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

Supporting Information

Magnesium Catalyzed [3+3] Heteroannulation of α-Enolic dithioesters with MBH Acetate: Access to Functionalized 3,4-Dihydro-2H-thiopyrans

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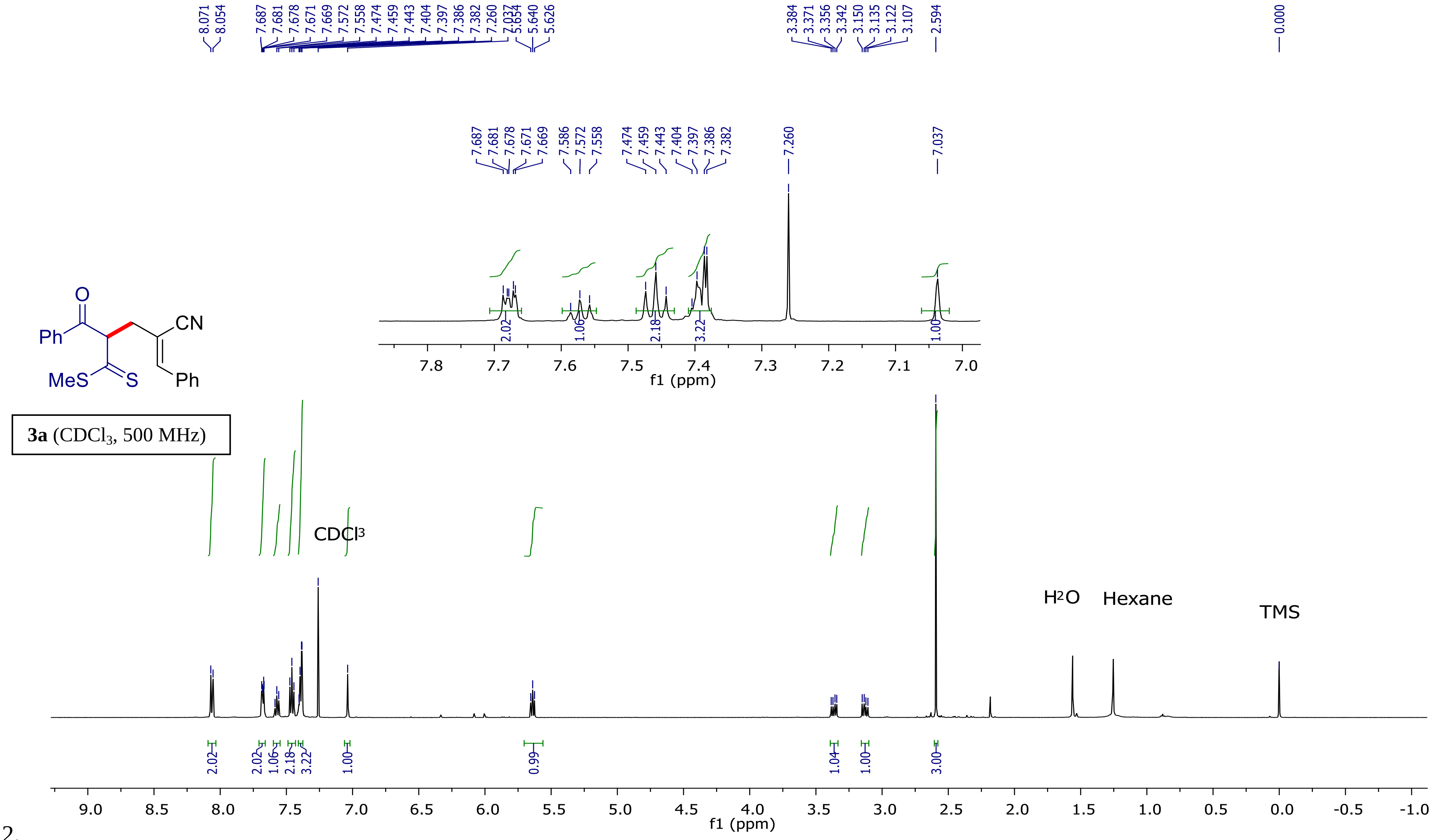
Table of Contents

1. Representative ^{1}H, ^{13}C, DEPT, COSY and HRMS Spectra S2
2. Crystal Data of **6l** and **6i** S95
3. Quantum Chemical Calculations S116
4. References S132

Representative ^{1}H, $^{13}C\{^{1}H\}$, DEPT, COSY and HRMS Spectra

1. ^{1}H (500 MHz, $CDCl_3$) and ^{13}C(^{1}H) (125 MHz, $CDCl_3$) NMR of Compound 3a



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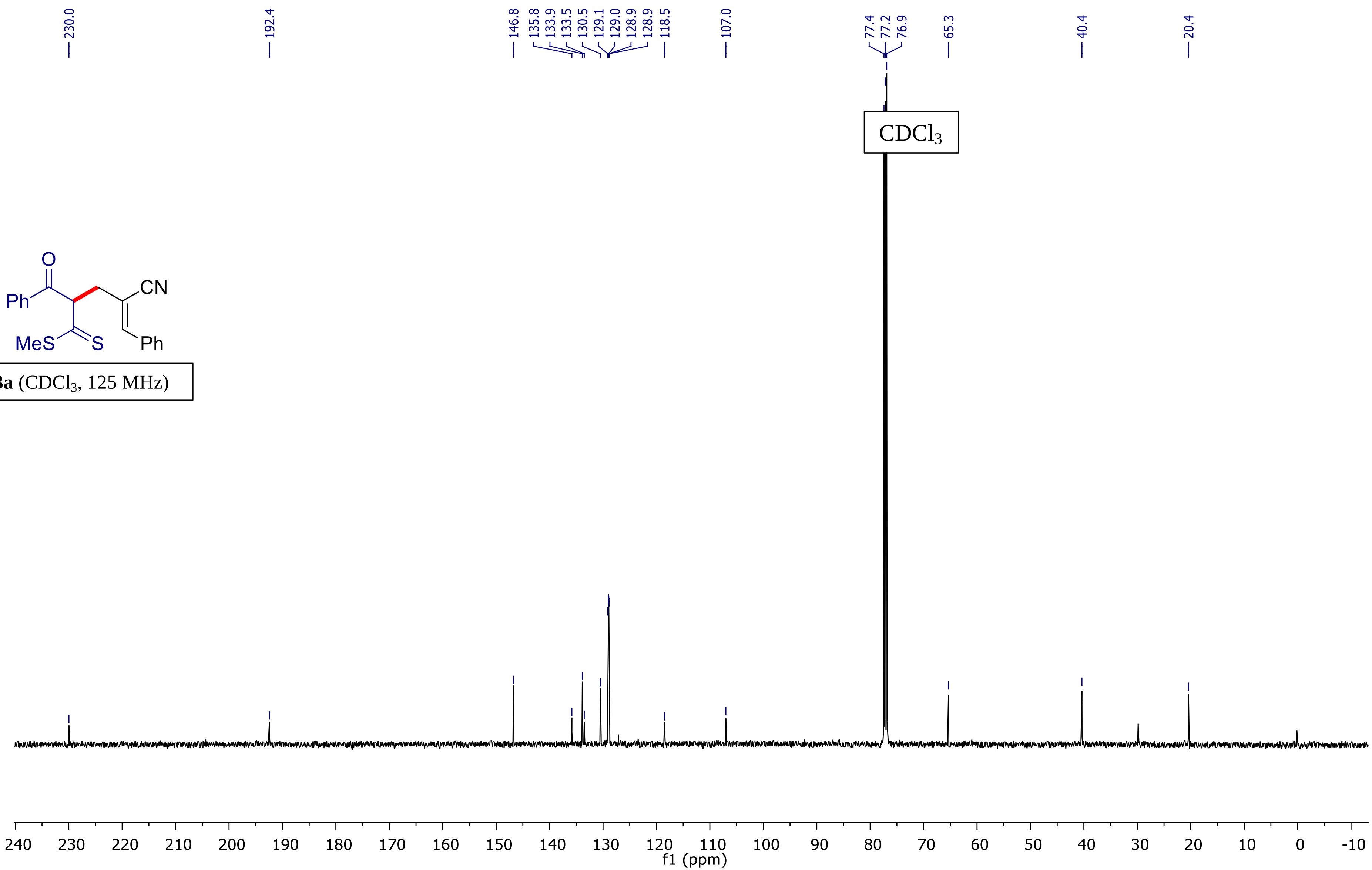
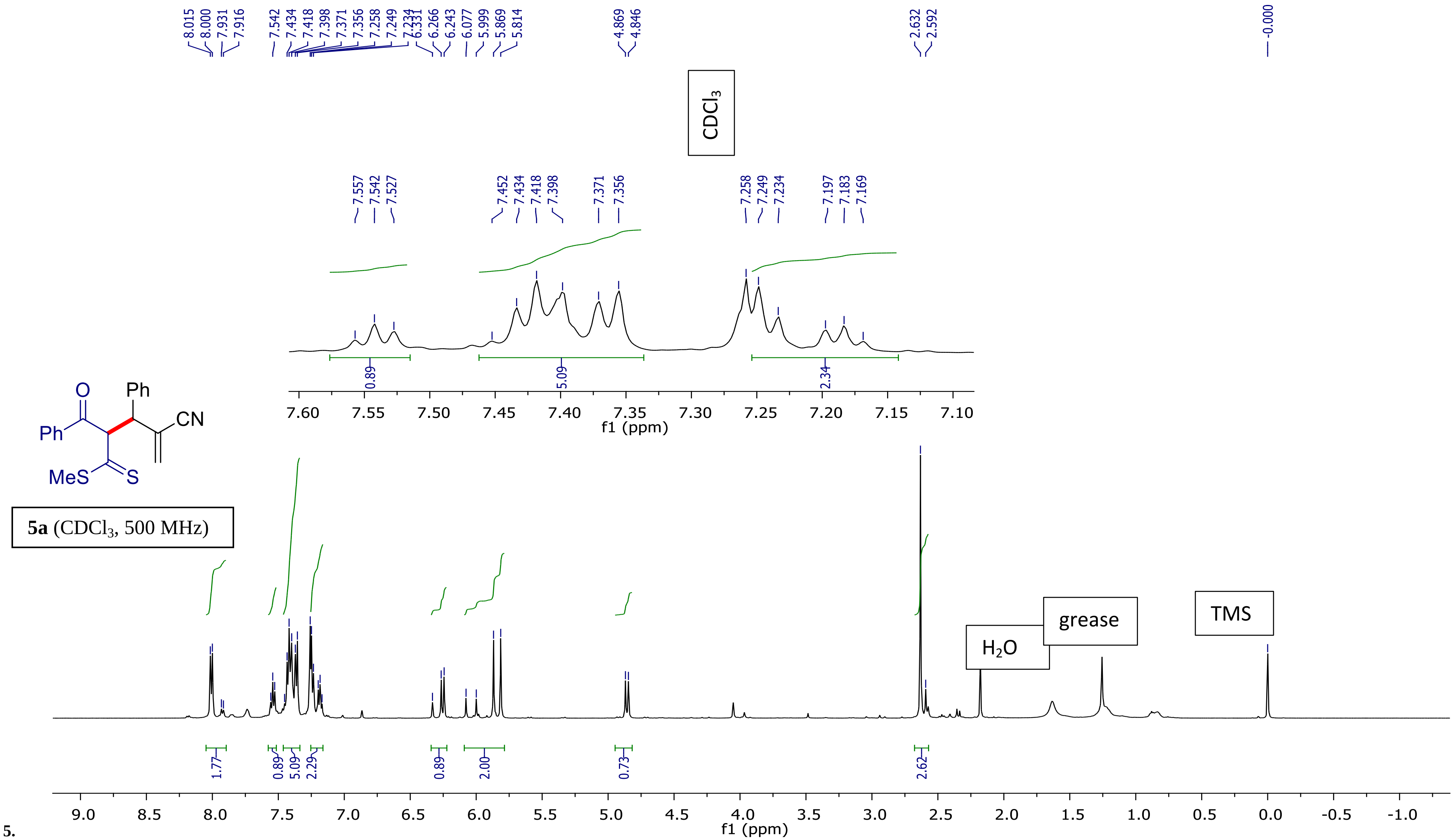


3a ($CDCl_3$, 125 MHz)

3.

4. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C(^{1}H)$ (125 MHz, $CDCl_3$) NMR of Compound 5a



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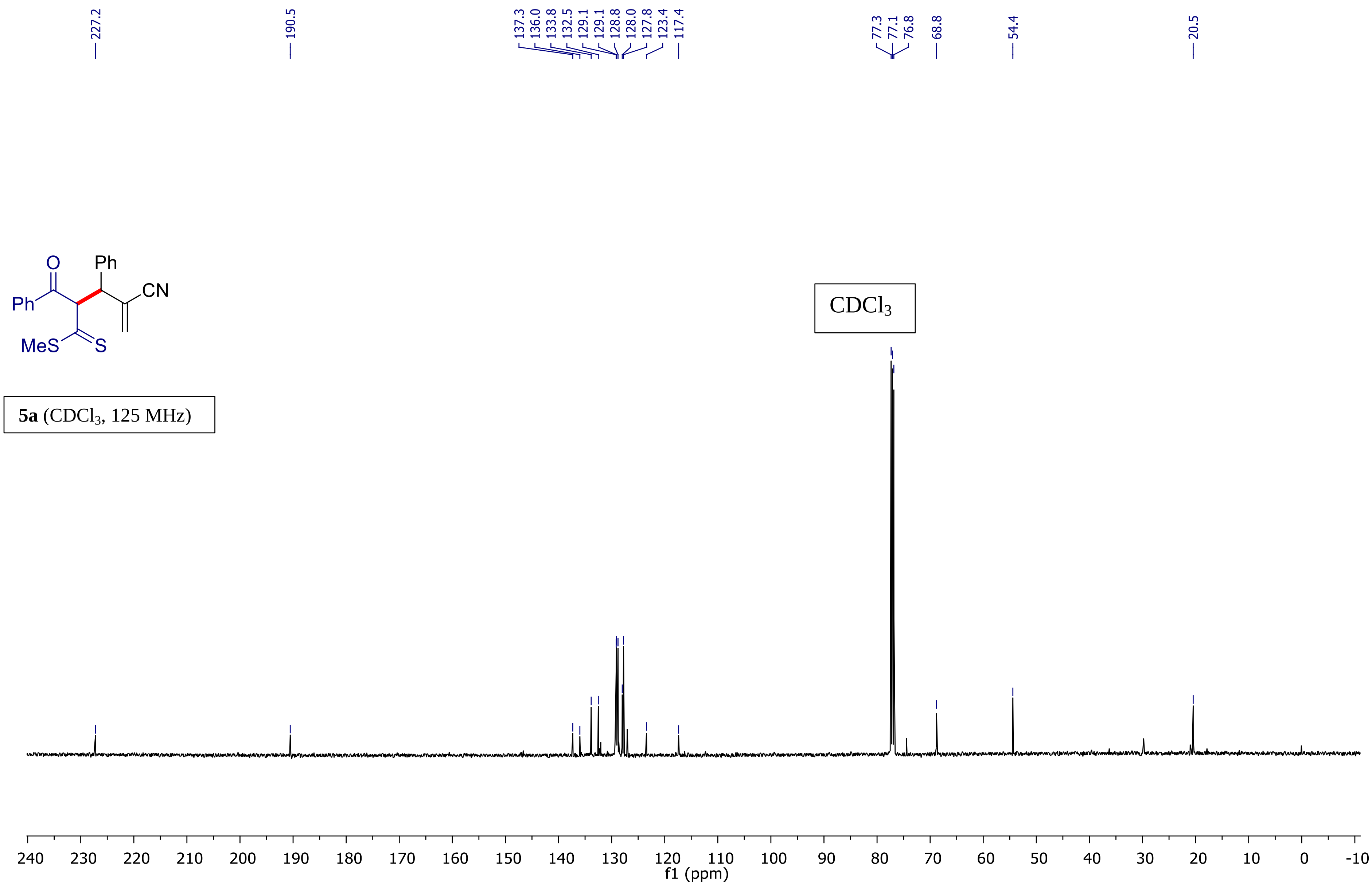
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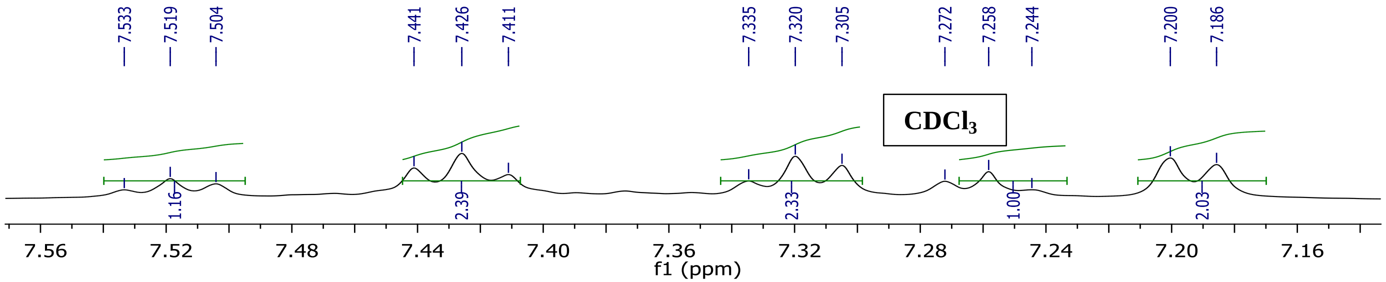
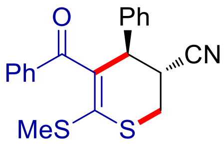
132.5
129.1
129.1
128.8
128.0
127.8
123.4
117.4
77.3
77.1
76.8
68.8
54.4
20.5
O
Ph
CN
Ph
MeS
S
CDCl3
5a (CDCl3, 125 MHz)
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

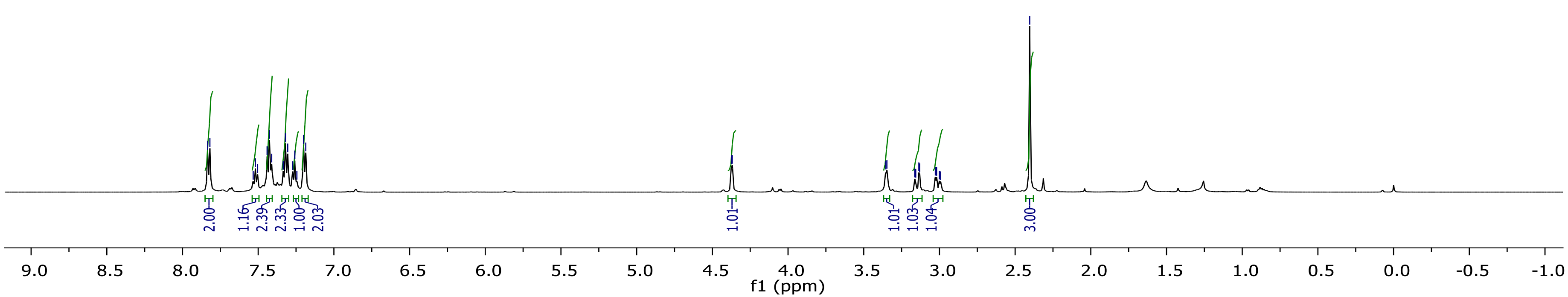
6.

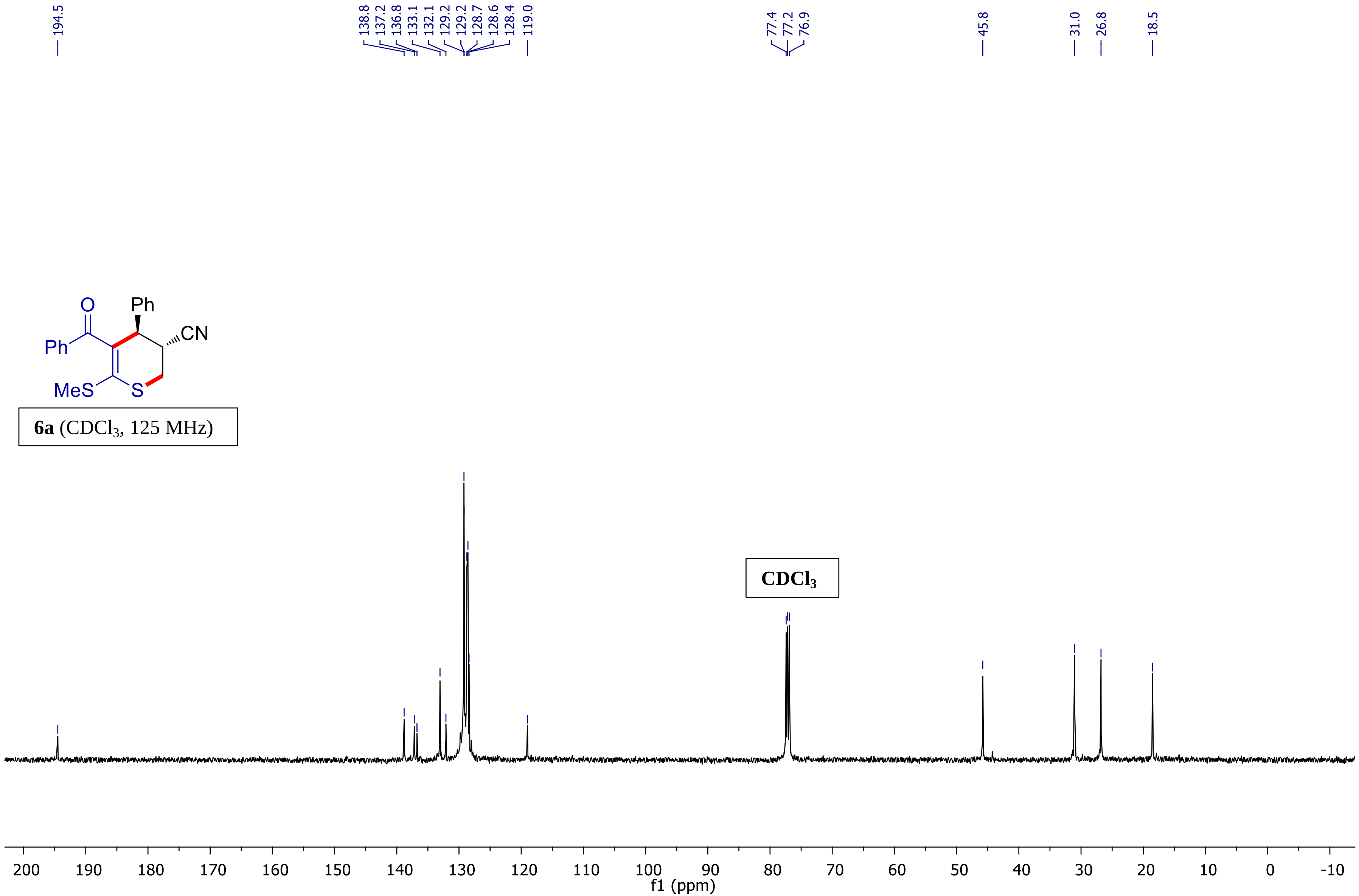
^{1}H (500 MHz, $CDCl_3$) and ^{13}C(^{1}H) (125 MHz, $CDCl_3$) NMR of Compound 6a





6a ($CDCl_3$, 500 MHz)

