Regio- and Stereoselective synthesis of Sulfur-Bearing Four-Membered Heterocycles: Direct Access to 2,4-disubstituted thietane 1-oxides

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Supporting Information

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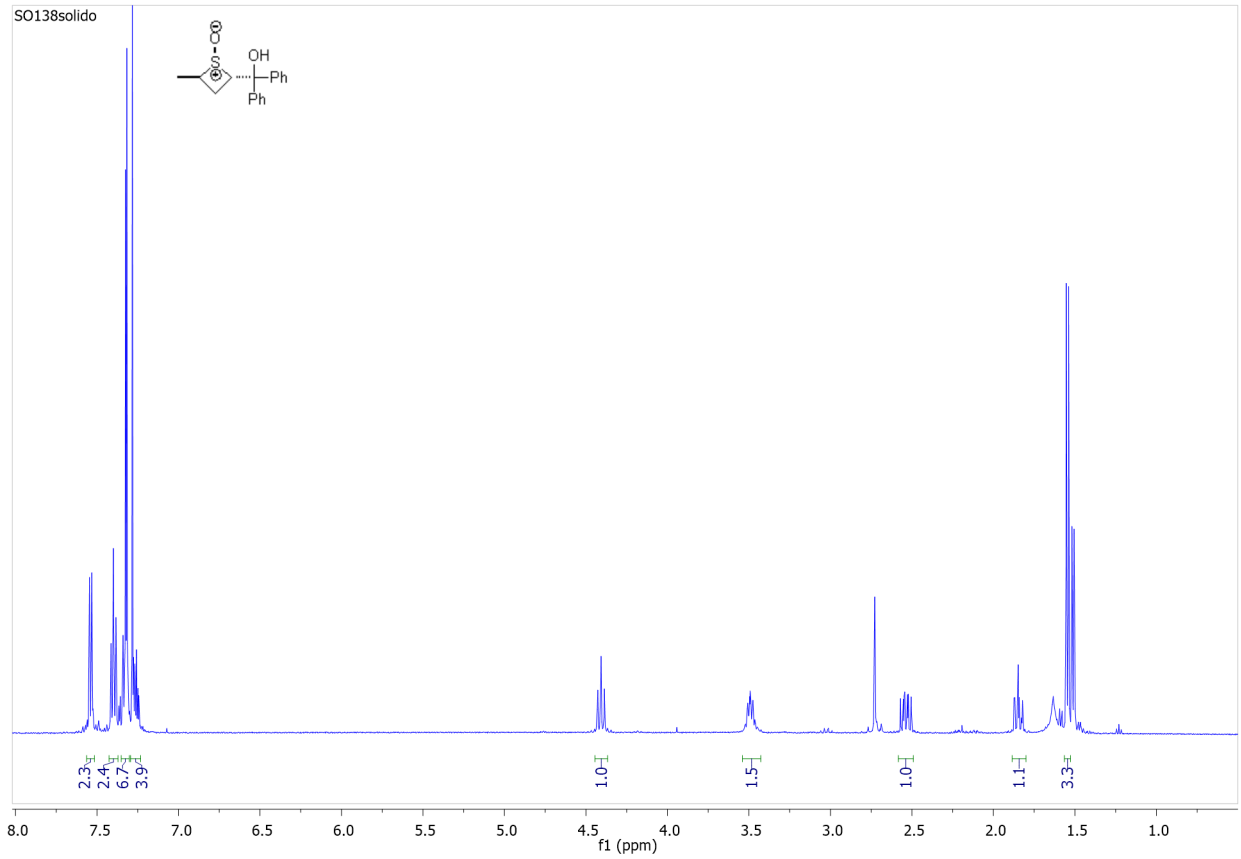
(1*R*$_S$,2S*,4R**)-4a**


SO138solido
OH
Ph
Ph
2.3
2.4
6.7
3.9
1.0
1.5
1.0
1.1
3.3
8.0
7.5
7.0
6.5
6.0
5.5
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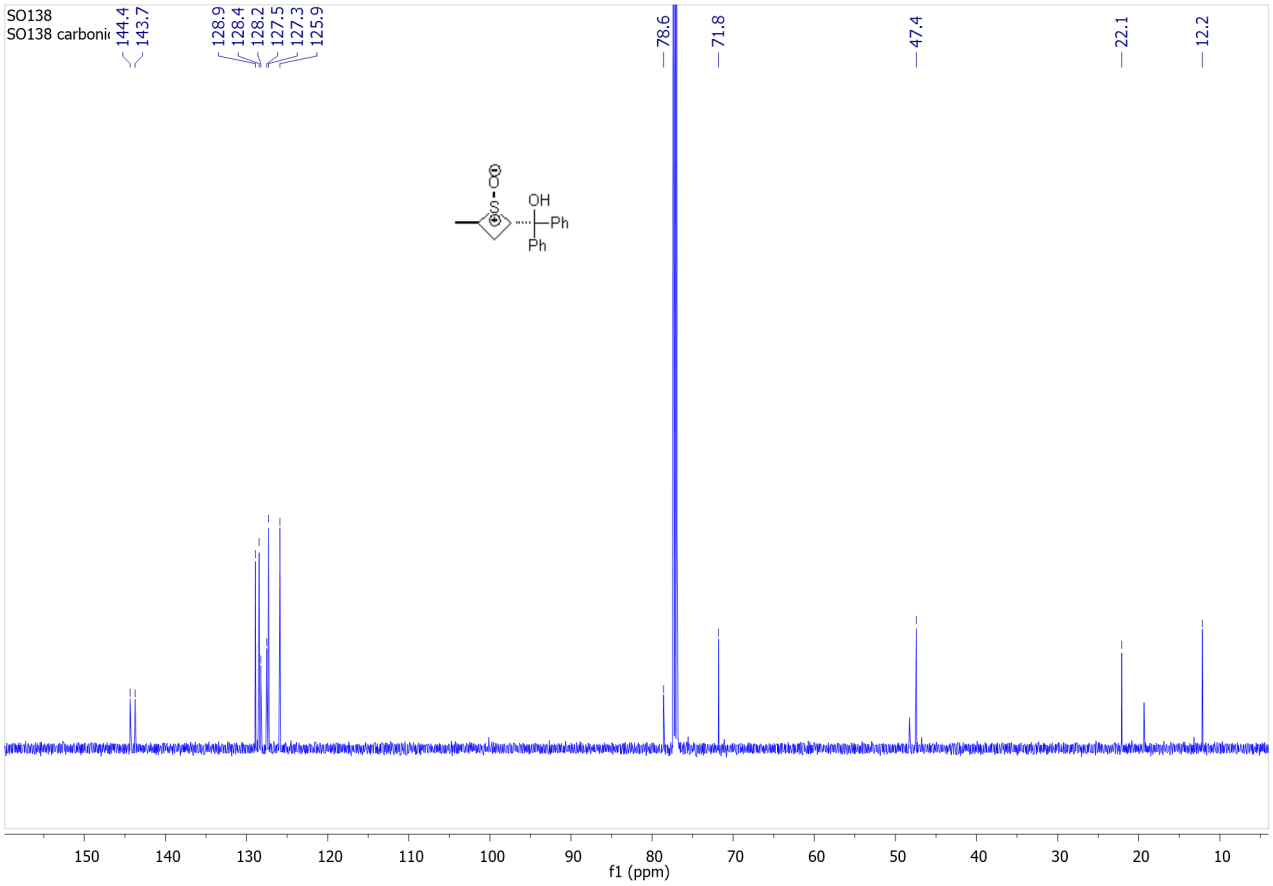
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)


SO138
SO138 carboni
144.4
143.7
128.9
128.4
128.2
127.5
127.3
125.9
78.6
71.8
47.4
22.1
12.2
OH
Ph
Ph
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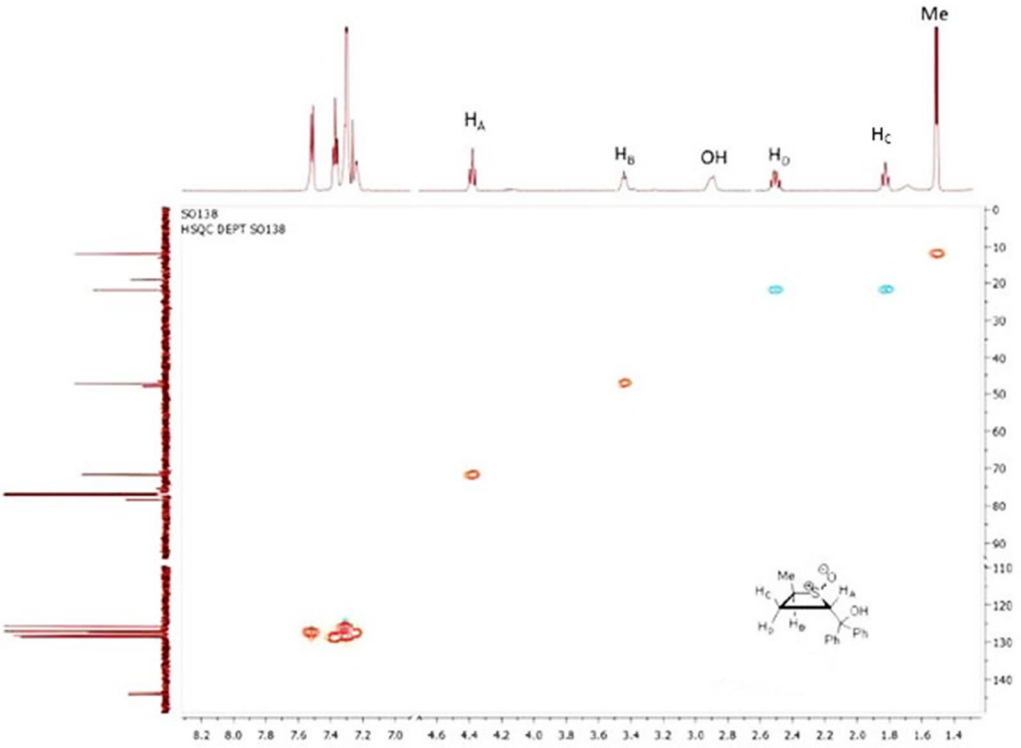
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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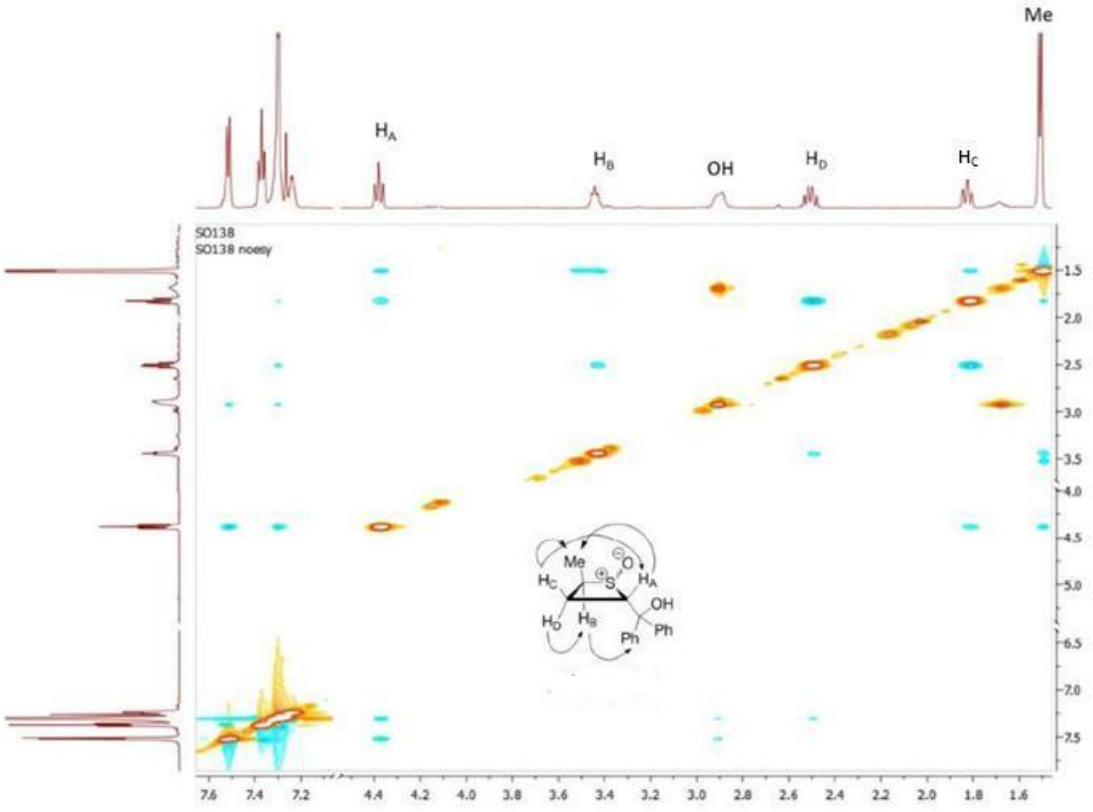
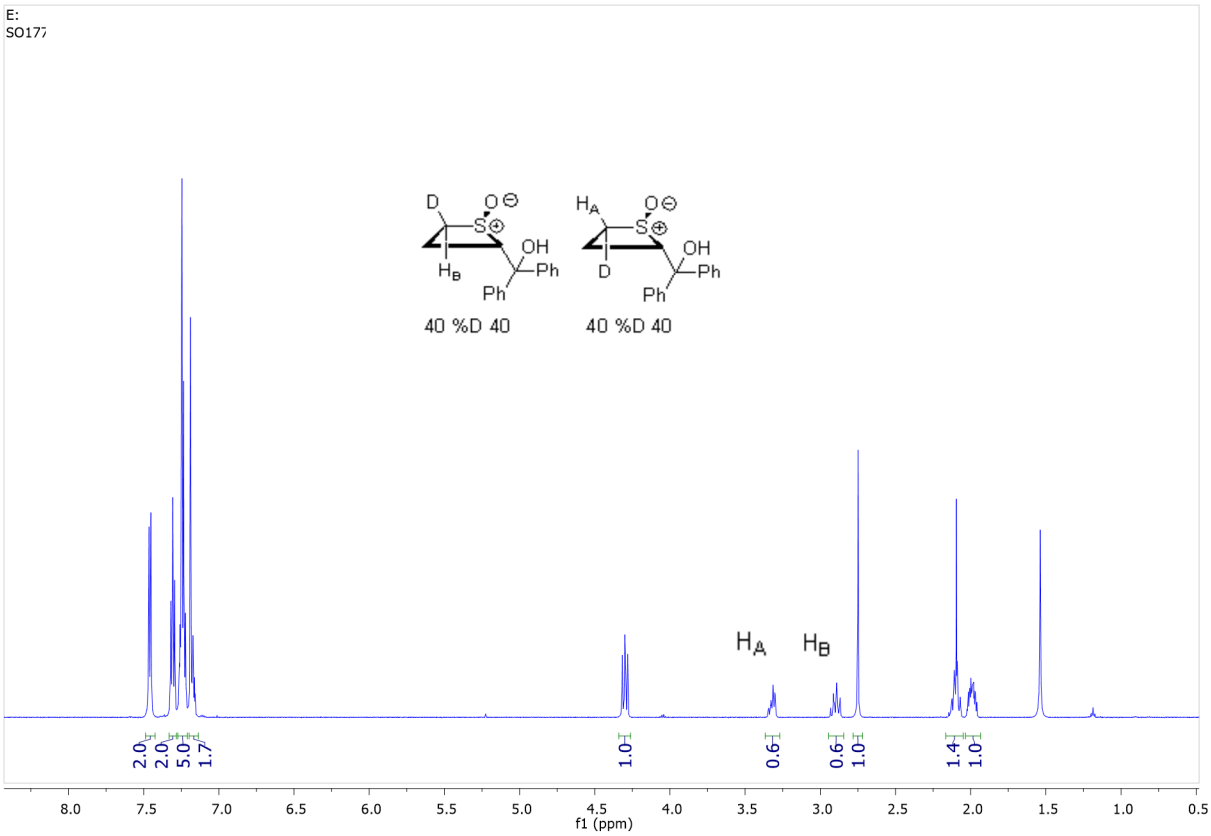
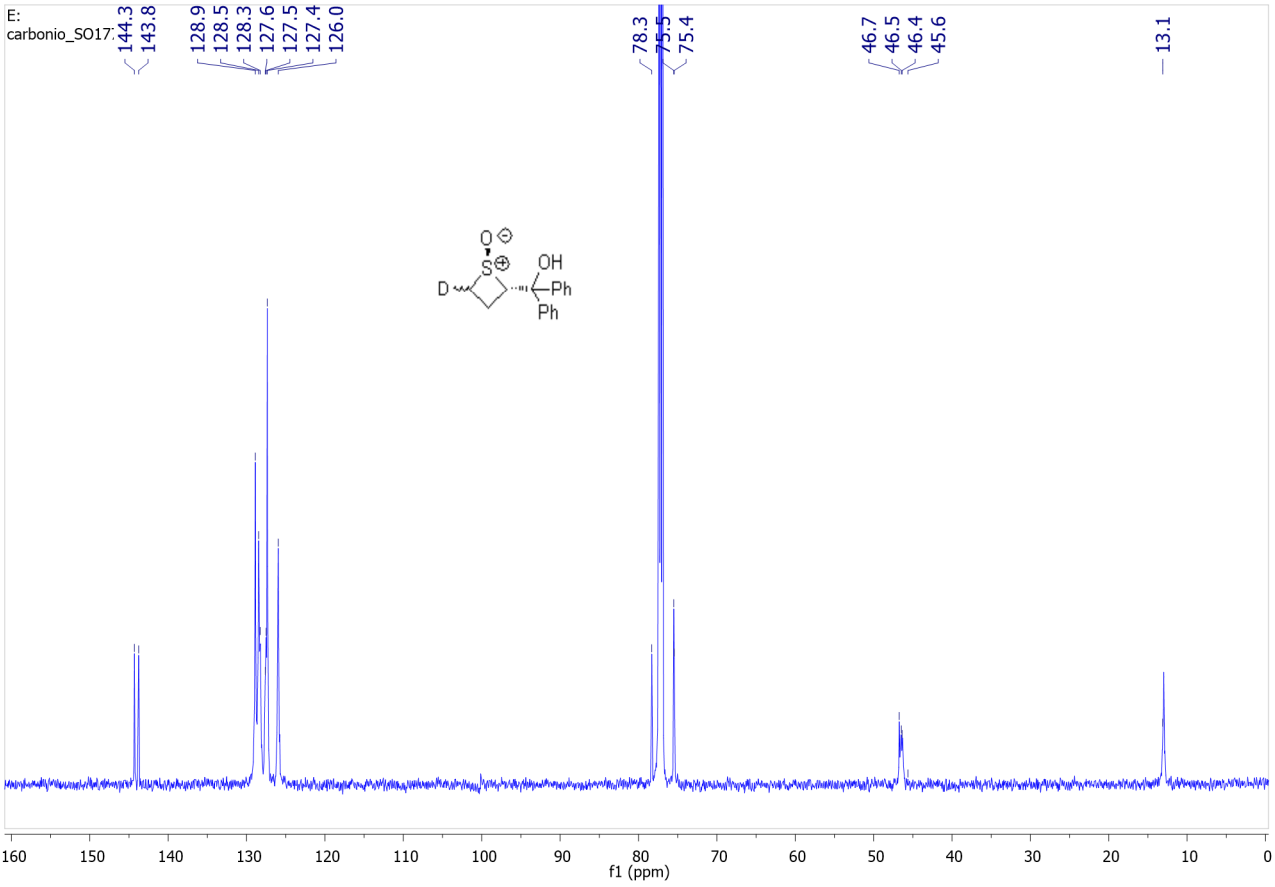
H_A
H_B
OH
H_D
H_C
S0138
HSQC DEPT S0138

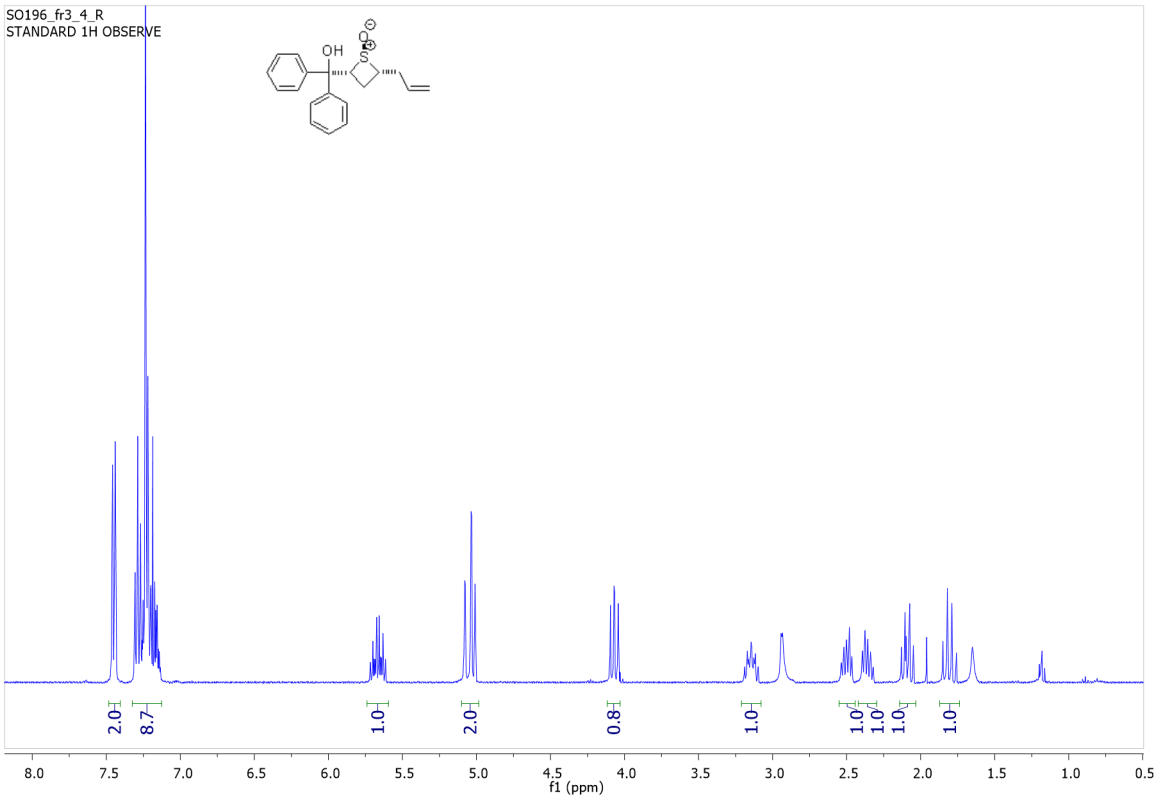

Me
H_A
H_B
OH
H_D
H_C
S0138
S0138 noesy

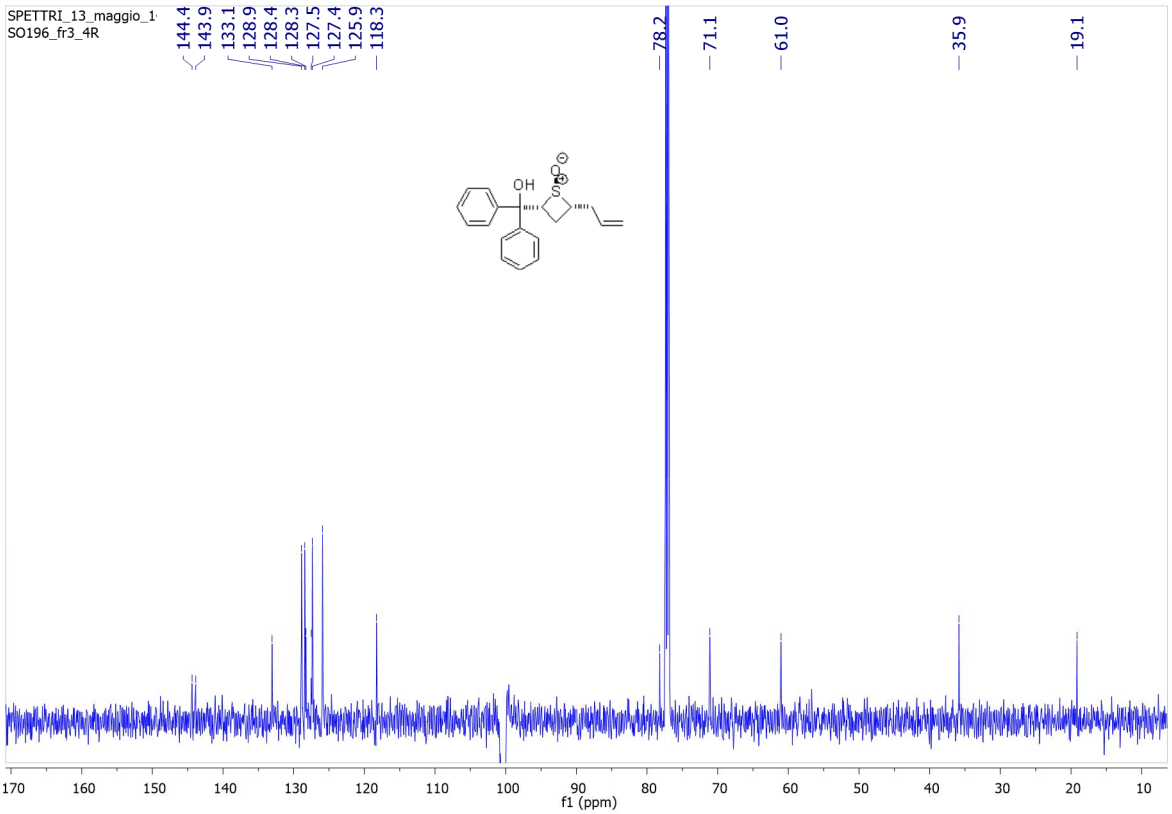
(*1R*$_S$,2S*,4R*)/(1R*$_S$**,2S*,4S*)-4b**



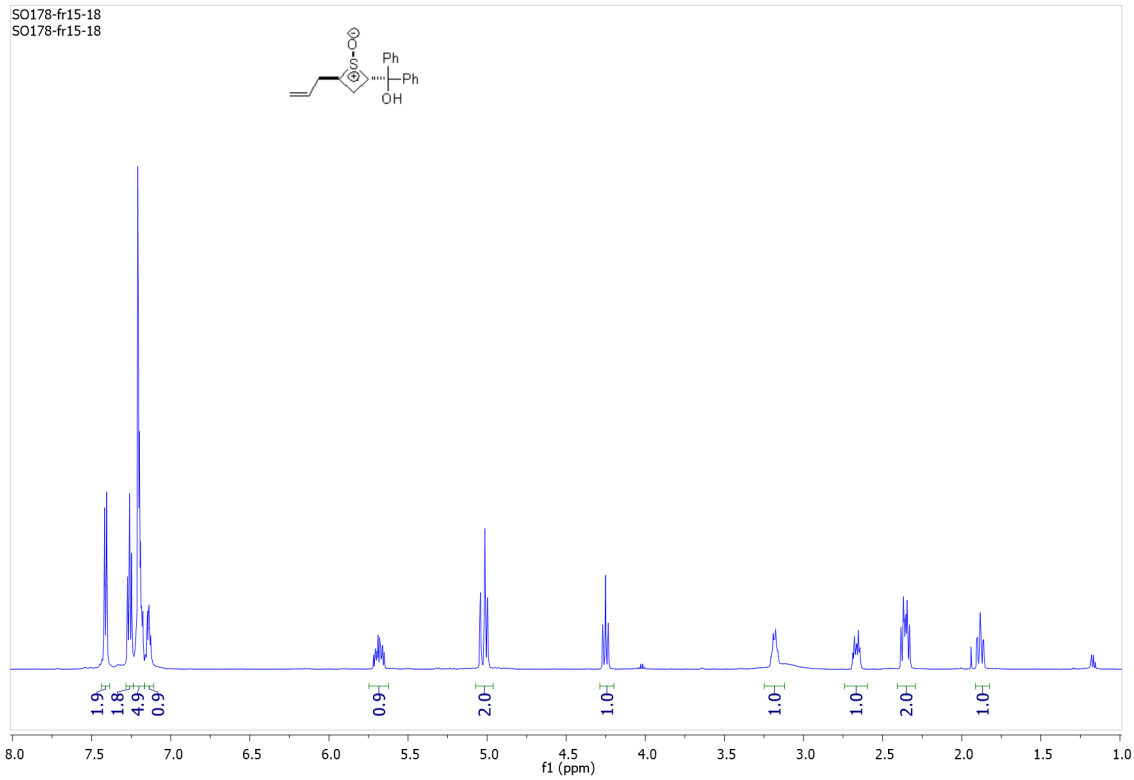


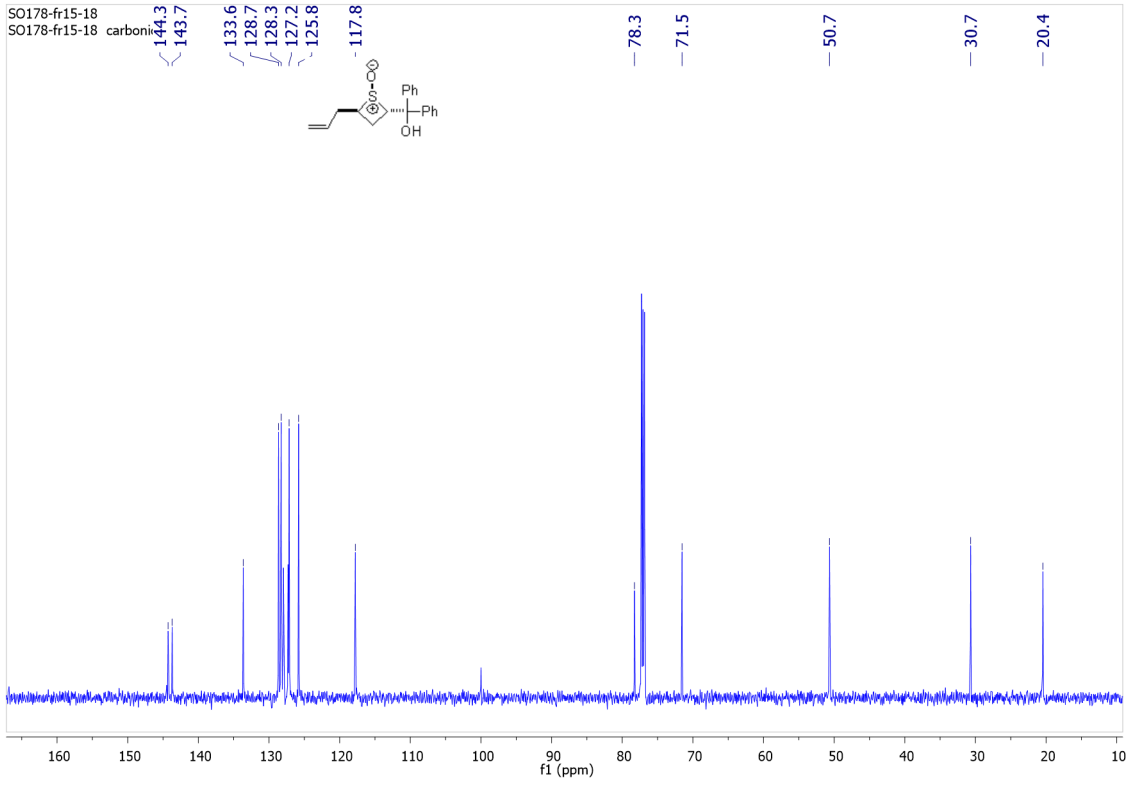
(1R_S*,2*S,4*S**)-4c *minor***

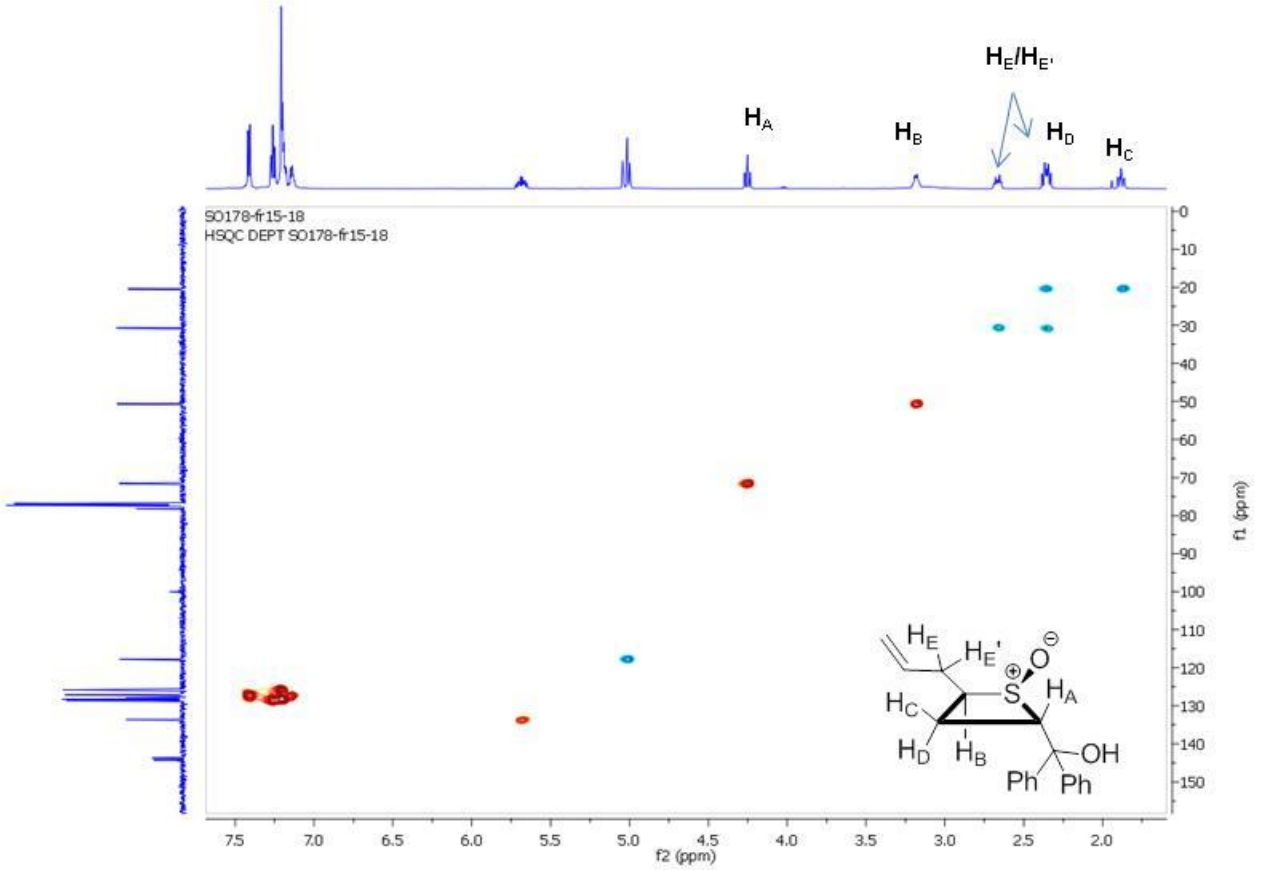


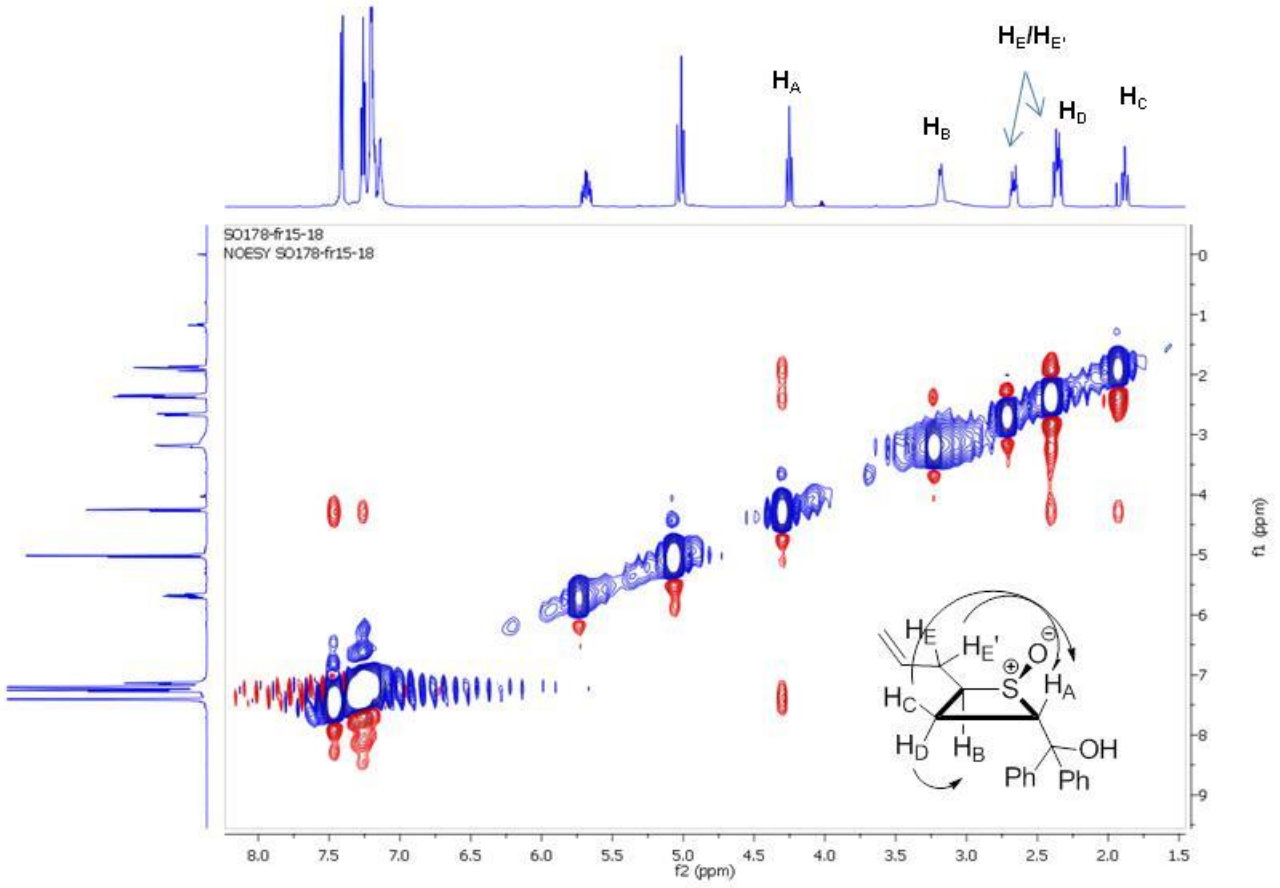


(1R_S*, 2*S, 4*R**)-4c *major***

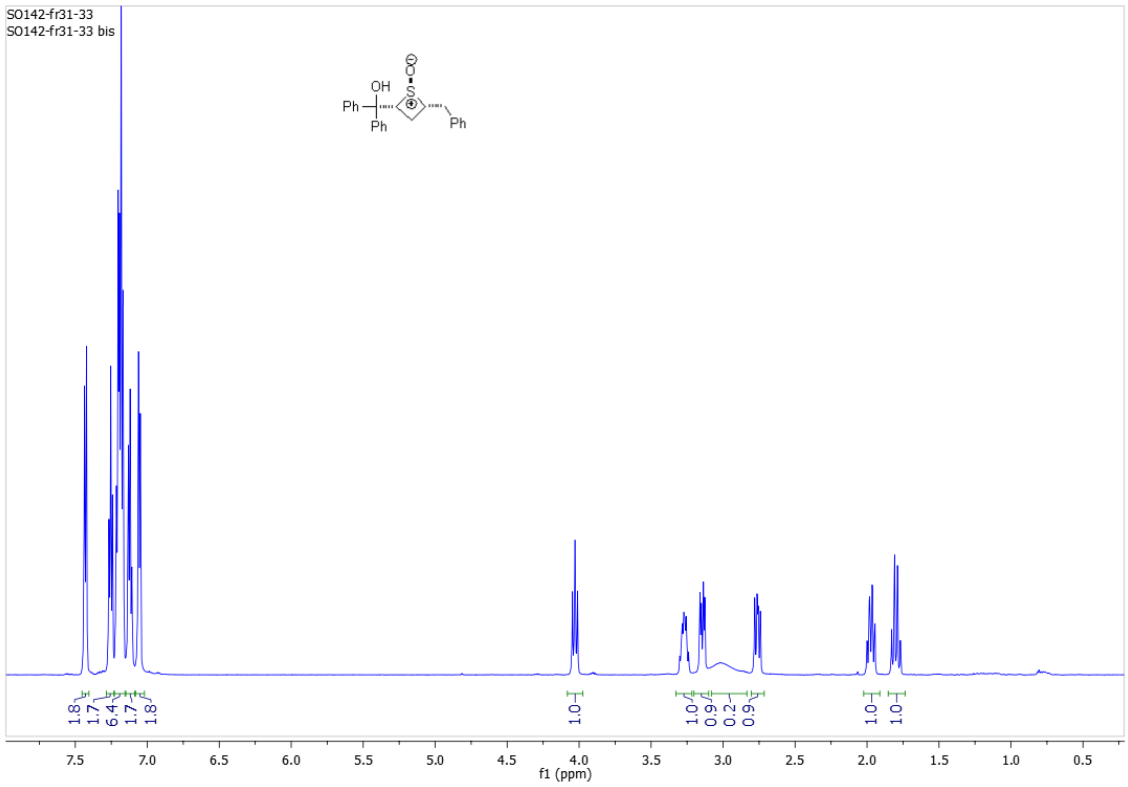


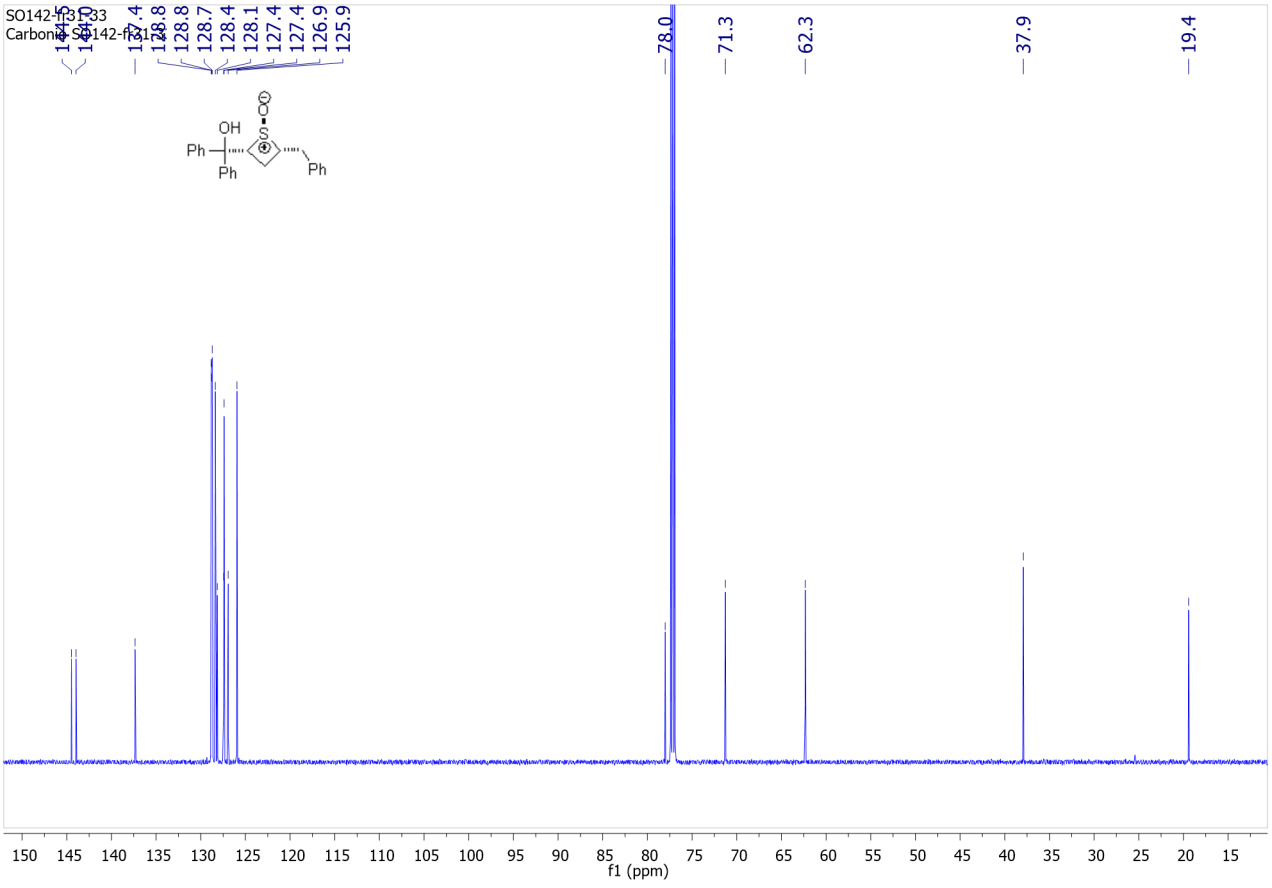


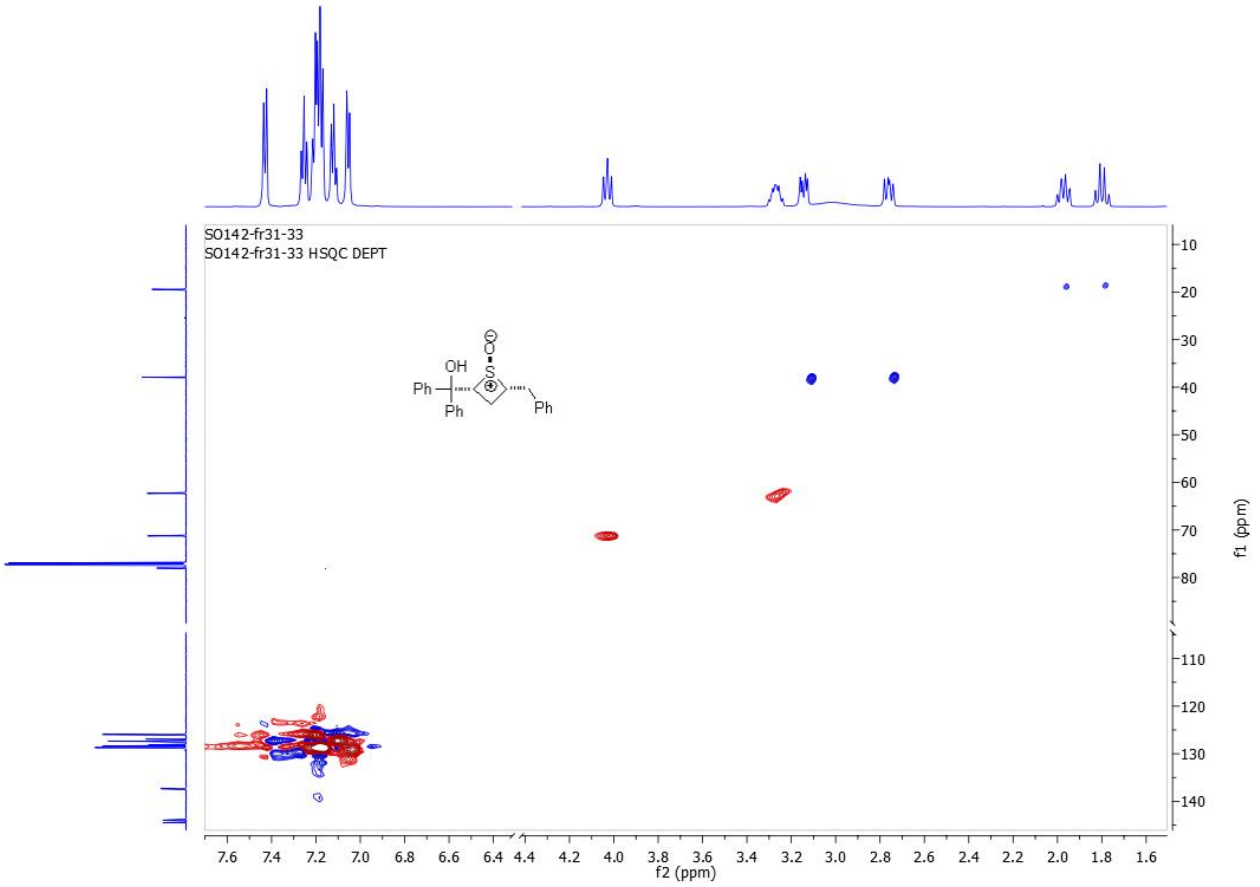

HE/HE'
HA
HB
HD
HC
SO178-fr15-18
HSQC DEPT SO178-fr15-18
f2 (ppm)
f1 (ppm)
HE
HE'
O
S
HA
HC
HD
HB
OH
Ph
Ph

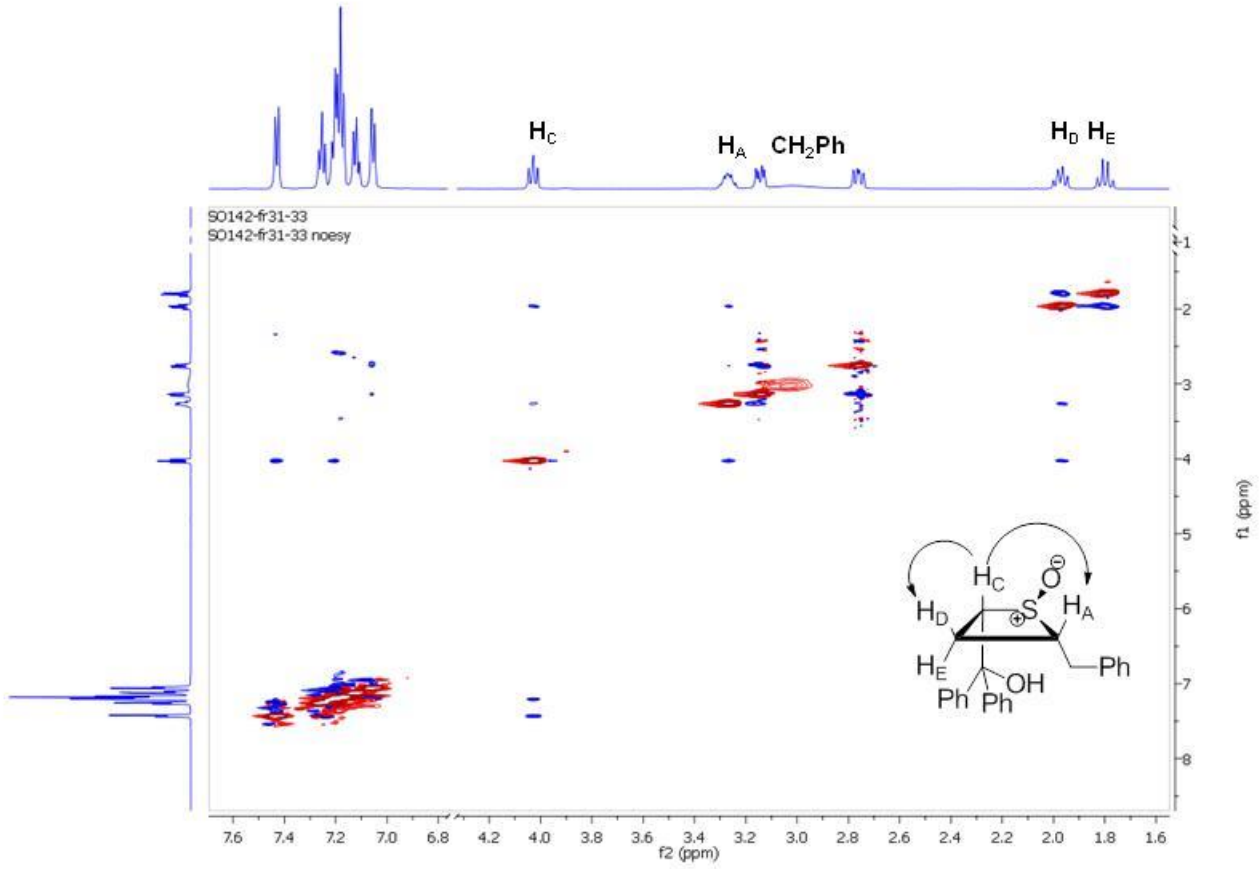

HE/HE'
HA
HB
HD
HC
SO178-fr15-18
NOESY SO178-fr15-18
f2 (ppm)
f1 (ppm)
HE
HE'
O
S
HA
HC
HD
HB
OH
Ph
Ph

(1R_S*,2*S,4*S**)-4d *minor***

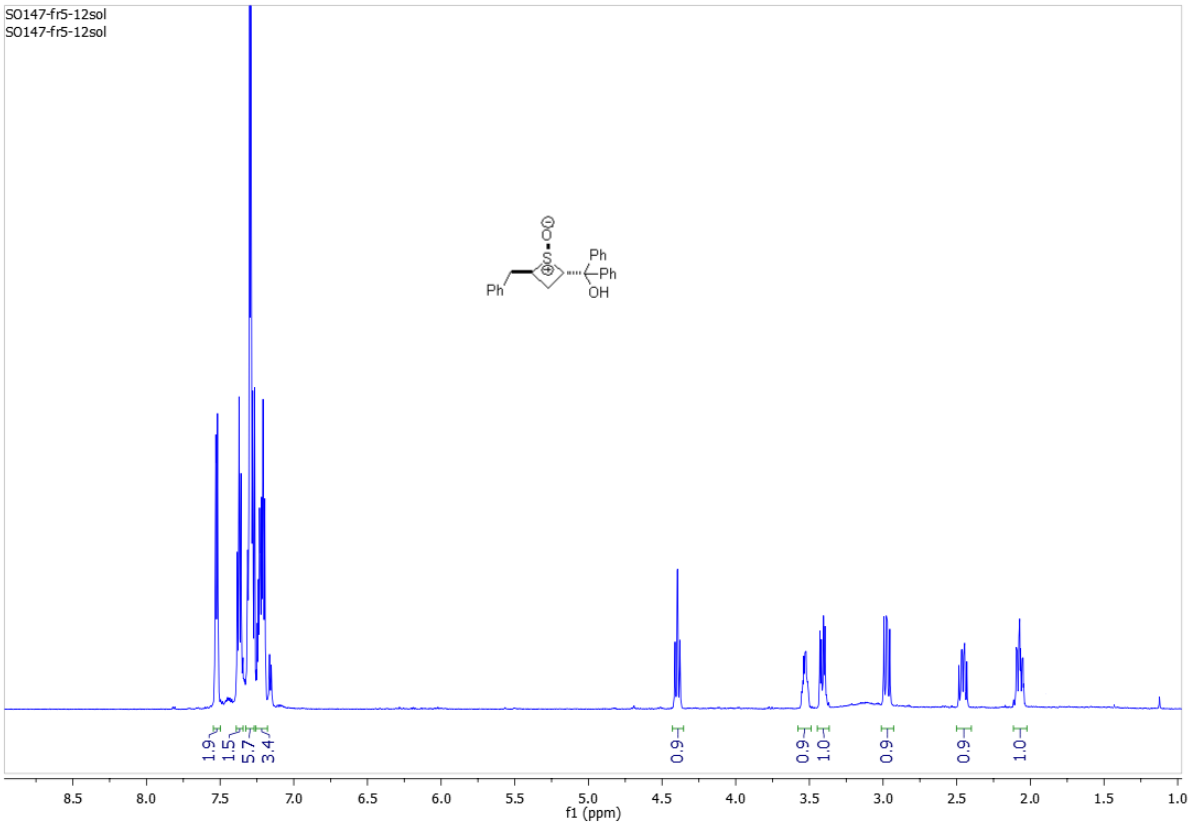


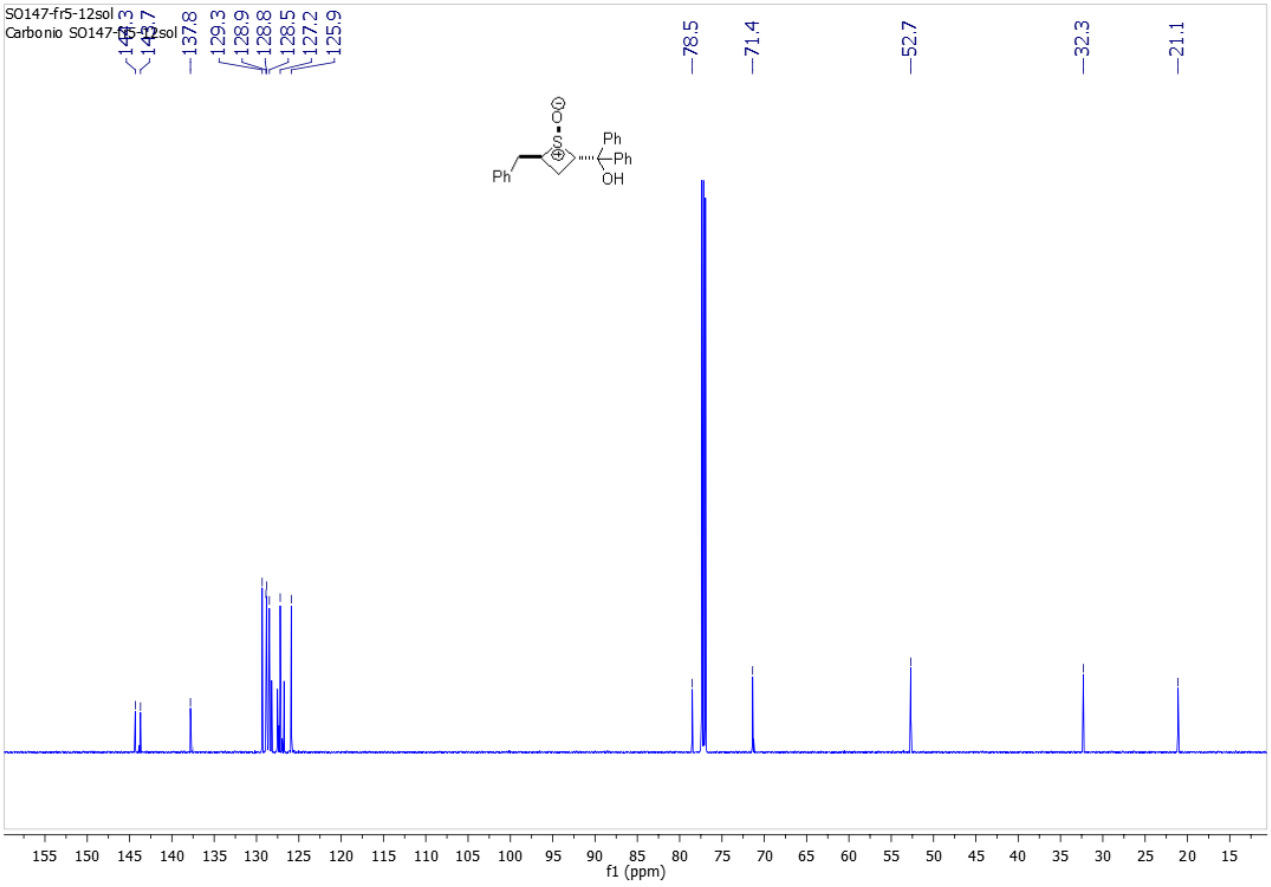


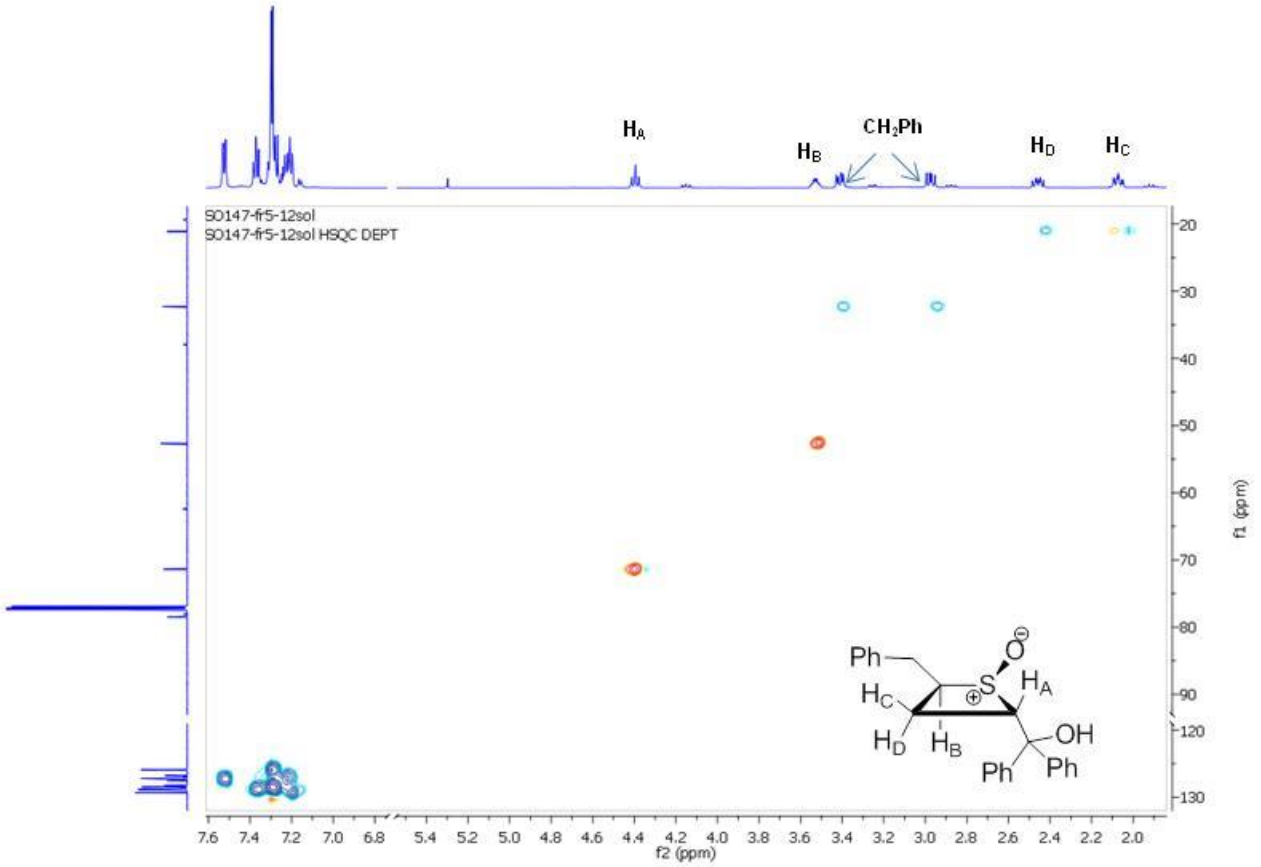

SO142-fr31-33
SO142-fr31-33 HSQC DEPT
OH
Ph
Ph
Ph
f1 (ppm)
f2 (ppm)

