Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Diels-Alder reactions of 4-halo masked *o*-benzoquinones. Experimental and theoretical investigations

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Supplementary Information

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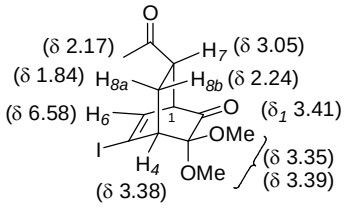
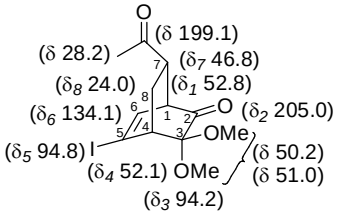
Table S1: Complete connectivity assignment of **11c**.



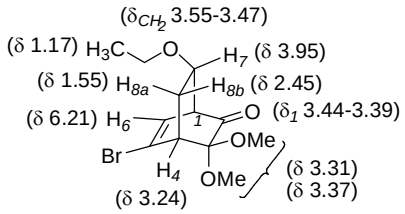
11c (^{1}H chemical shifts)



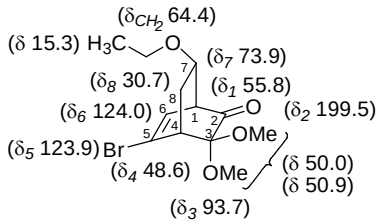
11c (^{13}C chemical shifts)

Carbon	^{13}C (ppm)	COSY (^{1}H-^{1}H)	Connectivity from		ROESY
			HMQC	HMBC	
1	52.8	H_1-H_6	H_1		H_1-H_6, H_1-H_7
2	205.0		-		
3	94.2				
4	52.1		H_4	H_6 H_7	H_4-H_{8a} H_4-H_{8b}
5	94.8		-	H_1 H_4 H_6	
6	134.1	H_6-H_1	H_6	H_1 H_4 H_7	H_6-CH_3 H_6-H_7 (weak)
7	46.8	H_7-H_{8a} H_7-H_{8b}	H_7	H_1 H_7 H_{8a} H_{8b}	H_7-H_1 H_7-H_6 H_7-H_{8a} (weak) H_7-H_{8b}
8	24.0	H_{8a}- H_7 H_{8b}- H_7	H_{8a} H_{8b}	H_6 H_1 H_7	H_{8a}-H_4 H_{8b}-H_4 H_{8a}-H_{8b} H_{8a}-CH_3
OMe	50.2 51.0		-		
CO (Acetyl)	199.1				
CH_3 (Acetyl)	28.2				CH_3- H_6 CH_3- H_{8a}

Table S2: Complete connectivity assignment of **14c**.



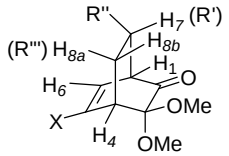
14c (^{1}H chemical shifts)



14c (^{13}C chemical shifts)

Carbon	^{13}C (ppm)	COSY (^{1}H-^{1}H)	Connectivity from		ROESY
			HMQC	HMBC	
1	55.8	H_1-H_6	H_1	H_6	H_1-H_7
2	199.5		-		
3	93.7				
4	48.6		H_4	H_6 OMe	H_4-H_{8a}
5	123.9		-	H_4 H_6 C_1-H_a	
6	124.0	H_6-H_1	H_6	H_1 H_4 H_7	H_6-H_1 H_6-CH_2
7	74.0	H_7-H_{8a}	H_7	H_1 H_4 OCH_2	H_7-H_{8a} H_7-H_{8b}
8	30.7	H_{8a}-H_7 H_{8b}-H_{8a}	H_{8a} H_{8b}	H_1	H_{8a}-H_{8b}
OMe	50.0 50.9			H_4	
CH_2 (ethyl)	64.4	CH_3-CH_2	-		
CH_3 (ethyl)	15.3		-		H_1-H_7

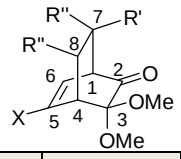
Table S3: Selected ^{1}H chemical shifts (in ppm) of Diels-Alder adducts derived from 4-halo MOBs.



S.No.	Adduct	H-1	H-4	H-6	H-7	H-8a	H-8b
1	**9a**	3.52	3.17	5.35-5.31	3.02-3.00	2.11	2.29
2	**9b**	3.34	3.09	5.36-5.33	-	1.84	2.61
3	**9c**	3.46	3.18	5.28	3.04-3.01	2.06	2.22
4	**10a**	3.57	3.24	6.05	3.04	2.02	2.34
5	**10b**	3.40	3.17	6.07	-	1.90	2.52
6	**10c**	3.50	3.25	6.02	3.07	1.92	2.30
7	**11a**	3.45	3.37	6.60	3.02	1.95	2.26
8	**11b**	3.30	3.30	6.63	-	1.84	2.45
9	**11c**	3.41-3.40	3.38-3.37	6.58	3.05	1.84	2.24
10	**12a**	3.21	3.26	5.32	3.38-3.35	1.89	2.57
11	**13a**	3.40-3.38	3.32-3.31	6.04	3.27	1.85	2.58
12	**13b**	3.57	3.16	5.99	3.97-3.94	1.56	2.46
13	**13c***	3.58	3.27	6.03-6.01	3.00	-	4.33
14	**13d**	3.56	3.15	5.97	3.95-3.92	1.55	2.45
15	**13e**	3.68-3.62	3.28	6.10	3.21	1.44	2.51
16	**14a**	3.35-3.30	3.35-3.30	6.27	3.25	1.84	2.56
17	**14b**	3.55-3.53	3.25-3.23	6.21	3.96-3.94	1.55	2.45
18	**14c***	3.56	3.37-3.36	6.26	3.04	-	4.33
19	**14d**	3.54	3.24	6.20	3.94-3.91	1.54	2.44
20	**14e**	3.66-3.60	3.30	6.33	3.26	1.49	2.60
21	**15a**	3.45	3.39-3.35	6.59	3.15	1.81	2.48
22	**15b**	3.52-3.39	3.28-3.27	6.53	3.96-3.93	1.52	2.38
23	**15c***	3.51	3.48	6.61	3.12-3.06	-	4.35
24	**15d**	3.45	3.27	6.52	3.95-3.90	1.53-1.48	2.36
25	**15e**	3.66-3.24	3.37-3.35	6.66	3.20	1.48	2.54

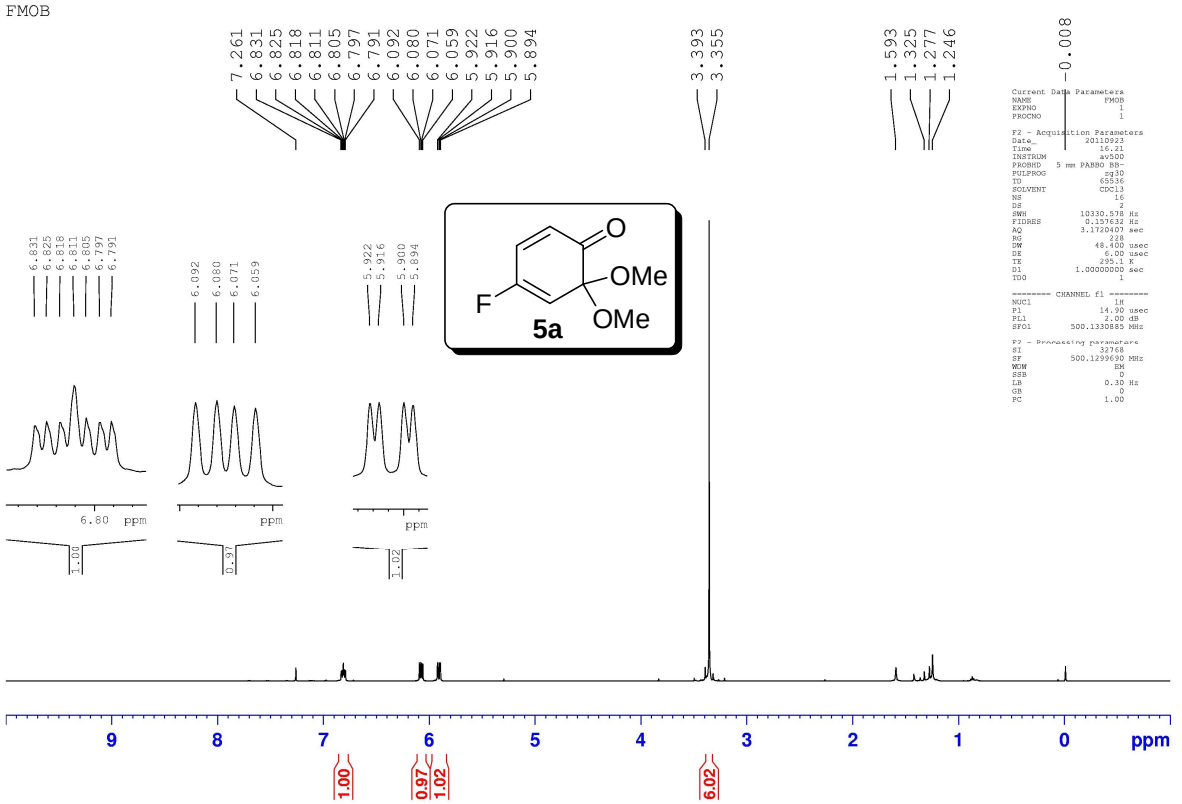
* The numbering of protons of these compounds is based on 3,3-dimethoxybicyclo[2.2.2]octen-2-one system.

Table S4: Selected ^{13}C chemical shifts (in ppm) of Diels-Alder adducts derived from 4-halo MOBs.



S.No.	Adduct	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8
1	**9a**	48.1 48.2	199.6	93.6	41.4 41.6	162.8 165.1	97.0 97.1	39.1	24.2
2	**9b**	54.4 54.5	200.8	93.9	41.5 41.6	163.2 165.4	98.8 98.9	46.8	30.6
3	**9c**	47.7 47.8	205.0	93.8	41.5 41.6	162.5 164.8	96.7 96.8	47.0	23.1
4	**10a**	50.1	199.2	93.5	47.4	137.1	120.4	39.0	24.7
5	**10b**	57.2	200.4	93.7	47.6	137.1	122.2	46.7	31.9
6	**10c**	50.3	204.9	93.6	46.9†	136.2	120.4	47.4†	23.7
7	**11a**	53.3	198.7	93.9	52.0	95.8	133.9	38.7	24.8
8	**11b**	59.8	200.0	94.1	52.2	95.7	135.8	46.3	32.0
9	**11c**	52.8†	205.0	94.2	52.1†	94.8	134.1	46.8	24.0
10	**12a**	53.1	200.5	93.6	42.2 42.4	163.0 165.2	96.9	39.7	30.1
11	**13a**	56.1	200.3	93.6	48.3	136.8	120.4	40.1	30.2
12	**13b**	54.6	199.8	93.4	46.9	136.0	119.4	74.1	30.6
13	**13c***	56.6	199.5	93.0	51.3	134.6	120.8	39.2	78.1
14	**13d**	54.6	200.0	93.5	46.9	136.0	119.4	74.3	30.6
15	**13e**	53.6	199.4	93.6	47.6	136.5	121.0	42.2	28.8
16	**14a**	57.3	199.8	93.8	50.2	124.9	125.2	40.0	30.3
17	**14b**	55.8	199.5	93.7	48.6	123.9	124.0	74.0	30.7
18	**14c***	56.9	199.2	93.3	52.6	122.5	125.6	39.6	78.0
19	**14d**	55.8	199.6	93.7	48.6	123.9	124.1	74.1	30.7
20	**14e**	54.7	199.2	93.8	49.3	124.4	125.6	41.9	28.9
21	**15a**	58.8	199.6	94.0	53.1	95.9	134.2	39.8	30.1
22	**15b**	57.2	199.2	93.8	51.3	94.7	132.8	73.8	30.4
23	**15c***	58.5	199.0	93.6	54.7	93.1	134.5	39.9	77.9
24	**15d**	57.2	199.4	93.9	51.4	94.7	132.9	74.0	30.5
25	**15e**	56.2	199.0	94.0	52.3	95.3	134.5	41.7	28.7

* The numbering of carbons of these compounds is based on 3,3-dimethoxybicyclo[2.2.2]octen-2-one system.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5.916
5.900
5.894
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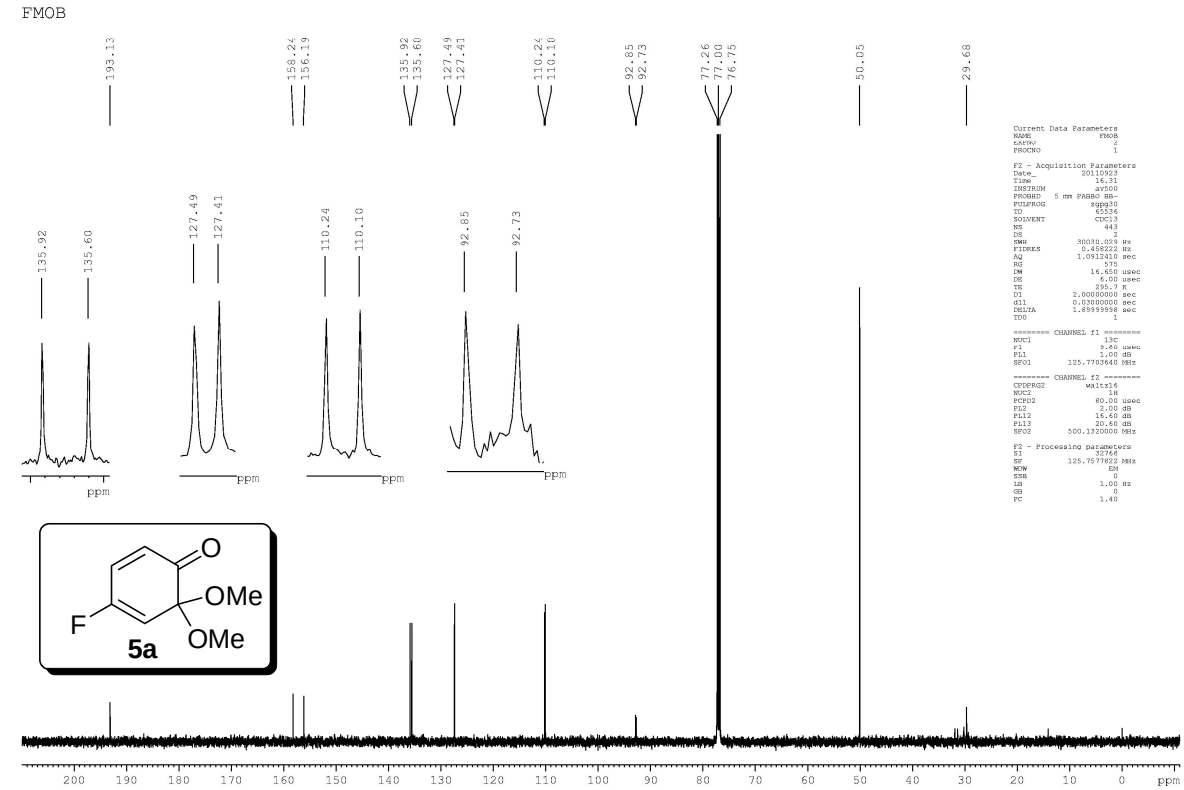
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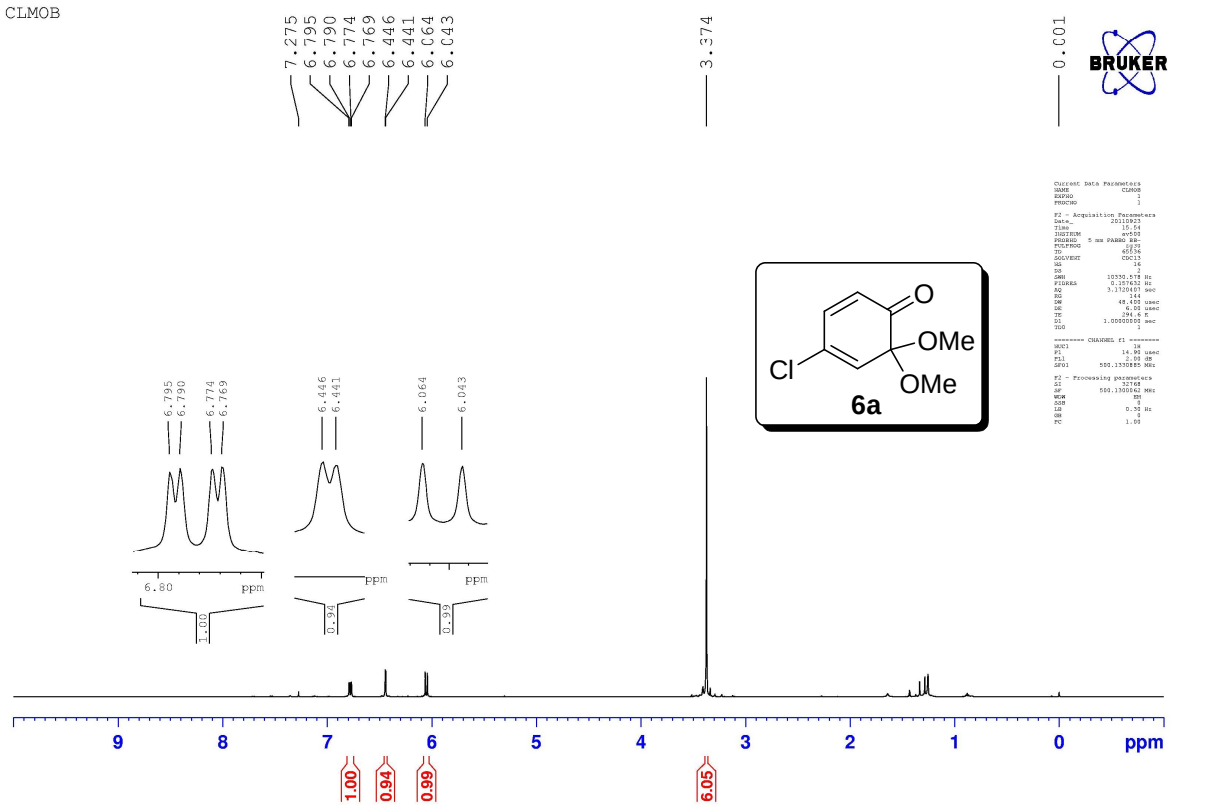
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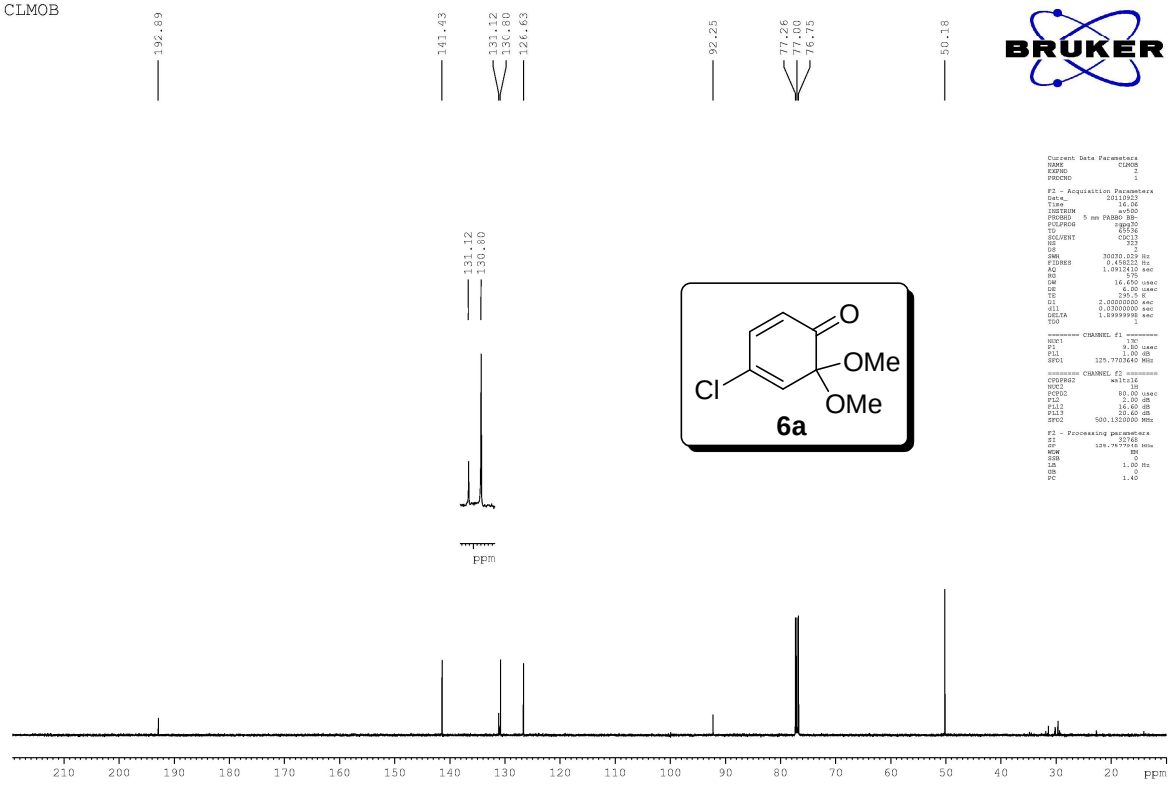
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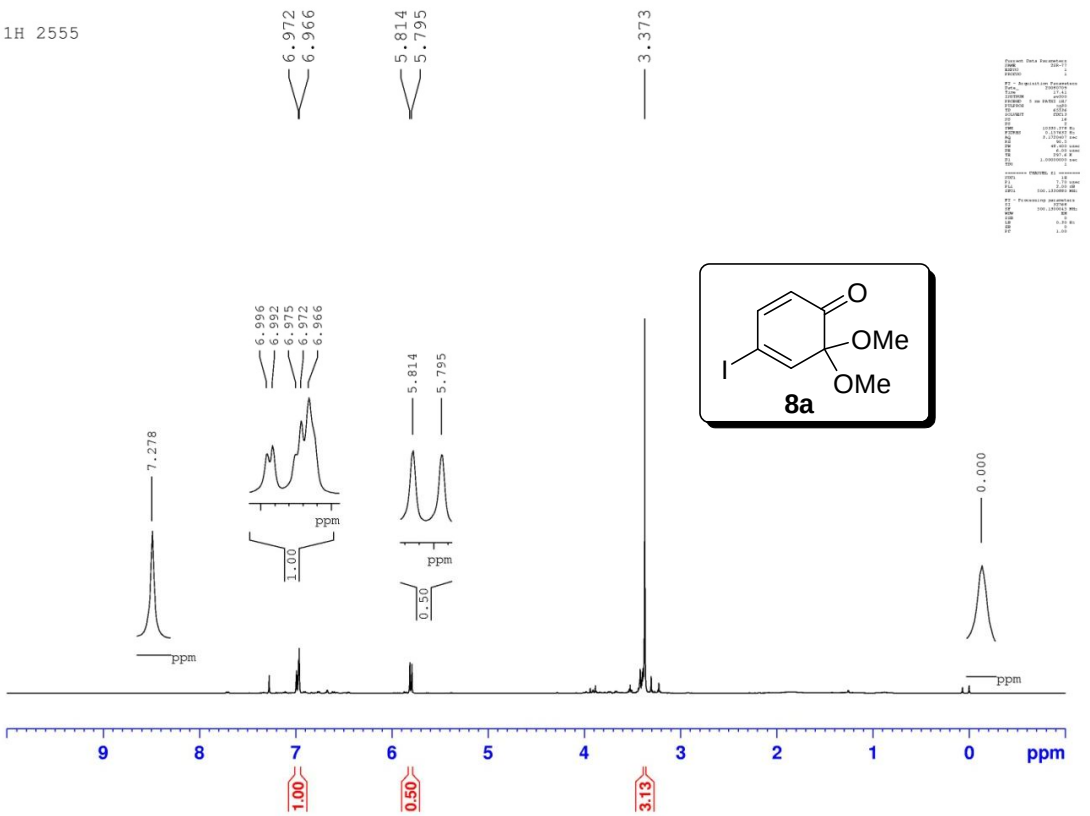
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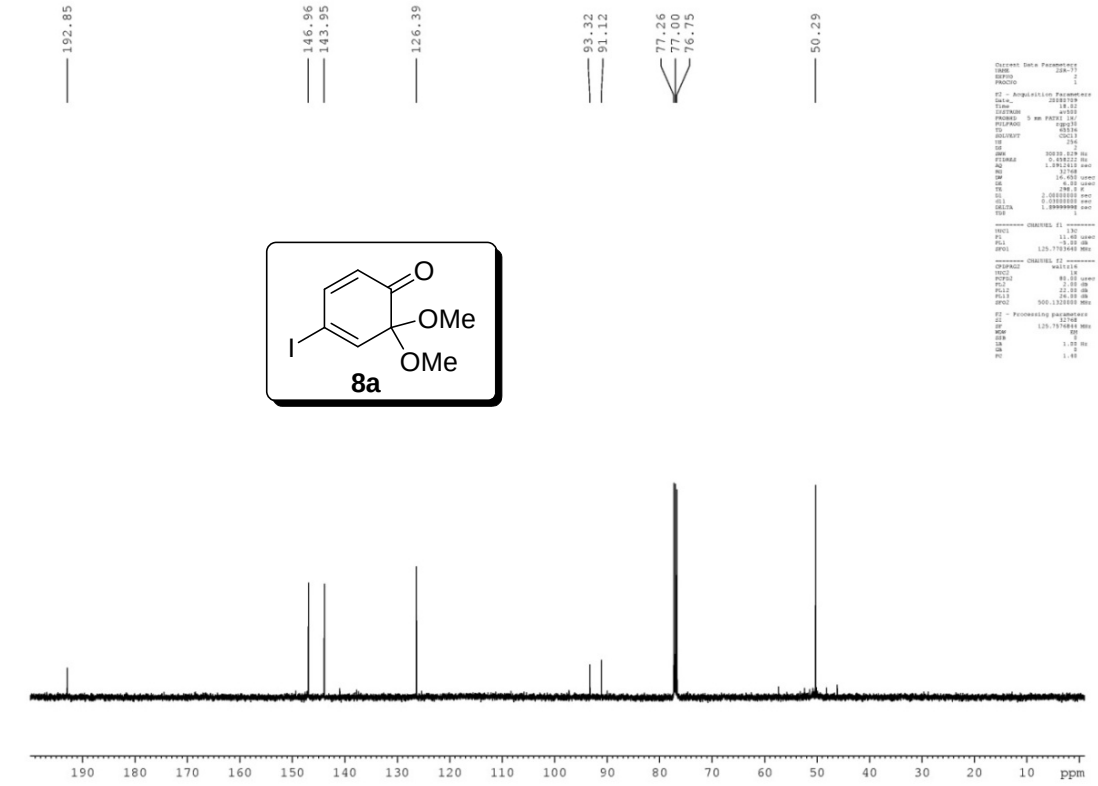
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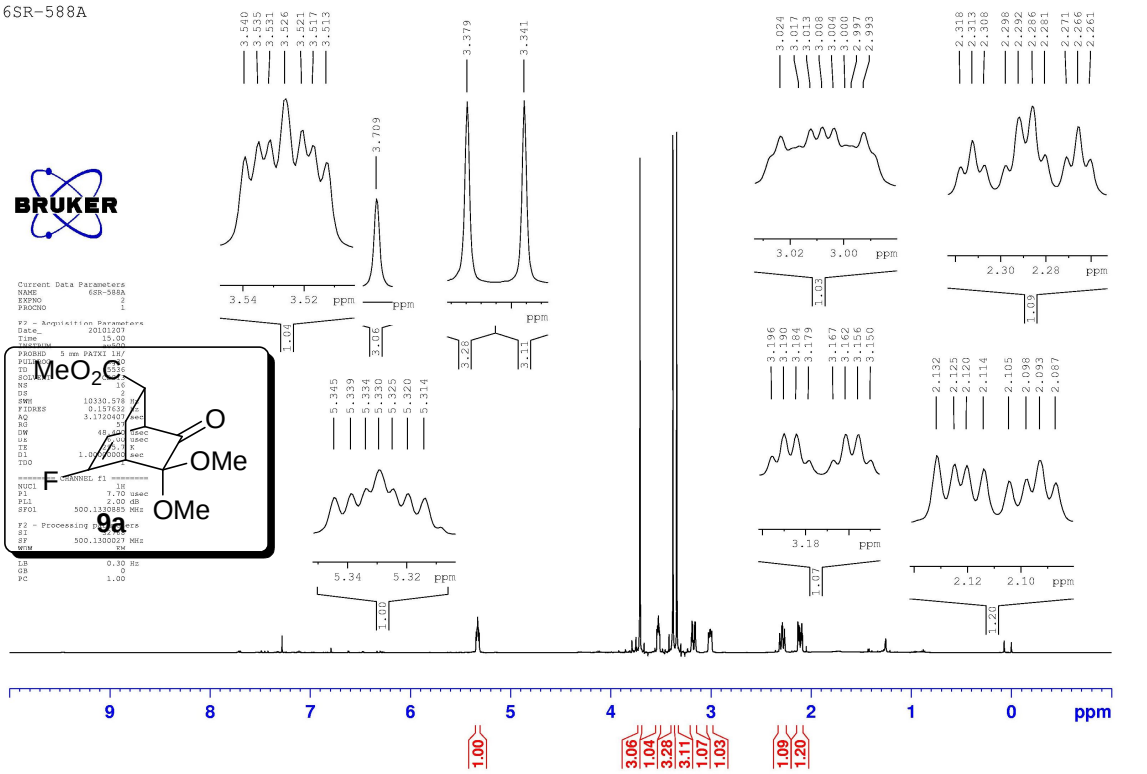
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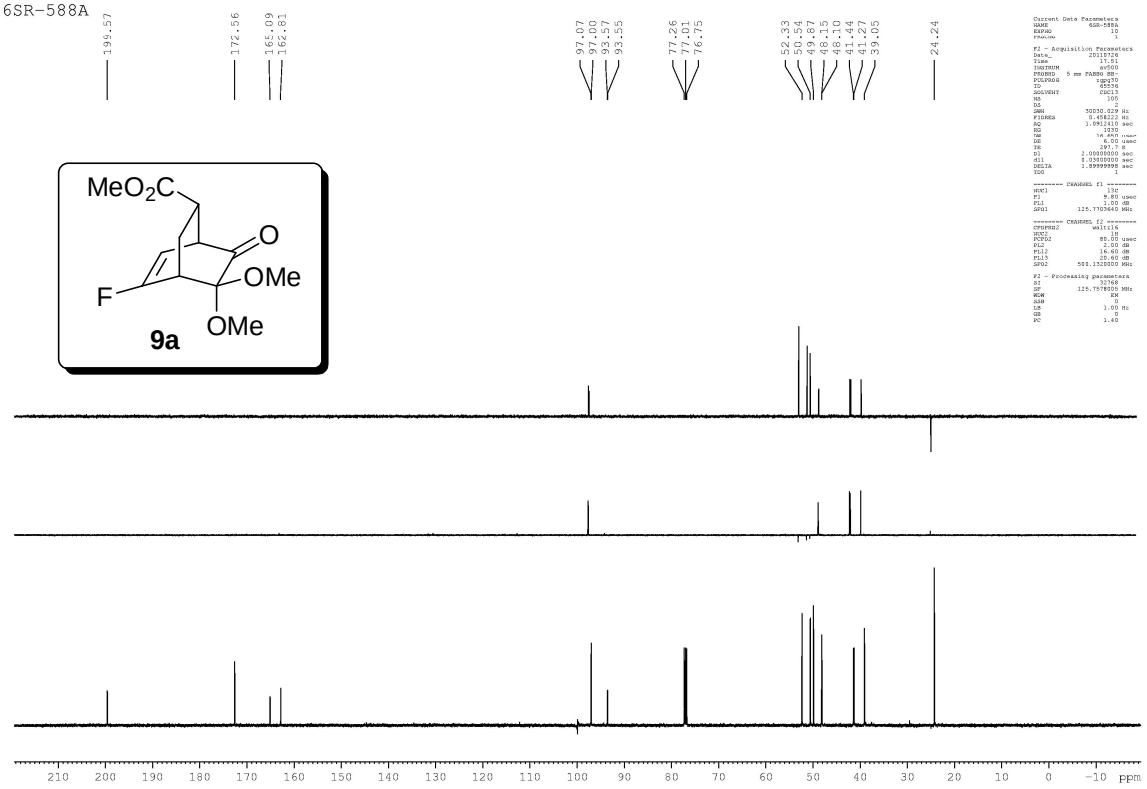
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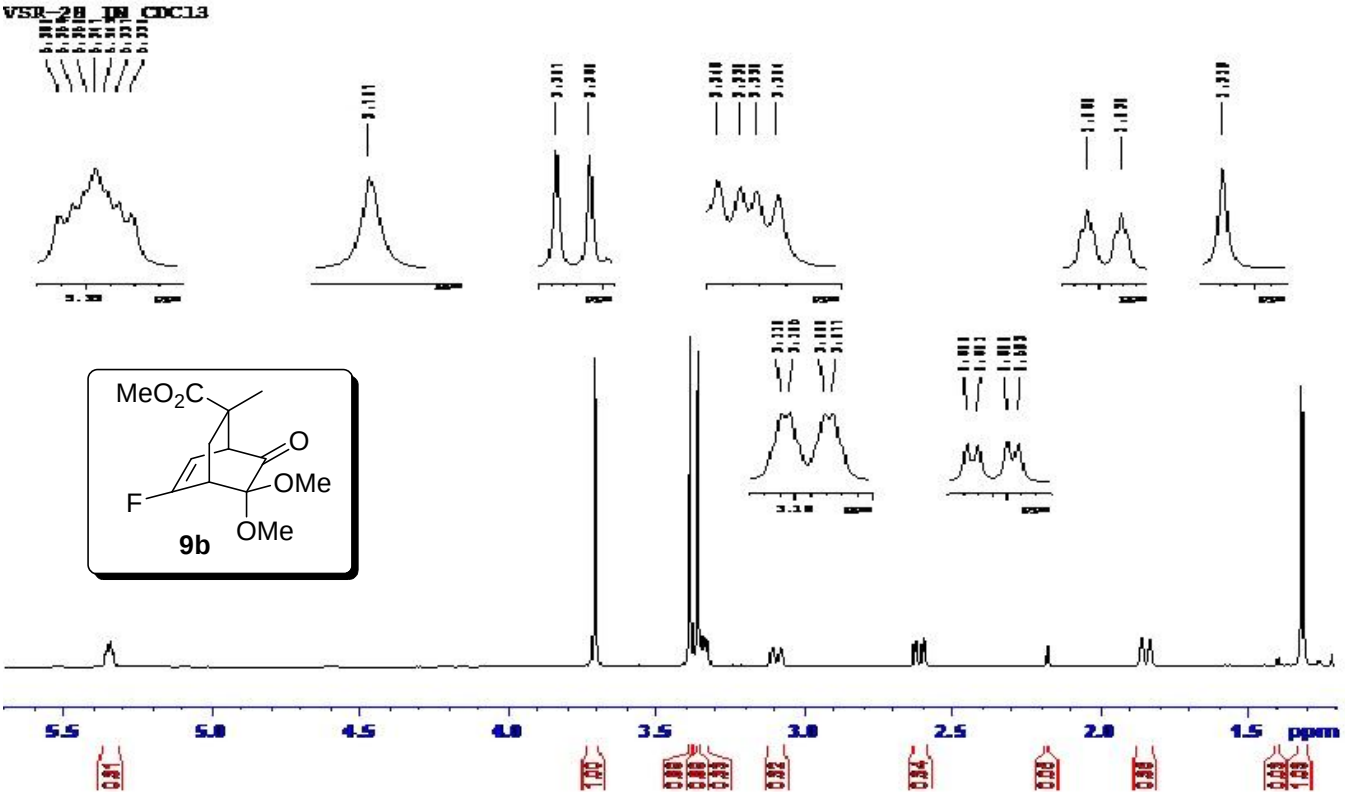
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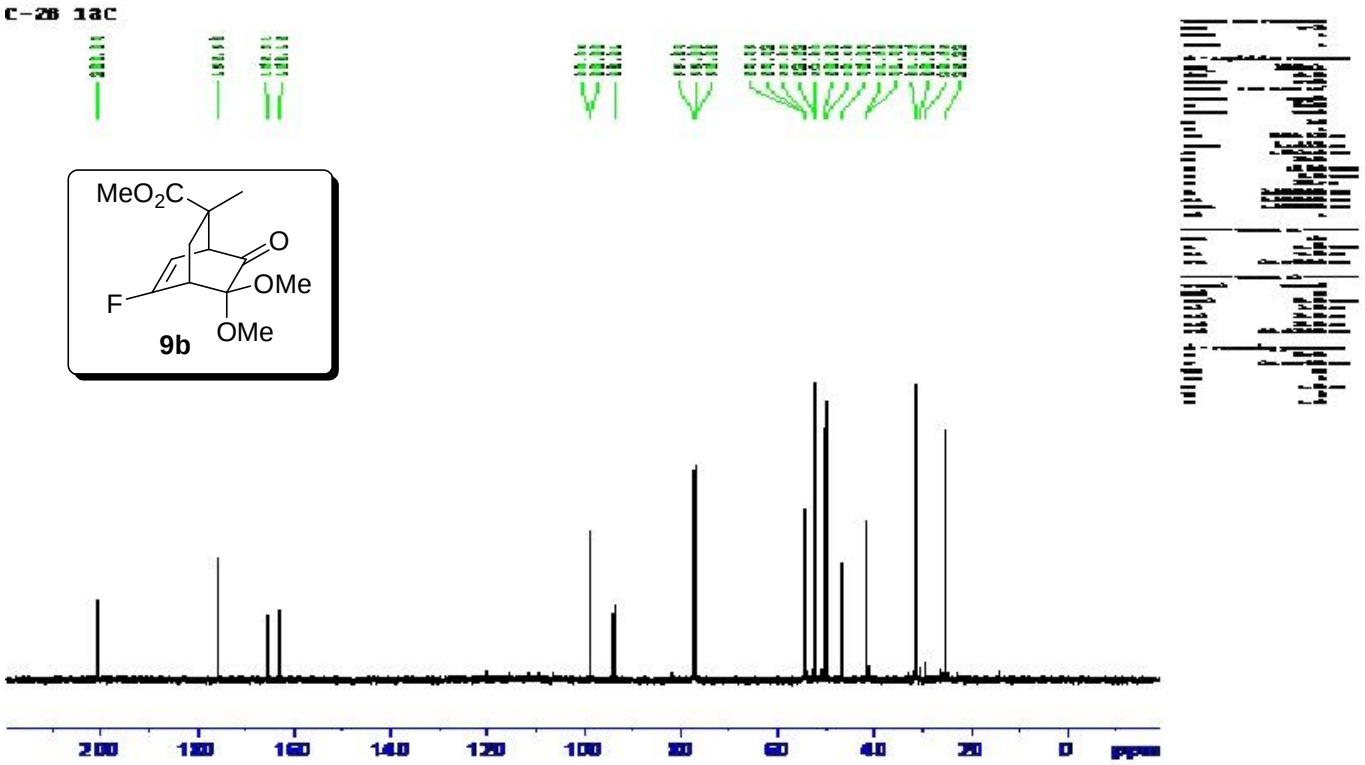
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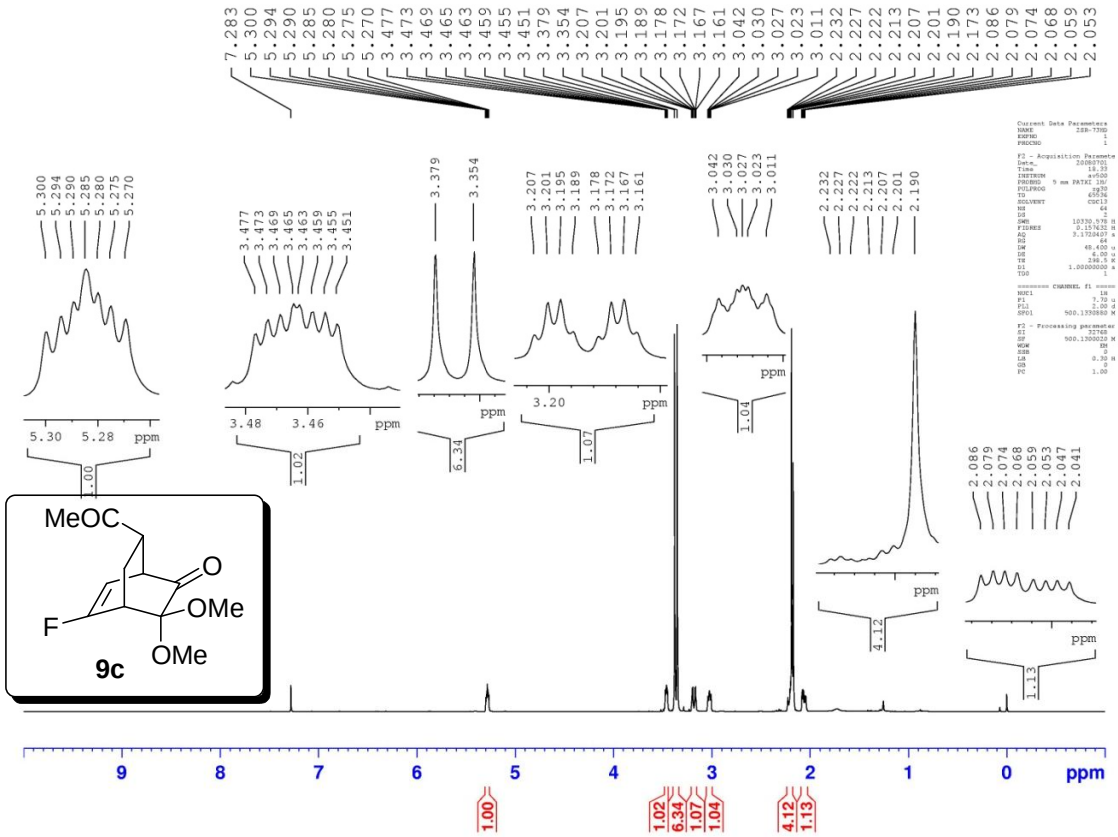
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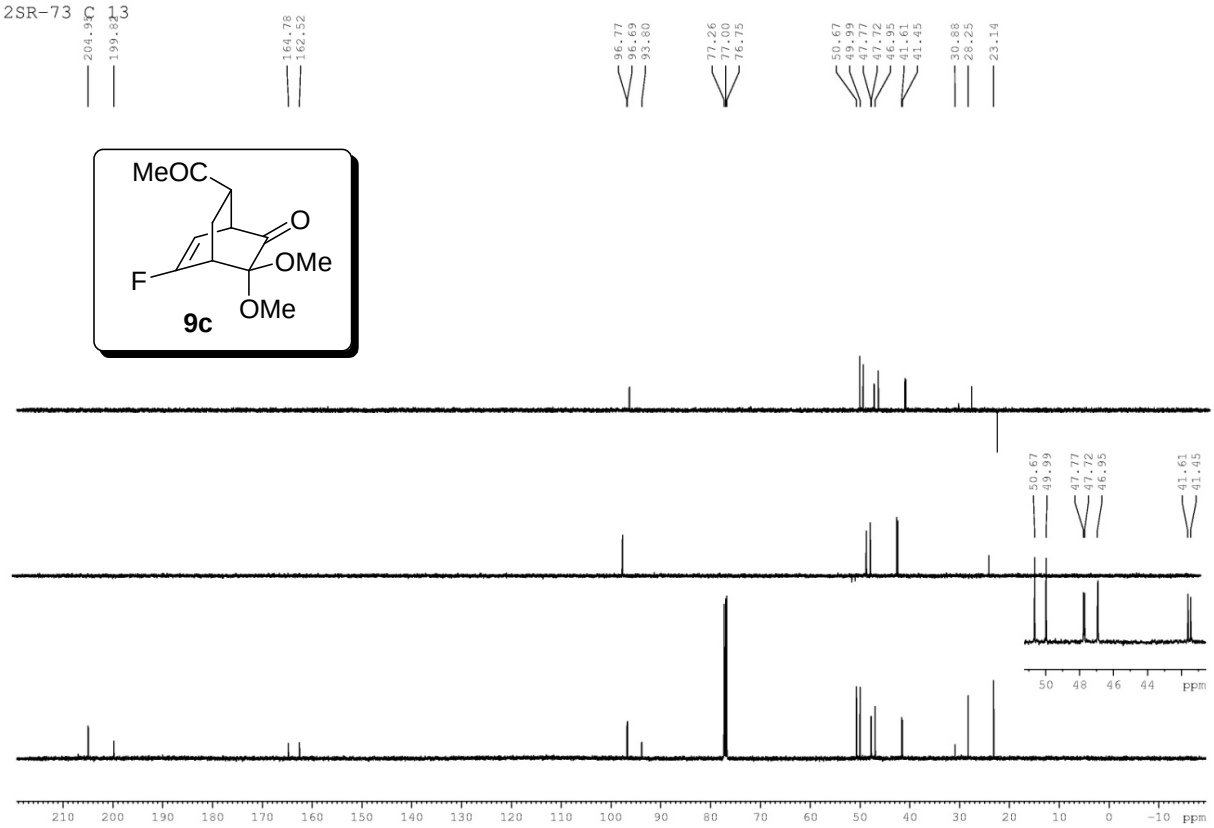
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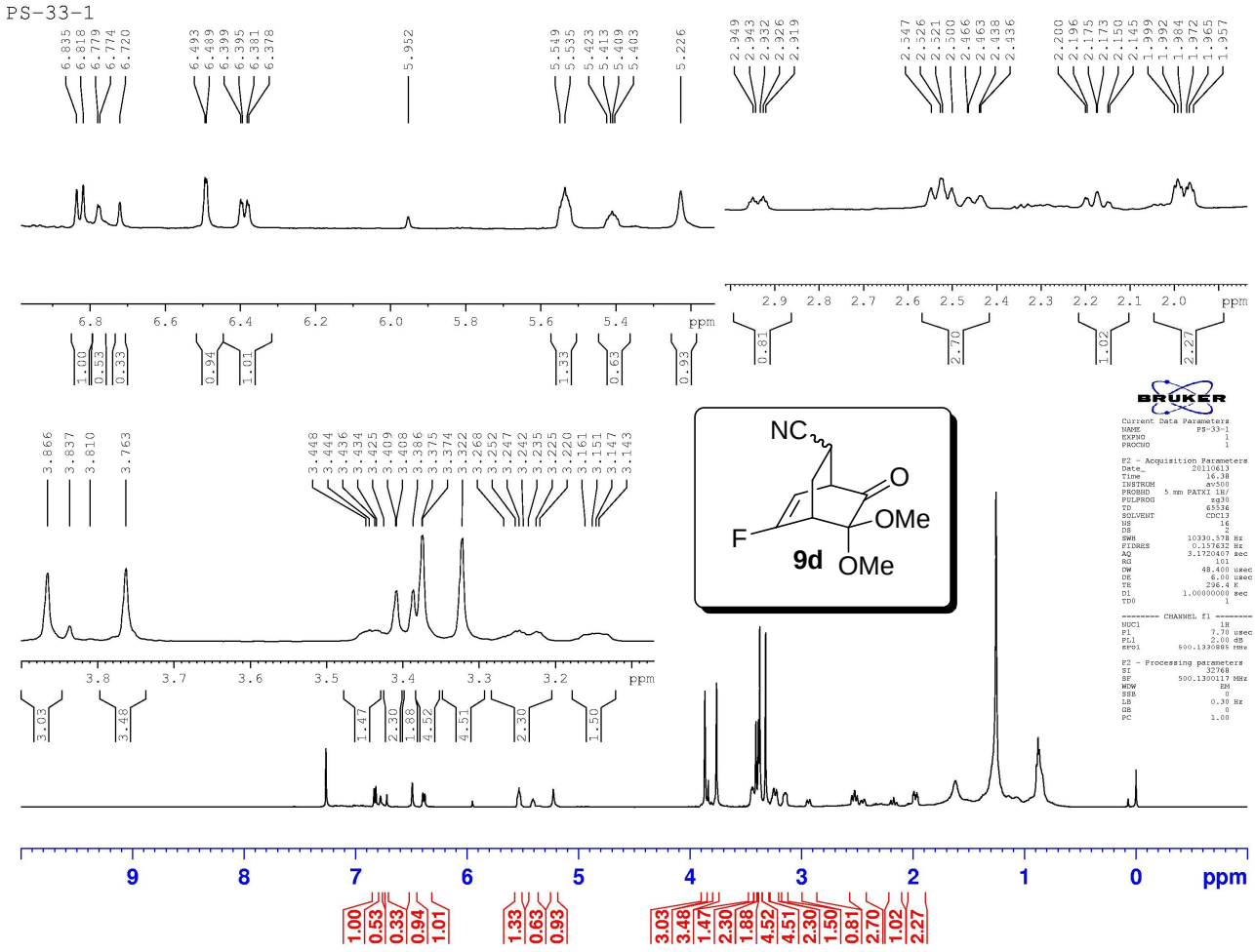
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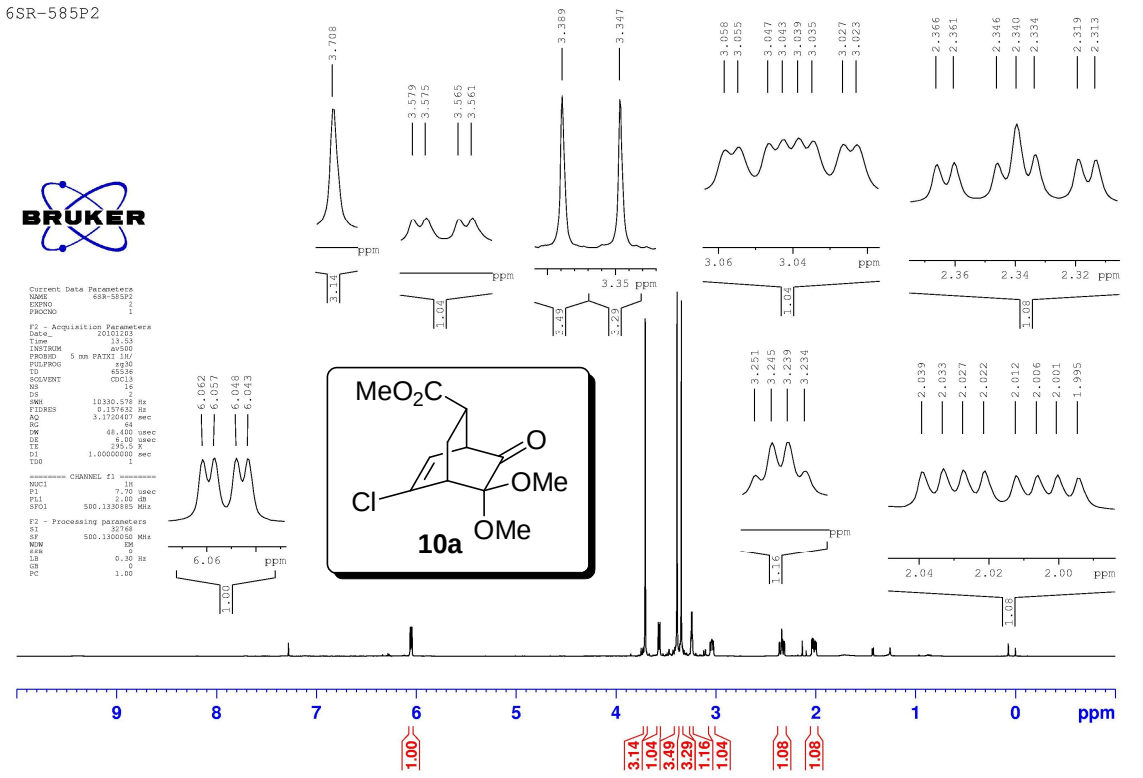
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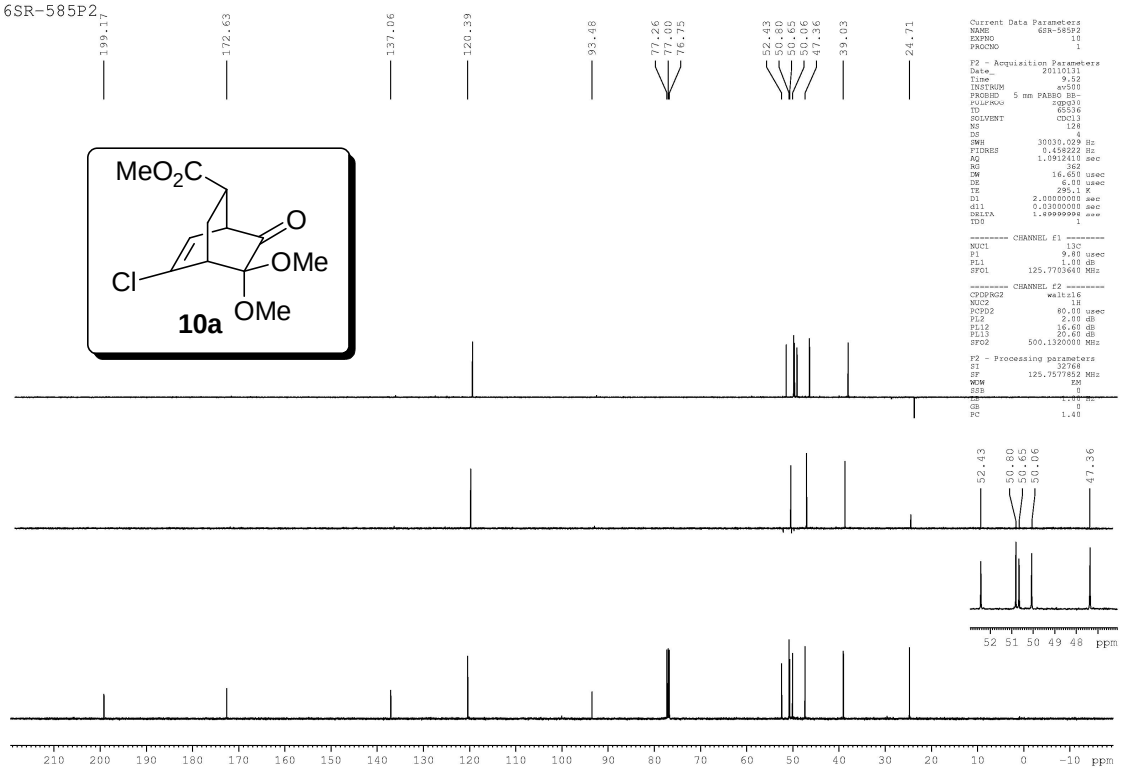
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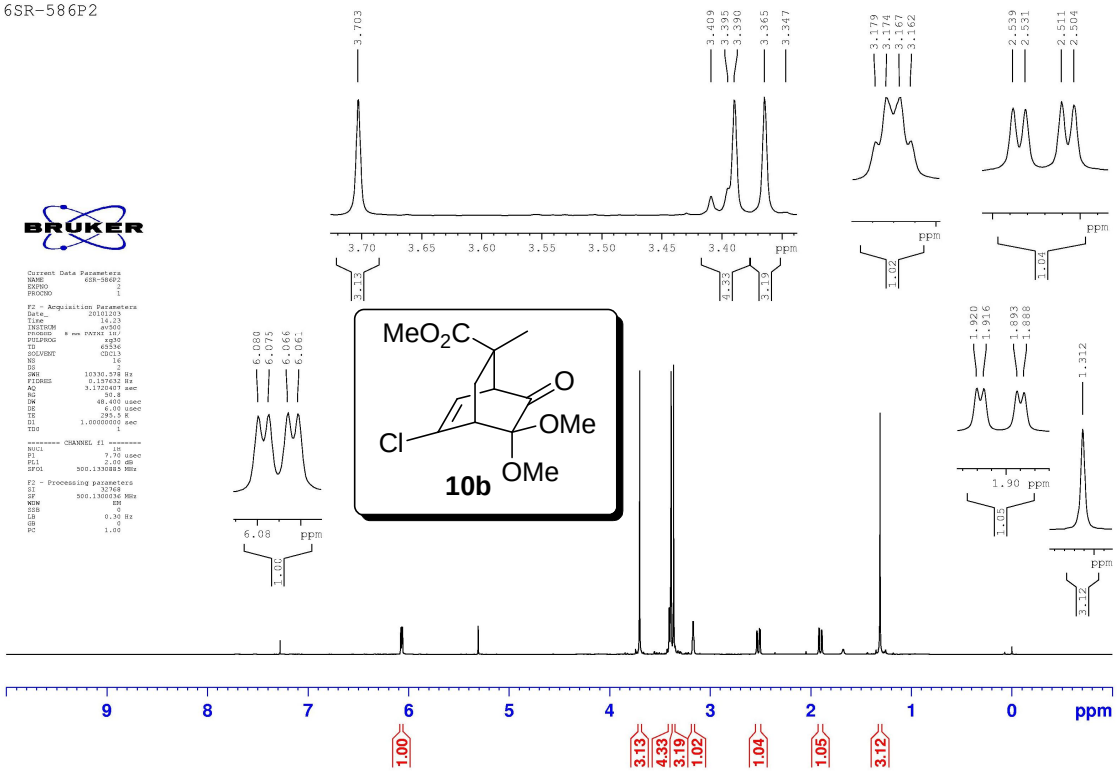

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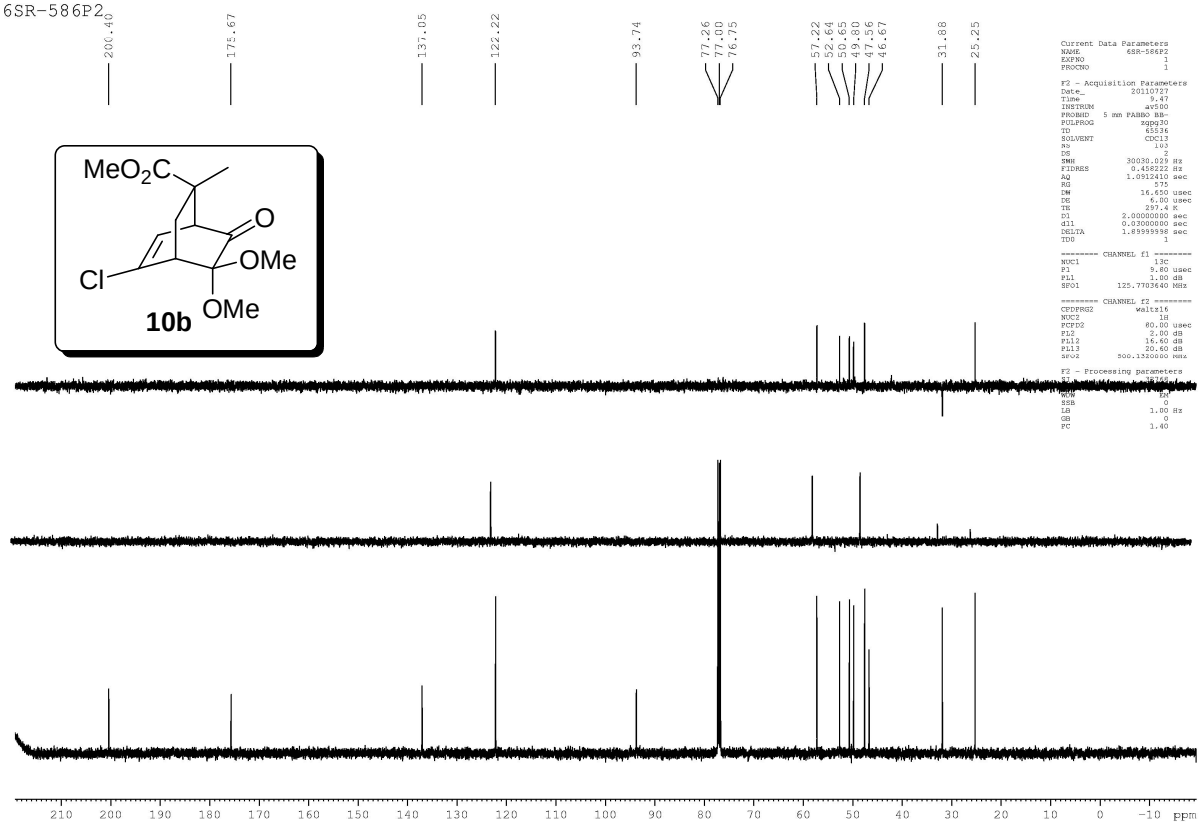