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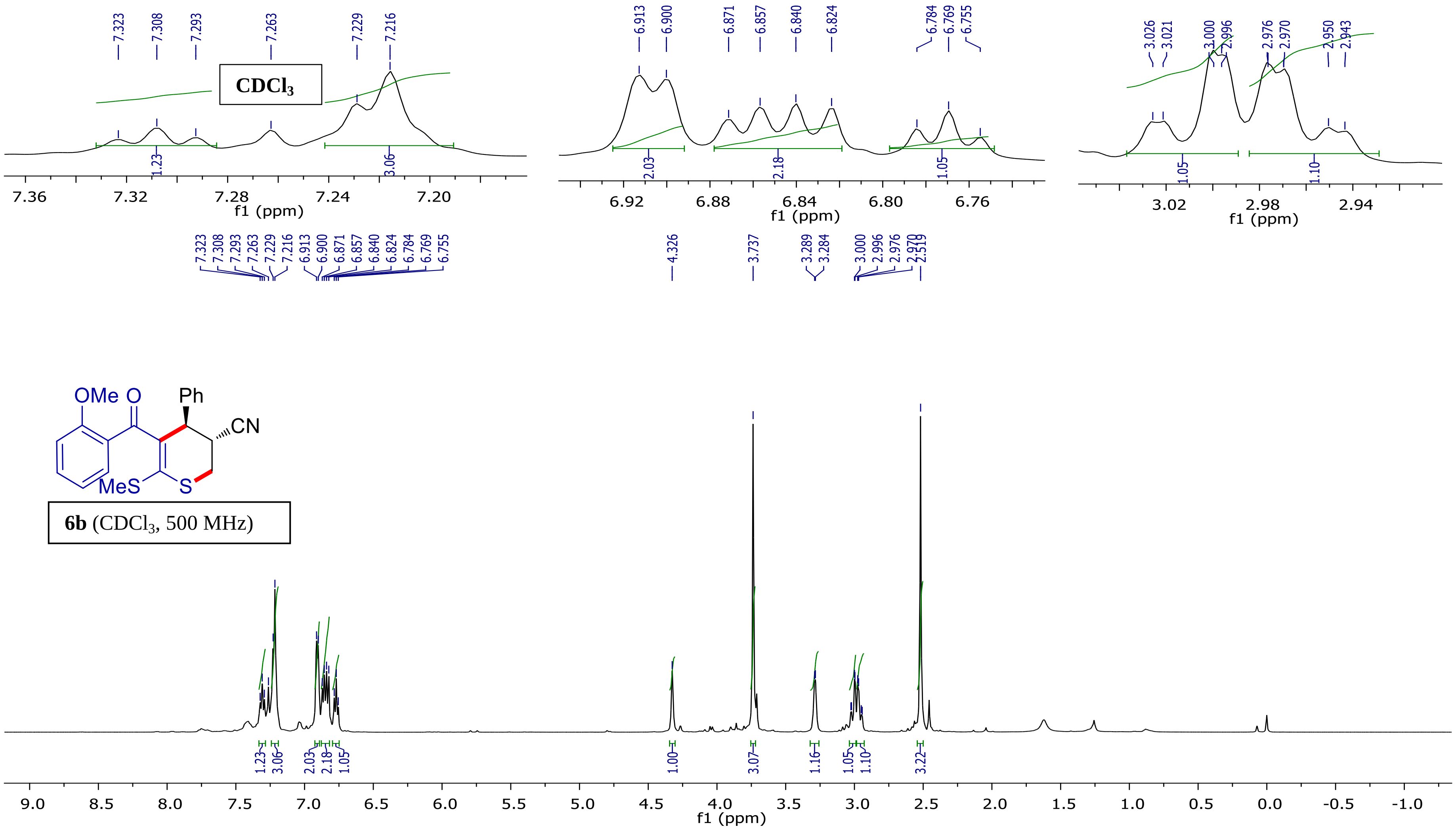
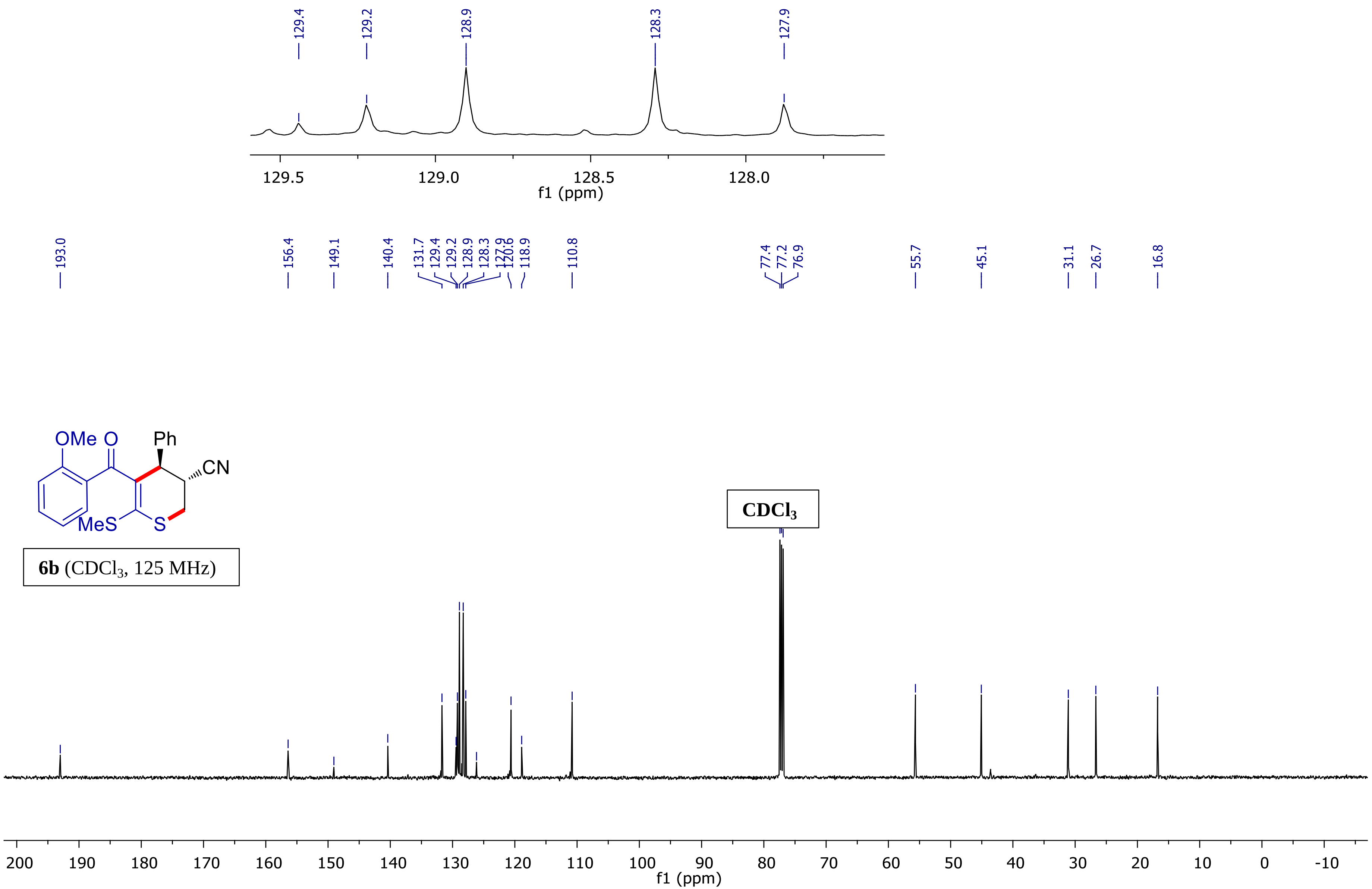
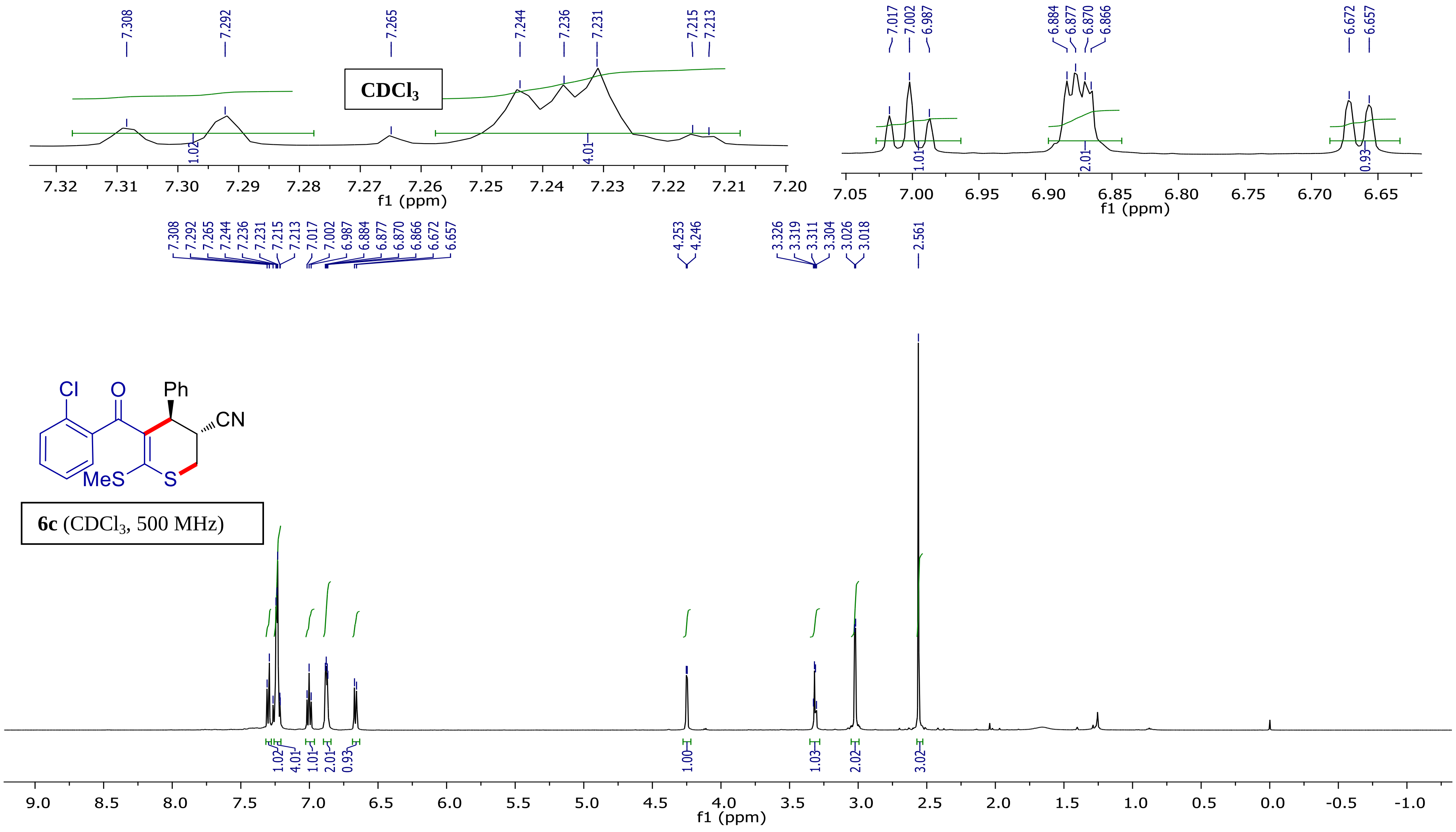
138.8
137.2
136.8
133.1
132.1
129.2
129.2
128.7
128.6
128.4
119.0
77.4
77.2
76.9
45.8
31.0
26.8
18.5
O
Ph
Ph
CN
MeS
S
6a (CDCl3, 125 MHz)
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

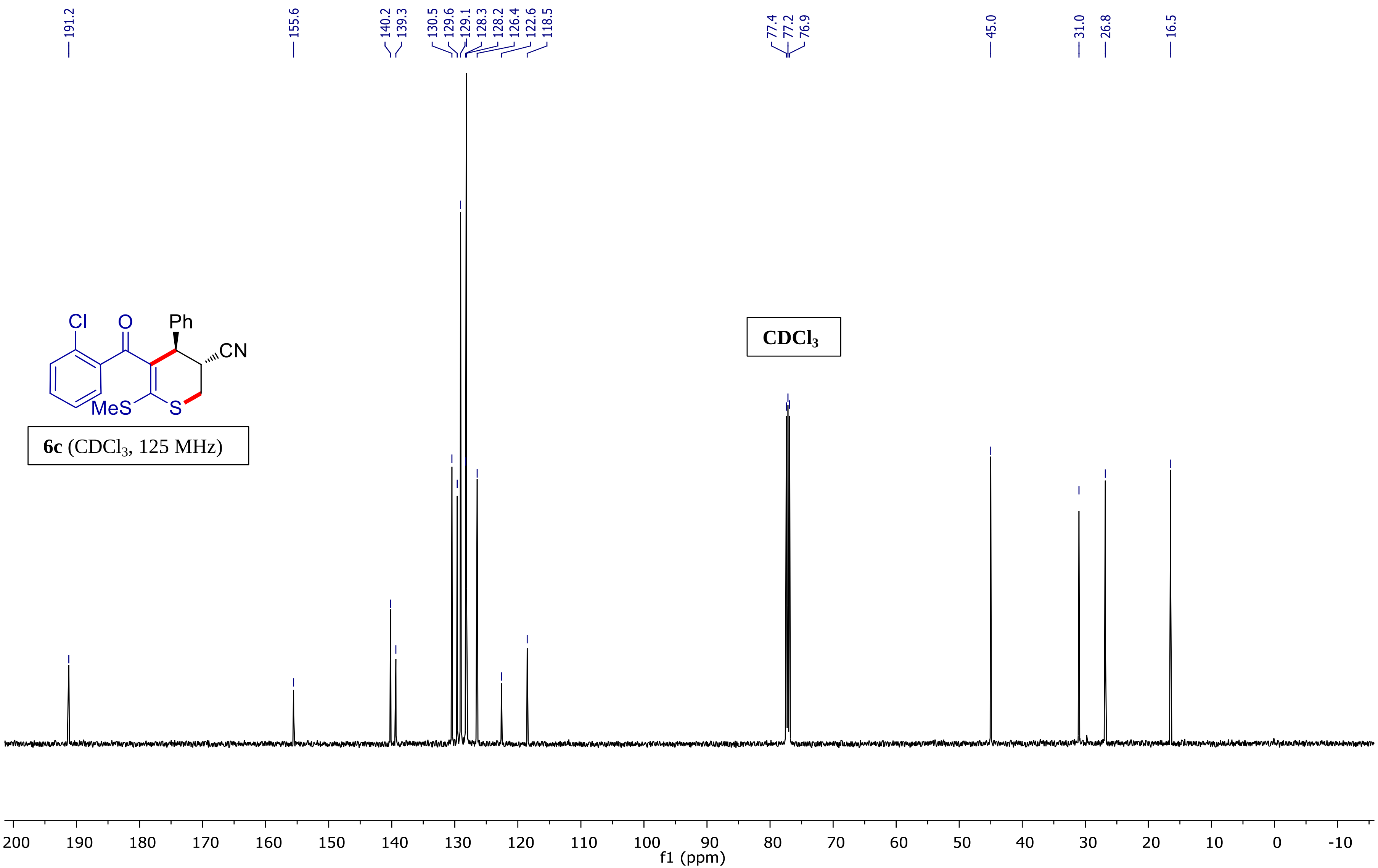
^{1}H (500 MHz, CDCl$_3$) and ^{13}C(^{1}H) (125 MHz, CDCl$_3$) NMR of Compound 6b