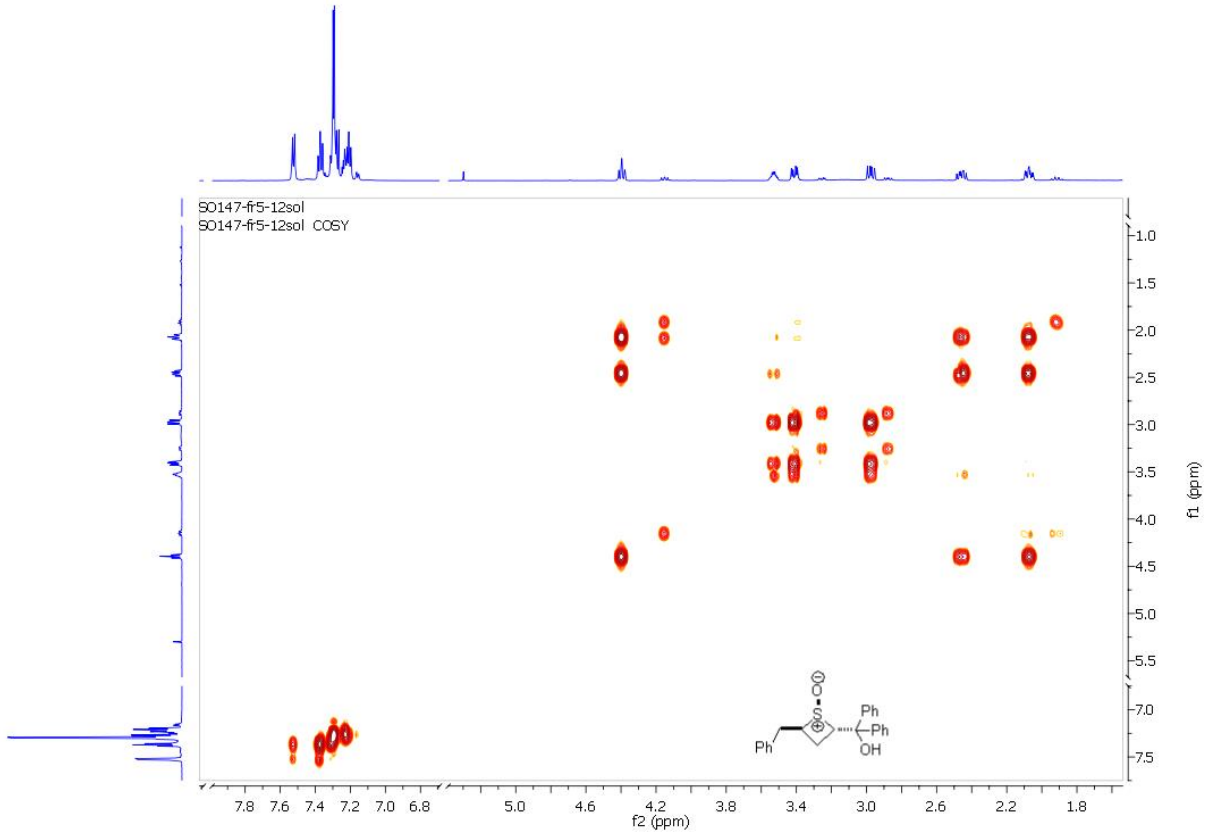

H_C
H_A
CH_2Ph
H_D H_E
SO142-fr31-33
SO142-fr31-33 noesy
H_C
H_D
H_A
H_E
Ph
OH
Ph
Ph
f1 (ppm)
f2 (ppm)

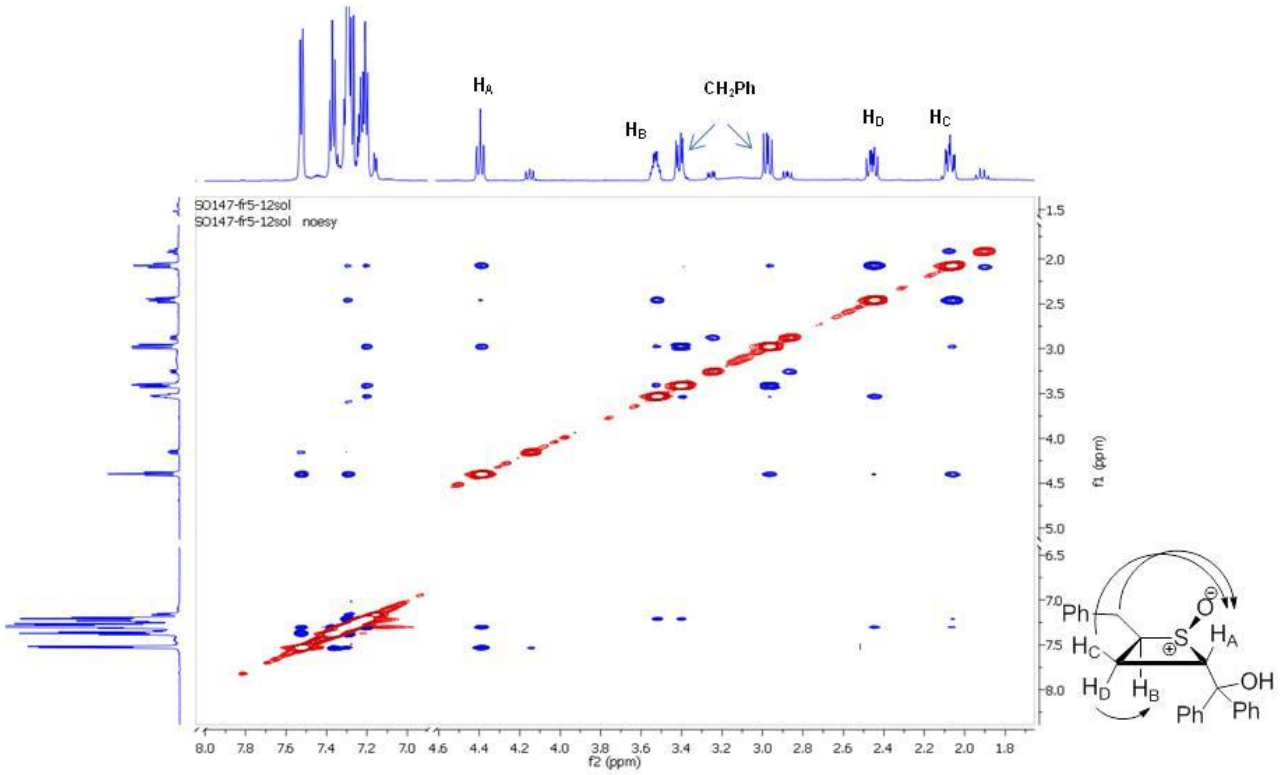
(1R_S*,2S*,4R*)-4d *major*



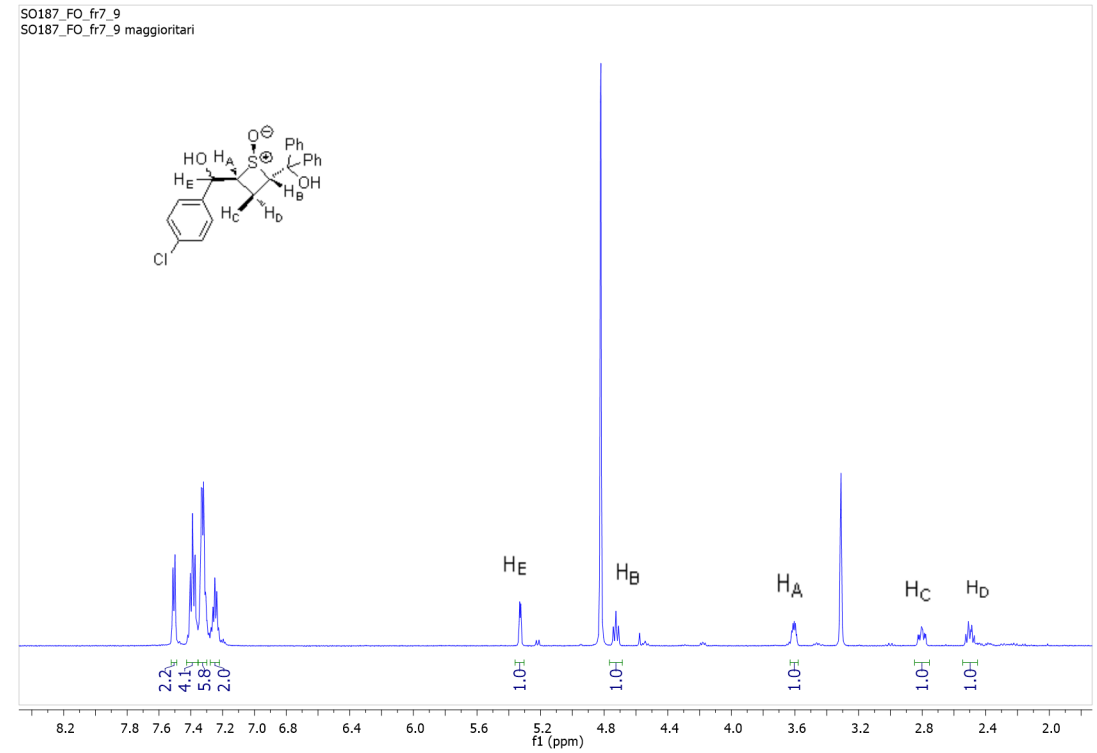


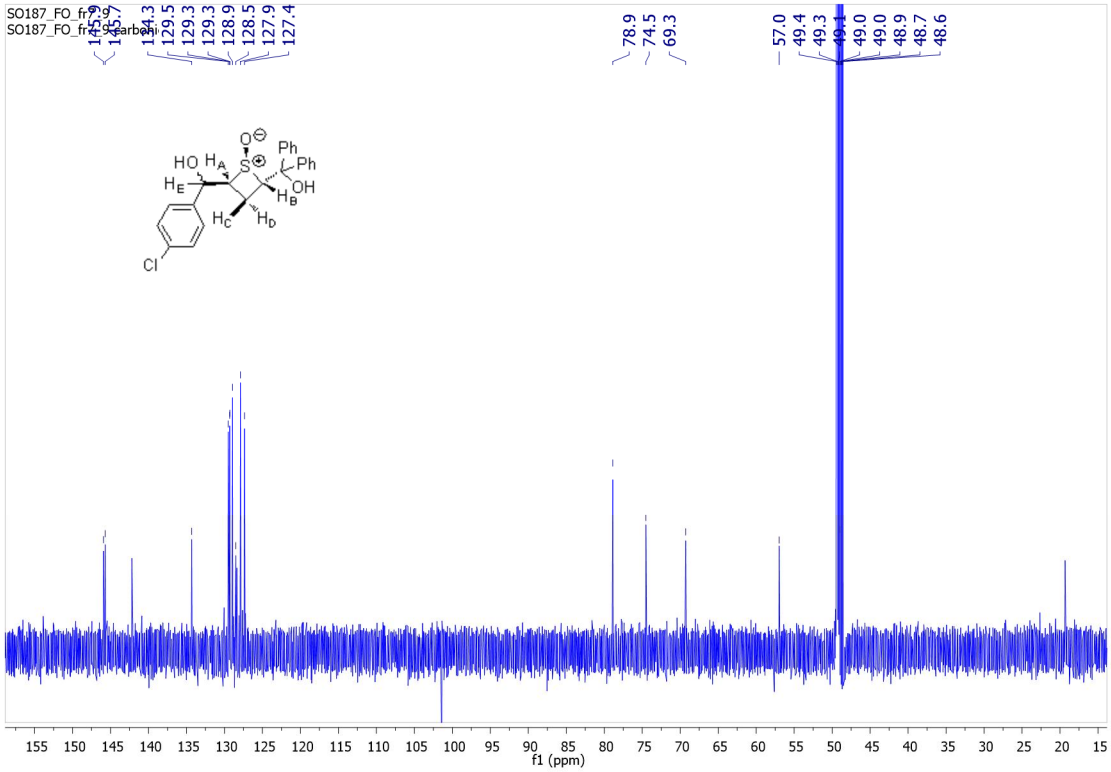

H_A
H_B
CH2Ph
H_D
H_C
SO147-fr5-12sol
SO147-fr5-12sol HSQC DEPT
f2 (ppm)
f1 (ppm)
Ph
H_C
H_D
H_B
S
H_A
O
OH
Ph
Ph

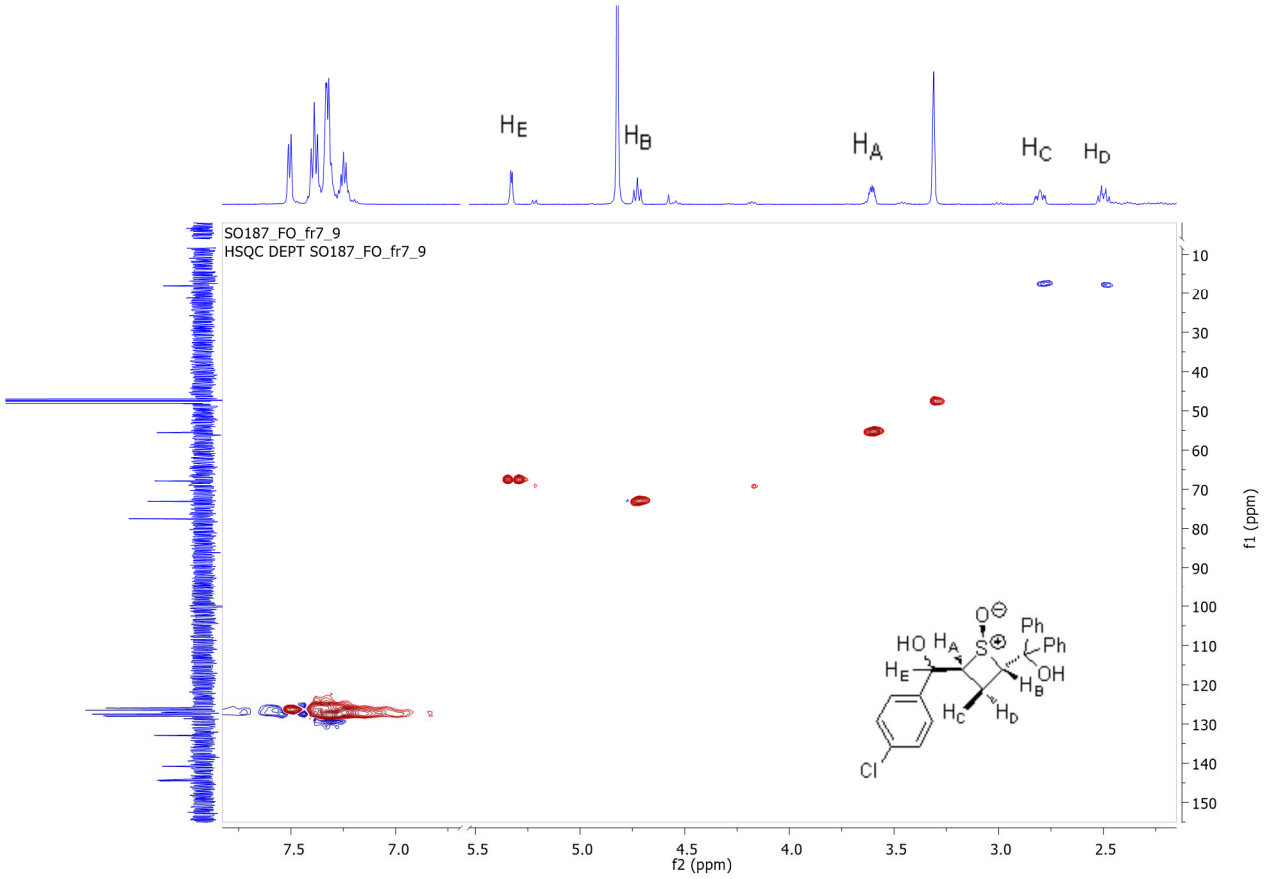

SO147-fr5-12sol
SO147-fr5-12sol COSY
f2 (ppm)
f1 (ppm)
Ph
Ph
Ph
OH

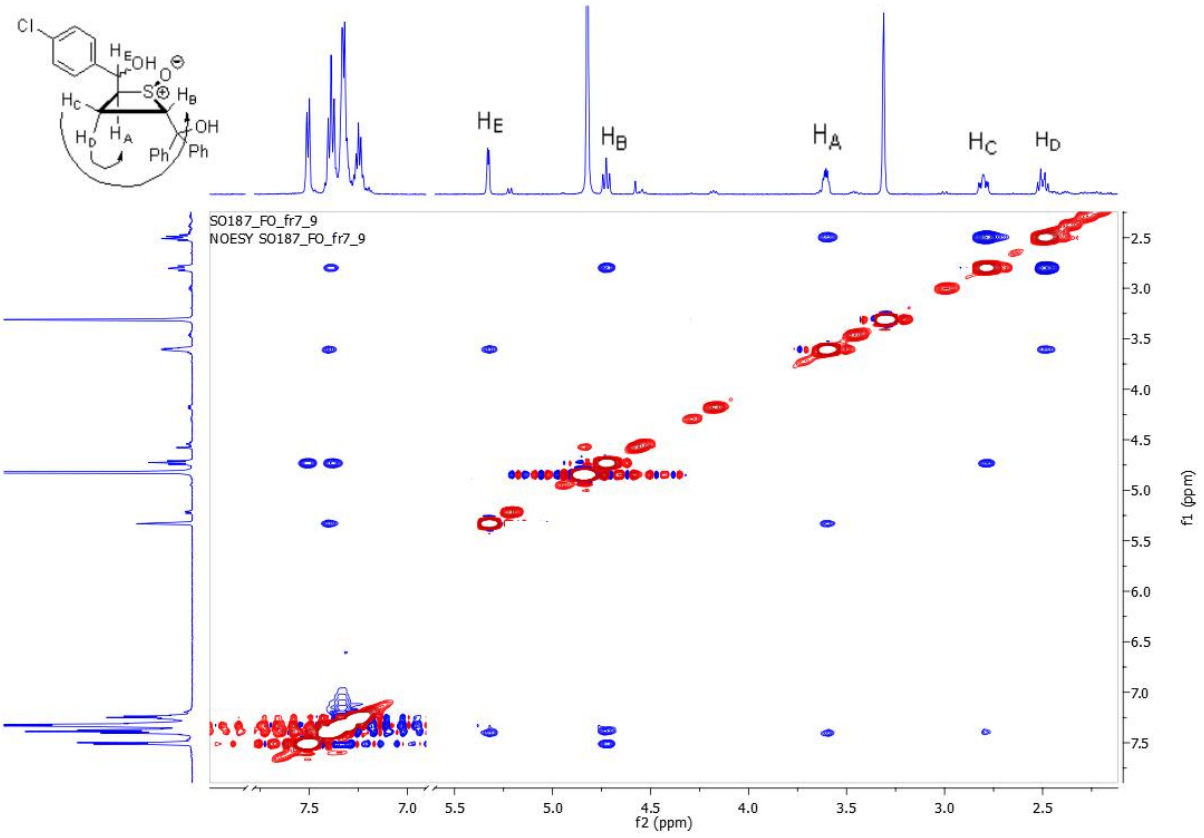

HA
CH2Ph
HB
HD
HC
SO147-fr5-12sol
SO147-fr5-12sol noesy
f2 (ppm)
f1 (ppm)
Ph
O
S
HA
HC
HD
HB
OH
Ph
Ph

(1*R*$_S$,2S*,4S*)*-4e** first eluted diastereoisomer

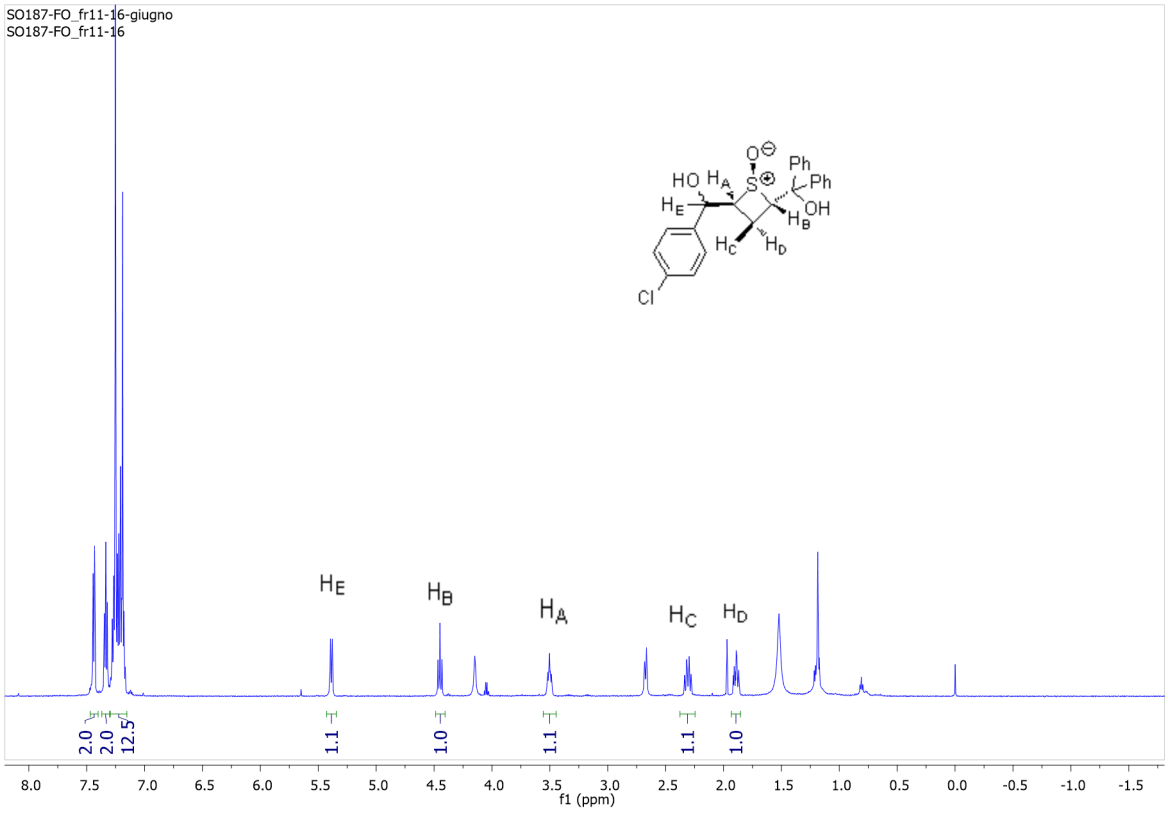


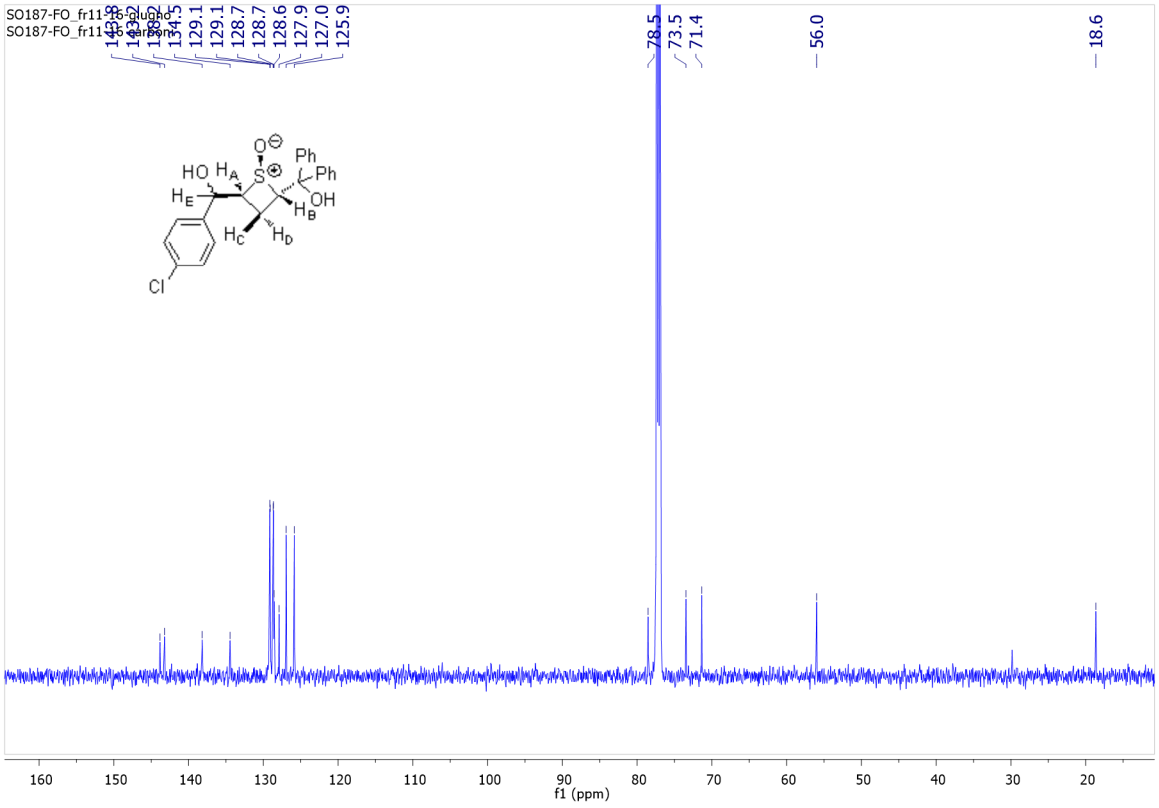


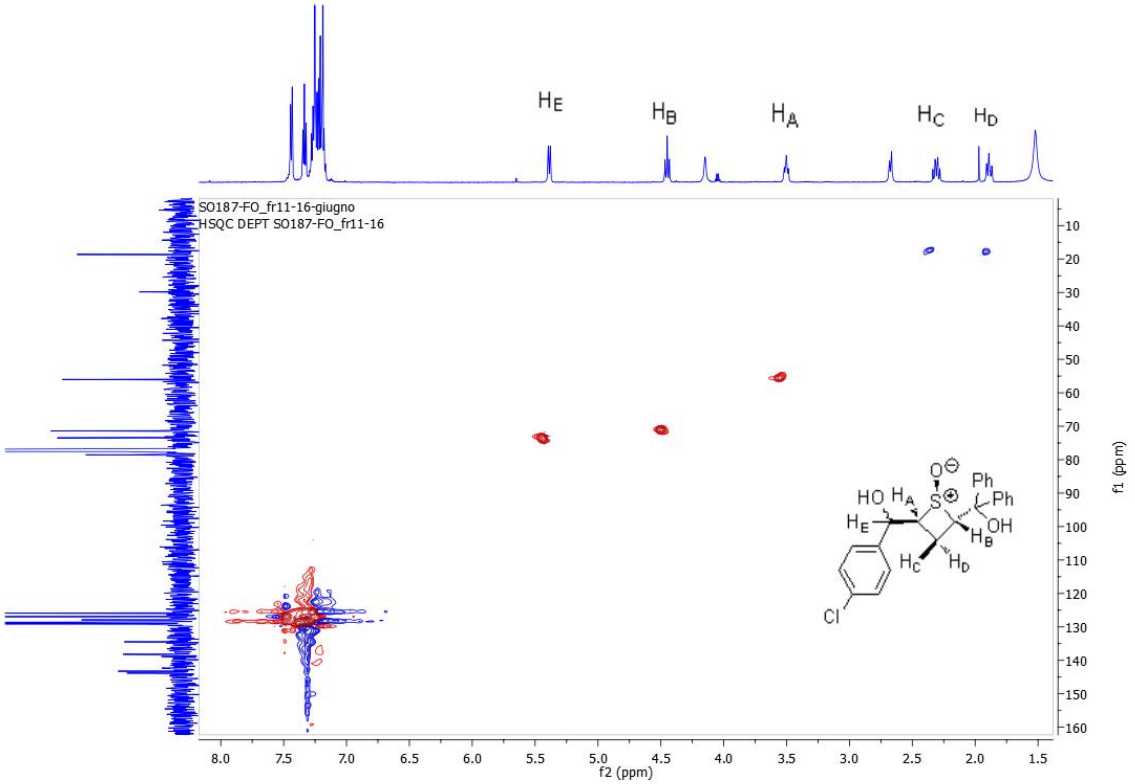

HE
HB
HA
HC
HD
SO187_FO_fr7_9
HSQC DEPT SO187_FO_fr7_9
f2 (ppm)
f1 (ppm)

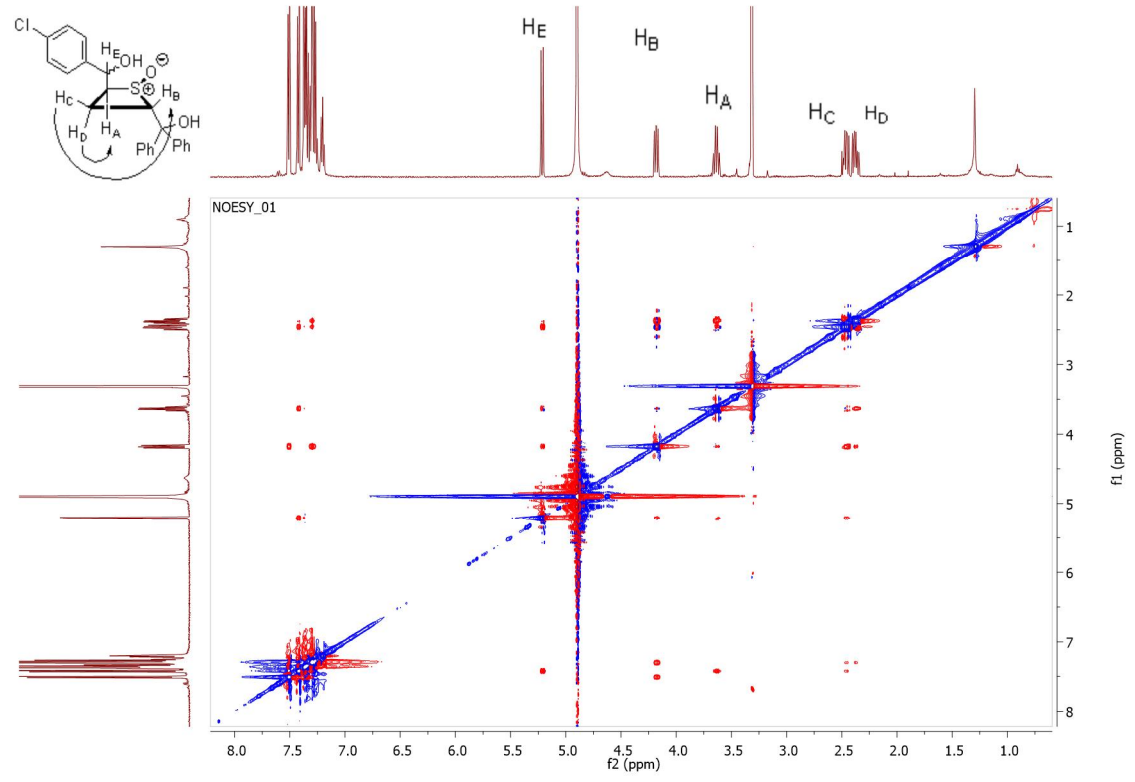

HE
HB
HA
HC
HD
SO187_FO_fr7_9
NOESY SO187_FO_fr7_9
f2 (ppm)
f1 (ppm)

(1*R*$_S$,2S*,4S*)*-4e** second eluted diastereoisomer



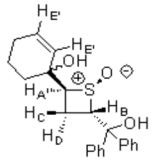


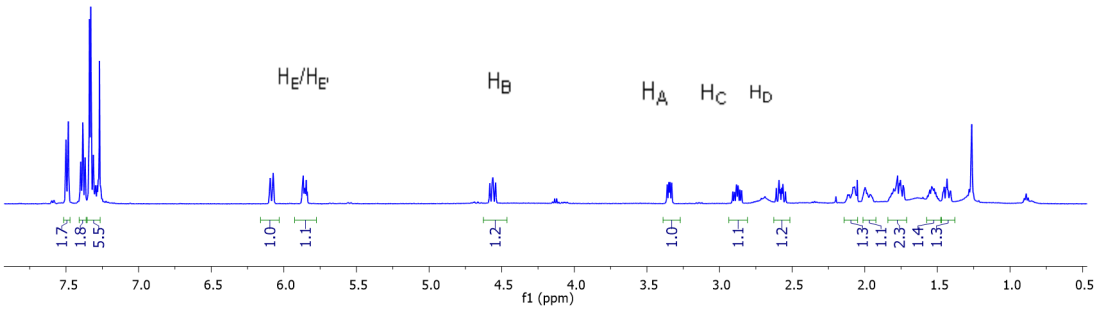

HE
HB
HA
HC
HD
SO187-FO_fr11-16-giugno
HSQC DEPT SO187-FO_fr11-16
f2 (ppm)
f1 (ppm)


HE
HB
HA
HC
HD
NOESY_01
f2 (ppm)
f1 (ppm)

(1*R*$_S$,2S*,4S*)-4f** first eluted diastereoisomer

PROTON_01





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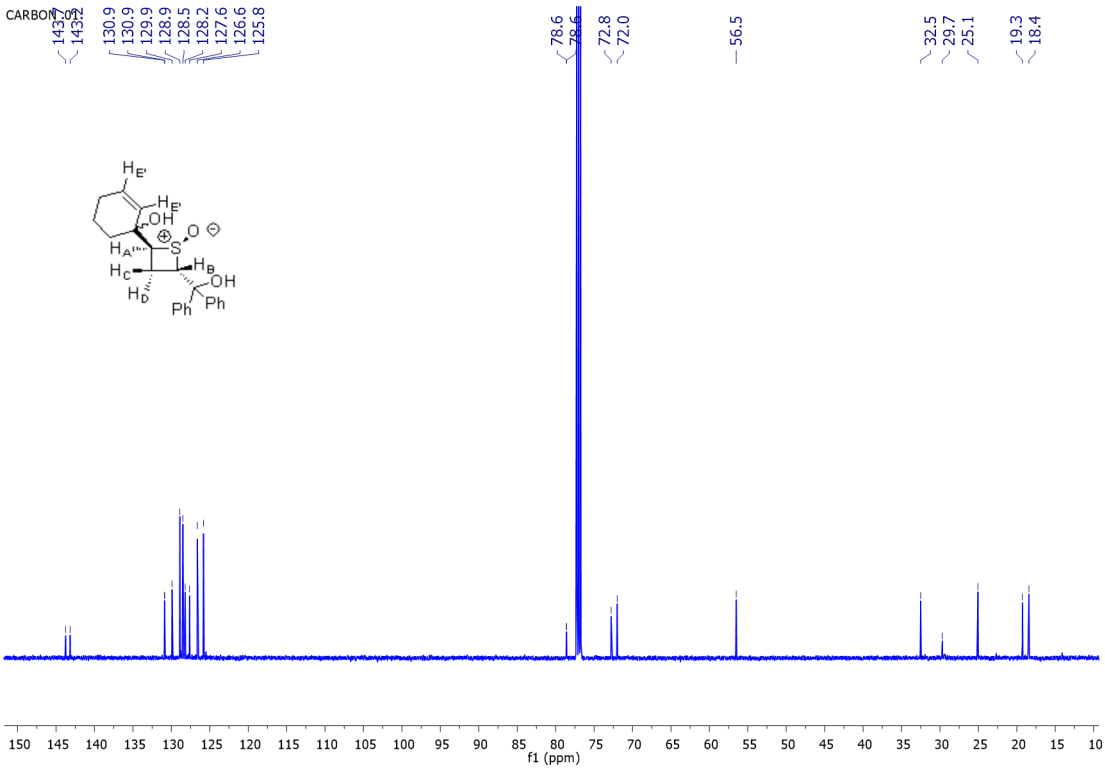
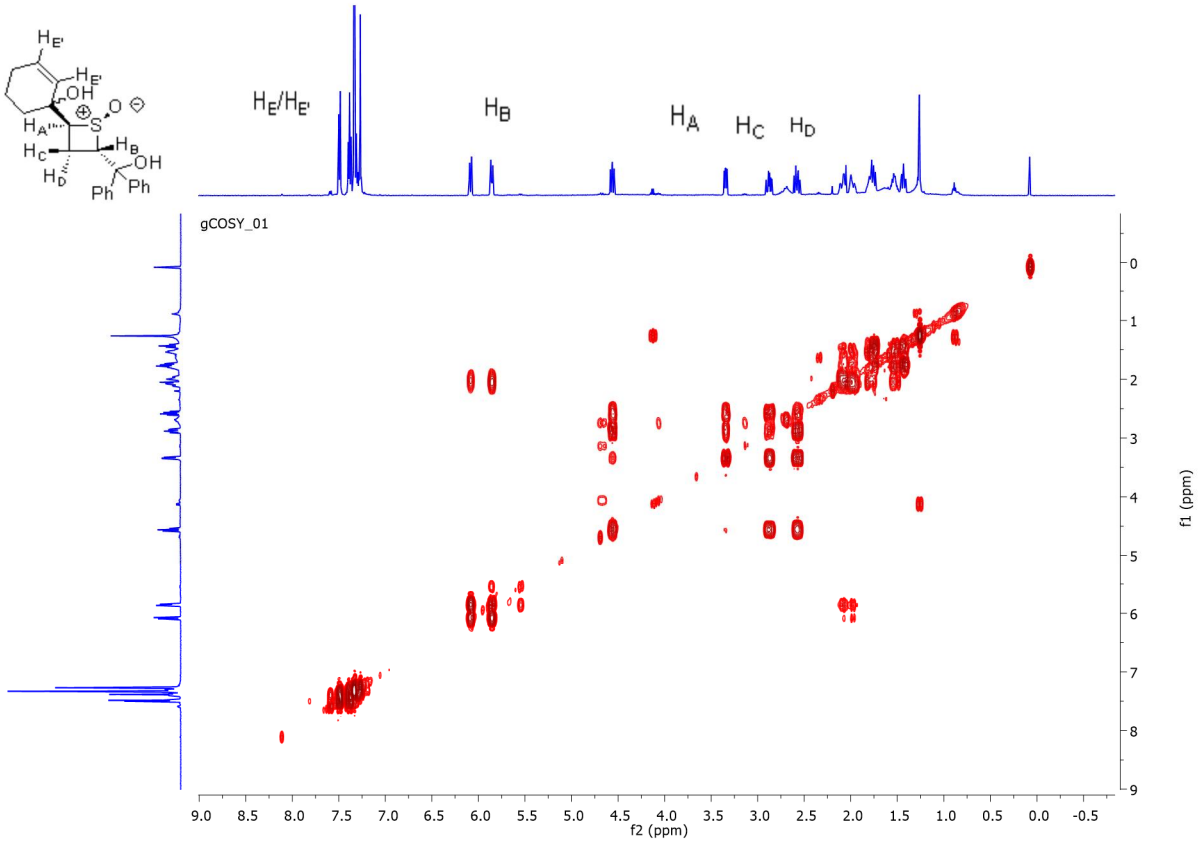
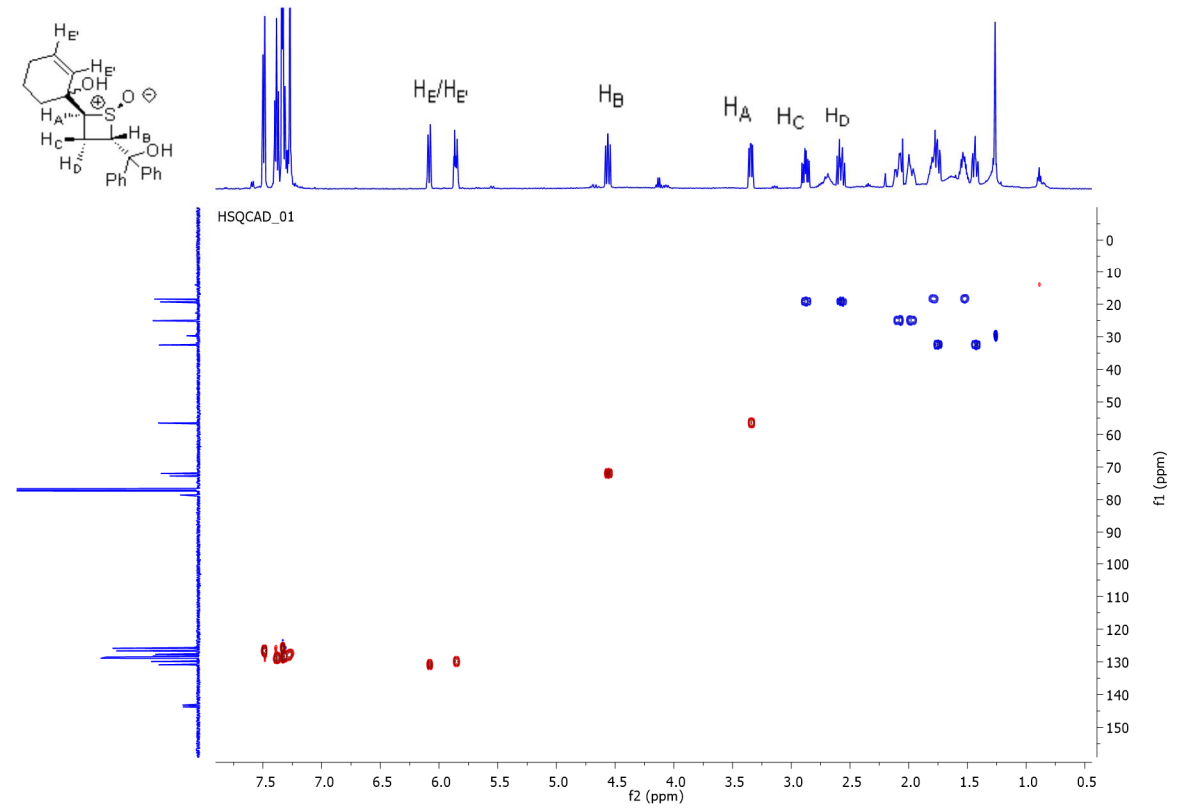
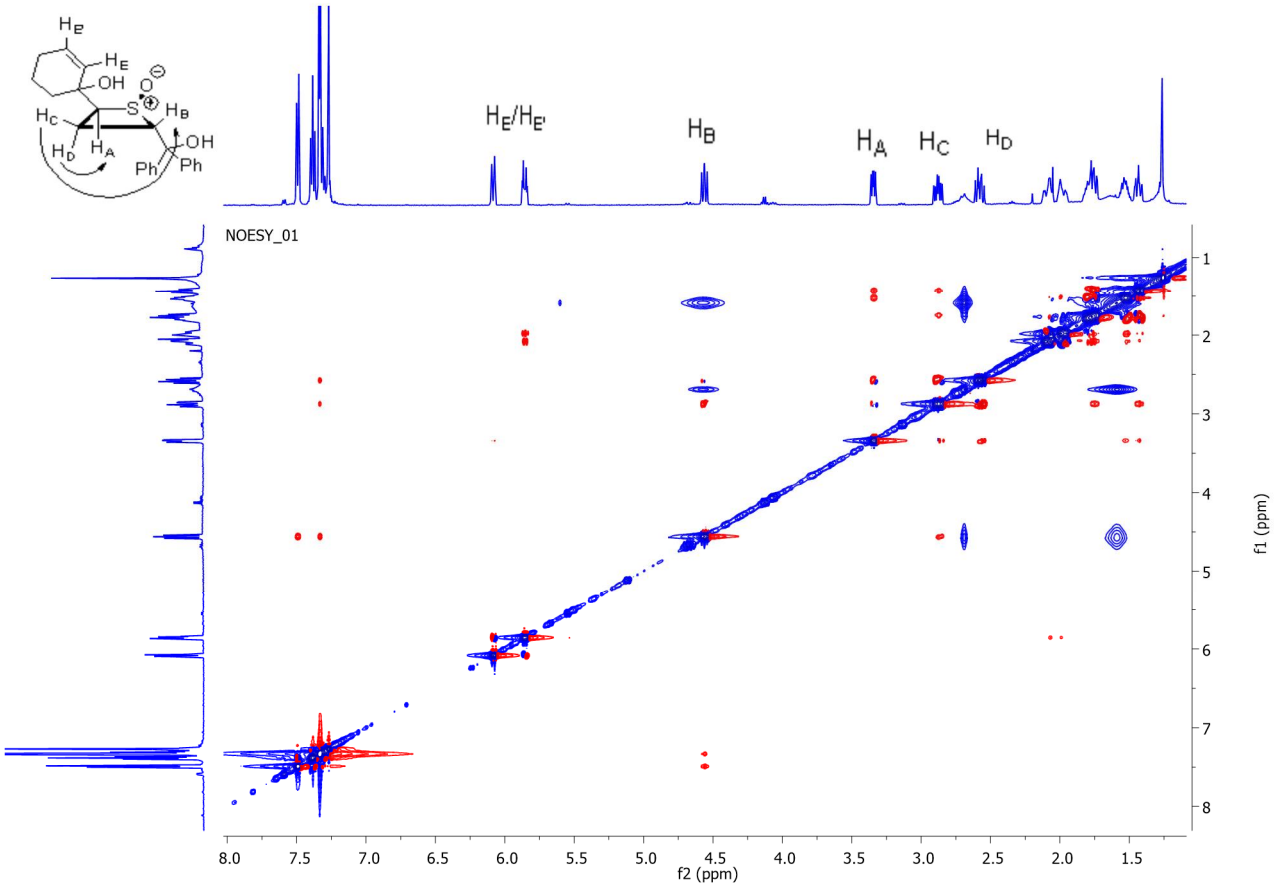
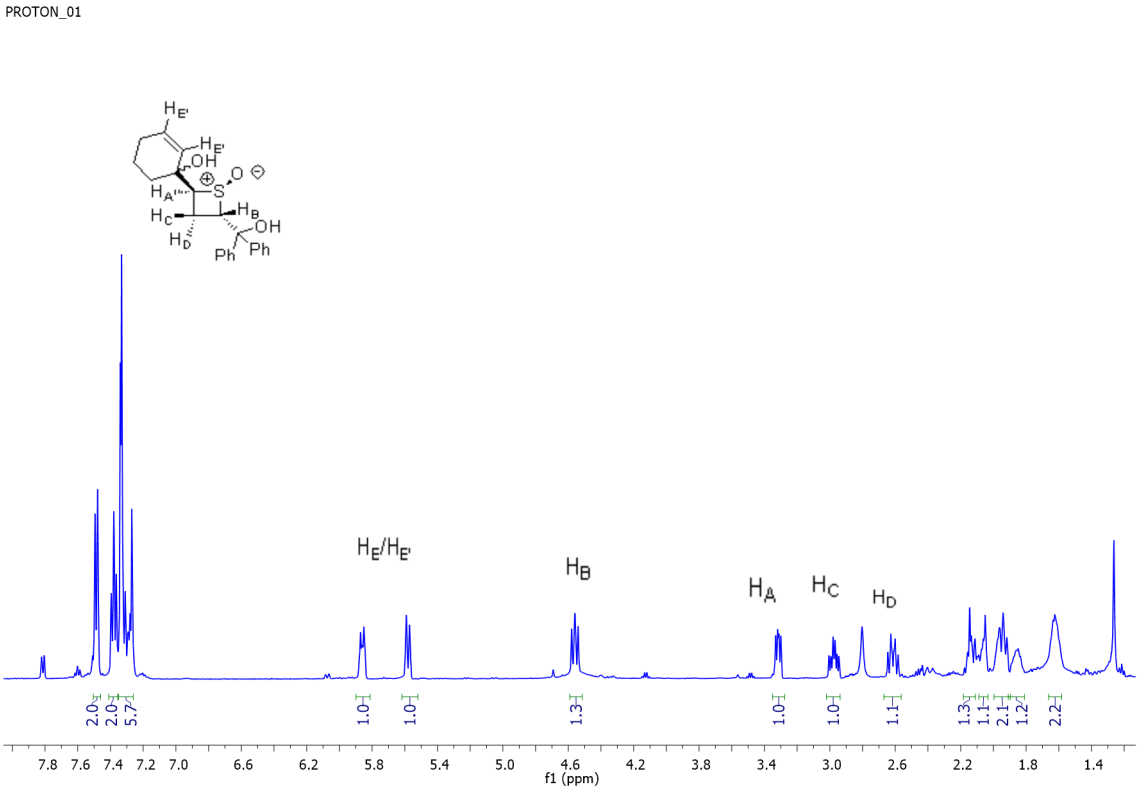


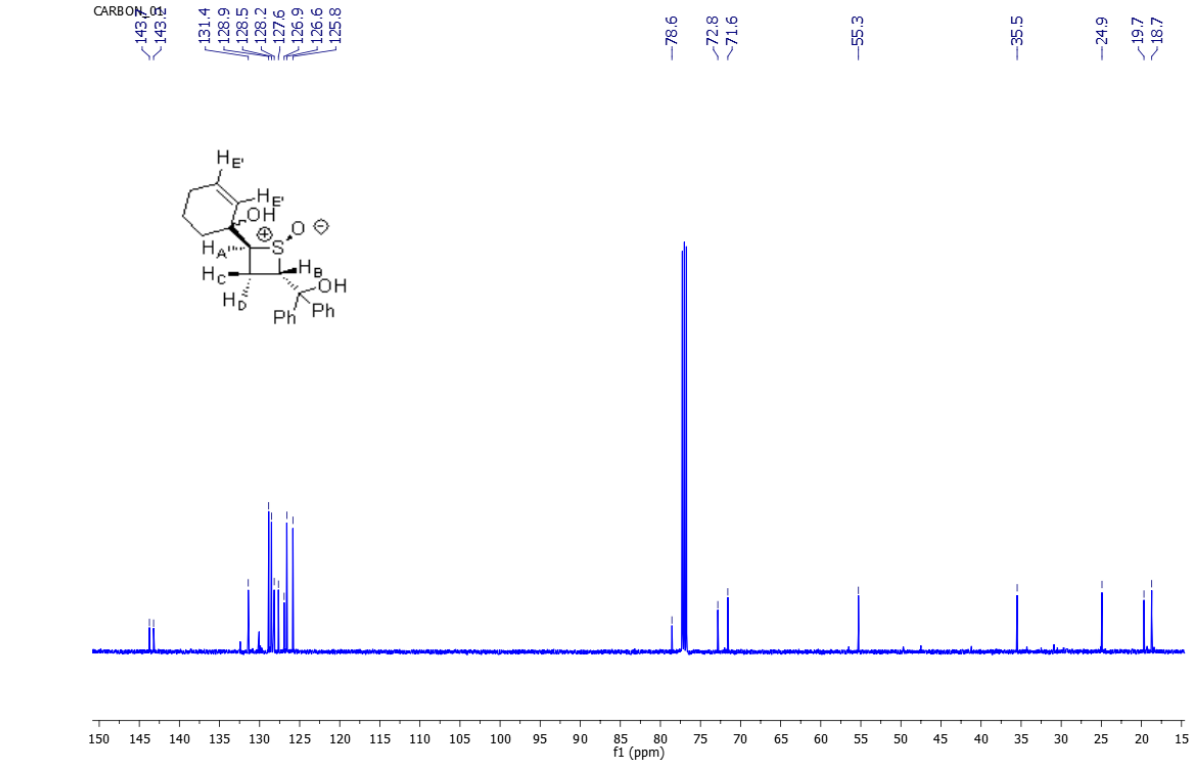

HE'
HE'
OH
O
HA
S
HB
HC
OH
HD
Ph
Ph
HE'/HE'
HB
HA
HC
HD
gCOSY_01
f1 (ppm)
f2 (ppm)

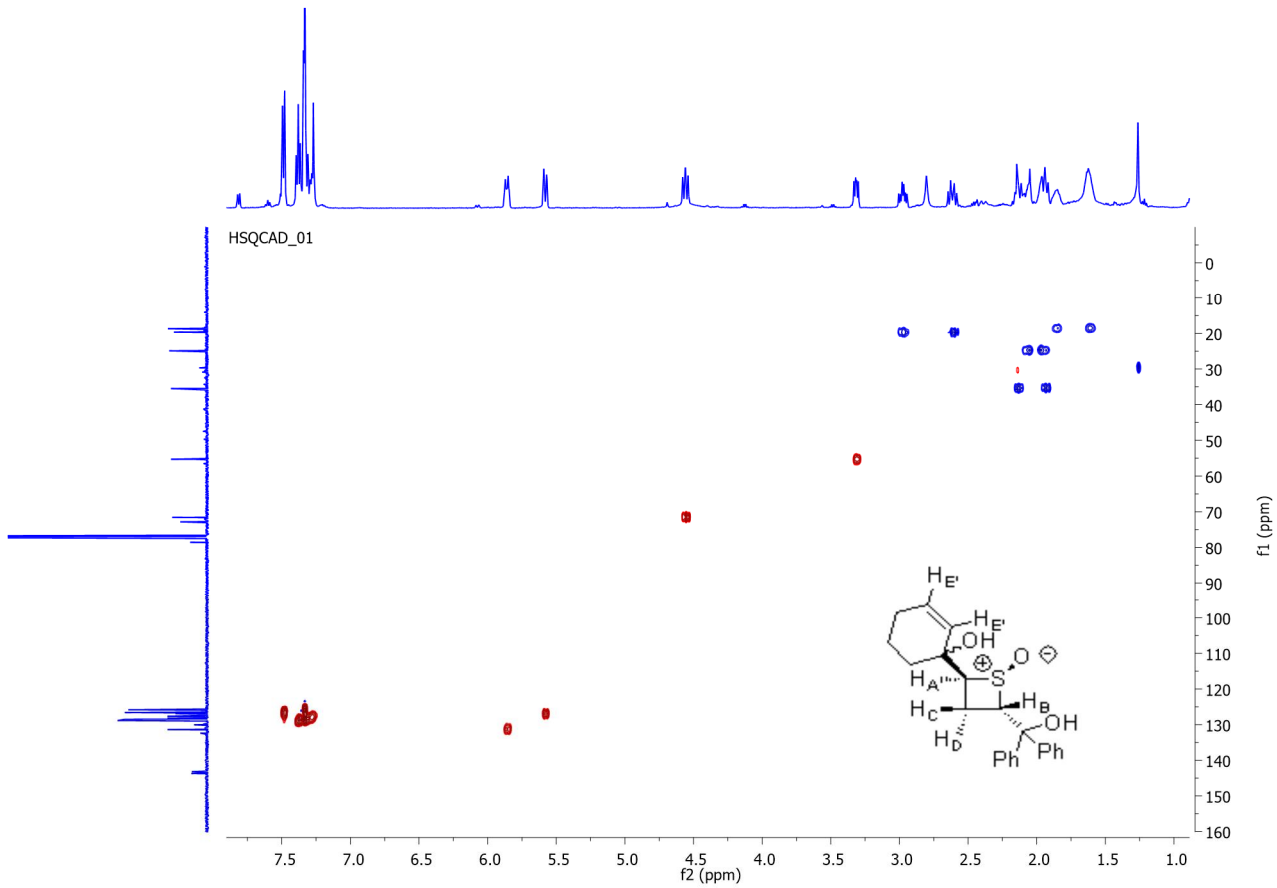

HE'
HE'
OH
O
HA
S
HB
HC
OH
HD
Ph
Ph
HE'/HE'
HB
HA
HC
HD
HSQCAD_01
f1 (ppm)
f2 (ppm)

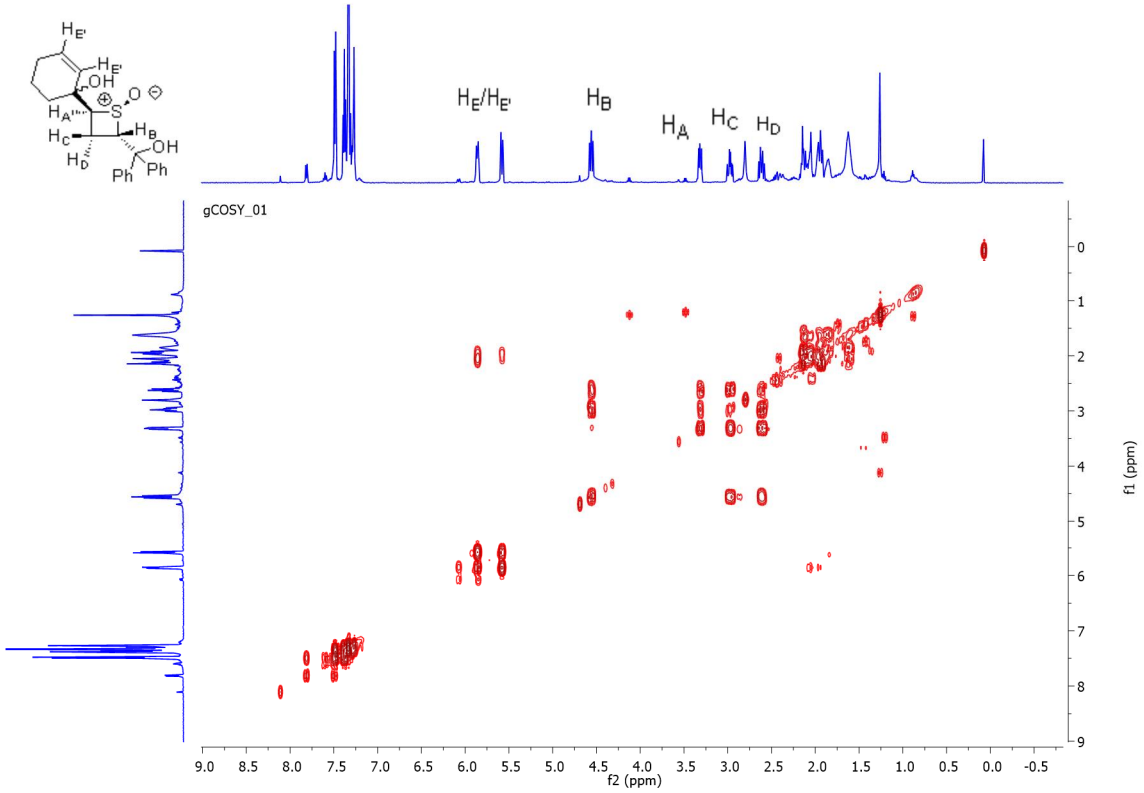


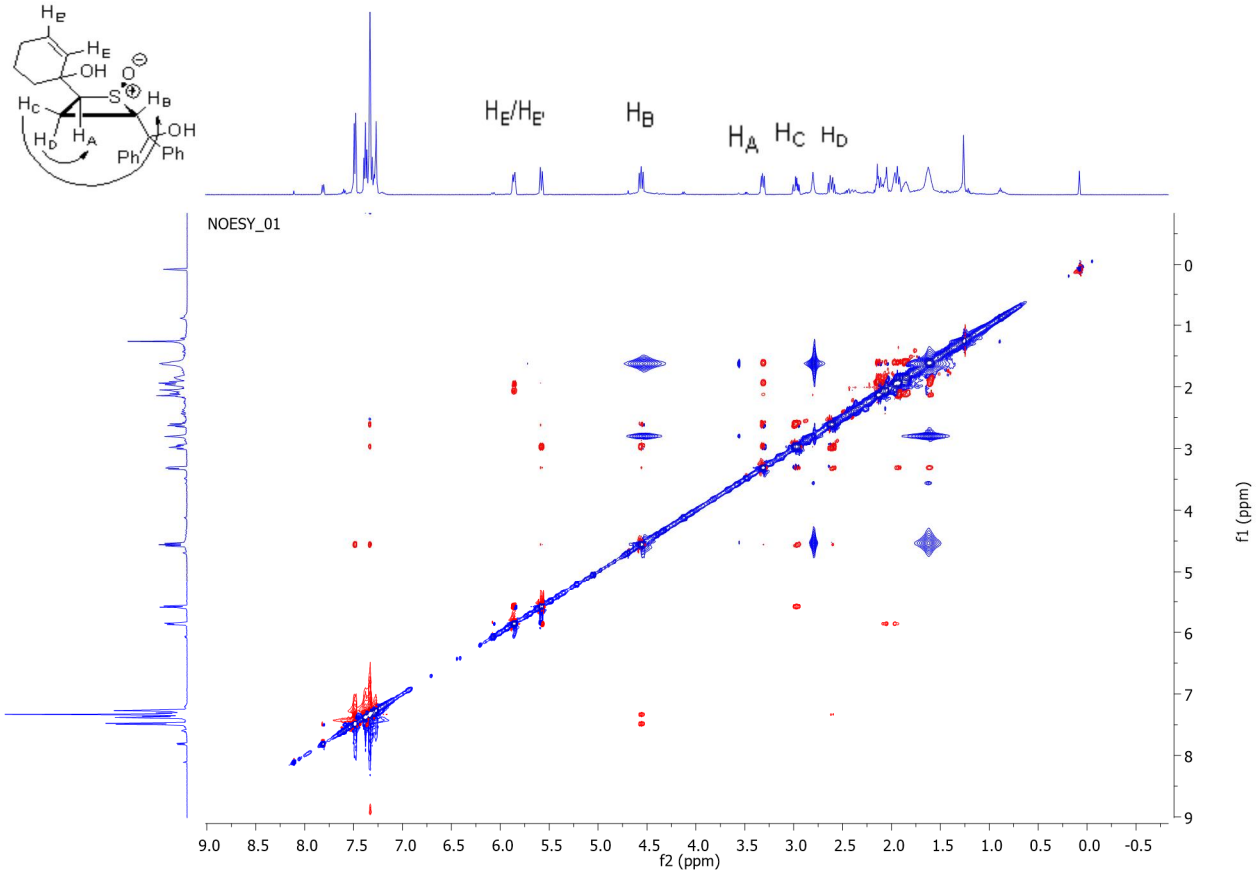
(1*R*$_S$,2S*,4S*)-4f** second eluted diastereoisomer



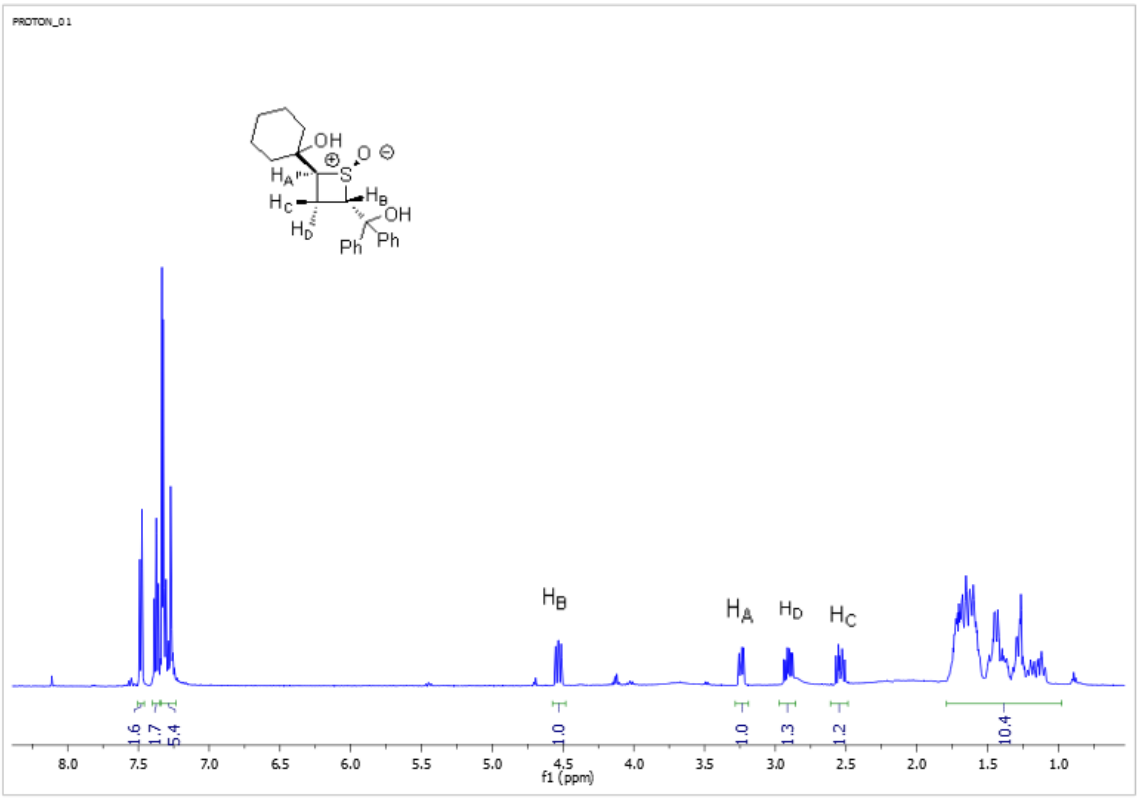

CARBON_01
143.2
143.1
131.4
128.9
128.5
128.2
127.6
126.9
126.6
125.8
78.6
72.8
71.6
55.3
35.5
24.9
19.7
18.7
f1 (ppm)