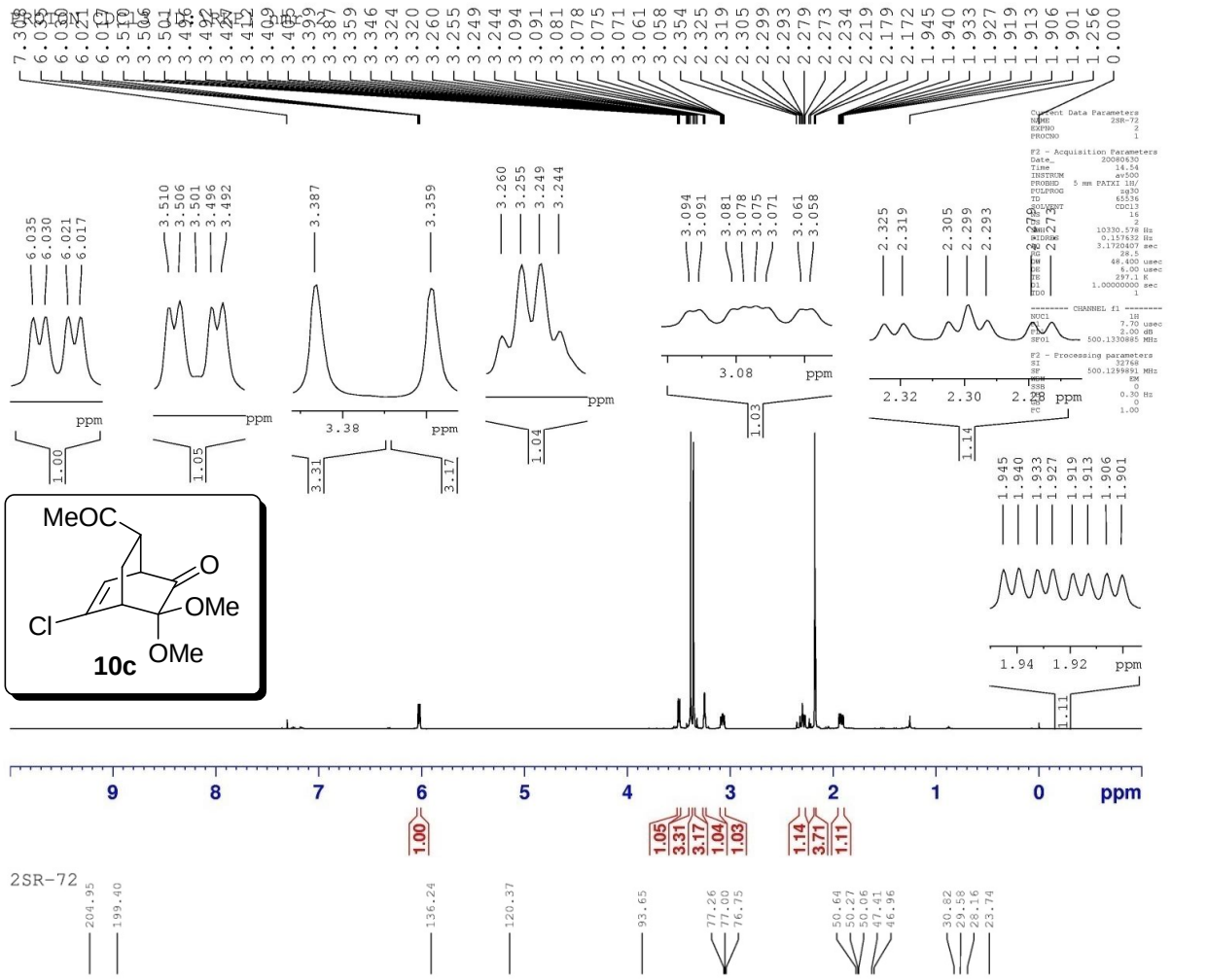
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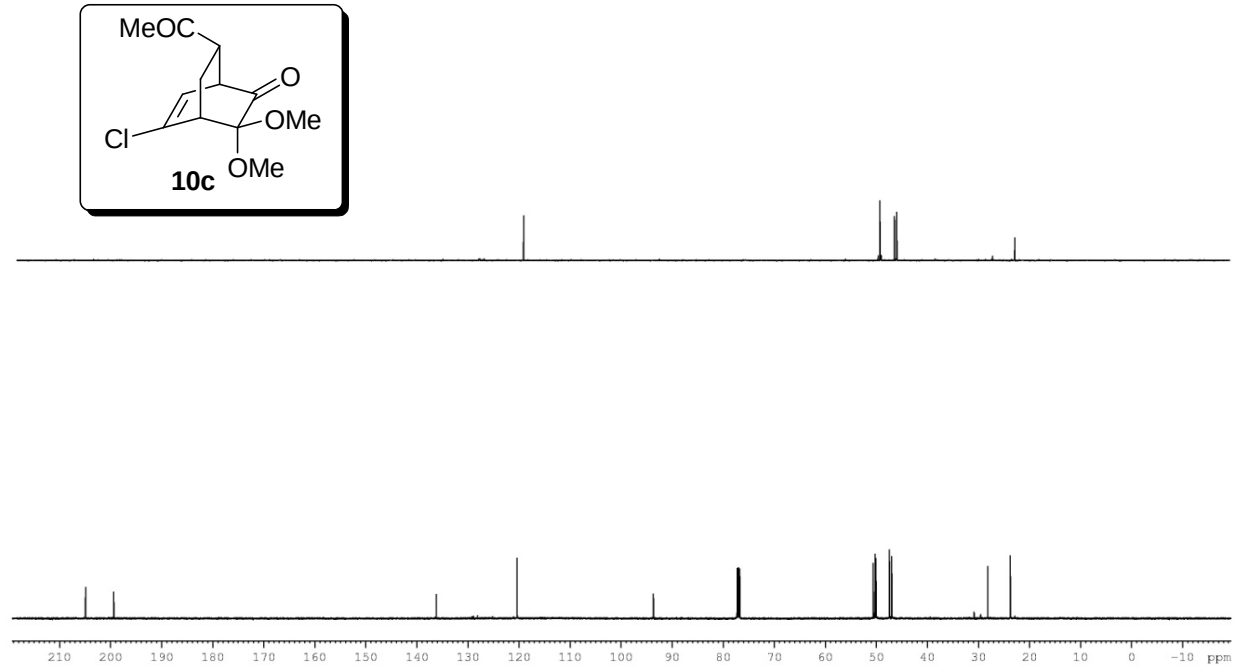
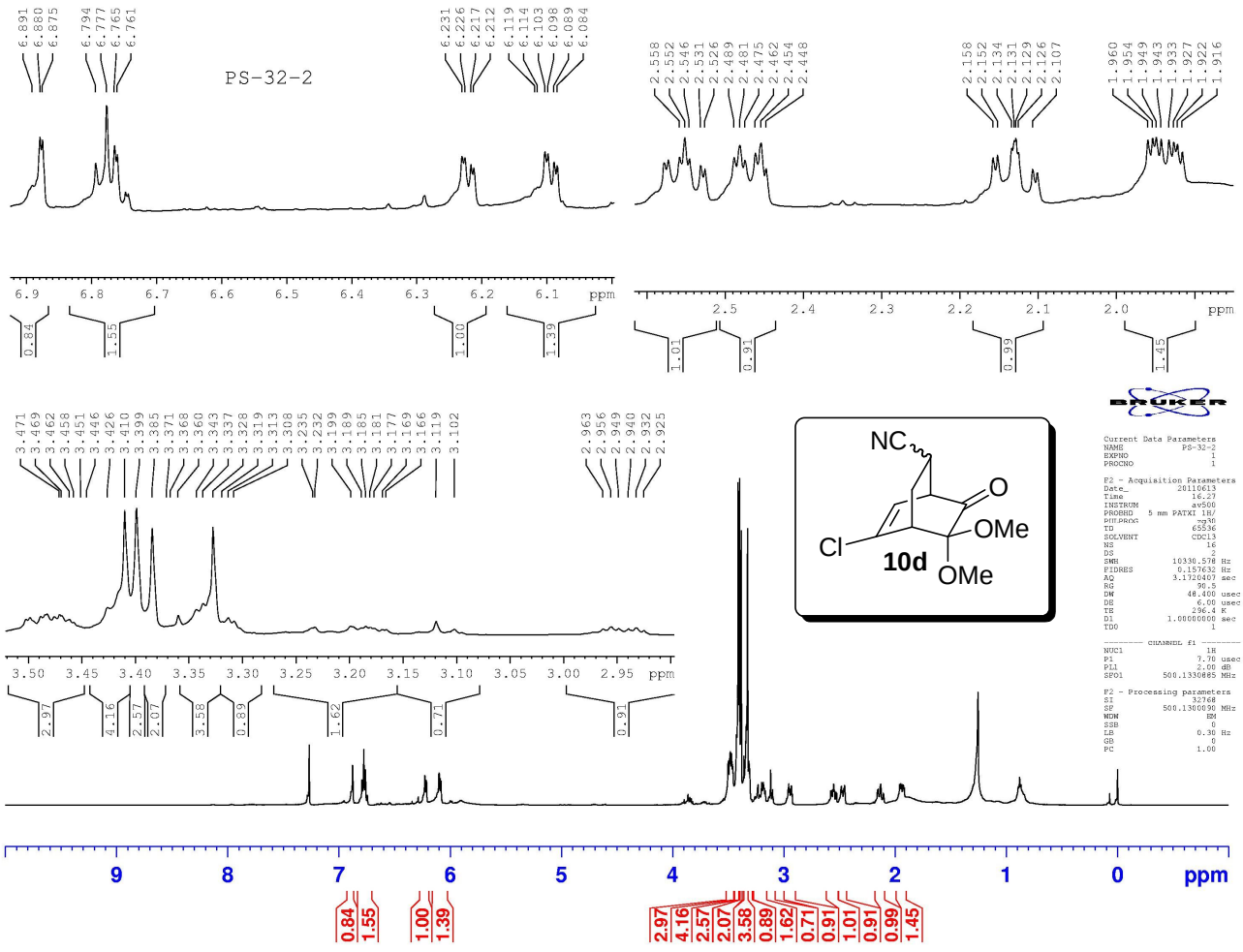
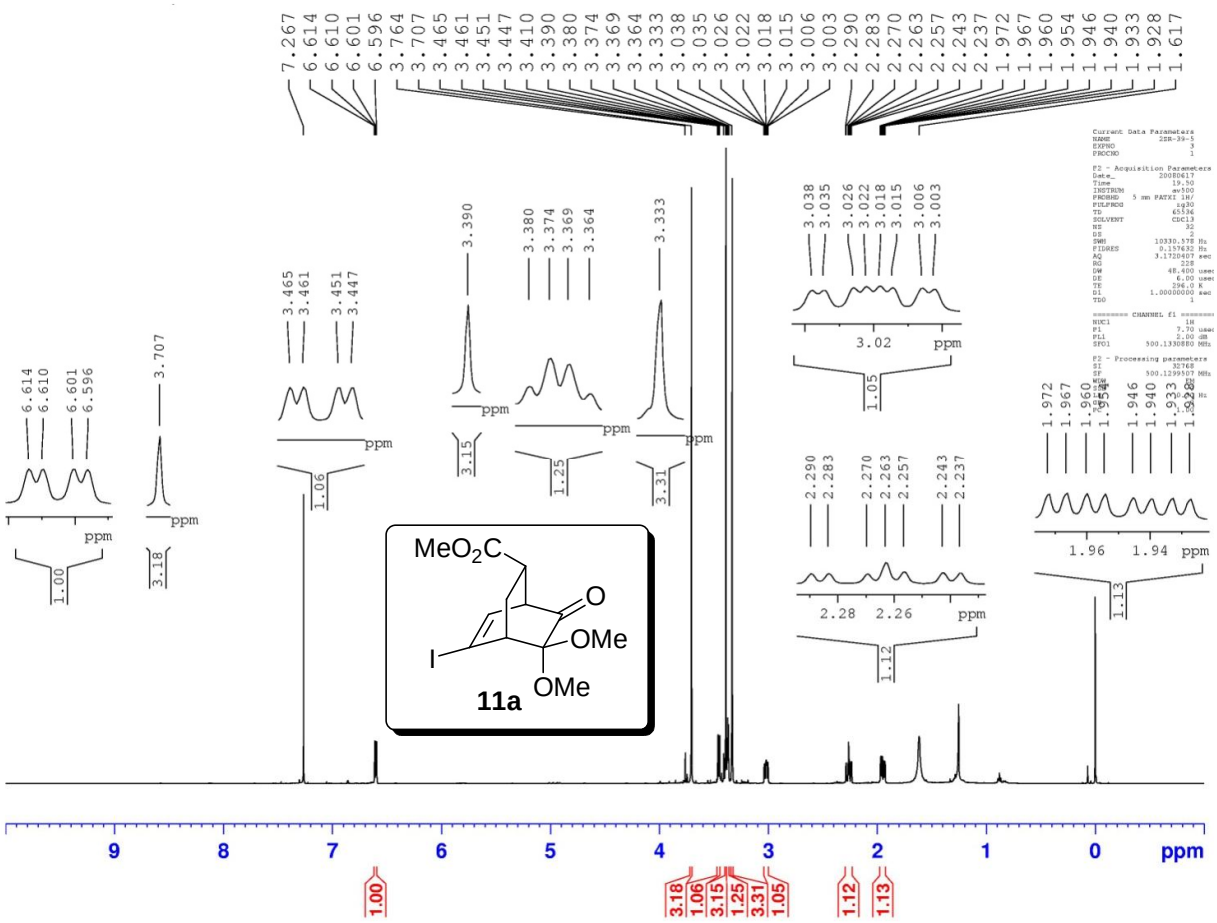
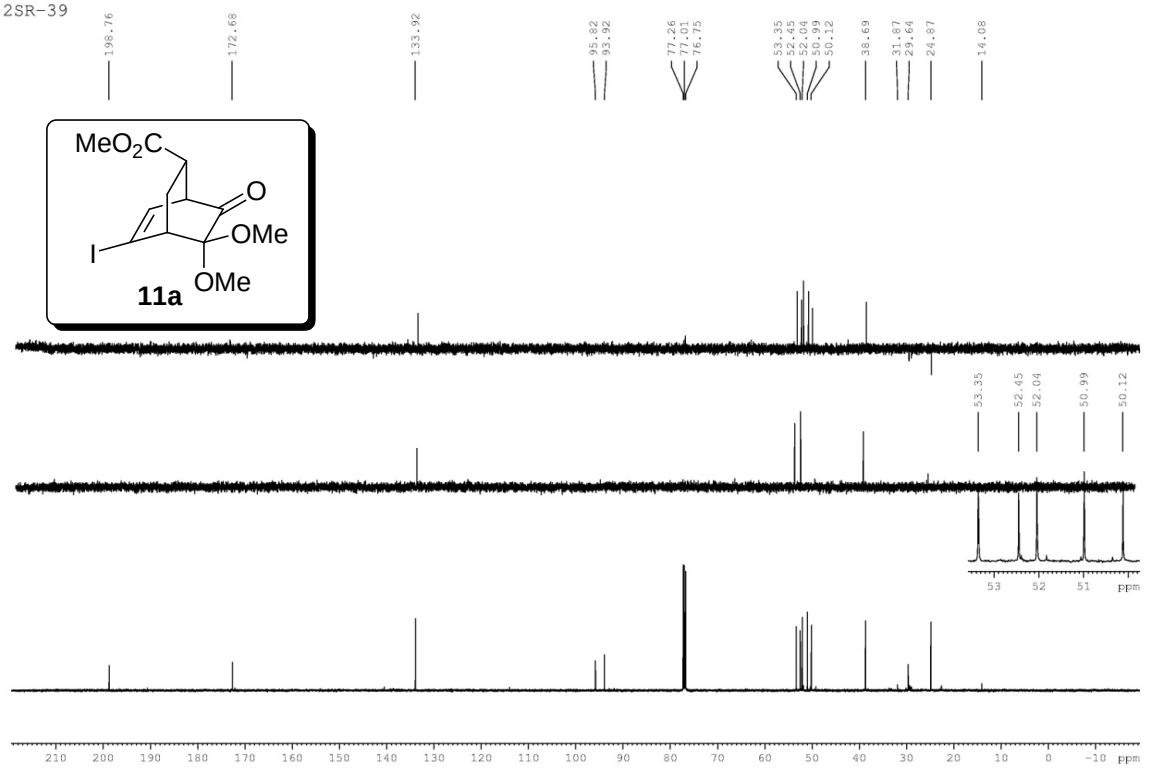
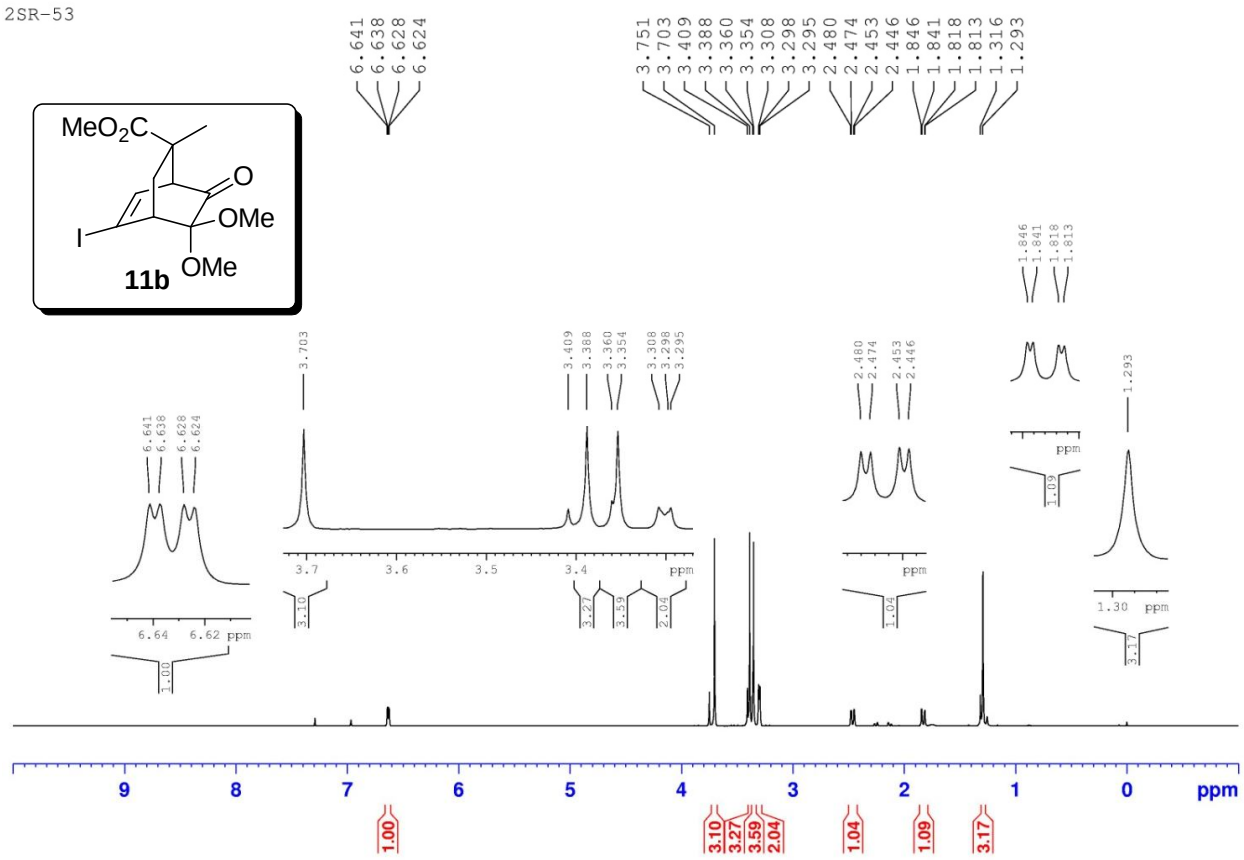
10c

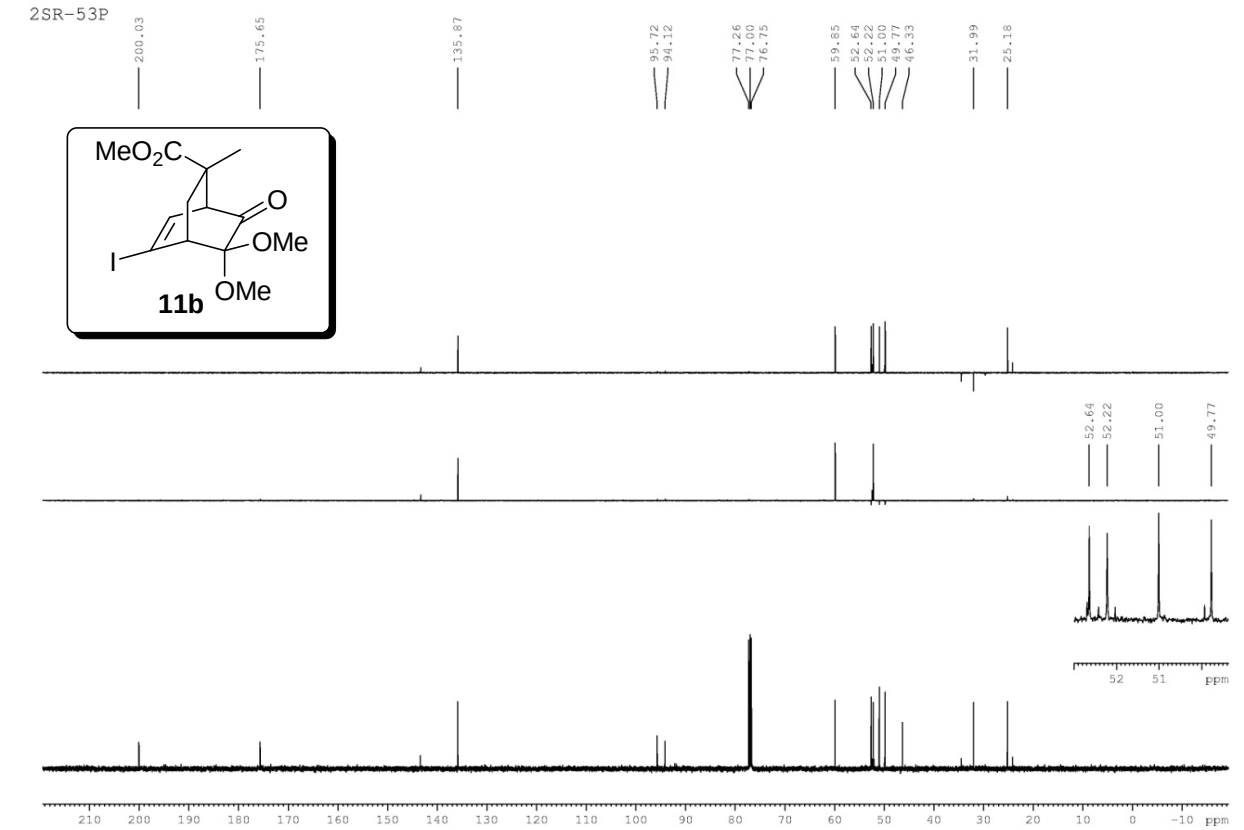

2SR-72
MeOC
O
Cl
OMe
OMe
10c

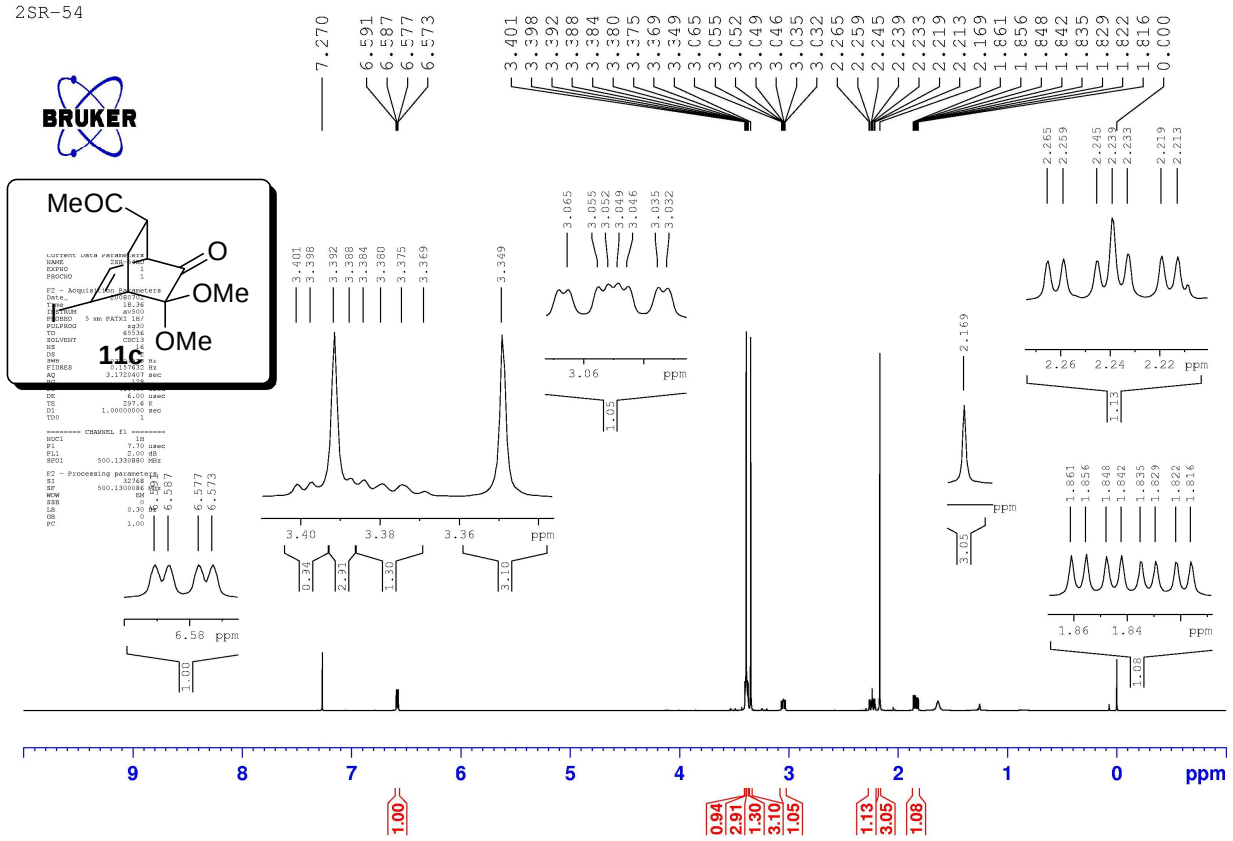

PS-32-2
NC
O
OMe
Cl
10d
OMe
ppm

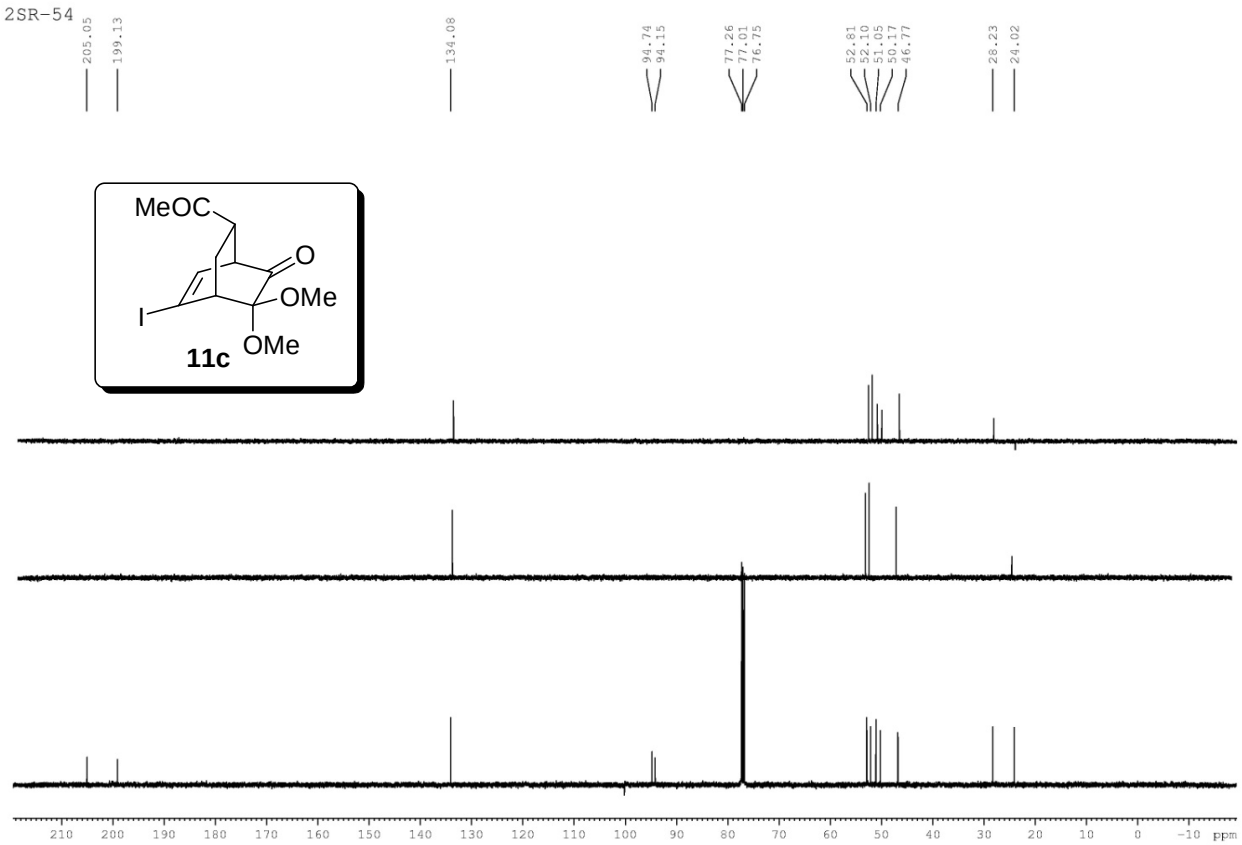

MeO2C
O
OMe
I
OMe
11a

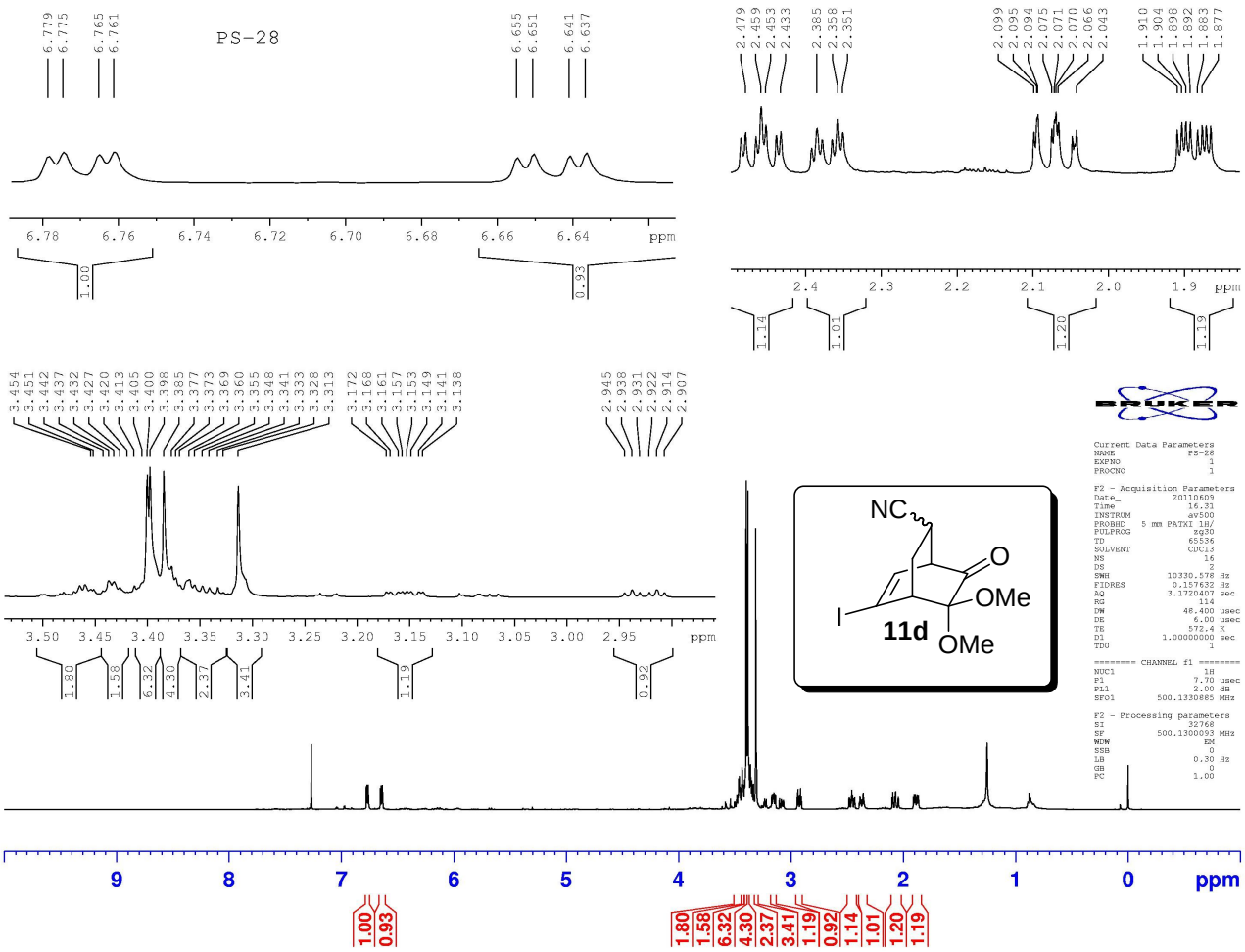

2SR-39
MeO2C
O
OMe
I
OMe
11a

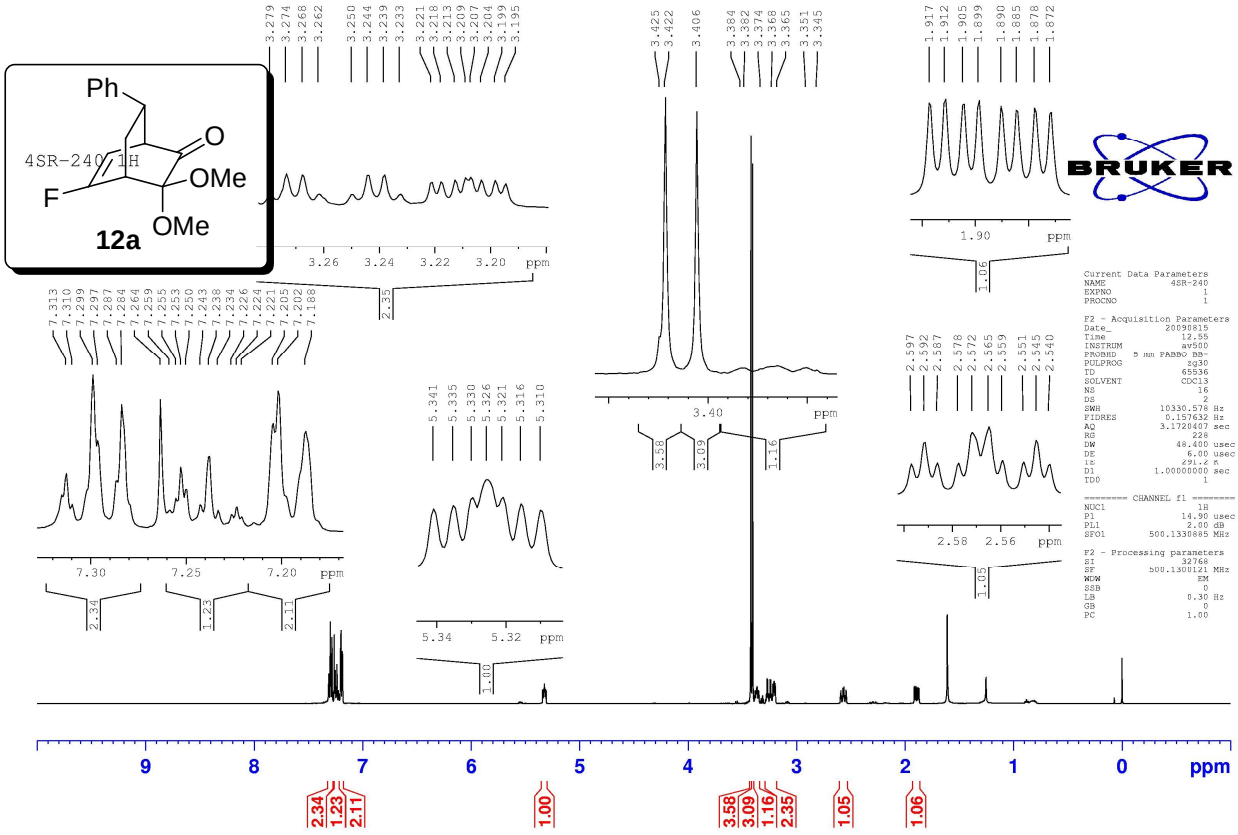

2SR-53
MeO2C
O
OMe
I
OMe
11b
6.641
6.638
6.628
6.624
3.751
3.703
3.409
3.388
3.360
3.354
3.308
3.298
3.295
2.480
2.474
2.453
2.446
1.846
1.841
1.818
1.813
1.316
1.293
ppm
9
8
7
6
5
4
3
2
1
0
1.00
3.10
3.27
3.59
2.04
1.04
1.09
3.17

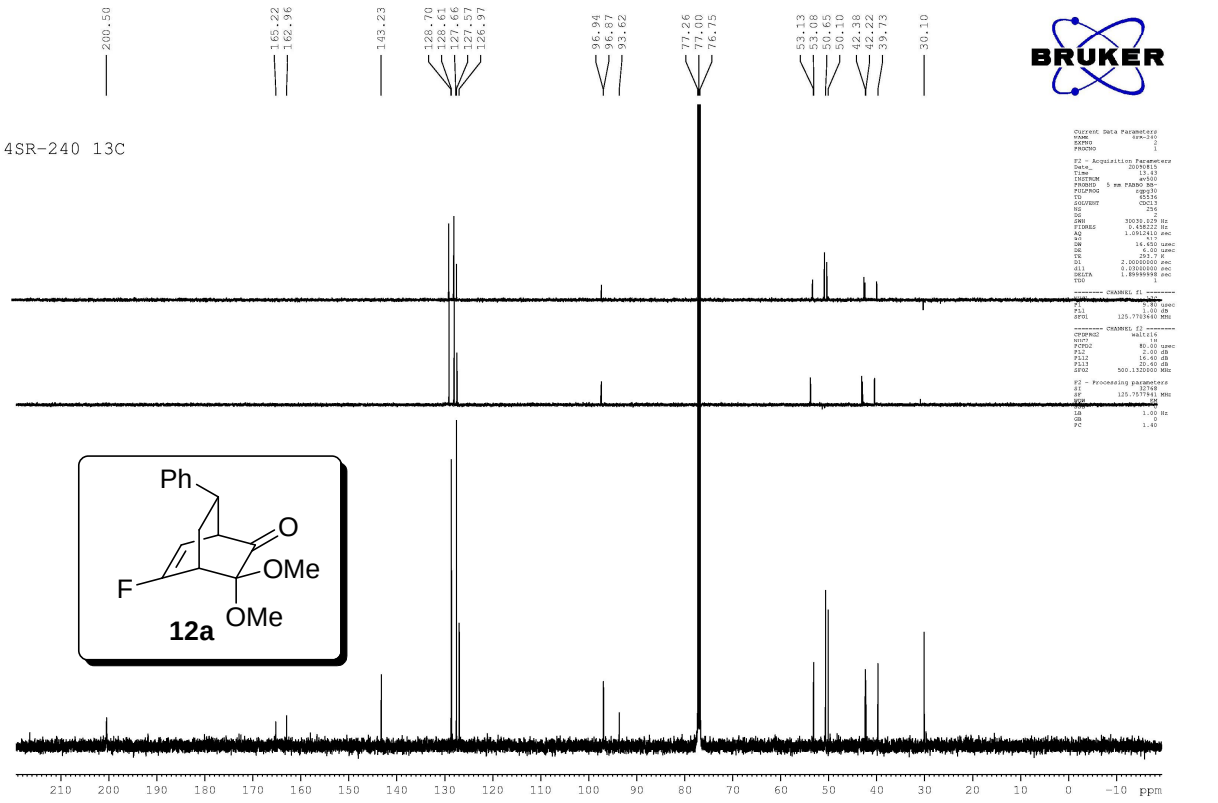

2SR-53P
200.03
175.65
135.87
95.72
94.12
77.26
77.00
76.75
59.85
52.64
52.22
51.00
49.77
46.33
31.99
25.18
MeO2C
O
OMe
I
OMe
11b
52.64
52.22
51.00
49.77
52
51
ppm
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

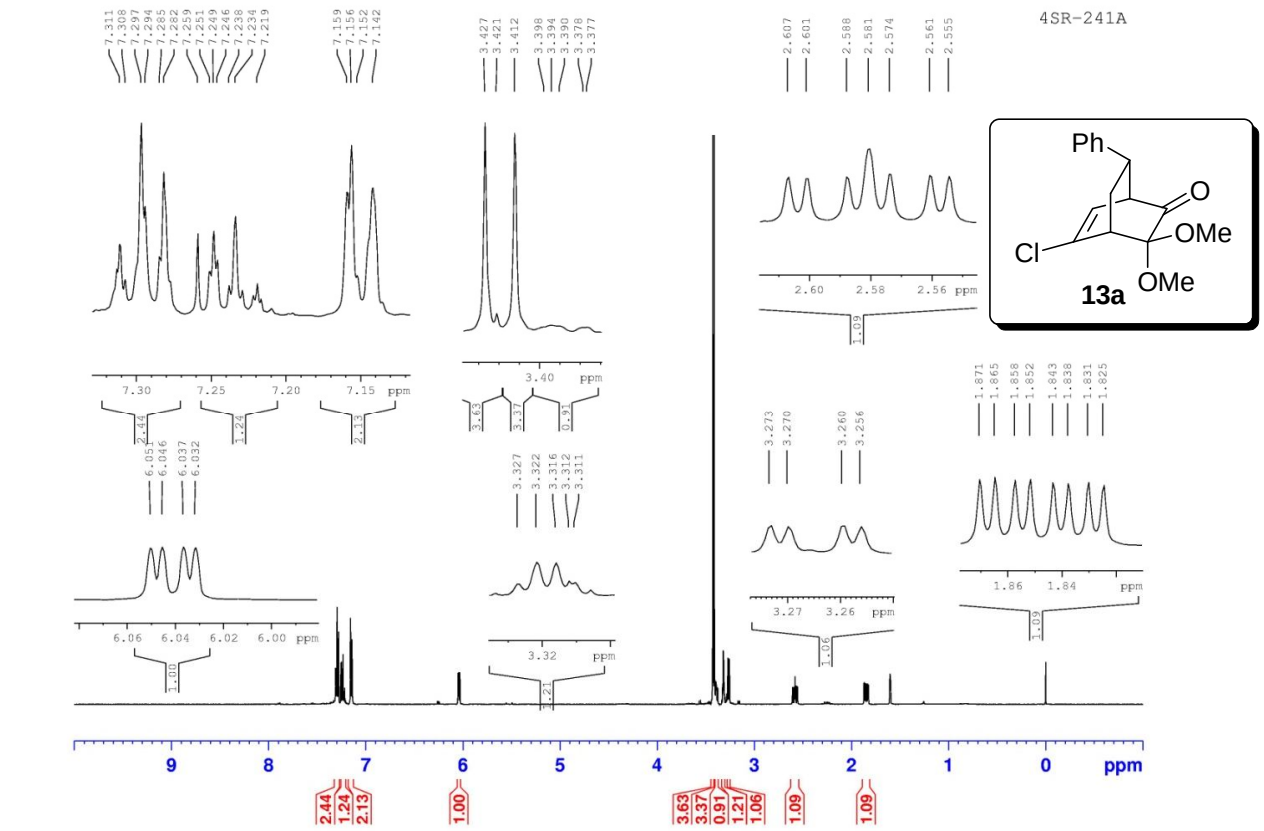

2SR-54
BRUKER
MeOC
O
OMe
OMe
11c
7.270
6.591
6.587
6.577
6.573
3.401
3.398
3.392
3.388
3.384
3.380
3.375
3.369
3.349
3.065
3.055
3.052
3.049
3.046
3.035
3.032
2.265
2.259
2.245
2.239
2.233
2.219
2.213
2.169
1.861
1.856
1.848
1.842
1.835
1.829
1.822
1.816
0.000
3.40
3.38
3.36
ppm
3.06
ppm
2.26
2.24
2.22
ppm
6.58
ppm
1.86
1.84
ppm
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.94
2.91
1.30
3.10
1.05
1.13
3.05
1.08

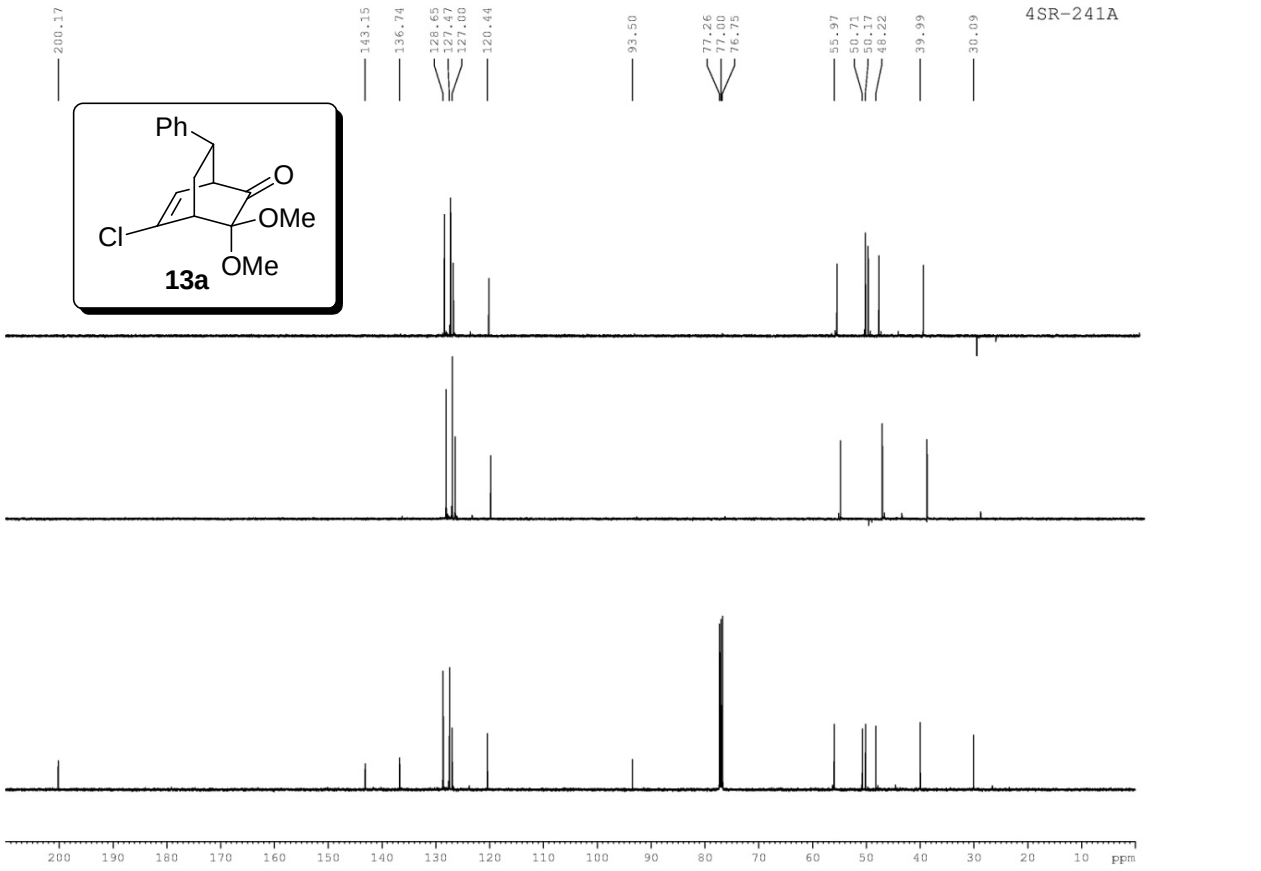

2SR-54
205.05
199.13
134.08
94.74
94.15
77.26
77.01
76.75
52.81
52.10
51.05
50.17
46.77
28.23
24.02
MeOC
O
OMe
I
OMe
11c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

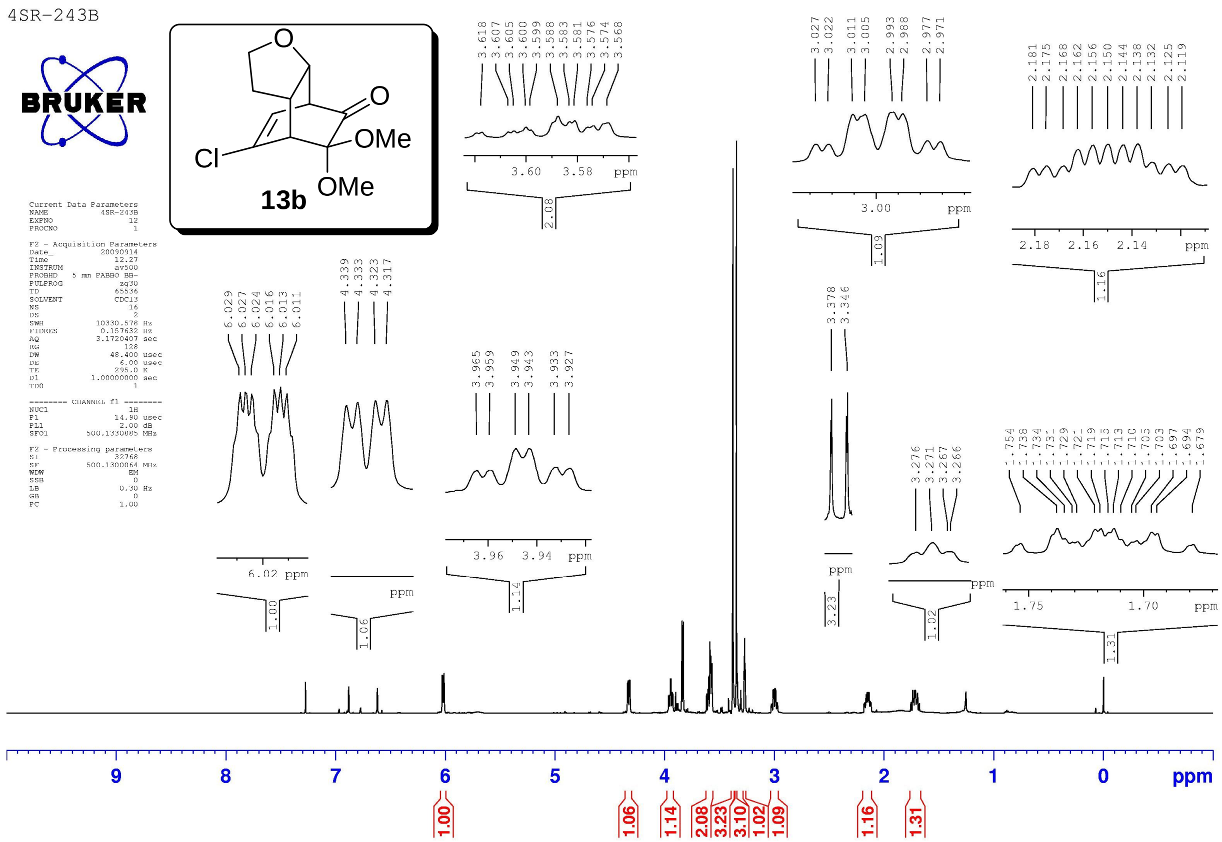

PS-28
11d
NC
O
OMe
I
OMe
ppm

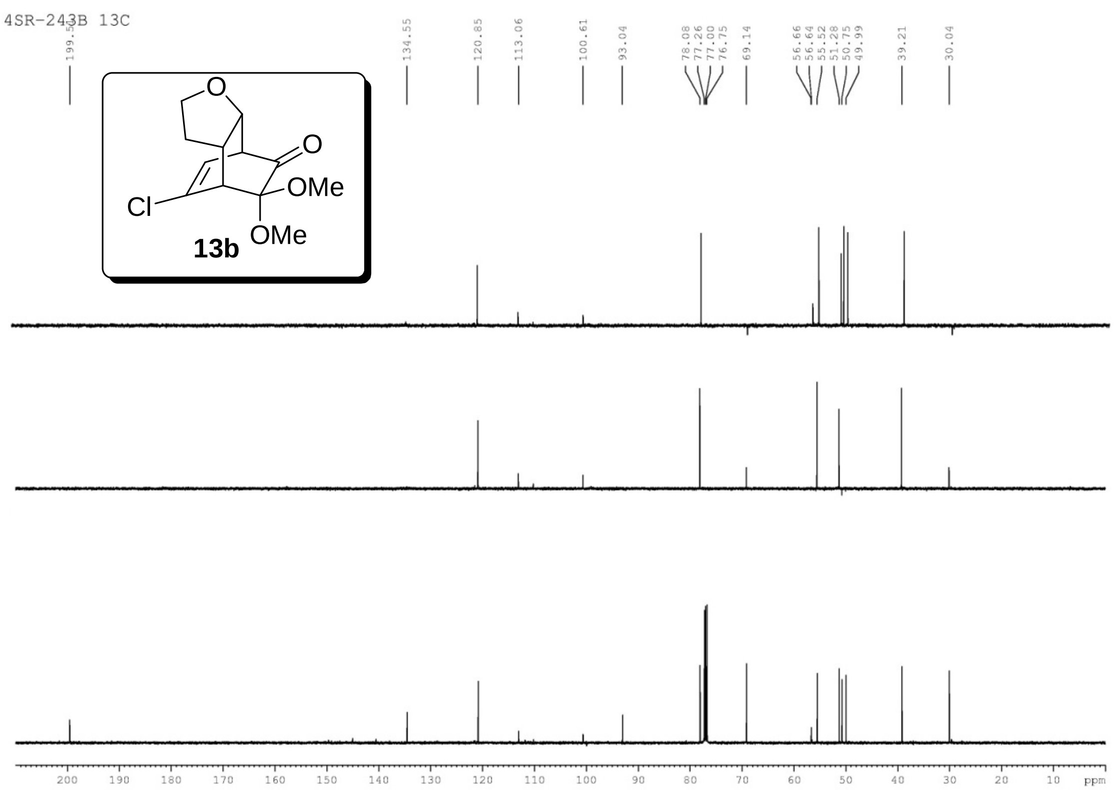

Ph
O
4SR-240 1H
OMe
F
OMe
12a
BRUKER
ppm
9
8
7
6
5
4
3
2
1
0

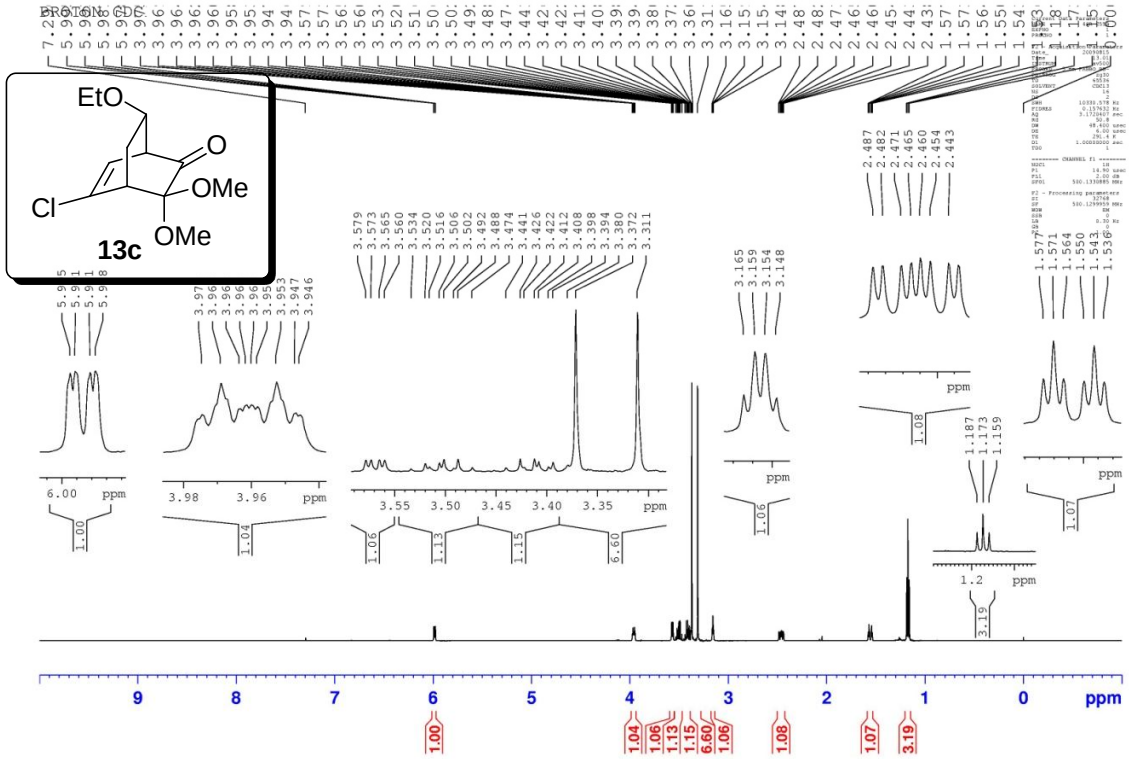

4SR-240 13C
BRUKER
Ph
O
OMe
F
OMe
12a
ppm

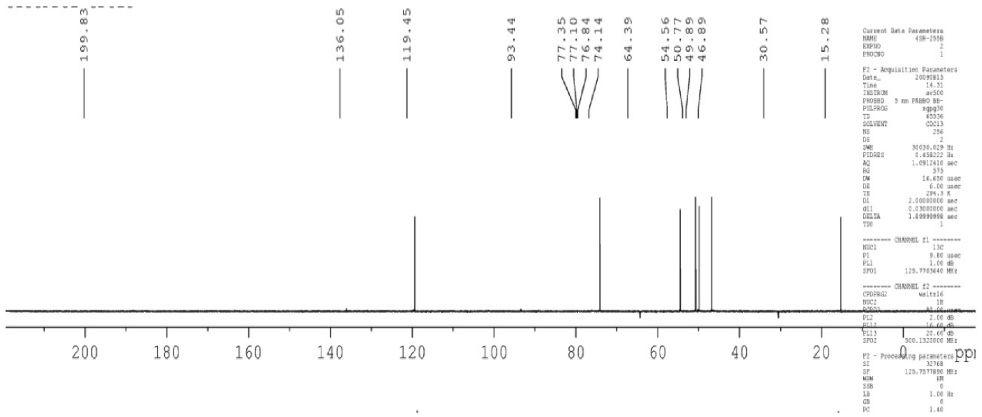

4SR-241A
Ph
O
Cl
OMe
OMe
13a

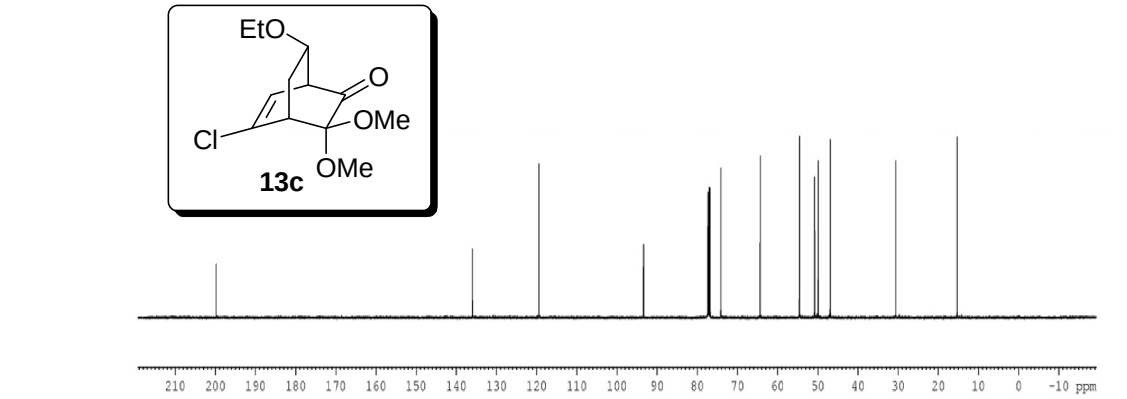

4SR-241A
Ph
O
Cl
OMe
OMe
13a

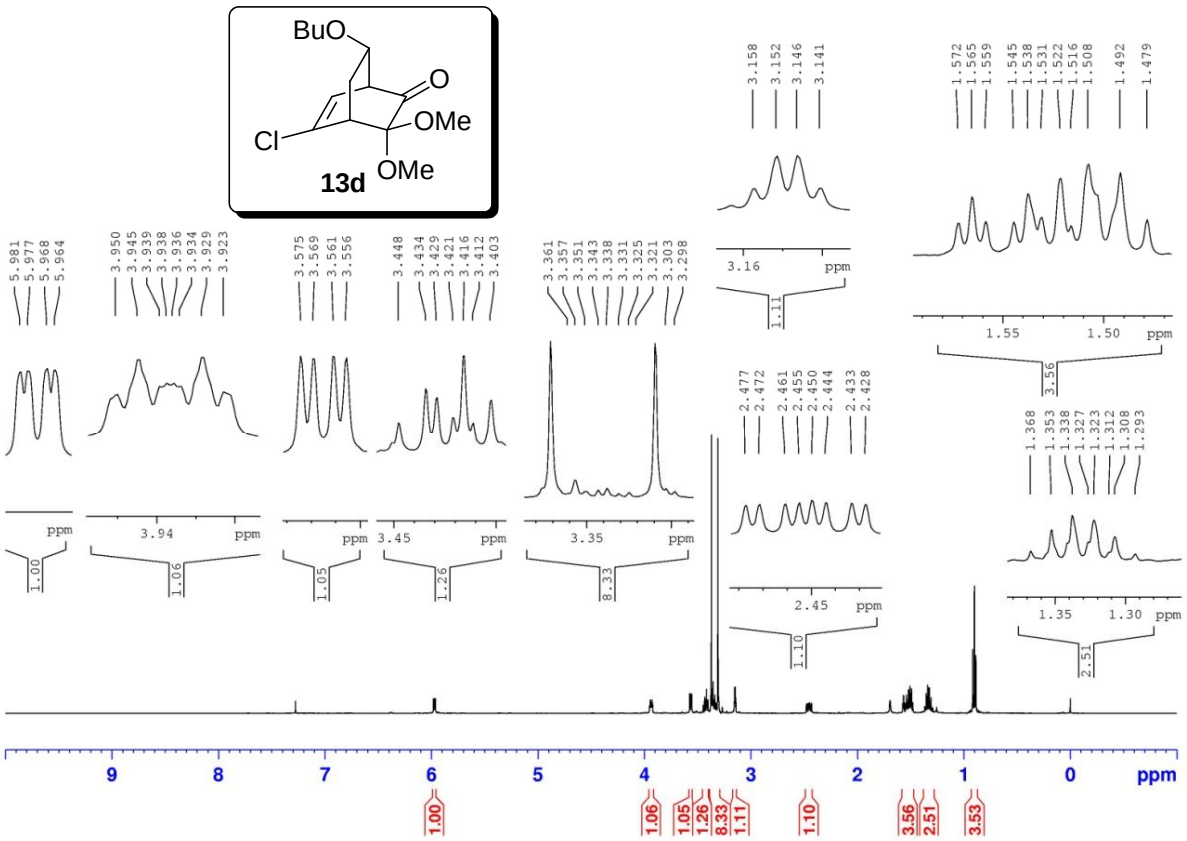

4SR-243B
BRUKER
Cl
OMe
OMe
13b
ppm

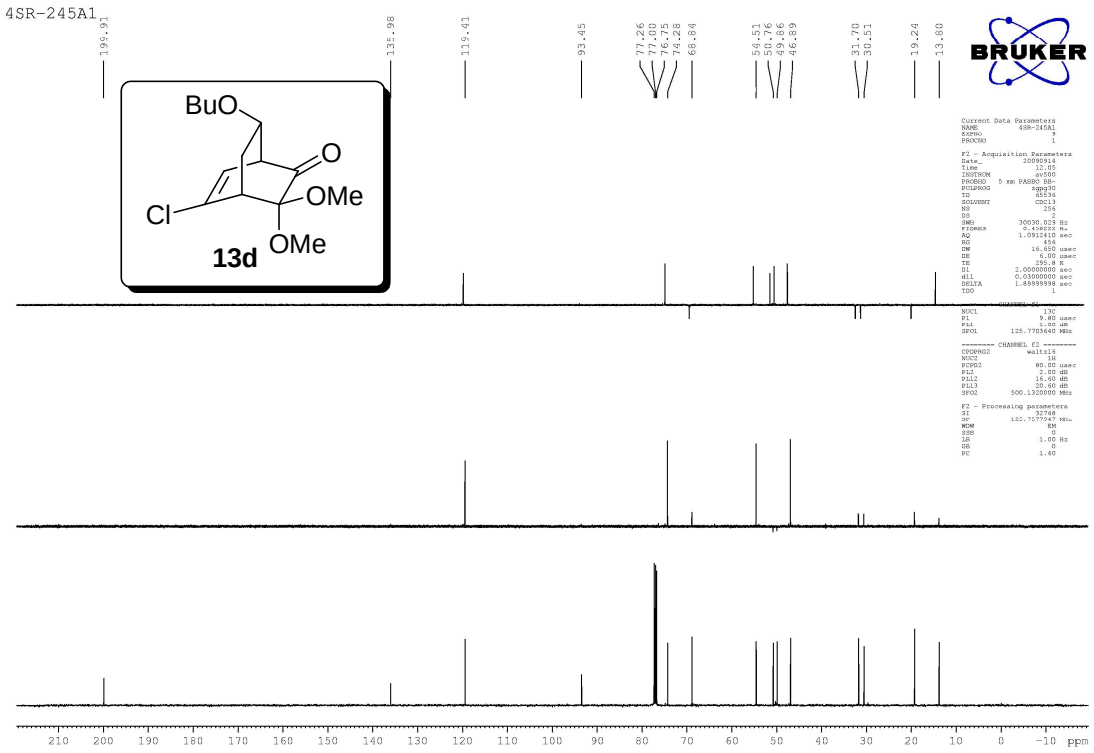

4SR-243B 13C
Cl
OMe
OMe
13b
134.55
120.85
113.06
100.61
93.04
78.08
77.26
77.00
76.75
69.14
56.66
56.64
55.52
51.28
50.75
49.99
39.21
30.04
ppm

