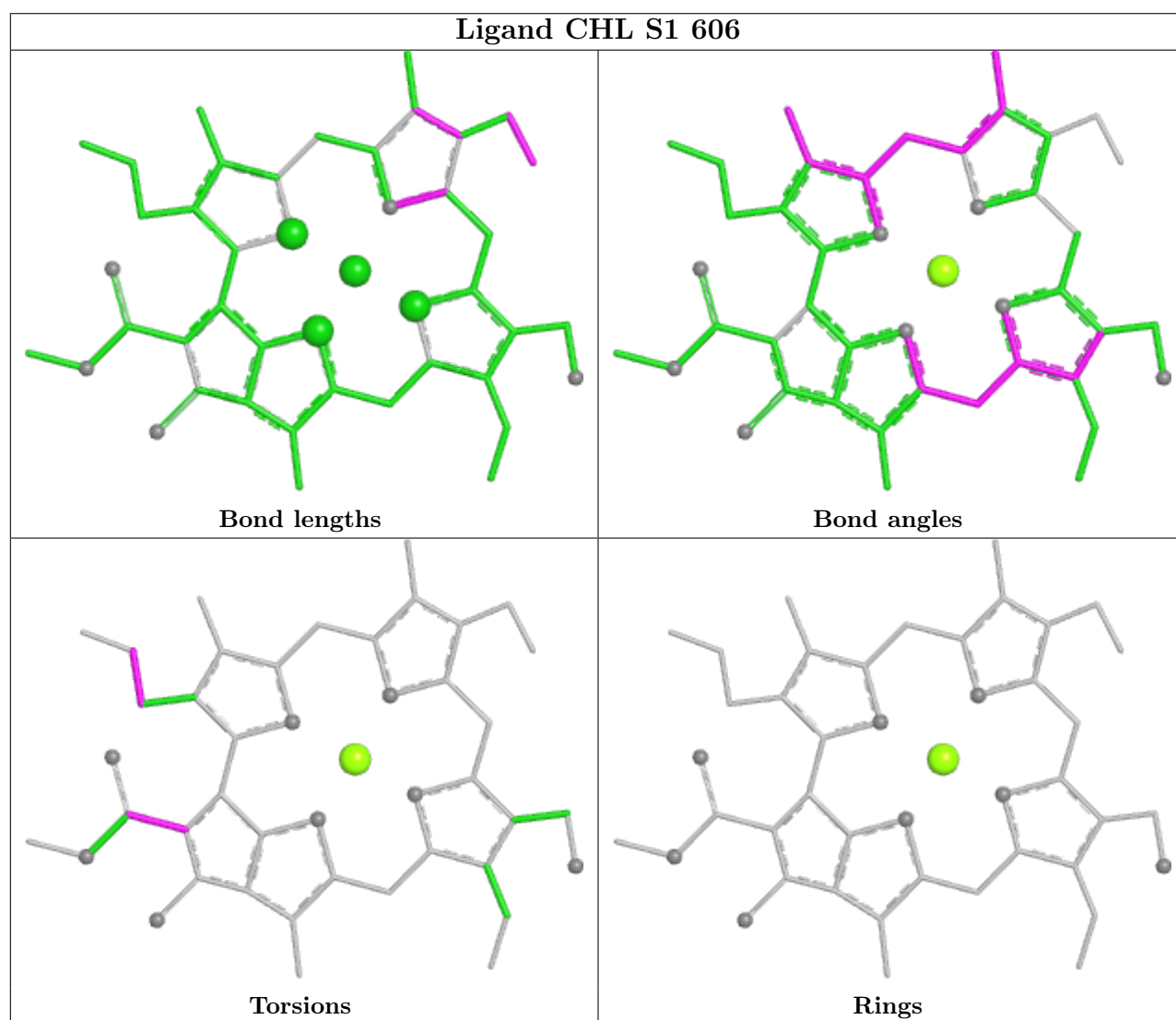
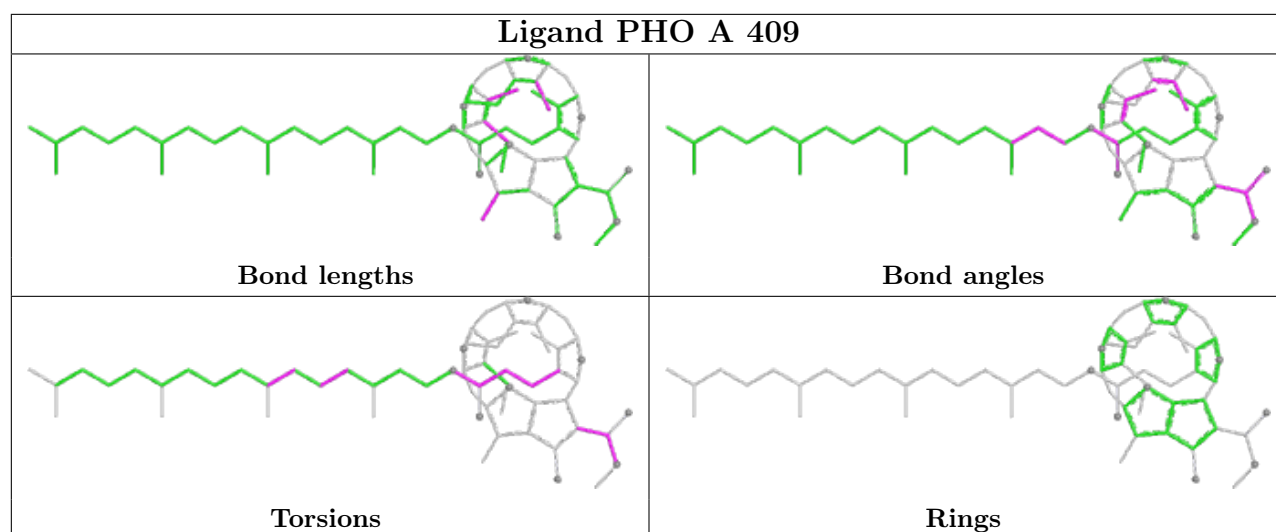


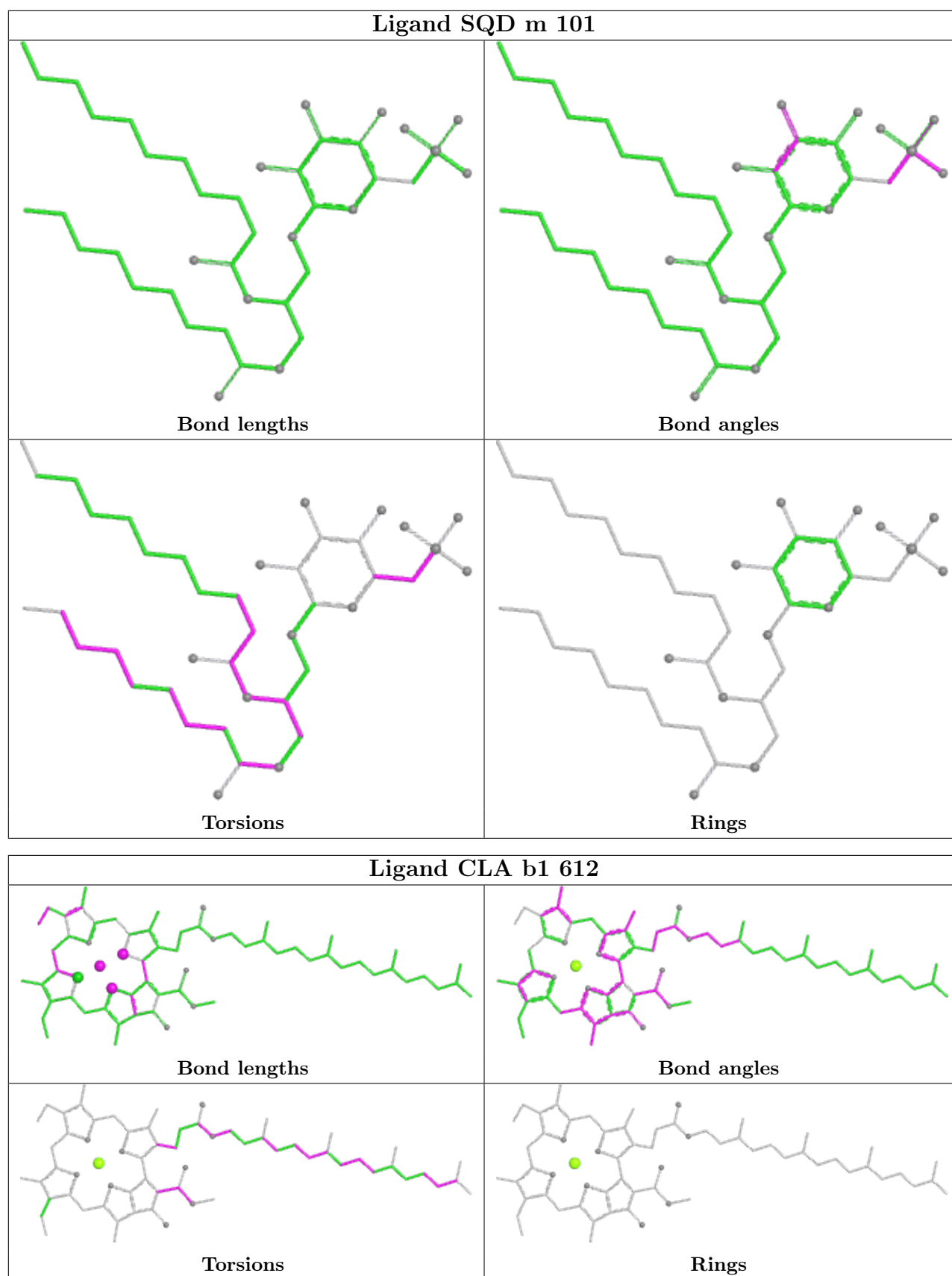


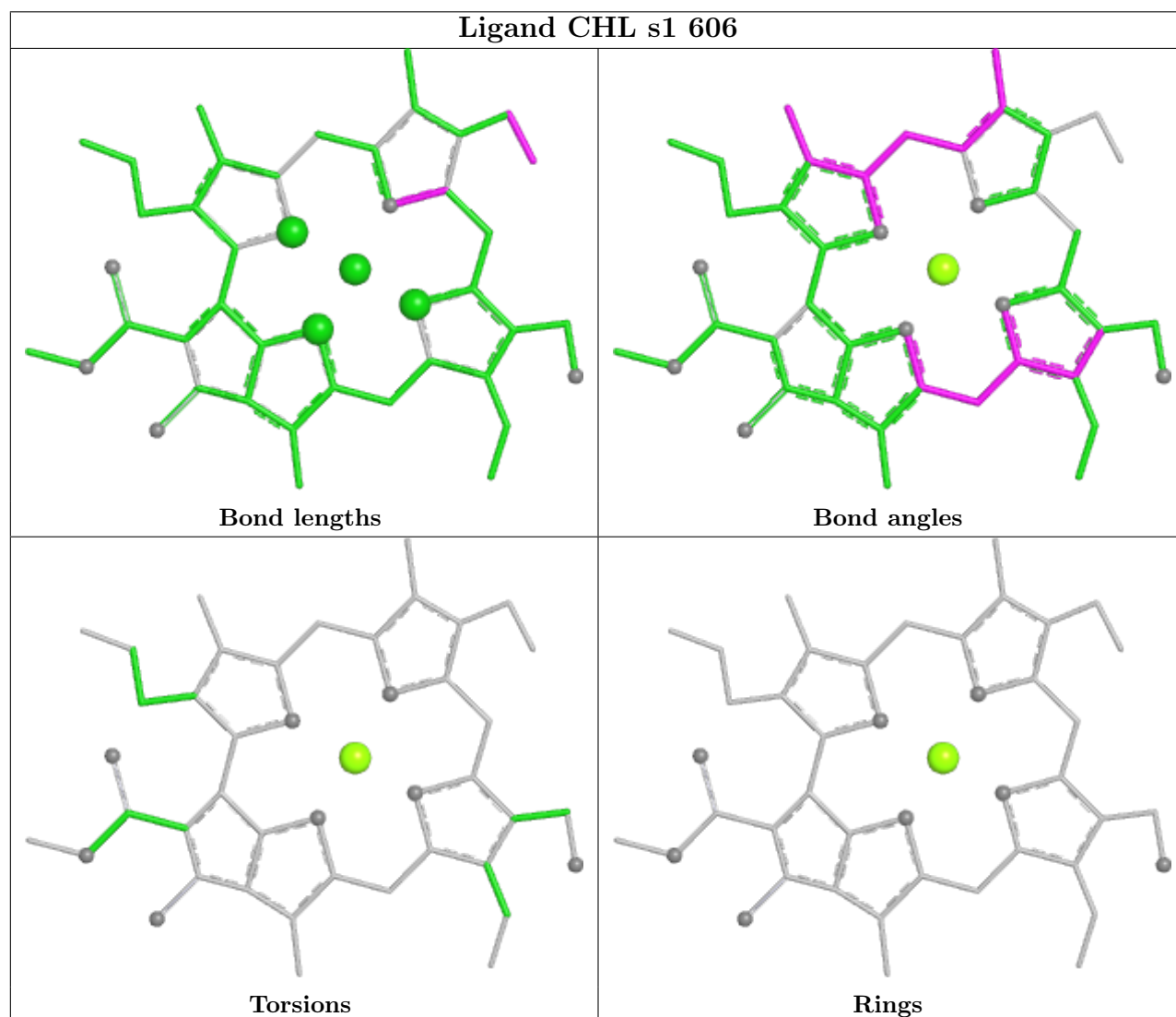
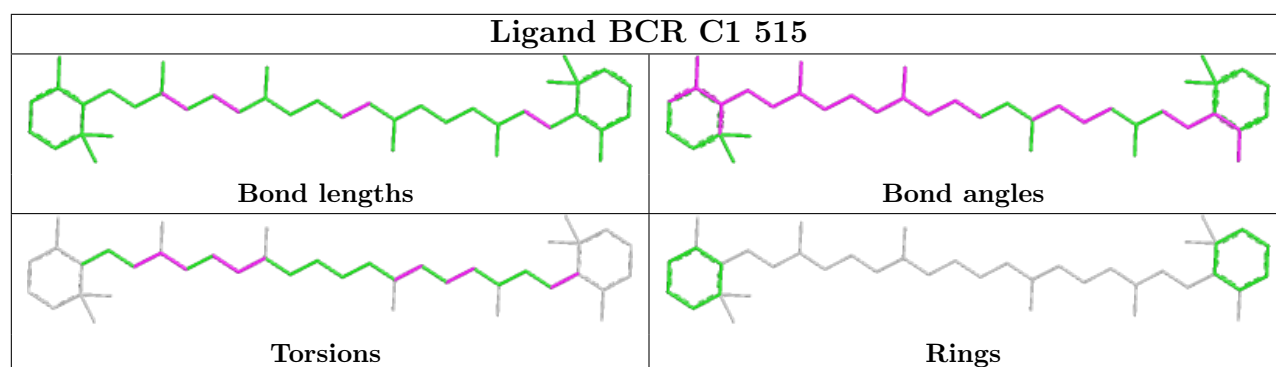
Ligand BCR C1 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

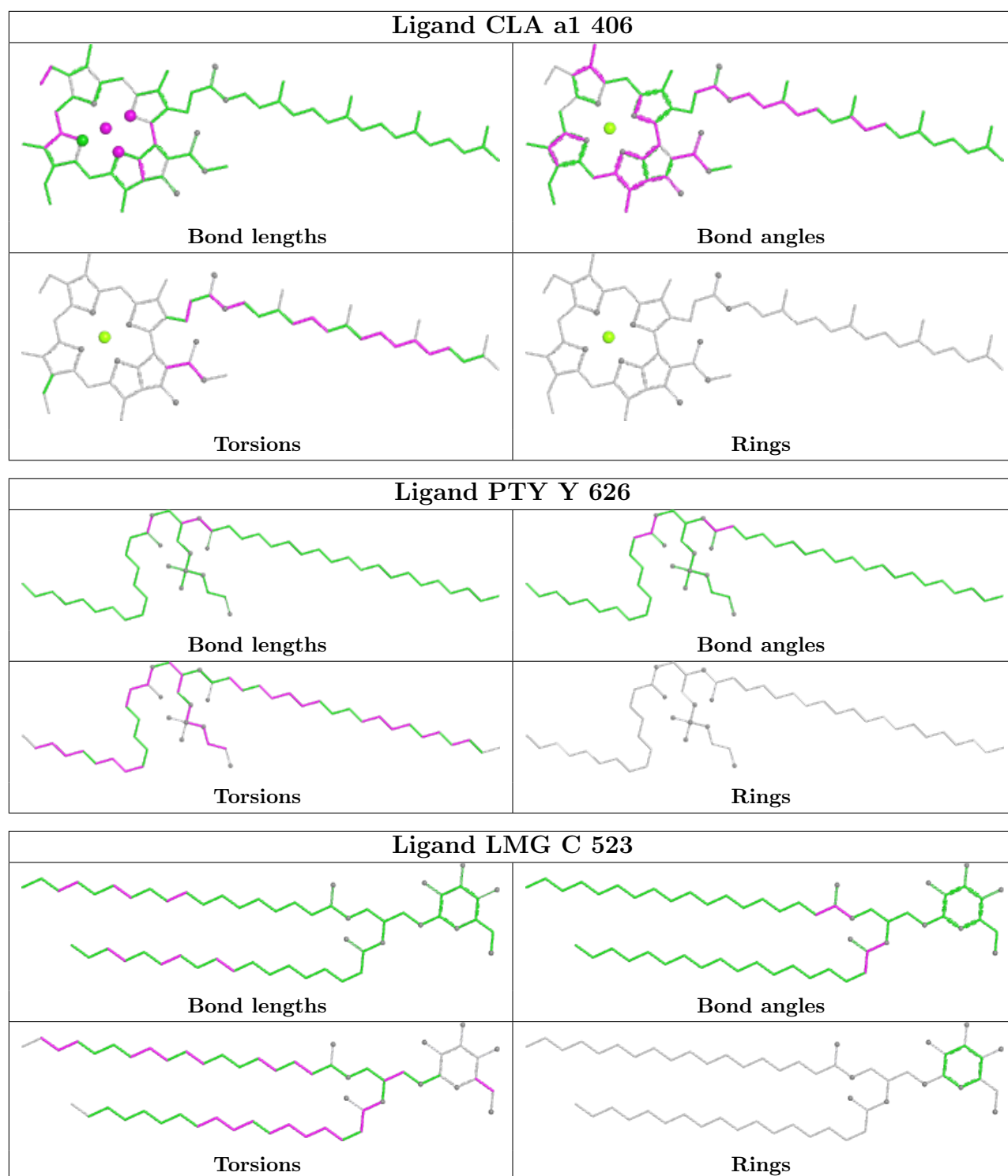
Ligand CLA A1 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

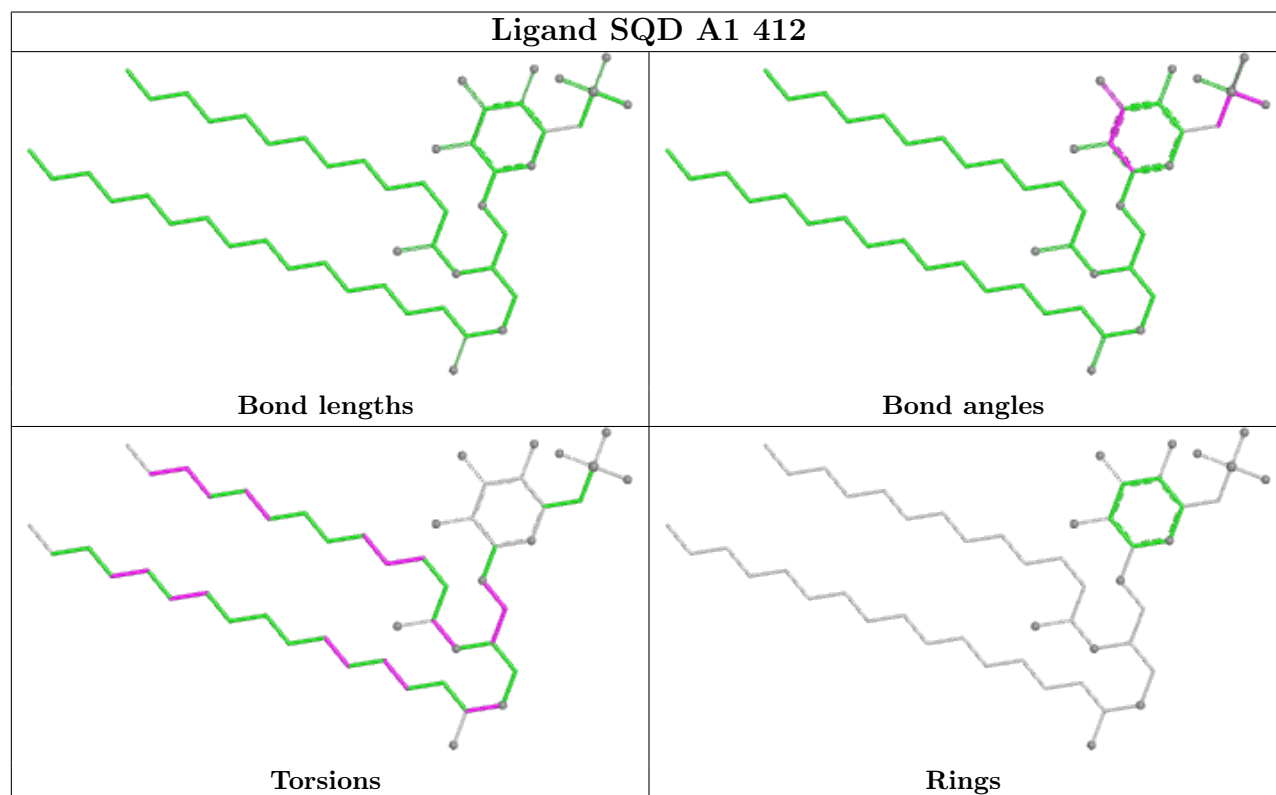
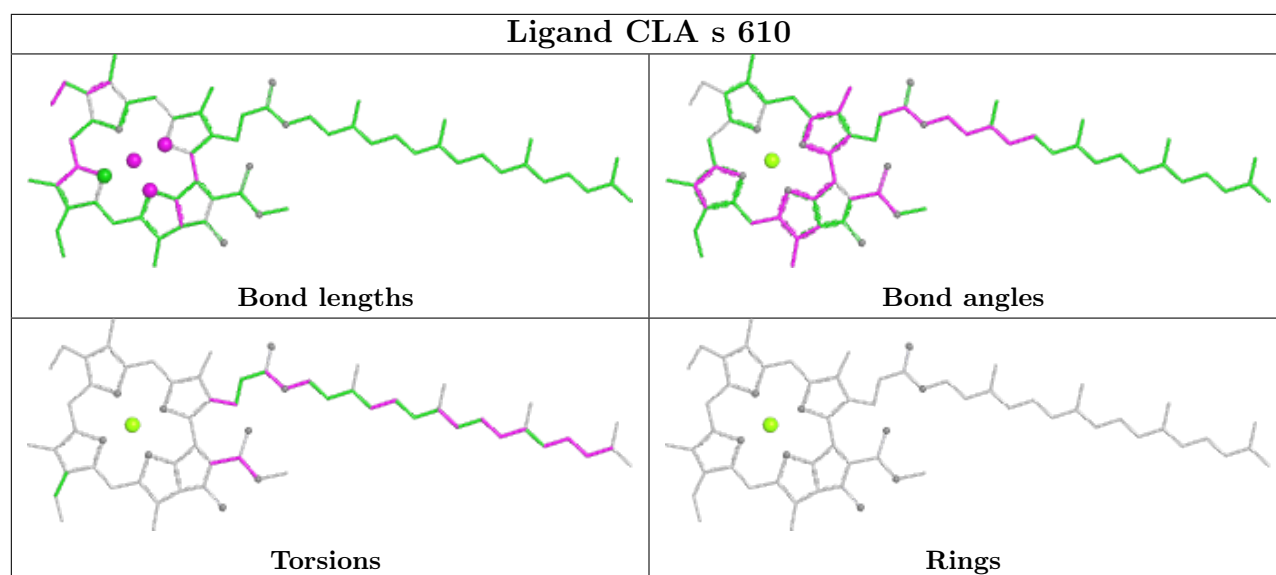
Ligand PHO A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