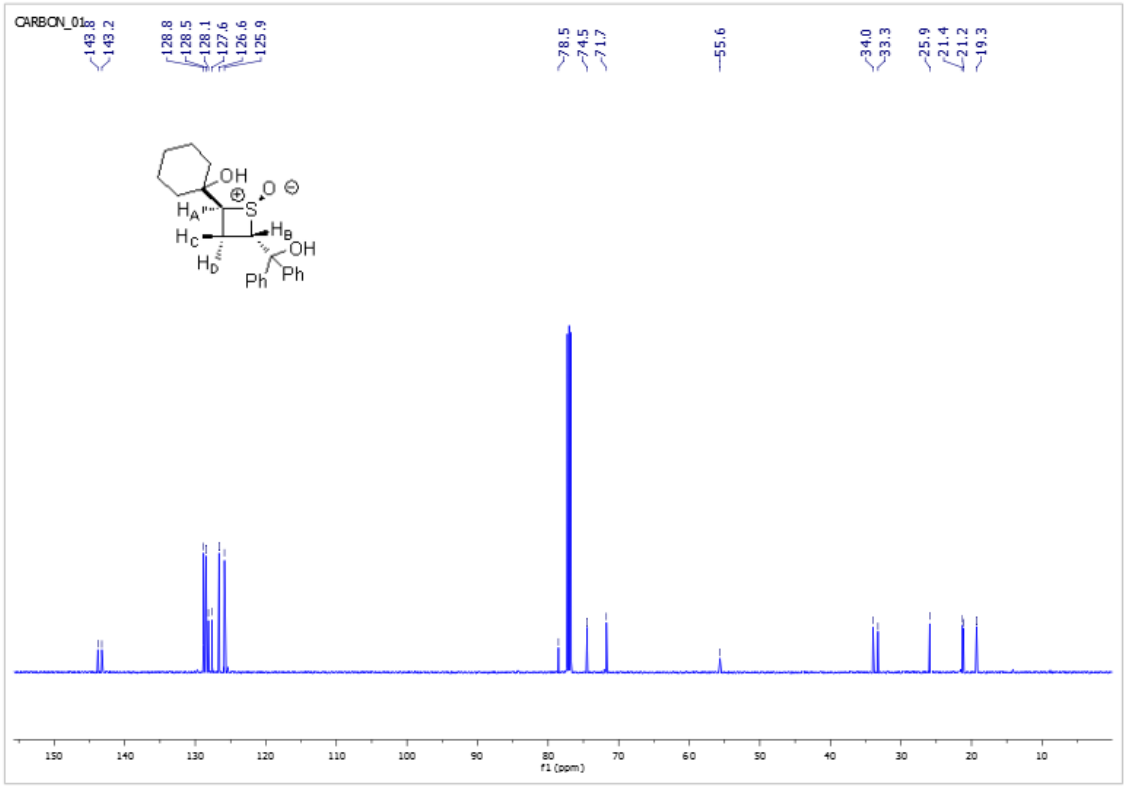

HSQCAD_01
f2 (ppm)
f1 (ppm)

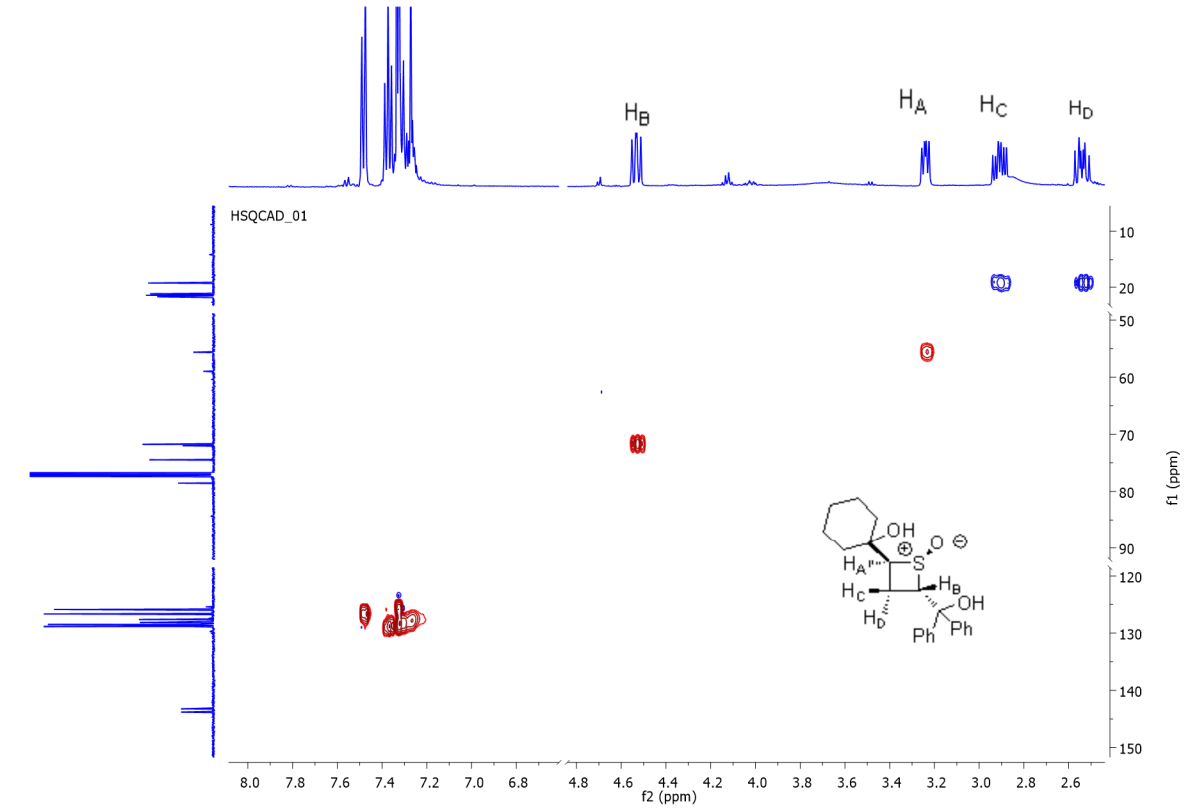

gCOSY_01
HE/HE'
HB
HA
HC
HD
f1 (ppm)
f2 (ppm)

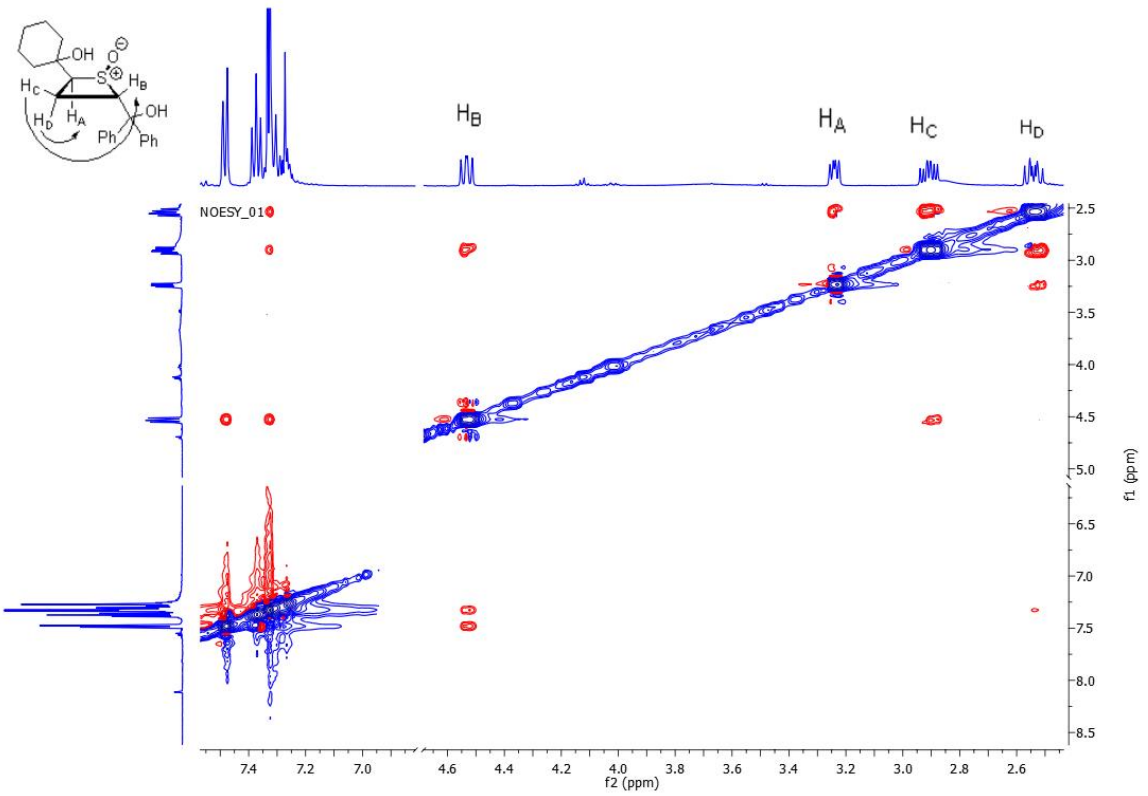

NOESY_01
HE/HE'
HB
HA
HC
HD
f1 (ppm)
f2 (ppm)

(1R_S*,2*S,4*S**)-4g**

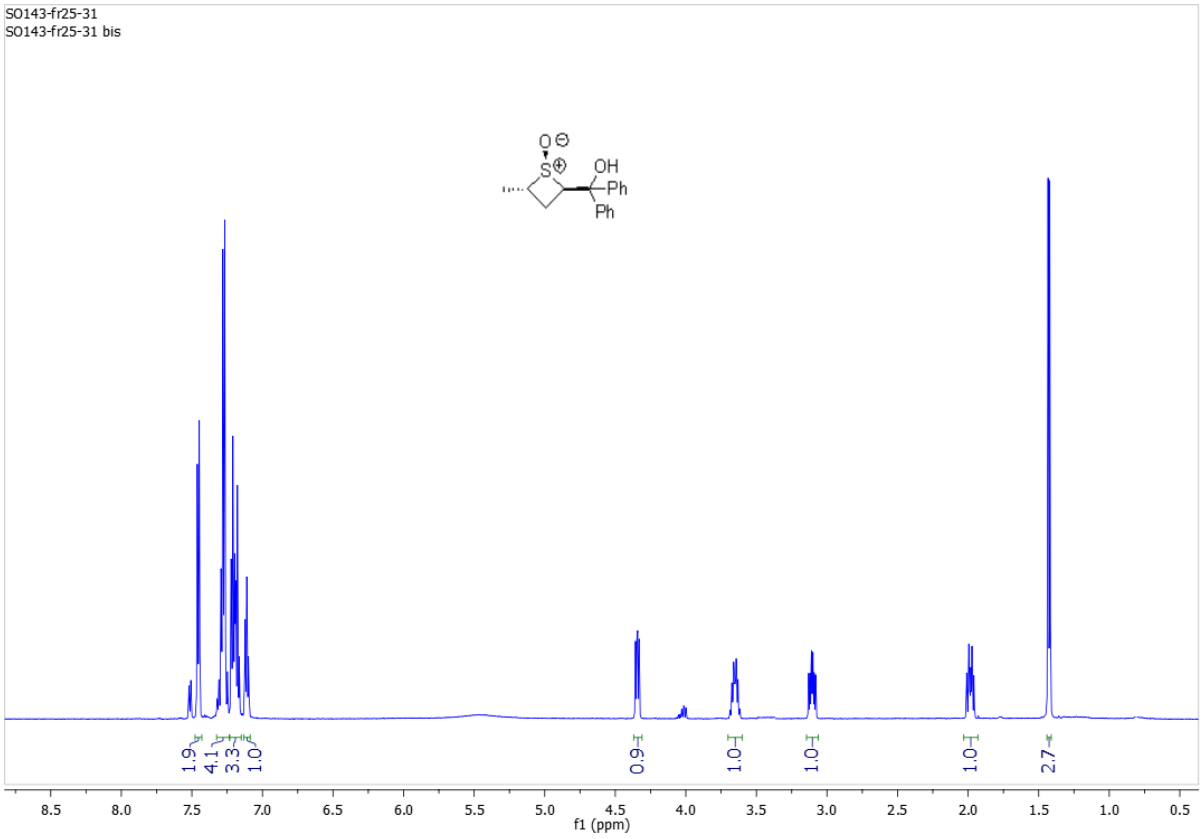

PROTON_01
OH
O
HA
S
HB
HC
HD
OH
Ph
Ph
HB
HA
HD
HC
1.6
1.7
5.4
1.0
1.0
1.3
1.2
10.4
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

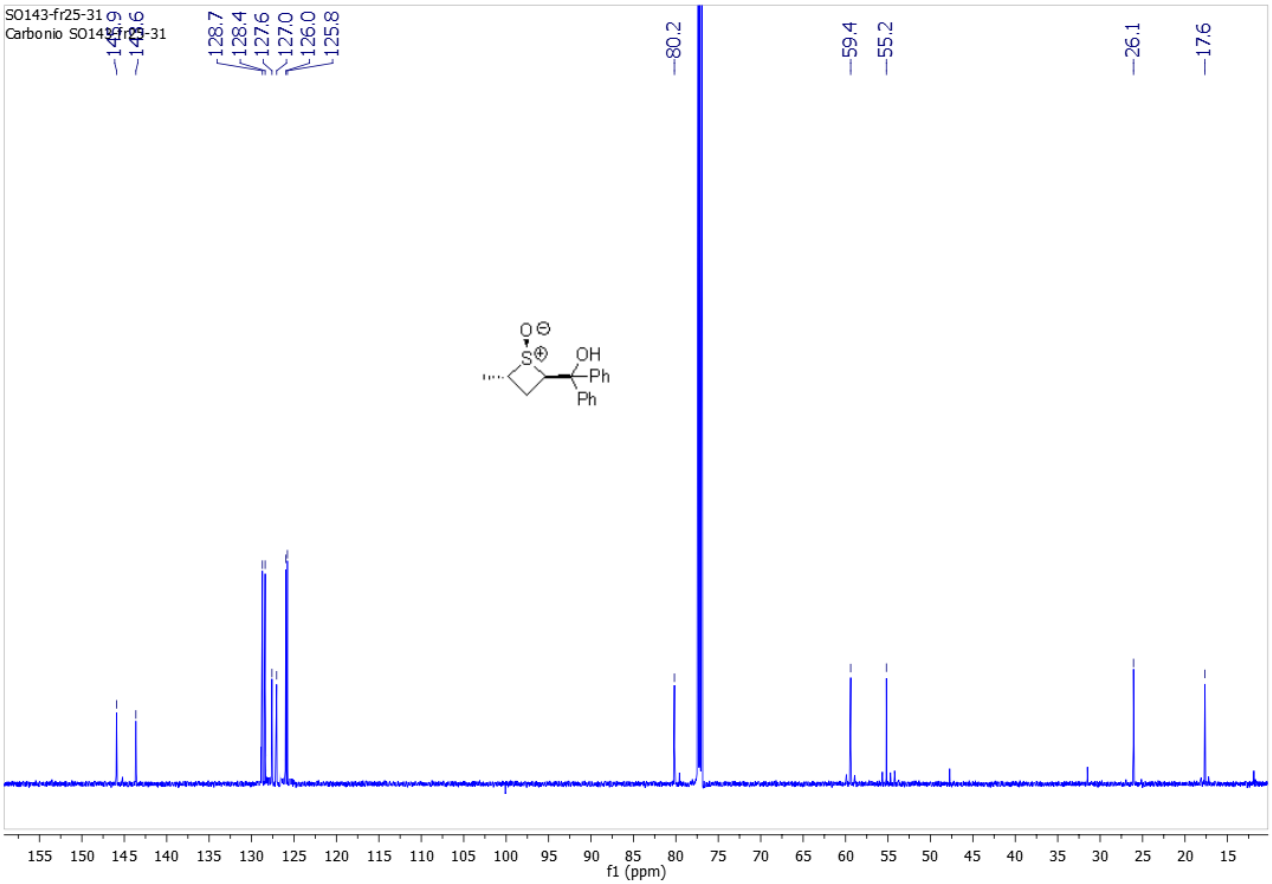

CARBON_01
143.8
143.2
128.8
128.5
128.1
127.6
126.6
125.9
78.5
74.5
71.7
55.6
34.0
33.3
25.9
21.4
21.2
19.3
OH
O
HA
S
HB
HC
HD
OH
Ph
Ph
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

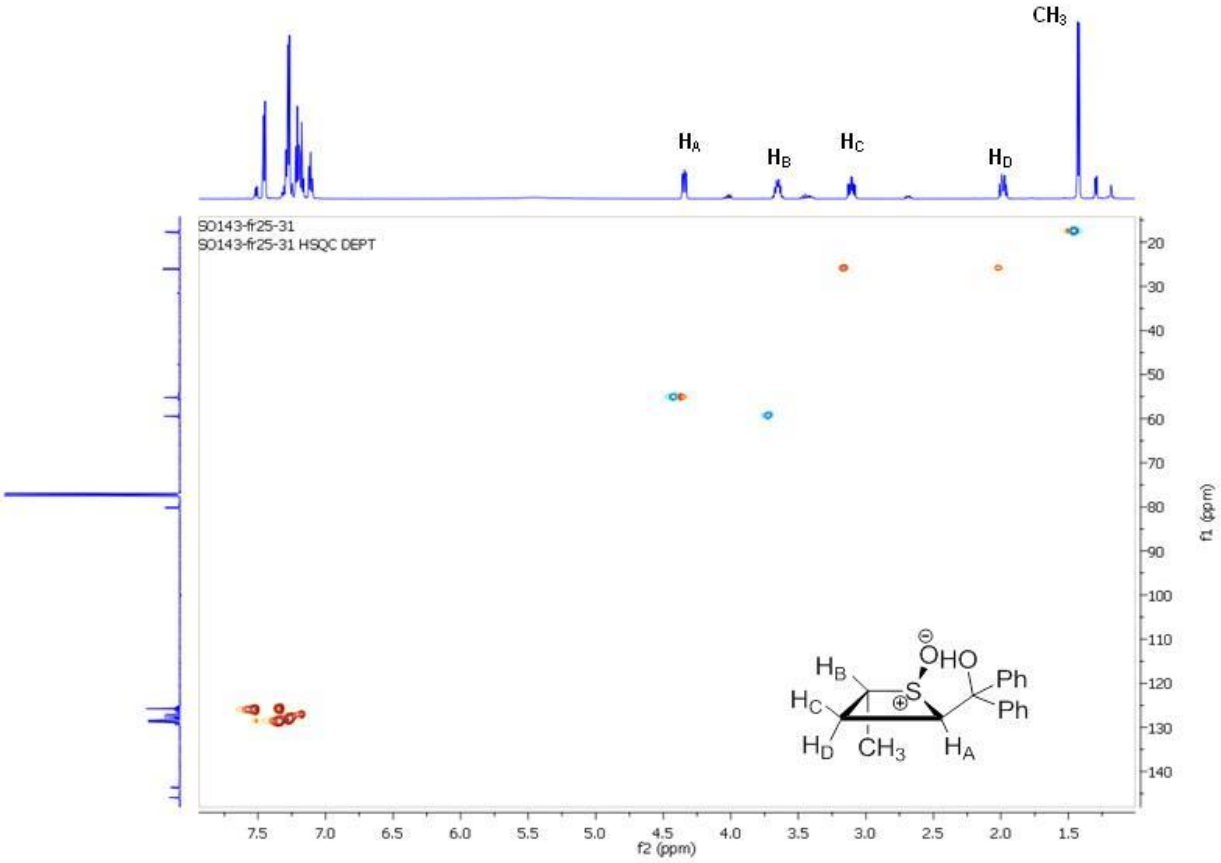

HB
HA
HC
HD
HSQCAD_01
f2 (ppm)
f1 (ppm)

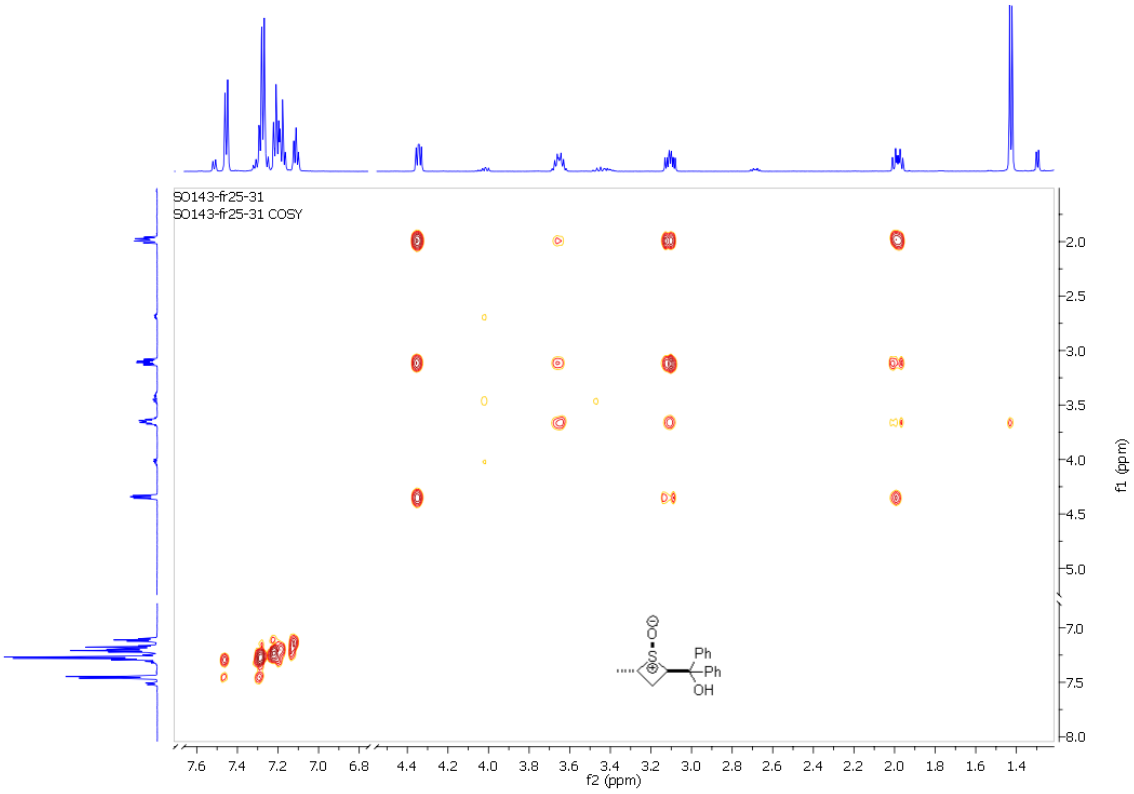

HB
HA
HC
HD
NOESY_01
f2 (ppm)
f1 (ppm)

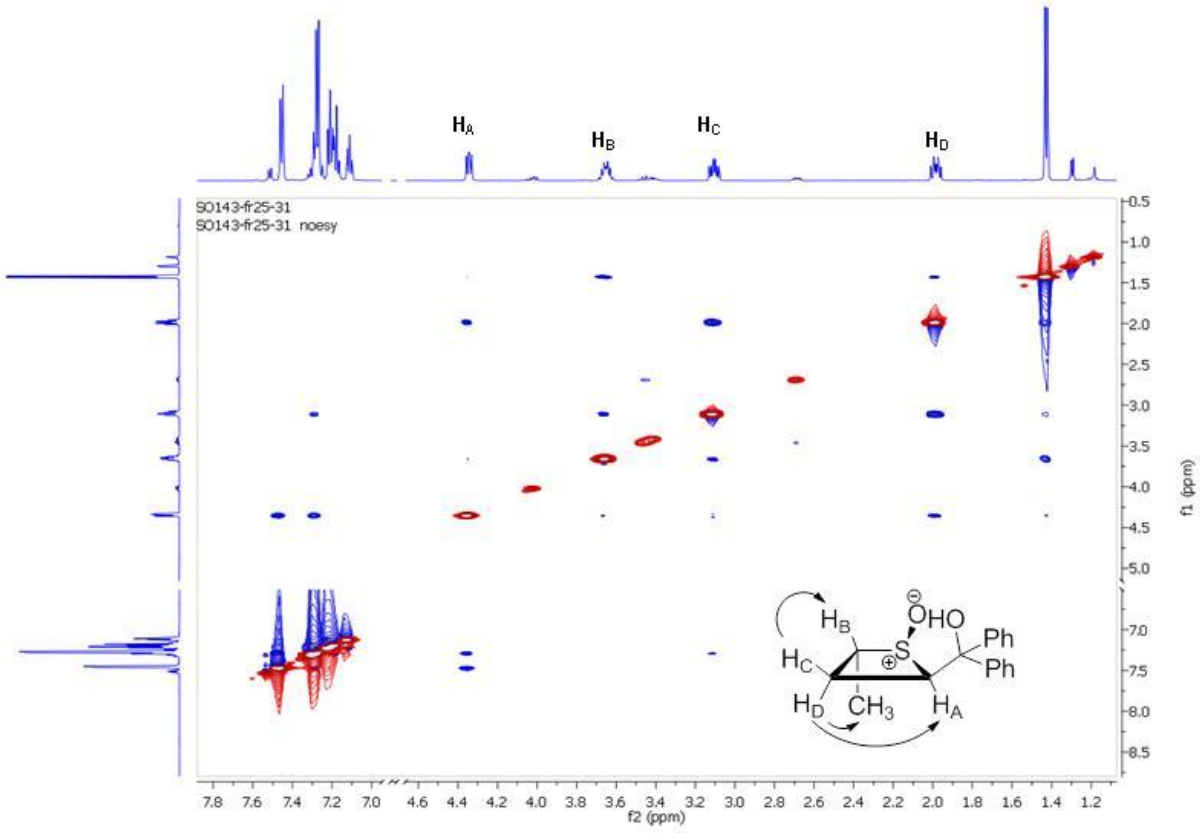
(1R_S*,2*R,4*S**)-5a *major***



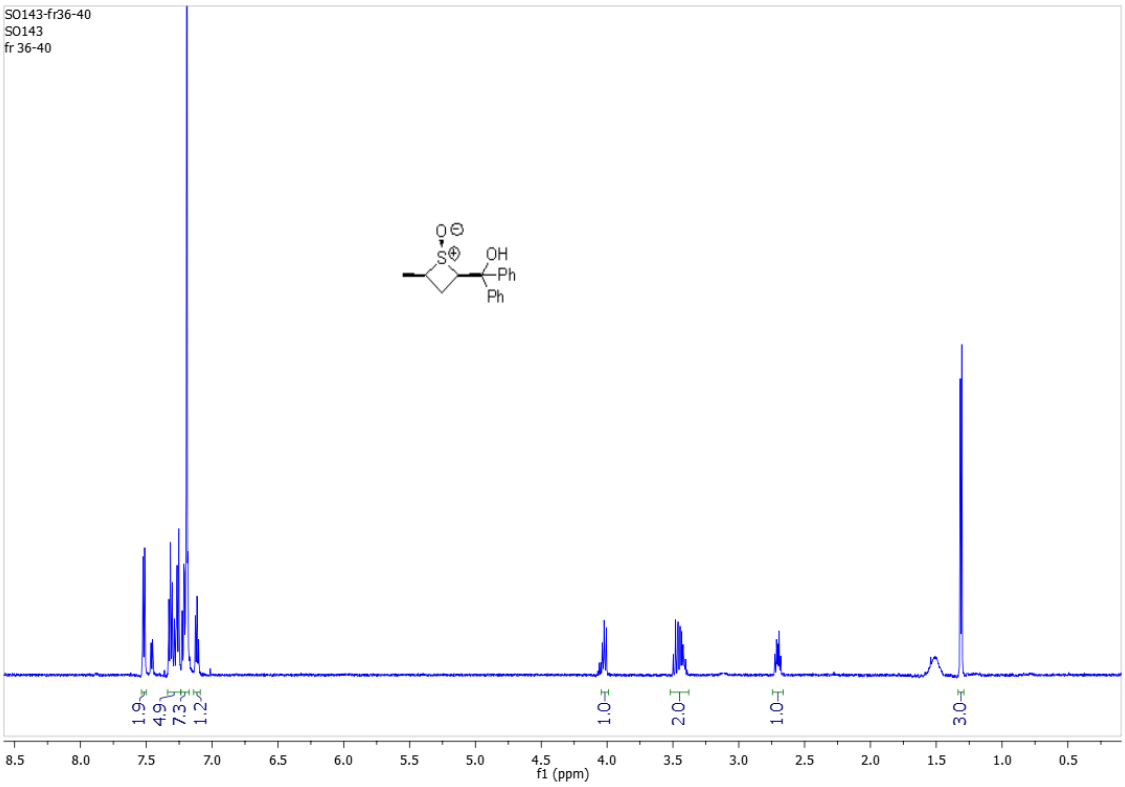


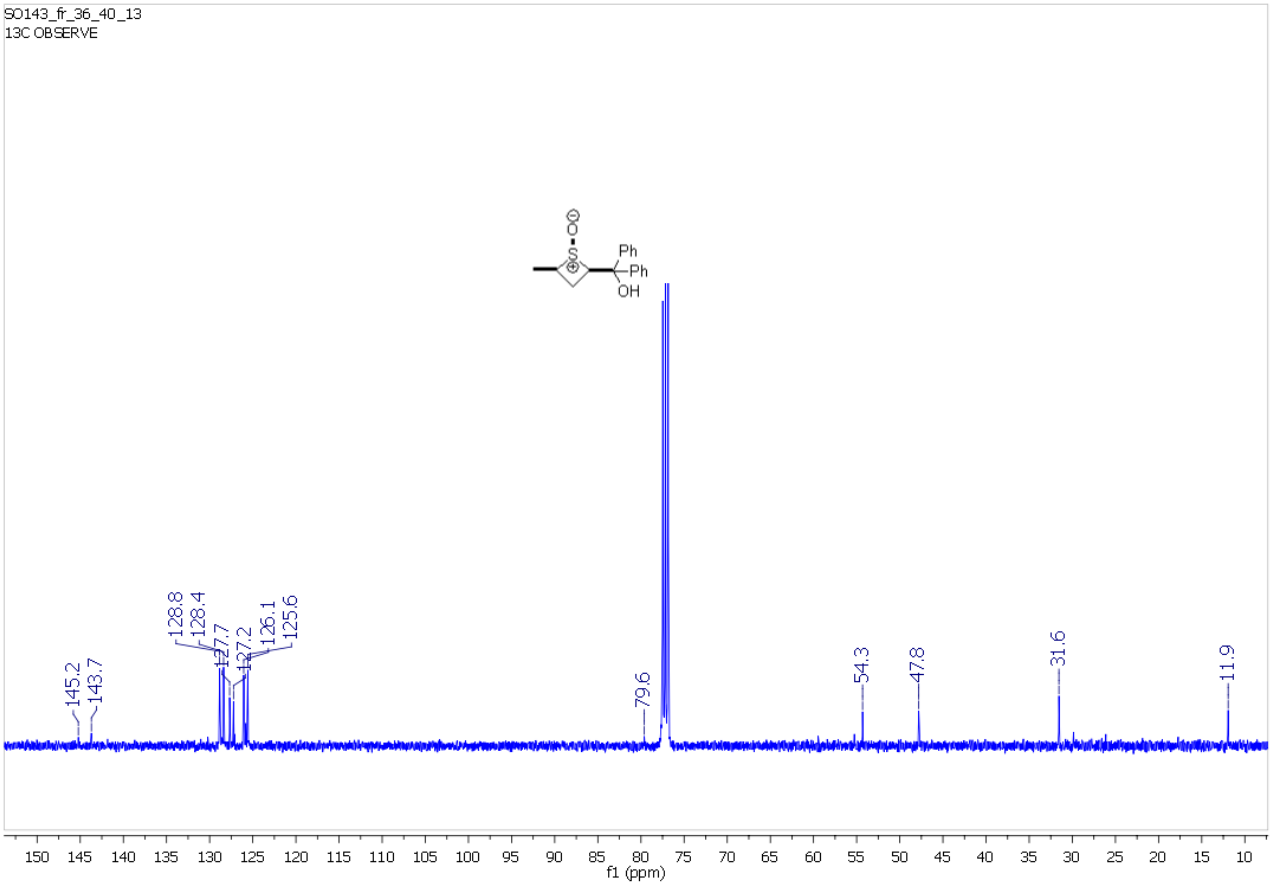

CH3
HA
HB
HC
HD
SO143-fr25-31
SO143-fr25-31 HSQC DEPT
f1 (ppm)
f2 (ppm)
HB
HC
HD
CH3
HA
OHO
S
Ph
Ph


SO143-fr25-31
SO143-fr25-31 COSY
f1 (ppm)
f2 (ppm)
Ph
Ph
OH

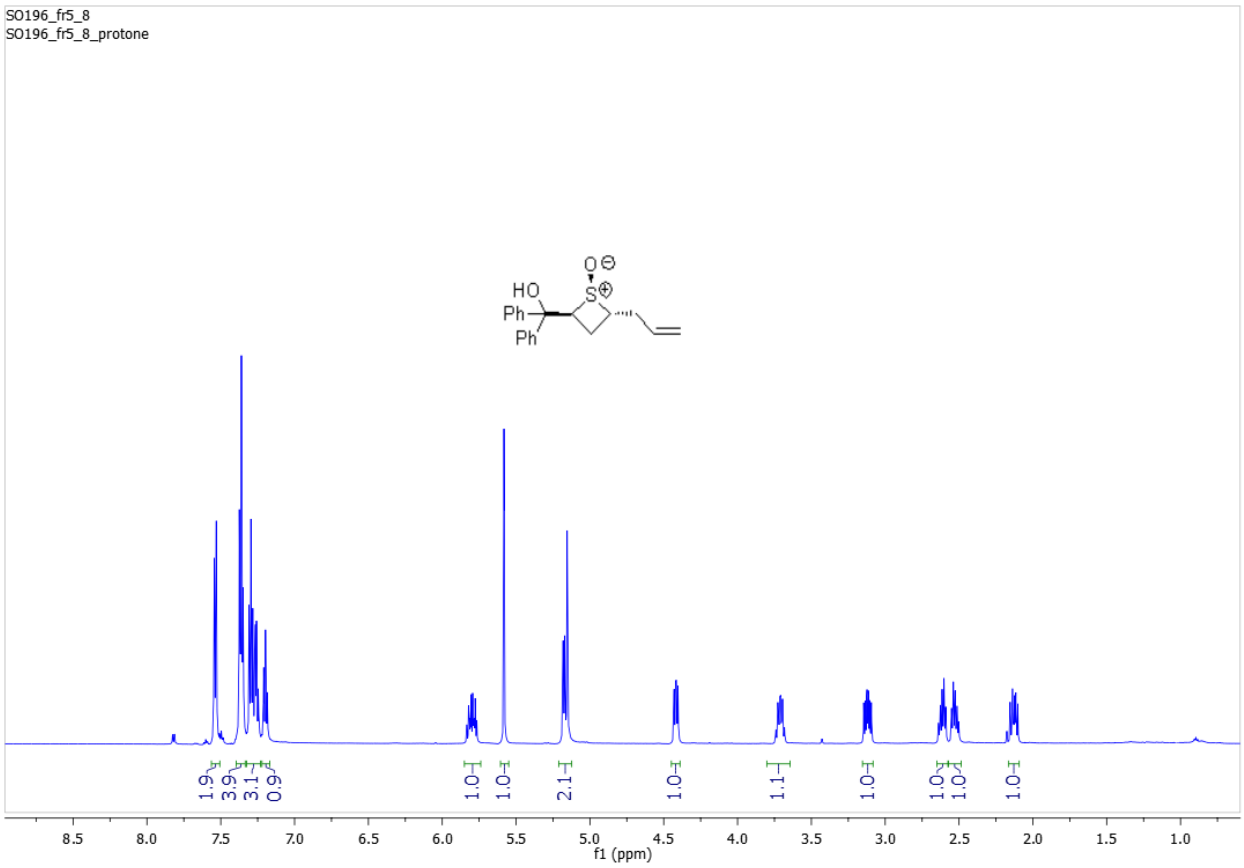

HA
HB
HC
HD
SO143-fr25-31
SO143-fr25-31 noesy
f2 (ppm)
f1 (ppm)
HB
HC
HD
CH3
HA
OHO
S
Ph
Ph

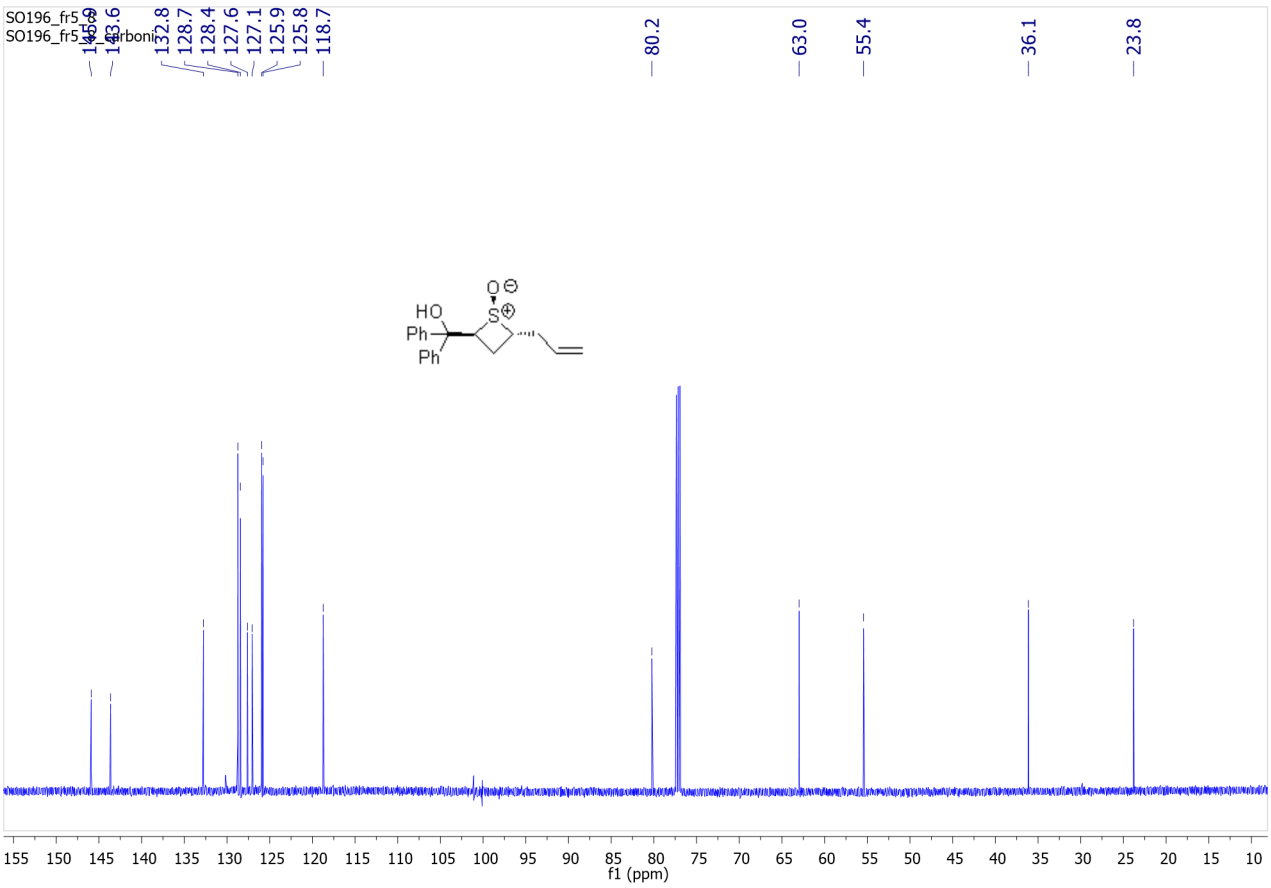
(1R_S*,2*R,4*R**)-5a *minor***



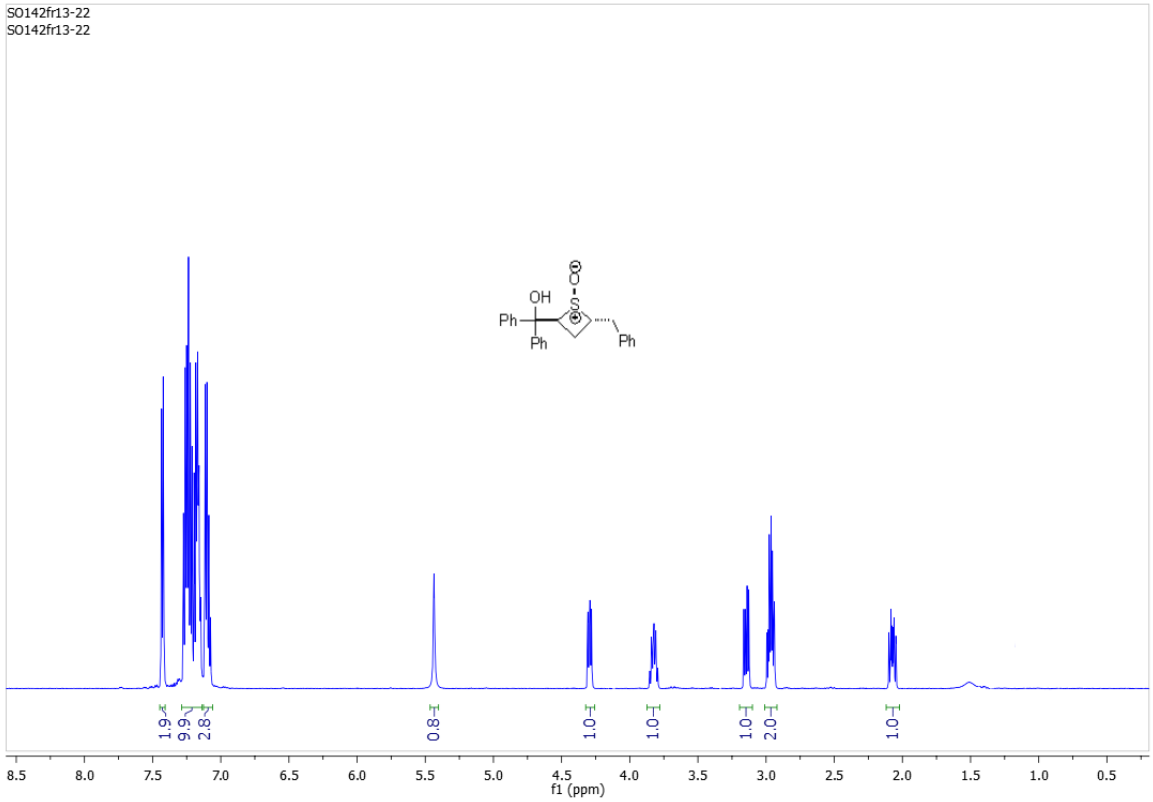


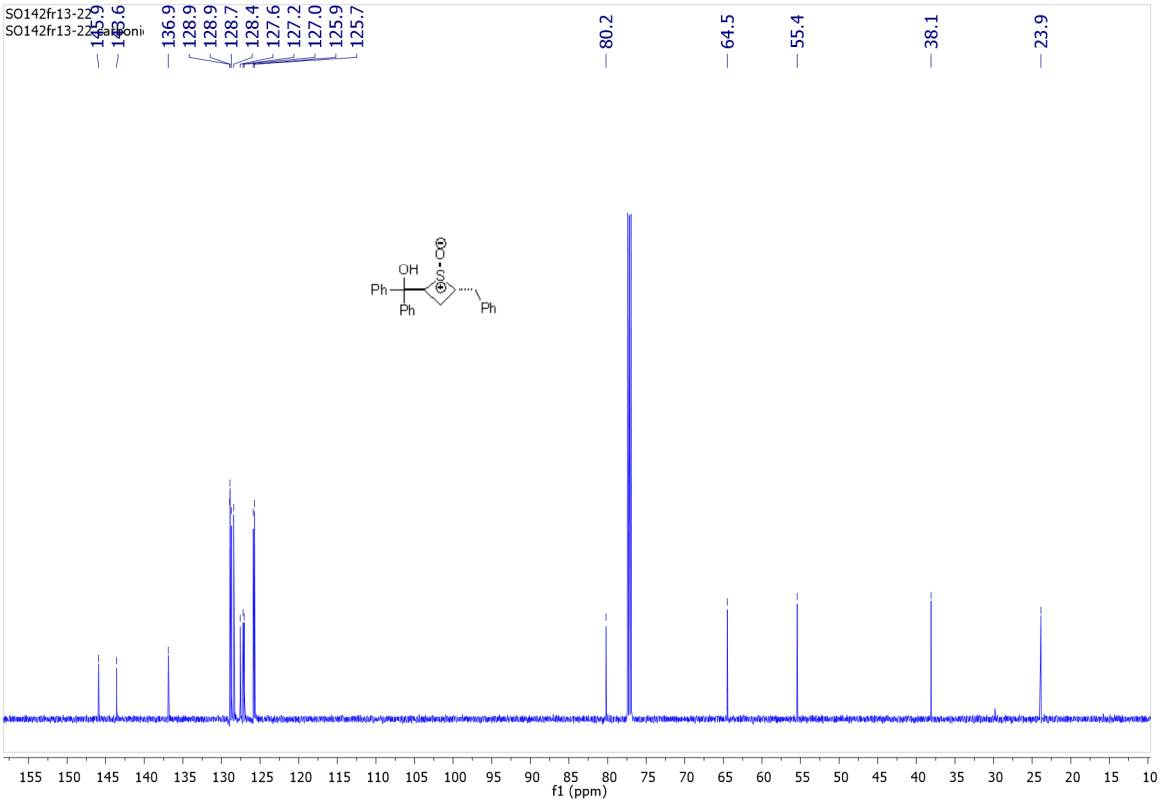
(1R_S*,2R*,4S*)-5c

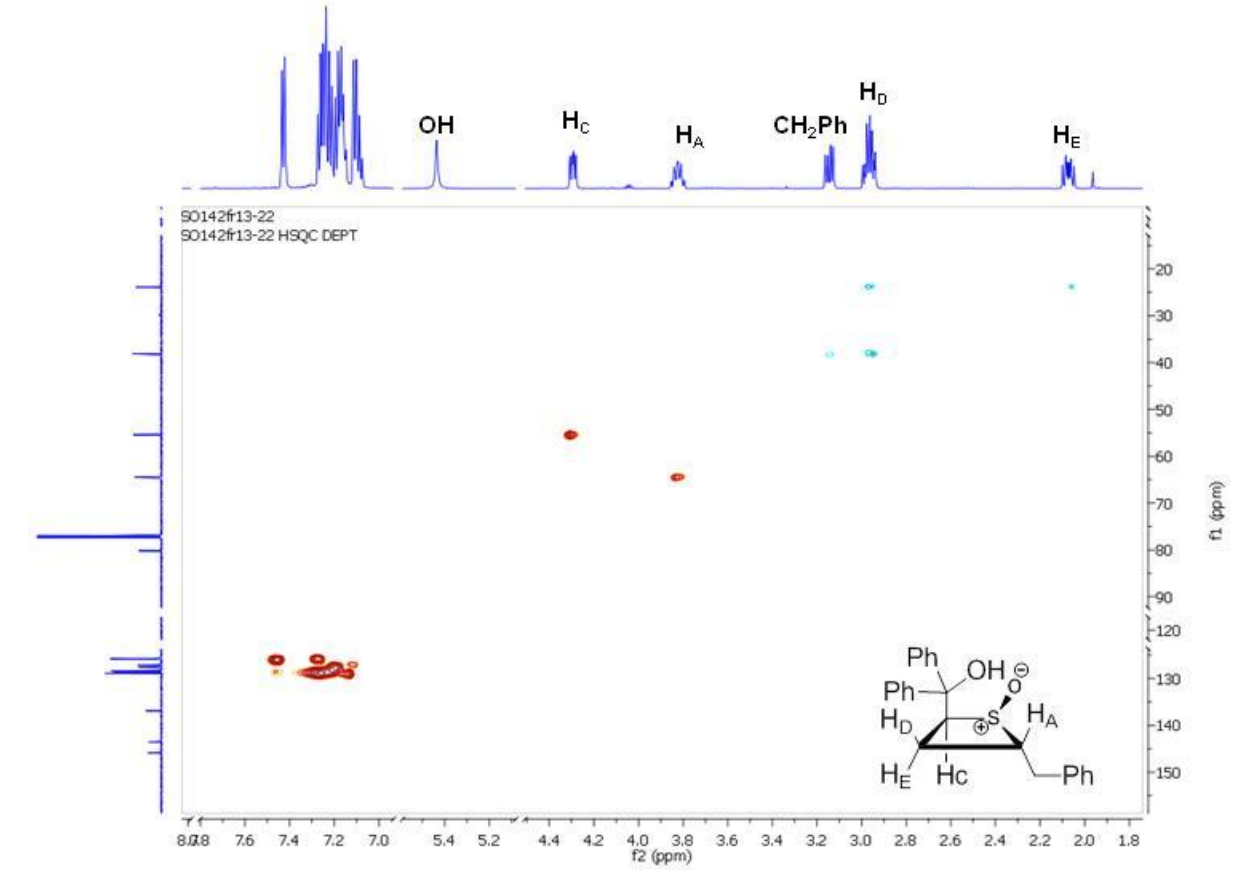

SO196_fr5_8
SO196_fr5_8_protone
HO
Ph
Ph
1.9
3.9
3.1
0.9
1.0
1.0
2.1
1.0
1.1
1.0
1.0
1.0
1.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

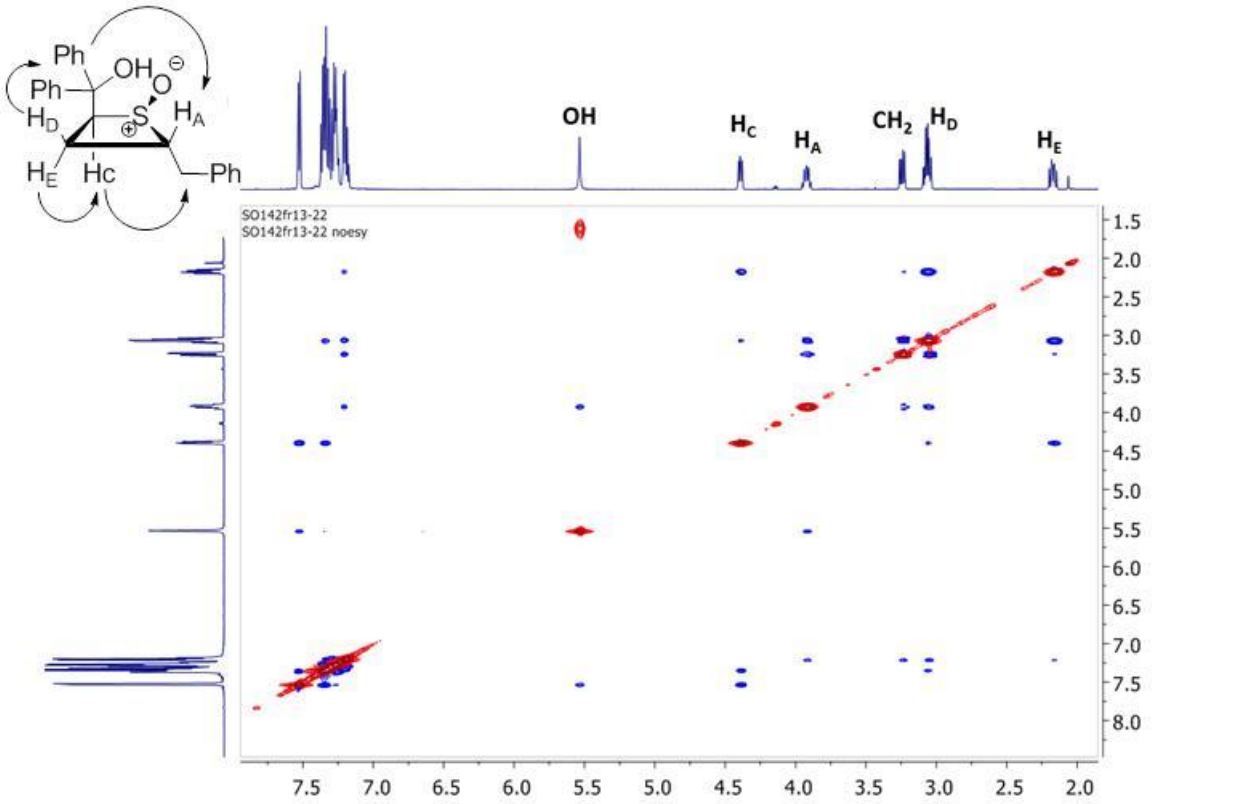

SO196_fr5_
SO196_fr5_8_carbon
145.9
143.6
132.8
128.7
128.4
127.6
127.1
125.9
125.8
118.7
80.2
63.0
55.4
36.1
23.8
HO
Ph
Ph
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)

(1R_S*, 2R*, 4S*)-5d

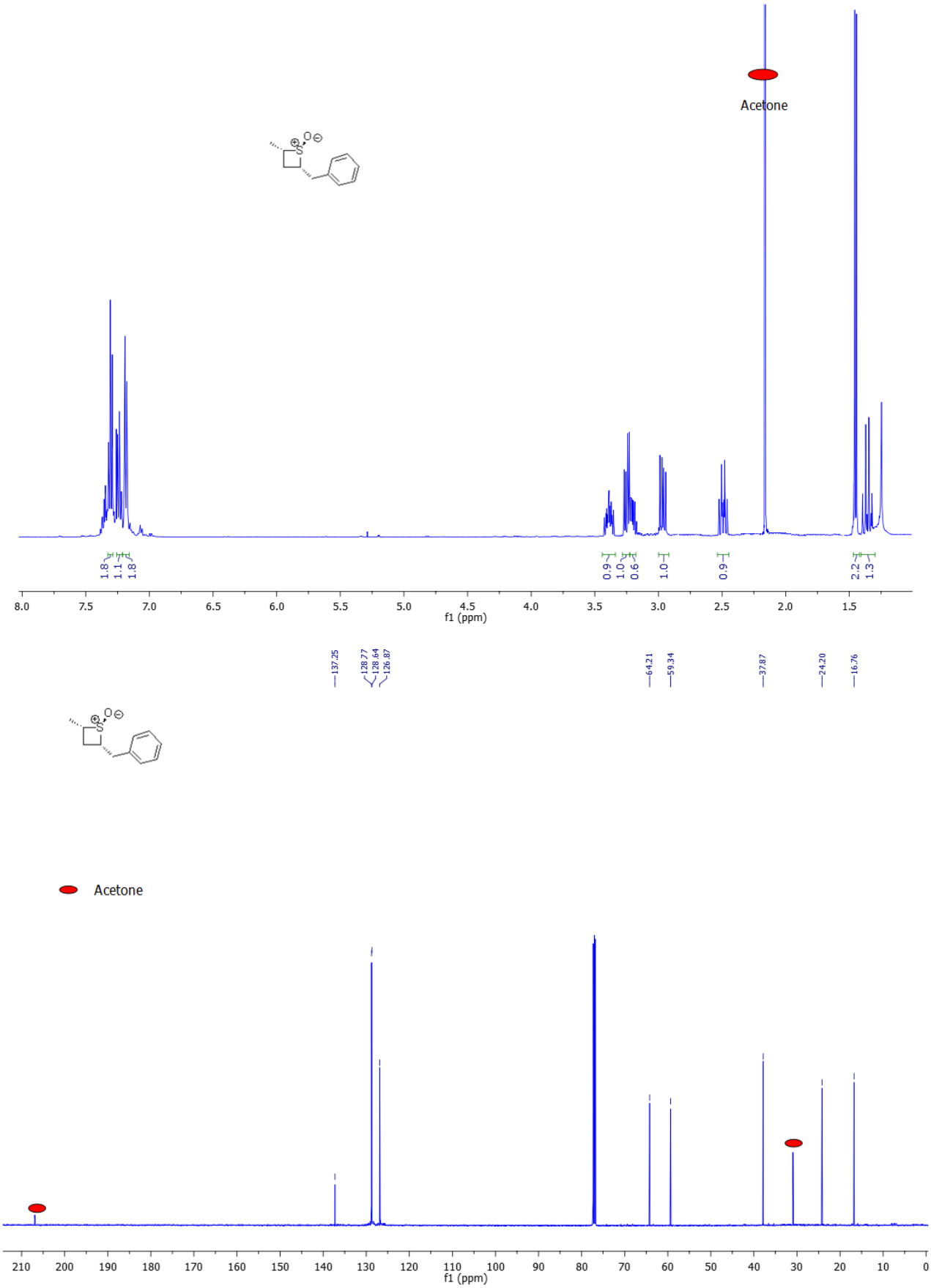

SO142fr13-22
SO142fr13-22
OH
Ph
Ph
Ph
1.9
9.9
2.8
0.8
1.0
1.0
1.0
2.0
1.0
f1 (ppm)

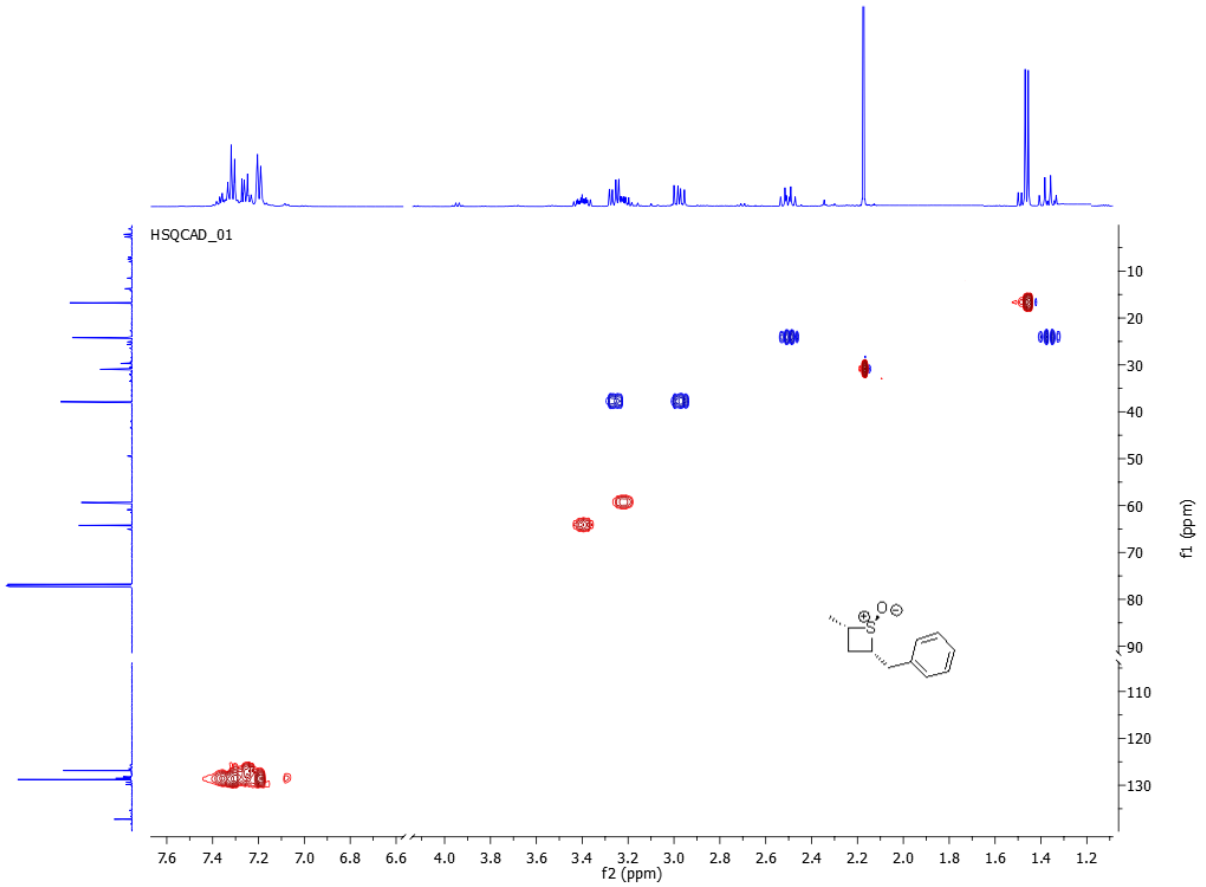

SO142fr13-22
SO142fr13-22
145.9
143.6
136.9
128.9
128.9
128.7
128.4
127.6
127.2
127.0
125.9
125.7
80.2
64.5
55.4
38.1
23.9
OH
Ph
Ph
Ph
f1 (ppm)