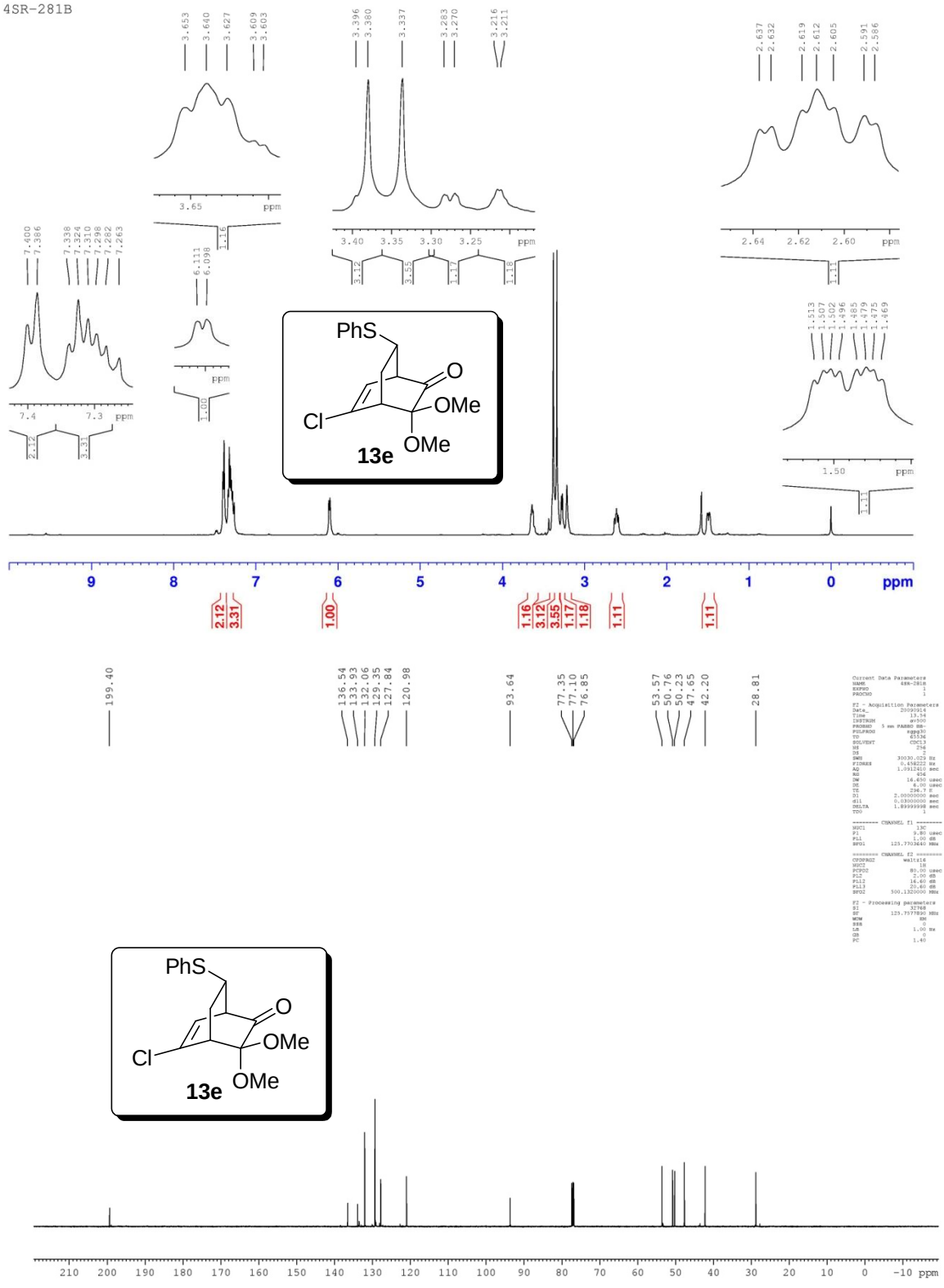

EtO
O
OMe
Cl
OMe
13c
ppm

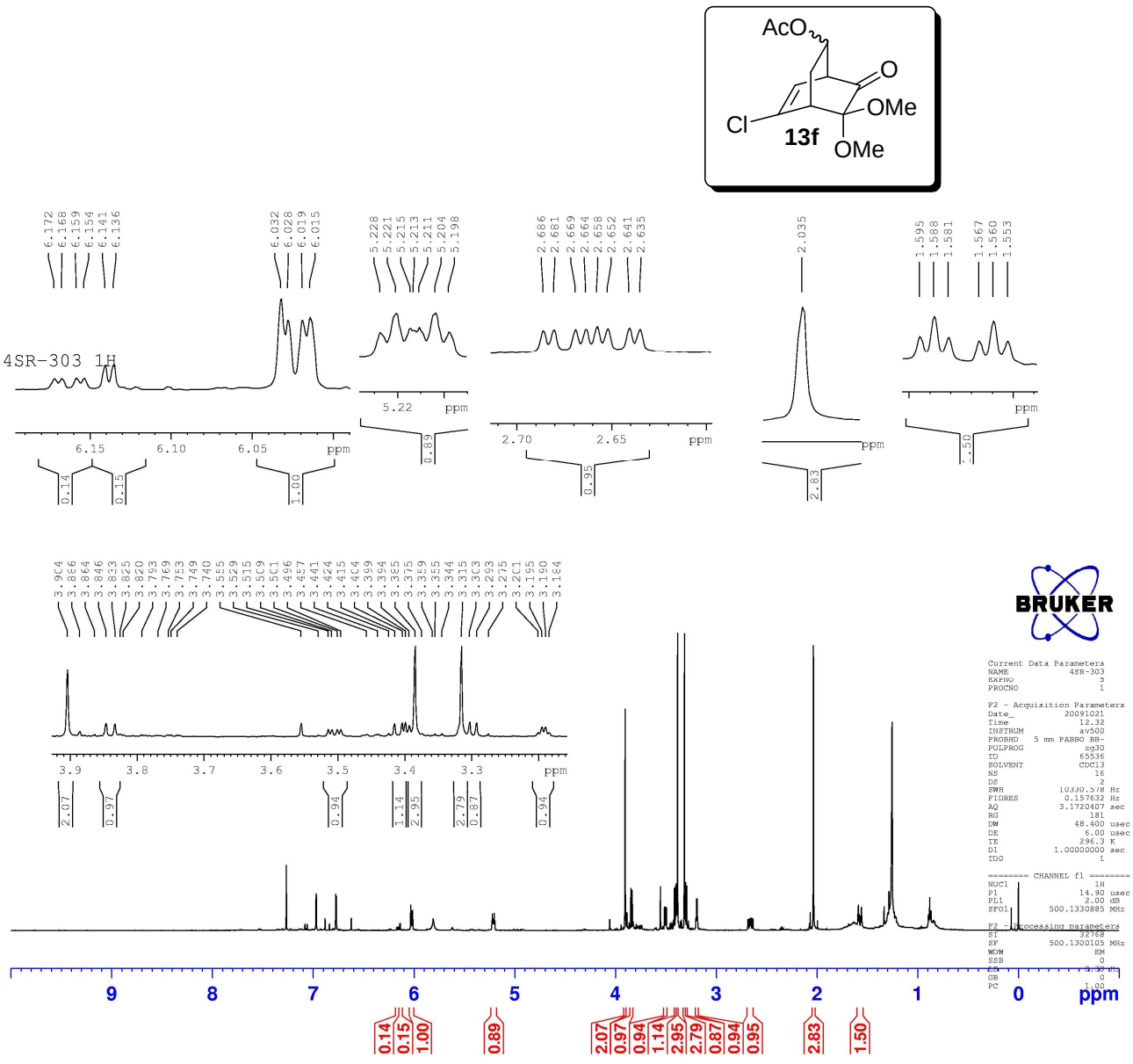

199.83
136.05
119.45
93.44
77.35
77.10
76.84
74.14
64.39
54.56
50.77
46.89
30.57
15.28
ppm


EtO
O
OMe
Cl
OMe
13c
ppm


BuO
O
Cl
OMe
OMe
13d
ppm


4SR-245A1
BuO
O
Cl
OMe
OMe
13d
BRUKER
ppm


4SR-281B
PhS
O
OMe
Cl
OMe
13e
PhS
O
OMe
Cl
OMe
13e


AcO
O
OMe
Cl
13f
OMe
4SR-303 1H
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6.168
6.159
6.154
6.141
6.136
6.032
6.028
6.019
6.015
5.228
5.221
5.215
5.213
5.211
5.204
5.198
2.686
2.681
2.669
2.664
2.658
2.652
2.641
2.635
2.035
1.595
1.588
1.581
1.567
1.560
1.553
6.15
6.10
6.05
ppm
0.14
0.15
1.00
5.22
ppm
0.89
2.70
2.65
ppm
0.95
ppm
2.83
ppm
1.50
3.904
3.886
3.864
3.846
3.833
3.825
3.820
3.793
3.769
3.753
3.749
3.740
3.555
3.529
3.515
3.509
3.501
3.496
3.457
3.441
3.424
3.415
3.404
3.399
3.394
3.385
3.375
3.359
3.355
3.344
3.315
3.303
3.293
3.275
3.201
3.195
3.190
3.184
3.9
3.8
3.7
3.6
3.5
3.4
3.3
ppm
2.07
0.97
0.94
1.14
2.95
2.79
0.87
0.94
BRUKER
Current Data Parameters
NAME 4SR-303
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091021
Time 12.32
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.90 usec
PL1 2.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
0.14
0.15
1.00
0.89
2.07
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0.87
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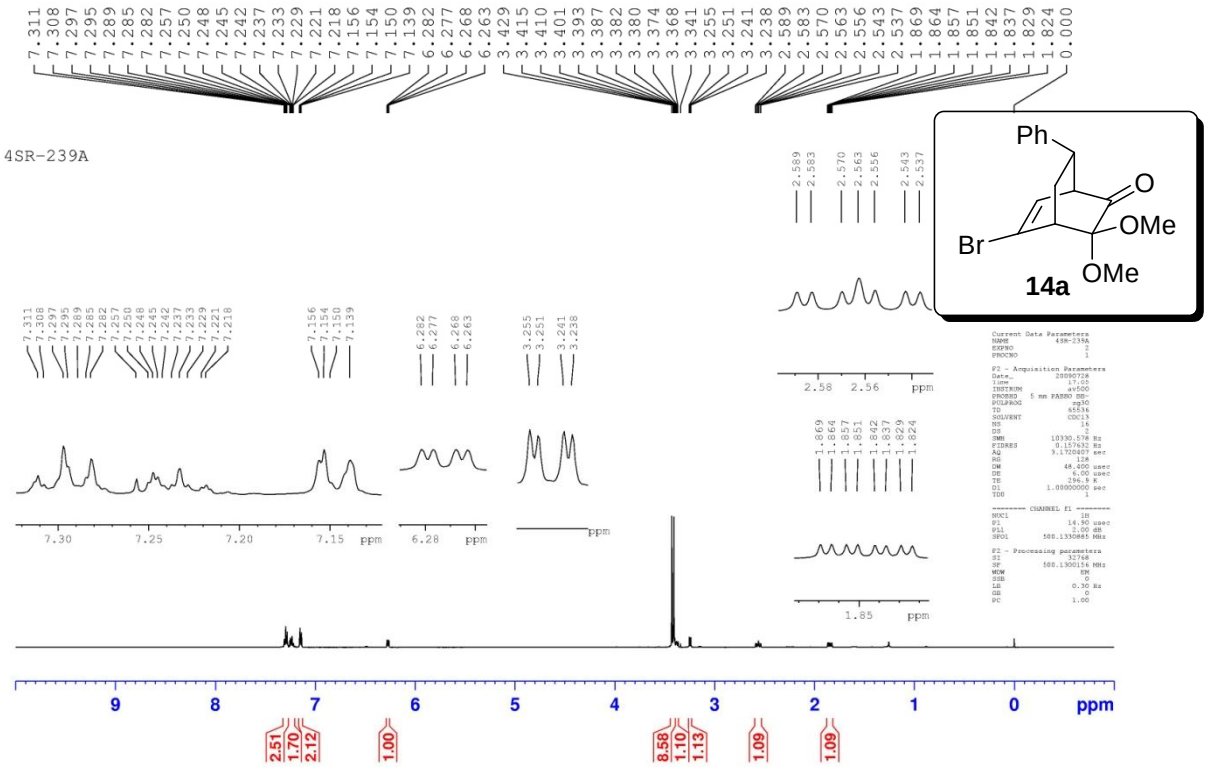
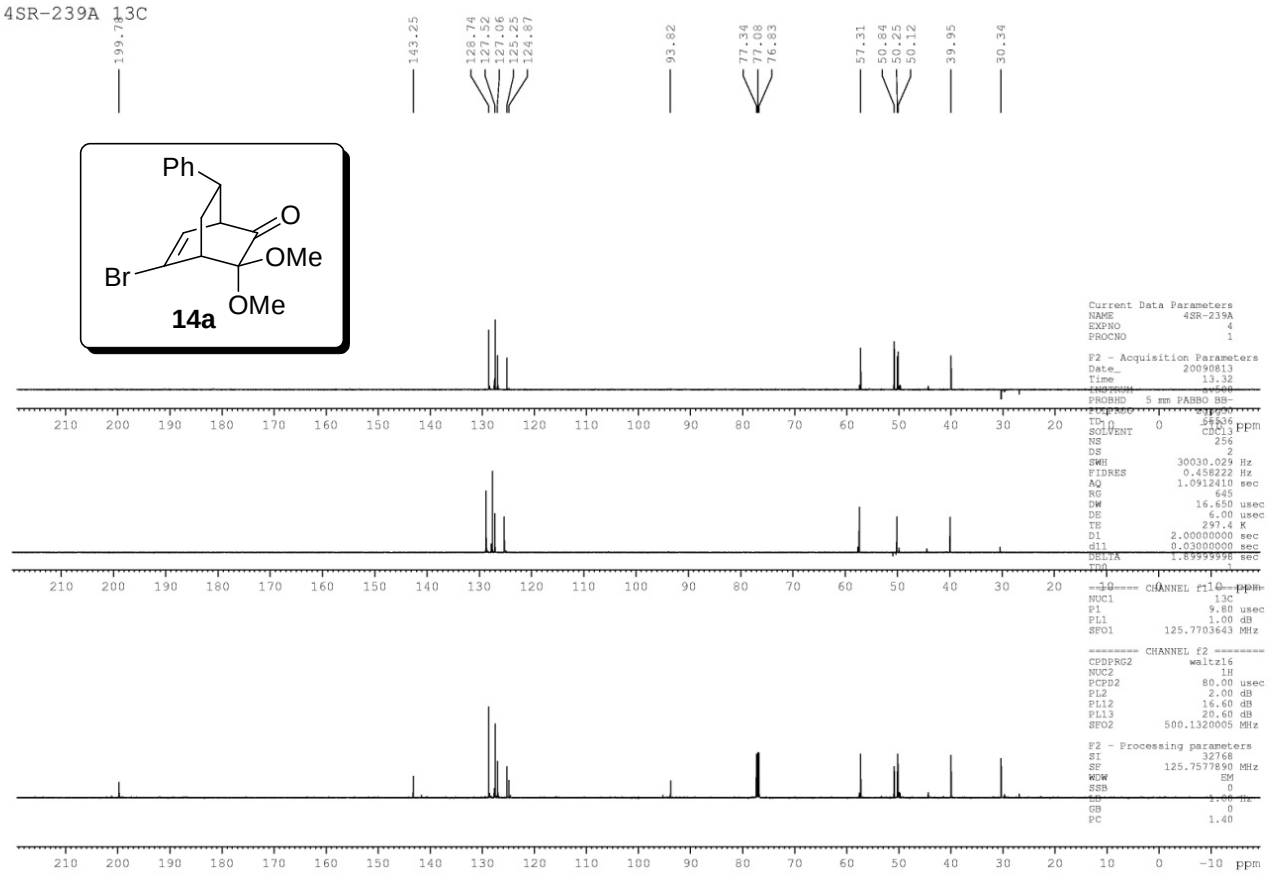
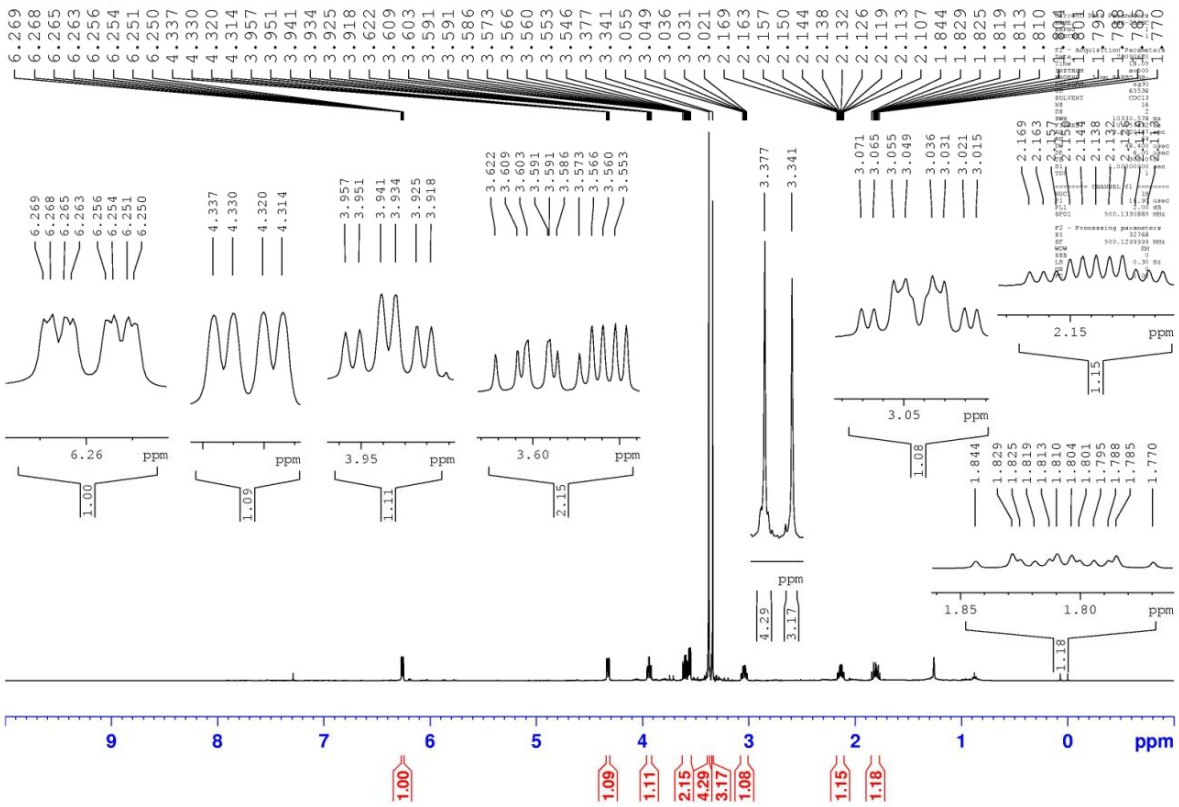
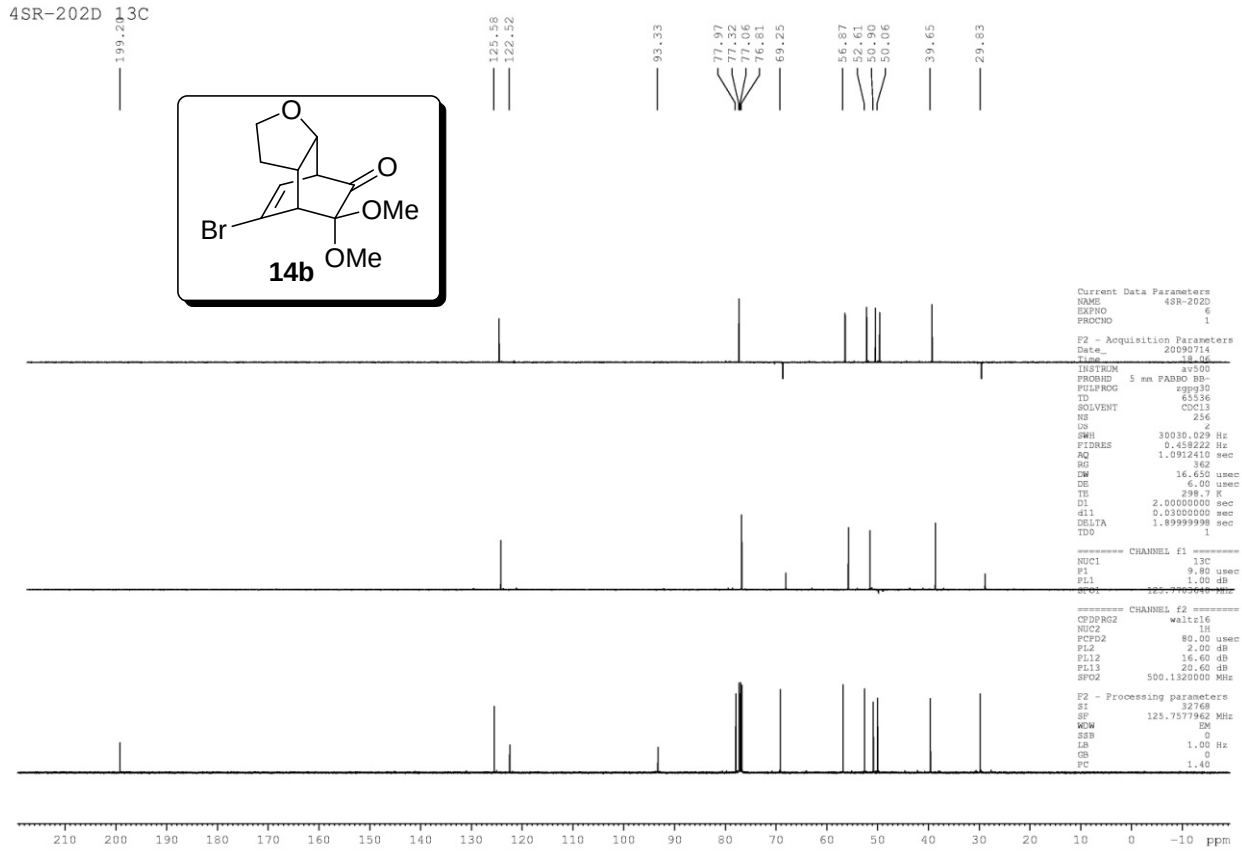
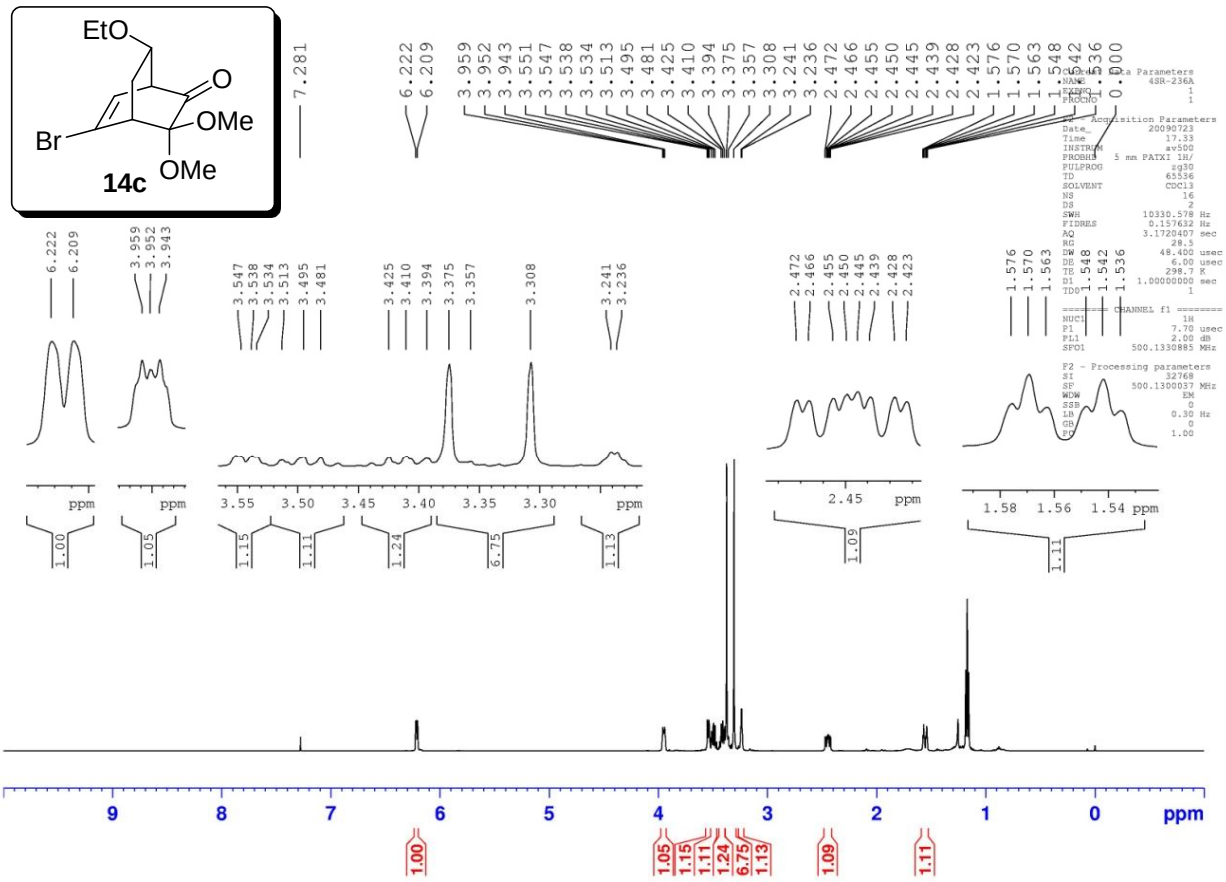
0.95
2.83
1.50

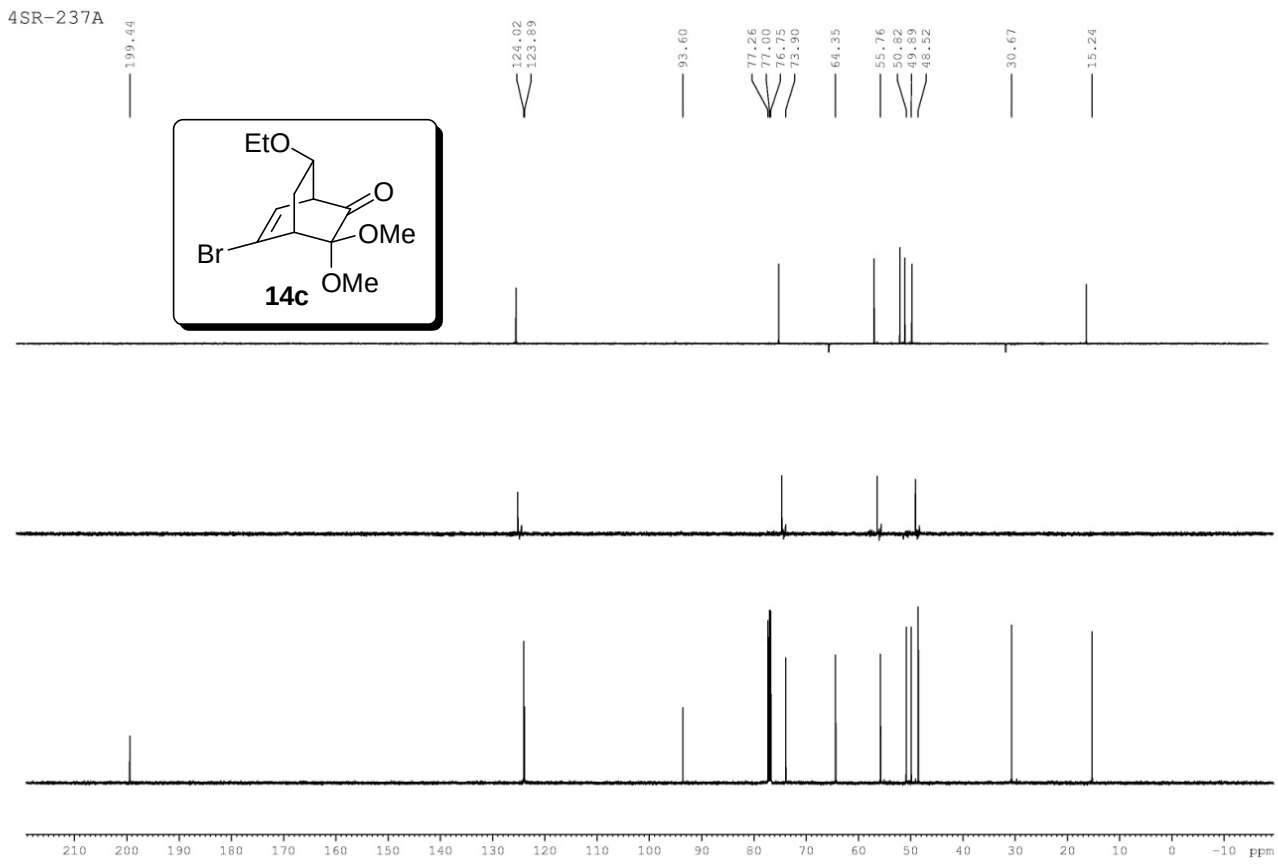

4SR-239A
Ph
O
OMe
Br
OMe
14a
9
8
7
6
5
4
3
2
1
0
ppm

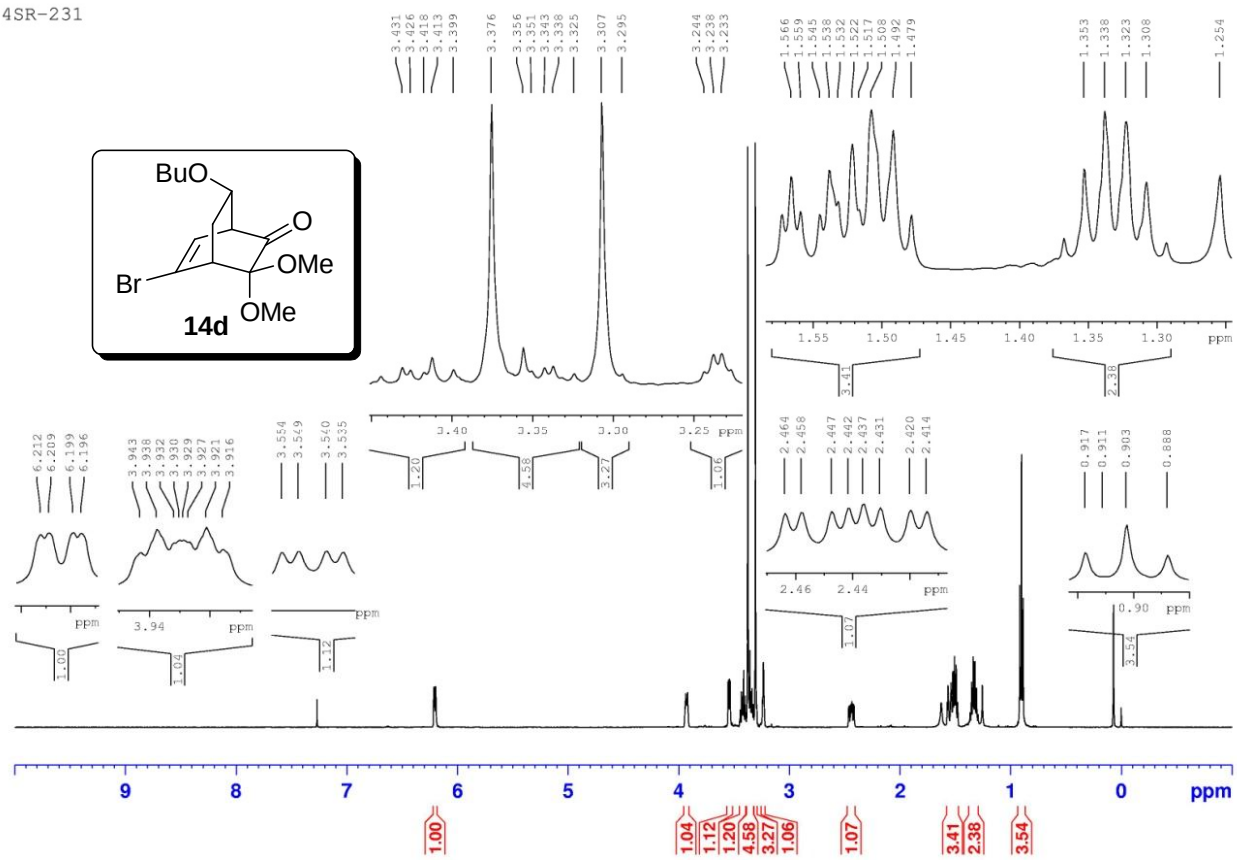

4SR-239A 13C
Ph
O
OMe
Br
OMe
14a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