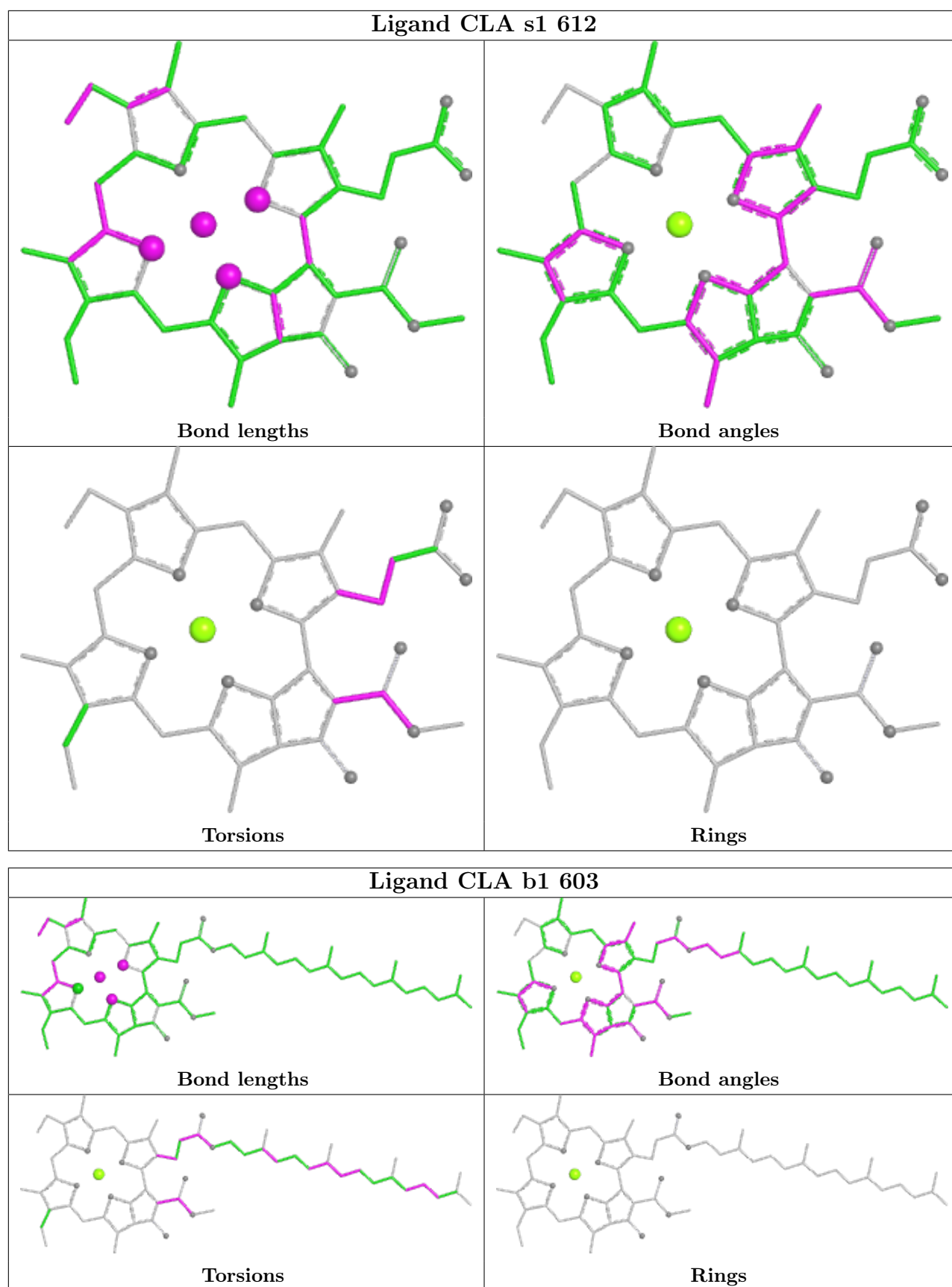




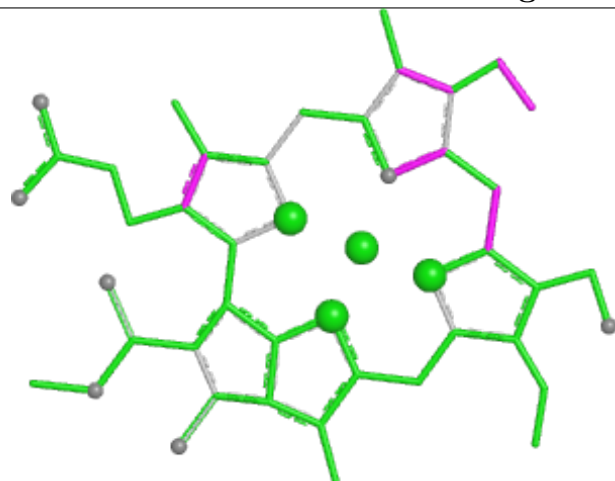




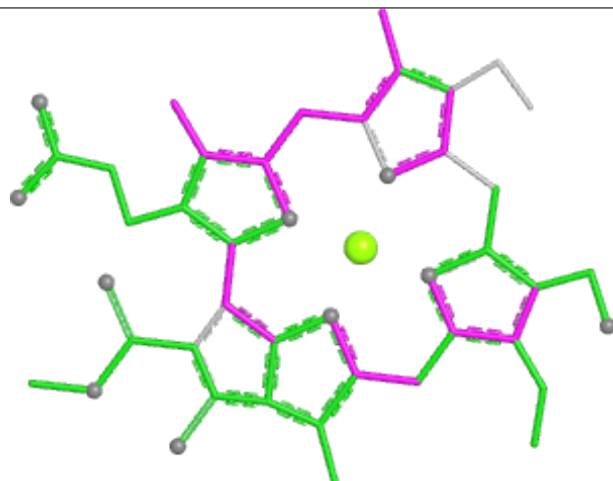




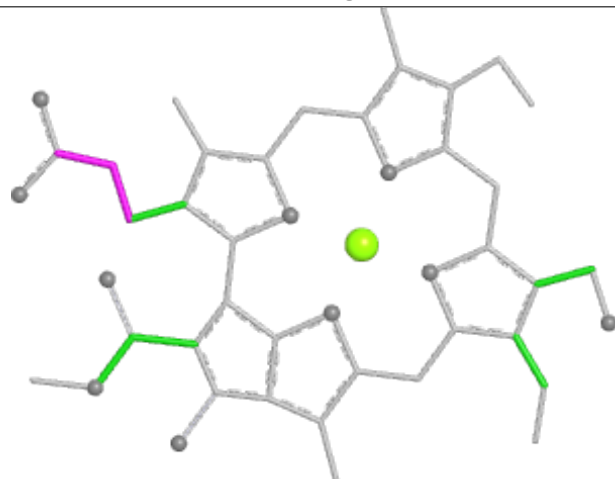
Ligand CHL S 601



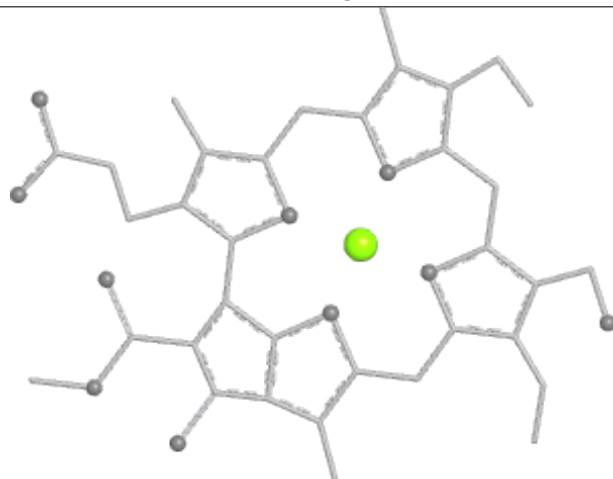
Bond lengths



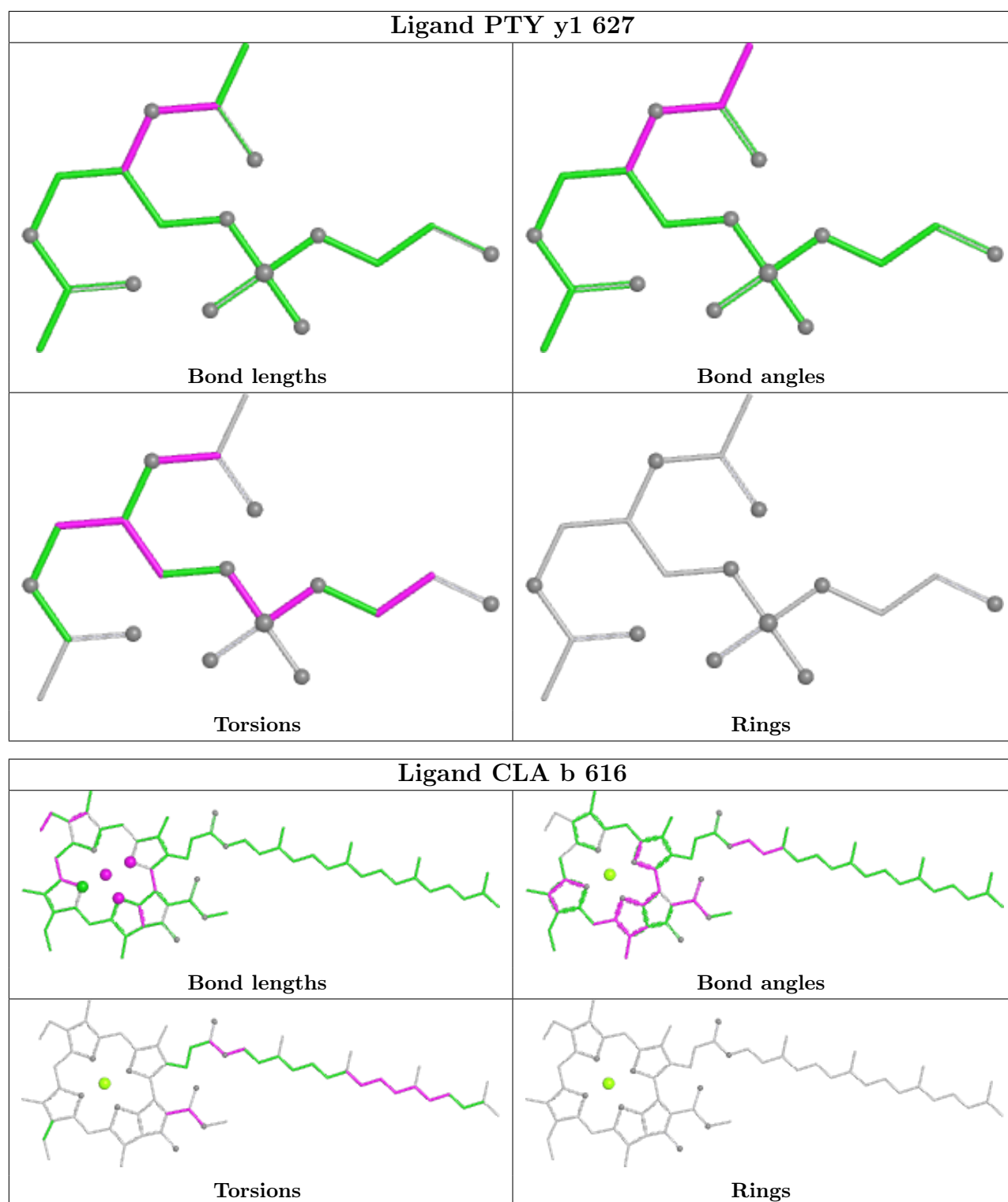
Bond angles

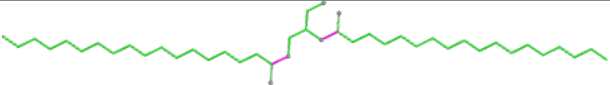
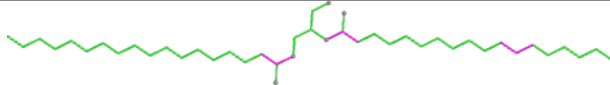
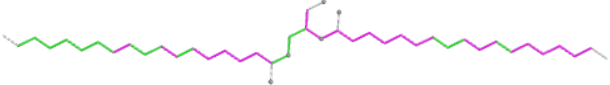
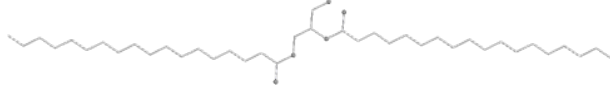
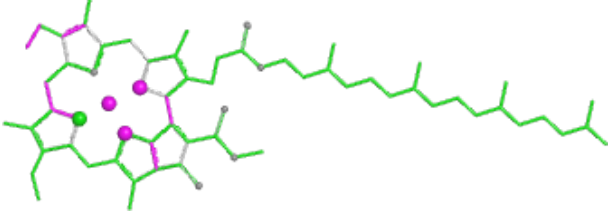
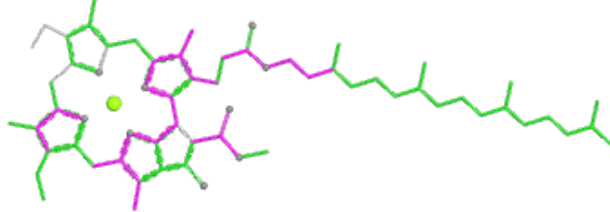
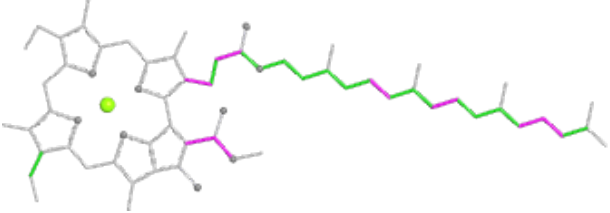
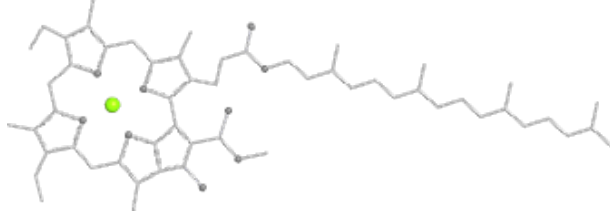
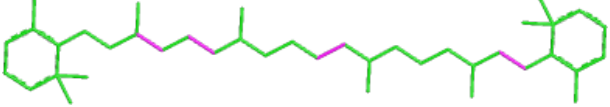
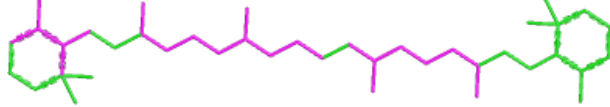
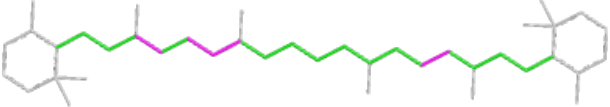
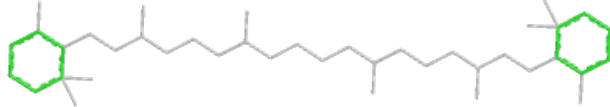


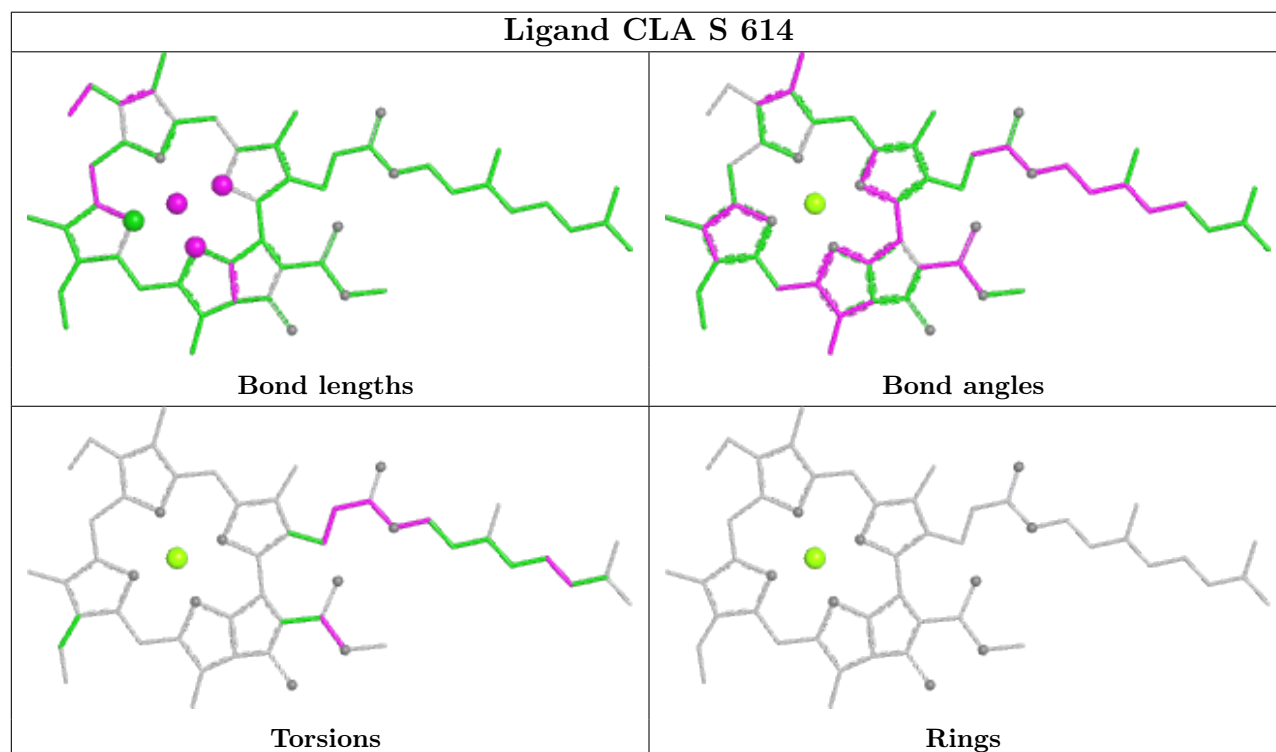
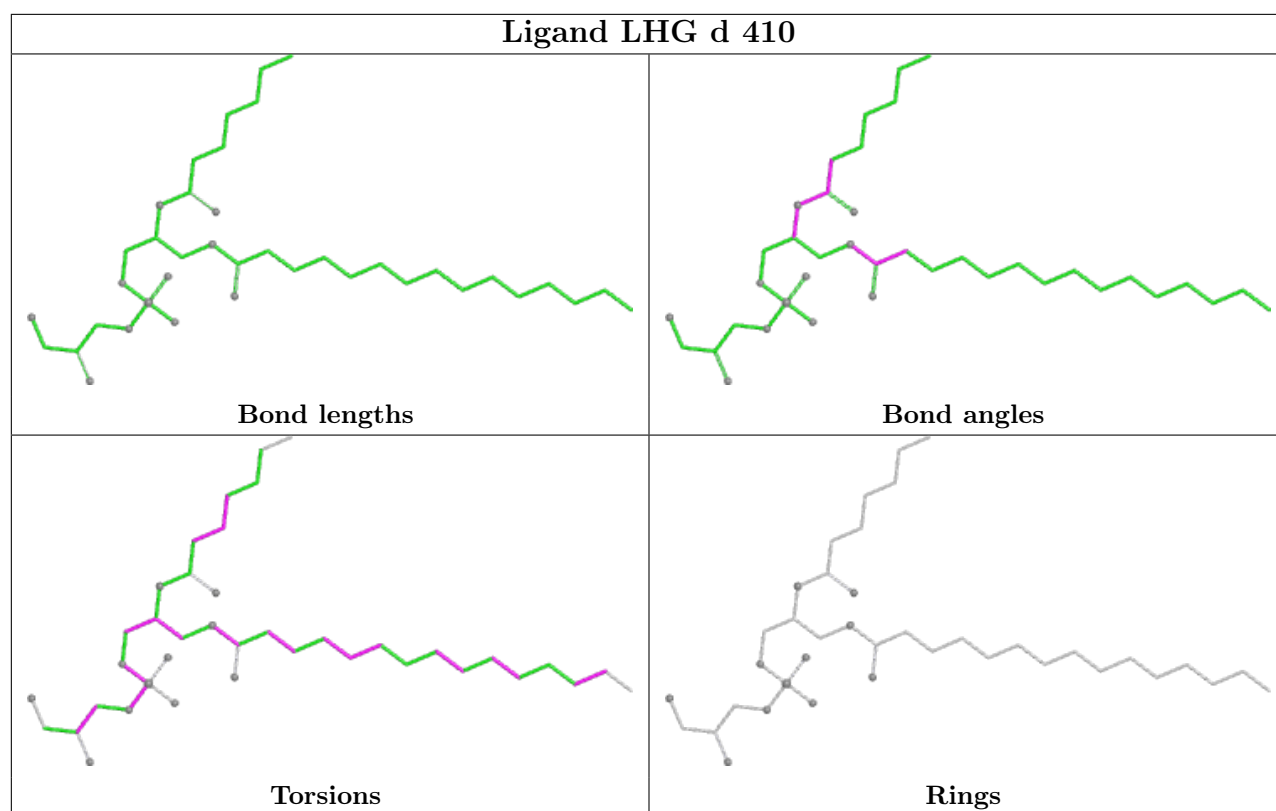
Torsions

