wwPDB EM Validation Summary Report (i)

Apr 30, 2024 – 03:49 PM JST

PDB ID	:	8WA2
EMDB ID	:	EMD-37389
Title	:	cryo-EM structure of native mastigonemes isolated from Chlamydomonas reinhardtii at 3.0 angstrom resolution
Authors	:	Huang, J.; Tao, H.; Chen, J.; Pan, J.; Yan, C.; Yan, N.
Deposited on	:	2023-09-06
Resolution	:	3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

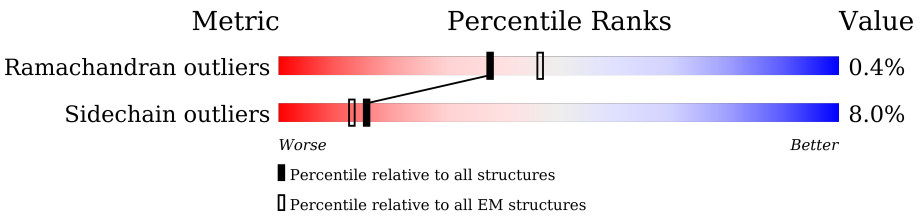
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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 <=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	1987	86% 10% •
1	B	1987	87% 9% •
1	C	1987	18% 69% 6% 25%
1	D	1987	23% 71% 7% 21%
1	E	1987	36% 66% 7% 27%
1	F	1987	35% 66% 7% 27%
2	G	64	8% 38% 62%
2	H	64	8% 20% 27% 53%
2	I	64	9% 19% 33% • 47%

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Mol	Chain	Length	Quality of chain
3	0	3	67% 33%
3	0A	3	67% 33%
3	1	3	67% 33%
3	2	3	67% 33%
3	8C	3	100%
3	9C	3	33% 67%
3	BC	3	33% 67%
3	CC	3	33% 67%
3	DD	3	67% 33%
3	EB	3	100% 67% 33%
3	ED	3	67% 33%
3	FD	3	67% 33%
3	GC	3	67% 33%
3	HA	3	33% 67%
3	HC	3	67% 33%
3	IA	3	67% 33%
3	IC	3	67% 33%
3	ID	3	67% 33%
3	J	3	100%
3	K	3	100%
3	KD	3	67% 33%
3	LB	3	100%
3	LC	3	100%
3	MA	3	100%
3	NA	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	NC	3	100%
3	O	3	67% 33%
3	OA	3	67% 33%
3	OB	3	100% 100%
3	P	3	67% 33%
3	PB	3	33% 67% 33%
3	Q	3	67% 33%
3	QB	3	33% 67% 33%
3	QD	3	100%
3	RA	3	67% 33%
3	RB	3	67% 33% 67%
3	SB	3	100%
3	T	3	67% 33%
3	TA	3	33% 67%
3	TB	3	67% 33%
3	TC	3	100%
3	TD	3	100%
3	UB	3	67% 33%
3	V	3	67% 33%
3	WC	3	33% 67%
3	XA	3	33% 67% 33%
3	ZA	3	67% 33%
3	aD	3	33% 100%
3	b	3	67% 33%
3	bD	3	100%

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Mol	Chain	Length	Quality of chain
3	cA	3	33% 67%
3	dC	3	67% 33%
3	e	3	67% 33%
3	eC	3	100%
3	hB	3	100% 100%
3	iD	3	67% 33%
3	jA	3	33% 67%
3	kA	3	100%
3	l	3	100%
3	lC	3	100%
3	lD	3	67% 100%
3	m	3	100%
3	mD	3	33% 67% 33%
3	nD	3	33% 100%
3	oB	3	67% 33% 67%
3	oC	3	33% 100%
3	oD	3	33% 67% 33%
3	pC	3	33% 67%
3	pD	3	67% 33% 67%
3	qC	3	100%
3	qD	3	67% 100%
3	rA	3	100%
3	rB	3	67% 67% 33%
3	rC	3	100% 67% 33%
3	rD	3	67% 67% 33%

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Mol	Chain	Length	Quality of chain
3	sB	3	33% 100%
3	sC	3	100% 33% 67%
3	t	3	67% 33%
3	tB	3	33% 100%
3	tC	3	33% 67% 33%
3	uA	3	67% 33%
3	uB	3	67% 33%
3	uC	3	67% 67% 33%
3	vA	3	67% 33%
3	vB	3	33% 67% 33%
3	w	3	67% 33%
3	wA	3	67% 33%
3	wB	3	100%
3	x	3	33% 67%
3	xA	3	100%
3	xB	3	67% 33%
3	y	3	67% 33%
3	yA	3	67% 33%
3	z	3	67% 33%
3	zA	3	100%
4	AD	4	50% 50%
4	DC	4	50% 50%
4	JA	4	75% 25%
4	JB	4	50% 75% 25%
4	L	4	75% 25%

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Mol	Chain	Length	Quality of chain
4	LD	4	50% 50%
4	MD	4	100%
4	NB	4	50% 50% 50%
4	OC	4	75% 25%
4	OD	4	50% 50%
4	PC	4	75% 25%
4	RC	4	75% 25%
4	RD	4	50% 50%
4	SD	4	50% 50%
4	UA	4	75% 25%
4	UC	4	100%
4	VA	4	75% 25%
4	VC	4	75% 25%
4	VD	4	50% 50%
4	W	4	75% 25%
4	X	4	75% 25%
4	YC	4	50% 50%
4	Z	4	25% 75%
4	ZD	4	25% 75% 25%
4	aA	4	100%
4	bA	4	100%
4	c	4	75% 25%
4	cC	4	50% 50% 50%
4	d	4	25% 75%
4	eA	4	100%

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Mol	Chain	Length	Quality of chain
4	g	4	75% 25%
4	gD	4	25% 50% 50%
4	iA	4	50% 50%
4	jC	4	75% 25%
4	k	4	100%
4	kD	4	25% 100%
4	mB	4	75% 50% 50%
4	nC	4	25% 50% 50%
4	pA	4	100%
4	qB	4	75% 25% 75%
4	r	4	100%
4	tA	4	50% 50%
4	v	4	75% 25%
5	BD	5	60% 40%
5	EC	5	40% 60%
5	KA	5	40% 60%
5	M	5	20% 80%
6	0B	3	33% 33% 33% 33%
6	0C	3	100% 33% 67%
6	1C	3	100% 67% 33%
6	2C	3	100% 33% 67%
6	3A	3	67% 33%
6	3B	3	100%
6	3D	3	100% 100%
6	4B	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	5	3	67% 33%
6	5B	3	33% 67%
6	6A	3	33% 67%
6	6C	3	100% 100%
6	6D	3	100%
6	7A	3	33% 67%
6	7D	3	33% 67%
6	8	3	33% 67%
6	8A	3	100%
6	8D	3	100%
6	9	3	33% 67%
6	9B	3	33% 67%
6	AA	3	33% 67%
6	CB	3	33% 67%
6	CD	3	33% 33% 33%
6	EA	3	33% 67%
6	FC	3	100%
6	GD	3	33% 67%
6	JC	3	33% 67%
6	LA	3	33% 33% 33%
6	ME	3	67% 33%
6	N	3	33% 33% 33%
6	OE	3	67% 33%
6	PA	3	67% 33%
6	R	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	XB	3	33% 33% 33% 33%
6	ZE	3	33% 67%
6	aB	3	33% 67%
6	bB	3	100%
6	bE	3	67% 33%
6	cB	3	100%
6	gB	3	67% 33%
6	mE	3	33% 67%
6	nE	3	33% 67%
6	oE	3	33% 67%
6	uD	3	100% 33% 33% 33%
6	xC	3	100% 67% 33%
6	xD	3	100% 33% 67%
6	yD	3	100% 100%
6	zD	3	100% 33% 67%
7	HD	4	50% 50%
7	KC	4	50% 50%
7	QA	4	50% 50%
7	S	4	25% 75%
7	UD	4	75% 25%
7	WD	4	75% 25%
7	XC	4	75% 25%
7	ZC	4	75% 25%
7	dA	4	50% 50%
7	f	4	25% 75%

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Mol	Chain	Length	Quality of chain
7	fA	4	100%
7	h	4	75% 25%
8	JD	5	80% 20%
8	MC	5	40% 60%
8	SA	5	80% 20%
8	U	5	40% 60%
9	ND	2	50% 50%
9	QC	2	100%
9	WA	2	100%
9	Y	2	100%
9	YD	2	100%
9	bC	2	100%
9	hA	2	50% 50%
9	j	2	50% 50%
10	1A	5	20% 80%
10	3	5	40% 60%
10	MB	5	80% 40% 60%
10	PD	5	60% 40%
10	SC	5	80% 20%
10	VB	5	20% 60% 40%
10	YA	5	80% 20%
10	a	5	20% 80%
10	jD	5	20% 60% 40%
10	mC	5	40% 40% 60%
10	pB	5	100% 60% 40%

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Mol	Chain	Length	Quality of chain
10	sA	5	60% 40%
10	sD	5	60% 80% 20%
10	u	5	60% 40%
10	vC	5	40% 40% 60%
10	yB	5	80% 20%
11	XD	3	100%
11	aC	3	33% 67%
11	gA	3	33% 67%
11	i	3	100%
12	FB	5	100% 40% 40% 20%
12	IB	5	80% 20% 60% 20%
12	cD	5	20% 60% 20% 20%
12	fC	5	20% 40% 40% 20%
12	fD	5	20% 60% 20%
12	iB	5	100% 60% 20% 20%
12	iC	5	20% 80% 20%
12	lA	5	40% 40% 20%
12	lB	5	80% 40% 40% 20%
12	n	5	40% 40% 20%
12	oA	5	40% 40% 20%
12	q	5	20% 60% 20%
13	0D	4	100% 75% 25%
13	1B	4	75% 25%
13	2A	4	75% 25%
13	2B	4	50% 50%

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Mol	Chain	Length	Quality of chain
13	3C	4	100%, 50%, 50%
13	4	4	25%, 50%, 25%
13	4A	4	50%, 50%
13	5A	4	50%, 50%
13	6	4	50%, 50%
13	6B	4	50%, 50%
13	7	4	50%, 50%
13	9A	4	50%, 50%
13	BA	4	50%, 50%
13	GB	4	100%, 75%, 25%
13	WB	4	25%, 25%, 50%, 25%
13	YB	4	50%, 50%
13	ZB	4	75%, 25%
13	dB	4	50%, 50%
13	dD	4	25%, 75%, 25%
13	gC	4	25%, 50%, 25%, 25%
13	jB	4	100%, 50%, 25%, 25%
13	mA	4	50%, 25%, 25%
13	o	4	50%, 25%, 25%
13	tD	4	75%, 25%, 50%, 25%
13	vD	4	75%, 50%, 50%
13	wC	4	75%, 25%, 50%, 25%
13	wD	4	50%, 25%, 75%
13	yC	4	50%, 50%, 50%
13	zB	4	25%, 75%, 25%

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Mol	Chain	Length	Quality of chain
13	zC	4	100%; 25%, 75%
14	HB	4	100%; 50%, 25%, 25%
14	KB	4	100%; 50%, 25%, 25%
14	eD	4	50%, 25%, 25%
14	hC	4	50%, 25%, 25%
14	hD	4	25%, 50%, 25%
14	kB	4	100%; 25%, 50%, 25%
14	kC	4	50%, 25%, 25%
14	nA	4	75%, 25%
14	nB	4	75%; 25%, 50%, 25%
14	p	4	50%, 25%, 25%
14	qA	4	75%, 25%
14	s	4	75%, 25%
15	1D	5	100%; 40%, 60%
15	2D	5	100%; 40%, 60%
15	4C	5	100%; 40%, 60%
15	5C	5	100%; 20%, 80%
15	7B	5	60%, 40%
15	8B	5	40%, 60%
15	AB	5	20%, 80%
15	BB	5	40%, 60%
15	CA	5	40%, 60%
15	DA	5	20%, 80%
15	eB	5	40%, 60%
15	fB	5	40%, 60%

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Mol	Chain	Length	Quality of chain
16	4D	2	50% / 50% / 50%
16	AC	2	100% / 100%
16	FA	2	50% / 50%
17	5D	6	50% / 50%
17	7C	6	50% / 50%
17	DB	6	17% / 83%
17	GA	6	50% / 50%
18	0E	5	60% / 40%
18	9D	5	20% / 80%
18	BE	5	20% / 40% / 60%
18	DE	5	20% / 40% / 60%
18	IE	5	20% / 80%
18	JE	5	40% / 60%
18	KE	5	60% / 40%
18	PE	5	60% / 40%
18	SE	5	60% / 40%
18	cE	5	60% / 40%
18	fE	5	40% / 60%
18	pE	5	100%
18	rE	5	20% / 40% / 60%
18	tE	5	40% / 60%
18	yE	5	20% / 40% / 60%
18	zE	5	20% / 60% / 40%
19	1E	4	50% / 100%
19	AE	4	50% / 50%

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Mol	Chain	Length	Quality of chain
19	LE	4	25% 50% 50%
19	NE	4	75% 25%
19	aE	4	25% 50% 50%
19	qE	4	50% 50%
20	CE	4	75% 25%
20	EE	4	50% 50%
20	HE	4	50% 50%
20	TE	4	50% 50%
20	UE	4	75% 25%
20	WE	4	50% 50%
20	gE	4	50% 50%
20	hE	4	75% 25%
20	jE	4	75% 25%
20	sE	4	25% 75%
20	uE	4	50% 50%
20	xE	4	50% 50%
21	FE	5	20% 80%
21	kE	5	20% 80%
21	vE	5	40% 60%
22	GE	6	33% 67%
22	QE	6	17% 33% 67%
22	RE	6	33% 50% 17%
22	VE	6	33% 67%
22	dE	6	17% 83%
22	eE	6	17% 17% 67% 17%

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Mol	Chain	Length	Quality of chain
22	iE	6	17% 50% 50%
22	wE	6	67% 33%
23	XE	6	33% 67%
24	YE	6	17% 83%
24	lE	6	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
10	AHR	1A	4	X	-	-	-
10	AHR	3	4	X	-	-	-
10	AHR	VB	4	X	-	-	-
10	AHR	sD	4	X	-	-	-
10	AHR	vC	4	X	-	-	-
10	AHR	yB	4	X	-	-	-
12	GZL	FB	3	X	-	-	-
12	GZL	IB	3	X	-	-	-
12	GZL	cD	3	X	-	-	-
12	GZL	fC	3	X	-	-	-
12	GZL	fD	3	X	-	-	-
12	GZL	iB	3	X	-	-	-
12	GZL	iC	3	X	-	-	-
12	GZL	lA	3	X	-	-	-
12	GZL	lB	3	X	-	-	-
12	GZL	n	3	X	-	-	-
12	GZL	oA	3	X	-	-	-
12	GZL	q	3	X	-	-	-
12	AHR	q	5	X	-	-	-
13	FUB	0D	2	X	-	-	-
13	GZL	1B	3	X	-	-	-
13	GZL	2A	3	X	-	-	-
13	GZL	2B	3	X	-	-	-
13	FUB	3C	2	X	-	-	-
13	GZL	4	3	X	X	-	-
13	GZL	4A	3	X	-	-	-
13	GZL	5A	3	X	-	-	-
13	GZL	6	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	FUB	6B	2	X	-	-	-
13	GZL	7	3	X	-	-	-
13	FUB	9A	2	X	-	-	-
13	FUB	BA	2	X	-	-	-
13	GZL	GB	3	X	-	-	-
13	GZL	WB	3	X	-	-	-
13	GZL	YB	3	X	-	-	-
13	GZL	ZB	3	X	-	-	-
13	FUB	dB	2	X	-	-	-
13	GZL	dD	3	X	-	-	-
13	GZL	gC	3	X	-	-	-
13	GZL	jB	3	X	-	-	-
13	GZL	mA	3	X	-	-	-
13	GZL	o	3	X	-	-	-
13	GZL	tD	3	X	-	-	-
13	GZL	vD	3	X	-	-	-
13	GZL	wC	3	X	-	-	-
13	GZL	wD	3	X	-	-	-
13	GZL	yC	3	X	-	-	-
13	GZL	zB	3	X	-	-	-
13	GZL	zC	3	X	-	-	-
14	GZL	HB	3	X	-	-	-
14	GZL	KB	3	X	-	-	-
14	GZL	eD	3	X	-	-	-
14	GZL	hC	3	X	-	-	-
14	GZL	hD	3	X	-	-	-
14	GZL	kB	3	X	-	-	-
14	GZL	kC	3	X	-	-	-
14	GZL	nA	3	X	-	-	-
14	GZL	nB	3	X	-	-	-
14	GZL	p	3	X	-	-	-
14	GZL	qA	3	X	-	-	-
14	GZL	s	3	X	-	-	-
15	GZL	1D	3	X	-	-	-
15	AHR	1D	5	X	-	-	-
15	GZL	2D	3	X	-	-	-
15	GZL	4C	3	X	-	-	-
15	AHR	4C	5	X	-	-	-
15	GZL	5C	3	X	-	-	-
15	GZL	7B	3	X	-	-	-
15	AHR	7B	5	X	-	-	-
15	GZL	8B	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	GZL	AB	3	X	-	-	-
15	AHR	AB	5	X	-	-	-
15	GZL	BB	3	X	-	-	-
15	GZL	CA	3	X	-	-	-
15	AHR	CA	5	X	-	-	-
15	GZL	DA	3	X	-	-	-
15	GZL	eB	3	X	-	-	-
15	AHR	eB	5	X	-	-	-
15	GZL	fB	3	X	-	-	-
17	MAN	5D	4	X	-	-	-
17	MAN	5D	6	X	-	-	-
17	MAN	7C	4	X	-	-	-
17	MAN	7C	6	X	-	-	-
17	MAN	DB	4	X	-	-	-
17	MAN	DB	6	X	-	-	-
17	MAN	GA	4	X	-	-	-
17	MAN	GA	6	X	-	-	-
18	GZL	0E	3	X	-	-	-
18	AHR	0E	4	X	-	-	-
18	AHR	0E	5	X	-	-	-
18	GZL	9D	3	X	-	-	-
18	AHR	9D	4	X	-	-	-
18	GZL	BE	3	X	-	-	-
18	AHR	BE	4	X	-	-	-
18	AHR	BE	5	X	-	-	-
18	GZL	DE	3	X	-	-	-
18	AHR	DE	5	X	-	-	-
18	GZL	IE	3	X	-	-	-
18	AHR	IE	4	X	-	-	-
18	GZL	JE	3	X	-	-	-
18	AHR	JE	5	X	-	-	-
18	GZL	KE	3	X	-	-	-
18	AHR	KE	4	X	-	-	-
18	AHR	KE	5	X	-	-	-
18	GZL	PE	3	X	-	-	-
18	AHR	PE	4	X	-	-	-
18	AHR	PE	5	X	-	-	-
18	FUB	SE	1	X	-	-	-
18	GZL	SE	3	X	-	-	-
18	AHR	SE	4	X	-	-	-
18	AHR	SE	5	X	-	-	-
18	GZL	cE	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AHR	cE	4	X	-	-	-
18	AHR	cE	5	X	-	-	-
18	FUB	fE	1	X	-	-	-
18	GZL	fE	3	X	-	-	-
18	AHR	fE	4	X	-	-	-
18	AHR	fE	5	X	-	-	-
18	GZL	pE	3	X	-	-	-
18	AHR	pE	4	X	-	-	-
18	GZL	rE	3	X	-	-	-
18	AHR	rE	4	X	-	-	-
18	AHR	rE	5	X	-	-	-
18	GZL	tE	3	X	-	-	-
18	AHR	tE	5	X	-	-	-
18	GZL	yE	3	X	-	-	-
18	AHR	yE	4	X	-	-	-
18	GZL	zE	3	X	-	-	-
18	AHR	zE	5	X	-	-	-
19	GZL	1E	3	X	-	-	-
19	AHR	1E	4	X	-	-	-
19	GZL	AE	3	X	-	-	-
19	GZL	LE	3	X	-	-	-
19	AHR	LE	4	X	-	-	-
19	GZL	NE	3	X	-	-	-
19	AHR	NE	4	X	-	-	-
19	GZL	aE	3	X	-	-	-
19	AHR	aE	4	X	-	-	-
19	GZL	qE	3	X	-	-	-
2	HYP	G	23	X	-	-	-
2	HYP	G	26	X	-	-	-
2	HYP	I	23	X	-	-	-
2	HYP	I	26	X	-	-	-
20	GZL	CE	3	X	-	-	-
20	GZL	EE	3	X	-	-	-
20	GZL	HE	3	X	-	-	-
20	GZL	TE	3	X	-	-	-
20	AHR	TE	4	X	-	-	-
20	GZL	UE	3	X	-	-	-
20	GZL	WE	3	X	-	-	-
20	AHR	WE	4	X	-	-	-
20	GZL	gE	3	X	-	-	-
20	AHR	gE	4	X	-	-	-
20	GZL	hE	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	GZL	jE	3	X	-	-	-
20	AHR	jE	4	X	-	-	-
20	GZL	sE	3	X	-	-	-
20	GZL	uE	3	X	-	-	-
20	GZL	xE	3	X	-	-	-
21	GZL	FE	3	X	-	-	-
21	AHR	FE	4	X	-	-	-
21	AHR	FE	5	X	-	-	-
21	GZL	kE	3	X	-	-	-
21	AHR	kE	4	X	-	-	-
21	GZL	vE	3	X	-	-	-
21	AHR	vE	4	X	-	-	-
21	AHR	vE	5	X	-	-	-
22	GZL	GE	3	X	-	-	-
22	GZL	QE	3	X	-	-	-
22	AHR	QE	4	X	-	-	-
22	AHR	QE	6	X	-	-	-
22	GZL	RE	3	X	-	-	-
22	AHR	RE	4	X	-	-	-
22	GZL	VE	3	X	-	-	-
22	AHR	VE	4	X	-	-	-
22	GZL	dE	3	X	-	-	-
22	AHR	dE	4	X	-	-	-
22	AHR	dE	6	X	-	-	-
22	GZL	eE	3	X	-	-	-
22	AHR	eE	4	X	-	-	-
22	GZL	iE	3	X	-	-	-
22	AHR	iE	4	X	-	-	-
22	GZL	wE	3	X	-	-	-
23	GZL	XE	3	X	-	-	-
23	AHR	XE	4	X	-	-	-
23	AHR	XE	5	X	-	-	-
24	GZL	YE	3	X	-	-	-
24	AHR	YE	4	X	-	-	-
24	GZL	lE	3	X	-	-	-
24	AHR	lE	4	X	-	-	-
27	GLA	A	2007	X	-	-	-
27	GLA	B	2008	X	-	-	-
27	GLA	B	2014	X	-	-	-
27	GLA	E	2007	X	-	-	-
27	GLA	F	2009	X	-	-	-
3	FUB	XA	2	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUB	AD	1	X	-	-	-
4	FUB	DC	1	X	-	-	-
4	FUB	JA	1	X	-	-	-
4	FUB	L	1	X	-	-	-
4	FUB	OD	2	X	-	-	-
4	AHR	PC	4	X	-	-	-
4	FUB	RC	2	X	-	-	-
4	AHR	VA	4	X	-	-	-
4	FUB	Z	2	X	-	-	-
5	AHR	BD	5	X	-	-	-
6	GZL	0B	3	X	-	-	-
6	GZL	1C	3	X	-	-	-
6	FUB	2C	2	X	-	-	-
6	GZL	2C	3	X	-	-	-
6	GZL	3A	3	X	-	-	-
6	GZL	3D	3	X	-	-	-
6	GZL	4B	3	X	-	-	-
6	GZL	5	3	X	-	-	-
6	FUB	5B	2	X	-	-	-
6	GZL	5B	3	X	-	-	-
6	GZL	6C	3	X	-	-	-
6	GZL	6D	3	X	-	-	-
6	GZL	7A	3	X	-	-	-
6	GZL	7D	3	X	-	-	-
6	GZL	8	3	X	-	-	-
6	FUB	8A	2	X	-	-	-
6	GZL	8A	3	X	-	-	-
6	GZL	8D	3	X	-	-	-
6	GZL	9	3	X	-	-	-
6	GZL	9B	3	X	-	-	-
6	FUB	AA	2	X	-	-	-
6	GZL	AA	3	X	-	-	-
6	GZL	CB	3	X	-	-	-
6	GZL	CD	3	X	-	-	-
6	GZL	EA	3	X	-	-	-
6	GZL	FC	3	X	-	-	-
6	GZL	GD	3	X	-	-	-
6	GZL	JC	3	X	-	-	-
6	GZL	LA	3	X	-	-	-
6	GZL	ME	3	X	-	-	-
6	GZL	N	3	X	-	-	-
6	GZL	OE	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GZL	PA	3	X	-	-	-
6	GZL	R	3	X	-	-	-
6	GZL	XB	3	X	-	-	-
6	GZL	ZE	3	X	-	-	-
6	GZL	bB	3	X	-	-	-
6	GZL	bE	3	X	-	-	-
6	FUB	cB	2	X	-	-	-
6	GZL	cB	3	X	-	-	-
6	GZL	gB	3	X	-	-	-
6	GZL	mE	3	X	-	-	-
6	GZL	nE	3	X	-	-	-
6	GZL	oE	3	X	-	-	-
6	GZL	uD	3	X	-	-	-
6	GZL	xC	3	X	-	-	-
6	GZL	yD	3	X	-	-	-
6	FUB	zD	2	X	-	-	-
6	GZL	zD	3	X	-	-	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 85288 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.

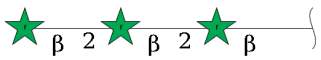
- Molecule 1 is a protein called Mst1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1907	13862	8723	2261	2797	81	0	0
1	B	1907	13862	8723	2261	2797	81	0	0
1	C	1494	10840	6862	1753	2179	46	0	0
1	D	1566	11377	7199	1841	2286	51	0	0
1	E	1449	10491	6595	1712	2105	79	0	0
1	F	1443	10455	6573	1705	2098	79	0	0

- Molecule 2 is a protein called Mstax.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	G	64	438	269	65	104	0	0
2	H	30	201	125	30	46	0	0
2	I	34	238	145	35	58	0	0

- Molecule 3 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	J	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	K	3	27	15	12	0	0
3	O	3	27	15	12	0	0
3	P	3	27	15	12	0	0
3	Q	3	27	15	12	0	0
3	T	3	27	15	12	0	0
3	V	3	27	15	12	0	0
3	b	3	27	15	12	0	0
3	e	3	27	15	12	0	0
3	l	3	27	15	12	0	0
3	m	3	27	15	12	0	0
3	t	3	27	15	12	0	0
3	w	3	27	15	12	0	0
3	x	3	27	15	12	0	0
3	y	3	27	15	12	0	0
3	z	3	27	15	12	0	0
3	0	3	27	15	12	0	0
3	1	3	27	15	12	0	0
3	2	3	27	15	12	0	0
3	HA	3	27	15	12	0	0
3	IA	3	27	15	12	0	0
3	MA	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	NA	3	27	15	12	0	0
3	OA	3	27	15	12	0	0
3	RA	3	27	15	12	0	0
3	TA	3	27	15	12	0	0
3	XA	3	27	15	12	0	0
3	ZA	3	27	15	12	0	0
3	cA	3	27	15	12	0	0
3	jA	3	27	15	12	0	0
3	kA	3	27	15	12	0	0
3	rA	3	27	15	12	0	0
3	uA	3	27	15	12	0	0
3	vA	3	27	15	12	0	0
3	wA	3	27	15	12	0	0
3	xA	3	27	15	12	0	0
3	yA	3	27	15	12	0	0
3	zA	3	27	15	12	0	0
3	0A	3	27	15	12	0	0
3	EB	3	27	15	12	0	0
3	LB	3	27	15	12	0	0
3	OB	3	27	15	12	0	0
3	PB	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	QB	3	27	15	12	0	0
3	RB	3	27	15	12	0	0
3	SB	3	27	15	12	0	0
3	TB	3	27	15	12	0	0
3	UB	3	27	15	12	0	0
3	hB	3	27	15	12	0	0
3	oB	3	27	15	12	0	0
3	rB	3	27	15	12	0	0
3	sB	3	27	15	12	0	0
3	tB	3	27	15	12	0	0
3	uB	3	27	15	12	0	0
3	vB	3	27	15	12	0	0
3	wB	3	27	15	12	0	0
3	xB	3	27	15	12	0	0
3	BC	3	27	15	12	0	0
3	CC	3	27	15	12	0	0
3	GC	3	27	15	12	0	0
3	HC	3	27	15	12	0	0
3	IC	3	27	15	12	0	0
3	LC	3	27	15	12	0	0
3	NC	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	TC	3	27	15	12	0	0
3	WC	3	27	15	12	0	0
3	dC	3	27	15	12	0	0
3	eC	3	27	15	12	0	0
3	lC	3	27	15	12	0	0
3	oC	3	27	15	12	0	0
3	pC	3	27	15	12	0	0
3	qC	3	27	15	12	0	0
3	rC	3	27	15	12	0	0
3	sC	3	27	15	12	0	0
3	tC	3	27	15	12	0	0
3	uC	3	27	15	12	0	0
3	8C	3	27	15	12	0	0
3	9C	3	27	15	12	0	0
3	DD	3	27	15	12	0	0
3	ED	3	27	15	12	0	0
3	FD	3	27	15	12	0	0
3	ID	3	27	15	12	0	0
3	KD	3	27	15	12	0	0
3	QD	3	27	15	12	0	0
3	TD	3	27	15	12	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	aD	3	27	15	12	0	0
3	bD	3	27	15	12	0	0
3	iD	3	27	15	12	0	0
3	lD	3	27	15	12	0	0
3	mD	3	27	15	12	0	0
3	nD	3	27	15	12	0	0
3	oD	3	27	15	12	0	0
3	pD	3	27	15	12	0	0
3	qD	3	27	15	12	0	0
3	rD	3	27	15	12	0	0

- Molecule 4 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
4	L	4	36	20	16	0	0
4	W	4	36	20	16	0	0
4	X	4	36	20	16	0	0
4	Z	4	36	20	16	0	0
4	c	4	36	20	16	0	0
4	d	4	36	20	16	0	0
4	g	4	36	20	16	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
4	k	4	36	20	16	0	0
4	r	4	36	20	16	0	0
4	v	4	36	20	16	0	0
4	JA	4	36	20	16	0	0
4	UA	4	36	20	16	0	0
4	VA	4	36	20	16	0	0
4	aA	4	36	20	16	0	0
4	bA	4	36	20	16	0	0
4	eA	4	36	20	16	0	0
4	iA	4	36	20	16	0	0
4	pA	4	36	20	16	0	0
4	tA	4	36	20	16	0	0
4	JB	4	36	20	16	0	0
4	NB	4	36	20	16	0	0
4	mB	4	36	20	16	0	0
4	qB	4	36	20	16	0	0
4	DC	4	36	20	16	0	0
4	OC	4	36	20	16	0	0
4	PC	4	36	20	16	0	0
4	RC	4	36	20	16	0	0
4	UC	4	36	20	16	0	0

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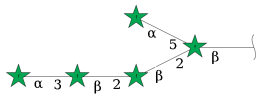
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
4	VC	4	36	20	16	0	0
4	YC	4	36	20	16	0	0
4	cC	4	36	20	16	0	0
4	jC	4	36	20	16	0	0
4	nC	4	36	20	16	0	0
4	AD	4	36	20	16	0	0
4	LD	4	36	20	16	0	0
4	MD	4	36	20	16	0	0
4	OD	4	36	20	16	0	0
4	RD	4	36	20	16	0	0
4	SD	4	36	20	16	0	0
4	VD	4	36	20	16	0	0
4	ZD	4	36	20	16	0	0
4	gD	4	36	20	16	0	0
4	kD	4	36	20	16	0	0

- Molecule 5 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
5	M	5	45	25	20	0	0
5	KA	5	45	25	20	0	0

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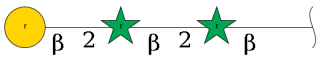
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
5	EC	5	45	25	20	0	0
5	BD	5	45	25	20	0	0

- Molecule 6 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
6	N	3	29	16	13	0	0
6	R	3	29	16	13	0	0
6	5	3	29	16	13	0	0
6	8	3	29	16	13	0	0
6	9	3	29	16	13	0	0
6	AA	3	29	16	13	0	0
6	EA	3	29	16	13	0	0
6	LA	3	29	16	13	0	0
6	PA	3	29	16	13	0	0
6	3A	3	29	16	13	0	0
6	6A	3	29	16	13	0	0
6	7A	3	29	16	13	0	0
6	8A	3	29	16	13	0	0
6	CB	3	29	16	13	0	0
6	XB	3	29	16	13	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
6	aB	3	29	16	13	0	0
6	bB	3	29	16	13	0	0
6	cB	3	29	16	13	0	0
6	gB	3	29	16	13	0	0
6	0B	3	29	16	13	0	0
6	3B	3	29	16	13	0	0
6	4B	3	29	16	13	0	0
6	5B	3	29	16	13	0	0
6	9B	3	29	16	13	0	0
6	FC	3	29	16	13	0	0
6	JC	3	29	16	13	0	0
6	xC	3	29	16	13	0	0
6	0C	3	29	16	13	0	0
6	1C	3	29	16	13	0	0
6	2C	3	29	16	13	0	0
6	6C	3	29	16	13	0	0
6	CD	3	29	16	13	0	0
6	GD	3	29	16	13	0	0
6	uD	3	29	16	13	0	0
6	xD	3	29	16	13	0	0
6	yD	3	29	16	13	0	0

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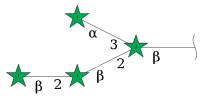
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
6	zD	3	29	16	13	0	0
6	3D	3	29	16	13	0	0
6	6D	3	29	16	13	0	0
6	7D	3	29	16	13	0	0
6	8D	3	29	16	13	0	0
6	ME	3	29	16	13	0	0
6	OE	3	29	16	13	0	0
6	ZE	3	29	16	13	0	0
6	bE	3	29	16	13	0	0
6	mE	3	29	16	13	0	0
6	nE	3	29	16	13	0	0
6	oE	3	29	16	13	0	0

- Molecule 7 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
7	S	4	36	20	16	0	0
7	f	4	36	20	16	0	0
7	h	4	36	20	16	0	0
7	QA	4	36	20	16	0	0
7	dA	4	36	20	16	0	0

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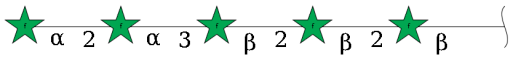
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
7	fA	4	36	20	16	0	0
7	KC	4	36	20	16	0	0
7	XC	4	36	20	16	0	0
7	ZC	4	36	20	16	0	0
7	HD	4	36	20	16	0	0
7	UD	4	36	20	16	0	0
7	WD	4	36	20	16	0	0

- Molecule 8 is an oligosaccharide called alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
8	U	5	45	25	20	0	0
8	SA	5	45	25	20	0	0
8	MC	5	45	25	20	0	0
8	JD	5	45	25	20	0	0

- Molecule 9 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
9	Y	2	18	10	8	0	0

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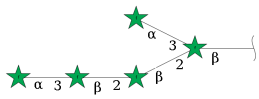
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
9	j	2	18	10	8	0	0
9	WA	2	18	10	8	0	0
9	hA	2	18	10	8	0	0
9	QC	2	18	10	8	0	0
9	bC	2	18	10	8	0	0
9	ND	2	18	10	8	0	0
9	YD	2	18	10	8	0	0

- Molecule 10 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
10	a	5	45	25	20	0	0
10	u	5	45	25	20	0	0
10	3	5	45	25	20	0	0
10	YA	5	45	25	20	0	0
10	sA	5	45	25	20	0	0
10	1A	5	45	25	20	0	0
10	MB	5	45	25	20	0	0
10	VB	5	45	25	20	0	0
10	pB	5	45	25	20	0	0

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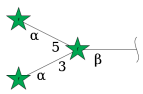
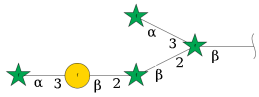
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
10	yB	5	45	25	20	0	0
10	SC	5	45	25	20	0	0
10	mC	5	45	25	20	0	0
10	vC	5	45	25	20	0	0
10	PD	5	45	25	20	0	0
10	jD	5	45	25	20	0	0
10	sD	5	45	25	20	0	0

- Molecule 11 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
11	i	3	27	15	12	0	0
11	gA	3	27	15	12	0	0
11	aC	3	27	15	12	0	0
11	XD	3	27	15	12	0	0

- Molecule 12 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
12	n	5	47	26	21	0	0
12	q	5	47	26	21	0	0
12	lA	5	47	26	21	0	0
12	oA	5	47	26	21	0	0
12	FB	5	47	26	21	0	0
12	IB	5	47	26	21	0	0
12	iB	5	47	26	21	0	0
12	lB	5	47	26	21	0	0
12	fC	5	47	26	21	0	0
12	iC	5	47	26	21	0	0
12	cD	5	47	26	21	0	0
12	fD	5	47	26	21	0	0

- Molecule 13 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
13	o	4	38	21	17	0	0
13	4	4	38	21	17	0	0
13	6	4	38	21	17	0	0
13	7	4	38	21	17	0	0
13	BA	4	38	21	17	0	0

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Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
13	mA	4	38	21	17	0	0
13	2A	4	38	21	17	0	0
13	4A	4	38	21	17	0	0
13	5A	4	38	21	17	0	0
13	9A	4	38	21	17	0	0
13	GB	4	38	21	17	0	0
13	WB	4	38	21	17	0	0
13	YB	4	38	21	17	0	0
13	ZB	4	38	21	17	0	0
13	dB	4	38	21	17	0	0
13	jB	4	38	21	17	0	0
13	zB	4	38	21	17	0	0
13	1B	4	38	21	17	0	0
13	2B	4	38	21	17	0	0
13	6B	4	38	21	17	0	0
13	gC	4	38	21	17	0	0
13	wC	4	38	21	17	0	0
13	yC	4	38	21	17	0	0
13	zC	4	38	21	17	0	0
13	3C	4	38	21	17	0	0
13	dD	4	38	21	17	0	0

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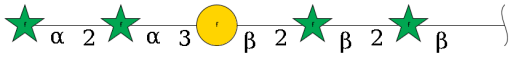
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
13	tD	4	38	21	17	0	0
13	vD	4	38	21	17	0	0
13	wD	4	38	21	17	0	0
13	0D	4	38	21	17	0	0

- Molecule 14 is an oligosaccharide called beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
14	p	4	38	21	17	0	0
14	s	4	38	21	17	0	0
14	nA	4	38	21	17	0	0
14	qA	4	38	21	17	0	0
14	HB	4	38	21	17	0	0
14	KB	4	38	21	17	0	0
14	kB	4	38	21	17	0	0
14	nB	4	38	21	17	0	0
14	hC	4	38	21	17	0	0
14	kC	4	38	21	17	0	0
14	eD	4	38	21	17	0	0
14	hD	4	38	21	17	0	0

- Molecule 15 is an oligosaccharide called alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
15	CA	5	Total	C	O		0	0
			47	26	21			
15	DA	5	Total	C	O		0	0
			47	26	21			
15	AB	5	Total	C	O		0	0
			47	26	21			
15	BB	5	Total	C	O		0	0
			47	26	21			
15	eB	5	Total	C	O		0	0
			47	26	21			
15	fB	5	Total	C	O		0	0
			47	26	21			
15	7B	5	Total	C	O		0	0
			47	26	21			
15	8B	5	Total	C	O		0	0
			47	26	21			
15	4C	5	Total	C	O		0	0
			47	26	21			
15	5C	5	Total	C	O		0	0
			47	26	21			
15	1D	5	Total	C	O		0	0
			47	26	21			
15	2D	5	Total	C	O		0	0
			47	26	21			

- Molecule 16 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	FA	2	Total	C	N	O	0	0
			28	16	2	10		

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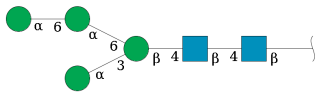
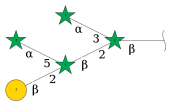
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	AC	2	28	16	2	10	0	0
16	4D	2	28	16	2	10	0	0

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	GA	6	72	40	2	30	0	0
17	DB	6	72	40	2	30	0	0
17	7C	6	72	40	2	30	0	0
17	5D	6	72	40	2	30	0	0

- Molecule 18 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
18	9D	5	47	26	21	0	0
18	BE	5	47	26	21	0	0
18	DE	5	47	26	21	0	0
18	IE	5	47	26	21	0	0
18	JE	5	47	26	21	0	0

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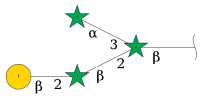
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
18	KE	5	47	26	21	0	0
18	PE	5	47	26	21	0	0
18	SE	5	47	26	21	0	0
18	cE	5	47	26	21	0	0
18	fE	5	47	26	21	0	0
18	pE	5	47	26	21	0	0
18	rE	5	47	26	21	0	0
18	tE	5	47	26	21	0	0
18	yE	5	47	26	21	0	0
18	zE	5	47	26	21	0	0
18	0E	5	47	26	21	0	0

- Molecule 19 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.

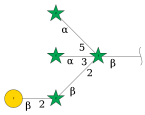


Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
19	AE	4	38	21	17	0	0
19	LE	4	38	21	17	0	0
19	NE	4	38	21	17	0	0
19	aE	4	38	21	17	0	0
19	qE	4	38	21	17	0	0
19	1E	4	38	21	17	0	0

- Molecule 20 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
20	CE	4	38	21	17	0	0
20	EE	4	38	21	17	0	0
20	HE	4	38	21	17	0	0
20	TE	4	38	21	17	0	0
20	UE	4	38	21	17	0	0
20	WE	4	38	21	17	0	0
20	gE	4	38	21	17	0	0
20	hE	4	38	21	17	0	0
20	jE	4	38	21	17	0	0
20	sE	4	38	21	17	0	0
20	uE	4	38	21	17	0	0
20	xE	4	38	21	17	0	0

- Molecule 21 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
21	FE	5	47	26	21	0	0

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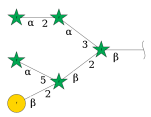
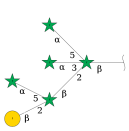
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
21	kE	5	47	26	21	0	0
21	vE	5	47	26	21	0	0

- Molecule 22 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose.



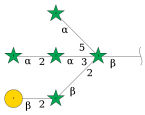
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
22	GE	6	56	31	25	0	0
22	QE	6	56	31	25	0	0
22	RE	6	56	31	25	0	0
22	VE	6	56	31	25	0	0
22	dE	6	56	31	25	0	0
22	eE	6	56	31	25	0	0
22	iE	6	56	31	25	0	0
22	wE	6	56	31	25	0	0

- Molecule 23 is an oligosaccharide called beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
23	XE	6	56	31	25	0	0

- Molecule 24 is an oligosaccharide called beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.

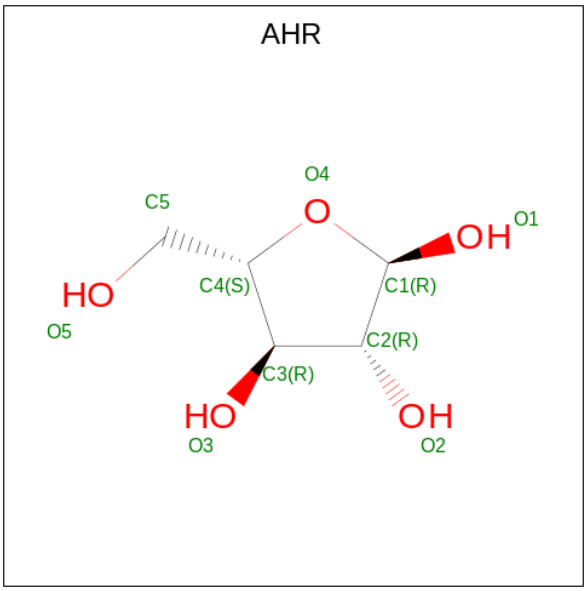


Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
24	YE	6	56	31	25	0	0
			Total	C	O		
24	lE	6	56	31	25	0	0

- Molecule 25 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
25	A	1	1	1	0
			Total	Ca	
25	B	1	1	1	0
			Total	Ca	
25	C	1	1	1	0
			Total	Ca	
25	D	1	1	1	0
			Total	Ca	
25	E	1	1	1	0
			Total	Ca	
25	F	1	1	1	0

- Molecule 26 is alpha-L-arabinofuranose (three-letter code: AHR) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	A	1	9	5	4	0
			Total	C	O	
26	A	1	9	5	4	0
			Total	C	O	
26	A	1	9	5	4	0
			Total	C	O	
26	A	1	9	5	4	0
			Total	C	O	
26	B	1	9	5	4	0
			Total	C	O	
26	B	1	9	5	4	0
			Total	C	O	
26	B	1	9	5	4	0
			Total	C	O	
26	B	1	9	5	4	0
			Total	C	O	
26	C	1	9	5	4	0
			Total	C	O	
26	C	1	9	5	4	0
			Total	C	O	
26	D	1	9	5	4	0
			Total	C	O	
26	D	1	9	5	4	0
			Total	C	O	
26	D	1	9	5	4	0
			Total	C	O	
26	E	1	9	5	4	0

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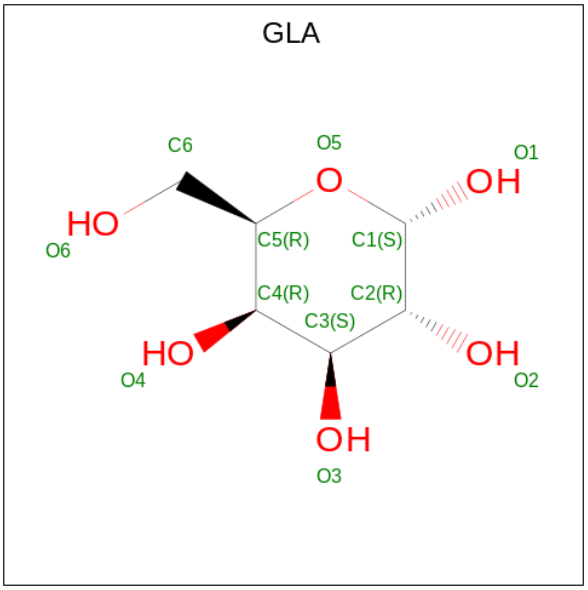
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	E	1	9	5	4	0
26	F	1	9	5	4	0
26	F	1	9	5	4	0
26	F	1	9	5	4	0
26	F	1	9	5	4	0
26	F	1	9	5	4	0

- Molecule 27 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	A	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0
27	B	1	11	6	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	C	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	D	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	E	1	11	6	5	0

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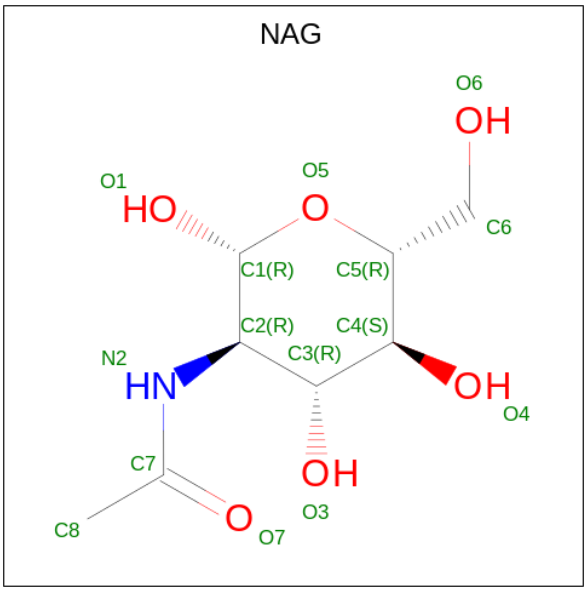
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	E	1	11	6	5	0
27	E	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0
27	F	1	11	6	5	0

- Molecule 28 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



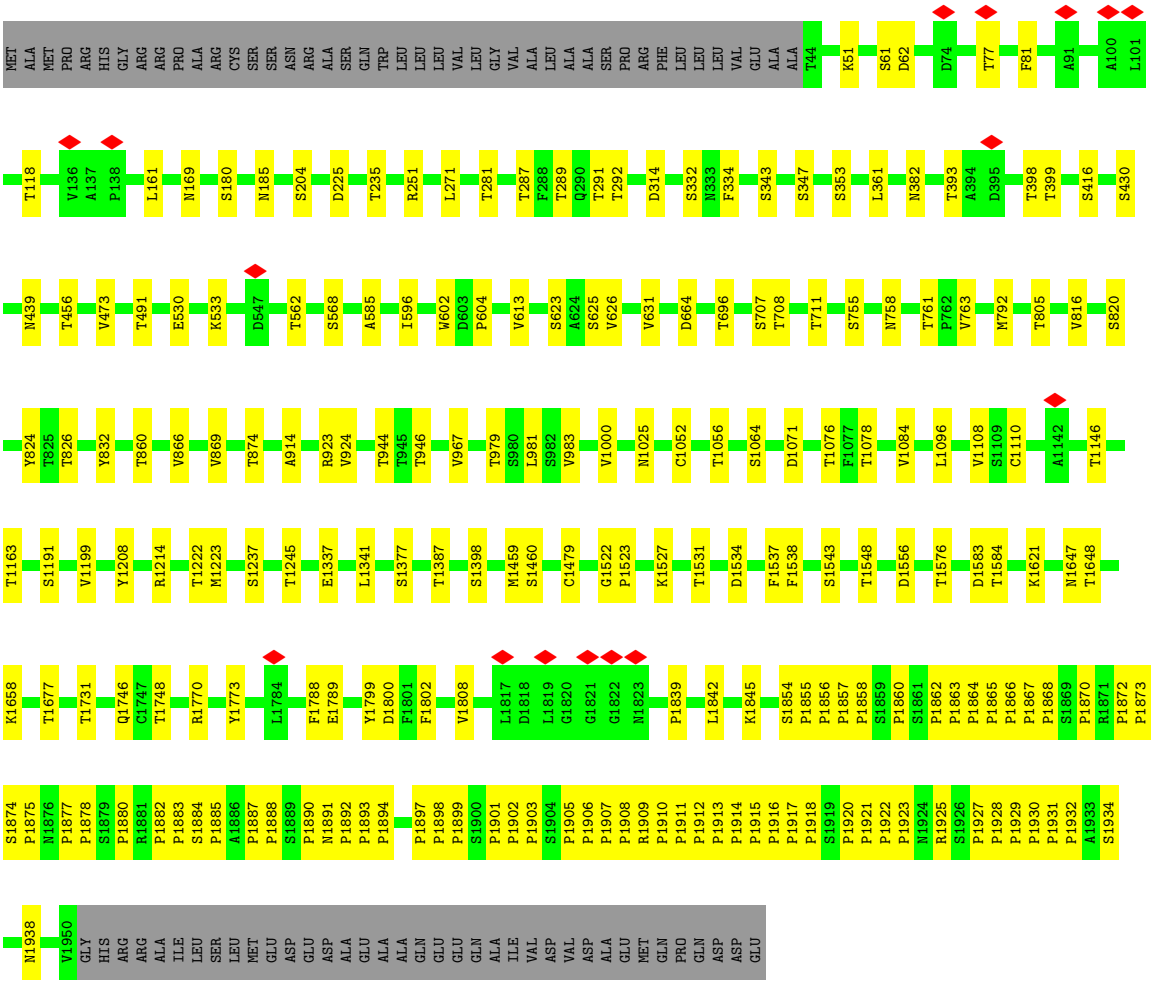
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	N	O	0
			14	8	1	5	
28	B	1	Total	C	N	O	0
			14	8	1	5	
28	B	1	Total	C	N	O	0
			14	8	1	5	
28	C	1	Total	C	N	O	0
			14	8	1	5	
28	C	1	Total	C	N	O	0
			14	8	1	5	
28	D	1	Total	C	N	O	0
			14	8	1	5	
28	E	1	Total	C	N	O	0
			14	8	1	5	

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.

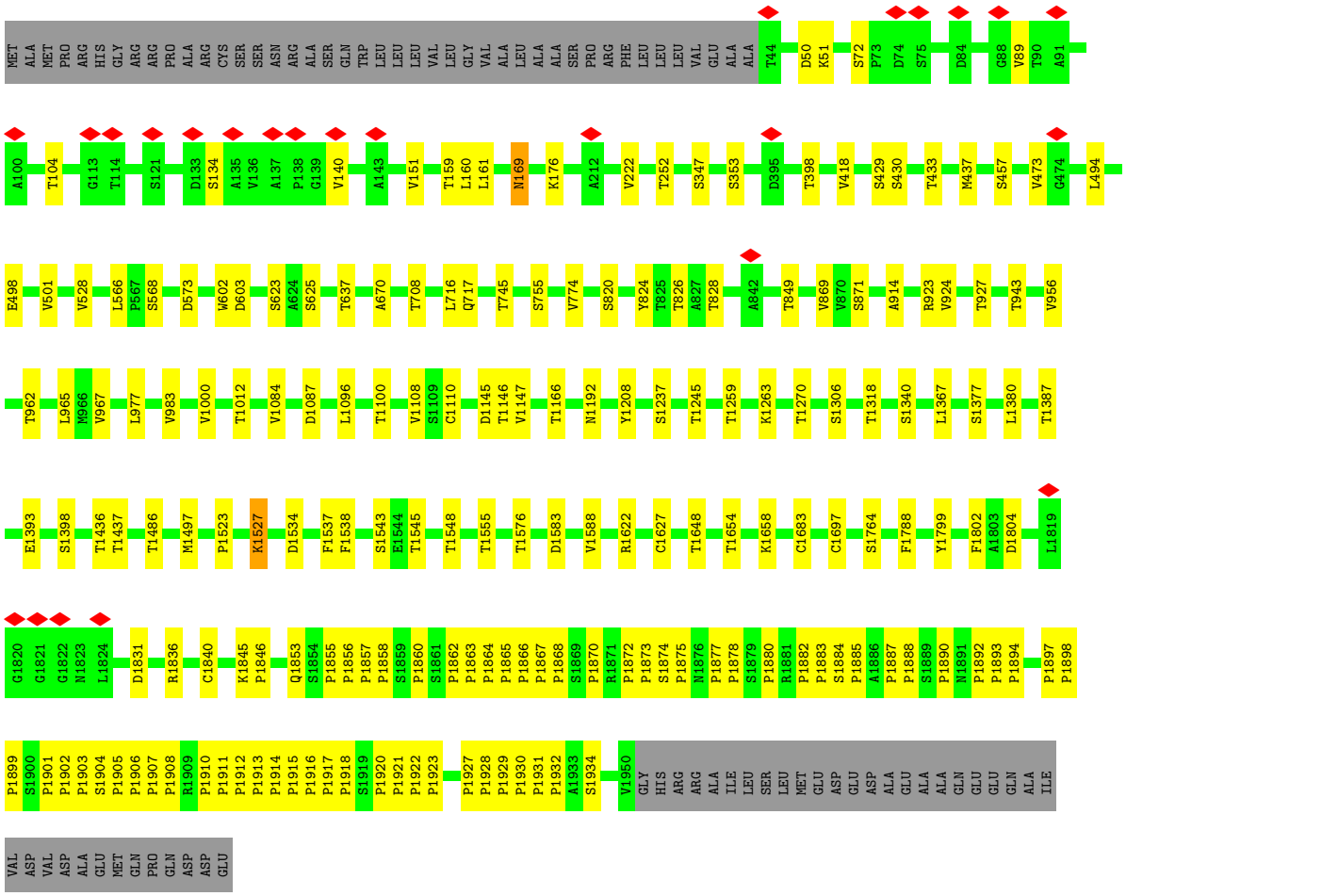
- Molecule 1: Mst1

Chain A: 86% 10%



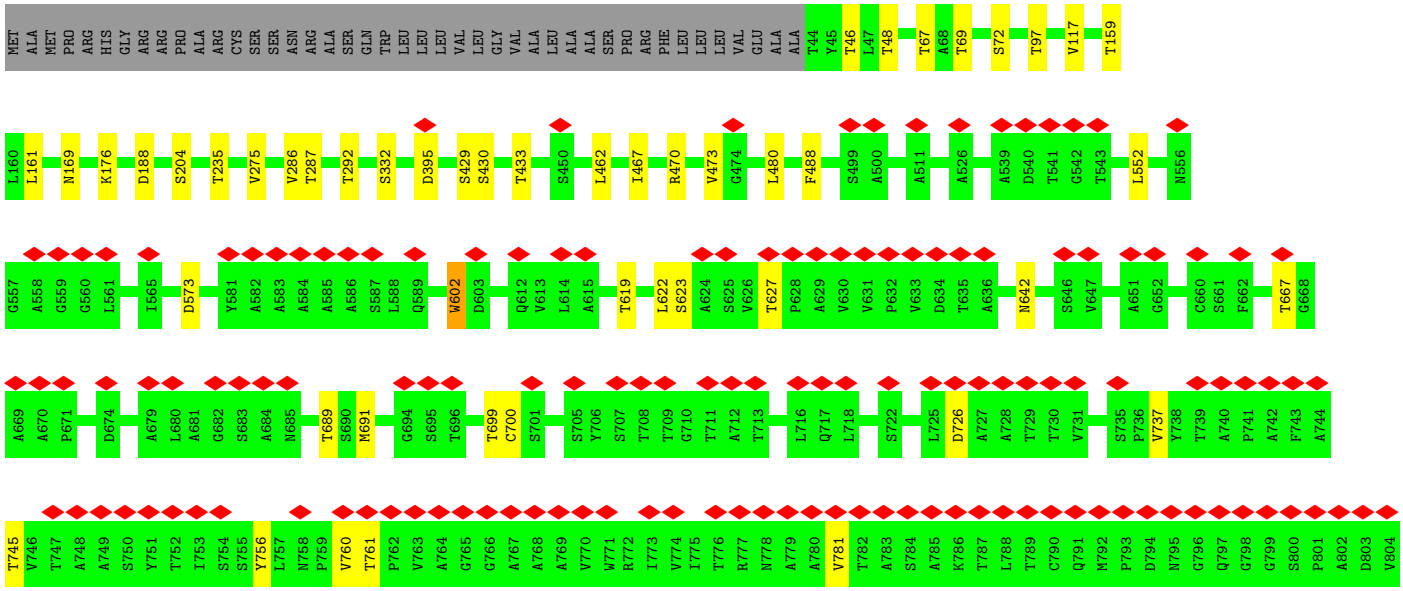
- Molecule 1: Mst1

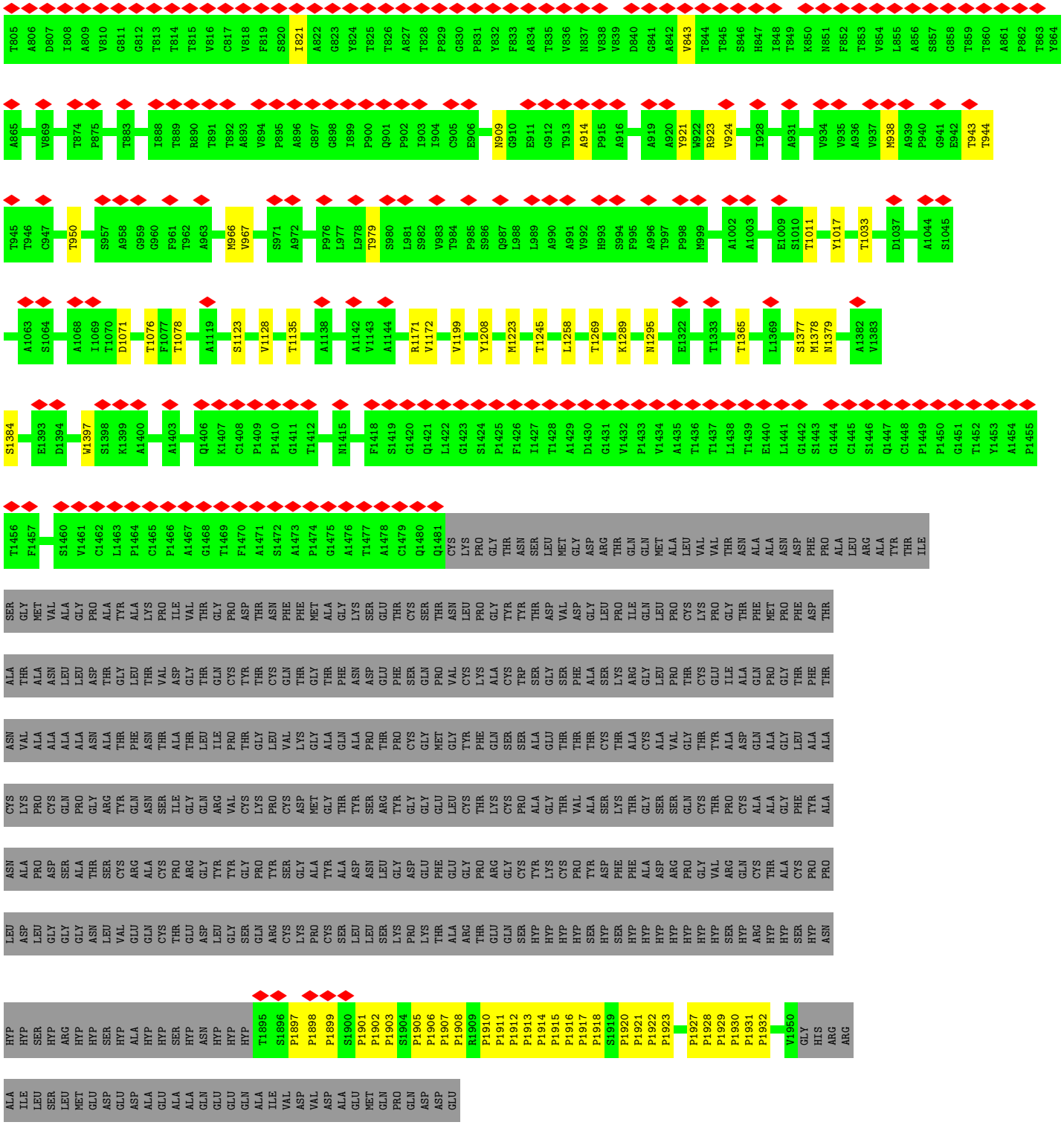
Chain B: 87% 9%



- Molecule 1: Mst1

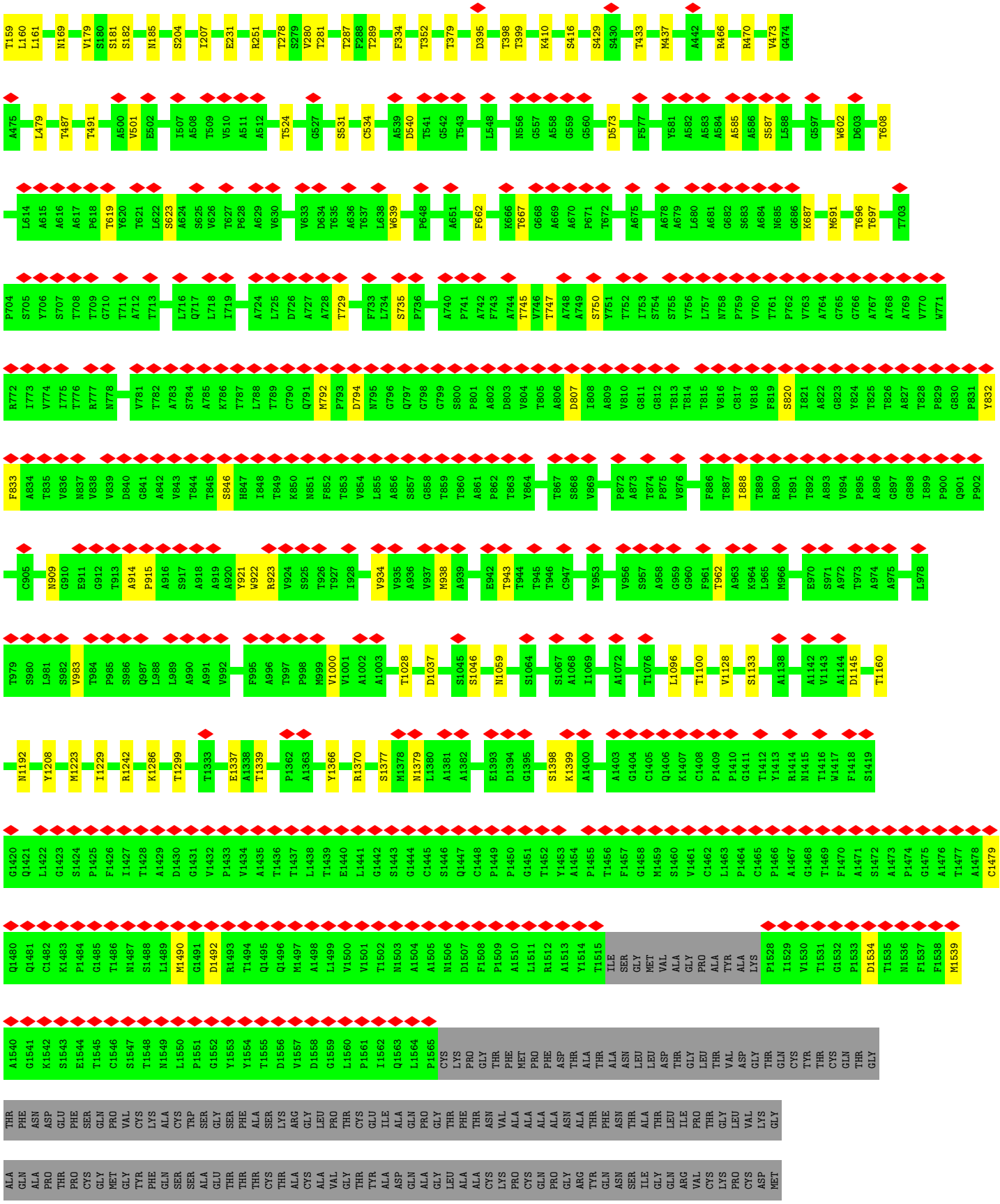
Chain C:





- Molecule 1: Mst1

Chain D: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A475 L479 T487 T491 A500 V501 E502 I507 A508 T509 V510 A511 A512 T524 G527 S531 C534 A539 D540 T541 G542 T543 L548 N556 G557 A558 G559 G560 D573 F577 Y581 A582 A583 A584 A585 A586 S587 L588 G597 W602 D603 T608
L614 A615 A616 A617 P618 T619 Y620 T621 L622 S623 A624 S625 V626 T627 P628 A629 V630 V633 D634 T635 A636 T637 L638 W639 P648 A651 F662 K666 T667 G668 A669 A670 P671 T672 A675 A678 A679 L680 A681 G682 S683 A684 N685 G686 K687 M691 T696 T697 T703
P704 S705 Y706 S707 T708 T709 G710 T711 A712 T713 L716 Q717 L718 I719 A724 L725 D726 A727 A728 T729 F733 L734 S735 P736 A740 P741 A742 F743 A744 T745 V746 T747 A748 A749 S750 Y751 T752 I753 S754 S755 Y756 L757 N758 P759 V760 T761 P762 V763 A764 G765 G766 A767 A768 A769 V770 W771
R772 I773 V774 I775 T776 R777 N778 V781 T782 A783 S784 A785 K786 T787 L788 T789 C790 Q791 M792 P793 D794 N795 G796 Q797 G798 G799 S800 P801 A802 D803 V804 T805 A806 D807 I808 A809 V810 G811 G812 T813 T814 T815 V816 C817 V818 F819 S820 I821 A822 G823 Y824 T825 T826 A827 T828 P829 G830 P831 Y832
F833 A834 T835 V836 N837 V838 V839 D840 G841 A842 V843 T844 T845 S846 H847 I848 T849 K850 N851 F852 T853 V854 L855 A856 S857 G858 T859 T860 A861 P862 T863 Y864 T867 S868 V869 P872 A873 T874 P875 V876 T886 T887 I888 T889 R890 T891 T892 A893 V894 P895 A896 G897 G898 I899 P900 Q901 P902
C905 N909 G910 E911 G912 T913 A914 P915 A916 S917 A918 A919 A920 Y921 W922 R923 V924 S925 T926 T927 I928 V934 V935 A936 V937 M938 A939 E942 T943 T944 T945 T946 C947 Y953 V956 S957 A958 G959 G960 F961 T962 A963 K964 L965 M966 E970 S971 A972 T973 A974 A975 L978
T979 S980 L981 S982 V983 T984 P985 S986 Q987 L988 L989 A990 A991 V992 F995 A996 T997 P998 M999 V1000 V1001 A1002 A1003 T1028 D1037 S1045 S1046 N1059 S1064 S1067 A1068 I1069 A1072 T1076 L1096 T1100 V1128 S1133 A1138 A1142 V1143 A1144 D1145 T1160
N1192 Y1208 M1223 I1229 R1242 K1286 T1299 T1333 E1337 A1338 T1339 P1362 A1363 Y1366 R1370 S1377 M1378 N1379 L1380 A1381 A1382 E1393 D1394 G1395 S1398 K1399 A1400 A1403 G1404 C1405 Q1406 K1407 C1408 P1409 P1410 G1411 T1412 Y1413 R1414 N1415 T1416 W1417 F1418 S1419
G1420 Q1421 L1422 G1423 S1424 P1425 F1426 I1427 T1428 A1429 D1430 G1431 V1432 P1433 V1434 A1435 T1436 T1437 L1438 T1439 E1440 L1441 G1442 S1443 G1444 C1445 S1446 Q1447 C1448 P1449 P1450 G1451 L1511 T1452 Y1453 A1454 P1455 T1456 F1457 G1458 M1459 S1460 V1461 C1462 L1463 P1464 C1465 P1466 A1467 G1468 T1469 F1470 A1471 S1472 A1473 P1474 G1475 F1538 A1476 T1477 A1478 C1479
Q1480 Q1481 C1482 K1483 P1484 G1485 T1486 N1487 S1488 L1489 M1490 G1491 D1492 R1493 T1494 Q1495 Q1496 M1497 A1498 L1499 V1500 V1501 T1502 N1503 A1504 A1505 N1506 D1507 F1508 P1509 A1510 L1511 R1512 A1513 Y1514 T1515 ILE SER GLY MET VAL ALA GLY PRO ALA TYR ALA LYS P1528 I1529 V1530 T1531 G1532 P1533 D1534 T1535 N1536 F1537 F1538 M1539
A1540 G1541 K1542 S1543 E1544 T1545 C1546 S1547 T1548 N1549 L1550 P1551 G1552 Y1553 Y1554 T1555 D1556 V1557 D1558 G1559 L1560 P1561 I1562 Q1563 L1564 P1565 CYS LYS PRO GLY THR PHE MET PRO PHE ASP THR ALA THR ALA ASN LEU LEU ASP THR GLY LEU THR VAL ASP GLY THR GLN CYS TYR THR CYS GLN THR GLY
THR PHE ASN ASP GLU PHE SER GLN PRO VAL CYS LYS ALA CYS TRP SER GLY SER PHE ALA SER LYS ARG GLY LEU PRO THR CYS GLU ILE ALA GLN PRO GLY THR PHE THR ASN VAL ALA ALA ALA ALA ASN ALA THR PHE ASN THR ALA THR LEU ILE PRO THR GLY LEU VAL LYS GLY
ALA GLN ALA PRO THR PRO CYS GLY MET GLY TYR PHE GLN SER SER ALA GLU THR THR THR CYS THR ALA CYS ALA VAL GLY THR TYR ALA ASP GLN ALA GLY LEU ALA ALA CYS LYS PRO CYS GLN PRO GLY ARG TYR GLN ASN SER ILE GLY GLN ARG VAL CYS LYS PRO CYS ASP MET

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

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

CYS SER LEU LEU SER LYS PRO LYS THR ALA ARG THR GLU GLN SER HYP HYP HYP HYP HYP SER HYP SER HYP HYP HYP HYP HYP HYP HYP HYP SER HYP ARG HYP HYP HYP HYP SER HYP HYP HYP HYP HYP ASN HYP HYP HYP SER HYP ARG HYP HYP SER HYP HYP HYP ASN HYP HYP HYP T1895 S1896 P1897 P1898 P1899

S1900 P1901 P1902 P1903 S1904 P1905 P1906 P1907 P1908 R1909 P1910 P1911 P1912 P1913 P1914 P1915 P1916 P1917 P1918 S1919 P1920 P1921 P1922 P1923 N1924 R1925 S1926 P1927 P1928 P1929 P1930 P1931 P1932 V1950 GLY HIS ARG ARG ALA ILE LEU SER LEU MET GLU GLU ASP GLU ASP ALA GLU GLU ALA ALA GLN GLU GLU GLN ALA ILE VAL

ASP VAL ASP ALA GLU MET GLN PRO GLN ASP ASP GLU

- Molecule 1: Mst1

Chain E:

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

SER ASP ALA VAL THR PHE THR ALA THR VAL ALA SER PRO ASP SER THR THR ALA VAL PHE PHE THR LEU ASP TYR GLY ASP GLY VAL THR ALA GLU THR ARG THR THR THR GLY ALA LEU SER THR THR PRO THR ALA ASN LEU VAL SER ALA GLY THR TYR THR VAL THR TYR ALA

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

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

TYR ASP ALA PRO VAL GLY GLY THR LEU LEU ARG THR PHE THR PRO ALA ALA ALA ASN ALA VAL TYR VAL VAL ASP PRO SER LYS TYR VAL LEU THR LEU THR VAL GLY PRO THR THR SER VAL THR THR ALA ASP GLN VAL THR PHE THR GLN THR THR THR GLU VAL SER TYR SER ALA SER

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

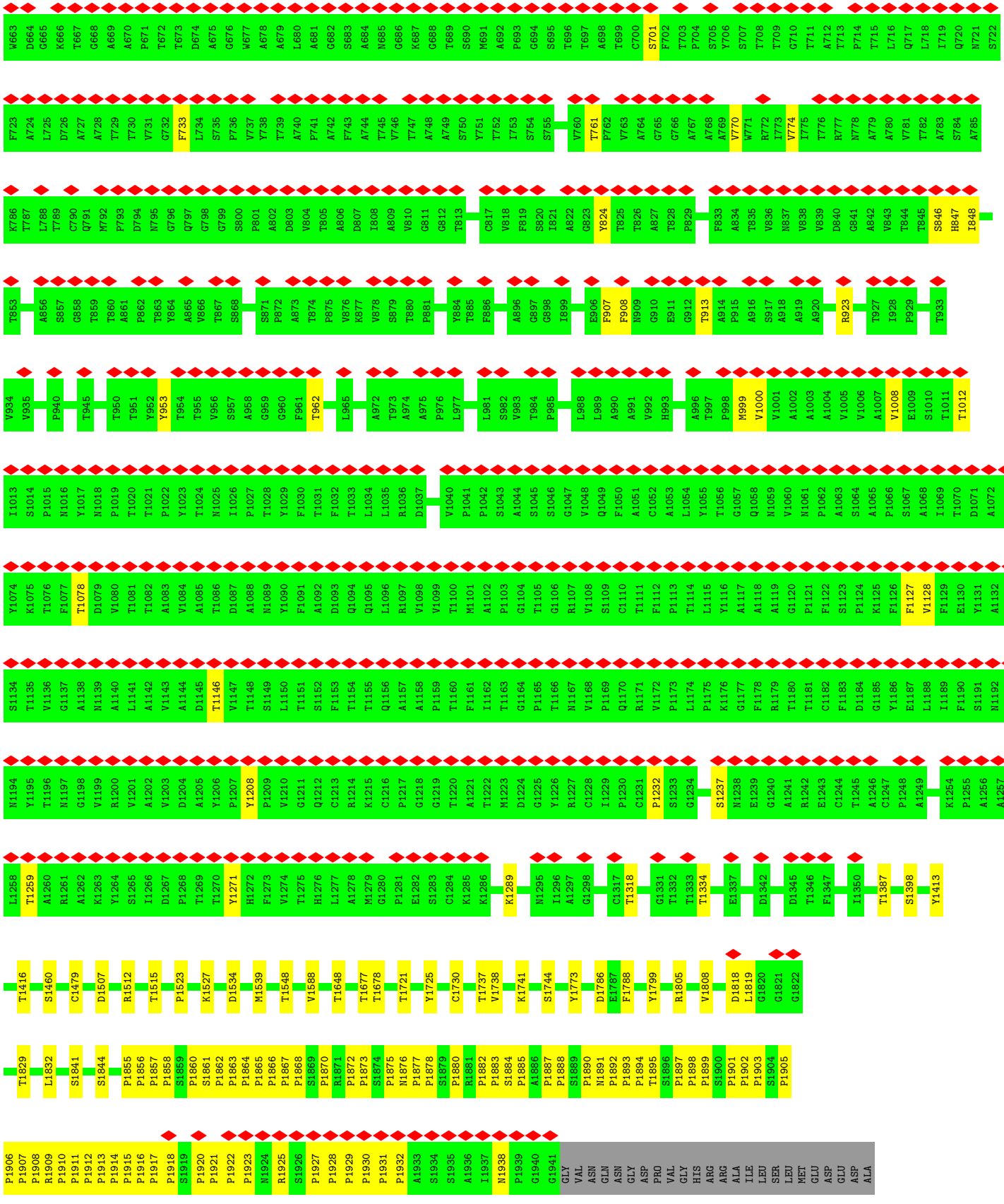
LEU ARG LEU TYR ASP GLY ALA ASN ASN VAL ILE ALA GLU LYS ILE VAL VAL ILE THR VAL SER ASN ALA GLY TYR THR LEU ALA LEU ALA LYS THR THR ALA ASP PRO VAL THR THR ASP ASP THR LYS LEU ALA PHE SER ALA GLY HIS LEU SER SER THR SER GLN VAL TRP TRP

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

LEU ALA SER THR THR VAL THR PHE THR VAL THR PRO V493 L494 Y495 A496 L497 E498 S499 A500 V501 E502 P503 F504 S505 P506 I507 A508 T509 V510 A511 A512 K513 W514 S515 F516 R517 I518 Q519 R520 S521 K522 A523 T524 P525 A526 G527 V528 T529 E530 S531 I532 K533 C534 A535 F536 F537 G538 A539 D540

T541 G542 T543 A544 P545 A546 D547 L548 A549 A550 W551 L552 T553 A554 A555 N556 G557 A558 G559 G560 L561 T562 A563 T564 I565 L566 P567 S568 S569 I570 P571 S572 D573 I574 I575 S576 F577 T578 R579 T580 Y581 A582 A583 A584 A585 A586 S587 L588 Q589 G590 G591 L592 Q593 C594 F595 I596 G597 S598 T599 P600

L601 W602 D603 P604 Y605 Y606 P607 T608 P609 V610 F611 Q612 V613 L614 A615 A616 A617 P618 T619 Y620 T621 L622 S623 A624 S625 V626 T627 P628 A629 V630 D634 T635 A636 T637 L638 W639 T640 Y641 N642 I643 I644 R645 S646 V647 P648 V649 P650 A651 G652 G653 P654 S655 L656 P657 I658 L659 C660 S661 F662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F723 A724 L725 D726 A727 A728 T729 T730 V731 G732 F733 L734 S735 P736 V737 Y738 T739 A740 P741 A742 F743 A744 T745 V746 T747 A748 A749 S750 Y751 T752 I753 S754 S755 V760 T761 P762 V763 A764 G765 G766 A767 A768 A769 V770 W771 R772 T773 V774 I775 T776 R777 N778 A779 A780 V781 T782 A783 S784 A785
K786 T787 L788 T789 C790 Q791 M792 P793 D794 N795 G796 Q797 G798 G799 S800 P801 A802 D803 V804 T805 A806 D807 I808 A809 V810 G811 G812 T813 C817 V818 F819 S820 I821 A822 G823 Y824 T825 T826 A827 T828 P829 F833 A834 T835 V836 N837 V838 V839 D840 G841 A842 V843 T844 T845 S846 H847 I848
T853 A856 S857 G858 T859 T860 A861 P862 T863 Y864 A865 V866 T867 S868 S871 P872 A873 T874 P875 V876 K877 V878 S879 T880 P881 Y884 T885 F886 A896 G897 G898 I899 E906 F907 F908 N909 G910 E911 G912 T913 A914 P915 A916 S917 A918 A919 A920 R923 T927 I928 P929 T933
V934 V935 P940 T945 T950 T951 Y952 Y953 T954 T955 V956 S957 A958 G959 G960 F961 T962 L965 A972 T973 A974 A975 P976 L977 L981 S982 V983 T984 P985 L988 L989 A990 A991 V992 H993 A996 T997 P998 M999 V1000 V1001 A1002 A1003 A1004 V1005 V1006 A1007 V1008 E1009 S1010 T1011 T1012
I1013 S1014 P1015 N1016 Y1017 N1018 P1019 T1020 T1021 P1022 Y1023 T1024 N1025 I1026 P1027 T1028 Y1029 F1030 T1031 F1032 T1033 L1034 L1035 R1036 D1037 V1040 P1041 P1042 S1043 A1044 S1045 S1046 G1047 V1048 Q1049 F1050 A1051 C1052 A1053 L1054 Y1055 T1056 G1057 Q1058 N1059 V1060 N1061 P1062 A1063 S1064 A1065 P1066 S1067 A1068 I1069 T1070 D1071 A1072 V1073
Y1074 K1075 T1076 F1077 T1078 D1079 V1080 T1081 T1082 A1083 V1084 A1085 T1086 D1087 A1088 N1089 Y1090 F1091 A1092 D1093 Q1094 Q1095 L1096 R1097 V1098 V1099 T1100 M1101 A1102 P1103 G1104 T1105 G1106 R1107 V1108 S1109 C1110 T1111 F1112 P1113 T1114 L1115 Y1116 A1117 A1118 A1119 G1120 P1121 F1122 S1123 P1124 K1125 F1126 F1127 V1128 F1129 E1130 Y1131 A1132 S1133
S1134 T1135 V1136 G1137 A1138 N1139 A1140 L1141 A1142 V1143 A1144 D1145 T1146 V1147 T1148 S1149 L1150 T1151 S1152 F1153 T1154 T1155 Q1156 A1157 A1158 P1159 T1160 F1161 I1162 T1163 G1164 P1165 T1166 N1167 V1168 P1169 Q1170 R1171 V1172 P1173 L1174 P1175 K1176 G1177 F1178 R1179 T1180 T1181 C1182 F1183 D1184 G1185 Y1186 E1187 L1188 I1189 F1190 S1191 N1192 D1193
N1194 Y1195 T1196 N1197 G1198 V1199 R1200 V1201 A1202 V1203 D1204 A1205 Y1206 P1207 Y1208 P1209 V1210 G1211 Q1212 C1213 R1214 K1215 C1216 P1217 G1218 G1219 T1220 A1221 T1222 M1223 D1224 G1225 Y1226 R1227 C1228 I1229 P1230 C1231 P1232 S1233 G1234 S1237 N1238 E1239 G1240 A1241 R1242 E1243 C1244 T1245 A1246 C1247 P1248 A1249 K1254 P1255 A1256 A1257
L1258 T1259 A1260 R1261 A1262 K1263 Y1264 S1265 I1266 D1267 P1268 T1269 T1270 Y1271 H1272 F1273 V1274 T1275 H1276 L1277 A1278 M1279 G1280 P1281 E1282 S1283 C1284 K1285 K1286 K1289 N1295 I1296 A1297 G1298 C1317 T1318 G1331 T1332 T1333 T1334 E1337 D1342 D1345 T1346 F1347 I1350 T1387 S1398 Y1413
T1416 S1460 C1479 D1507 R1512 T1515 P1523 K1527 D1534 M1539 T1548 V1588 T1648 T1677 T1678 T1721 Y1725 C1730 T1737 V1738 K1741 S1744 Y1773 D1786 E1787 F1788 Y1799 R1805 V1808 D1818 L1819 G1820 G1821 G1822
T1829 L1832 S1841 S1844 P1855 P1856 P1857 P1858 S1859 P1860 S1861 P1862 P1863 P1864 P1865 P1866 P1867 P1868 S1869 P1870 R1871 P1872 P1873 S1874 P1875 N1876 P1877 P1878 S1879 P1880 R1881 P1882 P1883 S1884 P1885 A1886 P1887 P1888 S1889 P1890 N1891 P1892 P1893 P1894 T1895 S1896 P1897 P1898 P1899 S1900 P1901 P1902 P1903 S1904 P1905
P1906 P1907 P1908 R1909 P1910 P1911 P1912 P1913 P1914 P1915 P1916 P1917 P1918 S1919 P1920 P1921 P1922 P1923 N1924 R1925 S1926 P1927 P1928 P1929 P1930 P1931 P1932 A1933 S1934 S1935 A1936 I1937 N1938 P1939 G1940 G1941 GLY VAL ASN GLN ASN GLY ASP PRO VAL GLY HIS ARG ARG ALA ILE LEU SER LEU MET GLU ASP GLU ASP ALA

GLU ALA ALA GLN GLU GLU GLN ALA ILE VAL ASP VAL ASP ALA GLU MET GLN PRO GLN ASP ASP GLU

- Molecule 1: Mst1

Chain F: 35% 66% 7% 27%

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

SER ASP ALA VAL THR PHE THR ALA THR VAL ALA SER PRO ASP SER THR THR ALA VAL PHE PHE THR LEU ASP TYR GLY ASP GLY VAL THR ALA GLU THR THR ARG THR THR THR GLY ALA LEU SER THR THR PRO THR ALA ASN LEU VAL SER ALA GLY THR TYR THR VAL THR TYR ALA

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

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

TYR ASP ALA PRO VAL GLY GLY THR LEU LEU ARG THR PHE THR PRO ALA ALA ALA ASN ALA VAL TYR VAL VAL ASP PRO SER LYS TYR VAL LEU THR LEU THR VAL GLY PRO THR THR SER VAL THR THR ALA ASP GLN VAL THR PHE THR GLN THR THR GLU VAL SER TYR SER VAL ALA SER

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

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

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

LEU ALA SER THR THR VAL THR PHE THR VAL THR PRO V493 L494 Y495 A496 L497 E498 S499 A500 V501 E502 P503 F504 S505 P506 I507 A508 T509 V510 A511 A512 K513 W514 S515 F516 R517 I518 Q519 R520 S521 K522 A523 T524 P525 A526 G527 V528 T529 E530 S531 I532 K533 C534 A535 F536 F537 G538 A539 D540

T541 G542 T543 A544 P545 A546 D547 L548 A549 A550 W551 L552 T553 A554 A555 N556 G557 A558 G559 G560 L561 T562 A563 T564 I565 L566 P567 S568 S569 I570 P571 S572 D573 I574 I575 S576 F577 T578 R579 T580 Y581 A582 A583 A584 A585 A586 S587 L588 Q589 G590 K591 L592 Q593 C594 F595 I596 G597 S598 T599 P600

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G665 K666 T667 G668 A669 A670 P671 T672 T673 D674 A675 G676 W677 A678 A679 L680 A681 G682 S683 A684 N685 G686 K687 G688 T689 S690 M691 A692 P693 G694 S695 T696 T697 A698 T699 C700 S701 F702 T703 P704 S705 Y706 S707 T708 T709 G710 T711 A712 T713 P714 T715 L716 Q717 L718 I719 Q720 N721 S722 F723 A724

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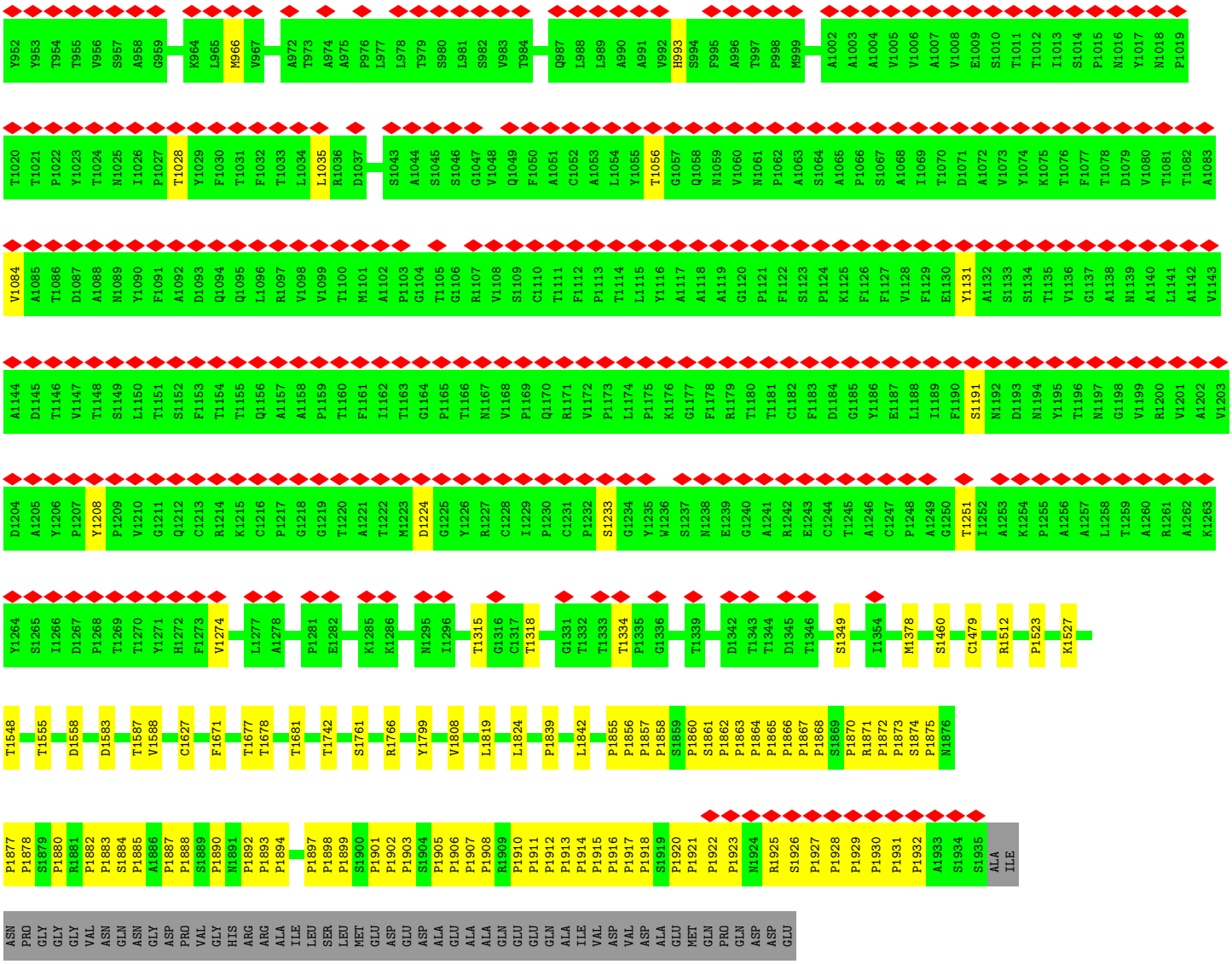
T789 C790 Q791 M792 P793 D794 N795 G798 G799 S800 P801 A802 D803 V804 T805 A806 D807 I808 A809 V810 G811 G812 C817 S820 I821 A822 G823 Y824 T825 T826 A827 T828 P829 G830 P831 Y832 F833 V836 N837 V838 V839 D840 G841 A842 V843 T844 T845 S846 H847 I848 T853 V854 L855 A856 S857

G858 T859 T860 A861 P862 T863 Y864 A865 V866 T867 V870 S871 P872 A873 T874 P875 V876 K877 V878 S879 T880 P881 V882 F886 T891 A896 G897 G898 C905 F908 E911 G912 T913 A914 P915 A916 S917 A918 A919 R923 T926 T927 I928 P929 V937 C947 T950 T951



- Molecule 2: Mstax

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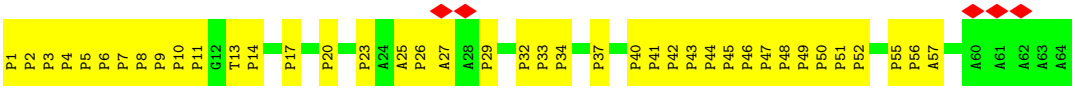
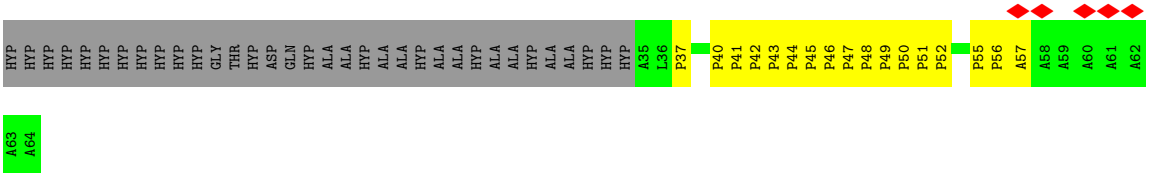
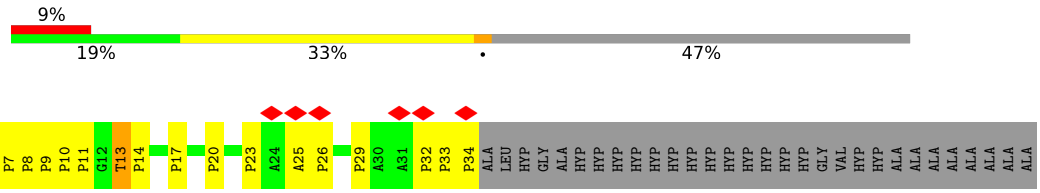


- Molecule 2: Mstax

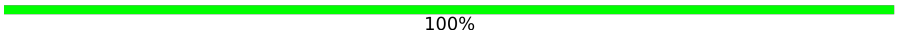
Chain H:



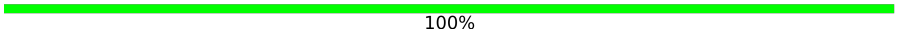
• Molecule 2: Mstax

Chain I: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain J: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain K: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain O: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain P: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain Q: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain T: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain V: 

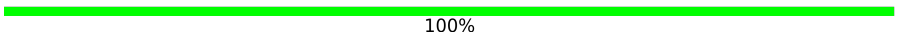
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b: 

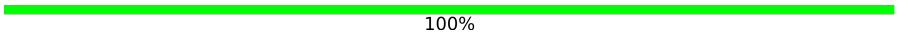
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain l: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain m: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain t: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain w: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain x: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain y: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain z: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HA: 33% 67%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain IA: 67% 33%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain MA: 100%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain NA: 33% 67%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain OA: 67% 33%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain RA: 67% 33%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TA: 33% 67%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain XA: 

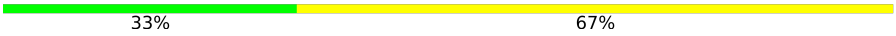
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ZA: 

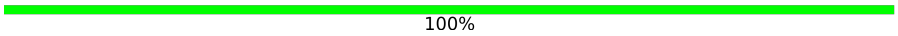
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain cA: 

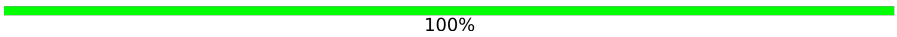
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain jA: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain kA: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain rA: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uA: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain vA: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain wA: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xA: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain yA: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain zA: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0A: 67% 33%

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain EB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain LB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain OB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain PB: 

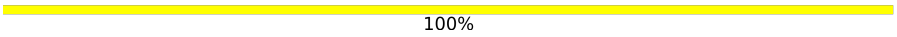
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain QB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain RB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain SB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain UB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain hB: 

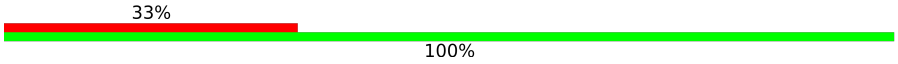
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain oB: 

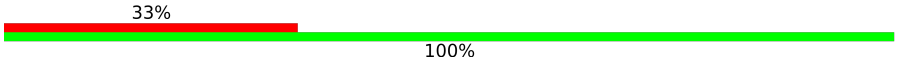
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain rB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain sB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain tB: 

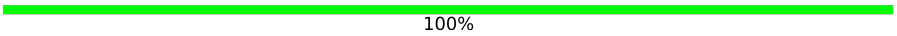
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain vB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain wB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xB: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain BC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain GC: 

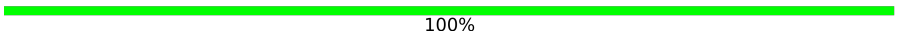
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain IC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain LC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain NC: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TC: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WC: 33% 67%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain dC: 67% 33%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain eC: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain lC: 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

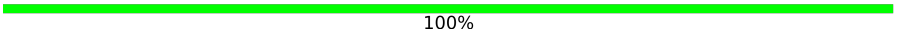
Chain oC: 33% 100%

FUB1 FUB2 FUB3

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain pC: 

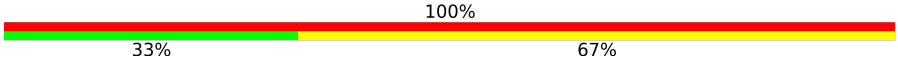
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain qC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain rC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain sC: 

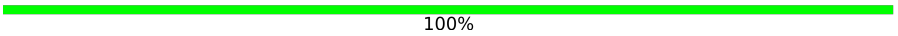
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain tC: 

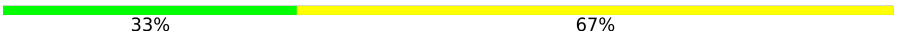
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uC: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8C: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9C: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain DD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ED: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain FD: 

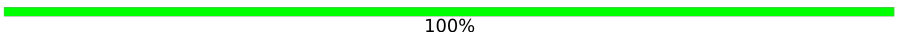
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ID: 

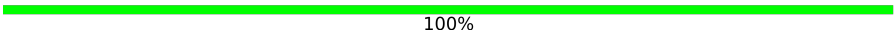
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain KD: 

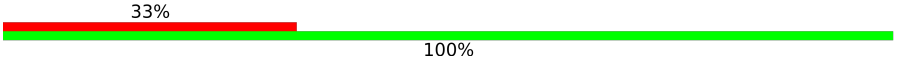
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain QD: 

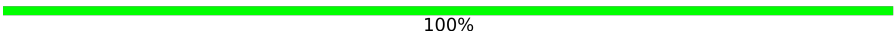
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain aD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain iD: 

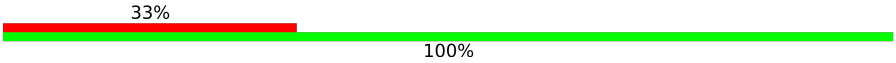
• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain lD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain mD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain nD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain oD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain pD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain qD: 

• Molecule 3: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain rD: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain L: 75% 25%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain W: 75% 25%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain X: 75% 25%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain Z: 25% 75%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain c: 75% 25%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain d: 25% 75%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain g: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain k: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain r: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain v: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain JA: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain UA: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain VA: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain aA: 100%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain bA: 100%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain eA: 100%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain iA: 50% 50%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain pA: 100%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain tA: 50% 50%

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain JB: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain NB: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain mB: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain qB: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain DC: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain OC: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain PC: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain RC: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain UC: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain VC: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain YC: 

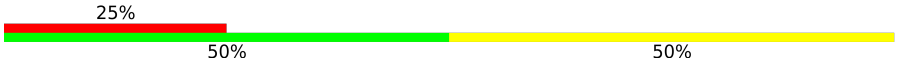
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain cC: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain jC: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain nC: 

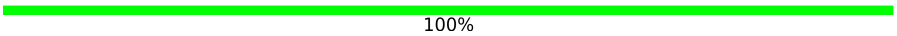
• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain AD: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain LD: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain MD: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain OD: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain RD: 

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain SD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain VD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

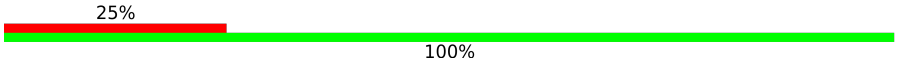
Chain ZD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain gD:

• Molecule 4: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain kD:



• Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain M:

• Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain KA: 

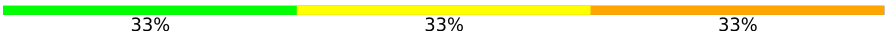
• Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain EC: 

• Molecule 5: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain BD: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain N: 

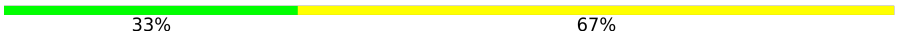
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain R: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 5: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9: 

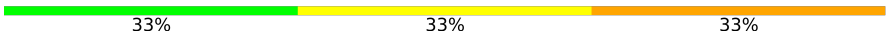
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain AA: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain EA: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain LA: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain PA: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 3A: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6A: 33% 67%

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 7A: 33% 67%

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8A: 100%

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CB: 33% 67%

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain XB: 33% 33% 33% 33%

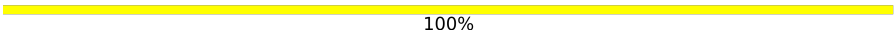
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain aB: 33% 67%

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bB: 100%

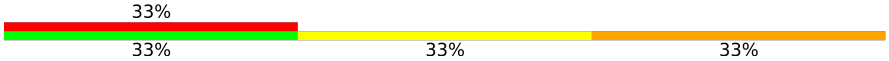
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain cB: 

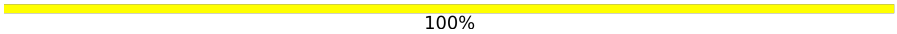
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain gB: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0B: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 3B: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4B: 

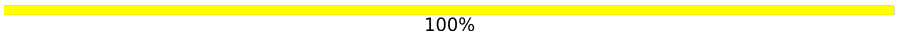
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 5B: 

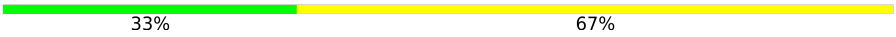
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 9B: 

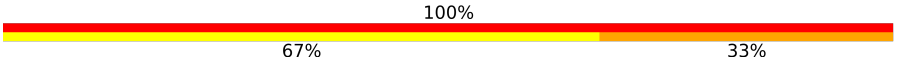
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain FC: 

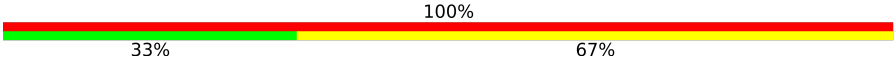
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain JC: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xC: 

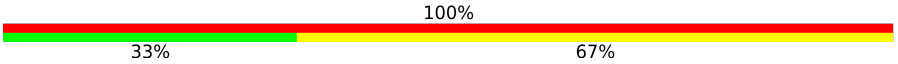
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0C: 

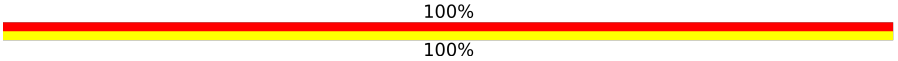
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1C: 

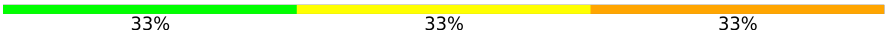
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2C: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6C: 

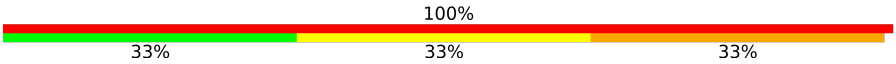
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CD: 

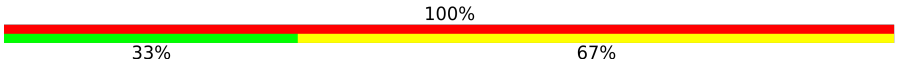
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain GD: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uD: 

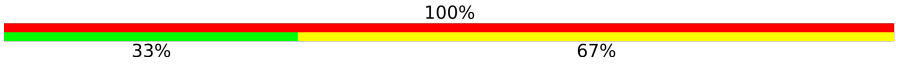
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xD: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain yD: 

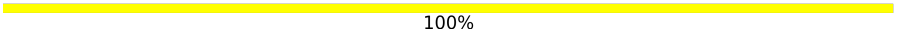
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain zD: 

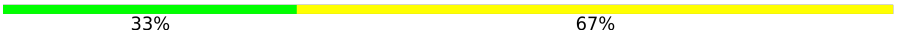
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 3D: 

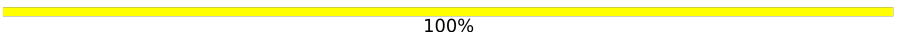
• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6D: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 7D: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 8D: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ME: 

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain OE: 67% 33%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ZE: 33% 67%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bE: 67% 33%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain mE: 33% 67%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain nE: 33% 67%

FUB1 FUB2 GZL3

• Molecule 6: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain oE: 33% 67%

FUB1 FUB2 GZL3

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain S: 25% 75%

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain f: 

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain h: 

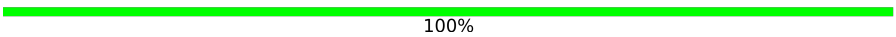
• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain QA: 

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain dA: 

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain fA: 

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain KC: 

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain XC: 

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain ZC: 

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain HD: 

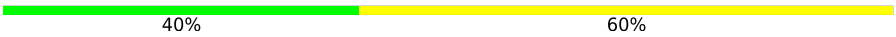
• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain UD: 

• Molecule 7: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain WD: 

• Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain U: 

• Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain SA: 80% 20%

• Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain MC: 40% 60%

• Molecule 8: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain JD: 80% 20%

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain Y: 100%

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain j: 50% 50%

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WA: 100%

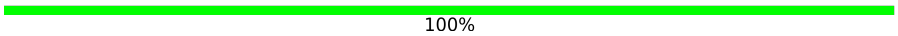
• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain hA: 50% 50%

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain QC: 100%

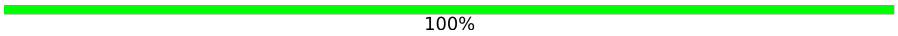
• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain bC: 

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain ND: 

• Molecule 9: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain YD: 

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain a: 

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain u: 

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 3: 

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain YA: 

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

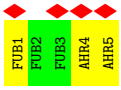
Chain sA:

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 1A:

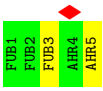
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain MB:



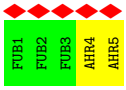
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain VB:



• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain pB:



• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

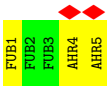
Chain yB:

• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain SC:

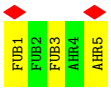
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain mC:



• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain vC:

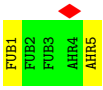


• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain PD:

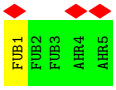
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain jD:



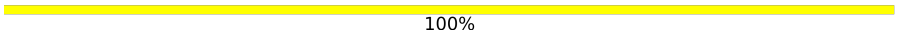
• Molecule 10: alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain sD:



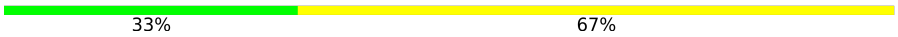
• Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain i:



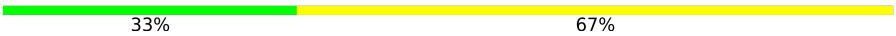
• Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain gA:



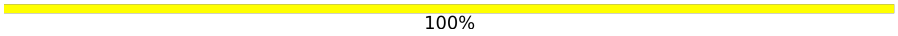
• Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain aC:



• Molecule 11: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain XD:

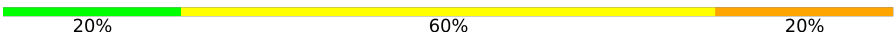


• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain n:

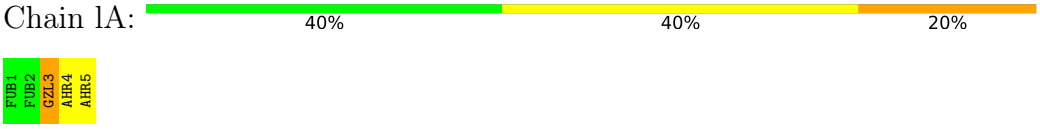
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain q:



• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain lA:

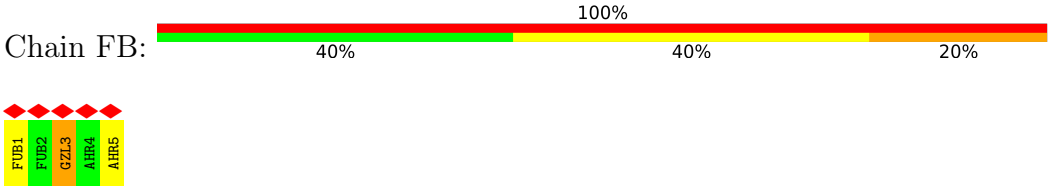


• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain oA:

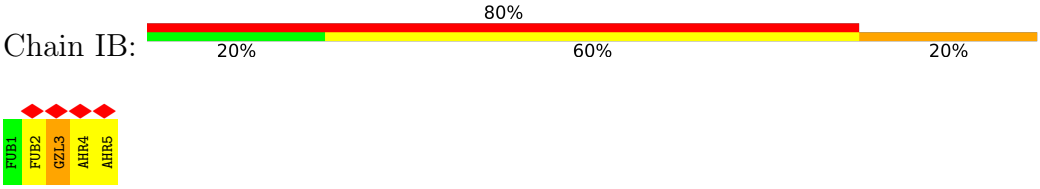
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain FB:



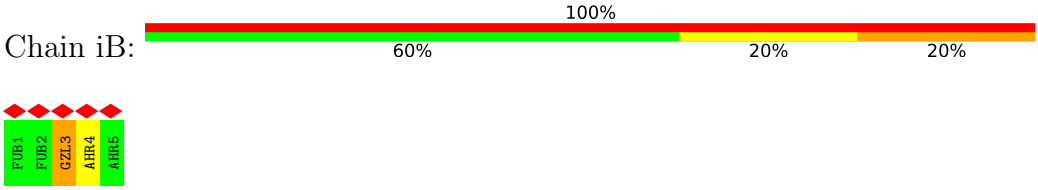
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain IB:



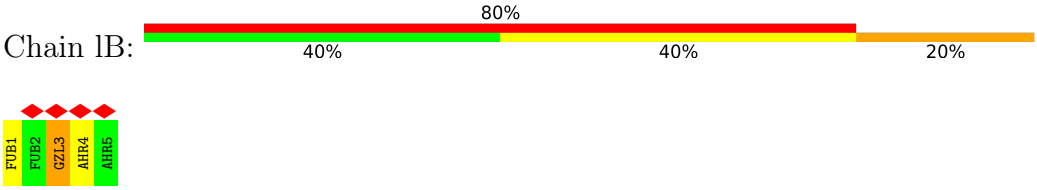
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain iB:



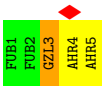
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain lB:



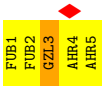
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain fC: 



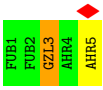
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain iC: 

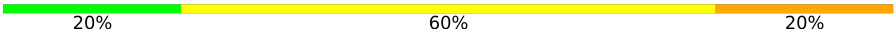


• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain cD: 



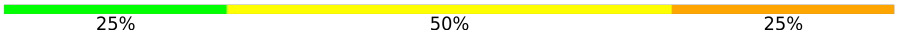
• Molecule 12: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain fD: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain o: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 7: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain BA: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain mA: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2A: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4A: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

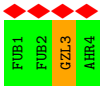
Chain 5A: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

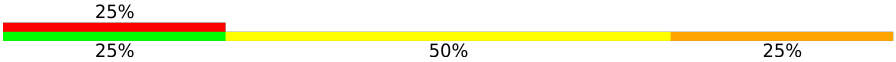
Chain 9A: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain GB: 



• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WB: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain YB: 

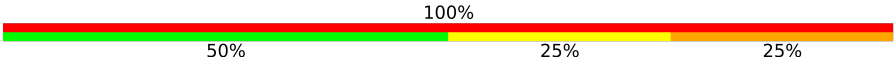
• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

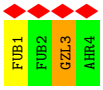
Chain ZB: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain dB: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain jB: 



• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain zB: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1B: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2B: 

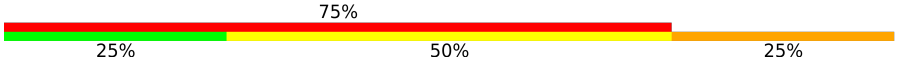
• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 6B: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain gC: 

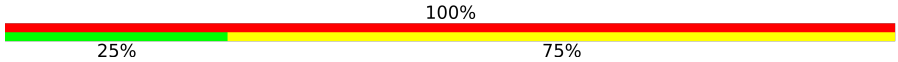
• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

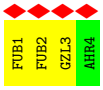
Chain wC: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

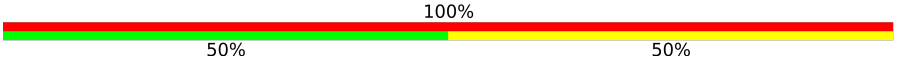
Chain yC: 

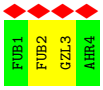
• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain zC: 



• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

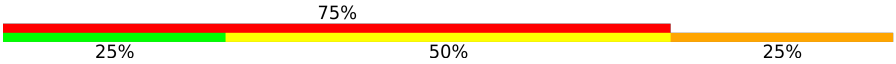
Chain 3C: 



• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain dD: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain tD: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

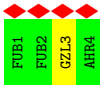
Chain vD: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain wD: 

• Molecule 13: alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 0D: 



• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain p: 

• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain s: 

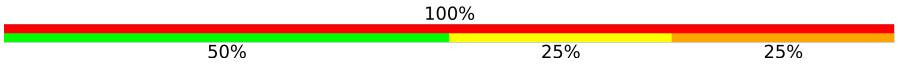
• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

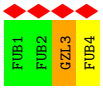
Chain nA: 

• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

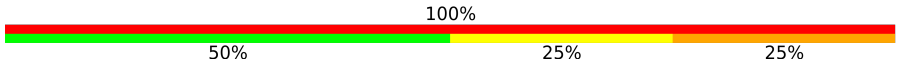
Chain qA: 

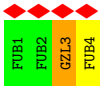
• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain HB: 

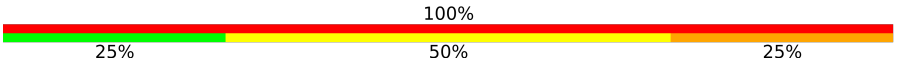


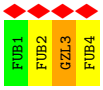
• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain KB: 

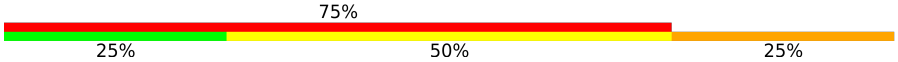


• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain kB: 



• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain nB: 

• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain hC: 

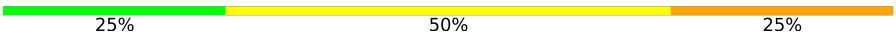
• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain kC: 

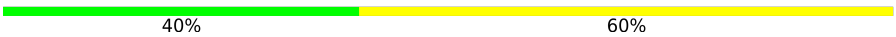
• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain eD: 

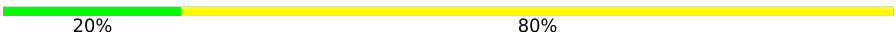
• Molecule 14: beta-L-arabinofuranose-(1-5)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose -(1-2)-beta-L-arabinofuranose

Chain hD: 

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CA: 

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain DA: 

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain AB: 

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain BB: 40% 60%

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain eB: 40% 60%

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain fB: 40% 60%

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

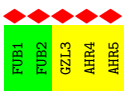
Chain 7B: 60% 40%

• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

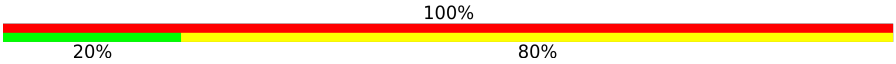
Chain 8B: 40% 60%

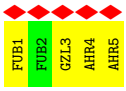
• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 4C: 100% 40% 60%

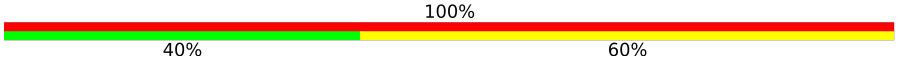


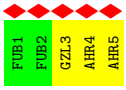
• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 5C: 

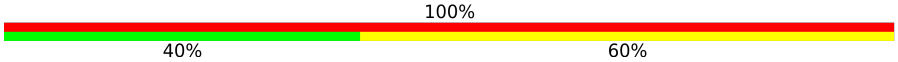


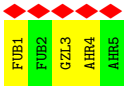
• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 1D: 



• Molecule 15: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain 2D: 



• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA: 

• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AC: 

• Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4D: 

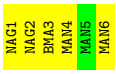
• Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-aceta

mido-2-deoxy-beta-D-glucopyranose

Chain GA: 

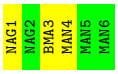
• Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DB: 



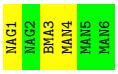
• Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7C: 



• Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5D: 

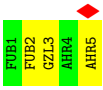


• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 9D: 

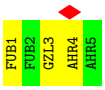
• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain BE: 



• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain DE: 



• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain IE: 

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain JE: 

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain KE: 

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain PE: 

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain SE: 

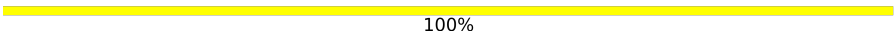
• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain cE: 

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

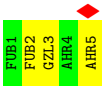
Chain fE: 

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

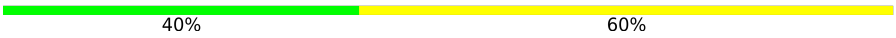
Chain pE: 

• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain rE: 

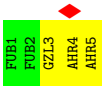


• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain tE: 

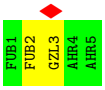
• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain yE: 



• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain zE: 



• Molecule 18: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 0E: 

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain AE: 

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain LE: 

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain NE: 

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain aE: 

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain qE: 

• Molecule 19: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain 1E: 

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain CE: 

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain EE: 

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain HE: 

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain TE: 

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain UE: 

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain WE: 50% 50%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain gE: 50% 50%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain hE: 75% 25%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain jE: 75% 25%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain sE: 25% 75%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain uE: 50% 50%

• Molecule 20: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain xE: 

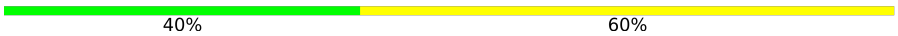
• Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain FE: 

• Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

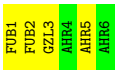
Chain kE: 

• Molecule 21: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain vE: 

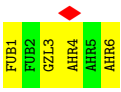
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain GE: 

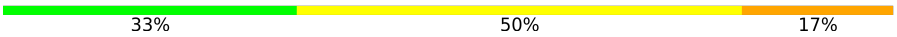


• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain QE: 



• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain RE: 

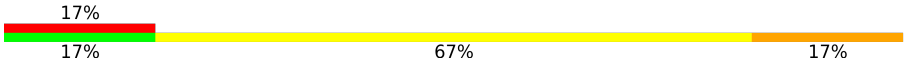
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

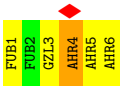
Chain VE: 

• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain dE: 

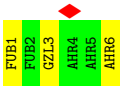
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain eE: 



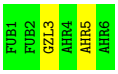
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain iE: 

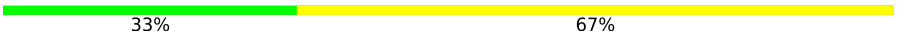


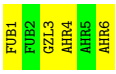
• Molecule 22: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]beta-L-arabinofuranose

Chain wE: 

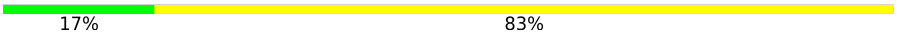


• Molecule 23: beta-D-galactofuranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

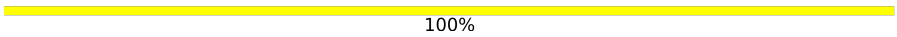
Chain XE: 



• Molecule 24: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain YE: 

• Molecule 24: beta-D-galactofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)][alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain lE: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69065	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.527	Depositor
Minimum map value	-0.673	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	554.24, 554.24, 554.24	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FUB, GZL, MAN, HYP, CA, BMA, GLA, AHR, NAG

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	0.29	0/13724	0.54	2/18848 (0.0%)
1	B	0.29	0/13724	0.54	3/18848 (0.0%)
1	C	0.27	0/10873	0.51	0/14984
1	D	0.27	0/11422	0.53	2/15734 (0.0%)
1	E	0.27	0/10283	0.51	0/14106
1	F	0.31	2/10246 (0.0%)	0.56	4/14055 (0.0%)
2	G	0.25	0/139	0.58	0/174
2	H	0.21	0/69	0.43	0/89
2	I	0.23	0/71	0.45	0/87
All	All	0.28	2/70551 (0.0%)	0.53	11/96925 (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	2
1	B	0	1
1	E	0	2
1	F	0	1
2	G	2	0
2	I	2	0
All	All	4	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	632	PRO	CB-CG	-10.50	0.97	1.50
1	F	632	PRO	CG-CD	-9.54	1.19	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	632	PRO	N-CD-CG	-16.73	78.11	103.20
1	F	632	PRO	CB-CG-CD	14.79	164.20	106.50
1	F	632	PRO	CA-CB-CG	-13.73	77.91	104.00
1	B	1846	PRO	CA-N-CD	-12.21	94.40	111.50
1	A	1839	PRO	CA-N-CD	-11.07	96.00	111.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	23	HYP	CA
2	G	26	HYP	CA
2	I	23	HYP	CA
2	I	26	HYP	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1522	GLY	Peptide
1	A	1527	LYS	Peptide
1	B	1527	LYS	Peptide
1	E	1527	LYS	Peptide
1	E	1725	TYR	Peptide

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	1848/1987 (93%)	1690 (92%)	150 (8%)	8 (0%)	34 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1848/1987 (93%)	1691 (92%)	150 (8%)	7 (0%)	34	72
1	C	1461/1987 (74%)	1342 (92%)	115 (8%)	4 (0%)	41	76
1	D	1531/1987 (77%)	1411 (92%)	114 (7%)	6 (0%)	34	72
1	E	1390/1987 (70%)	1289 (93%)	97 (7%)	4 (0%)	41	76
1	F	1384/1987 (70%)	1273 (92%)	108 (8%)	3 (0%)	47	82
2	G	27/64 (42%)	17 (63%)	6 (22%)	4 (15%)	0	1
2	H	12/64 (19%)	11 (92%)	0	1 (8%)	1	4
2	I	14/64 (22%)	9 (64%)	3 (21%)	2 (14%)	0	1
All	All	9515/12114 (78%)	8733 (92%)	743 (8%)	39 (0%)	38	72

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	585	ALA
1	A	1523	PRO
1	B	1523	PRO
1	E	1523	PRO
1	F	1523	PRO

5.3.2 Protein sidechains (i)

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	1451/1514 (96%)	1314 (91%)	137 (9%)	8	32
1	B	1451/1514 (96%)	1331 (92%)	120 (8%)	11	39
1	C	1149/1514 (76%)	1064 (93%)	85 (7%)	13	44
1	D	1209/1514 (80%)	1099 (91%)	110 (9%)	9	34
1	E	1081/1514 (71%)	1005 (93%)	76 (7%)	15	47
1	F	1078/1514 (71%)	1009 (94%)	69 (6%)	17	51
2	G	5/5 (100%)	5 (100%)	0	100	100
2	H	2/5 (40%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	I	3/5 (60%)	2 (67%)	1 (33%)	0 1
All	All	7429/9099 (82%)	6831 (92%)	598 (8%)	16 40

5 of 598 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	846	SER
1	F	1558	ASP
1	E	1078	THR
1	E	824	TYR
1	E	1844	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1672	GLN
1	D	1212	GLN
1	B	1536	ASN
1	C	612	GLN
1	B	1293	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

358 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	$\#\|Z\| > 2$
1	HYP	F	1857	1	6,8,9	0.52	0	5,10,12	1.58	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	HYP	I	10	2	6,8,9	0.52	0	5,10,12	1.70	1 (20%)
1	HYP	C	1916	1	6,8,9	0.50	0	5,10,12	1.18	1 (20%)
1	HYP	A	1920	1	6,8,9	0.53	0	5,10,12	1.55	1 (20%)
1	HYP	A	1917	1	6,8,9	0.51	0	5,10,12	1.59	1 (20%)
1	HYP	B	1929	1	6,8,9	0.41	0	5,10,12	1.36	1 (20%)
1	HYP	D	1901	1	6,8,9	0.37	0	5,10,12	1.18	1 (20%)
1	HYP	B	1912	1	6,8,9	0.38	0	5,10,12	1.24	1 (20%)
1	HYP	E	1870	1	6,8,9	0.48	0	5,10,12	1.56	2 (40%)
2	HYP	H	44	2	6,8,9	0.50	0	5,10,12	1.63	1 (20%)
1	HYP	F	1878	1	6,8,9	0.55	0	5,10,12	1.54	1 (20%)
1	HYP	D	1911	1	6,8,9	0.45	0	5,10,12	1.19	1 (20%)
1	HYP	F	1912	1	6,8,9	0.41	0	5,10,12	1.15	1 (20%)
2	HYP	G	43	2	6,8,9	0.49	0	5,10,12	1.47	1 (20%)
1	HYP	A	1908	1	6,8,9	0.53	0	5,10,12	2.18	3 (60%)
1	HYP	B	1878	1	6,8,9	0.51	0	5,10,12	1.84	2 (40%)
1	HYP	B	1908	1	6,8,9	0.57	0	5,10,12	2.10	3 (60%)
1	HYP	A	1864	1	6,8,9	0.51	0	5,10,12	1.48	1 (20%)
1	HYP	E	1899	1	6,8,9	0.37	0	5,10,12	1.29	1 (20%)
1	HYP	A	1873	1	6,8,9	0.47	0	5,10,12	1.21	1 (20%)
2	HYP	G	44	2	6,8,9	0.52	0	5,10,12	1.52	1 (20%)
1	HYP	D	1931	1	6,8,9	0.45	0	5,10,12	1.39	1 (20%)
1	HYP	B	1892	1	6,8,9	0.37	0	5,10,12	1.23	1 (20%)
1	HYP	D	1917	1	6,8,9	0.51	0	5,10,12	1.51	1 (20%)
1	HYP	B	1872	1	6,8,9	0.44	0	5,10,12	1.33	1 (20%)
2	HYP	G	42	2	6,8,9	0.37	0	5,10,12	1.25	1 (20%)
1	HYP	B	1906	1	6,8,9	0.39	0	5,10,12	1.16	1 (20%)
2	HYP	G	7	2	6,8,9	0.38	0	5,10,12	1.36	1 (20%)
1	HYP	C	1907	1	6,8,9	0.51	0	5,10,12	1.73	2 (40%)
1	HYP	B	1857	1	6,8,9	0.55	0	5,10,12	1.60	1 (20%)
1	HYP	D	1918	1	6,8,9	0.49	0	5,10,12	1.82	2 (40%)
1	HYP	A	1905	1	6,8,9	0.39	0	5,10,12	1.21	1 (20%)
1	HYP	E	1901	1	6,8,9	0.53	0	5,10,12	1.42	1 (20%)
2	HYP	I	29	2	6,8,9	0.43	0	5,10,12	1.20	1 (20%)
1	HYP	A	1910	1	6,8,9	0.39	0	5,10,12	1.15	1 (20%)
1	HYP	B	1890	1	6,8,9	0.45	0	5,10,12	1.19	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	C	1899	1	6,8,9	0.37	0	5,10,12	1.28	1 (20%)
1	HYP	F	1882	1	6,8,9	0.42	0	5,10,12	1.17	1 (20%)
2	HYP	G	6	2	6,8,9	0.46	0	5,10,12	1.52	1 (20%)
2	HYP	H	50	2	6,8,9	0.38	0	5,10,12	1.20	1 (20%)
1	HYP	C	1903	1	6,8,9	0.51	0	5,10,12	1.79	2 (40%)
2	HYP	G	52	2	6,8,9	0.51	0	5,10,12	1.65	1 (20%)
2	HYP	I	6	2	6,8,9	0.35	0	5,10,12	1.29	1 (20%)
1	HYP	A	1855	1	6,8,9	0.49	0	5,10,12	1.16	1 (20%)
2	HYP	G	32	2	6,8,9	0.49	0	5,10,12	1.41	1 (20%)
1	HYP	E	1907	1	6,8,9	0.44	0	5,10,12	1.64	2 (40%)
1	HYP	A	1863	1	6,8,9	0.48	0	5,10,12	1.36	1 (20%)
1	HYP	F	1902	1	6,8,9	0.50	0	5,10,12	1.69	1 (20%)
1	HYP	C	1897	1	6,8,9	0.46	0	5,10,12	1.28	1 (20%)
1	HYP	F	1913	1	6,8,9	0.38	0	5,10,12	1.24	1 (20%)
2	HYP	G	50	2	6,8,9	0.41	0	5,10,12	1.18	1 (20%)
1	HYP	F	1911	1	6,8,9	0.43	0	5,10,12	1.15	1 (20%)
2	HYP	H	52	2	6,8,9	0.49	0	5,10,12	1.73	2 (40%)
1	HYP	D	1928	1	6,8,9	0.43	0	5,10,12	1.13	1 (20%)
1	HYP	E	1866	1	6,8,9	0.54	0	5,10,12	1.41	1 (20%)
1	HYP	A	1928	1	6,8,9	0.42	0	5,10,12	1.13	1 (20%)
2	HYP	G	20	2	6,8,9	0.51	0	5,10,12	1.32	1 (20%)
1	HYP	F	1923	1	6,8,9	0.53	0	5,10,12	2.08	3 (60%)
2	HYP	I	34	2	6,8,9	0.50	0	5,10,12	1.61	1 (20%)
1	HYP	C	1929	1	6,8,9	0.38	0	5,10,12	1.25	1 (20%)
1	HYP	B	1887	1	6,8,9	0.40	0	5,10,12	1.27	1 (20%)
2	HYP	I	26	2	6,8,9	0.52	0	5,10,12	1.48	2 (40%)
1	HYP	D	1927	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	A	1913	1	6,8,9	0.38	0	5,10,12	1.27	1 (20%)
1	HYP	E	1931	1	6,8,9	0.43	0	5,10,12	1.32	1 (20%)
1	HYP	F	1915	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
2	HYP	I	17	2	6,8,9	0.43	0	5,10,12	1.20	1 (20%)
1	HYP	B	1915	1	6,8,9	0.43	0	5,10,12	1.26	1 (20%)
1	HYP	F	1890	1	6,8,9	0.39	0	5,10,12	1.15	1 (20%)
1	HYP	B	1902	1	6,8,9	0.52	0	5,10,12	1.59	1 (20%)
1	HYP	A	1882	1	6,8,9	0.40	0	5,10,12	1.21	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	B	1860	1	6,8,9	0.51	0	5,10,12	1.71	2 (40%)
2	HYP	H	56	2	6,8,9	0.44	0	5,10,12	1.24	1 (20%)
2	HYP	I	11	2	6,8,9	0.48	0	5,10,12	1.79	2 (40%)
2	HYP	I	5	2	6,8,9	0.36	0	5,10,12	1.42	1 (20%)
1	HYP	A	1887	1	6,8,9	0.41	0	5,10,12	1.23	1 (20%)
1	HYP	D	1907	1	6,8,9	0.50	0	5,10,12	1.58	1 (20%)
1	HYP	F	1927	1	6,8,9	0.39	0	5,10,12	1.14	1 (20%)
1	HYP	E	1877	1	6,8,9	0.51	0	5,10,12	1.76	2 (40%)
1	HYP	F	1917	1	6,8,9	0.51	0	5,10,12	1.39	1 (20%)
1	HYP	F	1920	1	6,8,9	0.54	0	5,10,12	1.55	1 (20%)
1	HYP	D	1920	1	6,8,9	0.53	0	5,10,12	1.48	1 (20%)
1	HYP	F	1862	1	6,8,9	0.49	0	5,10,12	1.35	1 (20%)
2	HYP	G	56	2	6,8,9	0.44	0	5,10,12	1.25	1 (20%)
1	HYP	F	1866	1	6,8,9	0.52	0	5,10,12	1.35	1 (20%)
1	HYP	B	1883	1	6,8,9	0.47	0	5,10,12	2.01	2 (40%)
2	HYP	G	33	2	6,8,9	0.51	0	5,10,12	1.61	1 (20%)
2	HYP	H	49	2	6,8,9	0.52	0	5,10,12	1.47	1 (20%)
1	HYP	B	1910	1	6,8,9	0.45	0	5,10,12	1.16	1 (20%)
1	HYP	D	1913	1	6,8,9	0.38	0	5,10,12	1.23	1 (20%)
2	HYP	G	10	2	6,8,9	0.54	0	5,10,12	1.64	1 (20%)
1	HYP	F	1908	1	6,8,9	0.57	0	5,10,12	1.79	2 (40%)
1	HYP	B	1931	1	6,8,9	0.46	0	5,10,12	1.41	1 (20%)
1	HYP	A	1923	1	6,8,9	0.52	0	5,10,12	1.88	3 (60%)
1	HYP	B	1901	1	6,8,9	0.42	0	5,10,12	1.16	1 (20%)
1	HYP	C	1912	1	6,8,9	0.38	0	5,10,12	1.18	1 (20%)
1	HYP	C	1921	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	E	1930	1	6,8,9	0.36	0	5,10,12	1.21	1 (20%)
1	HYP	F	1907	1	6,8,9	0.52	0	5,10,12	1.74	2 (40%)
2	HYP	H	40	2	6,8,9	0.39	0	5,10,12	1.12	1 (20%)
1	HYP	A	1927	1	6,8,9	0.52	0	5,10,12	1.41	1 (20%)
1	HYP	E	1920	1	6,8,9	0.53	0	5,10,12	1.45	1 (20%)
2	HYP	I	9	2	6,8,9	0.51	0	5,10,12	1.55	1 (20%)
1	HYP	A	1915	1	6,8,9	0.40	0	5,10,12	1.23	1 (20%)
1	HYP	A	1898	1	6,8,9	0.42	0	5,10,12	1.21	1 (20%)
2	HYP	G	51	2	6,8,9	0.51	0	5,10,12	1.59	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HYP	G	11	2	6,8,9	0.48	0	5,10,12	1.93	2 (40%)
1	HYP	B	1921	1	6,8,9	0.40	0	5,10,12	1.22	1 (20%)
1	HYP	D	1930	1	6,8,9	0.40	0	5,10,12	1.26	1 (20%)
1	HYP	F	1929	1	6,8,9	0.43	0	5,10,12	1.19	1 (20%)
1	HYP	A	1932	1	6,8,9	0.52	0	5,10,12	1.78	3 (60%)
2	HYP	I	2	2	6,8,9	0.48	0	5,10,12	1.45	1 (20%)
2	HYP	H	41	2	6,8,9	0.43	0	5,10,12	1.27	1 (20%)
1	HYP	F	1880	1	6,8,9	0.42	0	5,10,12	1.42	1 (20%)
1	HYP	A	1878	1	6,8,9	0.52	0	5,10,12	1.70	2 (40%)
1	HYP	C	1906	1	6,8,9	0.40	0	5,10,12	1.16	1 (20%)
1	HYP	B	1888	1	6,8,9	0.54	0	5,10,12	1.68	2 (40%)
1	HYP	E	1856	1	6,8,9	0.51	0	5,10,12	1.30	1 (20%)
2	HYP	H	37	2	6,8,9	0.49	0	5,10,12	1.15	1 (20%)
1	HYP	E	1863	1	6,8,9	0.50	0	5,10,12	1.42	1 (20%)
1	HYP	B	1866	1	6,8,9	0.48	0	5,10,12	1.30	1 (20%)
1	HYP	E	1885	1	6,8,9	0.51	0	5,10,12	1.39	1 (20%)
1	HYP	E	1864	1	6,8,9	0.54	0	5,10,12	1.55	1 (20%)
2	HYP	I	20	2	6,8,9	0.49	0	5,10,12	1.27	1 (20%)
2	HYP	G	41	2	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	A	1857	1	6,8,9	0.50	0	5,10,12	1.32	1 (20%)
2	HYP	G	47	2	6,8,9	0.39	0	5,10,12	1.27	1 (20%)
1	HYP	E	1914	1	6,8,9	0.50	0	5,10,12	1.25	1 (20%)
1	HYP	F	1883	1	6,8,9	0.48	0	5,10,12	1.96	2 (40%)
1	HYP	B	1885	1	6,8,9	0.42	0	5,10,12	1.16	1 (20%)
1	HYP	E	1855	1	6,8,9	0.51	0	5,10,12	1.20	1 (20%)
1	HYP	A	1902	1	6,8,9	0.54	0	5,10,12	1.60	1 (20%)
1	HYP	B	1864	1	6,8,9	0.51	0	5,10,12	1.47	1 (20%)
2	HYP	G	34	2	6,8,9	0.48	0	5,10,12	1.67	2 (40%)
2	HYP	H	42	2	6,8,9	0.37	0	5,10,12	1.23	1 (20%)
1	HYP	A	1922	1	6,8,9	0.55	0	5,10,12	1.72	1 (20%)
1	HYP	A	1916	1	6,8,9	0.52	0	5,10,12	1.45	1 (20%)
1	HYP	F	1865	1	6,8,9	0.55	0	5,10,12	1.64	1 (20%)
2	HYP	G	46	2	6,8,9	0.52	0	5,10,12	1.54	1 (20%)
1	HYP	F	1870	1	6,8,9	0.50	0	5,10,12	1.57	1 (20%)
1	HYP	D	1910	1	6,8,9	0.43	0	5,10,12	1.14	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	A	1880	1	6,8,9	0.41	0	5,10,12	1.38	1 (20%)
1	HYP	F	1888	1	6,8,9	0.44	0	5,10,12	1.85	2 (40%)
1	HYP	D	1905	1	6,8,9	0.39	0	5,10,12	1.18	1 (20%)
1	HYP	F	1887	1	6,8,9	0.40	0	5,10,12	1.15	1 (20%)
1	HYP	F	1858	1	6,8,9	0.54	0	5,10,12	1.69	1 (20%)
1	HYP	D	1915	1	6,8,9	0.39	0	5,10,12	1.23	1 (20%)
1	HYP	B	1928	1	6,8,9	0.53	0	5,10,12	1.52	1 (20%)
1	HYP	E	1868	1	6,8,9	0.52	0	5,10,12	1.79	2 (40%)
1	HYP	D	1906	1	6,8,9	0.44	0	5,10,12	1.34	1 (20%)
1	HYP	F	1867	1	6,8,9	0.50	0	5,10,12	1.64	1 (20%)
1	HYP	B	1862	1	6,8,9	0.53	0	5,10,12	1.45	1 (20%)
1	HYP	E	1913	1	6,8,9	0.36	0	5,10,12	1.18	1 (20%)
2	HYP	I	8	2	6,8,9	0.51	0	5,10,12	1.50	1 (20%)
1	HYP	A	1930	1	6,8,9	0.52	0	5,10,12	1.66	1 (20%)
1	HYP	B	1867	1	6,8,9	0.49	0	5,10,12	1.64	1 (20%)
1	HYP	E	1912	1	6,8,9	0.46	0	5,10,12	1.27	1 (20%)
1	HYP	F	1868	1	6,8,9	0.52	0	5,10,12	2.02	3 (60%)
1	HYP	A	1883	1	6,8,9	0.50	0	5,10,12	2.15	2 (40%)
1	HYP	B	1899	1	6,8,9	0.38	0	5,10,12	1.42	1 (20%)
2	HYP	G	5	2	6,8,9	0.36	0	5,10,12	1.17	1 (20%)
1	HYP	B	1920	1	6,8,9	0.53	0	5,10,12	1.37	1 (20%)
1	HYP	A	1890	1	6,8,9	0.48	0	5,10,12	1.23	1 (20%)
1	HYP	F	1860	1	6,8,9	0.57	0	5,10,12	1.56	1 (20%)
1	HYP	B	1877	1	6,8,9	0.51	0	5,10,12	1.64	1 (20%)
1	HYP	E	1905	1	6,8,9	0.43	0	5,10,12	1.23	1 (20%)
2	HYP	G	3	2	6,8,9	0.53	0	5,10,12	1.61	1 (20%)
1	HYP	D	1898	1	6,8,9	0.41	0	5,10,12	1.23	1 (20%)
1	HYP	A	1856	1	6,8,9	0.52	0	5,10,12	1.33	1 (20%)
1	HYP	E	1915	1	6,8,9	0.37	0	5,10,12	1.14	1 (20%)
1	HYP	C	1910	1	6,8,9	0.46	0	5,10,12	1.17	1 (20%)
1	HYP	E	1894	1	6,8,9	0.38	0	5,10,12	1.25	1 (20%)
1	HYP	C	1914	1	6,8,9	0.49	0	5,10,12	1.42	1 (20%)
1	HYP	C	1905	1	6,8,9	0.42	0	5,10,12	1.17	1 (20%)
1	HYP	D	1932	1	6,8,9	0.53	0	5,10,12	1.81	3 (60%)
1	HYP	E	1882	1	6,8,9	0.41	0	5,10,12	1.22	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	F	1914	1	6,8,9	0.51	0	5,10,12	1.45	1 (20%)
1	HYP	A	1865	1	6,8,9	0.51	0	5,10,12	1.65	1 (20%)
1	HYP	F	1930	1	6,8,9	0.49	0	5,10,12	1.52	1 (20%)
1	HYP	A	1867	1	6,8,9	0.48	0	5,10,12	1.58	1 (20%)
2	HYP	G	8	2	6,8,9	0.50	0	5,10,12	1.59	1 (20%)
1	HYP	B	1930	1	6,8,9	0.52	0	5,10,12	1.62	1 (20%)
1	HYP	C	1902	1	6,8,9	0.54	0	5,10,12	1.77	2 (40%)
1	HYP	F	1875	1	6,8,9	0.39	0	5,10,12	1.15	1 (20%)
1	HYP	A	1911	1	6,8,9	0.39	0	5,10,12	1.20	1 (20%)
1	HYP	A	1858	1	6,8,9	0.38	0	5,10,12	1.22	1 (20%)
1	HYP	F	1921	1	6,8,9	0.37	0	5,10,12	1.34	1 (20%)
1	HYP	E	1862	1	6,8,9	0.53	0	5,10,12	1.47	1 (20%)
1	HYP	F	1897	1	6,8,9	0.45	0	5,10,12	1.28	1 (20%)
1	HYP	B	1903	1	6,8,9	0.55	0	5,10,12	1.92	3 (60%)
1	HYP	F	1872	1	6,8,9	0.48	0	5,10,12	1.23	1 (20%)
1	HYP	E	1918	1	6,8,9	0.48	0	5,10,12	1.70	2 (40%)
1	HYP	F	1855	1	6,8,9	0.56	0	5,10,12	1.43	1 (20%)
1	HYP	A	1907	1	6,8,9	0.44	0	5,10,12	1.86	2 (40%)
1	HYP	D	1929	1	6,8,9	0.38	0	5,10,12	1.20	1 (20%)
1	HYP	E	1906	1	6,8,9	0.37	0	5,10,12	1.22	1 (20%)
1	HYP	D	1899	1	6,8,9	0.46	0	5,10,12	1.70	2 (40%)
1	HYP	E	1932	1	6,8,9	0.52	0	5,10,12	1.45	1 (20%)
1	HYP	A	1899	1	6,8,9	0.38	0	5,10,12	1.39	1 (20%)
2	HYP	G	26	2	6,8,9	0.38	0	5,10,12	1.15	1 (20%)
1	HYP	B	1863	1	6,8,9	0.51	0	5,10,12	1.43	1 (20%)
1	HYP	A	1866	1	6,8,9	0.51	0	5,10,12	1.46	1 (20%)
2	HYP	I	33	2	6,8,9	0.47	0	5,10,12	1.25	1 (20%)
1	HYP	A	1903	1	6,8,9	0.55	0	5,10,12	1.77	2 (40%)
1	HYP	C	1920	1	6,8,9	0.52	0	5,10,12	1.47	1 (20%)
1	HYP	A	1872	1	6,8,9	0.47	0	5,10,12	1.31	1 (20%)
1	HYP	A	1860	1	6,8,9	0.52	0	5,10,12	1.77	2 (40%)
1	HYP	A	1901	1	6,8,9	0.40	0	5,10,12	1.16	1 (20%)
1	HYP	A	1897	1	6,8,9	0.43	0	5,10,12	1.26	1 (20%)
1	HYP	E	1898	1	6,8,9	0.41	0	5,10,12	1.18	1 (20%)
2	HYP	H	48	2	6,8,9	0.38	0	5,10,12	1.20	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	D	1922	1	6,8,9	0.50	0	5,10,12	1.40	1 (20%)
1	HYP	D	1916	1	6,8,9	0.51	0	5,10,12	1.39	1 (20%)
1	HYP	B	1905	1	6,8,9	0.39	0	5,10,12	1.19	1 (20%)
1	HYP	D	1923	1	6,8,9	0.50	0	5,10,12	1.82	3 (60%)
2	HYP	H	45	2	6,8,9	0.38	0	5,10,12	1.19	1 (20%)
2	HYP	I	14	2	6,8,9	0.37	0	5,10,12	1.26	1 (20%)
1	HYP	A	1931	1	6,8,9	0.49	0	5,10,12	1.41	1 (20%)
1	HYP	C	1908	1	6,8,9	0.54	0	5,10,12	1.91	3 (60%)
1	HYP	F	1893	1	6,8,9	0.38	0	5,10,12	1.30	1 (20%)
1	HYP	D	1914	1	6,8,9	0.46	0	5,10,12	1.10	1 (20%)
2	HYP	H	43	2	6,8,9	0.49	0	5,10,12	1.48	1 (20%)
1	HYP	A	1929	1	6,8,9	0.40	0	5,10,12	1.24	1 (20%)
1	HYP	B	1894	1	6,8,9	0.50	0	5,10,12	1.95	2 (40%)
2	HYP	H	47	2	6,8,9	0.39	0	5,10,12	1.26	1 (20%)
1	HYP	B	1882	1	6,8,9	0.39	0	5,10,12	1.21	1 (20%)
1	HYP	C	1917	1	6,8,9	0.53	0	5,10,12	1.46	1 (20%)
1	HYP	F	1928	1	6,8,9	0.44	0	5,10,12	1.25	1 (20%)
2	HYP	G	29	2	6,8,9	0.41	0	5,10,12	1.21	1 (20%)
1	HYP	A	1875	1	6,8,9	0.45	0	5,10,12	1.19	1 (20%)
1	HYP	A	1921	1	6,8,9	0.40	0	5,10,12	1.37	1 (20%)
1	HYP	C	1918	1	6,8,9	0.52	0	5,10,12	1.76	2 (40%)
1	HYP	F	1922	1	6,8,9	0.54	0	5,10,12	1.57	1 (20%)
1	HYP	E	1916	1	6,8,9	0.51	0	5,10,12	1.33	1 (20%)
1	HYP	A	1877	1	6,8,9	0.47	0	5,10,12	1.32	1 (20%)
1	HYP	E	1873	1	6,8,9	0.46	0	5,10,12	1.32	1 (20%)
1	HYP	F	1892	1	6,8,9	0.35	0	5,10,12	1.24	1 (20%)
1	HYP	F	1906	1	6,8,9	0.42	0	5,10,12	1.30	1 (20%)
1	HYP	B	1918	1	6,8,9	0.56	0	5,10,12	1.59	1 (20%)
1	HYP	F	1885	1	6,8,9	0.45	0	5,10,12	1.22	1 (20%)
1	HYP	F	1894	1	6,8,9	0.48	0	5,10,12	1.93	2 (40%)
1	HYP	E	1880	1	6,8,9	0.48	0	5,10,12	1.44	1 (20%)
2	HYP	G	48	2	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
2	HYP	I	4	2	6,8,9	0.49	0	5,10,12	1.27	1 (20%)
1	HYP	B	1868	1	6,8,9	0.49	0	5,10,12	1.97	2 (40%)
2	HYP	G	37	2	6,8,9	0.45	0	5,10,12	0.96	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	E	1865	1	6,8,9	0.52	0	5,10,12	1.63	1 (20%)
1	HYP	A	1862	1	6,8,9	0.53	0	5,10,12	1.43	1 (20%)
1	HYP	B	1913	1	6,8,9	0.38	0	5,10,12	1.31	1 (20%)
1	HYP	F	1931	1	6,8,9	0.41	0	5,10,12	1.35	1 (20%)
2	HYP	I	1	2	6,8,9	0.49	0	5,10,12	1.25	1 (20%)
2	HYP	G	23	2	6,8,9	0.39	0	5,10,12	1.46	1 (20%)
1	HYP	C	1928	1	6,8,9	0.39	0	5,10,12	1.26	1 (20%)
1	HYP	E	1922	1	6,8,9	0.55	0	5,10,12	1.52	1 (20%)
1	HYP	A	1892	1	6,8,9	0.37	0	5,10,12	1.34	1 (20%)
1	HYP	E	1890	1	6,8,9	0.41	0	5,10,12	1.12	1 (20%)
1	HYP	B	1898	1	6,8,9	0.40	0	5,10,12	1.25	1 (20%)
1	HYP	F	1918	1	6,8,9	0.49	0	5,10,12	1.98	2 (40%)
1	HYP	F	1877	1	6,8,9	0.51	0	5,10,12	1.55	1 (20%)
1	HYP	D	1912	1	6,8,9	0.46	0	5,10,12	1.30	1 (20%)
1	HYP	E	1888	1	6,8,9	0.44	0	5,10,12	1.82	2 (40%)
2	HYP	H	46	2	6,8,9	0.48	0	5,10,12	1.60	1 (20%)
1	HYP	F	1932	1	6,8,9	0.49	0	5,10,12	1.71	2 (40%)
1	HYP	E	1911	1	6,8,9	0.41	0	5,10,12	1.22	1 (20%)
1	HYP	B	1916	1	6,8,9	0.52	0	5,10,12	1.45	1 (20%)
1	HYP	E	1883	1	6,8,9	0.47	0	5,10,12	2.01	2 (40%)
1	HYP	A	1912	1	6,8,9	0.39	0	5,10,12	1.21	1 (20%)
1	HYP	C	1913	1	6,8,9	0.38	0	5,10,12	1.24	1 (20%)
1	HYP	B	1873	1	6,8,9	0.48	0	5,10,12	1.35	1 (20%)
1	HYP	B	1865	1	6,8,9	0.49	0	5,10,12	1.68	1 (20%)
1	HYP	E	1858	1	6,8,9	0.51	0	5,10,12	1.67	1 (20%)
1	HYP	E	1887	1	6,8,9	0.44	0	5,10,12	1.22	1 (20%)
1	HYP	E	1928	1	6,8,9	0.43	0	5,10,12	1.22	1 (20%)
1	HYP	D	1897	1	6,8,9	0.42	0	5,10,12	1.23	1 (20%)
2	HYP	G	17	2	6,8,9	0.37	0	5,10,12	1.26	1 (20%)
2	HYP	I	23	2	6,8,9	0.37	0	5,10,12	1.41	1 (20%)
1	HYP	E	1867	1	6,8,9	0.53	0	5,10,12	1.78	1 (20%)
1	HYP	F	1864	1	6,8,9	0.51	0	5,10,12	1.43	1 (20%)
1	HYP	A	1885	1	6,8,9	0.38	0	5,10,12	1.20	1 (20%)
1	HYP	C	1911	1	6,8,9	0.42	0	5,10,12	1.20	1 (20%)
2	HYP	G	1	2	6,8,9	0.47	0	5,10,12	1.19	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	HYP	B	1855	1	6,8,9	0.51	0	5,10,12	1.17	1 (20%)
1	HYP	D	1903	1	6,8,9	0.55	0	5,10,12	1.74	2 (40%)
1	HYP	B	1914	1	6,8,9	0.47	0	5,10,12	1.52	1 (20%)
1	HYP	F	1901	1	6,8,9	0.38	0	5,10,12	1.14	1 (20%)
2	HYP	G	40	2	6,8,9	0.39	0	5,10,12	1.14	1 (20%)
1	HYP	F	1863	1	6,8,9	0.51	0	5,10,12	1.39	1 (20%)
1	HYP	C	1901	1	6,8,9	0.37	0	5,10,12	1.16	1 (20%)
1	HYP	C	1923	1	6,8,9	0.53	0	5,10,12	1.93	2 (40%)
1	HYP	F	1916	1	6,8,9	0.49	0	5,10,12	1.26	1 (20%)
1	HYP	E	1893	1	6,8,9	0.43	0	5,10,12	1.24	1 (20%)
1	HYP	F	1898	1	6,8,9	0.42	0	5,10,12	1.16	1 (20%)
1	HYP	E	1917	1	6,8,9	0.53	0	5,10,12	1.37	1 (20%)
1	HYP	A	1870	1	6,8,9	0.50	0	5,10,12	1.57	2 (40%)
1	HYP	E	1878	1	6,8,9	0.52	0	5,10,12	1.90	2 (40%)
1	HYP	E	1860	1	6,8,9	0.55	0	5,10,12	1.86	3 (60%)
1	HYP	C	1927	1	6,8,9	0.40	0	5,10,12	1.20	1 (20%)
1	HYP	B	1922	1	6,8,9	0.53	0	5,10,12	1.61	1 (20%)
1	HYP	E	1903	1	6,8,9	0.51	0	5,10,12	1.87	2 (40%)
2	HYP	G	14	2	6,8,9	0.39	0	5,10,12	1.32	1 (20%)
2	HYP	G	9	2	6,8,9	0.48	0	5,10,12	1.76	2 (40%)
1	HYP	C	1915	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	C	1898	1	6,8,9	0.46	0	5,10,12	1.19	1 (20%)
1	HYP	E	1872	1	6,8,9	0.52	0	5,10,12	1.27	1 (20%)
1	HYP	D	1908	1	6,8,9	0.54	0	5,10,12	1.70	2 (40%)
1	HYP	F	1905	1	6,8,9	0.37	0	5,10,12	1.26	1 (20%)
1	HYP	E	1897	1	6,8,9	0.45	0	5,10,12	1.19	1 (20%)
1	HYP	C	1932	1	6,8,9	0.51	0	5,10,12	1.84	2 (40%)
1	HYP	E	1923	1	6,8,9	0.48	0	5,10,12	2.08	2 (40%)
1	HYP	E	1929	1	6,8,9	0.36	0	5,10,12	1.23	1 (20%)
1	HYP	F	1903	1	6,8,9	0.55	0	5,10,12	1.70	2 (40%)
1	HYP	D	1921	1	6,8,9	0.43	0	5,10,12	1.22	1 (20%)
1	HYP	B	1858	1	6,8,9	0.36	0	5,10,12	1.38	1 (20%)
1	HYP	E	1927	1	6,8,9	0.40	0	5,10,12	1.19	1 (20%)
2	HYP	I	32	2	6,8,9	0.42	0	5,10,12	1.15	1 (20%)
1	HYP	A	1868	1	6,8,9	0.50	0	5,10,12	1.92	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	A	1893	1	6,8,9	0.37	0	5,10,12	1.28	1 (20%)
1	HYP	B	1870	1	6,8,9	0.52	0	5,10,12	1.54	1 (20%)
1	HYP	B	1897	1	6,8,9	0.43	0	5,10,12	1.14	1 (20%)
1	HYP	E	1908	1	6,8,9	0.54	0	5,10,12	2.07	3 (60%)
1	HYP	A	1888	1	6,8,9	0.52	0	5,10,12	1.52	1 (20%)
1	HYP	F	1910	1	6,8,9	0.40	0	5,10,12	1.13	1 (20%)
1	HYP	E	1875	1	6,8,9	0.45	0	5,10,12	1.17	1 (20%)
1	HYP	B	1923	1	6,8,9	0.54	0	5,10,12	1.96	3 (60%)
1	HYP	E	1921	1	6,8,9	0.38	0	5,10,12	1.31	1 (20%)
1	HYP	C	1931	1	6,8,9	0.44	0	5,10,12	1.38	1 (20%)
1	HYP	B	1856	1	6,8,9	0.49	0	5,10,12	1.26	1 (20%)
1	HYP	B	1875	1	6,8,9	0.42	0	5,10,12	1.16	1 (20%)
2	HYP	G	4	2	6,8,9	0.52	0	5,10,12	1.38	1 (20%)
1	HYP	E	1857	1	6,8,9	0.52	0	5,10,12	1.56	1 (20%)
2	HYP	I	7	2	6,8,9	0.50	0	5,10,12	1.63	1 (20%)
2	HYP	I	3	2	6,8,9	0.52	0	5,10,12	1.63	1 (20%)
2	HYP	H	51	2	6,8,9	0.50	0	5,10,12	1.62	1 (20%)
1	HYP	B	1880	1	6,8,9	0.42	0	5,10,12	1.34	1 (20%)
1	HYP	A	1894	1	6,8,9	0.50	0	5,10,12	1.88	2 (40%)
1	HYP	B	1927	1	6,8,9	0.41	0	5,10,12	1.20	1 (20%)
1	HYP	B	1893	1	6,8,9	0.40	0	5,10,12	1.23	1 (20%)
2	HYP	G	2	2	6,8,9	0.50	0	5,10,12	1.63	1 (20%)
2	HYP	H	55	2	6,8,9	0.44	0	5,10,12	1.19	1 (20%)
1	HYP	C	1922	1	6,8,9	0.53	0	5,10,12	1.47	1 (20%)
1	HYP	B	1932	1	6,8,9	0.51	0	5,10,12	1.55	1 (20%)
1	HYP	E	1892	1	6,8,9	0.38	0	5,10,12	1.27	1 (20%)
1	HYP	E	1902	1	6,8,9	0.48	0	5,10,12	1.67	1 (20%)
1	HYP	A	1914	1	6,8,9	0.50	0	5,10,12	1.38	1 (20%)
1	HYP	A	1918	1	6,8,9	0.51	0	5,10,12	1.60	1 (20%)
1	HYP	F	1873	1	6,8,9	0.45	0	5,10,12	1.27	1 (20%)
1	HYP	B	1911	1	6,8,9	0.39	0	5,10,12	1.18	1 (20%)
2	HYP	G	55	2	6,8,9	0.46	0	5,10,12	1.19	1 (20%)
2	HYP	G	45	2	6,8,9	0.41	0	5,10,12	1.26	1 (20%)
1	HYP	D	1902	1	6,8,9	0.49	0	5,10,12	1.74	2 (40%)
1	HYP	B	1907	1	6,8,9	0.51	0	5,10,12	1.65	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	A	1906	1	6,8,9	0.39	0	5,10,12	1.35	1 (20%)
1	HYP	F	1899	1	6,8,9	0.37	0	5,10,12	1.29	1 (20%)
1	HYP	B	1917	1	6,8,9	0.54	0	5,10,12	1.65	1 (20%)
1	HYP	C	1930	1	6,8,9	0.53	0	5,10,12	1.72	1 (20%)
1	HYP	E	1910	1	6,8,9	0.42	0	5,10,12	1.18	1 (20%)
2	HYP	G	49	2	6,8,9	0.51	0	5,10,12	1.48	1 (20%)
1	HYP	F	1856	1	6,8,9	0.52	0	5,10,12	1.35	1 (20%)

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
1	HYP	F	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	I	10	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1870	1	-	0/0/11/13	0/1/1/1
2	HYP	H	44	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1912	1	-	0/0/11/13	0/1/1/1
2	HYP	G	43	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1873	1	-	0/0/11/13	0/1/1/1
2	HYP	G	44	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1872	1	-	0/0/11/13	0/1/1/1
2	HYP	G	42	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1906	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	G	7	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1857	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1901	1	-	0/0/11/13	0/1/1/1
2	HYP	I	29	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1882	1	-	0/0/11/13	0/1/1/1
2	HYP	G	6	2	-	0/0/11/13	0/1/1/1
2	HYP	H	50	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1903	1	-	0/0/11/13	0/1/1/1
2	HYP	G	52	2	-	0/0/11/13	0/1/1/1
2	HYP	I	6	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1855	1	-	0/0/11/13	0/1/1/1
2	HYP	G	32	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	G	50	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1911	1	-	0/0/11/13	0/1/1/1
2	HYP	H	52	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1928	1	-	0/0/11/13	0/1/1/1
2	HYP	G	20	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	I	34	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1887	1	-	0/0/11/13	0/1/1/1
2	HYP	I	26	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	D	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1915	1	-	0/0/11/13	0/1/1/1
2	HYP	I	17	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1890	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1860	1	-	0/0/11/13	0/1/1/1
2	HYP	H	56	2	-	0/0/11/13	0/1/1/1
2	HYP	I	11	2	-	0/0/11/13	0/1/1/1
2	HYP	I	5	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1862	1	-	0/0/11/13	0/1/1/1
2	HYP	G	56	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1883	1	-	0/0/11/13	0/1/1/1
2	HYP	G	33	2	-	0/0/11/13	0/1/1/1
2	HYP	H	49	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	G	10	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1907	1	-	0/0/11/13	0/1/1/1
2	HYP	H	40	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1920	1	-	0/0/11/13	0/1/1/1
2	HYP	I	9	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1898	1	-	0/0/11/13	0/1/1/1
2	HYP	G	51	2	-	0/0/11/13	0/1/1/1
2	HYP	G	11	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1932	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	I	2	2	-	0/0/11/13	0/1/1/1
2	HYP	H	41	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1856	1	-	0/0/11/13	0/1/1/1
2	HYP	H	37	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1864	1	-	0/0/11/13	0/1/1/1
2	HYP	I	20	2	-	0/0/11/13	0/1/1/1
2	HYP	G	41	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	G	47	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1864	1	-	0/0/11/13	0/1/1/1
2	HYP	G	34	2	-	0/0/11/13	0/1/1/1
2	HYP	H	42	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1865	1	-	0/0/11/13	0/1/1/1
2	HYP	G	46	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1913	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	I	8	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1899	1	-	0/0/11/13	0/1/1/1
2	HYP	G	5	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1905	1	-	0/0/11/13	0/1/1/1
2	HYP	G	3	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1867	1	-	0/0/11/13	0/1/1/1
2	HYP	G	8	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1929	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1932	1	-	0/0/11/13	0/1/1/1
2	HYP	G	26	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	A	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1866	1	-	0/0/11/13	0/1/1/1
2	HYP	I	33	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1898	1	-	0/0/11/13	0/1/1/1
2	HYP	H	48	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1923	1	-	0/0/11/13	0/1/1/1
2	HYP	H	45	2	-	0/0/11/13	0/1/1/1
2	HYP	I	14	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1914	1	-	0/0/11/13	0/1/1/1
2	HYP	H	43	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1894	1	-	0/0/11/13	0/1/1/1
2	HYP	H	47	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1928	1	-	0/0/11/13	0/1/1/1
2	HYP	G	29	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1892	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1885	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1880	1	-	0/0/11/13	0/1/1/1
2	HYP	G	48	2	-	0/0/11/13	0/1/1/1
2	HYP	I	4	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1868	1	-	0/0/11/13	0/1/1/1
2	HYP	G	37	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	G	23	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	F	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	I	1	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1888	1	-	0/0/11/13	0/1/1/1
2	HYP	H	46	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	G	17	2	-	0/0/11/13	0/1/1/1
2	HYP	I	23	2	1/1/2/4	0/0/11/13	0/1/1/1
1	HYP	E	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1885	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	C	1911	1	-	0/0/11/13	0/1/1/1
2	HYP	G	1	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1901	1	-	0/0/11/13	0/1/1/1
2	HYP	G	40	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1903	1	-	0/0/11/13	0/1/1/1
2	HYP	G	14	2	-	0/0/11/13	0/1/1/1
2	HYP	G	9	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	D	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1927	1	-	0/0/11/13	0/1/1/1
2	HYP	I	32	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1908	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1888	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1875	1	-	0/0/11/13	0/1/1/1
2	HYP	G	4	2	-	0/0/11/13	0/1/1/1
1	HYP	E	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	I	7	2	-	0/0/11/13	0/1/1/1
2	HYP	I	3	2	-	0/0/11/13	0/1/1/1
2	HYP	H	51	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1893	1	-	0/0/11/13	0/1/1/1
2	HYP	G	2	2	-	0/0/11/13	0/1/1/1
2	HYP	H	55	2	-	0/0/11/13	0/1/1/1
1	HYP	C	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1911	1	-	0/0/11/13	0/1/1/1
2	HYP	G	55	2	-	0/0/11/13	0/1/1/1
2	HYP	G	45	2	-	0/0/11/13	0/1/1/1
1	HYP	D	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	F	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	C	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	E	1910	1	-	0/0/11/13	0/1/1/1
2	HYP	G	49	2	-	0/0/11/13	0/1/1/1
1	HYP	F	1856	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 434 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1883	HYP	CG-CB-CA	-3.50	99.55	103.96
1	A	1883	HYP	CG-CB-CA	-3.47	99.59	103.96
1	E	1923	HYP	CG-CB-CA	-3.37	99.71	103.96
1	F	1918	HYP	CG-CB-CA	-3.31	99.79	103.96
1	B	1883	HYP	CG-CB-CA	-3.27	99.84	103.96

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	23	HYP	CA
2	I	23	HYP	CA
2	G	26	HYP	CA
2	I	26	HYP	CA

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

1348 monosaccharides 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	$\#\|Z\| > 2$
3	FUB	0	1	3	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
3	FUB	0	2	3	9,9,10	0.55	0	10,12,14	0.90	0
3	FUB	0	3	3	9,9,10	0.58	0	10,12,14	0.96	0
3	FUB	0A	1	3	9,9,10	0.57	0	10,12,14	0.98	1 (10%)
3	FUB	0A	2	3	9,9,10	0.54	0	10,12,14	0.78	0
3	FUB	0A	3	3	9,9,10	0.56	0	10,12,14	0.90	0
6	FUB	0B	1	6	9,9,10	0.57	0	10,12,14	1.01	0
6	FUB	0B	2	6	9,9,10	0.58	0	10,12,14	1.23	1 (10%)
6	GZL	0B	3	6	11,11,12	6.99	6 (54%)	14,15,17	3.96	4 (28%)
6	FUB	0C	1	6	9,9,10	0.59	0	10,12,14	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FUB	0C	2	6	9,9,10	0.57	0	10,12,14	1.17	1 (10%)
6	GZL	0C	3	6	11,11,12	6.70	7 (63%)	14,15,17	1.49	2 (14%)
13	FUB	0D	1	13	9,9,10	0.59	0	10,12,14	0.88	0
13	FUB	0D	2	13	9,9,10	0.57	0	10,12,14	1.04	0
13	GZL	0D	3	13	11,11,12	6.70	7 (63%)	14,15,17	1.50	3 (21%)
13	AHR	0D	4	13	9,9,10	0.56	0	10,12,14	0.89	0
18	FUB	0E	1	18	9,9,10	0.59	0	10,12,14	0.99	0
18	FUB	0E	2	18	9,9,10	0.56	0	10,12,14	0.87	0
18	GZL	0E	3	18	11,11,12	6.73	7 (63%)	14,15,17	1.45	2 (14%)
18	AHR	0E	4	18	9,9,10	0.58	0	10,12,14	0.96	0
18	AHR	0E	5	18	9,9,10	0.58	0	10,12,14	1.08	1 (10%)
3	FUB	1	1	3	9,9,10	0.57	0	10,12,14	0.82	0
3	FUB	1	2	3	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	1	3	3	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
10	FUB	1A	1	10	9,9,10	0.52	0	10,12,14	1.11	1 (10%)
10	FUB	1A	2	10	9,9,10	0.54	0	10,12,14	0.76	0
10	FUB	1A	3	10	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
10	AHR	1A	4	10	9,9,10	0.58	0	10,12,14	0.85	1 (10%)
10	AHR	1A	5	10	9,9,10	0.57	0	10,12,14	0.96	1 (10%)
13	FUB	1B	1	13	9,9,10	0.55	0	10,12,14	0.86	0
13	FUB	1B	2	13	9,9,10	0.57	0	10,12,14	0.88	0
13	GZL	1B	3	13	11,11,12	6.77	7 (63%)	14,15,17	1.37	1 (7%)
13	AHR	1B	4	13	9,9,10	0.57	0	10,12,14	0.98	0
6	FUB	1C	1	6	9,9,10	0.55	0	10,12,14	0.70	0
6	FUB	1C	2	6	9,9,10	0.57	0	10,12,14	0.89	0
6	GZL	1C	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.58	2 (14%)
15	FUB	1D	1	15	9,9,10	0.58	0	10,12,14	1.00	0
15	FUB	1D	2	15	9,9,10	0.59	0	10,12,14	0.97	0
15	GZL	1D	3	15	11,11,12	6.74	7 (63%)	14,15,17	1.30	1 (7%)
15	AHR	1D	4	15	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
15	AHR	1D	5	15	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
19	FUB	1E	1	19	9,9,10	0.56	0	10,12,14	1.12	1 (10%)
19	FUB	1E	2	19	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
19	GZL	1E	3	19	11,11,12	6.72	7 (63%)	14,15,17	1.64	2 (14%)
19	AHR	1E	4	19	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
3	FUB	2	1	3	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	2	2	3	9,9,10	0.54	0	10,12,14	0.74	0
3	FUB	2	3	3	9,9,10	0.57	0	10,12,14	1.01	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	FUB	2A	1	13	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
13	FUB	2A	2	13	9,9,10	0.48	0	10,12,14	1.37	2 (20%)
13	GZL	2A	3	13	11,11,12	6.85	7 (63%)	14,15,17	0.98	0
13	AHR	2A	4	13	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
13	FUB	2B	1	13	9,9,10	0.57	0	10,12,14	1.04	0
13	FUB	2B	2	13	9,9,10	0.57	0	10,12,14	0.89	0
13	GZL	2B	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.52	2 (14%)
13	AHR	2B	4	13	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
6	FUB	2C	1	6	9,9,10	0.59	0	10,12,14	0.93	0
6	FUB	2C	2	6	9,9,10	0.58	0	10,12,14	1.10	1 (10%)
6	GZL	2C	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.57	2 (14%)
15	FUB	2D	1	15	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
15	FUB	2D	2	15	9,9,10	0.59	0	10,12,14	0.91	0
15	GZL	2D	3	15	11,11,12	6.74	7 (63%)	14,15,17	1.49	2 (14%)
15	AHR	2D	4	15	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
15	AHR	2D	5	15	9,9,10	0.59	0	10,12,14	0.98	0
10	FUB	3	1	10	9,9,10	0.55	0	10,12,14	1.10	1 (10%)
10	FUB	3	2	10	9,9,10	0.55	0	10,12,14	0.66	0
10	FUB	3	3	10	9,9,10	0.60	0	10,12,14	1.06	1 (10%)
10	AHR	3	4	10	9,9,10	0.57	0	10,12,14	0.95	0
10	AHR	3	5	10	9,9,10	0.58	0	10,12,14	0.88	1 (10%)
6	FUB	3A	1	6	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
6	FUB	3A	2	6	9,9,10	0.54	0	10,12,14	1.17	1 (10%)
6	GZL	3A	3	6	11,11,12	6.88	6 (54%)	14,15,17	4.71	4 (28%)
6	FUB	3B	1	6	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
6	FUB	3B	2	6	9,9,10	0.55	0	10,12,14	1.28	1 (10%)
6	GZL	3B	3	6	11,11,12	6.70	7 (63%)	14,15,17	1.60	2 (14%)
13	FUB	3C	1	13	9,9,10	0.58	0	10,12,14	0.97	0
13	FUB	3C	2	13	9,9,10	0.56	0	10,12,14	1.18	1 (10%)
13	GZL	3C	3	13	11,11,12	6.68	7 (63%)	14,15,17	1.51	2 (14%)
13	AHR	3C	4	13	9,9,10	0.59	0	10,12,14	0.85	0
6	FUB	3D	1	6	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
6	FUB	3D	2	6	9,9,10	0.57	0	10,12,14	1.06	1 (10%)
6	GZL	3D	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.43	2 (14%)
13	FUB	4	1	13	9,9,10	0.53	0	10,12,14	0.86	0
13	FUB	4	2	13	9,9,10	0.51	0	10,12,14	1.37	1 (10%)
13	GZL	4	3	13	11,11,12	6.84	7 (63%)	14,15,17	3.32	7 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	AHR	4	4	13	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
13	FUB	4A	1	13	9,9,10	0.53	0	10,12,14	0.89	0
13	FUB	4A	2	13	9,9,10	0.56	0	10,12,14	0.82	0
13	GZL	4A	3	13	11,11,12	6.78	7 (63%)	14,15,17	1.46	1 (7%)
13	AHR	4A	4	13	9,9,10	0.55	0	10,12,14	1.12	1 (10%)
6	FUB	4B	1	6	9,9,10	0.57	0	10,12,14	0.87	1 (10%)
6	FUB	4B	2	6	9,9,10	0.58	0	10,12,14	0.84	0
6	GZL	4B	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.72	2 (14%)
15	FUB	4C	1	15	9,9,10	0.58	0	10,12,14	0.91	0
15	FUB	4C	2	15	9,9,10	0.58	0	10,12,14	0.98	0
15	GZL	4C	3	15	11,11,12	6.73	7 (63%)	14,15,17	1.43	1 (7%)
15	AHR	4C	4	15	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
15	AHR	4C	5	15	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
16	NAG	4D	1	1,16	14,14,15	0.34	0	17,19,21	0.55	0
16	NAG	4D	2	16	14,14,15	0.45	0	17,19,21	1.36	2 (11%)
6	FUB	5	1	6	9,9,10	0.55	0	10,12,14	0.97	1 (10%)
6	FUB	5	2	6	9,9,10	0.52	0	10,12,14	1.27	1 (10%)
6	GZL	5	3	6	11,11,12	6.73	6 (54%)	14,15,17	1.55	1 (7%)
13	FUB	5A	1	13	9,9,10	0.56	0	10,12,14	0.90	0
13	FUB	5A	2	13	9,9,10	0.55	0	10,12,14	0.78	0
13	GZL	5A	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.31	1 (7%)
13	AHR	5A	4	13	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	FUB	5B	1	6	9,9,10	0.55	0	10,12,14	0.80	0
6	FUB	5B	2	6	9,9,10	0.59	0	10,12,14	1.08	1 (10%)
6	GZL	5B	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.38	1 (7%)
15	FUB	5C	1	15	9,9,10	0.56	0	10,12,14	1.09	1 (10%)
15	FUB	5C	2	15	9,9,10	0.58	0	10,12,14	0.97	0
15	GZL	5C	3	15	11,11,12	6.71	7 (63%)	14,15,17	1.64	2 (14%)
15	AHR	5C	4	15	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
15	AHR	5C	5	15	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
17	NAG	5D	1	17,1	14,14,15	0.33	0	17,19,21	0.98	1 (5%)
17	NAG	5D	2	17	14,14,15	0.30	0	17,19,21	0.76	0
17	BMA	5D	3	17	11,11,12	0.26	0	15,15,17	1.30	3 (20%)
17	MAN	5D	4	17	11,11,12	0.41	0	15,15,17	2.40	3 (20%)
17	MAN	5D	5	17	11,11,12	0.27	0	15,15,17	0.61	0
17	MAN	5D	6	17	11,11,12	0.30	0	15,15,17	0.85	0
13	FUB	6	1	13	9,9,10	0.54	0	10,12,14	0.77	0
13	FUB	6	2	13	9,9,10	0.58	0	10,12,14	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	GZL	6	3	13	11,11,12	6.78	6 (54%)	14,15,17	1.39	1 (7%)
13	AHR	6	4	13	9,9,10	0.58	0	10,12,14	1.09	1 (10%)
6	FUB	6A	1	6	9,9,10	0.56	0	10,12,14	0.88	0
6	FUB	6A	2	6	9,9,10	0.53	0	10,12,14	1.45	1 (10%)
6	GZL	6A	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.48	1 (7%)
13	FUB	6B	1	13	9,9,10	0.56	0	10,12,14	0.89	0
13	FUB	6B	2	13	9,9,10	0.55	0	10,12,14	1.19	2 (20%)
13	GZL	6B	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.84	4 (28%)
13	AHR	6B	4	13	9,9,10	0.55	0	10,12,14	0.97	0
6	FUB	6C	1	6	9,9,10	0.58	0	10,12,14	0.97	1 (10%)
6	FUB	6C	2	6	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
6	GZL	6C	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.48	1 (7%)
6	FUB	6D	1	6	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	FUB	6D	2	6	9,9,10	0.57	0	10,12,14	1.15	1 (10%)
6	GZL	6D	3	6	11,11,12	6.68	7 (63%)	14,15,17	1.90	3 (21%)
13	FUB	7	1	13	9,9,10	0.58	0	10,12,14	0.98	0
13	FUB	7	2	13	9,9,10	0.57	0	10,12,14	0.77	0
13	GZL	7	3	13	11,11,12	6.73	7 (63%)	14,15,17	1.44	2 (14%)
13	AHR	7	4	13	9,9,10	0.56	0	10,12,14	1.15	1 (10%)
6	FUB	7A	1	6	9,9,10	0.56	0	10,12,14	0.98	1 (10%)
6	FUB	7A	2	6	9,9,10	0.58	0	10,12,14	0.96	0
6	GZL	7A	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.43	1 (7%)
15	FUB	7B	1	15	9,9,10	0.51	0	10,12,14	0.96	0
15	FUB	7B	2	15	9,9,10	0.55	0	10,12,14	0.86	0
15	GZL	7B	3	15	11,11,12	6.75	7 (63%)	14,15,17	1.40	1 (7%)
15	AHR	7B	4	15	9,9,10	0.60	0	10,12,14	1.22	2 (20%)
15	AHR	7B	5	15	9,9,10	0.59	0	10,12,14	0.89	0
17	NAG	7C	1	17,1	14,14,15	0.32	0	17,19,21	0.84	1 (5%)
17	NAG	7C	2	17	14,14,15	0.35	0	17,19,21	0.99	0
17	BMA	7C	3	17	11,11,12	0.20	0	15,15,17	1.21	1 (6%)
17	MAN	7C	4	17	11,11,12	0.31	0	15,15,17	1.15	2 (13%)
17	MAN	7C	5	17	11,11,12	0.24	0	15,15,17	0.74	0
17	MAN	7C	6	17	11,11,12	0.29	0	15,15,17	0.98	0
6	FUB	7D	1	6	9,9,10	0.58	0	10,12,14	0.97	0
6	FUB	7D	2	6	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
6	GZL	7D	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.57	2 (14%)
6	FUB	8	1	6	9,9,10	0.56	0	10,12,14	0.99	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FUB	8	2	6	9,9,10	0.55	0	10,12,14	0.81	0
6	GZL	8	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.42	1 (7%)
6	FUB	8A	1	6	9,9,10	0.54	0	10,12,14	1.04	1 (10%)
6	FUB	8A	2	6	9,9,10	0.60	0	10,12,14	1.08	1 (10%)
6	GZL	8A	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.52	1 (7%)
15	FUB	8B	1	15	9,9,10	0.58	0	10,12,14	0.95	0
15	FUB	8B	2	15	9,9,10	0.56	0	10,12,14	0.92	0
15	GZL	8B	3	15	11,11,12	6.74	7 (63%)	14,15,17	1.25	1 (7%)
15	AHR	8B	4	15	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
15	AHR	8B	5	15	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
3	FUB	8C	1	3	9,9,10	0.58	0	10,12,14	0.82	0
3	FUB	8C	2	3	9,9,10	0.55	0	10,12,14	0.81	0
3	FUB	8C	3	3	9,9,10	0.58	0	10,12,14	0.91	0
6	FUB	8D	1	6	9,9,10	0.56	0	10,12,14	0.91	1 (10%)
6	FUB	8D	2	6	9,9,10	0.57	0	10,12,14	0.92	1 (10%)
6	GZL	8D	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.58	2 (14%)
6	FUB	9	1	6	9,9,10	0.54	0	10,12,14	0.88	1 (10%)
6	FUB	9	2	6	9,9,10	0.56	0	10,12,14	0.79	0
6	GZL	9	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.33	1 (7%)
13	FUB	9A	1	13	9,9,10	0.56	0	10,12,14	0.89	0
13	FUB	9A	2	13	9,9,10	0.54	0	10,12,14	1.20	2 (20%)
13	GZL	9A	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.93	4 (28%)
13	AHR	9A	4	13	9,9,10	0.56	0	10,12,14	1.01	0
6	FUB	9B	1	6	9,9,10	0.57	0	10,12,14	0.87	0
6	FUB	9B	2	6	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
6	GZL	9B	3	6	11,11,12	6.69	7 (63%)	14,15,17	1.61	2 (14%)
3	FUB	9C	1	3	9,9,10	0.58	0	10,12,14	1.03	0
3	FUB	9C	2	3	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
3	FUB	9C	3	3	9,9,10	0.57	0	10,12,14	0.89	1 (10%)
18	FUB	9D	1	18	9,9,10	0.59	0	10,12,14	2.72	5 (50%)
18	FUB	9D	2	18	9,9,10	0.56	0	10,12,14	0.91	0
18	GZL	9D	3	18	11,11,12	6.74	7 (63%)	14,15,17	1.42	2 (14%)
18	AHR	9D	4	18	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
18	AHR	9D	5	18	9,9,10	0.59	0	10,12,14	1.26	1 (10%)
6	FUB	AA	1	6	9,9,10	0.53	0	10,12,14	0.77	0
6	FUB	AA	2	6	9,9,10	0.59	0	10,12,14	1.12	1 (10%)
6	GZL	AA	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.27	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	FUB	AB	1	15	9,9,10	0.54	0	10,12,14	1.00	1 (10%)
15	FUB	AB	2	15	9,9,10	0.58	0	10,12,14	0.90	0
15	GZL	AB	3	15	11,11,12	6.73	7 (63%)	14,15,17	1.25	1 (7%)
15	AHR	AB	4	15	9,9,10	0.63	0	10,12,14	1.22	1 (10%)
15	AHR	AB	5	15	9,9,10	0.58	0	10,12,14	1.14	1 (10%)
16	NAG	AC	1	1,16	14,14,15	0.53	0	17,19,21	1.02	1 (5%)
16	NAG	AC	2	16	14,14,15	0.40	0	17,19,21	1.32	2 (11%)
4	FUB	AD	1	4	9,9,10	0.56	0	10,12,14	0.95	1 (10%)
4	FUB	AD	2	4	9,9,10	0.55	0	10,12,14	0.81	0
4	FUB	AD	3	4	9,9,10	0.55	0	10,12,14	0.77	0
4	AHR	AD	4	4	9,9,10	0.55	0	10,12,14	1.12	1 (10%)
19	FUB	AE	1	19	9,9,10	0.56	0	10,12,14	1.26	1 (10%)
19	FUB	AE	2	19	9,9,10	0.57	0	10,12,14	0.87	0
19	GZL	AE	3	19	11,11,12	6.75	7 (63%)	14,15,17	1.43	1 (7%)
19	AHR	AE	4	19	9,9,10	0.56	0	10,12,14	0.83	0
13	FUB	BA	1	13	9,9,10	0.56	0	10,12,14	0.75	0
13	FUB	BA	2	13	9,9,10	0.54	0	10,12,14	1.41	3 (30%)
13	GZL	BA	3	13	11,11,12	6.67	7 (63%)	14,15,17	1.91	4 (28%)
13	AHR	BA	4	13	9,9,10	0.55	0	10,12,14	0.85	0
15	FUB	BB	1	15	9,9,10	0.55	0	10,12,14	1.00	1 (10%)
15	FUB	BB	2	15	9,9,10	0.56	0	10,12,14	0.69	0
15	GZL	BB	3	15	11,11,12	6.75	7 (63%)	14,15,17	1.15	1 (7%)
15	AHR	BB	4	15	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
15	AHR	BB	5	15	9,9,10	0.59	0	10,12,14	0.91	0
3	FUB	BC	1	3	9,9,10	0.56	0	10,12,14	1.00	1 (10%)
3	FUB	BC	2	3	9,9,10	0.55	0	10,12,14	0.93	1 (10%)
3	FUB	BC	3	3	9,9,10	0.56	0	10,12,14	0.87	0
5	FUB	BD	1	5	9,9,10	0.55	0	10,12,14	1.02	1 (10%)
5	FUB	BD	2	5	9,9,10	0.52	0	10,12,14	0.86	0
5	FUB	BD	3	5	9,9,10	0.57	0	10,12,14	0.93	0
5	AHR	BD	4	5	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
5	AHR	BD	5	5	9,9,10	0.56	0	10,12,14	0.81	0
18	FUB	BE	1	18	9,9,10	0.60	0	10,12,14	0.91	0
18	FUB	BE	2	18	9,9,10	0.53	0	10,12,14	1.05	1 (10%)
18	GZL	BE	3	18	11,11,12	6.70	7 (63%)	14,15,17	1.55	2 (14%)
18	AHR	BE	4	18	9,9,10	0.56	0	10,12,14	0.80	0
18	AHR	BE	5	18	9,9,10	0.54	0	10,12,14	1.15	1 (10%)
15	FUB	CA	1	15	9,9,10	0.55	0	10,12,14	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	FUB	CA	2	15	9,9,10	0.54	0	10,12,14	0.83	0
15	GZL	CA	3	15	11,11,12	6.75	7 (63%)	14,15,17	1.18	1 (7%)
15	AHR	CA	4	15	9,9,10	0.60	0	10,12,14	1.27	2 (20%)
15	AHR	CA	5	15	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	FUB	CB	1	6	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
6	FUB	CB	2	6	9,9,10	0.56	0	10,12,14	0.87	0
6	GZL	CB	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.48	3 (21%)
3	FUB	CC	1	3	9,9,10	0.57	0	10,12,14	0.95	1 (10%)
3	FUB	CC	2	3	9,9,10	0.55	0	10,12,14	0.91	1 (10%)
3	FUB	CC	3	3	9,9,10	0.56	0	10,12,14	0.79	0
6	FUB	CD	1	6	9,9,10	0.56	0	10,12,14	0.96	0
6	FUB	CD	2	6	9,9,10	0.50	0	10,12,14	1.12	1 (10%)
6	GZL	CD	3	6	11,11,12	7.12	7 (63%)	14,15,17	4.08	5 (35%)
20	FUB	CE	1	20	9,9,10	0.56	0	10,12,14	0.79	0
20	FUB	CE	2	20	9,9,10	0.51	0	10,12,14	0.84	0
20	GZL	CE	3	20	11,11,12	6.69	7 (63%)	14,15,17	1.62	2 (14%)
20	AHR	CE	4	20	9,9,10	0.59	0	10,12,14	0.86	0
15	FUB	DA	1	15	9,9,10	0.57	0	10,12,14	0.99	1 (10%)
15	FUB	DA	2	15	9,9,10	0.56	0	10,12,14	0.82	0
15	GZL	DA	3	15	11,11,12	6.74	6 (54%)	14,15,17	1.34	1 (7%)
15	AHR	DA	4	15	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
15	AHR	DA	5	15	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
17	NAG	DB	1	17,1	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
17	NAG	DB	2	17	14,14,15	0.32	0	17,19,21	1.09	1 (5%)
17	BMA	DB	3	17	11,11,12	0.23	0	15,15,17	1.23	2 (13%)
17	MAN	DB	4	17	11,11,12	0.31	0	15,15,17	1.18	2 (13%)
17	MAN	DB	5	17	11,11,12	0.24	0	15,15,17	0.73	0
17	MAN	DB	6	17	11,11,12	0.40	0	15,15,17	1.52	2 (13%)
4	FUB	DC	1	4	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
4	FUB	DC	2	4	9,9,10	0.56	0	10,12,14	0.83	0
4	FUB	DC	3	4	9,9,10	0.56	0	10,12,14	0.81	0
4	AHR	DC	4	4	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
3	FUB	DD	1	3	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
3	FUB	DD	2	3	9,9,10	0.57	0	10,12,14	0.80	0
3	FUB	DD	3	3	9,9,10	0.57	0	10,12,14	0.97	0
18	FUB	DE	1	18	9,9,10	0.52	0	10,12,14	1.09	1 (10%)
18	FUB	DE	2	18	9,9,10	0.51	0	10,12,14	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	GZL	DE	3	18	11,11,12	6.70	7 (63%)	14,15,17	1.66	2 (14%)
18	AHR	DE	4	18	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
18	AHR	DE	5	18	9,9,10	0.58	0	10,12,14	0.92	0
6	FUB	EA	1	6	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
6	FUB	EA	2	6	9,9,10	0.55	0	10,12,14	0.91	0
6	GZL	EA	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.37	1 (7%)
3	FUB	EB	1	3	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
3	FUB	EB	2	3	9,9,10	0.58	0	10,12,14	0.84	0
3	FUB	EB	3	3	9,9,10	0.57	0	10,12,14	0.98	0
5	FUB	EC	1	5	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
5	FUB	EC	2	5	9,9,10	0.59	0	10,12,14	1.16	0
5	FUB	EC	3	5	9,9,10	0.58	0	10,12,14	1.08	1 (10%)
5	AHR	EC	4	5	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
5	AHR	EC	5	5	9,9,10	0.56	0	10,12,14	0.80	0
3	FUB	ED	1	3	9,9,10	0.54	0	10,12,14	1.05	1 (10%)
3	FUB	ED	2	3	9,9,10	0.56	0	10,12,14	0.80	0
3	FUB	ED	3	3	9,9,10	0.58	0	10,12,14	0.80	0
20	FUB	EE	1	20	9,9,10	0.53	0	10,12,14	0.88	0
20	FUB	EE	2	20	9,9,10	0.55	0	10,12,14	1.10	1 (10%)
20	GZL	EE	3	20	11,11,12	6.73	7 (63%)	14,15,17	1.51	1 (7%)
20	AHR	EE	4	20	9,9,10	0.60	0	10,12,14	0.81	0
16	NAG	FA	1	1,16	14,14,15	0.42	0	17,19,21	0.59	0
16	NAG	FA	2	16	14,14,15	0.39	0	17,19,21	1.39	2 (11%)
12	FUB	FB	1	12	9,9,10	0.59	0	10,12,14	1.02	1 (10%)
12	FUB	FB	2	12	9,9,10	0.58	0	10,12,14	0.96	0
12	GZL	FB	3	12	11,11,12	6.67	7 (63%)	14,15,17	1.70	2 (14%)
12	AHR	FB	4	12	9,9,10	0.58	0	10,12,14	0.93	0
12	AHR	FB	5	12	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
6	FUB	FC	1	6	9,9,10	0.56	0	10,12,14	1.29	2 (20%)
6	FUB	FC	2	6	9,9,10	0.60	0	10,12,14	1.20	1 (10%)
6	GZL	FC	3	6	11,11,12	6.60	7 (63%)	14,15,17	2.44	4 (28%)
3	FUB	FD	1	3	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
3	FUB	FD	2	3	9,9,10	0.54	0	10,12,14	0.72	0
3	FUB	FD	3	3	9,9,10	0.58	0	10,12,14	0.90	0
21	FUB	FE	1	21	9,9,10	0.55	0	10,12,14	1.12	1 (10%)
21	FUB	FE	2	21	9,9,10	0.53	0	10,12,14	0.70	0
21	GZL	FE	3	21	11,11,12	6.75	6 (54%)	14,15,17	1.35	1 (7%)
21	AHR	FE	4	21	9,9,10	0.57	0	10,12,14	1.00	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	AHR	FE	5	21	9,9,10	0.60	0	10,12,14	1.02	1 (10%)
17	NAG	GA	1	17,1	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
17	NAG	GA	2	17	14,14,15	0.33	0	17,19,21	0.94	0
17	BMA	GA	3	17	11,11,12	0.25	0	15,15,17	1.64	4 (26%)
17	MAN	GA	4	17	11,11,12	0.31	0	15,15,17	0.72	0
17	MAN	GA	5	17	11,11,12	0.24	0	15,15,17	0.62	0
17	MAN	GA	6	17	11,11,12	0.29	0	15,15,17	1.00	1 (6%)
13	FUB	GB	1	13	9,9,10	0.58	0	10,12,14	0.87	0
13	FUB	GB	2	13	9,9,10	0.59	0	10,12,14	0.92	0
13	GZL	GB	3	13	11,11,12	6.74	7 (63%)	14,15,17	1.29	1 (7%)
13	AHR	GB	4	13	9,9,10	0.56	0	10,12,14	0.99	0
3	FUB	GC	1	3	9,9,10	0.56	0	10,12,14	0.99	1 (10%)
3	FUB	GC	2	3	9,9,10	0.54	0	10,12,14	0.71	0
3	FUB	GC	3	3	9,9,10	0.58	0	10,12,14	0.87	0
6	FUB	GD	1	6	9,9,10	0.55	0	10,12,14	1.08	1 (10%)
6	FUB	GD	2	6	9,9,10	0.55	0	10,12,14	0.84	0
6	GZL	GD	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.45	2 (14%)
22	FUB	GE	1	22	9,9,10	0.57	0	10,12,14	1.20	1 (10%)
22	FUB	GE	2	22	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
22	GZL	GE	3	22	11,11,12	6.71	7 (63%)	14,15,17	1.46	2 (14%)
22	AHR	GE	4	22	9,9,10	0.56	0	10,12,14	0.76	0
22	AHR	GE	5	22	9,9,10	0.59	0	10,12,14	1.48	3 (30%)
22	AHR	GE	6	22	9,9,10	0.54	0	10,12,14	0.77	0
3	FUB	HA	1	3	9,9,10	0.55	0	10,12,14	0.93	1 (10%)
3	FUB	HA	2	3	9,9,10	0.58	0	10,12,14	0.79	0
3	FUB	HA	3	3	9,9,10	0.59	0	10,12,14	1.02	1 (10%)
14	FUB	HB	1	14	9,9,10	0.55	0	10,12,14	0.76	0
14	FUB	HB	2	14	9,9,10	0.56	0	10,12,14	0.87	0
14	GZL	HB	3	14	11,11,12	6.65	7 (63%)	14,15,17	1.76	3 (21%)
14	FUB	HB	4	14	9,9,10	0.59	0	10,12,14	1.08	1 (10%)
3	FUB	HC	1	3	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
3	FUB	HC	2	3	9,9,10	0.56	0	10,12,14	0.74	0
3	FUB	HC	3	3	9,9,10	0.57	0	10,12,14	0.92	0
7	FUB	HD	1	7	9,9,10	0.58	0	10,12,14	1.16	1 (10%)
7	FUB	HD	2	7	9,9,10	0.56	0	10,12,14	0.86	0
7	FUB	HD	3	7	9,9,10	0.56	0	10,12,14	0.99	0
7	AHR	HD	4	7	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
20	FUB	HE	1	20	9,9,10	0.59	0	10,12,14	1.15	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	FUB	HE	2	20	9,9,10	0.54	0	10,12,14	0.96	0
20	GZL	HE	3	20	11,11,12	6.72	7 (63%)	14,15,17	1.64	2 (14%)
20	AHR	HE	4	20	9,9,10	0.56	0	10,12,14	0.99	0
3	FUB	IA	1	3	9,9,10	0.54	0	10,12,14	0.74	0
3	FUB	IA	2	3	9,9,10	0.54	0	10,12,14	0.92	1 (10%)
3	FUB	IA	3	3	9,9,10	0.56	0	10,12,14	0.78	0
12	FUB	IB	1	12	9,9,10	0.58	0	10,12,14	0.92	0
12	FUB	IB	2	12	9,9,10	0.56	0	10,12,14	0.95	1 (10%)
12	GZL	IB	3	12	11,11,12	6.72	7 (63%)	14,15,17	1.43	1 (7%)
12	AHR	IB	4	12	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
12	AHR	IB	5	12	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
3	FUB	IC	1	3	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
3	FUB	IC	2	3	9,9,10	0.52	0	10,12,14	0.80	0
3	FUB	IC	3	3	9,9,10	0.56	0	10,12,14	0.85	0
3	FUB	ID	1	3	9,9,10	0.57	0	10,12,14	1.05	1 (10%)
3	FUB	ID	2	3	9,9,10	0.54	0	10,12,14	0.80	0
3	FUB	ID	3	3	9,9,10	0.59	0	10,12,14	0.86	0
18	FUB	IE	1	18	9,9,10	0.58	0	10,12,14	1.10	1 (10%)
18	FUB	IE	2	18	9,9,10	0.52	0	10,12,14	0.89	0
18	GZL	IE	3	18	11,11,12	6.68	7 (63%)	14,15,17	1.71	3 (21%)
18	AHR	IE	4	18	9,9,10	0.55	0	10,12,14	1.12	1 (10%)
18	AHR	IE	5	18	9,9,10	0.56	0	10,12,14	1.17	1 (10%)
3	FUB	J	1	3	9,9,10	0.55	0	10,12,14	0.83	0
3	FUB	J	2	3	9,9,10	0.56	0	10,12,14	0.95	0
3	FUB	J	3	3	9,9,10	0.60	0	10,12,14	0.92	0
4	FUB	JA	1	4	9,9,10	0.58	0	10,12,14	0.86	0
4	FUB	JA	2	4	9,9,10	0.58	0	10,12,14	1.04	0
4	FUB	JA	3	4	9,9,10	0.57	0	10,12,14	0.94	0
4	AHR	JA	4	4	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
4	FUB	JB	1	4	9,9,10	0.57	0	10,12,14	0.99	1 (10%)
4	FUB	JB	2	4	9,9,10	0.58	0	10,12,14	0.99	0
4	FUB	JB	3	4	9,9,10	0.58	0	10,12,14	0.88	0
4	AHR	JB	4	4	9,9,10	0.56	0	10,12,14	0.74	0
6	FUB	JC	1	6	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
6	FUB	JC	2	6	9,9,10	0.56	0	10,12,14	0.83	0
6	GZL	JC	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.44	1 (7%)
8	FUB	JD	1	8	9,9,10	0.56	0	10,12,14	0.81	0
8	FUB	JD	2	8	9,9,10	0.56	0	10,12,14	0.76	0
8	FUB	JD	3	8	9,9,10	0.59	0	10,12,14	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	AHR	JD	4	8	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
8	AHR	JD	5	8	9,9,10	0.58	0	10,12,14	0.96	0
18	FUB	JE	1	18	9,9,10	0.58	0	10,12,14	1.10	1 (10%)
18	FUB	JE	2	18	9,9,10	0.57	0	10,12,14	0.90	0
18	GZL	JE	3	18	11,11,12	6.70	7 (63%)	14,15,17	1.59	2 (14%)
18	AHR	JE	4	18	9,9,10	0.58	0	10,12,14	0.80	0
18	AHR	JE	5	18	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	K	1	3	9,9,10	0.56	0	10,12,14	0.63	0
3	FUB	K	2	3	9,9,10	0.54	0	10,12,14	0.81	0
3	FUB	K	3	3	9,9,10	0.55	0	10,12,14	0.76	0
5	FUB	KA	1	5	9,9,10	0.56	0	10,12,14	0.94	0
5	FUB	KA	2	5	9,9,10	0.59	0	10,12,14	0.96	0
5	FUB	KA	3	5	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
5	AHR	KA	4	5	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
5	AHR	KA	5	5	9,9,10	0.59	0	10,12,14	1.01	1 (10%)
14	FUB	KB	1	14	9,9,10	0.58	0	10,12,14	0.98	0
14	FUB	KB	2	14	9,9,10	0.59	0	10,12,14	0.99	0
14	GZL	KB	3	14	11,11,12	6.64	7 (63%)	14,15,17	1.85	2 (14%)
14	FUB	KB	4	14	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
7	FUB	KC	1	7	9,9,10	0.57	0	10,12,14	1.14	1 (10%)
7	FUB	KC	2	7	9,9,10	0.56	0	10,12,14	0.77	0
7	FUB	KC	3	7	9,9,10	0.58	0	10,12,14	0.97	0
7	AHR	KC	4	7	9,9,10	0.56	0	10,12,14	1.00	1 (10%)
3	FUB	KD	1	3	9,9,10	0.57	0	10,12,14	0.98	1 (10%)
3	FUB	KD	2	3	9,9,10	0.56	0	10,12,14	0.92	0
3	FUB	KD	3	3	9,9,10	0.57	0	10,12,14	0.98	0
18	FUB	KE	1	18	9,9,10	0.59	0	10,12,14	1.10	0
18	FUB	KE	2	18	9,9,10	0.56	0	10,12,14	0.93	0
18	GZL	KE	3	18	11,11,12	6.68	7 (63%)	14,15,17	1.54	2 (14%)
18	AHR	KE	4	18	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
18	AHR	KE	5	18	9,9,10	0.57	0	10,12,14	1.01	0
4	FUB	L	1	4	9,9,10	0.59	0	10,12,14	0.64	0
4	FUB	L	2	4	9,9,10	0.56	0	10,12,14	0.92	0
4	FUB	L	3	4	9,9,10	0.60	0	10,12,14	0.82	0
4	AHR	L	4	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
6	FUB	LA	1	6	9,9,10	0.59	0	10,12,14	0.97	0
6	FUB	LA	2	6	9,9,10	0.56	0	10,12,14	1.26	1 (10%)
6	GZL	LA	3	6	11,11,12	7.12	7 (63%)	14,15,17	4.03	5 (35%)
3	FUB	LB	1	3	9,9,10	0.58	0	10,12,14	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	LB	2	3	9,9,10	0.57	0	10,12,14	0.85	0
3	FUB	LB	3	3	9,9,10	0.57	0	10,12,14	0.97	0
3	FUB	LC	1	3	9,9,10	0.58	0	10,12,14	1.02	0
3	FUB	LC	2	3	9,9,10	0.55	0	10,12,14	0.79	0
3	FUB	LC	3	3	9,9,10	0.58	0	10,12,14	0.84	0
4	FUB	LD	1	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
4	FUB	LD	2	4	9,9,10	0.57	0	10,12,14	0.79	0
4	FUB	LD	3	4	9,9,10	0.58	0	10,12,14	0.80	0
4	AHR	LD	4	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
19	FUB	LE	1	19	9,9,10	0.58	0	10,12,14	1.11	0
19	FUB	LE	2	19	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
19	GZL	LE	3	19	11,11,12	6.74	7 (63%)	14,15,17	1.38	1 (7%)
19	AHR	LE	4	19	9,9,10	0.55	0	10,12,14	0.96	0
5	FUB	M	1	5	9,9,10	0.56	0	10,12,14	0.93	0
5	FUB	M	2	5	9,9,10	0.58	0	10,12,14	1.29	2 (20%)
5	FUB	M	3	5	9,9,10	0.56	0	10,12,14	1.12	1 (10%)
5	AHR	M	4	5	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
5	AHR	M	5	5	9,9,10	0.56	0	10,12,14	1.17	1 (10%)
3	FUB	MA	1	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	MA	2	3	9,9,10	0.55	0	10,12,14	0.83	0
3	FUB	MA	3	3	9,9,10	0.58	0	10,12,14	0.87	0
10	FUB	MB	1	10	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
10	FUB	MB	2	10	9,9,10	0.58	0	10,12,14	1.04	0
10	FUB	MB	3	10	9,9,10	0.58	0	10,12,14	0.83	0
10	AHR	MB	4	10	9,9,10	0.57	0	10,12,14	1.06	1 (10%)
10	AHR	MB	5	10	9,9,10	0.57	0	10,12,14	1.19	1 (10%)
8	FUB	MC	1	8	9,9,10	0.55	0	10,12,14	1.02	1 (10%)
8	FUB	MC	2	8	9,9,10	0.56	0	10,12,14	0.78	0
8	FUB	MC	3	8	9,9,10	0.56	0	10,12,14	0.83	0
8	AHR	MC	4	8	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
8	AHR	MC	5	8	9,9,10	0.59	0	10,12,14	1.05	1 (10%)
4	FUB	MD	1	4	9,9,10	0.53	0	10,12,14	0.90	0
4	FUB	MD	2	4	9,9,10	0.55	0	10,12,14	0.84	0
4	FUB	MD	3	4	9,9,10	0.59	0	10,12,14	0.97	0
4	AHR	MD	4	4	9,9,10	0.56	0	10,12,14	0.79	0
6	FUB	ME	1	6	9,9,10	0.58	0	10,12,14	0.89	0
6	FUB	ME	2	6	9,9,10	0.57	0	10,12,14	0.80	0
6	GZL	ME	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.47	1 (7%)
6	FUB	N	1	6	9,9,10	0.58	0	10,12,14	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FUB	N	2	6	9,9,10	0.62	0	10,12,14	1.15	2 (20%)
6	GZL	N	3	6	11,11,12	6.64	7 (63%)	14,15,17	3.38	5 (35%)
3	FUB	NA	1	3	9,9,10	0.54	0	10,12,14	1.10	1 (10%)
3	FUB	NA	2	3	9,9,10	0.54	0	10,12,14	0.78	0
3	FUB	NA	3	3	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
4	FUB	NB	1	4	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
4	FUB	NB	2	4	9,9,10	0.58	0	10,12,14	0.95	0
4	FUB	NB	3	4	9,9,10	0.57	0	10,12,14	0.91	0
4	AHR	NB	4	4	9,9,10	0.56	0	10,12,14	1.00	1 (10%)
3	FUB	NC	1	3	9,9,10	0.58	0	10,12,14	0.91	0
3	FUB	NC	2	3	9,9,10	0.57	0	10,12,14	0.85	0
3	FUB	NC	3	3	9,9,10	0.56	0	10,12,14	0.98	0
9	FUB	ND	1	9	9,9,10	0.62	0	10,12,14	1.04	0
9	FUB	ND	2	9	9,9,10	0.58	0	10,12,14	1.09	1 (10%)
19	FUB	NE	1	19	9,9,10	0.58	0	10,12,14	0.92	0
19	FUB	NE	2	19	9,9,10	0.57	0	10,12,14	0.76	0
19	GZL	NE	3	19	11,11,12	6.71	7 (63%)	14,15,17	1.53	2 (14%)
19	AHR	NE	4	19	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	O	1	3	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
3	FUB	O	2	3	9,9,10	0.56	0	10,12,14	0.83	0
3	FUB	O	3	3	9,9,10	0.59	0	10,12,14	0.98	0
3	FUB	OA	1	3	9,9,10	0.58	0	10,12,14	1.08	1 (10%)
3	FUB	OA	2	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	OA	3	3	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	OB	1	3	9,9,10	0.59	0	10,12,14	0.98	0
3	FUB	OB	2	3	9,9,10	0.59	0	10,12,14	0.90	0
3	FUB	OB	3	3	9,9,10	0.58	0	10,12,14	0.98	0
4	FUB	OC	1	4	9,9,10	0.53	0	10,12,14	0.89	0
4	FUB	OC	2	4	9,9,10	0.58	0	10,12,14	0.69	0
4	FUB	OC	3	4	9,9,10	0.56	0	10,12,14	0.82	0
4	AHR	OC	4	4	9,9,10	0.56	0	10,12,14	1.13	1 (10%)
4	FUB	OD	1	4	9,9,10	0.53	0	10,12,14	1.05	1 (10%)
4	FUB	OD	2	4	9,9,10	0.51	0	10,12,14	0.81	0
4	FUB	OD	3	4	9,9,10	0.58	0	10,12,14	0.86	0
4	AHR	OD	4	4	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
6	FUB	OE	1	6	9,9,10	0.62	0	10,12,14	0.78	0
6	FUB	OE	2	6	9,9,10	0.58	0	10,12,14	0.90	0
6	GZL	OE	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.60	2 (14%)
3	FUB	P	1	3	9,9,10	0.57	0	10,12,14	1.11	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	P	2	3	9,9,10	0.56	0	10,12,14	0.87	0
3	FUB	P	3	3	9,9,10	0.59	0	10,12,14	0.94	0
6	FUB	PA	1	6	9,9,10	0.58	0	10,12,14	1.00	0
6	FUB	PA	2	6	9,9,10	0.57	0	10,12,14	0.90	0
6	GZL	PA	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.44	1 (7%)
3	FUB	PB	1	3	9,9,10	0.56	0	10,12,14	0.92	1 (10%)
3	FUB	PB	2	3	9,9,10	0.57	0	10,12,14	0.90	0
3	FUB	PB	3	3	9,9,10	0.56	0	10,12,14	0.88	0
4	FUB	PC	1	4	9,9,10	0.53	0	10,12,14	0.97	0
4	FUB	PC	2	4	9,9,10	0.54	0	10,12,14	0.82	0
4	FUB	PC	3	4	9,9,10	0.57	0	10,12,14	0.95	0
4	AHR	PC	4	4	9,9,10	0.64	0	10,12,14	1.23	2 (20%)
10	FUB	PD	1	10	9,9,10	0.54	0	10,12,14	1.06	1 (10%)
10	FUB	PD	2	10	9,9,10	0.59	0	10,12,14	0.94	0
10	FUB	PD	3	10	9,9,10	0.59	0	10,12,14	0.87	0
10	AHR	PD	4	10	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
10	AHR	PD	5	10	9,9,10	0.58	0	10,12,14	1.00	0
18	FUB	PE	1	18	9,9,10	0.55	0	10,12,14	1.02	1 (10%)
18	FUB	PE	2	18	9,9,10	0.55	0	10,12,14	0.74	0
18	GZL	PE	3	18	11,11,12	6.75	7 (63%)	14,15,17	1.40	1 (7%)
18	AHR	PE	4	18	9,9,10	0.56	0	10,12,14	0.82	0
18	AHR	PE	5	18	9,9,10	0.57	0	10,12,14	1.03	0
3	FUB	Q	1	3	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
3	FUB	Q	2	3	9,9,10	0.55	0	10,12,14	0.80	0
3	FUB	Q	3	3	9,9,10	0.56	0	10,12,14	0.80	0
7	FUB	QA	1	7	9,9,10	0.55	0	10,12,14	1.17	1 (10%)
7	FUB	QA	2	7	9,9,10	0.59	0	10,12,14	0.88	0
7	FUB	QA	3	7	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
7	AHR	QA	4	7	9,9,10	0.55	0	10,12,14	0.87	0
3	FUB	QB	1	3	9,9,10	0.59	0	10,12,14	0.95	1 (10%)
3	FUB	QB	2	3	9,9,10	0.59	0	10,12,14	0.87	0
3	FUB	QB	3	3	9,9,10	0.54	0	10,12,14	0.80	0
9	FUB	QC	1	9	9,9,10	0.56	0	10,12,14	0.93	0
9	FUB	QC	2	9	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	QD	1	3	9,9,10	0.57	0	10,12,14	0.76	0
3	FUB	QD	2	3	9,9,10	0.59	0	10,12,14	0.96	0
3	FUB	QD	3	3	9,9,10	0.56	0	10,12,14	0.88	0
22	FUB	QE	1	22	9,9,10	0.56	0	10,12,14	0.86	1 (10%)
22	FUB	QE	2	22	9,9,10	0.57	0	10,12,14	0.95	0
22	GZL	QE	3	22	11,11,12	6.75	7 (63%)	14,15,17	1.43	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	AHR	QE	4	22	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
22	AHR	QE	5	22	9,9,10	0.57	0	10,12,14	0.87	0
22	AHR	QE	6	22	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
6	FUB	R	1	6	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
6	FUB	R	2	6	9,9,10	0.57	0	10,12,14	0.91	0
6	GZL	R	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.49	1 (7%)
3	FUB	RA	1	3	9,9,10	0.56	0	10,12,14	1.09	1 (10%)
3	FUB	RA	2	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	RA	3	3	9,9,10	0.58	0	10,12,14	0.94	0
3	FUB	RB	1	3	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
3	FUB	RB	2	3	9,9,10	0.60	0	10,12,14	1.00	0
3	FUB	RB	3	3	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
4	FUB	RC	1	4	9,9,10	0.55	0	10,12,14	0.94	0
4	FUB	RC	2	4	9,9,10	0.55	0	10,12,14	0.71	0
4	FUB	RC	3	4	9,9,10	0.59	0	10,12,14	0.94	0
4	AHR	RC	4	4	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
4	FUB	RD	1	4	9,9,10	0.55	0	10,12,14	0.81	0
4	FUB	RD	2	4	9,9,10	0.58	0	10,12,14	0.97	1 (10%)
4	FUB	RD	3	4	9,9,10	0.59	0	10,12,14	0.95	0
4	AHR	RD	4	4	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
22	FUB	RE	1	22	9,9,10	0.58	0	10,12,14	1.05	0
22	FUB	RE	2	22	9,9,10	0.56	0	10,12,14	0.90	0
22	GZL	RE	3	22	11,11,12	6.75	7 (63%)	14,15,17	1.36	1 (7%)
22	AHR	RE	4	22	9,9,10	0.57	0	10,12,14	1.05	1 (10%)
22	AHR	RE	5	22	9,9,10	0.55	0	10,12,14	1.19	2 (20%)
22	AHR	RE	6	22	9,9,10	0.62	0	10,12,14	1.23	1 (10%)
7	FUB	S	1	7	9,9,10	0.56	0	10,12,14	1.15	1 (10%)
7	FUB	S	2	7	9,9,10	0.56	0	10,12,14	0.81	0
7	FUB	S	3	7	9,9,10	0.55	0	10,12,14	1.04	1 (10%)
7	AHR	S	4	7	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
8	FUB	SA	1	8	9,9,10	0.57	0	10,12,14	0.97	0
8	FUB	SA	2	8	9,9,10	0.57	0	10,12,14	0.85	0
8	FUB	SA	3	8	9,9,10	0.55	0	10,12,14	0.96	1 (10%)
8	AHR	SA	4	8	9,9,10	0.60	0	10,12,14	1.00	0
8	AHR	SA	5	8	9,9,10	0.58	0	10,12,14	0.85	0
3	FUB	SB	1	3	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
3	FUB	SB	2	3	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
3	FUB	SB	3	3	9,9,10	0.58	0	10,12,14	1.02	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	FUB	SC	1	10	9,9,10	0.57	0	10,12,14	0.93	0
10	FUB	SC	2	10	9,9,10	0.57	0	10,12,14	0.82	0
10	FUB	SC	3	10	9,9,10	0.60	0	10,12,14	0.89	0
10	AHR	SC	4	10	9,9,10	0.57	0	10,12,14	0.88	0
10	AHR	SC	5	10	9,9,10	0.59	0	10,12,14	1.05	1 (10%)
4	FUB	SD	1	4	9,9,10	0.57	0	10,12,14	1.01	0
4	FUB	SD	2	4	9,9,10	0.58	0	10,12,14	1.09	1 (10%)
4	FUB	SD	3	4	9,9,10	0.58	0	10,12,14	0.87	0
4	AHR	SD	4	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
18	FUB	SE	1	18	9,9,10	0.56	0	10,12,14	1.16	1 (10%)
18	FUB	SE	2	18	9,9,10	0.53	0	10,12,14	0.86	0
18	GZL	SE	3	18	11,11,12	6.75	7 (63%)	14,15,17	1.40	1 (7%)
18	AHR	SE	4	18	9,9,10	0.57	0	10,12,14	0.99	0
18	AHR	SE	5	18	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	T	1	3	9,9,10	0.54	0	10,12,14	1.10	1 (10%)
3	FUB	T	2	3	9,9,10	0.56	0	10,12,14	0.82	0
3	FUB	T	3	3	9,9,10	0.58	0	10,12,14	0.96	0
3	FUB	TA	1	3	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	TA	2	3	9,9,10	0.54	0	10,12,14	1.02	1 (10%)
3	FUB	TA	3	3	9,9,10	0.57	0	10,12,14	0.81	0
3	FUB	TB	1	3	9,9,10	0.55	0	10,12,14	0.74	0
3	FUB	TB	2	3	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
3	FUB	TB	3	3	9,9,10	0.57	0	10,12,14	0.86	0
3	FUB	TC	1	3	9,9,10	0.59	0	10,12,14	1.13	1 (10%)
3	FUB	TC	2	3	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
3	FUB	TC	3	3	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
3	FUB	TD	1	3	9,9,10	0.56	0	10,12,14	0.79	0
3	FUB	TD	2	3	9,9,10	0.59	0	10,12,14	0.91	0
3	FUB	TD	3	3	9,9,10	0.57	0	10,12,14	0.90	0
20	FUB	TE	1	20	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
20	FUB	TE	2	20	9,9,10	0.57	0	10,12,14	0.76	0
20	GZL	TE	3	20	11,11,12	6.74	7 (63%)	14,15,17	1.56	1 (7%)
20	AHR	TE	4	20	9,9,10	0.56	0	10,12,14	0.83	0
8	FUB	U	1	8	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
8	FUB	U	2	8	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
8	FUB	U	3	8	9,9,10	0.58	0	10,12,14	0.90	0
8	AHR	U	4	8	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
8	AHR	U	5	8	9,9,10	0.59	0	10,12,14	0.92	0
4	FUB	UA	1	4	9,9,10	0.57	0	10,12,14	1.03	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FUB	UA	2	4	9,9,10	0.57	0	10,12,14	0.83	0
4	FUB	UA	3	4	9,9,10	0.57	0	10,12,14	0.88	0
4	AHR	UA	4	4	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	UB	1	3	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
3	FUB	UB	2	3	9,9,10	0.56	0	10,12,14	0.74	0
3	FUB	UB	3	3	9,9,10	0.57	0	10,12,14	0.96	0
4	FUB	UC	1	4	9,9,10	0.52	0	10,12,14	0.89	0
4	FUB	UC	2	4	9,9,10	0.56	0	10,12,14	0.93	0
4	FUB	UC	3	4	9,9,10	0.57	0	10,12,14	0.94	0
4	AHR	UC	4	4	9,9,10	0.59	0	10,12,14	0.93	0
7	FUB	UD	1	7	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
7	FUB	UD	2	7	9,9,10	0.56	0	10,12,14	0.70	0
7	FUB	UD	3	7	9,9,10	0.57	0	10,12,14	0.84	0
7	AHR	UD	4	7	9,9,10	0.57	0	10,12,14	0.77	0
20	FUB	UE	1	20	9,9,10	0.54	0	10,12,14	0.87	0
20	FUB	UE	2	20	9,9,10	0.49	0	10,12,14	0.99	0
20	GZL	UE	3	20	11,11,12	6.75	7 (63%)	14,15,17	1.31	1 (7%)
20	AHR	UE	4	20	9,9,10	0.58	0	10,12,14	0.77	0
3	FUB	V	1	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	V	2	3	9,9,10	0.56	0	10,12,14	0.90	0
3	FUB	V	3	3	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
4	FUB	VA	1	4	9,9,10	0.55	0	10,12,14	0.95	0
4	FUB	VA	2	4	9,9,10	0.57	0	10,12,14	0.90	0
4	FUB	VA	3	4	9,9,10	0.55	0	10,12,14	0.83	0
4	AHR	VA	4	4	9,9,10	0.60	0	10,12,14	0.76	0
10	FUB	VB	1	10	9,9,10	0.54	0	10,12,14	0.95	0
10	FUB	VB	2	10	9,9,10	0.56	0	10,12,14	0.81	0
10	FUB	VB	3	10	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
10	AHR	VB	4	10	9,9,10	0.58	0	10,12,14	0.79	0
10	AHR	VB	5	10	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
4	FUB	VC	1	4	9,9,10	0.55	0	10,12,14	0.85	0
4	FUB	VC	2	4	9,9,10	0.58	0	10,12,14	0.93	0
4	FUB	VC	3	4	9,9,10	0.58	0	10,12,14	0.85	0
4	AHR	VC	4	4	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
4	FUB	VD	1	4	9,9,10	0.57	0	10,12,14	0.92	0
4	FUB	VD	2	4	9,9,10	0.58	0	10,12,14	0.99	1 (10%)
4	FUB	VD	3	4	9,9,10	0.58	0	10,12,14	0.86	0
4	AHR	VD	4	4	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
22	FUB	VE	1	22	9,9,10	0.56	0	10,12,14	1.33	1 (10%)
22	FUB	VE	2	22	9,9,10	0.53	0	10,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	GZL	VE	3	22	11,11,12	6.73	7 (63%)	14,15,17	1.41	1 (7%)
22	AHR	VE	4	22	9,9,10	0.57	0	10,12,14	1.15	1 (10%)
22	AHR	VE	5	22	9,9,10	0.58	0	10,12,14	0.96	1 (10%)
22	AHR	VE	6	22	9,9,10	0.58	0	10,12,14	0.94	0
4	FUB	W	1	4	9,9,10	0.57	0	10,12,14	0.84	0
4	FUB	W	2	4	9,9,10	0.57	0	10,12,14	0.76	0
4	FUB	W	3	4	9,9,10	0.57	0	10,12,14	0.83	0
4	AHR	W	4	4	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
9	FUB	WA	1	9	9,9,10	0.56	0	10,12,14	0.84	0
9	FUB	WA	2	9	9,9,10	0.58	0	10,12,14	0.95	0
13	FUB	WB	1	13	9,9,10	0.54	0	10,12,14	0.95	0
13	FUB	WB	2	13	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
13	GZL	WB	3	13	11,11,12	6.80	7 (63%)	14,15,17	1.26	1 (7%)
13	AHR	WB	4	13	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
3	FUB	WC	1	3	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
3	FUB	WC	2	3	9,9,10	0.57	0	10,12,14	0.93	0
3	FUB	WC	3	3	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
7	FUB	WD	1	7	9,9,10	0.60	0	10,12,14	0.93	0
7	FUB	WD	2	7	9,9,10	0.59	0	10,12,14	1.10	0
7	FUB	WD	3	7	9,9,10	0.58	0	10,12,14	0.95	0
7	AHR	WD	4	7	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
20	FUB	WE	1	20	9,9,10	0.54	0	10,12,14	0.93	0
20	FUB	WE	2	20	9,9,10	0.56	0	10,12,14	0.81	0
20	GZL	WE	3	20	11,11,12	6.73	7 (63%)	14,15,17	1.36	1 (7%)
20	AHR	WE	4	20	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
4	FUB	X	1	4	9,9,10	0.54	0	10,12,14	0.95	1 (10%)
4	FUB	X	2	4	9,9,10	0.55	0	10,12,14	0.79	0
4	FUB	X	3	4	9,9,10	0.57	0	10,12,14	0.83	0
4	AHR	X	4	4	9,9,10	0.58	0	10,12,14	0.98	0
3	FUB	XA	1	3	9,9,10	0.57	0	10,12,14	1.04	0
3	FUB	XA	2	3	9,9,10	0.53	0	10,12,14	0.65	0
3	FUB	XA	3	3	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
6	FUB	XB	1	6	9,9,10	0.57	0	10,12,14	1.02	0
6	FUB	XB	2	6	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	GZL	XB	3	6	11,11,12	7.02	6 (54%)	14,15,17	3.89	4 (28%)
7	FUB	XC	1	7	9,9,10	0.58	0	10,12,14	1.04	0
7	FUB	XC	2	7	9,9,10	0.53	0	10,12,14	0.99	1 (10%)
7	FUB	XC	3	7	9,9,10	0.59	0	10,12,14	0.87	0
7	AHR	XC	4	7	9,9,10	0.58	0	10,12,14	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	FUB	XD	1	11	9,9,10	0.66	0	10,12,14	1.19	1 (10%)
11	AHR	XD	2	11	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
11	AHR	XD	3	11	9,9,10	0.56	0	10,12,14	1.09	1 (10%)
23	FUB	XE	1	23	9,9,10	0.56	0	10,12,14	1.20	1 (10%)
23	FUB	XE	2	23	9,9,10	0.56	0	10,12,14	0.71	0
23	GZL	XE	3	23	11,11,12	6.72	7 (63%)	14,15,17	1.41	1 (7%)
23	AHR	XE	4	23	9,9,10	0.56	0	10,12,14	0.88	1 (10%)
23	AHR	XE	5	23	9,9,10	0.57	0	10,12,14	0.92	0
23	AHR	XE	6	23	9,9,10	0.56	0	10,12,14	0.98	1 (10%)
9	FUB	Y	1	9	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
9	FUB	Y	2	9	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
10	FUB	YA	1	10	9,9,10	0.57	0	10,12,14	0.82	0
10	FUB	YA	2	10	9,9,10	0.58	0	10,12,14	0.85	0
10	FUB	YA	3	10	9,9,10	0.57	0	10,12,14	0.82	0
10	AHR	YA	4	10	9,9,10	0.58	0	10,12,14	0.99	0
10	AHR	YA	5	10	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
13	FUB	YB	1	13	9,9,10	0.53	0	10,12,14	0.76	0
13	FUB	YB	2	13	9,9,10	0.57	0	10,12,14	0.75	0
13	GZL	YB	3	13	11,11,12	6.78	7 (63%)	14,15,17	1.14	1 (7%)
13	AHR	YB	4	13	9,9,10	0.56	0	10,12,14	1.12	1 (10%)
4	FUB	YC	1	4	9,9,10	0.57	0	10,12,14	0.87	0
4	FUB	YC	2	4	9,9,10	0.55	0	10,12,14	0.97	1 (10%)
4	FUB	YC	3	4	9,9,10	0.57	0	10,12,14	0.81	0
4	AHR	YC	4	4	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
9	FUB	YD	1	9	9,9,10	0.55	0	10,12,14	0.60	0
9	FUB	YD	2	9	9,9,10	0.55	0	10,12,14	0.78	0
24	FUB	YE	1	24	9,9,10	0.54	0	10,12,14	1.47	1 (10%)
24	FUB	YE	2	24	9,9,10	0.55	0	10,12,14	0.80	0
24	GZL	YE	3	24	11,11,12	6.73	7 (63%)	14,15,17	1.39	1 (7%)
24	AHR	YE	4	24	9,9,10	0.59	0	10,12,14	1.10	2 (20%)
24	AHR	YE	5	24	9,9,10	0.58	0	10,12,14	1.18	1 (10%)
24	AHR	YE	6	24	9,9,10	0.59	0	10,12,14	1.00	1 (10%)
4	FUB	Z	1	4	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
4	FUB	Z	2	4	9,9,10	0.55	0	10,12,14	0.96	1 (10%)
4	FUB	Z	3	4	9,9,10	0.56	0	10,12,14	0.81	0
4	AHR	Z	4	4	9,9,10	0.58	0	10,12,14	1.15	1 (10%)
3	FUB	ZA	1	3	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
3	FUB	ZA	2	3	9,9,10	0.56	0	10,12,14	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	ZA	3	3	9,9,10	0.57	0	10,12,14	0.94	0
13	FUB	ZB	1	13	9,9,10	0.59	0	10,12,14	1.00	0
13	FUB	ZB	2	13	9,9,10	0.57	0	10,12,14	0.93	0
13	GZL	ZB	3	13	11,11,12	6.73	7 (63%)	14,15,17	1.57	3 (21%)
13	AHR	ZB	4	13	9,9,10	0.57	0	10,12,14	0.94	0
7	FUB	ZC	1	7	9,9,10	0.55	0	10,12,14	0.82	0
7	FUB	ZC	2	7	9,9,10	0.57	0	10,12,14	0.91	0
7	FUB	ZC	3	7	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
7	AHR	ZC	4	7	9,9,10	0.57	0	10,12,14	1.01	0
4	FUB	ZD	1	4	9,9,10	0.57	0	10,12,14	0.99	1 (10%)
4	FUB	ZD	2	4	9,9,10	0.57	0	10,12,14	0.85	0
4	FUB	ZD	3	4	9,9,10	0.59	0	10,12,14	0.92	0
4	AHR	ZD	4	4	9,9,10	0.58	0	10,12,14	1.00	0
6	FUB	ZE	1	6	9,9,10	0.57	0	10,12,14	0.86	0
6	FUB	ZE	2	6	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
6	GZL	ZE	3	6	11,11,12	6.70	7 (63%)	14,15,17	1.41	1 (7%)
10	FUB	a	1	10	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
10	FUB	a	2	10	9,9,10	0.56	0	10,12,14	0.97	1 (10%)
10	FUB	a	3	10	9,9,10	0.57	0	10,12,14	0.82	0
10	AHR	a	4	10	9,9,10	0.55	0	10,12,14	1.18	1 (10%)
10	AHR	a	5	10	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
4	FUB	aA	1	4	9,9,10	0.55	0	10,12,14	0.77	0
4	FUB	aA	2	4	9,9,10	0.58	0	10,12,14	0.92	0
4	FUB	aA	3	4	9,9,10	0.57	0	10,12,14	0.96	0
4	AHR	aA	4	4	9,9,10	0.57	0	10,12,14	0.98	0
6	FUB	aB	1	6	9,9,10	0.57	0	10,12,14	0.89	0
6	FUB	aB	2	6	9,9,10	0.54	0	10,12,14	1.25	2 (20%)
6	GZL	aB	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.48	2 (14%)
11	FUB	aC	1	11	9,9,10	0.64	0	10,12,14	1.07	0
11	AHR	aC	2	11	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
11	AHR	aC	3	11	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
3	FUB	aD	1	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	aD	2	3	9,9,10	0.57	0	10,12,14	0.95	0
3	FUB	aD	3	3	9,9,10	0.58	0	10,12,14	0.89	0
19	FUB	aE	1	19	9,9,10	0.59	0	10,12,14	0.85	0
19	FUB	aE	2	19	9,9,10	0.57	0	10,12,14	0.98	0
19	GZL	aE	3	19	11,11,12	6.69	7 (63%)	14,15,17	1.69	3 (21%)
19	AHR	aE	4	19	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
3	FUB	b	1	3	9,9,10	0.58	0	10,12,14	1.12	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	b	2	3	9,9,10	0.57	0	10,12,14	0.94	0
3	FUB	b	3	3	9,9,10	0.58	0	10,12,14	0.92	0
4	FUB	bA	1	4	9,9,10	0.55	0	10,12,14	0.88	0
4	FUB	bA	2	4	9,9,10	0.57	0	10,12,14	0.88	0
4	FUB	bA	3	4	9,9,10	0.57	0	10,12,14	0.98	0
4	AHR	bA	4	4	9,9,10	0.57	0	10,12,14	0.88	0
6	FUB	bB	1	6	9,9,10	0.55	0	10,12,14	1.05	1 (10%)
6	FUB	bB	2	6	9,9,10	0.59	0	10,12,14	0.96	1 (10%)
6	GZL	bB	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.43	1 (7%)
9	FUB	bC	1	9	9,9,10	0.56	0	10,12,14	0.70	0
9	FUB	bC	2	9	9,9,10	0.54	0	10,12,14	0.82	0
3	FUB	bD	1	3	9,9,10	0.51	0	10,12,14	0.87	0
3	FUB	bD	2	3	9,9,10	0.58	0	10,12,14	0.87	0
3	FUB	bD	3	3	9,9,10	0.57	0	10,12,14	0.82	0
6	FUB	bE	1	6	9,9,10	0.61	0	10,12,14	1.01	0
6	FUB	bE	2	6	9,9,10	0.55	0	10,12,14	0.86	0
6	GZL	bE	3	6	11,11,12	6.77	7 (63%)	14,15,17	1.55	1 (7%)
4	FUB	c	1	4	9,9,10	0.56	0	10,12,14	0.79	0
4	FUB	c	2	4	9,9,10	0.58	0	10,12,14	0.89	0
4	FUB	c	3	4	9,9,10	0.55	0	10,12,14	0.92	0
4	AHR	c	4	4	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
3	FUB	cA	1	3	9,9,10	0.56	0	10,12,14	0.83	0
3	FUB	cA	2	3	9,9,10	0.58	0	10,12,14	0.99	1 (10%)
3	FUB	cA	3	3	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
6	FUB	cB	1	6	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
6	FUB	cB	2	6	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
6	GZL	cB	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.59	2 (14%)
4	FUB	cC	1	4	9,9,10	0.56	0	10,12,14	1.19	1 (10%)
4	FUB	cC	2	4	9,9,10	0.57	0	10,12,14	0.85	0
4	FUB	cC	3	4	9,9,10	0.57	0	10,12,14	0.95	0
4	AHR	cC	4	4	9,9,10	0.57	0	10,12,14	1.06	1 (10%)
12	FUB	cD	1	12	9,9,10	0.57	0	10,12,14	0.80	0
12	FUB	cD	2	12	9,9,10	0.59	0	10,12,14	0.96	0
12	GZL	cD	3	12	11,11,12	6.72	7 (63%)	14,15,17	1.45	2 (14%)
12	AHR	cD	4	12	9,9,10	0.58	0	10,12,14	0.98	0
12	AHR	cD	5	12	9,9,10	0.59	0	10,12,14	1.02	1 (10%)
18	FUB	cE	1	18	9,9,10	0.55	0	10,12,14	1.05	1 (10%)
18	FUB	cE	2	18	9,9,10	0.59	0	10,12,14	0.88	0
18	GZL	cE	3	18	11,11,12	6.74	7 (63%)	14,15,17	1.66	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	AHR	cE	4	18	9,9,10	0.57	0	10,12,14	0.95	0
18	AHR	cE	5	18	9,9,10	0.57	0	10,12,14	0.87	0
4	FUB	d	1	4	9,9,10	0.55	0	10,12,14	0.97	1 (10%)
4	FUB	d	2	4	9,9,10	0.57	0	10,12,14	0.92	0
4	FUB	d	3	4	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
4	AHR	d	4	4	9,9,10	0.56	0	10,12,14	1.15	1 (10%)
7	FUB	dA	1	7	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
7	FUB	dA	2	7	9,9,10	0.54	0	10,12,14	1.07	1 (10%)
7	FUB	dA	3	7	9,9,10	0.56	0	10,12,14	0.88	0
7	AHR	dA	4	7	9,9,10	0.57	0	10,12,14	0.78	0
13	FUB	dB	1	13	9,9,10	0.58	0	10,12,14	0.74	0
13	FUB	dB	2	13	9,9,10	0.56	0	10,12,14	1.12	0
13	GZL	dB	3	13	11,11,12	6.75	7 (63%)	14,15,17	1.87	4 (28%)
13	AHR	dB	4	13	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
3	FUB	dC	1	3	9,9,10	0.56	0	10,12,14	0.86	0
3	FUB	dC	2	3	9,9,10	0.58	0	10,12,14	0.86	0
3	FUB	dC	3	3	9,9,10	0.58	0	10,12,14	1.09	1 (10%)
13	FUB	dD	1	13	9,9,10	0.59	0	10,12,14	0.86	0
13	FUB	dD	2	13	9,9,10	0.56	0	10,12,14	0.84	0
13	GZL	dD	3	13	11,11,12	6.72	7 (63%)	14,15,17	1.27	1 (7%)
13	AHR	dD	4	13	9,9,10	0.56	0	10,12,14	0.93	0
22	FUB	dE	1	22	9,9,10	0.56	0	10,12,14	0.97	1 (10%)
22	FUB	dE	2	22	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
22	GZL	dE	3	22	11,11,12	6.72	7 (63%)	14,15,17	1.53	1 (7%)
22	AHR	dE	4	22	9,9,10	0.55	0	10,12,14	1.14	1 (10%)
22	AHR	dE	5	22	9,9,10	0.58	0	10,12,14	1.10	0
22	AHR	dE	6	22	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
3	FUB	e	1	3	9,9,10	0.59	0	10,12,14	0.83	0
3	FUB	e	2	3	9,9,10	0.58	0	10,12,14	0.93	0
3	FUB	e	3	3	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
4	FUB	eA	1	4	9,9,10	0.58	0	10,12,14	0.98	0
4	FUB	eA	2	4	9,9,10	0.56	0	10,12,14	0.82	0
4	FUB	eA	3	4	9,9,10	0.58	0	10,12,14	0.99	0
4	AHR	eA	4	4	9,9,10	0.58	0	10,12,14	0.95	0
15	FUB	eB	1	15	9,9,10	0.55	0	10,12,14	1.00	1 (10%)
15	FUB	eB	2	15	9,9,10	0.57	0	10,12,14	0.92	0
15	GZL	eB	3	15	11,11,12	6.75	7 (63%)	14,15,17	1.49	2 (14%)
15	AHR	eB	4	15	9,9,10	0.61	0	10,12,14	1.21	1 (10%)
15	AHR	eB	5	15	9,9,10	0.59	0	10,12,14	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	eC	1	3	9,9,10	0.55	0	10,12,14	0.69	0
3	FUB	eC	2	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	eC	3	3	9,9,10	0.58	0	10,12,14	0.90	0
14	FUB	eD	1	14	9,9,10	0.56	0	10,12,14	0.90	0
14	FUB	eD	2	14	9,9,10	0.58	0	10,12,14	0.84	0
14	GZL	eD	3	14	11,11,12	6.70	7 (63%)	14,15,17	1.76	2 (14%)
14	FUB	eD	4	14	9,9,10	0.59	0	10,12,14	1.01	1 (10%)
22	FUB	eE	1	22	9,9,10	0.61	0	10,12,14	1.17	1 (10%)
22	FUB	eE	2	22	9,9,10	0.57	0	10,12,14	0.91	0
22	GZL	eE	3	22	11,11,12	6.74	6 (54%)	14,15,17	1.57	1 (7%)
22	AHR	eE	4	22	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
22	AHR	eE	5	22	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
22	AHR	eE	6	22	9,9,10	0.59	0	10,12,14	1.19	1 (10%)
7	FUB	f	1	7	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
7	FUB	f	2	7	9,9,10	0.55	0	10,12,14	1.04	1 (10%)
7	FUB	f	3	7	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
7	AHR	f	4	7	9,9,10	0.53	0	10,12,14	0.80	0
7	FUB	fA	1	7	9,9,10	0.57	0	10,12,14	0.99	0
7	FUB	fA	2	7	9,9,10	0.58	0	10,12,14	0.92	0
7	FUB	fA	3	7	9,9,10	0.58	0	10,12,14	0.96	0
7	AHR	fA	4	7	9,9,10	0.57	0	10,12,14	0.98	0
15	FUB	fB	1	15	9,9,10	0.57	0	10,12,14	1.01	0
15	FUB	fB	2	15	9,9,10	0.58	0	10,12,14	0.88	0
15	GZL	fB	3	15	11,11,12	6.74	7 (63%)	14,15,17	1.31	1 (7%)
15	AHR	fB	4	15	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
15	AHR	fB	5	15	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
12	FUB	fC	1	12	9,9,10	0.59	0	10,12,14	0.93	0
12	FUB	fC	2	12	9,9,10	0.56	0	10,12,14	0.87	0
12	GZL	fC	3	12	11,11,12	6.75	7 (63%)	14,15,17	1.31	1 (7%)
12	AHR	fC	4	12	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
12	AHR	fC	5	12	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
12	FUB	fD	1	12	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
12	FUB	fD	2	12	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
12	GZL	fD	3	12	11,11,12	6.70	7 (63%)	14,15,17	1.25	1 (7%)
12	AHR	fD	4	12	9,9,10	0.56	0	10,12,14	0.91	0
12	AHR	fD	5	12	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
18	FUB	fE	1	18	9,9,10	0.54	0	10,12,14	1.14	1 (10%)
18	FUB	fE	2	18	9,9,10	0.54	0	10,12,14	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	GZL	fE	3	18	11,11,12	6.73	7 (63%)	14,15,17	1.34	1 (7%)
18	AHR	fE	4	18	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
18	AHR	fE	5	18	9,9,10	0.58	0	10,12,14	0.85	0
4	FUB	g	1	4	9,9,10	0.56	0	10,12,14	1.03	0
4	FUB	g	2	4	9,9,10	0.58	0	10,12,14	0.89	0
4	FUB	g	3	4	9,9,10	0.57	0	10,12,14	0.90	0
4	AHR	g	4	4	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
11	FUB	gA	1	11	9,9,10	0.66	0	10,12,14	1.36	1 (10%)
11	AHR	gA	2	11	9,9,10	0.57	0	10,12,14	0.94	0
11	AHR	gA	3	11	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
6	FUB	gB	1	6	9,9,10	0.57	0	10,12,14	0.85	0
6	FUB	gB	2	6	9,9,10	0.56	0	10,12,14	0.90	0
6	GZL	gB	3	6	11,11,12	6.71	7 (63%)	14,15,17	1.54	2 (14%)
13	FUB	gC	1	13	9,9,10	0.58	0	10,12,14	0.85	0
13	FUB	gC	2	13	9,9,10	0.59	0	10,12,14	1.01	0
13	GZL	gC	3	13	11,11,12	6.75	7 (63%)	14,15,17	1.28	1 (7%)
13	AHR	gC	4	13	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
4	FUB	gD	1	4	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
4	FUB	gD	2	4	9,9,10	0.56	0	10,12,14	0.99	1 (10%)
4	FUB	gD	3	4	9,9,10	0.57	0	10,12,14	0.78	0
4	AHR	gD	4	4	9,9,10	0.57	0	10,12,14	0.79	0
20	FUB	gE	1	20	9,9,10	0.56	0	10,12,14	0.95	0
20	FUB	gE	2	20	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
20	GZL	gE	3	20	11,11,12	6.74	7 (63%)	14,15,17	1.28	1 (7%)
20	AHR	gE	4	20	9,9,10	0.58	0	10,12,14	0.87	0
7	FUB	h	1	7	9,9,10	0.56	0	10,12,14	1.01	0
7	FUB	h	2	7	9,9,10	0.59	0	10,12,14	0.97	0
7	FUB	h	3	7	9,9,10	0.57	0	10,12,14	1.00	0
7	AHR	h	4	7	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
9	FUB	hA	1	9	9,9,10	0.54	0	10,12,14	0.87	1 (10%)
9	FUB	hA	2	9	9,9,10	0.55	0	10,12,14	0.78	0
3	FUB	hB	1	3	9,9,10	0.58	0	10,12,14	0.81	0
3	FUB	hB	2	3	9,9,10	0.58	0	10,12,14	0.85	0
3	FUB	hB	3	3	9,9,10	0.59	0	10,12,14	0.94	0
14	FUB	hC	1	14	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
14	FUB	hC	2	14	9,9,10	0.57	0	10,12,14	0.87	0
14	GZL	hC	3	14	11,11,12	6.72	7 (63%)	14,15,17	1.67	2 (14%)
14	FUB	hC	4	14	9,9,10	0.59	0	10,12,14	0.85	0
14	FUB	hD	1	14	9,9,10	0.57	0	10,12,14	0.98	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FUB	hD	2	14	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
14	GZL	hD	3	14	11,11,12	6.61	7 (63%)	14,15,17	1.61	2 (14%)
14	FUB	hD	4	14	9,9,10	0.57	0	10,12,14	0.94	0
20	FUB	hE	1	20	9,9,10	0.57	0	10,12,14	0.96	0
20	FUB	hE	2	20	9,9,10	0.56	0	10,12,14	0.83	0
20	GZL	hE	3	20	11,11,12	6.72	7 (63%)	14,15,17	1.44	1 (7%)
20	AHR	hE	4	20	9,9,10	0.56	0	10,12,14	0.88	0
11	FUB	i	1	11	9,9,10	0.65	0	10,12,14	1.31	1 (10%)
11	AHR	i	2	11	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
11	AHR	i	3	11	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
4	FUB	iA	1	4	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
4	FUB	iA	2	4	9,9,10	0.57	0	10,12,14	0.97	0
4	FUB	iA	3	4	9,9,10	0.56	0	10,12,14	0.87	0
4	AHR	iA	4	4	9,9,10	0.57	0	10,12,14	1.18	1 (10%)
12	FUB	iB	1	12	9,9,10	0.60	0	10,12,14	0.94	0
12	FUB	iB	2	12	9,9,10	0.59	0	10,12,14	1.01	0
12	GZL	iB	3	12	11,11,12	6.71	7 (63%)	14,15,17	1.53	2 (14%)
12	AHR	iB	4	12	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
12	AHR	iB	5	12	9,9,10	0.60	0	10,12,14	0.97	0
12	FUB	iC	1	12	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
12	FUB	iC	2	12	9,9,10	0.58	0	10,12,14	0.99	1 (10%)
12	GZL	iC	3	12	11,11,12	6.68	7 (63%)	14,15,17	1.43	1 (7%)
12	AHR	iC	4	12	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
12	AHR	iC	5	12	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
3	FUB	iD	1	3	9,9,10	0.57	0	10,12,14	0.98	1 (10%)
3	FUB	iD	2	3	9,9,10	0.55	0	10,12,14	0.79	0
3	FUB	iD	3	3	9,9,10	0.57	0	10,12,14	0.92	0
22	FUB	iE	1	22	9,9,10	0.55	0	10,12,14	1.17	1 (10%)
22	FUB	iE	2	22	9,9,10	0.55	0	10,12,14	0.89	0
22	GZL	iE	3	22	11,11,12	6.75	7 (63%)	14,15,17	1.33	1 (7%)
22	AHR	iE	4	22	9,9,10	0.60	0	10,12,14	0.99	0
22	AHR	iE	5	22	9,9,10	0.56	0	10,12,14	0.64	0
22	AHR	iE	6	22	9,9,10	0.57	0	10,12,14	1.14	1 (10%)
9	FUB	j	1	9	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
9	FUB	j	2	9	9,9,10	0.56	0	10,12,14	0.78	0
3	FUB	jA	1	3	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	jA	2	3	9,9,10	0.58	0	10,12,14	0.90	0
3	FUB	jA	3	3	9,9,10	0.56	0	10,12,14	1.06	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	FUB	jB	1	13	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
13	FUB	jB	2	13	9,9,10	0.56	0	10,12,14	0.89	0
13	GZL	jB	3	13	11,11,12	6.75	7 (63%)	14,15,17	1.33	1 (7%)
13	AHR	jB	4	13	9,9,10	0.59	0	10,12,14	0.98	0
4	FUB	jC	1	4	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
4	FUB	jC	2	4	9,9,10	0.58	0	10,12,14	0.97	0
4	FUB	jC	3	4	9,9,10	0.57	0	10,12,14	0.99	0
4	AHR	jC	4	4	9,9,10	0.57	0	10,12,14	0.93	0
10	FUB	jD	1	10	9,9,10	0.55	0	10,12,14	1.20	1 (10%)
10	FUB	jD	2	10	9,9,10	0.59	0	10,12,14	0.98	0
10	FUB	jD	3	10	9,9,10	0.58	0	10,12,14	0.92	0
10	AHR	jD	4	10	9,9,10	0.58	0	10,12,14	0.96	0
10	AHR	jD	5	10	9,9,10	0.57	0	10,12,14	1.05	1 (10%)
20	FUB	jE	1	20	9,9,10	0.59	0	10,12,14	1.01	0
20	FUB	jE	2	20	9,9,10	0.57	0	10,12,14	0.91	0
20	GZL	jE	3	20	11,11,12	6.72	7 (63%)	14,15,17	1.58	2 (14%)
20	AHR	jE	4	20	9,9,10	0.57	0	10,12,14	0.89	0
4	FUB	k	1	4	9,9,10	0.58	0	10,12,14	0.83	0
4	FUB	k	2	4	9,9,10	0.58	0	10,12,14	0.96	0
4	FUB	k	3	4	9,9,10	0.55	0	10,12,14	0.94	0
4	AHR	k	4	4	9,9,10	0.58	0	10,12,14	0.96	0
3	FUB	kA	1	3	9,9,10	0.53	0	10,12,14	0.77	0
3	FUB	kA	2	3	9,9,10	0.55	0	10,12,14	0.80	0
3	FUB	kA	3	3	9,9,10	0.58	0	10,12,14	0.87	0
14	FUB	kB	1	14	9,9,10	0.59	0	10,12,14	0.90	0
14	FUB	kB	2	14	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
14	GZL	kB	3	14	11,11,12	6.65	7 (63%)	14,15,17	1.63	3 (21%)
14	FUB	kB	4	14	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
14	FUB	kC	1	14	9,9,10	0.57	0	10,12,14	0.97	1 (10%)
14	FUB	kC	2	14	9,9,10	0.58	0	10,12,14	0.99	0
14	GZL	kC	3	14	11,11,12	6.66	7 (63%)	14,15,17	1.91	2 (14%)
14	FUB	kC	4	14	9,9,10	0.60	0	10,12,14	0.85	0
4	FUB	kD	1	4	9,9,10	0.60	0	10,12,14	0.96	0
4	FUB	kD	2	4	9,9,10	0.58	0	10,12,14	0.85	0
4	FUB	kD	3	4	9,9,10	0.56	0	10,12,14	0.90	0
4	AHR	kD	4	4	9,9,10	0.57	0	10,12,14	0.93	0
21	FUB	kE	1	21	9,9,10	0.55	0	10,12,14	1.16	2 (20%)
21	FUB	kE	2	21	9,9,10	0.56	0	10,12,14	1.01	1 (10%)
21	GZL	kE	3	21	11,11,12	6.75	7 (63%)	14,15,17	1.24	1 (7%)
21	AHR	kE	4	21	9,9,10	0.58	0	10,12,14	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	AHR	kE	5	21	9,9,10	0.56	0	10,12,14	1.10	1 (10%)
3	FUB	l	1	3	9,9,10	0.58	0	10,12,14	0.92	0
3	FUB	l	2	3	9,9,10	0.53	0	10,12,14	0.82	0
3	FUB	l	3	3	9,9,10	0.57	0	10,12,14	0.88	0
12	FUB	lA	1	12	9,9,10	0.55	0	10,12,14	0.92	0
12	FUB	lA	2	12	9,9,10	0.58	0	10,12,14	0.94	0
12	GZL	lA	3	12	11,11,12	6.73	7 (63%)	14,15,17	1.24	1 (7%)
12	AHR	lA	4	12	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
12	AHR	lA	5	12	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
12	FUB	lB	1	12	9,9,10	0.54	0	10,12,14	1.16	1 (10%)
12	FUB	lB	2	12	9,9,10	0.57	0	10,12,14	0.94	0
12	GZL	lB	3	12	11,11,12	6.71	7 (63%)	14,15,17	1.36	1 (7%)
12	AHR	lB	4	12	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
12	AHR	lB	5	12	9,9,10	0.58	0	10,12,14	0.97	0
3	FUB	lC	1	3	9,9,10	0.57	0	10,12,14	0.81	0
3	FUB	lC	2	3	9,9,10	0.56	0	10,12,14	0.87	0
3	FUB	lC	3	3	9,9,10	0.58	0	10,12,14	1.01	0
3	FUB	lD	1	3	9,9,10	0.59	0	10,12,14	0.87	0
3	FUB	lD	2	3	9,9,10	0.56	0	10,12,14	0.95	0
3	FUB	lD	3	3	9,9,10	0.59	0	10,12,14	0.86	0
24	FUB	lE	1	24	9,9,10	0.54	0	10,12,14	1.33	1 (10%)
24	FUB	lE	2	24	9,9,10	0.55	0	10,12,14	1.04	1 (10%)
24	GZL	lE	3	24	11,11,12	6.71	7 (63%)	14,15,17	1.48	1 (7%)
24	AHR	lE	4	24	9,9,10	0.59	0	10,12,14	1.15	2 (20%)
24	AHR	lE	5	24	9,9,10	0.55	0	10,12,14	1.10	1 (10%)
24	AHR	lE	6	24	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
3	FUB	m	1	3	9,9,10	0.53	0	10,12,14	0.88	0
3	FUB	m	2	3	9,9,10	0.57	0	10,12,14	0.79	0
3	FUB	m	3	3	9,9,10	0.57	0	10,12,14	0.88	0
13	FUB	mA	1	13	9,9,10	0.56	0	10,12,14	0.83	0
13	FUB	mA	2	13	9,9,10	0.60	0	10,12,14	0.88	0
13	GZL	mA	3	13	11,11,12	6.76	7 (63%)	14,15,17	1.28	1 (7%)
13	AHR	mA	4	13	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
4	FUB	mB	1	4	9,9,10	0.55	0	10,12,14	1.00	1 (10%)
4	FUB	mB	2	4	9,9,10	0.56	0	10,12,14	0.94	0
4	FUB	mB	3	4	9,9,10	0.57	0	10,12,14	1.02	0
4	AHR	mB	4	4	9,9,10	0.58	0	10,12,14	0.95	1 (10%)
10	FUB	mC	1	10	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
10	FUB	mC	2	10	9,9,10	0.58	0	10,12,14	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	FUB	mC	3	10	9,9,10	0.57	0	10,12,14	0.82	0
10	AHR	mC	4	10	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
10	AHR	mC	5	10	9,9,10	0.57	0	10,12,14	1.19	1 (10%)
3	FUB	mD	1	3	9,9,10	0.56	0	10,12,14	0.69	0
3	FUB	mD	2	3	9,9,10	0.58	0	10,12,14	0.99	0
3	FUB	mD	3	3	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
6	FUB	mE	1	6	9,9,10	0.58	0	10,12,14	0.98	0
6	FUB	mE	2	6	9,9,10	0.58	0	10,12,14	0.97	1 (10%)
6	GZL	mE	3	6	11,11,12	6.72	7 (63%)	14,15,17	1.70	2 (14%)
12	FUB	n	1	12	9,9,10	0.55	0	10,12,14	0.87	0
12	FUB	n	2	12	9,9,10	0.58	0	10,12,14	0.84	0
12	GZL	n	3	12	11,11,12	6.73	7 (63%)	14,15,17	1.29	1 (7%)
12	AHR	n	4	12	9,9,10	0.55	0	10,12,14	1.14	1 (10%)
12	AHR	n	5	12	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
14	FUB	nA	1	14	9,9,10	0.52	0	10,12,14	0.90	0
14	FUB	nA	2	14	9,9,10	0.59	0	10,12,14	0.86	0
14	GZL	nA	3	14	11,11,12	6.72	7 (63%)	14,15,17	1.90	4 (28%)
14	FUB	nA	4	14	9,9,10	0.59	0	10,12,14	1.07	0
14	FUB	nB	1	14	9,9,10	0.57	0	10,12,14	0.89	0
14	FUB	nB	2	14	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
14	GZL	nB	3	14	11,11,12	6.67	7 (63%)	14,15,17	1.60	3 (21%)
14	FUB	nB	4	14	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
4	FUB	nC	1	4	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
4	FUB	nC	2	4	9,9,10	0.57	0	10,12,14	0.99	0
4	FUB	nC	3	4	9,9,10	0.58	0	10,12,14	0.97	0
4	AHR	nC	4	4	9,9,10	0.58	0	10,12,14	1.02	1 (10%)
3	FUB	nD	1	3	9,9,10	0.60	0	10,12,14	1.00	0
3	FUB	nD	2	3	9,9,10	0.58	0	10,12,14	0.95	0
3	FUB	nD	3	3	9,9,10	0.54	0	10,12,14	0.65	0
6	FUB	nE	1	6	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
6	FUB	nE	2	6	9,9,10	0.57	0	10,12,14	0.97	0
6	GZL	nE	3	6	11,11,12	6.69	7 (63%)	14,15,17	1.64	2 (14%)
13	FUB	o	1	13	9,9,10	0.57	0	10,12,14	0.77	0
13	FUB	o	2	13	9,9,10	0.58	0	10,12,14	0.85	0
13	GZL	o	3	13	11,11,12	6.76	7 (63%)	14,15,17	1.26	1 (7%)
13	AHR	o	4	13	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
12	FUB	oA	1	12	9,9,10	0.54	0	10,12,14	1.11	1 (10%)
12	FUB	oA	2	12	9,9,10	0.56	0	10,12,14	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	GZL	oA	3	12	11,11,12	6.75	7 (63%)	14,15,17	1.30	1 (7%)
12	AHR	oA	4	12	9,9,10	0.59	0	10,12,14	0.90	0
12	AHR	oA	5	12	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
3	FUB	oB	1	3	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
3	FUB	oB	2	3	9,9,10	0.56	0	10,12,14	0.82	0
3	FUB	oB	3	3	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
3	FUB	oC	1	3	9,9,10	0.60	0	10,12,14	0.91	0
3	FUB	oC	2	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	oC	3	3	9,9,10	0.59	0	10,12,14	0.87	0
3	FUB	oD	1	3	9,9,10	0.59	0	10,12,14	0.96	0
3	FUB	oD	2	3	9,9,10	0.57	0	10,12,14	0.87	0
3	FUB	oD	3	3	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
6	FUB	oE	1	6	9,9,10	0.57	0	10,12,14	0.86	0
6	FUB	oE	2	6	9,9,10	0.57	0	10,12,14	0.99	1 (10%)
6	GZL	oE	3	6	11,11,12	6.69	7 (63%)	14,15,17	1.67	2 (14%)
14	FUB	p	1	14	9,9,10	0.54	0	10,12,14	0.86	0
14	FUB	p	2	14	9,9,10	0.58	0	10,12,14	0.89	0
14	GZL	p	3	14	11,11,12	6.70	7 (63%)	14,15,17	1.69	4 (28%)
14	FUB	p	4	14	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
4	FUB	pA	1	4	9,9,10	0.56	0	10,12,14	0.74	0
4	FUB	pA	2	4	9,9,10	0.57	0	10,12,14	0.84	0
4	FUB	pA	3	4	9,9,10	0.57	0	10,12,14	0.80	0
4	AHR	pA	4	4	9,9,10	0.56	0	10,12,14	0.92	0
10	FUB	pB	1	10	9,9,10	0.58	0	10,12,14	1.09	0
10	FUB	pB	2	10	9,9,10	0.58	0	10,12,14	1.05	0
10	FUB	pB	3	10	9,9,10	0.57	0	10,12,14	0.84	0
10	AHR	pB	4	10	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
10	AHR	pB	5	10	9,9,10	0.58	0	10,12,14	1.17	1 (10%)
3	FUB	pC	1	3	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
3	FUB	pC	2	3	9,9,10	0.58	0	10,12,14	1.02	1 (10%)
3	FUB	pC	3	3	9,9,10	0.58	0	10,12,14	0.90	0
3	FUB	pD	1	3	9,9,10	0.59	0	10,12,14	1.09	1 (10%)
3	FUB	pD	2	3	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	pD	3	3	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
18	FUB	pE	1	18	9,9,10	0.55	0	10,12,14	2.39	5 (50%)
18	FUB	pE	2	18	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
18	GZL	pE	3	18	11,11,12	6.71	7 (63%)	14,15,17	1.53	2 (14%)
18	AHR	pE	4	18	9,9,10	0.59	0	10,12,14	1.05	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	AHR	pE	5	18	9,9,10	0.61	0	10,12,14	1.20	1 (10%)
12	FUB	q	1	12	9,9,10	0.56	0	10,12,14	1.02	1 (10%)
12	FUB	q	2	12	9,9,10	0.57	0	10,12,14	0.94	0
12	GZL	q	3	12	11,11,12	6.72	7 (63%)	14,15,17	1.35	1 (7%)
12	AHR	q	4	12	9,9,10	0.58	0	10,12,14	0.97	1 (10%)
12	AHR	q	5	12	9,9,10	0.55	0	10,12,14	1.04	1 (10%)
14	FUB	qA	1	14	9,9,10	0.59	0	10,12,14	0.75	0
14	FUB	qA	2	14	9,9,10	0.59	0	10,12,14	0.90	0
14	GZL	qA	3	14	11,11,12	6.73	7 (63%)	14,15,17	1.72	2 (14%)
14	FUB	qA	4	14	9,9,10	0.58	0	10,12,14	1.02	0
4	FUB	qB	1	4	9,9,10	0.59	0	10,12,14	1.05	1 (10%)
4	FUB	qB	2	4	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
4	FUB	qB	3	4	9,9,10	0.58	0	10,12,14	0.99	0
4	AHR	qB	4	4	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
3	FUB	qC	1	3	9,9,10	0.57	0	10,12,14	0.98	0
3	FUB	qC	2	3	9,9,10	0.56	0	10,12,14	0.81	0
3	FUB	qC	3	3	9,9,10	0.54	0	10,12,14	0.63	0
3	FUB	qD	1	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	qD	2	3	9,9,10	0.58	0	10,12,14	0.93	0
3	FUB	qD	3	3	9,9,10	0.56	0	10,12,14	0.93	0
19	FUB	qE	1	19	9,9,10	0.57	0	10,12,14	1.27	1 (10%)
19	FUB	qE	2	19	9,9,10	0.58	0	10,12,14	0.88	0
19	GZL	qE	3	19	11,11,12	6.73	7 (63%)	14,15,17	1.54	2 (14%)
19	AHR	qE	4	19	9,9,10	0.59	0	10,12,14	0.80	0
4	FUB	r	1	4	9,9,10	0.55	0	10,12,14	0.78	0
4	FUB	r	2	4	9,9,10	0.57	0	10,12,14	0.87	0
4	FUB	r	3	4	9,9,10	0.57	0	10,12,14	0.90	0
4	AHR	r	4	4	9,9,10	0.58	0	10,12,14	0.83	0
3	FUB	rA	1	3	9,9,10	0.54	0	10,12,14	0.80	0
3	FUB	rA	2	3	9,9,10	0.55	0	10,12,14	0.81	0
3	FUB	rA	3	3	9,9,10	0.59	0	10,12,14	0.92	0
3	FUB	rB	1	3	9,9,10	0.56	0	10,12,14	0.95	1 (10%)
3	FUB	rB	2	3	9,9,10	0.57	0	10,12,14	0.83	0
3	FUB	rB	3	3	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	rC	1	3	9,9,10	0.57	0	10,12,14	1.06	1 (10%)
3	FUB	rC	2	3	9,9,10	0.57	0	10,12,14	0.92	0
3	FUB	rC	3	3	9,9,10	0.59	0	10,12,14	0.99	0
3	FUB	rD	1	3	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
3	FUB	rD	2	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	rD	3	3	9,9,10	0.57	0	10,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	FUB	rE	1	18	9,9,10	0.61	0	10,12,14	1.03	0
18	FUB	rE	2	18	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
18	GZL	rE	3	18	11,11,12	6.76	7 (63%)	14,15,17	1.46	2 (14%)
18	AHR	rE	4	18	9,9,10	0.55	0	10,12,14	0.77	0
18	AHR	rE	5	18	9,9,10	0.58	0	10,12,14	1.16	1 (10%)
14	FUB	s	1	14	9,9,10	0.55	0	10,12,14	0.86	0
14	FUB	s	2	14	9,9,10	0.59	0	10,12,14	0.94	0
14	GZL	s	3	14	11,11,12	6.70	7 (63%)	14,15,17	1.98	3 (21%)
14	FUB	s	4	14	9,9,10	0.60	0	10,12,14	0.88	0
10	FUB	sA	1	10	9,9,10	0.57	0	10,12,14	1.05	0
10	FUB	sA	2	10	9,9,10	0.57	0	10,12,14	0.85	0
10	FUB	sA	3	10	9,9,10	0.55	0	10,12,14	0.79	0
10	AHR	sA	4	10	9,9,10	0.58	0	10,12,14	1.13	1 (10%)
10	AHR	sA	5	10	9,9,10	0.57	0	10,12,14	1.16	1 (10%)
3	FUB	sB	1	3	9,9,10	0.60	0	10,12,14	0.93	0
3	FUB	sB	2	3	9,9,10	0.57	0	10,12,14	1.05	0
3	FUB	sB	3	3	9,9,10	0.58	0	10,12,14	0.83	0
3	FUB	sC	1	3	9,9,10	0.54	0	10,12,14	1.07	1 (10%)
3	FUB	sC	2	3	9,9,10	0.58	0	10,12,14	0.86	0
3	FUB	sC	3	3	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
10	FUB	sD	1	10	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
10	FUB	sD	2	10	9,9,10	0.57	0	10,12,14	0.82	0
10	FUB	sD	3	10	9,9,10	0.58	0	10,12,14	1.00	0
10	AHR	sD	4	10	9,9,10	0.57	0	10,12,14	0.90	0
10	AHR	sD	5	10	9,9,10	0.58	0	10,12,14	0.80	0
20	FUB	sE	1	20	9,9,10	0.56	0	10,12,14	1.05	1 (10%)
20	FUB	sE	2	20	9,9,10	0.57	0	10,12,14	1.00	0
20	GZL	sE	3	20	11,11,12	6.73	7 (63%)	14,15,17	1.59	2 (14%)
20	AHR	sE	4	20	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
3	FUB	t	1	3	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
3	FUB	t	2	3	9,9,10	0.56	0	10,12,14	0.77	0
3	FUB	t	3	3	9,9,10	0.57	0	10,12,14	0.97	0
4	FUB	tA	1	4	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
4	FUB	tA	2	4	9,9,10	0.57	0	10,12,14	0.81	0
4	FUB	tA	3	4	9,9,10	0.56	0	10,12,14	0.79	0
4	AHR	tA	4	4	9,9,10	0.56	0	10,12,14	1.15	1 (10%)
3	FUB	tB	1	3	9,9,10	0.59	0	10,12,14	0.81	0
3	FUB	tB	2	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	tB	3	3	9,9,10	0.55	0	10,12,14	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	tC	1	3	9,9,10	0.59	0	10,12,14	1.01	0
3	FUB	tC	2	3	9,9,10	0.59	0	10,12,14	0.93	0
3	FUB	tC	3	3	9,9,10	0.59	0	10,12,14	1.08	1 (10%)
13	FUB	tD	1	13	9,9,10	0.57	0	10,12,14	1.06	0
13	FUB	tD	2	13	9,9,10	0.56	0	10,12,14	1.14	1 (10%)
13	GZL	tD	3	13	11,11,12	6.79	6 (54%)	14,15,17	1.14	2 (14%)
13	AHR	tD	4	13	9,9,10	0.59	0	10,12,14	1.18	1 (10%)
18	FUB	tE	1	18	9,9,10	0.54	0	10,12,14	0.93	1 (10%)
18	FUB	tE	2	18	9,9,10	0.53	0	10,12,14	0.76	0
18	GZL	tE	3	18	11,11,12	6.71	7 (63%)	14,15,17	1.59	2 (14%)
18	AHR	tE	4	18	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
18	AHR	tE	5	18	9,9,10	0.59	0	10,12,14	0.98	0
10	FUB	u	1	10	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
10	FUB	u	2	10	9,9,10	0.58	0	10,12,14	0.88	0
10	FUB	u	3	10	9,9,10	0.56	0	10,12,14	0.93	0
10	AHR	u	4	10	9,9,10	0.59	0	10,12,14	0.98	0
10	AHR	u	5	10	9,9,10	0.56	0	10,12,14	1.18	1 (10%)
3	FUB	uA	1	3	9,9,10	0.55	0	10,12,14	0.81	0
3	FUB	uA	2	3	9,9,10	0.58	0	10,12,14	0.82	0
3	FUB	uA	3	3	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
3	FUB	uB	1	3	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
3	FUB	uB	2	3	9,9,10	0.58	0	10,12,14	0.86	0
3	FUB	uB	3	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	uC	1	3	9,9,10	0.55	0	10,12,14	0.92	0
3	FUB	uC	2	3	9,9,10	0.57	0	10,12,14	0.97	0
3	FUB	uC	3	3	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
6	FUB	uD	1	6	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
6	FUB	uD	2	6	9,9,10	0.60	0	10,12,14	1.03	0
6	GZL	uD	3	6	11,11,12	7.02	6 (54%)	14,15,17	3.92	4 (28%)
20	FUB	uE	1	20	9,9,10	0.54	0	10,12,14	0.95	1 (10%)
20	FUB	uE	2	20	9,9,10	0.52	0	10,12,14	0.93	0
20	GZL	uE	3	20	11,11,12	6.71	7 (63%)	14,15,17	1.52	2 (14%)
20	AHR	uE	4	20	9,9,10	0.59	0	10,12,14	0.84	0
4	FUB	v	1	4	9,9,10	0.57	0	10,12,14	1.08	1 (10%)
4	FUB	v	2	4	9,9,10	0.56	0	10,12,14	0.88	0
4	FUB	v	3	4	9,9,10	0.56	0	10,12,14	0.90	0
4	AHR	v	4	4	9,9,10	0.58	0	10,12,14	1.01	0
3	FUB	vA	1	3	9,9,10	0.58	0	10,12,14	0.80	0
3	FUB	vA	2	3	9,9,10	0.57	0	10,12,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUB	vA	3	3	9,9,10	0.57	0	10,12,14	1.09	1 (10%)
3	FUB	vB	1	3	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
3	FUB	vB	2	3	9,9,10	0.58	0	10,12,14	0.85	0
3	FUB	vB	3	3	9,9,10	0.59	0	10,12,14	0.90	0
10	FUB	vC	1	10	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
10	FUB	vC	2	10	9,9,10	0.56	0	10,12,14	0.80	0
10	FUB	vC	3	10	9,9,10	0.58	0	10,12,14	0.99	1 (10%)
10	AHR	vC	4	10	9,9,10	0.61	0	10,12,14	0.87	0
10	AHR	vC	5	10	9,9,10	0.57	0	10,12,14	0.93	1 (10%)
13	FUB	vD	1	13	9,9,10	0.55	0	10,12,14	0.95	0
13	FUB	vD	2	13	9,9,10	0.58	0	10,12,14	0.94	0
13	GZL	vD	3	13	11,11,12	6.70	7 (63%)	14,15,17	1.54	2 (14%)
13	AHR	vD	4	13	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
21	FUB	vE	1	21	9,9,10	0.53	0	10,12,14	1.01	1 (10%)
21	FUB	vE	2	21	9,9,10	0.56	0	10,12,14	0.82	0
21	GZL	vE	3	21	11,11,12	6.74	7 (63%)	14,15,17	1.37	1 (7%)
21	AHR	vE	4	21	9,9,10	0.58	0	10,12,14	1.00	0
21	AHR	vE	5	21	9,9,10	0.57	0	10,12,14	0.68	0
3	FUB	w	1	3	9,9,10	0.58	0	10,12,14	0.84	0
3	FUB	w	2	3	9,9,10	0.58	0	10,12,14	0.93	0
3	FUB	w	3	3	9,9,10	0.55	0	10,12,14	1.03	1 (10%)
3	FUB	wA	1	3	9,9,10	0.57	0	10,12,14	0.72	0
3	FUB	wA	2	3	9,9,10	0.57	0	10,12,14	0.81	0
3	FUB	wA	3	3	9,9,10	0.55	0	10,12,14	0.87	1 (10%)
3	FUB	wB	1	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	wB	2	3	9,9,10	0.56	0	10,12,14	0.84	0
3	FUB	wB	3	3	9,9,10	0.59	0	10,12,14	0.85	0
13	FUB	wC	1	13	9,9,10	0.56	0	10,12,14	0.97	0
13	FUB	wC	2	13	9,9,10	0.54	0	10,12,14	1.09	1 (10%)
13	GZL	wC	3	13	11,11,12	6.84	7 (63%)	14,15,17	1.25	2 (14%)
13	AHR	wC	4	13	9,9,10	0.60	0	10,12,14	1.19	1 (10%)
13	FUB	wD	1	13	9,9,10	0.56	0	10,12,14	0.99	1 (10%)
13	FUB	wD	2	13	9,9,10	0.57	0	10,12,14	0.81	0
13	GZL	wD	3	13	11,11,12	6.72	7 (63%)	14,15,17	1.55	3 (21%)
13	AHR	wD	4	13	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
22	FUB	wE	1	22	9,9,10	0.59	0	10,12,14	1.05	0
22	FUB	wE	2	22	9,9,10	0.58	0	10,12,14	0.92	0
22	GZL	wE	3	22	11,11,12	6.75	7 (63%)	14,15,17	1.40	1 (7%)
22	AHR	wE	4	22	9,9,10	0.56	0	10,12,14	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	AHR	wE	5	22	9,9,10	0.59	0	10,12,14	1.53	3 (30%)
22	AHR	wE	6	22	9,9,10	0.55	0	10,12,14	0.75	0
3	FUB	x	1	3	9,9,10	0.57	0	10,12,14	0.76	0
3	FUB	x	2	3	9,9,10	0.59	0	10,12,14	0.98	1 (10%)
3	FUB	x	3	3	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
3	FUB	xA	1	3	9,9,10	0.60	0	10,12,14	0.87	0
3	FUB	xA	2	3	9,9,10	0.58	0	10,12,14	0.89	0
3	FUB	xA	3	3	9,9,10	0.57	0	10,12,14	0.97	0
3	FUB	xB	1	3	9,9,10	0.55	0	10,12,14	1.07	1 (10%)
3	FUB	xB	2	3	9,9,10	0.55	0	10,12,14	0.79	0
3	FUB	xB	3	3	9,9,10	0.57	0	10,12,14	1.01	0
6	FUB	xC	1	6	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
6	FUB	xC	2	6	9,9,10	0.59	0	10,12,14	1.05	1 (10%)
6	GZL	xC	3	6	11,11,12	7.01	6 (54%)	14,15,17	3.90	4 (28%)
6	FUB	xD	1	6	9,9,10	0.57	0	10,12,14	0.81	0
6	FUB	xD	2	6	9,9,10	0.58	0	10,12,14	1.21	2 (20%)
6	GZL	xD	3	6	11,11,12	6.65	7 (63%)	14,15,17	1.71	2 (14%)
20	FUB	xE	1	20	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
20	FUB	xE	2	20	9,9,10	0.56	0	10,12,14	0.71	0
20	GZL	xE	3	20	11,11,12	6.69	7 (63%)	14,15,17	1.59	2 (14%)
20	AHR	xE	4	20	9,9,10	0.56	0	10,12,14	0.98	0
3	FUB	y	1	3	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	y	2	3	9,9,10	0.58	0	10,12,14	0.91	0
3	FUB	y	3	3	9,9,10	0.54	0	10,12,14	0.86	0
3	FUB	yA	1	3	9,9,10	0.58	0	10,12,14	1.10	1 (10%)
3	FUB	yA	2	3	9,9,10	0.55	0	10,12,14	0.78	0
3	FUB	yA	3	3	9,9,10	0.58	0	10,12,14	0.86	0
10	FUB	yB	1	10	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
10	FUB	yB	2	10	9,9,10	0.58	0	10,12,14	0.73	0
10	FUB	yB	3	10	9,9,10	0.59	0	10,12,14	1.09	0
10	AHR	yB	4	10	9,9,10	0.58	0	10,12,14	0.92	0
10	AHR	yB	5	10	9,9,10	0.57	0	10,12,14	0.79	0
13	FUB	yC	1	13	9,9,10	0.56	0	10,12,14	0.93	0
13	FUB	yC	2	13	9,9,10	0.56	0	10,12,14	1.00	1 (10%)
13	GZL	yC	3	13	11,11,12	6.70	7 (63%)	14,15,17	1.52	1 (7%)
13	AHR	yC	4	13	9,9,10	0.59	0	10,12,14	0.97	0
6	FUB	yD	1	6	9,9,10	0.54	0	10,12,14	0.91	1 (10%)
6	FUB	yD	2	6	9,9,10	0.56	0	10,12,14	1.08	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GZL	yD	3	6	11,11,12	6.74	7 (63%)	14,15,17	1.49	2 (14%)
18	FUB	yE	1	18	9,9,10	0.56	0	10,12,14	0.93	0
18	FUB	yE	2	18	9,9,10	0.52	0	10,12,14	0.91	0
18	GZL	yE	3	18	11,11,12	6.64	7 (63%)	14,15,17	1.79	3 (21%)
18	AHR	yE	4	18	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
18	AHR	yE	5	18	9,9,10	0.56	0	10,12,14	1.13	1 (10%)
3	FUB	z	1	3	9,9,10	0.55	0	10,12,14	0.97	1 (10%)
3	FUB	z	2	3	9,9,10	0.56	0	10,12,14	0.90	0
3	FUB	z	3	3	9,9,10	0.57	0	10,12,14	0.84	0
3	FUB	zA	1	3	9,9,10	0.52	0	10,12,14	0.87	0
3	FUB	zA	2	3	9,9,10	0.59	0	10,12,14	0.87	0
3	FUB	zA	3	3	9,9,10	0.56	0	10,12,14	0.87	0
13	FUB	zB	1	13	9,9,10	0.54	0	10,12,14	1.03	1 (10%)
13	FUB	zB	2	13	9,9,10	0.54	0	10,12,14	1.06	1 (10%)
13	GZL	zB	3	13	11,11,12	6.77	7 (63%)	14,15,17	1.21	1 (7%)
13	AHR	zB	4	13	9,9,10	0.59	0	10,12,14	1.10	1 (10%)
13	FUB	zC	1	13	9,9,10	0.56	0	10,12,14	0.93	1 (10%)
13	FUB	zC	2	13	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
13	GZL	zC	3	13	11,11,12	6.71	7 (63%)	14,15,17	1.53	3 (21%)
13	AHR	zC	4	13	9,9,10	0.57	0	10,12,14	0.99	0
6	FUB	zD	1	6	9,9,10	0.57	0	10,12,14	1.02	0
6	FUB	zD	2	6	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
6	GZL	zD	3	6	11,11,12	6.73	7 (63%)	14,15,17	1.51	2 (14%)
18	FUB	zE	1	18	9,9,10	0.60	0	10,12,14	1.04	0
18	FUB	zE	2	18	9,9,10	0.59	0	10,12,14	1.07	1 (10%)
18	GZL	zE	3	18	11,11,12	6.66	7 (63%)	14,15,17	1.75	3 (21%)
18	AHR	zE	4	18	9,9,10	0.58	0	10,12,14	0.80	0
18	AHR	zE	5	18	9,9,10	0.58	0	10,12,14	0.95	0