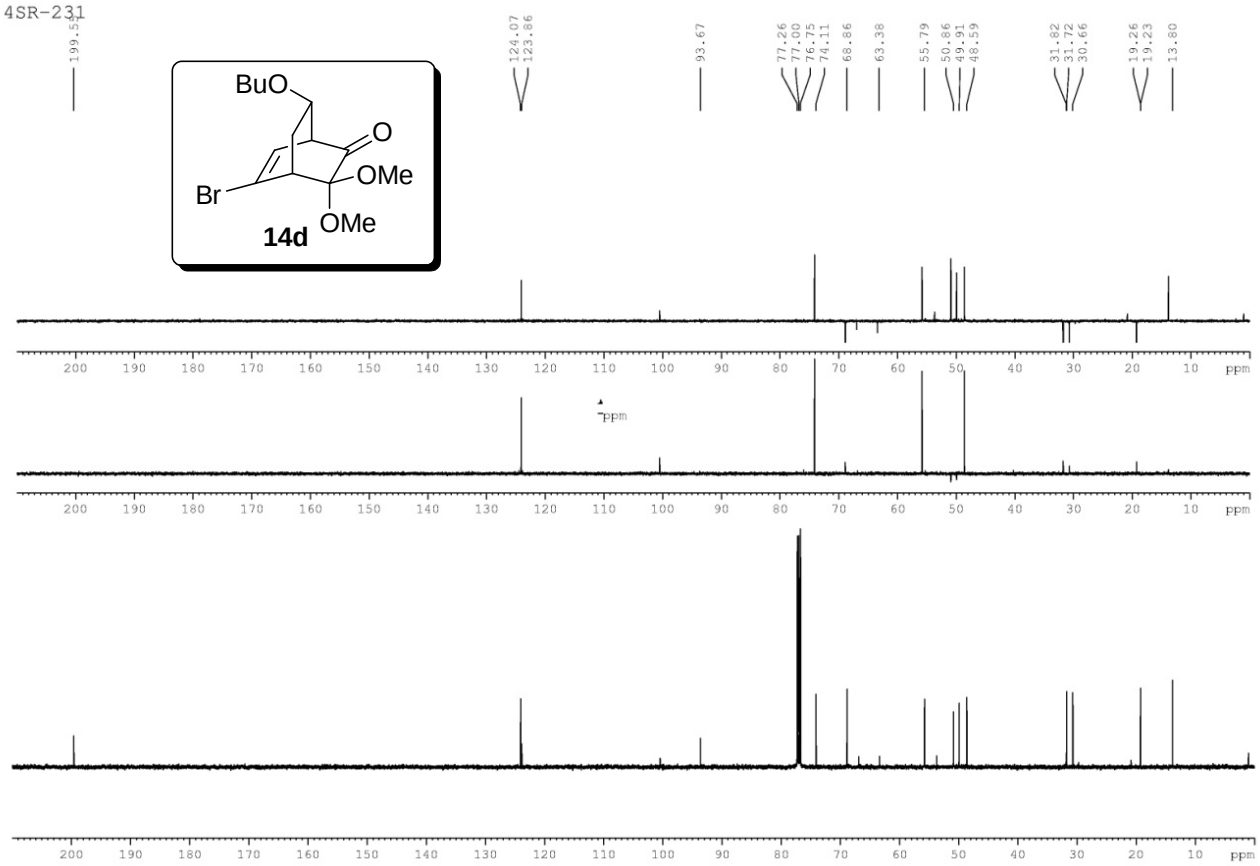


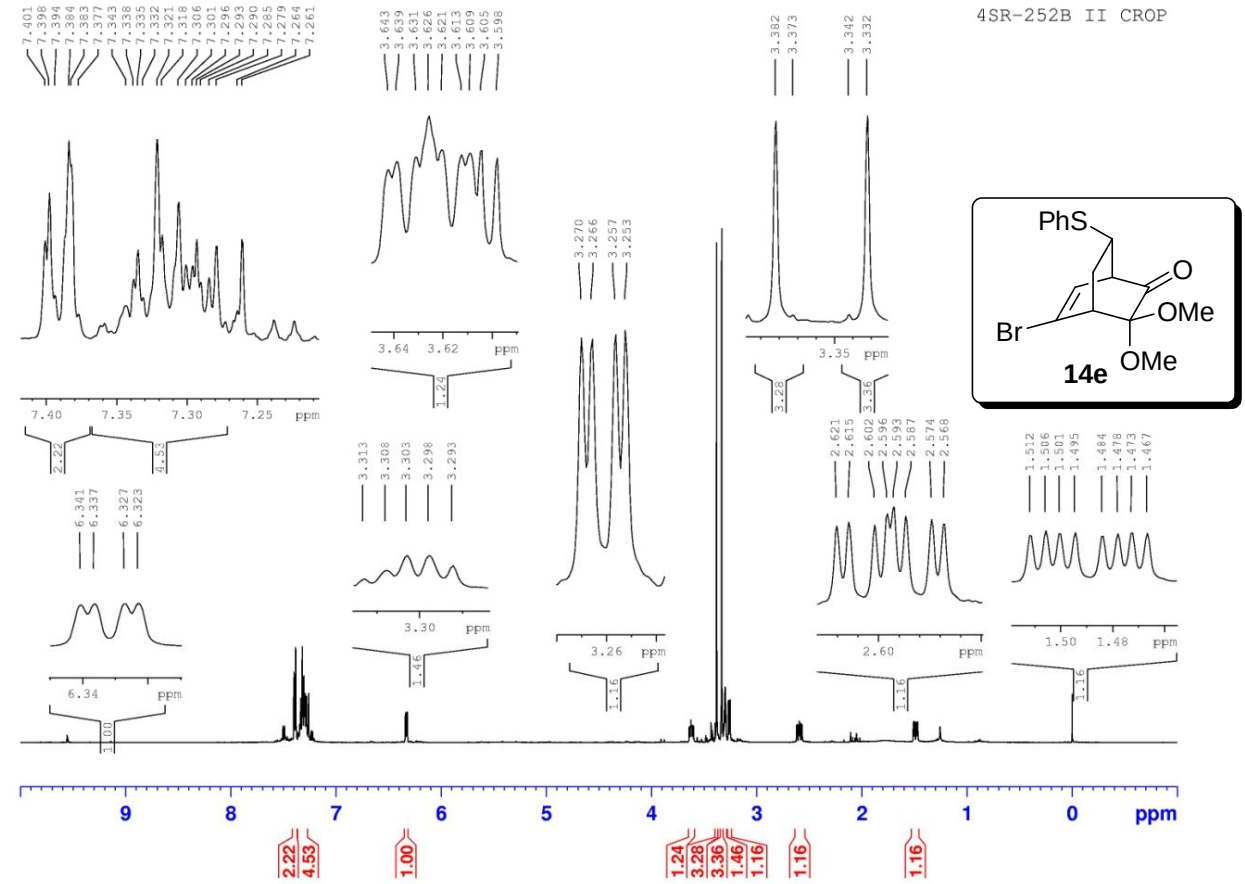

4SR-202D 13C
Br
OMe
OMe
O
O
14b

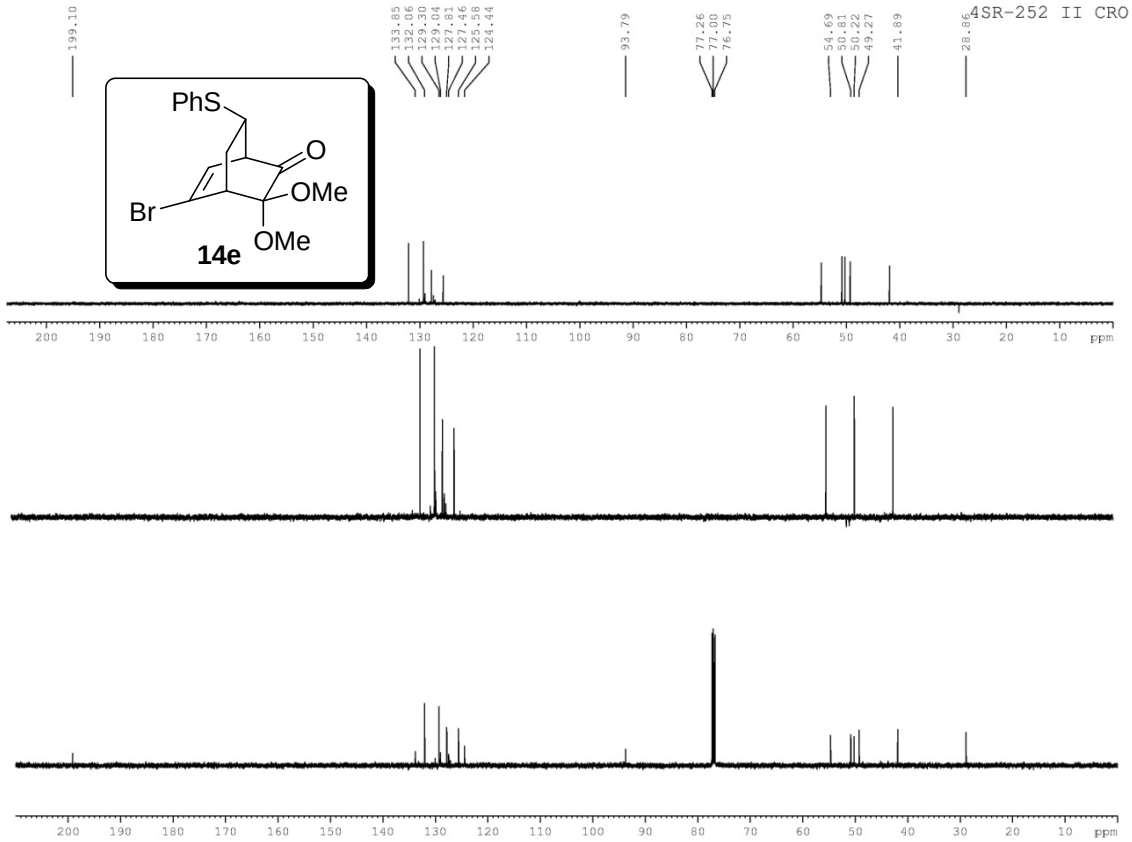

EtO
O
OMe
Br
OMe
14c

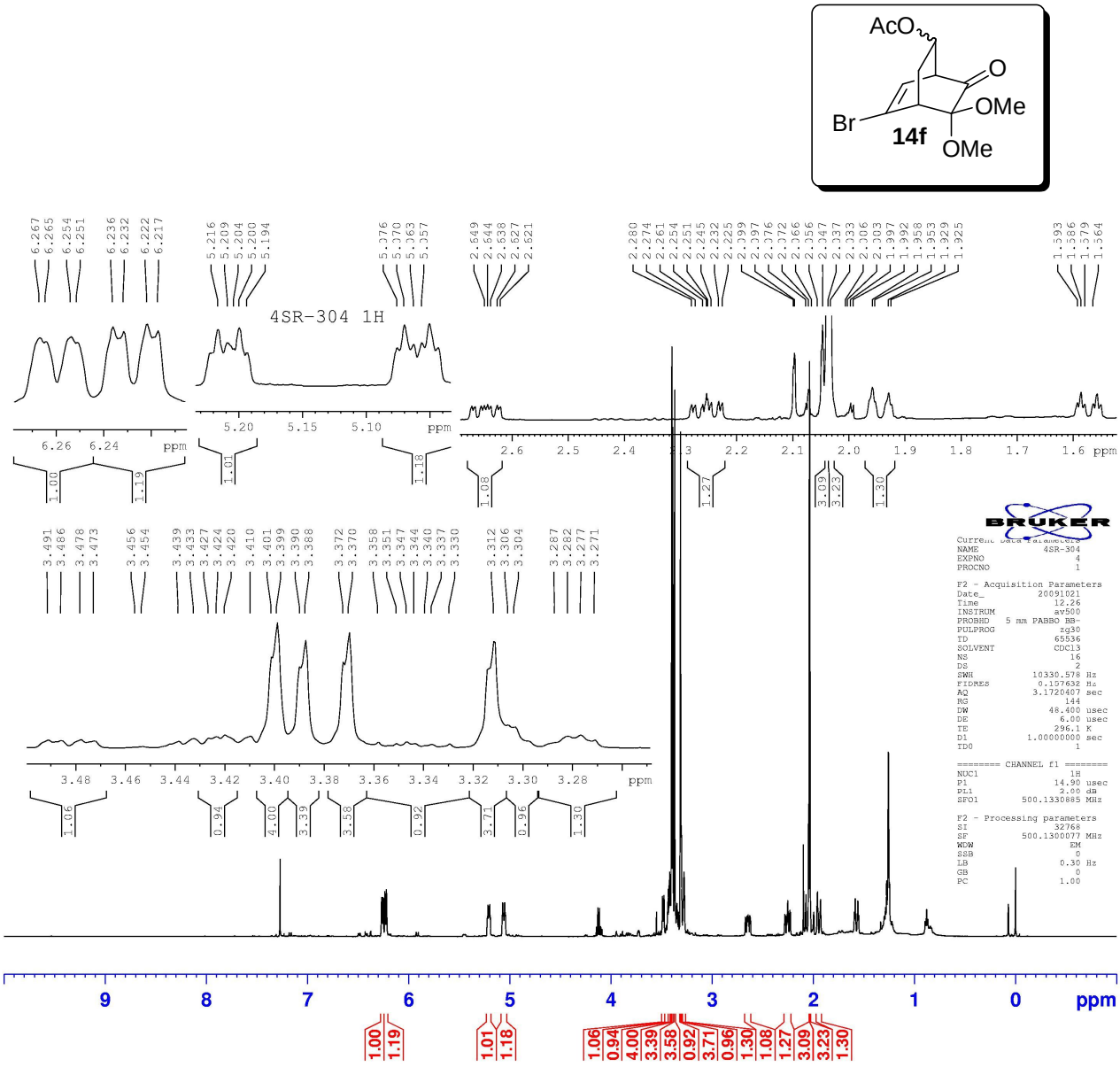

4SR-237A
EtO
O
OMe
Br
OMe
14c

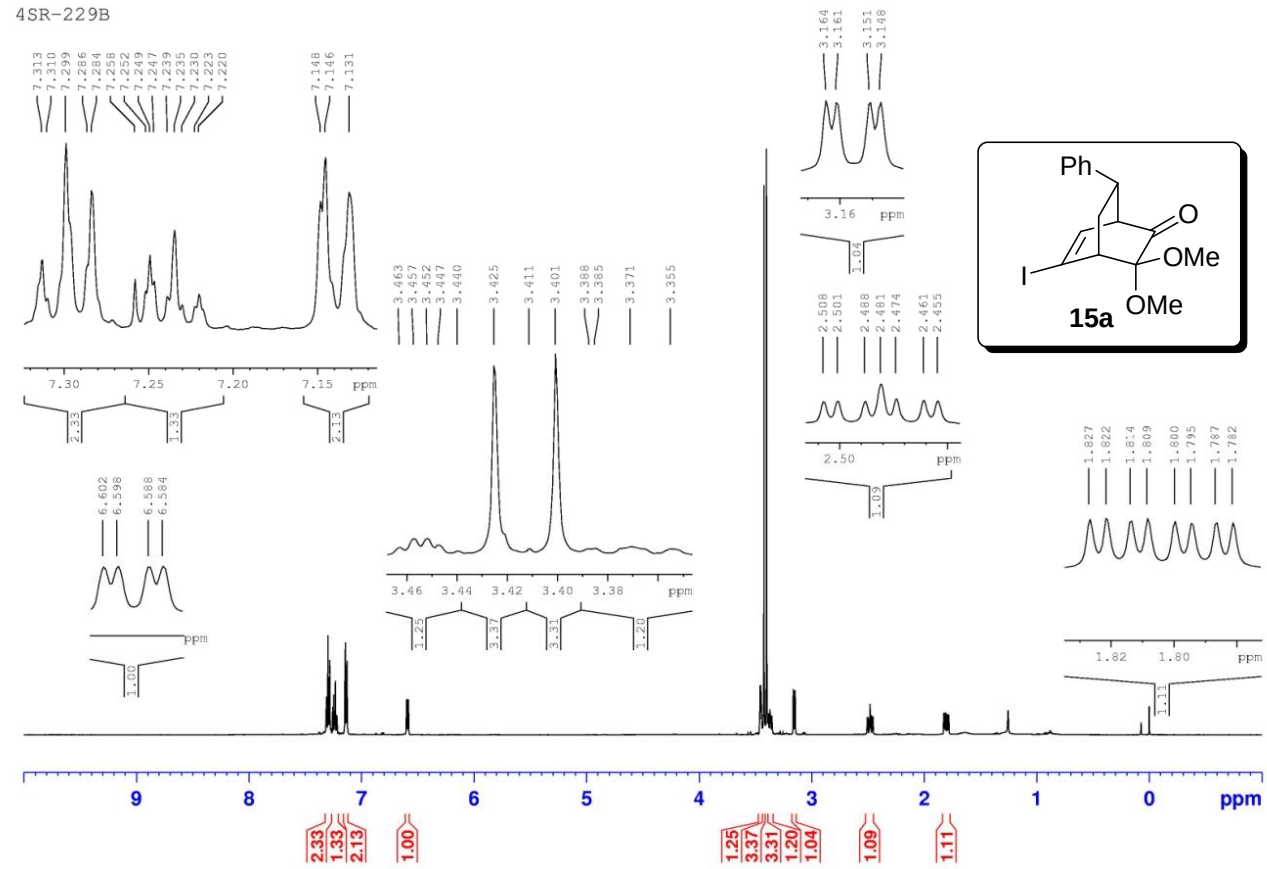

4SR-231
BuO
O
OMe
Br
OMe
14d

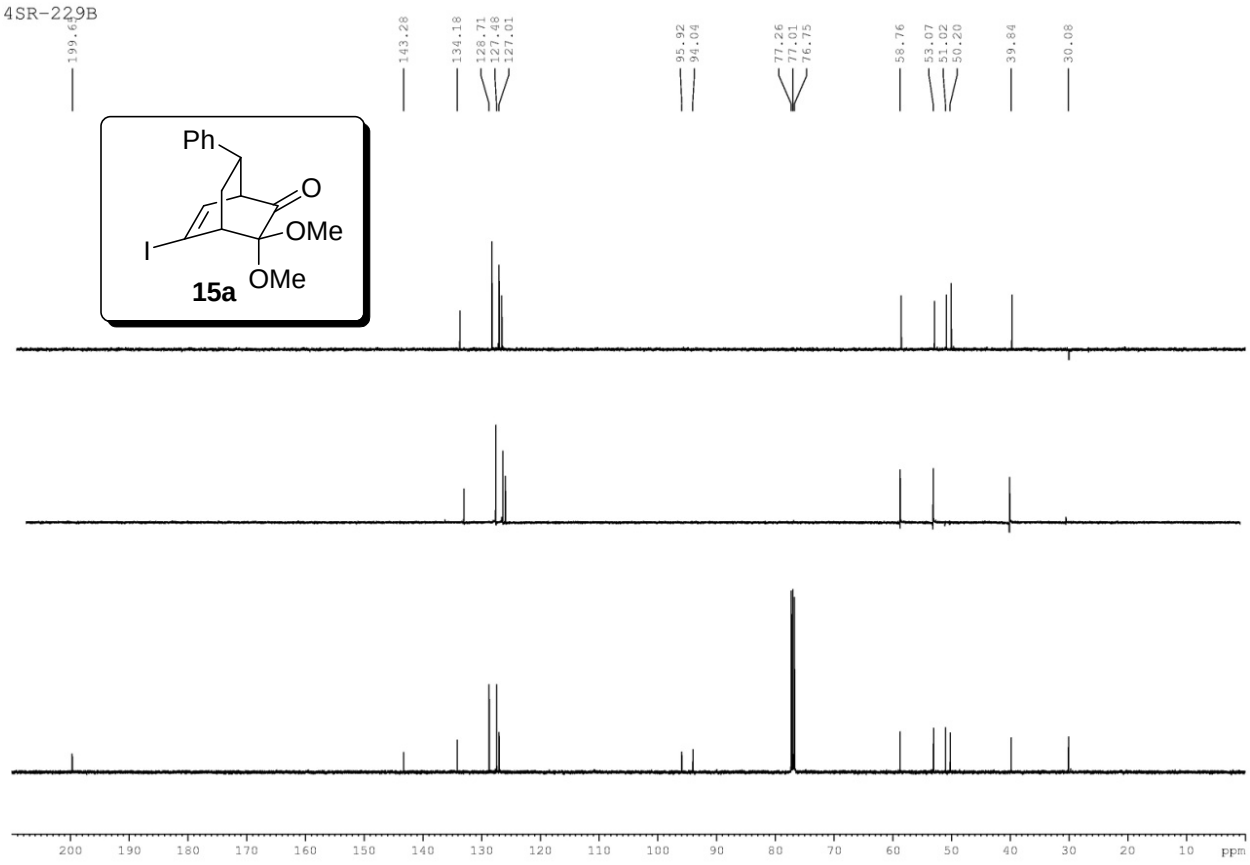

4SR-231
BuO
O
OMe
Br
OMe
14d

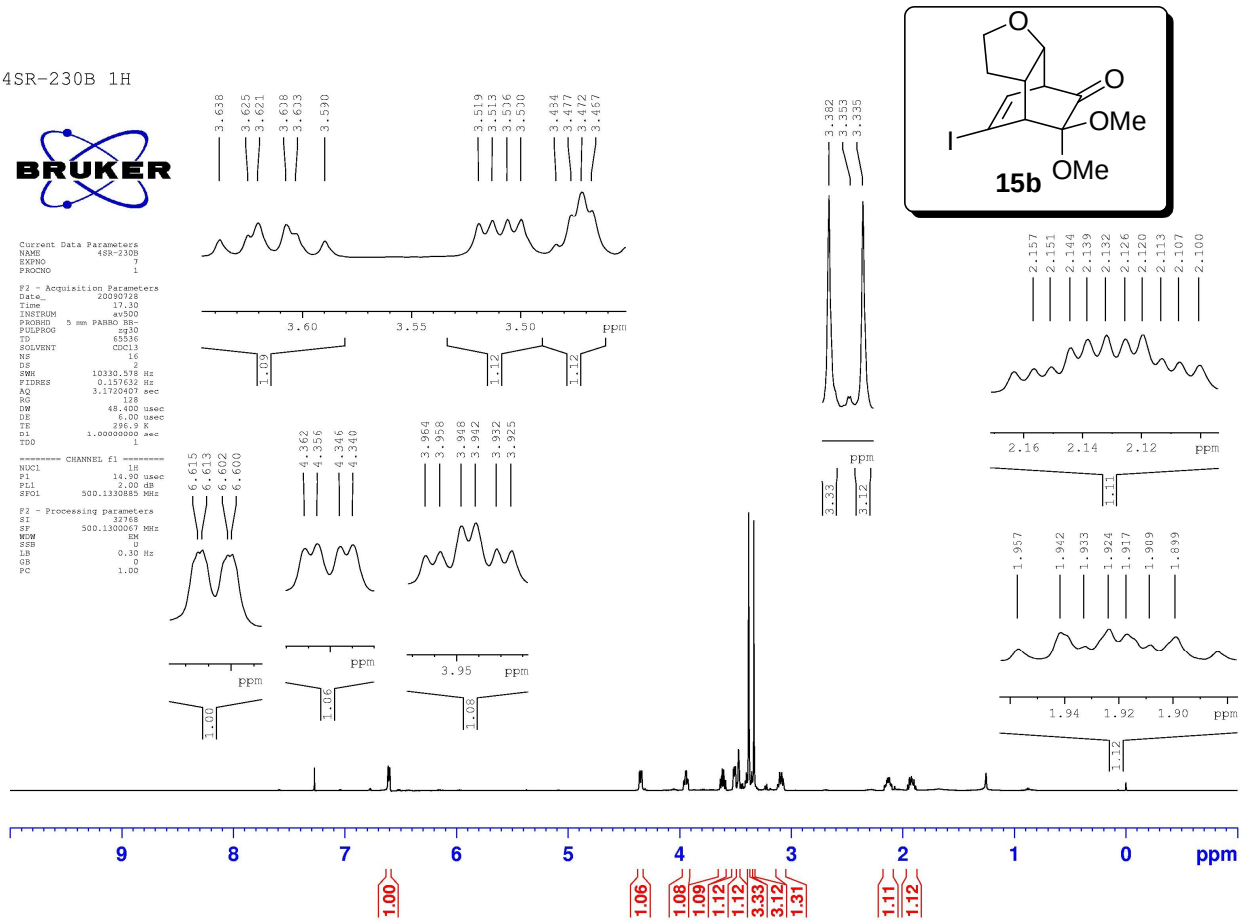

4SR-252B II CROP
PhS
O
OMe
Br
OMe
14e

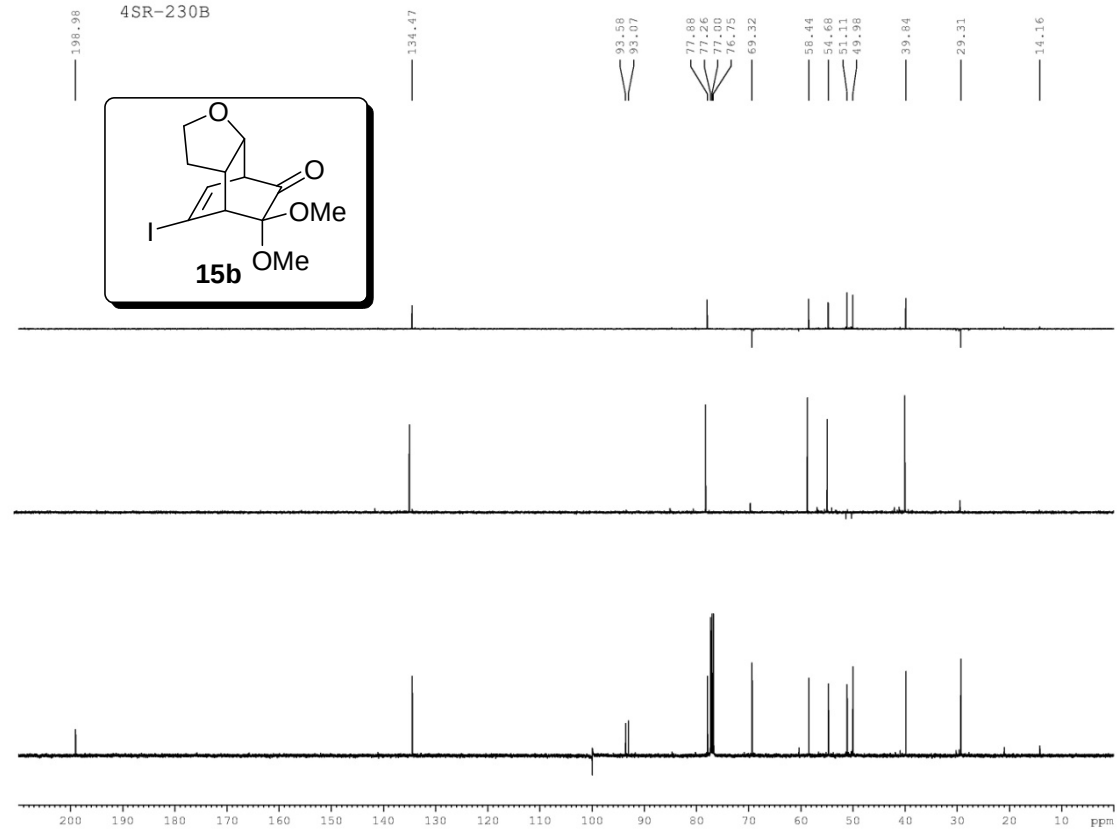

4SR-252 II CRO
PhS
O
OMe
Br
OMe
14e

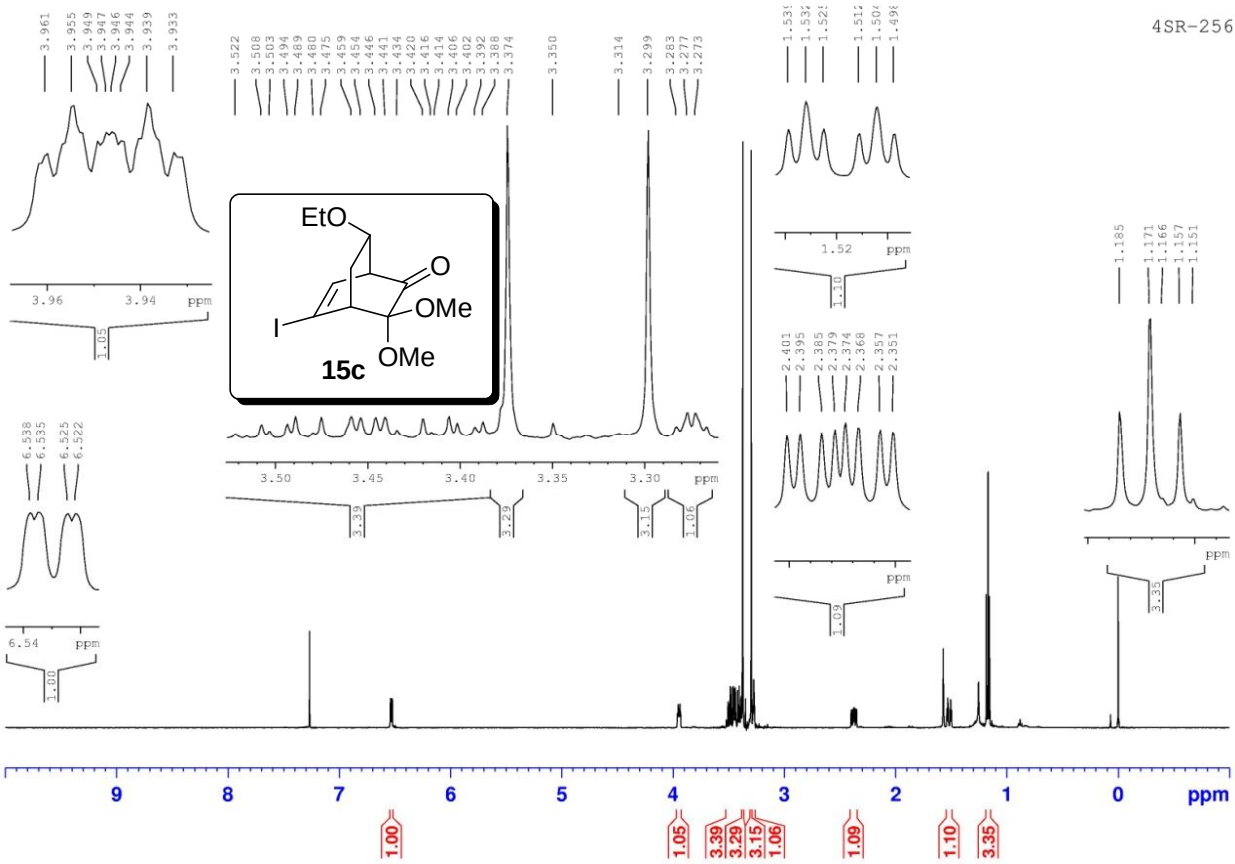

AcO
O
OMe
Br
14f
OMe
4SR-304 1H
ppm

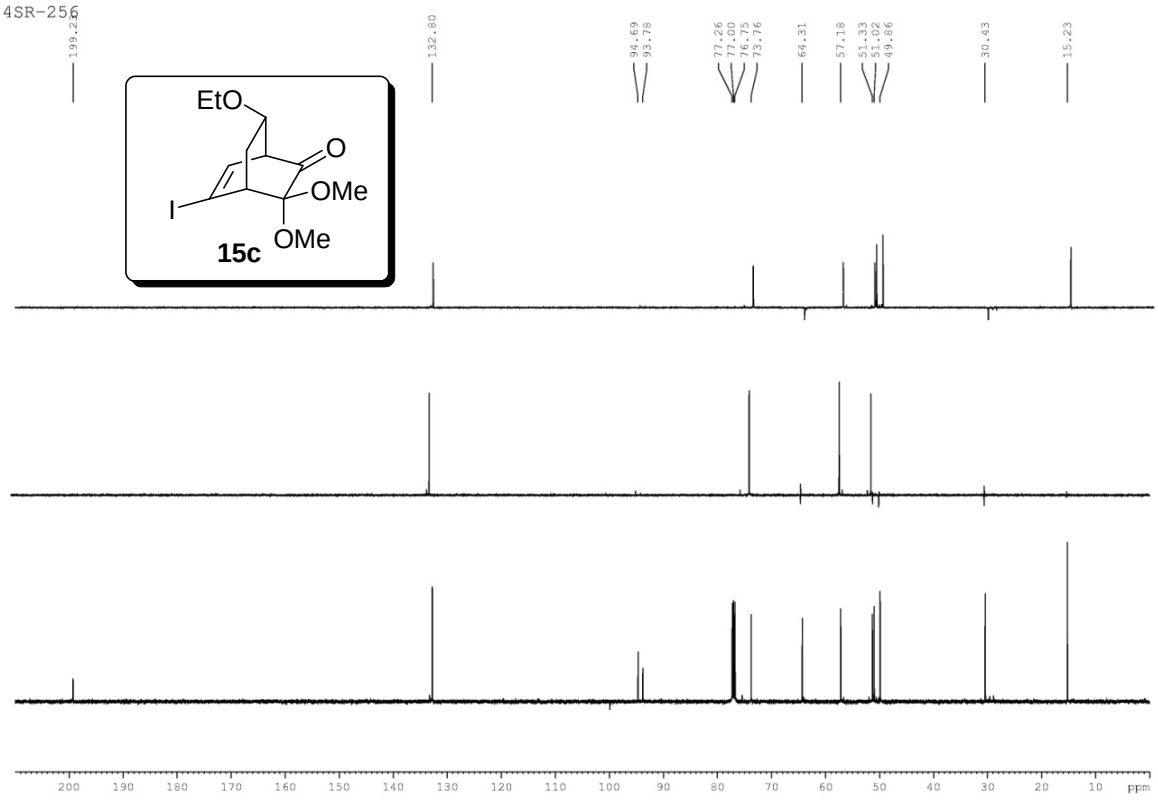

4SR-229B
Ph
O
OMe
I
OMe
15a
ppm

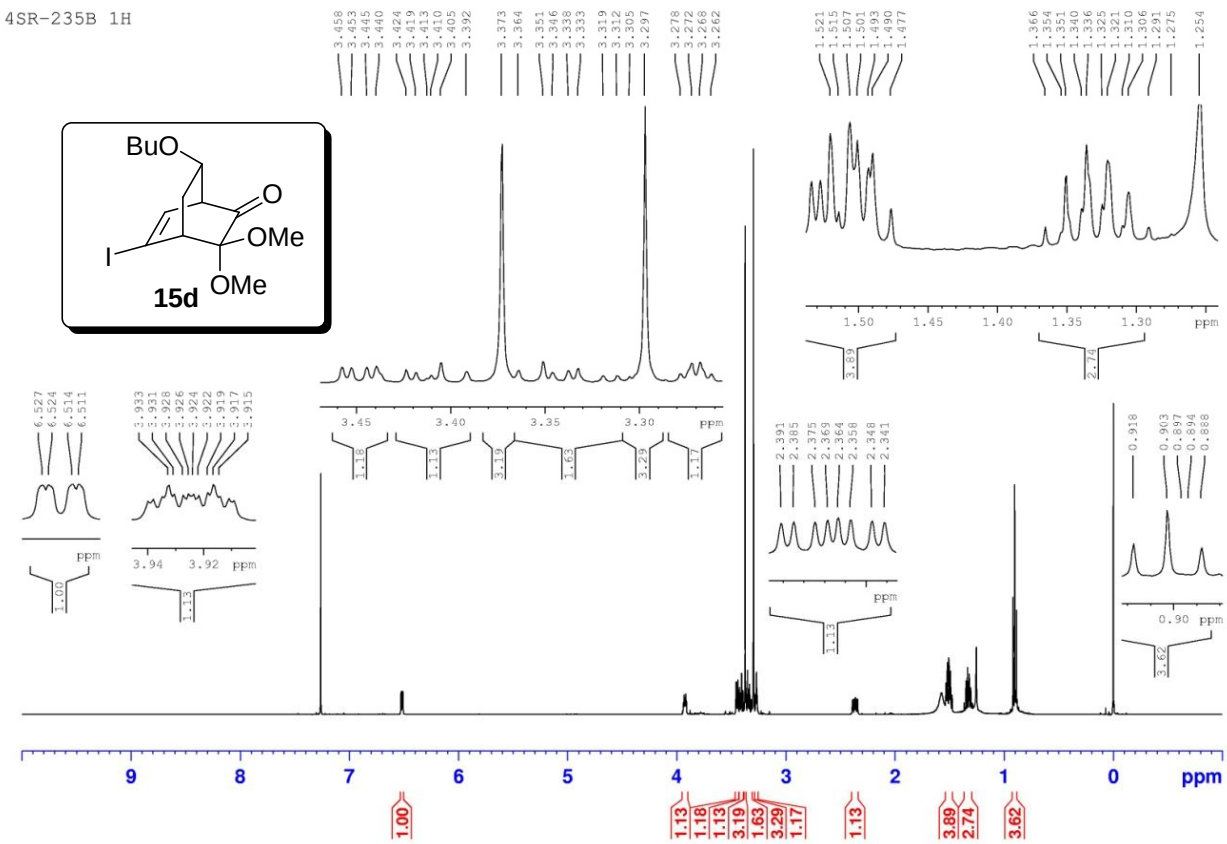

4SR-229B
Ph
O
OMe
I
OMe
15a
ppm

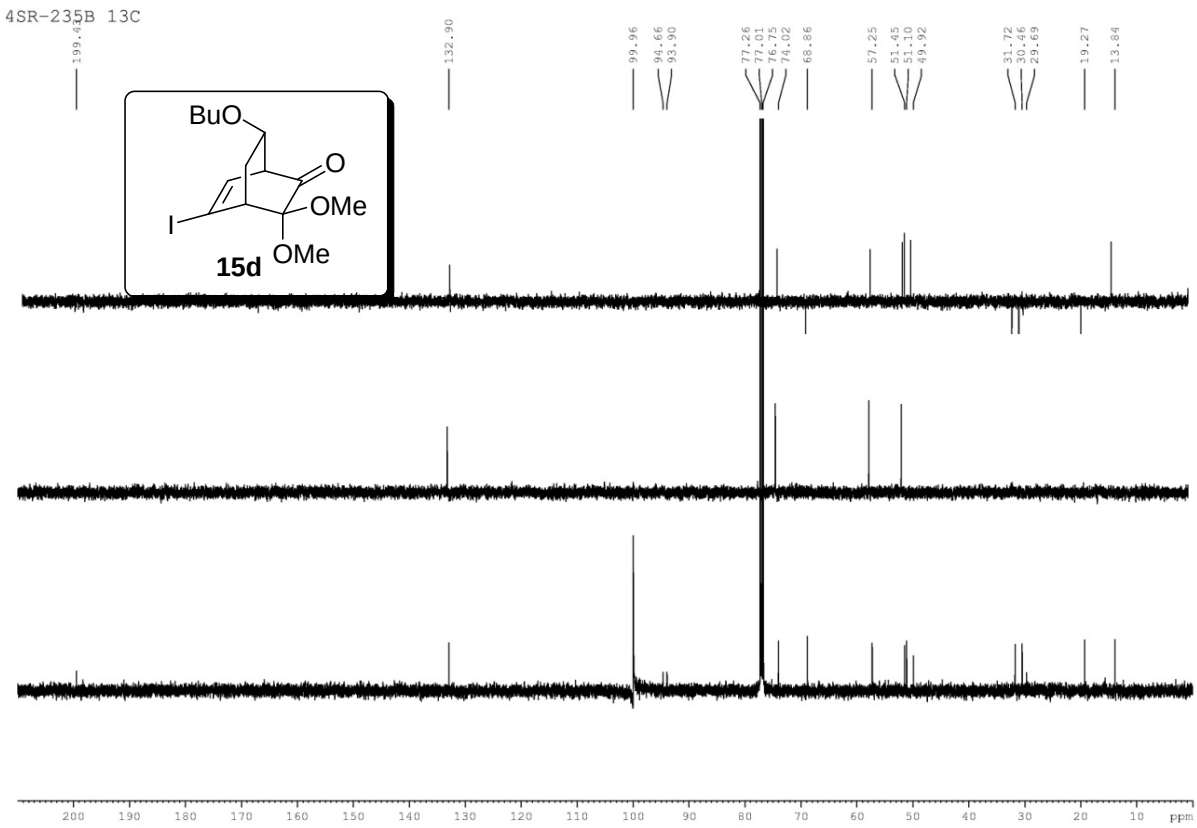

4SR-230B 1H
15b

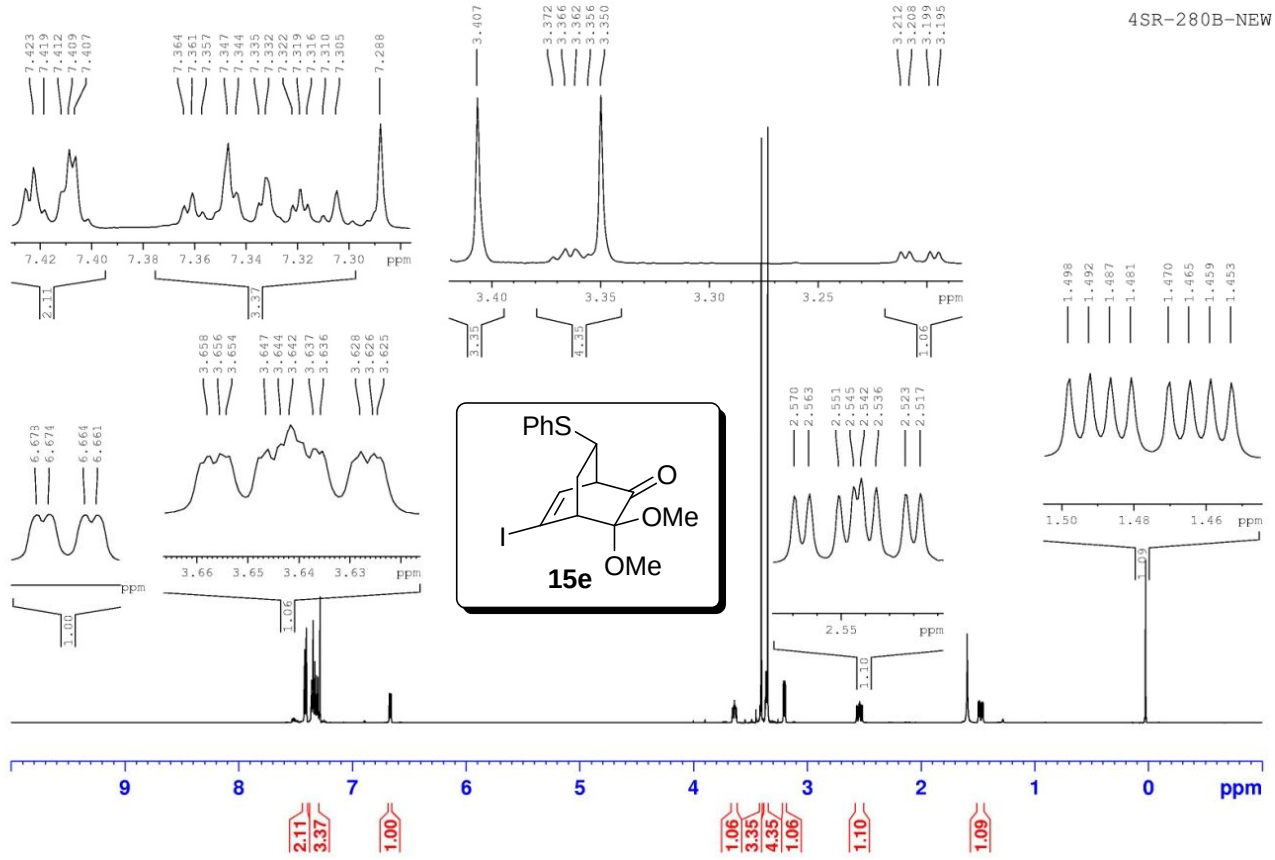

4SR-230B
15b

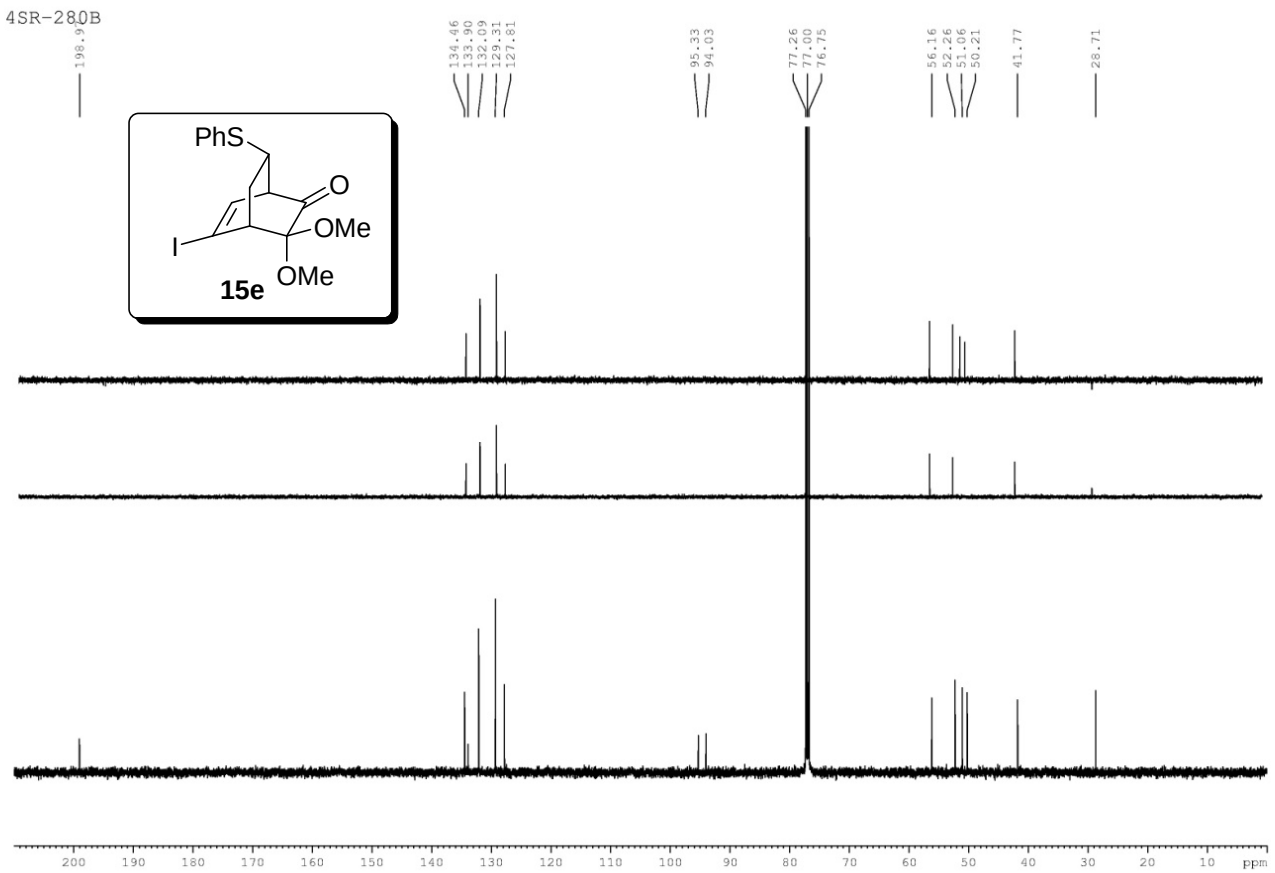

4SR-256
EtO
O
OMe
I
OMe
15c
ppm

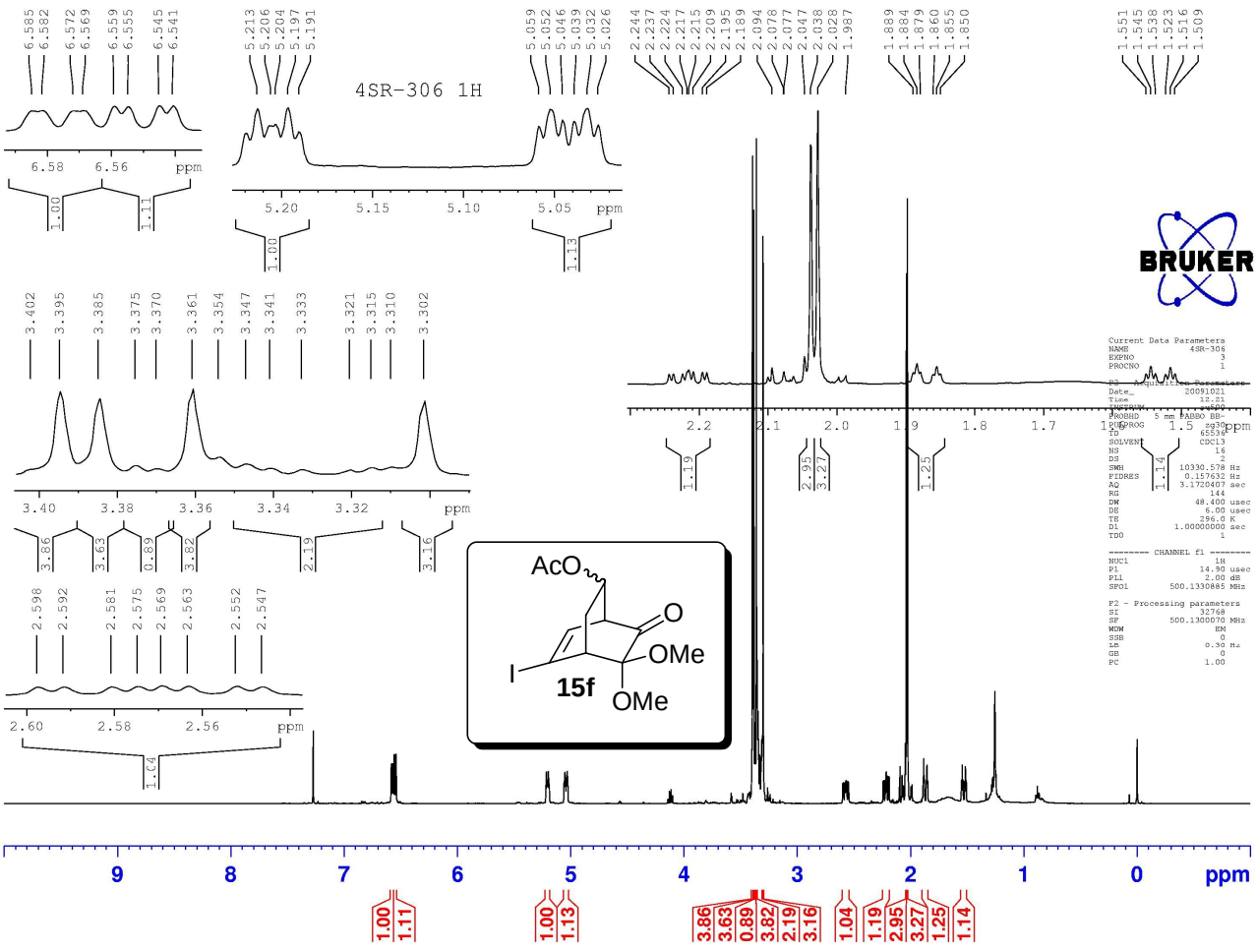

4SR-256
EtO
O
OMe
I
OMe
15c
ppm


4SR-235B 1H
BuO
O
OMe
I
OMe
15d


4SR-235B 13C
BuO
O
OMe
I
OMe
15d


4SR-280B-NEW
PhS
O
OMe
I
OMe
15e


4SR-280B
PhS
O
OMe
I
OMe
15e


4SR-306 1H
AcO
O
OMe
I
15f
OMe
BRUKER
ppm

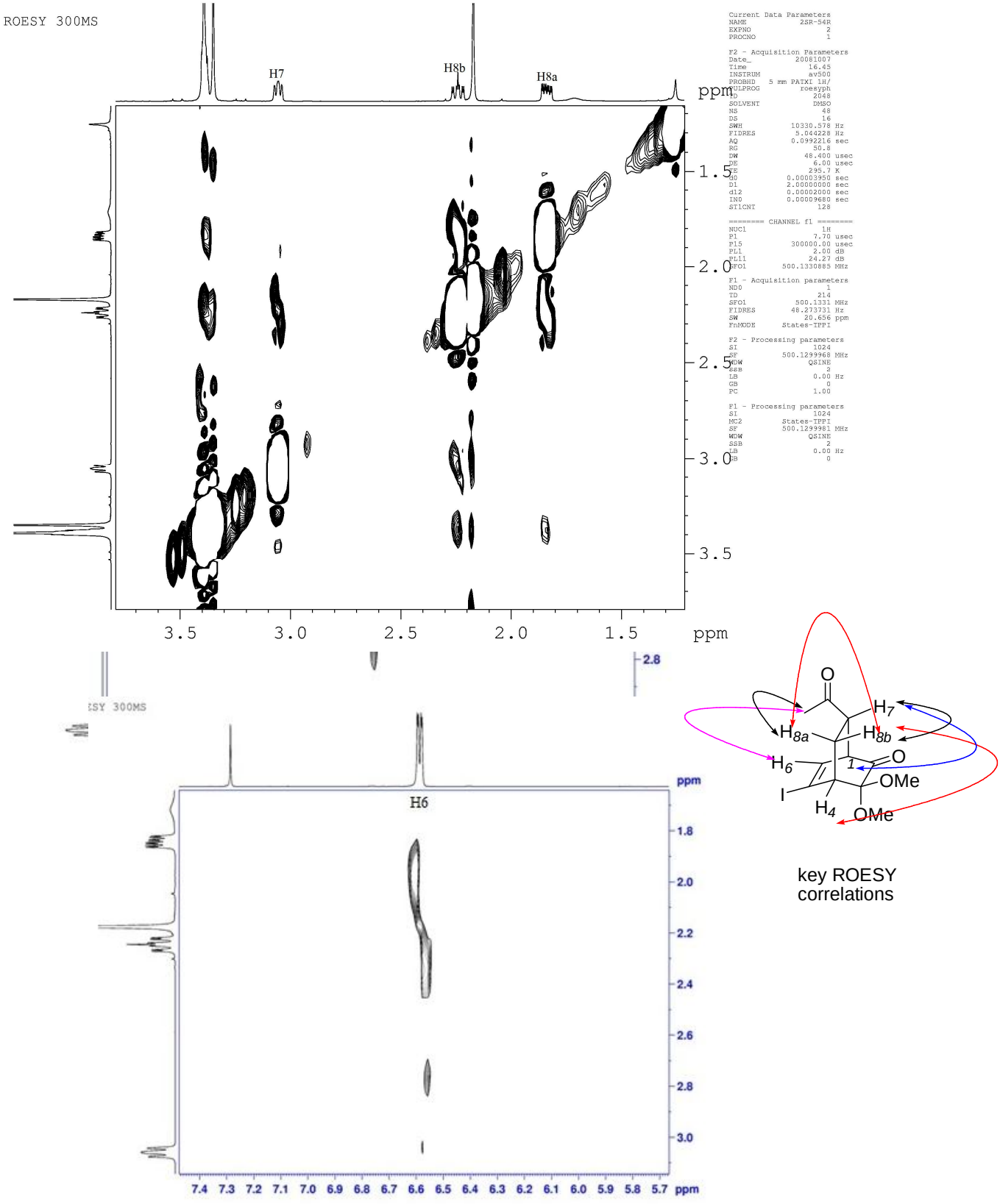


Figure S1: ^{1}H-^{1}H ROESY Spectrum of **11c**.

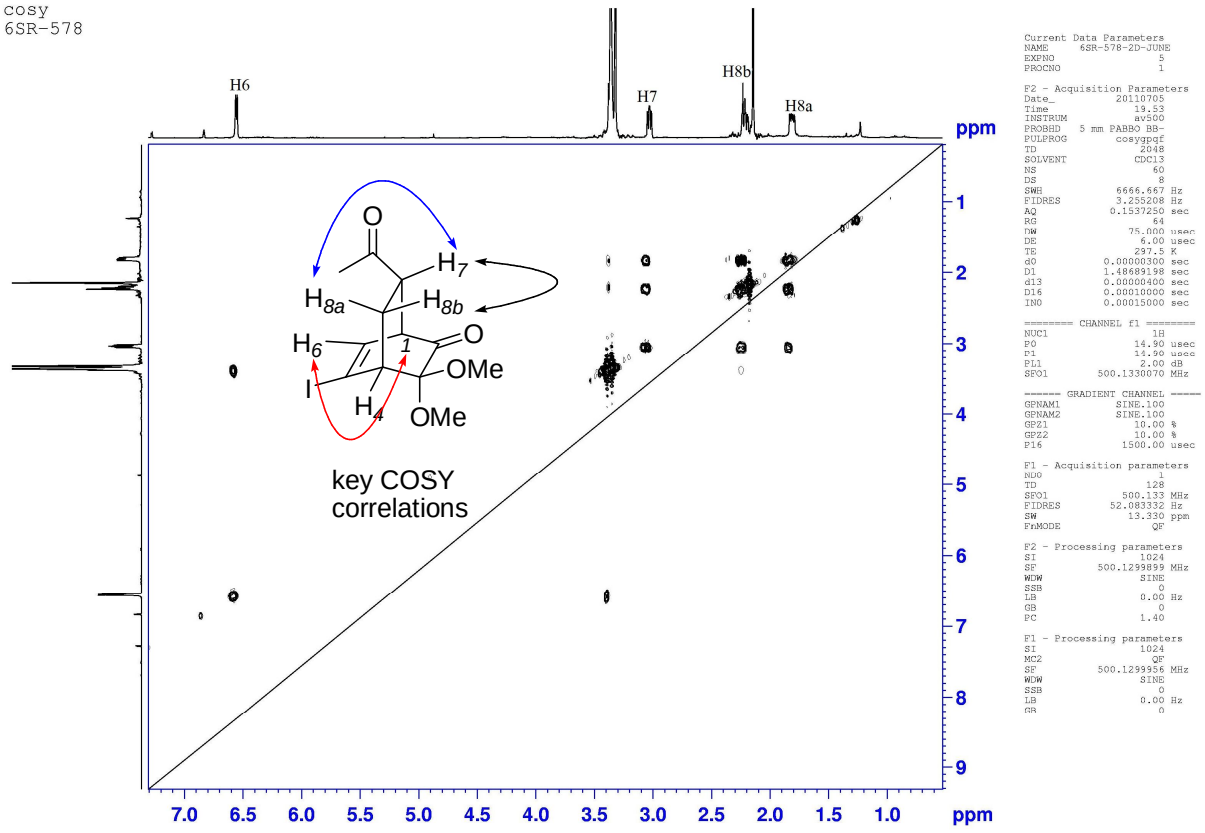


Figure S2: ^{1}H-^{1}H COSY Spectrum of **11c**.

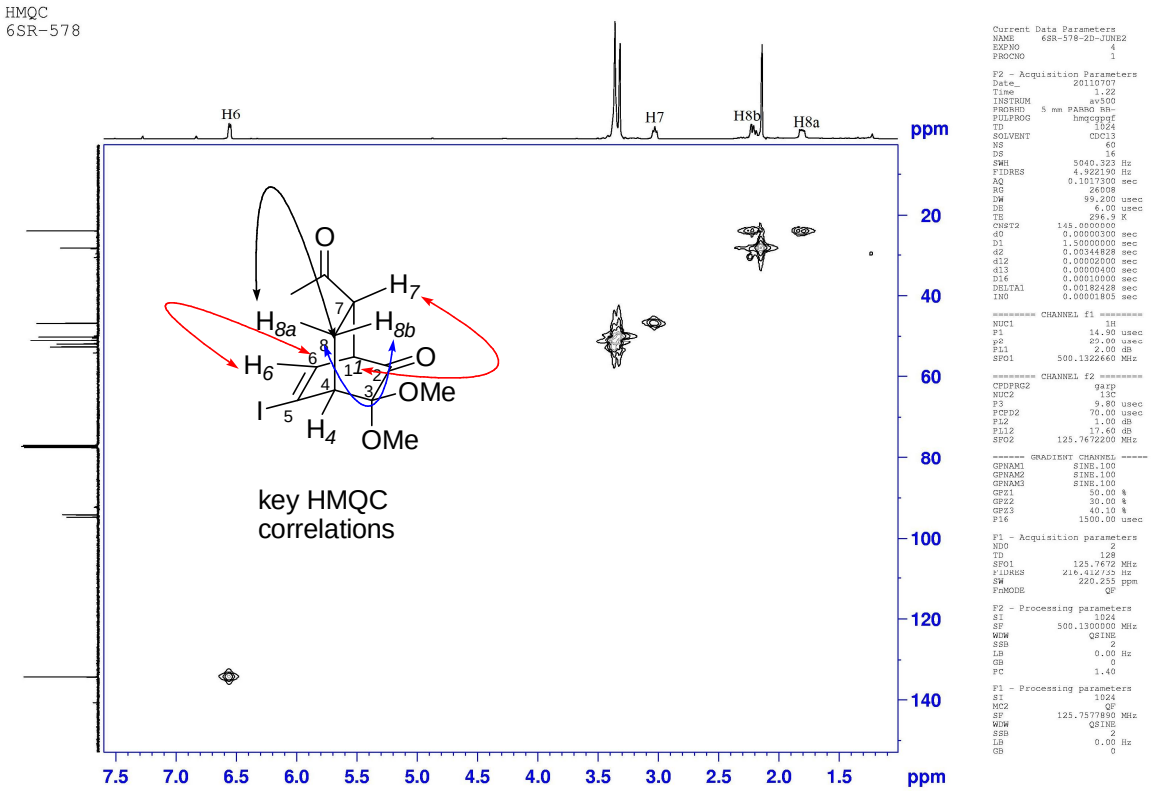


Figure S3: ^{1}H-^{13}C COSY HMQC Spectrum of **11c**.

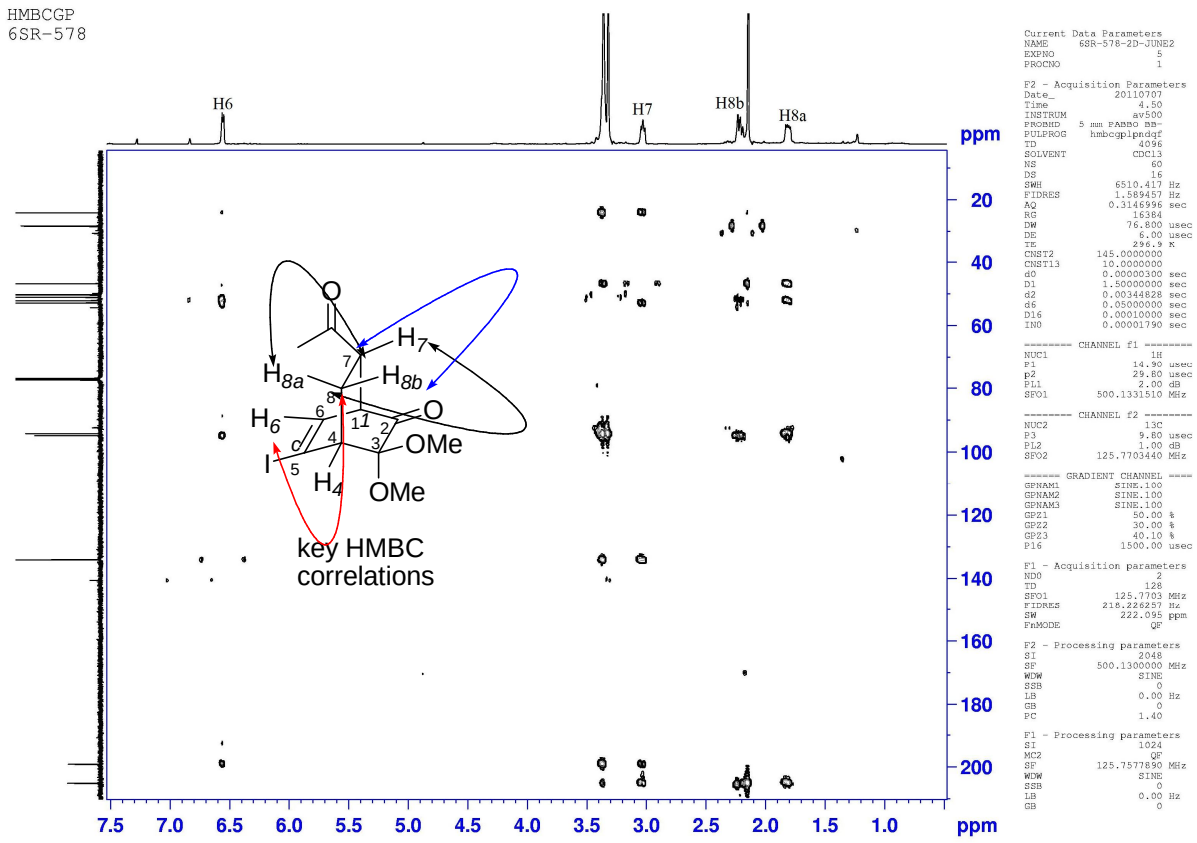


Figure S4: ^{1}H-^{13}C COSY (HMBC) Spectrum of **11c**.

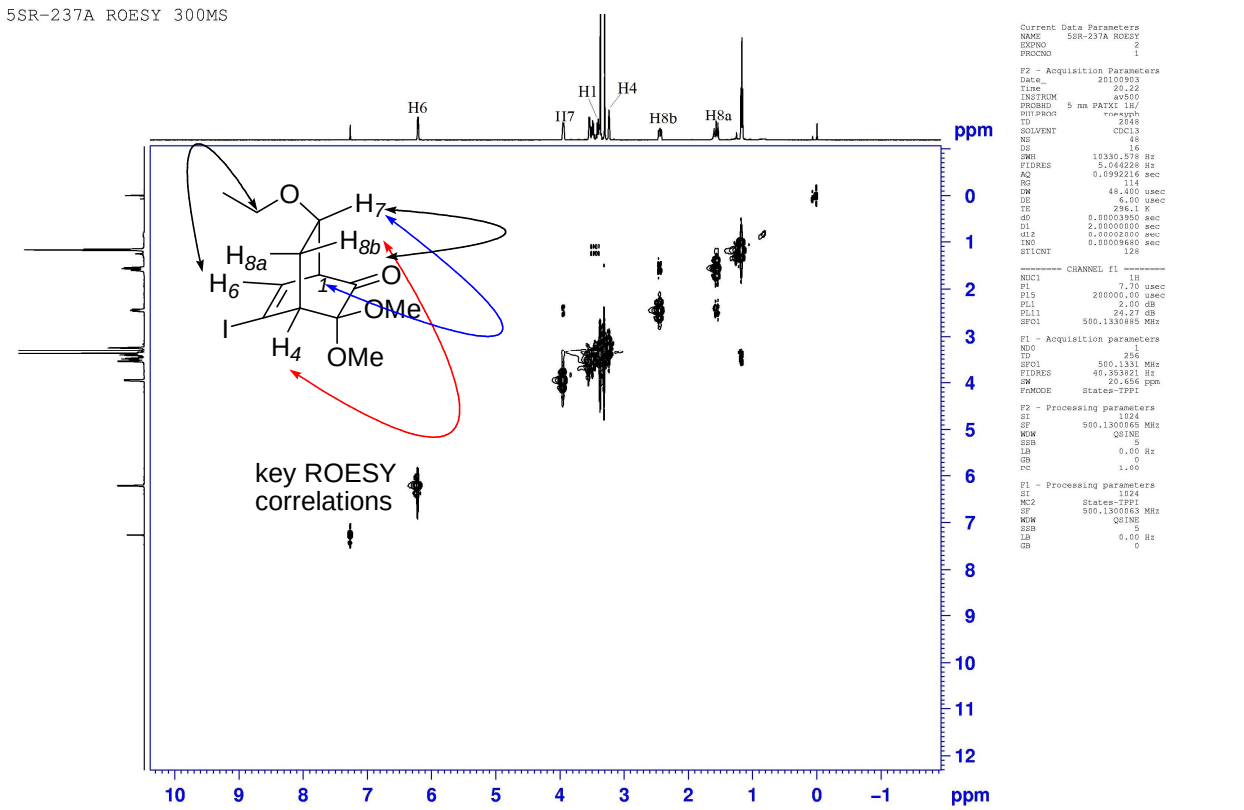


Figure S5: ^{1}H-^{1}H ROESY Spectrum of **14c**.

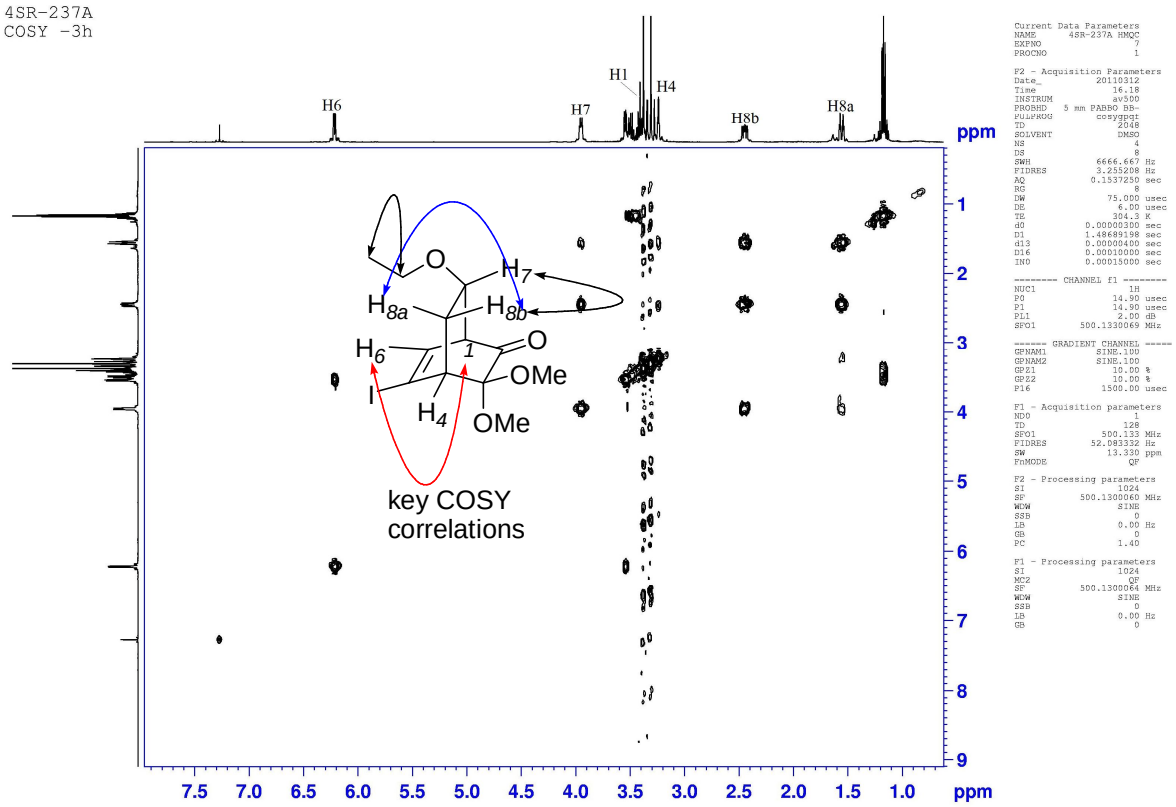


Figure S6: ^{1}H-^{1}H COSY Spectrum of **14c**.

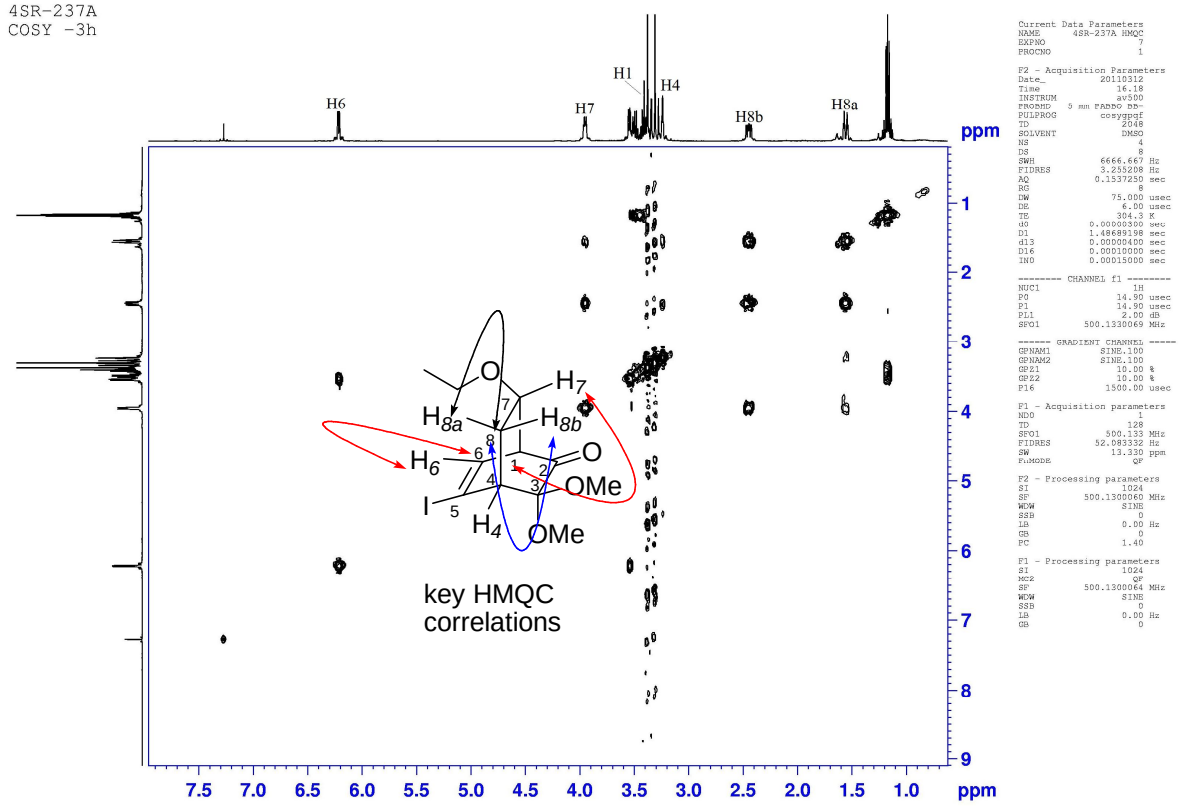


Figure S7: ^{1}H-^{13}C COSY (HMQC) Spectrum of **14c**.

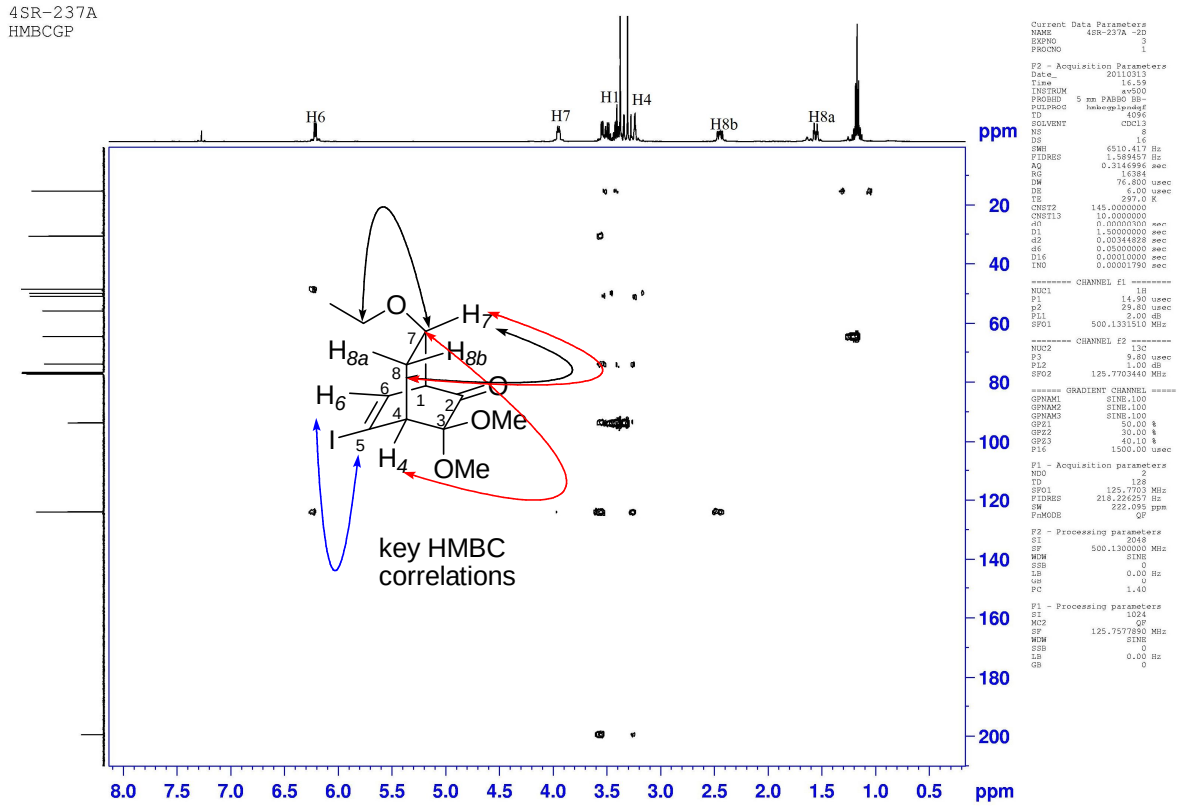


Figure S8: ^{1}H-^{13}C COSY (HMBC) Spectrum of **14c**.

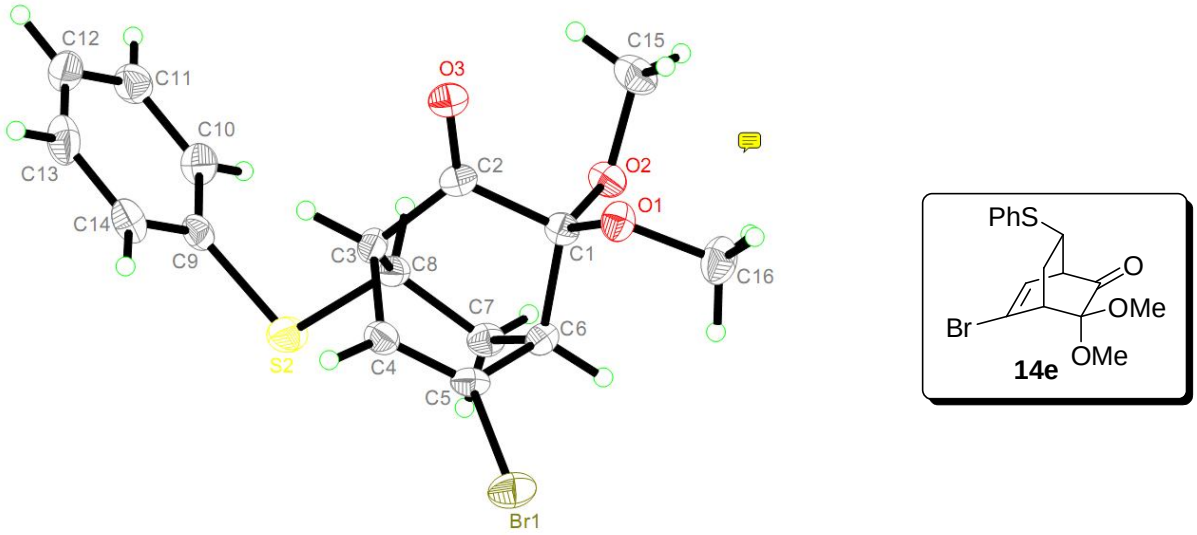


Figure S9: ORTEP Plot of the crystal structure of adduct **14e** (numbering is arbitrary).

Table S5: Crystallographic data for the compound **14e.**

Empirical formula	C16 H17 Br O3 S	
Formula weight	369.27	
Temperature	240	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2(1)/c	
Unit cell dimensions	a = 10.6073(17) Å	α= 90.00
	b = 7.7726(13) Å	β= 119.150(6)
	c = 21.494(3+) Å	γ = 90.00
Volume	1547.7(4) $Å^3$	
Z	4	
Density (calculated)	1.585 Mg/m^3	
Absorption coefficient	2.798 mm^{-1}	
F(000)	316	
Crystal size	0.28 x 0.21 x 0.14 mm^3	
Theta range for data collection	2.17 to 25.00°	
Reflections collected	6397	
Independent reflections	2431 [R(int) = 0.0283]	
Completeness to theta = 25.84°	93.4 %	
Absorption correction	empirical	
Max. and min. transmission	0.9774 and 0.9685	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2431 / 0 / 200	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0547, wR2 = 0.1347	
R indices (all data)	R1 = 0.0674, wR2 = 0.1440	
Largest diff. peak and hole	0.225 and -0.229 e.Å$^-$	

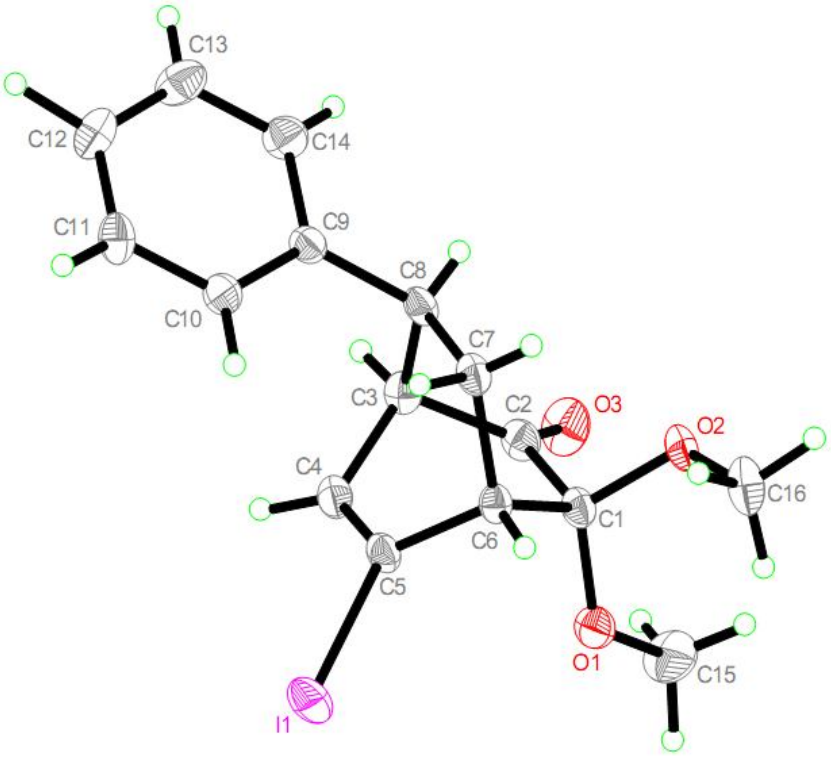


Figure S10: ORTEP Plot of the crystal structure of adduct **15a** (numbering is arbitrary).

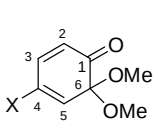
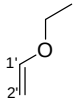
Table S6: Crystallographic data for the compound **15a**.

Empirical formula	$C_{16}H_{17}IO_3$	
Formula weight	384.20	
Temperature	293(2)	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.541(2) Å	α= 79.510(5)
	b =10.227(3)Å	β= 74.206(5)
	c = 10.666(3)Å	γ = 70.686(5)
Volume	743.1(4)Å^3	
Z	2	

Density (calculated)	1.717Mg/m^3
Absorption coefficient	2.159mm^{-1}
F(000)	380
Crystal size	0.29 x 0.22 x 0.15mm^3
Theta range for data collection	2.00 to 26.37°
Reflections collected	6397
Independent reflections	2431 [R(int) = 0.0283]
Completeness to theta = 25.84°	93.4 %
Absorption correction	'empirical'
Max. and min. transmission	0.9774 and 0.9685
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2431 / 0 / 200
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0547, wR2 = 0.1347
R indices (all data)	R1 = 0.0674, wR2 = 0.1440
Largest diff. peak and hole	0.225 and -0.229 e.Å$^-$

Table S7. HOMO-LUMO energies of MOBs **5-8** and dienophiles MVK and EVE

Reactant	**HOMO (eV)**	**LUMO (eV)**
FMOB	–6.643984256	–2.51571242
ClMOB	–6.715550764	–2.609864556
BrMOB	–6.694869948	–2.604422236
IMOB	–6.92127046	–2.94429512
MVK	–6.731333492	–1.490651448
EVE	–6.085602224	1.225610464

Table S8. Fukui indices for MOBs **5-8** and dienophiles MVK and EVE.   

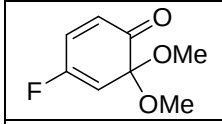
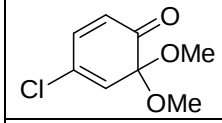
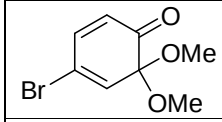
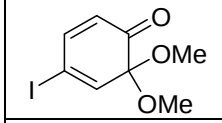
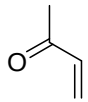
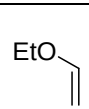
	F(+)						F(–)					
	1	2	3	4	5	6	1	2	3	4	5	6
	0.1068	0.1341	0.2148	0.0346	0.1126	0.0165	0.0338	0.1218	0.0201	0.0219	0.0490	0.0955
	0.1001	0.1266	0.1938	0.0474	0.1375	0.0167	0.0346	0.1202	0.0190	0.0185	0.0395	0.1012
	0.0986	0.1261	0.1932	0.0456	0.1382	0.0174	0.0300	0.1161	0.0205	0.0278	0.0558	0.0893
	0.1142	0.1472	0.2246	0.0628	0.1851	0.0090	0.0090	0.0819	0.0233	0.0795	0.1629	0.0178
	0.1363 **(C1')**	0.3355 **(C2')**					0.1759 **(C1')**	0.0130 **(C2')**				
	0.6209 **(C1')**	0.5056 **(C2')**					0.1021 **(C1')**	0.2667 **(C2')**				

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Table S9. Ab Initio RHF/6-31G** calculations of energies (eV) and coefficients (*Ci*) of the frontier molecular orbitals for dienes **5**-**8** and dienophiles MVK and EVE.

MOB/ dienophile	**HOMO**					**LUMO**				
	E	**C2**	**C3**	**C4**	**C5**	**E**	**C2**	**C3**	**C4**	**C5**
FMOB	–9.430996328	–0.27568	–0.19207	0.24387	0.30597	1.29527216	–0.21339	0.26328	0.14983	–0.19784
ClMOB	–9.42473766	–0.27259	–0.18918	0.24283	0.29782	1.226426812	–0.20732	0.25658	0.15613	–0.22146
BrMOB	–9.354803848	–0.2619	–0.17841	0.24146	0.29825	1.216086404	–0.20687	0.25545	0.15723	–0.22708
IMOB	–9.391539508	0.17568	0.26733	–0.27018	–0.33869	0.806279708	–0.24973	0.29914	0.18585	–0.27353
MVK	–10.401089868	0.34183(**C2'**)	0.36325(**C1'**)			2.739391772	0.31155(**C2'**)	–0.20329(**C1'**)		
EVE	–9.18527558	0.38725(**C2'**)	0.29508(**C1'**)			5.60967134	–0.31470(**C2'**)	0.40919(**C1'**)		

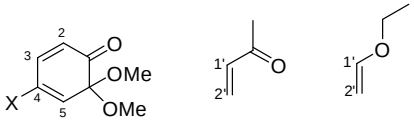


Table S10. Total energies (au) and relative energies[a] (kcal/mol) for the stationary points corresponding to the cycloaddition reaction between halo masked *o*-benzoquinones and MVK.

	B3LYP/6-31G**		B3LYP/6-31G** in methanol	
	Total Energy (au)	Rel energy[a] (kcal/mol)	Total Energy (au)	Rel energy[a] (kcal/mol)
5	–635.7149181		–635.7226627	
MVK	–231.2441998		–231.2498995	
9c (ortho-endo) **TS**	–866.9401133	11.93	–866.9514379	13.26
9c (ortho-exo) **TS**	–866.9336468	15.98	–866.9458184	16.78
9c (meta-endo) **TS**	–866.9323442	16.80	–866.9438834	18.01
9c (meta-endo) **TS**	–866.9251091	21.34	–866.9370876	22.26
6	–996.0772566		–996.084898	
MVK	–231.2441998		–231.2498995	
10c (ortho-endo) **TS**	–1227.3019549	12.24	–1227.3133613	13.45
10c (ortho-exo) **TS**	–1227.2968698	15.43	–1227.3089205	16.24
10c (meta-endo) **TS**	–1227.2942833	17.05	–1227.3060688	18.03
10c (meta-endo) **TS**	–1227.2889173	20.42	–1227.3008031	21.33
7	–3107.586208		–3107.5938828	
MVK	–231.2441998		–231.2498995	
(7+MVK) (ortho-endo) **TS**	–3338.812108	11.48	–3338.8233909	12.80
(7+MVK) (ortho-exo) **TS**	–3338.8069004	14.75	–3338.818928	15.60
(7+MVK) (meta-endo) **TS**	–3338.8054029	15.69	–3338.8167992	16.93
(7+MVK) (meta-endo) **TS**	–3338.7988166	19.82	–3338.8106631	20.78
8	–7455.7985121		–7455.8252912	
MVK	–231.2441998		–231.2498995	
11c (ortho-endo) **TS**	–7687.0411318	0.99	–7687.0774479	-1.42
11c (ortho-exo) **TS**	–7687.034717	5.02	–7687.0721328	1.92
11c (meta-endo) **TS**	–7687.0332597	5.93	–7687.0698017	3.38
11c (meta-endo) **TS**	–7687.0276703	9.44	–7687.0647103	6.58

[a] Relative to that of halo-MOB + MVK.

Table S11. Total energies (au) and relative energies[a] (kcal/mol, in parentheses) for the stationary points corresponding to the cycloaddition reaction between halo masked *o*-benzoquinone and MVK.

	B3LYP/6-31G**	ΔE(R-P)	B3LYP/6-31G** in methanol	ΔE(R-P)
5	–635.7149181		–635.7226627	
MVK	–231.2441998		–231.2498995	
9c (ortho-endo) **P**	–867.0013632	–26.51	–867.0129779	–25.36
9c (ortho-exo) **P**	–867.0002599	–25.82	–867.011487	–24.43
9c (meta-endo) **P**	–867.0008939	–26.21	–867.0125463	–25.09
9c (meta-endo) **P**	–867.0006984	–26.09	–867.0123501	–24.97
6	–996.0772566		–996.084898	
MVK	–231.2441998		–231.2498995	
10c (ortho-endo) **P**	–1227.3646539	–27.11	–1227.376628	–26.25
10c (ortho-exo) **P**	–1227.3636805	–26.50	–1227.3750736	–25.27
10c (meta-endo) **P**	–1227.3643855	–26.94	–1227.3761766	–25.97
10c (meta-endo) **P**	–1227.3645175	–27.02	–1227.3761898	–25.97
7	–3107.586208		–3107.5938828	
MVK	–231.2441998		–231.2498995	
(7+MVK) (ortho-endo) **P**	–3338.8748525	–27.89	–3338.8866608	–26.91
(7+MVK) (ortho-exo) **P**	–3338.87384	-27.25	–3338.8851382	–25.95
(7+MVK) (meta-endo) **P**	–3338.8749906	–27.98	–3338.8865929	–26.86
(7+MVK) (meta-endo) **P**	–3338.8748538	–27.89	–3338.88637	–26.72
8	–7455.7985121		–7455.8252912	
MVK	–-231.2441998		–231.2498995	
11c (ortho-endo) **P**	–7687.1064146	–39.97	–7687.1437025	–42.99
11c (ortho-exo) **P**	–7687.1045829	–38.82	–7687.1413423	–41.51
11c (meta-endo) **P**	–7687.1058104	–39.59	–7687.142908	–42.49
11c (meta-endo) **P**	–7687.1056479	–39.49	–7687.1426045	–42.30

[a] Relative to that of halo-MOB + MVK.

Table S12. Total energies (au) and relative energies[a] (kcal/mol, in parentheses) for the stationary points corresponding to the cycloaddition reaction between halo masked *o*-benzoquinone and EVE.

	B3LYP/6-31G**		B3LYP/6-31G** in methanol	
5	–635.7149181		–635.7226627	
EVE	–232.4448713		–232.447664	
(5+EVE) (ortho-endo) **P**	–868.1913854	–19.83	–868.2006138	–34.96
(5+EVE) (ortho-exo) **P**	–868.1943538	–21.67	–868.2030358	–36.48
(5+EVE) (meta-endo) **P**	–868.1899045	–18.90	–868.1986372	–33.72
(5+EVE) (meta-endo) **P**	–868.1874233	–17.34	–868.1966494	–32.48
6	–996.0772566		–996.084898	
EVE	–232.4448713		–232.447664	
13c (ortho-endo) **P**	–1228.5553184	–20.83	–1228.5645886	–20.10
13c (ortho-exo) **P**	–1228.557802	–22.39	–1228.5665478	–21.33
13c (meta-endo) **P**	–1228.551528	–18.45	–1228.5603823	–17.46
13c (meta-endo) **P**	–1228.5510404	–18.14	–1228.5605419	–17.56
7	–3107.586208		–3107.5938828	
EVE	–232.4448713		–232.447664	
14c (ortho-endo) **P**	–3340.0655352	–21.62	–3340.0776884	–22.68
14c (ortho-exo) **P**	–3340.0679791	–23.15	–3340.0766506	–22.03
14c (meta-endo) **P**	–3340.0639571	–20.63	–3340.0727356	–19.57
14c (meta-endo) **P**	–3340.061313	–18.97	–3340.0707101	–18.30
8	–7455.7985121		–7455.8252912	
EVE	–232.4448713		–232.447664	
15c (ortho-endo) **P**	–7688.2961072	–33.08	–7688.3332136	–37.81
15c (ortho-exo) **P**	–7688.2976053	–34.02	–7688.3310194	–36.44
15c (meta-endo) **P**	–7688.2910238	–29.90	–7688.3246147	–32.42
15c (meta-endo) **P**	–7688.2910786	–29.93	–7688.3254774	–32.96

[a] Relative to that of halo-MOB + EVE

Table S13. Total energies (au) and relative energies[a] (kcal/mol) for the stationary points corresponding to the cycloaddition reaction between halo masked *o*-benzoquinones and EVE.

Reactant/TS	B3LYP/6-31G**		B3LYP/6-31G** in methanol	
	Total Energy (au)	Rel energy[a] (kcal/mol)	Total Energy (au)	Rel energy[a] (kcal/mol)
5	–635.7149181		–635.7226627	
EVE	–232.4448713		–232.447664	
(5+EVE) (ortho-endo) **TS**	–868.1290825	19.27	–868.1448944	15.96
(5+EVE) (ortho-exo) **TS**	–868.1290204	19.31	–868.1396219	19.27
(5+EVE) (meta-endo) **TS**	–868.128417	19.69	–868.1381465	20.19
(5+EVE) (meta-endo) **TS**	–868.1199958	24.97	–868.1293679	25.70
6	–996.0772566		–996.084898	
EVE	–232.4448713		–232.447664	
13c (ortho-endo) **TS**	–1228.4946613	17.24	–1228.5057711	16.81
13c (ortho-exo) **TS**	–1228.495579	16.66	–1228.505966	16.67
13c (meta-endo) **TS**	–1228.4905152	19.84	–1228.5002031	20.30
13c (meta-endo) **TS**	–1228.4837049	24.11	–1228.4931831	24.71
7	–3107.586208		–3107.5938828	
EVE	–232.4448713		–232.447664	
14c (ortho-endo) **TS**	–3340.0073707	14.88	–3340.0182789	14.60
14c (ortho-exo) **TS**	–3340.0061677	15.63	–3340.0163859	15.79
14c (meta-endo) **TS**	–3340.0021762	18.14	–3340.0117456	18.70
14c (meta-endo) **TS**	–3339.9933393	23.68	–3340.00272381	24.36
8	–7455.7985121		–7455.8252912	
EVE	–232.4448713		–232.447664	
15c (ortho-endo) **TS**	–7688.2332563	6.35	–7688.2687806	2.62
15c (ortho-exo) **TS**	–7688.2334107	6.26	–7688.2684179	2.85
15c (meta-endo) **TS**	–7688.2282164	9.52	–7688.2623154	6.68
15c (meta-endo) **TS**	–7688.2218882	13.49	–7688.2556605	10.85

[a] Relative to that of halo-MOB + EVE

Table S14. Bond distances in the transition states.