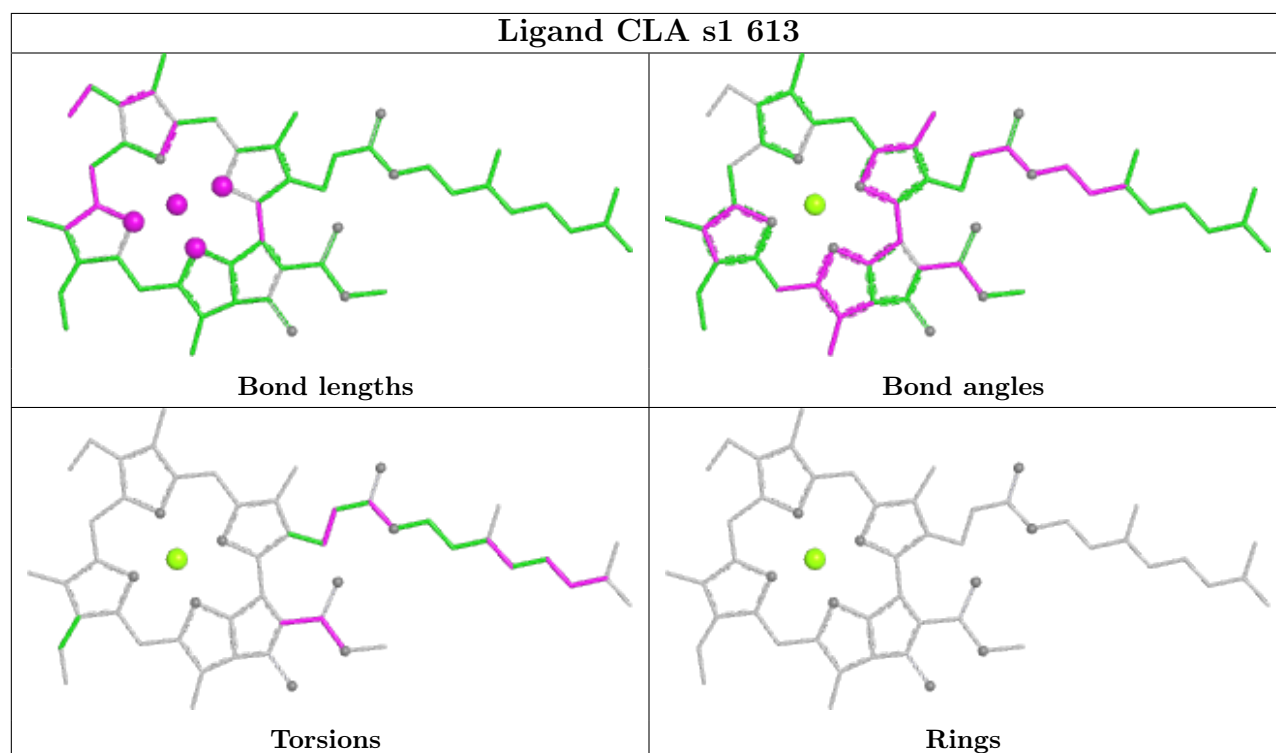
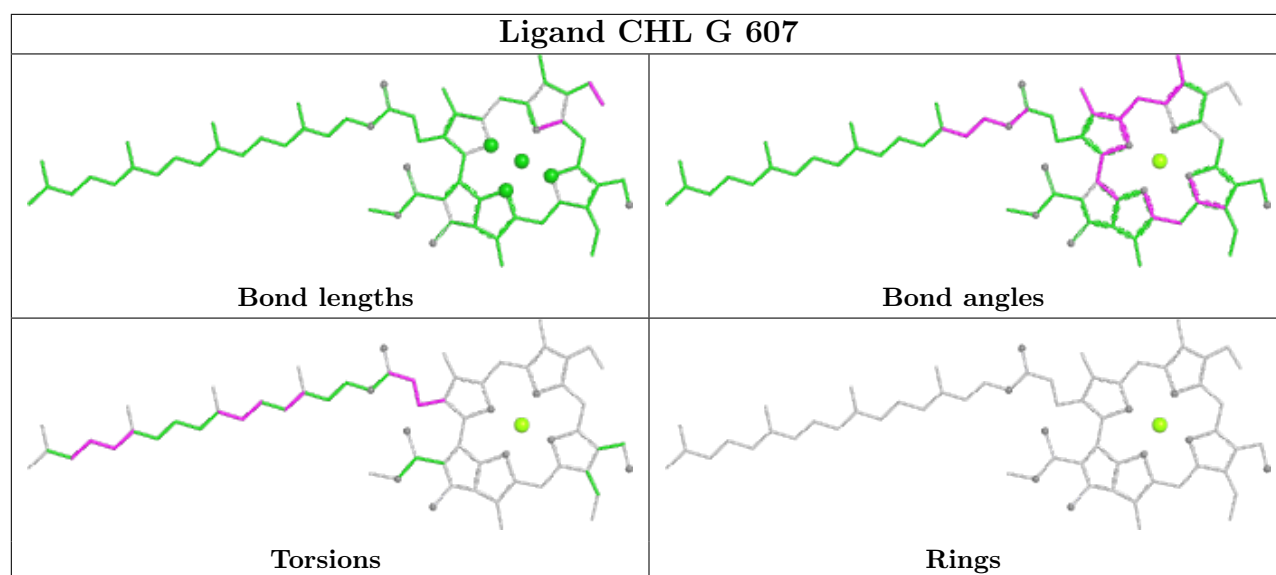


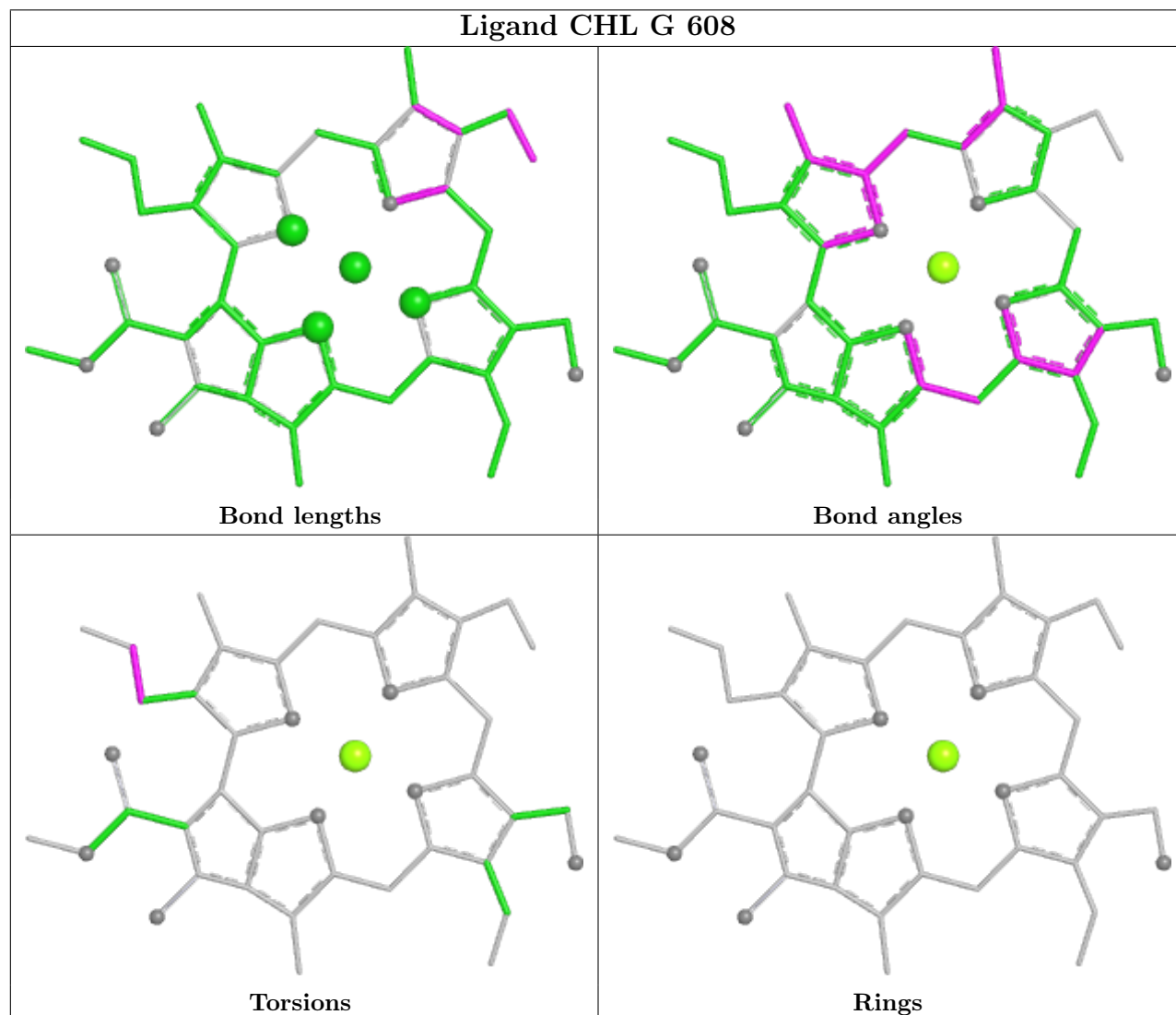
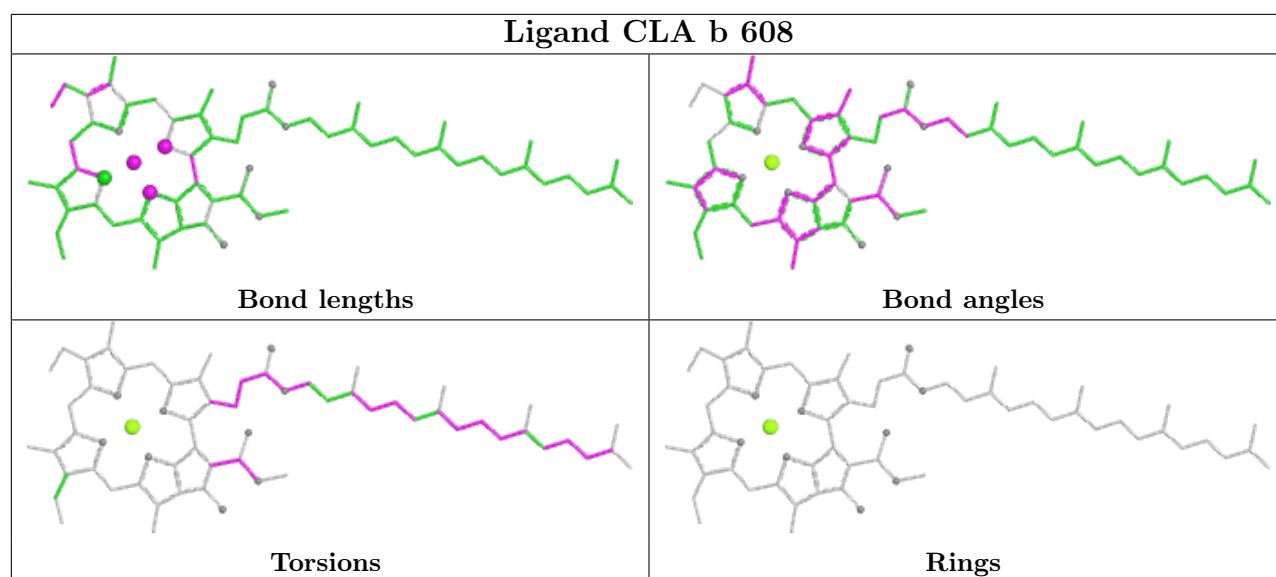
Rings

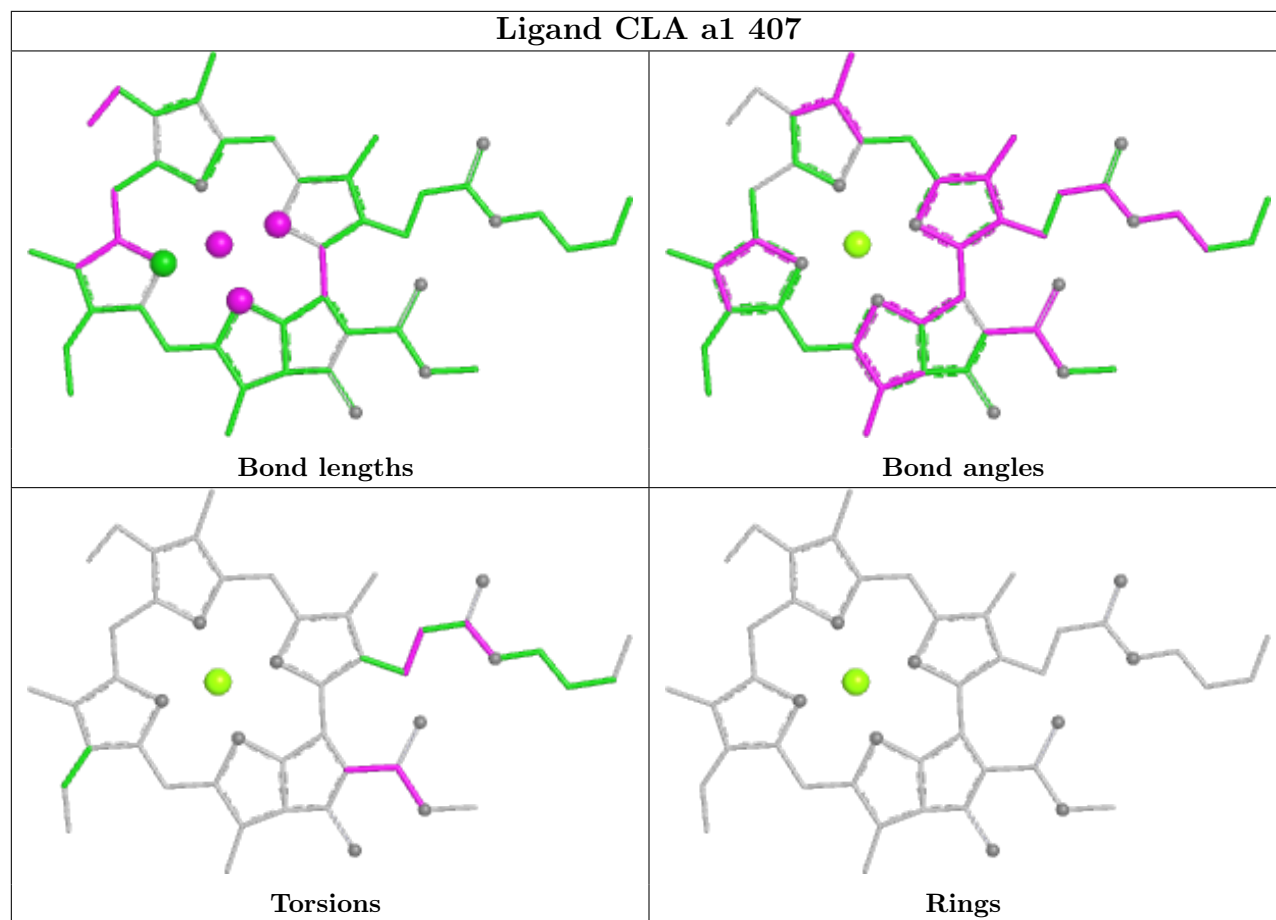


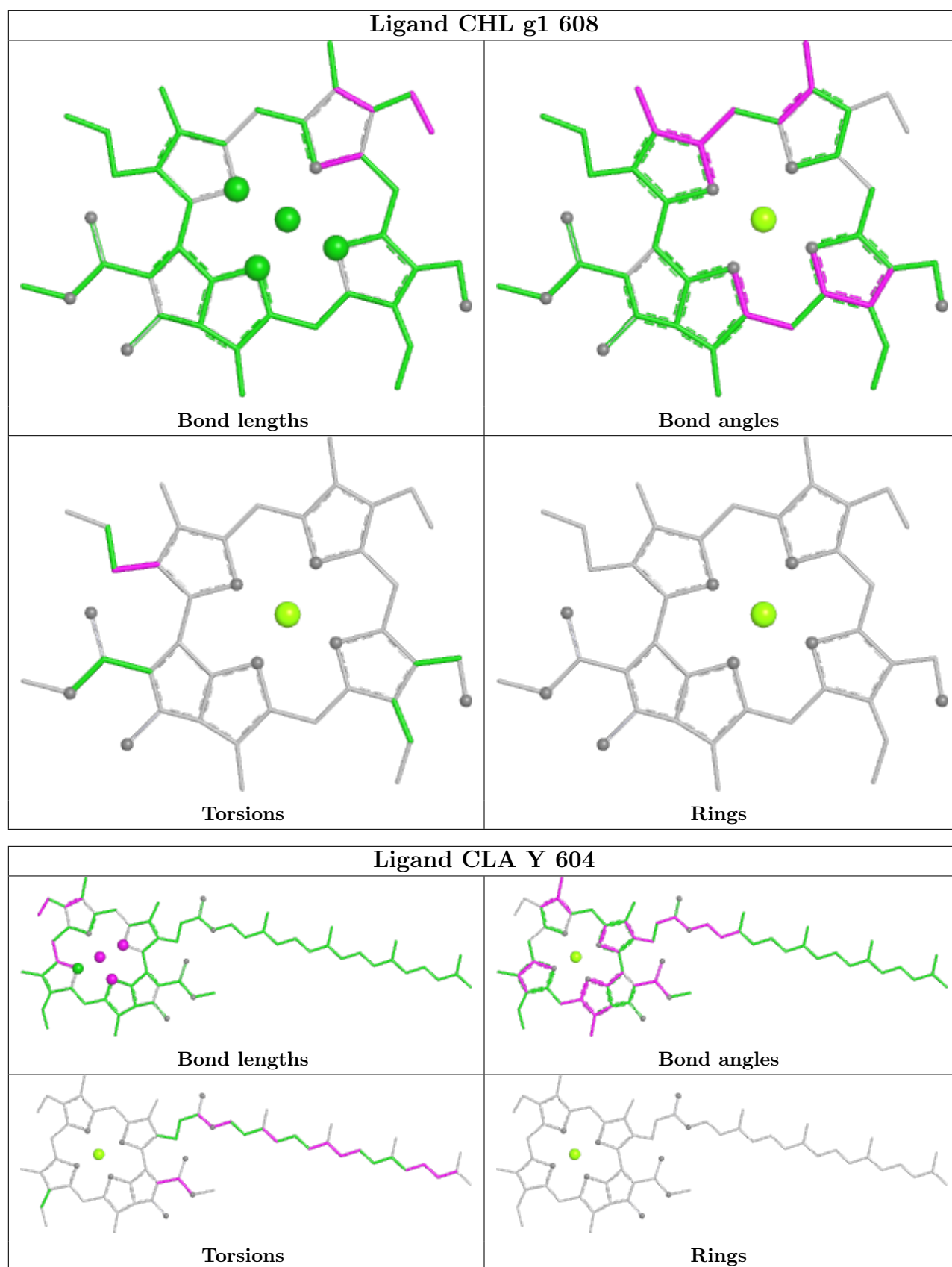
Ligand DGA b 625	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA b1 607	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B1 619	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