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
3	FUB	0	1	3	-	0/2/15/18	0/1/1/1
3	FUB	0	2	3	-	0/2/15/18	0/1/1/1
3	FUB	0	3	3	-	0/2/15/18	0/1/1/1
3	FUB	0A	1	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	0A	2	3	-	0/2/15/18	0/1/1/1
3	FUB	0A	3	3	-	0/2/15/18	0/1/1/1
6	FUB	0B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	0B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	0B	3	6	2/2/4/5	5/6/19/22	0/1/1/1
6	FUB	0C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	0C	2	6	-	0/2/15/18	0/1/1/1
6	GZL	0C	3	6	-	2/6/19/22	0/1/1/1
13	FUB	0D	1	13	-	0/2/15/18	0/1/1/1
13	FUB	0D	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	0D	3	13	-	6/6/19/22	0/1/1/1
13	AHR	0D	4	13	-	0/2/15/18	0/1/1/1
18	FUB	0E	1	18	-	0/2/15/18	0/1/1/1
18	FUB	0E	2	18	-	0/2/15/18	0/1/1/1
18	GZL	0E	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	0E	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	0E	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	1	1	3	-	0/2/15/18	0/1/1/1
3	FUB	1	2	3	-	0/2/15/18	0/1/1/1
3	FUB	1	3	3	-	0/2/15/18	0/1/1/1
10	FUB	1A	1	10	-	0/2/15/18	0/1/1/1
10	FUB	1A	2	10	-	0/2/15/18	0/1/1/1
10	FUB	1A	3	10	-	0/2/15/18	0/1/1/1
10	AHR	1A	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	1A	5	10	-	0/2/15/18	0/1/1/1
13	FUB	1B	1	13	-	0/2/15/18	0/1/1/1
13	FUB	1B	2	13	-	0/2/15/18	0/1/1/1
13	GZL	1B	3	13	1/1/4/5	3/6/19/22	0/1/1/1
13	AHR	1B	4	13	-	0/2/15/18	0/1/1/1
6	FUB	1C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	1C	2	6	-	0/2/15/18	0/1/1/1
6	GZL	1C	3	6	1/1/4/5	0/6/19/22	0/1/1/1
15	FUB	1D	1	15	-	0/2/15/18	0/1/1/1
15	FUB	1D	2	15	-	0/2/15/18	0/1/1/1
15	GZL	1D	3	15	1/1/4/5	4/6/19/22	0/1/1/1
15	AHR	1D	4	15	-	0/2/15/18	0/1/1/1
15	AHR	1D	5	15	1/1/3/4	0/2/15/18	0/1/1/1
19	FUB	1E	1	19	-	0/2/15/18	0/1/1/1
19	FUB	1E	2	19	-	0/2/15/18	0/1/1/1
19	GZL	1E	3	19	1/1/4/5	4/6/19/22	0/1/1/1
19	AHR	1E	4	19	1/1/3/4	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	2	1	3	-	0/2/15/18	0/1/1/1
3	FUB	2	2	3	-	0/2/15/18	0/1/1/1
3	FUB	2	3	3	-	0/2/15/18	0/1/1/1
13	FUB	2A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	2A	2	13	-	0/2/15/18	0/1/1/1
13	GZL	2A	3	13	3/3/4/5	2/6/19/22	0/1/1/1
13	AHR	2A	4	13	-	0/2/15/18	0/1/1/1
13	FUB	2B	1	13	-	0/2/15/18	0/1/1/1
13	FUB	2B	2	13	-	0/2/15/18	0/1/1/1
13	GZL	2B	3	13	1/1/4/5	0/6/19/22	0/1/1/1
13	AHR	2B	4	13	-	0/2/15/18	0/1/1/1
6	FUB	2C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	2C	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	2C	3	6	1/1/4/5	4/6/19/22	0/1/1/1
15	FUB	2D	1	15	-	0/2/15/18	0/1/1/1
15	FUB	2D	2	15	-	0/2/15/18	0/1/1/1
15	GZL	2D	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	2D	4	15	-	0/2/15/18	0/1/1/1
15	AHR	2D	5	15	-	0/2/15/18	0/1/1/1
10	FUB	3	1	10	-	0/2/15/18	0/1/1/1
10	FUB	3	2	10	-	0/2/15/18	0/1/1/1
10	FUB	3	3	10	-	0/2/15/18	0/1/1/1
10	AHR	3	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	3	5	10	-	0/2/15/18	0/1/1/1
6	FUB	3A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	3A	2	6	-	0/2/15/18	0/1/1/1
6	GZL	3A	3	6	2/2/4/5	4/6/19/22	0/1/1/1
6	FUB	3B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	3B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	3B	3	6	-	2/6/19/22	0/1/1/1
13	FUB	3C	1	13	-	0/2/15/18	0/1/1/1
13	FUB	3C	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	3C	3	13	-	4/6/19/22	0/1/1/1
13	AHR	3C	4	13	-	0/2/15/18	0/1/1/1
6	FUB	3D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	3D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	3D	3	6	1/1/4/5	0/6/19/22	0/1/1/1
13	FUB	4	1	13	-	0/2/15/18	0/1/1/1
13	FUB	4	2	13	-	0/2/15/18	0/1/1/1
13	GZL	4	3	13	2/2/4/5	5/6/19/22	0/1/1/1
13	AHR	4	4	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FUB	4A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	4A	2	13	-	0/2/15/18	0/1/1/1
13	GZL	4A	3	13	1/1/4/5	0/6/19/22	0/1/1/1
13	AHR	4A	4	13	-	0/2/15/18	0/1/1/1
6	FUB	4B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	4B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	4B	3	6	1/1/4/5	4/6/19/22	0/1/1/1
15	FUB	4C	1	15	-	0/2/15/18	0/1/1/1
15	FUB	4C	2	15	-	0/2/15/18	0/1/1/1
15	GZL	4C	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	4C	4	15	-	0/2/15/18	0/1/1/1
15	AHR	4C	5	15	1/1/3/4	0/2/15/18	0/1/1/1
16	NAG	4D	1	1,16	-	4/6/23/26	0/1/1/1
16	NAG	4D	2	16	-	0/6/23/26	0/1/1/1
6	FUB	5	1	6	-	0/2/15/18	0/1/1/1
6	FUB	5	2	6	-	0/2/15/18	0/1/1/1
6	GZL	5	3	6	3/3/4/5	2/6/19/22	0/1/1/1
13	FUB	5A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	5A	2	13	-	0/2/15/18	0/1/1/1
13	GZL	5A	3	13	1/1/4/5	2/6/19/22	0/1/1/1
13	AHR	5A	4	13	-	0/2/15/18	0/1/1/1
6	FUB	5B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	5B	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	5B	3	6	1/1/4/5	6/6/19/22	0/1/1/1
15	FUB	5C	1	15	-	0/2/15/18	0/1/1/1
15	FUB	5C	2	15	-	0/2/15/18	0/1/1/1
15	GZL	5C	3	15	1/1/4/5	0/6/19/22	0/1/1/1
15	AHR	5C	4	15	-	0/2/15/18	0/1/1/1
15	AHR	5C	5	15	-	0/2/15/18	0/1/1/1
17	NAG	5D	1	17,1	-	1/6/23/26	0/1/1/1
17	NAG	5D	2	17	-	2/6/23/26	0/1/1/1
17	BMA	5D	3	17	-	2/2/19/22	0/1/1/1
17	MAN	5D	4	17	1/1/4/5	2/2/19/22	0/1/1/1
17	MAN	5D	5	17	-	0/2/19/22	0/1/1/1
17	MAN	5D	6	17	1/1/4/5	2/2/19/22	0/1/1/1
13	FUB	6	1	13	-	0/2/15/18	0/1/1/1
13	FUB	6	2	13	-	0/2/15/18	0/1/1/1
13	GZL	6	3	13	1/1/4/5	3/6/19/22	0/1/1/1
13	AHR	6	4	13	-	0/2/15/18	0/1/1/1
6	FUB	6A	1	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUB	6A	2	6	-	0/2/15/18	0/1/1/1
6	GZL	6A	3	6	-	2/6/19/22	0/1/1/1
13	FUB	6B	1	13	-	0/2/15/18	0/1/1/1
13	FUB	6B	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	6B	3	13	-	4/6/19/22	0/1/1/1
13	AHR	6B	4	13	-	0/2/15/18	0/1/1/1
6	FUB	6C	1	6	-	0/2/15/18	0/1/1/1
6	FUB	6C	2	6	-	0/2/15/18	0/1/1/1
6	GZL	6C	3	6	1/1/4/5	2/6/19/22	0/1/1/1
6	FUB	6D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	6D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	6D	3	6	1/1/4/5	4/6/19/22	0/1/1/1
13	FUB	7	1	13	-	0/2/15/18	0/1/1/1
13	FUB	7	2	13	-	0/2/15/18	0/1/1/1
13	GZL	7	3	13	1/1/4/5	0/6/19/22	0/1/1/1
13	AHR	7	4	13	-	0/2/15/18	0/1/1/1
6	FUB	7A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	7A	2	6	-	0/2/15/18	0/1/1/1
6	GZL	7A	3	6	1/1/4/5	2/6/19/22	0/1/1/1
15	FUB	7B	1	15	-	0/2/15/18	0/1/1/1
15	FUB	7B	2	15	-	0/2/15/18	0/1/1/1
15	GZL	7B	3	15	1/1/4/5	6/6/19/22	0/1/1/1
15	AHR	7B	4	15	-	0/2/15/18	0/1/1/1
15	AHR	7B	5	15	1/1/3/4	0/2/15/18	0/1/1/1
17	NAG	7C	1	17,1	-	1/6/23/26	0/1/1/1
17	NAG	7C	2	17	-	0/6/23/26	0/1/1/1
17	BMA	7C	3	17	-	2/2/19/22	0/1/1/1
17	MAN	7C	4	17	1/1/4/5	2/2/19/22	0/1/1/1
17	MAN	7C	5	17	-	2/2/19/22	0/1/1/1
17	MAN	7C	6	17	1/1/4/5	1/2/19/22	0/1/1/1
6	FUB	7D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	7D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	7D	3	6	1/1/4/5	6/6/19/22	0/1/1/1
6	FUB	8	1	6	-	0/2/15/18	0/1/1/1
6	FUB	8	2	6	-	0/2/15/18	0/1/1/1
6	GZL	8	3	6	1/1/4/5	0/6/19/22	0/1/1/1
6	FUB	8A	1	6	-	0/2/15/18	0/1/1/1
6	FUB	8A	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	8A	3	6	1/1/4/5	4/6/19/22	0/1/1/1
15	FUB	8B	1	15	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FUB	8B	2	15	-	0/2/15/18	0/1/1/1
15	GZL	8B	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	8B	4	15	-	0/2/15/18	0/1/1/1
15	AHR	8B	5	15	-	0/2/15/18	0/1/1/1
3	FUB	8C	1	3	-	0/2/15/18	0/1/1/1
3	FUB	8C	2	3	-	0/2/15/18	0/1/1/1
3	FUB	8C	3	3	-	0/2/15/18	0/1/1/1
6	FUB	8D	1	6	-	0/2/15/18	0/1/1/1
6	FUB	8D	2	6	-	0/2/15/18	0/1/1/1
6	GZL	8D	3	6	1/1/4/5	2/6/19/22	0/1/1/1
6	FUB	9	1	6	-	0/2/15/18	0/1/1/1
6	FUB	9	2	6	-	0/2/15/18	0/1/1/1
6	GZL	9	3	6	1/1/4/5	1/6/19/22	0/1/1/1
13	FUB	9A	1	13	-	0/2/15/18	0/1/1/1
13	FUB	9A	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	9A	3	13	-	4/6/19/22	0/1/1/1
13	AHR	9A	4	13	-	0/2/15/18	0/1/1/1
6	FUB	9B	1	6	-	0/2/15/18	0/1/1/1
6	FUB	9B	2	6	-	0/2/15/18	0/1/1/1
6	GZL	9B	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	9C	1	3	-	0/2/15/18	0/1/1/1
3	FUB	9C	2	3	-	0/2/15/18	0/1/1/1
3	FUB	9C	3	3	-	0/2/15/18	0/1/1/1
18	FUB	9D	1	18	-	0/2/15/18	0/1/1/1
18	FUB	9D	2	18	-	0/2/15/18	0/1/1/1
18	GZL	9D	3	18	1/1/4/5	3/6/19/22	0/1/1/1
18	AHR	9D	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	9D	5	18	-	0/2/15/18	0/1/1/1
6	FUB	AA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	AA	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	AA	3	6	1/1/4/5	6/6/19/22	0/1/1/1
15	FUB	AB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	AB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	AB	3	15	1/1/4/5	4/6/19/22	0/1/1/1
15	AHR	AB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	AB	5	15	1/1/3/4	0/2/15/18	0/1/1/1
16	NAG	AC	1	1,16	-	3/6/23/26	0/1/1/1
16	NAG	AC	2	16	-	2/6/23/26	0/1/1/1
4	FUB	AD	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	AD	2	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	AD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	AD	4	4	-	0/2/15/18	0/1/1/1
19	FUB	AE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	AE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	AE	3	19	1/1/4/5	6/6/19/22	0/1/1/1
19	AHR	AE	4	19	-	0/2/15/18	0/1/1/1
13	FUB	BA	1	13	-	0/2/15/18	0/1/1/1
13	FUB	BA	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	BA	3	13	-	4/6/19/22	0/1/1/1
13	AHR	BA	4	13	-	0/2/15/18	0/1/1/1
15	FUB	BB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	BB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	BB	3	15	1/1/4/5	1/6/19/22	0/1/1/1
15	AHR	BB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	BB	5	15	-	0/2/15/18	0/1/1/1
3	FUB	BC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	BC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	BC	3	3	-	0/2/15/18	0/1/1/1
5	FUB	BD	1	5	-	0/2/15/18	0/1/1/1
5	FUB	BD	2	5	-	0/2/15/18	0/1/1/1
5	FUB	BD	3	5	-	0/2/15/18	0/1/1/1
5	AHR	BD	4	5	-	0/2/15/18	0/1/1/1
5	AHR	BD	5	5	1/1/3/4	0/2/15/18	0/1/1/1
18	FUB	BE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	BE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	BE	3	18	1/1/4/5	4/6/19/22	0/1/1/1
18	AHR	BE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	BE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
15	FUB	CA	1	15	-	0/2/15/18	0/1/1/1
15	FUB	CA	2	15	-	0/2/15/18	0/1/1/1
15	GZL	CA	3	15	1/1/4/5	4/6/19/22	0/1/1/1
15	AHR	CA	4	15	-	0/2/15/18	0/1/1/1
15	AHR	CA	5	15	1/1/3/4	0/2/15/18	0/1/1/1
6	FUB	CB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	CB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	CB	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	CC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	CC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	CC	3	3	-	0/2/15/18	0/1/1/1
6	FUB	CD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	CD	2	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GZL	CD	3	6	3/3/4/5	1/6/19/22	0/1/1/1
20	FUB	CE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	CE	2	20	-	1/2/15/18	0/1/1/1
20	GZL	CE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	CE	4	20	-	0/2/15/18	0/1/1/1
15	FUB	DA	1	15	-	0/2/15/18	0/1/1/1
15	FUB	DA	2	15	-	0/2/15/18	0/1/1/1
15	GZL	DA	3	15	1/1/4/5	2/6/19/22	0/1/1/1
15	AHR	DA	4	15	-	0/2/15/18	0/1/1/1
15	AHR	DA	5	15	-	0/2/15/18	0/1/1/1
17	NAG	DB	1	17,1	-	2/6/23/26	0/1/1/1
17	NAG	DB	2	17	-	2/6/23/26	0/1/1/1
17	BMA	DB	3	17	-	2/2/19/22	0/1/1/1
17	MAN	DB	4	17	1/1/4/5	2/2/19/22	0/1/1/1
17	MAN	DB	5	17	-	2/2/19/22	0/1/1/1
17	MAN	DB	6	17	1/1/4/5	1/2/19/22	0/1/1/1
4	FUB	DC	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	DC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	DC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	DC	4	4	-	0/2/15/18	0/1/1/1
3	FUB	DD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	DD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	DD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	DE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	DE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	DE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	DE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	DE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
6	FUB	EA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	EA	2	6	-	0/2/15/18	0/1/1/1
6	GZL	EA	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	EB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	EB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	EB	3	3	-	0/2/15/18	0/1/1/1
5	FUB	EC	1	5	-	0/2/15/18	0/1/1/1
5	FUB	EC	2	5	-	0/2/15/18	0/1/1/1
5	FUB	EC	3	5	-	0/2/15/18	0/1/1/1
5	AHR	EC	4	5	-	0/2/15/18	0/1/1/1
5	AHR	EC	5	5	-	0/2/15/18	0/1/1/1
3	FUB	ED	1	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	ED	2	3	-	0/2/15/18	0/1/1/1
3	FUB	ED	3	3	-	0/2/15/18	0/1/1/1
20	FUB	EE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	EE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	EE	3	20	1/1/4/5	0/6/19/22	0/1/1/1
20	AHR	EE	4	20	-	0/2/15/18	0/1/1/1
16	NAG	FA	1	1,16	-	4/6/23/26	0/1/1/1
16	NAG	FA	2	16	-	2/6/23/26	0/1/1/1
12	FUB	FB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	FB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	FB	3	12	2/2/4/5	3/6/19/22	0/1/1/1
12	AHR	FB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	FB	5	12	-	0/2/15/18	0/1/1/1
6	FUB	FC	1	6	-	0/2/15/18	0/1/1/1
6	FUB	FC	2	6	-	0/2/15/18	0/1/1/1
6	GZL	FC	3	6	1/1/4/5	4/6/19/22	0/1/1/1
3	FUB	FD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	FD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	FD	3	3	-	0/2/15/18	0/1/1/1
21	FUB	FE	1	21	-	0/2/15/18	0/1/1/1
21	FUB	FE	2	21	-	0/2/15/18	0/1/1/1
21	GZL	FE	3	21	1/1/4/5	2/6/19/22	0/1/1/1
21	AHR	FE	4	21	1/1/3/4	0/2/15/18	0/1/1/1
21	AHR	FE	5	21	1/1/3/4	0/2/15/18	0/1/1/1
17	NAG	GA	1	17,1	-	1/6/23/26	0/1/1/1
17	NAG	GA	2	17	-	2/6/23/26	0/1/1/1
17	BMA	GA	3	17	-	2/2/19/22	0/1/1/1
17	MAN	GA	4	17	1/1/4/5	1/2/19/22	0/1/1/1
17	MAN	GA	5	17	-	1/2/19/22	0/1/1/1
17	MAN	GA	6	17	1/1/4/5	1/2/19/22	0/1/1/1
13	FUB	GB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	GB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	GB	3	13	2/2/4/5	3/6/19/22	0/1/1/1
13	AHR	GB	4	13	-	0/2/15/18	0/1/1/1
3	FUB	GC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	GC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	GC	3	3	-	0/2/15/18	0/1/1/1
6	FUB	GD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	GD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	GD	3	6	1/1/4/5	4/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	FUB	GE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	GE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	GE	3	22	1/1/4/5	6/6/19/22	0/1/1/1
22	AHR	GE	4	22	-	0/2/15/18	0/1/1/1
22	AHR	GE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	GE	6	22	-	0/2/15/18	0/1/1/1
3	FUB	HA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	HA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	HA	3	3	-	0/2/15/18	0/1/1/1
14	FUB	HB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	HB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	HB	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	HB	4	14	-	0/2/15/18	0/1/1/1
3	FUB	HC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	HC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	HC	3	3	-	0/2/15/18	0/1/1/1
7	FUB	HD	1	7	-	0/2/15/18	0/1/1/1
7	FUB	HD	2	7	-	0/2/15/18	0/1/1/1
7	FUB	HD	3	7	-	0/2/15/18	0/1/1/1
7	AHR	HD	4	7	-	0/2/15/18	0/1/1/1
20	FUB	HE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	HE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	HE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	HE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	IA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	IA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	IA	3	3	-	0/2/15/18	0/1/1/1
12	FUB	IB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	IB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	IB	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	IB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	IB	5	12	-	0/2/15/18	0/1/1/1
3	FUB	IC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	IC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	IC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	ID	1	3	-	0/2/15/18	0/1/1/1
3	FUB	ID	2	3	-	0/2/15/18	0/1/1/1
3	FUB	ID	3	3	-	0/2/15/18	0/1/1/1
18	FUB	IE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	IE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	IE	3	18	1/1/4/5	6/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	AHR	IE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	IE	5	18	-	0/2/15/18	0/1/1/1
3	FUB	J	1	3	-	0/2/15/18	0/1/1/1
3	FUB	J	2	3	-	0/2/15/18	0/1/1/1
3	FUB	J	3	3	-	0/2/15/18	0/1/1/1
4	FUB	JA	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	JA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	JA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	JA	4	4	-	0/2/15/18	0/1/1/1
4	FUB	JB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	JB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	JB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	JB	4	4	-	0/2/15/18	0/1/1/1
6	FUB	JC	1	6	-	0/2/15/18	0/1/1/1
6	FUB	JC	2	6	-	0/2/15/18	0/1/1/1
6	GZL	JC	3	6	1/1/4/5	0/6/19/22	0/1/1/1
8	FUB	JD	1	8	-	0/2/15/18	0/1/1/1
8	FUB	JD	2	8	-	0/2/15/18	0/1/1/1
8	FUB	JD	3	8	-	0/2/15/18	0/1/1/1
8	AHR	JD	4	8	-	0/2/15/18	0/1/1/1
8	AHR	JD	5	8	-	0/2/15/18	0/1/1/1
18	FUB	JE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	JE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	JE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	JE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	JE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	K	1	3	-	0/2/15/18	0/1/1/1
3	FUB	K	2	3	-	0/2/15/18	0/1/1/1
3	FUB	K	3	3	-	0/2/15/18	0/1/1/1
5	FUB	KA	1	5	-	0/2/15/18	0/1/1/1
5	FUB	KA	2	5	-	0/2/15/18	0/1/1/1
5	FUB	KA	3	5	-	0/2/15/18	0/1/1/1
5	AHR	KA	4	5	-	0/2/15/18	0/1/1/1
5	AHR	KA	5	5	-	0/2/15/18	0/1/1/1
14	FUB	KB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	KB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	KB	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	KB	4	14	-	0/2/15/18	0/1/1/1
7	FUB	KC	1	7	-	0/2/15/18	0/1/1/1
7	FUB	KC	2	7	-	0/2/15/18	0/1/1/1
7	FUB	KC	3	7	-	0/2/15/18	0/1/1/1
7	AHR	KC	4	7	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	KD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	KD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	KD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	KE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	KE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	KE	3	18	1/1/4/5	4/6/19/22	0/1/1/1
18	AHR	KE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	KE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	L	1	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	L	2	4	-	0/2/15/18	0/1/1/1
4	FUB	L	3	4	-	0/2/15/18	0/1/1/1
4	AHR	L	4	4	-	0/2/15/18	0/1/1/1
6	FUB	LA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	LA	2	6	-	0/2/15/18	0/1/1/1
6	GZL	LA	3	6	2/2/4/5	2/6/19/22	0/1/1/1
3	FUB	LB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	LB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	LB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	LC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	LC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	LC	3	3	-	0/2/15/18	0/1/1/1
4	FUB	LD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	LD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	LD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	LD	4	4	-	0/2/15/18	0/1/1/1
19	FUB	LE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	LE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	LE	3	19	1/1/4/5	2/6/19/22	0/1/1/1
19	AHR	LE	4	19	1/1/3/4	0/2/15/18	0/1/1/1
5	FUB	M	1	5	-	0/2/15/18	0/1/1/1
5	FUB	M	2	5	-	0/2/15/18	0/1/1/1
5	FUB	M	3	5	-	0/2/15/18	0/1/1/1
5	AHR	M	4	5	-	0/2/15/18	0/1/1/1
5	AHR	M	5	5	-	0/2/15/18	0/1/1/1
3	FUB	MA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	MA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	MA	3	3	-	0/2/15/18	0/1/1/1
10	FUB	MB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	MB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	MB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	MB	4	10	-	0/2/15/18	0/1/1/1
10	AHR	MB	5	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FUB	MC	1	8	-	0/2/15/18	0/1/1/1
8	FUB	MC	2	8	-	0/2/15/18	0/1/1/1
8	FUB	MC	3	8	-	0/2/15/18	0/1/1/1
8	AHR	MC	4	8	-	0/2/15/18	0/1/1/1
8	AHR	MC	5	8	-	0/2/15/18	0/1/1/1
4	FUB	MD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	MD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	MD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	MD	4	4	-	0/2/15/18	0/1/1/1
6	FUB	ME	1	6	-	0/2/15/18	0/1/1/1
6	FUB	ME	2	6	-	0/2/15/18	0/1/1/1
6	GZL	ME	3	6	1/1/4/5	4/6/19/22	0/1/1/1
6	FUB	N	1	6	-	0/2/15/18	0/1/1/1
6	FUB	N	2	6	-	0/2/15/18	0/1/1/1
6	GZL	N	3	6	2/2/4/5	2/6/19/22	0/1/1/1
3	FUB	NA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	NA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	NA	3	3	-	0/2/15/18	0/1/1/1
4	FUB	NB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	NB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	NB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	NB	4	4	-	0/2/15/18	0/1/1/1
3	FUB	NC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	NC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	NC	3	3	-	0/2/15/18	0/1/1/1
9	FUB	ND	1	9	-	0/2/15/18	0/1/1/1
9	FUB	ND	2	9	-	0/2/15/18	0/1/1/1
19	FUB	NE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	NE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	NE	3	19	1/1/4/5	2/6/19/22	0/1/1/1
19	AHR	NE	4	19	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	O	1	3	-	0/2/15/18	0/1/1/1
3	FUB	O	2	3	-	0/2/15/18	0/1/1/1
3	FUB	O	3	3	-	0/2/15/18	0/1/1/1
3	FUB	OA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	OA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	OA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	OB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	OB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	OB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	OC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	OC	2	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	OC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	OC	4	4	-	0/2/15/18	0/1/1/1
4	FUB	OD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	OD	2	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	OD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	OD	4	4	-	0/2/15/18	0/1/1/1
6	FUB	OE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	OE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	OE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
3	FUB	P	1	3	-	0/2/15/18	0/1/1/1
3	FUB	P	2	3	-	0/2/15/18	0/1/1/1
3	FUB	P	3	3	-	0/2/15/18	0/1/1/1
6	FUB	PA	1	6	-	0/2/15/18	0/1/1/1
6	FUB	PA	2	6	-	0/2/15/18	0/1/1/1
6	GZL	PA	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	PB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	PB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	PB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	PC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	PC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	PC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	PC	4	4	1/1/3/4	0/2/15/18	0/1/1/1
10	FUB	PD	1	10	-	0/2/15/18	0/1/1/1
10	FUB	PD	2	10	-	0/2/15/18	0/1/1/1
10	FUB	PD	3	10	-	0/2/15/18	0/1/1/1
10	AHR	PD	4	10	-	0/2/15/18	0/1/1/1
10	AHR	PD	5	10	-	0/2/15/18	0/1/1/1
18	FUB	PE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	PE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	PE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	PE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	PE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	Q	1	3	-	0/2/15/18	0/1/1/1
3	FUB	Q	2	3	-	0/2/15/18	0/1/1/1
3	FUB	Q	3	3	-	0/2/15/18	0/1/1/1
7	FUB	QA	1	7	-	0/2/15/18	0/1/1/1
7	FUB	QA	2	7	-	0/2/15/18	0/1/1/1
7	FUB	QA	3	7	-	0/2/15/18	0/1/1/1
7	AHR	QA	4	7	-	0/2/15/18	0/1/1/1
3	FUB	QB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	QB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	QB	3	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FUB	QC	1	9	-	0/2/15/18	0/1/1/1
9	FUB	QC	2	9	-	0/2/15/18	0/1/1/1
3	FUB	QD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	QD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	QD	3	3	-	0/2/15/18	0/1/1/1
22	FUB	QE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	QE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	QE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	QE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	QE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	QE	6	22	1/1/3/4	0/2/15/18	0/1/1/1
6	FUB	R	1	6	-	0/2/15/18	0/1/1/1
6	FUB	R	2	6	-	0/2/15/18	0/1/1/1
6	GZL	R	3	6	1/1/4/5	2/6/19/22	0/1/1/1
3	FUB	RA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	RA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	RA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	RB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	RB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	RB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	RC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	RC	2	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	RC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	RC	4	4	-	0/2/15/18	0/1/1/1
4	FUB	RD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	RD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	RD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	RD	4	4	-	0/2/15/18	0/1/1/1
22	FUB	RE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	RE	2	22	-	1/2/15/18	0/1/1/1
22	GZL	RE	3	22	1/1/4/5	3/6/19/22	0/1/1/1
22	AHR	RE	4	22	2/2/3/4	0/2/15/18	0/1/1/1
22	AHR	RE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	RE	6	22	-	0/2/15/18	0/1/1/1
7	FUB	S	1	7	-	0/2/15/18	0/1/1/1
7	FUB	S	2	7	-	0/2/15/18	0/1/1/1
7	FUB	S	3	7	-	0/2/15/18	0/1/1/1
7	AHR	S	4	7	-	0/2/15/18	0/1/1/1
8	FUB	SA	1	8	-	0/2/15/18	0/1/1/1
8	FUB	SA	2	8	-	0/2/15/18	0/1/1/1
8	FUB	SA	3	8	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	AHR	SA	4	8	-	0/2/15/18	0/1/1/1
8	AHR	SA	5	8	-	0/2/15/18	0/1/1/1
3	FUB	SB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	SB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	SB	3	3	-	0/2/15/18	0/1/1/1
10	FUB	SC	1	10	-	0/2/15/18	0/1/1/1
10	FUB	SC	2	10	-	0/2/15/18	0/1/1/1
10	FUB	SC	3	10	-	0/2/15/18	0/1/1/1
10	AHR	SC	4	10	-	0/2/15/18	0/1/1/1
10	AHR	SC	5	10	-	0/2/15/18	0/1/1/1
4	FUB	SD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	SD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	SD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	SD	4	4	-	0/2/15/18	0/1/1/1
18	FUB	SE	1	18	1/1/3/4	0/2/15/18	0/1/1/1
18	FUB	SE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	SE	3	18	1/1/4/5	3/6/19/22	0/1/1/1
18	AHR	SE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	SE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	T	1	3	-	0/2/15/18	0/1/1/1
3	FUB	T	2	3	-	0/2/15/18	0/1/1/1
3	FUB	T	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	TD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	TD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	TD	3	3	-	0/2/15/18	0/1/1/1
20	FUB	TE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	TE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	TE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	TE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
8	FUB	U	1	8	-	0/2/15/18	0/1/1/1
8	FUB	U	2	8	-	0/2/15/18	0/1/1/1
8	FUB	U	3	8	-	0/2/15/18	0/1/1/1
8	AHR	U	4	8	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	AHR	U	5	8	-	0/2/15/18	0/1/1/1
4	FUB	UA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	UA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	UA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	UA	4	4	-	0/2/15/18	0/1/1/1
3	FUB	UB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	UB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	UB	3	3	-	0/2/15/18	0/1/1/1
4	FUB	UC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	UC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	UC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	UC	4	4	-	0/2/15/18	0/1/1/1
7	FUB	UD	1	7	-	0/2/15/18	0/1/1/1
7	FUB	UD	2	7	-	0/2/15/18	0/1/1/1
7	FUB	UD	3	7	-	0/2/15/18	0/1/1/1
7	AHR	UD	4	7	-	0/2/15/18	0/1/1/1
20	FUB	UE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	UE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	UE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	UE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	V	1	3	-	0/2/15/18	0/1/1/1
3	FUB	V	2	3	-	0/2/15/18	0/1/1/1
3	FUB	V	3	3	-	0/2/15/18	0/1/1/1
4	FUB	VA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	VA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	VA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	VA	4	4	2/2/3/4	0/2/15/18	0/1/1/1
10	FUB	VB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	VB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	VB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	VB	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	VB	5	10	-	0/2/15/18	0/1/1/1
4	FUB	VC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	VC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	VC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	VC	4	4	-	0/2/15/18	0/1/1/1
4	FUB	VD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	VD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	VD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	VD	4	4	-	0/2/15/18	0/1/1/1
22	FUB	VE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	VE	2	22	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	GZL	VE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	VE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	VE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	VE	6	22	-	0/2/15/18	0/1/1/1
4	FUB	W	1	4	-	0/2/15/18	0/1/1/1
4	FUB	W	2	4	-	0/2/15/18	0/1/1/1
4	FUB	W	3	4	-	0/2/15/18	0/1/1/1
4	AHR	W	4	4	-	0/2/15/18	0/1/1/1
9	FUB	WA	1	9	-	0/2/15/18	0/1/1/1
9	FUB	WA	2	9	-	0/2/15/18	0/1/1/1
13	FUB	WB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	WB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	WB	3	13	3/3/4/5	1/6/19/22	0/1/1/1
13	AHR	WB	4	13	-	0/2/15/18	0/1/1/1
3	FUB	WC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	WC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	WC	3	3	-	0/2/15/18	0/1/1/1
7	FUB	WD	1	7	-	0/2/15/18	0/1/1/1
7	FUB	WD	2	7	-	0/2/15/18	0/1/1/1
7	FUB	WD	3	7	-	0/2/15/18	0/1/1/1
7	AHR	WD	4	7	-	0/2/15/18	0/1/1/1
20	FUB	WE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	WE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	WE	3	20	1/1/4/5	2/6/19/22	0/1/1/1
20	AHR	WE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	X	1	4	-	0/2/15/18	0/1/1/1
4	FUB	X	2	4	-	0/2/15/18	0/1/1/1
4	FUB	X	3	4	-	0/2/15/18	0/1/1/1
4	AHR	X	4	4	-	0/2/15/18	0/1/1/1
3	FUB	XA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	XA	2	3	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	XA	3	3	-	0/2/15/18	0/1/1/1
6	FUB	XB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	XB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	XB	3	6	2/2/4/5	5/6/19/22	0/1/1/1
7	FUB	XC	1	7	-	0/2/15/18	0/1/1/1
7	FUB	XC	2	7	-	0/2/15/18	0/1/1/1
7	FUB	XC	3	7	-	0/2/15/18	0/1/1/1
7	AHR	XC	4	7	-	0/2/15/18	0/1/1/1
11	FUB	XD	1	11	-	0/2/15/18	0/1/1/1
11	AHR	XD	2	11	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	AHR	XD	3	11	-	0/2/15/18	0/1/1/1
23	FUB	XE	1	23	-	0/2/15/18	0/1/1/1
23	FUB	XE	2	23	-	1/2/15/18	0/1/1/1
23	GZL	XE	3	23	1/1/4/5	2/6/19/22	0/1/1/1
23	AHR	XE	4	23	1/1/3/4	0/2/15/18	0/1/1/1
23	AHR	XE	5	23	1/1/3/4	0/2/15/18	0/1/1/1
23	AHR	XE	6	23	-	0/2/15/18	0/1/1/1
9	FUB	Y	1	9	-	0/2/15/18	0/1/1/1
9	FUB	Y	2	9	-	0/2/15/18	0/1/1/1
10	FUB	YA	1	10	-	0/2/15/18	0/1/1/1
10	FUB	YA	2	10	-	0/2/15/18	0/1/1/1
10	FUB	YA	3	10	-	0/2/15/18	0/1/1/1
10	AHR	YA	4	10	-	0/2/15/18	0/1/1/1
10	AHR	YA	5	10	-	0/2/15/18	0/1/1/1
13	FUB	YB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	YB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	YB	3	13	1/1/4/5	4/6/19/22	0/1/1/1
13	AHR	YB	4	13	-	0/2/15/18	0/1/1/1
4	FUB	YC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	YC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	YC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	YC	4	4	-	0/2/15/18	0/1/1/1
9	FUB	YD	1	9	-	0/2/15/18	0/1/1/1
9	FUB	YD	2	9	-	0/2/15/18	0/1/1/1
24	FUB	YE	1	24	-	0/2/15/18	0/1/1/1
24	FUB	YE	2	24	-	0/2/15/18	0/1/1/1
24	GZL	YE	3	24	1/1/4/5	4/6/19/22	0/1/1/1
24	AHR	YE	4	24	1/1/3/4	0/2/15/18	0/1/1/1
24	AHR	YE	5	24	-	0/2/15/18	0/1/1/1
24	AHR	YE	6	24	-	0/2/15/18	0/1/1/1
4	FUB	Z	1	4	-	0/2/15/18	0/1/1/1
4	FUB	Z	2	4	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	Z	3	4	-	0/2/15/18	0/1/1/1
4	AHR	Z	4	4	-	0/2/15/18	0/1/1/1
3	FUB	ZA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	ZA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	ZA	3	3	-	0/2/15/18	0/1/1/1
13	FUB	ZB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	ZB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	ZB	3	13	1/1/4/5	2/6/19/22	0/1/1/1
13	AHR	ZB	4	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUB	ZC	1	7	-	0/2/15/18	0/1/1/1
7	FUB	ZC	2	7	-	0/2/15/18	0/1/1/1
7	FUB	ZC	3	7	-	0/2/15/18	0/1/1/1
7	AHR	ZC	4	7	-	0/2/15/18	0/1/1/1
4	FUB	ZD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	ZD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	ZD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	ZD	4	4	-	0/2/15/18	0/1/1/1
6	FUB	ZE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	ZE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	ZE	3	6	1/1/4/5	2/6/19/22	0/1/1/1
10	FUB	a	1	10	-	0/2/15/18	0/1/1/1
10	FUB	a	2	10	-	0/2/15/18	0/1/1/1
10	FUB	a	3	10	-	0/2/15/18	0/1/1/1
10	AHR	a	4	10	-	0/2/15/18	0/1/1/1
10	AHR	a	5	10	-	0/2/15/18	0/1/1/1
4	FUB	aA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	aA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	aA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	aA	4	4	-	0/2/15/18	0/1/1/1
6	FUB	aB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	aB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	aB	3	6	-	2/6/19/22	0/1/1/1
11	FUB	aC	1	11	-	0/2/15/18	0/1/1/1
11	AHR	aC	2	11	-	0/2/15/18	0/1/1/1
11	AHR	aC	3	11	-	0/2/15/18	0/1/1/1
3	FUB	aD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	aD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	aD	3	3	-	0/2/15/18	0/1/1/1
19	FUB	aE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	aE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	aE	3	19	1/1/4/5	2/6/19/22	0/1/1/1
19	AHR	aE	4	19	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	b	1	3	-	0/2/15/18	0/1/1/1
3	FUB	b	2	3	-	0/2/15/18	0/1/1/1
3	FUB	b	3	3	-	0/2/15/18	0/1/1/1
4	FUB	bA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	bA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	bA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	bA	4	4	-	0/2/15/18	0/1/1/1
6	FUB	bB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	bB	2	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GZL	bB	3	6	1/1/4/5	4/6/19/22	0/1/1/1
9	FUB	bC	1	9	-	0/2/15/18	0/1/1/1
9	FUB	bC	2	9	-	0/2/15/18	0/1/1/1
3	FUB	bD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	bD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	bD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	bE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	bE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	bE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
4	FUB	c	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c	2	4	-	0/2/15/18	0/1/1/1
4	FUB	c	3	4	-	0/2/15/18	0/1/1/1
4	AHR	c	4	4	-	0/2/15/18	0/1/1/1
3	FUB	cA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	cA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	cA	3	3	-	0/2/15/18	0/1/1/1
6	FUB	cB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	cB	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	cB	3	6	1/1/4/5	4/6/19/22	0/1/1/1
4	FUB	cC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	cC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	cC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	cC	4	4	-	0/2/15/18	0/1/1/1
12	FUB	cD	1	12	-	0/2/15/18	0/1/1/1
12	FUB	cD	2	12	-	0/2/15/18	0/1/1/1
12	GZL	cD	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	cD	4	12	-	0/2/15/18	0/1/1/1
12	AHR	cD	5	12	-	0/2/15/18	0/1/1/1
18	FUB	cE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	cE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	cE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	cE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	cE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	d	1	4	-	0/2/15/18	0/1/1/1
4	FUB	d	2	4	-	0/2/15/18	0/1/1/1
4	FUB	d	3	4	-	0/2/15/18	0/1/1/1
4	AHR	d	4	4	-	0/2/15/18	0/1/1/1
7	FUB	dA	1	7	-	0/2/15/18	0/1/1/1
7	FUB	dA	2	7	-	0/2/15/18	0/1/1/1
7	FUB	dA	3	7	-	0/2/15/18	0/1/1/1
7	AHR	dA	4	7	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FUB	dB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	dB	2	13	1/1/3/4	0/2/15/18	0/1/1/1
13	GZL	dB	3	13	-	4/6/19/22	0/1/1/1
13	AHR	dB	4	13	-	0/2/15/18	0/1/1/1
3	FUB	dC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	dC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	dC	3	3	-	0/2/15/18	0/1/1/1
13	FUB	dD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	dD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	dD	3	13	2/2/4/5	3/6/19/22	0/1/1/1
13	AHR	dD	4	13	-	0/2/15/18	0/1/1/1
22	FUB	dE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	dE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	dE	3	22	1/1/4/5	4/6/19/22	0/1/1/1
22	AHR	dE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	dE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	dE	6	22	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	e	1	3	-	0/2/15/18	0/1/1/1
3	FUB	e	2	3	-	0/2/15/18	0/1/1/1
3	FUB	e	3	3	-	0/2/15/18	0/1/1/1
4	FUB	eA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	eA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	eA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	eA	4	4	-	0/2/15/18	0/1/1/1
15	FUB	eB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	eB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	eB	3	15	1/1/4/5	6/6/19/22	0/1/1/1
15	AHR	eB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	eB	5	15	1/1/3/4	0/2/15/18	0/1/1/1
3	FUB	eC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	eC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	eC	3	3	-	0/2/15/18	0/1/1/1
14	FUB	eD	1	14	-	0/2/15/18	0/1/1/1
14	FUB	eD	2	14	-	0/2/15/18	0/1/1/1
14	GZL	eD	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	eD	4	14	-	0/2/15/18	0/1/1/1
22	FUB	eE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	eE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	eE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	eE	4	22	2/2/3/4	0/2/15/18	0/1/1/1
22	AHR	eE	5	22	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	AHR	eE	6	22	-	0/2/15/18	0/1/1/1
7	FUB	f	1	7	-	0/2/15/18	0/1/1/1
7	FUB	f	2	7	-	0/2/15/18	0/1/1/1
7	FUB	f	3	7	-	0/2/15/18	0/1/1/1
7	AHR	f	4	7	-	0/2/15/18	0/1/1/1
7	FUB	fA	1	7	-	0/2/15/18	0/1/1/1
7	FUB	fA	2	7	-	0/2/15/18	0/1/1/1
7	FUB	fA	3	7	-	0/2/15/18	0/1/1/1
7	AHR	fA	4	7	-	0/2/15/18	0/1/1/1
15	FUB	fB	1	15	-	0/2/15/18	0/1/1/1
15	FUB	fB	2	15	-	0/2/15/18	0/1/1/1
15	GZL	fB	3	15	1/1/4/5	0/6/19/22	0/1/1/1
15	AHR	fB	4	15	-	0/2/15/18	0/1/1/1
15	AHR	fB	5	15	-	0/2/15/18	0/1/1/1
12	FUB	fC	1	12	-	0/2/15/18	0/1/1/1
12	FUB	fC	2	12	-	0/2/15/18	0/1/1/1
12	GZL	fC	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	fC	4	12	-	0/2/15/18	0/1/1/1
12	AHR	fC	5	12	-	0/2/15/18	0/1/1/1
12	FUB	fD	1	12	-	0/2/15/18	0/1/1/1
12	FUB	fD	2	12	-	0/2/15/18	0/1/1/1
12	GZL	fD	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	fD	4	12	-	0/2/15/18	0/1/1/1
12	AHR	fD	5	12	-	0/2/15/18	0/1/1/1
18	FUB	fE	1	18	1/1/3/4	0/2/15/18	0/1/1/1
18	FUB	fE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	fE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	fE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	fE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	g	1	4	-	0/2/15/18	0/1/1/1
4	FUB	g	2	4	-	0/2/15/18	0/1/1/1
4	FUB	g	3	4	-	0/2/15/18	0/1/1/1
4	AHR	g	4	4	-	0/2/15/18	0/1/1/1
11	FUB	gA	1	11	-	1/2/15/18	0/1/1/1
11	AHR	gA	2	11	-	0/2/15/18	0/1/1/1
11	AHR	gA	3	11	-	0/2/15/18	0/1/1/1
6	FUB	gB	1	6	-	0/2/15/18	0/1/1/1
6	FUB	gB	2	6	-	0/2/15/18	0/1/1/1
6	GZL	gB	3	6	1/1/4/5	6/6/19/22	0/1/1/1
13	FUB	gC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	gC	2	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GZL	gC	3	13	2/2/4/5	2/6/19/22	0/1/1/1
13	AHR	gC	4	13	-	0/2/15/18	0/1/1/1
4	FUB	gD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	gD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	gD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	gD	4	4	-	0/2/15/18	0/1/1/1
20	FUB	gE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	gE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	gE	3	20	1/1/4/5	2/6/19/22	0/1/1/1
20	AHR	gE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
7	FUB	h	1	7	-	0/2/15/18	0/1/1/1
7	FUB	h	2	7	-	0/2/15/18	0/1/1/1
7	FUB	h	3	7	-	0/2/15/18	0/1/1/1
7	AHR	h	4	7	-	0/2/15/18	0/1/1/1
9	FUB	hA	1	9	-	0/2/15/18	0/1/1/1
9	FUB	hA	2	9	-	0/2/15/18	0/1/1/1
3	FUB	hB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	hB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	hB	3	3	-	0/2/15/18	0/1/1/1
14	FUB	hC	1	14	-	0/2/15/18	0/1/1/1
14	FUB	hC	2	14	-	0/2/15/18	0/1/1/1
14	GZL	hC	3	14	2/2/4/5	3/6/19/22	0/1/1/1
14	FUB	hC	4	14	-	0/2/15/18	0/1/1/1
14	FUB	hD	1	14	-	0/2/15/18	0/1/1/1
14	FUB	hD	2	14	-	0/2/15/18	0/1/1/1
14	GZL	hD	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	hD	4	14	-	0/2/15/18	0/1/1/1
20	FUB	hE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	hE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	hE	3	20	1/1/4/5	3/6/19/22	0/1/1/1
20	AHR	hE	4	20	-	0/2/15/18	0/1/1/1
11	FUB	i	1	11	-	0/2/15/18	0/1/1/1
11	AHR	i	2	11	-	0/2/15/18	0/1/1/1
11	AHR	i	3	11	-	0/2/15/18	0/1/1/1
4	FUB	iA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	iA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	iA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	iA	4	4	-	0/2/15/18	0/1/1/1
12	FUB	iB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	iB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	iB	3	12	2/2/4/5	6/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	AHR	iB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	iB	5	12	-	0/2/15/18	0/1/1/1
12	FUB	iC	1	12	-	0/2/15/18	0/1/1/1
12	FUB	iC	2	12	-	0/2/15/18	0/1/1/1
12	GZL	iC	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	iC	4	12	-	0/2/15/18	0/1/1/1
12	AHR	iC	5	12	-	0/2/15/18	0/1/1/1
3	FUB	iD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	iD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	iD	3	3	-	0/2/15/18	0/1/1/1
22	FUB	iE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	iE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	iE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	iE	4	22	1/1/3/4	0/2/15/18	0/1/1/1
22	AHR	iE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	iE	6	22	-	0/2/15/18	0/1/1/1
9	FUB	j	1	9	-	0/2/15/18	0/1/1/1
9	FUB	j	2	9	-	0/2/15/18	0/1/1/1
3	FUB	jA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	jA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	jA	3	3	-	0/2/15/18	0/1/1/1
13	FUB	jB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	jB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	jB	3	13	2/2/4/5	3/6/19/22	0/1/1/1
13	AHR	jB	4	13	-	0/2/15/18	0/1/1/1
4	FUB	jC	1	4	-	0/2/15/18	0/1/1/1
4	FUB	jC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	jC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	jC	4	4	-	0/2/15/18	0/1/1/1
10	FUB	jD	1	10	-	0/2/15/18	0/1/1/1
10	FUB	jD	2	10	-	0/2/15/18	0/1/1/1
10	FUB	jD	3	10	-	0/2/15/18	0/1/1/1
10	AHR	jD	4	10	-	0/2/15/18	0/1/1/1
10	AHR	jD	5	10	-	0/2/15/18	0/1/1/1
20	FUB	jE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	jE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	jE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	jE	4	20	1/1/3/4	0/2/15/18	0/1/1/1
4	FUB	k	1	4	-	0/2/15/18	0/1/1/1
4	FUB	k	2	4	-	0/2/15/18	0/1/1/1
4	FUB	k	3	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	k	4	4	-	0/2/15/18	0/1/1/1
3	FUB	kA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	kA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	kA	3	3	-	0/2/15/18	0/1/1/1
14	FUB	kB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	kB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	kB	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	kB	4	14	-	0/2/15/18	0/1/1/1
14	FUB	kC	1	14	-	0/2/15/18	0/1/1/1
14	FUB	kC	2	14	-	0/2/15/18	0/1/1/1
14	GZL	kC	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	kC	4	14	-	0/2/15/18	0/1/1/1
4	FUB	kD	1	4	-	0/2/15/18	0/1/1/1
4	FUB	kD	2	4	-	0/2/15/18	0/1/1/1
4	FUB	kD	3	4	-	0/2/15/18	0/1/1/1
4	AHR	kD	4	4	-	0/2/15/18	0/1/1/1
21	FUB	kE	1	21	-	0/2/15/18	0/1/1/1
21	FUB	kE	2	21	-	0/2/15/18	0/1/1/1
21	GZL	kE	3	21	1/1/4/5	0/6/19/22	0/1/1/1
21	AHR	kE	4	21	1/1/3/4	0/2/15/18	0/1/1/1
21	AHR	kE	5	21	-	0/2/15/18	0/1/1/1
3	FUB	l	1	3	-	0/2/15/18	0/1/1/1
3	FUB	l	2	3	-	0/2/15/18	0/1/1/1
3	FUB	l	3	3	-	0/2/15/18	0/1/1/1
12	FUB	lA	1	12	-	0/2/15/18	0/1/1/1
12	FUB	lA	2	12	-	0/2/15/18	0/1/1/1
12	GZL	lA	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	lA	4	12	-	0/2/15/18	0/1/1/1
12	AHR	lA	5	12	-	0/2/15/18	0/1/1/1
12	FUB	lB	1	12	-	0/2/15/18	0/1/1/1
12	FUB	lB	2	12	-	0/2/15/18	0/1/1/1
12	GZL	lB	3	12	2/2/4/5	6/6/19/22	0/1/1/1
12	AHR	lB	4	12	-	0/2/15/18	0/1/1/1
12	AHR	lB	5	12	-	0/2/15/18	0/1/1/1
3	FUB	lC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	lC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	lC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	lD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	lD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	lD	3	3	-	0/2/15/18	0/1/1/1
24	FUB	lE	1	24	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	FUB	lE	2	24	-	0/2/15/18	0/1/1/1
24	GZL	lE	3	24	1/1/4/5	5/6/19/22	0/1/1/1
24	AHR	lE	4	24	1/1/3/4	0/2/15/18	0/1/1/1
24	AHR	lE	5	24	-	0/2/15/18	0/1/1/1
24	AHR	lE	6	24	-	0/2/15/18	0/1/1/1
3	FUB	m	1	3	-	0/2/15/18	0/1/1/1
3	FUB	m	2	3	-	0/2/15/18	0/1/1/1
3	FUB	m	3	3	-	0/2/15/18	0/1/1/1
13	FUB	mA	1	13	-	0/2/15/18	0/1/1/1
13	FUB	mA	2	13	-	0/2/15/18	0/1/1/1
13	GZL	mA	3	13	2/2/4/5	4/6/19/22	0/1/1/1
13	AHR	mA	4	13	-	0/2/15/18	0/1/1/1
4	FUB	mB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	mB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	mB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	mB	4	4	-	0/2/15/18	0/1/1/1
10	FUB	mC	1	10	-	0/2/15/18	0/1/1/1
10	FUB	mC	2	10	-	0/2/15/18	0/1/1/1
10	FUB	mC	3	10	-	0/2/15/18	0/1/1/1
10	AHR	mC	4	10	-	0/2/15/18	0/1/1/1
10	AHR	mC	5	10	-	0/2/15/18	0/1/1/1
3	FUB	mD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	mD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	mD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	mE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	mE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	mE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
12	FUB	n	1	12	-	0/2/15/18	0/1/1/1
12	FUB	n	2	12	-	0/2/15/18	0/1/1/1
12	GZL	n	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	n	4	12	-	0/2/15/18	0/1/1/1
12	AHR	n	5	12	-	0/2/15/18	0/1/1/1
14	FUB	nA	1	14	-	0/2/15/18	0/1/1/1
14	FUB	nA	2	14	-	0/2/15/18	0/1/1/1
14	GZL	nA	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	nA	4	14	-	0/2/15/18	0/1/1/1
14	FUB	nB	1	14	-	0/2/15/18	0/1/1/1
14	FUB	nB	2	14	-	0/2/15/18	0/1/1/1
14	GZL	nB	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	nB	4	14	-	0/2/15/18	0/1/1/1
4	FUB	nC	1	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	nC	2	4	-	0/2/15/18	0/1/1/1
4	FUB	nC	3	4	-	0/2/15/18	0/1/1/1
4	AHR	nC	4	4	-	0/2/15/18	0/1/1/1
3	FUB	nD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	nD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	nD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	nE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	nE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	nE	3	6	1/1/4/5	6/6/19/22	0/1/1/1
13	FUB	o	1	13	-	0/2/15/18	0/1/1/1
13	FUB	o	2	13	-	0/2/15/18	0/1/1/1
13	GZL	o	3	13	2/2/4/5	2/6/19/22	0/1/1/1
13	AHR	o	4	13	-	0/2/15/18	0/1/1/1
12	FUB	oA	1	12	-	0/2/15/18	0/1/1/1
12	FUB	oA	2	12	-	0/2/15/18	0/1/1/1
12	GZL	oA	3	12	2/2/4/5	2/6/19/22	0/1/1/1
12	AHR	oA	4	12	-	0/2/15/18	0/1/1/1
12	AHR	oA	5	12	-	0/2/15/18	0/1/1/1
3	FUB	oB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	oB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	oB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	oC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	oC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	oC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	oD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	oD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	oD	3	3	-	0/2/15/18	0/1/1/1
6	FUB	oE	1	6	-	0/2/15/18	0/1/1/1
6	FUB	oE	2	6	-	0/2/15/18	0/1/1/1
6	GZL	oE	3	6	1/1/4/5	4/6/19/22	0/1/1/1
14	FUB	p	1	14	-	0/2/15/18	0/1/1/1
14	FUB	p	2	14	-	0/2/15/18	0/1/1/1
14	GZL	p	3	14	2/2/4/5	6/6/19/22	0/1/1/1
14	FUB	p	4	14	-	0/2/15/18	0/1/1/1
4	FUB	pA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	pA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	pA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	pA	4	4	-	0/2/15/18	0/1/1/1
10	FUB	pB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	pB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	pB	3	10	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	AHR	pB	4	10	-	0/2/15/18	0/1/1/1
10	AHR	pB	5	10	-	0/2/15/18	0/1/1/1
3	FUB	pC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	pC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	pC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	pD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	pE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	pE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	pE	3	18	1/1/4/5	4/6/19/22	0/1/1/1
18	AHR	pE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	pE	5	18	-	0/2/15/18	0/1/1/1
12	FUB	q	1	12	-	0/2/15/18	0/1/1/1
12	FUB	q	2	12	-	0/2/15/18	0/1/1/1
12	GZL	q	3	12	2/2/4/5	0/6/19/22	0/1/1/1
12	AHR	q	4	12	-	0/2/15/18	0/1/1/1
12	AHR	q	5	12	1/1/3/4	0/2/15/18	0/1/1/1
14	FUB	qA	1	14	-	0/2/15/18	0/1/1/1
14	FUB	qA	2	14	-	0/2/15/18	0/1/1/1
14	GZL	qA	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	qA	4	14	-	0/2/15/18	0/1/1/1
4	FUB	qB	1	4	-	0/2/15/18	0/1/1/1
4	FUB	qB	2	4	-	0/2/15/18	0/1/1/1
4	FUB	qB	3	4	-	0/2/15/18	0/1/1/1
4	AHR	qB	4	4	-	0/2/15/18	0/1/1/1
3	FUB	qC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	qC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	qC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	qD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	qD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	qD	3	3	-	0/2/15/18	0/1/1/1
19	FUB	qE	1	19	-	0/2/15/18	0/1/1/1
19	FUB	qE	2	19	-	0/2/15/18	0/1/1/1
19	GZL	qE	3	19	1/1/4/5	4/6/19/22	0/1/1/1
19	AHR	qE	4	19	-	0/2/15/18	0/1/1/1
4	FUB	r	1	4	-	0/2/15/18	0/1/1/1
4	FUB	r	2	4	-	0/2/15/18	0/1/1/1
4	FUB	r	3	4	-	0/2/15/18	0/1/1/1
4	AHR	r	4	4	-	0/2/15/18	0/1/1/1
3	FUB	rA	1	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	rA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	rB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	rC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rC	3	3	-	0/2/15/18	0/1/1/1
3	FUB	rD	1	3	-	0/2/15/18	0/1/1/1
3	FUB	rD	2	3	-	0/2/15/18	0/1/1/1
3	FUB	rD	3	3	-	0/2/15/18	0/1/1/1
18	FUB	rE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	rE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	rE	3	18	1/1/4/5	3/6/19/22	0/1/1/1
18	AHR	rE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	rE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
14	FUB	s	1	14	-	0/2/15/18	0/1/1/1
14	FUB	s	2	14	-	0/2/15/18	0/1/1/1
14	GZL	s	3	14	2/2/4/5	4/6/19/22	0/1/1/1
14	FUB	s	4	14	-	0/2/15/18	0/1/1/1
10	FUB	sA	1	10	-	0/2/15/18	0/1/1/1
10	FUB	sA	2	10	-	0/2/15/18	0/1/1/1
10	FUB	sA	3	10	-	0/2/15/18	0/1/1/1
10	AHR	sA	4	10	-	0/2/15/18	0/1/1/1
10	AHR	sA	5	10	-	0/2/15/18	0/1/1/1
3	FUB	sB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	sB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	sB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	sC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	sC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	sC	3	3	-	0/2/15/18	0/1/1/1
10	FUB	sD	1	10	-	0/2/15/18	0/1/1/1
10	FUB	sD	2	10	-	0/2/15/18	0/1/1/1
10	FUB	sD	3	10	-	0/2/15/18	0/1/1/1
10	AHR	sD	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	sD	5	10	-	0/2/15/18	0/1/1/1
20	FUB	sE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	sE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	sE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	sE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	t	1	3	-	0/2/15/18	0/1/1/1
3	FUB	t	2	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	t	3	3	-	0/2/15/18	0/1/1/1
4	FUB	tA	1	4	-	0/2/15/18	0/1/1/1
4	FUB	tA	2	4	-	0/2/15/18	0/1/1/1
4	FUB	tA	3	4	-	0/2/15/18	0/1/1/1
4	AHR	tA	4	4	-	0/2/15/18	0/1/1/1
3	FUB	tB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	tB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	tB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	tC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	tC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	tC	3	3	-	0/2/15/18	0/1/1/1
13	FUB	tD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	tD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	tD	3	13	3/3/4/5	0/6/19/22	0/1/1/1
13	AHR	tD	4	13	-	0/2/15/18	0/1/1/1
18	FUB	tE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	tE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	tE	3	18	1/1/4/5	2/6/19/22	0/1/1/1
18	AHR	tE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	tE	5	18	1/1/3/4	0/2/15/18	0/1/1/1
10	FUB	u	1	10	-	0/2/15/18	0/1/1/1
10	FUB	u	2	10	-	0/2/15/18	0/1/1/1
10	FUB	u	3	10	-	0/2/15/18	0/1/1/1
10	AHR	u	4	10	-	0/2/15/18	0/1/1/1
10	AHR	u	5	10	-	0/2/15/18	0/1/1/1
3	FUB	uA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	uA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	uA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	uB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	uB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	uB	3	3	-	0/2/15/18	0/1/1/1
3	FUB	uC	1	3	-	0/2/15/18	0/1/1/1
3	FUB	uC	2	3	-	0/2/15/18	0/1/1/1
3	FUB	uC	3	3	-	0/2/15/18	0/1/1/1
6	FUB	uD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	uD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	uD	3	6	2/2/4/5	6/6/19/22	0/1/1/1
20	FUB	uE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	uE	2	20	-	0/2/15/18	0/1/1/1
20	GZL	uE	3	20	1/1/4/5	4/6/19/22	0/1/1/1
20	AHR	uE	4	20	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	v	1	4	-	0/2/15/18	0/1/1/1
4	FUB	v	2	4	-	0/2/15/18	0/1/1/1
4	FUB	v	3	4	-	0/2/15/18	0/1/1/1
4	AHR	v	4	4	-	0/2/15/18	0/1/1/1
3	FUB	vA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	vA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	vA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	vB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	vB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	vB	3	3	-	0/2/15/18	0/1/1/1
10	FUB	vC	1	10	-	0/2/15/18	0/1/1/1
10	FUB	vC	2	10	-	0/2/15/18	0/1/1/1
10	FUB	vC	3	10	-	0/2/15/18	0/1/1/1
10	AHR	vC	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	vC	5	10	-	0/2/15/18	0/1/1/1
13	FUB	vD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	vD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	vD	3	13	1/1/4/5	4/6/19/22	0/1/1/1
13	AHR	vD	4	13	-	0/2/15/18	0/1/1/1
21	FUB	vE	1	21	-	0/2/15/18	0/1/1/1
21	FUB	vE	2	21	-	0/2/15/18	0/1/1/1
21	GZL	vE	3	21	1/1/4/5	4/6/19/22	0/1/1/1
21	AHR	vE	4	21	1/1/3/4	0/2/15/18	0/1/1/1
21	AHR	vE	5	21	2/2/3/4	0/2/15/18	0/1/1/1
3	FUB	w	1	3	-	0/2/15/18	0/1/1/1
3	FUB	w	2	3	-	0/2/15/18	0/1/1/1
3	FUB	w	3	3	-	0/2/15/18	0/1/1/1
3	FUB	wA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	wA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	wA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	wB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	wB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	wB	3	3	-	0/2/15/18	0/1/1/1
13	FUB	wC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	wC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	wC	3	13	3/3/4/5	1/6/19/22	0/1/1/1
13	AHR	wC	4	13	-	0/2/15/18	0/1/1/1
13	FUB	wD	1	13	-	0/2/15/18	0/1/1/1
13	FUB	wD	2	13	-	0/2/15/18	0/1/1/1
13	GZL	wD	3	13	1/1/4/5	6/6/19/22	0/1/1/1
13	AHR	wD	4	13	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	FUB	wE	1	22	-	0/2/15/18	0/1/1/1
22	FUB	wE	2	22	-	0/2/15/18	0/1/1/1
22	GZL	wE	3	22	1/1/4/5	2/6/19/22	0/1/1/1
22	AHR	wE	4	22	-	0/2/15/18	0/1/1/1
22	AHR	wE	5	22	-	0/2/15/18	0/1/1/1
22	AHR	wE	6	22	-	0/2/15/18	0/1/1/1
3	FUB	x	1	3	-	0/2/15/18	0/1/1/1
3	FUB	x	2	3	-	0/2/15/18	0/1/1/1
3	FUB	x	3	3	-	0/2/15/18	0/1/1/1
3	FUB	xA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	xA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	xA	3	3	-	0/2/15/18	0/1/1/1
3	FUB	xB	1	3	-	0/2/15/18	0/1/1/1
3	FUB	xB	2	3	-	0/2/15/18	0/1/1/1
3	FUB	xB	3	3	-	0/2/15/18	0/1/1/1
6	FUB	xC	1	6	-	0/2/15/18	0/1/1/1
6	FUB	xC	2	6	-	0/2/15/18	0/1/1/1
6	GZL	xC	3	6	2/2/4/5	5/6/19/22	0/1/1/1
6	FUB	xD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	xD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	xD	3	6	-	6/6/19/22	0/1/1/1
20	FUB	xE	1	20	-	0/2/15/18	0/1/1/1
20	FUB	xE	2	20	-	2/2/15/18	0/1/1/1
20	GZL	xE	3	20	1/1/4/5	6/6/19/22	0/1/1/1
20	AHR	xE	4	20	-	0/2/15/18	0/1/1/1
3	FUB	y	1	3	-	0/2/15/18	0/1/1/1
3	FUB	y	2	3	-	0/2/15/18	0/1/1/1
3	FUB	y	3	3	-	0/2/15/18	0/1/1/1
3	FUB	yA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	yA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	yA	3	3	-	0/2/15/18	0/1/1/1
10	FUB	yB	1	10	-	0/2/15/18	0/1/1/1
10	FUB	yB	2	10	-	0/2/15/18	0/1/1/1
10	FUB	yB	3	10	-	0/2/15/18	0/1/1/1
10	AHR	yB	4	10	1/1/3/4	0/2/15/18	0/1/1/1
10	AHR	yB	5	10	-	0/2/15/18	0/1/1/1
13	FUB	yC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	yC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	yC	3	13	1/1/4/5	2/6/19/22	0/1/1/1
13	AHR	yC	4	13	-	0/2/15/18	0/1/1/1
6	FUB	yD	1	6	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUB	yD	2	6	-	0/2/15/18	0/1/1/1
6	GZL	yD	3	6	1/1/4/5	2/6/19/22	0/1/1/1
18	FUB	yE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	yE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	yE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	yE	4	18	1/1/3/4	0/2/15/18	0/1/1/1
18	AHR	yE	5	18	-	0/2/15/18	0/1/1/1
3	FUB	z	1	3	-	0/2/15/18	0/1/1/1
3	FUB	z	2	3	-	0/2/15/18	0/1/1/1
3	FUB	z	3	3	-	0/2/15/18	0/1/1/1
3	FUB	zA	1	3	-	0/2/15/18	0/1/1/1
3	FUB	zA	2	3	-	0/2/15/18	0/1/1/1
3	FUB	zA	3	3	-	0/2/15/18	0/1/1/1
13	FUB	zB	1	13	-	0/2/15/18	0/1/1/1
13	FUB	zB	2	13	-	0/2/15/18	0/1/1/1
13	GZL	zB	3	13	3/3/4/5	2/6/19/22	0/1/1/1
13	AHR	zB	4	13	-	0/2/15/18	0/1/1/1
13	FUB	zC	1	13	-	0/2/15/18	0/1/1/1
13	FUB	zC	2	13	-	0/2/15/18	0/1/1/1
13	GZL	zC	3	13	1/1/4/5	6/6/19/22	0/1/1/1
13	AHR	zC	4	13	-	0/2/15/18	0/1/1/1
6	FUB	zD	1	6	-	0/2/15/18	0/1/1/1
6	FUB	zD	2	6	1/1/3/4	0/2/15/18	0/1/1/1
6	GZL	zD	3	6	1/1/4/5	2/6/19/22	0/1/1/1
18	FUB	zE	1	18	-	0/2/15/18	0/1/1/1
18	FUB	zE	2	18	-	0/2/15/18	0/1/1/1
18	GZL	zE	3	18	1/1/4/5	6/6/19/22	0/1/1/1
18	AHR	zE	4	18	-	0/2/15/18	0/1/1/1
18	AHR	zE	5	18	1/1/3/4	0/2/15/18	0/1/1/1

The worst 5 of 1123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CD	3	GZL	C2-C3	-19.62	1.22	1.53
6	LA	3	GZL	C2-C3	-19.56	1.22	1.53
6	uD	3	GZL	C2-C3	-19.38	1.22	1.53
6	xC	3	GZL	C2-C3	-19.37	1.22	1.53
6	XB	3	GZL	C2-C3	-19.34	1.22	1.53

The worst 5 of 834 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	3A	3	GZL	C1-O4-C4	-12.65	82.02	107.84
6	N	3	GZL	C5-C4-C3	-9.92	102.60	115.86
6	CD	3	GZL	C1-O4-C4	-9.73	87.98	107.84
6	0B	3	GZL	C1-O4-C4	-9.43	88.59	107.84
6	LA	3	GZL	C1-O4-C4	-9.36	88.73	107.84

5 of 302 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	XA	2	FUB	C1
4	L	1	FUB	C4
4	Z	2	FUB	C1
4	JA	1	FUB	C4
4	VA	4	AHR	C2

5 of 605 torsion outliers are listed below:

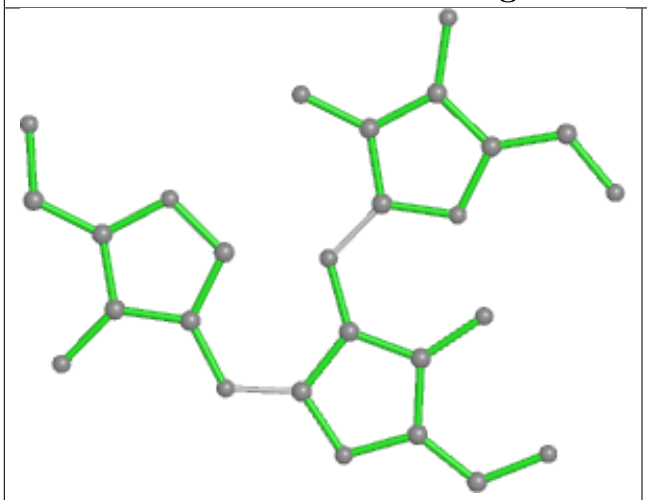
Mol	Chain	Res	Type	Atoms
6	N	3	GZL	C4-C5-C6-O6
6	N	3	GZL	O5-C5-C6-O6
6	5	3	GZL	O5-C5-C6-O6
6	AA	3	GZL	C3-C4-C5-C6
6	AA	3	GZL	O4-C4-C5-C6

There are no ring outliers.

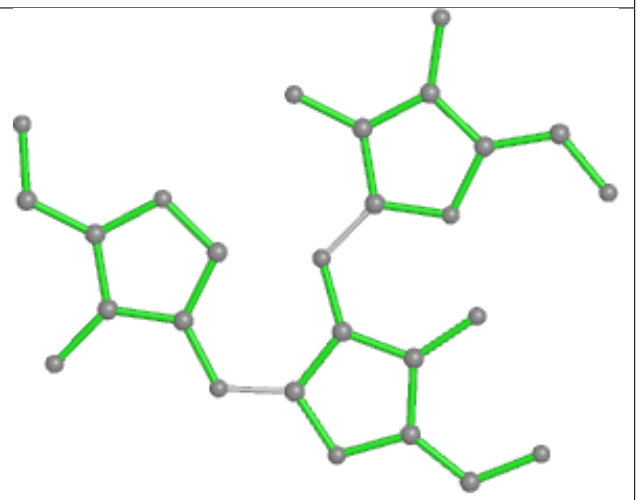
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

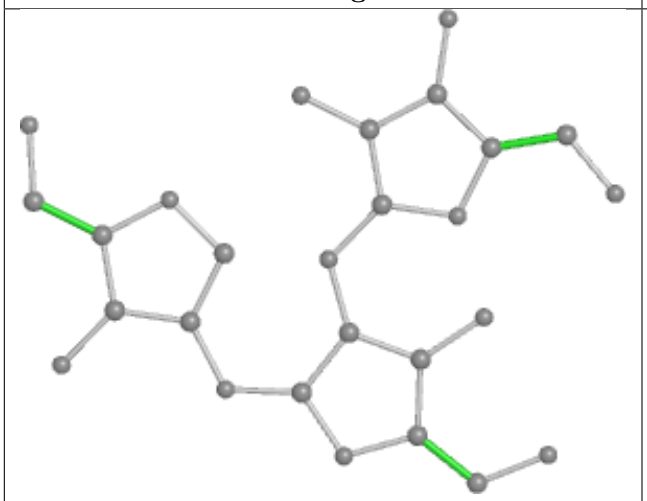
Oligosaccharide Chain J



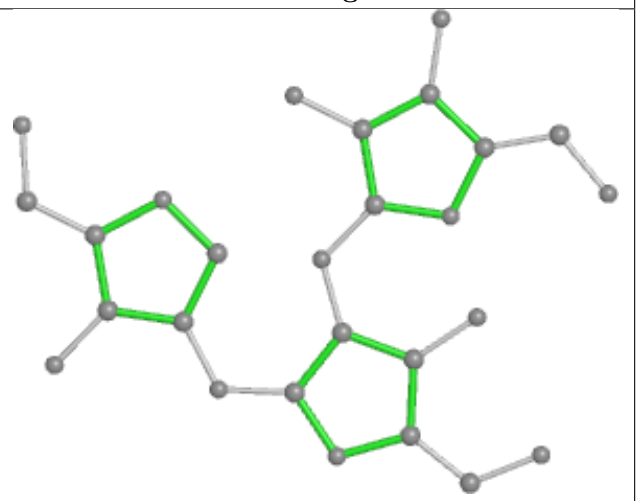
Bond lengths



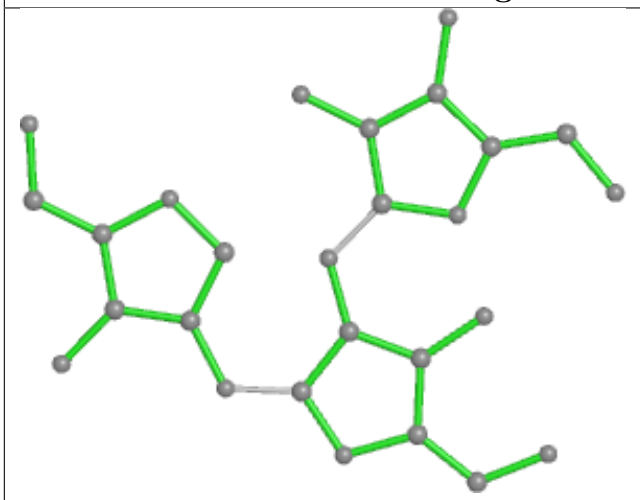
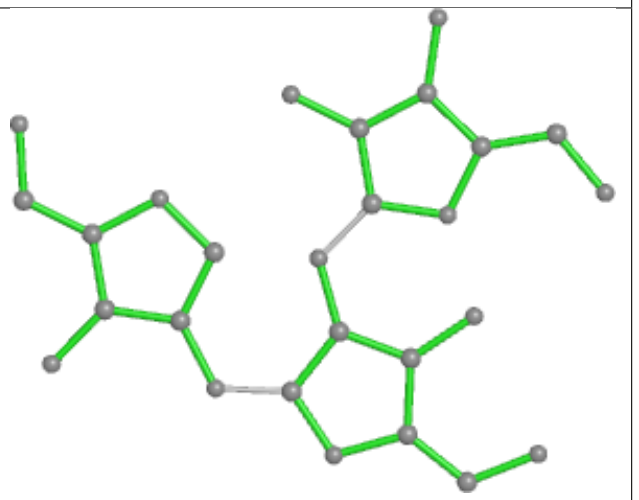
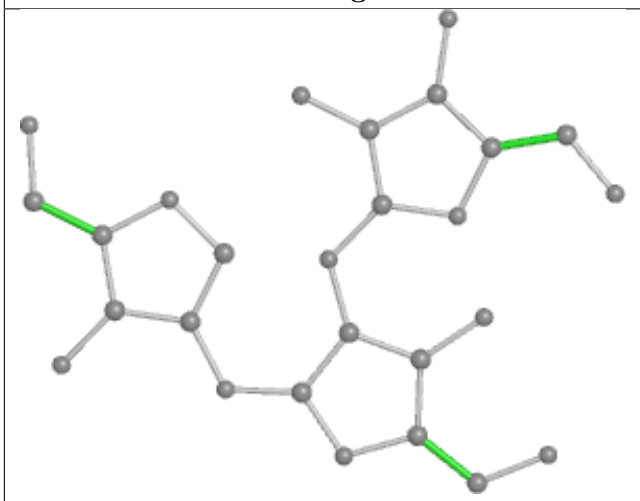
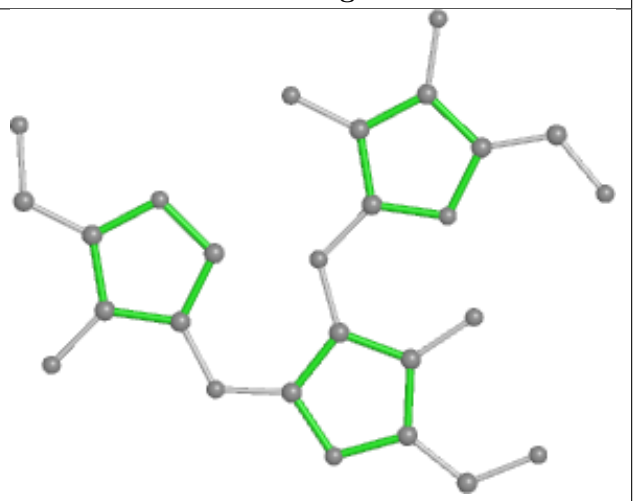
Bond angles

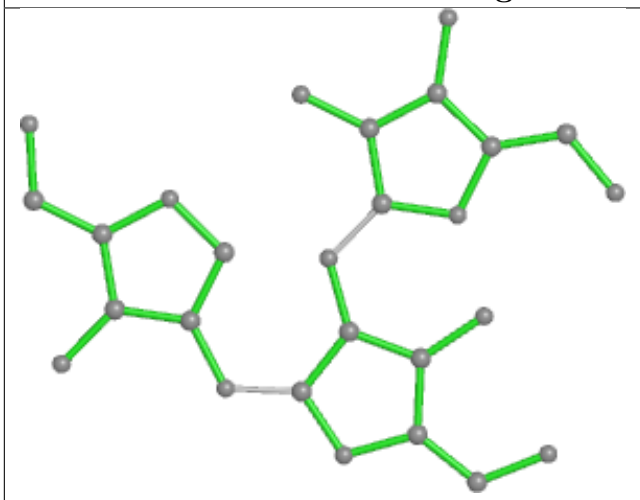
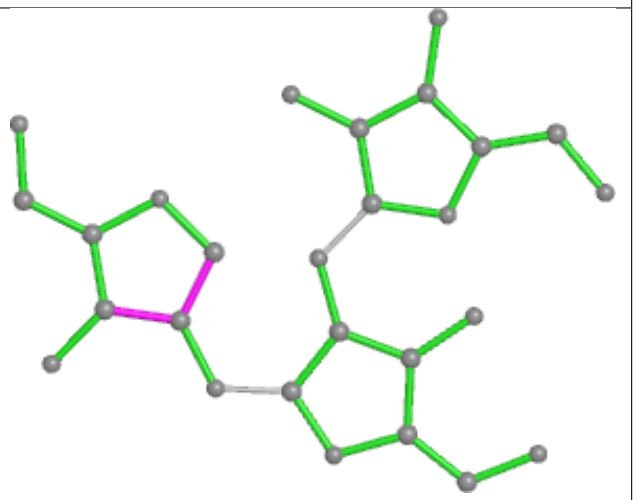
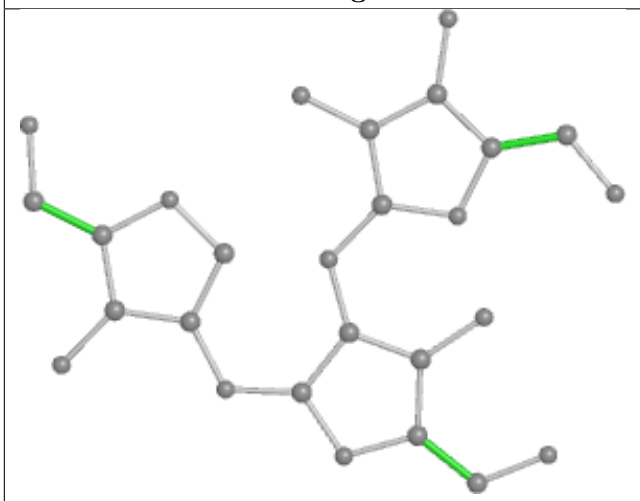
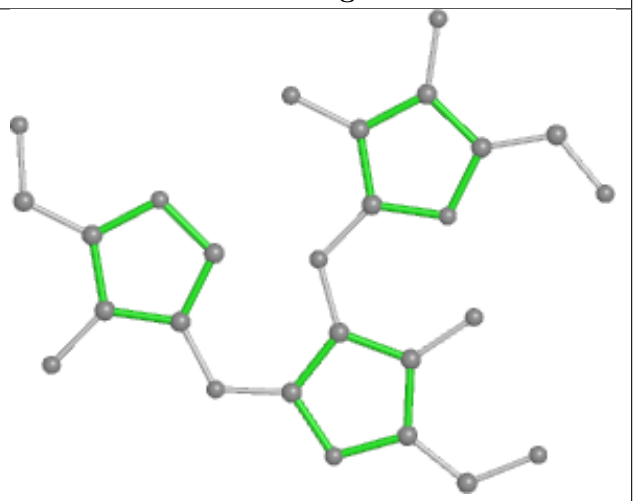


Torsions

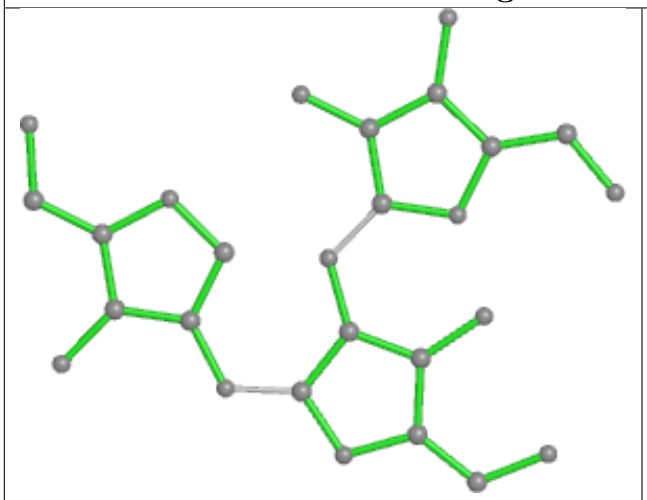


Rings

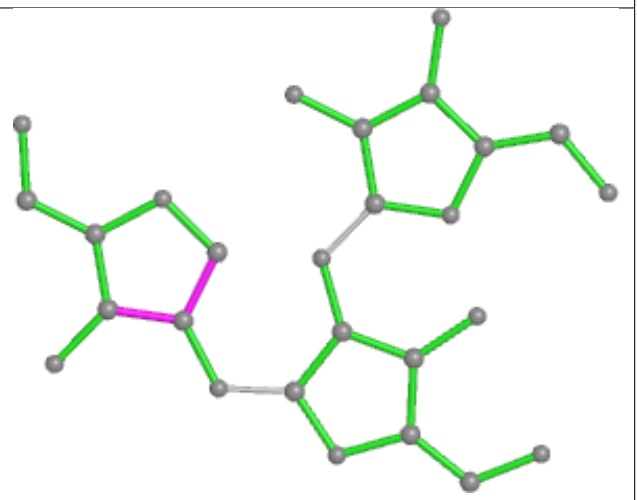
Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

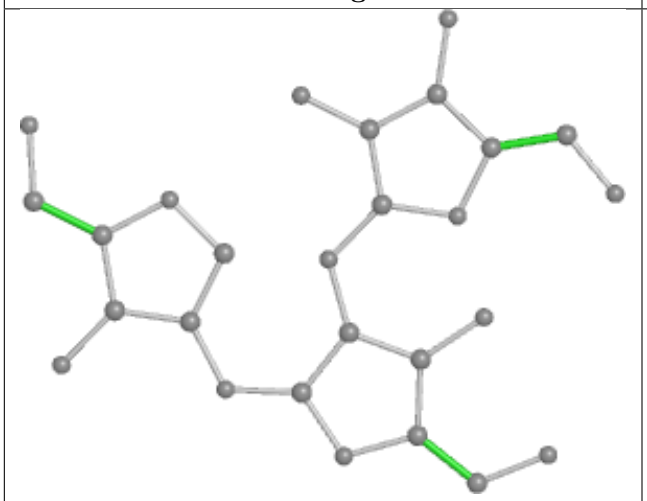
Oligosaccharide Chain P



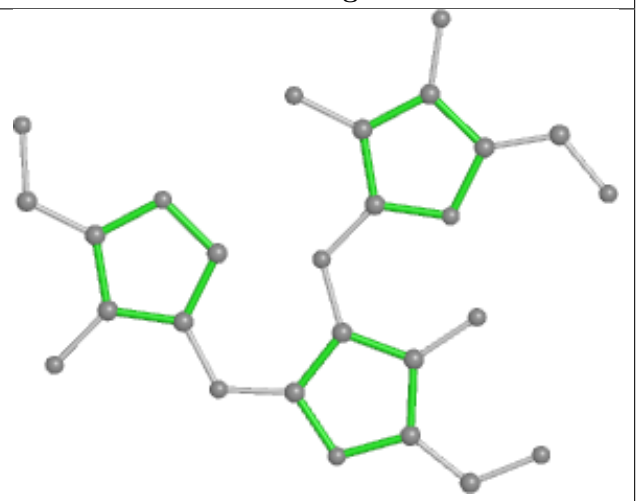
Bond lengths



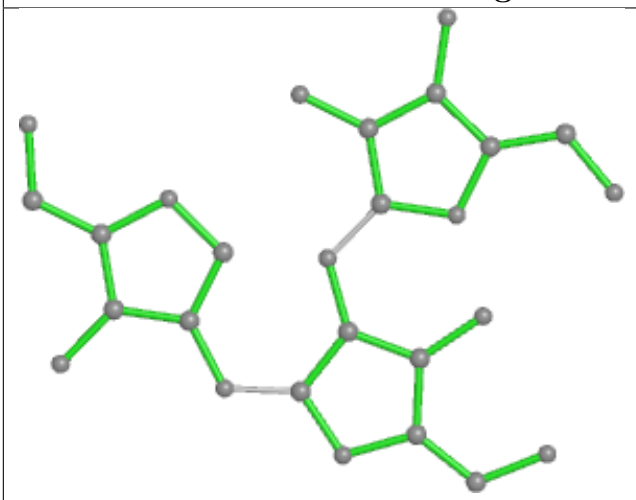
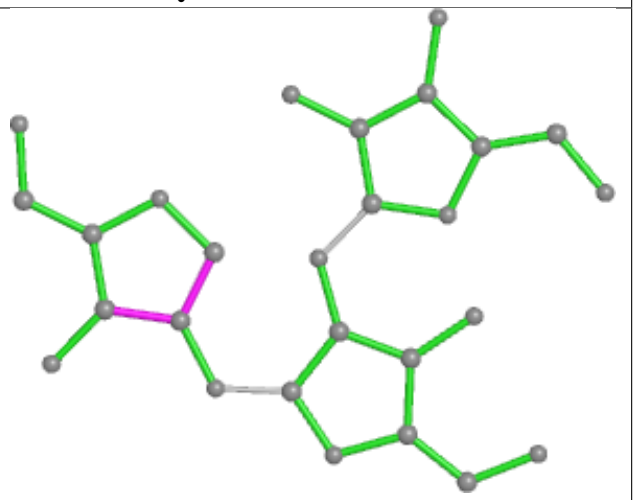
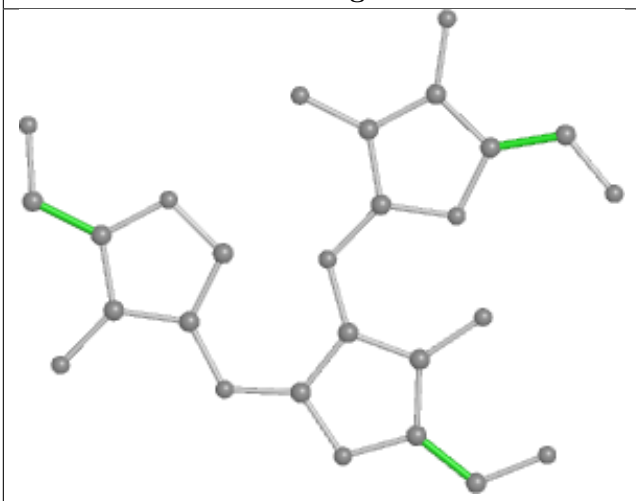
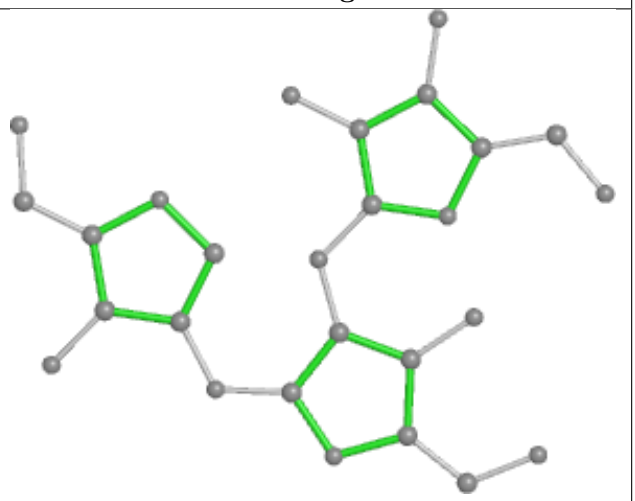
Bond angles



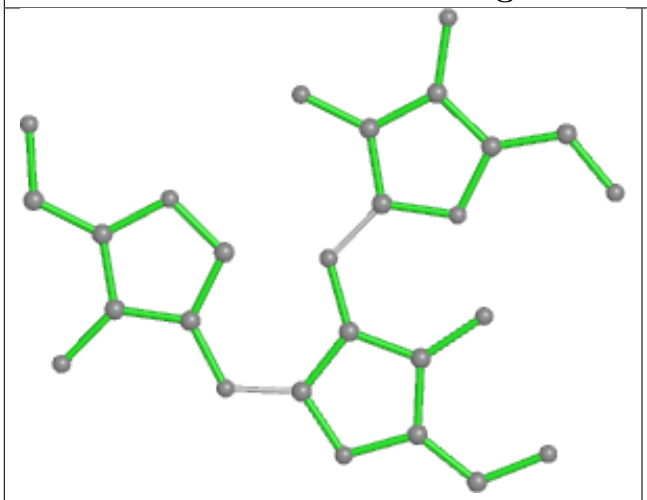
Torsions



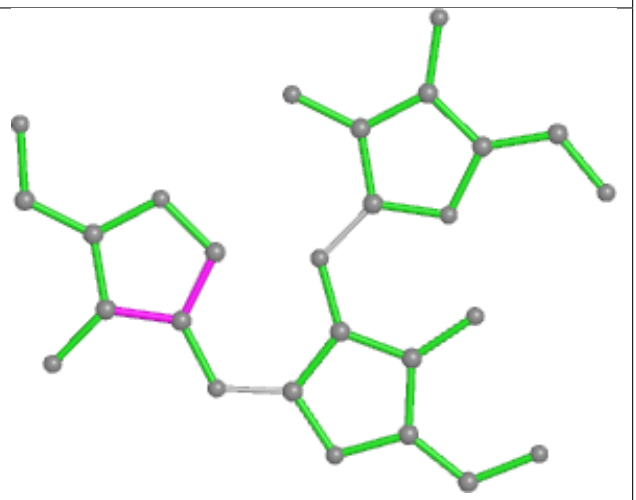
Rings

Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

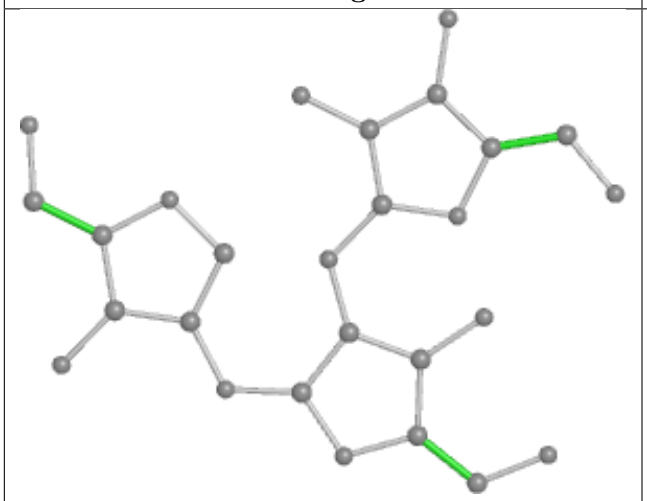
Oligosaccharide Chain T



Bond lengths



Bond angles



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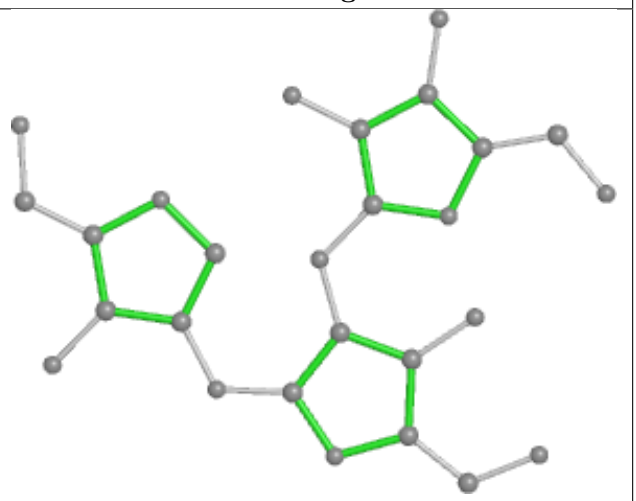
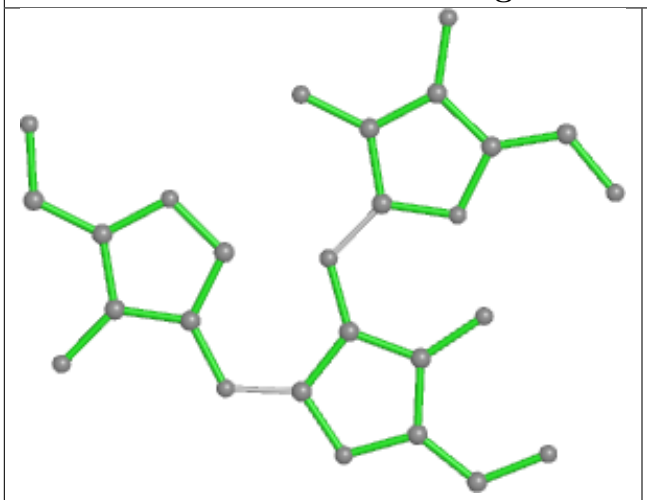


Rings

Oligosaccharide Chain V



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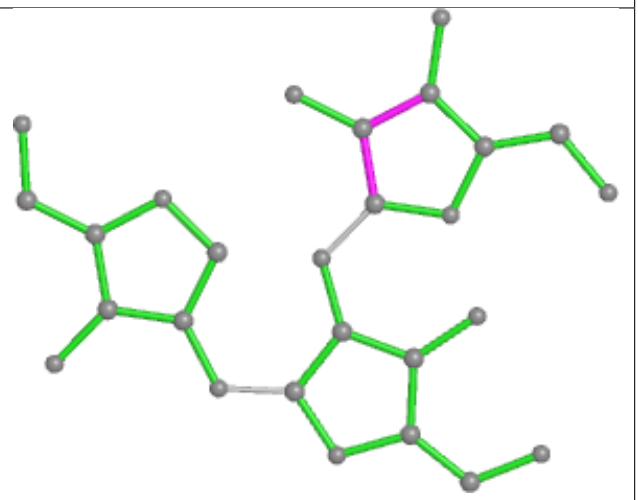

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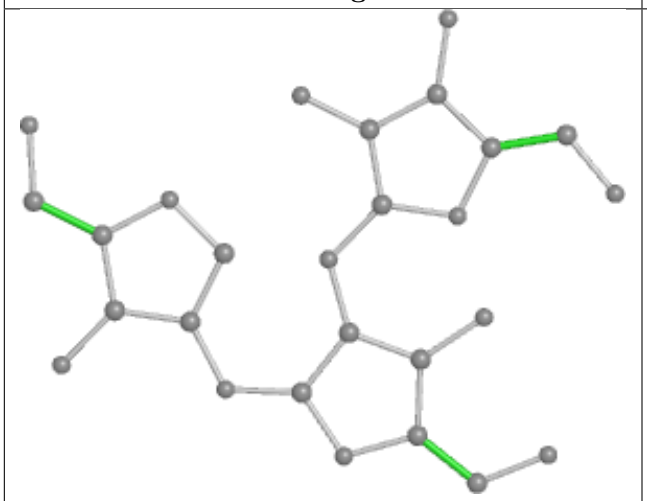

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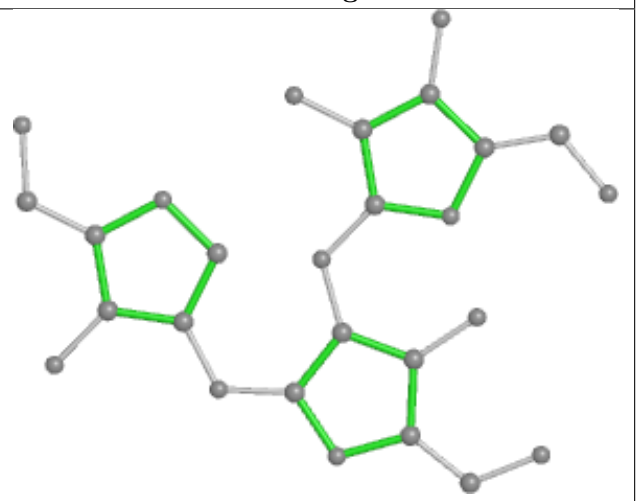
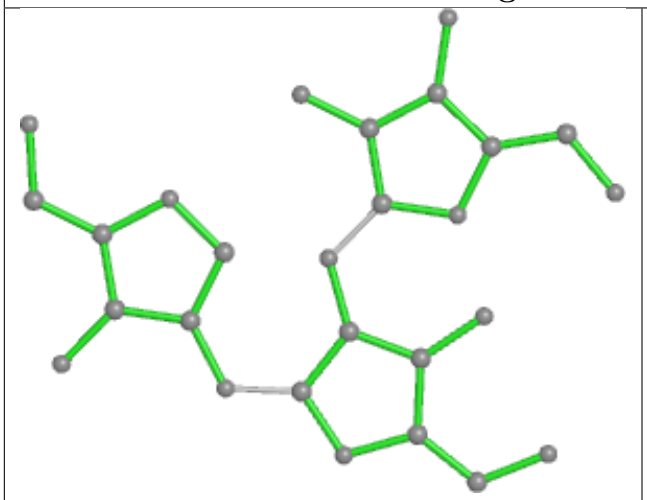


Rings

Oligosaccharide Chain b



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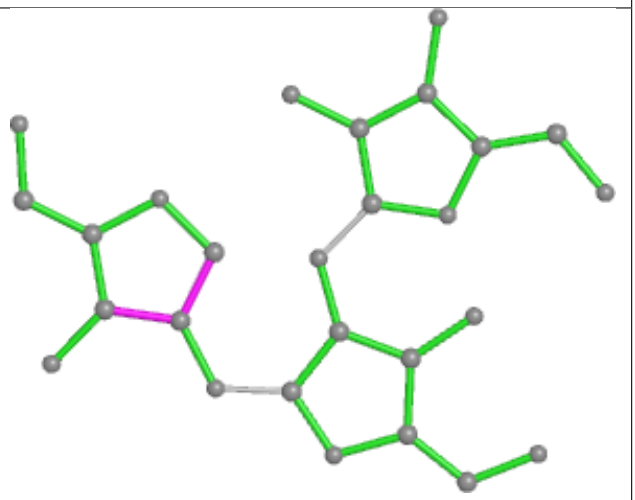

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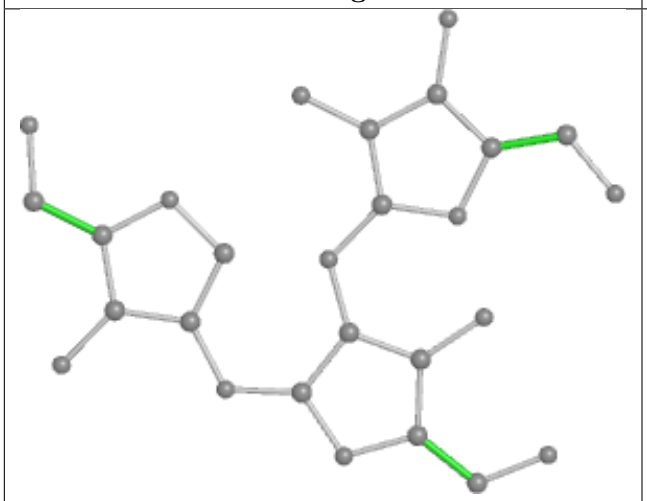

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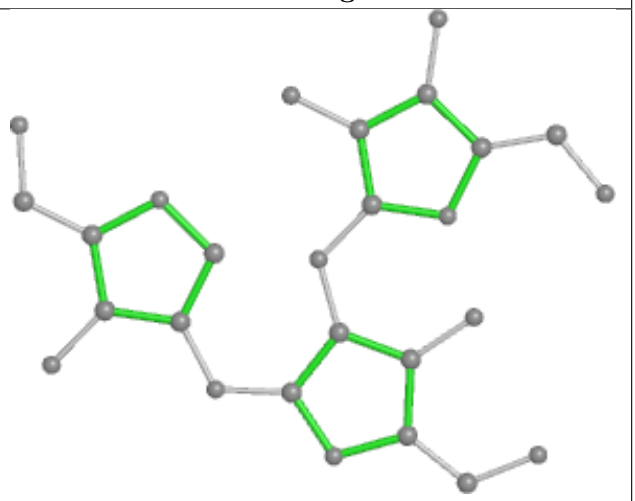
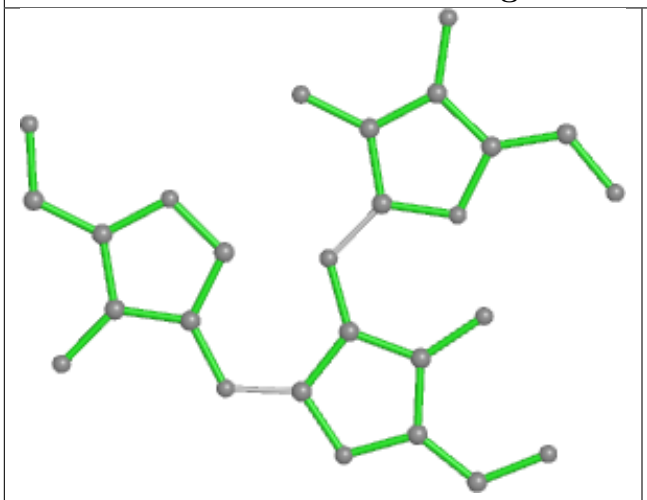


Rings

Oligosaccharide Chain e



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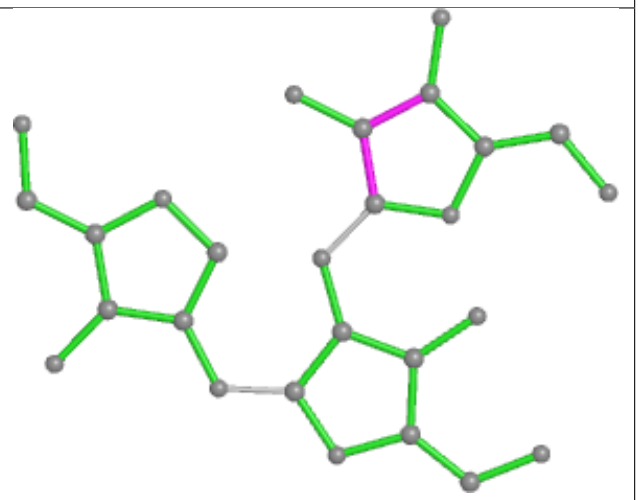

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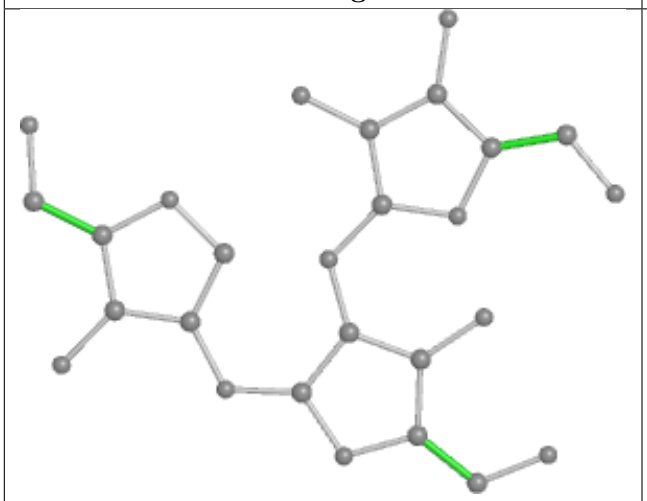

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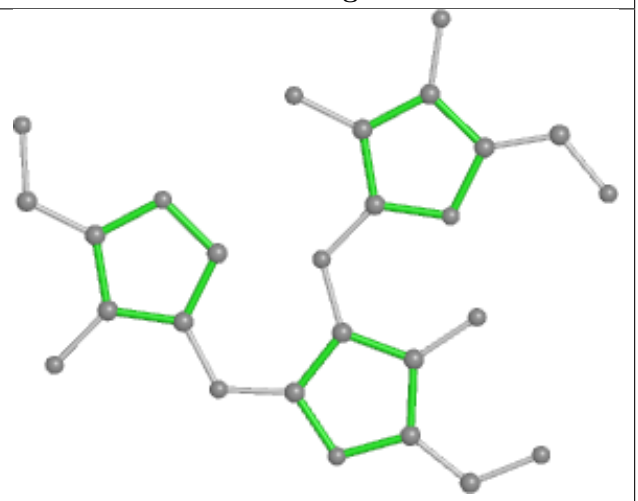
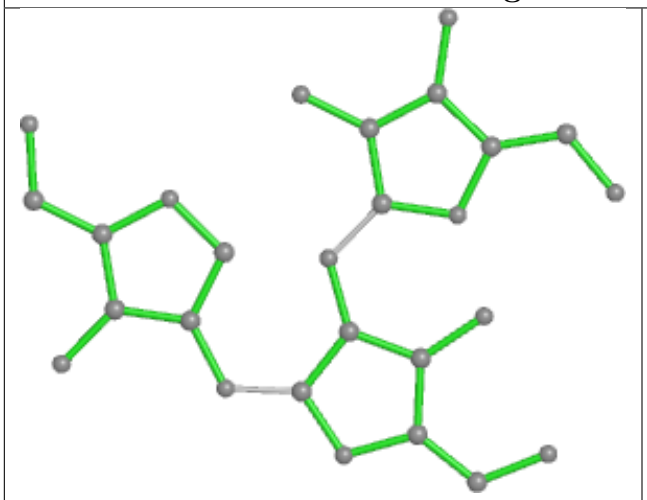


Rings

Oligosaccharide Chain l



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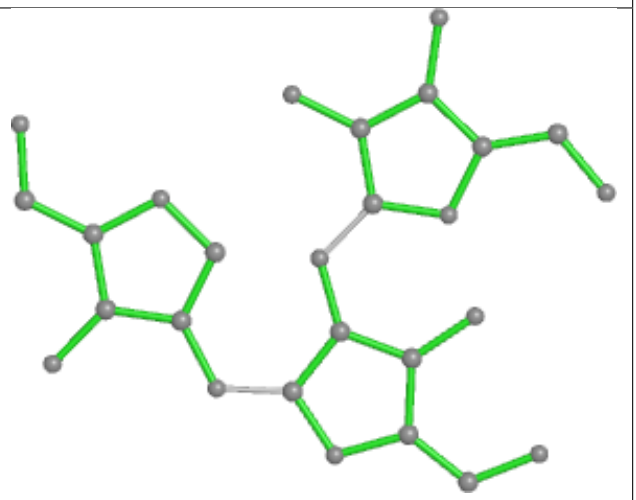

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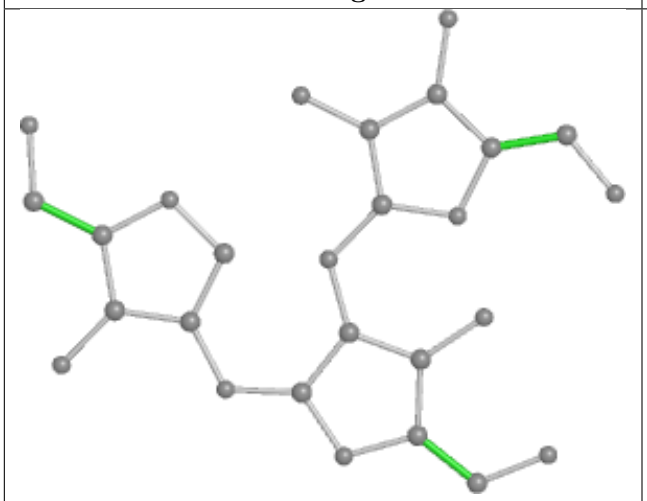

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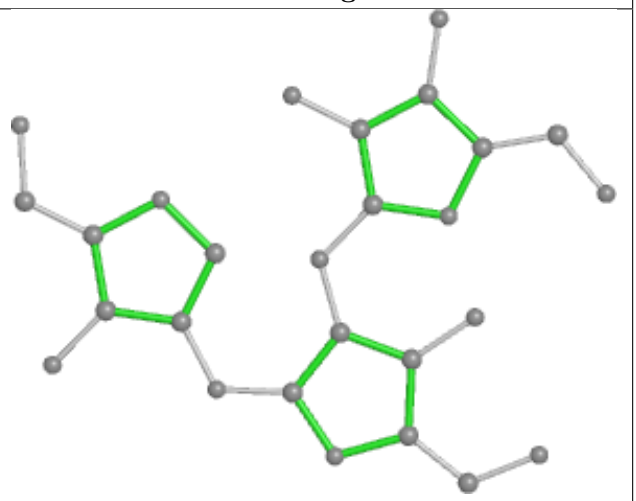
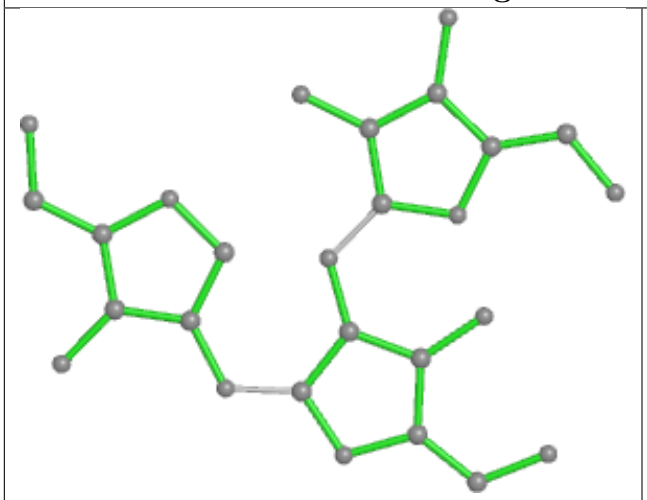


Rings

Oligosaccharide Chain m



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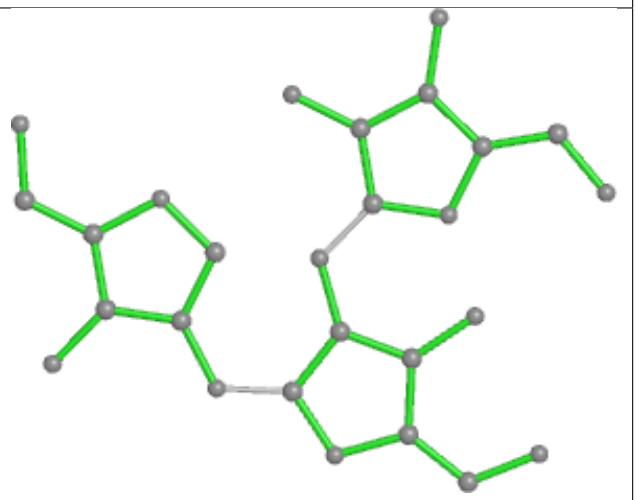

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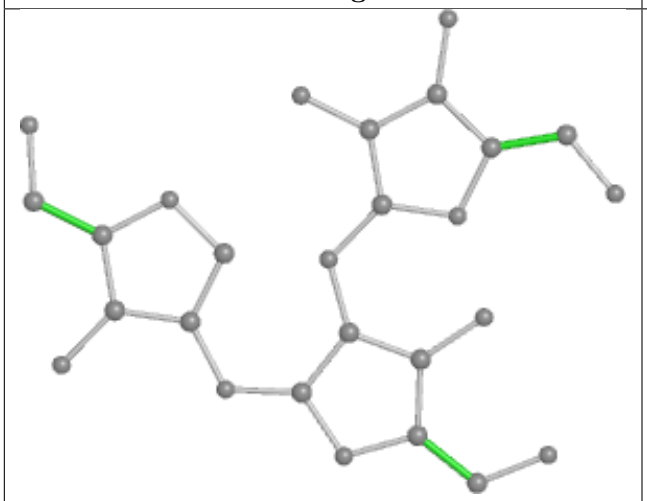

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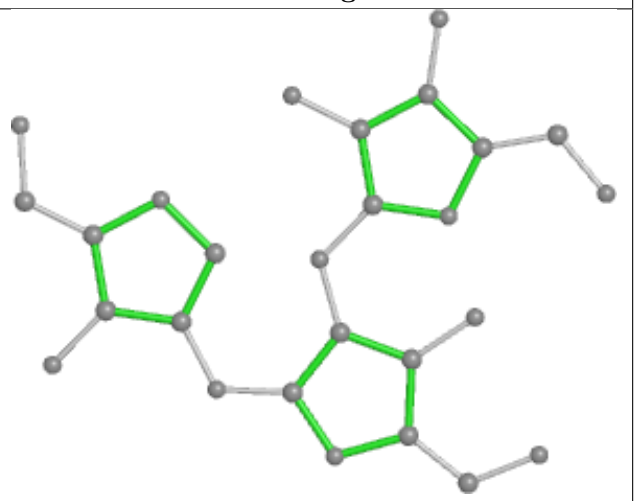
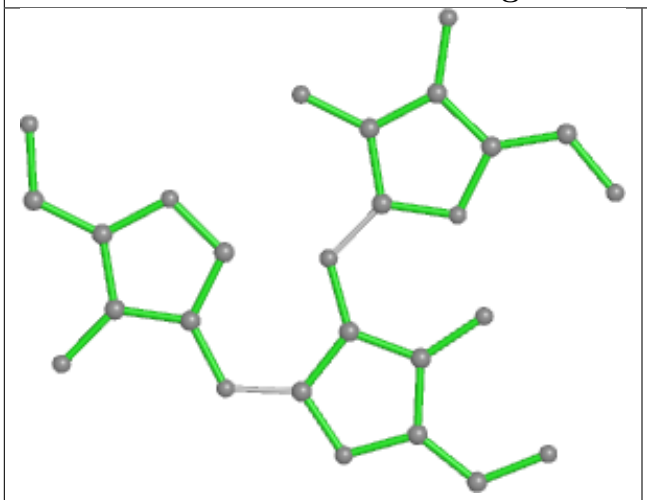


Rings

Oligosaccharide Chain t



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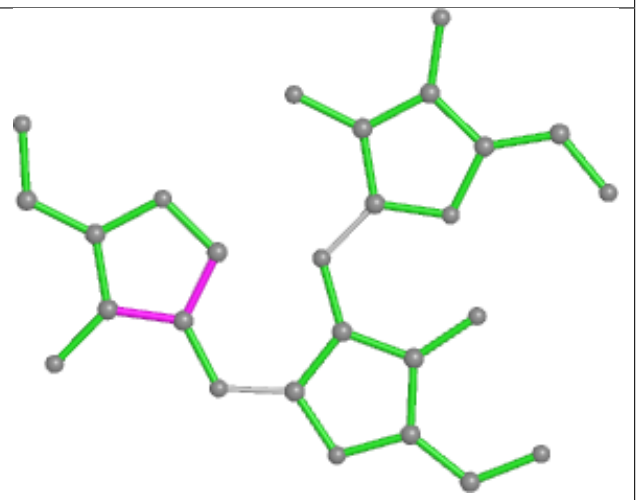

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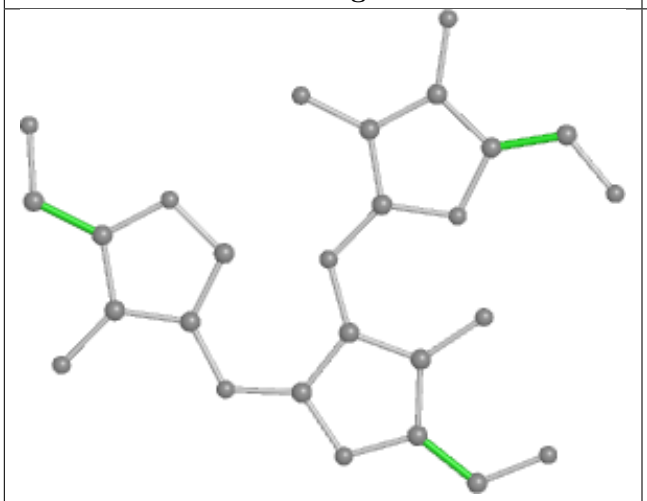

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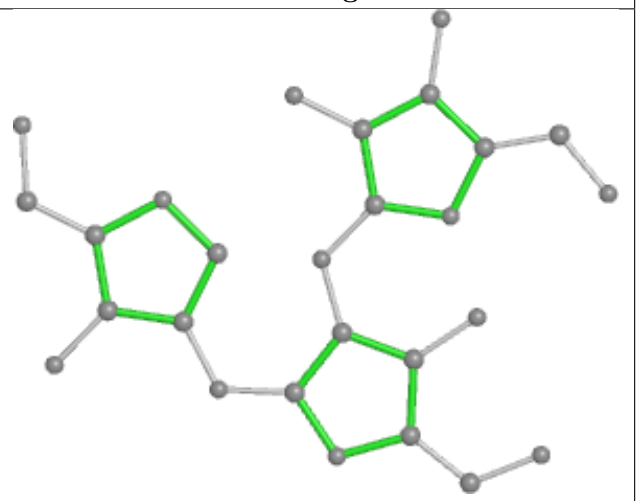
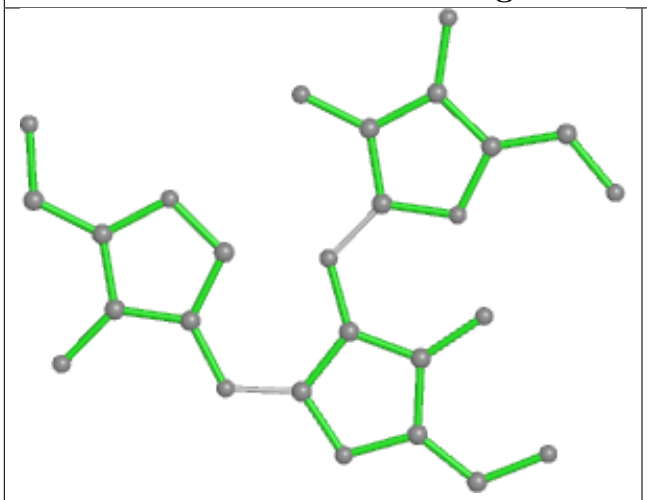


Rings

Oligosaccharide Chain w



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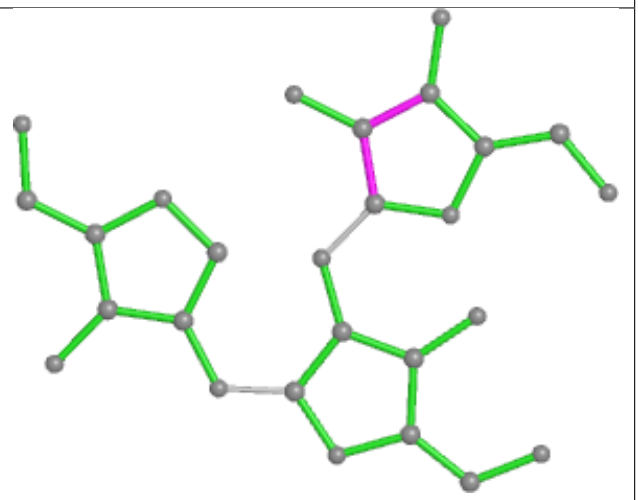

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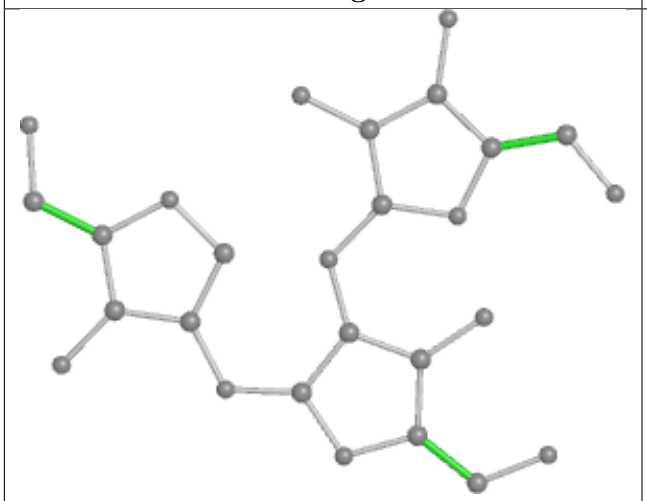

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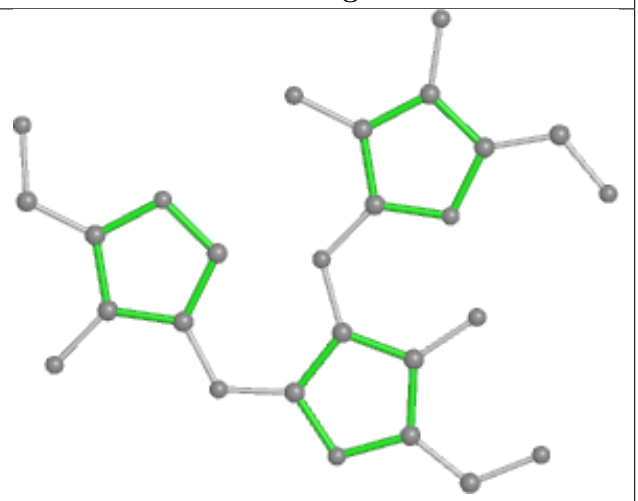
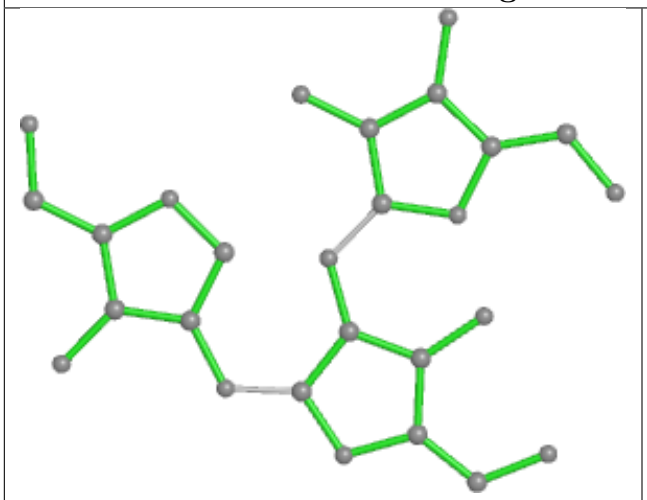


Rings

Oligosaccharide Chain x



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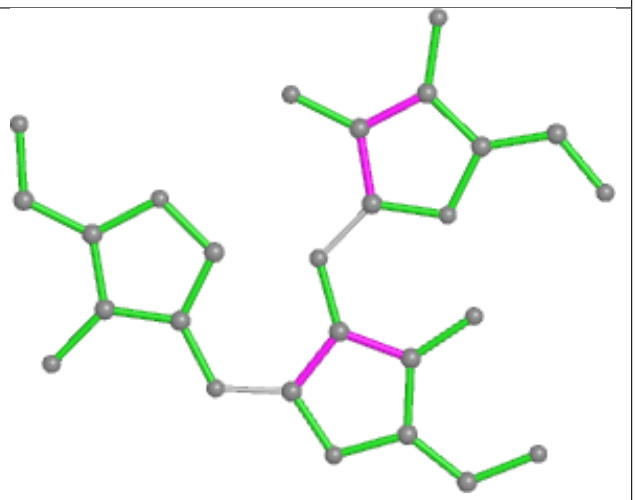

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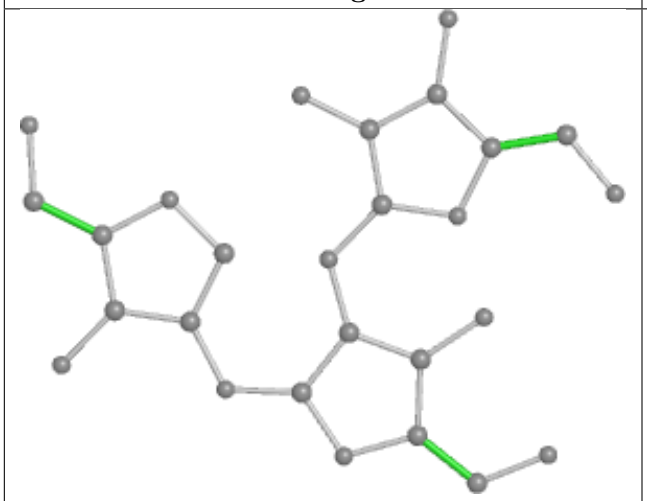

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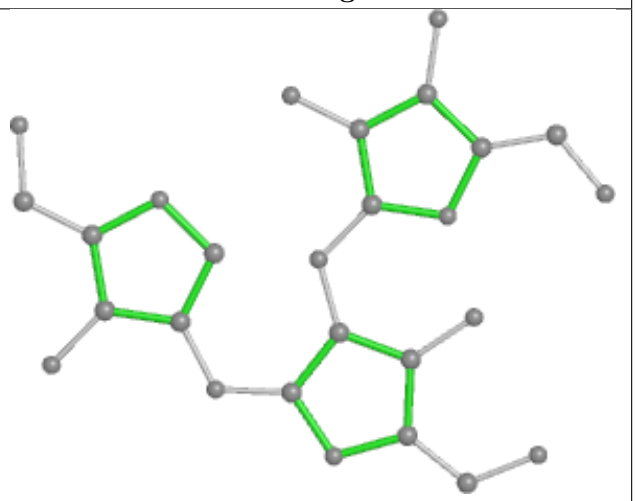
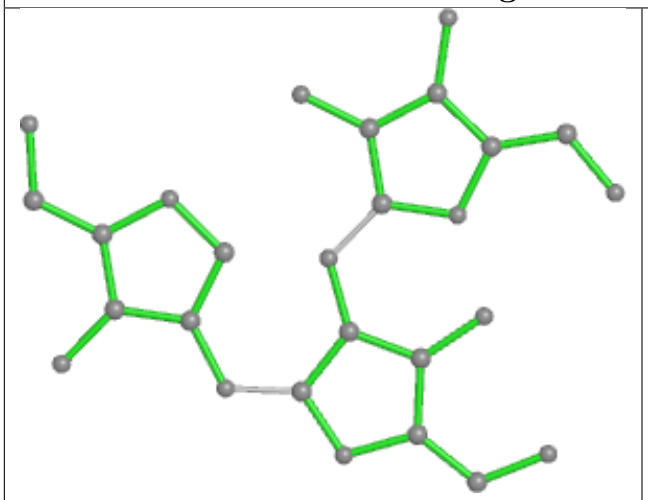


Rings

Oligosaccharide Chain y



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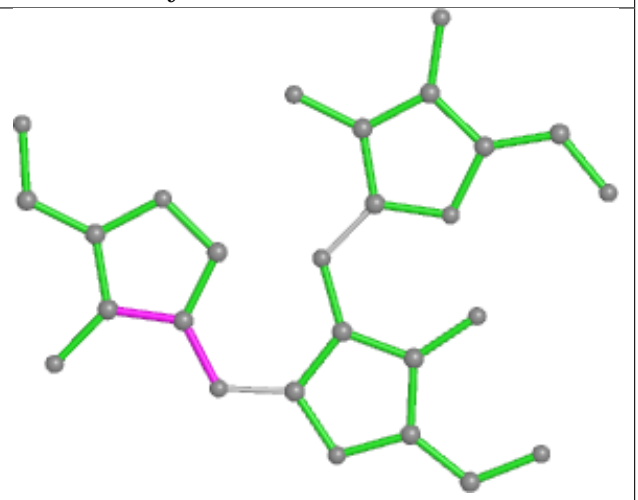

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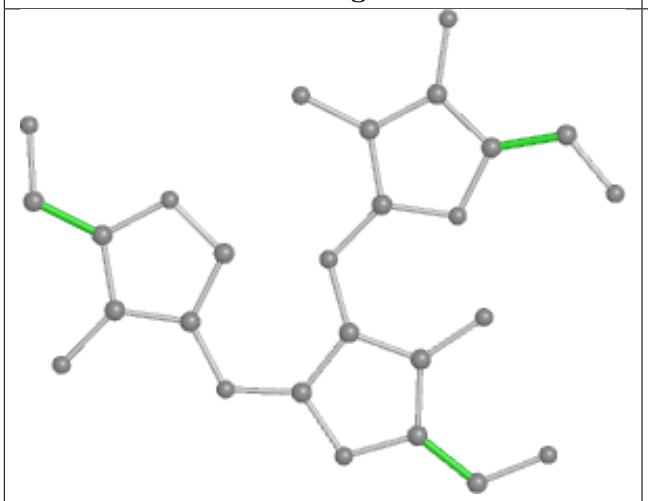

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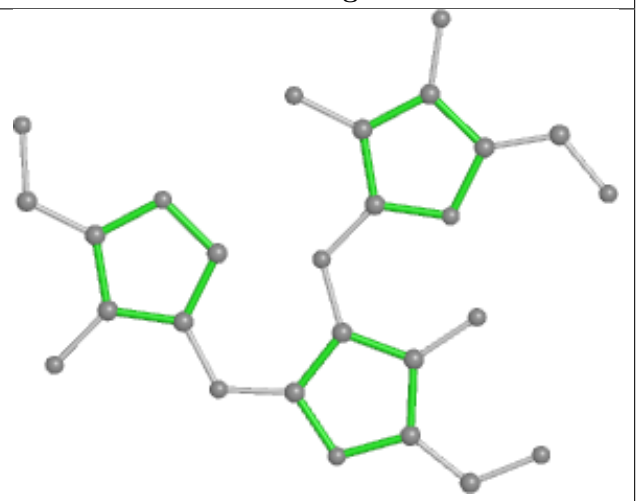

Rings

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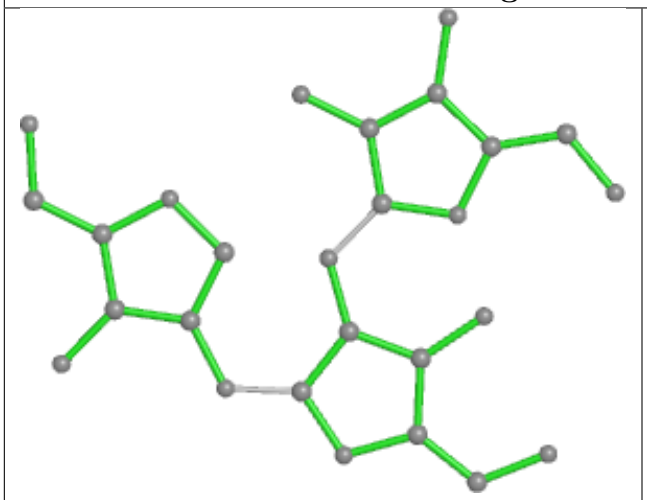

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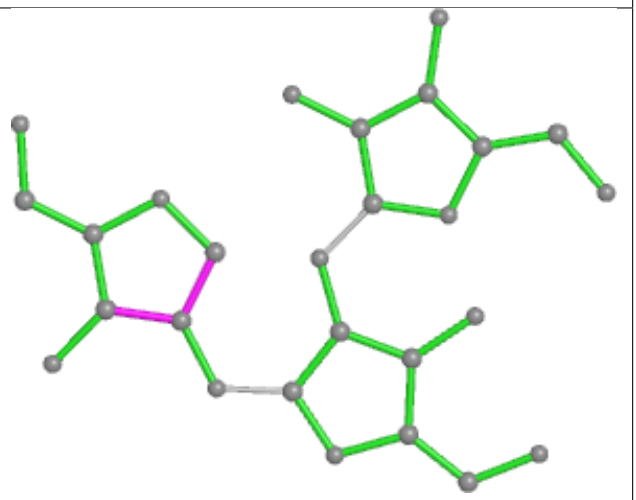
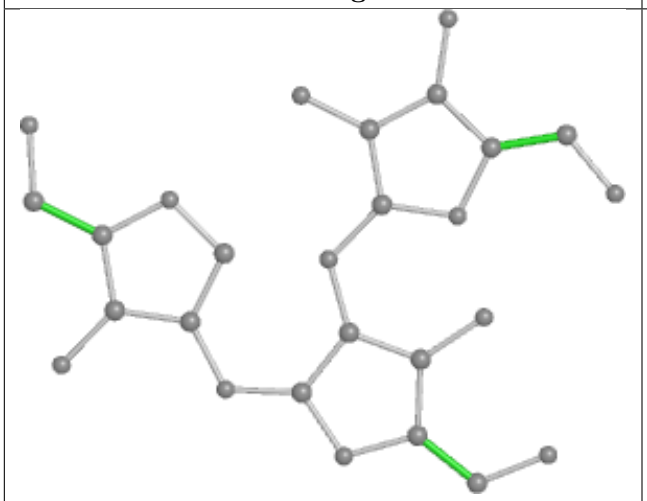


Bond angles



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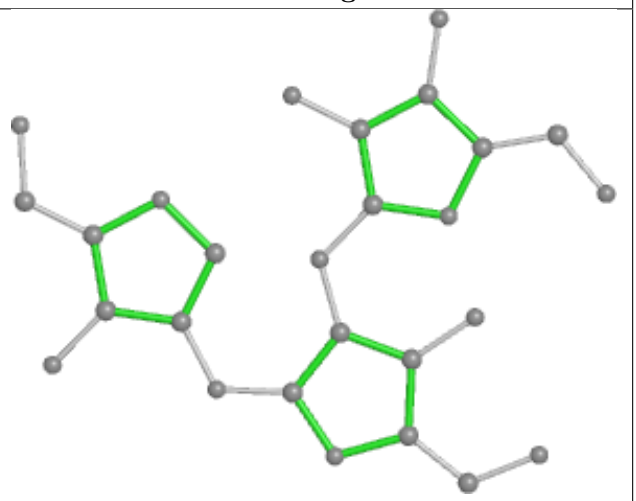

Rings

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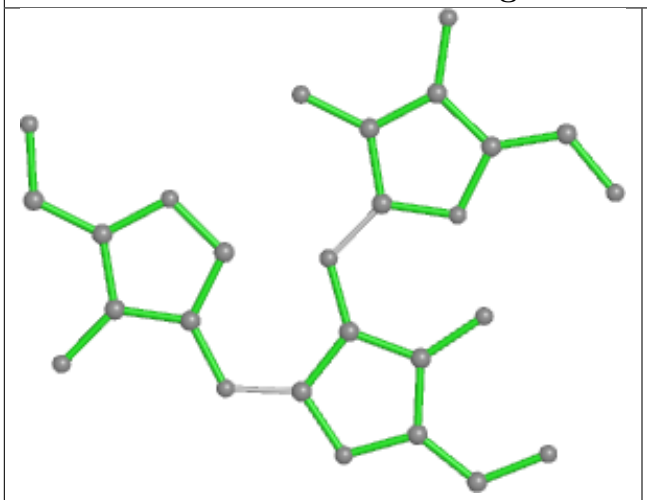

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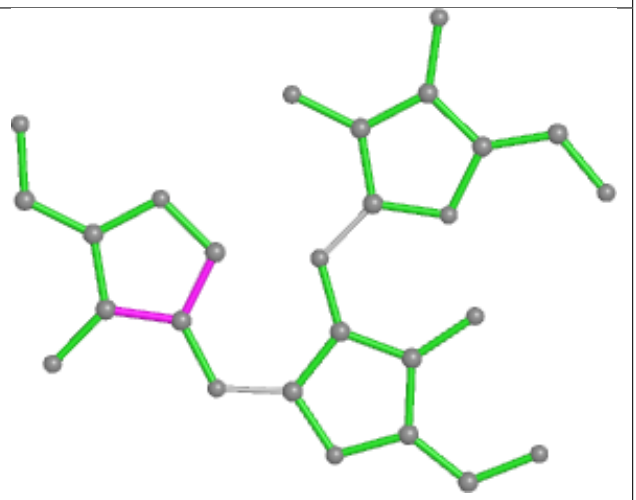

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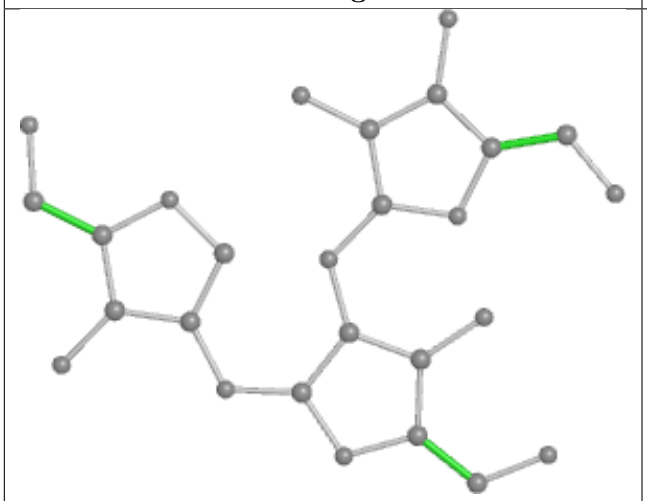

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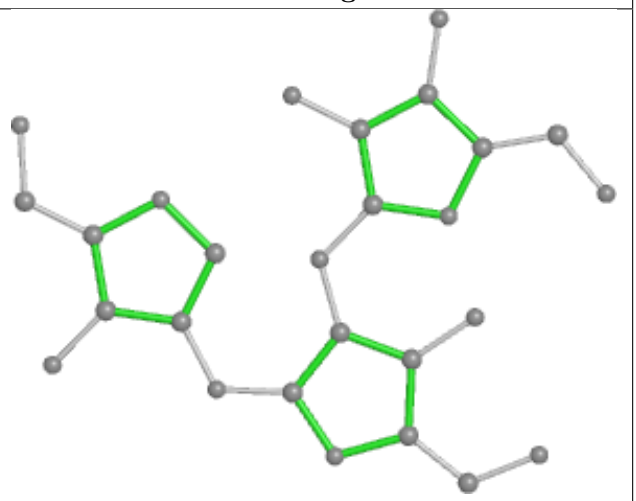
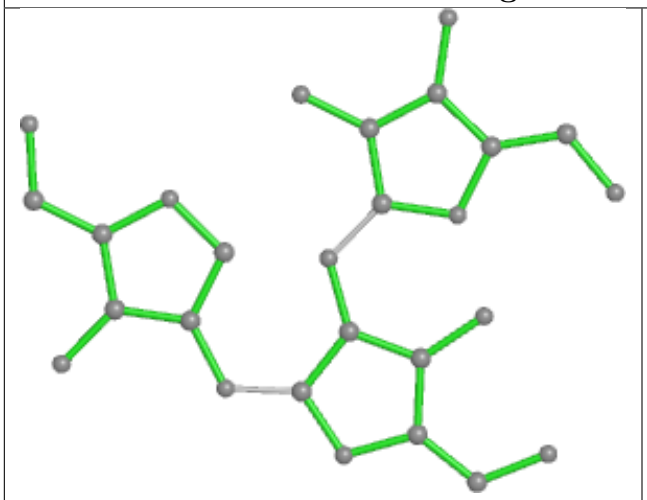


Rings

Oligosaccharide Chain 1



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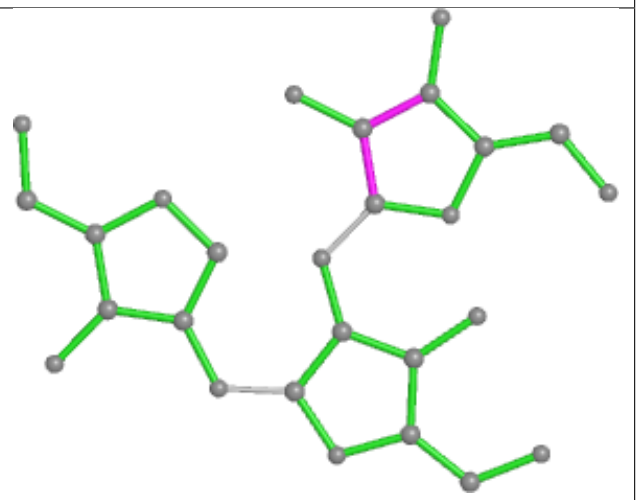

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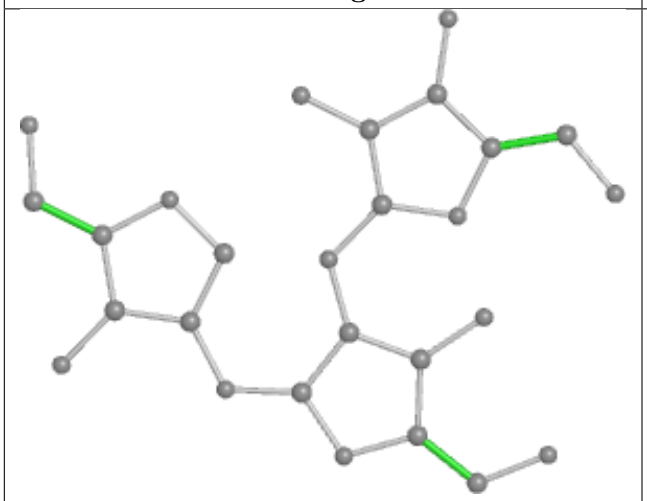

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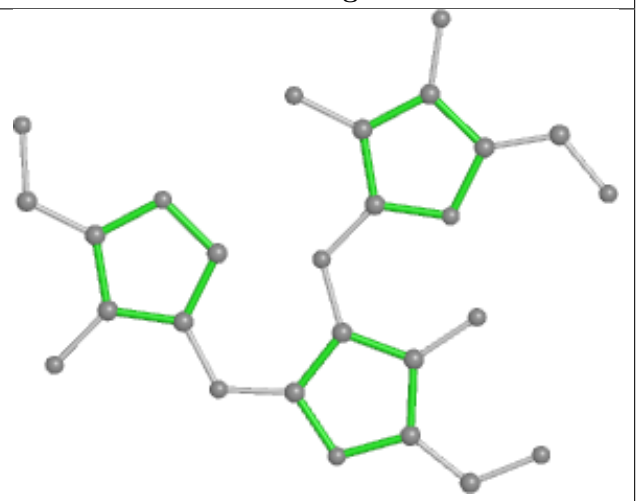
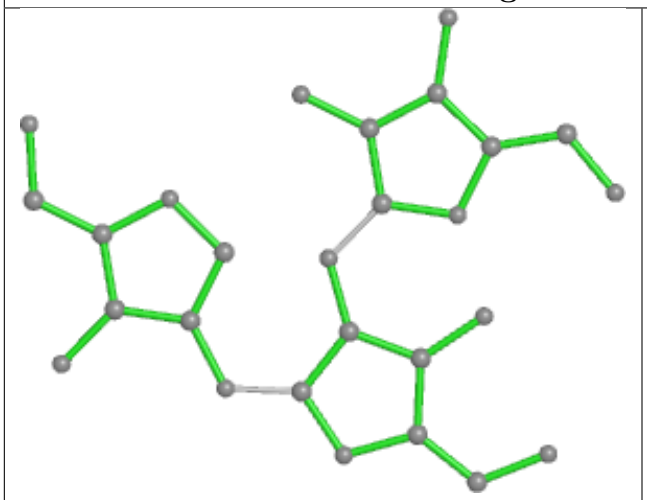


Rings

Oligosaccharide Chain 2



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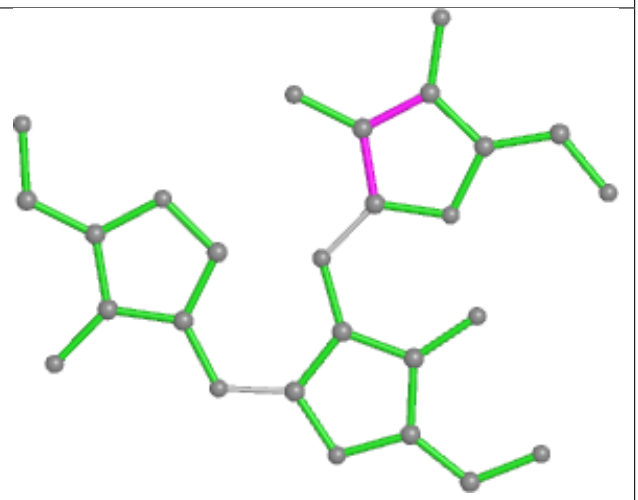

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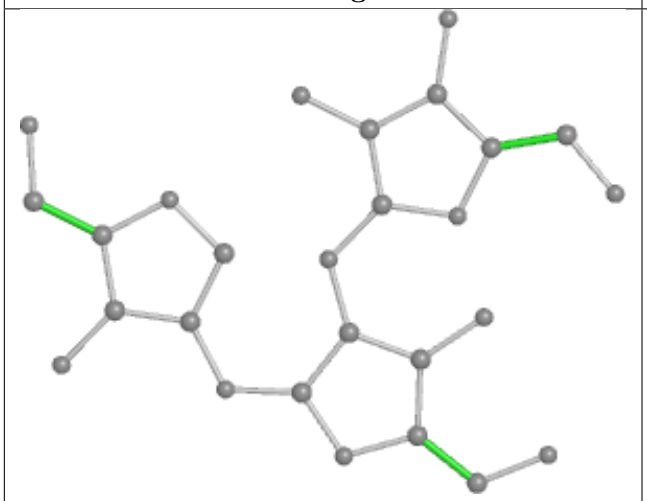

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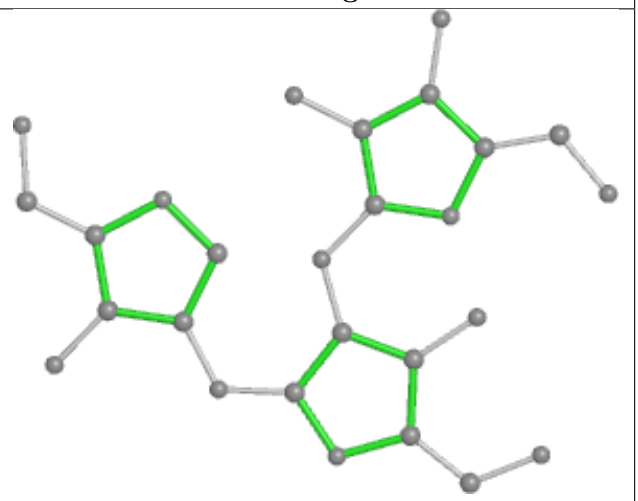
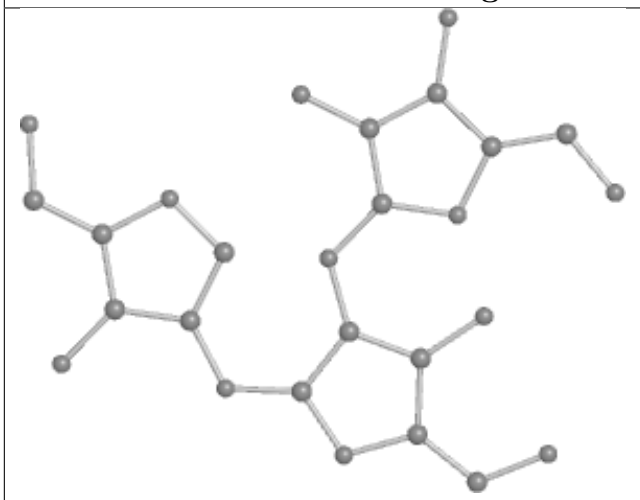
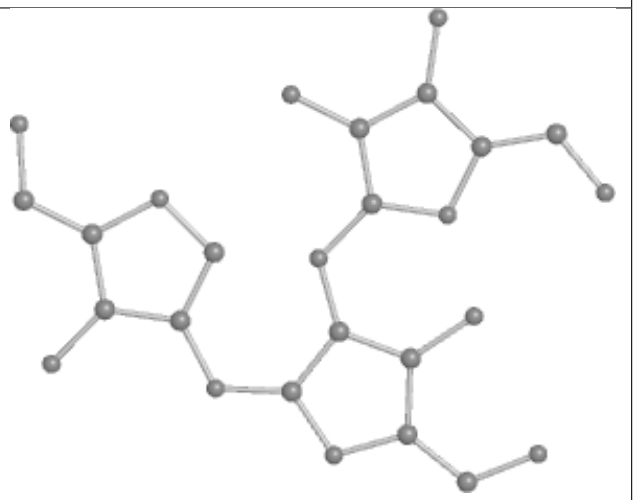
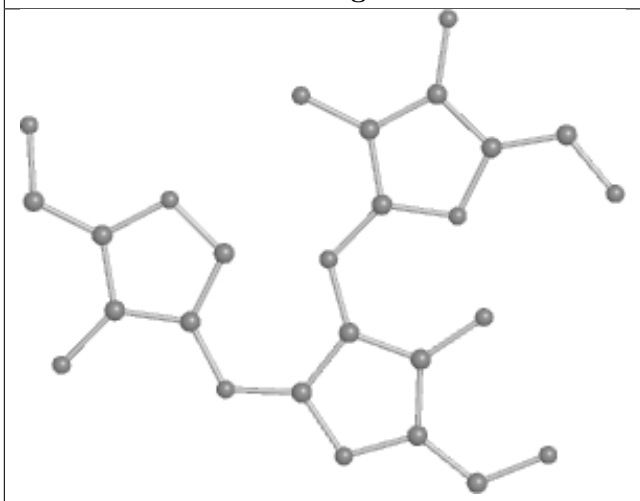
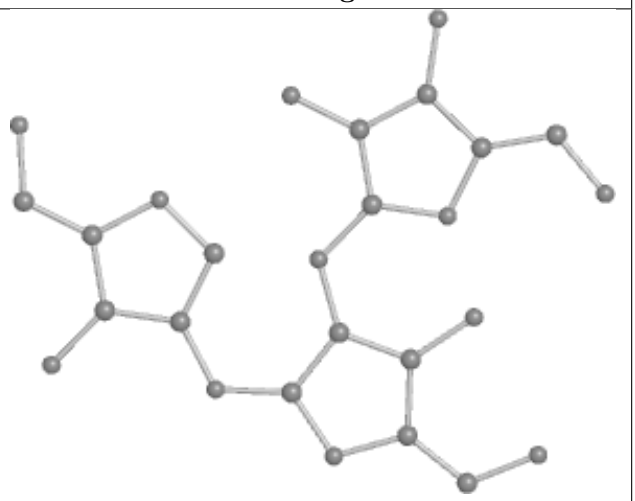
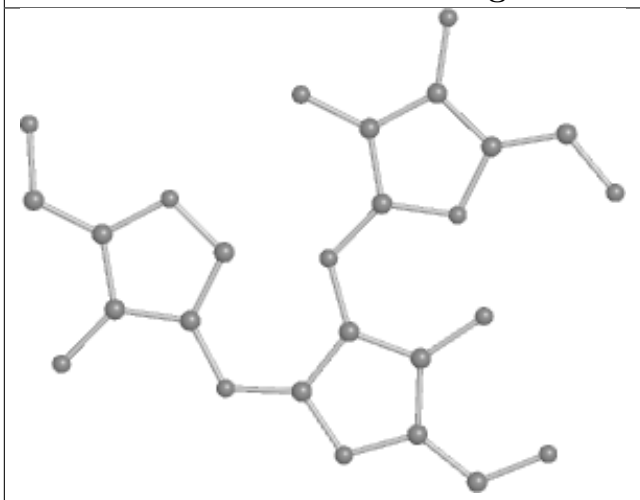
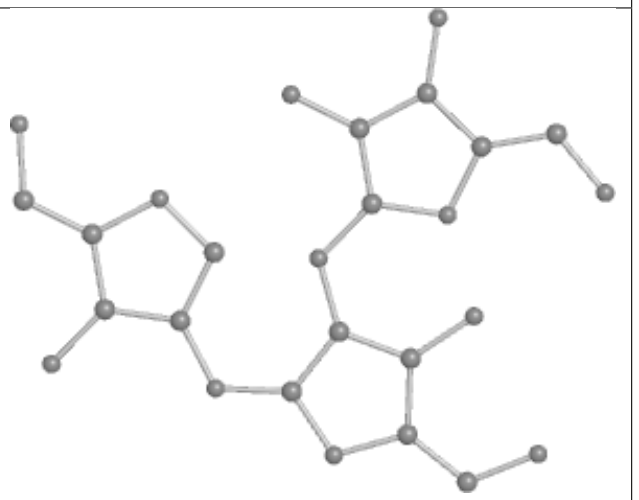
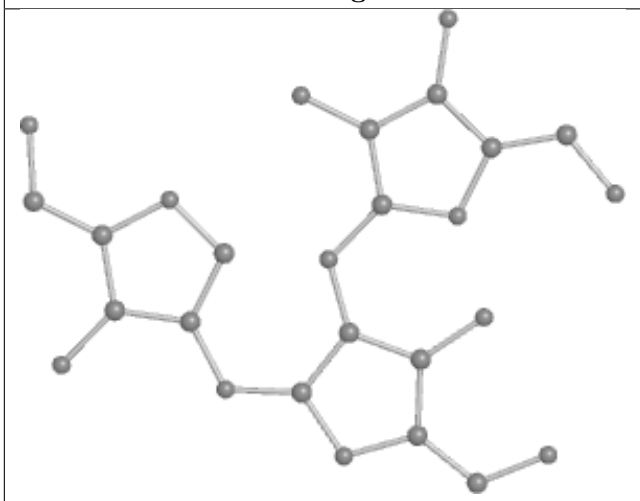
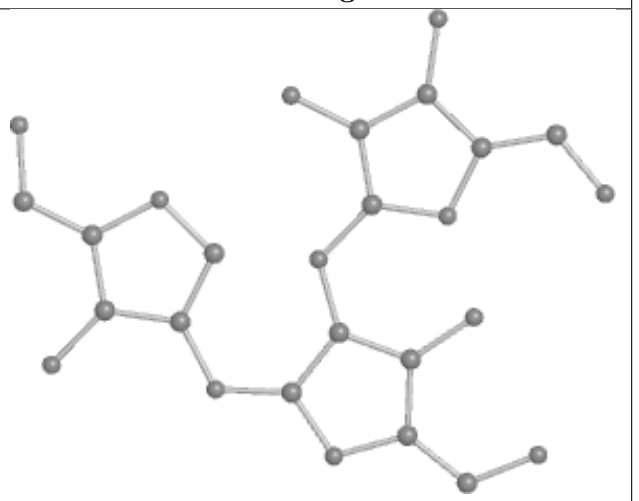
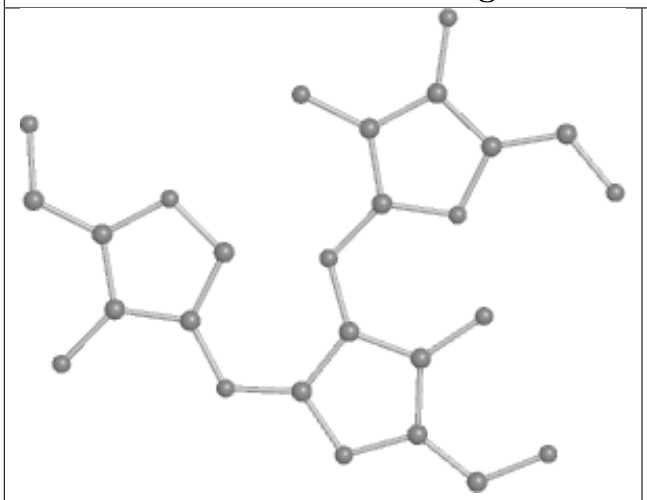


Rings

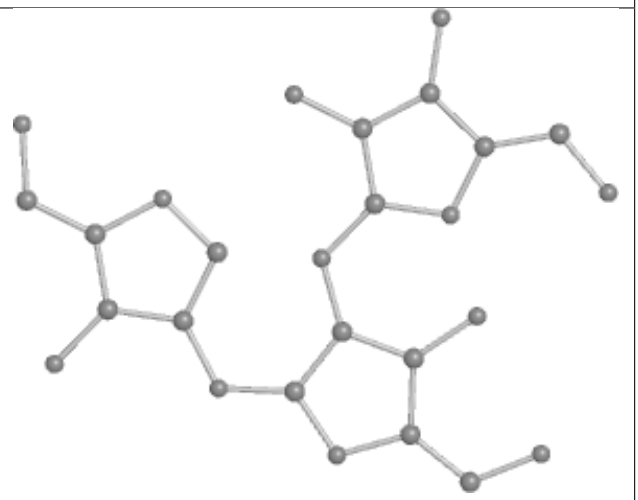
Oligosaccharide Chain HA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain IA	
 Bond lengths	 Bond angles
 Torsions	 Rings

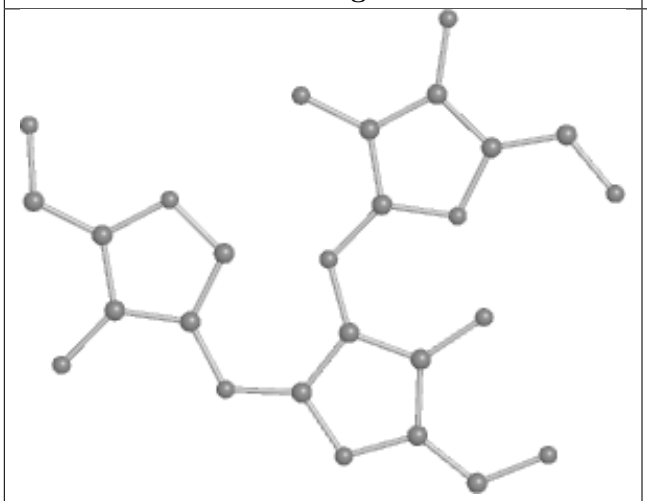
Oligosaccharide Chain MA



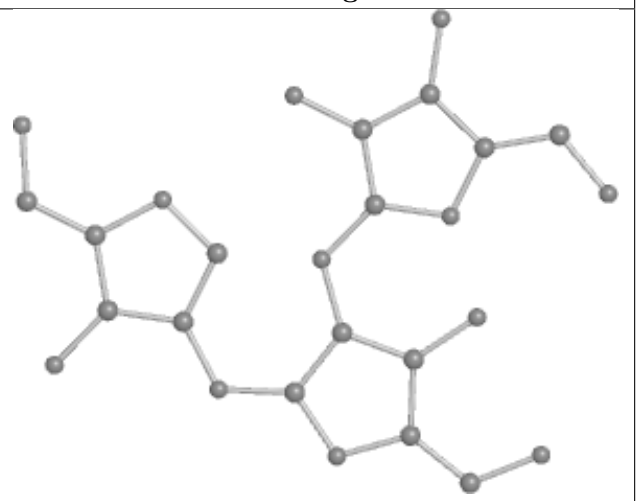
Bond lengths



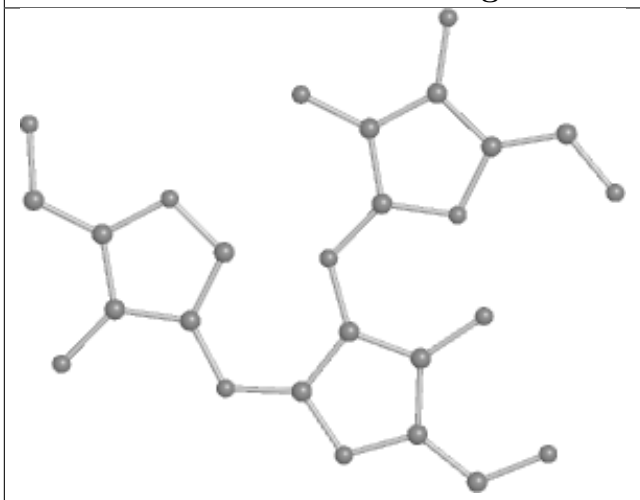
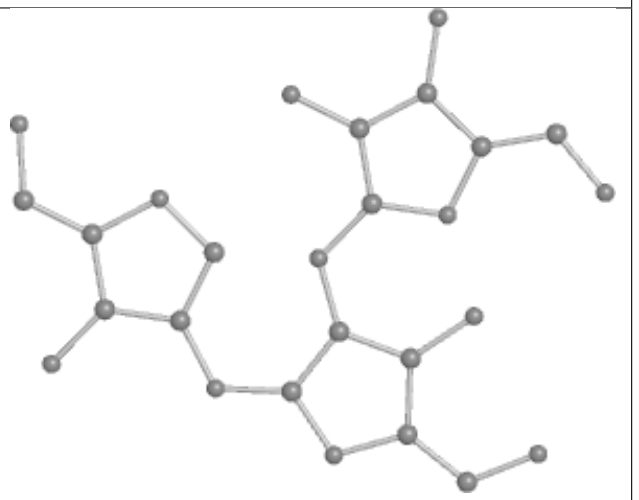
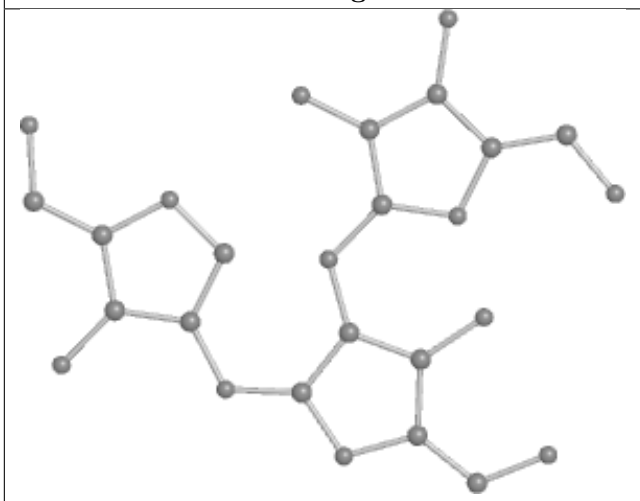
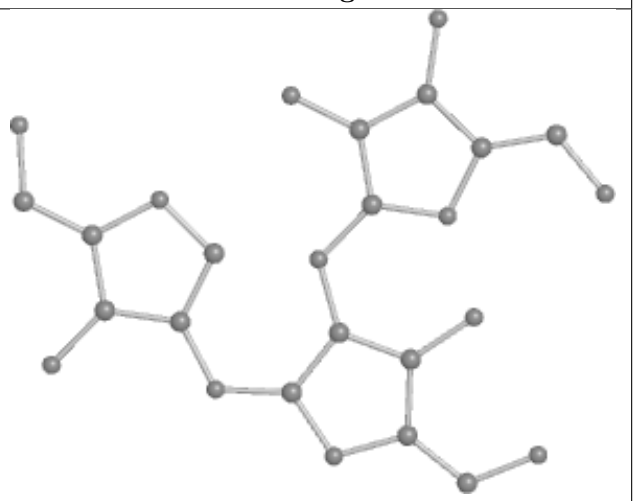
Bond angles

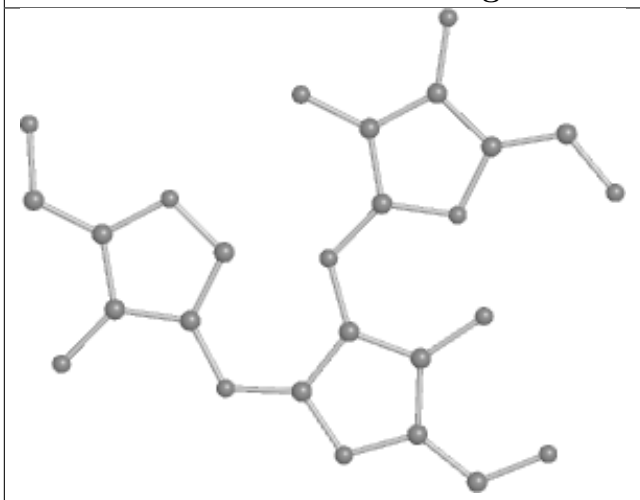
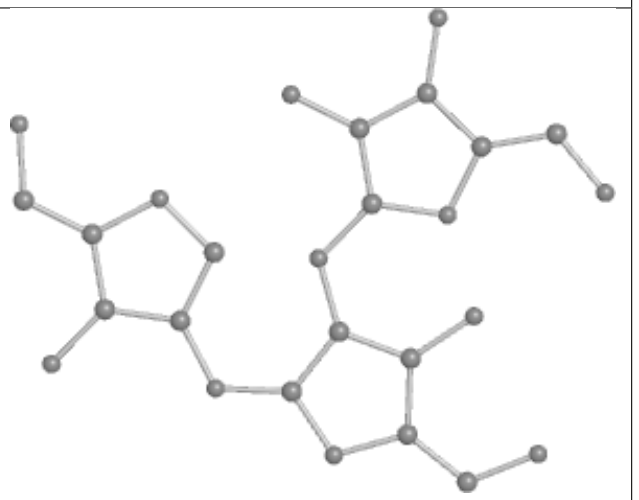
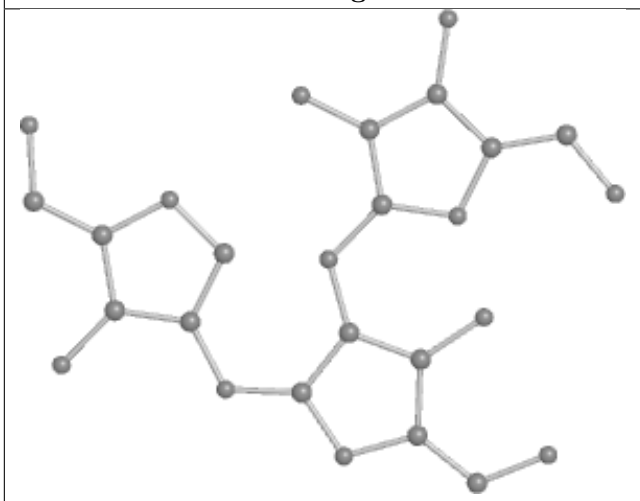
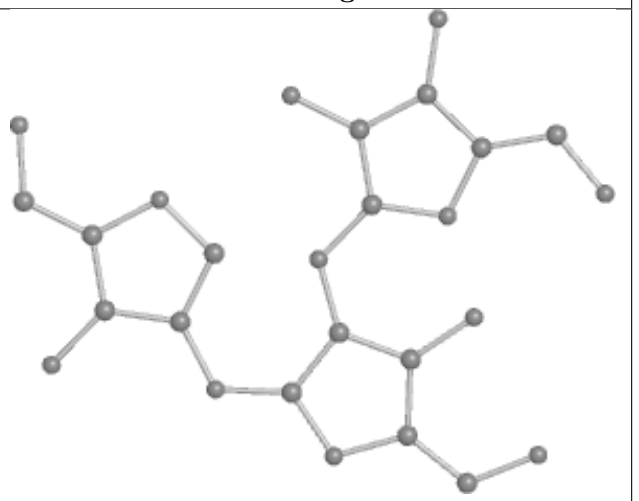


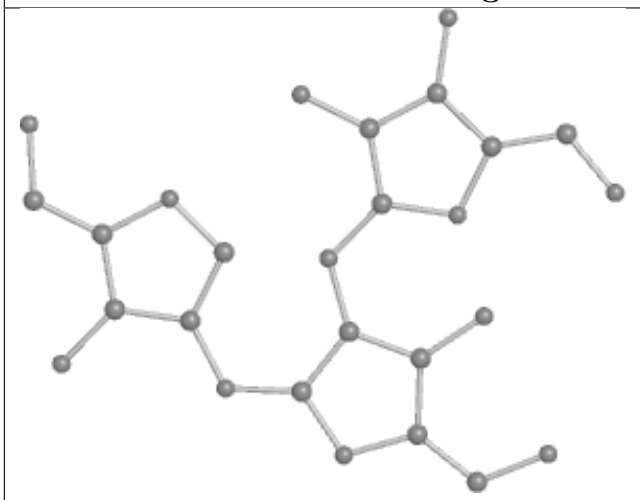
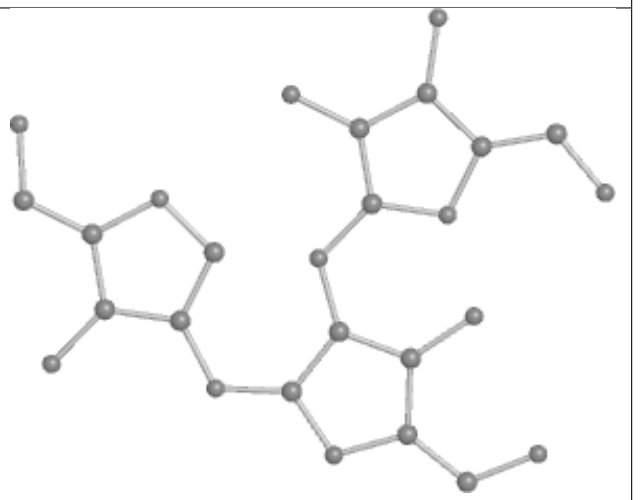
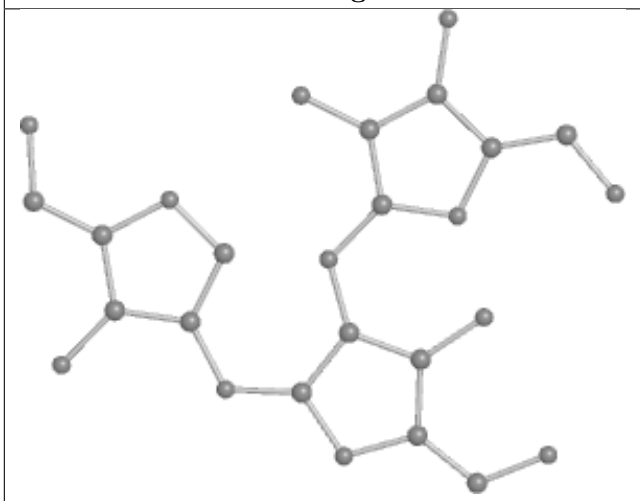
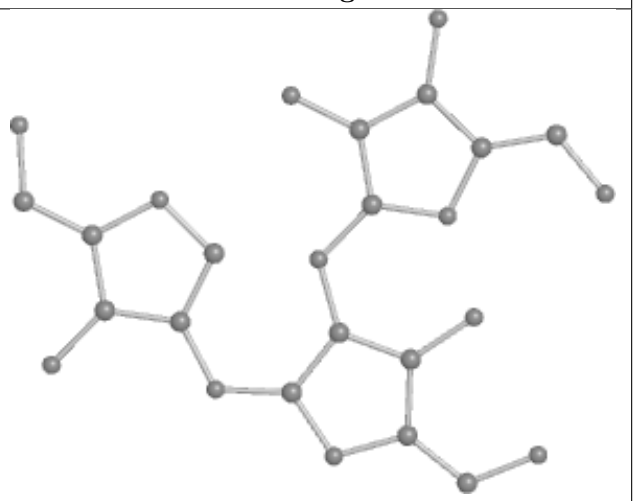
Torsions

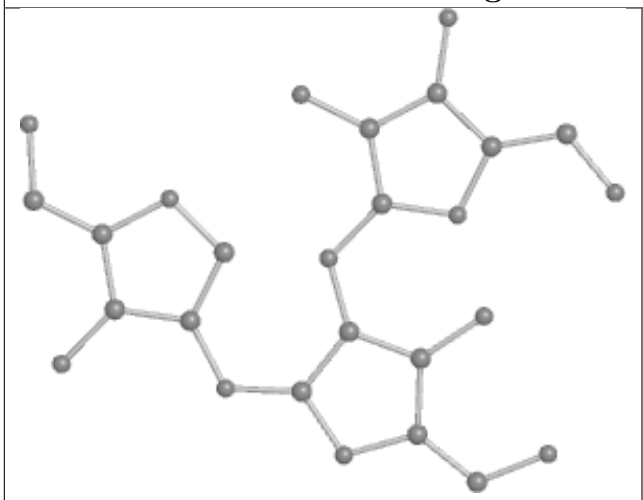
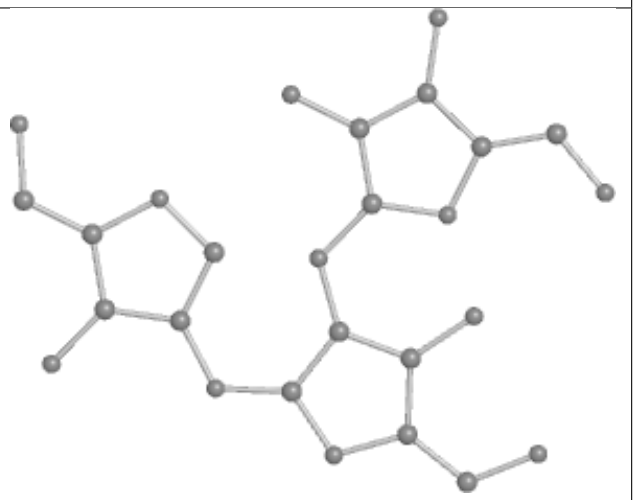
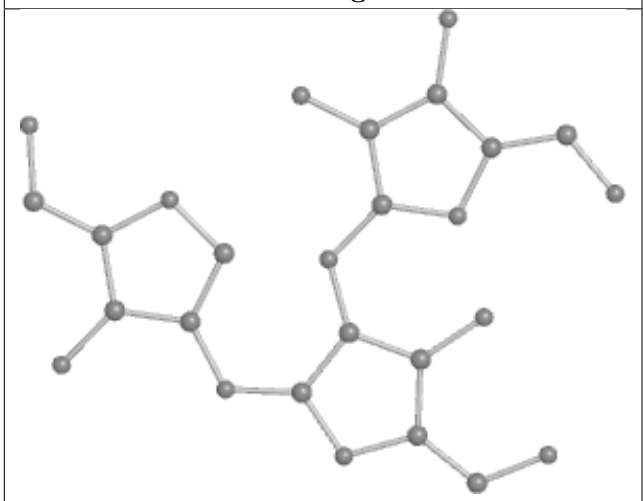
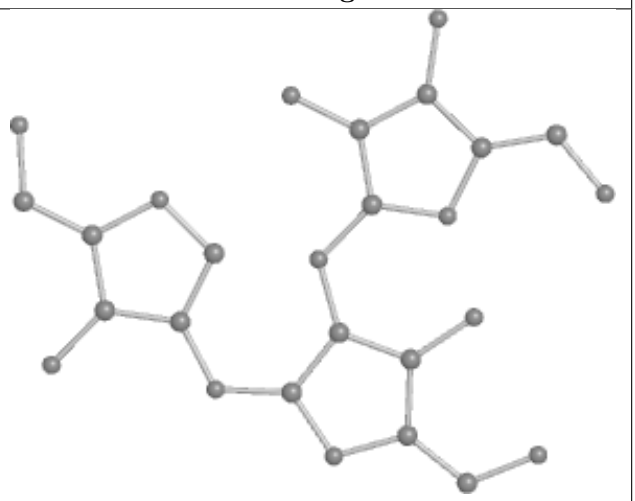


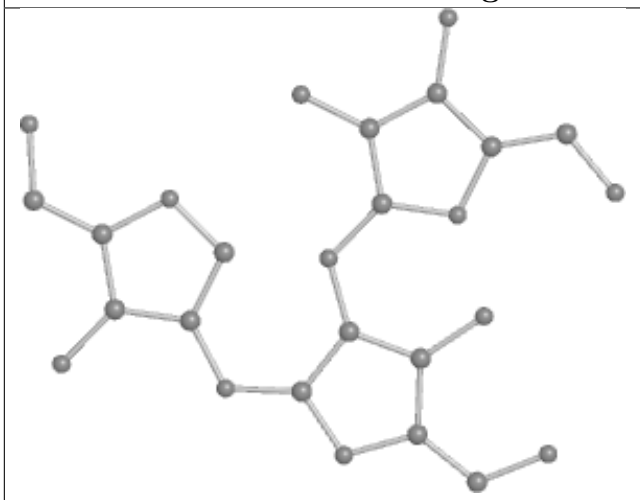
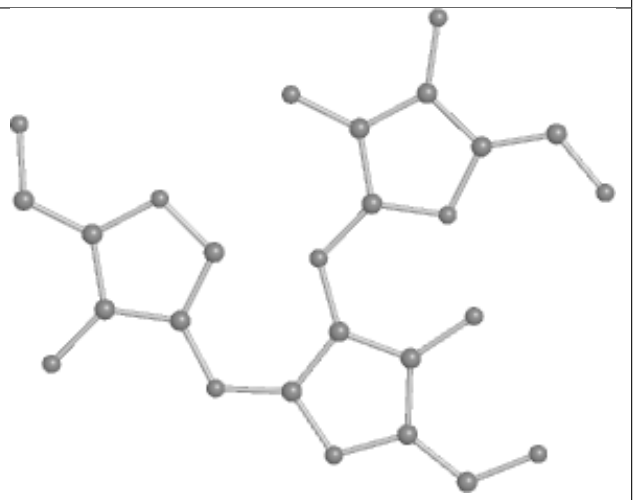
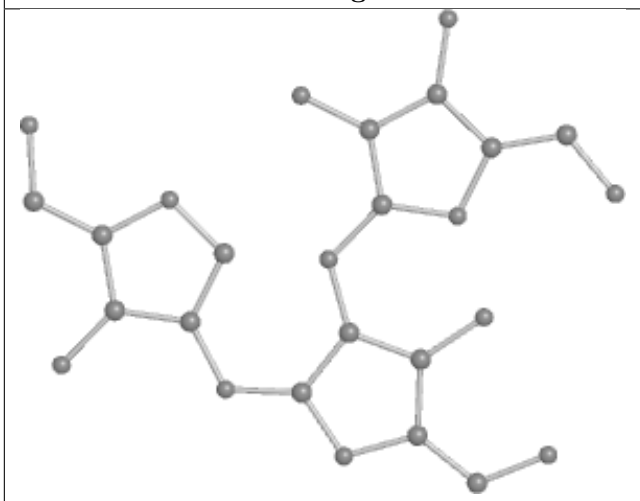
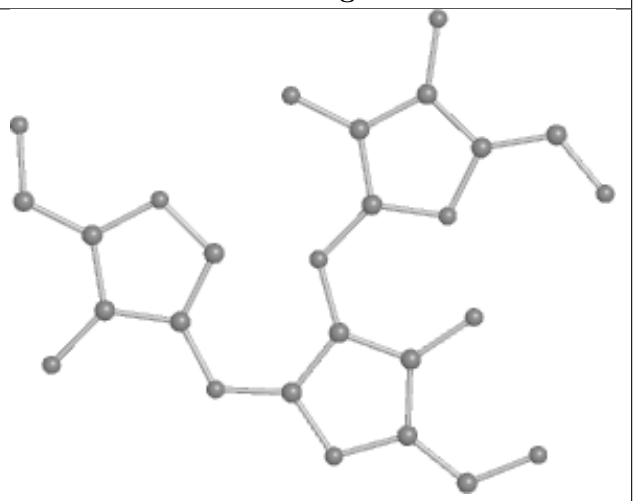
Rings

Oligosaccharide Chain NA	
 Bond lengths	 Bond angles
 Torsions	 Rings

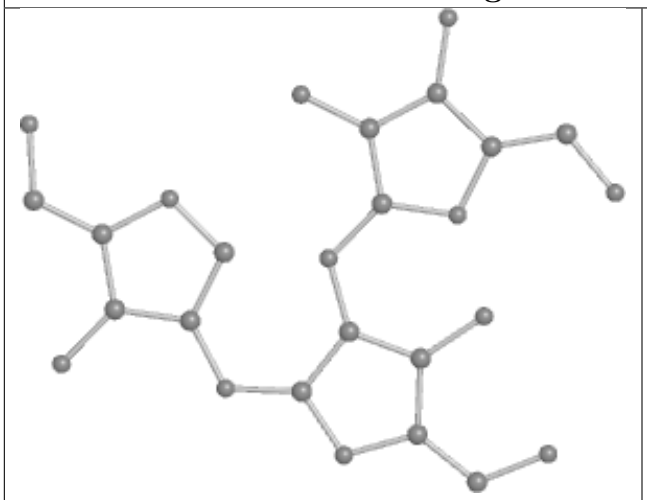
Oligosaccharide Chain OA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain RA	
 Bond lengths	 Bond angles
 Torsions	 Rings

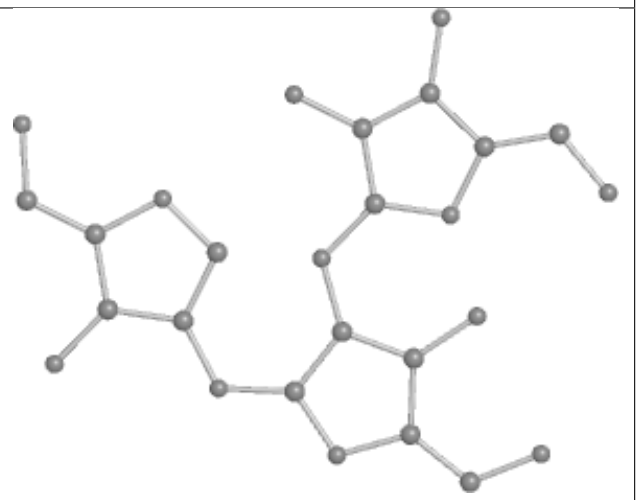
Oligosaccharide Chain TA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain XA	
 Bond lengths	 Bond angles
 Torsions	 Rings

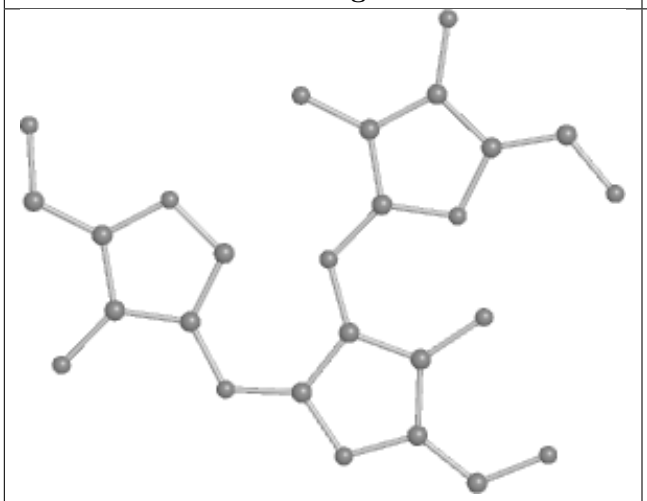
Oligosaccharide Chain ZA



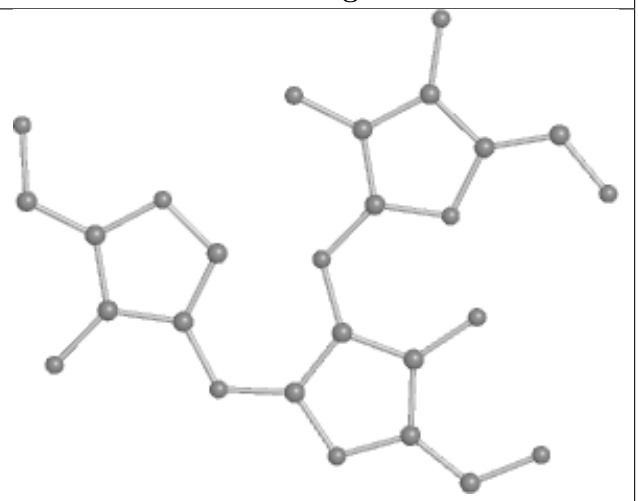
Bond lengths



Bond angles

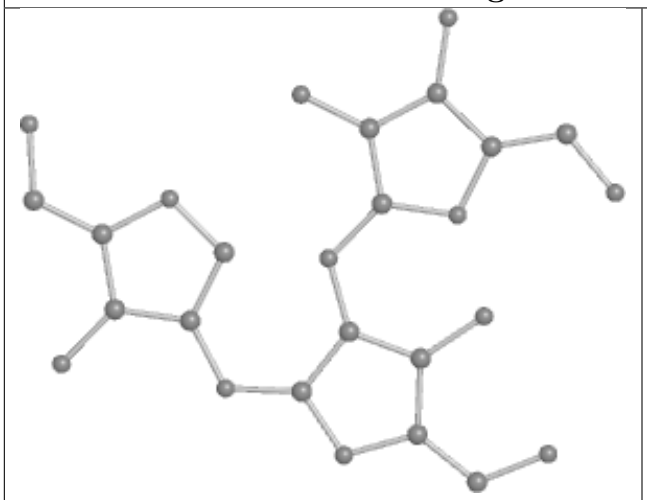


Torsions

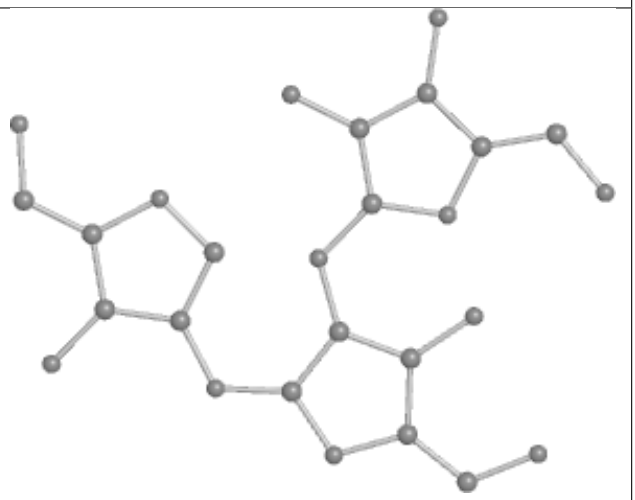


Rings

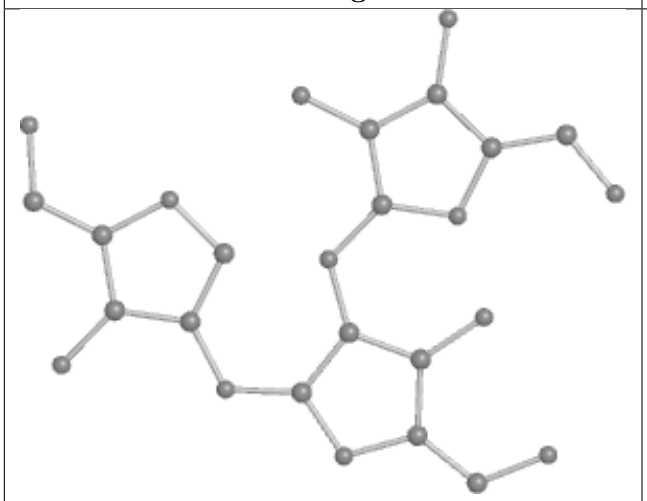
Oligosaccharide Chain cA



Bond lengths



Bond angles



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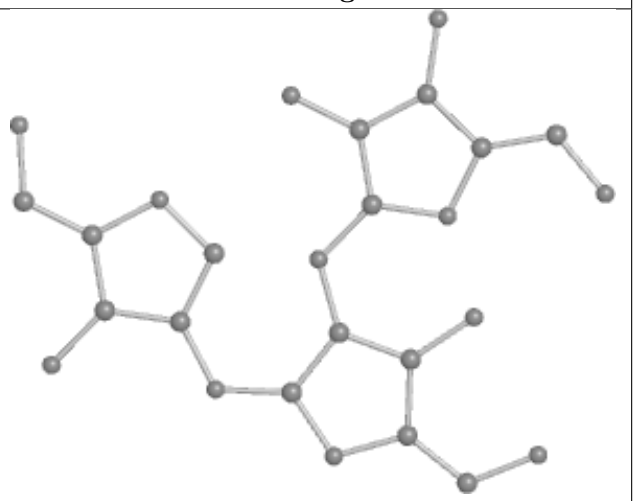
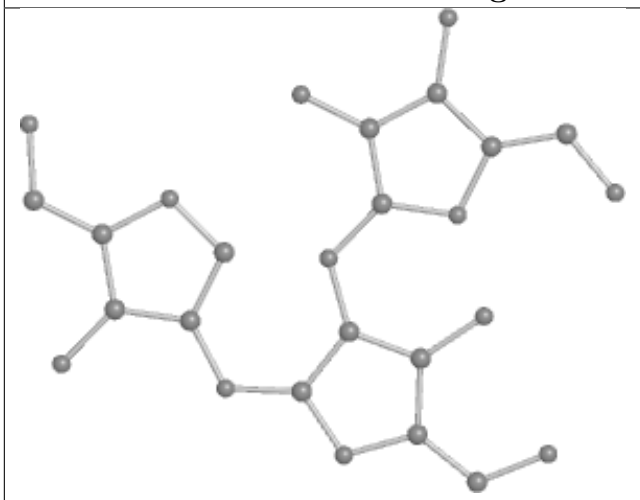
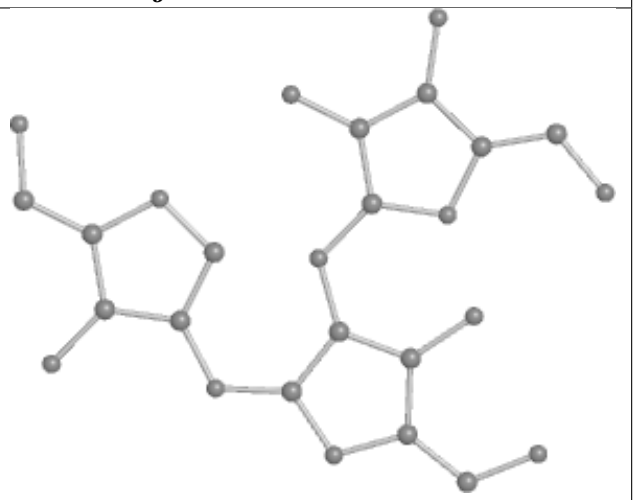
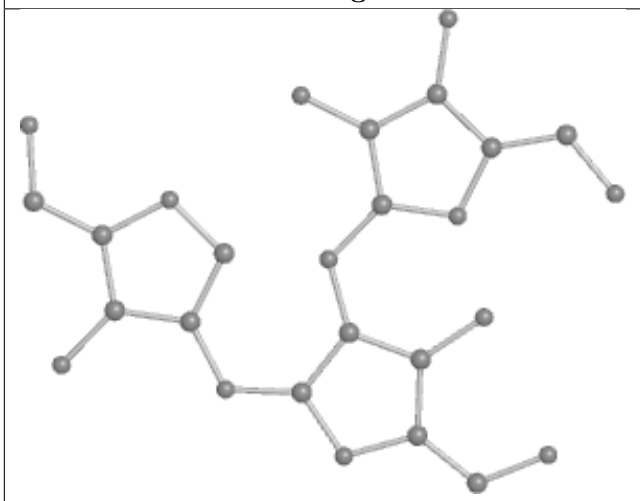
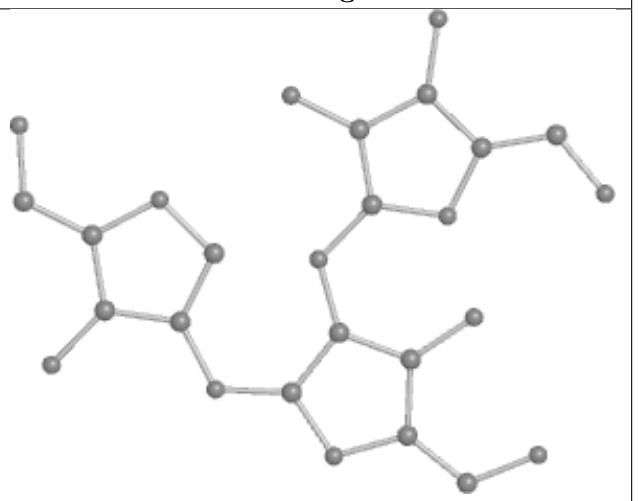
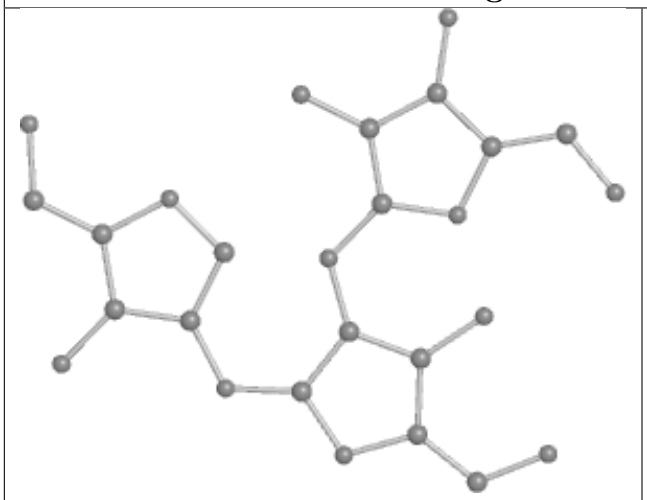


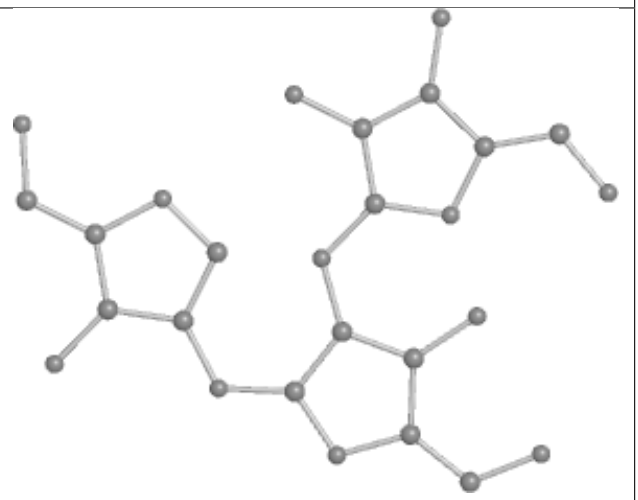
Rings

Oligosaccharide Chain jA	
 Bond lengths	 Bond angles
 Torsions	 Rings

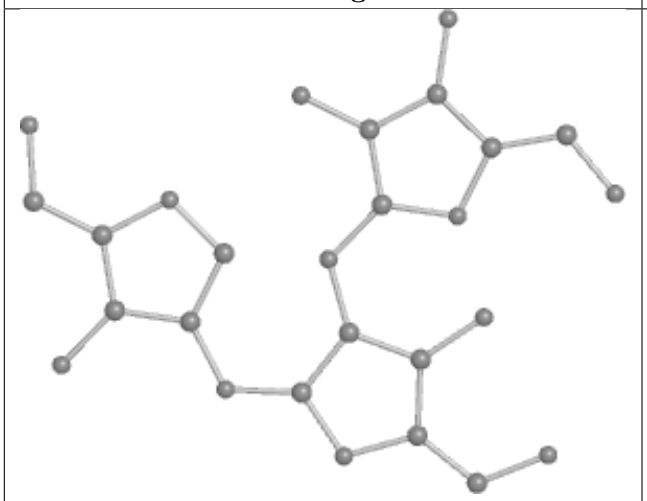
Oligosaccharide Chain kA



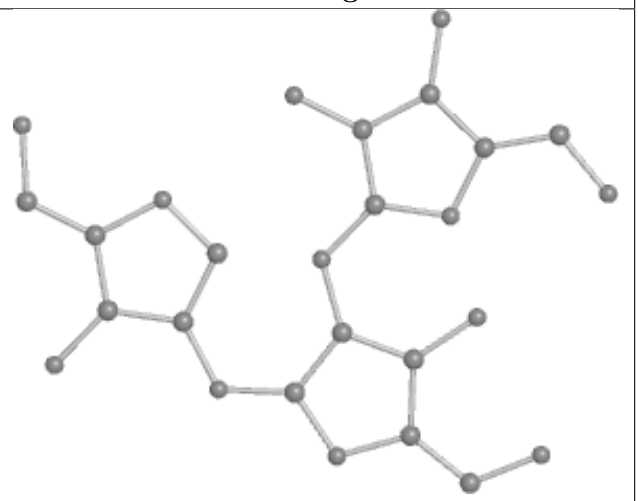
Bond lengths



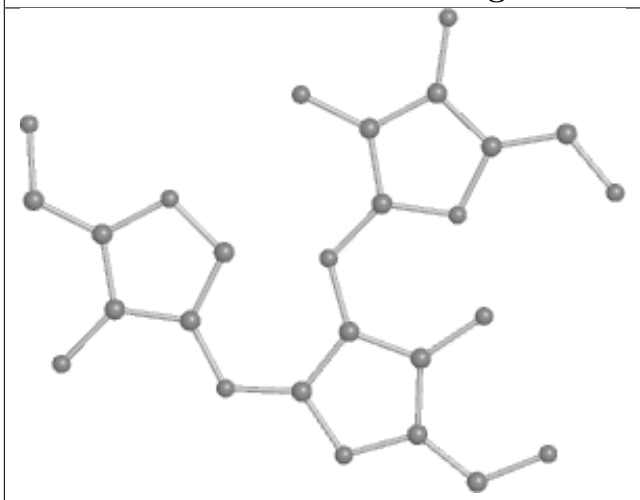
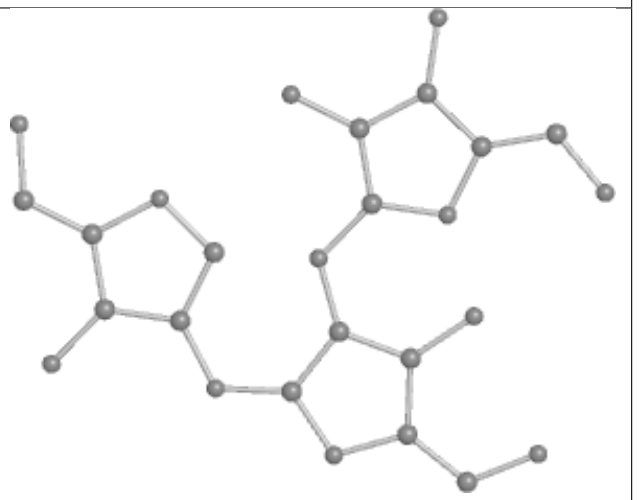
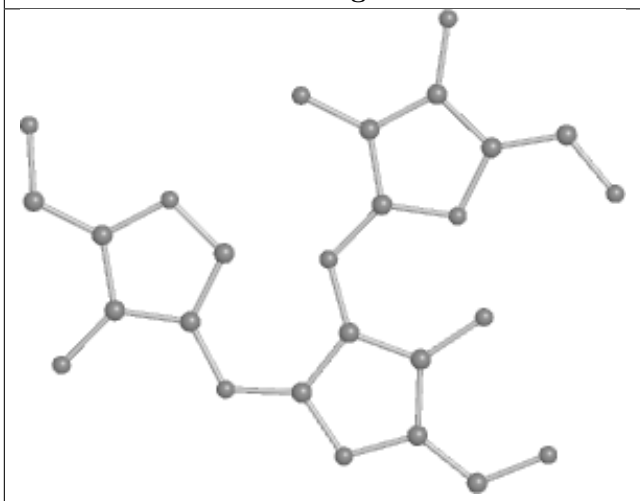
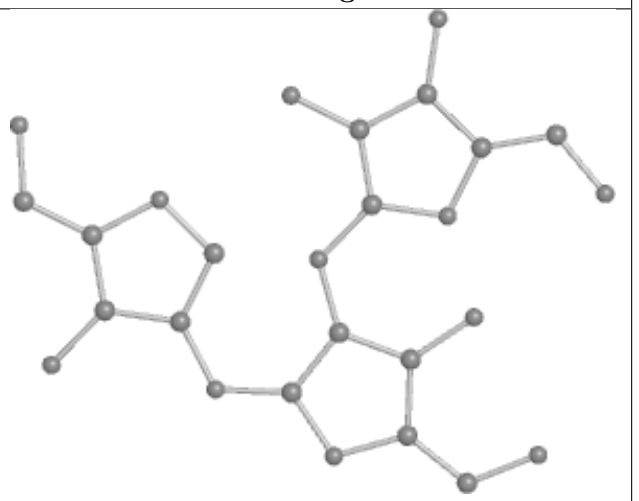
Bond angles



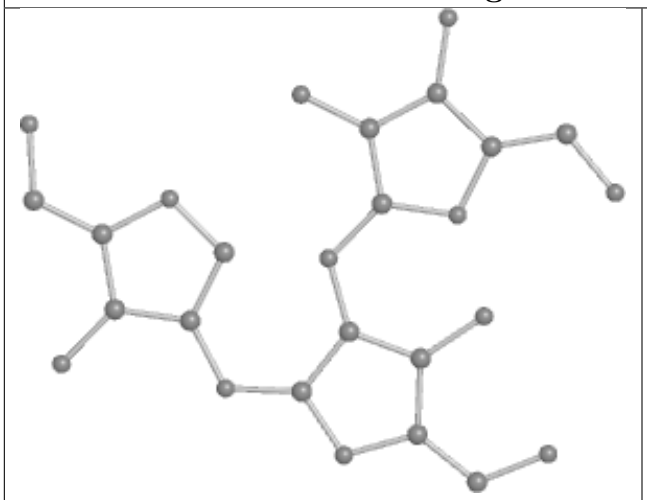
Torsions



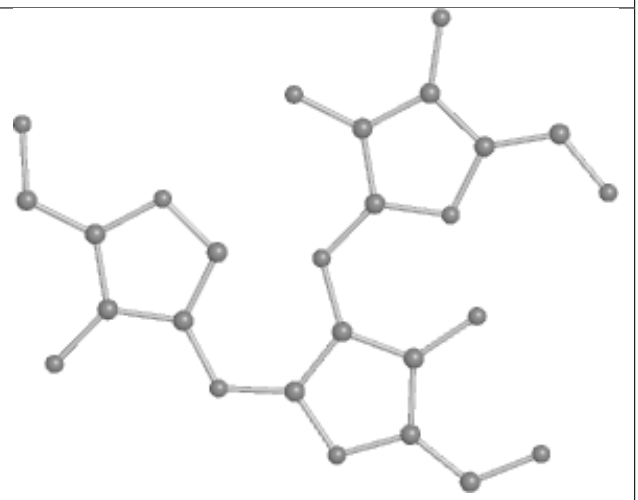
Rings

Oligosaccharide Chain rA	
 Bond lengths	 Bond angles
 Torsions	 Rings

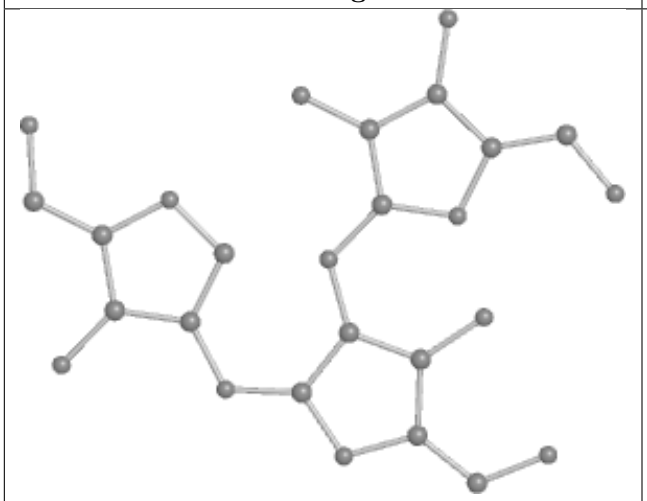
Oligosaccharide Chain uA



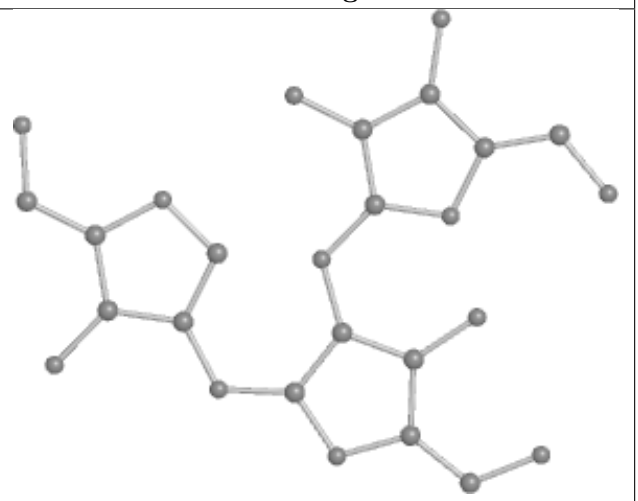
Bond lengths



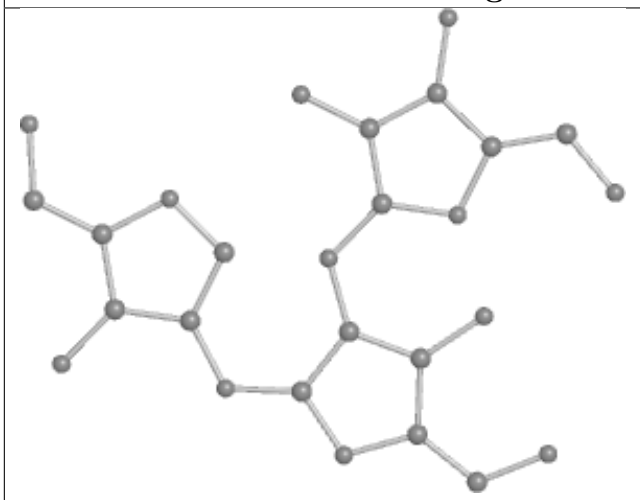
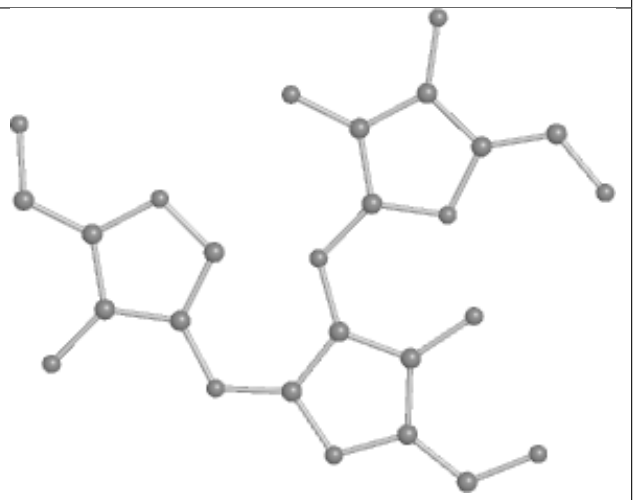
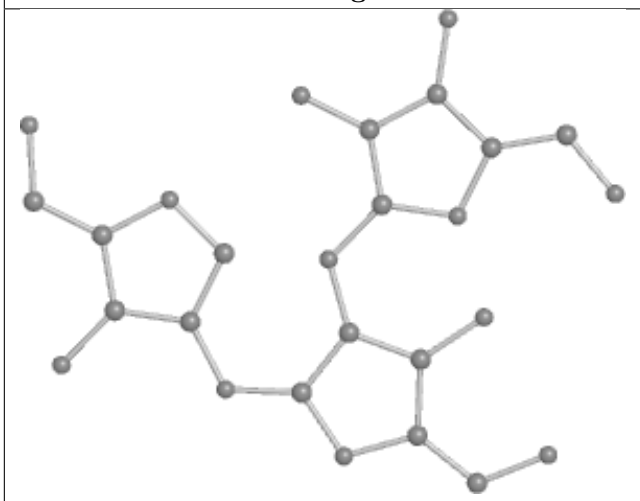
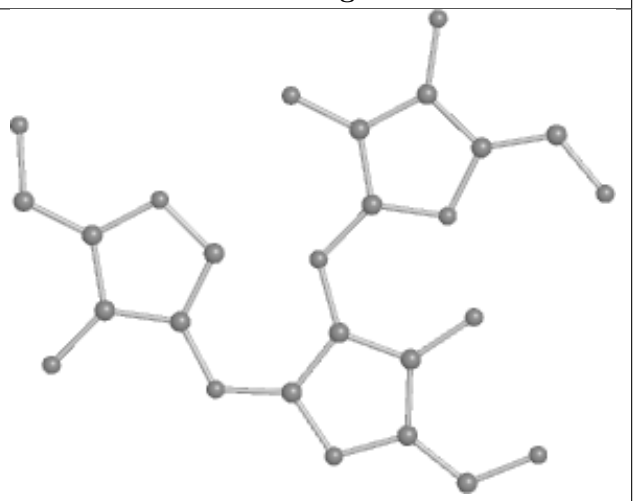
Bond angles



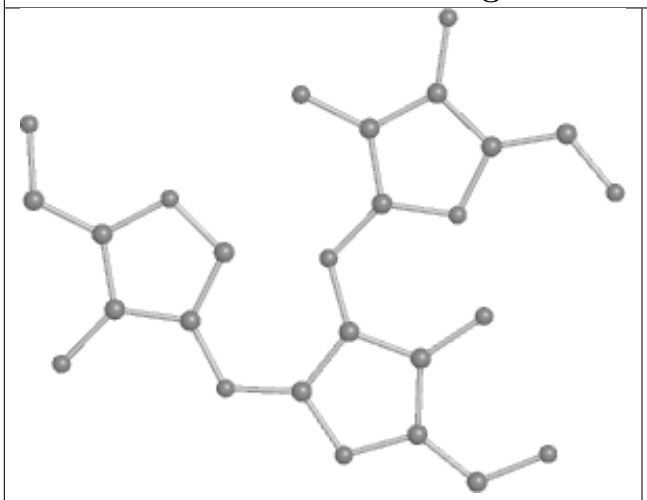
Torsions



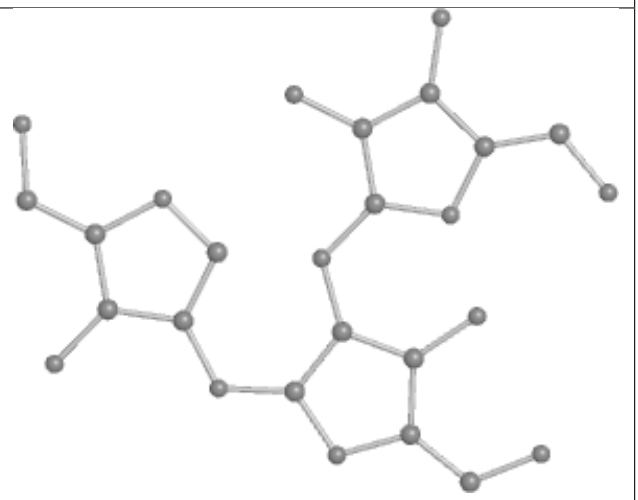
Rings

Oligosaccharide Chain vA	
 Bond lengths	 Bond angles
 Torsions	 Rings

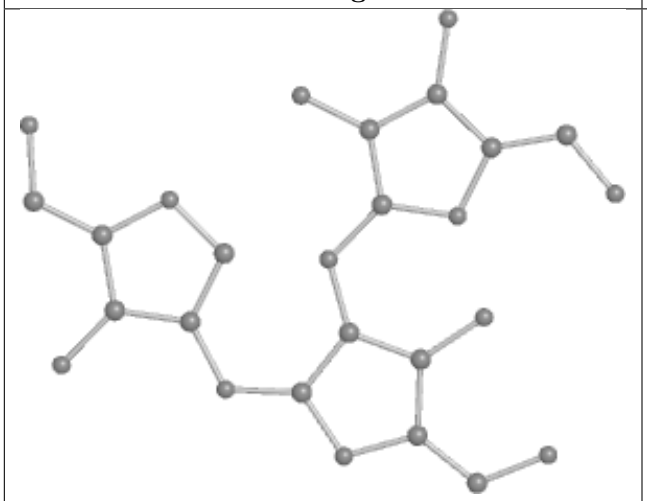
Oligosaccharide Chain wA



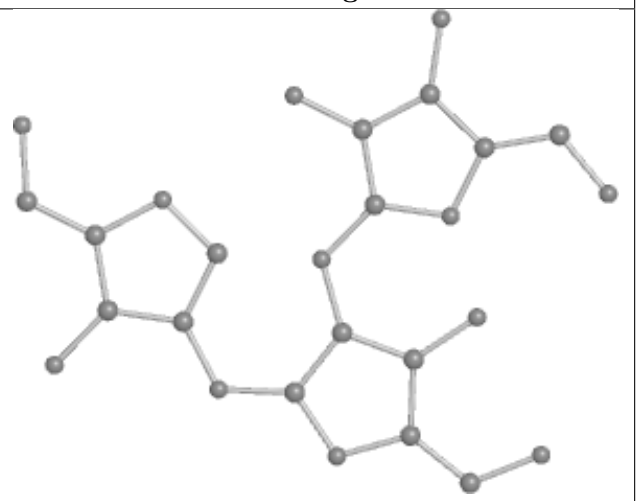
Bond lengths



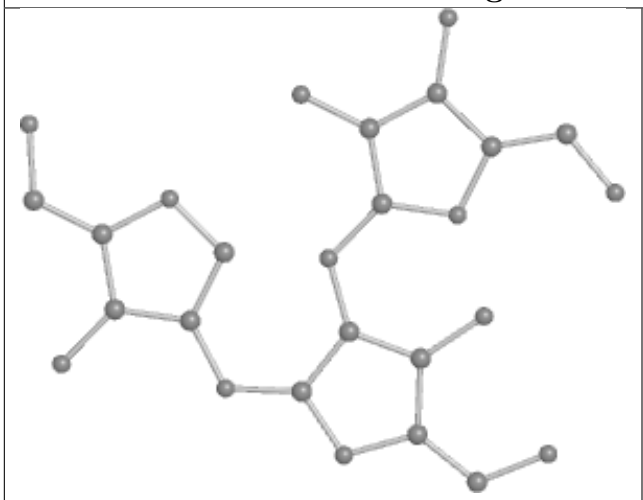
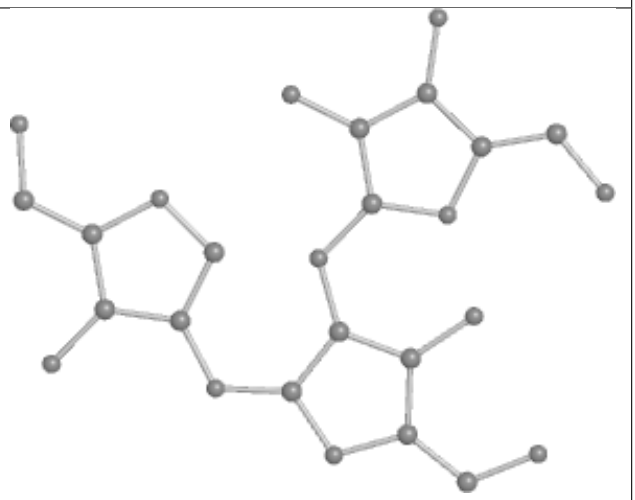
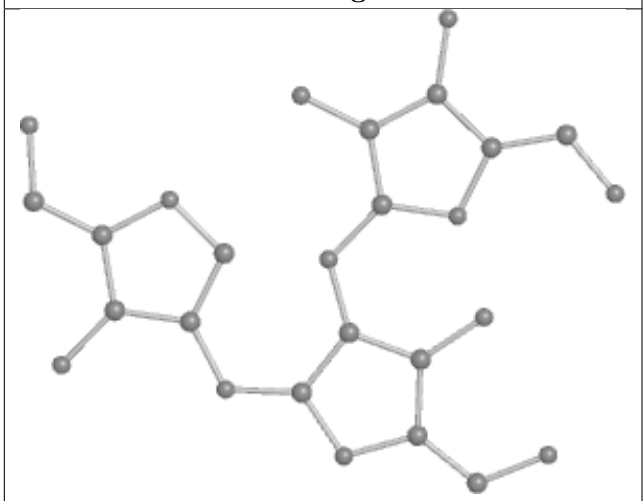
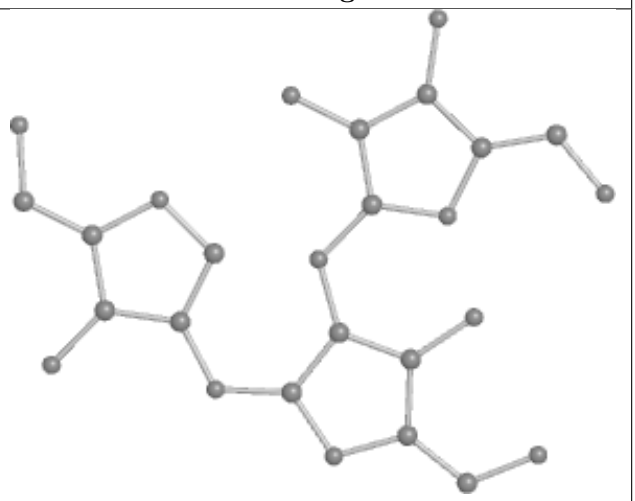
Bond angles



Torsions



Rings

Oligosaccharide Chain xA	
 Bond lengths	 Bond angles
 Torsions	 Rings

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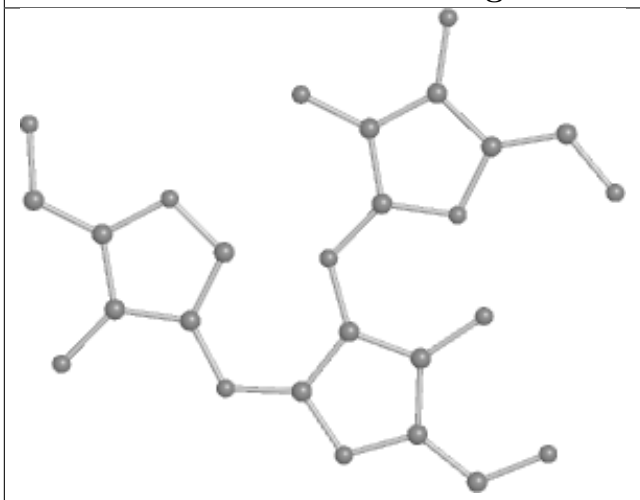
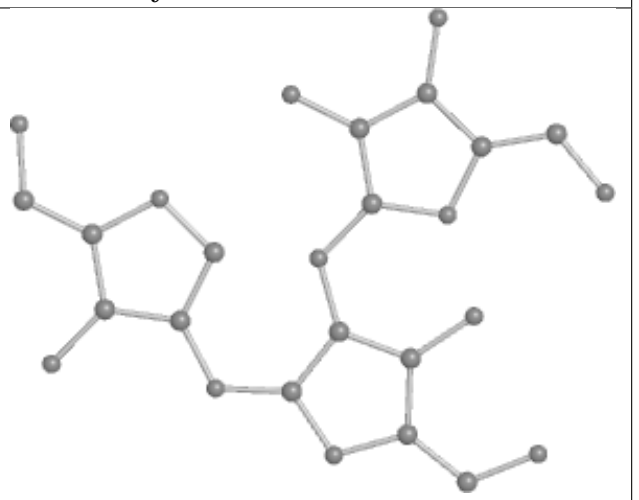
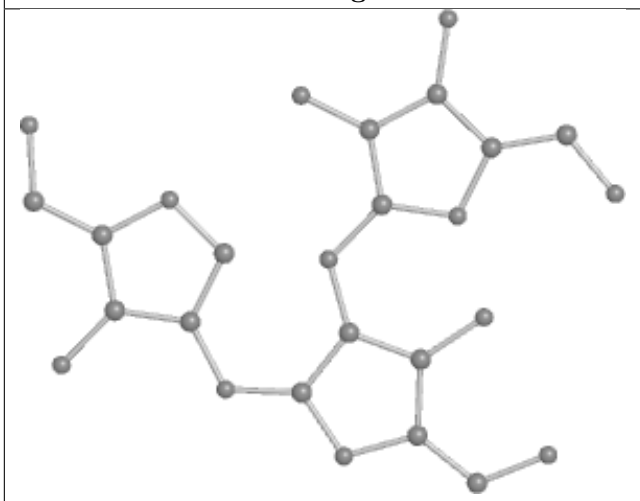
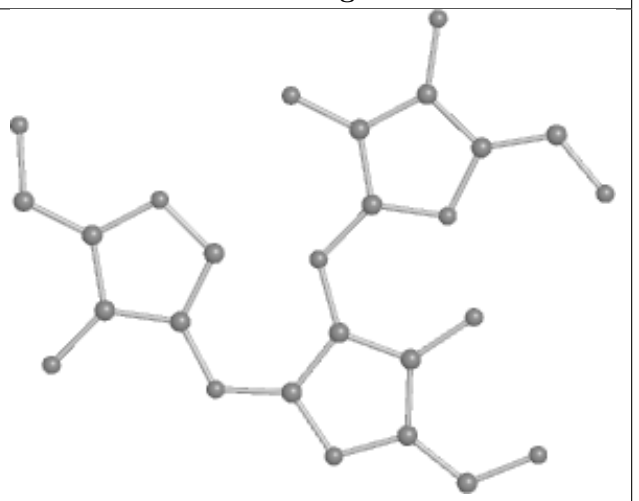
 Bond lengths	 Bond angles
 Torsions	 Rings

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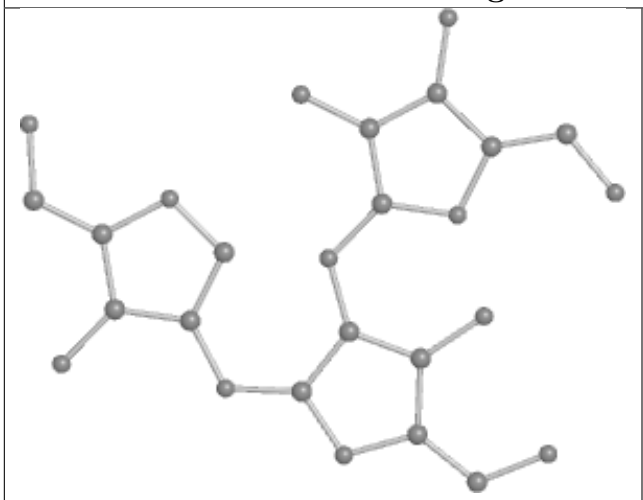
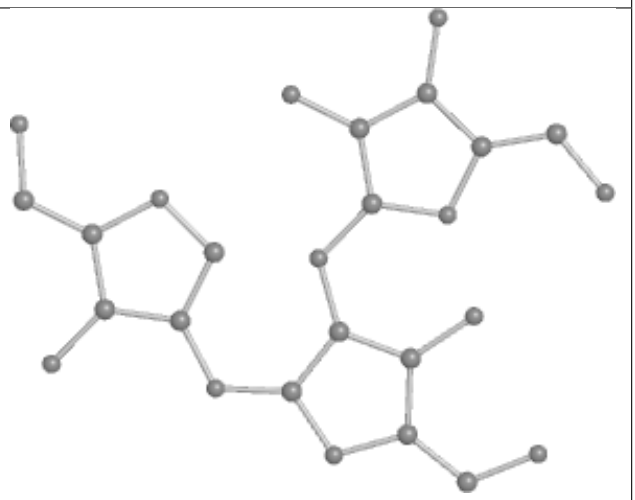
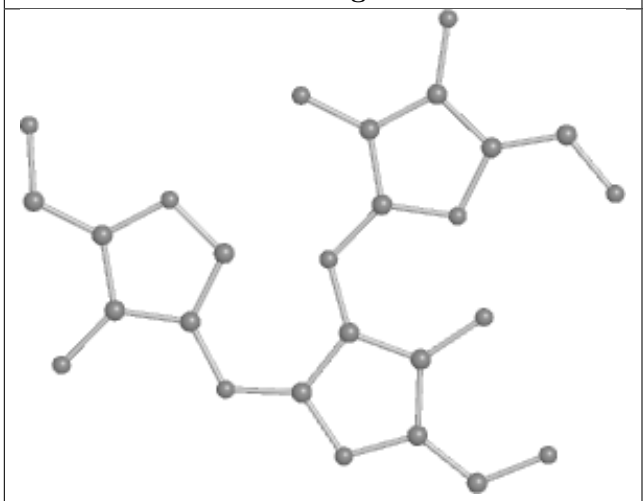
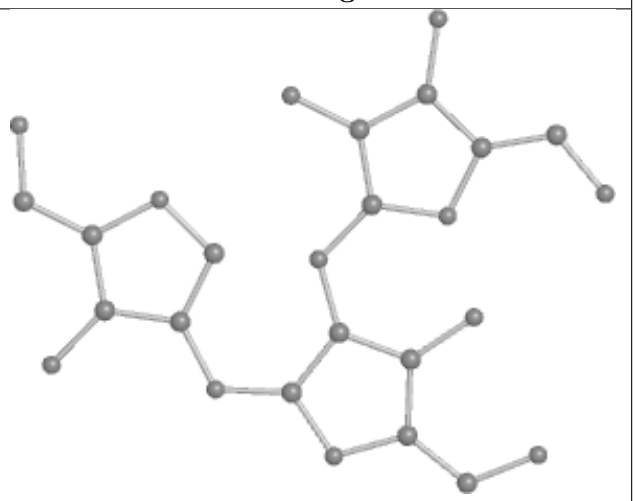
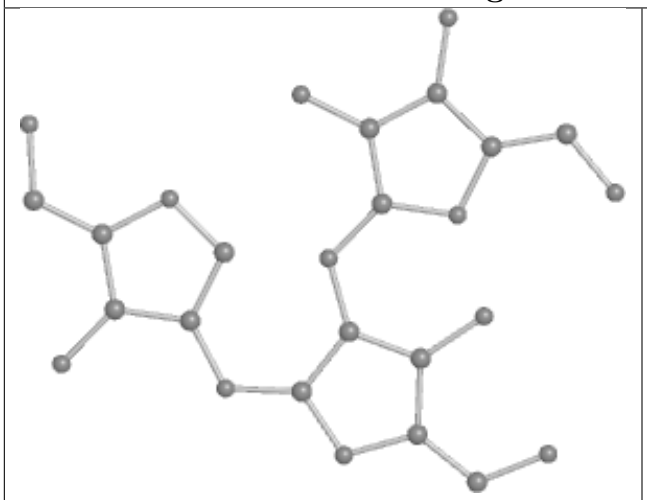
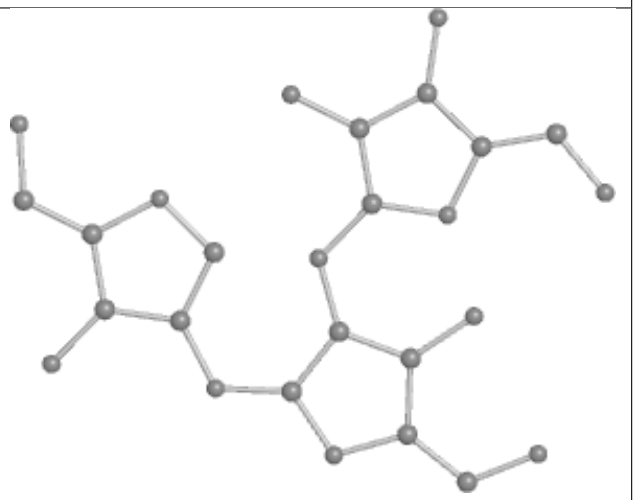
 Bond lengths	 Bond angles
 Torsions	 Rings

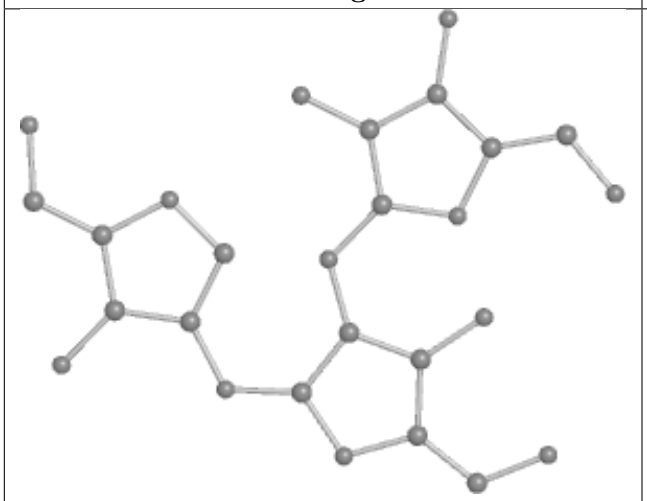
Oligosaccharide Chain 0A



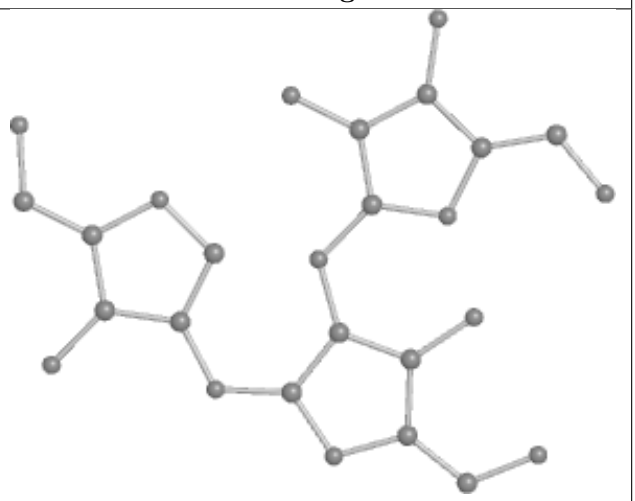
Bond lengths



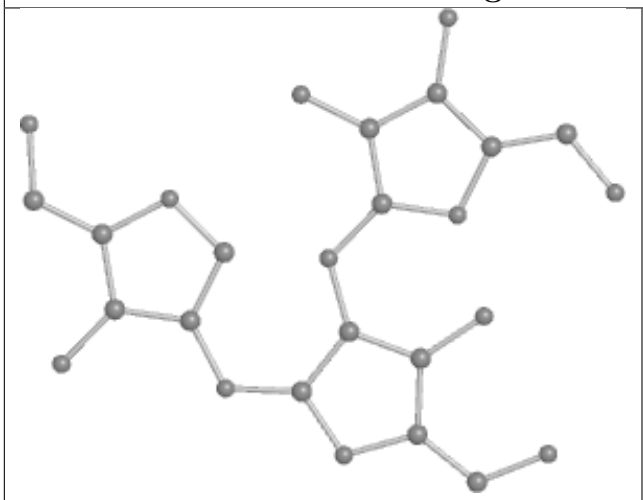
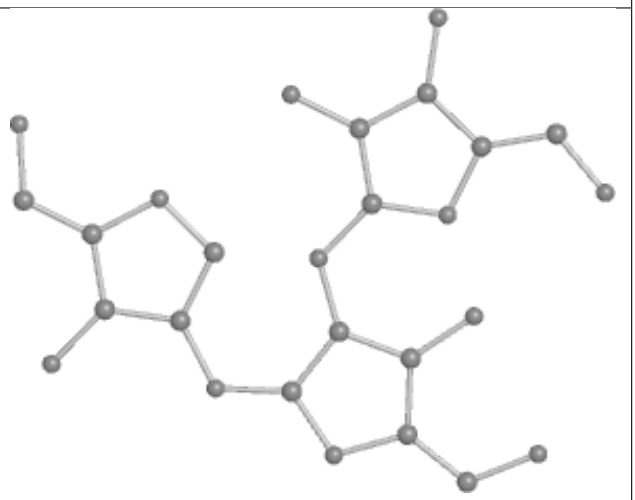
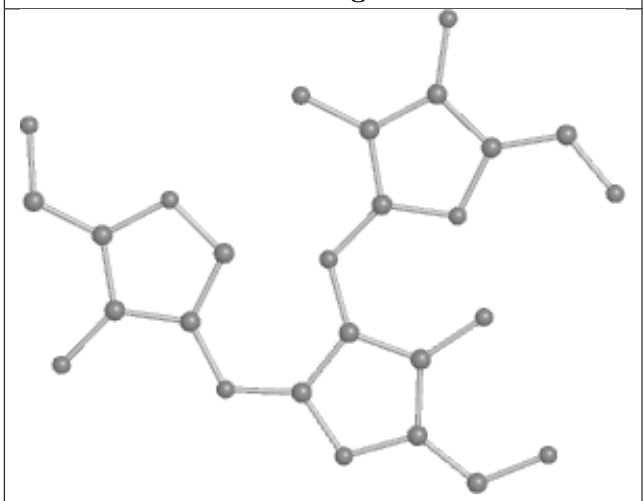
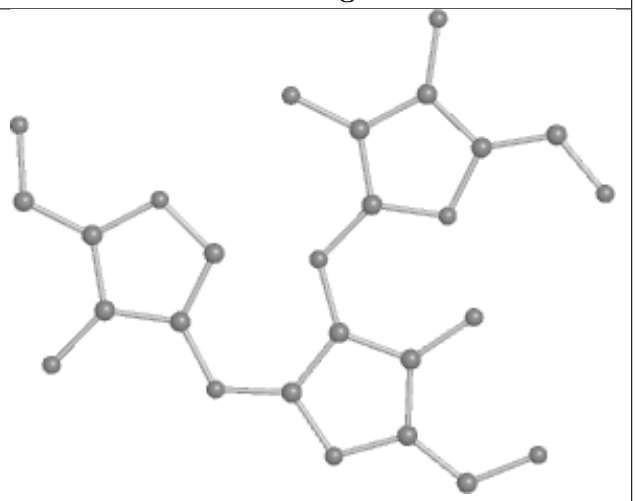
Bond angles



Torsions



Rings

Oligosaccharide Chain EB	
 Bond lengths	 Bond angles
 Torsions	 Rings

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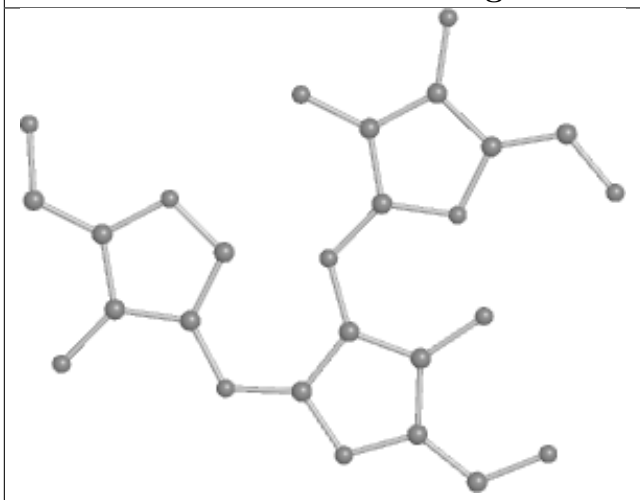
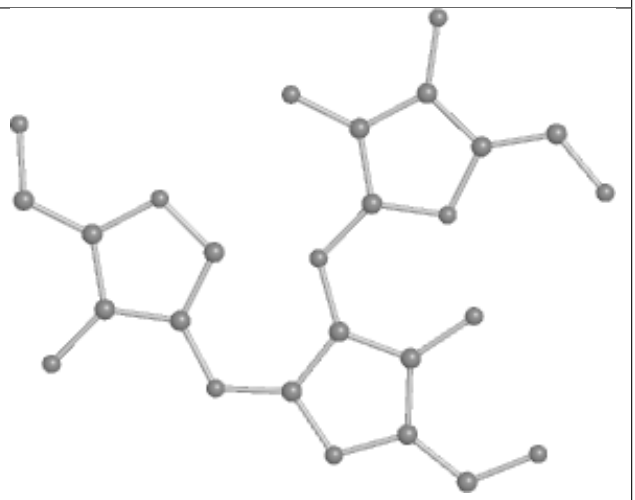
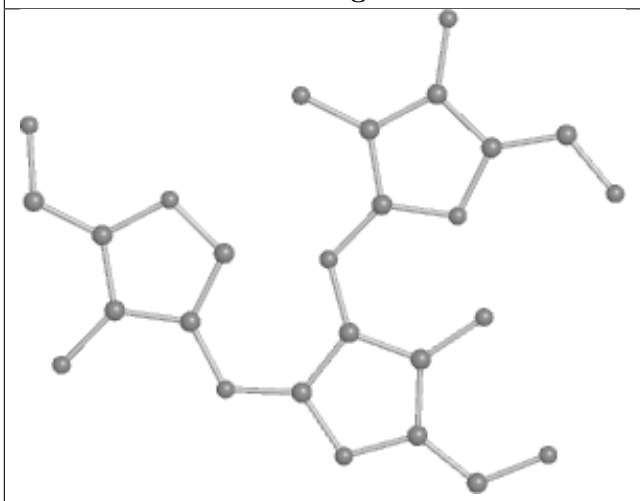
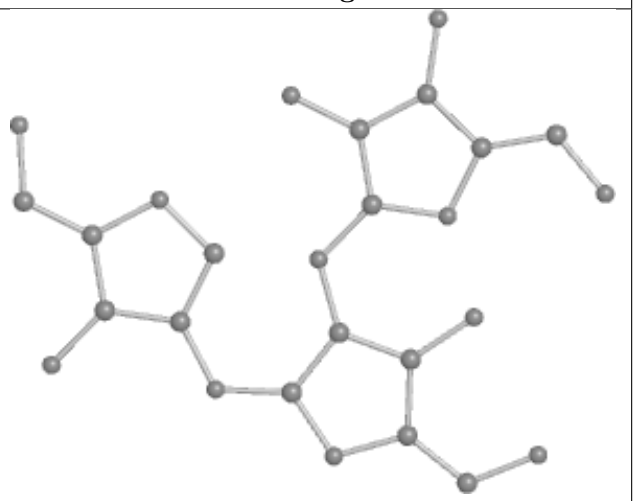
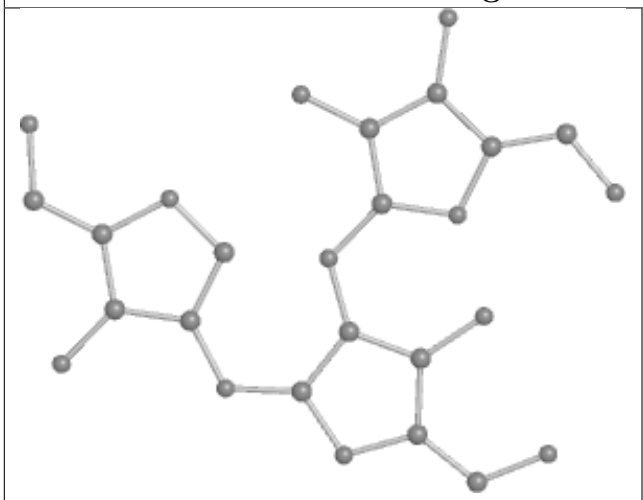
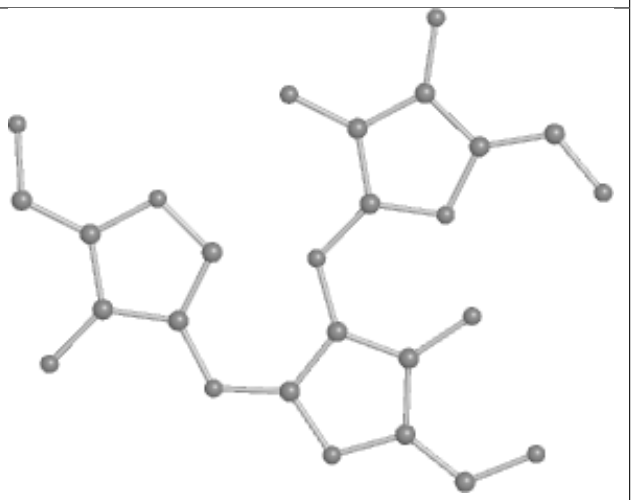
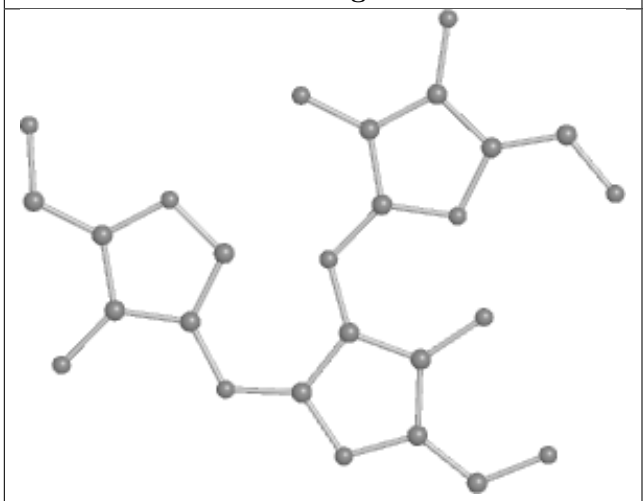
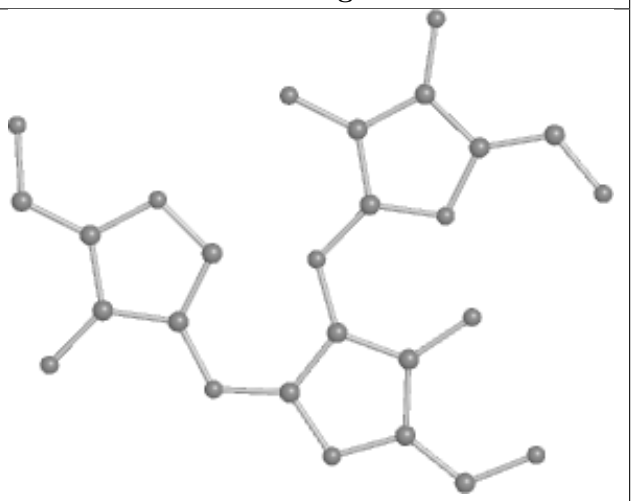
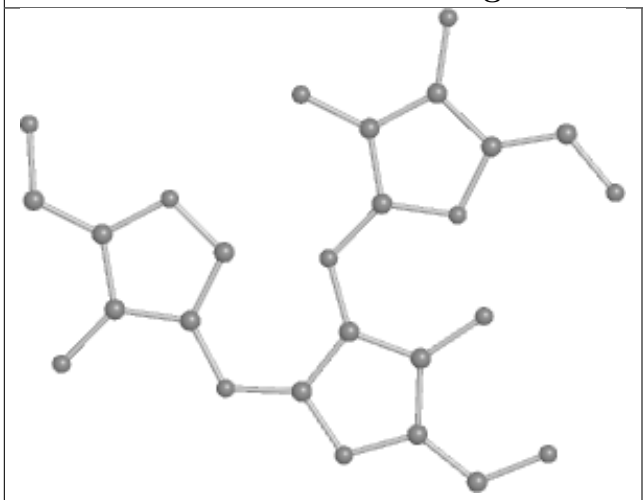
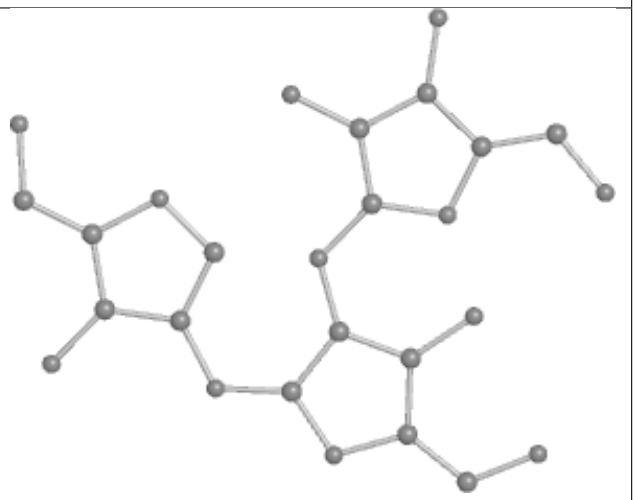
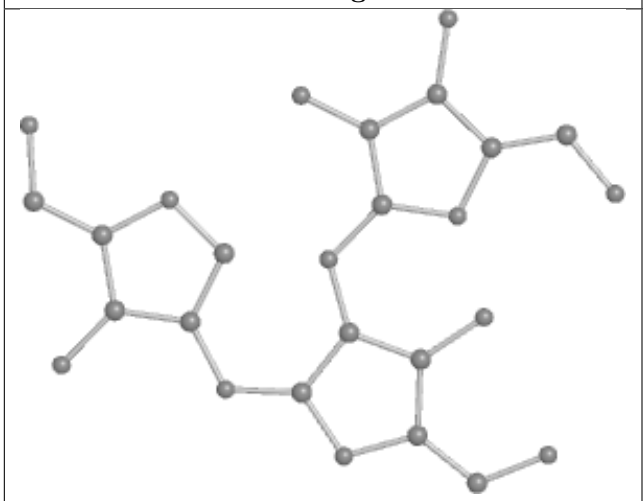
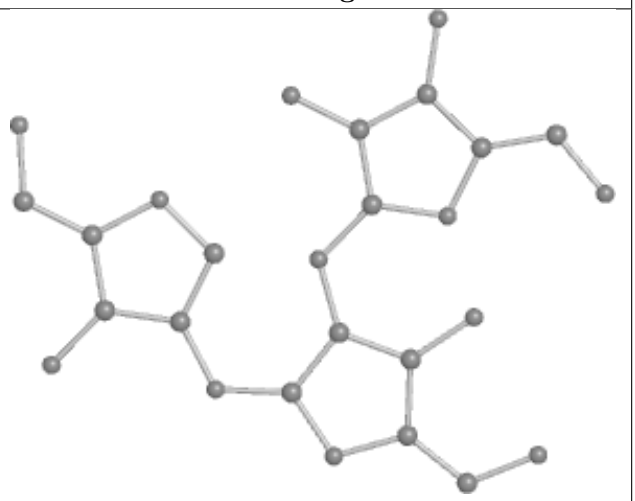
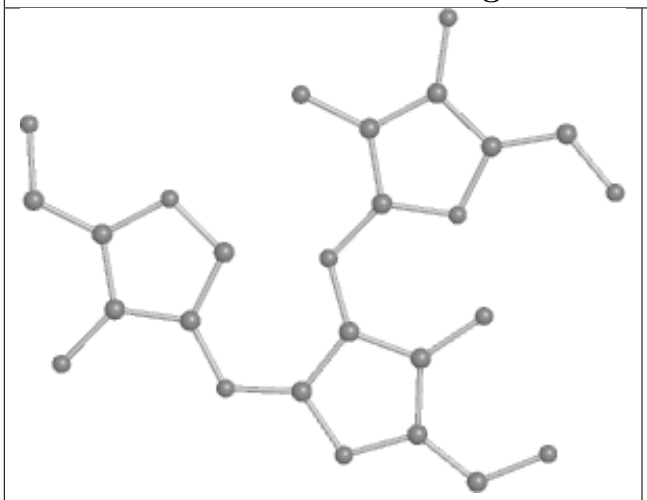
 Bond lengths	 Bond angles
 Torsions	 Rings