TS		Bond distance	
		C_5-$C_{n'}$† (Å)	C_2-$C_{n'}$† (Å)
9c (ortho-endo) **TS**	ortho-endo	1.91888	2.78550
9c (ortho-exo) **TS**	ortho-exo	2.03426	2.74058
9c (meta-endo) **TS**	meta-endo	2.35963	2.23286
9c (meta-exo) **TS**	meta-exo	2.43103	2.17443
10c (ortho-endo) **TS**	ortho-endo	2.02331	2.79346
10c (ortho-exo) **TS**	ortho-exo	2.06667	2.80647
10c (meta-endo) **TS**	meta-endo	2.31512	2.21854
10c (meta-exo) **TS**	meta-exo	2.38832	2.17023
(7+MVK) (ortho-endo) **TS**	ortho-endo	2.01599	2.82903
(7+MVK) (ortho-exo) **TS**	ortho-exo	2.02861	2.74718
(7+MVK) (meta-endo) **TS**	meta-endo	2.31229	2.21997
(7+MVK) (meta-exo) **TS**	meta-exo	2.39481	2.18982
11c (ortho-endo) **TS**	ortho-endo	2.03928	2.80180
11c (ortho-exo) **TS**	ortho-exo	2.25001	3.00372
11c (meta-endo) **TS**	meta-endo	2.28616	2.17562
11c (meta-exo) **TS**	meta-exo	2.31084	2.07949
(5+EVE) (ortho-endo) **TS**	ortho-endo	1.94055	2.78403
(5+EVE) (ortho-exo) **TS**	ortho-exo	1.99628	2.87542
(5+EVE) (meta-endo) **TS**	meta-endo	2.41458	2.29710
(5+EVE) (meta-exo) **TS**	meta-exo	2.57943	2.03486
13c (ortho-endo) **TS**	ortho-endo	1.90104	2.75090
13c (ortho-exo) **TS**	ortho-exo	2.03186	2.97621
13c (meta-endo) **TS**	meta-endo	2.44226	2.30749
13c (meta-exo) **TS**	meta-exo	2.54196	2.06447
14c (ortho-endo) **TS**	ortho-endo	1.95316	2.88237
14c (ortho-exo) **TS**	ortho-exo	2.00415	2.93764
14c (meta-endo) **TS**	meta-endo	2.33821	2.22190
14c (meta-exo) **TS**	meta-exo	2.51228	2.08551
15c (ortho-endo) **TS**	ortho-endo	1.97379	2.90106
15c (ortho-exo) **TS**	ortho-exo	1.77610	2.76643
15c (meta-endo) **TS**	meta-endo	2.23009	2.08860
15c (meta-exo) **TS**	meta-exo	2.44381	1.88664

†The distances are of C_5-$C_{2'}$ for ortho TS and C_5-$C_{1'}$ for meta TS.

Table S15. Imaginary frequencies and total energies of transition states.

TS	Imaginary frequency (cm^{-1})	Total energy (a.u.)
9c (ortho-endo) **TS**	–371.4684	–866.9401133
9c (ortho-exo) **TS**	–393.7123	–866.9336468
9c (meta-endo) **TS**	–440.5551	–866.9323442
9c (meta-exo) **TS**	–461.5369	–866.9251091
10c (ortho-endo) **TS**	–374.6994	–1227.3019549
10c (ortho-exo) **TS**	–396.9304	–1227.2968698
10c (meta-endo) **TS**	–432.6676	–1227.2942833
10c (meta-exo) **TS**	–454.3963	–1227.2889173
(7+MVK) (ortho-endo) **TS**	–370.8943	–3338.812108
(7+MVK) (ortho-exo) **TS**	–392.8237	–3338.8069004
(7+MVK) (meta-endo) **TS**	–426.6280	–3338.8054029
(7+MVK) (meta-exo) **TS**	–453.9831	–3338.7988166
11c (ortho-endo) **TS**	–378.4059	–7687.0411318
11c (ortho-exo) **TS**	–399.3135	–7687.034717
11c (meta-endo) **TS**	–434.3585	–7687.0332597
11c (meta-exo) **TS**	–457.6114	–7687.0276703
(5+EVE) (ortho-endo) **TS**	–410.6655	–868.1290825
(5+EVE) (ortho-exo) **TS**	–411.4020	–868.1290204
(5+EVE) (meta-endo) **TS**	–481.4355	–868.128417
(5+EVE) (meta-exo) **TS**	–474.9753	–868.1199958
13c (ortho-endo) **TS**	–396.0362	–1228.4946613
13c (ortho-exo) **TS**	–395.0851	–1228.495579
13c (meta-endo) **TS**	–466.9261	–1228.4905152
13c (meta-exo) **TS**	–474.1158	–1228.4837049
14c (ortho-endo) **TS**	–379.6638	–3340.0073707
14c (ortho-exo) **TS**	–388.3635	–3340.0061677
14c (meta-endo) **TS**	–470.5185	–3340.0021762
14 (meta-exo) **TS**	–475.8273	–3339.9933393
15 (ortho-endo) **TS**	–392.1105	–7688.2332563
15 (ortho-exo) **TS**	–397.8849	–7688.2334107
15 (meta-endo) **TS**	–466.9047	–7688.2282164
15 (meta-exo) **TS**	–469.9066	–7688.2218882

Table S16. Total energies (in au) and relative energies (in kcal/mol) for the stationary points corresponding to the cycloaddition reaction between chloro MOB and ACN/VA

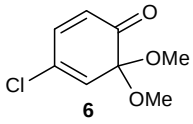
4-Halo MOB	Config.	Cycloaddition with ACN				Cycloaddition with VA			
		B3LYP/6-31G**	Rel ene[a] (kcal/mol)	C_5-$C_{\pi'}$† (Å)	C_2-$C_{\pi'}$† (Å)	B3LYP/6-31G**	Rel ene[b] (kcal/mol)	C_5-$C_{\pi'}$† (Å)	C_2-$C_{\pi'}$† (Å)
 **6**	ortho-endo	–1166.8891900	15.25	2.00658	2.73373	–1302.5223887	21.80	1.97540	2.70111
	ortho-exo	–1166.8882247	15.86	1.78589	2.71587	–1302.5233617	21.19	1.99305	2.77792
	meta-endo	–1166.8824111	19.51	2.26016	2.25775	–1302.5133245	27.49	2.18927	2.32253
	meta-exo	–1166.8766507	23.12	2.29199	2.24626	–1302.5168219	25.29	2.51300	2.32470

Table S17. Gibbs Free Energies of Transition States

TS	**Gibbs free energy** (kcal/mol)
9c (ortho-endo) **TS**	–866.733072
9c (ortho-exo) **TS**	–866.725968
9c (meta-endo) **TS**	–866.724741
9c (meta-exo) **TS**	–866.717165
10c (ortho-endo) **TS**	–1227.096583
10c (ortho-exo) **TS**	–1227.091174
10c (meta-endo) **TS**	–1227.089034
10c (meta-exo) **TS**	–1227.083804
(7+MVK) (ortho-endo) **TS**	–3338.608441
(7+MVK) (ortho-exo) **TS**	–3338.602771
(7+MVK) (meta-endo) **TS**	–3338.601177
(7+MVK) (meta-exo) **TS**	–3338.595236
11c (ortho-endo) **TS**	–7686.839513
11c (ortho-exo) **TS**	–7686.832718
11c (meta-endo) **TS**	–7686.831201
11c (meta-exo) **TS**	–7686.826371
(5+EVE) (ortho-endo) **TS**	–867.897553
(5+EVE) (ortho-exo) **TS**	–867.897332
(5+EVE) (meta-endo) **TS**	–867.897732
(5+EVE) (meta-exo) **TS**	–867.889389
13c (ortho-endo) **TS**	–1228.265774
13c (ortho-exo) **TS**	–1228.266415
13c (meta-endo) **TS**	–1228.262410
13c (meta-exo) **TS**	–1228.255934
14c (ortho-endo) **TS**	–3339.779786
14c (ortho-exo) **TS**	–3339.778273
14c (meta-endo) **TS**	–3339.774844
14c (meta-exo) **TS**	–3339.767364
15c (ortho-endo) **TS**	–7688.008211
15c (ortho-exo) **TS**	–7688.007751
15c (meta-endo) **TS**	–7688.003331
15c (meta-exo) **TS**	–7687.997418

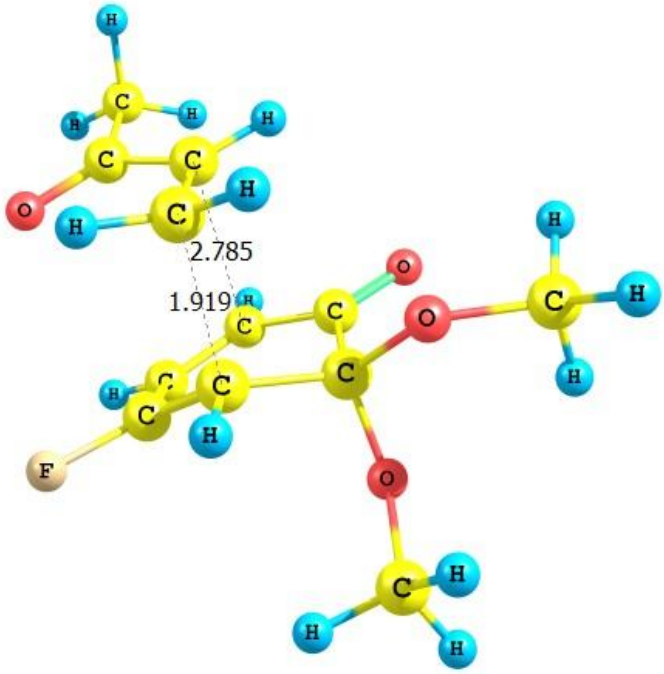
Table S18. Gibbs Free Energies of Products

Product	**Gibbs free energy** (kcal/mol)
9c (ortho-endo) **P**	–866.787220
9c (ortho-exo) **P**	–866.784979
9c (meta-endo) **P**	–866.786556
9c (meta-exo) **P**	–866.785012
10c (ortho-endo) **P**	–1227.152768
10c (ortho-exo) **P**	–1227.151076
10c (meta-endo) **P**	–1227.152616
10c (meta-exo) **P**	–1227.151013
(7+MVK) (ortho-endo) **P**	–3338.661756
(7+MVK) (ortho-exo) **P**	–3338.662300
(7+MVK) (meta-endo) **P**	–3338.660391
(7+MVK) (meta-exo) **P**	–3338.662555
11c (ortho-endo) **P**	–7686.898265
11c (ortho-exo) **P**	–7686.896683
11c (meta-endo) **P**	–7686.898097
11c (meta-exo) **P**	–7686.896979
(5+EVE) (ortho-endo) **P**	–867.953164
(5+EVE) (ortho-exo) **P**	–867.951328
(5+EVE) (meta-endo) **P**	–867.950931
(5+EVE) (meta-exo) **P**	–867.948517
13c (ortho-endo) **P**	–1228.319300
13c (ortho-exo) **P**	–1228.317473
13c (meta-endo) **P**	–1228.315028
13c (meta-exo) **P**	–1228.310712
14c (ortho-endo) **P**	–3339.830980
14c (ortho-exo) **P**	–3339.831840
14c (meta-endo) **P**	–3339.823256
14c (meta-exo) **P**	–3339.826356
15c (ortho-endo) **P**	–7688.064651
15c (ortho-exo) **P**	–7688.064627
15c (meta-endo) **P**	–7688.058182
15c (meta-exo) **P**	–7688.058831

Table S19. Gibbs Free Energies of Reactants

Reactant	**Gibbs free energy** (kcal/mol)
F-MOB	–635.590480
Cl-MOB	–995.955342
Br-MOB	–3107.467458
I-MOB	–7455.681568
MVK	–231.181528
EVE	–232.354946

Transition State Structures halo-MOBs, MVK & EVE



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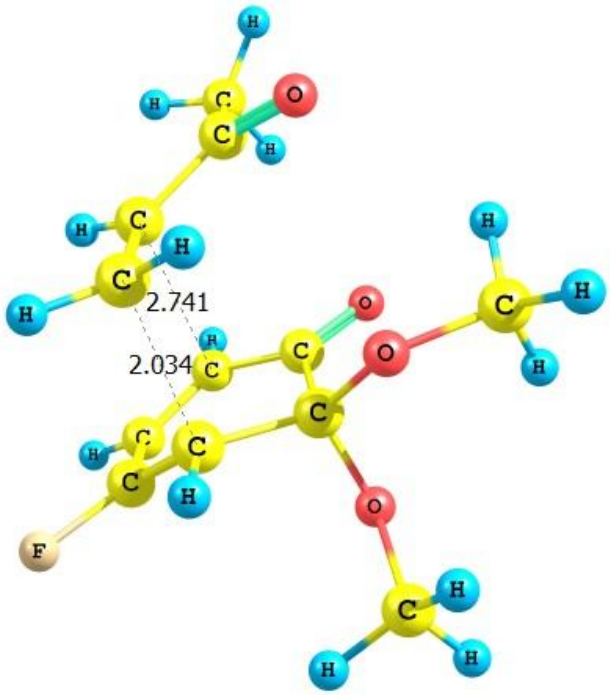

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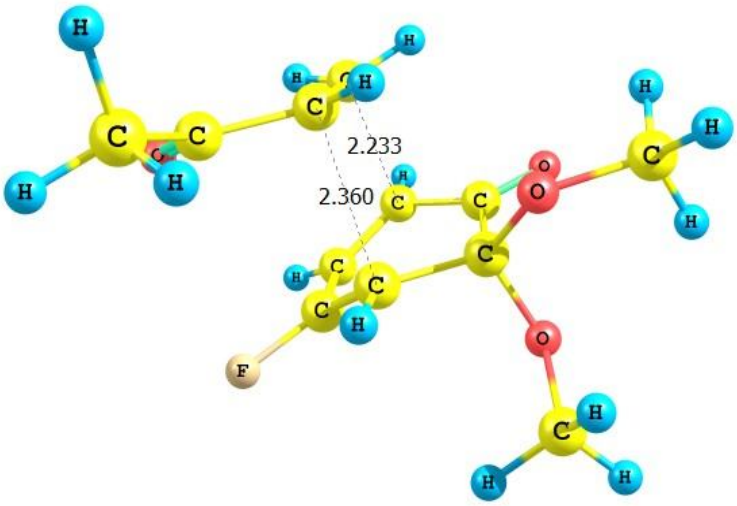

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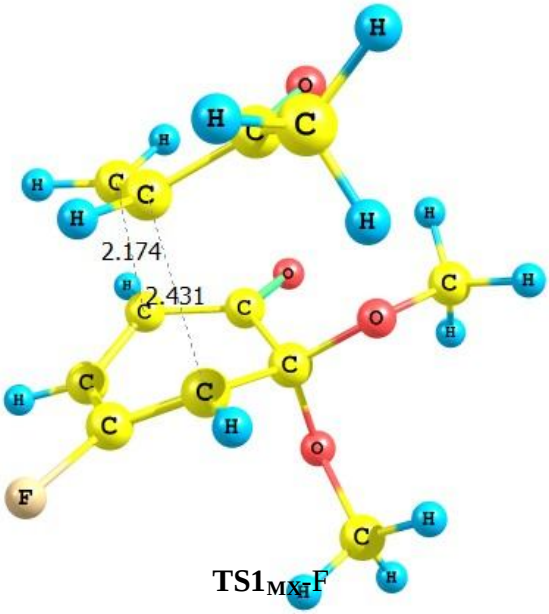

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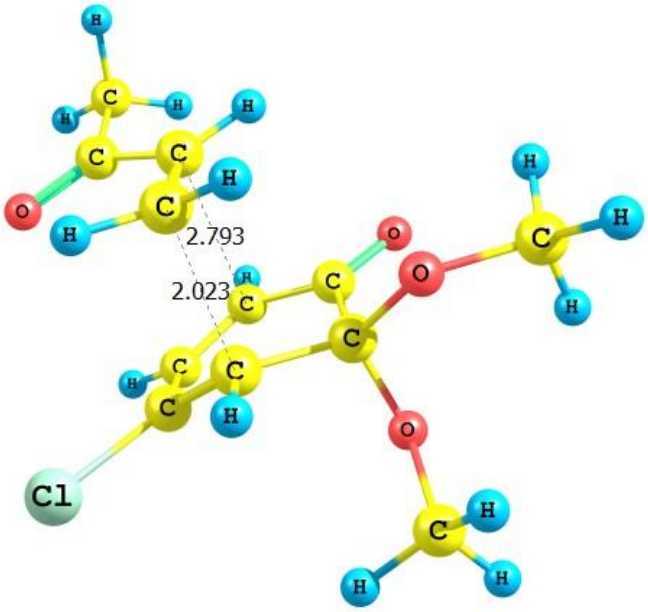

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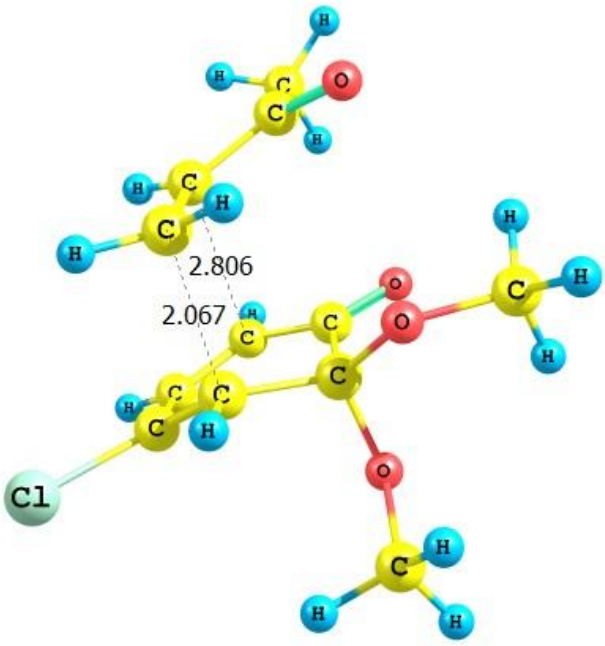

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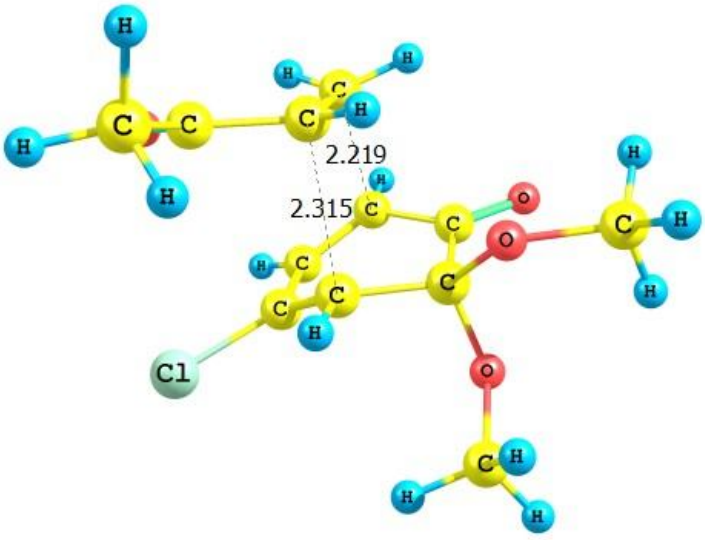

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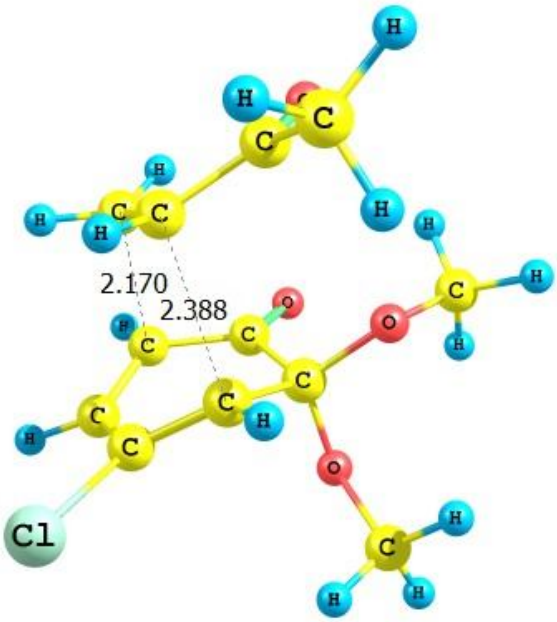

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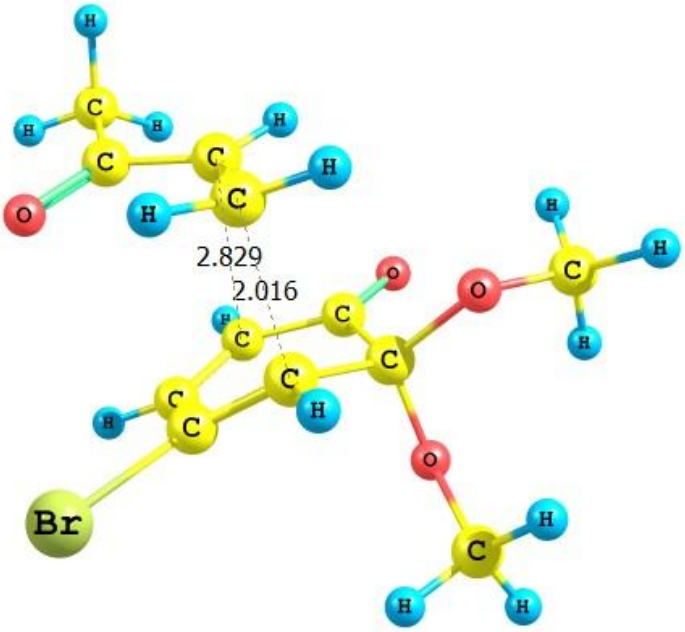

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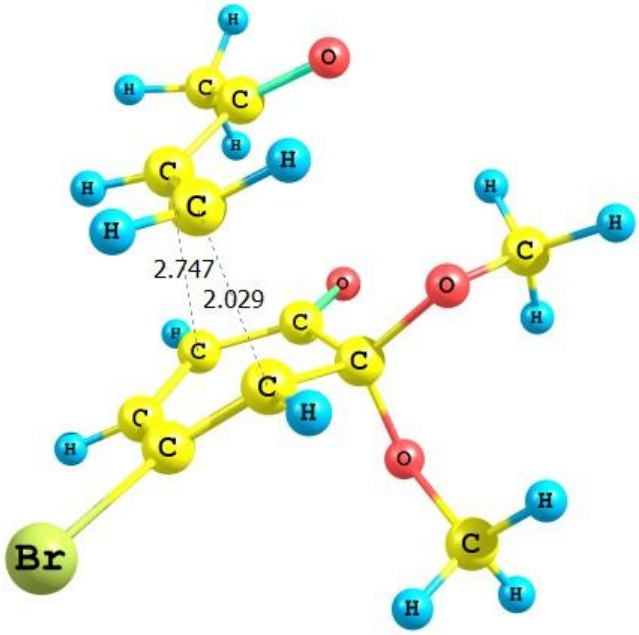

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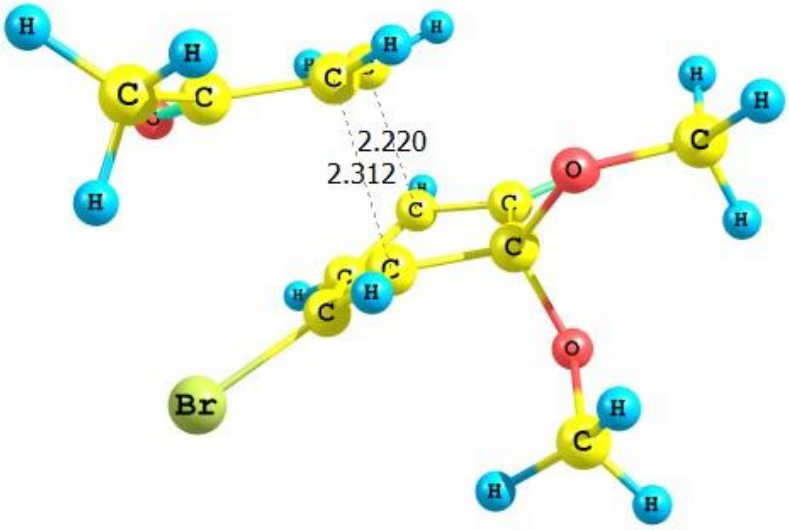

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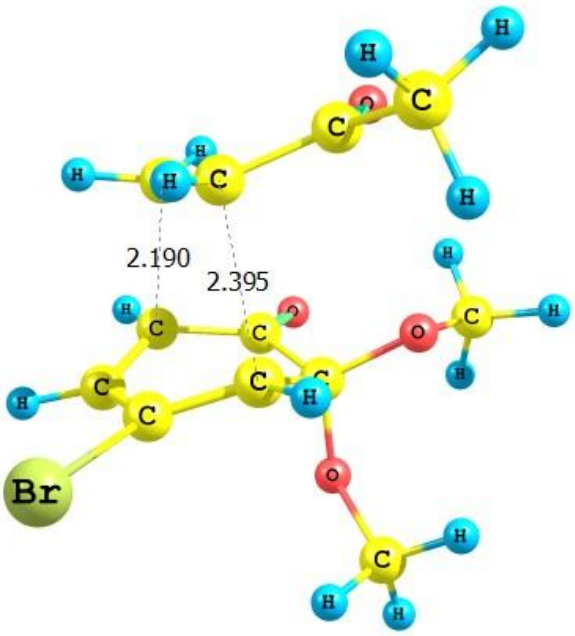

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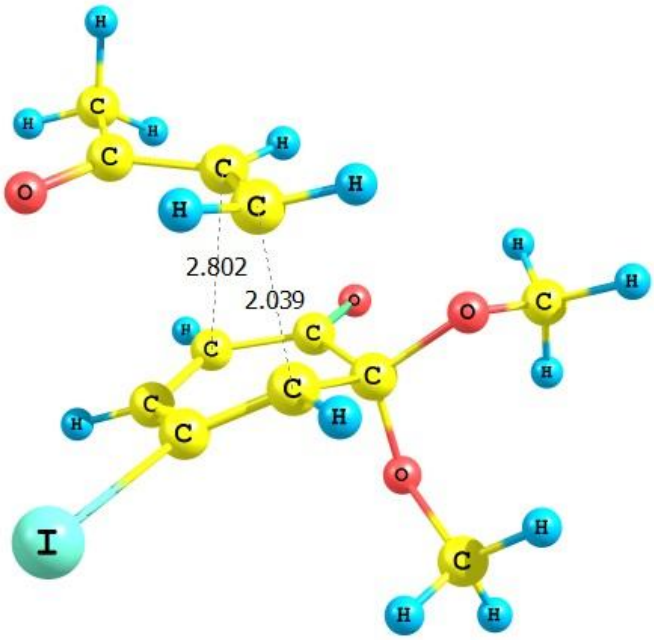

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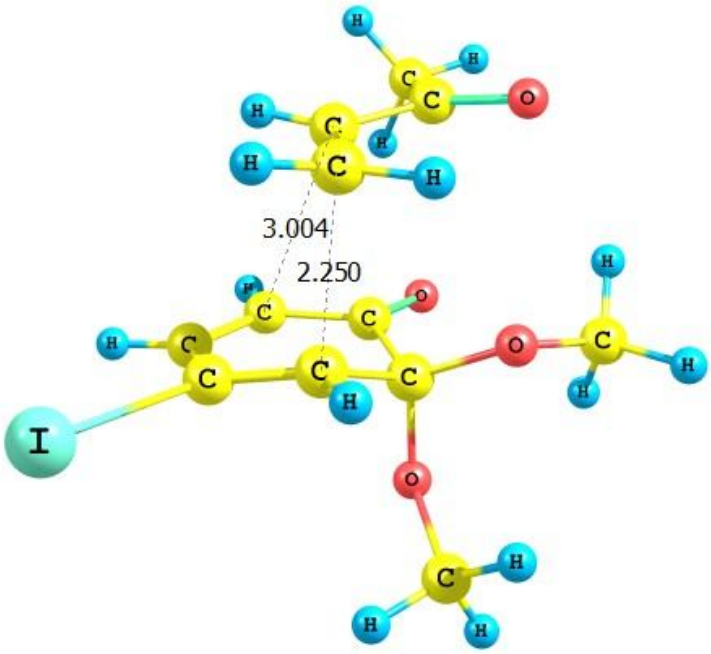

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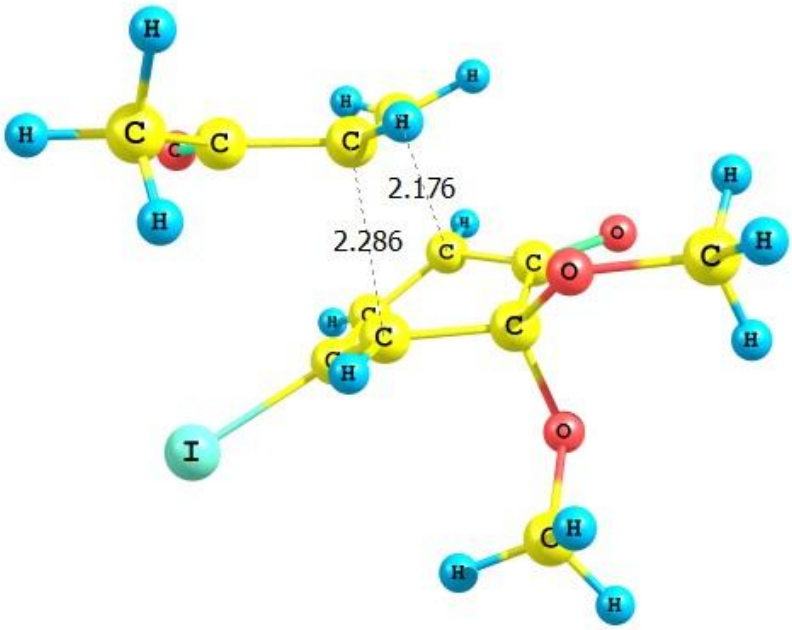

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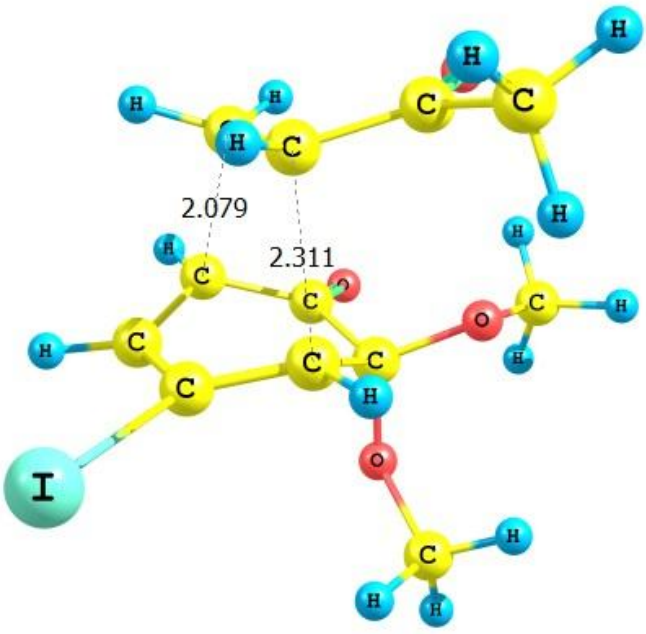

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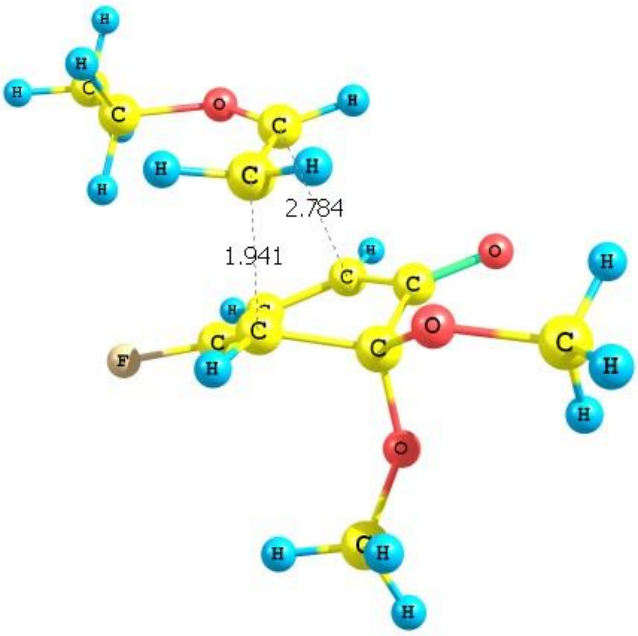

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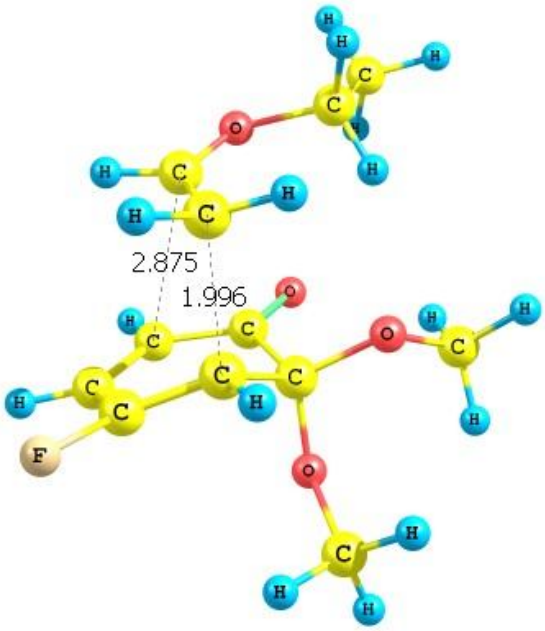

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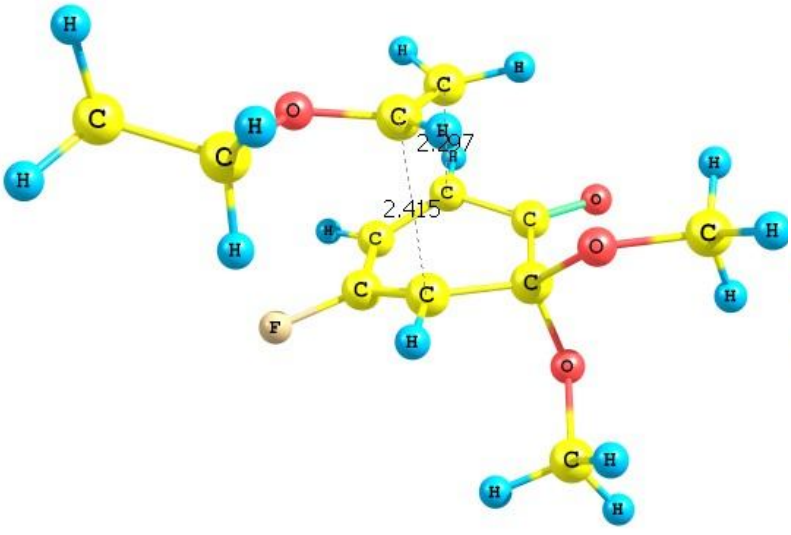

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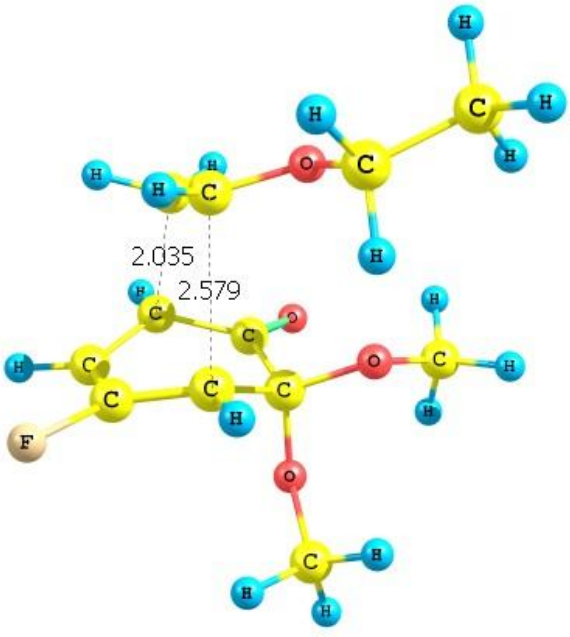

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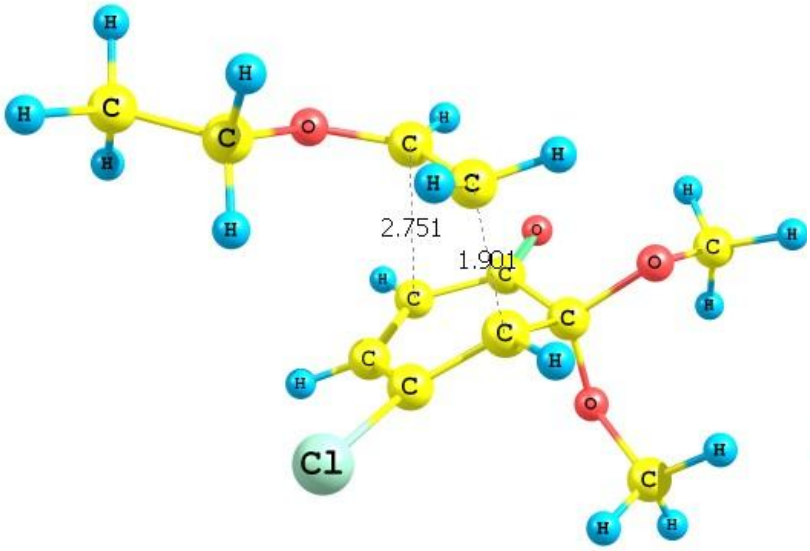

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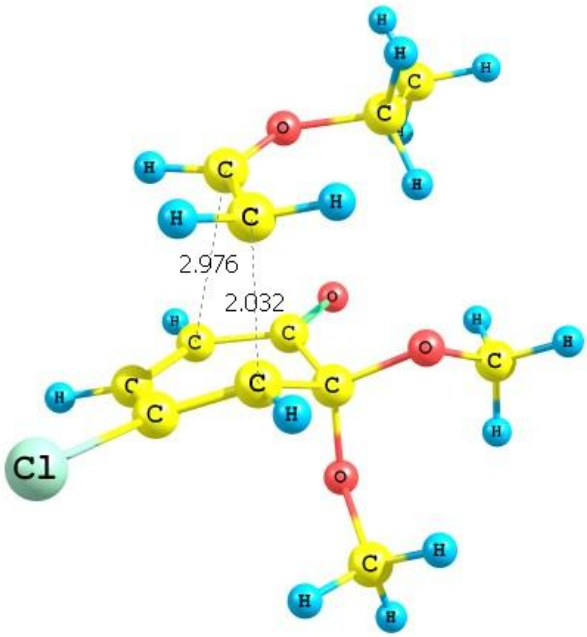

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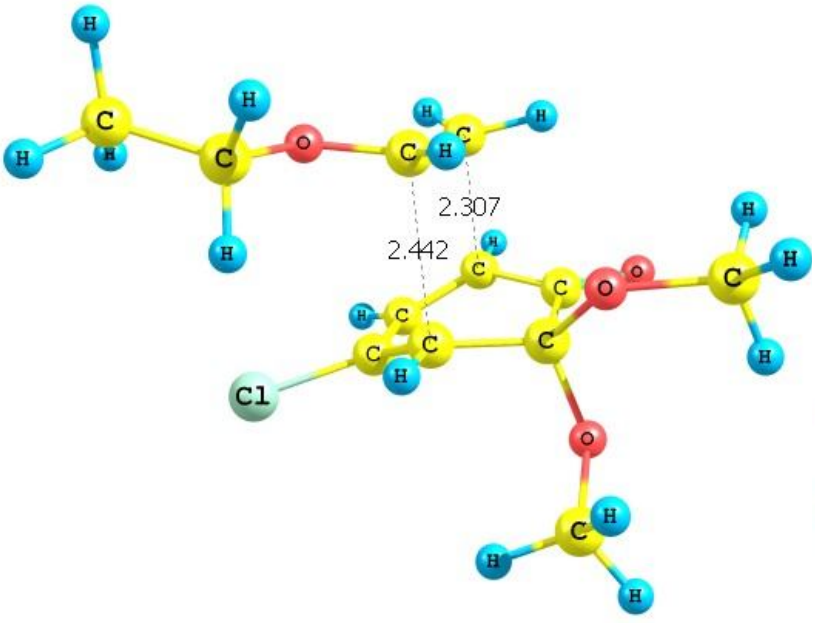
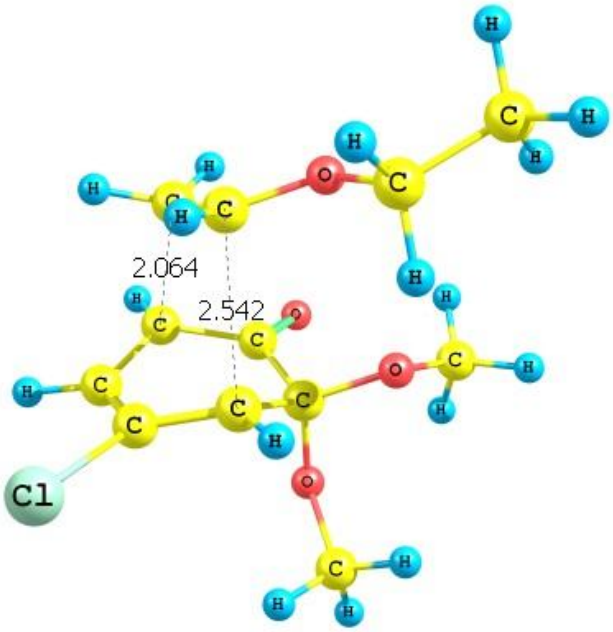


TS2$_{MN}$-Cl



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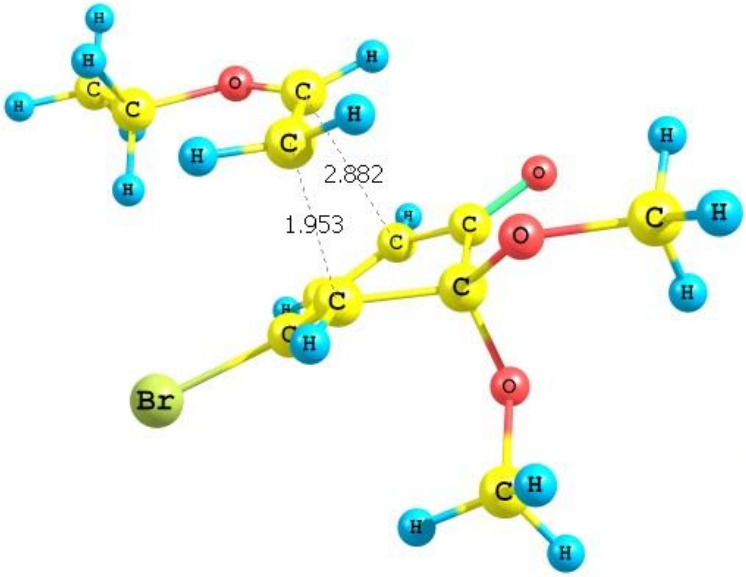
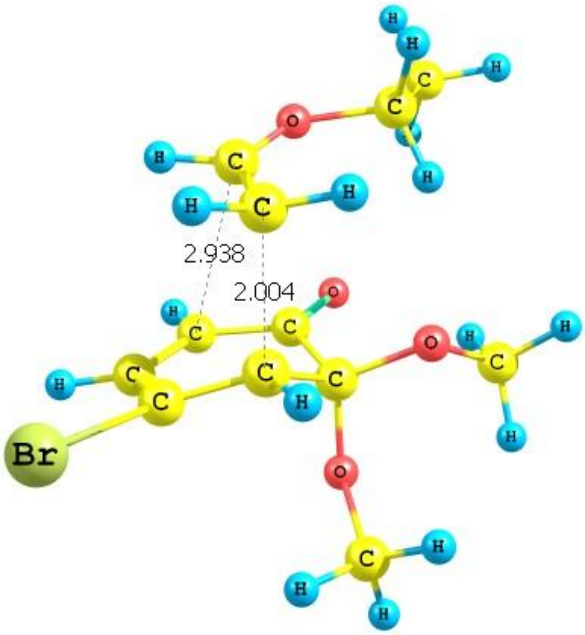


TS2$_{ON}$-Br



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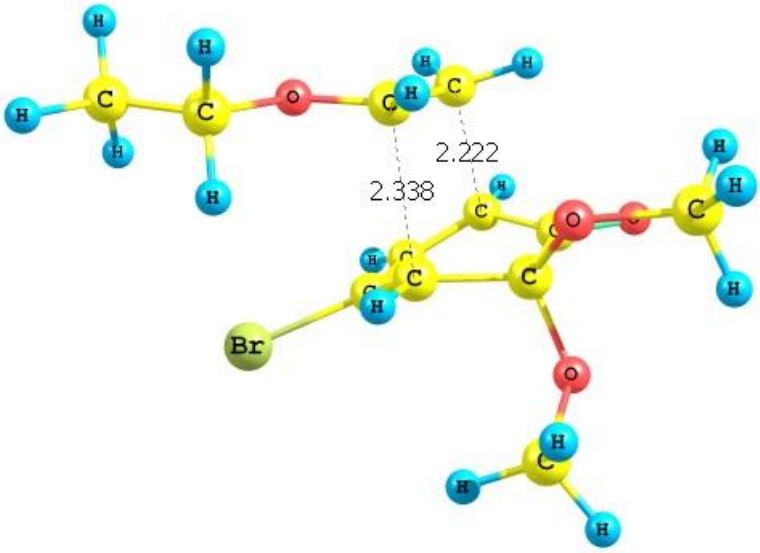

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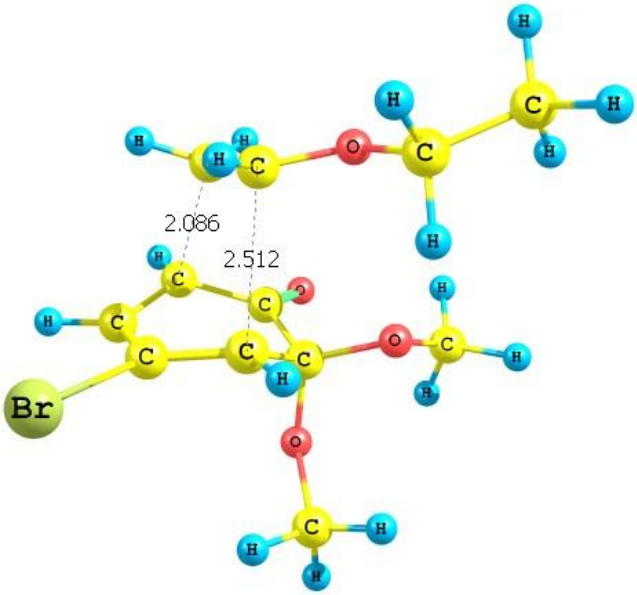

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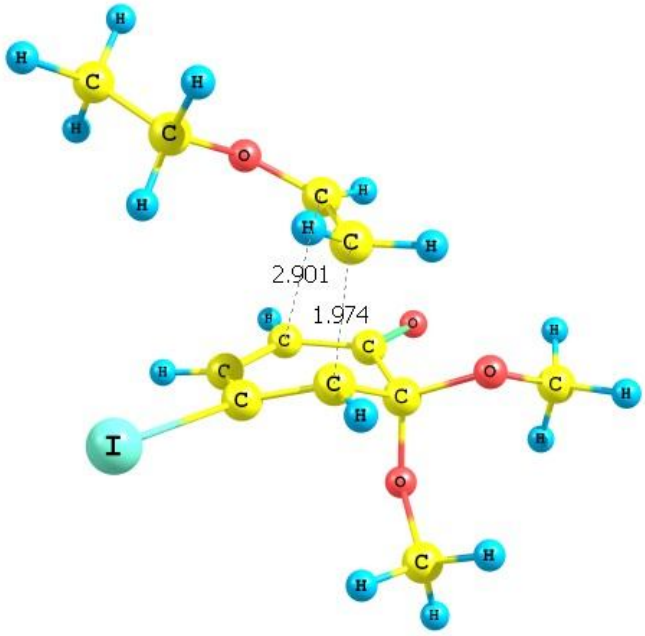
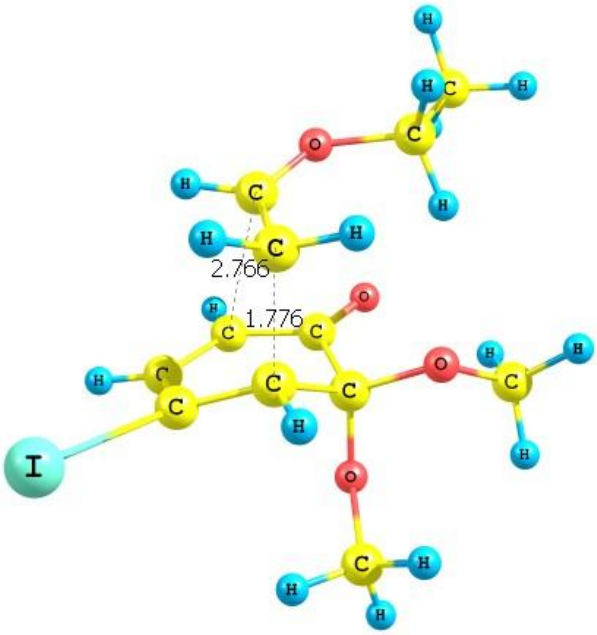


TS2$_{ON}$-I



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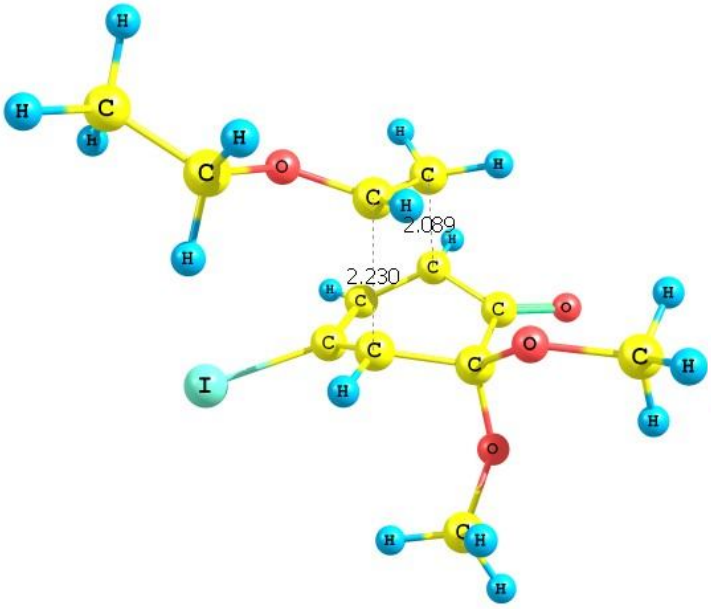
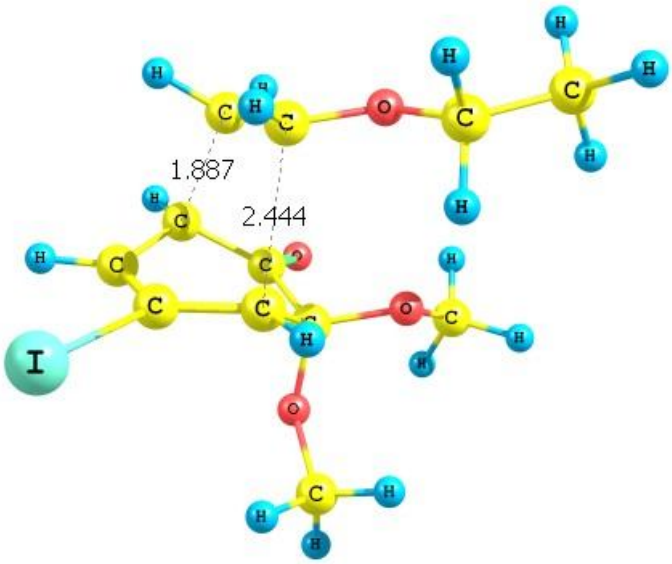
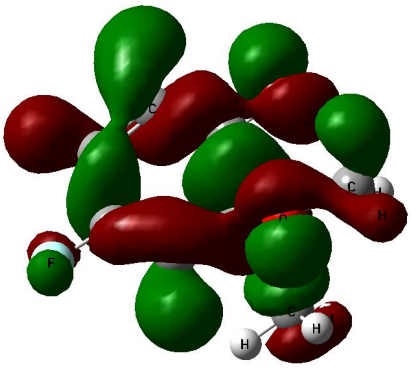


TS2$_{MN}$-I

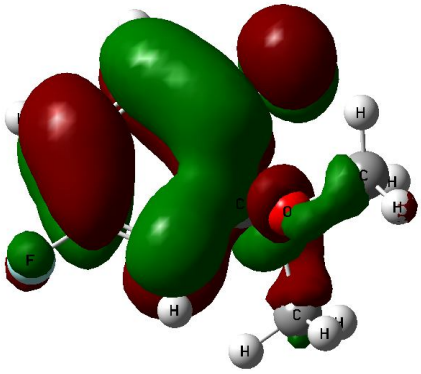


TS2$_{MX}$-I

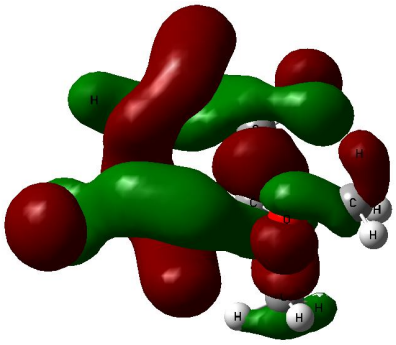
HOMO and LUMO figures of MOBs 5-8 and MVK and EVE



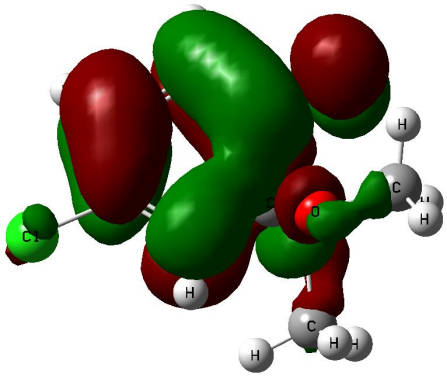
HOMO of FMOB (**5**)



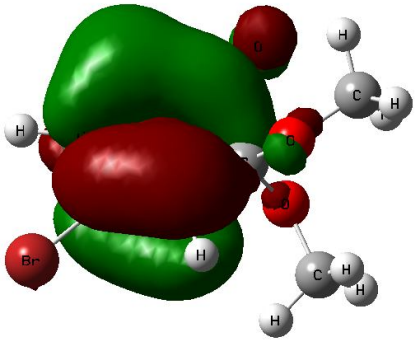
LUMO of FMOB (**5**)



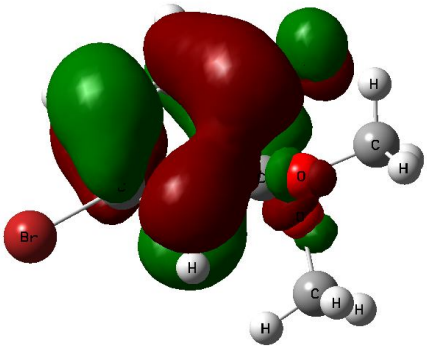
HOMO of ClMOB (**6**)



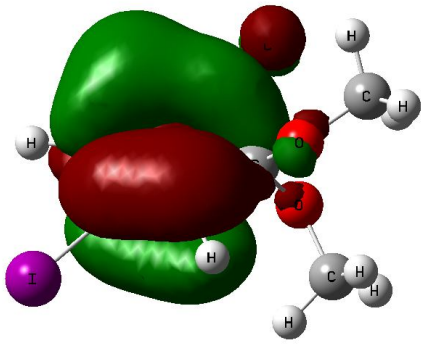
LUMO of ClMOB (**6**)



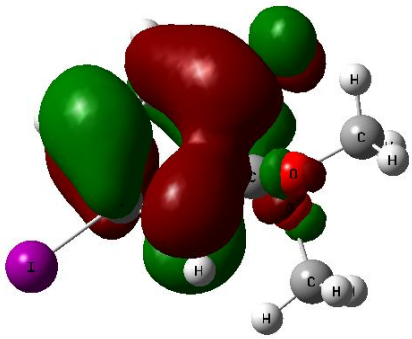
HOMO of BrMOB (**7**)



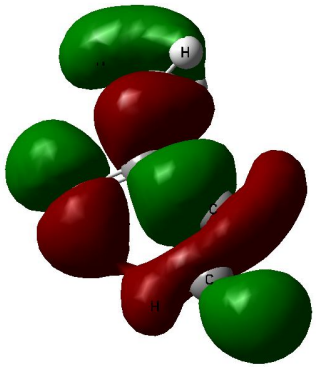
LUMO of BrMOB (**7**)



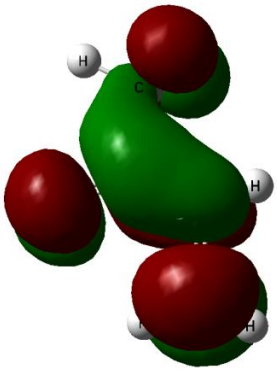
HOMO of IMOB (**8**)



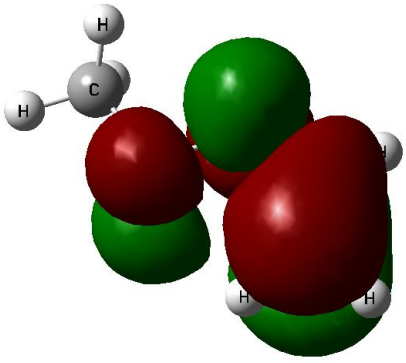
LUMO of IMOB (**8**)



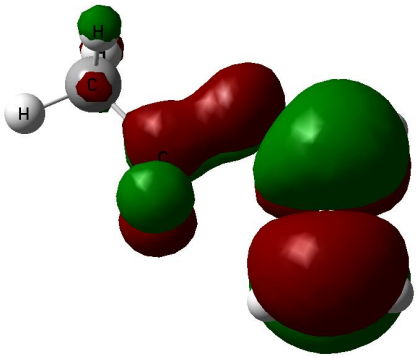
HOMO of MVK



LUMO of MVK

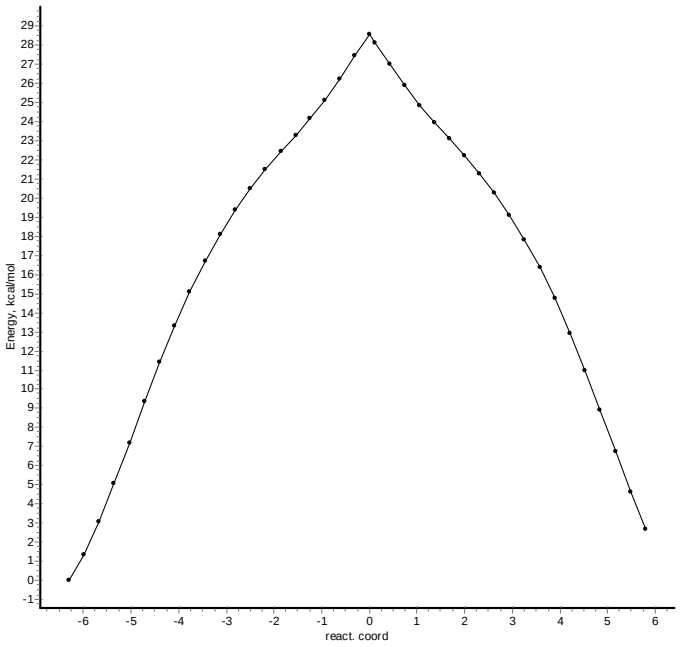


HOMO of EVE

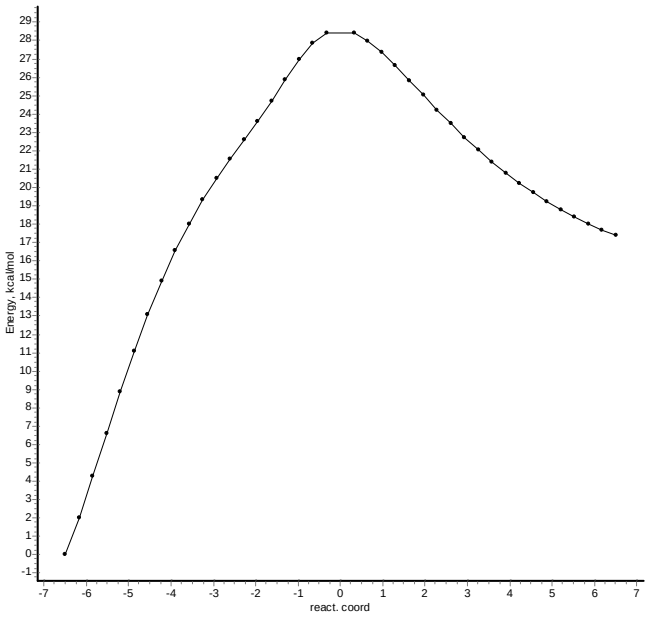


LUMO of EVE

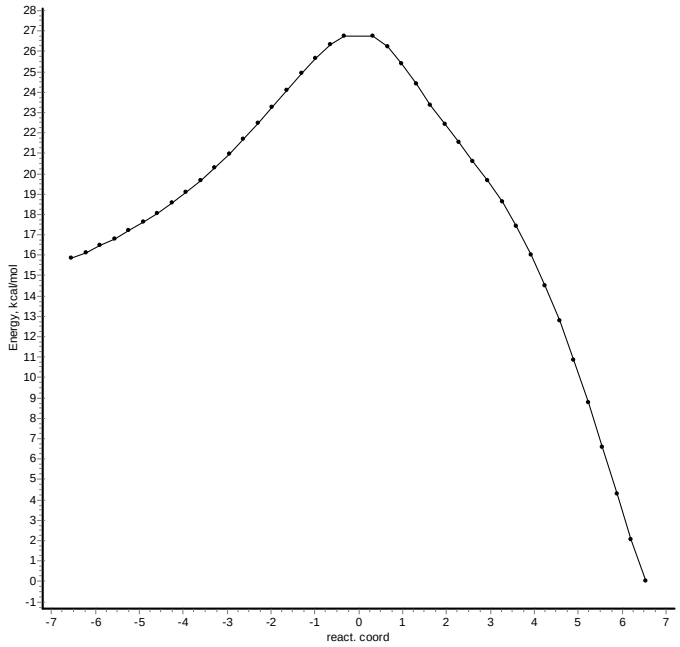
Intrinsic Reaction Coordinate (IRC) plots of Transition states