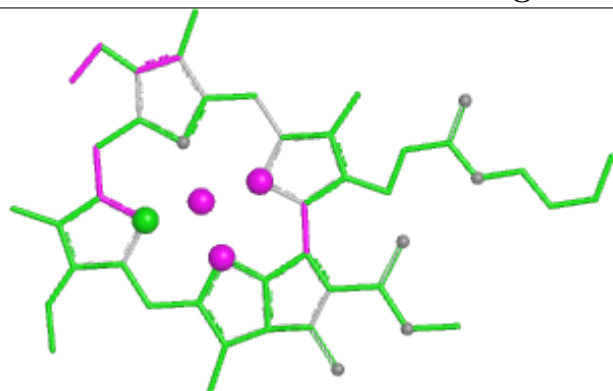




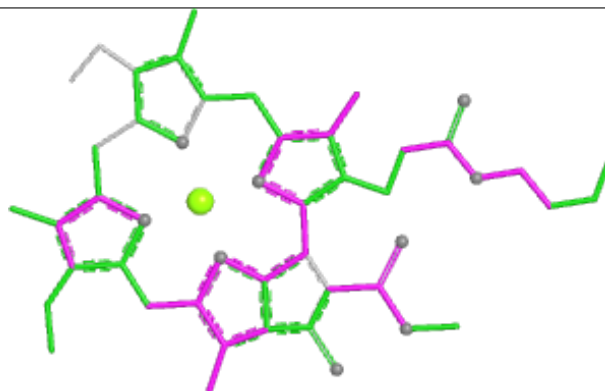




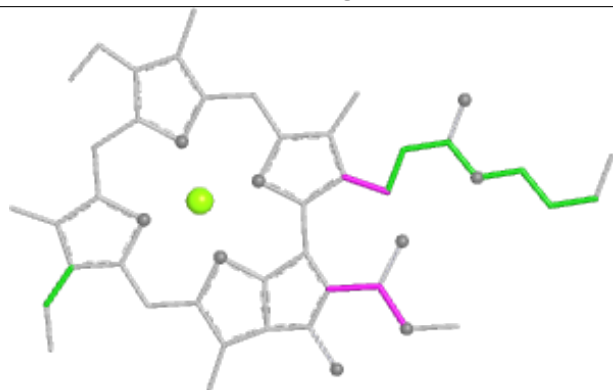
Ligand CLA N 614



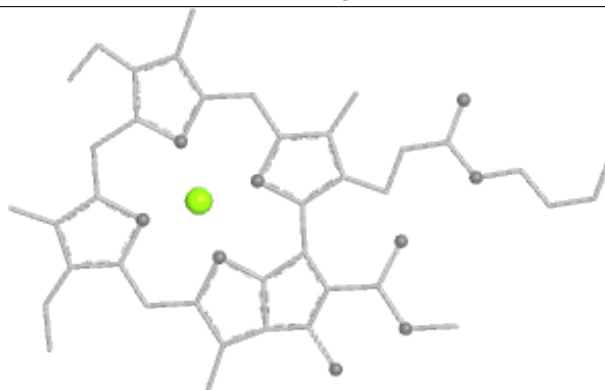
Bond lengths



Bond angles

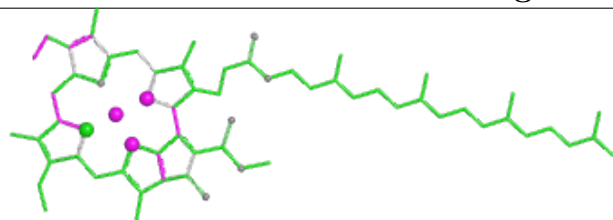


Torsions

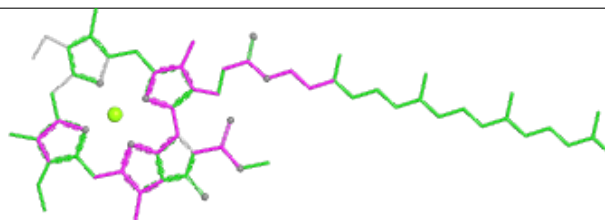


Rings

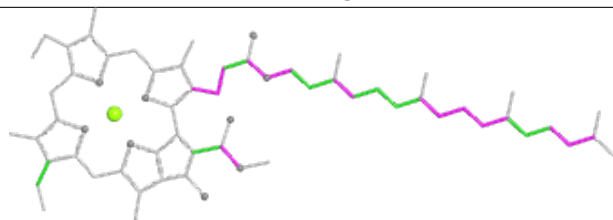
Ligand CLA C 501



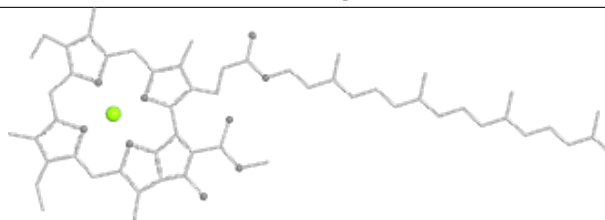
Bond lengths



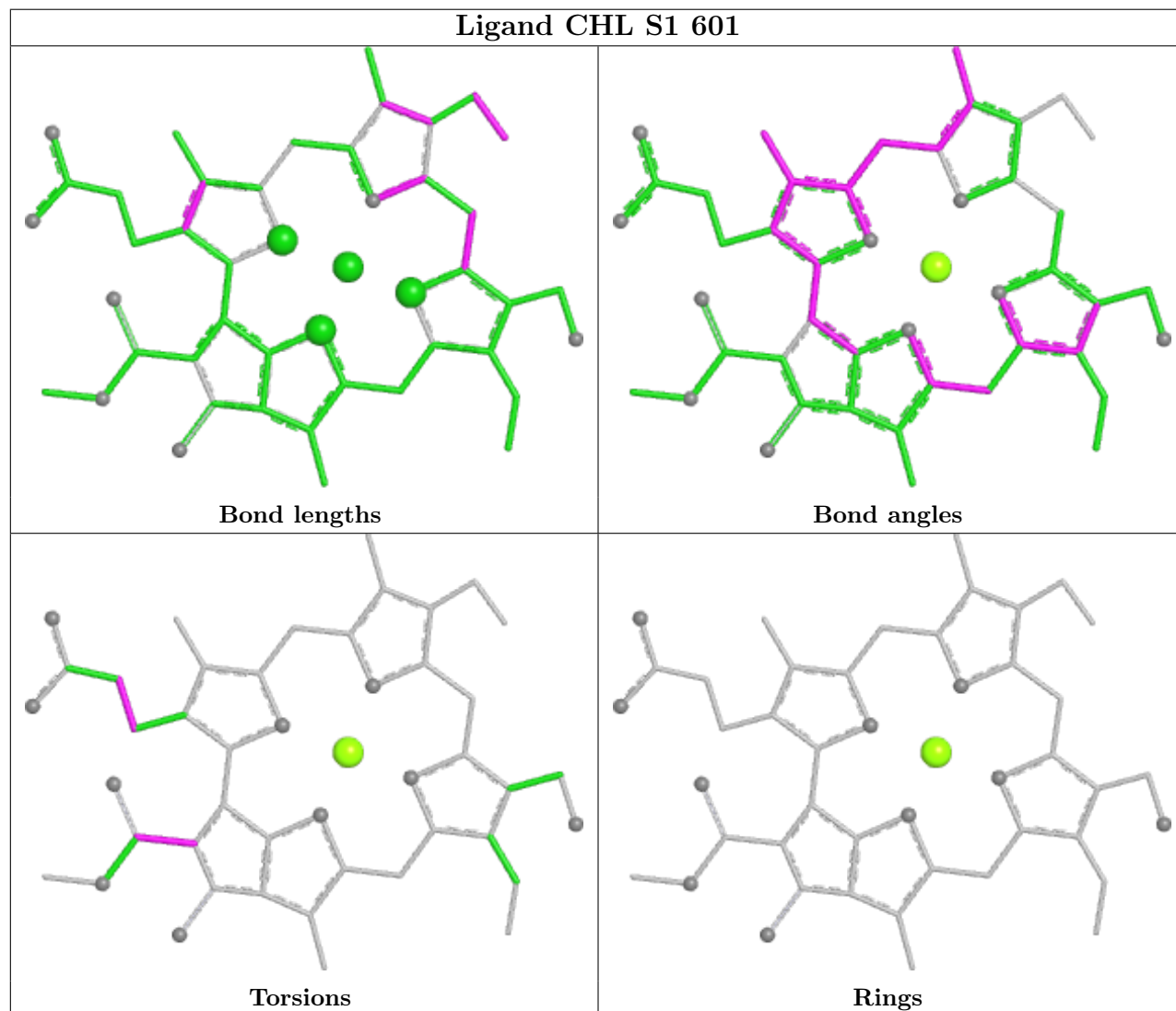
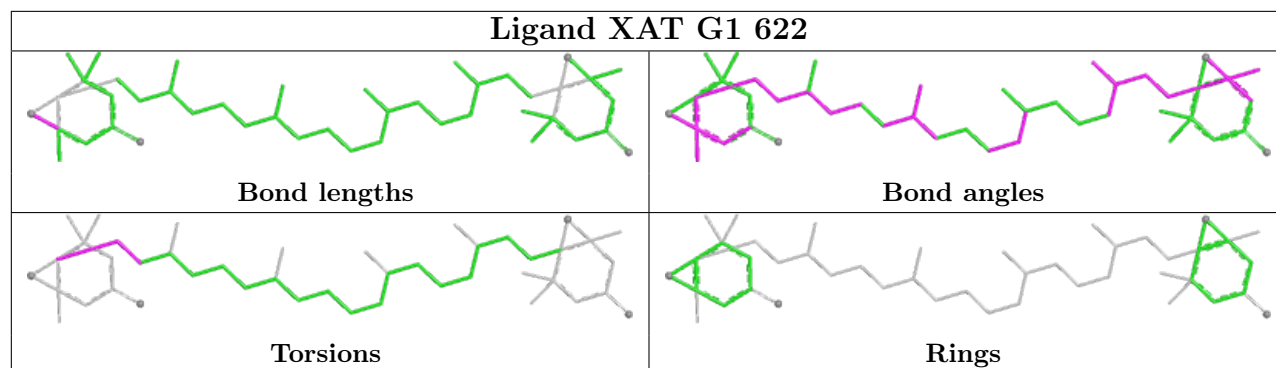
Bond angles