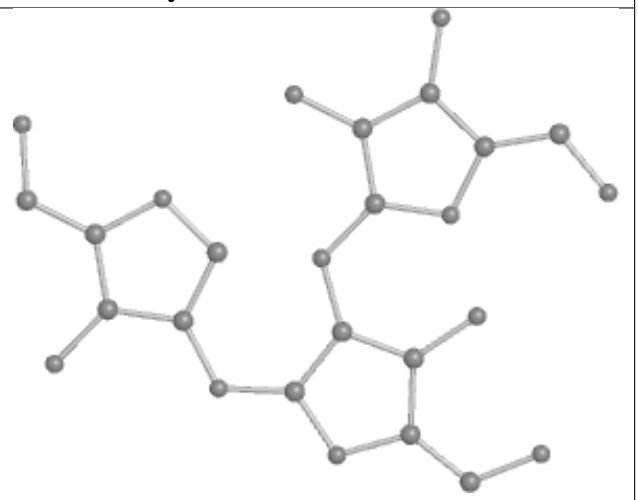
Oligosaccharide Chain OB	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain PB	
 Bond lengths	 Bond angles
 Torsions	 Rings

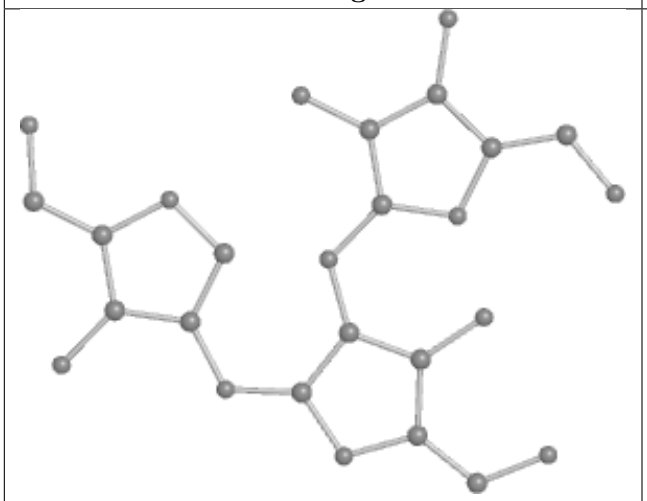
Oligosaccharide Chain QB



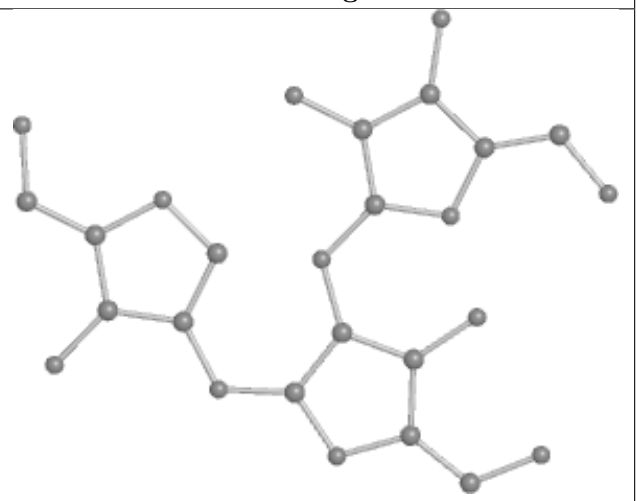
Bond lengths



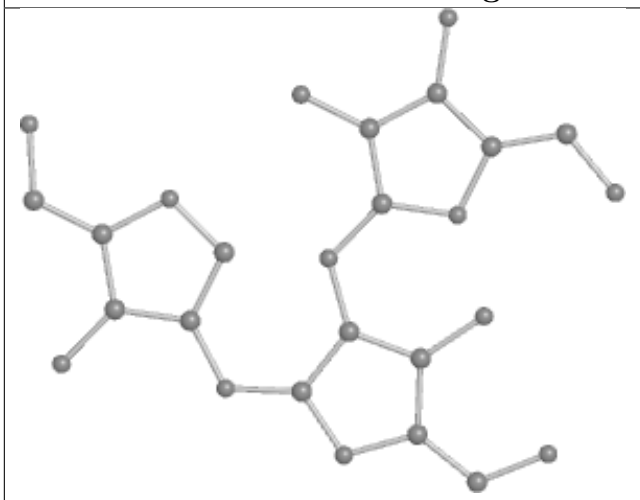
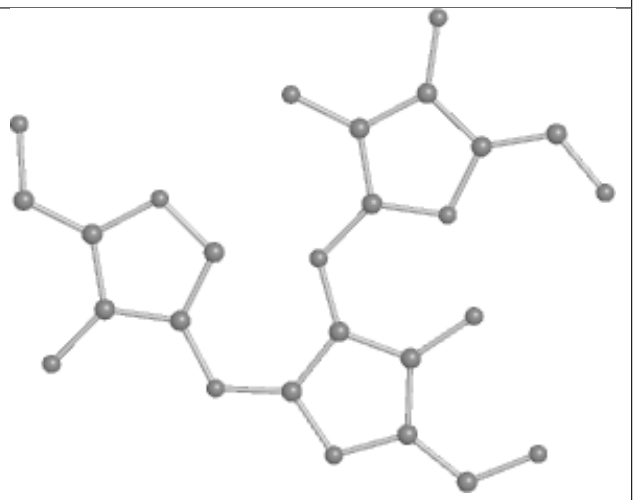
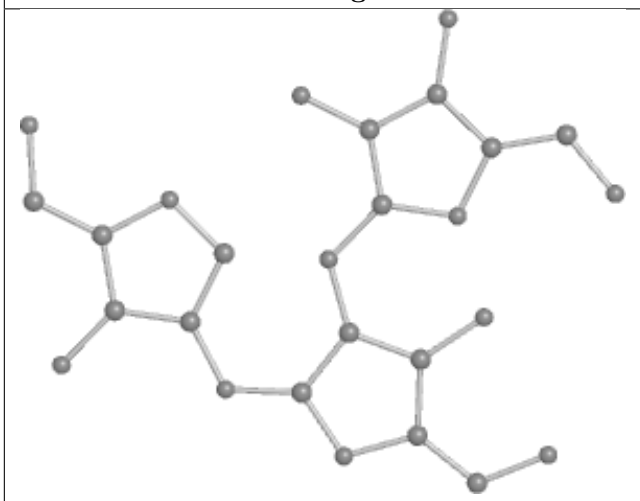
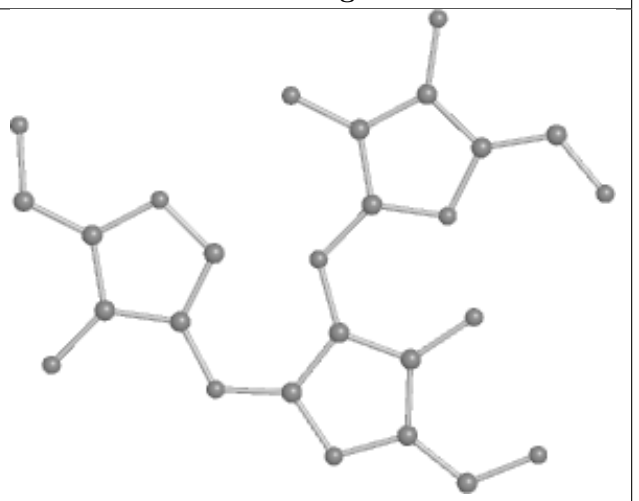
Bond angles



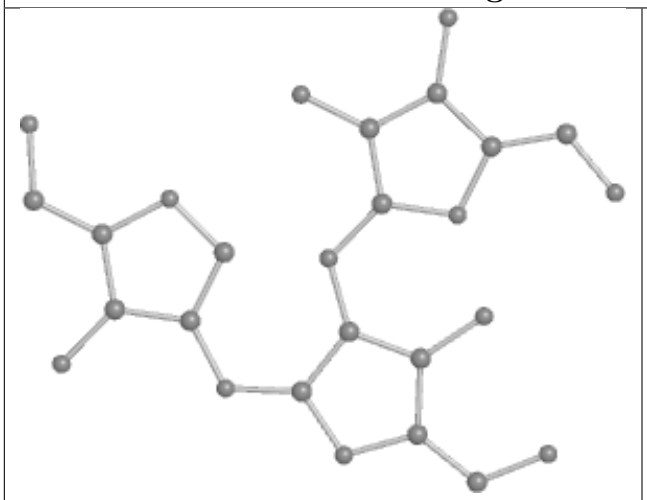
Torsions



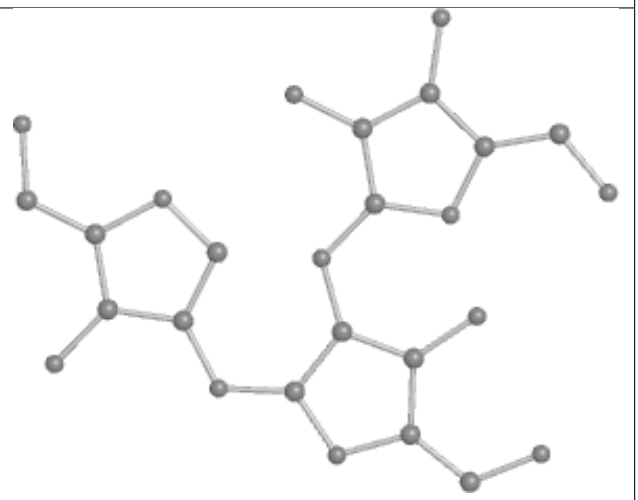
Rings

Oligosaccharide Chain RB	
 Bond lengths	 Bond angles
 Torsions	 Rings

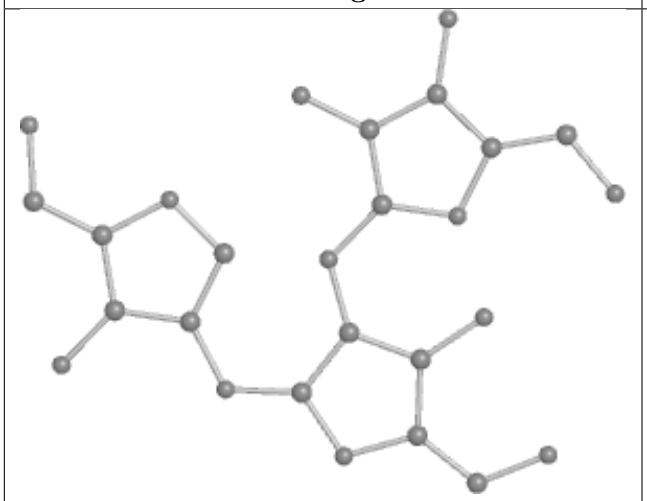
Oligosaccharide Chain SB



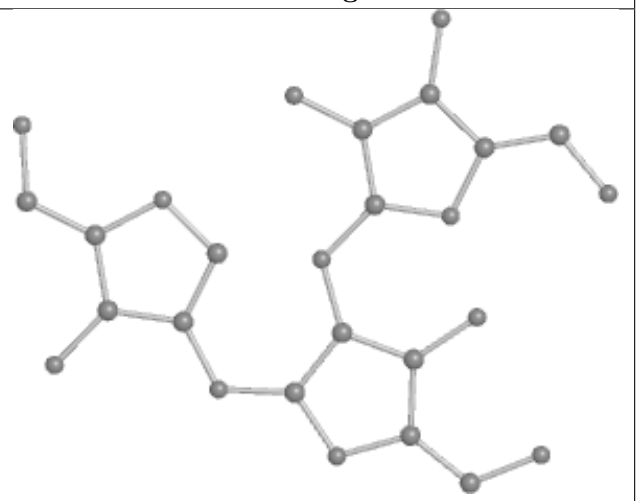
Bond lengths



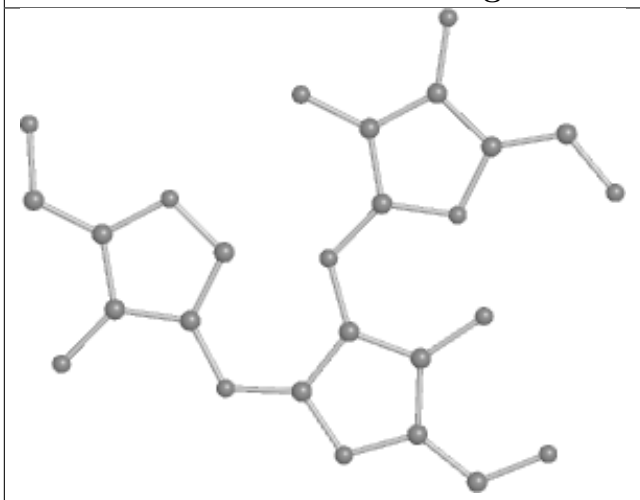
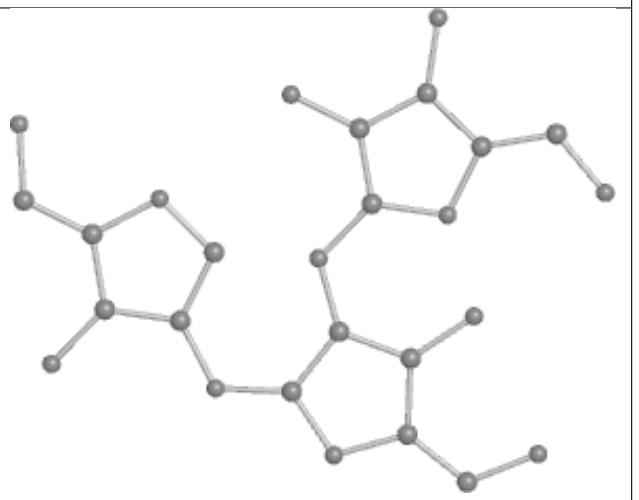
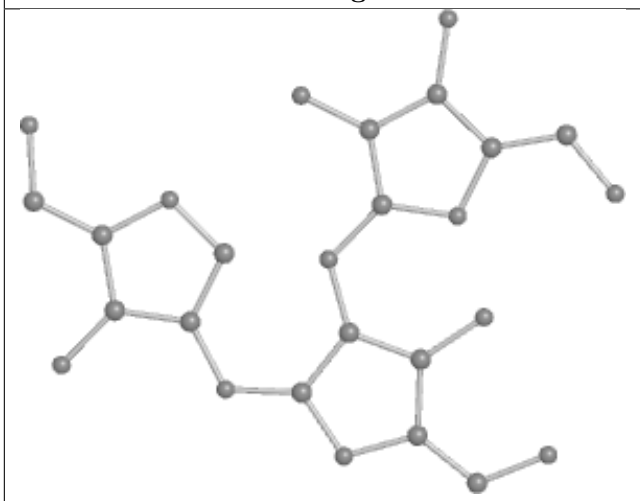
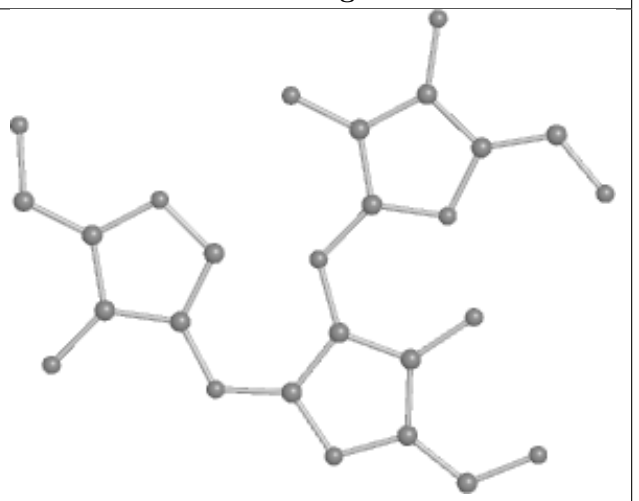
Bond angles

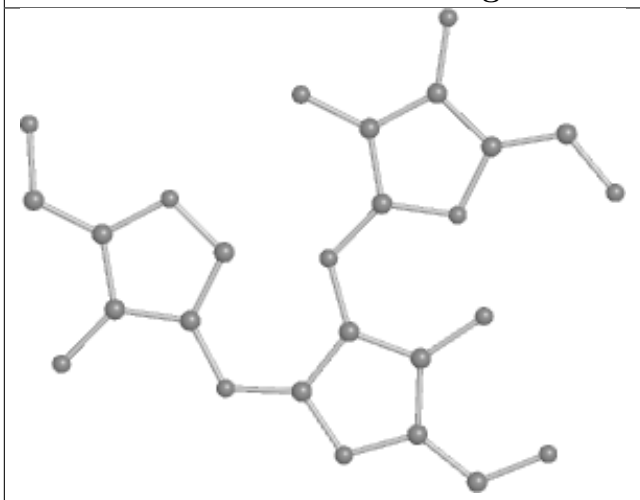
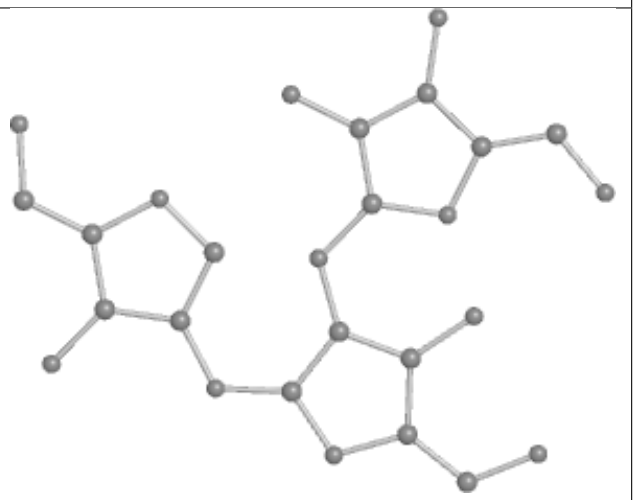
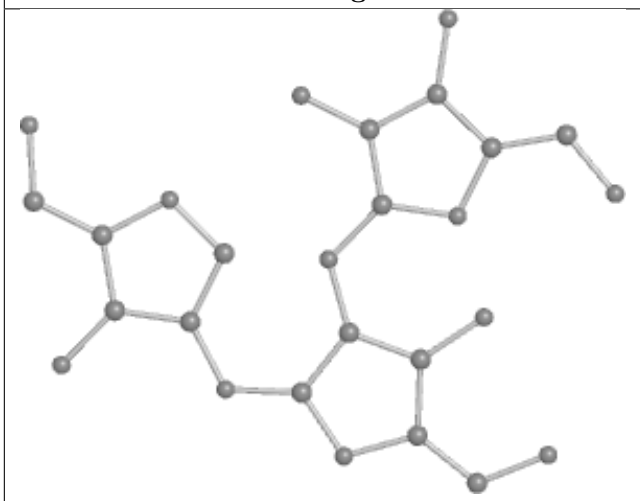
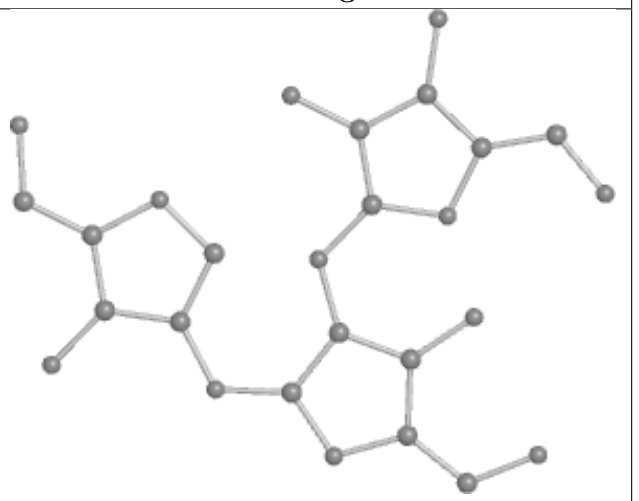


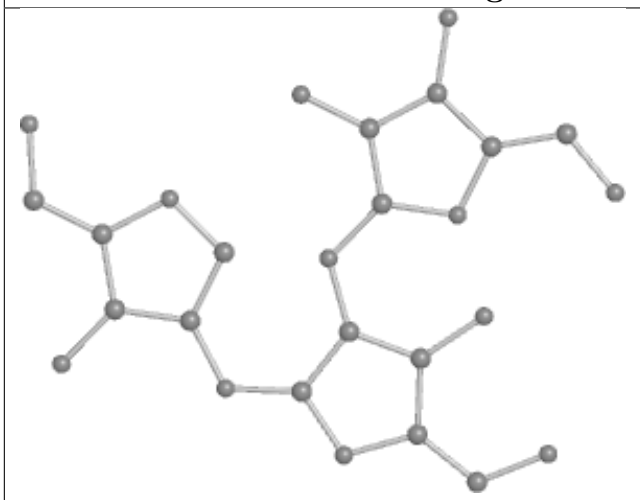
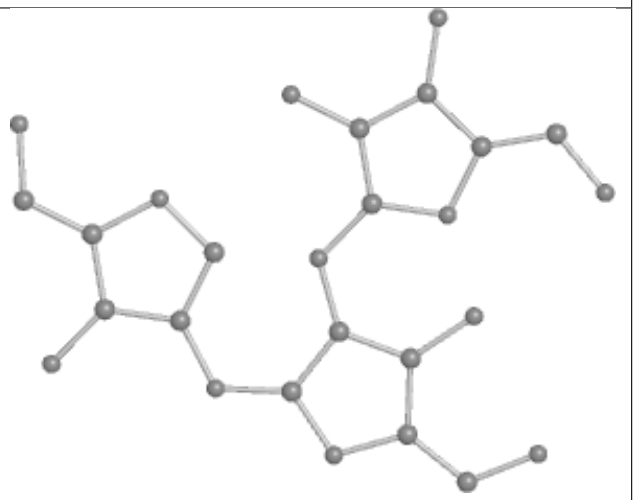
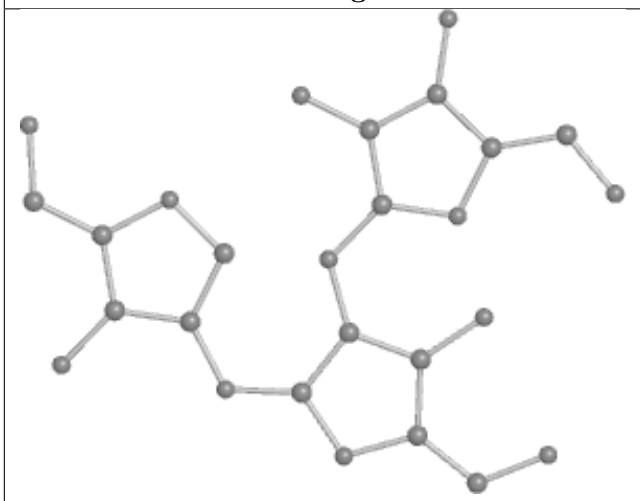
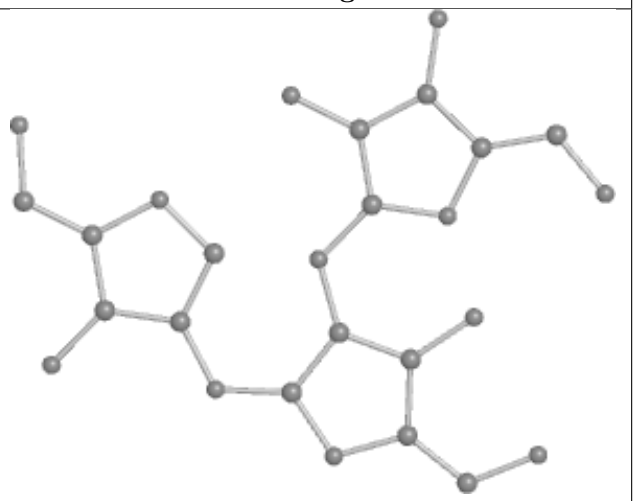
Torsions

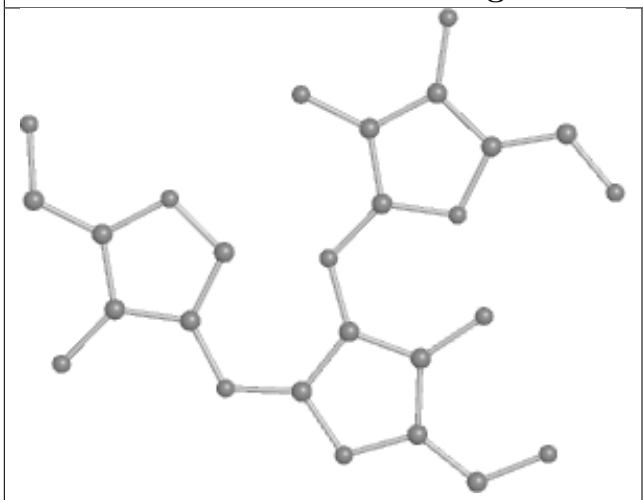
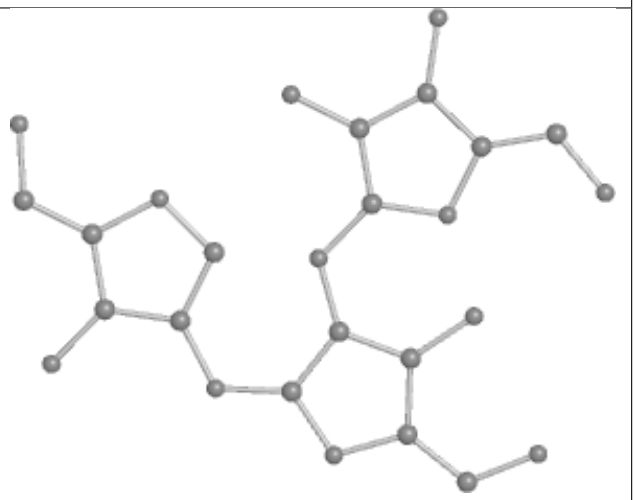
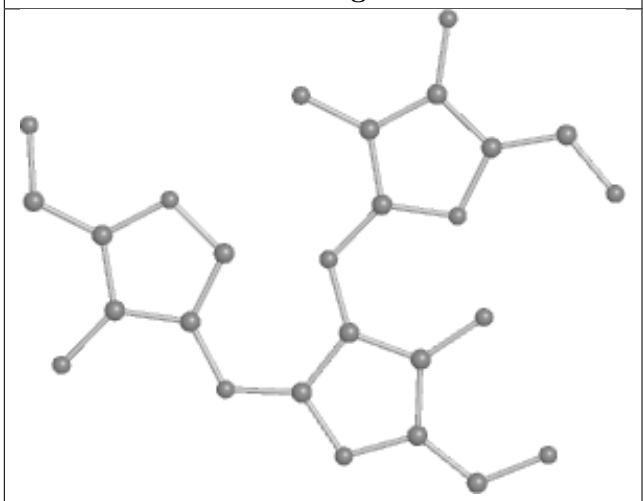
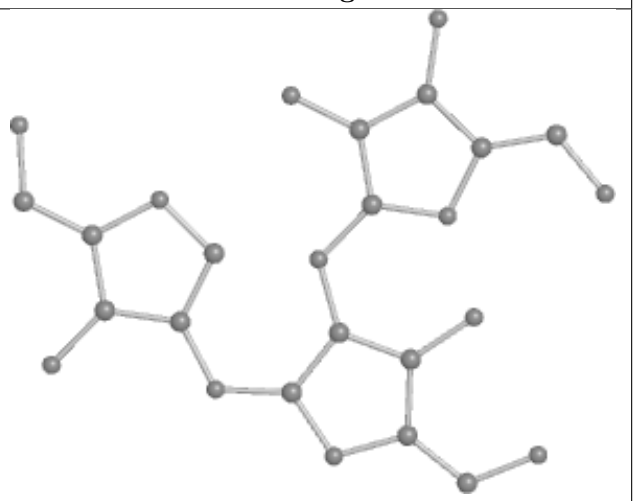


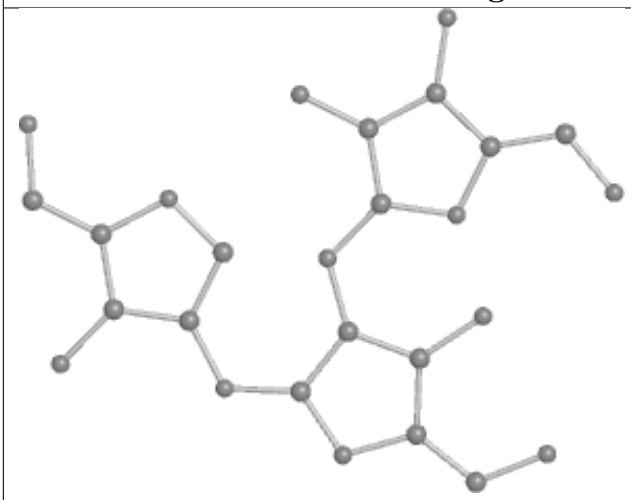
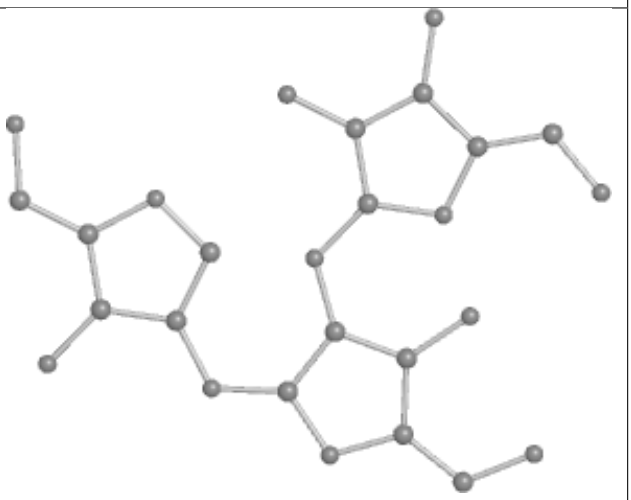
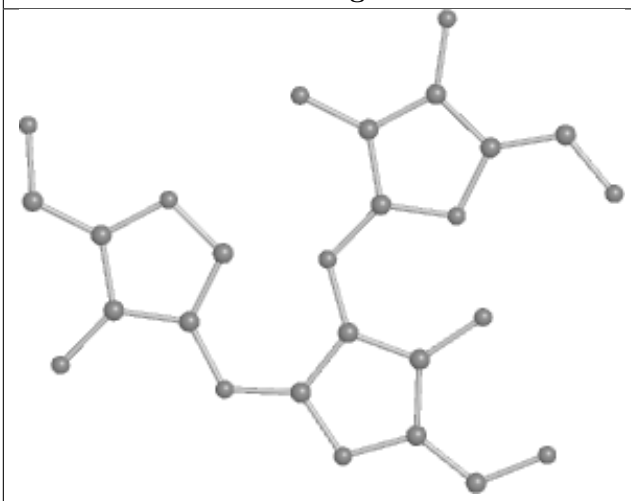
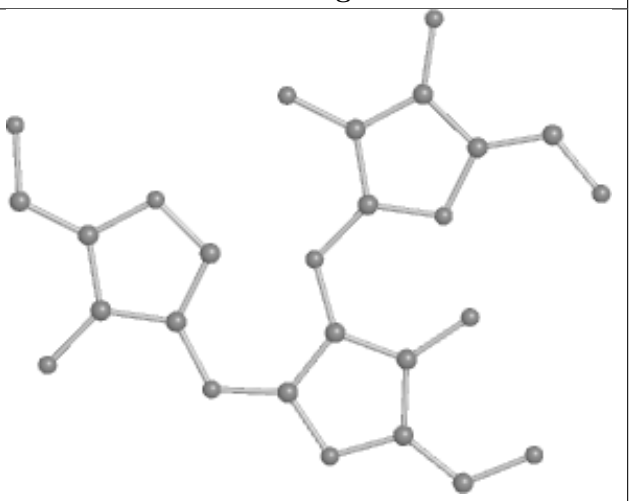
Rings

Oligosaccharide Chain TB	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain UB	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain hB	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain oB	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain rB	
 Bond lengths	 Bond angles
 Torsions	 Rings

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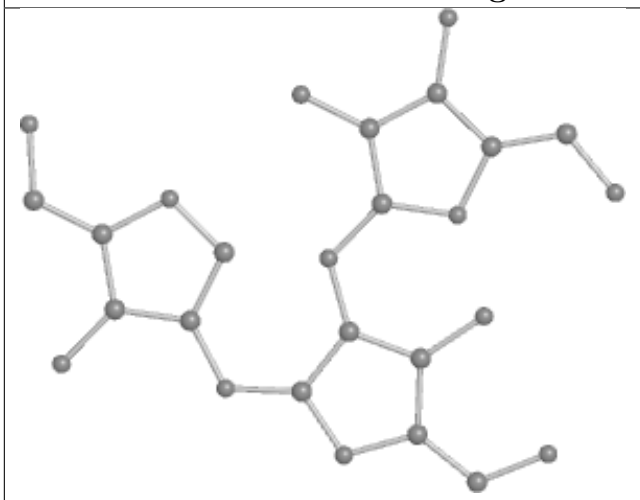
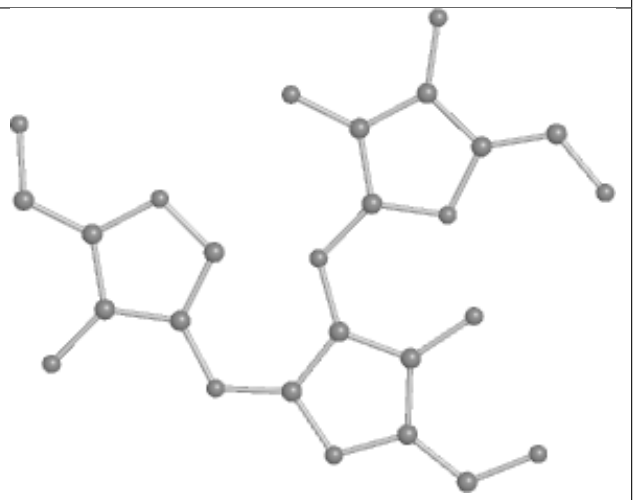
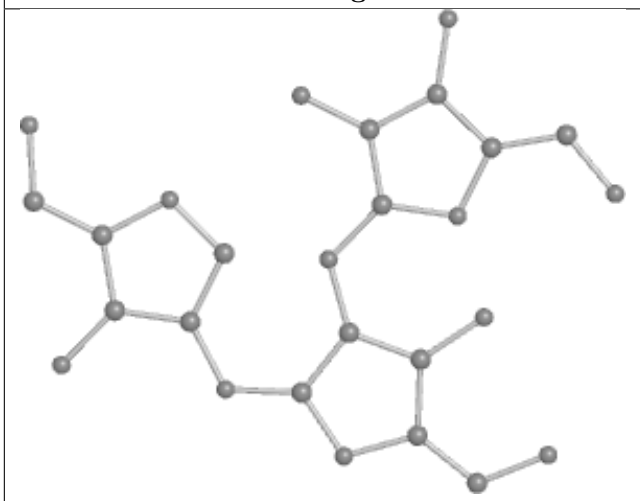
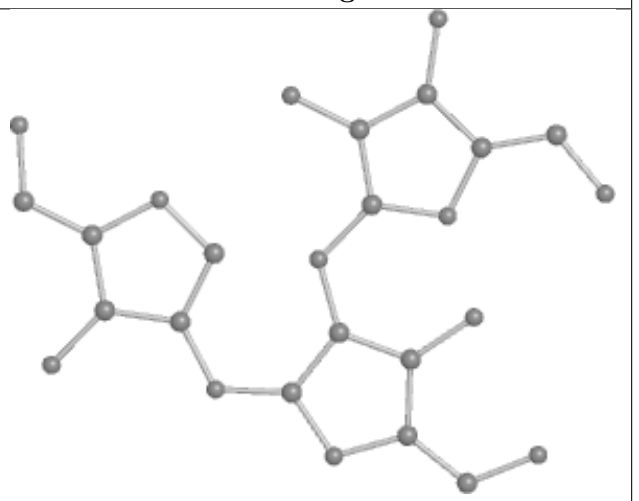
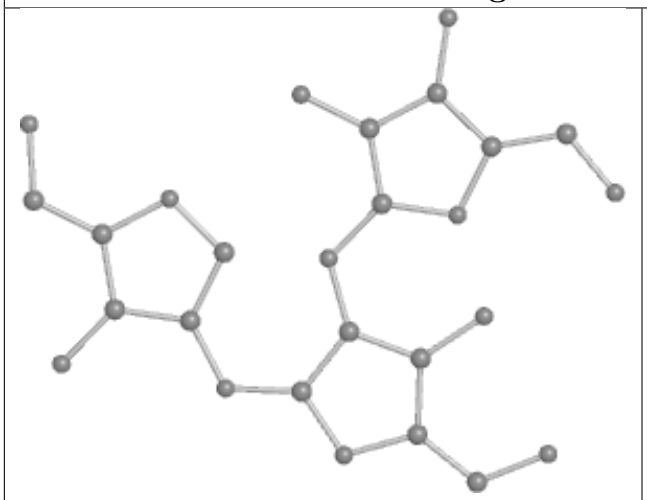
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain tB



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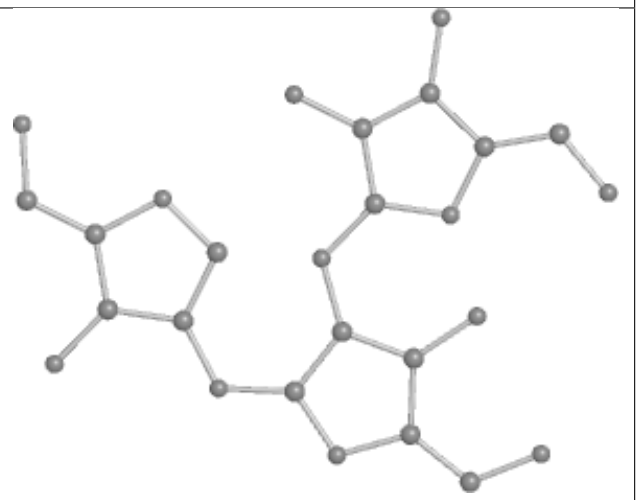

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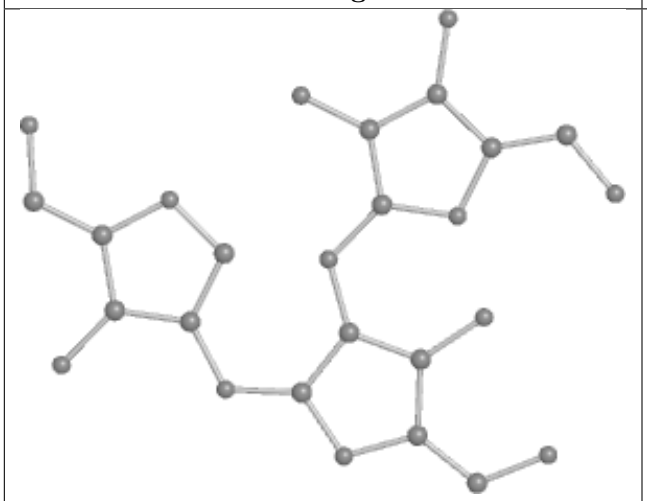

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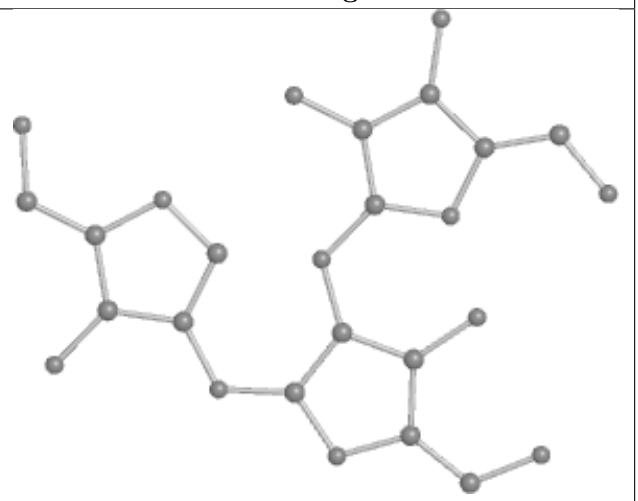
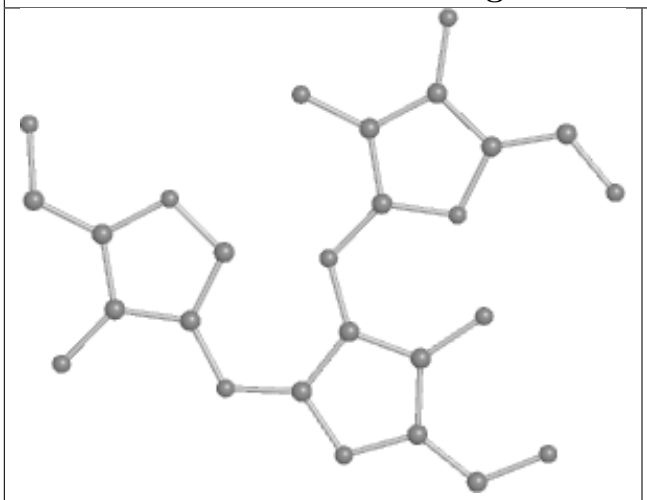


Rings

Oligosaccharide Chain uB



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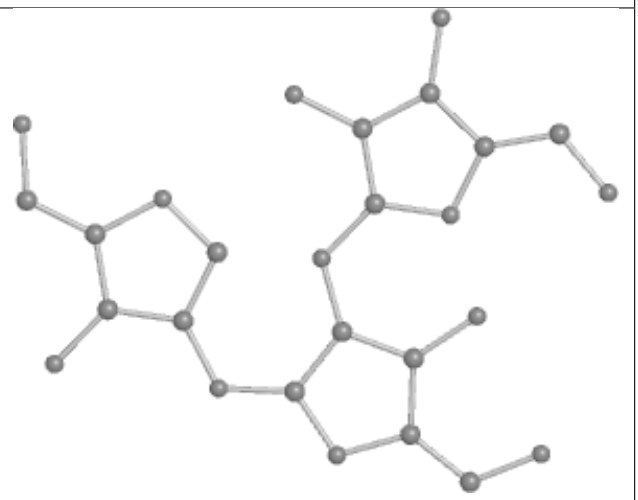

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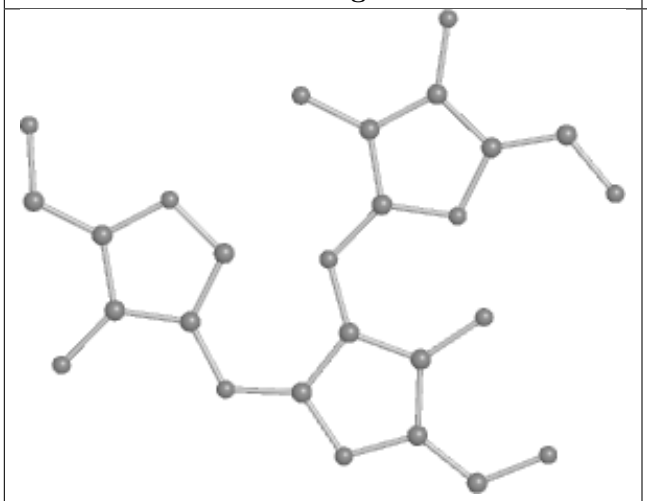

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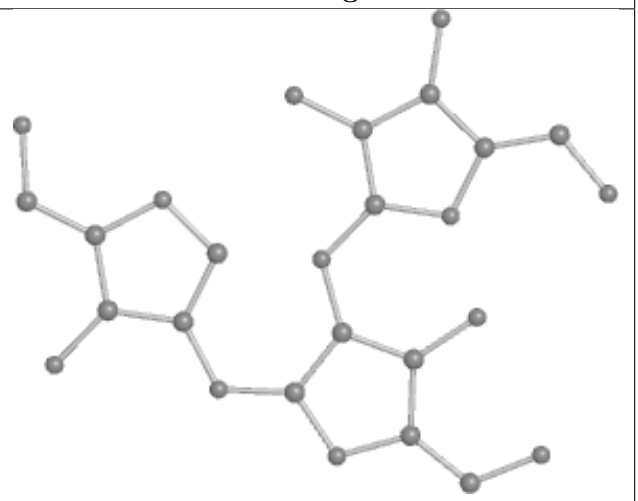
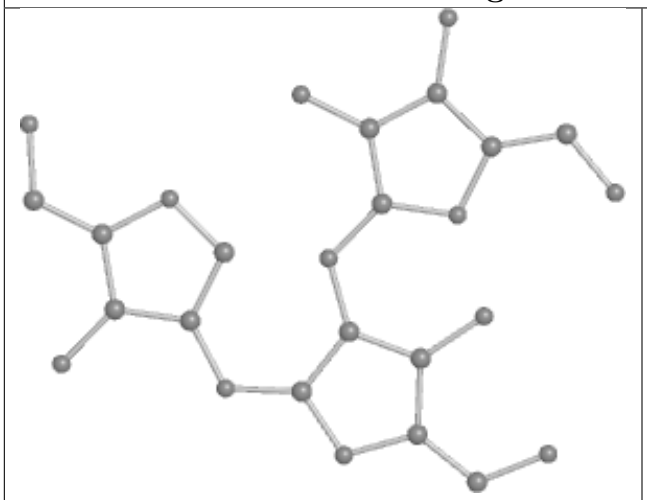


Rings

Oligosaccharide Chain vB



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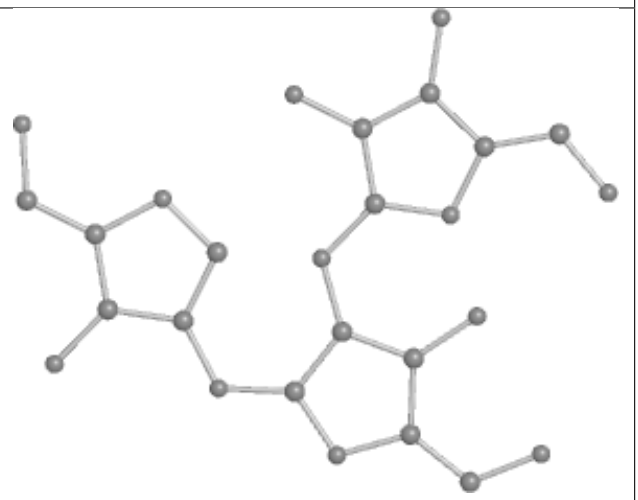

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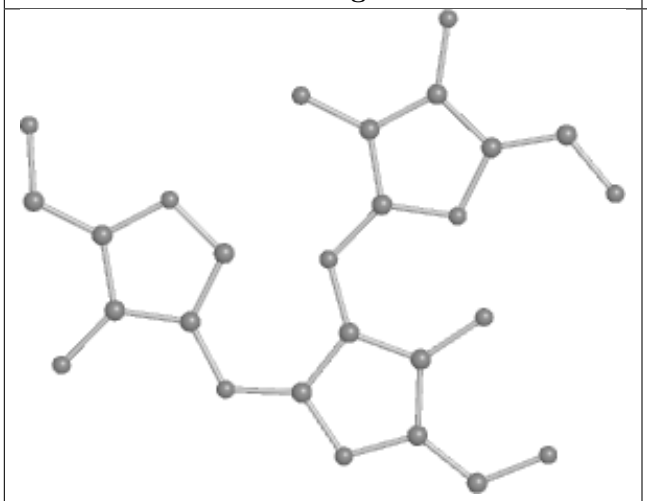

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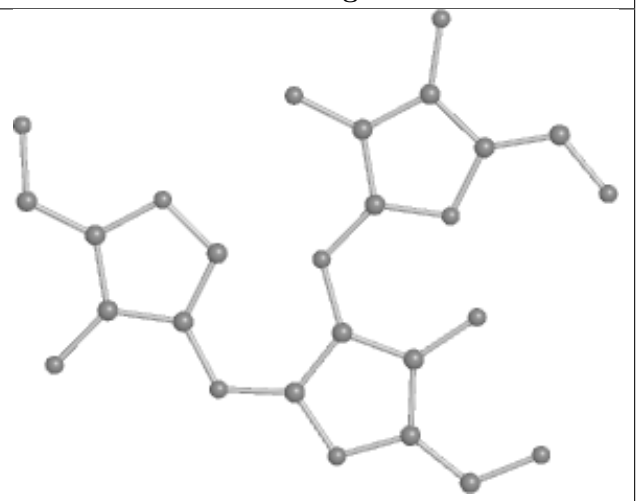
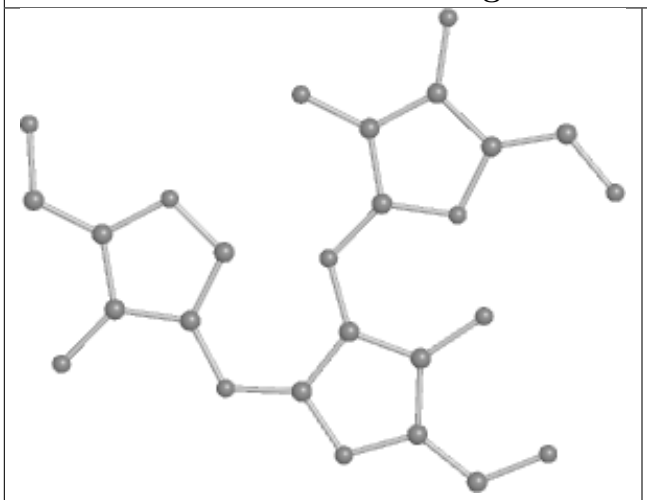


Rings

Oligosaccharide Chain wB



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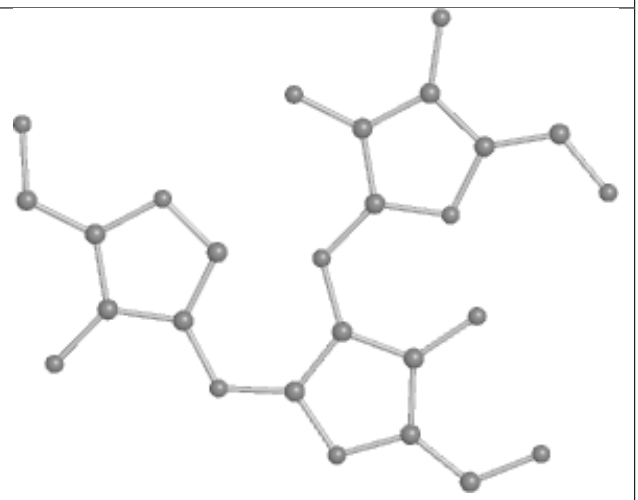
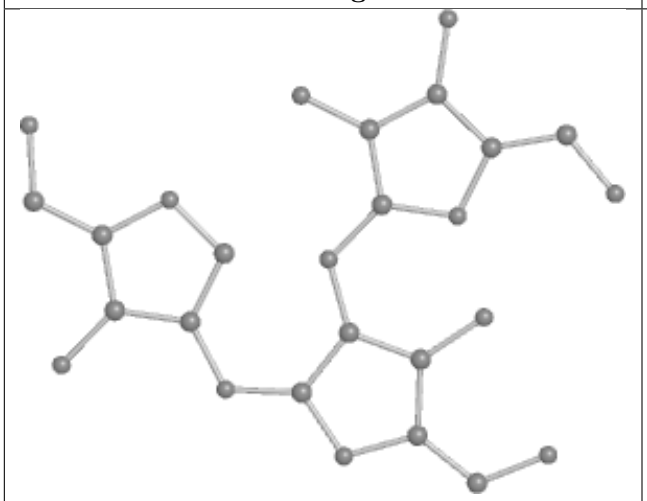


Bond angles



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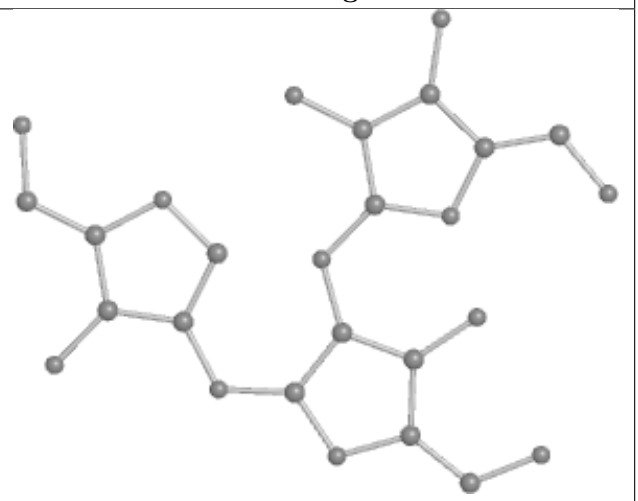
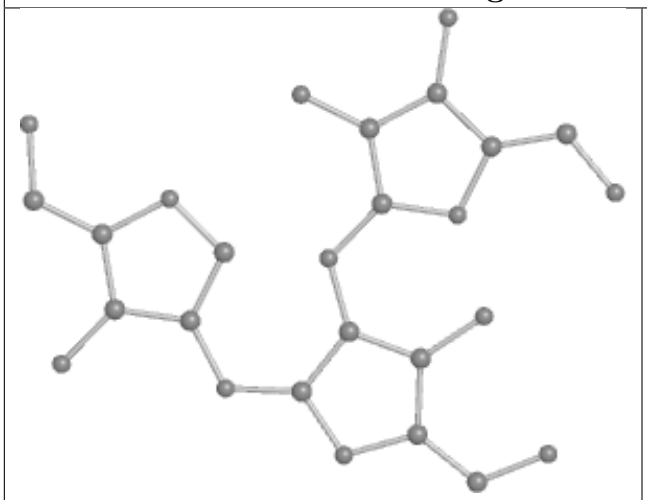


Rings

Oligosaccharide Chain xB



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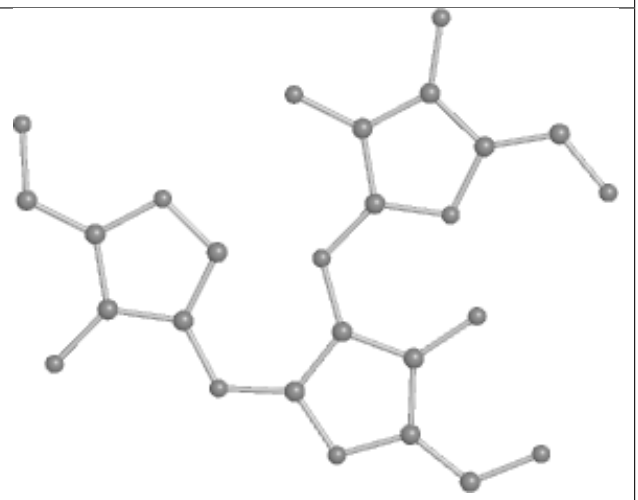
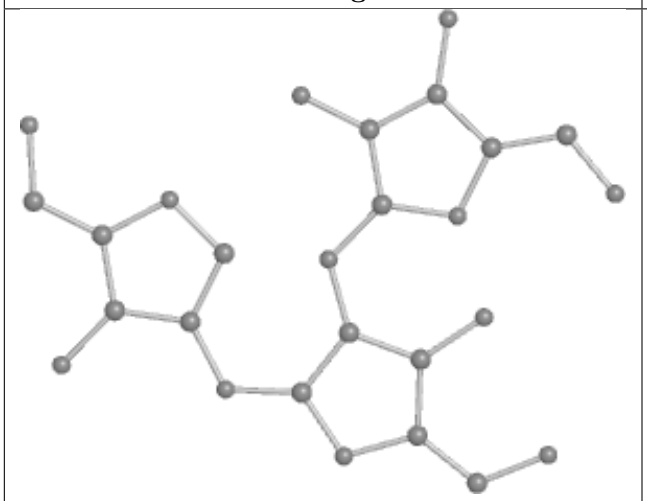


Bond angles



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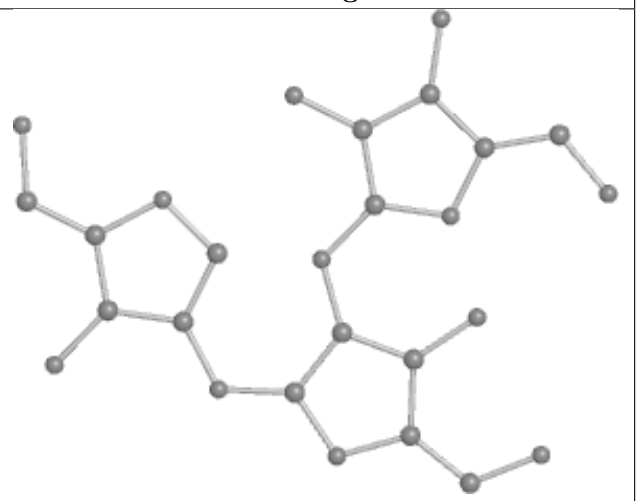
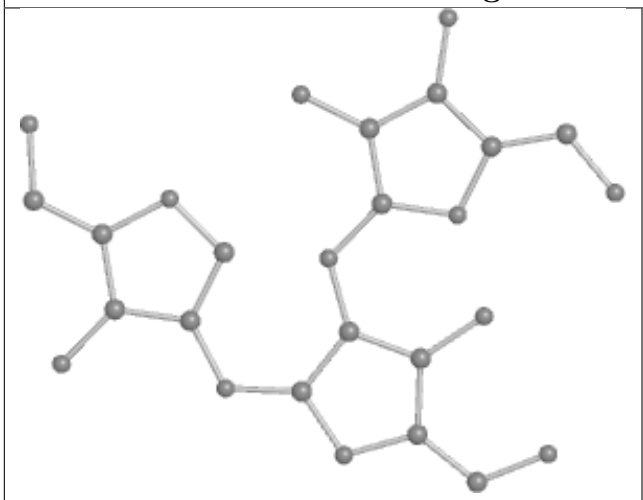
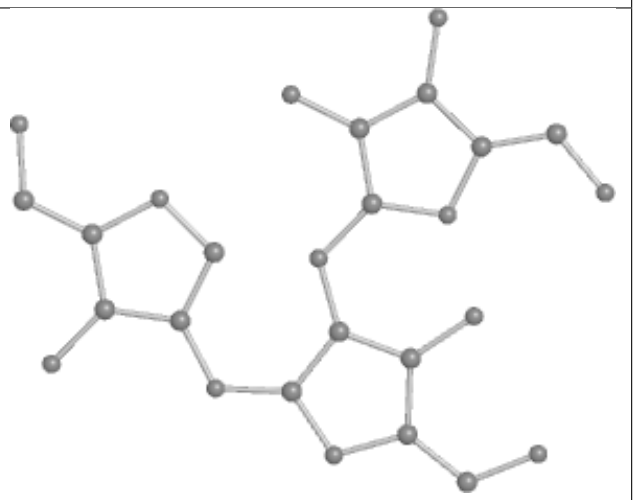
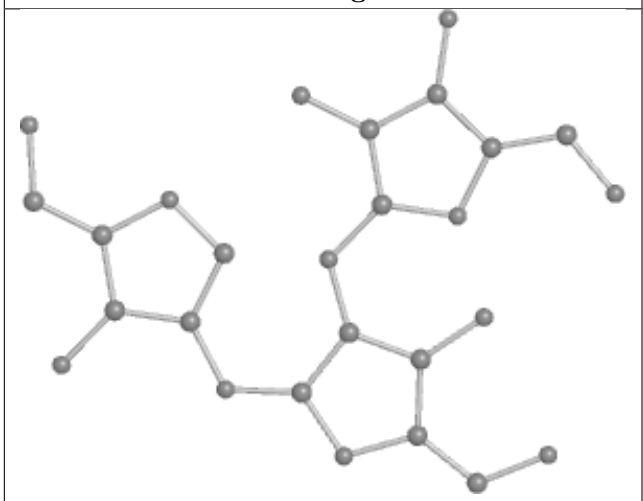
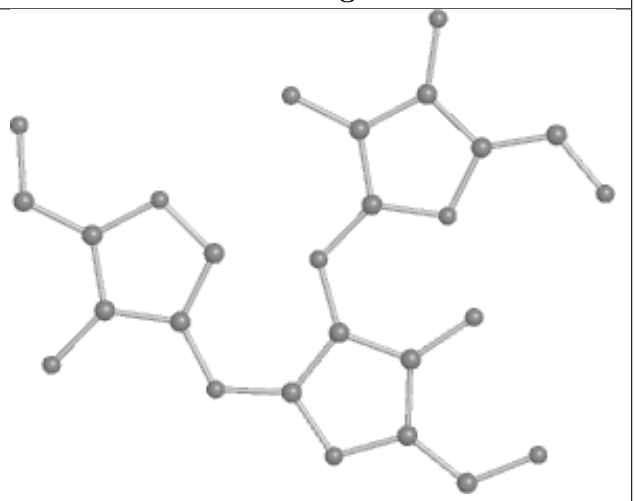


Rings

Oligosaccharide Chain BC	
 Bond lengths	 Bond angles
 Torsions	 Rings

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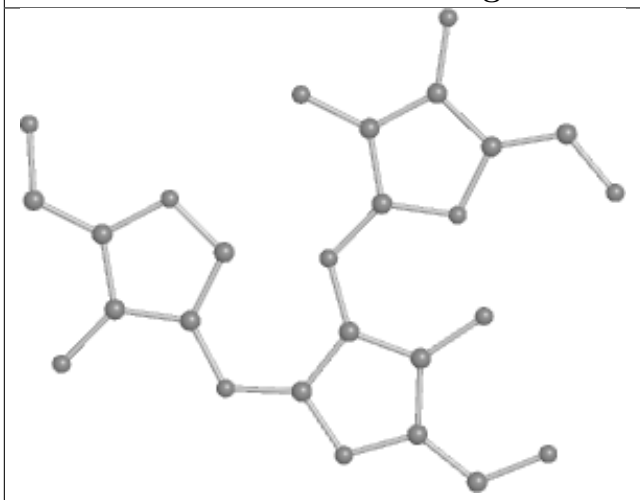
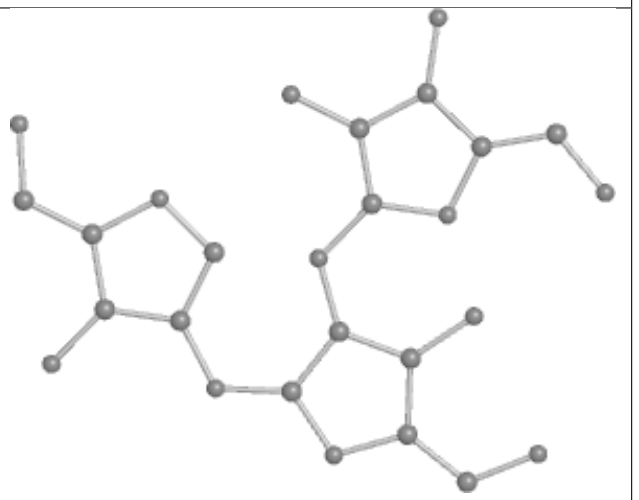
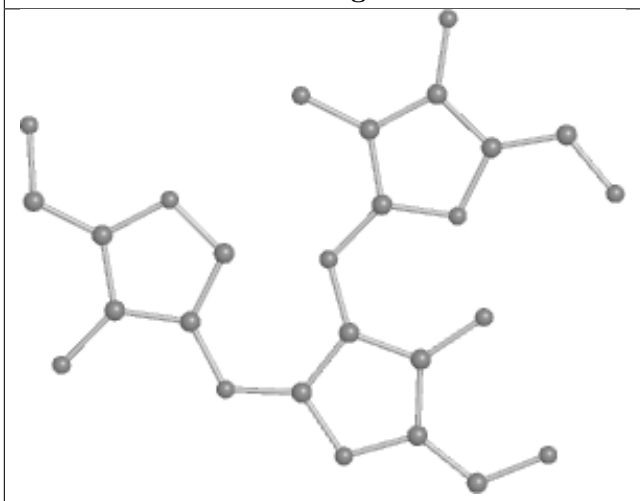
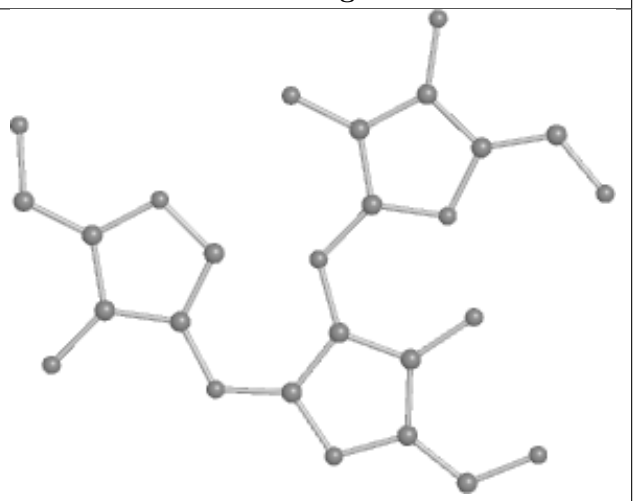
 Bond lengths	 Bond angles
 Torsions	 Rings

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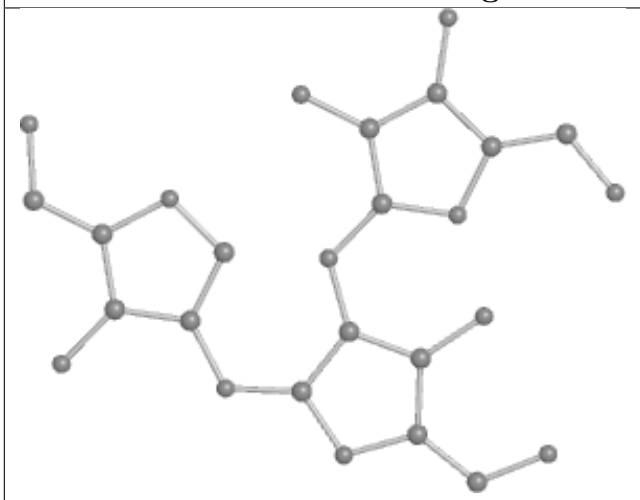
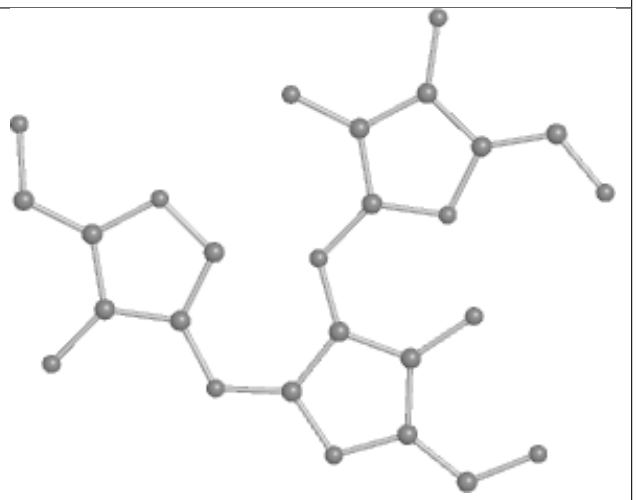
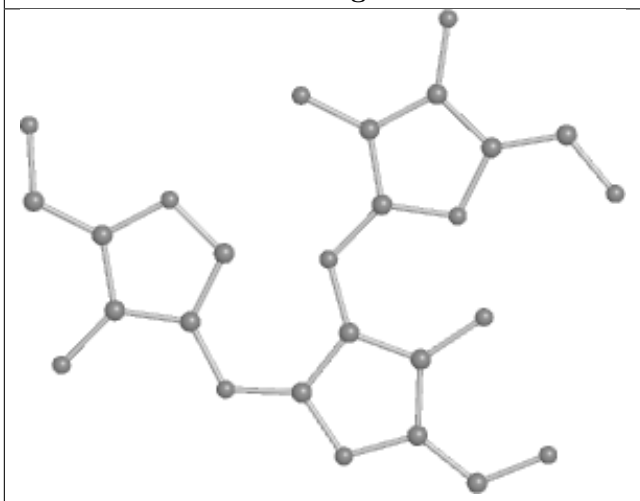
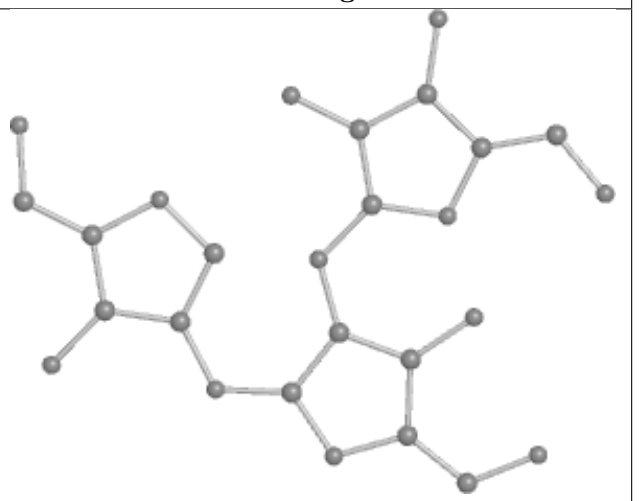
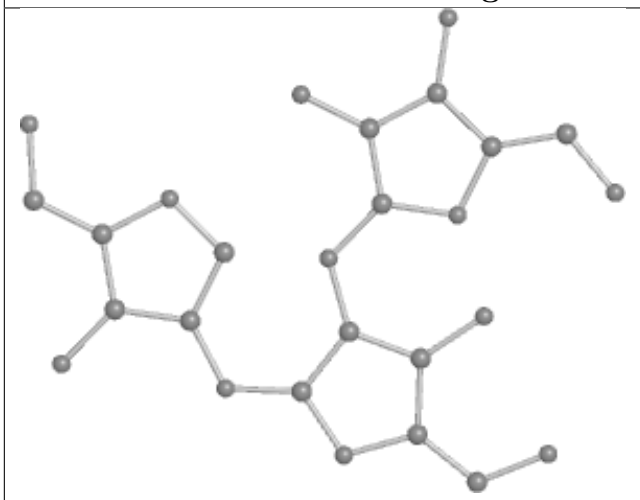
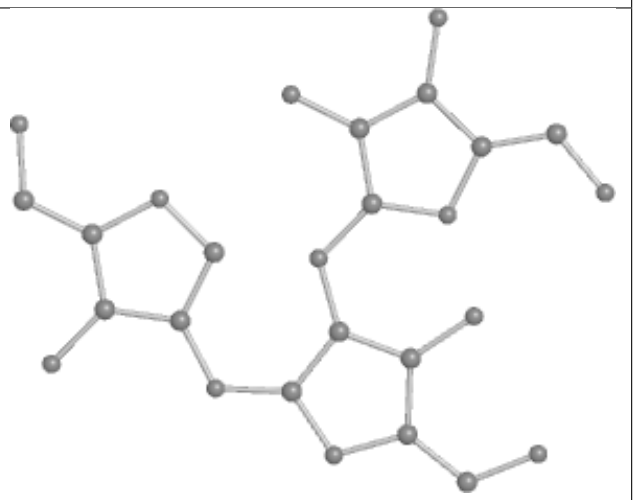
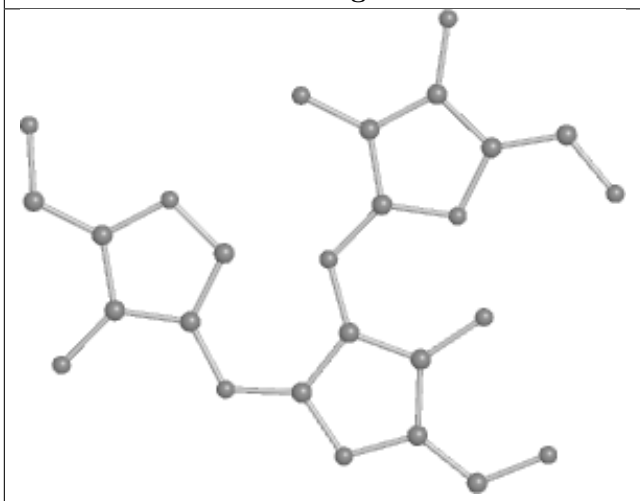
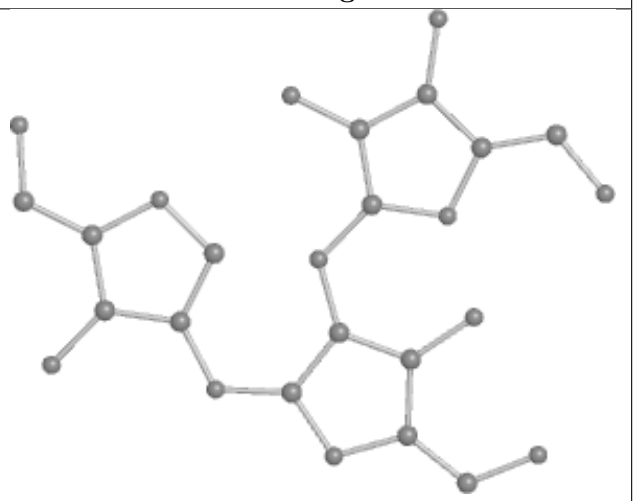
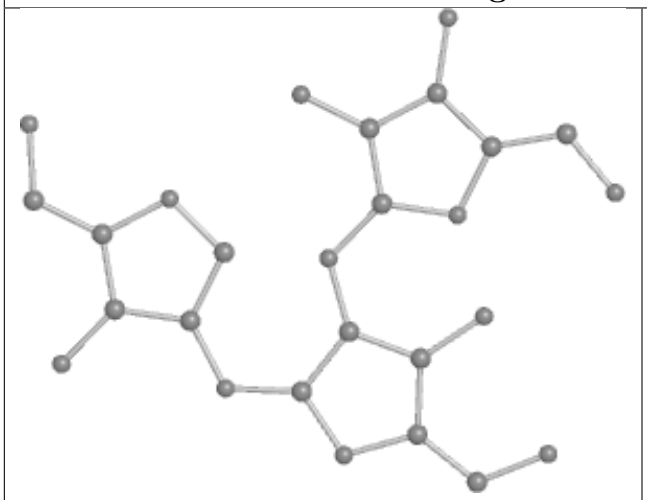
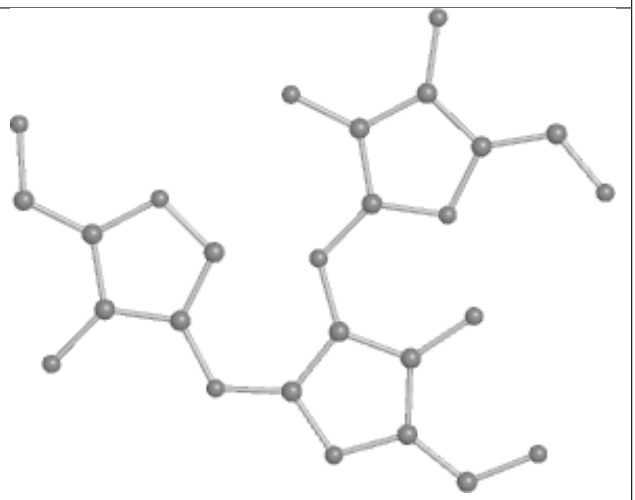
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain HC	
 Bond lengths	 Bond angles
 Torsions	 Rings

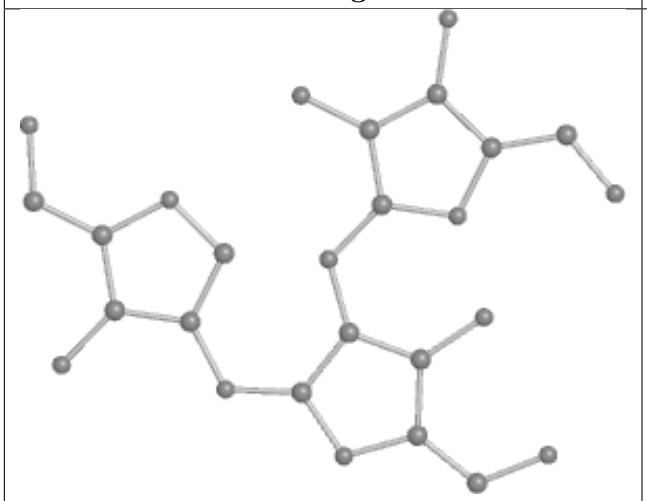
Oligosaccharide Chain IC



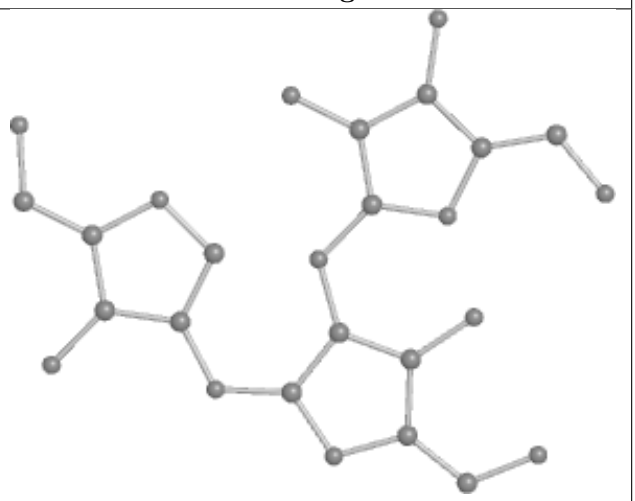
Bond lengths



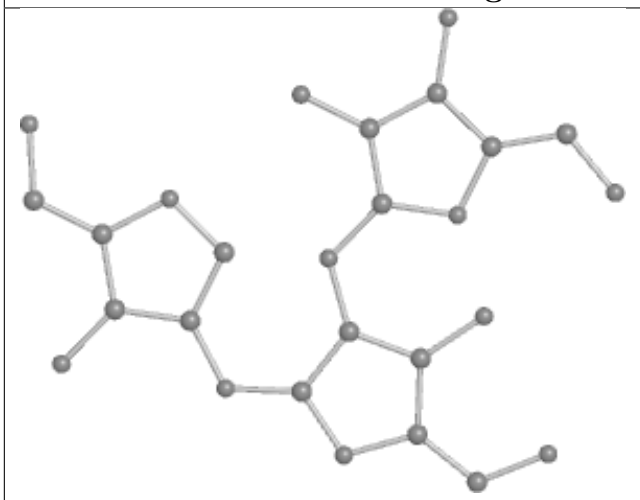
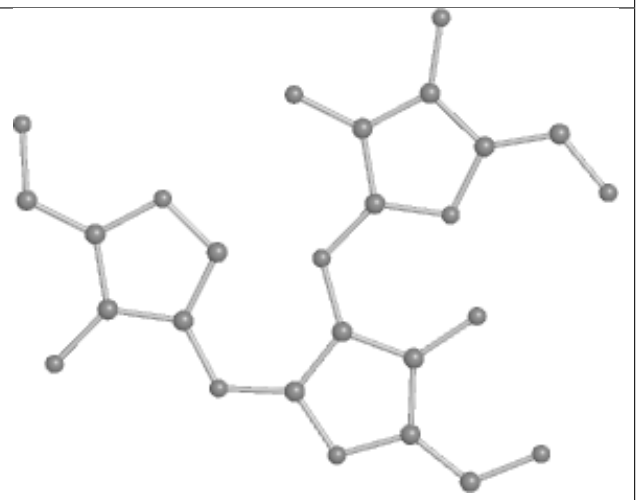
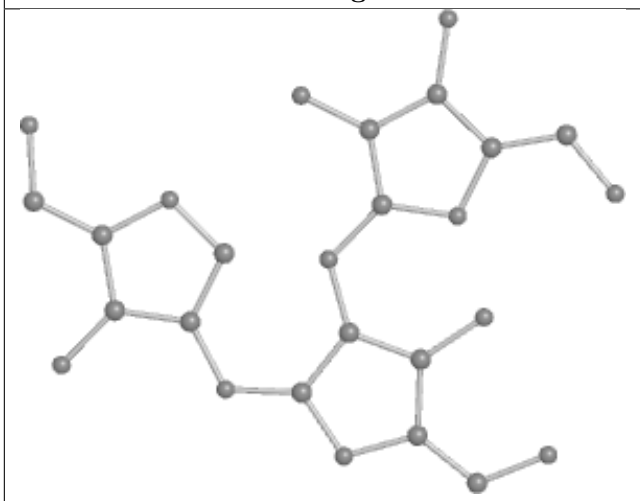
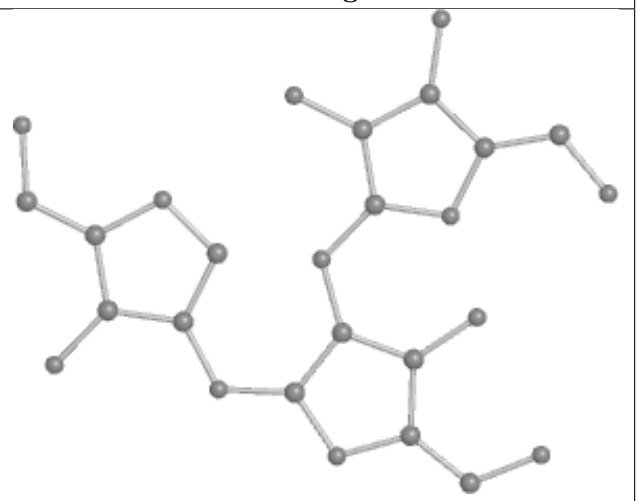
Bond angles

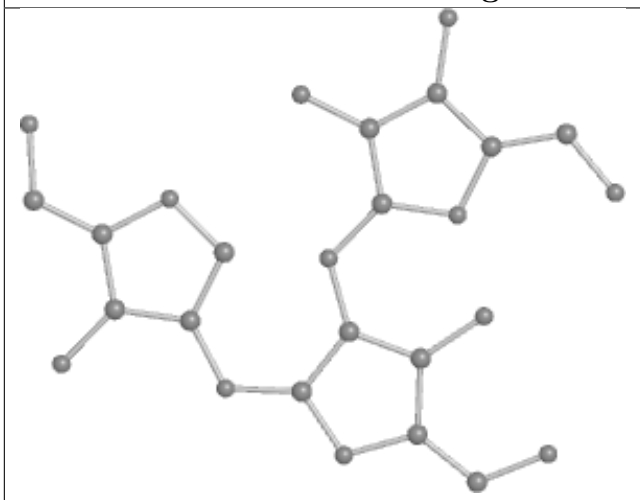
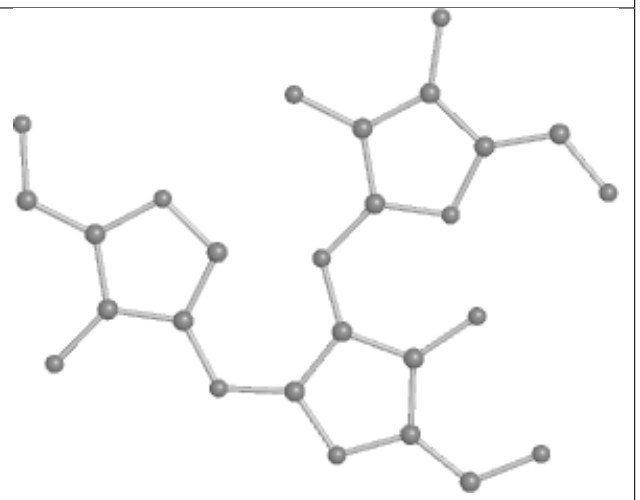
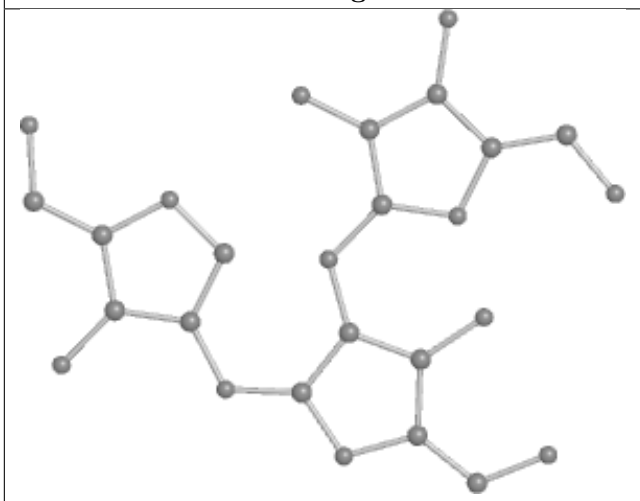
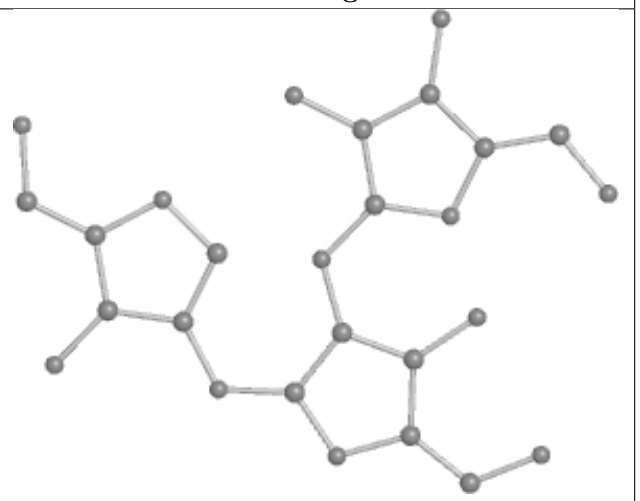


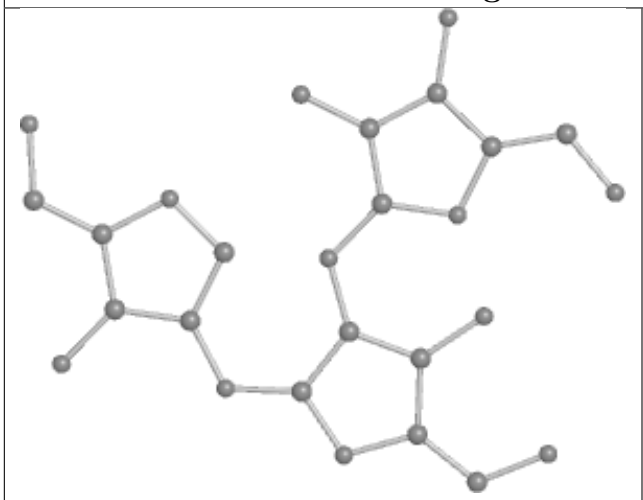
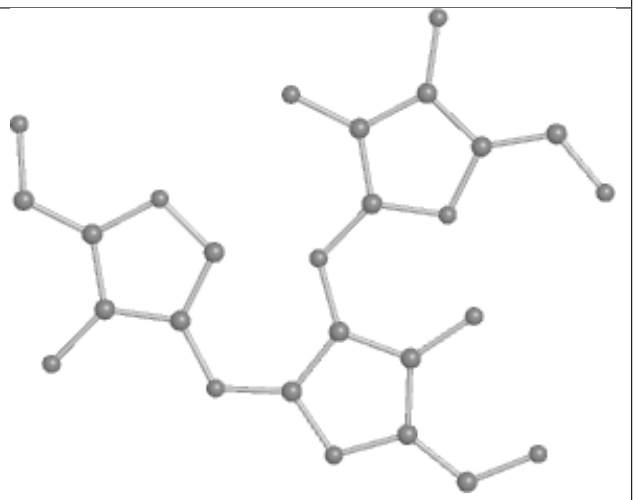
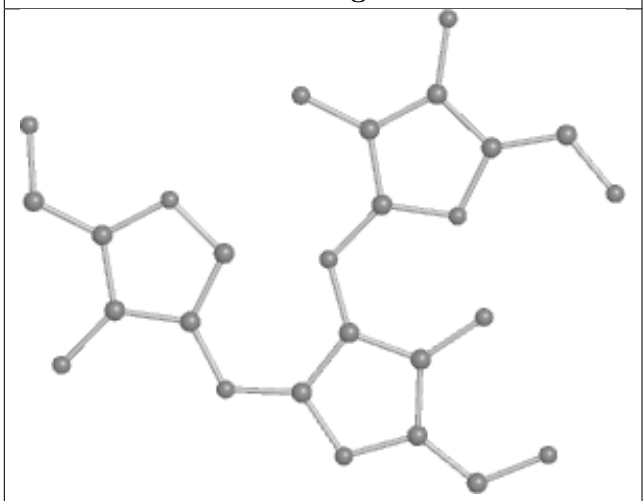
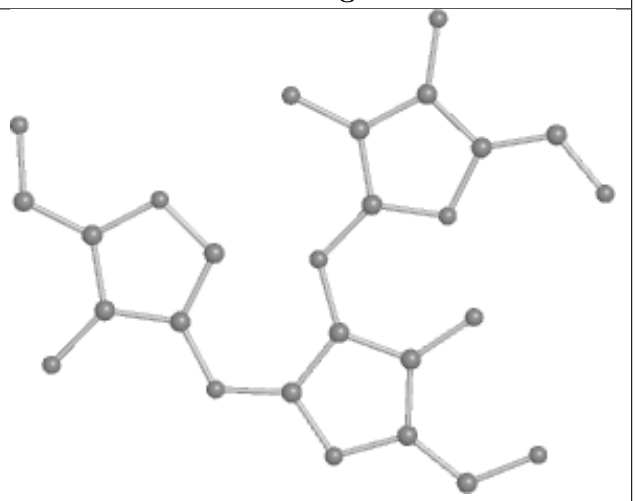
Torsions

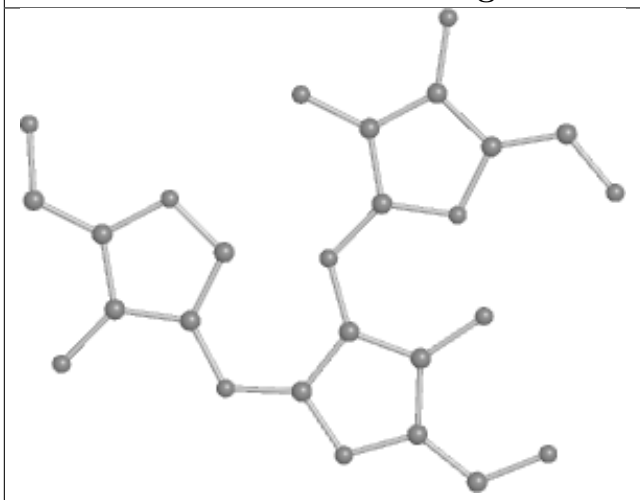
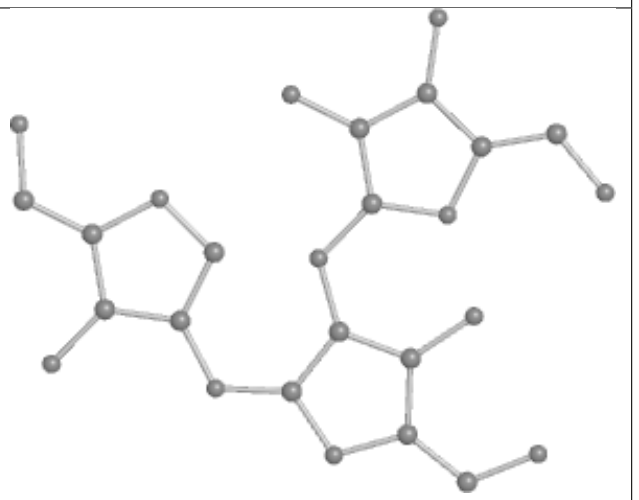
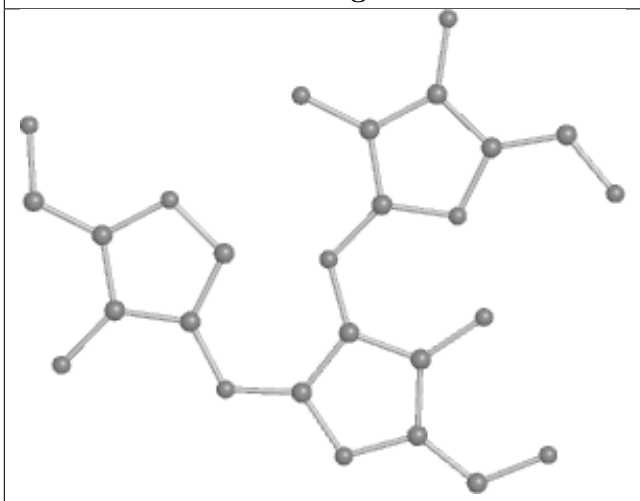
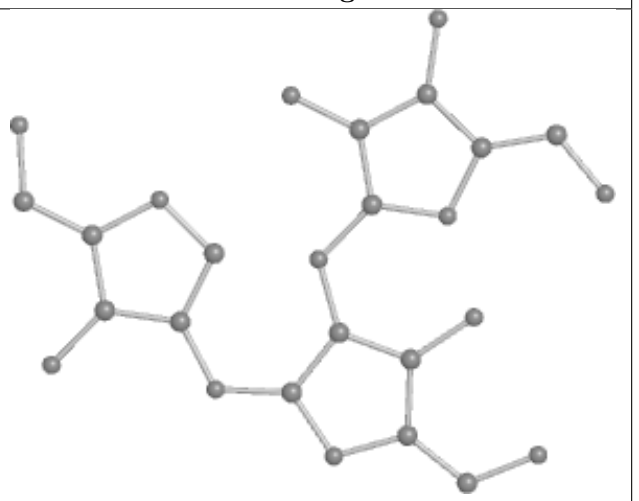


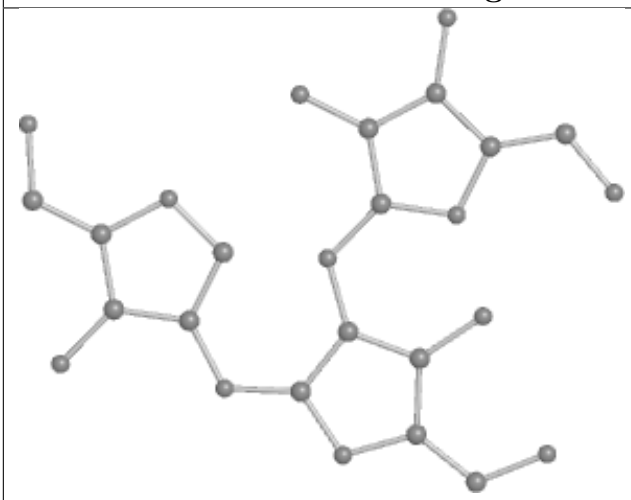
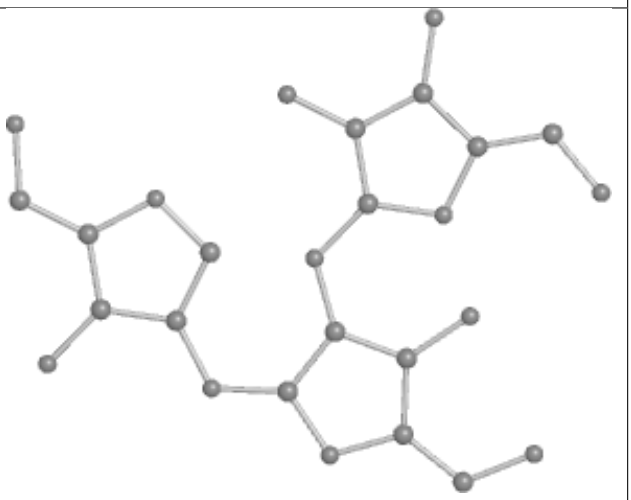
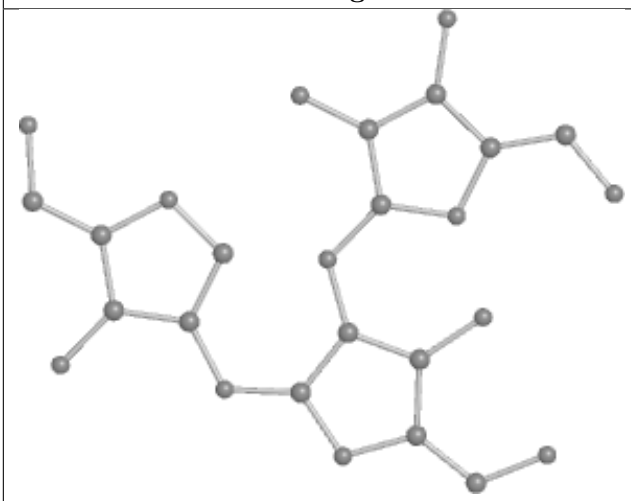
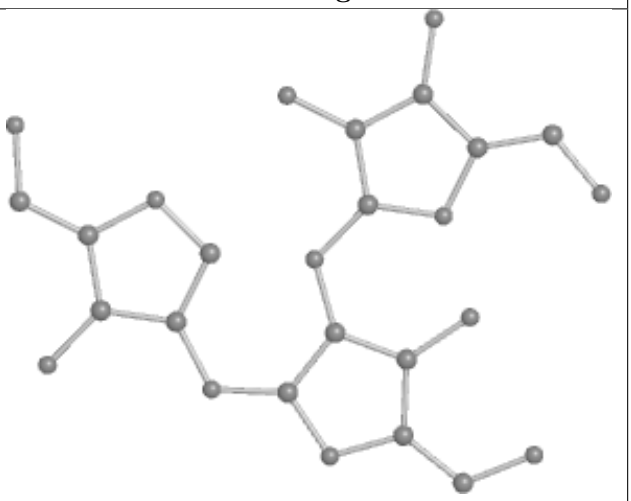
Rings

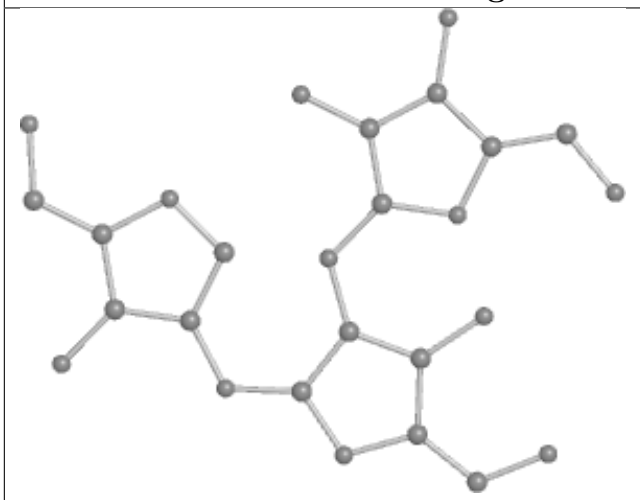
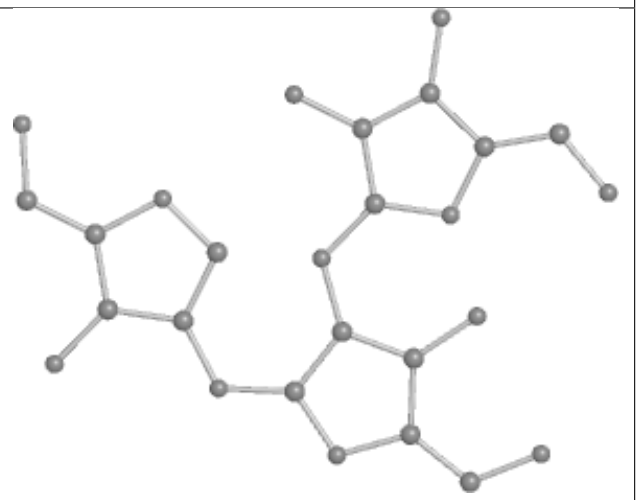
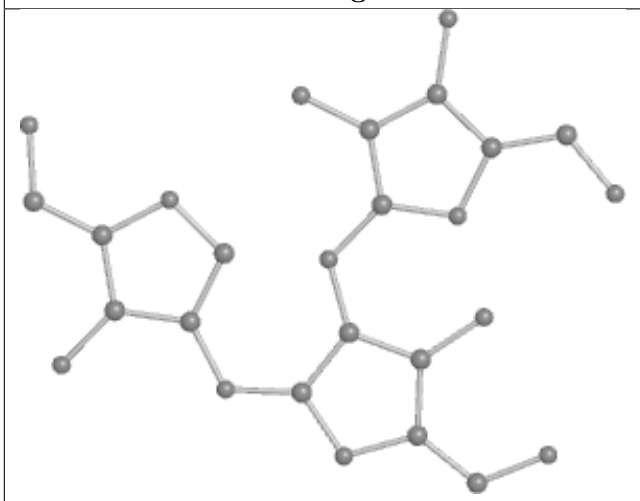
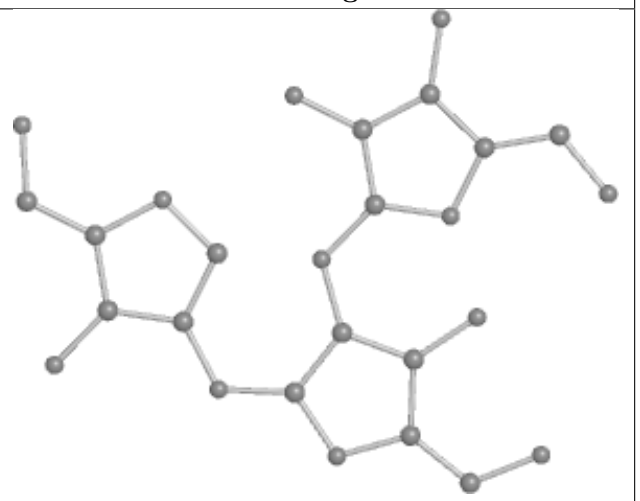
Oligosaccharide Chain LC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

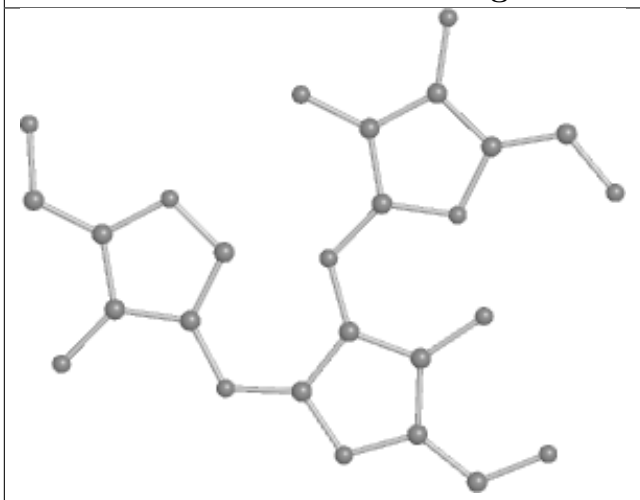
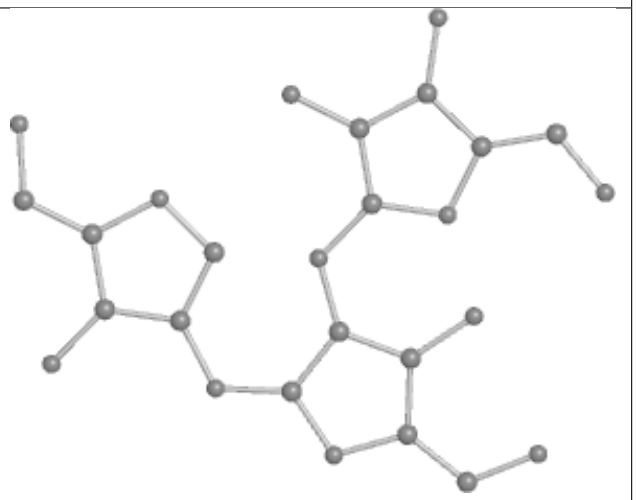
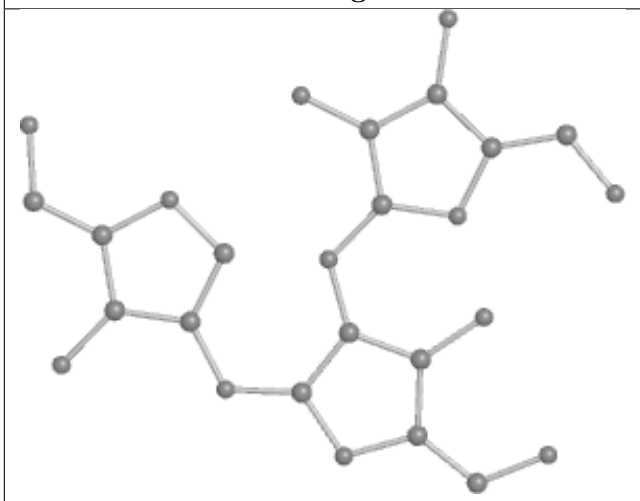
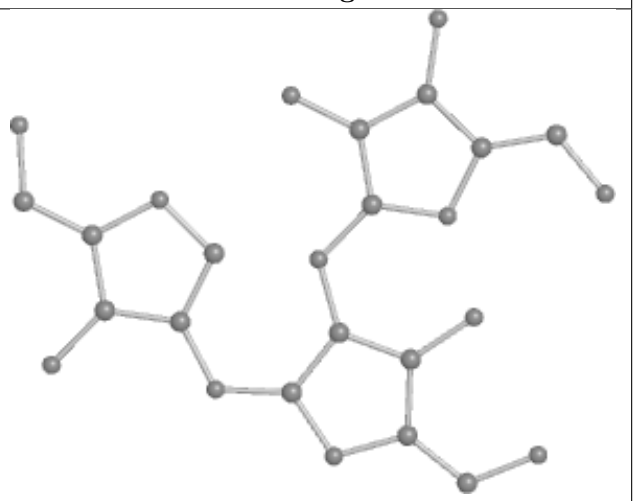
Oligosaccharide Chain NC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

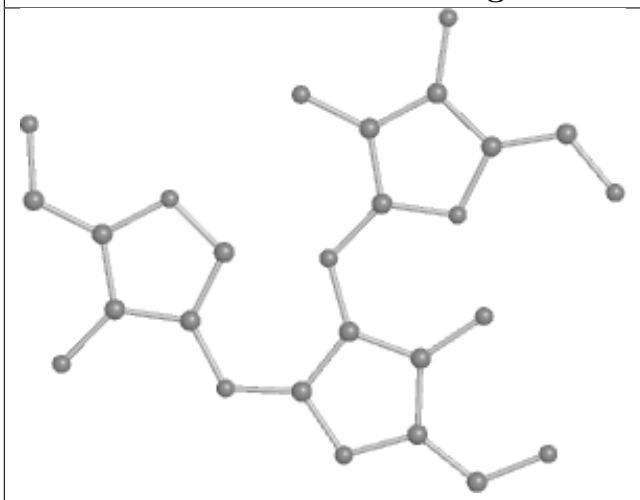
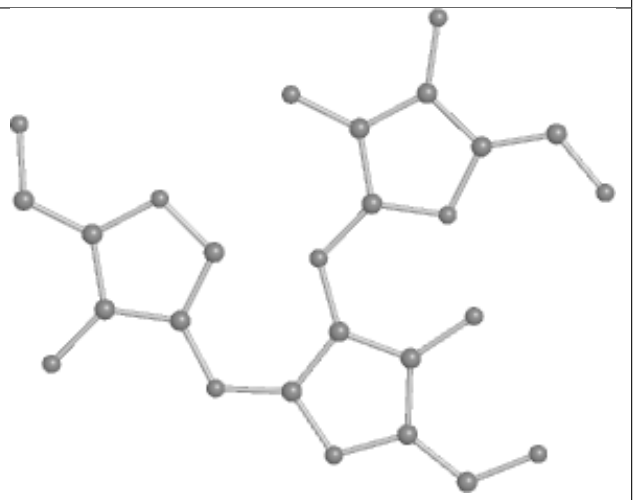
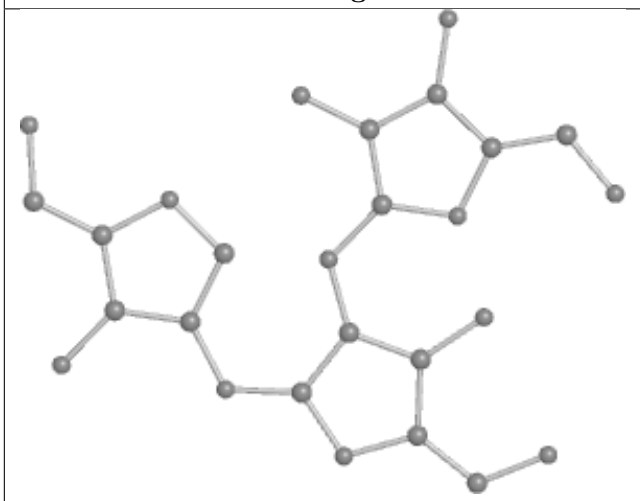
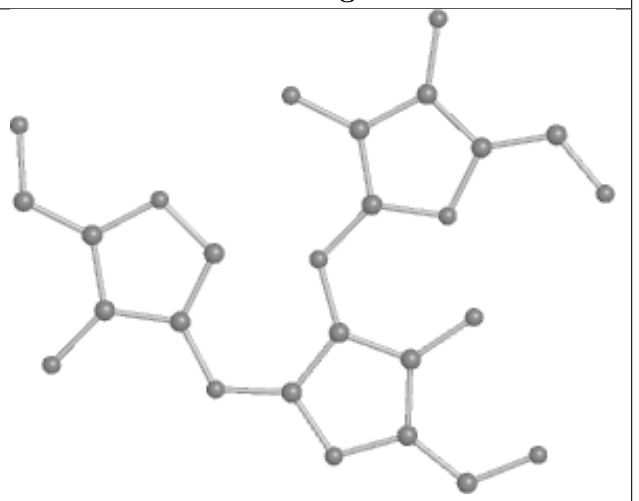
Oligosaccharide Chain TC	
 Bond lengths	 Bond angles
 Torsions	 Rings

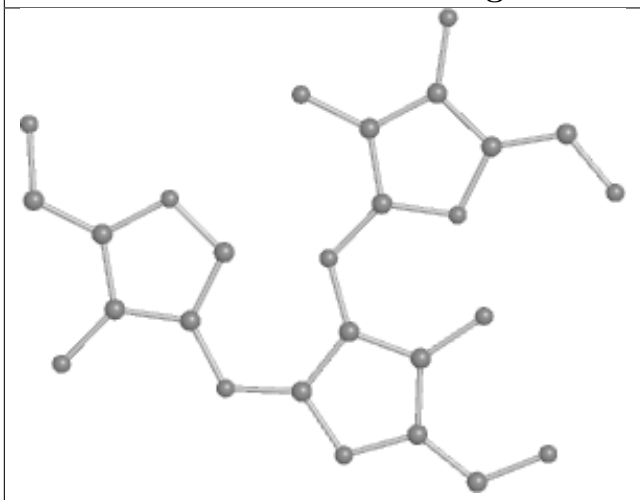
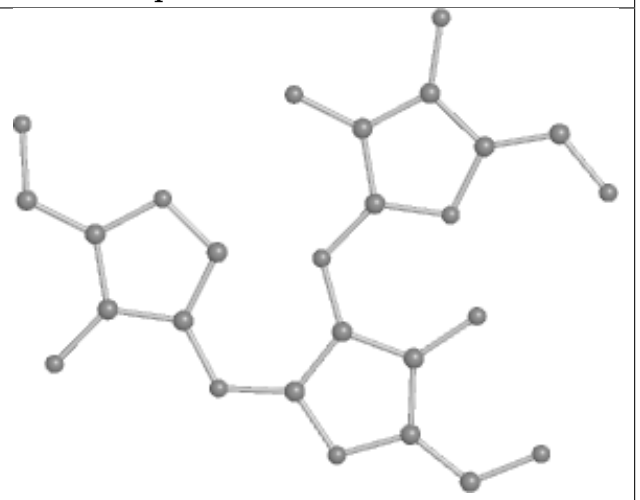
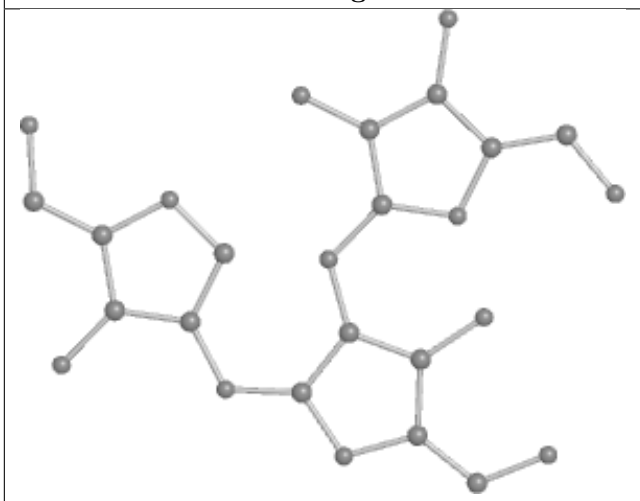
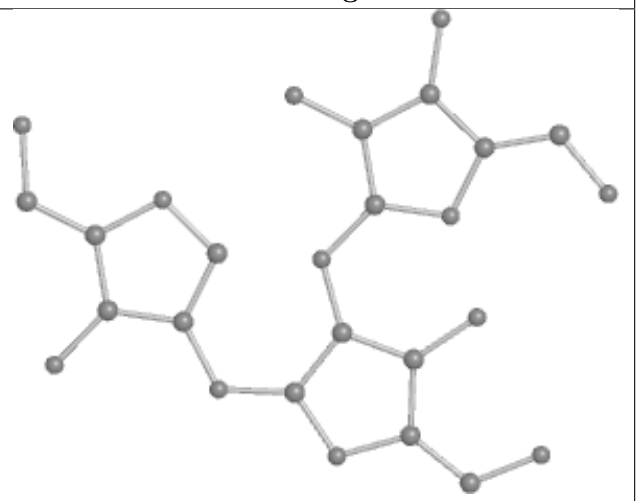
Oligosaccharide Chain WC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

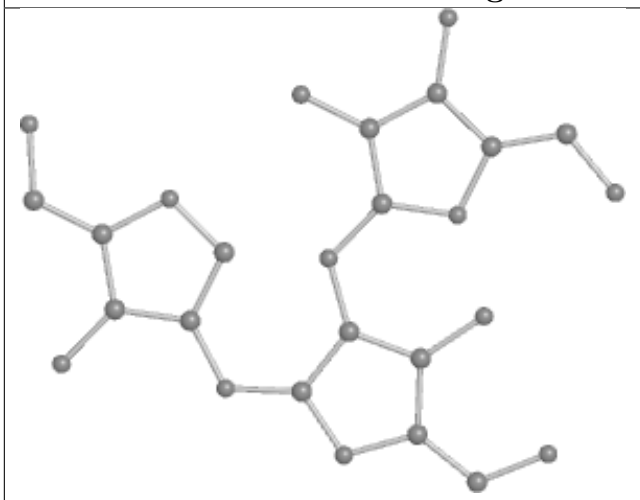
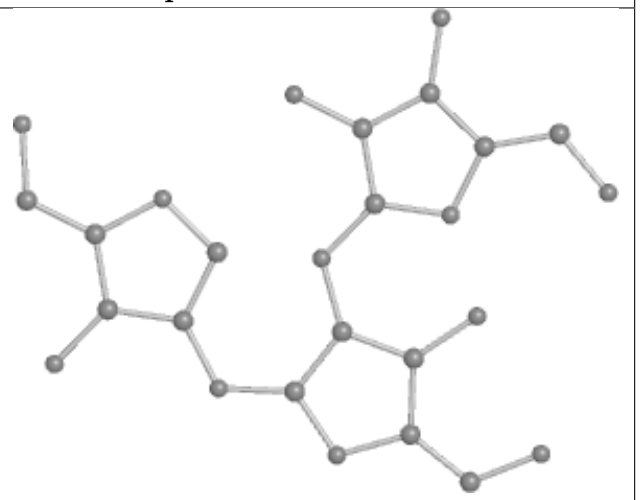
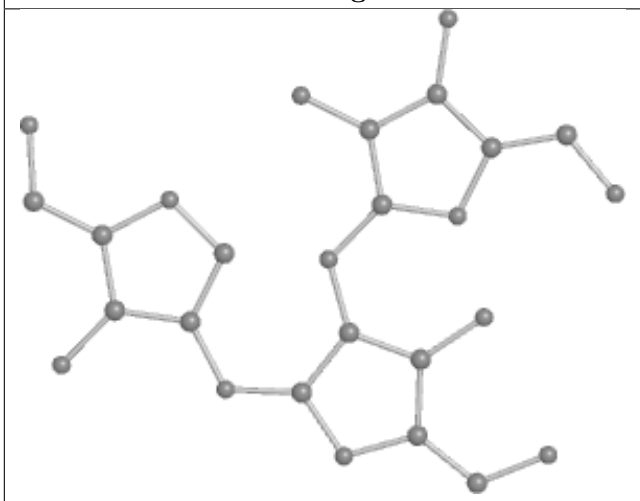
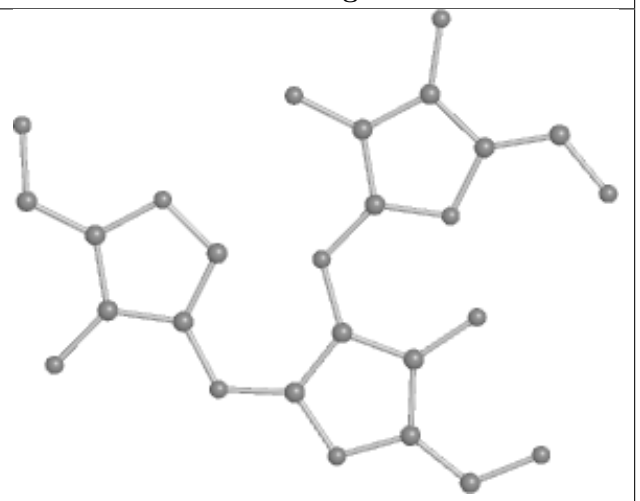
Oligosaccharide Chain dC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

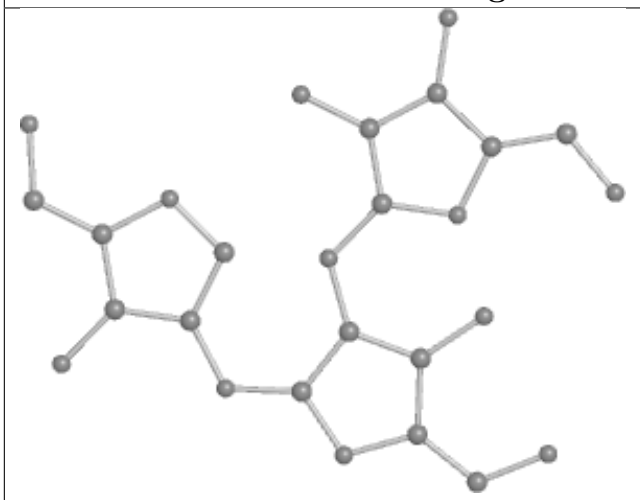
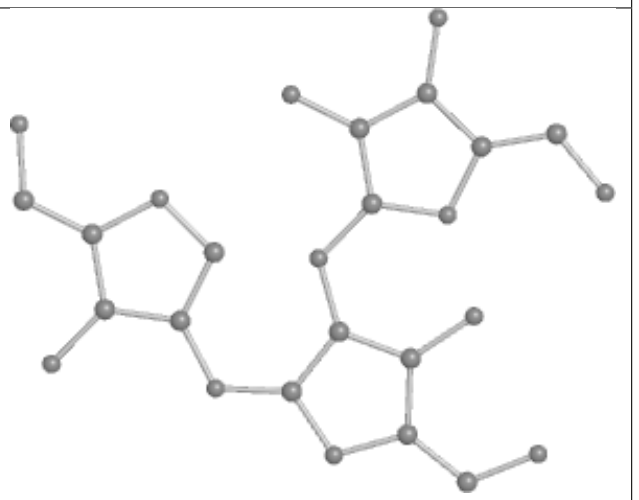
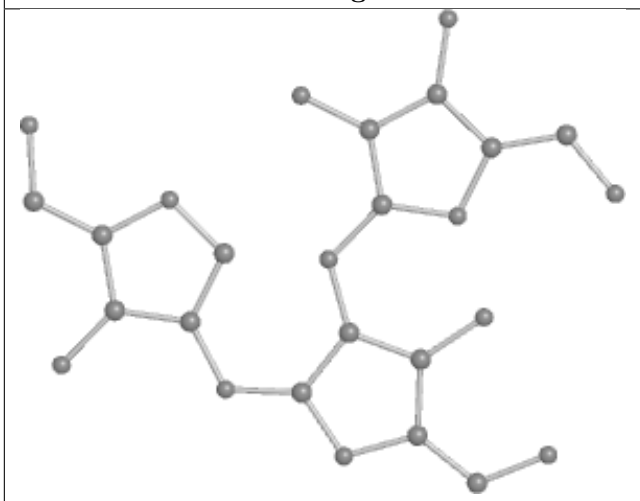
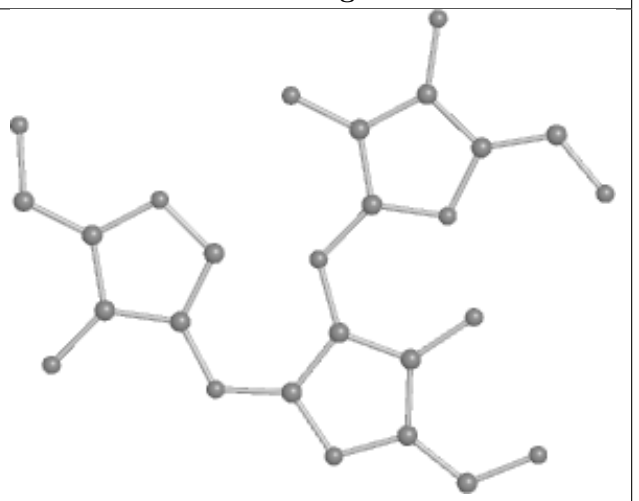
Oligosaccharide Chain eC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

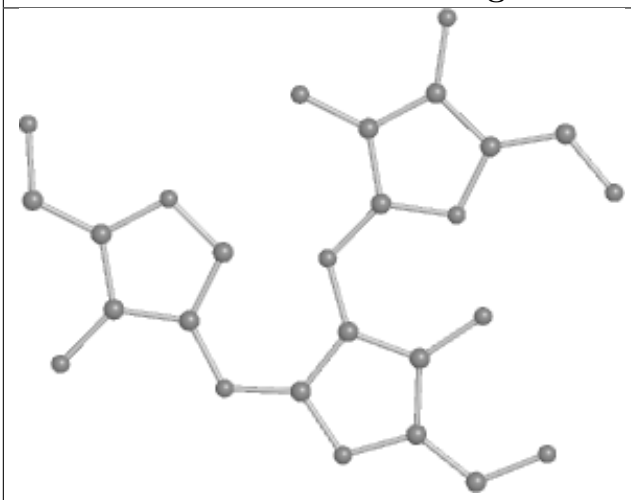
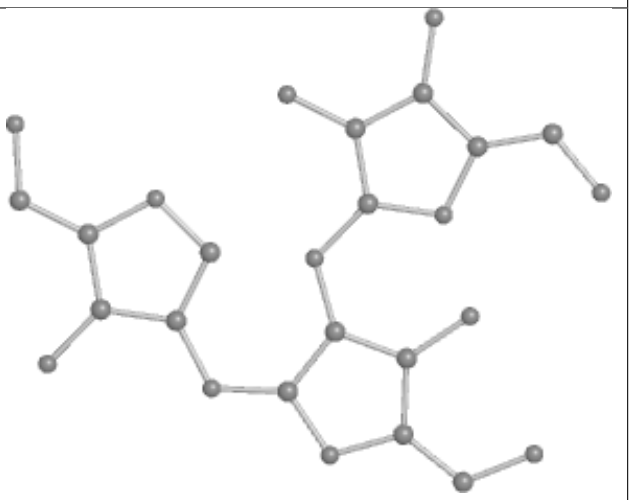
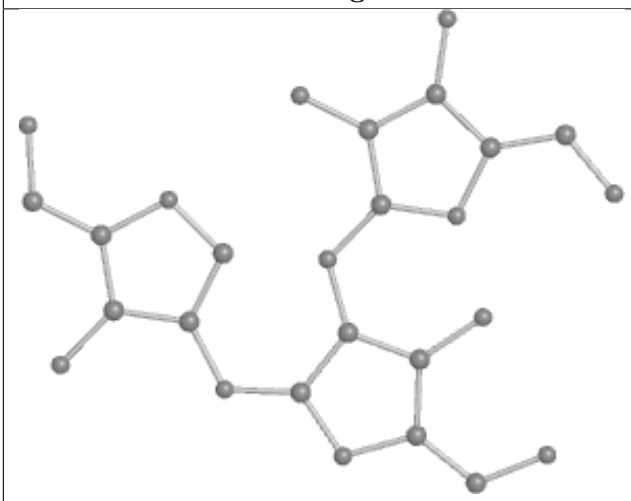
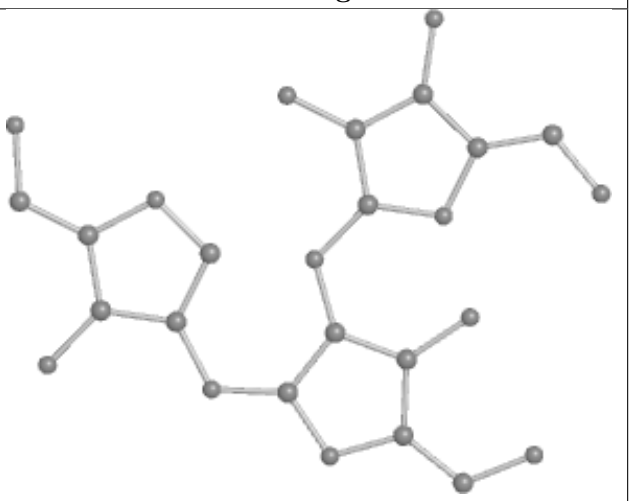
Oligosaccharide Chain lC	
 Bond lengths	 Bond angles
 Torsions	 Rings

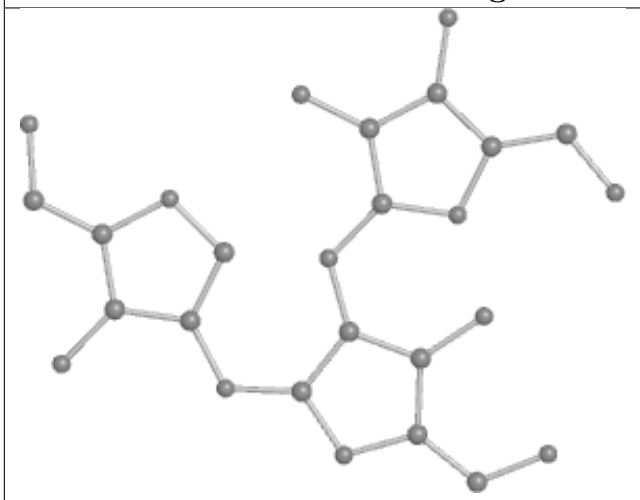
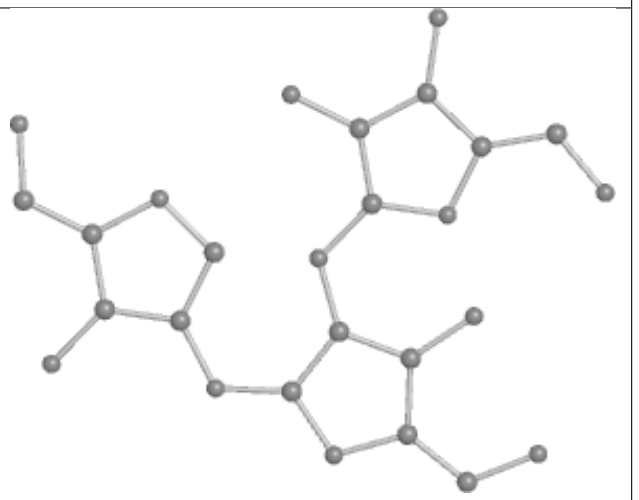
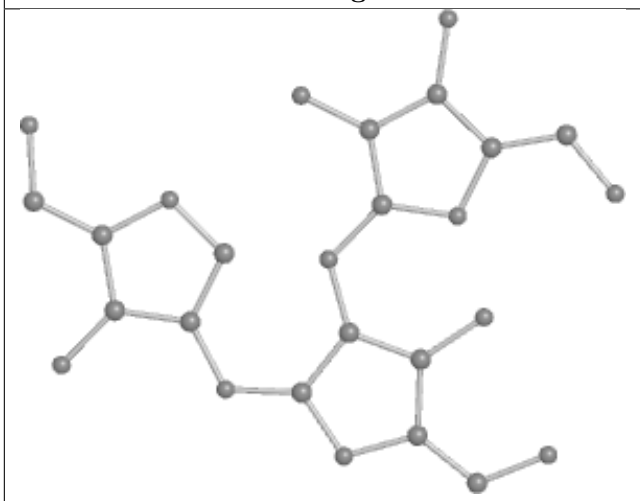
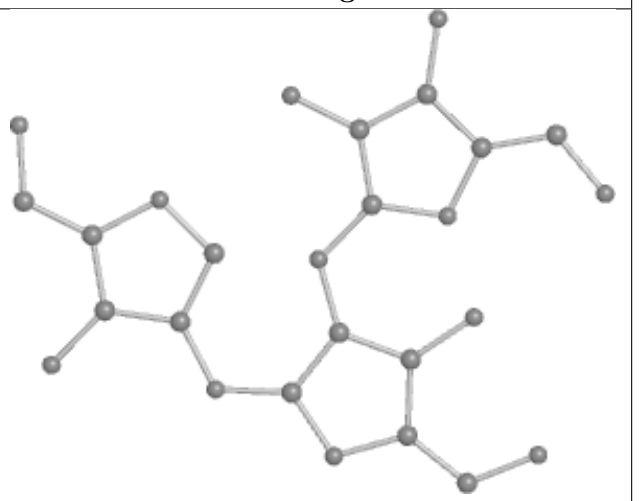
Oligosaccharide Chain oC	
 Bond lengths	 Bond angles
 Torsions	 Rings

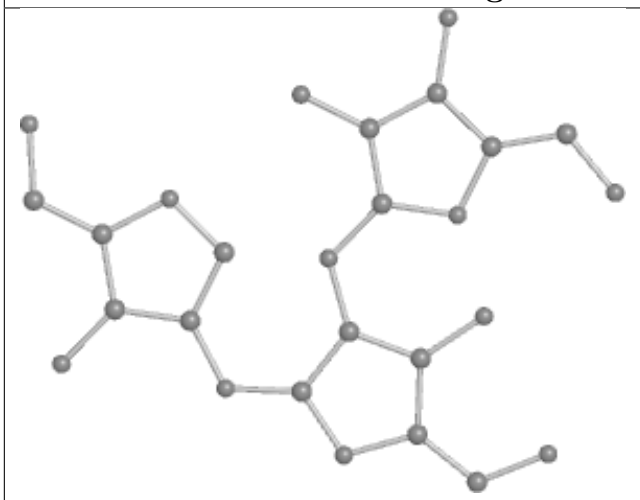
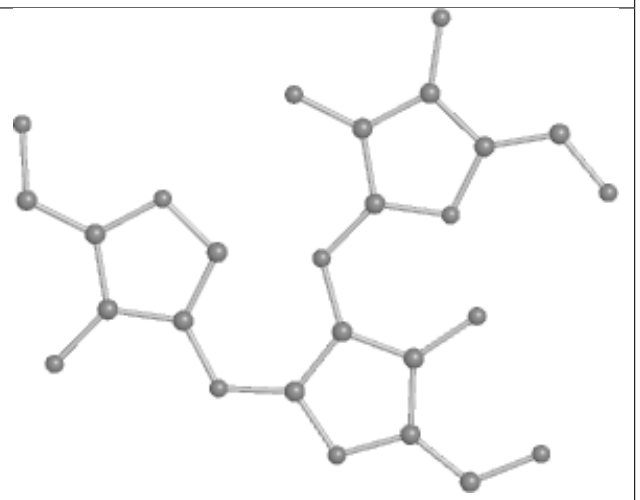
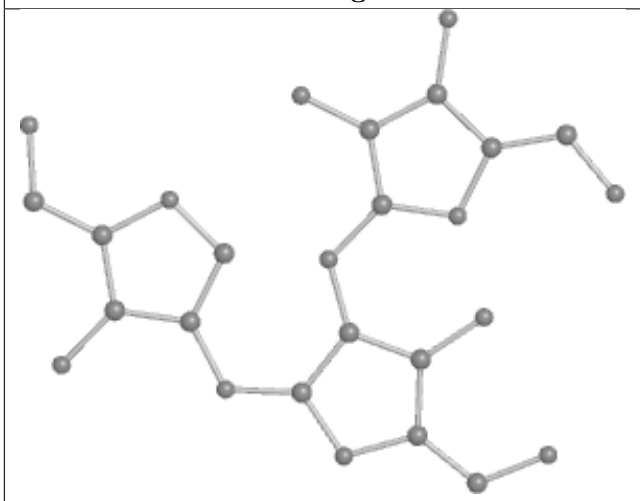
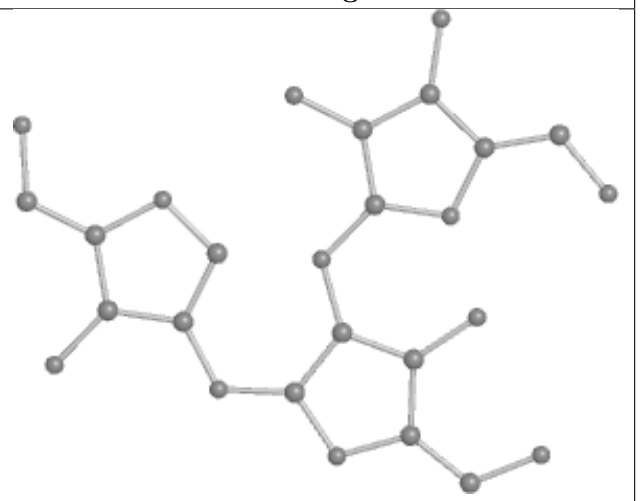
Oligosaccharide Chain pC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

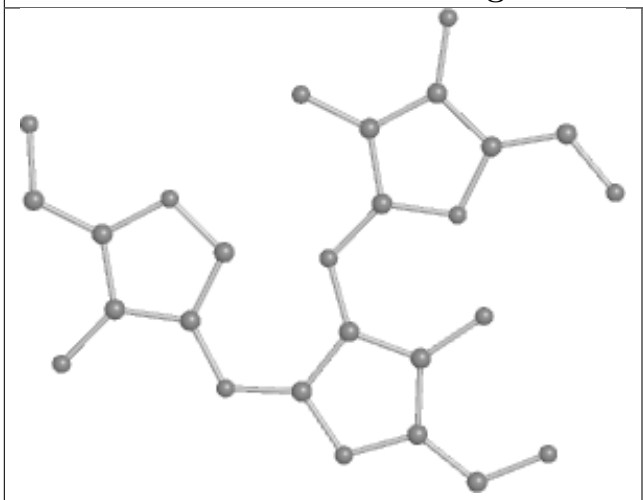
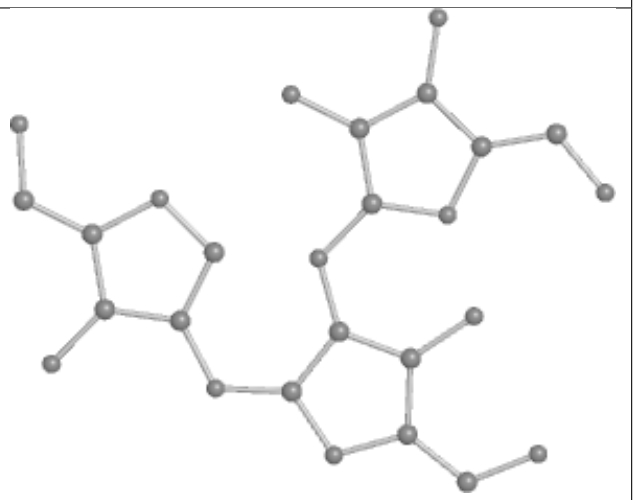
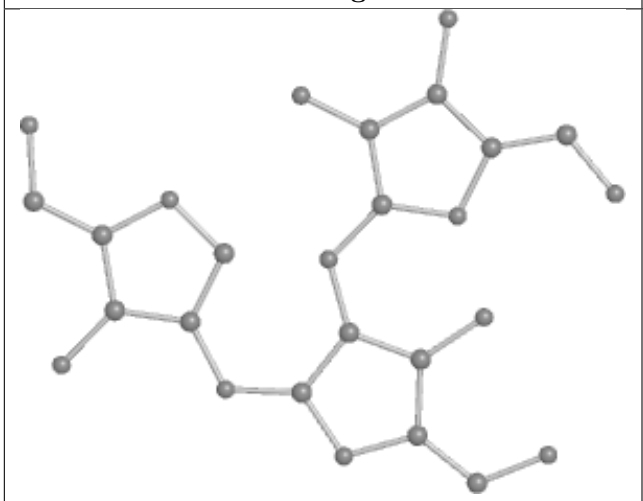
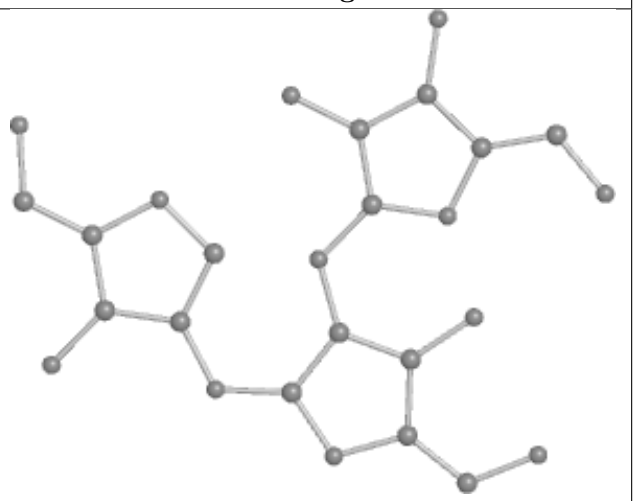
Oligosaccharide Chain qC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

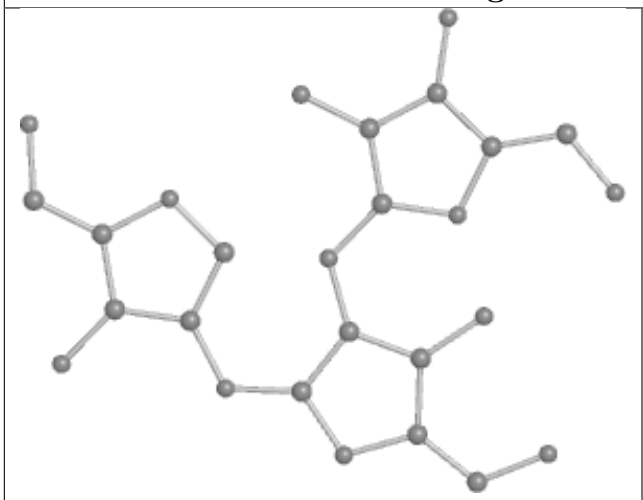
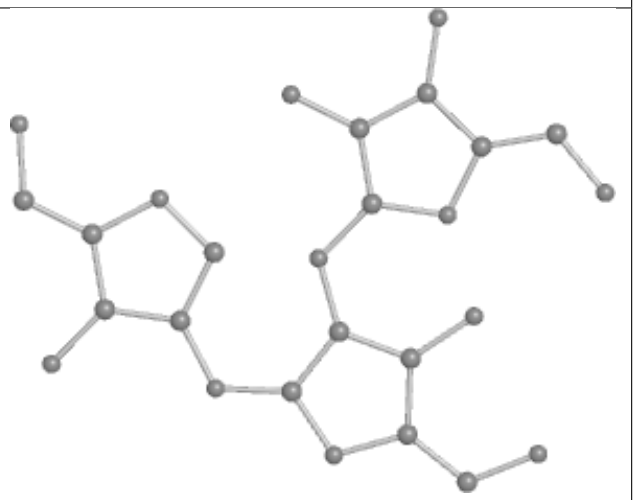
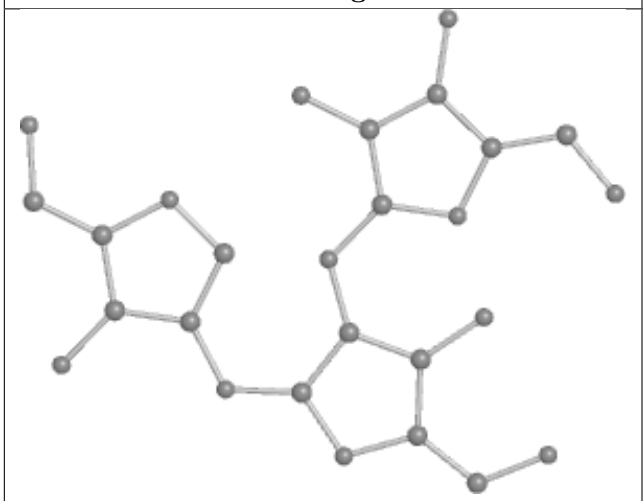
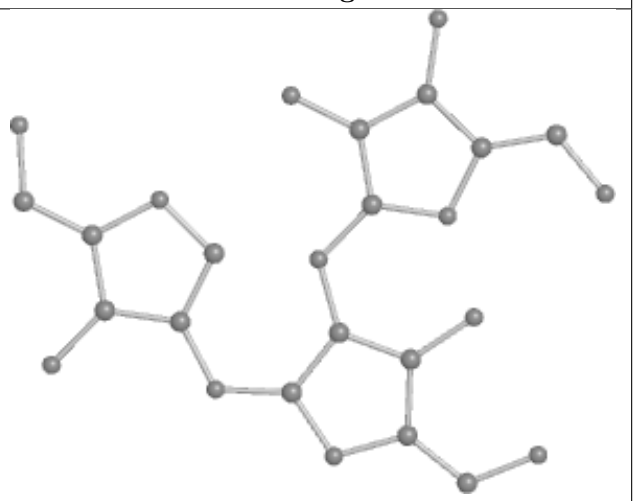
Oligosaccharide Chain rC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain sC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

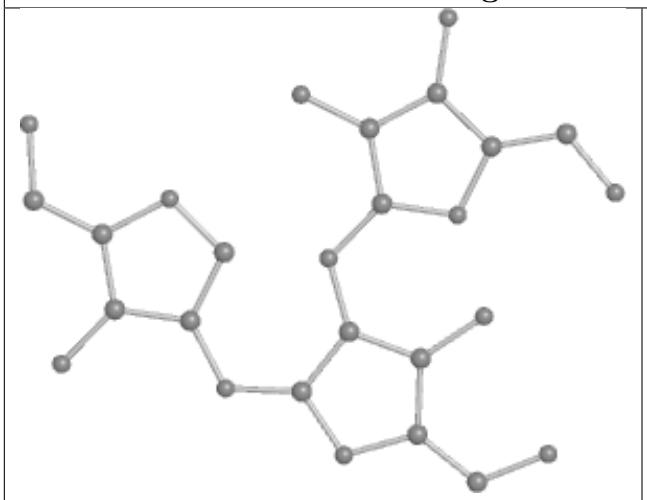
Oligosaccharide Chain tC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain uC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

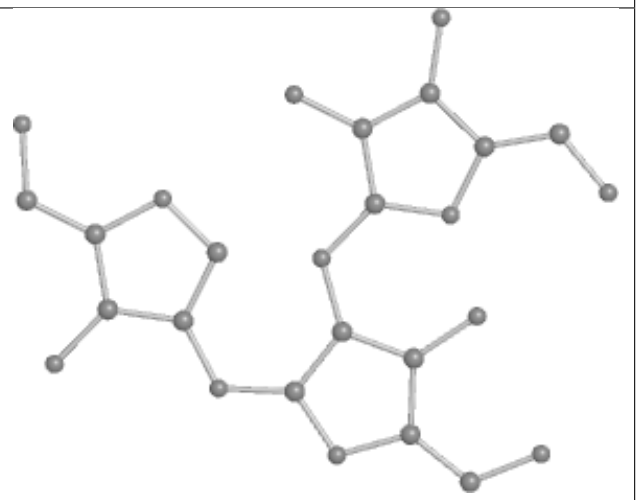
Oligosaccharide Chain 8C	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 9C	
 Bond lengths	 Bond angles
 Torsions	 Rings

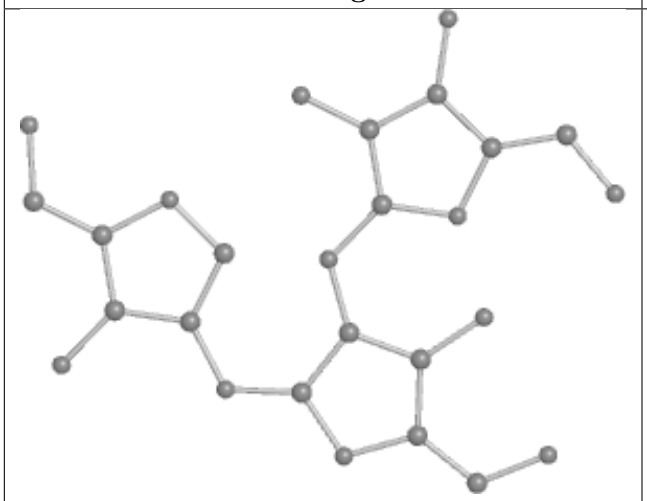
Oligosaccharide Chain DD



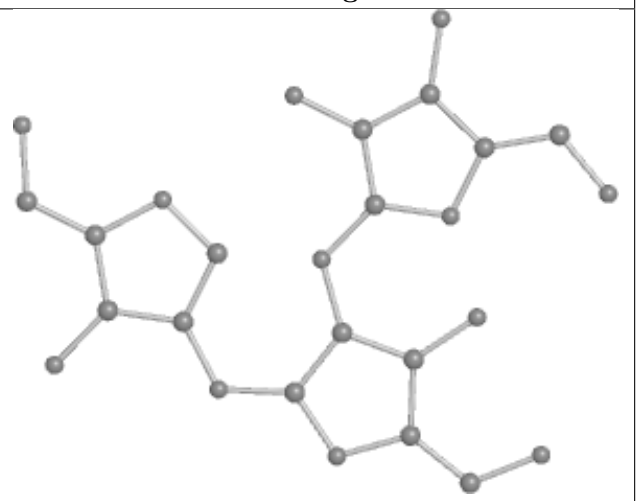
Bond lengths



Bond angles

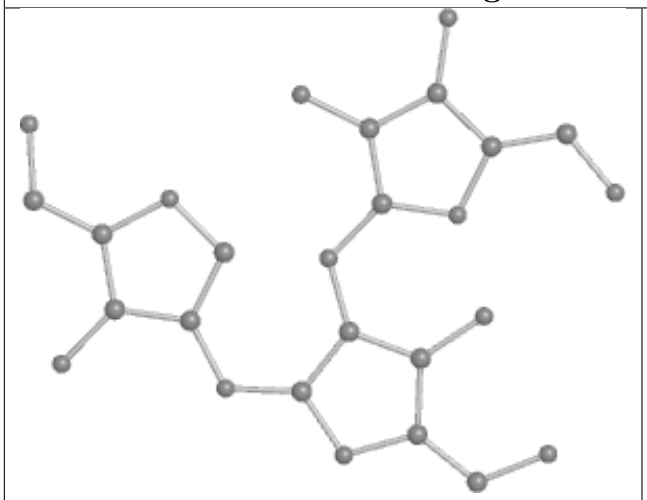


Torsions

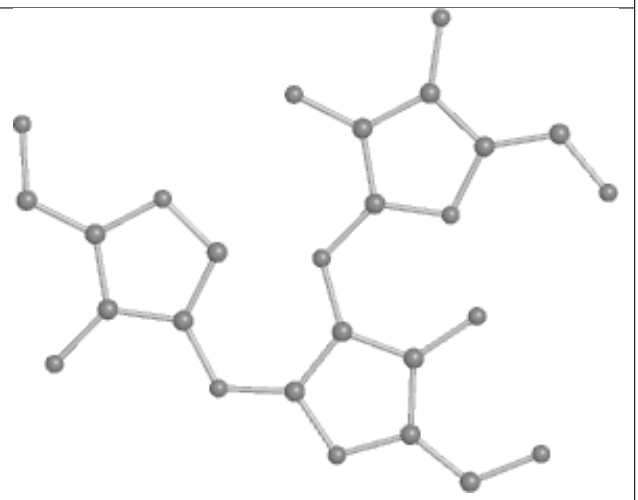


Rings

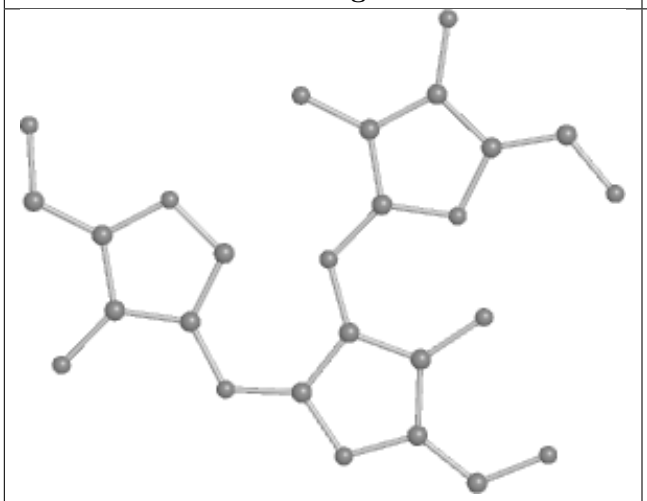
Oligosaccharide Chain ED



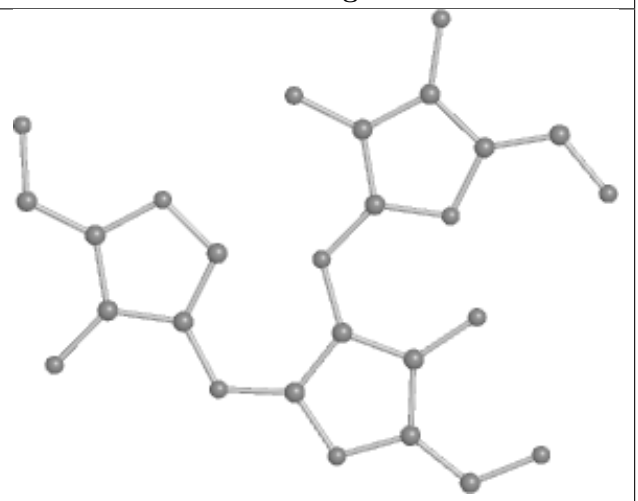
Bond lengths



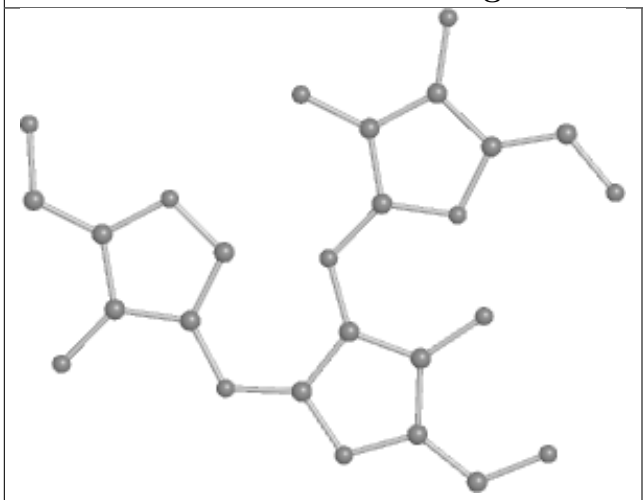
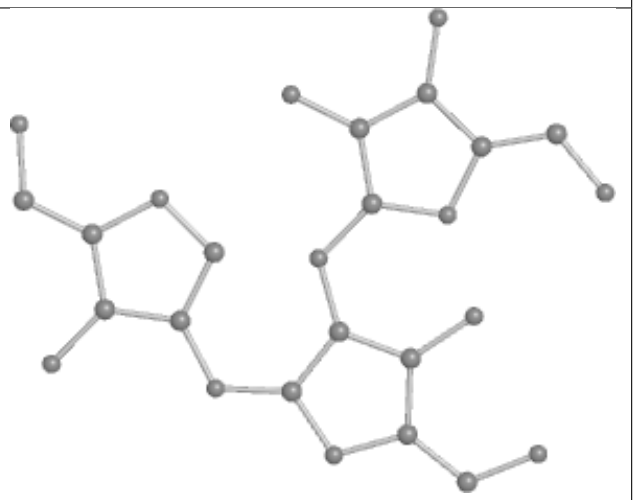
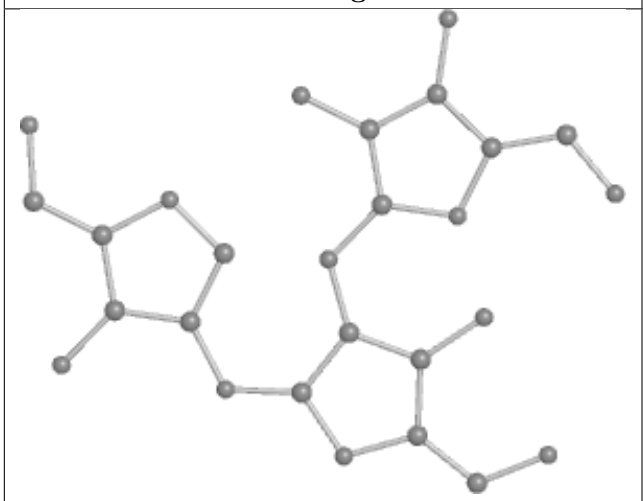
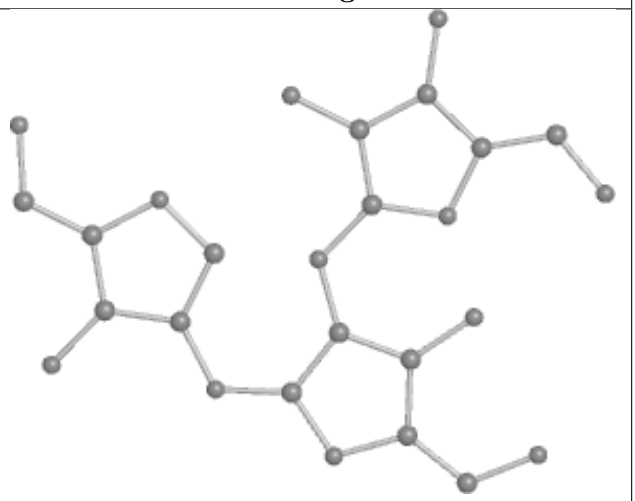
Bond angles

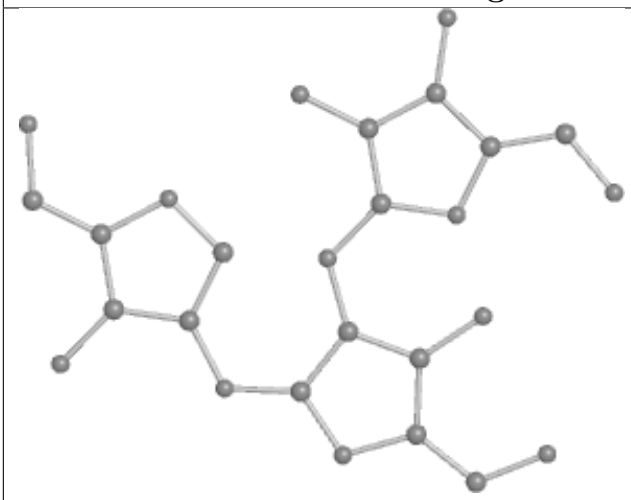
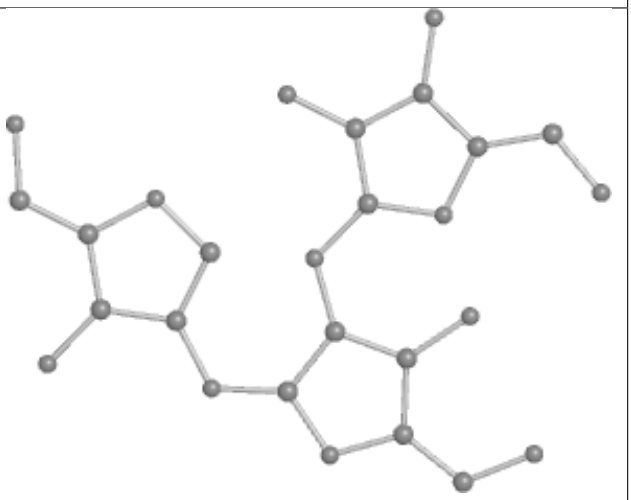
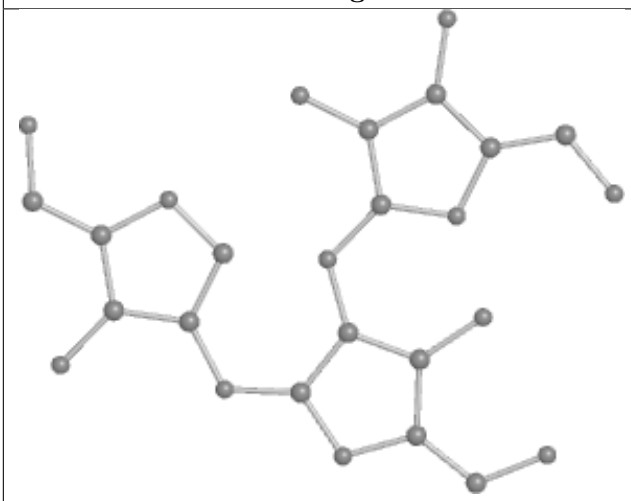
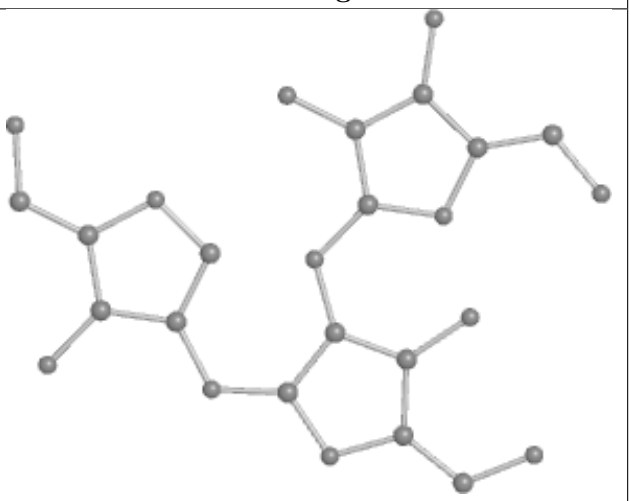


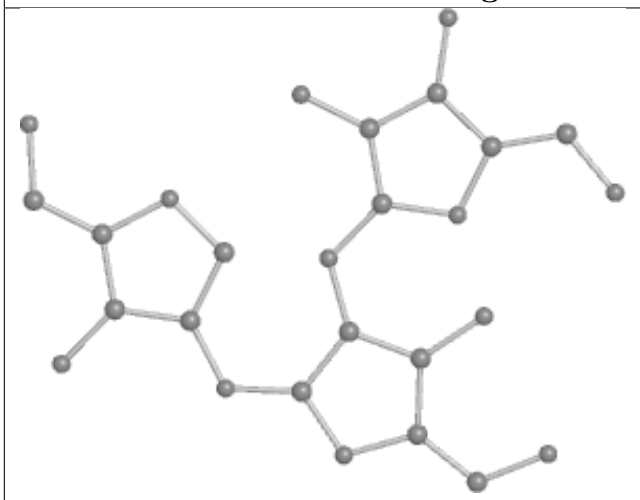
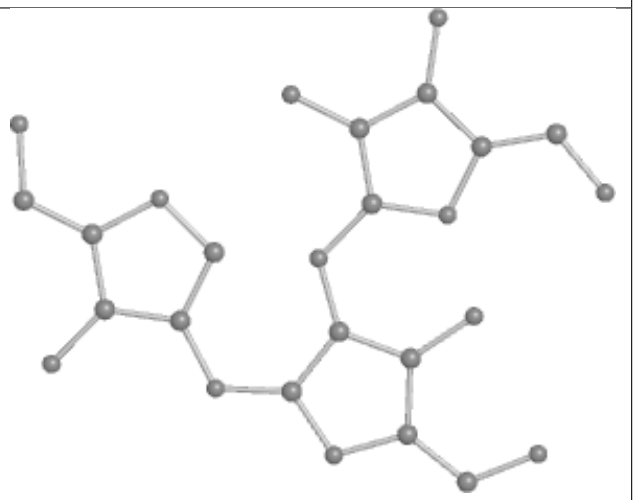
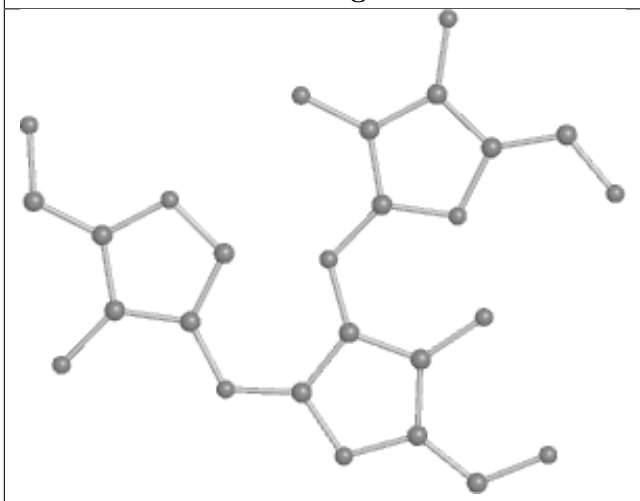
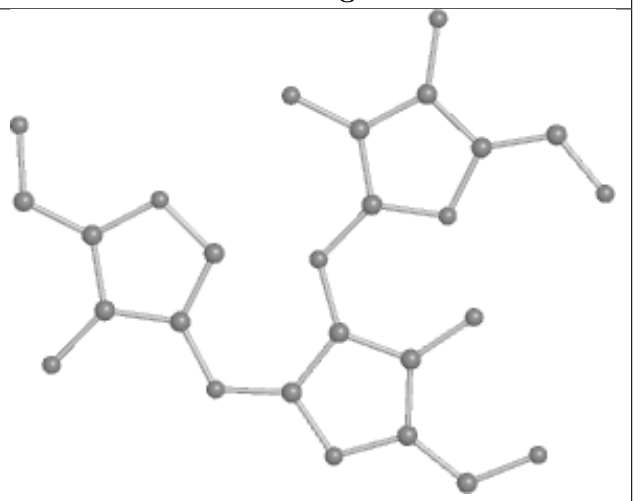
Torsions



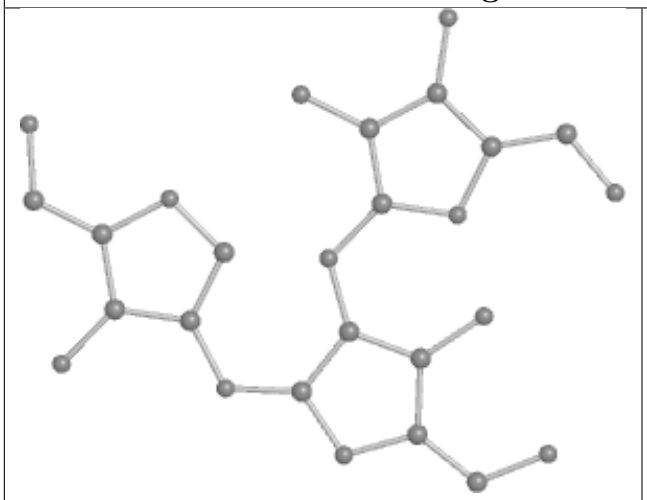
Rings

Oligosaccharide Chain FD	
 Bond lengths	 Bond angles
 Torsions	 Rings

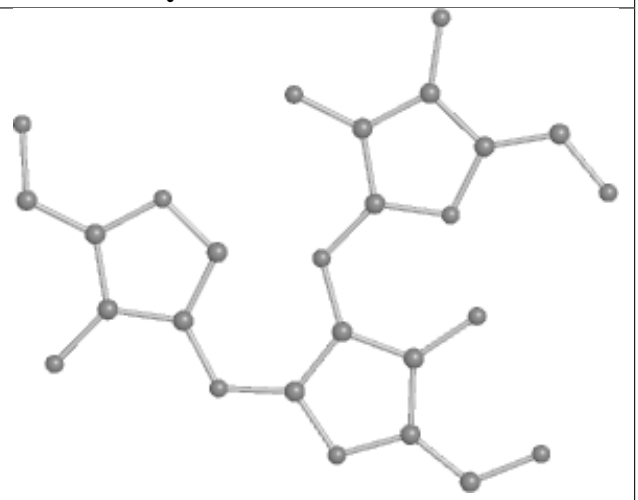
Oligosaccharide Chain ID	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain KD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

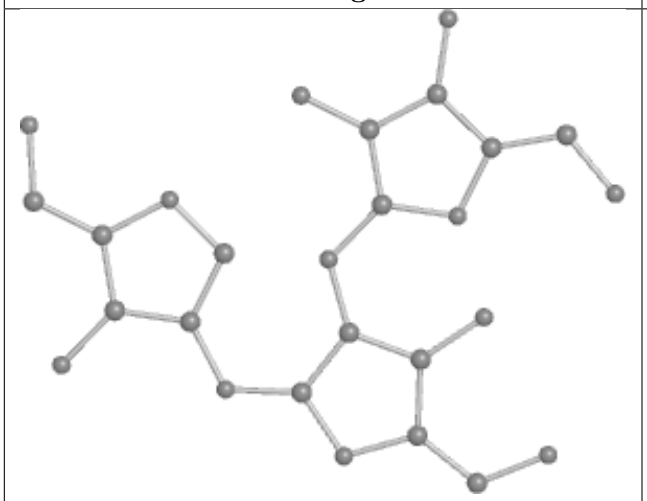
Oligosaccharide Chain QD



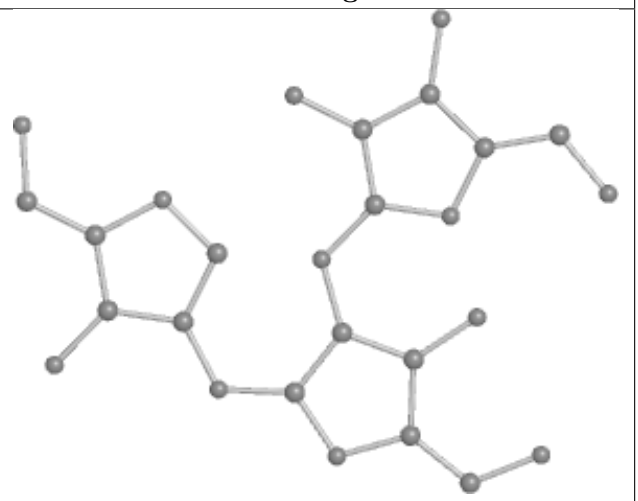
Bond lengths



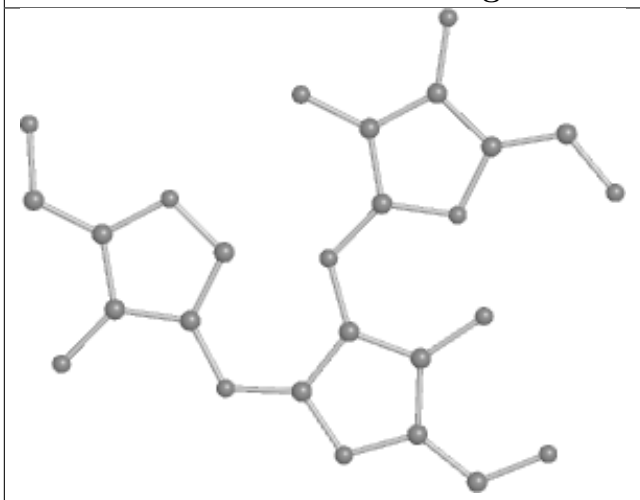
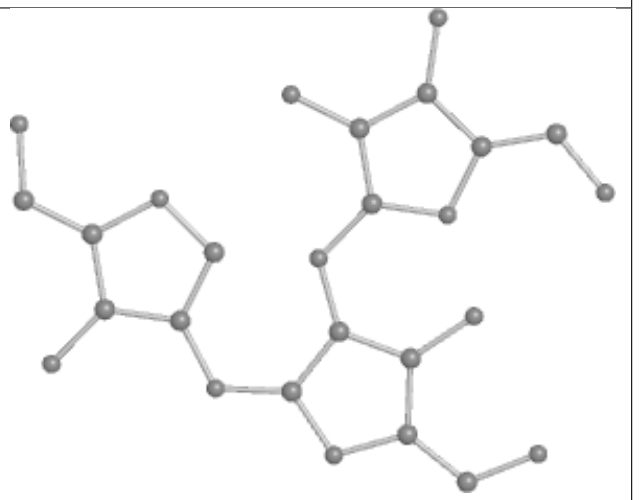
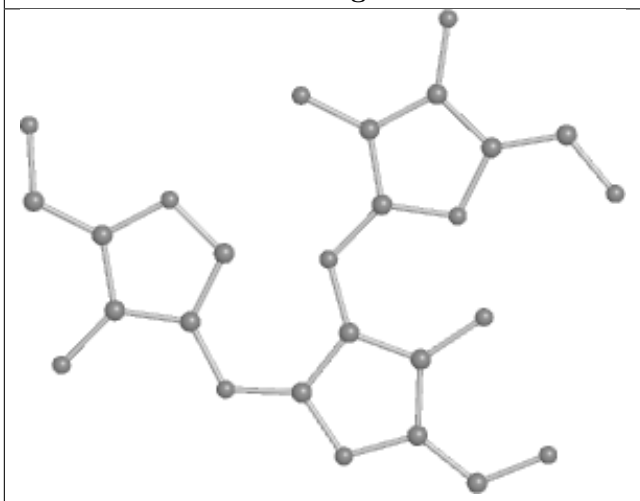
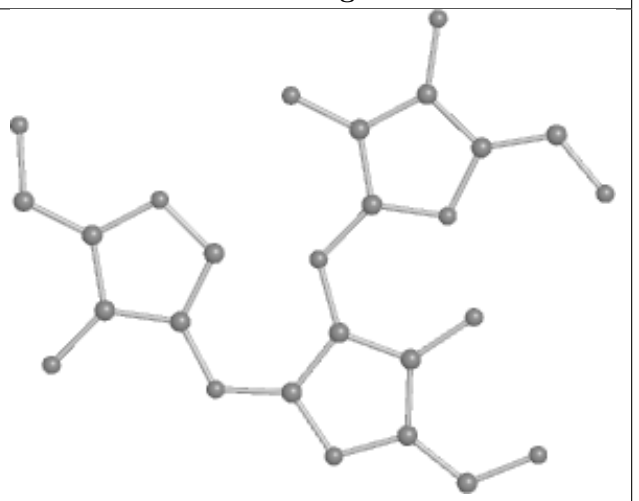
Bond angles

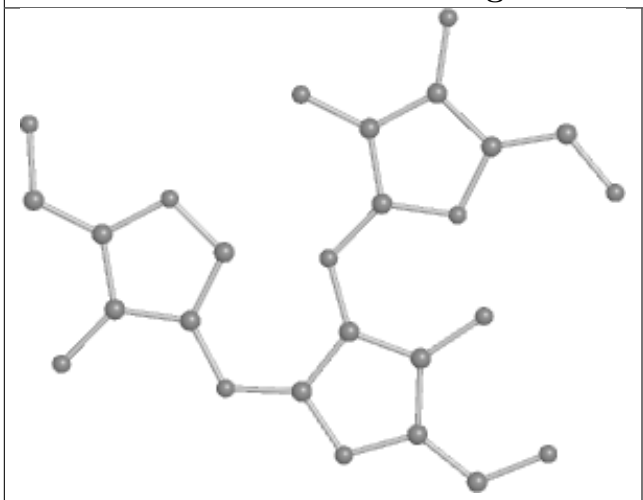
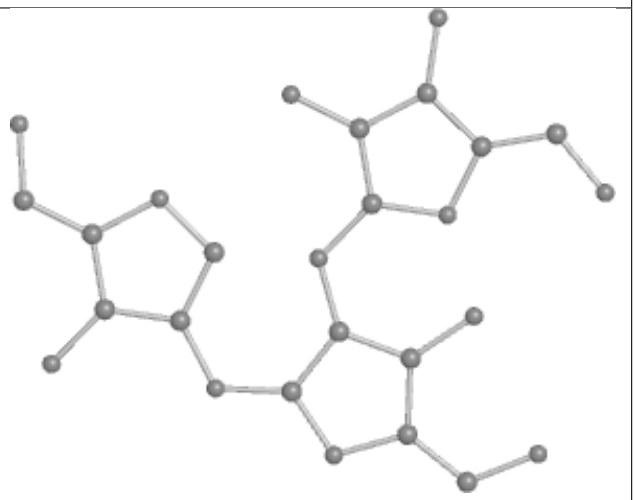
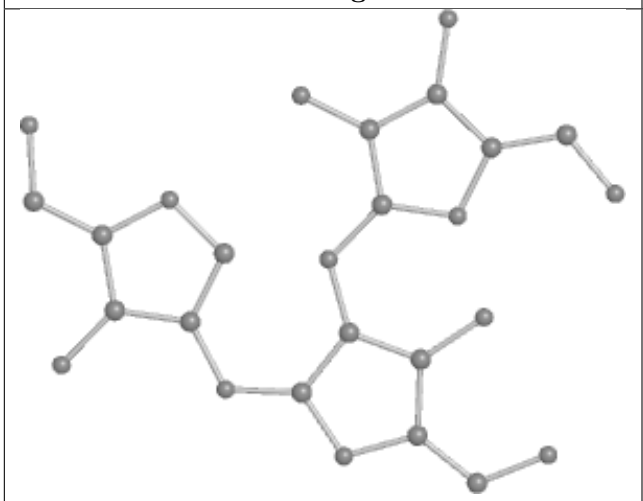
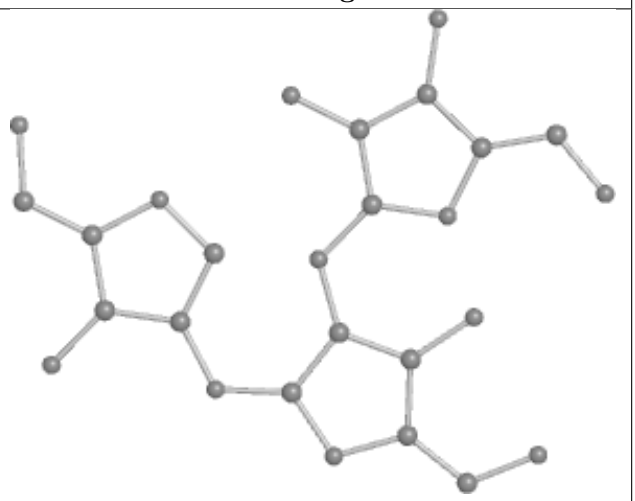


Torsions

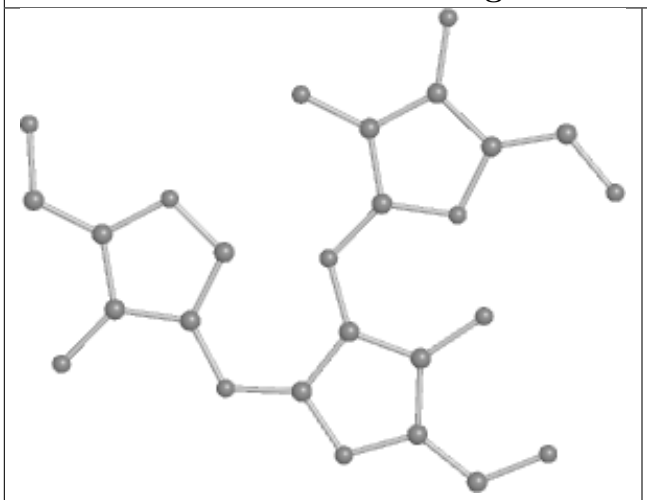


Rings

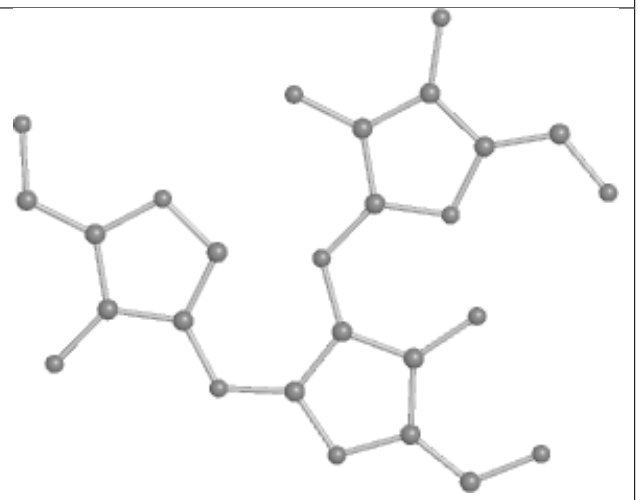
Oligosaccharide Chain TD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain aD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

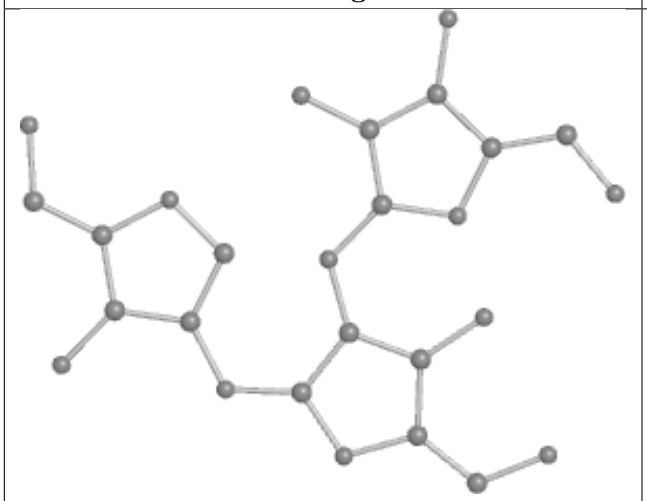
Oligosaccharide Chain bD



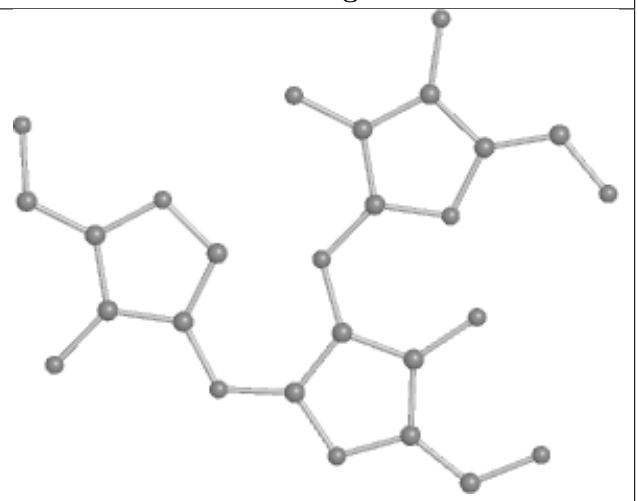
Bond lengths



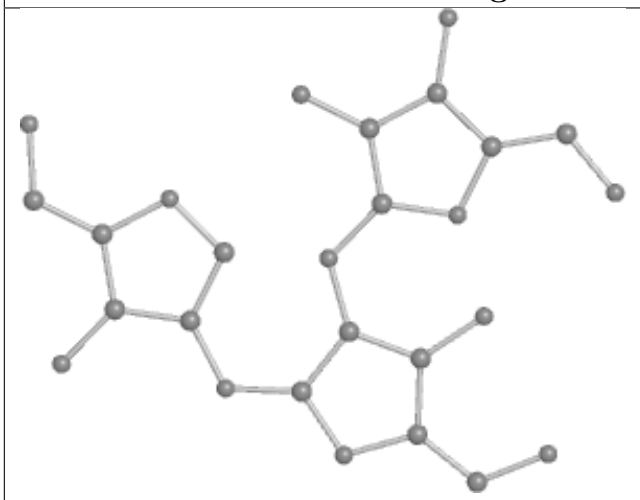
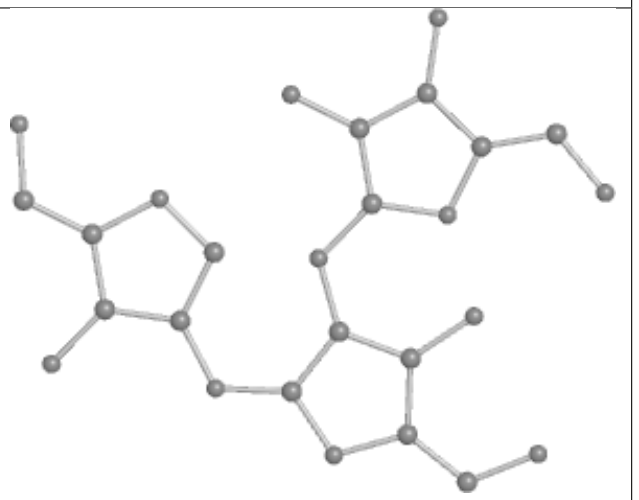
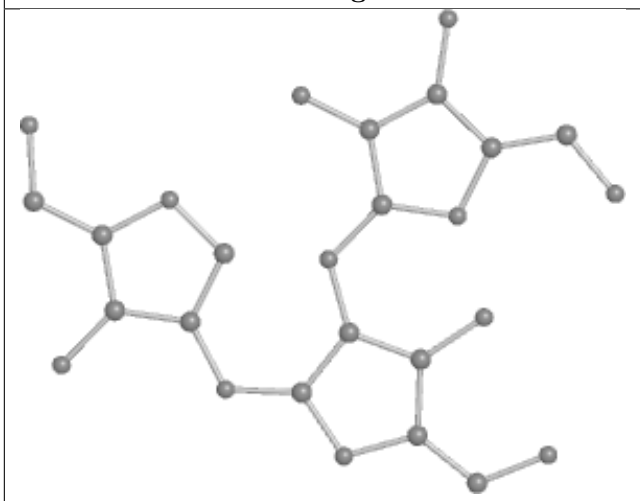
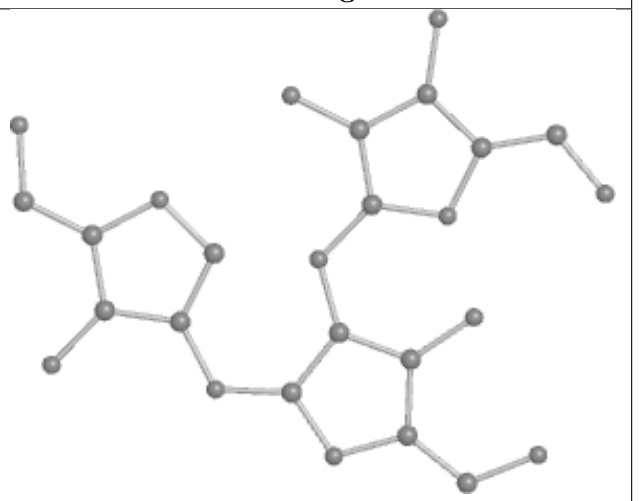
Bond angles



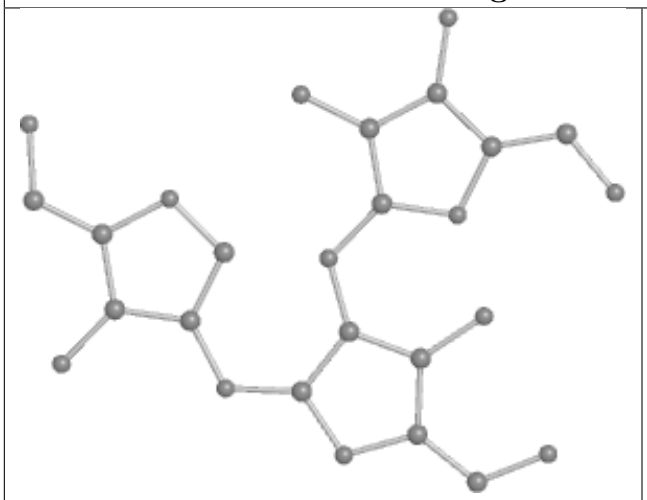
Torsions



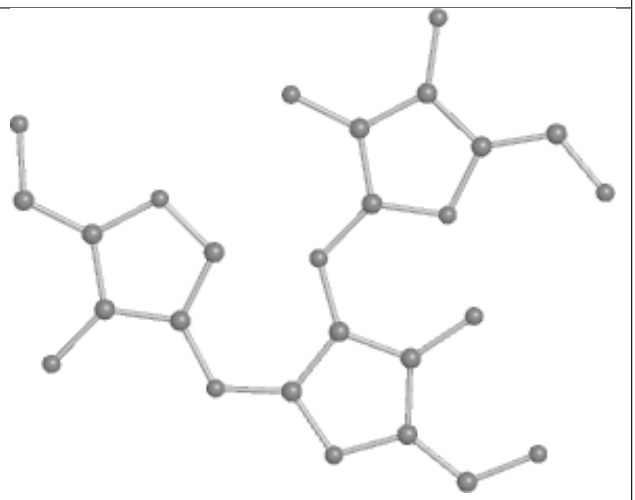
Rings

Oligosaccharide Chain iD	
 Bond lengths	 Bond angles
 Torsions	 Rings

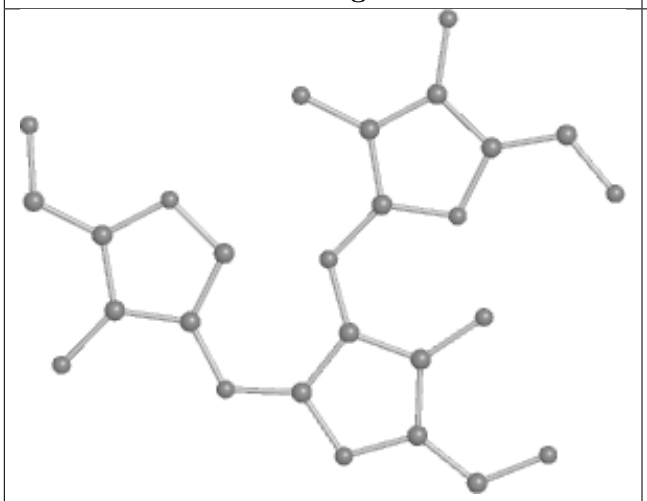
Oligosaccharide Chain lD



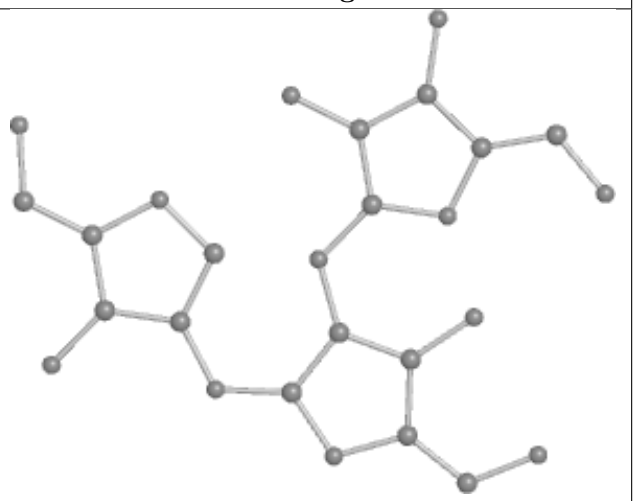
Bond lengths



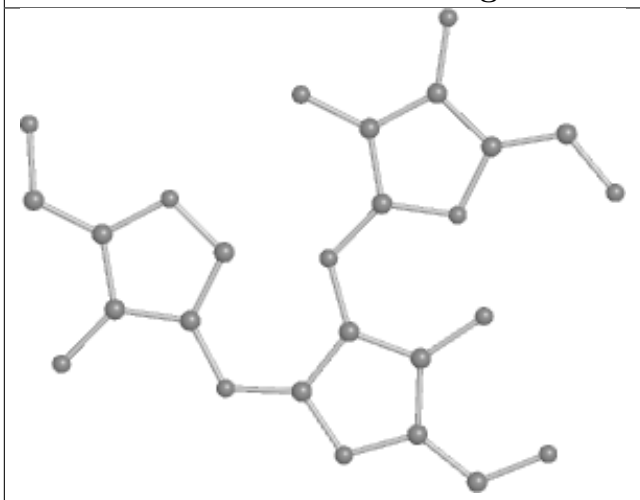
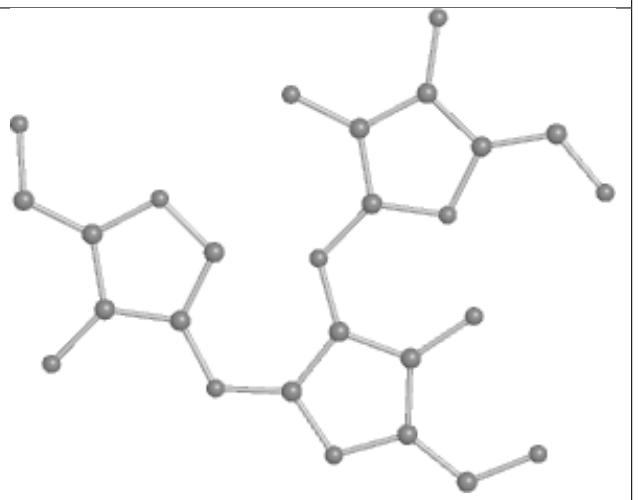
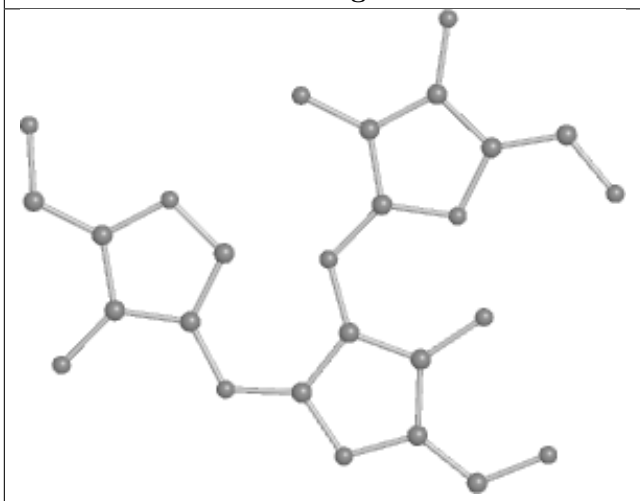
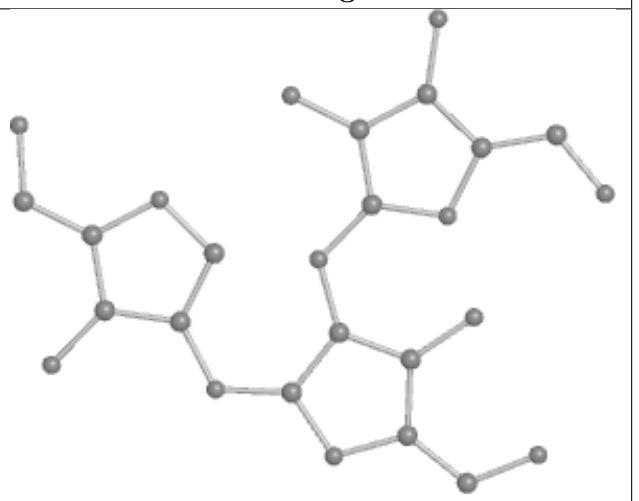
Bond angles

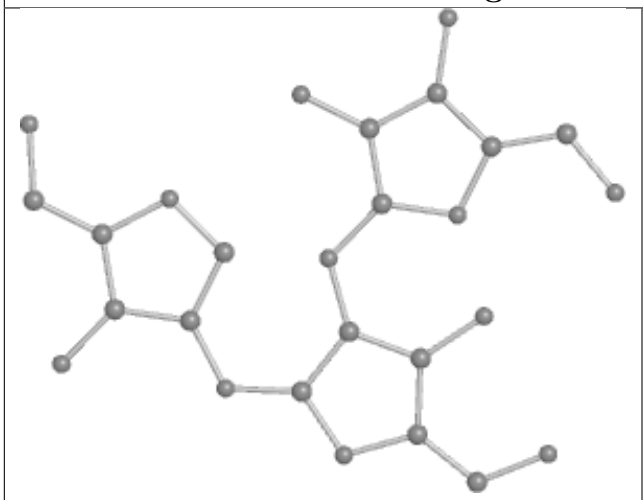
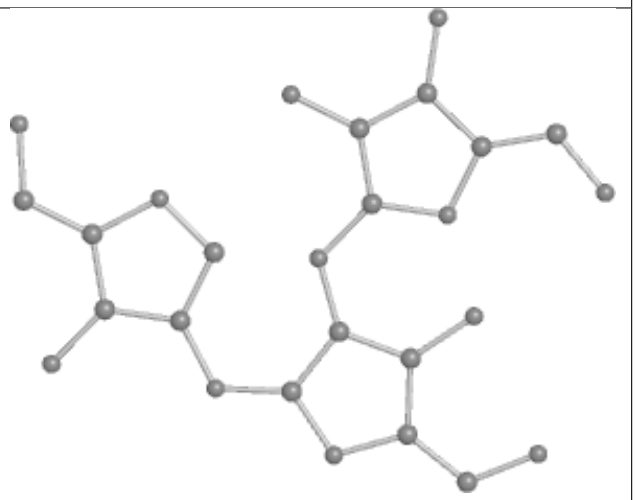
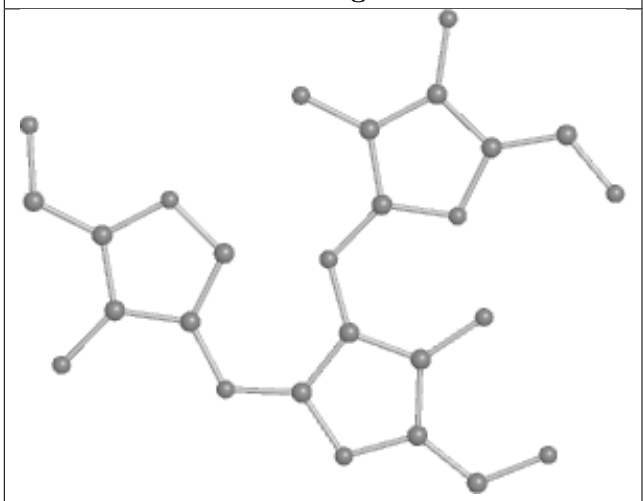
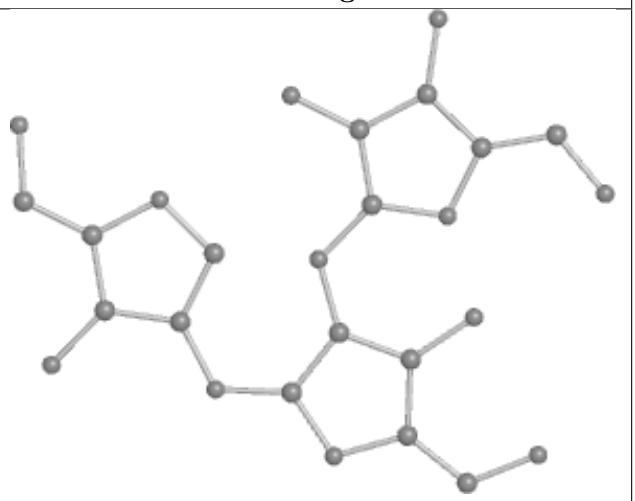


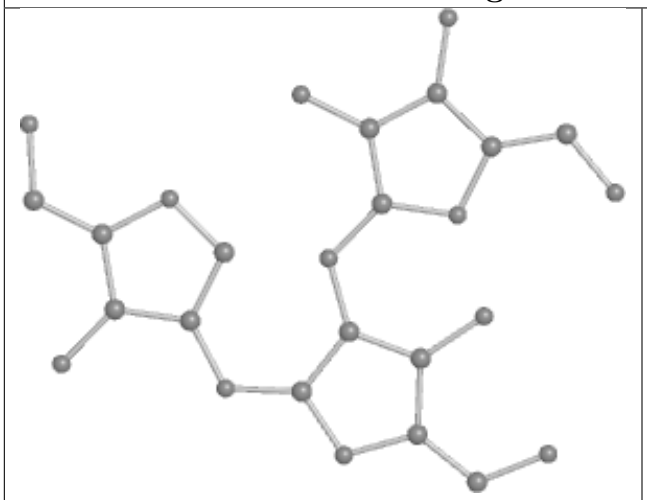
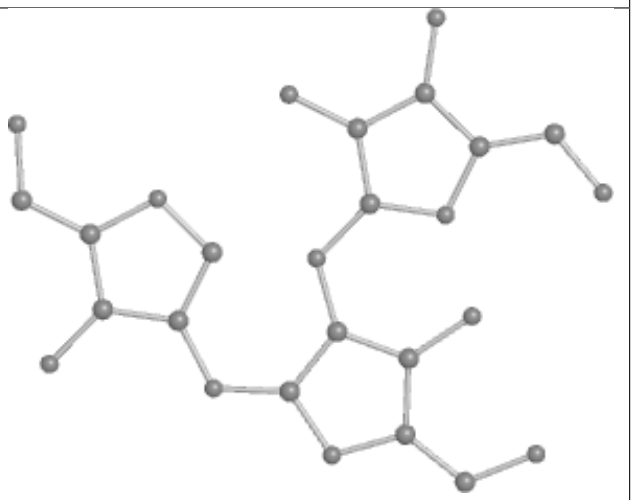
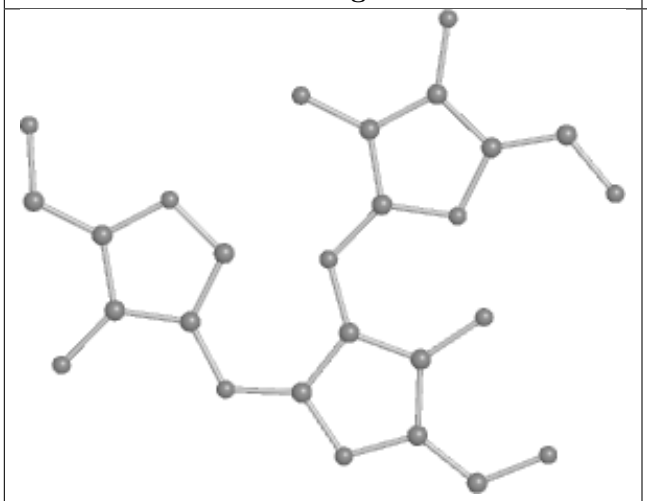
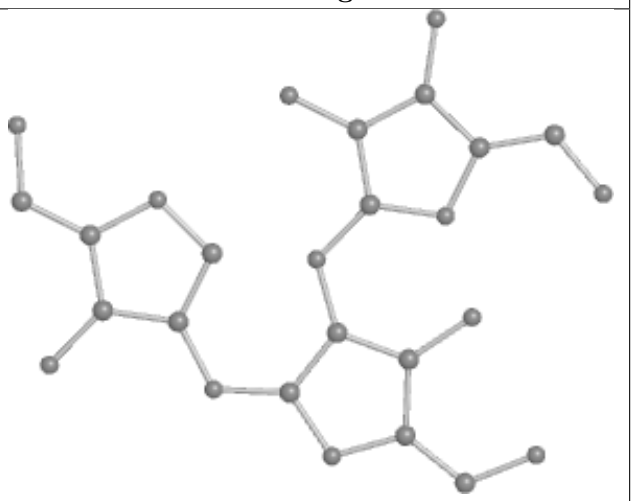
Torsions



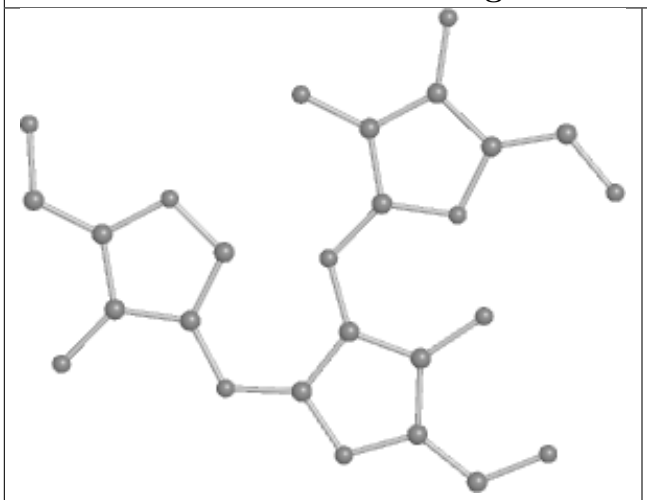
Rings

Oligosaccharide Chain mD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

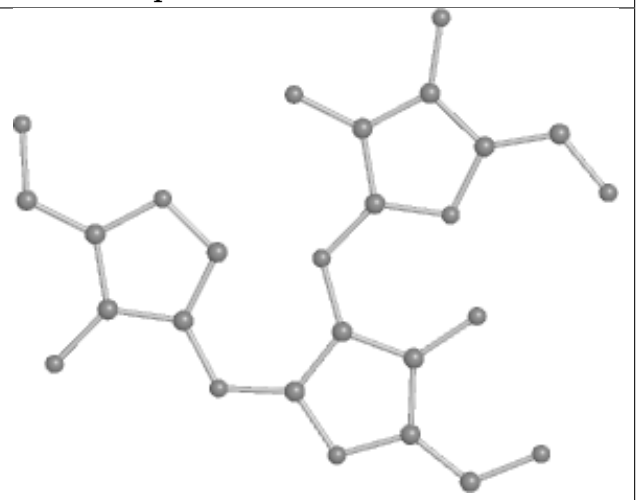
Oligosaccharide Chain nD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain oD	
 Bond lengths	 Bond angles
 Torsions	 Rings

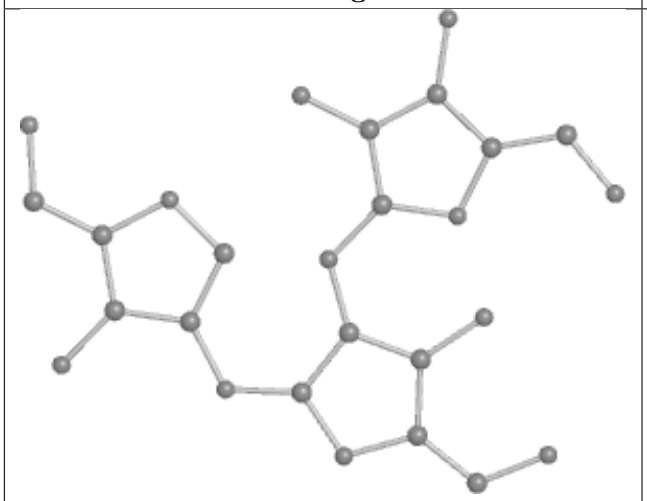
Oligosaccharide Chain pD



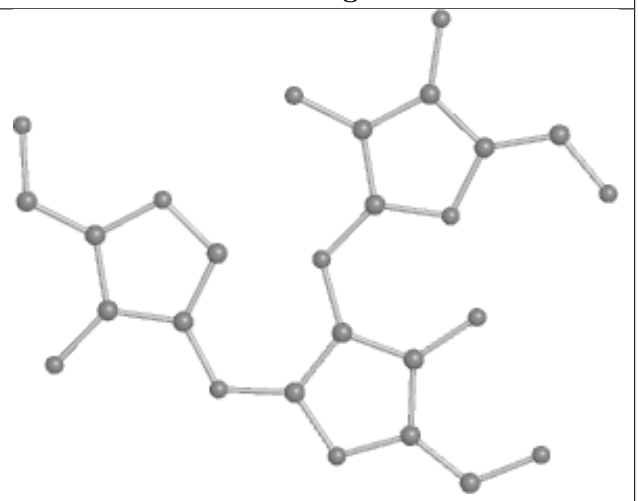
Bond lengths



Bond angles

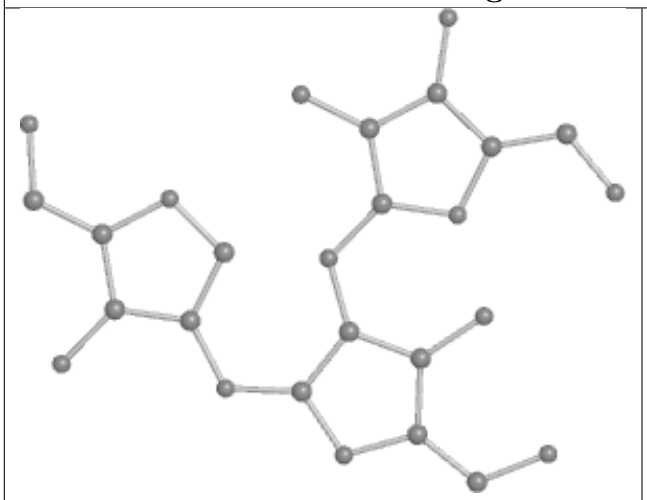


Torsions

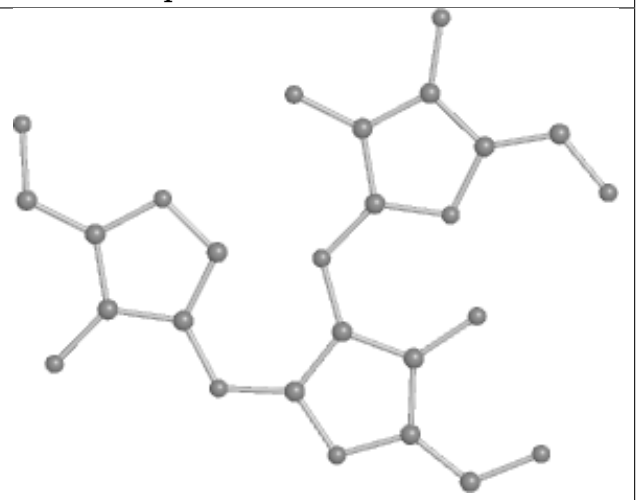


Rings

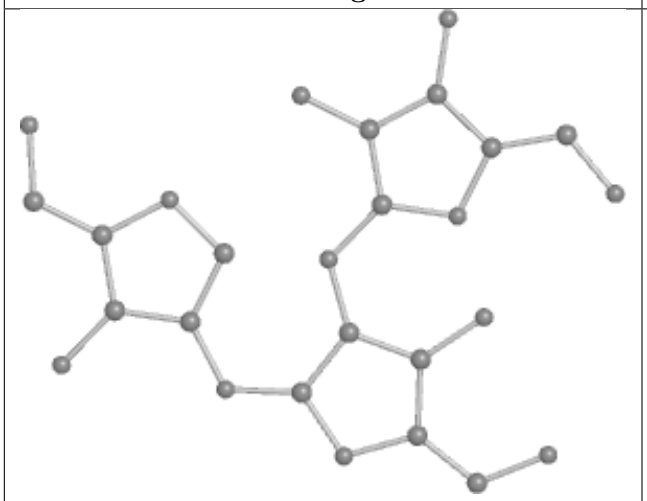
Oligosaccharide Chain qD



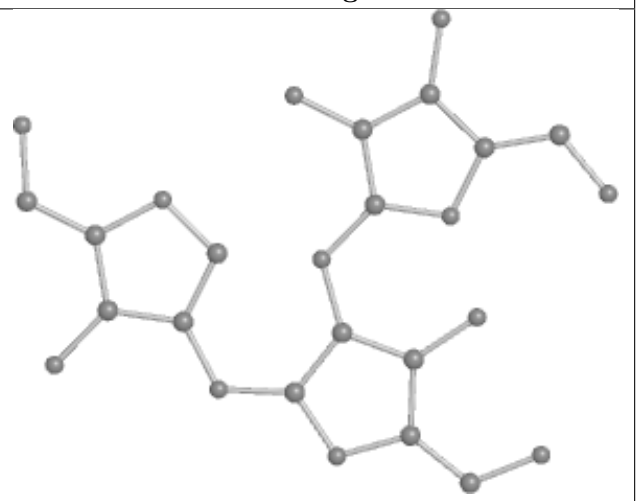
Bond lengths



Bond angles

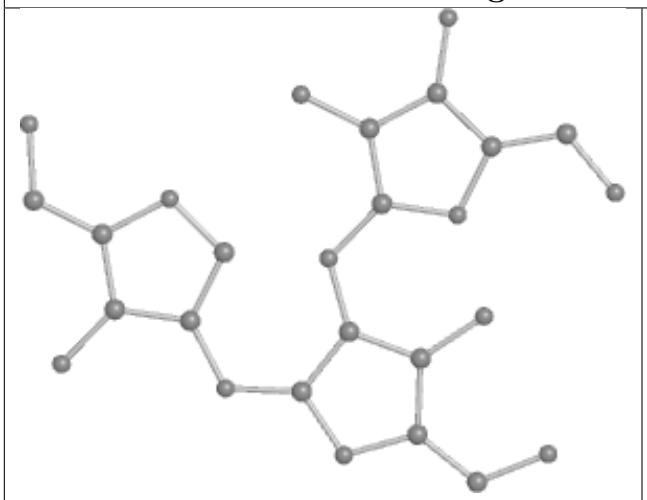


Torsions

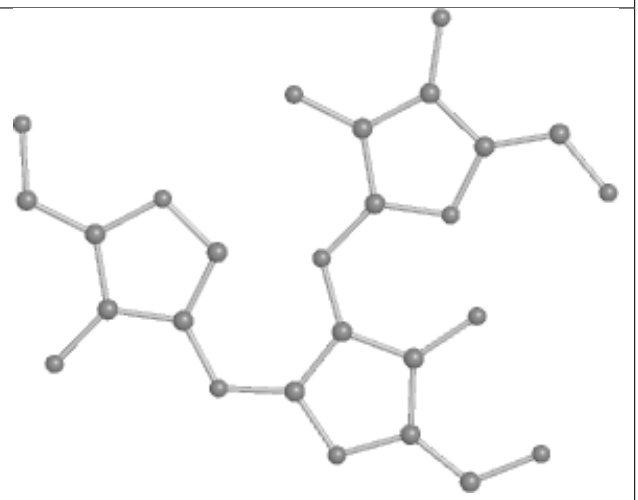


Rings

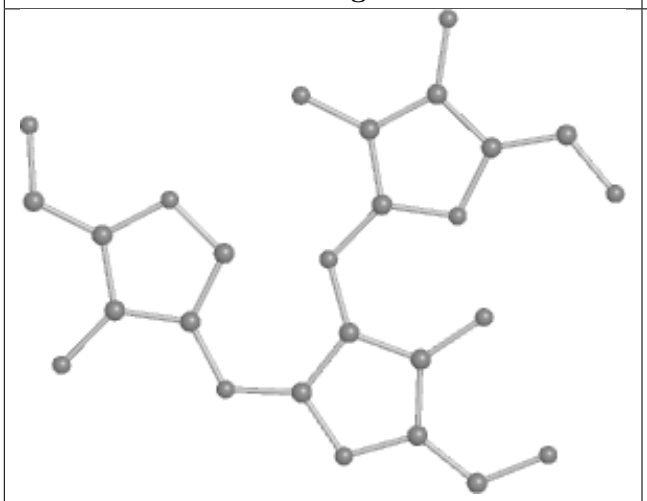
Oligosaccharide Chain rD



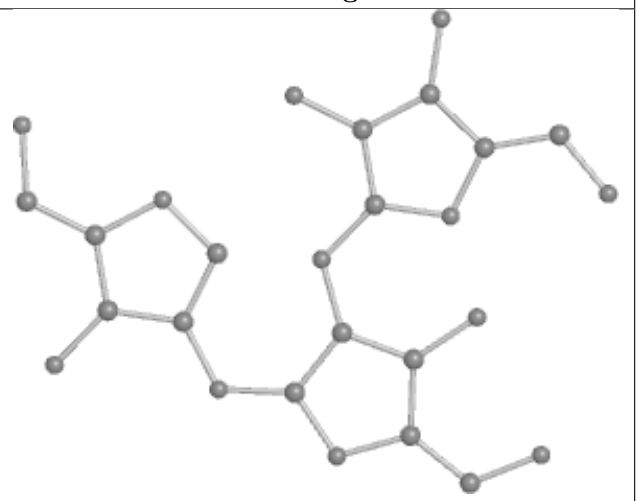
Bond lengths



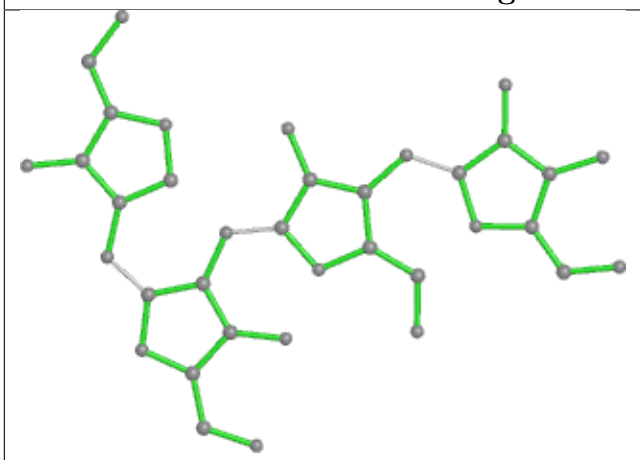
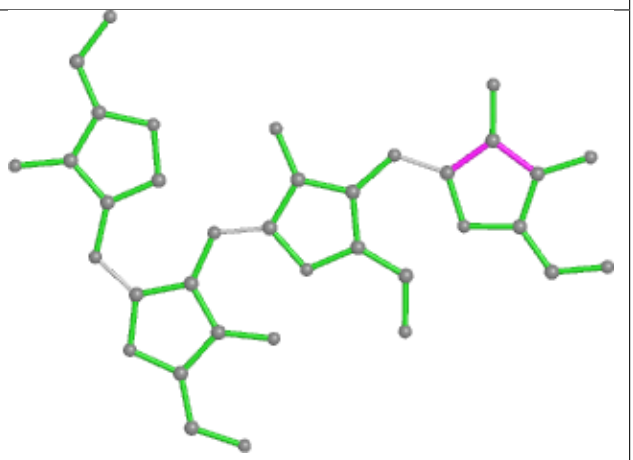
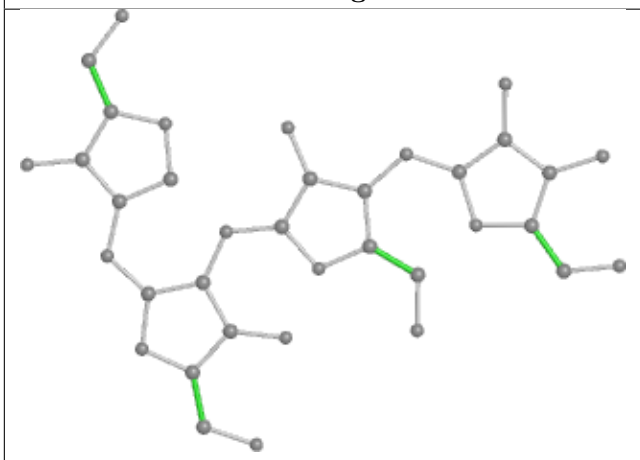
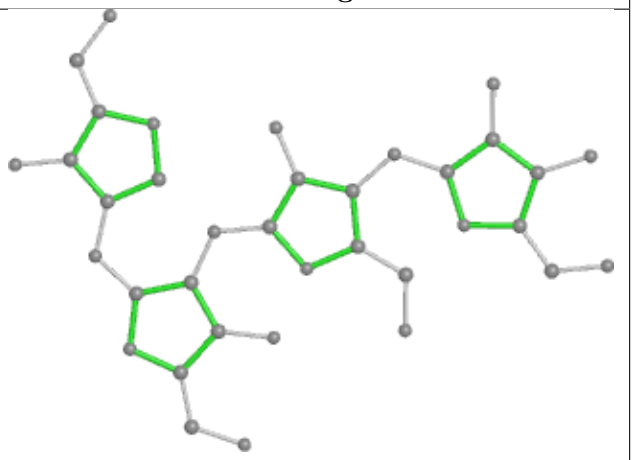
Bond angles



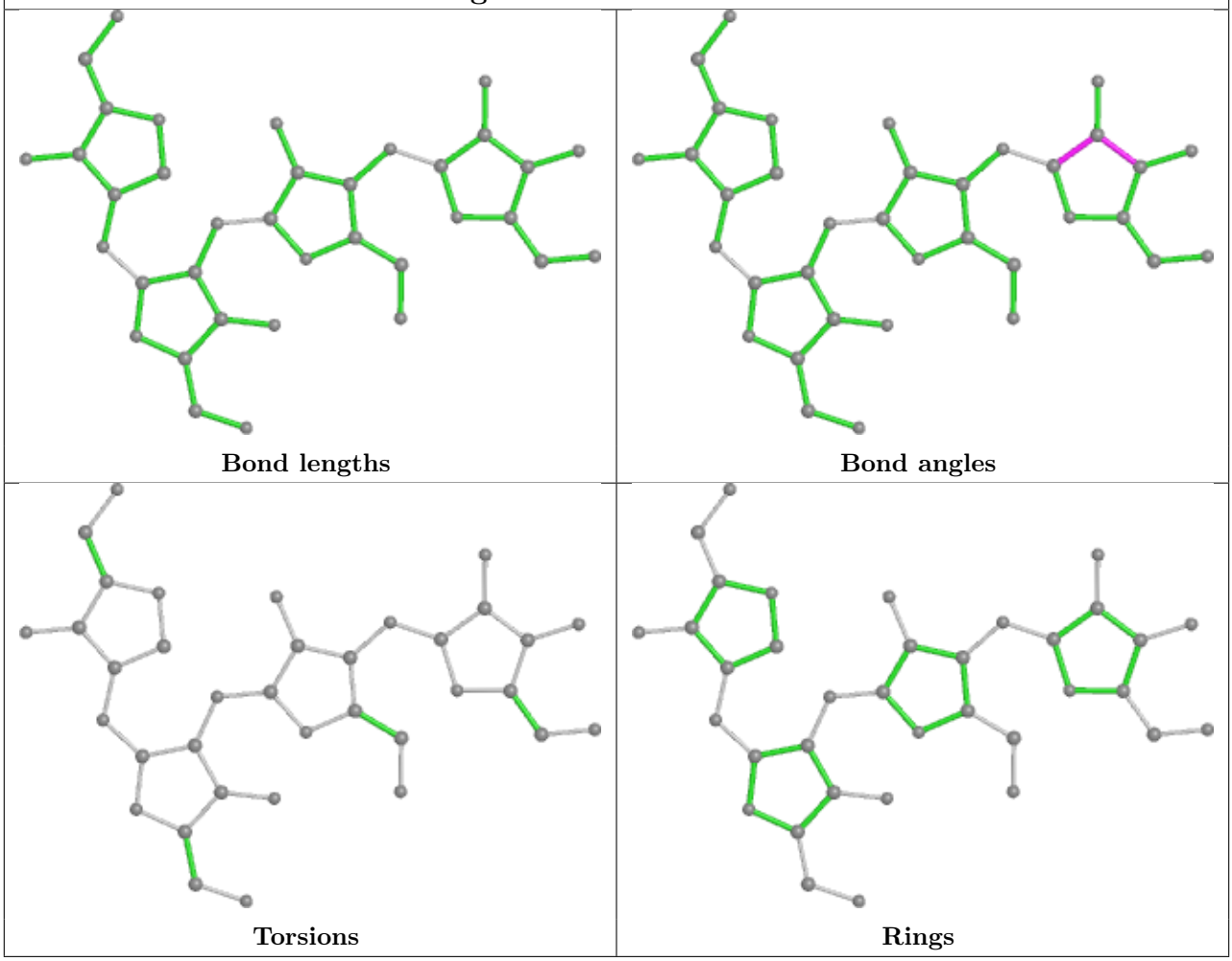
Torsions



Rings

Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain W



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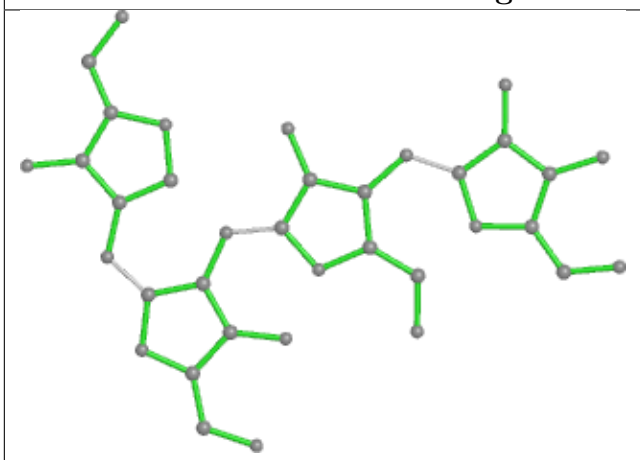
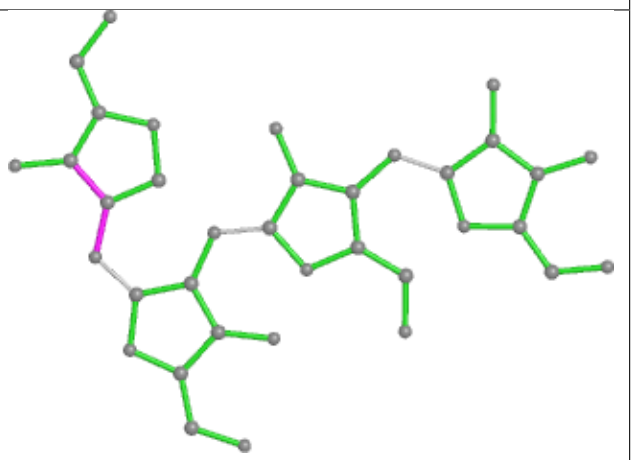
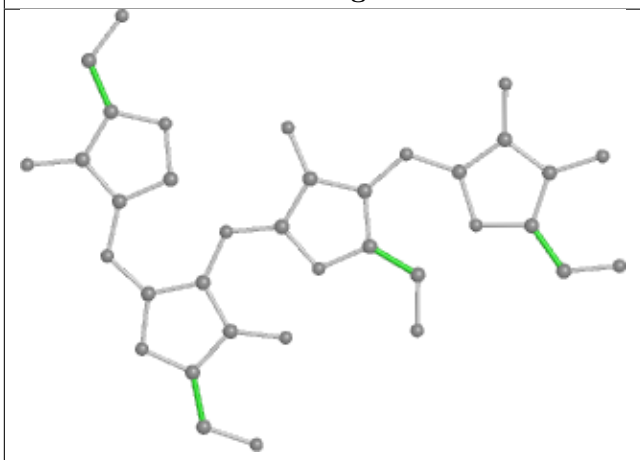
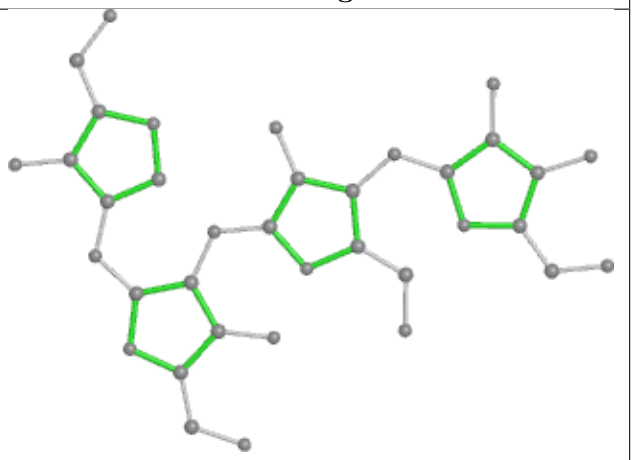
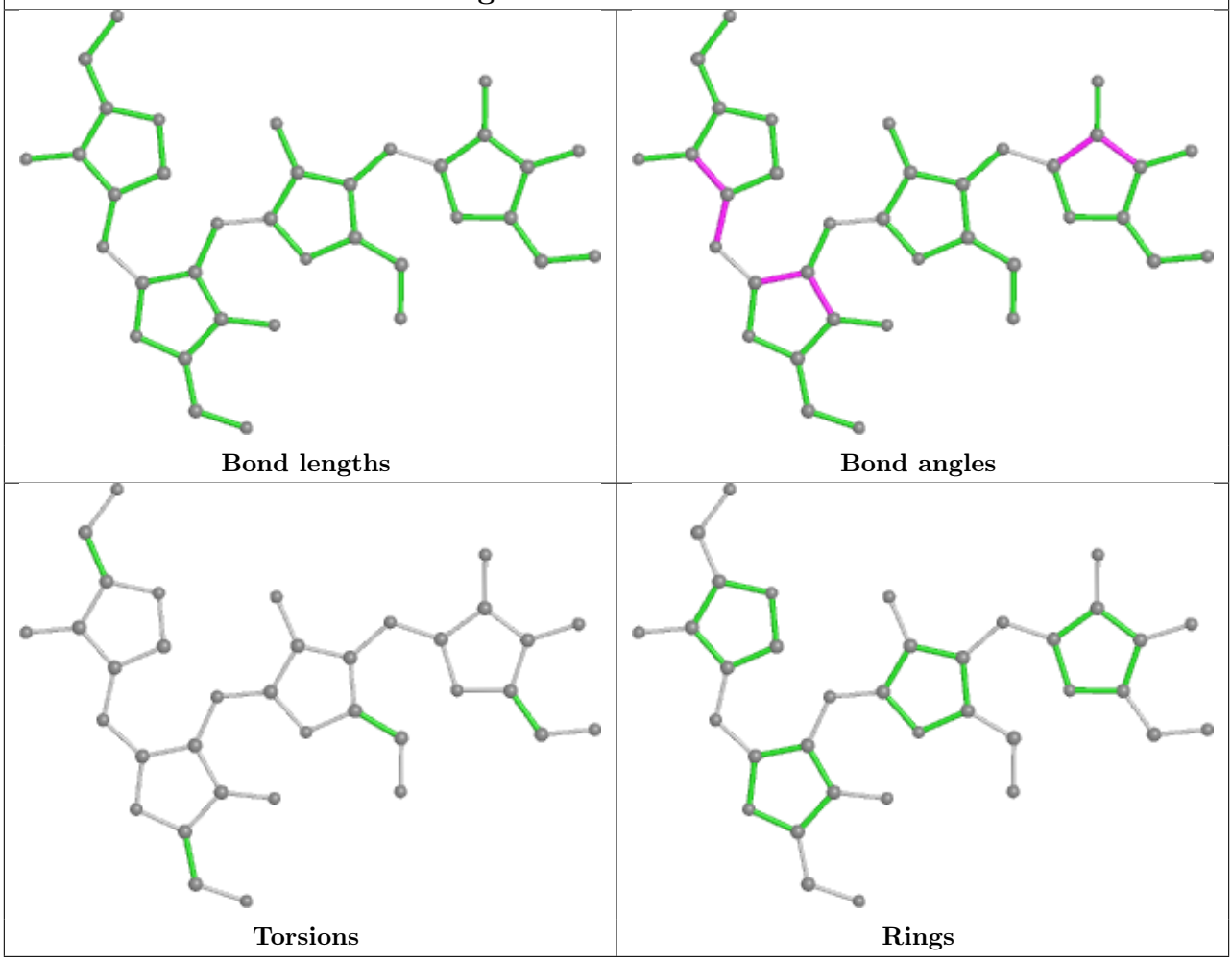
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Z



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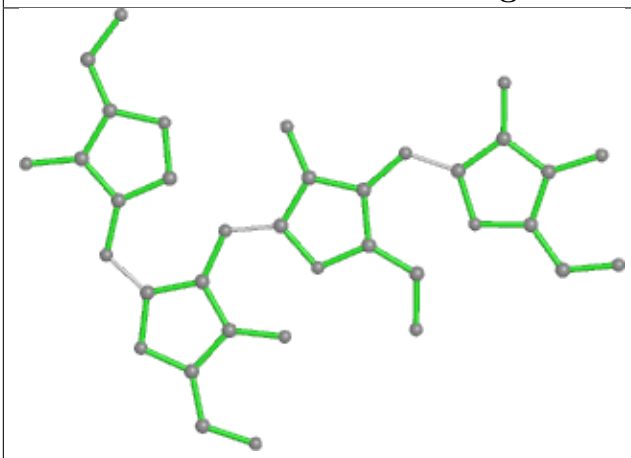
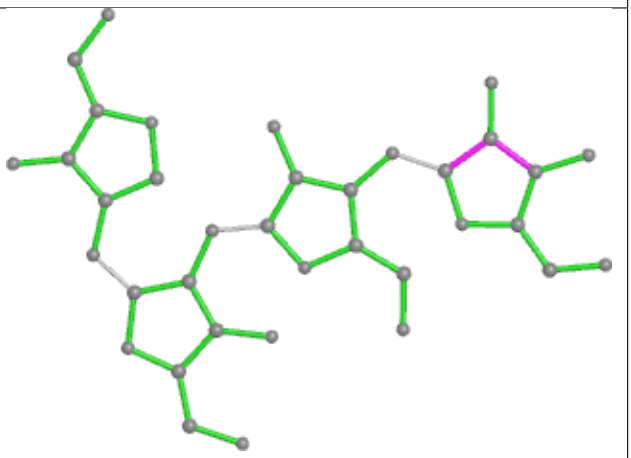
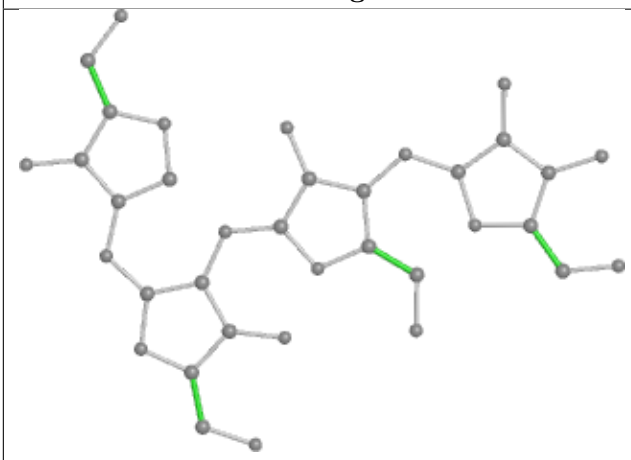
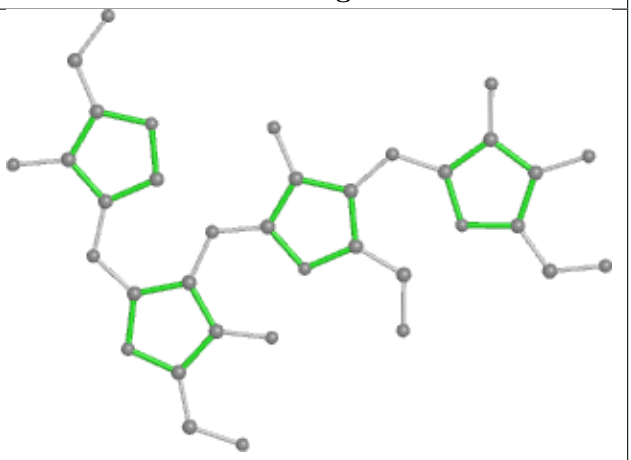
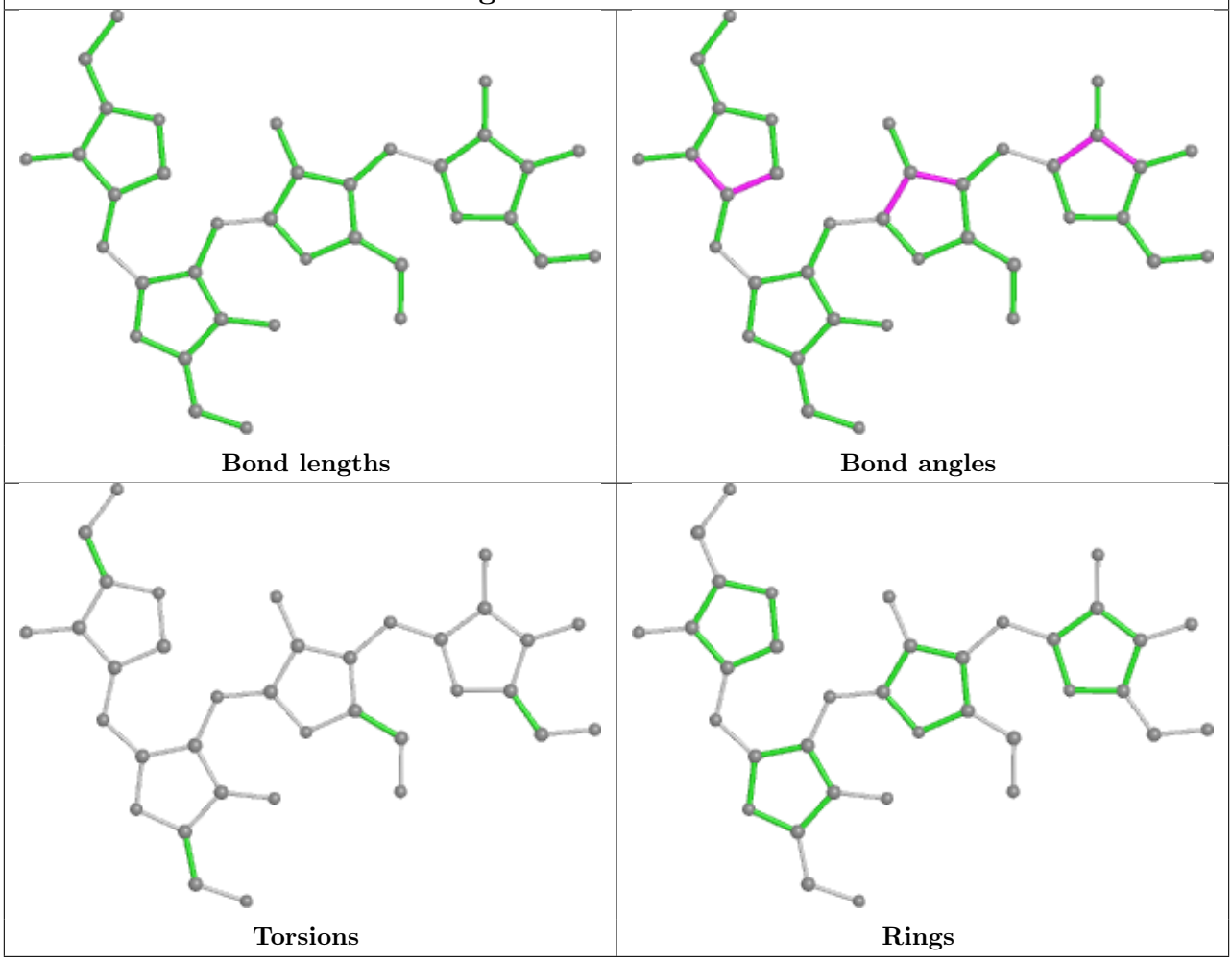
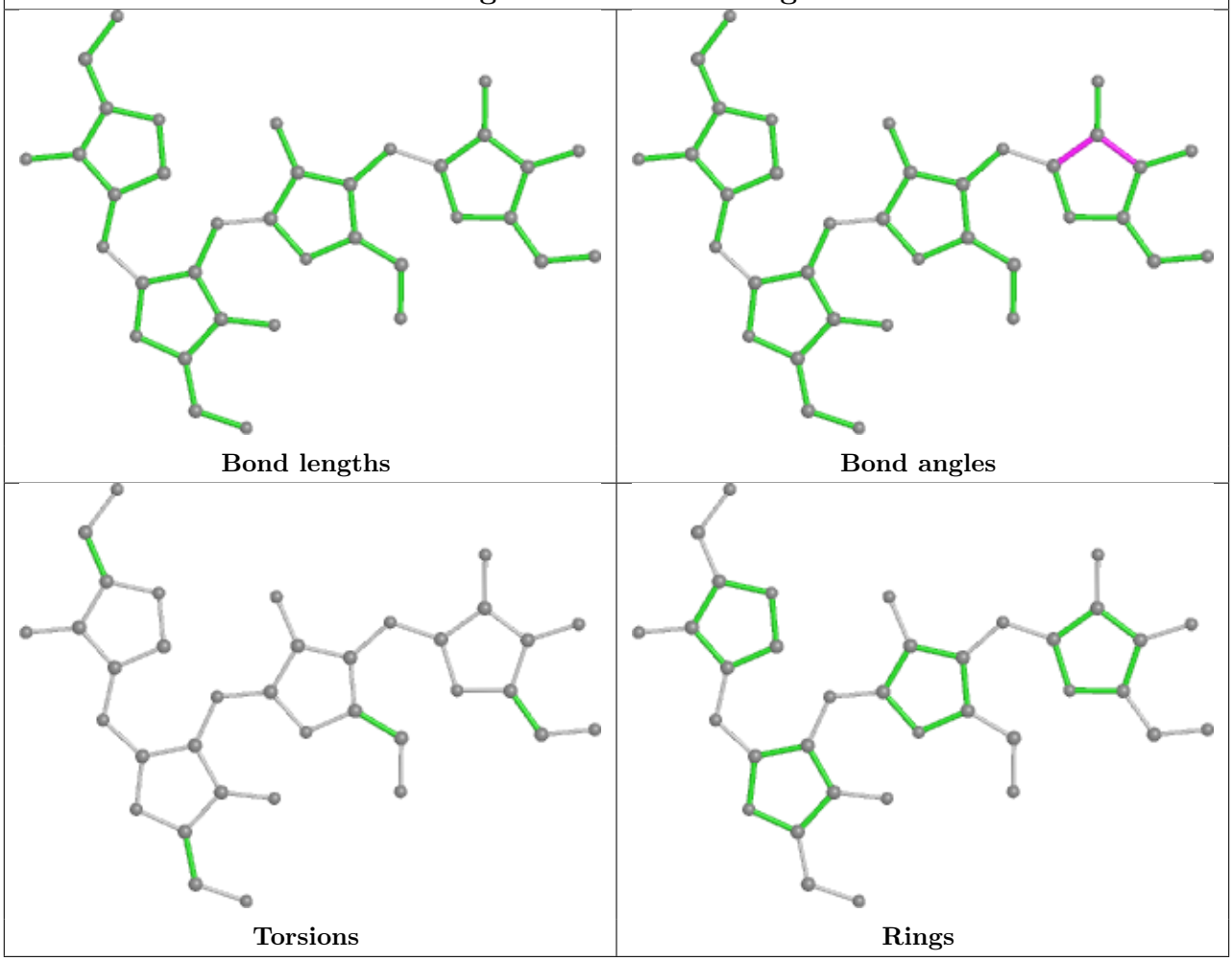
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain d



Oligosaccharide Chain g



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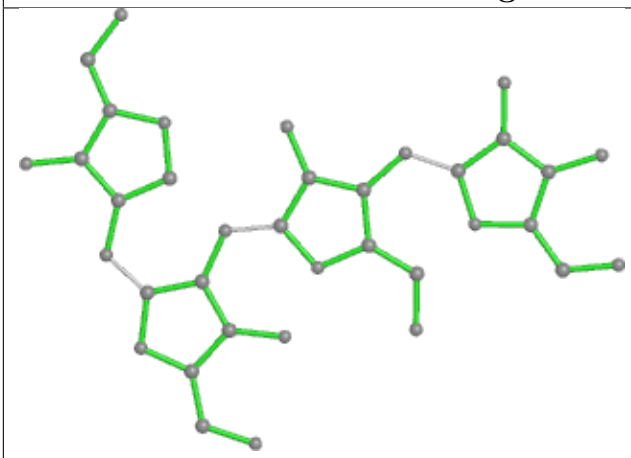
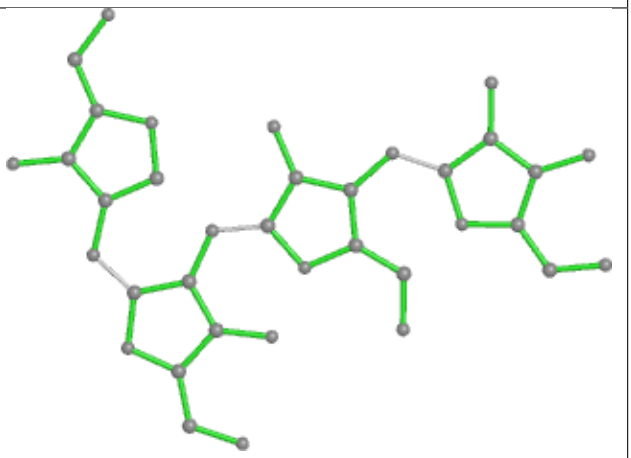
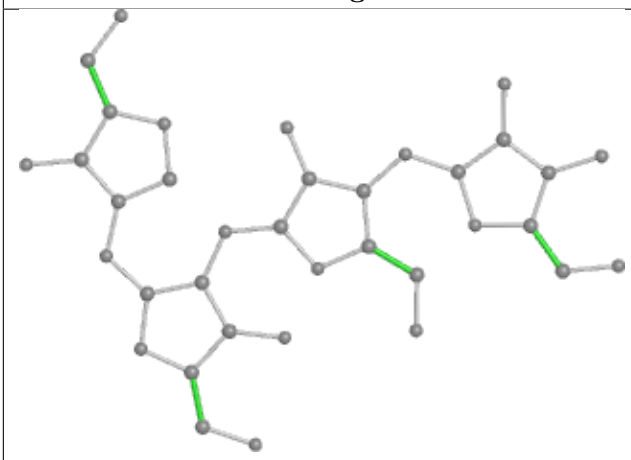
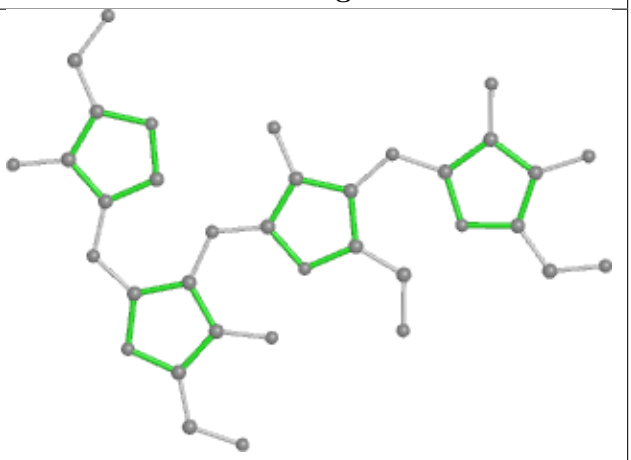
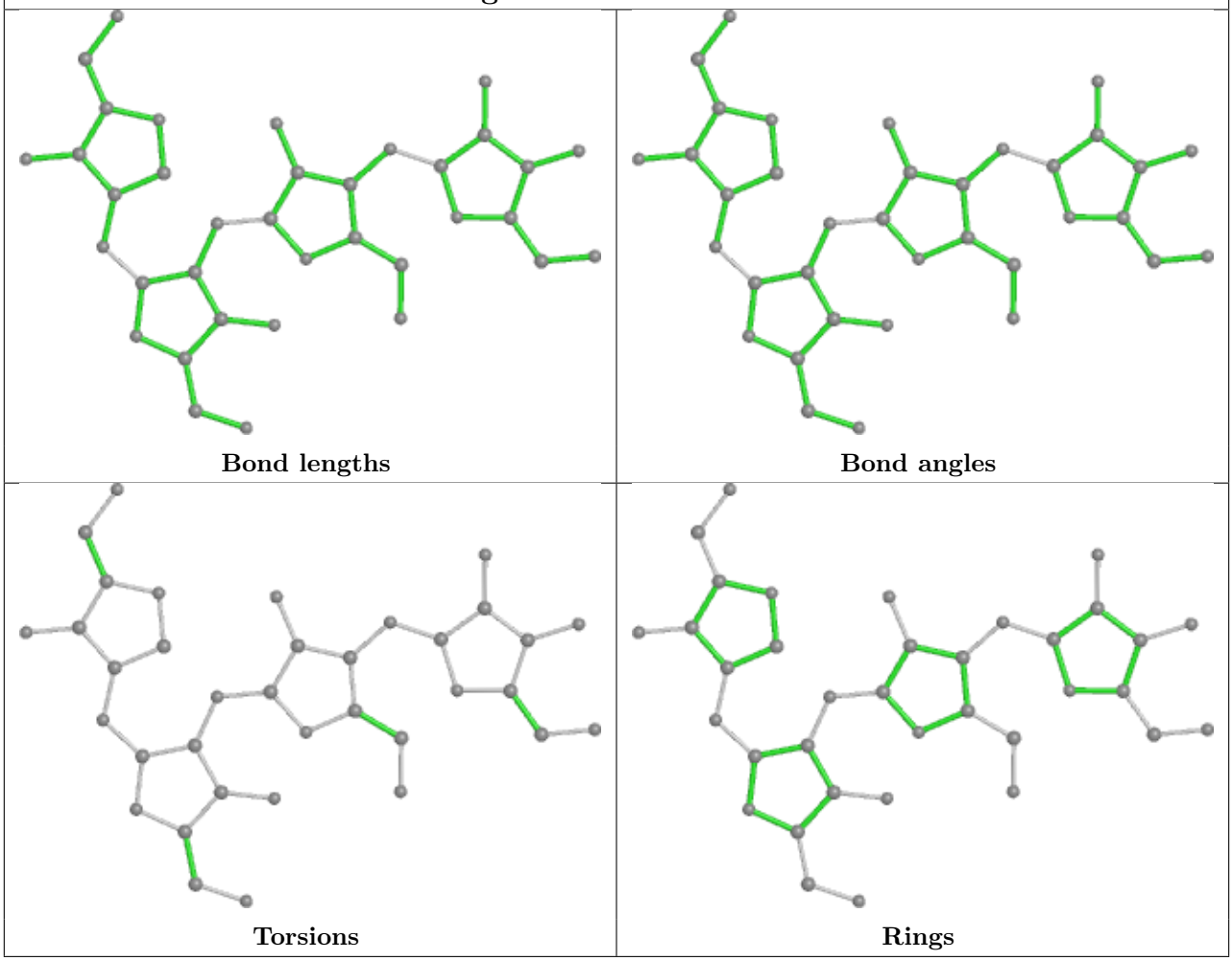
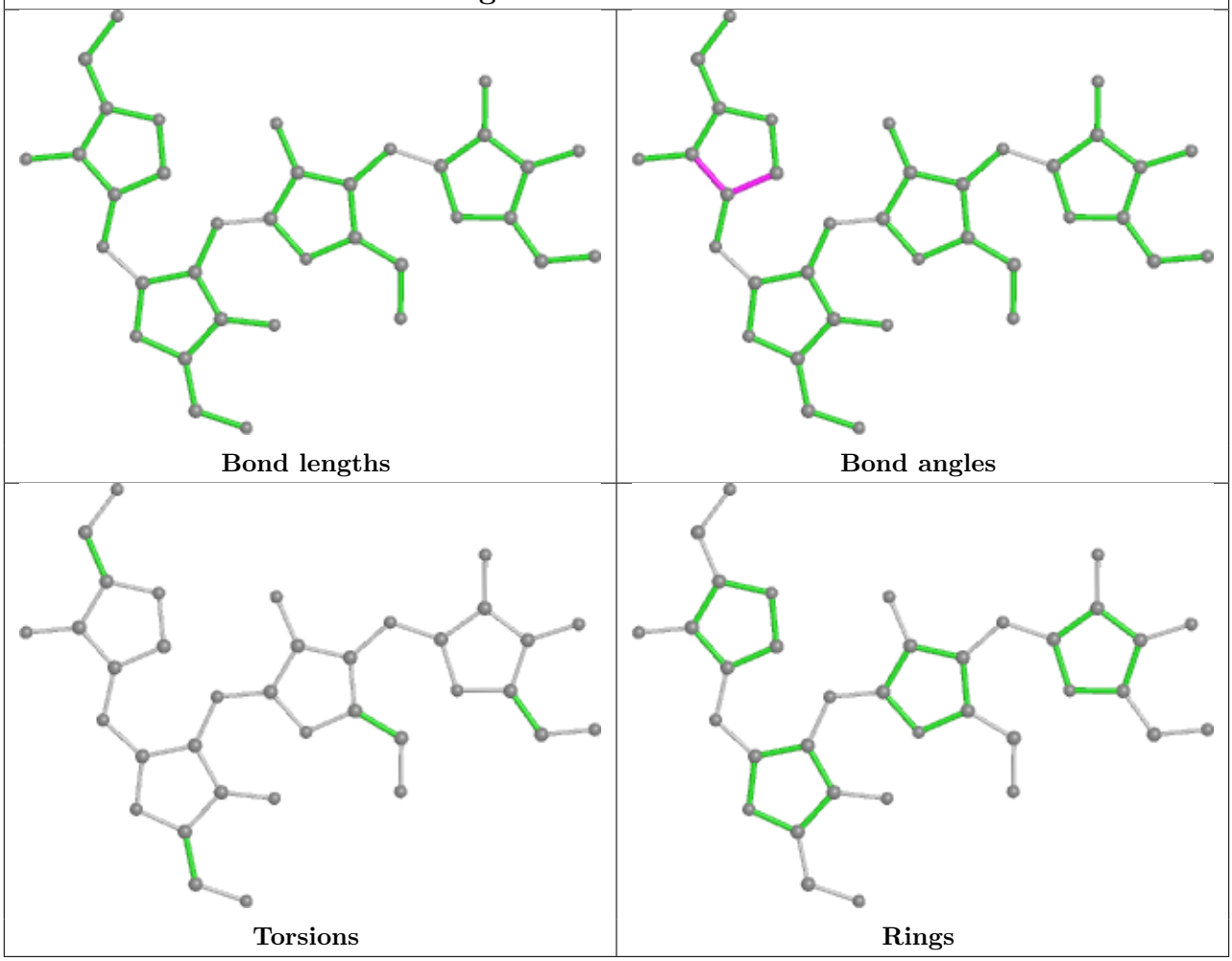
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain r



Oligosaccharide Chain v



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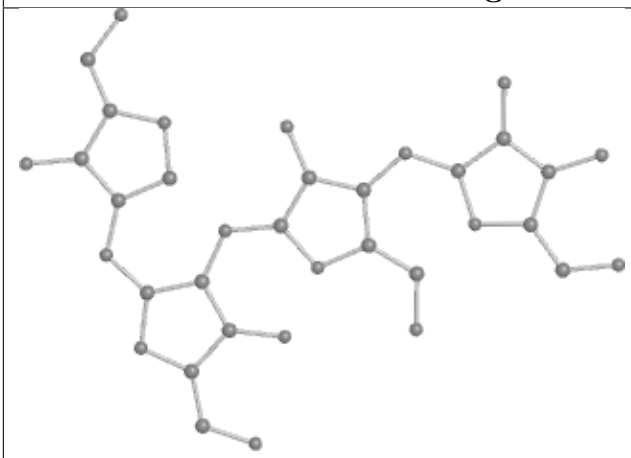
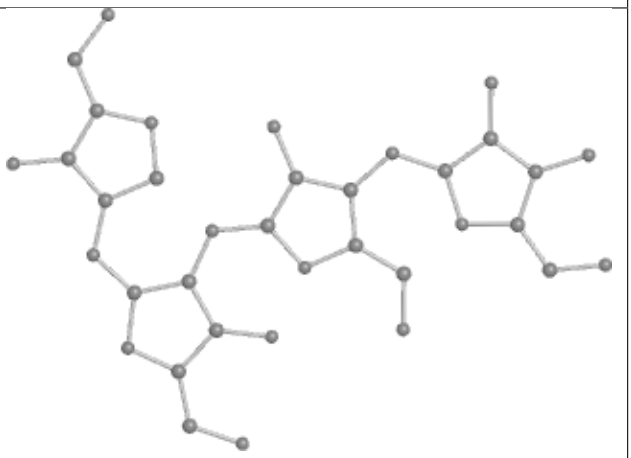
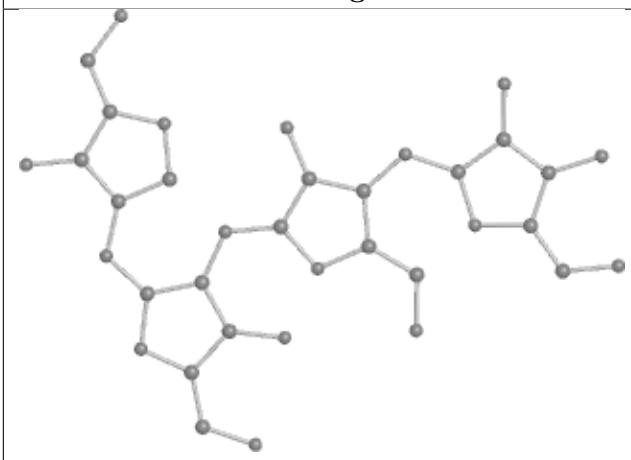
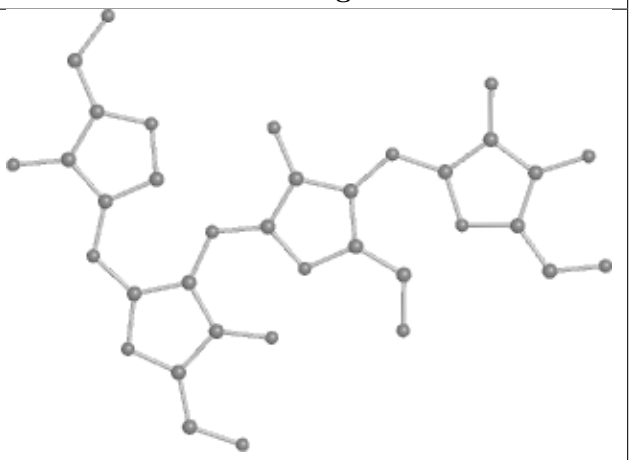
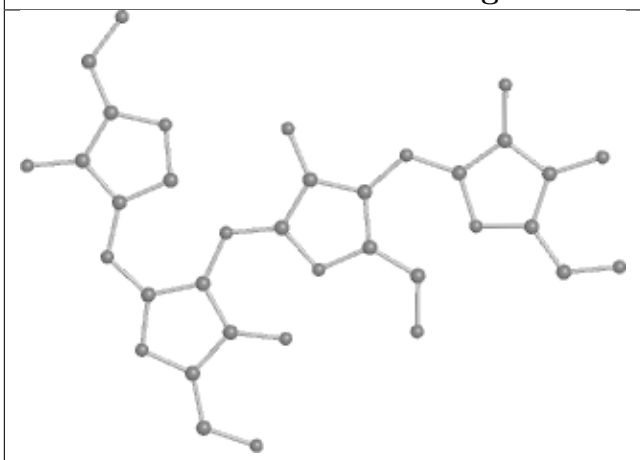
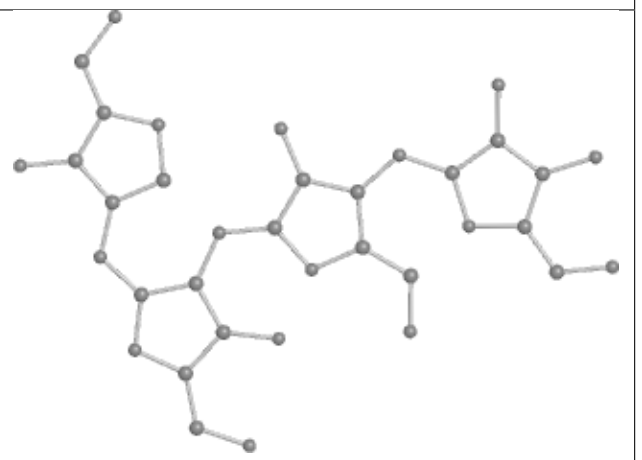
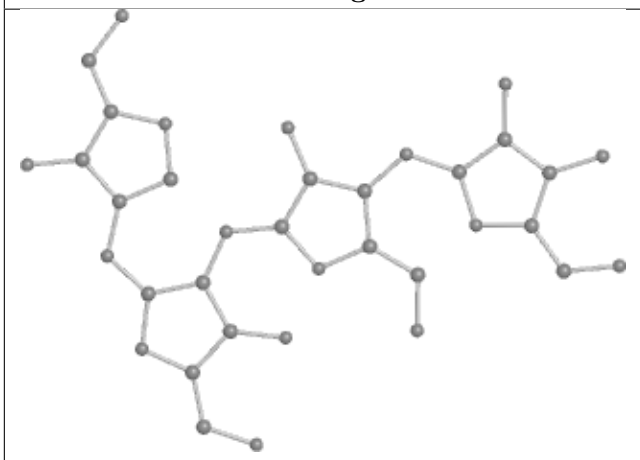
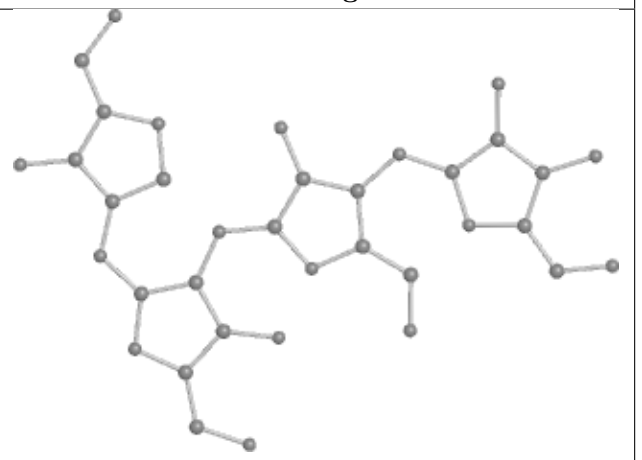
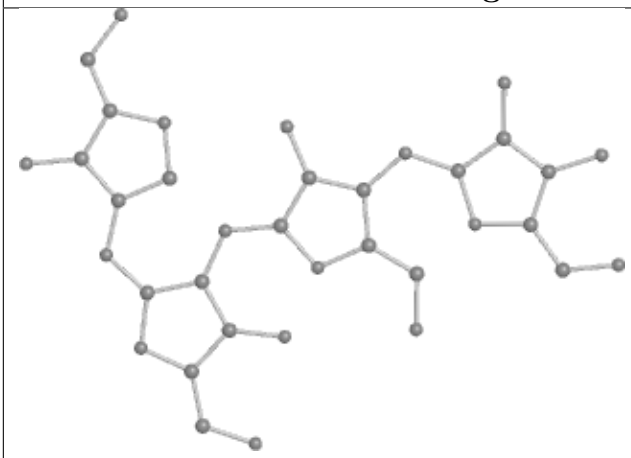
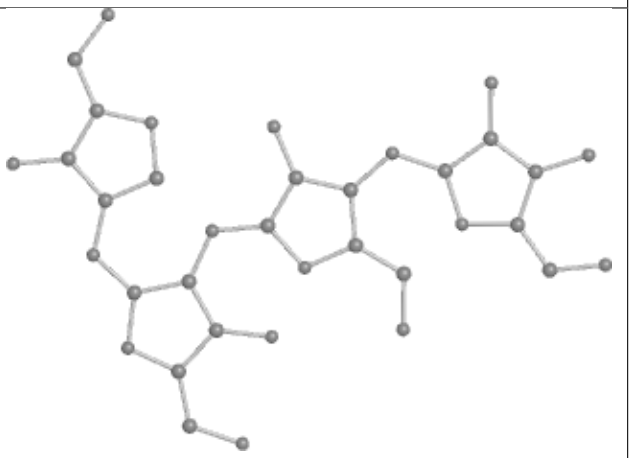
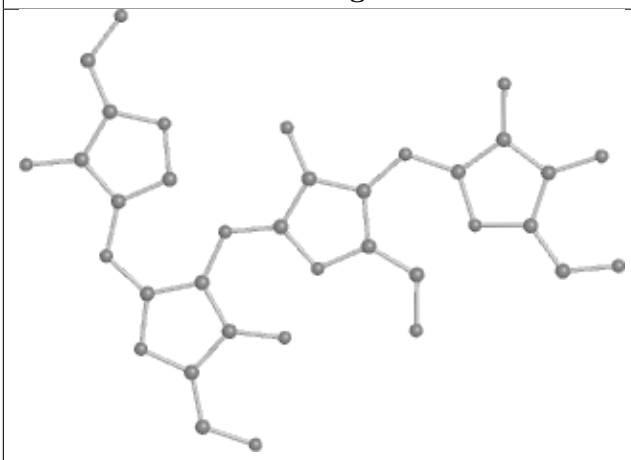
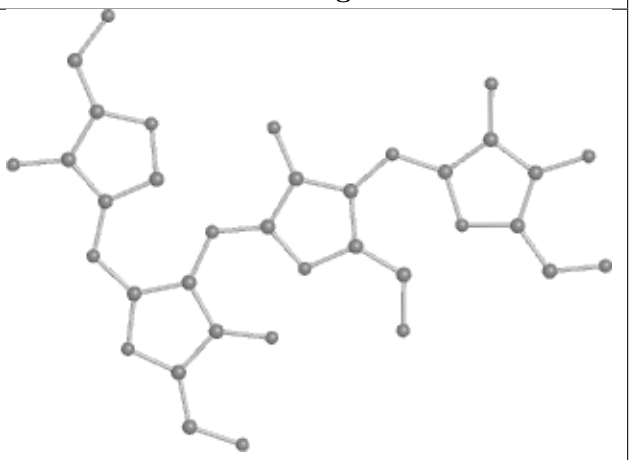
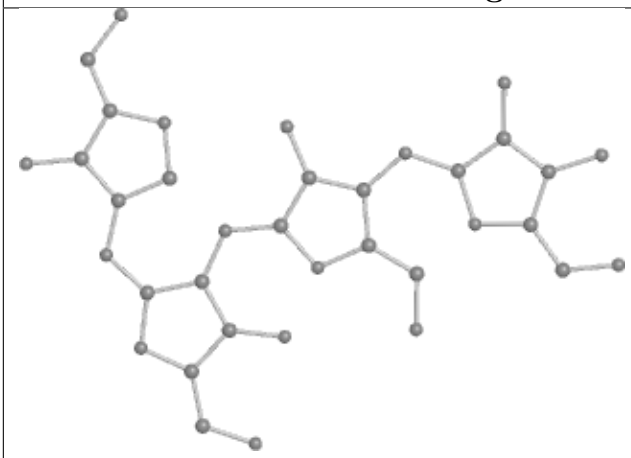
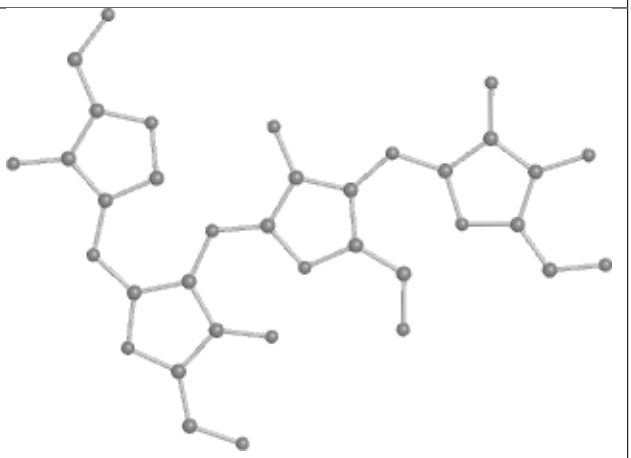
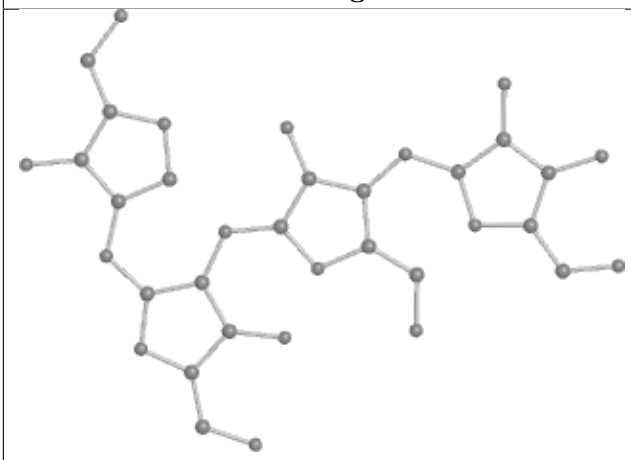
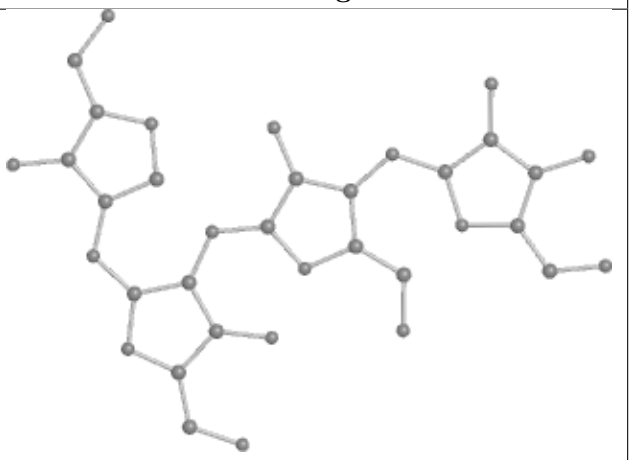
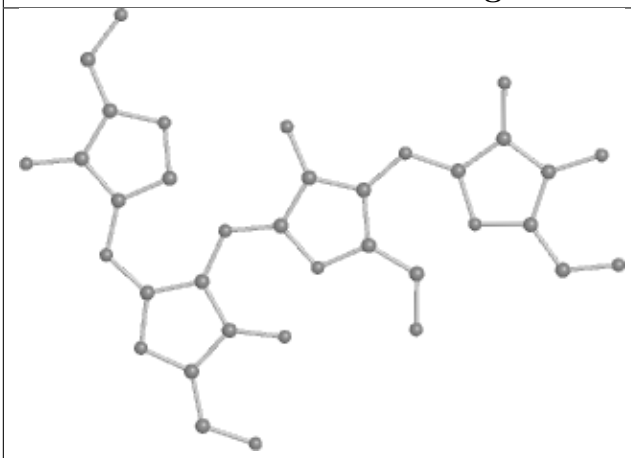
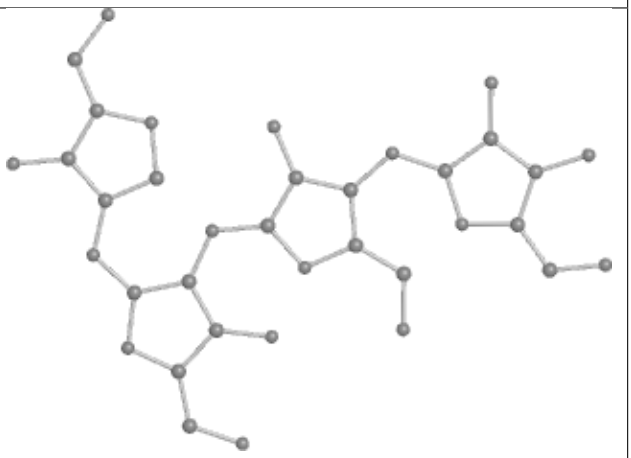
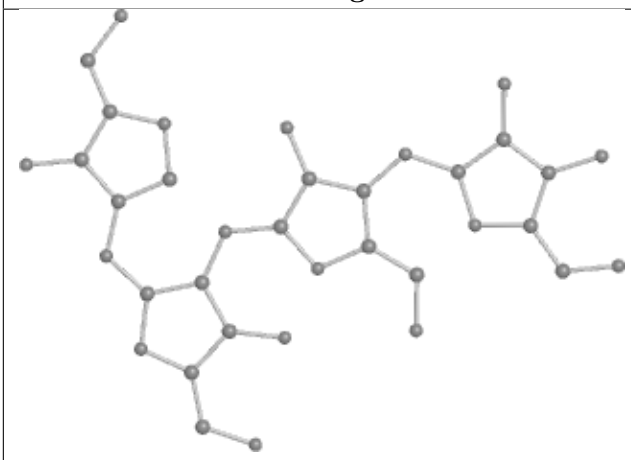
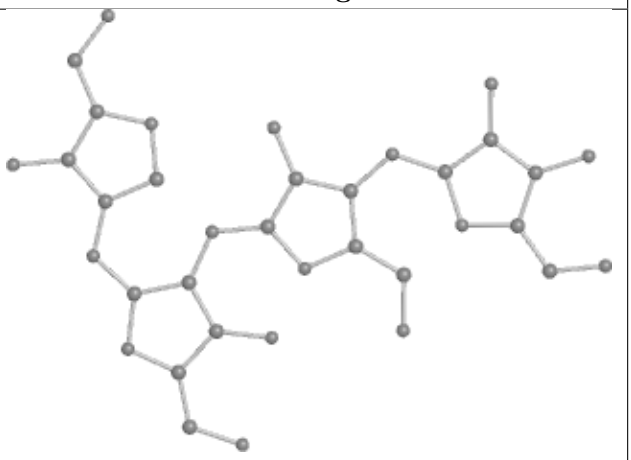
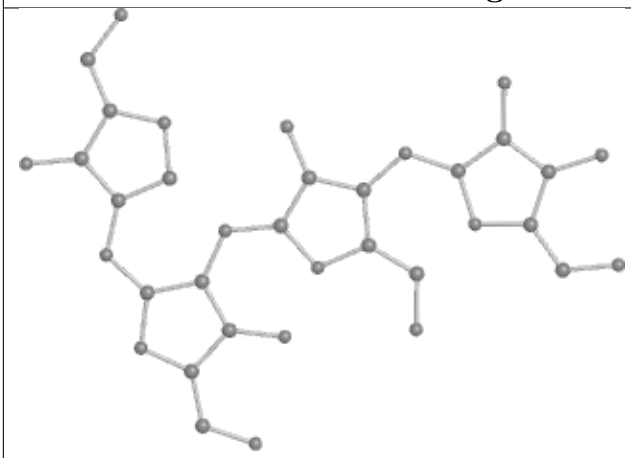
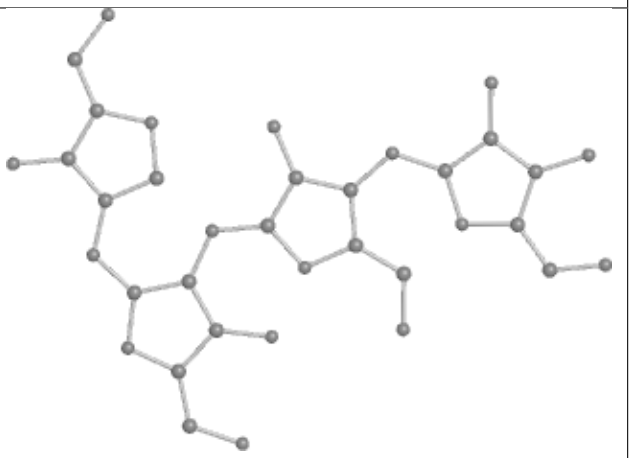
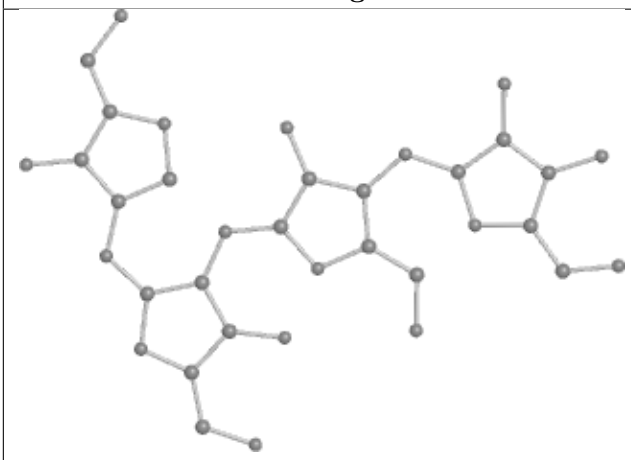
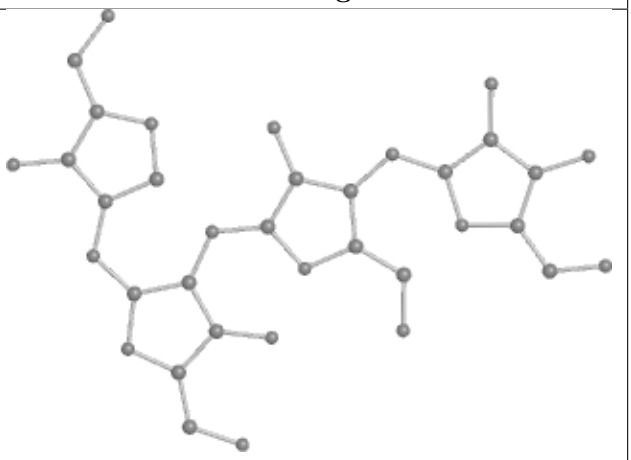
 Bond lengths	 Bond angles
 Torsions	 Rings