129.4
129.2
128.9
128.3
127.9
129.5
129.0
128.5
128.0
f1 (ppm)
193.0
156.4
149.1
140.4
131.7
129.4
129.2
128.9
128.3
127.9
126.6
118.9
110.8
77.4
77.2
76.9
55.7
45.1
31.1
26.7
16.8
OMe
O
Ph
CN
MeS
S
6b ($CDCl_3$, 125 MHz)
$CDCl_3$
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

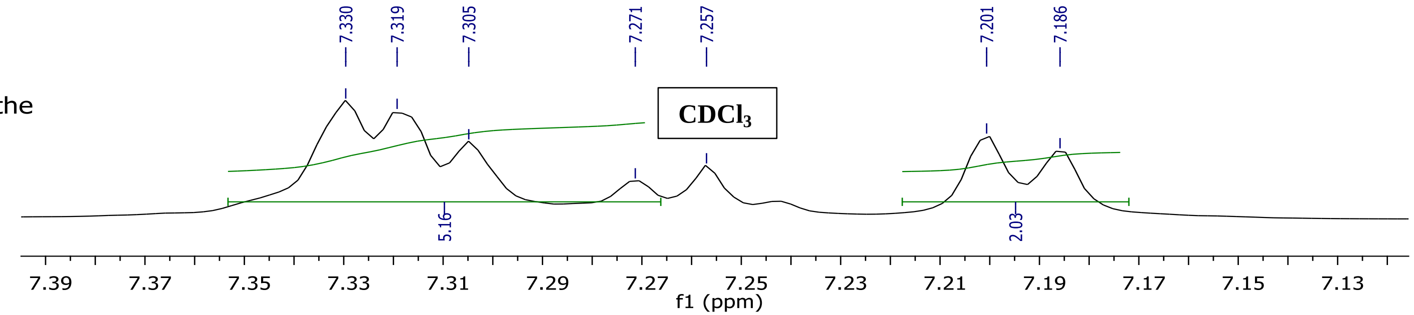
^{1}H (500 MHz, CDCl$_3$) and ^{13}C(^{1}H) (125 MHz, CDCl$_3$) NMR of Compound 6c

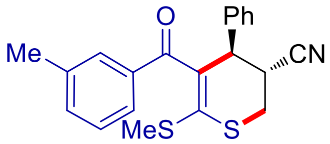



191.2
155.6
140.2
139.3
130.5
129.6
129.1
128.3
128.2
126.4
122.6
118.5
77.4
77.2
76.9
45.0
31.0
26.8
16.5
Cl
O
Ph
CN
MeS
S
6c (CDCl3, 125 MHz)
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

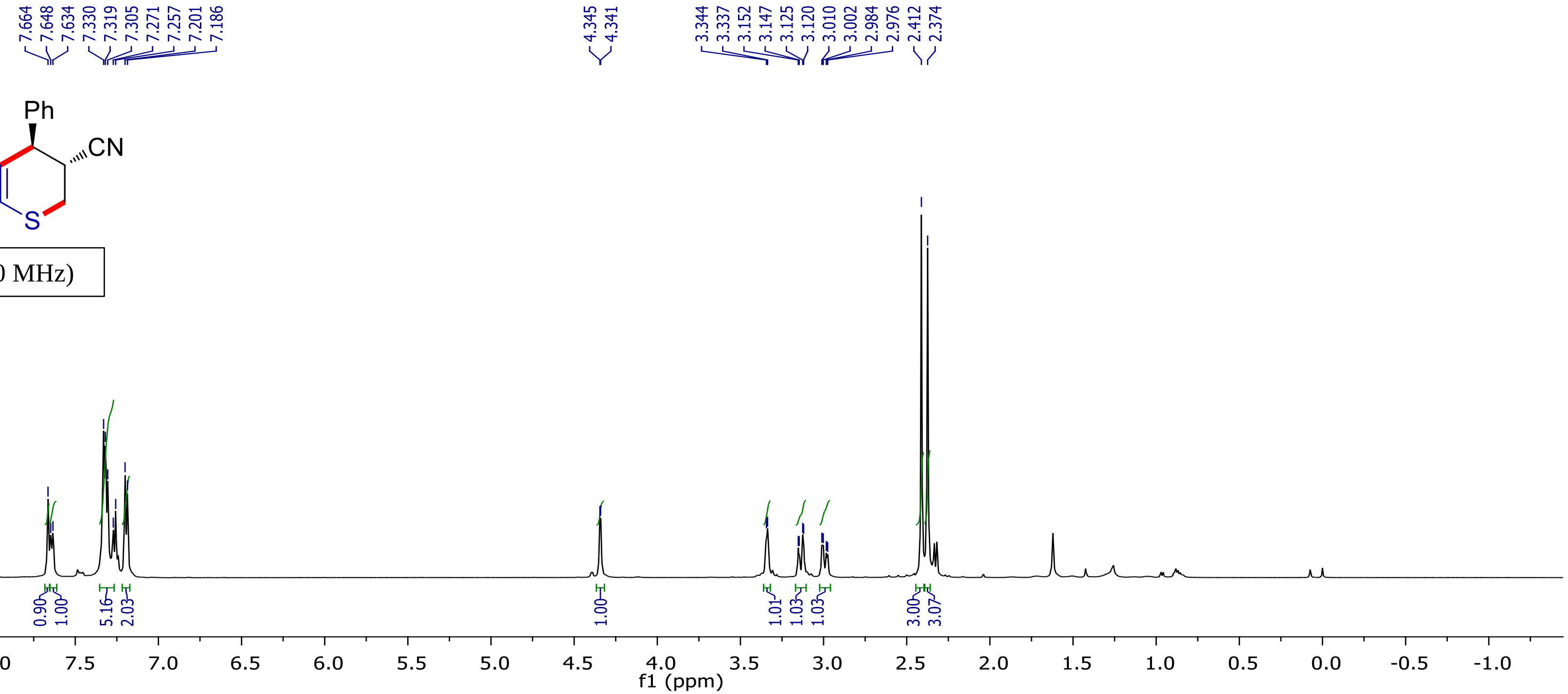
[1]H (500 MHz, CDCl$_3$) and [13]C([1]H) (125 MHz, CDCl$_3$) NMR of Compound 6d

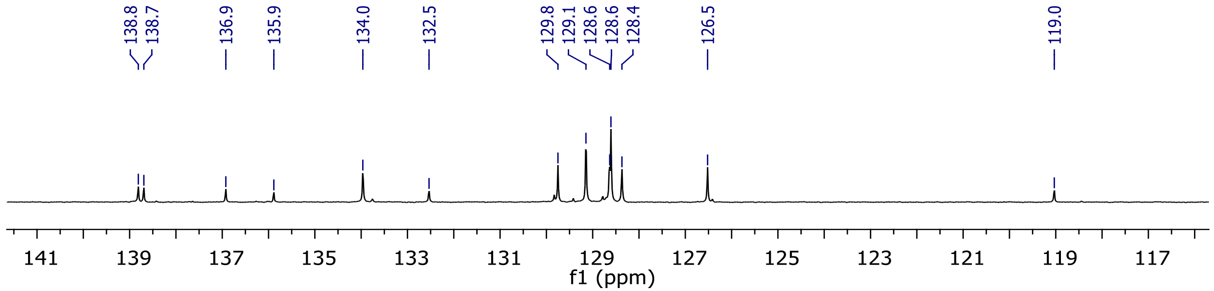
The trace amount of impurity is the inseparable diastereomer.

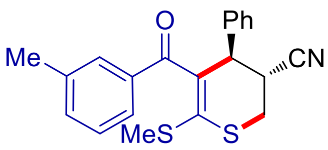




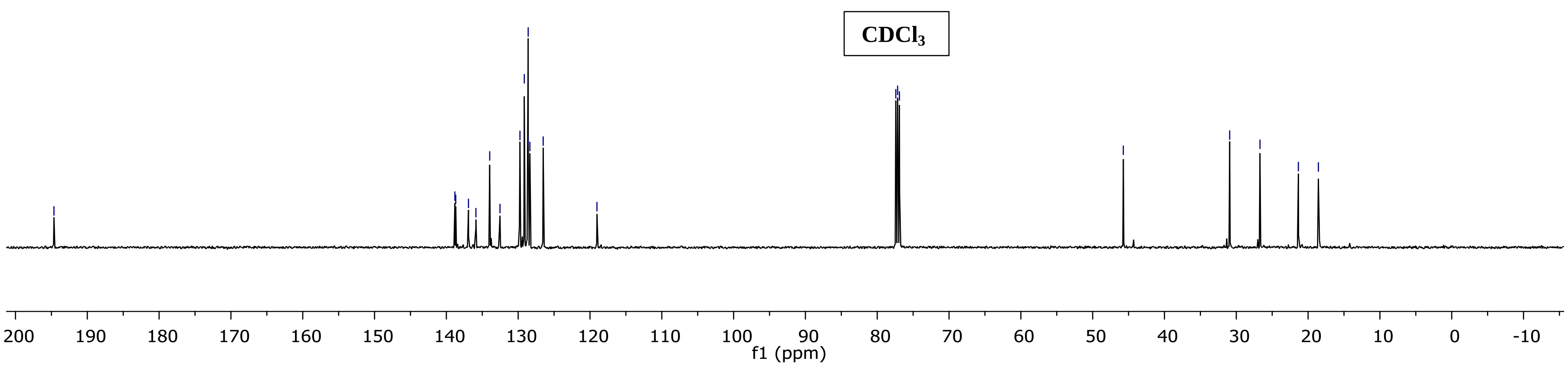
6d (CDCl$_3$, 500 MHz)



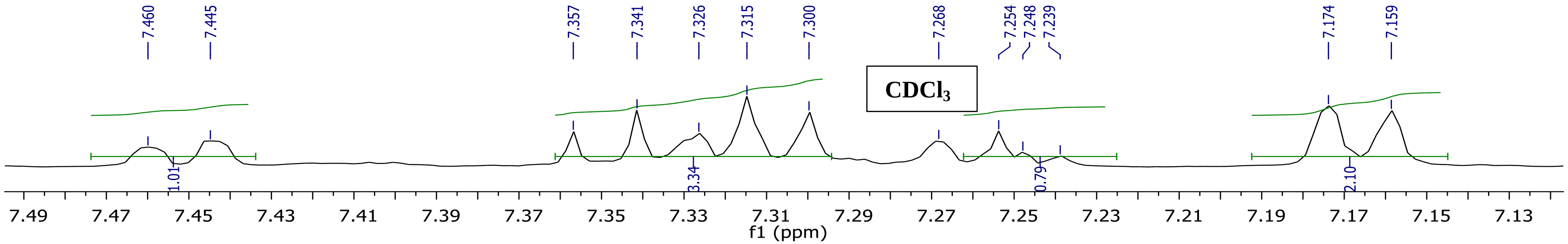


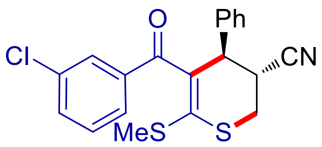


6d ($CDCl_3$, 125 MHz)

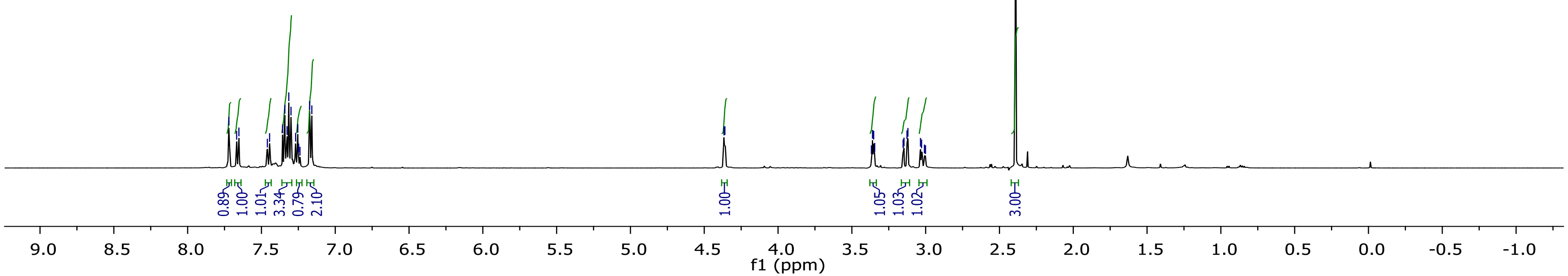


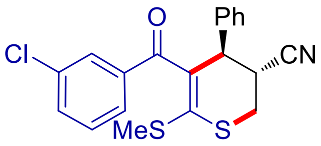
^{1}H (500 MHz, $CDCl_3$) and ^{13}C(^{1}H) (125 MHz, $CDCl_3$) NMR of Compound 6e