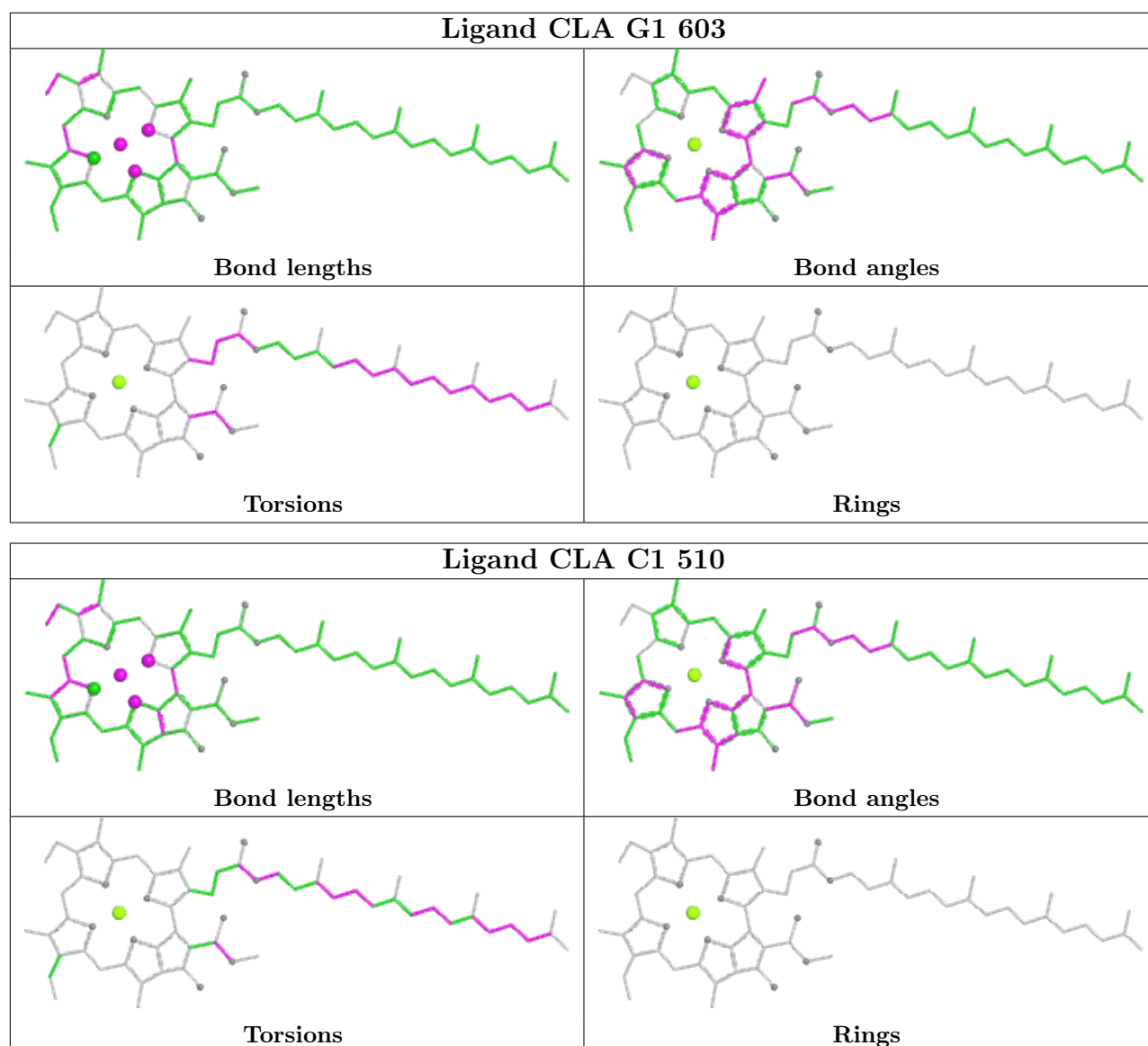


Torsions

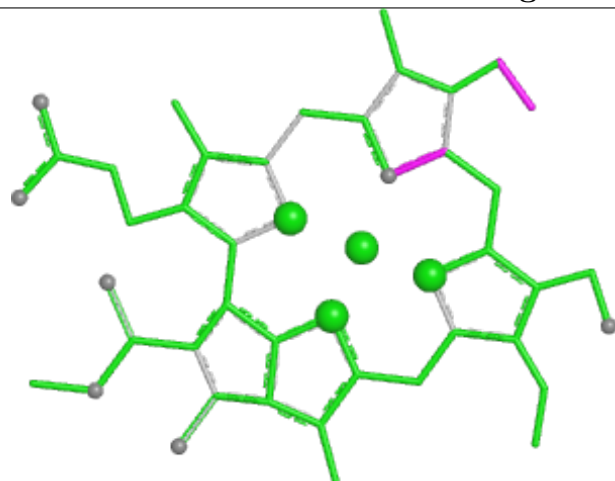


Rings

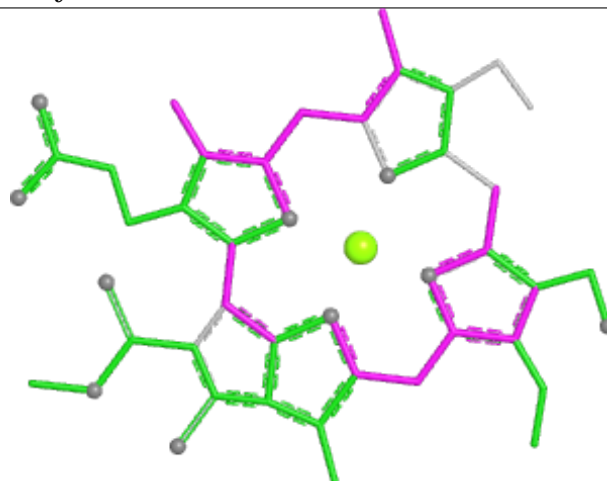




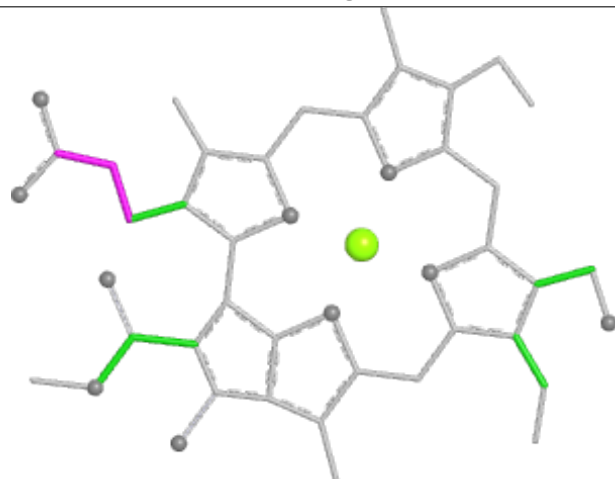
Ligand CHL y 605



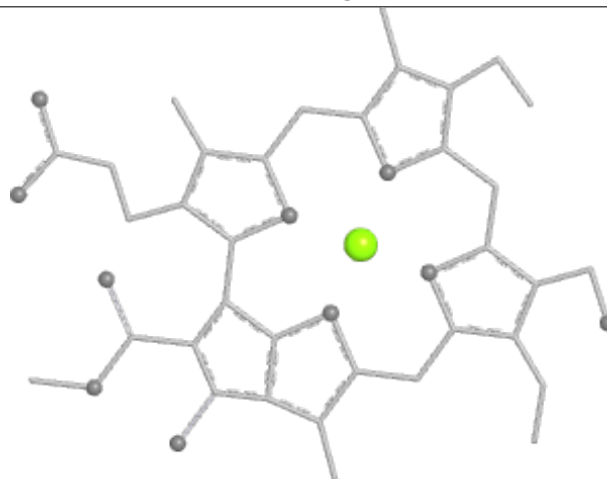
Bond lengths



Bond angles

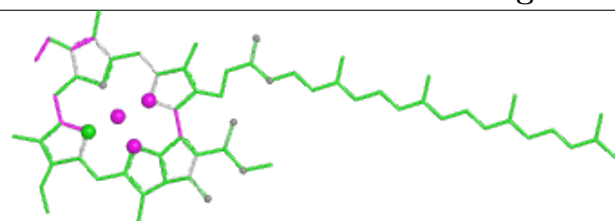


Torsions

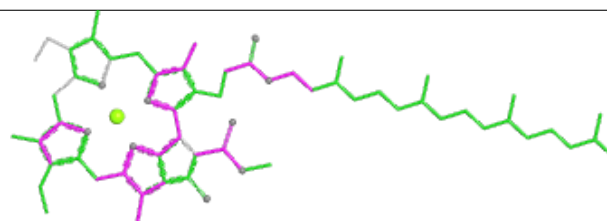


Rings

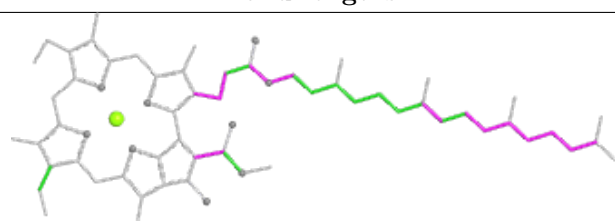
Ligand CLA B 602



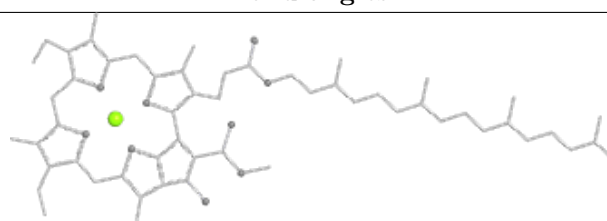
Bond lengths



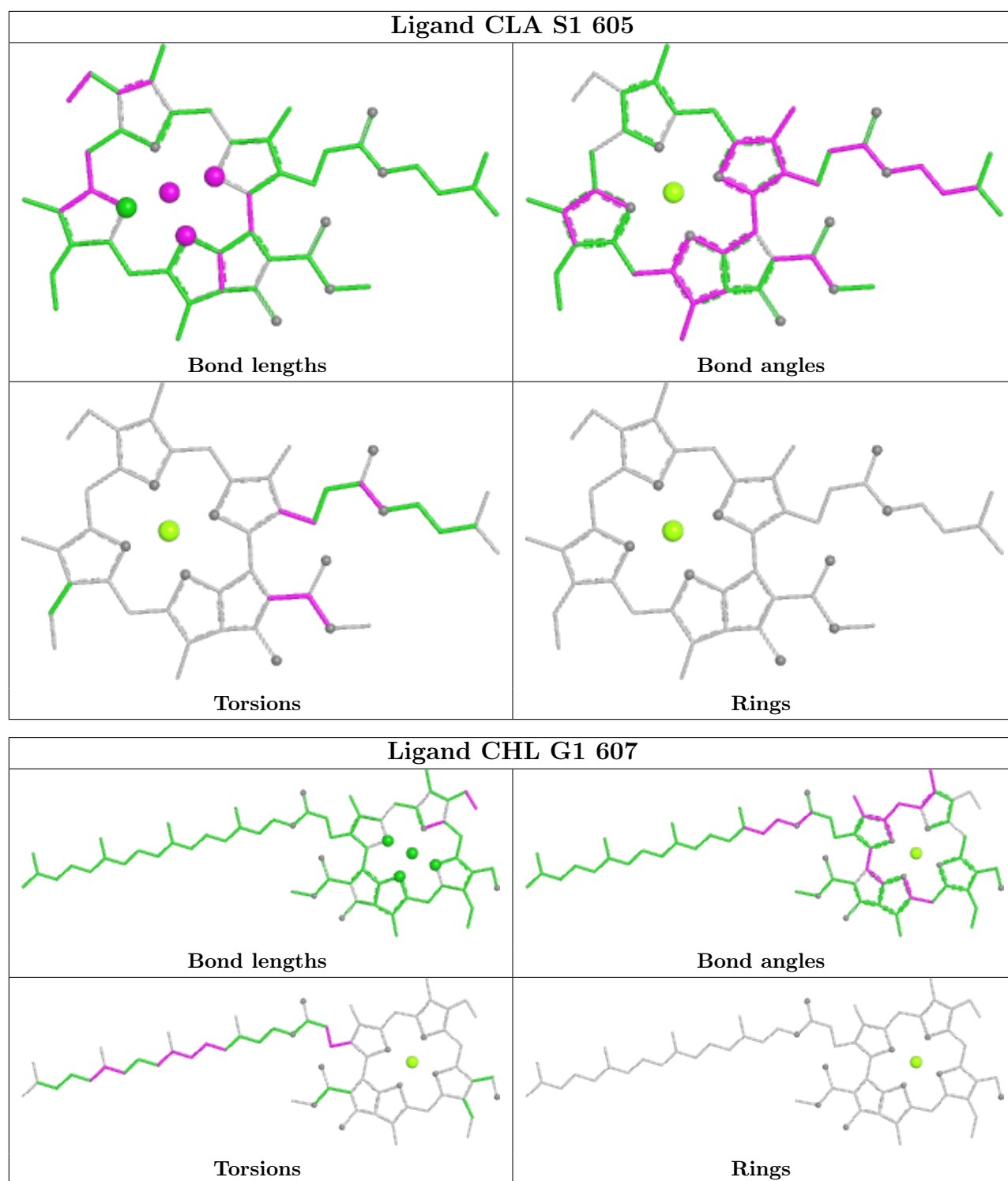
Bond angles

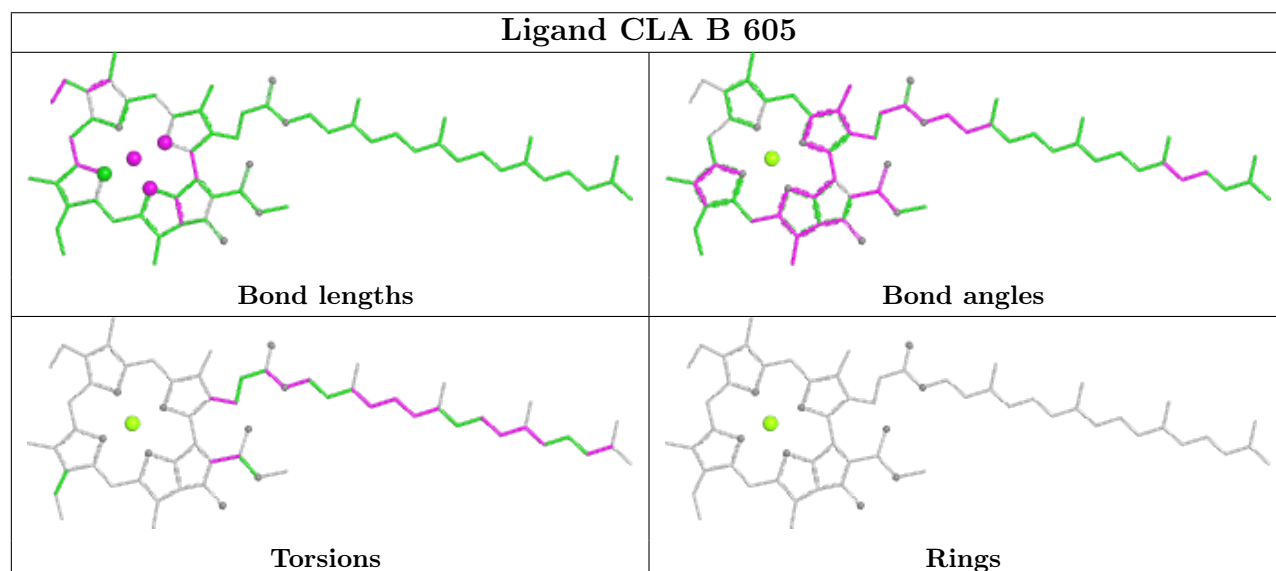
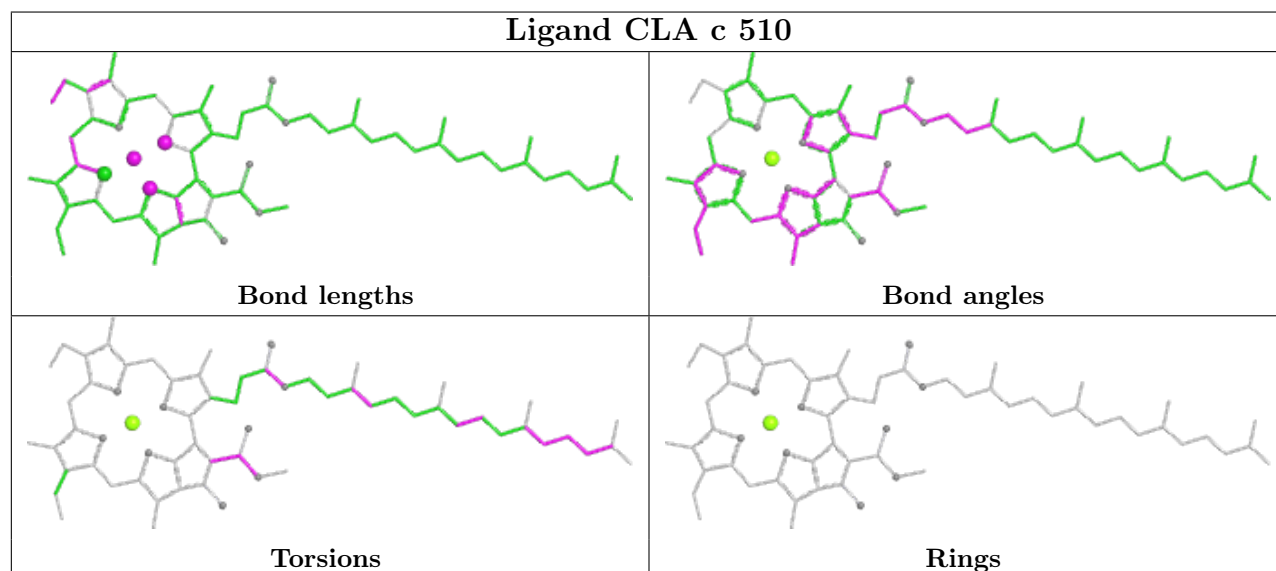
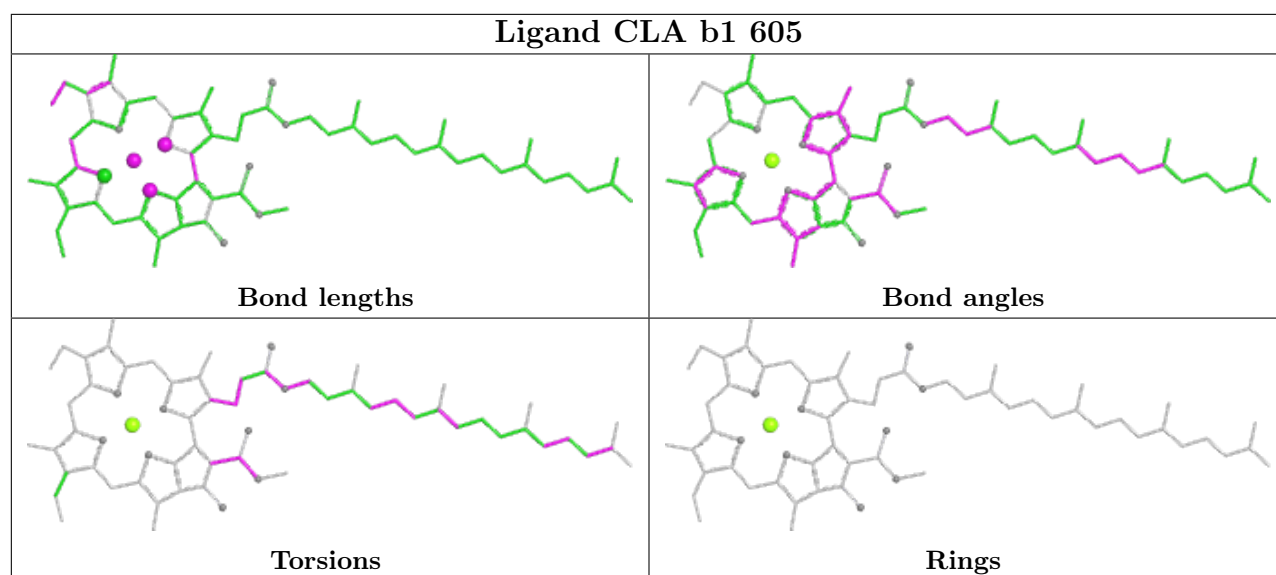


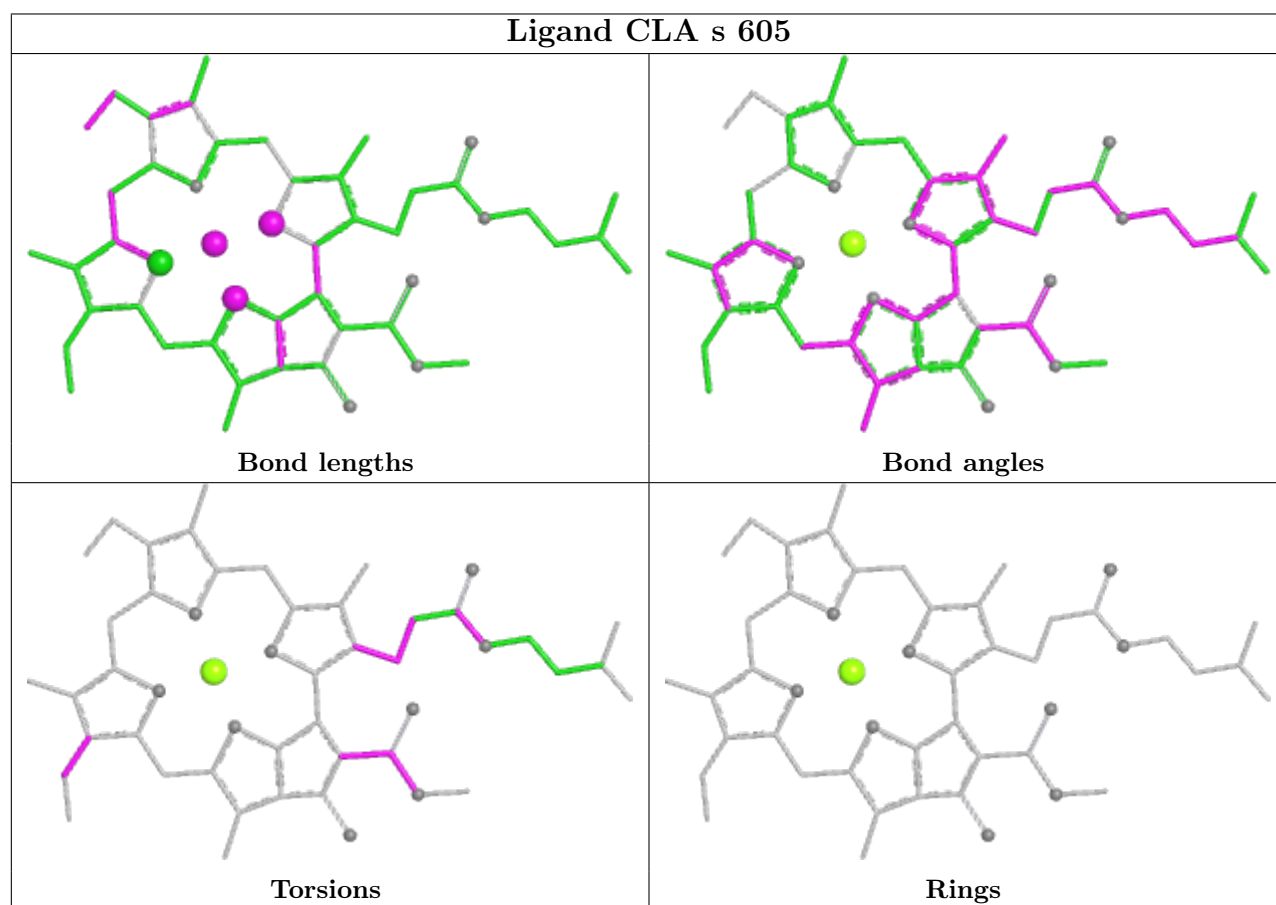
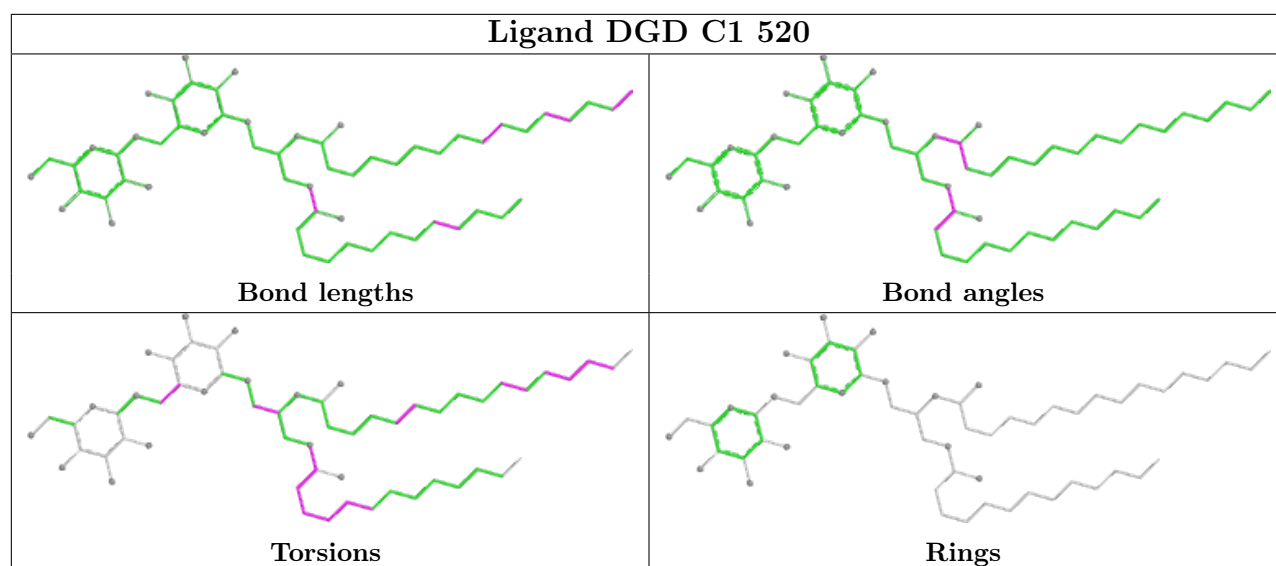
Torsions

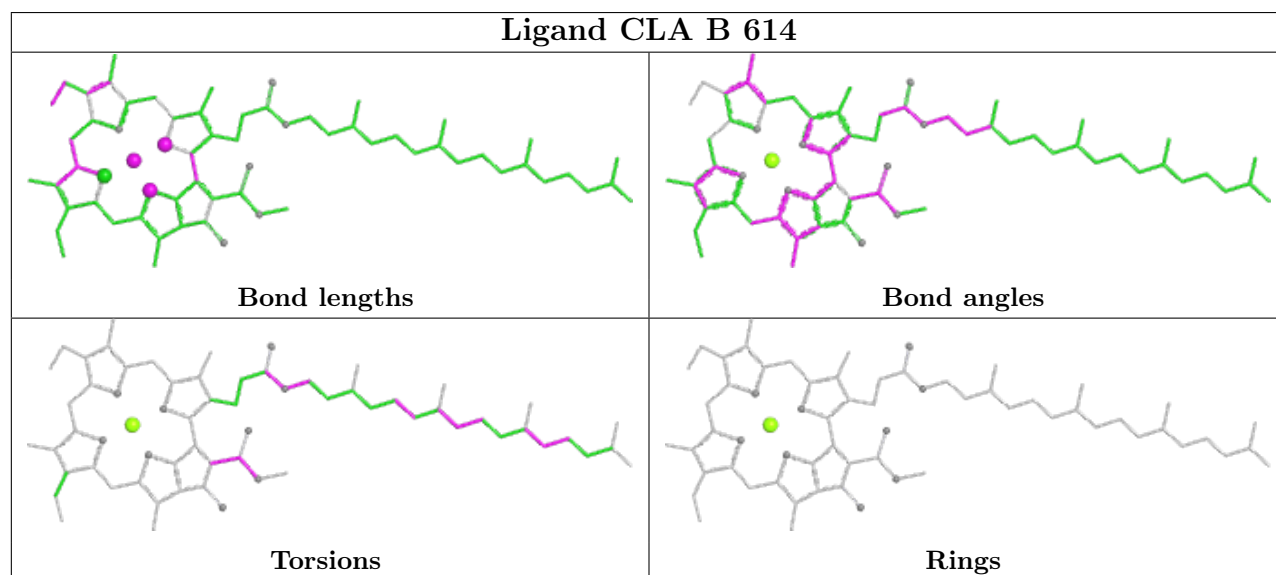
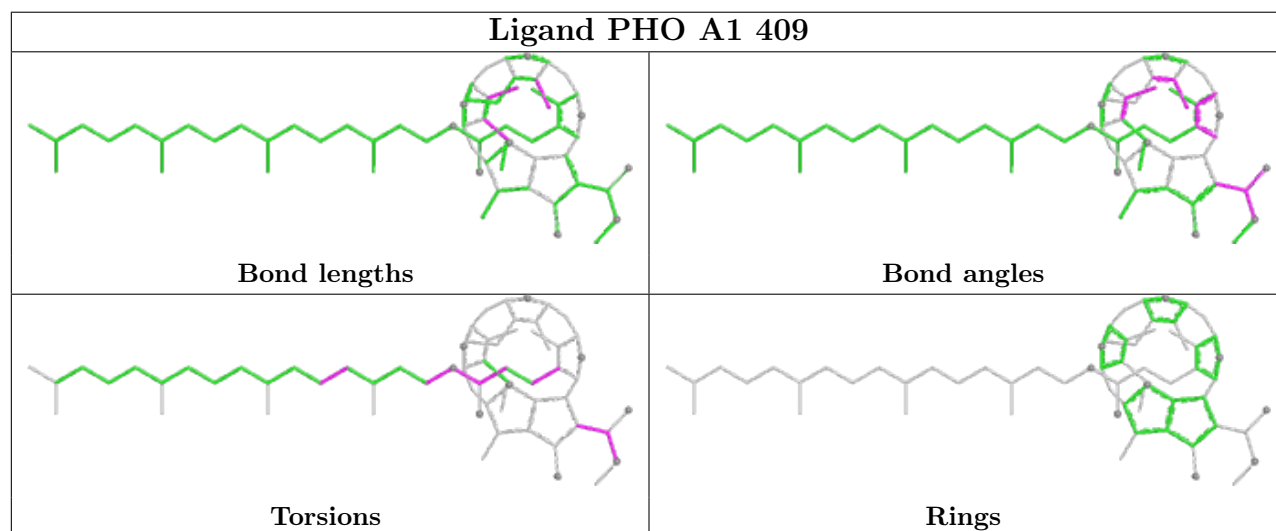
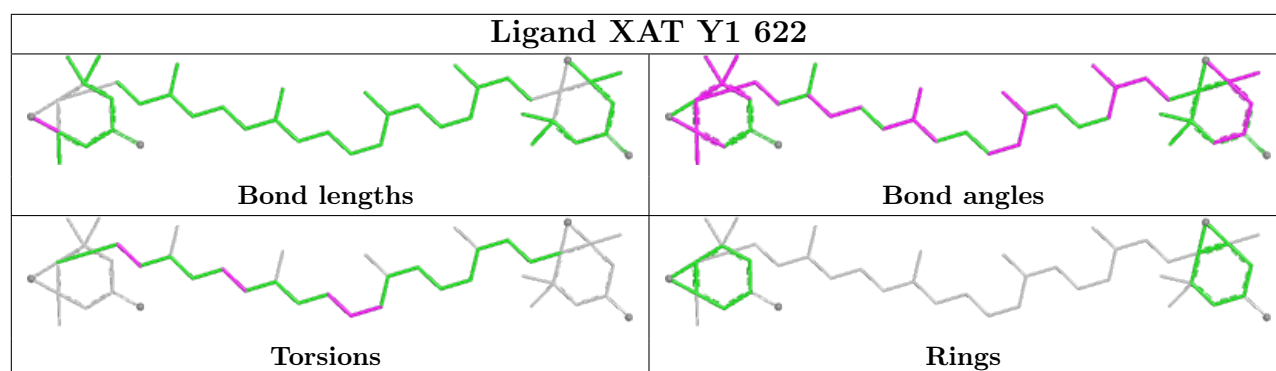