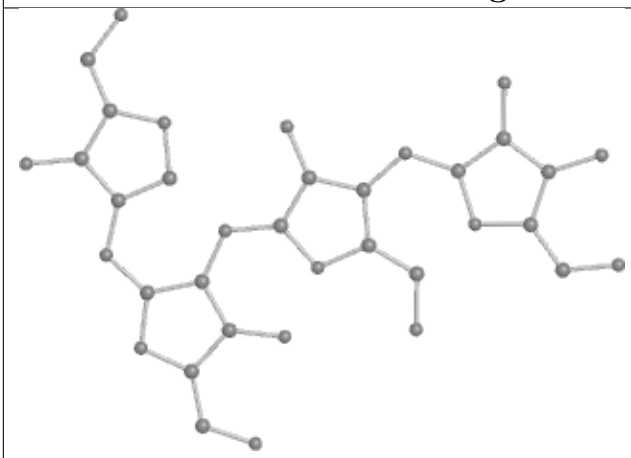
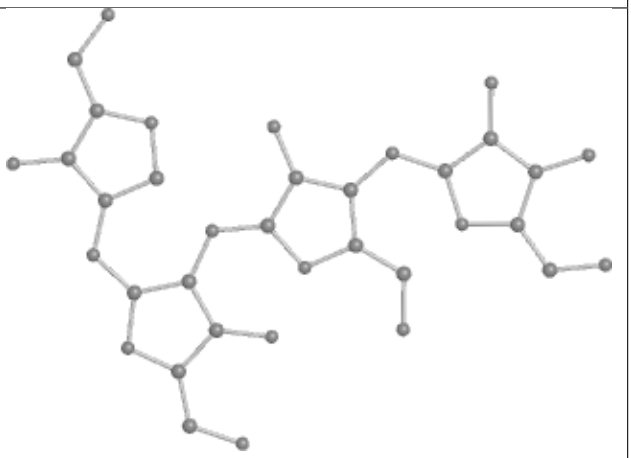
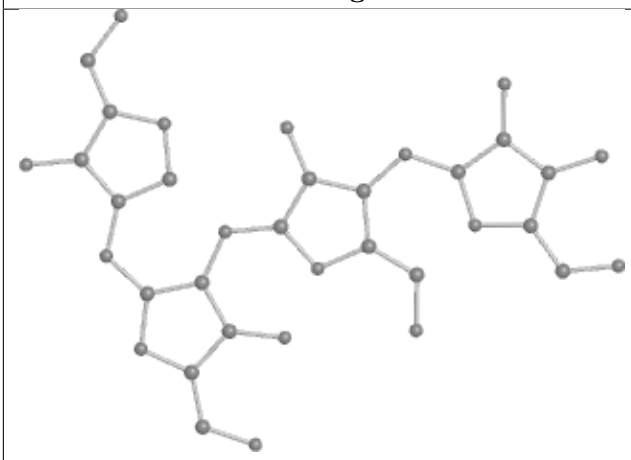
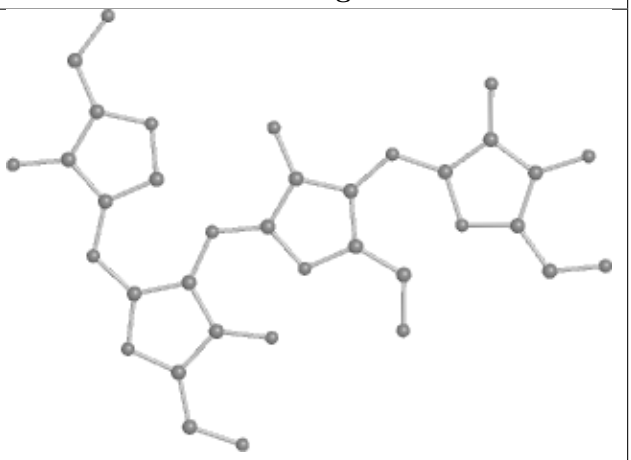
Oligosaccharide Chain UA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

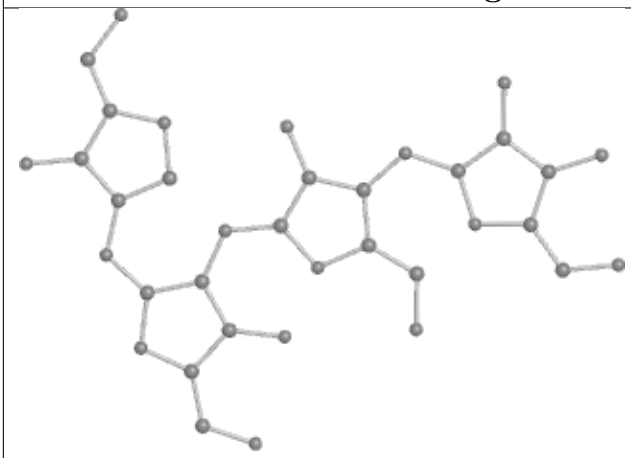
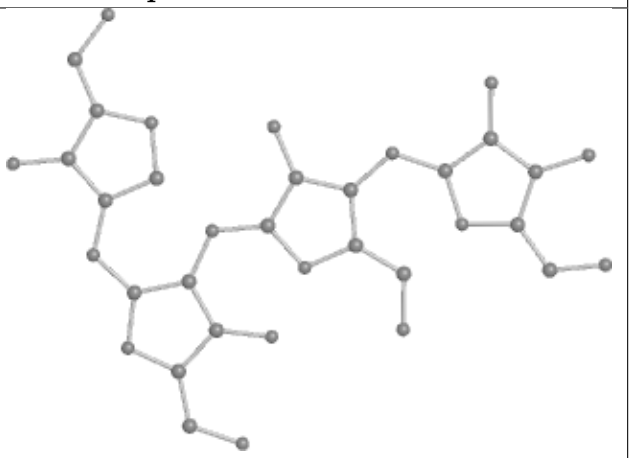
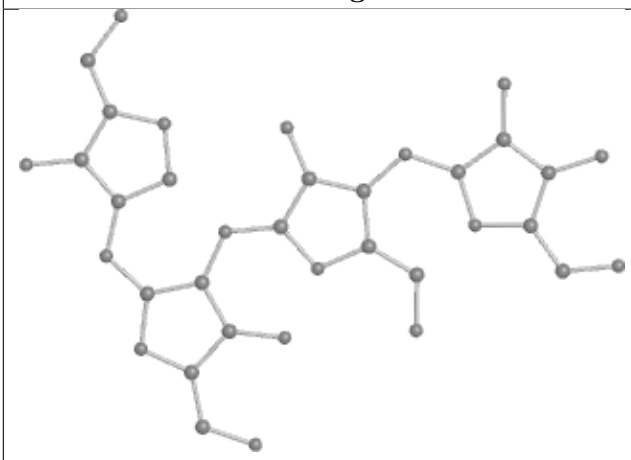
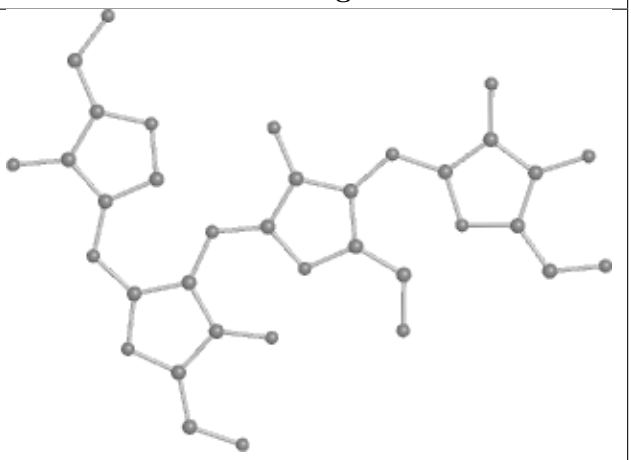
Oligosaccharide Chain VA	
 Bond lengths	 Bond angles
 Torsions	 Rings

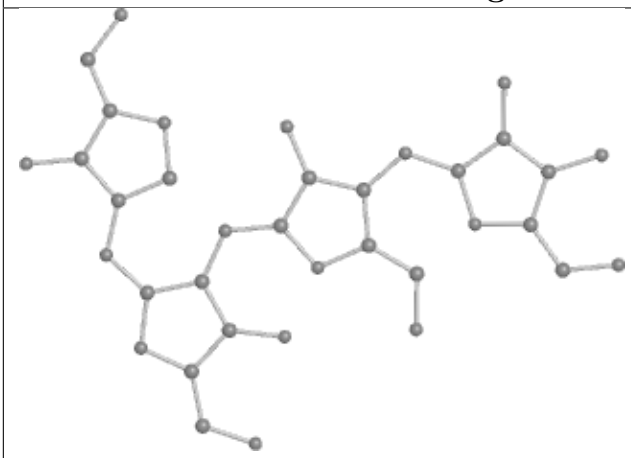
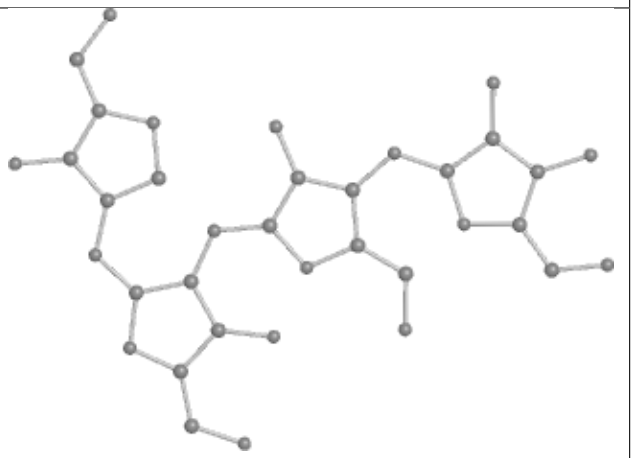
Oligosaccharide Chain aA	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain bA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain eA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain iA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain pA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain tA	
	
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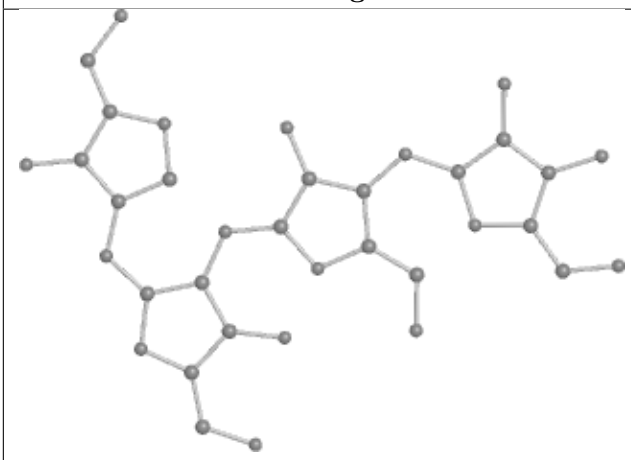	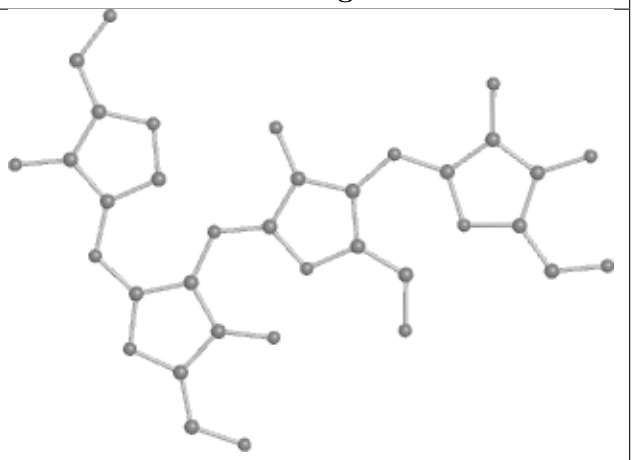
Torsions	**Rings**

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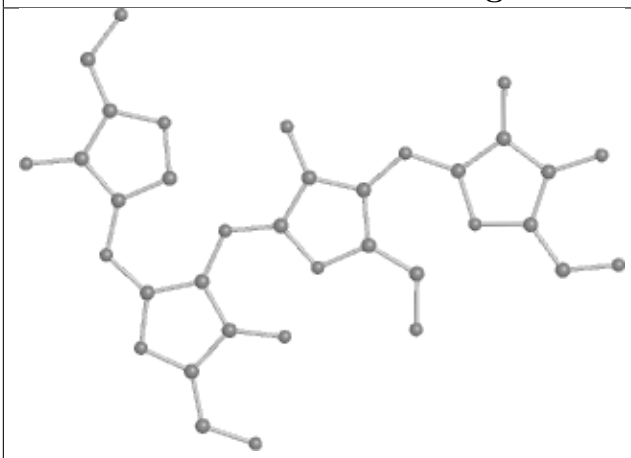	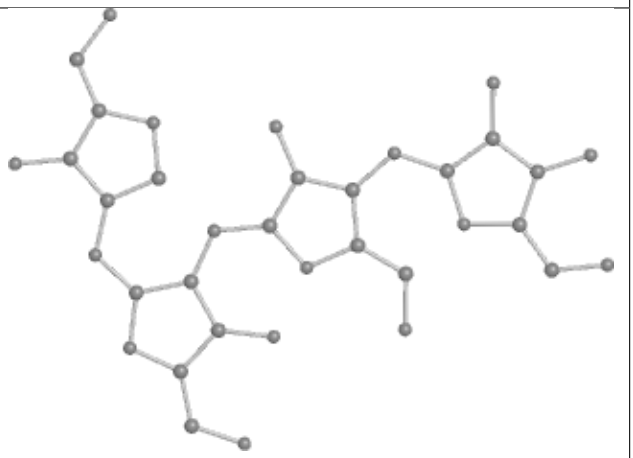
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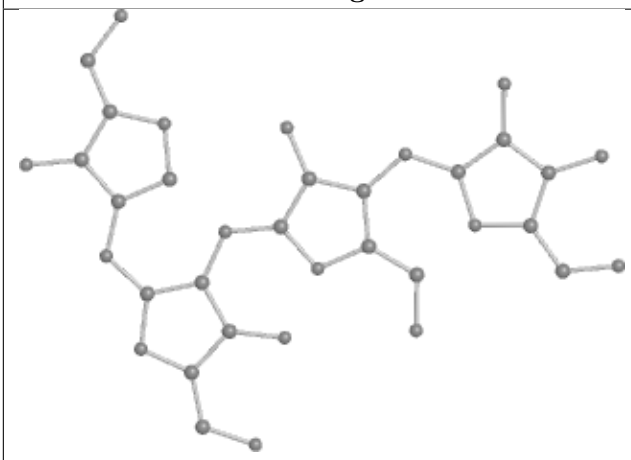	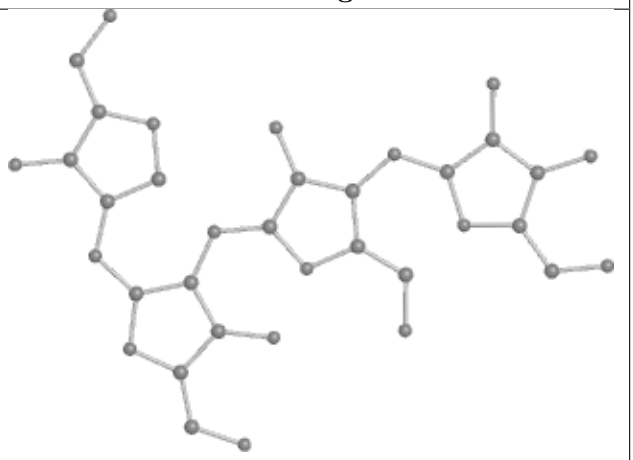
Torsions	**Rings**

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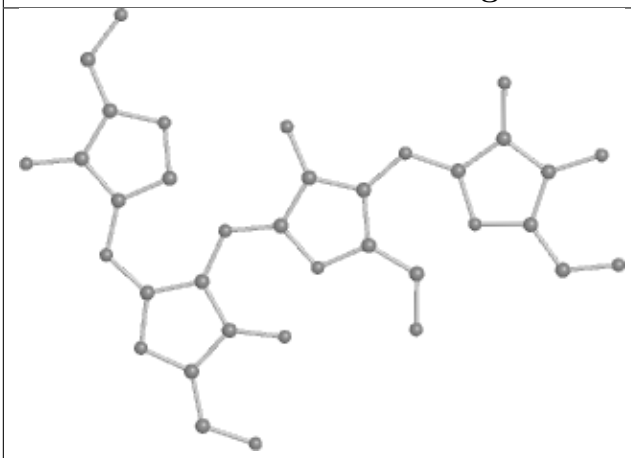
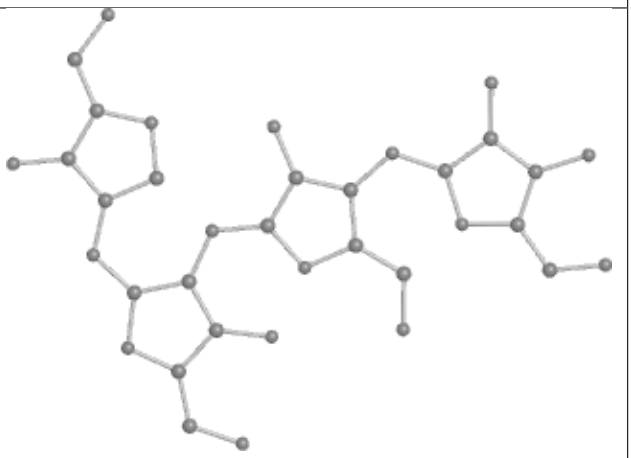
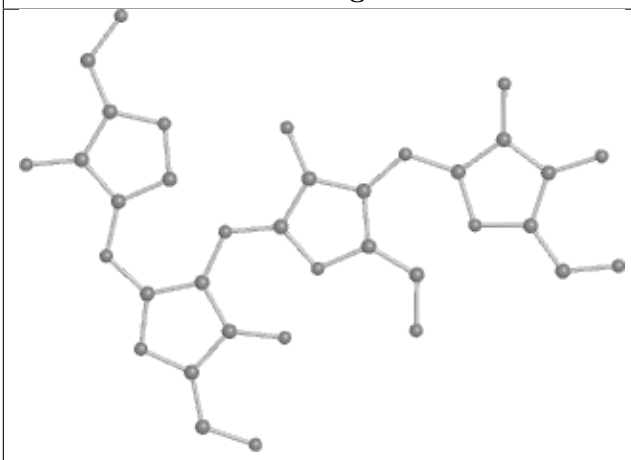
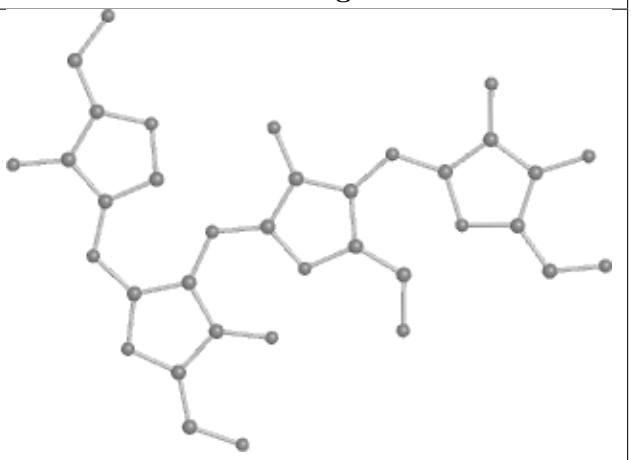
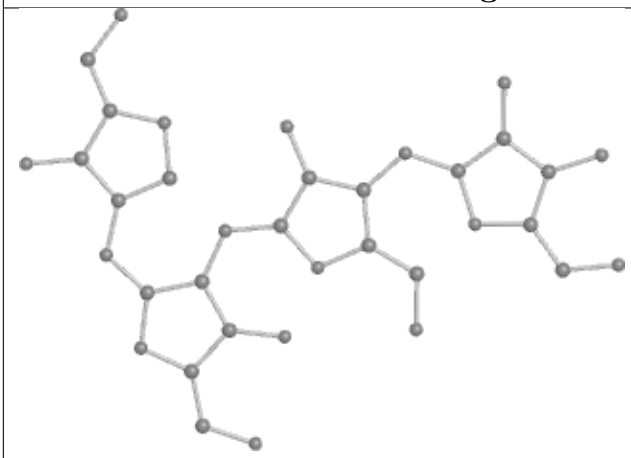
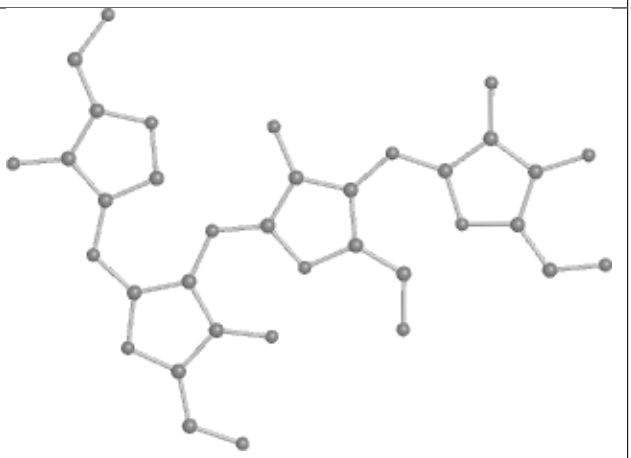
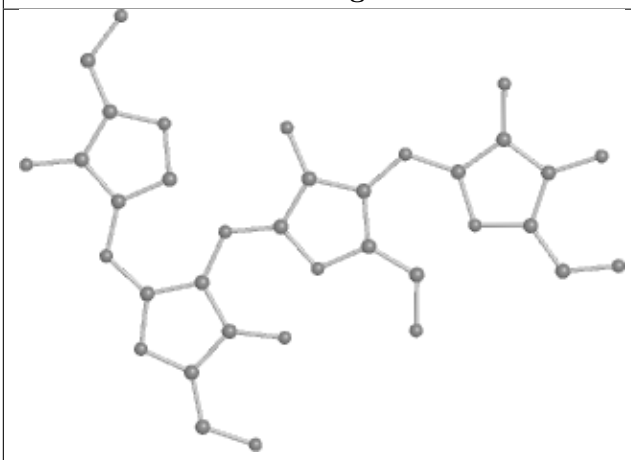
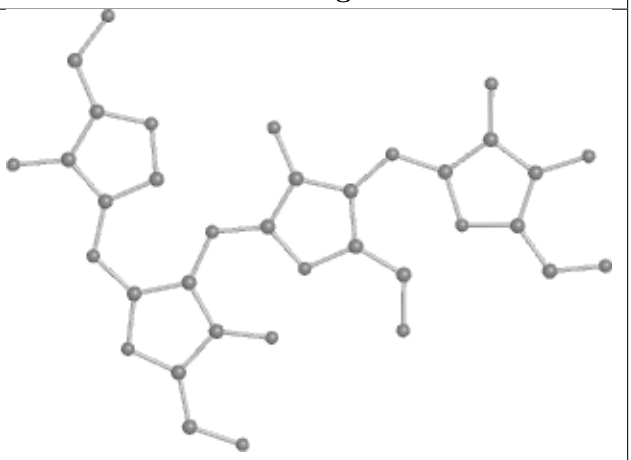
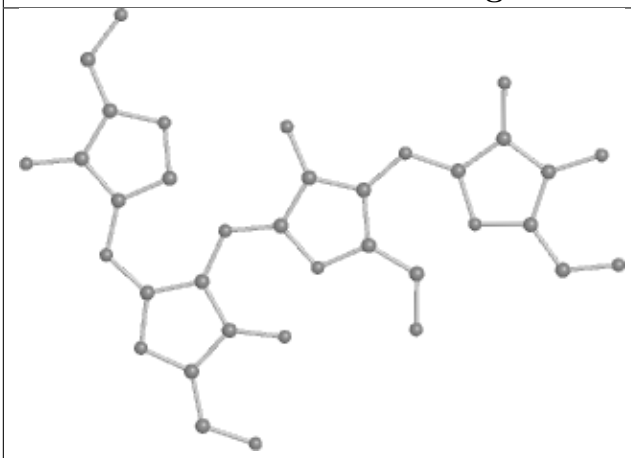
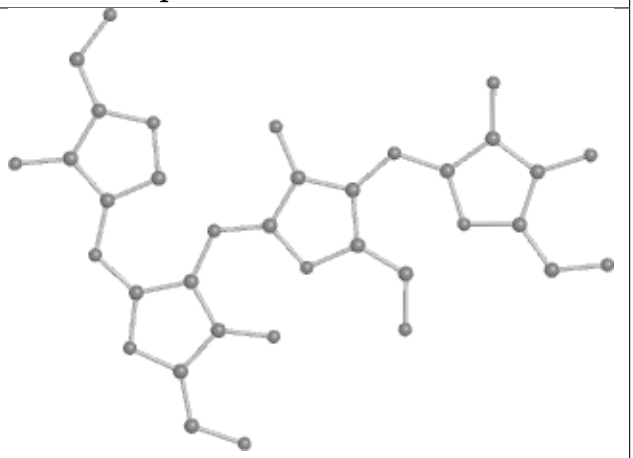
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain mB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain qB	
	
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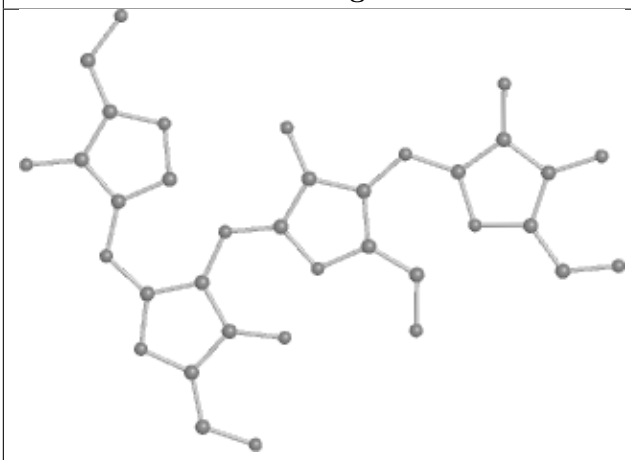
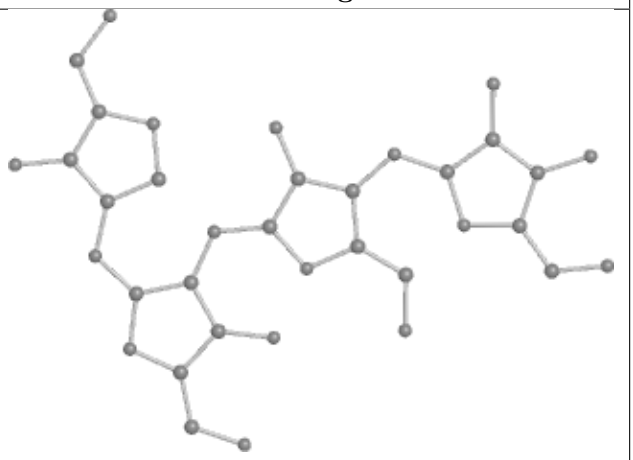
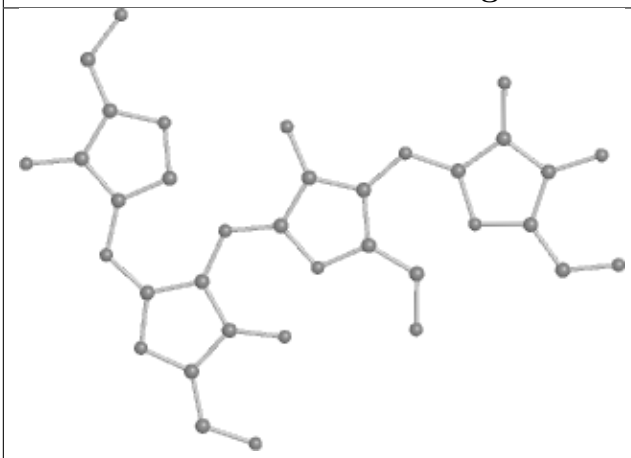
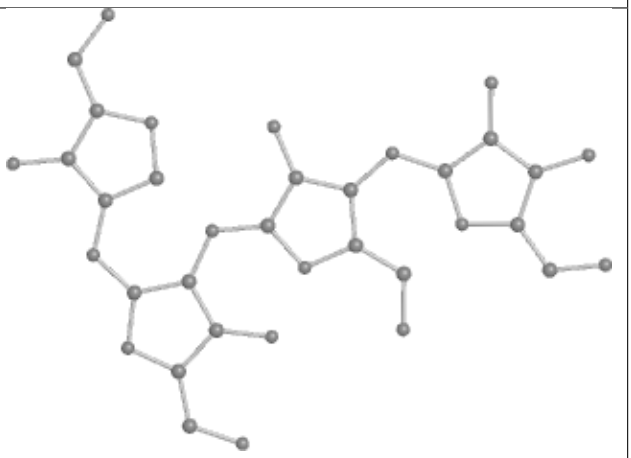
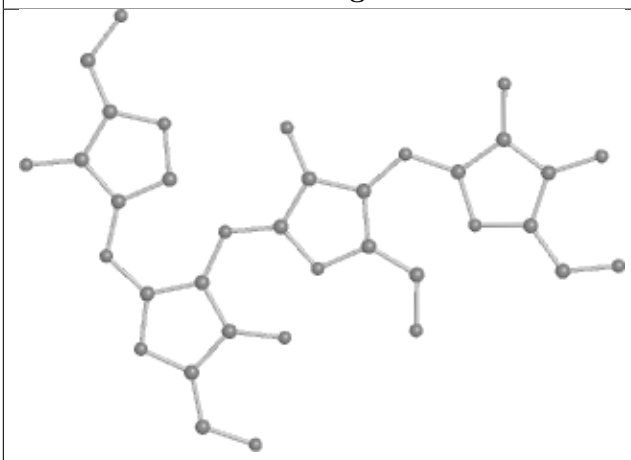
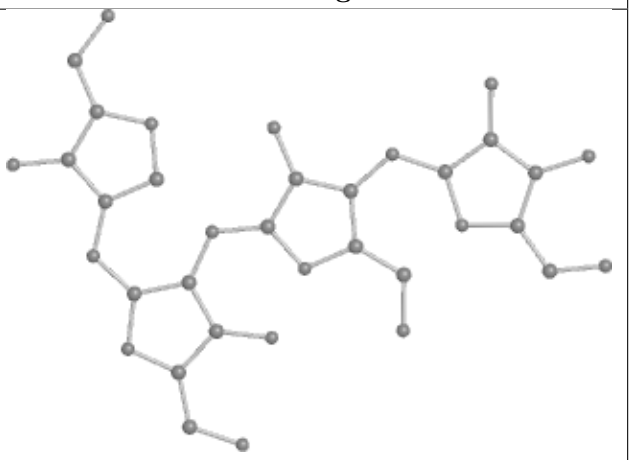
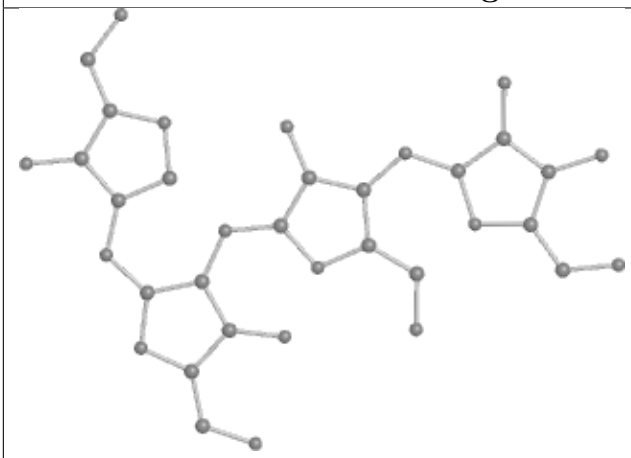
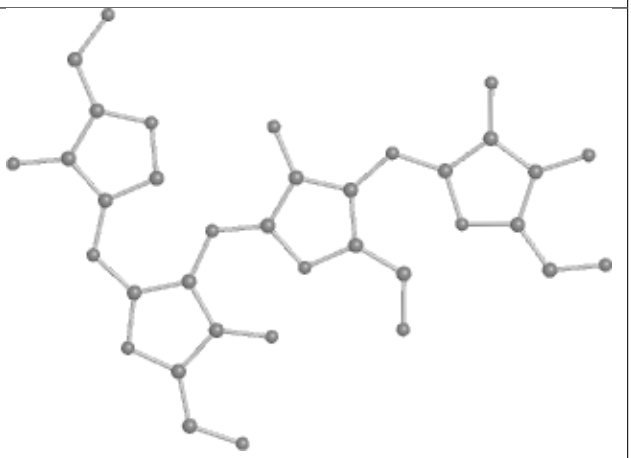
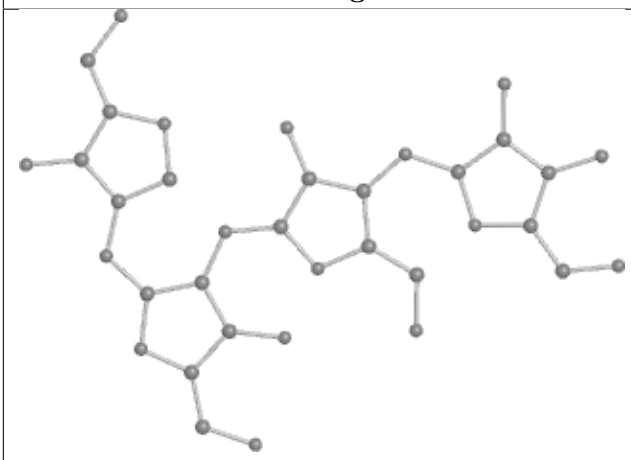
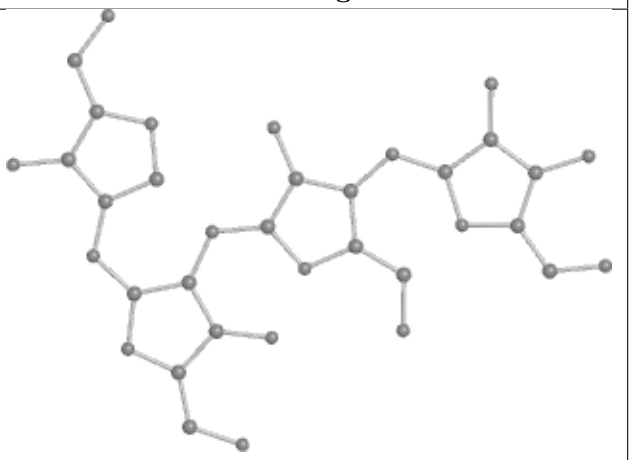
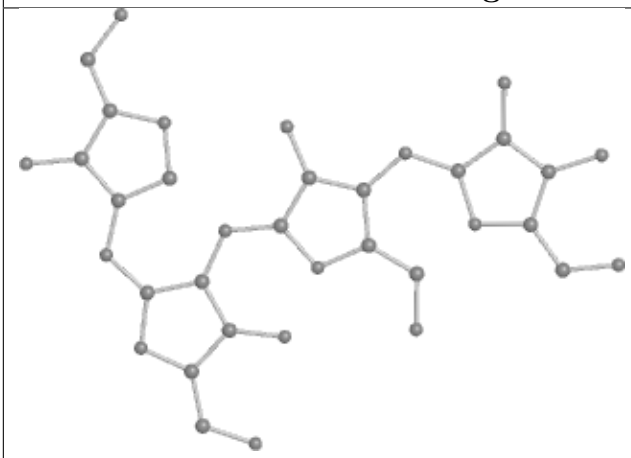
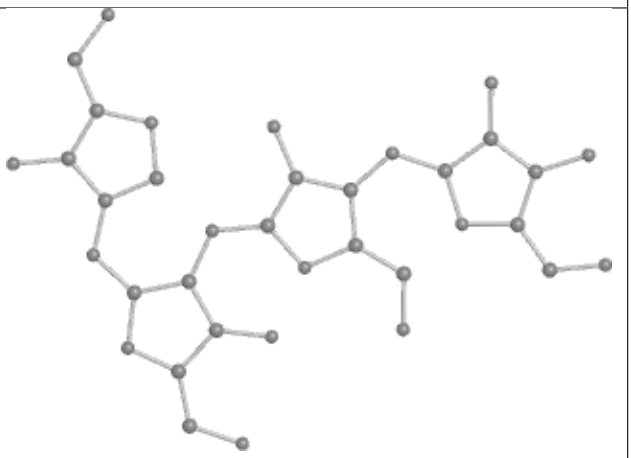
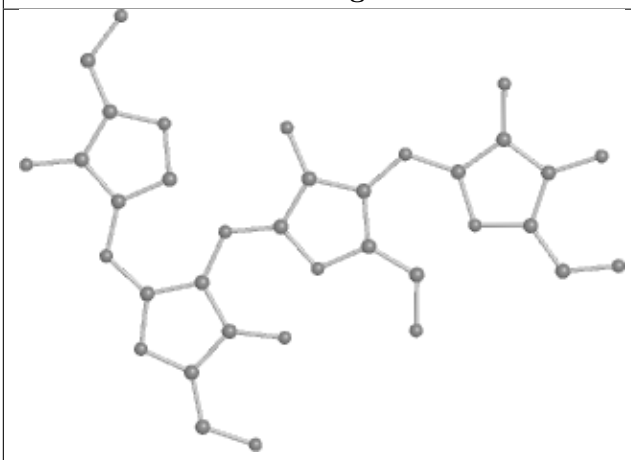
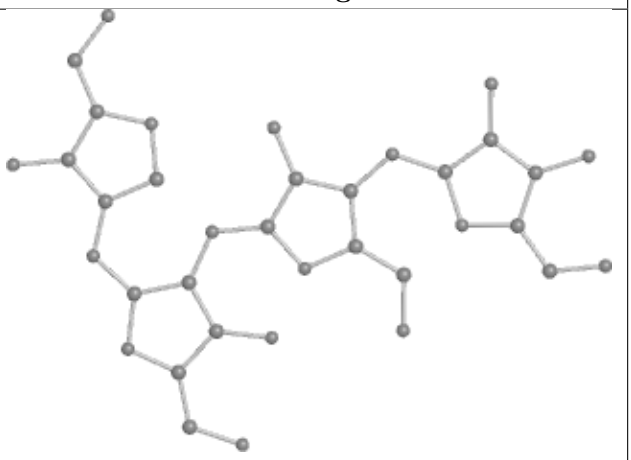
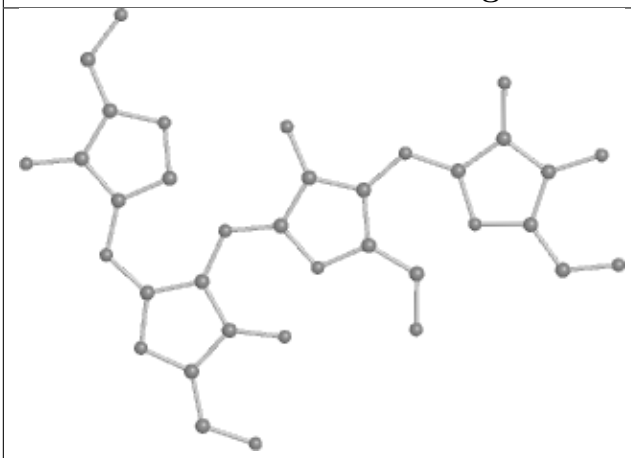
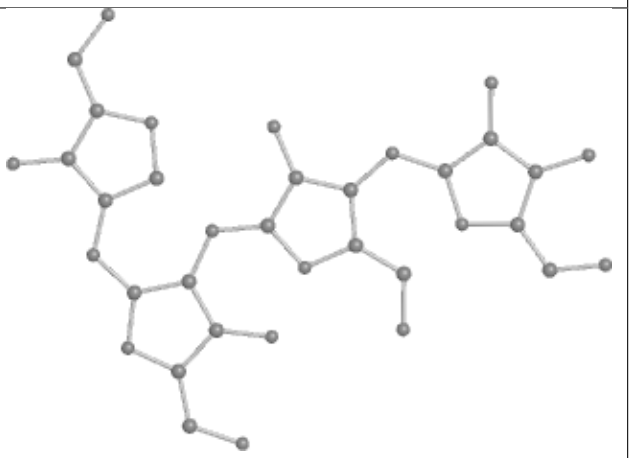
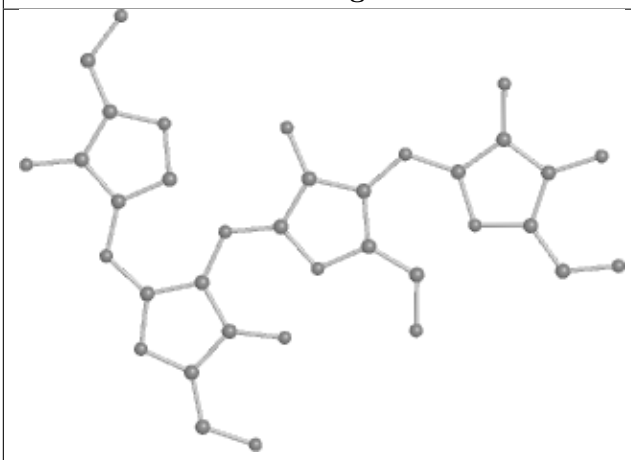
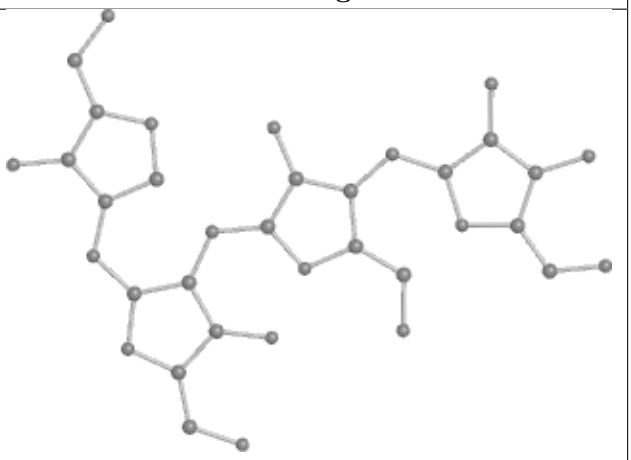
	
Torsions	**Rings**

Oligosaccharide Chain DC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain OC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain PC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain RC	
 Bond lengths	 Bond angles
 Torsions	 Rings

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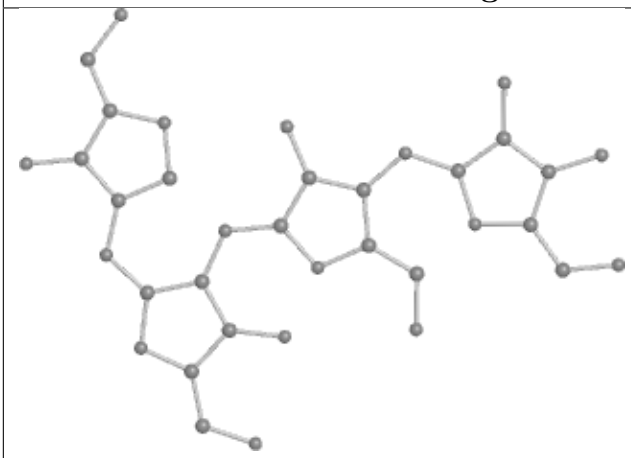
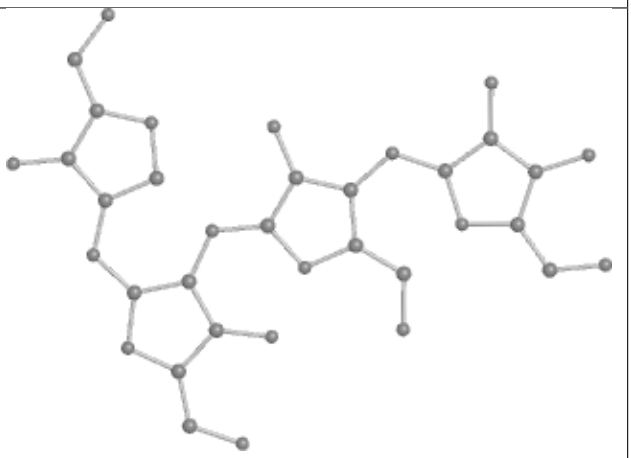
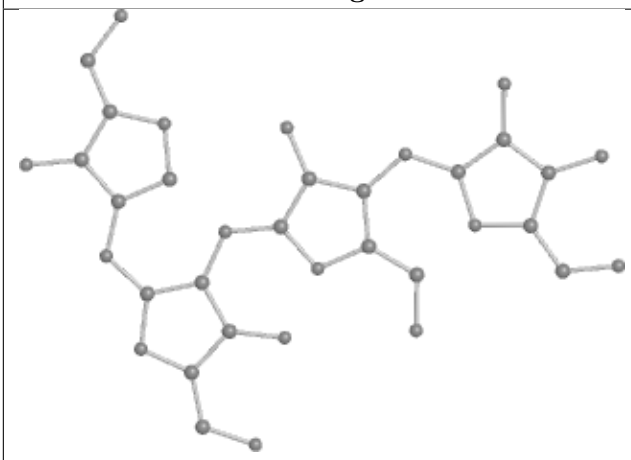
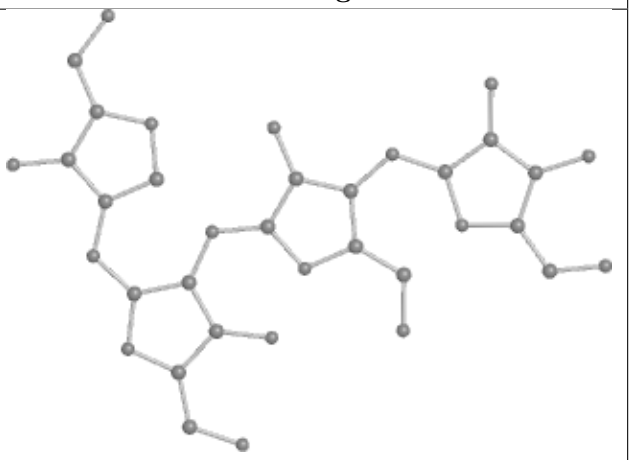
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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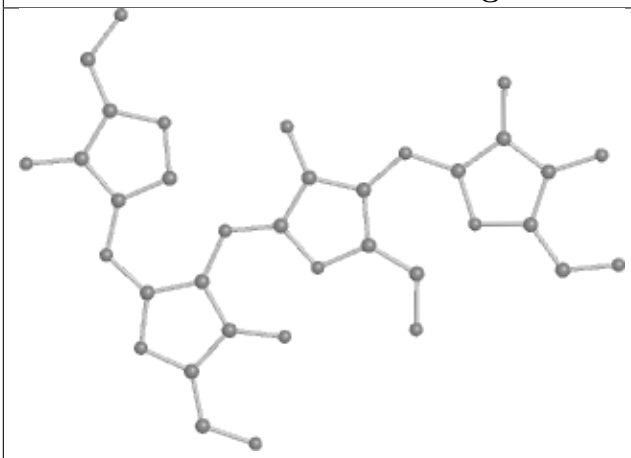
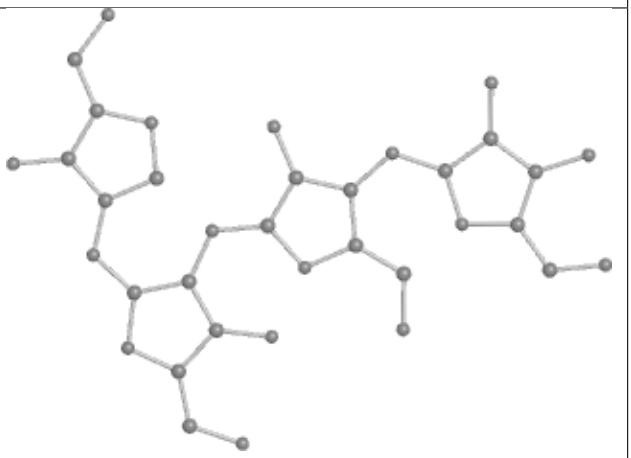
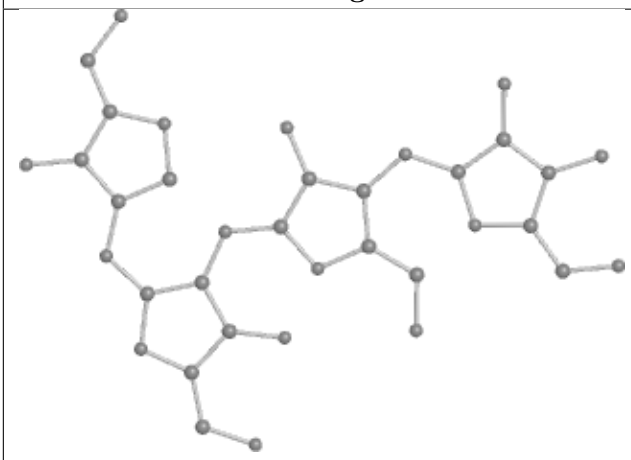
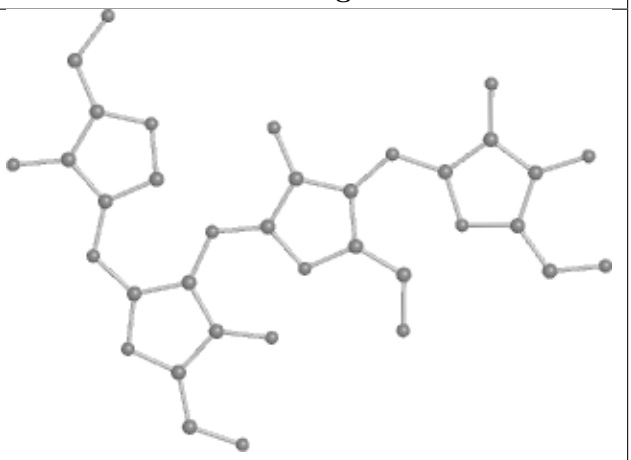
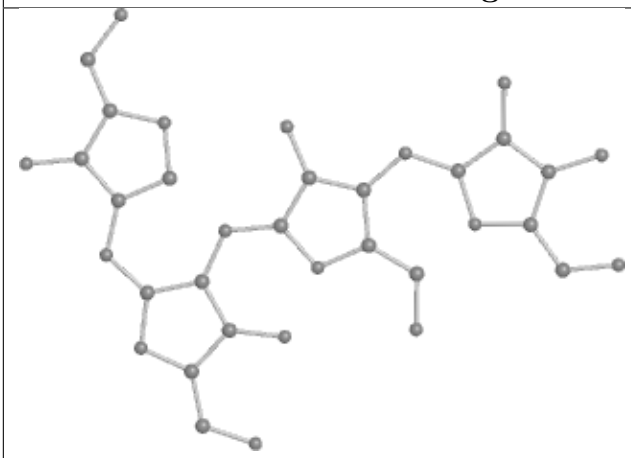
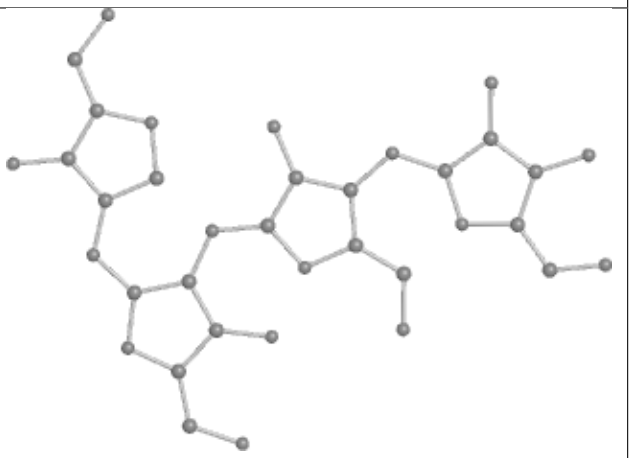
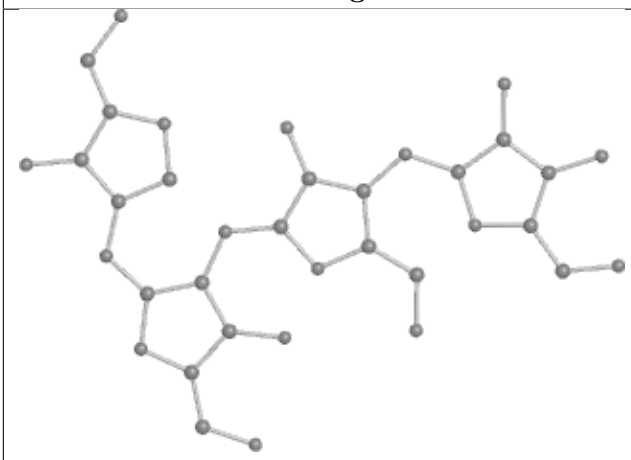
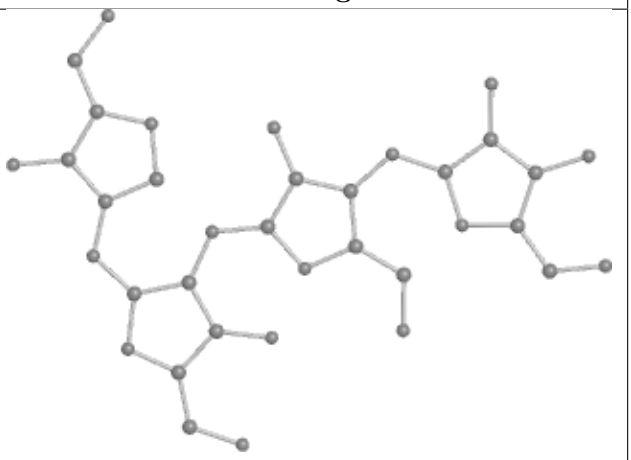
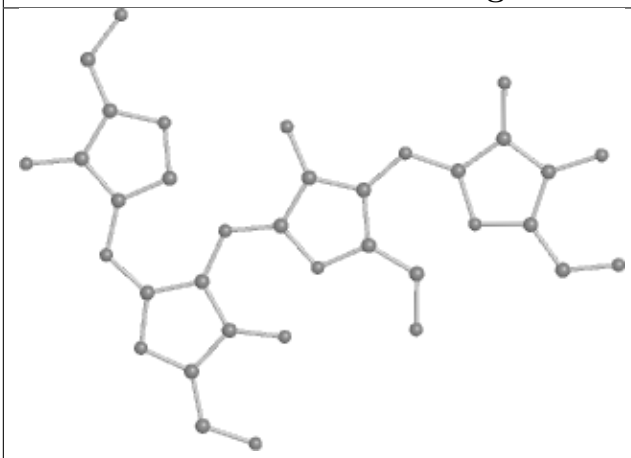
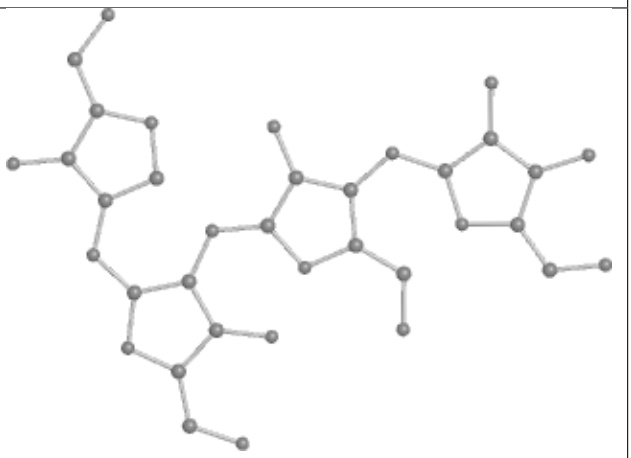
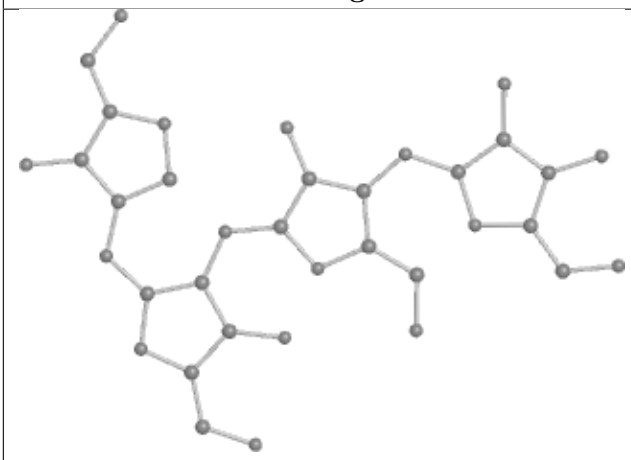
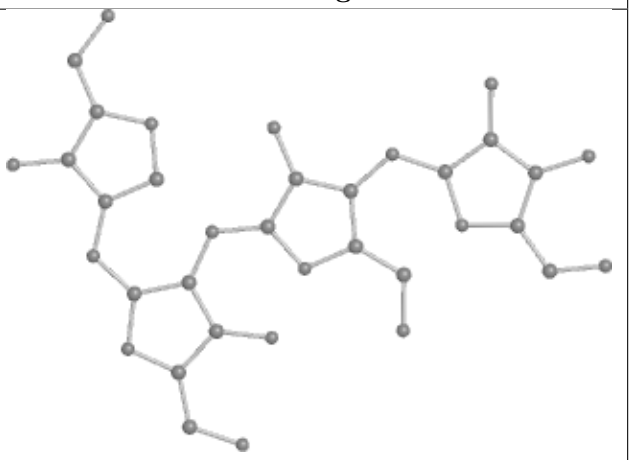
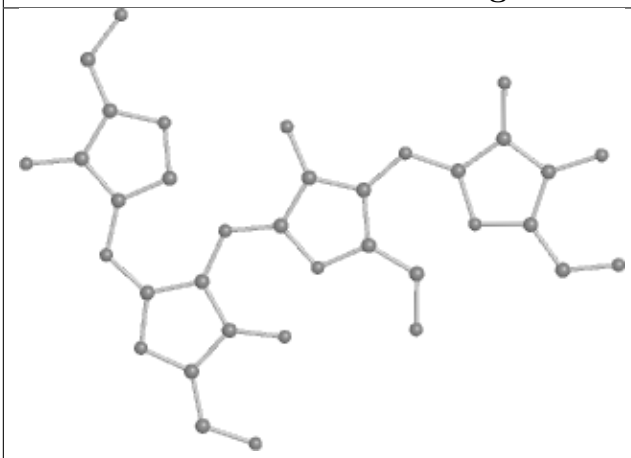
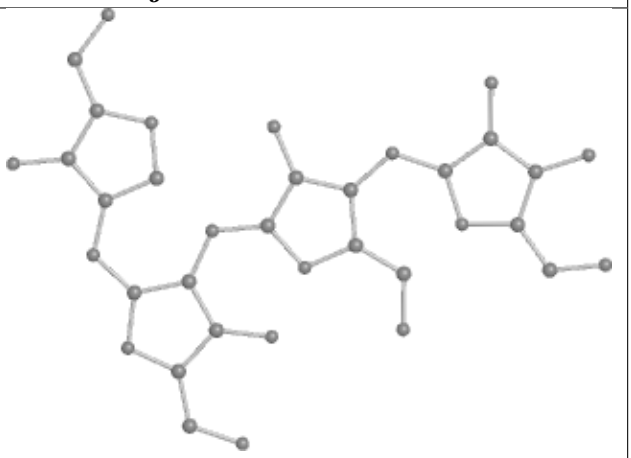
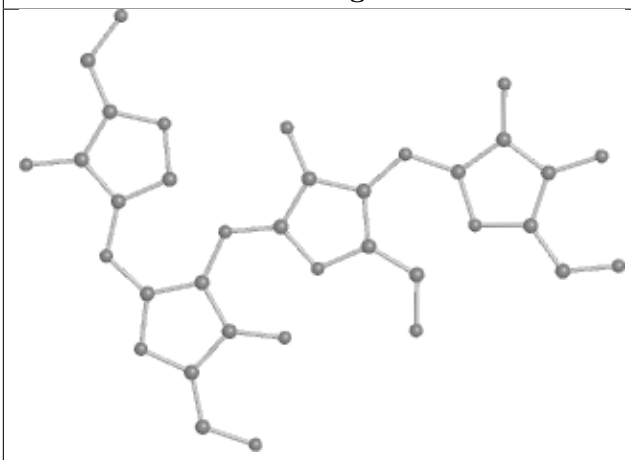
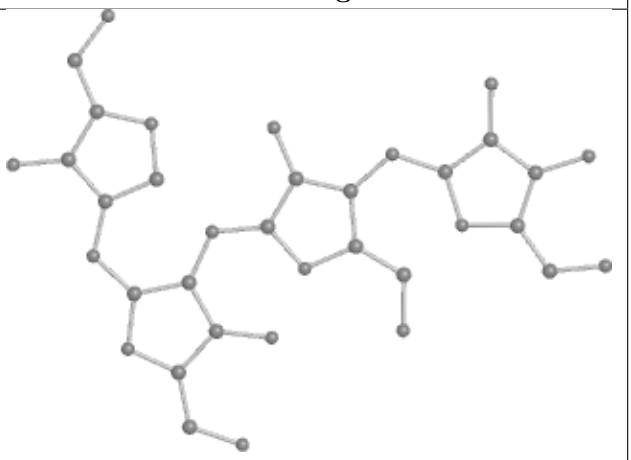
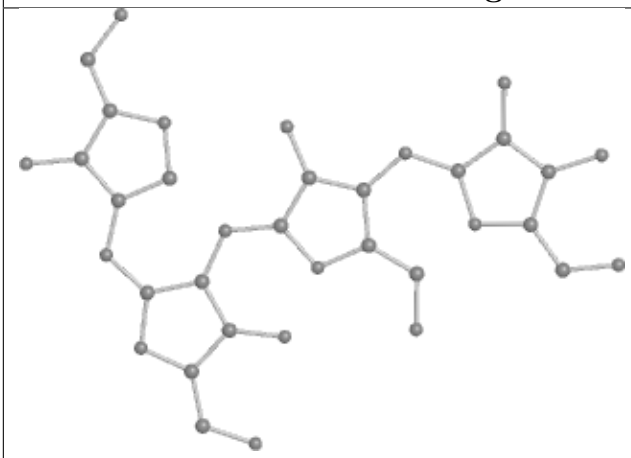
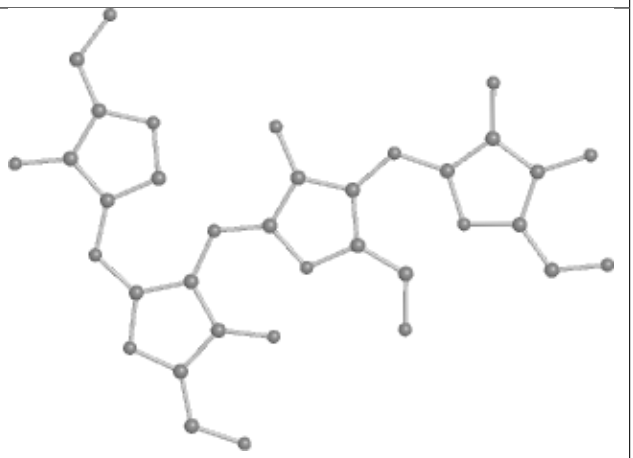
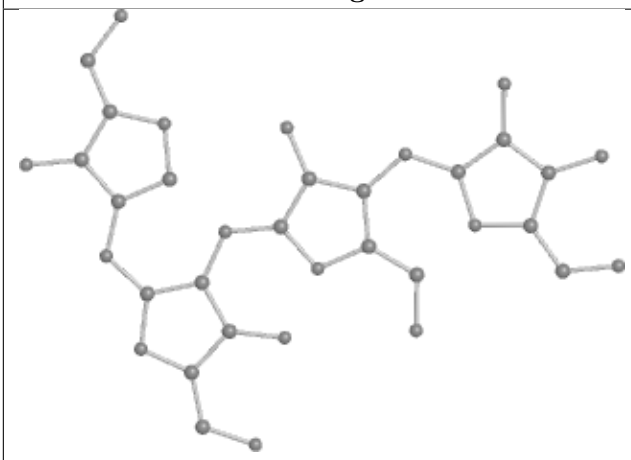
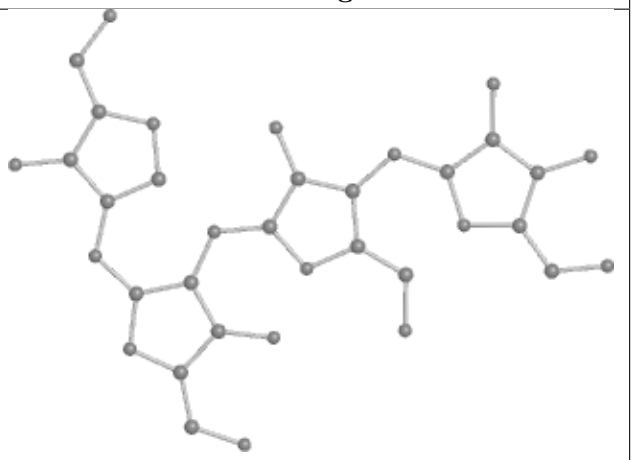
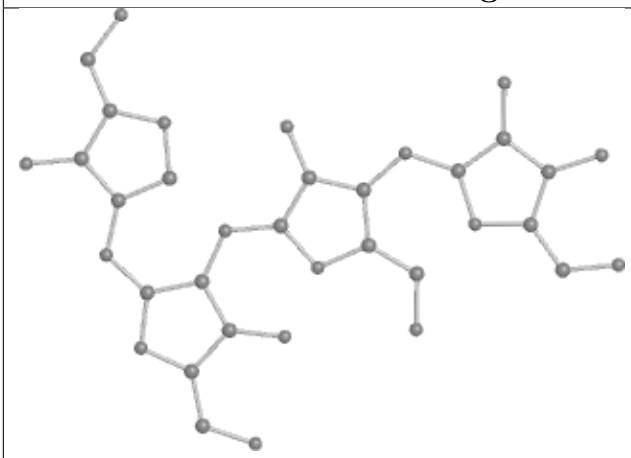
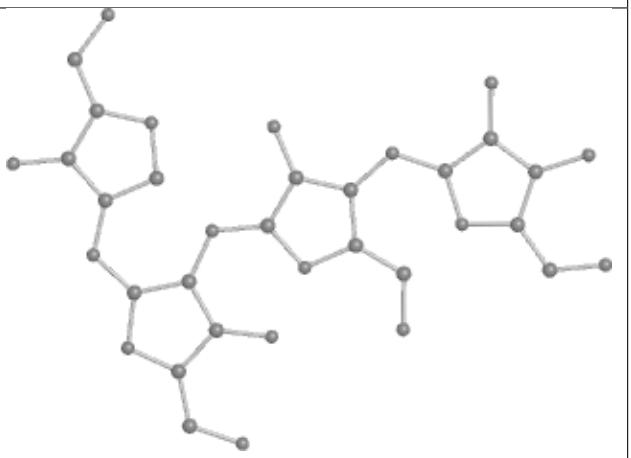
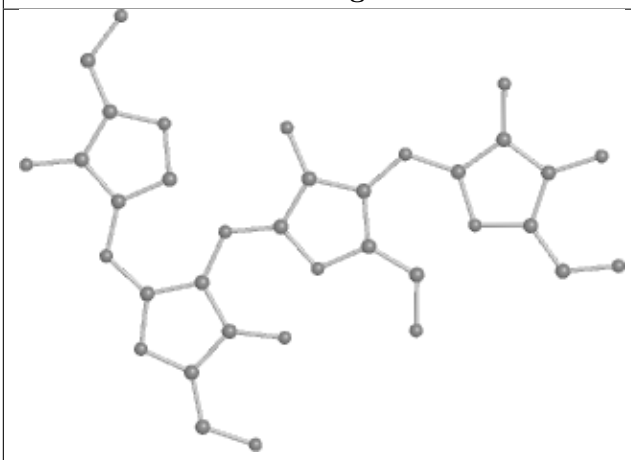
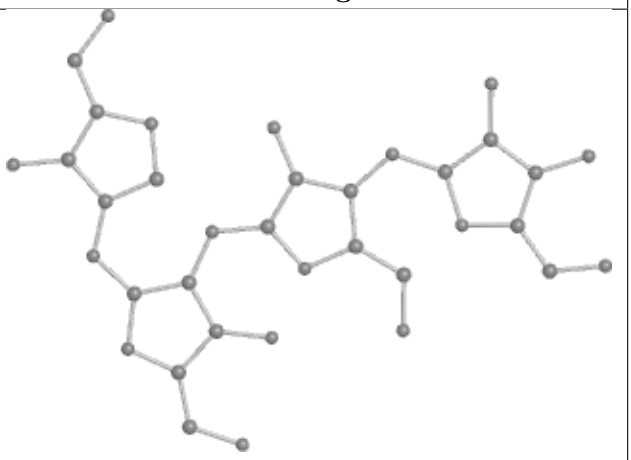
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain YC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain cC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain jC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain nC	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain AD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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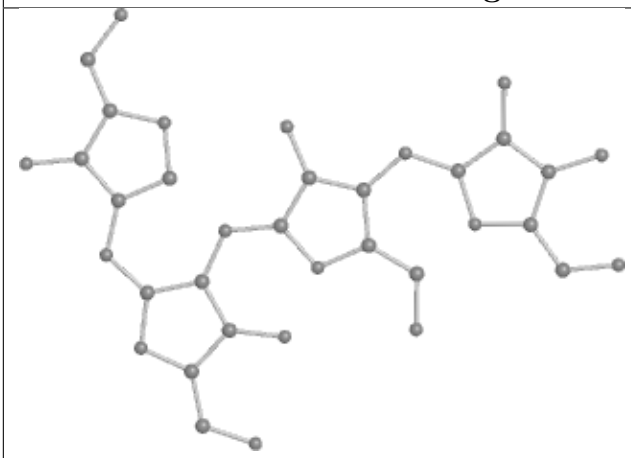
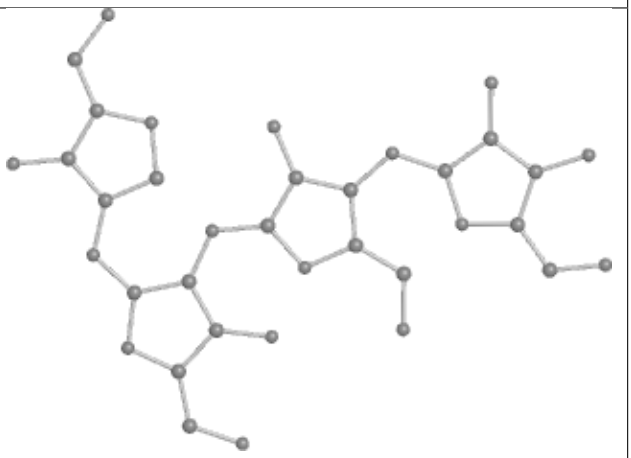
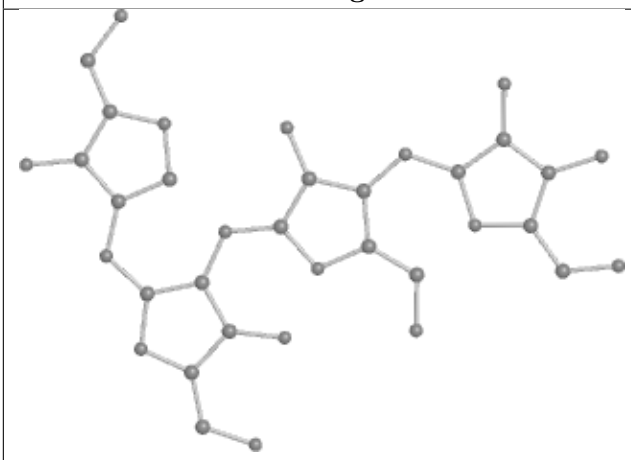
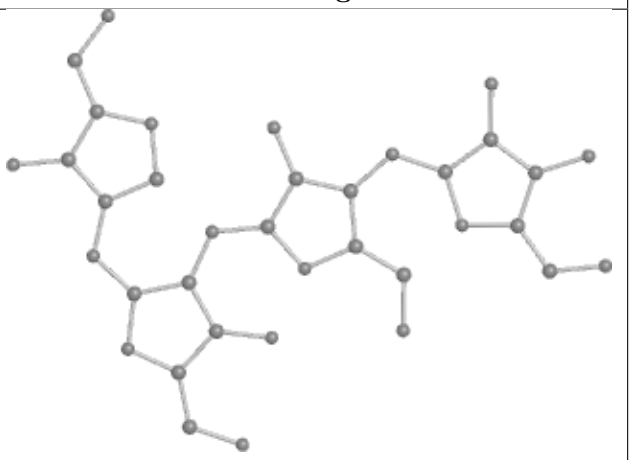
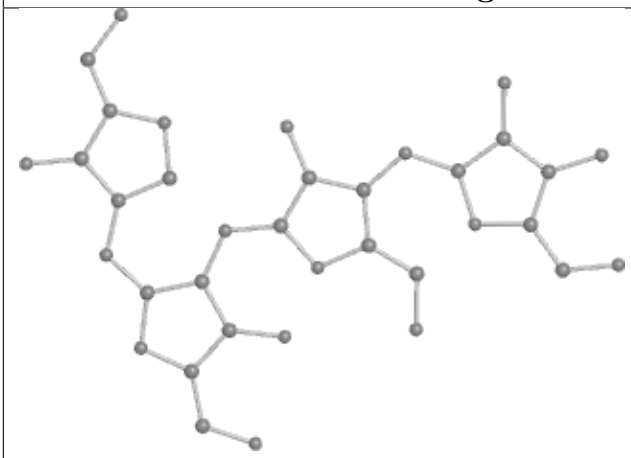
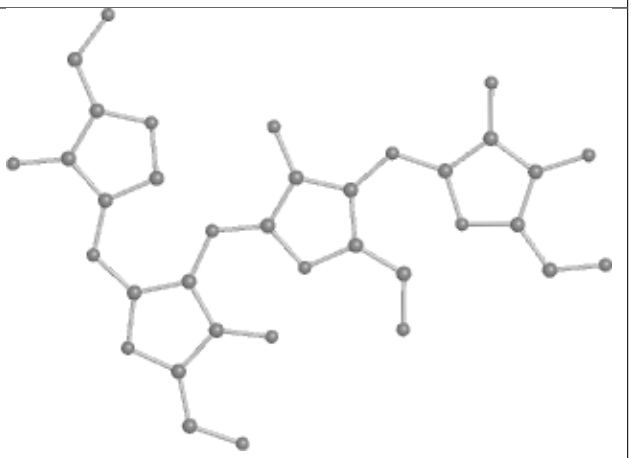
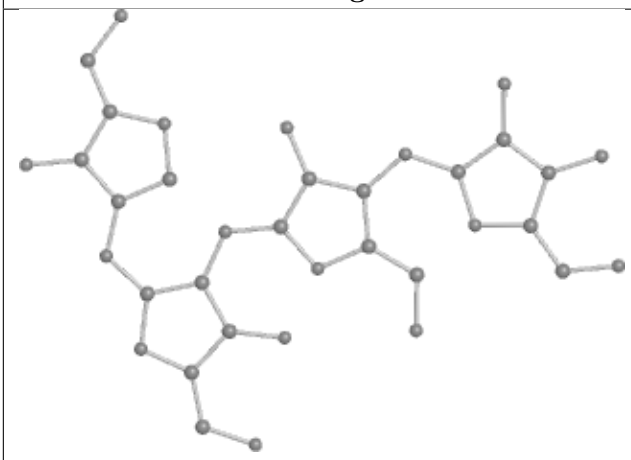
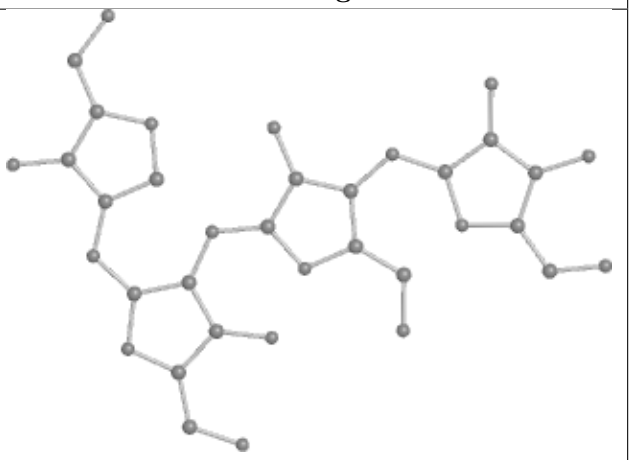
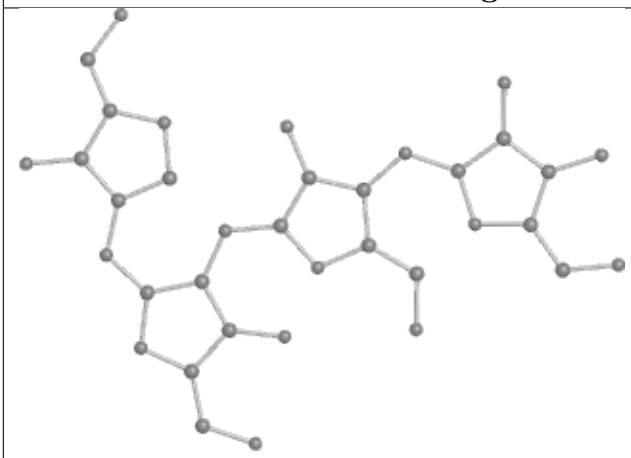
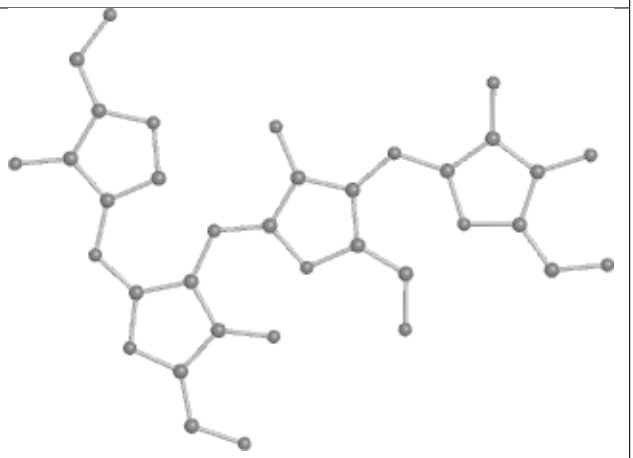
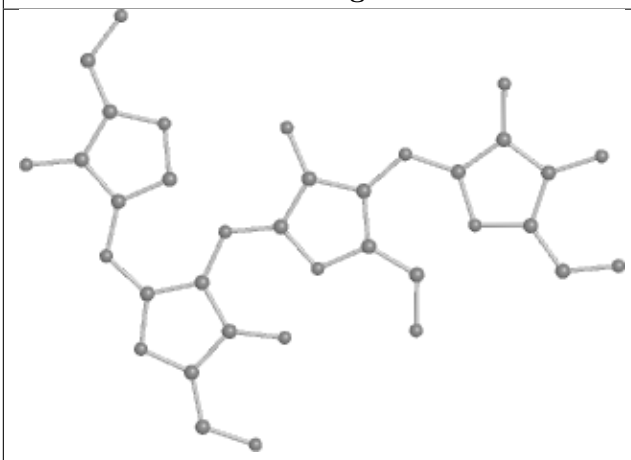
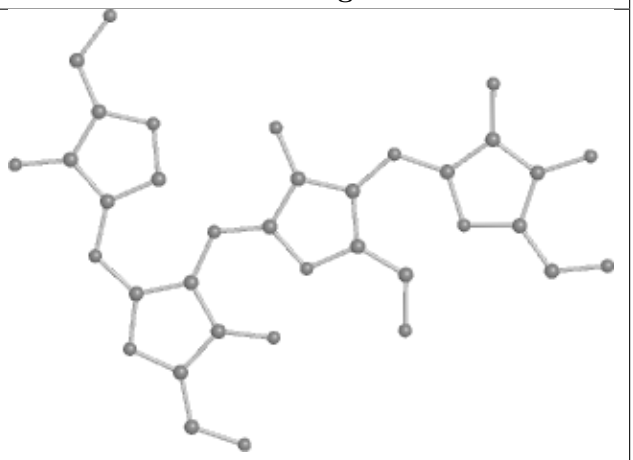
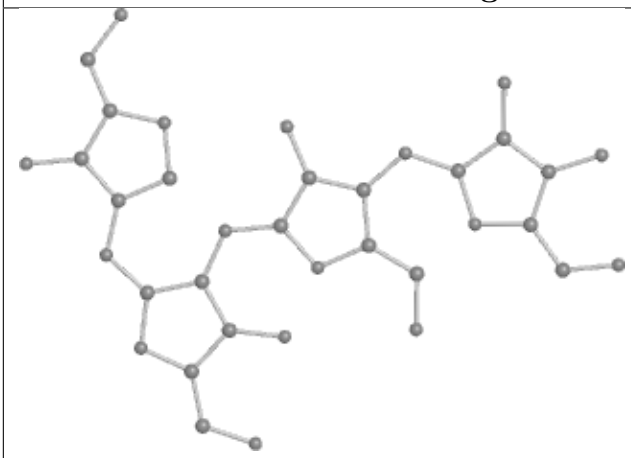
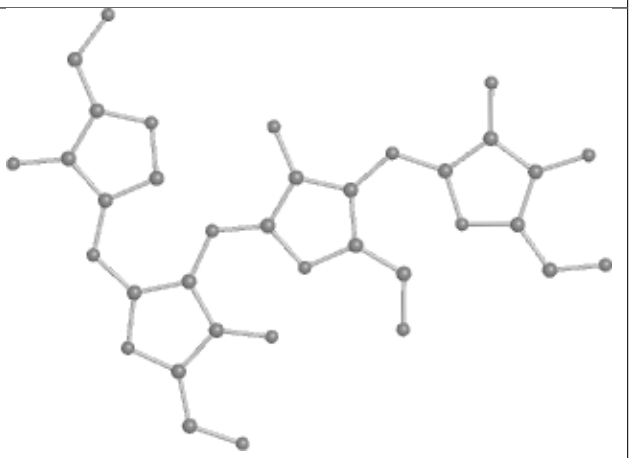
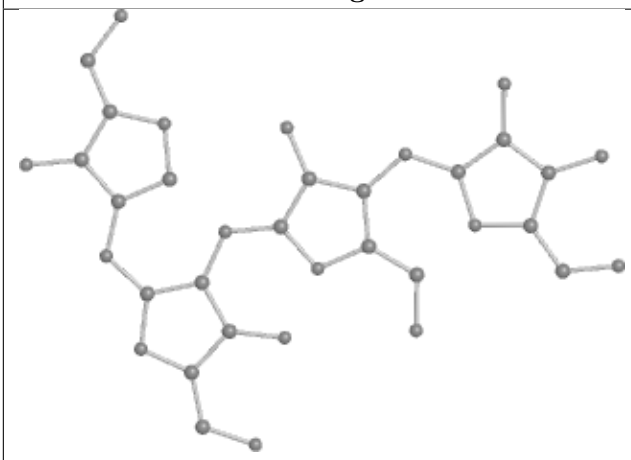
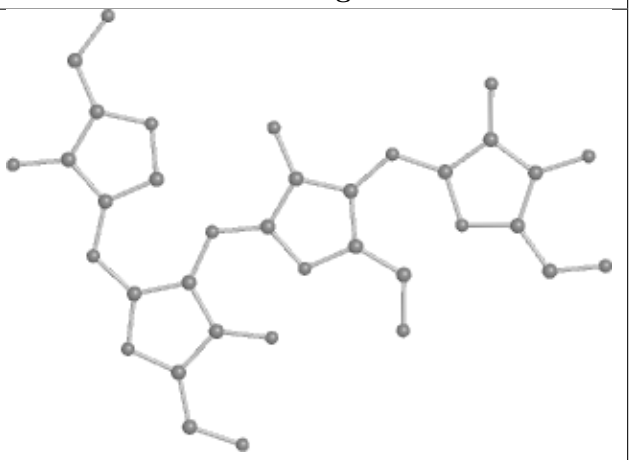
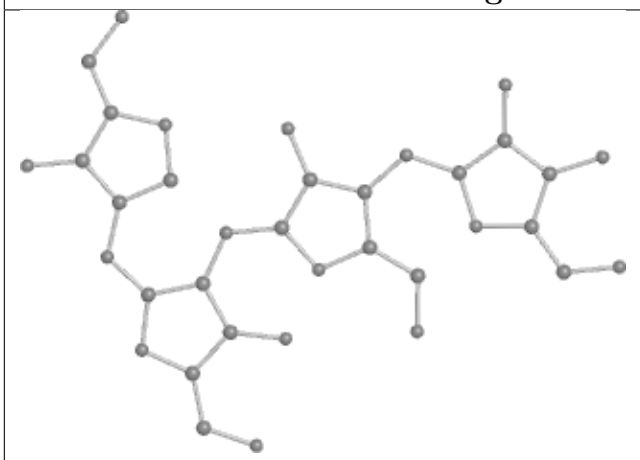
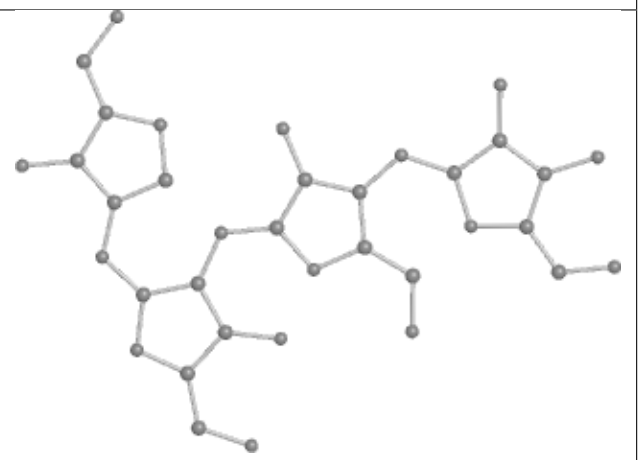
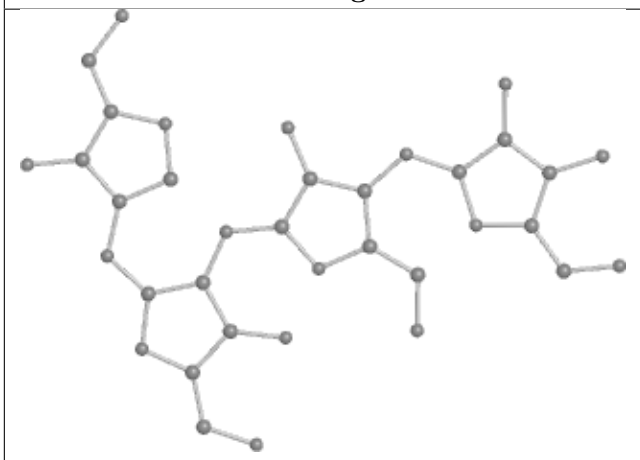
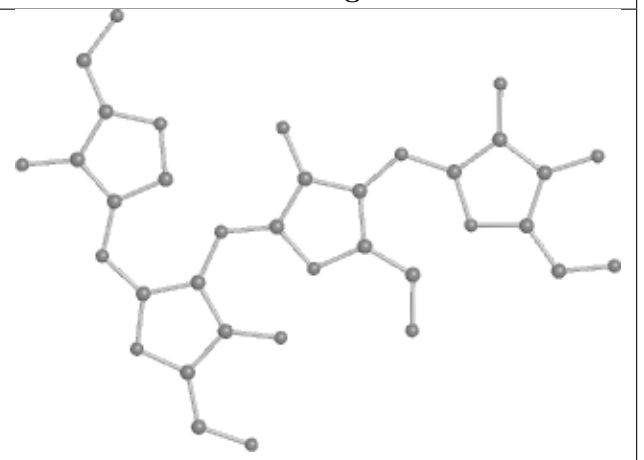
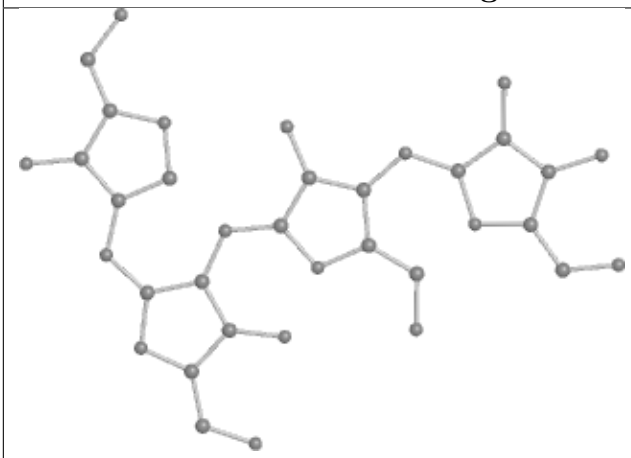
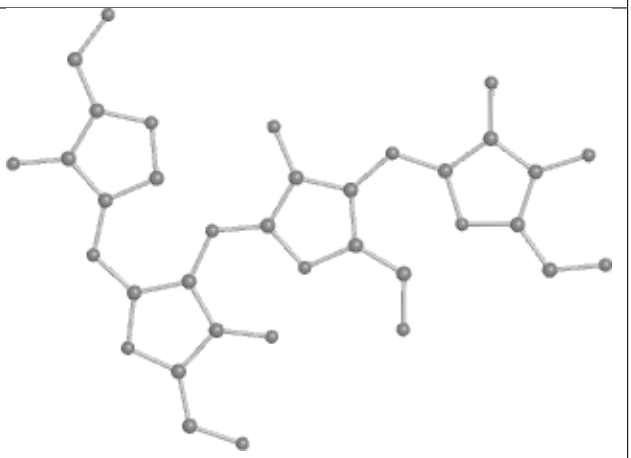
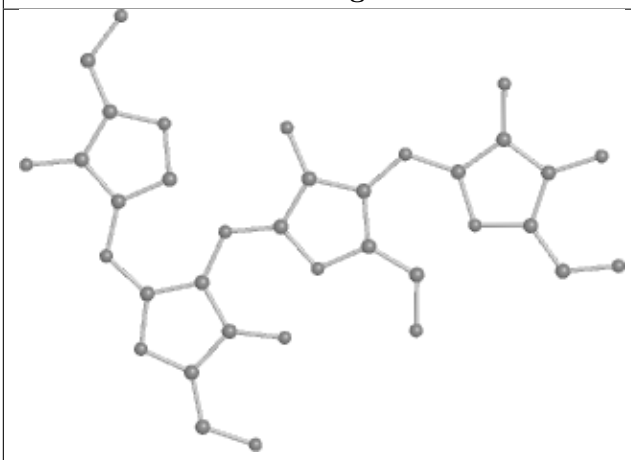
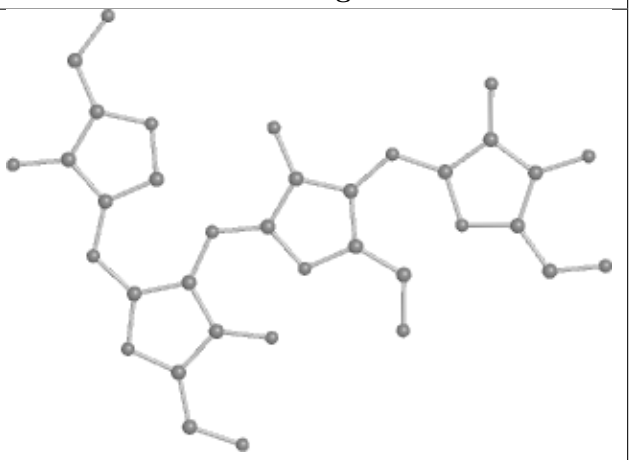
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

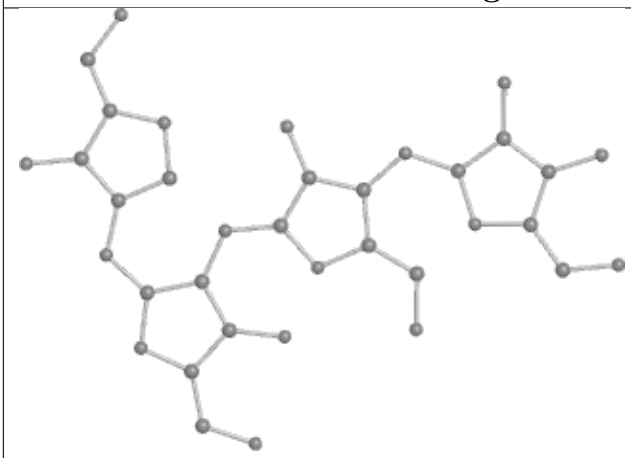
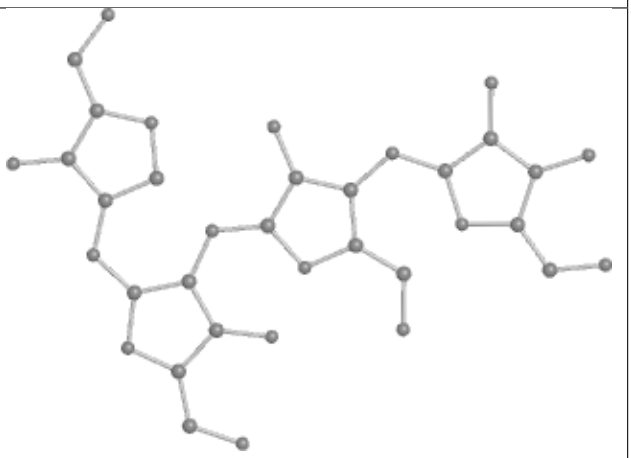
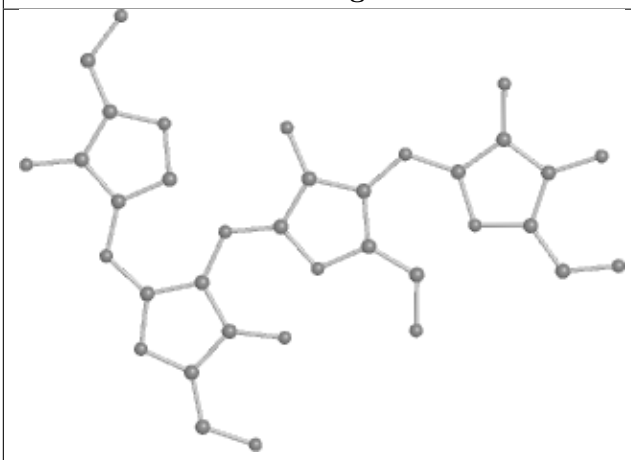
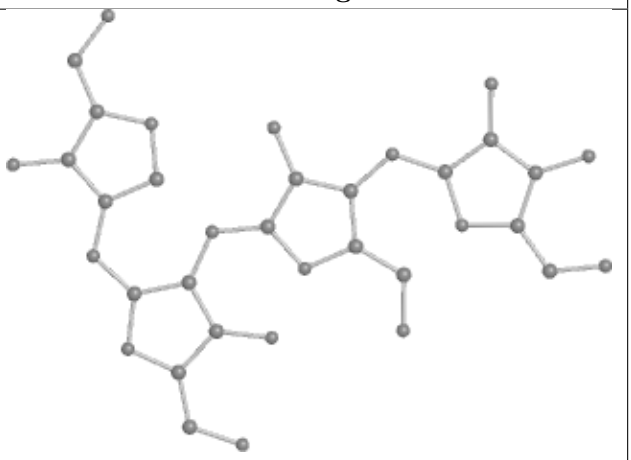
Oligosaccharide Chain MD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

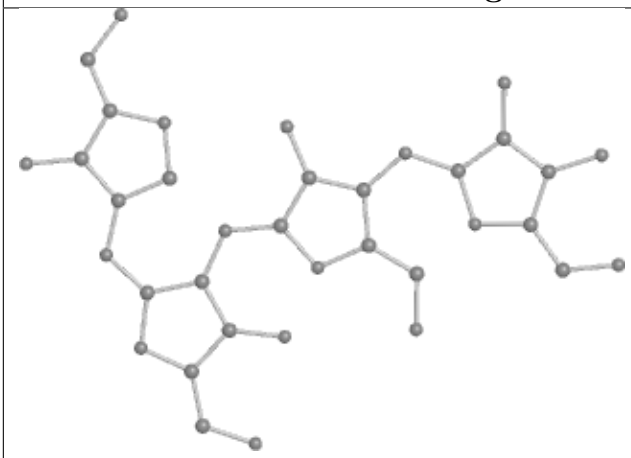
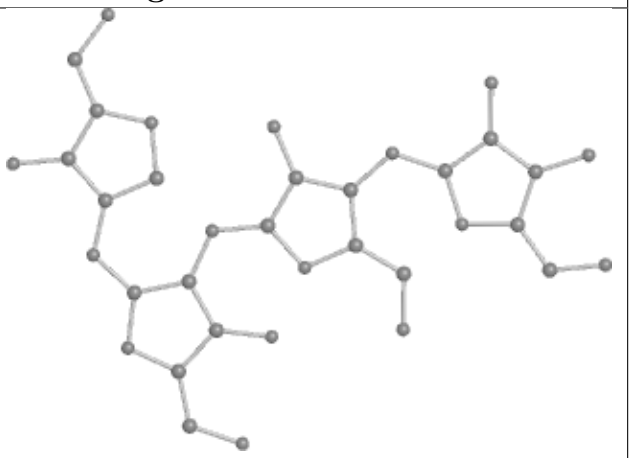
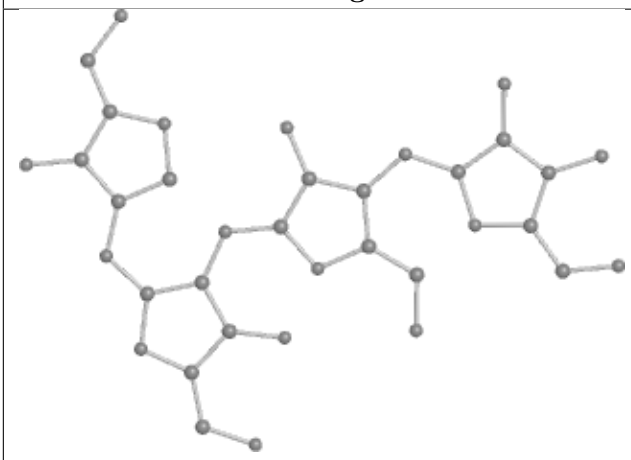
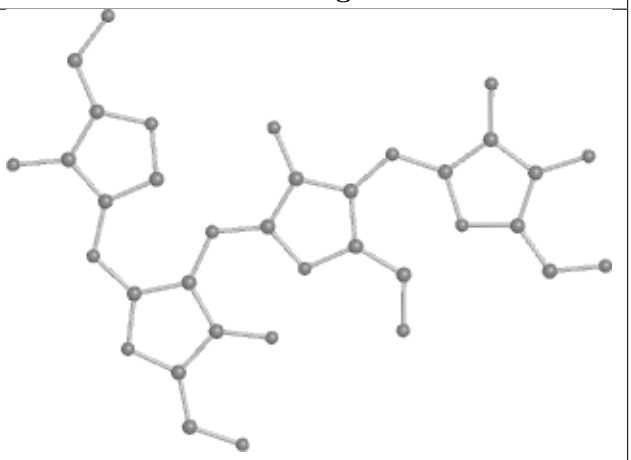
Oligosaccharide Chain OD	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

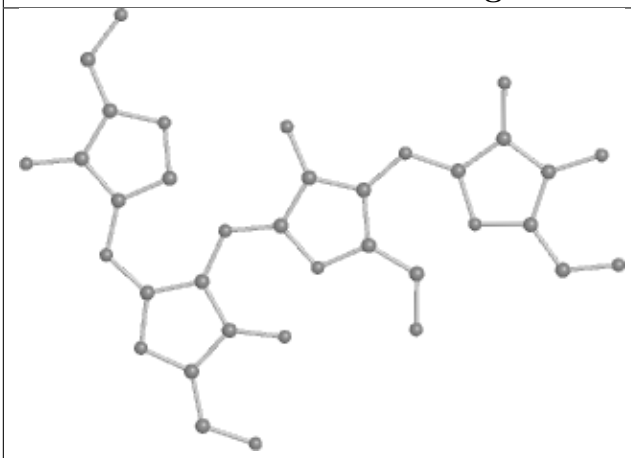
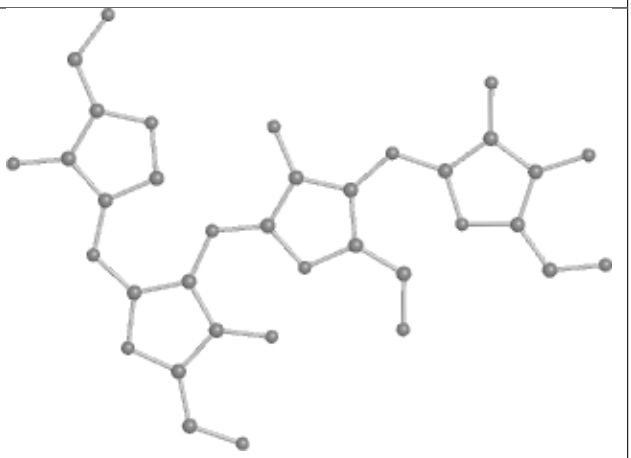
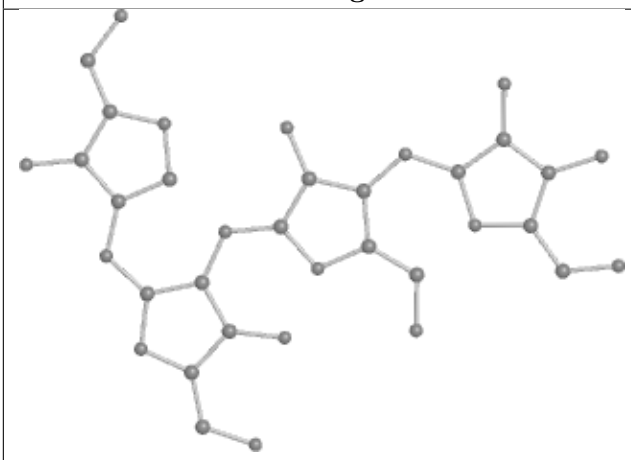
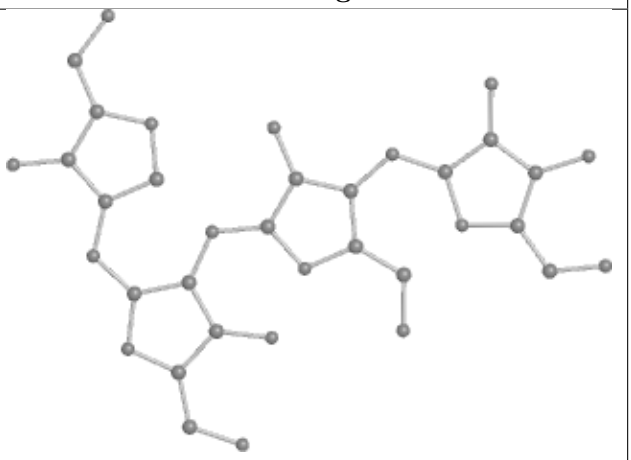
Oligosaccharide Chain RD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

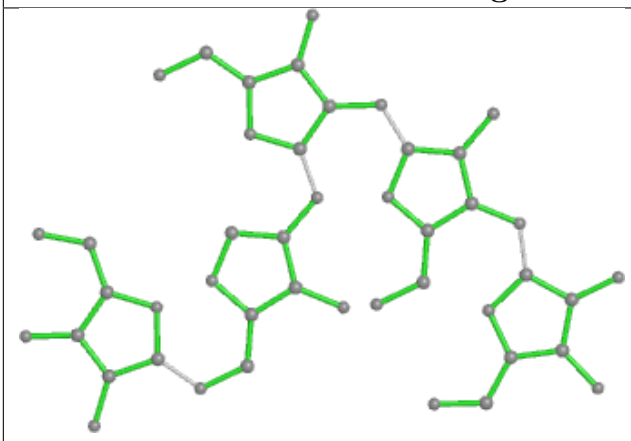
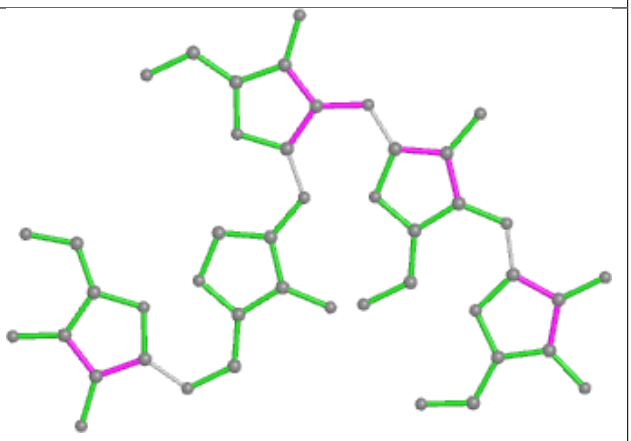
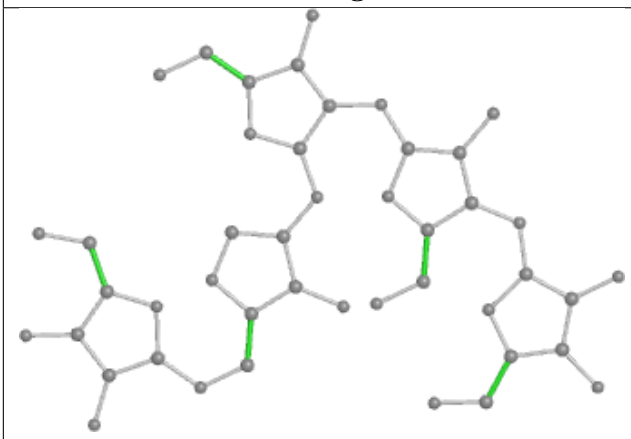
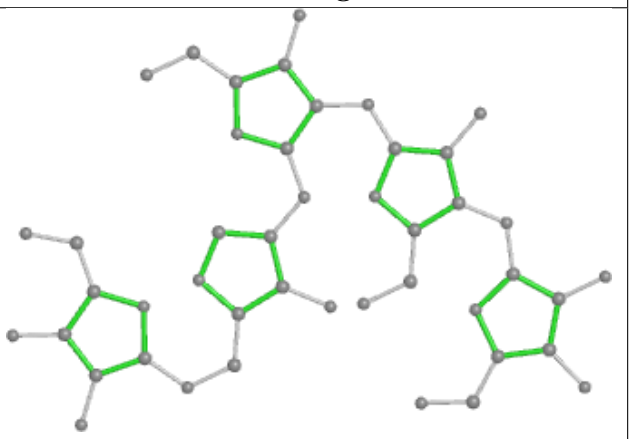
Oligosaccharide Chain SD	
 Bond lengths	 Bond angles
 Torsions	 Rings

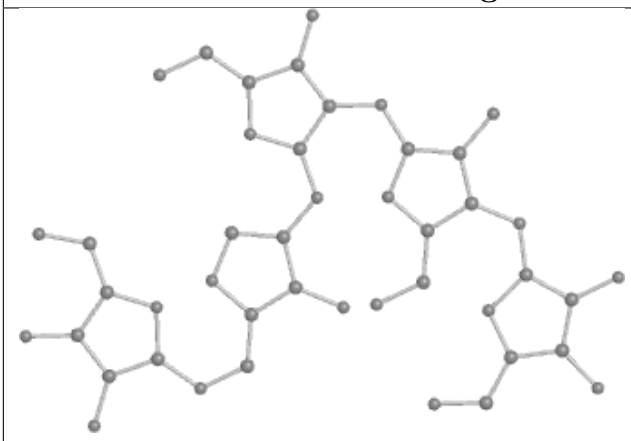
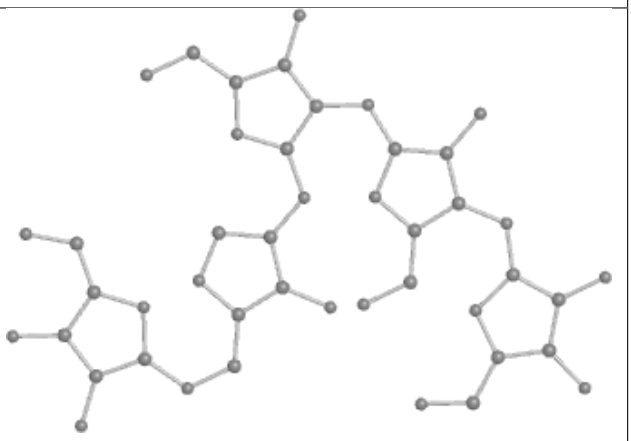
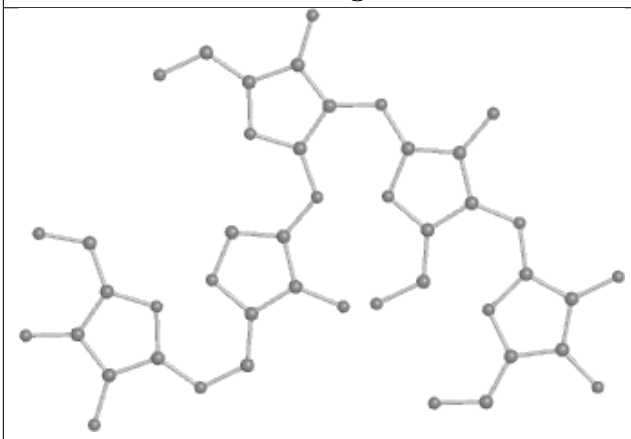
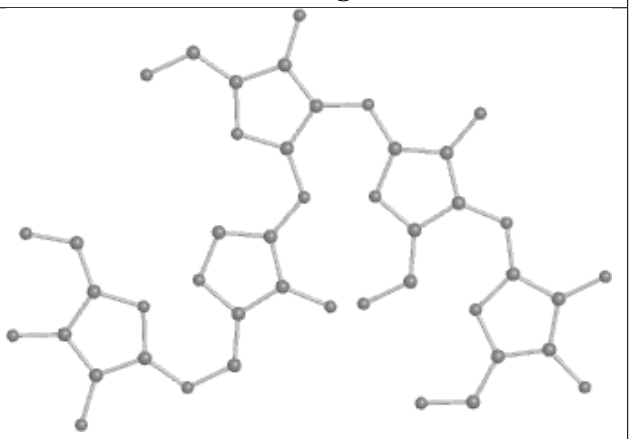
Oligosaccharide Chain VD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

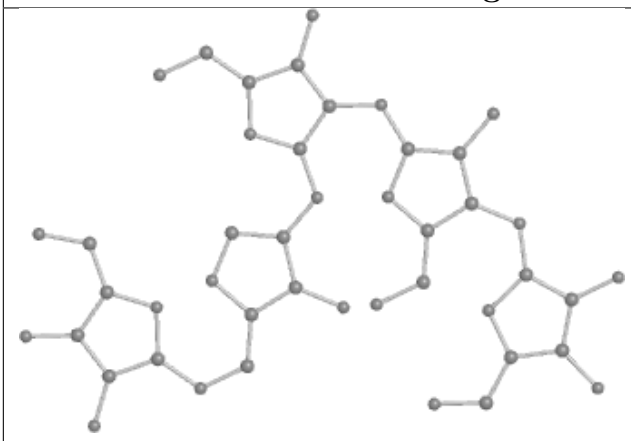
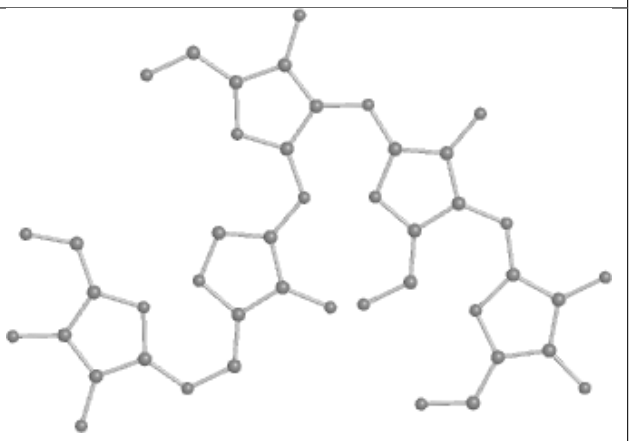
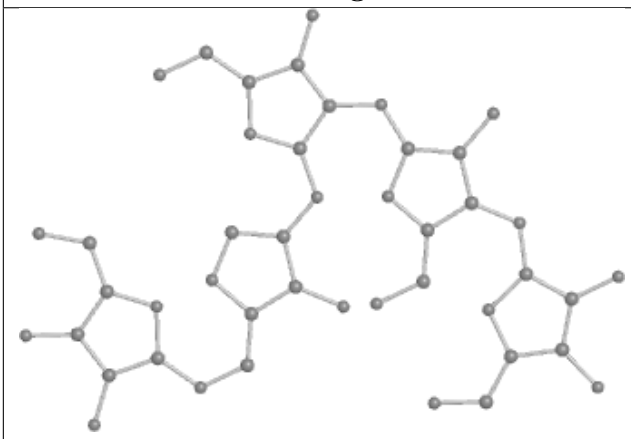
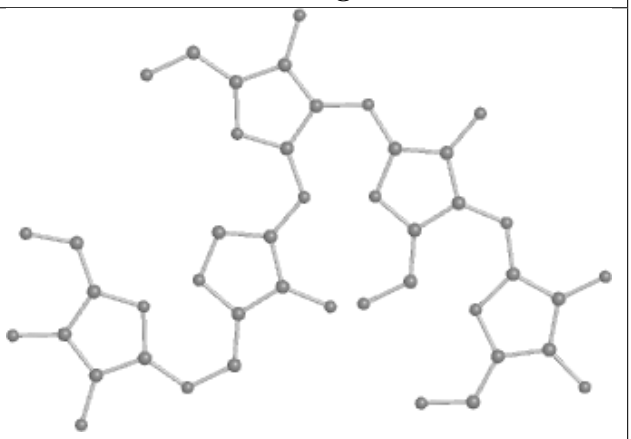
Oligosaccharide Chain ZD	
 Bond lengths	 Bond angles
 Torsions	 Rings

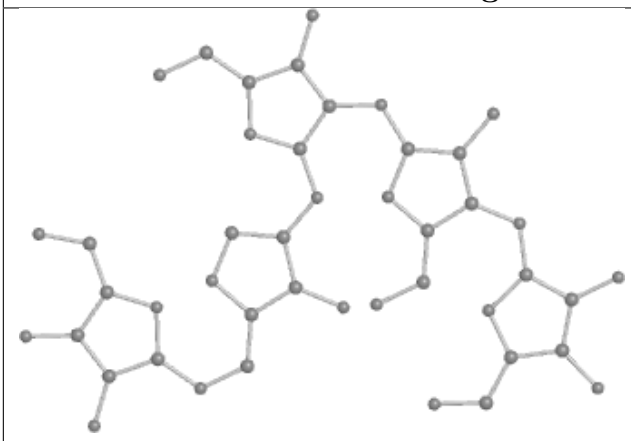
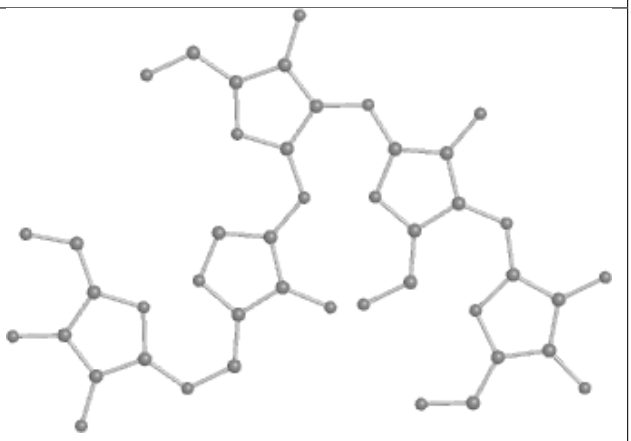
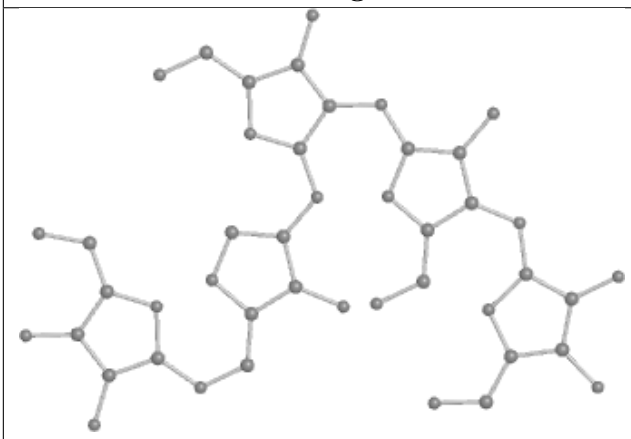
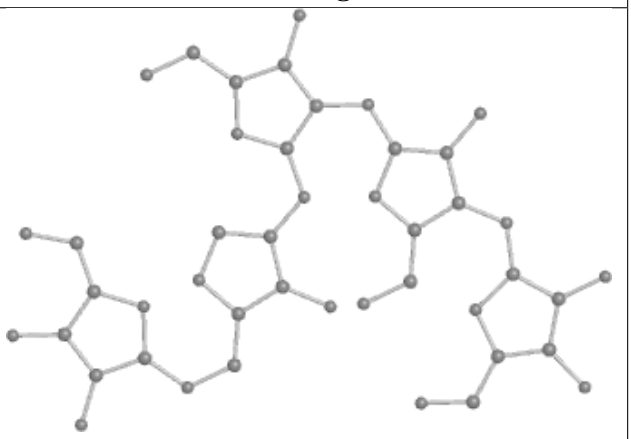
Oligosaccharide Chain gD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain kD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

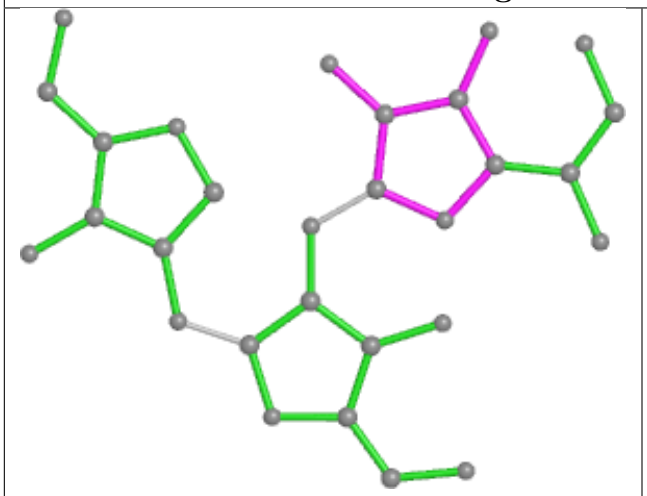
Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain KA	
 Bond lengths	 Bond angles
 Torsions	 Rings

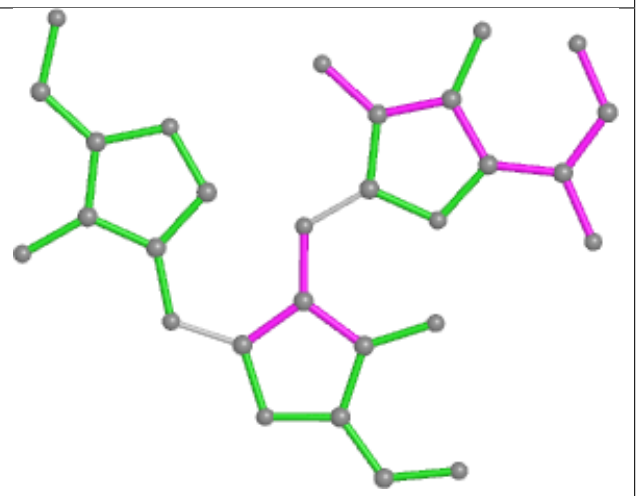
Oligosaccharide Chain EC	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain BD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

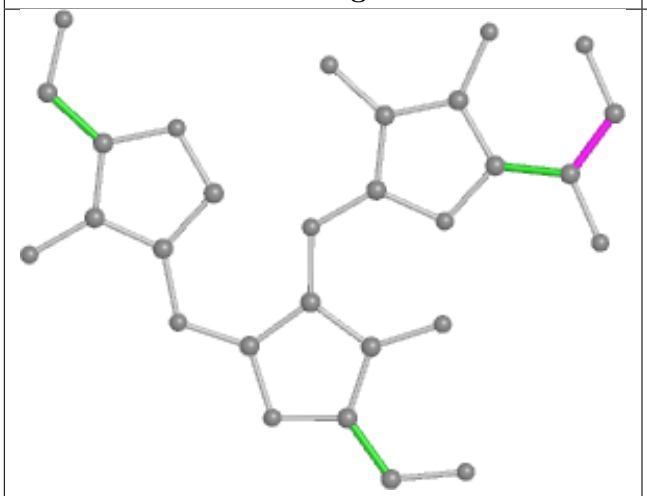
Oligosaccharide Chain N



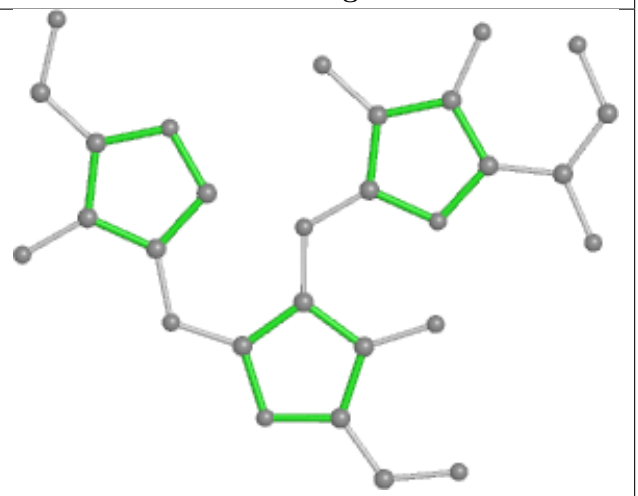
Bond lengths



Bond angles

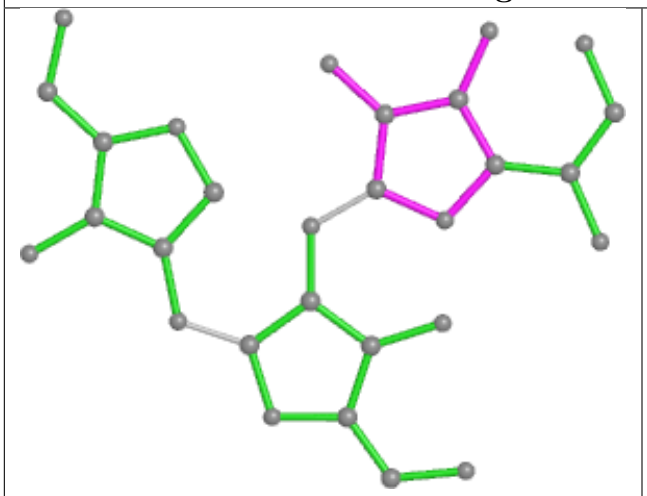


Torsions

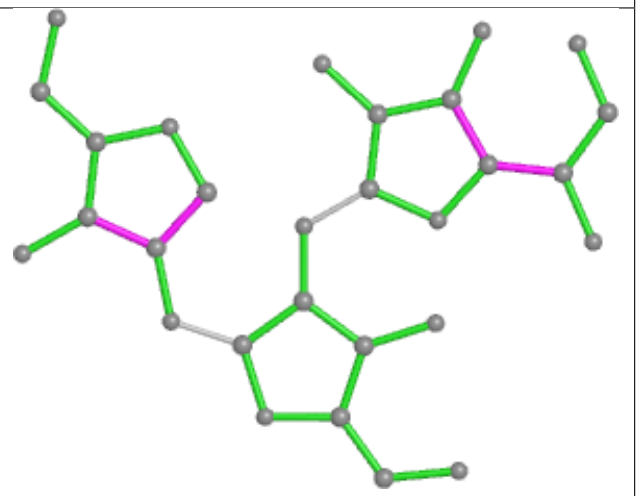


Rings

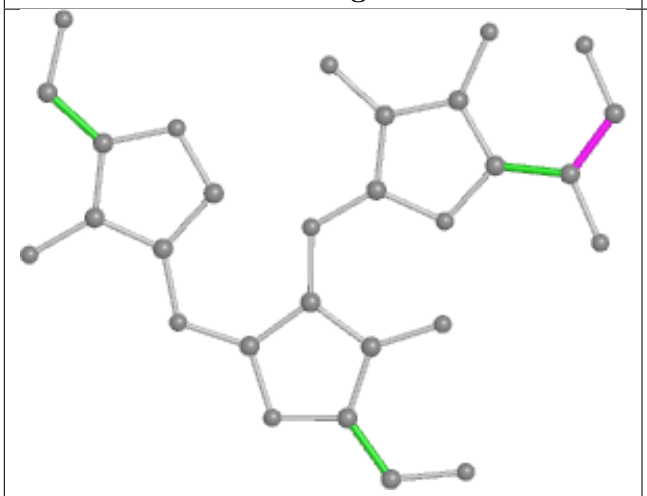
Oligosaccharide Chain R



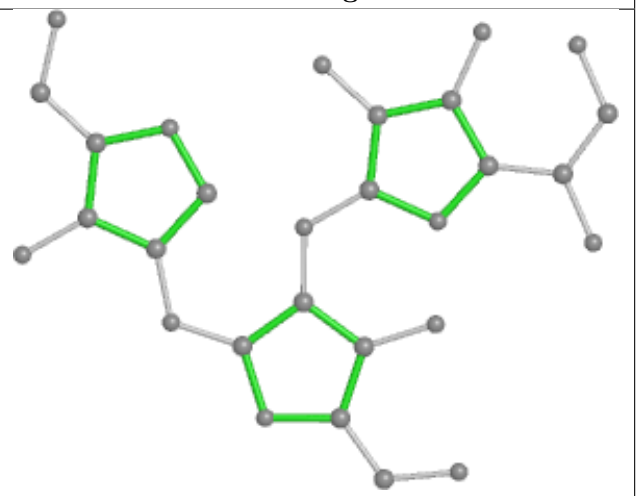
Bond lengths



Bond angles

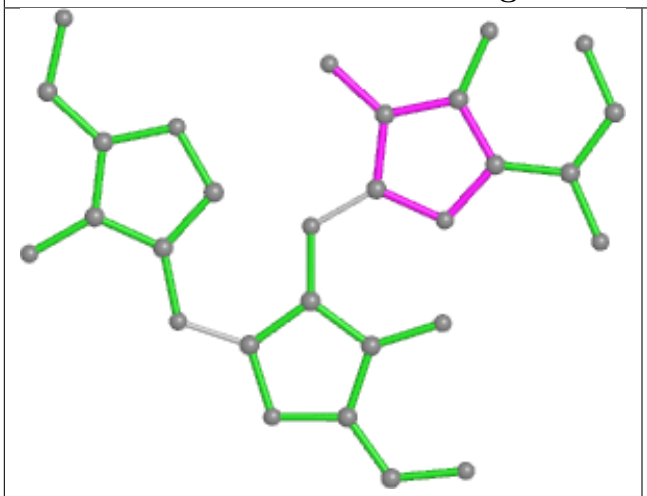


Torsions

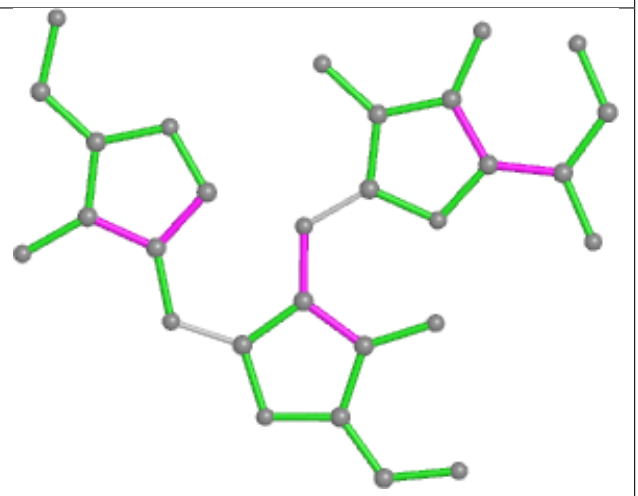


Rings

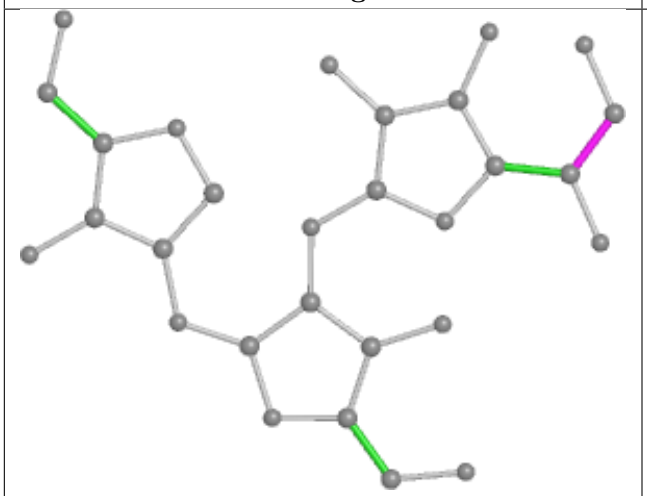
Oligosaccharide Chain 5



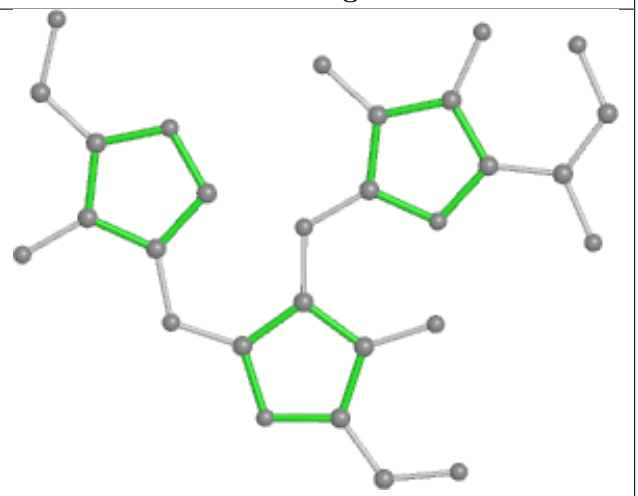
Bond lengths



Bond angles

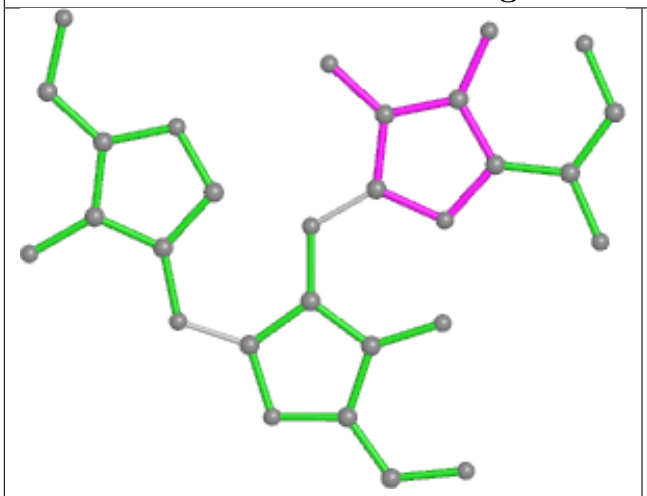


Torsions

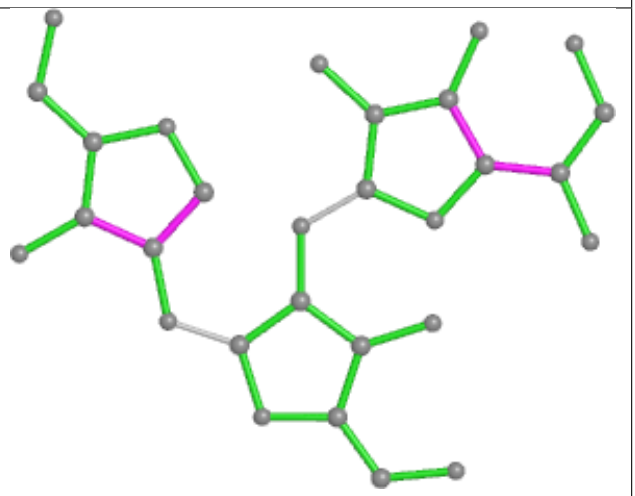


Rings

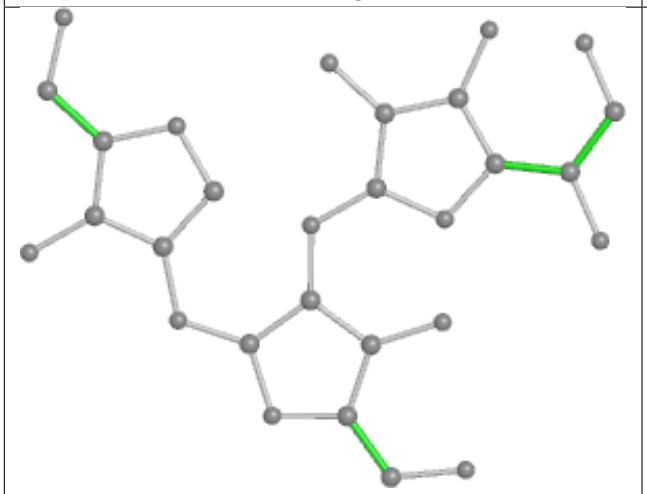
Oligosaccharide Chain 8



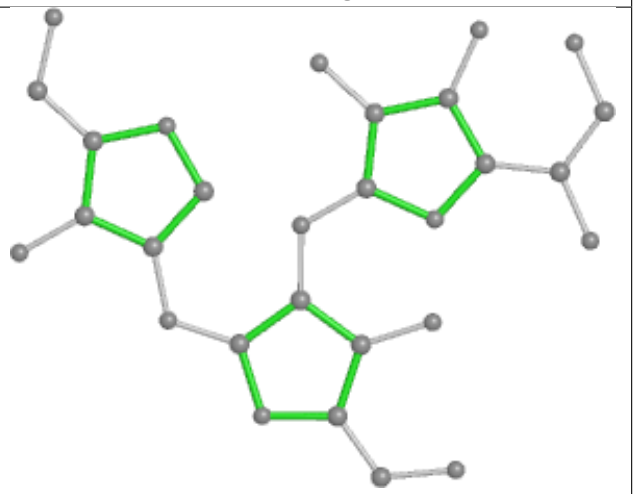
Bond lengths



Bond angles

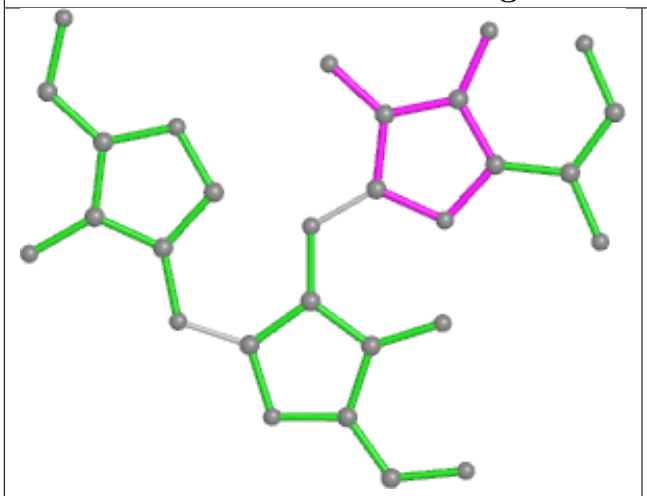


Torsions

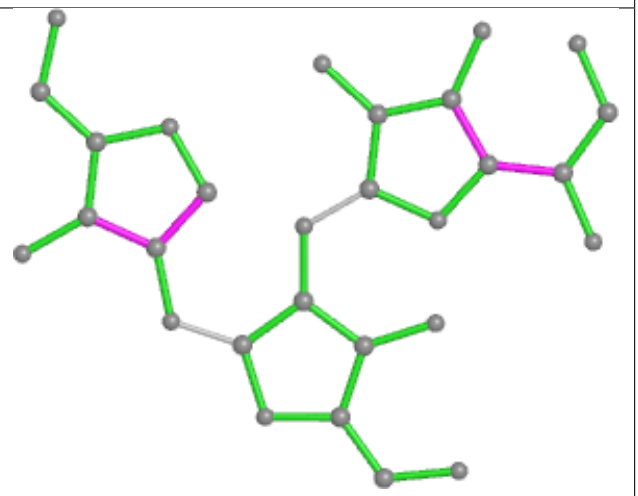


Rings

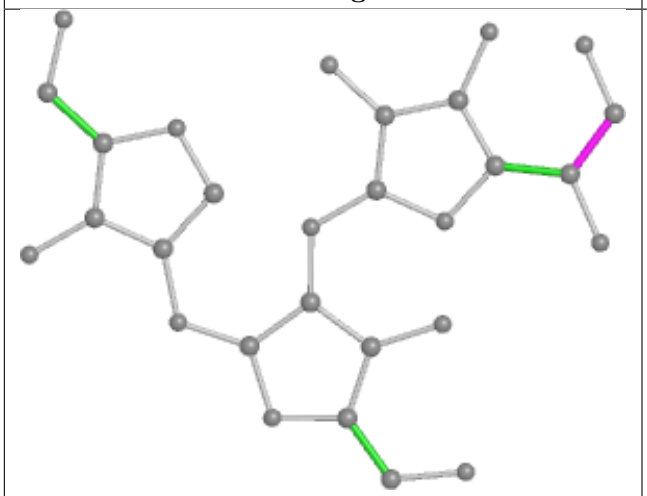
Oligosaccharide Chain 9



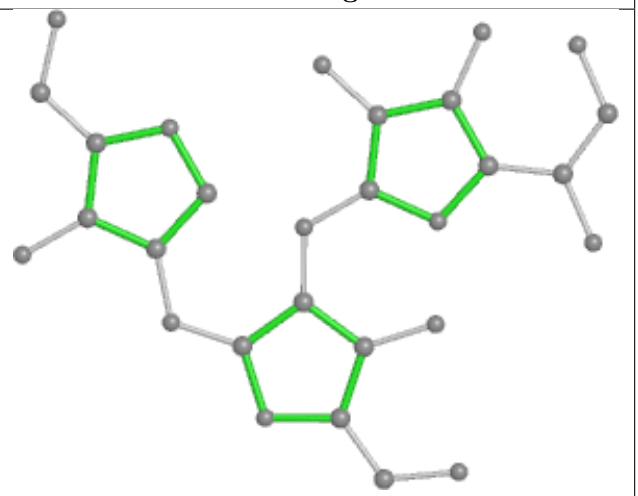
Bond lengths



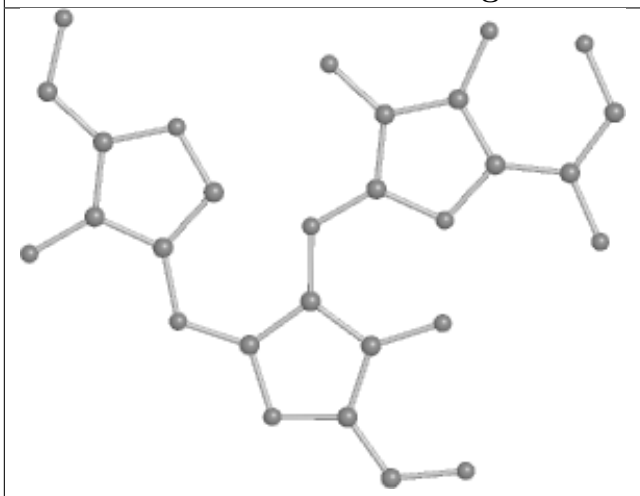
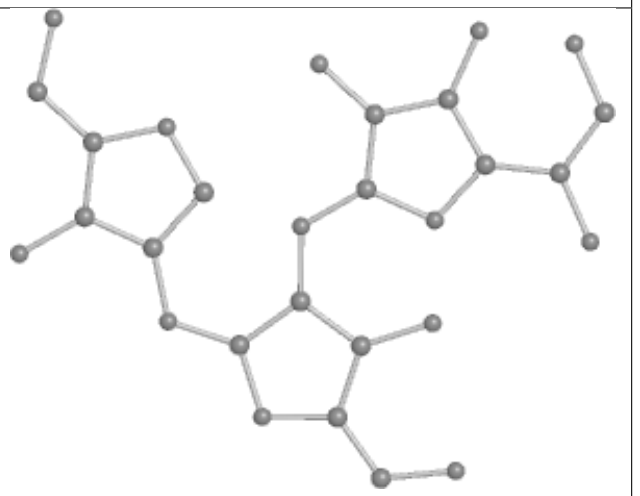
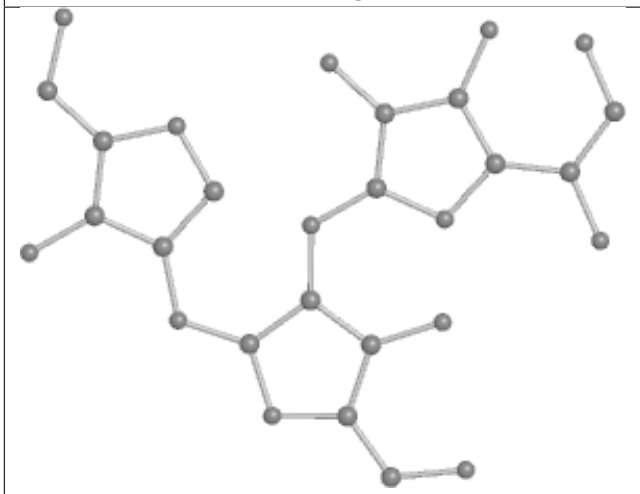
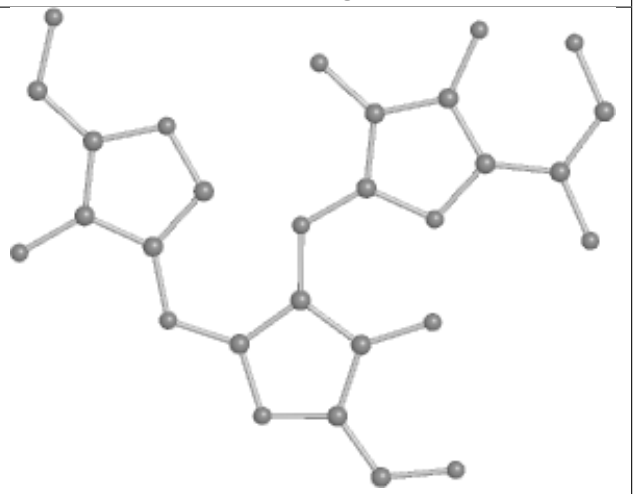
Bond angles

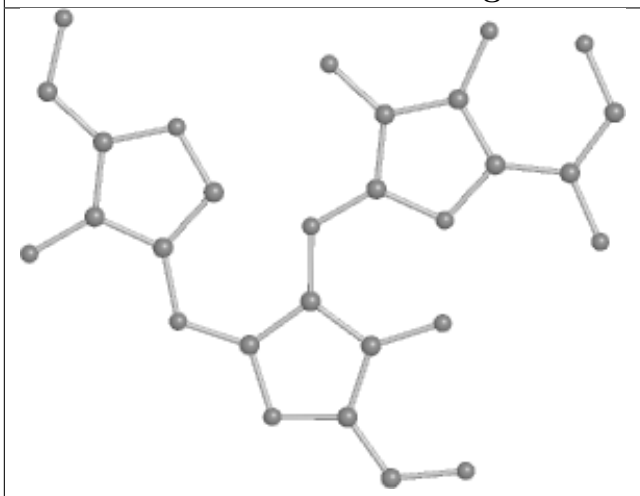
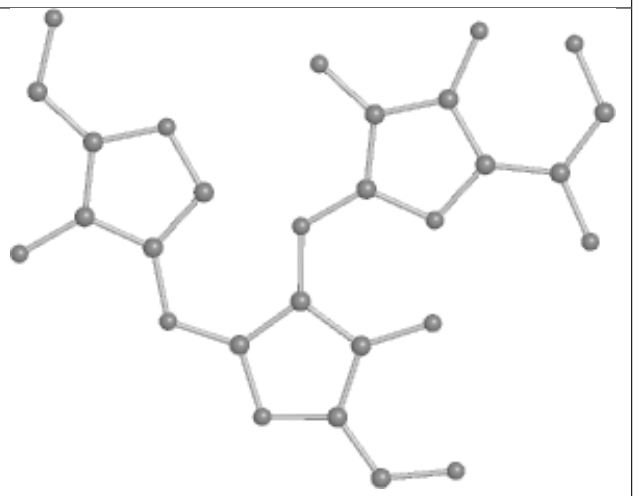
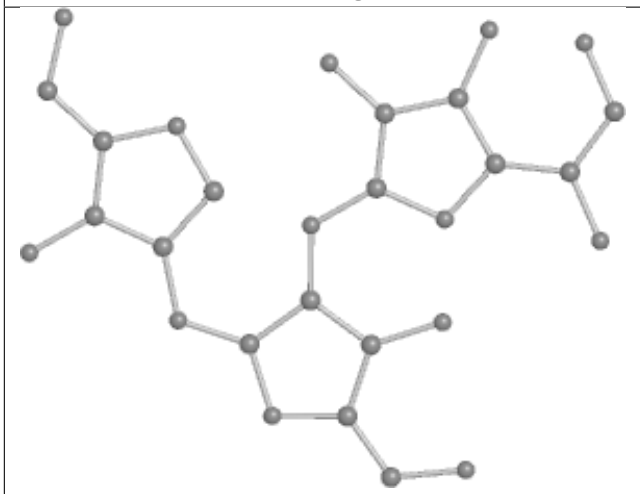
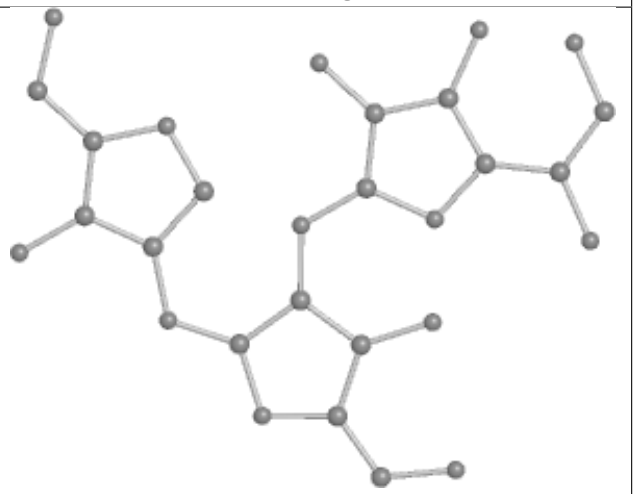


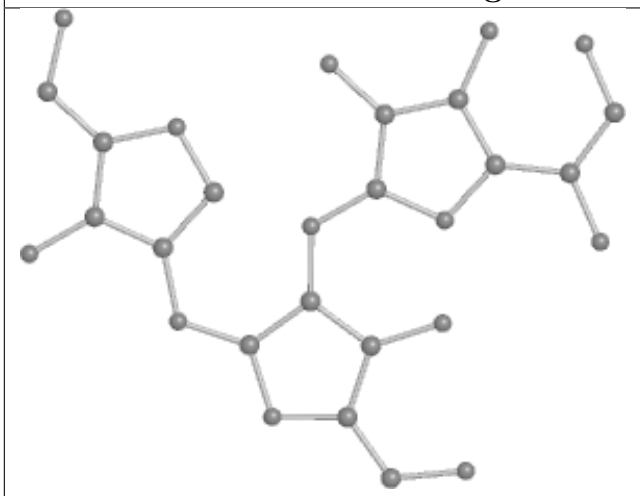
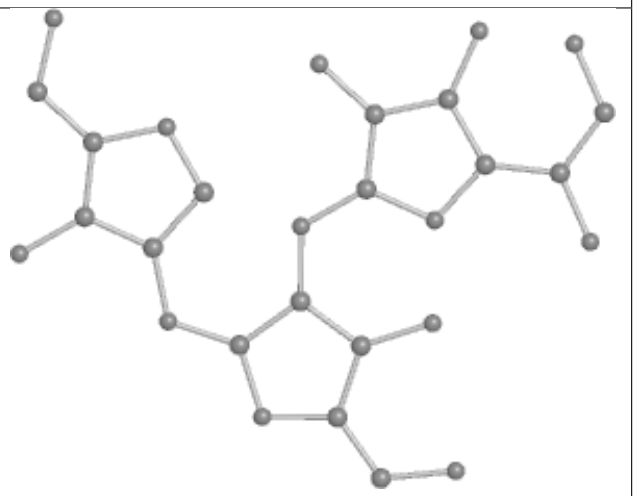
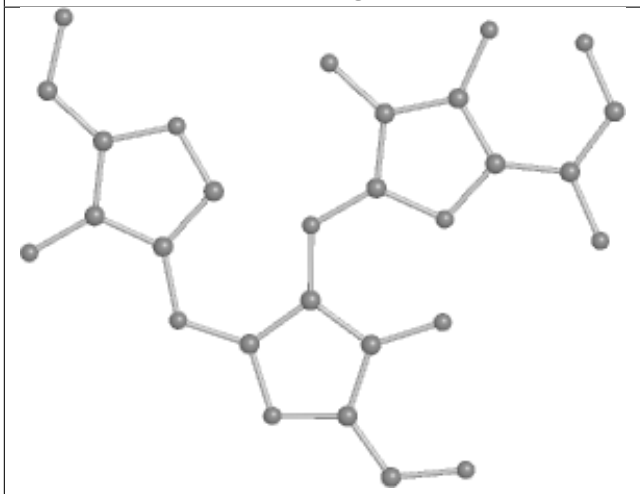
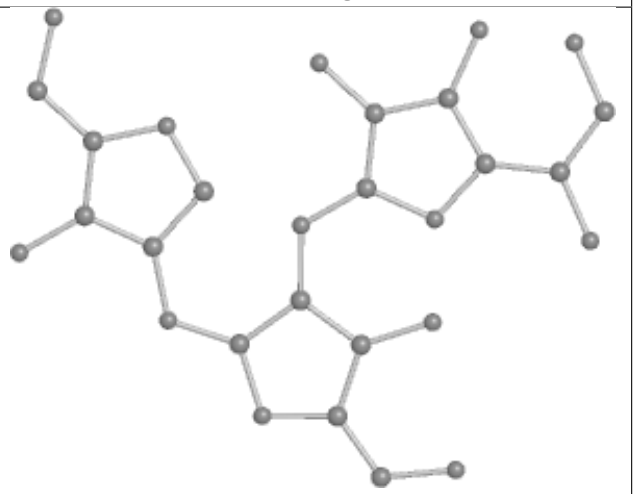
Torsions

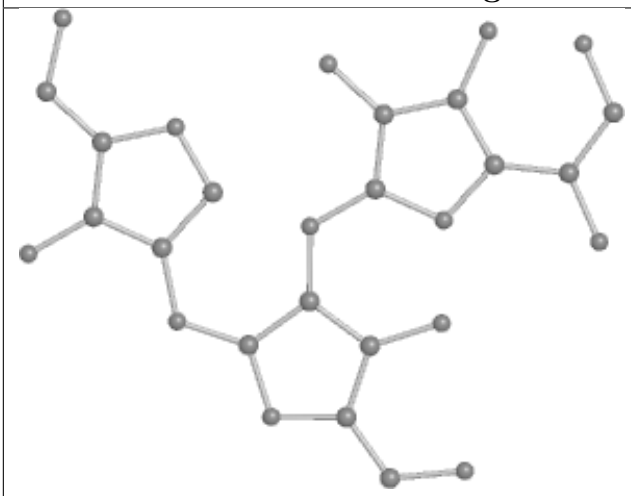
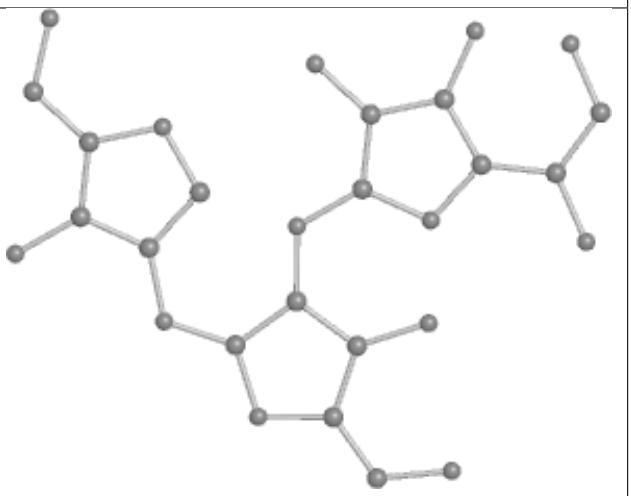
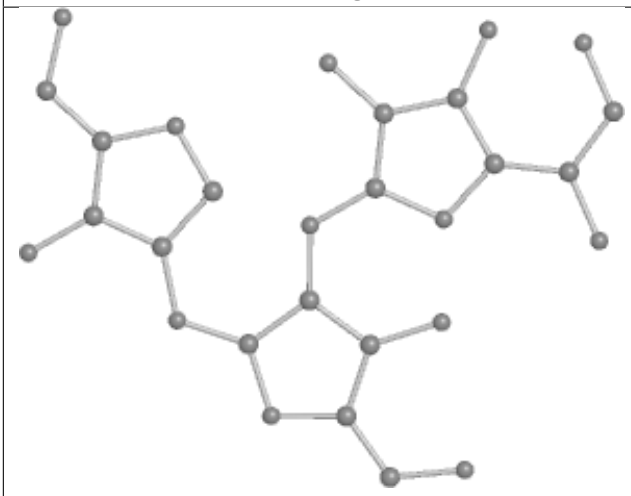
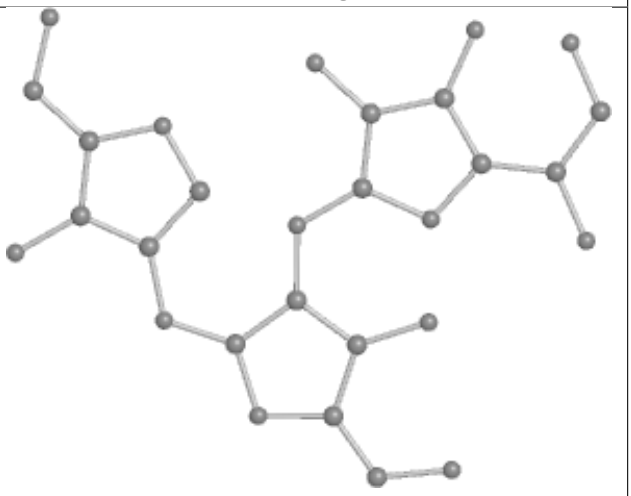


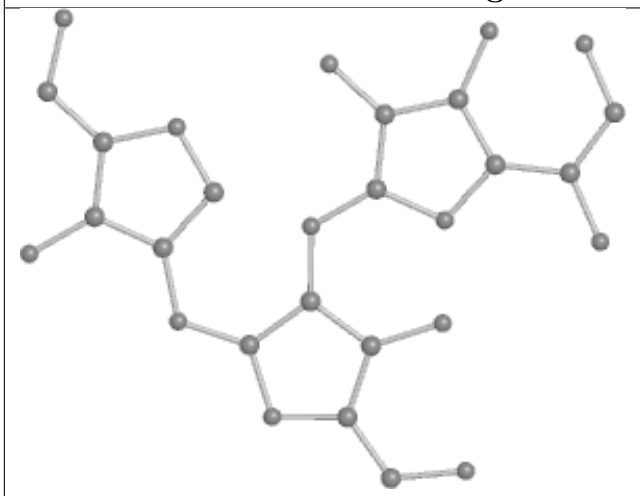
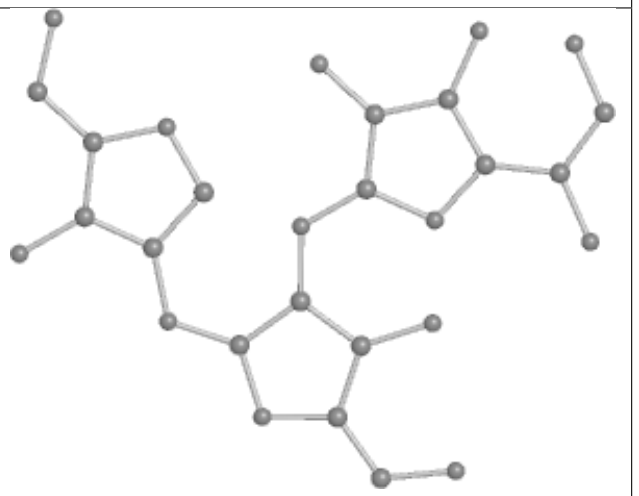
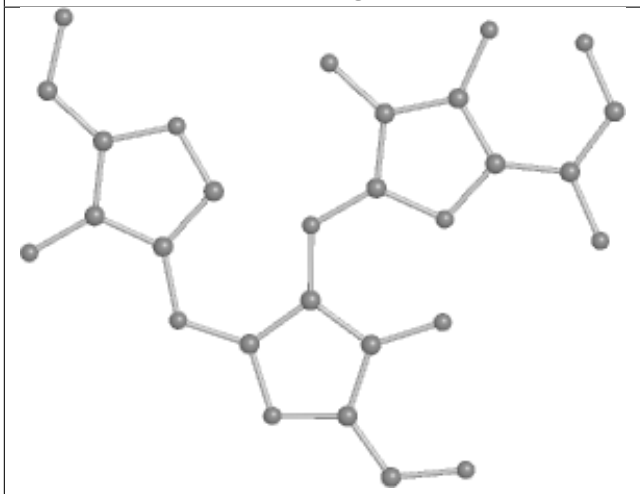
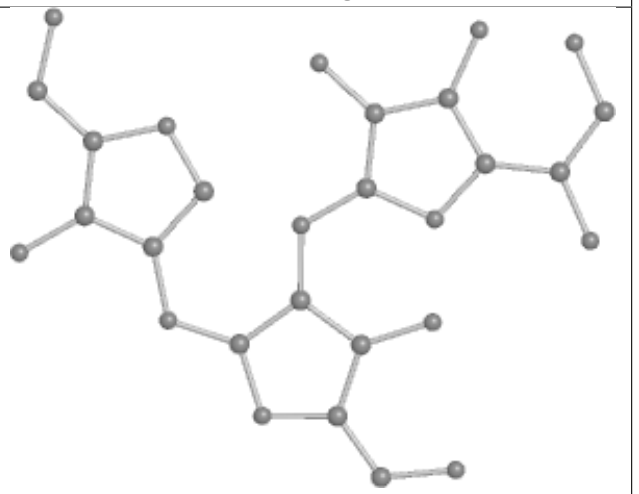
Rings

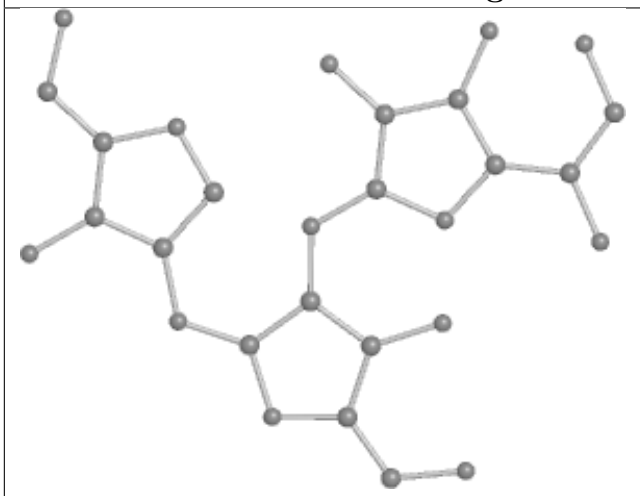
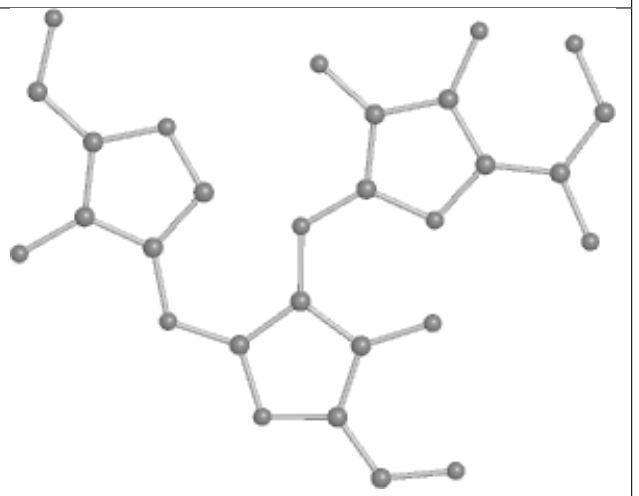
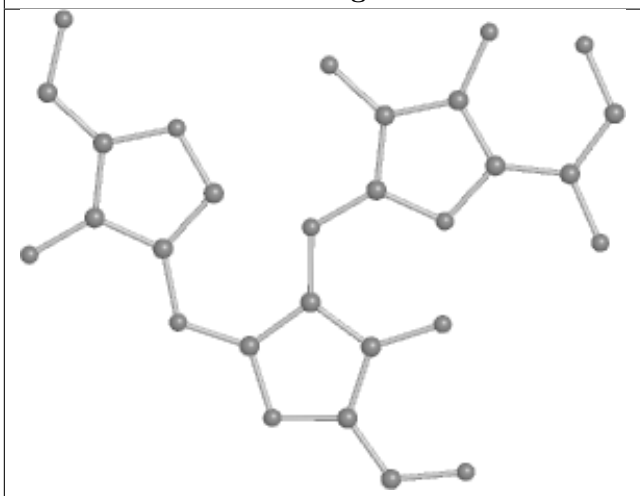
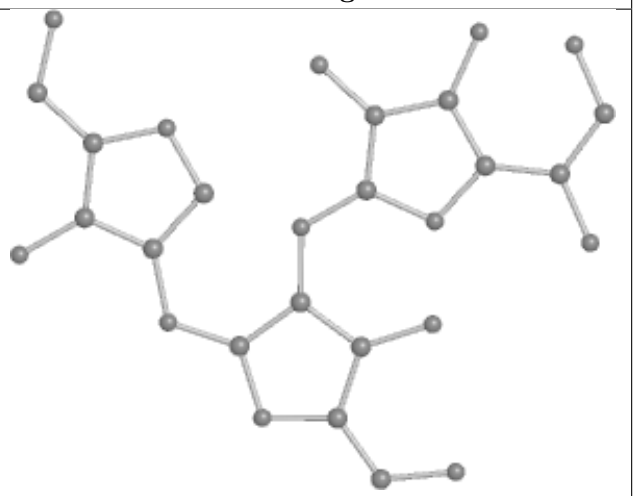
Oligosaccharide Chain AA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

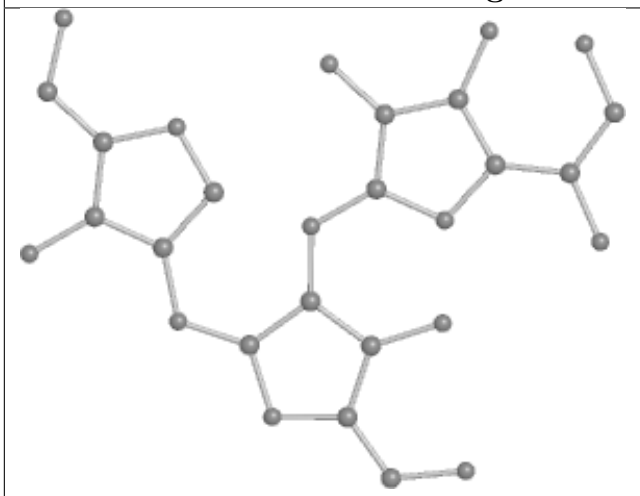
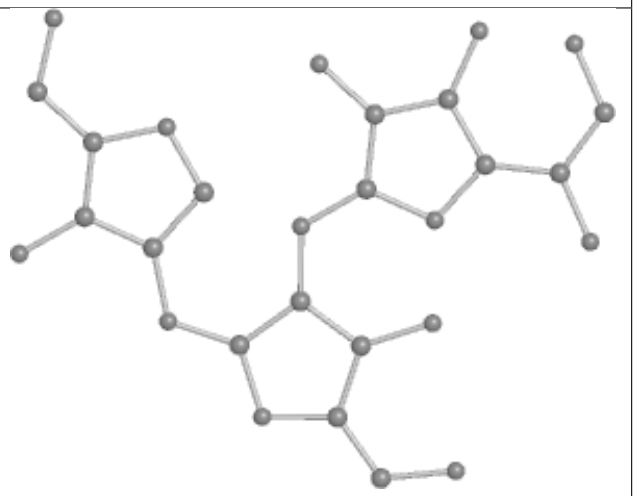
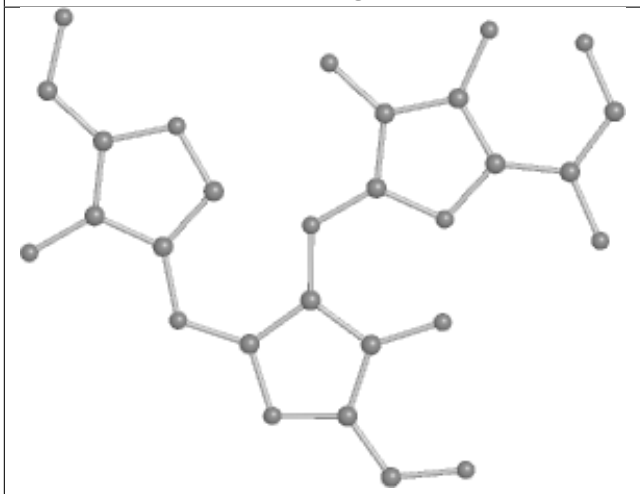
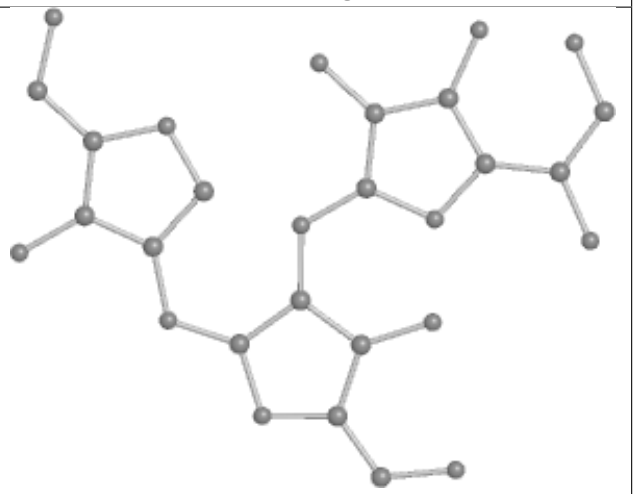
Oligosaccharide Chain EA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain LA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

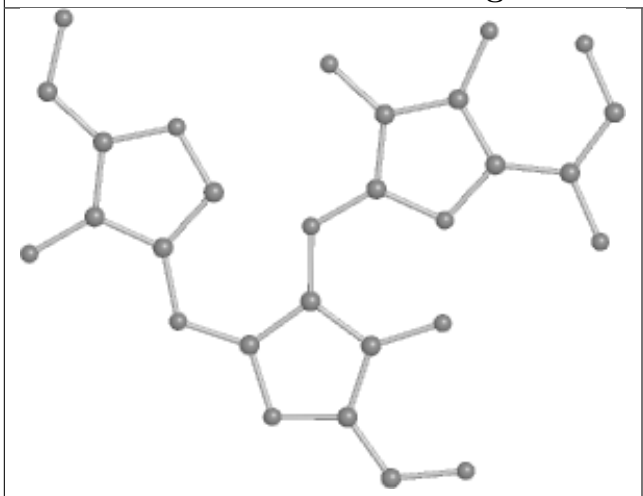
Oligosaccharide Chain PA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 3A	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

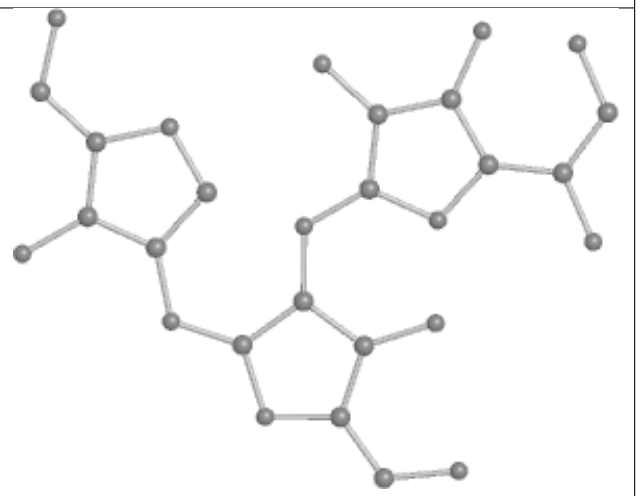
Oligosaccharide Chain 6A	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain 7A	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

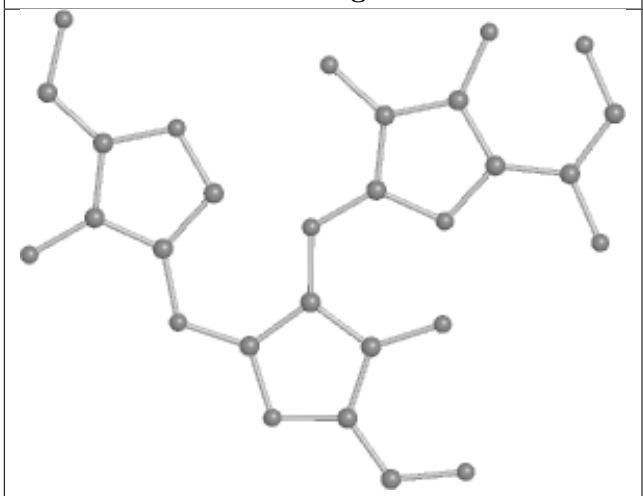
Oligosaccharide Chain 8A



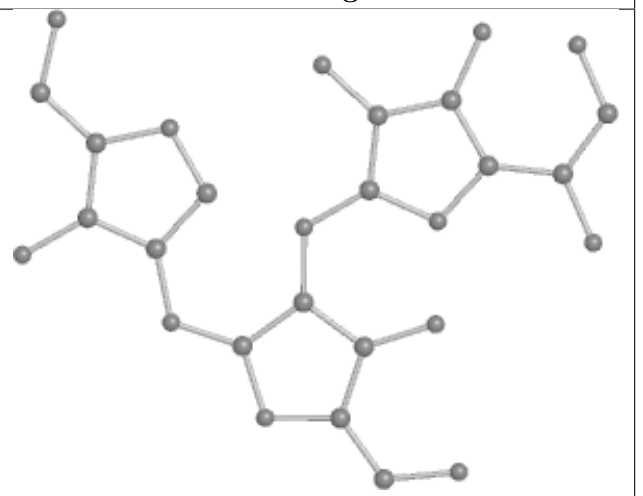
Bond lengths



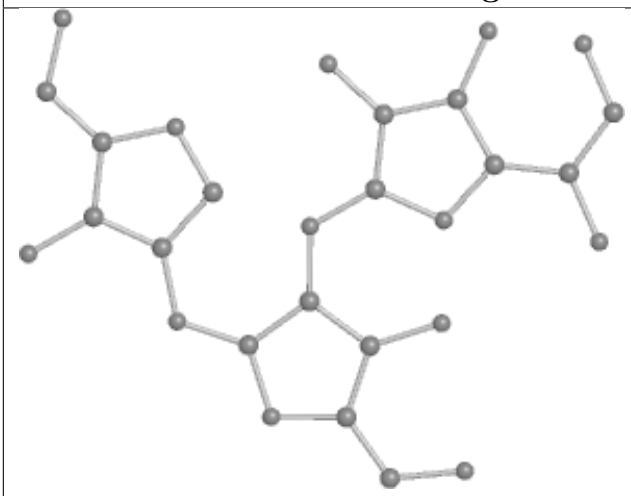
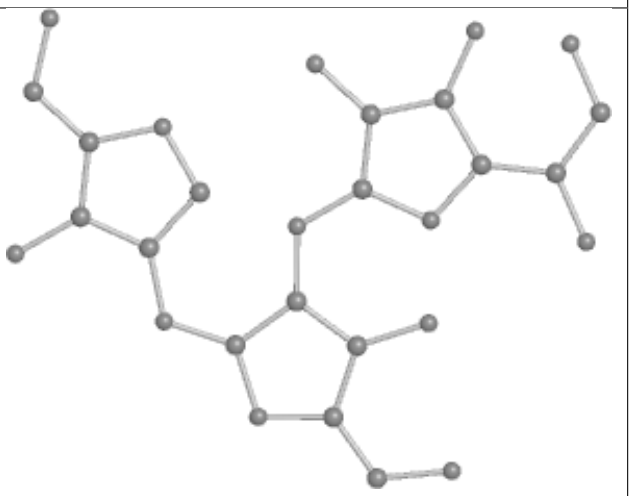
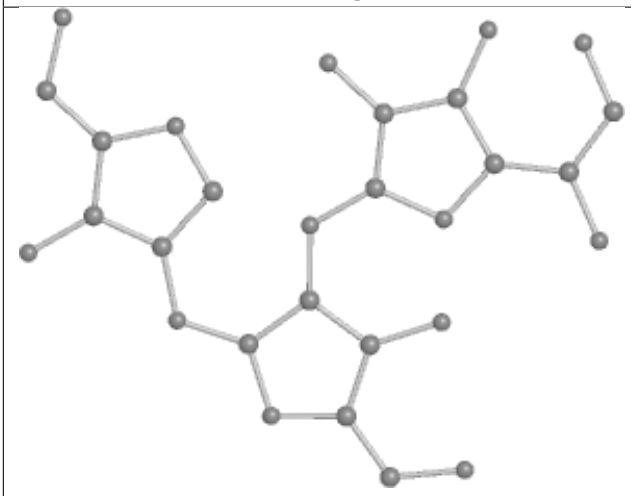
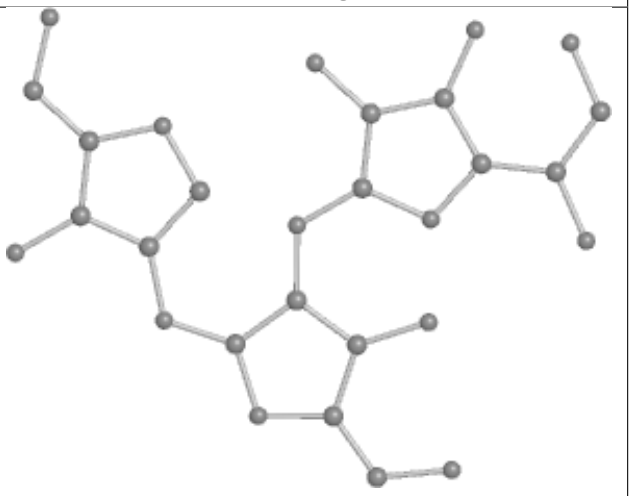
Bond angles

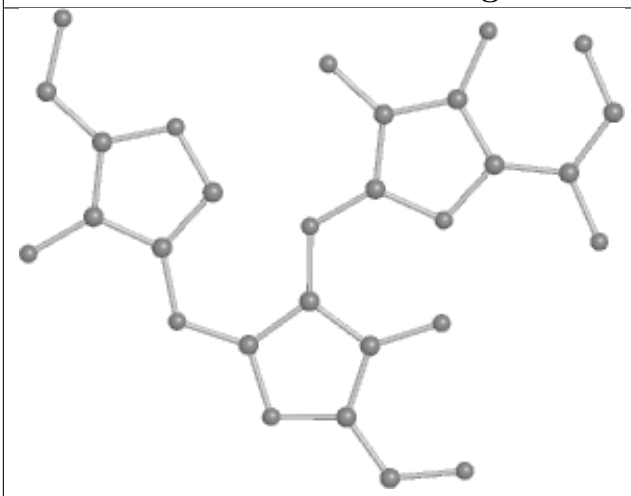
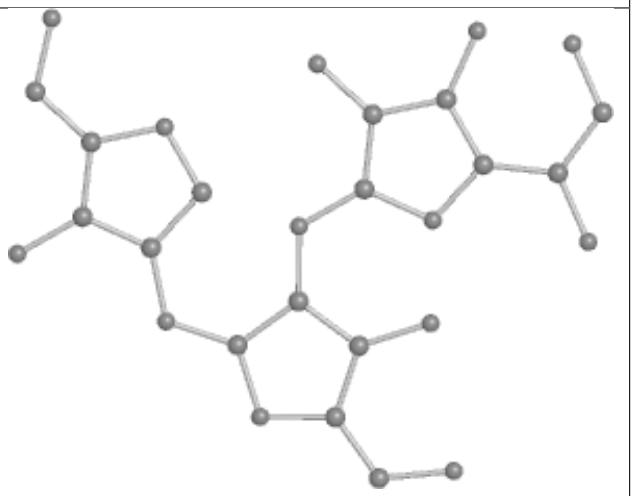
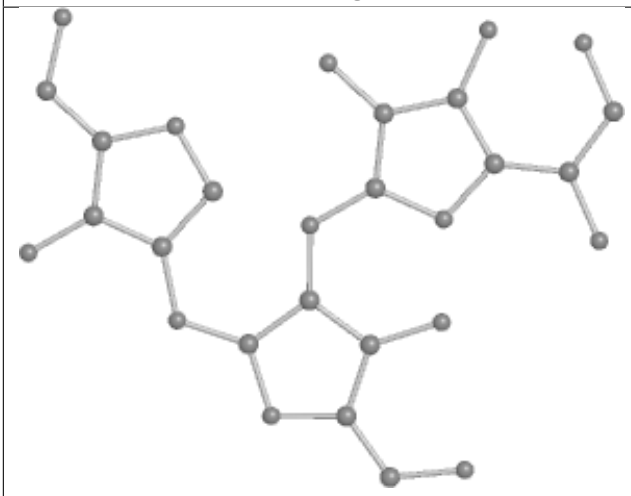
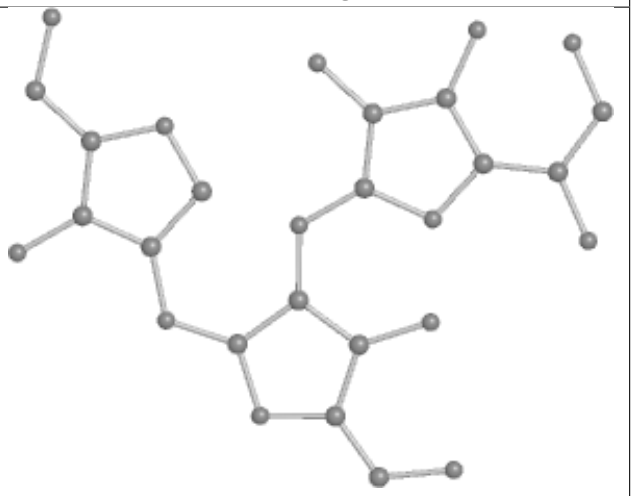


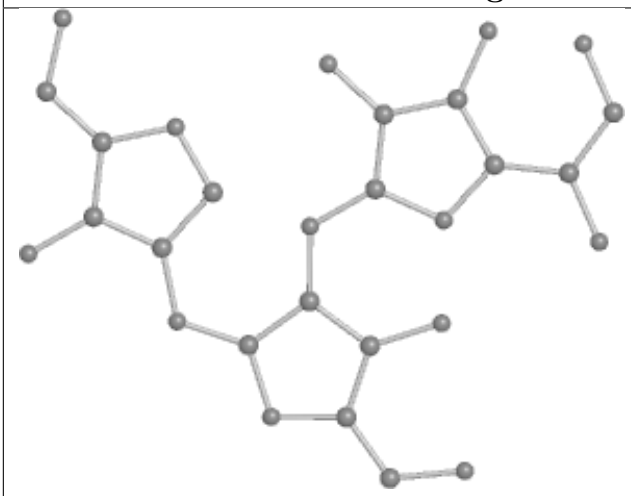
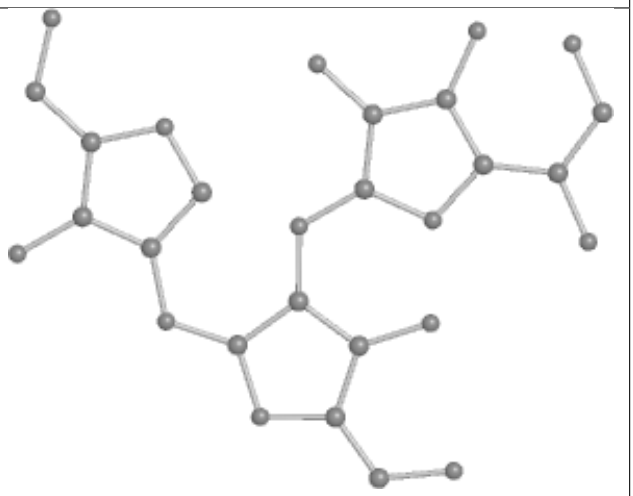
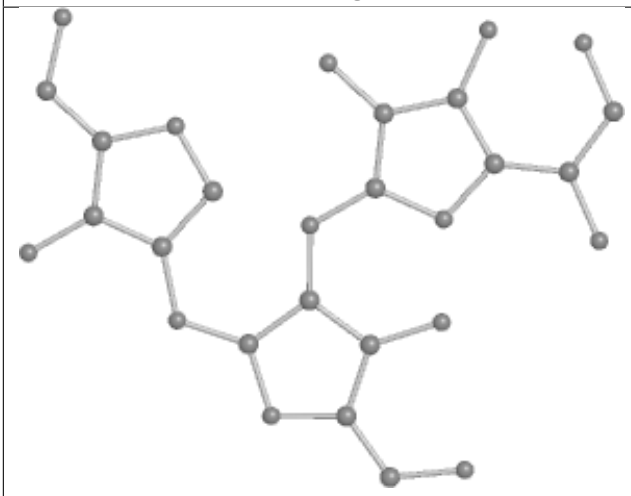
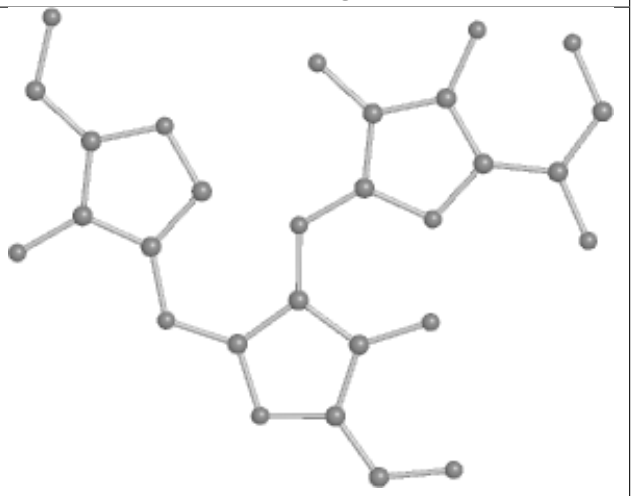
Torsions

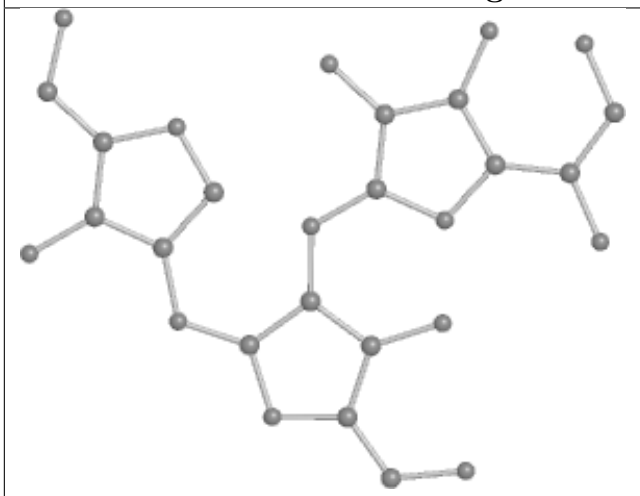
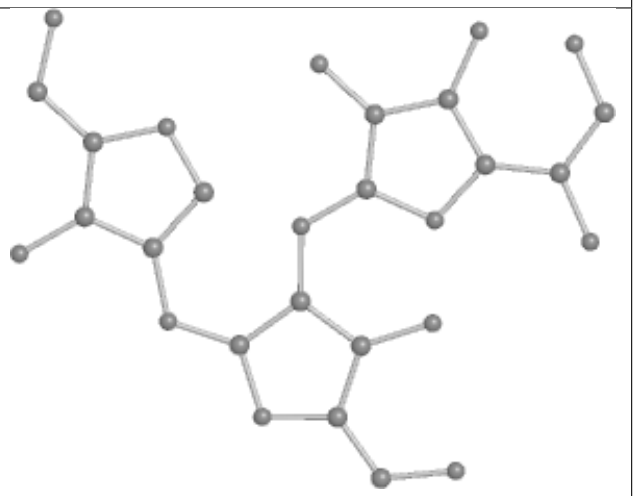
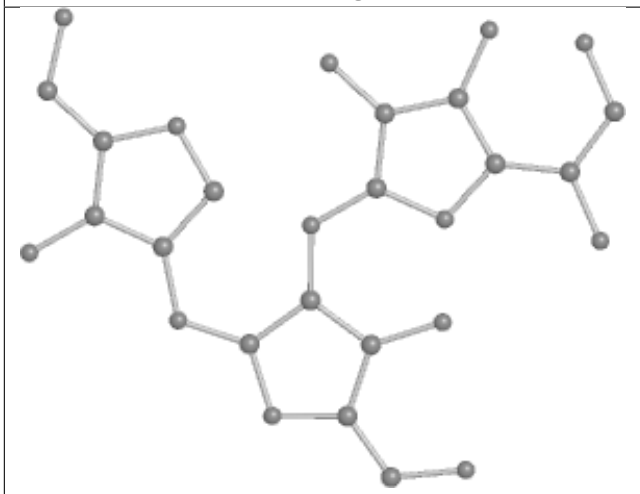
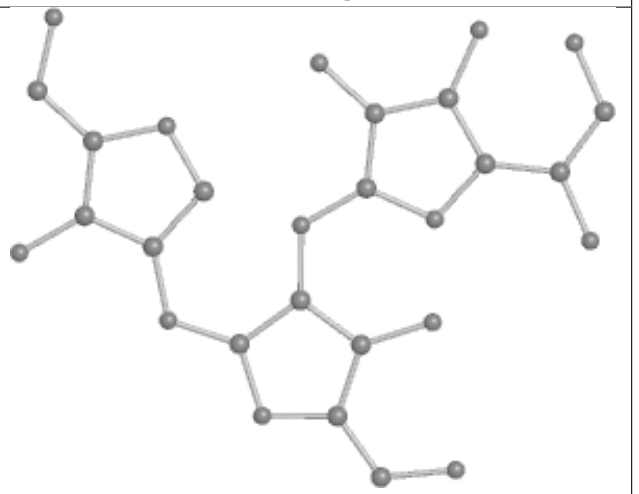


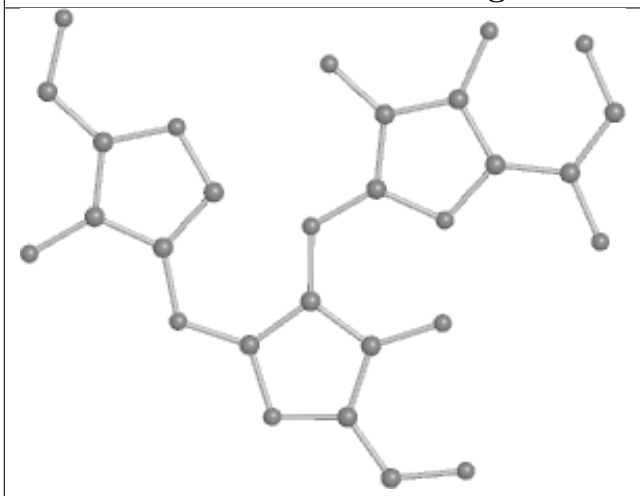
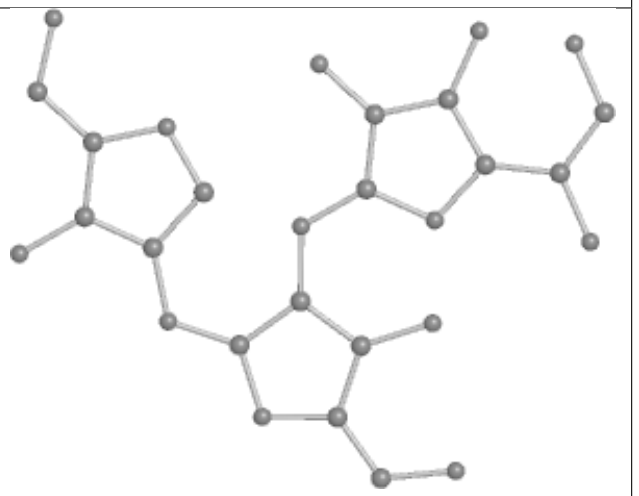
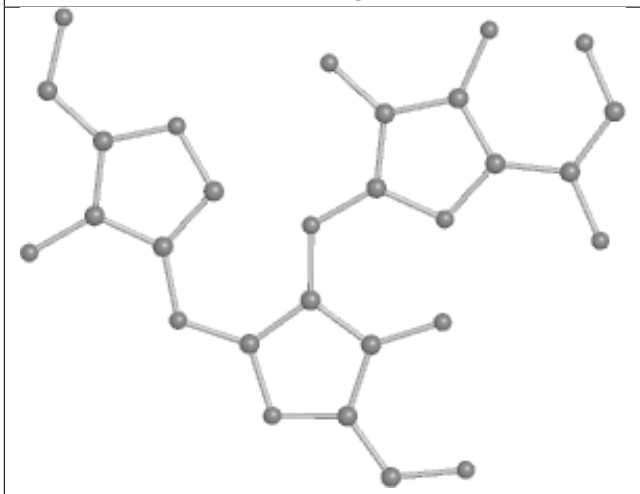
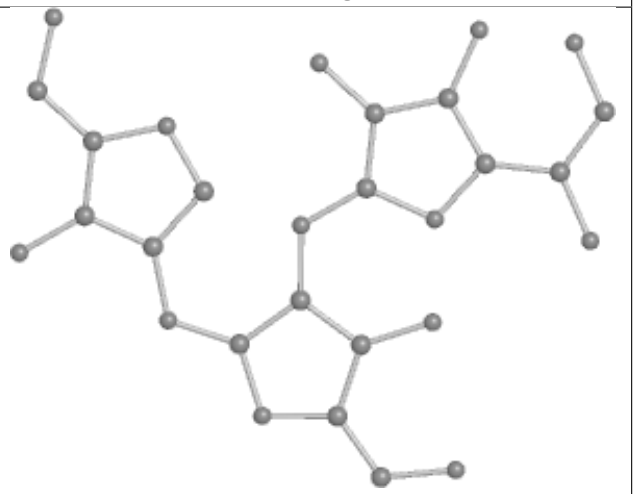
Rings

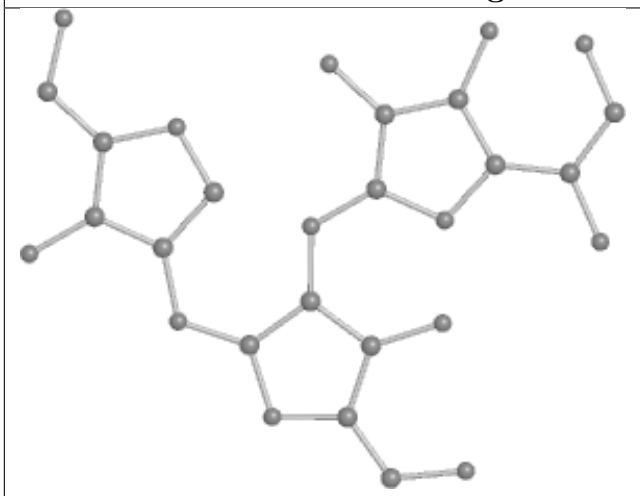
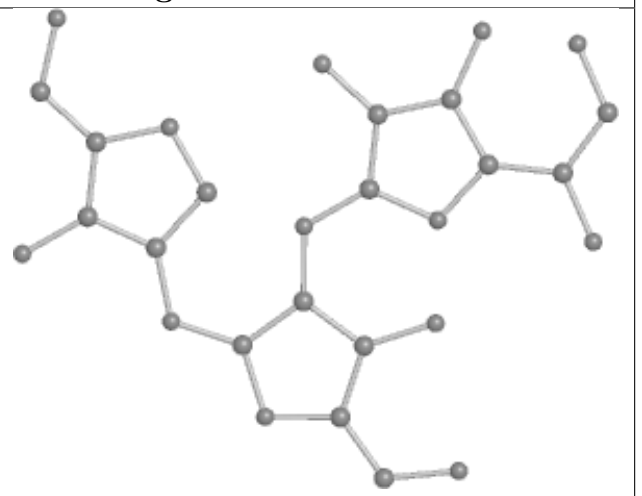
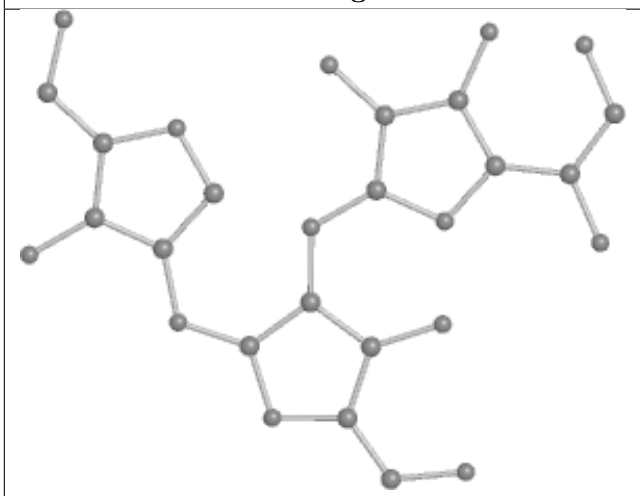
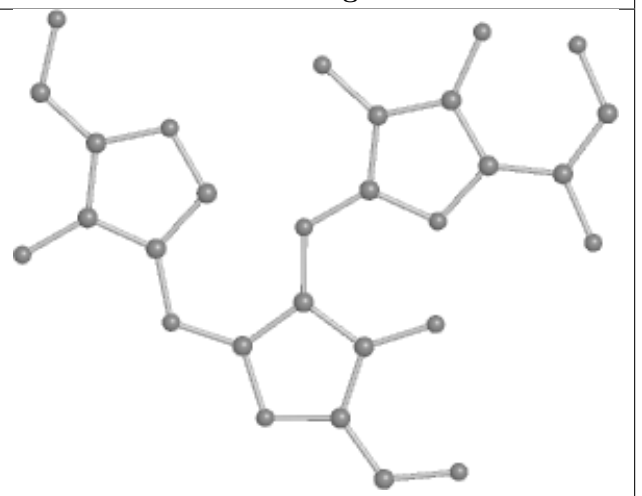
Oligosaccharide Chain CB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain XB	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

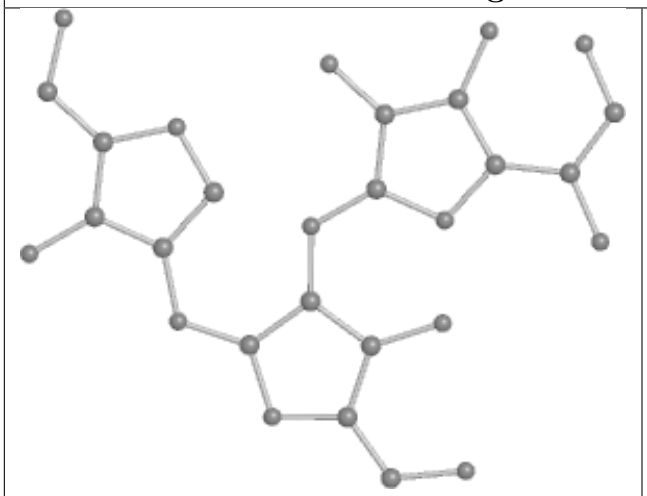
Oligosaccharide Chain aB	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain bB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

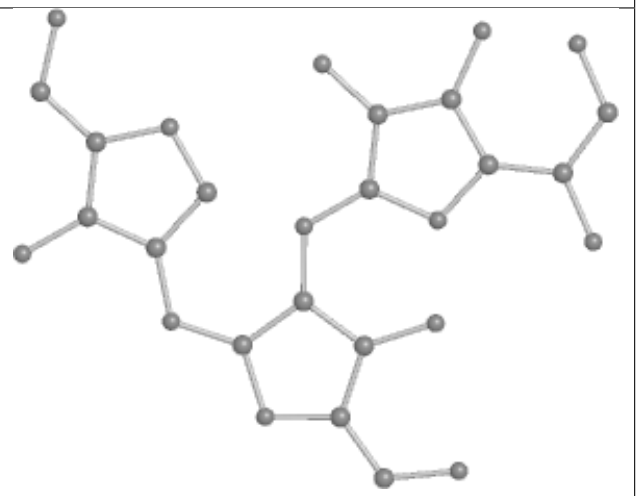
Oligosaccharide Chain cB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain gB	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

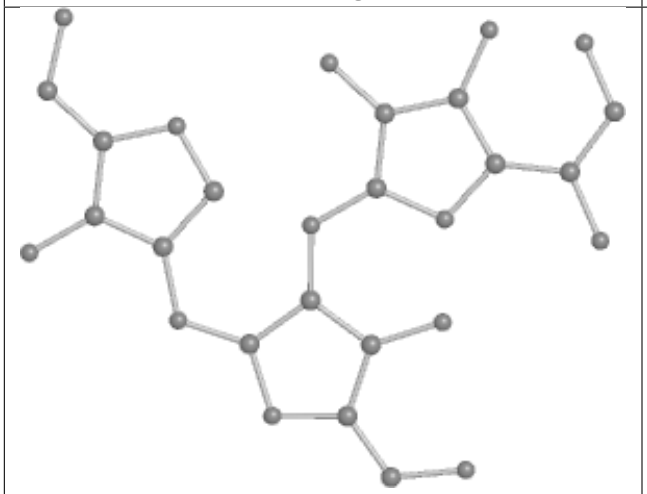
Oligosaccharide Chain 0B



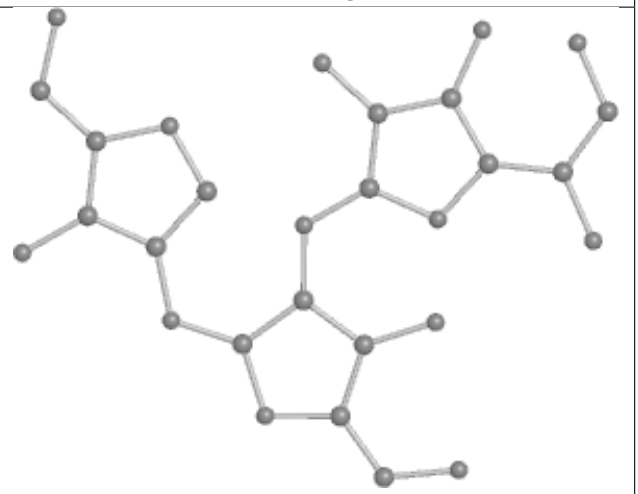
Bond lengths



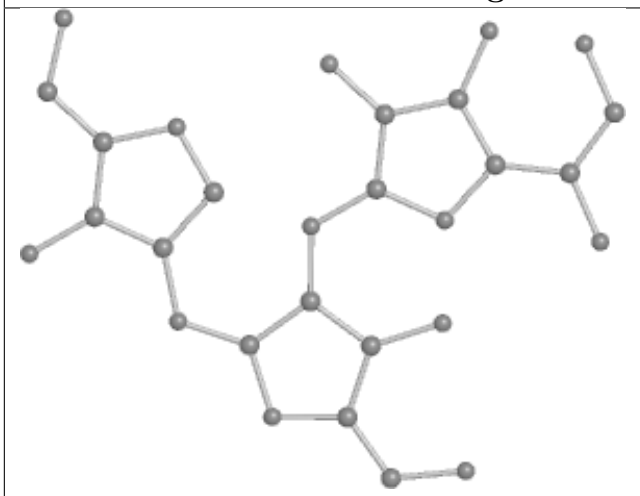
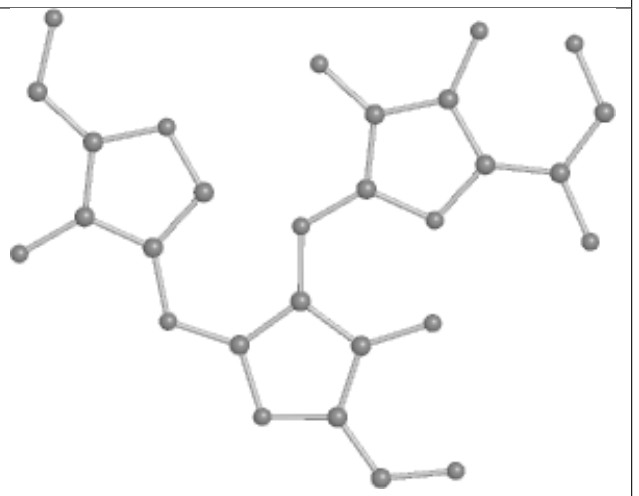
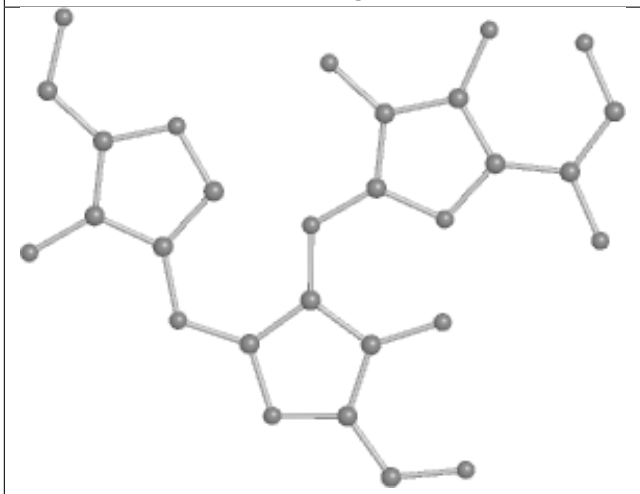
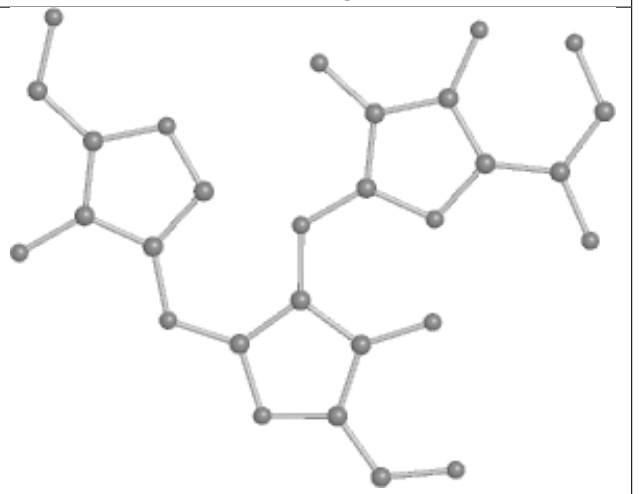
Bond angles

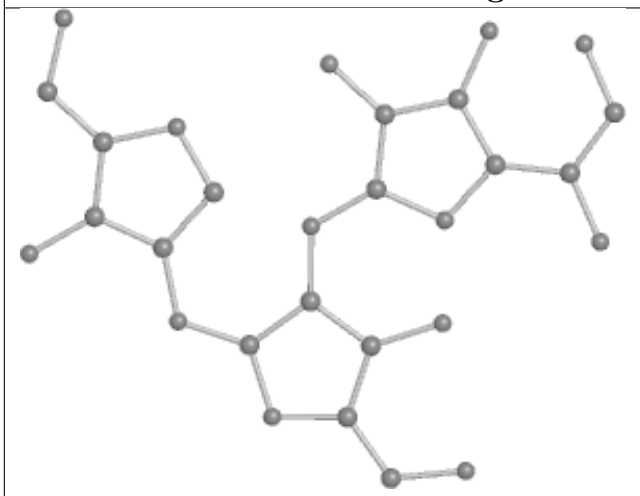
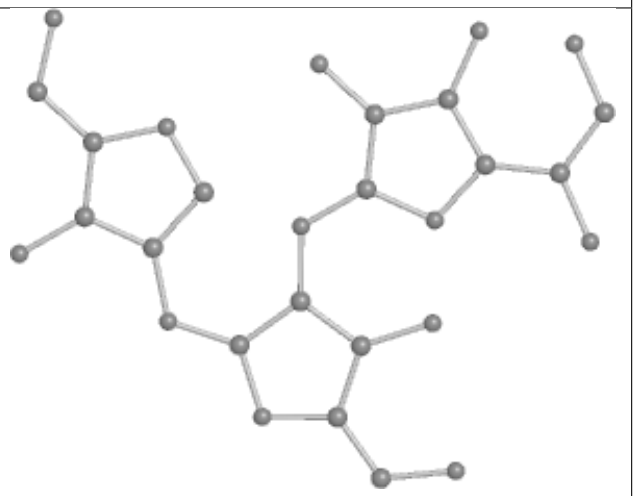
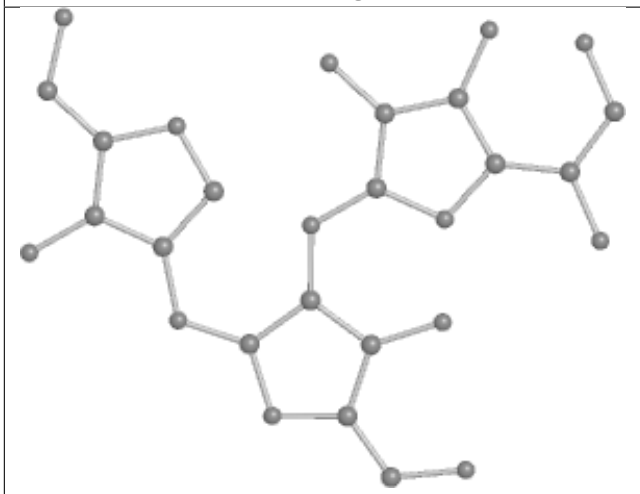
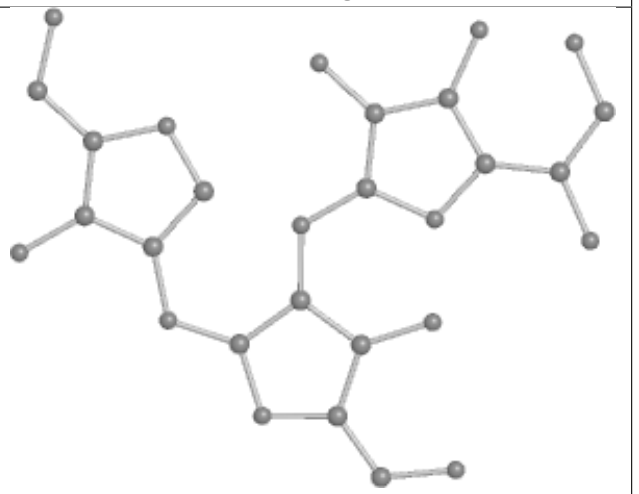


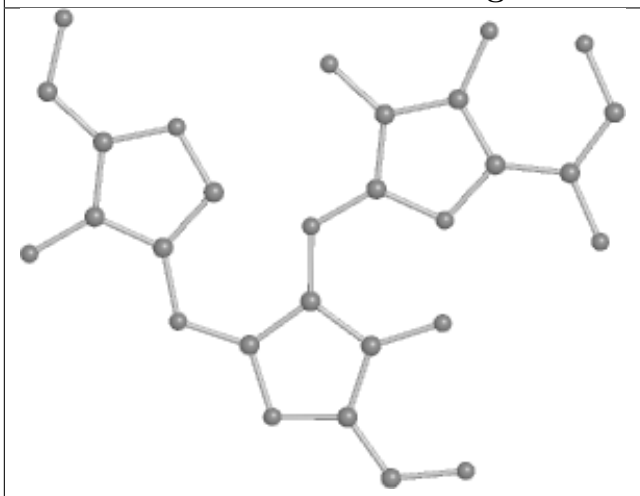
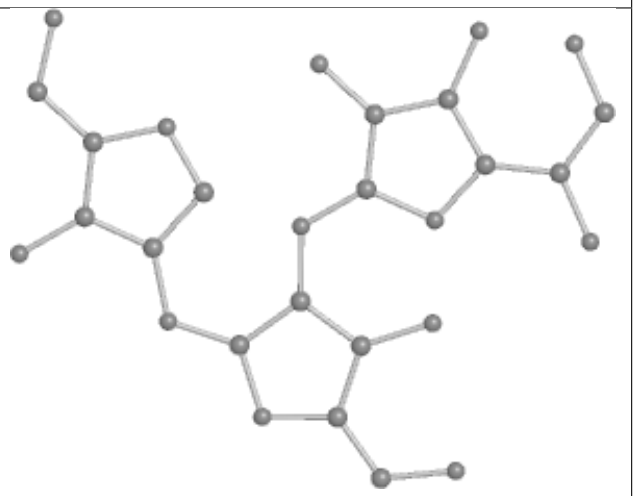
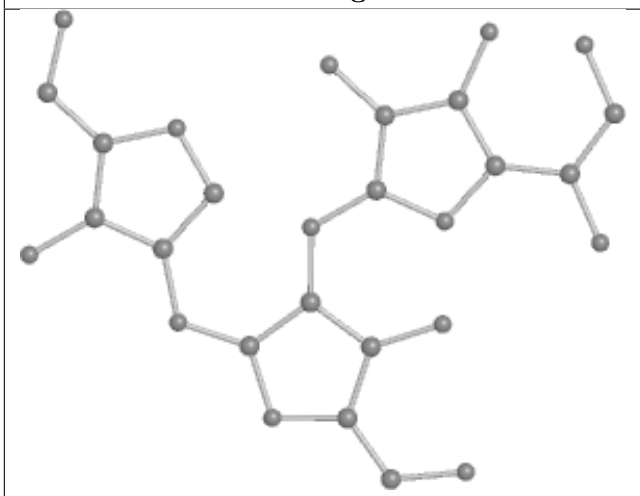
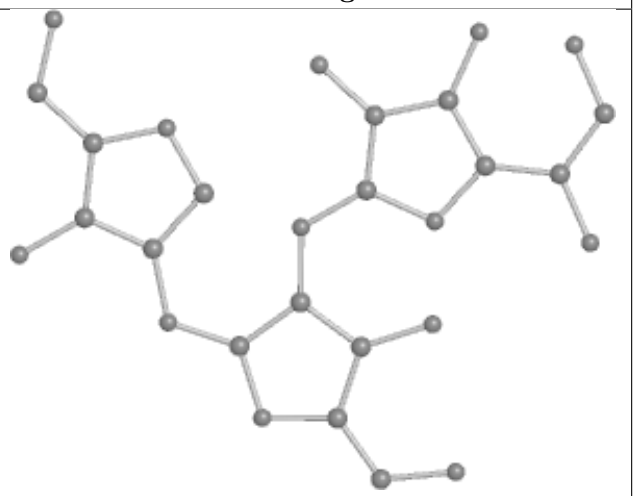
Torsions

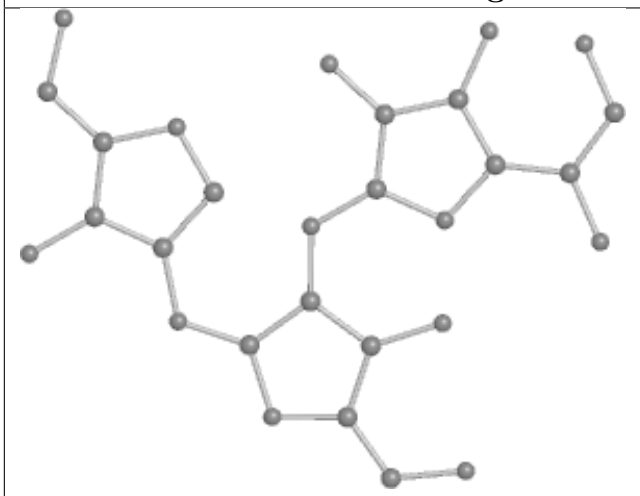
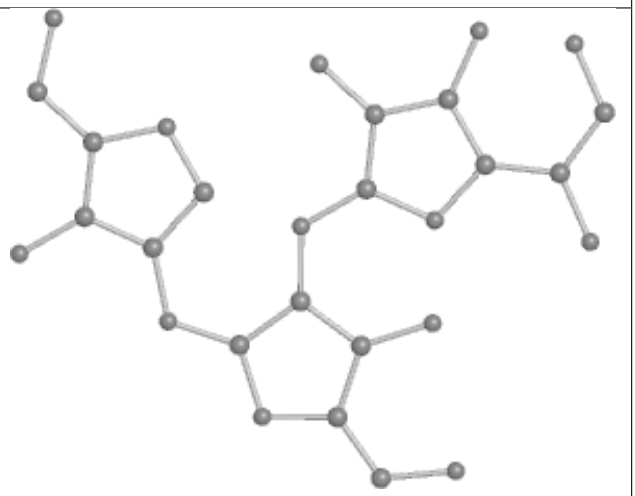
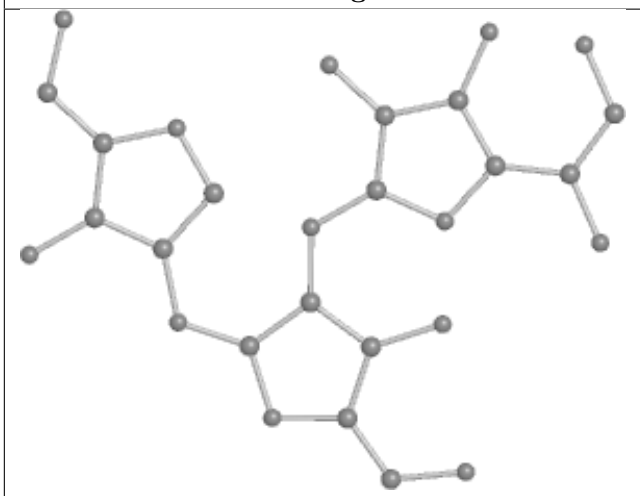
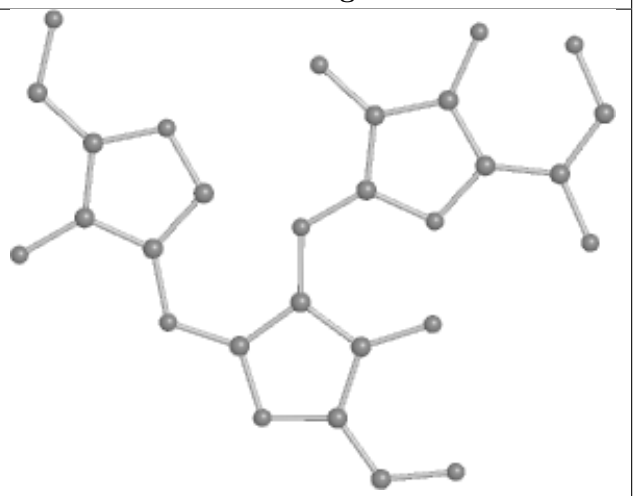


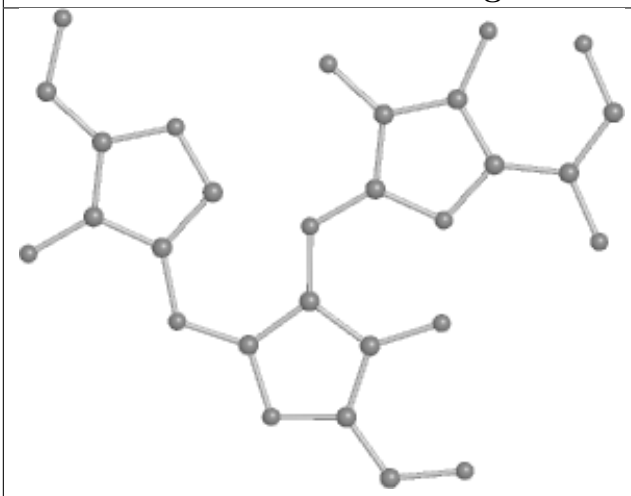
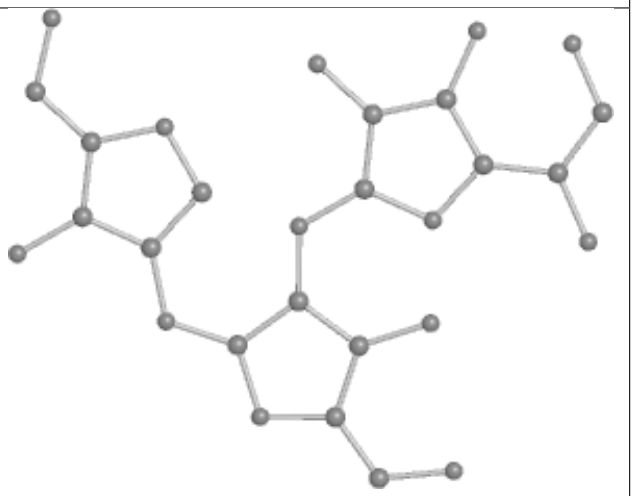
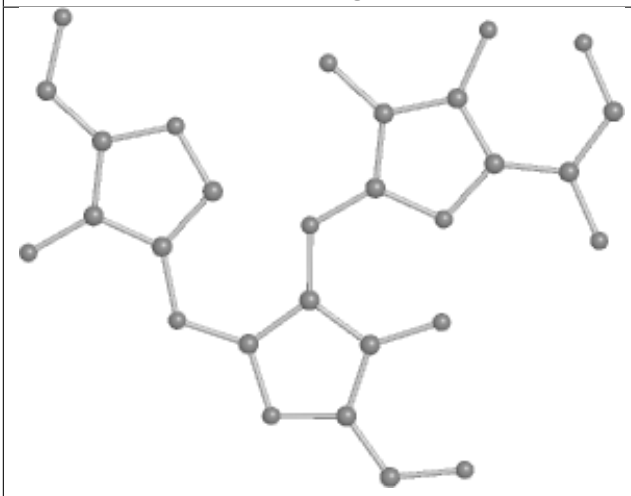
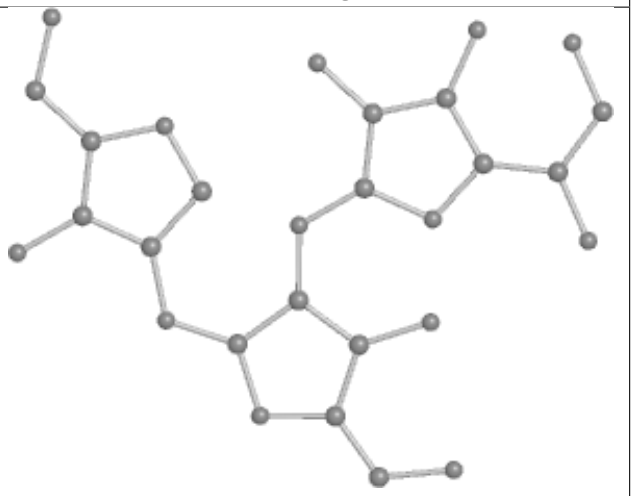
Rings

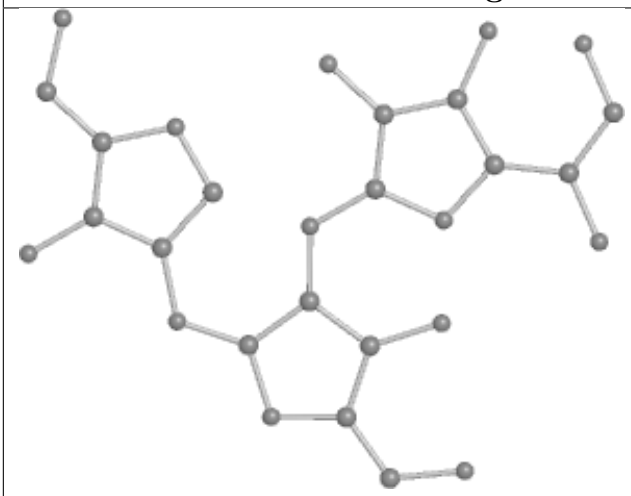
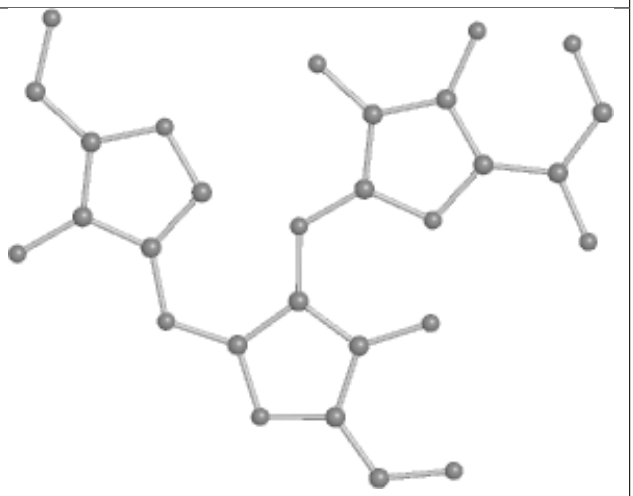
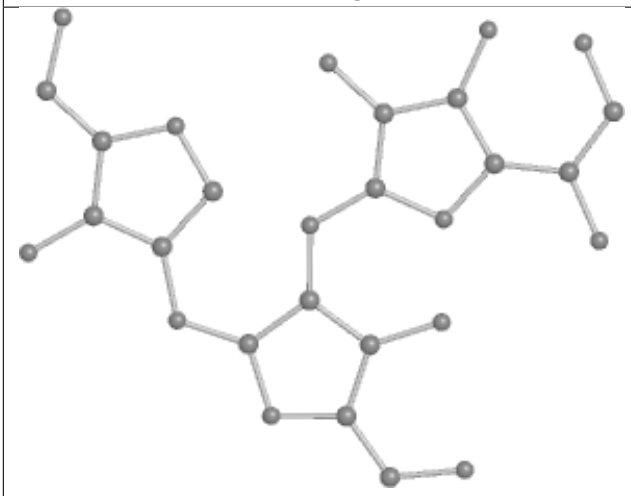
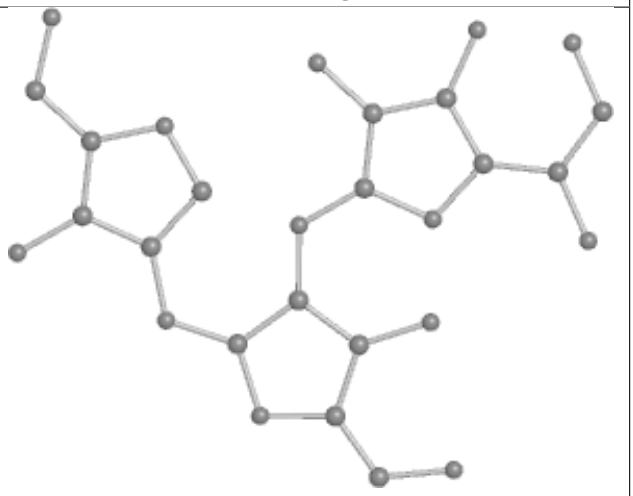
Oligosaccharide Chain 3B	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

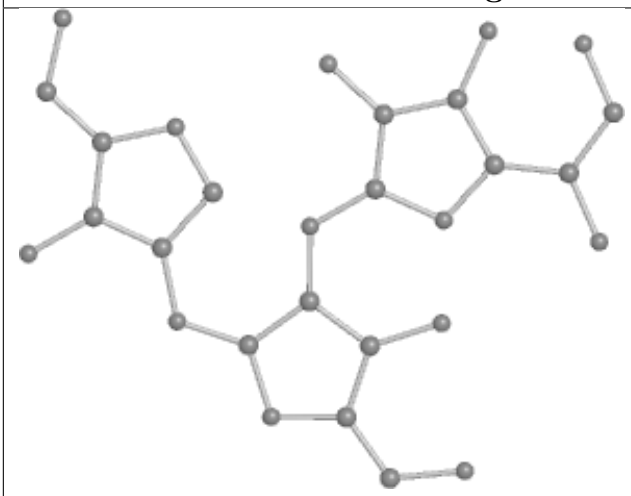
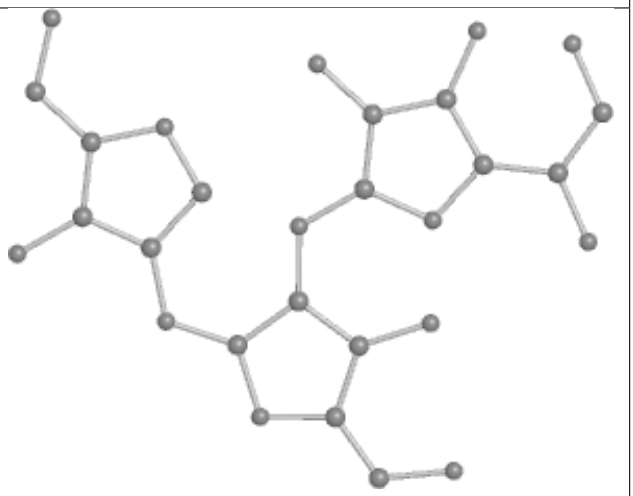
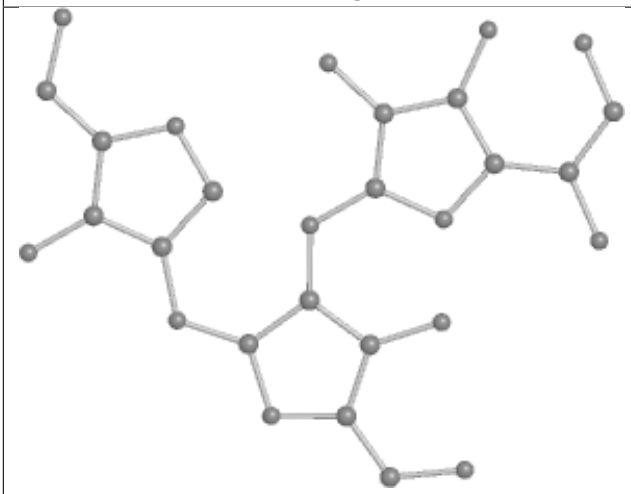
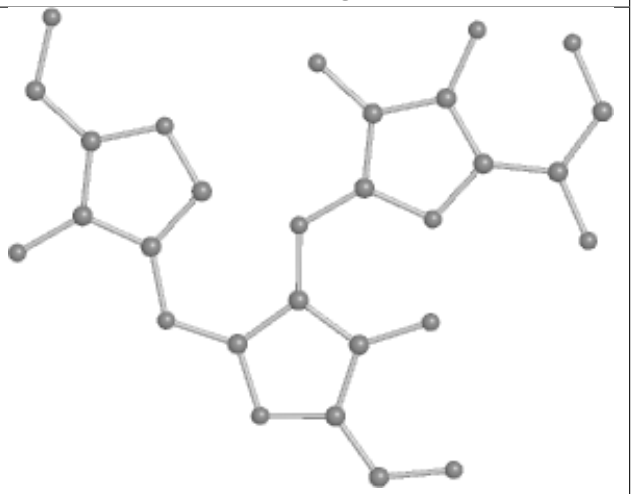
Oligosaccharide Chain 4B	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

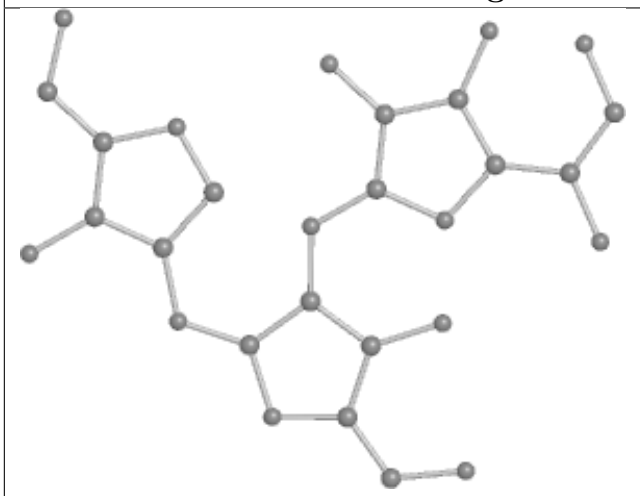
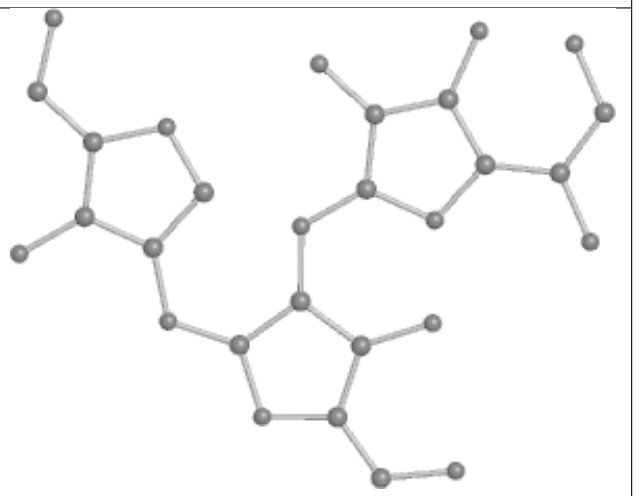
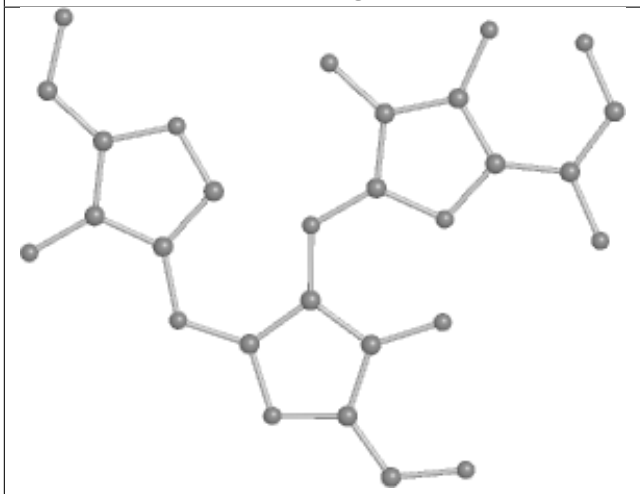
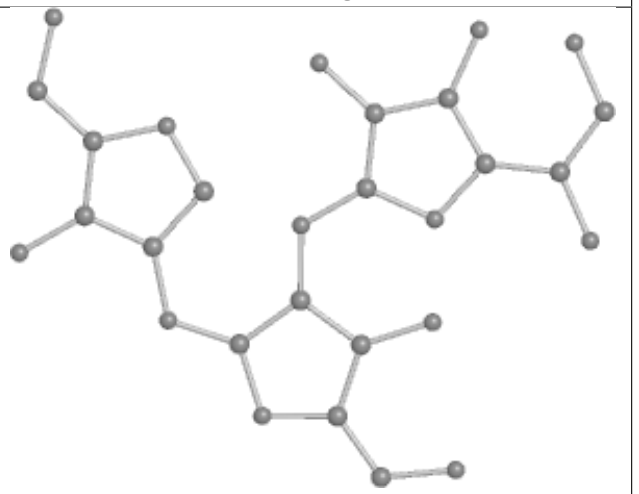
Oligosaccharide Chain 5B	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

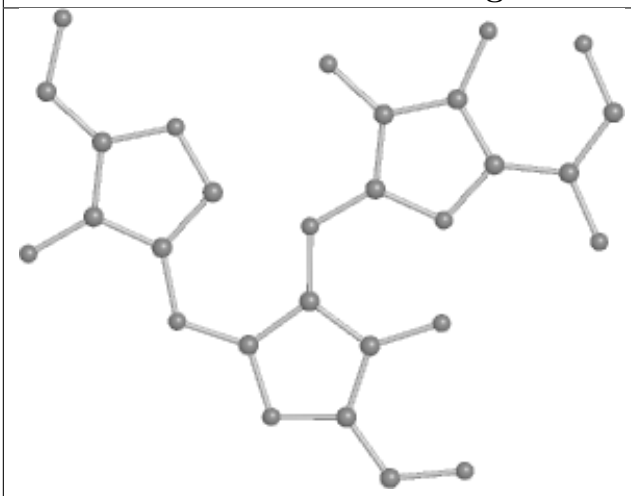
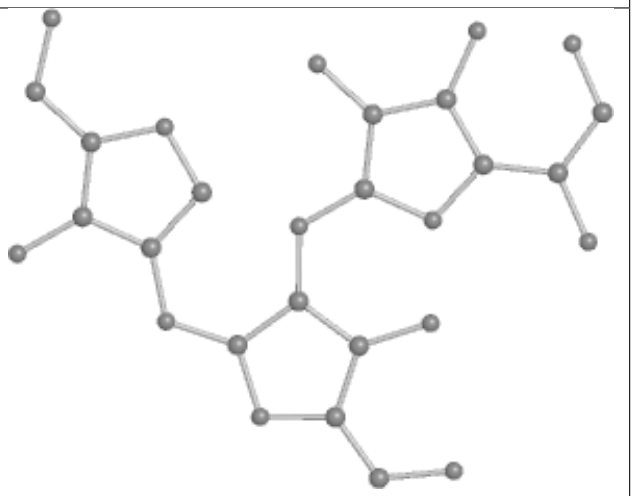
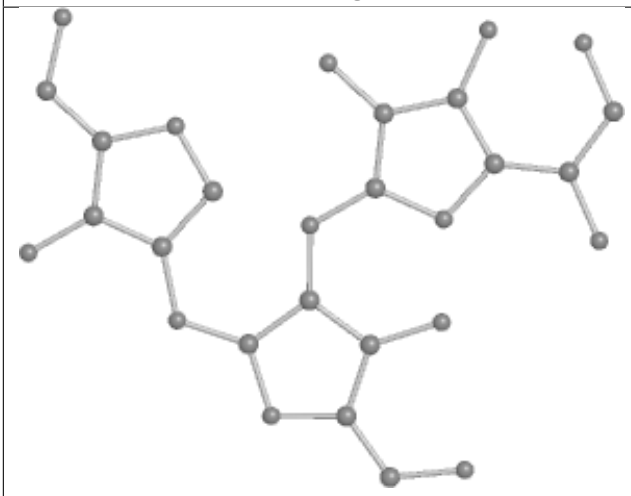
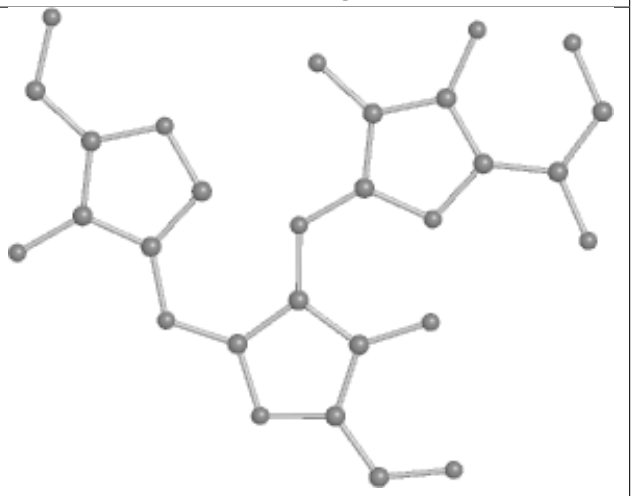
Oligosaccharide Chain 9B	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

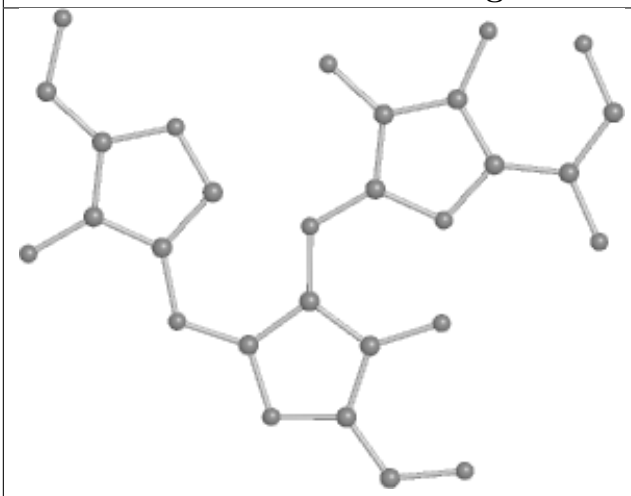
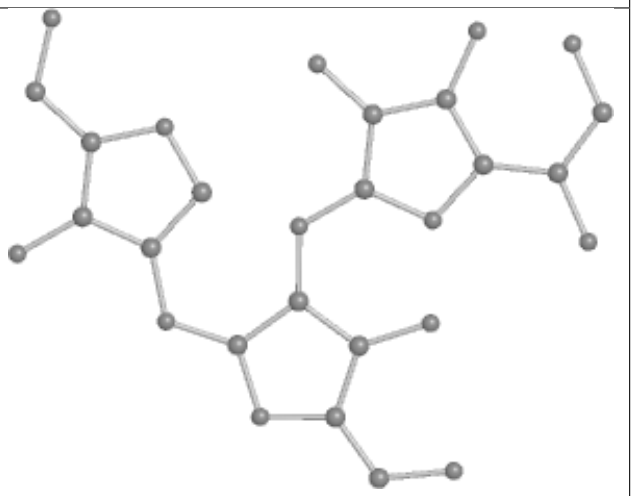
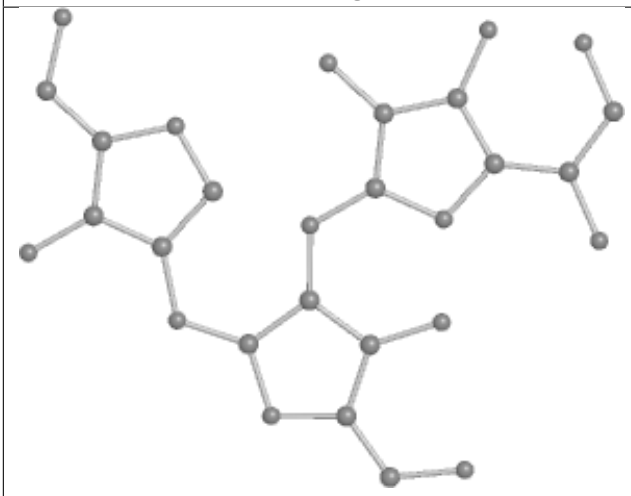
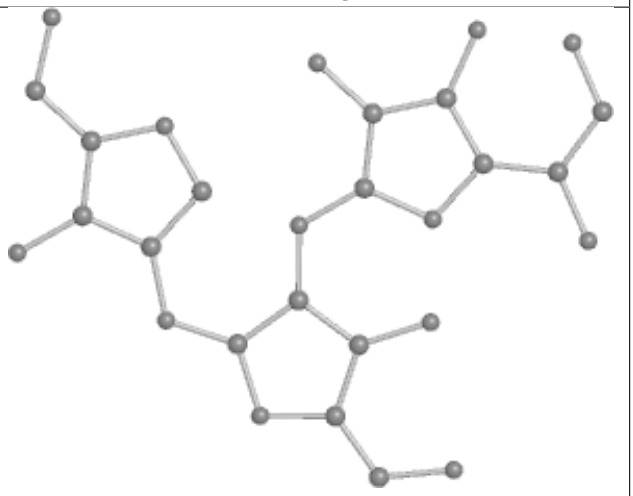
Oligosaccharide Chain FC	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

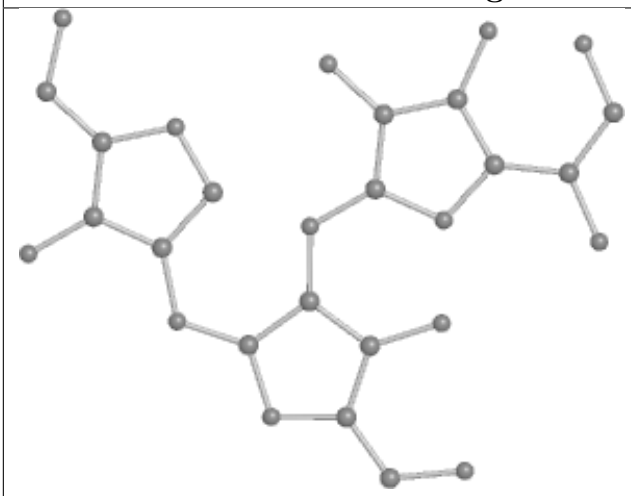
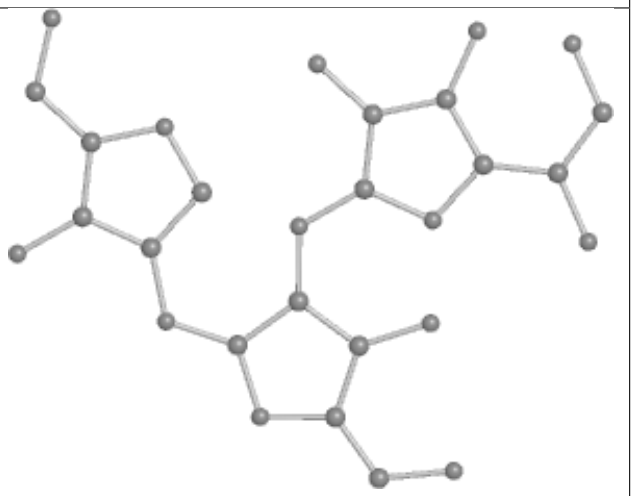
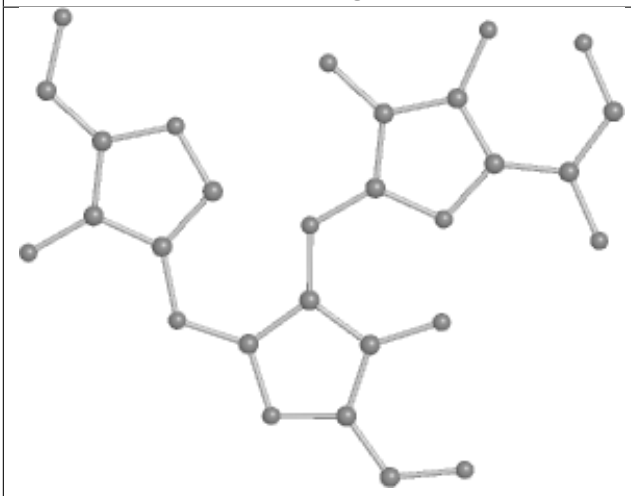
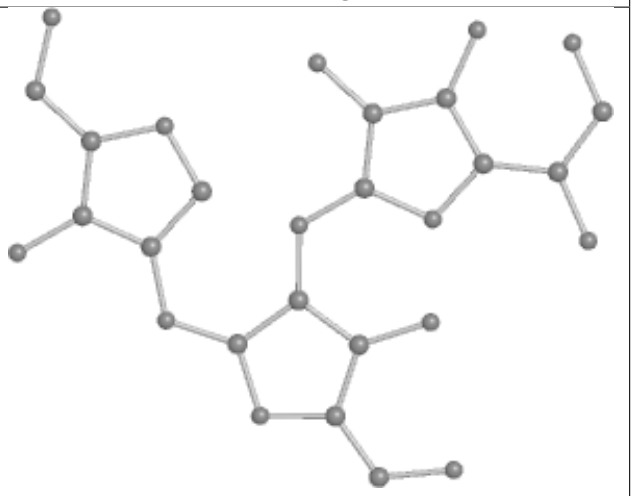
Oligosaccharide Chain JC	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

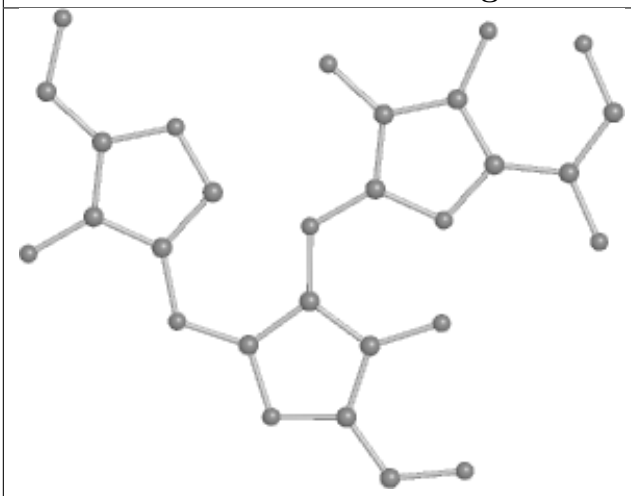
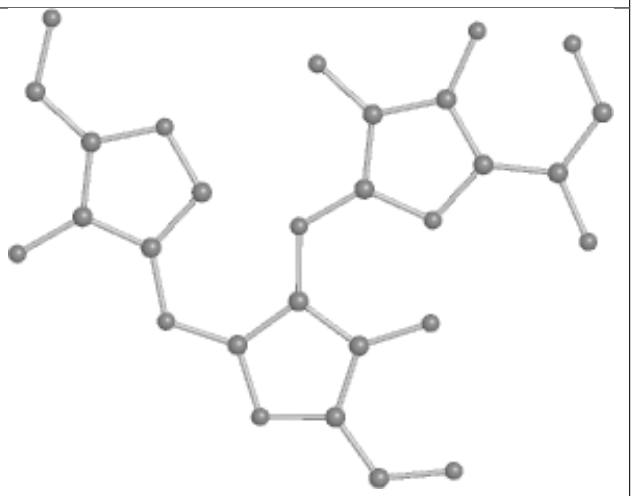
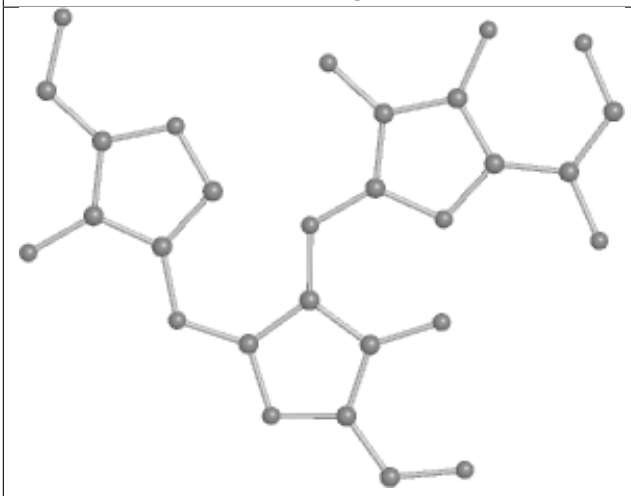
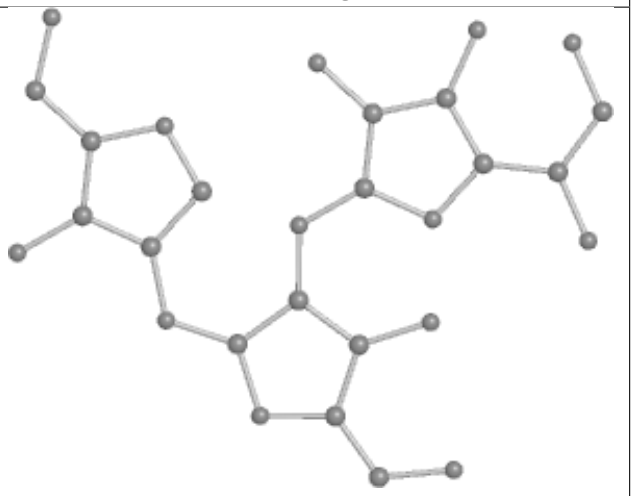
Oligosaccharide Chain xC	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

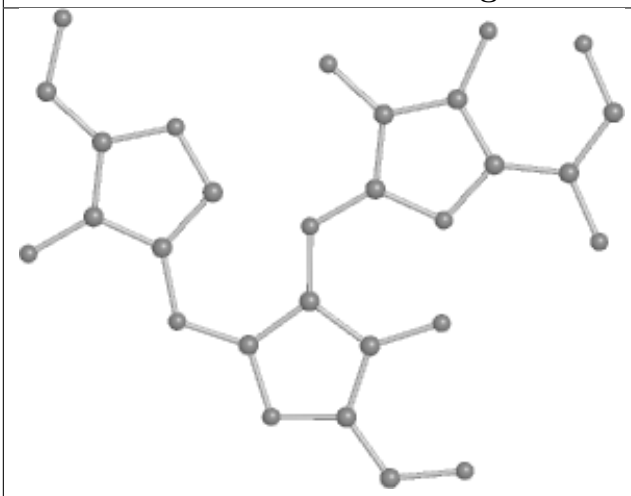
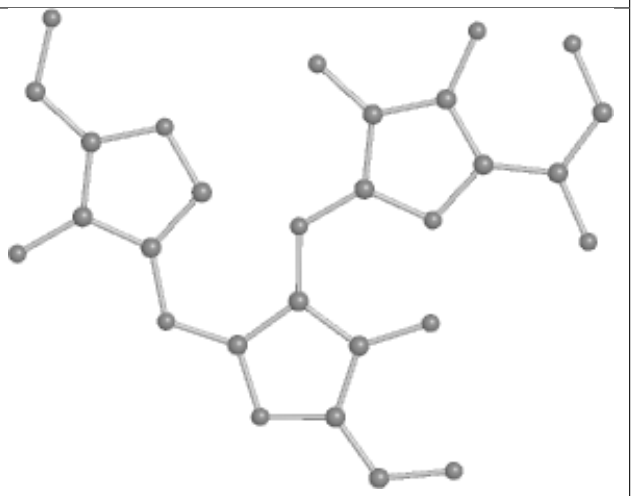
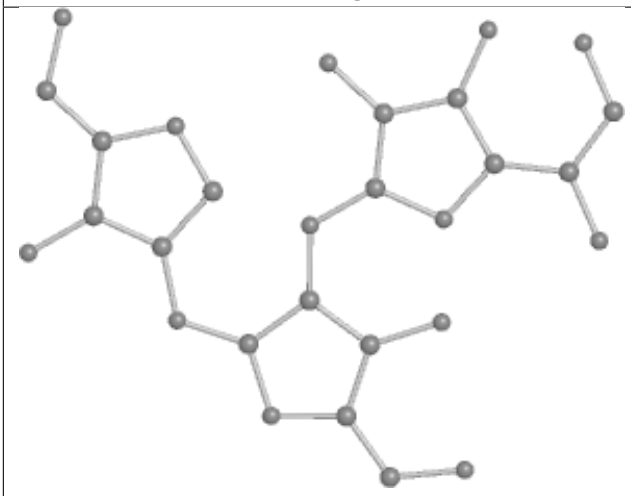
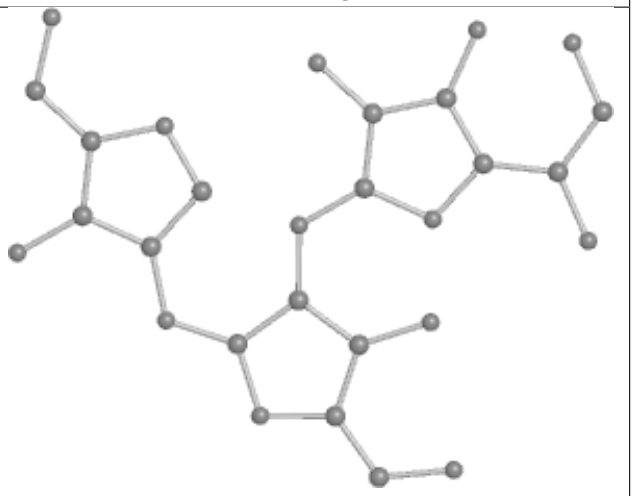
Oligosaccharide Chain 0C	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