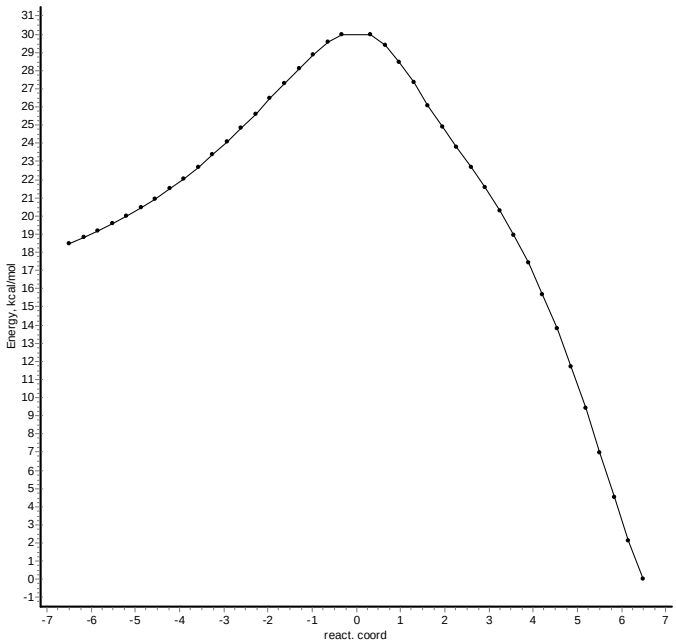
$TS1_{ON}$-F



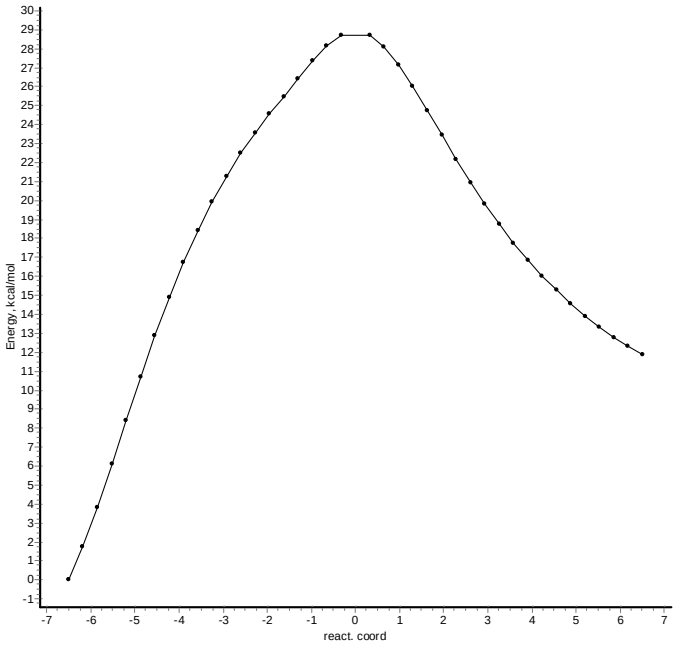
$TS1_{ON}$-Cl



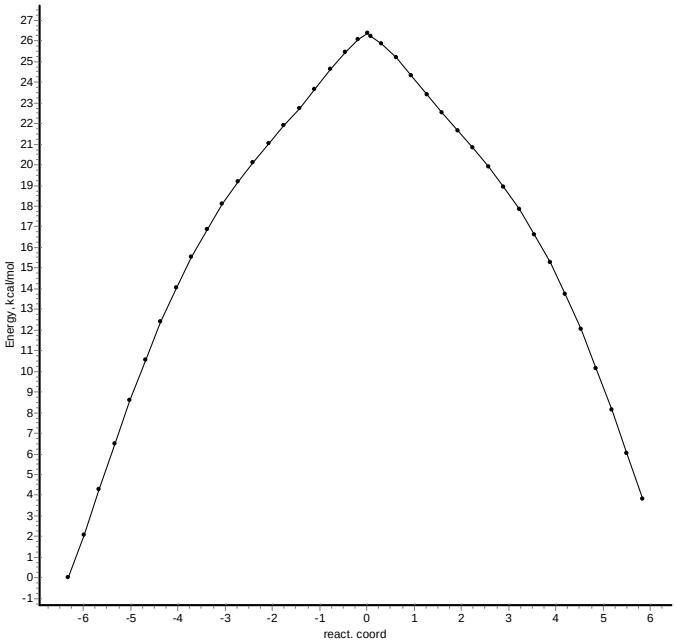
$TS1_{ON}$-Br



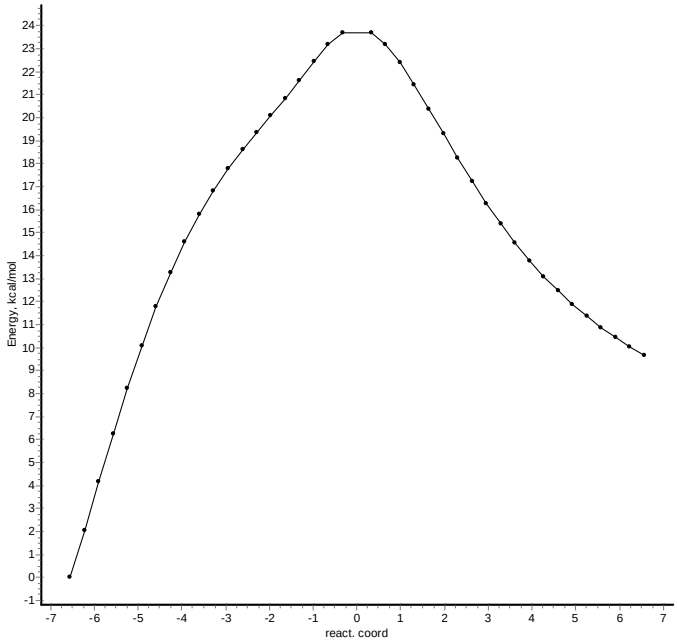
$TS1_{ON}$-I



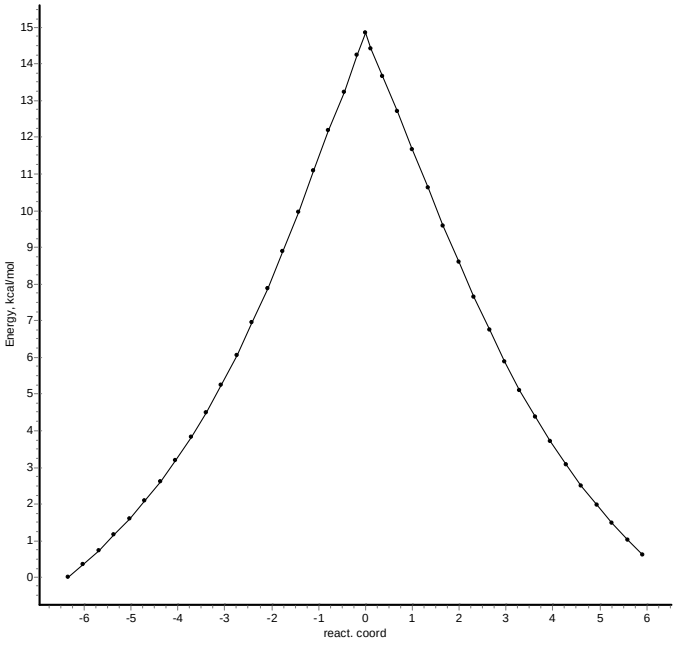
TS2$_{ON}$-F



TS2$_{ON}$-Cl



TS2$_{ON}$-Br



TS2$_{ON}$-I

Cartesian coordinates of reactants **5**, **6**, **7**, **8**, **MVK**, **EVE** and Transition State geometries

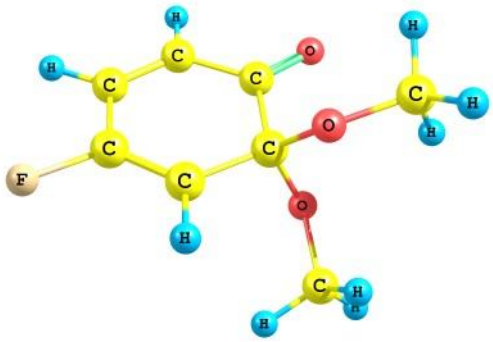
9c (ortho-endo) TS	**9c** (ortho-exo) TS	**9c** (meta-endo) TS	**9c** (meta-exo) TS
10c (ortho-endo) TS	**10c** (ortho-exo) TS	**10c** (meta-endo) TS	**10c** (meta-exo) TS
(**7+MVK**) (ortho-endo) TS	(**7+MVK**) (ortho-exo) TS	(**7+MVK**) (meta-endo) TS	(**7+MVK**) (meta-exo) TS
11c (ortho-endo) TS	**11c** (ortho-exo) TS	**11c** (meta-endo) TS	**11c** (meta-exo) TS
(**5+EVE**) (ortho-endo) TS	(**5+EVE**) (ortho-exo) TS	(**5+EVE**) (meta-endo) TS	(**5+EVE**) (meta-exo) TS
13c (ortho-endo) TS	**13c** (ortho-exo) TS	**13c** (meta-endo) TS	**13c** (meta-exo) TS
14c (ortho-endo) TS	**14c** (ortho-exo) TS	**14c** (meta-endo) TS	**14c** (meta-exo) TS
15c (ortho-endo) TS	**15c** (ortho-exo) TS	**15c** (meta-endo) TS	**15c** (meta-exo) TS

Products

9c (ortho-endo) P	**9c** (ortho-exo) P	**9c** (meta-endo) P	**9c** (meta-exo) P
10c (ortho-endo) P	**10c** (ortho-exo) P	**10c** (meta-endo) P	**10c** (meta-exo) P
(**7+MVK**) (ortho-endo) P	(**7+MVK**) (ortho-exo) P	(**7+MVK**) (meta-endo) P	(**7+MVK**) (meta-exo) P
11c (ortho-endo) P	**11c** (ortho-exo) P	**11c** (meta-endo) P	**11c** (meta-exo) P
(**5+EVE**) (ortho-endo) P	(**5+EVE**) (ortho-exo) P	(**5+EVE**) (meta-endo) P	(**5+EVE**) (meta-exo) P
13c (ortho-endo) P	**13c** (ortho-exo) P	**13c** (meta-endo) P	**13c** (meta-exo) P
14c (ortho-endo) P	**14c** (ortho-exo) P	**14c** (meta-endo) P	**14c** (meta-exo) P
15c (ortho-endo) P	**15c** (ortho-exo) P	**15c** (meta-endo) P	**15c** (meta-exo) P

5

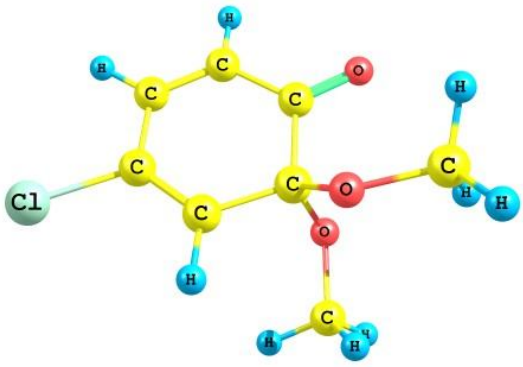
6	1.590577000	-0.048999000	0.088143000
6	0.723523000	1.086335000	-0.407059000
6	0.903257000	-0.952286000	1.167924000
1	1.086935000	1.683427000	-1.234669000
8	1.466287000	-1.960942000	1.560767000
6	-0.461950000	1.336836000	0.152545000
6	-0.407954000	-0.544611000	1.699190000
1	-0.826400000	-1.169292000	2.481058000
6	-1.046995000	0.539778000	1.219696000
1	-2.017237000	0.850260000	1.596069000
8	1.917364000	-0.766556000	-1.080552000
8	2.739147000	0.411927000	0.781448000
6	3.566890000	1.342702000	0.083444000
1	4.511874000	1.372662000	0.629018000
1	3.753903000	1.019296000	-0.946079000
1	3.129699000	2.348439000	0.075283000
6	2.783169000	-1.904485000	-0.957234000
1	3.576457000	-1.723972000	-0.228658000
1	2.229225000	-2.798590000	-0.659709000



1	3.212661000	-2.050836000	-1.951414000
9	-1.230196000	2.362953000	-0.271092000

6

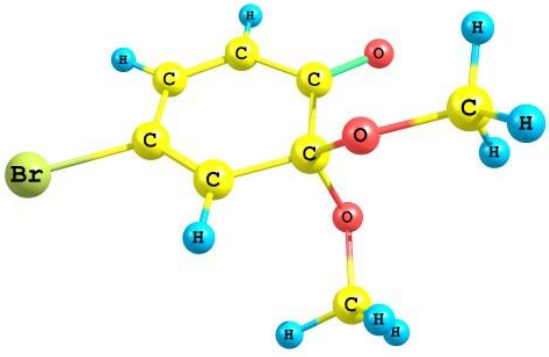
6	1.542877000	-0.045336000	0.126674000
6	0.721086000	1.122638000	-0.381650000
6	0.800051000	-0.936490000	1.173485000
1	1.141037000	1.695330000	-1.199946000
8	1.311820000	-1.974886000	1.559245000
6	-0.466659000	1.428339000	0.151952000
6	-0.498453000	-0.475624000	1.685920000
1	-0.956422000	-1.087265000	2.456168000
6	-1.090084000	0.637515000	1.210425000
1	-2.051593000	0.968177000	1.589669000
8	1.884150000	-0.749588000	-1.043534000
8	2.678981000	0.384562000	0.857928000
6	3.554682000	1.298055000	0.194023000
1	4.491319000	1.276980000	0.754091000
1	3.744471000	0.990691000	-0.839673000
1	3.158081000	2.320273000	0.204648000
6	2.710656000	-1.917000000	-0.915538000
1	3.484225000	-1.774398000	-0.157979000



1	2.119382000	-2.798047000	-0.654018000
1	3.167921000	-2.056809000	-1.898039000
17	-1.390448000	2.810624000	-0.425615000

7

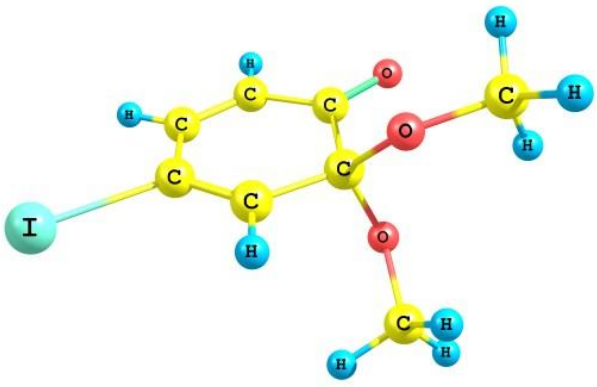
6	-1.637045000	-0.567139000	0.141729000
6	-0.284516000	-1.069568000	-0.326846000
6	-1.555945000	0.611728000	1.164113000
1	-0.289055000	-1.801443000	-1.125629000
8	-2.576644000	1.178308000	1.519821000
6	0.853559000	-0.627045000	0.216787000
6	-0.236472000	0.989909000	1.690189000
1	-0.224763000	1.772449000	2.441750000
6	0.894343000	0.404030000	1.249676000
1	1.864533000	0.693292000	1.639998000
8	-2.292495000	-0.209366000	-1.051645000
8	-2.340420000	-1.552191000	0.879286000
6	-2.528600000	-2.814934000	0.237272000
1	-3.320322000	-3.319654000	0.793889000
1	-2.841419000	-2.691024000	-0.804691000
1	-1.620963000	-3.428991000	0.276157000
6	-3.638171000	0.284475000	-0.963626000



1	-4.211382000	-0.258297000	-0.209007000
1	-3.657006000	1.349936000	-0.721631000
1	-4.071077000	0.121817000	-1.953596000
35	2.547204000	-1.306468000	-0.362255000

8

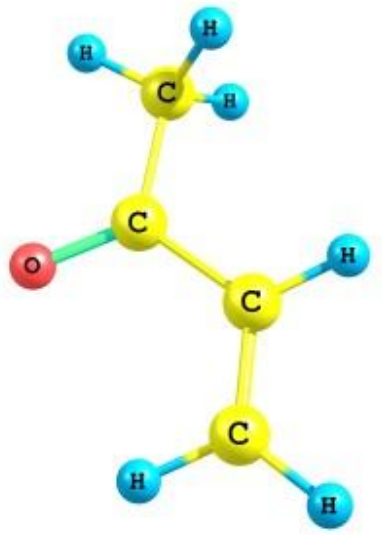
6	-1.485593000	-1.248724000	0.112396000
6	-0.056421000	-1.008222000	-0.349545000
6	-1.999258000	-0.192763000	1.143527000
1	0.276983000	-1.613479000	-1.186025000
8	-3.182077000	-0.165228000	1.456455000
6	0.735392000	-0.098018000	0.234466000
6	-1.018722000	0.729560000	1.737385000
1	-1.387507000	1.389103000	2.518263000
6	0.264532000	0.770543000	1.317543000
1	0.966171000	1.468460000	1.765806000
8	-2.223887000	-1.263306000	-1.088872000
8	-1.604180000	-2.458940000	0.849882000
6	-1.115126000	-3.650032000	0.215773000
1	-1.530050000	-4.480777000	0.789824000
1	-1.456355000	-3.719933000	-0.822485000
1	-0.020832000	-3.702053000	0.251770000



6	-3.641204000	-1.523712000	-1.023598000
1	-3.872378000	-2.275430000	-0.265593000
1	-4.197642000	-0.609590000	-0.803708000
1	-3.909922000	-1.894498000	-2.016001000
53	2.748691000	0.183459000	-0.416549000

MVK (cis)

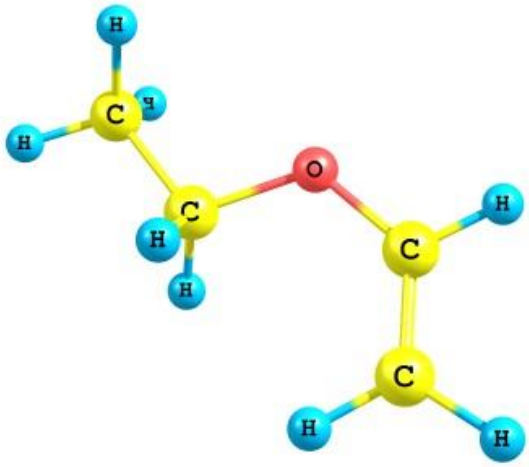
6	-0.825025000	-0.340864000	-1.783100000
6	-1.497502000	-1.281508000	-1.114635000
6	-3.457225000	-2.121515000	0.302789000
1	-2.788220000	-2.527740000	1.070931000
1	-3.672218000	-2.939407000	-0.395376000
1	-1.125581000	-2.302216000	-1.053270000
1	-1.217002000	0.671092000	-1.829813000
1	0.111831000	-0.550430000	-2.289187000
1	-4.383571000	-1.780092000	0.765449000
6	-2.787878000	-0.970369000	-0.423815000
8	-3.275262000	0.148398000	-0.443742000



EVE

6	0.579843000	-0.918281000	0.250752000
6	1.784868000	-1.402945000	-0.064480000
6	2.540182000	-1.688731000	2.171615000

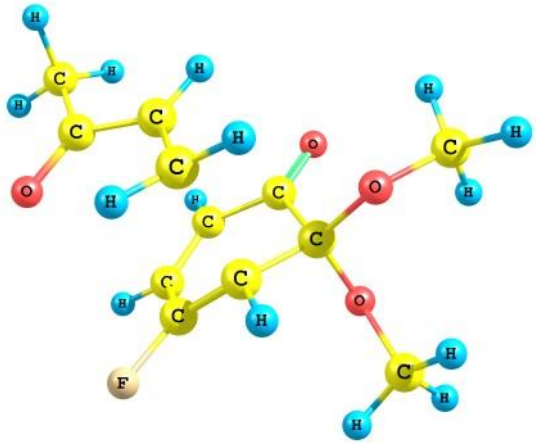
1	1.659260000	-2.289669000	2.438264000
1	2.318457000	-0.642637000	2.426139000
1	2.096478000	-1.535257000	-1.097158000
1	0.236987000	-0.773439000	1.267581000
1	-0.101964000	-0.651310000	-0.547300000
8	2.782012000	-1.795824000	0.768139000
6	3.780125000	-2.179657000	2.896577000
1	3.634712000	-2.113940000	3.979271000
1	3.991618000	-3.221035000	2.637999000
1	4.650249000	-1.574668000	2.626522000



9c (ortho-endo) TS

6	1.355543000	-0.112830000	-0.040260000
6	0.485498000	0.967790000	-0.692706000
6	0.502712000	-0.943765000	0.962727000
1	0.978973000	1.535079000	-1.478672000
8	0.791463000	-2.097834000	1.249554000
6	-0.318971000	1.702128000	0.190172000
6	-0.584561000	-0.203753000	1.609122000
1	-1.085598000	-0.722415000	2.420251000
6	-0.865038000	1.120370000	1.336613000
1	-1.595984000	1.678048000	1.911130000

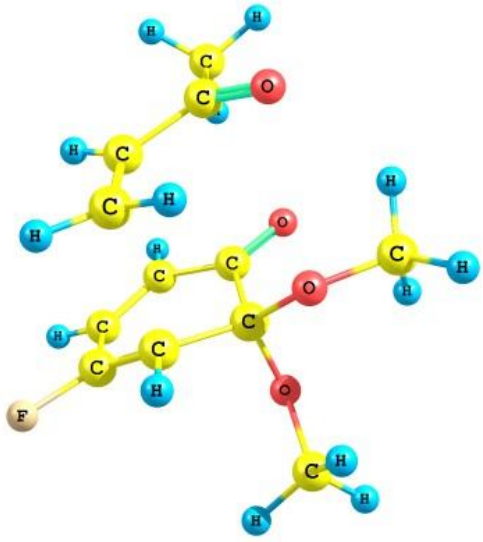
8	1.913225000	-0.848590000	-1.091598000
8	2.349892000	0.449109000	0.804703000
6	3.237006000	1.394249000	0.205987000
1	4.076331000	1.499163000	0.895995000
1	3.607031000	1.041240000	-0.762490000
1	2.760331000	2.374050000	0.079074000
6	2.823635000	-1.910598000	-0.763571000
1	3.423873000	-1.656006000	0.112655000
1	2.286043000	-2.839459000	-0.568379000
1	3.472746000	-2.023858000	-1.635630000
6	-0.768206000	-0.053302000	-1.726003000
6	-1.507518000	-0.935508000	-0.915097000
6	-3.682927000	-1.514563000	0.298682000
1	-3.110062000	-2.184324000	0.947678000
1	-4.171678000	-2.136322000	-0.461222000
1	-1.191425000	-1.963936000	-0.781004000
1	-1.330680000	0.779736000	-2.137210000
1	-0.014744000	-0.486150000	-2.377537000
1	-4.455075000	-1.003625000	0.876131000
6	-2.788817000	-0.488443000	-0.376237000
8	-3.123824000	0.696898000	-0.467298000



9	-0.714030000	2.931274000	-0.171136000

9c (ortho-exo) TS

6	-0.684152000	0.748053000	0.004667000
6	-1.321512000	-0.381615000	-0.799977000
6	0.231544000	0.176182000	1.134104000
1	-1.801198000	-0.105466000	-1.734408000
8	1.120254000	0.844747000	1.639636000
6	-1.823723000	-1.441010000	-0.087953000
6	-0.181396000	-1.139647000	1.661403000
1	0.350137000	-1.486444000	2.545176000
6	-1.236337000	-1.837711000	1.145659000
1	-1.577950000	-2.765200000	1.601647000
8	-0.074211000	1.586388000	-0.928061000
8	-1.654701000	1.437640000	0.798994000
6	-2.694671000	2.073583000	0.039650000
1	-3.032567000	2.935502000	0.626086000
1	-2.308093000	2.422789000	-0.925720000
1	-3.547854000	1.397720000	-0.126396000
6	0.654480000	2.709970000	-0.379042000
1	0.227949000	3.013355000	0.581998000
1	1.710151000	2.450456000	-0.274334000

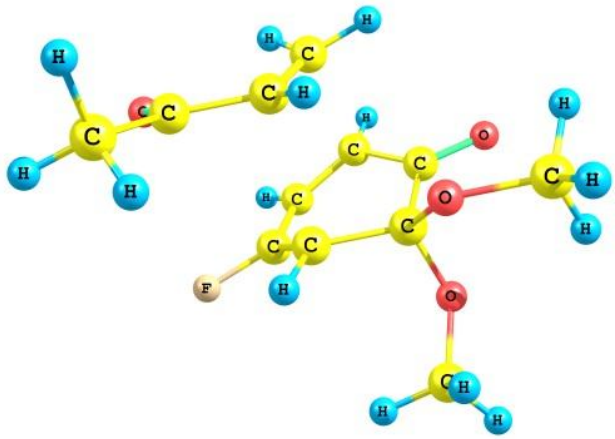


1	0.539299000	3.519739000	-1.109793000
6	0.491678000	-1.219103000	-1.694357000
6	1.421439000	-1.488545000	-0.722995000
6	3.445663000	-0.807849000	0.697680000
1	4.276551000	-0.097623000	0.677741000
1	3.823154000	-1.838272000	0.654122000
1	1.457427000	-2.453401000	-0.223145000
1	-0.096325000	-2.005174000	-2.150565000
1	0.644520000	-0.296562000	-2.246814000
1	2.882872000	-0.672053000	1.631903000
6	2.500779000	-0.495548000	-0.456307000
8	2.599129000	0.527028000	-1.118619000
9	-2.699399000	-2.285151000	-0.657588000

9c (meta-endo) TS

6	-1.256817000	0.168872000	0.146821000
6	0.085924000	0.872658000	0.268781000
6	-1.233880000	-0.884567000	-1.001863000
1	0.226545000	1.500248000	1.141346000
8	-2.151989000	-1.670488000	-1.156752000
6	0.752836000	1.179636000	-0.899922000
6	-0.050704000	-0.843460000	-1.889273000

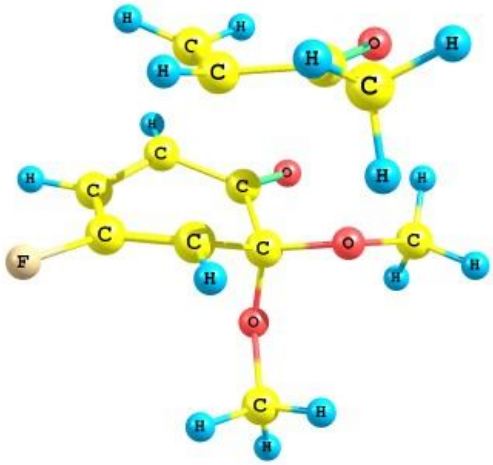
1	-0.075430000	-1.557203000	-2.707593000
6	0.703154000	0.323982000	-1.999970000
1	1.373615000	0.490785000	-2.835571000
8	-1.541671000	-0.376993000	1.411920000
8	-2.275952000	1.060034000	-0.285546000
6	-2.472055000	2.233605000	0.504971000
1	-3.438219000	2.640963000	0.201664000
1	-2.498894000	1.997230000	1.574091000
1	-1.695120000	2.983748000	0.316299000
6	-2.800881000	-1.045726000	1.581360000
1	-3.597700000	-0.527843000	1.043629000
1	-2.752498000	-2.079145000	1.230591000
1	-3.000975000	-1.025285000	2.655437000
6	1.271337000	-1.114299000	0.732110000
6	1.028325000	-2.000498000	-0.313643000
6	3.026284000	0.183211000	2.087251000
1	2.199014000	0.664890000	2.617072000
1	3.833693000	0.895807000	1.913649000
1	1.833083000	-2.189879000	-1.013693000
1	0.675030000	-1.168188000	1.635618000
1	3.402237000	-0.616954000	2.737243000



6	2.583603000	-0.421267000	0.767464000
8	3.289782000	-0.364477000	-0.232324000
1	0.271149000	-2.768497000	-0.213376000
9	1.651150000	2.184648000	-0.899923000

9c (meta-exo) TS

6	-0.473647000	0.839529000	-0.031656000
6	-0.723559000	-0.352045000	-0.943230000
6	-0.413545000	0.376033000	1.456929000
1	-0.523126000	-0.216306000	-2.000790000
8	0.029308000	1.082370000	2.340656000
6	-1.693931000	-1.247724000	-0.541667000
6	-1.008663000	-0.961726000	1.727311000
1	-1.087502000	-1.204845000	2.782565000
6	-1.891306000	-1.535962000	0.807751000
1	-2.561630000	-2.340253000	1.092973000
8	0.657365000	1.484262000	-0.535860000
8	-1.598164000	1.716691000	0.010937000
6	-2.031242000	2.241638000	-1.243981000
1	-2.709427000	3.063816000	-1.008155000
1	-1.188294000	2.623651000	-1.829176000
1	-2.573720000	1.491859000	-1.832982000

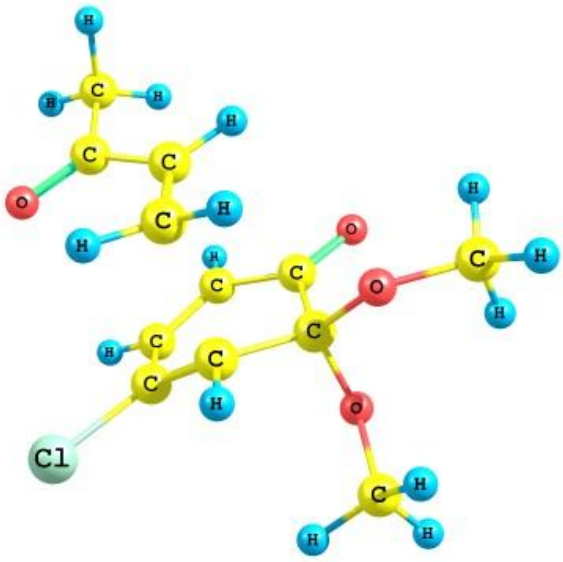


6	1.196661000	2.599713000	0.194240000
1	0.400799000	3.190736000	0.651213000
1	1.889593000	2.252719000	0.961912000
1	1.731348000	3.200595000	-0.545385000
6	1.157693000	-1.664644000	-0.138310000
6	0.855303000	-1.946877000	1.195083000
6	2.727770000	-0.618366000	-1.887203000
1	2.570323000	-1.538041000	-2.459030000
1	3.776572000	-0.321209000	-1.935715000
1	0.429515000	-2.905102000	1.462726000
1	0.868932000	-2.361055000	-0.917063000
1	2.122303000	0.173838000	-2.340338000
6	2.311943000	-0.760714000	-0.435580000
8	2.918551000	-0.187981000	0.458128000
1	1.464298000	-1.460104000	1.951211000
9	-2.305258000	-2.025129000	-1.464774000

10c (ortho-endo) TS

6	1.429509000	-0.220317000	-0.033662000
6	0.509472000	0.855488000	-0.627160000
6	0.645547000	-1.106556000	0.977563000
1	0.945863000	1.424968000	-1.442186000

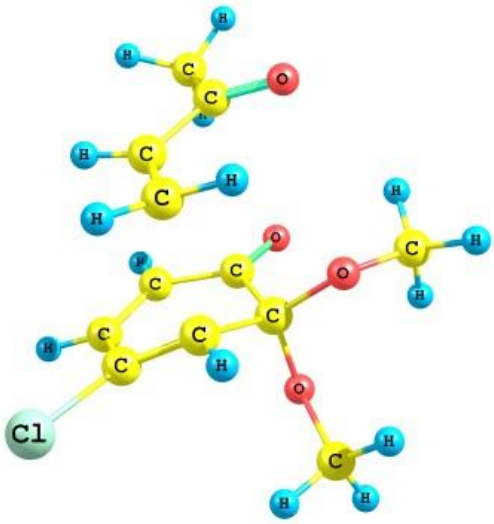
8	1.031454000	-2.228395000	1.275146000
6	-0.317506000	1.528037000	0.275630000
6	-0.507064000	-0.463613000	1.613753000
1	-0.986960000	-1.034653000	2.402478000
6	-0.853750000	0.849535000	1.384928000
1	-1.618502000	1.331267000	1.983503000
8	1.976810000	-0.912094000	-1.122975000
8	2.431152000	0.355324000	0.790200000
6	3.264264000	1.346274000	0.185339000
1	4.131742000	1.450244000	0.839637000
1	3.597517000	1.035958000	-0.810619000
1	2.754180000	2.314402000	0.116100000
6	2.945774000	-1.937976000	-0.851526000
1	3.568604000	-1.672476000	0.005194000
1	2.458751000	-2.894043000	-0.653575000
1	3.562783000	-2.006852000	-1.751028000
6	-0.771107000	-0.272234000	-1.714431000
6	-1.392193000	-1.236266000	-0.920609000
6	-3.476234000	-2.131401000	0.261388000
1	-2.830562000	-2.716551000	0.924145000
1	-3.828630000	-2.807973000	-0.526759000



1	-0.959537000	-2.224950000	-0.811053000
1	-1.395728000	0.549393000	-2.052362000
1	0.022329000	-0.595356000	-2.379028000
1	-4.340183000	-1.757313000	0.812507000
6	-2.725592000	-0.967670000	-0.362213000
8	-3.216361000	0.159283000	-0.419519000
17	-0.904284000	3.126540000	-0.116104000

10c (ortho-exo) TS

6	-0.212943000	1.071815000	0.027831000
6	-1.142291000	0.065975000	-0.666678000
6	0.578528000	0.370982000	1.173351000
1	-1.600259000	0.426636000	-1.582221000
8	1.610663000	0.841706000	1.630391000
6	-1.877283000	-0.775995000	0.165625000
6	-0.075407000	-0.805831000	1.760022000
1	0.410358000	-1.225436000	2.635722000
6	-1.323913000	-1.238743000	1.372881000
1	-1.838395000	-2.010141000	1.936604000
8	0.537925000	1.654260000	-0.987893000
8	-0.958263000	2.036889000	0.763426000
6	-1.912506000	2.799481000	0.023435000

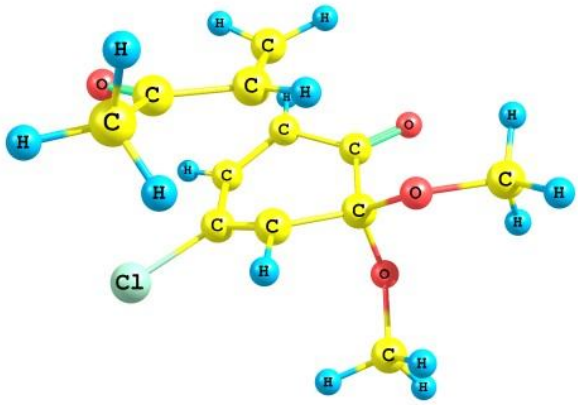


1	-2.173988000	3.650051000	0.655651000
1	-1.488613000	3.164367000	-0.917814000
1	-2.820416000	2.219876000	-0.183712000
6	1.538317000	2.627009000	-0.636439000
1	1.196282000	3.262002000	0.183957000
1	2.471297000	2.136095000	-0.362808000
1	1.683275000	3.229782000	-1.536172000
6	0.211829000	-1.227555000	-1.540907000
6	1.103582000	-1.746855000	-0.606562000
6	3.372146000	-1.818270000	0.583394000
1	4.418680000	-1.651381000	0.324526000
1	3.186177000	-2.885946000	0.736117000
1	0.868154000	-2.658081000	-0.067713000
1	-0.571079000	-1.866158000	-1.936468000
1	0.614356000	-0.473114000	-2.210885000
1	3.162343000	-1.294477000	1.523646000
6	2.486940000	-1.224272000	-0.494979000
8	2.899855000	-0.343555000	-1.240195000
17	-3.336565000	-1.536760000	-0.440594000

10c (meta-endo) TS

6	1.365133000	0.147775000	-0.197114000

6	-0.077330000	0.539956000	-0.500890000
6	1.479245000	-0.484353000	1.219214000
1	-0.277593000	0.810843000	-1.532174000
8	2.500788000	-1.035272000	1.589786000
6	-0.801947000	1.133518000	0.524281000
6	0.277433000	-0.349684000	2.071078000
1	0.384848000	-0.758693000	3.071134000
6	-0.640309000	0.677422000	1.833531000
1	-1.320337000	1.004895000	2.611755000
8	1.782491000	-0.697037000	-1.240617000
8	2.193582000	1.294558000	-0.083005000
6	2.201354000	2.188585000	-1.198307000
1	3.074259000	2.829409000	-1.061693000
1	2.295163000	1.646563000	-2.145327000
1	1.301361000	2.813853000	-1.221771000
6	3.143384000	-1.155922000	-1.221414000
1	3.817603000	-0.372764000	-0.868935000
1	3.256656000	-2.033711000	-0.581248000
1	3.380316000	-1.415102000	-2.256122000
6	-0.891844000	-1.621555000	-0.345294000
6	-0.570510000	-2.060361000	0.941264000

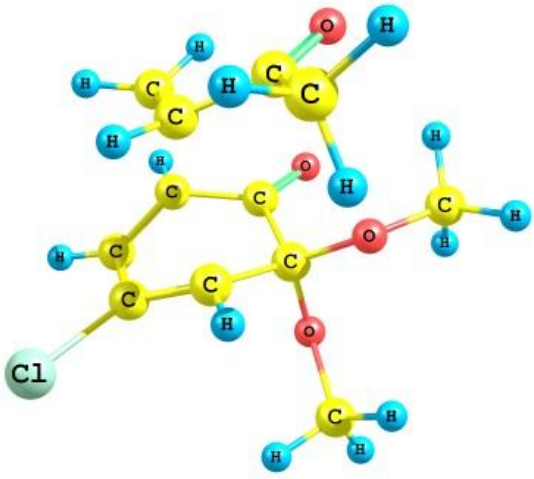


6	-2.752554000	-1.213043000	-2.068337000
1	-2.054786000	-0.635295000	-2.682978000
1	-3.752196000	-0.782082000	-2.132395000
1	-1.380916000	-2.150635000	1.655461000
1	-0.245031000	-1.874750000	-1.177039000
1	-2.773759000	-2.230032000	-2.478966000
6	-2.309439000	-1.262259000	-0.618131000
8	-3.085658000	-1.035027000	0.300570000
17	-2.097892000	2.257964000	0.148786000
1	0.293254000	-2.696147000	1.097776000

10c (meta-exo) TS

6	0.226995000	1.014303000	-0.086885000
6	-0.751407000	-0.000950000	-0.666515000
6	0.389019000	0.788940000	1.445124000
1	-0.722579000	-0.131306000	-1.742609000
8	1.294872000	1.284552000	2.085073000
6	-1.928618000	-0.210549000	0.032859000
6	-0.694372000	-0.012070000	2.076213000
1	-0.647722000	-0.041244000	3.160857000
6	-1.924690000	-0.169656000	1.428484000
1	-2.810729000	-0.453457000	1.986289000

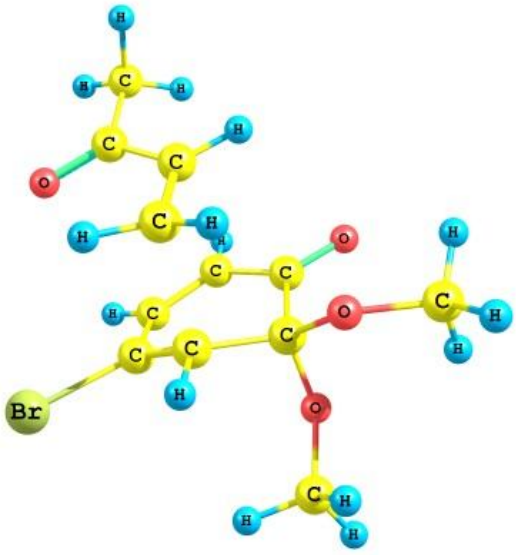
8	1.383622000	0.916648000	-0.861328000
8	-0.308589000	2.334627000	-0.107021000
6	-0.723662000	2.826053000	-1.382478000
1	-0.855664000	3.902654000	-1.260821000
1	0.036034000	2.638157000	-2.148231000
1	-1.676983000	2.384126000	-1.696414000
6	2.533195000	1.685803000	-0.467478000
1	2.235922000	2.657198000	-0.067774000
1	3.117163000	1.140904000	0.275534000
1	3.120696000	1.819879000	-1.378811000
6	0.386447000	-1.942438000	0.133479000
6	0.284238000	-1.869487000	1.526475000
6	1.857665000	-2.106154000	-1.970644000
1	1.233720000	-2.953823000	-2.271310000
1	2.901216000	-2.302746000	-2.220639000
1	-0.477954000	-2.438585000	2.042931000
1	-0.354936000	-2.499845000	-0.428538000
1	1.525130000	-1.224990000	-2.529197000
6	1.743665000	-1.812614000	-0.487287000
8	2.723345000	-1.517000000	0.181102000
17	-3.350683000	-0.830288000	-0.803997000



1	1.201447000	-1.679733000	2.075995000

7 + MVK (ortho-endo) TS

6	-1.649419000	-0.348088000	-0.034930000
6	-0.271850000	-0.730314000	-0.591647000
6	-1.520615000	0.849230000	0.950611000
1	-0.296111000	-1.458662000	-1.396180000
8	-2.469327000	1.581392000	1.195180000
6	0.768828000	-0.804457000	0.334843000
6	-0.229096000	0.958731000	1.634823000
1	-0.173615000	1.708510000	2.418128000
6	0.799890000	0.065081000	1.440996000
1	1.685158000	0.099453000	2.065485000
8	-2.469948000	-0.116256000	-1.146638000
8	-2.166413000	-1.368008000	0.806458000
6	-2.227375000	-2.683075000	0.251034000
1	-2.883931000	-3.256839000	0.907651000
1	-2.647470000	-2.672246000	-0.760539000
1	-1.238599000	-3.156849000	0.233615000
6	-3.854652000	0.185668000	-0.909473000
1	-4.231961000	-0.360931000	-0.042737000
1	-3.998966000	1.254805000	-0.746474000

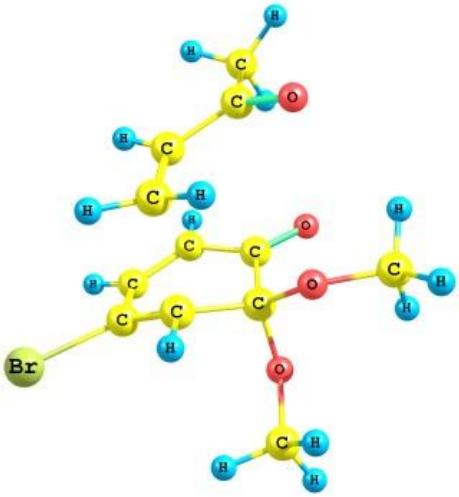


1	-4.386008000	-0.135357000	-1.809014000
6	0.186433000	0.883661000	-1.709357000
6	0.190972000	2.048036000	-0.942072000
6	1.489430000	3.915689000	0.229467000
1	0.618924000	4.105309000	0.865617000
1	1.466688000	4.656277000	-0.579282000
1	-0.698993000	2.662880000	-0.859114000
1	1.156282000	0.512058000	-2.027328000
1	-0.651376000	0.717358000	-2.377212000
1	2.408634000	4.050626000	0.801271000
6	1.453660000	2.515940000	-0.357231000
8	2.450103000	1.791781000	-0.359809000
35	2.294251000	-1.856408000	-0.069651000

7 + MVK (ortho-exo) TS

6	0.509451000	1.186348000	0.034253000
6	-0.662422000	0.408018000	-0.579823000
6	1.177638000	0.344847000	1.161650000
1	-1.079897000	0.858505000	-1.474844000
8	2.309426000	0.580930000	1.559871000
6	-1.528900000	-0.210430000	0.323268000
6	0.314503000	-0.661912000	1.793701000

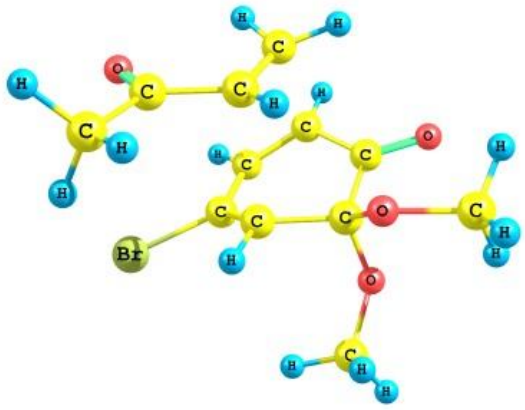
1	0.746185000	-1.182100000	2.643418000
6	-1.029069000	-0.781065000	1.502902000
1	-1.673474000	-1.401206000	2.117072000
8	1.320647000	1.550170000	-1.034860000
8	0.045521000	2.314887000	0.768156000
6	-0.751868000	3.253950000	0.045176000
1	-0.767723000	4.164290000	0.647327000
1	-0.316763000	3.475164000	-0.934868000
1	-1.780819000	2.895015000	-0.082164000
6	2.546648000	2.251465000	-0.759696000
1	2.427043000	2.933567000	0.084792000
1	3.351425000	1.545291000	-0.557482000
1	2.765784000	2.818690000	-1.667542000
6	0.265811000	-1.165244000	-1.462135000
6	1.054935000	-1.877357000	-0.556072000
6	3.293056000	-2.496181000	0.530098000
1	4.305613000	-2.695265000	0.174755000
1	2.799937000	-3.432175000	0.808283000
1	0.630029000	-2.697535000	0.011982000
1	-0.664379000	-1.608793000	-1.803521000
1	0.808581000	-0.557071000	-2.180441000



1	3.364835000	-1.863628000	1.423084000
6	2.529071000	-1.720675000	-0.526537000
8	3.111688000	-0.977026000	-1.307294000
35	-3.300793000	-0.634143000	-0.232501000

7 + MVK (meta-endo) TS

6	-1.619917000	-0.353039000	-0.188570000
6	-0.128389000	-0.316126000	-0.503232000
6	-1.909652000	0.303357000	1.190634000
1	0.136577000	-0.563123000	-1.525240000
8	-3.046517000	0.552311000	1.551075000
6	0.742883000	-0.606700000	0.535756000
6	-0.717703000	0.574759000	2.025075000
1	-0.937134000	0.989731000	3.004164000
6	0.463457000	-0.146126000	1.822353000
1	1.212262000	-0.214347000	2.602997000
8	-2.273571000	0.259428000	-1.271115000
8	-2.062908000	-1.685879000	0.015700000
6	-1.754935000	-2.626063000	-1.016584000
1	-2.379986000	-3.499310000	-0.821823000
1	-1.992623000	-2.225138000	-2.007937000
1	-0.701123000	-2.926831000	-0.984809000

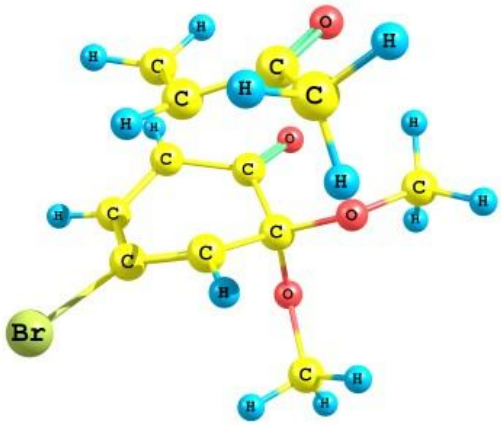


6	-3.709473000	0.284877000	-1.253568000
1	-4.114076000	-0.647403000	-0.854194000
1	-4.083969000	1.118328000	-0.655162000
1	-4.013278000	0.406726000	-2.295994000
6	0.033018000	1.990264000	-0.468405000
6	-0.426161000	2.394245000	0.787041000
6	2.018445000	1.798342000	-2.115069000
1	1.230352000	1.820435000	-2.871664000
1	2.527047000	0.828721000	-2.151924000
1	0.310837000	2.766387000	1.489402000
1	-0.640300000	1.990936000	-1.317101000
1	2.766177000	2.563551000	-2.339935000
6	1.500927000	2.006728000	-0.702318000
8	2.279504000	2.149068000	0.232535000
1	-1.442734000	2.750948000	0.905049000
35	2.456998000	-1.348175000	0.140570000

7 + MVK (meta-exo) TS

6	0.826081000	1.005496000	-0.135706000
6	-0.369276000	0.143518000	-0.521679000
6	1.135645000	0.843717000	1.381190000
1	-0.488824000	-0.059163000	-1.579878000

8	2.184262000	1.207478000	1.875247000
6	-1.467748000	0.179323000	0.316638000
6	0.015895000	0.292605000	2.191748000
1	0.189797000	0.318258000	3.263484000
6	-1.291220000	0.305196000	1.696372000
1	-2.137564000	0.214909000	2.368683000
8	1.843121000	0.667219000	-1.028045000
8	0.514357000	2.395100000	-0.195013000
6	-0.014894000	2.867879000	-1.435024000
1	0.043397000	3.956896000	-1.391099000
1	0.575785000	2.507237000	-2.283702000
1	-1.062844000	2.571446000	-1.564917000
6	3.145348000	1.240107000	-0.821630000
1	3.067784000	2.274556000	-0.480802000
1	3.709067000	0.650394000	-0.097392000
1	3.636988000	1.203295000	-1.796502000
6	0.506262000	-1.928380000	0.300392000
6	0.596978000	-1.756578000	1.683324000
6	1.646153000	-2.474540000	-1.938199000
1	0.862343000	-3.223254000	-2.091526000
1	2.604305000	-2.855915000	-2.293783000

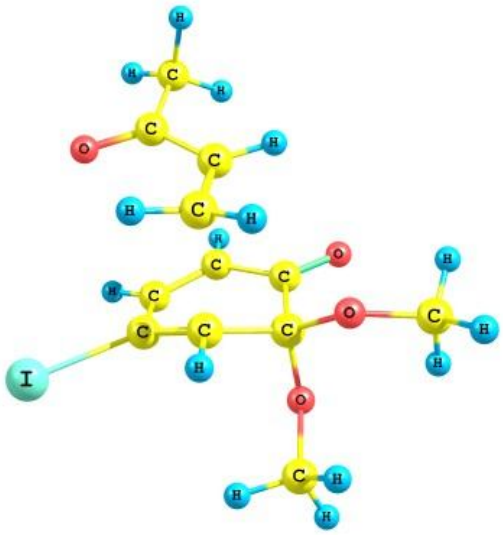


1	-0.182390000	-2.136992000	2.330478000
1	-0.391781000	-2.359967000	-0.128365000
1	1.385614000	-1.585900000	-2.523261000
6	1.774841000	-2.074658000	-0.481866000
8	2.867410000	-1.910038000	0.040618000
1	1.594144000	-1.694042000	2.108843000
35	-3.191526000	-0.300627000	-0.365602000

11c (ortho-endo) TS

6	-1.635298000	-1.013474000	-0.027930000
6	-0.231261000	-0.701611000	-0.576166000
6	-2.088480000	0.094601000	0.968559000
1	0.080499000	-1.352007000	-1.388898000
8	-3.273617000	0.269535000	1.232951000
6	0.724719000	-0.276208000	0.351450000
6	-1.005198000	0.830069000	1.627640000
1	-1.311611000	1.526745000	2.404072000
6	0.327906000	0.523044000	1.446804000
1	1.078999000	0.987717000	2.077676000
8	-2.466214000	-1.177392000	-1.150356000
8	-1.616372000	-2.169431000	0.799115000
6	-1.099484000	-3.374010000	0.215596000

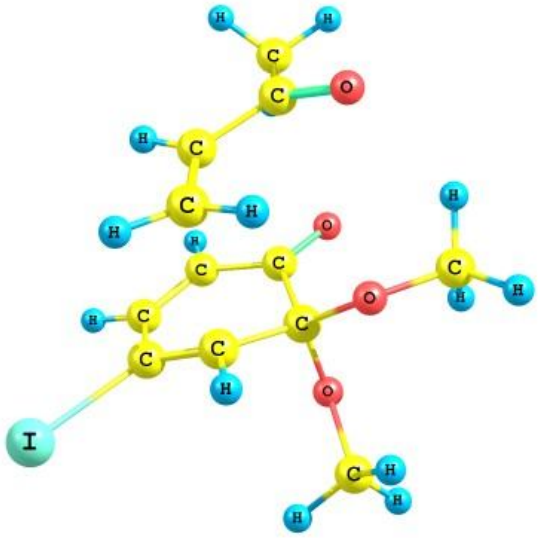
1	-1.422257000	-4.183338000	0.873567000
1	-1.504191000	-3.539054000	-0.788633000
1	-0.004059000	-3.361190000	0.177189000
6	-3.831217000	-1.592872000	-0.933768000
1	-3.902690000	-2.298272000	-0.102843000
1	-4.470578000	-0.732155000	-0.729640000
1	-4.137124000	-2.081165000	-1.862735000
6	-0.595959000	0.962679000	-1.696782000
6	-1.200382000	1.960276000	-0.928655000
6	-1.133501000	4.250044000	0.211820000
1	-2.024323000	3.950245000	0.772879000
1	-1.468563000	4.890764000	-0.613510000
1	-2.282974000	2.016881000	-0.860524000
1	0.432244000	1.134502000	-2.003301000
1	-1.224466000	0.399346000	-2.379057000
1	-0.465160000	4.832456000	0.849070000
6	-0.392354000	3.051986000	-0.357146000
8	0.841521000	3.002783000	-0.367973000
53	2.786920000	-0.563822000	-0.044222000



11c (ortho-exo) TS

6	0.981100000	1.136661000	0.051808000

6	-0.284305000	0.480344000	-0.505945000
6	1.575998000	0.278356000	1.224703000
1	-0.632773000	0.859097000	-1.460774000
8	2.738612000	0.392919000	1.591864000
6	-1.167014000	-0.087264000	0.377338000
6	0.600137000	-0.531941000	1.974404000
1	0.971442000	-1.006224000	2.879594000
6	-0.718941000	-0.612880000	1.627405000
1	-1.416544000	-1.164607000	2.251830000
8	1.787878000	1.385397000	-1.061772000
8	0.648455000	2.337208000	0.756454000
6	-0.008094000	3.361095000	-0.008237000
1	0.263068000	4.312570000	0.455486000
1	0.329457000	3.360223000	-1.049014000
1	-1.097596000	3.239541000	0.032086000
6	3.102712000	1.975236000	-0.893270000
1	3.157681000	2.578742000	0.012552000
1	3.850050000	1.180819000	-0.876744000
1	3.255491000	2.610820000	-1.771053000
6	0.667196000	-1.332355000	-1.439375000
6	1.490569000	-1.939015000	-0.525520000

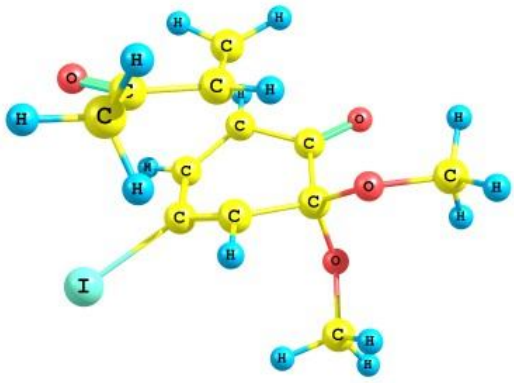


6	3.757390000	-2.366921000	0.578417000
1	4.825928000	-2.212095000	0.418039000
1	3.539583000	-3.437799000	0.658851000
1	1.098882000	-2.679018000	0.166635000
1	-0.328925000	-1.705497000	-1.641964000
1	1.130670000	-0.674156000	-2.167812000
1	3.460778000	-1.872140000	1.511724000
6	2.970080000	-1.723016000	-0.545557000
8	3.519855000	-1.077351000	-1.431547000
53	-3.203143000	-0.368405000	-0.184084000

11c (meta-endo) TS

6	-1.843099000	-0.546424000	-0.197335000
6	-0.391508000	-0.164675000	-0.506049000
6	-2.241979000	-0.056584000	1.224741000
1	-0.109862000	-0.276583000	-1.548634000
8	-3.403593000	-0.061841000	1.602746000
6	0.544152000	-0.378296000	0.506431000
6	-1.114163000	0.388598000	2.075313000
1	-1.395919000	0.654414000	3.092324000
6	0.182870000	-0.091221000	1.824554000
1	0.923653000	-0.095612000	2.618002000

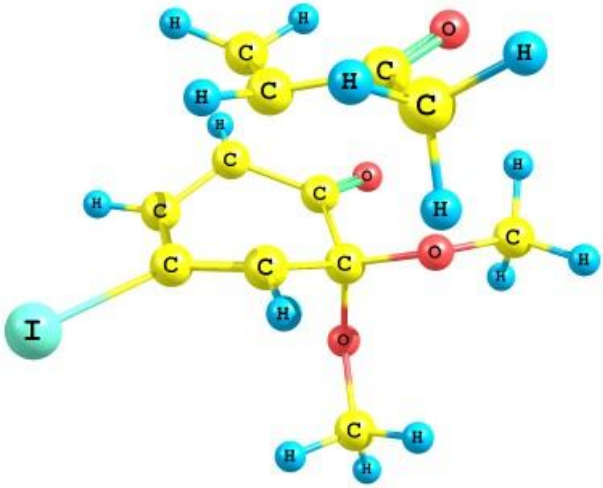
8	-2.629581000	-0.012701000	-1.237670000
8	-1.990442000	-1.955925000	-0.085747000
6	-1.543453000	-2.742907000	-1.199219000
1	-1.975904000	-3.734518000	-1.051730000
1	-1.897550000	-2.330832000	-2.150421000
1	-0.450950000	-2.828546000	-1.214763000
6	-4.039859000	-0.312221000	-1.236782000
1	-4.225674000	-1.342233000	-0.923822000
1	-4.583844000	0.365848000	-0.575035000
1	-4.366785000	-0.171303000	-2.270117000
6	-0.728685000	2.084211000	-0.270734000
6	-1.186236000	2.301631000	1.041669000
6	0.982480000	2.726581000	-2.077484000
1	0.843121000	1.792115000	-2.632007000
1	2.015402000	3.061350000	-2.183925000
1	-0.501909000	2.777467000	1.737166000
1	-1.456103000	2.032413000	-1.075254000
1	0.309154000	3.467370000	-2.524887000
6	0.652416000	2.536319000	-0.607987000
8	1.479917000	2.755291000	0.272367000
1	-2.244176000	2.466840000	1.218866000



53	2.562817000	-0.869941000	0.030339000

11c (meta-exo) TS

6	-1.298504000	-0.975953000	-0.173073000
6	-0.042633000	-0.146567000	-0.443009000
6	-1.638733000	-0.935627000	1.348617000
1	0.136734000	0.070431000	-1.491751000
8	-2.682243000	-1.377535000	1.795605000
6	1.033132000	-0.309887000	0.432790000
6	-0.564503000	-0.380374000	2.219015000
1	-0.782455000	-0.470198000	3.281252000
6	0.777264000	-0.487645000	1.790408000
1	1.581677000	-0.515141000	2.519432000
8	-2.264890000	-0.481466000	-1.058862000
8	-1.064475000	-2.370050000	-0.370900000
6	-0.563555000	-2.753200000	-1.659597000
1	-0.670390000	-3.838712000	-1.706357000
1	-1.145932000	-2.295042000	-2.465855000
1	0.496007000	-2.493507000	-1.770380000
6	-3.621455000	-0.966805000	-0.954853000
1	-3.643018000	-2.029765000	-0.706283000
1	-4.168230000	-0.392003000	-0.204530000

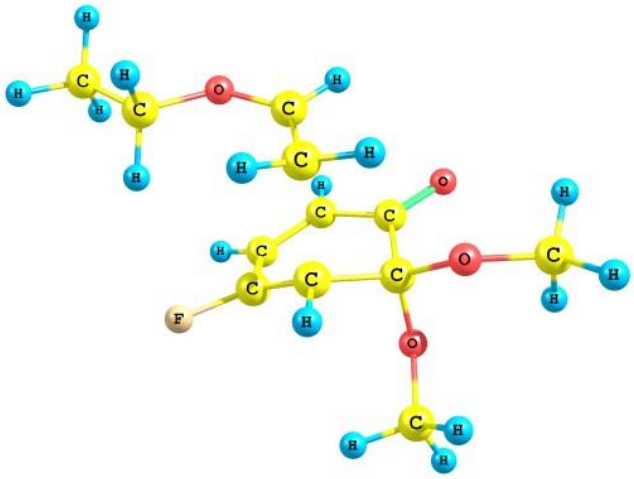


1	-4.062150000	-0.801832000	-1.941158000
6	-0.762173000	1.873019000	0.419269000
6	-0.973631000	1.613655000	1.793875000
6	-1.677913000	2.660387000	-1.850412000
1	-0.804904000	3.318670000	-1.905159000
1	-2.557852000	3.170819000	-2.246621000
1	-0.249396000	1.986805000	2.509512000
1	0.173466000	2.331702000	0.114334000
1	-1.477986000	1.777655000	-2.469200000
6	-1.952882000	2.188054000	-0.436795000
8	-3.096047000	2.127689000	0.005283000
1	-2.008507000	1.631175000	2.131304000
53	3.014296000	0.133689000	-0.217641000

5 + EVE (ortho-endo) TS

6	1.547867000	0.017835000	-0.085534000
6	0.366026000	0.782807000	-0.704286000
6	1.014597000	-0.880630000	1.075161000
1	0.600145000	1.304738000	-1.629338000
8	1.554886000	-1.951065000	1.348552000
6	-0.414605000	1.473857000	0.241527000
6	-0.106908000	-0.322577000	1.805529000

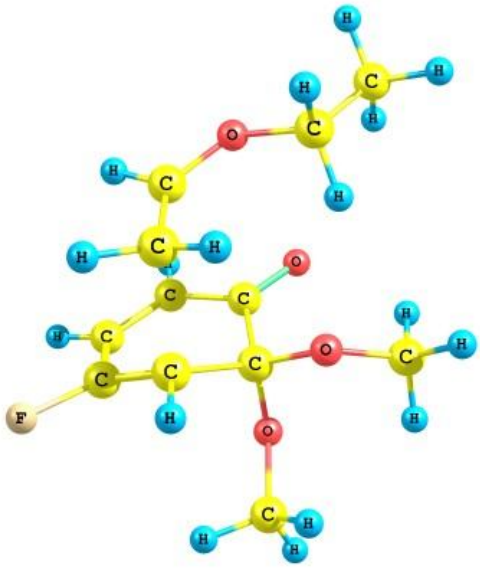
1	-0.409296000	-0.854172000	2.701638000
6	-0.689897000	0.896789000	1.471663000
1	-1.442759000	1.346002000	2.112714000
8	2.169162000	-0.675177000	-1.138382000
8	2.457671000	0.883292000	0.575301000
6	3.015621000	1.933992000	-0.211099000
1	3.868407000	2.315850000	0.353966000
1	3.361655000	1.568423000	-1.184200000
1	2.297586000	2.749317000	-0.362290000
6	3.344849000	-1.441503000	-0.832489000
1	3.934523000	-0.957099000	-0.051015000
1	3.081910000	-2.448036000	-0.505537000
1	3.924578000	-1.479531000	-1.759028000
6	-0.686853000	-0.687660000	-1.407781000
6	-1.375904000	-1.412540000	-0.419877000
6	-3.417385000	-0.148435000	-0.679505000
1	-3.530403000	-0.431631000	-1.734233000
1	-2.914694000	0.821865000	-0.631692000
1	-0.978824000	-2.313362000	0.029672000
1	-1.289351000	-0.111713000	-2.104037000
1	0.132758000	-1.225613000	-1.870820000



8	-2.624895000	-1.155578000	-0.012969000
6	-4.762384000	-0.104875000	0.020318000
1	-5.406553000	0.636326000	-0.462017000
1	-5.256992000	-1.078721000	-0.026640000
1	-4.642747000	0.172453000	1.070951000
9	-1.199407000	2.503419000	-0.196652000

5 + EVE (ortho-exo) TS

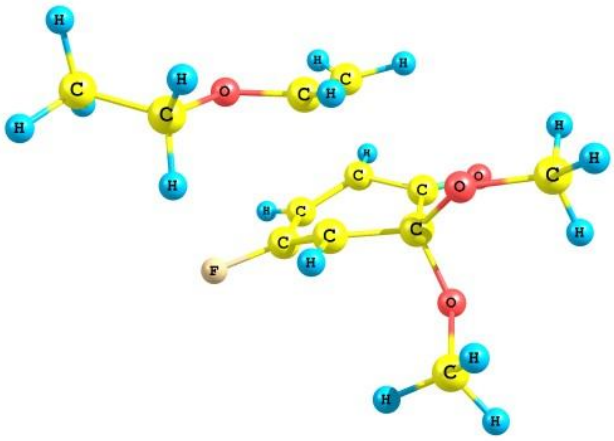
6	-0.656785000	0.792983000	-0.008857000
6	-1.277427000	-0.325444000	-0.847205000
6	0.051023000	0.163634000	1.237167000
1	-1.632264000	-0.024907000	-1.829816000
8	1.063274000	0.670537000	1.723034000
6	-2.088520000	-1.201502000	-0.109697000
6	-0.613767000	-1.003622000	1.779071000
1	-0.240826000	-1.373502000	2.728375000
6	-1.734135000	-1.571426000	1.180904000
1	-2.275129000	-2.378962000	1.665776000
8	0.191652000	1.526184000	-0.863909000
8	-1.646569000	1.627825000	0.572943000
6	-2.615807000	2.179449000	-0.316408000
1	-3.095343000	2.996597000	0.226853000