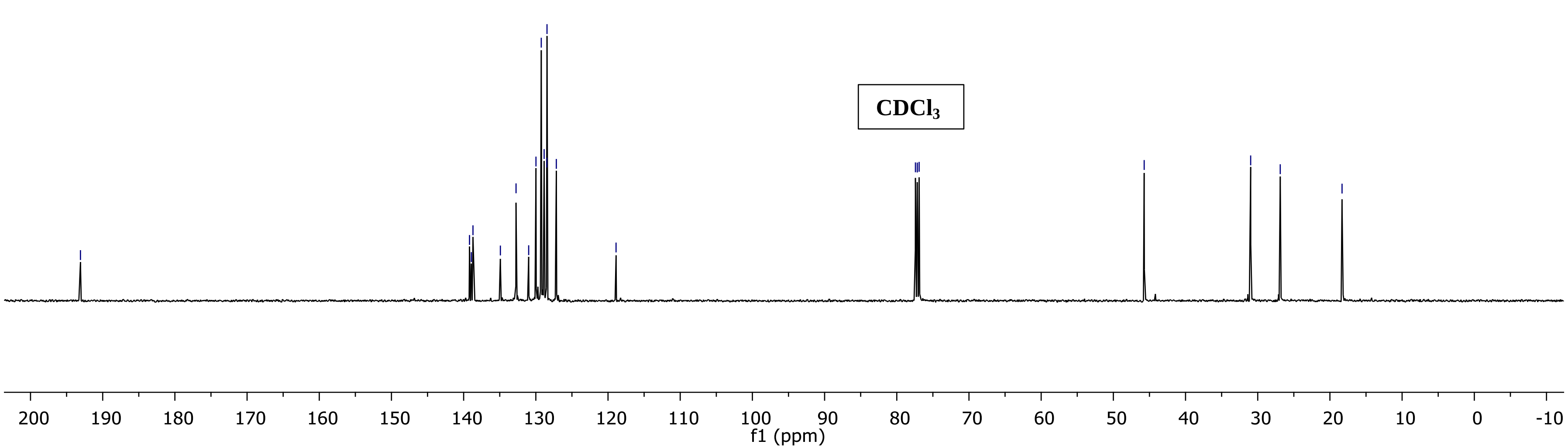


6e ($CDCl_3$, 500 MHz)

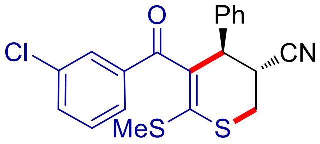




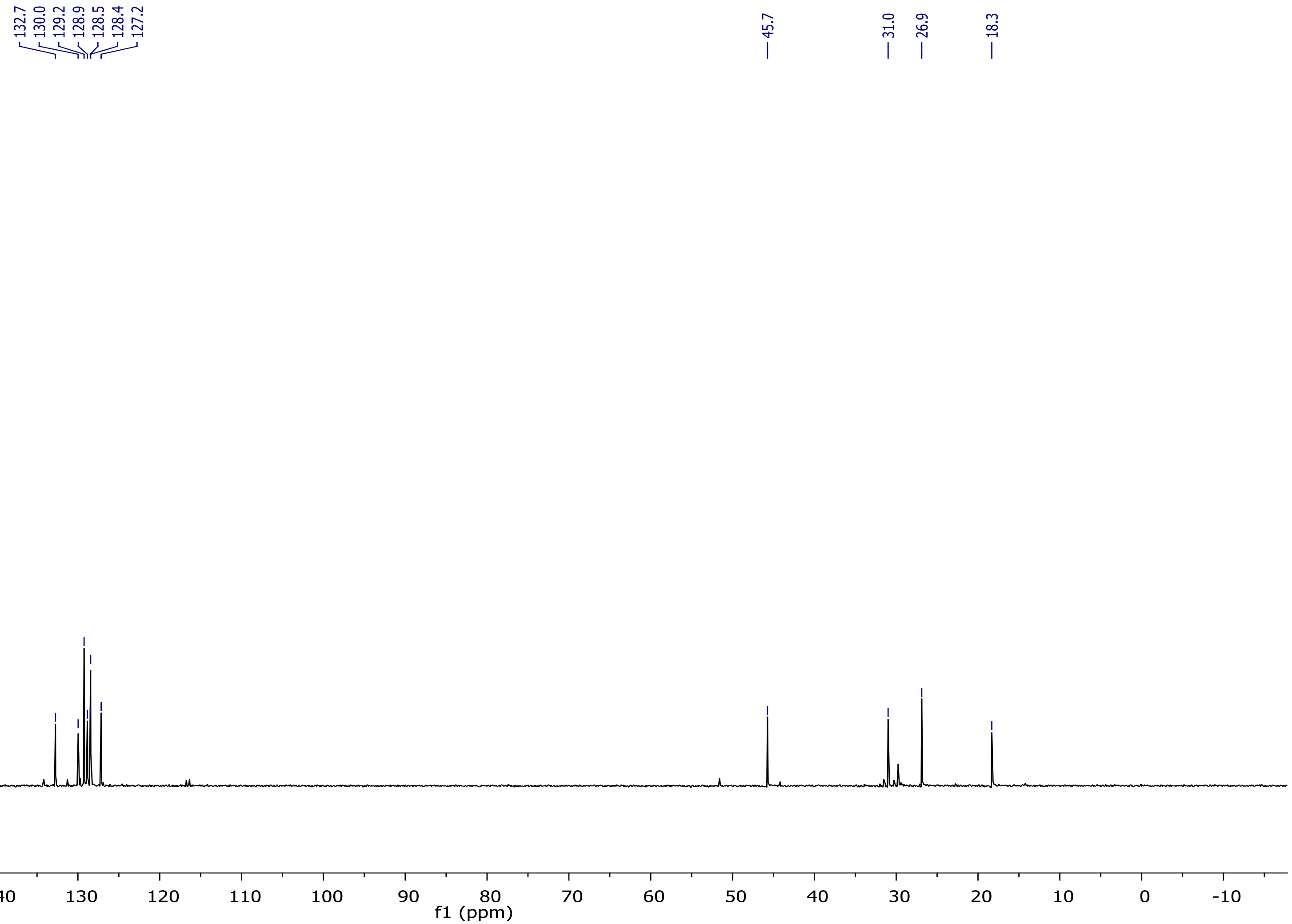
6e ($CDCl_3$, 125 MHz)



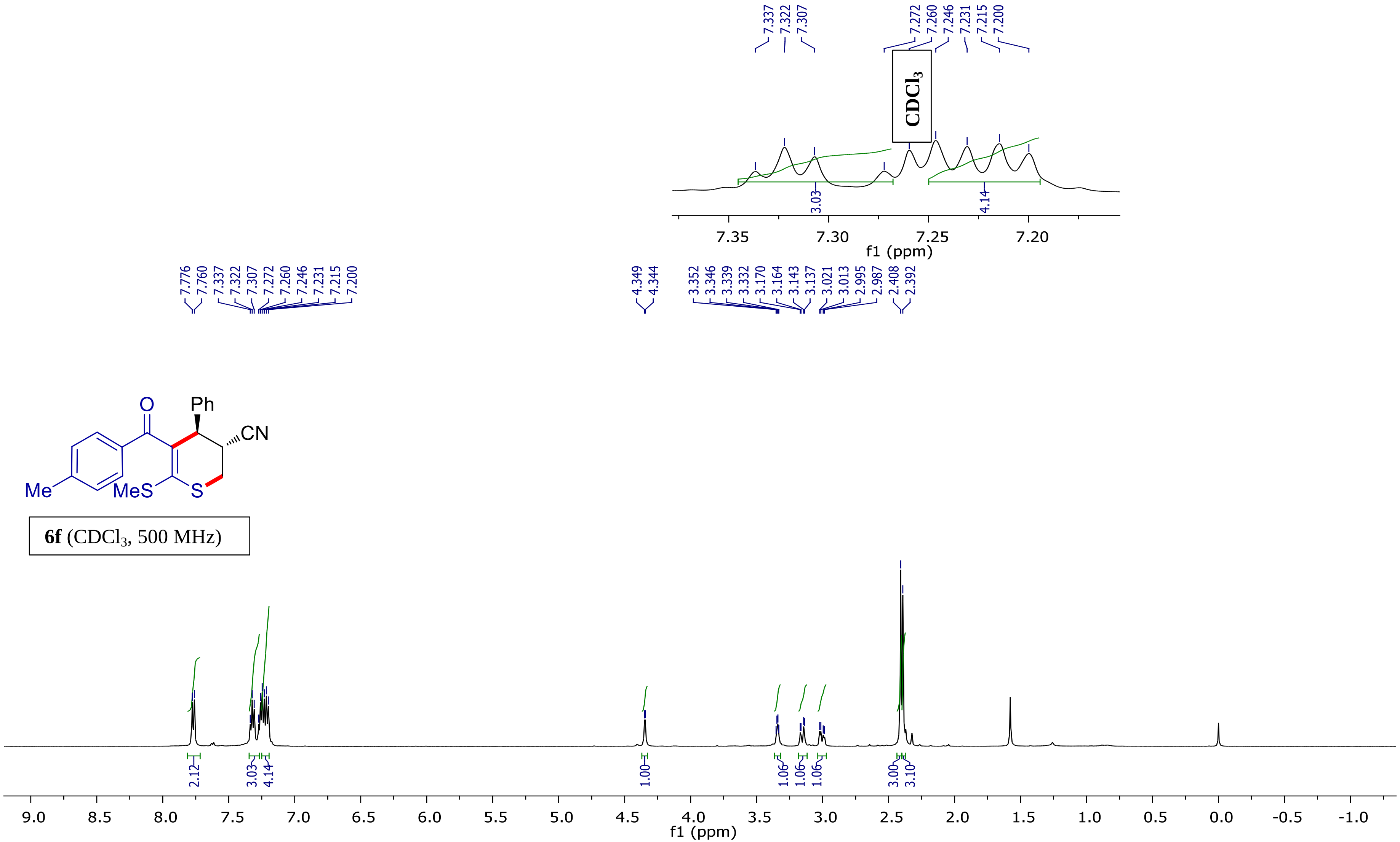
DEPT-45 NMR of Compound 6e

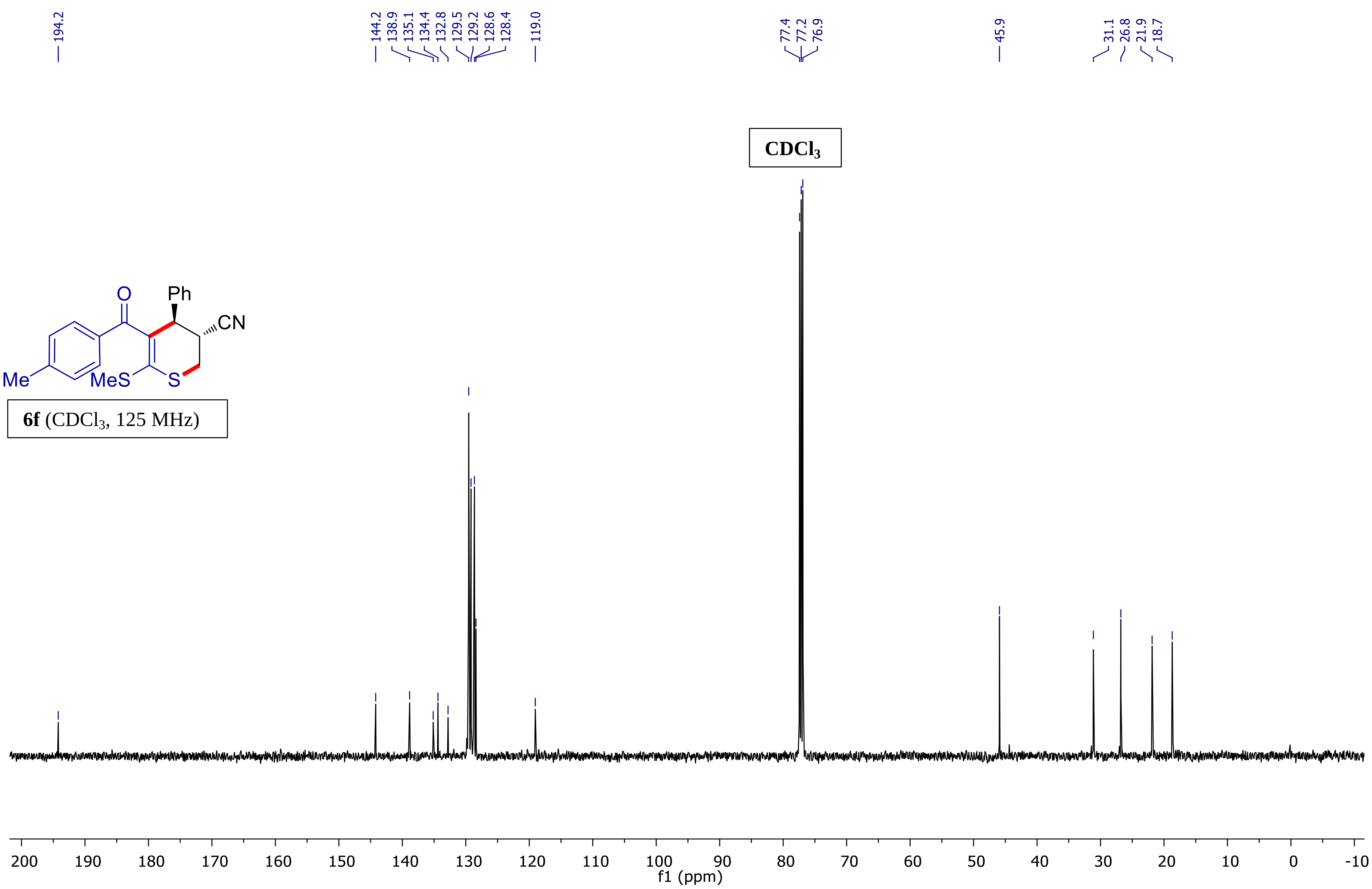


6e DEPT-45 ($CDCl_3$, 125 MHz)