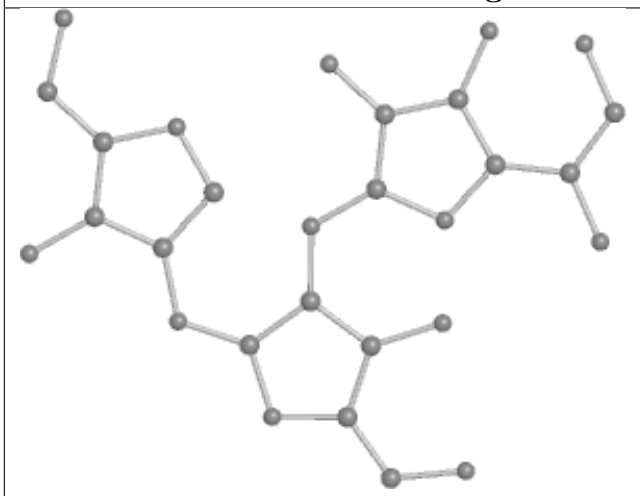
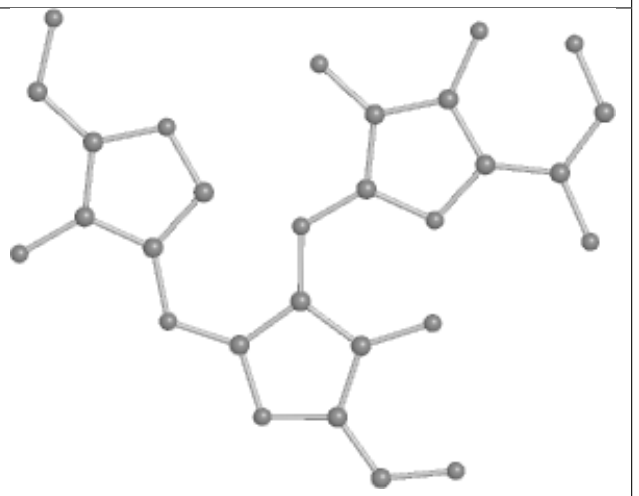
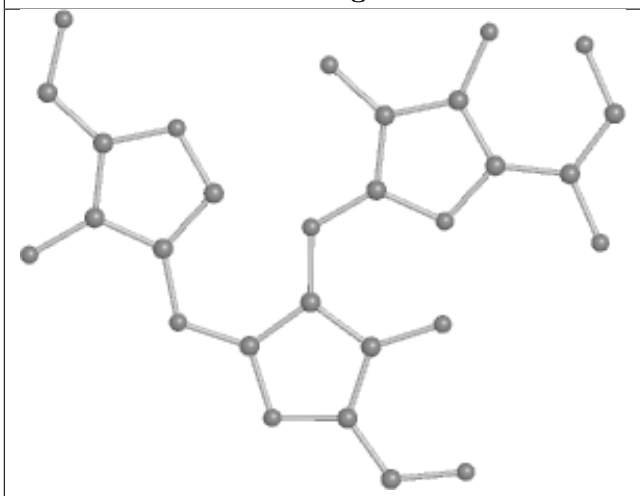
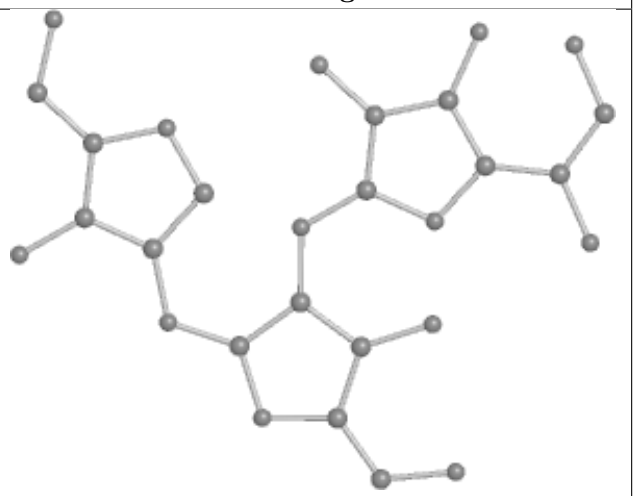
Oligosaccharide Chain 1C	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

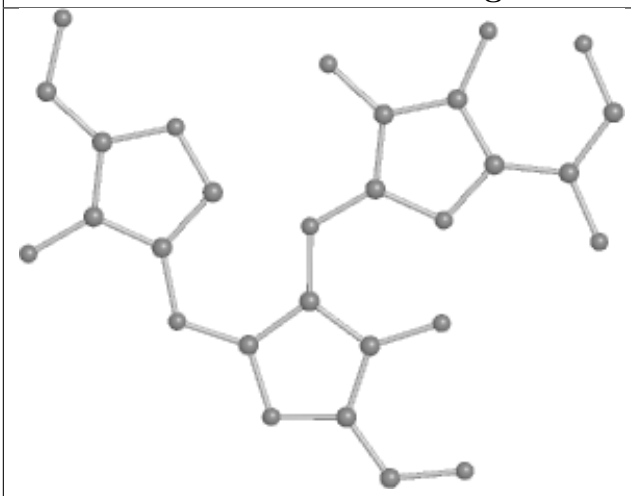
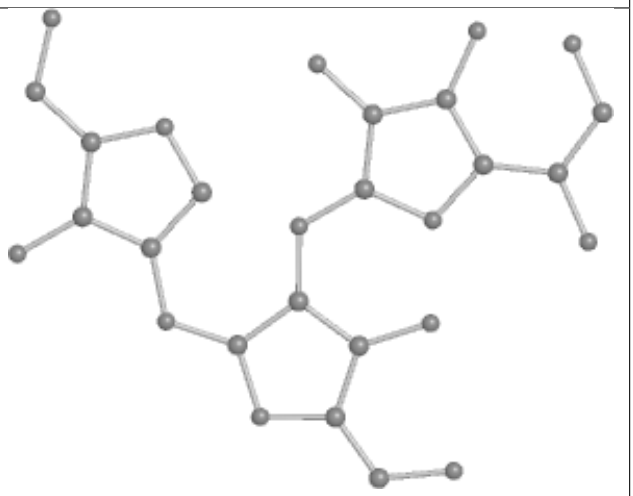
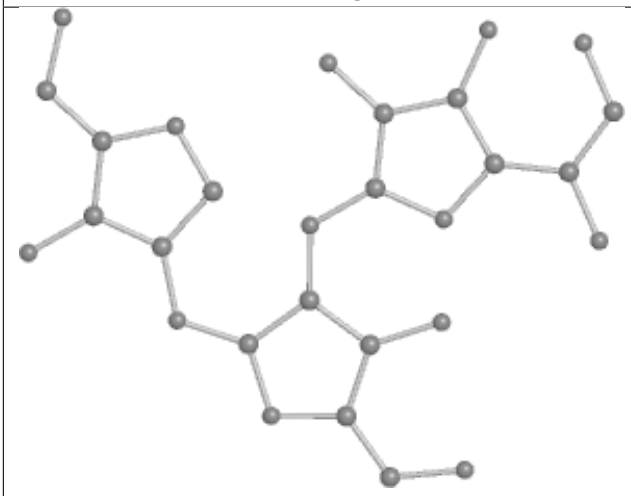
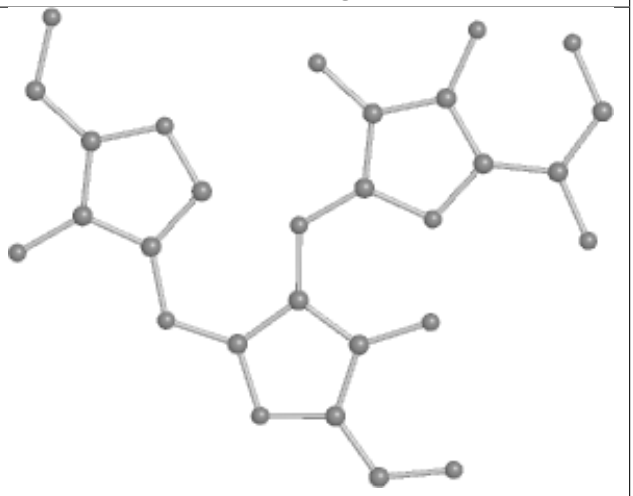
Oligosaccharide Chain 2C	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

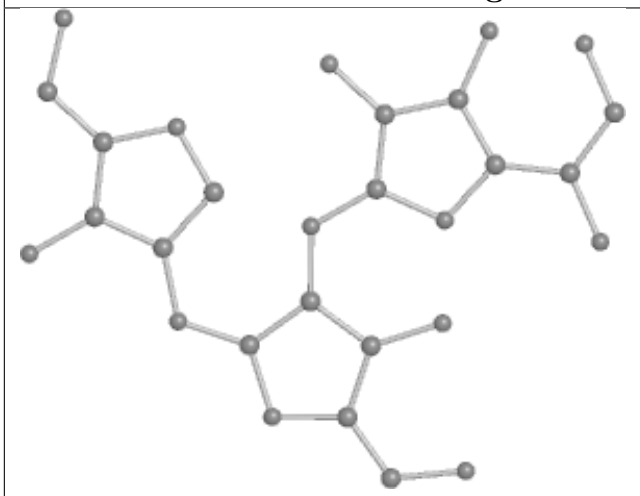
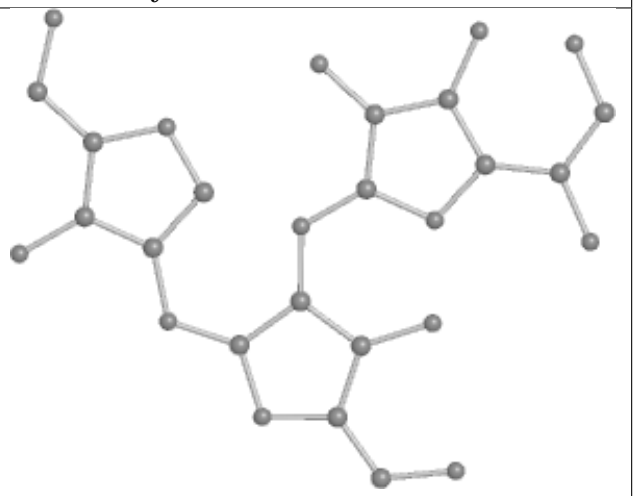
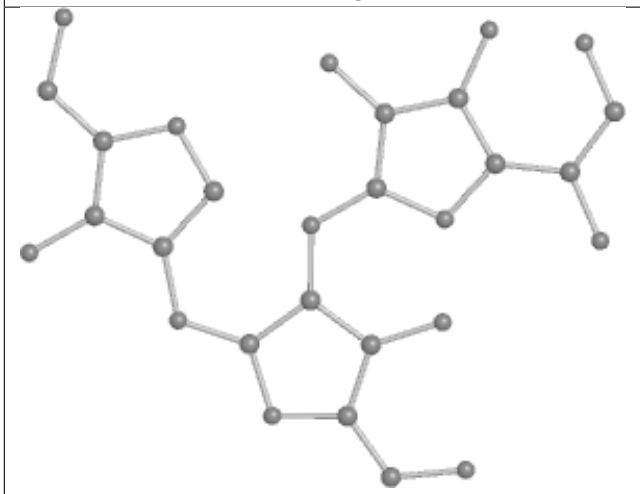
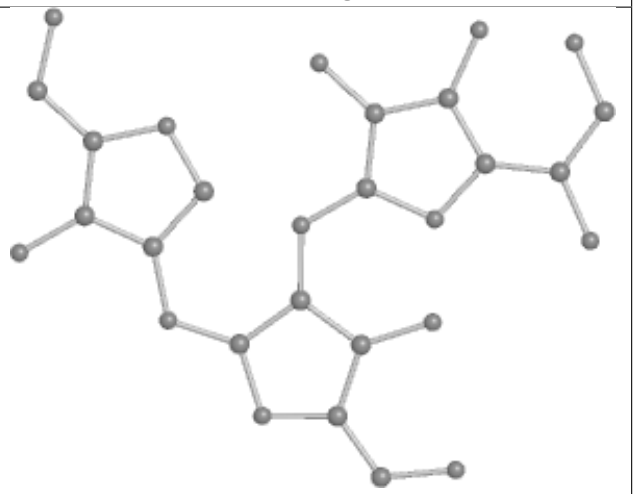
Oligosaccharide Chain 6C	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

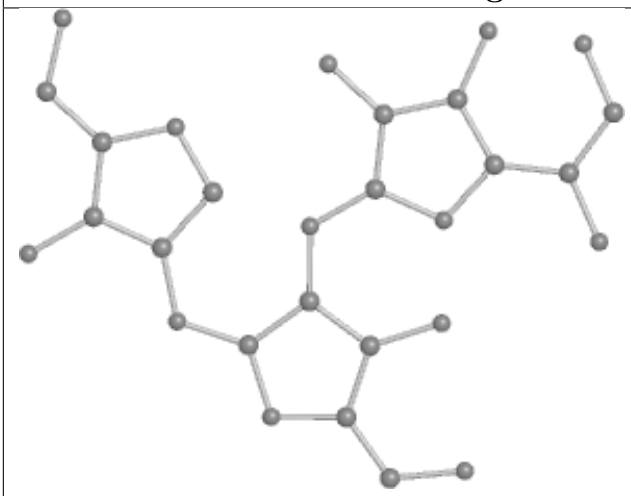
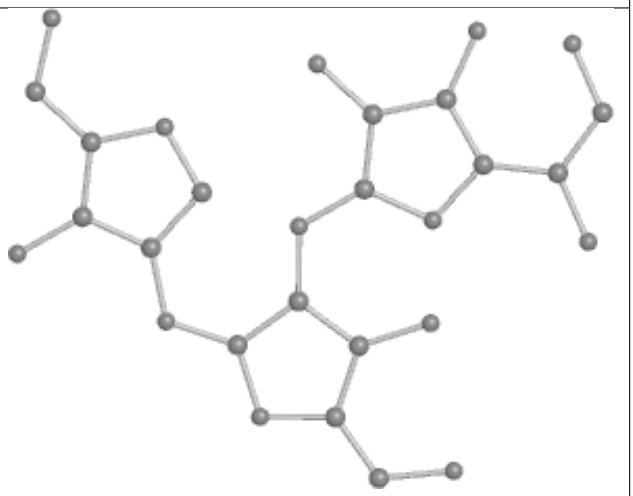
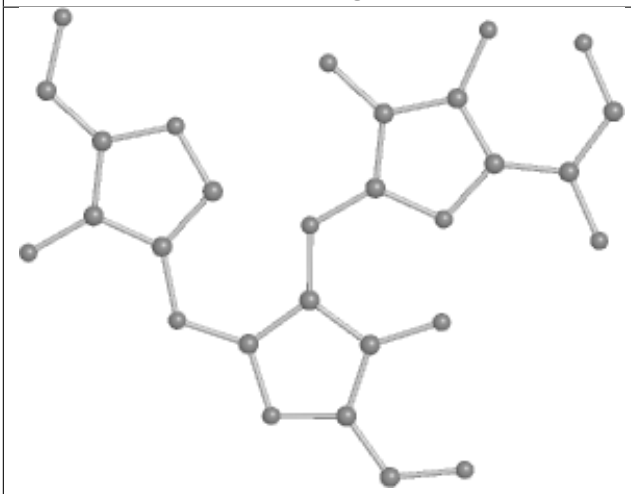
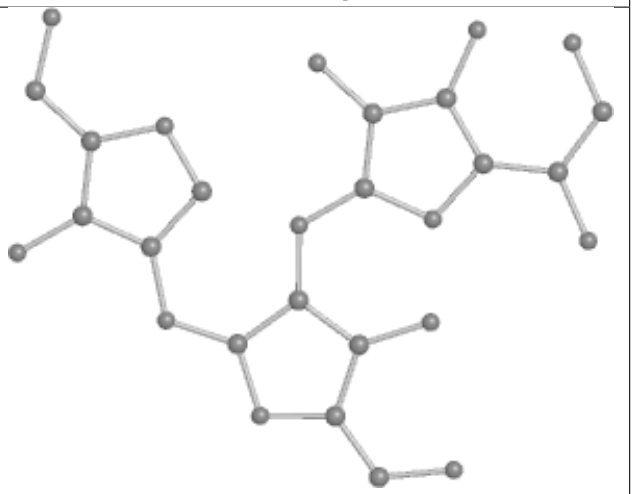
Oligosaccharide Chain CD	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain GD	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

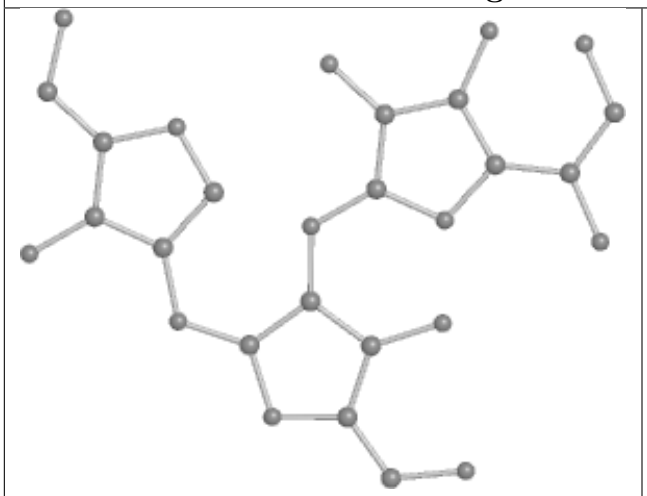
Oligosaccharide Chain uD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain xD	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

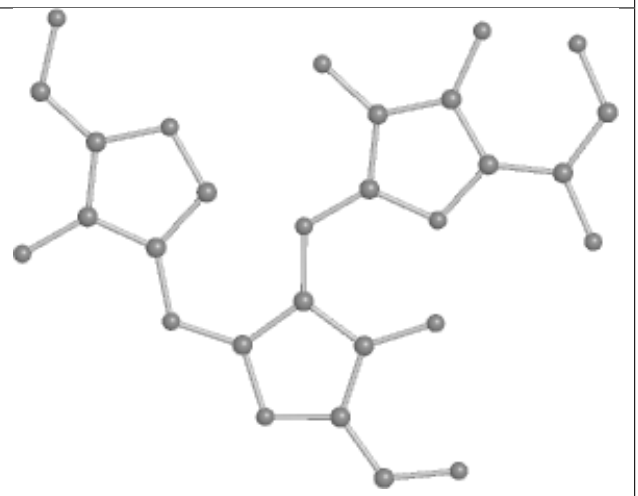
Oligosaccharide Chain yD	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain zD	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

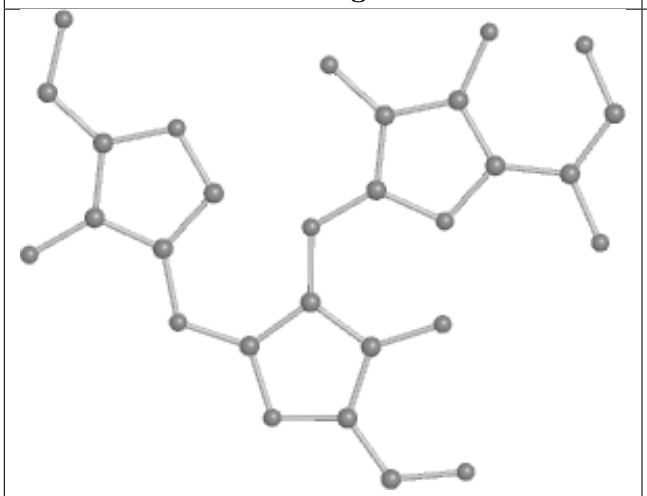
Oligosaccharide Chain 3D



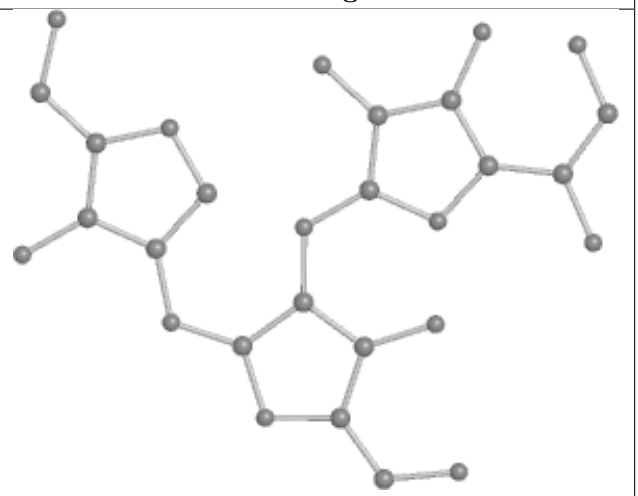
Bond lengths



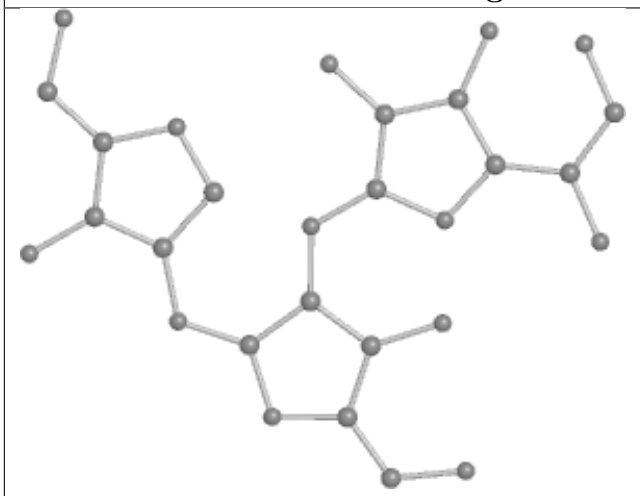
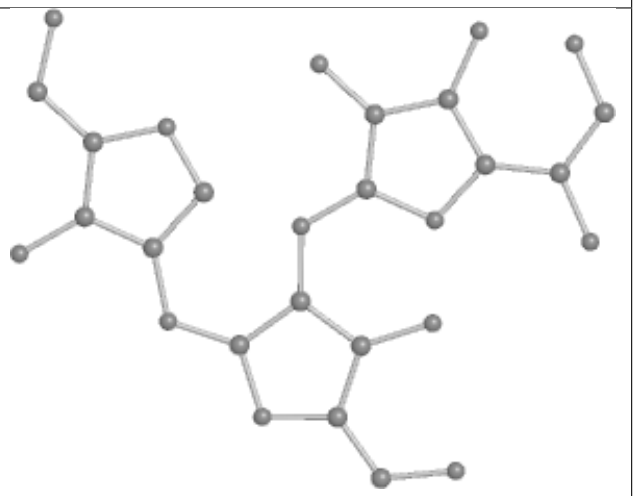
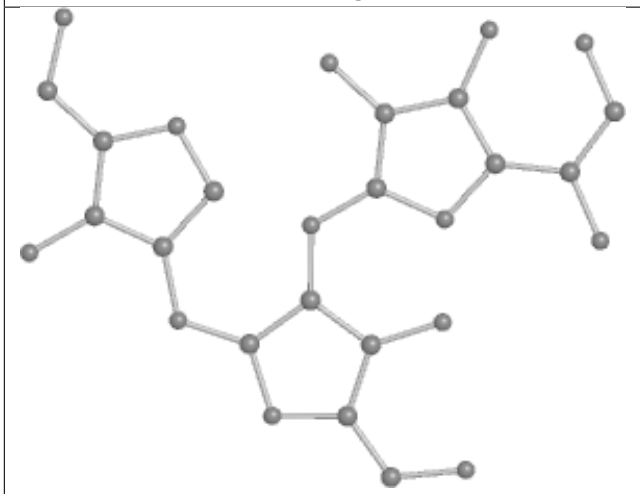
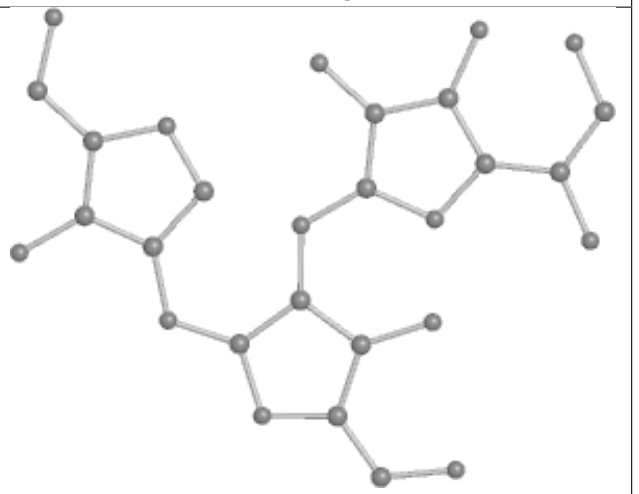
Bond angles



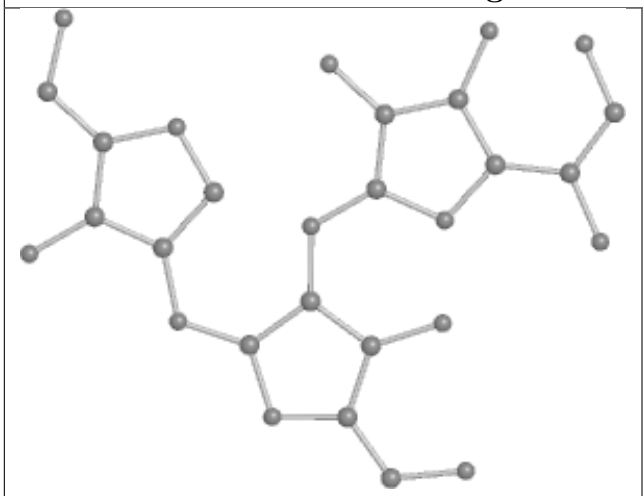
Torsions



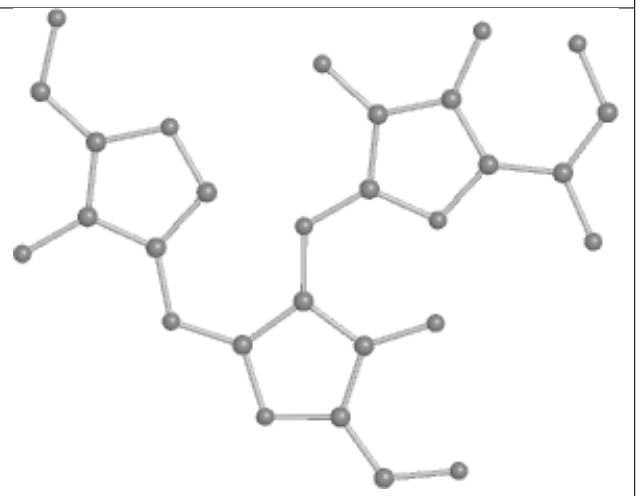
Rings

Oligosaccharide Chain 6D	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

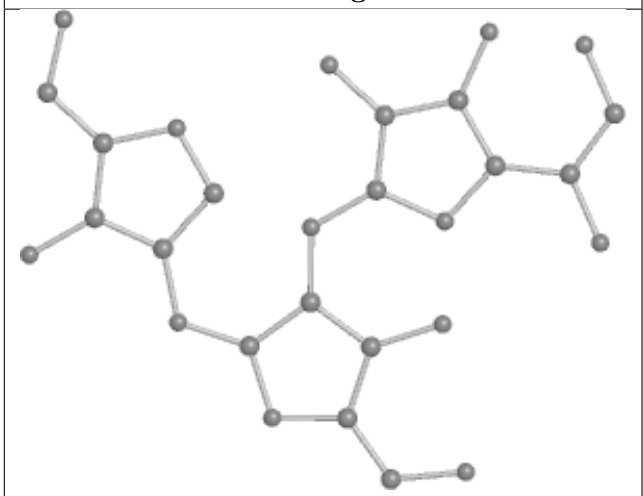
Oligosaccharide Chain 7D



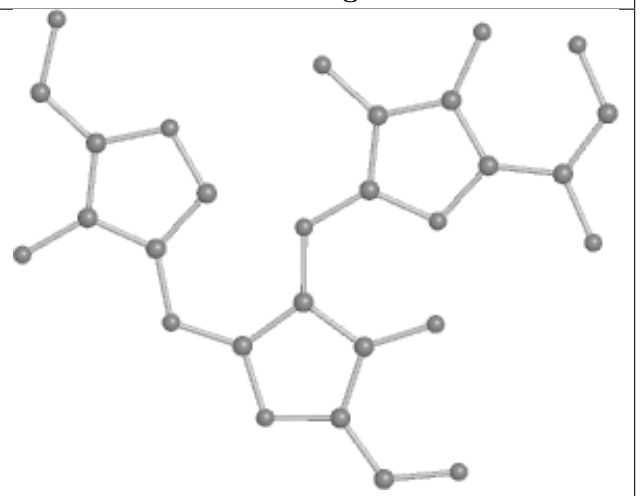
Bond lengths



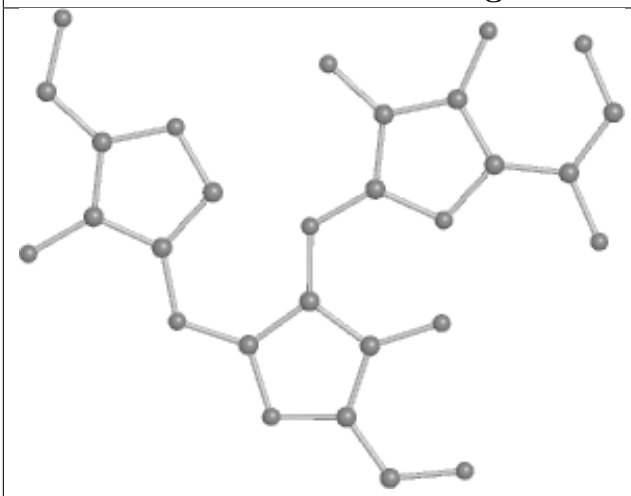
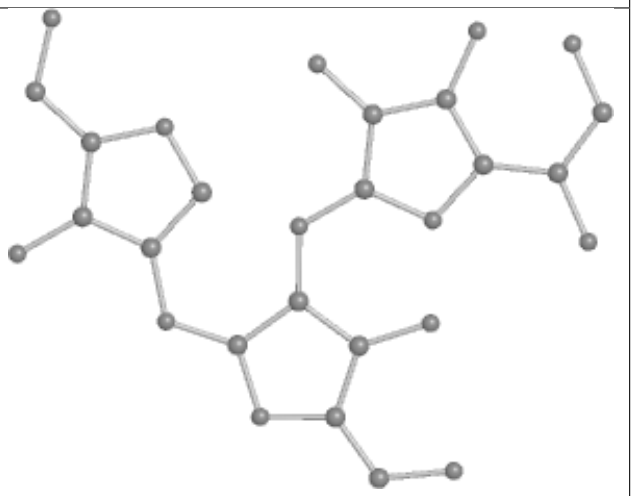
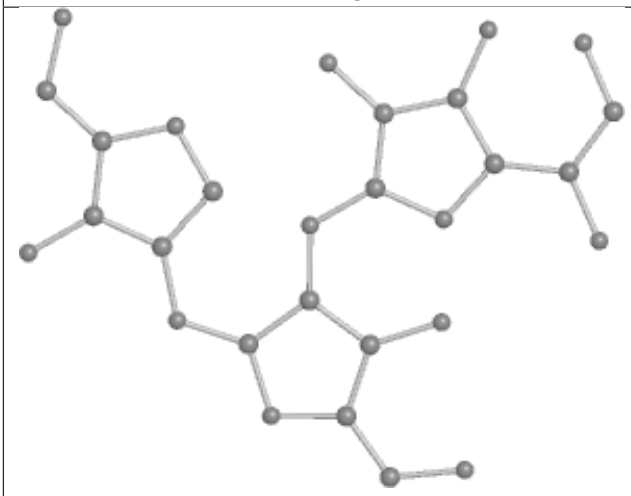
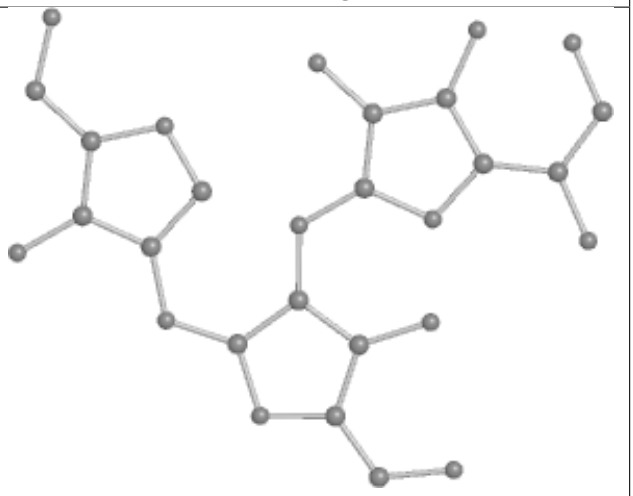
Bond angles

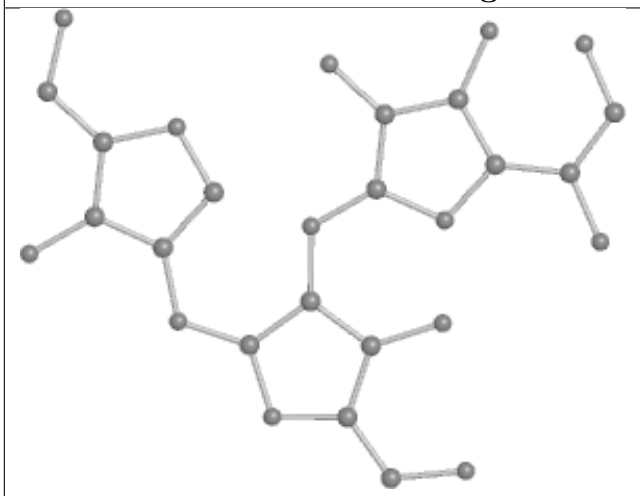
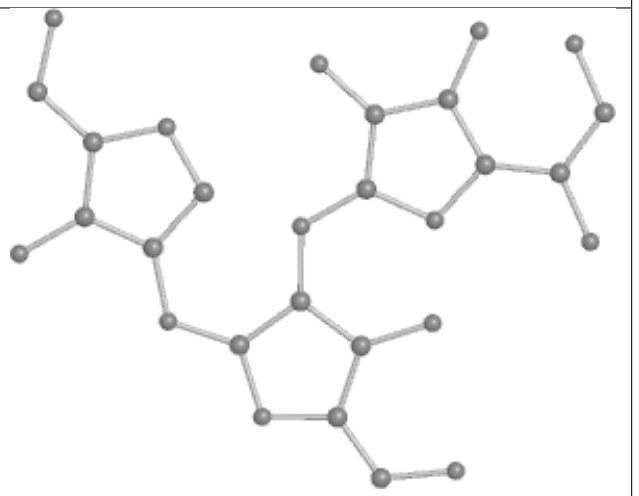
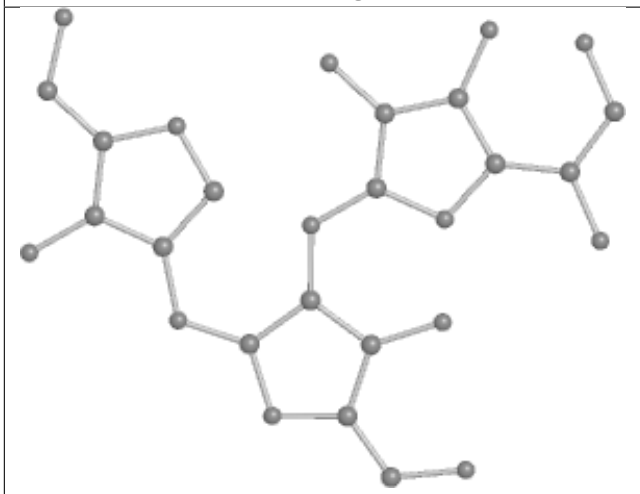
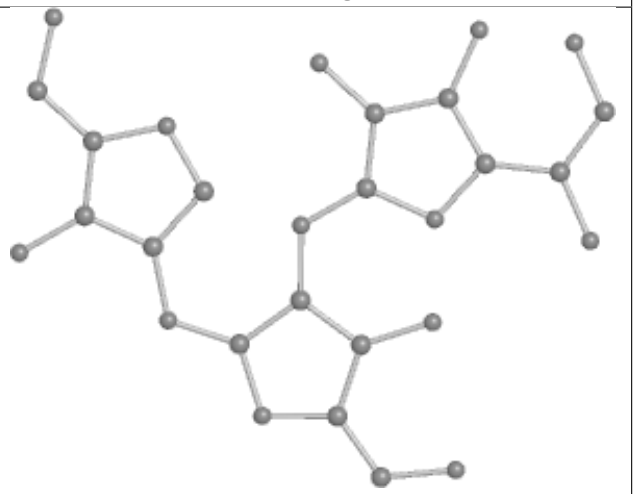


Torsions

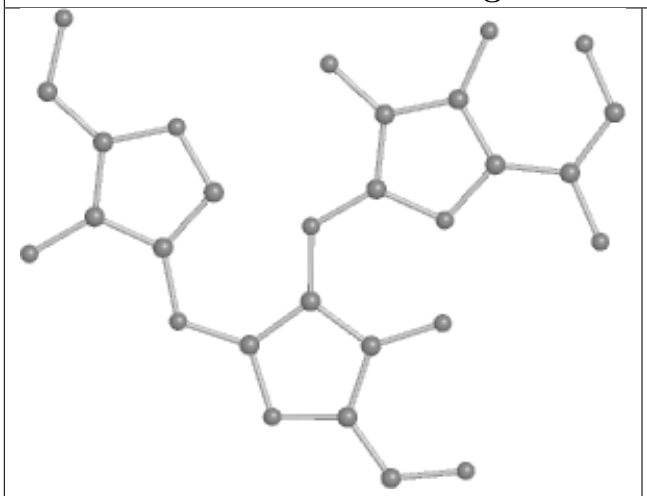


Rings

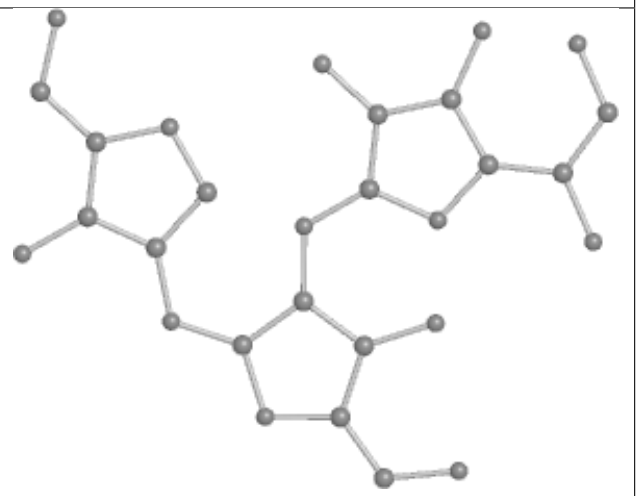
Oligosaccharide Chain 8D	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain ME	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

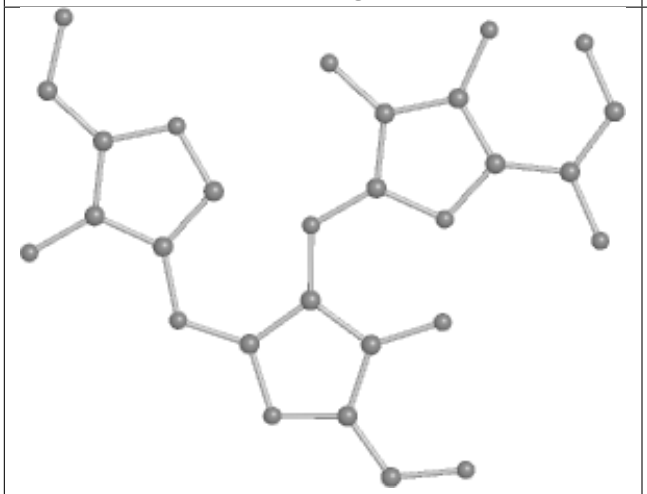
Oligosaccharide Chain OE



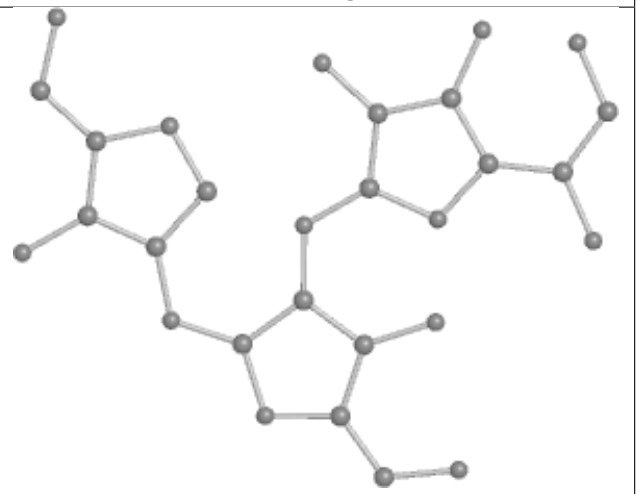
Bond lengths



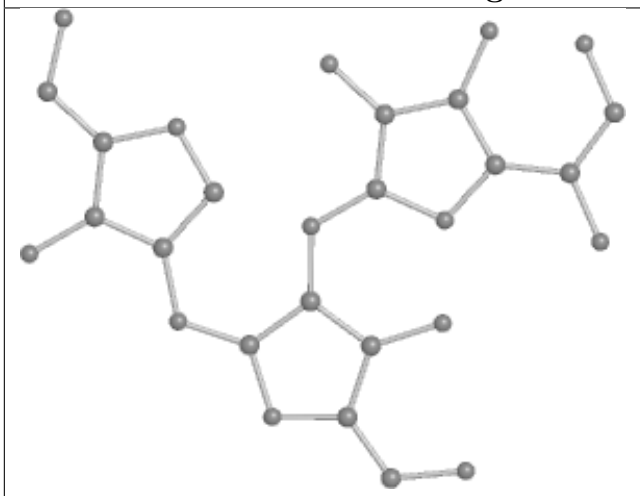
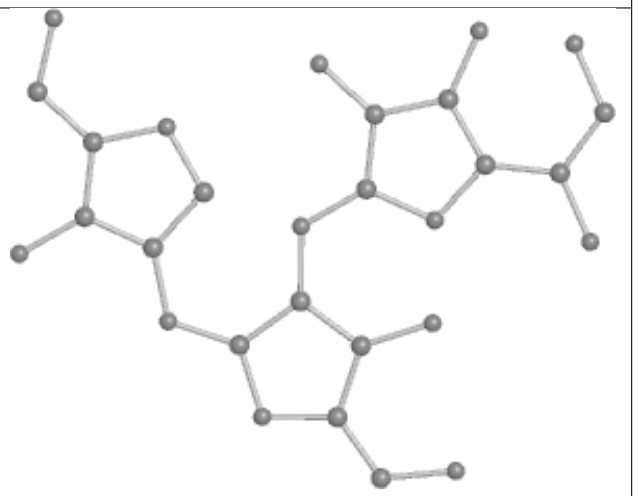
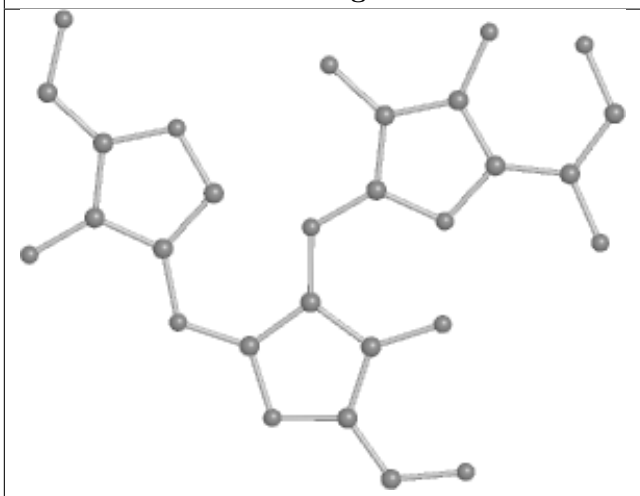
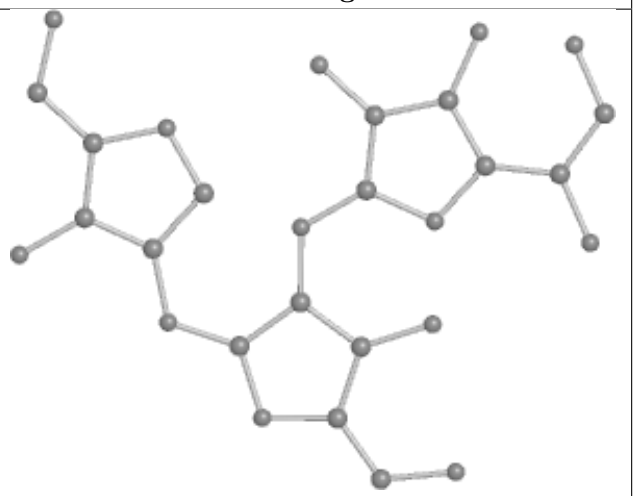
Bond angles

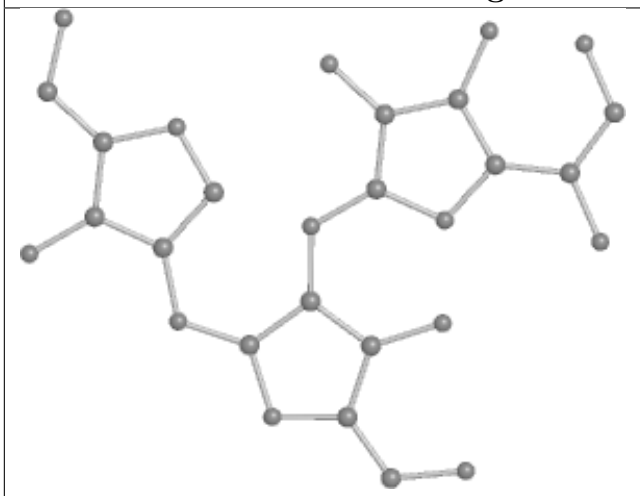
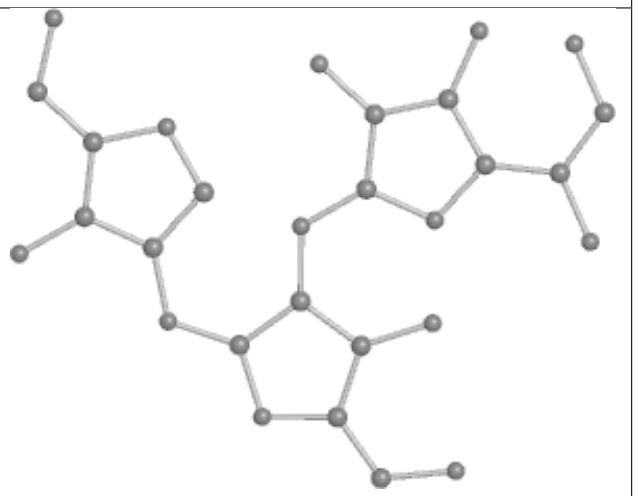
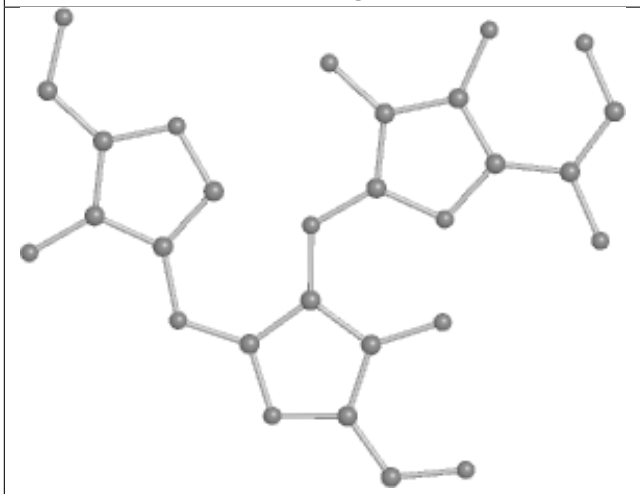
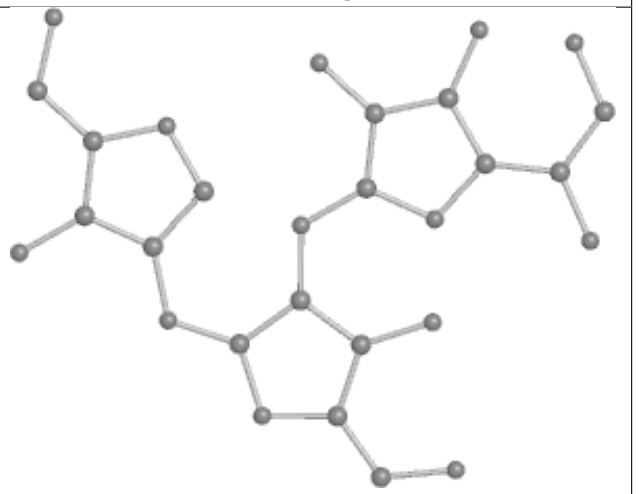


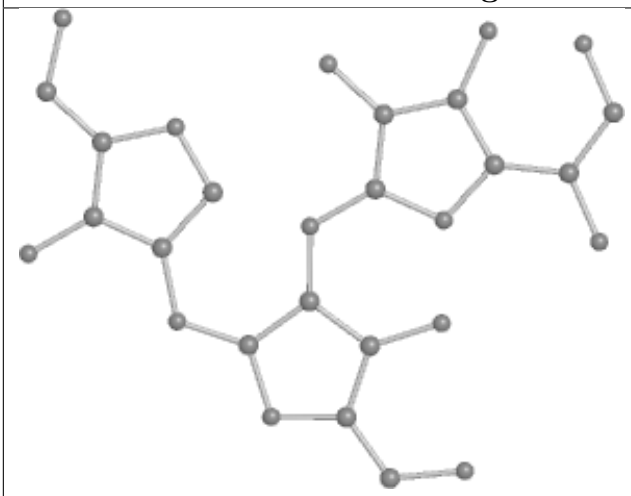
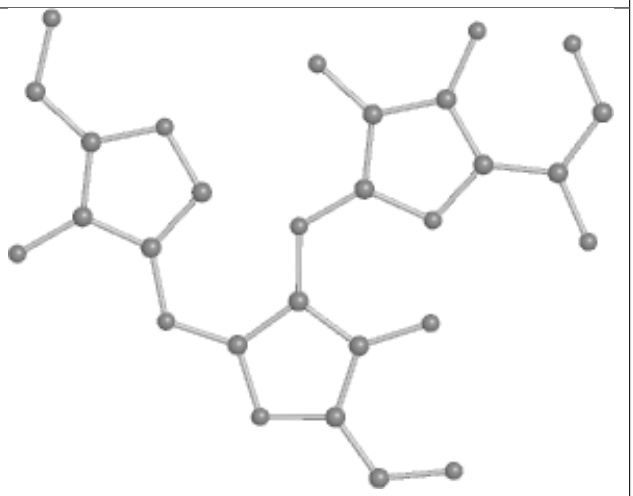
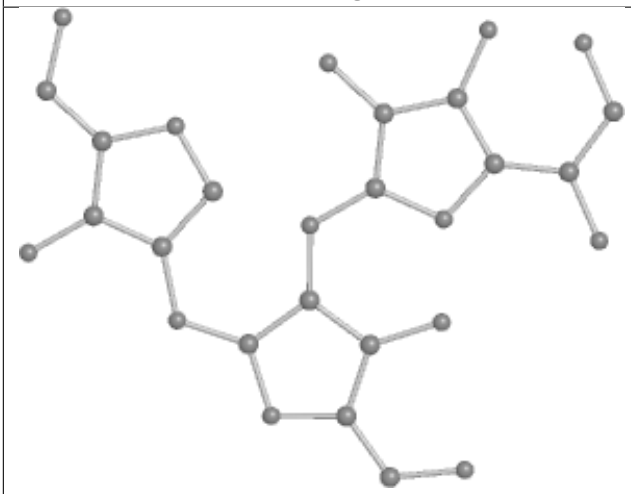
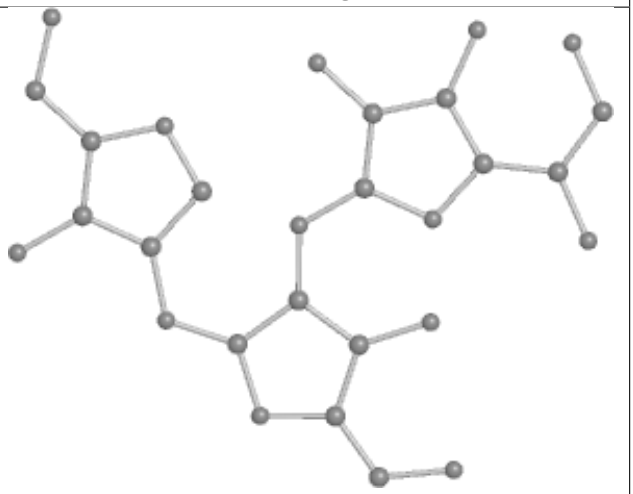
Torsions

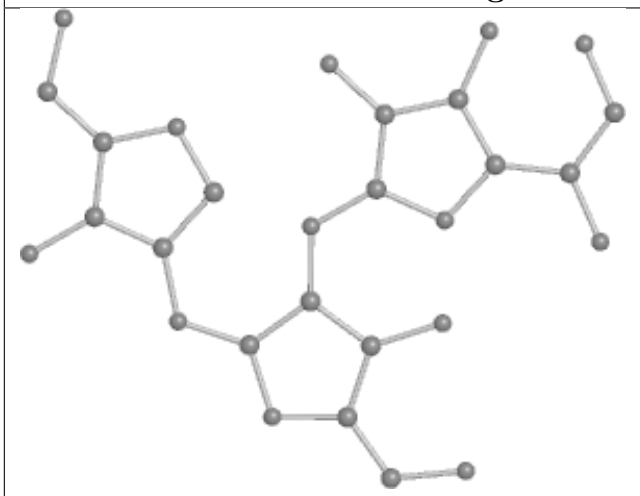
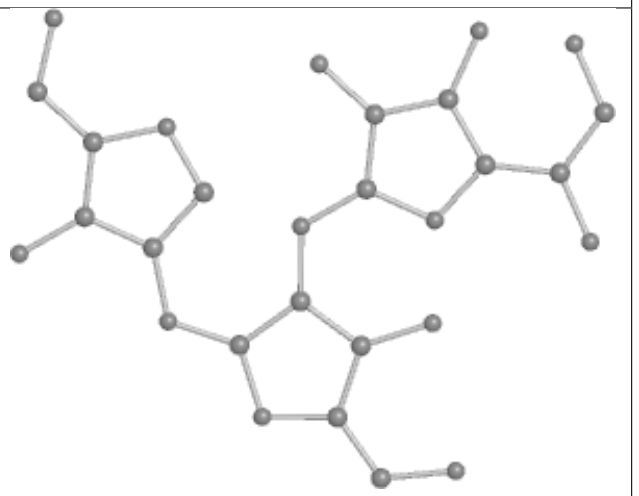
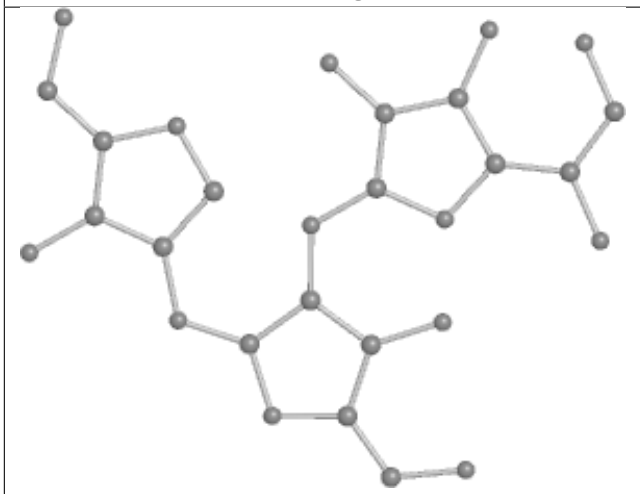
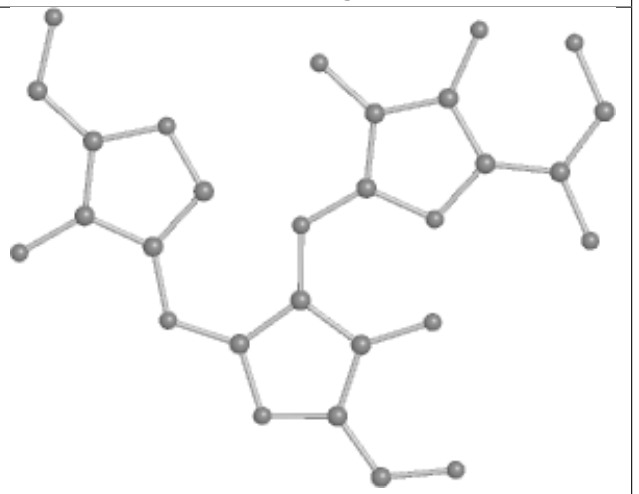


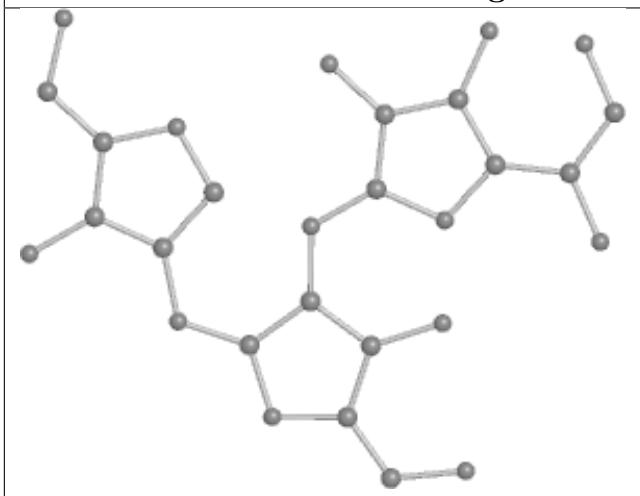
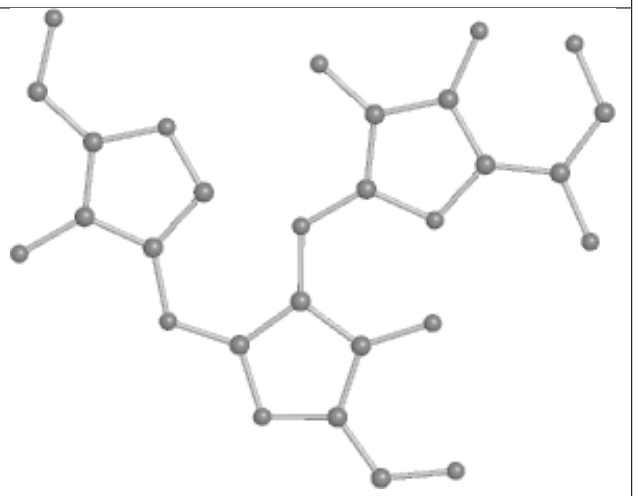
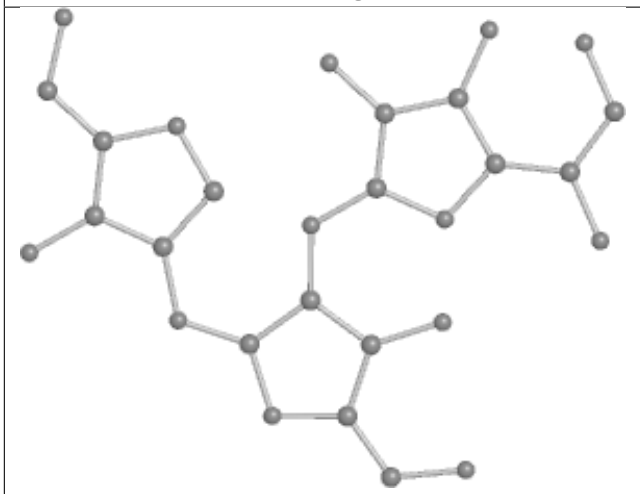
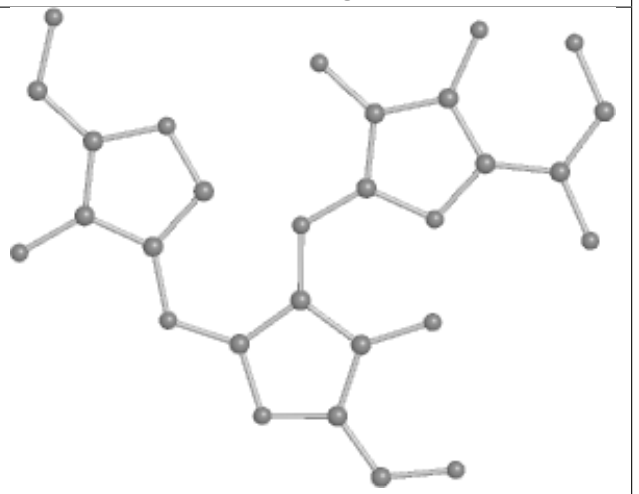
Rings

Oligosaccharide Chain ZE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

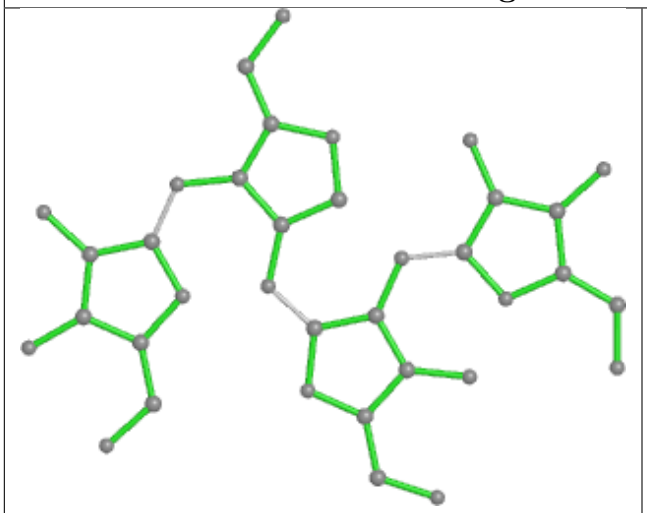
Oligosaccharide Chain bE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain mE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

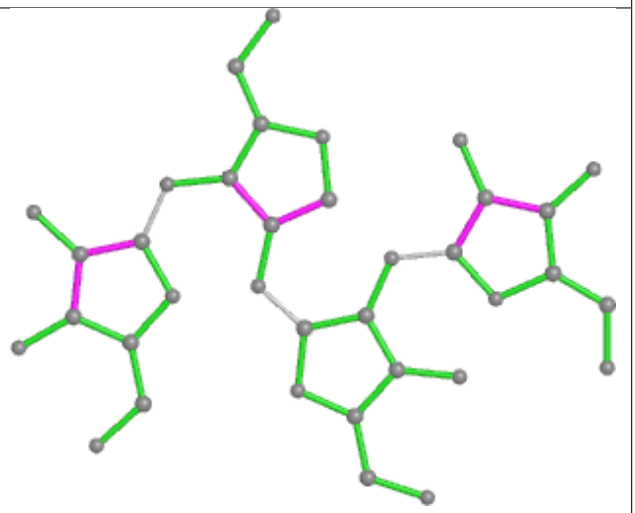
Oligosaccharide Chain nE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain oE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

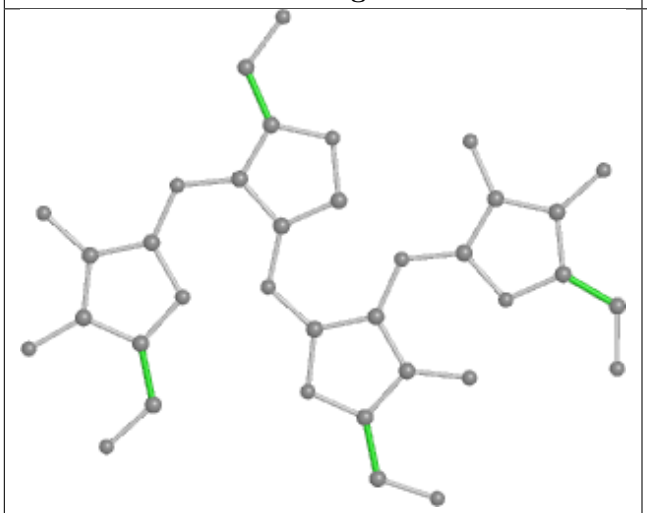
Oligosaccharide Chain S



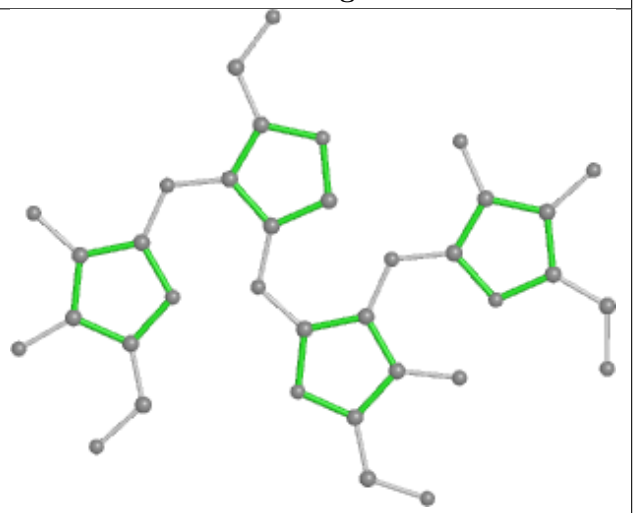
Bond lengths



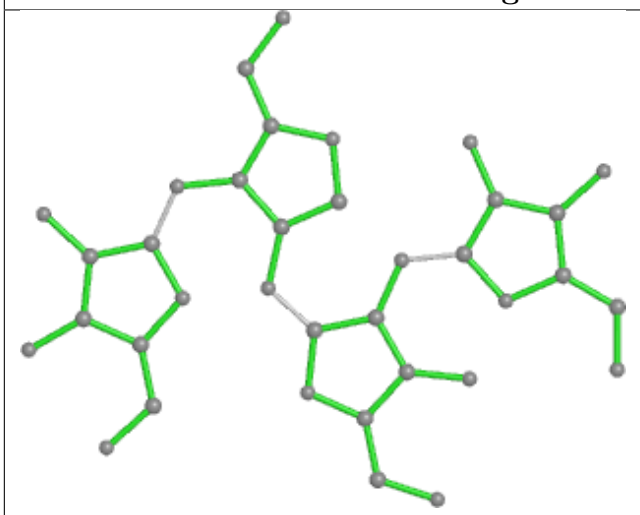
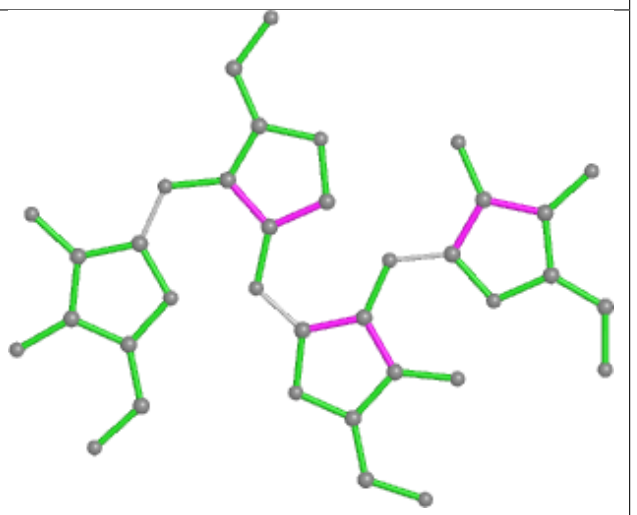
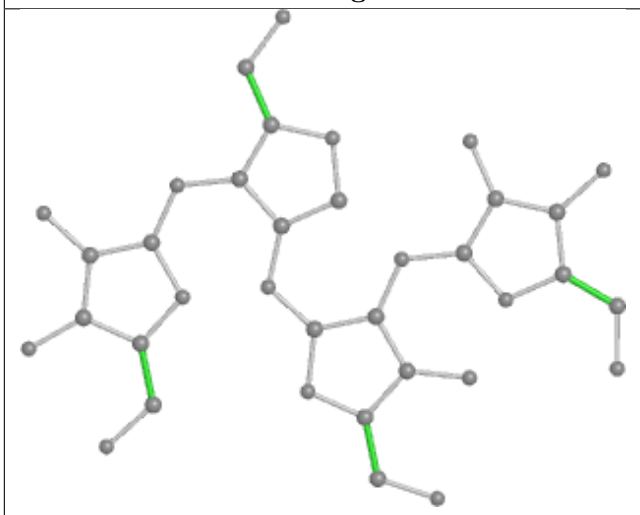
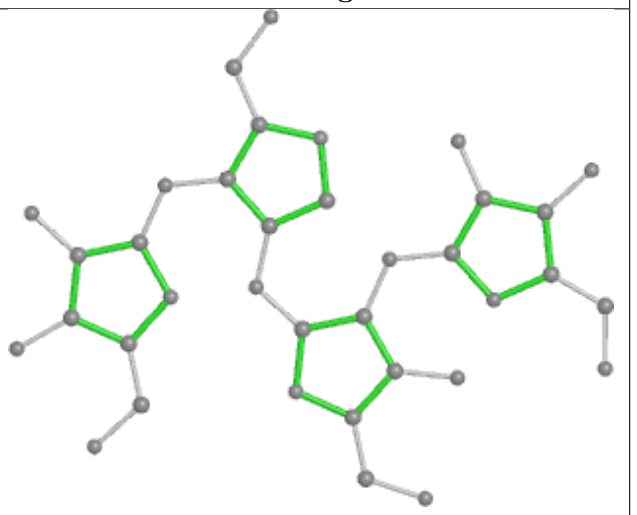
Bond angles



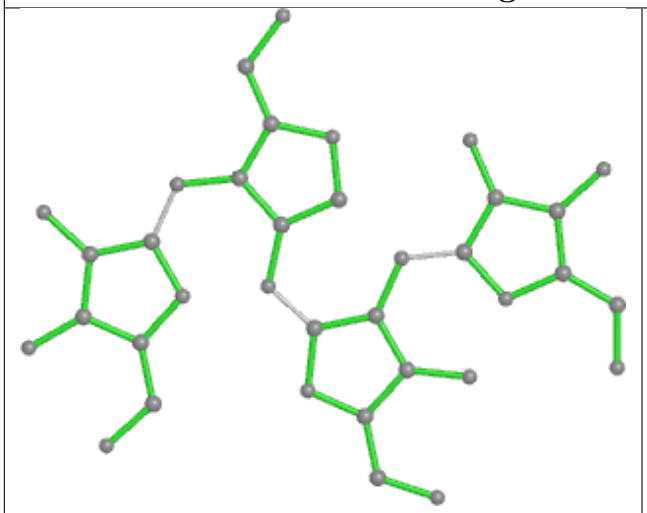
Torsions



Rings

Oligosaccharide Chain f	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain h



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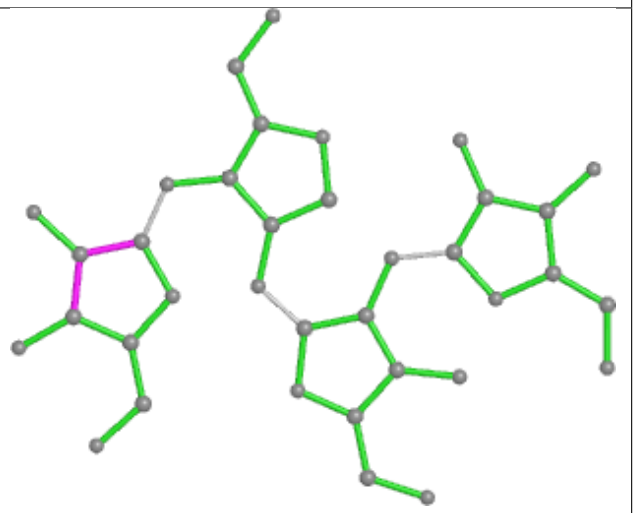
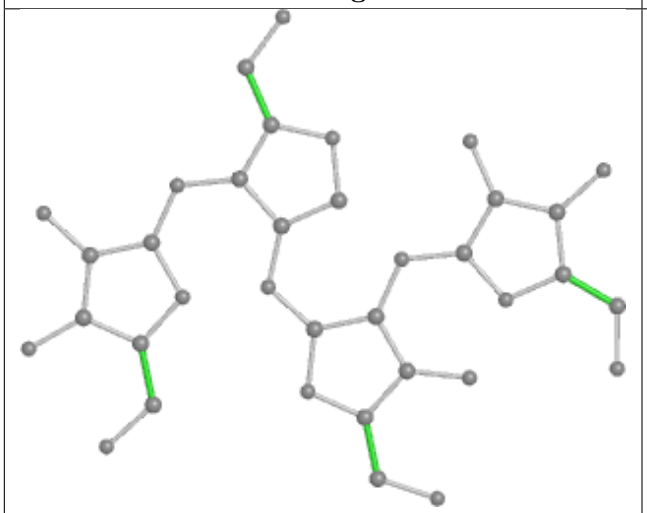


Bond angles



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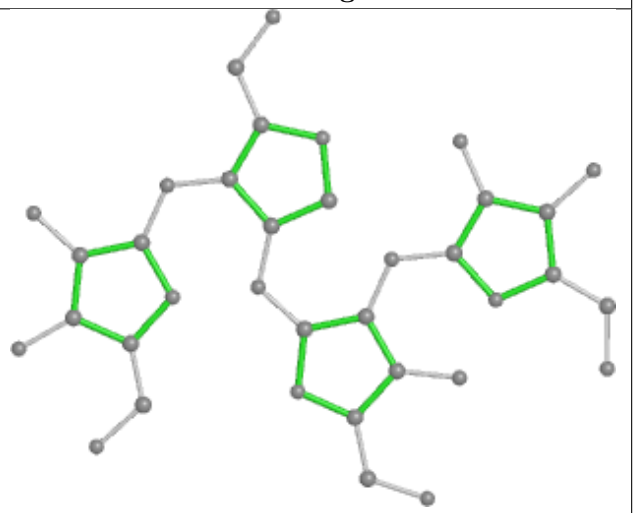
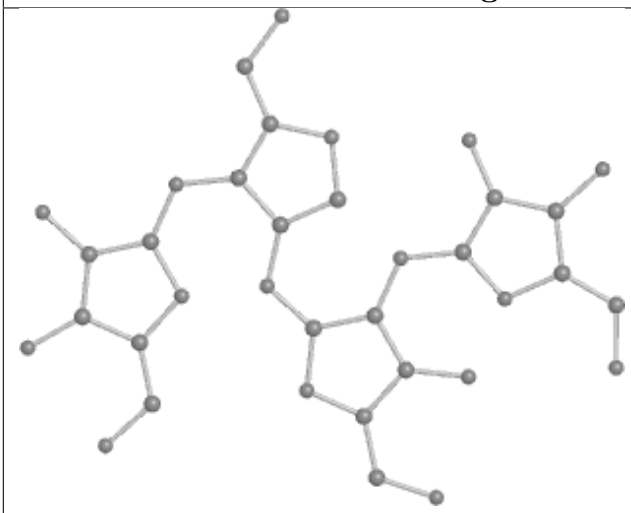
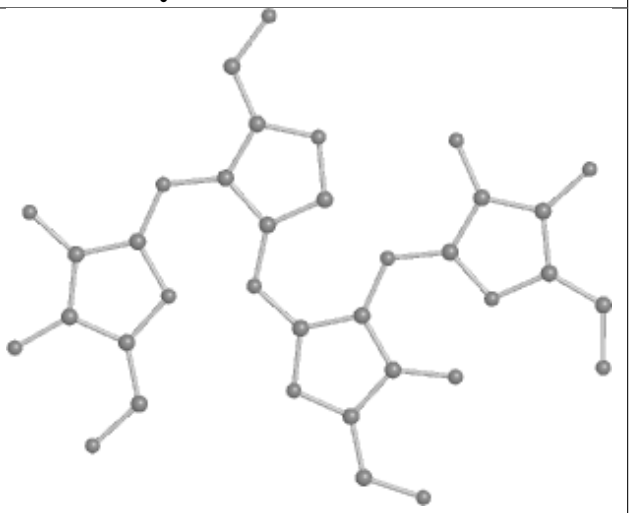
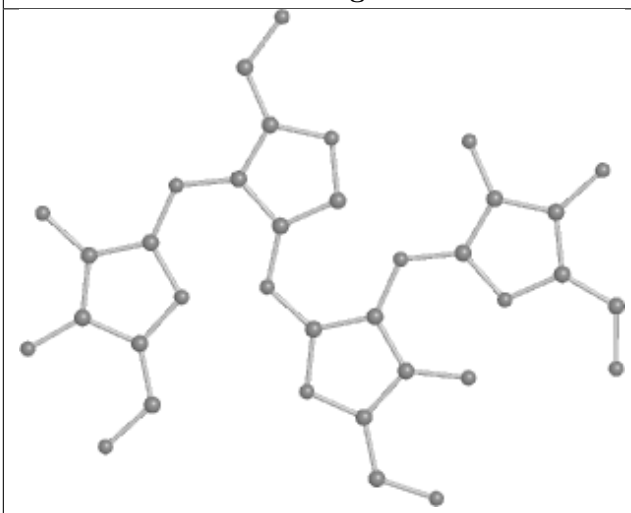
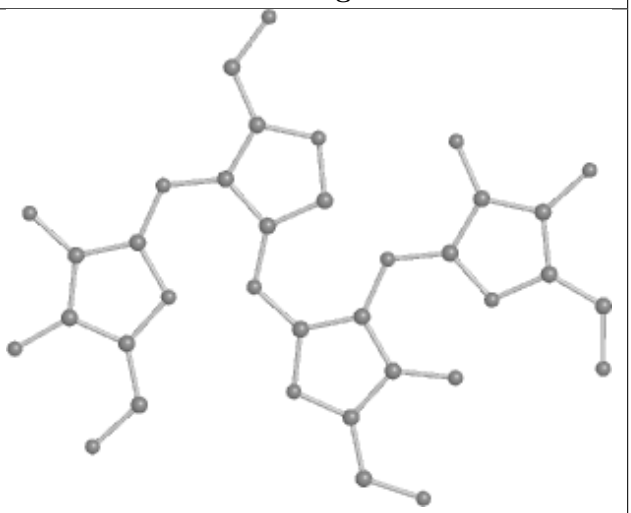


Rings

Oligosaccharide Chain QA	
 Bond lengths	 Bond angles
 Torsions	 Rings

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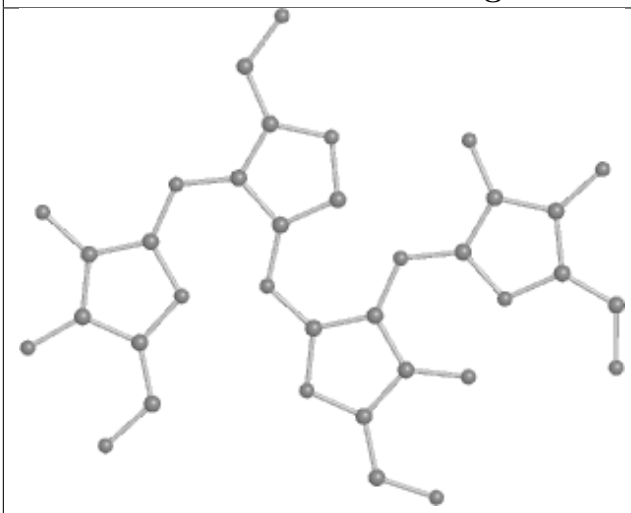
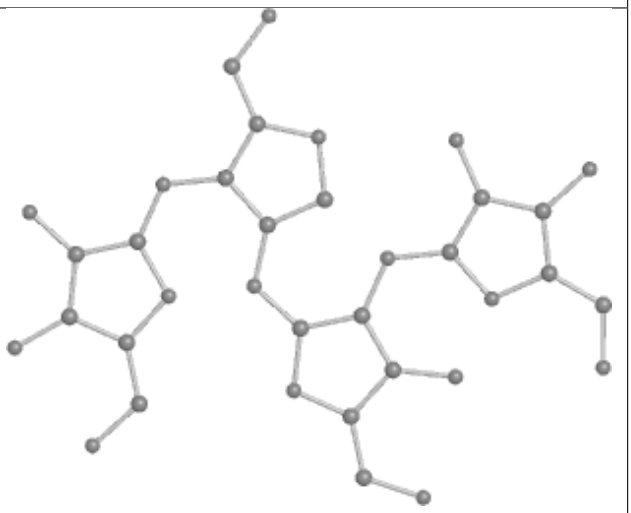
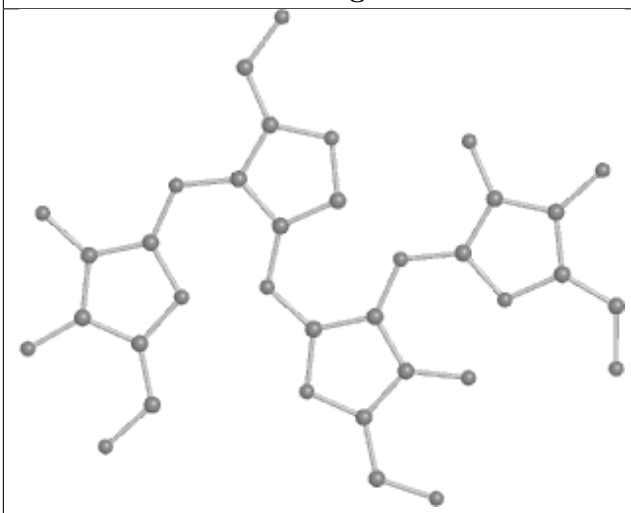
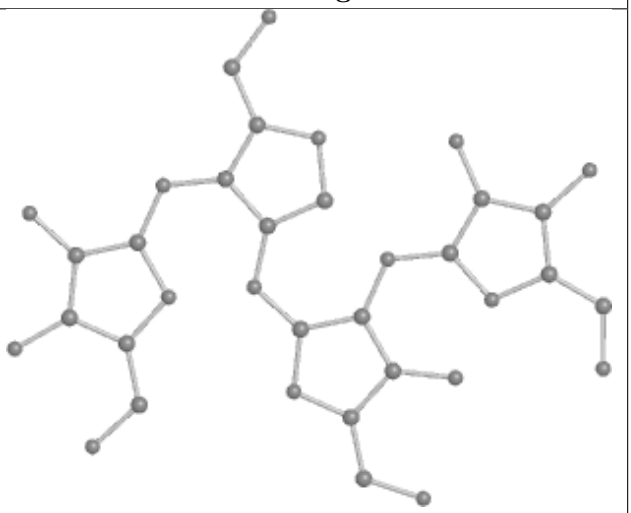
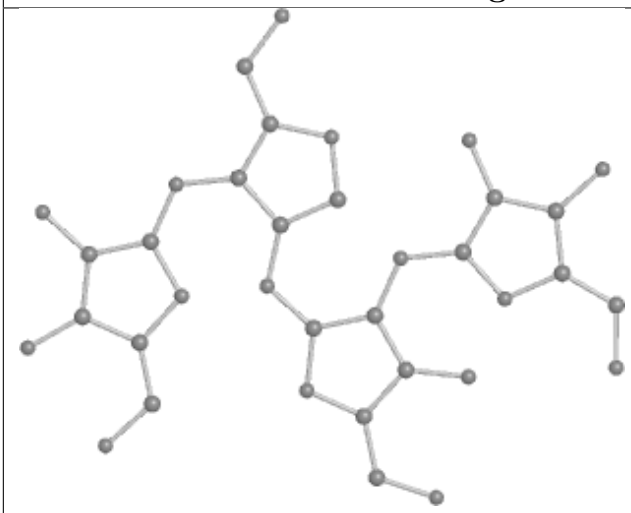
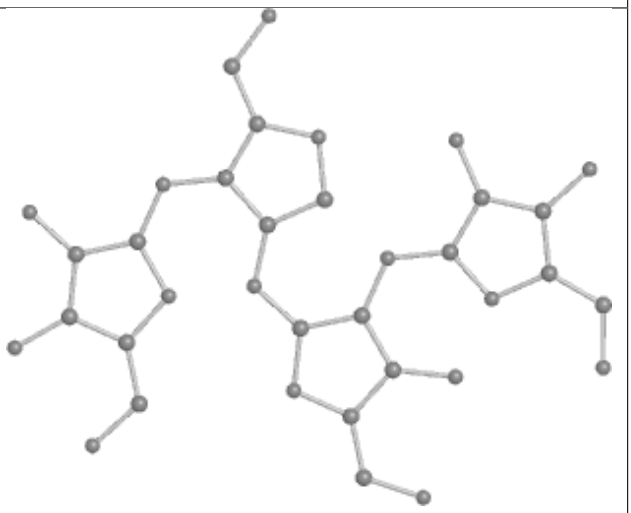
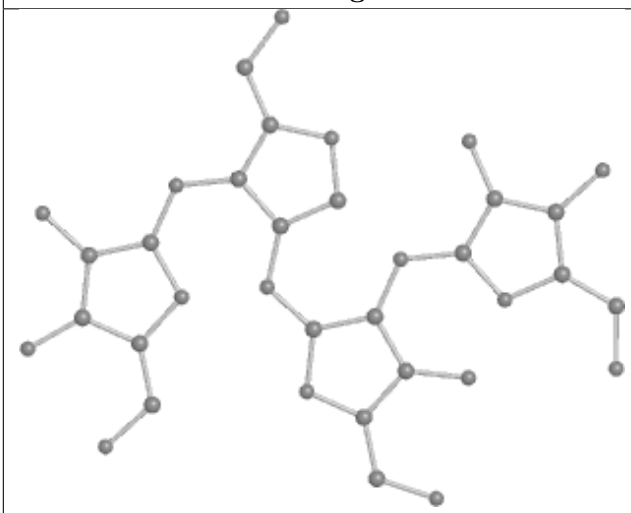
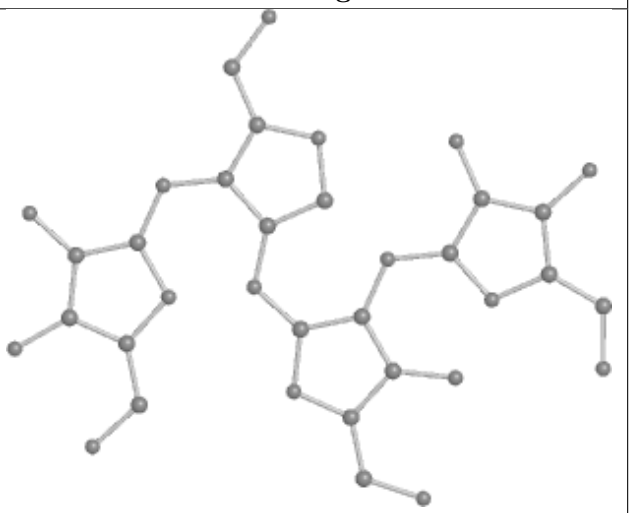
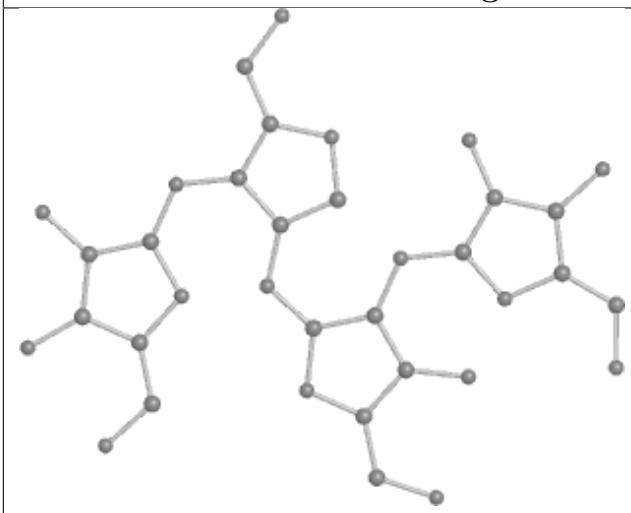
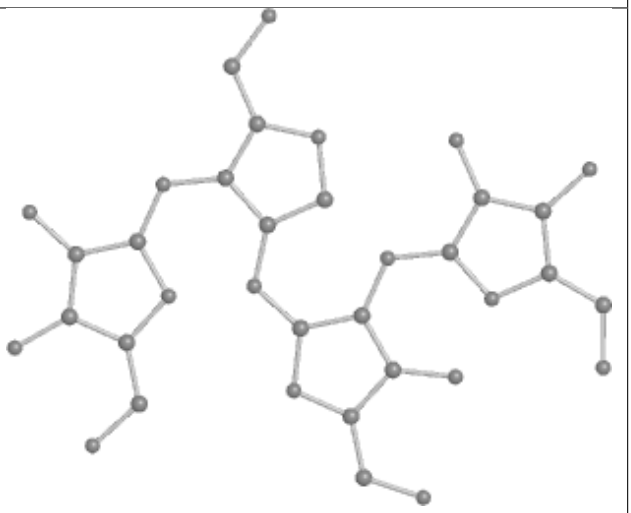
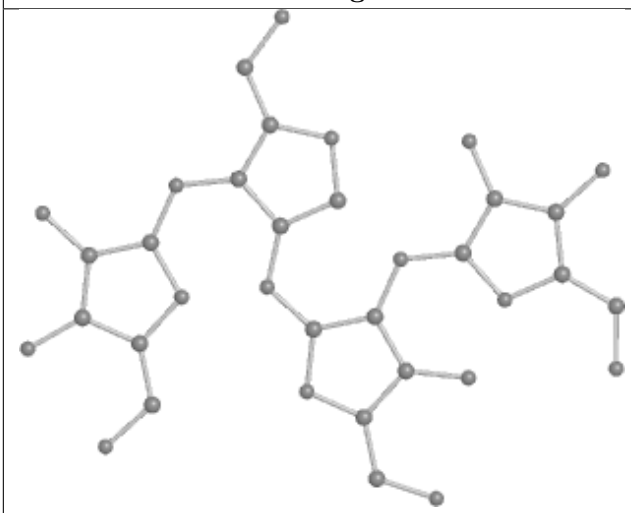
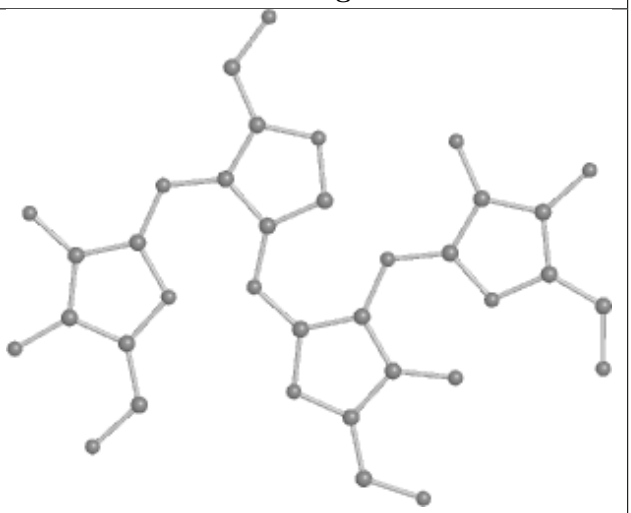
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain fA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain KC	
 Bond lengths	 Bond angles
 Torsions	 Rings

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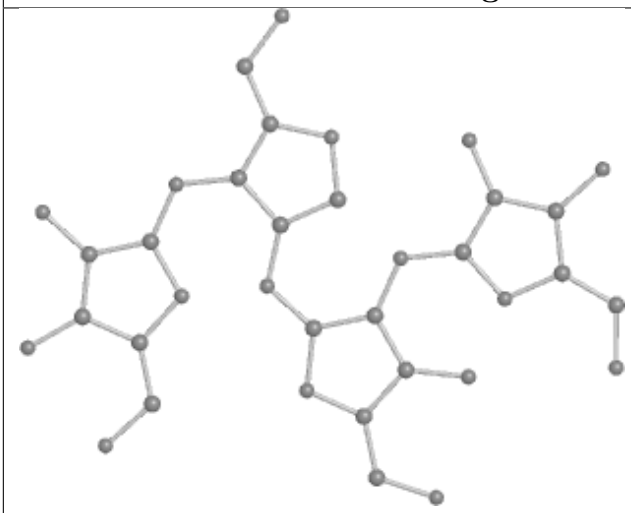
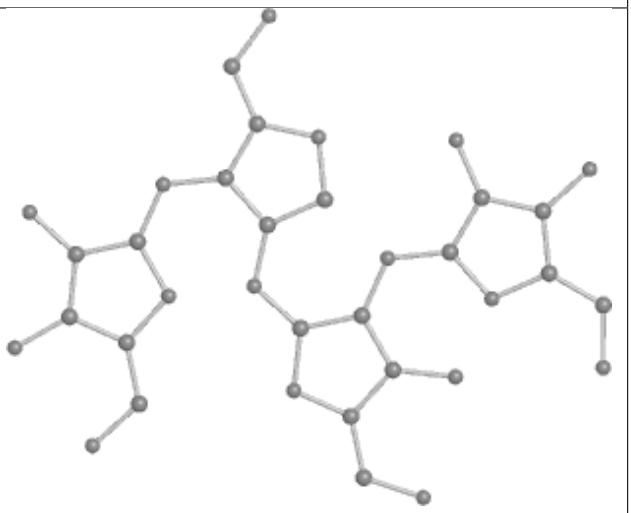
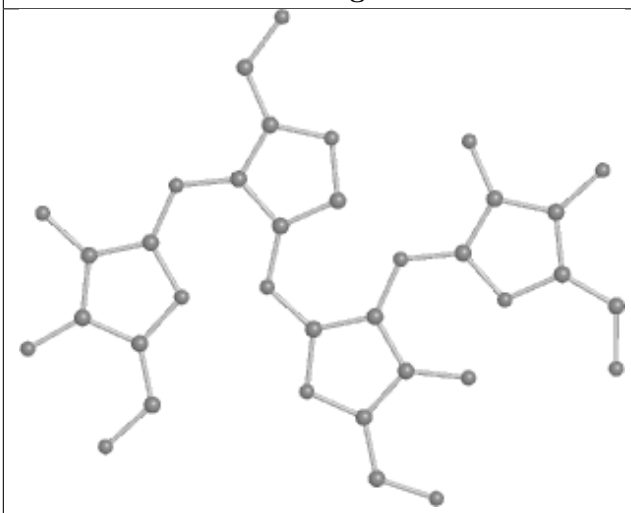
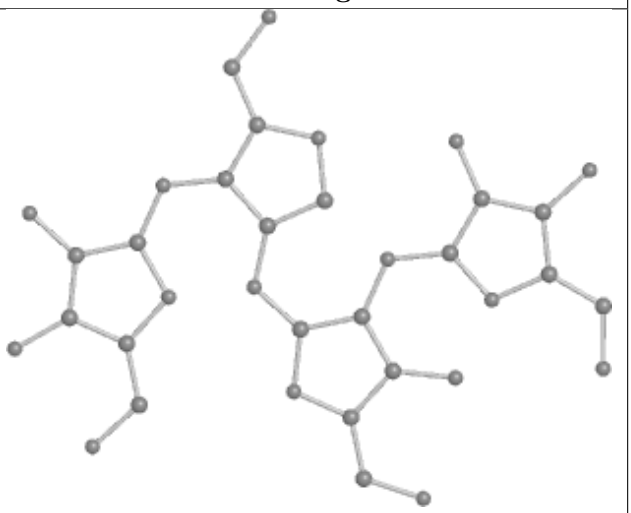
 Bond lengths	 Bond angles
 Torsions	 Rings

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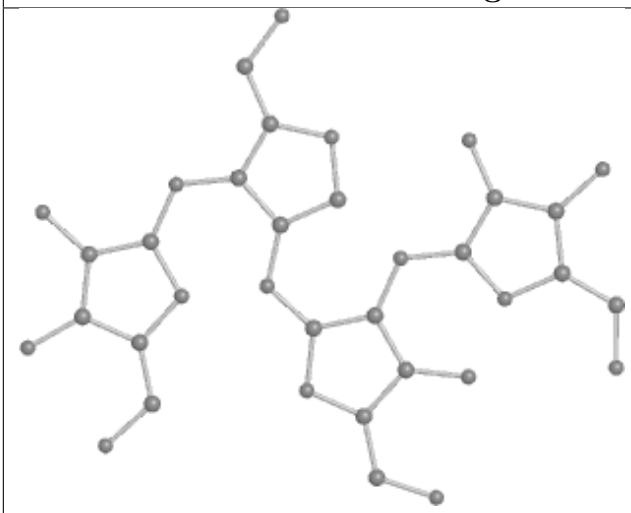
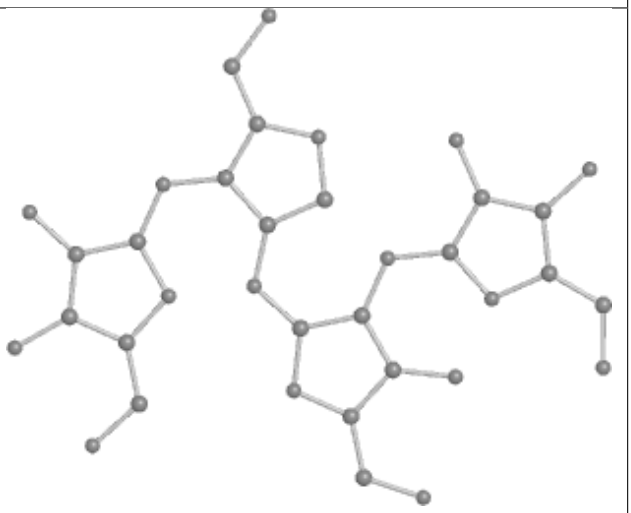
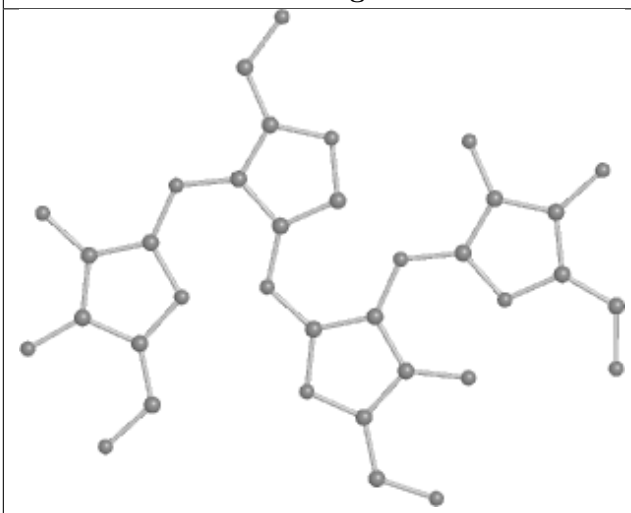
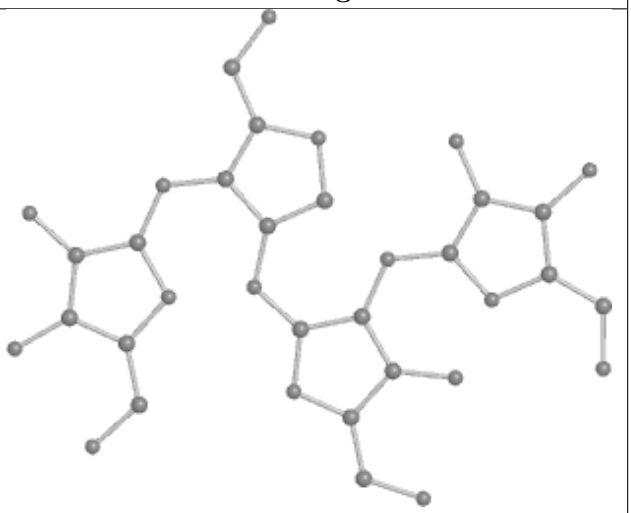
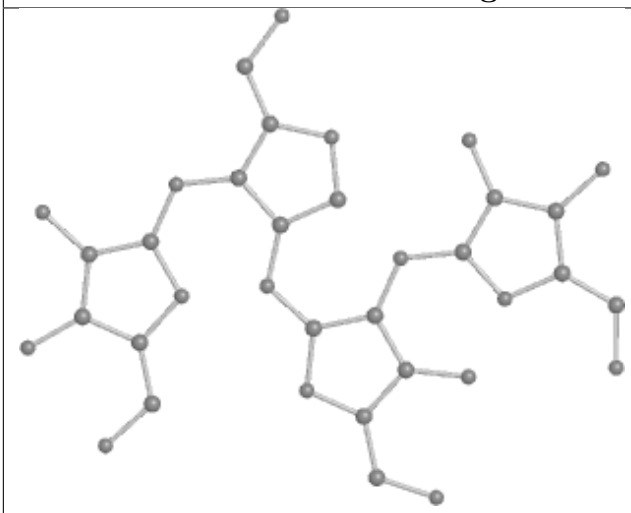
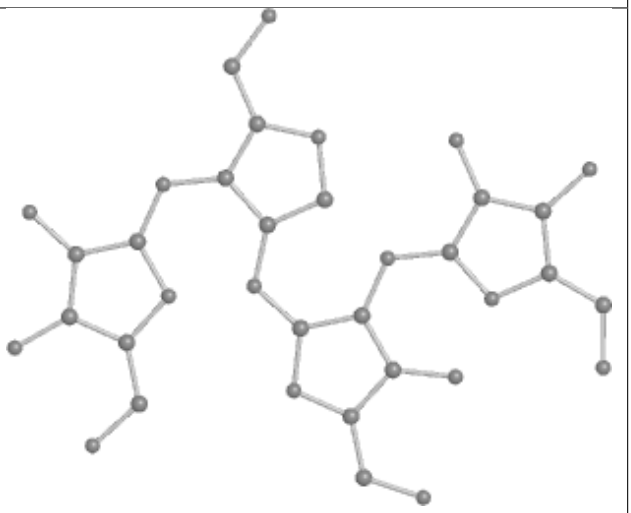
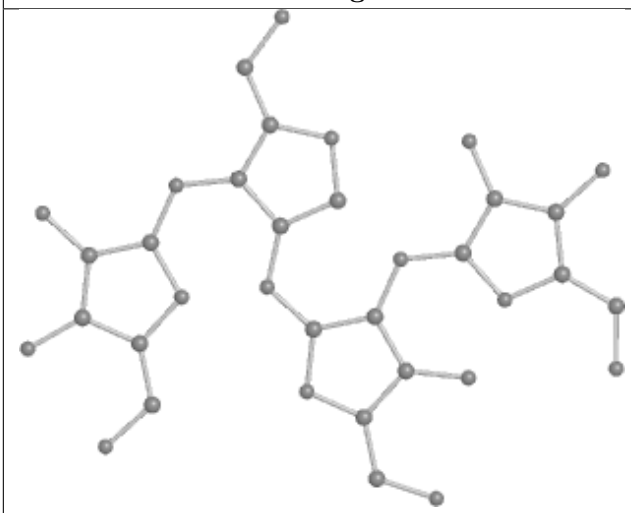
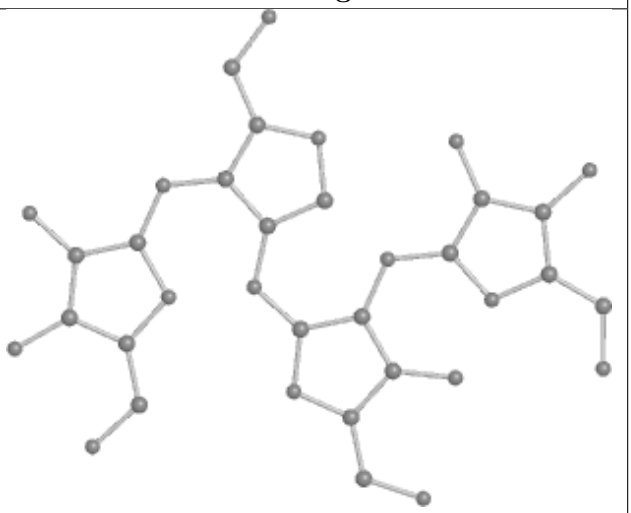
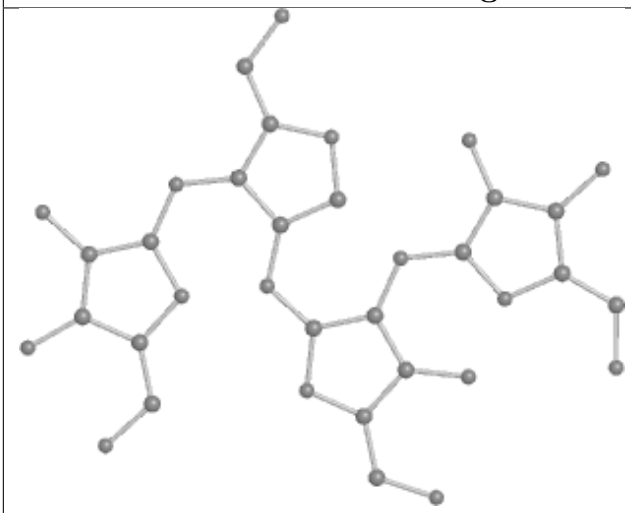
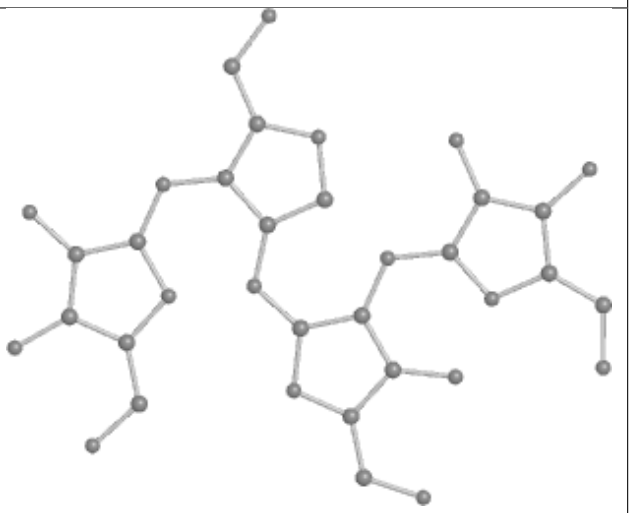
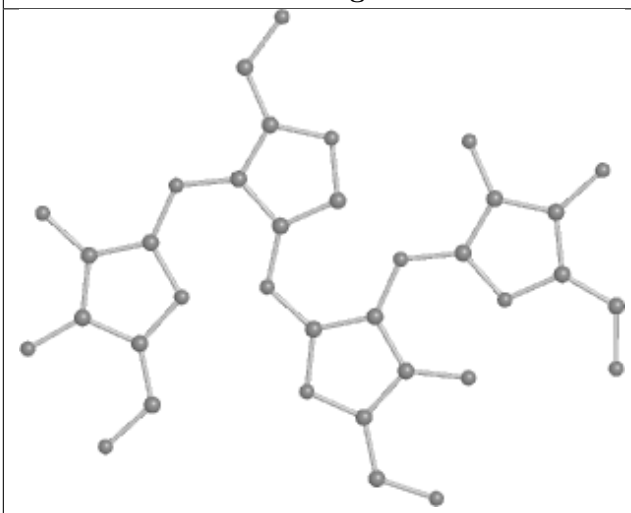
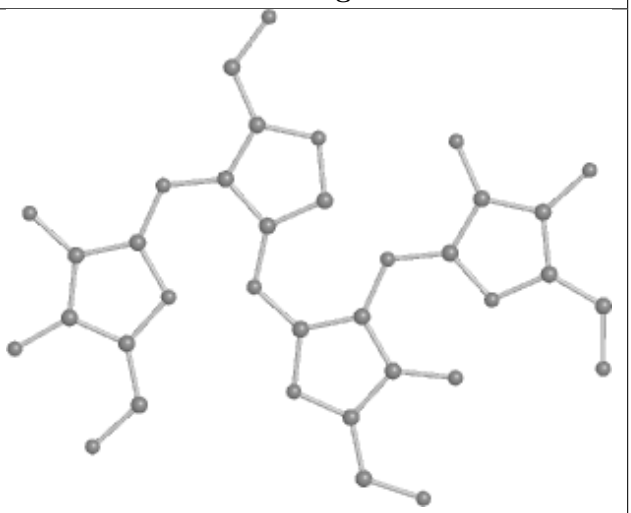
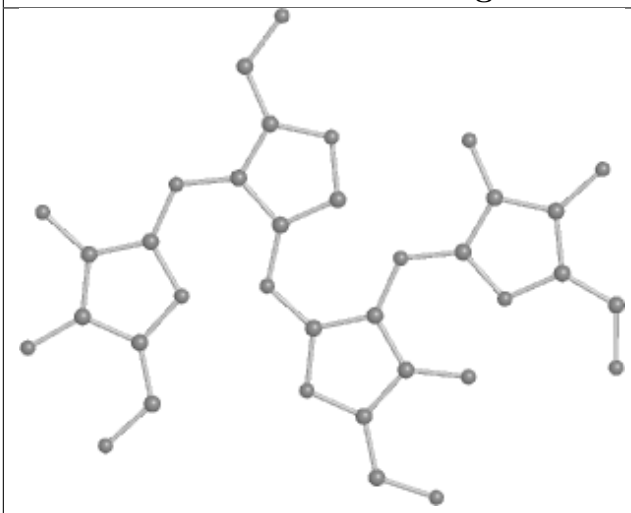
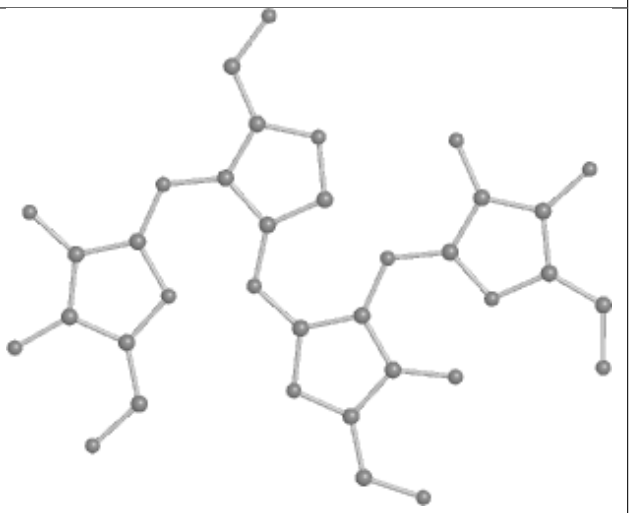
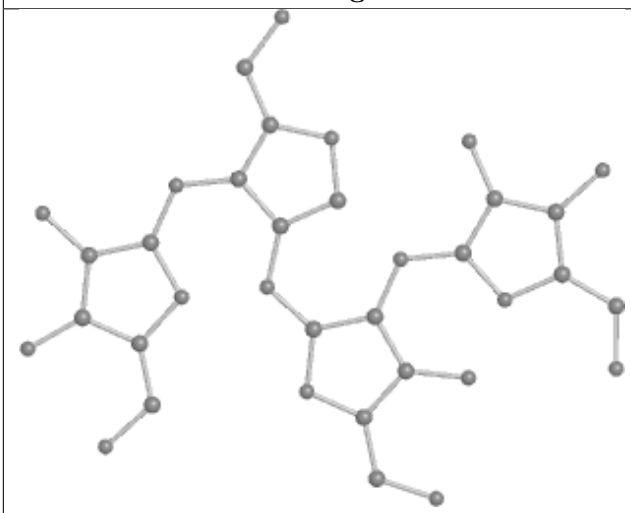
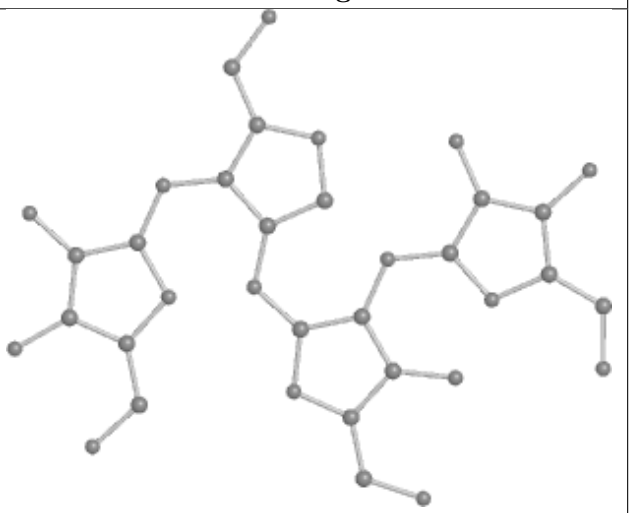
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain HD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain UD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain WD	
 Bond lengths	 Bond angles
 Torsions	 Rings

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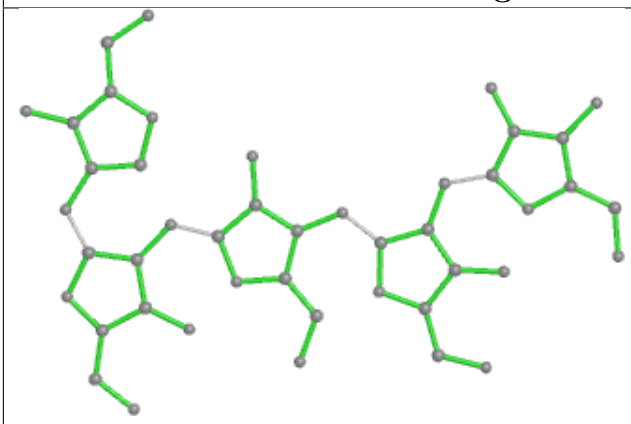
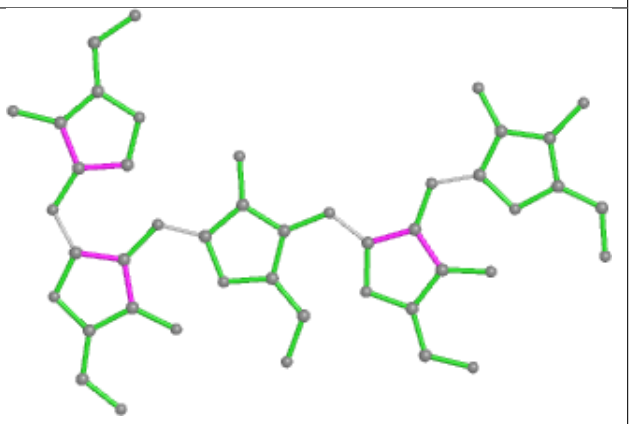
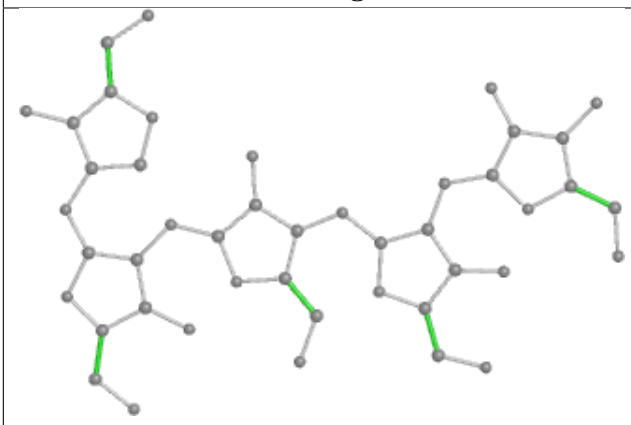
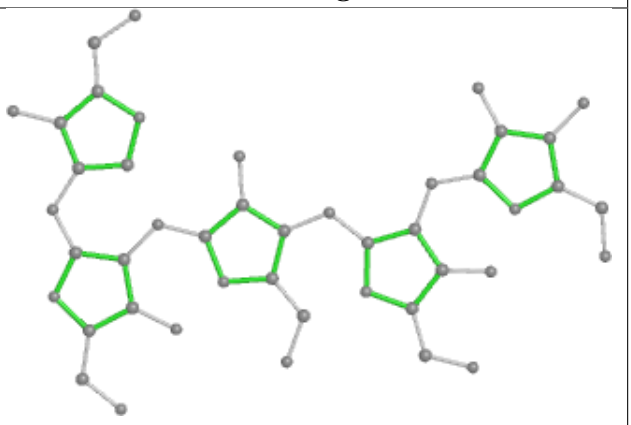
 Bond lengths	 Bond angles
 Torsions	 Rings

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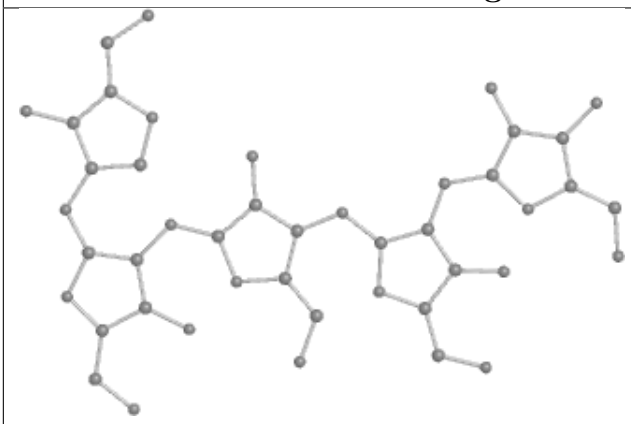
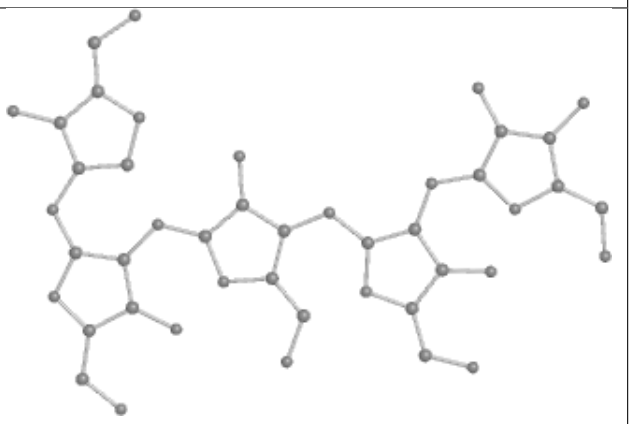
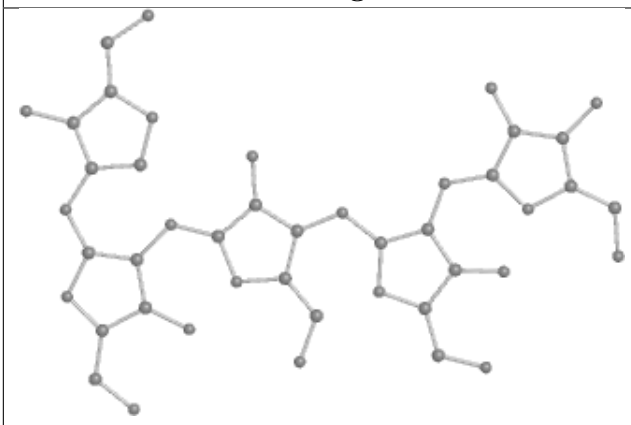
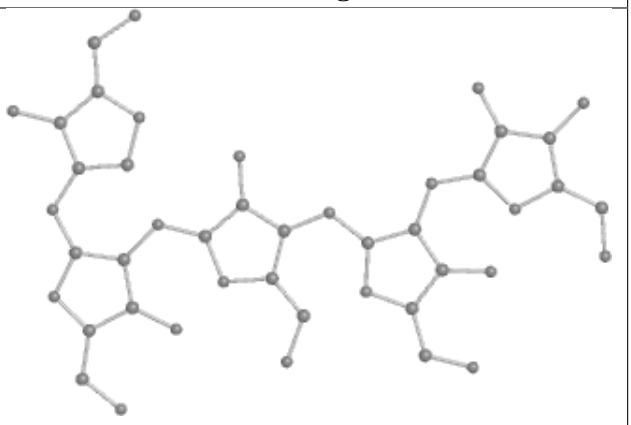
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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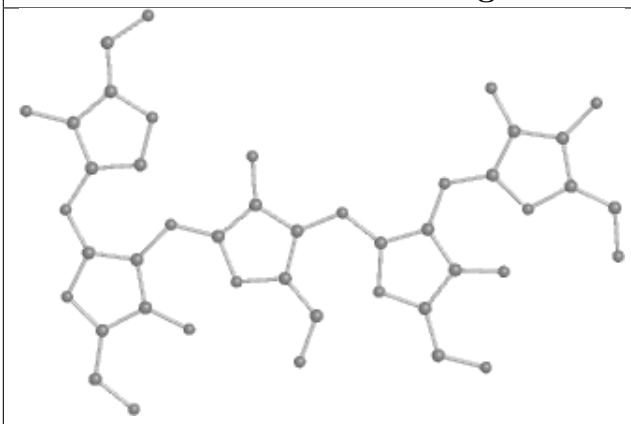
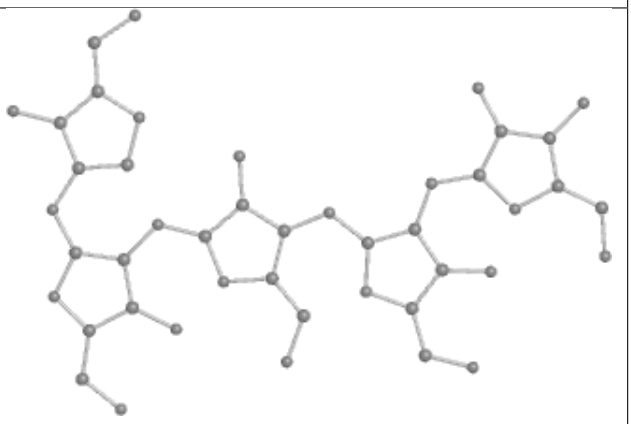
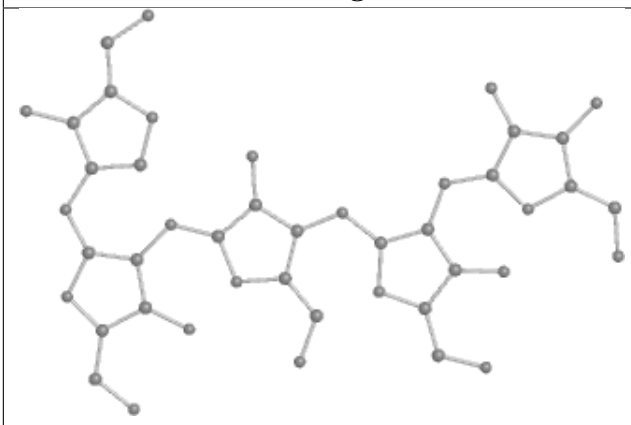
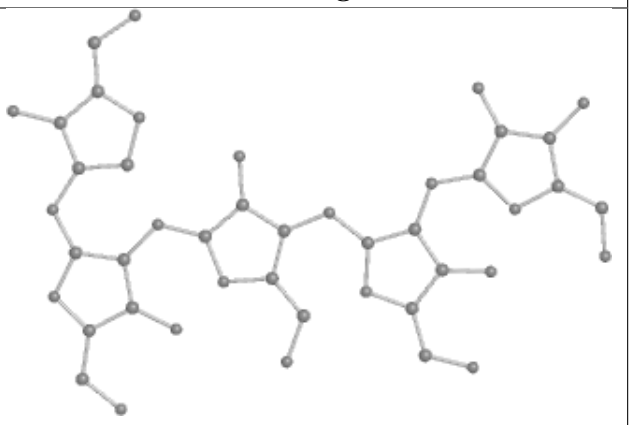
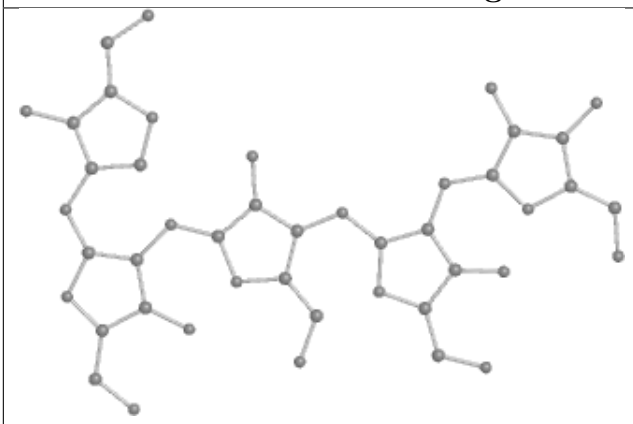
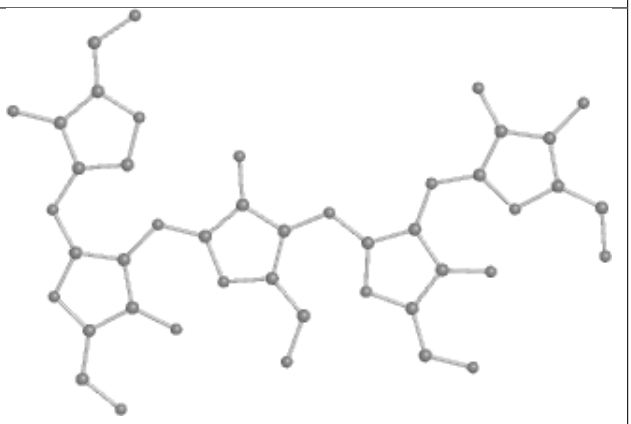
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

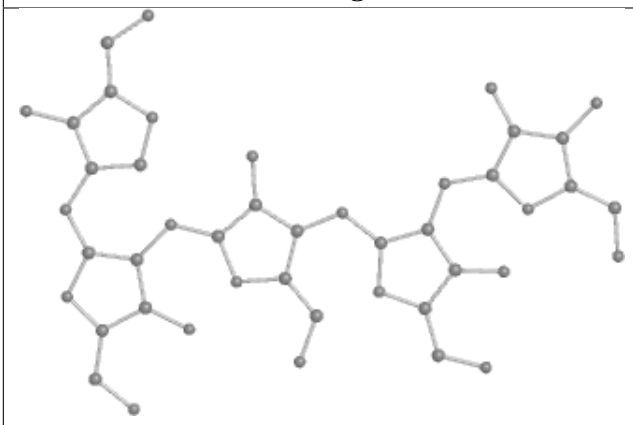
Oligosaccharide Chain JD



Bond lengths



Bond angles



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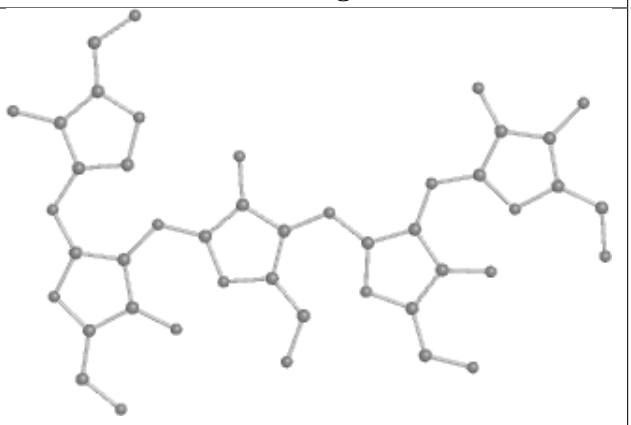
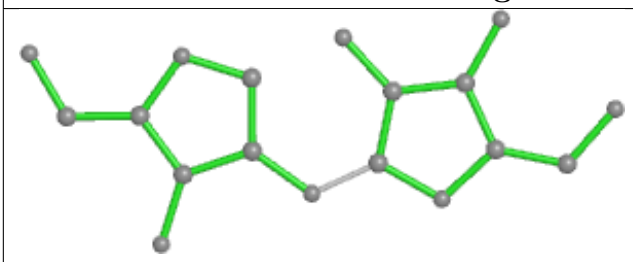


Rings

Oligosaccharide Chain Y



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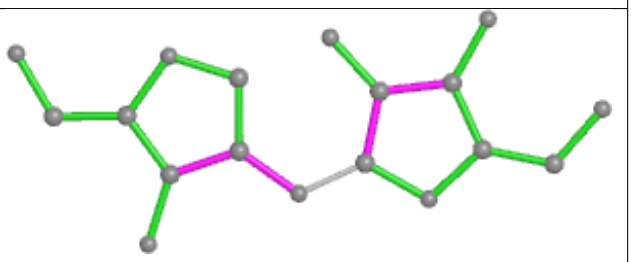

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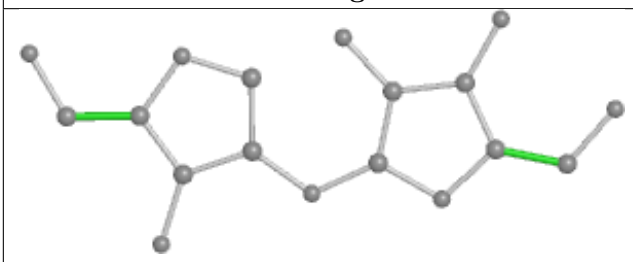

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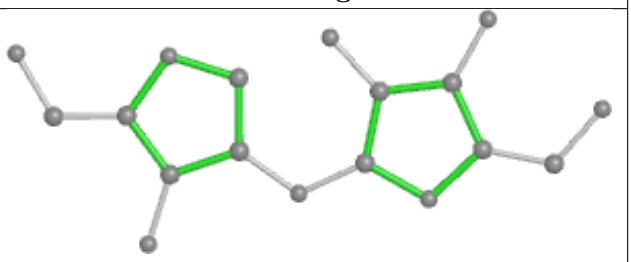
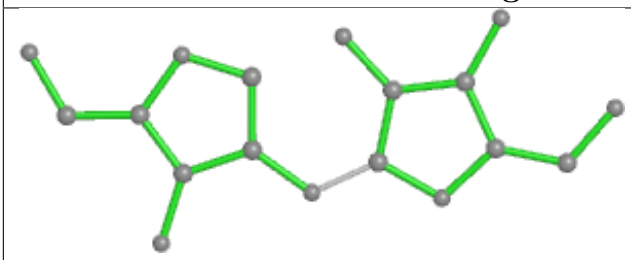
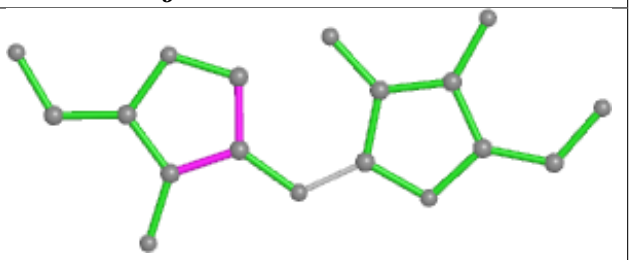
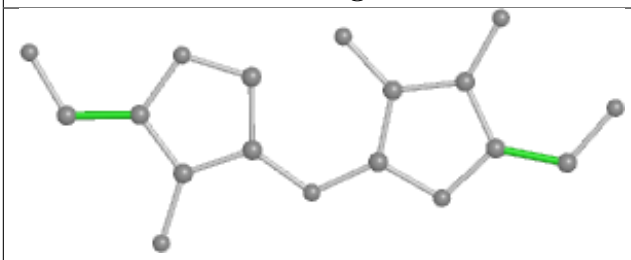
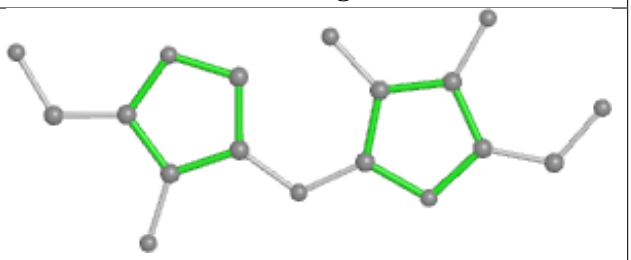


Rings

Oligosaccharide Chain j	
 Bond lengths	 Bond angles
 Torsions	 Rings

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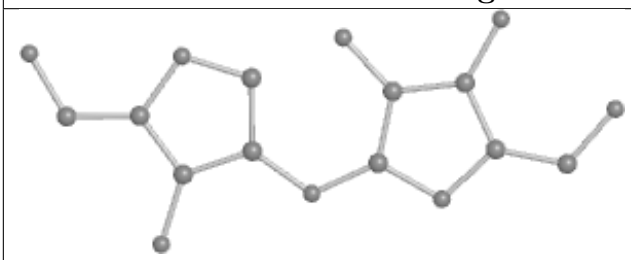
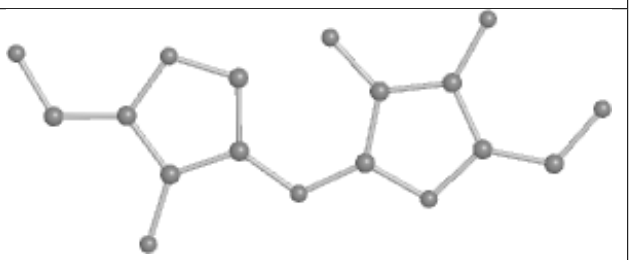
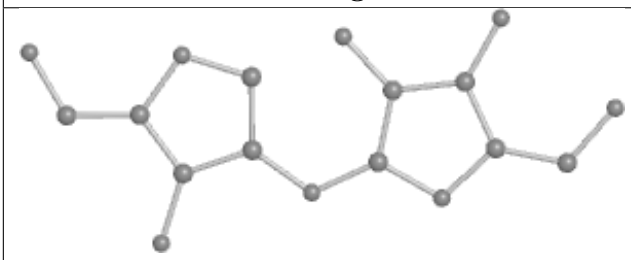
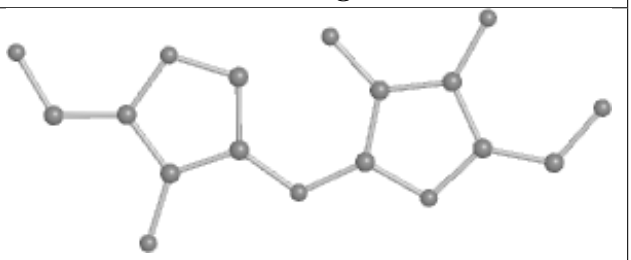
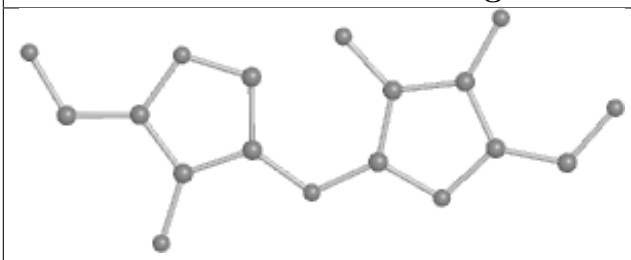
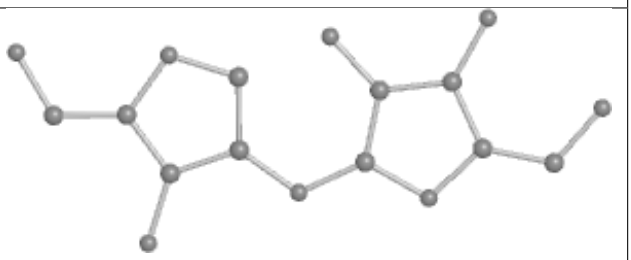
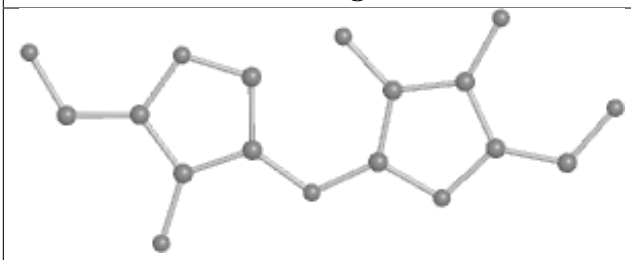
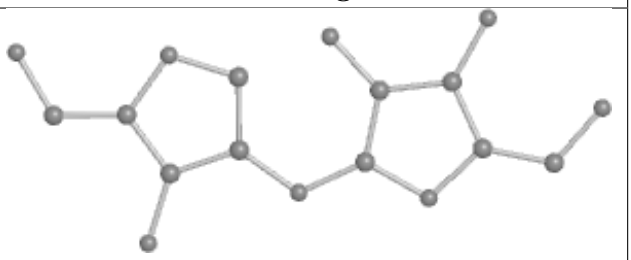
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain hA	
 Bond lengths	 Bond angles
 Torsions	 Rings

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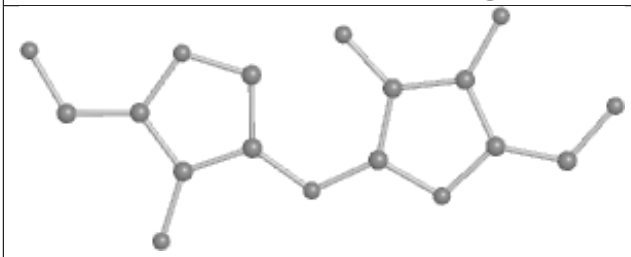
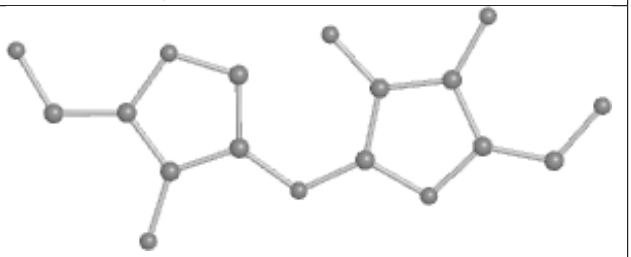
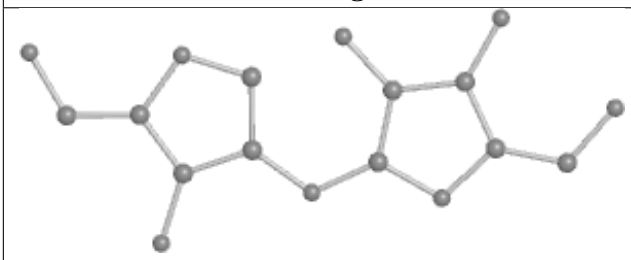
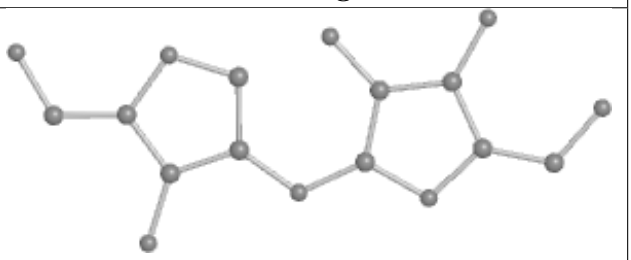
 Bond lengths	 Bond angles
 Torsions	 Rings

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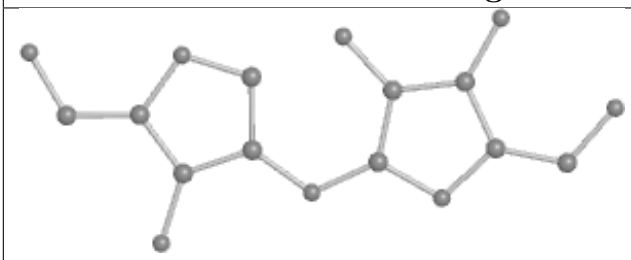
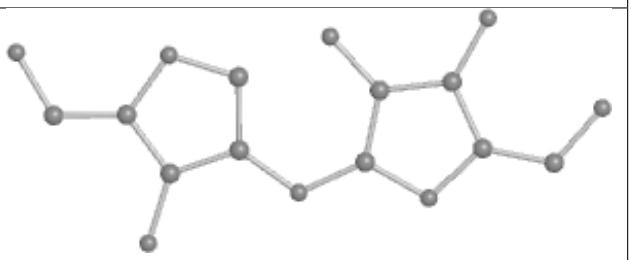
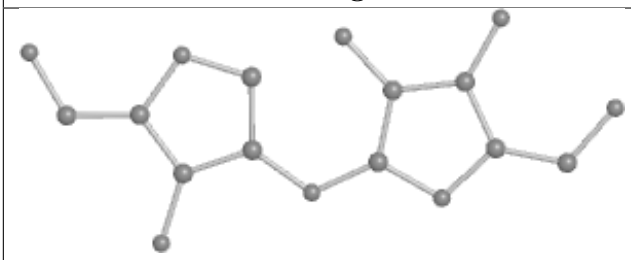
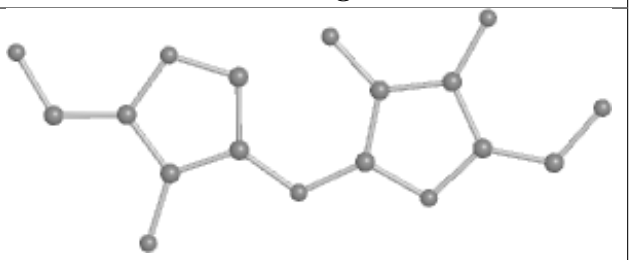
 Bond lengths	 Bond angles
 Torsions	 Rings

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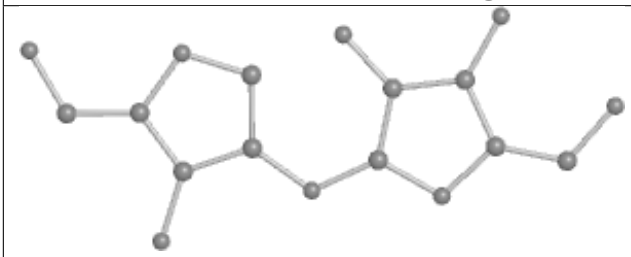
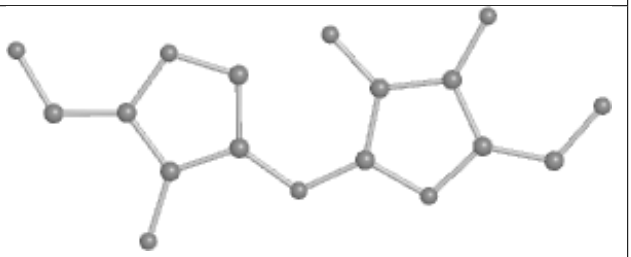
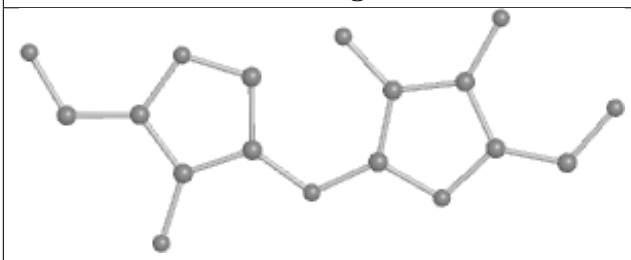
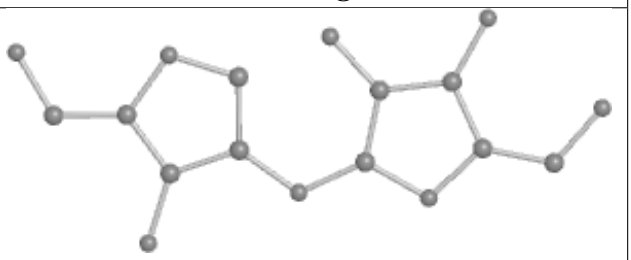
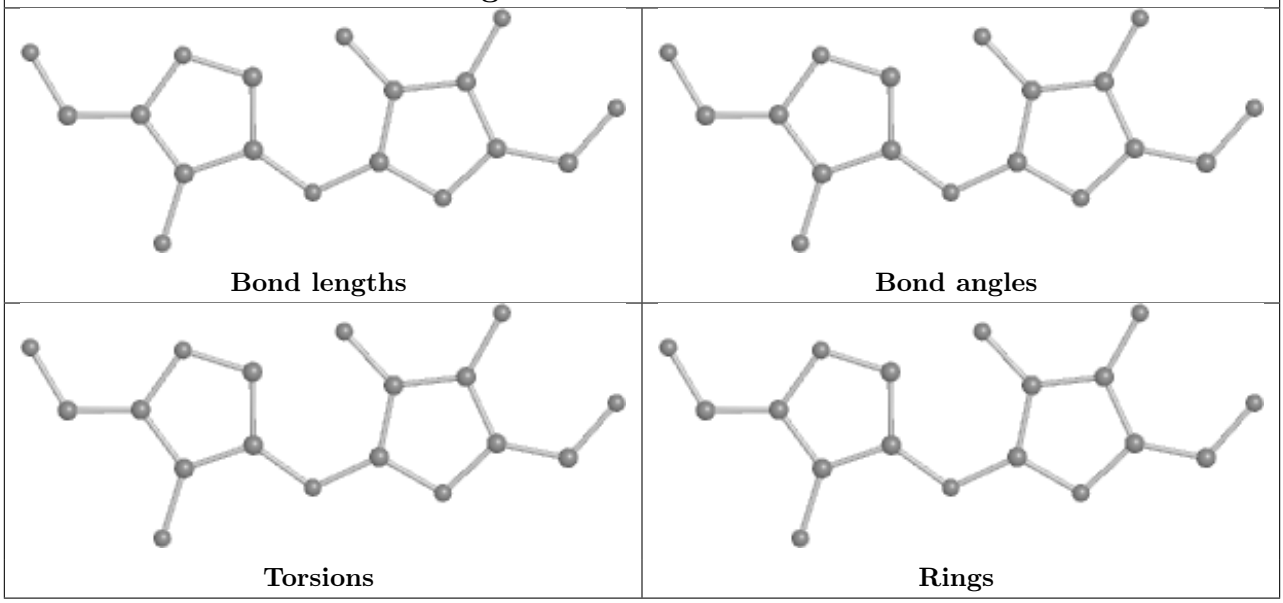
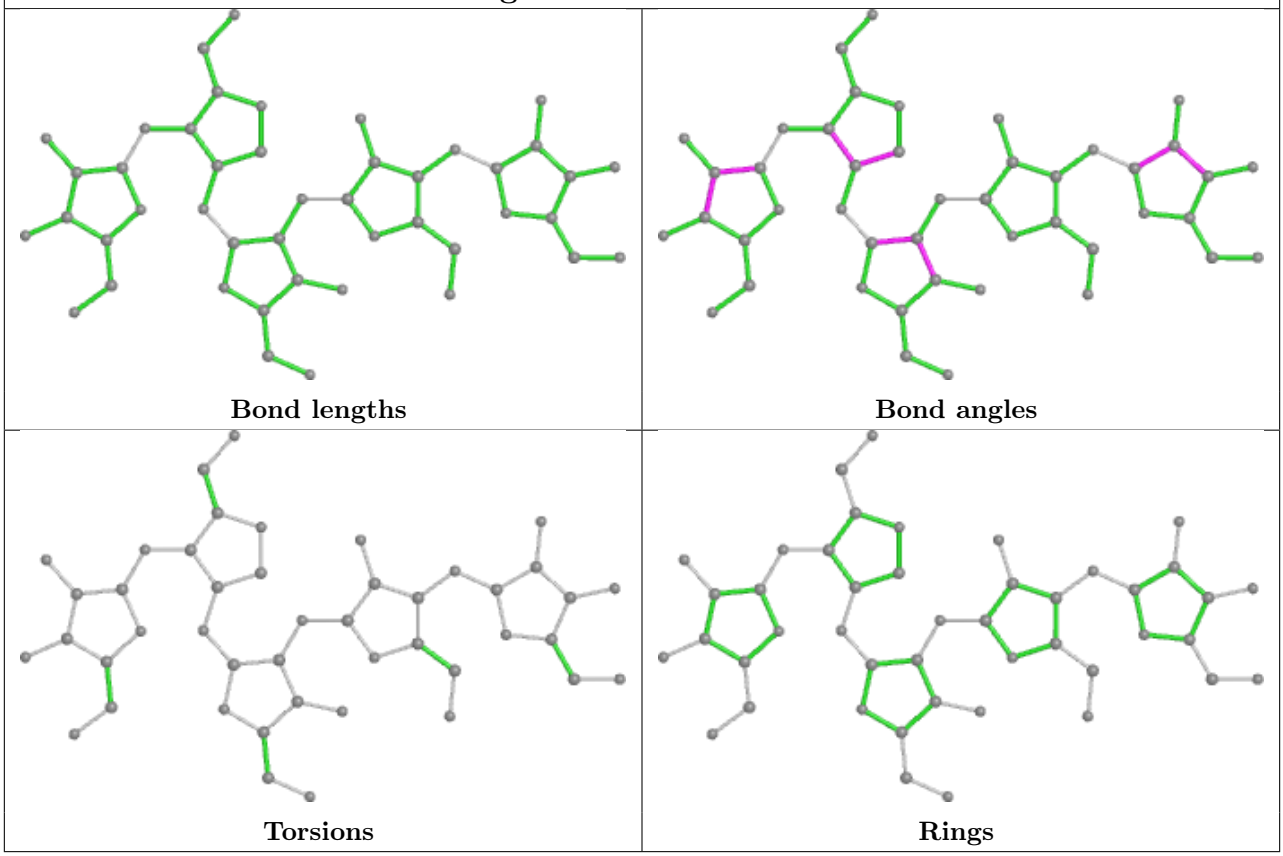
 Bond lengths	 Bond angles
 Torsions	 Rings

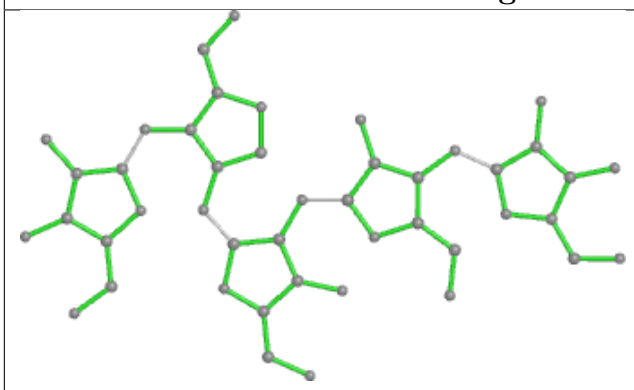
Oligosaccharide Chain YD



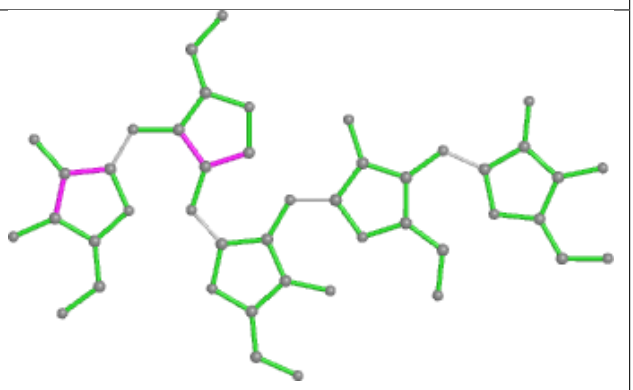
Oligosaccharide Chain a



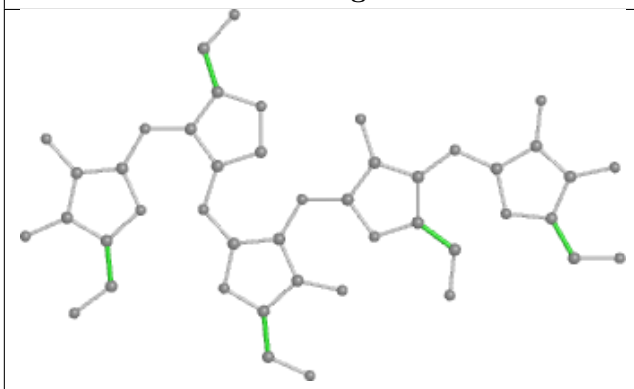
Oligosaccharide Chain u



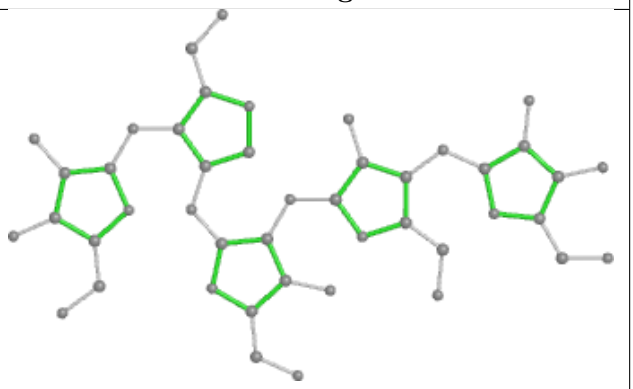
Bond lengths



Bond angles

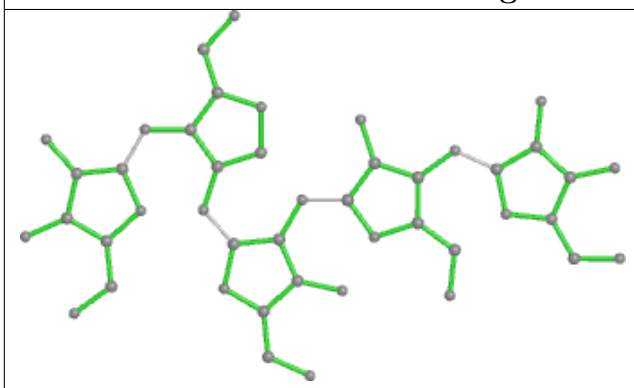


Torsions



Rings

Oligosaccharide Chain 3



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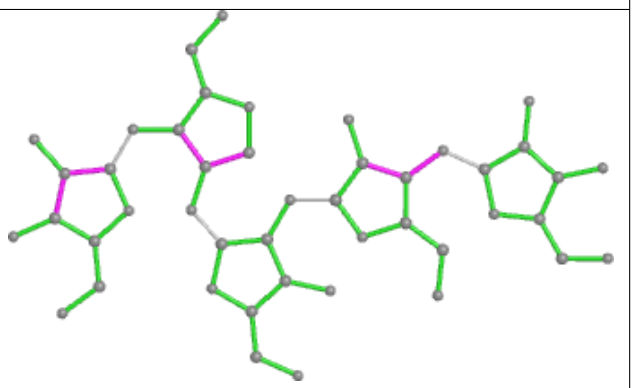
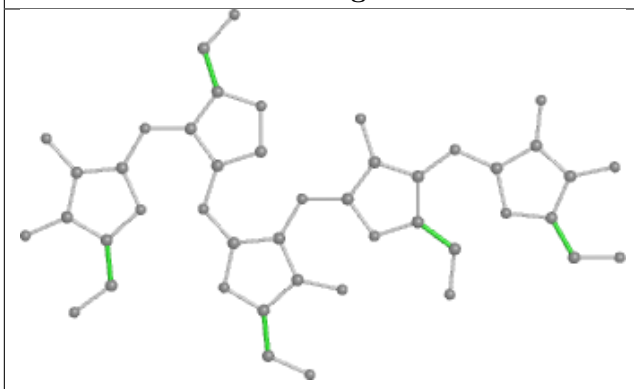


Bond angles



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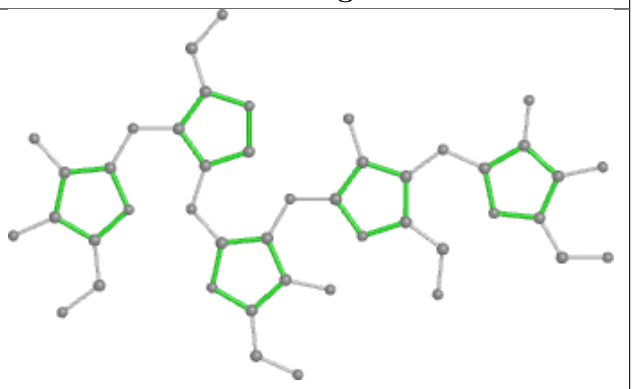
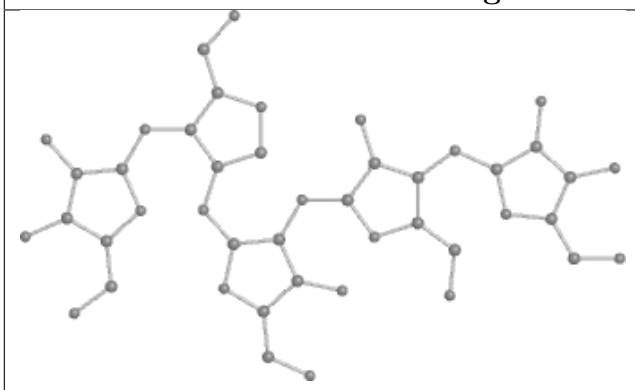
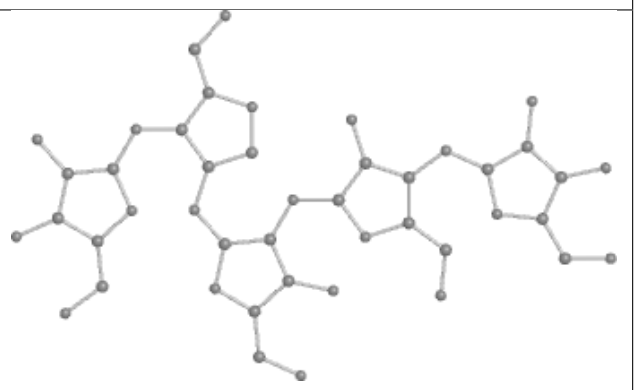


Rings

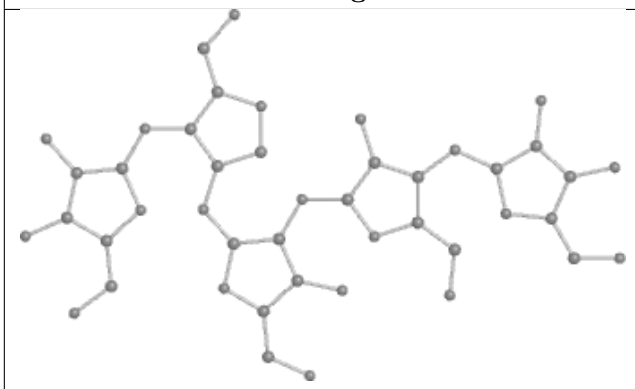
Oligosaccharide Chain YA



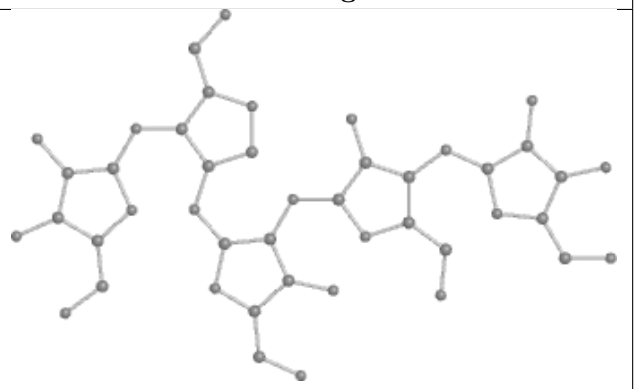
Bond lengths



Bond angles

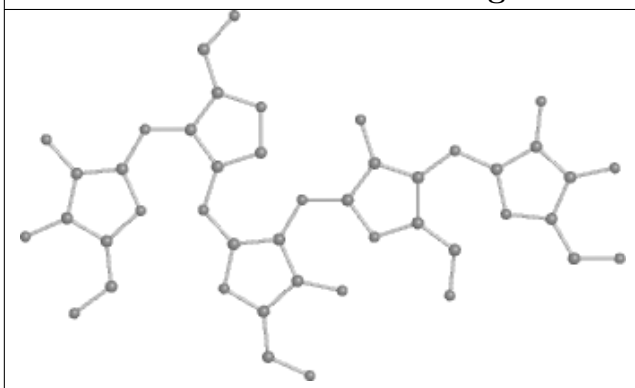


Torsions

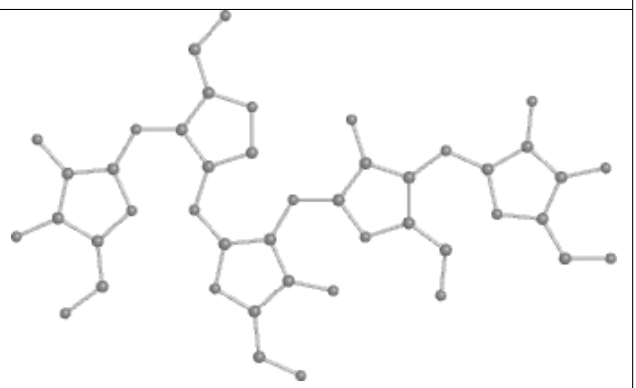


Rings

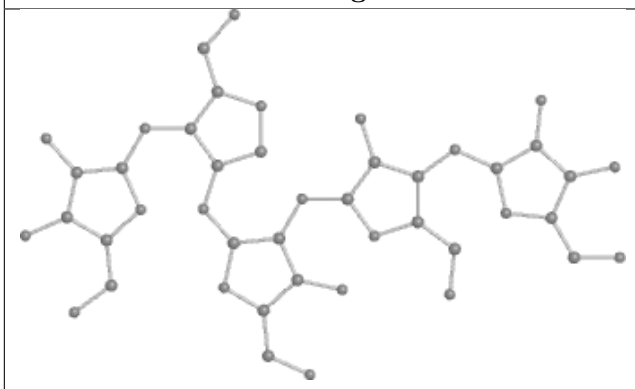
Oligosaccharide Chain sA



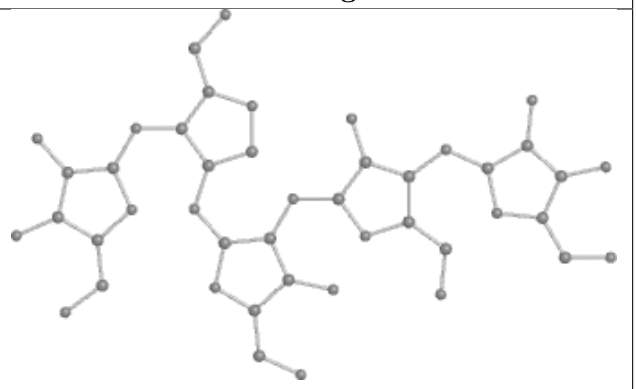
Bond lengths



Bond angles

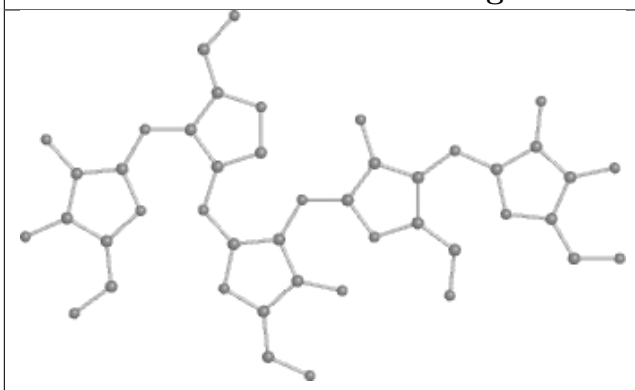


Torsions



Rings

Oligosaccharide Chain 1A



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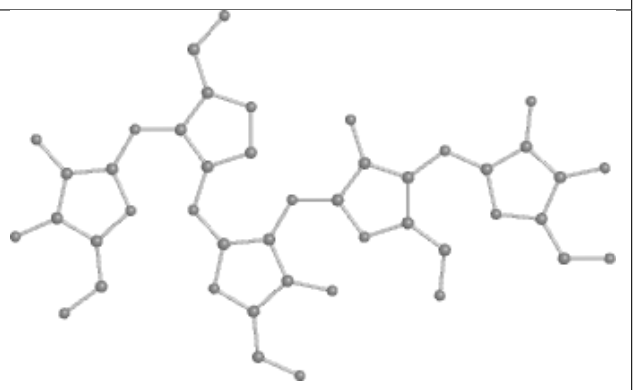

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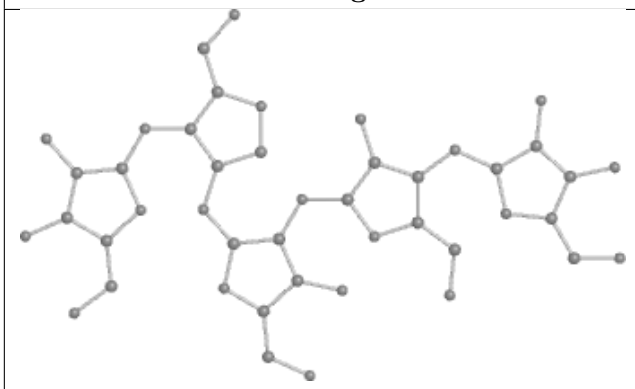

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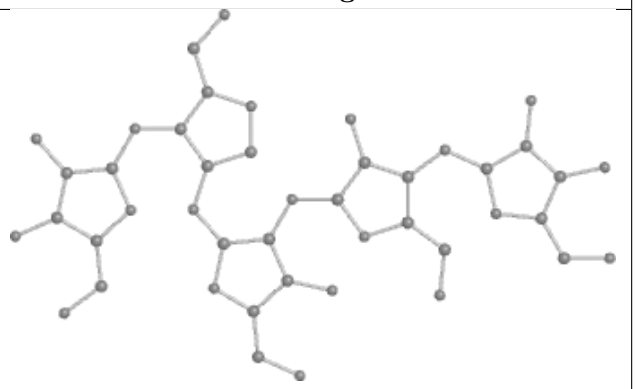
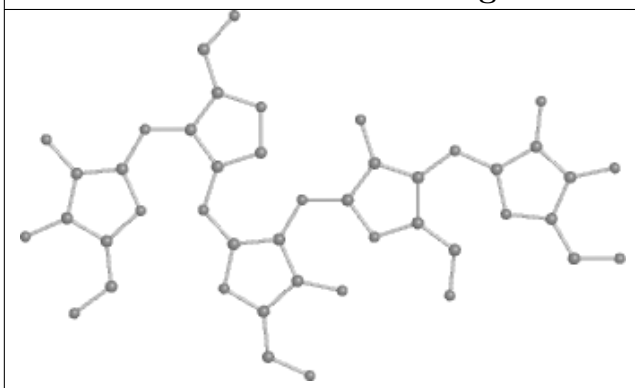


Rings

Oligosaccharide Chain MB



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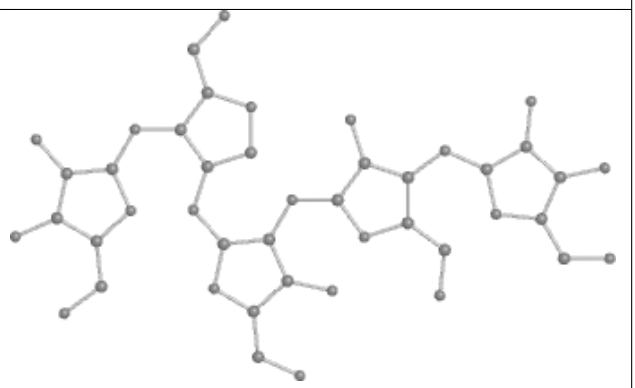

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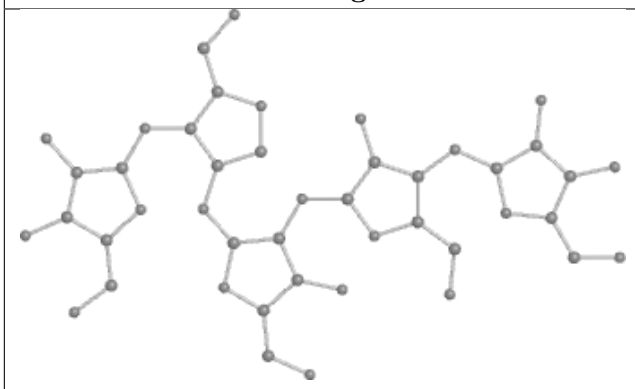

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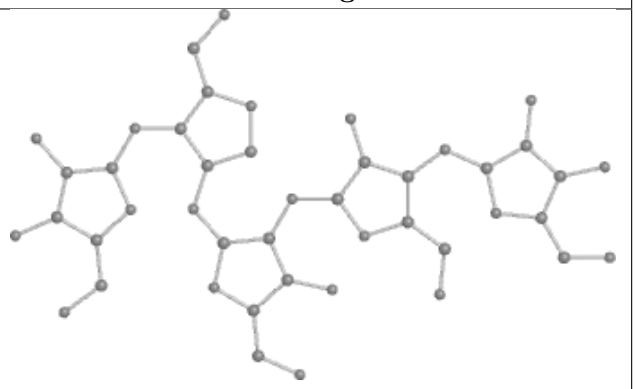
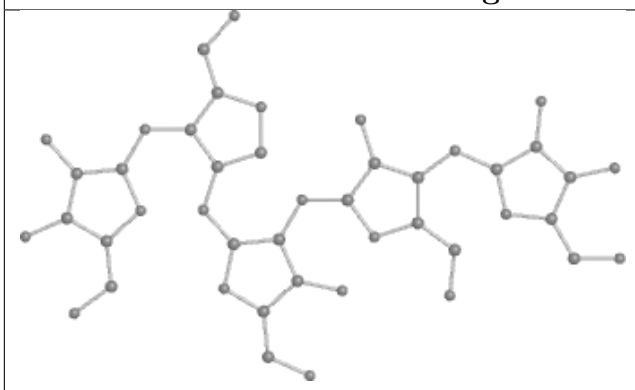
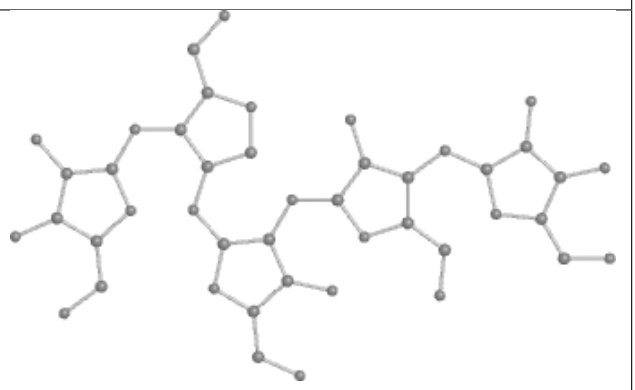


Rings

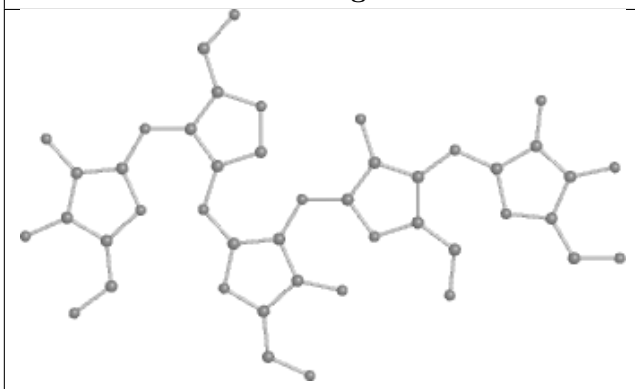
Oligosaccharide Chain VB



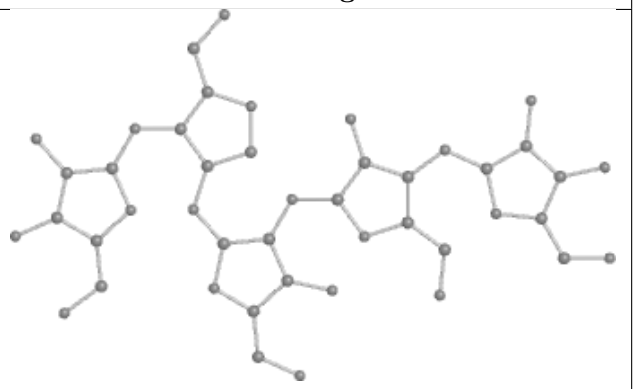
Bond lengths



Bond angles

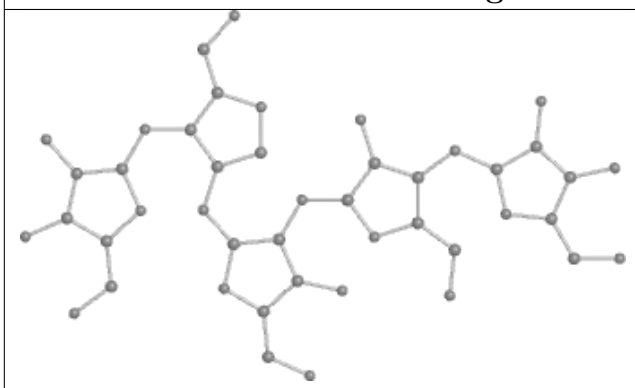


Torsions



Rings

Oligosaccharide Chain pB



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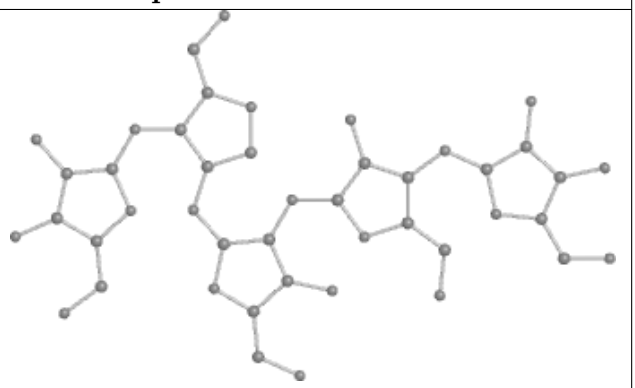
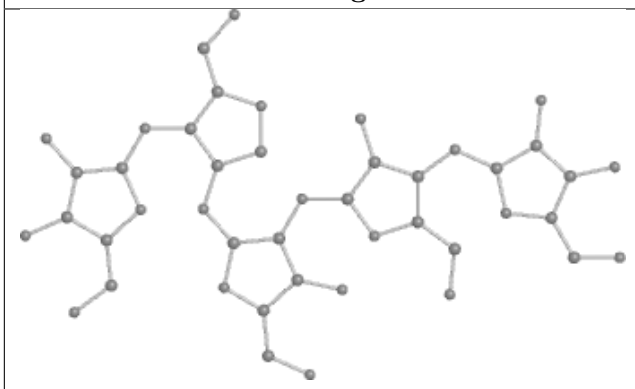


Bond angles



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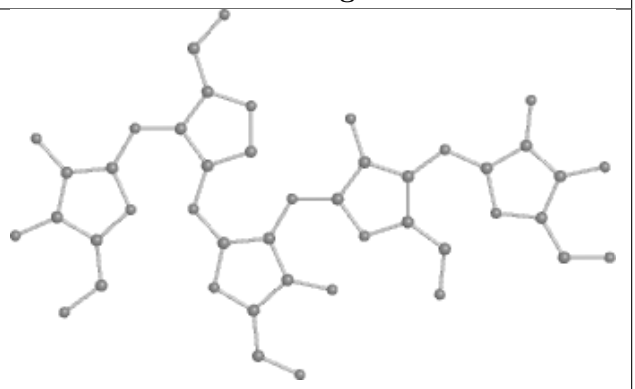
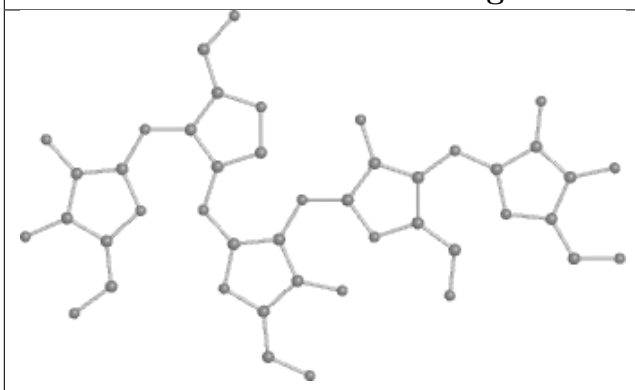


Rings

Oligosaccharide Chain yB



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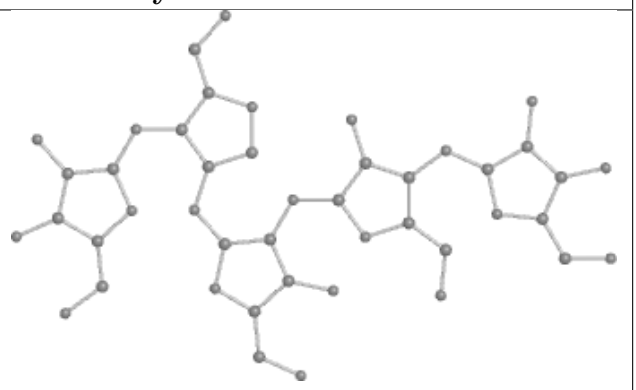
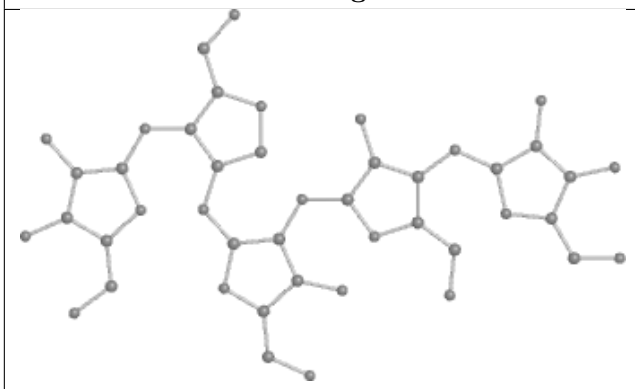
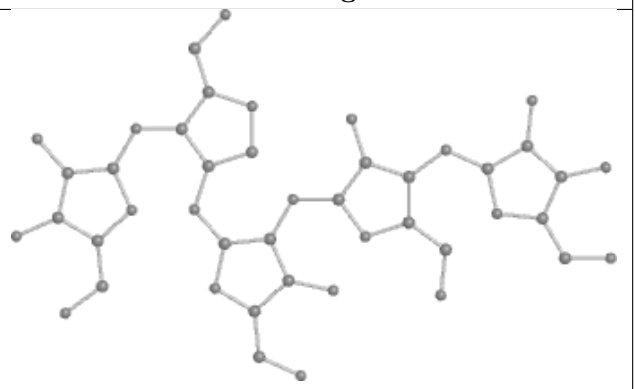


Bond angles

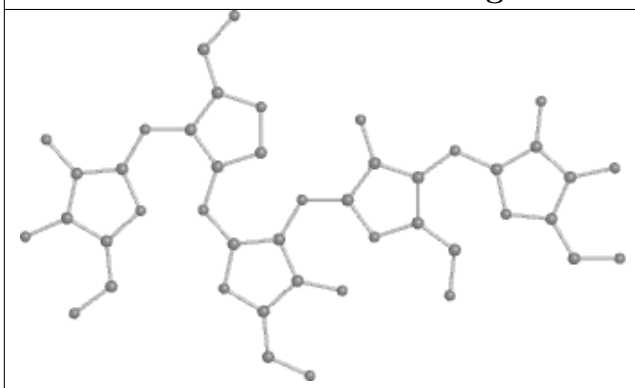


Torsions

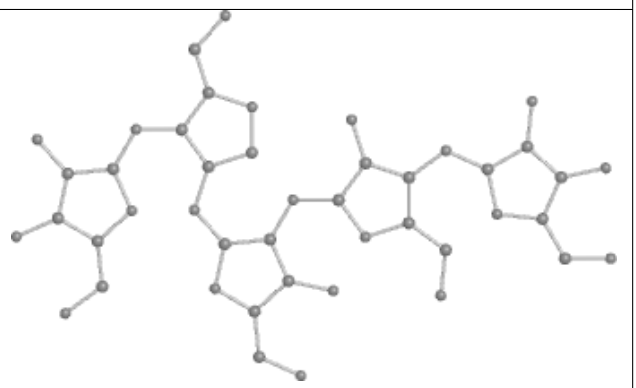


Rings

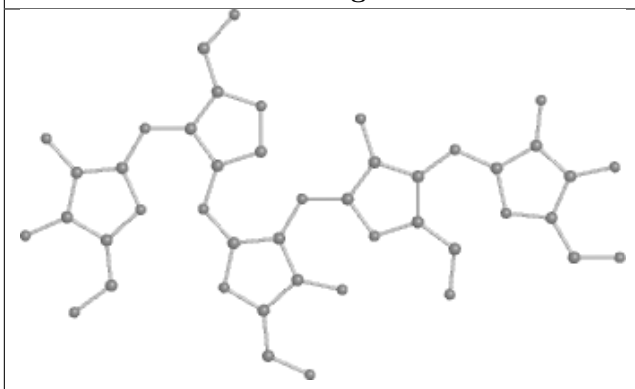
Oligosaccharide Chain SC



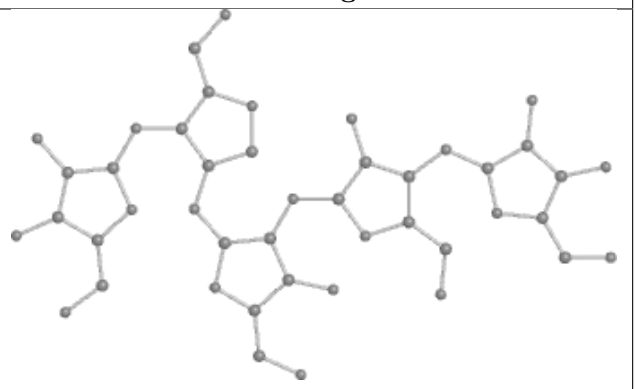
Bond lengths



Bond angles

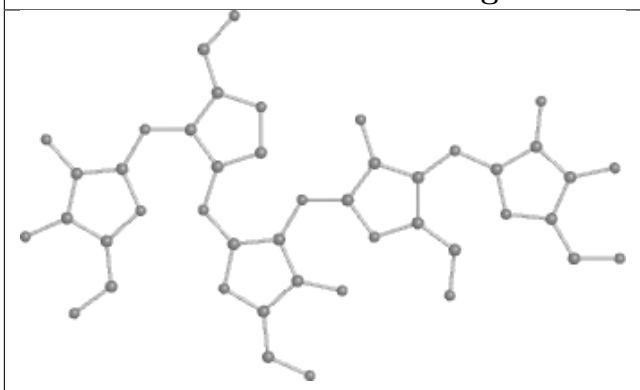


Torsions



Rings

Oligosaccharide Chain mC



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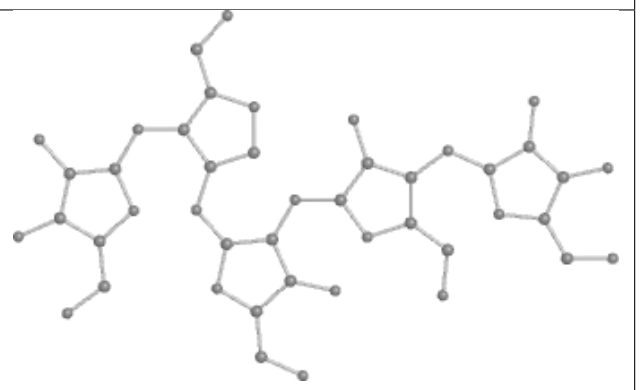
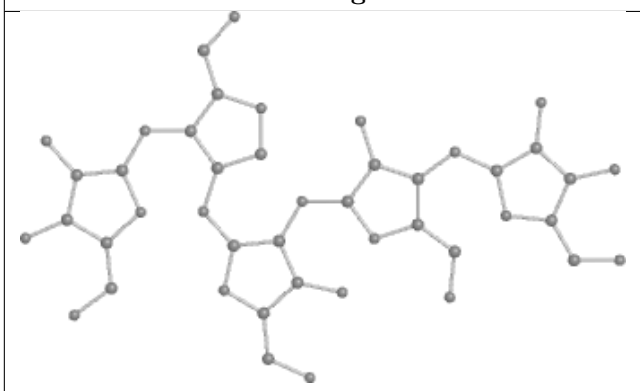


Bond angles



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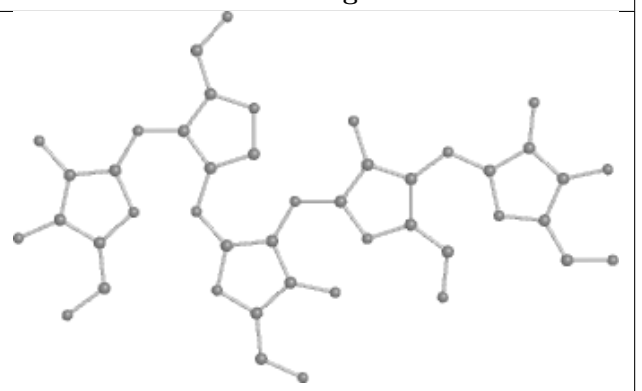
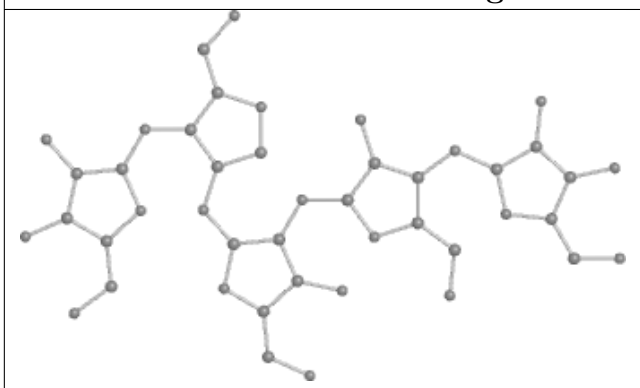
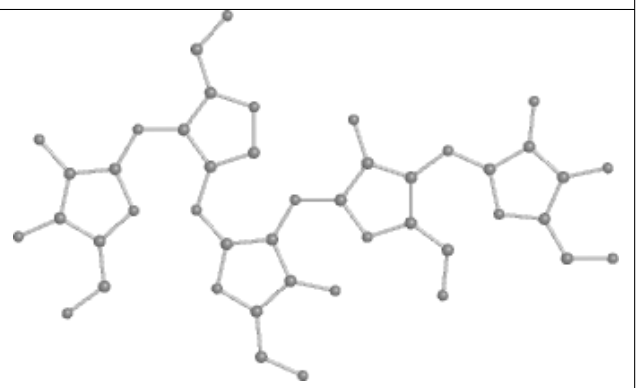


Rings

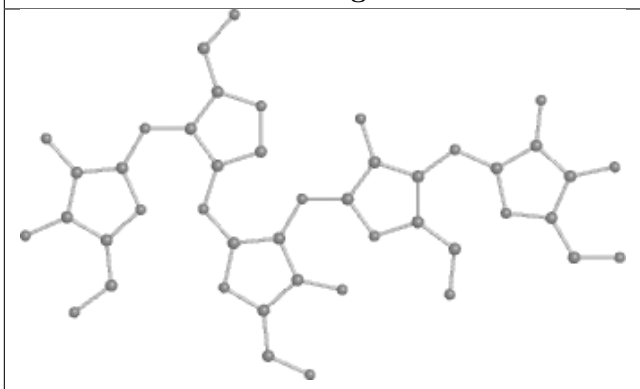
Oligosaccharide Chain vC



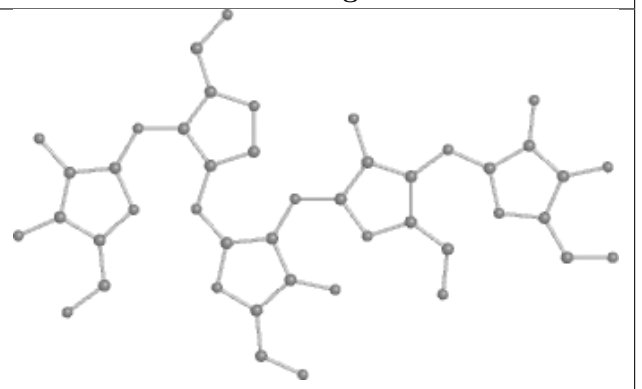
Bond lengths



Bond angles

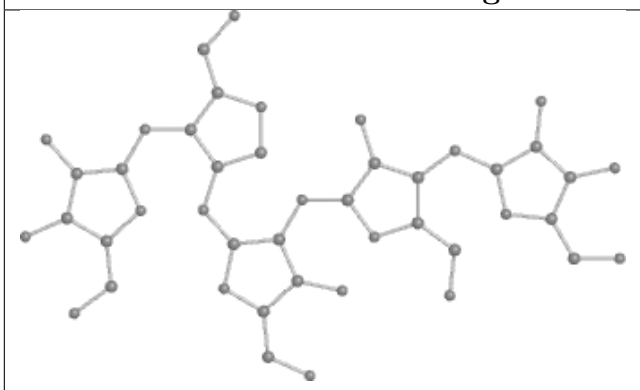


Torsions

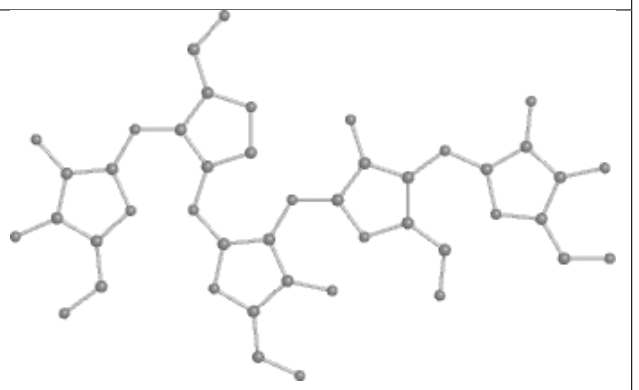


Rings

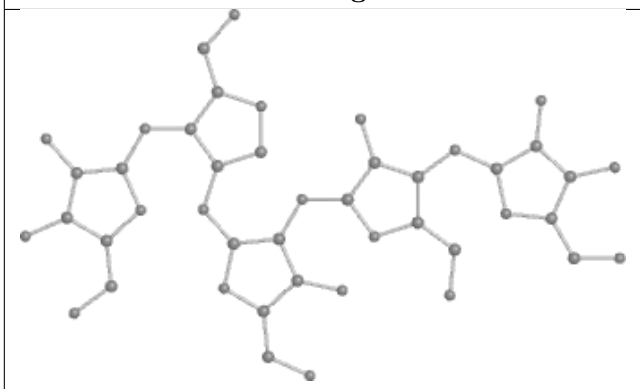
Oligosaccharide Chain PD



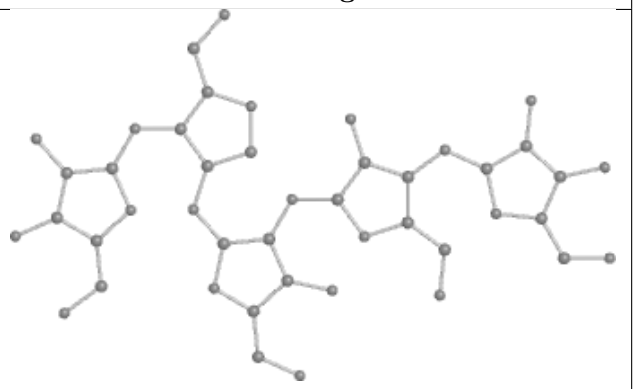
Bond lengths



Bond angles

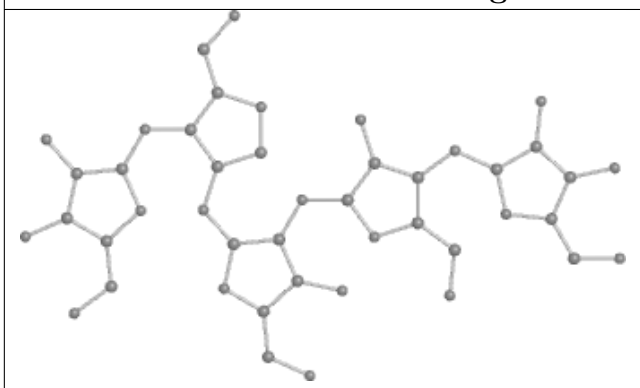


Torsions

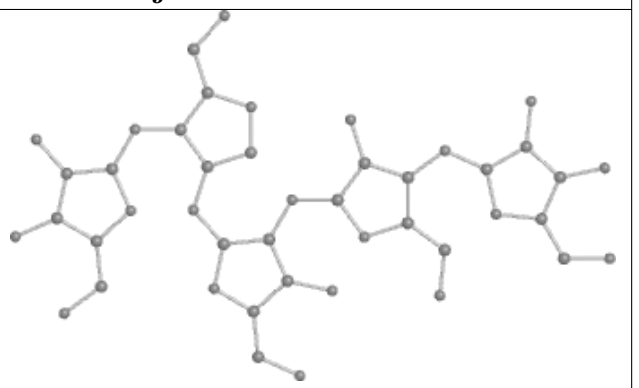


Rings

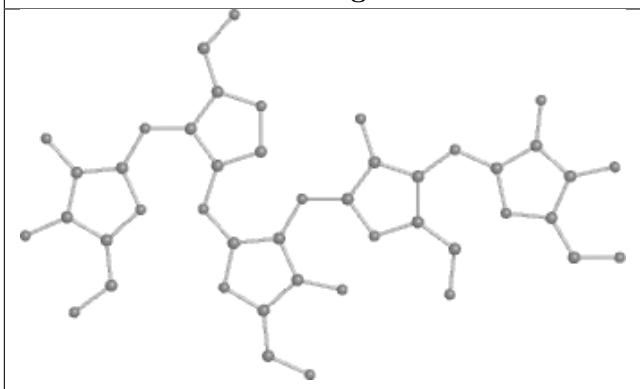
Oligosaccharide Chain jD



Bond lengths



Bond angles



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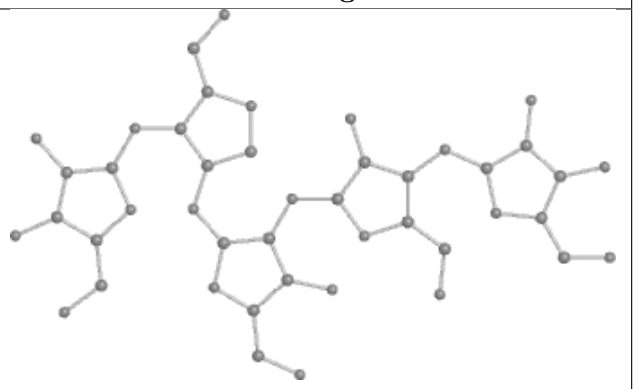
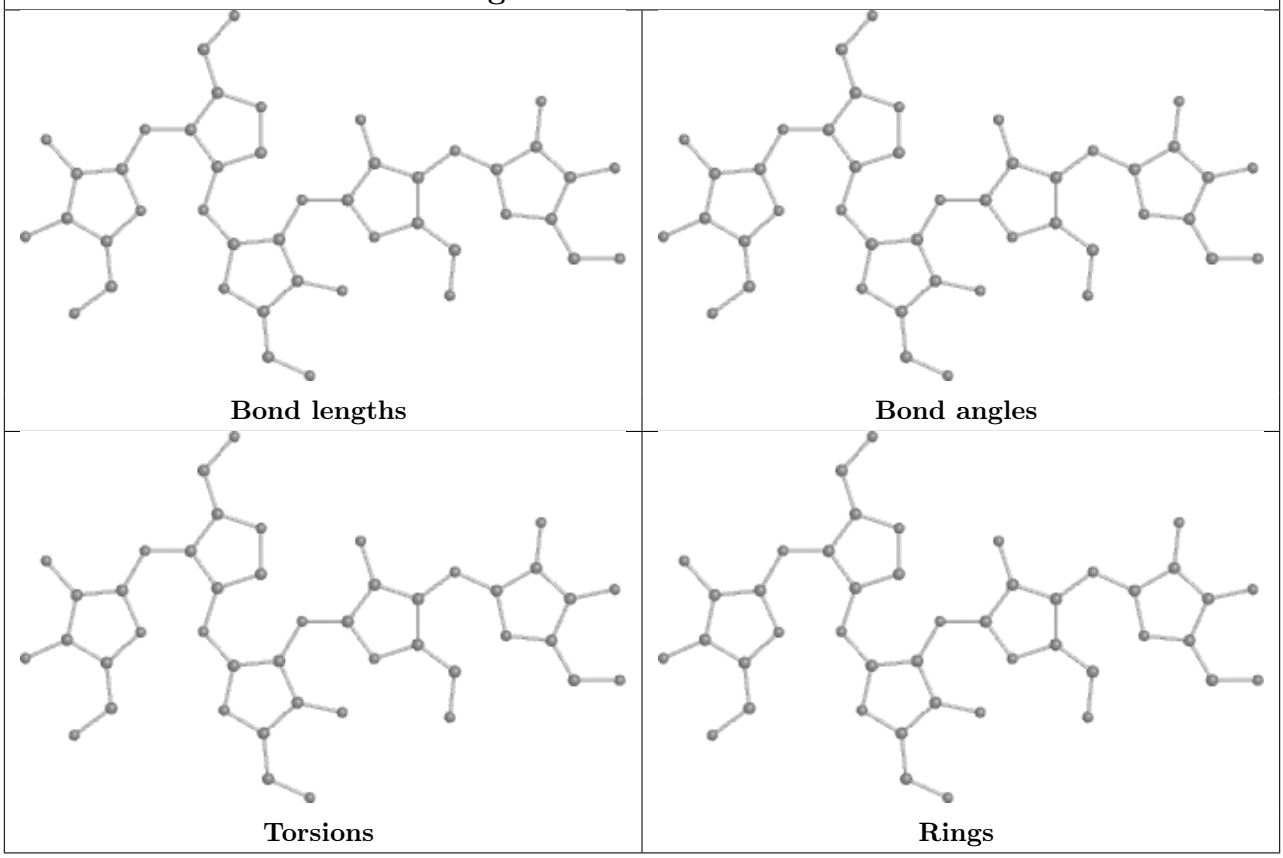
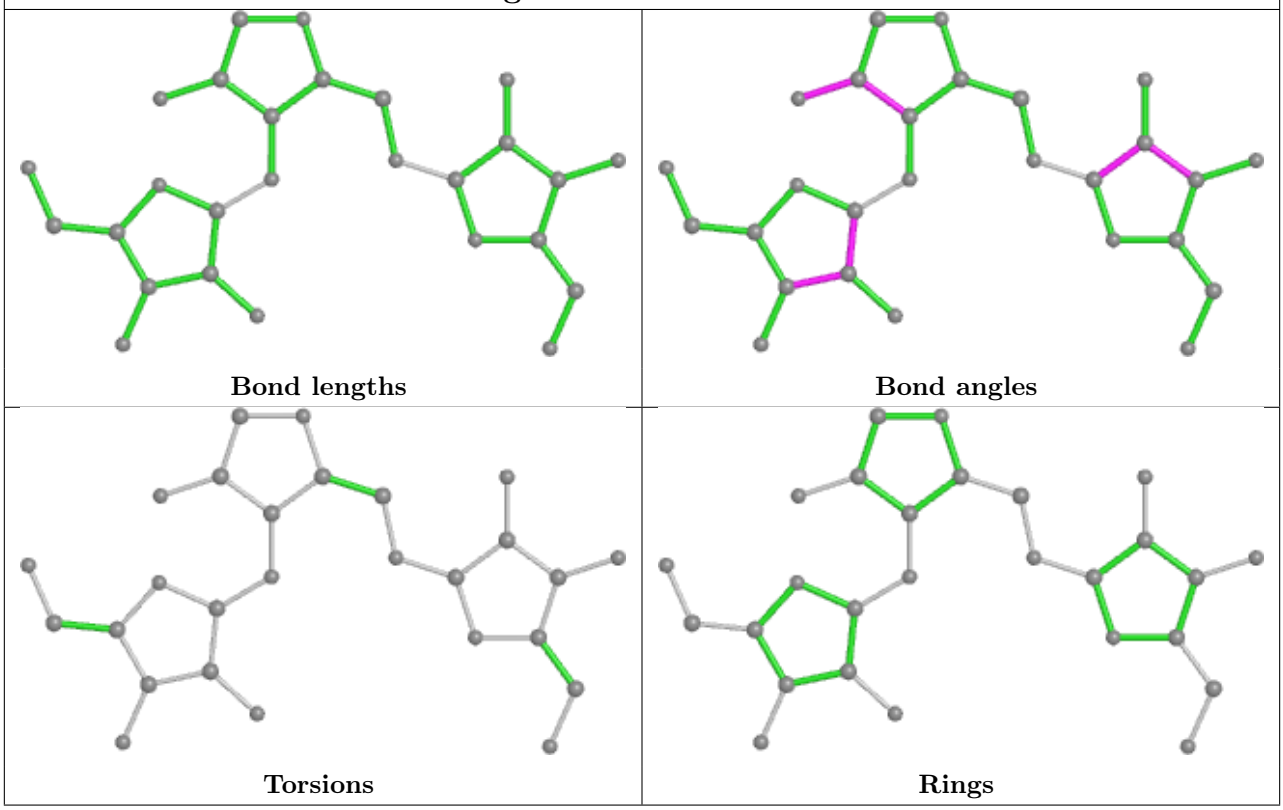


Rings

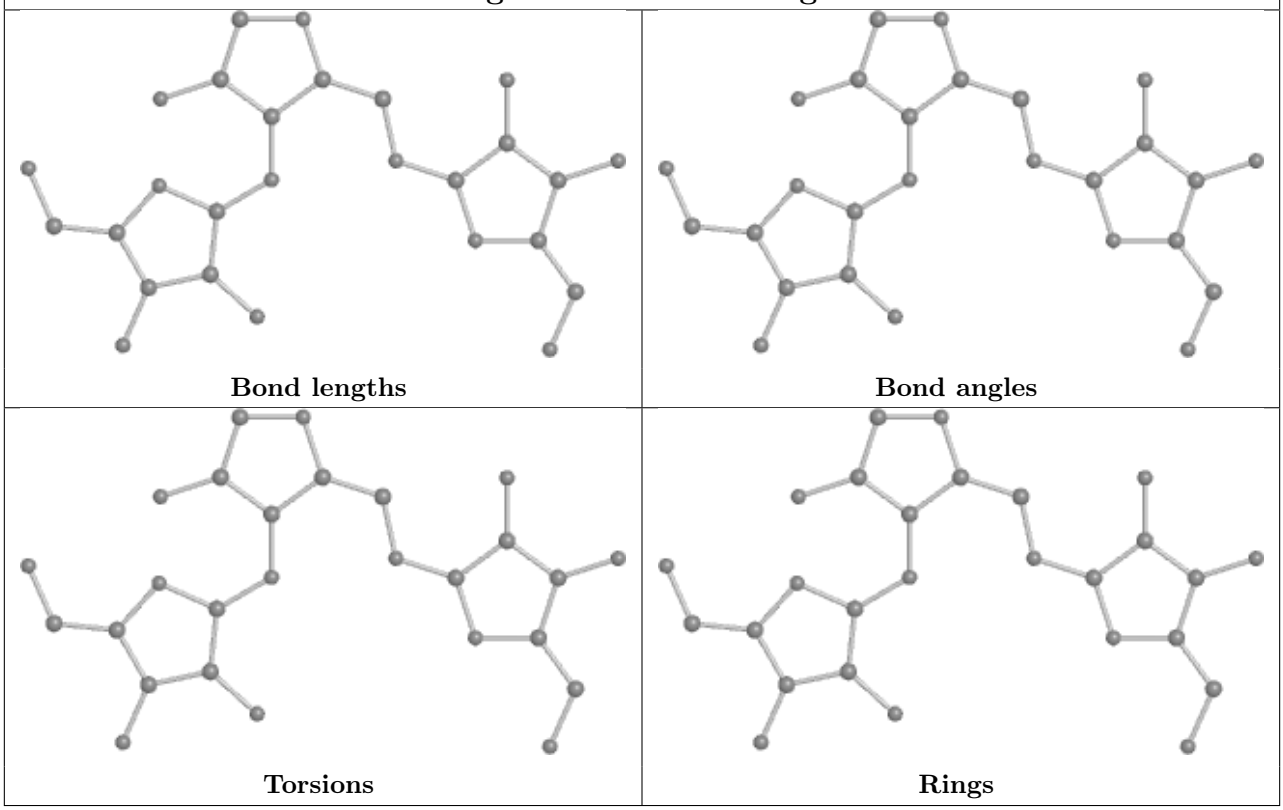
Oligosaccharide Chain sD



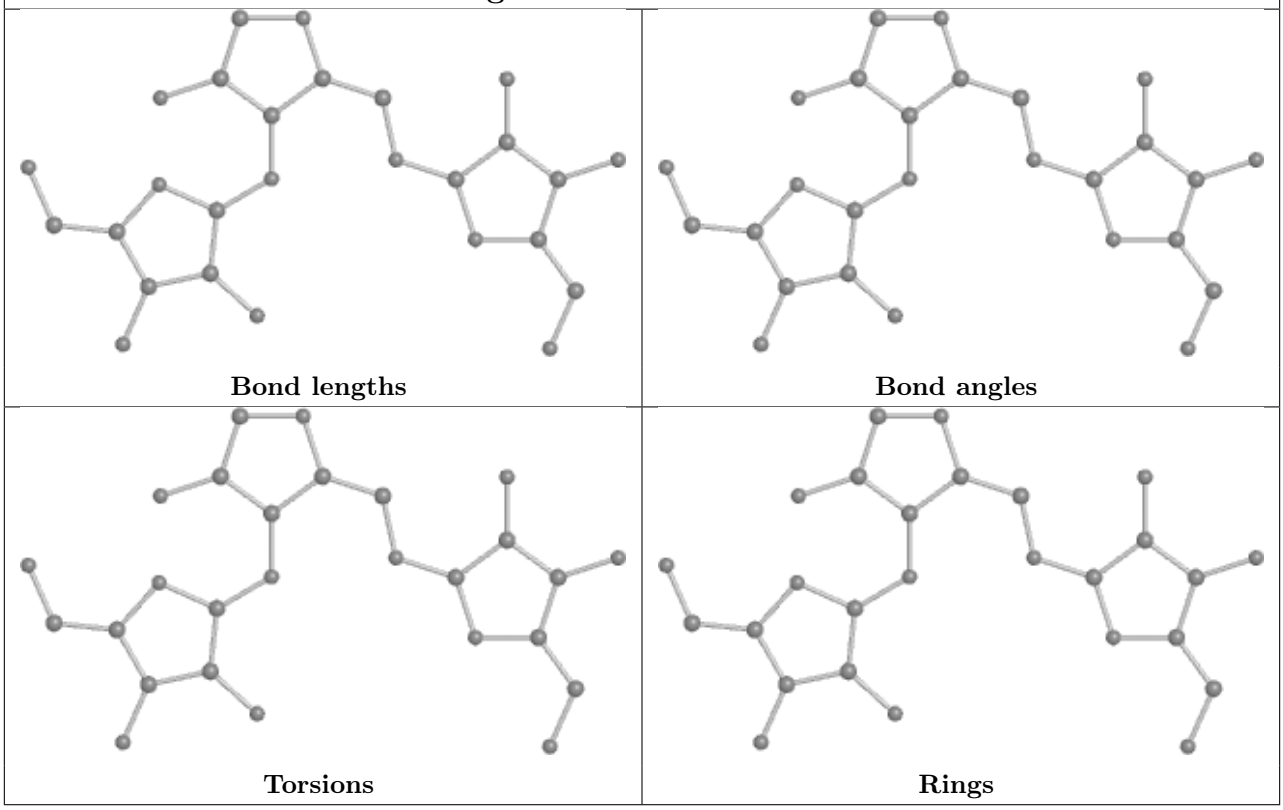
Oligosaccharide Chain i

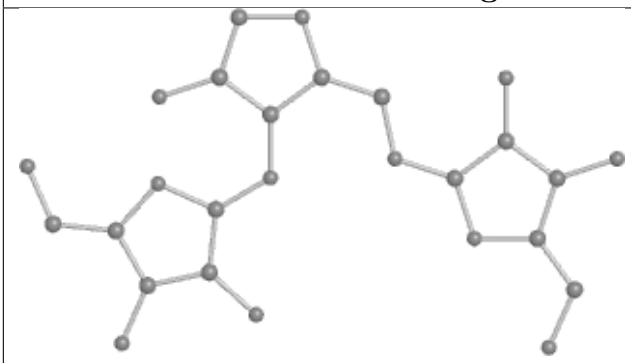
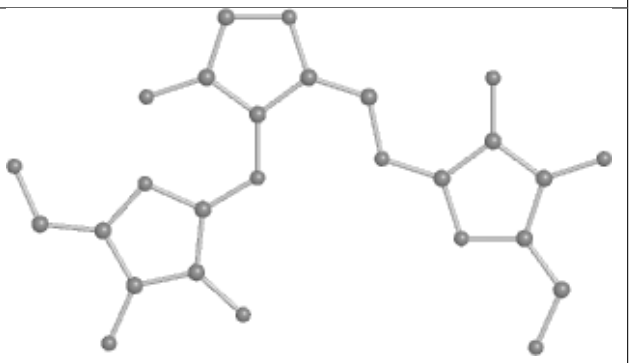
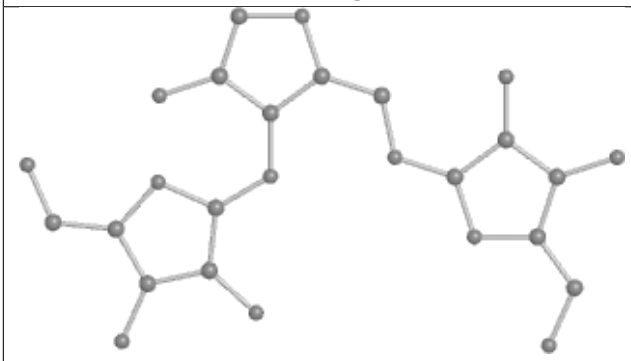
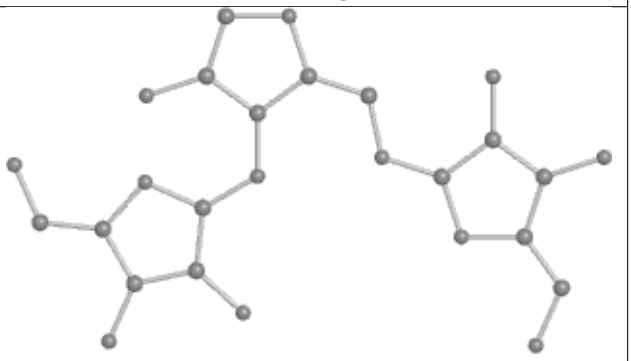


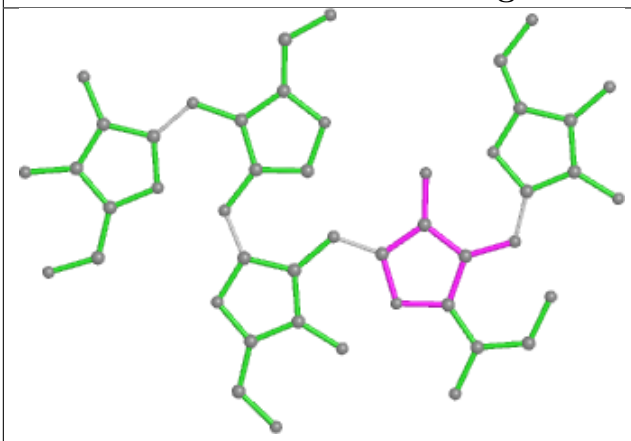
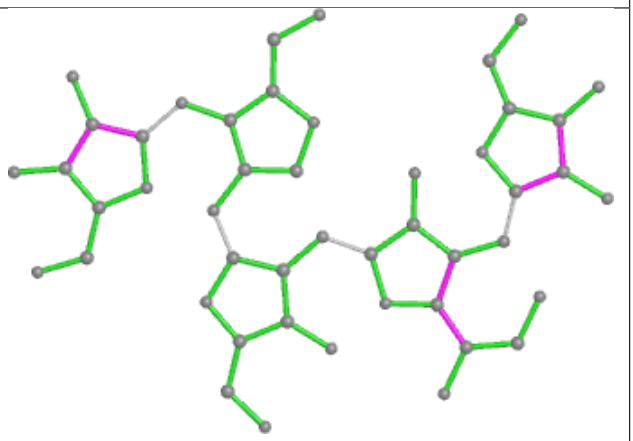
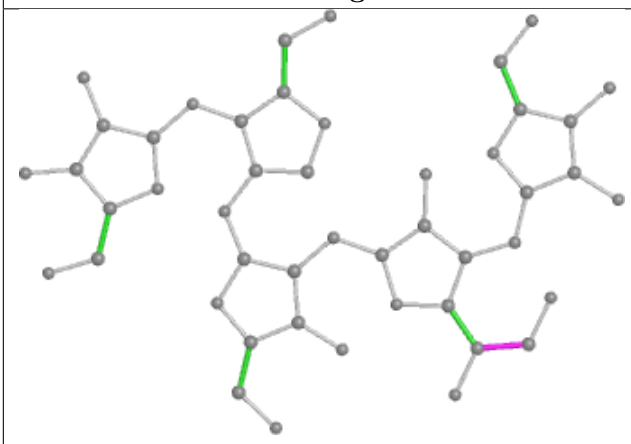
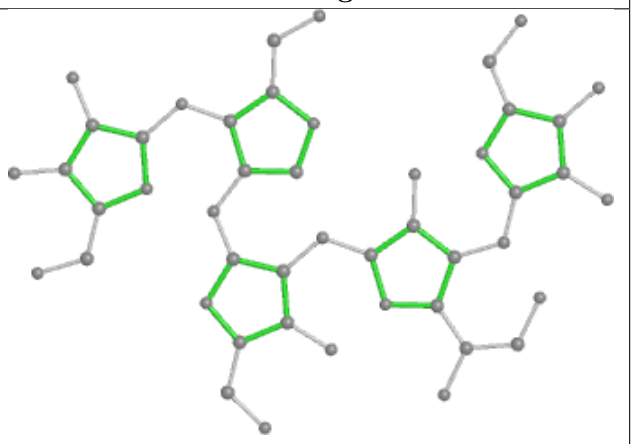
Oligosaccharide Chain gA

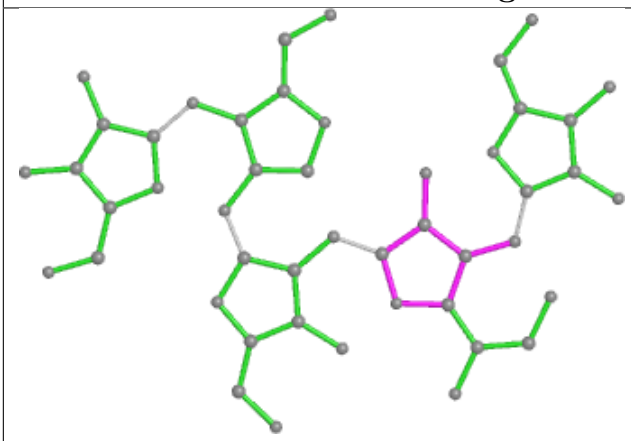
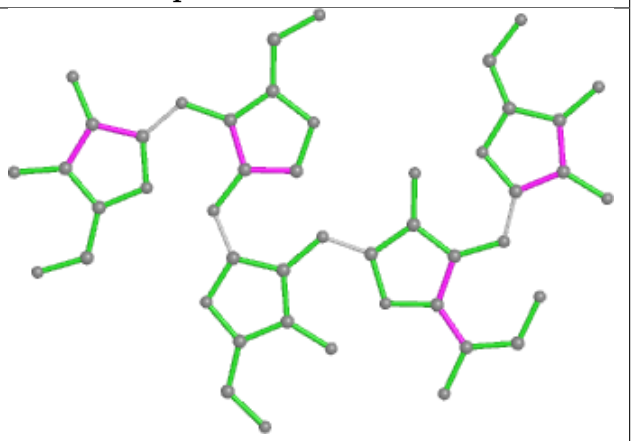
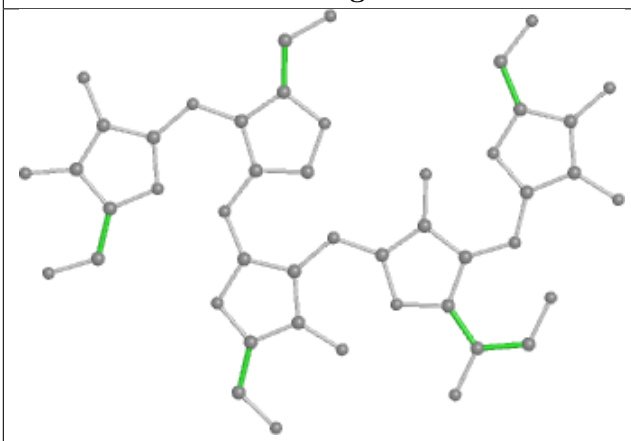
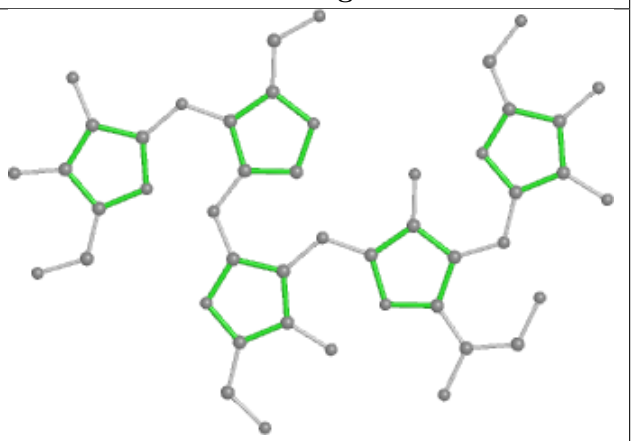


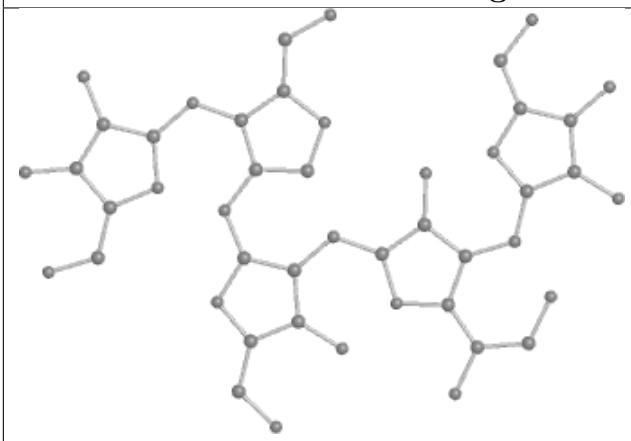
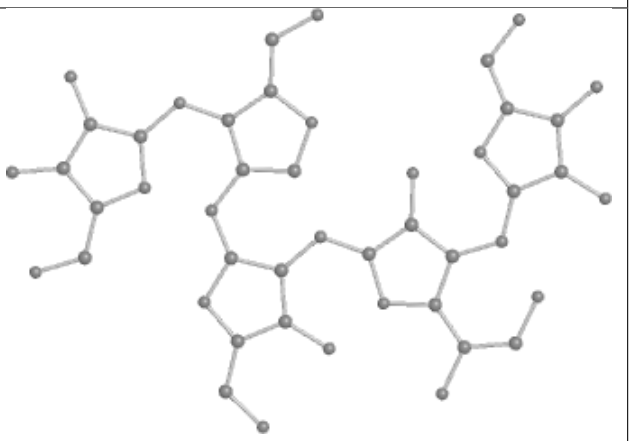
Oligosaccharide Chain aC



Oligosaccharide Chain XD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain n	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain q	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain lA	
	
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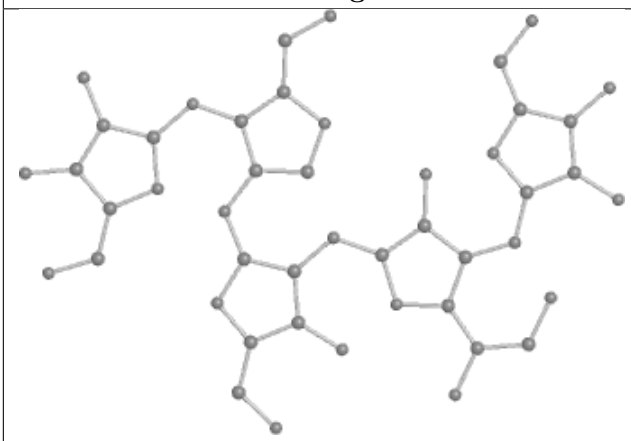	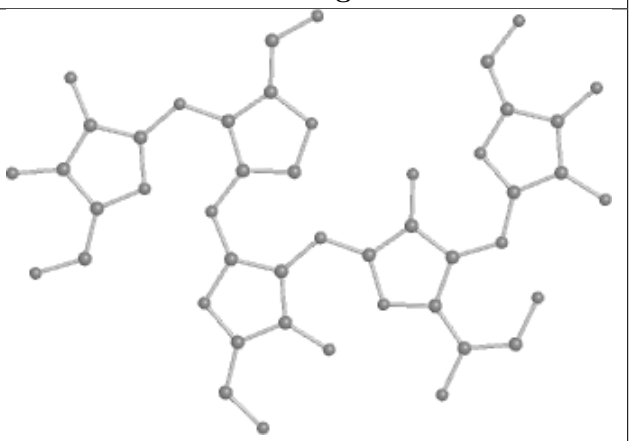
Torsions	**Rings**

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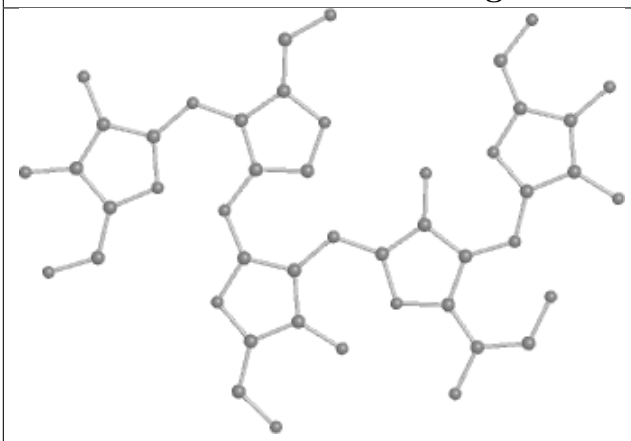	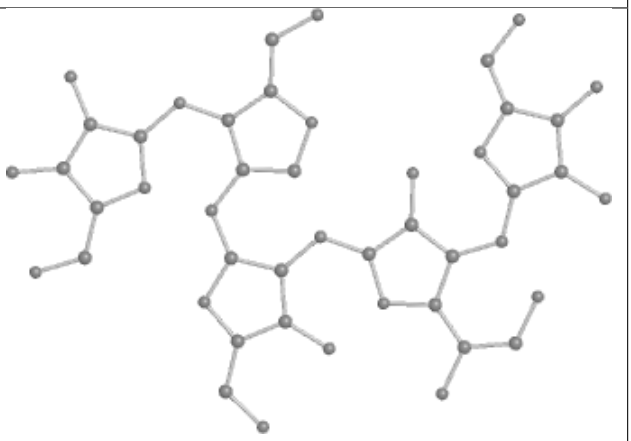
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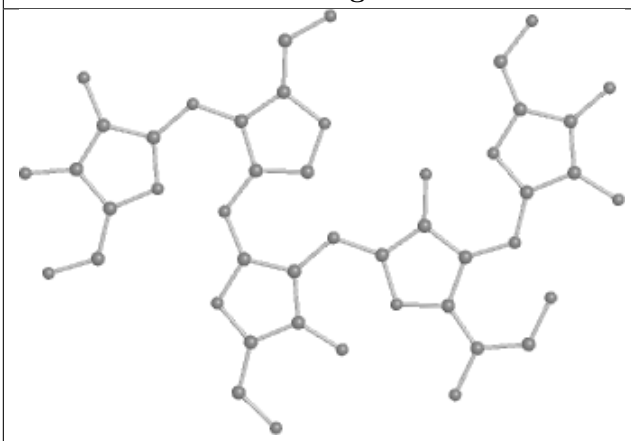
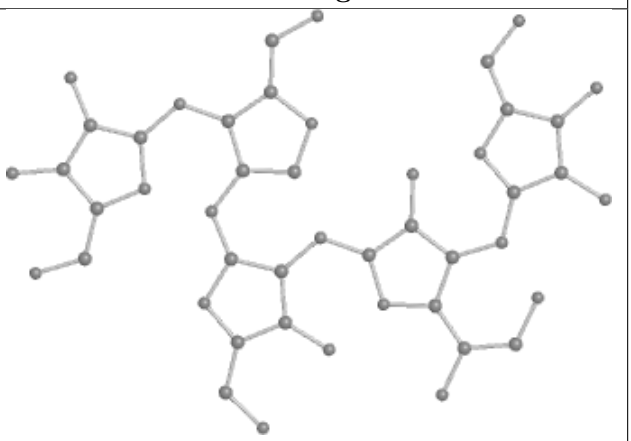
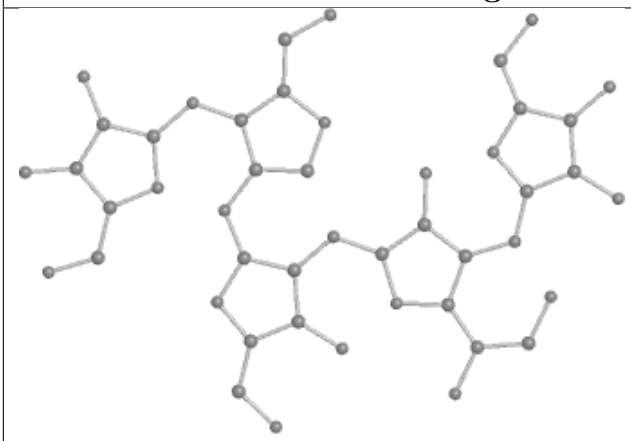
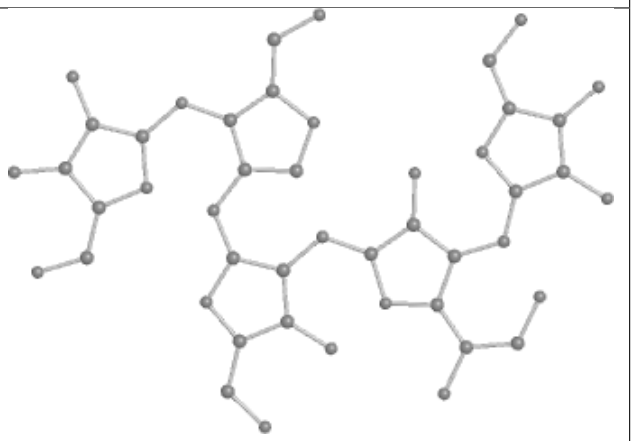
	
Torsions	**Rings**

Oligosaccharide Chain FB	
	
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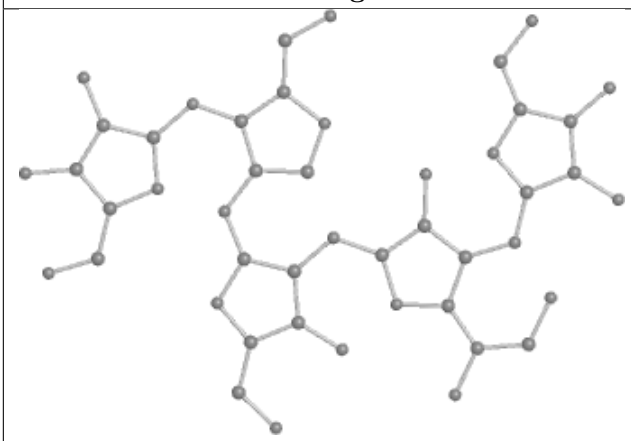
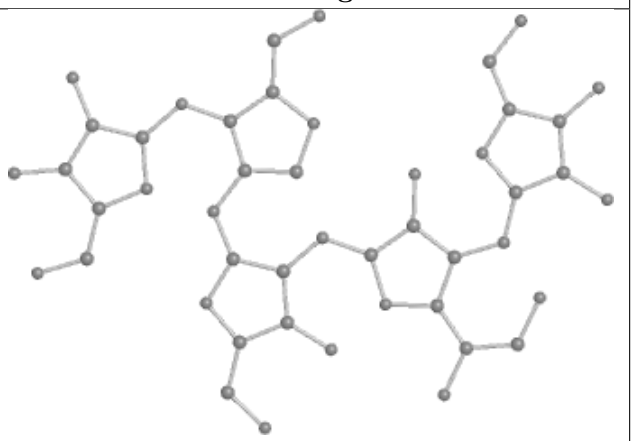
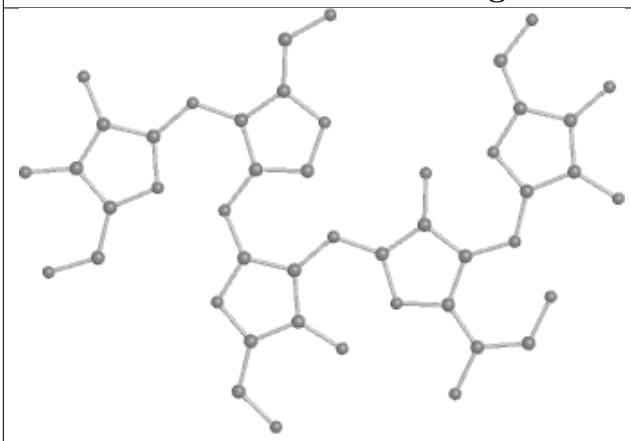
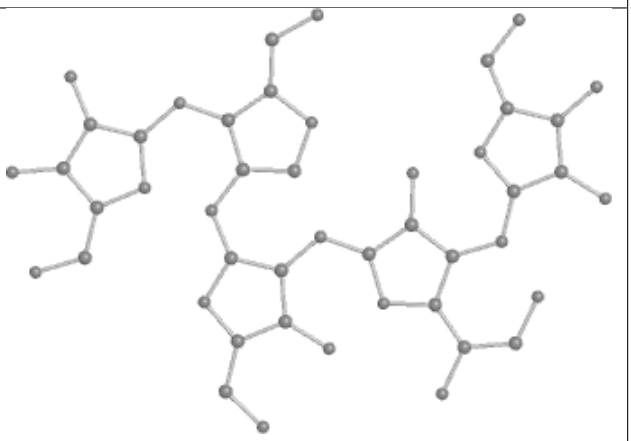
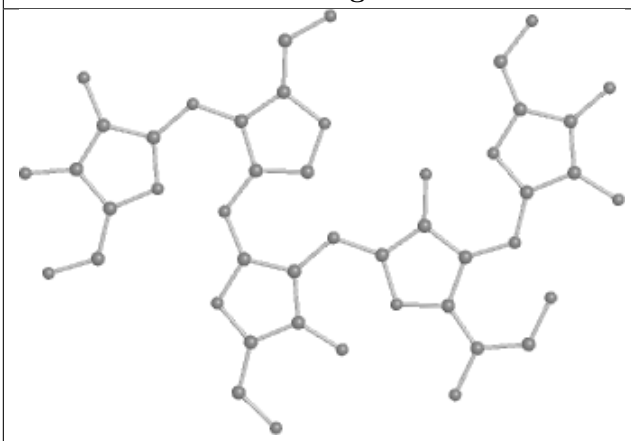
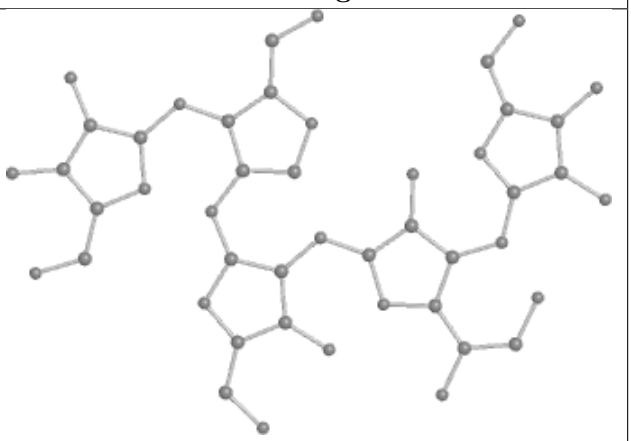
	
Torsions	**Rings**

Oligosaccharide Chain IB	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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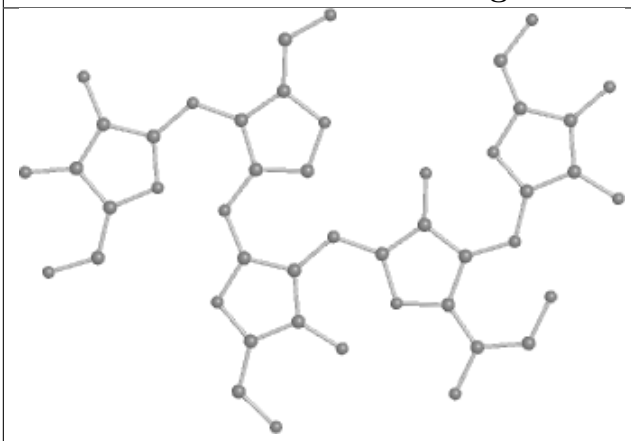	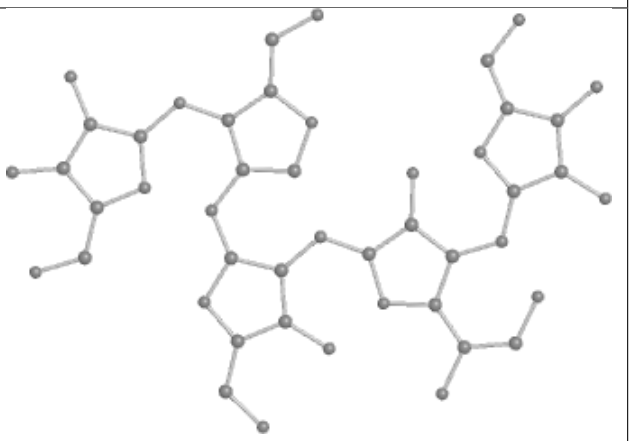
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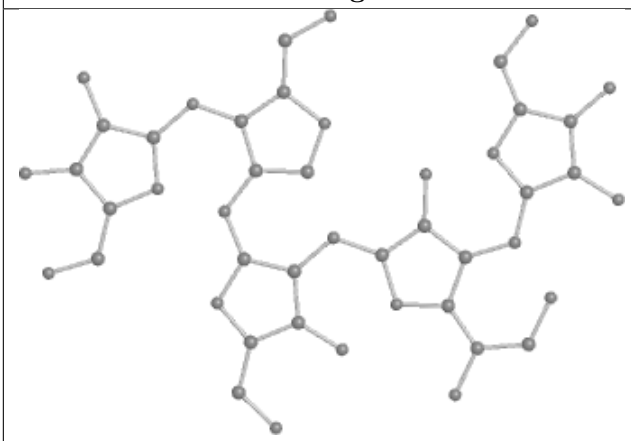	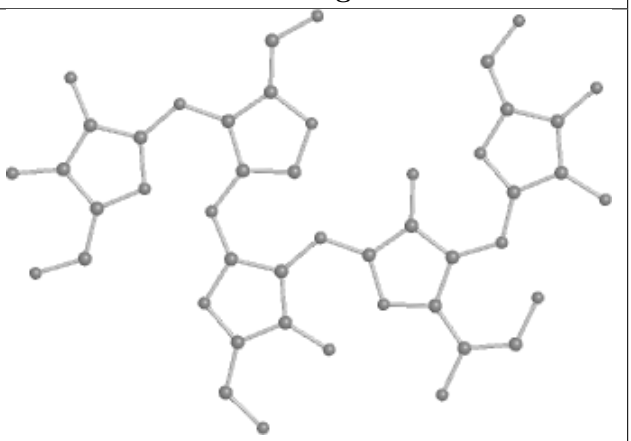
Torsions	**Rings**

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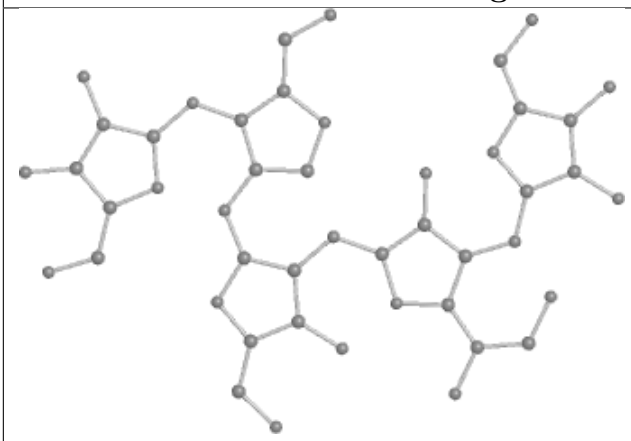
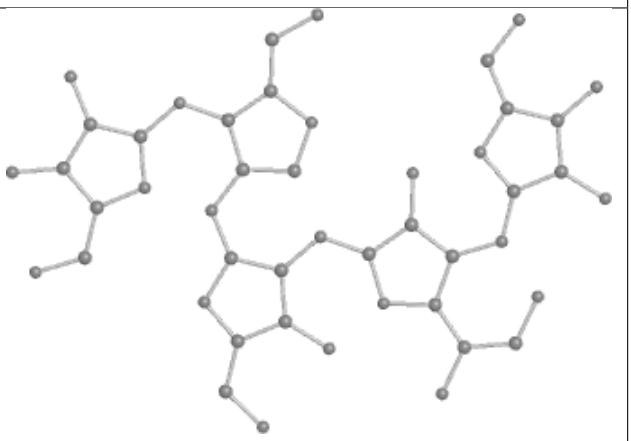
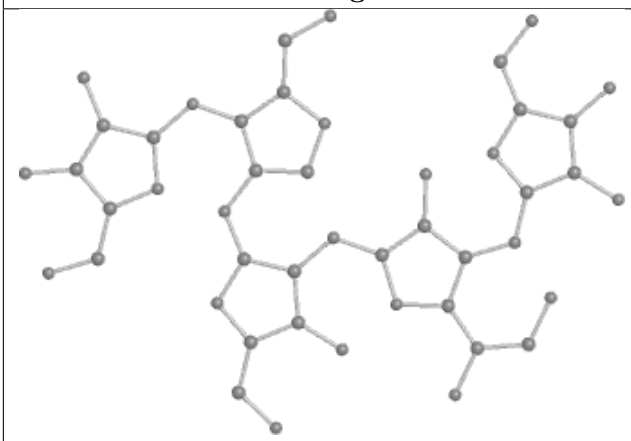
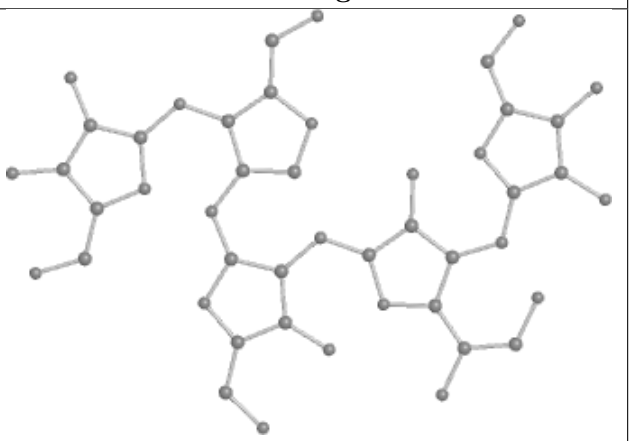
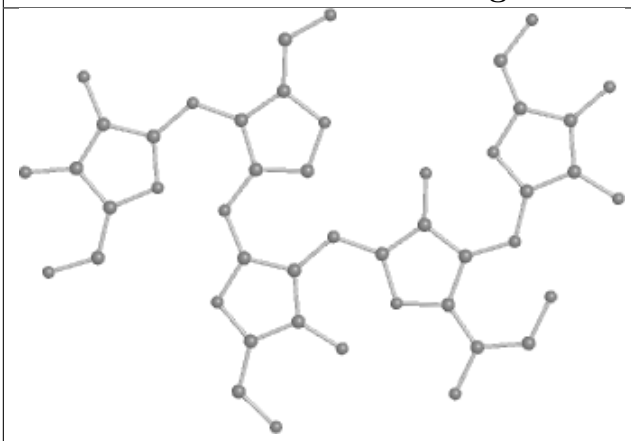
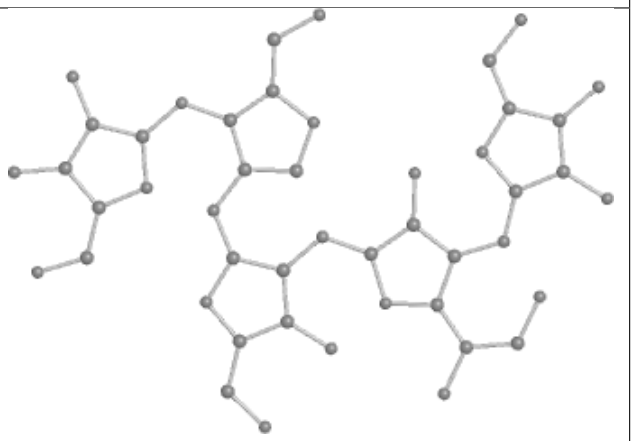
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain fC	
	
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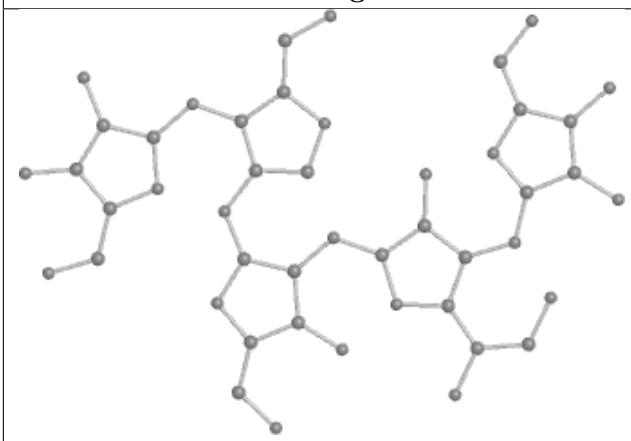	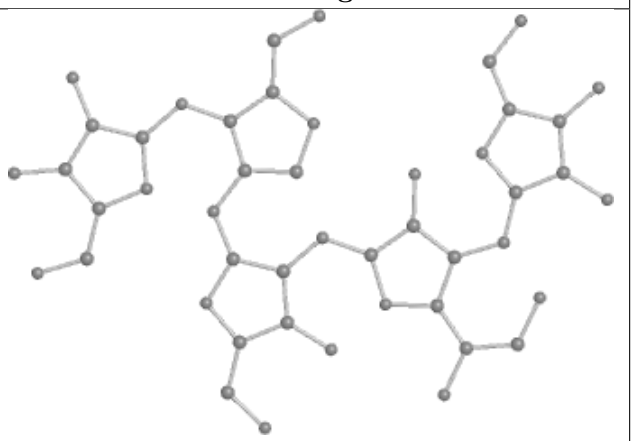
Torsions	**Rings**

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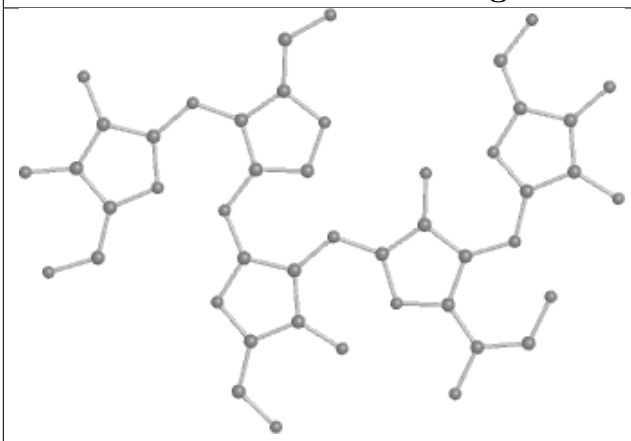	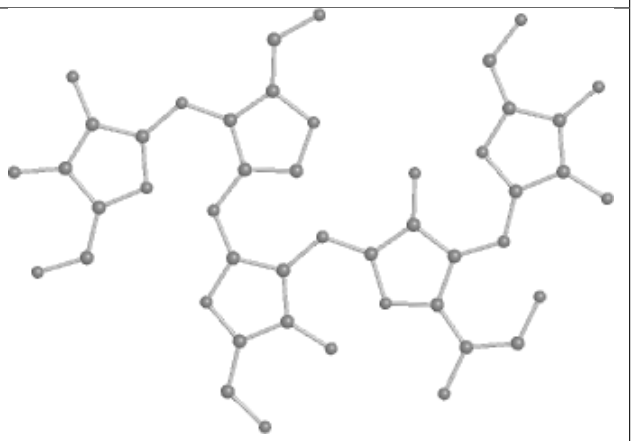
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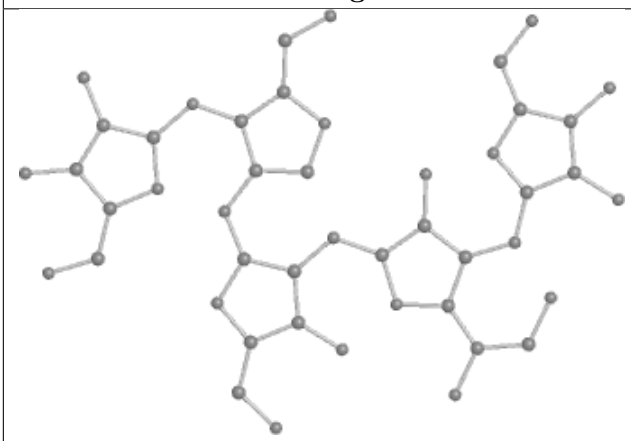
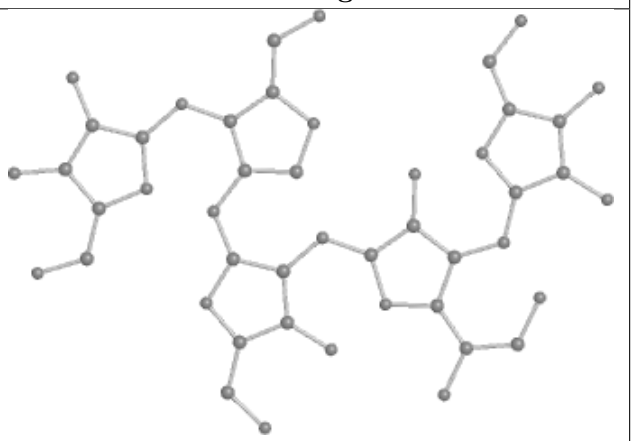
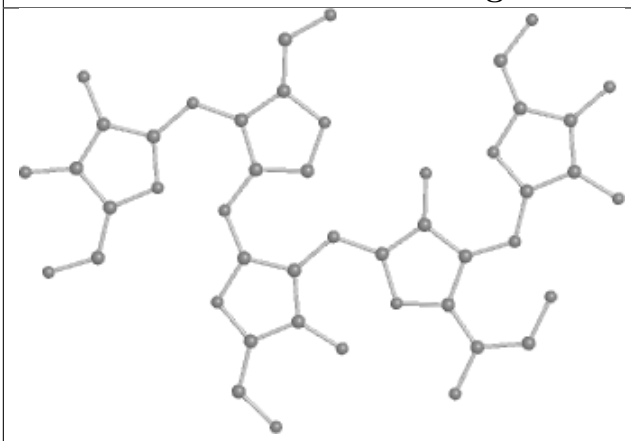
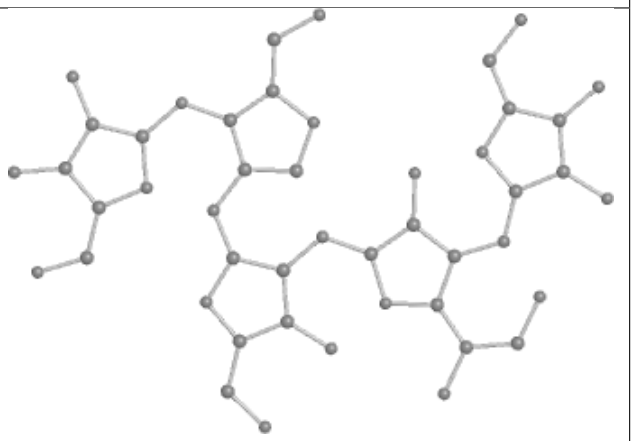
	
Torsions	**Rings**

Oligosaccharide Chain cD	
	
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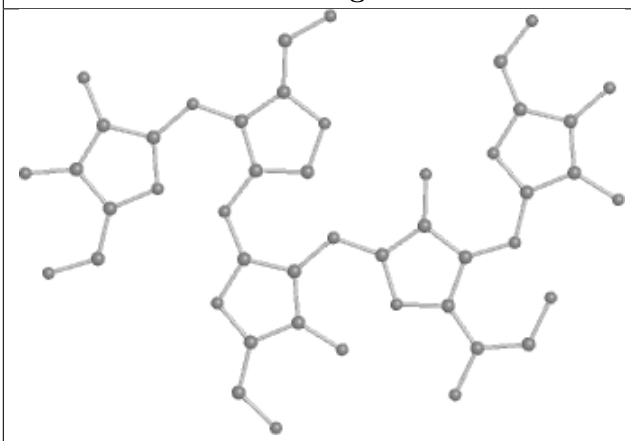	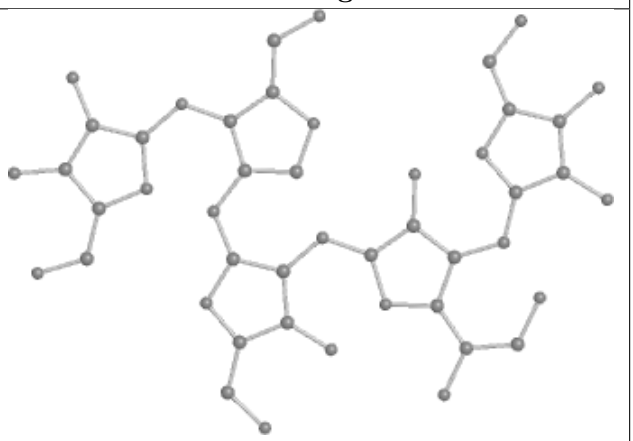
Torsions	**Rings**

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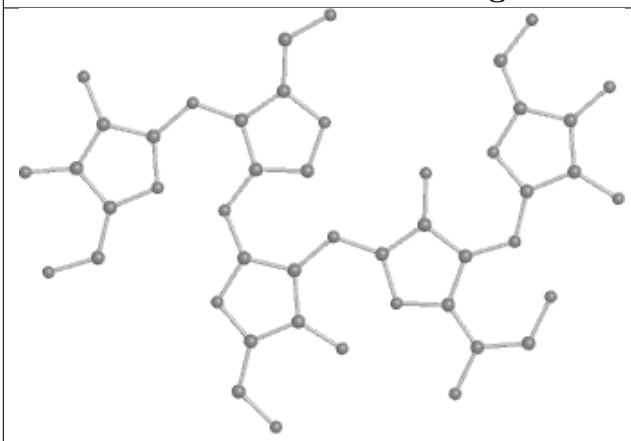
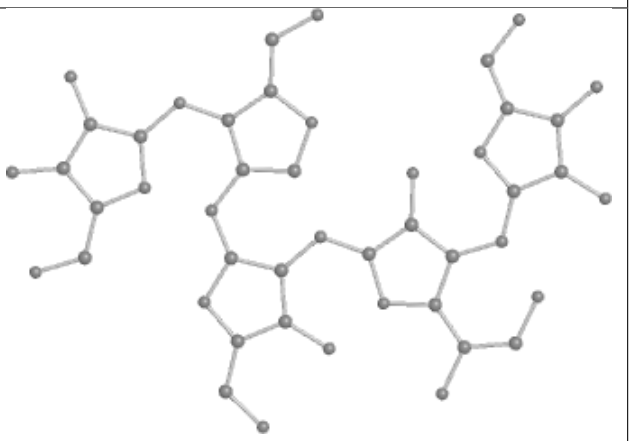
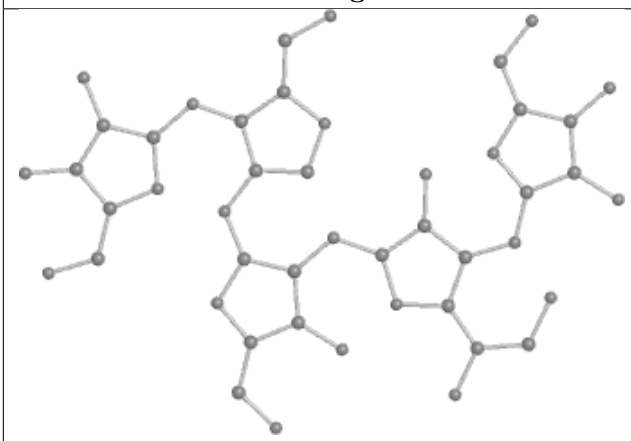
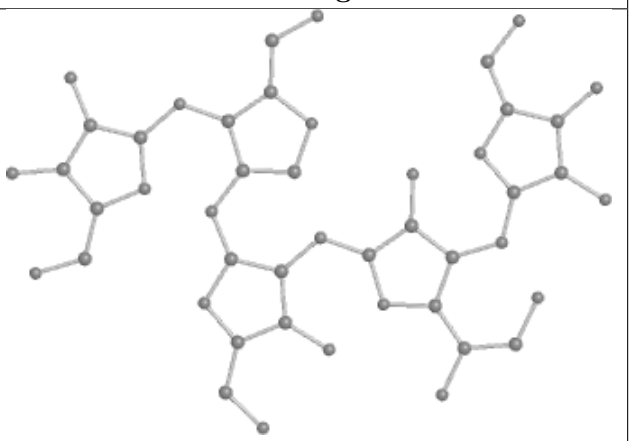
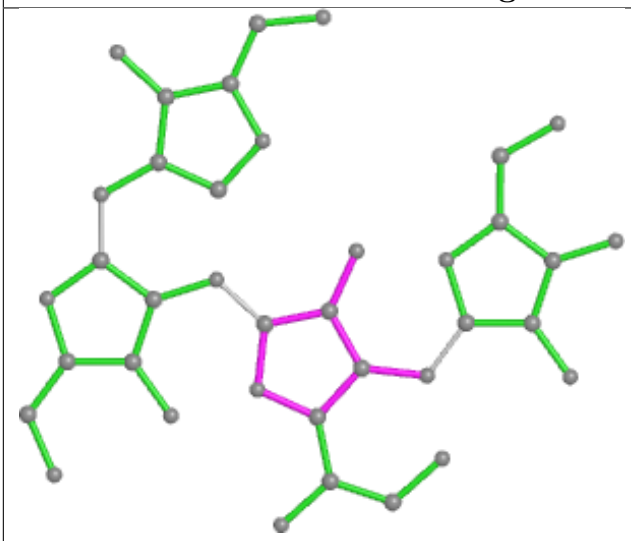
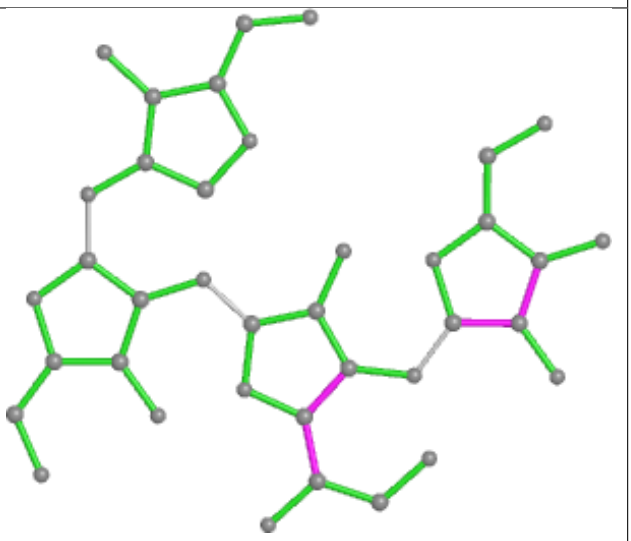
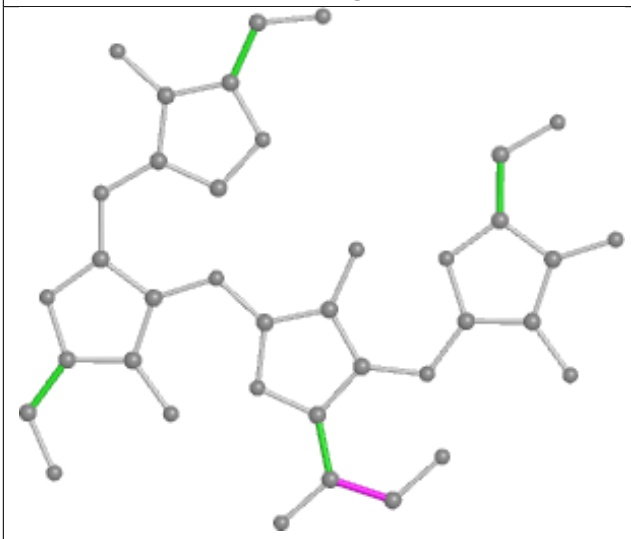
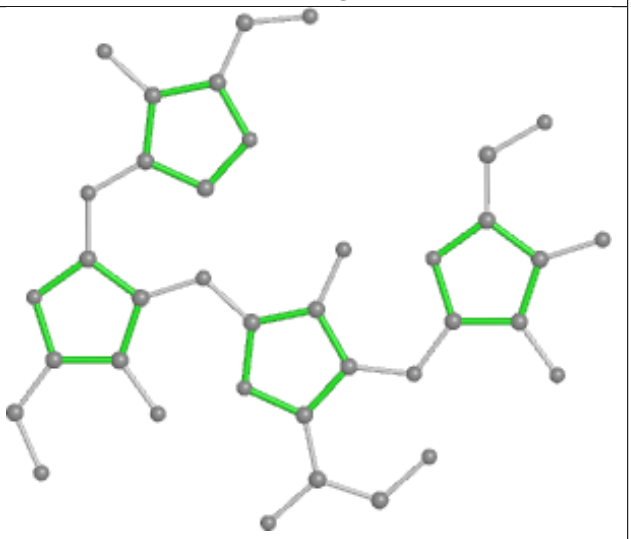
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain o	
 Bond lengths	 Bond angles
 Torsions	 Rings