1	-2.151779000	2.576093000	-1.226946000
1	-3.377434000	1.440156000	-0.591043000
6	0.692025000	2.776335000	-0.359413000
1	-0.124753000	3.471774000	-0.145858000
1	1.287253000	2.626063000	0.540909000
1	1.308996000	3.183783000	-1.163732000
6	0.314527000	-1.386277000	-1.417671000
6	1.122682000	-1.834340000	-0.356971000
6	2.959415000	-0.318364000	-0.728806000
1	3.233484000	-0.726585000	-1.711548000
1	2.262321000	0.507795000	-0.868953000
1	-0.287289000	-2.158631000	-1.885295000
1	0.749306000	-0.678839000	-2.115469000
8	2.309923000	-1.369370000	0.023140000
6	4.177422000	0.107139000	0.066261000
1	4.855242000	-0.735936000	0.227703000
1	4.719857000	0.887753000	-0.476252000
1	3.865416000	0.501506000	1.035828000
1	0.860928000	-2.723912000	0.202828000
9	-3.032017000	-1.922560000	-0.773918000

5 + EVE (meta-endo) TS

6	1.384685000	0.249675000	-0.179378000
6	0.000603000	0.858786000	-0.127839000
6	1.576051000	-0.828119000	0.930504000
1	-0.262941000	1.528790000	-0.938514000
8	2.585559000	-1.511030000	0.975162000
6	-0.611543000	0.994163000	1.095440000
6	0.459971000	-0.977445000	1.887337000
1	0.599022000	-1.761601000	2.623756000
6	-0.404150000	0.081804000	2.134877000
1	-1.035807000	0.108493000	3.015615000
8	1.530685000	-0.271074000	-1.487654000
8	2.406348000	1.187624000	0.126702000
6	2.413000000	2.388550000	-0.642242000
1	3.382894000	2.856121000	-0.461181000
1	2.306905000	2.182559000	-1.713324000
1	1.621257000	3.078047000	-0.325775000
6	2.795619000	-0.852715000	-1.831587000
1	3.622575000	-0.274604000	-1.413918000
1	2.874471000	-1.882991000	-1.474657000
1	2.840994000	-0.834329000	-2.923555000
6	-1.211969000	-1.158320000	-0.667435000

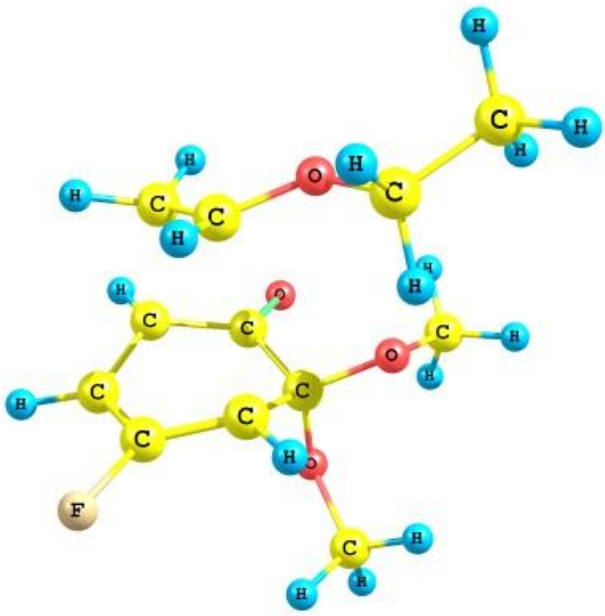


6	-0.560008000	-2.069952000	0.142989000
6	-3.120561000	0.156652000	-1.148123000
1	-2.951748000	-0.083652000	-2.206636000
1	-2.656793000	1.127406000	-0.938531000
1	0.308564000	-2.581044000	-0.249264000
1	-0.860542000	-0.912569000	-1.663623000
8	-2.485712000	-0.838308000	-0.335353000
6	-4.603659000	0.167961000	-0.809424000
1	-5.053665000	1.121370000	-1.100724000
1	-5.142802000	-0.638562000	-1.313374000
1	-4.731482000	0.047541000	0.269589000
1	-1.136956000	-2.589704000	0.897271000
9	-1.636357000	1.878311000	1.219474000

5 + EVE (meta-exo) TS

6	-0.555653000	0.846987000	-0.010537000
6	-0.716244000	-0.262432000	-1.027460000
6	-0.740484000	0.294004000	1.433536000
1	-0.378540000	-0.059900000	-2.038072000
8	-0.398998000	0.921037000	2.417682000
6	-1.769544000	-1.135623000	-0.825377000
6	-1.389988000	-1.050417000	1.517021000

1	-1.664472000	-1.321471000	2.533212000
6	-2.200597000	-1.487402000	0.447795000
1	-2.958929000	-2.250526000	0.580171000
8	0.686873000	1.451359000	-0.264522000
8	-1.610978000	1.811792000	-0.062858000
6	-1.870988000	2.381408000	-1.343075000
1	-2.531371000	3.232917000	-1.166285000
1	-0.949466000	2.732898000	-1.821170000
1	-2.374917000	1.671564000	-2.009803000
6	1.082064000	2.546088000	0.572052000
1	0.224169000	3.163180000	0.846891000
1	1.569916000	2.188339000	1.481739000
1	1.786142000	3.135766000	-0.021762000
6	1.052261000	-1.741166000	0.129785000
6	0.373663000	-2.046767000	1.323411000
6	2.793468000	-0.656702000	-1.043338000
1	2.934015000	-1.580108000	-1.622775000
1	2.134300000	0.017145000	-1.598937000
1	0.925693000	-2.334409000	-0.770627000
8	2.157660000	-0.980812000	0.203190000
6	4.123536000	0.001683000	-0.732983000

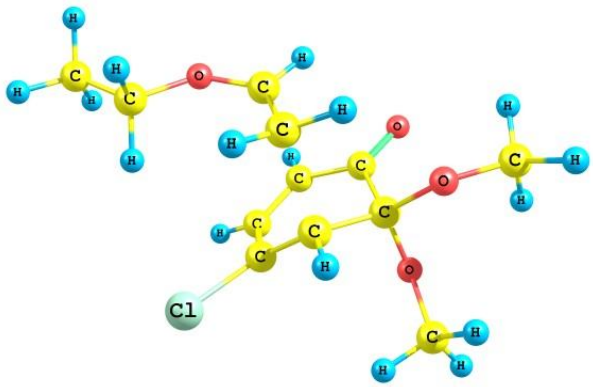


1	4.769058000	-0.669030000	-0.158916000
1	4.635746000	0.263754000	-1.663760000
1	3.970455000	0.915772000	-0.153604000
1	-0.099105000	-3.019129000	1.374487000
1	0.869147000	-1.727077000	2.235986000
9	-2.291917000	-1.791630000	-1.891077000

13c (ortho-endo) TS

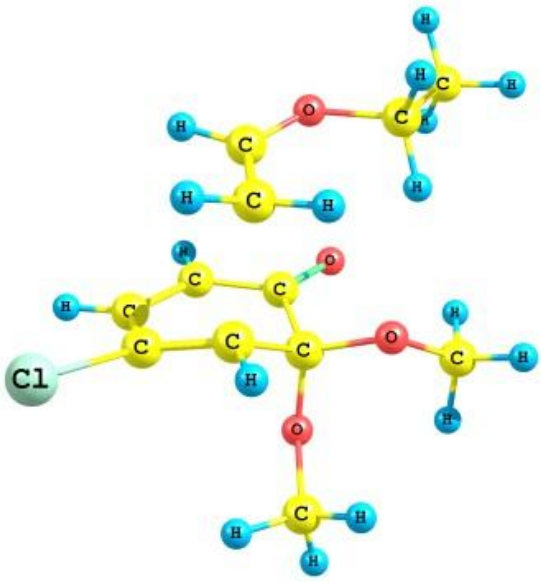
6	1.648291000	-0.088770000	-0.072002000
6	0.458047000	0.704470000	-0.646856000
6	1.125242000	-1.044087000	1.041094000
1	0.708256000	1.259761000	-1.548499000
8	1.663113000	-2.128718000	1.256756000
6	-0.310250000	1.375812000	0.336161000
6	-0.002485000	-0.525973000	1.791407000
1	-0.304427000	-1.101241000	2.660678000
6	-0.580571000	0.713465000	1.530939000
1	-1.315858000	1.121456000	2.218126000
8	2.257854000	-0.726398000	-1.166183000
8	2.560834000	0.742067000	0.623698000
6	3.104971000	1.839491000	-0.108314000
1	3.957048000	2.197825000	0.472808000

1	3.450032000	1.529346000	-1.100877000
1	2.378306000	2.654144000	-0.211281000
6	3.429449000	-1.516001000	-0.907363000
1	4.031780000	-1.071117000	-0.111976000
1	3.160369000	-2.533525000	-0.621721000
1	3.998911000	-1.518326000	-1.840817000
6	-0.591564000	-0.683872000	-1.411554000
6	-1.182569000	-1.555679000	-0.470126000
6	-3.390930000	-0.579218000	-0.615883000
1	-3.452718000	-0.748853000	-1.698400000
1	-3.047430000	0.445219000	-0.444723000
1	-0.674137000	-2.444447000	-0.117534000
1	-1.264879000	-0.088247000	-2.021015000
1	0.221433000	-1.139216000	-1.968253000
8	-2.449994000	-1.519938000	-0.053501000
6	-4.727681000	-0.830269000	0.054367000
1	-5.475300000	-0.138376000	-0.344780000
1	-5.068729000	-1.853218000	-0.126181000
1	-4.654025000	-0.674665000	1.133859000
17	-1.340164000	2.724186000	-0.161576000



13c (ortho-exo) TS

6	-0.246102000	1.020164000	0.001912000
6	-1.139156000	-0.009630000	-0.695871000
6	0.399458000	0.368526000	1.265391000
1	-1.462242000	0.276088000	-1.692834000
8	1.529237000	0.680519000	1.640197000
6	-2.062816000	-0.642249000	0.149335000
6	-0.463201000	-0.564473000	1.963578000
1	-0.122131000	-0.908553000	2.934506000
6	-1.696501000	-0.950851000	1.465444000
1	-2.349651000	-1.577620000	2.065446000
8	0.672904000	1.487120000	-0.962542000
8	-1.009318000	2.083208000	0.547574000
6	-1.909574000	2.747108000	-0.339614000
1	-2.182612000	3.682940000	0.152528000
1	-1.436967000	2.971856000	-1.302733000
1	-2.816717000	2.155612000	-0.507640000
6	1.459946000	2.637404000	-0.609046000
1	0.828949000	3.445857000	-0.231675000
1	2.205661000	2.385753000	0.145889000
1	1.941830000	2.955188000	-1.536619000

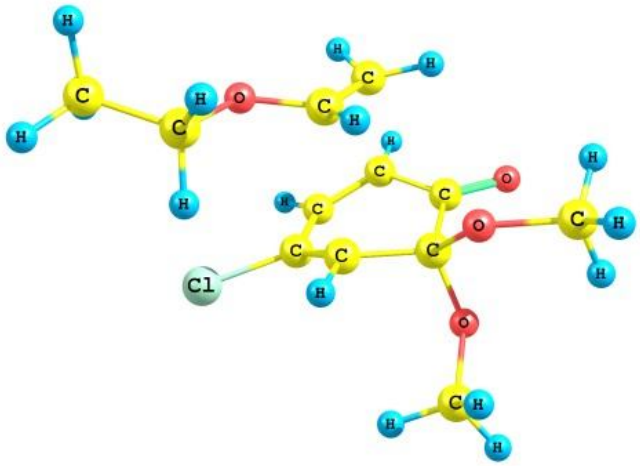


6	0.186323000	-1.431166000	-1.288138000
6	0.942276000	-1.980320000	-0.245008000
6	3.012813000	-0.872669000	-0.769681000
1	3.110913000	-1.336864000	-1.760313000
1	2.493537000	0.080014000	-0.867532000
1	-0.607035000	-2.072235000	-1.658258000
1	0.707658000	-0.862314000	-2.049907000
8	2.214096000	-1.752561000	0.058823000
6	4.353076000	-0.712520000	-0.081771000
1	4.841638000	-1.681003000	0.058381000
1	5.006970000	-0.080817000	-0.690915000
1	4.215385000	-0.240163000	0.893432000
1	0.524121000	-2.743527000	0.401491000
17	-3.480819000	-1.417203000	-0.560286000

13c (meta-endo) TS

6	1.493874000	0.133148000	-0.279504000
6	0.065549000	0.609098000	-0.464183000
6	1.728174000	-0.420173000	1.155736000
1	-0.220837000	0.849803000	-1.480393000
8	2.777798000	-0.961783000	1.459527000
6	-0.566138000	1.214884000	0.600238000

6	0.624489000	-0.204839000	2.113737000
1	0.810342000	-0.593322000	3.110591000
6	-0.292532000	0.819989000	1.919541000
1	-0.899452000	1.188804000	2.738303000
8	1.717461000	-0.829967000	-1.290887000
8	2.428069000	1.199778000	-0.353380000
6	2.384862000	2.000369000	-1.533649000
1	3.312346000	2.576295000	-1.539840000
1	2.337703000	1.382870000	-2.437564000
1	1.535786000	2.693953000	-1.522977000
6	3.031854000	-1.395809000	-1.390596000
1	3.800858000	-0.638737000	-1.223396000
1	3.175308000	-2.205103000	-0.670296000
1	3.107311000	-1.786442000	-2.408635000
6	-0.932706000	-1.587225000	-0.084330000
6	-0.291452000	-2.038737000	1.054306000
6	-2.905756000	-0.896778000	-1.196110000
1	-2.655456000	-1.617038000	-1.987086000
1	-2.534528000	0.089034000	-1.502010000
1	0.625620000	-2.600031000	0.950151000
1	-0.520251000	-1.751115000	-1.075127000

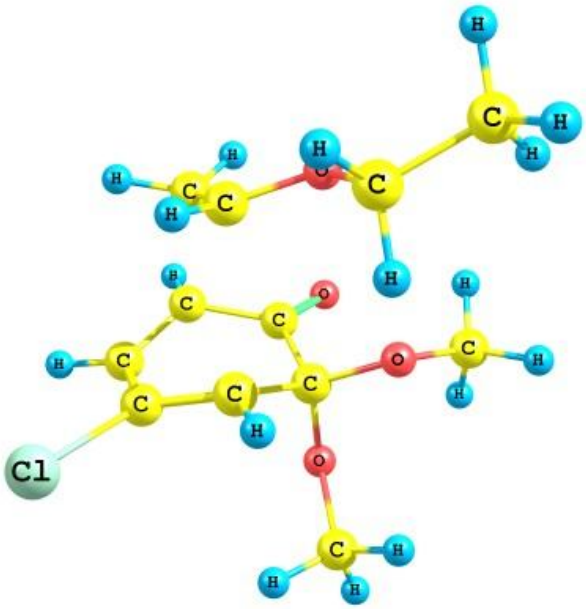


8	-2.250256000	-1.291487000	0.016635000
6	-4.402350000	-0.861707000	-0.934110000
1	-4.907667000	-0.266138000	-1.699861000
1	-4.835863000	-1.865394000	-0.932968000
1	-4.594208000	-0.400029000	0.037899000
1	-0.878226000	-2.212271000	1.946674000
17	-1.980622000	2.234660000	0.310289000

13c (meta-exo) TS

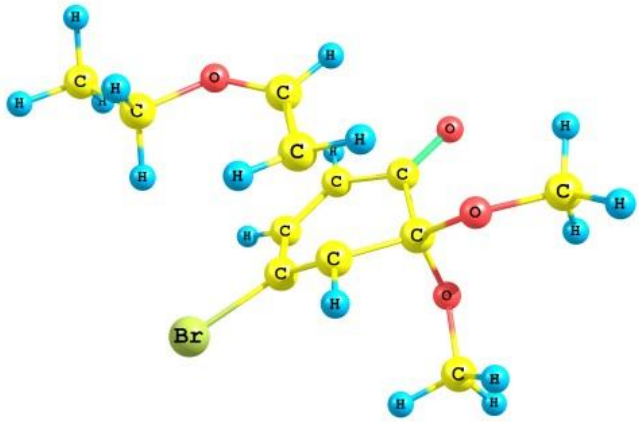
6	-0.098218000	1.058064000	-0.087227000
6	-0.727033000	-0.168964000	-0.722146000
6	-0.131201000	0.943693000	1.463326000
1	-0.507022000	-0.335025000	-1.770482000
8	0.558444000	1.638183000	2.184855000
6	-1.923900000	-0.604335000	-0.177218000
6	-1.101406000	-0.060568000	1.991314000
1	-1.238453000	0.004182000	3.067701000
6	-2.180935000	-0.475847000	1.186436000
1	-3.077823000	-0.894686000	1.627248000
8	1.177388000	1.191196000	-0.657481000
8	-0.873645000	2.242103000	-0.281759000
6	-1.240941000	2.534584000	-1.628518000

1	-1.618178000	3.559225000	-1.621982000
1	-0.378652000	2.471833000	-2.302042000
1	-2.031232000	1.865278000	-1.987900000
6	1.989629000	2.291641000	-0.226024000
1	1.382400000	3.180099000	-0.040716000
1	2.540542000	2.039945000	0.682889000
1	2.687493000	2.485592000	-1.045176000
6	0.768726000	-1.778213000	0.556368000
6	0.271564000	-1.596512000	1.857582000
6	2.494649000	-1.567175000	-1.047578000
1	2.270420000	-2.594514000	-1.367477000
1	1.958976000	-0.866220000	-1.694840000
1	0.331475000	-2.499366000	-0.127656000
8	2.028826000	-1.384674000	0.298892000
6	3.987705000	-1.302949000	-1.065526000
1	4.516487000	-1.993719000	-0.402781000
1	4.376216000	-1.429848000	-2.080568000
1	4.198239000	-0.280875000	-0.740243000
1	-0.438955000	-2.329917000	2.214595000
1	0.990085000	-1.246654000	2.593094000
17	-3.043644000	-1.545313000	-1.174380000



14c (ortho-endo) TS

6	1.871050000	-0.036352000	-0.068987000
6	0.527971000	0.490769000	-0.607118000
6	1.599866000	-1.091664000	1.046704000
1	0.623573000	1.096067000	-1.504669000
8	2.376365000	-2.025118000	1.238933000
6	-0.355470000	0.933988000	0.395348000
6	0.416025000	-0.837292000	1.845324000
1	0.276594000	-1.468058000	2.717293000
6	-0.442805000	0.222469000	1.594387000
1	-1.240618000	0.449366000	2.295018000
8	2.583880000	-0.517162000	-1.180720000
8	2.590854000	0.974198000	0.616462000
6	2.829176000	2.183223000	-0.103651000
1	3.597361000	2.721632000	0.455080000
1	3.194534000	1.982574000	-1.117059000
1	1.926216000	2.803356000	-0.154727000
6	3.918153000	-1.001381000	-0.960108000
1	4.419417000	-0.421590000	-0.181774000
1	3.909834000	-2.052631000	-0.670340000
1	4.443216000	-0.870238000	-1.910265000

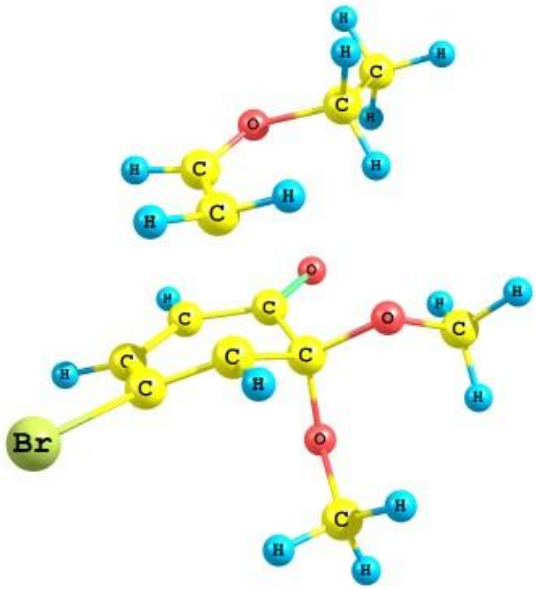


6	-0.207724000	-1.111451000	-1.447633000
6	-0.607041000	-2.098955000	-0.535770000
6	-2.950021000	-1.527751000	-0.622374000
1	-3.010176000	-1.721805000	-1.700936000
1	-2.778777000	-0.457886000	-0.470991000
1	0.074106000	-2.858574000	-0.171830000
1	-0.985469000	-0.628331000	-2.031337000
1	0.694196000	-1.351576000	-1.999717000
8	-1.845747000	-2.288087000	-0.080531000
6	-4.204246000	-1.992711000	0.091639000
1	-5.071882000	-1.452243000	-0.298152000
1	-4.365086000	-3.063555000	-0.059221000
1	-4.131654000	-1.800625000	1.165333000
35	-1.759652000	2.147032000	-0.082326000

14c (ortho-exo) TS

6	0.402527000	1.145409000	0.009953000
6	-0.693876000	0.258218000	-0.587017000
6	0.994823000	0.444172000	1.274677000
1	-1.018527000	0.554489000	-1.580316000
8	2.181323000	0.564539000	1.579156000
6	-1.667621000	-0.152191000	0.337881000

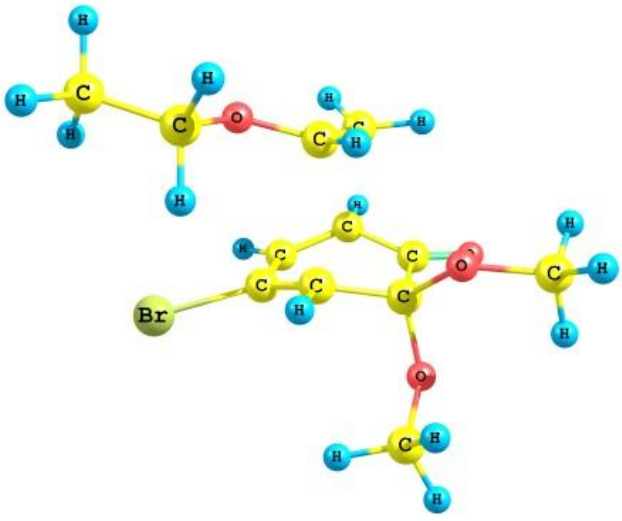
6	0.023507000	-0.293384000	2.058372000
1	0.355458000	-0.655099000	3.026144000
6	-1.289029000	-0.467863000	1.646175000
1	-2.007383000	-0.936906000	2.311730000
8	1.334423000	1.393985000	-1.017846000
8	-0.129823000	2.351533000	0.530624000
6	-0.985709000	3.098760000	-0.333708000
1	-1.085541000	4.086261000	0.121555000
1	-0.555500000	3.206853000	-1.336446000
1	-1.977184000	2.637891000	-0.410558000
6	2.300524000	2.430010000	-0.770107000
1	1.819072000	3.409375000	-0.693351000
1	2.870217000	2.228065000	0.136750000
1	2.959184000	2.422871000	-1.641688000
6	0.294725000	-1.392117000	-1.148872000
6	1.011989000	-2.008141000	-0.112401000
6	3.210944000	-1.349841000	-0.844615000
1	3.182018000	-1.920376000	-1.782802000
1	2.853209000	-0.337049000	-1.029747000
1	-0.622563000	-1.901125000	-1.427968000
1	0.858596000	-0.984905000	-1.980868000



8	2.321843000	-2.000786000	0.096401000
6	4.592310000	-1.350977000	-0.222151000
1	4.926370000	-2.369942000	-0.006907000
1	5.307527000	-0.891384000	-0.911369000
1	4.579390000	-0.777514000	0.707307000
35	-3.365371000	-0.736379000	-0.327563000
1	0.510841000	-2.644733000	0.607442000

14c (meta-endo) TS

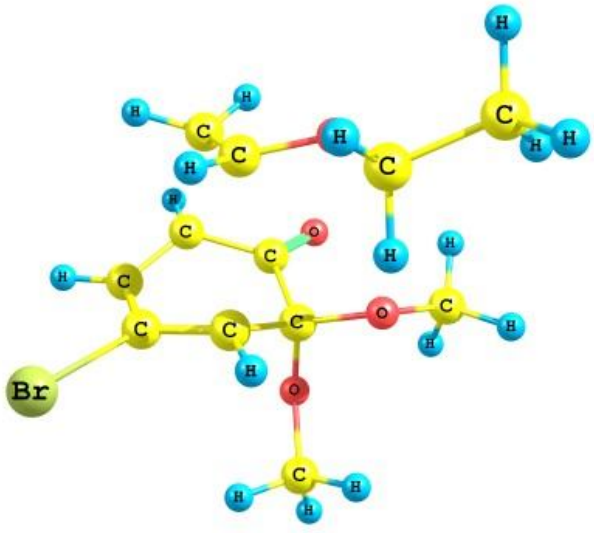
6	-1.746646000	-0.219089000	-0.276983000
6	-0.247722000	-0.308189000	-0.498361000
6	-2.076479000	0.236621000	1.172858000
1	0.056111000	-0.490775000	-1.523066000
8	-3.223127000	0.454762000	1.523911000
6	0.538190000	-0.756059000	0.551776000
6	-0.912879000	0.362030000	2.078493000
1	-1.162773000	0.695761000	3.081690000
6	0.227662000	-0.421545000	1.868230000
1	0.921398000	-0.628930000	2.674245000
8	-2.232701000	0.669615000	-1.263461000
8	-2.381401000	-1.485680000	-0.354930000
6	-2.097073000	-2.267352000	-1.514221000



1	-2.838007000	-3.069123000	-1.525539000
1	-2.192642000	-1.676290000	-2.432240000
1	-1.094405000	-2.708678000	-1.467878000
6	-3.650377000	0.880051000	-1.321117000
1	-4.193941000	-0.051188000	-1.148673000
1	-3.976309000	1.618001000	-0.583340000
1	-3.854063000	1.249324000	-2.329532000
6	0.228703000	1.956392000	-0.163799000
6	-0.498541000	2.253757000	0.989217000
6	2.333442000	1.725943000	-1.232847000
1	2.050454000	2.462161000	-1.998087000
1	2.094915000	0.724682000	-1.611616000
1	-1.514228000	2.610222000	0.876562000
1	-0.199390000	2.076622000	-1.154124000
8	1.577765000	1.972714000	-0.040254000
6	3.804973000	1.824931000	-0.879519000
1	4.418176000	1.589390000	-1.754458000
1	4.061050000	2.830717000	-0.534972000
1	4.040924000	1.109647000	-0.087606000
35	2.228271000	-1.584560000	0.174459000
1	0.049450000	2.621808000	1.848086000

14c (meta-exo) TS

6	0.599248000	1.130891000	-0.193630000
6	-0.399783000	0.031500000	-0.507419000
6	0.770868000	1.281027000	1.344508000
1	-0.380488000	-0.360301000	-1.517534000
8	1.713909000	1.863028000	1.845526000
6	-1.573940000	0.040562000	0.224533000
6	-0.336561000	0.688726000	2.150374000
1	-0.290692000	0.955283000	3.203179000
6	-1.590394000	0.454073000	1.553941000
1	-2.489229000	0.379523000	2.154057000
8	1.765598000	0.825313000	-0.910198000
8	0.110586000	2.430021000	-0.532767000
6	-0.426996000	2.572784000	-1.846533000
1	-0.552104000	3.645717000	-2.005682000
1	0.255528000	2.172741000	-2.605280000
1	-1.401991000	2.080031000	-1.938950000
6	2.877857000	1.722333000	-0.787527000
1	2.541523000	2.759254000	-0.722292000
1	3.477712000	1.484826000	0.093679000
1	3.473019000	1.583932000	-1.694234000

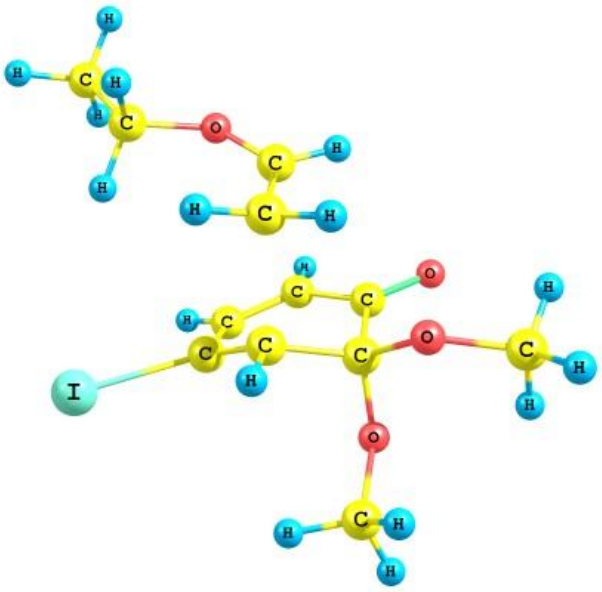


6	0.789844000	-1.696898000	0.874247000
6	0.579337000	-1.184846000	2.164776000
6	2.225292000	-2.236749000	-0.927775000
1	1.685420000	-3.189665000	-1.020922000
1	1.799727000	-1.515711000	-1.632355000
1	0.072863000	-2.362304000	0.402126000
8	2.050233000	-1.727345000	0.403215000
6	3.711229000	-2.424791000	-1.164325000
1	4.136415000	-3.131534000	-0.446179000
1	3.882157000	-2.810563000	-2.173960000
1	4.236577000	-1.471370000	-1.065214000
35	-3.147662000	-0.773377000	-0.521573000
1	-0.229386000	-1.617210000	2.738055000
1	1.472521000	-0.934253000	2.729336000

15c (ortho-endo) TS

6	-2.089906000	-0.214792000	-0.063804000
6	-0.650266000	-0.408889000	-0.588293000
6	-2.092293000	0.866149000	1.062433000
1	-0.601170000	-1.012355000	-1.491827000
8	-3.085185000	1.569837000	1.263200000
6	0.316126000	-0.624648000	0.416229000

6	-0.880286000	0.919186000	1.858057000
1	-0.900974000	1.566030000	2.731076000
6	0.210883000	0.093868000	1.618461000
1	1.026263000	0.073560000	2.337081000
8	-2.882687000	0.092226000	-1.188173000
8	-2.559222000	-1.374377000	0.608639000
6	-2.524707000	-2.603403000	-0.126706000
1	-3.152879000	-3.301406000	0.430999000
1	-2.929934000	-2.480214000	-1.137355000
1	-1.506432000	-3.005808000	-0.181178000
6	-4.306461000	0.224631000	-0.998108000
1	-4.667420000	-0.465153000	-0.231814000
1	-4.564039000	1.245521000	-0.711932000
1	-4.756073000	-0.027838000	-1.962695000
6	-0.311551000	1.336887000	-1.444667000
6	-0.227577000	2.410502000	-0.543207000
6	2.183971000	2.584684000	-0.614904000
1	2.173118000	2.766388000	-1.696679000
1	2.359091000	1.519372000	-0.439857000
1	-1.107284000	2.947894000	-0.205759000
1	0.586160000	1.068412000	-1.994377000

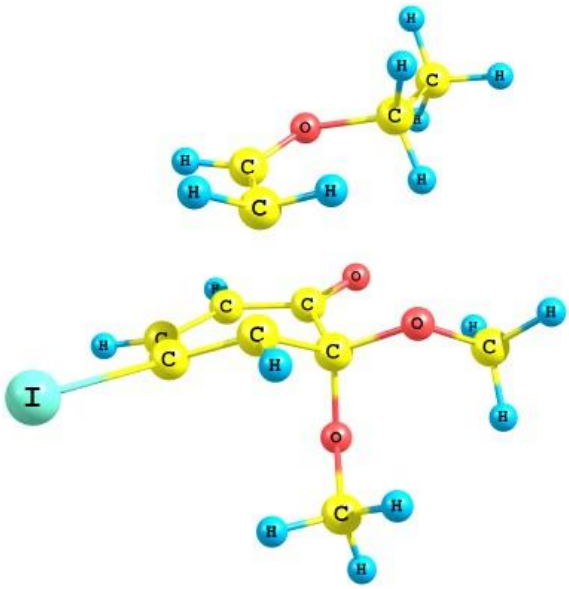


1	-1.224839000	1.320476000	-2.030563000
8	0.894574000	2.966904000	-0.073499000
6	3.235157000	3.435228000	0.076553000
1	4.225547000	3.182580000	-0.315498000
1	3.053797000	4.499774000	-0.097625000
1	3.234589000	3.253611000	1.155050000
53	2.125172000	-1.647245000	-0.055673000

15c (ortho-exo) TS

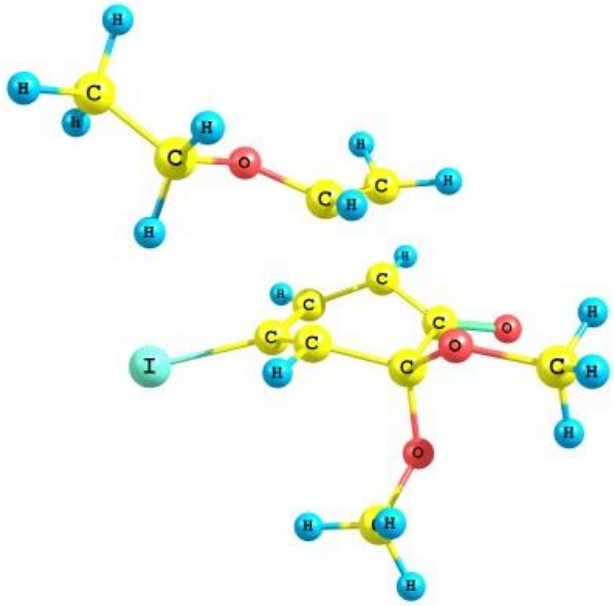
6	0.923637000	1.179987000	0.017792000
6	-0.228520000	0.328663000	-0.549730000
6	1.520495000	0.422844000	1.244271000
1	-0.588704000	0.726685000	-1.498865000
8	2.731522000	0.456303000	1.501433000
6	-1.238338000	0.011667000	0.433811000
6	0.534071000	-0.236755000	2.060268000
1	0.875352000	-0.616264000	3.019920000
6	-0.828456000	-0.304642000	1.714713000
1	-1.539517000	-0.692960000	2.439416000
8	1.835606000	1.376332000	-1.047779000
8	0.471025000	2.407737000	0.558009000
6	-0.392267000	3.189375000	-0.275335000

1	-0.403751000	4.188709000	0.164787000
1	-0.016282000	3.250594000	-1.302713000
1	-1.411024000	2.786371000	-0.276021000
6	2.887582000	2.340379000	-0.825529000
1	2.483983000	3.356538000	-0.796086000
1	3.429087000	2.129030000	0.095797000
1	3.547781000	2.240602000	-1.690370000
6	0.535185000	-1.182439000	-1.086238000
6	1.209007000	-1.908893000	-0.037723000
6	3.446682000	-1.491436000	-0.851906000
1	3.256051000	-1.961450000	-1.824624000
1	3.249237000	-0.422370000	-0.911176000
1	-0.339372000	-1.721216000	-1.455354000
1	1.176711000	-0.874387000	-1.909330000
8	2.511936000	-2.081696000	0.103673000
6	4.844967000	-1.787582000	-0.347064000
1	5.061815000	-2.859405000	-0.377191000
1	5.574045000	-1.270958000	-0.979752000
1	4.957216000	-1.425793000	0.677589000
1	0.653396000	-2.526955000	0.658132000
53	-3.200962000	-0.470626000	-0.225299000



15c (meta-endo) TS

6	-1.983190000	-0.302254000	-0.308683000
6	-0.481749000	-0.086761000	-0.490530000
6	-2.385934000	-0.089818000	1.179500000
1	-0.160985000	-0.153075000	-1.527192000
8	-3.550537000	-0.134671000	1.542069000
6	0.356609000	-0.594495000	0.515155000
6	-1.253923000	0.183118000	2.099531000
1	-1.565936000	0.321950000	3.133702000
6	-0.016856000	-0.457751000	1.845092000
1	0.666066000	-0.680963000	2.658231000
8	-2.612983000	0.610154000	-1.187348000
8	-2.383794000	-1.638817000	-0.551989000
6	-1.971448000	-2.220982000	-1.790739000
1	-2.599365000	-3.103717000	-1.930434000
1	-2.126510000	-1.536262000	-2.632120000
1	-0.921625000	-2.534276000	-1.757360000
6	-4.048523000	0.586587000	-1.248132000
1	-4.431083000	-0.435719000	-1.205781000
1	-4.488784000	1.166981000	-0.432646000
1	-4.310031000	1.040242000	-2.207816000

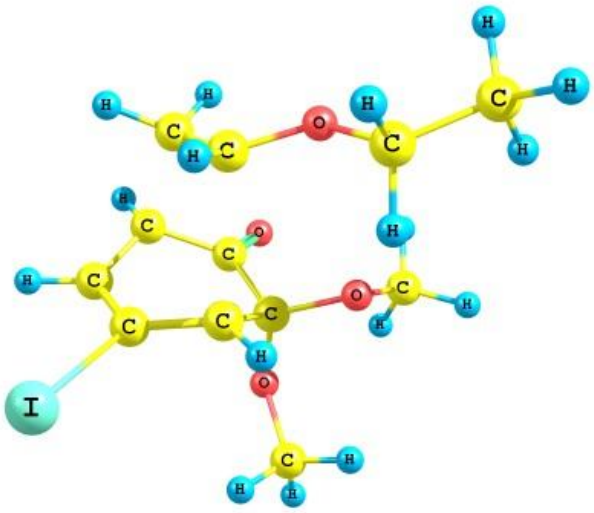


6	-0.343757000	2.073068000	0.047448000
6	-1.068779000	2.088845000	1.265148000
6	1.657365000	2.642072000	-1.095348000
1	1.035451000	3.278974000	-1.738515000
1	1.809866000	1.683792000	-1.607168000
1	-2.119415000	2.357150000	1.186226000
1	-0.850848000	2.315189000	-0.884901000
8	0.970490000	2.411308000	0.143913000
6	2.988243000	3.307054000	-0.791202000
1	3.561069000	3.427244000	-1.716517000
1	2.843710000	4.293663000	-0.341522000
1	3.575119000	2.689393000	-0.105666000
1	-0.555945000	2.533316000	2.113559000
53	2.312556000	-1.309807000	0.038855000

15c (meta-exo) TS

6	-1.095207000	-1.125842000	-0.215862000
6	0.014441000	-0.104074000	-0.413484000
6	-1.363718000	-1.326575000	1.305974000
1	0.097932000	0.305821000	-1.414547000
8	-2.363532000	-1.881682000	1.725451000
6	1.147909000	-0.243581000	0.397985000

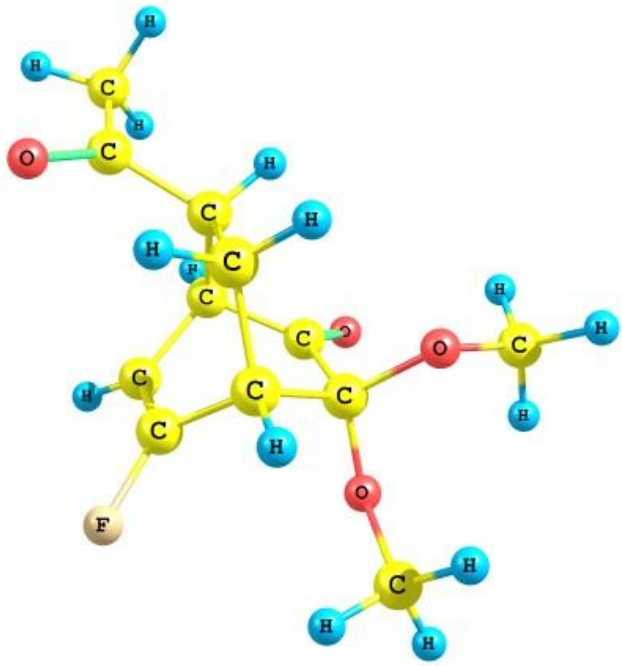
6	-0.326258000	-0.723030000	2.210404000
1	-0.454020000	-1.059905000	3.240000000
6	1.018164000	-0.652825000	1.711872000
1	1.864260000	-0.713124000	2.388115000
8	-2.195630000	-0.660492000	-0.959969000
8	-0.715065000	-2.445310000	-0.611342000
6	-0.196745000	-2.583970000	-1.937924000
1	-0.218702000	-3.653571000	-2.158625000
1	-0.816231000	-2.052923000	-2.669491000
1	0.837660000	-2.226884000	-2.002962000
6	-3.396472000	-1.452590000	-0.948508000
1	-3.171628000	-2.517026000	-0.857307000
1	-4.050338000	-1.149658000	-0.126330000
1	-3.890724000	-1.261034000	-1.905586000
6	-1.026500000	1.661885000	0.916951000
6	-0.963185000	1.052844000	2.213392000
6	-2.304169000	2.498517000	-0.890154000
1	-1.742695000	3.441922000	-0.859233000
1	-1.821599000	1.819789000	-1.600097000
1	-0.231174000	2.323038000	0.573370000
8	-2.254387000	1.886225000	0.412626000



6	-3.761943000	2.738087000	-1.251955000
1	-4.308687000	3.125533000	-0.386946000
1	-3.832568000	3.476615000	-2.056895000
1	-4.244872000	1.815328000	-1.583004000
1	-0.225566000	1.486785000	2.882703000
1	-1.941544000	0.941818000	2.681392000
53	3.054745000	0.420273000	-0.325865000

9c (ortho-endo) P

6	1.492198000	-0.202411000	-0.065235000
6	0.434366000	0.745471000	-0.698654000
6	0.736708000	-1.087082000	0.976689000
1	0.903223000	1.435788000	-1.401849000
8	1.276849000	-1.953958000	1.627172000
6	-0.216225000	1.466940000	0.445866000
6	-0.759711000	-0.757731000	1.046051000
1	-1.218774000	-1.381598000	1.814251000
6	-0.854331000	0.725299000	1.350762000
1	-1.356005000	1.114925000	2.227285000
8	2.017830000	-0.977735000	-1.119944000
8	2.490956000	0.461657000	0.666659000
6	3.233612000	1.456029000	-0.041671000

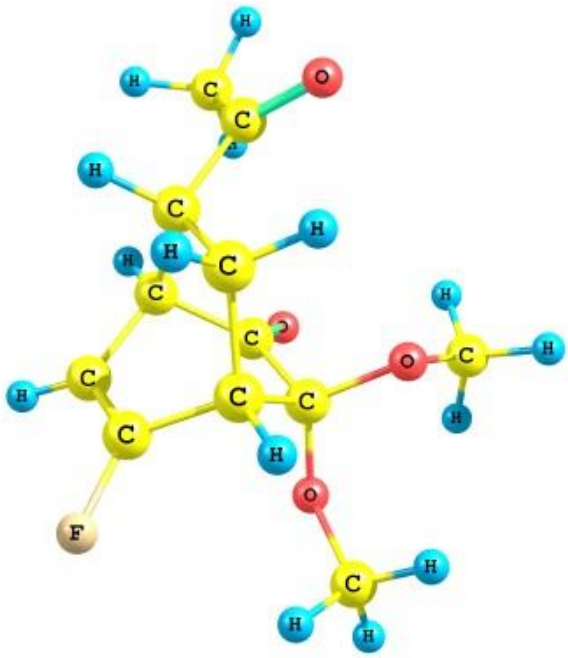


1	4.128664000	1.646710000	0.553389000
1	3.528323000	1.104545000	-1.036116000
1	2.665445000	2.389218000	-0.134543000
6	3.010613000	-1.953812000	-0.777294000
1	3.738252000	-1.545152000	-0.071694000
1	2.558988000	-2.847942000	-0.338124000
1	3.506429000	-2.212740000	-1.715358000
6	-0.659866000	-0.102451000	-1.405203000
6	-1.331013000	-1.062355000	-0.394524000
6	-3.628050000	-2.124072000	0.191257000
1	-3.172368000	-2.512244000	1.107230000
1	-3.614153000	-2.940729000	-0.541424000
1	-1.081688000	-2.106680000	-0.620034000
1	-1.418300000	0.569014000	-1.813575000
1	-0.206193000	-0.662154000	-2.224689000
1	-4.663479000	-1.837136000	0.378495000
6	-2.861320000	-0.943276000	-0.376188000
8	-3.434352000	0.040953000	-0.801281000
9	-0.116044000	2.806873000	0.489974000

9c (ortho-exo) P

6	-0.295677000	1.132195000	0.055156000

6	-1.066238000	-0.003671000	-0.684186000
6	0.512308000	0.448377000	1.205062000
1	-1.680683000	0.411183000	-1.484918000
8	1.284839000	1.046069000	1.923205000
6	-1.893153000	-0.689947000	0.365019000
6	0.262523000	-1.061784000	1.275331000
1	0.793774000	-1.474107000	2.133065000
6	-1.239984000	-1.251718000	1.381273000
1	-1.708817000	-1.749347000	2.220879000
8	0.541351000	1.728696000	-0.901920000
8	-1.130382000	2.062971000	0.701373000
6	-2.085073000	2.730612000	-0.126612000
1	-2.428959000	3.595033000	0.444425000
1	-1.634152000	3.072133000	-1.064154000
1	-2.945139000	2.086397000	-0.345125000
6	1.416125000	2.773269000	-0.454490000
1	0.906436000	3.443181000	0.242556000
1	2.306962000	2.365363000	0.030440000
1	1.705966000	3.320118000	-1.354157000
6	-0.042034000	-1.028348000	-1.246399000
6	0.768016000	-1.661706000	-0.086951000

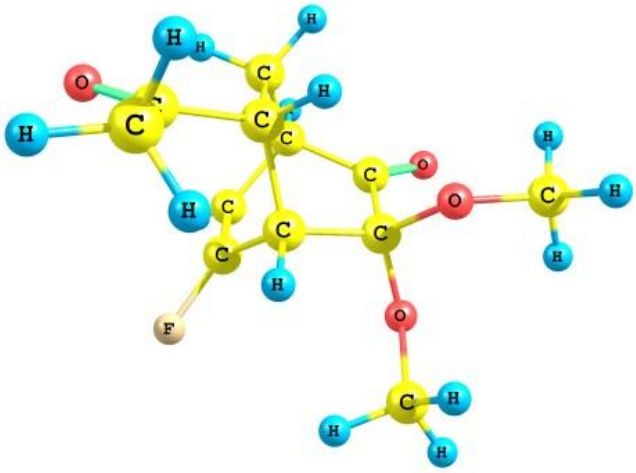


6	3.170434000	-1.919426000	0.901975000
1	4.195616000	-2.056663000	0.556027000
1	2.815529000	-2.828009000	1.399768000
1	0.574955000	-2.741897000	-0.030846000
1	-0.580334000	-1.797028000	-1.806456000
1	0.639512000	-0.527045000	-1.934604000
1	3.151459000	-1.110605000	1.642142000
6	2.292077000	-1.536740000	-0.274982000
8	2.775818000	-1.166326000	-1.326950000
9	-3.231747000	-0.680920000	0.229321000

9c (meta-endo) P

6	1.422742000	0.148075000	-0.184439000
6	-0.108740000	0.322175000	-0.420110000
6	1.594215000	-0.453151000	1.249197000
1	-0.291610000	0.786571000	-1.390439000
8	2.674954000	-0.751279000	1.707526000
6	-0.613364000	1.170818000	0.711413000
6	0.253544000	-0.644071000	1.960529000
1	0.432300000	-1.020506000	2.968680000
6	-0.436264000	0.708808000	1.947222000
1	-0.734624000	1.227999000	2.849163000

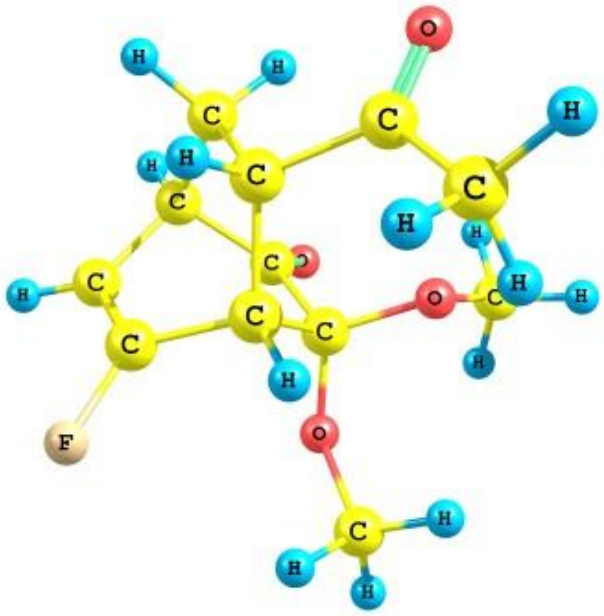
8	1.885947000	-0.723477000	-1.190496000
8	2.128139000	1.362838000	-0.160428000
6	2.009902000	2.187905000	-1.321131000
1	2.824906000	2.911561000	-1.261908000
1	2.111553000	1.603500000	-2.241752000
1	1.056948000	2.730428000	-1.331342000
6	3.276849000	-1.074462000	-1.158210000
1	3.897026000	-0.202612000	-0.936620000
1	3.476368000	-1.847748000	-0.411545000
1	3.509031000	-1.453422000	-2.155935000
6	-0.778584000	-1.096451000	-0.324244000
6	-0.584578000	-1.647037000	1.109716000
6	-2.540258000	-0.956624000	-2.227237000
1	-1.857875000	-0.286880000	-2.759413000
1	-3.573767000	-0.651283000	-2.394619000
1	-1.561591000	-1.770270000	1.582960000
1	-0.259472000	-1.721236000	-1.056590000
1	-2.393716000	-1.958775000	-2.649309000
6	-2.253633000	-1.008081000	-0.736915000
8	-3.153389000	-0.996415000	0.081175000
1	-0.087633000	-2.621748000	1.083527000



9	-1.192353000	2.346233000	0.401814000

9c (meta-exo) P

6	0.201345000	1.042351000	0.004680000
6	-0.585666000	-0.212485000	-0.475028000
6	0.228741000	0.995305000	1.568940000
1	-0.703659000	-0.205844000	-1.559322000
8	0.786854000	1.835305000	2.237969000
6	-1.916663000	-0.151031000	0.223583000
6	-0.499345000	-0.232475000	2.120968000
1	-0.476841000	-0.200261000	3.211132000
6	-1.909834000	-0.165450000	1.555313000
1	-2.793059000	-0.089070000	2.177143000
8	1.487397000	0.940993000	-0.560008000
8	-0.427115000	2.259820000	-0.309472000
6	-0.699030000	2.496743000	-1.691547000
1	-0.918274000	3.562469000	-1.777776000
1	0.165011000	2.254609000	-2.319386000
1	-1.573175000	1.928530000	-2.032086000
6	2.455773000	1.930234000	-0.178027000
1	2.006100000	2.925476000	-0.151507000
1	2.885626000	1.705585000	0.801239000

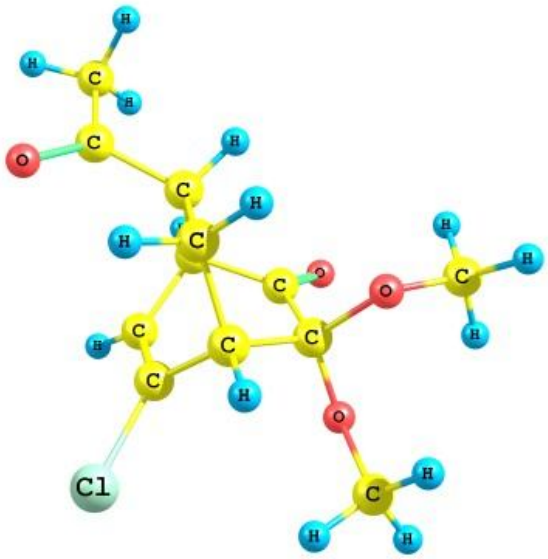


1	3.235509000	1.889910000	-0.941117000
6	0.132047000	-1.514667000	0.019383000
6	0.242646000	-1.481379000	1.563632000
6	1.490262000	-1.802871000	-2.189935000
1	0.581634000	-2.241553000	-2.616165000
1	2.367513000	-2.345177000	-2.545424000
1	-0.196509000	-2.380583000	2.003823000
1	-0.521953000	-2.342996000	-0.286215000
1	1.553784000	-0.764462000	-2.529606000
6	1.473085000	-1.823026000	-0.672240000
8	2.456519000	-2.143599000	-0.034249000
1	1.297648000	-1.462508000	1.849600000
9	-3.022085000	-0.064619000	-0.541288000

10c (ortho-endo) P

6	1.483383000	-0.173511000	-0.049278000
6	0.429043000	0.781594000	-0.681291000
6	0.734245000	-1.043352000	1.006806000
1	0.907651000	1.456581000	-1.391493000
8	1.276876000	-1.891637000	1.678718000
6	-0.236161000	1.513132000	0.459204000
6	-0.765514000	-0.731224000	1.057519000

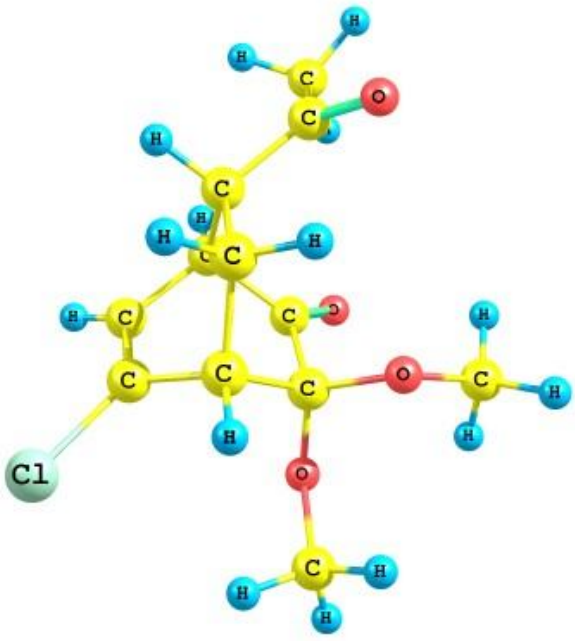
1	-1.228798000	-1.354500000	1.823954000
6	-0.874919000	0.751043000	1.351462000
1	-1.402279000	1.127722000	2.219237000
8	1.976324000	-0.970945000	-1.105823000
8	2.505008000	0.477326000	0.657851000
6	3.291783000	1.411218000	-0.085085000
1	4.189013000	1.589812000	0.510394000
1	3.579327000	1.007087000	-1.061293000
1	2.764875000	2.362547000	-0.223176000
6	2.950646000	-1.966400000	-0.765904000
1	3.687283000	-1.573506000	-0.060859000
1	2.481971000	-2.852012000	-0.326637000
1	3.439179000	-2.235410000	-1.704944000
6	-0.669636000	-0.059583000	-1.389522000
6	-1.318913000	-1.042805000	-0.389118000
6	-3.585678000	-2.187495000	0.155702000
1	-3.123354000	-2.583147000	1.065303000
1	-3.540850000	-2.985432000	-0.596110000
1	-1.036064000	-2.077717000	-0.617514000
1	-1.437123000	0.616102000	-1.773456000
1	-0.224087000	-0.600679000	-2.225673000



1	-4.630830000	-1.938112000	0.342577000
6	-2.852634000	-0.970013000	-0.377296000
8	-3.451563000	0.007910000	-0.779986000
17	-0.178776000	3.258496000	0.530196000

10c (ortho-exo) P

6	-0.314158000	1.120491000	0.066717000
6	-1.085512000	-0.016218000	-0.673567000
6	0.488111000	0.442893000	1.221648000
1	-1.687524000	0.406418000	-1.478436000
8	1.244447000	1.044005000	1.953589000
6	-1.917286000	-0.723183000	0.370094000
6	0.259587000	-1.070486000	1.279659000
1	0.792682000	-1.483922000	2.135870000
6	-1.239515000	-1.276997000	1.378713000
1	-1.689772000	-1.803514000	2.211629000
8	0.536229000	1.699231000	-0.892367000
8	-1.141249000	2.063926000	0.698885000
6	-2.041748000	2.779985000	-0.149685000
1	-2.386556000	3.636528000	0.432425000
1	-1.541255000	3.134807000	-1.056268000
1	-2.908654000	2.168384000	-0.425891000

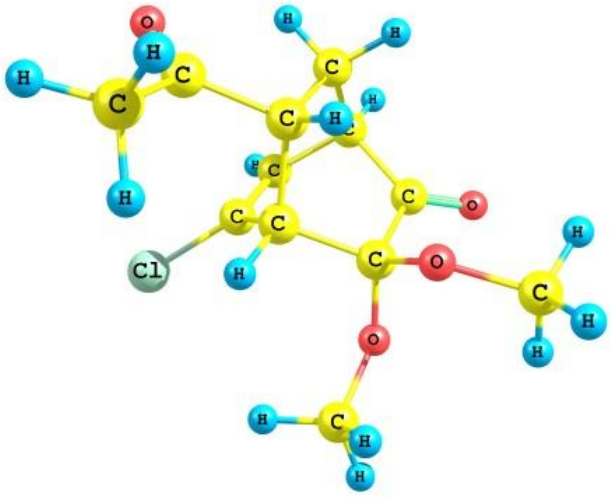


6	1.415951000	2.741506000	-0.449984000
1	0.905879000	3.425775000	0.232737000
1	2.298269000	2.332320000	0.049411000
1	1.720182000	3.273075000	-1.353923000
6	-0.059905000	-1.037093000	-1.239711000
6	0.766657000	-1.659060000	-0.087316000
6	3.178473000	-1.883200000	0.889240000
1	4.204896000	-1.995862000	0.538079000
1	2.843374000	-2.805035000	1.376180000
1	0.594631000	-2.742732000	-0.032861000
1	-0.599664000	-1.811333000	-1.790454000
1	0.611904000	-0.533245000	-1.935355000
1	3.146536000	-1.084413000	1.639696000
6	2.288632000	-1.504779000	-0.280424000
8	2.760692000	-1.115444000	-1.330677000
17	-3.657590000	-0.794963000	0.208187000

10c (meta-endo) P

6	1.418032000	0.166316000	-0.179092000
6	-0.115536000	0.326910000	-0.424960000
6	1.592807000	-0.415267000	1.259672000
1	-0.286115000	0.777186000	-1.403219000

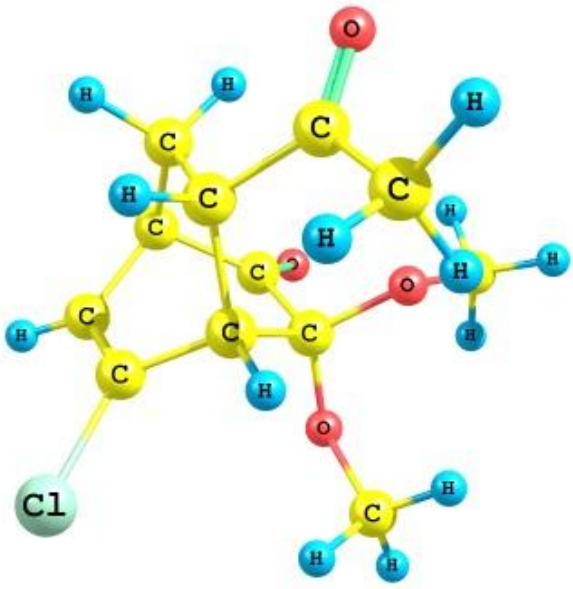
8	2.675200000	-0.678087000	1.734573000
6	-0.651416000	1.171697000	0.705572000
6	0.251339000	-0.645850000	1.955075000
1	0.426735000	-1.021122000	2.964372000
6	-0.471050000	0.687354000	1.936395000
1	-0.792841000	1.181657000	2.844982000
8	1.885287000	-0.726351000	-1.166787000
8	2.120314000	1.380605000	-0.177750000
6	2.059487000	2.152372000	-1.379223000
1	2.865756000	2.884484000	-1.307012000
1	2.214694000	1.528433000	-2.265484000
1	1.106162000	2.686412000	-1.468161000
6	3.276706000	-1.074299000	-1.122396000
1	3.894626000	-0.199002000	-0.908284000
1	3.473383000	-1.837749000	-0.364699000
1	3.514921000	-1.466392000	-2.113585000
6	-0.773878000	-1.097042000	-0.333710000
6	-0.552152000	-1.664197000	1.088327000
6	-2.571305000	-0.898150000	-2.201562000
1	-1.943206000	-0.149482000	-2.693241000
1	-3.624432000	-0.647426000	-2.332961000



1	-1.521176000	-1.837231000	1.562346000
1	-0.260165000	-1.708905000	-1.081174000
1	-2.369607000	-1.856547000	-2.696150000
6	-2.258430000	-1.034747000	-0.722130000
8	-3.145614000	-1.121322000	0.104873000
17	-1.460483000	2.682511000	0.351271000
1	-0.015092000	-2.616702000	1.045836000

10c (meta-exo) P

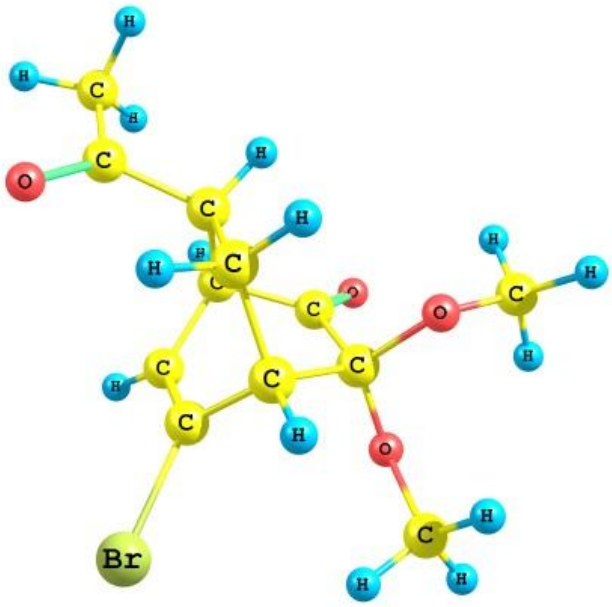
6	0.181264000	1.045921000	0.003535000
6	-0.599739000	-0.216352000	-0.472550000
6	0.208543000	1.010479000	1.565533000
1	-0.702650000	-0.211019000	-1.557631000
8	0.752927000	1.860761000	2.232446000
6	-1.939309000	-0.181035000	0.228358000
6	-0.495321000	-0.226602000	2.124598000
1	-0.469718000	-0.192393000	3.214738000
6	-1.905671000	-0.189616000	1.563139000
1	-2.780855000	-0.146960000	2.200377000
8	1.471633000	0.934158000	-0.552504000
8	-0.440407000	2.261245000	-0.323094000
6	-0.644487000	2.520028000	-1.713110000



1	-0.880517000	3.582931000	-1.788647000
1	0.256252000	2.307346000	-2.298069000
1	-1.487072000	1.943497000	-2.113088000
6	2.443351000	1.919911000	-0.169833000
1	1.999624000	2.918013000	-0.150081000
1	2.866783000	1.697758000	0.812873000
1	3.227122000	1.871007000	-0.928212000
6	0.132200000	-1.511055000	0.022086000
6	0.260459000	-1.467690000	1.563619000
6	1.472591000	-1.800854000	-2.198693000
1	0.558763000	-2.236564000	-2.616567000
1	2.344831000	-2.347299000	-2.560196000
1	-0.157810000	-2.371011000	2.015294000
1	-0.520661000	-2.344472000	-0.272146000
1	1.537833000	-0.763561000	-2.541300000
6	1.467987000	-1.817310000	-0.681078000
8	2.456705000	-2.135199000	-0.049836000
17	-3.411956000	-0.147400000	-0.718033000
1	1.317804000	-1.428666000	1.838363000