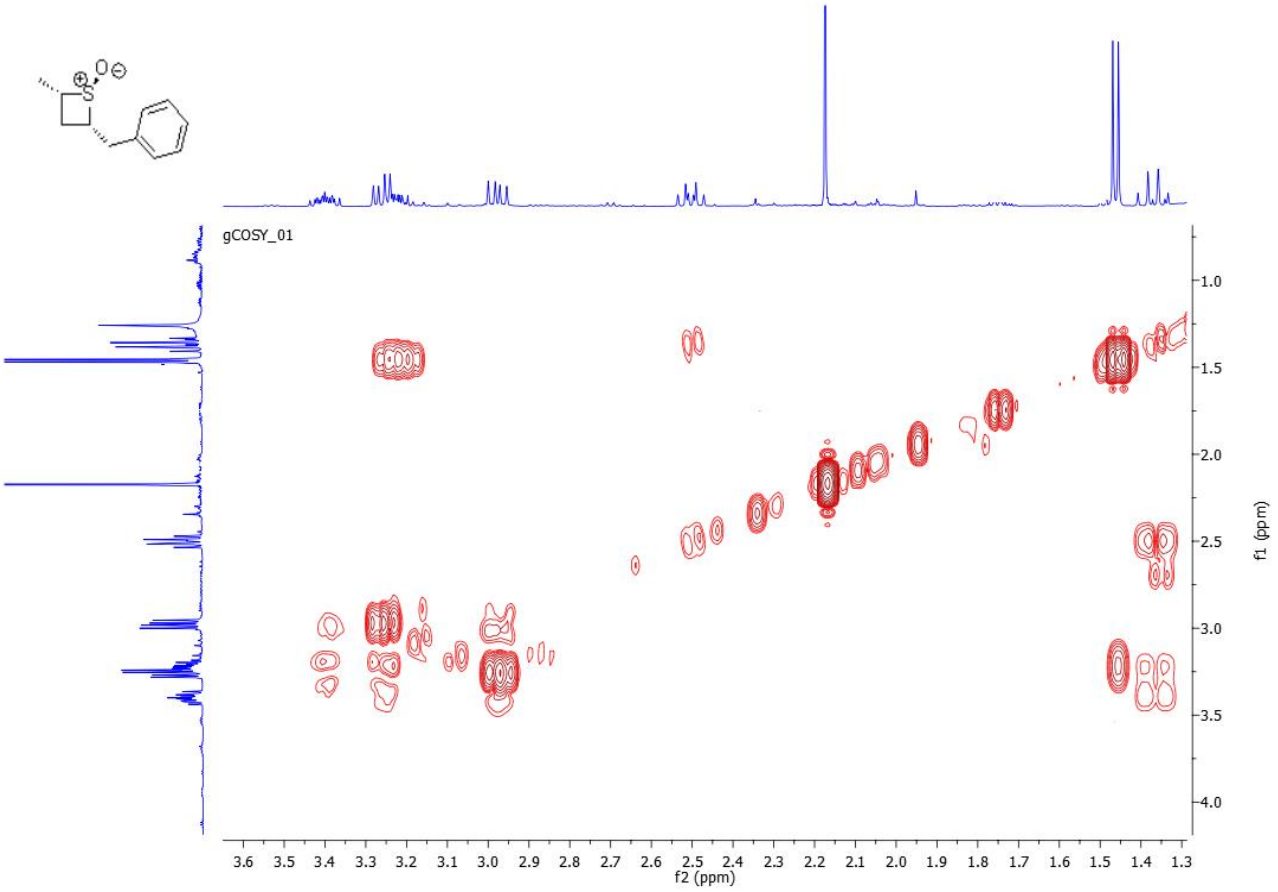

OH
H_C
H_A
CH_2Ph
H_D
H_E
SO142fr13-22
SO142fr13-22 HSQC DEPT
f2 (ppm)
f1 (ppm)
Ph
OH
Ph
H_D
H_A
H_E
Hc
Ph


Ph
OH
Ph
H_D
H_A
H_E
Hc
Ph
OH
H_C
H_A
CH_2
H_D
H_E
SO142fr13-22
SO142fr13-22 noesy

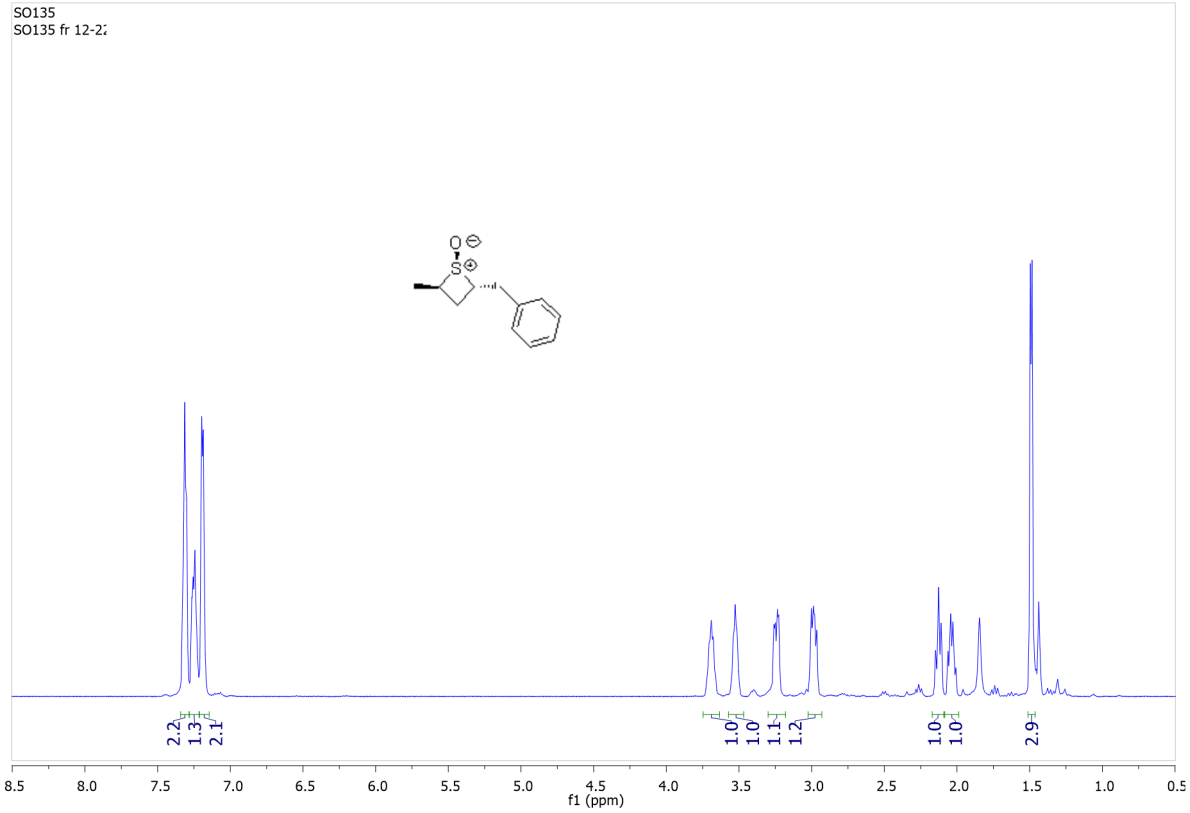
(1R_S*, 2*R, 4*S**)-6a *major***

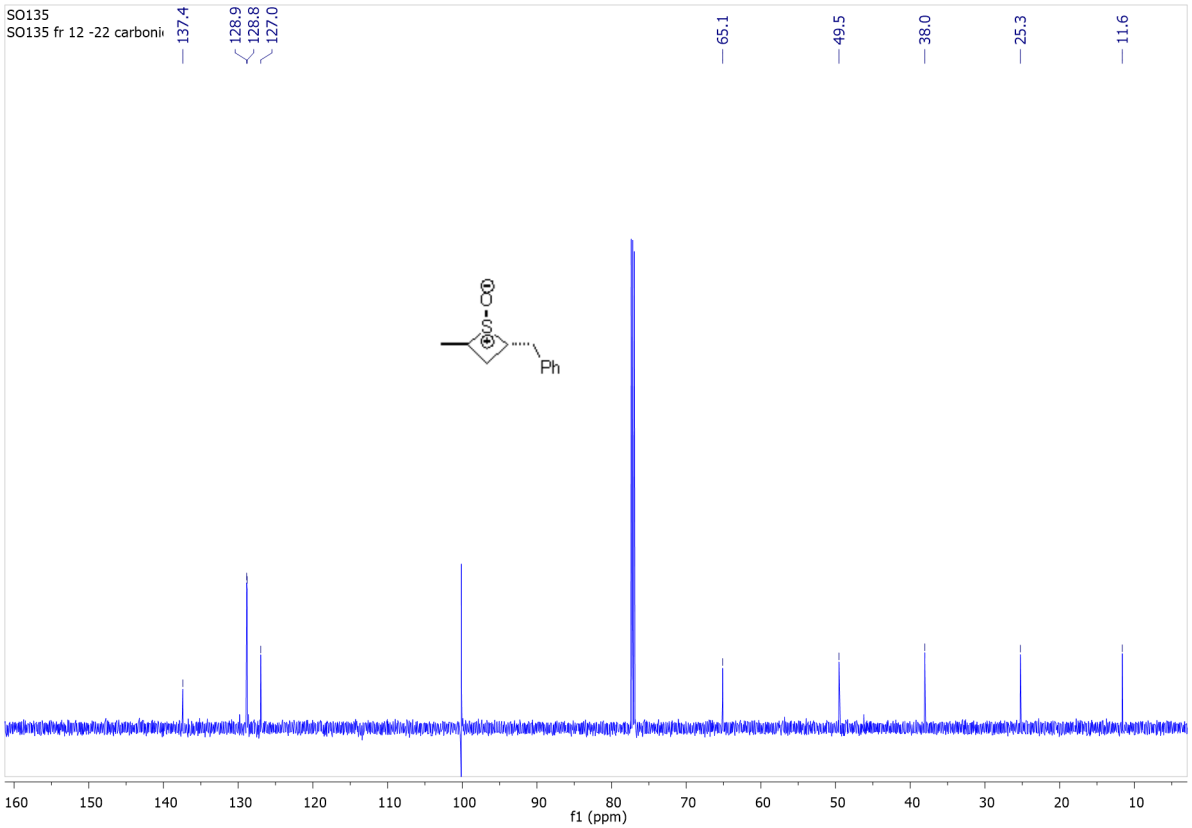


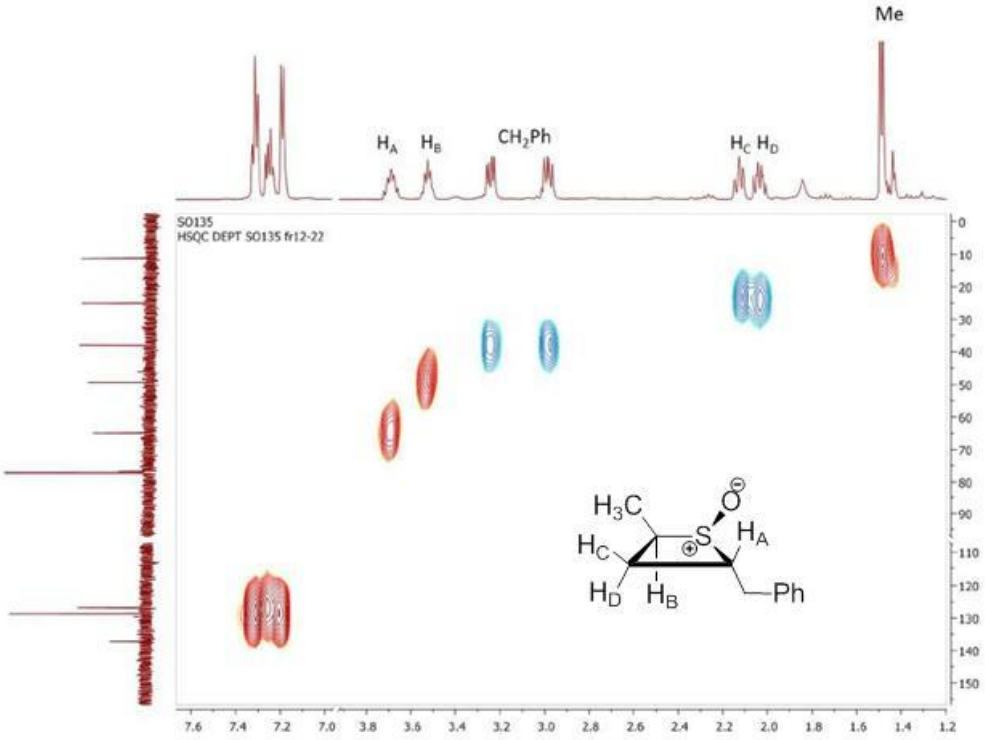

HSQCAD_01
f2 (ppm)
f1 (ppm)

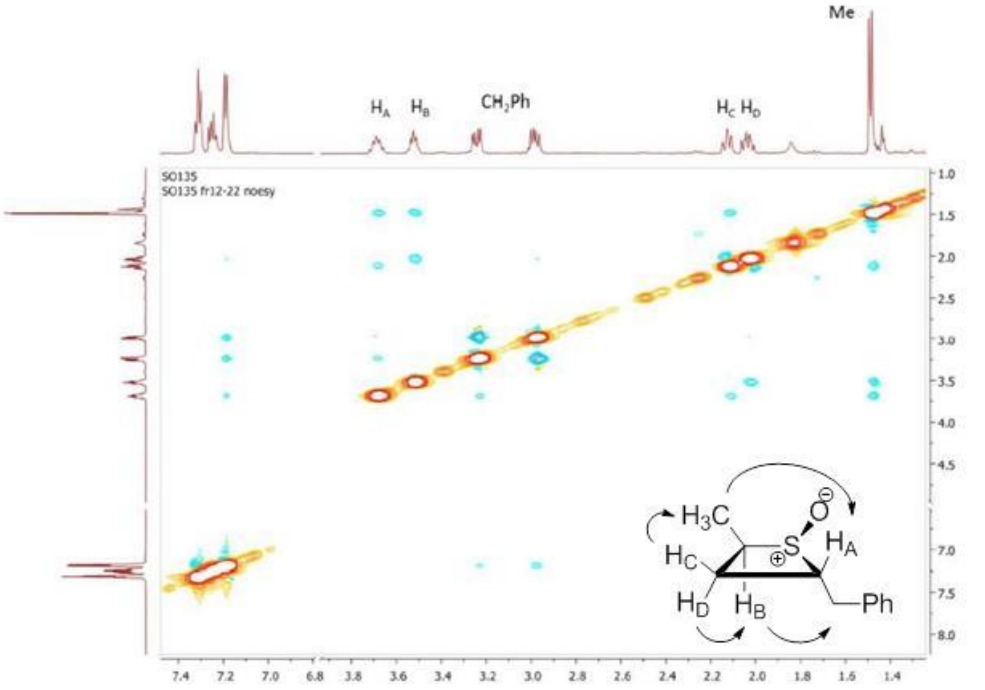

gCOSY_01
f2 (ppm)
f1 (ppm)

(1R_S*, 2*R, 4*R**)-6a *minor***

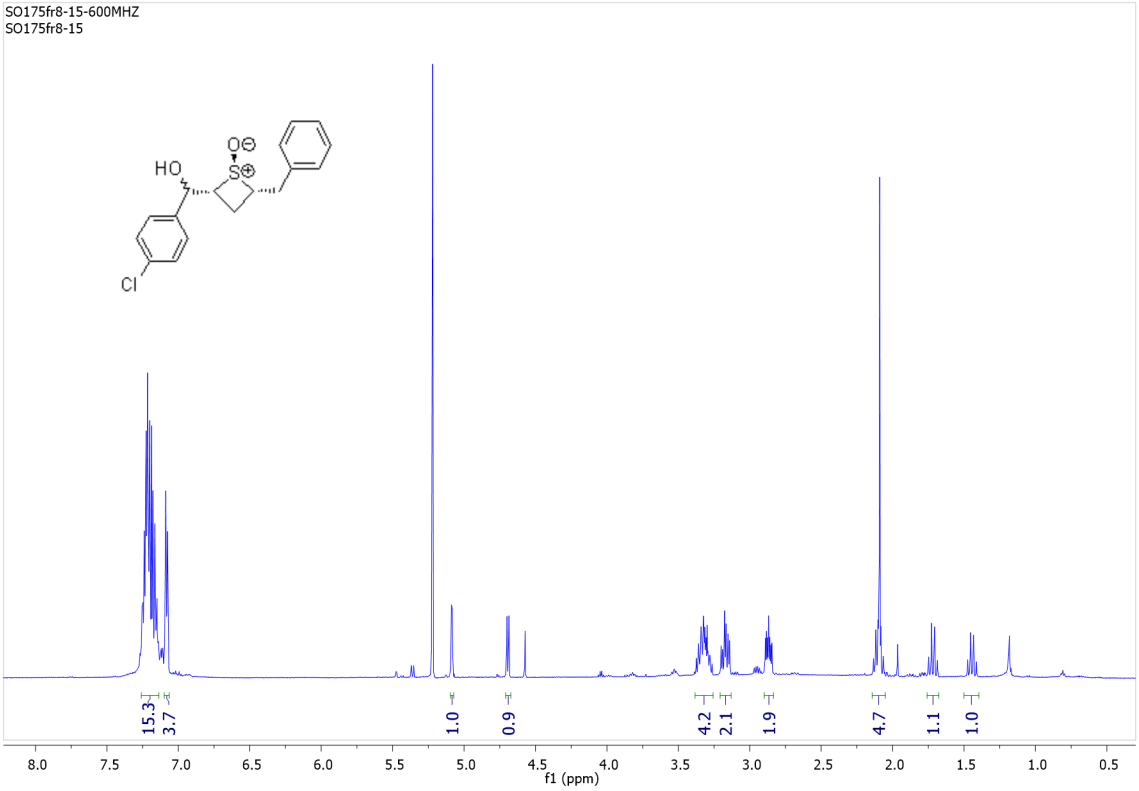


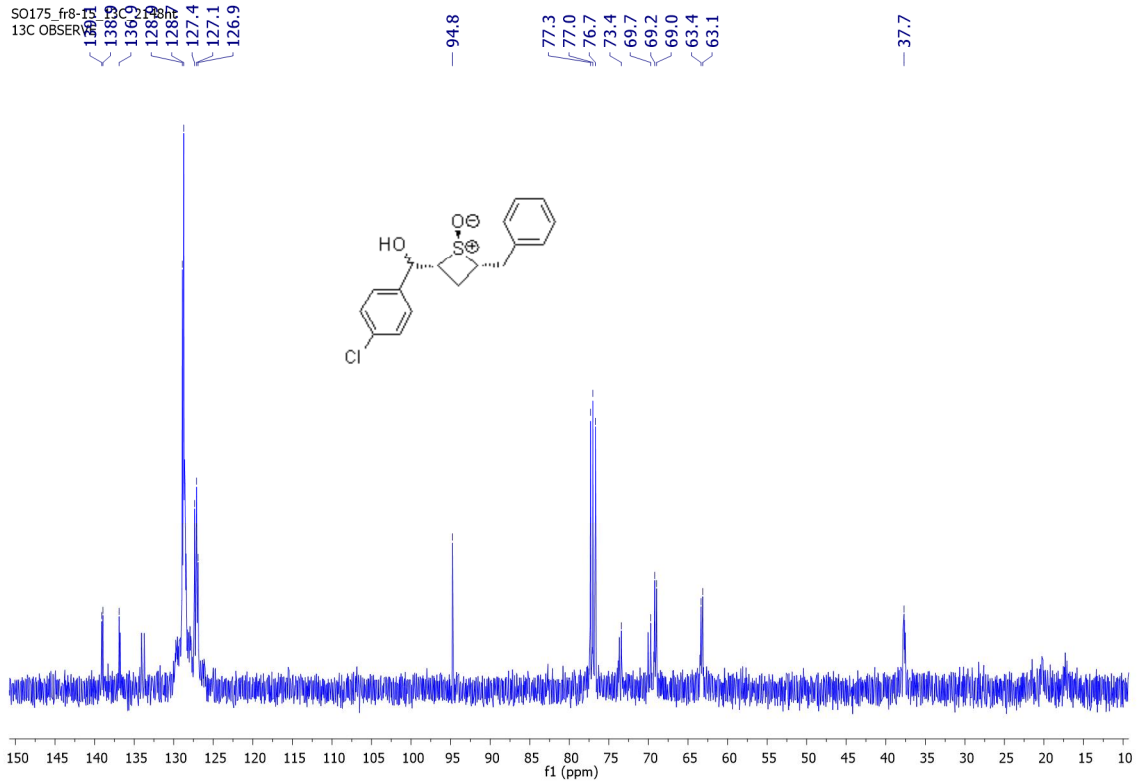


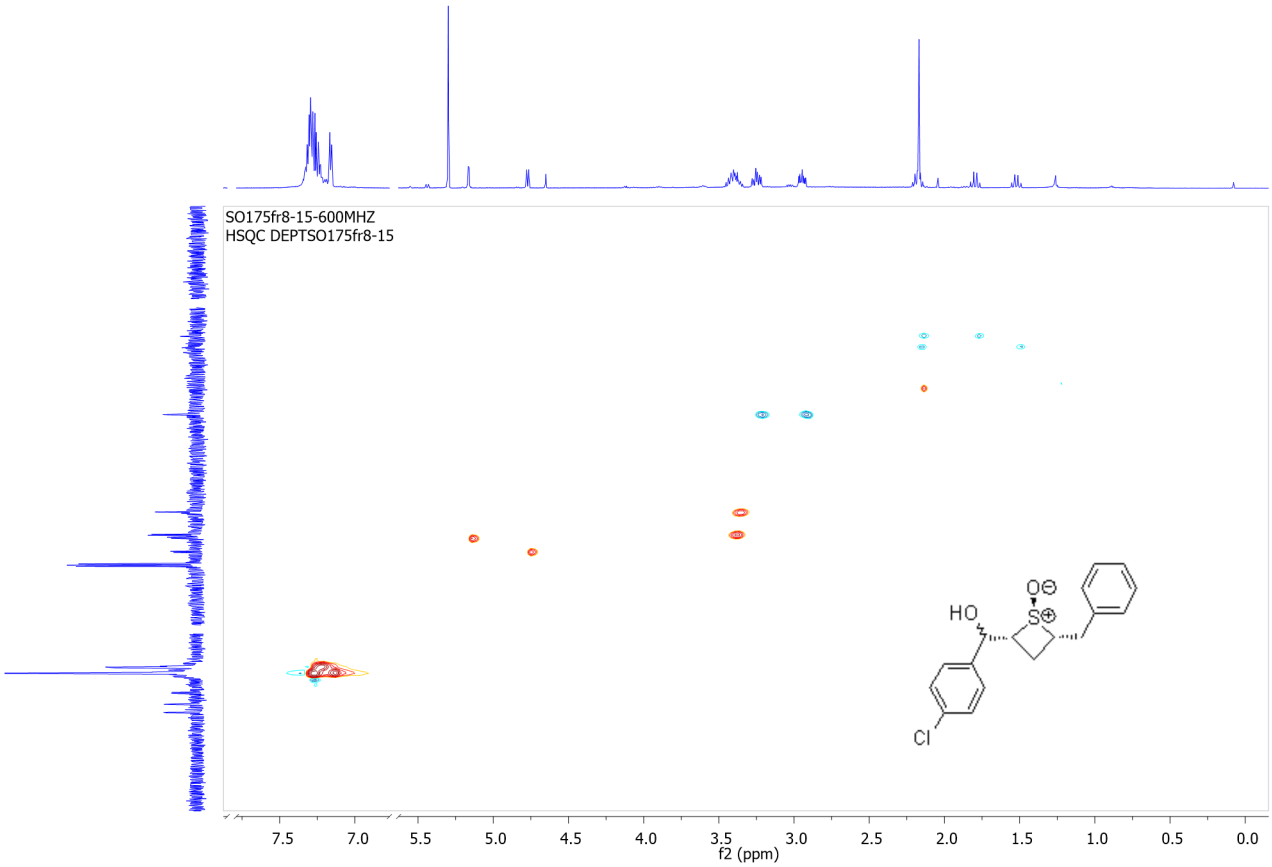

Me
H_A H_B
CH_2Ph
H_C H_D
SO135
HSQC DEPT SO135 fr12-22
H_3C
H_C
H_D
H_B
H_A
Ph

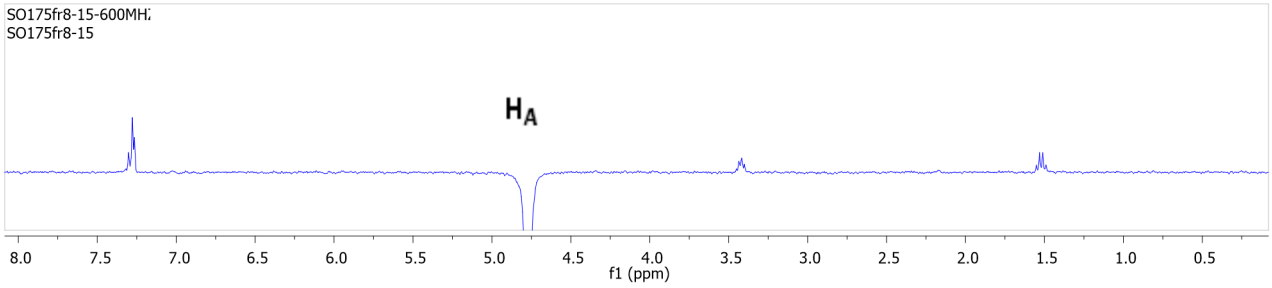

Me
H_A H_B
CH_2Ph
H_C H_D
SO135
SO135 fr12-22 noesy
H_3C
H_C
H_D
H_B
H_A
Ph

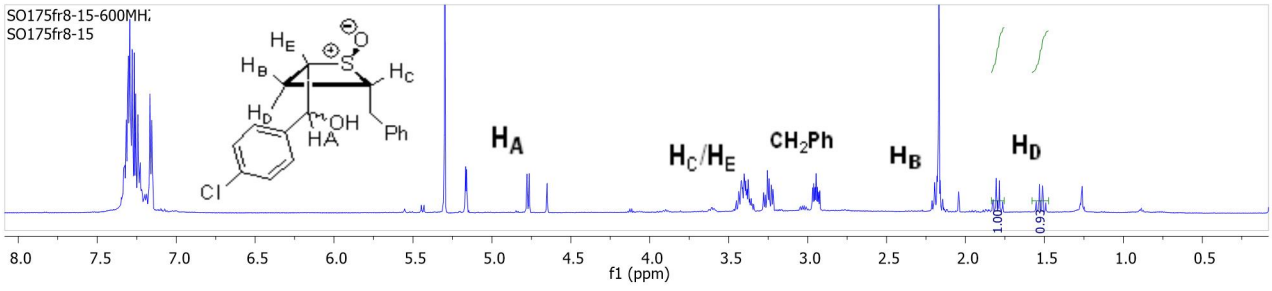
(1R$_S$*, 2*S, 4*S**) 6b**

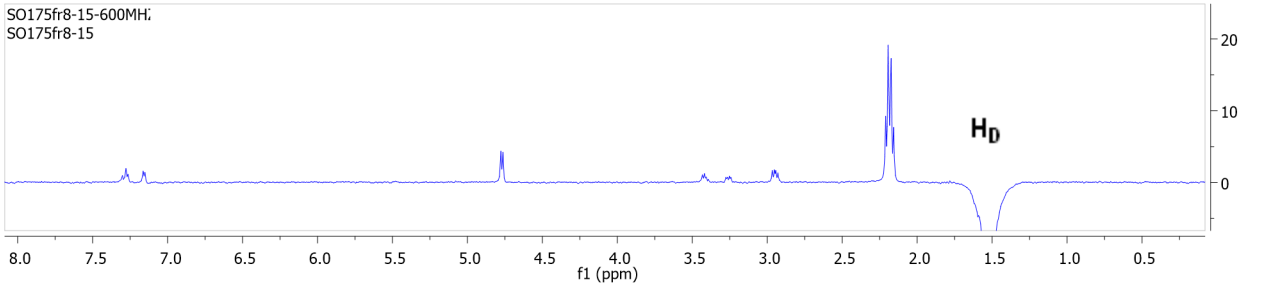

SO175fr8-15-600MHZ
SO175fr8-15
HO
O
S
Cl
15.3
3.7
1.0
0.9
4.2
2.1
1.9
4.7
1.1
1.0
f1 (ppm)


SO175_fr8-15_13C_21-8ht
13C OBSERVE
138.2
138.0
136.9
128.7
128.4
127.4
127.1
126.9
94.8
77.3
77.0
76.7
73.4
69.7
69.2
69.0
63.4
63.1
37.7
HO
O
S
Cl
f1 (ppm)

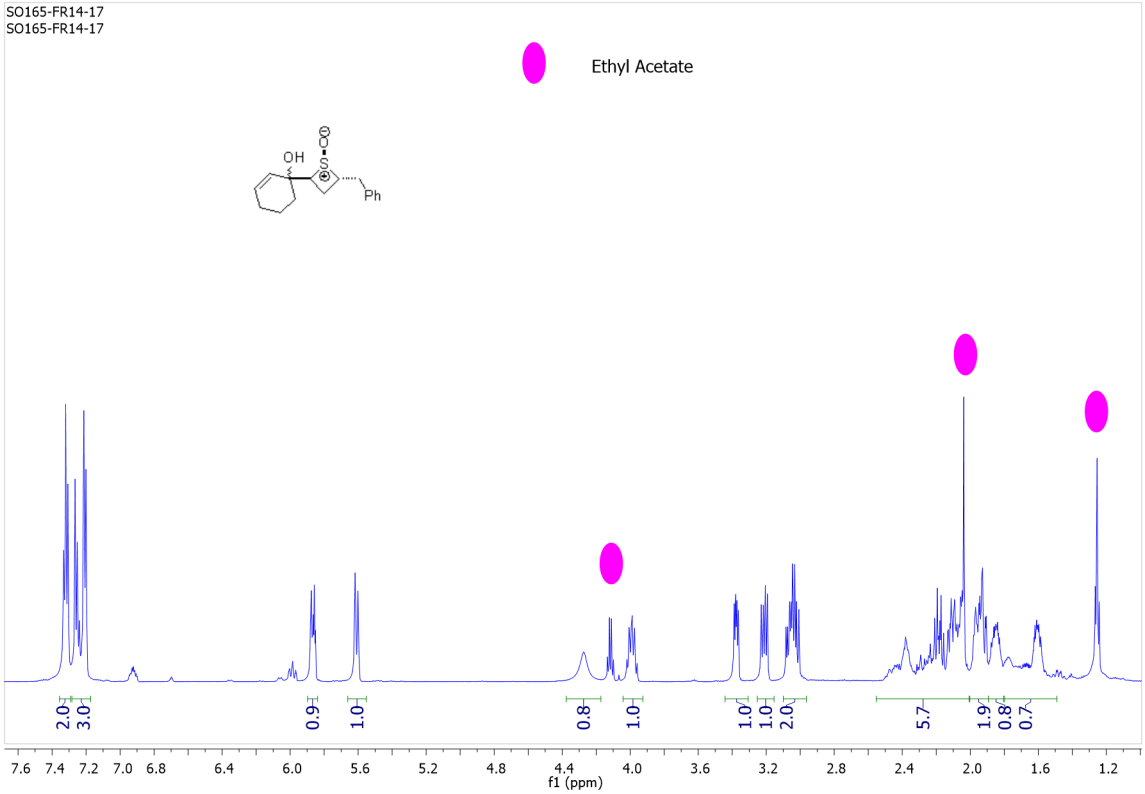

SO175fr8-15-600MHZ
HSQC DEPTSO175fr8-15
HO
Cl
7.5 7.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f2 (ppm)

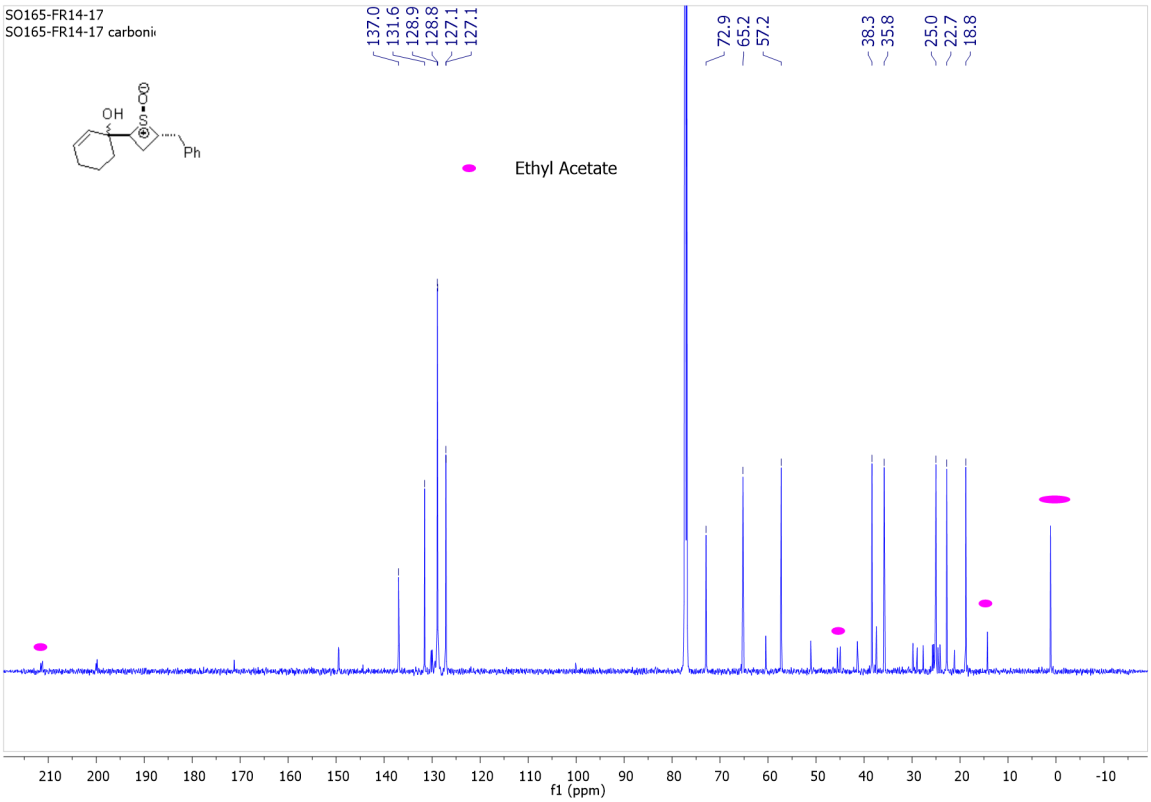

SO175fr8-15-600MH;
SO175fr8-15
HA
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

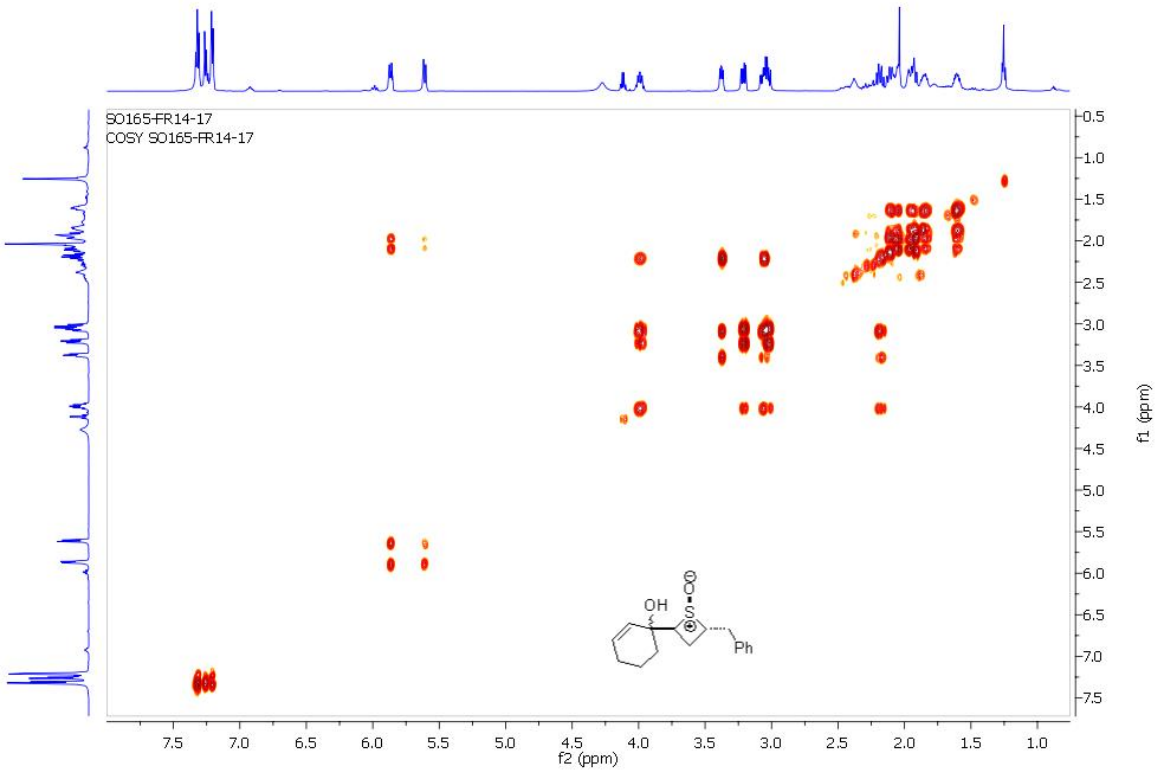

SO175fr8-15-600MH;
SO175fr8-15
HE
HB
HC
HD
OH
HA
Ph
Cl
HA
HC/HE
CH2Ph
HB
HD
1.00
0.93
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

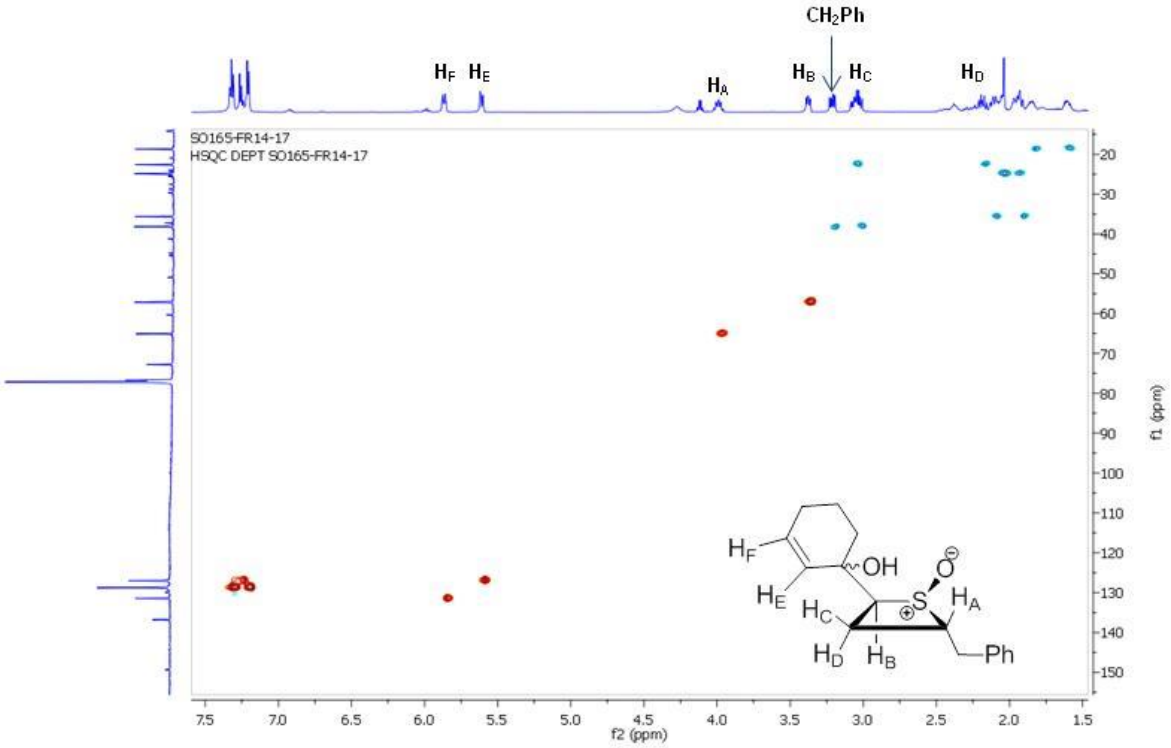

SO175fr8-15-600MH;
SO175fr8-15
HD
20
10
0
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

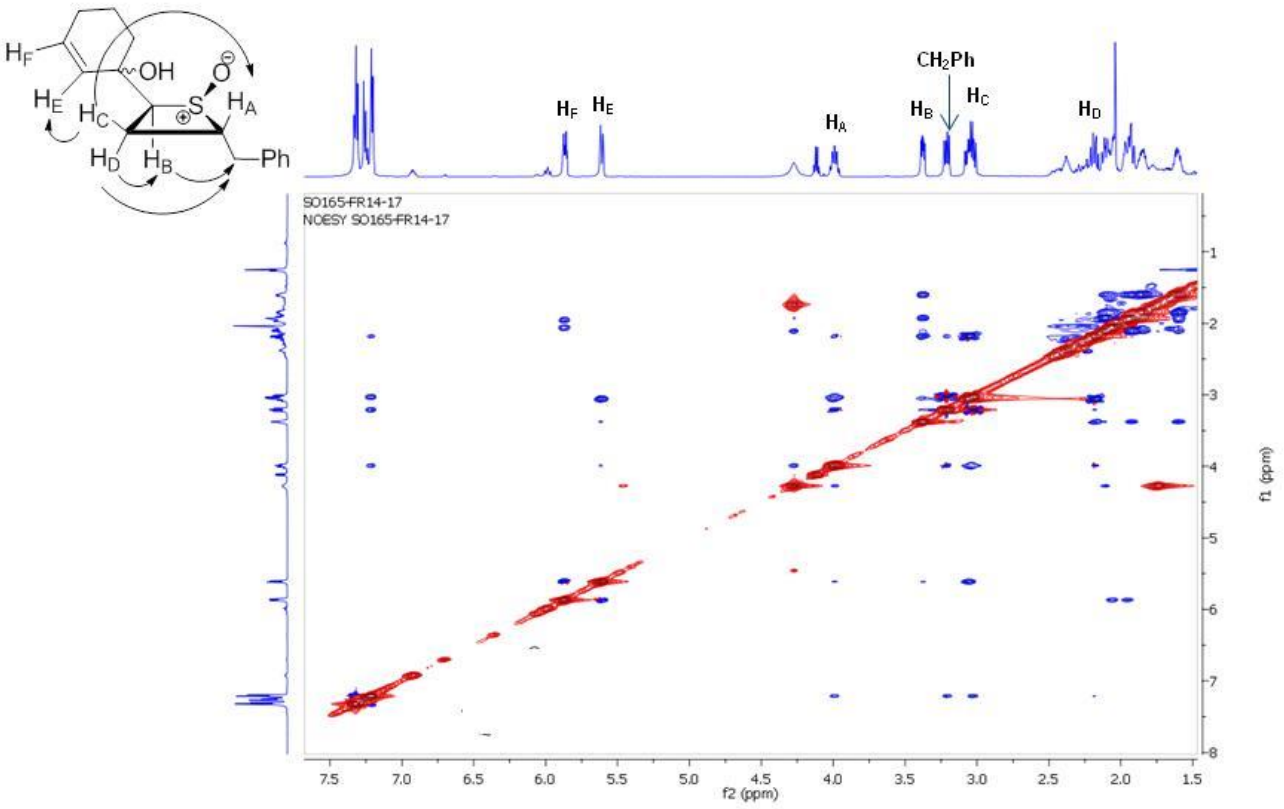
(1R$_S$, 2R*, 4S*) 6c major*



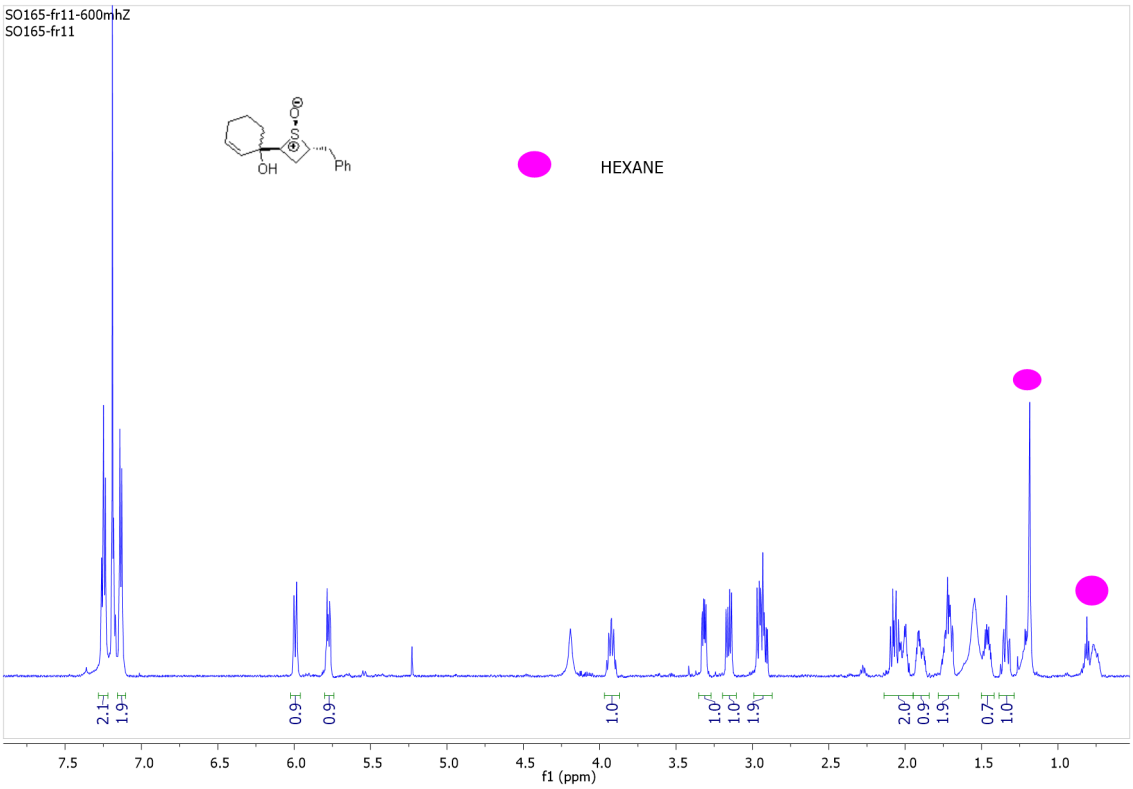


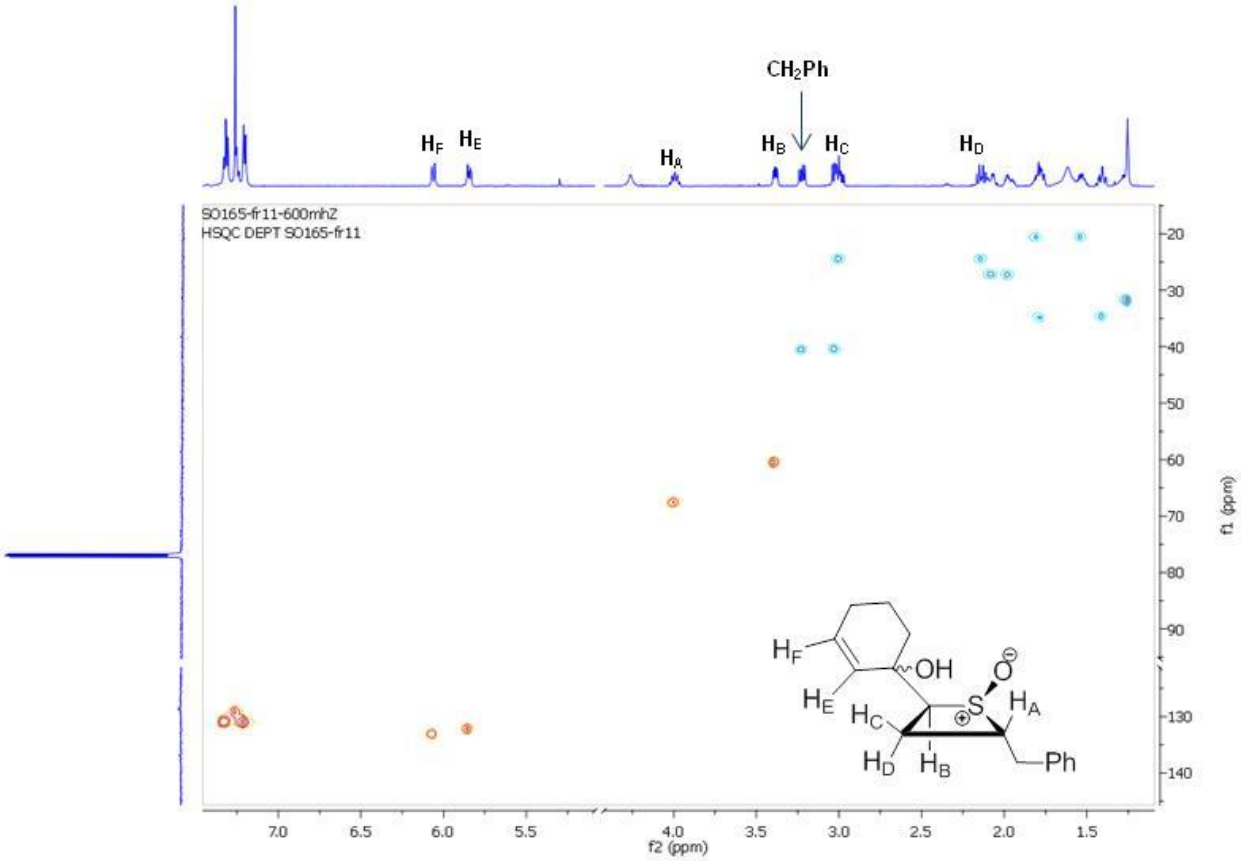

SO165-FR14-17
COSY SO165-FR14-17
OH
Ph
f2 (ppm)
f1 (ppm)

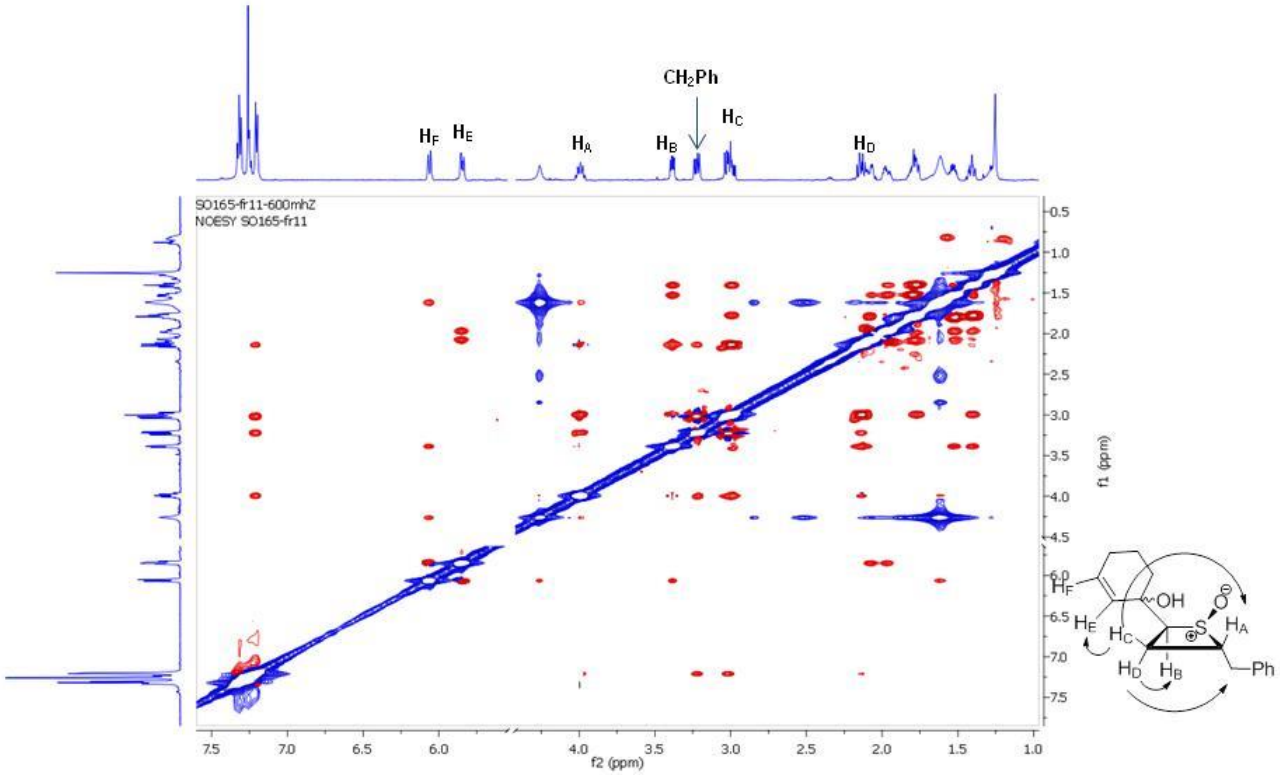

CH2Ph
HF HE
HA
HB HC
HD
SO165-FR14-17
HSQC DEPT SO165-FR14-17
OH
Ph
f2 (ppm)
f1 (ppm)


HF
OH
O
HE
HC
S
HA
HD
HB
Ph
HF HE
HA
CH2Ph
HB
HC
HD
SO165-FR14-17
NOESY SO165-FR14-17
f2 (ppm)
f1 (ppm)

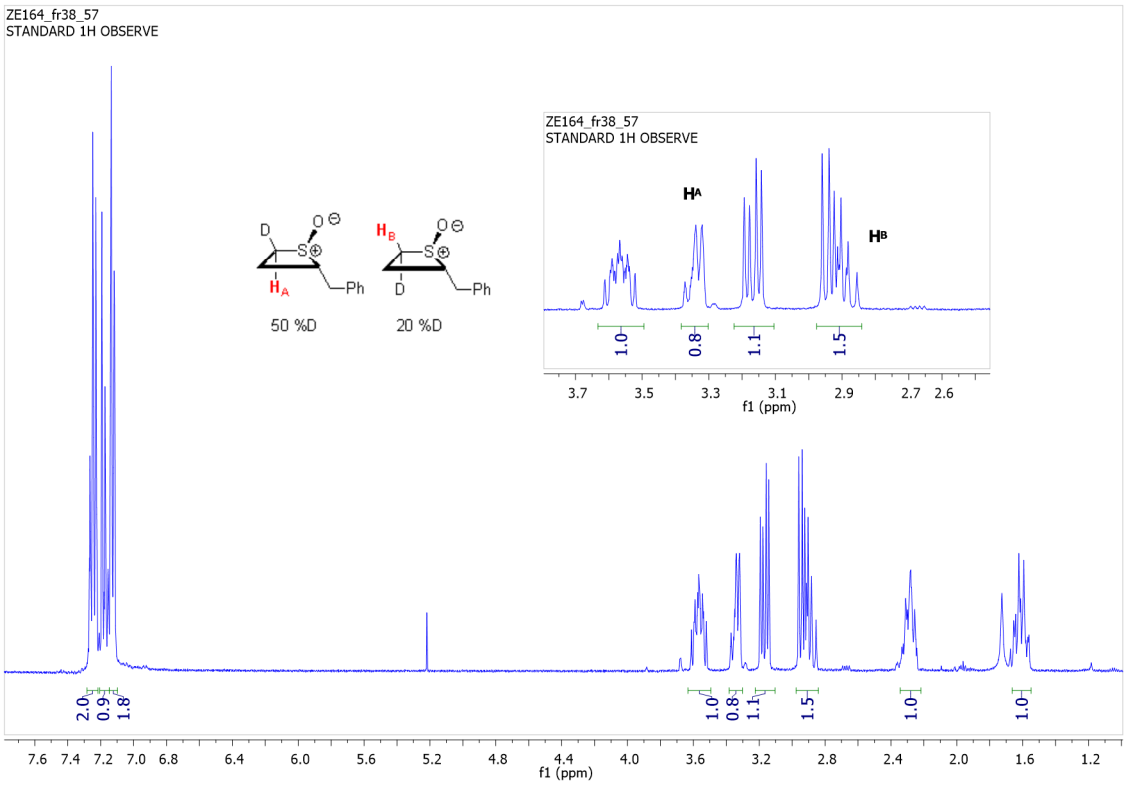
(1R$_S$*, 2R*, 4S*) 6c minor

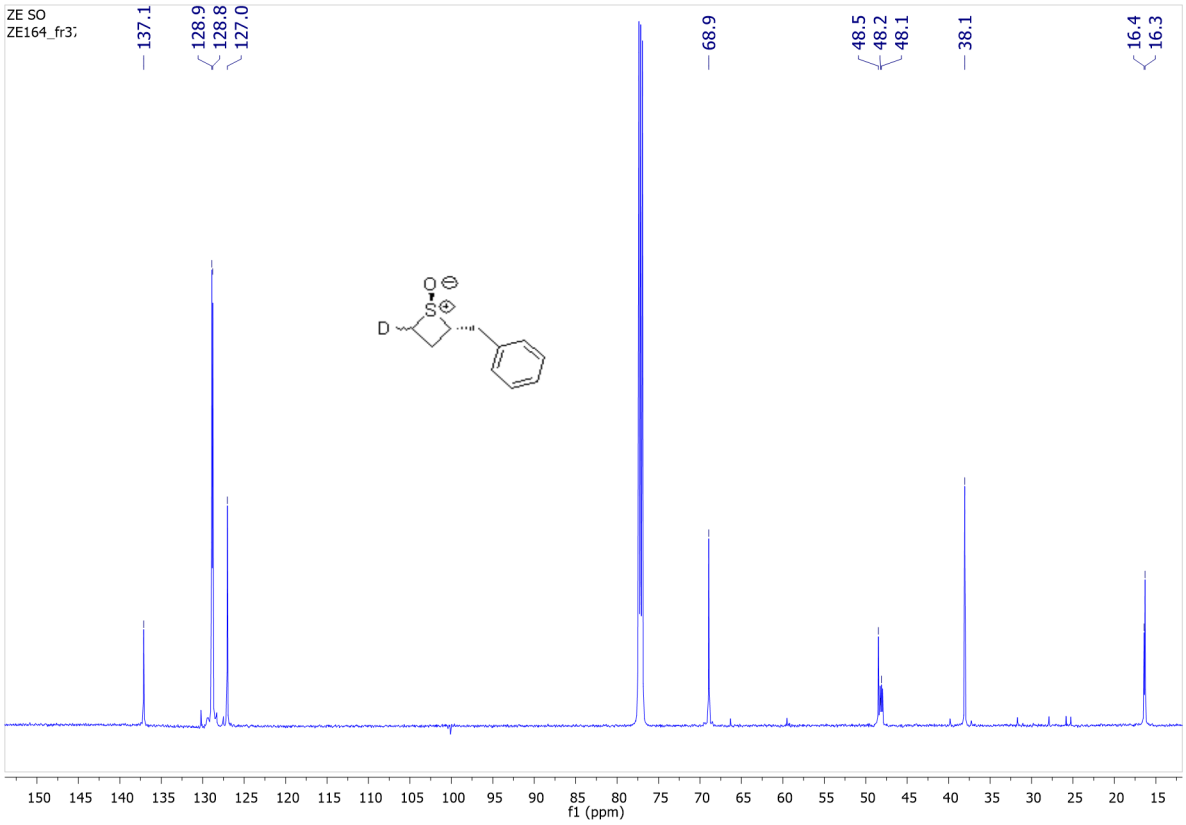




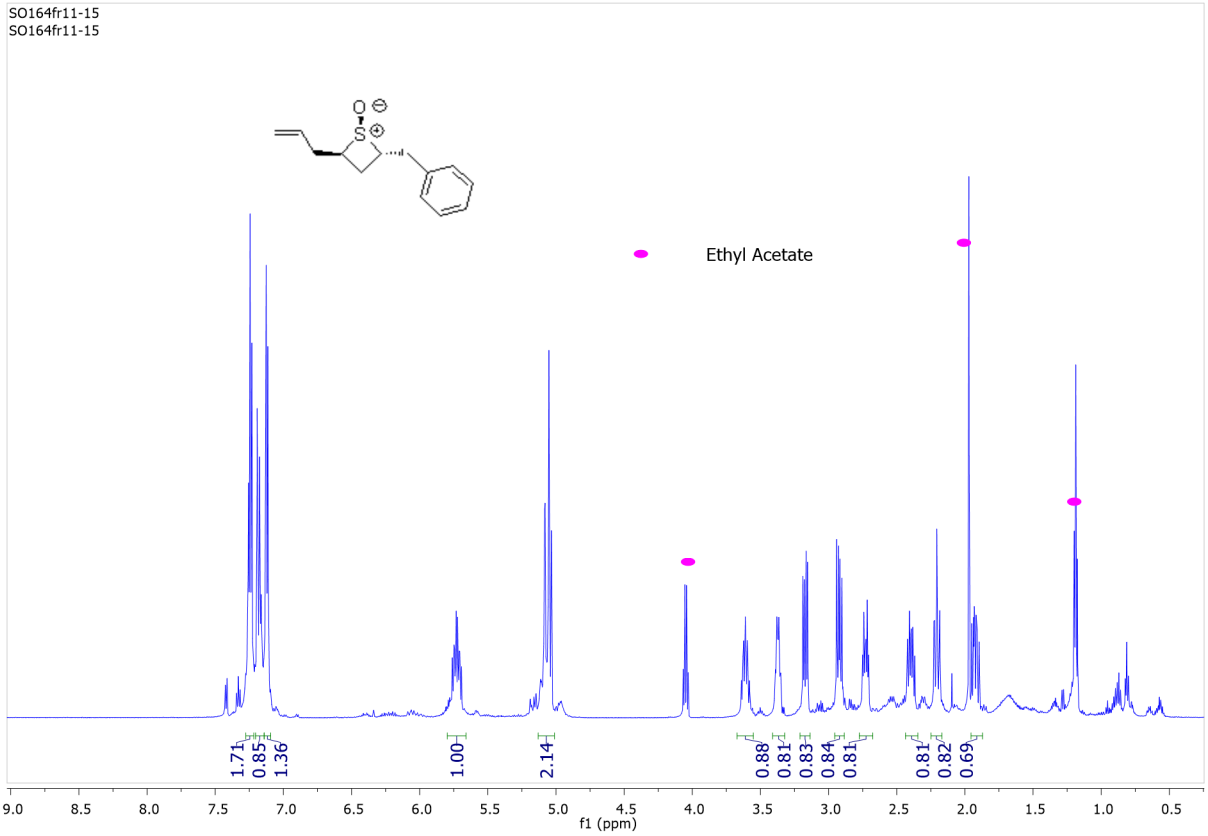

CH2Ph
HF
HE
HA
HB
HC
HD
SO165-fr11-600mhZ
NOESY SO165-fr11
f2 (ppm)
f1 (ppm)
OH
S
Ph

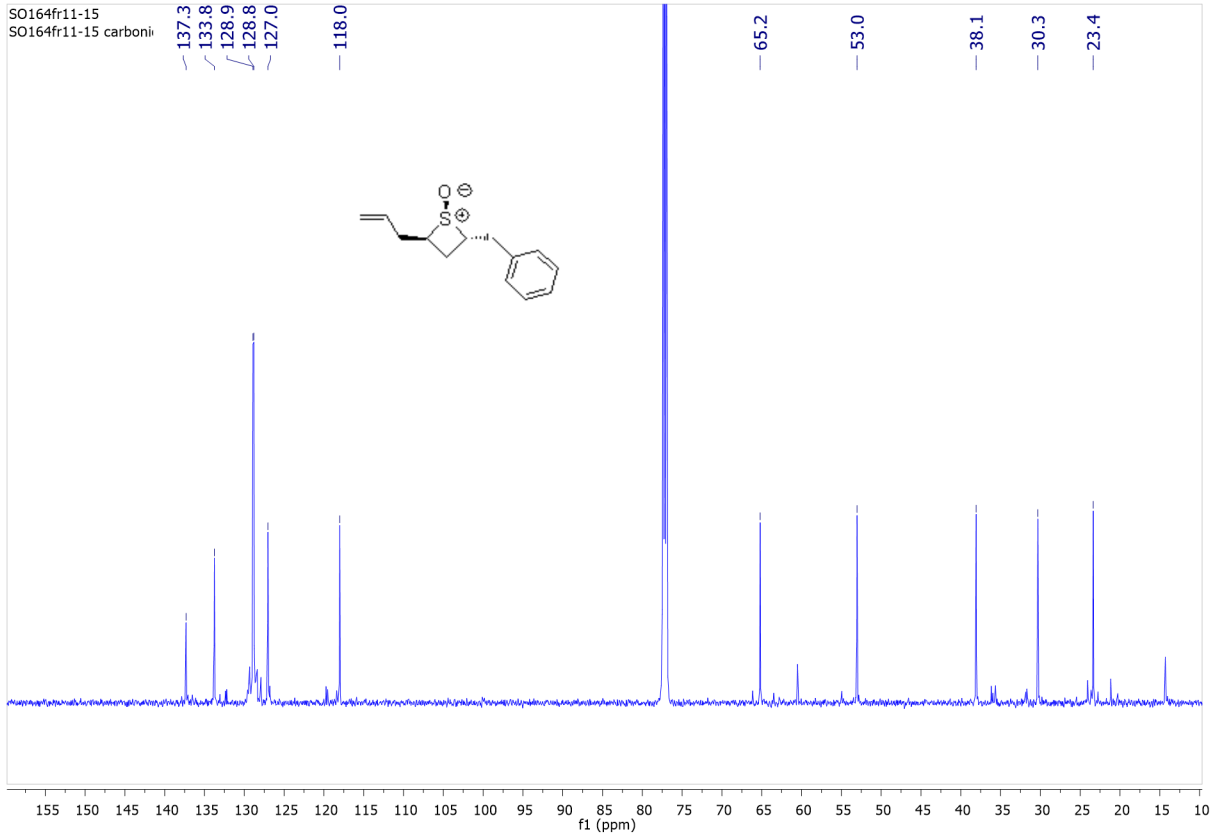
(*1R*$_S$*,*2R,*4R**)/(*1R*$_S$*,*2R**,*4S**)- 6d**