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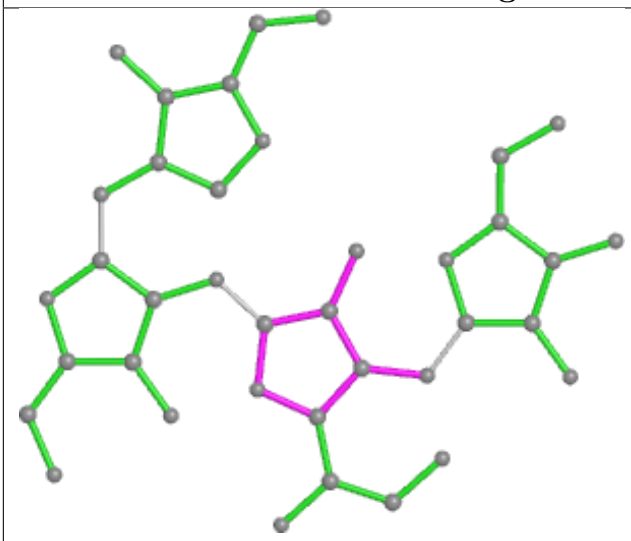
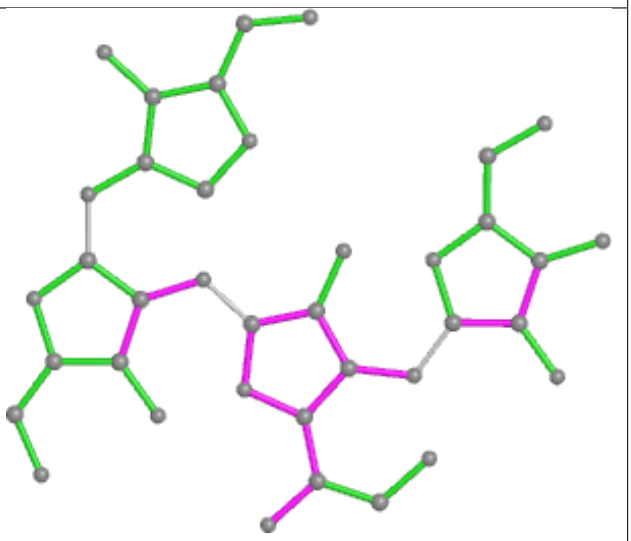
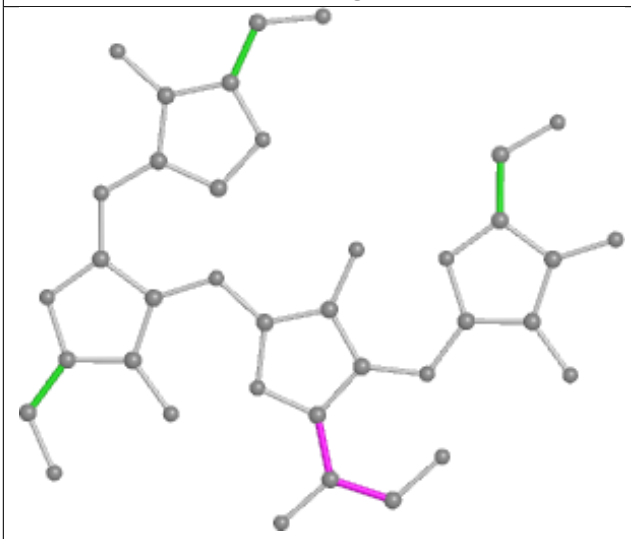
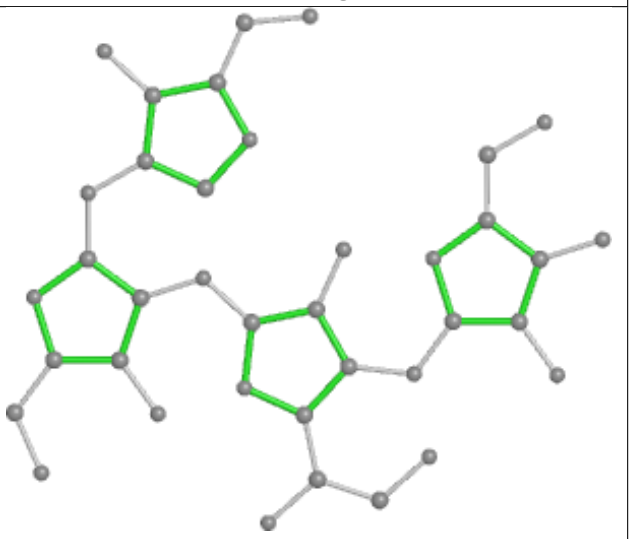
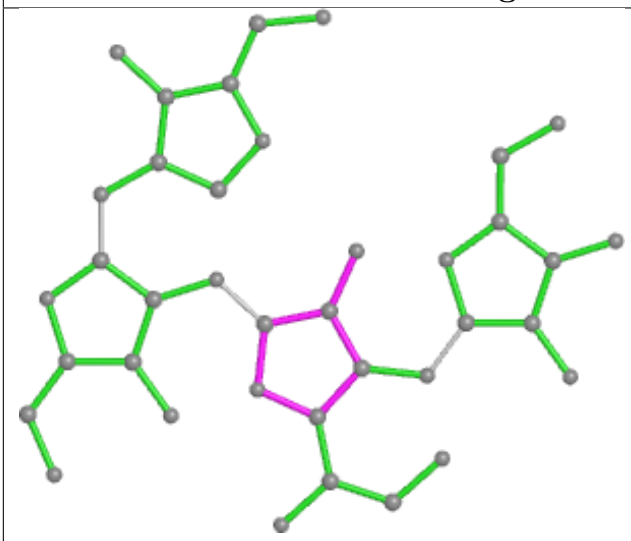
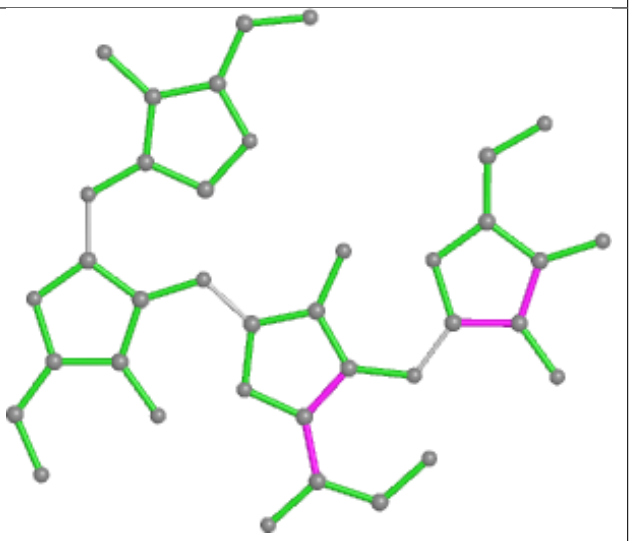
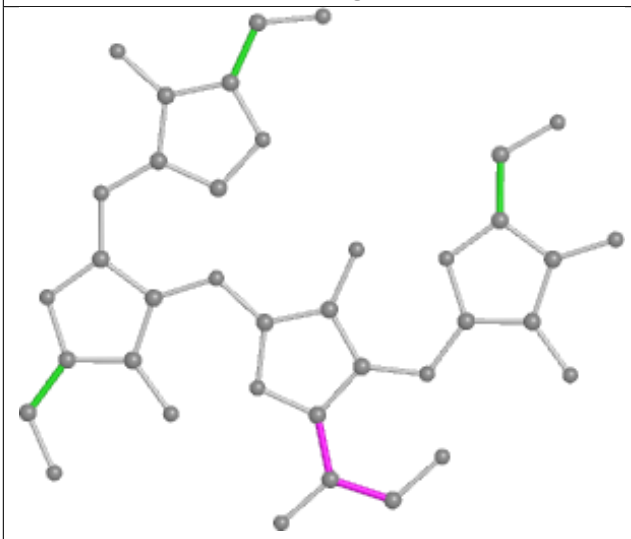
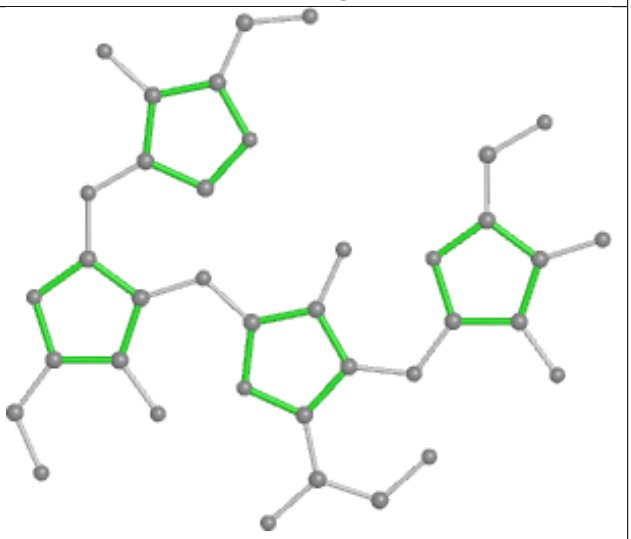
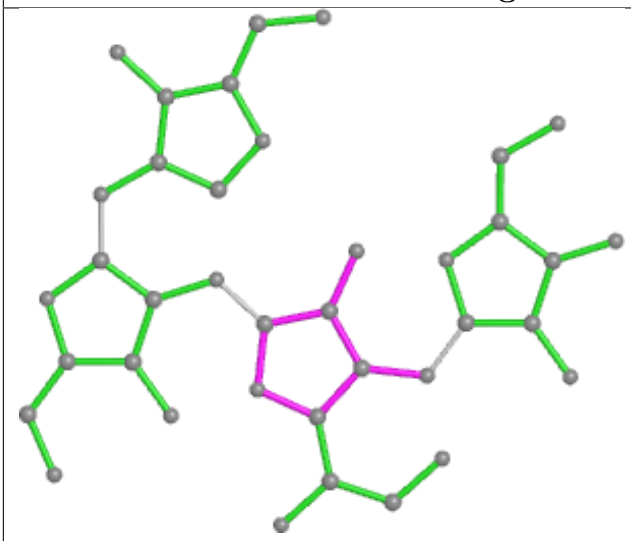
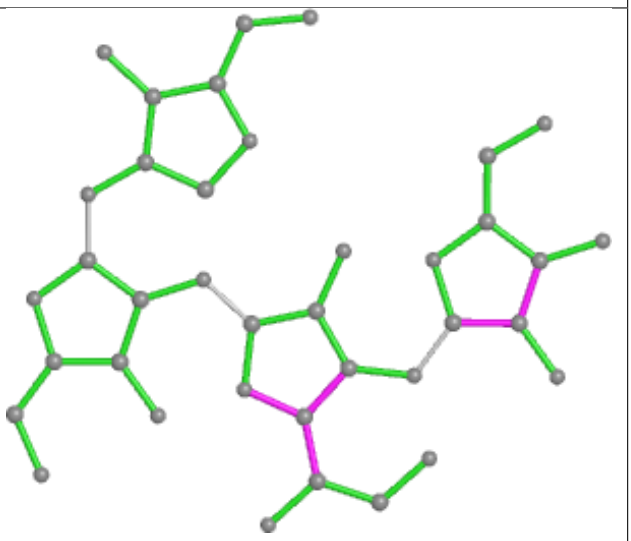
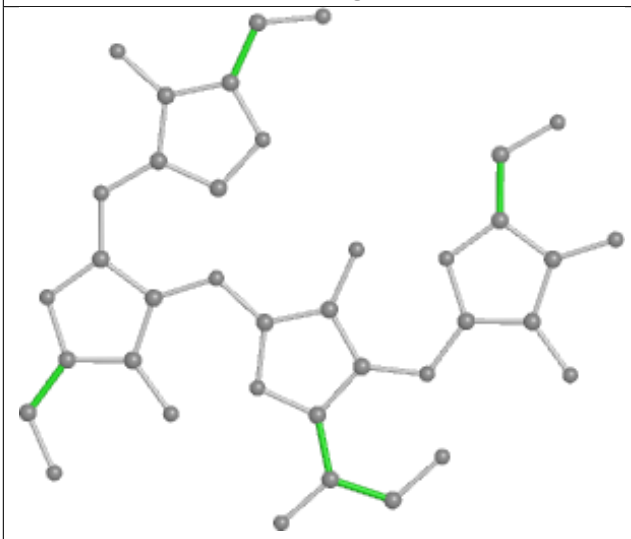
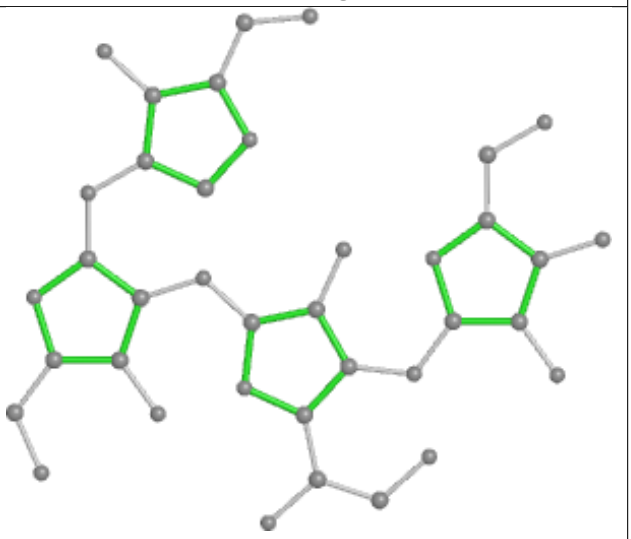
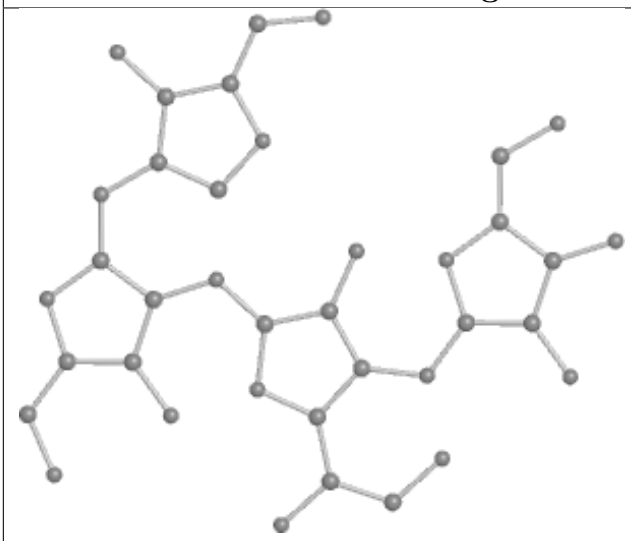
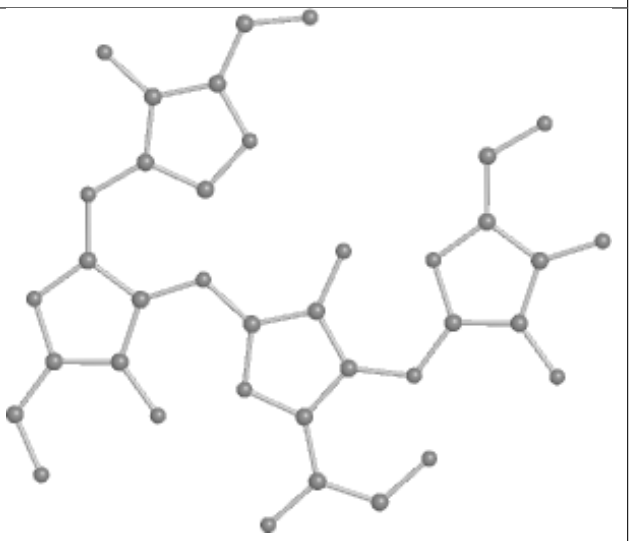
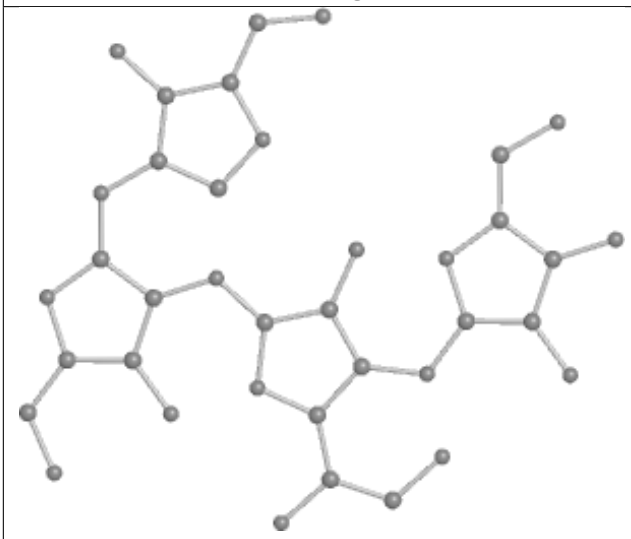
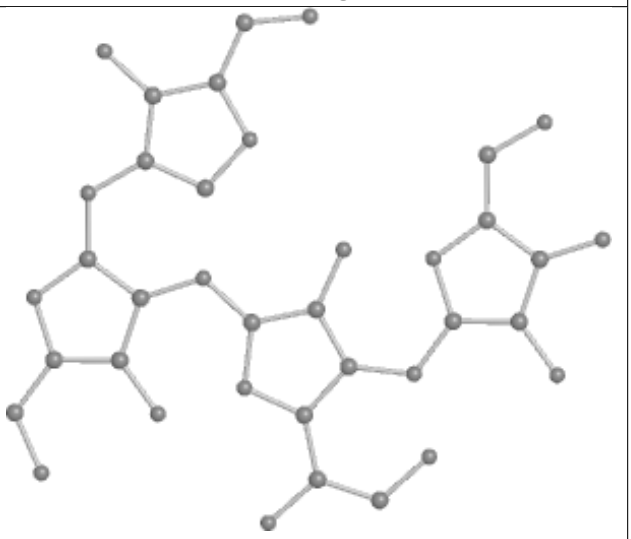
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 6	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 7	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain BA	
 Bond lengths	 Bond angles
 Torsions	 Rings

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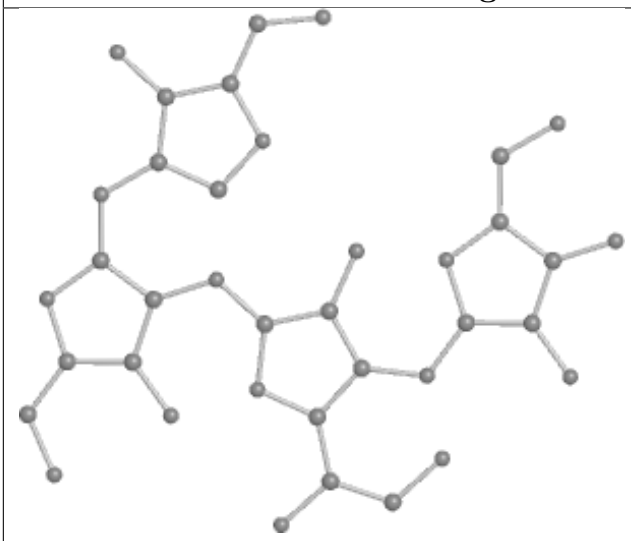
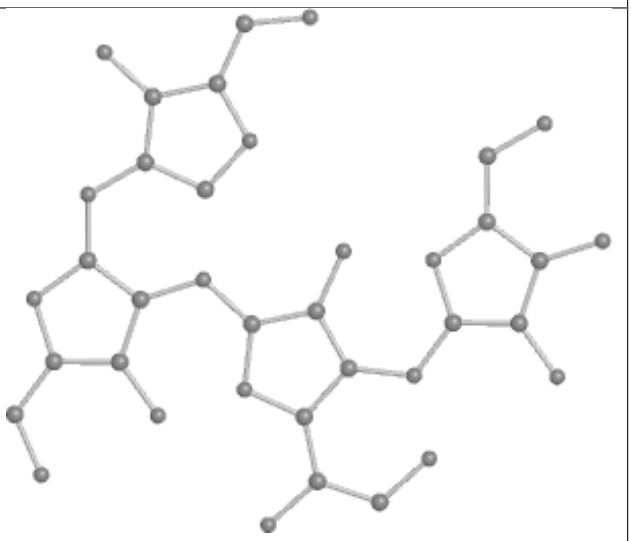
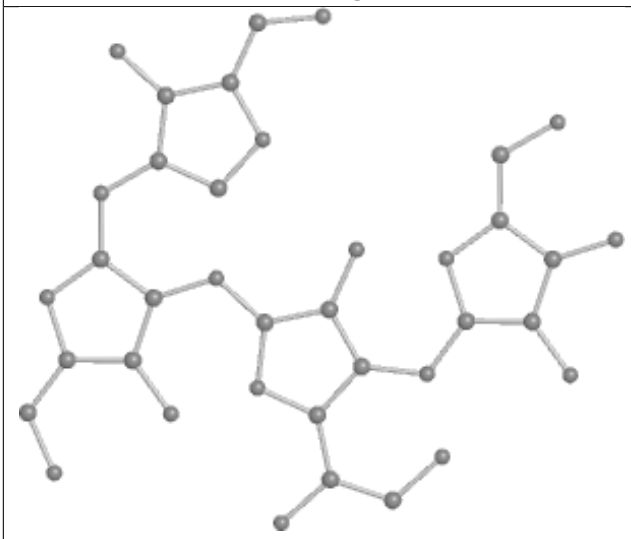
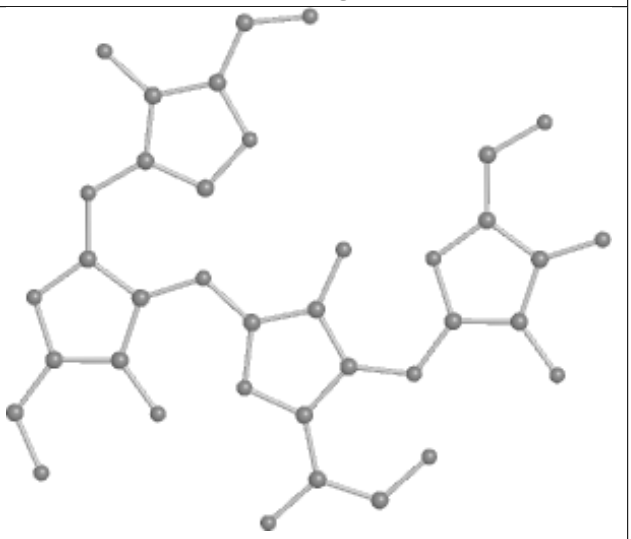
 Bond lengths	 Bond angles
 Torsions	 Rings

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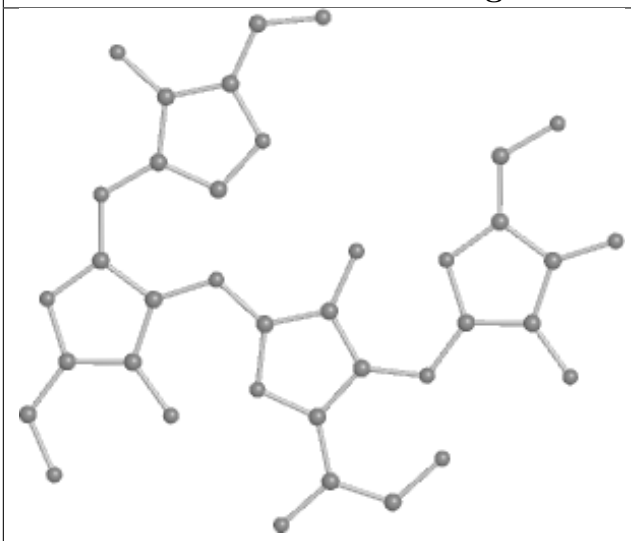
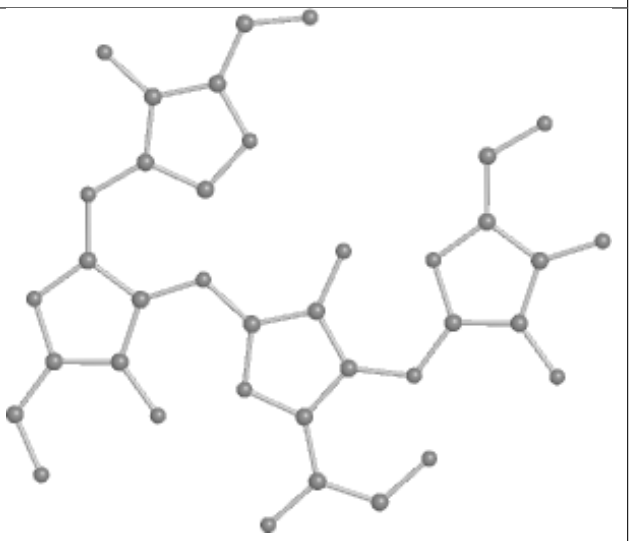
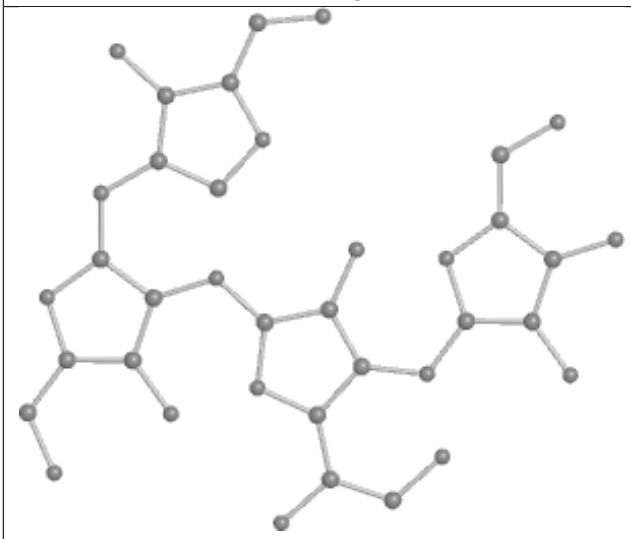
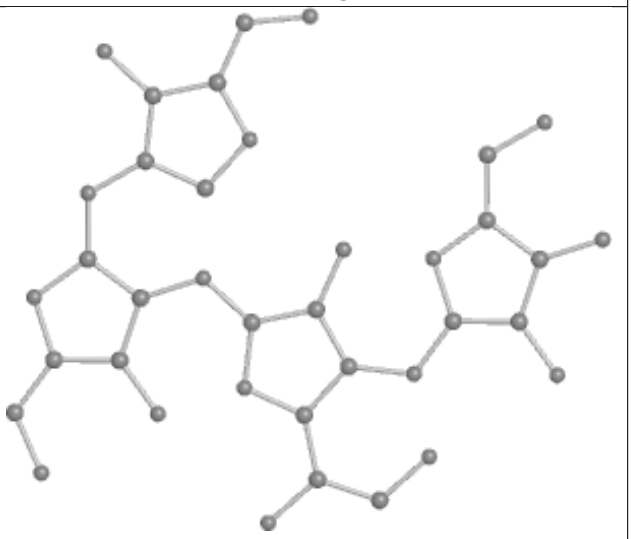
 Bond lengths	 Bond angles
 Torsions	 Rings

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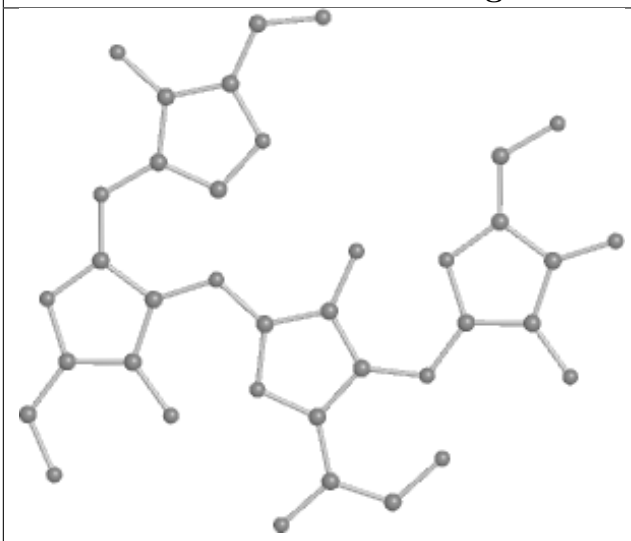
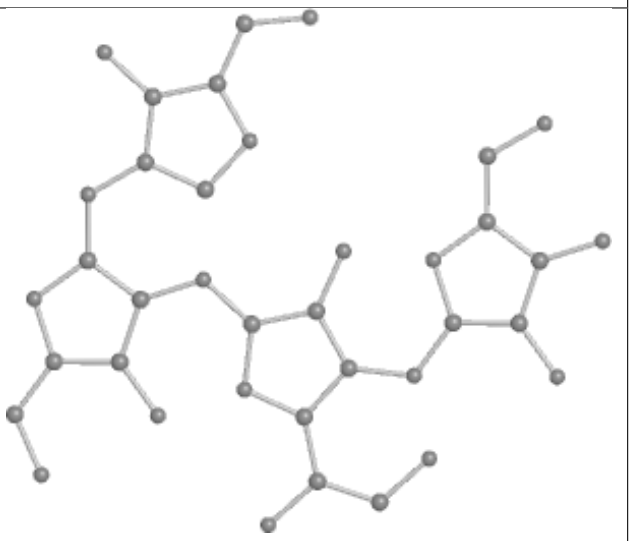
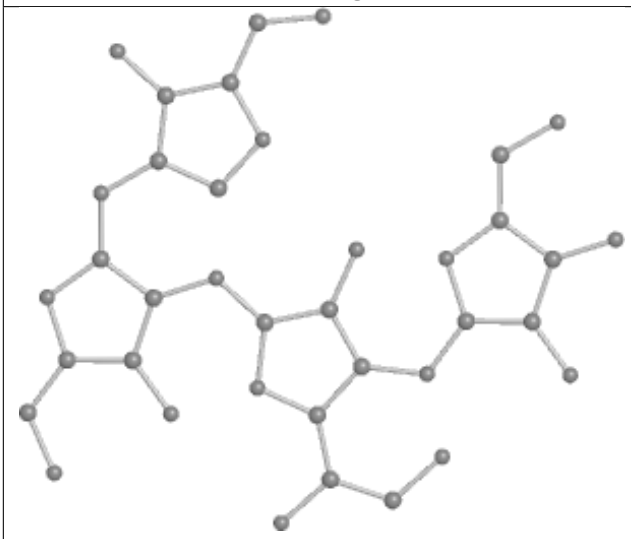
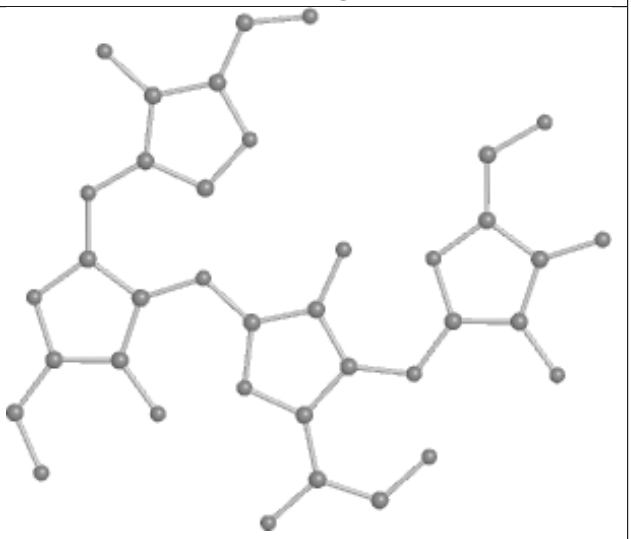
 Bond lengths	 Bond angles
 Torsions	 Rings

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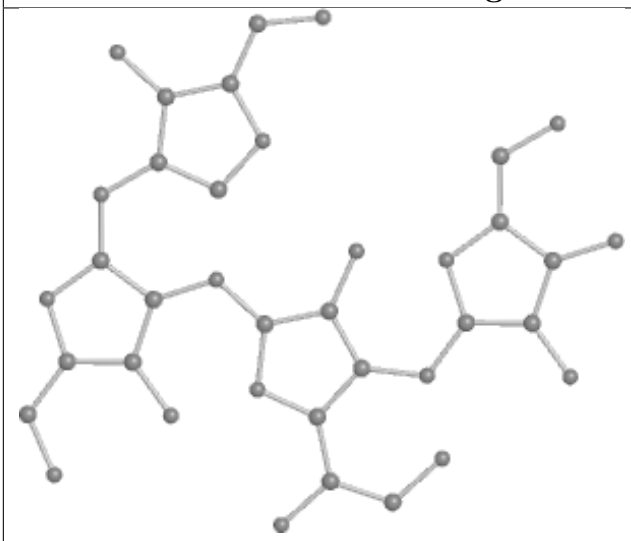
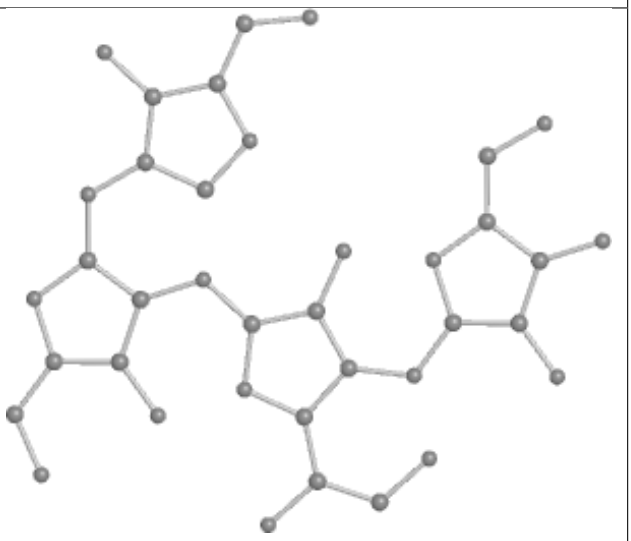
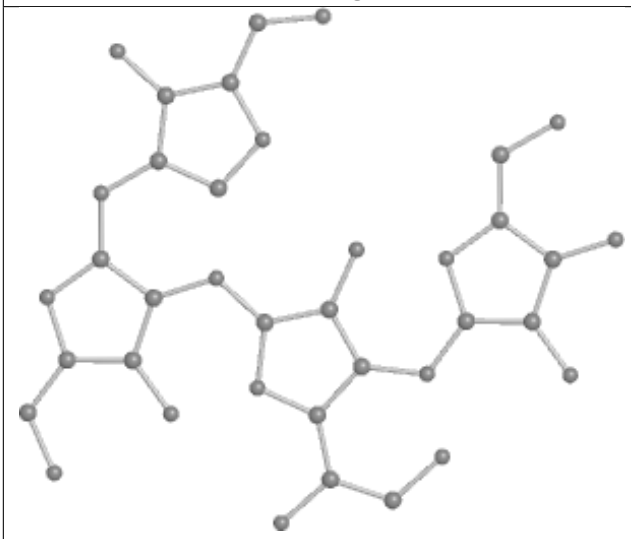
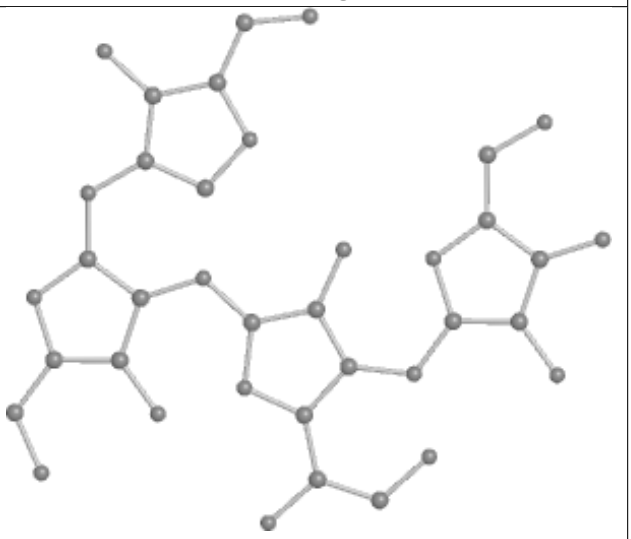
 Bond lengths	 Bond angles
 Torsions	 Rings

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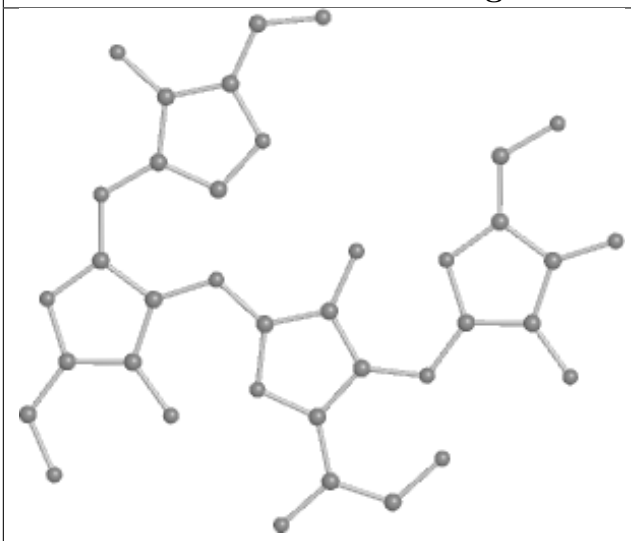
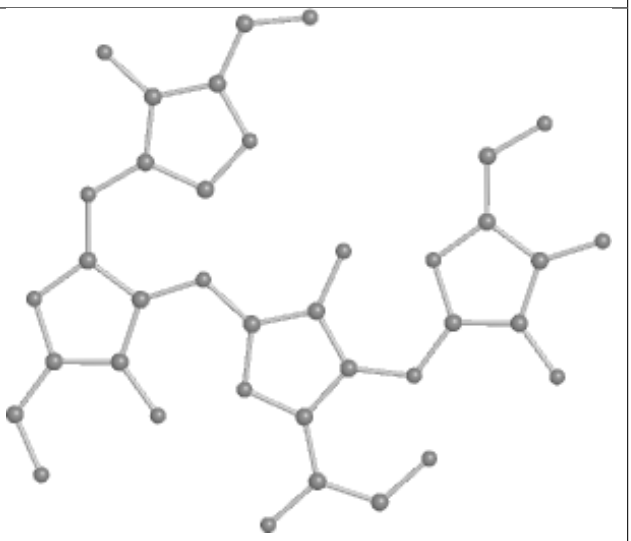
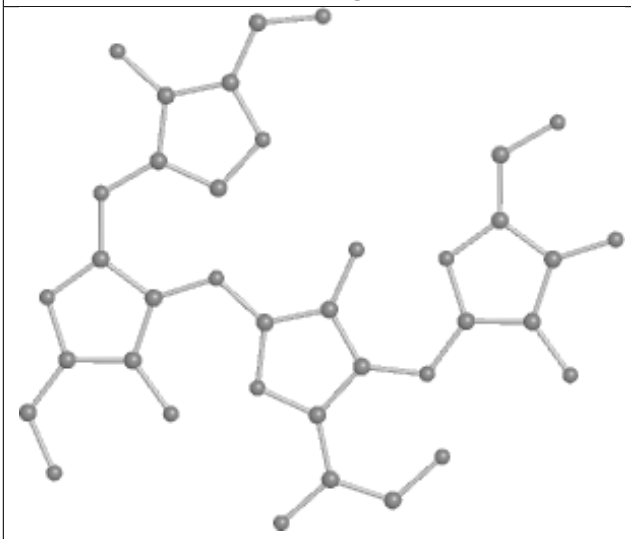
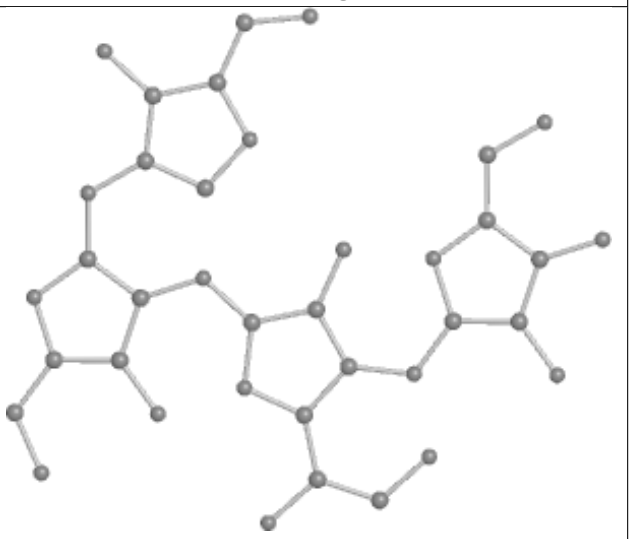
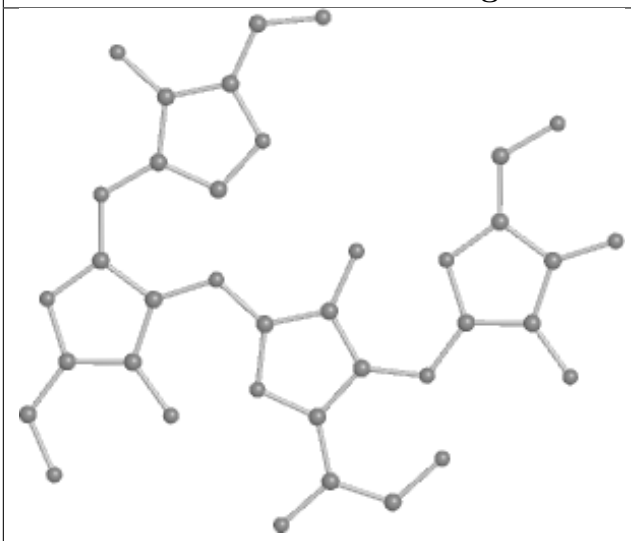
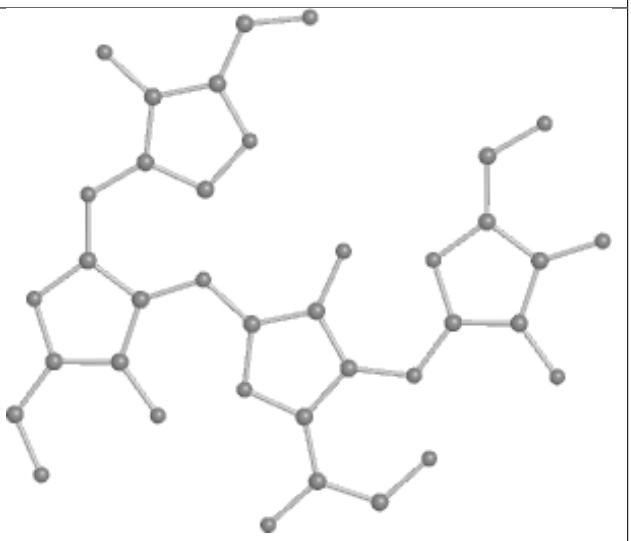
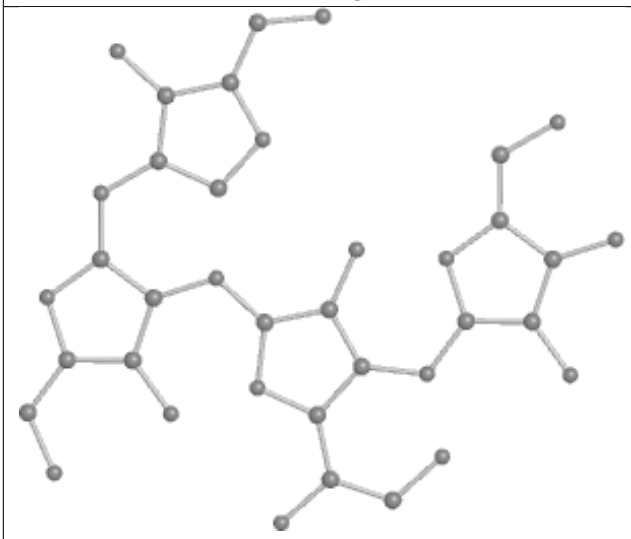
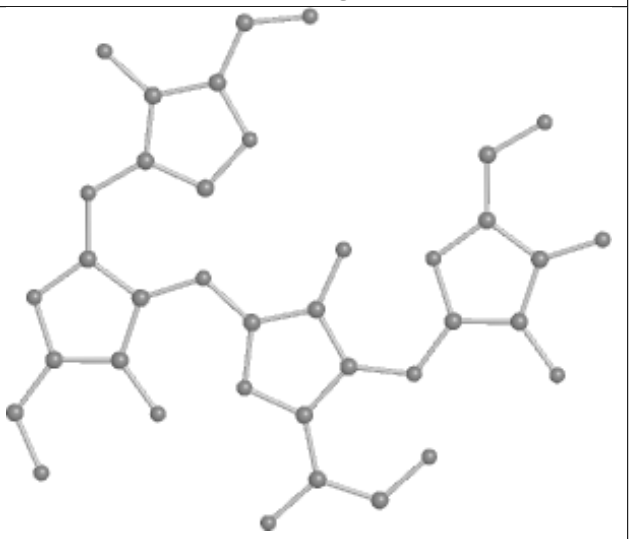
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain GB	
 Bond lengths	 Bond angles
 Torsions	 Rings

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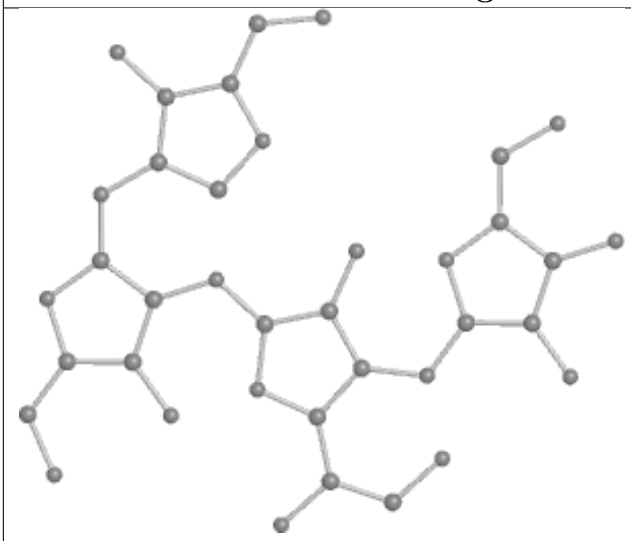
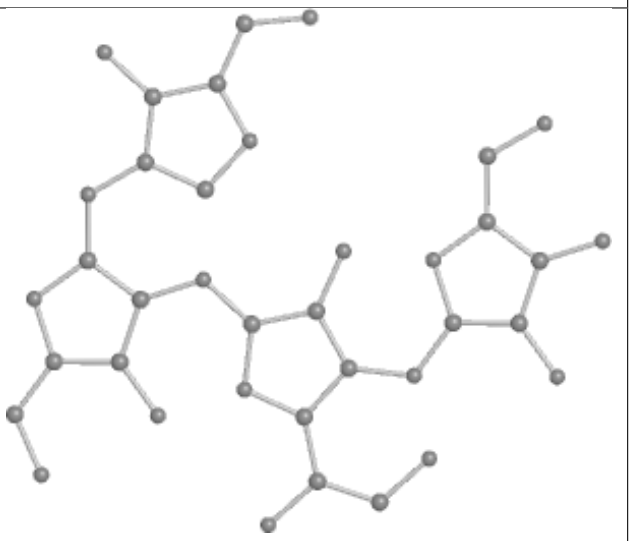
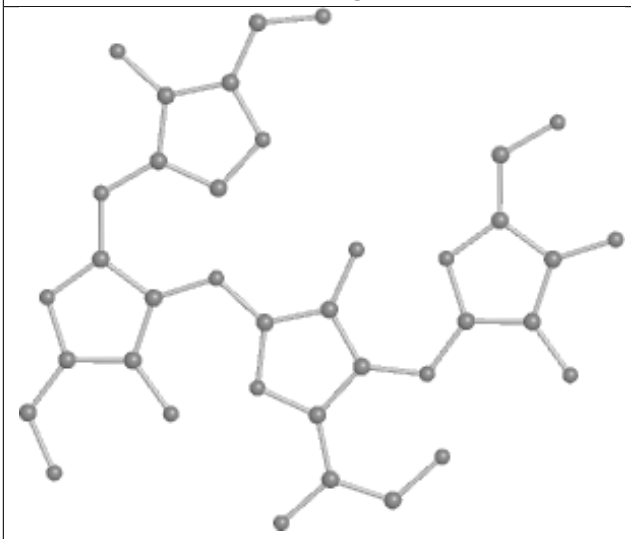
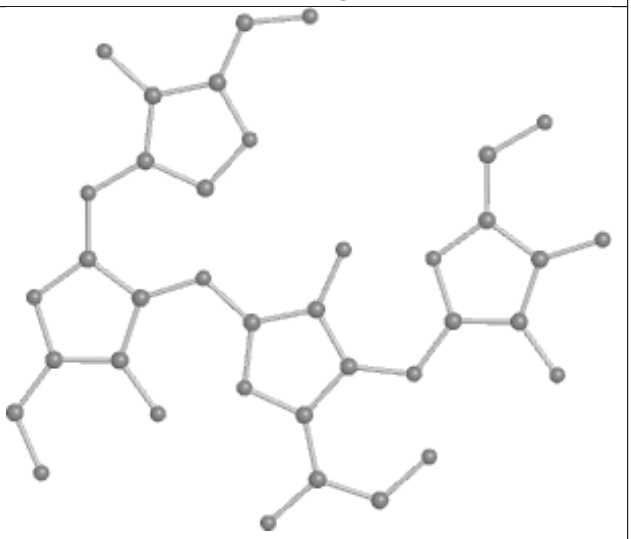
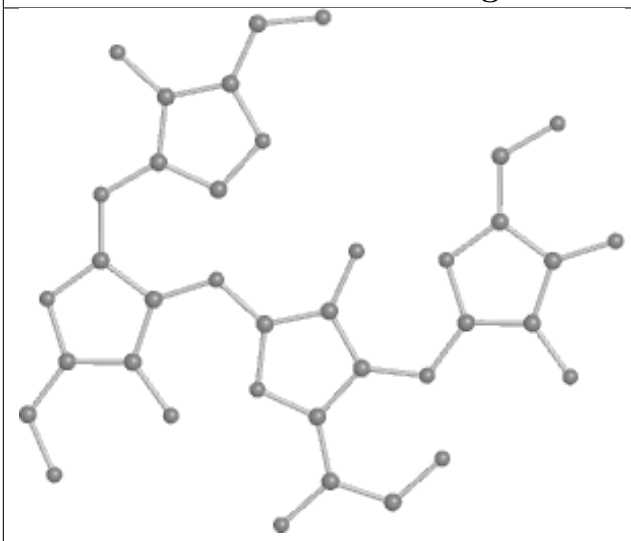
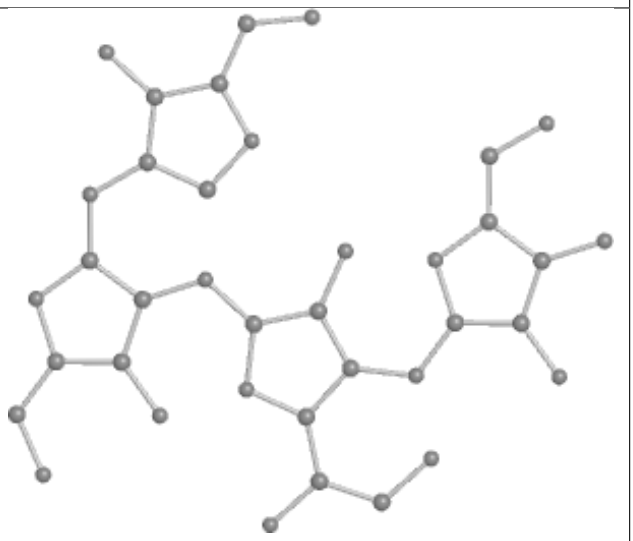
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain YB	
	
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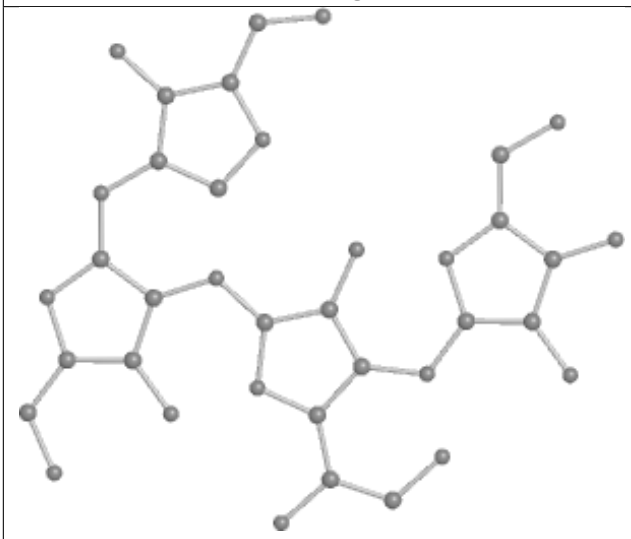
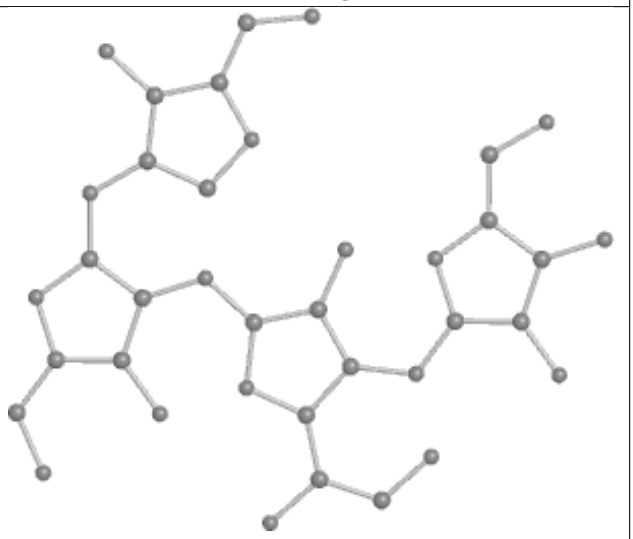
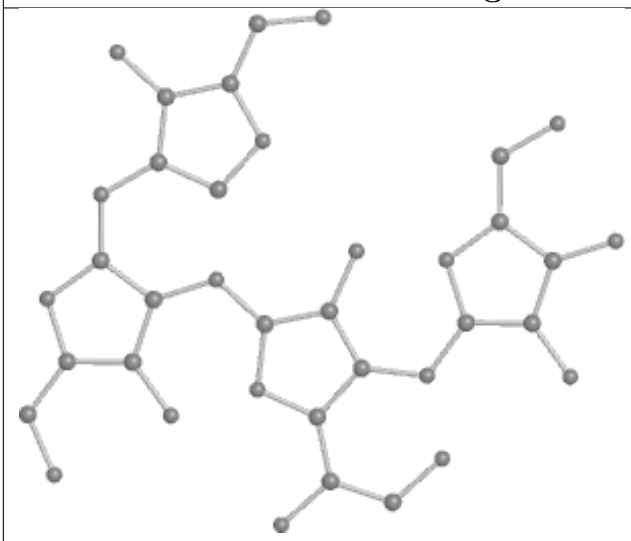
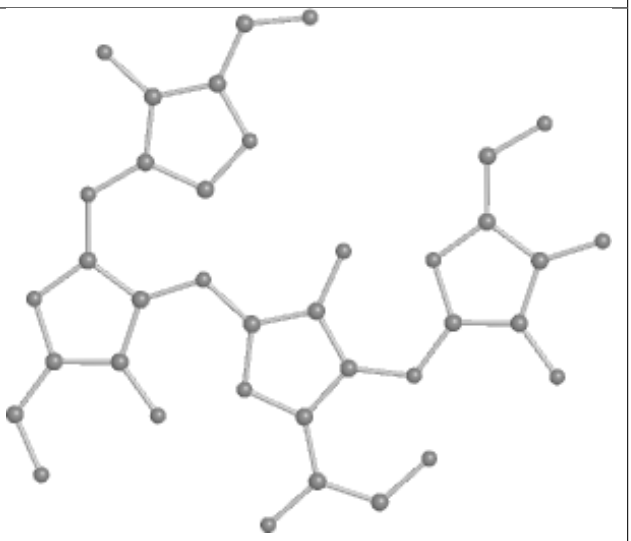
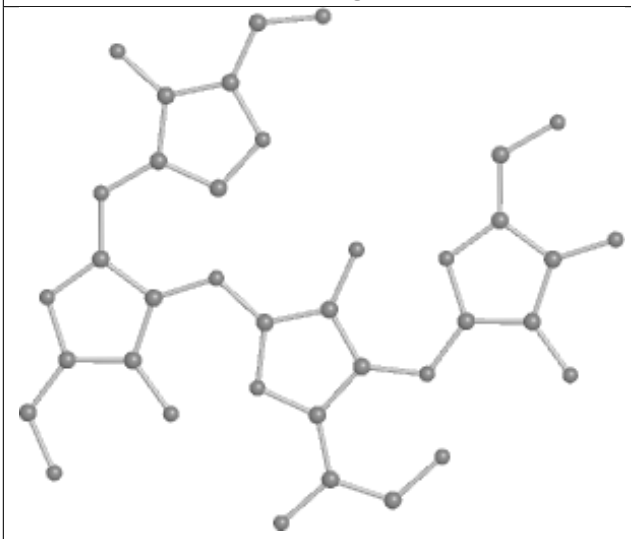
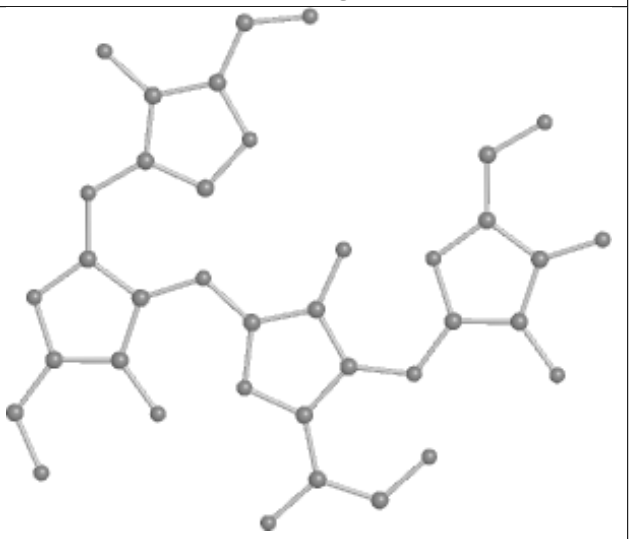
	
Torsions	**Rings**

Oligosaccharide Chain ZB	
 Bond lengths	 Bond angles
 Torsions	 Rings

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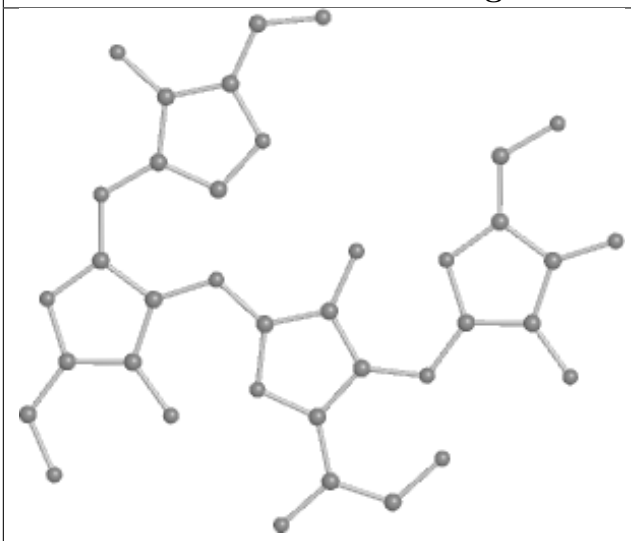
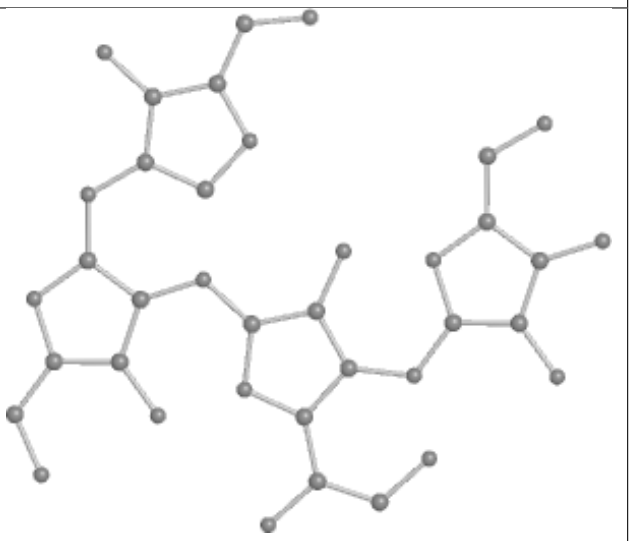
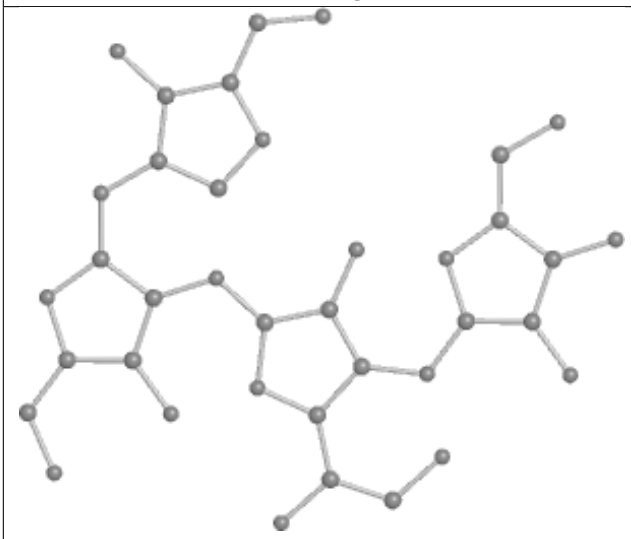
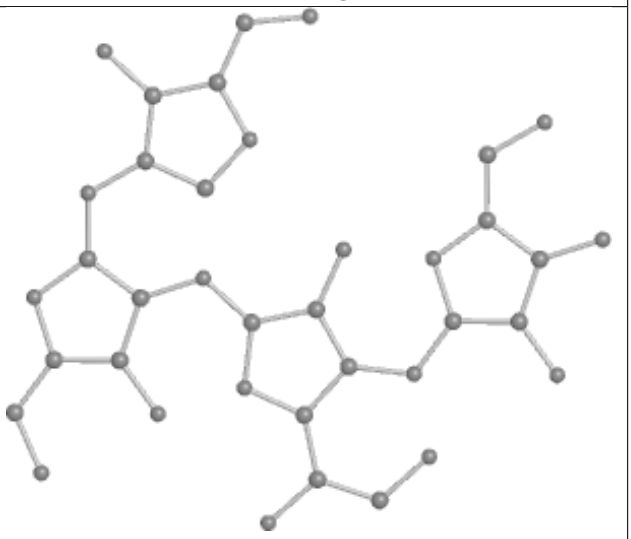
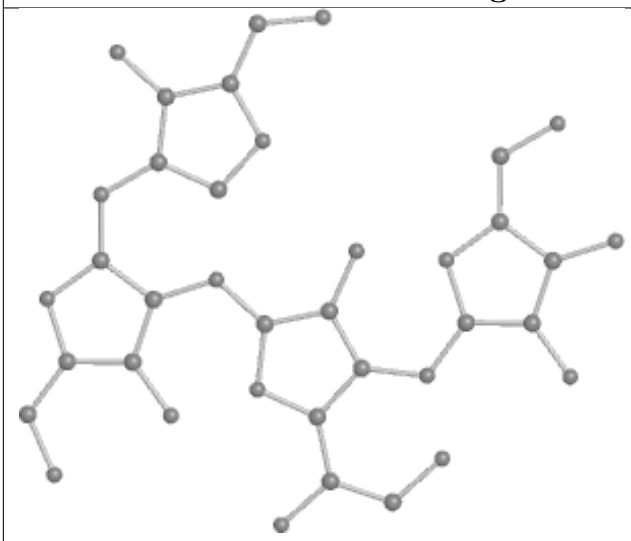
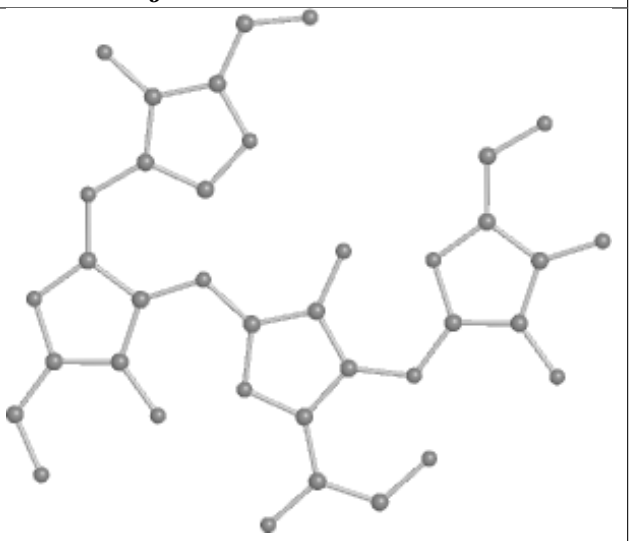
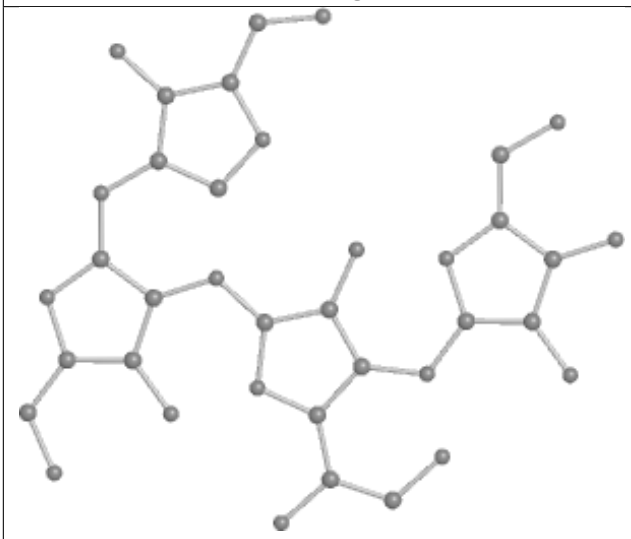
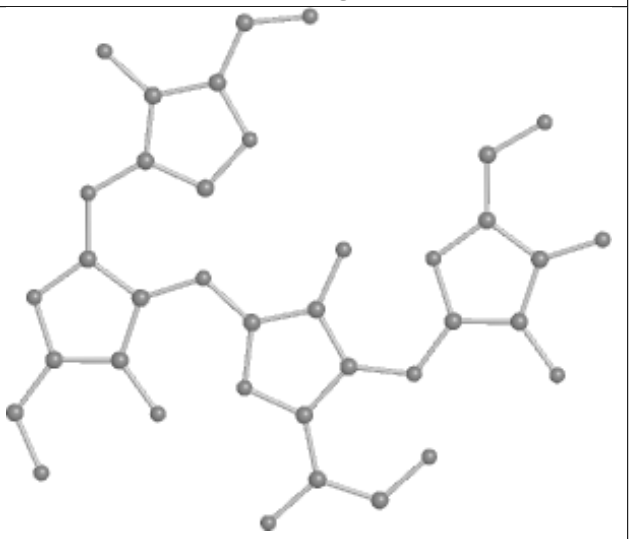
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain jB	
 Bond lengths	 Bond angles
 Torsions	 Rings

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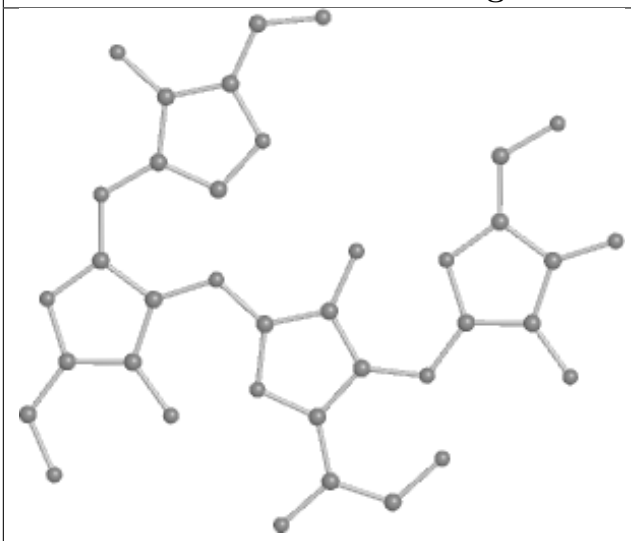
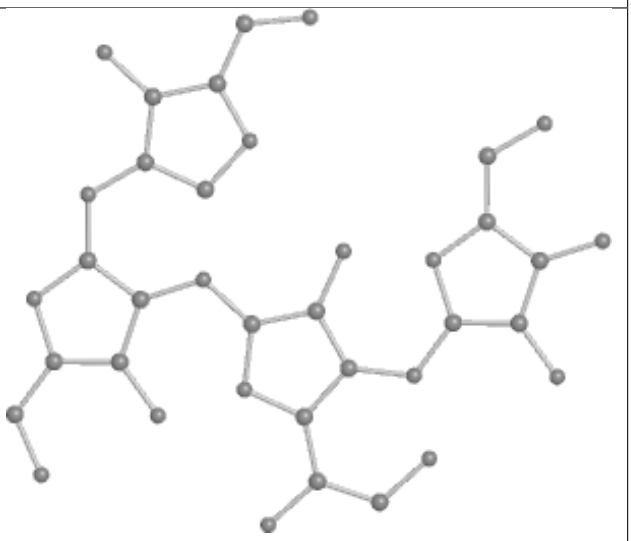
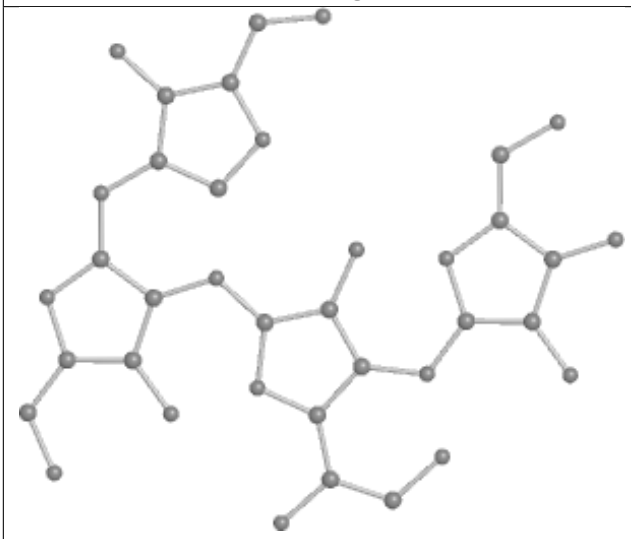
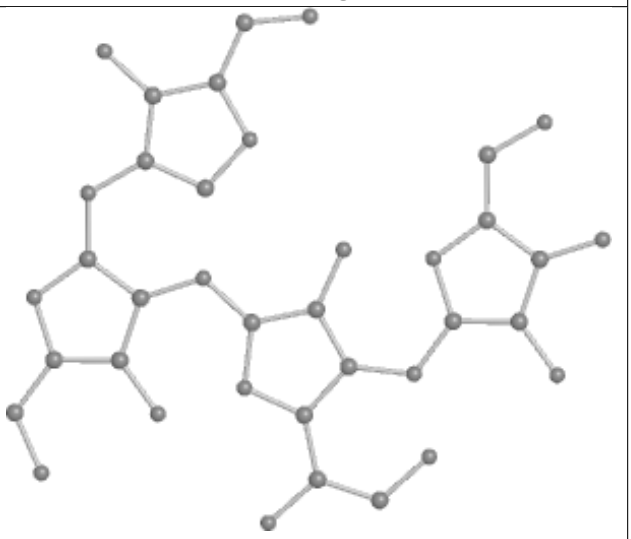
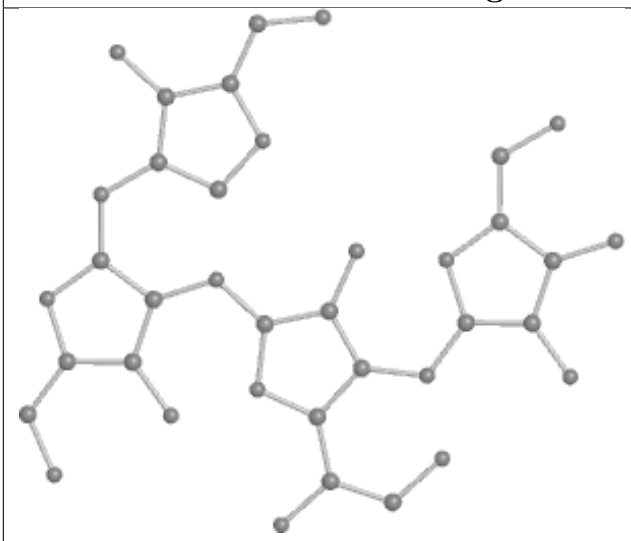
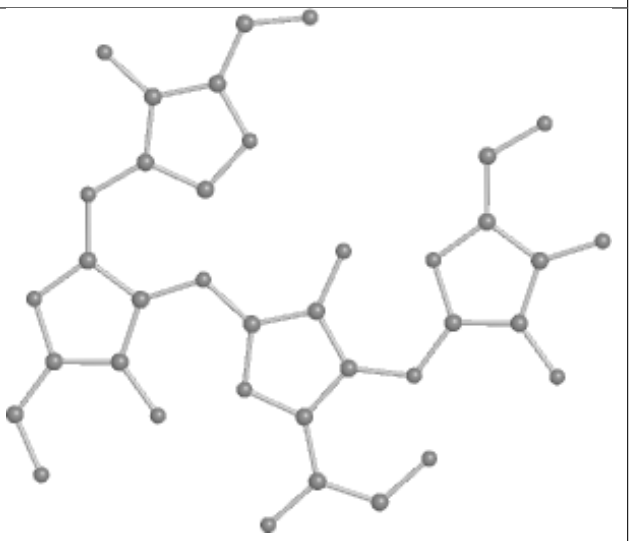
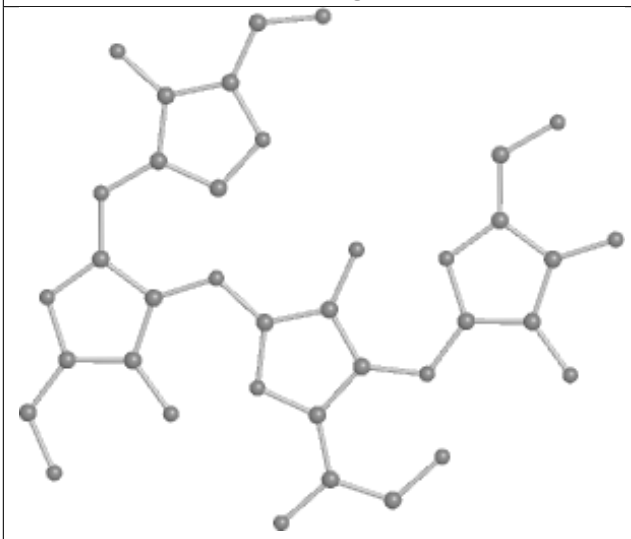
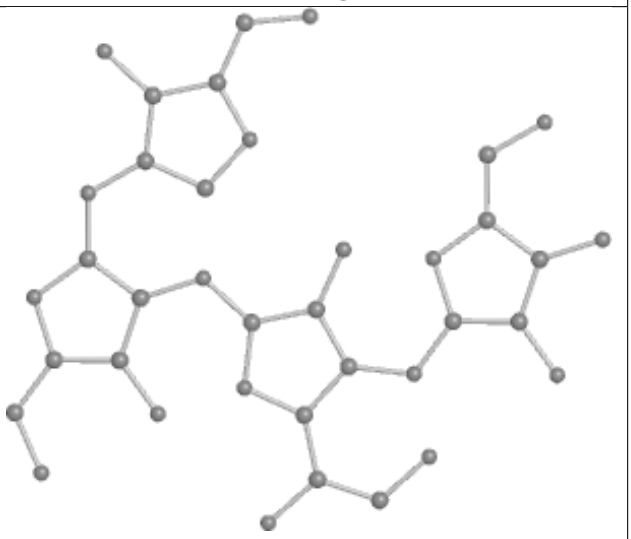
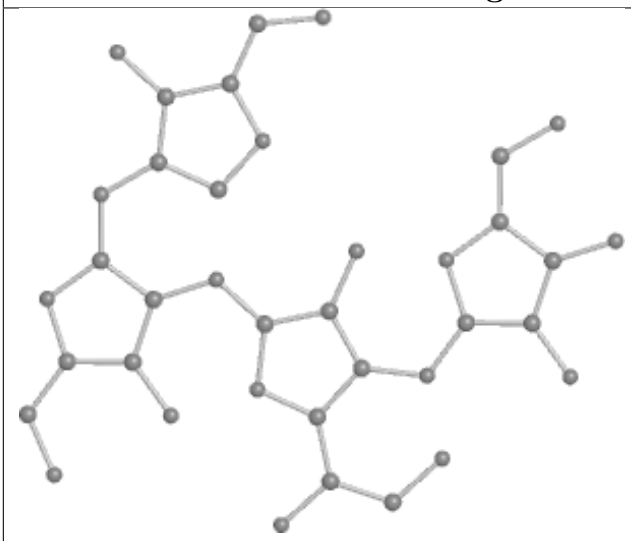
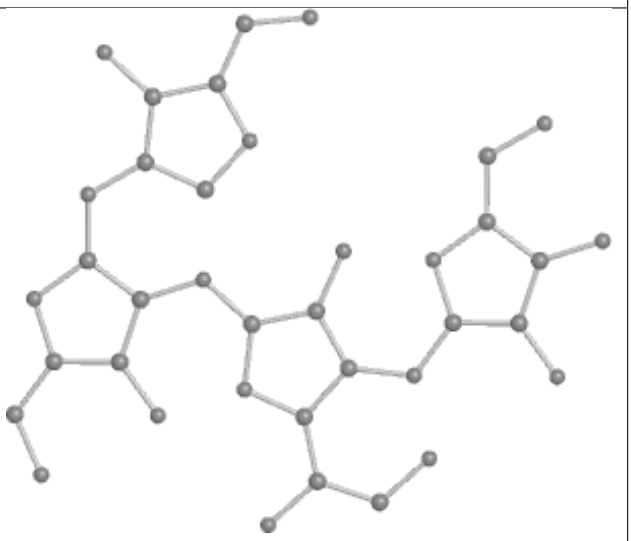
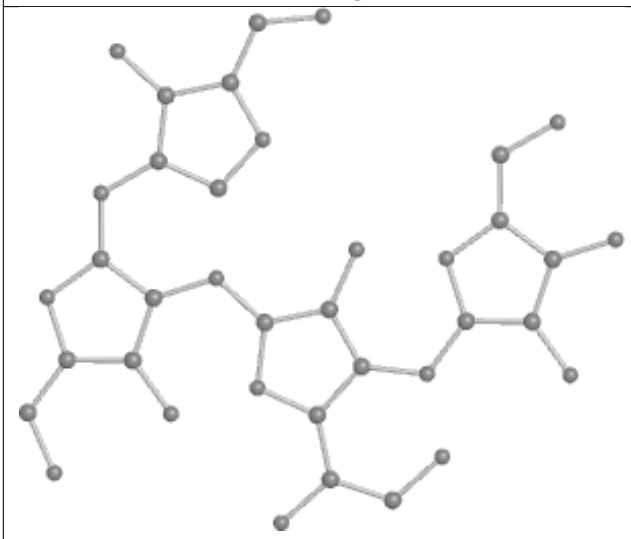
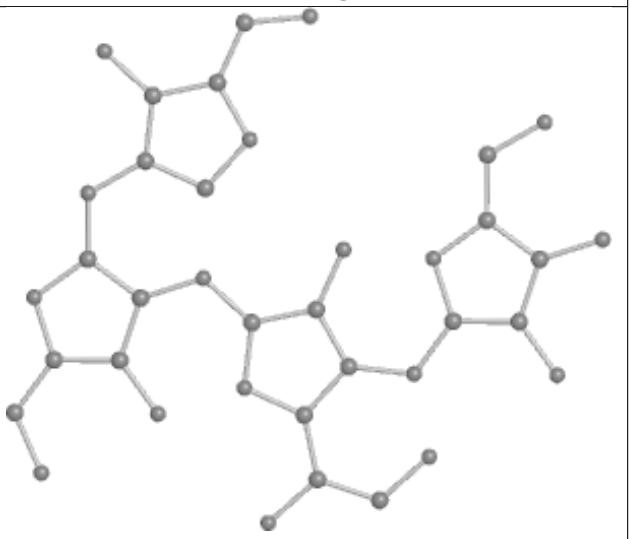
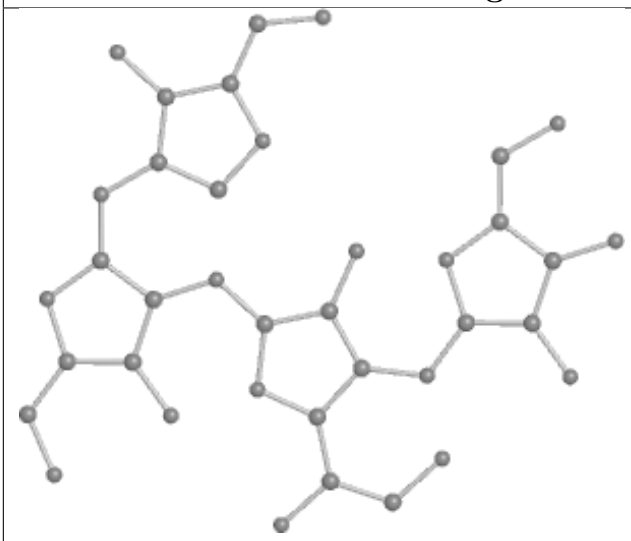
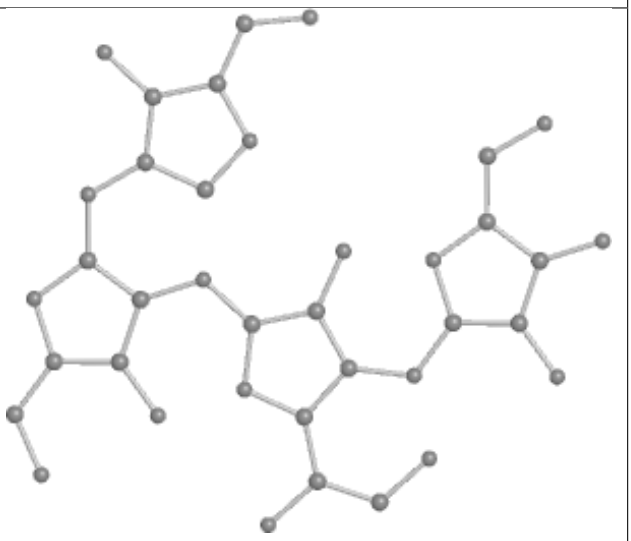
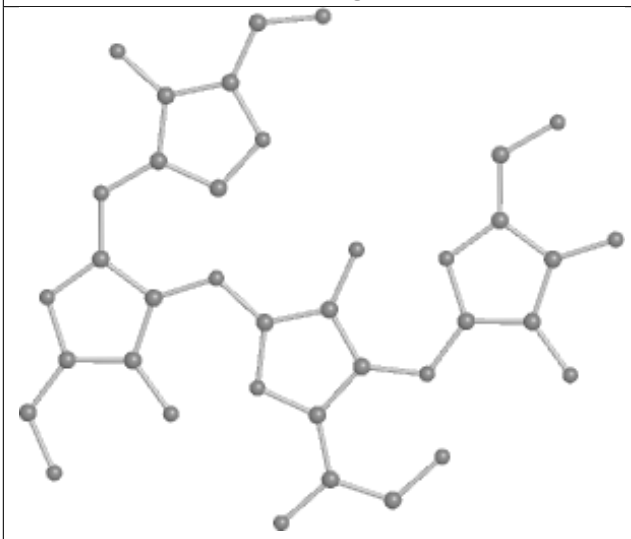
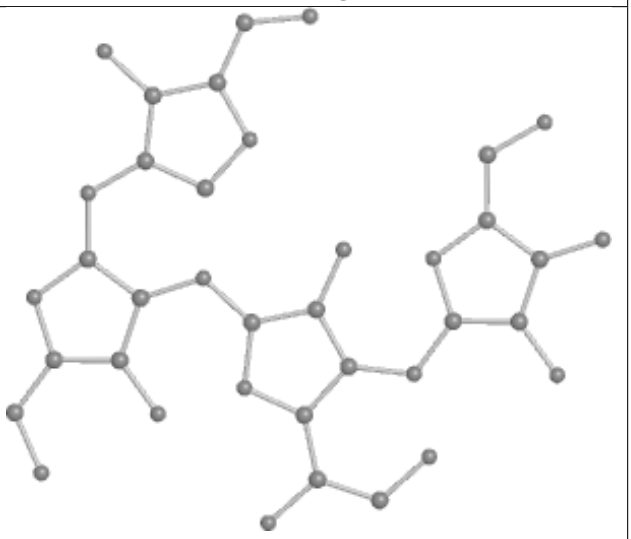
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 1B	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 2B	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 6B	
 Bond lengths	 Bond angles
 Torsions	 Rings

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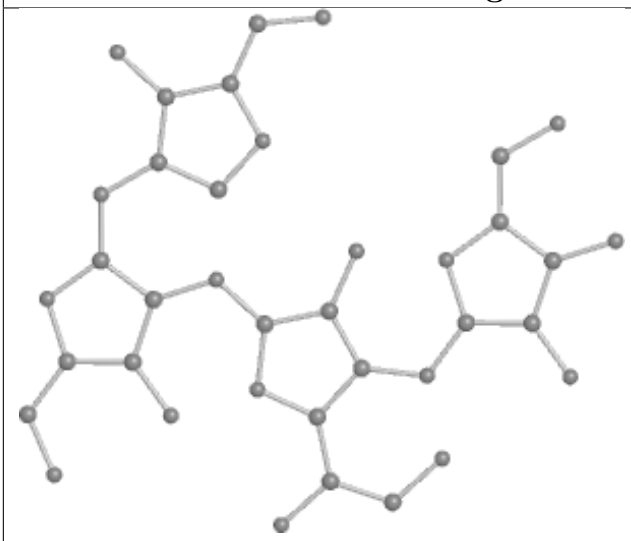
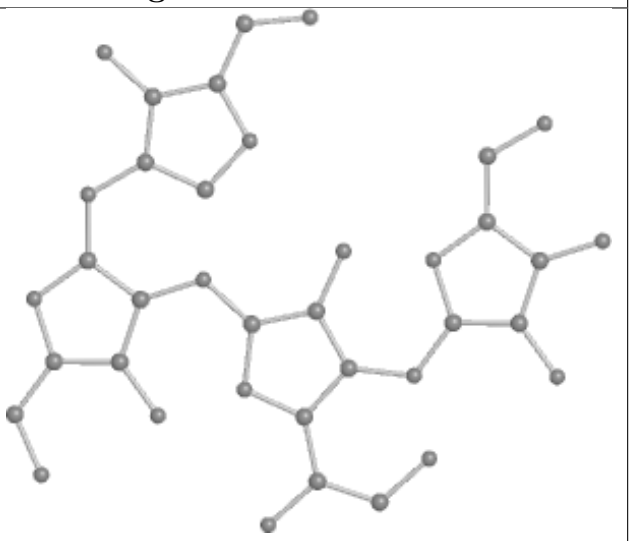
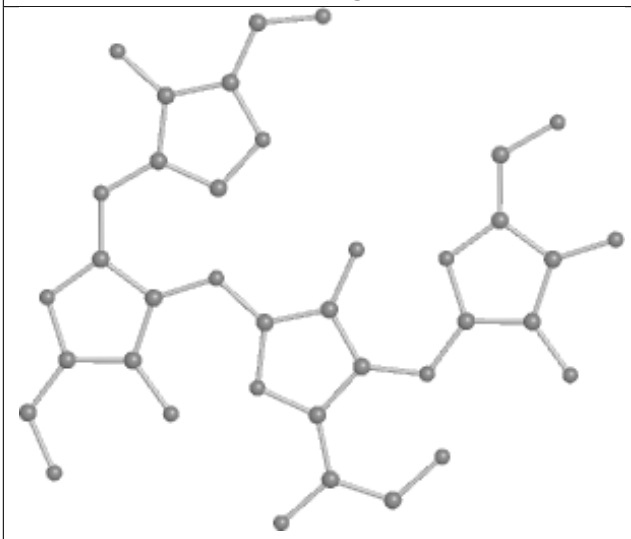
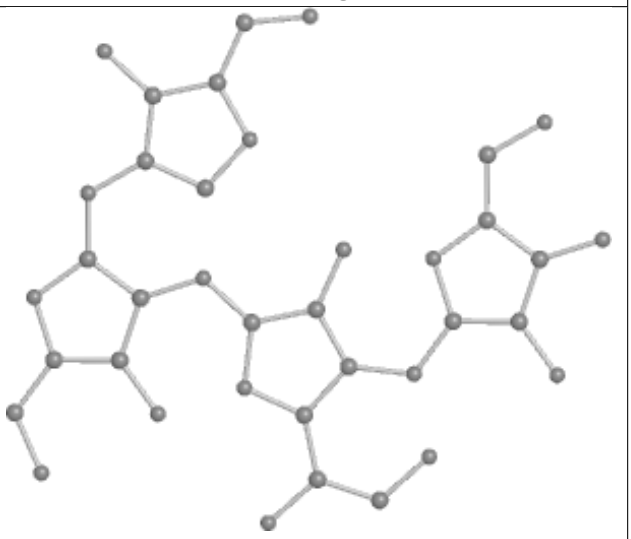
 Bond lengths	 Bond angles
 Torsions	 Rings

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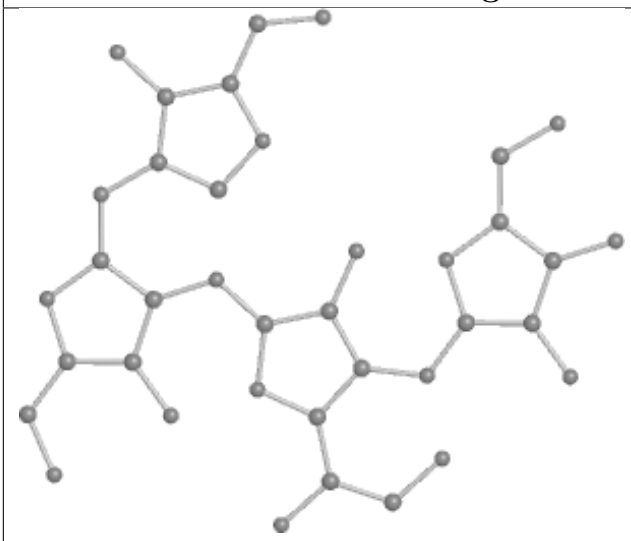
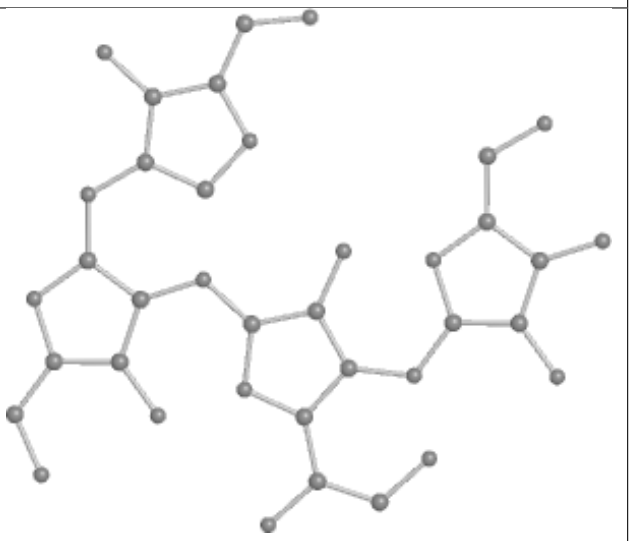
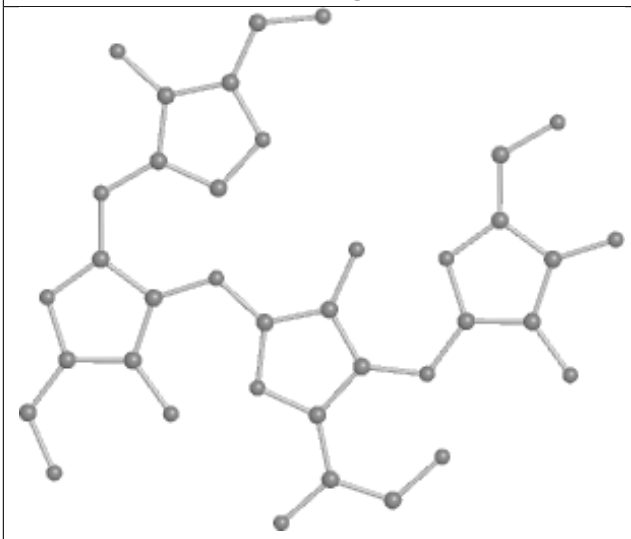
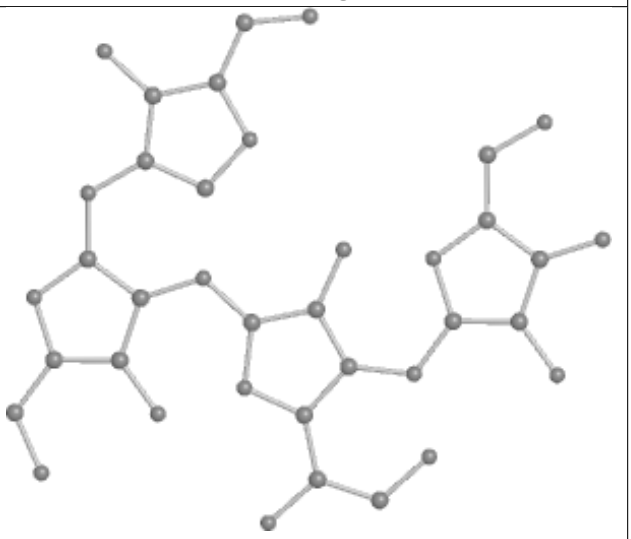
 Bond lengths	 Bond angles
 Torsions	 Rings

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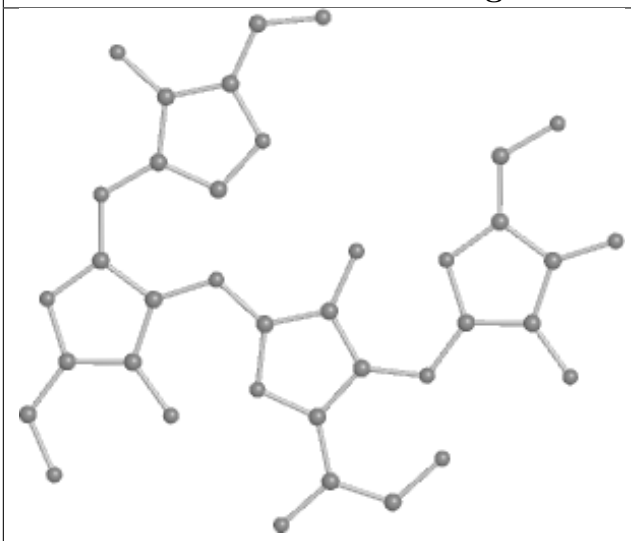
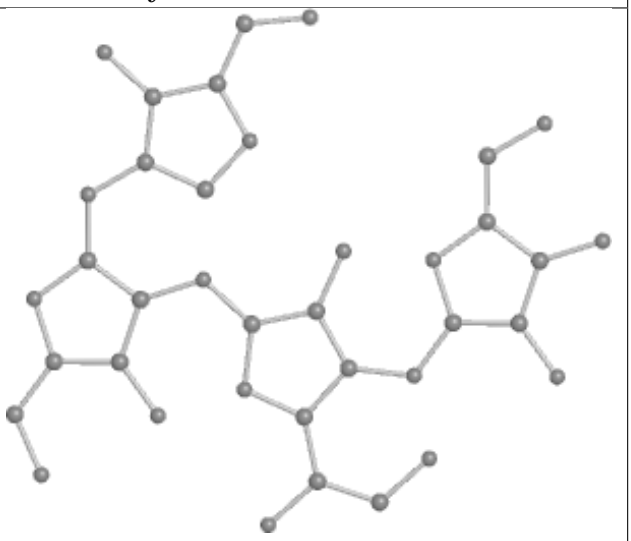
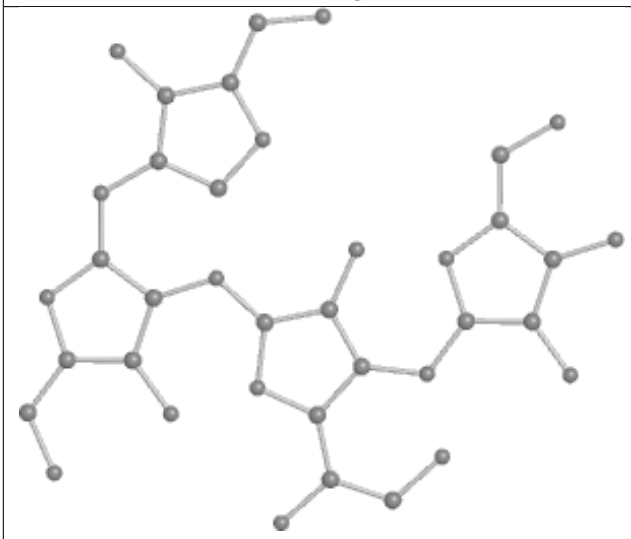
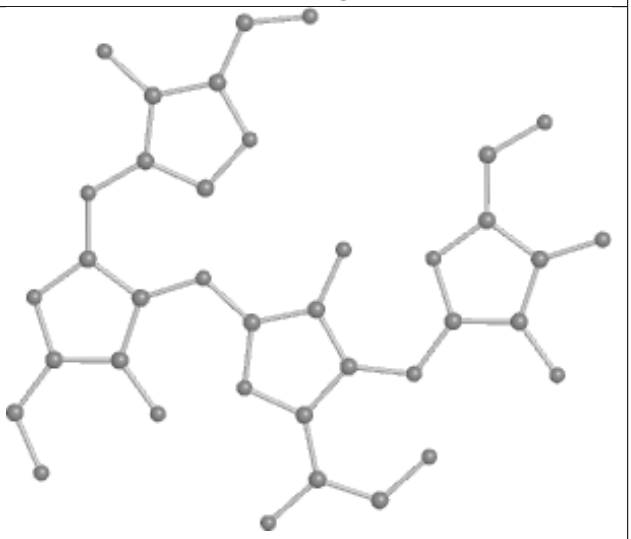
 Bond lengths	 Bond angles
 Torsions	 Rings

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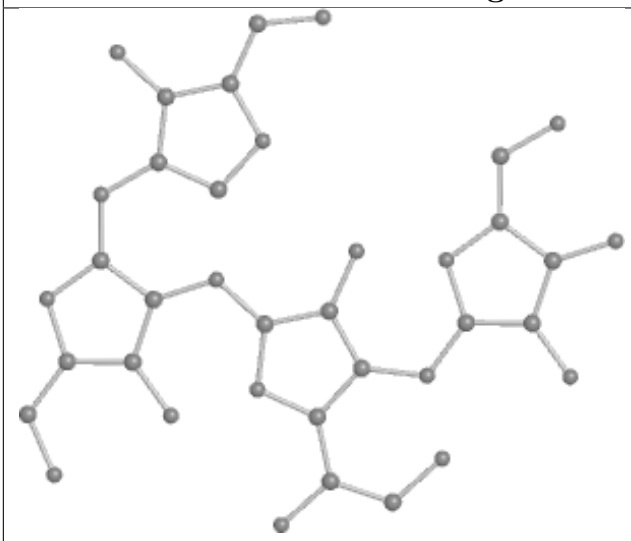
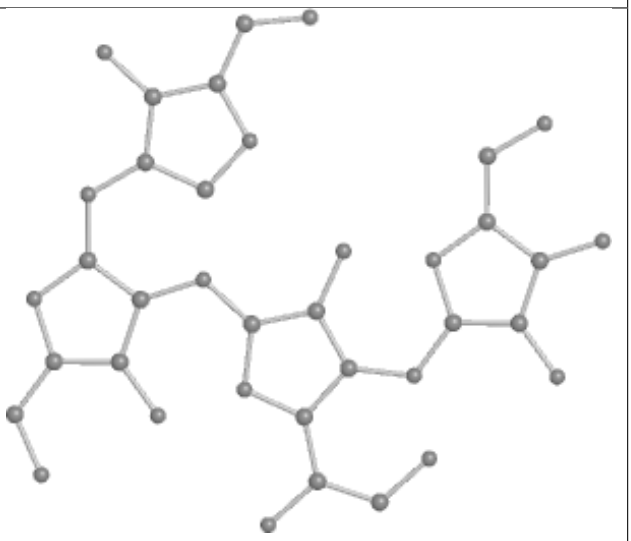
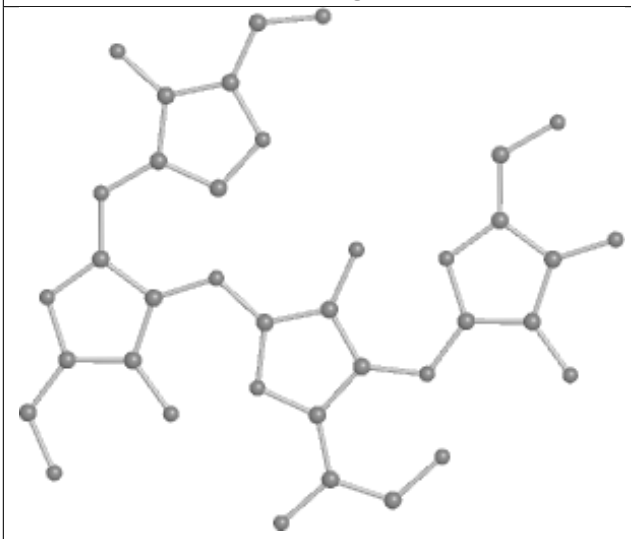
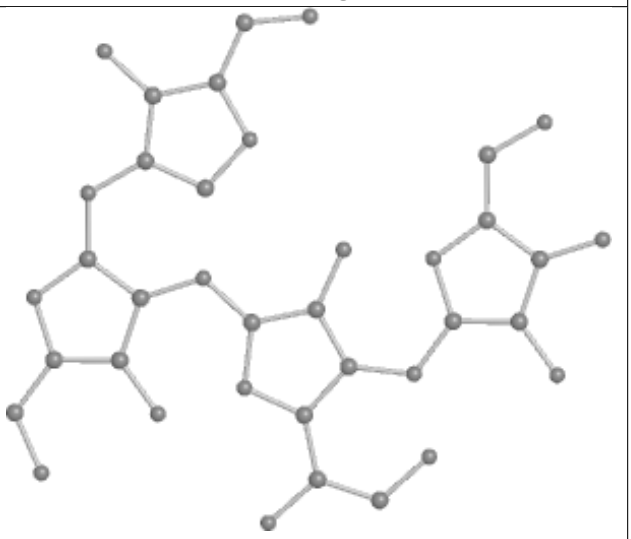
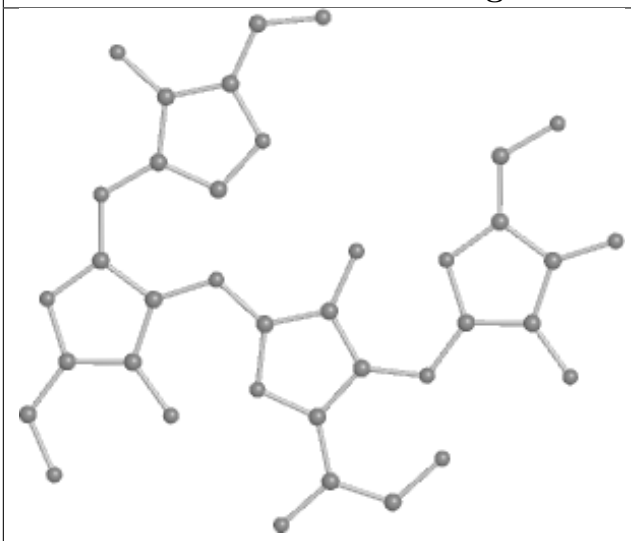
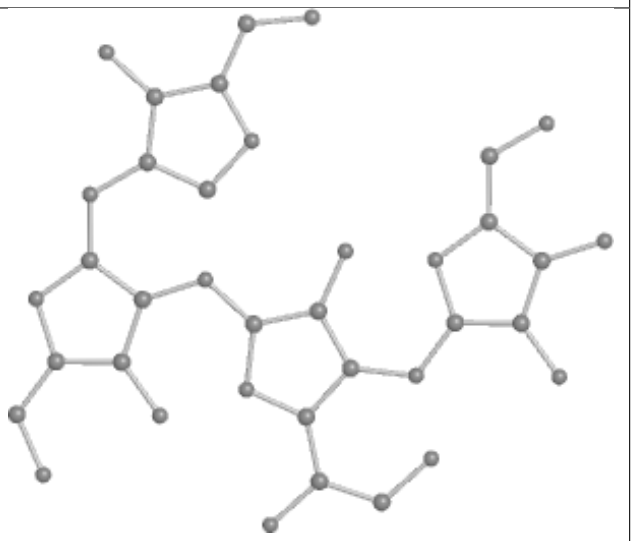
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 3C	
	
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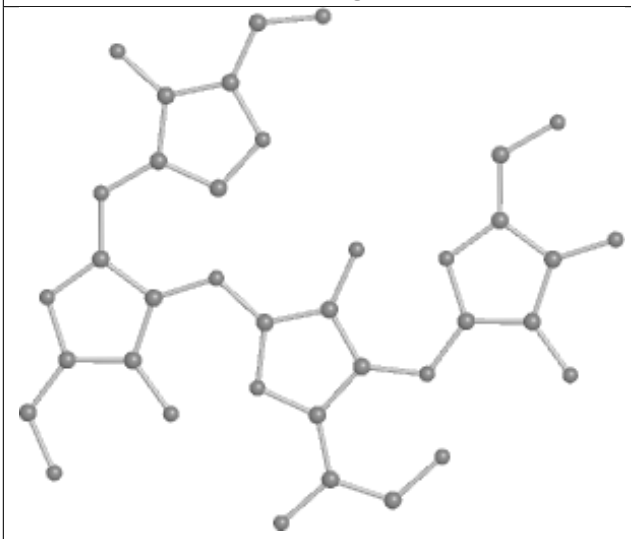
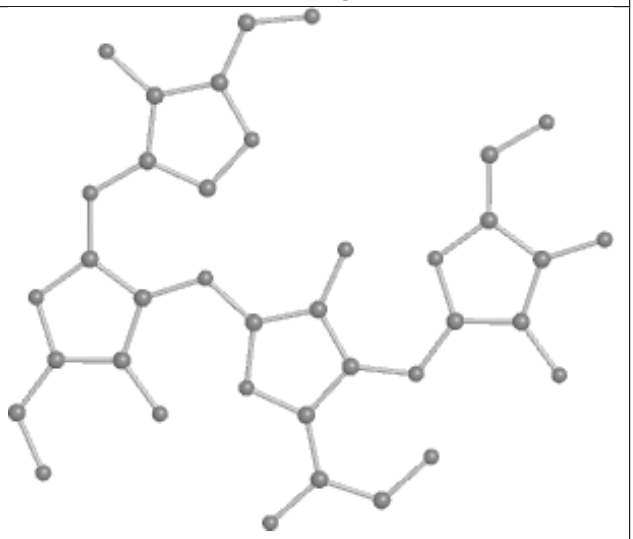
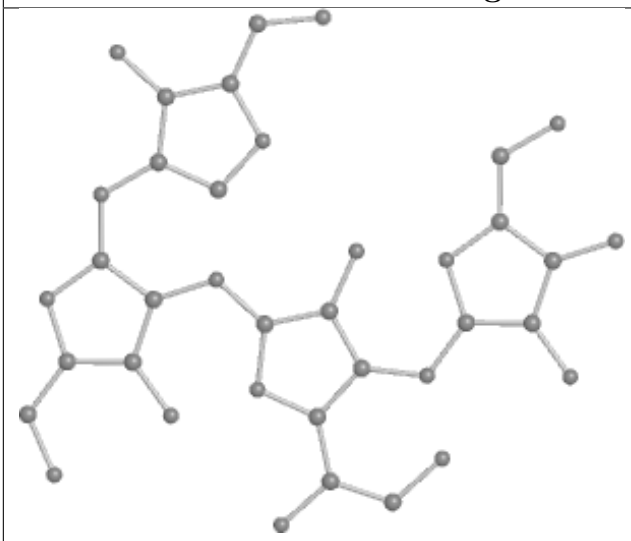
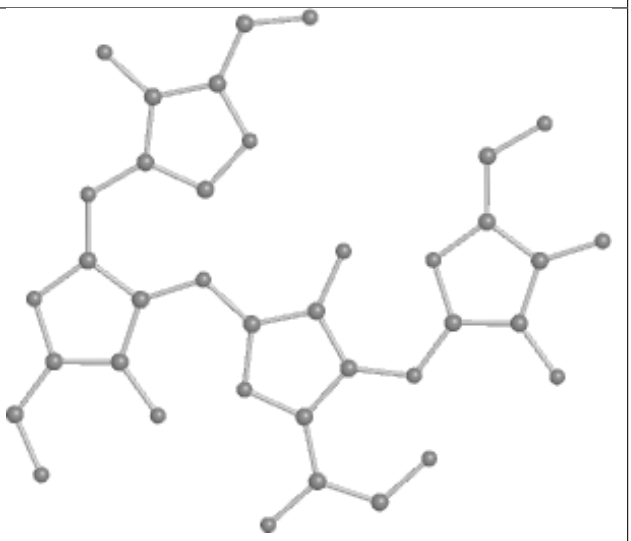
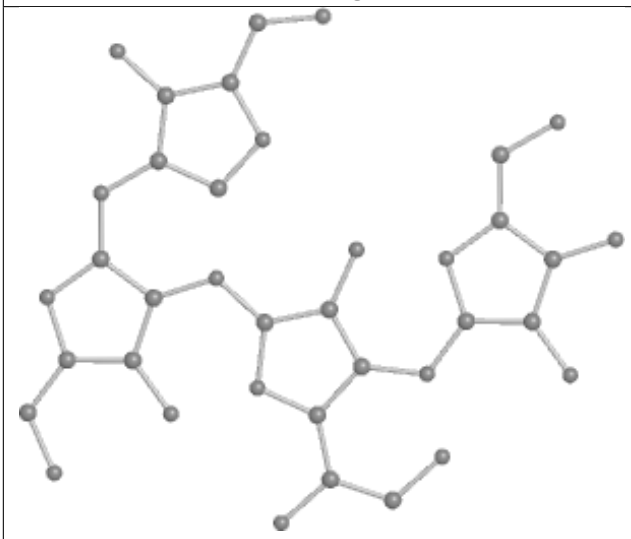
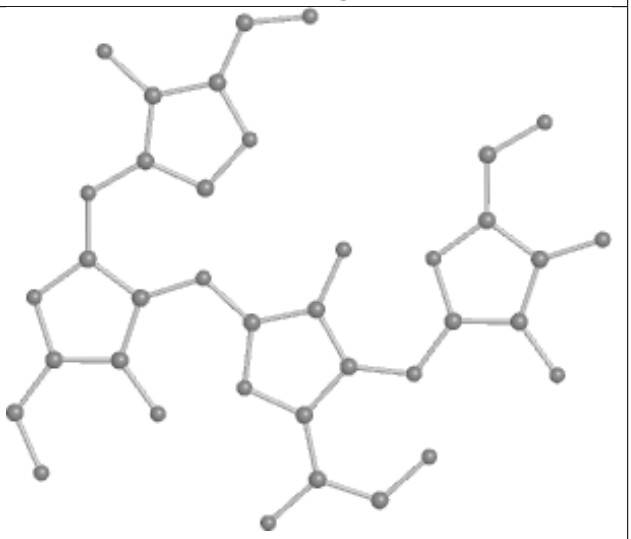
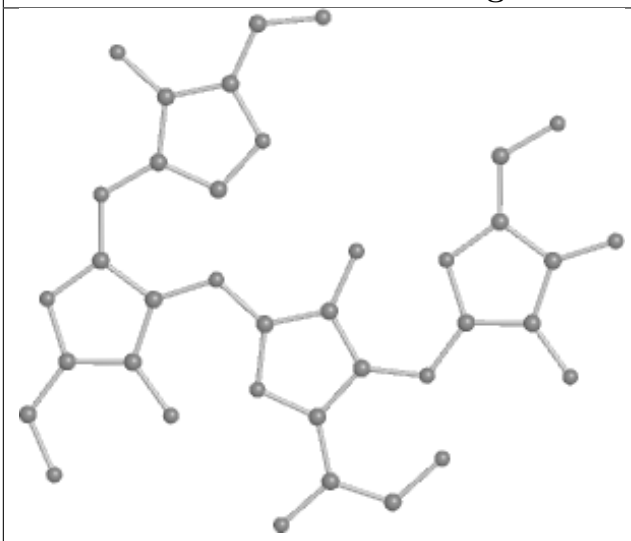
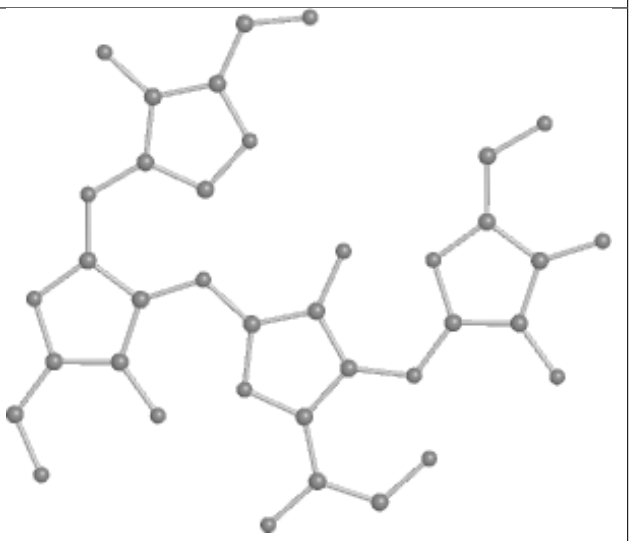
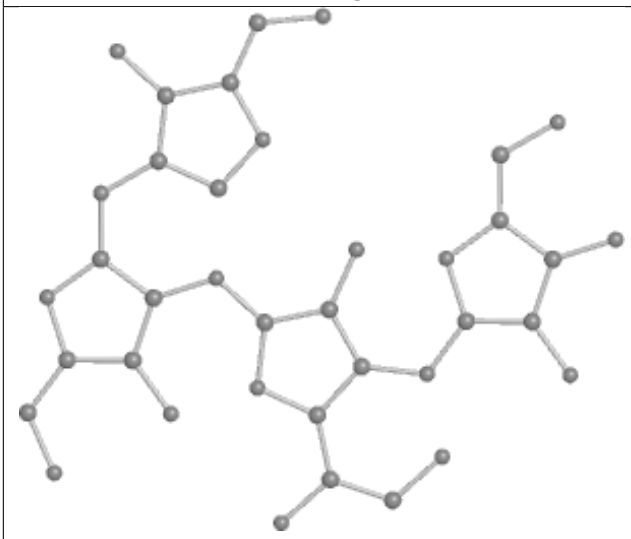
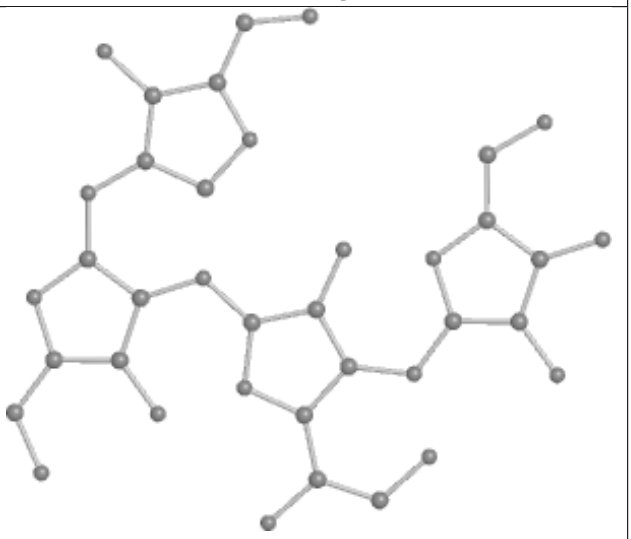
	
Torsions	**Rings**

Oligosaccharide Chain dD	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain tD	
 Bond lengths	 Bond angles
 Torsions	 Rings

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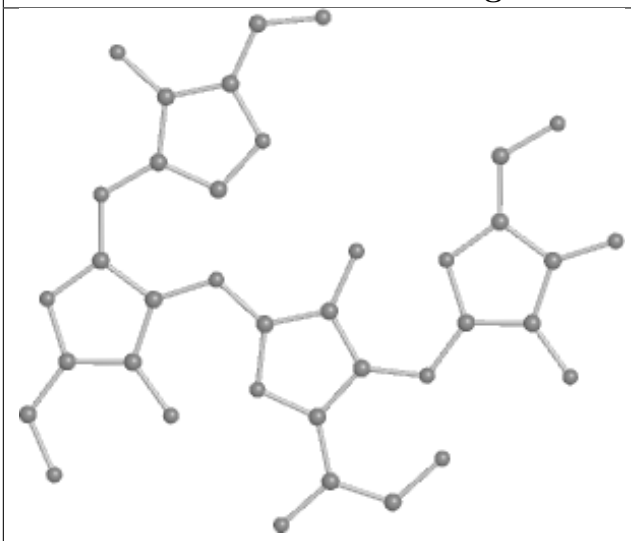
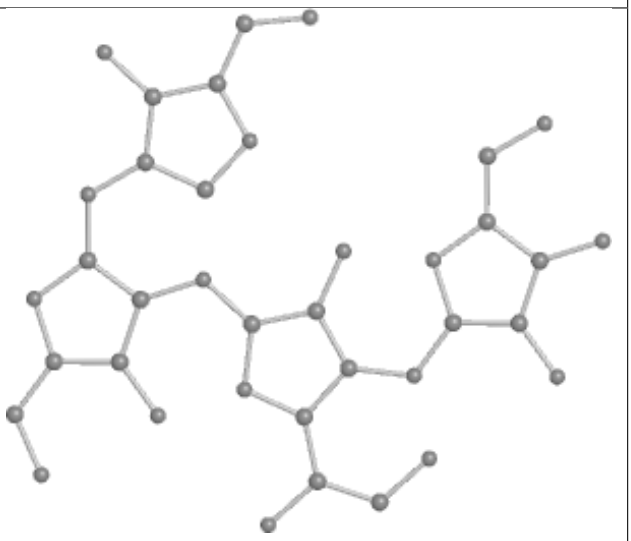
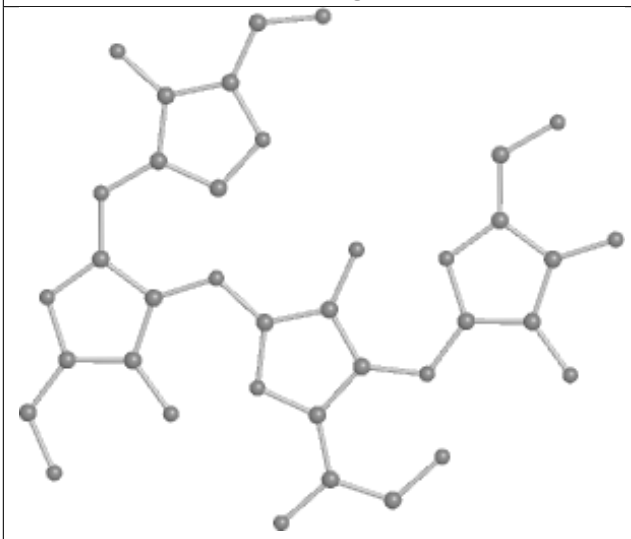
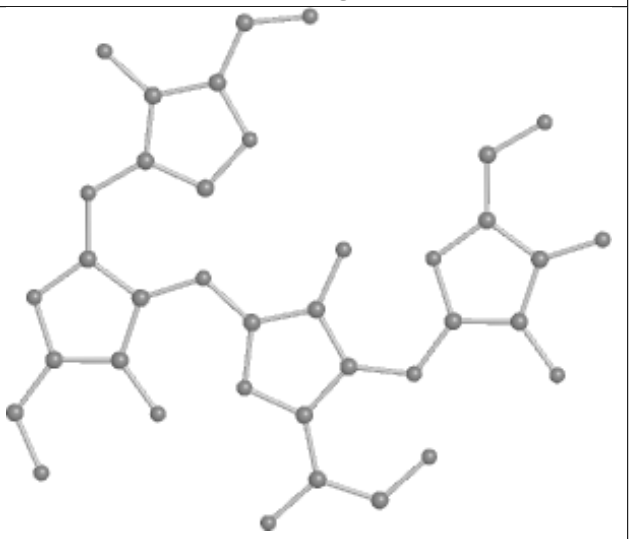
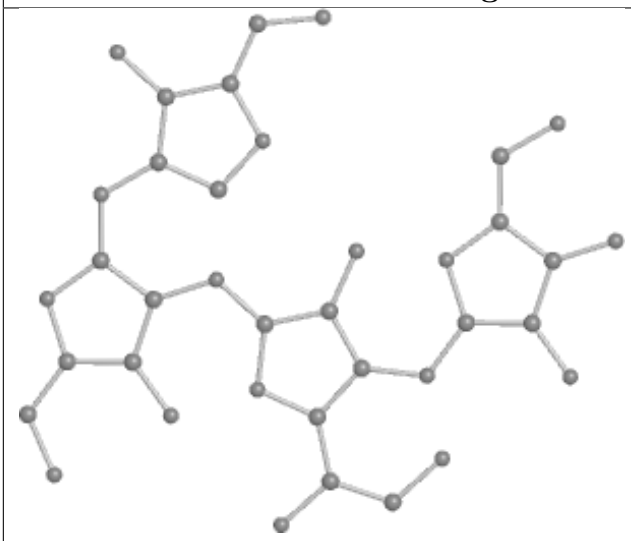
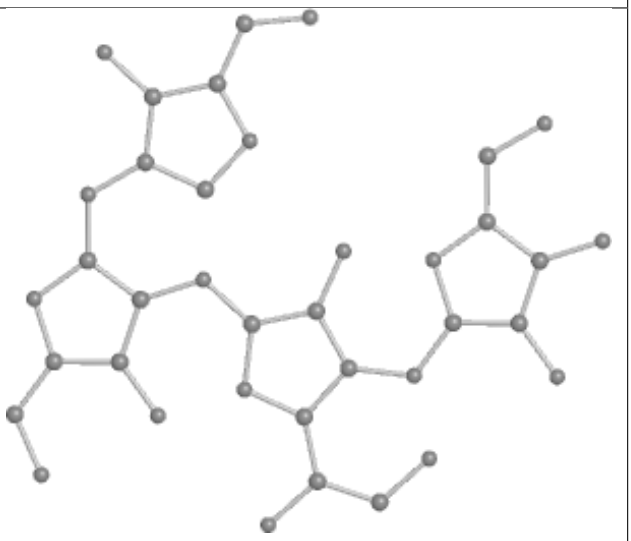
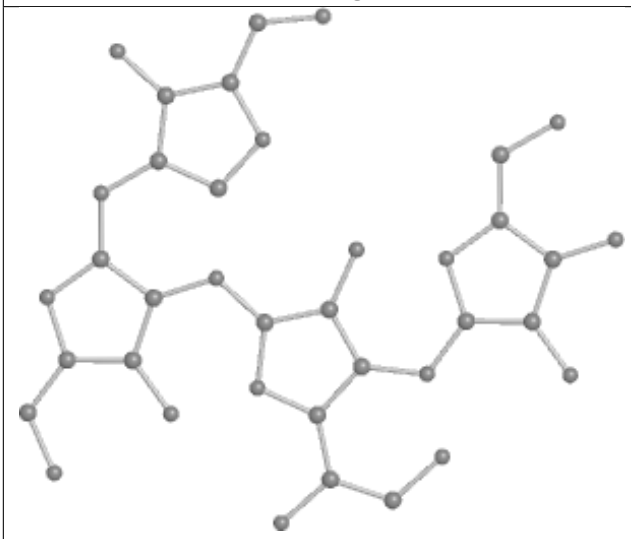
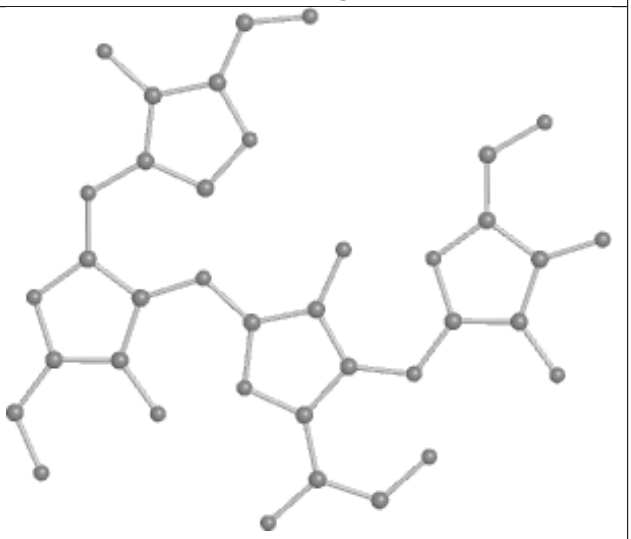
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain wD	
 Bond lengths	 Bond angles
 Torsions	 Rings

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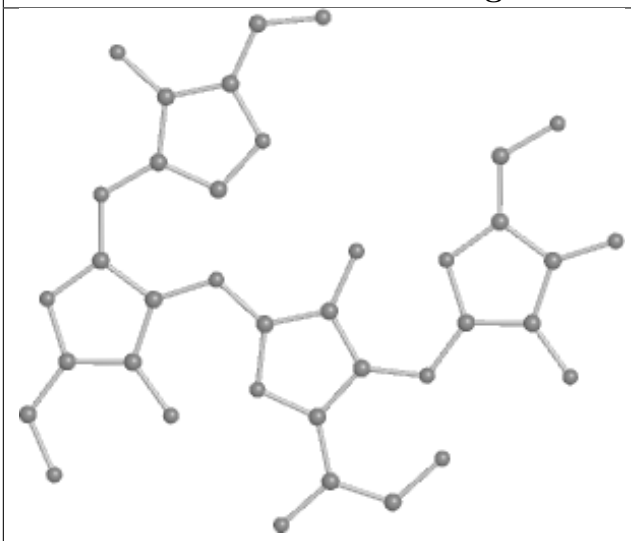
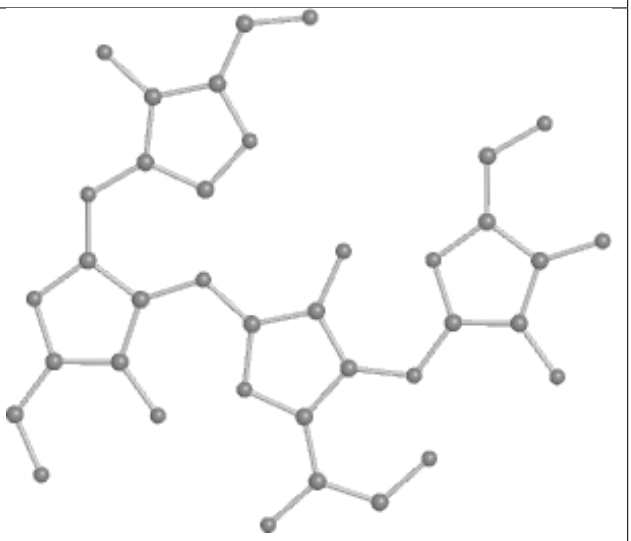
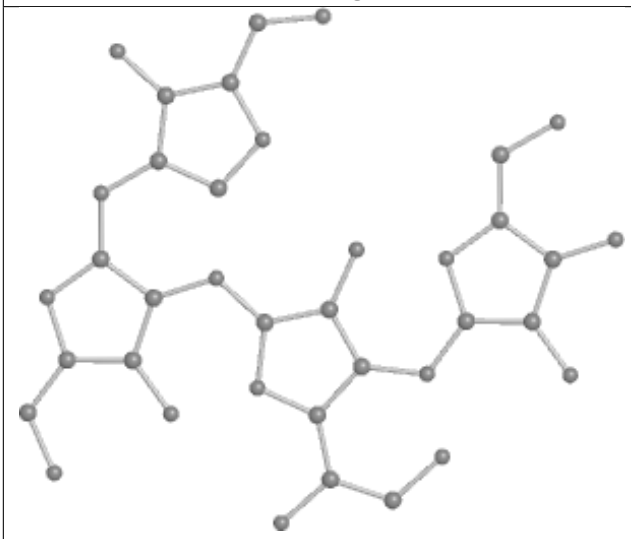
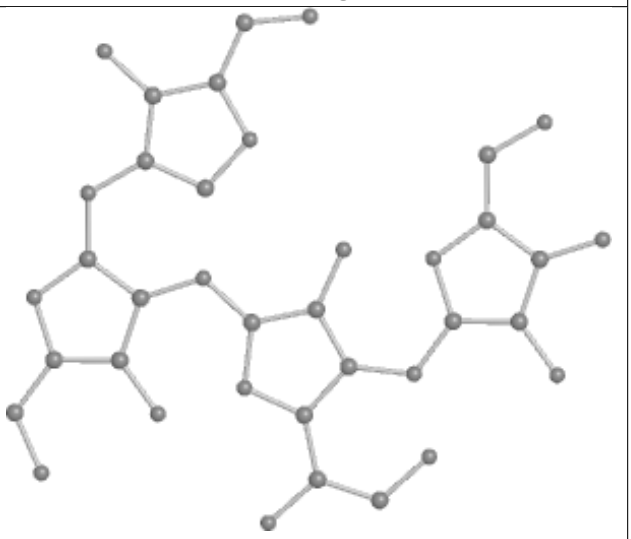
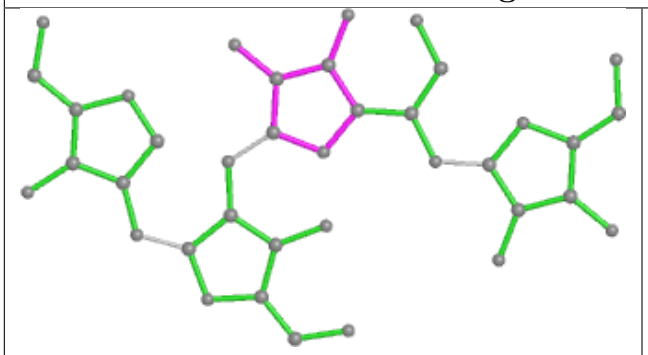
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain p



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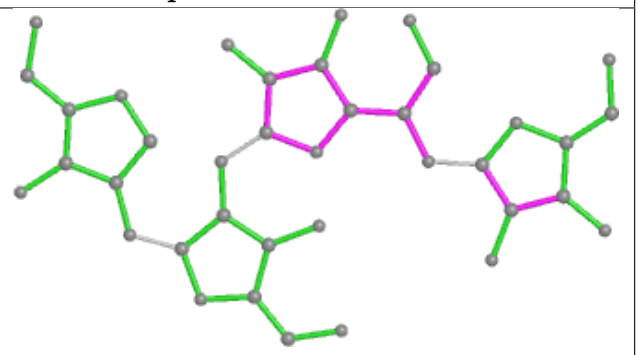
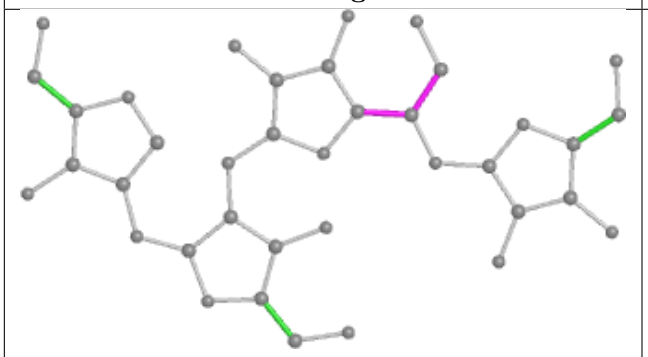


Bond angles



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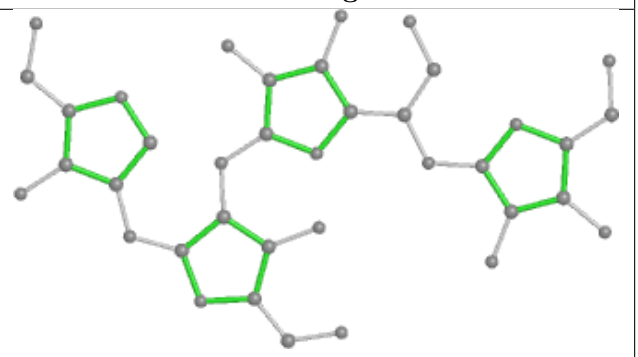
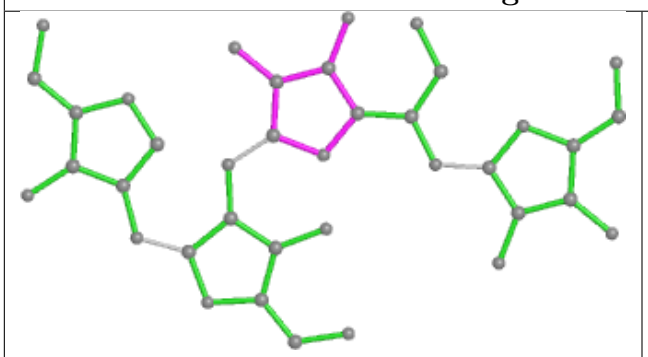


Rings

Oligosaccharide Chain s



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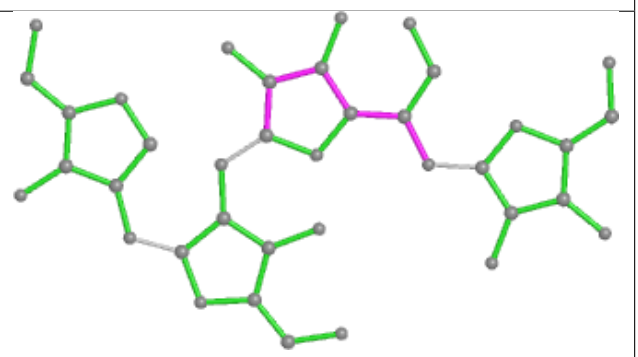

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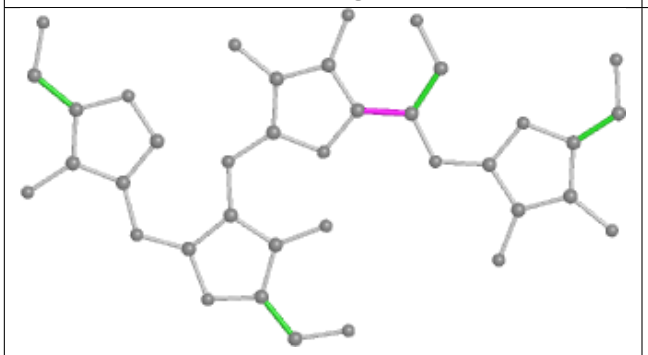

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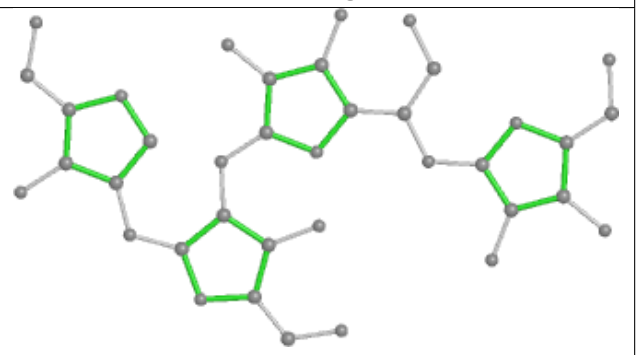
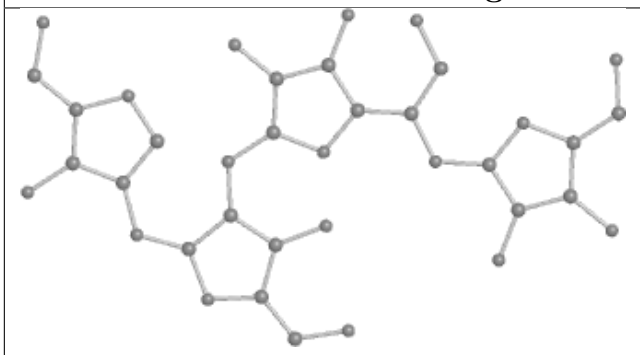


Rings

Oligosaccharide Chain nA



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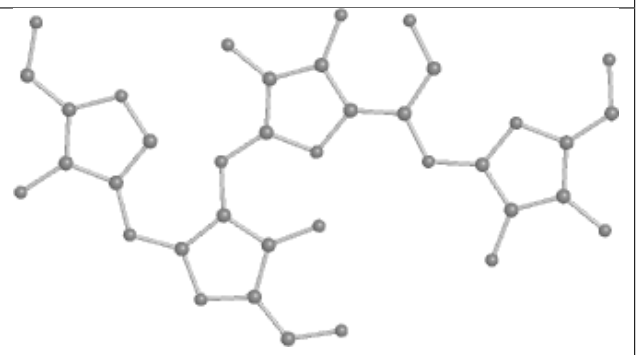

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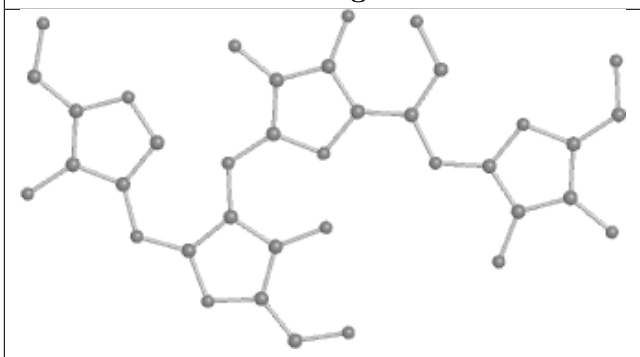

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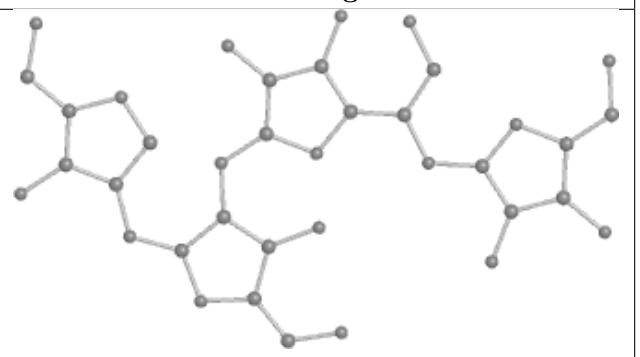
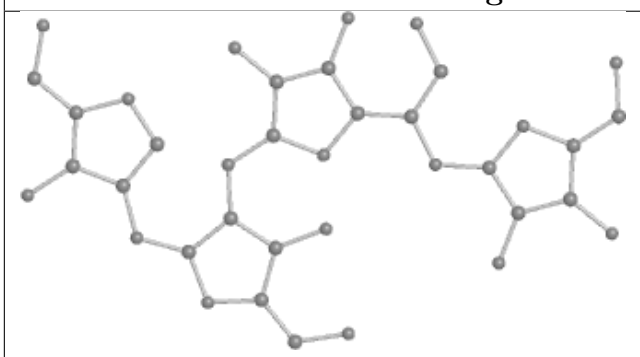
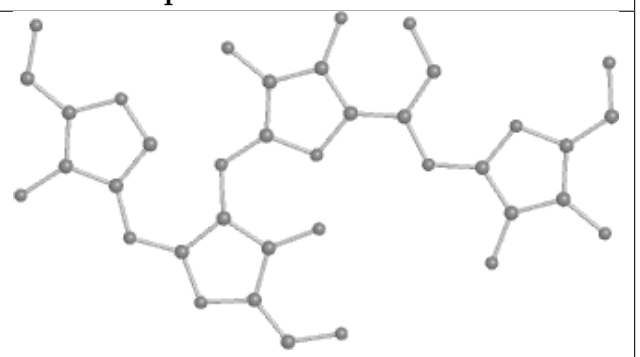


Rings

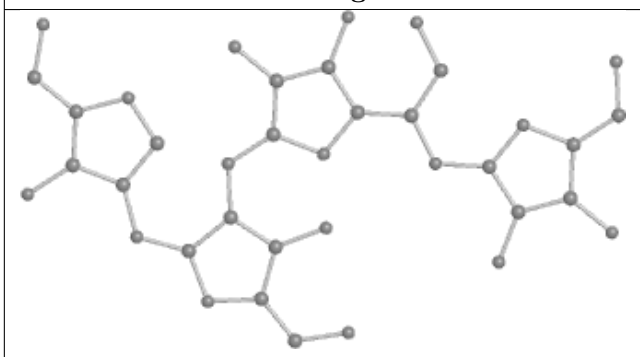
Oligosaccharide Chain qA



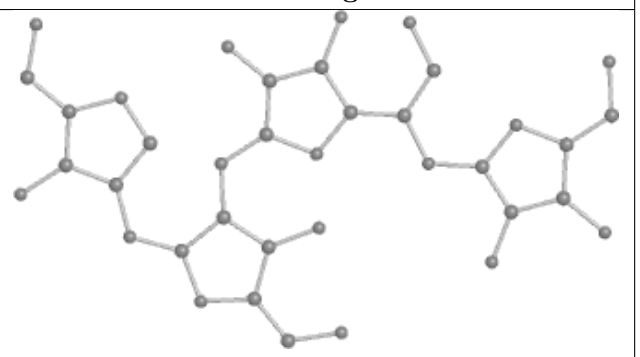
Bond lengths



Bond angles

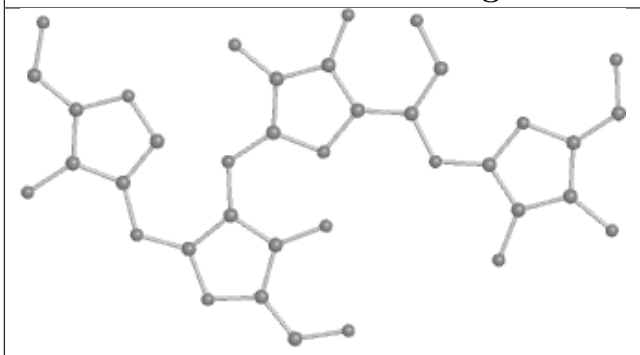


Torsions

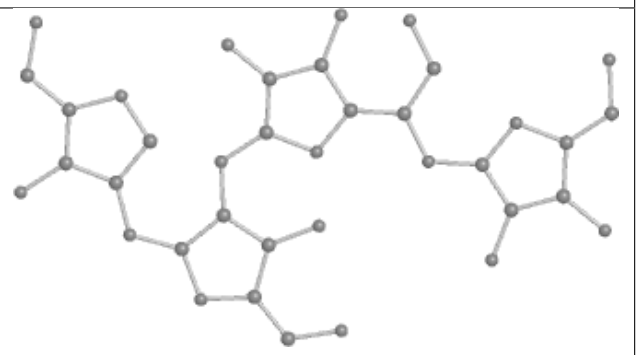


Rings

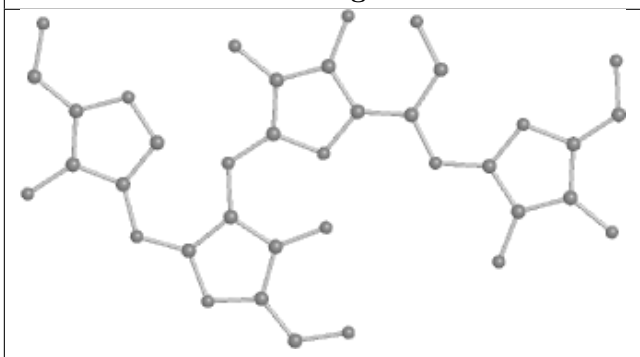
Oligosaccharide Chain HB



Bond lengths



Bond angles



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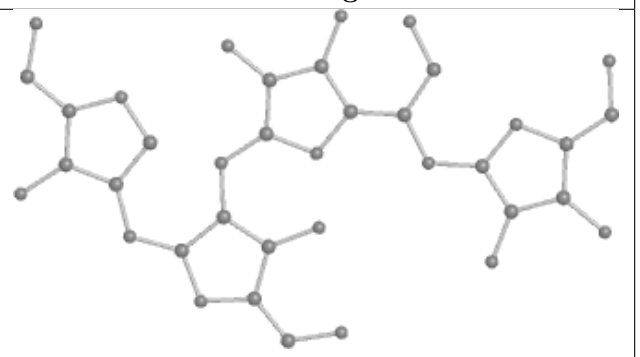
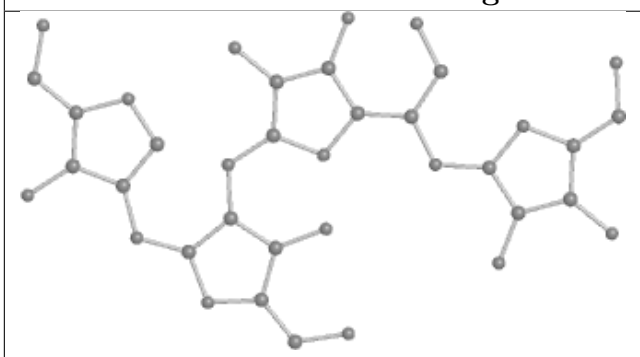


Rings

Oligosaccharide Chain KB



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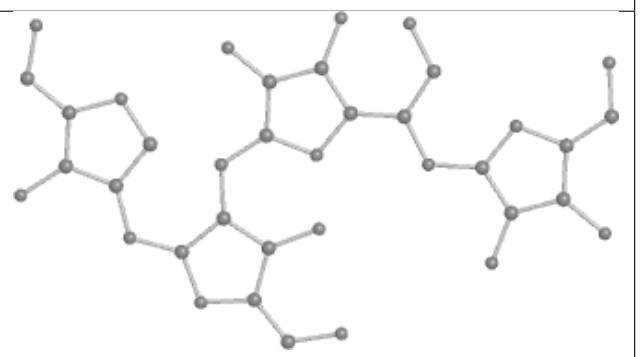
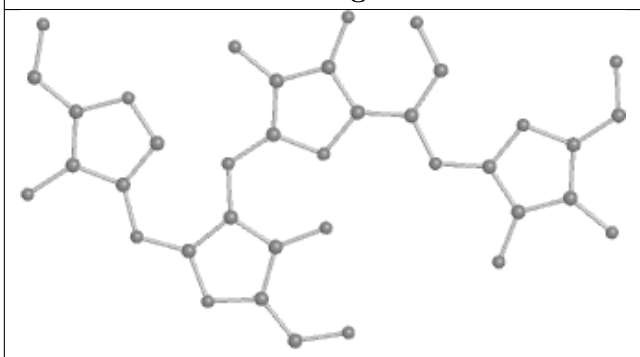


Bond angles



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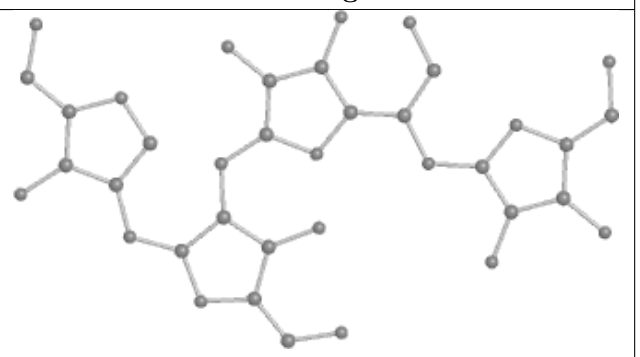
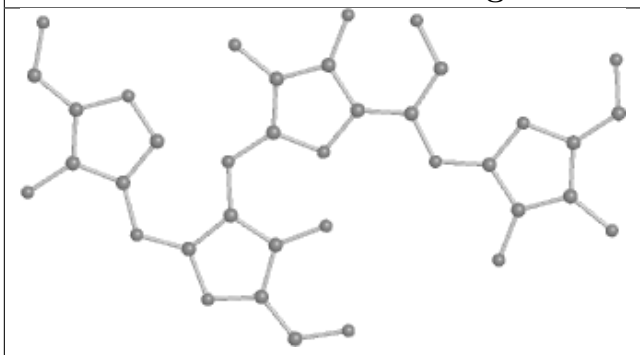


Rings

Oligosaccharide Chain kB



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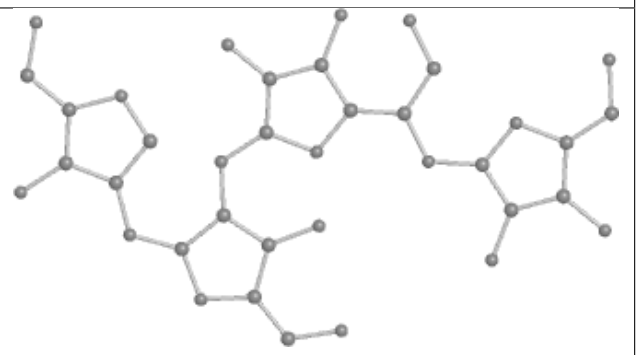

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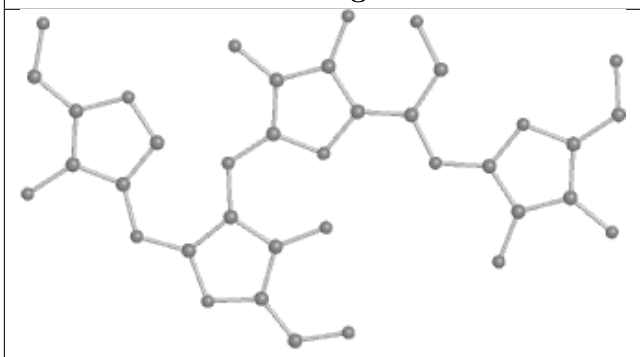

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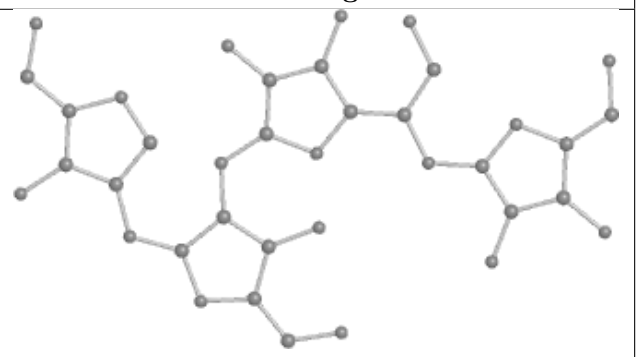
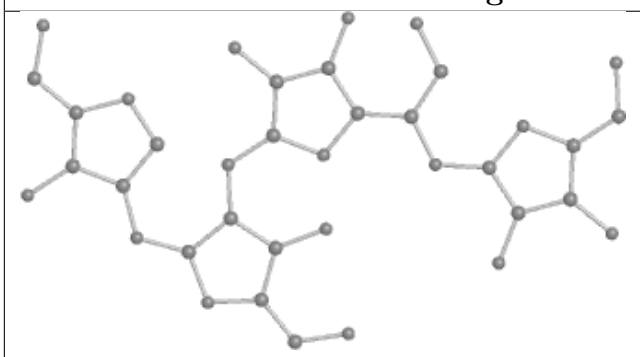


Rings

Oligosaccharide Chain nB



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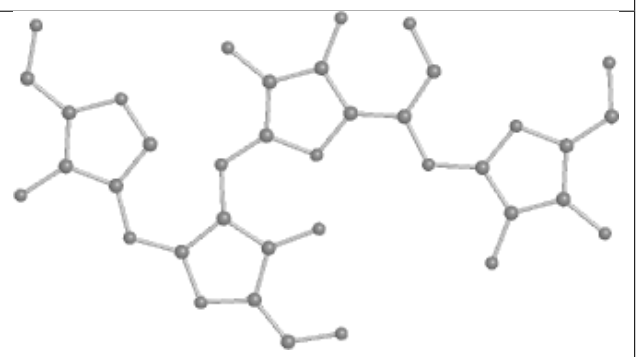
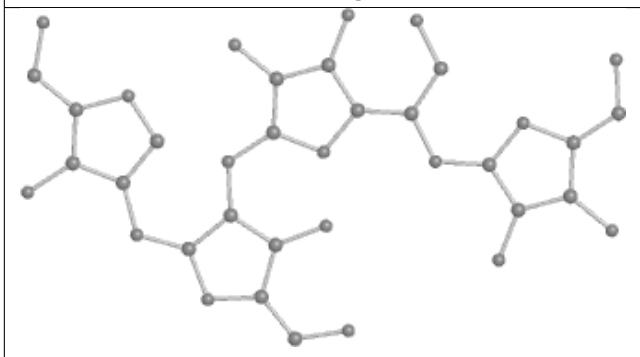


Bond angles



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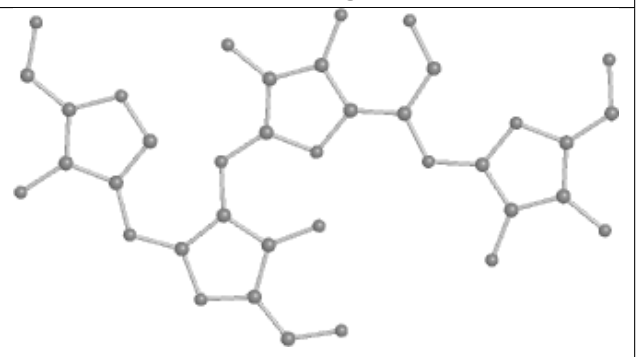
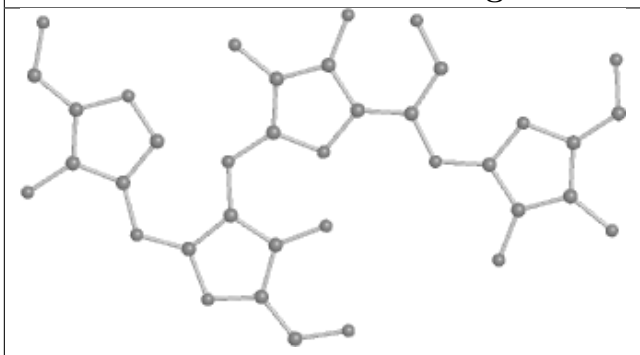


Rings

Oligosaccharide Chain hC



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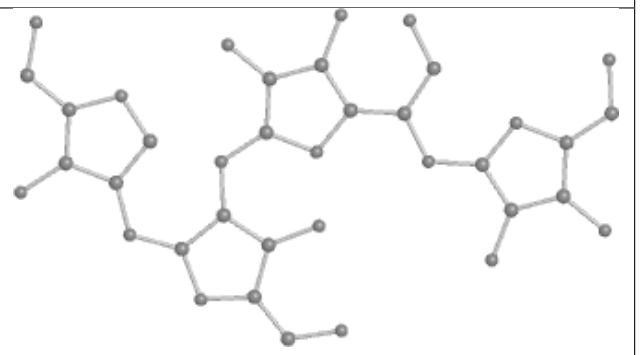
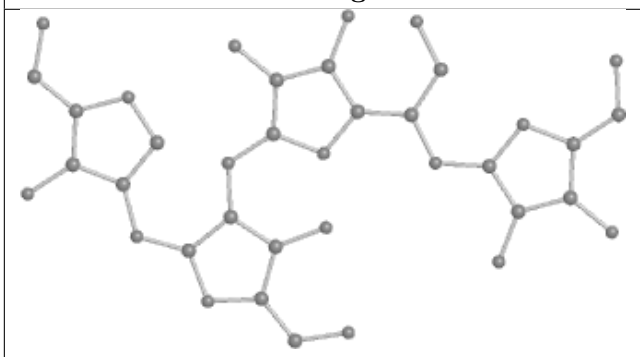


Bond angles



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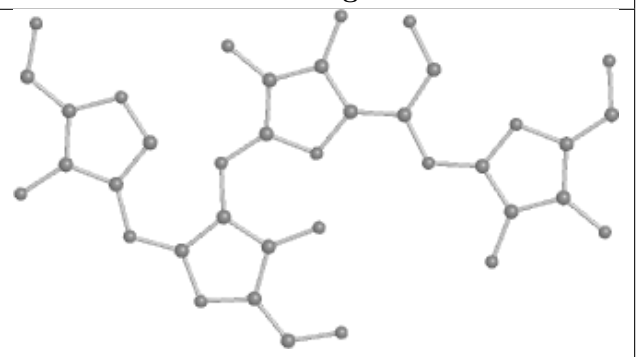
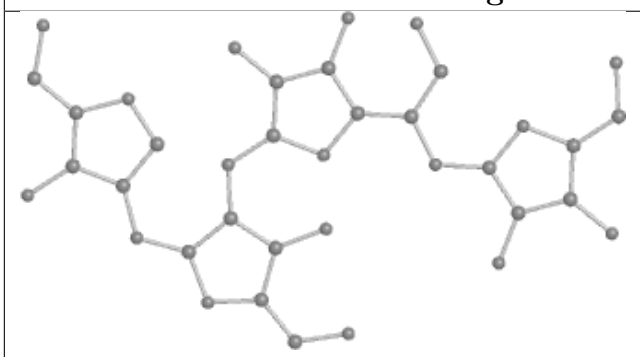


Rings

Oligosaccharide Chain kC



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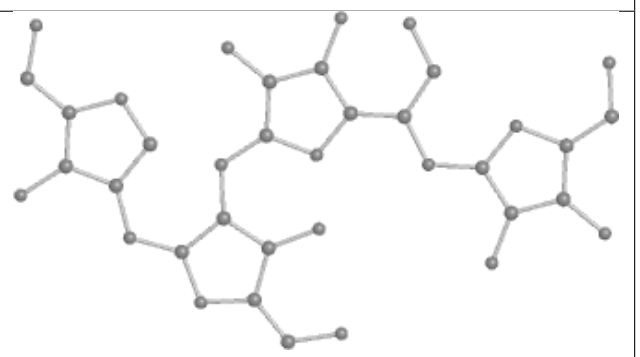
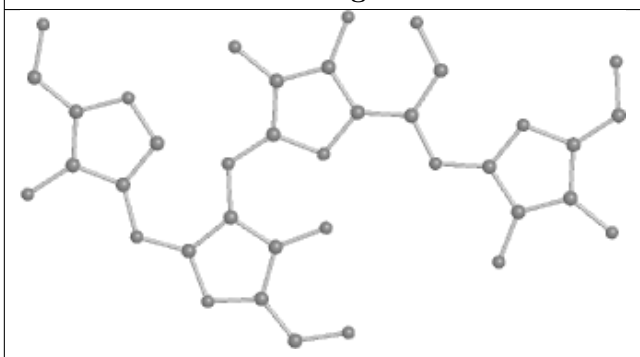


Bond angles



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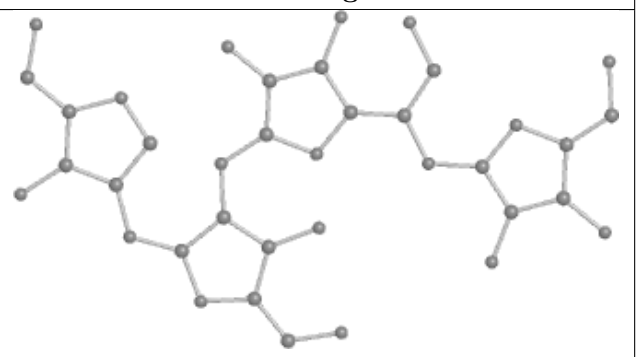
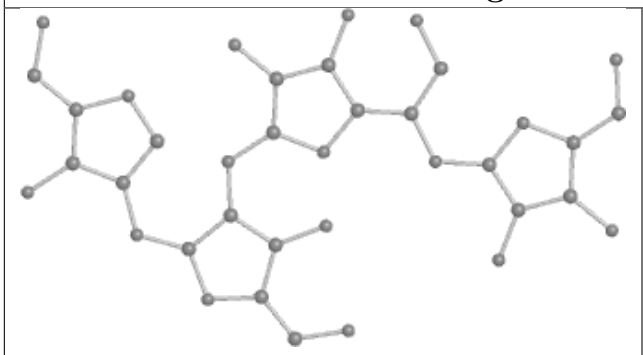


Rings

Oligosaccharide Chain eD



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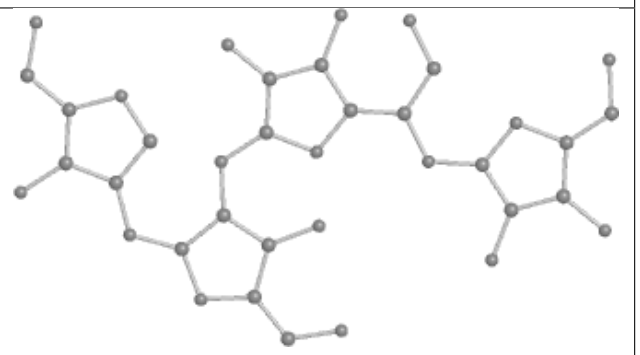
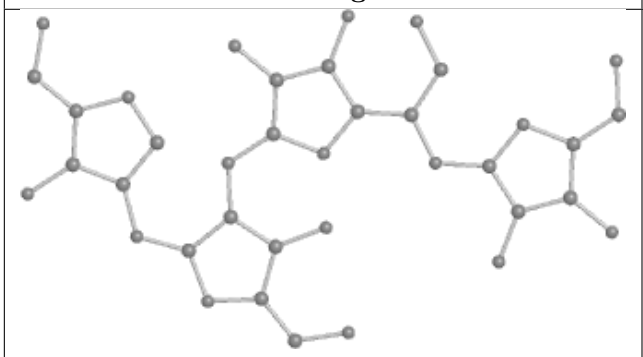


Bond angles



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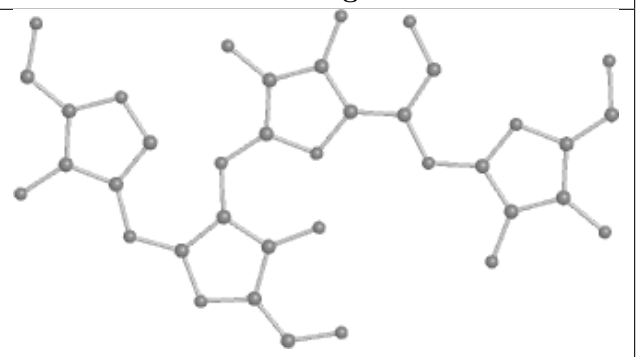
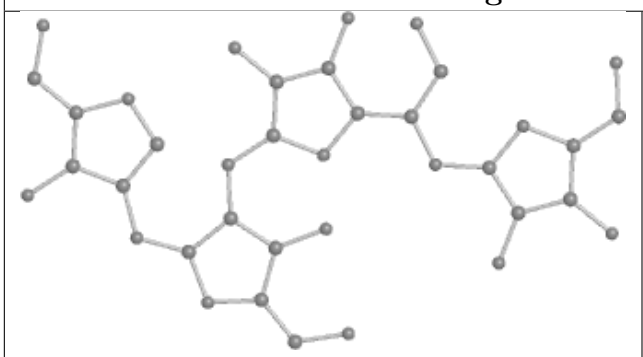


Rings

Oligosaccharide Chain hD



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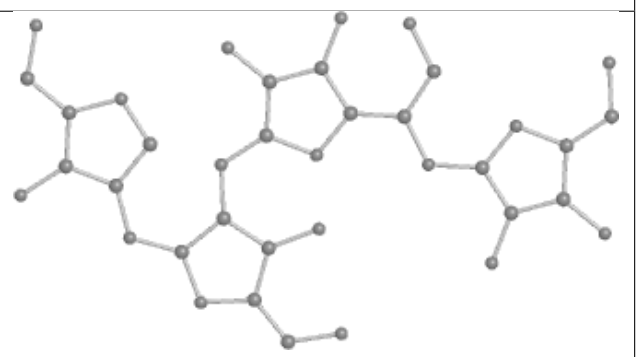
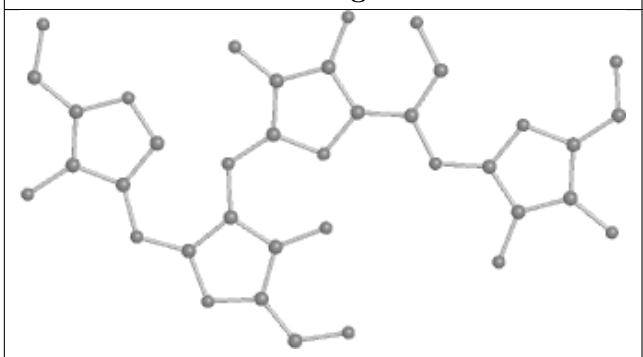


Bond angles



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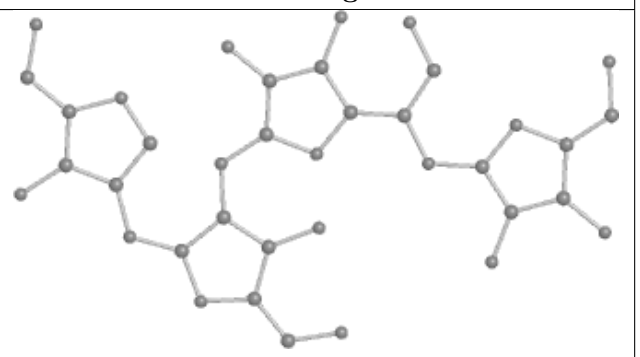
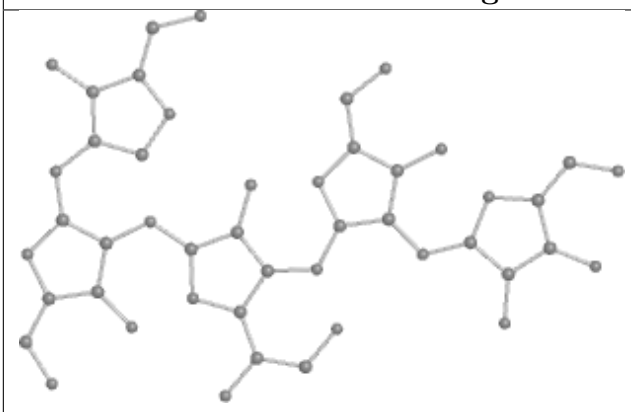
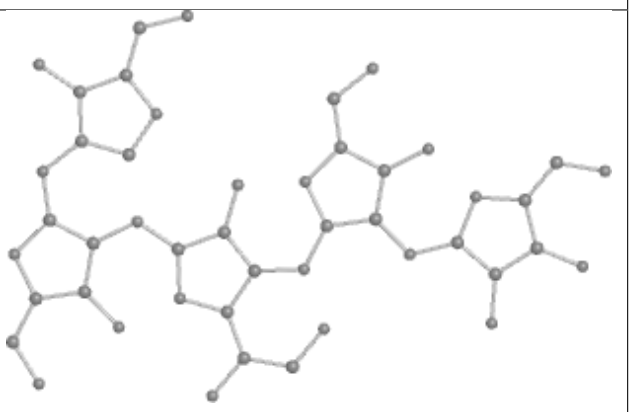
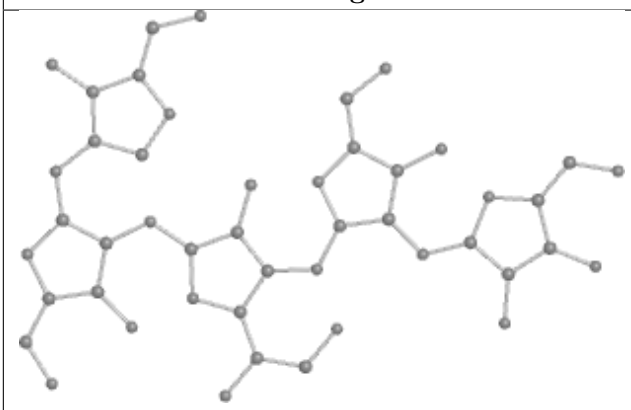
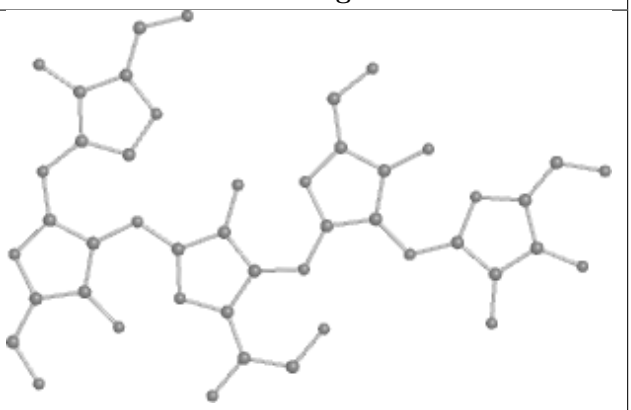


Rings

Oligosaccharide Chain CA	
 Bond lengths	 Bond angles
 Torsions	 Rings

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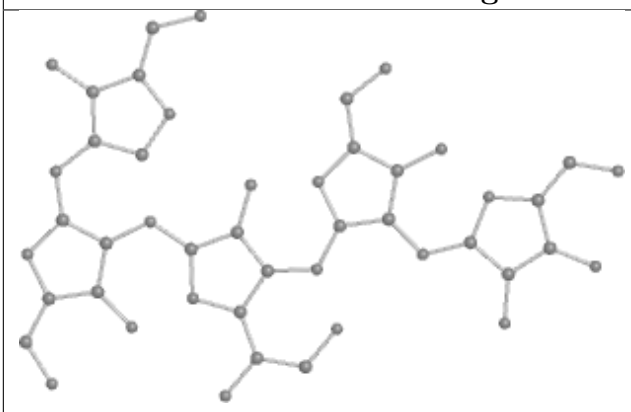
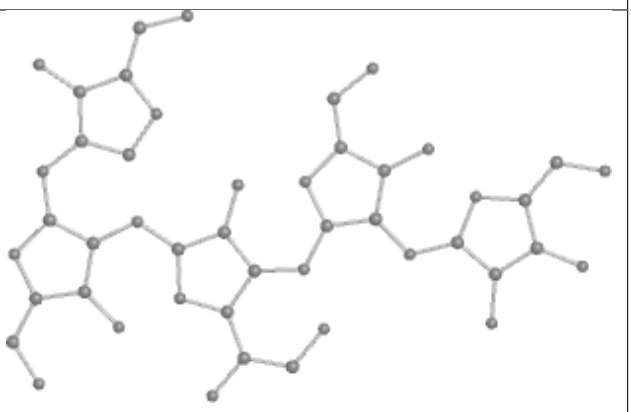
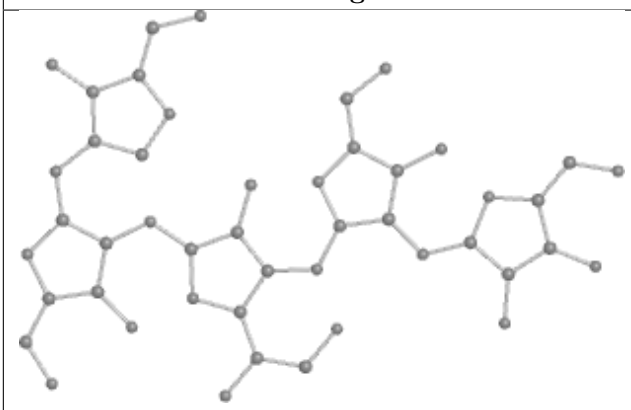
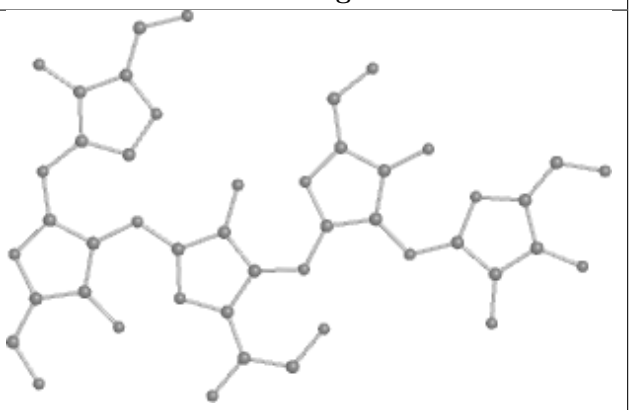
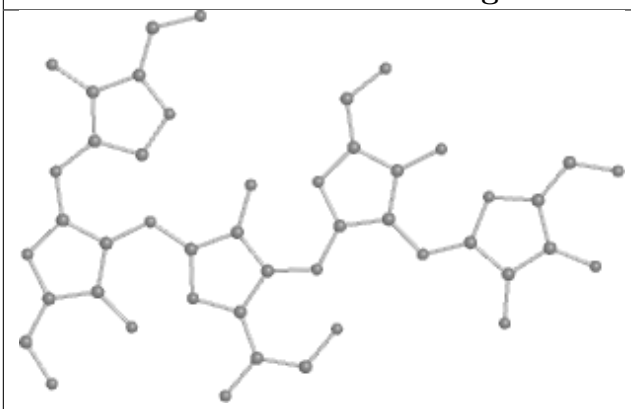
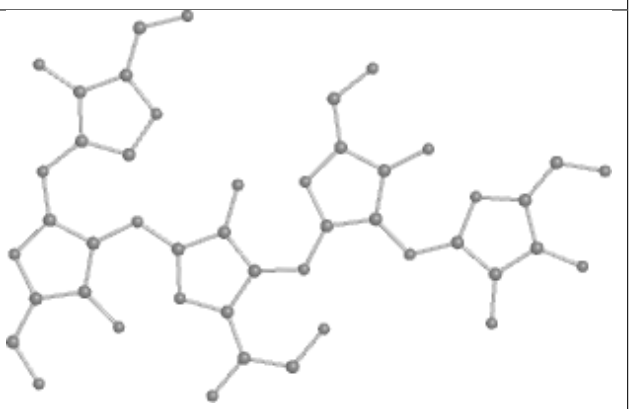
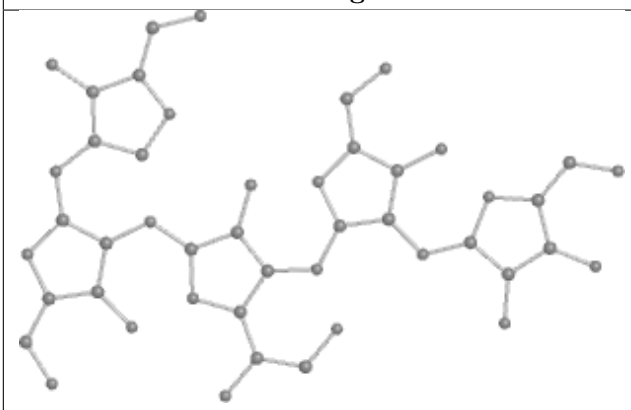
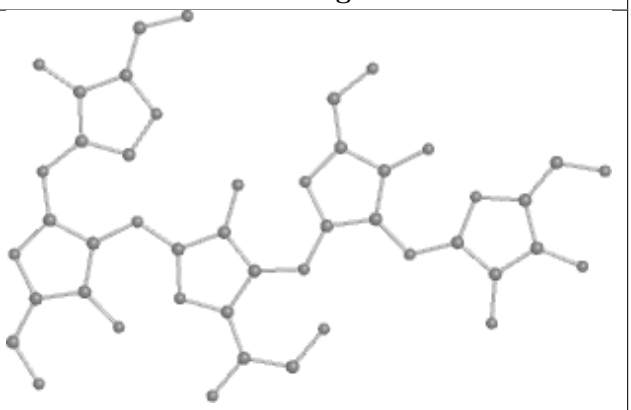
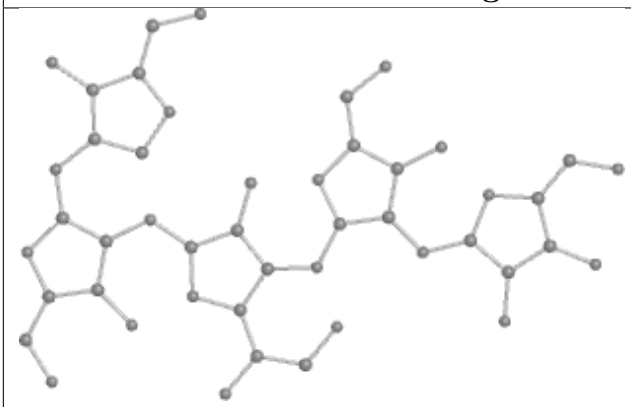
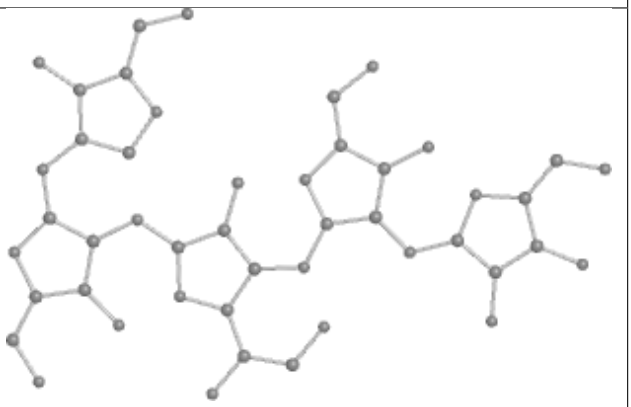
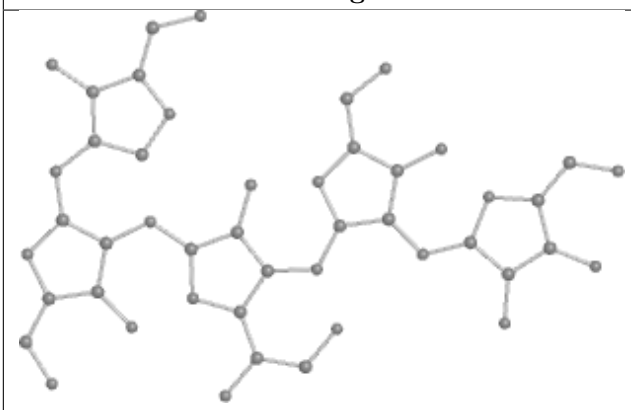
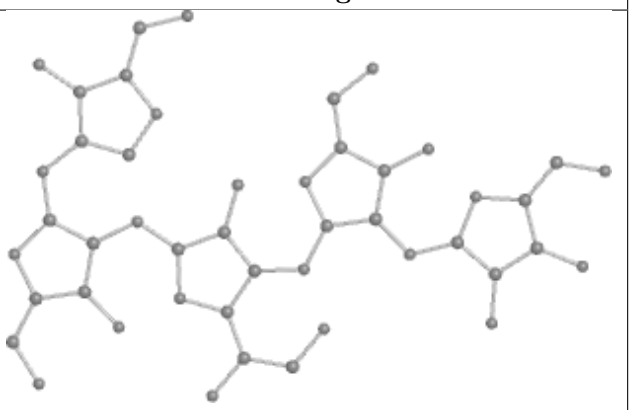
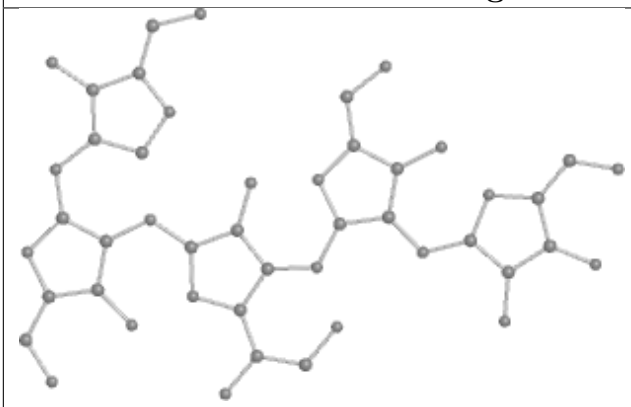
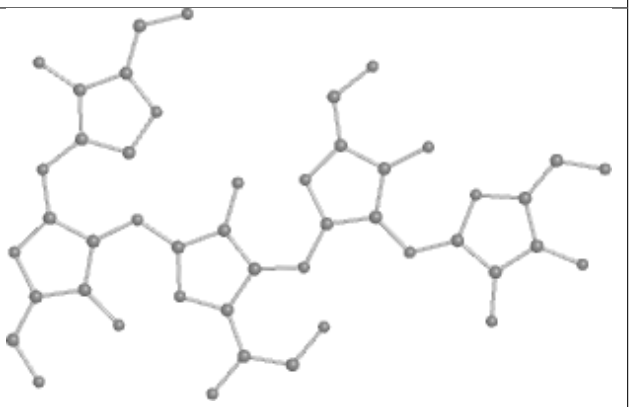
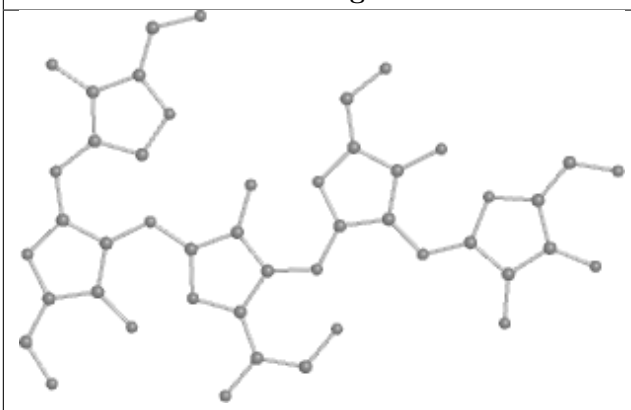
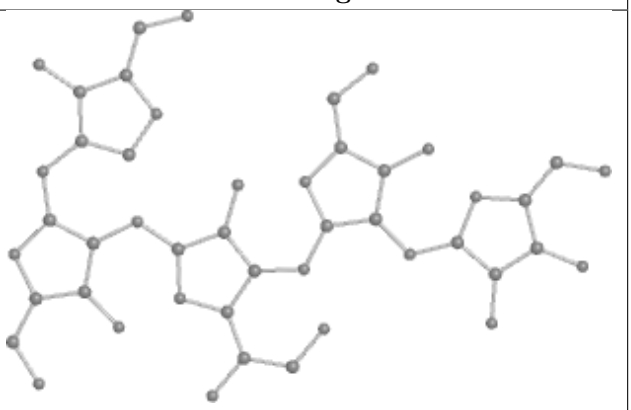
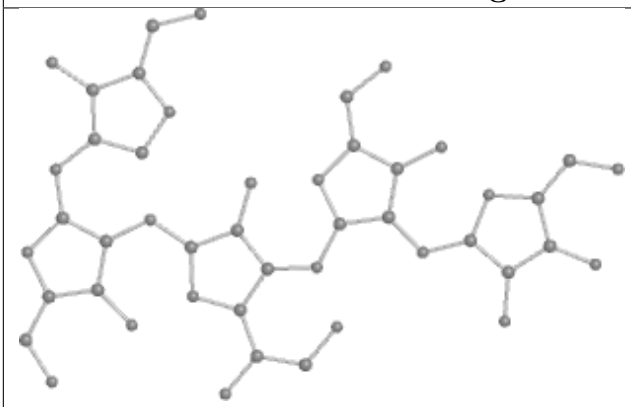
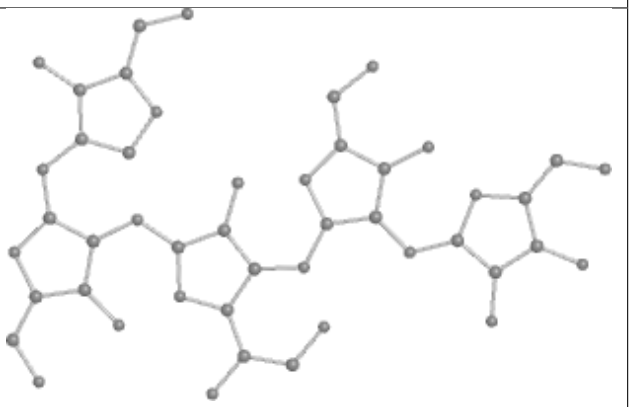
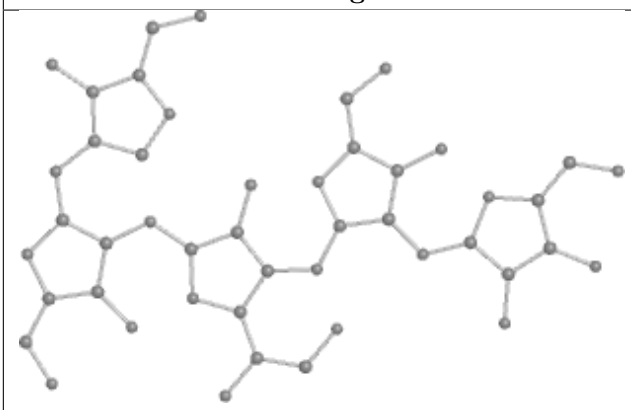
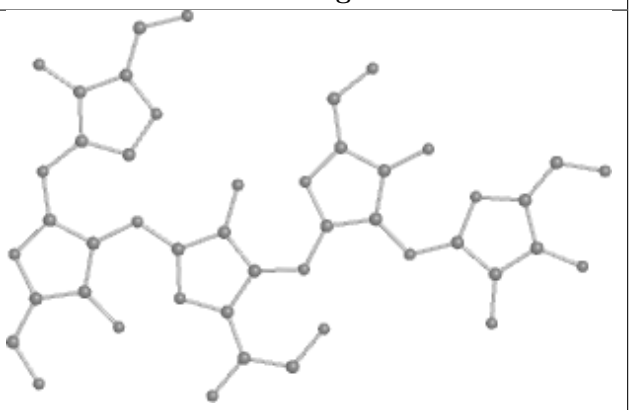
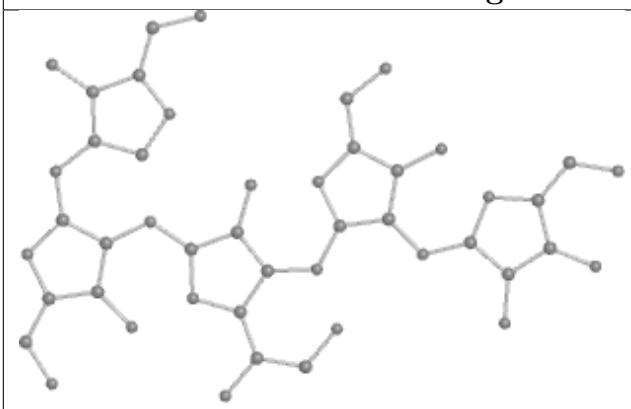
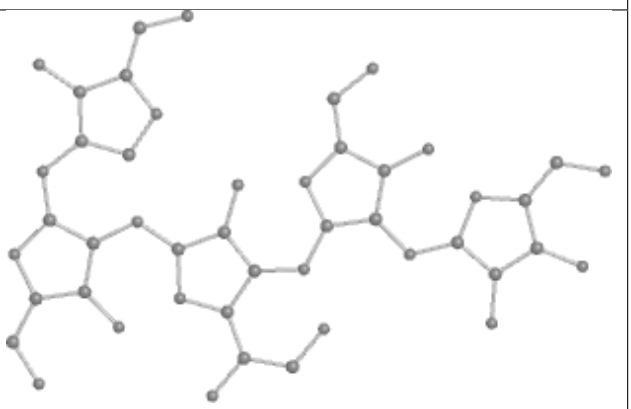
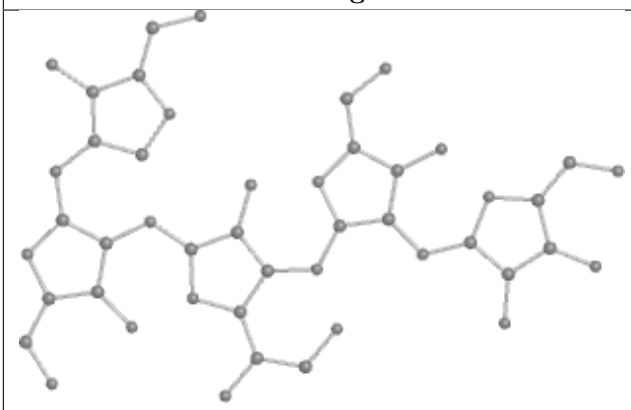
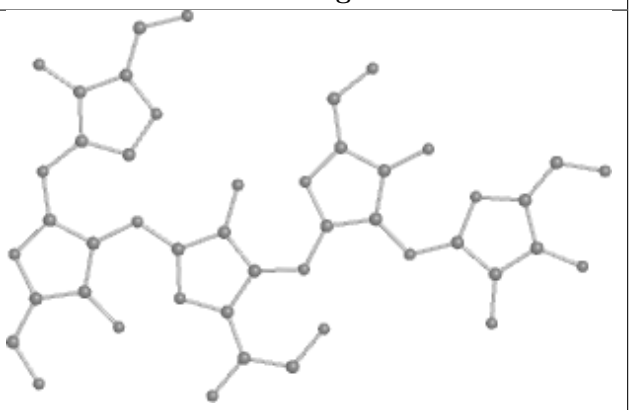
 Bond lengths	 Bond angles
 Torsions	 Rings

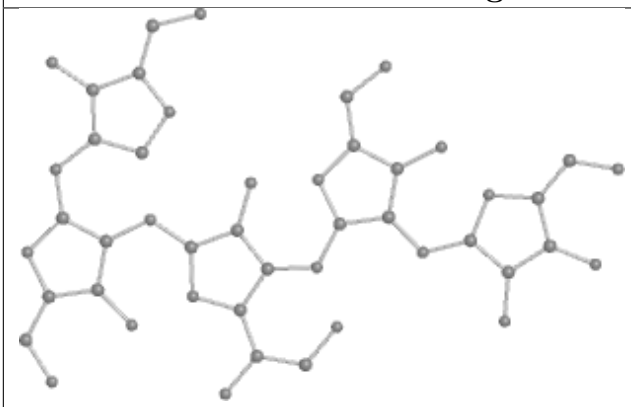
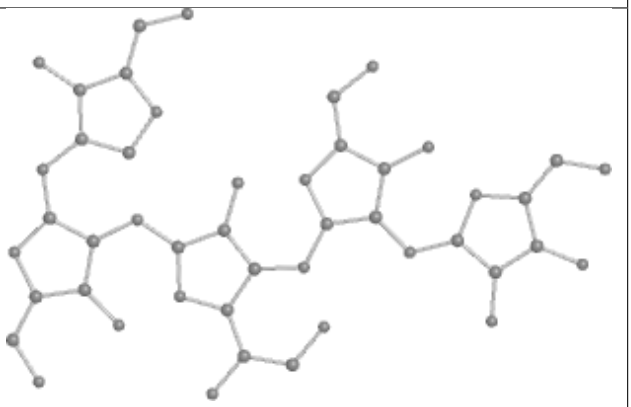
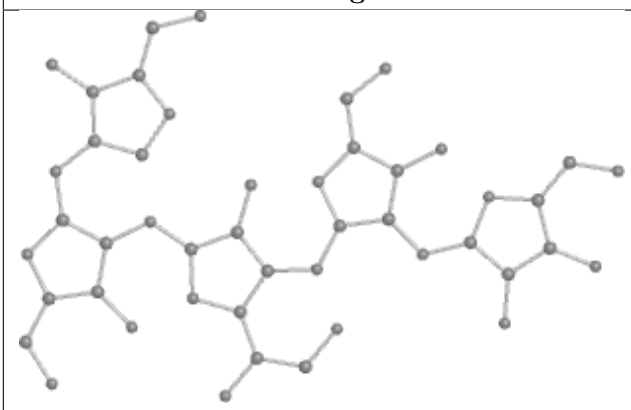
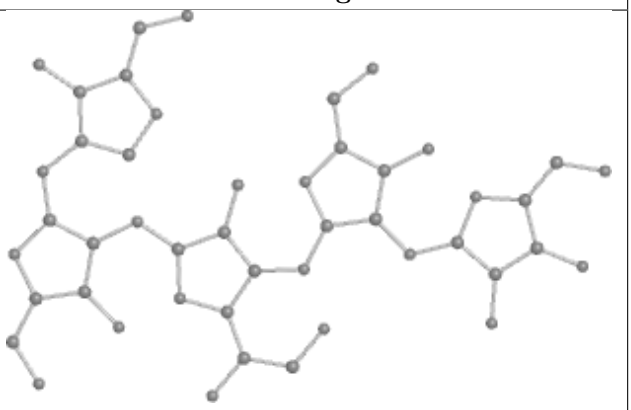
Oligosaccharide Chain AB	
 Bond lengths	 Bond angles
 Torsions	 Rings

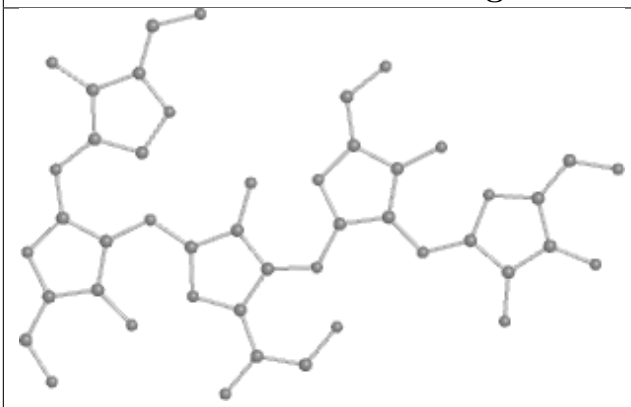
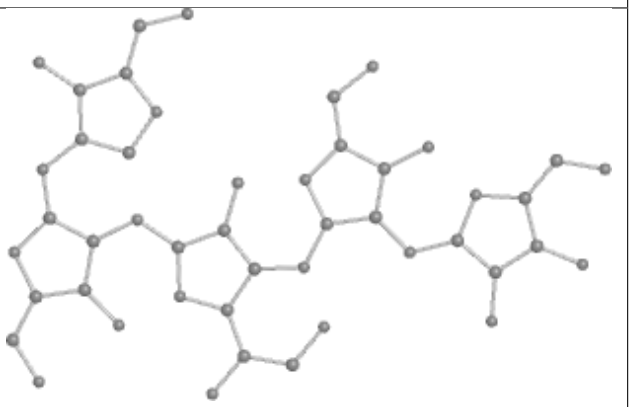
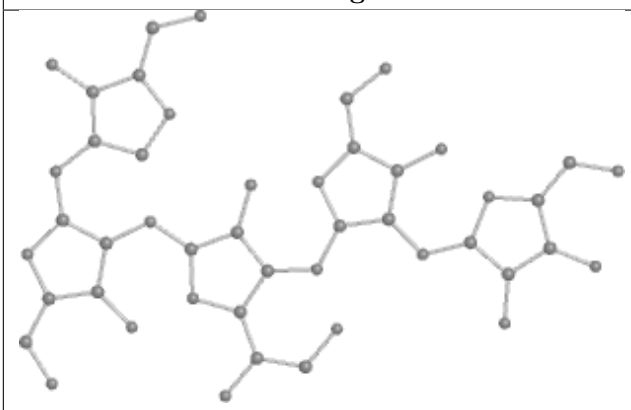
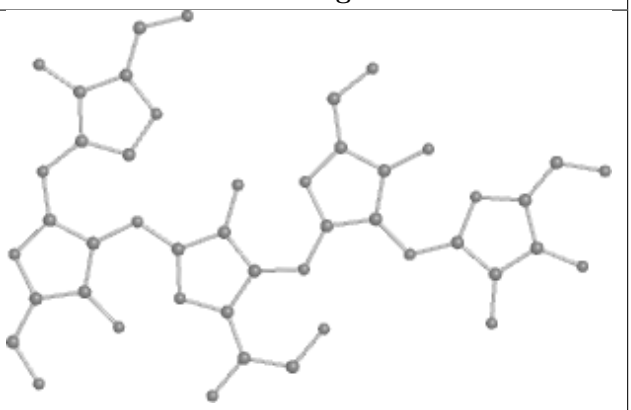
Oligosaccharide Chain BB	
 Bond lengths	 Bond angles
 Torsions	 Rings

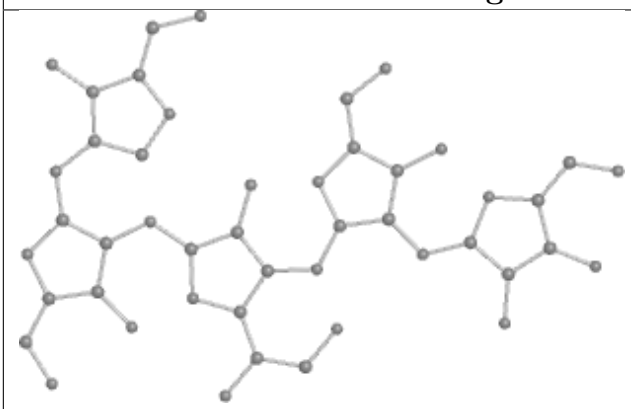
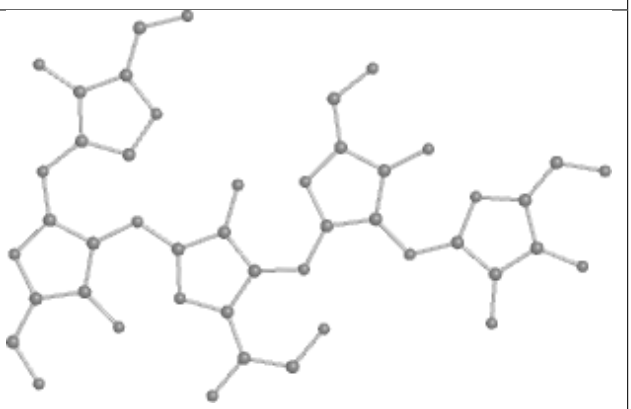
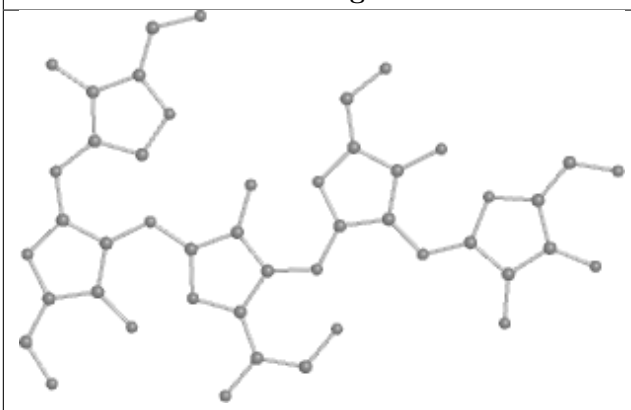
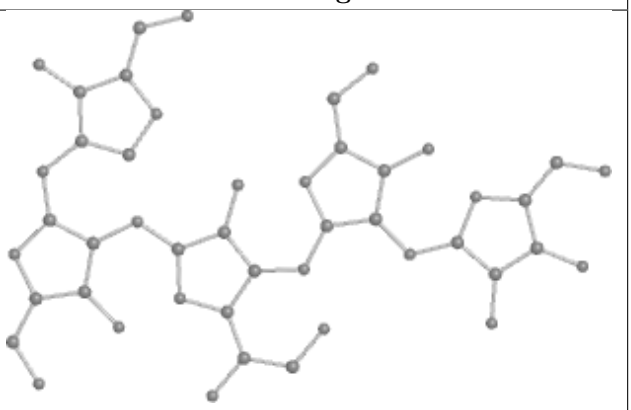
Oligosaccharide Chain eB	
 Bond lengths	 Bond angles
 Torsions	 Rings

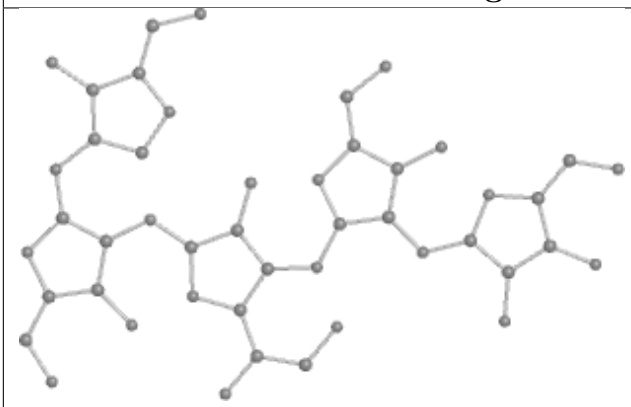
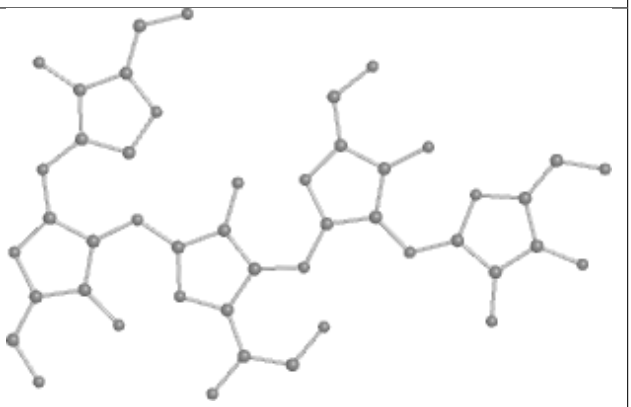
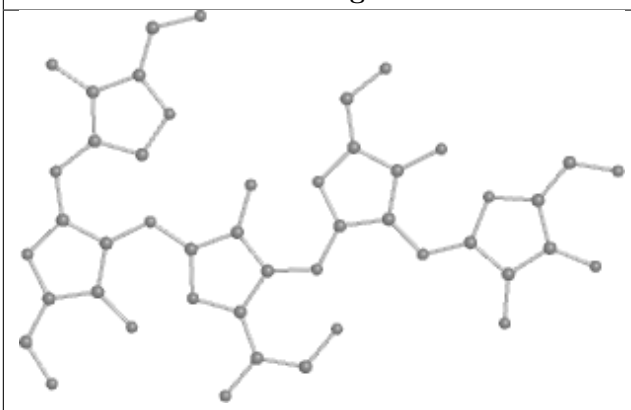
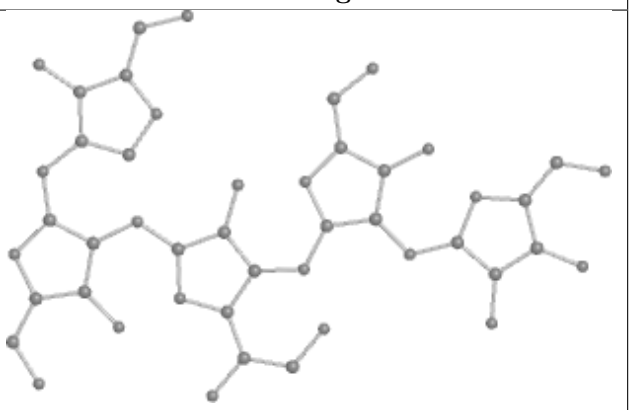
Oligosaccharide Chain fB	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 7B	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 8B	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 4C	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 5C	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 1D	
 Bond lengths	 Bond angles
 Torsions	 Rings

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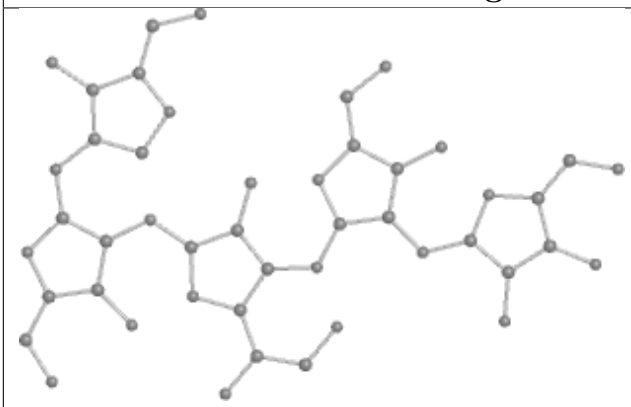
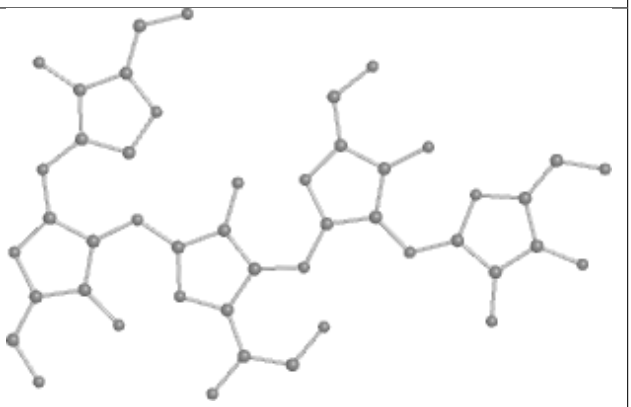
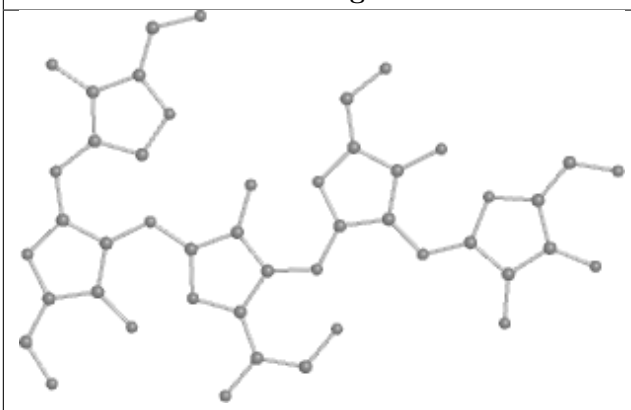
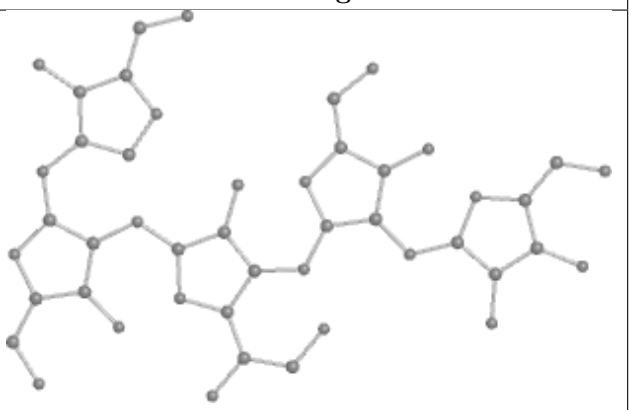
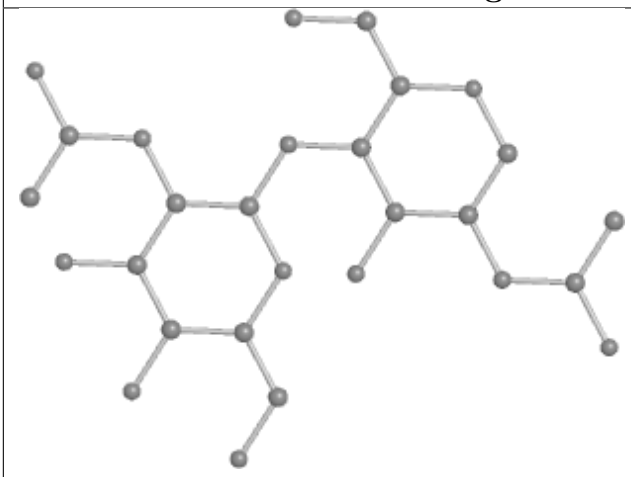
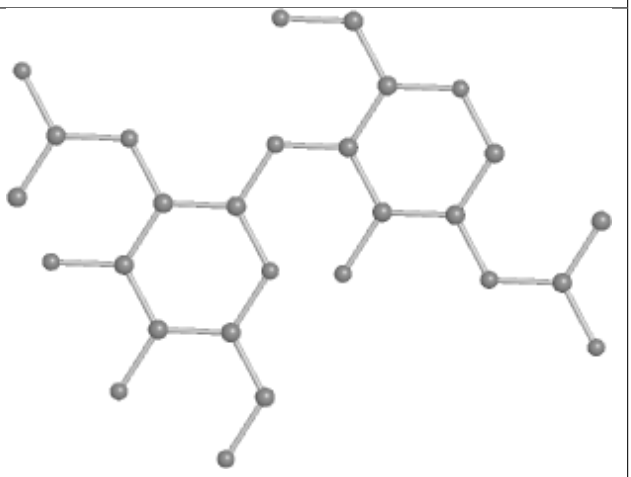
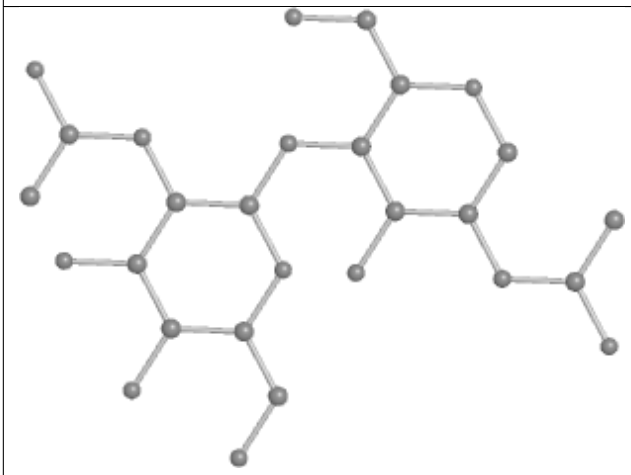
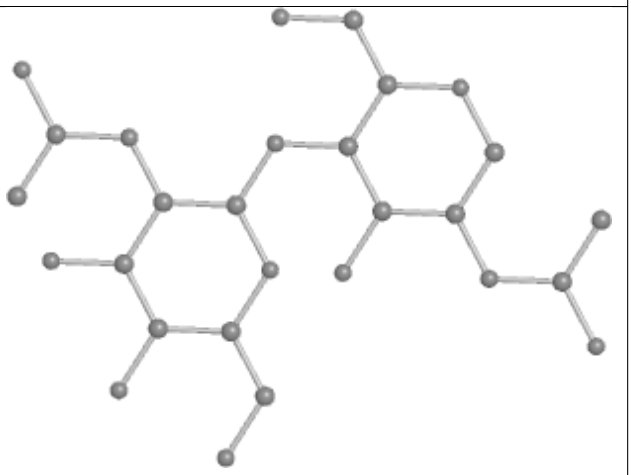
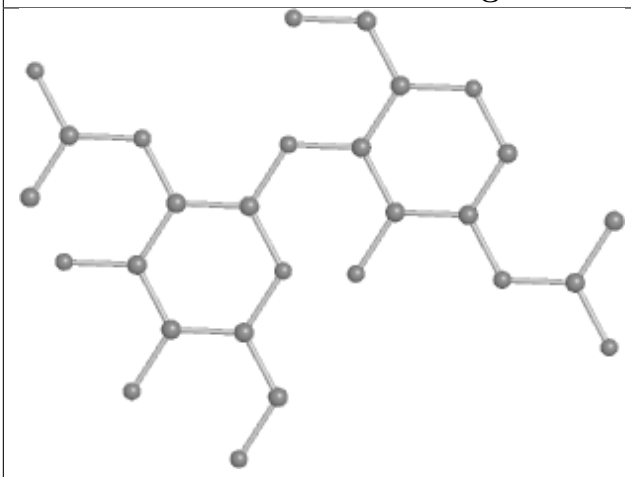
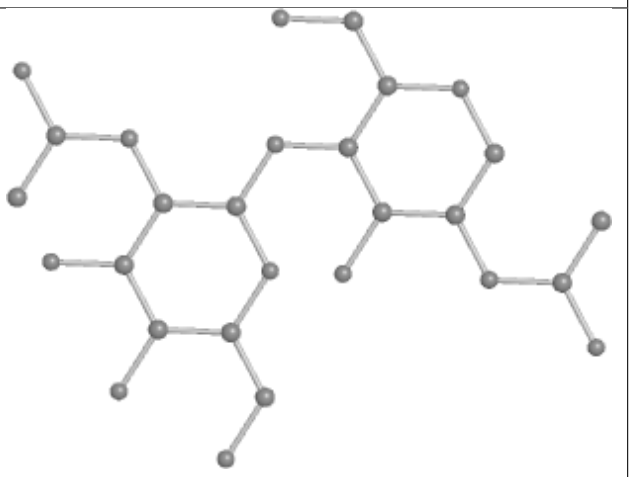
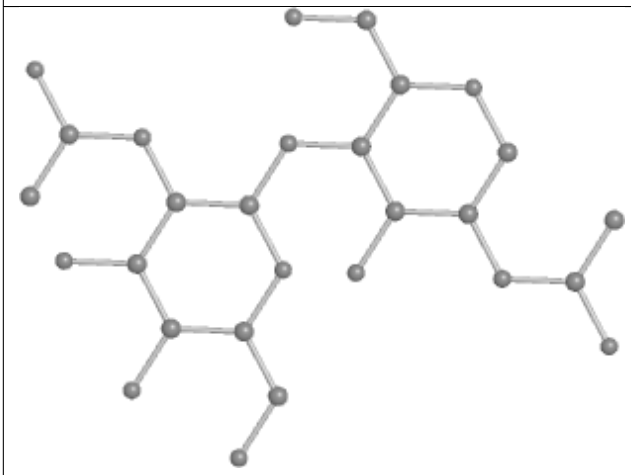
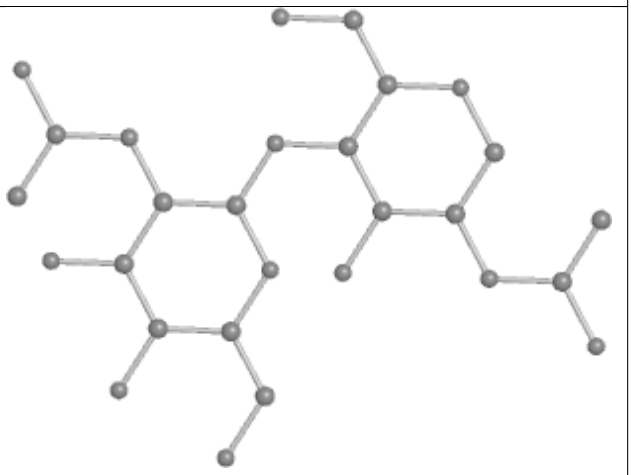
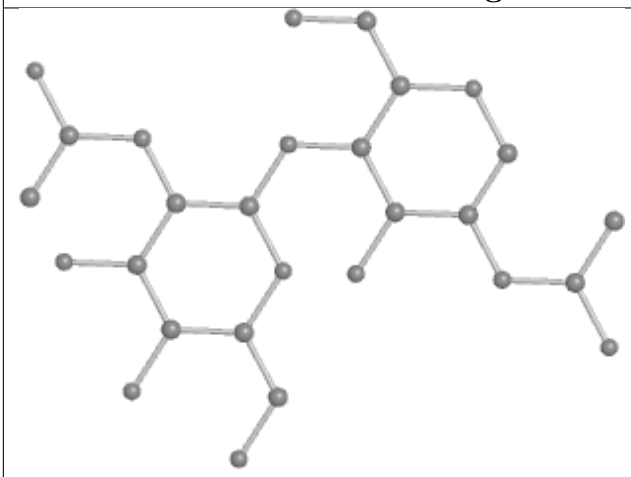
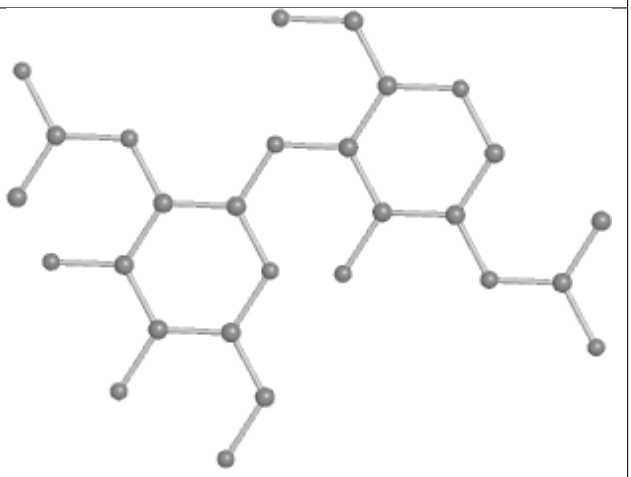
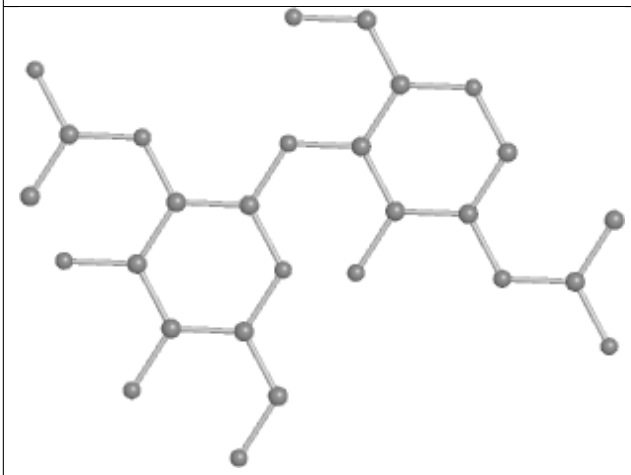
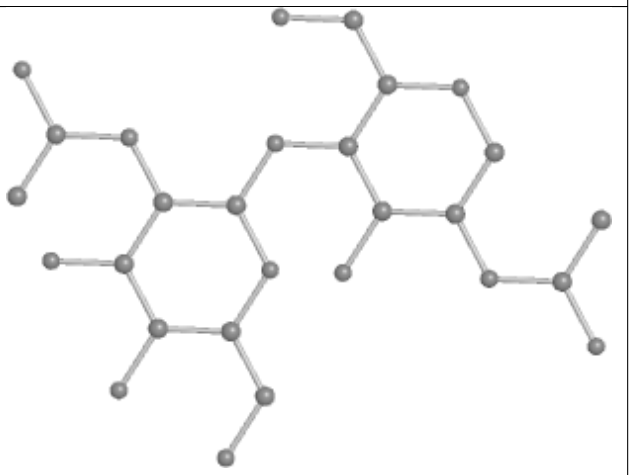
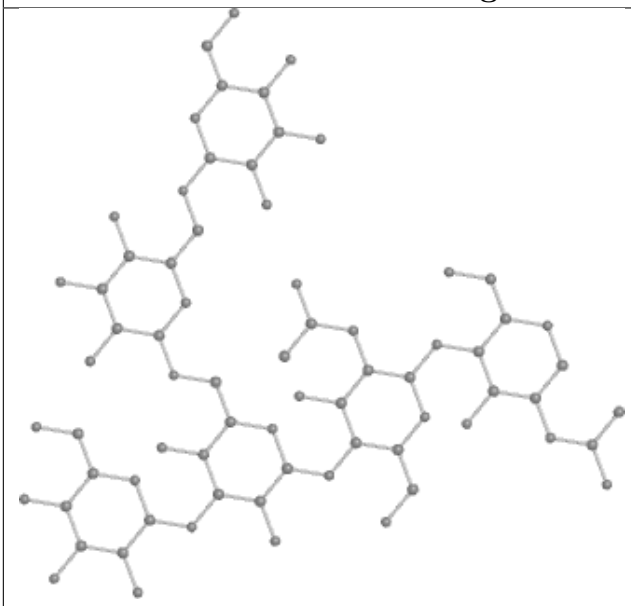
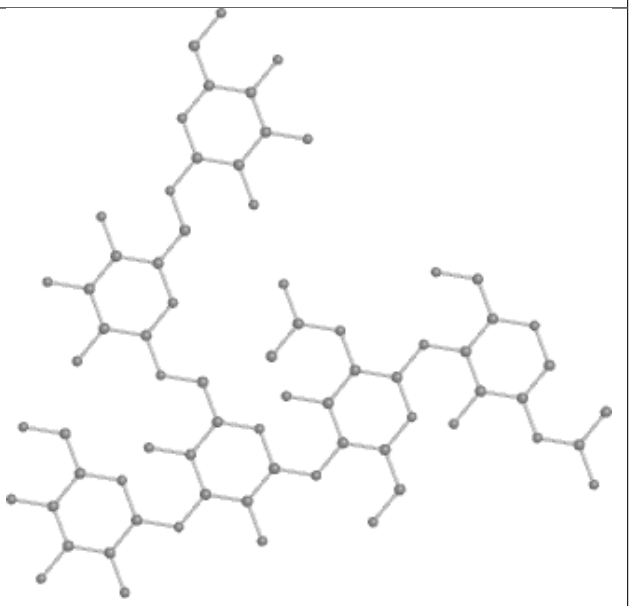
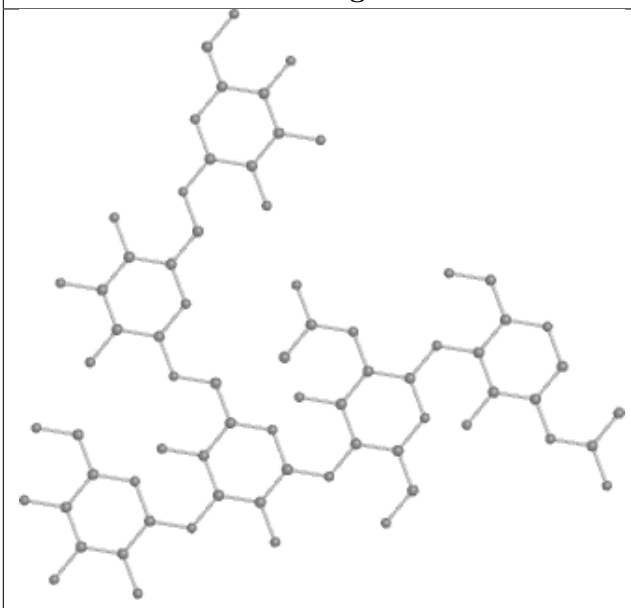
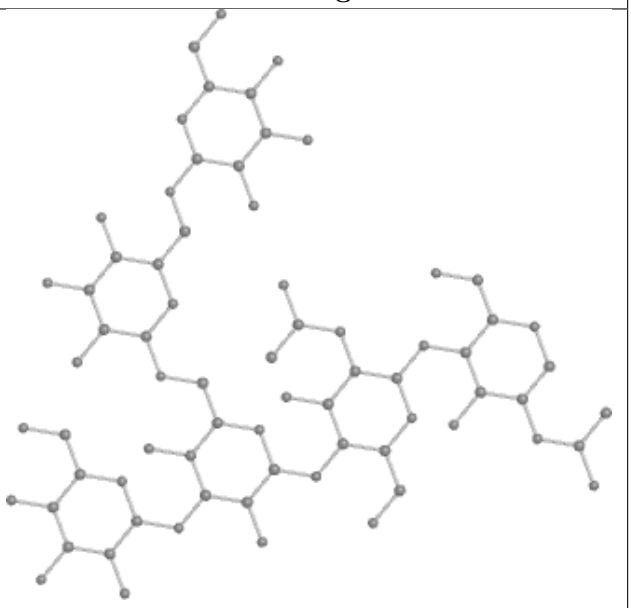
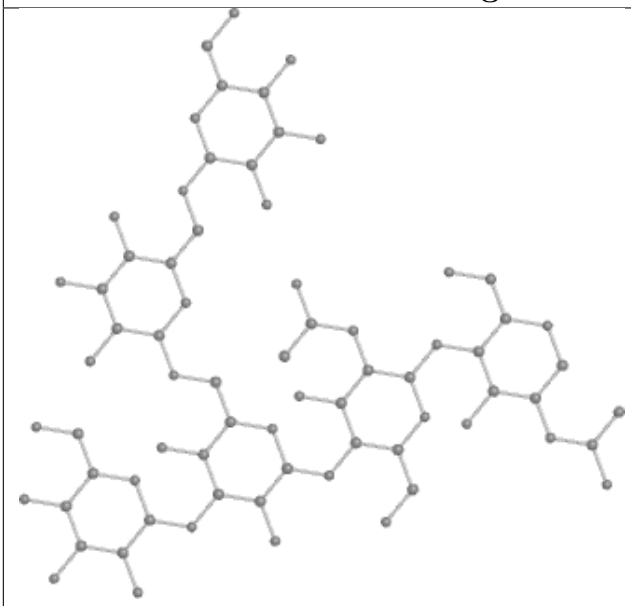
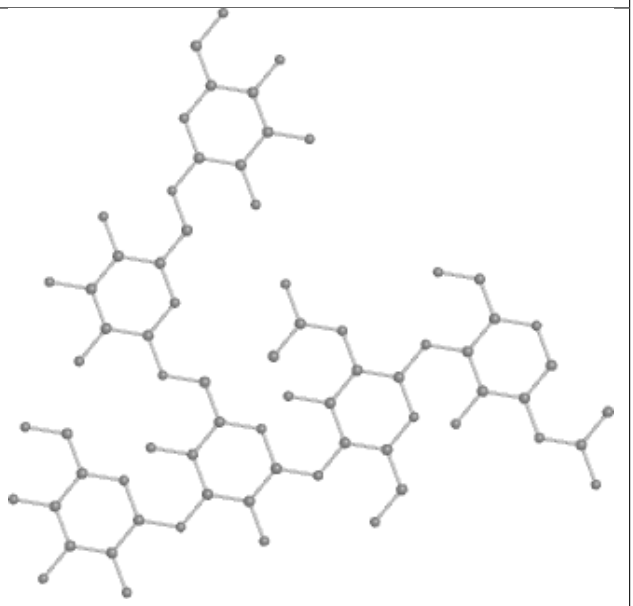
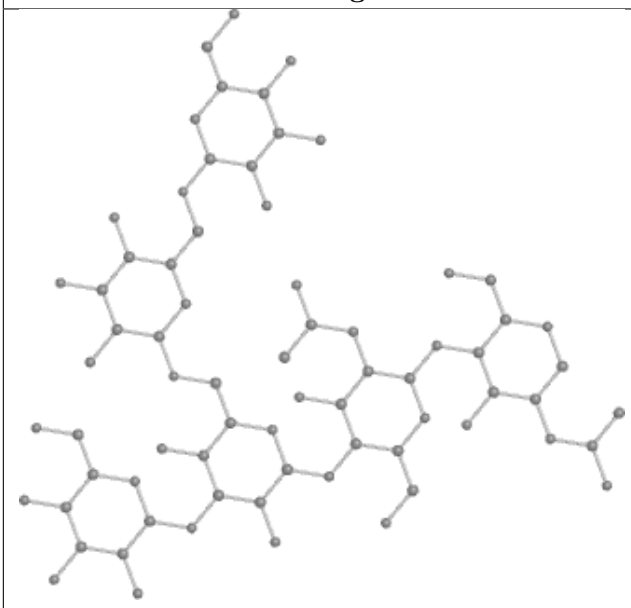
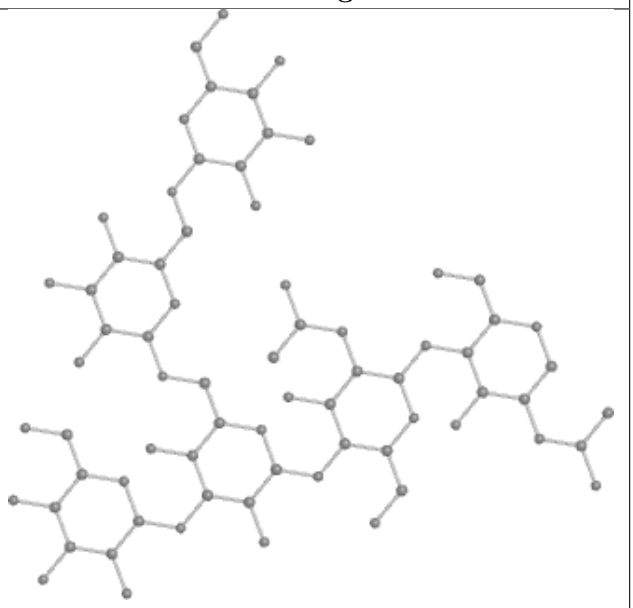
 Bond lengths	 Bond angles
 Torsions	 Rings

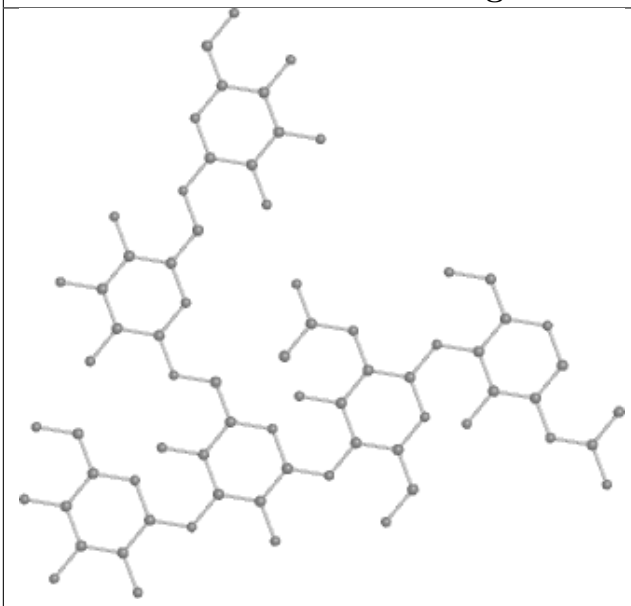
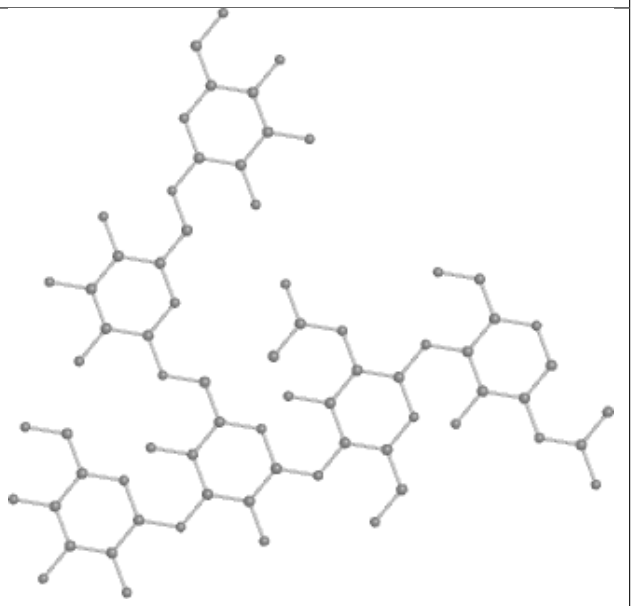
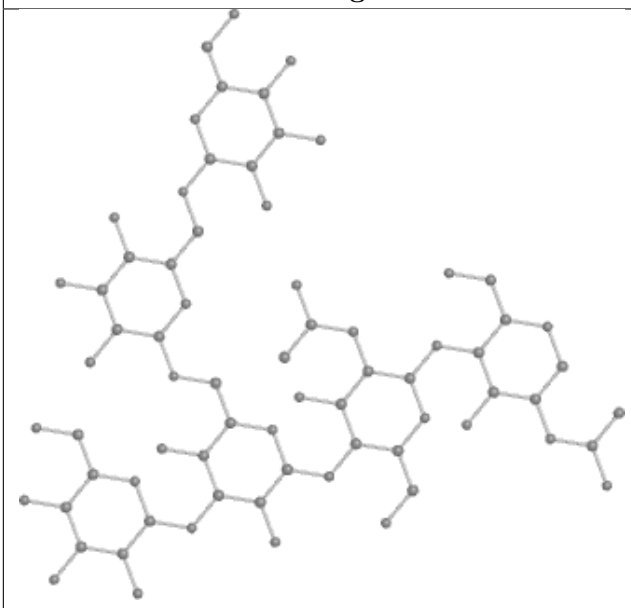
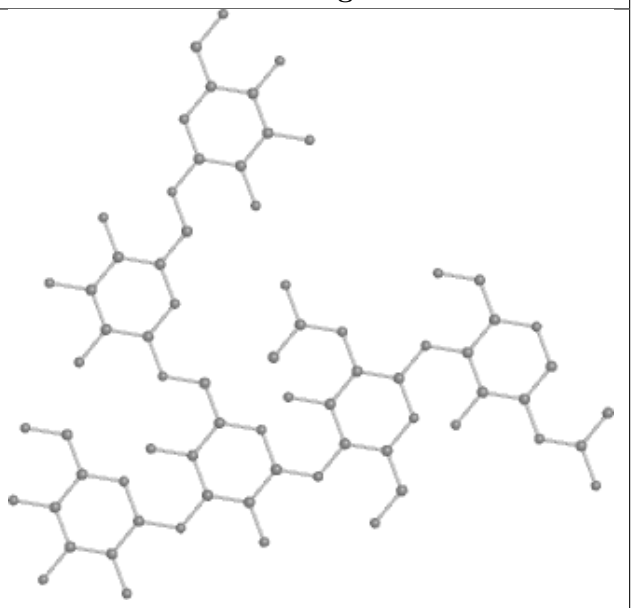
Oligosaccharide Chain FA	
 Bond lengths	 Bond angles
 Torsions	 Rings

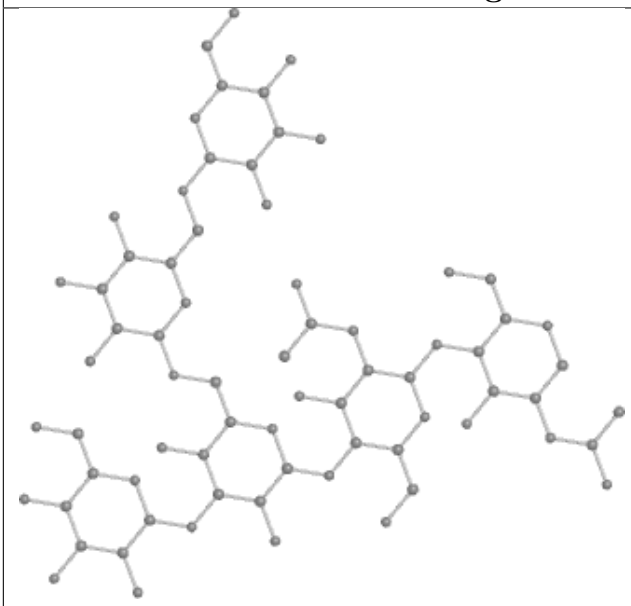
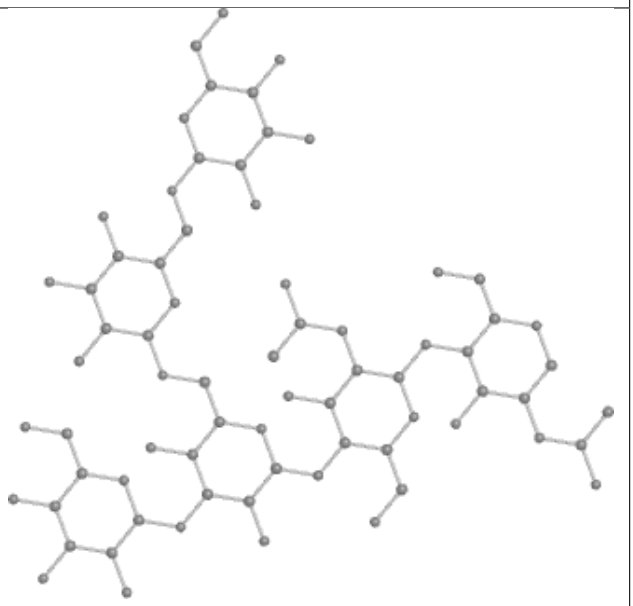
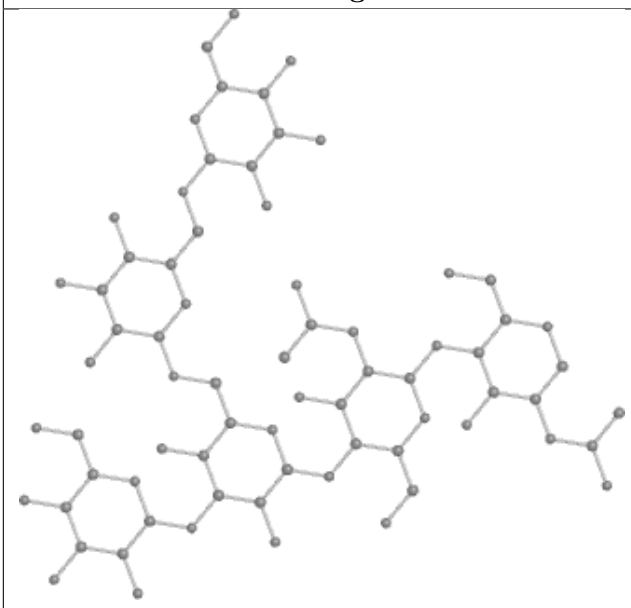
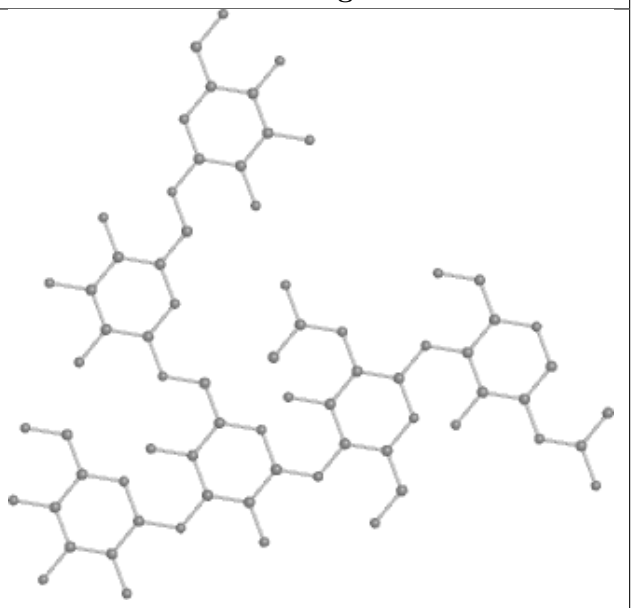
Oligosaccharide Chain AC	
 Bond lengths	 Bond angles
 Torsions	 Rings

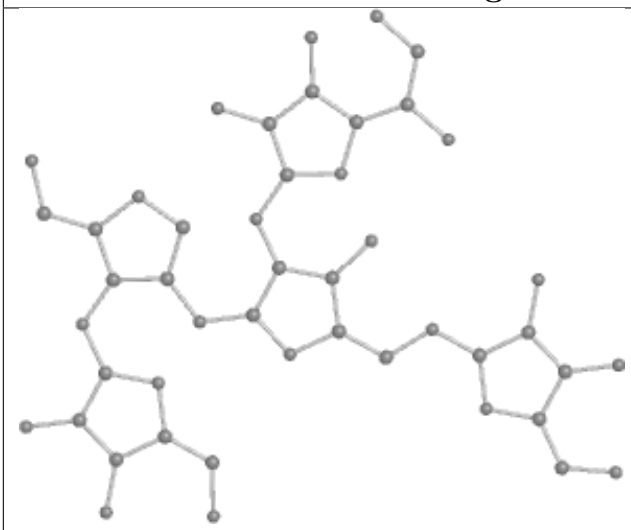
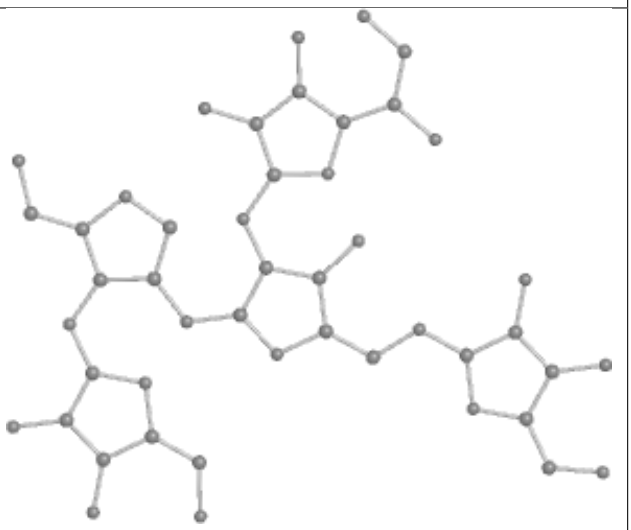
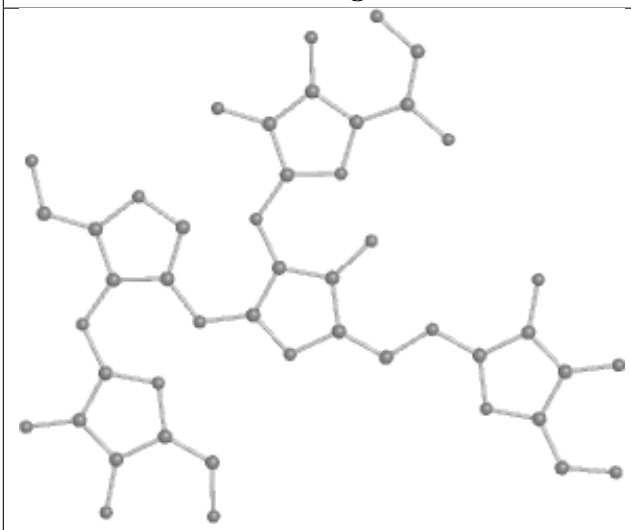
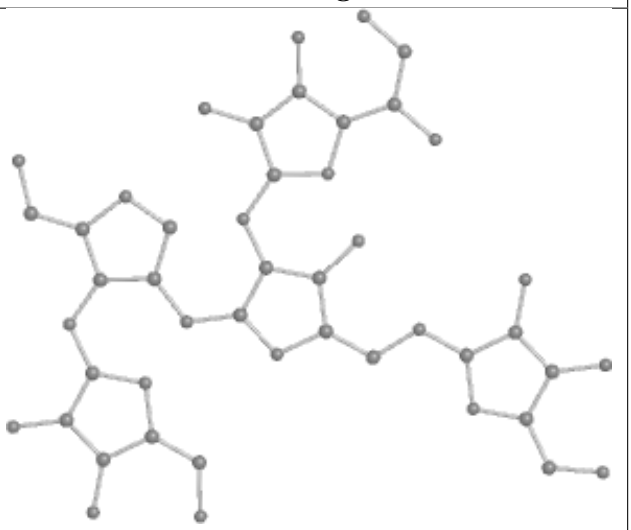
Oligosaccharide Chain 4D	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

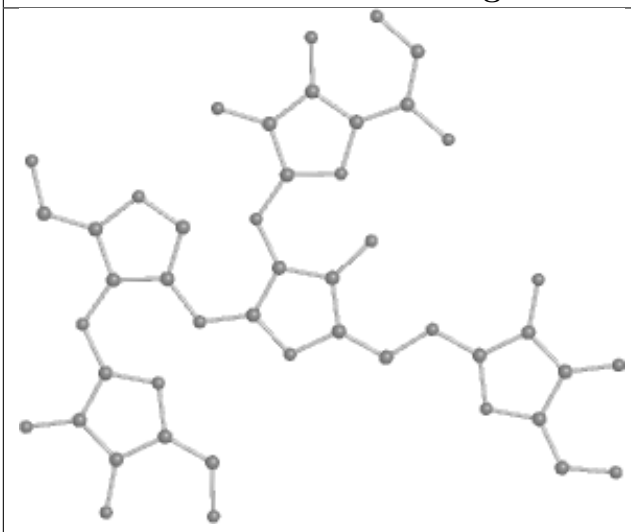
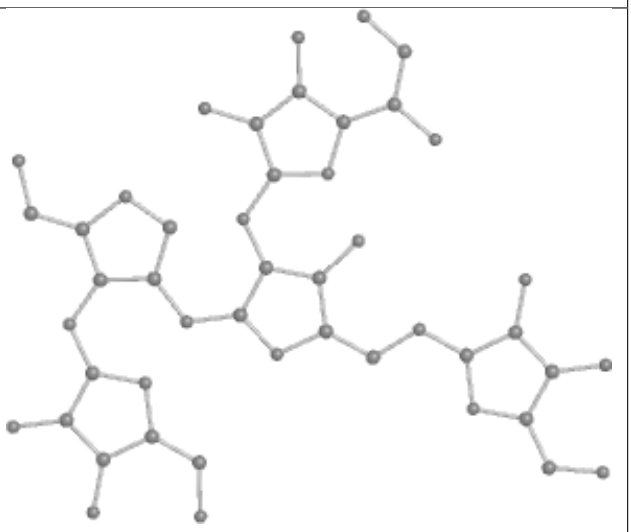
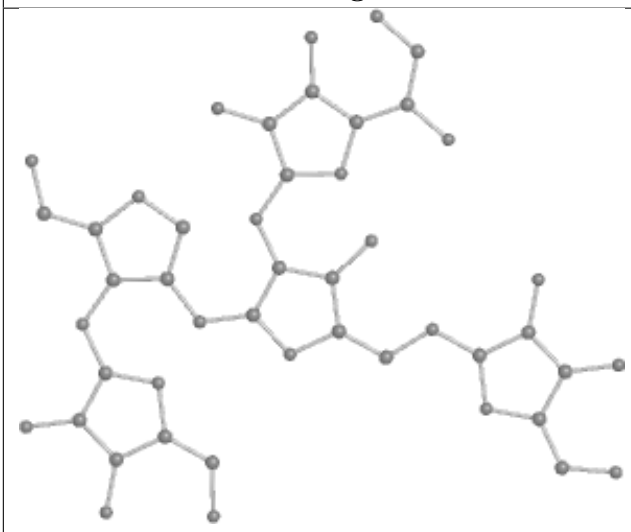
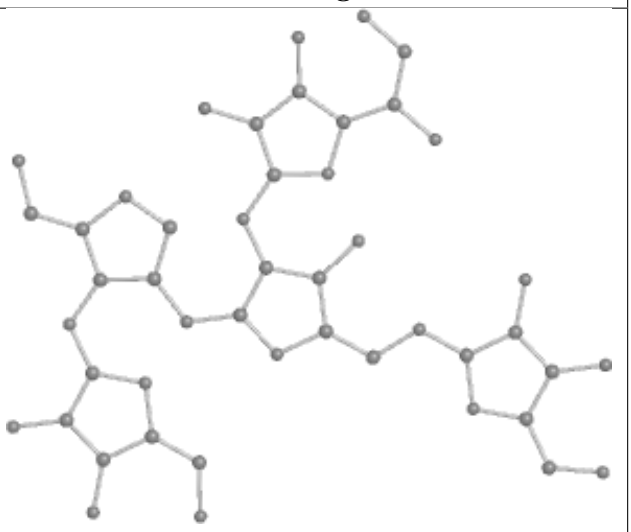
Oligosaccharide Chain GA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

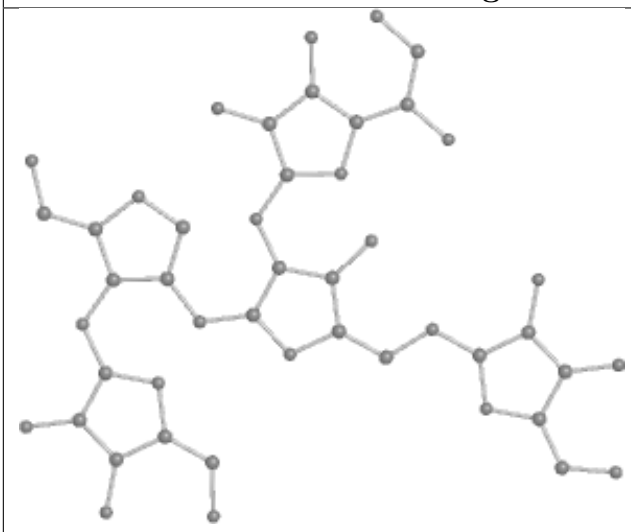
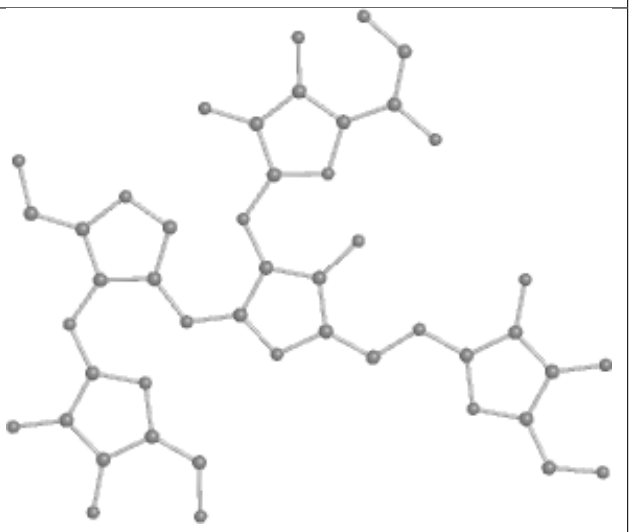
Oligosaccharide Chain DB	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain 7C	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 5D	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain 9D	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain BE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain DE	
	
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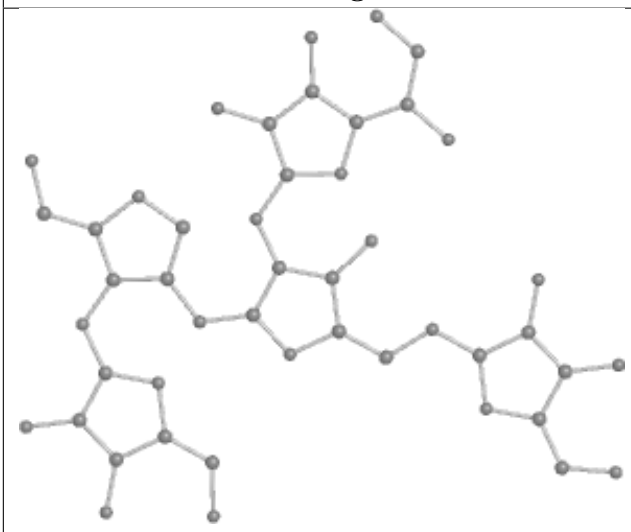	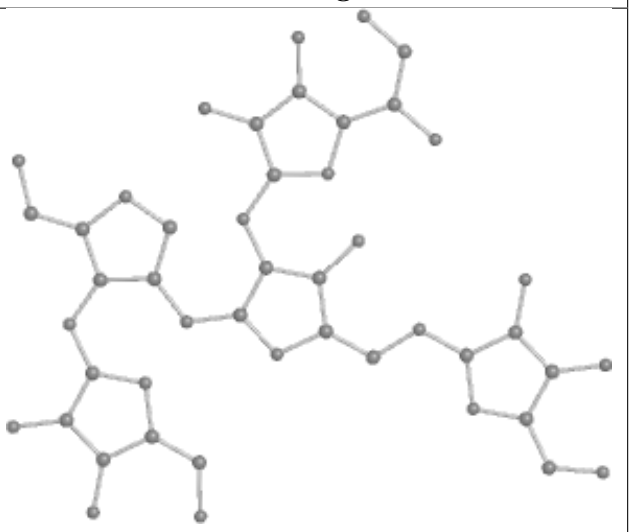
Torsions	**Rings**

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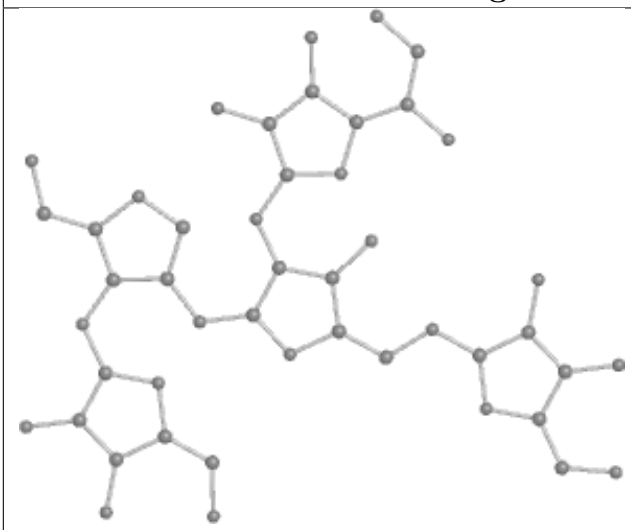	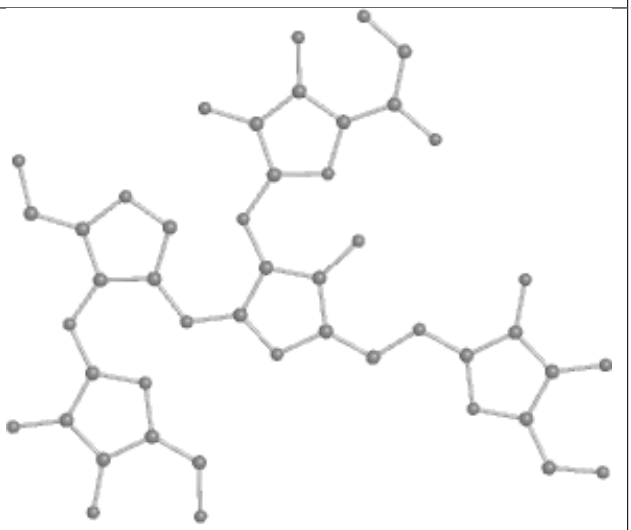
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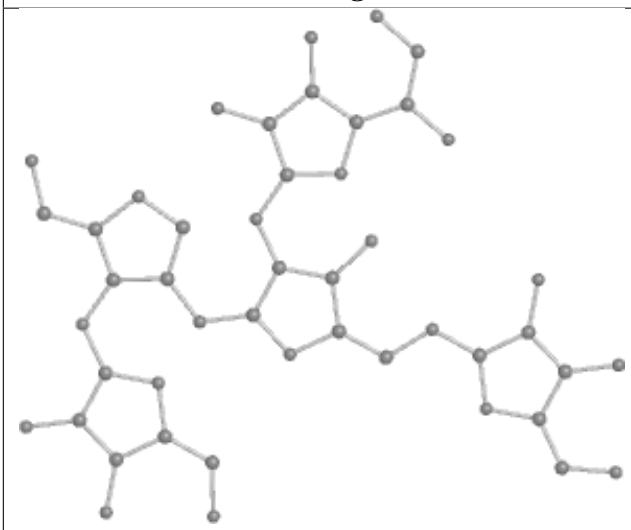	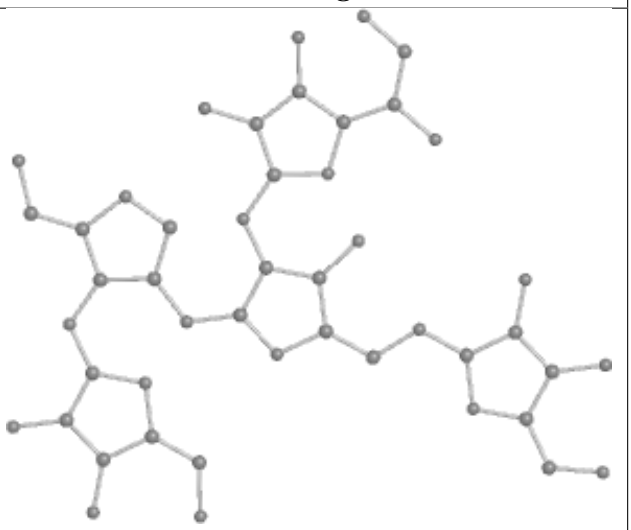
Torsions	**Rings**

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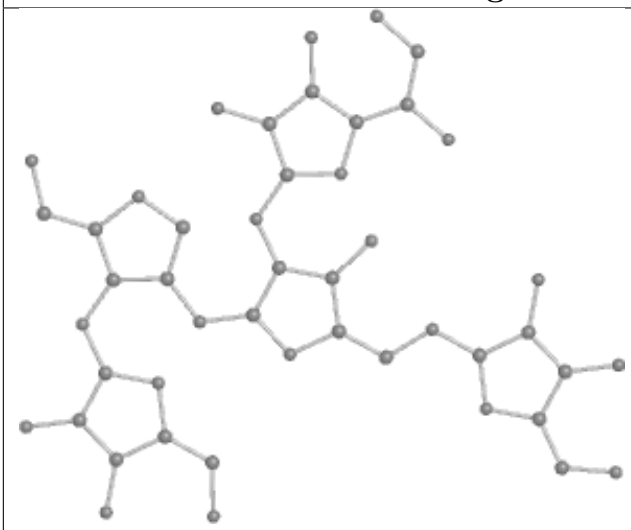	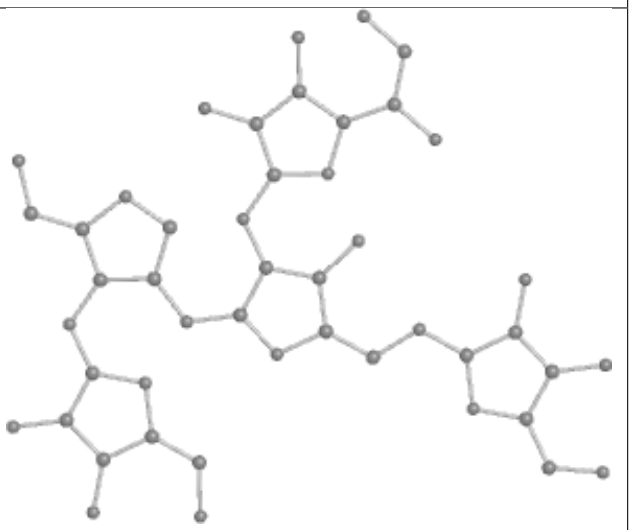
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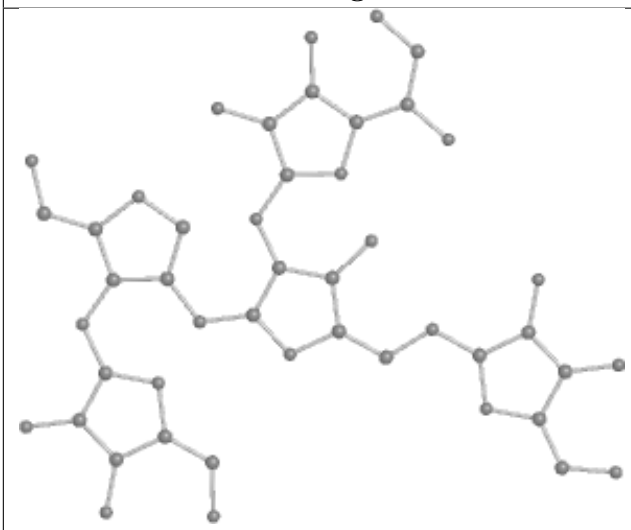	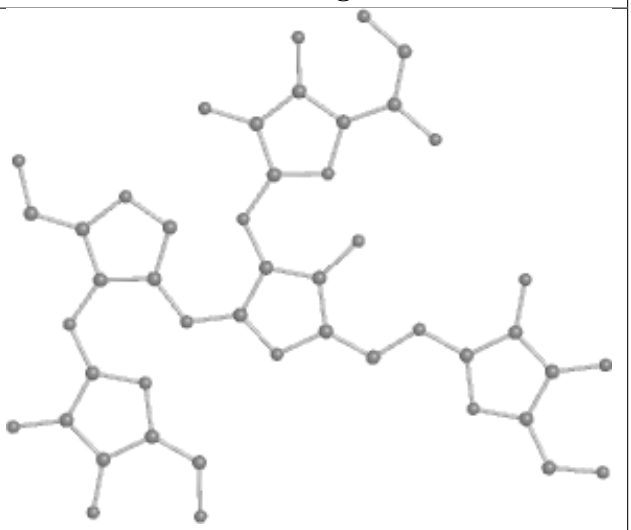
Torsions	**Rings**