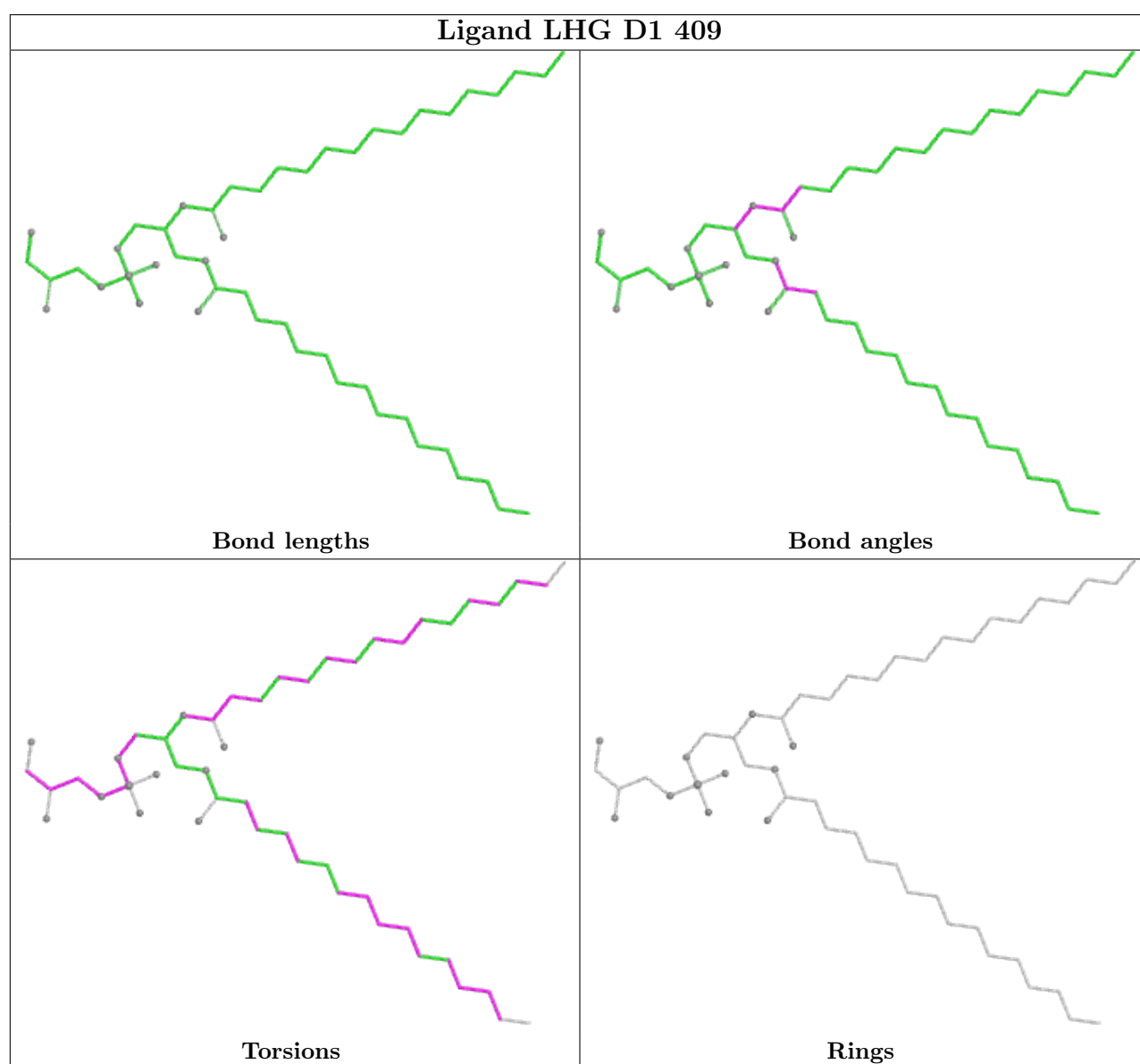
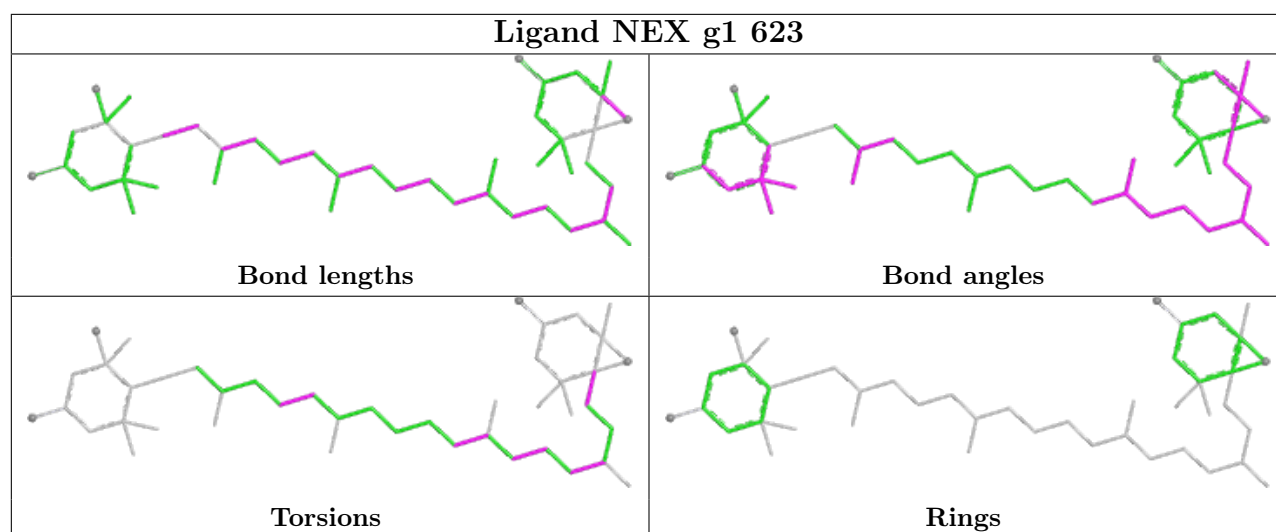
Rings

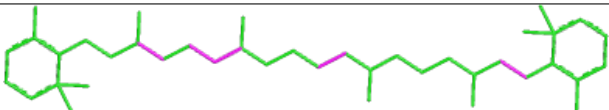
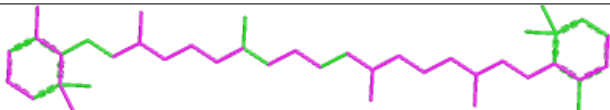
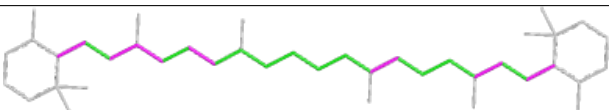
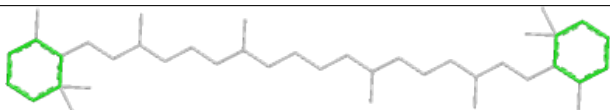


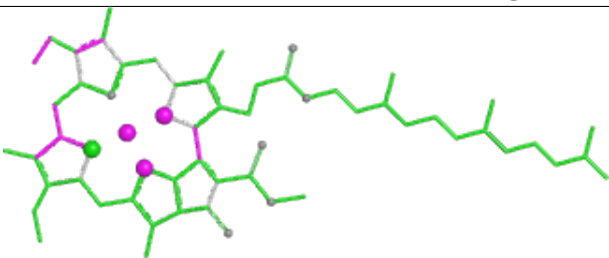
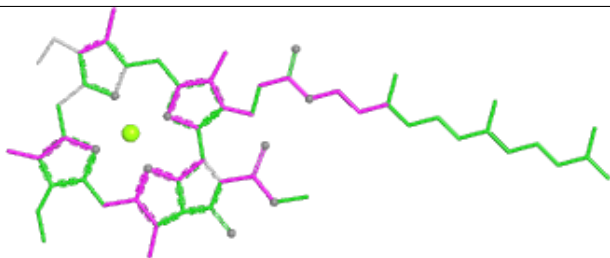
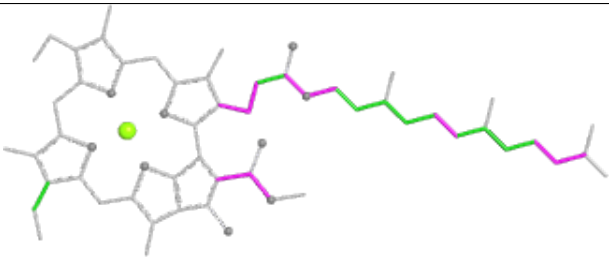
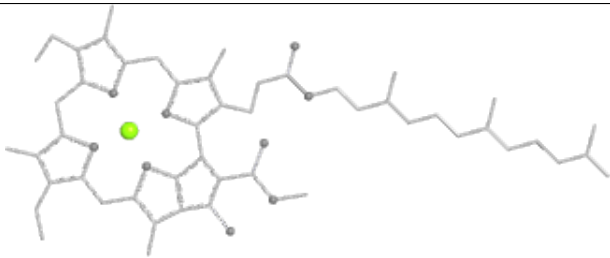


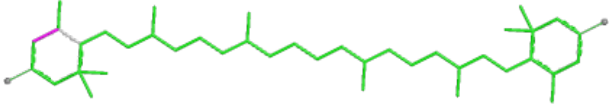
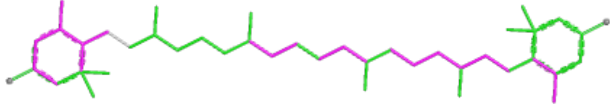
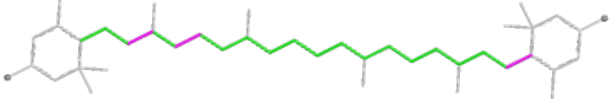
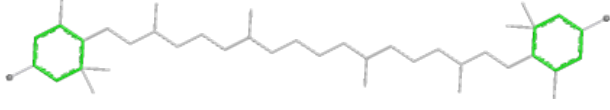


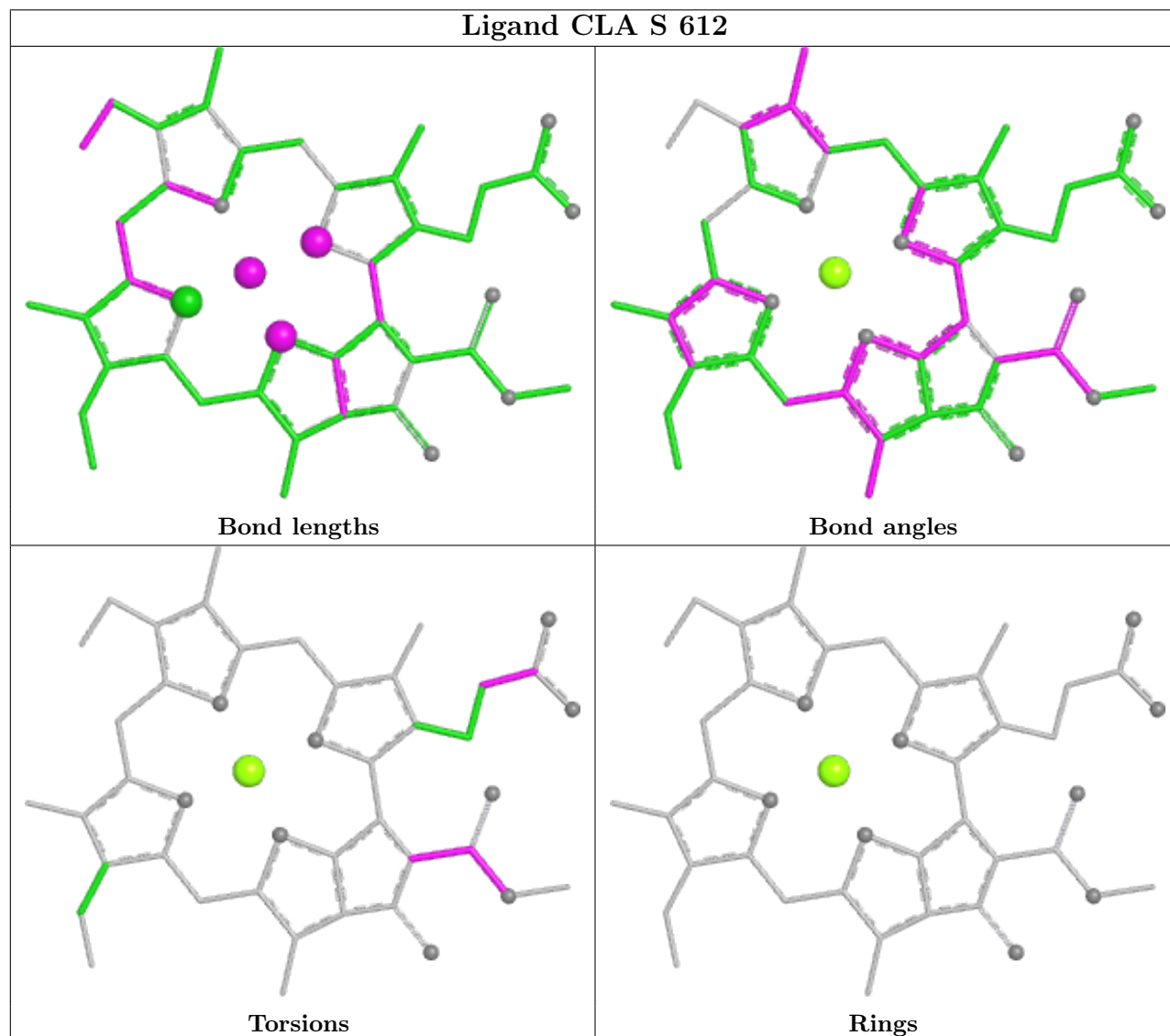
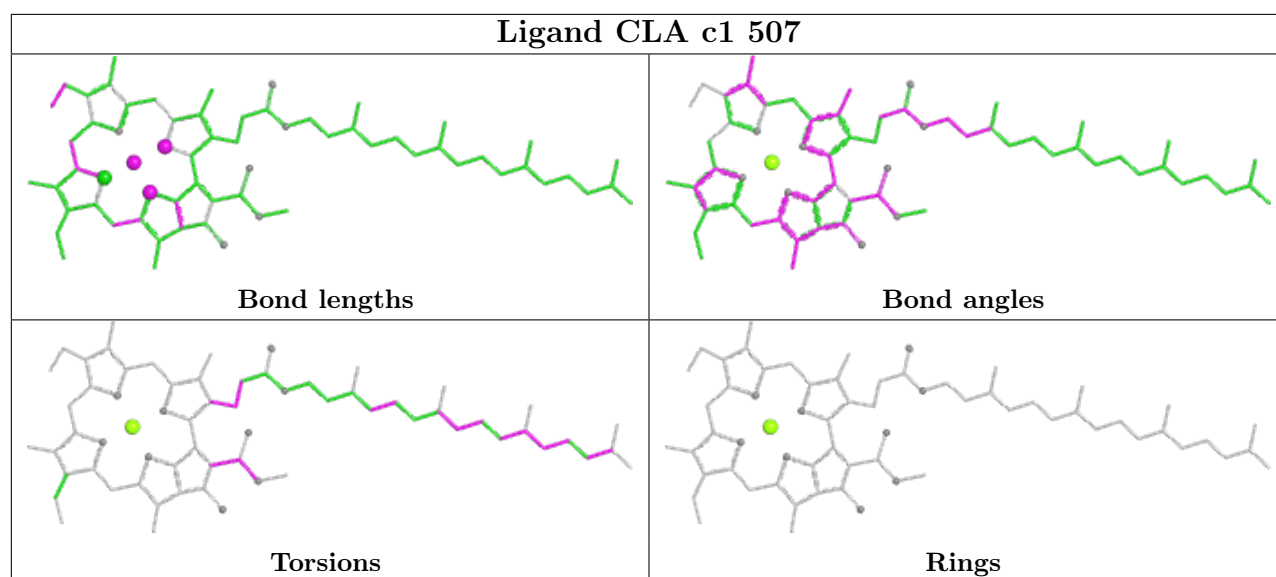


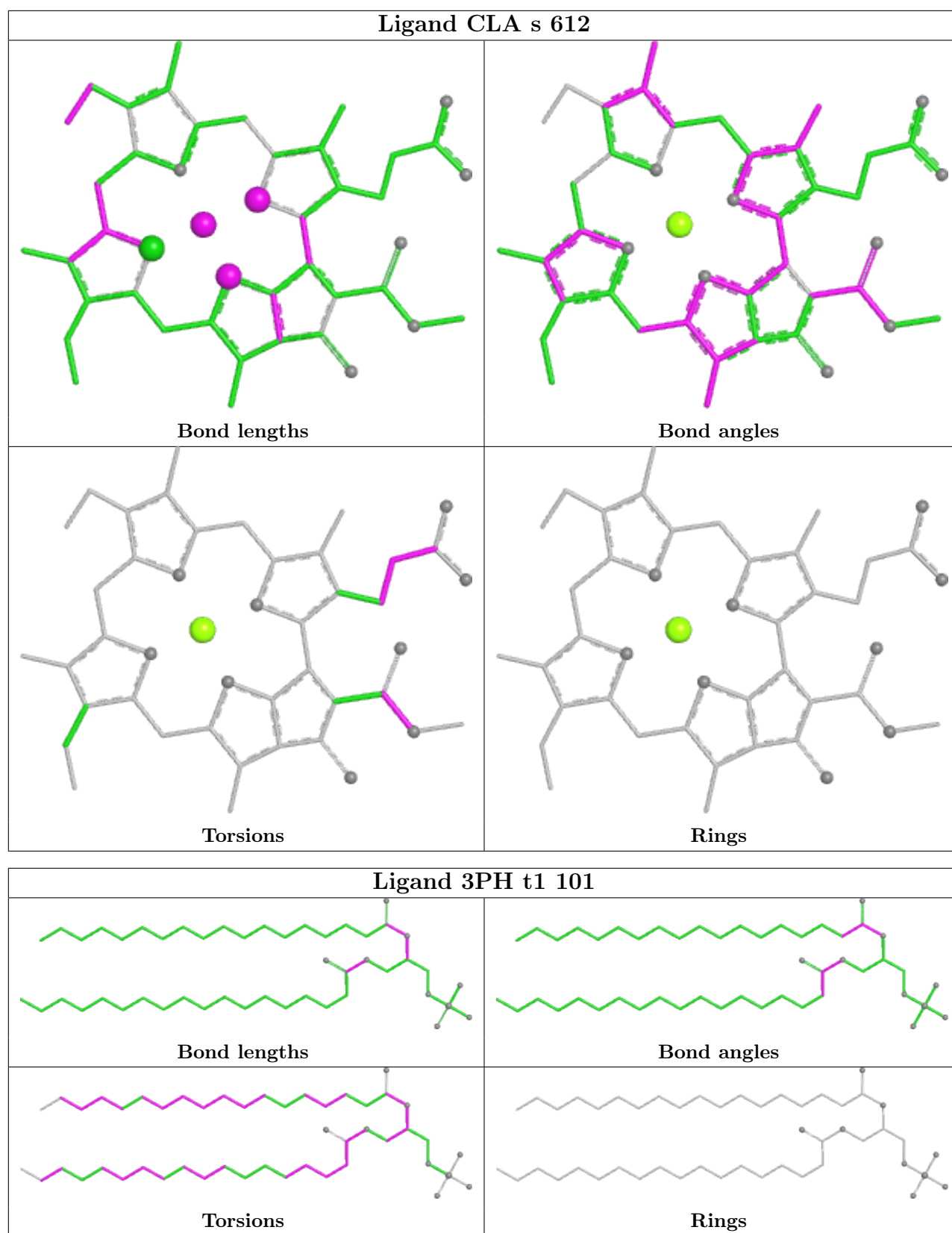


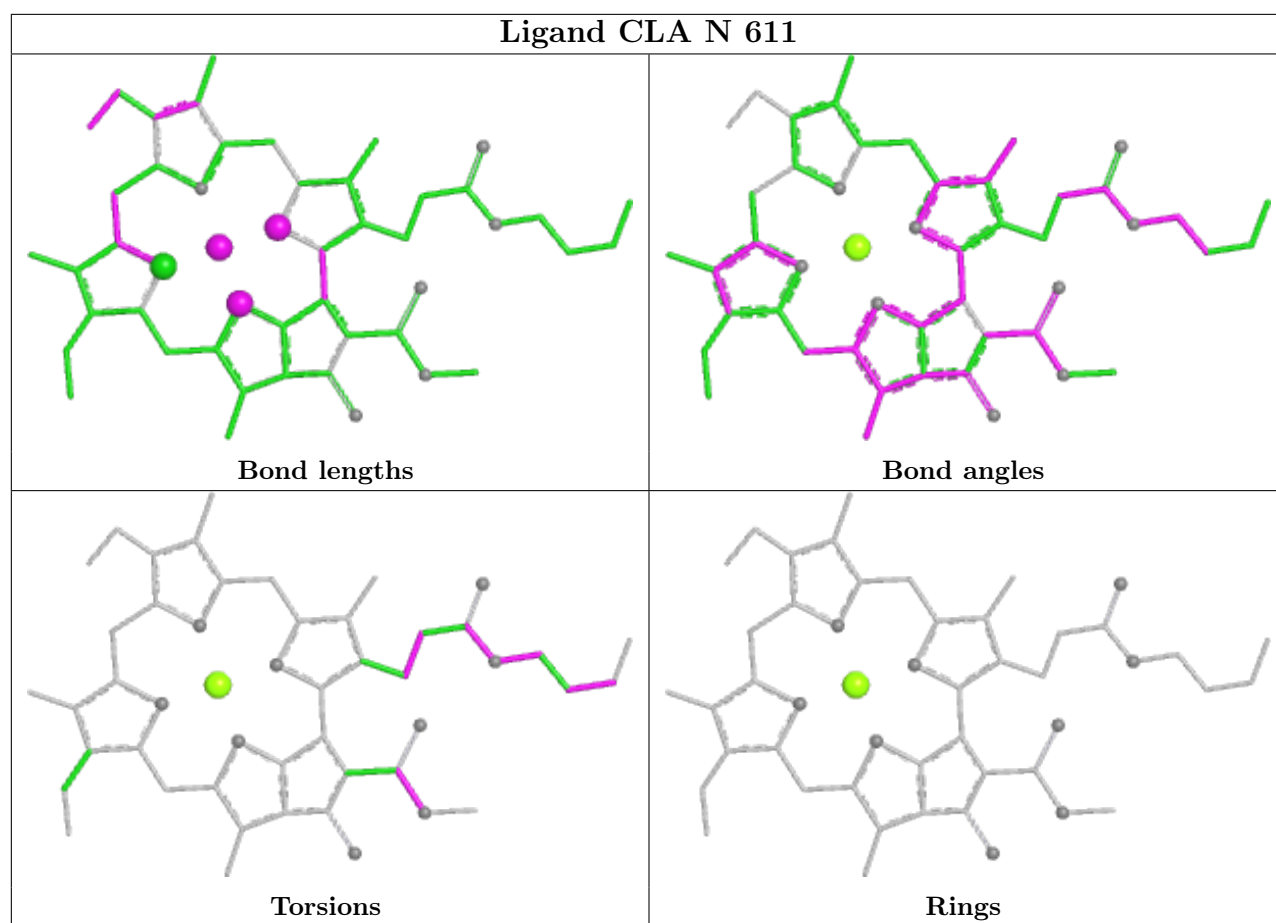
Ligand BCR C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