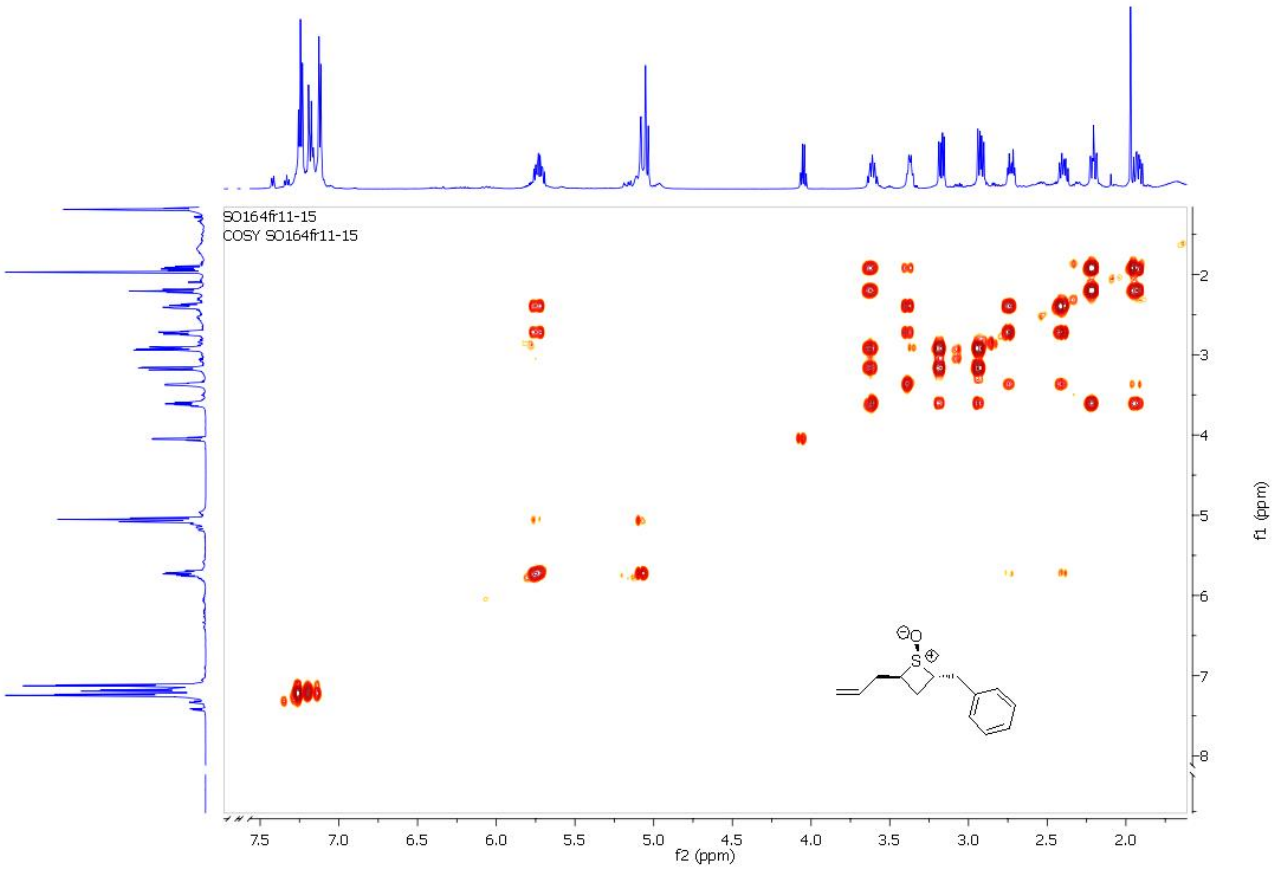


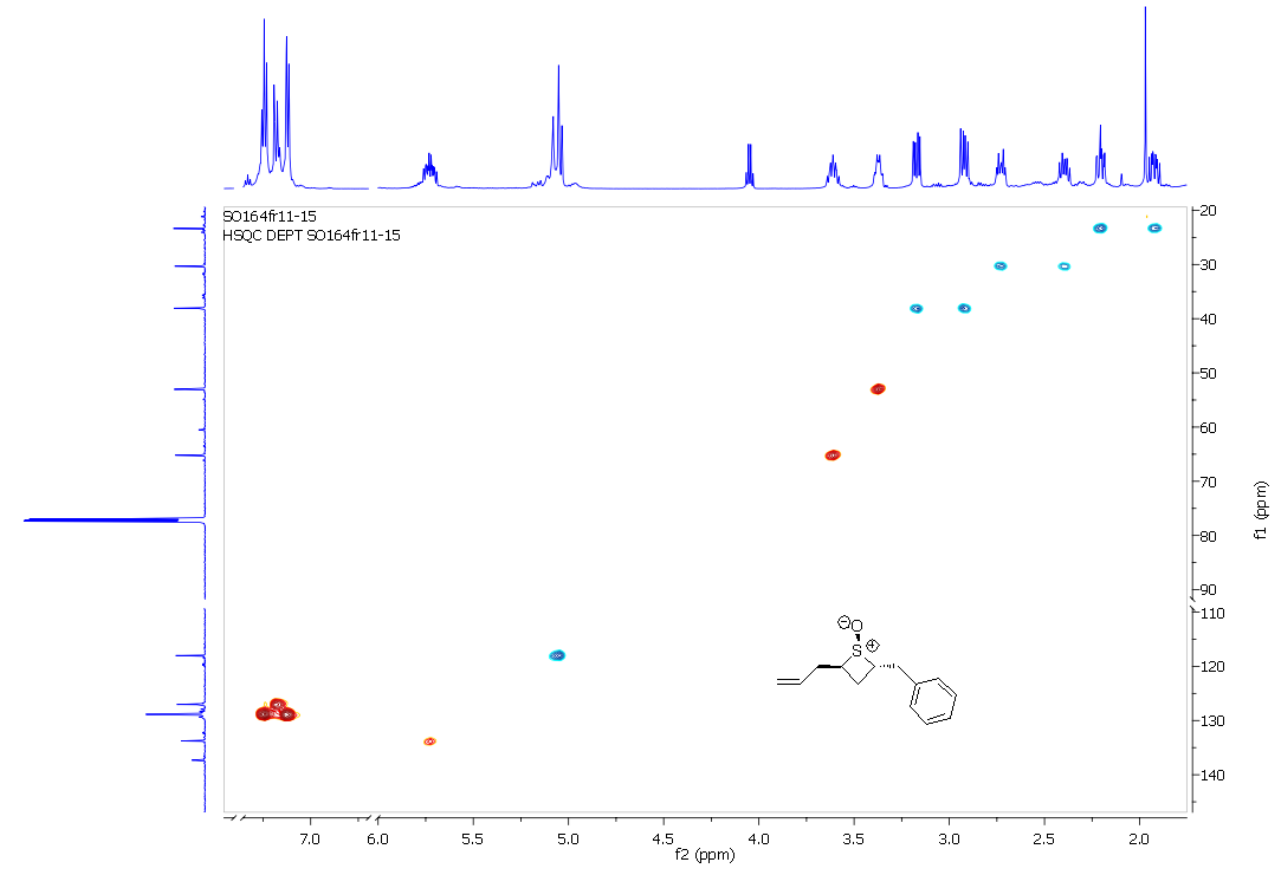


(1R$_S$*, 2R*, 4R*) 6e minor

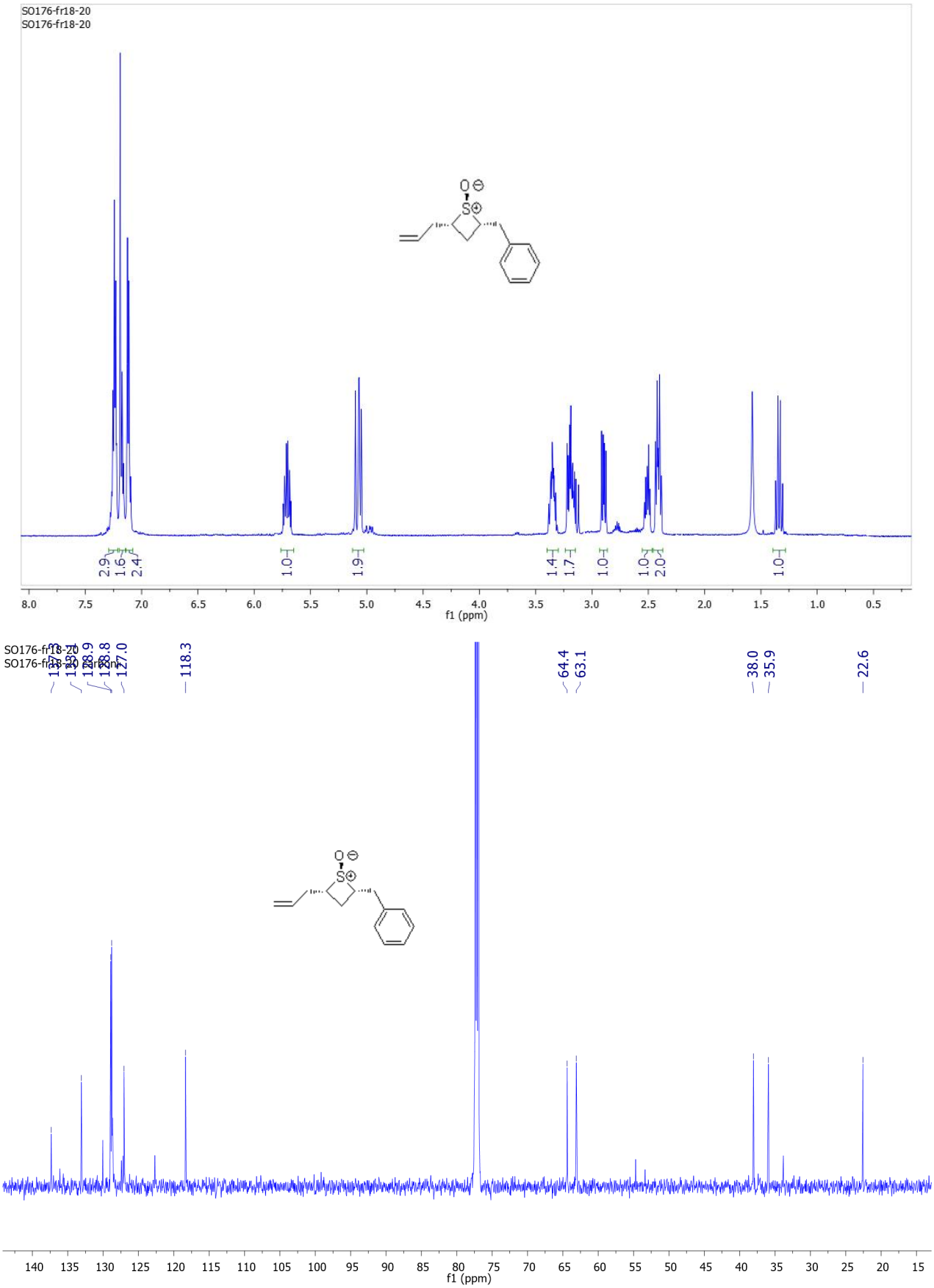


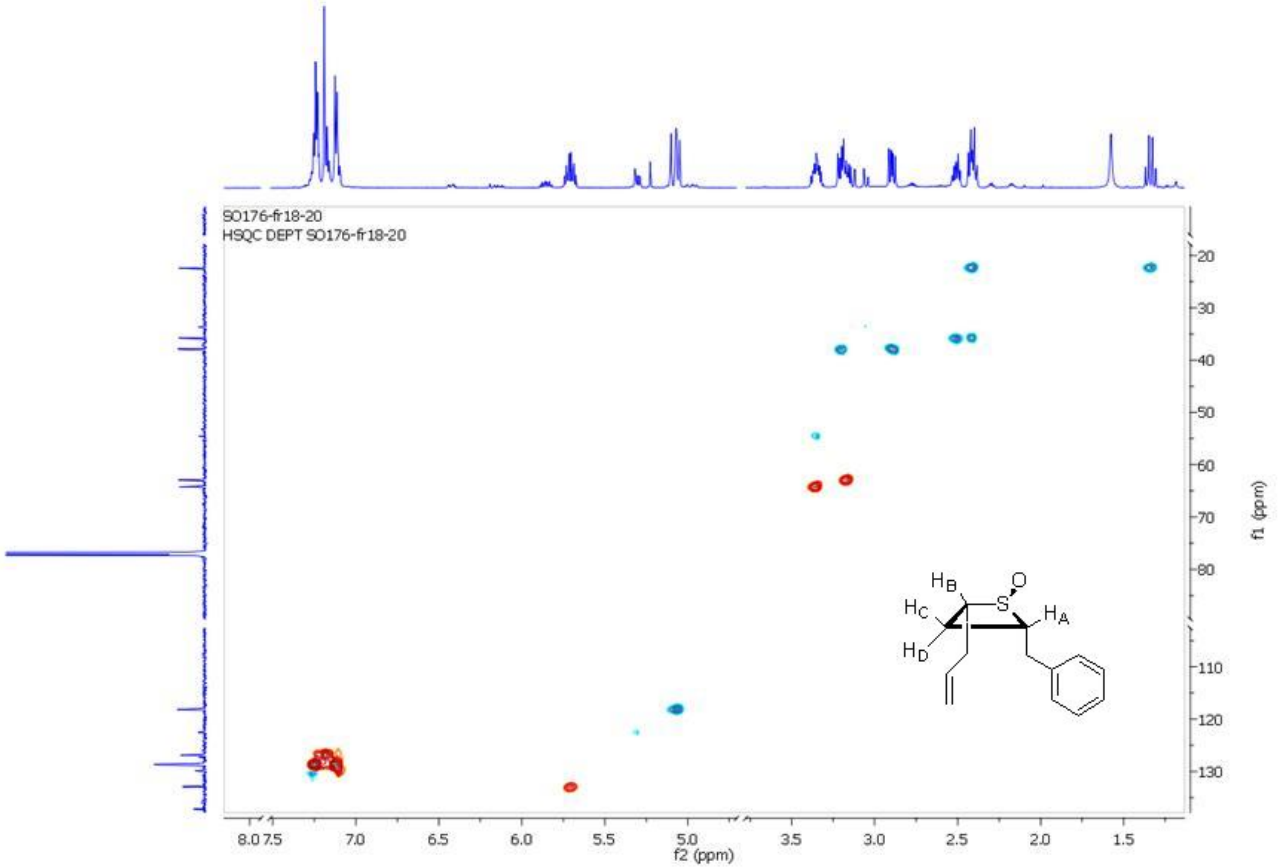


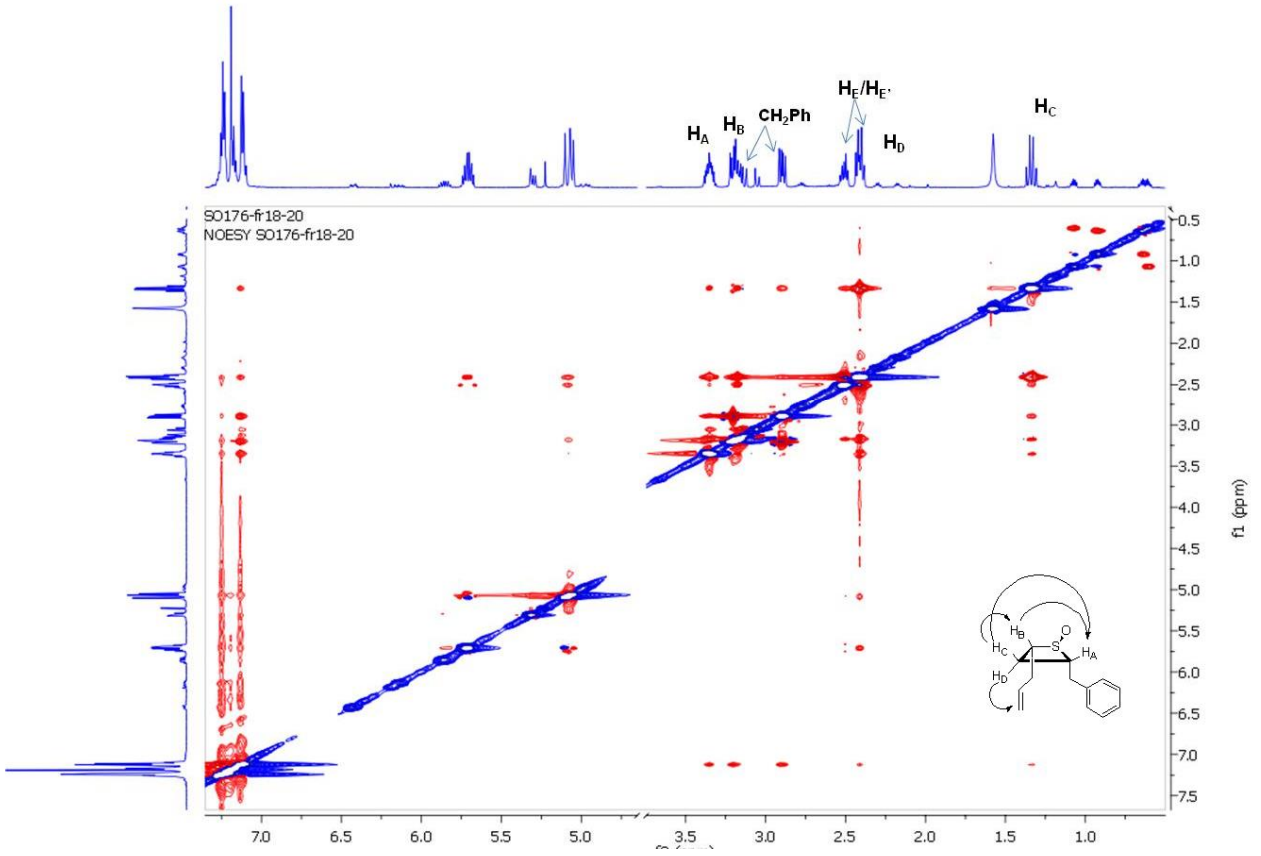

SO164fr11-15
COSY SO164fr11-15
f2 (ppm)
f1 (ppm)


SO164fr11-15
HSQC DEPT SO164fr11-15
f2 (ppm)
f1 (ppm)

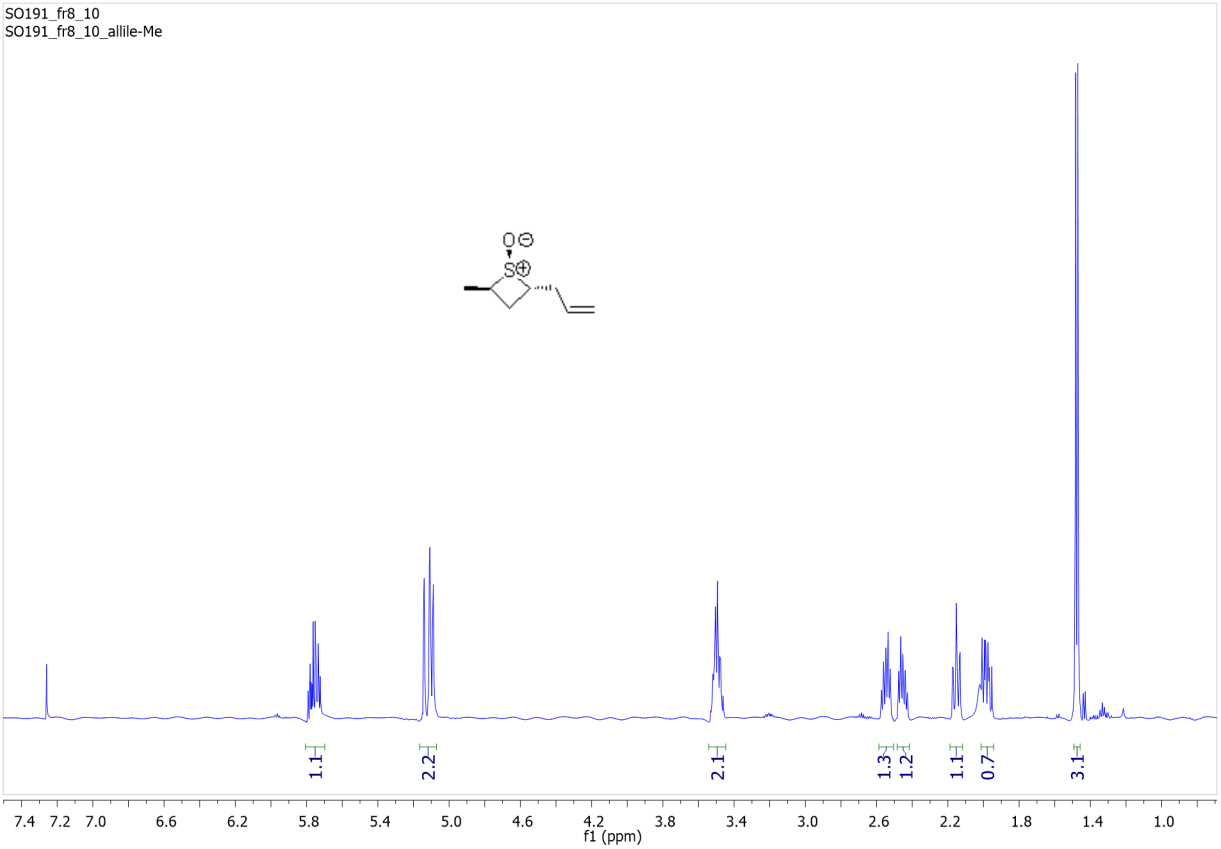
(1R$_S$*, 2R*, 4S*) 6e major

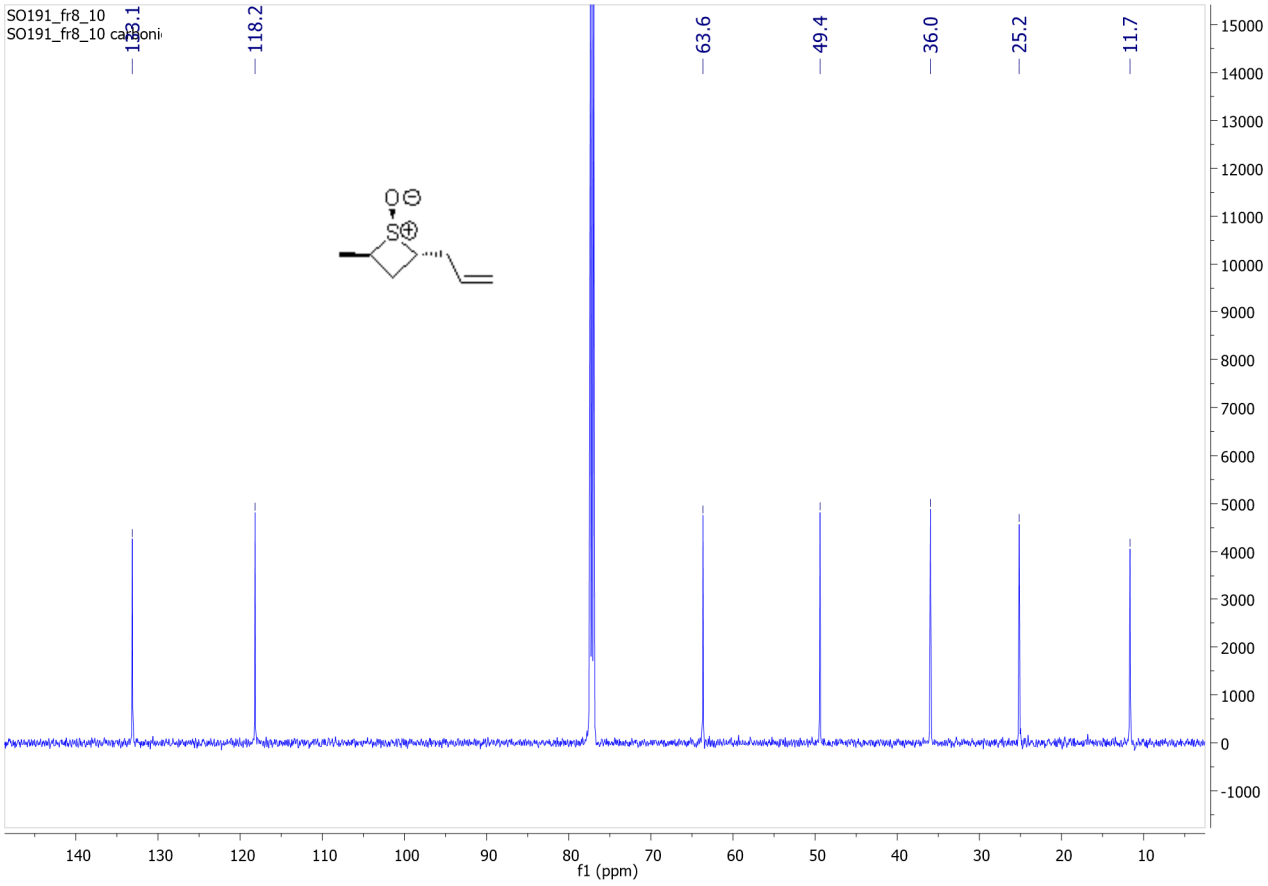


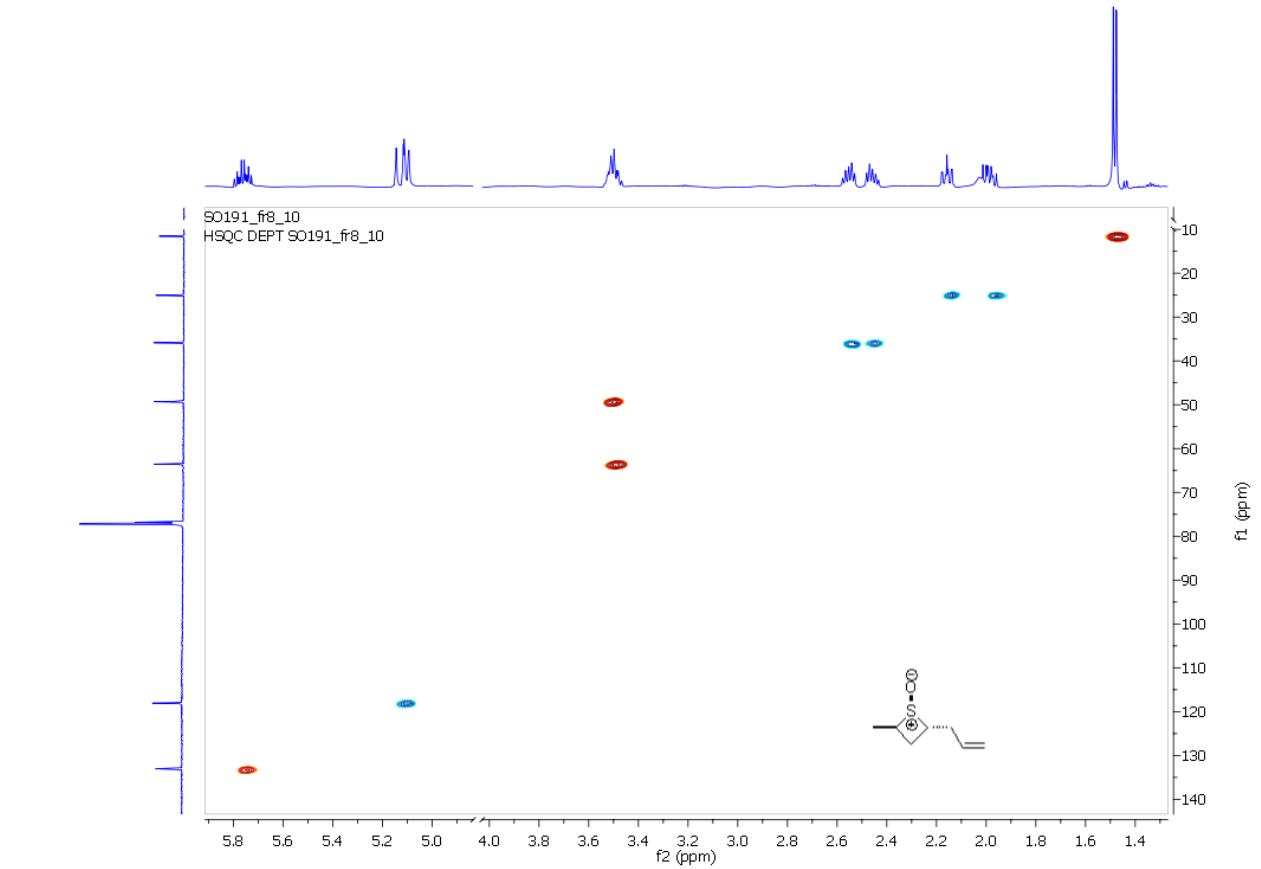

SO176-fr18-20
HSQC DEPT SO176-fr18-20
f2 (ppm)
f1 (ppm)
H_B
O
H_C
S
H_A
H_D

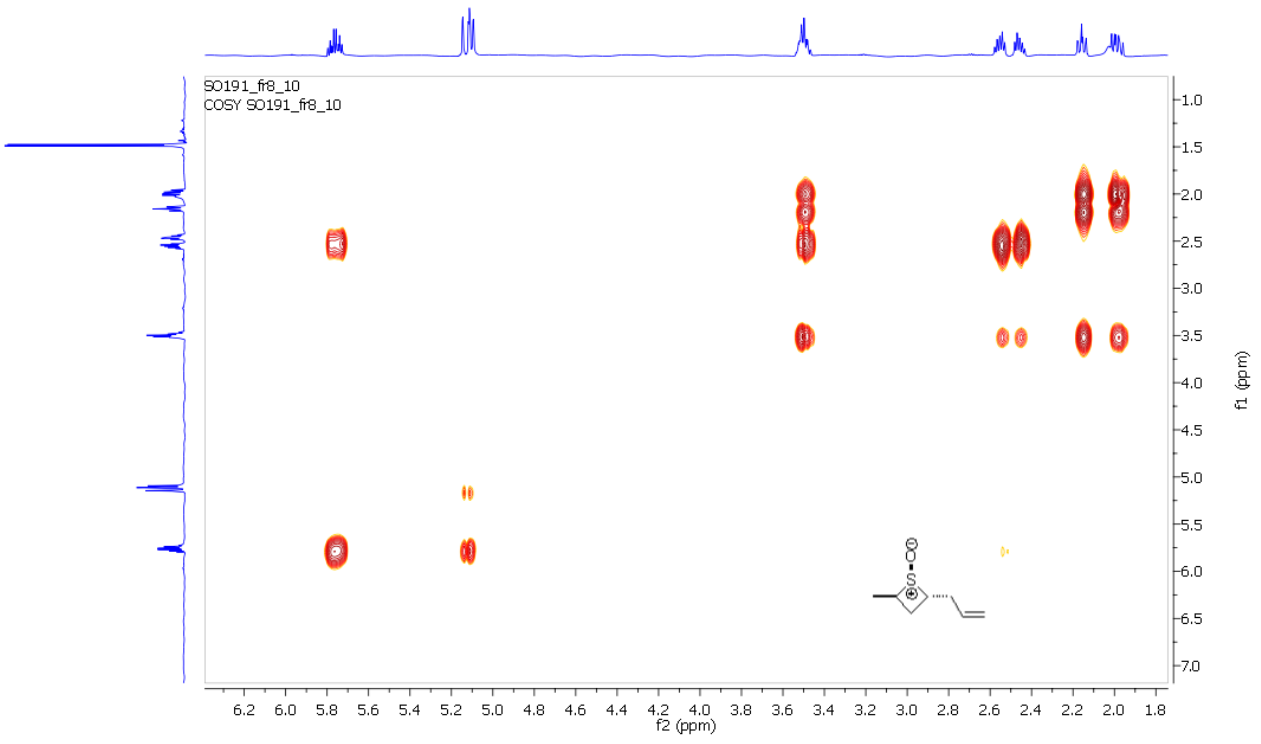

H_A
H_B
CH_2Ph
H_E/H_E'
H_D
H_C
SO176-fr18-20
NOESY SO176-fr18-20
f1 (ppm)
H_B
O
H_C
S
H_A
H_D

(1R$_S$, 2R*, 4R*) 7a major*

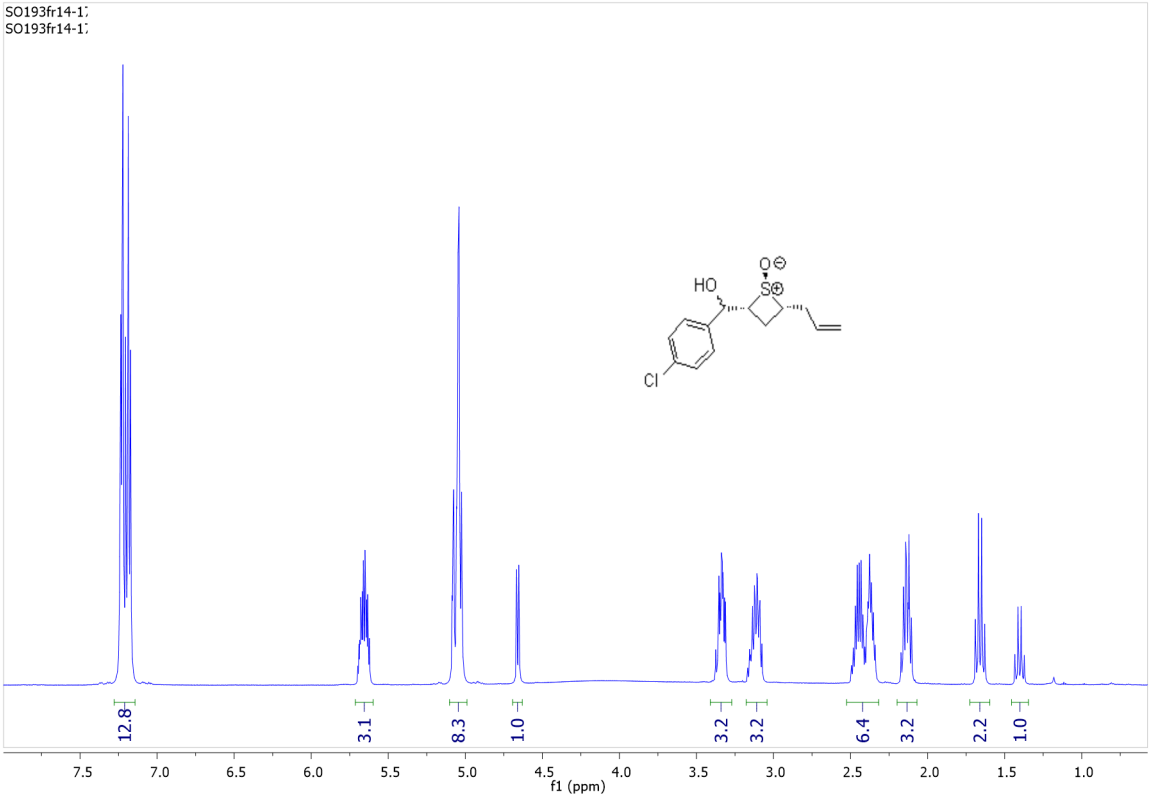


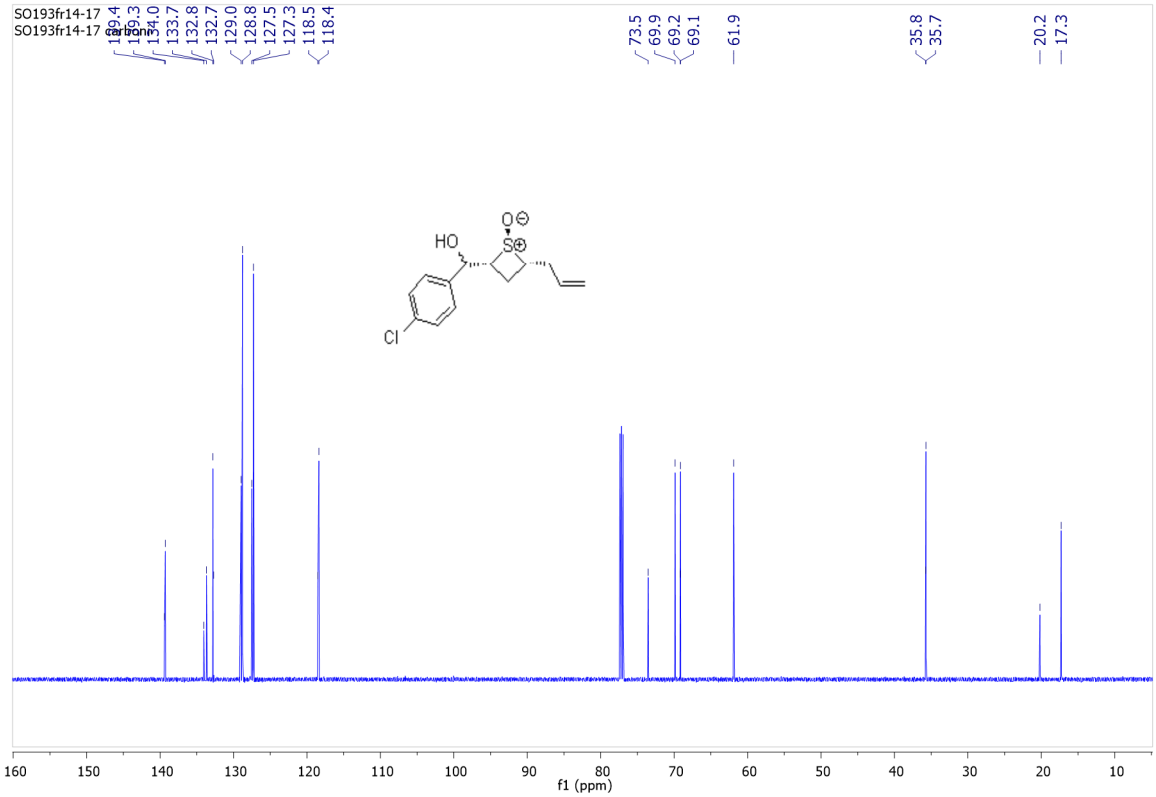


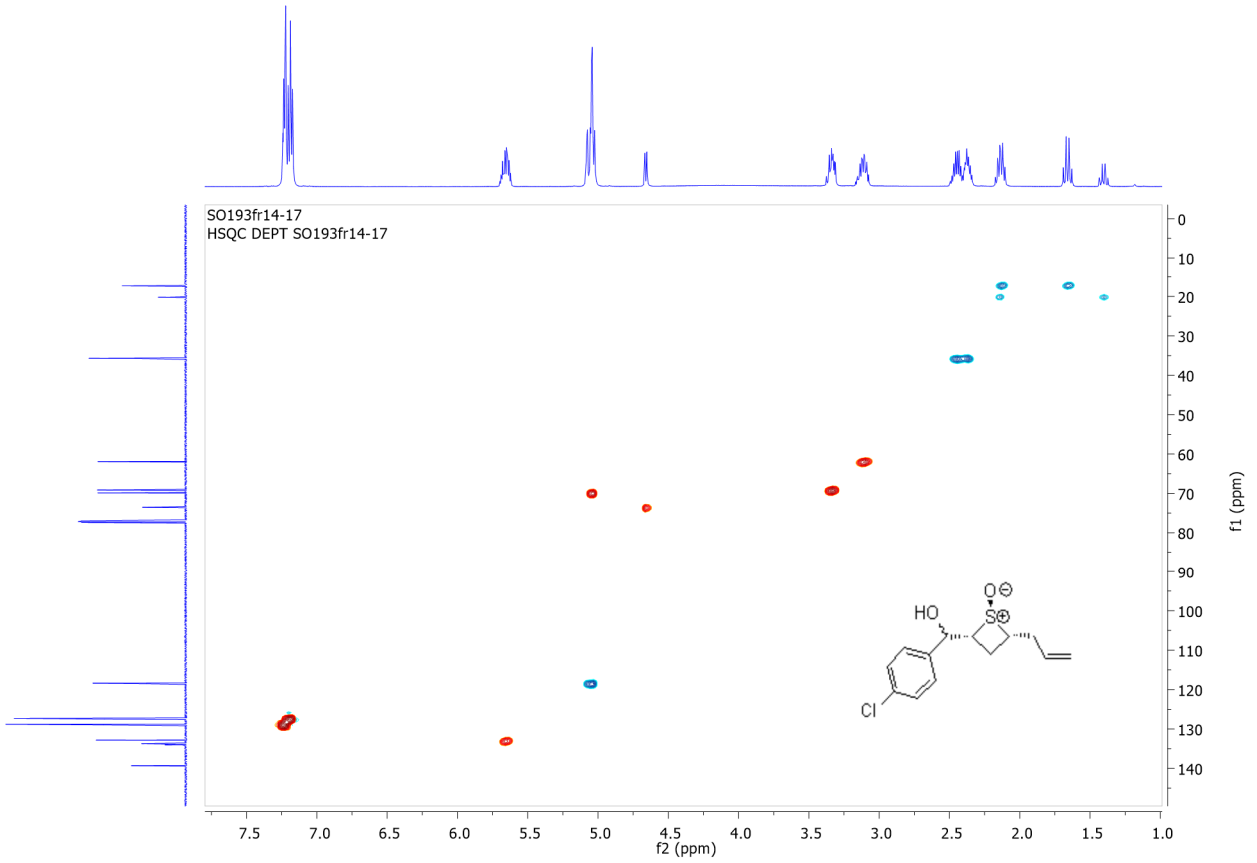

SO191_fr8_10
HSQC DEPT SO191_fr8_10
f2 (ppm)
f1 (ppm)

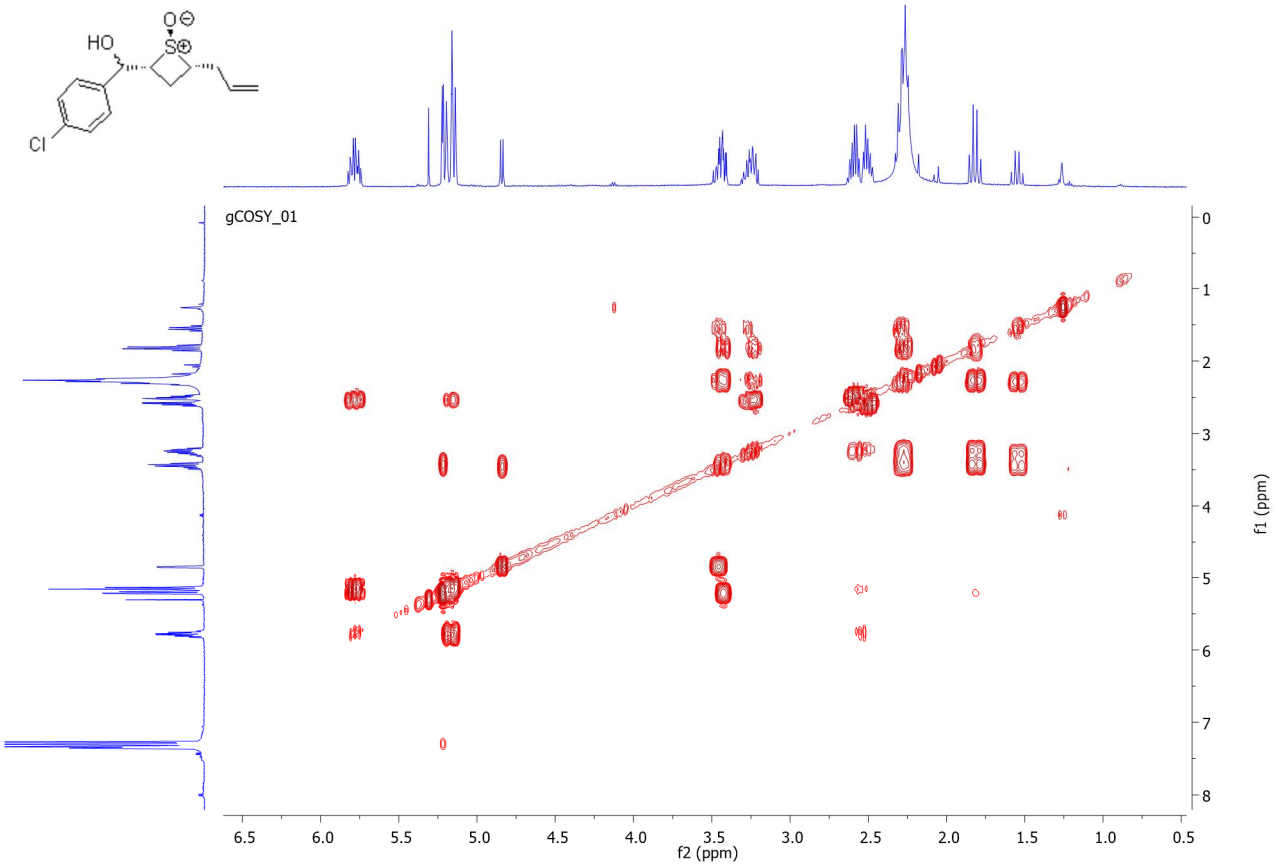

SO191_fr8_10
COSY SO191_fr8_10
f2 (ppm)
f1 (ppm)

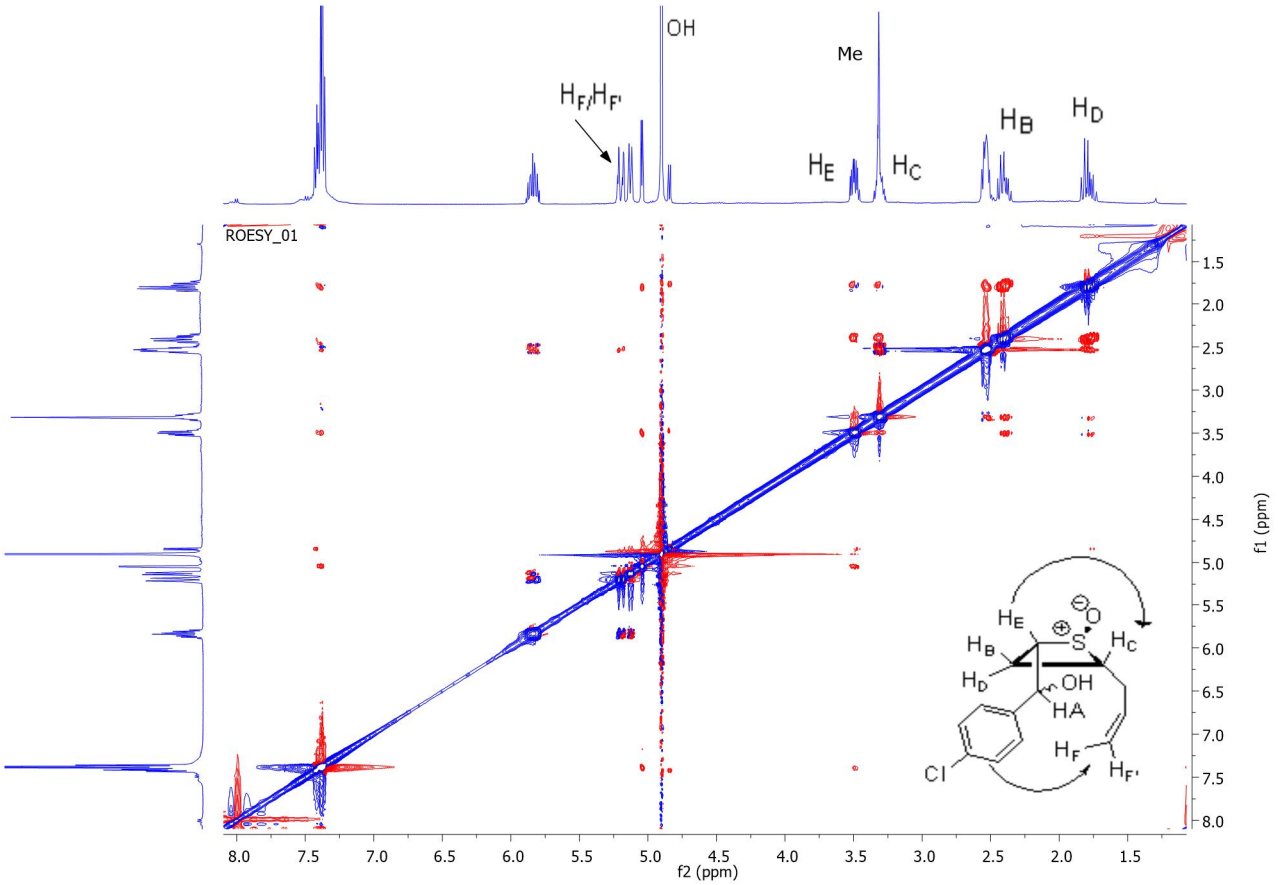
(1R_S*, 2S*, 4S*) 7b


SO193fr14-17
SO193fr14-17
HO
Cl
12.8
3.1
8.3
1.0
3.2
3.2
6.4
3.2
2.2
1.0
f1 (ppm)

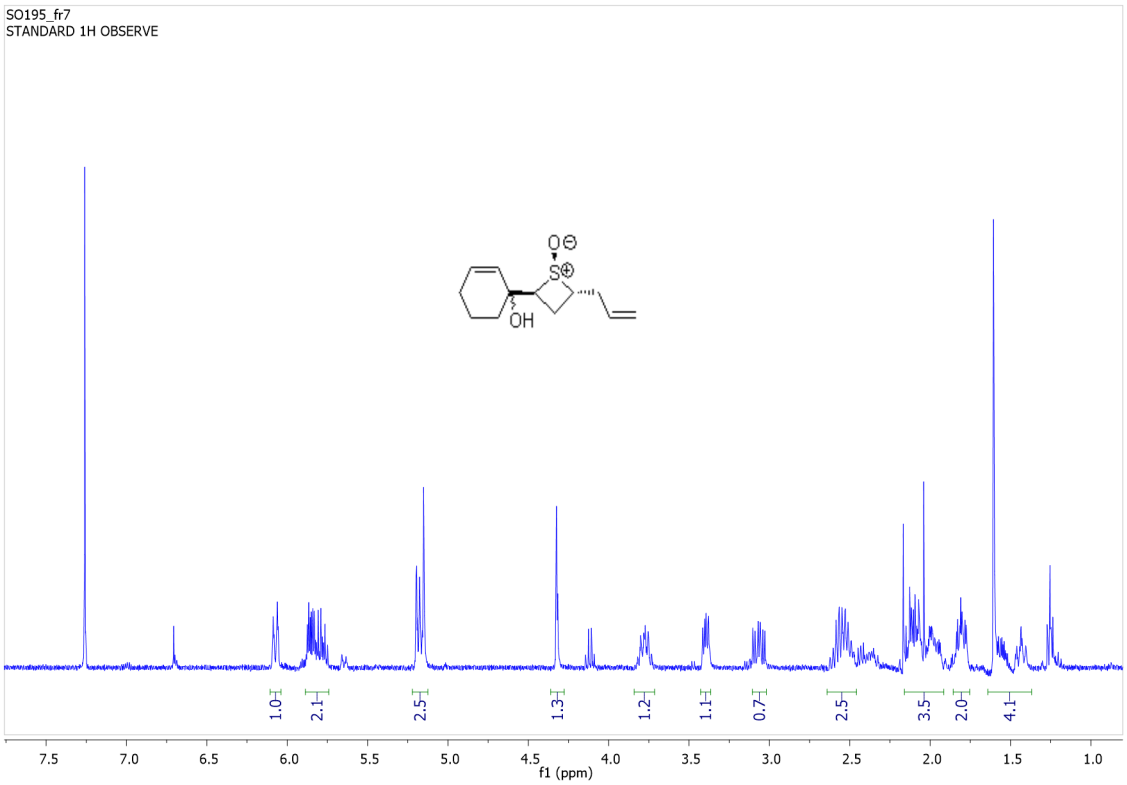

SO193fr14-17
SO193fr14-17 carbon
169.4
169.3
134.0
133.7
132.8
132.7
129.0
128.8
127.5
127.3
118.5
118.4
73.5
69.9
69.2
69.1
61.9
35.8
35.7
20.2
17.3
HO
Cl
f1 (ppm)

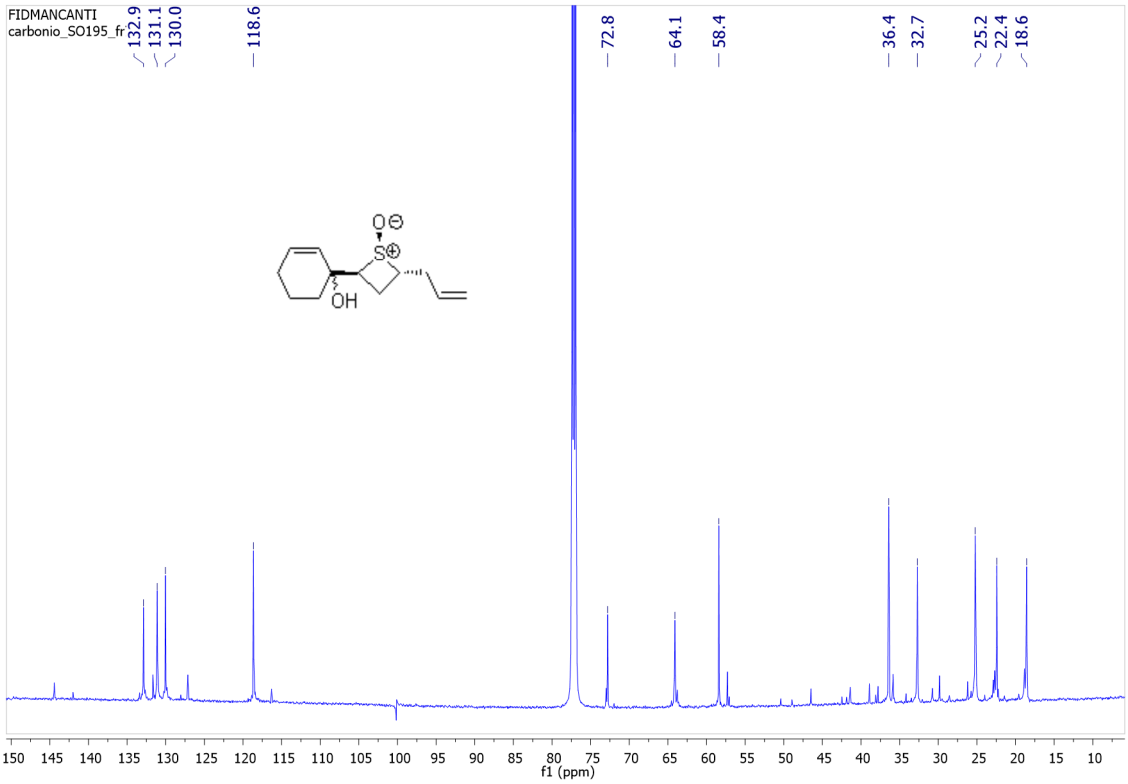

SO193fr14-17
HSQC DEPT SO193fr14-17
HO
Cl
f2 (ppm)
f1 (ppm)

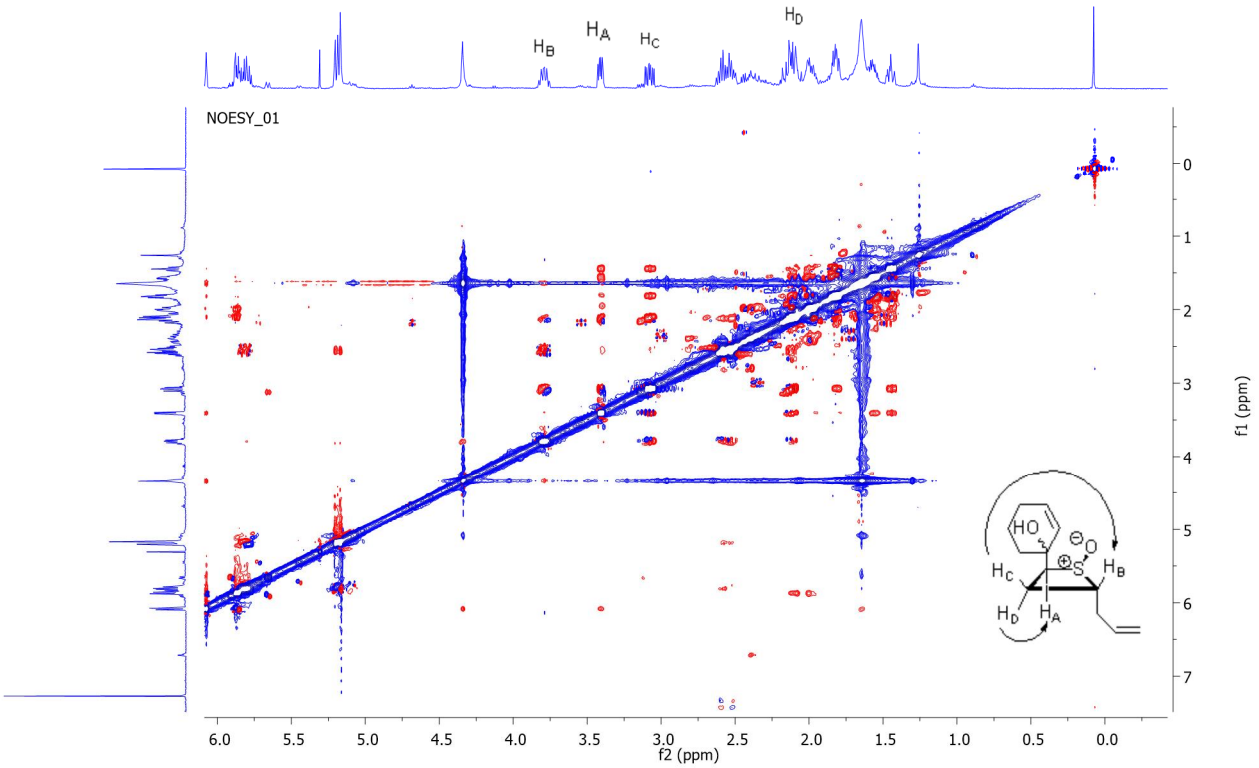

HO
Cl
gCOSY_01
f2 (ppm)
f1 (ppm)