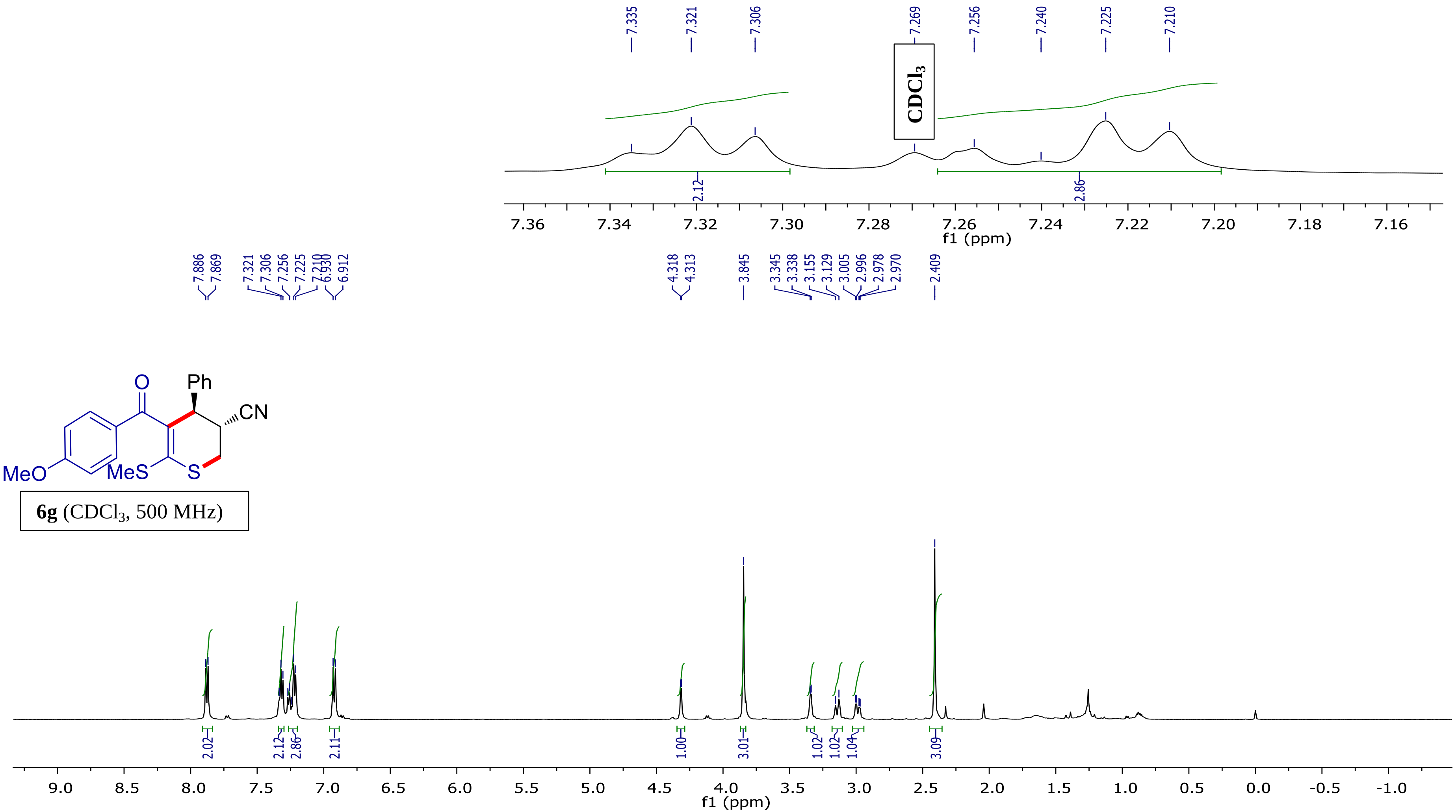
[1]H (500 MHz, CDCl$_3$) and [13]C([1]H) (125 MHz, CDCl$_3$) NMR of Compound 6f

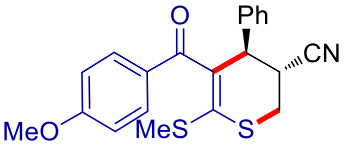




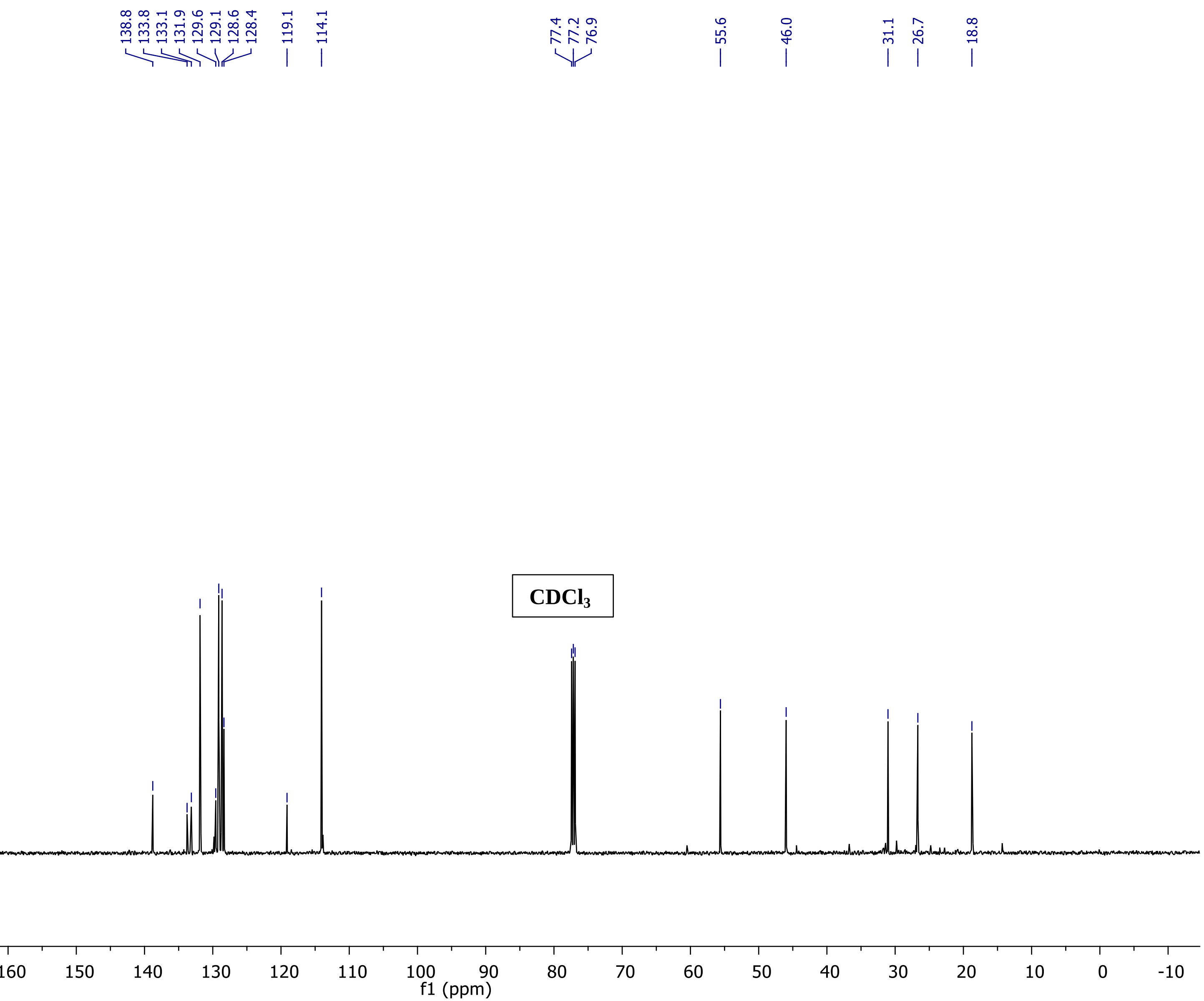
194.2
144.2
138.9
135.1
134.4
132.8
129.5
129.2
128.6
128.4
119.0
77.4
77.2
76.9
45.9
31.1
26.8
21.9
18.7
CDCl3
O
Ph
CN
Me
MeS
S
6f (CDCl3, 125 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

^{1}H (500 MHz, CDCl$_3$) and ^{13}C(^{1}H) (125 MHz, CDCl$_3$) NMR of Compound 6g

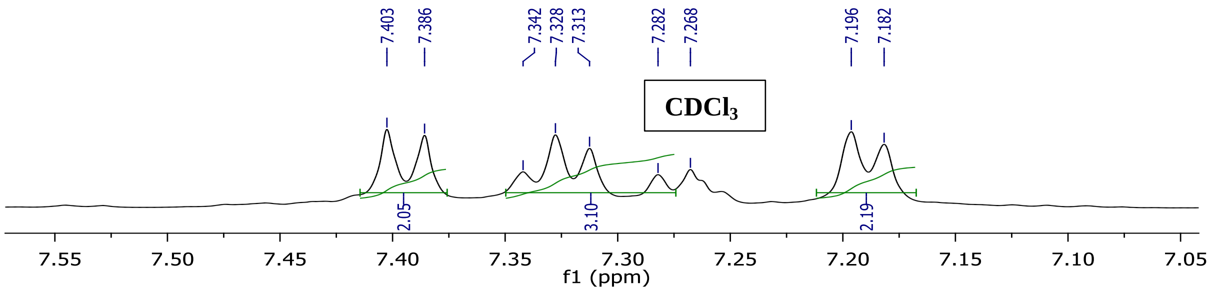


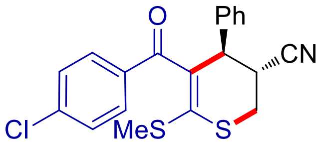


6g ($CDCl_3$, 125 MHz)