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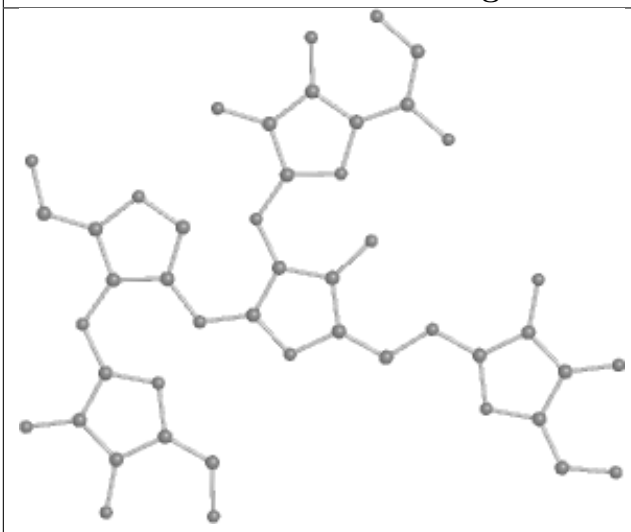	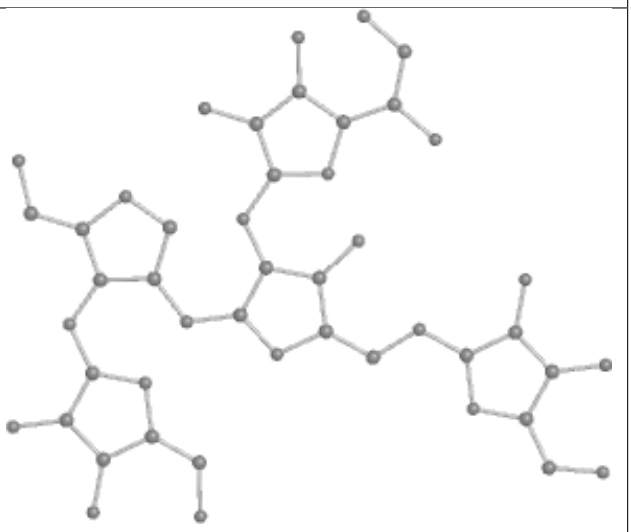
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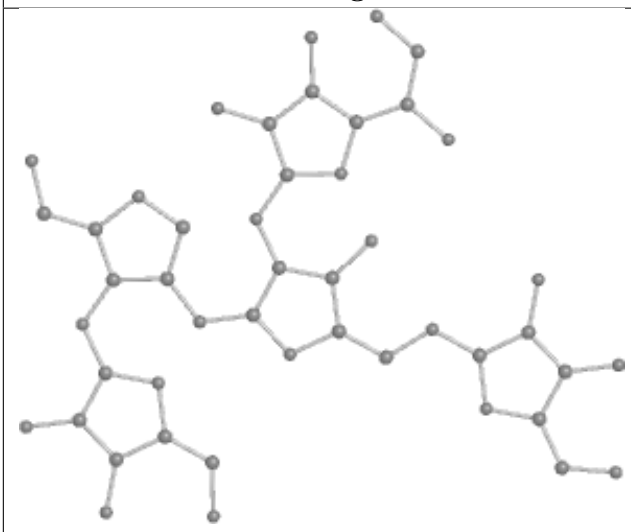
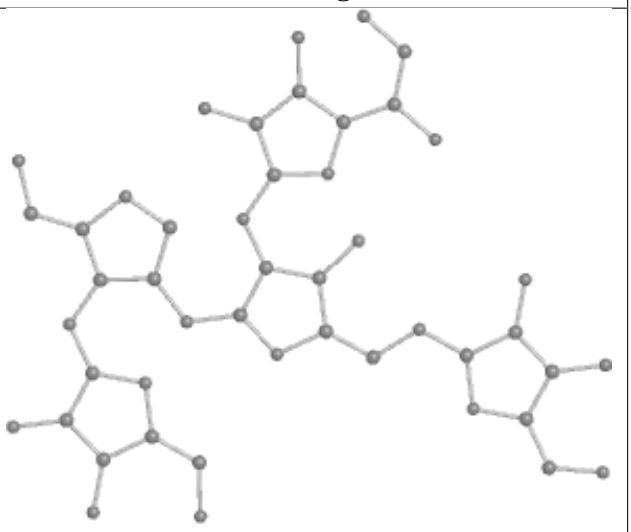
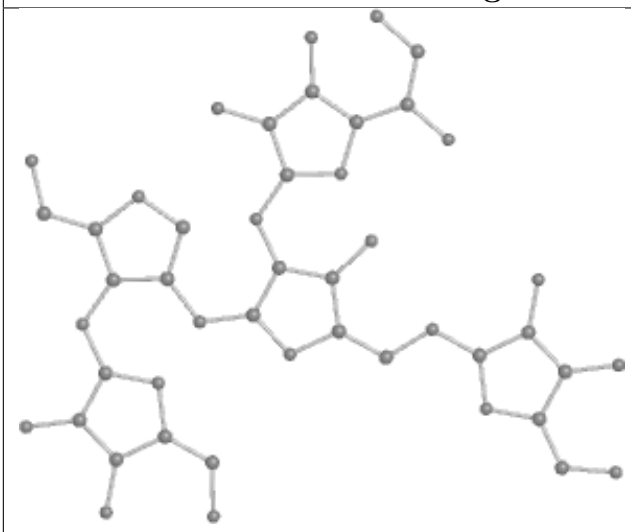
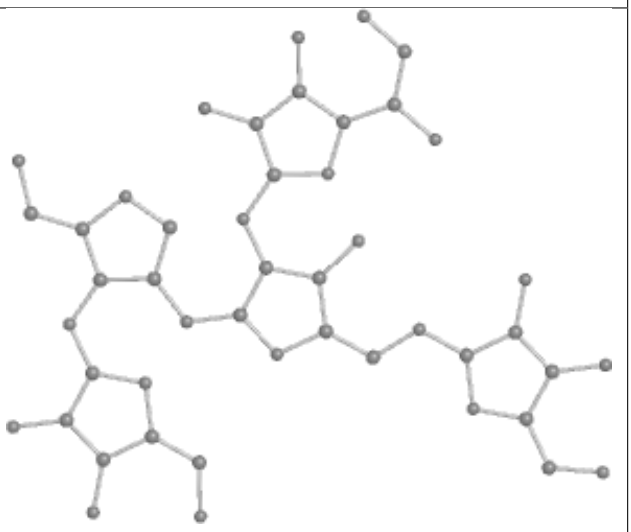
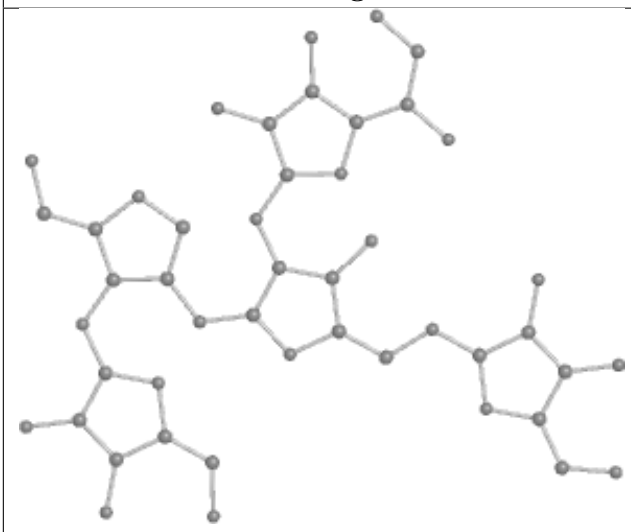
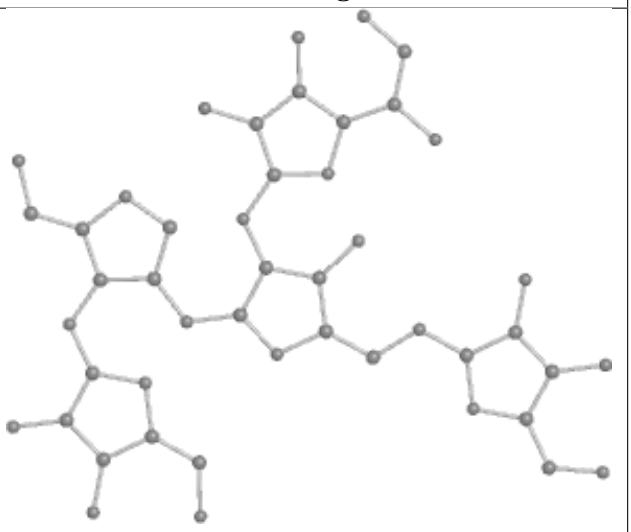
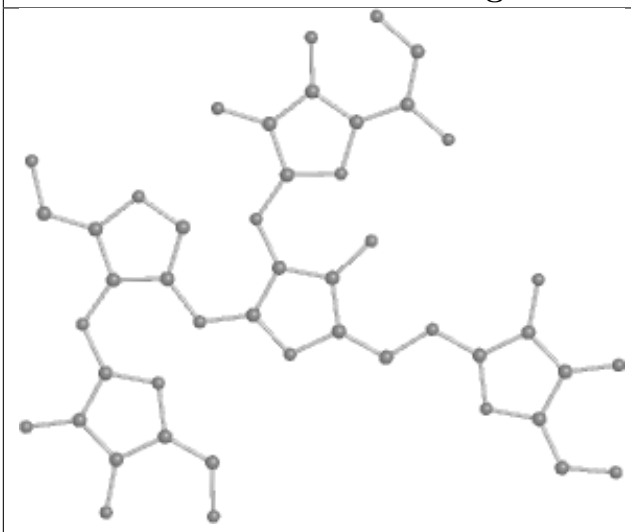
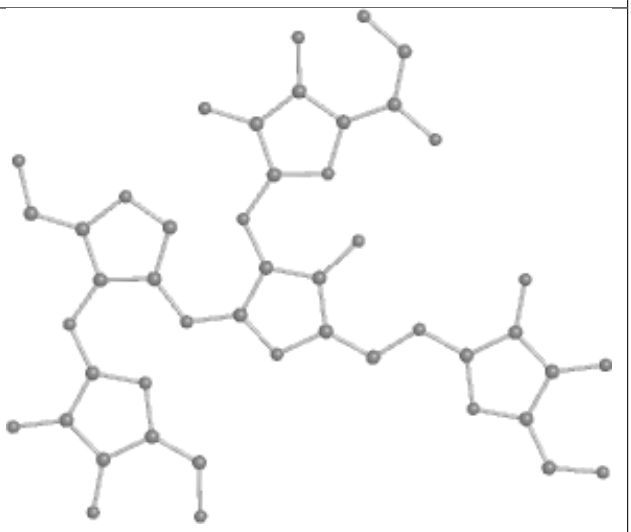
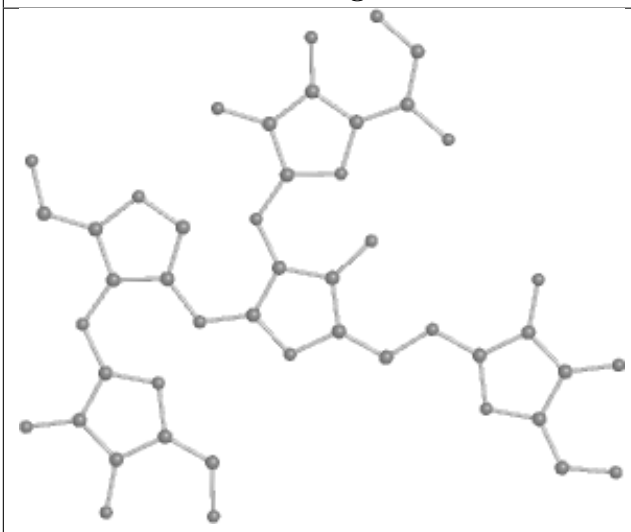
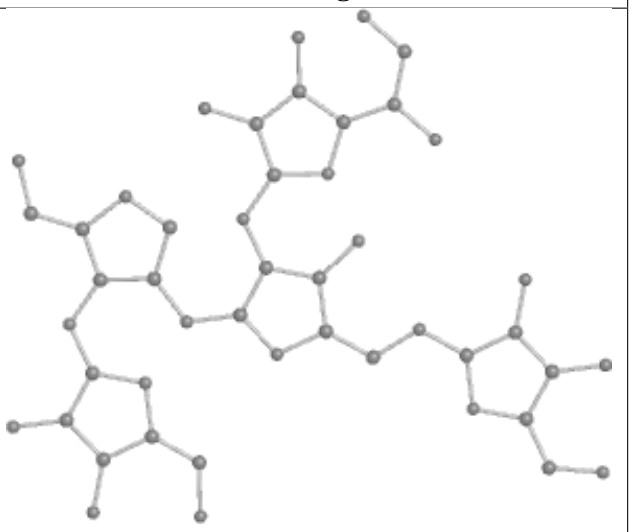
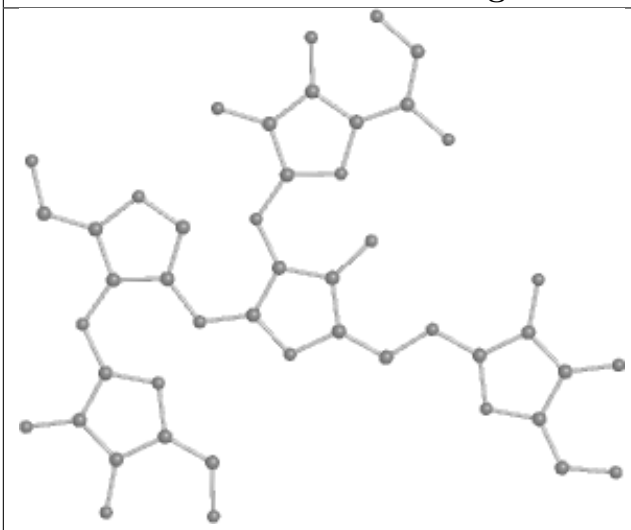
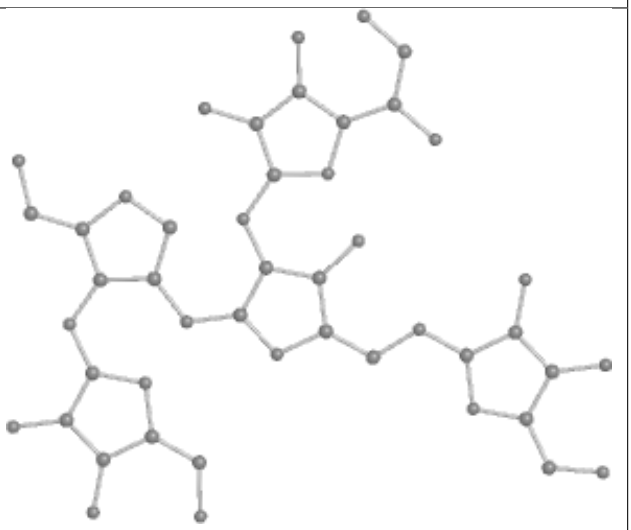
	
Torsions	**Rings**

Oligosaccharide Chain PE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain SE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain cE	
	
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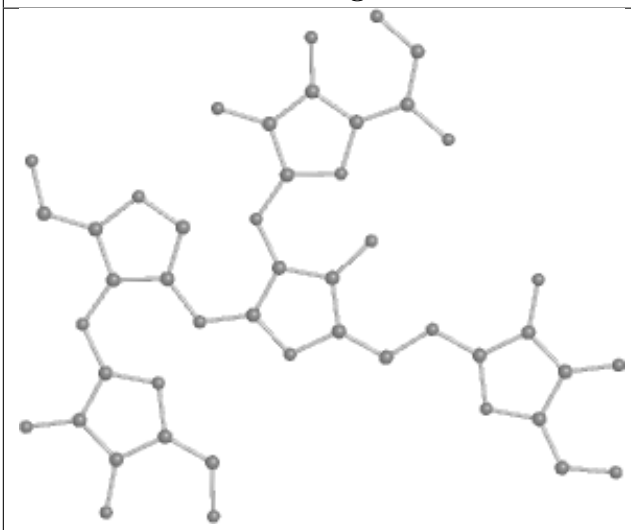	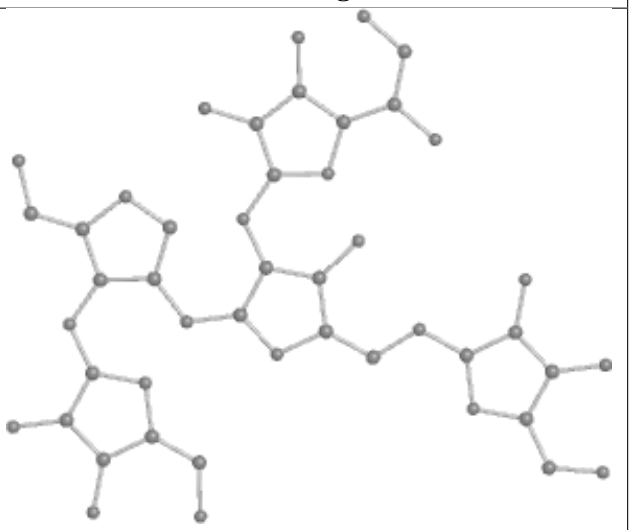
Torsions	**Rings**

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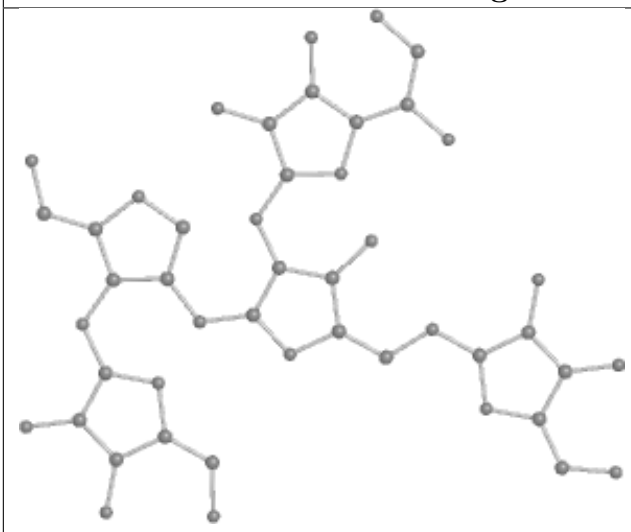	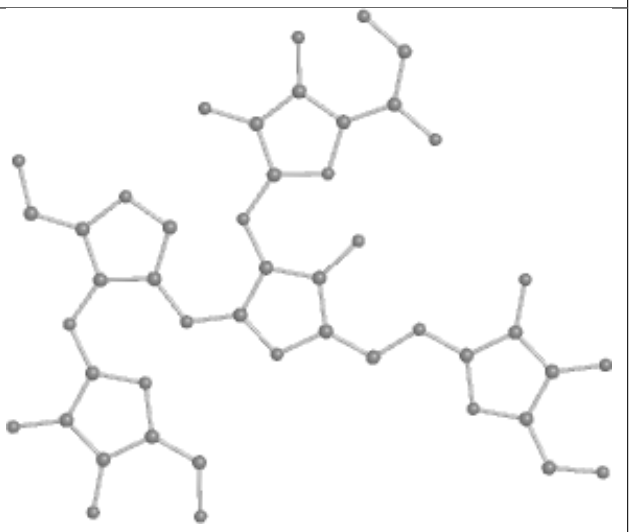
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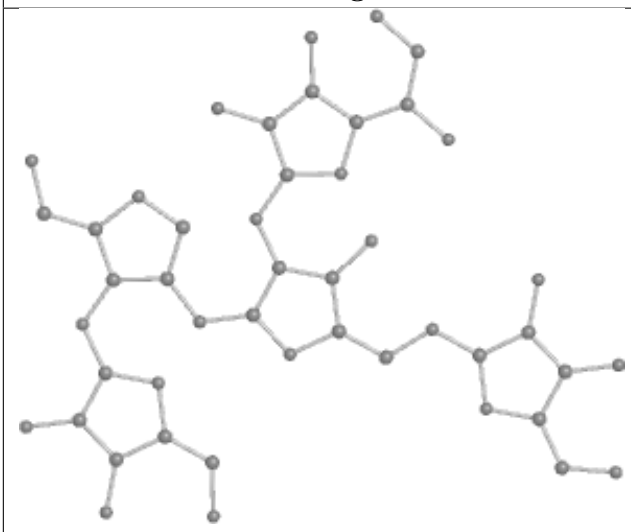
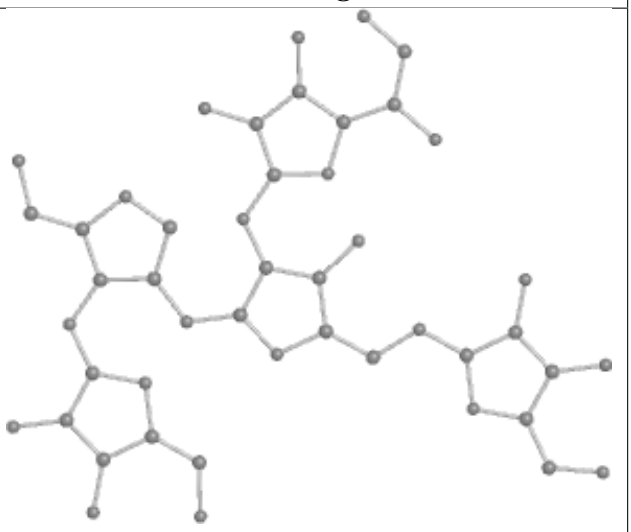
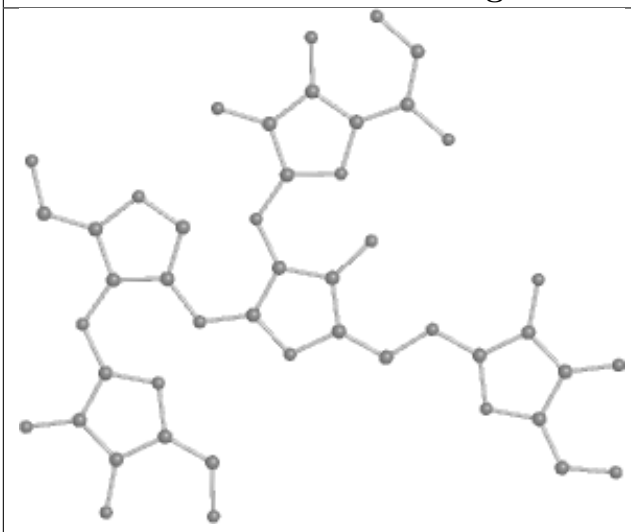
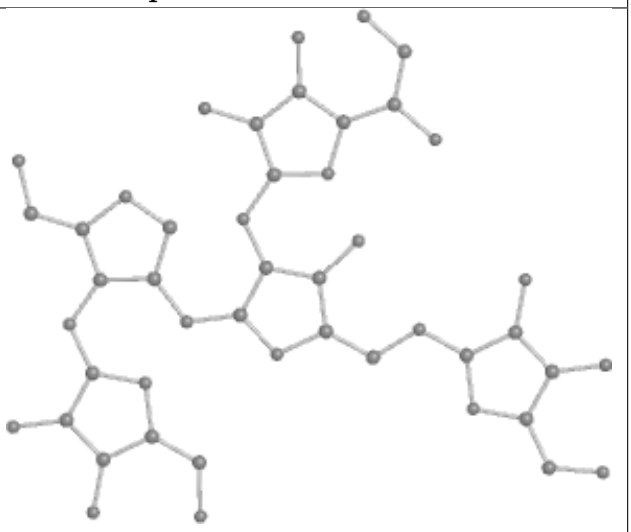
	
Torsions	**Rings**

Oligosaccharide Chain pE	
	
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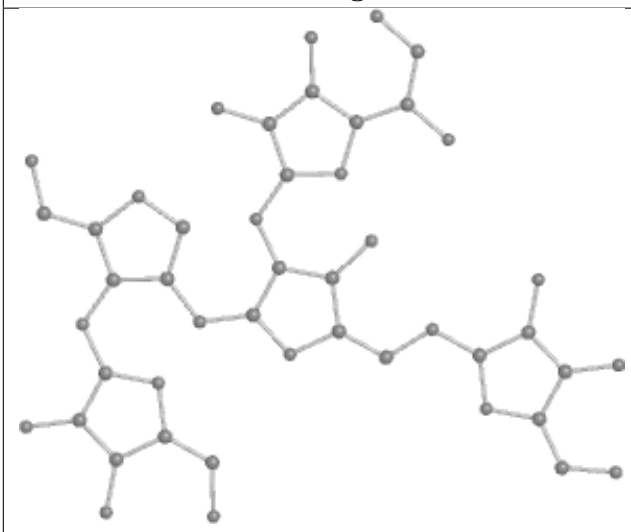
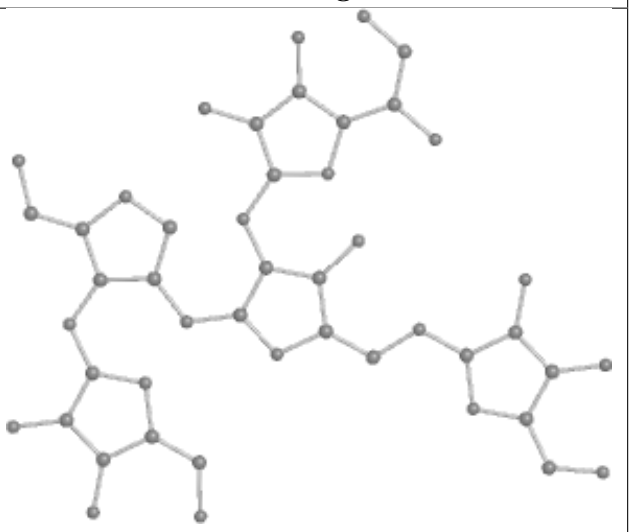
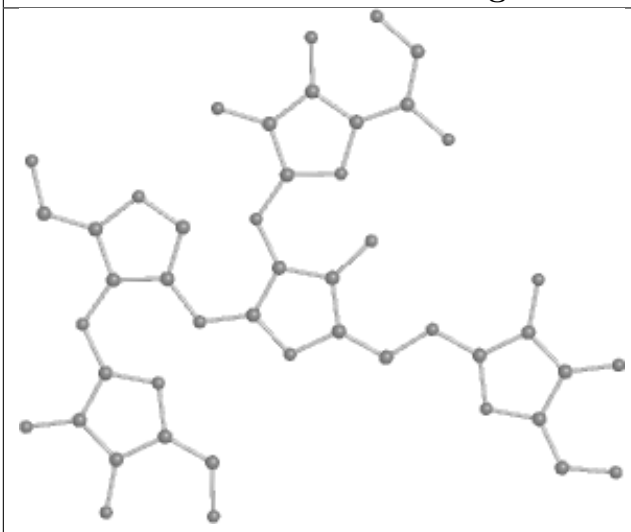
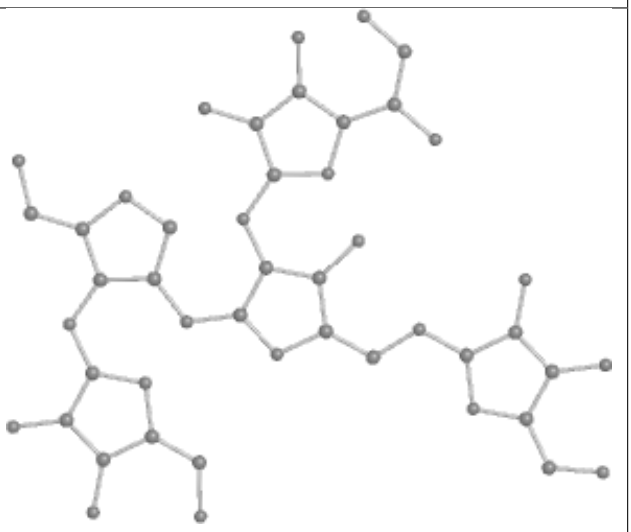
	
Torsions	**Rings**

Oligosaccharide Chain rE	
	
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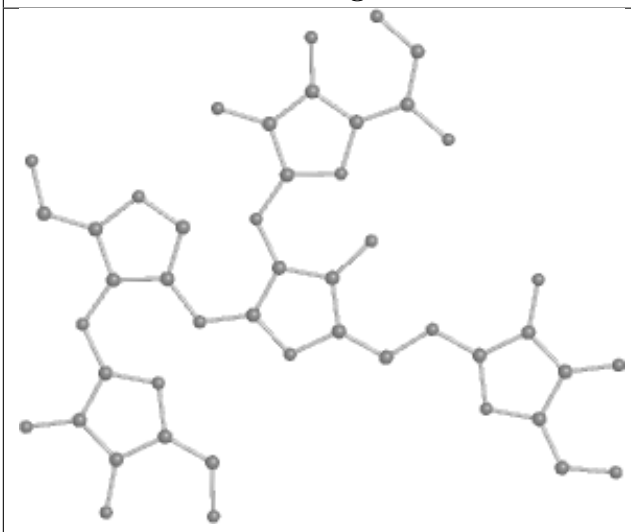	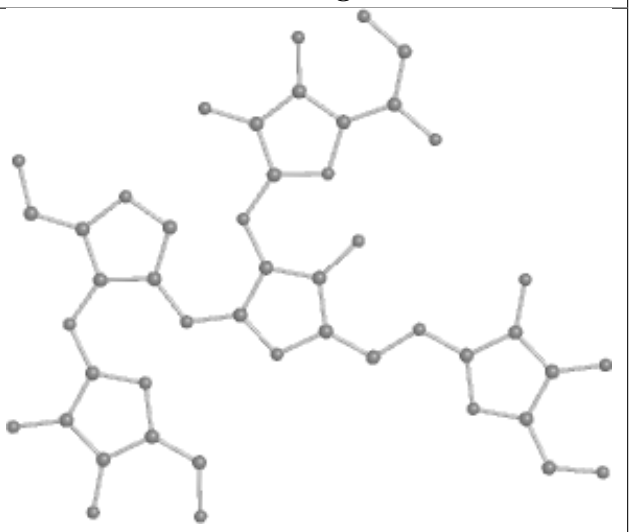
Torsions	**Rings**

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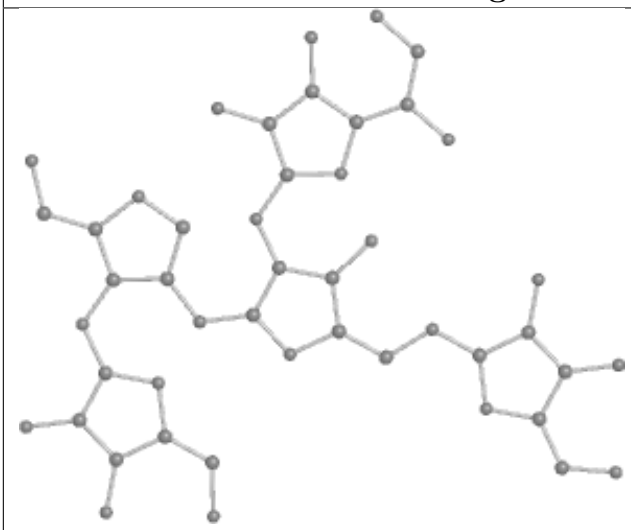
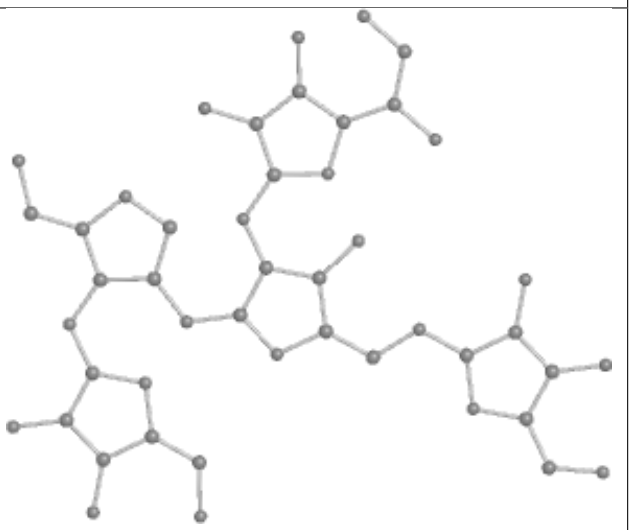
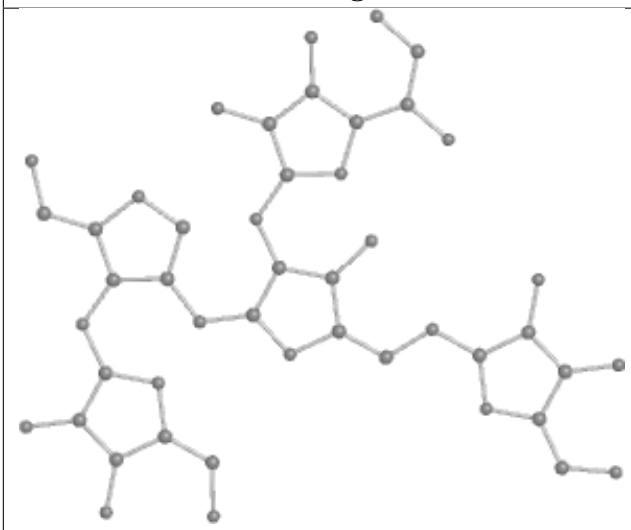
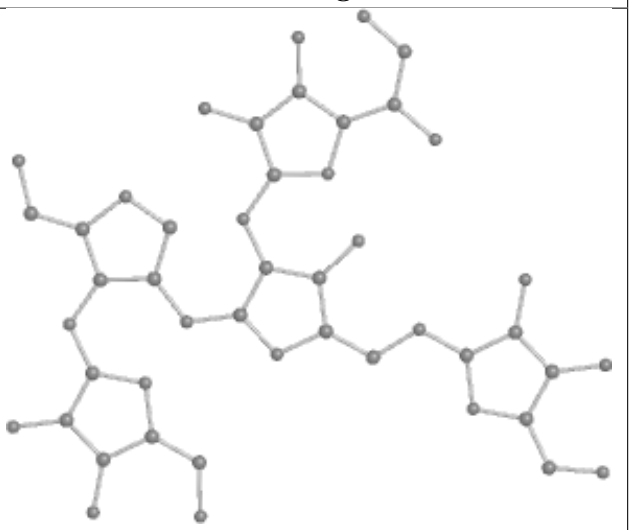
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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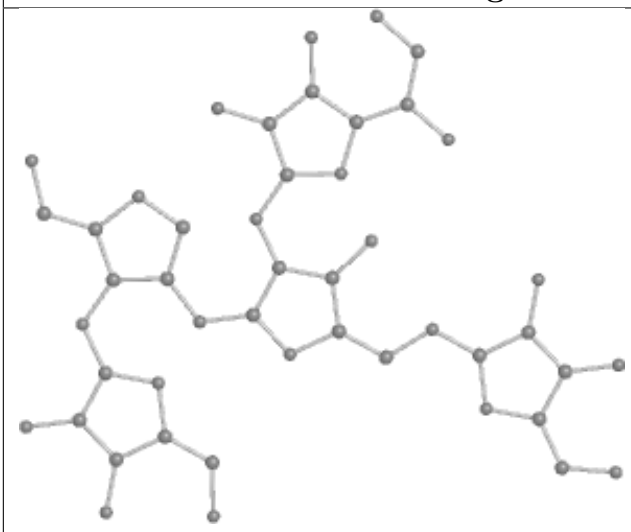	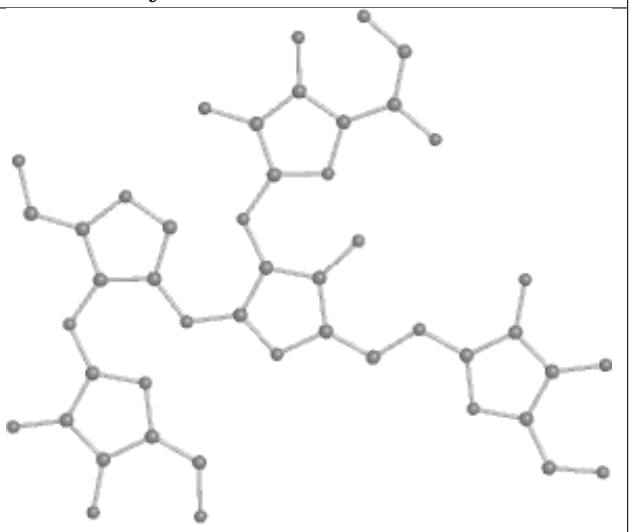
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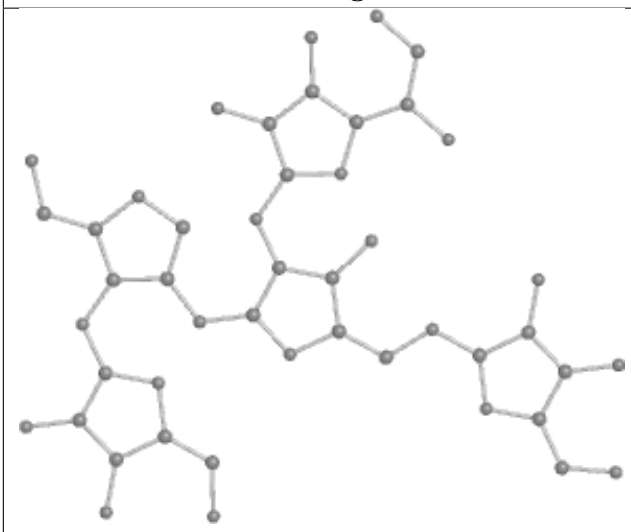	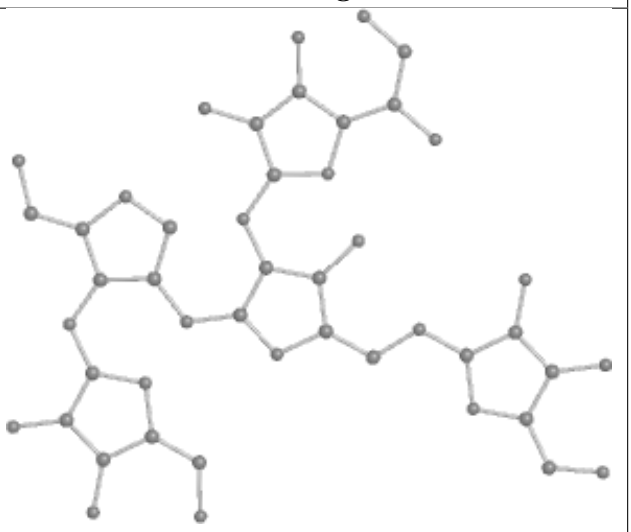
Torsions	**Rings**

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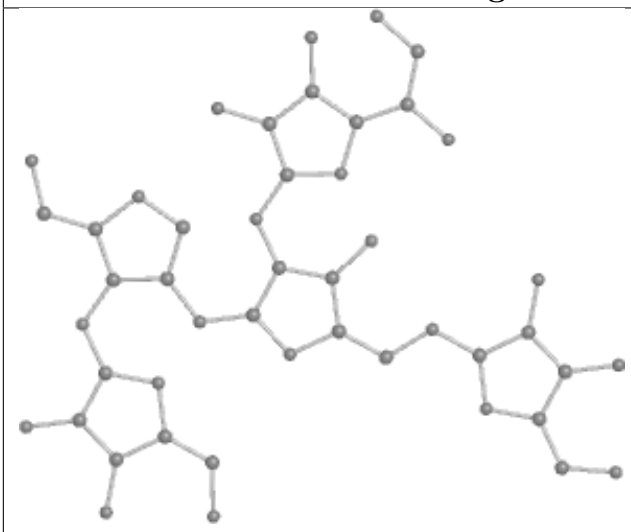	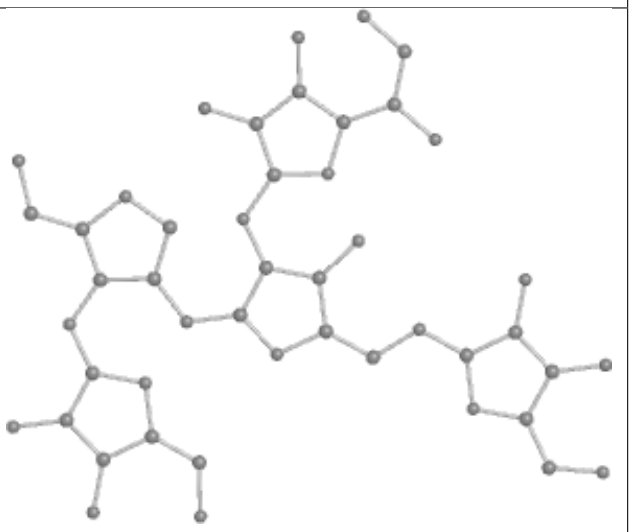
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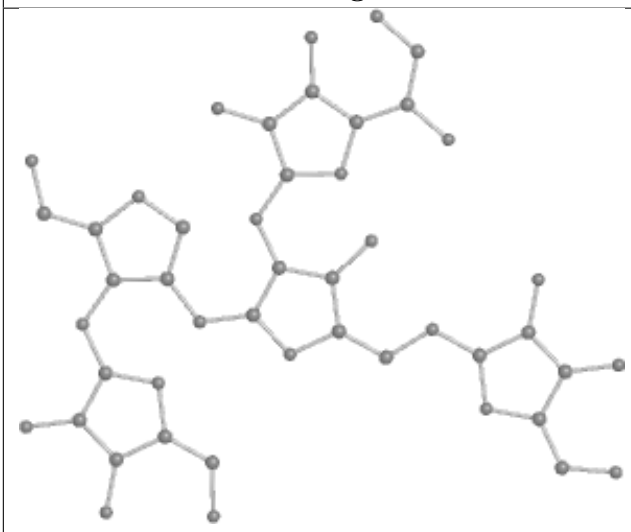	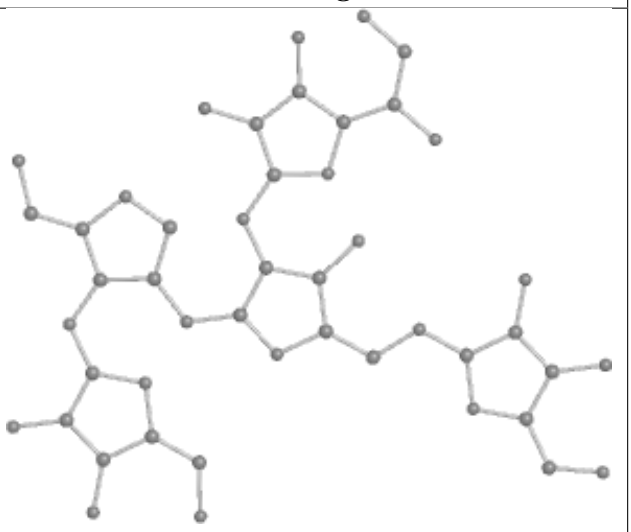
Torsions	**Rings**

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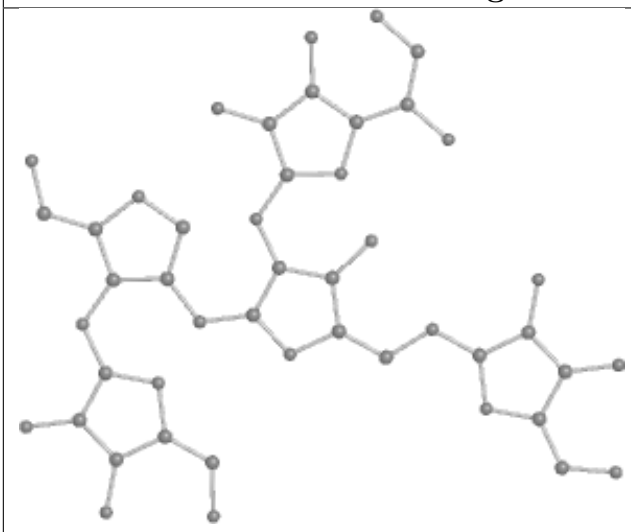
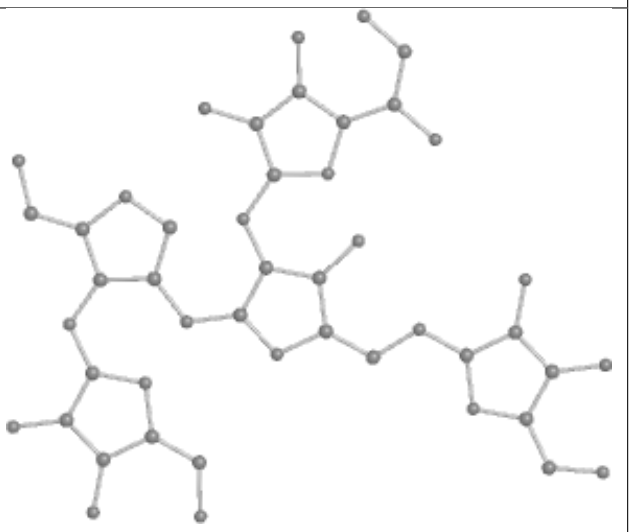
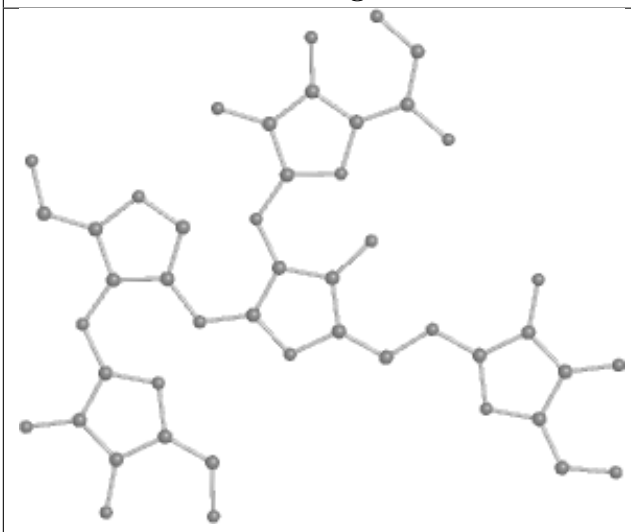
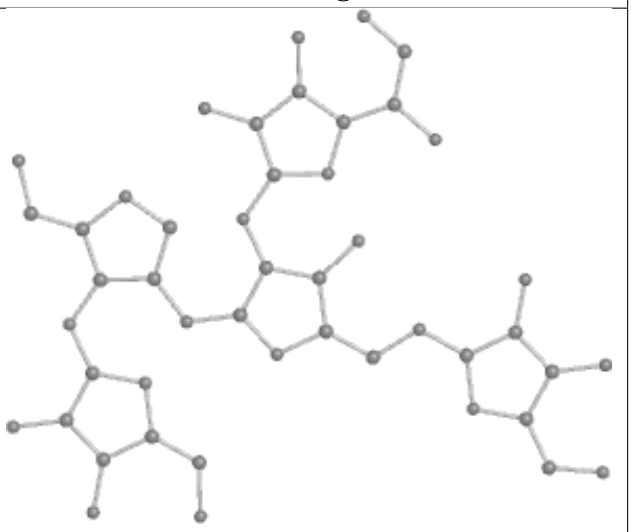
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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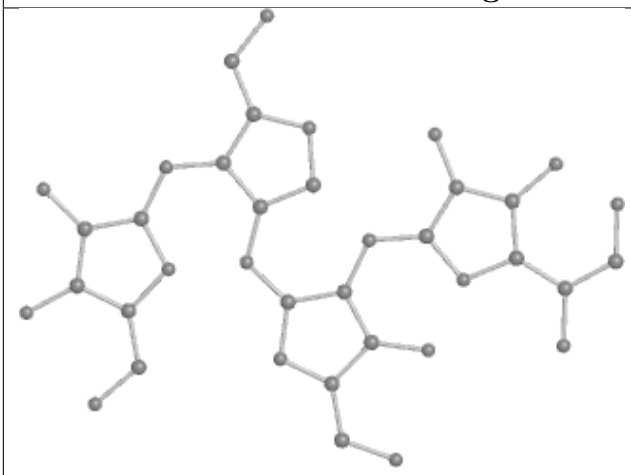
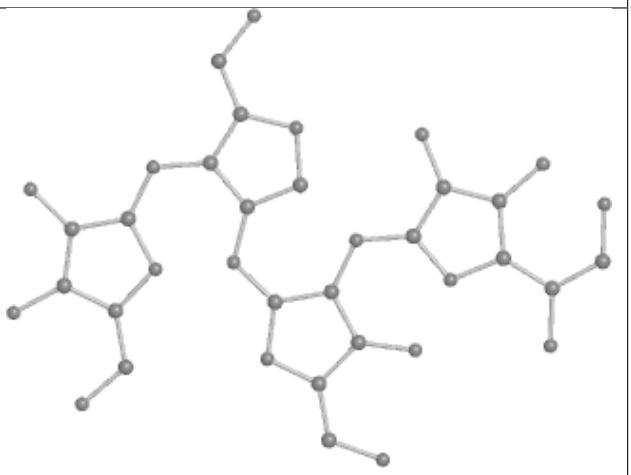
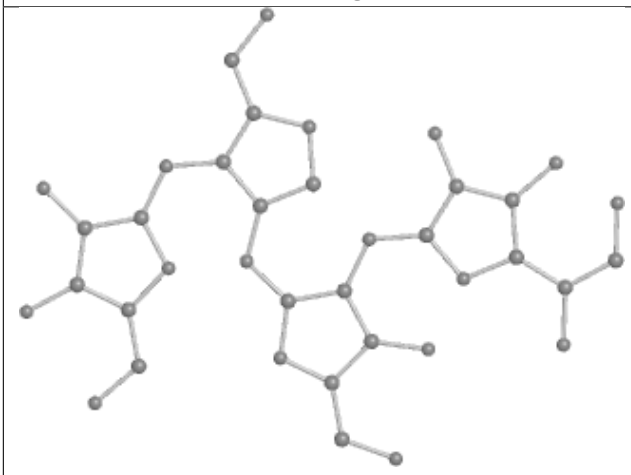
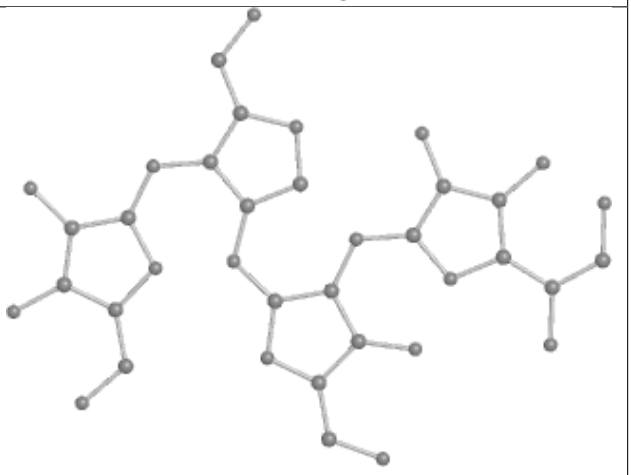
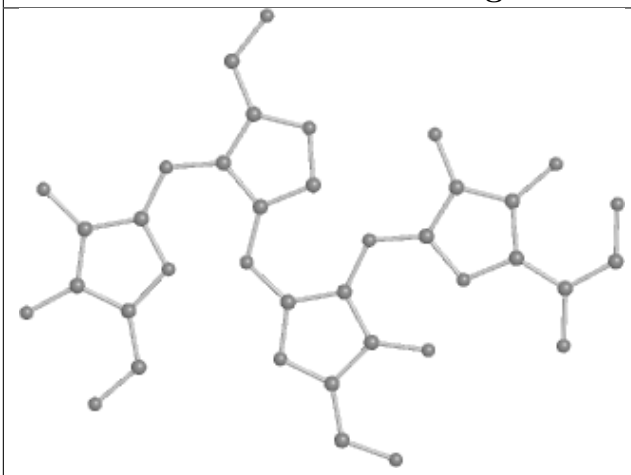
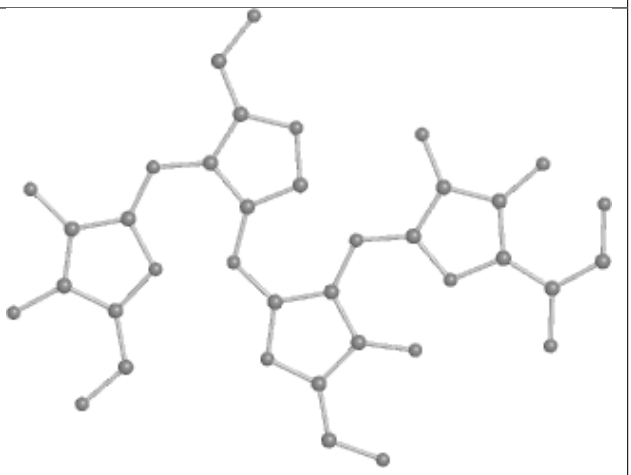
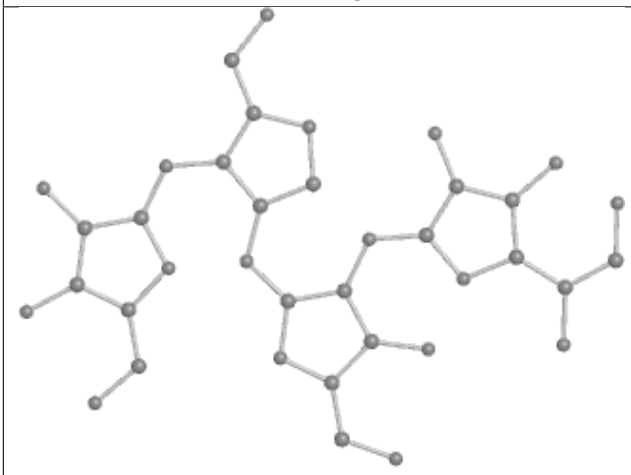
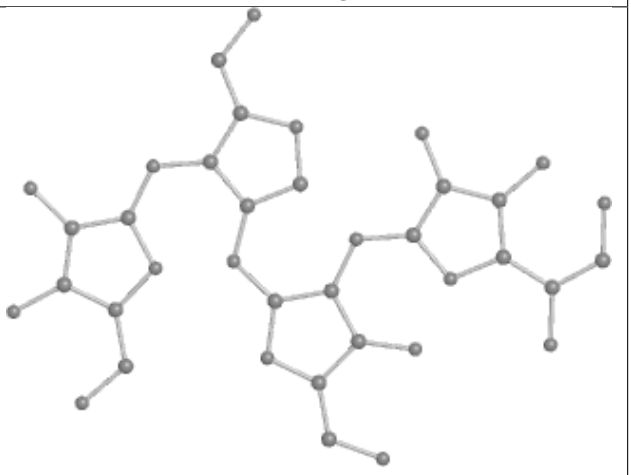
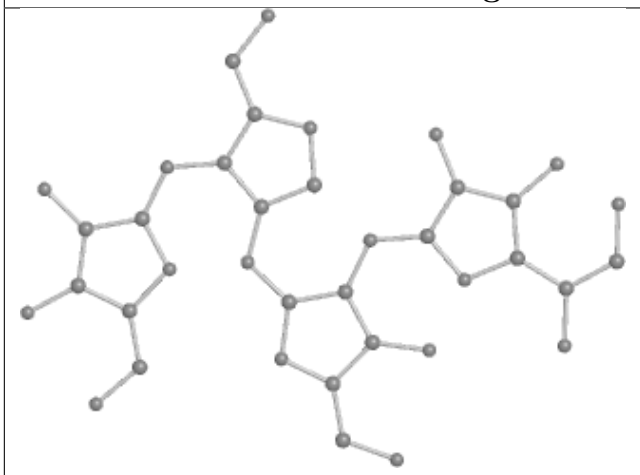
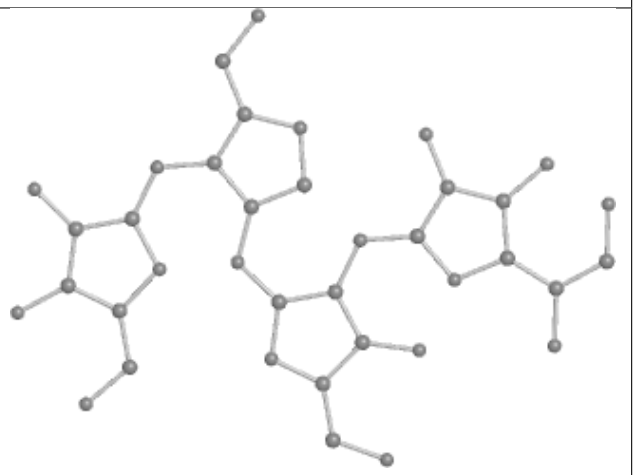
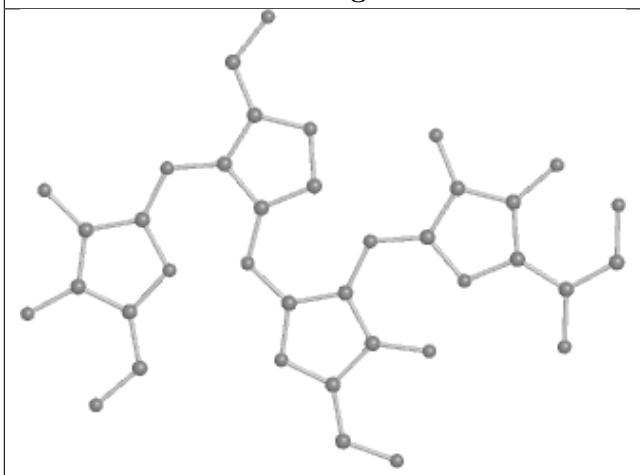
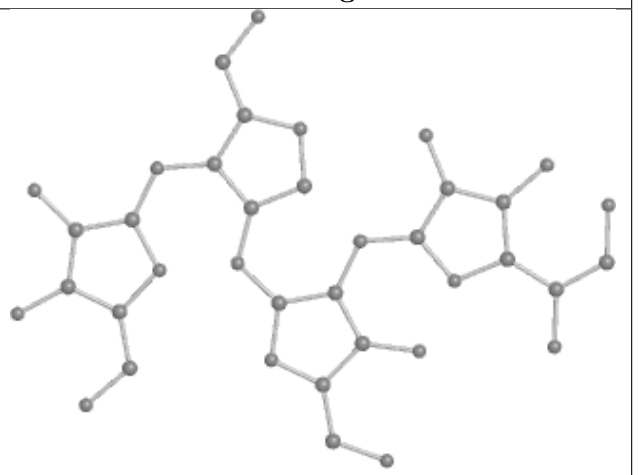
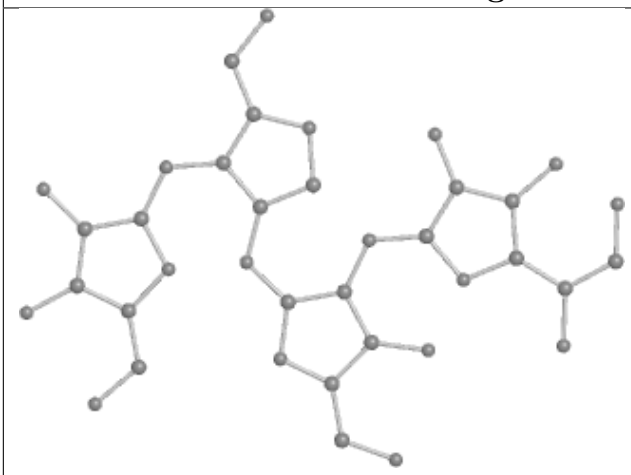
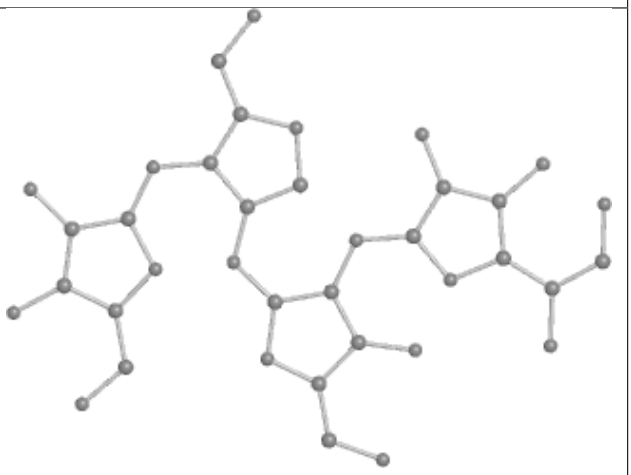
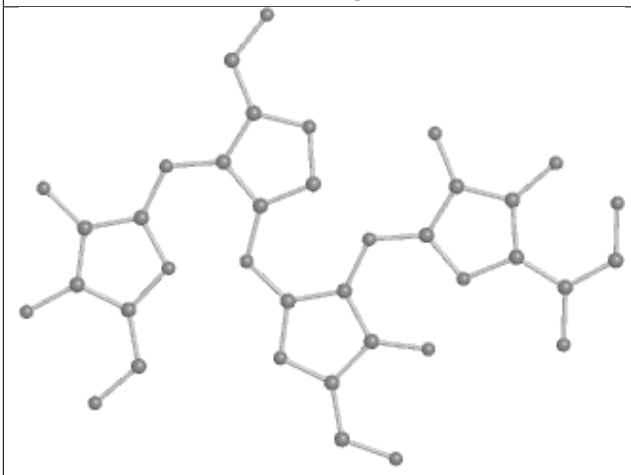
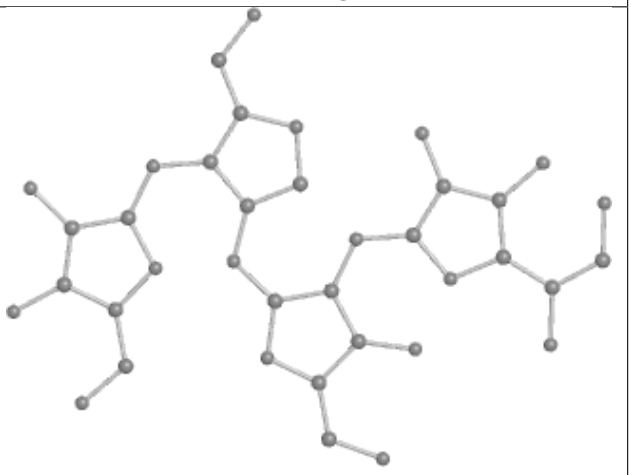
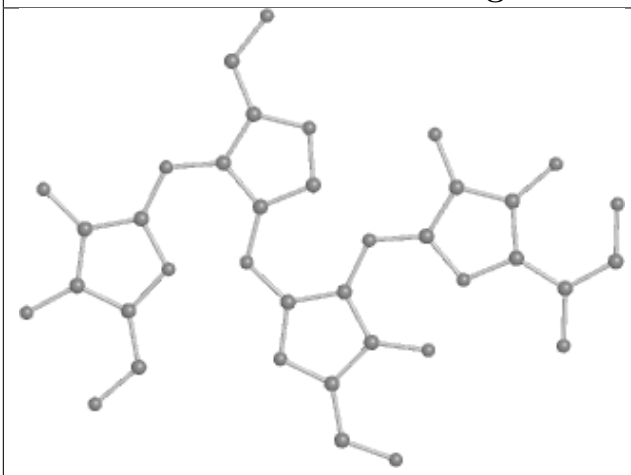
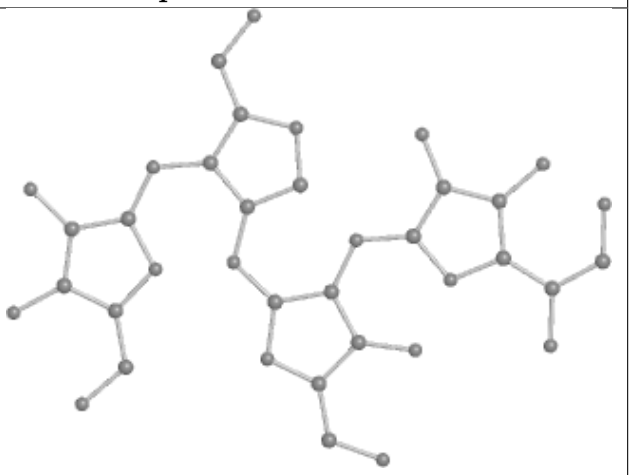
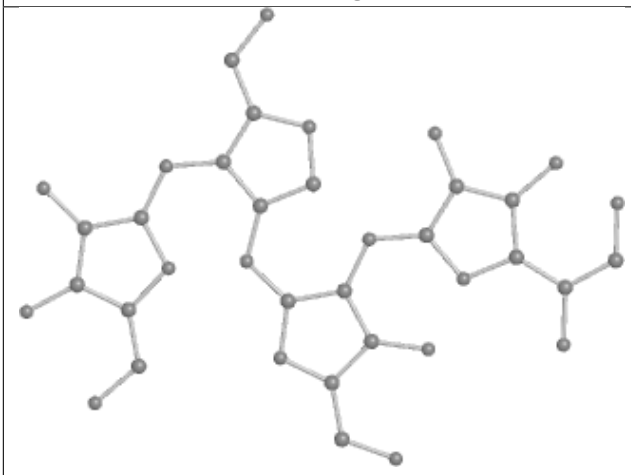
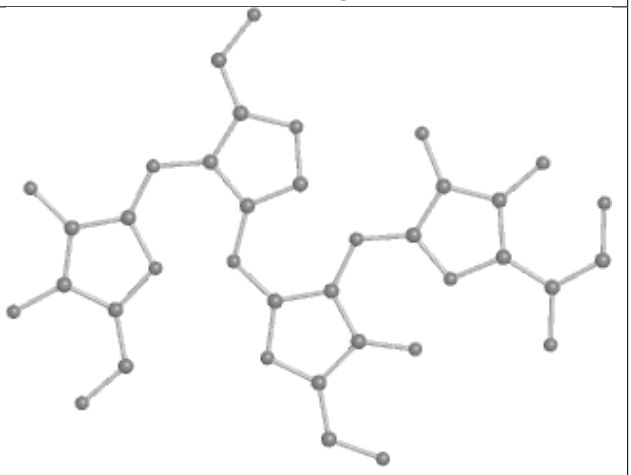
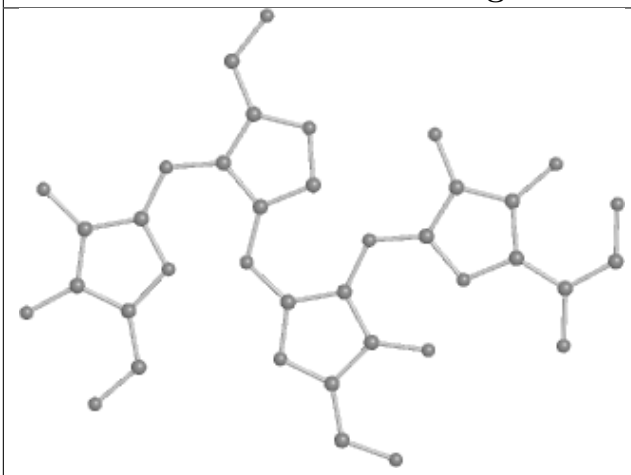
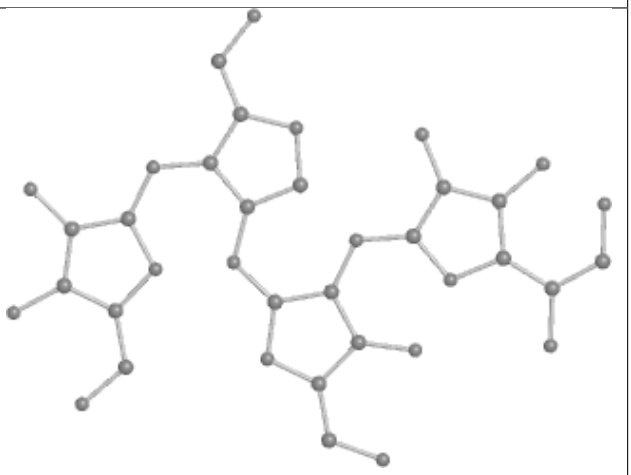
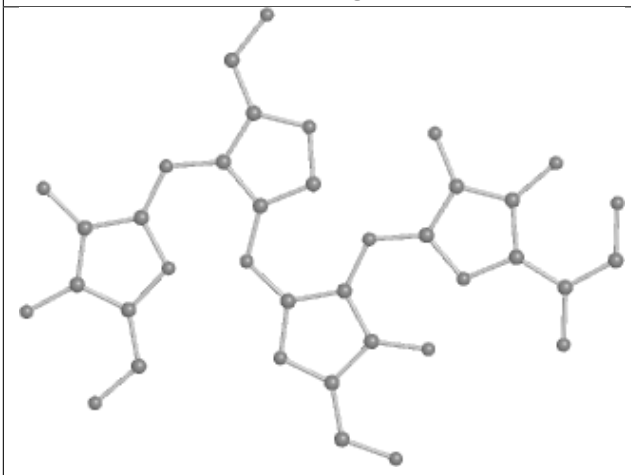
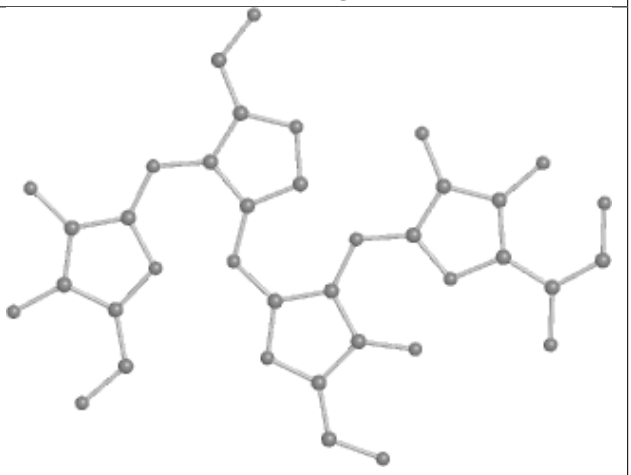
 Bond lengths	 Bond angles
 Torsions	 Rings

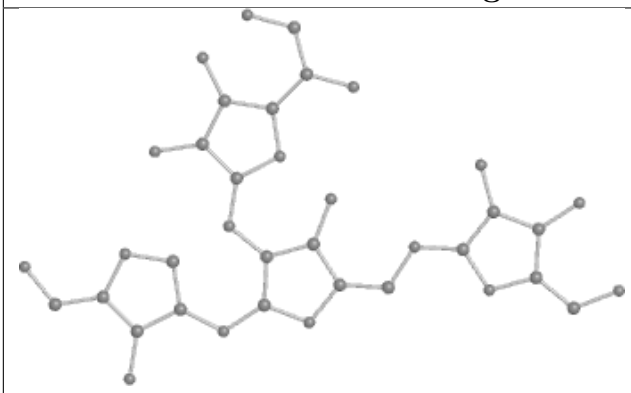
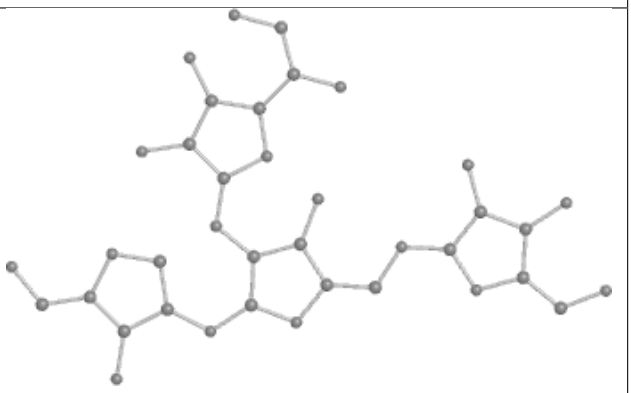
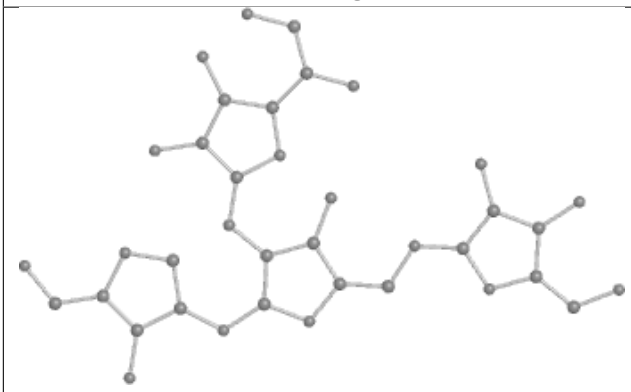
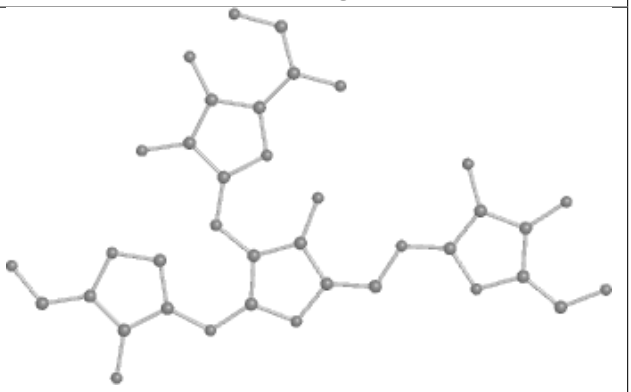
Oligosaccharide Chain LE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

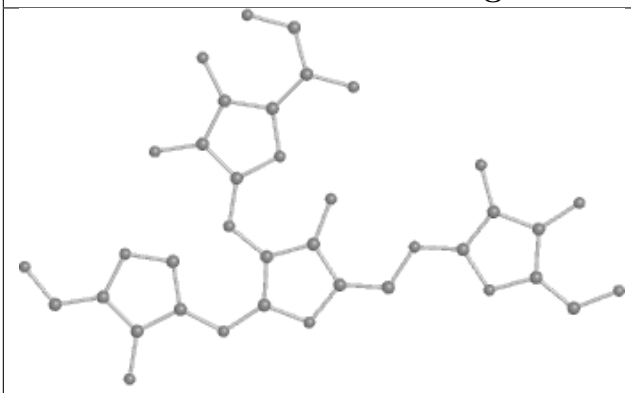
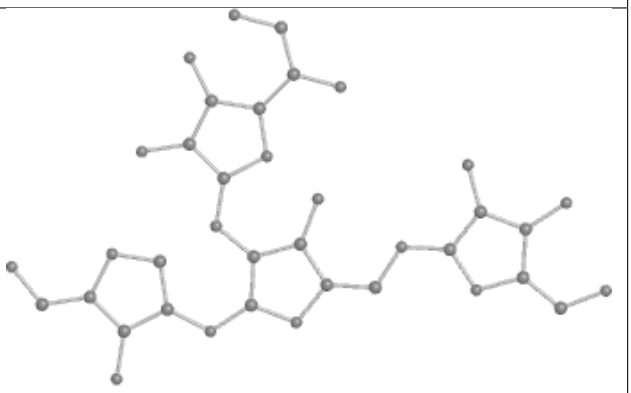
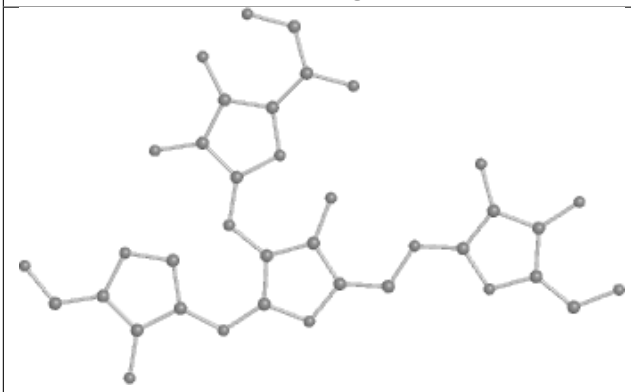
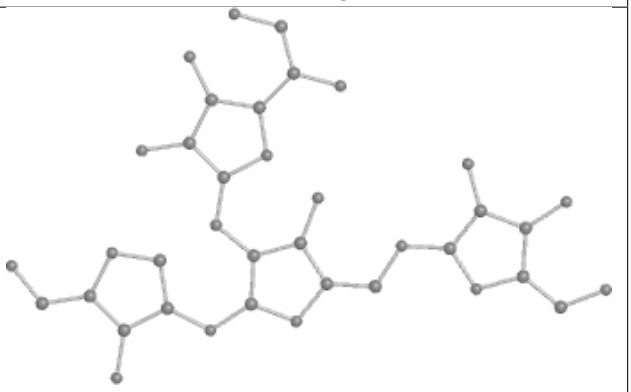
Oligosaccharide Chain NE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

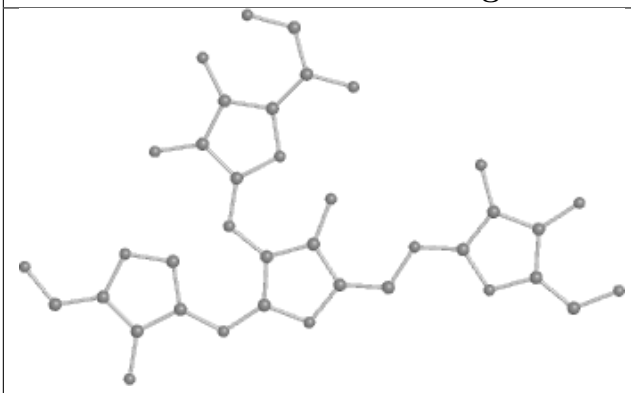
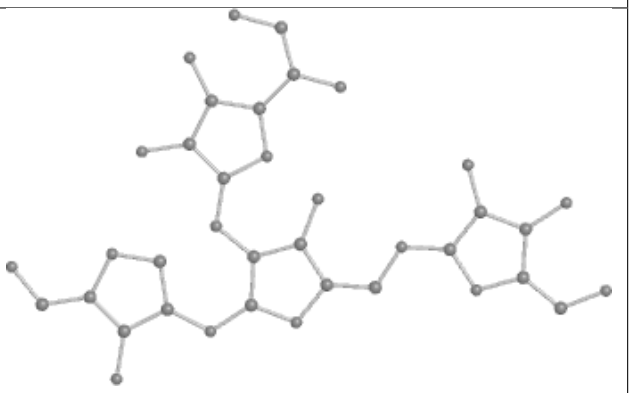
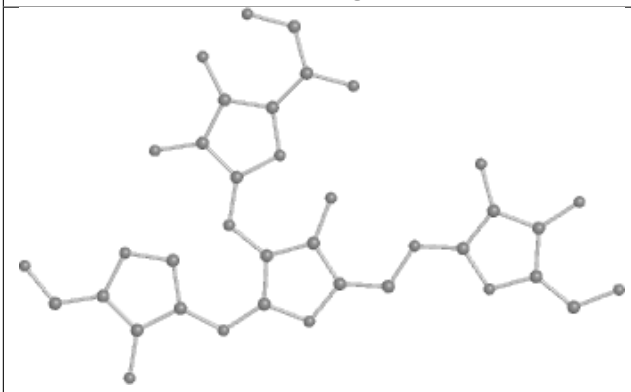
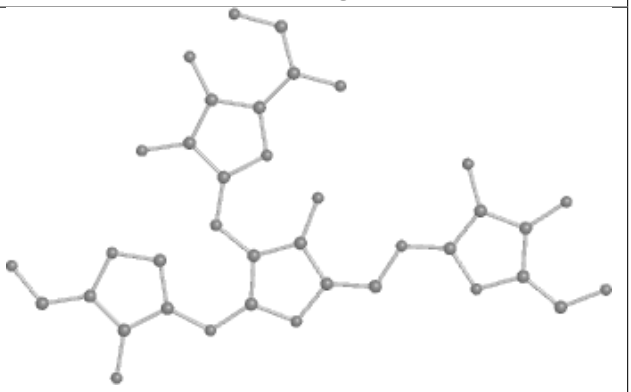
Oligosaccharide Chain aE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

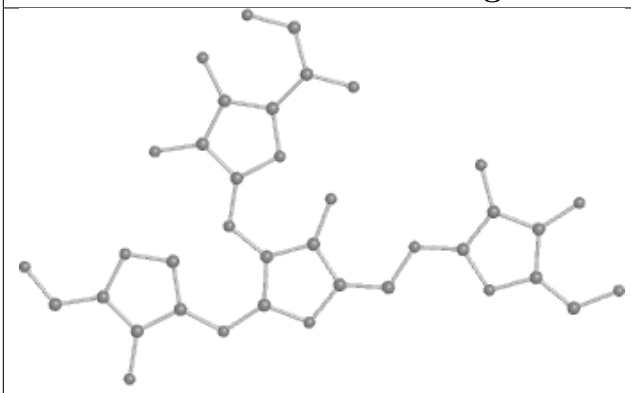
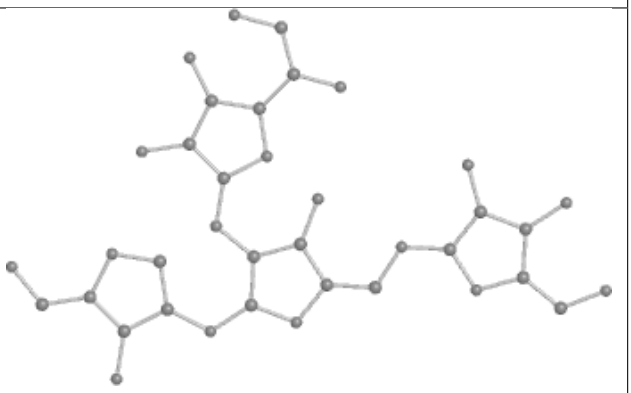
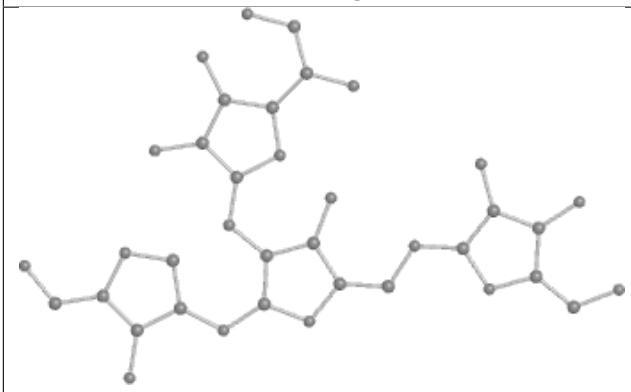
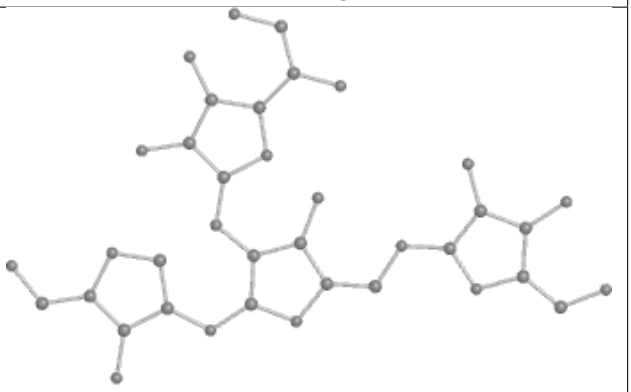
Oligosaccharide Chain qE	
 Bond lengths	 Bond angles
 Torsions	 Rings

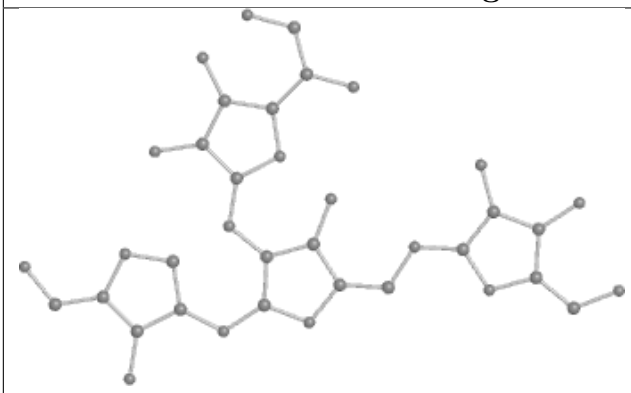
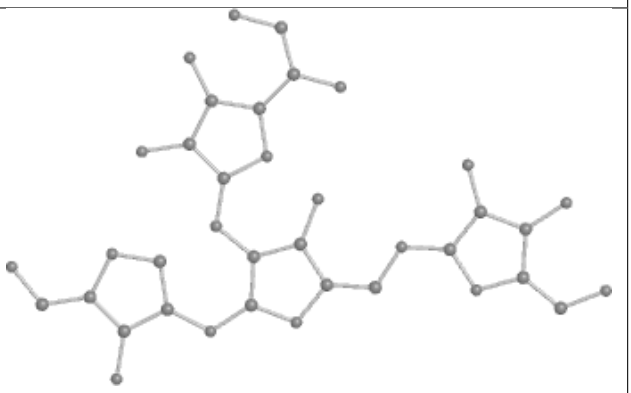
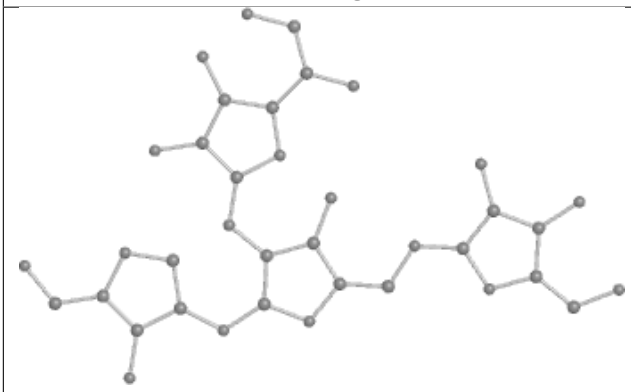
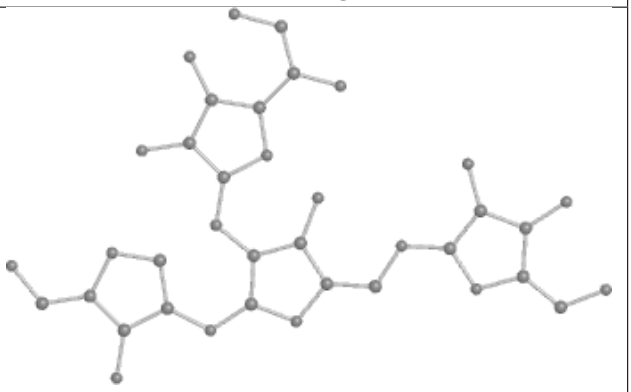
Oligosaccharide Chain 1E	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

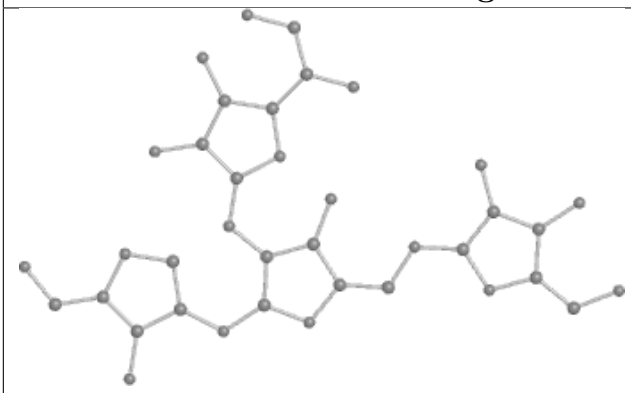
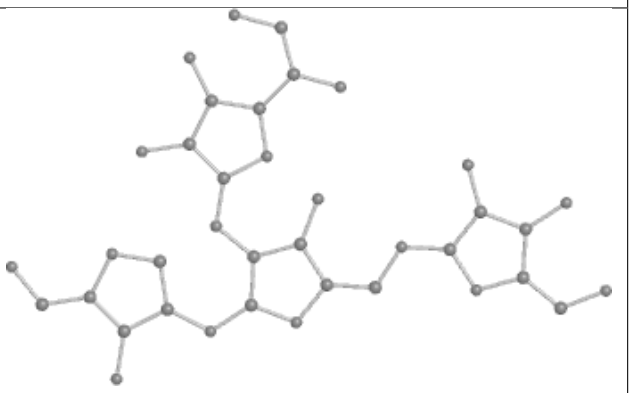
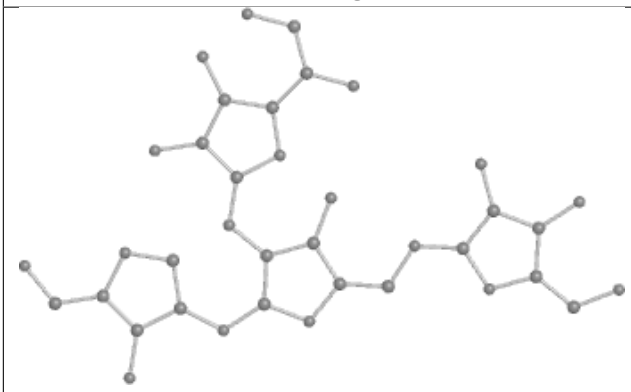
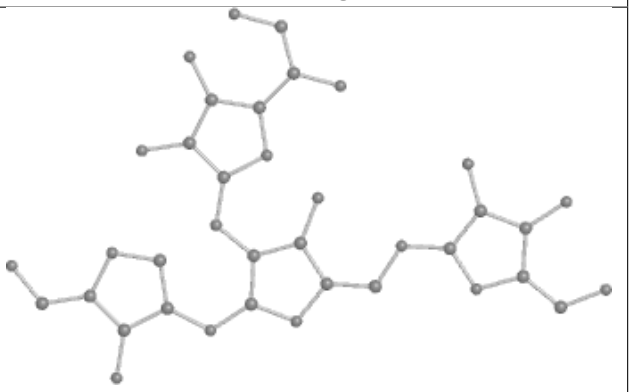
Oligosaccharide Chain CE	
 Bond lengths	 Bond angles
 Torsions	 Rings

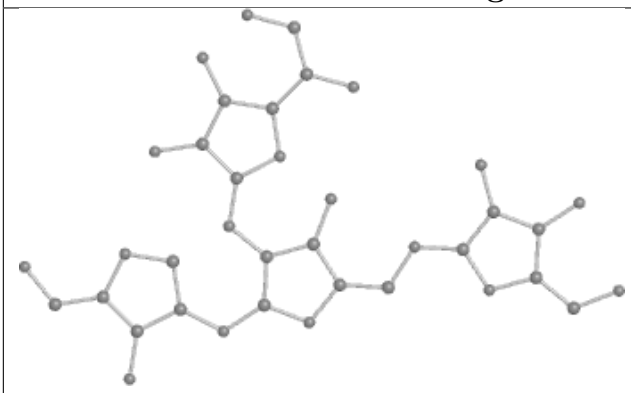
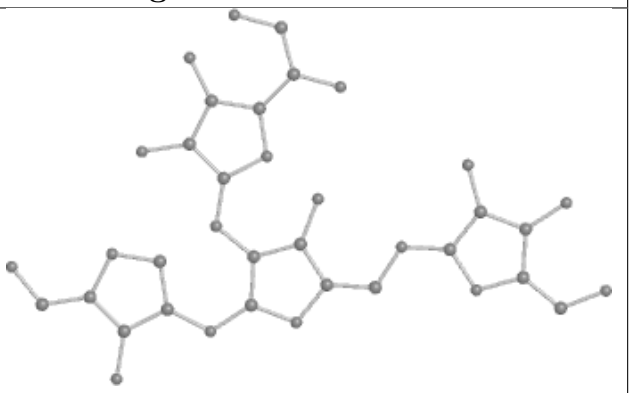
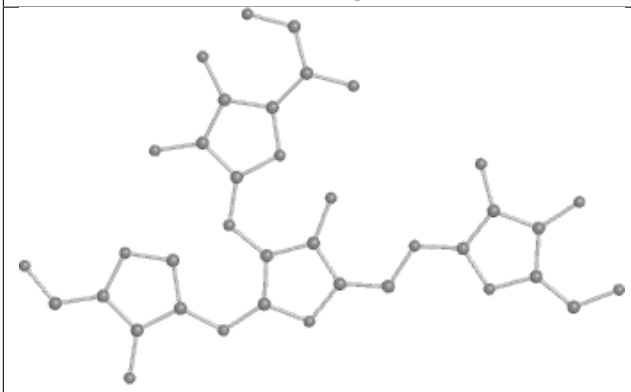
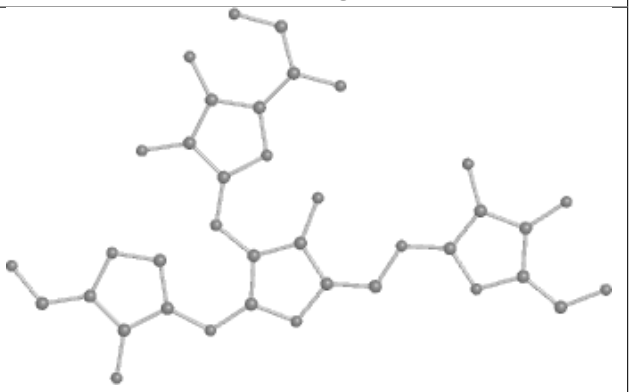
Oligosaccharide Chain EE	
 Bond lengths	 Bond angles
 Torsions	 Rings

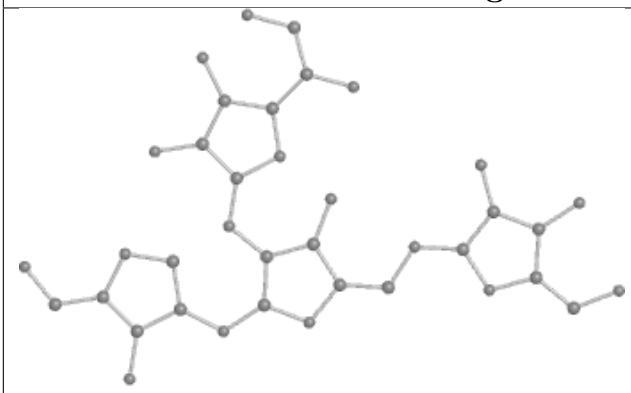
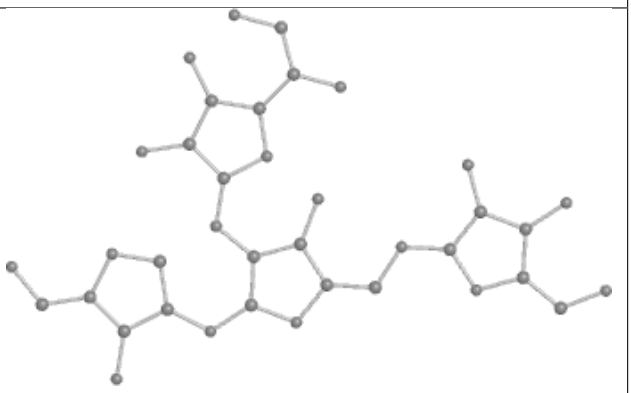
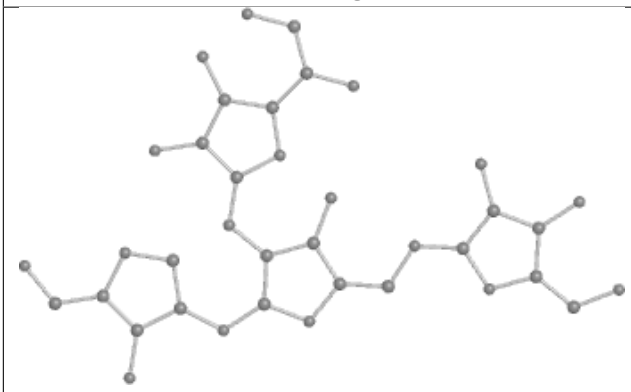
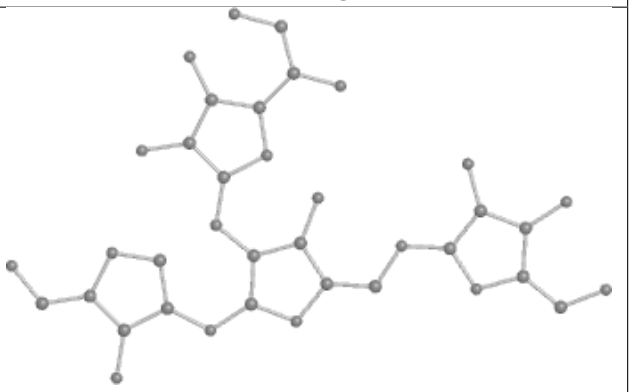
Oligosaccharide Chain HE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

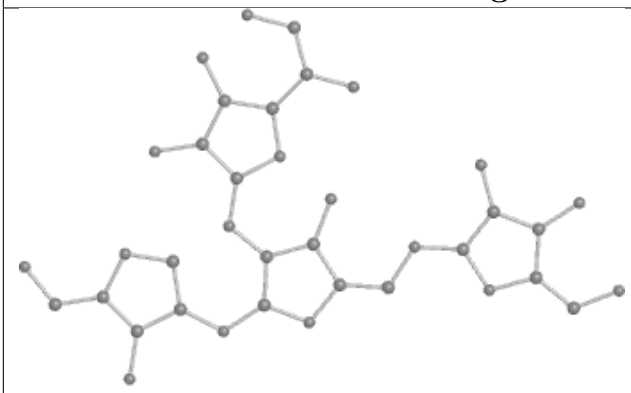
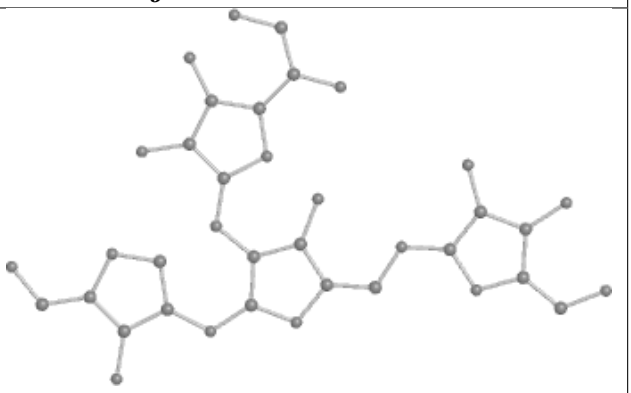
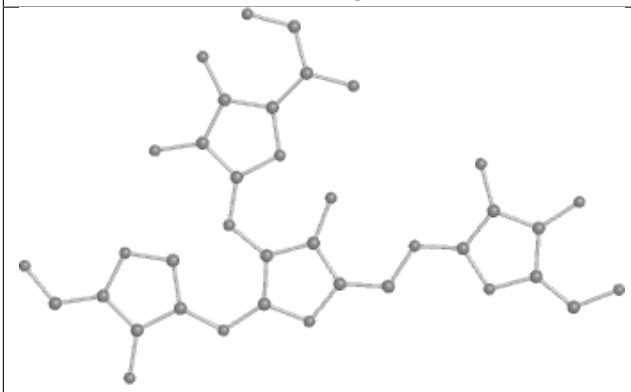
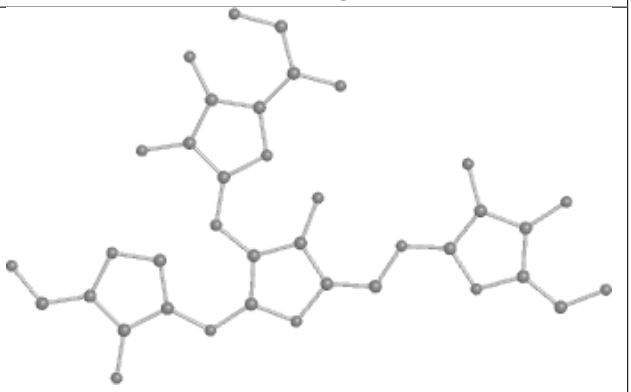
Oligosaccharide Chain TE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain UE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain WE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain gE	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain hE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain jE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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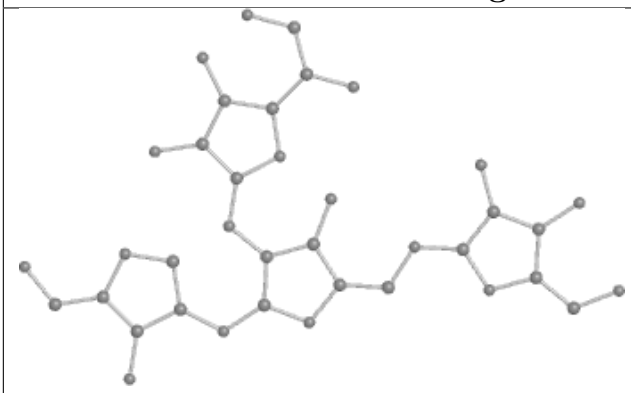
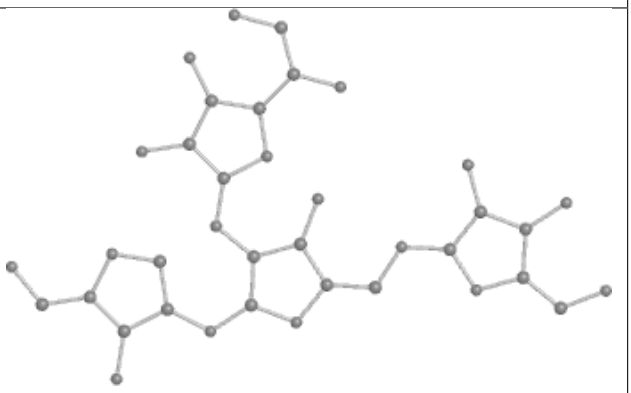
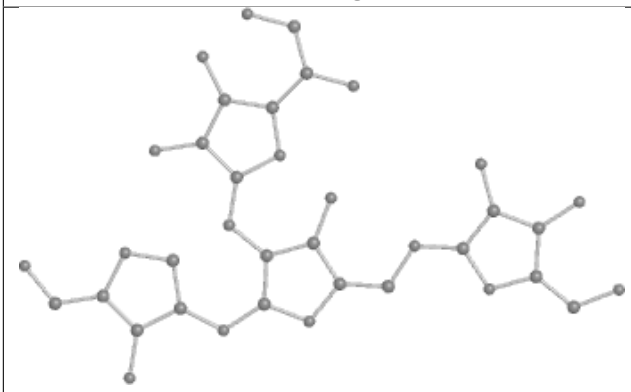
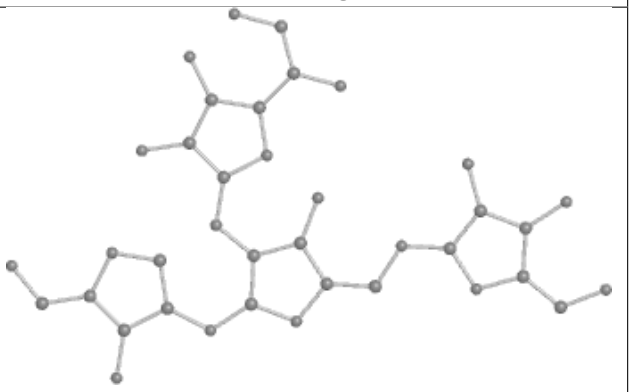
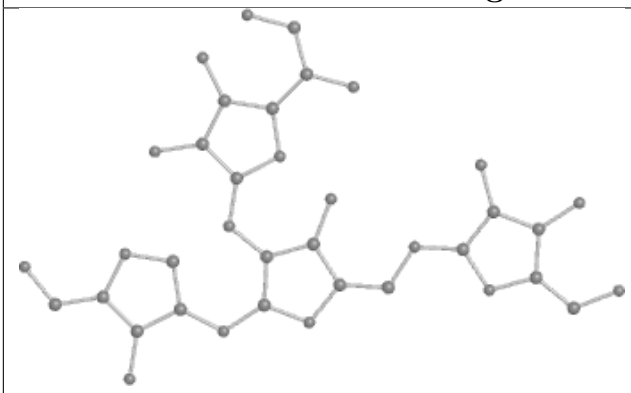
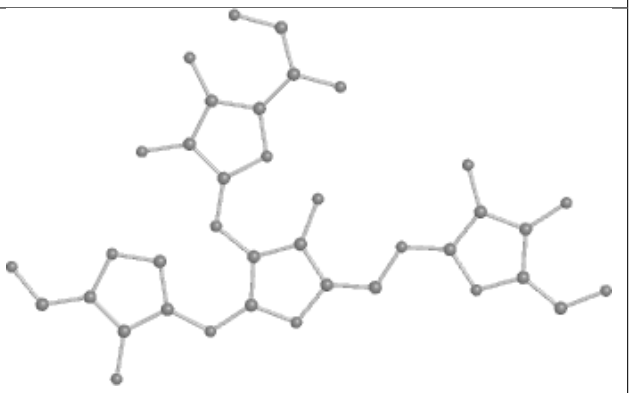
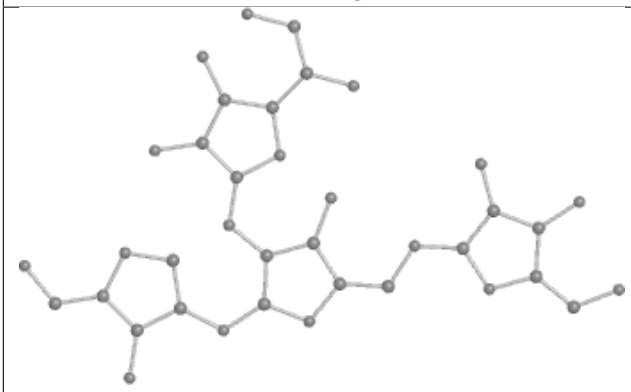
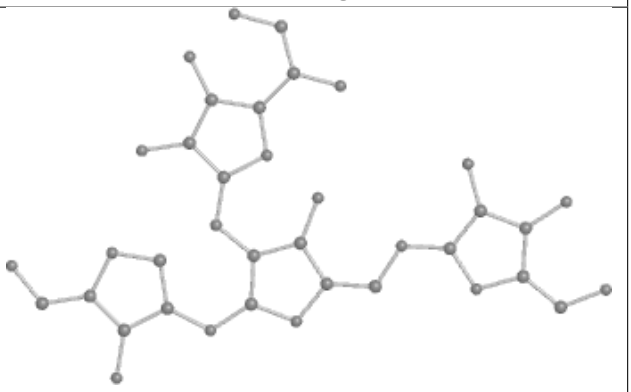
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain uE	
 Bond lengths	 Bond angles
 Torsions	 Rings

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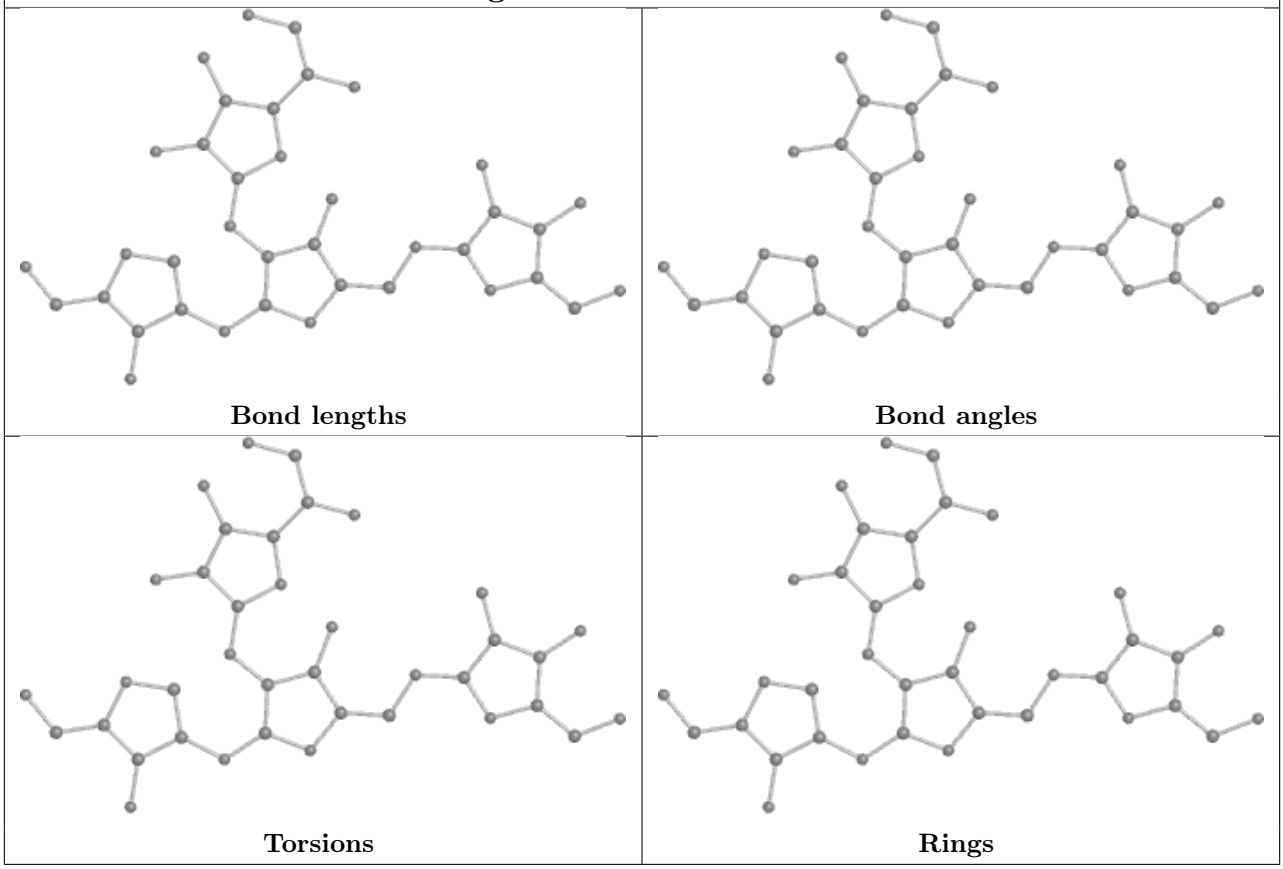

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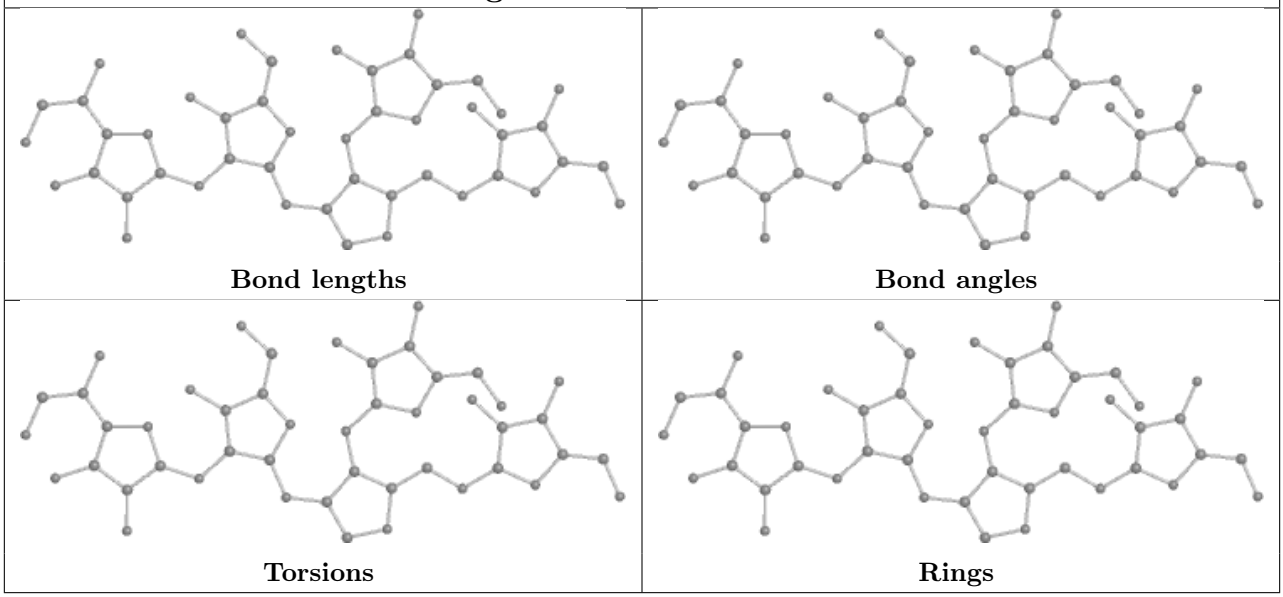

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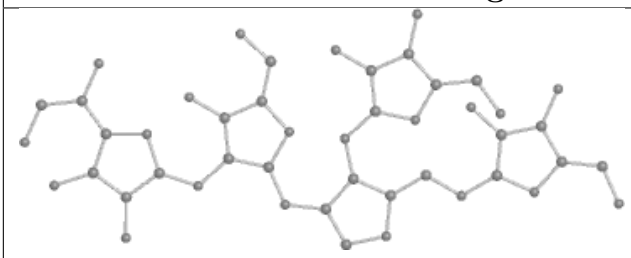
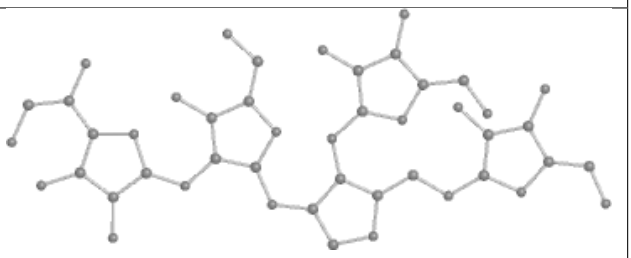
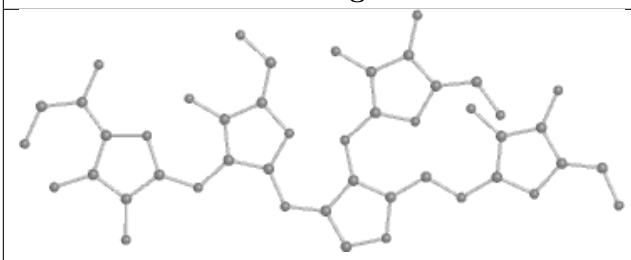
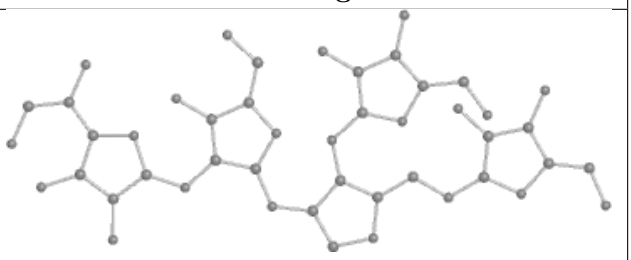
 Bond lengths	 Bond angles
 Torsions	 Rings

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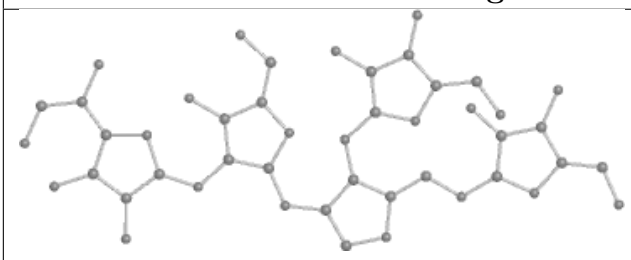
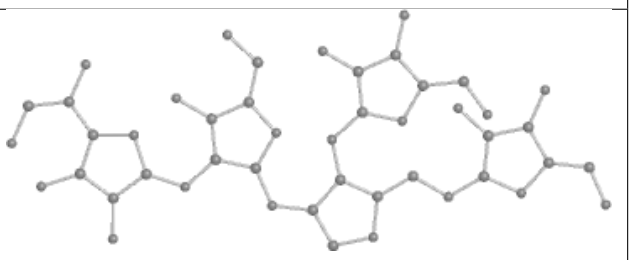
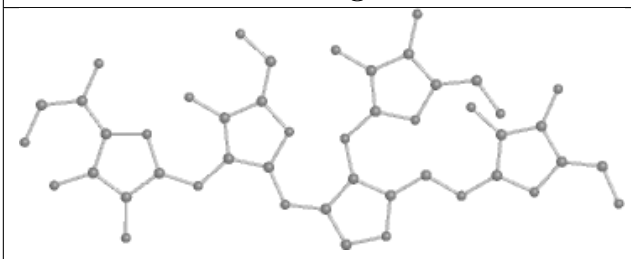
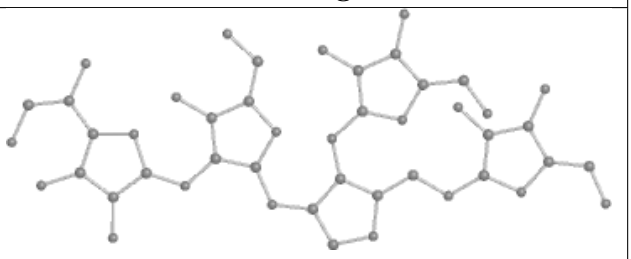
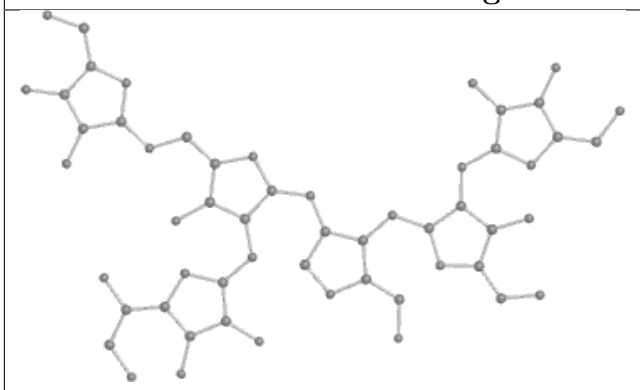
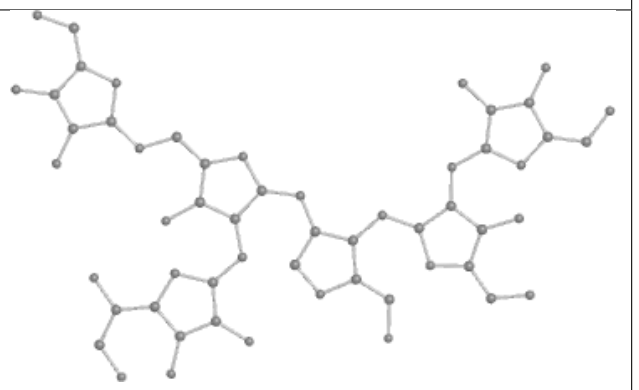
 Bond lengths	 Bond angles
 Torsions	 Rings

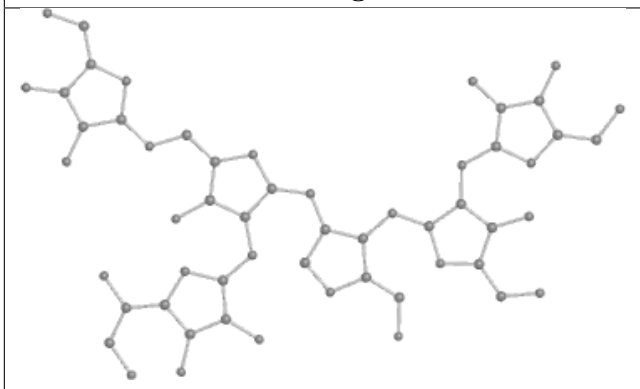
Oligosaccharide Chain GE



Bond lengths



Bond angles



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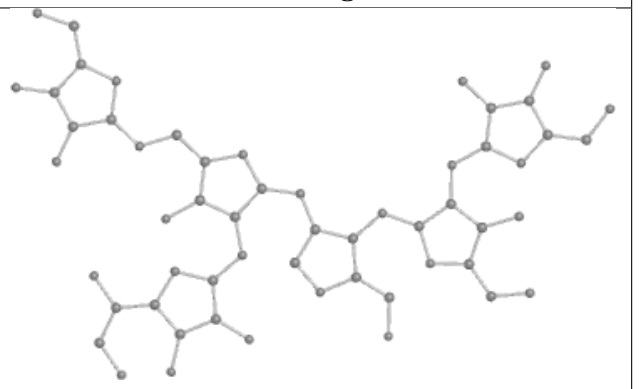
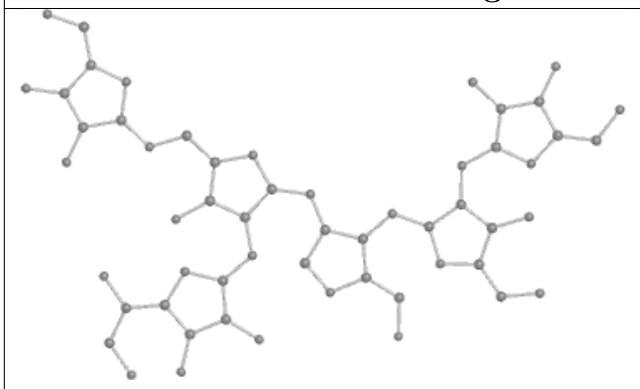


Rings

Oligosaccharide Chain QE



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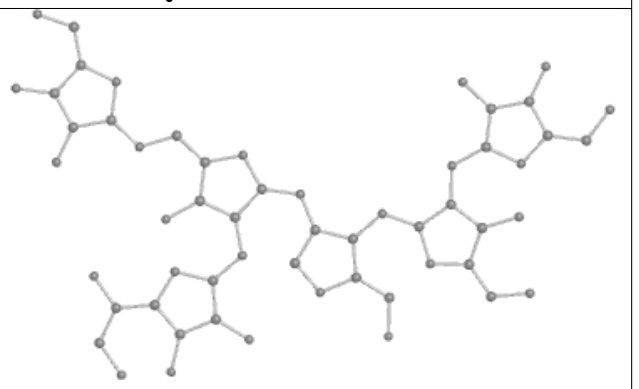

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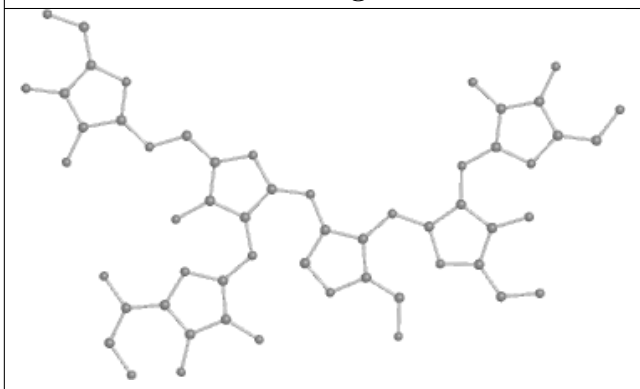

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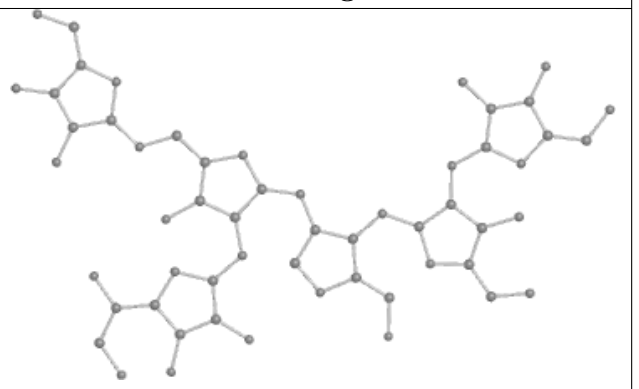
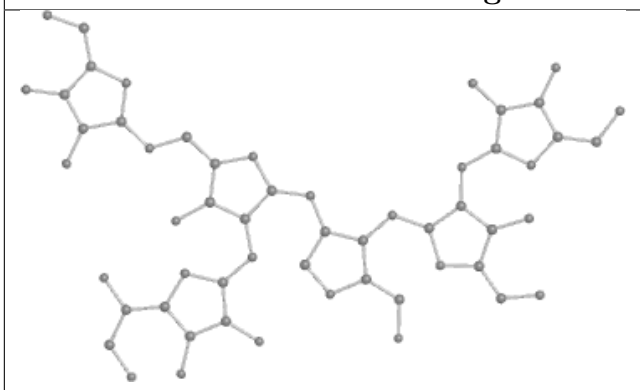


Rings

Oligosaccharide Chain RE



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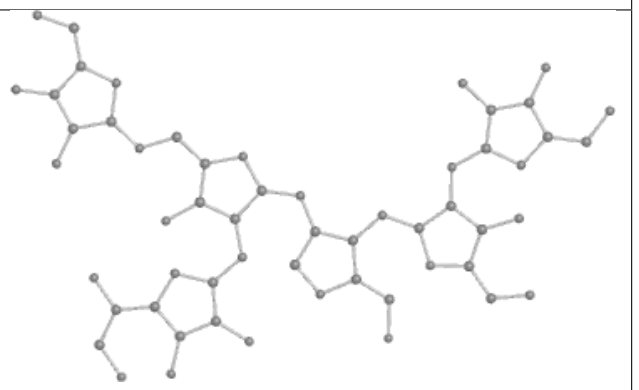
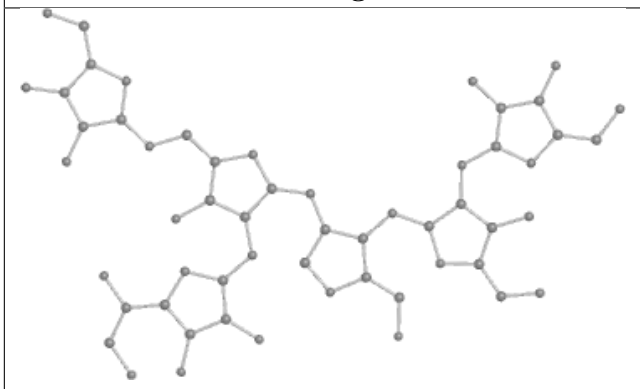


Bond angles



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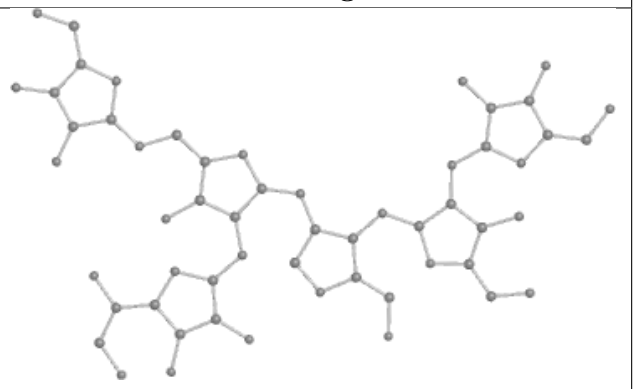
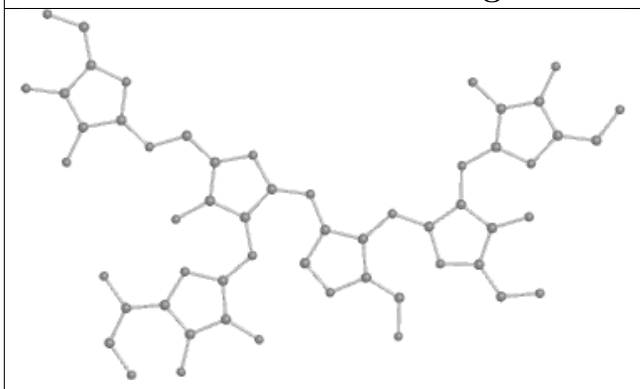


Rings

Oligosaccharide Chain VE



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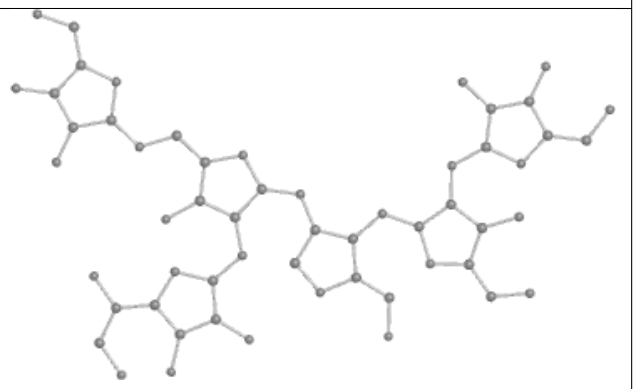

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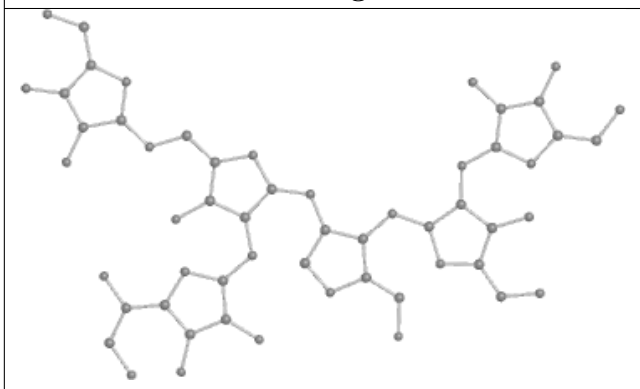

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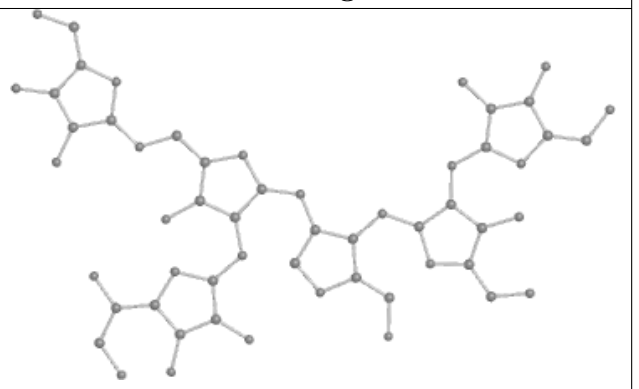
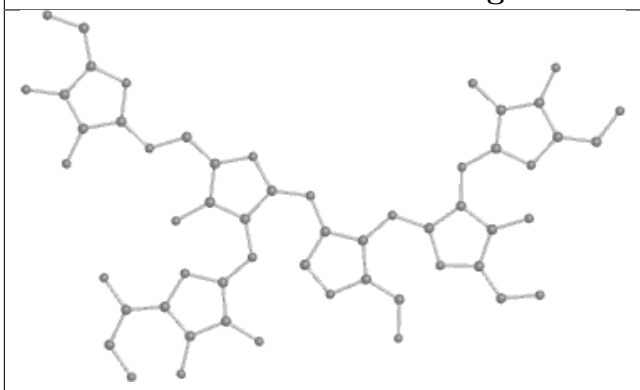


Rings

Oligosaccharide Chain dE



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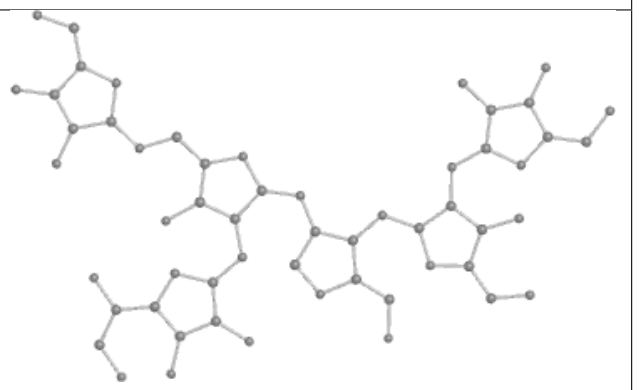

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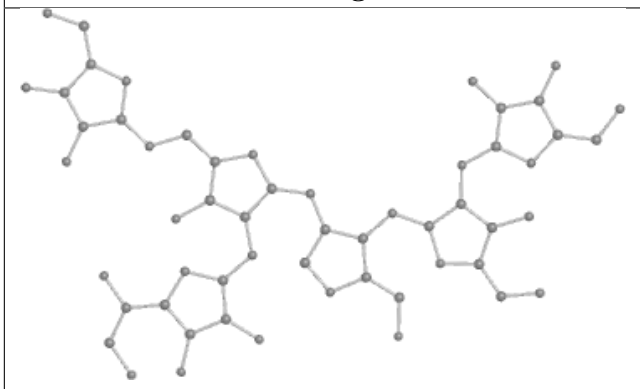

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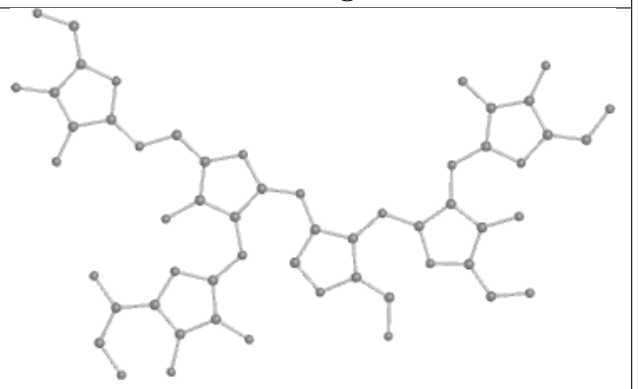
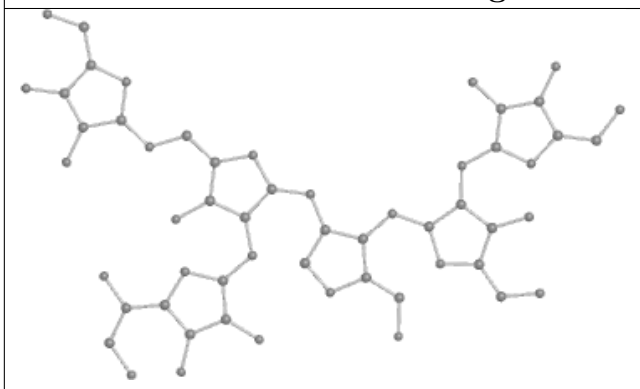


Rings

Oligosaccharide Chain eE



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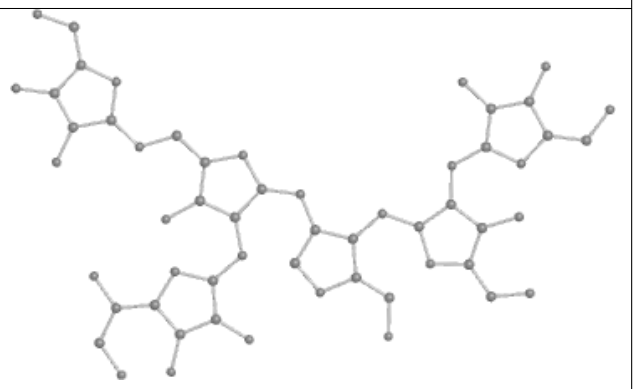

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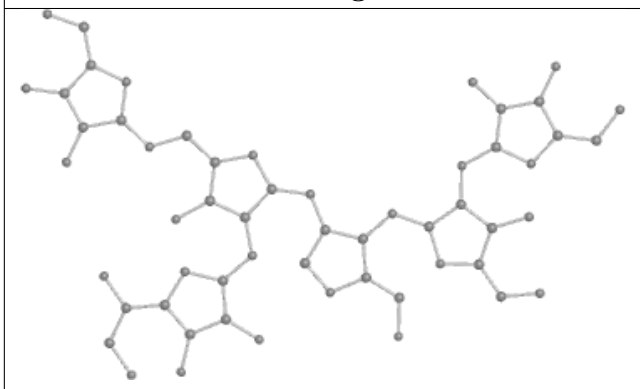

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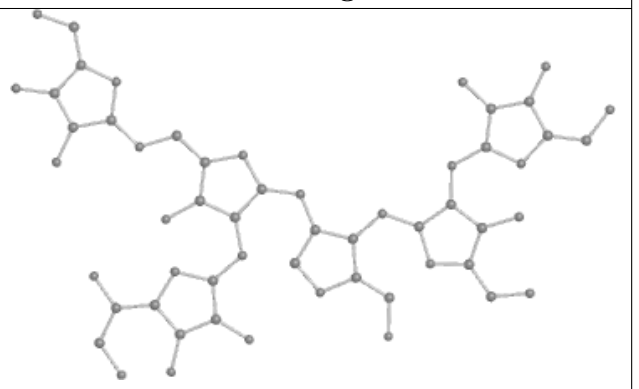
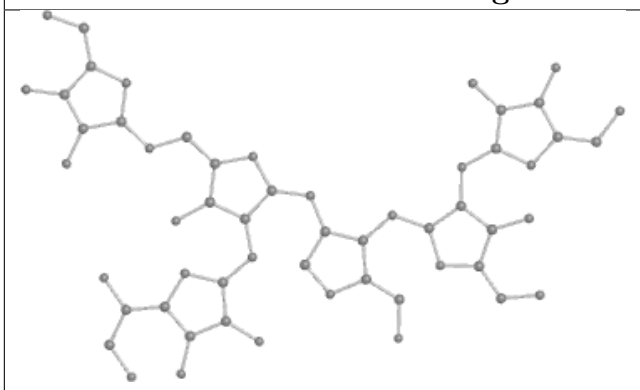


Rings

Oligosaccharide Chain iE



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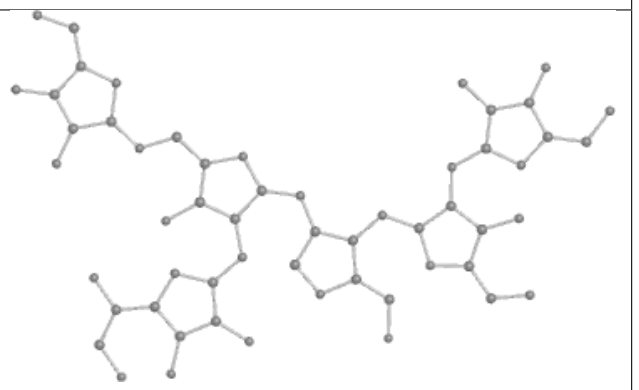

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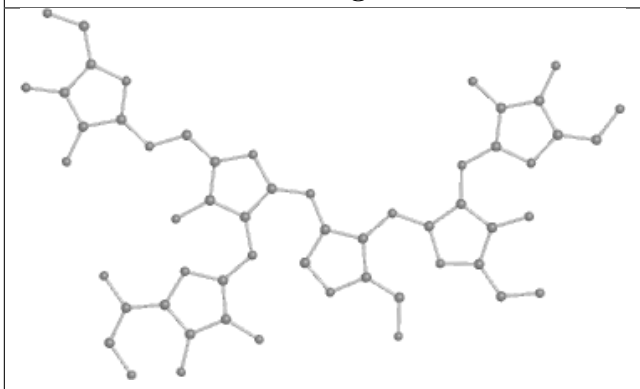

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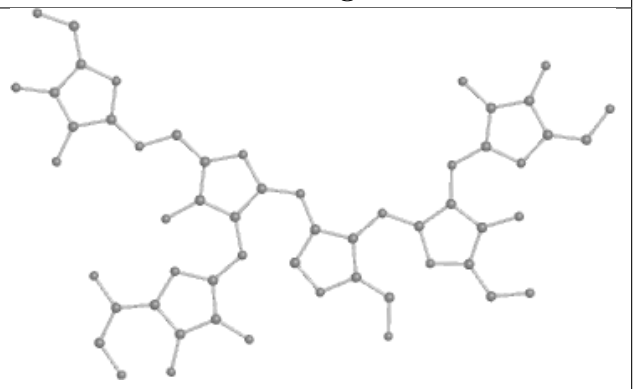
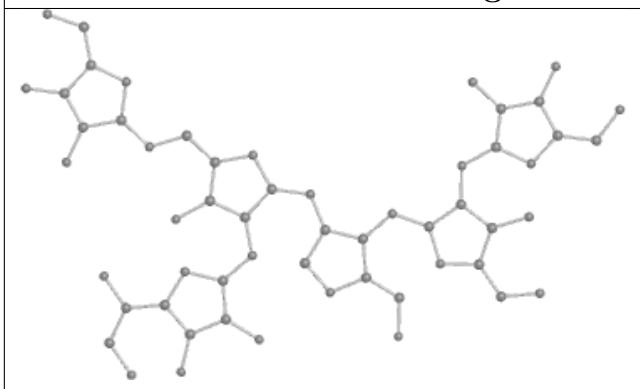


Rings

Oligosaccharide Chain wE



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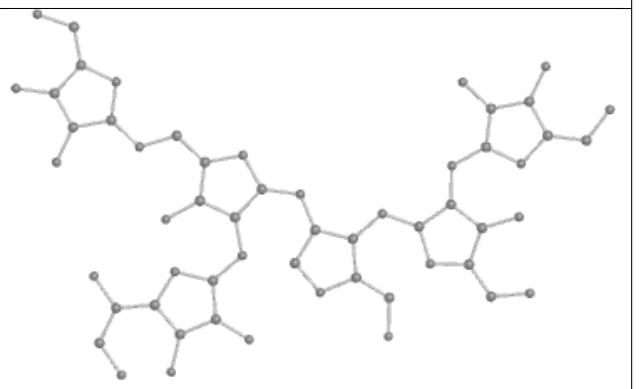
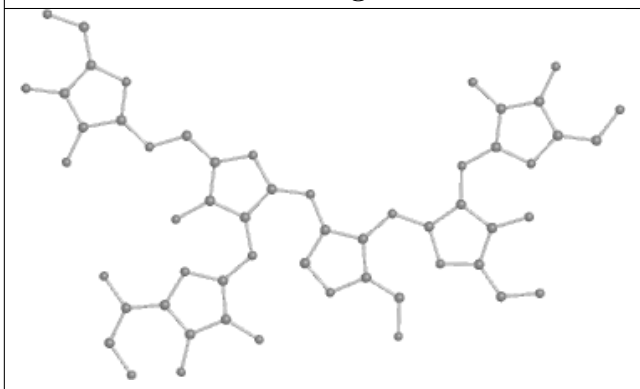


Bond angles



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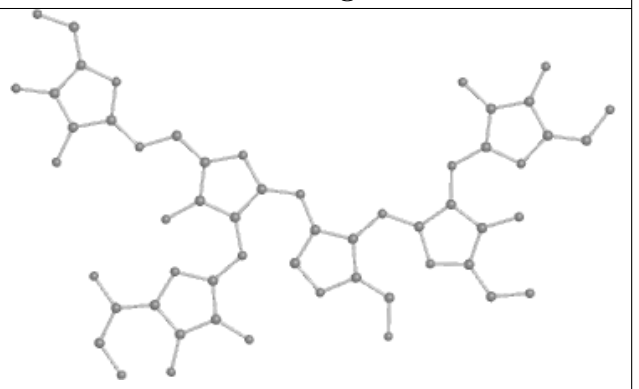
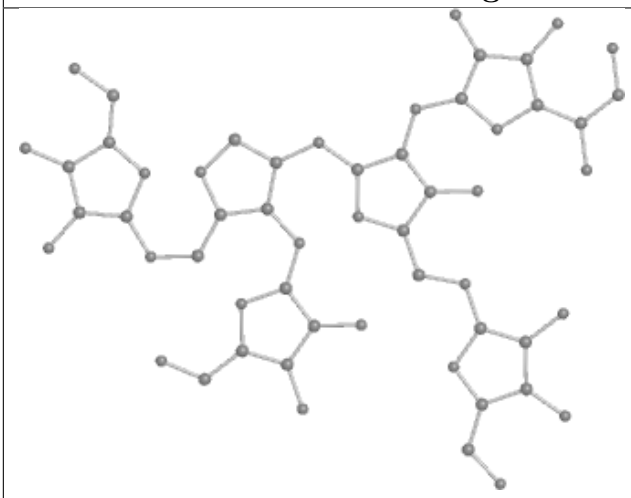
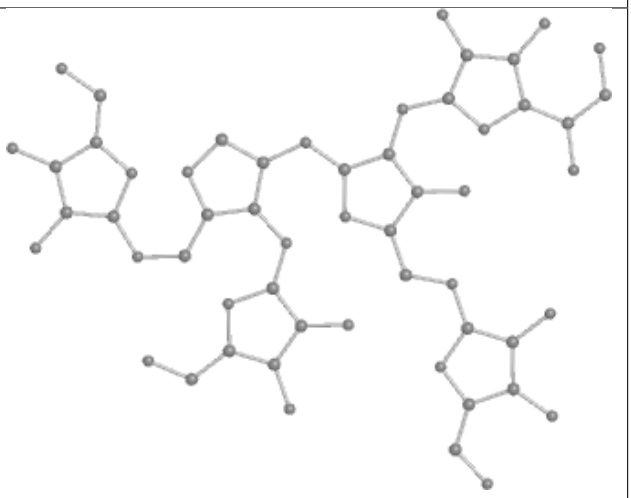
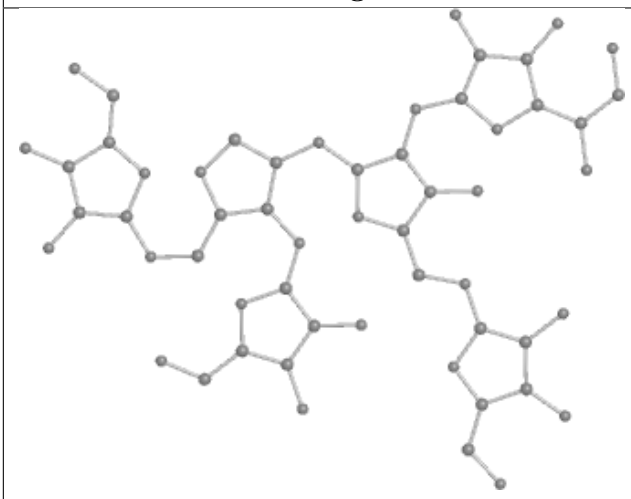
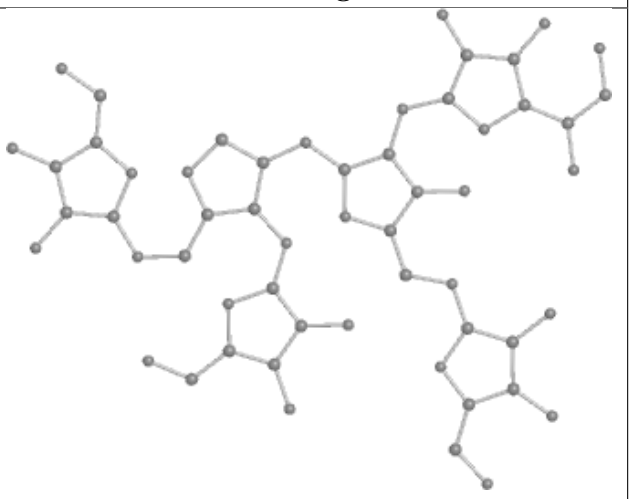
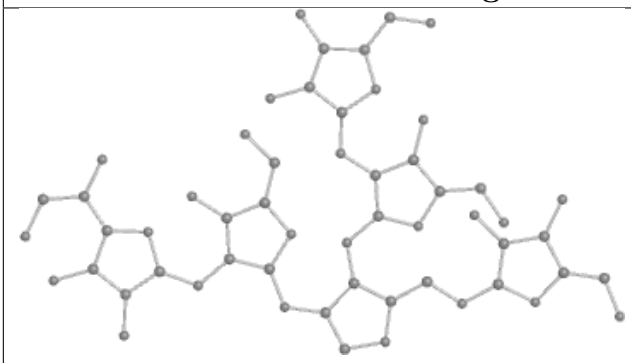


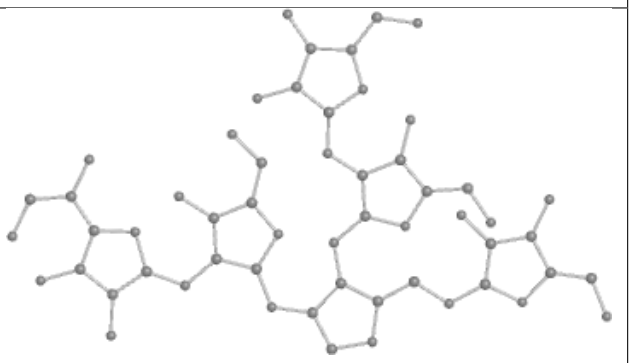
Rings

Oligosaccharide Chain XE	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

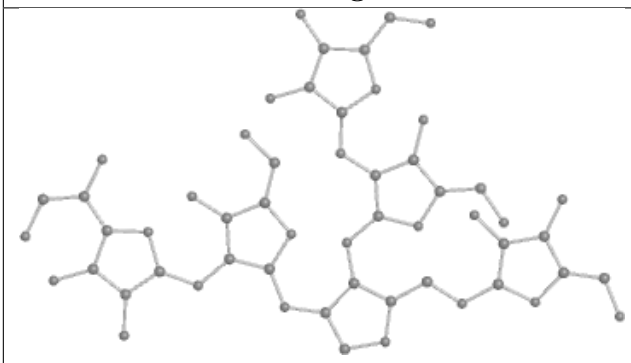
Oligosaccharide Chain YE



Bond lengths



Bond angles



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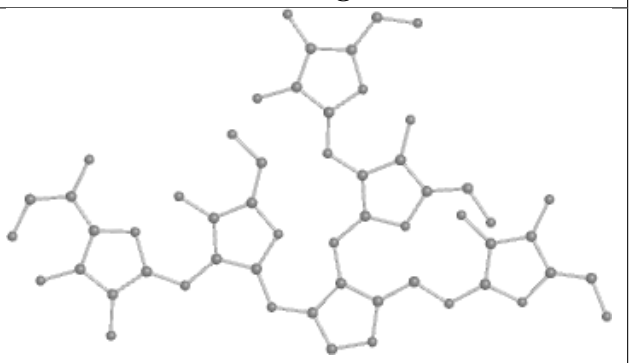
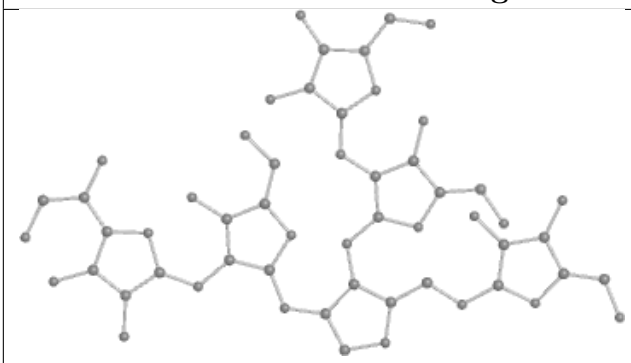


Rings

Oligosaccharide Chain lE



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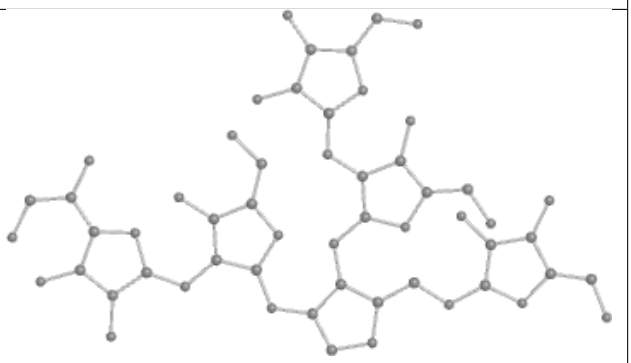

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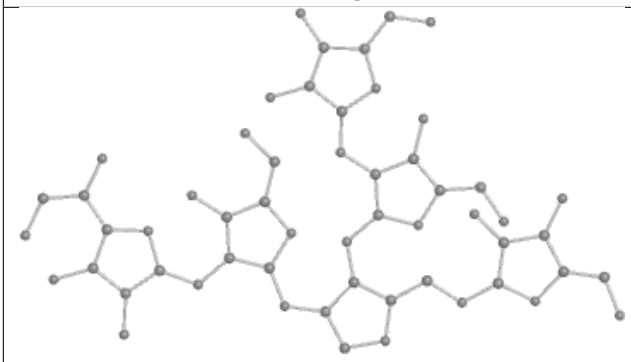
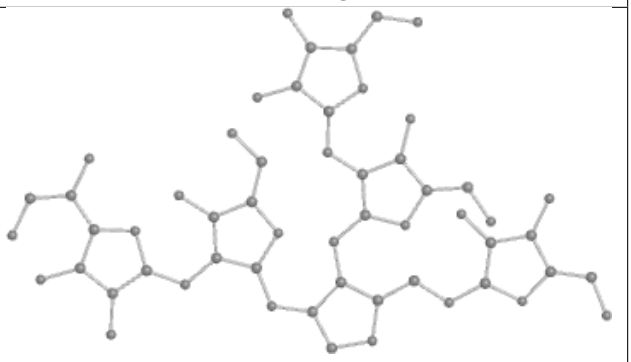


Torsions



Rings

5.6 Ligand geometry (i)

Of 95 ligands modelled in this entry, 6 are monoatomic - leaving 89 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	$\#\|Z\| > 2$
26	AHR	B	2020	-	9,9,10	0.90	0	10,12,14	1.02	1 (10%)
26	AHR	B	2004	-	9,9,10	0.80	0	10,12,14	1.79	4 (40%)
26	AHR	A	2002	-	9,9,10	0.87	1 (11%)	10,12,14	1.47	2 (20%)
27	GLA	F	2007	1	11,11,12	1.70	3 (27%)	15,15,17	1.09	1 (6%)
26	AHR	F	2001	-	9,9,10	0.68	0	10,12,14	1.57	3 (30%)
28	NAG	B	2019	1	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
27	GLA	E	2008	-	11,11,12	1.76	3 (27%)	15,15,17	1.12	1 (6%)
27	GLA	E	2011	1	11,11,12	1.74	3 (27%)	15,15,17	0.91	0
27	GLA	F	2013	1	11,11,12	1.78	2 (18%)	15,15,17	1.02	1 (6%)
26	AHR	D	2001	-	9,9,10	0.68	0	10,12,14	1.55	2 (20%)
27	GLA	E	2004	1	11,11,12	1.89	3 (27%)	15,15,17	2.03	4 (26%)
27	GLA	F	2010	-	11,11,12	1.80	3 (27%)	15,15,17	0.90	0
27	GLA	E	2016	1	11,11,12	1.85	3 (27%)	15,15,17	0.85	0
27	GLA	A	2004	1	11,11,12	1.89	3 (27%)	15,15,17	1.92	4 (26%)
27	GLA	D	2007	1	11,11,12	1.73	2 (18%)	15,15,17	0.93	0
27	GLA	F	2006	1	11,11,12	1.83	3 (27%)	15,15,17	2.17	4 (26%)
27	GLA	D	2006	1	11,11,12	1.70	2 (18%)	15,15,17	1.06	1 (6%)
27	GLA	A	2007	1	11,11,12	1.77	3 (27%)	15,15,17	0.67	0
27	GLA	A	2015	1	11,11,12	1.81	3 (27%)	15,15,17	0.84	0
27	GLA	B	2006	1	11,11,12	1.77	3 (27%)	15,15,17	0.75	0
26	AHR	B	2003	-	9,9,10	0.91	0	10,12,14	1.83	4 (40%)
26	AHR	A	2003	-	9,9,10	0.79	1 (11%)	10,12,14	1.57	2 (20%)
28	NAG	C	2009	1	14,14,15	0.36	0	17,19,21	0.78	0
26	AHR	E	2003	-	9,9,10	0.67	0	10,12,14	1.58	3 (30%)
28	NAG	D	2010	1	14,14,15	0.31	0	17,19,21	0.74	0
28	NAG	E	2017	1	14,14,15	0.32	0	17,19,21	1.00	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	AHR	A	2018	-	9,9,10	0.56	0	10,12,14	1.09	1 (10%)
27	GLA	A	2014	1	11,11,12	1.80	2 (18%)	15,15,17	0.93	0
26	AHR	D	2003	-	9,9,10	0.84	0	10,12,14	1.56	2 (20%)
27	GLA	C	2004	1	11,11,12	1.77	3 (27%)	15,15,17	0.81	0
27	GLA	B	2010	1	11,11,12	1.78	3 (27%)	15,15,17	0.86	0
26	AHR	A	2019	-	9,9,10	0.56	0	10,12,14	0.89	0
27	GLA	B	2014	1	11,11,12	1.68	2 (18%)	15,15,17	0.86	1 (6%)
27	GLA	B	2017	1	11,11,12	1.67	2 (18%)	15,15,17	1.55	2 (13%)
27	GLA	A	2009	1	11,11,12	1.73	3 (27%)	15,15,17	1.12	1 (6%)
26	AHR	F	2005	-	9,9,10	0.67	0	10,12,14	1.57	3 (30%)
27	GLA	C	2007	1	11,11,12	1.80	3 (27%)	15,15,17	0.89	0
26	AHR	D	2004	-	9,9,10	0.69	0	10,12,14	1.59	3 (30%)
27	GLA	F	2014	1	11,11,12	1.79	3 (27%)	15,15,17	0.88	0
27	GLA	D	2008	1	11,11,12	1.77	3 (27%)	15,15,17	0.78	0
27	GLA	E	2006	1	11,11,12	1.79	3 (27%)	15,15,17	0.82	0
27	GLA	C	2006	1	11,11,12	1.71	2 (18%)	15,15,17	0.84	0
27	GLA	B	2009	-	11,11,12	1.78	2 (18%)	15,15,17	1.72	2 (13%)
26	AHR	C	2003	-	9,9,10	0.82	0	10,12,14	1.58	2 (20%)
26	AHR	F	2019	-	9,9,10	0.56	0	10,12,14	0.63	0
27	GLA	E	2009	1	11,11,12	1.73	3 (27%)	15,15,17	1.13	1 (6%)
27	GLA	B	2008	1	11,11,12	1.76	2 (18%)	15,15,17	0.81	0
27	GLA	F	2018	1	11,11,12	1.78	3 (27%)	15,15,17	0.69	0
27	GLA	A	2012	1	11,11,12	1.76	3 (27%)	15,15,17	0.94	1 (6%)
26	AHR	F	2004	-	9,9,10	0.67	0	10,12,14	1.59	3 (30%)
28	NAG	B	2018	1	14,14,15	0.35	0	17,19,21	0.81	0
27	GLA	B	2012	1	11,11,12	1.81	3 (27%)	15,15,17	0.77	0
27	GLA	F	2017	1	11,11,12	1.75	3 (27%)	15,15,17	1.18	1 (6%)
27	GLA	A	2005	1	11,11,12	1.72	2 (18%)	15,15,17	0.93	1 (6%)
27	GLA	E	2012	1	11,11,12	1.66	2 (18%)	15,15,17	1.32	1 (6%)
27	GLA	B	2015	1	11,11,12	1.77	2 (18%)	15,15,17	0.86	0
27	GLA	E	2007	1	11,11,12	1.82	3 (27%)	15,15,17	1.47	3 (20%)
27	GLA	B	2005	1	11,11,12	1.88	3 (27%)	15,15,17	1.86	4 (26%)
27	GLA	E	2015	1	11,11,12	1.71	2 (18%)	15,15,17	1.36	1 (6%)
26	AHR	F	2003	-	9,9,10	0.57	0	10,12,14	1.59	1 (10%)
27	GLA	A	2016	1	11,11,12	1.77	2 (18%)	15,15,17	1.10	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	GLA	A	2008	-	11,11,12	1.79	2 (18%)	15,15,17	1.59	2 (13%)
27	GLA	E	2010	1	11,11,12	1.70	2 (18%)	15,15,17	1.43	1 (6%)
27	GLA	A	2011	1	11,11,12	1.79	3 (27%)	15,15,17	0.94	1 (6%)
27	GLA	E	2014	1	11,11,12	1.75	2 (18%)	15,15,17	0.98	0
27	GLA	A	2006	1	11,11,12	1.81	3 (27%)	15,15,17	1.02	1 (6%)
28	NAG	A	2017	1	14,14,15	0.32	0	17,19,21	0.66	0
27	GLA	C	2005	1	11,11,12	1.70	2 (18%)	15,15,17	0.99	1 (6%)
27	GLA	A	2010	1	11,11,12	1.74	3 (27%)	15,15,17	0.92	1 (6%)
27	GLA	F	2008	1	11,11,12	1.76	3 (27%)	15,15,17	1.04	2 (13%)
27	GLA	A	2013	1	11,11,12	1.78	3 (27%)	15,15,17	0.69	0
26	AHR	C	2001	-	9,9,10	0.55	0	10,12,14	1.61	1 (10%)
27	GLA	F	2016	1	11,11,12	1.70	2 (18%)	15,15,17	0.97	1 (6%)
26	AHR	B	2002	-	9,9,10	0.56	0	10,12,14	1.16	1 (10%)
27	GLA	F	2011	1	11,11,12	1.78	3 (27%)	15,15,17	0.91	0
26	AHR	E	2002	-	9,9,10	0.82	1 (11%)	10,12,14	1.59	2 (20%)
27	GLA	F	2009	1	11,11,12	1.68	2 (18%)	15,15,17	0.89	1 (6%)
27	GLA	B	2013	1	11,11,12	1.73	2 (18%)	15,15,17	0.99	1 (6%)
27	GLA	B	2016	1	11,11,12	1.85	3 (27%)	15,15,17	0.84	0
27	GLA	E	2013	1	11,11,12	1.82	3 (27%)	15,15,17	0.84	0
27	GLA	C	2008	1	11,11,12	1.80	3 (27%)	15,15,17	1.01	1 (6%)
27	GLA	D	2009	1	11,11,12	1.82	3 (27%)	15,15,17	0.84	1 (6%)
28	NAG	C	2010	1	14,14,15	0.32	0	17,19,21	0.91	1 (5%)
27	GLA	F	2015	1	11,11,12	1.78	3 (27%)	15,15,17	0.70	0
27	GLA	E	2005	1	11,11,12	1.77	3 (27%)	15,15,17	0.95	1 (6%)
27	GLA	B	2007	1	11,11,12	1.81	3 (27%)	15,15,17	0.90	0
27	GLA	F	2012	1	11,11,12	1.75	3 (27%)	15,15,17	0.90	1 (6%)
27	GLA	B	2011	1	11,11,12	1.72	3 (27%)	15,15,17	1.04	2 (13%)
27	GLA	D	2005	1	11,11,12	1.79	3 (27%)	15,15,17	0.95	0

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
26	AHR	B	2020	-	-	1/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	AHR	B	2004	-	-	2/2/15/18	0/1/1/1
26	AHR	A	2002	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2007	1	-	2/2/19/22	0/1/1/1
26	AHR	F	2001	-	-	2/2/15/18	0/1/1/1
28	NAG	B	2019	1	-	2/6/23/26	0/1/1/1
27	GLA	E	2008	-	-	2/2/19/22	0/1/1/1
27	GLA	E	2011	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2013	1	-	0/2/19/22	0/1/1/1
26	AHR	D	2001	-	-	1/2/15/18	0/1/1/1
27	GLA	E	2004	1	-	0/2/19/22	0/1/1/1
27	GLA	F	2010	-	-	2/2/19/22	0/1/1/1
27	GLA	E	2016	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2004	1	-	0/2/19/22	0/1/1/1
27	GLA	D	2007	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	D	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	A	2007	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	A	2015	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2006	1	-	0/2/19/22	0/1/1/1
26	AHR	B	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	A	2003	-	-	2/2/15/18	0/1/1/1
28	NAG	C	2009	1	-	4/6/23/26	0/1/1/1
26	AHR	E	2003	-	-	2/2/15/18	0/1/1/1
28	NAG	D	2010	1	-	0/6/23/26	0/1/1/1
28	NAG	E	2017	1	-	4/6/23/26	0/1/1/1
26	AHR	A	2018	-	-	0/2/15/18	0/1/1/1
27	GLA	A	2014	1	-	2/2/19/22	0/1/1/1
26	AHR	D	2003	-	-	2/2/15/18	0/1/1/1
27	GLA	C	2004	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2010	1	-	2/2/19/22	0/1/1/1
26	AHR	A	2019	-	-	0/2/15/18	0/1/1/1
27	GLA	B	2014	1	1/1/4/5	0/2/19/22	0/1/1/1
27	GLA	B	2017	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2009	1	-	1/2/19/22	0/1/1/1
26	AHR	F	2005	-	-	2/2/15/18	0/1/1/1
27	GLA	C	2007	1	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	AHR	D	2004	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	D	2008	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2006	1	-	2/2/19/22	0/1/1/1
27	GLA	C	2006	1	-	0/2/19/22	0/1/1/1
27	GLA	B	2009	-	-	2/2/19/22	0/1/1/1
26	AHR	C	2003	-	-	2/2/15/18	0/1/1/1
26	AHR	F	2019	-	-	0/2/15/18	0/1/1/1
27	GLA	E	2009	1	-	0/2/19/22	0/1/1/1
27	GLA	B	2008	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	F	2018	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2012	1	-	2/2/19/22	0/1/1/1
26	AHR	F	2004	-	-	2/2/15/18	0/1/1/1
28	NAG	B	2018	1	-	4/6/23/26	0/1/1/1
27	GLA	B	2012	1	-	1/2/19/22	0/1/1/1
27	GLA	F	2017	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2005	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2012	1	-	1/2/19/22	0/1/1/1
27	GLA	E	2007	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	B	2015	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2005	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2015	1	-	0/2/19/22	0/1/1/1
26	AHR	F	2003	-	-	1/2/15/18	0/1/1/1
27	GLA	A	2016	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2008	-	-	2/2/19/22	0/1/1/1
27	GLA	E	2010	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2011	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2014	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2006	1	-	1/2/19/22	0/1/1/1
28	NAG	A	2017	1	-	2/6/23/26	0/1/1/1
27	GLA	C	2005	1	-	2/2/19/22	0/1/1/1
27	GLA	A	2010	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2008	1	-	1/2/19/22	0/1/1/1
27	GLA	A	2013	1	-	0/2/19/22	0/1/1/1
26	AHR	C	2001	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2016	1	-	2/2/19/22	0/1/1/1
26	AHR	B	2002	-	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GLA	F	2011	1	-	1/2/19/22	0/1/1/1
26	AHR	E	2002	-	-	2/2/15/18	0/1/1/1
27	GLA	F	2009	1	1/1/4/5	2/2/19/22	0/1/1/1
27	GLA	B	2013	1	-	1/2/19/22	0/1/1/1
27	GLA	B	2016	1	-	2/2/19/22	0/1/1/1
27	GLA	E	2013	1	-	2/2/19/22	0/1/1/1
27	GLA	C	2008	1	-	2/2/19/22	0/1/1/1
27	GLA	D	2009	1	-	2/2/19/22	0/1/1/1
28	NAG	C	2010	1	-	4/6/23/26	0/1/1/1
27	GLA	F	2015	1	-	0/2/19/22	0/1/1/1
27	GLA	E	2005	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2007	1	-	2/2/19/22	0/1/1/1
27	GLA	F	2012	1	-	2/2/19/22	0/1/1/1
27	GLA	B	2011	1	-	1/2/19/22	0/1/1/1
27	GLA	D	2005	1	-	2/2/19/22	0/1/1/1

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	2004	GLA	O5-C1	4.89	1.51	1.43
27	B	2005	GLA	O5-C1	4.86	1.51	1.43
27	B	2009	GLA	O5-C1	4.77	1.51	1.43
27	E	2004	GLA	O5-C1	4.73	1.51	1.43
27	A	2008	GLA	O5-C1	4.73	1.51	1.43

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	F	2006	GLA	O5-C1-C2	5.56	119.35	110.77
27	B	2009	GLA	C1-C2-C3	4.96	115.76	109.67
27	E	2004	GLA	O5-C1-C2	4.71	118.04	110.77
27	B	2005	GLA	O5-C1-C2	4.65	117.95	110.77
27	A	2004	GLA	O5-C1-C2	4.47	117.67	110.77

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	2007	GLA	C1
27	B	2008	GLA	C1

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Mol	Chain	Res	Type	Atom
27	B	2014	GLA	C1
27	E	2007	GLA	C1
27	F	2009	GLA	C1

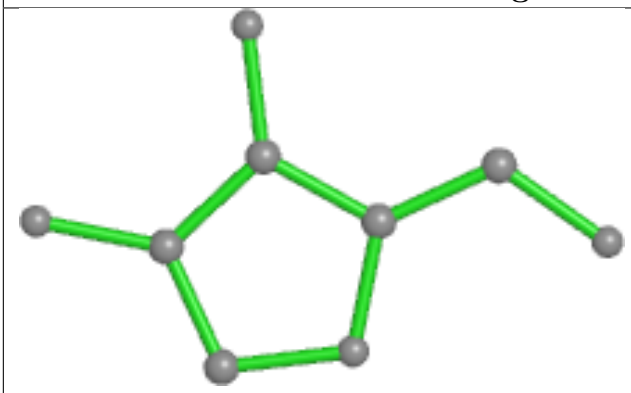
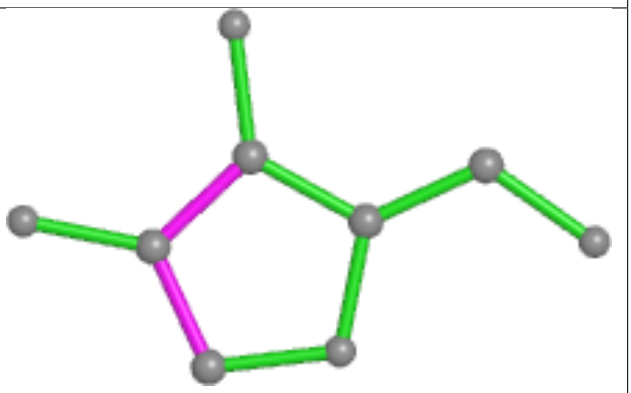
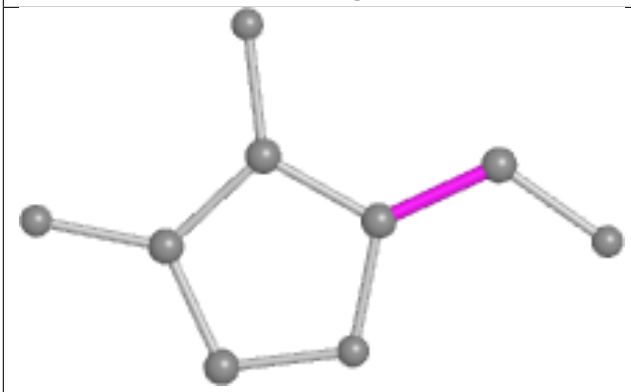
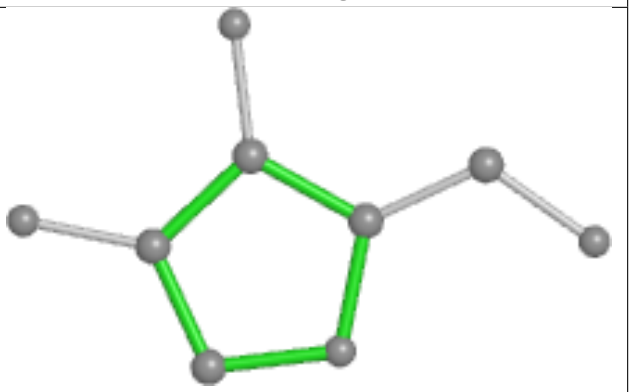
5 of 135 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	B	2018	NAG	C3-C2-N2-C7
28	B	2018	NAG	C8-C7-N2-C2
28	B	2018	NAG	O7-C7-N2-C2
28	C	2009	NAG	C3-C2-N2-C7
28	C	2009	NAG	C8-C7-N2-C2

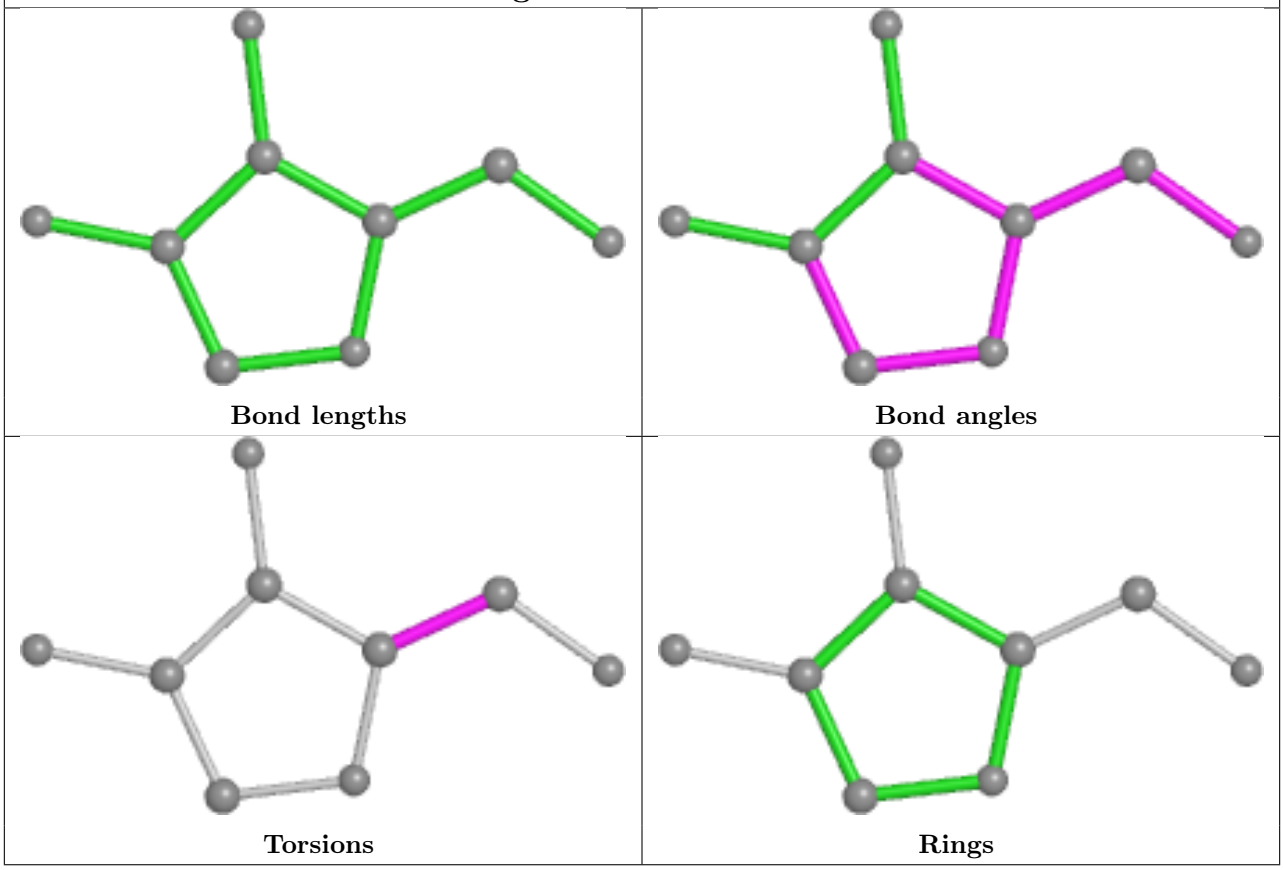
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 AHR B 2020	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AHR B 2004



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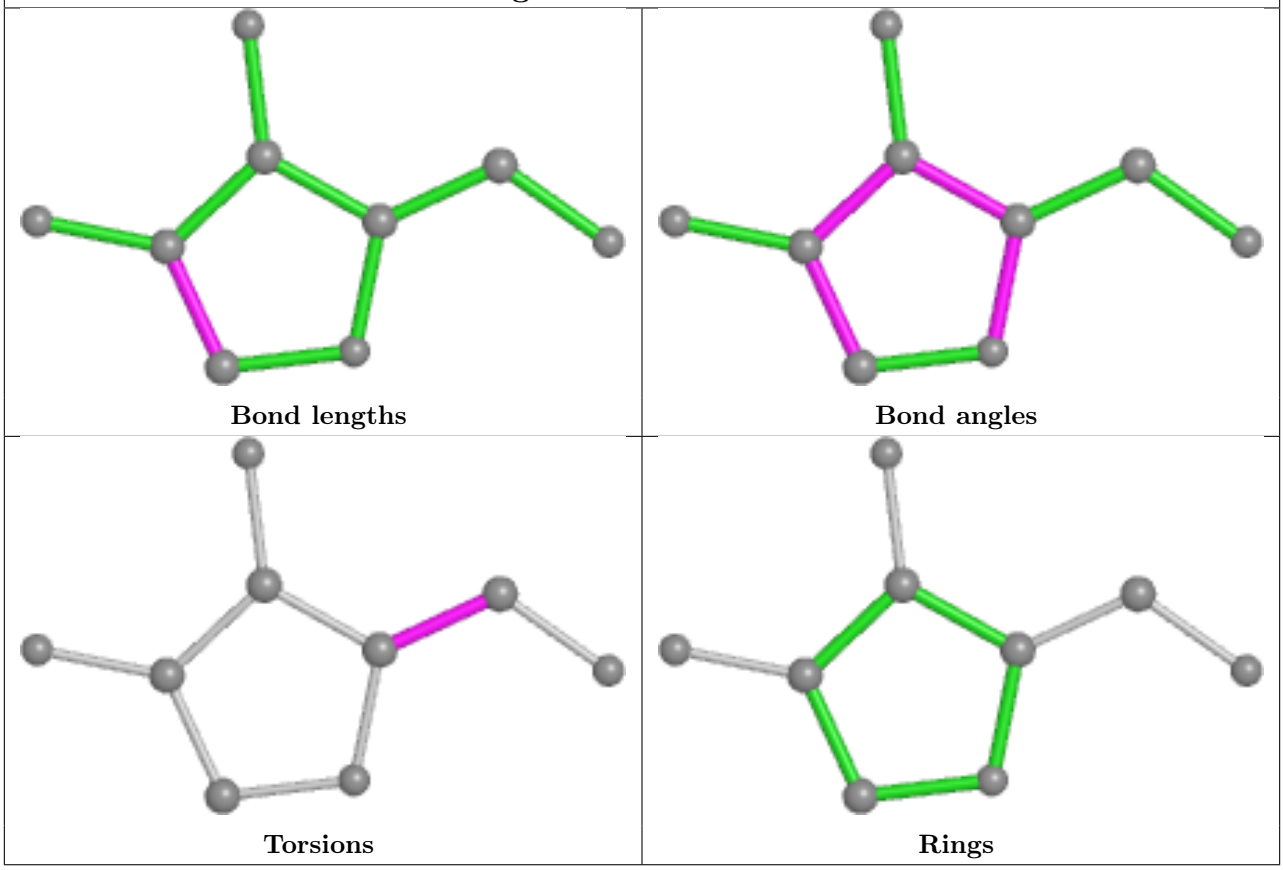

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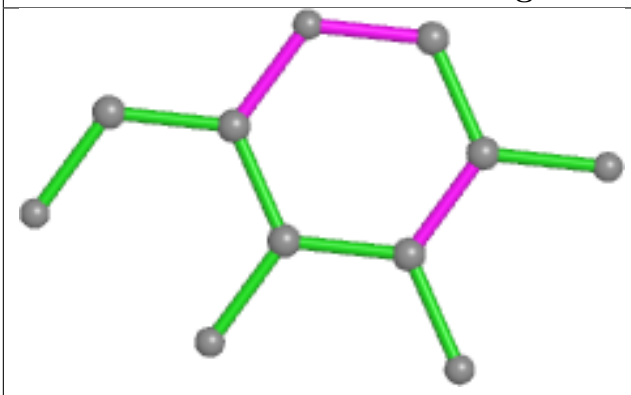
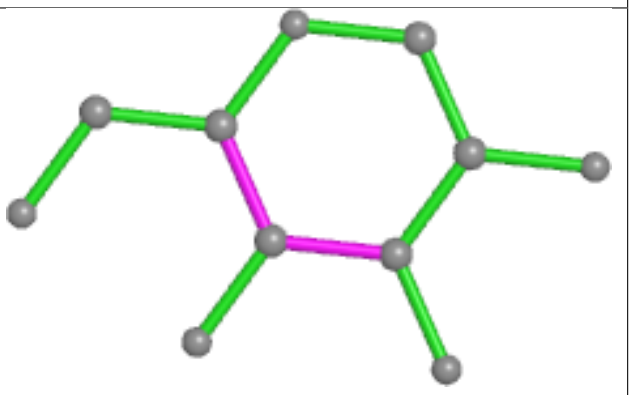
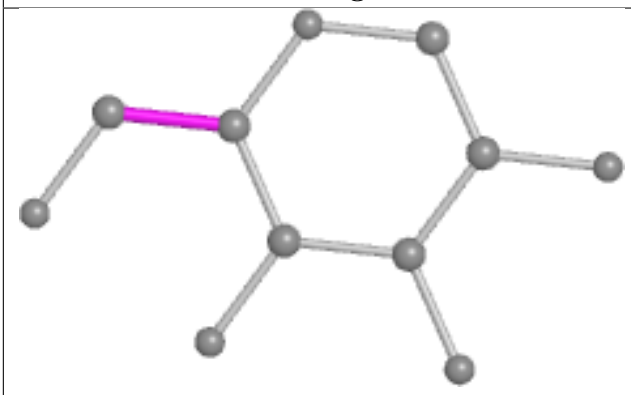
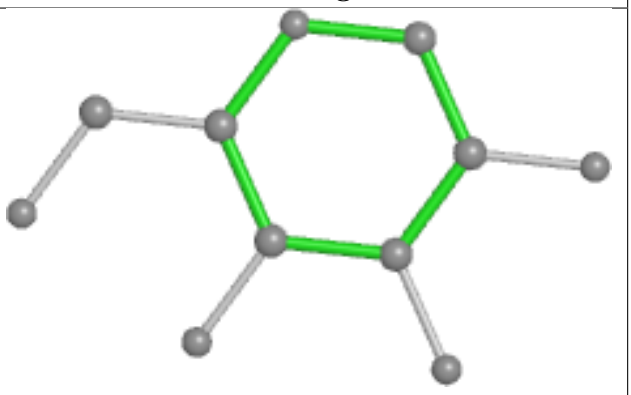
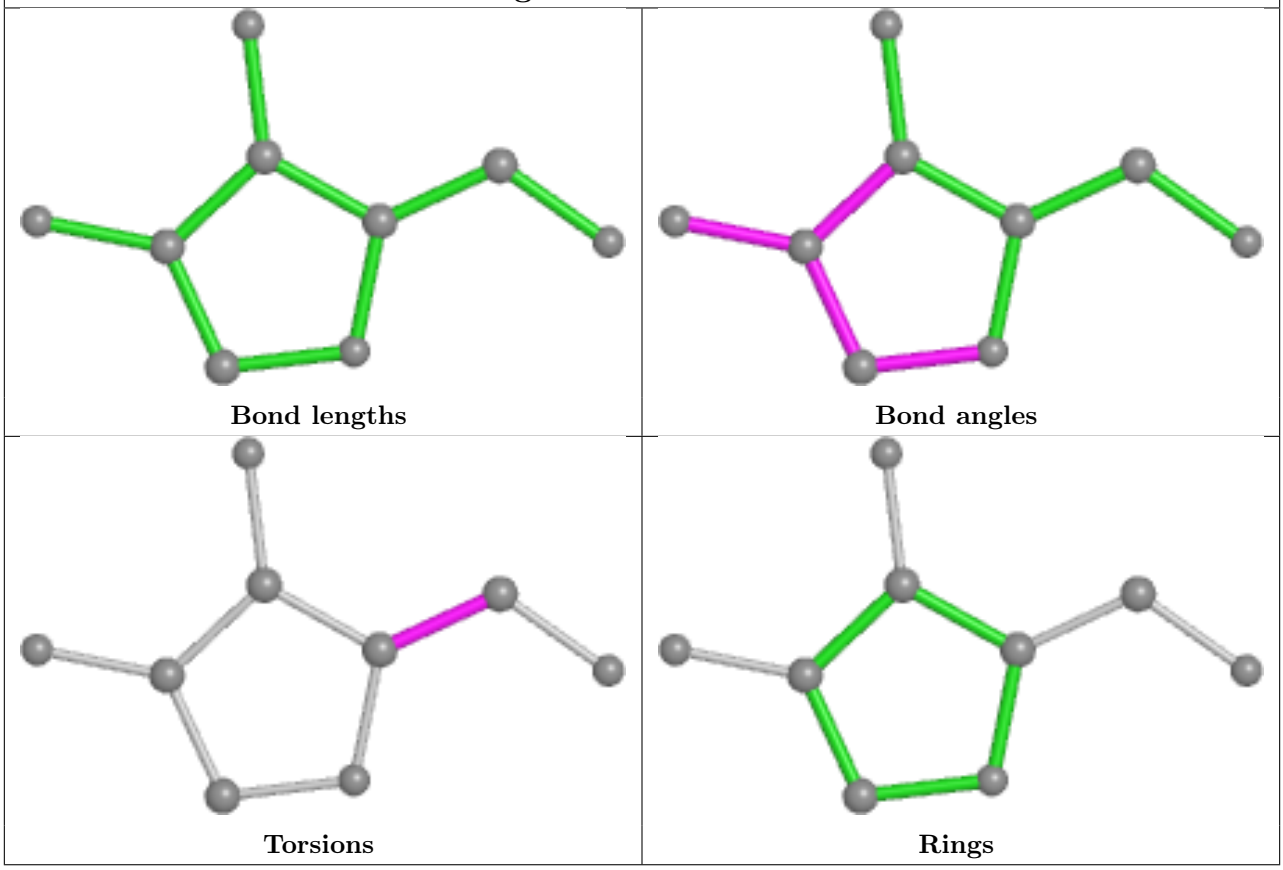
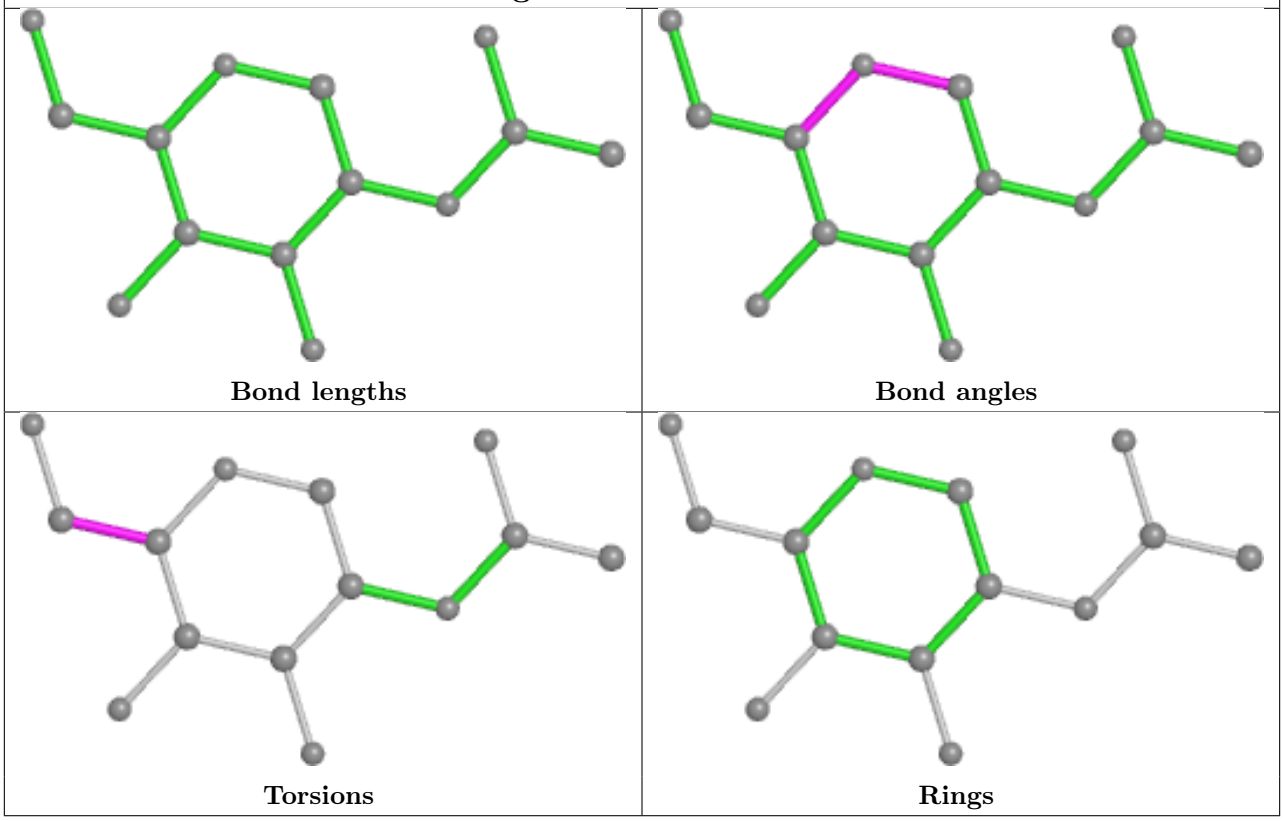
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AHR F 2001



Ligand NAG B 2019



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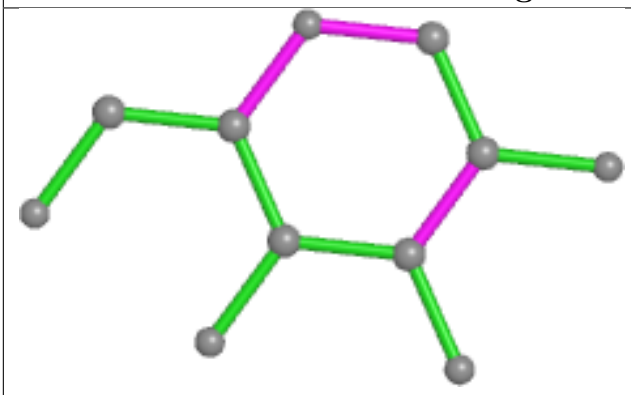	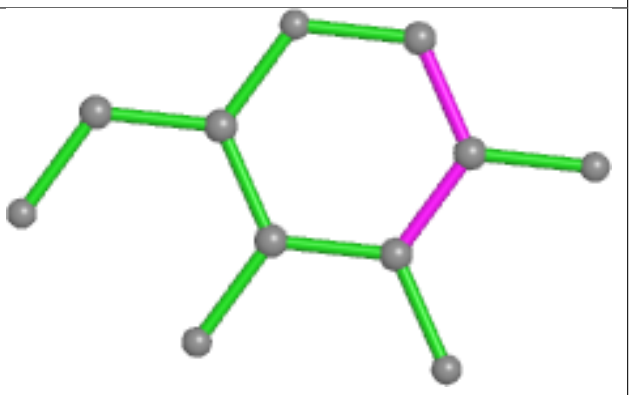
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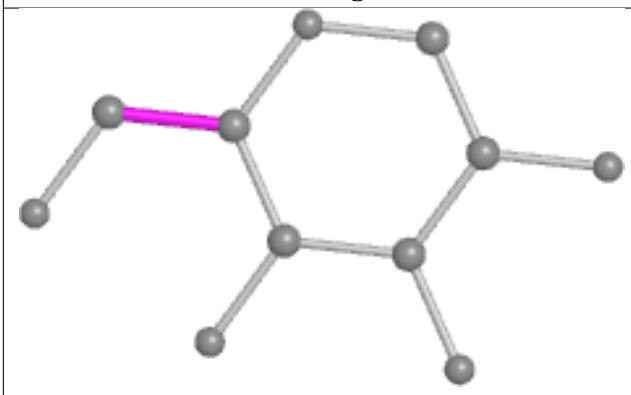	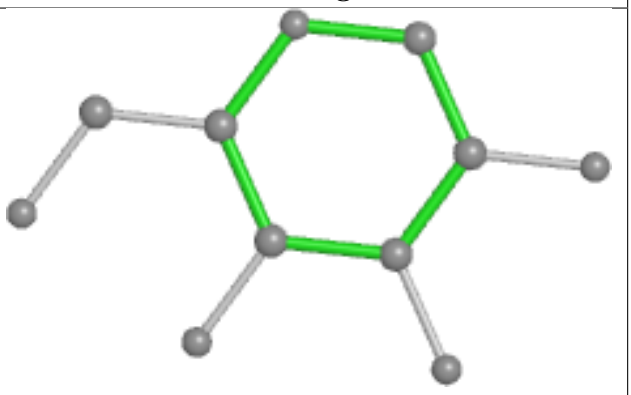
Torsions	**Rings**

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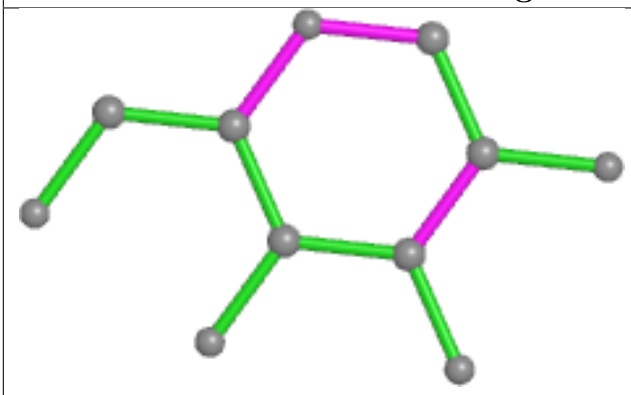
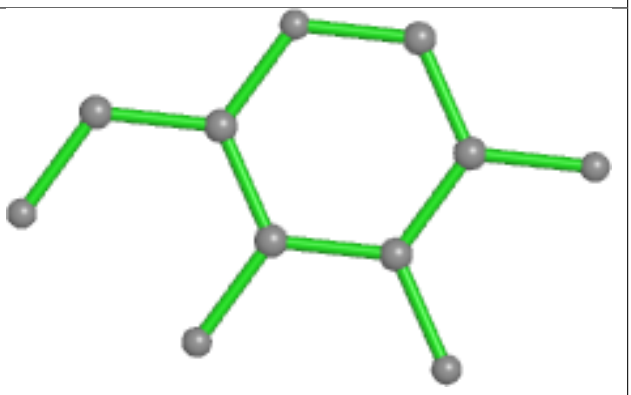
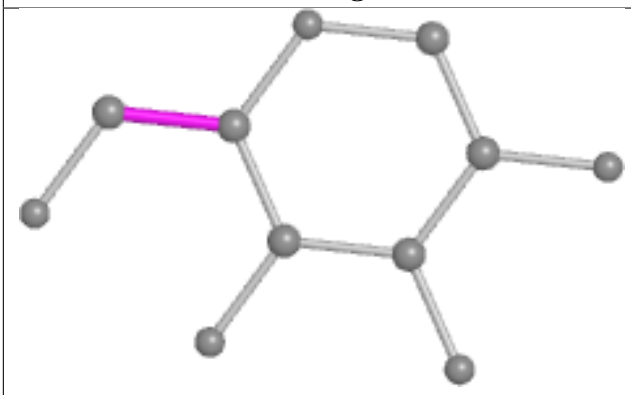
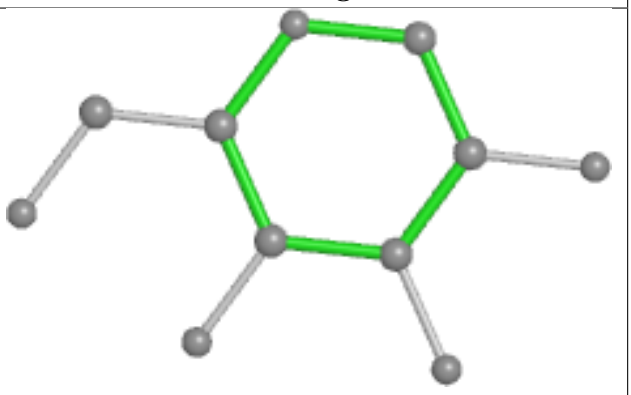
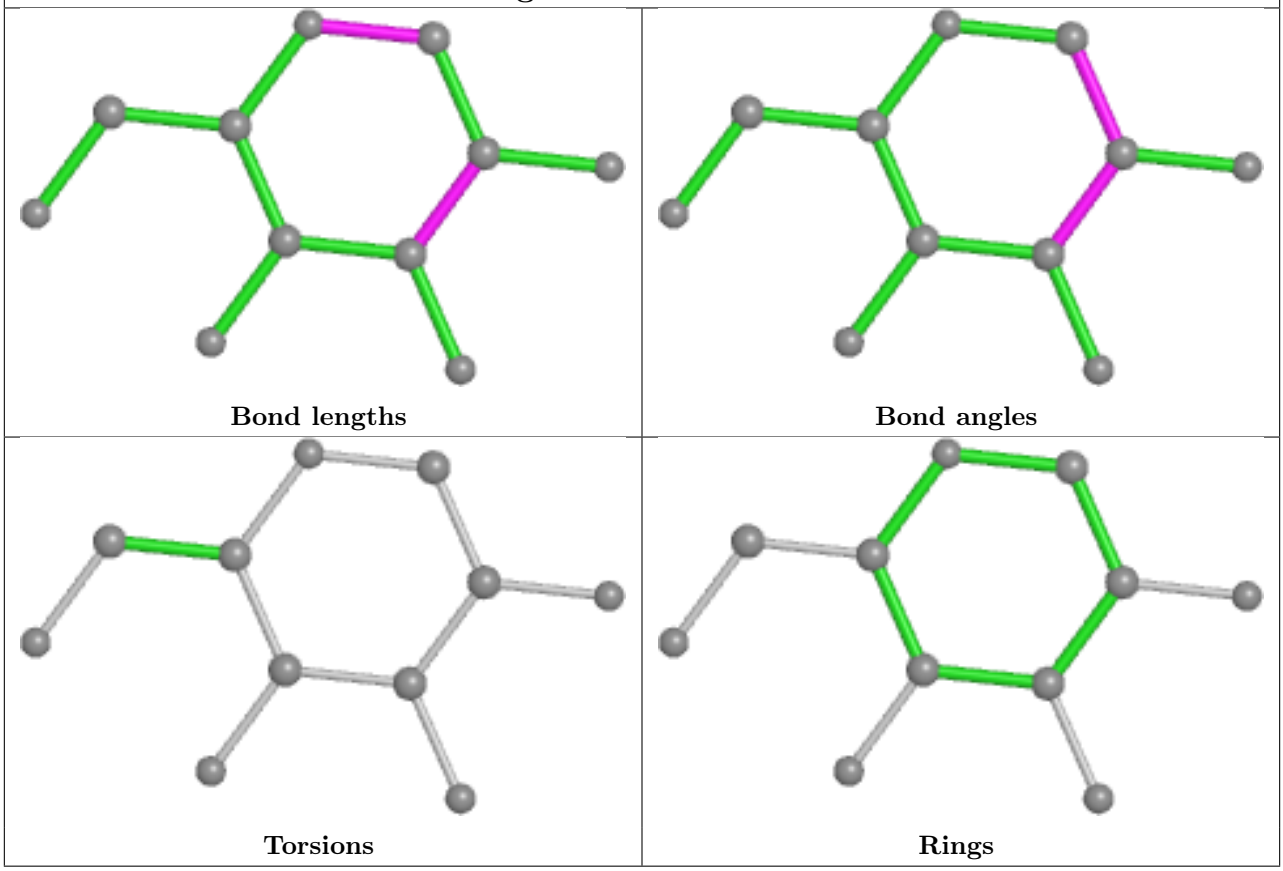
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA F 2013



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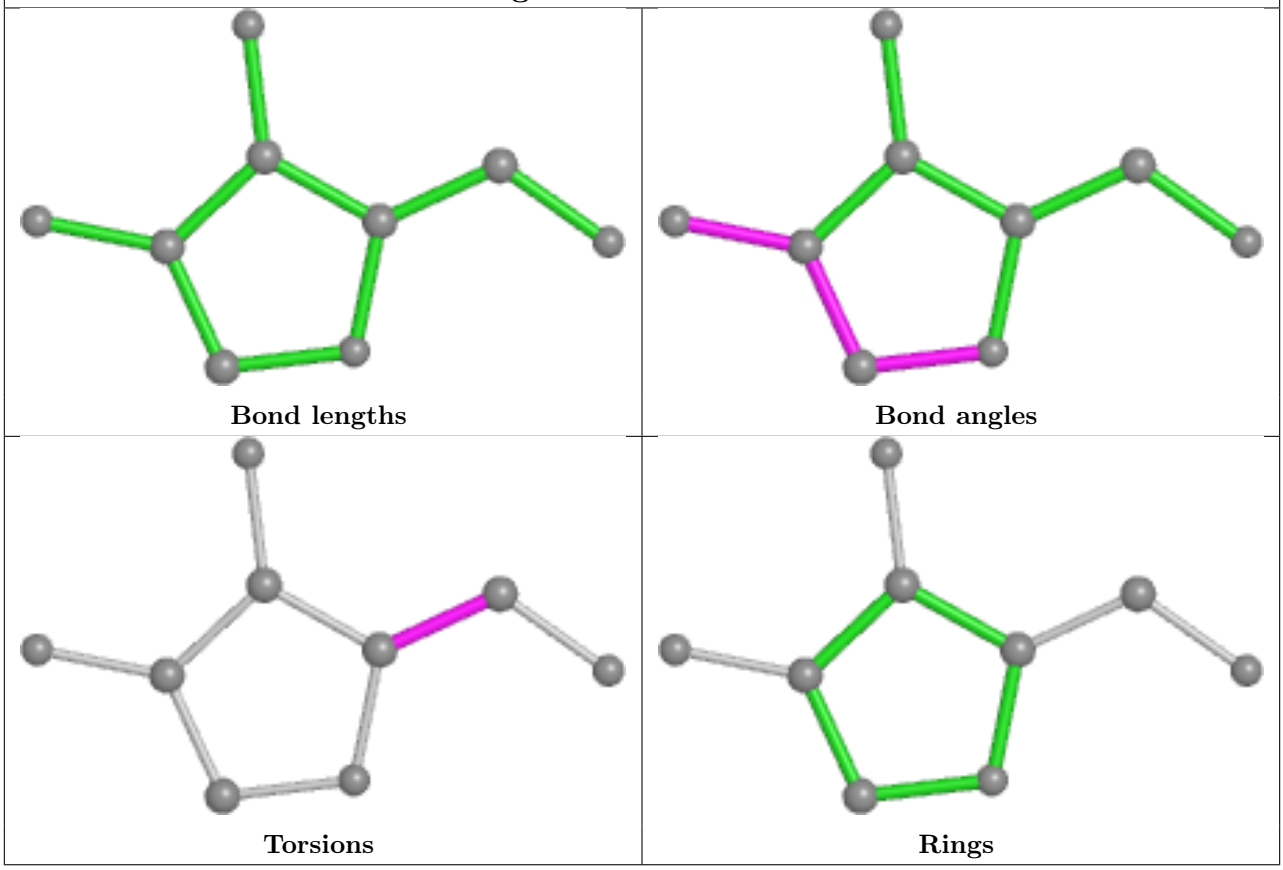

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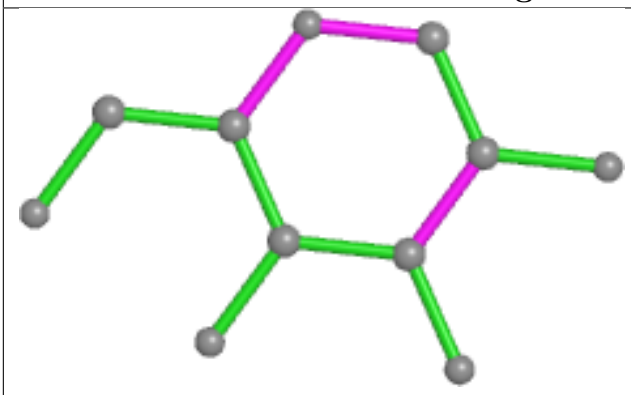
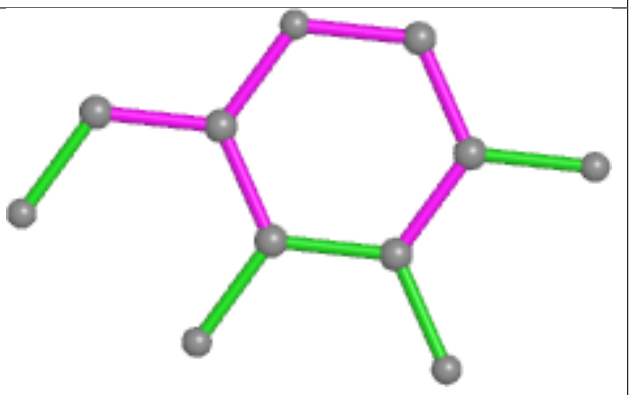
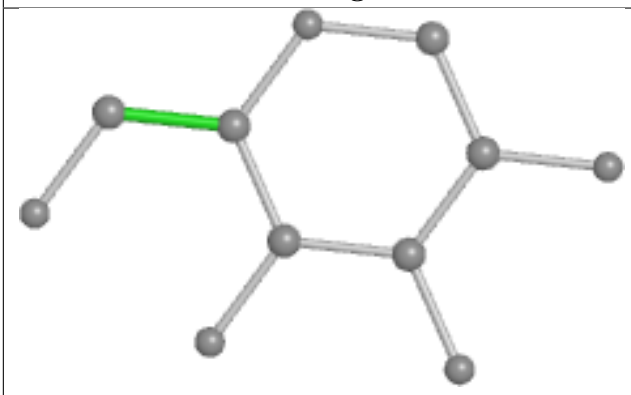
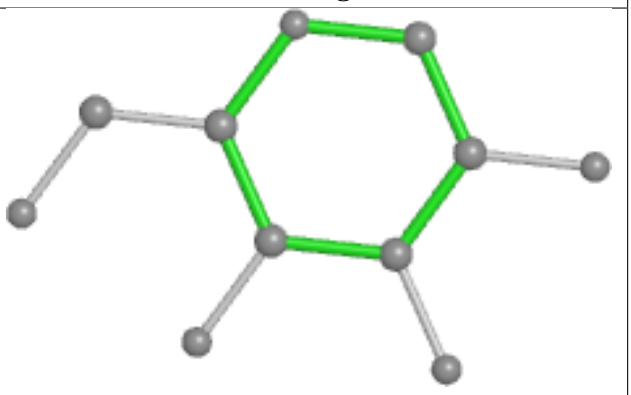
 Bond lengths	 Bond angles
 Torsions	 Rings

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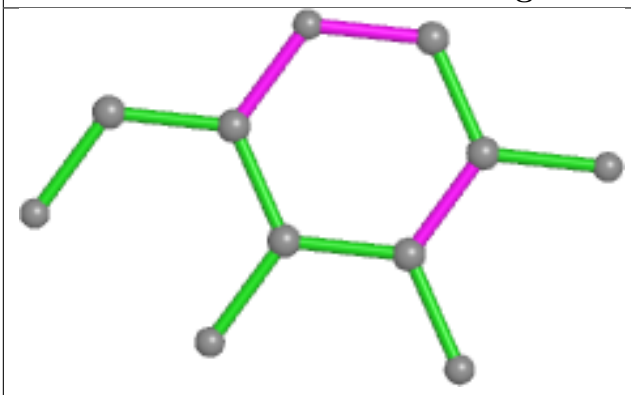
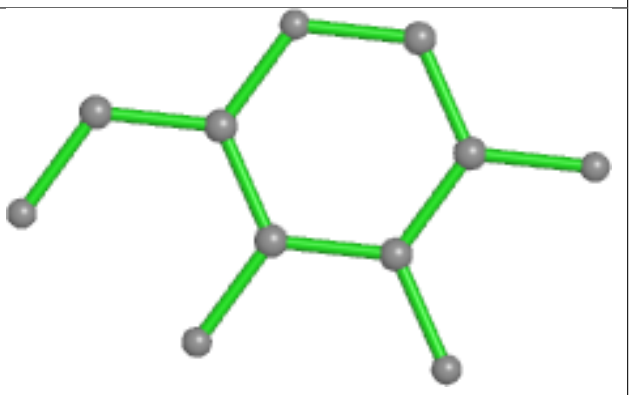
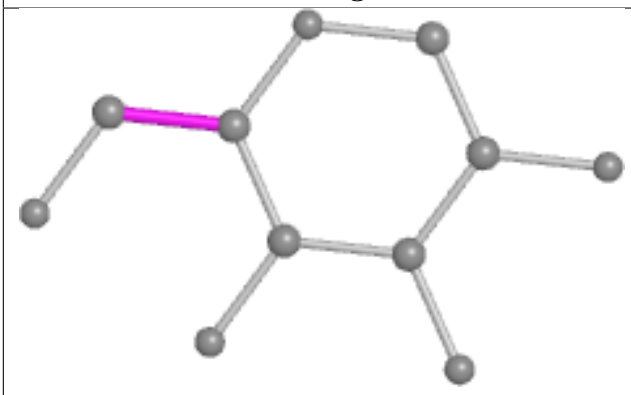
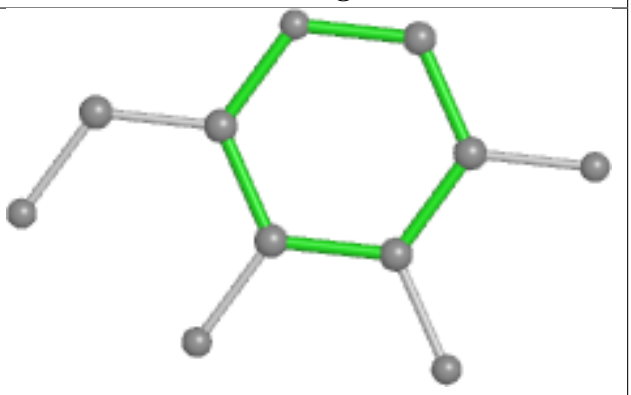
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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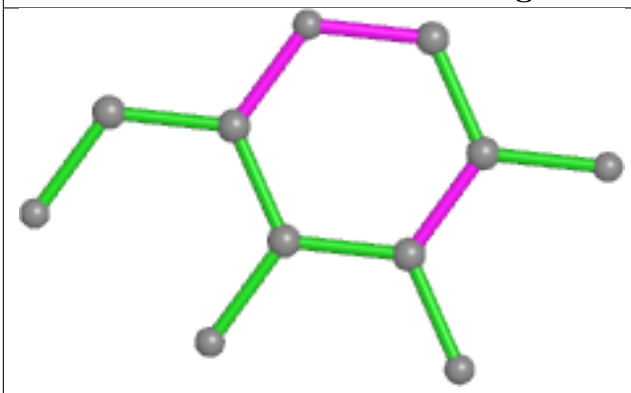	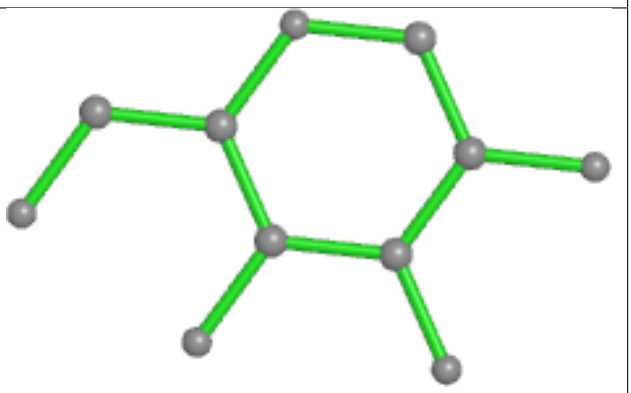
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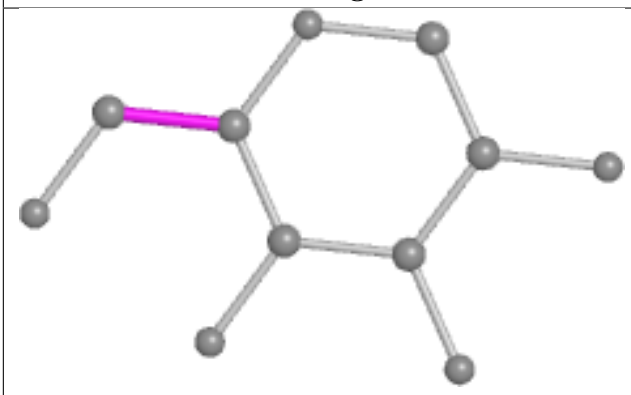	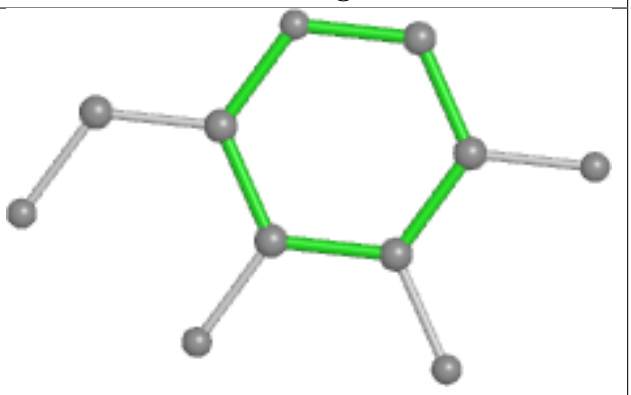
Torsions	**Rings**

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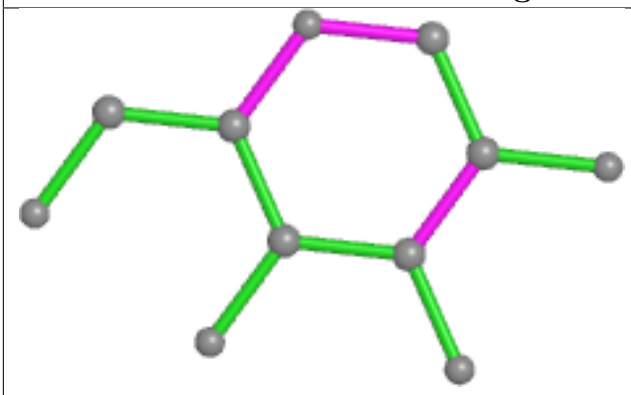
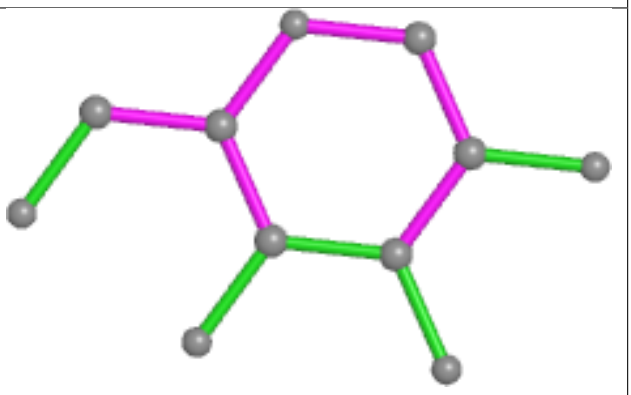
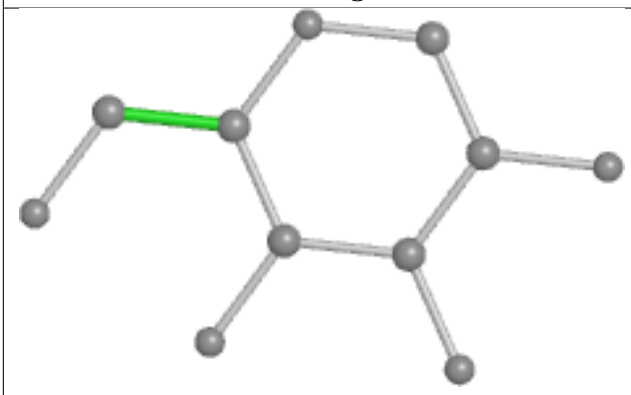
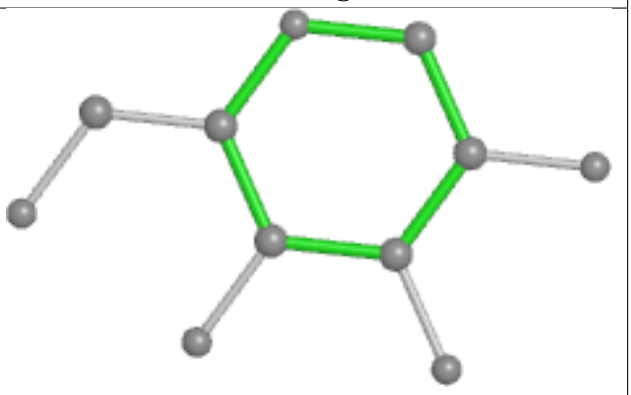
 Bond lengths	 Bond angles
 Torsions	 Rings

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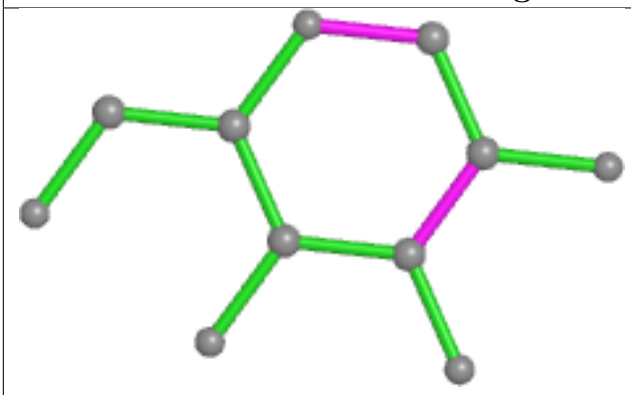
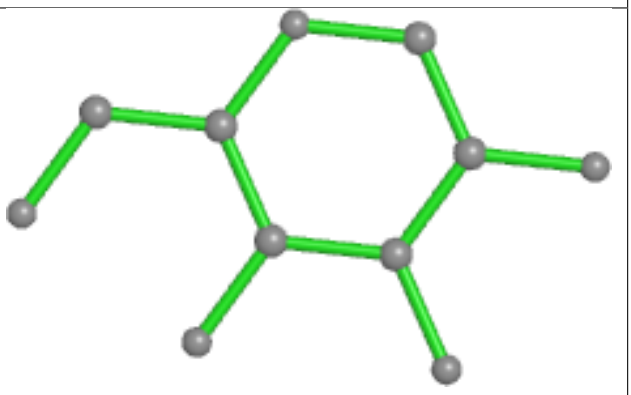
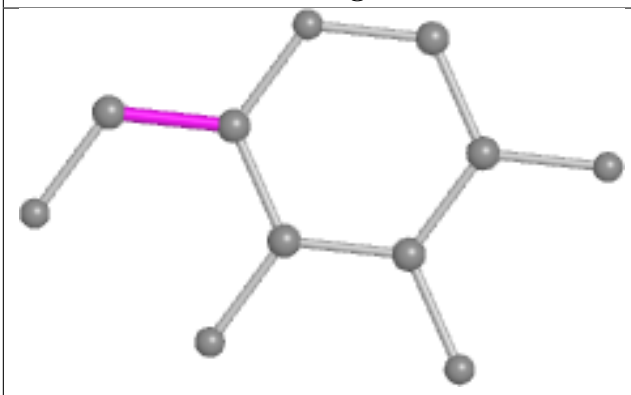
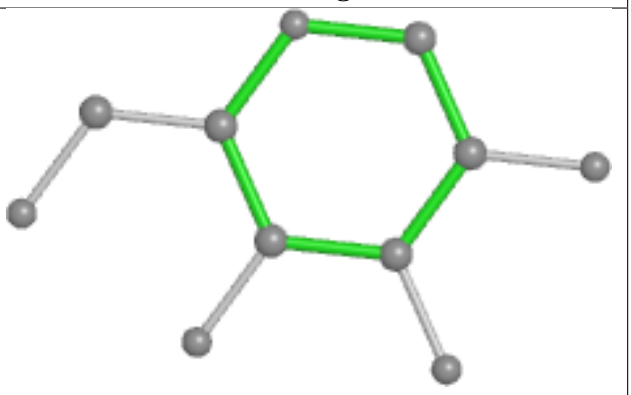
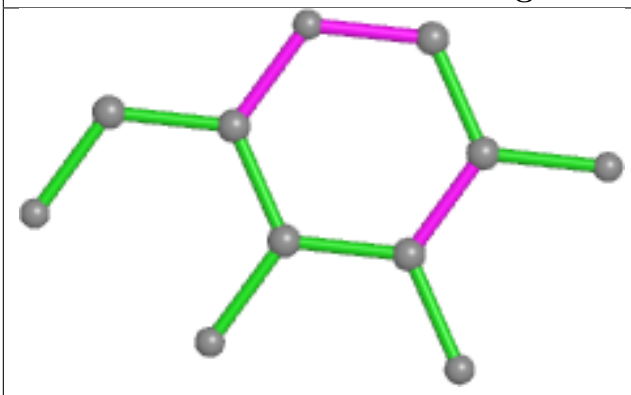
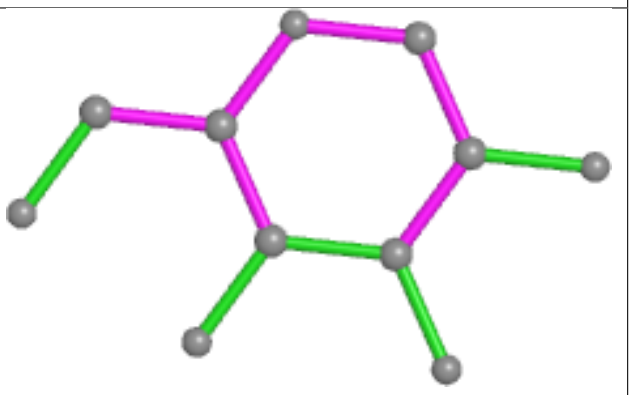
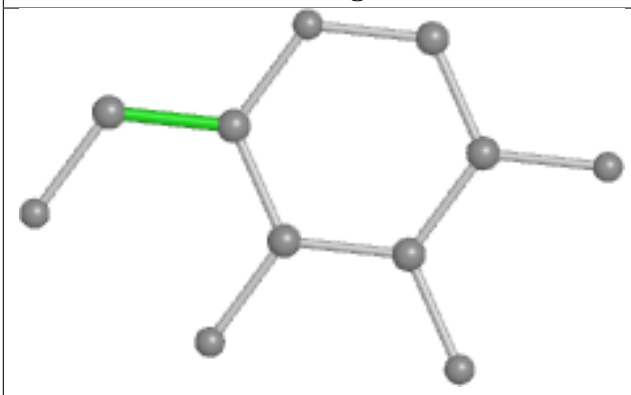
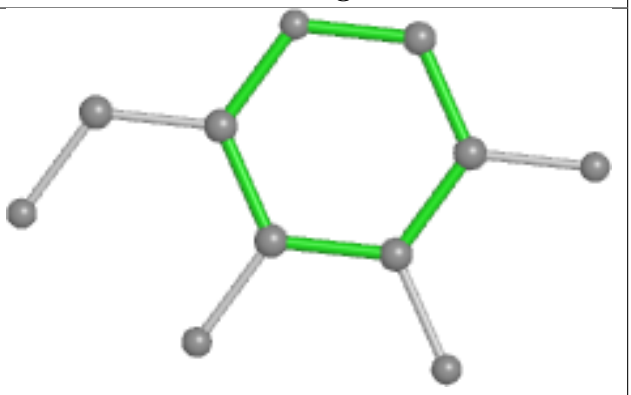
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA F 2006	
 Bond lengths	 Bond angles
 Torsions	 Rings

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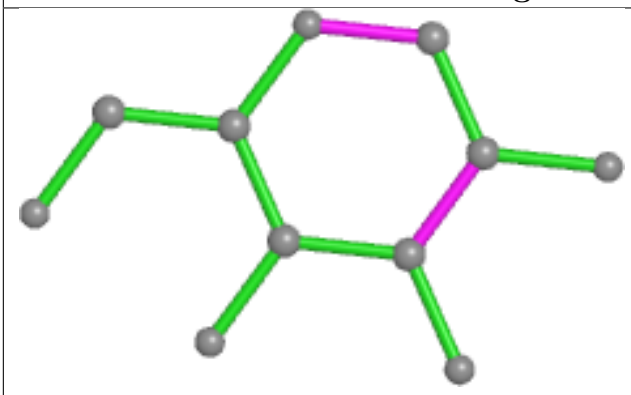	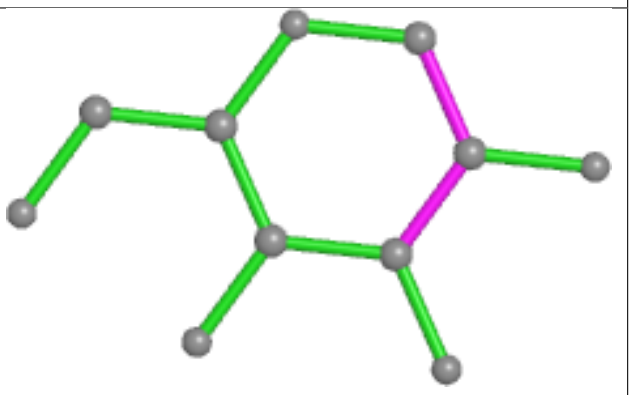
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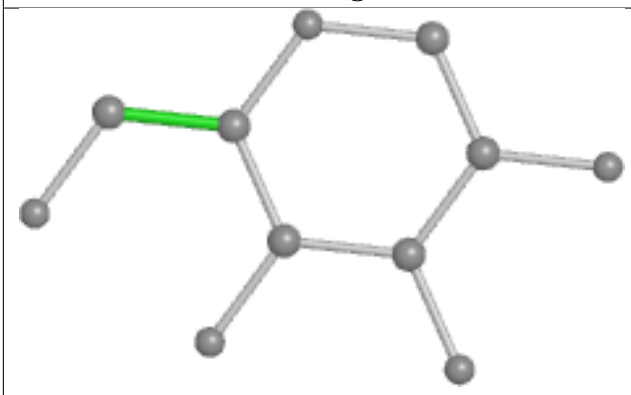	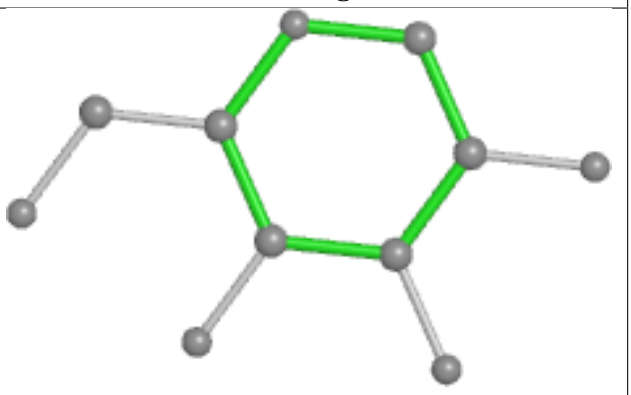
Torsions	**Rings**

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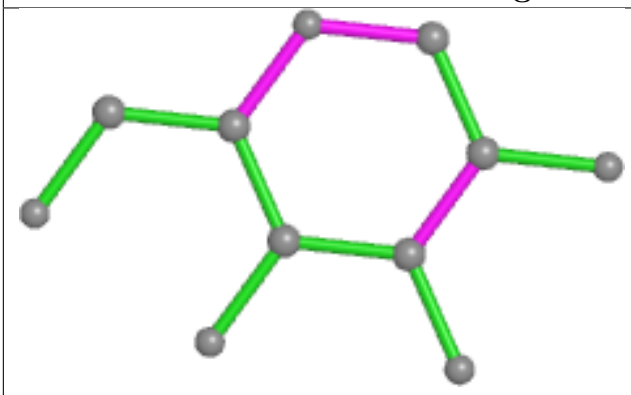
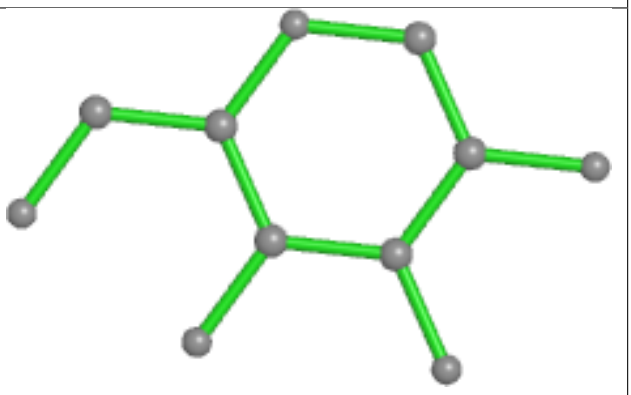
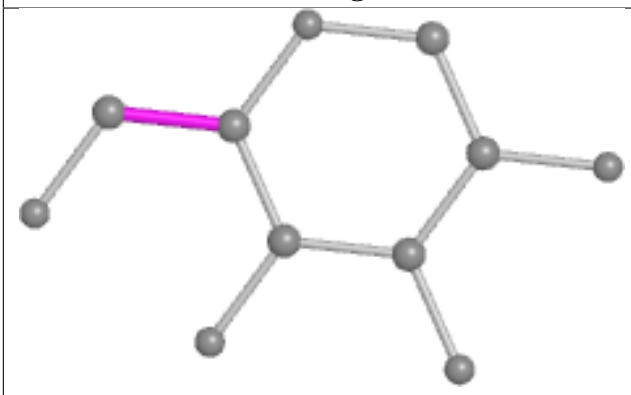
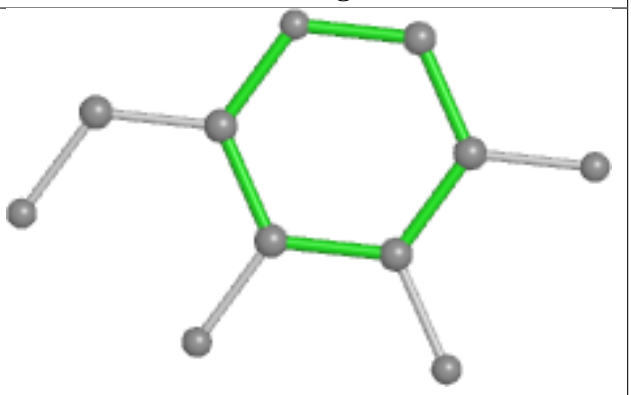
 Bond lengths	 Bond angles
 Torsions	 Rings

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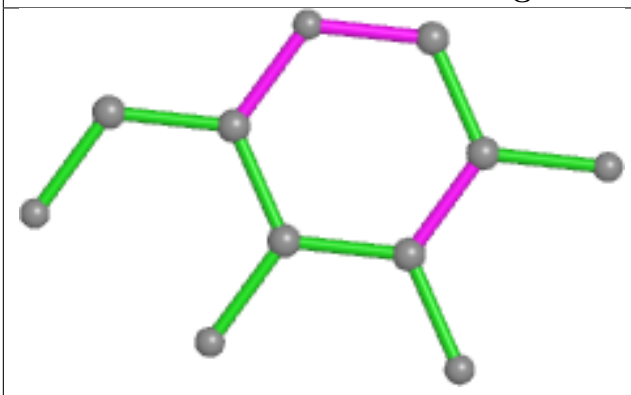	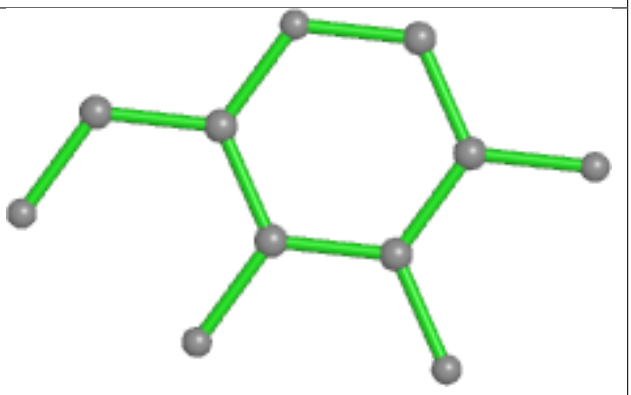
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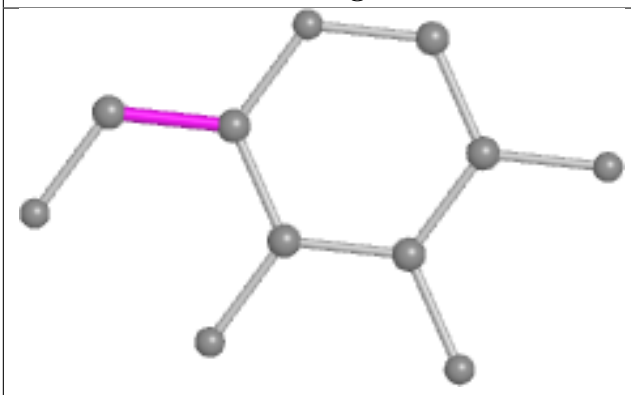
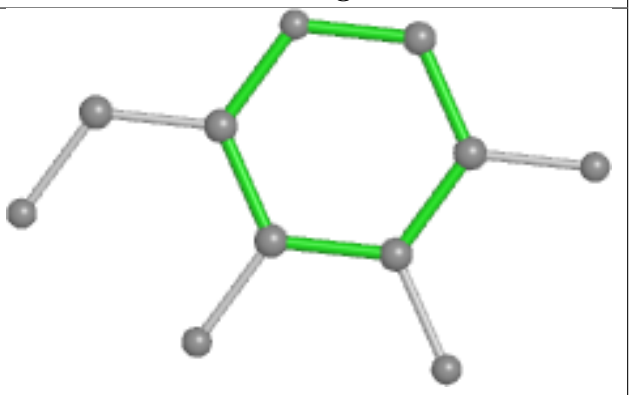
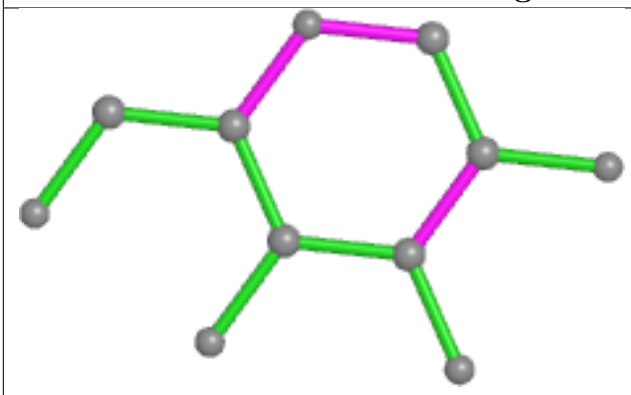
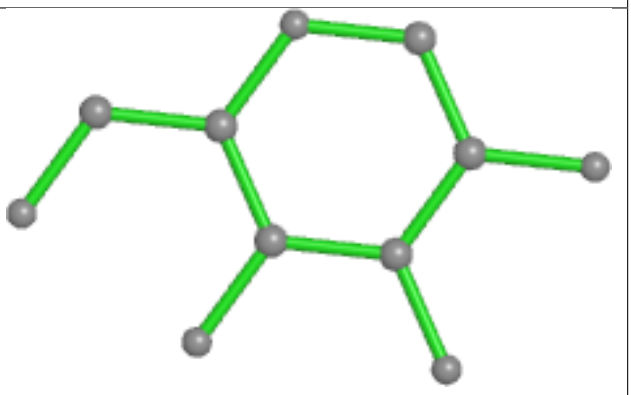
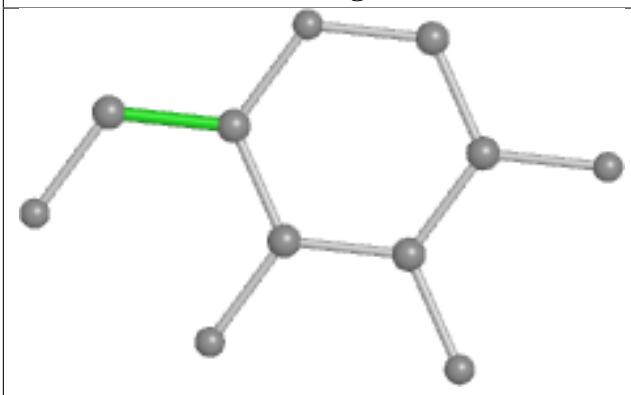
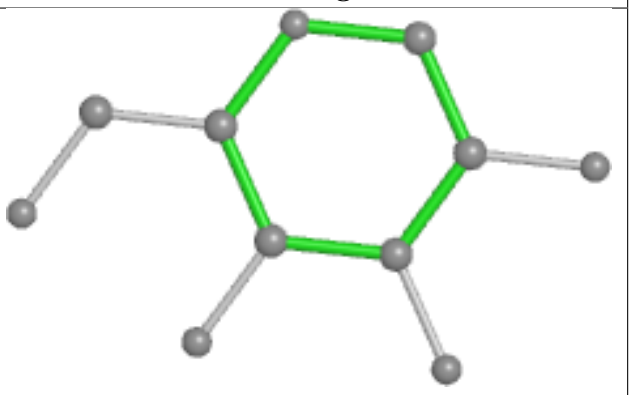
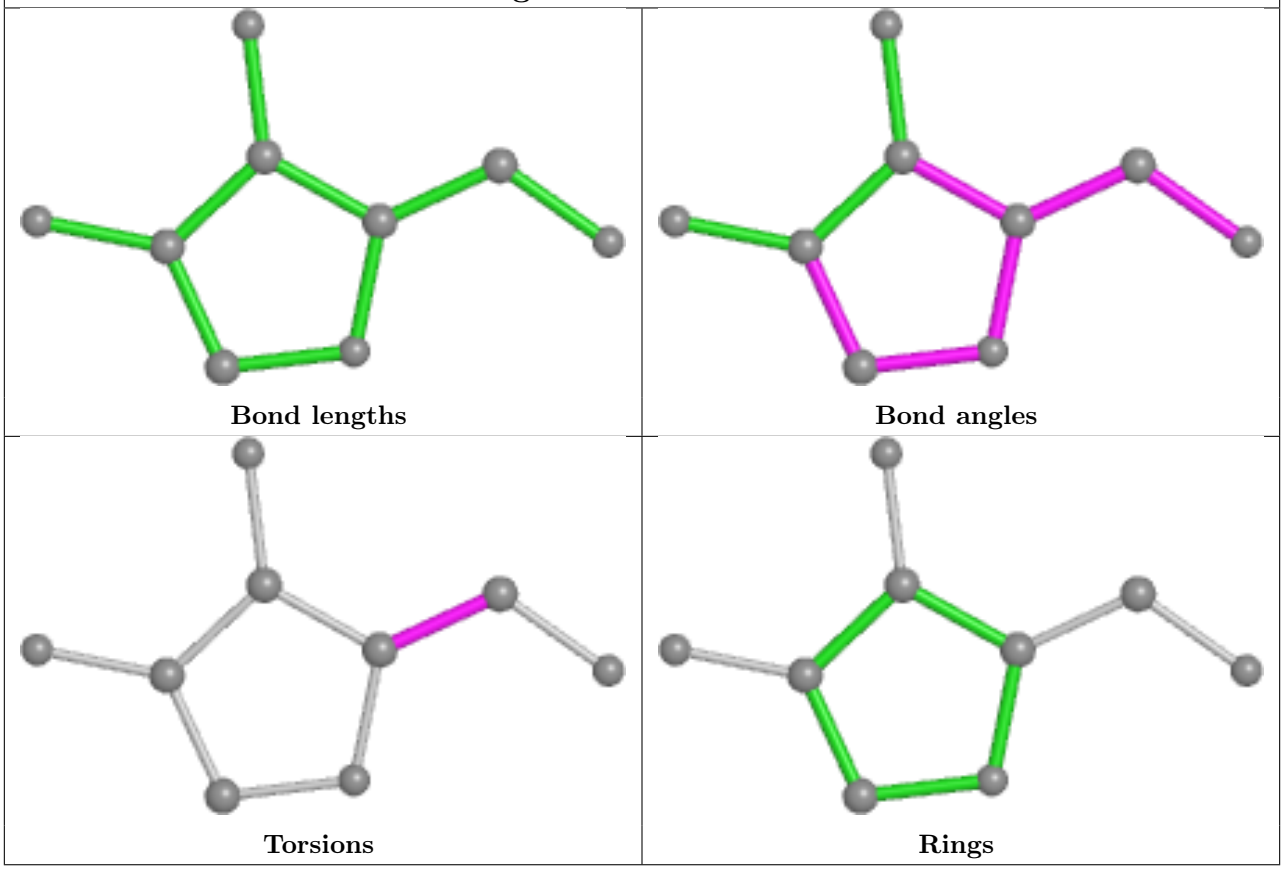
	
Torsions	**Rings**

Ligand GLA B 2006	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AHR B 2003



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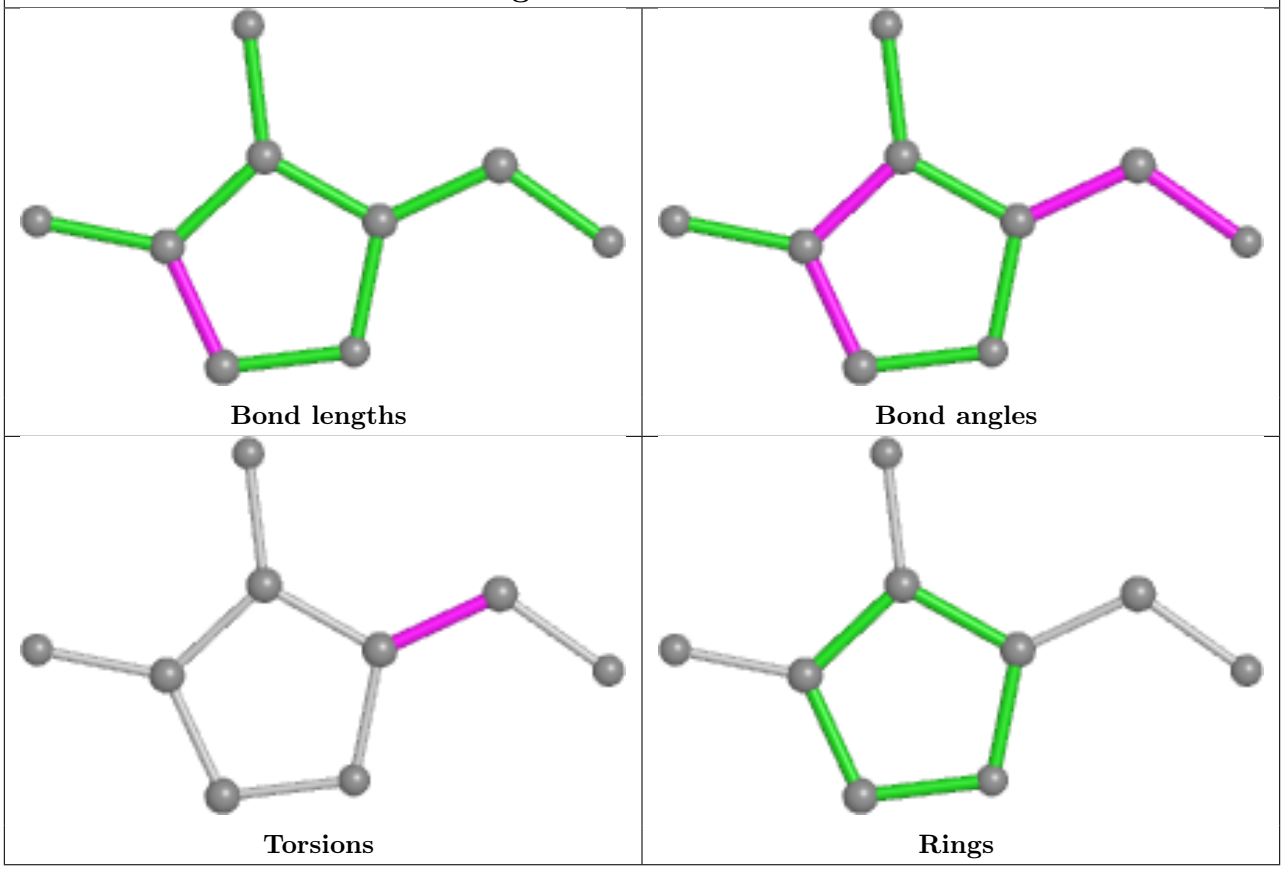
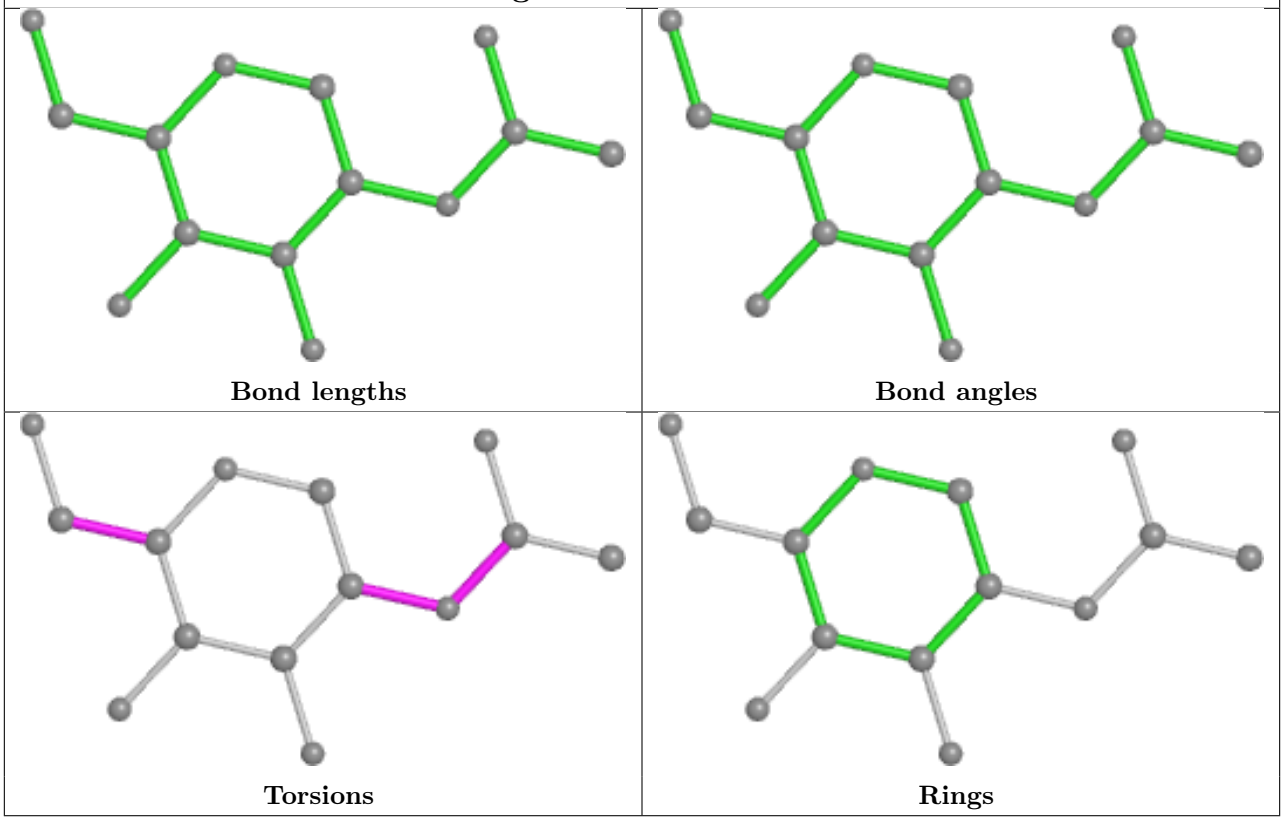
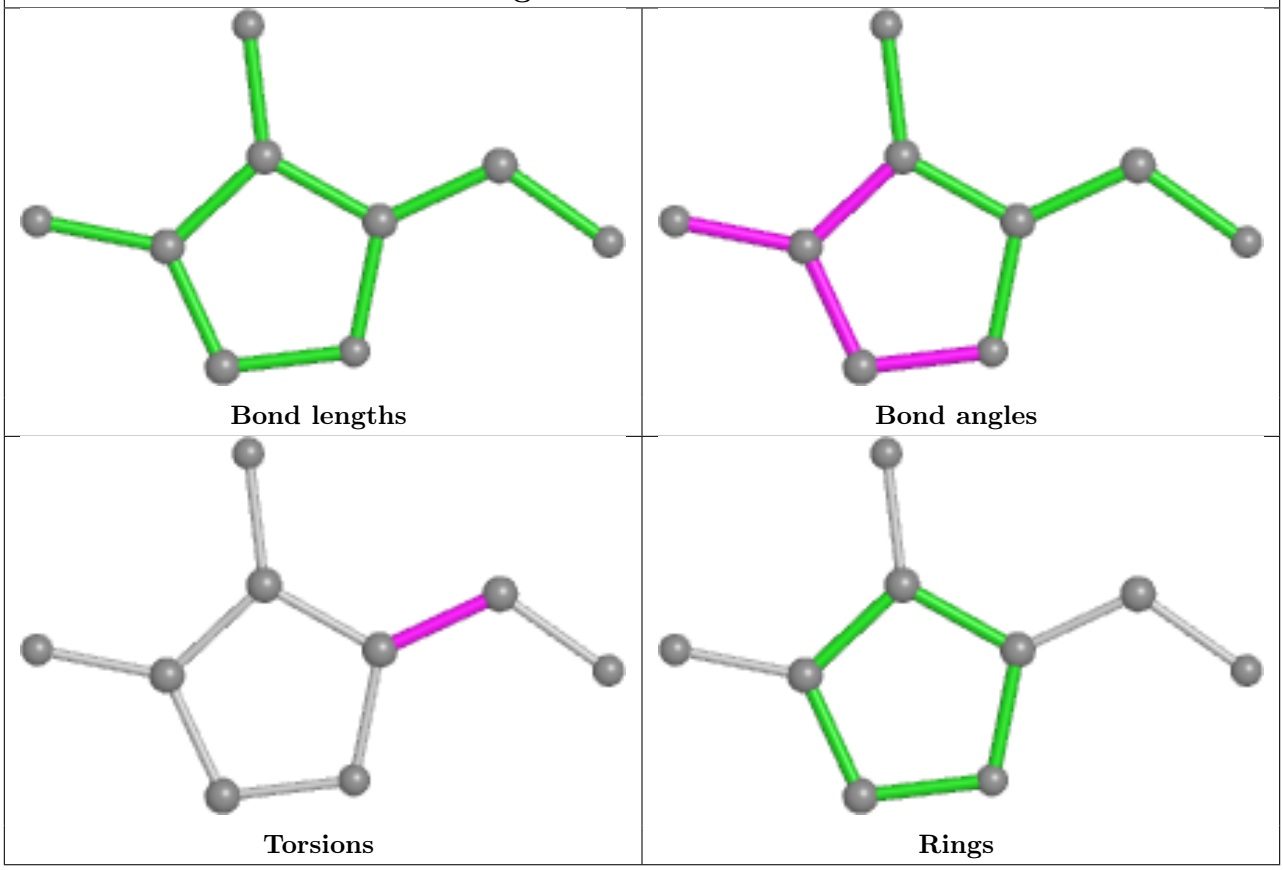


Ligand NAG C 2009



Ligand AHR E 2003



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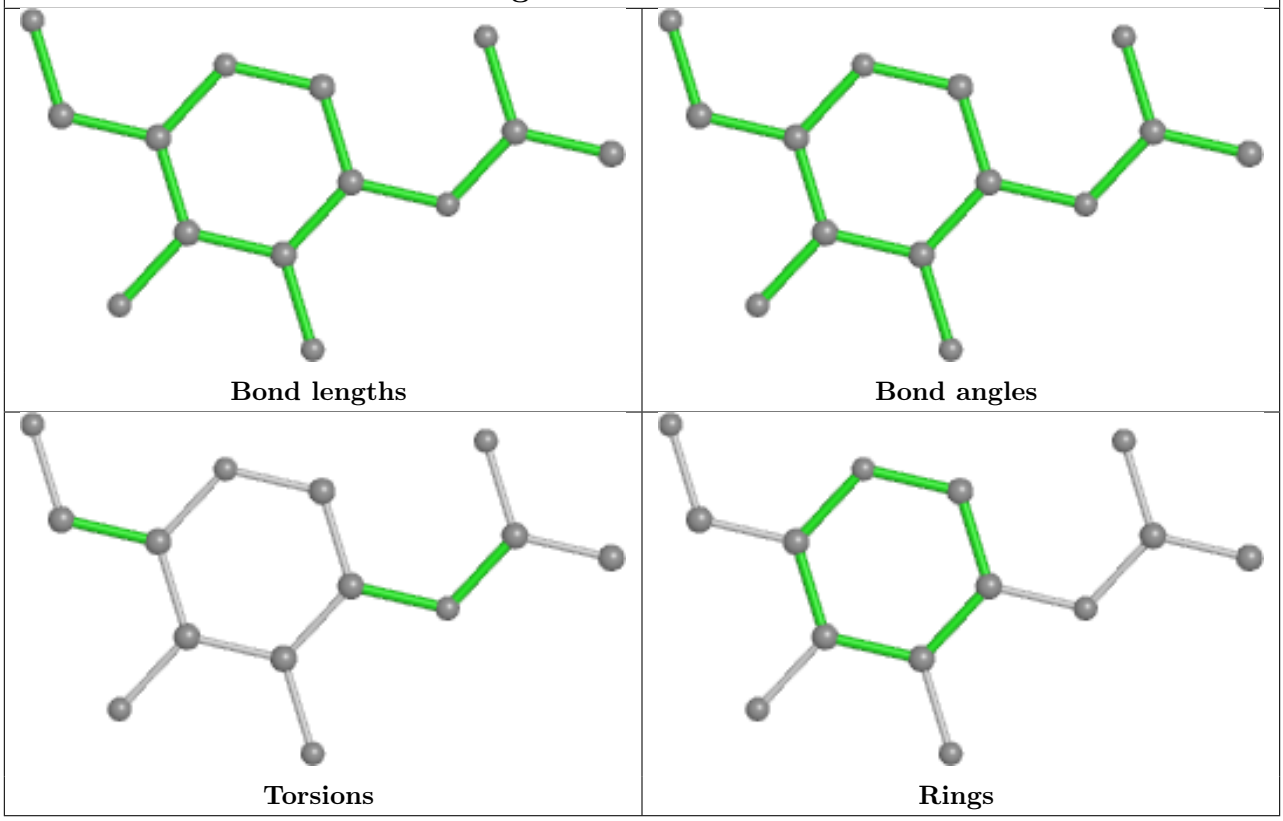

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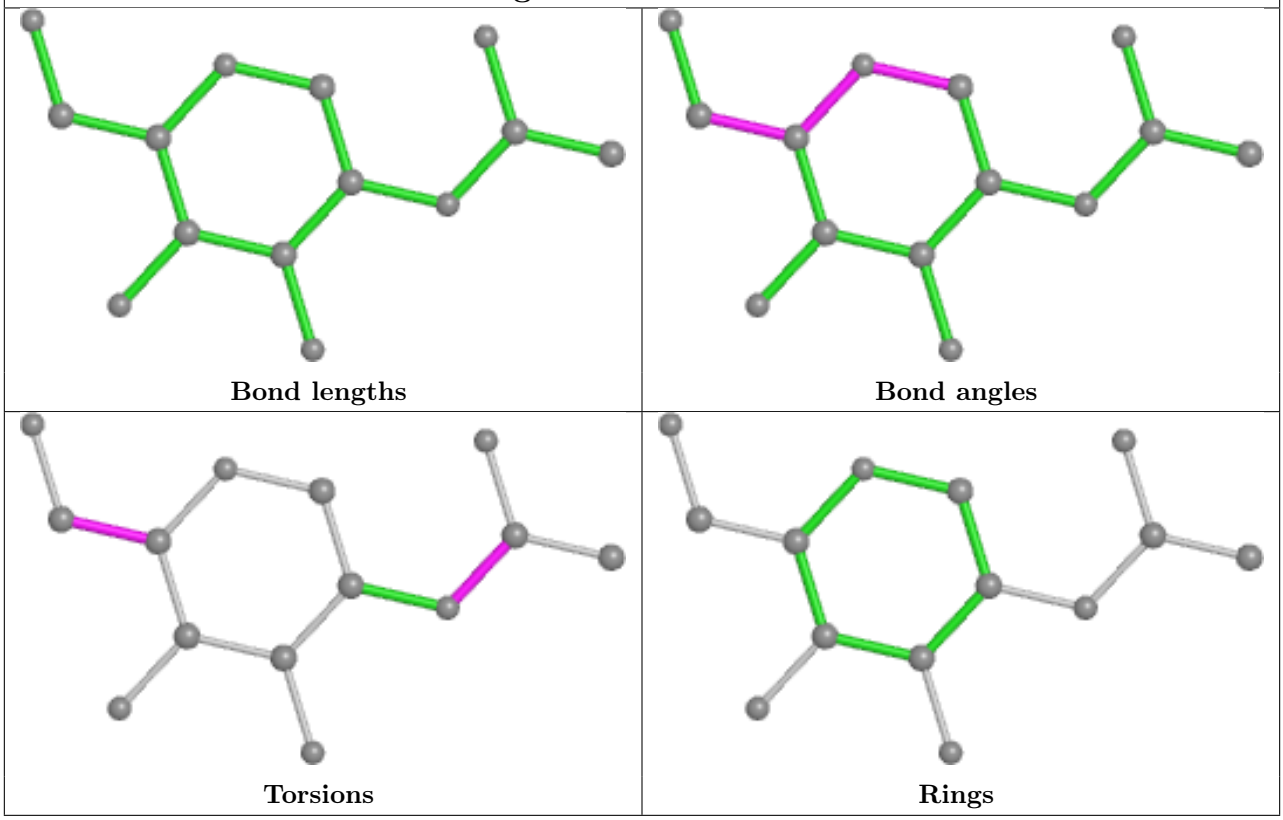

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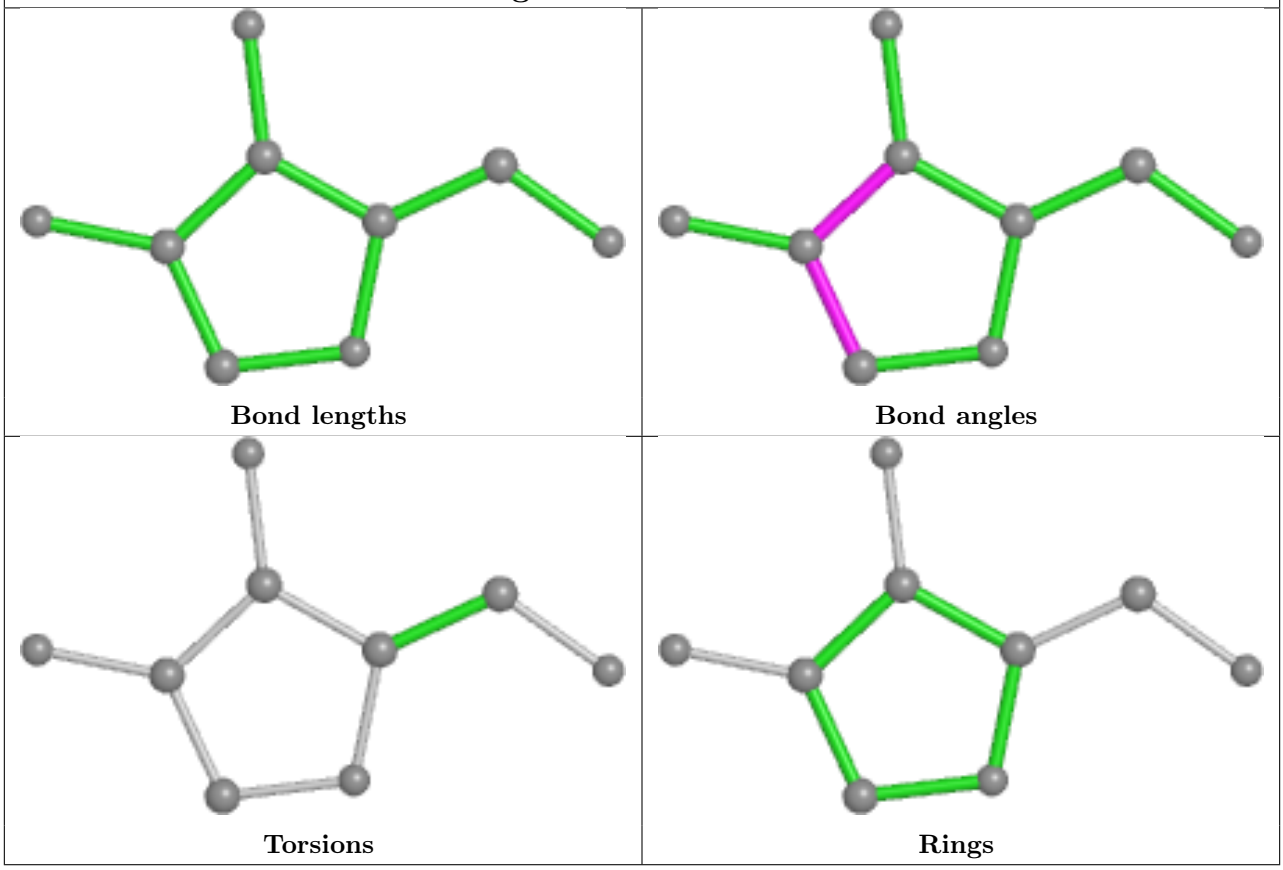
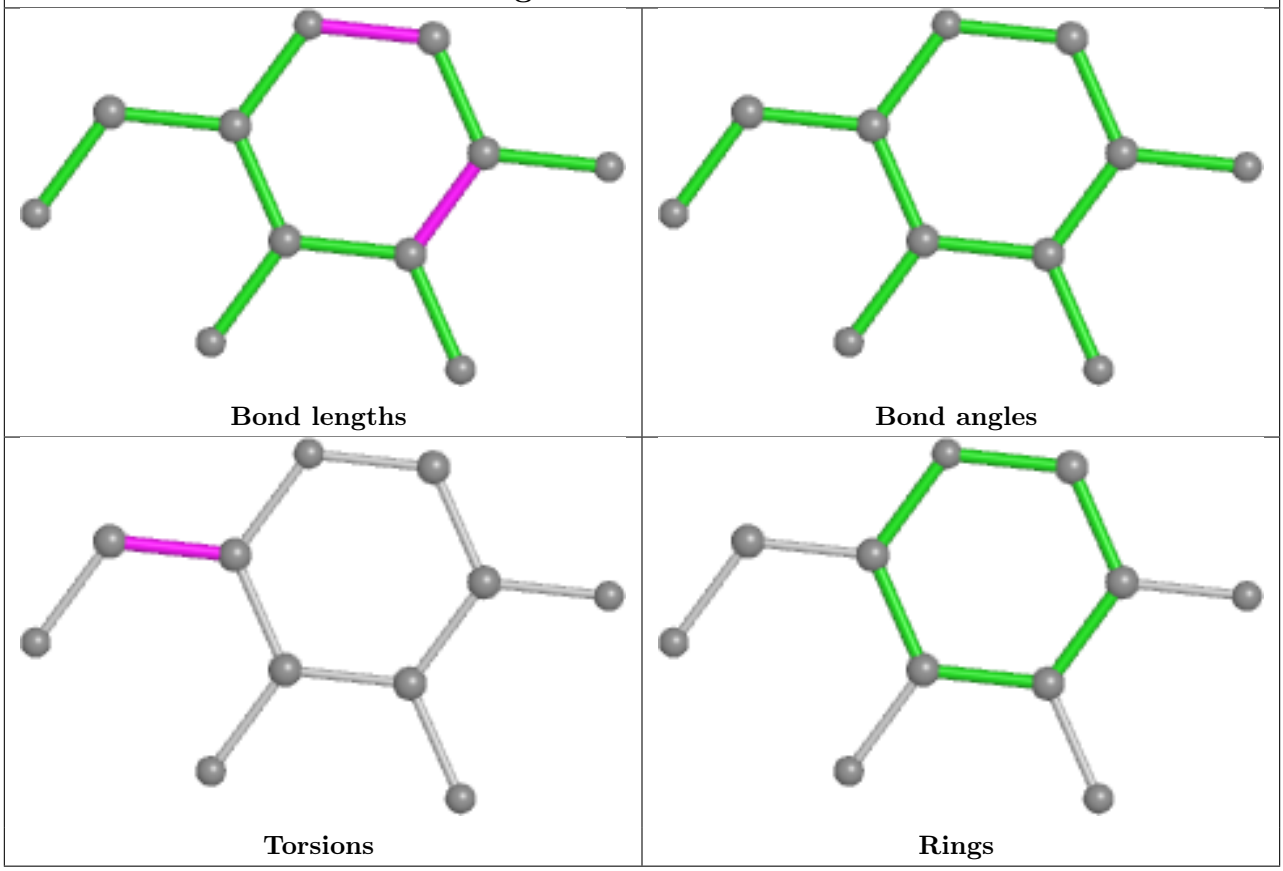