OH
Me
$H_F/H_{F'}$
H_E
H_C
H_B
H_D
ROESY_01
f2 (ppm)
f1 (ppm)
H_A
Cl

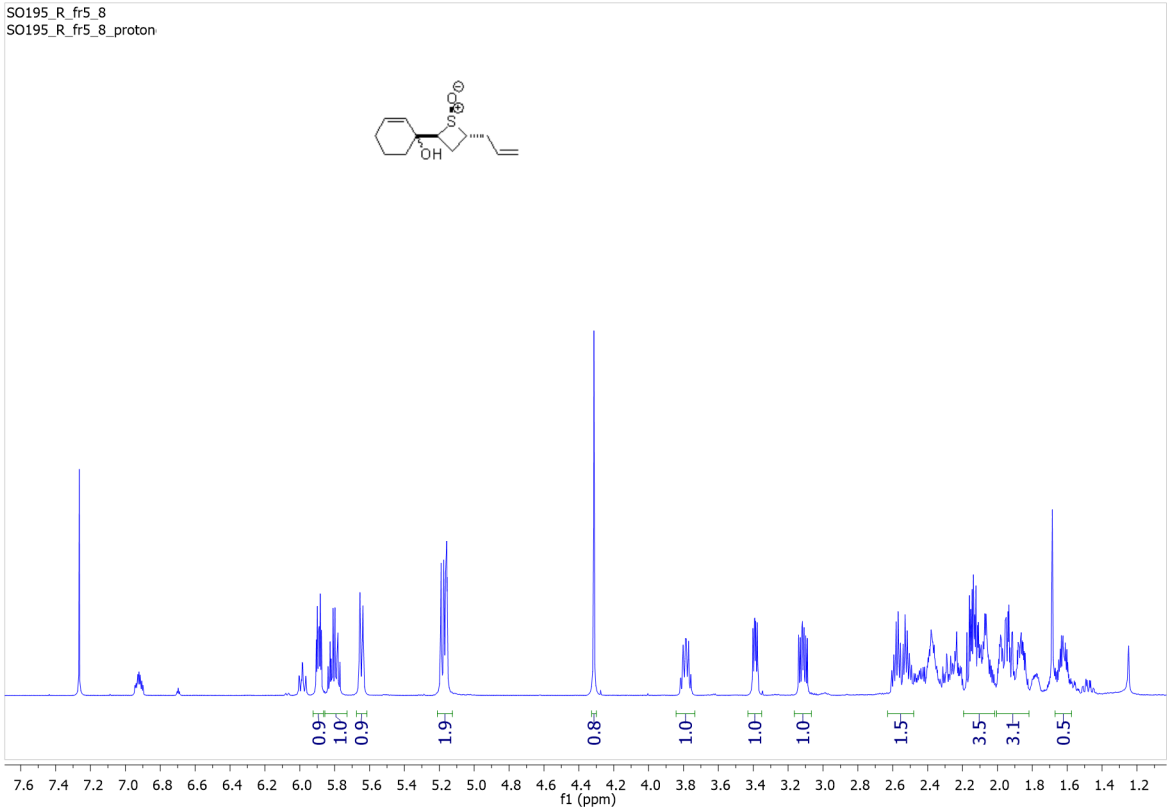
(1R_S*, 2*R, 4*S**) 7c *minor***

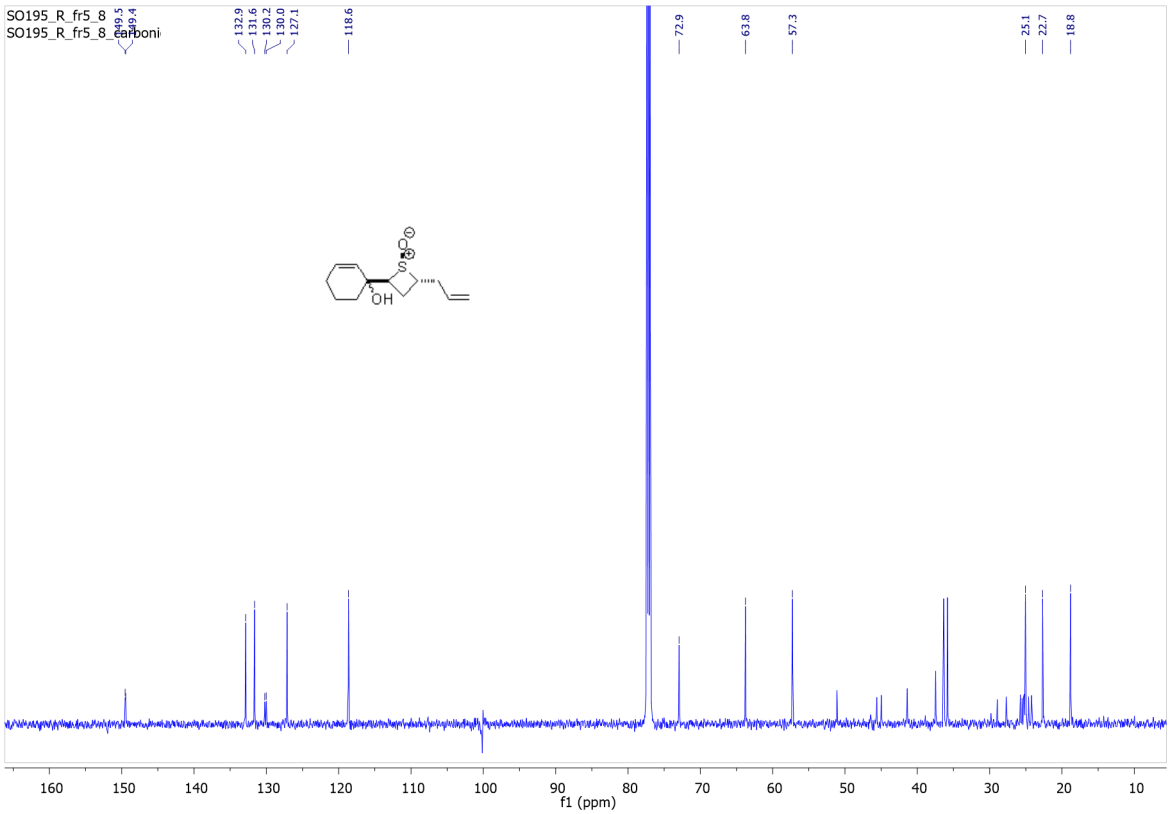




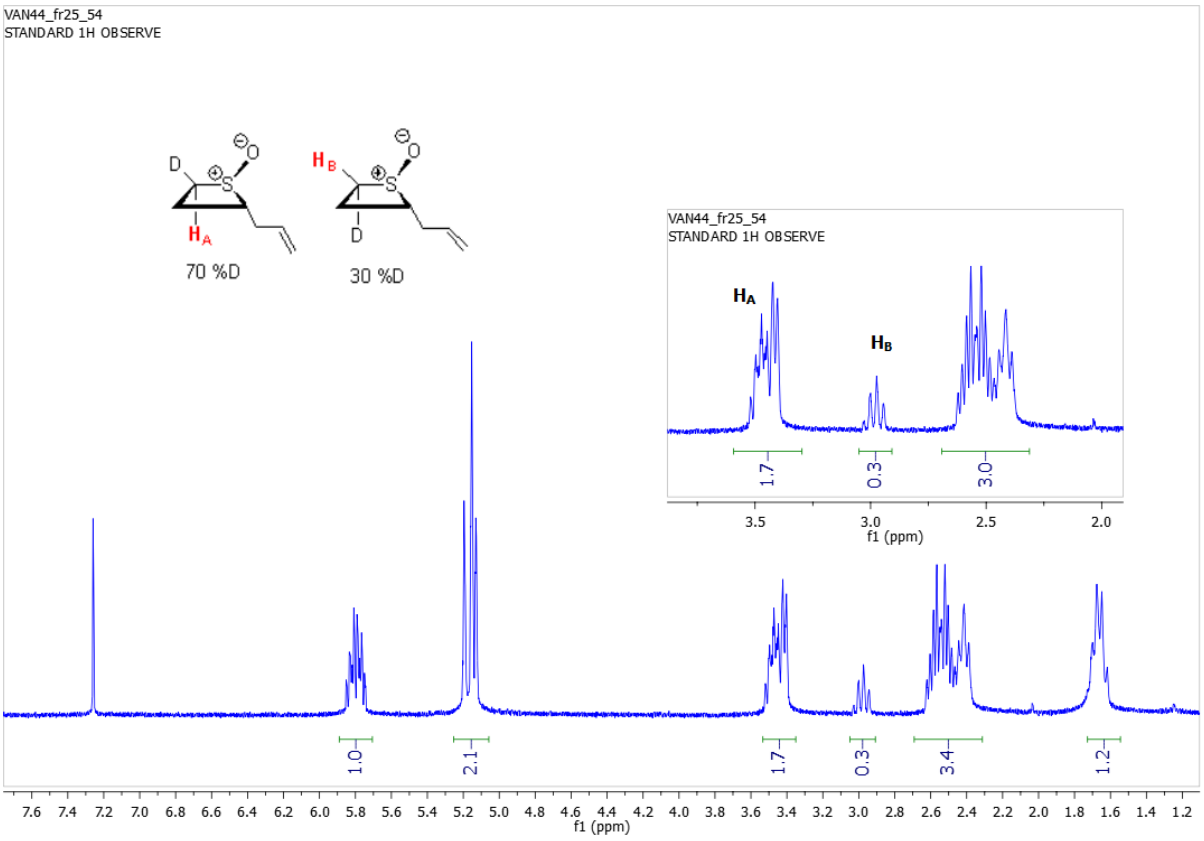

NOESY_01
H_B
H_A
H_C
H_D
HO
O
S
H_C
H_B
H_D
H_A
f2 (ppm)
f1 (ppm)

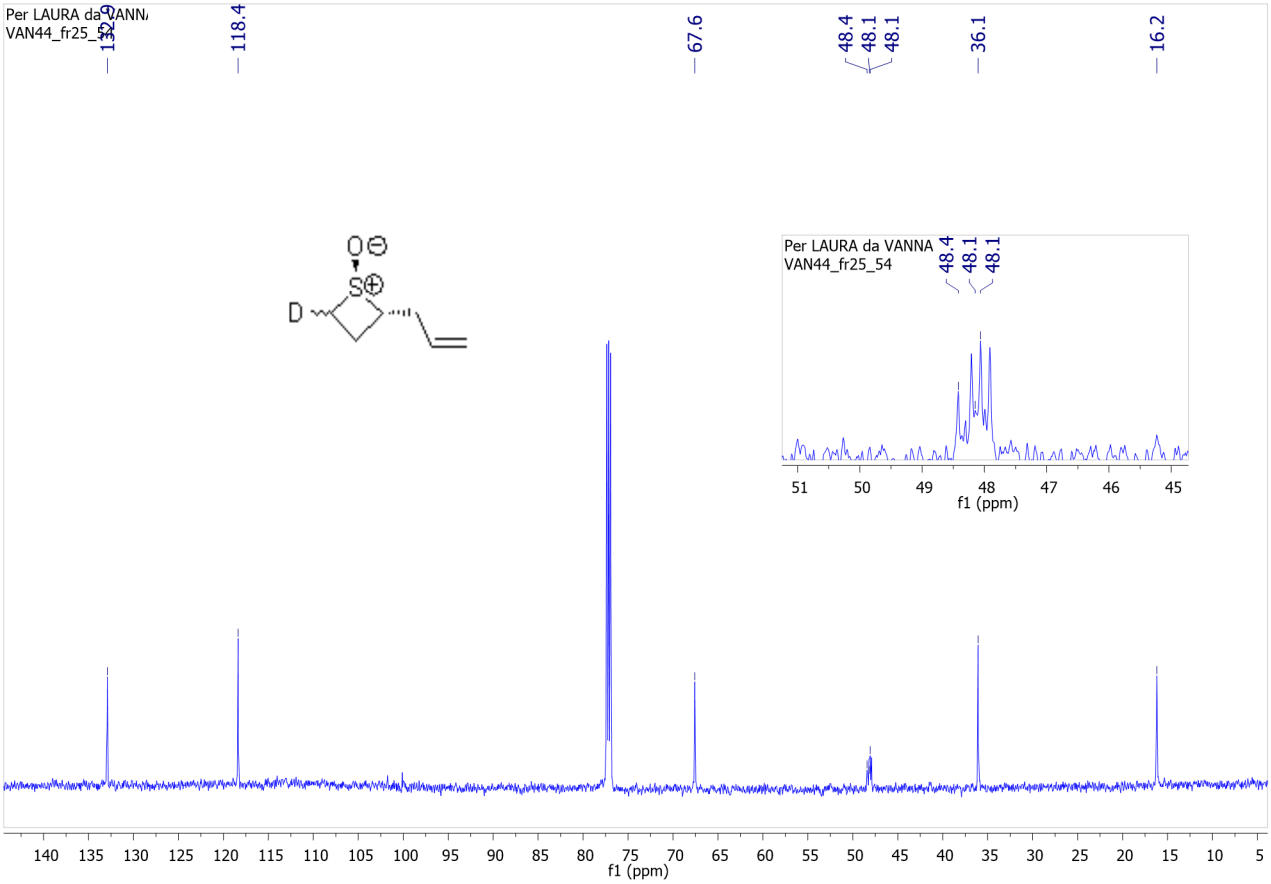
(1R_S*, 2*R, 4*S**) 7c *major***



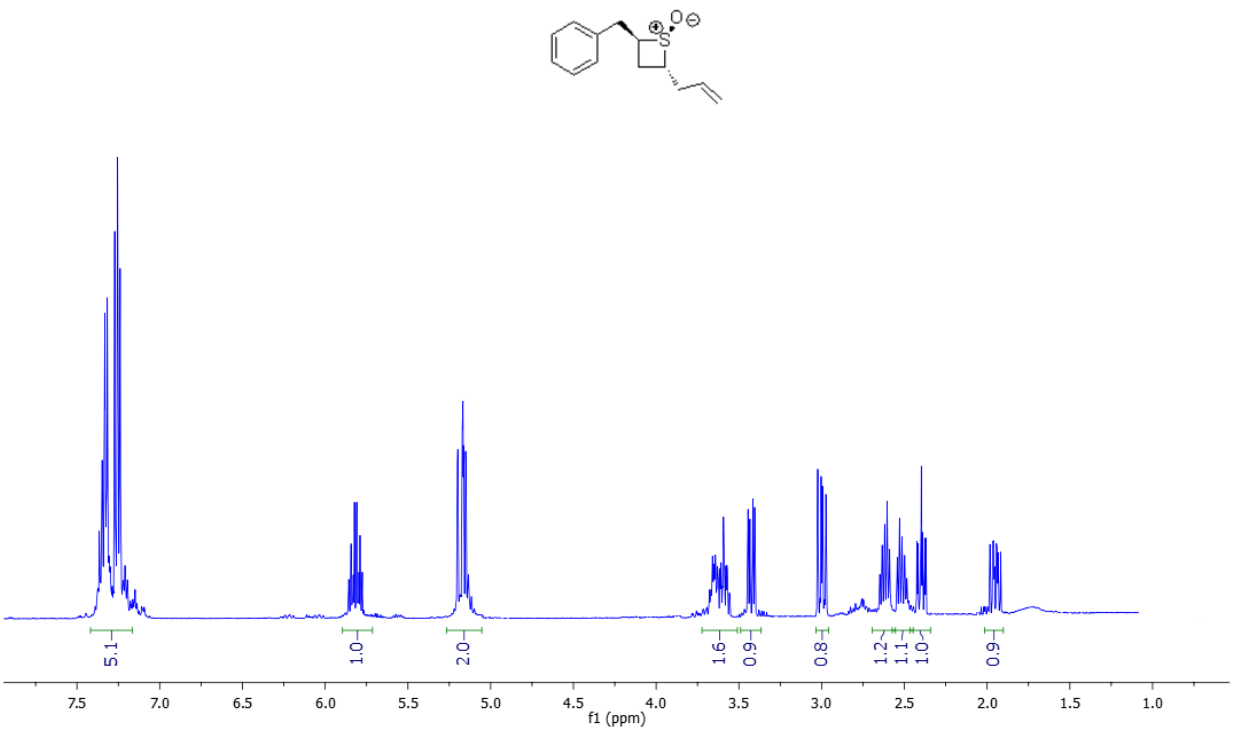


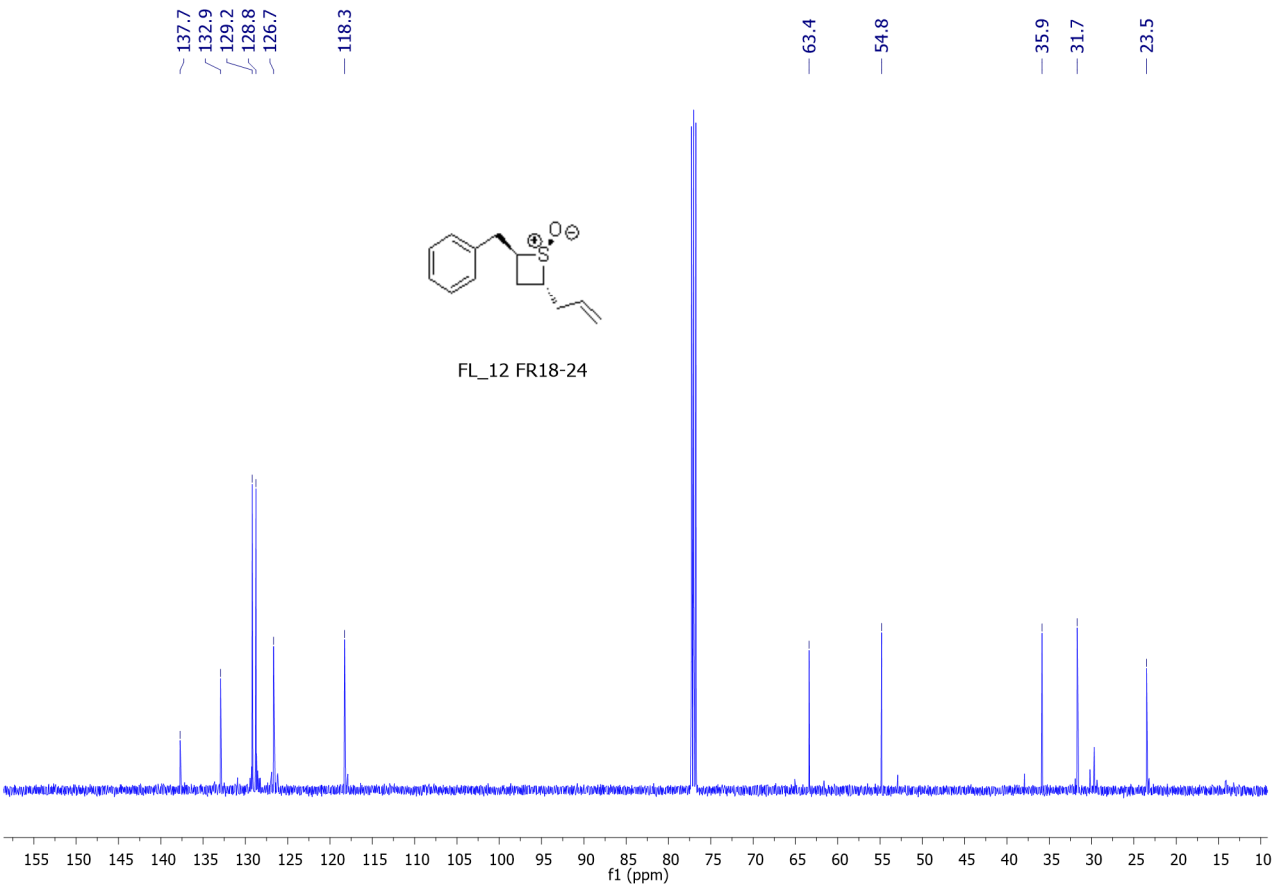
(1R_S*,2*R,4*R**)/(1R_S*,2*R**,4*S**)-7d**

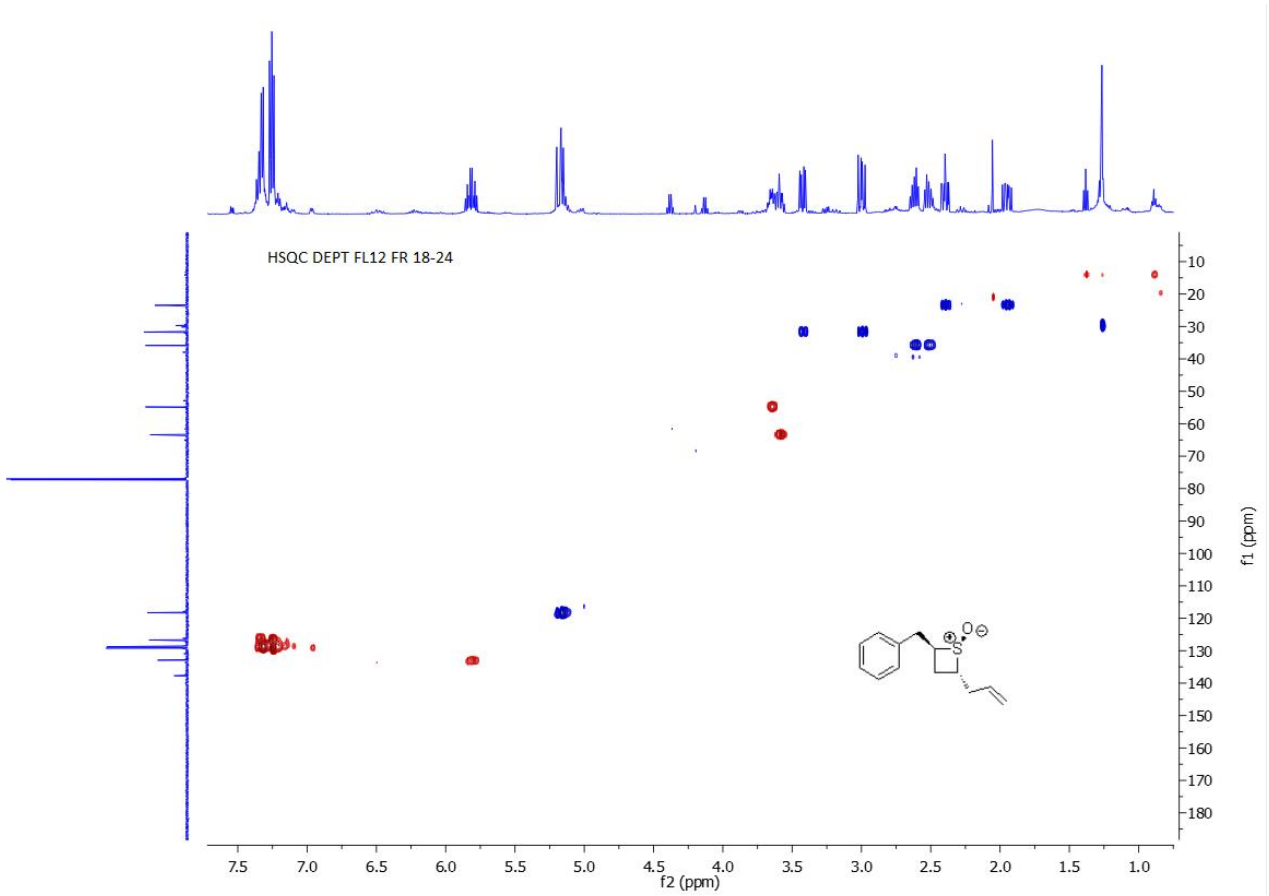


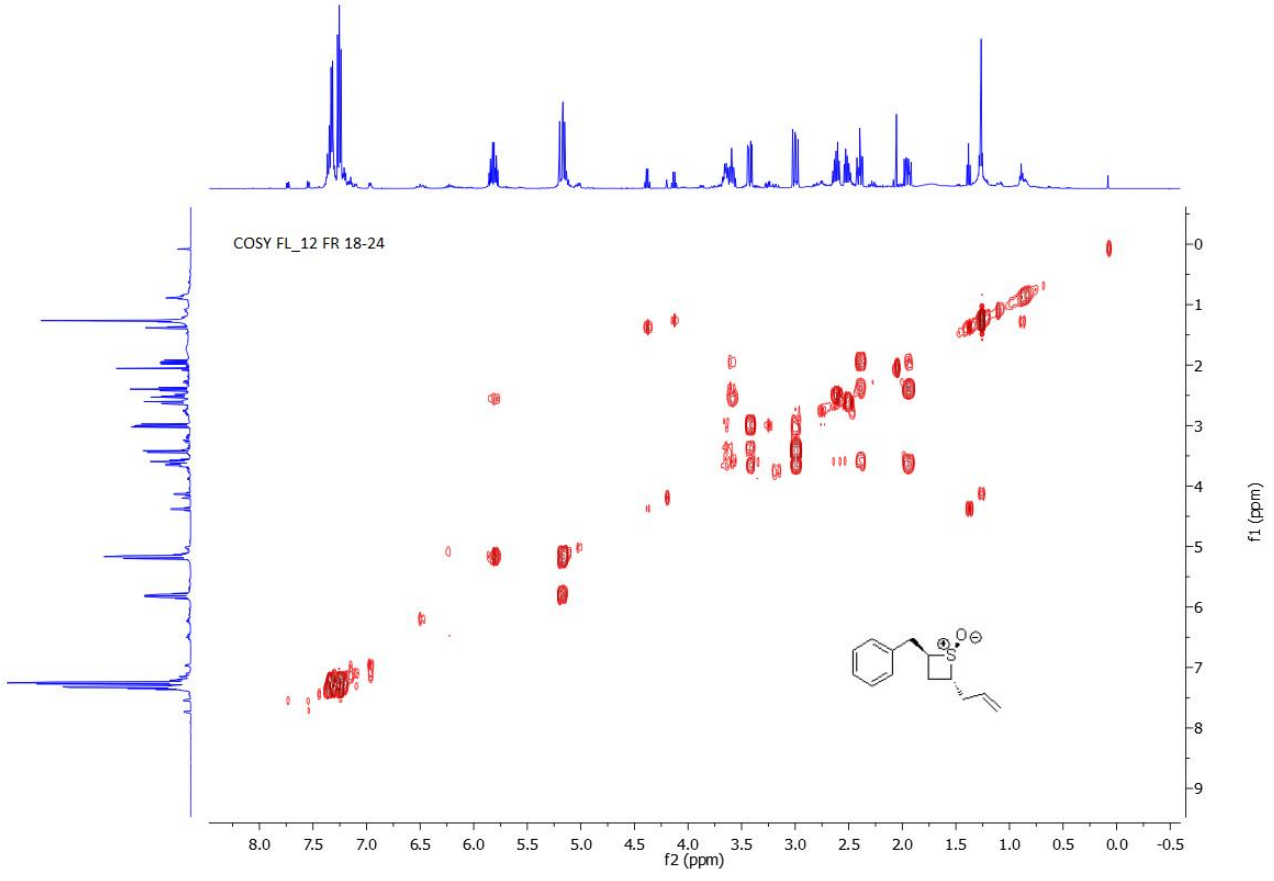


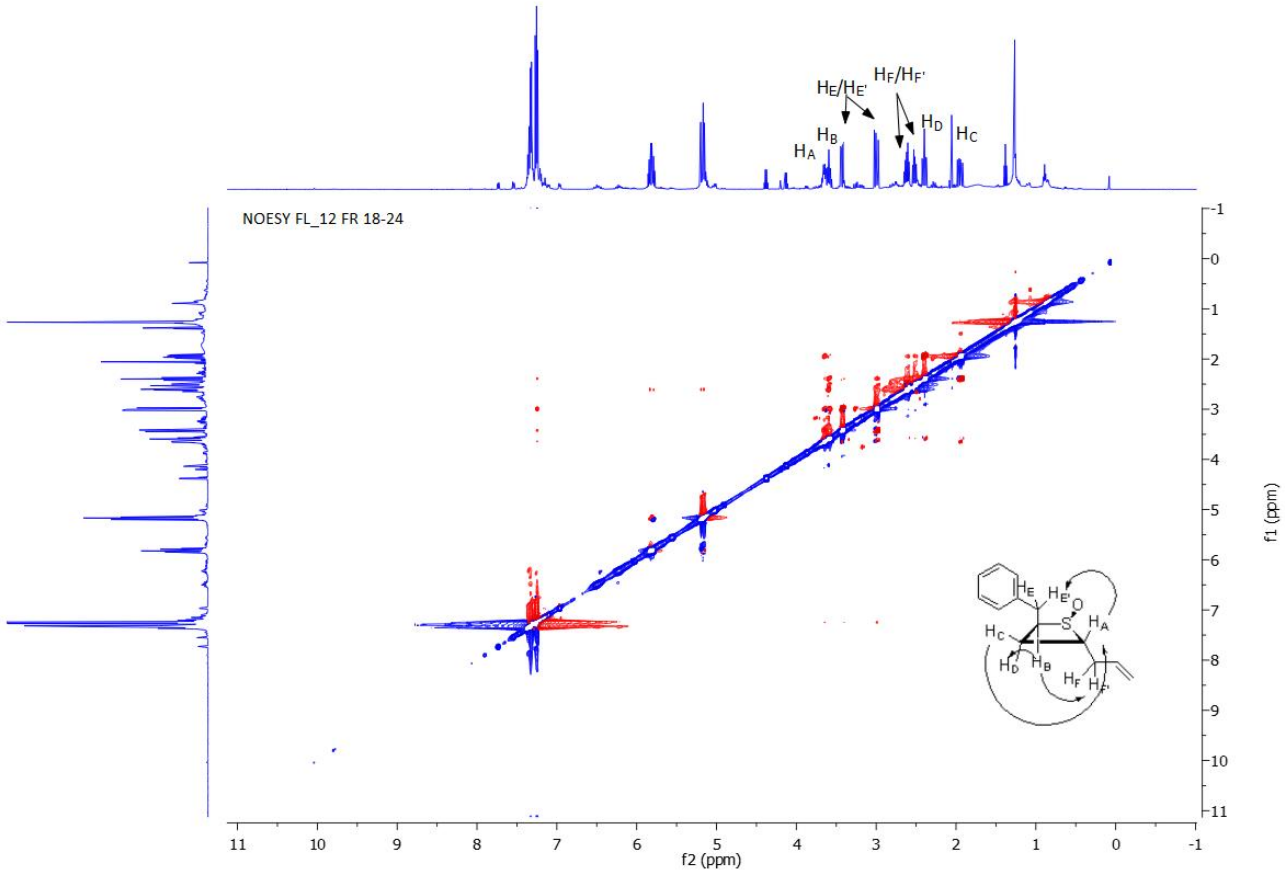
(1R_S*, 2*S, 4*S**)-7e**


5.1
1.0
2.0
1.6
0.9
0.8
1.2
1.1
1.0
0.9
f1 (ppm)

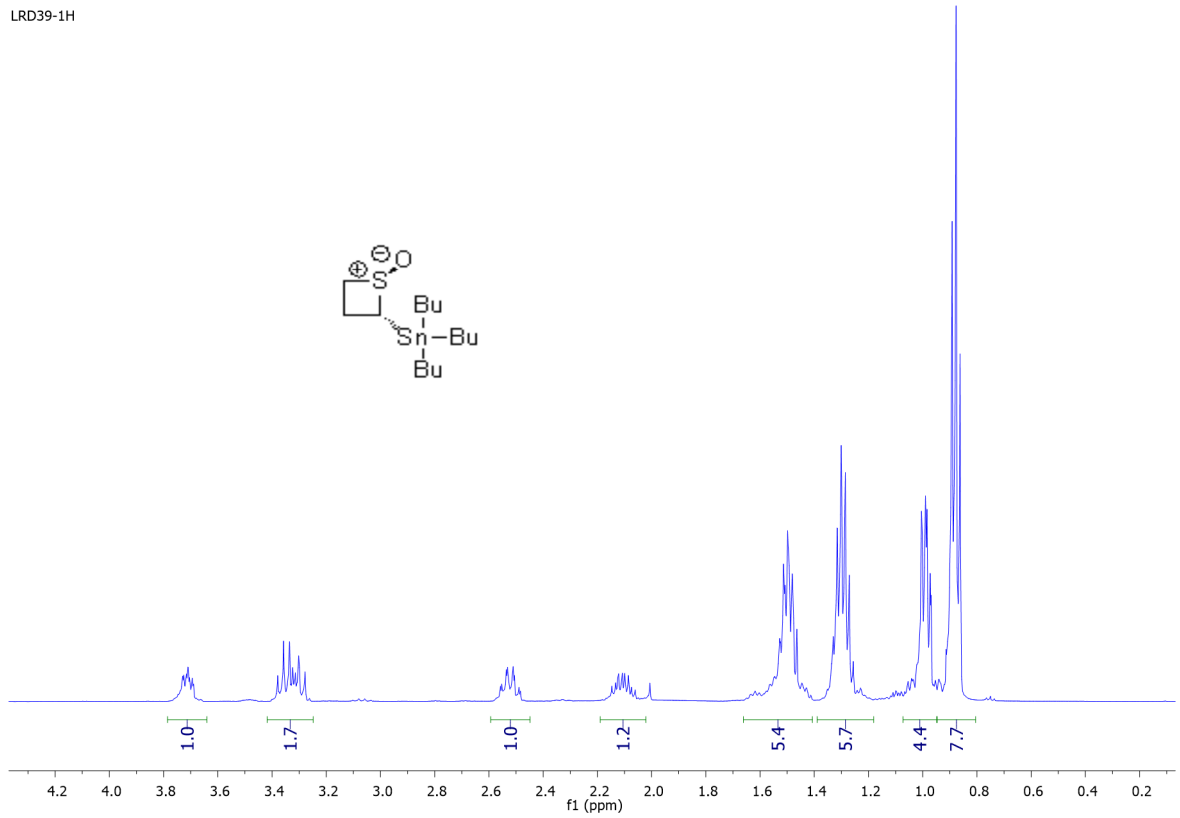

137.7
132.9
129.2
128.8
126.7
118.3
63.4
54.8
35.9
31.7
23.5
FL_12 FR18-24
f1 (ppm)

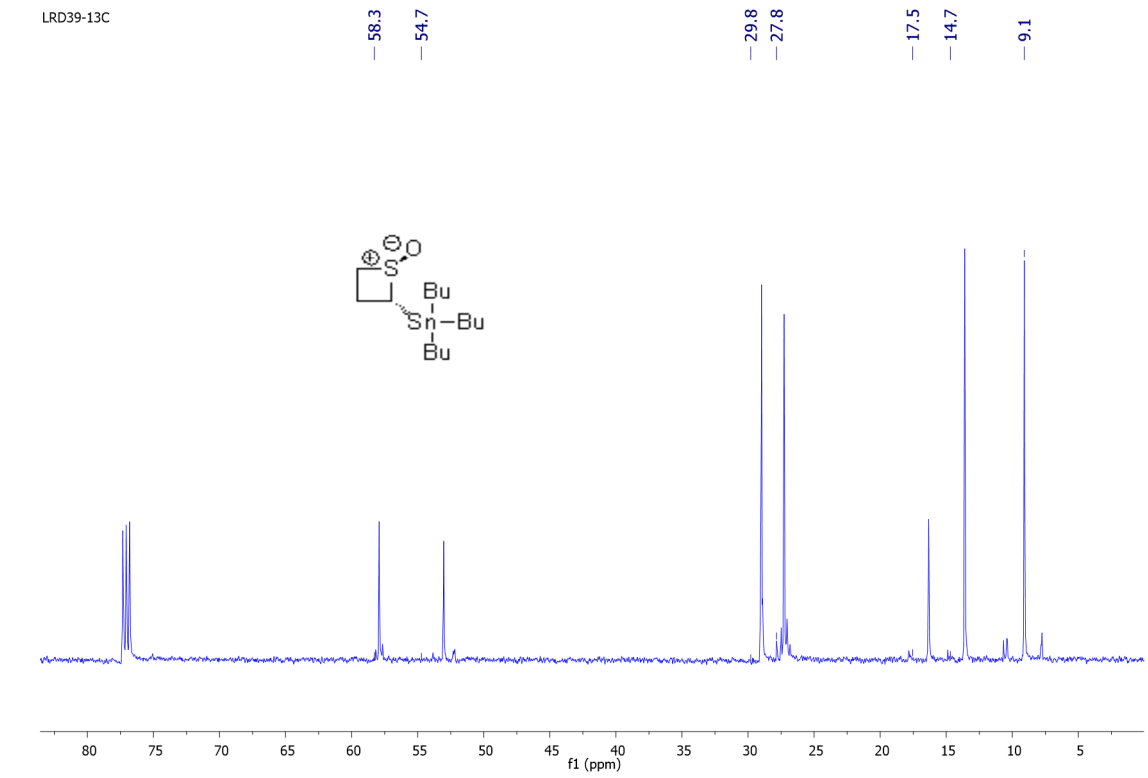

HSQC DEPT FL12 FR 18-24
f2 (ppm)
f1 (ppm)

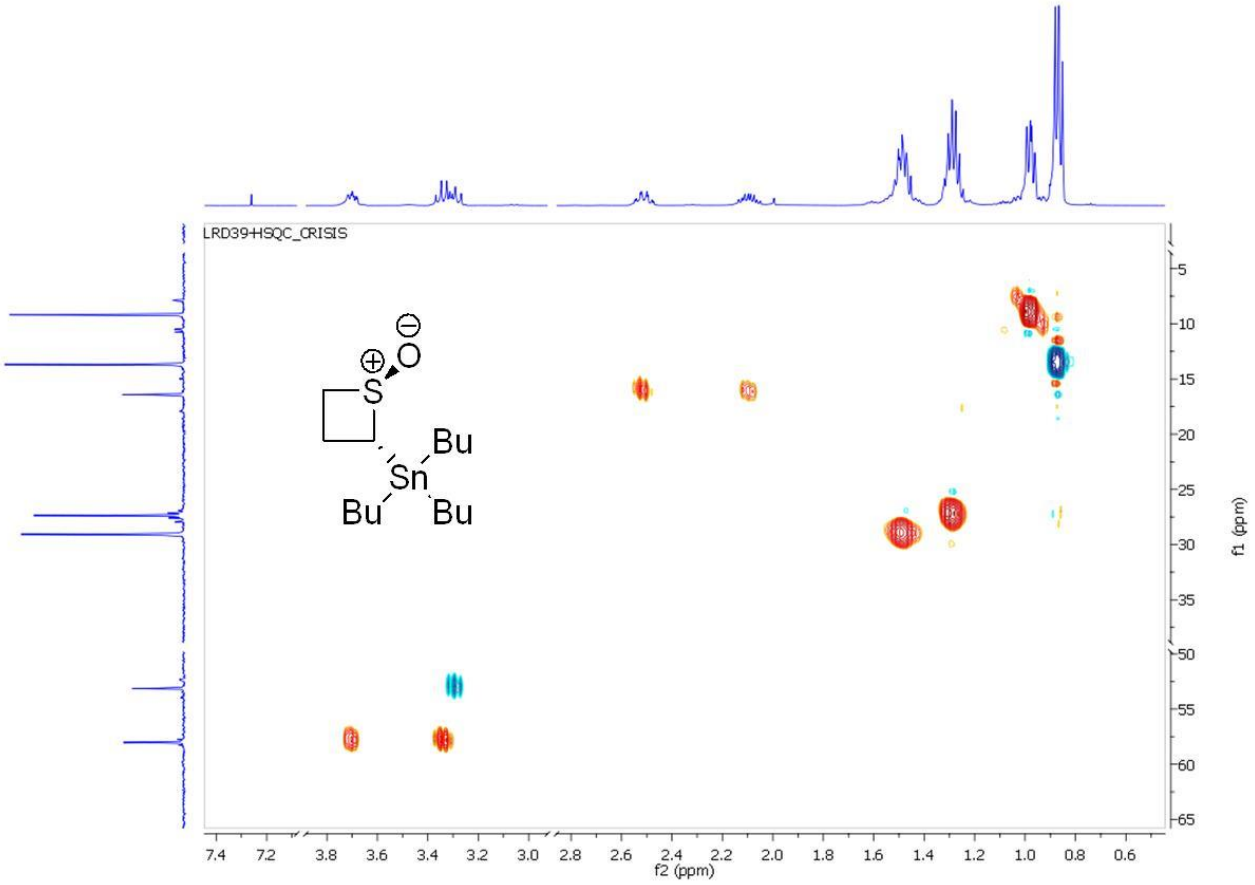

COSY FL_12 FR 18-24
f2 (ppm)
f1 (ppm)


NOESY FL_12 FR 18-24
HE/HE'
HF/HF'
HD
HC
HB
HA
f2 (ppm)
f1 (ppm)

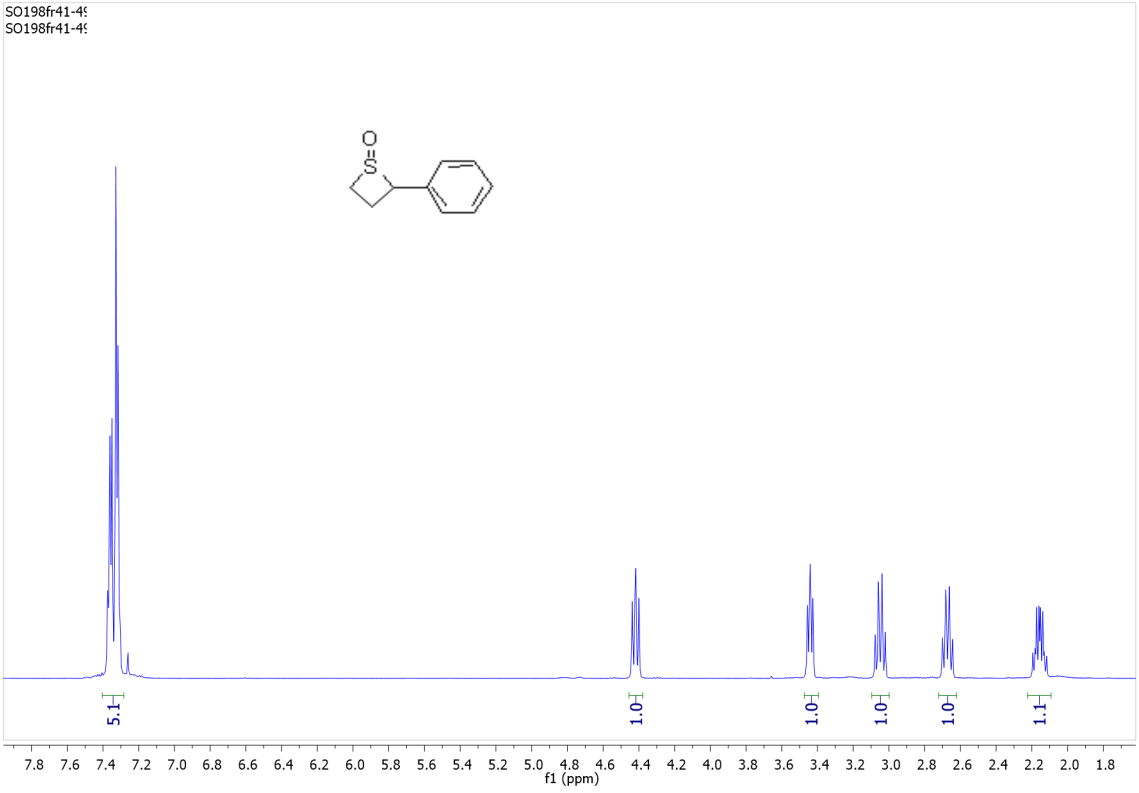
(1R_S*, 2R*)-8

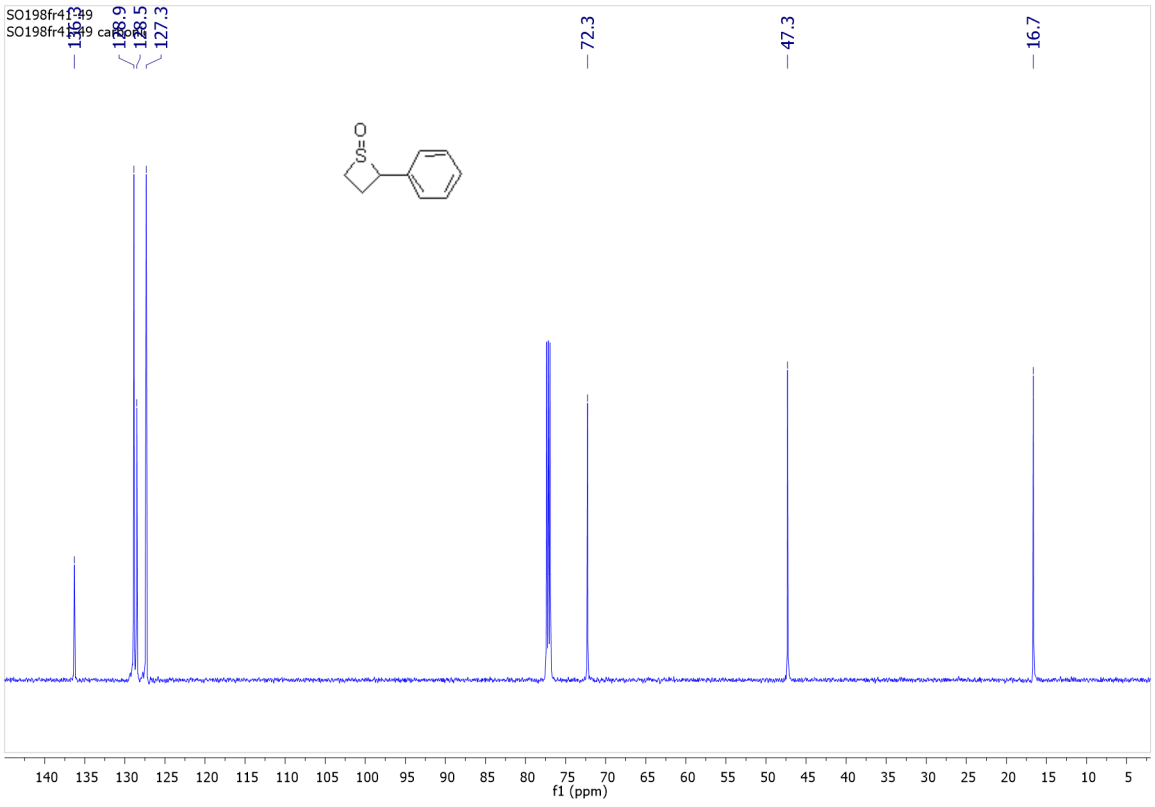

LRD39-1H
Bu
Sn–Bu
Bu
1.0
1.7
1.0
1.2
5.4
5.7
4.4
7.7
f1 (ppm)

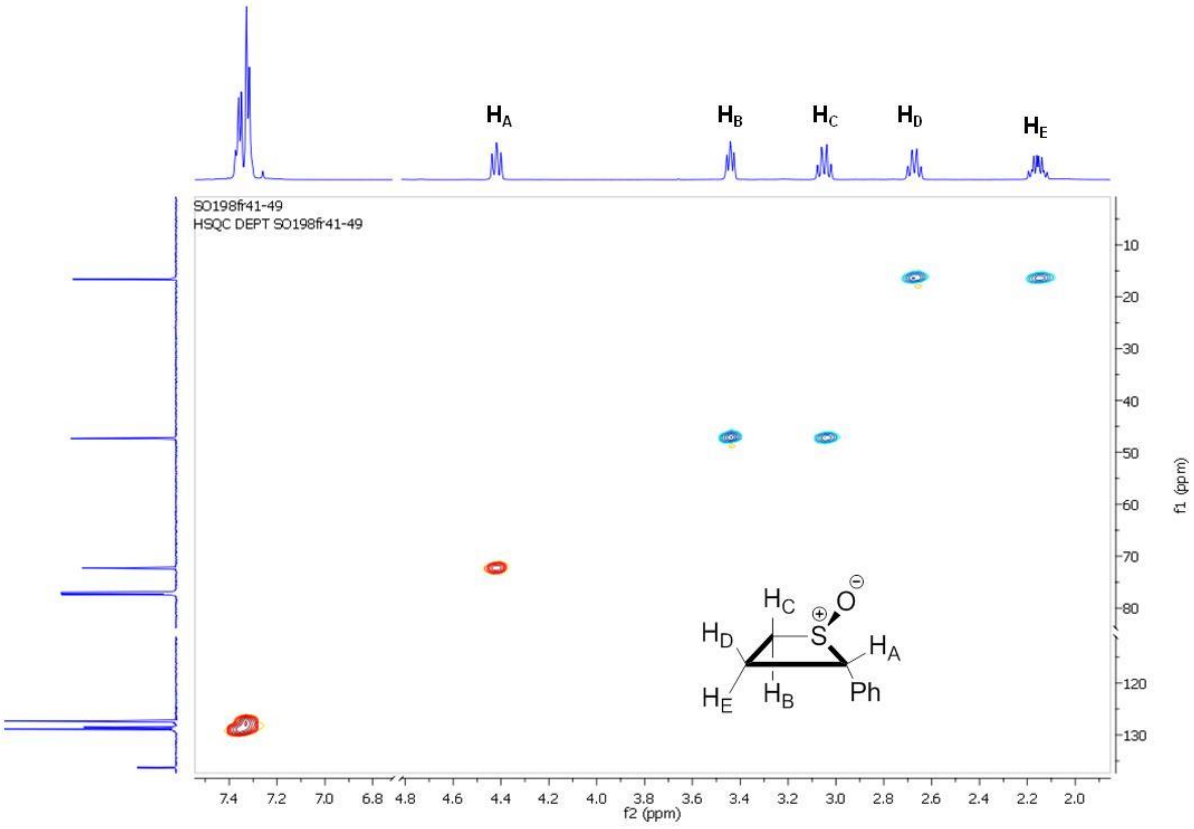

LRD39-13C
58.3
54.7
29.8
27.8
17.5
14.7
9.1
Bu
Sn–Bu
Bu
f1 (ppm)

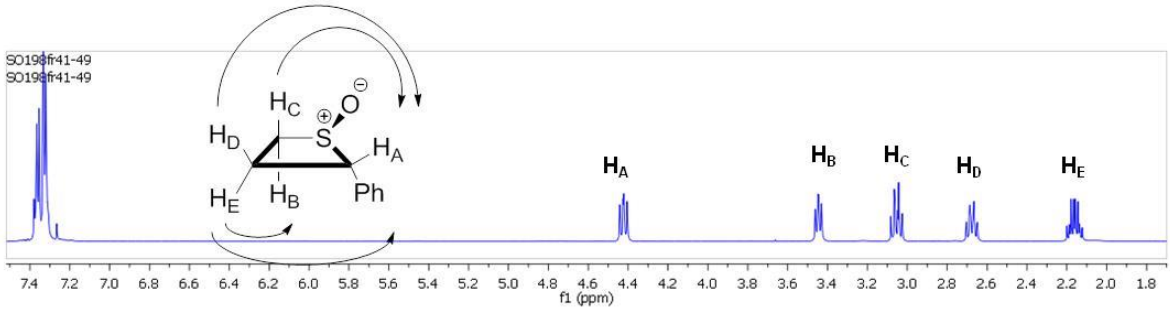

LRD39-HSQC_CRISIS
O
S
Bu
Sn
Bu
Bu
f2 (ppm)
f1 (ppm)

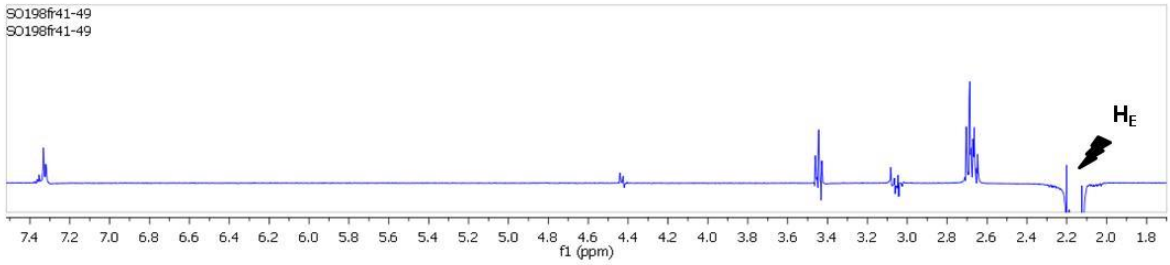
9

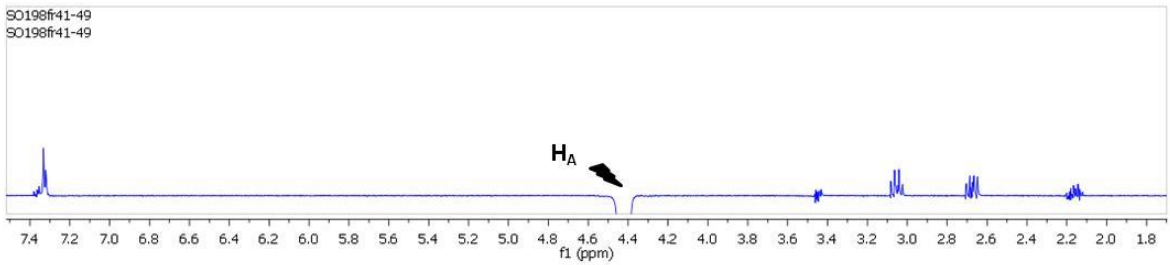

SO198fr41-49
SO198fr41-49
O
S
5.1
1.0
1.0
1.0
1.0
1.1
7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8
f1 (ppm)


SO198fr41-49
SO198fr41-49 carbon
139.2
128.9
128.5
127.3
72.3
47.3
16.7
O
S
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
f1 (ppm)

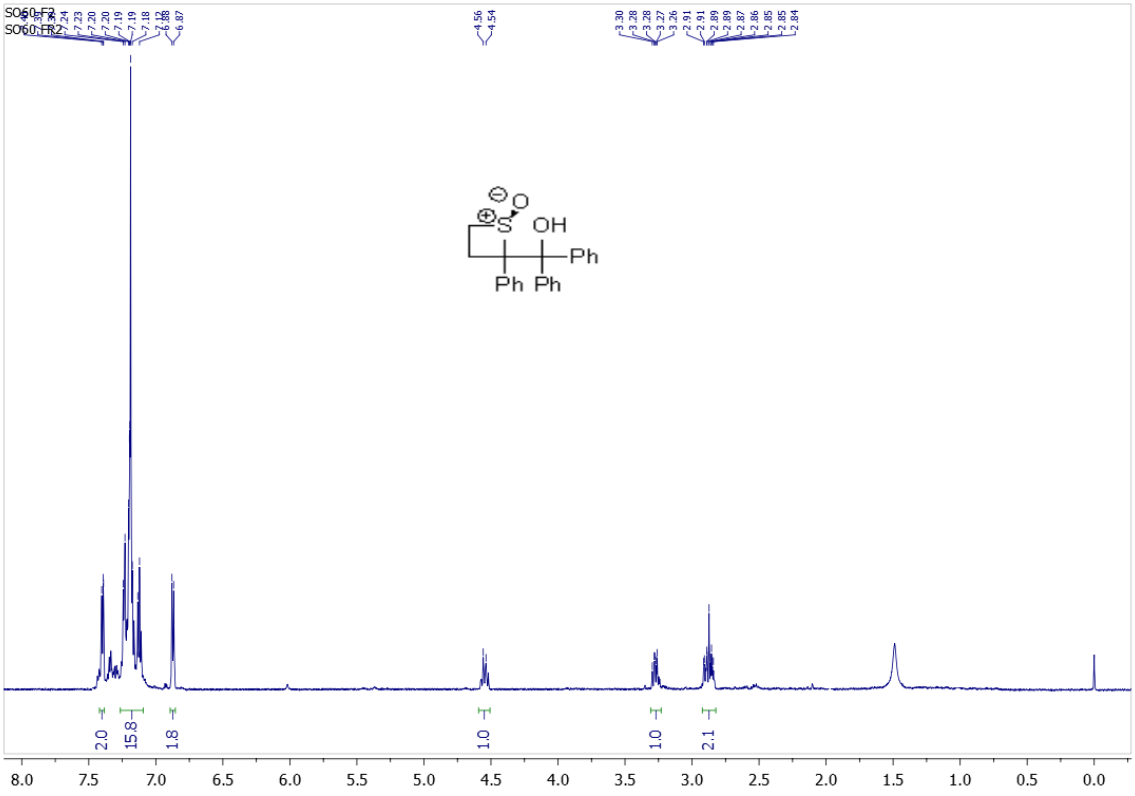

HA
HB
HC
HD
HE
SO198fr41-49
HSQC DEPT SO198fr41-49
f1 (ppm)
f2 (ppm)
HC
O
HD
S
HA
HE
HB
Ph

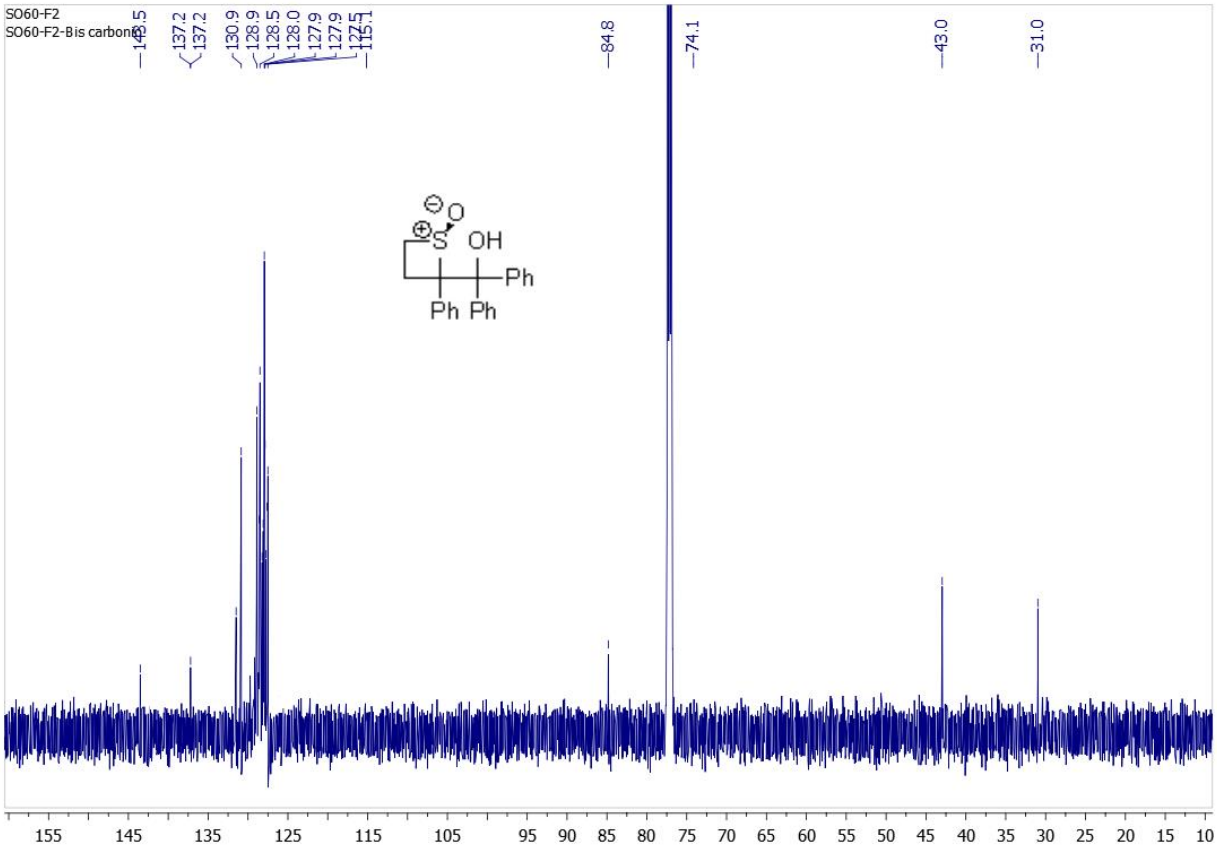

SO198fr41-49
SO198fr41-49
HC
O
HD
S
HA
HE
HB
Ph
HA
HB
HC
HD
HE
f1 (ppm)

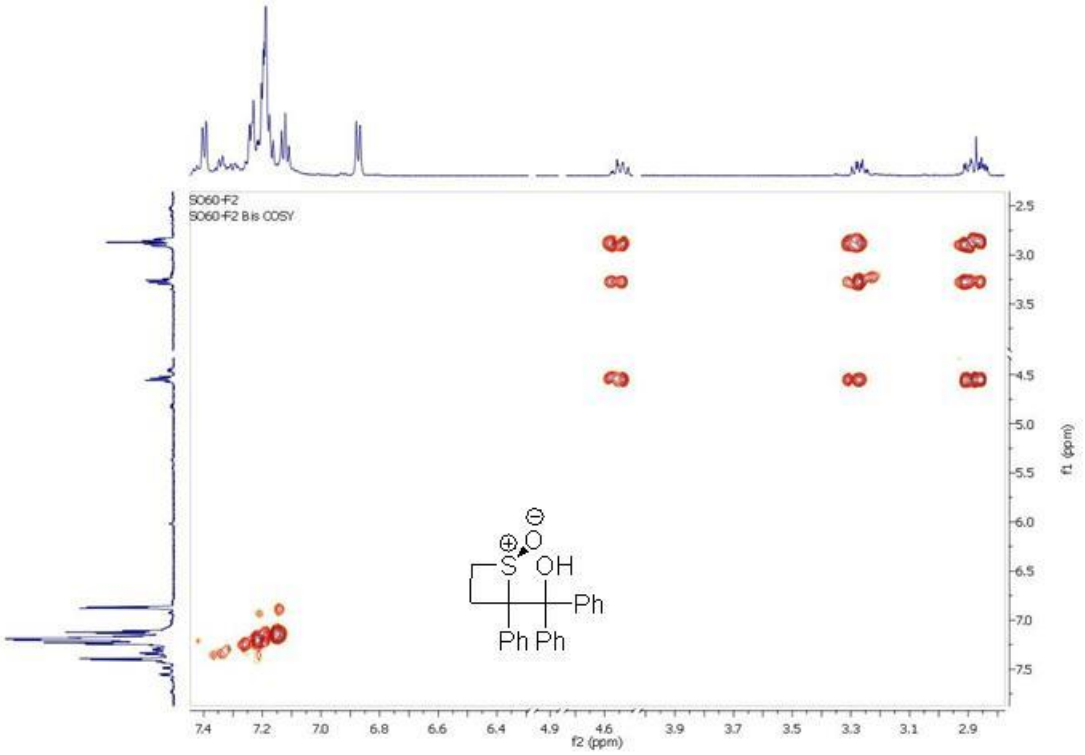

SO198fr41-49
SO198fr41-49
HE
f1 (ppm)

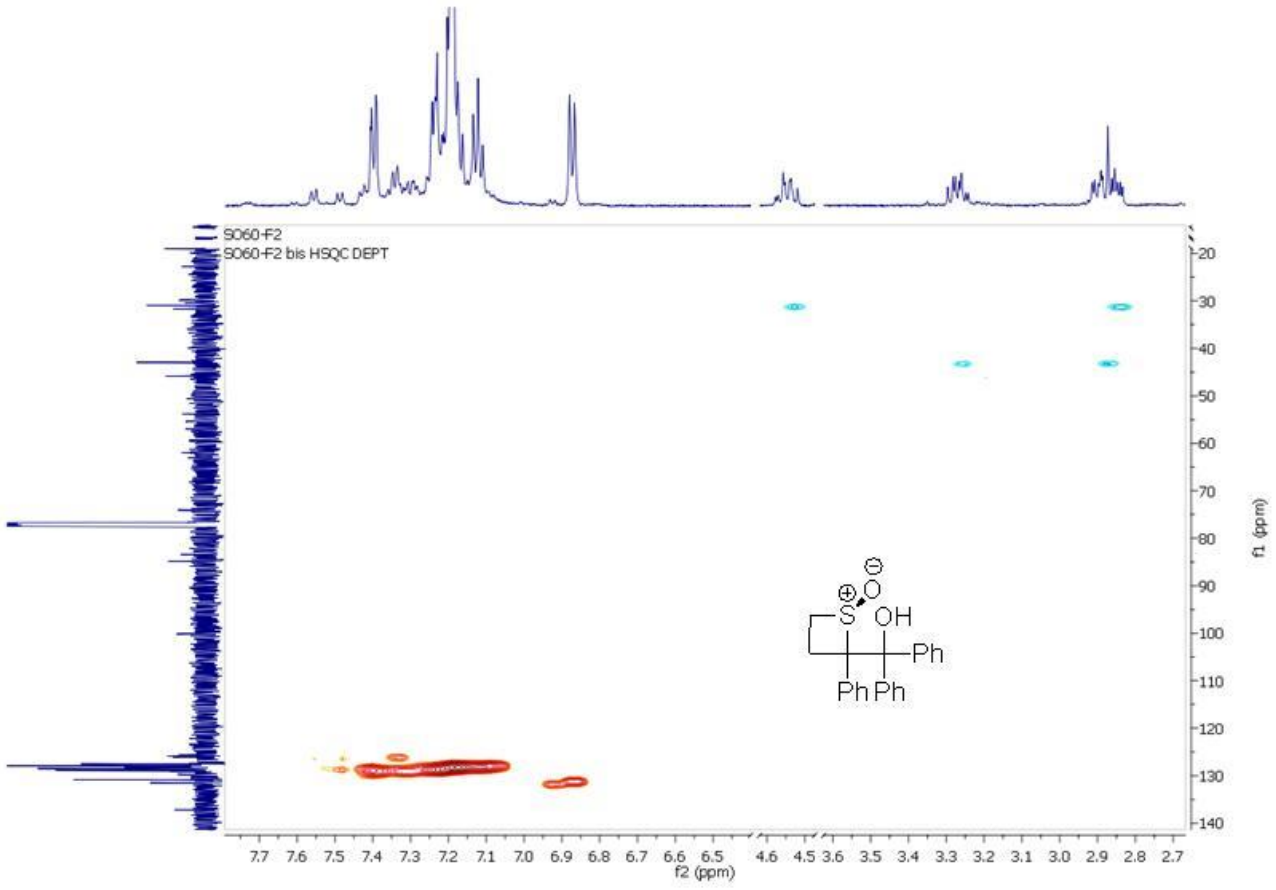

SO198fr41-49
SO198fr41-49
HA
f1 (ppm)