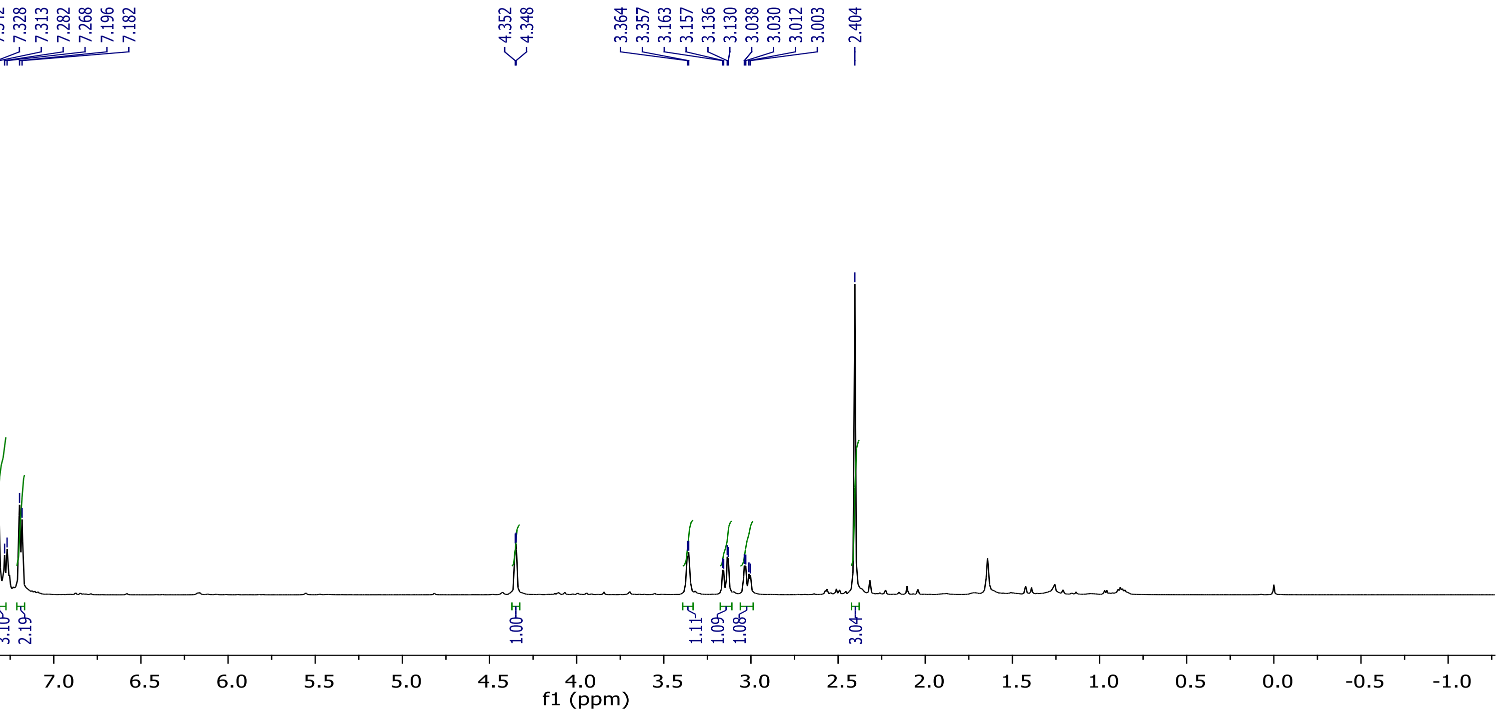


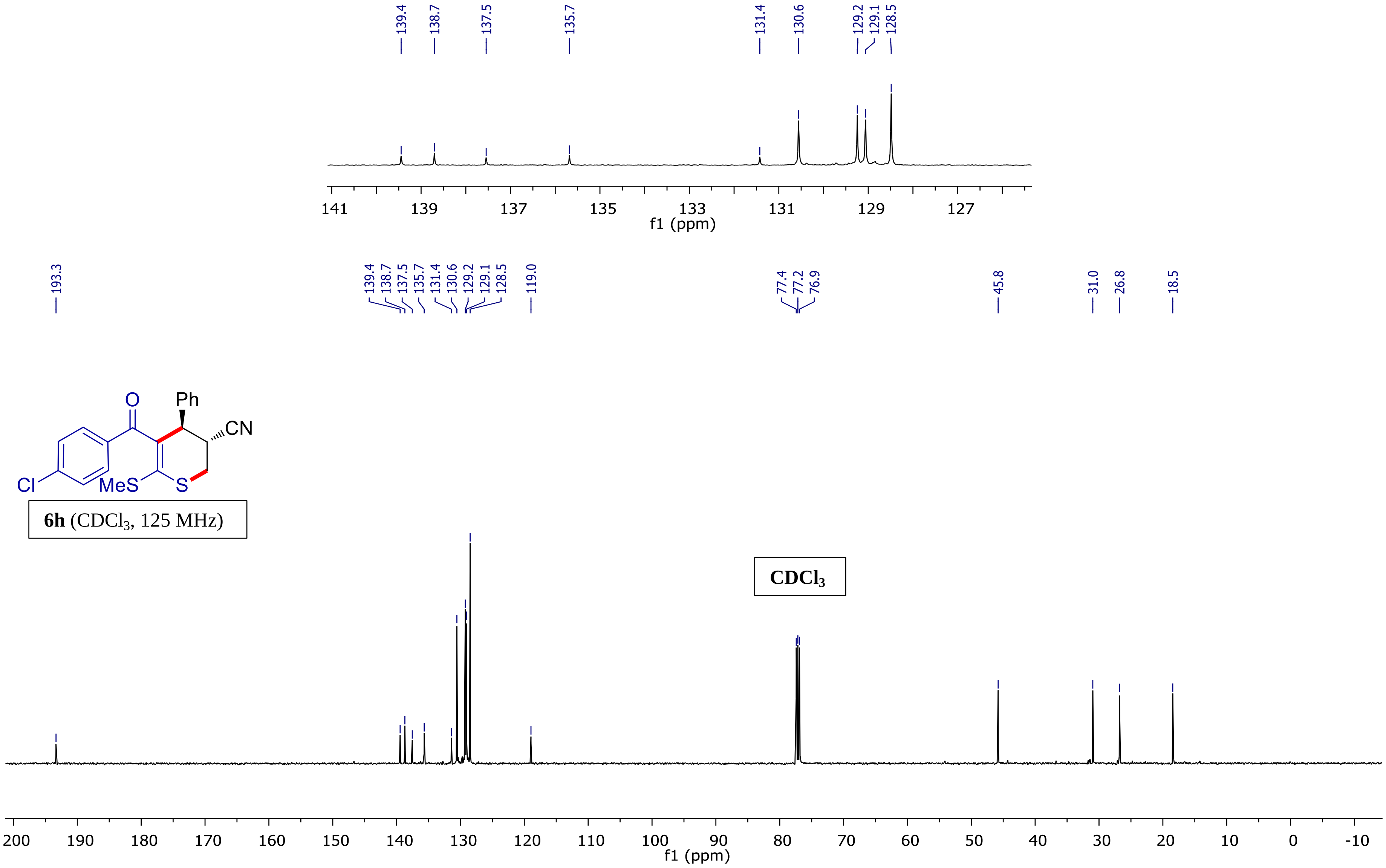
^{1}H (500 MHz, CDCl$_3$) and ^{13}C(^{1}H) (125 MHz, CDCl$_3$) NMR of Compound 6h



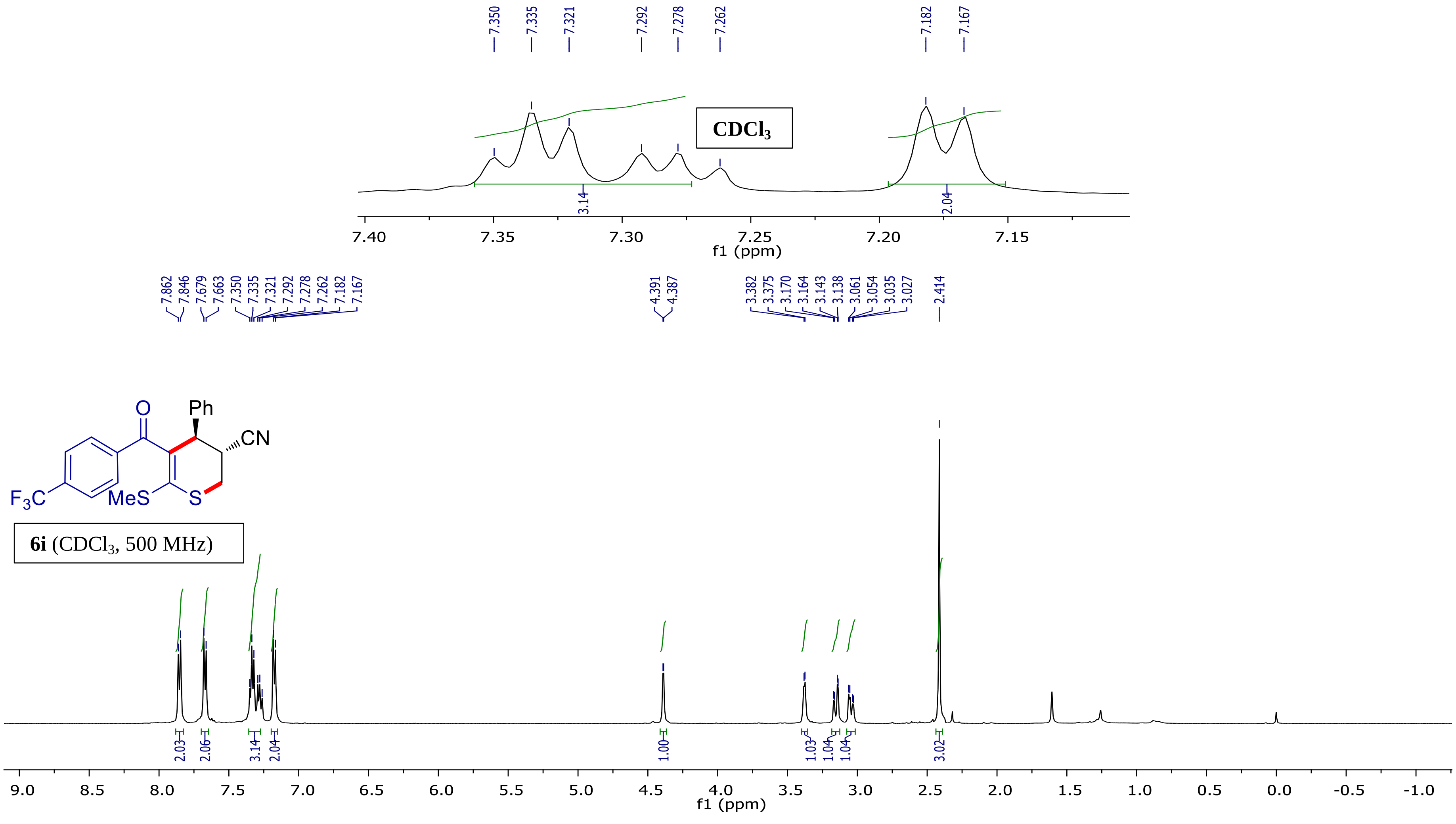


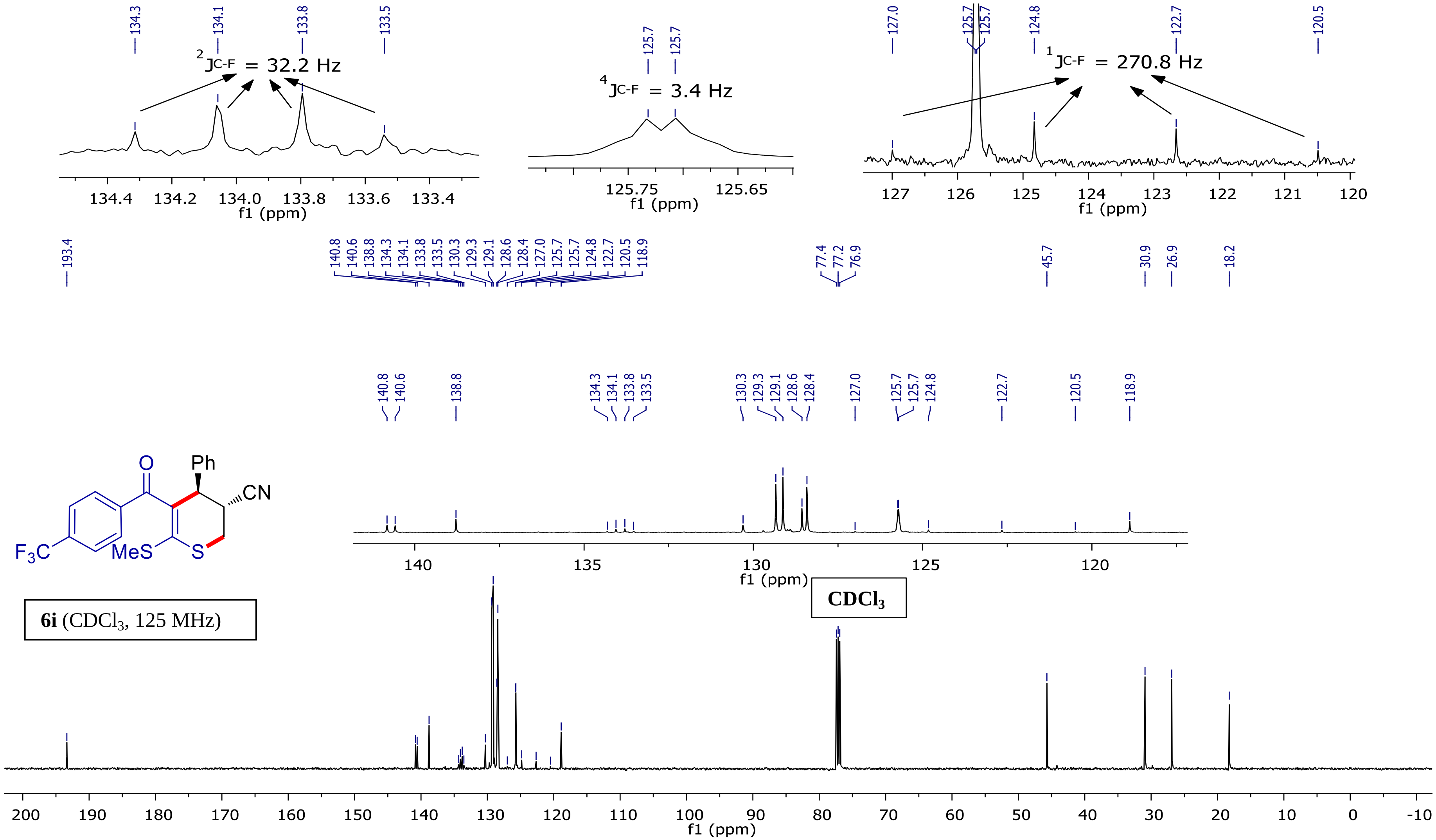
6h (CDCl$_3$, 500 MHz)




139.4
138.7
137.5
135.7
131.4
130.6
129.2
129.1
128.5
141
139
137
135
133
131
129
127
f1 (ppm)
193.3
119.0
77.4
77.2
76.9
45.8
31.0
26.8
18.5
O
Ph
CN
Cl
MeS
S
6h (CDCl3, 125 MHz)
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