7 + MVK (ortho-endo) P

6	1.491853000	-0.197157000	-0.056639000
6	0.440709000	0.760460000	-0.689711000
6	0.736386000	-1.075773000	0.986396000
1	0.922061000	1.428016000	-1.404509000
8	1.268593000	-1.946783000	1.637422000
6	-0.216921000	1.496784000	0.449605000
6	-0.758685000	-0.742506000	1.054413000
1	-1.222826000	-1.361285000	1.823880000
6	-0.854872000	0.741693000	1.346824000
1	-1.376119000	1.121192000	2.216934000
8	1.997516000	-0.978318000	-1.118562000
8	2.503959000	0.448014000	0.669549000
6	3.245166000	1.450531000	-0.030681000
1	4.152921000	1.616760000	0.552493000
1	3.519371000	1.118652000	-1.037768000
1	2.682785000	2.389546000	-0.088141000
6	2.981561000	-1.966599000	-0.786290000
1	3.720709000	-1.568061000	-0.086941000
1	2.523151000	-2.856022000	-0.344168000
1	3.465398000	-2.230745000	-1.729117000
6	-0.663059000	-0.077842000	-1.393823000

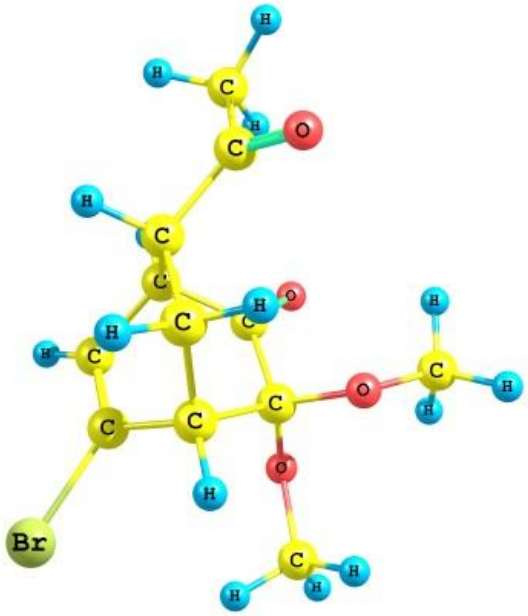


6	-1.324608000	-1.048115000	-0.388928000
6	-3.605308000	-2.150477000	0.185115000
1	-3.145335000	-2.535715000	1.100254000
1	-3.574888000	-2.962760000	-0.551913000
1	-1.059235000	-2.088178000	-0.615496000
1	-1.422760000	0.602360000	-1.785480000
1	-0.219029000	-0.628445000	-2.224653000
1	-4.646129000	-1.882673000	0.370649000
6	-2.857391000	-0.953498000	-0.373172000
8	-3.444545000	0.023717000	-0.794251000
35	-0.133800000	3.393335000	0.519664000

7 + MVK (ortho-exo) P

6	-0.298314000	1.131484000	0.059175000
6	-1.071262000	-0.004282000	-0.681127000
6	0.512654000	0.451013000	1.205427000
1	-1.664608000	0.419331000	-1.491835000
8	1.293824000	1.044306000	1.917391000
6	-1.910176000	-0.700594000	0.361085000
6	0.260349000	-1.058097000	1.281615000
1	0.787627000	-1.470815000	2.141907000
6	-1.241638000	-1.252222000	1.375642000

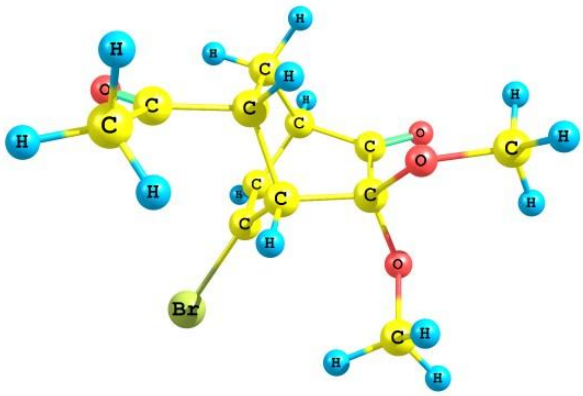
1	-1.697036000	-1.770968000	2.210519000
8	0.536973000	1.721082000	-0.905216000
8	-1.121885000	2.066249000	0.708445000
6	-2.082955000	2.736534000	-0.111381000
1	-2.405400000	3.612014000	0.455477000
1	-1.643750000	3.061927000	-1.060117000
1	-2.952852000	2.097899000	-0.303468000
6	1.415653000	2.766076000	-0.466583000
1	0.912699000	3.434857000	0.236298000
1	2.311928000	2.357692000	0.008041000
1	1.695433000	3.313844000	-1.368876000
6	-0.050057000	-1.034110000	-1.239251000
6	0.764938000	-1.660640000	-0.081077000
6	3.170129000	-1.913331000	0.904906000
1	4.195245000	-2.045126000	0.556645000
1	2.818380000	-2.826442000	1.396556000
1	0.578968000	-2.741706000	-0.021315000
1	-0.594390000	-1.805152000	-1.789986000
1	0.628828000	-0.537924000	-1.933835000
1	3.150428000	-1.109870000	1.650845000
6	2.289259000	-1.525007000	-0.268584000



8	2.769616000	-1.142382000	-1.317363000
35	-3.801616000	-0.758563000	0.176478000

7 + MVK (meta-endo) P

6	1.432630000	0.144921000	-0.184947000
6	-0.098601000	0.313664000	-0.434279000
6	1.599641000	-0.446444000	1.249915000
1	-0.263308000	0.749062000	-1.419640000
8	2.674933000	-0.752681000	1.715064000
6	-0.631887000	1.173978000	0.682035000
6	0.257551000	-0.630515000	1.958158000
1	0.429999000	-0.993364000	2.972523000
6	-0.452387000	0.709861000	1.919600000
1	-0.778313000	1.213268000	2.821629000
8	1.895665000	-0.734337000	-1.185264000
8	2.141920000	1.355363000	-0.162728000
6	2.016994000	2.189767000	-1.317360000
1	2.840693000	2.904036000	-1.263324000
1	2.101902000	1.611071000	-2.243383000
1	1.069245000	2.740359000	-1.306254000
6	3.287086000	-1.082768000	-1.152870000
1	3.906014000	-0.208192000	-0.938803000

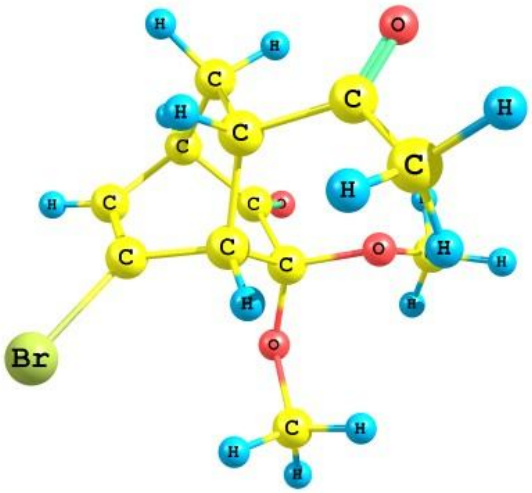


1	3.489055000	-1.850765000	-0.401343000
1	3.518195000	-1.468220000	-2.148338000
6	-0.771739000	-1.102325000	-0.324257000
6	-0.567308000	-1.648260000	1.108746000
6	-2.554680000	-0.915698000	-2.206483000
1	-1.875634000	-0.234101000	-2.726671000
1	-3.588458000	-0.599960000	-2.351368000
1	-1.541512000	-1.789143000	1.582829000
1	-0.261038000	-1.731727000	-1.059308000
1	-2.421418000	-1.905922000	-2.660154000
6	-2.252712000	-1.018477000	-0.722099000
8	-3.145459000	-1.064286000	0.101930000
1	-0.051962000	-2.613286000	1.086279000
35	-1.531074000	2.794521000	0.258969000

7 + MVK (meta-exo) P

6	0.200794000	1.048680000	0.007164000
6	-0.583856000	-0.207403000	-0.477626000
6	0.229981000	1.000991000	1.568644000
1	-0.673839000	-0.200444000	-1.563496000
8	0.794110000	1.832823000	2.242344000
6	-1.927005000	-0.161452000	0.211250000

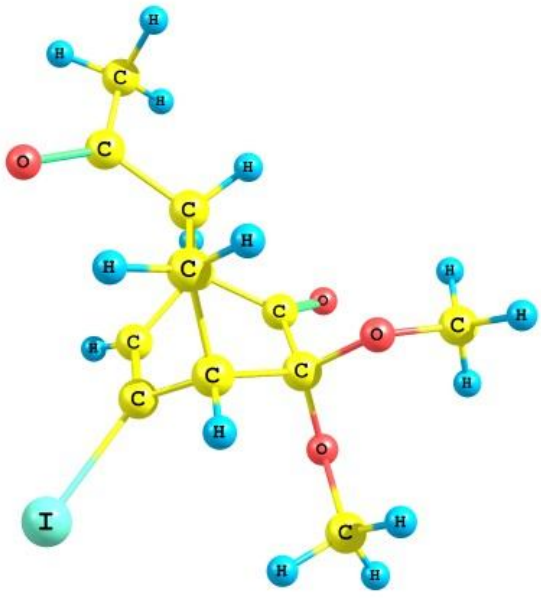
6	-0.501141000	-0.224479000	2.120466000
1	-0.485059000	-0.192003000	3.210907000
6	-1.906522000	-0.170866000	1.545322000
1	-2.785653000	-0.120493000	2.176423000
8	1.487498000	0.939951000	-0.557590000
8	-0.419445000	2.268798000	-0.303360000
6	-0.702351000	2.507637000	-1.683961000
1	-0.887152000	3.579785000	-1.772653000
1	0.145438000	2.235181000	-2.321479000
1	-1.600192000	1.966103000	-2.004223000
6	2.458278000	1.929592000	-0.182919000
1	2.011531000	2.926369000	-0.166743000
1	2.885915000	1.713154000	0.799219000
1	3.239265000	1.879673000	-0.944119000
6	0.131216000	-1.509940000	0.020614000
6	0.243418000	-1.474169000	1.563298000
6	1.486485000	-1.808524000	-2.188824000
1	0.572877000	-2.238507000	-2.612954000
1	2.358076000	-2.360155000	-2.543875000
1	-0.191918000	-2.373336000	2.007091000
1	-0.528307000	-2.334226000	-0.283943000



1	1.560187000	-0.771438000	-2.530461000
6	1.470793000	-1.824012000	-0.671316000
8	2.453699000	-2.144244000	-0.032334000
1	1.298120000	-1.449905000	1.849853000
35	-3.513341000	-0.104147000	-0.837681000

11c (ortho-endo) P

6	1.475225000	-0.160884000	-0.030886000
6	0.430316000	0.807649000	-0.663130000
6	0.719367000	-1.011534000	1.037347000
1	0.920281000	1.463227000	-1.383553000
8	1.255869000	-1.853621000	1.728446000
6	-0.233067000	1.554993000	0.473699000
6	-0.777246000	-0.696148000	1.075574000
1	-1.249313000	-1.309771000	1.844753000
6	-0.880310000	0.789959000	1.362089000
1	-1.422495000	1.160098000	2.225543000
8	1.940803000	-0.980603000	-1.090589000
8	2.518620000	0.478114000	0.658914000
6	3.332699000	1.379010000	-0.104411000
1	4.223026000	1.559277000	0.501428000
1	3.627163000	0.941041000	-1.063938000

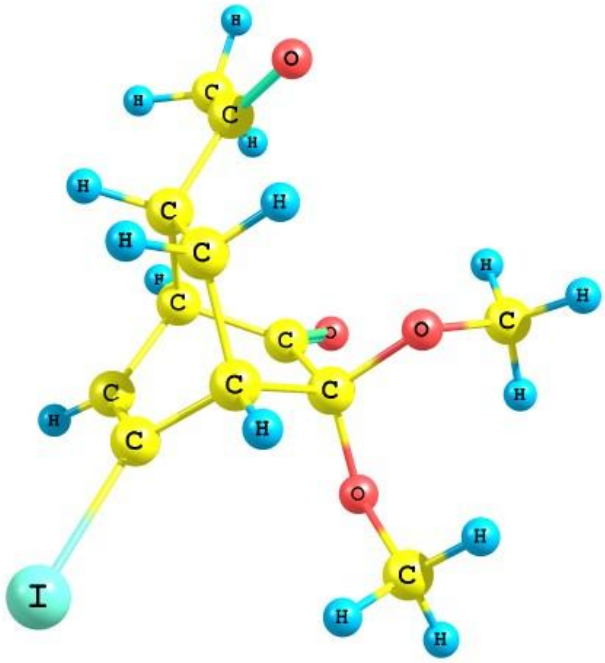


1	2.821110000	2.333464000	-0.274321000
6	2.921939000	-1.981616000	-0.762116000
1	3.693506000	-1.579985000	-0.100176000
1	2.458555000	-2.848719000	-0.282123000
1	3.365012000	-2.278802000	-1.715425000
6	-0.685549000	-0.015916000	-1.367728000
6	-1.320884000	-1.012429000	-0.372419000
6	-3.550424000	-2.251713000	0.108871000
1	-3.048624000	-2.706933000	0.968707000
1	-3.517318000	-2.987210000	-0.705080000
1	-1.013538000	-2.039150000	-0.604915000
1	-1.450163000	0.674868000	-1.730440000
1	-0.260726000	-0.545686000	-2.222244000
1	-4.594344000	-2.042263000	0.348464000
6	-2.855277000	-0.983672000	-0.355915000
8	-3.486859000	0.000722000	-0.702316000
53	-0.199184000	3.673228000	0.560192000

11c (ortho-exo) P

6	-0.329554000	1.136011000	0.073459000
6	-1.087970000	-0.014238000	-0.662947000
6	0.478722000	0.470849000	1.232012000

1	-1.683766000	0.402261000	-1.475632000
8	1.209113000	1.087383000	1.982275000
6	-1.914461000	-0.737963000	0.380201000
6	0.281722000	-1.045210000	1.287225000
1	0.819328000	-1.449541000	2.145374000
6	-1.217330000	-1.274095000	1.389705000
1	-1.645424000	-1.814679000	2.227577000
8	0.519206000	1.717833000	-0.891386000
8	-1.168773000	2.078117000	0.698889000
6	-2.053816000	2.809175000	-0.161139000
1	-2.428870000	3.640843000	0.438671000
1	-1.529309000	3.199176000	-1.039397000
1	-2.901739000	2.192304000	-0.481029000
6	1.388377000	2.781848000	-0.461007000
1	0.871386000	3.470359000	0.212535000
1	2.275865000	2.386320000	0.040640000
1	1.684474000	3.301846000	-1.374799000
6	-0.051905000	-1.025793000	-1.228675000
6	0.776524000	-1.645991000	-0.076726000
6	3.185975000	-1.963333000	0.883287000
1	4.199797000	-2.136730000	0.518147000

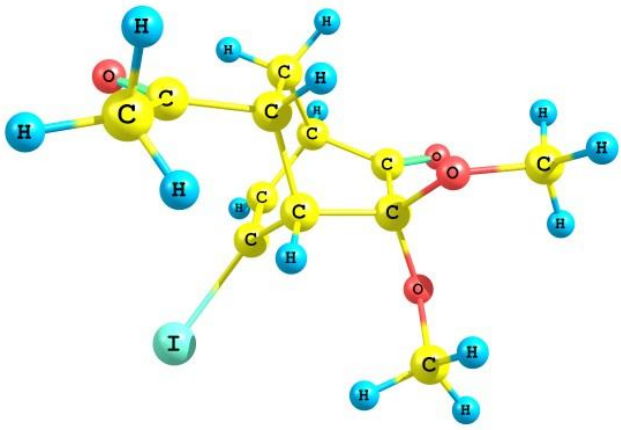


1	2.806273000	-2.864381000	1.377169000
1	0.584944000	-2.725733000	-0.011598000
1	-0.586920000	-1.803695000	-1.779855000
1	0.610767000	-0.516236000	-1.928949000
1	3.216396000	-1.165826000	1.635076000
6	2.300737000	-1.534150000	-0.274482000
8	2.783921000	-1.149382000	-1.326348000
53	-4.019902000	-0.916721000	0.188464000

11c (meta-endo) P

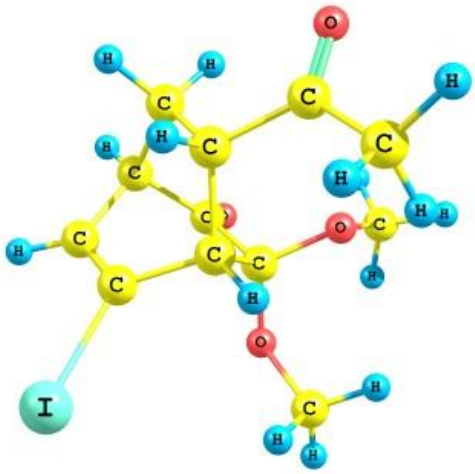
6	1.413755000	0.179226000	-0.169024000
6	-0.123412000	0.338147000	-0.412640000
6	1.590500000	-0.399296000	1.271793000
1	-0.287091000	0.782963000	-1.394248000
8	2.676252000	-0.645105000	1.757562000
6	-0.669505000	1.178088000	0.722473000
6	0.251894000	-0.651989000	1.959800000
1	0.425887000	-1.031438000	2.968071000
6	-0.481829000	0.676845000	1.949184000
1	-0.806030000	1.150420000	2.869909000
8	1.877548000	-0.723808000	-1.156241000
8	2.117918000	1.395193000	-0.177336000

6	2.079776000	2.152377000	-1.394767000
1	2.878929000	2.891307000	-1.308640000
1	2.261971000	1.518784000	-2.269118000
1	1.124401000	2.677745000	-1.509385000
6	3.276163000	-1.069259000	-1.127912000
1	3.898822000	-0.188264000	-0.952863000
1	3.483554000	-1.811891000	-0.352472000
1	3.491399000	-1.490304000	-2.112746000
6	-0.779151000	-1.087812000	-0.328249000
6	-0.544450000	-1.668301000	1.085521000
6	-2.570282000	-0.888257000	-2.204057000
1	-1.870920000	-0.224521000	-2.720309000
1	-3.593918000	-0.534610000	-2.338579000
1	-1.504534000	-1.863281000	1.568853000
1	-0.269014000	-1.692968000	-1.083600000
1	-2.480178000	-1.876892000	-2.672174000
6	-2.262224000	-1.034286000	-0.722875000
8	-3.158270000	-1.148353000	0.097622000
1	0.005475000	-2.612990000	1.028686000
53	-1.681237000	3.003597000	0.340593000



11c (meta-exo) P

6	0.166467000	1.056886000	0.016748000
6	-0.605334000	-0.212693000	-0.461575000
6	0.179928000	1.027651000	1.579770000
1	-0.695383000	-0.205160000	-1.547381000
8	0.694451000	1.896101000	2.253643000
6	-1.950890000	-0.200831000	0.238881000
6	-0.490992000	-0.225800000	2.136067000
1	-0.466263000	-0.196370000	3.226663000
6	-1.904505000	-0.213216000	1.576899000
1	-2.772176000	-0.191871000	2.228229000
8	1.467554000	0.937305000	-0.523756000
8	-0.454661000	2.270205000	-0.328708000
6	-0.606859000	2.539813000	-1.728327000
1	-0.881798000	3.594071000	-1.797358000
1	0.326826000	2.370728000	-2.274852000
1	-1.409000000	1.936801000	-2.170301000
6	2.439646000	1.935514000	-0.153456000
1	2.004072000	2.937619000	-0.180984000
1	2.839104000	1.742750000	0.845588000
1	3.238828000	1.850980000	-0.892944000
6	0.133153000	-1.504525000	0.030193000

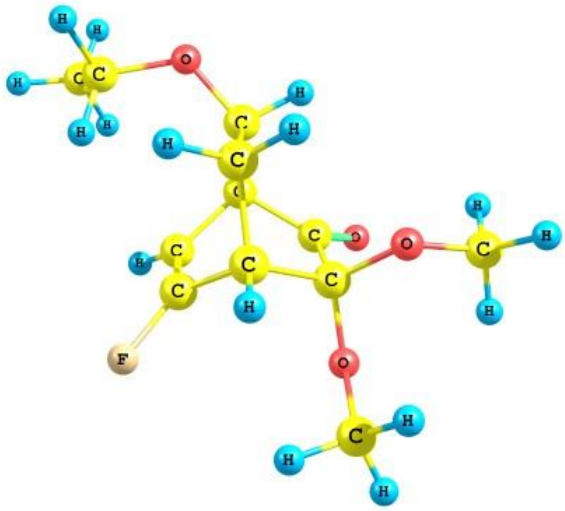


6	0.284872000	-1.450679000	1.568882000
6	1.421885000	-1.816597000	-2.220306000
1	0.482817000	-2.216077000	-2.618720000
1	2.263673000	-2.397764000	-2.601505000
1	-0.104808000	-2.361426000	2.031681000
1	-0.530372000	-2.336689000	-0.242439000
1	1.521070000	-0.783621000	-2.568907000
6	1.447195000	-1.833329000	-0.701480000
8	2.446008000	-2.176873000	-0.090898000
1	1.342926000	-1.384138000	1.834789000
53	-3.756743000	-0.215546000	-0.877168000

5 + EVE (ortho-endo) P

6	-0.214275000	1.020465000	-0.989136000
6	-0.587585000	0.181365000	0.266783000
6	1.336837000	1.216787000	-0.960348000
1	-1.669965000	0.075193000	0.354450000
8	1.935421000	1.850243000	-1.800682000
6	0.003496000	0.913807000	1.437939000
6	1.990990000	0.481194000	0.216089000
1	3.069919000	0.634911000	0.184572000
6	1.328641000	1.062156000	1.455129000

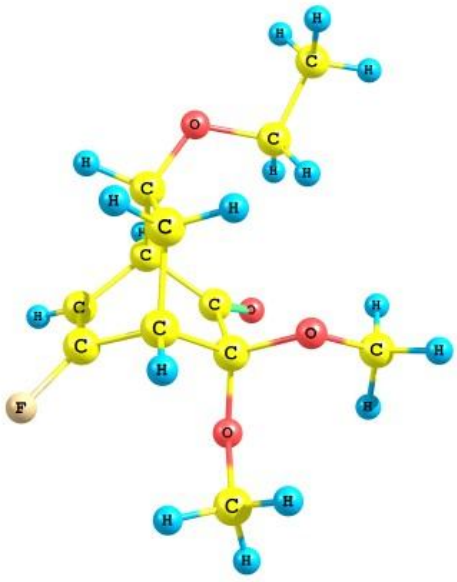
1	1.878667000	1.591339000	2.223409000
8	-0.610548000	0.258072000	-2.108736000
8	-0.759686000	2.314698000	-0.992676000
6	-2.181368000	2.400230000	-0.883665000
1	-2.448920000	3.411672000	-1.195191000
1	-2.679311000	1.676560000	-1.537681000
1	-2.513493000	2.249912000	0.150708000
6	-0.342636000	0.816191000	-3.402332000
1	-0.610022000	1.875291000	-3.438424000
1	0.711492000	0.710498000	-3.674026000
1	-0.963000000	0.251266000	-4.101320000
6	0.102924000	-1.208831000	0.189393000
6	1.636391000	-1.035869000	0.011310000
6	2.396012000	-1.925594000	2.181314000
1	2.255033000	-2.964536000	2.505387000
1	1.545595000	-1.346240000	2.554907000
1	1.900770000	-1.278327000	-1.023158000
1	-0.108941000	-1.759052000	1.110147000
1	-0.311981000	-1.780894000	-0.641751000
8	2.428756000	-1.946907000	0.750856000
6	3.701729000	-1.382690000	2.751669000



1	3.707786000	-1.473070000	3.843574000
1	4.551640000	-1.945114000	2.354733000
1	3.843477000	-0.328230000	2.496726000
9	-0.831367000	1.375900000	2.387544000

5 + EVE (ortho-exo) P

6	0.424726000	0.803062000	-1.194802000
6	0.187732000	-0.094666000	0.055202000
6	1.965193000	1.058418000	-1.276209000
1	-0.877895000	-0.280832000	0.198407000
8	2.470323000	1.718352000	-2.158409000
6	0.786952000	0.674912000	1.202830000
6	2.735064000	0.401271000	-0.124760000
1	3.795857000	0.642241000	-0.206042000
6	2.086541000	0.962921000	1.134174000
1	2.629908000	1.549481000	1.864253000
8	-0.047087000	0.080818000	-2.312265000
8	-0.160320000	2.077202000	-1.097427000
6	-1.567638000	2.107866000	-0.850256000
1	-1.894080000	3.121850000	-1.088638000
1	-2.103905000	1.395997000	-1.486757000
1	-1.792896000	1.902132000	0.202802000

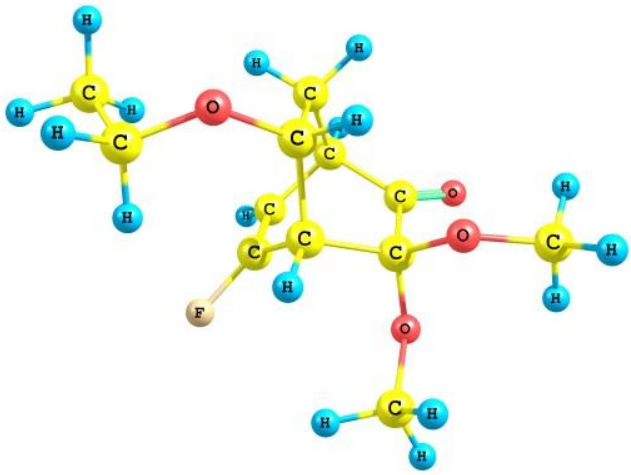


6	0.069184000	0.719388000	-3.591810000
1	-0.215718000	1.772441000	-3.533239000
1	1.089042000	0.651844000	-3.980512000
1	-0.615771000	0.183492000	-4.252497000
6	0.971990000	-1.420895000	-0.117889000
6	2.505685000	-1.150596000	-0.081754000
6	3.127356000	-1.640975000	-2.398426000
1	2.070322000	-1.552002000	-2.685238000
1	3.617446000	-0.690054000	-2.646435000
1	0.694942000	-2.119796000	0.675410000
1	0.689831000	-1.876610000	-1.068170000
6	3.784580000	-2.787274000	-3.149907000
1	4.833850000	-2.884474000	-2.856743000
1	3.279569000	-3.732299000	-2.930244000
1	3.741272000	-2.609945000	-4.229126000
8	3.259618000	-1.915245000	-1.002730000
1	2.898751000	-1.472016000	0.886628000
9	-0.030823000	1.067904000	2.197132000

5 + EVE (meta-endo) P

6	-0.202228000	1.009959000	-1.040474000
6	-0.371333000	0.168833000	0.265321000

6	1.323101000	1.339835000	-1.171874000
1	-1.420750000	-0.078643000	0.432535000
8	1.785826000	1.936255000	-2.118661000
6	0.206102000	1.020606000	1.358601000
6	2.138080000	0.798508000	0.007565000
1	3.179303000	1.103085000	-0.107577000
6	1.488864000	1.365725000	1.259412000
1	2.009744000	2.011532000	1.955351000
8	-0.669152000	0.212824000	-2.102721000
8	-0.841341000	2.261190000	-0.988423000
6	-2.246009000	2.240359000	-0.724504000
1	-2.620462000	3.227034000	-1.003357000
1	-2.755838000	1.477170000	-1.321637000
1	-2.450151000	2.072372000	0.339539000
6	-0.577727000	0.764600000	-3.424117000
1	-0.865770000	1.818487000	-3.431324000
1	0.434948000	0.672989000	-3.825895000
1	-1.272375000	0.183462000	-4.034497000
6	0.471553000	-1.136999000	0.094797000
6	1.979135000	-0.751096000	0.012997000
6	0.014262000	-1.943086000	2.410186000

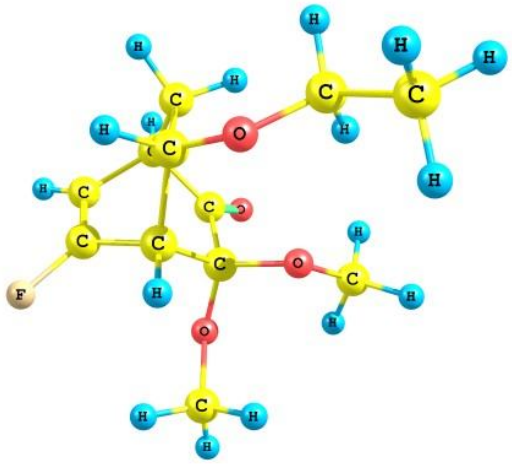


1	-0.615868000	-2.772750000	2.749161000
1	-0.548965000	-1.022330000	2.601953000
1	2.427724000	-1.178344000	-0.889542000
1	0.168661000	-1.560780000	-0.863474000
8	0.168288000	-2.180535000	1.010355000
6	1.314690000	-1.949182000	3.213921000
1	1.083066000	-1.977124000	4.284567000
1	1.908389000	-2.835421000	2.970264000
1	1.920925000	-1.058537000	3.030060000
1	2.518500000	-1.161817000	0.867703000
9	-0.613121000	1.408966000	2.358888000

5 + EVE (meta-exo) P

6	-0.285463000	1.615078000	-1.062539000
6	-0.742412000	0.553900000	-0.021951000
6	1.222556000	1.912587000	-0.776850000
1	-1.801016000	0.317410000	-0.133498000
8	1.877233000	2.692484000	-1.432303000
6	-0.420910000	1.160934000	1.316123000
6	1.761733000	1.078476000	0.390326000
1	2.806483000	1.340508000	0.563249000
6	0.862441000	1.414587000	1.571844000

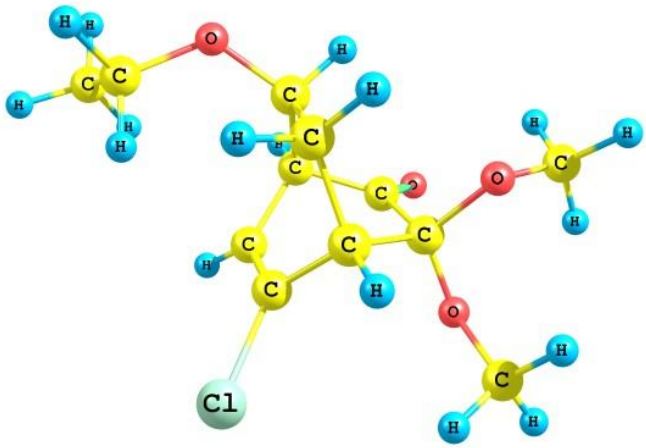
1	1.231304000	1.874321000	2.480256000
8	-0.477404000	1.068424000	-2.347434000
8	-0.937703000	2.853969000	-0.911537000
6	-2.365181000	2.828634000	-0.982984000
1	-2.677354000	3.859582000	-1.160594000
1	-2.715824000	2.197395000	-1.806146000
1	-2.806389000	2.483032000	-0.040880000
6	-0.116532000	1.897881000	-3.462258000
1	-0.437499000	2.929958000	-3.304774000
1	0.963266000	1.888113000	-3.635350000
1	-0.634175000	1.473098000	-4.325079000
6	0.092964000	-0.776880000	-0.076105000
6	1.603479000	-0.414683000	-0.022654000
6	0.423381000	-1.894650000	-2.267310000
1	0.700868000	-0.953281000	-2.752058000
1	1.345134000	-2.444409000	-2.020315000
8	-0.348419000	-1.660665000	-1.093379000
6	-0.441175000	-2.725866000	-3.201513000
1	-0.746018000	-3.657915000	-2.716925000
1	-1.342431000	-2.171252000	-3.476952000
1	0.111719000	-2.972334000	-4.113652000



1	2.127263000	-1.053468000	0.693588000
1	-0.161185000	-1.295675000	0.854848000
1	2.082715000	-0.563402000	-0.993194000
9	-1.433537000	1.403260000	2.168967000

13c (ortho-endo) P

6	-0.220796000	1.038784000	-0.968670000
6	-0.595125000	0.202547000	0.290565000
6	1.326170000	1.245433000	-0.939547000
1	-1.677415000	0.092845000	0.364139000
8	1.923522000	1.890642000	-1.771306000
6	-0.000107000	0.925617000	1.476294000
6	1.985091000	0.495371000	0.223775000
1	3.064664000	0.644743000	0.189980000
6	1.329888000	1.061557000	1.469795000
1	1.899690000	1.562925000	2.243121000
8	-0.597758000	0.256150000	-2.083720000
8	-0.779947000	2.324239000	-0.993652000
6	-2.206455000	2.392986000	-0.952219000
1	-2.468739000	3.404939000	-1.266309000
1	-2.663111000	1.670784000	-1.636901000
1	-2.589015000	2.227921000	0.061980000

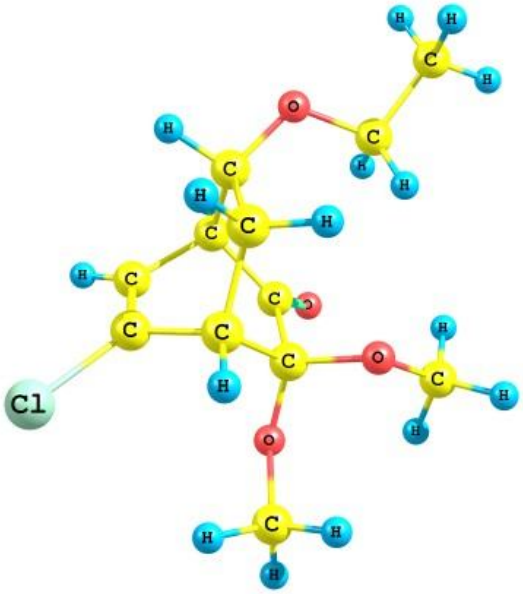


6	-0.326601000	0.803242000	-3.381425000
1	-0.608986000	1.857797000	-3.433150000
1	0.731480000	0.710255000	-3.642659000
1	-0.931896000	0.220614000	-4.079017000
6	0.091778000	-1.189849000	0.214133000
6	1.621186000	-1.021053000	0.013750000
6	2.404110000	-1.921745000	2.169136000
1	2.236391000	-2.957850000	2.489544000
1	1.573339000	-1.321534000	2.554010000
1	1.870425000	-1.256939000	-1.025781000
1	-0.110303000	-1.730989000	1.142490000
1	-0.335471000	-1.766959000	-0.607197000
8	2.425546000	-1.932572000	0.737891000
6	3.730134000	-1.418078000	2.728143000
1	3.745051000	-1.512994000	3.819460000
1	4.559983000	-2.001927000	2.319958000
1	3.898880000	-0.366853000	2.475364000
17	-1.036629000	1.493954000	2.766786000

13c (ortho-exo) P

6	0.429033000	0.809868000	-1.172680000
6	0.194528000	-0.085927000	0.080915000

6	1.966228000	1.070081000	-1.260378000
1	-0.871635000	-0.274108000	0.212658000
8	2.468223000	1.738680000	-2.137410000
6	0.803773000	0.672374000	1.242452000
6	2.743389000	0.401268000	-0.122100000
1	3.804548000	0.639684000	-0.207944000
6	2.106981000	0.950126000	1.145334000
1	2.675356000	1.509887000	1.878264000
8	-0.032612000	0.073331000	-2.287333000
8	-0.164266000	2.078656000	-1.089110000
6	-1.583640000	2.102746000	-0.921889000
1	-1.896623000	3.121210000	-1.159104000
1	-2.080578000	1.402964000	-1.601804000
1	-1.872239000	1.876457000	0.111039000
6	0.086508000	0.703124000	-3.571245000
1	-0.189666000	1.758699000	-3.519056000
1	1.105364000	0.625820000	-3.961518000
1	-0.602586000	0.167899000	-4.228176000
6	0.973769000	-1.415606000	-0.094239000
6	2.508211000	-1.152094000	-0.079255000
6	3.101148000	-1.631813000	-2.404662000

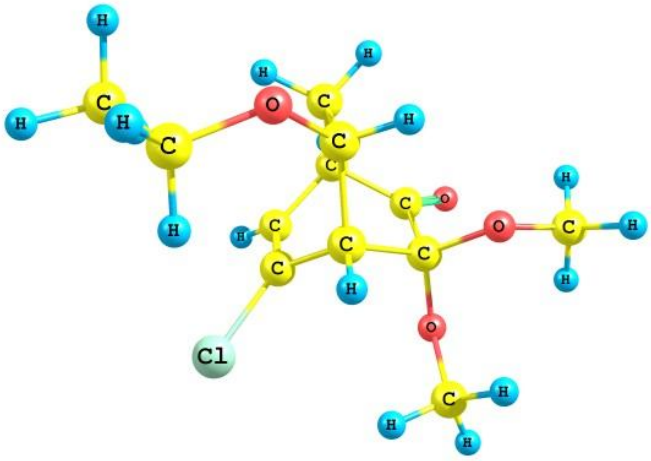


1	2.040340000	-1.550695000	-2.678313000
1	3.580165000	-0.674905000	-2.651568000
1	0.703154000	-2.106774000	0.707894000
1	0.678840000	-1.876781000	-1.037969000
6	3.761922000	-2.767122000	-3.169322000
1	4.815041000	-2.855369000	-2.887447000
1	3.268662000	-3.718542000	-2.950635000
1	3.705818000	-2.583607000	-4.246882000
8	3.251009000	-1.912100000	-1.011847000
1	2.914345000	-1.477537000	0.882383000
17	-0.197067000	1.151239000	2.595300000

13c (meta-endo) P

6	-0.205531000	1.022159000	-1.011882000
6	-0.363089000	0.187193000	0.304769000
6	1.318662000	1.340804000	-1.165927000
1	-1.411223000	-0.062402000	0.473415000
8	1.773544000	1.934263000	-2.117974000
6	0.233019000	1.049326000	1.393675000
6	2.150415000	0.794161000	0.000096000
1	3.191744000	1.092392000	-0.130878000
6	1.520585000	1.375887000	1.251540000

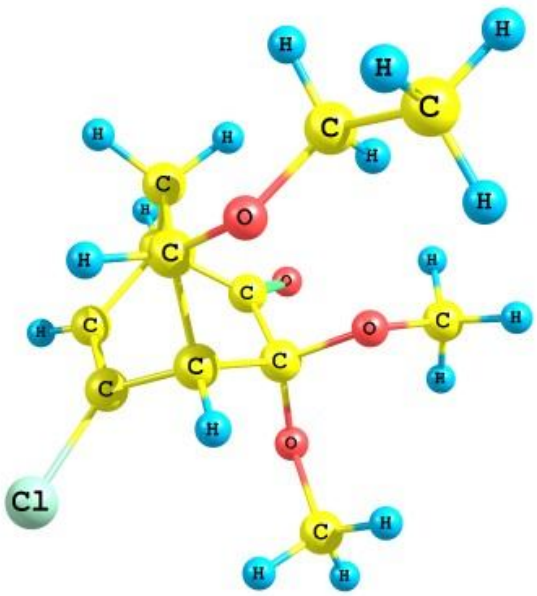
1	2.066106000	2.028776000	1.922541000
8	-0.681162000	0.215503000	-2.064735000
8	-0.841160000	2.273013000	-0.968209000
6	-2.258684000	2.254318000	-0.781362000
1	-2.607742000	3.256025000	-1.038376000
1	-2.740012000	1.521693000	-1.436909000
1	-2.525325000	2.043855000	0.260621000
6	-0.594569000	0.753289000	-3.392346000
1	-0.864836000	1.811748000	-3.407626000
1	0.412555000	0.640991000	-3.802954000
1	-1.304426000	0.177352000	-3.989986000
6	0.472606000	-1.124549000	0.111209000
6	1.981371000	-0.752868000	0.028216000
6	0.009544000	-2.008131000	2.396383000
1	-0.565301000	-2.885852000	2.711268000
1	-0.612620000	-1.130980000	2.609143000
1	2.429494000	-1.194728000	-0.867230000
1	0.161792000	-1.517572000	-0.857516000
8	0.170172000	-2.196227000	0.991091000
6	1.306359000	-1.950721000	3.203526000
1	1.074528000	-2.024839000	4.271824000



1	1.958742000	-2.788203000	2.937811000
1	1.851782000	-1.016352000	3.049109000
1	2.517894000	-1.153392000	0.889429000
17	-0.769352000	1.638155000	2.707562000

13c (meta-exo) P

6	-0.289290000	1.635834000	-1.036865000
6	-0.738738000	0.564603000	-0.000524000
6	1.211624000	1.953942000	-0.748655000
1	-1.794423000	0.323371000	-0.122214000
8	1.850280000	2.768373000	-1.376711000
6	-0.406690000	1.145680000	1.355281000
6	1.772424000	1.087349000	0.382851000
1	2.818862000	1.347014000	0.549820000
6	0.887315000	1.391827000	1.580872000
1	1.282604000	1.817012000	2.495668000
8	-0.452541000	1.077409000	-2.322589000
8	-0.964159000	2.861526000	-0.900760000
6	-2.384900000	2.819873000	-1.053428000
1	-2.700150000	3.852032000	-1.217608000
1	-2.678547000	2.209102000	-1.913255000
1	-2.876678000	2.440035000	-0.150444000

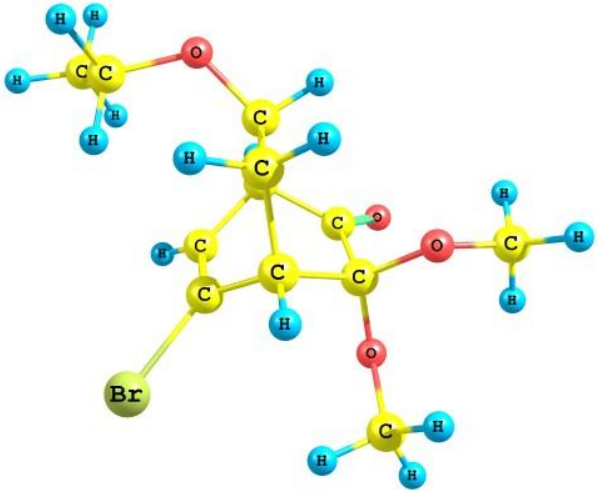


6	-0.087737000	1.907519000	-3.435717000
1	-0.437769000	2.932618000	-3.294905000
1	0.995716000	1.924805000	-3.584476000
1	-0.574295000	1.462618000	-4.306335000
6	0.097854000	-0.763468000	-0.080822000
6	1.606637000	-0.397066000	-0.060774000
6	0.400991000	-1.902017000	-2.265526000
1	0.688070000	-0.974099000	-2.770967000
1	1.317643000	-2.454385000	-2.005800000
8	-0.369546000	-1.633876000	-1.098745000
6	-0.470658000	-2.745118000	-3.182451000
1	-0.780416000	-3.666382000	-2.680751000
1	-1.369074000	-2.190034000	-3.466063000
1	0.078706000	-3.011090000	-4.091227000
1	2.153603000	-1.049726000	0.624825000
1	-0.133057000	-1.289611000	0.852095000
1	2.059578000	-0.519034000	-1.047289000
17	-1.669944000	1.405958000	2.537279000

14c (ortho-endo) P

6	-0.211664000	1.013155000	-1.004120000
6	-0.578489000	0.162551000	0.247570000

6	1.337608000	1.205176000	-0.990228000
1	-1.659260000	0.036891000	0.312407000
8	1.937181000	1.815123000	-1.846892000
6	0.002691000	0.885335000	1.436857000
6	1.998806000	0.488224000	0.192840000
1	3.076485000	0.652005000	0.164370000
6	1.328285000	1.047868000	1.433252000
1	1.889487000	1.551321000	2.211217000
8	-0.622066000	0.256084000	-2.123132000
8	-0.747222000	2.309106000	-0.999272000
6	-2.165619000	2.409193000	-0.853151000
1	-2.432436000	3.417410000	-1.175903000
1	-2.687760000	1.679481000	-1.481190000
1	-2.465597000	2.281086000	0.193535000
6	-0.373508000	0.824439000	-3.416415000
1	-0.620285000	1.888840000	-3.432278000
1	0.671724000	0.700832000	-3.713886000
1	-1.021346000	0.280843000	-4.107426000
6	0.125545000	-1.220507000	0.162532000
6	1.657958000	-1.036936000	-0.001636000
6	2.381579000	-1.904651000	2.189746000

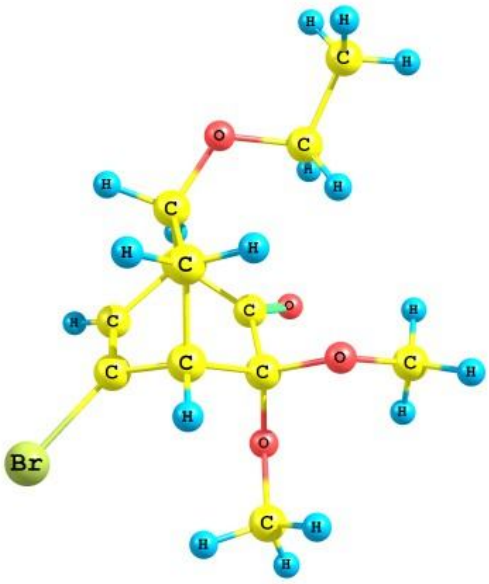


1	2.230214000	-2.943057000	2.510728000
1	1.522264000	-1.324636000	2.541405000
1	1.938802000	-1.286183000	-1.029948000
1	-0.090978000	-1.780089000	1.076491000
1	-0.279819000	-1.786847000	-0.677551000
8	2.453976000	-1.924912000	0.759835000
6	3.673904000	-1.364044000	2.791660000
1	3.651455000	-1.449672000	3.883658000
1	4.531787000	-1.930915000	2.419047000
1	3.826943000	-0.311133000	2.535960000
35	-1.137808000	1.460200000	2.845665000

14c (ortho-exo) P

6	0.424083000	0.808431000	-1.192300000
6	0.182583000	-0.089759000	0.057953000
6	1.961716000	1.062844000	-1.275186000
1	-0.883425000	-0.283866000	0.178622000
8	2.470991000	1.720424000	-2.156447000
6	0.780063000	0.669072000	1.222843000
6	2.731886000	0.403269000	-0.126280000
1	3.792978000	0.644808000	-0.204073000
6	2.082361000	0.950550000	1.136606000

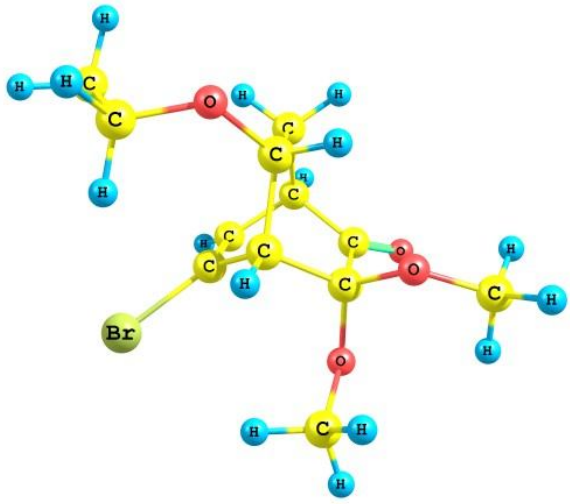
1	2.645248000	1.511837000	1.872506000
8	-0.042573000	0.076868000	-2.307603000
8	-0.160544000	2.081179000	-1.108257000
6	-1.570884000	2.116465000	-0.874474000
1	-1.897022000	3.121335000	-1.149689000
1	-2.100043000	1.383301000	-1.492256000
1	-1.800126000	1.946534000	0.183565000
6	0.076970000	0.708502000	-3.590424000
1	-0.190943000	1.765986000	-3.534296000
1	1.093811000	0.623354000	-3.984097000
1	-0.619002000	0.180543000	-4.246000000
6	0.966450000	-1.417122000	-0.111619000
6	2.500143000	-1.151011000	-0.083914000
6	3.111197000	-1.640768000	-2.404228000
1	2.051848000	-1.574227000	-2.687325000
1	3.581154000	-0.680385000	-2.654064000
1	0.691477000	-2.108455000	0.688840000
1	0.677474000	-1.877674000	-1.057391000
6	3.790206000	-2.774139000	-3.155708000
1	4.842570000	-2.847814000	-2.866882000
1	3.306718000	-3.729469000	-2.932251000



1	3.738367000	-2.599954000	-4.235052000
35	-0.325208000	1.189954000	2.680066000
8	3.253334000	-1.910734000	-1.008317000
1	2.898249000	-1.474471000	0.881762000

14c (meta-endo) P

6	-0.201474000	1.013582000	-1.034614000
6	-0.364312000	0.178229000	0.280819000
6	1.322951000	1.331928000	-1.182472000
1	-1.411612000	-0.081863000	0.435905000
8	1.786755000	1.906182000	-2.141983000
6	0.213806000	1.042332000	1.374677000
6	2.146016000	0.808010000	0.000352000
1	3.185919000	1.115551000	-0.120547000
6	1.497269000	1.385004000	1.245416000
1	2.032877000	2.037577000	1.924415000
8	-0.680913000	0.206394000	-2.084914000
8	-0.830500000	2.267758000	-0.994865000
6	-2.237444000	2.261533000	-0.735166000
1	-2.603602000	3.244104000	-1.038843000
1	-2.749913000	1.488359000	-1.316750000
1	-2.440216000	2.121045000	0.332410000

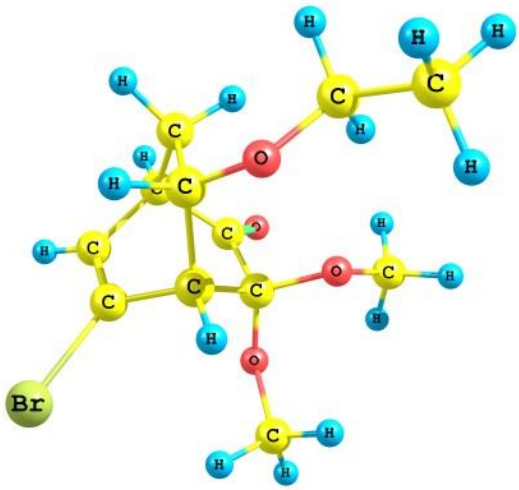


6	-0.601775000	0.745141000	-3.412473000
1	-0.877970000	1.802089000	-3.425045000
1	0.404392000	0.637856000	-3.826608000
1	-1.311283000	0.166451000	-4.007882000
6	0.485343000	-1.126710000	0.099624000
6	1.991418000	-0.741330000	0.035694000
6	0.000964000	-2.001977000	2.383912000
1	-0.580514000	-2.876677000	2.694812000
1	-0.617633000	-1.120682000	2.588183000
1	2.456843000	-1.184015000	-0.850408000
1	0.189893000	-1.524694000	-0.872148000
8	0.179582000	-2.196000000	0.980729000
6	1.288077000	-1.942839000	3.206048000
1	1.042984000	-2.009676000	4.271873000
1	1.943708000	-2.781989000	2.953974000
1	1.835214000	-1.009256000	3.052285000
35	-0.894519000	1.650930000	2.801778000
1	2.519327000	-1.130383000	0.907560000

14c (meta-exo) P

6	-0.284811000	1.626209000	-1.057775000
6	-0.744105000	0.555780000	-0.025608000

6	1.218147000	1.931708000	-0.766054000
1	-1.796144000	0.310020000	-0.164633000
8	1.873650000	2.720287000	-1.409576000
6	-0.432884000	1.143083000	1.330252000
6	1.760211000	1.085719000	0.390368000
1	2.803446000	1.349475000	0.570689000
6	0.855710000	1.395327000	1.573354000
1	1.238977000	1.823278000	2.491758000
8	-0.462275000	1.075217000	-2.343959000
8	-0.943240000	2.860398000	-0.914770000
6	-2.370509000	2.830107000	-1.002980000
1	-2.682344000	3.858312000	-1.196904000
1	-2.709355000	2.188823000	-1.823278000
1	-2.818076000	2.495480000	-0.060251000
6	-0.097606000	1.905337000	-3.457238000
1	-0.428056000	2.935172000	-3.304718000
1	0.983924000	1.903638000	-3.620067000
1	-0.603595000	1.474909000	-4.324111000
6	0.096761000	-0.772509000	-0.081409000
6	1.604469000	-0.403528000	-0.043149000
6	0.411685000	-1.896079000	-2.271744000

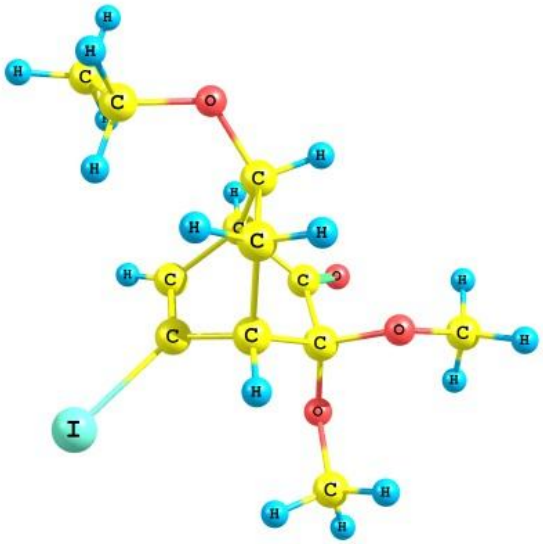


1	0.669904000	-0.954433000	-2.766484000
1	1.343756000	-2.431139000	-2.031651000
8	-0.348917000	-1.663325000	-1.089826000
6	-0.452441000	-2.746701000	-3.188783000
1	-0.736389000	-3.680276000	-2.694546000
1	-1.365839000	-2.208064000	-3.455752000
1	0.092018000	-2.990344000	-4.106762000
1	2.143595000	-1.050147000	0.654300000
1	-0.149441000	-1.284525000	0.855102000
1	2.070447000	-0.531027000	-1.023088000
35	-1.828623000	1.420499000	2.591070000

15c (ortho-endo) P

6	-0.225648000	1.046025000	-0.968902000
6	-0.599310000	0.207816000	0.292338000
6	1.323157000	1.252624000	-0.937284000
1	-1.681201000	0.086307000	0.350498000
8	1.926761000	1.897473000	-1.771155000
6	-0.009714000	0.927532000	1.487898000
6	1.981436000	0.505448000	0.224386000
1	3.060708000	0.659148000	0.193392000
6	1.322862000	1.066098000	1.472597000

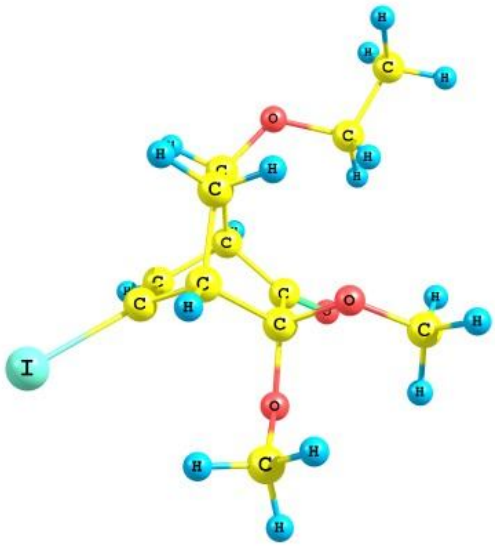
1	1.904557000	1.554469000	2.247728000
8	-0.604601000	0.259088000	-2.086009000
8	-0.787670000	2.332962000	-0.995160000
6	-2.219685000	2.404512000	-0.982958000
1	-2.469168000	3.420411000	-1.296290000
1	-2.664890000	1.688484000	-1.681756000
1	-2.619773000	2.236498000	0.023916000
6	-0.343998000	0.806208000	-3.392433000
1	-0.617701000	1.863325000	-3.442693000
1	0.710333000	0.698530000	-3.663884000
1	-0.964267000	0.226222000	-4.079669000
6	0.092716000	-1.183492000	0.220490000
6	1.619590000	-1.011026000	0.017906000
6	2.417008000	-1.918205000	2.180614000
1	2.228454000	-2.953458000	2.490226000
1	1.598799000	-1.305164000	2.569867000
1	1.869429000	-1.251691000	-1.019509000
1	-0.109894000	-1.721664000	1.150407000
1	-0.333053000	-1.767999000	-0.596984000
8	2.437146000	-1.919032000	0.743476000
6	3.754813000	-1.444737000	2.744251000



1	3.758528000	-1.536233000	3.836882000
1	4.573026000	-2.051911000	2.344943000
1	3.951040000	-0.398601000	2.488290000
53	-1.234320000	1.579644000	3.094591000

15c (ortho-exo) P

6	0.427243000	0.826882000	-1.161319000
6	0.194203000	-0.074383000	0.091112000
6	1.964999000	1.091209000	-1.244714000
1	-0.871748000	-0.270053000	0.212600000
8	2.468911000	1.785386000	-2.105474000
6	0.808106000	0.669998000	1.264879000
6	2.744988000	0.403215000	-0.123545000
1	3.806832000	0.640643000	-0.207773000
6	2.115047000	0.941287000	1.155166000
1	2.704239000	1.482897000	1.887851000
8	-0.031696000	0.084134000	-2.278099000
8	-0.173365000	2.095298000	-1.079102000
6	-1.601377000	2.119862000	-0.950611000
1	-1.900475000	3.146331000	-1.172611000
1	-2.082759000	1.438506000	-1.659965000
1	-1.916589000	1.873142000	0.069877000

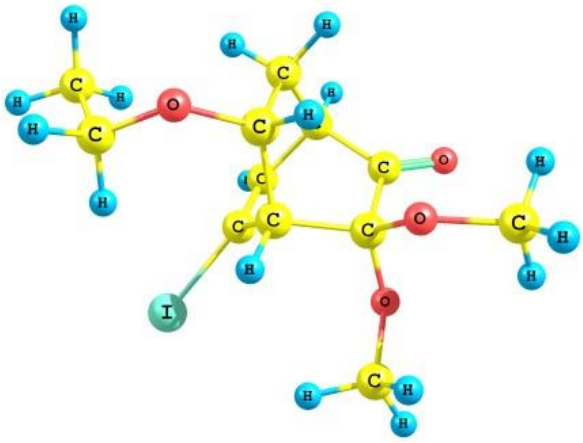


6	0.083969000	0.707362000	-3.570779000
1	-0.236153000	1.751931000	-3.538417000
1	1.112162000	0.663902000	-3.941787000
1	-0.573249000	0.134941000	-4.229480000
6	0.970302000	-1.406451000	-0.086412000
6	2.503538000	-1.147327000	-0.081758000
6	3.083609000	-1.658607000	-2.417472000
1	2.019698000	-1.621709000	-2.684952000
1	3.530457000	-0.689980000	-2.676212000
1	0.704584000	-2.091115000	0.723491000
1	0.664038000	-1.875969000	-1.022144000
6	3.781785000	-2.779991000	-3.173862000
1	4.841657000	-2.824536000	-2.904899000
1	3.326740000	-3.747527000	-2.940309000
1	3.706051000	-2.610361000	-4.253371000
8	3.248544000	-1.914536000	-1.016314000
1	2.915921000	-1.475729000	0.875459000
53	-0.358918000	1.209700000	2.953099000

15c (meta-endo) P

6	-0.209578000	1.033352000	-1.002133000
6	-0.368267000	0.201151000	0.320649000

6	1.317455000	1.348957000	-1.153438000
1	-1.416471000	-0.054348000	0.480485000
8	1.777357000	1.951022000	-2.102561000
6	0.231007000	1.064949000	1.413304000
6	2.149138000	0.794851000	0.005644000
1	3.191924000	1.089408000	-0.124515000
6	1.522600000	1.382545000	1.258078000
1	2.084729000	2.033997000	1.919302000
8	-0.681722000	0.217184000	-2.055413000
8	-0.848877000	2.285467000	-0.966601000
6	-2.277393000	2.268539000	-0.834943000
1	-2.604251000	3.288194000	-1.048037000
1	-2.739505000	1.578790000	-1.548423000
1	-2.584342000	2.004359000	0.183430000
6	-0.605984000	0.749585000	-3.392126000
1	-0.890649000	1.804393000	-3.417184000
1	0.402247000	0.643267000	-3.801987000
1	-1.310303000	0.156846000	-3.980545000
6	0.466545000	-1.113235000	0.124417000
6	1.974564000	-0.750232000	0.041429000
6	0.020379000	-2.031802000	2.412916000

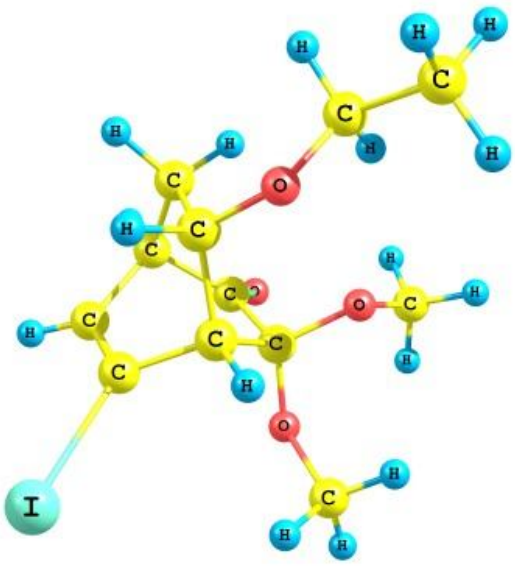


1	-0.549197000	-2.915505000	2.718949000
1	-0.599336000	-1.159032000	2.646846000
1	2.420813000	-1.198579000	-0.851917000
1	0.154094000	-1.503501000	-0.843783000
8	0.154737000	-2.195909000	0.996304000
6	1.329473000	-1.986644000	3.204592000
1	1.105167000	-2.077938000	4.273948000
1	1.979698000	-2.820925000	2.921419000
1	1.873861000	-1.049335000	3.062186000
1	2.513129000	-1.146434000	0.903205000
53	-0.941356000	1.827587000	3.020036000

15c (meta-exo) P

6	-0.288407000	1.664714000	-1.018949000
6	-0.738694000	0.577702000	0.004015000
6	1.208645000	1.991417000	-0.714371000
1	-1.791938000	0.335196000	-0.133932000
8	1.843839000	2.837613000	-1.310495000
6	-0.406428000	1.131470000	1.375470000
6	1.775645000	1.091832000	0.383930000
1	2.822895000	1.345687000	0.556370000
6	0.893863000	1.369818000	1.593831000

1	1.306039000	1.771739000	2.513673000
8	-0.428118000	1.105771000	-2.311986000
8	-0.980936000	2.883258000	-0.885337000
6	-2.399287000	2.836375000	-1.093496000
1	-2.713884000	3.874133000	-1.221796000
1	-2.656336000	2.262929000	-1.990167000
1	-2.918292000	2.414397000	-0.225075000
6	-0.057095000	1.939786000	-3.426145000
1	-0.419616000	2.962401000	-3.295618000
1	1.028608000	1.963641000	-3.560397000
1	-0.528801000	1.484605000	-4.300240000
6	0.099134000	-0.749813000	-0.091034000
6	1.605038000	-0.380014000	-0.096402000
6	0.374361000	-1.918091000	-2.275714000
1	0.626490000	-0.996677000	-2.810843000
1	1.307313000	-2.438244000	-2.011352000
8	-0.385523000	-1.632529000	-1.098530000
6	-0.487698000	-2.814227000	-3.154479000
1	-0.755891000	-3.734326000	-2.625944000
1	-1.409874000	-2.298422000	-3.438580000
1	0.056864000	-3.083457000	-4.066266000



1	2.171092000	-1.049018000	0.557761000
1	-0.115845000	-1.277276000	0.843590000
1	2.035895000	-0.469572000	-1.096126000
53	-1.908619000	1.403049000	2.851086000