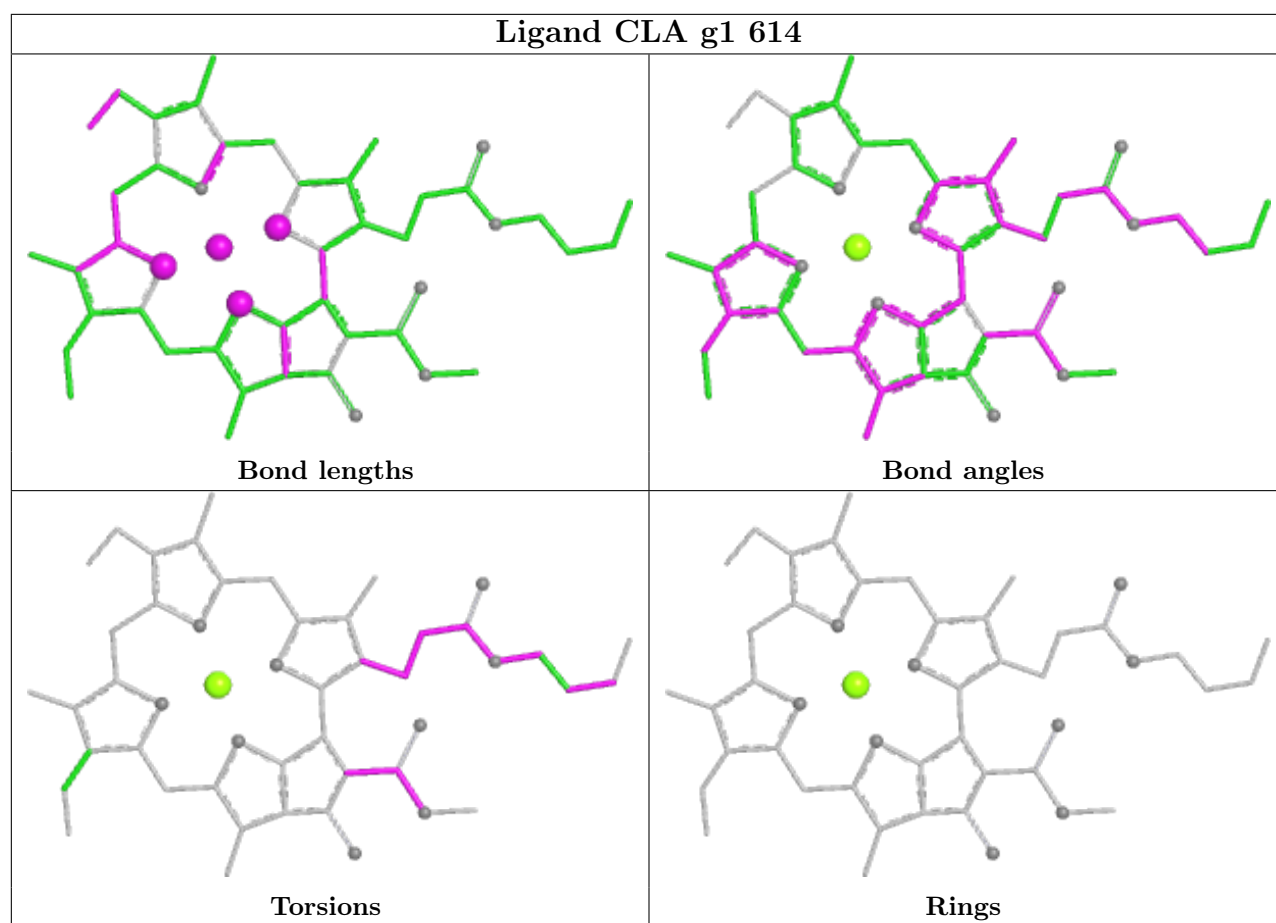
Ligand CLA r1 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

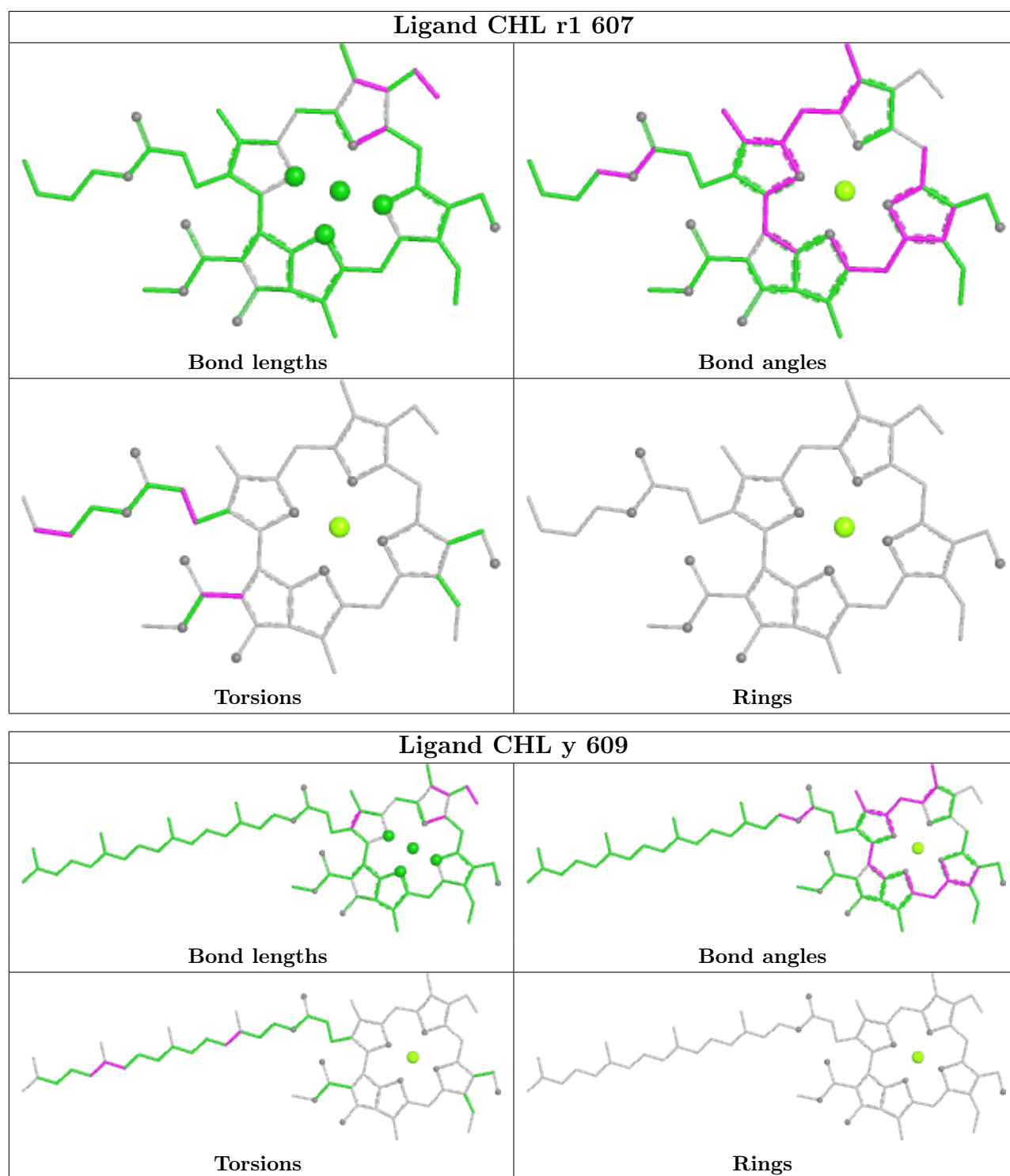
Ligand LUT n1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

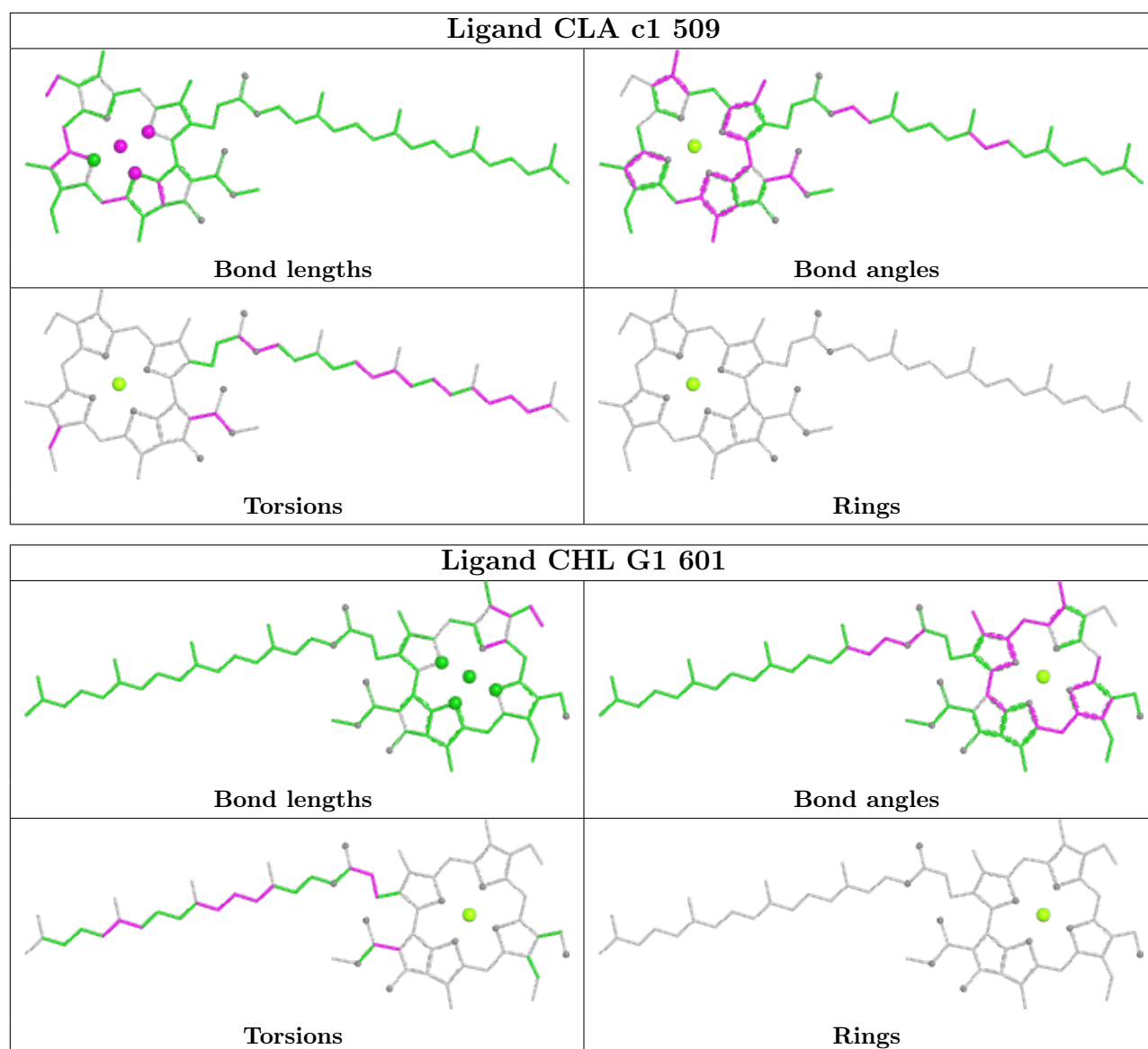


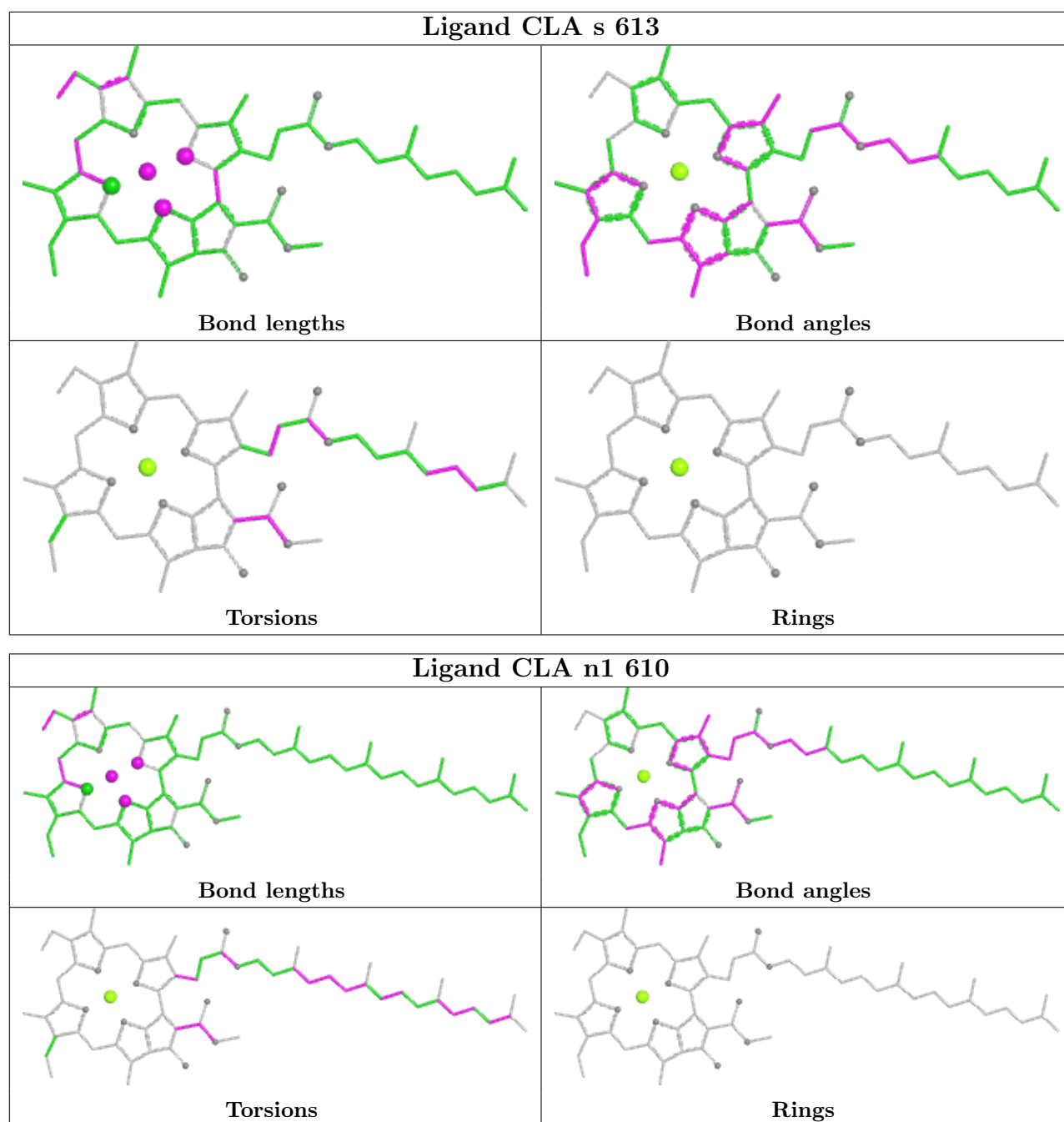












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	r1	1
22	R1	1
22	R	1
20	n1	1
20	n	1
21	G1	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.15
1	r1	110:PRO	C	126:GLU	N	13.08
1	R1	110:PRO	C	126:GLU	N	12.94
1	R	110:PRO	C	126:GLU	N	12.16
1	n1	57:PRO	C	58:PRO	N	3.54

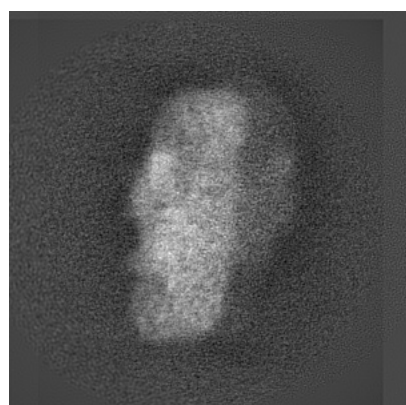
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13444. These allow visual inspection of the internal detail of the map and identification of artifacts.

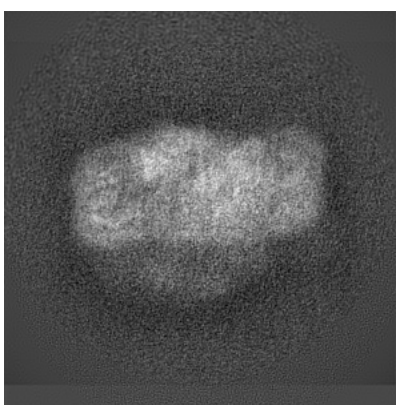
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

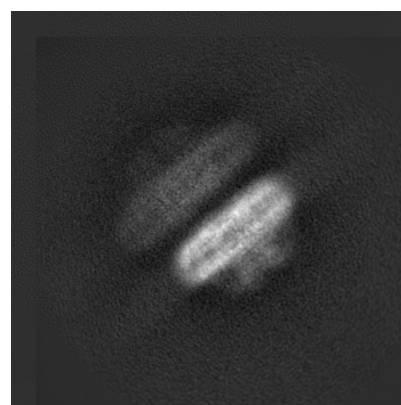
6.1.1 Primary map



X



Y

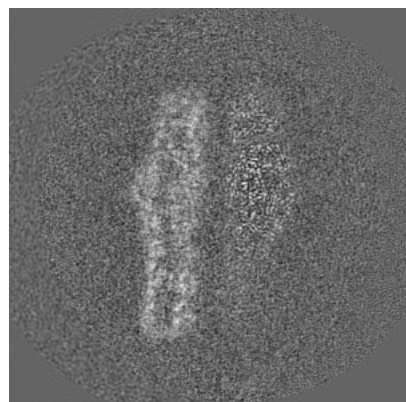


Z

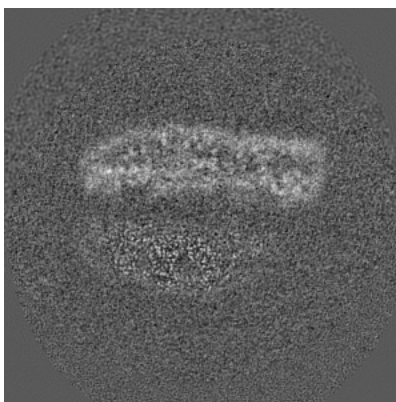
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

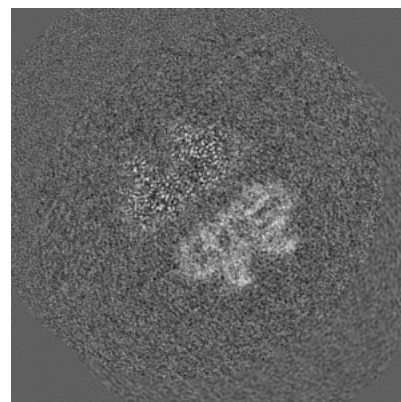
6.2.1 Primary map



X Index: 240



Y Index: 240

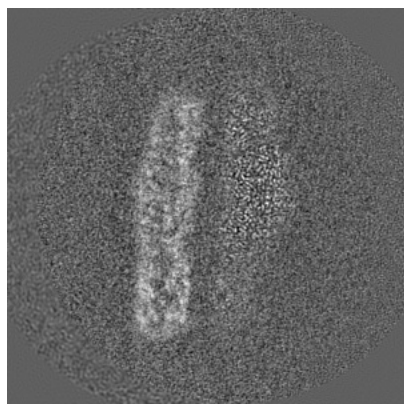


Z Index: 240

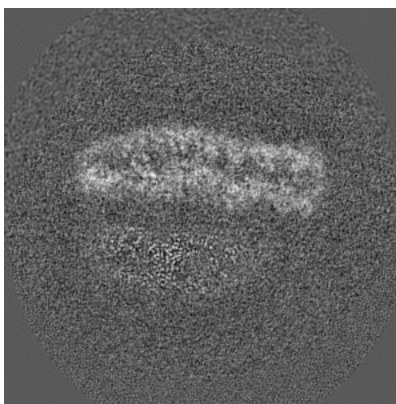
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

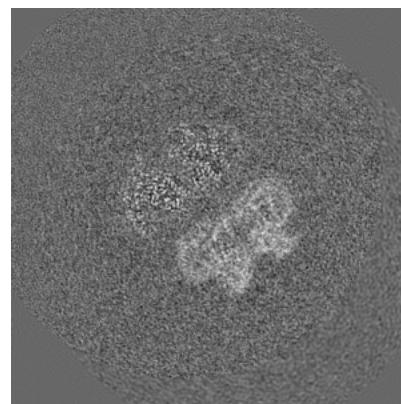
6.3.1 Primary map



X Index: 232



Y Index: 233

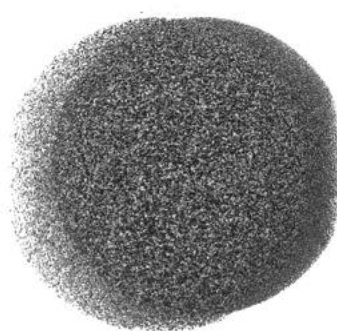


Z Index: 236

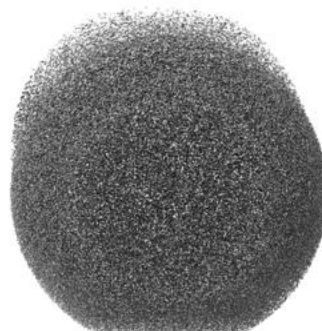
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