Ligand GLA A 2014



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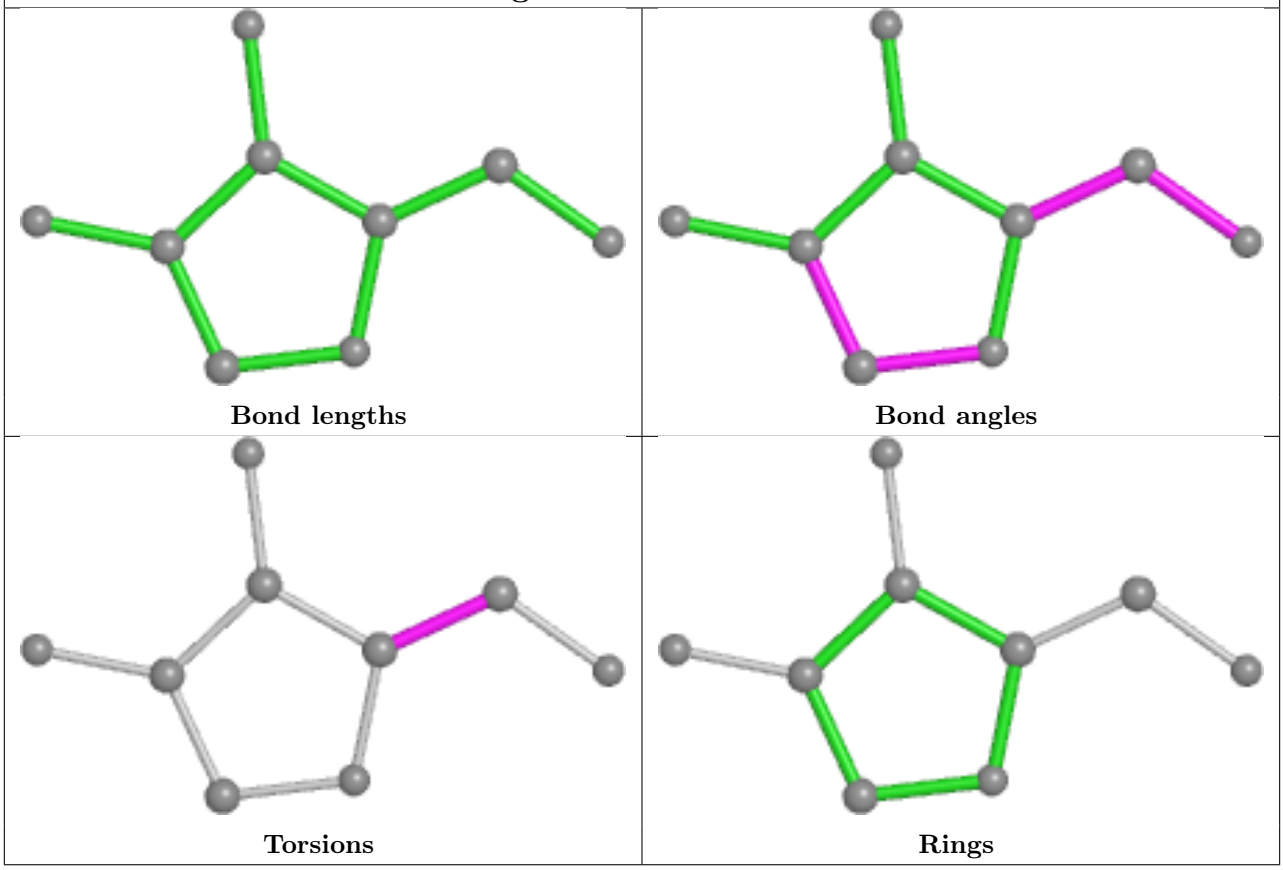
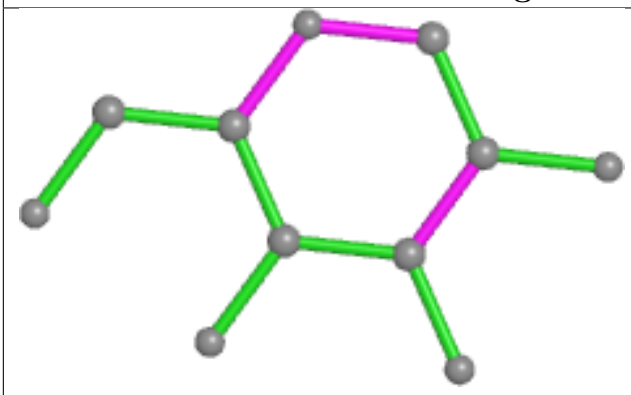
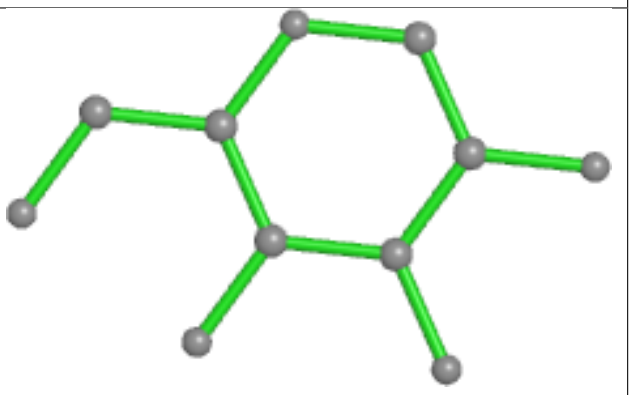
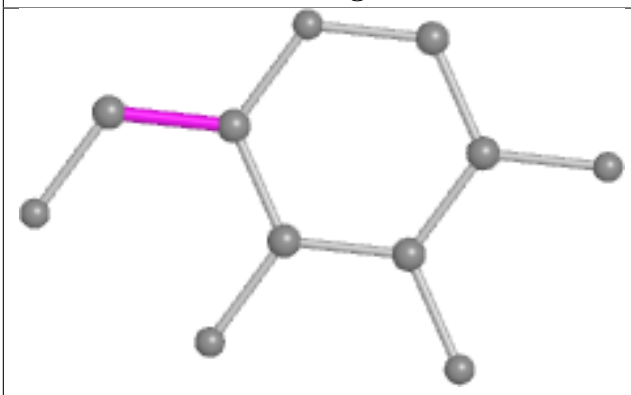
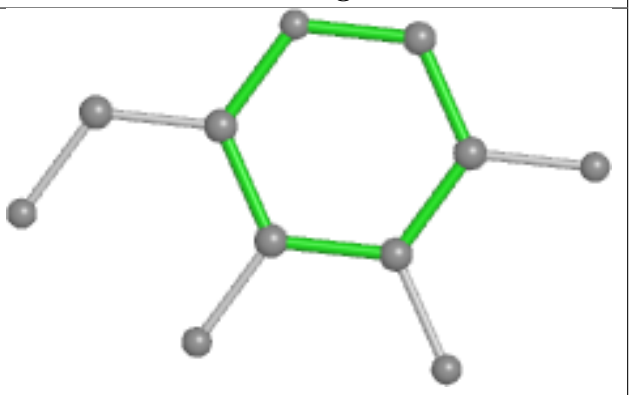


Ligand GLA C 2004	
 Bond lengths	 Bond angles
 Torsions	 Rings

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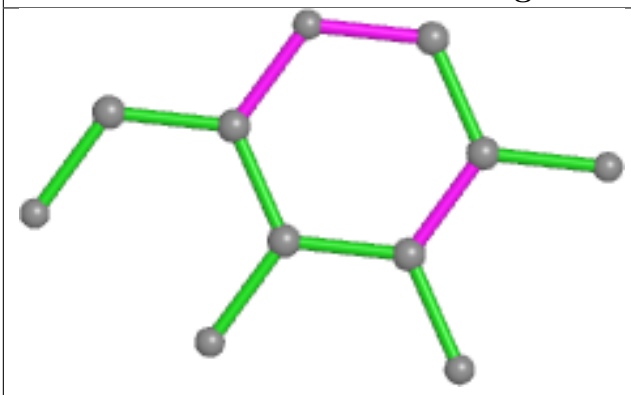	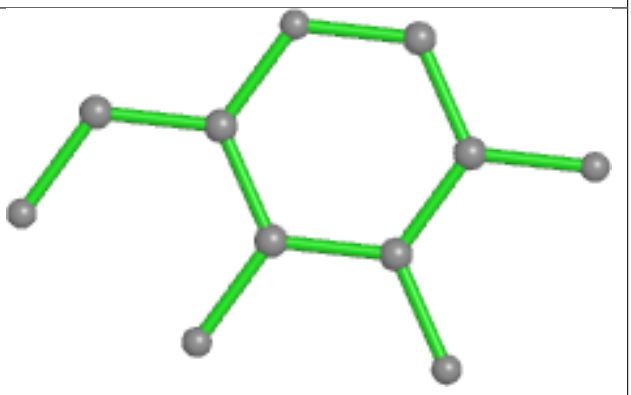
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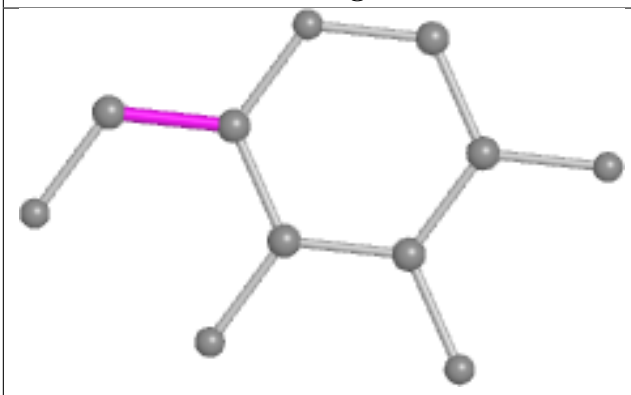
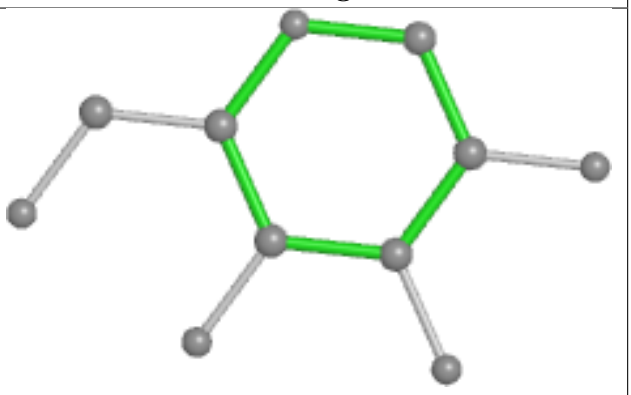
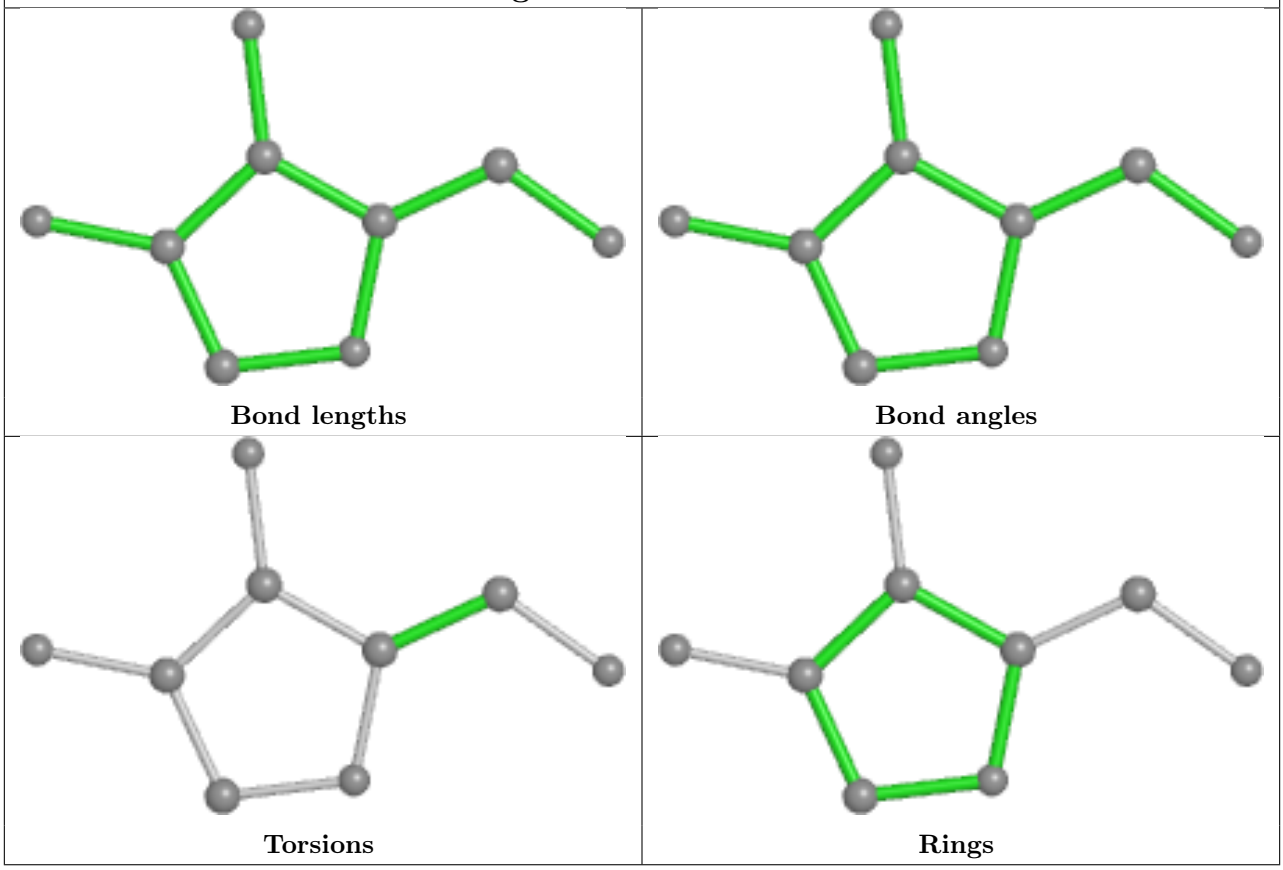
	
Torsions	**Rings**

Ligand AHR A 2019



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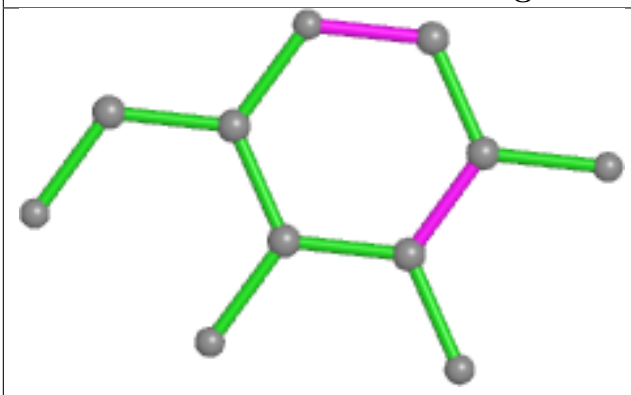	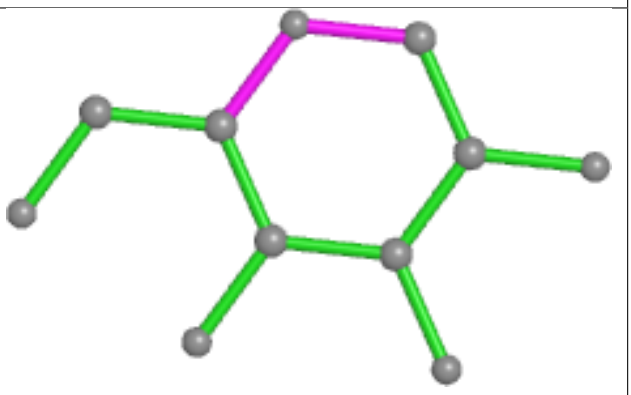
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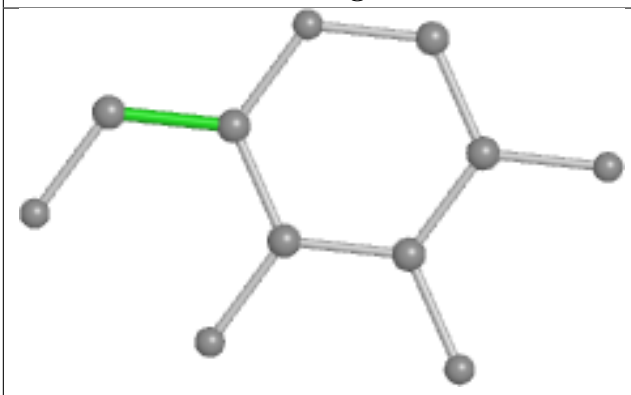	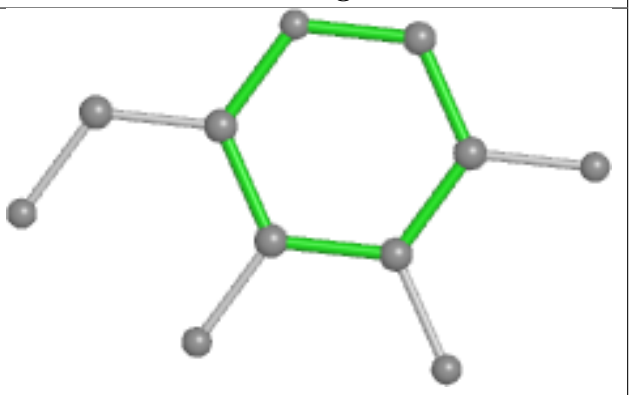
Torsions	**Rings**

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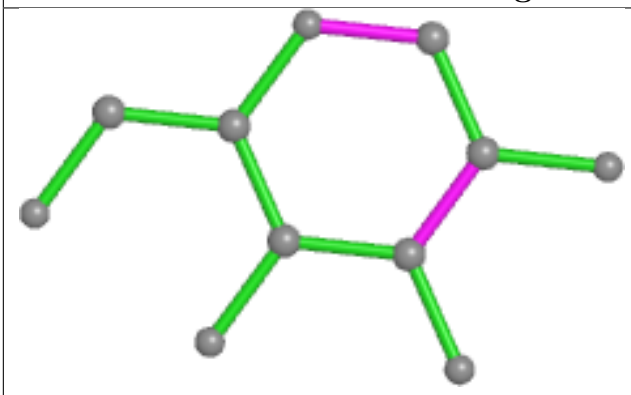	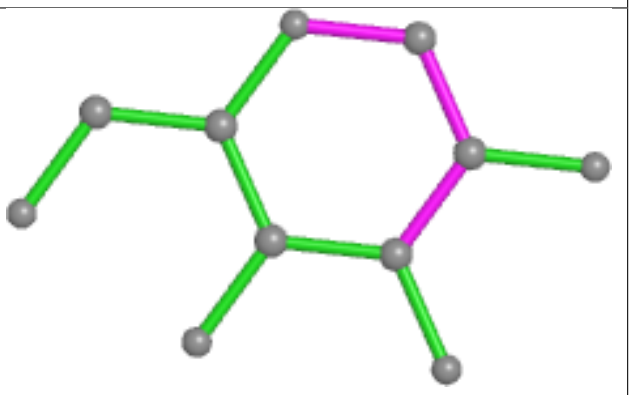
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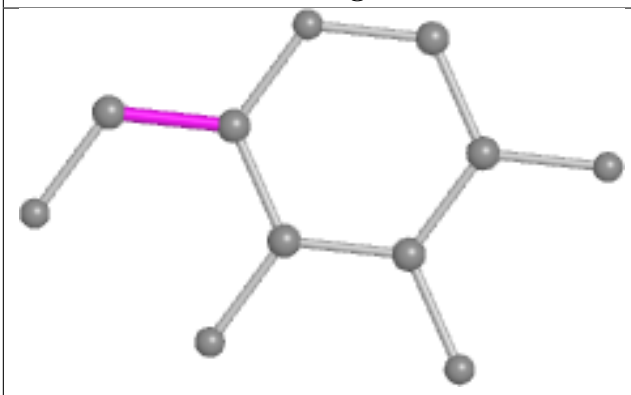
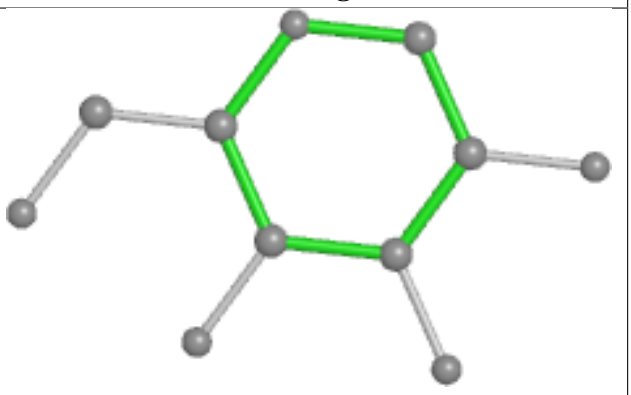
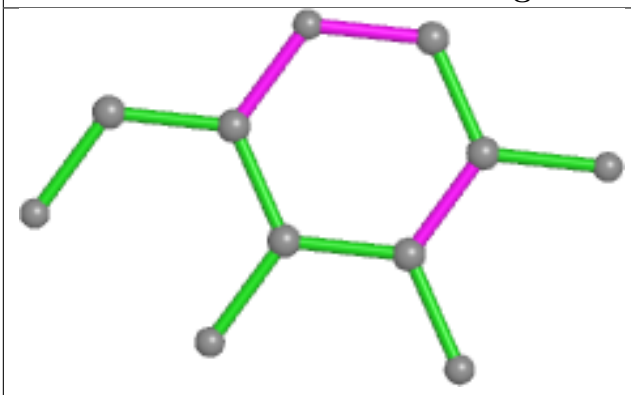
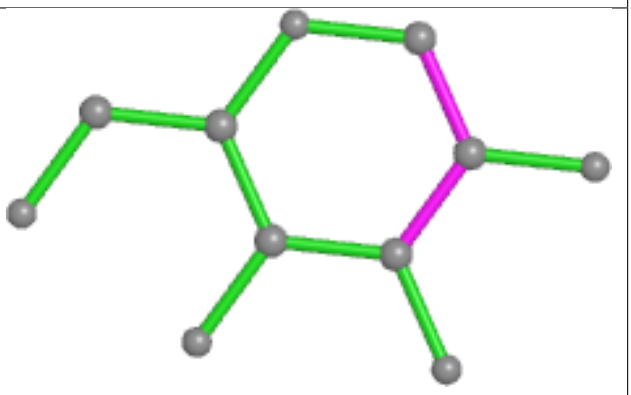
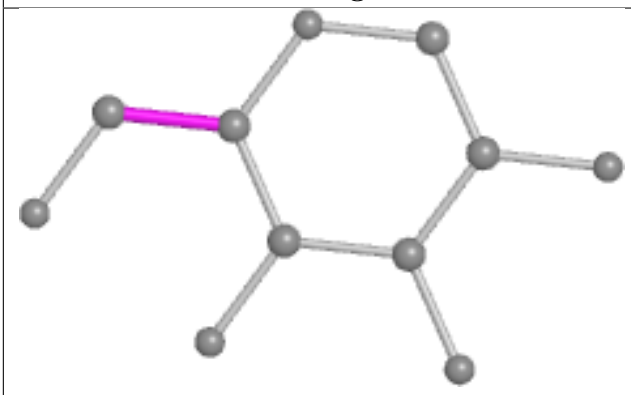
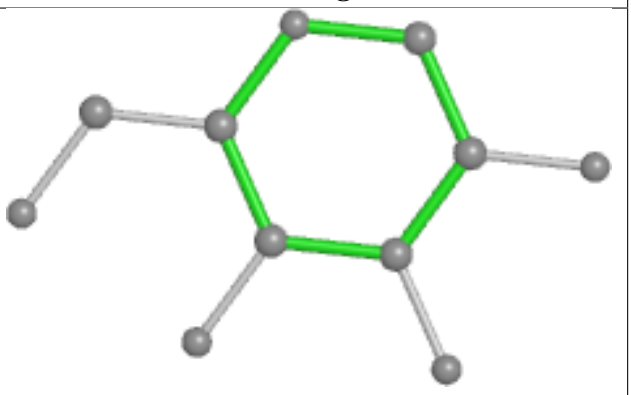
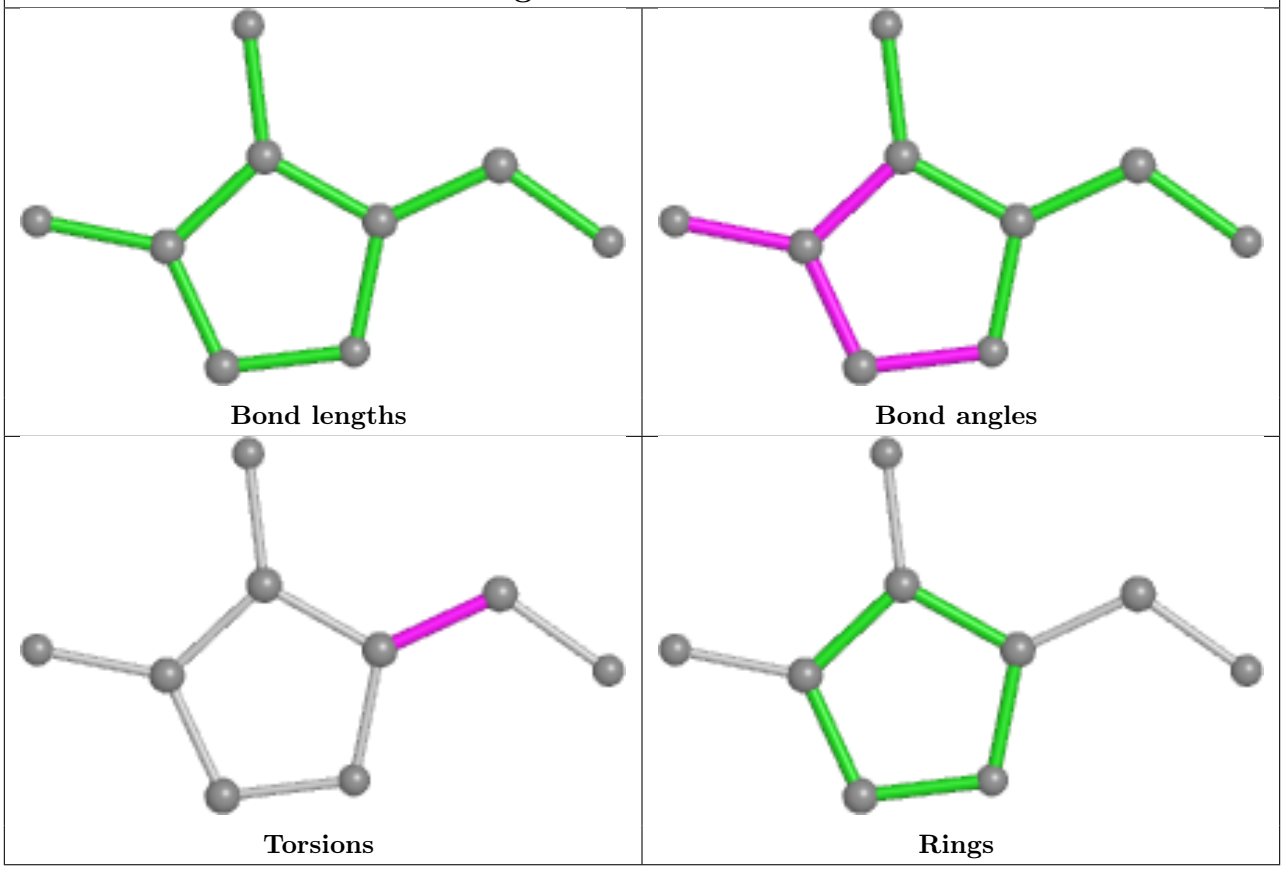
	
Torsions	**Rings**

Ligand GLA A 2009	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AHR F 2005



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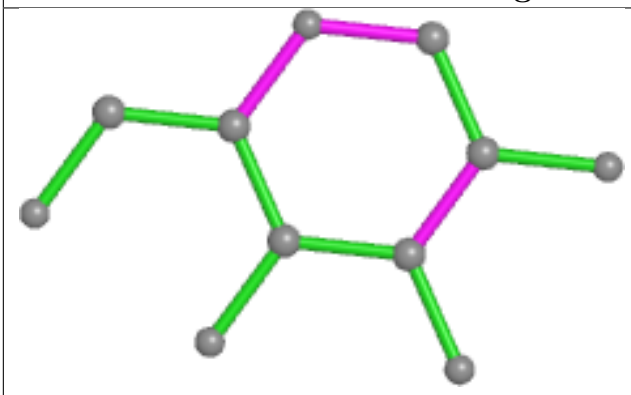
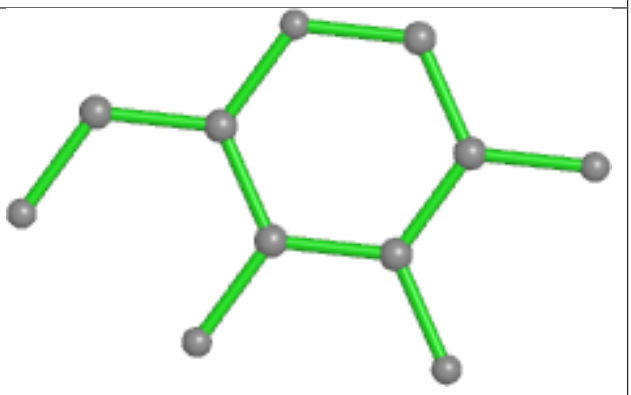
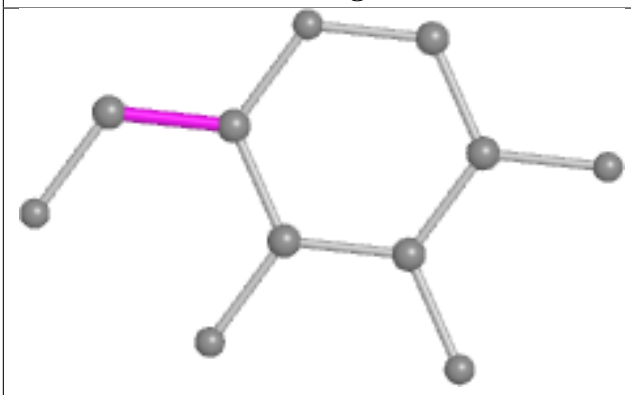
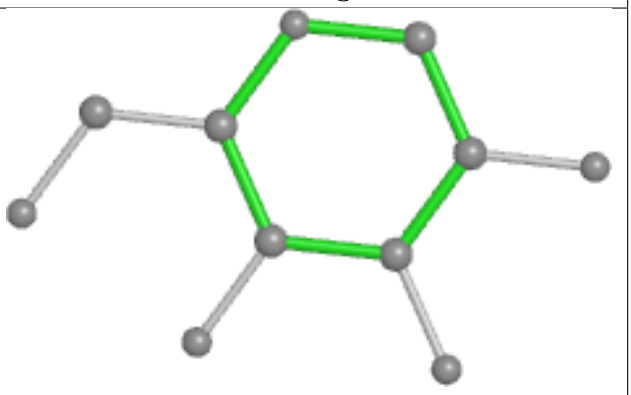
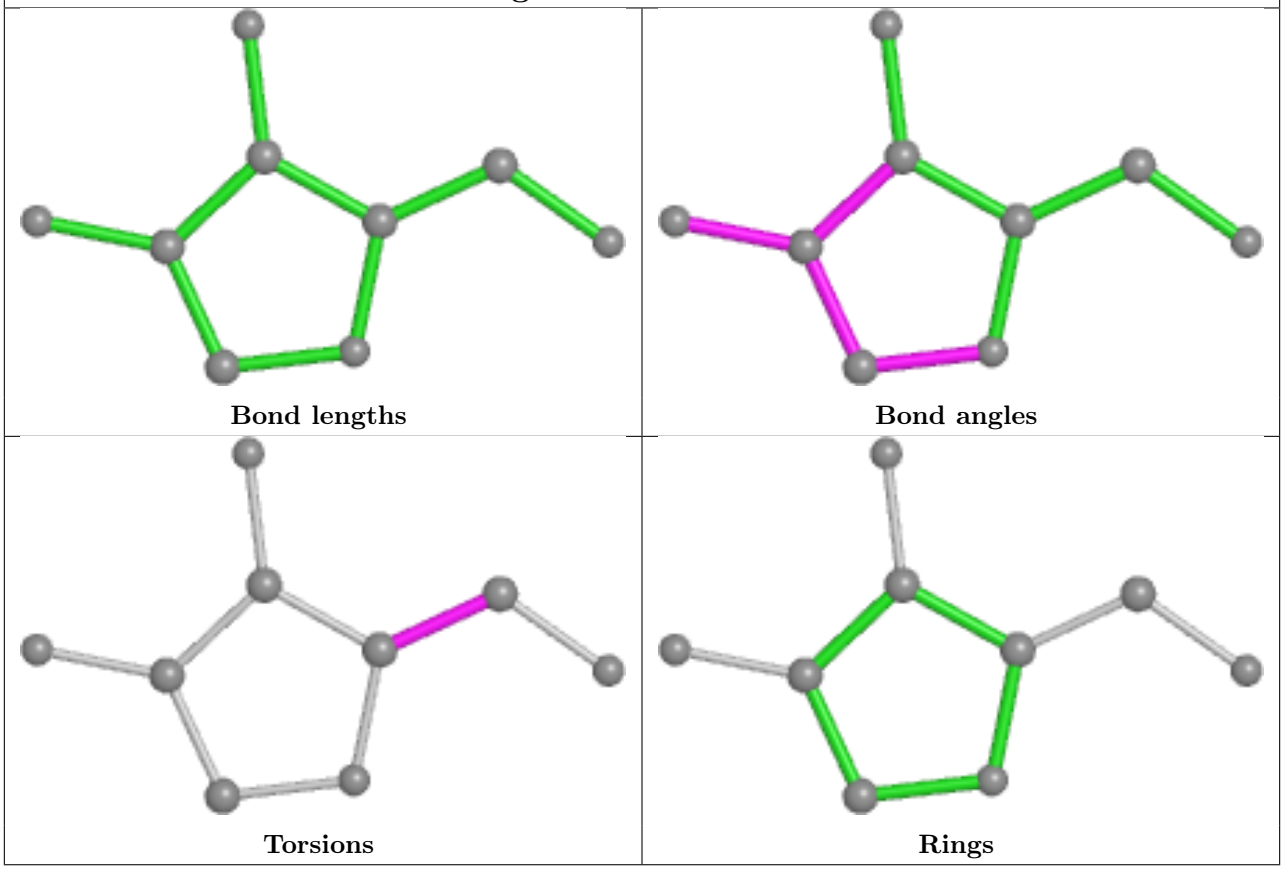
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AHR D 2004



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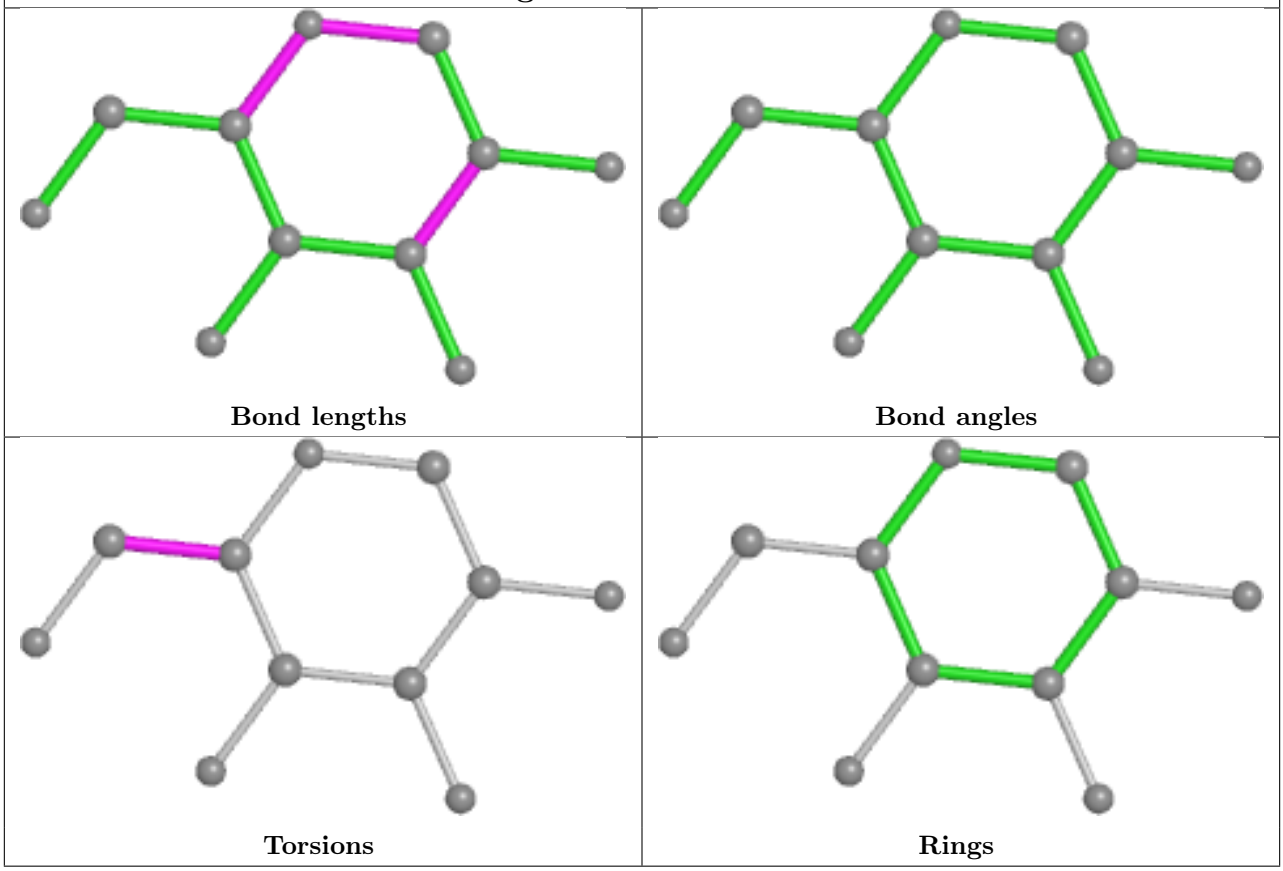
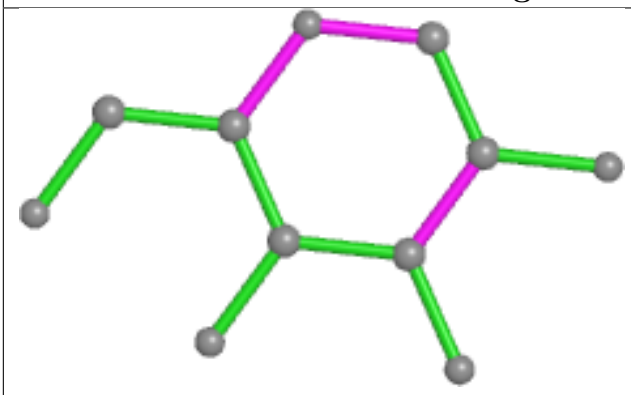
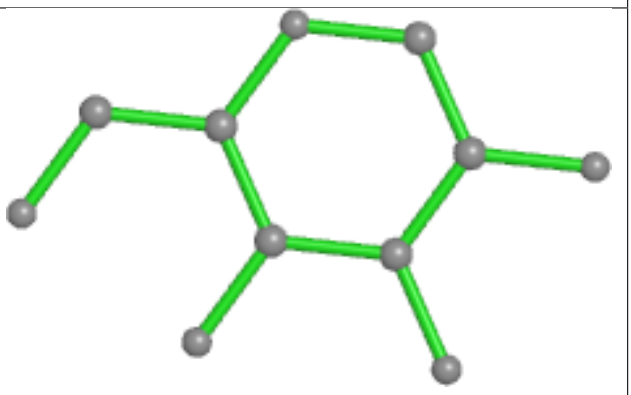
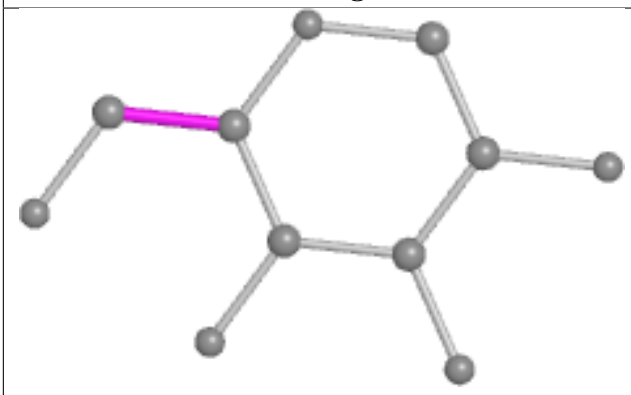
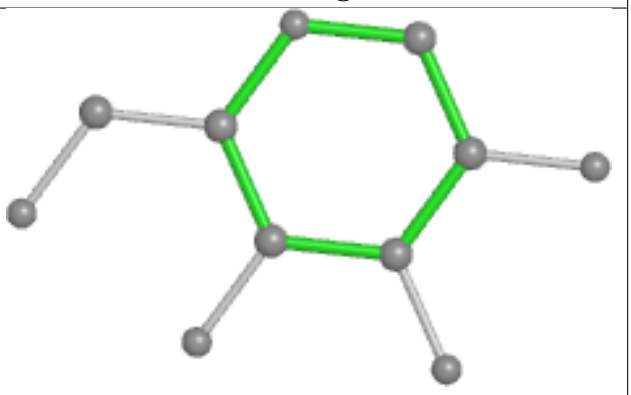
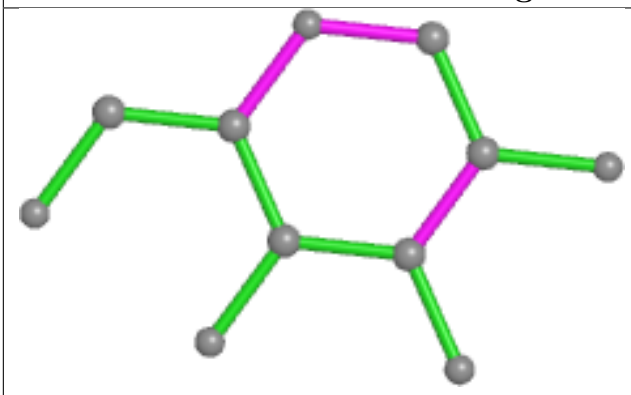
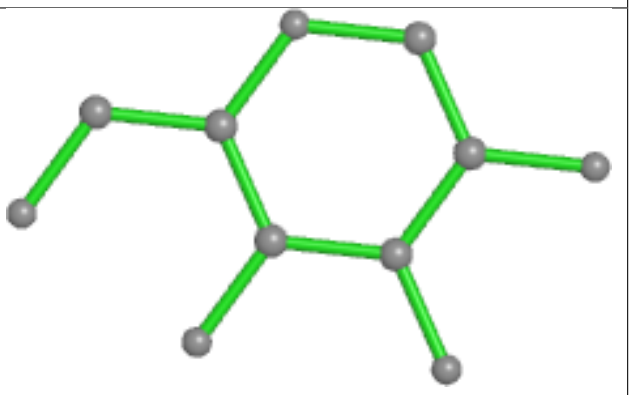
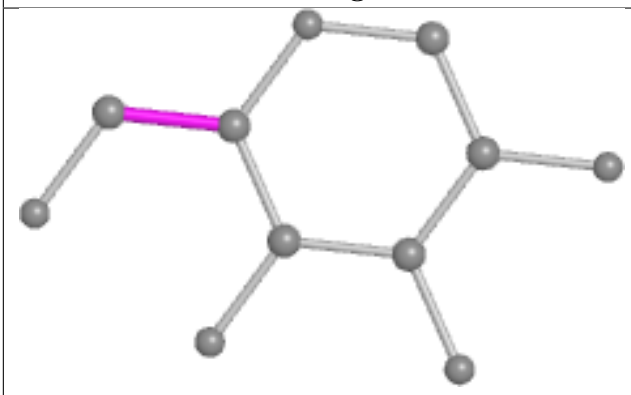
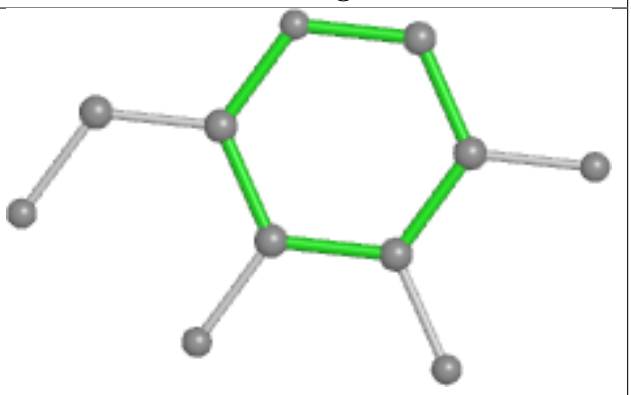
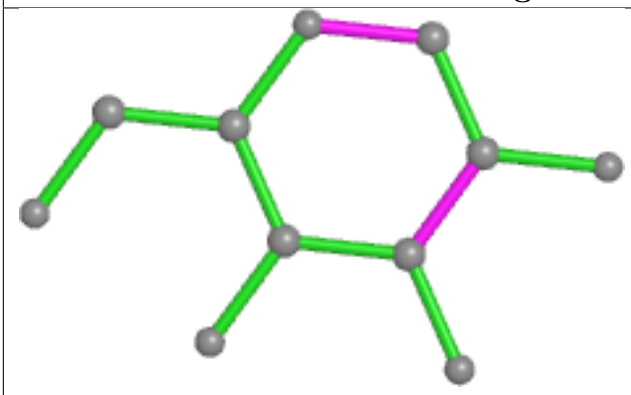
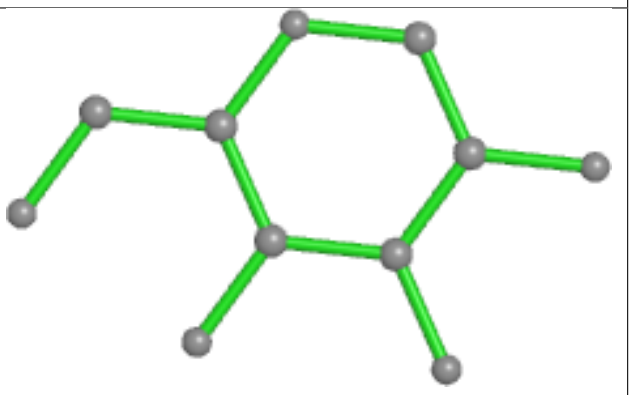
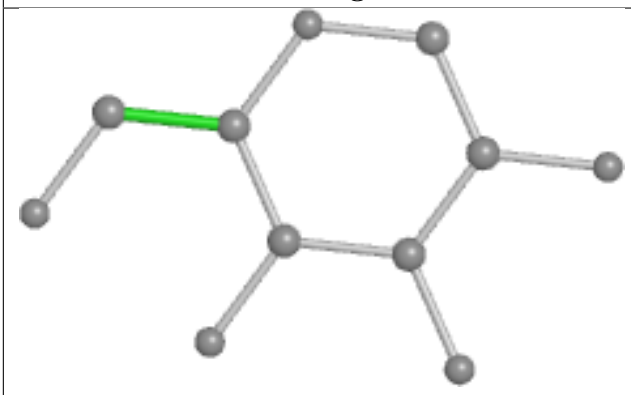
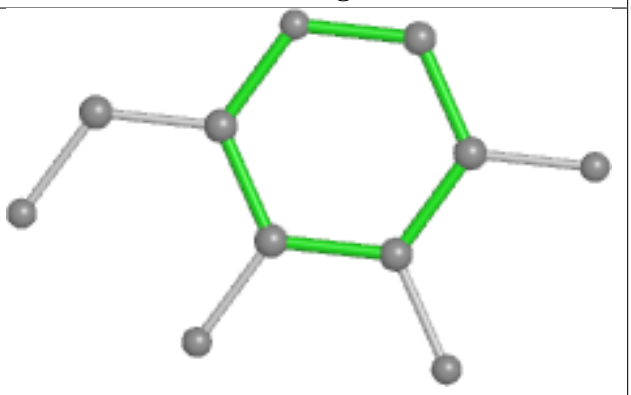
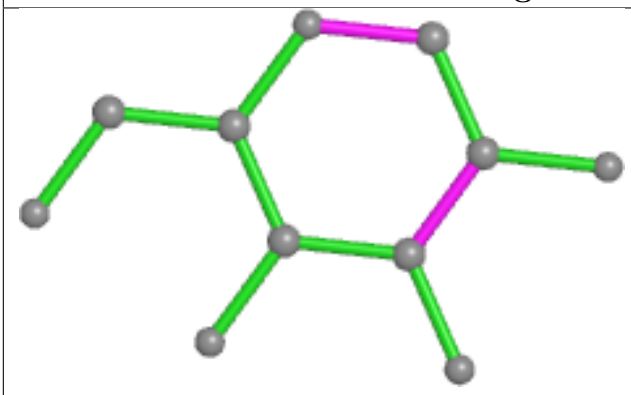
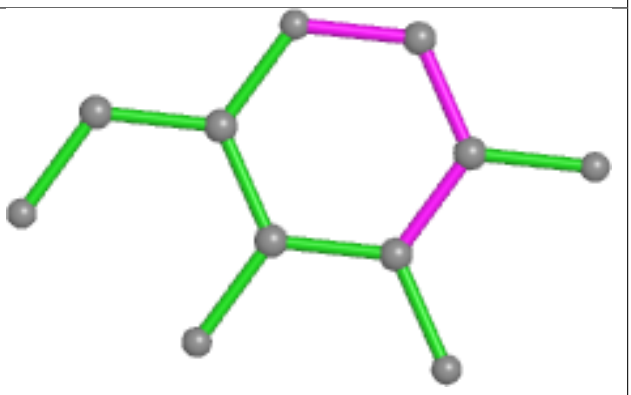
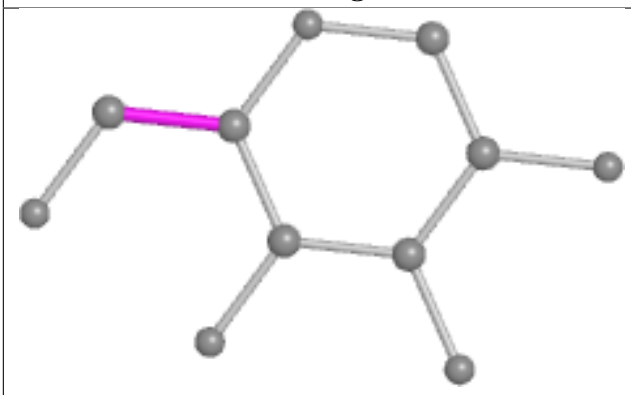
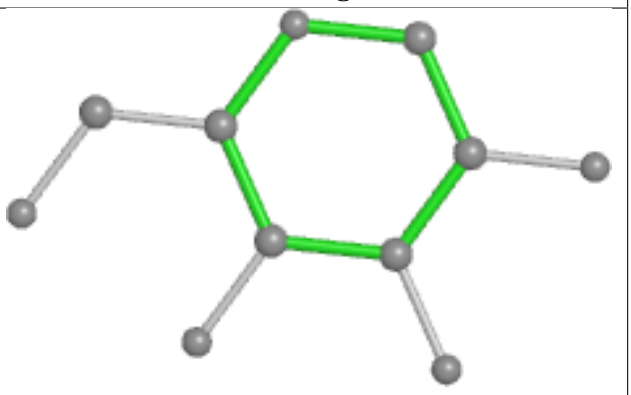


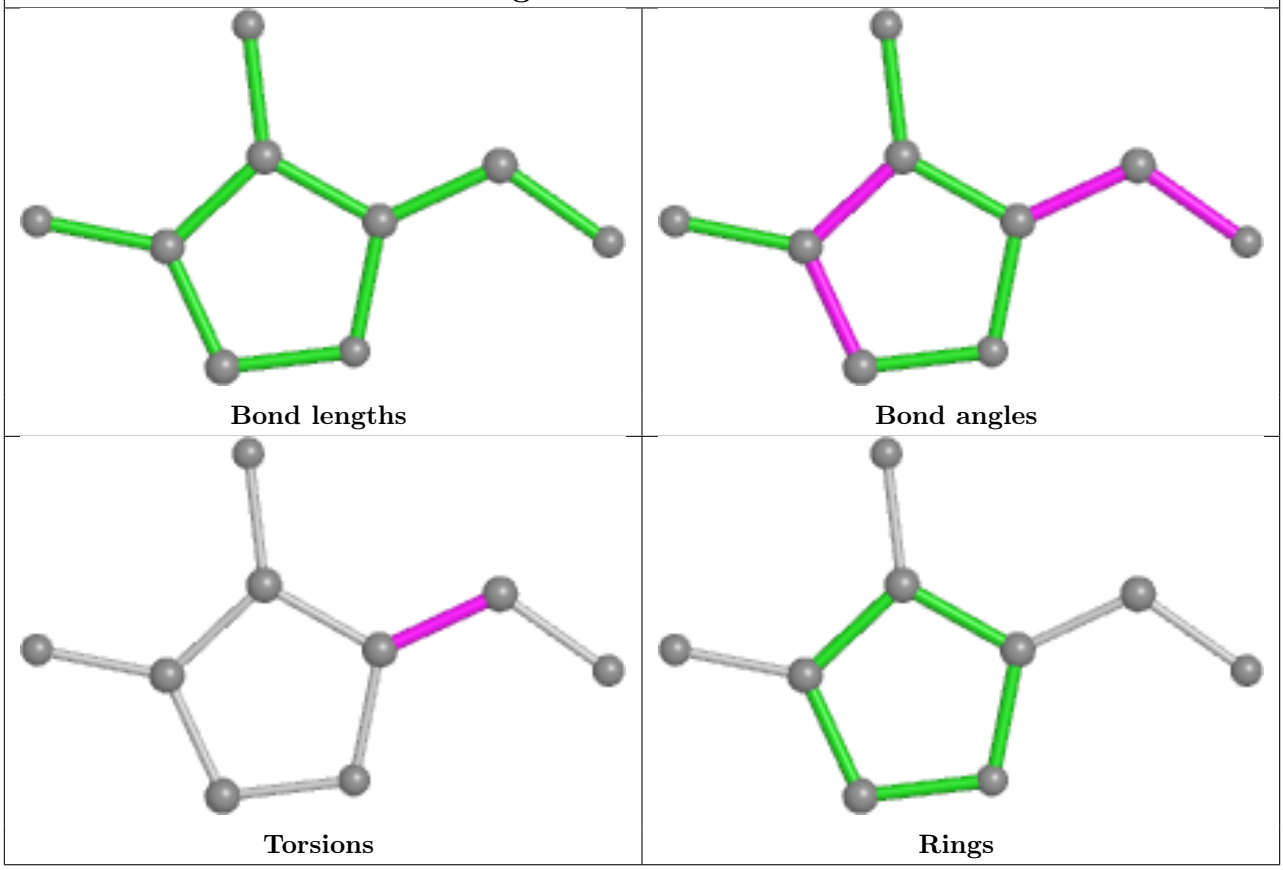
Ligand GLA D 2008	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA E 2006	
 Bond lengths	 Bond angles
 Torsions	 Rings

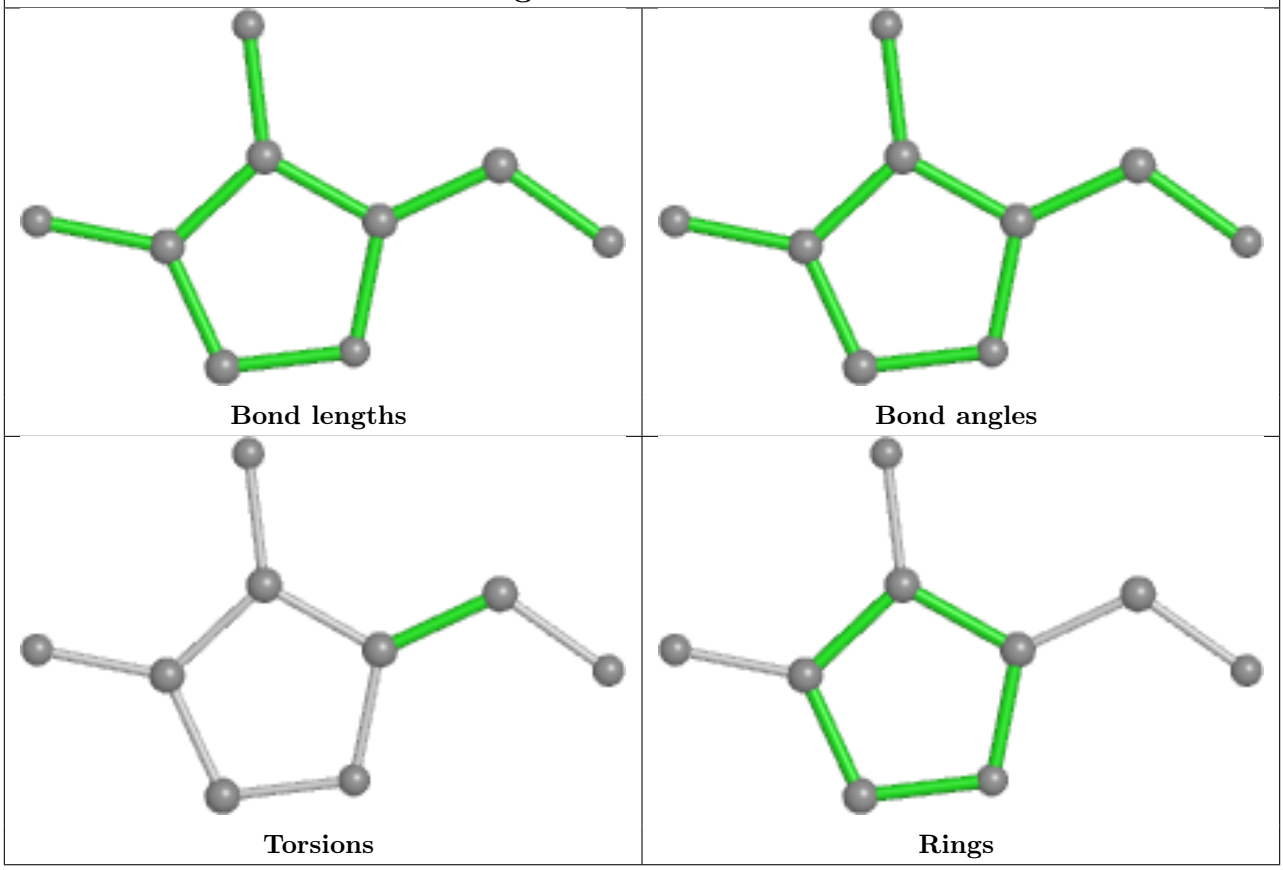
Ligand GLA C 2006	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA B 2009	
 Bond lengths	 Bond angles
 Torsions	 Rings

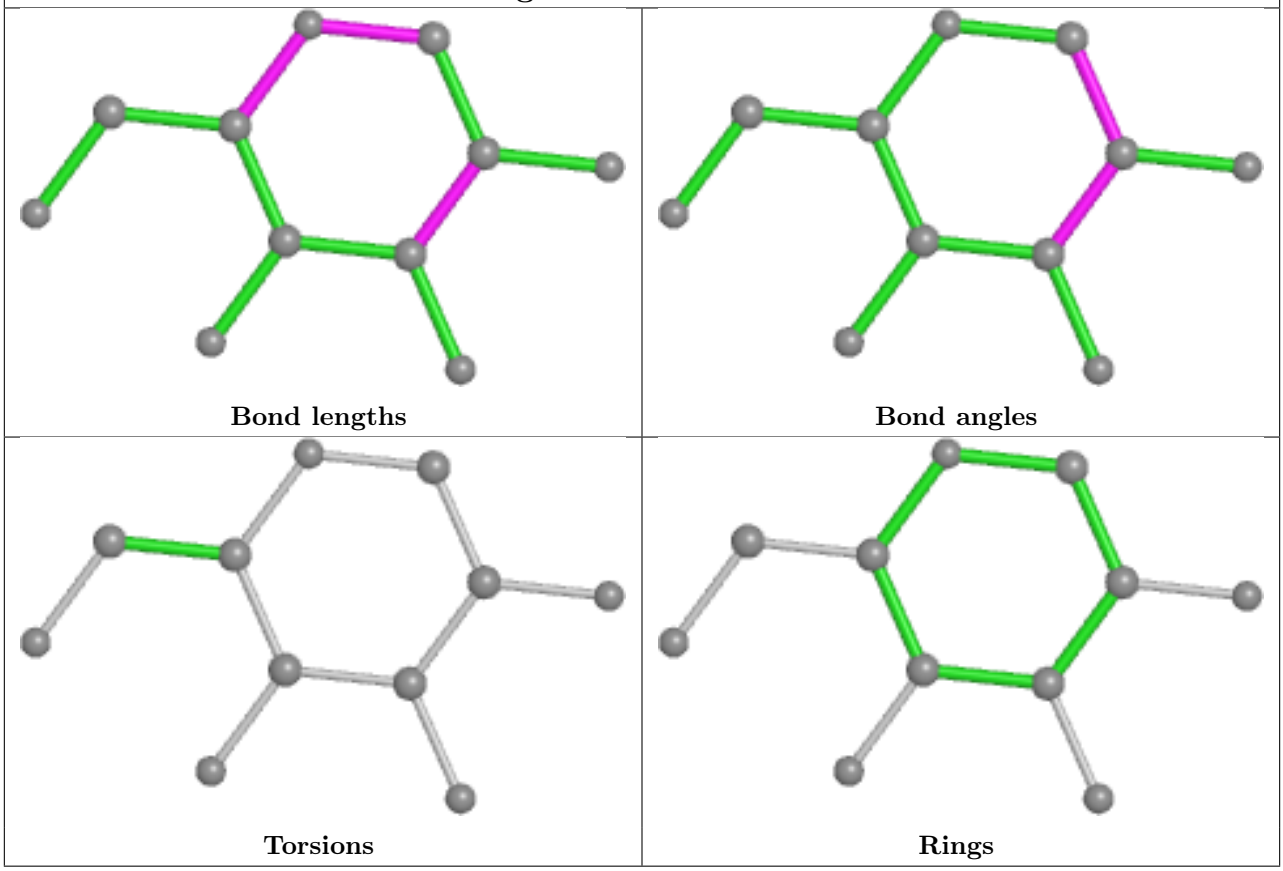
Ligand AHR C 2003

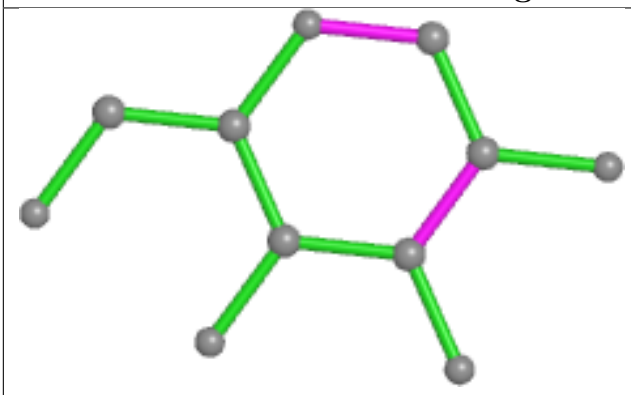
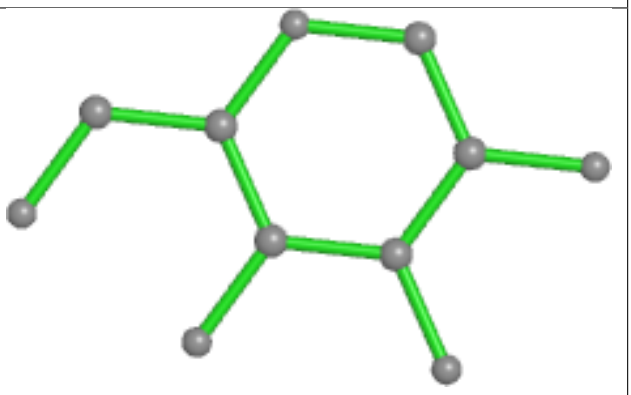
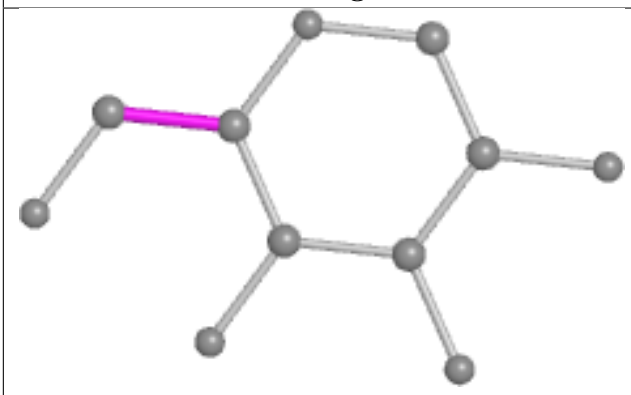
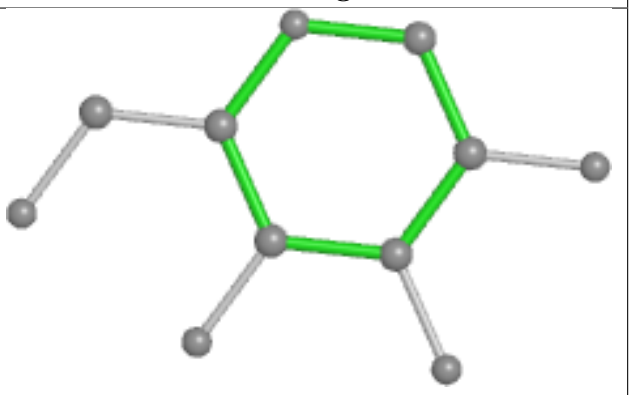


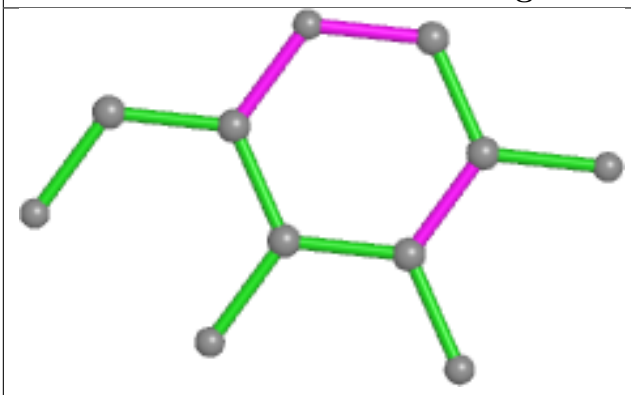
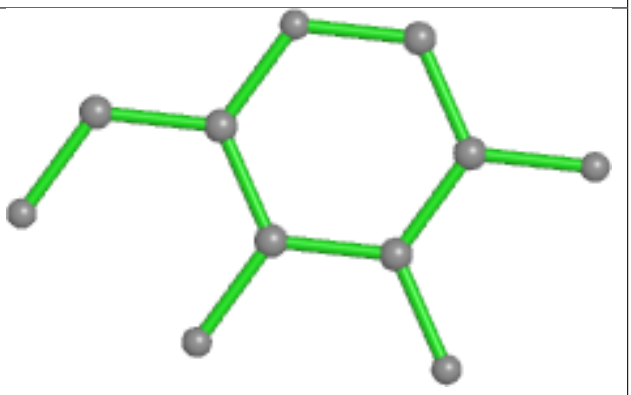
Ligand AHR F 2019



Ligand GLA E 2009



Ligand GLA B 2008	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA F 2018	
	
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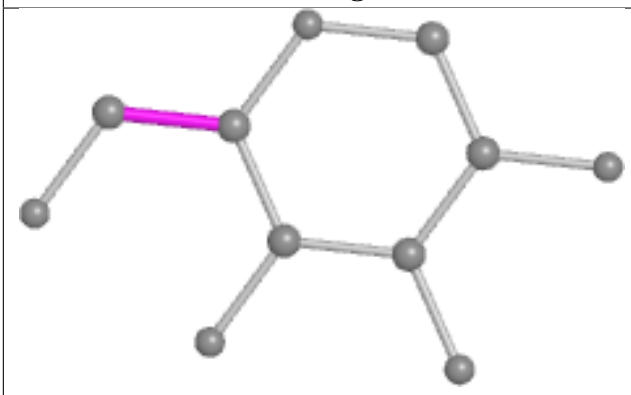
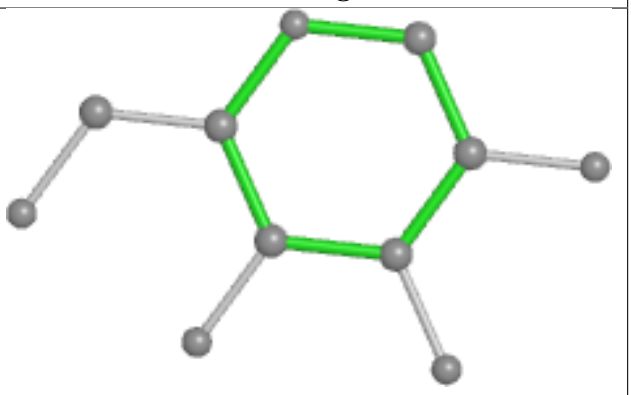
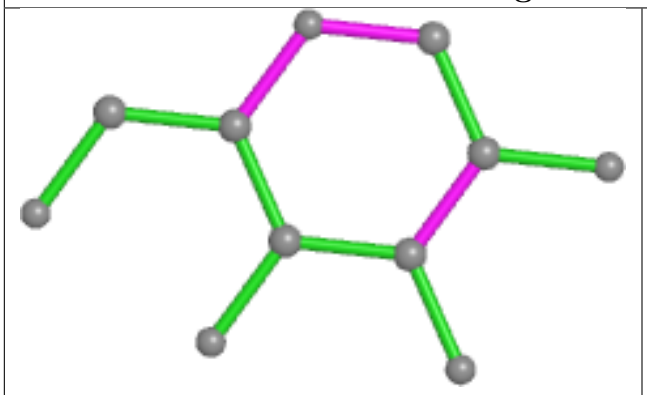
	
Torsions	**Rings**

Ligand GLA A 2012



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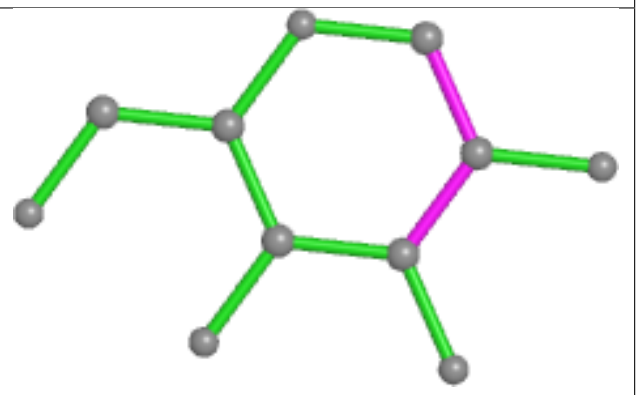

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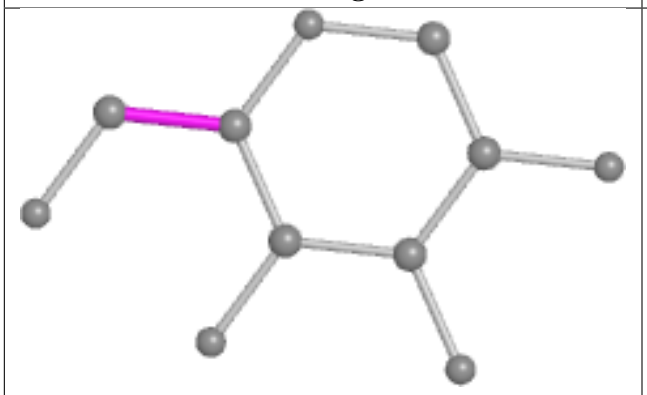

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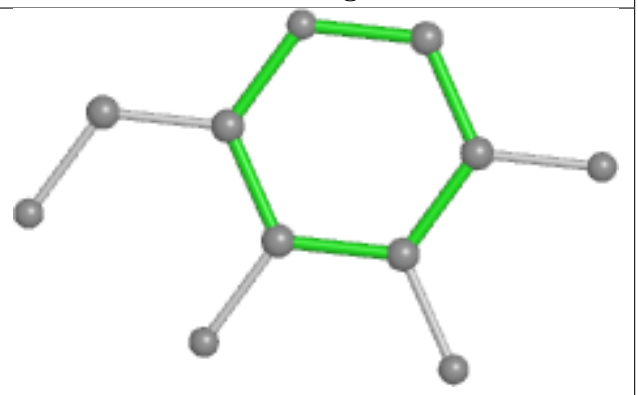
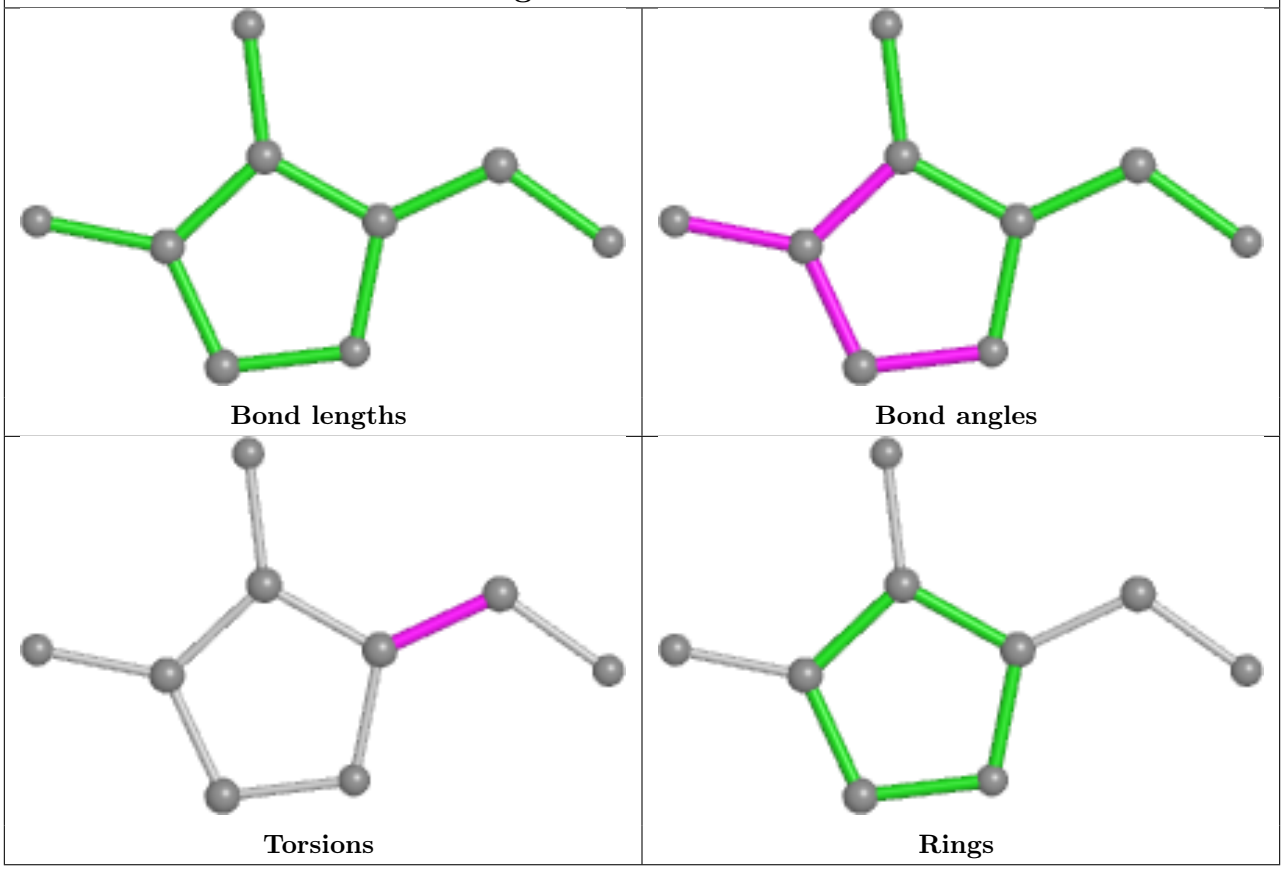
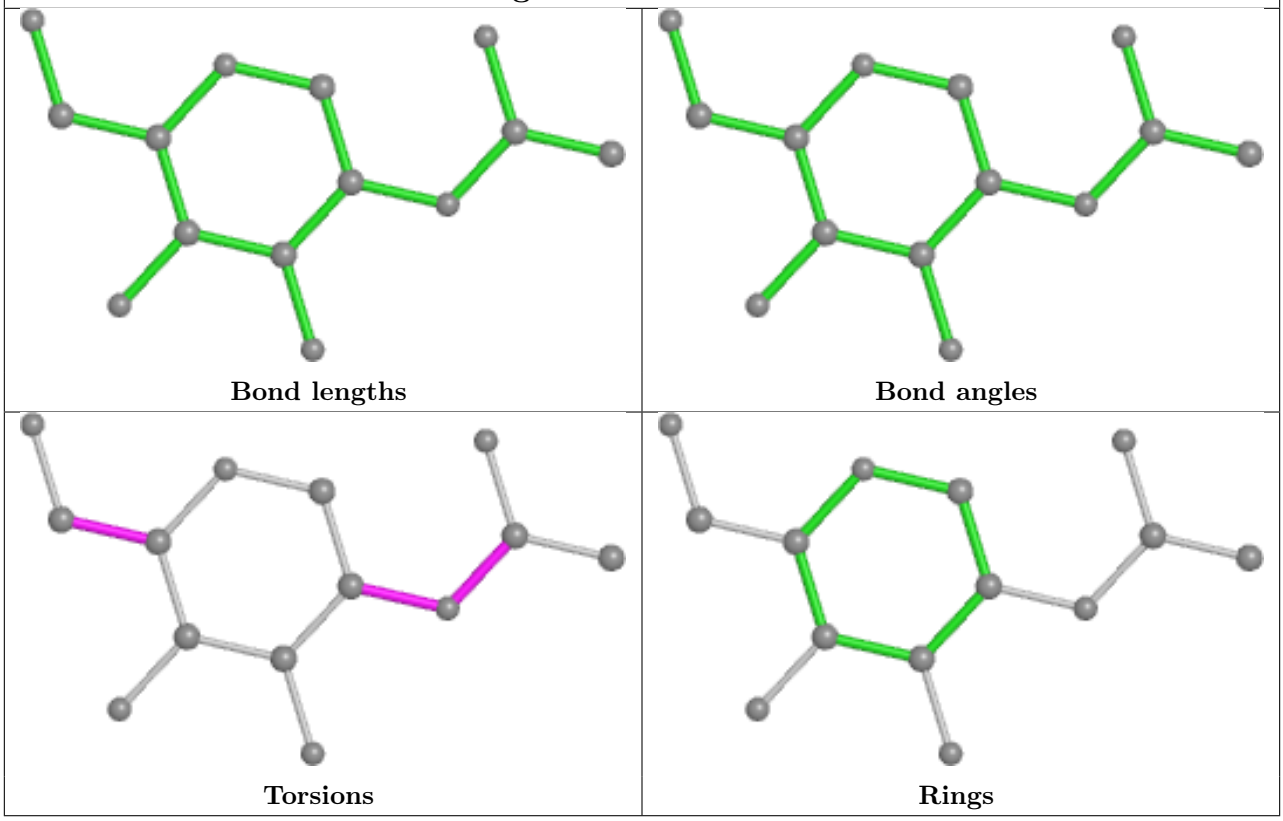


Rings

Ligand AHR F 2004



Ligand NAG B 2018



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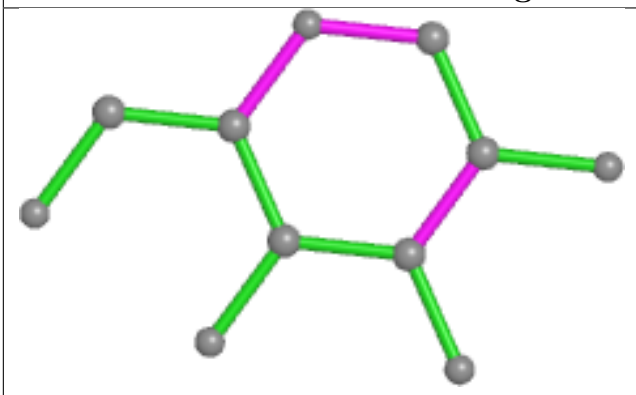
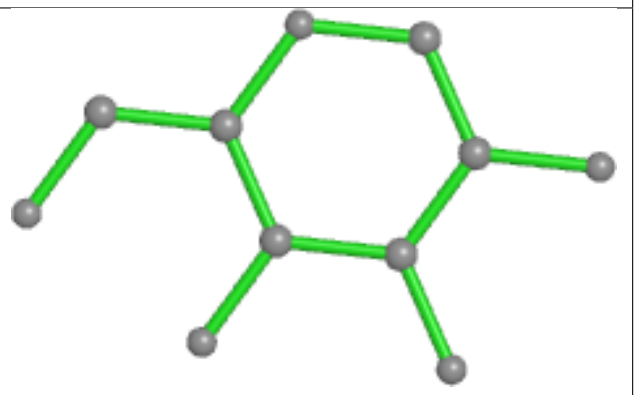
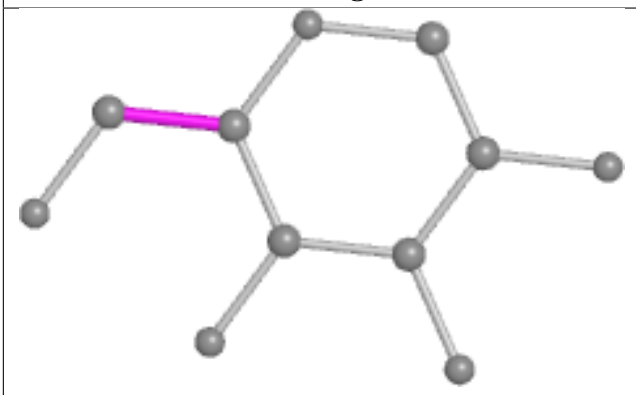
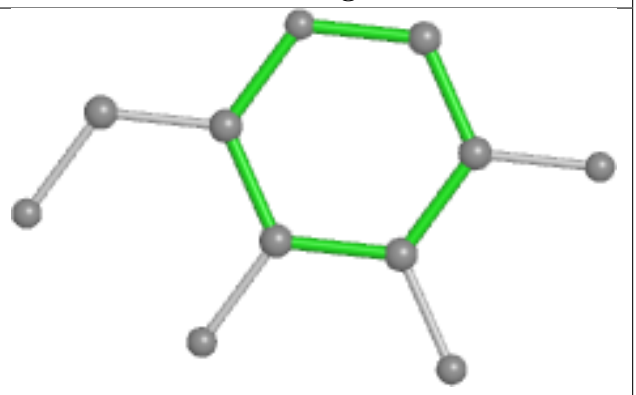
 Bond lengths	 Bond angles
 Torsions	 Rings

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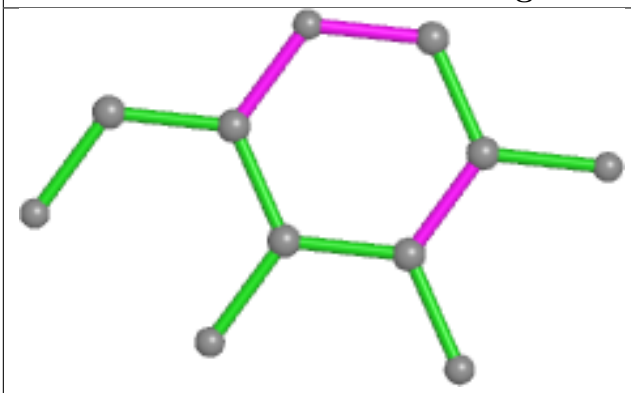
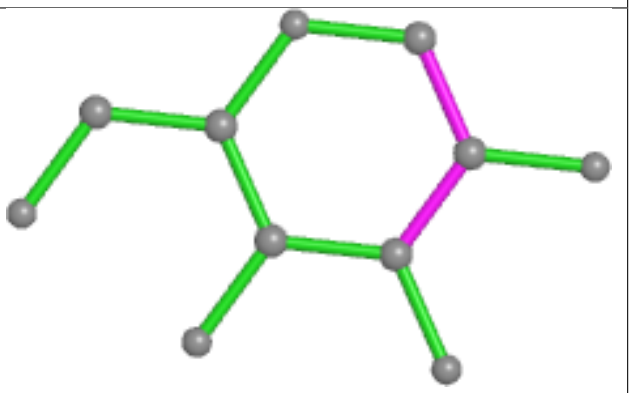
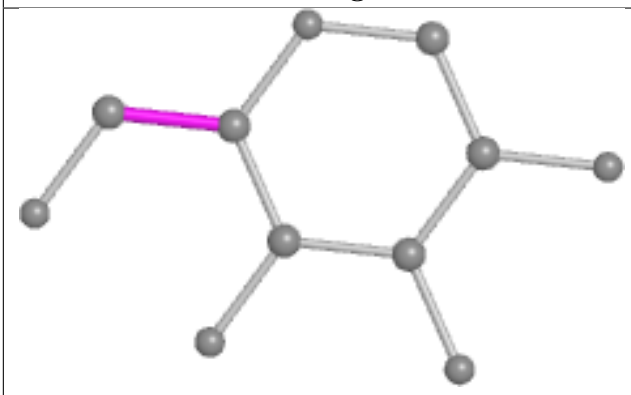
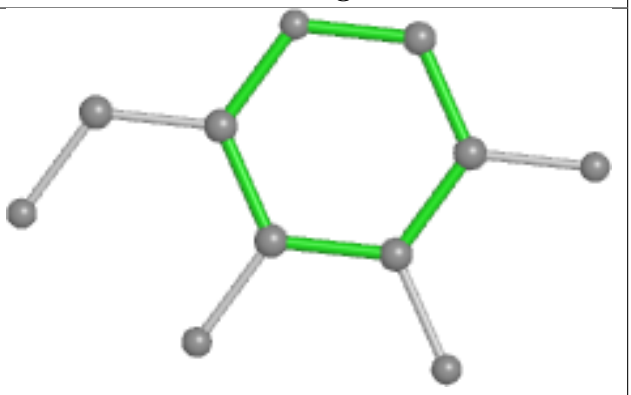
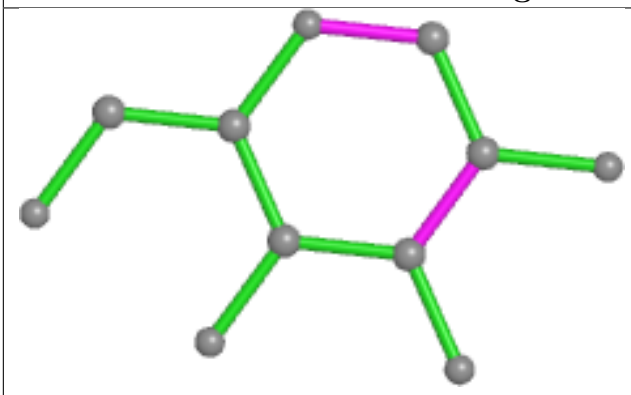
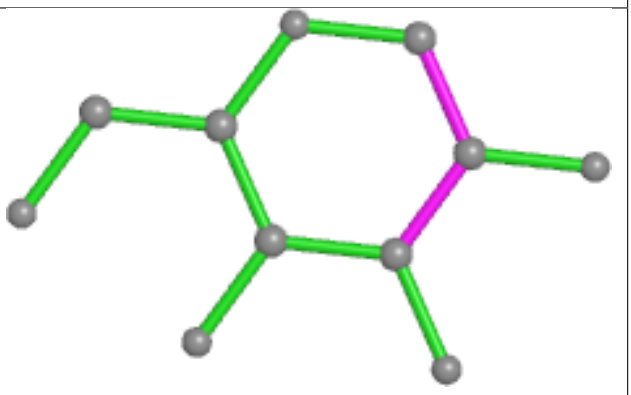
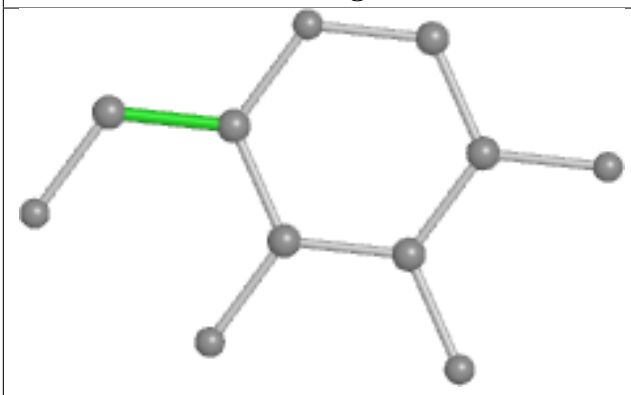
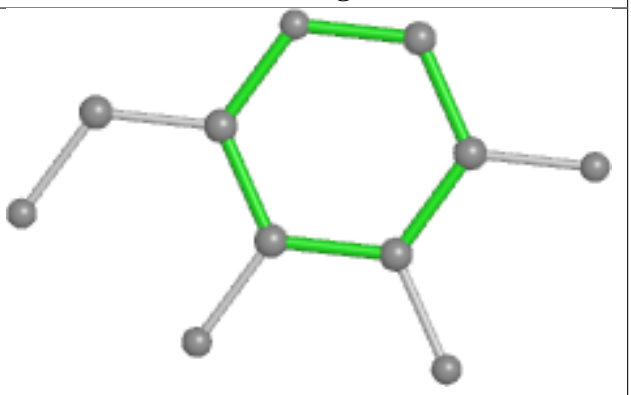
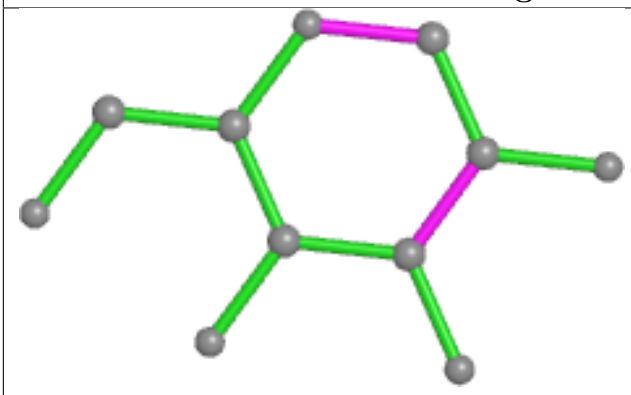
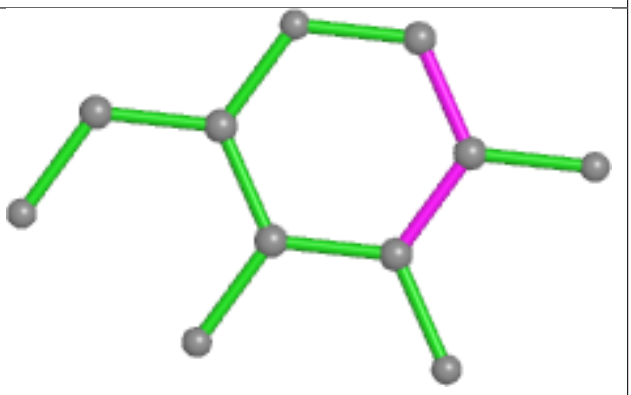
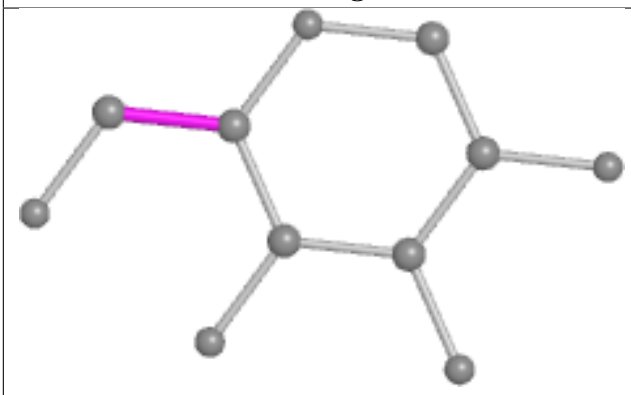
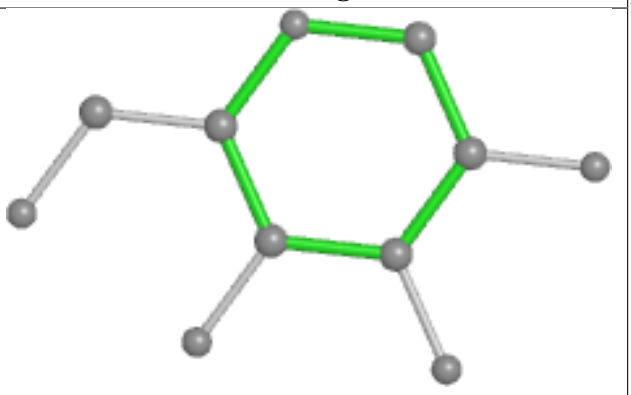
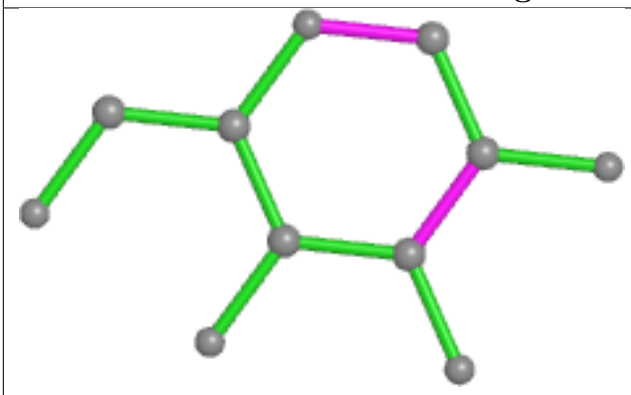
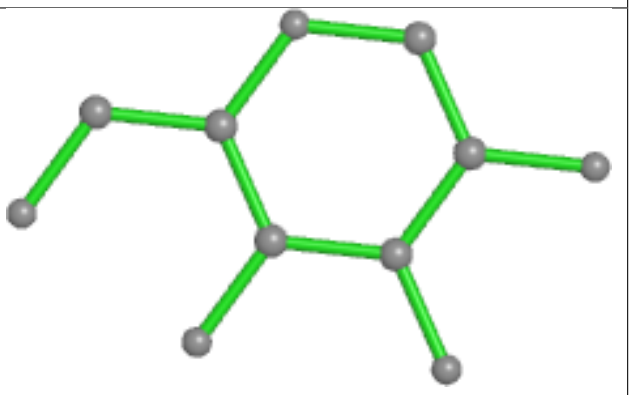
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA A 2005	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA E 2012	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA B 2015	
	
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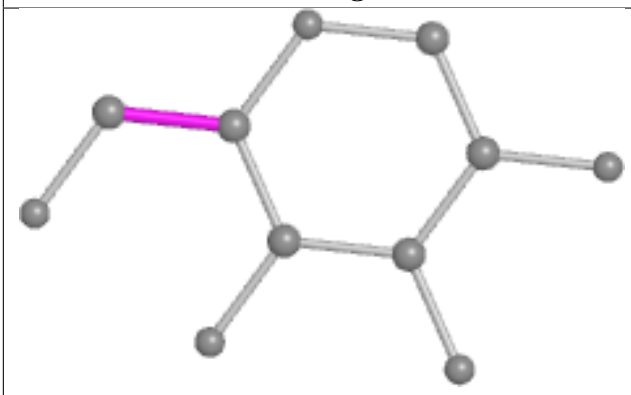	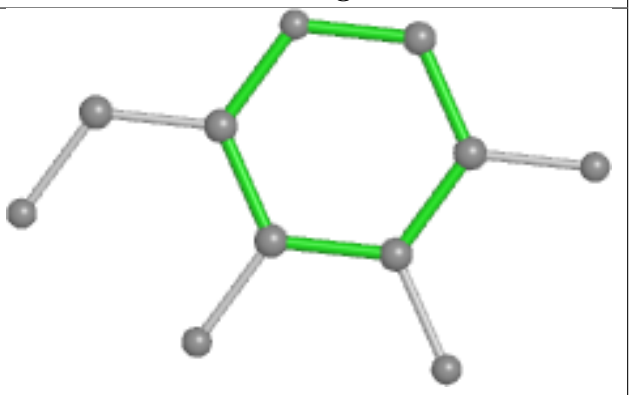
Torsions	**Rings**

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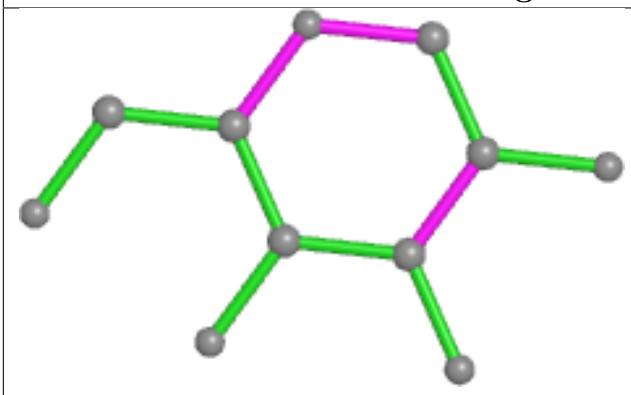
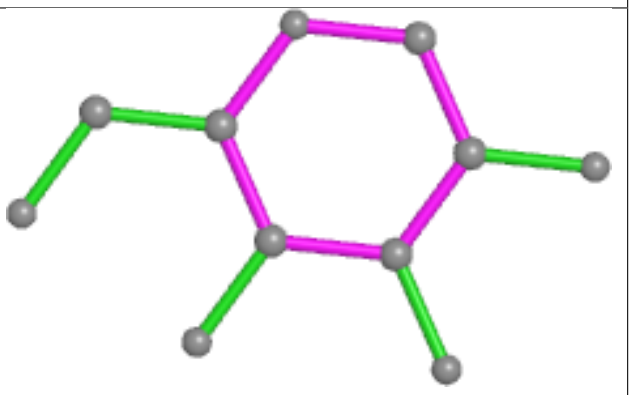
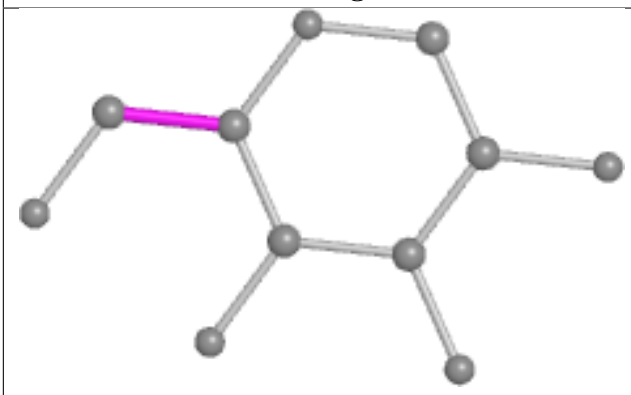
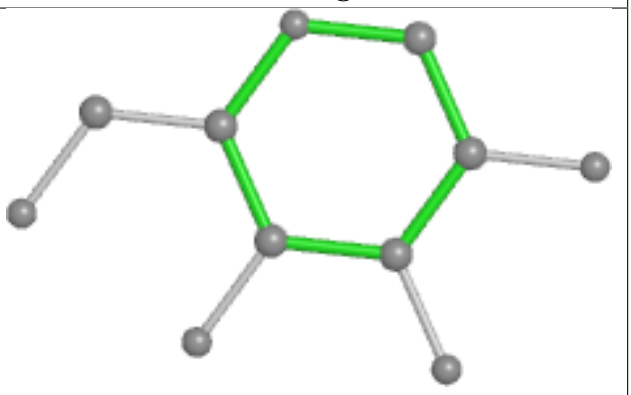
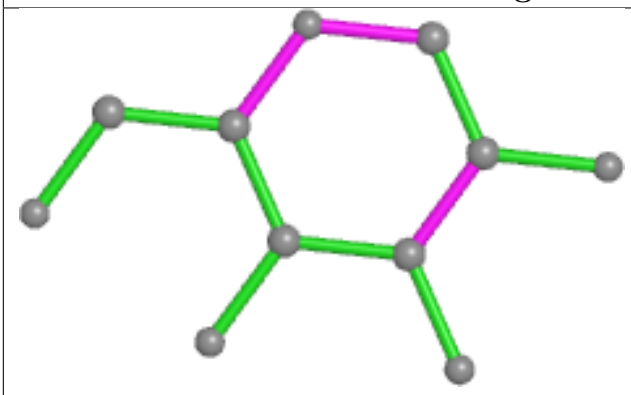
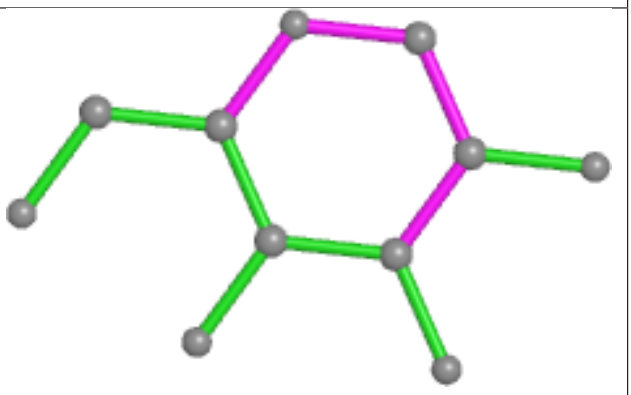
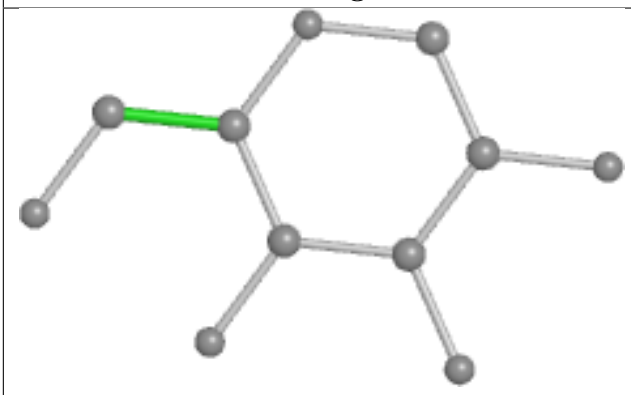
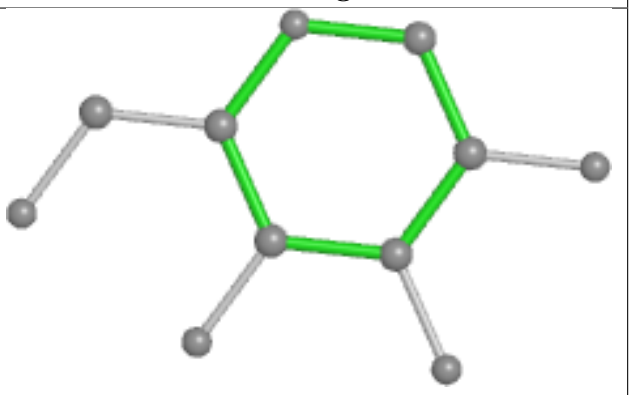
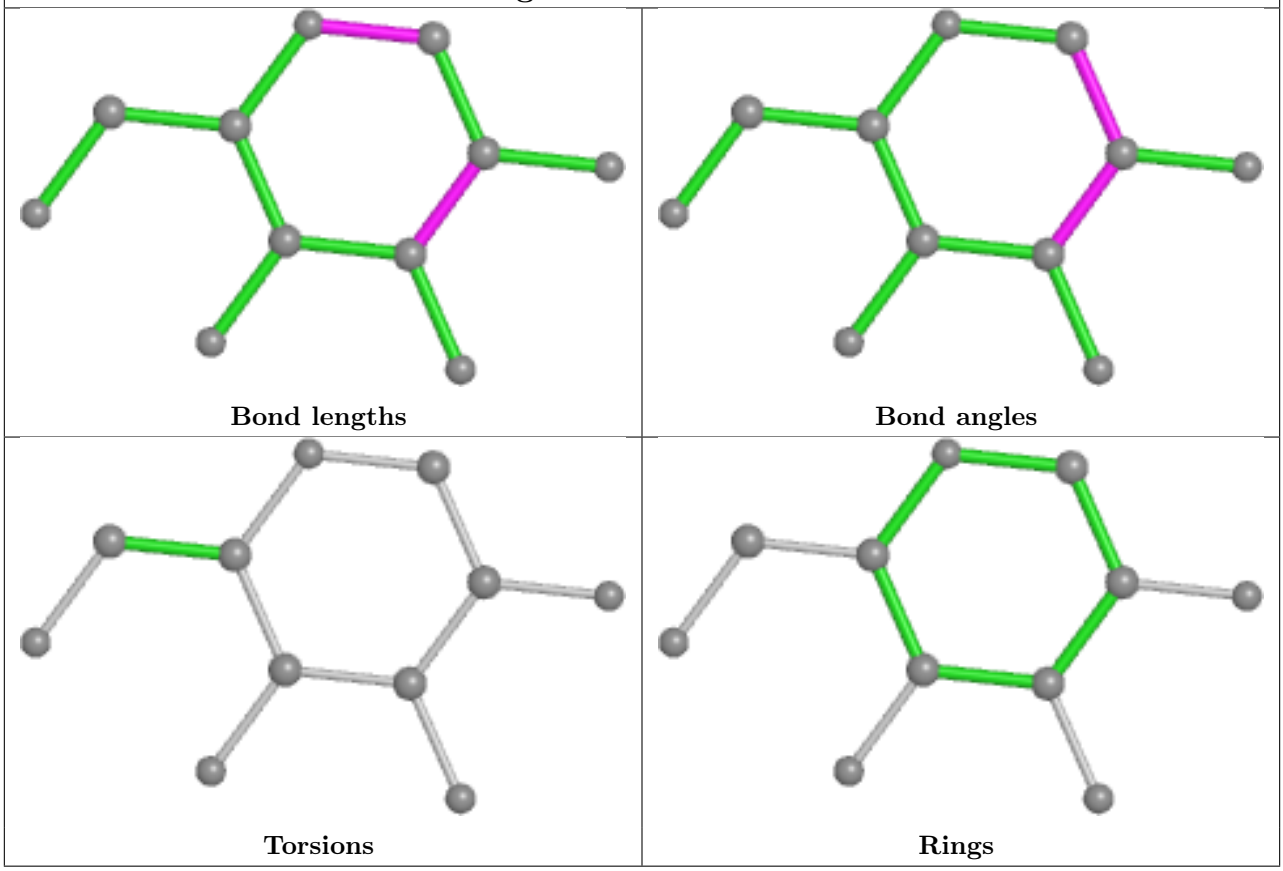
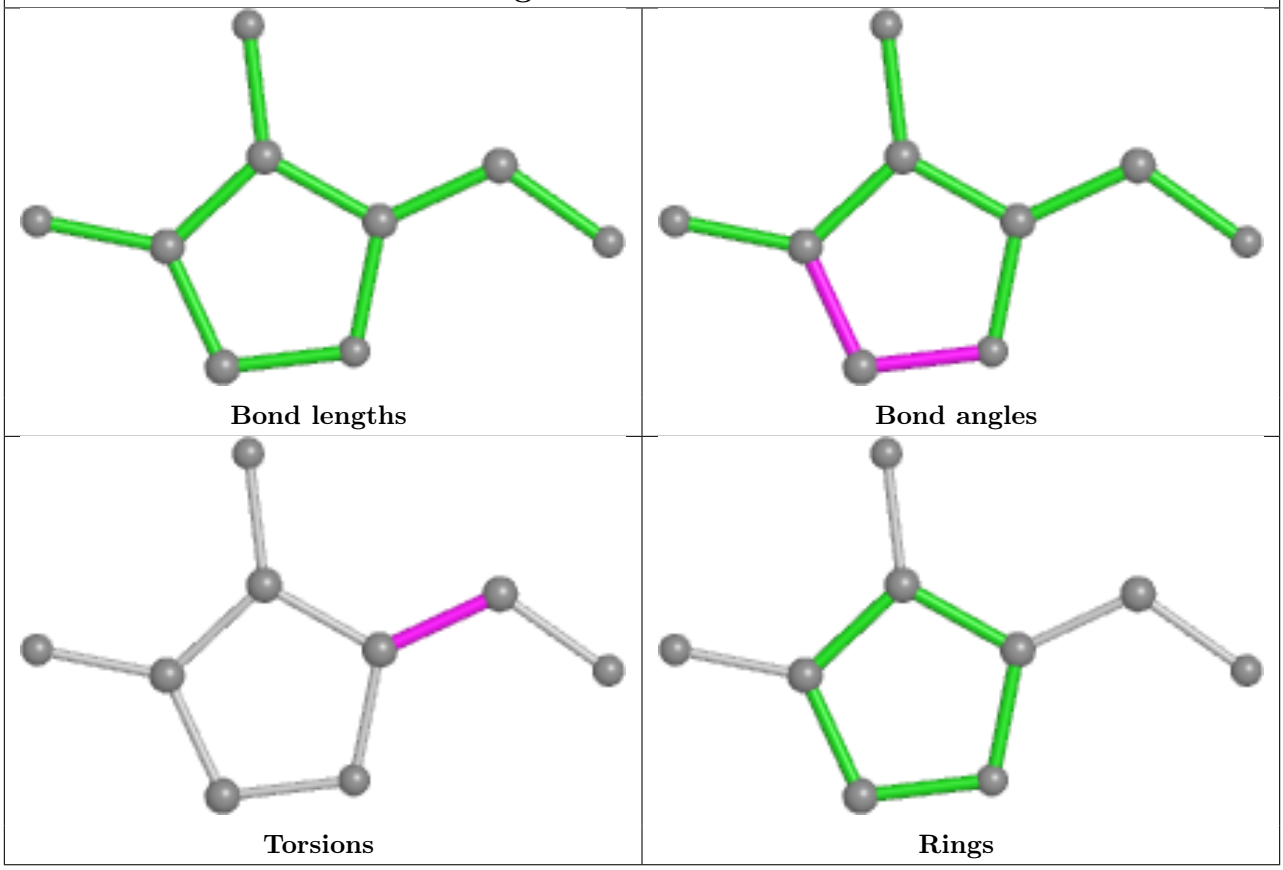
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA B 2005	
 Bond lengths	 Bond angles
 Torsions	 Rings

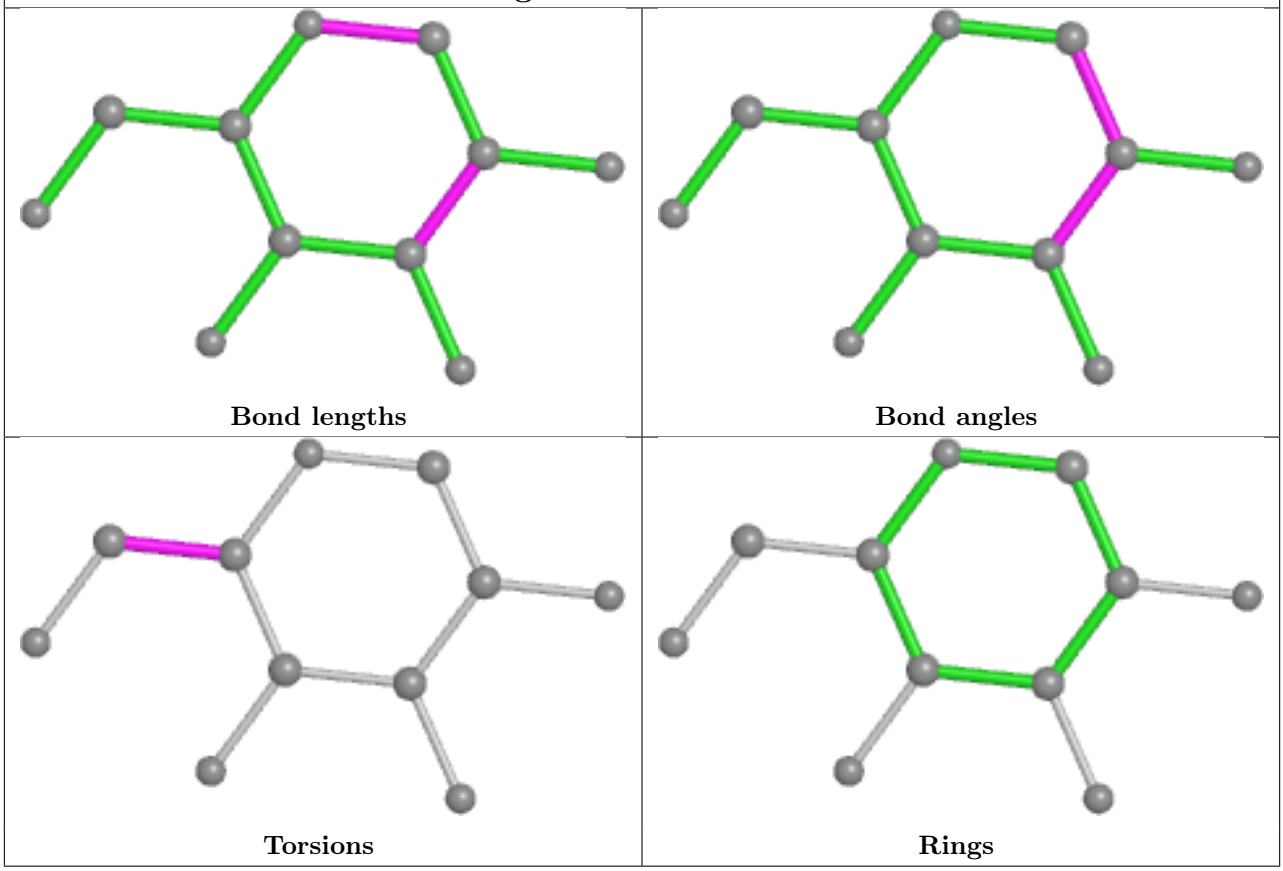
Ligand GLA E 2015



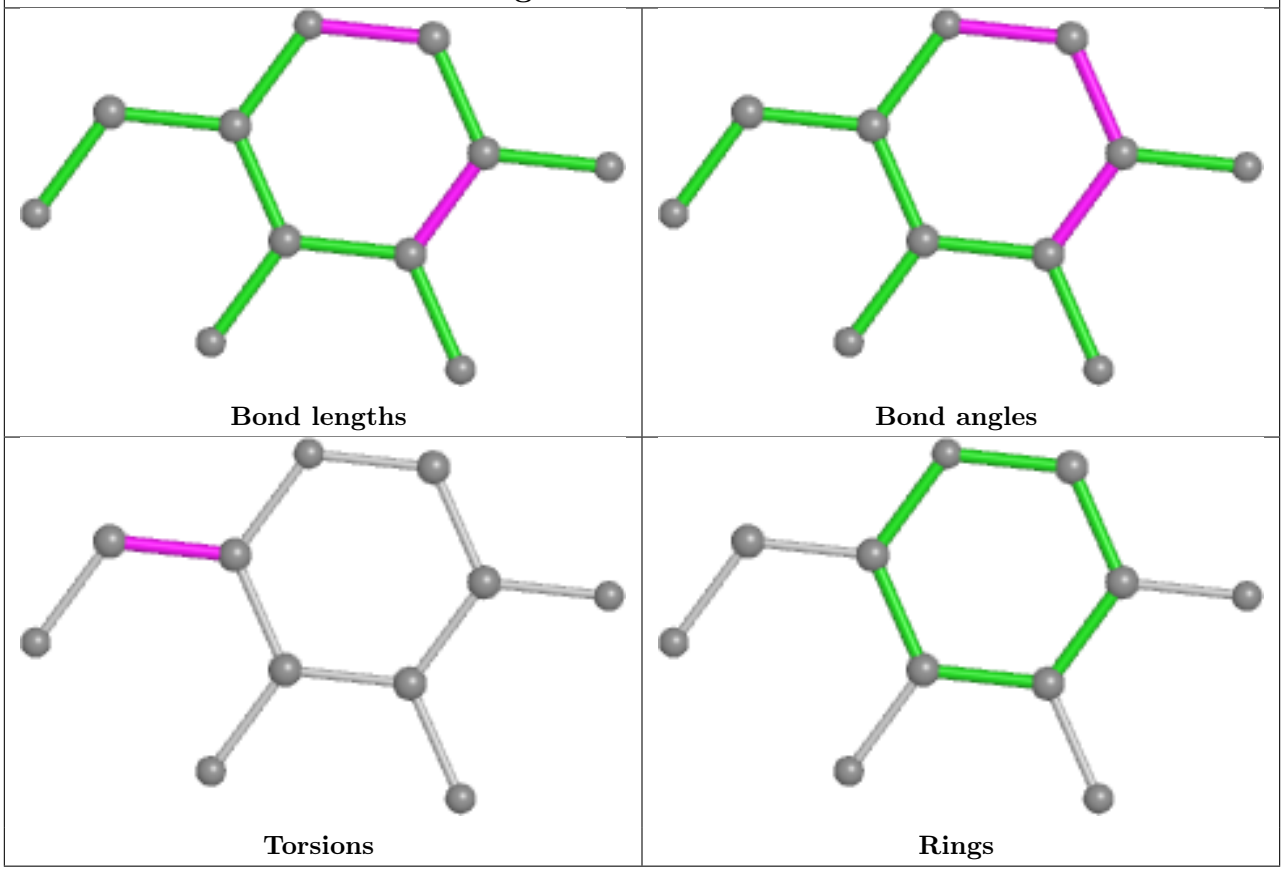
Ligand AHR F 2003



Ligand GLA A 2016



Ligand GLA A 2008



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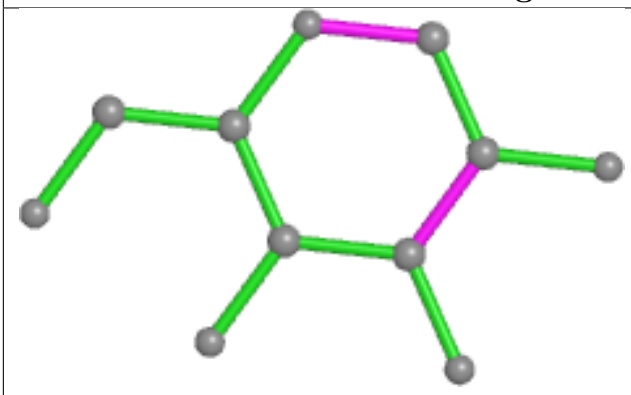
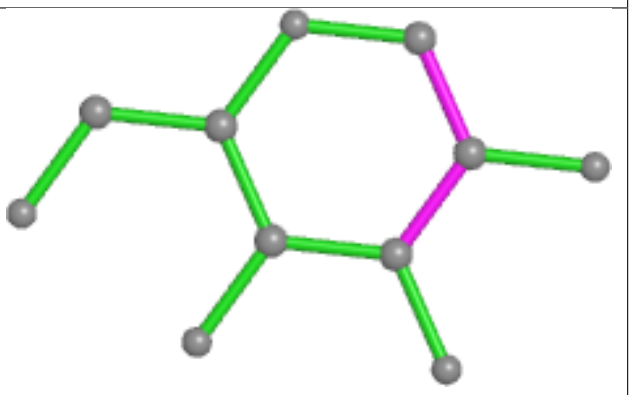
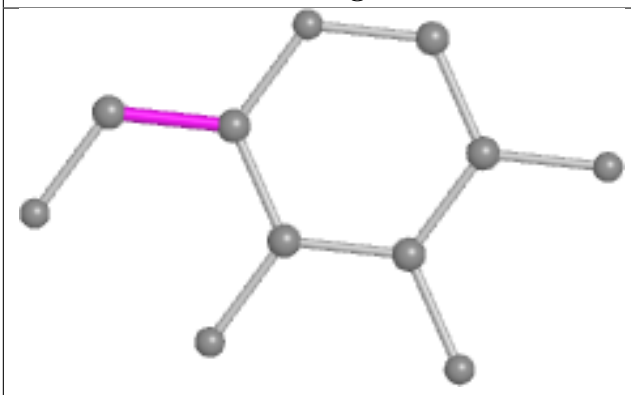
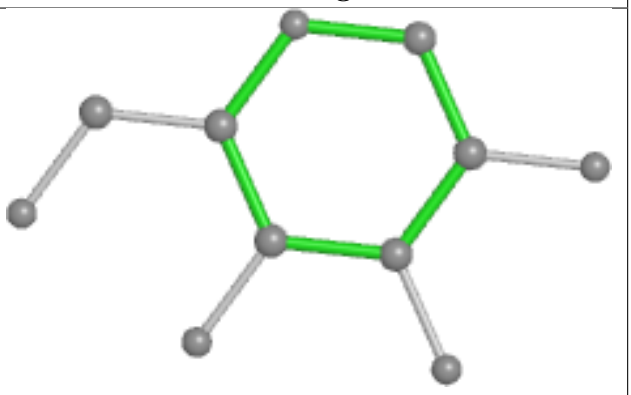
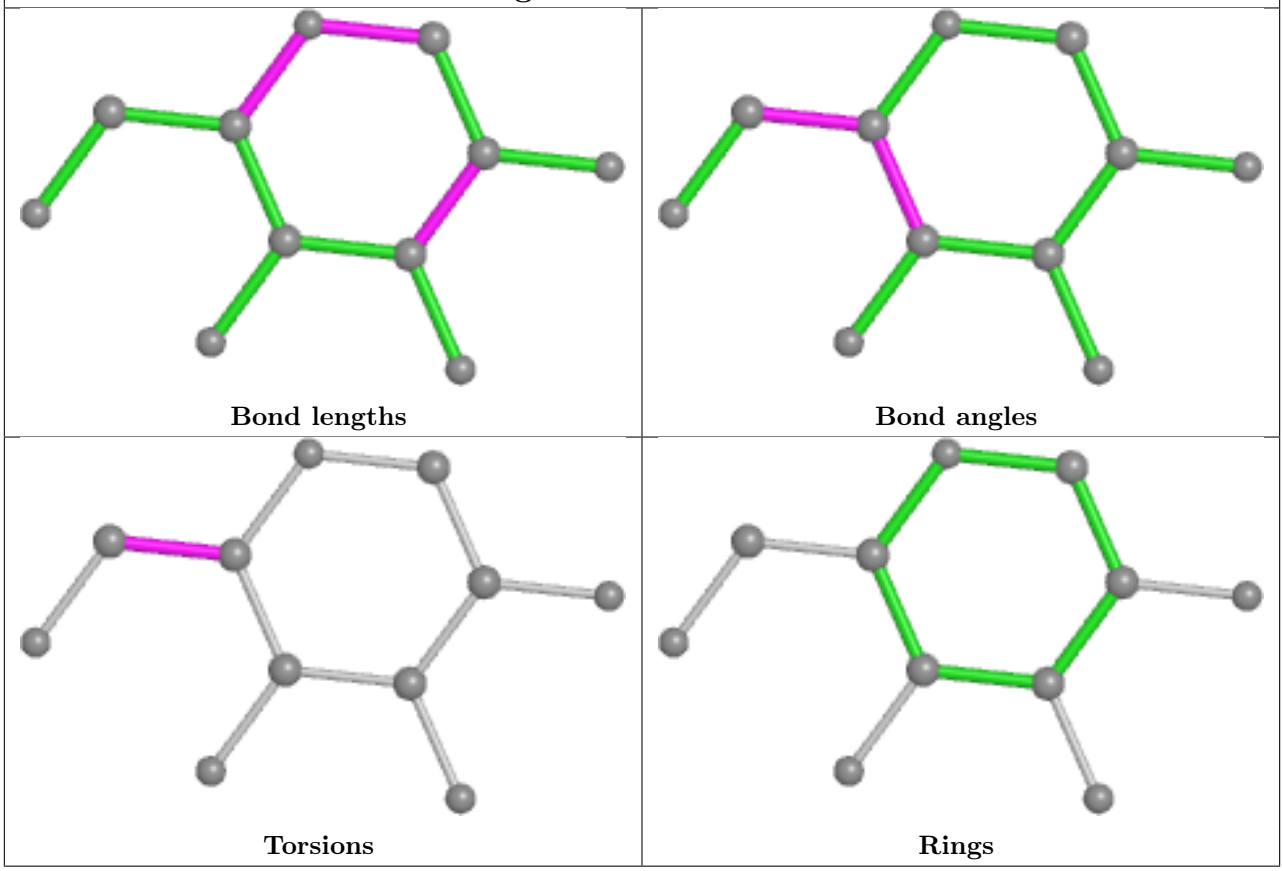
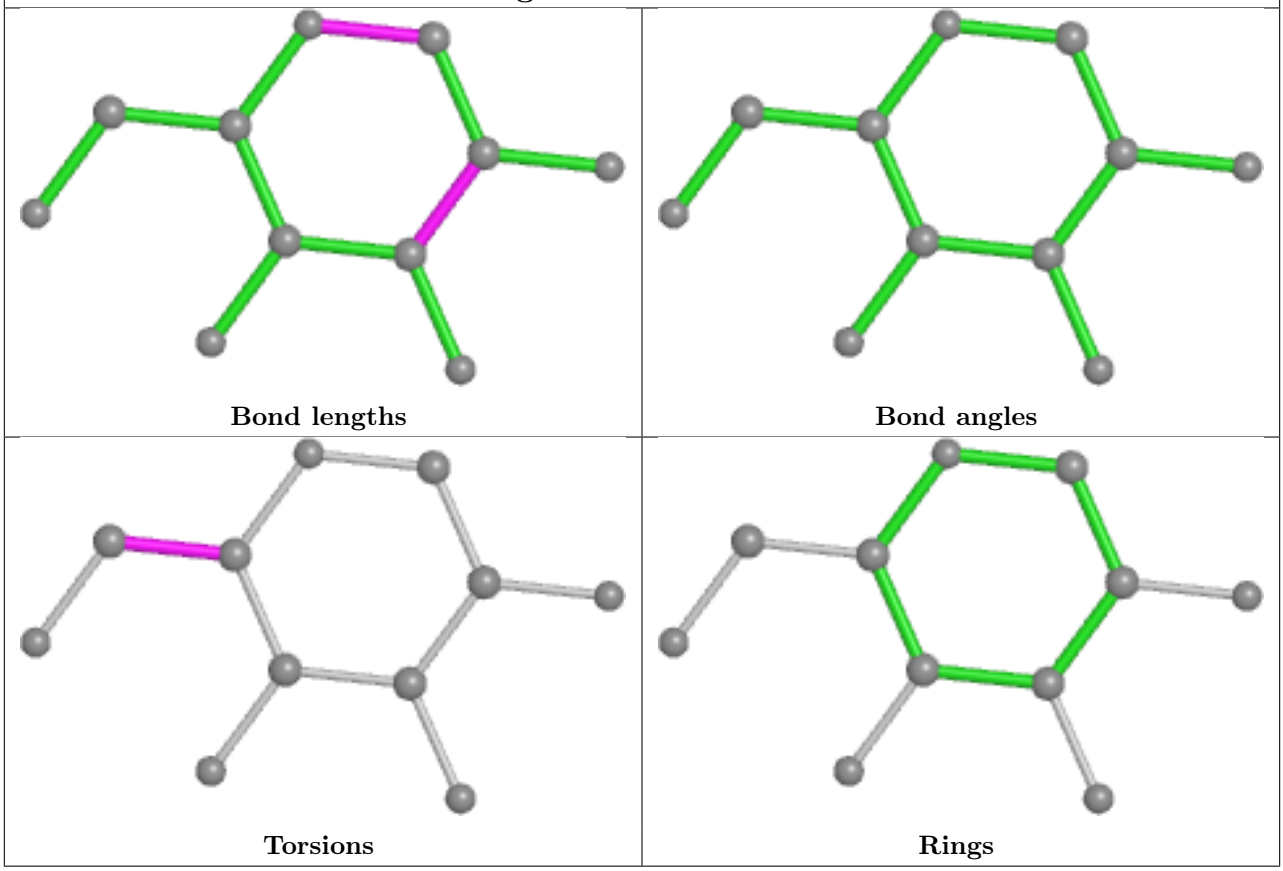
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA A 2011



Ligand GLA E 2014



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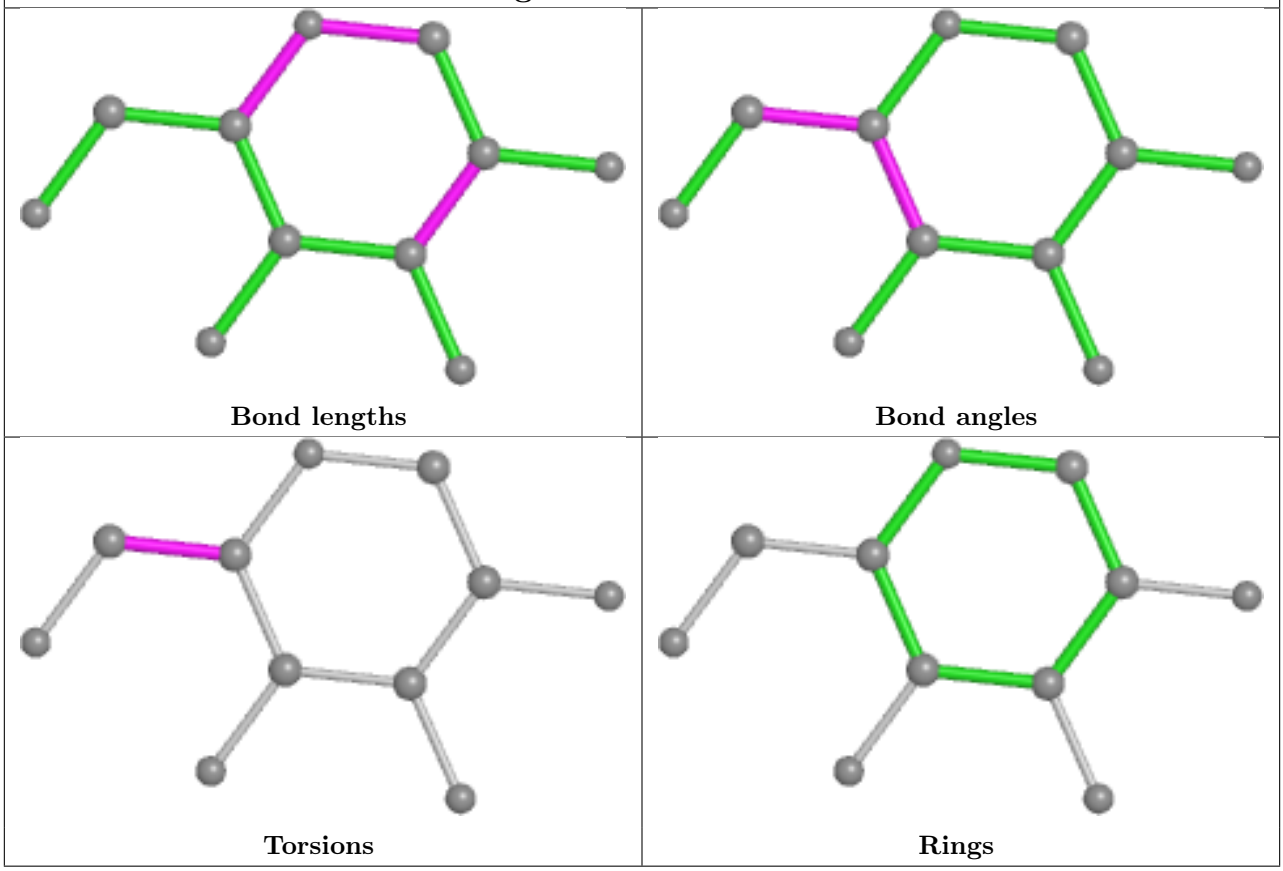
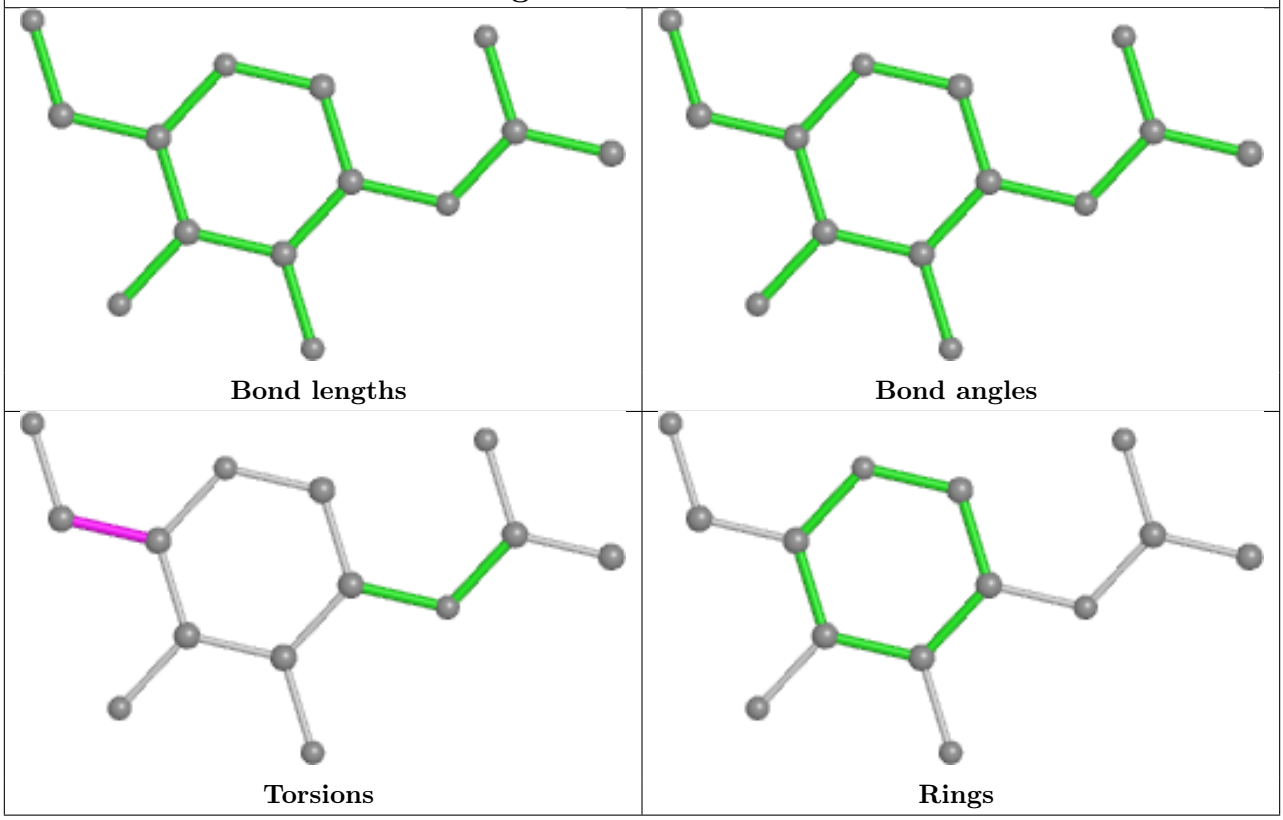
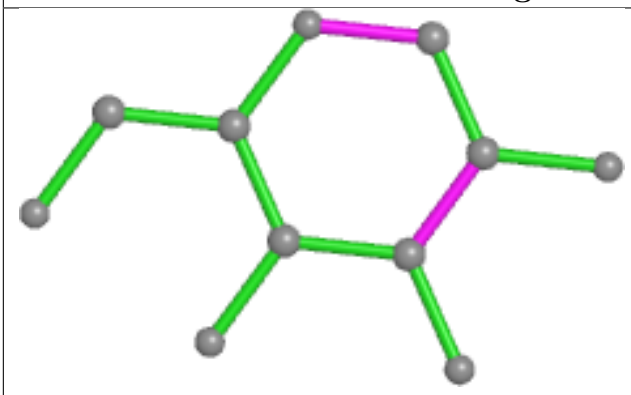
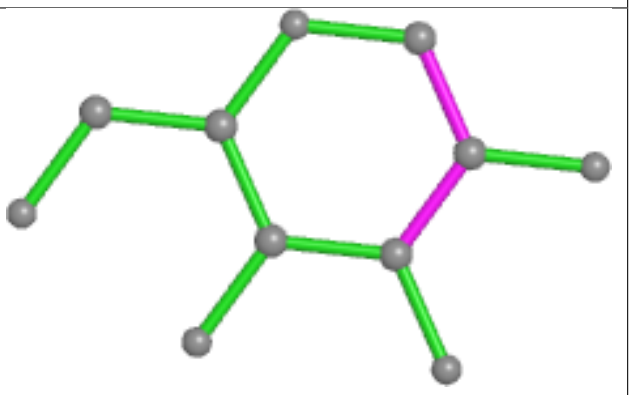
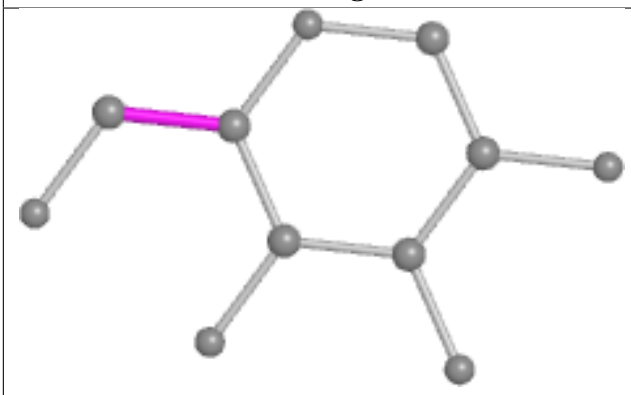
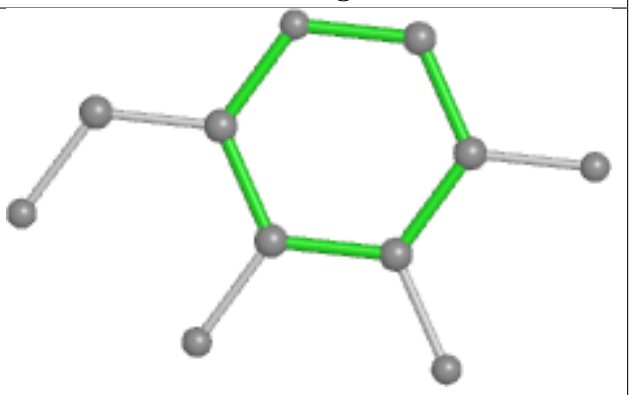
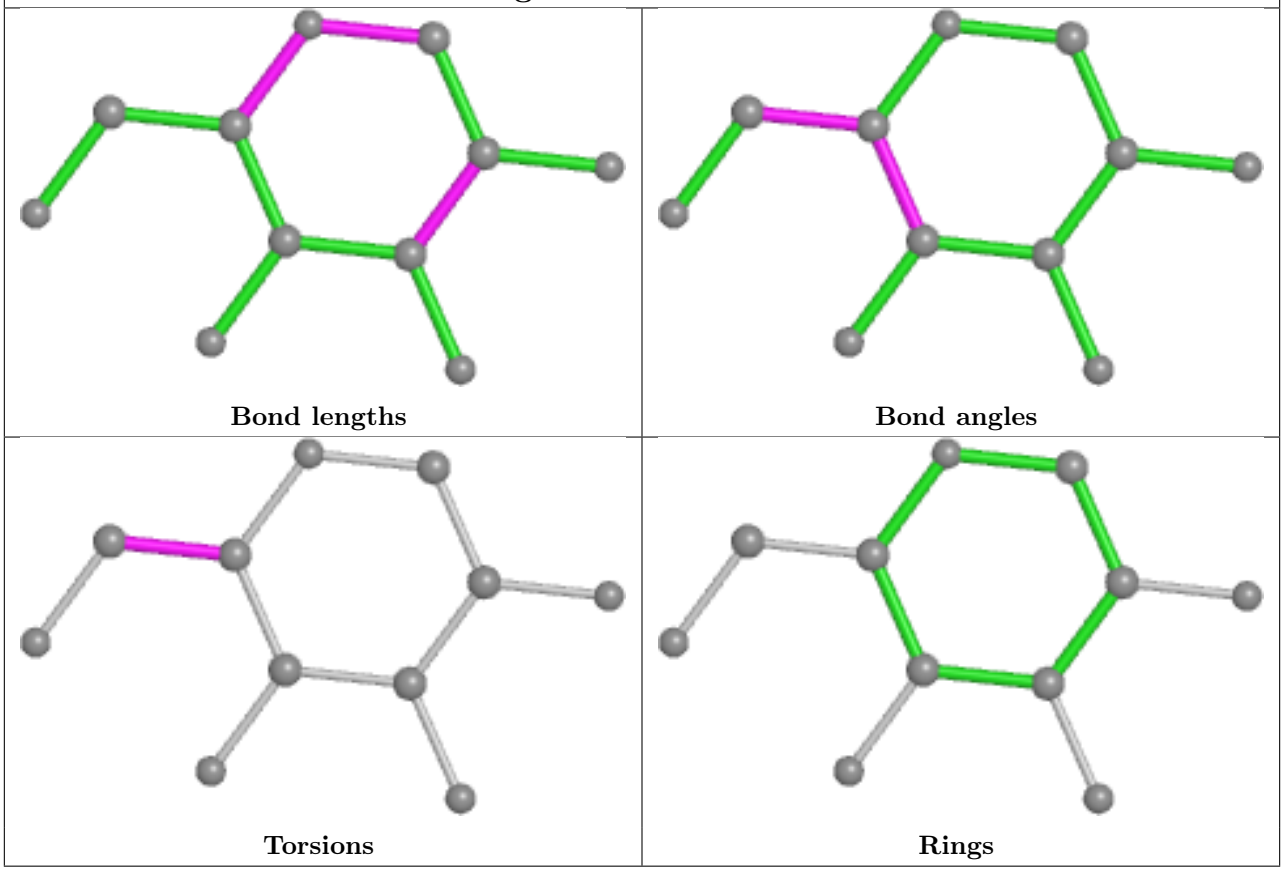


Ligand NAG A 2017

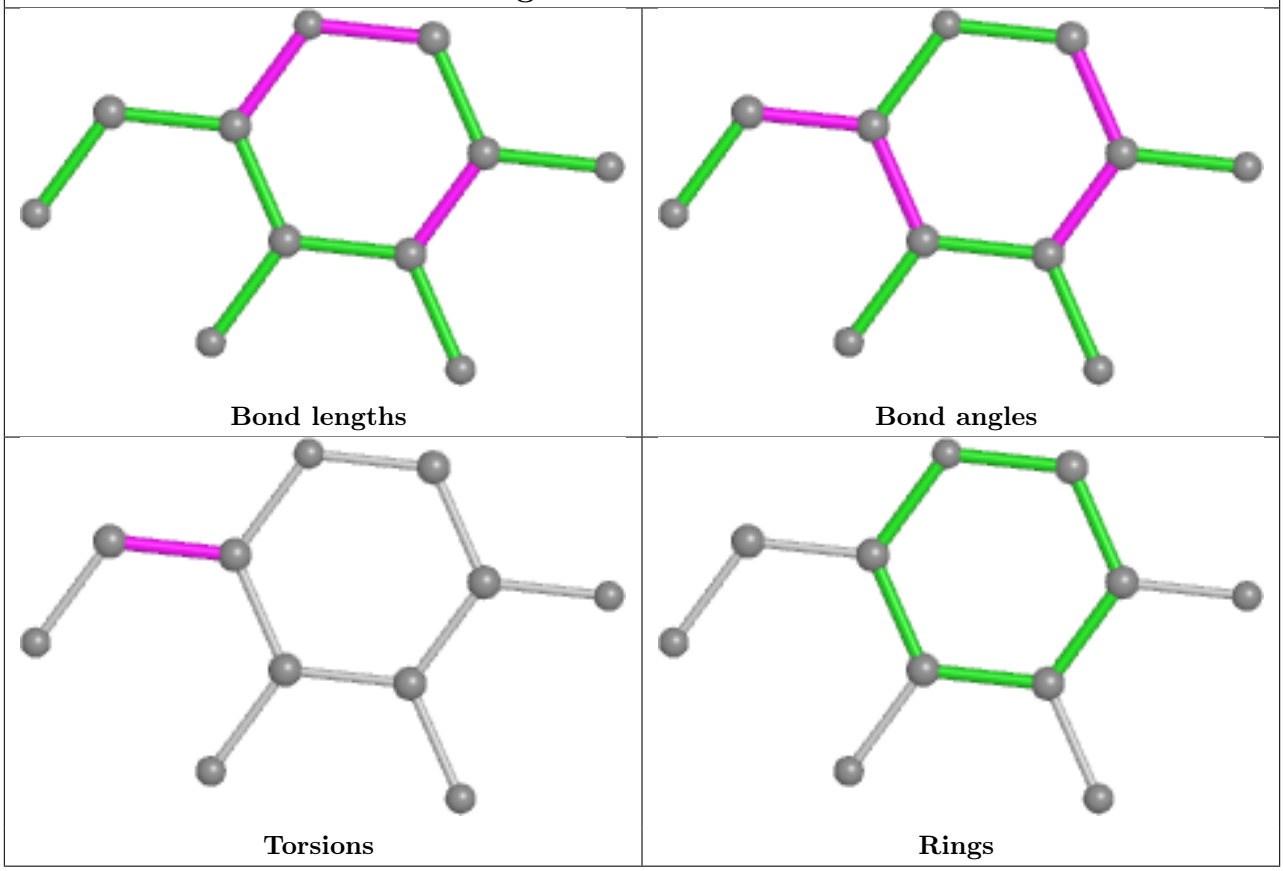


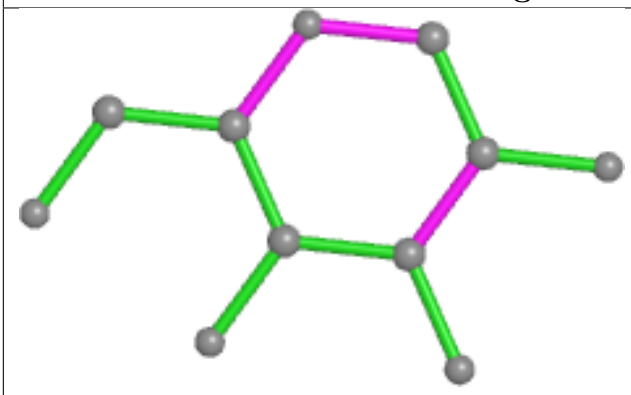
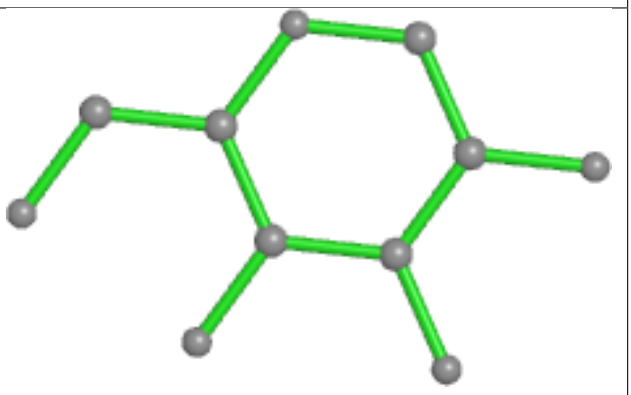
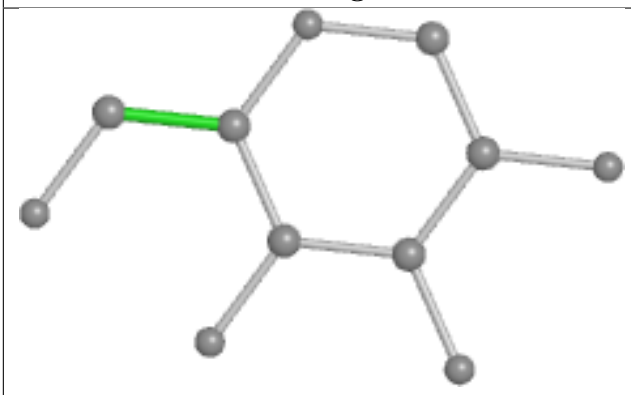
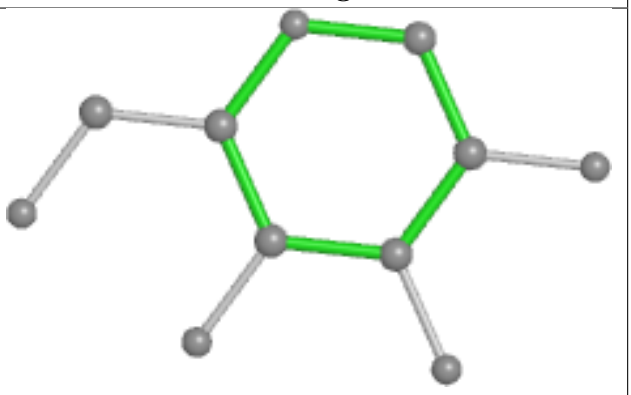
Ligand GLA C 2005	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA A 2010

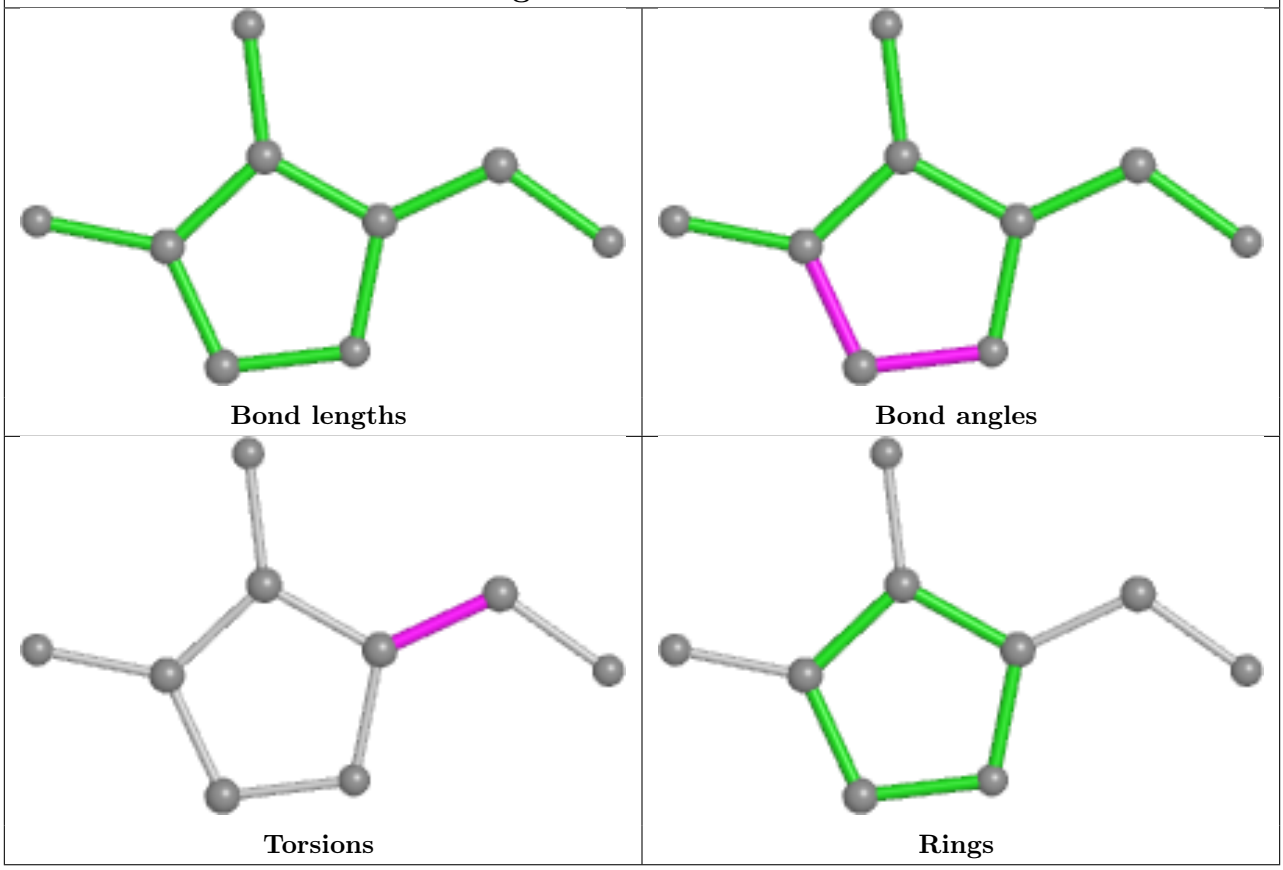


Ligand GLA F 2008

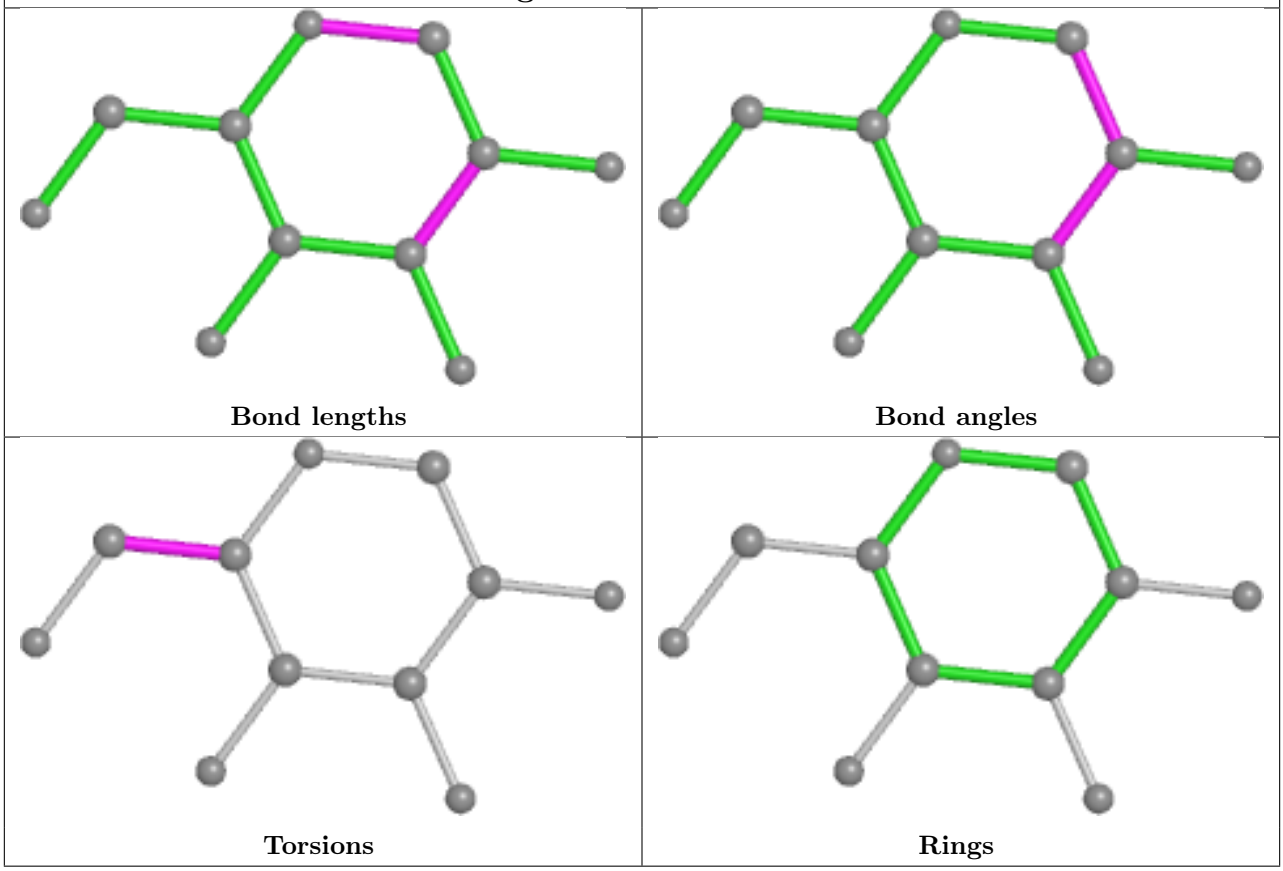


Ligand GLA A 2013	
 Bond lengths	 Bond angles
 Torsions	 Rings

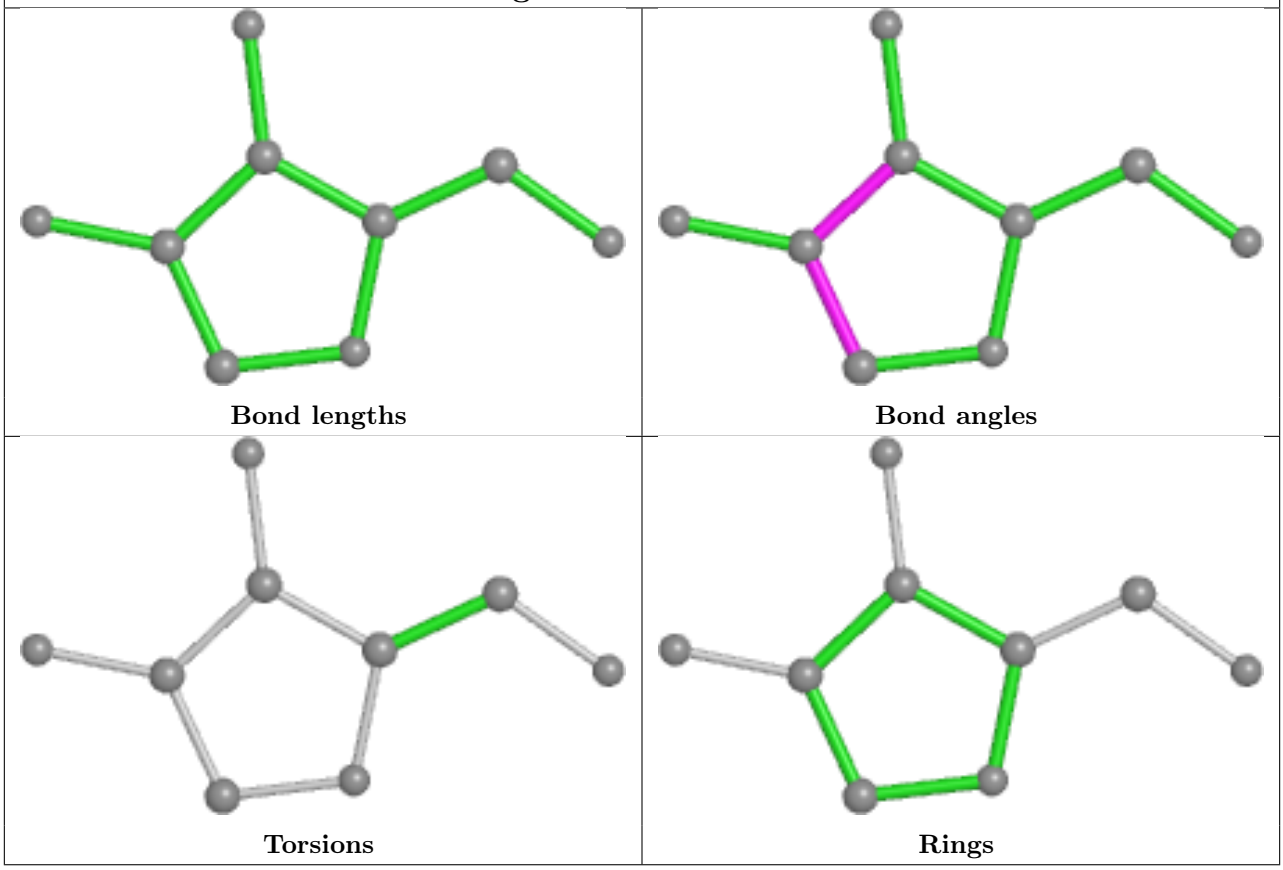
Ligand AHR C 2001



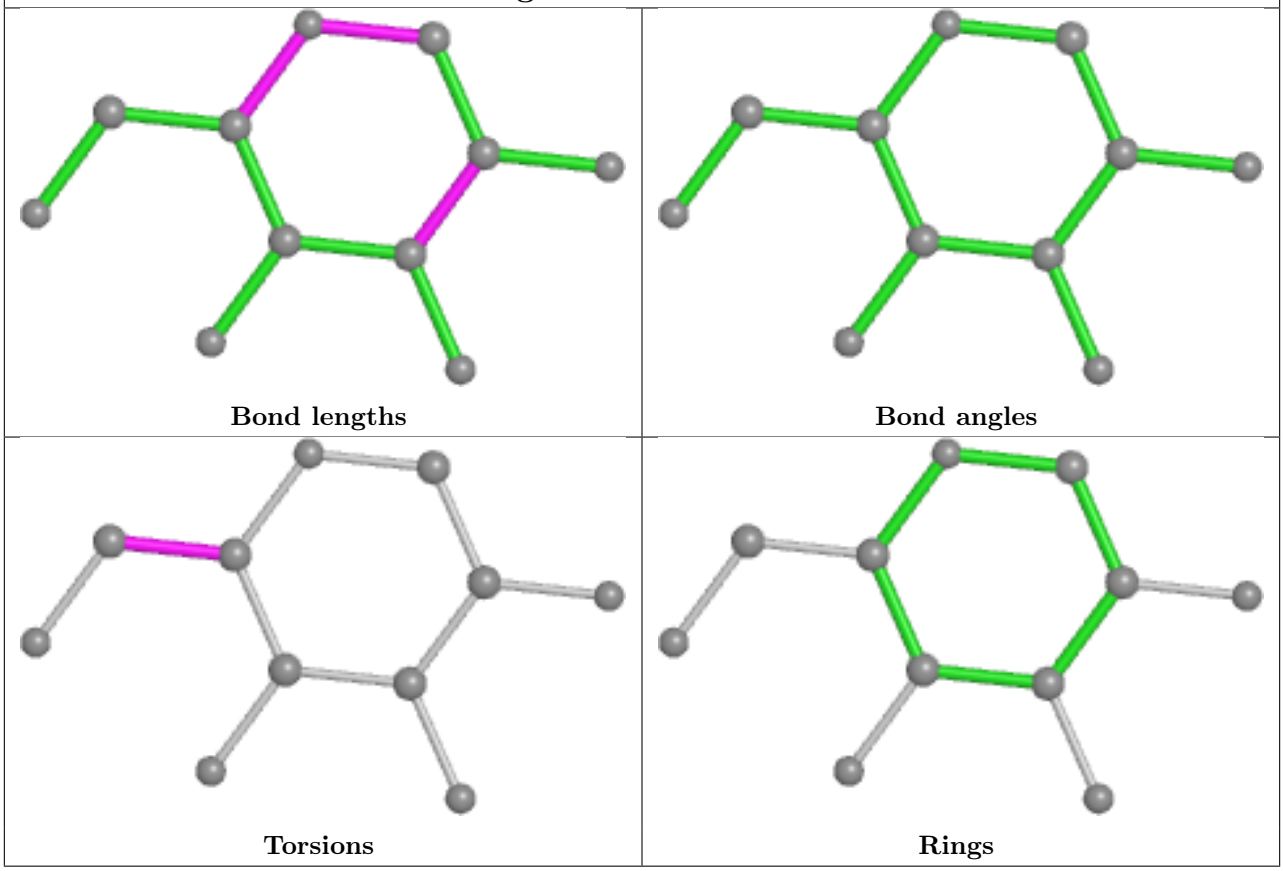
Ligand GLA F 2016



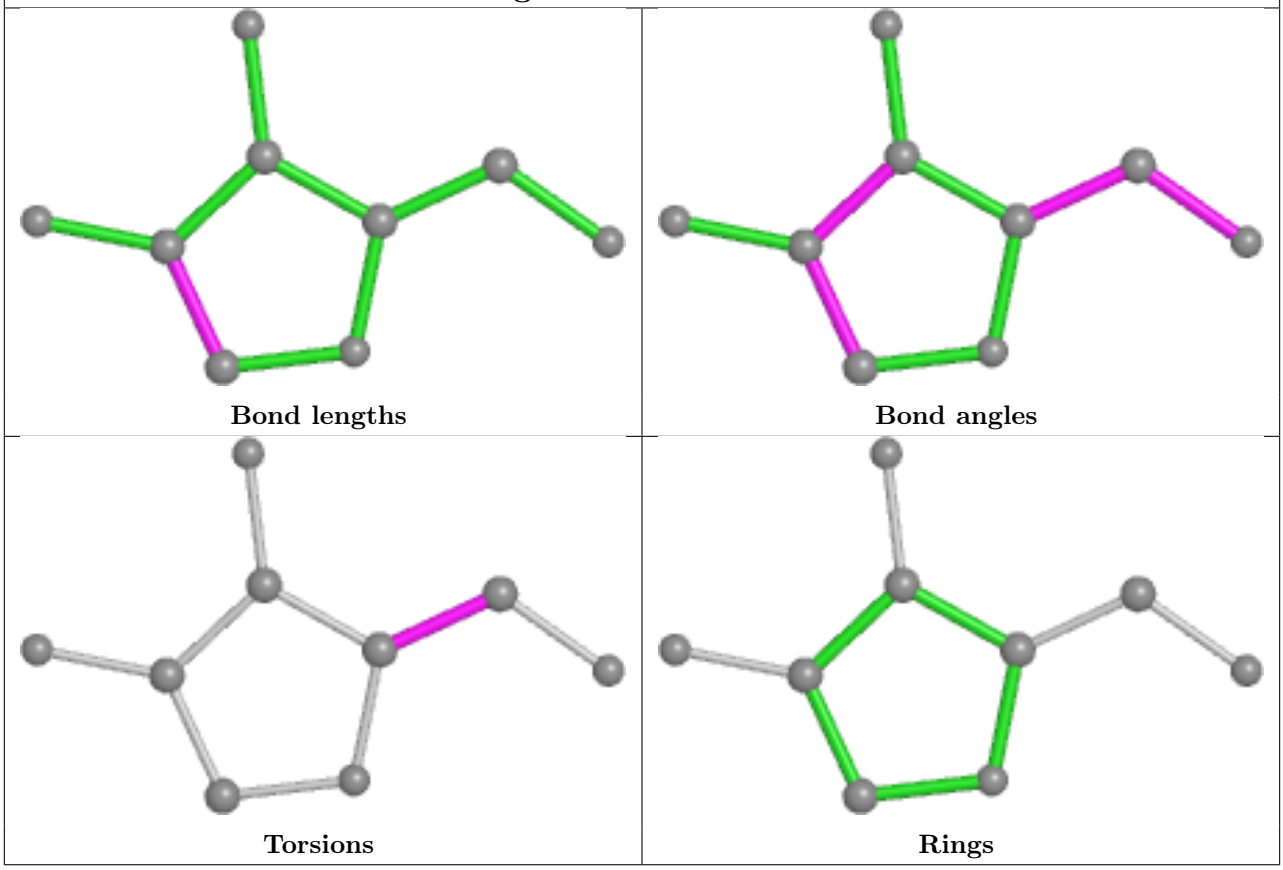
Ligand AHR B 2002



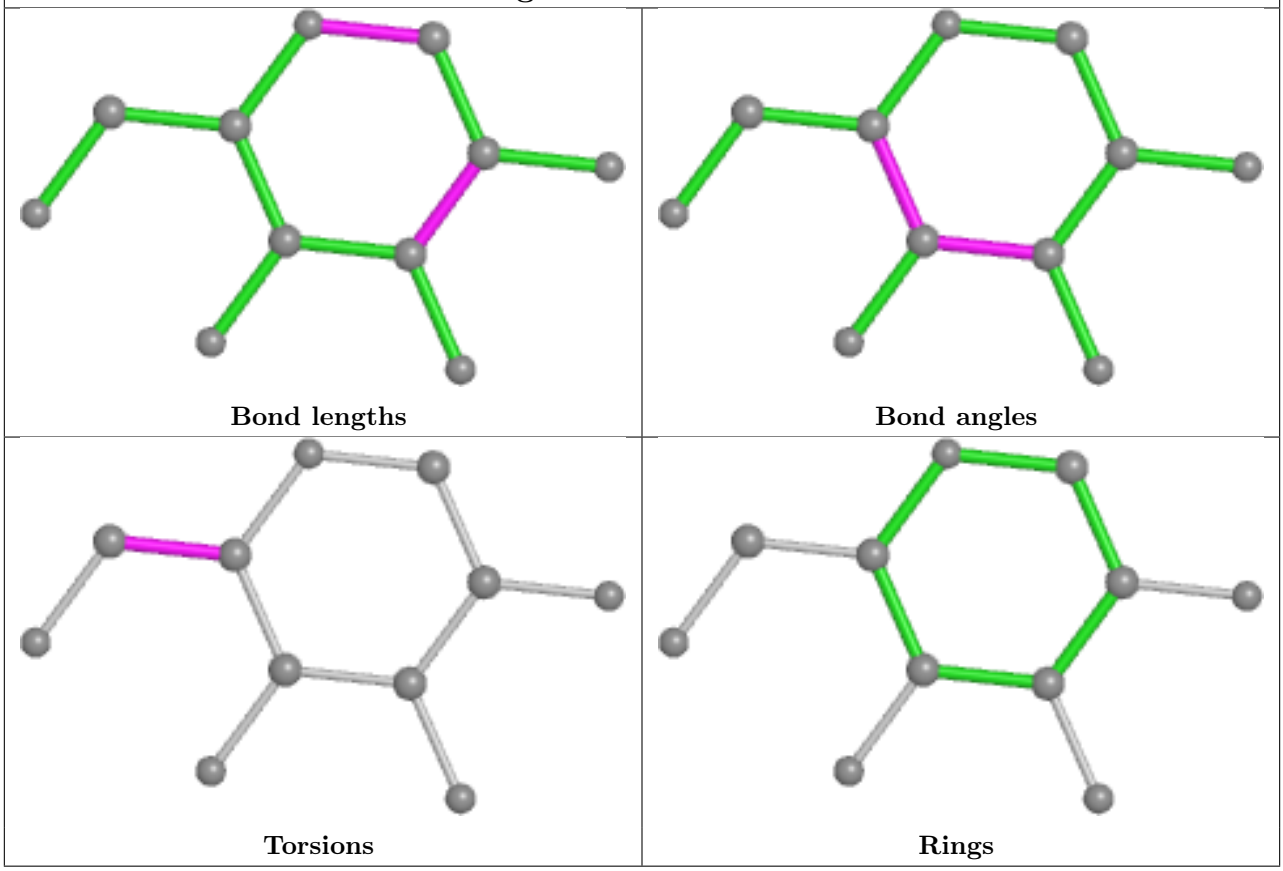
Ligand GLA F 2011

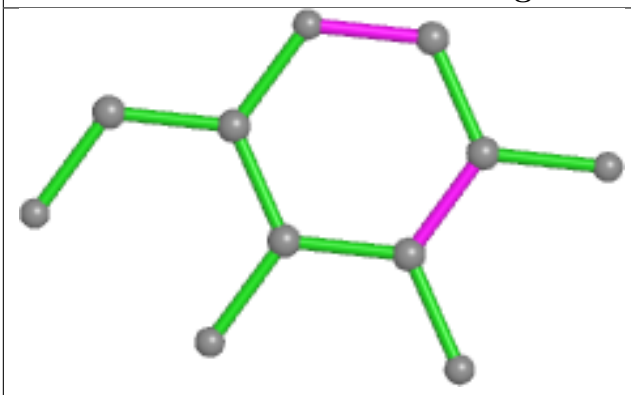
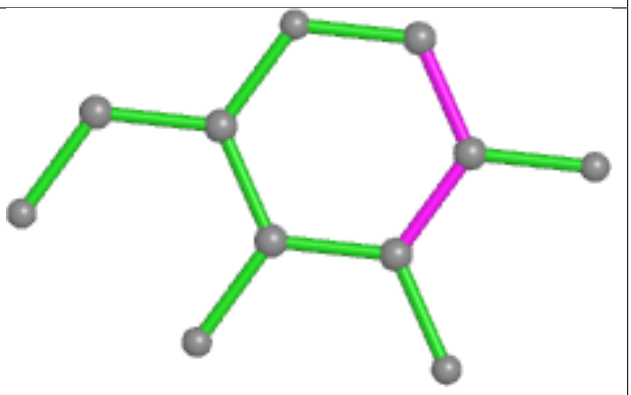
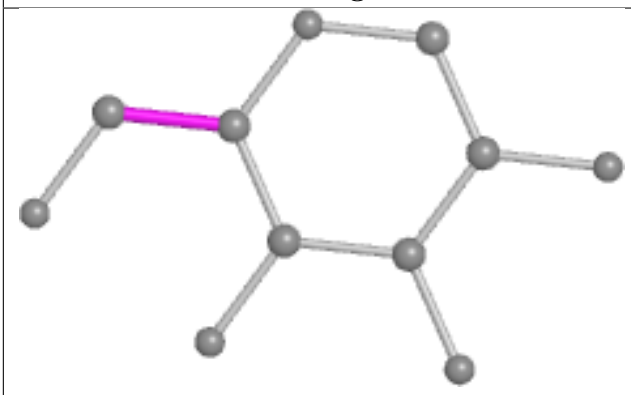
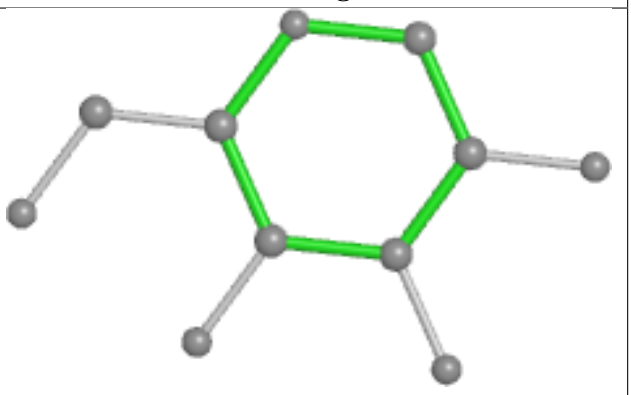


Ligand AHR E 2002

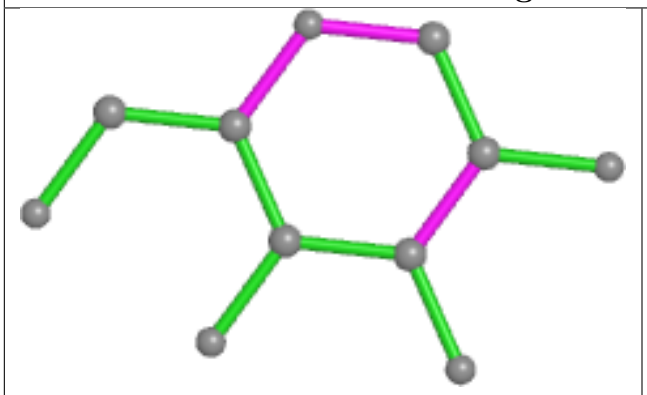


Ligand GLA F 2009

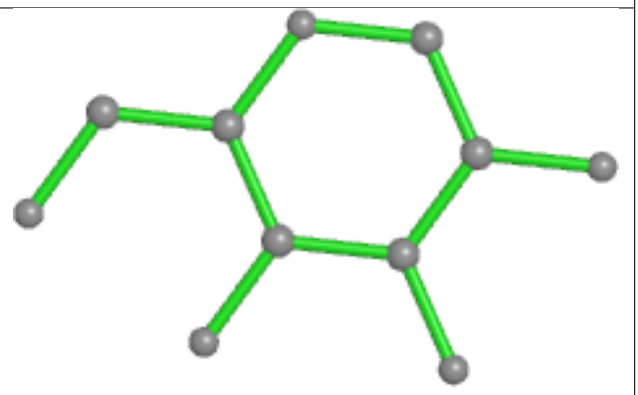


Ligand GLA B 2013	
 Bond lengths	 Bond angles
 Torsions	 Rings

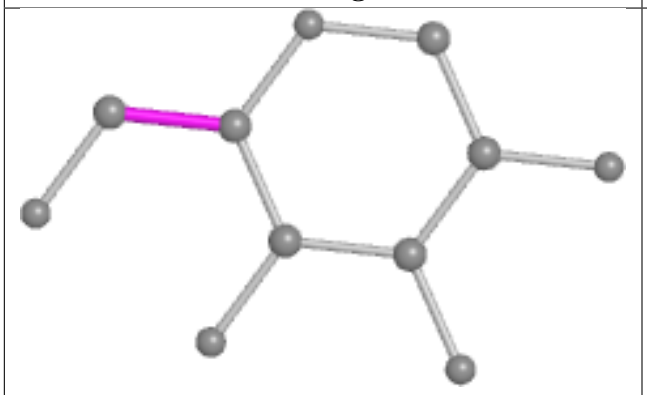
Ligand GLA B 2016



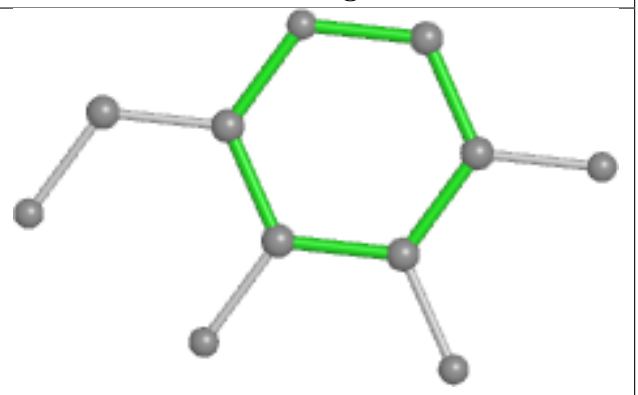
Bond lengths



Bond angles

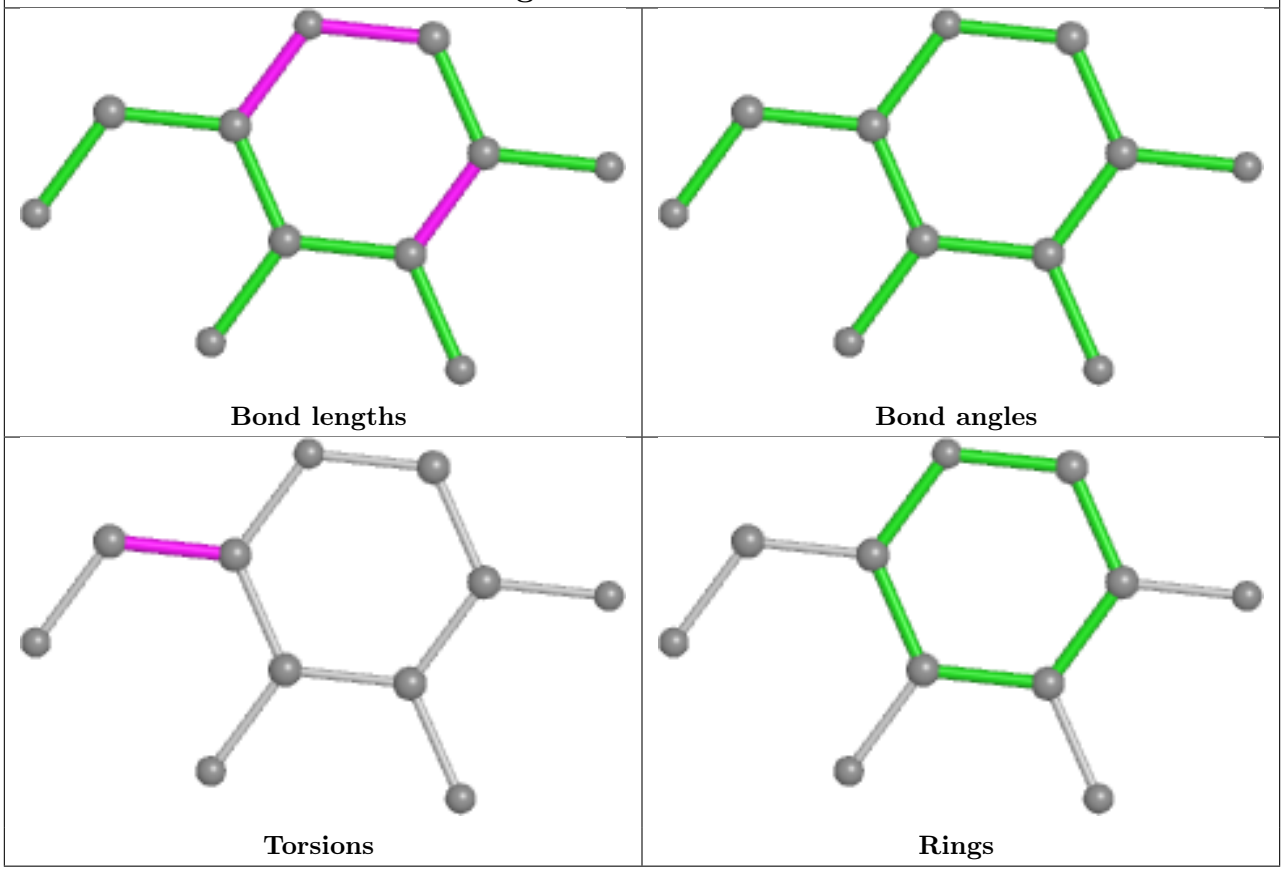


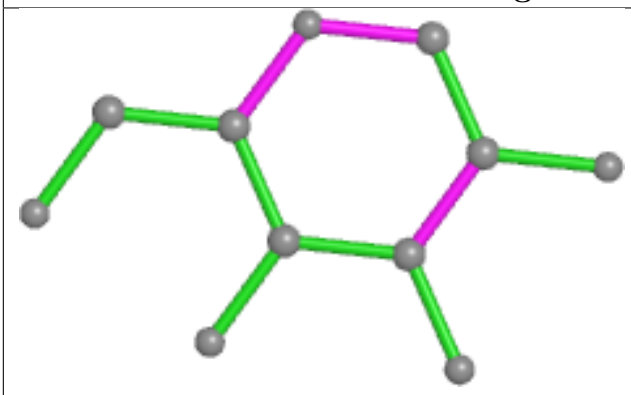
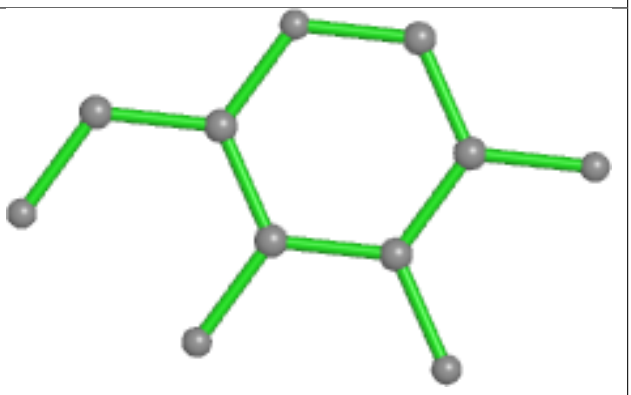
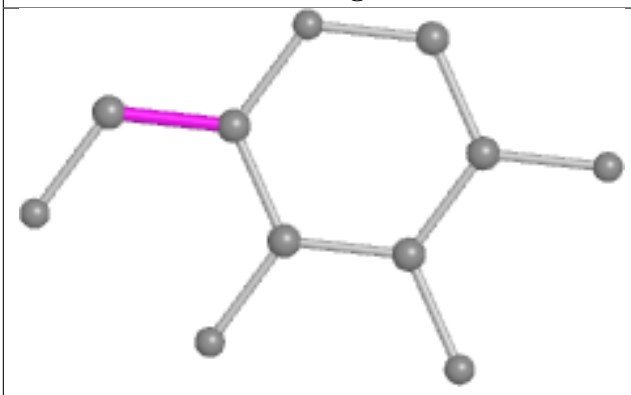
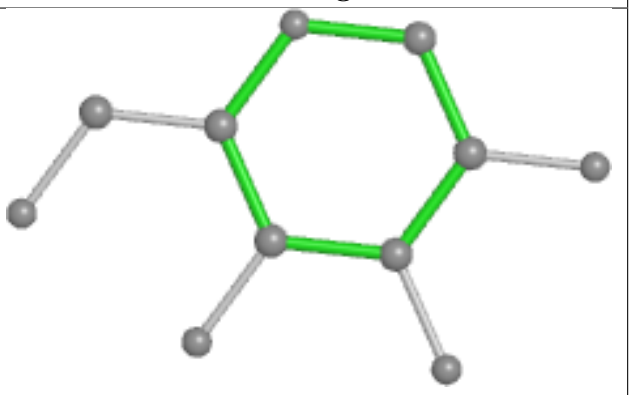
Torsions



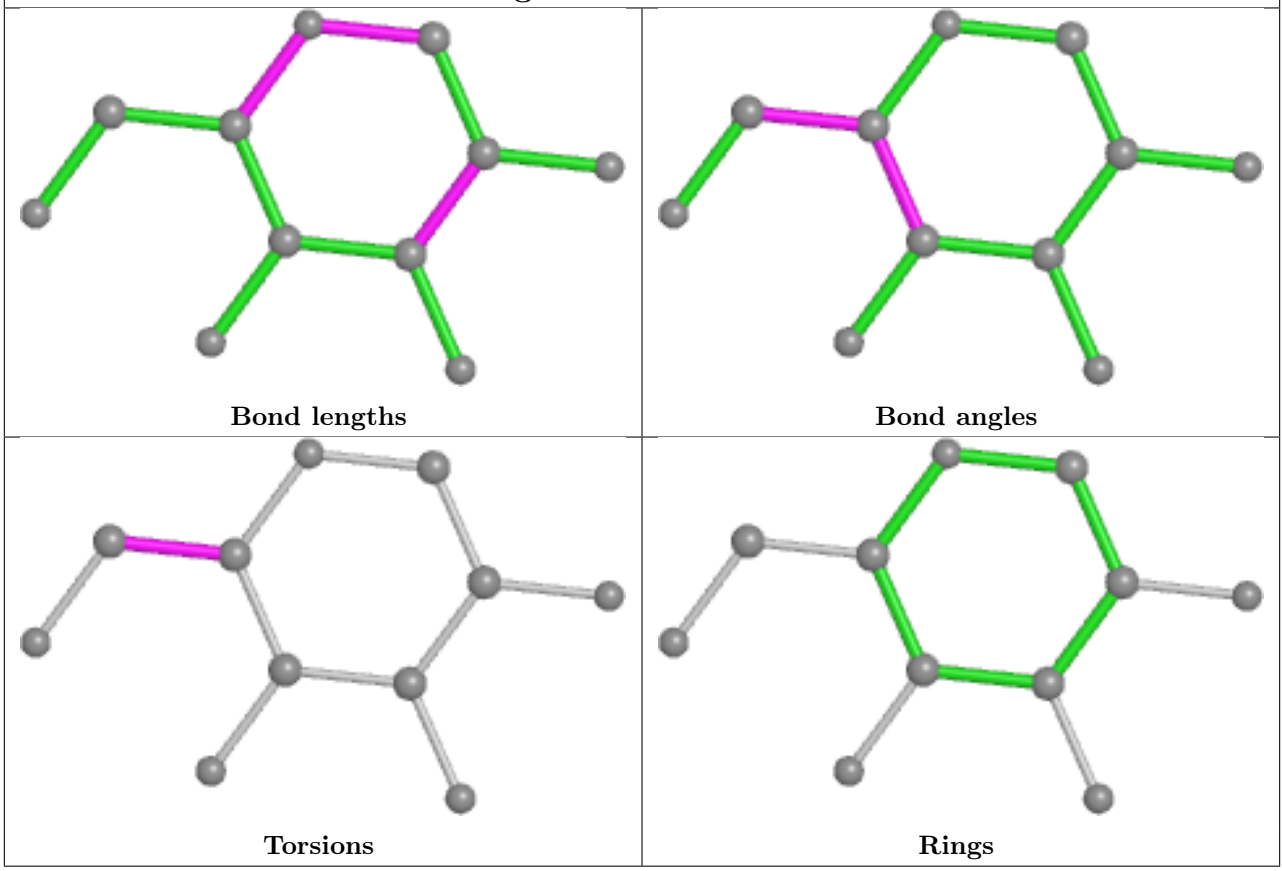
Rings

Ligand GLA E 2013

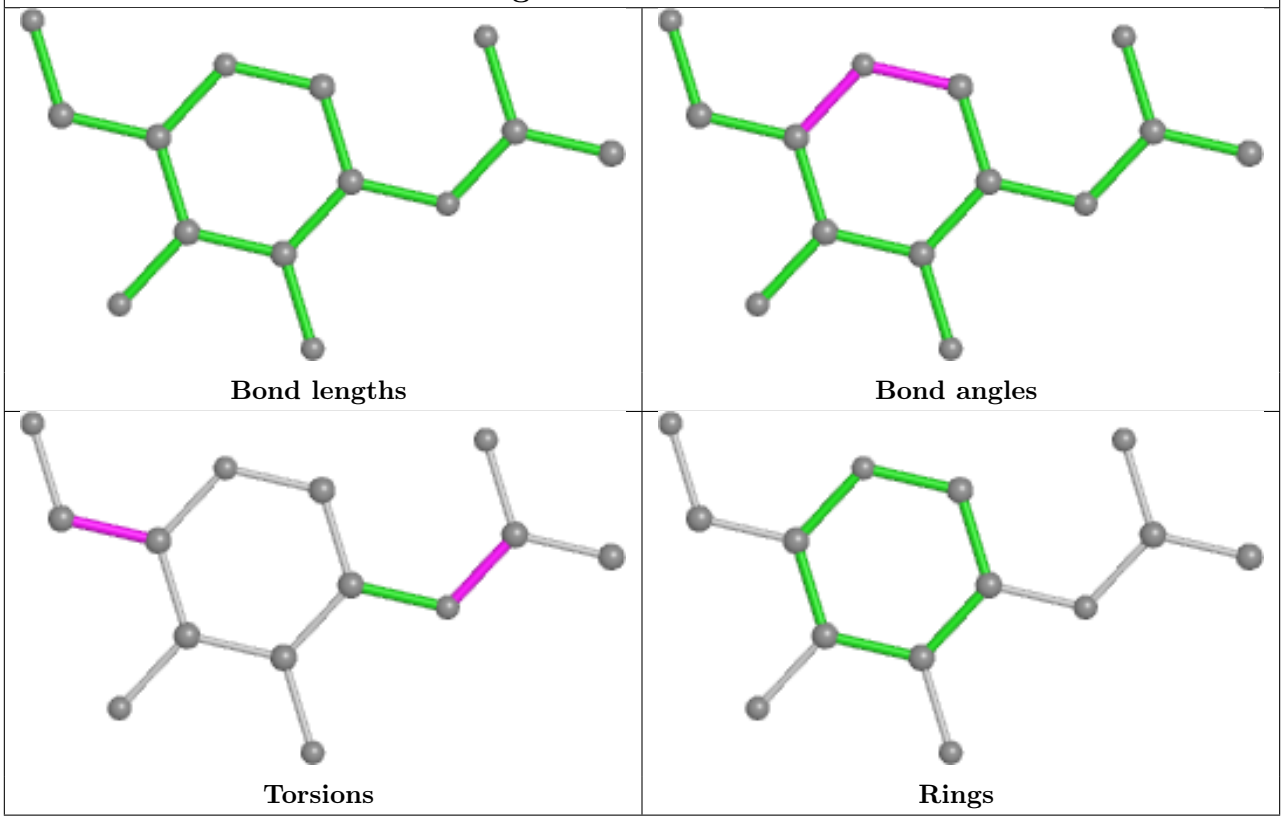


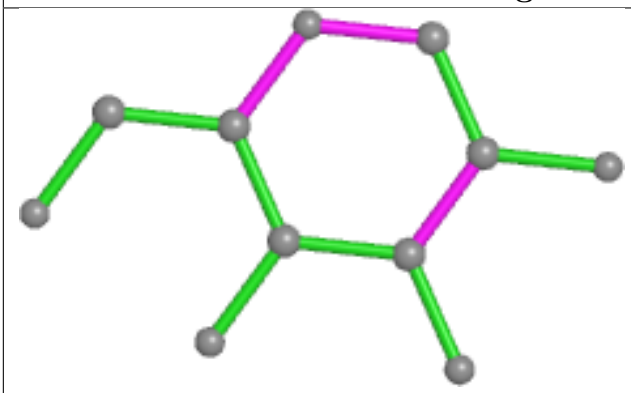
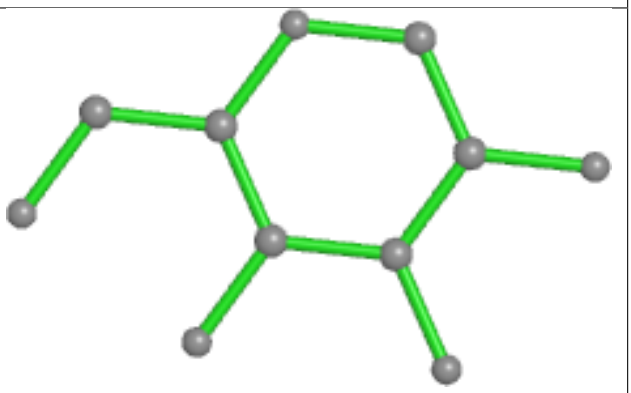
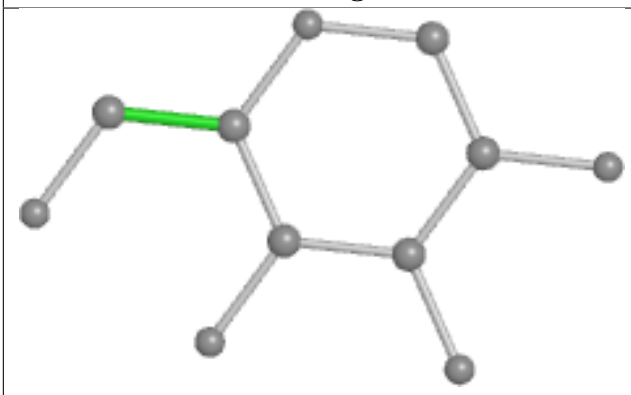
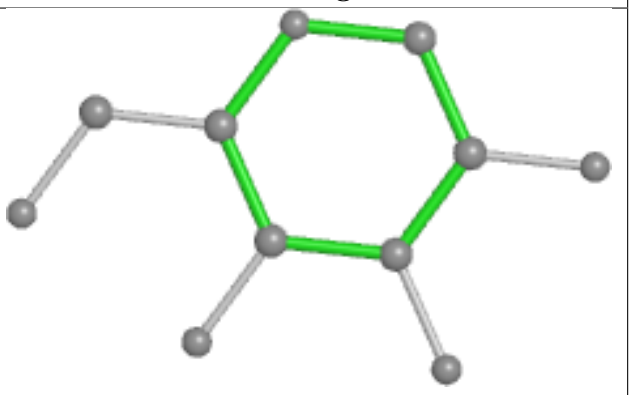
Ligand GLA C 2008	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

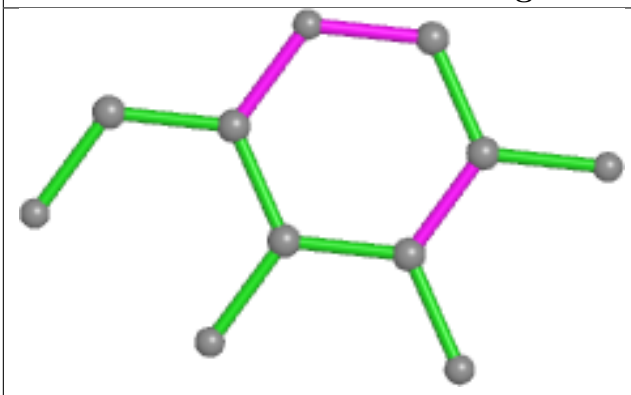
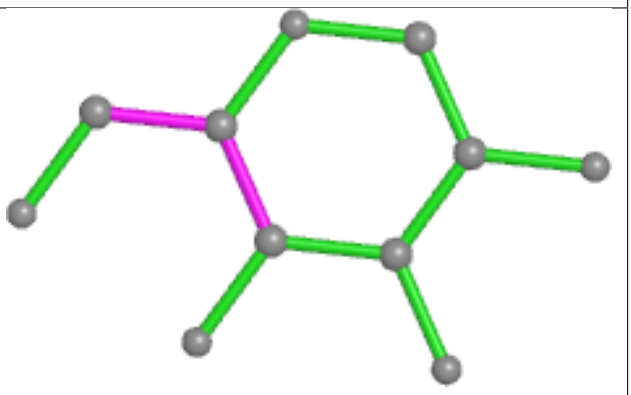
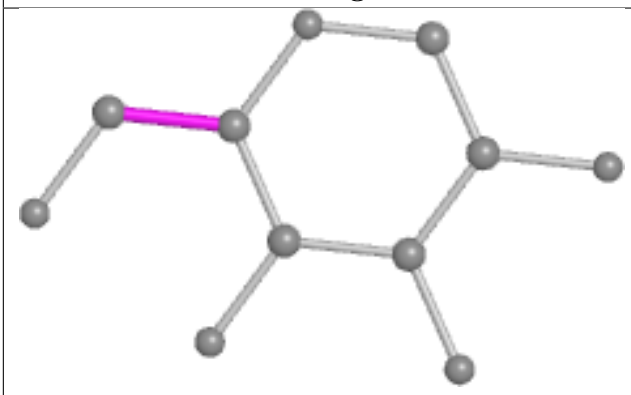
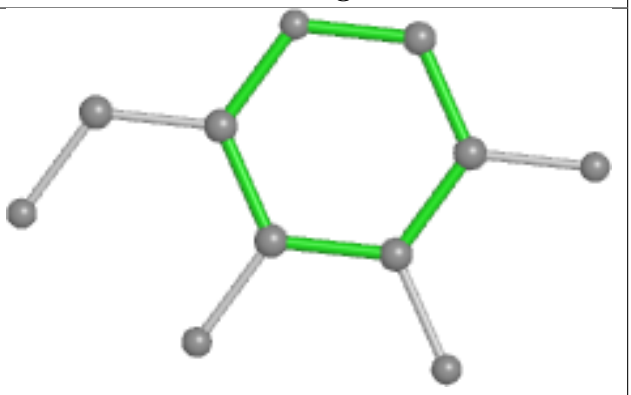
Ligand GLA D 2009

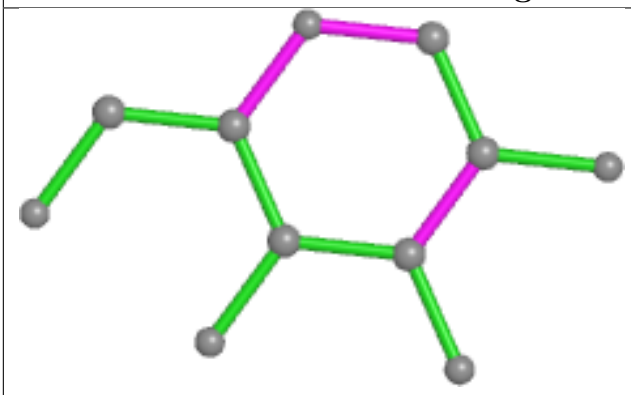
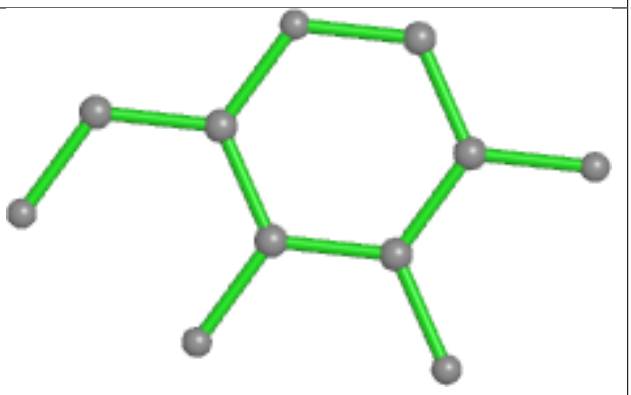
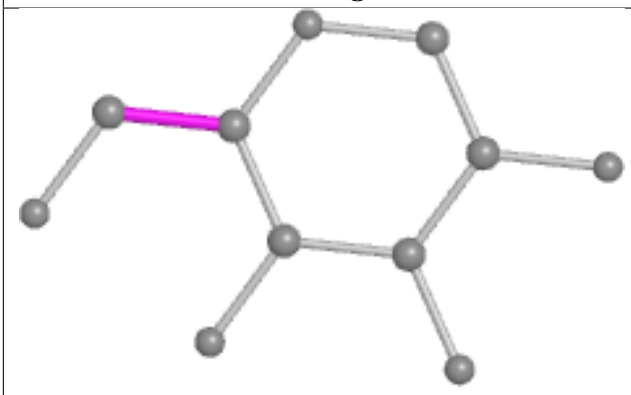
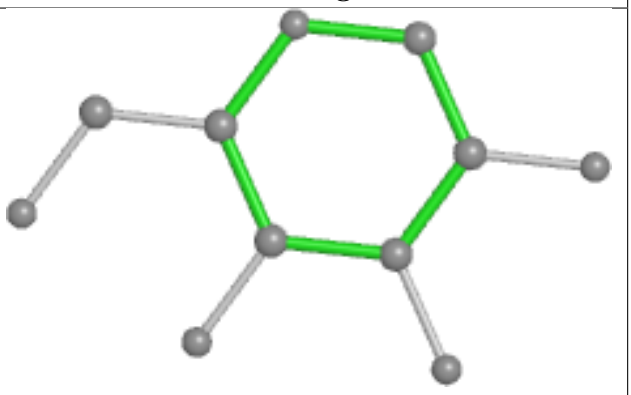


Ligand NAG C 2010

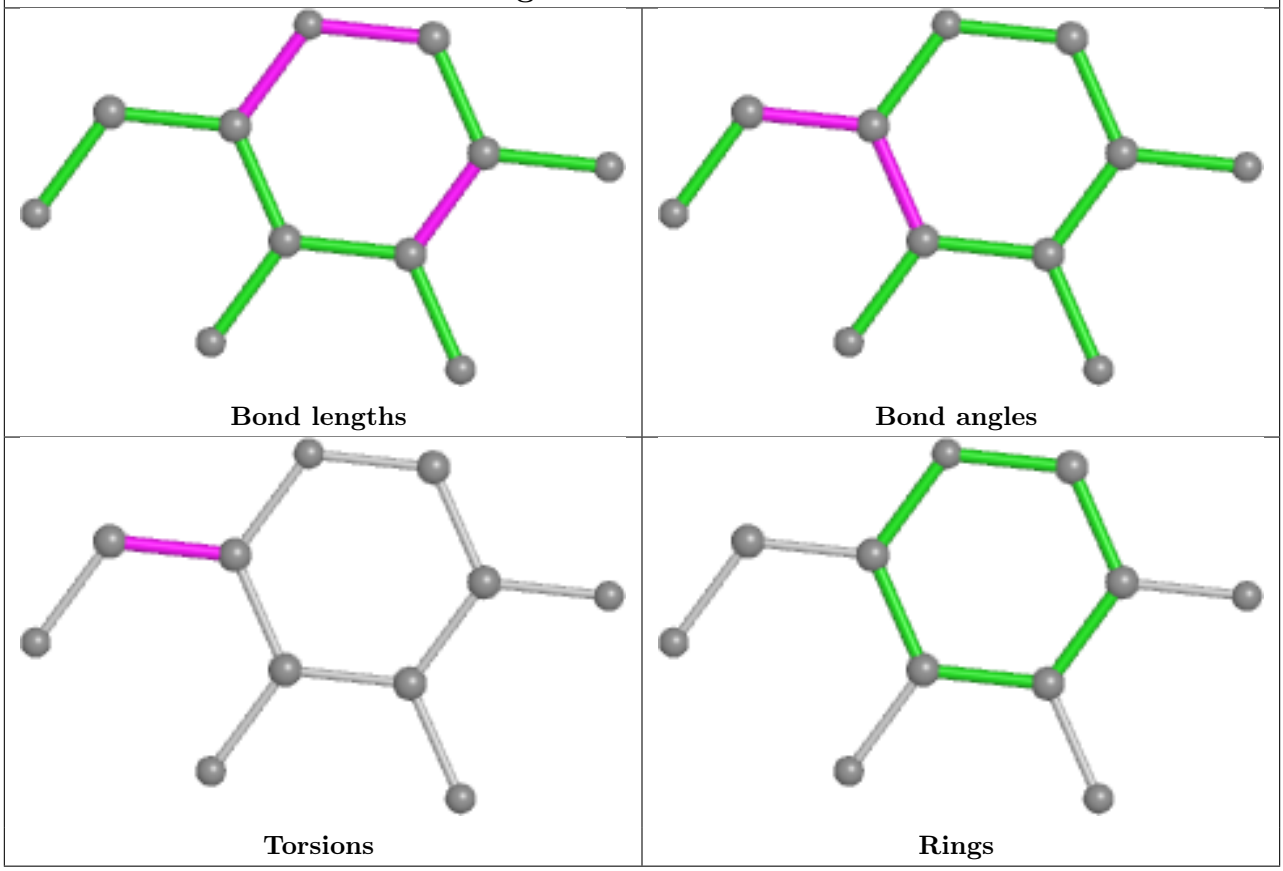


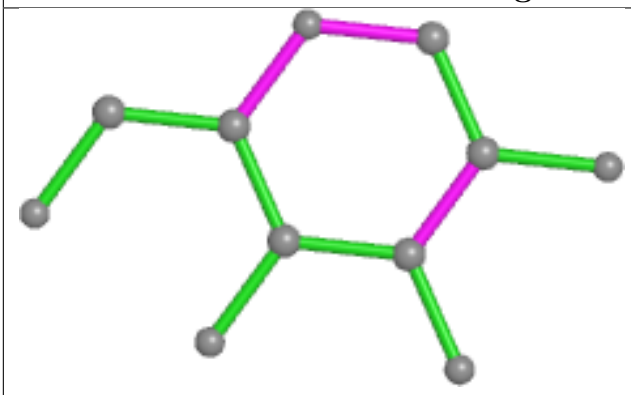
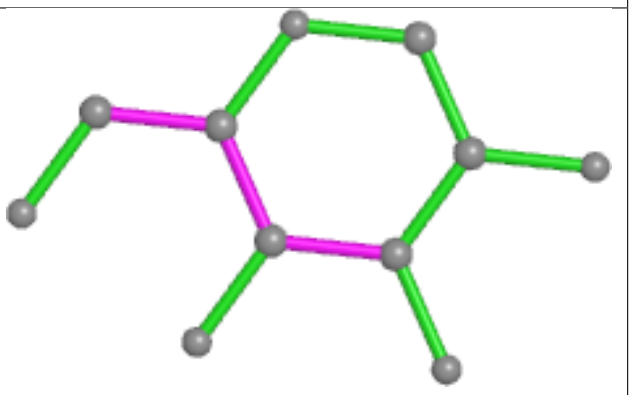
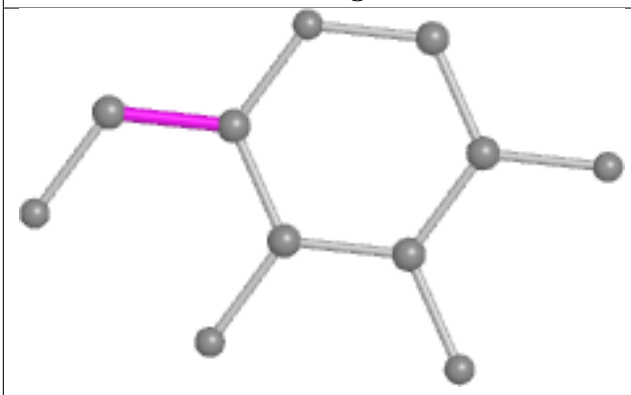
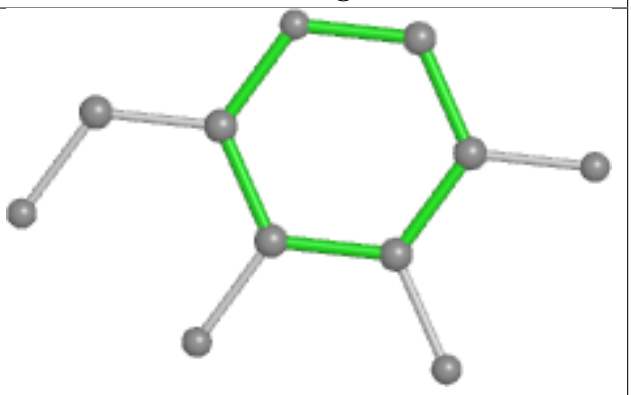
Ligand GLA F 2015	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

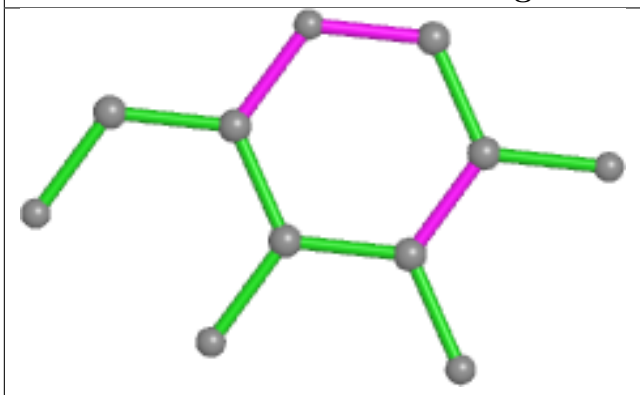
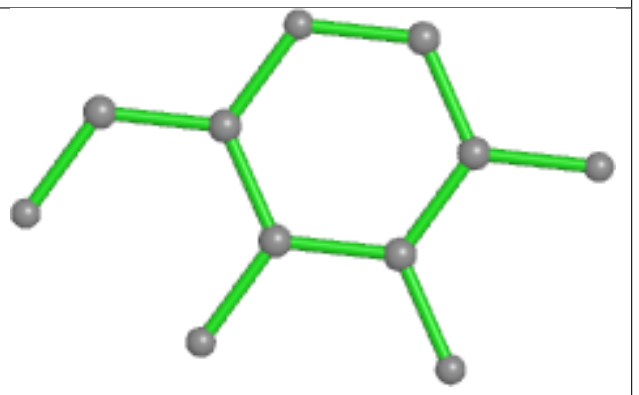
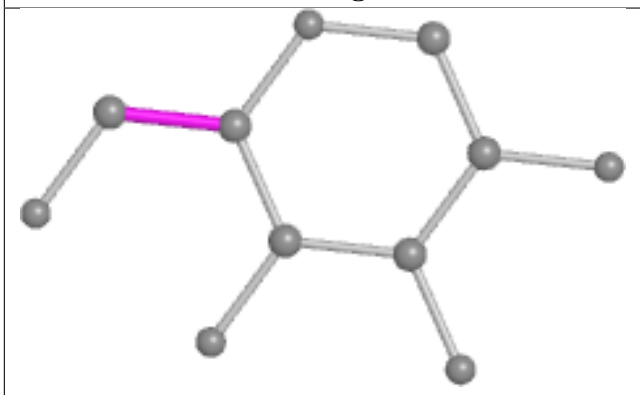
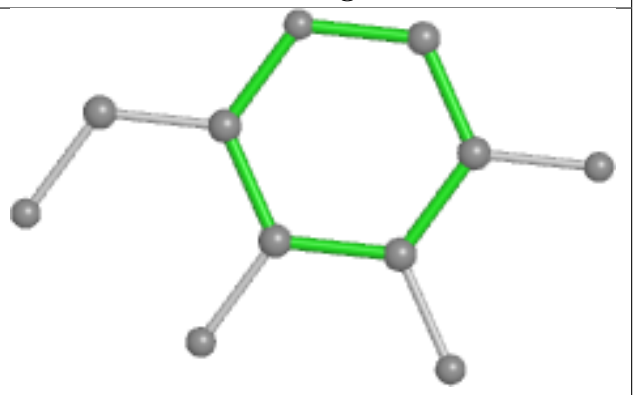
Ligand GLA E 2005	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA B 2007	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA F 2012



Ligand GLA B 2011	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLA D 2005	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

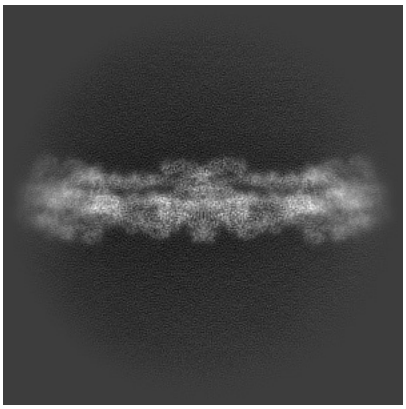
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37389. These allow visual inspection of the internal detail of the map and identification of artifacts.

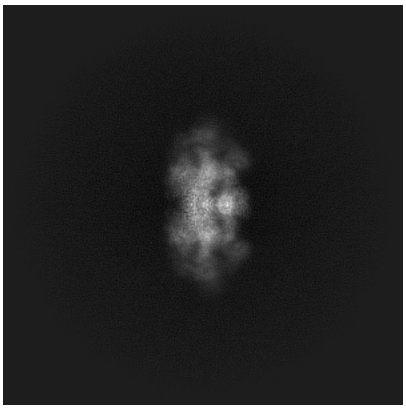
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

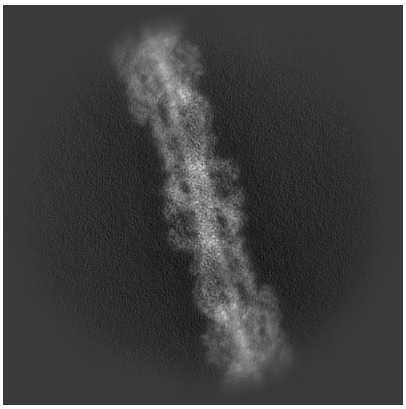
6.1.1 Primary map



X

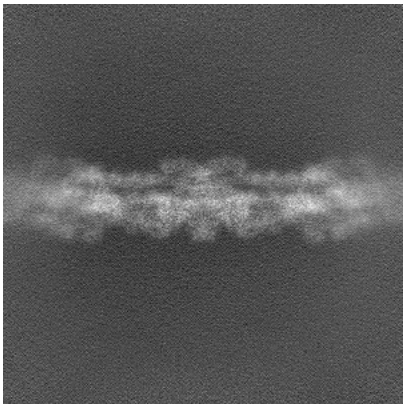


Y

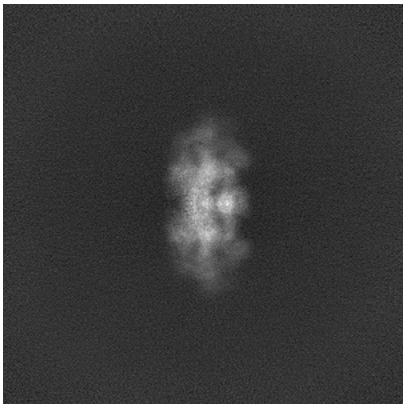


Z

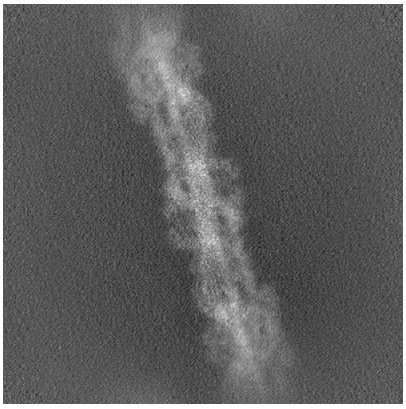
6.1.2 Raw map



X



Y

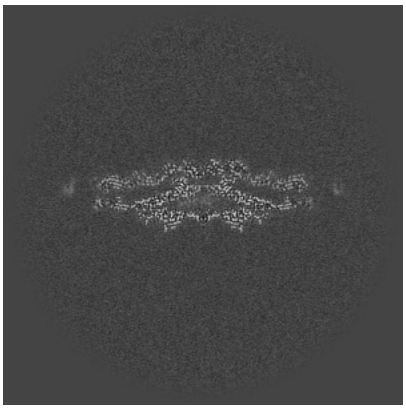


Z

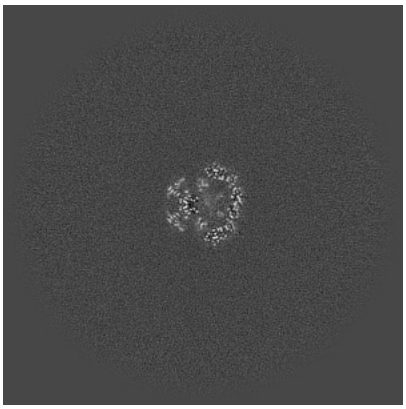
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

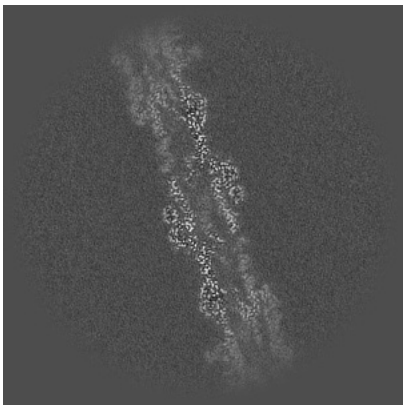
6.2.1 Primary map



X Index: 256

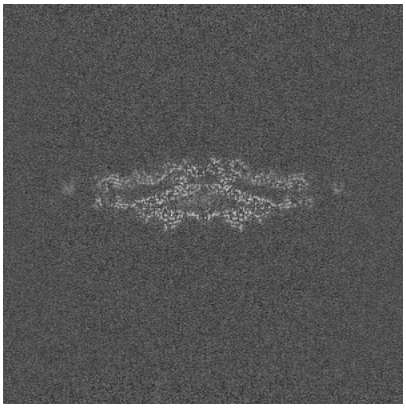


Y Index: 256

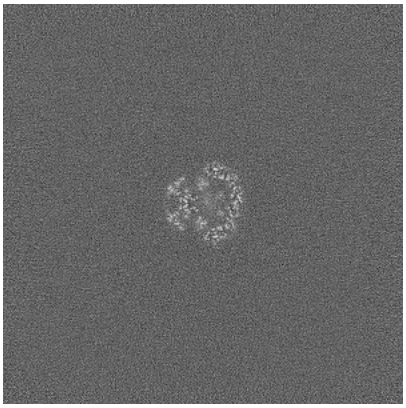


Z Index: 256

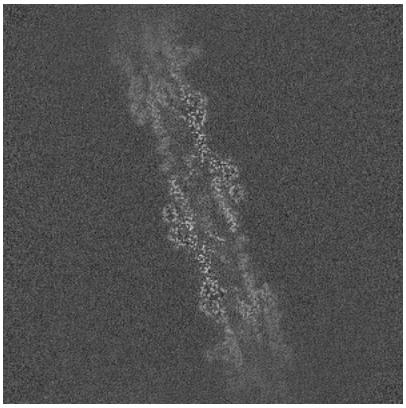
6.2.2 Raw map



X Index: 256



Y Index: 256

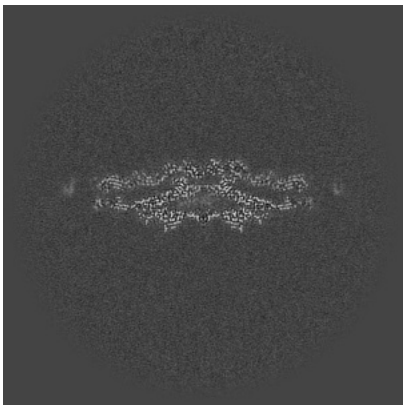


Z Index: 256

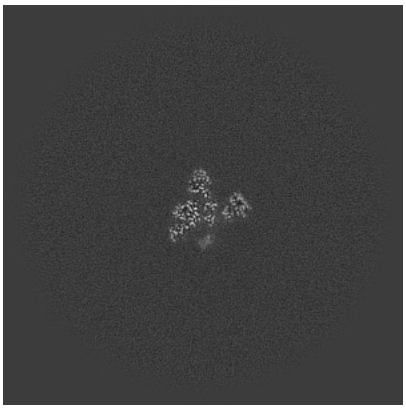
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

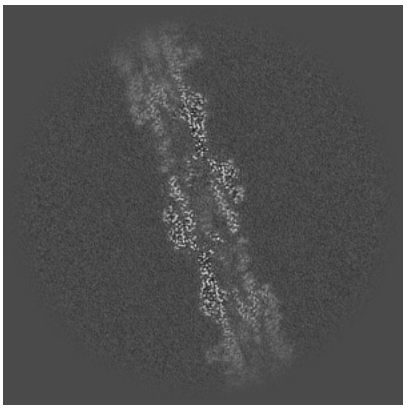
6.3.1 Primary map



X Index: 256

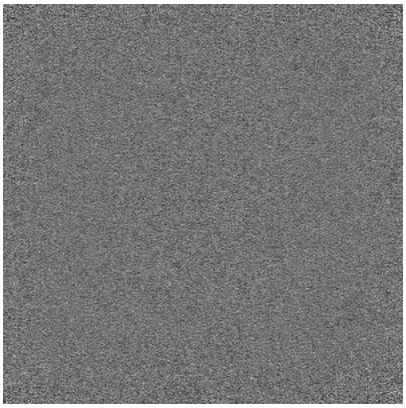


Y Index: 302

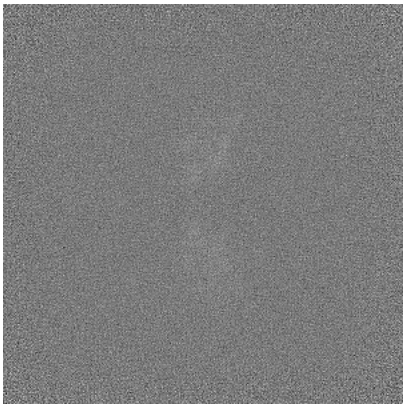


Z Index: 255

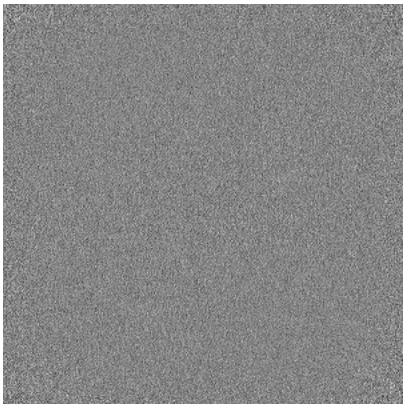
6.3.2 Raw map



X Index: 0



Y Index: 0

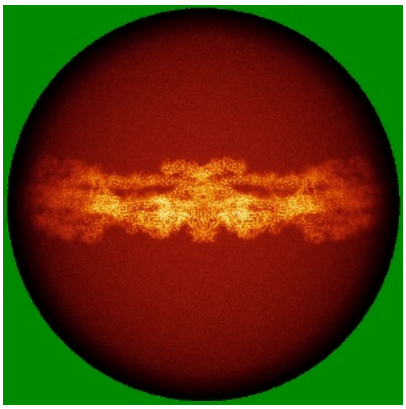


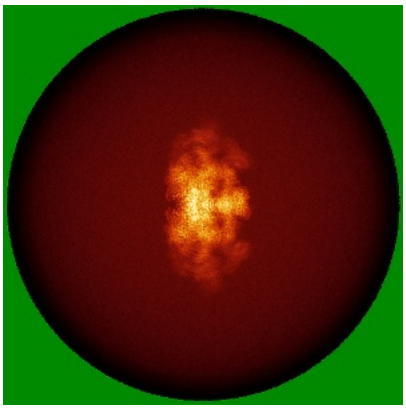
Z Index: 0

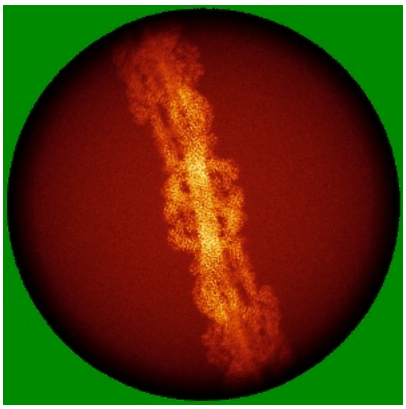
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

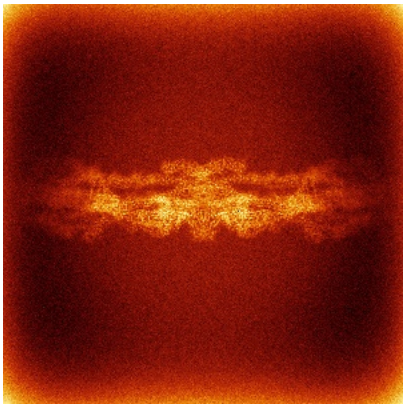
6.4.1 Primary map

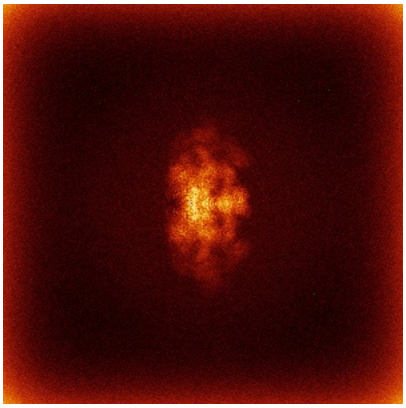

X

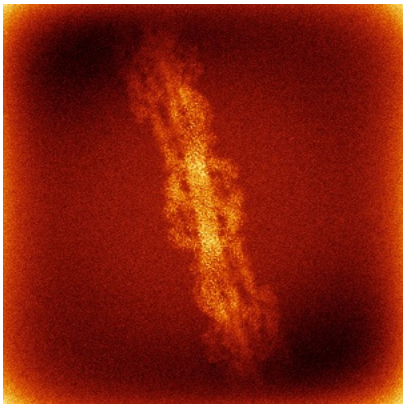

Y


Z

6.4.2 Raw map


X


Y


Z

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

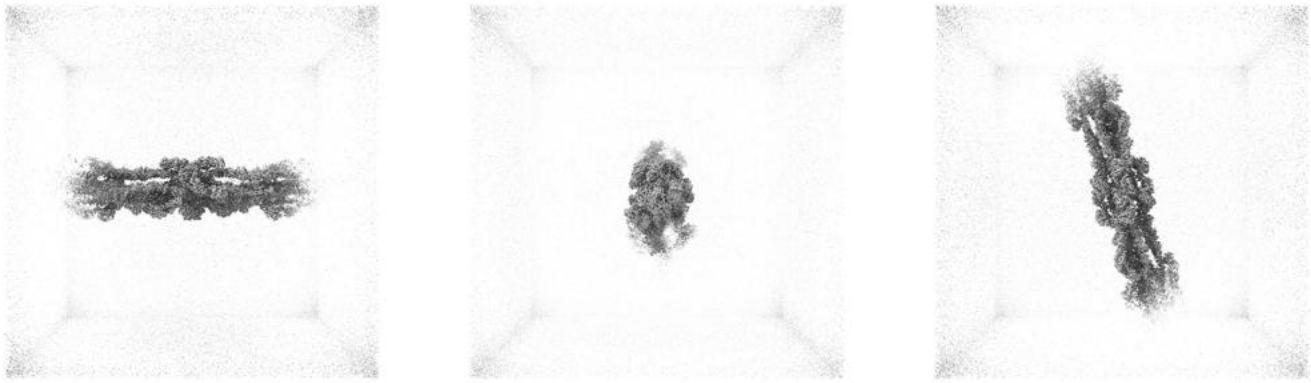
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

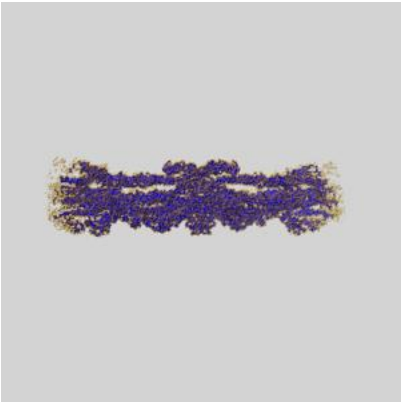
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

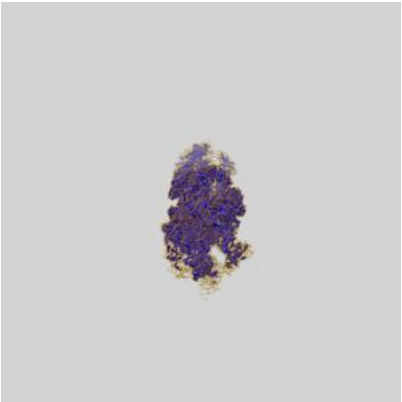
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

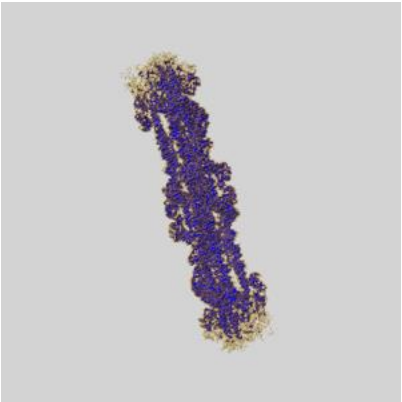
6.6.1 emd_37389_msk_1.map (i)



X



Y

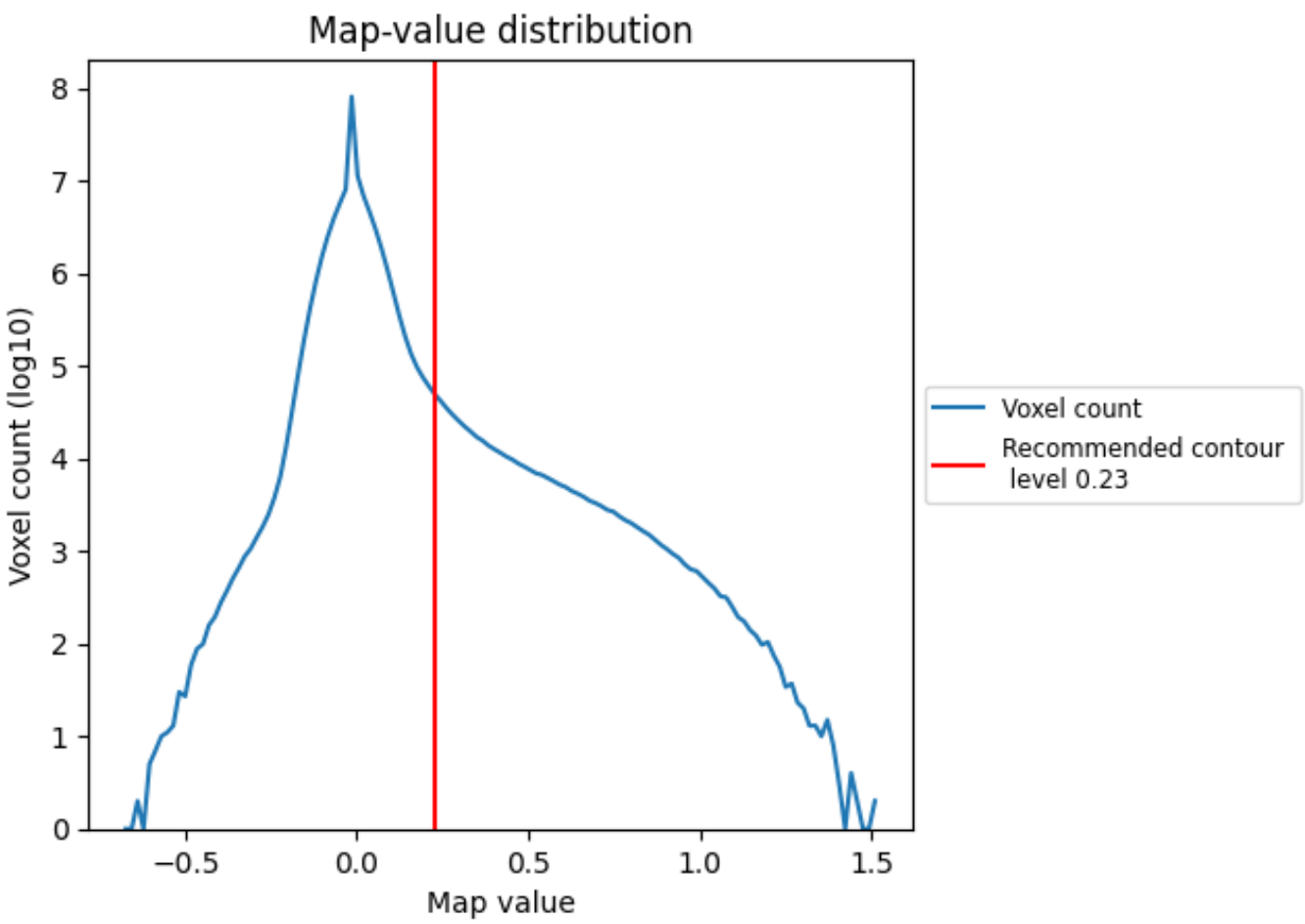


Z

7 Map analysis (i)

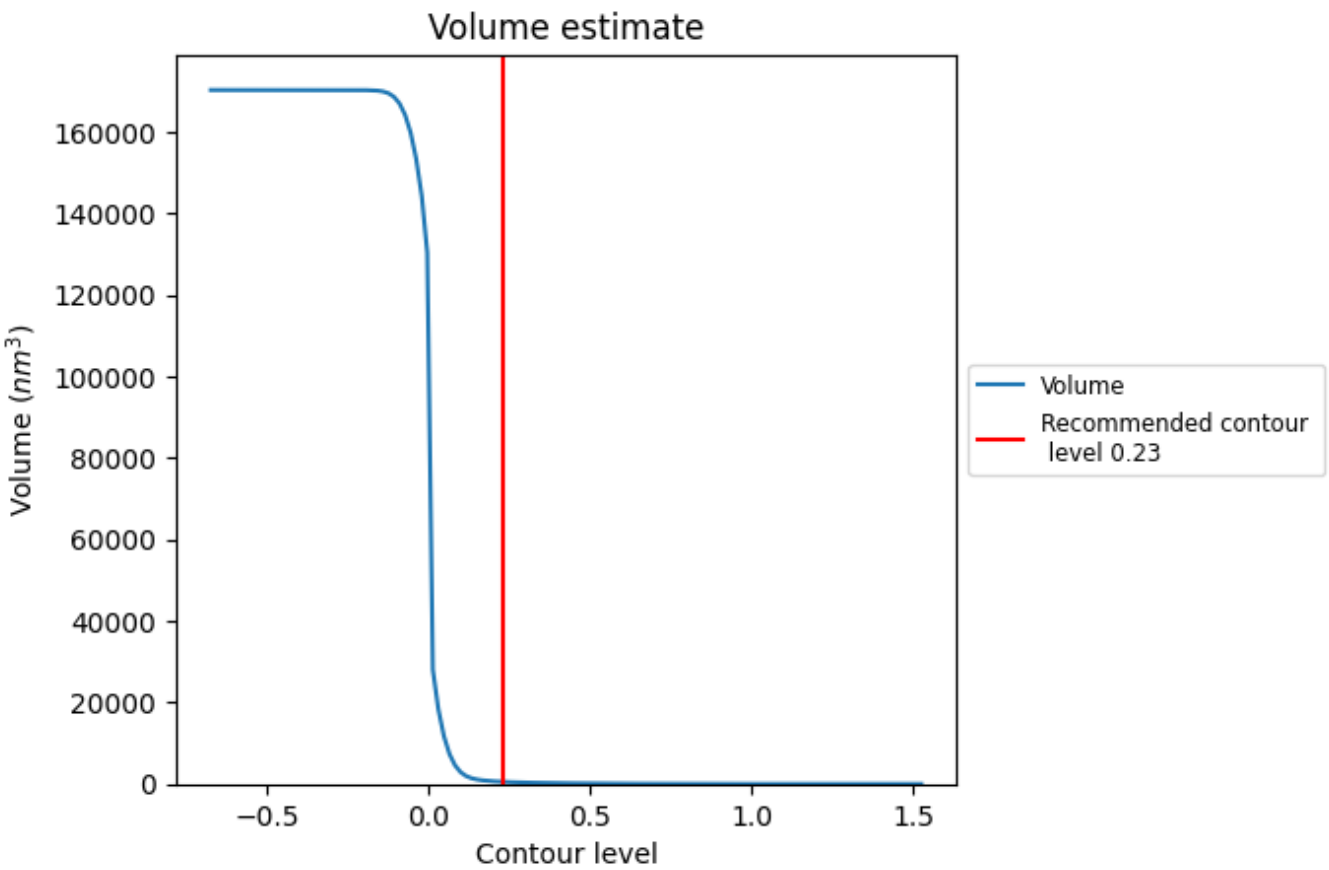
This section contains the results of statistical analysis of the map.

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.

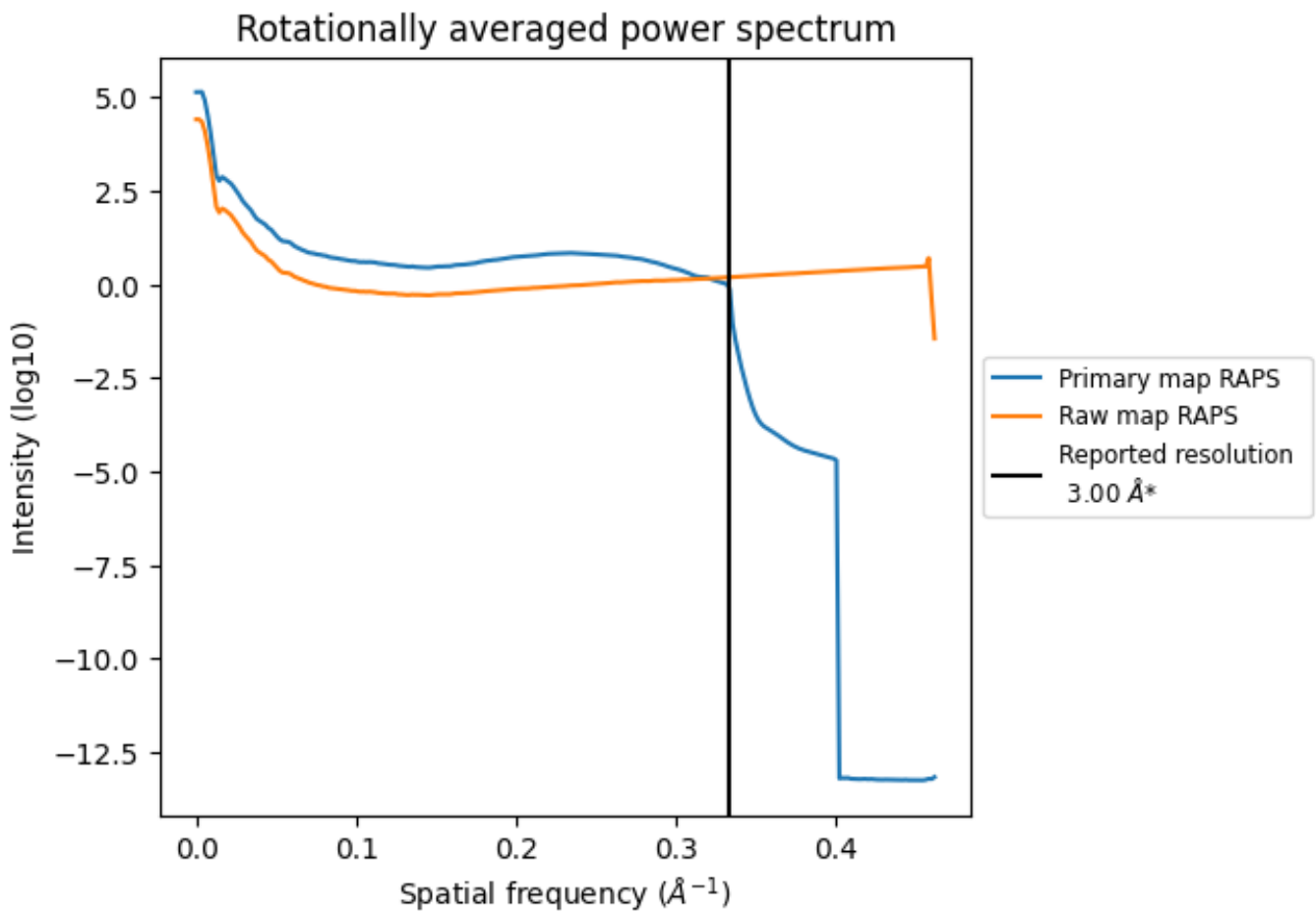
7.2 Volume estimate (i)



The volume at the recommended contour level is 527 nm^3; this corresponds to an approximate mass of 476 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 (i)

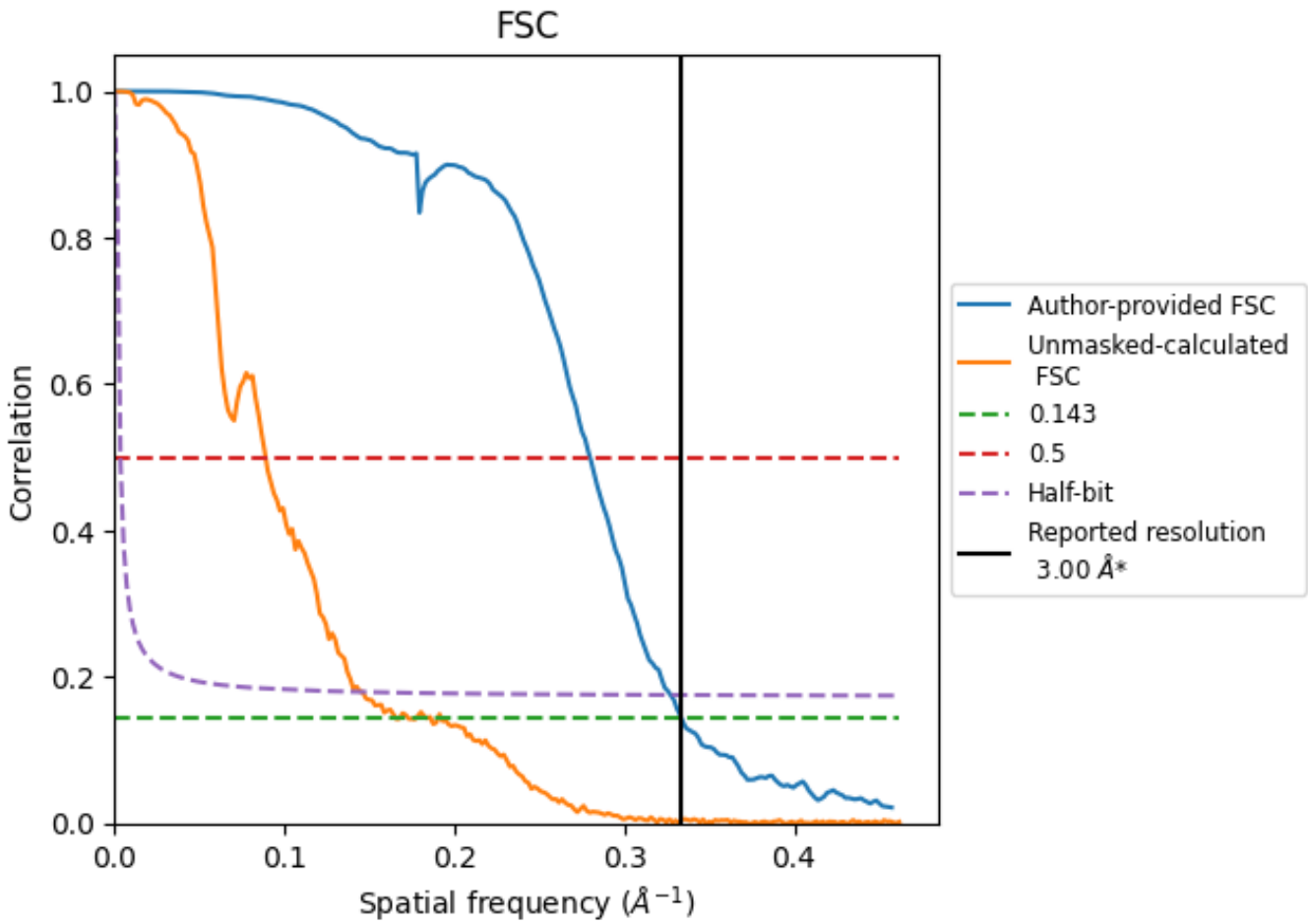


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

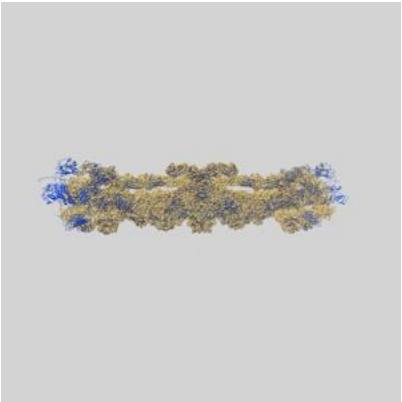
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.57	3.06
Unmasked-calculated*	6.04	11.24	6.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.04 differs from the reported value 3.0 by more than 10 %

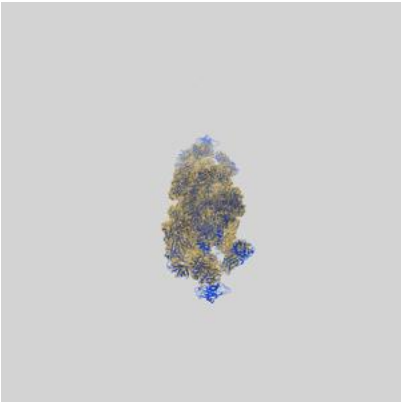
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37389 and PDB model 8WA2. Per-residue inclusion information can be found in section 3 on page 53.

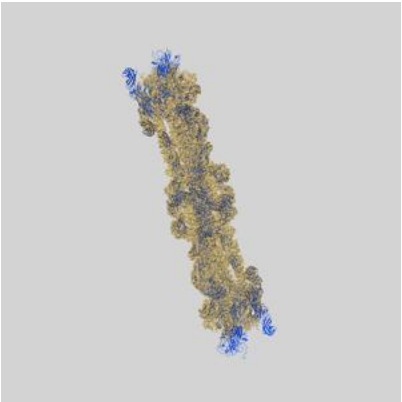
9.1 Map-model overlay (i)



X



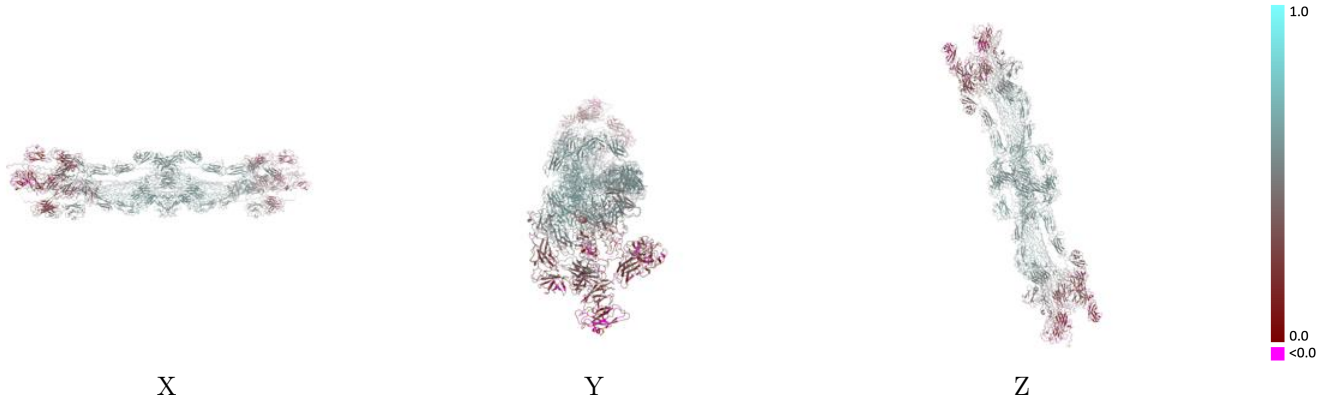
Y



Z

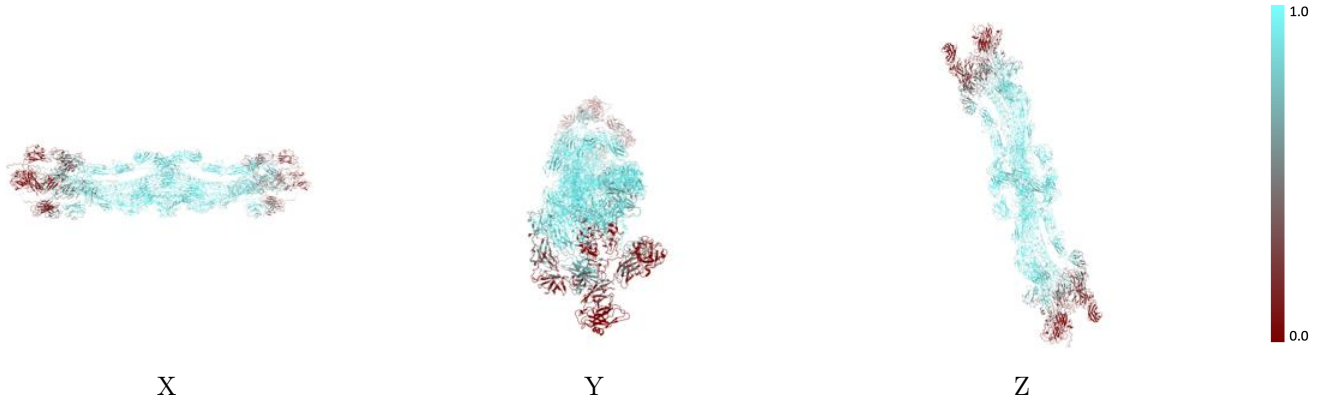
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



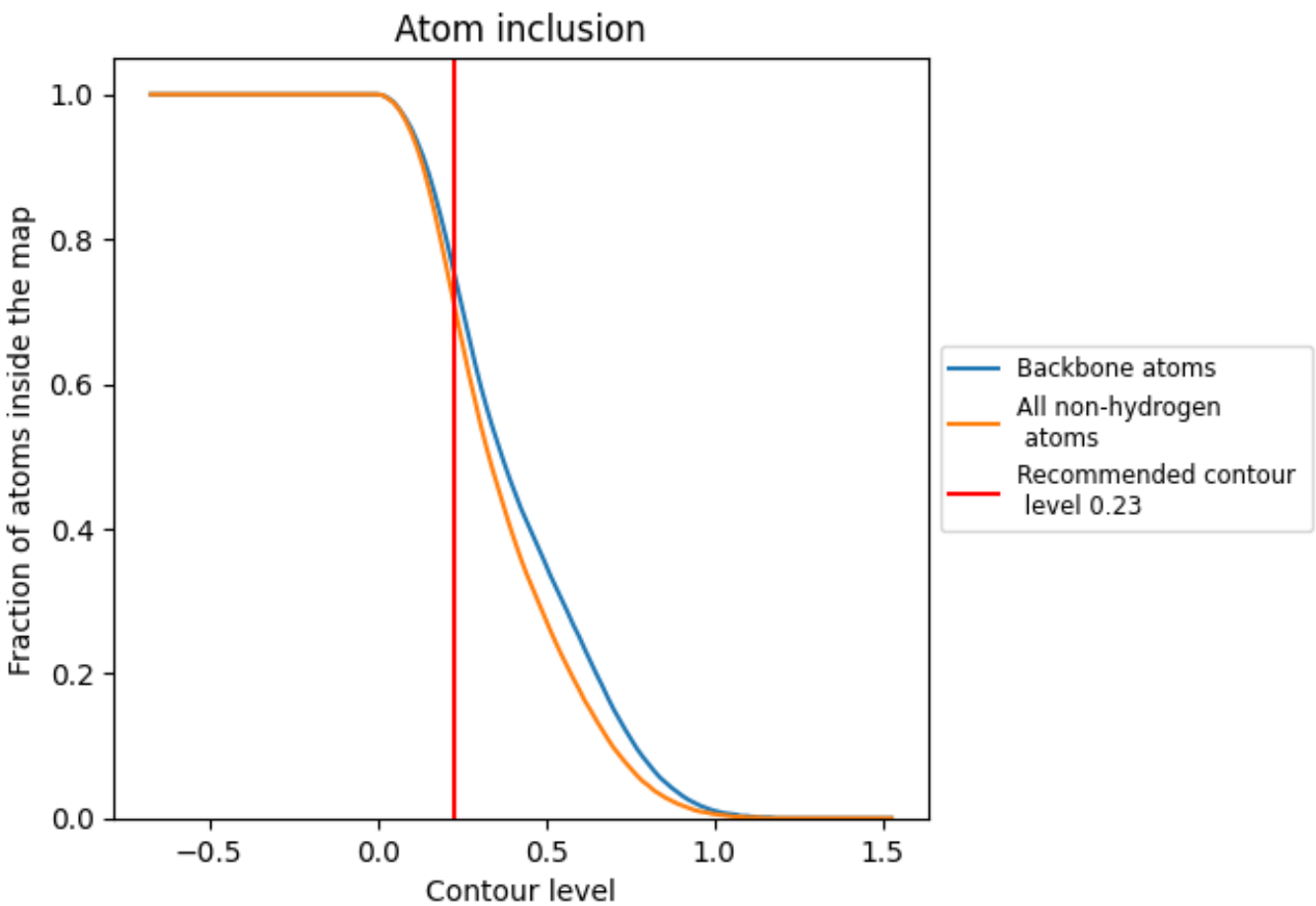
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.23).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.4570
0	0.7780	0.5390
0A	0.9630	0.5780
0B	0.5170	0.3330
0C	0.1030	0.2620
0D	0.0000	0.1240
0E	0.7020	0.3580
1	0.8520	0.5260
1A	0.8440	0.5240
1B	0.8680	0.5140
1C	0.0000	0.2620
1D	0.0000	0.2680
1E	0.3680	0.3570
2	0.9260	0.5380
2A	0.7110	0.4020
2B	0.6840	0.4460
2C	0.0000	0.0900
2D	0.0000	0.0530
3	0.9110	0.4940
3A	0.6900	0.3980
3B	0.7240	0.4480
3C	0.0000	0.2000
3D	0.0000	0.1280
4	0.8160	0.4770
4A	0.9470	0.5720
4B	0.8280	0.5020
4C	0.0000	0.1630
4D	0.5360	0.4130
5	0.7240	0.4800
5A	0.8420	0.5660
5B	0.8620	0.5280
5C	0.0000	0.1930
5D	0.9170	0.5420
6	0.9470	0.5720
6A	0.9310	0.5780

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Chain	Atom inclusion	Q-score
6B	0.8160	0.5310
6C	0.0000	0.1720
6D	0.6550	0.4610
7	0.8680	0.5540
7A	0.8620	0.5180
7B	0.9360	0.5350
7C	0.8750	0.5120
7D	0.7590	0.4250
8	0.8970	0.5490
8A	1.0000	0.6020
8B	0.7870	0.5060
8C	0.9260	0.5860
8D	0.7590	0.5330
9	0.8970	0.5620
9A	0.8680	0.5550
9B	0.9310	0.5480
9C	0.7780	0.5220
9D	0.7450	0.4270
A	0.9040	0.5460
AA	0.8970	0.5580
AB	0.9790	0.5770
AC	0.1070	0.1330
AD	0.9170	0.5680
AE	0.9470	0.5010
B	0.9040	0.5440
BA	0.8950	0.5540
BB	0.8940	0.5440
BC	0.9630	0.5780
BD	0.9330	0.5860
BE	0.7450	0.4390
C	0.6800	0.4450
CA	0.9790	0.5780
CB	0.9310	0.5860
CC	0.7780	0.4690
CD	0.7930	0.4910
CE	0.8420	0.5000
D	0.6430	0.4310
DA	0.8720	0.5340
DB	0.8470	0.5200
DC	0.8890	0.5450
DD	0.9260	0.5220
DE	0.8080	0.5160

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Chain	Atom inclusion	Q-score
E	0.4780	0.3750
EA	0.9310	0.5840
EB	0.0000	0.1940
EC	0.9560	0.5550
ED	0.8890	0.5400
EE	0.9210	0.5520
F	0.4870	0.3680
FA	0.7860	0.4320
FB	0.0000	0.2820
FC	0.7930	0.4170
FD	0.9260	0.5590
FE	0.9570	0.5680
G	0.8520	0.4770
GA	0.9030	0.5140
GB	0.0530	0.1760
GC	1.0000	0.5770
GD	0.8970	0.5680
GE	0.8390	0.5100
H	0.8010	0.4250
HA	0.7410	0.4240
HB	0.1050	0.3060
HC	0.9260	0.5570
HD	0.8610	0.5370
HE	0.8420	0.4860
I	0.7730	0.4450
IA	0.7410	0.4510
IB	0.2340	0.3620
IC	0.9260	0.5610
ID	0.9260	0.5270
IE	0.8940	0.5000
J	0.7780	0.3940
JA	0.7780	0.3850
JB	0.2500	0.3280
JC	0.8970	0.5550
JD	0.8440	0.4440
JE	0.8720	0.5120
K	0.7410	0.4130
KA	0.8440	0.4740
KB	0.1840	0.3940
KC	0.8890	0.5240
KD	0.8890	0.5280
KE	0.8080	0.4650

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Chain	Atom inclusion	Q-score
L	0.7780	0.4480
LA	0.6900	0.3950
LB	0.4810	0.3960
LC	0.8890	0.5170
LD	0.8890	0.5310
LE	0.5790	0.4390
M	0.8220	0.4470
MA	0.8520	0.4740
MB	0.2440	0.3120
MC	0.8440	0.5570
MD	0.8610	0.4970
ME	0.8970	0.5040
N	0.6210	0.2840
NA	0.8520	0.4270
NB	0.3330	0.3090
NC	0.8150	0.4630
ND	0.7220	0.4690
NE	0.7890	0.4830
O	0.7780	0.4630
OA	0.8520	0.5060
OB	0.1850	0.1930
OC	0.8060	0.4770
OD	0.6940	0.3100
OE	0.9310	0.5220
P	0.7780	0.4600
PA	0.8280	0.5150
PB	0.5180	0.4800
PC	0.8060	0.4790
PD	0.8670	0.4610
PE	0.8510	0.4710
Q	0.8520	0.4620
QA	0.7780	0.4610
QB	0.4810	0.2860
QC	0.8330	0.5180
QD	0.8890	0.5130
QE	0.7500	0.4370
R	0.9310	0.5370
RA	0.8150	0.4940
RB	0.4440	0.2560
RC	0.8060	0.3840
RD	0.7780	0.3870
RE	0.9110	0.5200

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Chain	Atom inclusion	Q-score
S	0.7780	0.4730
SA	0.7110	0.4530
SB	0.7410	0.4440
SC	0.8440	0.4550
SD	0.8060	0.3980
SE	0.9150	0.5260
T	0.8150	0.4580
TA	0.7410	0.4780
TB	0.6300	0.3990
TC	0.8150	0.4830
TD	0.8150	0.4730
TE	0.8420	0.4880
U	0.8000	0.4630
UA	0.8890	0.4630
UB	0.7040	0.4000
UC	0.7780	0.3260
UD	0.8610	0.3960
UE	0.8160	0.5000
V	0.7780	0.4470
VA	0.9170	0.4570
VB	0.6440	0.4450
VC	0.8890	0.4570
VD	0.8060	0.4110
VE	0.8750	0.5190
W	0.8330	0.4910
WA	0.7780	0.4080
WB	0.5530	0.3180
WC	0.7780	0.4970
WD	0.7780	0.4540
WE	0.7890	0.5130
X	0.8610	0.4700
XA	0.7780	0.3600
XB	0.4480	0.2390
XC	0.8610	0.4050
XD	0.8150	0.3350
XE	0.8040	0.5410
Y	0.8330	0.4590
YA	0.8000	0.3910
YB	0.7630	0.4680
YC	0.8890	0.4860
YD	0.7780	0.2770
YE	0.8930	0.5300

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Chain	Atom inclusion	Q-score
Z	0.8610	0.4340
ZA	0.7410	0.4490
ZB	0.7630	0.4570
ZC	0.6670	0.4550
ZD	0.6390	0.4140
ZE	0.7930	0.3920
a	0.8440	0.4410
aA	0.8330	0.4450
aB	0.7930	0.4980
aC	0.8520	0.4480
aD	0.5180	0.3540
aE	0.6050	0.3810
b	0.7780	0.4510
bA	0.8330	0.4410
bB	0.8280	0.5180
bC	0.5000	0.2290
bD	0.7780	0.4130
bE	0.7590	0.4020
c	0.8060	0.4370
cA	0.7780	0.4530
cB	0.8970	0.5360
cC	0.5280	0.3360
cD	0.6810	0.4300
cE	0.7660	0.3640
d	0.7780	0.4580
dA	0.8610	0.3890
dB	0.8420	0.4970
dC	0.6300	0.3600
dD	0.6580	0.4100
dE	0.7140	0.4370
e	0.8150	0.4870
eA	0.9170	0.4630
eB	0.9150	0.5530
eC	0.6300	0.4180
eD	0.7630	0.3990
eE	0.7860	0.4490
f	0.9440	0.5040
fA	0.6940	0.4290
fB	0.7870	0.5330
fC	0.5750	0.3830
fD	0.7230	0.4490
fE	0.8720	0.4850

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Chain	Atom inclusion	Q-score
g	0.8330	0.4840
gA	0.8150	0.4250
gB	0.8280	0.5060
gC	0.6580	0.4490
gD	0.6390	0.4450
gE	0.8160	0.4100
h	0.7500	0.4980
hA	0.8330	0.4740
hB	0.0000	0.1560
hC	0.7890	0.4280
hD	0.6320	0.3890
hE	0.8420	0.5460
i	0.8520	0.4700
iA	0.7780	0.4720
iB	0.0000	0.2310
iC	0.6170	0.4160
iD	0.6670	0.4500
iE	0.7680	0.4430
j	0.8890	0.4050
jA	0.8150	0.4760
jB	0.0260	0.2520
jC	0.7220	0.4740
jD	0.6670	0.3890
jE	0.6580	0.4430
k	0.6670	0.4760
kA	0.7780	0.4850
kB	0.0790	0.3290
kC	0.6050	0.4680
kD	0.5000	0.3100
kE	0.7870	0.5230
l	0.8520	0.5100
lA	0.7450	0.5000
lB	0.1280	0.2920
lC	0.7410	0.4410
lD	0.4070	0.3160
lE	0.7140	0.4250
m	0.8150	0.5080
mA	0.7630	0.4890
mB	0.1940	0.3010
mC	0.4890	0.3020
mD	0.4440	0.3290
mE	0.6900	0.3890

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Chain	Atom inclusion	Q-score
n	0.8080	0.5140
nA	0.8950	0.5250
nB	0.1840	0.3300
nC	0.5280	0.3920
nD	0.5560	0.3220
nE	0.6550	0.3630
o	0.7630	0.5030
oA	0.8510	0.5520
oB	0.3330	0.3180
oC	0.5180	0.3730
oD	0.4440	0.2630
oE	0.7590	0.4430
p	0.8680	0.5220
pA	0.8330	0.5440
pB	0.2220	0.2920
pC	0.6300	0.4570
pD	0.3330	0.2780
pE	0.7230	0.4180
q	0.8720	0.5400
qA	0.7890	0.5110
qB	0.3330	0.3340
qC	0.6300	0.4800
qD	0.4440	0.3680
qE	0.9470	0.4750
r	0.8890	0.5240
rA	0.8520	0.5530
rB	0.2220	0.3440
rC	0.2220	0.2050
rD	0.4440	0.3570
rE	0.6170	0.3780
s	0.8680	0.5100
sA	0.8220	0.5170
sB	0.5180	0.4020
sC	0.2960	0.1860
sD	0.3560	0.2430
sE	0.7630	0.4880
t	0.8890	0.5320
tA	0.8060	0.5160
tB	0.4810	0.3170
tC	0.5180	0.3590
tD	0.2630	0.1910
tE	0.8300	0.4560

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Chain	Atom inclusion	Q-score
u	0.8000	0.4770
uA	0.8150	0.5290
uB	0.5180	0.3210
uC	0.2960	0.4020
uD	0.1380	0.3240
uE	0.8420	0.4630
v	0.8060	0.5020
vA	0.8150	0.5300
vB	0.4810	0.3010
vC	0.4220	0.3310
vD	0.3160	0.3560
vE	0.8300	0.5180
w	0.7780	0.4950
wA	0.8520	0.5070
wB	0.7040	0.4330
wC	0.3420	0.1360
wD	0.3420	0.3580
wE	0.8210	0.4240
x	0.7040	0.4250
xA	0.8520	0.5250
xB	0.8520	0.5470
xC	0.1380	0.2600
xD	0.1030	0.2690
xE	0.7630	0.4430
y	0.8520	0.5030
yA	0.8520	0.5570
yB	0.7110	0.4230
yC	0.3420	0.2610
yD	0.0000	0.2070
yE	0.7660	0.4270
z	0.7780	0.4980
zA	0.8890	0.5340
zB	0.6320	0.3580
zC	0.1050	0.2530
zD	0.0000	0.1780
zE	0.6810	0.4300