(1R_S*,2S*)-10

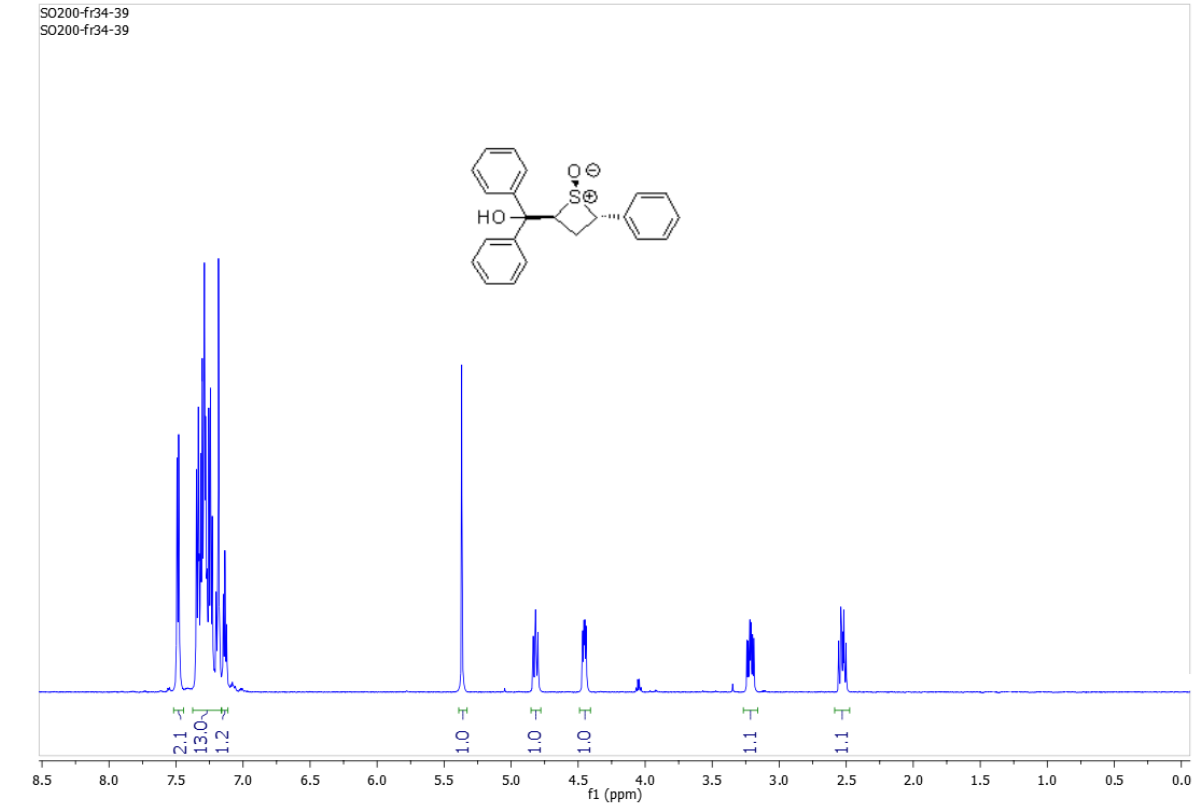

SO60-F2
SO60-FR2
OH
Ph
Ph Ph
2.0
15.8
1.8
1.0
1.0
2.1

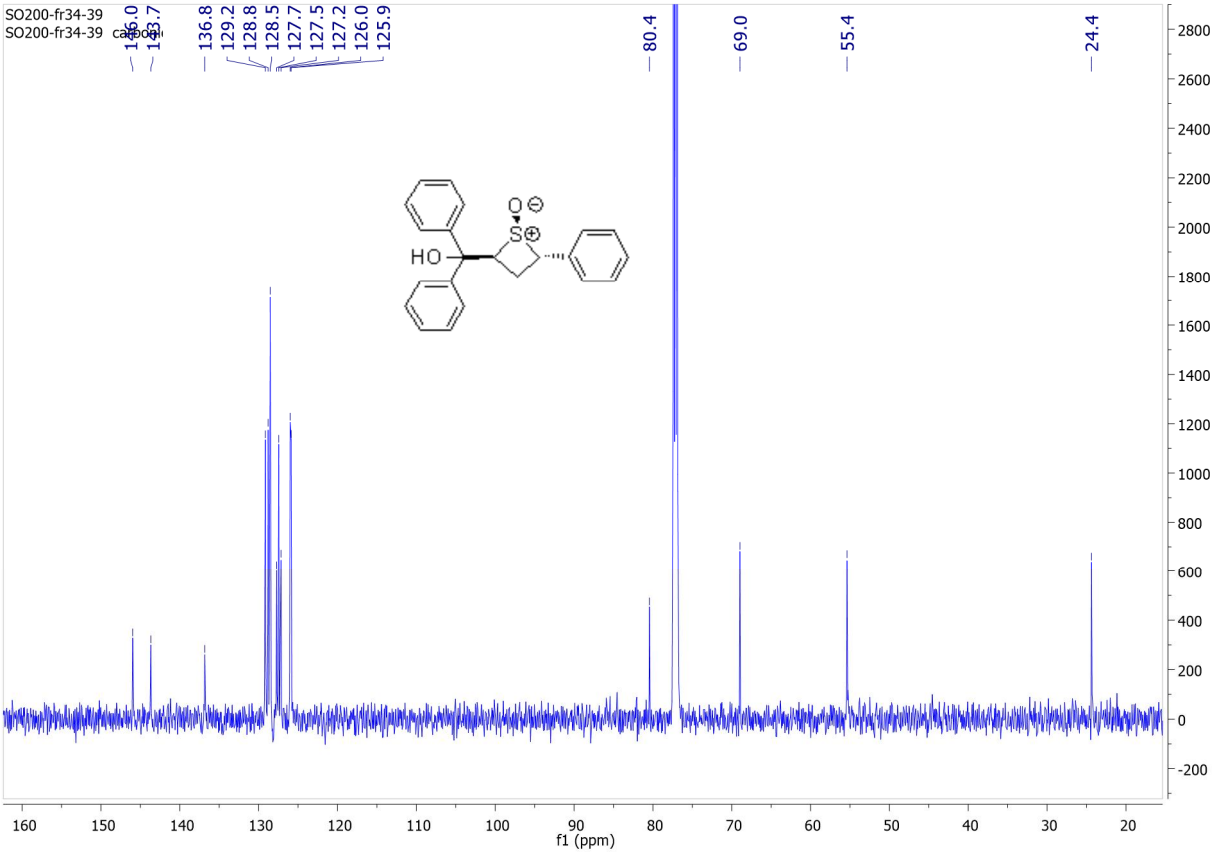

SO60-F2
SO60-F2-8is carbon6
145.5
137.2
137.2
130.9
128.9
128.5
128.0
127.9
127.9
84.8
74.1
43.0
31.0
OH
Ph
Ph Ph

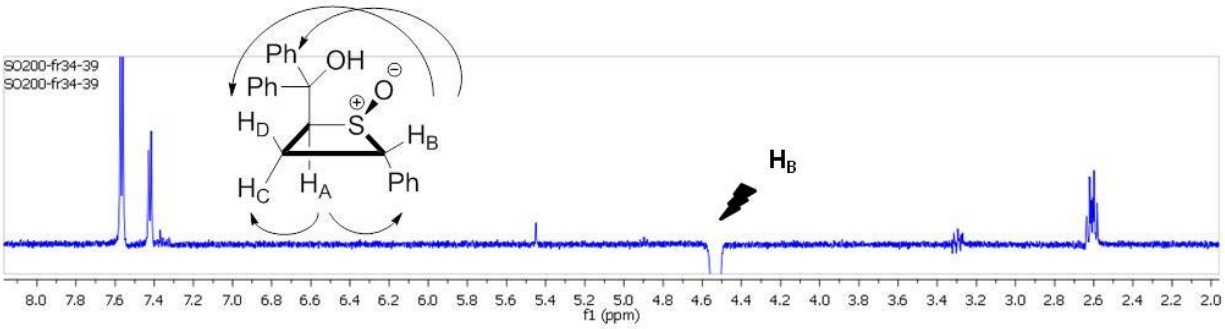

SO60-F2
SO60-F2 Bis COSY
f2 (ppm)
f1 (ppm)
OH
Ph
Ph Ph

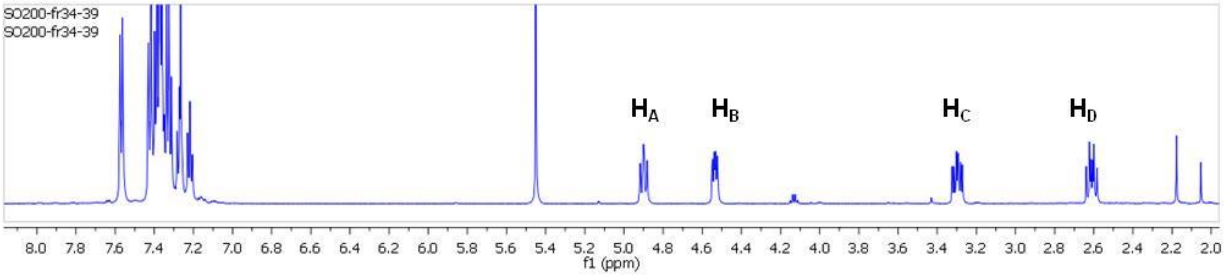

SO60-F2
SO60-F2 bis HSQC DEPT
f2 (ppm)
f1 (ppm)
OH
Ph
Ph Ph

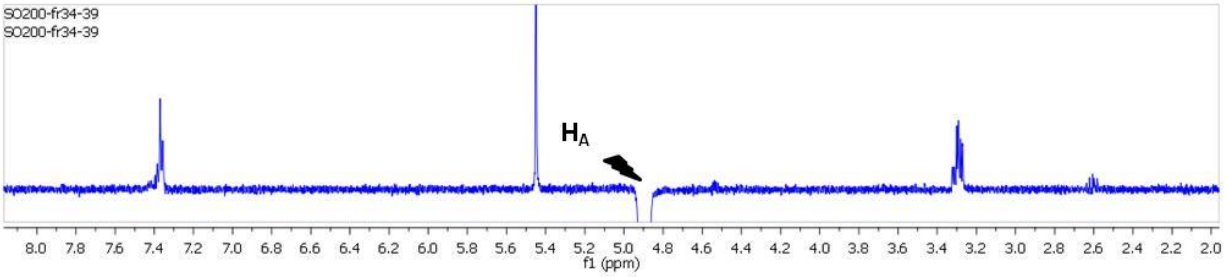
(1R_S*, 2*R, *4R**)-11**

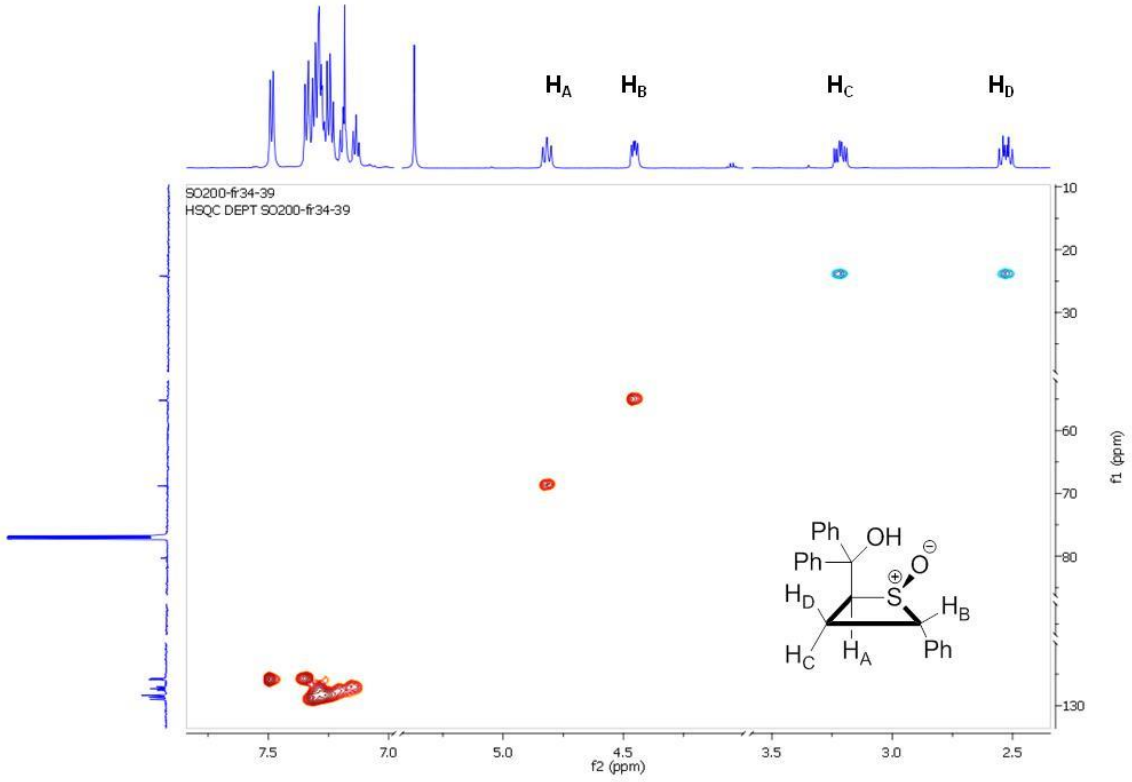

SO200-fr34-39
SO200-fr34-39
HO
O
S
2.1
13.0
1.2
1.0
1.0
1.0
1.1
1.1
f1 (ppm)


SO200-fr34-39
SO200-fr34-39 carbon
136.8
129.2
128.8
128.5
127.7
127.5
127.2
126.0
125.9
80.4
69.0
55.4
24.4
HO
O
S
f1 (ppm)

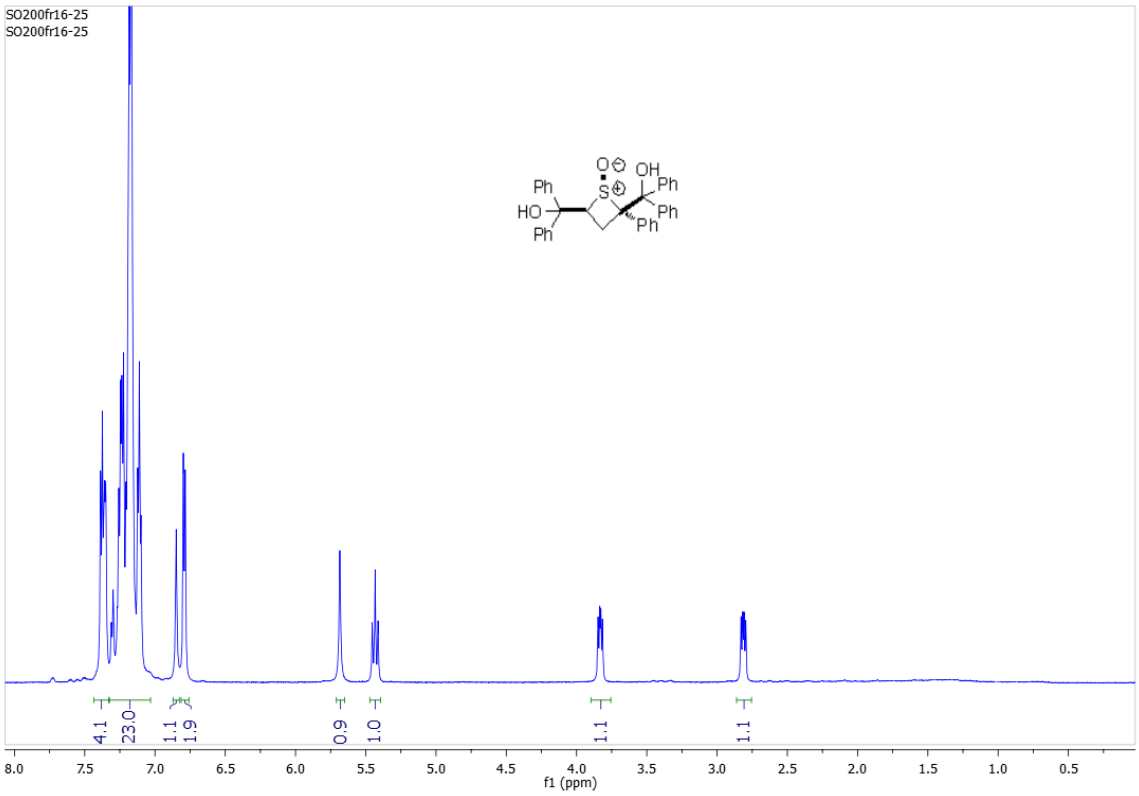

SO200-fr34-39
SO200-fr34-39
Ph
OH
Ph
O
S
H_D
H_B
H_C
H_A
Ph
H_B
f1 (ppm)

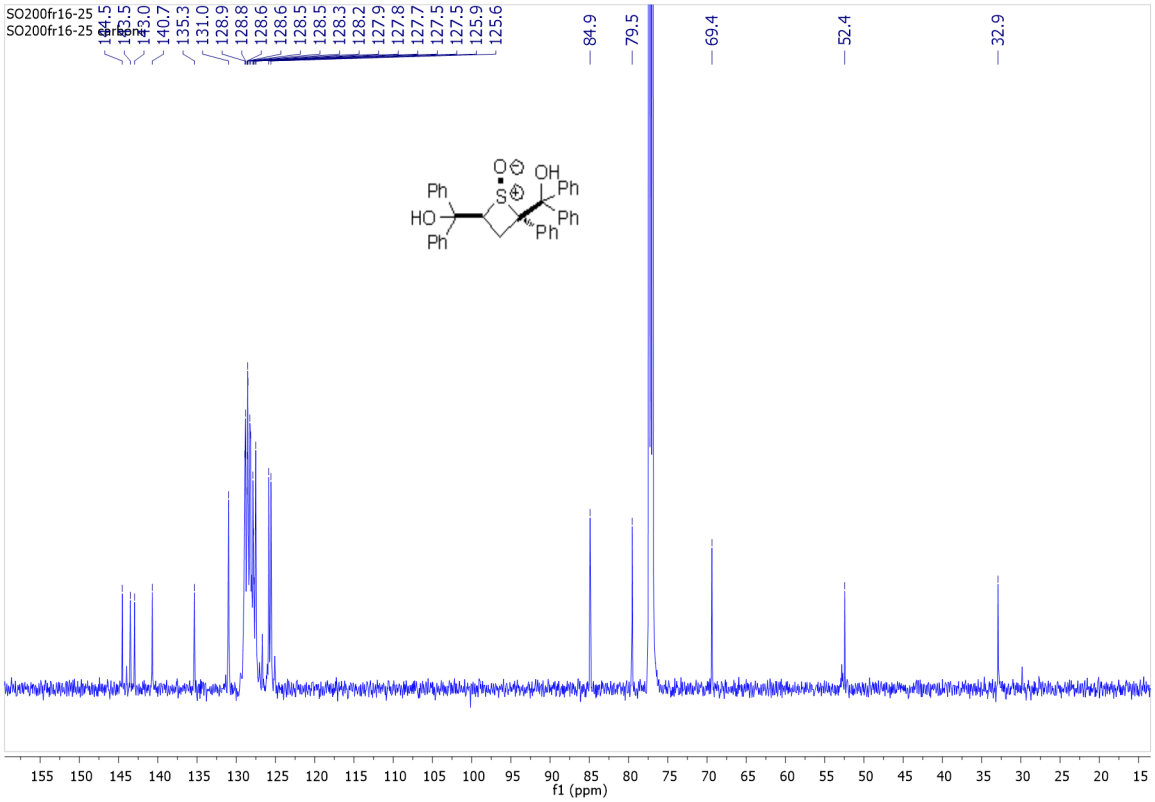

SO200-fr34-39
SO200-fr34-39
H_A
H_B
H_C
H_D
f1 (ppm)

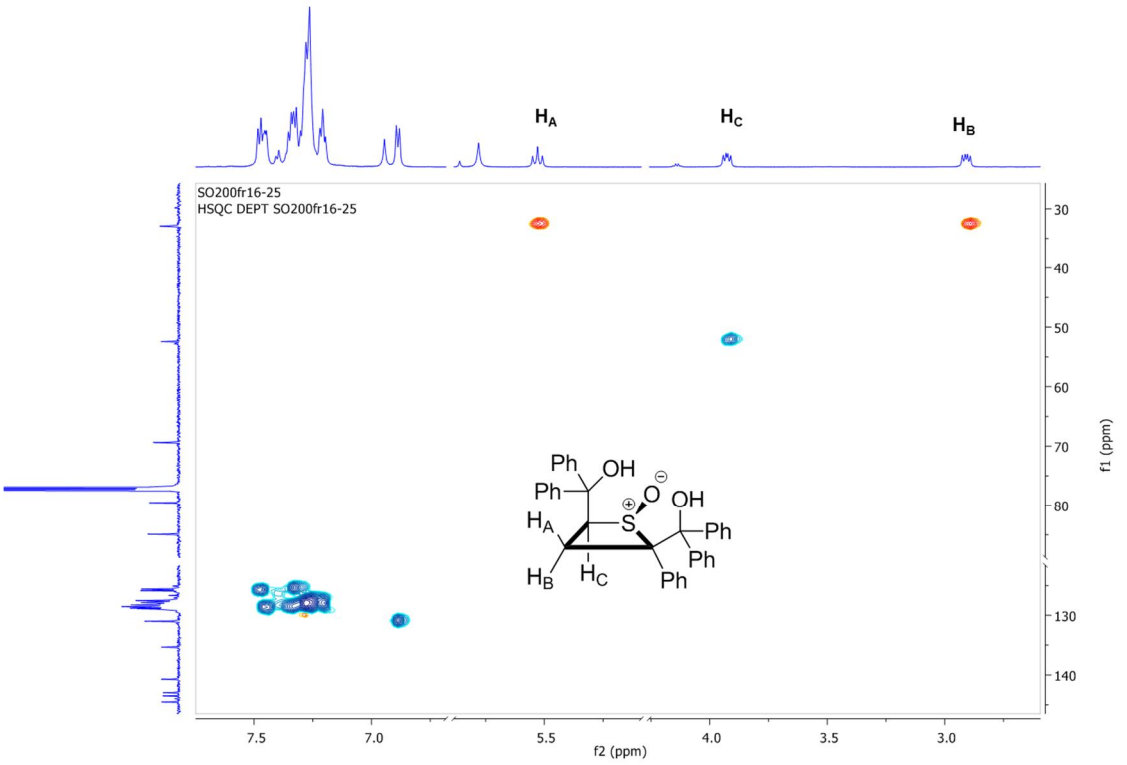

SO200-fr34-39
SO200-fr34-39
H_A
f1 (ppm)

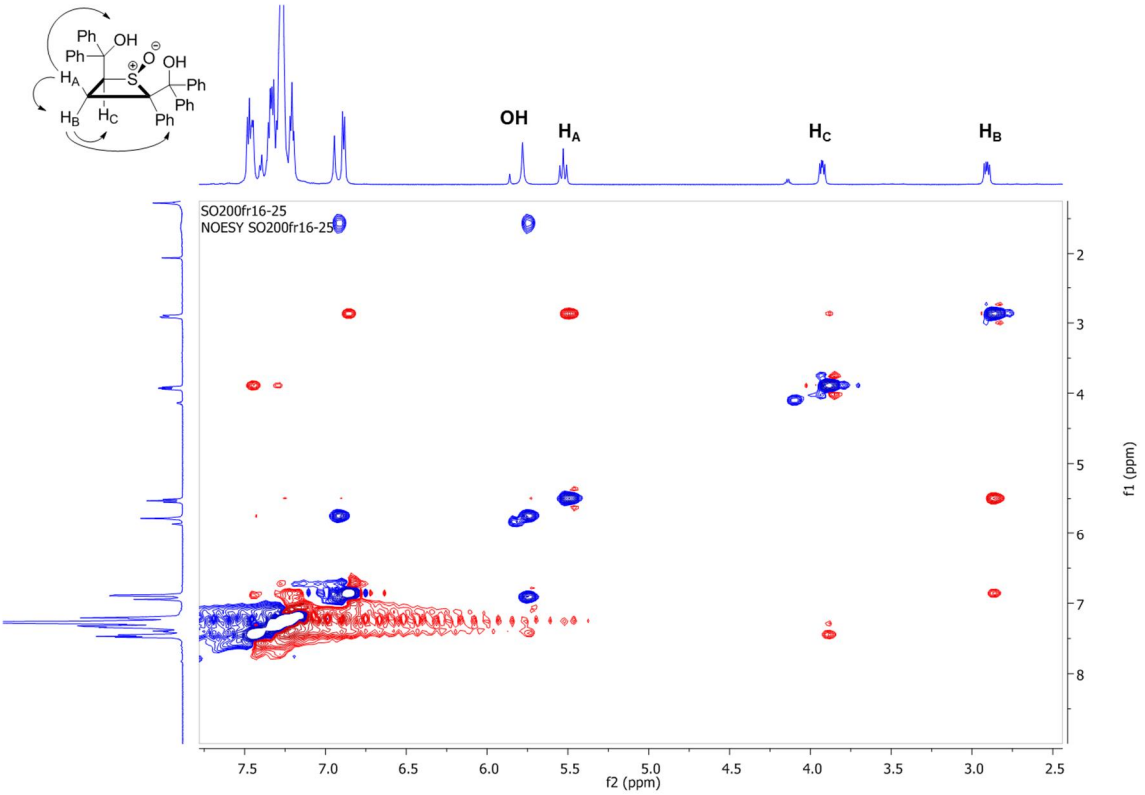

H_A
H_B
H_C
H_D
SO200-fr34-39
HSQC DEPT SO200-fr34-39
Ph
OH
Ph
O
S
H_D
H_B
H_C
H_A
Ph
f2 (ppm)
f1 (ppm)

(1R_S*, 2*S, 4*S**)-12**


SO200fr16-25
SO200fr16-25
4.1
23.0
1.1
1.9
0.9
1.0
1.1
1.1
f1 (ppm)


SO200fr16-25
SO200fr16-25
184.5
183.5
183.0
140.7
135.3
131.0
128.9
128.8
128.6
128.6
128.5
128.5
128.3
128.2
127.9
127.8
127.7
127.5
127.5
125.9
125.6
84.9
79.5
69.4
52.4
32.9
f1 (ppm)


HA
HC
HB
SO200fr16-25
HSQC DEPT SO200fr16-25
f2 (ppm)
f1 (ppm)


OH
HA
HC
HB
SO200fr16-25
NOESY SO200fr16-25
f2 (ppm)
f1 (ppm)

X-ray analysis[1]

X-ray diffraction intensities were collected at room temperature on a diffractometer with graphite-monochromated Mo *K*α radiation (λ = 0.71073 Å). The automatic data collection strategy was defined by *COLLECT* (Nonius, 2002), cell determination and refinement by *DIRAX* (Duisenberg, 1992; Duisenberg *et al*., 2000) and data reduction by *EVAL* (Nonius, 2002; Duisenberg *et al.*, 2003). Absorption corrections were performed using *SADABS* (Sheldrick, 2008a).

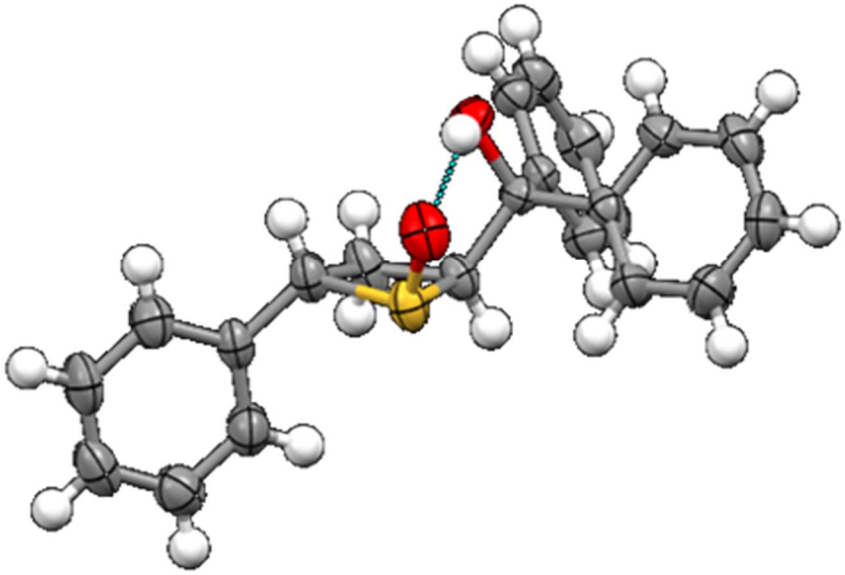
The crystal structure was solved by direct methods using *SIR2014* (Burla *et al.*, 2015) and refined by *SHELXL2014* (Sheldrick, 2008*b*). *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010) were used to prepare material for publication.

Refinement

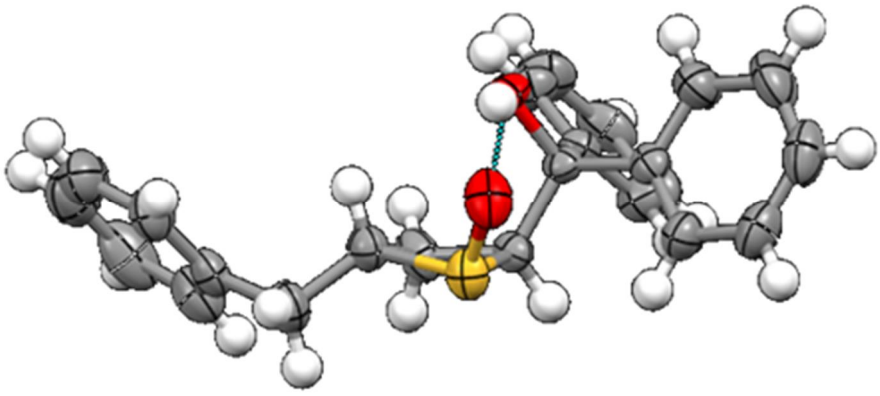
All non-hydrogen atoms were refined anisotropically. The hydrogen atoms of the hydroxyl groups were located by difference Fourier synthesis and freely isotropically refined.

The C-bonded H atoms were positioned geometrically with C—H = 0.96, 0.97 and 0.93 Å for methyl, methylene and aromatic H atoms, respectively, and constrained to ride on their parent atoms. The constraint U_{iso}(H) = kU_{eq}(C), where k = 1.5 for methyl and k = 1.2 for aromatic and methylene H atoms, was applied.

[1] a) Burla, M. C., Caliandro, R., Carrozzini, B., Cascarano, G. L., Cuocci, C., Giacovazzo, C., Mallamo, M., Mazzone, A. & Polidori, G. (2015). *J. Appl. Cryst.* **48**, 306–309. b) Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96. c) Duisenberg, A. J. M., Hooft, R. W. W., Schreurs, A. M. M. & Kroon, J. (2000). *J. Appl. Cryst.* **33**, 893–898. d) Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229. e) Farrugia, L. J. (20012). *J. Appl. Cryst.* **45**, 849–854. f) Nonius (2002). *COLLECT* and *EVAL*. Nonius BV, Delft, The Netherlands. g) Sheldrick, G. M. (2008*a*). *SADABS*. University of Göttingen, Germany. h) Sheldrick, G. M. (2008*b*). *Acta Cryst.* A**64**, 112–122. i)Westrip, S. P. (2010). *Acta Cryst.* **43**, 920-925.



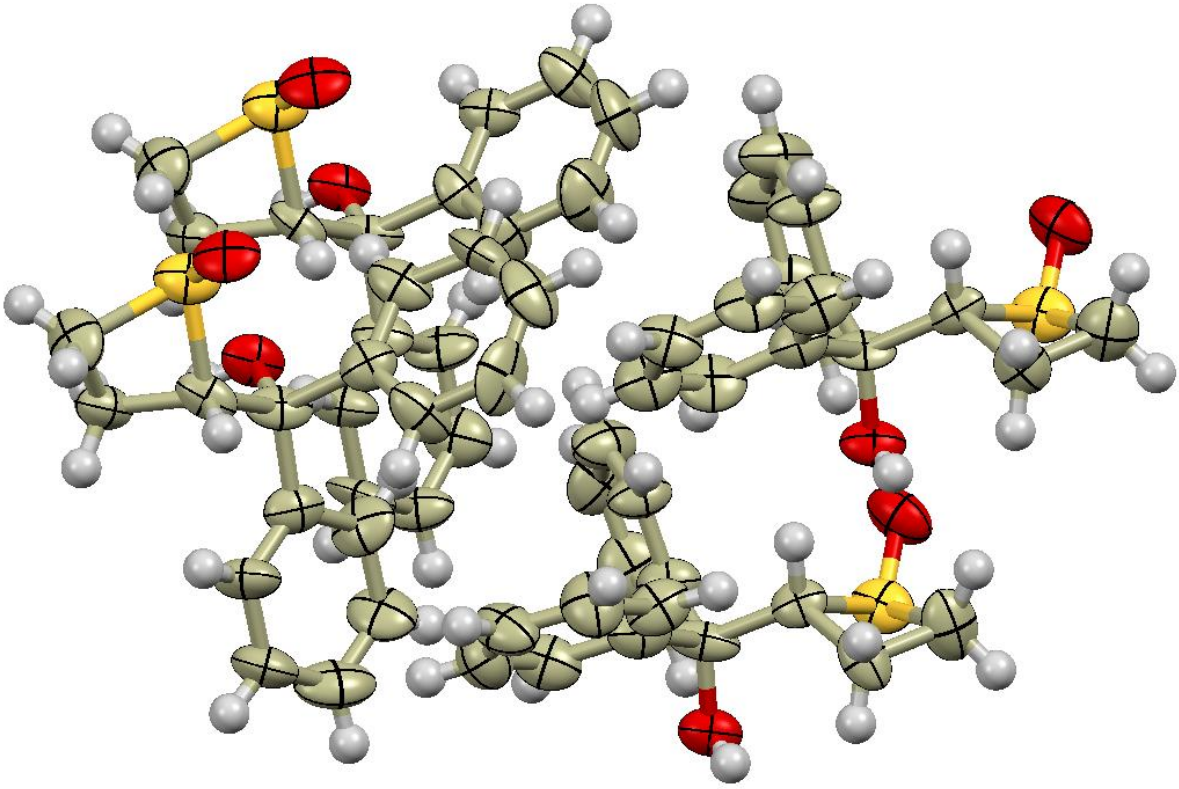
Other view of **11**
(probability level 50%, ellipsoid)



Other view of **5d**
(probability level 50%, ellipsoid)

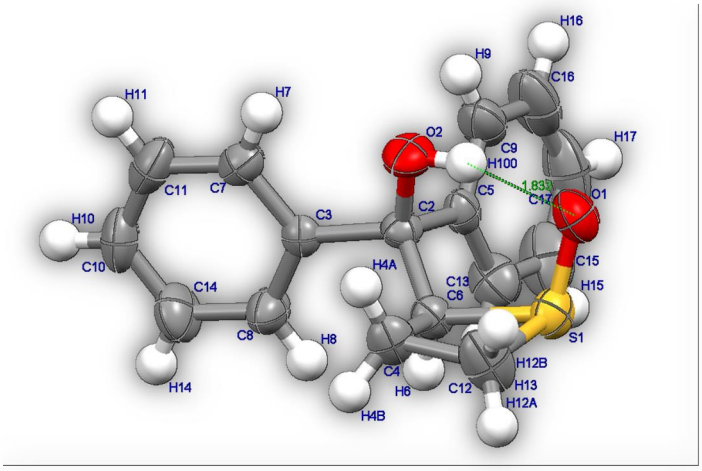
Ortep view of **2a**

50% ellipsoid probability

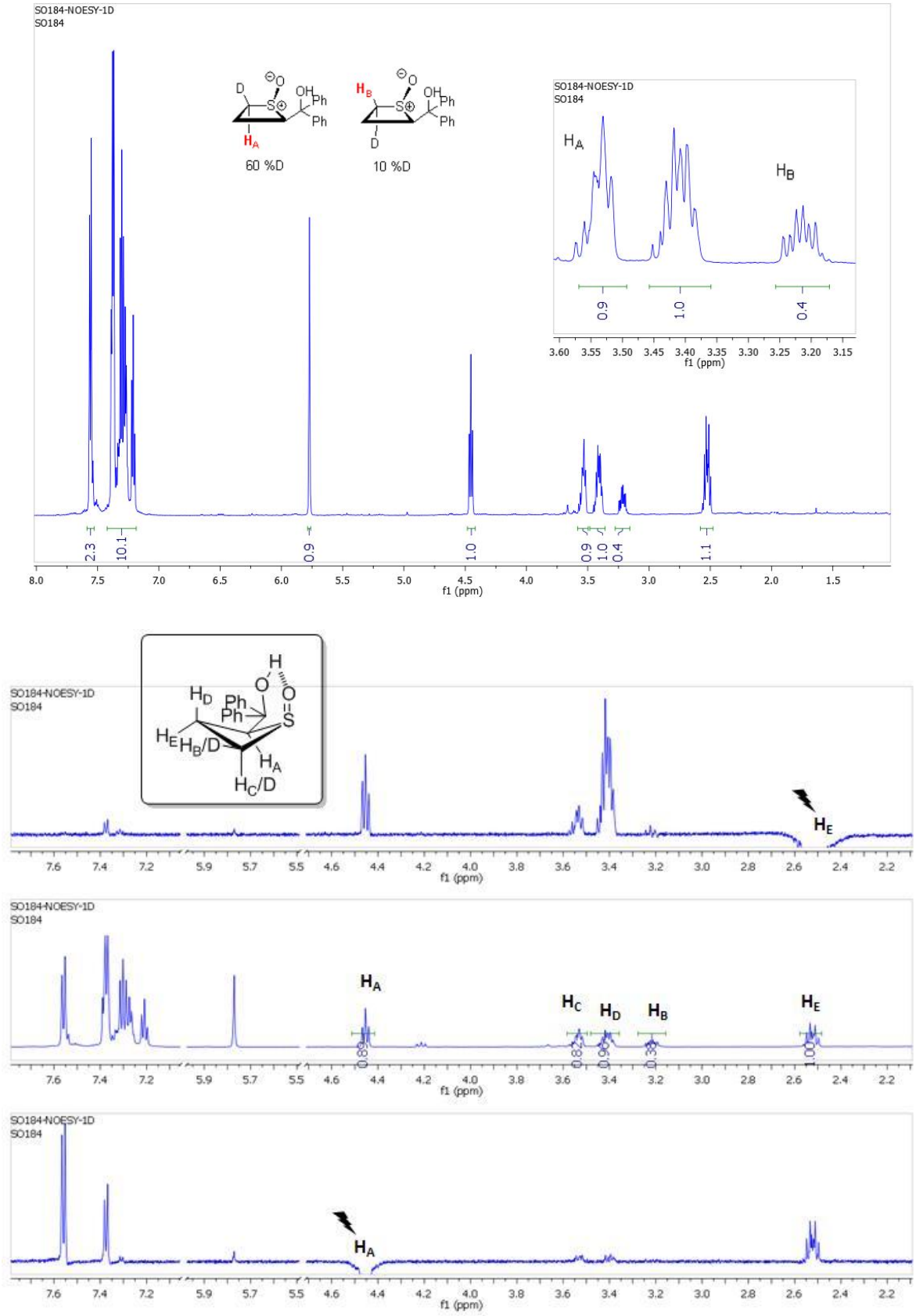


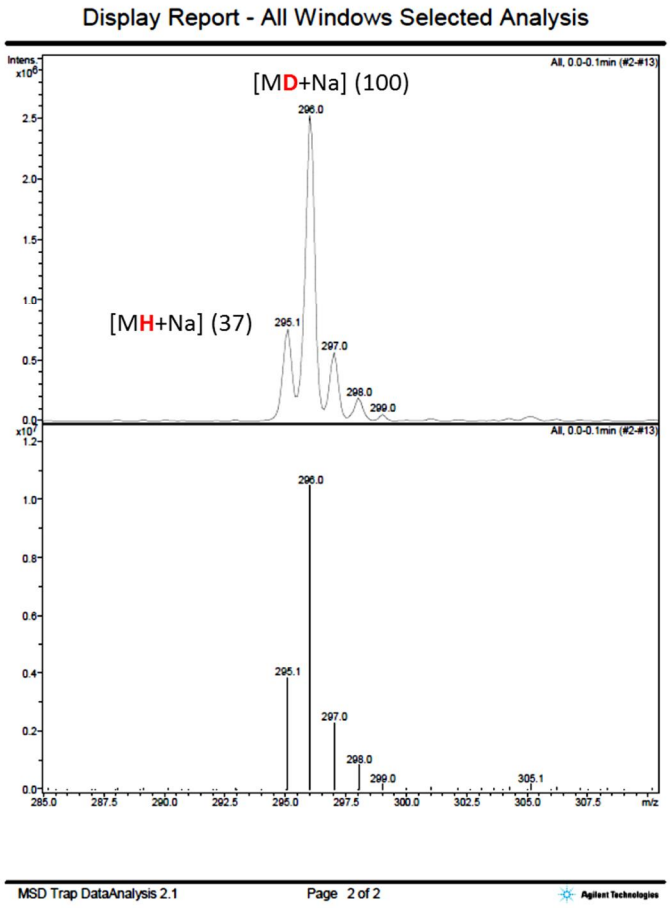
Ortep view of diast-**2a**

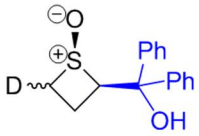
50% ellipsoid probability



Stereochemistry of deuterated thietane 1-oxides **(*1R*$_S$**,2R*,4R**)/(*1R*$_S$**,2R*,4S**)-5b** was ascertained by 1D-Noesy experiments.







Isotopic abundances for protonated m/z:
[MH+Na] 295.0769 (100.0%)
[MH+1+Na] 296.0802 (17.3%)
[MH+2+Na] 297.0727 (4.5%)
[MH+3+Na] 297.0836 (1.4%)

Deuterium content:
[MD+Na]/([MD+Na] + [MH+Na])
[100 – (37 x 0,173)] = 93,6 [MD+Na]
93,6/(93,6 + 37) = **71,7 %D**

Deuterated thietane 1-oxides (*1R*$_S$**,2R*,4R**)/(*1R*$_S$**,2R*,4S**)-6d and (*1R*$_S$**,2R*,4R**)/(*1R*$_S$**,2R*,4S**)-7d

Because of overlapping signals, the stereochemistry of deuterated thietane 1-oxides **(*1R*$_S$**,2R*,4R**)/(*1R*$_S$**,2R*,4S**)-6d** and **(*1R*$_S$**,2R*,4R**)/(*1R*$_S$**,2R*,4S**)-7d** was established by comparison with simulated NMR spectra of the equilibrium geometries at DFT level of calculations of thietanes **2b**,**c**. This approach has been found very reliable for strained heterocycles.[2] Simulated spectra for syn and anti C2-substituted thietane 1-oxides **2b**,**c** have been considered for sake of comparison. The stereochemistry of thietanes **2b**,**c** has been assigned previously.[3] 2D-NMR COSY and HSQC-DEPT experiments helped to assign the protons of the heterocyclic ring and DFT calculation to assign their stereochemistry.

[2] a) Azzena, U.; Dettori, G.; Pisano, L.; Musio, B.; Luisi, R. *J. Org. Chem.* **2011**, *76*, 2291. b) Degennaro, L.; Pisano, L.; Parisi, G.; Mansueto, R.; Clarkson, G. J.; Shipman, M.; Luisi, R., *J. Org. Chem*. **2015**, *80*, 6411. c) Zenzola, M.; Degennaro, L.; Trinchera, P.; Carroccia, L.; Giovine, A.; Romanazzi, G.; Mastrorilli, P.; Rizzi, R.; Pisano, L.; Luisi, R., *Chemistry Eur. J*. **2014**, *20*, 12190.

[3] Carroccia, L.; Degennaro, L.; Romanazzi, G.; Cuocci, C.; Pisano, L.; Luisi, R., *Org. Biomol. Chem*. **2014**, *12*, 2180.

syn 2-Allylthietane 1-oxide

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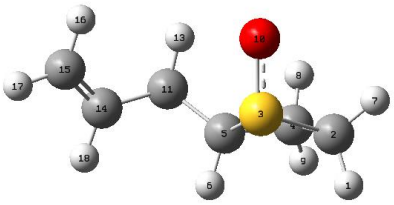

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C,0,0.0960491215,1.303240013,0.218454465
C,0,0.0409512575,-0.2346491318,0.2735393426
H,0,-0.4508271731,-0.6527443828,-0.6094374124
H,0,2.1534514513,2.1173423162,-0.2678847541
H,0,0.2180575829,1.72339433,1.2187589023
H,0,-0.7721550636,1.7720135866,-0.2503607712
O,0,2.6727034219,-0.2714455402,1.2101681819
C,0,-0.3973954721,-0.9214233109,1.5544773044
H,0,-1.3530506364,-0.4655261983,1.85019809
H,0,0.3217646888,-0.6954050222,2.3485863104
C,0,-0.571932352,-2.4082122605,1.4089058039
C,0,0.1036683369,-3.3264531486,2.0976982578
H,0,0.8542118109,-3.0485545245,2.8322796069
H,0,-0.0709474963,-4.3871177509,1.9479785012
H,0,-1.3107318259,-2.7316872738,0.6761697143

Zero-point correction= 0.147972 (Hartree/Particle)
Thermal correction to Energy= 0.156921
Thermal correction to Enthalpy= 0.157866
Thermal correction to Gibbs Free Energy= 0.113361
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Sum of electronic and thermal Energies= -707.961242
Sum of electronic and thermal Enthalpies= -707.960298
Sum of electronic and thermal Free Energies= -708.004803

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Calculating GIAO nuclear magnetic shielding tensors.

Rif **$\mathring{u}H_{TMS}$ (MPW/gen, THF) =31.4297, $\mathring{u}C_{TMS}$ (MPW/gen, THF) =186.1067**

SCF GIAO Magnetic shielding tensor (ppm):
1 H Isotropic = 28.1840 Anisotropy = 6.3316
XX= 29.7298 YX= 0.2784 ZX= 4.0055
XY= 0.9641 YY= 27.0121 ZY= 1.8717
XZ= 2.3985 YZ= 0.6421 ZZ= 27.8100
Eigenvalues: 25.1751 26.9718 32.4050
2 C Isotropic = 133.2135 Anisotropy = 56.4819
XX= 124.5887 YX= 28.1009 ZX= -9.4289
XY= 32.1215 YY= 151.0184 ZY= 22.2514
XZ= -24.2391 YZ= 6.1395 ZZ= 124.0335
Eigenvalues: 90.5952 138.1772 170.8681
3 S Isotropic = 98.9384 Anisotropy = 267.1385
XX= 73.0645 YX= -11.4464 ZX= 30.6736
XY= -25.9441 YY= -31.8577 ZY= 58.0235
XZ= 19.9564 YZ= 96.4875 ZZ= 255.6084
Eigenvalues: -55.9287 75.7132 277.0308
4 C Isotropic = 151.5896 Anisotropy = 48.6864
XX= 183.6775 YX= -2.0438 ZX= -6.0754
XY= -2.5125 YY= 146.3038 ZY= -15.9696
XZ= -2.3042 YZ= -2.2406 ZZ= 124.7876
Eigenvalues: 121.0960 149.6257 184.0472
5 C Isotropic = 116.6444 Anisotropy = 43.7949
XX= 108.4906 YX= -1.9578 ZX= 13.2283
XY= 2.8398 YY= 145.4062 ZY= 10.8345
XZ= 27.0276 YZ= -3.1279 ZZ= 96.0364
Eigenvalues: 81.0687 123.0236 145.8410
6 H Isotropic = 27.9588 Anisotropy = 2.9662
XX= 28.9976 YX= 0.3623 ZX= -0.7536
XY= -0.2572 YY= 26.5664 ZY= 2.5621
XZ= 0.1826 YZ= 2.0196 ZZ= 28.3124
Eigenvalues: 24.9773 28.9628 29.9362
7 H Isotropic = 29.0284 Anisotropy = 7.8580
XX= 32.6698 YX= -3.0787 ZX= -2.0758
XY= -2.6624 YY= 27.1781 ZY= 0.4706
XZ= -0.8297 YZ= 0.9471 ZZ= 27.2374
Eigenvalues: 25.9448 26.8733 34.2671
8 H Isotropic = 28.0530 Anisotropy = 4.8898
XX= 27.8259 YX= 0.6193 ZX= -1.6072
XY= 0.3309 YY= 26.9963 ZY= -3.9760
XZ= -0.7493 YZ= -0.8833 ZZ= 29.3369
Eigenvalues: 25.4457 27.4005 31.3129
9 H Isotropic = 28.6656 Anisotropy = 8.6026
XX= 27.6821 YX= 2.7071 ZX= 0.2783
XY= 2.4460 YY= 33.3716 ZY= 0.2181
XZ= -0.1495 YZ= -1.5124 ZZ= 24.9431
Eigenvalues: 24.8607 26.7354 34.4007
10 O Isotropic = 268.2795 Anisotropy = 328.9345
XX= 470.7513 YX= -62.3369 ZX= -66.9618
XY= -77.0825 YY= 140.9582 ZY= -179.9045
XZ= -33.0122 YZ= -51.0551 ZZ= 193.1291
Eigenvalues: 31.9290 285.3403 487.5692
11 C Isotropic = 148.1910 Anisotropy = 49.4254
XX= 173.4753 YX= 12.1590 ZX= -14.3614
XY= 8.6555 YY= 133.9244 ZY= -11.8795
XZ= -10.8631 YZ= -9.3100 ZZ= 137.1732
Eigenvalues: 124.8274 138.6042 181.1413
12 H Isotropic = 29.2194 Anisotropy = 7.3957
XX= 28.8356 YX= -0.4034 ZX= 0.8481
XY= -1.4972 YY= 31.8580 ZY= -3.5086
XZ= -0.0058 YZ= -4.1321 ZZ= 26.9646
Eigenvalues: 24.8727 28.6356 34.1499
13 H Isotropic = 28.3149 Anisotropy = 2.7720
XX= 28.9402 YX= -0.7379 ZX= 0.1774
XY= 0.2576 YY= 26.7013 ZY= 1.1491
XZ= 0.4561 YZ= 2.2344 ZZ= 29.3032
Eigenvalues: 25.8275 28.9543 30.1630

14 C Isotropic = 33.9095 Anisotropy = 175.9983
XX= 47.6579 YX= -18.0755 ZX= 95.4545
XY= -14.7172 YY= 62.9170 ZY= -64.5978
XZ= 88.9159 YZ= -69.8143 ZZ= -8.8463
Eigenvalues: -90.9965 41.4834 151.2418
15 C Isotropic = 54.4329 Anisotropy = 153.6211
XX= 57.4517 YX= -11.5851 ZX= 88.7205
XY= -12.9178 YY= 92.3324 ZY= -51.9761
XZ= 92.1365 YZ= -49.7823 ZZ= 13.5146
Eigenvalues: -64.6676 71.1194 156.8469
16 H Isotropic = 25.7756 Anisotropy = 6.5003
XX= 27.5955 YX= 3.3520 ZX= 2.8553
XY= 1.9541 YY= 26.8109 ZY= 1.0163
XZ= 0.5716 YZ= -1.1705 ZZ= 22.9202
Eigenvalues: 22.1376 25.0800 30.1091
17 H Isotropic = 25.8550 Anisotropy = 5.6456
XX= 27.4037 YX= 1.8723 ZX= 0.2281
XY= 3.0624 YY= 26.7550 ZY= -0.8330
XZ= 1.6297 YZ= 0.4026 ZZ= 23.4063
Eigenvalues: 22.9857 24.9605 29.6187
18 H Isotropic = 25.2253 Anisotropy = 4.4659
XX= 27.6122 YX= 1.7062 ZX= -0.3040
XY= 0.8258 YY= 25.0925 ZY= -0.0702
XZ= -0.7613 YZ= -0.3861 ZZ= 22.9712
Eigenvalues: 22.9070 24.5663 28.2026

---

anti 2-Allylthietane 1-oxide

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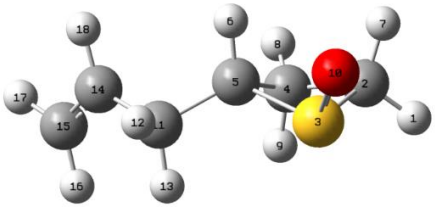

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C	1.23142	1.43621	0.49216
C	1.08684	-0.06524	0.10936
H	0.88073	-0.66535	0.97092
H	2.6427	0.68717	1.99121
H	0.50965	1.88659	1.14109
H	1.26951	2.04708	-0.38551
O	3.69295	-1.23329	-0.22348
C	0.06215	-0.4996	-0.95504
H	0.18741	-1.54095	-1.1667
H	0.21517	0.06712	-1.84964
C	-1.36303	-0.25084	-0.42724
C	-1.99221	0.97928	-0.66145
H	-1.48237	1.74567	-1.20699
H	-2.98243	1.15212	-0.29473
H	-1.87286	-1.01723	0.11831

Zero-point correction= 0.148295 (Hartree/Particle)
Thermal correction to Energy= 0.157178
Thermal correction to Enthalpy= 0.158123
Thermal correction to Gibbs Free Energy= 0.113840
Sum of electronic and zero-point Energies= -707.972457
Sum of electronic and thermal Energies= -707.963574
Sum of electronic and thermal Enthalpies= -707.962629
Sum of electronic and thermal Free Energies= -708.006912

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NMR=(readatoms)

Calculating GIAO nuclear magnetic shielding tensors.
Rif σHTMS (MPW/gen, SMD-$CDCl_3$) =31.4297
SCF GIAO Magnetic shielding tensor (ppm):
1 H Isotropic = 27.9973 Anisotropy = 7.6666
XX= 28.4739 YX= 2.5378 ZX= -1.2885
XY= 4.2852 YY= 29.3122 ZY= -2.6677
XZ= -1.3437 YZ= -1.1873 ZZ= 26.2057
Eigenvalues: 25.1652 25.7183 33.1083
2 C Isotropic = 127.0168 Anisotropy = 69.8638
XX= 108.8595 YX= -28.2893 ZX= 18.0981
XY= -17.3554 YY= 165.4551 ZY= 8.4447
XZ= 3.7896 YZ= 4.1440 ZZ= 106.7357
Eigenvalues: 90.9806 116.4771 173.5926
3 S Isotropic = 118.5332 Anisotropy = 329.9829
XX= 153.6108 YX= -38.7025 ZX= 126.9318
XY= -32.2292 YY= 57.0550 ZY= -121.8806
XZ= 152.7593 YZ= -135.1023 ZZ= 144.9337
Eigenvalues: -53.7661 70.8439 338.5218
4 C Isotropic = 163.5411 Anisotropy = 31.3739
XX= 162.6296 YX= 19.5787 ZX= 2.0675
XY= 15.2526 YY= 170.5303 ZY= -1.5229
XZ= -5.2008 YZ= 5.8488 ZZ= 157.4632
Eigenvalues: 148.0193 158.1469 184.4570
5 C Isotropic = 105.0682 Anisotropy = 72.4969
XX= 143.0367 YX= -22.4154 ZX= -14.7023
XY= -25.8538 YY= 85.7510 ZY= -4.2247
XZ= -6.6559 YZ= 5.0931 ZZ= 86.4170
Eigenvalues: 75.7945 86.0107 153.3995
6 H Isotropic = 27.9958 Anisotropy = 2.6347
XX= 28.0020 YX= 1.8846 ZX= 0.1409
XY= 1.9541 YY= 27.6280 ZY= -1.1319
XZ= 1.4769 YZ= -0.9242 ZZ= 28.3572
Eigenvalues: 25.3248 28.9103 29.7523
7 H Isotropic = 28.5269 Anisotropy = 6.1834
XX= 30.2516 YX= 1.6696 ZX= 2.9262
XY= 2.1571 YY= 26.8087 ZY= 2.0914
XZ= 1.5576 YZ= 0.2520 ZZ= 28.5203
Eigenvalues: 25.9379 26.9936 32.6491
8 H Isotropic = 29.1905 Anisotropy = 9.4984
XX= 28.7863 YX= -2.7035 ZX= -2.8584
XY= -2.4639 YY= 31.1444 ZY= 4.8484
XZ= -1.4749 YZ= 3.3565 ZZ= 27.6407
Eigenvalues: 24.8762 27.1725 35.5227
9 H Isotropic = 29.7606 Anisotropy = 6.2726
XX= 29.8918 YX= -0.7676 ZX= 2.3232
XY= -0.5698 YY= 29.1527 ZY= -3.2862
XZ= 2.4138 YZ= -2.5214 ZZ= 30.2373

```
 Eigenvalues:   26.3732   28.9663   33.9423
  10 O   Isotropic =   213.3363   Anisotropy =   282.9903
 XX=  258.3876  YX=  149.4290  ZX= -108.9161
 XY=  161.1556  YY=  224.0602  ZY=   64.2975
 XZ=   -2.4869  YZ=  -38.2890  ZZ=  157.5612
 Eigenvalues:   61.3807  176.6318  401.9965
  11 C   Isotropic =   140.9008   Anisotropy =    26.2872
 XX=  153.9111  YX=    7.3394  ZX=  -11.0695
 XY=    5.5105  YY=  132.0184  ZY=    9.9048
 XZ=   -7.9902  YZ=    6.9209  ZZ=  136.7731
 Eigenvalues:  121.8849  142.3920  158.4256
  12 H   Isotropic =    28.4741   Anisotropy =     6.7918
 XX=   27.6469  YX=    0.9002  ZX=    0.4098
 XY=   -0.4057  YY=   32.9611  ZY=    0.0870
 XZ=   -0.1765  YZ=    0.8849  ZZ=   24.8144
 Eigenvalues:   24.7818   27.6385   33.0020
  13 H   Isotropic =    29.1300   Anisotropy =     4.4448
 XX=   29.7836  YX=    1.2054  ZX=    0.2077
 XY=    0.2754  YY=   26.0394  ZY=    1.6433
 XZ=    1.4746  YZ=    0.0789  ZZ=   31.5670
 Eigenvalues:   25.8124   29.4844   32.0932
  14 C   Isotropic =    33.3274   Anisotropy =   179.4697
 XX=   30.4924  YX=   39.0218  ZX=   64.1219
 XY=   34.0536  YY=  130.1657  ZY=   26.6860
 XZ=   58.4371  YZ=   30.1156  ZZ=  -60.6758
 Eigenvalues:  -91.8525   38.8609  152.9739
  15 C   Isotropic =    56.6554   Anisotropy =   148.5074
 XX=   52.1389  YX=   25.5249  ZX=   65.4359
 XY=   26.7468  YY=  140.7377  ZY=   17.8979
 XZ=   65.4675  YZ=   16.6395  ZZ=  -22.9104
 Eigenvalues:  -60.8487   75.1545  155.6603
  16 H   Isotropic =    25.8915   Anisotropy =     6.0323
 XX=   28.3413  YX=   -1.1863  ZX=    4.1207
 XY=   -0.7674  YY=   25.6348  ZY=   -0.9833
 XZ=    1.4399  YZ=    0.0762  ZZ=   23.6985
 Eigenvalues:   22.3979   25.3636   29.9130
  17 H   Isotropic =    25.9501   Anisotropy =     5.6929
 XX=   28.7592  YX=   -1.0836  ZX=    0.6841
 XY=   -1.5971  YY=   25.4389  ZY=   -0.1078
 XZ=    2.7274  YZ=   -0.8445  ZZ=   23.6521
 Eigenvalues:   23.1326   24.9723   29.7454
  18 H   Isotropic =    25.2161   Anisotropy =     4.6041
 XX=   28.2516  YX=   -0.5047  ZX=    0.3233
 XY=   -0.2168  YY=   24.4426  ZY=   -0.9083
 XZ=   -0.5025  YZ=   -0.5552  ZZ=   22.9543
 Eigenvalues:   22.6461   24.7168   28.2855

%chk=D:\TTOAlli\TTOAlantiJgen1.chk
# rb3lyp/gen scrf=(smd,solvent=chloroform)
NMR=(spinspin,readatoms)
Total nuclear spin-spin coupling J (Hz):
           1             2             3             4
5
    1  0.000000D+00
    2  0.000000D+00  0.000000D+00
    3  0.000000D+00  0.000000D+00  0.000000D+00
    4  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
    5  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
    6 -0.121799D+01  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
    7 -0.153183D+02  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
    8  0.495258D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
    9  0.632158D+01  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
   10  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
   11  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
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0.000000D+00
   13 -0.599126D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
   14  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
   15  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
   16 -0.158428D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
   17 -0.222369D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
   18 -0.115489D+00  0.000000D+00  0.000000D+00  0.000000D+00
0.000000D+00
           6             7             8             9
10
    6  0.000000D+00
    7 -0.502806D+00  0.000000D+00
    8  0.937023D+01  0.973755D+01  0.000000D+00
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0.000000D+00
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0.000000D+00
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0.000000D+00
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0.000000D+00
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0.000000D+00
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0.000000D+00
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0.000000D+00
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0.000000D+00
   18  0.503518D-01 -0.332453D-01 -0.444295D-01 -0.105291D+00
0.000000D+00
          11            12            13            14
15
   11  0.000000D+00
   12  0.000000D+00  0.000000D+00
   13  0.000000D+00 -0.118845D+02  0.000000D+00
   14  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
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0.000000D+00
   16  0.000000D+00 -0.144741D+01 -0.871051D+00  0.000000D+00
0.000000D+00
   17  0.000000D+00 -0.120138D+00 -0.112066D+01  0.000000D+00
0.000000D+00
   18  0.000000D+00  0.647528D+01  0.780729D+01  0.000000D+00
0.000000D+00
          16            17            18
   16  0.000000D+00
   17  0.477029D+01  0.000000D+00
   18  0.147474D+02  0.864066D+01  0.000000D+00
```
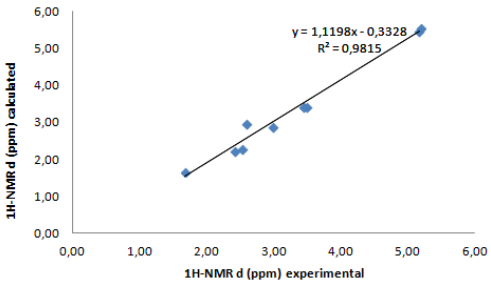
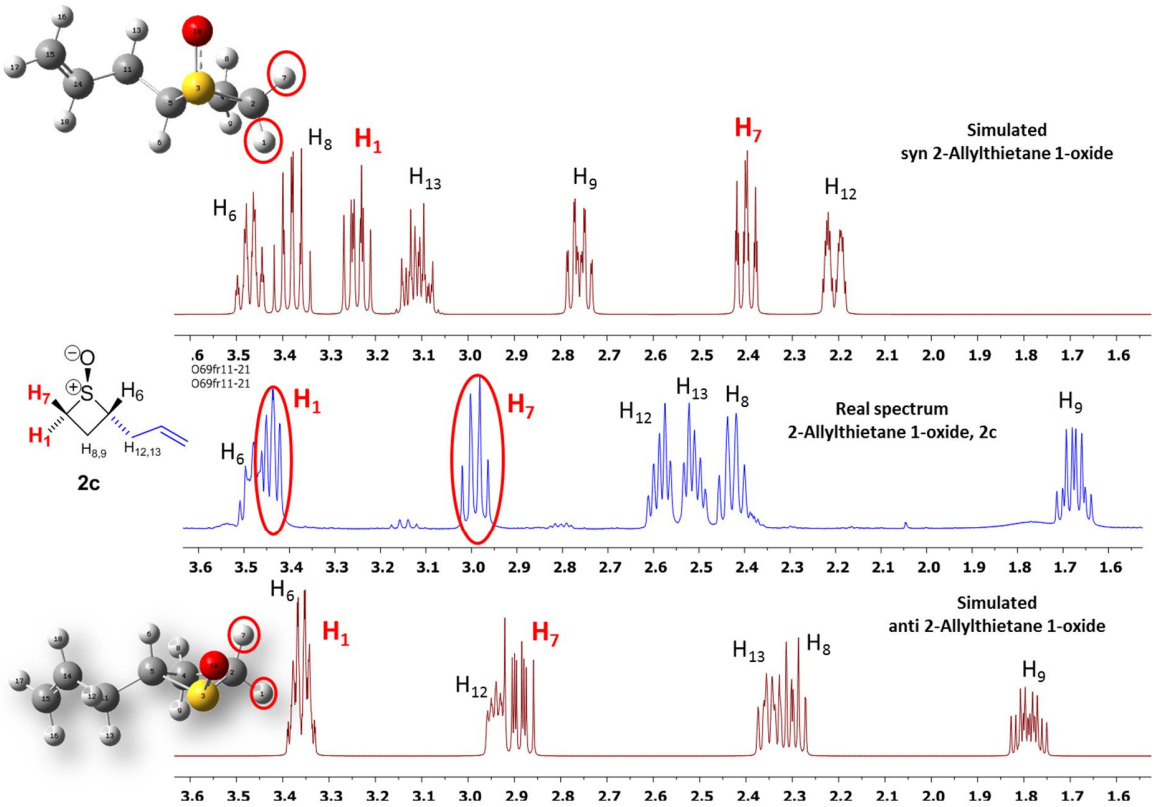