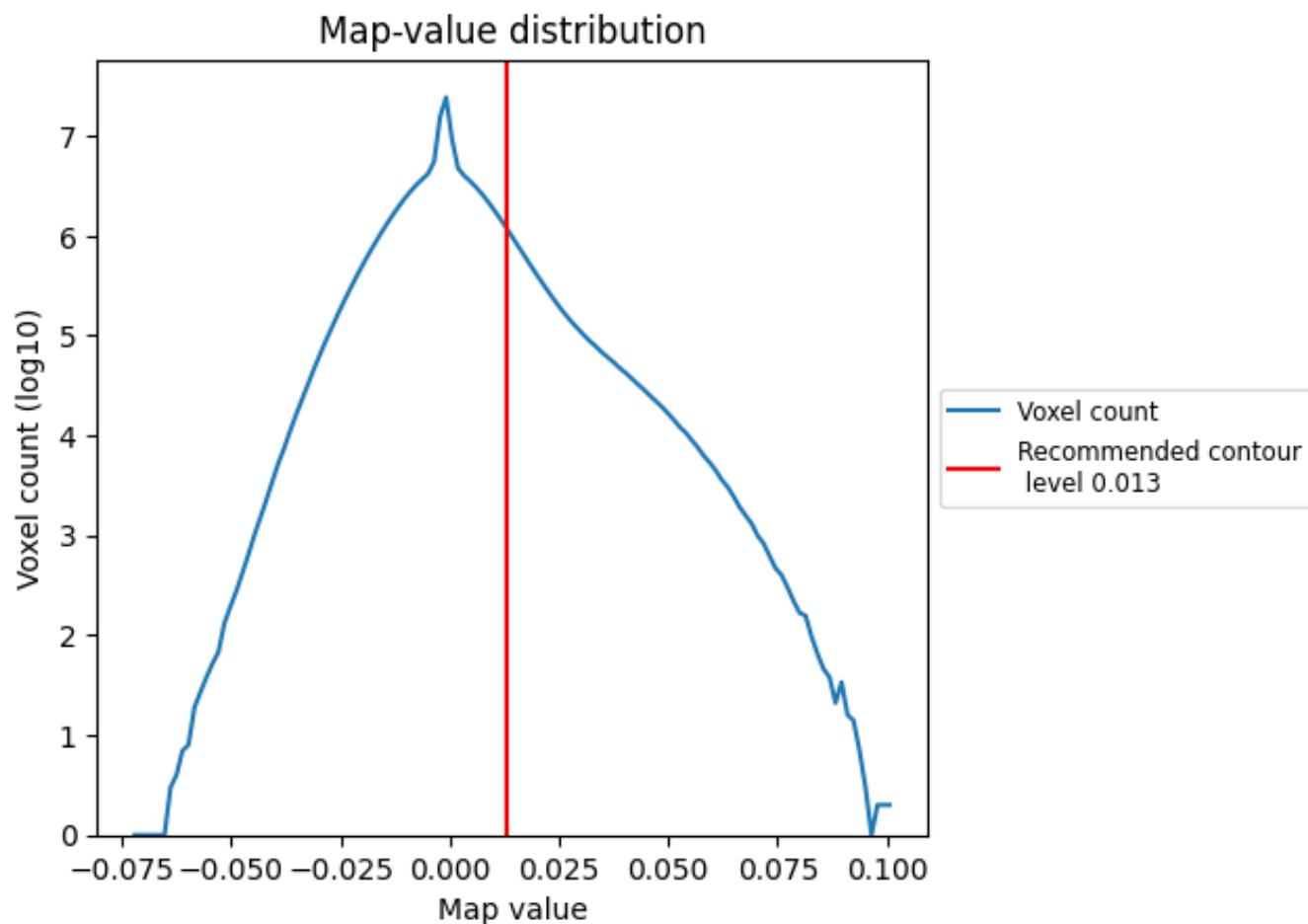
6.5 Mask visualisation

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

7 Map analysis [i](#)

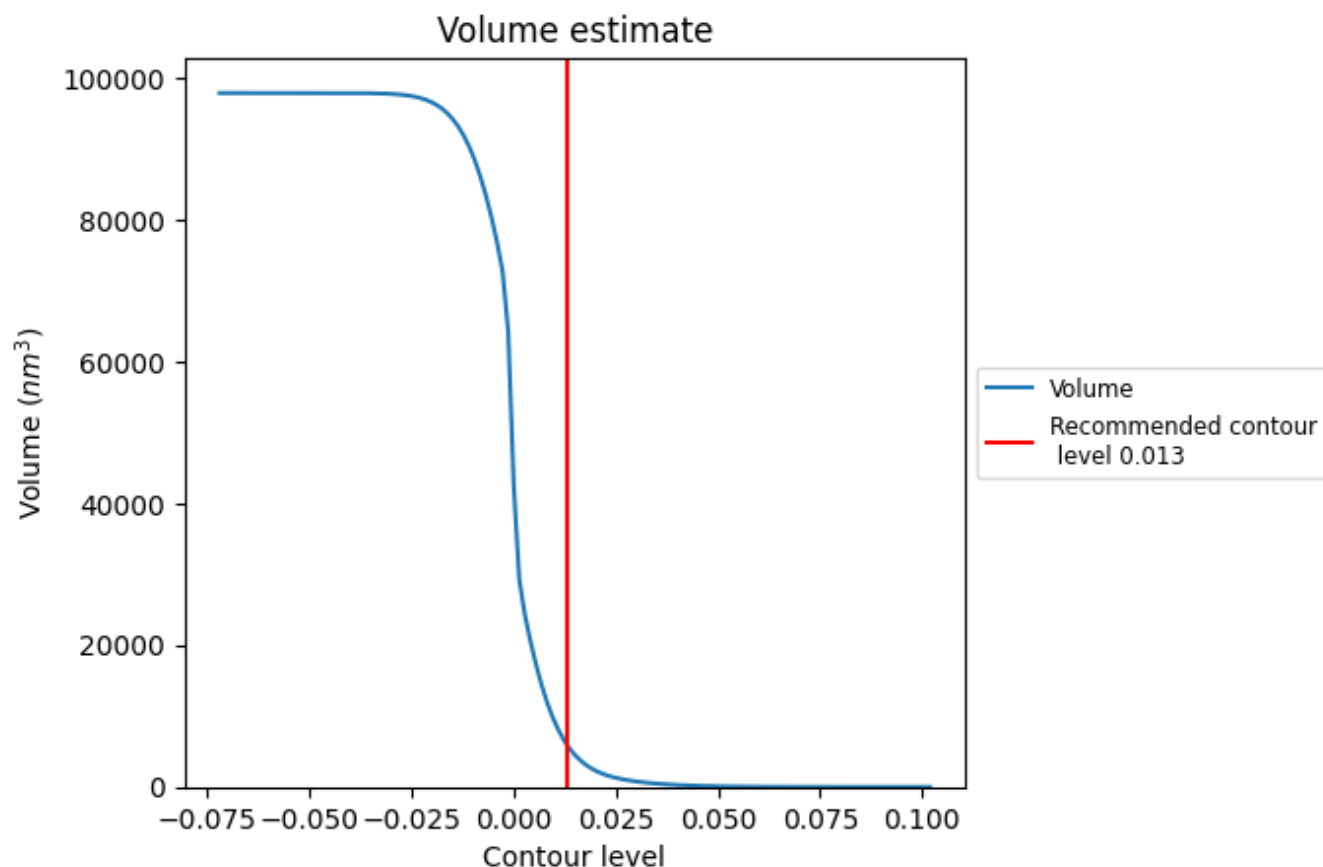
This section contains the results of statistical analysis of the map.

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.

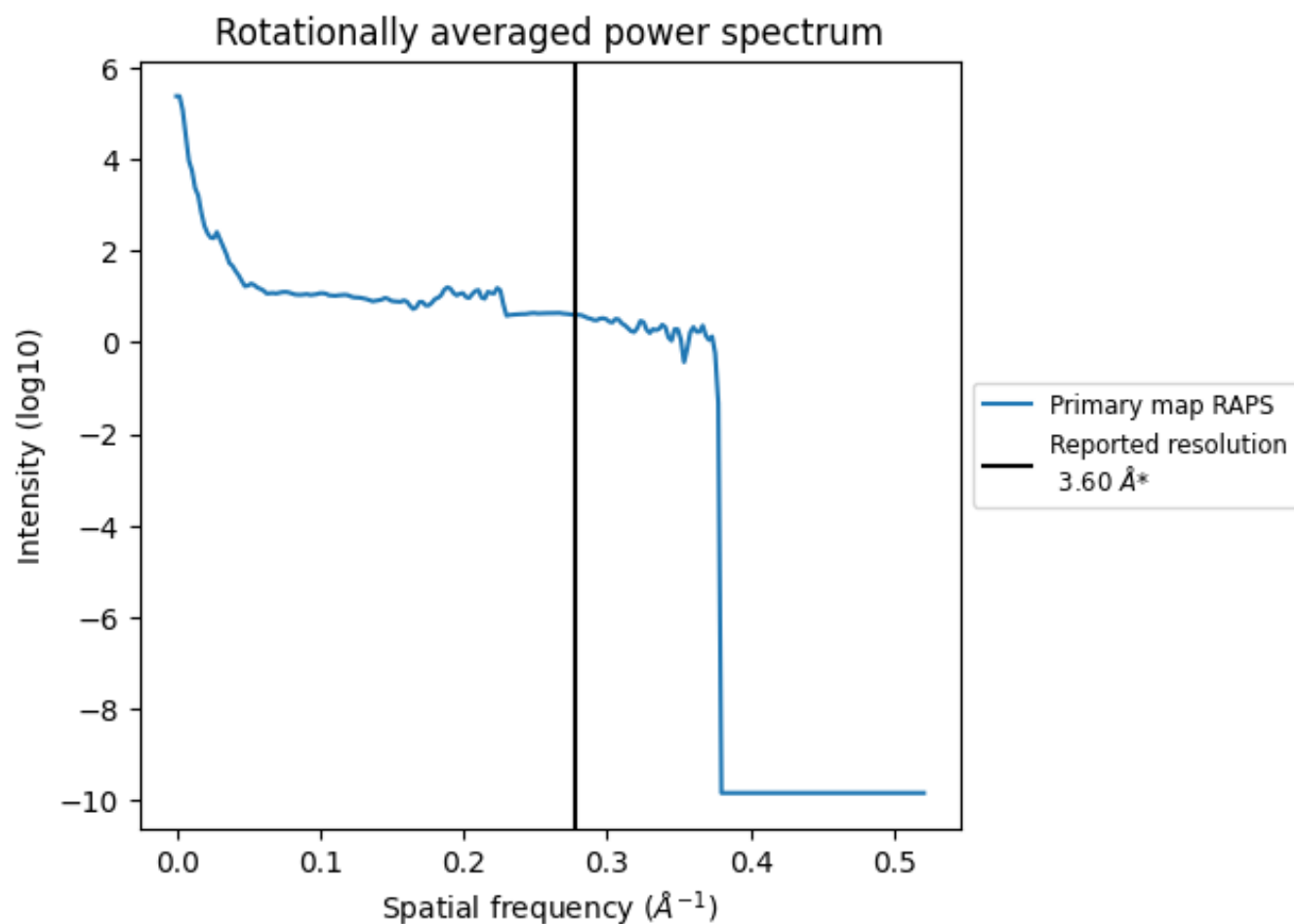
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5989 nm³; this corresponds to an approximate mass of 5410 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 ⓘ

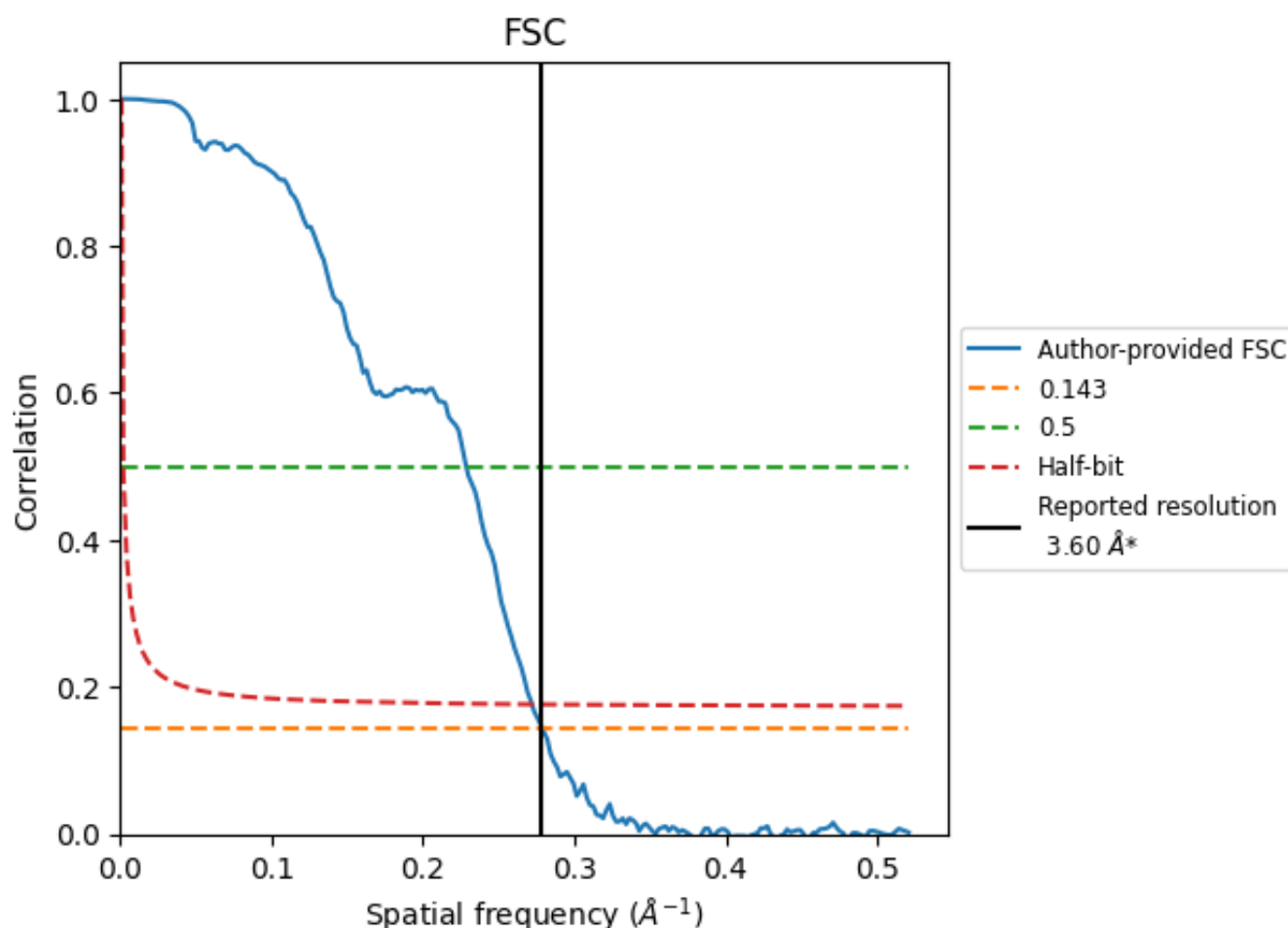


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

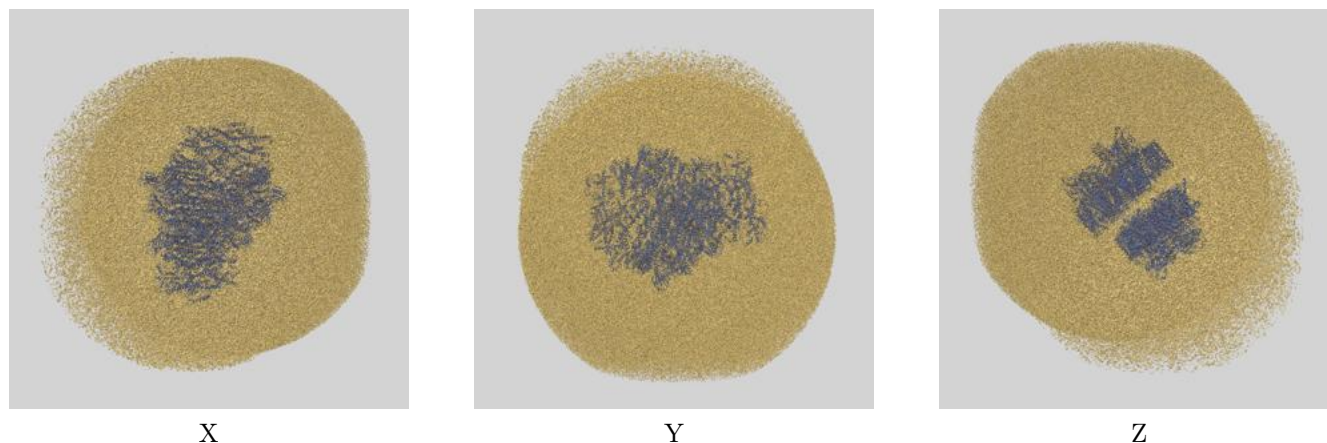
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.37	3.68
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

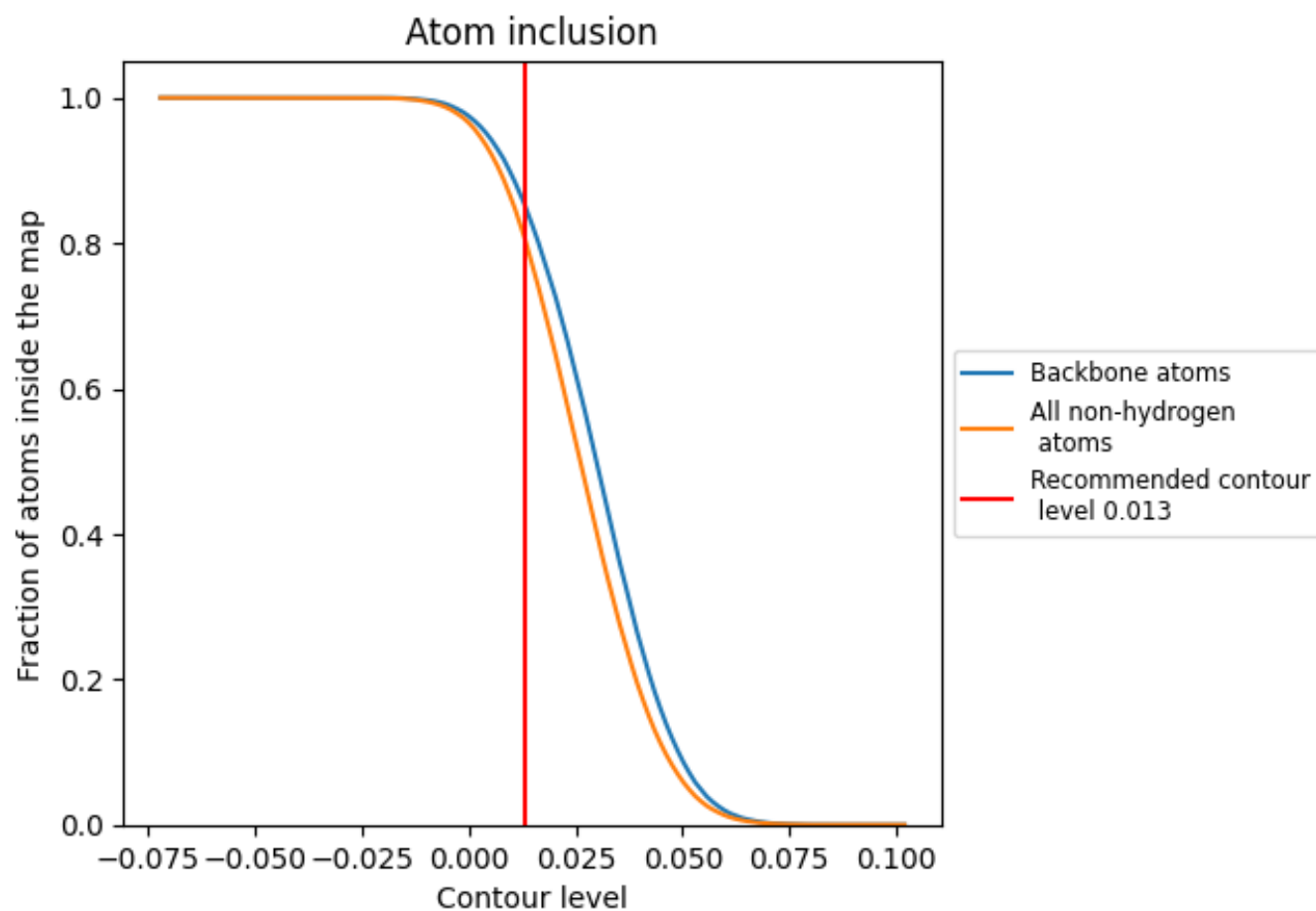
This section contains information regarding the fit between EMDB map EMD-13444 and PDB model 7PIN. Per-residue inclusion information can be found in section [3](#) on page [74](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.013 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 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.