Squares linear fitting parameter (R^2) of the correlation plot between computed (without scaling) and experimental data, Mean Absolute Error (MAE) and Corrected Mean Absolute Error (CMAE).[4]

TABLE. Experimental, calculated and scaled ^{1}H-NMR chemical shift (ppm)

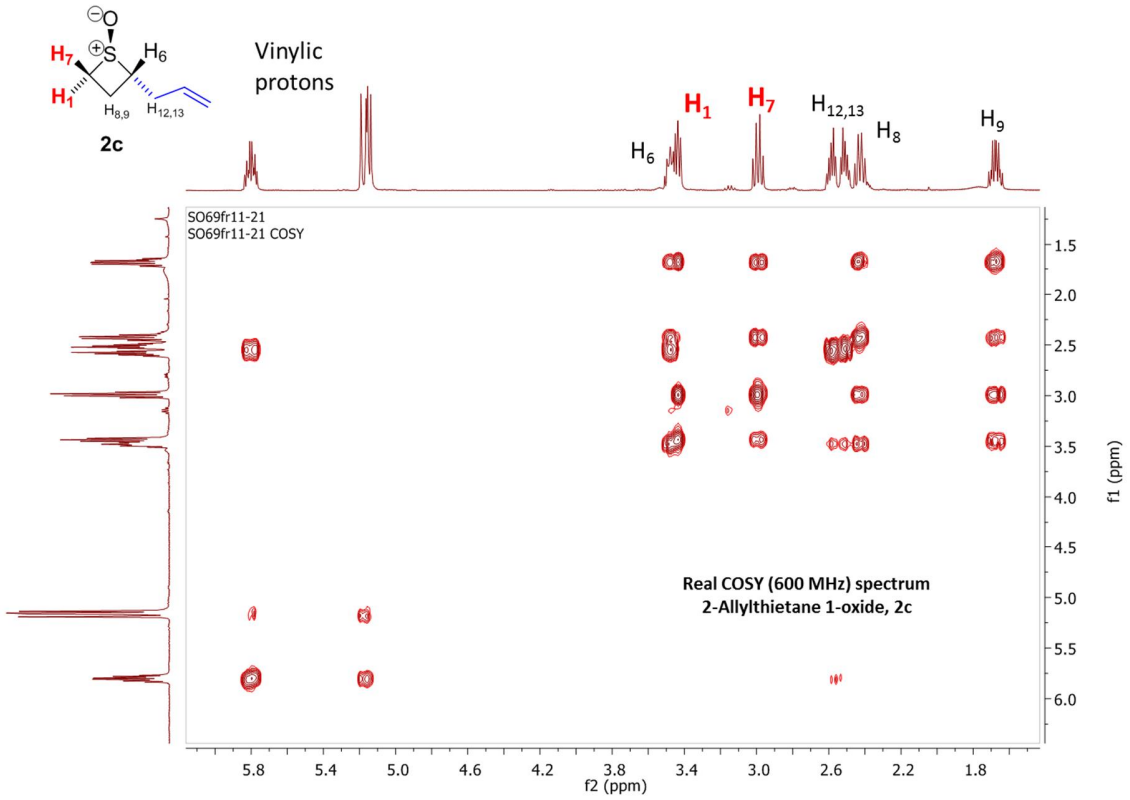
Atoms	δ_{exp}[a]	$\delta_{calculated}$[b]	δ_{scaled}[c]
H_9	1.68	1.67	1.79
H_8	2.42	2.24	2.30
H_7	2.98	2.90	2.89
H_{13}	2.52	2.30	2.49
H_{12}	2.58	2.96	3.06
H_1	3.44	3.43	3.36
H_6	3.48	3.43	3.36
H_{17}	5.15	5.48	5.19
H_{16}	5.18	5.54	5.24
H_{18}	5.80	6.21	5.84
R^2	-	0.981	-
MAE[c]	-	0.203	-
CMAE[c]	-	0.158	-

[a]Experimental values in $CDCl_3$ at 298 K. [b]SMD($CDCl_3$)/MPW1PW91/gen values. [c]The parameters MAE and CMAE are calculated as follow: $MAE = \frac{1}{N}\sum_i^N |\delta_{calc} - \delta_{exp}|$, $CMAE = \frac{1}{N}\sum_i^N |\delta_{scaled} - \delta_{exp}|$ with $\delta_{scaled} = \frac{\delta_{calc} - intercept}{slope}$





[4] U. Azzena, G. Dettori, L. Pisano, B. Musio, R. Luisi *J. Org. Chem.* **2011**, *76*, 2291-2295.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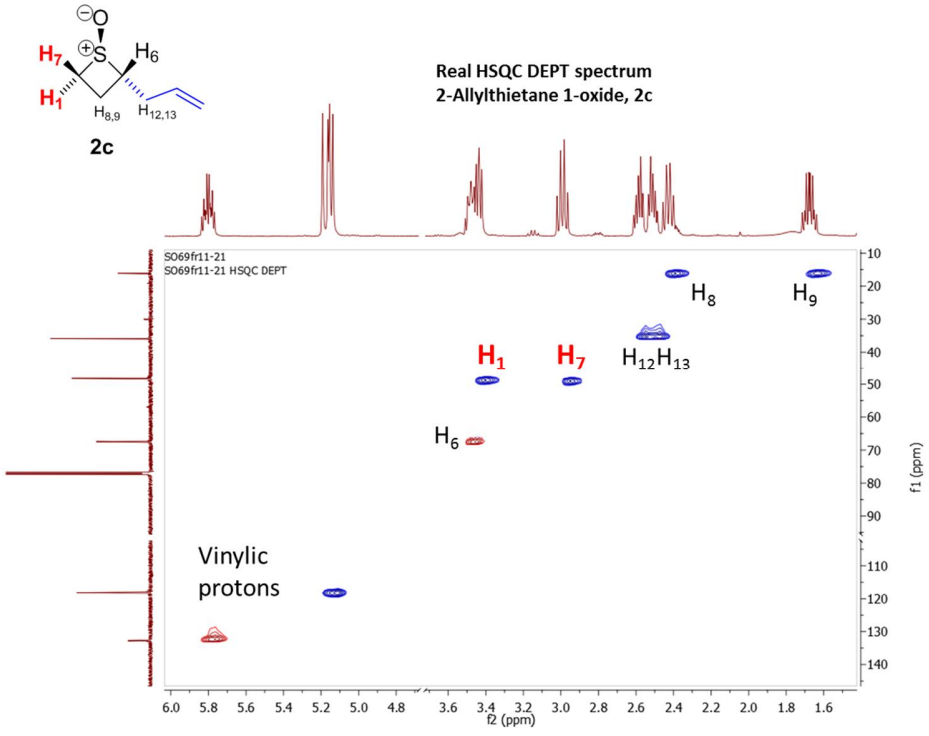
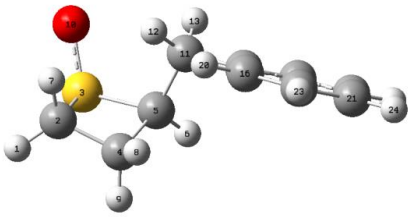
Vinylic
protons
H1
H7
H6
H12,13
H8
H9
SO69fr11-21
SO69fr11-21 COSY
Real COSY (600 MHz) spectrum
2-Allylthietane 1-oxide, 2c
f2 (ppm)
f1 (ppm)


2c
Real HSQC DEPT spectrum
2-Allylthietane 1-oxide, 2c
SO69fr11-21
SO69fr11-21 HSQC DEPT
H8
H9
H1
H7
H12H13
H6
Vinylic
protons
f2 (ppm)
f1 (ppm)

syn 2-Benzylthietane 1-oxide

%chk=D:\TTOBenz\TTOBzsinCDCl3NMR.chk
B3LYP/6-311++g(d,p) opt freq geom=check guess=read scrf(smd, solvent=chloroform)



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Zero-point correction= 0.196348 (Hartree/Particle)
Thermal correction to Energy= 0.207391
Thermal correction to Enthalpy= 0.208335
Thermal correction to Gibbs Free Energy= 0.158122
Sum of electronic and zero-point Energies= -861.620811
Sum of electronic and thermal Energies= -861.609768
Sum of electronic and thermal Enthalpies= -861.608824
Sum of electronic and thermal Free Energies= -861.659037

%chk=D:\TTOBenz\TTOBzsinCDCl3MPW.chk
MPW1PW91/6-311++g(d,p) geom=check guess=read scrf(smd, solvent=chloroform) NMR

Calculating GIAO nuclear magnetic shielding tensors.
Rif σHTMS (MPW/6-311++G(d,p), SMD-$CDCl_3$) =31.8426
SCF GIAO Magnetic shielding tensor (ppm):
1 H Isotropic = 28.2726 Anisotropy = 7.7559
XX= 29.5547 YX= -2.5200 ZX= 0.1194
XY= -4.8588 YY= 29.9054 ZY= 0.7281
XZ= -0.4467 YZ= 0.0584 ZZ= 25.3577
Eigenvalues: 25.3062 26.0684 33.4432
2 C Isotropic = 130.2538 Anisotropy = 79.0016
XX= 105.6358 YX= 26.4252 ZX= 20.8372
XY= 22.2150 YY= 168.9470 ZY= 11.7843
XZ= 8.5042 YZ= 19.1975 ZZ= 116.1785
Eigenvalues: 93.1073 114.7325 182.9215
3 S Isotropic = 138.3168 Anisotropy = 313.7172
XX= 32.2159 YX= -65.0498 ZX= 33.6768
XY= -47.1994 YY= 72.7307 ZY= 100.3856
XZ= 56.8998 YZ= 96.7829 ZZ= 310.0037
Eigenvalues: -34.3097 101.7985 347.4616
4 C Isotropic = 169.4036 Anisotropy = 28.0703
XX= 174.0261 YX= -11.1351 ZX= -0.1846
XY= -11.4209 YY= 179.0661 ZY= 0.3910
XZ= -2.8359 YZ= -4.5998 ZZ= 155.1185
Eigenvalues: 154.5103 165.5834 188.1171
5 C Isotropic = 116.2809 Anisotropy = 61.6945
XX= 144.3285 YX= 20.2478 ZX= 21.5068
XY= 8.5527 YY= 97.5946 ZY= 20.2691
XZ= 14.4584 YZ= 7.4639 ZZ= 106.9197
Eigenvalues: 87.5907 103.8415 157.4106
6 H Isotropic = 28.2366 Anisotropy = 4.9018
XX= 29.1352 YX= -2.8843 ZX= 0.5359
XY= -2.6219 YY= 27.1551 ZY= -1.9063
XZ= -2.3365 YZ= -3.7386 ZZ= 28.4194
Eigenvalues: 23.5445 29.6607 31.5045
7 H Isotropic = 28.3905 Anisotropy = 5.9373
XX= 28.8778 YX= -2.5911 ZX= 2.2756
XY= -1.6423 YY= 28.0314 ZY= -3.6252
XZ= 0.2274 YZ= -1.4820 ZZ= 28.2623
Eigenvalues: 25.4071 27.4158 32.3488
8 H Isotropic = 29.7927 Anisotropy = 8.5858
XX= 32.7673 YX= 3.2196 ZX= -1.3393
XY= 3.3150 YY= 31.5719 ZY= -0.4656
XZ= -1.6141 YZ= 2.4308 ZZ= 25.0388
Eigenvalues: 24.3702 29.4912 35.5165
9 H Isotropic = 29.7220 Anisotropy = 8.3296
XX= 27.6630 YX= -0.2684 ZX= -0.0096
XY= -1.2134 YY= 27.6784 ZY= 3.3201
XZ= -1.7431 YZ= 2.8824 ZZ= 33.8247
Eigenvalues: 26.2886 27.6024 35.2751
10 O Isotropic = 231.9668 Anisotropy = 331.0148
XX= 293.8259 YX= -152.2773 ZX= -43.1868
XY= -121.9345 YY= 304.2457 ZY= -135.7176
XZ= 59.3425 YZ= -56.6802 ZZ= 97.8288
Eigenvalues: 50.1037 193.1534 452.6433
11 C Isotropic = 153.1688 Anisotropy = 20.3694
XX= 165.2692 YX= 1.2334 ZX= 7.1098
XY= 4.0835 YY= 150.1588 ZY= -4.3501
XZ= 3.5587 YZ= -2.0885 ZZ= 144.0783
Eigenvalues: 141.2175 151.5404 166.7484
12 H Isotropic = 28.7232 Anisotropy = 5.3596
XX= 29.7564 YX= -0.9623 ZX= 0.5484
XY= 0.5074 YY= 26.1969 ZY= -2.8472
XZ= 1.0106 YZ= -3.7034 ZZ= 30.2163
Eigenvalues: 24.3576 29.5157 32.2962
13 H Isotropic = 28.5670 Anisotropy = 6.9549
XX= 28.7642 YX= 0.8168 ZX= -0.1832
XY= -0.3949 YY= 32.0627 ZY= 2.8583
XZ= 1.7132 YZ= 3.1584 ZZ= 24.8739
Eigenvalues: 23.6982 28.7992 33.2035
14 C Isotropic = 41.7584 Anisotropy = 197.7095
XX= -44.8728 YX= -27.4675 ZX= -44.9544

XY= -28.3918 YY= 35.7925 ZY= 61.3040
XZ= -49.1328 YZ= 51.6017 ZZ= 134.3557
Eigenvalues: -58.8985 10.6091 173.5648
15 C Isotropic = 52.1581 Anisotropy = 176.4791
XX= 26.8022 YX= -47.3976 ZX= -12.7149
XY= -50.2164 YY= -1.2590 ZY= 74.8779
XZ= -4.5559 YZ= 73.1499 ZZ= 130.9311
Eigenvalues: -55.6976 42.3611 169.8109
16 C Isotropic = 51.4020 Anisotropy = 168.4364
XX= 27.4425 YX= 23.8537 ZX= -50.8078
XY= 27.4384 YY= 19.6842 ZY= 82.7547
XZ= -43.3825 YZ= 84.8266 ZZ= 107.0793
Eigenvalues: -57.4655 47.9786 163.6929
17 C Isotropic = 52.8710 Anisotropy = 187.9408
XX= 21.5637 YX= 21.6865 ZX= -52.6176
XY= 21.1468 YY= 16.3768 ZY= 87.3176
XZ= -51.5948 YZ= 86.6713 ZZ= 120.6726
Eigenvalues: -58.9935 39.4417 178.1649
18 H Isotropic = 24.0730 Anisotropy = 8.8088
XX= 27.6917 YX= -3.1195 ZX= 2.3824
XY= -2.5107 YY= 23.1644 ZY= -1.5562
XZ= 2.3194 YZ= -1.5189 ZZ= 21.3628
Eigenvalues: 20.3729 21.9005 29.9455
19 C Isotropic = 53.5361 Anisotropy = 186.3187
XX= 26.5862 YX= -52.8362 ZX= -13.8160
XY= -51.8034 YY= -0.0492 ZY= 77.9270
XZ= -13.2440 YZ= 77.4054 ZZ= 134.0714
Eigenvalues: -57.7912 40.6510 177.7486
20 H Isotropic = 24.0297 Anisotropy = 8.4260
XX= 27.3299 YX= 3.5340 ZX= -1.3775
XY= 3.3094 YY= 23.3705 ZY= -1.0789
XZ= -0.8721 YZ= -1.7431 ZZ= 21.3888
Eigenvalues: 20.5511 21.8910 29.6470
21 C Isotropic = 55.5011 Anisotropy = 187.4095
XX= -41.0230 YX= -28.4069 ZX= -45.1735
XY= -28.0787 YY= 65.6746 ZY= 51.0182
XZ= -47.2723 YZ= 50.6346 ZZ= 141.8517
Eigenvalues: -54.3871 40.4497 180.4408
22 H Isotropic = 23.9950 Anisotropy = 5.1550
XX= 26.6416 YX= 1.6765 ZX= 0.4055
XY= 1.6272 YY= 23.9753 ZY= -1.1425
XZ= 0.6191 YZ= -1.2272 ZZ= 21.3680
Eigenvalues: 20.6986 23.8547 27.4316
23 H Isotropic = 23.9987 Anisotropy = 5.4261
XX= 26.9327 YX= -0.5130 ZX= 1.5651
XY= -0.4316 YY= 23.1709 ZY= -1.5121
XZ= 1.7299 YZ= -1.5832 ZZ= 21.8925
Eigenvalues: 20.6462 23.7338 27.6161
24 H Isotropic = 24.0582 Anisotropy = 4.4394
XX= 24.1952 YX= 0.1071 ZX= 0.5792
XY= 0.0618 YY= 25.7412 ZY= -2.4078
XZ= 0.5366 YZ= -2.5036 ZZ= 22.2381
Eigenvalues: 20.8867 24.2700 27.0178

%chk=D:\TTOBenz\TTOBzsinCDCl3NMR.chk
B3LYP/6-311++g(d,p) geom=check guess=read scrf(smd, solvent=chloroform) NMR=spinspin

Total nuclear spin-spin coupling J (Hz):

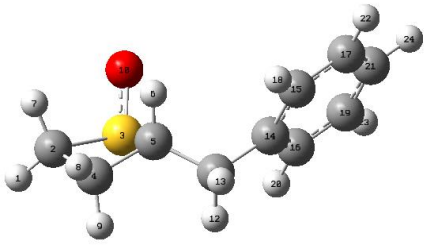
	1	2	3	4	5
1	0.000000D+00				
2	0.144682D+03	0.000000D+00			
3	0.610021D+01	-0.992546D+01	0.000000D+00		
4	-0.528228D+00	0.309168D+02	0.337879D+01	0.000000D+00	
5	0.110732D+02	-0.461553D+01	-0.831639D+01	0.320253D+02	0.000000D+00
6	0.247893D+01	0.821165D+01	0.645328D+01	-0.148780D+00	0.147232D+03
7	-0.941048D+01	0.142937D+03	0.127291D+01	-0.396062D+01	0.125329D+01
8	0.158693D+01	-0.197520D+01	0.605383D+01	0.135559D+03	-0.262556D+01
9	0.777164D+01	-0.366199D+01	-0.520518D-01	0.129380D+03	-0.286050D+01
10	-0.388660D+00	-0.413088D+01	0.477937D+02	0.124744D+01	-0.456975D+01
11	-0.568782D+00	0.471864D+00	0.815283D-01	-0.112284D+01	0.347462D+02
12	-0.249570D+00	-0.258141D+00	0.315562D+00	0.354114D+01	-0.515494D+01
13	-0.412882D+00	-0.370626D+00	0.871211D+00	0.873919D+01	-0.614607D+01
14	-0.992384D-01	-0.283089D+00	0.813385D+00	0.863474D+00	-0.168325D+01
15	0.347755D-01	0.103398D+00	-0.728007D-01	-0.936086D-01	0.109873D+01
16	0.181697D-01	0.128260D-01	0.119842D-01	-0.999546D-01	0.129699D+01
17	-0.294204D-01	0.149573D-01	0.303718D-01	0.420168D-01	-0.991404D+00
18	-0.151566D+00	-0.150450D-01	0.146747D-01	0.411599D-01	-0.645991D+00
19	-0.156588D-01	-0.287308D-02	0.649436D-01	0.352986D-01	-0.796981D+00
20	-0.360362D-01	0.164358D-01	0.149574D-01	0.189575D+00	-0.669490D+00
21	-0.330289D-01	-0.148568D-01	-0.303035D-01	-0.389277D-01	0.877809D+00
22	-0.120836D+00	-0.333361D-01	0.684121D-02	-0.573348D-01	0.313751D+00
23	-0.685287D-01	-0.110525D-01	-0.165988D-02	-0.150214D-01	0.308626D+00
24	-0.994430D-01	-0.154978D-01	0.162001D-01	-0.108579D-02	-0.681476D+00

	6	7	8	9	10
6	0.000000D+00				
7	-0.141808D+01	0.000000D+00			
8	0.188855D+01	0.106355D+02	0.000000D+00		
9	0.798378D+01	0.111347D+02	-0.122004D+02	0.000000D+00	
10	-0.228335D+00	-0.108512D+01	0.758823D+00	0.486061D+00	0.000000D+00
11	-0.152224D+01	-0.450208D-01	0.505107D+01	0.564151D+01	-0.798221D+00
12	0.114442D+02	0.593634D+00	-0.660254D-01	-0.472491D+00	-0.156036D+00
13	0.326622D+01	-0.520984D-02	-0.525609D+00	0.405873D+00	-0.382715D+00
14	0.260875D+01	0.630306D-01	-0.103194D+00	-0.191872D+00	-0.291758D+00
15	-0.424243D-01	0.170473D-02	0.382380D-01	0.681944D-01	0.272512D-03
16	-0.202495D-01	0.217452D-01	0.416780D+00	0.797628D-01	-0.108878D-01
17	0.778956D-01	-0.278328D-01	-0.336336D-01	-0.289922D-01	0.501019D-02
18	0.404851D+00	-0.997469D-01	-0.525369D-01	-0.276462D-01	-0.201653D-01

19 -0.306448D-02 0.516289D-02 0.742382D-01 -0.176262D-01 -0.320936D-02
20 -0.638388D-01 0.246932D+00 0.401350D+00 -0.173679D-01 0.273373D-01
21 -0.489609D-01 -0.352420D-01 -0.136417D-01 0.113597D-01 -0.925537D-02
22 0.149500D-01 -0.983644D-01 -0.943215D-01 -0.577335D-01 -0.213363D-02
23 -0.135568D+00 0.240701D-02 0.567603D-01 -0.514655D-01 0.144409D-02
24 -0.537451D-01 -0.726682D-01 -0.624084D-01 -0.822220D-01 0.137609D-01
11 12 13 14 15
11 0.000000D+00
12 0.124473D+03 0.000000D+00
13 0.125439D+03 -0.120097D+02 0.000000D+00
14 0.433372D+02 -0.428336D+01 -0.529695D+01 0.000000D+00
15 0.303153D+01 0.613920D+01 0.396466D+01 0.603679D+02 0.000000D+00
16 0.319216D+01 0.520710D+01 0.510938D+01 0.609914D+02 0.108946D+00
17 0.335433D+01 0.861585D+00 -0.557941D+00 -0.151942D+01 0.607738D+02
18 0.406906D+01 -0.321404D+00 -0.298019D+00 0.573002D+00 0.148203D+03
19 0.342273D+01 0.106981D+00 0.588874D-01 -0.153528D+01 0.868369D+01
20 0.419435D+01 0.116226D+00 -0.690378D+00 0.794191D+00 0.568759D+01
21 -0.694915D+00 0.412352D-01 0.526574D+00 0.911259D+01 -0.191905D+01
22 0.424967D+00 0.106709D+00 0.174925D+00 0.680321D+01 0.165037D+01
23 0.408839D+00 0.457941D-01 0.191673D+00 0.682394D+01 -0.117192D+01
24 0.511114D+00 -0.280159D+00 -0.660649D+00 -0.124659D+01 0.691969D+01
16 17 18 19 20
16 0.000000D+00
17 0.865773D+01 0.000000D+00
18 0.583826D+01 0.120561D+01 0.000000D+00
19 0.600536D+02 -0.150134D+01 -0.923995D+00 0.000000D+00
20 0.148802D+03 -0.891096D+00 0.129355D+01 0.144339D+01 0.000000D+00
21 -0.195078D+01 0.596752D+02 0.670352D+01 0.600443D+02 0.660981D+01
22 -0.116081D+01 0.150106D+03 0.714876D+01 0.699403D+01 0.374321D+00
23 0.170671D+01 0.702719D+01 0.396799D+00 0.150082D+03 0.699797D+01
24 0.689269D+01 0.178113D+01 0.620284D+00 0.173148D+01 0.635578D+00
21 22 23 24
21 0.000000D+00
22 0.150680D+01 0.000000D+00
23 0.141411D+01 0.783509D+00 0.000000D+00
24 0.151007D+03 0.677293D+01 0.685548D+01 0.000000D+00

anti 2-Benzylthietane 1-oxide

%chk=C:\G09W\TTO\TTOBz\TTOBzCDCL3.chk
opt freq B3LYP/6-311++g(d,p) scrf(smd, solvent=chloroform) NMR=spinspin



Charge = 0 Multiplicity = 1
H,0,4.285585068,-0.3243521691,-0.5034095451
C,0,3.4354091687,0.0587008662,0.0589030068
S,0,1.8912154372,-0.9772135773,-0.1004878928
C,0,2.6830150257,1.2868023102,-0.4768892294
C,0,1.2793686076,0.8151393904,-0.0436929055
H,0,1.1068440272,1.0128998489,1.0176632884
H,0,3.6692815832,0.1282973831,1.122721238
H,0,2.9947743345,2.2435045816,-0.0554015155
H,0,2.7534311597,1.351476447,-1.5655947155
O,0,1.590382174,-1.7685081215,1.1660207386
C,0,0.0774073995,1.1865861575,-0.9044752207
H,0,0.2645423909,0.8750086634,-1.9368840202
H,0,0.0188316631,2.2817654881,-0.9171603678
C,0,-1.2385448236,0.6142274018,-0.420957302
C,0,-1.9636550976,1.2463893936,0.5974072848
C,0,-1.7506993997,-0.5671183,-0.9690645194
C,0,-3.1645476216,0.7101676759,1.0585363638
H,0,-1.5880872057,2.1691062684,1.0293477564
C,0,-2.9513194435,-1.1082059568,-0.5085925513
H,0,-1.2093722798,-1.0672252144,-1.7658099363
C,0,-3.6618781595,-0.471353231,0.5072848801
H,0,-3.7140841606,1.2162011334,1.8450852149
H,0,-3.3306136857,-2.025587135,-0.9456362713
H,0,-4.5962183554,-0.8898371147,0.8649734451

Zero-point correction= 0.196009 (Hartree/Particle)
Thermal correction to Energy= 0.207145
Thermal correction to Enthalpy= 0.208090
Thermal correction to Gibbs Free Energy= 0.157198
Sum of electronic and zero-point Energies= -861.622404
Sum of electronic and thermal Energies= -861.611267
Sum of electronic and thermal Enthalpies= -861.610323
Sum of electronic and thermal Free Energies= -861.661215

MPW1PW91- SCF GIAO Magnetic shielding tensor (ppm):
Calculating GIAO nuclear magnetic shielding tensors.
Rif σHTMS (MPW/6-311++G(d,p), SMD-$CDCl_3$) =31.8426
SCF GIAO Magnetic shielding tensor (ppm):
1 H Isotropic = 28.3713 Anisotropy = 8.0237
XX= 33.0730 YX= 2.4014 ZX= 1.7870
XY= 0.9342 YY= 26.0989 ZY= -0.0983
XZ= 1.0541 YZ= 0.6547 ZZ= 25.9422
Eigenvalues: 25.6483 25.7452 33.7205
2 C Isotropic = 133.0252 Anisotropy = 67.9277
XX= 136.3199 YX= -33.6949 ZX= -10.5135
XY= -40.5655 YY= 144.2821 ZY= -15.5879
XZ= 3.2759 YZ= -7.6845 ZZ= 118.4735

Eigenvalues: 97.5860 123.1793 178.3103
3 S Isotropic = 116.5079 Anisotropy = 329.2913
XX= 56.2642 YX= 30.2969 ZX= 51.5194
XY= 27.0481 YY= 65.6489 ZY= -146.0678
XZ= 57.0919 YZ= -188.6605 ZZ= 227.6107
Eigenvalues: -63.3815 76.8698 336.0354
4 C Isotropic = 166.3446 Anisotropy = 34.5692
XX= 188.6128 YX= 3.3684 ZX= -2.5638
XY= 4.2720 YY= 157.3593 ZY= -0.1557
XZ= -5.1636 YZ= 7.9379 ZZ= 153.0617
Eigenvalues: 150.0422 159.6008 189.3907
5 C Isotropic = 105.5843 Anisotropy = 55.4267
XX= 90.2031 YX= 2.2805 ZX= 5.9766
XY= 20.0702 YY= 139.8371 ZY= -3.5409
XZ= -7.9834 YZ= -4.3750 ZZ= 86.7129
Eigenvalues: 86.3987 87.8189 142.5355
6 H Isotropic = 28.1943 Anisotropy = 5.3791
XX= 31.5578 YX= 0.2911 ZX= 0.5777
XY= 1.8870 YY= 24.8341 ZY= 1.2467
XZ= -1.7569 YZ= 0.9041 ZZ= 28.1909
Eigenvalues: 24.3162 28.4862 31.7803
7 H Isotropic = 28.9242 Anisotropy = 6.3711
XX= 29.9438 YX= 1.2040 ZX= -3.9418
XY= 1.8952 YY= 27.2063 ZY= -1.0577
XZ= -1.8833 YZ= -0.5315 ZZ= 29.6225
Eigenvalues: 26.3265 27.2745 33.1716
8 H Isotropic = 29.3899 Anisotropy = 10.2883
XX= 28.1074 YX= -3.6743 ZX= -1.6183
XY= -2.8242 YY= 33.5909 ZY= 4.0830
XZ= -1.2376 YZ= 1.9790 ZZ= 26.4714
Eigenvalues: 25.3230 26.5979 36.2488
9 H Isotropic = 29.8866 Anisotropy = 5.6901
XX= 29.4850 YX= -0.8392 ZX= 1.8652
XY= -0.7149 YY= 28.7256 ZY= -2.8105
XZ= 1.1501 YZ= -2.3317 ZZ= 31.4492
Eigenvalues: 27.1711 28.8088 33.6800
10 O Isotropic = 207.3052 Anisotropy = 300.0291
XX= 372.1265 YX= 91.6606 ZX= -42.5017
XY= 103.2475 YY= 136.7300 ZY= 124.9960
XZ= -10.8157 YZ= -6.4320 ZZ= 113.0590
Eigenvalues: 42.2482 172.3428 407.3246
11 C Isotropic = 145.3305 Anisotropy = 32.4418
XX= 165.3691 YX= -11.7536 ZX= 8.3369
XY= -2.1020 YY= 134.3308 ZY= -2.2797
XZ= -4.5440 YZ= 2.2027 ZZ= 136.2917
Eigenvalues: 132.8168 136.2164 166.9584
12 H Isotropic = 28.9422 Anisotropy = 4.6545
XX= 29.0335 YX= -0.6283 ZX= 0.4566
XY= -1.8080 YY= 25.8857 ZY= -0.7865
XZ= 0.7443 YZ= 0.6337 ZZ= 31.9075
Eigenvalues: 25.4670 29.3144 32.0452
13 H Isotropic = 28.6898 Anisotropy = 6.3193
XX= 28.6882 YX= 0.7571 ZX= 0.3153
XY= 0.9744 YY= 32.7138 ZY= 0.7170
XZ= 1.6231 YZ= -0.5204 ZZ= 24.6673
Eigenvalues: 24.4447 28.7219 32.9026
14 C Isotropic = 42.3515 Anisotropy = 198.1761
XX= -3.2728 YX= 74.4386 ZX= -62.0427
XY= 77.5370 YY= 57.9890 ZY= -58.0747
XZ= -63.5431 YZ= -52.1259 ZZ= 72.3382
Eigenvalues: -59.4079 11.9934 174.4689
15 C Isotropic = 52.9733 Anisotropy = 174.1056
XX= 57.5336 YX= 61.5998 ZX= -21.0490
XY= 58.6892 YY= 37.9849 ZY= -90.8826
XZ= -13.4063 YZ= -92.0860 ZZ= 63.4014
Eigenvalues: -53.6044 43.4806 169.0437
16 C Isotropic = 52.4232 Anisotropy = 170.9037
XX= 41.6628 YX= 20.8129 ZX= -76.7167
XY= 12.8704 YY= 85.5033 ZY= -73.7756
XZ= -70.7049 YZ= -76.9961 ZZ= 30.1034
Eigenvalues: -54.7250 45.6355 166.3589
17 C Isotropic = 52.8619 Anisotropy = 187.6424
XX= 42.6914 YX= 23.5781 ZX= -80.6074
XY= 23.5738 YY= 82.9782 ZY= -79.0015
XZ= -81.2913 YZ= -80.1591 ZZ= 32.9161
Eigenvalues: -58.7695 39.3984 177.9569
18 H Isotropic = 24.0426 Anisotropy = 8.2598
XX= 27.1966 YX= 0.2339 ZX= 4.4341
XY= -0.1078 YY= 21.7307 ZY= 1.0822
XZ= 3.4158 YZ= 0.8690 ZZ= 23.2593
Eigenvalues: 20.3611 22.1658 29.6597
19 C Isotropic = 54.0649 Anisotropy = 187.2401
XX= 61.8479 YX= 67.0457 ZX= -23.1071
XY= 67.6580 YY= 38.4124 ZY= -94.4969
XZ= -22.4410 YZ= -93.2682 ZZ= 61.9343
Eigenvalues: -56.9935 40.2965 178.8916
20 H Isotropic = 24.1816 Anisotropy = 7.8623
XX= 25.9711 YX= -3.8357 ZX= -1.6388
XY= -3.2601 YY= 23.7515 ZY= 1.6967
XZ= -1.3706 YZ= 2.1500 ZZ= 22.8223
Eigenvalues: 20.8102 22.3115 29.4231
21 C Isotropic = 55.9978 Anisotropy = 186.7200
XX= 4.3691 YX= 79.2788 ZX= -58.0264
XY= 81.0783 YY= 76.9976 ZY= -43.7166
XZ= -60.8203 YZ= -42.7863 ZZ= 86.6266
Eigenvalues: -53.4788 40.9943 180.4777
22 H Isotropic = 24.0115 Anisotropy = 5.2175
XX= 25.4642 YX= -2.5956 ZX= 0.7997
XY= -2.6177 YY= 24.0693 ZY= 1.5523
XZ= 0.7000 YZ= 1.4953 ZZ= 22.5011
Eigenvalues: 20.5984 23.9463 27.4899
23 H Isotropic = 24.0495 Anisotropy = 5.2625
XX= 26.1349 YX= -1.4811 ZX= 2.2748
XY= -1.4896 YY= 22.3958 ZY= 1.0310
XZ= 2.1648 YZ= 0.9779 ZZ= 23.6179
Eigenvalues: 20.6996 23.8911 27.5578
24 H Isotropic = 24.0620 Anisotropy = 4.4767
XX= 23.8912 YX= -0.7876 ZX= 1.2973
XY= -0.5748 YY= 23.7412 ZY= 2.8245
XZ= 1.0338 YZ= 2.7831 ZZ= 24.5534

%chk=C:\G09W\TTO\TTOBz\TTOBzCDCl3NMR.chk
B3LYP/6-311++g(d,p) geom=check guess=read scrf(smd, solvent=chloroform) NMR=spinspin

Total nuclear spin-spin coupling J (Hz):

	1	2	3	4	5
1	0.000000D+00				
2	0.146142D+03	0.000000D+00			
3	0.612807D+01	-0.998818D+01	0.000000D+00		
4	-0.564136D+00	0.313459D+02	0.348399D+01	0.000000D+00	
5	0.116171D+02	-0.301819D+01	-0.986576D+01	0.305047D+02	0.000000D+00
6	-0.128348D+01	0.149588D+01	0.762532D+00	-0.352645D+01	0.145675D+03

7 -0.896614D+01 0.143552D+03 0.107873D+01 -0.394796D+01 0.130240D+01
8 0.135775D+01 -0.200036D+01 0.703293D+01 0.136808D+03 -0.170606D+01
9 0.800287D+01 -0.389019D+01 0.333957D+00 0.128773D+03 -0.403427D+01
10 -0.364609D+00 -0.380118D+01 0.475808D+02 0.119463D+01 -0.398080D+01
11 0.185868D+01 0.639464D+01 0.270407D+01 0.422174D+00 0.355568D+02
12 -0.296768D+00 -0.400549D+00 0.152694D+01 0.174933D+01 -0.591212D+01
13 -0.214200D+00 -0.766089D+00 0.598386D+01 0.253683D+01 -0.318518D+01
14 -0.826958D-01 -0.707853D-02 0.213170D-01 0.467625D+01 -0.228653D+01
15 -0.197080D-01 -0.209126D-01 0.199886D-01 -0.804704D-01 0.109204D+01
16 -0.216541D-01 0.105265D+00 0.165028D+00 -0.473869D-01 0.107029D+01
17 -0.714931D-01 -0.796711D-02 0.232861D-01 0.577462D-01 -0.101669D+01
18 -0.167403D+00 -0.185081D-01 0.257473D-01 0.293742D-01 -0.726113D+00
19 -0.649980D-01 0.428958D-01 0.140302D-01 0.780107D-01 -0.945035D+00
20 -0.204949D+00 0.211725D-01 0.172022D+00 -0.365290D-02 -0.791731D+00
21 -0.212064D-01 -0.212101D-01 -0.947259D-02 0.109298D-01 0.909069D+00
22 -0.135161D+00 -0.480686D-01 -0.313061D-01 0.353156D-01 0.315445D+00
23 -0.137354D+00 -0.558489D-01 -0.155891D-01 0.263354D-01 0.287124D+00
24 -0.166226D+00 -0.347510D-01 0.838684D-02 -0.497146D-01 -0.725951D+00

	6	7	8	9	10
6	0.000000D+00				
7	-0.450929D-01	0.000000D+00			
8	0.891780D+01	0.100758D+02	0.000000D+00		
9	0.100384D+02	0.111401D+02	-0.113578D+02	0.000000D+00	
10	-0.921896D+00	-0.101788D+01	0.773868D+00	0.434928D+00	0.000000D+00
11	-0.116001D+01	-0.437626D+00	0.640786D+00	0.457083D+01	0.215385D+00
12	0.108352D+02	-0.964120D-01	-0.295462D+00	0.151308D+00	0.967141D-01
13	0.308437D+01	-0.123764D+00	-0.370922D+00	-0.175651D+00	-0.224699D+00
14	0.216406D+01	-0.491363D-02	-0.306588D+00	-0.180887D+00	-0.409075D-01
15	-0.782519D-01	-0.228004D-01	0.629269D-01	0.823517D-01	-0.246274D-01
16	-0.162681D-01	-0.115815D-01	-0.457694D-01	-0.414845D-01	-0.566268D-01
17	0.875523D-01	-0.219276D-01	-0.209703D-02	-0.652243D-02	-0.913508D-03
18	0.393066D+00	-0.255281D-01	0.702459D-01	-0.356803D-02	-0.163262D-01
19	0.475668D-02	-0.362059D-01	-0.530939D-01	-0.246025D-01	-0.601775D-02
20	-0.621299D-01	-0.230039D+00	-0.142754D+00	0.406642D-01	-0.172819D-01
21	-0.541868D-01	-0.352389D-01	-0.437295D-01	-0.579234D-01	-0.750842D-02
22	0.985346D-02	-0.822978D-01	-0.588596D-01	-0.106557D+00	-0.601093D-02
23	-0.151273D+00	-0.166278D+00	-0.133778D+00	-0.100406D+00	-0.180097D-01
24	-0.487912D-01	-0.119791D+00	-0.108836D+00	-0.108592D+00	-0.427234D-02

	11	12	13	14	15
11	0.000000D+00				
12	0.123257D+03	0.000000D+00			
13	0.120904D+03	-0.131207D+02	0.000000D+00		
14	0.437627D+02	-0.379561D+01	-0.534280D+01	0.000000D+00	
15	0.310817D+01	0.604020D+01	0.419881D+01	0.605646D+02	0.000000D+00
16	0.341581D+01	0.477229D+01	0.544976D+01	0.607173D+02	-0.990515D-03
17	0.340147D+01	0.787397D+00	-0.384723D+00	-0.152935D+01	0.607445D+02
18	0.424572D+01	-0.348642D+00	-0.235516D+00	0.724801D+00	0.147959D+03
19	0.349512D+01	-0.239862D-01	0.214541D+00	-0.155223D+01	0.875465D+01
20	0.438972D+01	0.851805D-01	-0.592889D+00	0.953330D+00	0.577537D+01
21	-0.716418D+00	0.101806D+00	0.398741D+00	0.921507D+01	-0.191440D+01
22	0.403279D+00	0.109793D+00	0.124897D+00	0.680907D+01	0.165952D+01
23	0.404179D+00	0.432351D-01	0.143674D+00	0.680942D+01	-0.117043D+01
24	0.535668D+00	-0.338101D+00	-0.578573D+00	-0.123443D+01	0.694286D+01

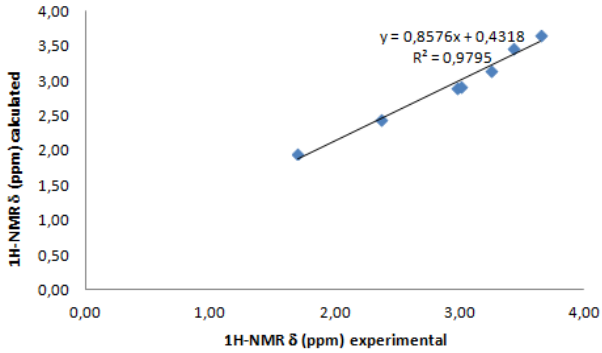
	16	17	18	19	20
16	0.000000D+00				
17	0.871827D+01	0.000000D+00			
18	0.578658D+01	0.118601D+01	0.000000D+00		
19	0.602542D+02	-0.151613D+01	-0.915643D+00	0.000000D+00	
20	0.148823D+03	-0.899833D+00	0.131708D+01	0.127264D+01	0.000000D+00
21	-0.192915D+01	0.597836D+02	0.666596D+01	0.600556D+02	0.661374D+01
22	-0.115491D+01	0.150022D+03	0.710268D+01	0.696444D+01	0.398476D+00
23	0.165556D+01	0.703716D+01	0.403284D+00	0.150439D+03	0.707306D+01
24	0.693165D+01	0.178556D+01	0.618314D+00	0.169167D+01	0.633293D+00

	21	22	23	24
21	0.000000D+00			
22	0.146038D+01	0.000000D+00		
23	0.144036D+01	0.773927D+00	0.000000D+00	
24	0.150911D+03	0.680151D+01	0.687090D+01	0.000000D+00

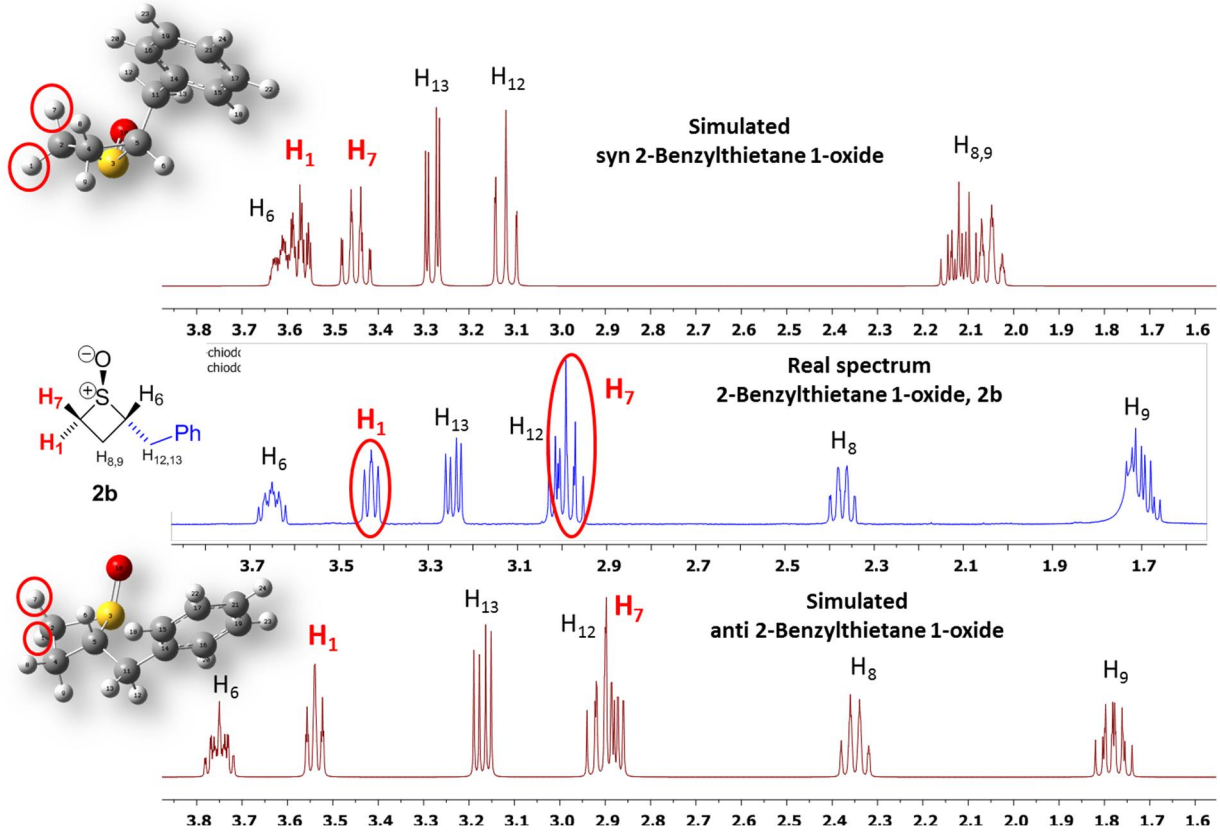
Squares linear fitting parameter (R^2) of the correlation plot between computed (without scaling) and experimental data, Mean Absolute Error (MAE) and Corrected Mean Absolute Error (CMAE).[5]

Table. Experimental, calculated and scaled ^{1}H-NMR chemical shift (ppm)

Atoms	δ_{exp}[a]	$\delta_{calculated}$[b]	δ_{scaled}[c]
H_9	1,70	1,96	1,78
H_8	2,37	2,45	2,35
H_{12}	2,980	2,900	2,88
H_7	3,01	2,93	2,91
H_{13}	3,25	3,15	3,17
H_1	3,430	3.47	3,54
H_6	3,65	3,65	3,75
R^2	-	0.979	-
MAE[c]	-	0.09	-
CMAE[c]	-	0.08	-

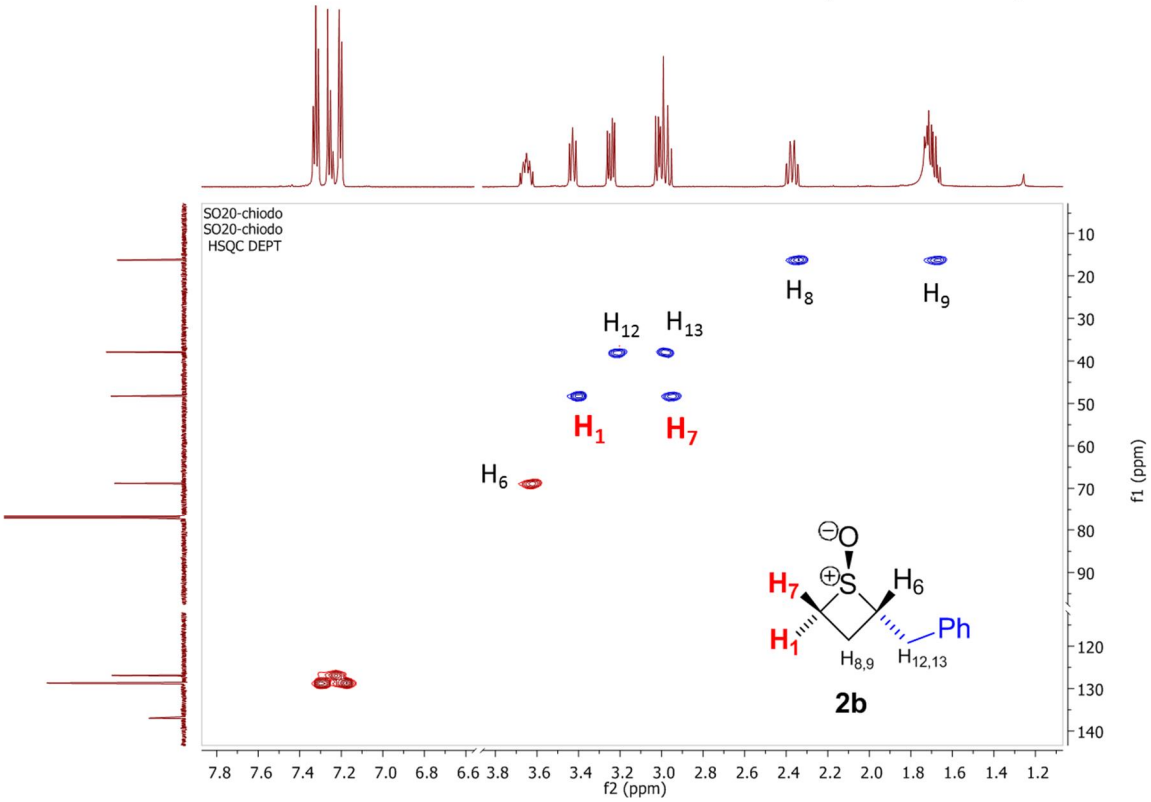


[a]Experimental values in $CDCl_3$ at 298 K. [b]SMD($CDCl_3$)/MPW1PW91/6-311++G(d,p) values. [c]The parameters MAE and CMAE are calculated as follow: $MAE = \frac{1}{N}\sum_i^N |\delta_{calc} - \delta_{exp}|$, $CMAE = \frac{1}{N}\sum_i^N |\delta_{scaled} - \delta_{exp}|$ with $\delta_{scaled} = \frac{\delta_{calc} - intercept}{slope}$

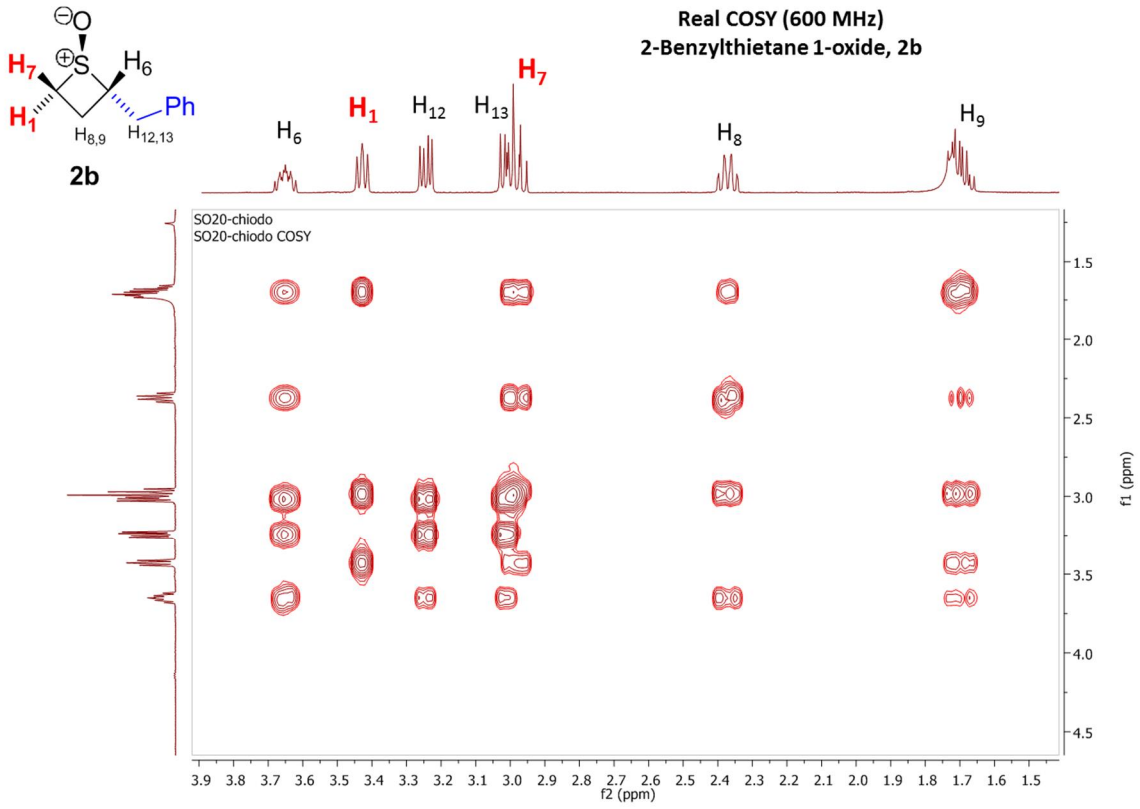


[5] U. Azzena, G. Dettori, L. Pisano, B. Musio, R. Luisi *J. Org. Chem.* **2011**, *76*, 2291-2295.

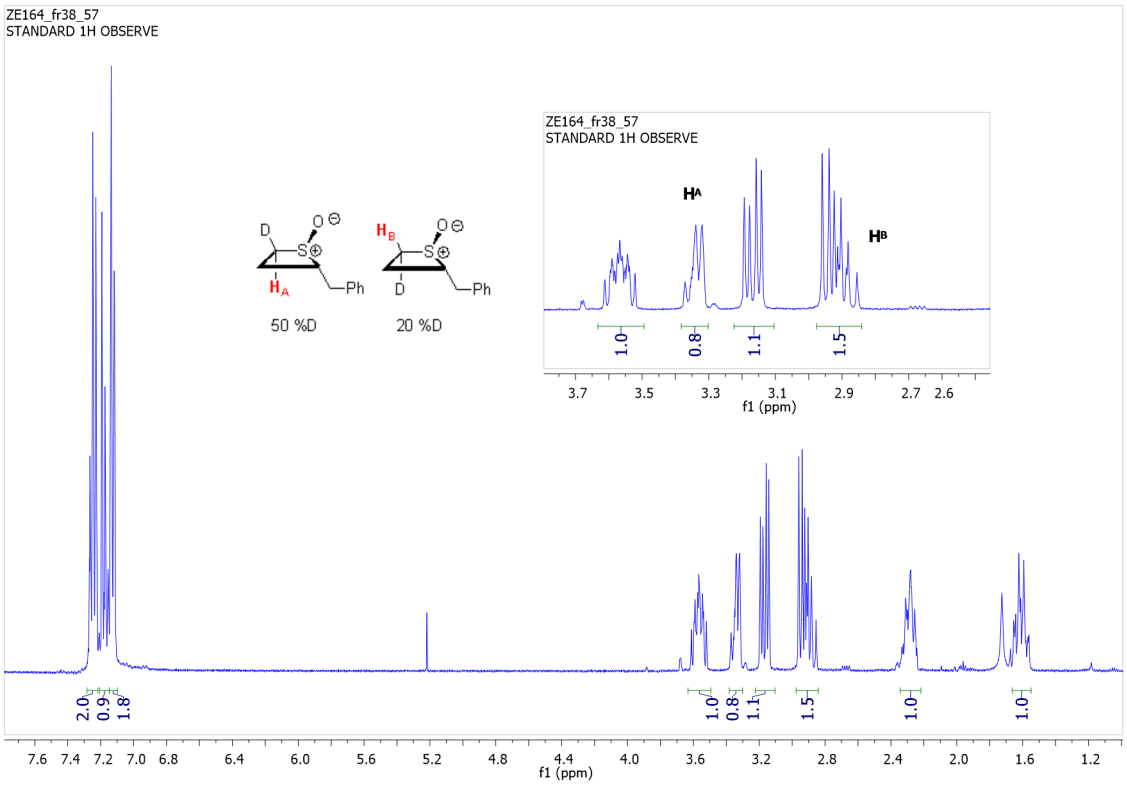
Real HSQC-DEPT spectrum
2-Benzylthietane 1-oxide, 2b

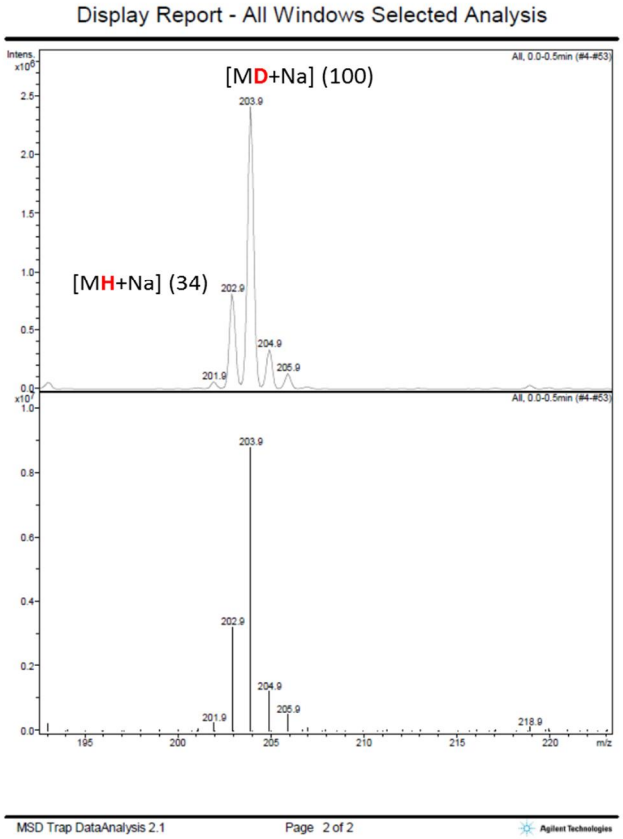


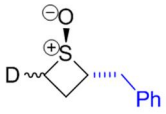
Real COSY (600 MHz)
2-Benzylthietane 1-oxide, 2b



(*1R*$_S$*,2R**,4R**)/(*1R*$_S$*,2R**,4S**)-6d



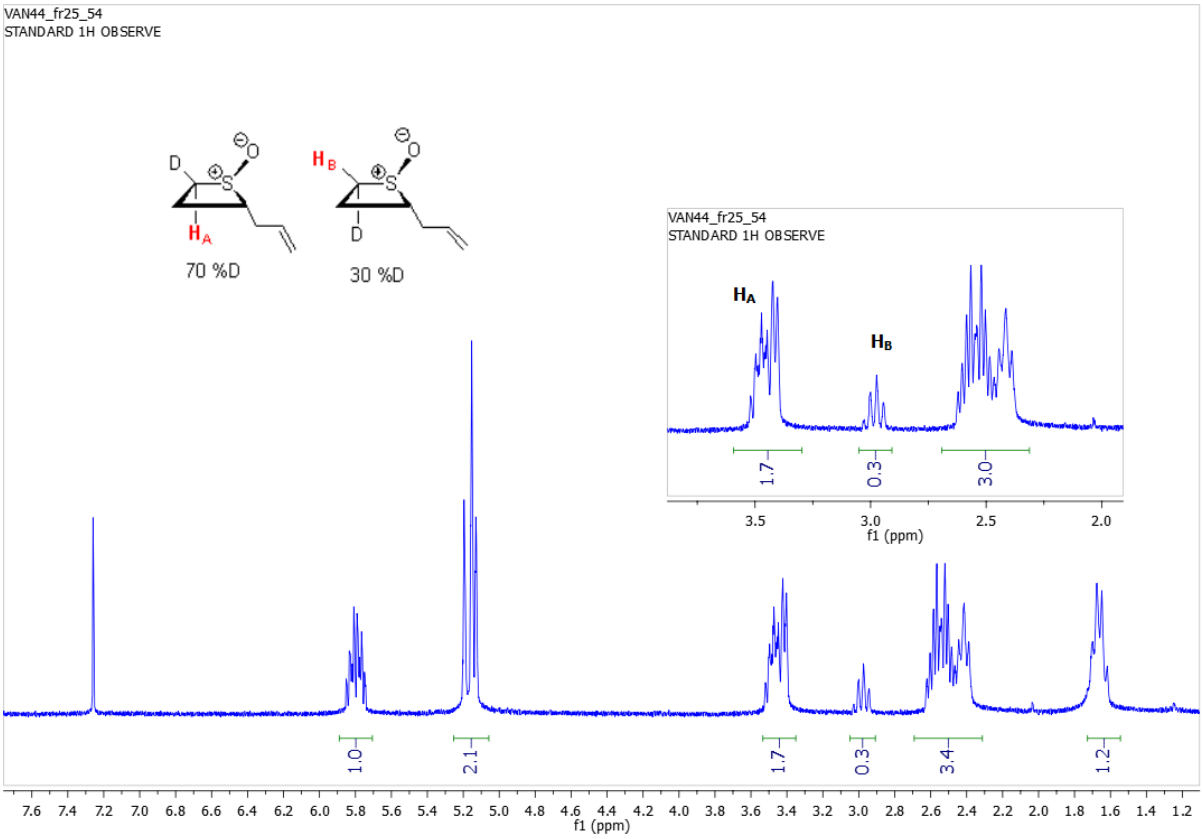


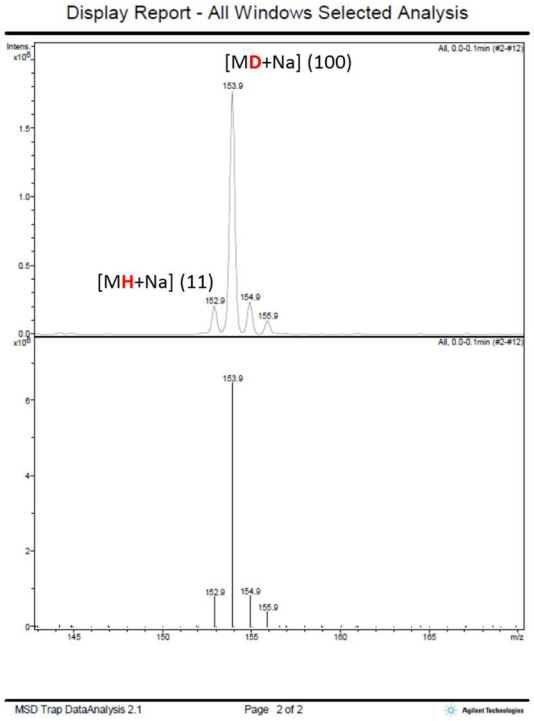


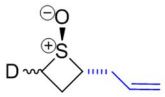
Isotopic abundances for protonated m/z:
[MH+Na] 203.0507 (100.0%)
[MH+1+Na] 204.0540 (10.8%)
[MH+2+Na] 205.0465 (4.5%)

Deuterium content:
[MD+Na]/([MD+Na] + [MH+Na])
[100 – (34 x 0,108)] = 96,3 [MD+Na]
96,3/(96,3 + 34) = **74 %D**

(*1R*$_S$*,*2R,*4R**)/(*1R*$_S$*,*2R**,*4S**)-7d**







Isotopic abundances for protonated m/z:
[MH+Na] 153.0350 (100.0%)
[MH+1+Na] 154.0384 (6.5%)
[MH+2+Na] 155.0308 (4.5%)

Deuterium content:
[MD+Na]/([MD+Na] + [MH+Na])
[100 – (11 x 0,065)] = 99,3 [MD+Na]
99,3/(99,3 + 11,1) = **90 %D**