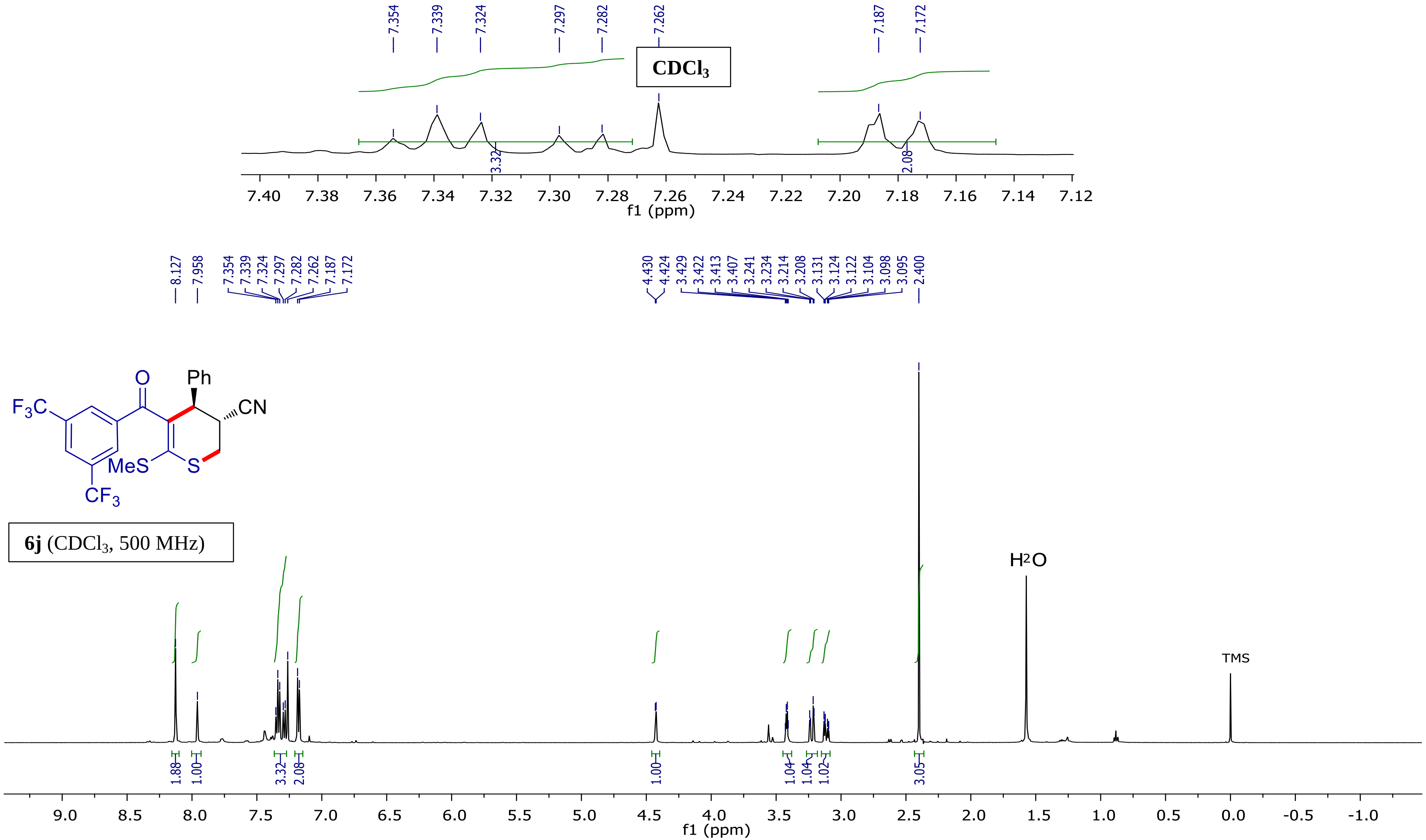
<u>^{1}H (500 MHz, CDCl$_3$) and ^{13}C(^{1}H) (125 MHz, CDCl$_3$) NMR of Compound 6i</u>

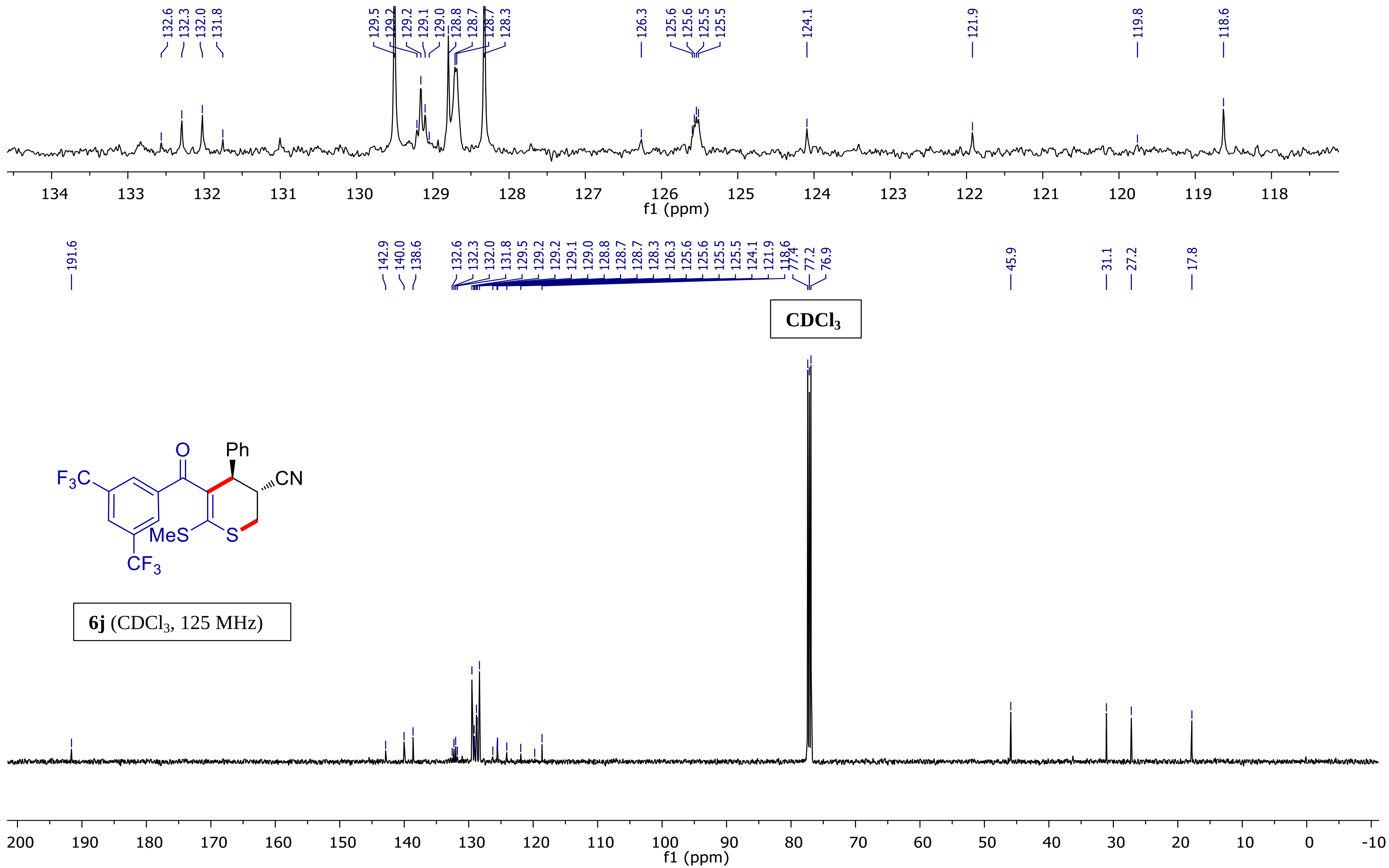




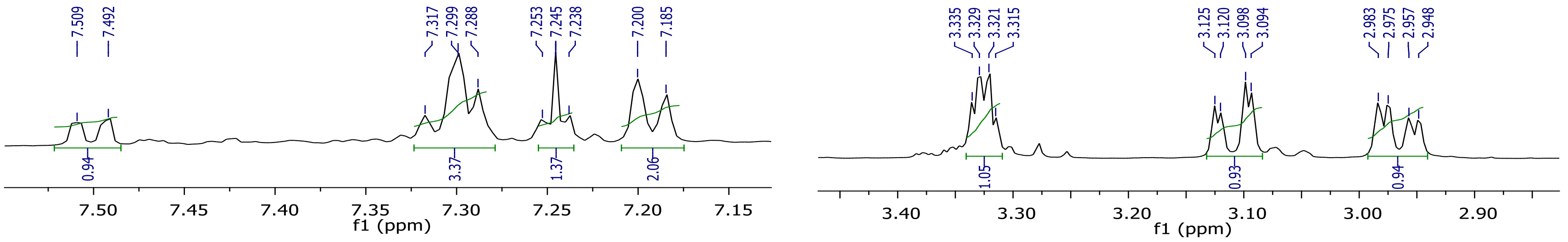
2JC-F = 32.2 Hz
4JC-F = 3.4 Hz
1JC-F = 270.8 Hz
f1 (ppm)
Ph
O
CN
F3C
MeS
S
6i (CDCl3, 125 MHz)
CDCl3

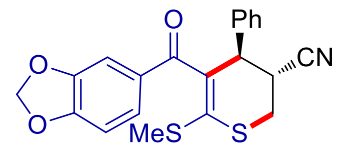
^{1}H (500 MHz, $CDCl_3$) and $^{13}C(^1H)$ (125 MHz, $CDCl_3$) NMR of Compound 6j



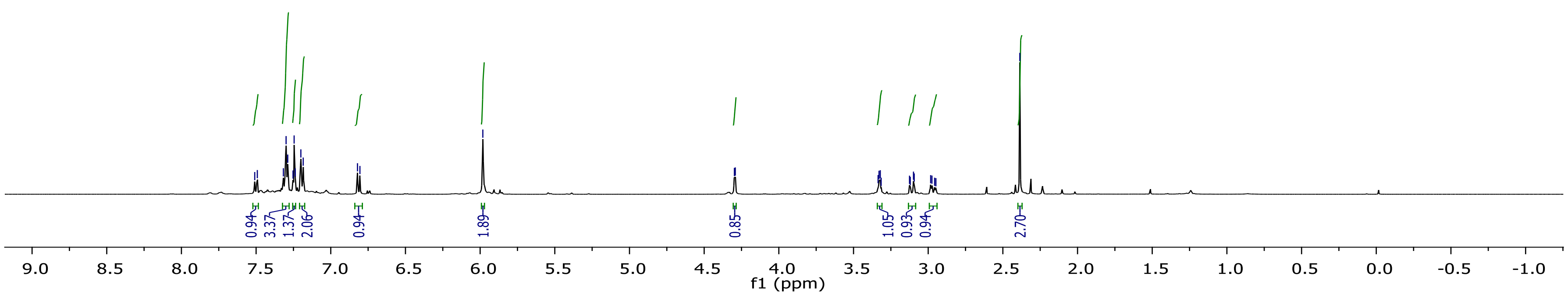

132.6
132.3
132.0
131.8
129.5
129.2
129.2
129.1
129.0
128.8
128.7
128.7
128.3
126.3
125.6
125.6
125.5
125.5
124.1
121.9
119.8
118.6
134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
191.6
142.9
140.0
138.6
132.6
132.3
132.0
131.8
129.5
129.2
129.2
129.1
129.0
128.8
128.7
128.7
128.3
126.3
125.6
125.6
125.5
125.5
124.1
121.9
118.6
77.4
77.2
76.9
45.9
31.1
27.2
17.8
CDCl3
O
Ph
F3C
CN
MeS
S
CF3
6j (CDCl3, 125 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

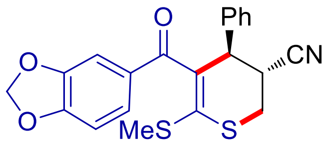
[1]H (500 MHz, $CDCl_3$) and [13]C([1]H) (125 MHz, $CDCl_3$) NMR of Compound 6k



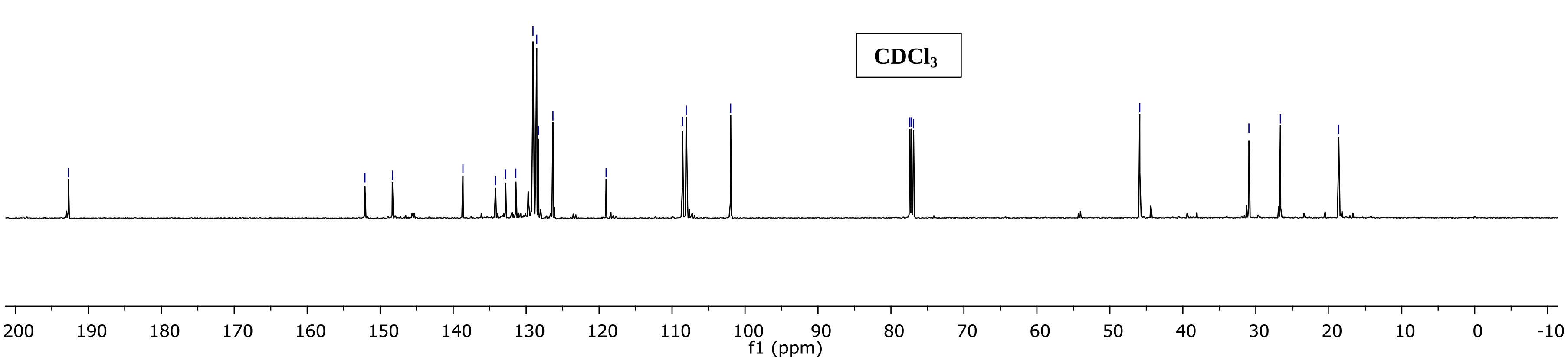


6k ($CDCl_3$, 500 MHz)

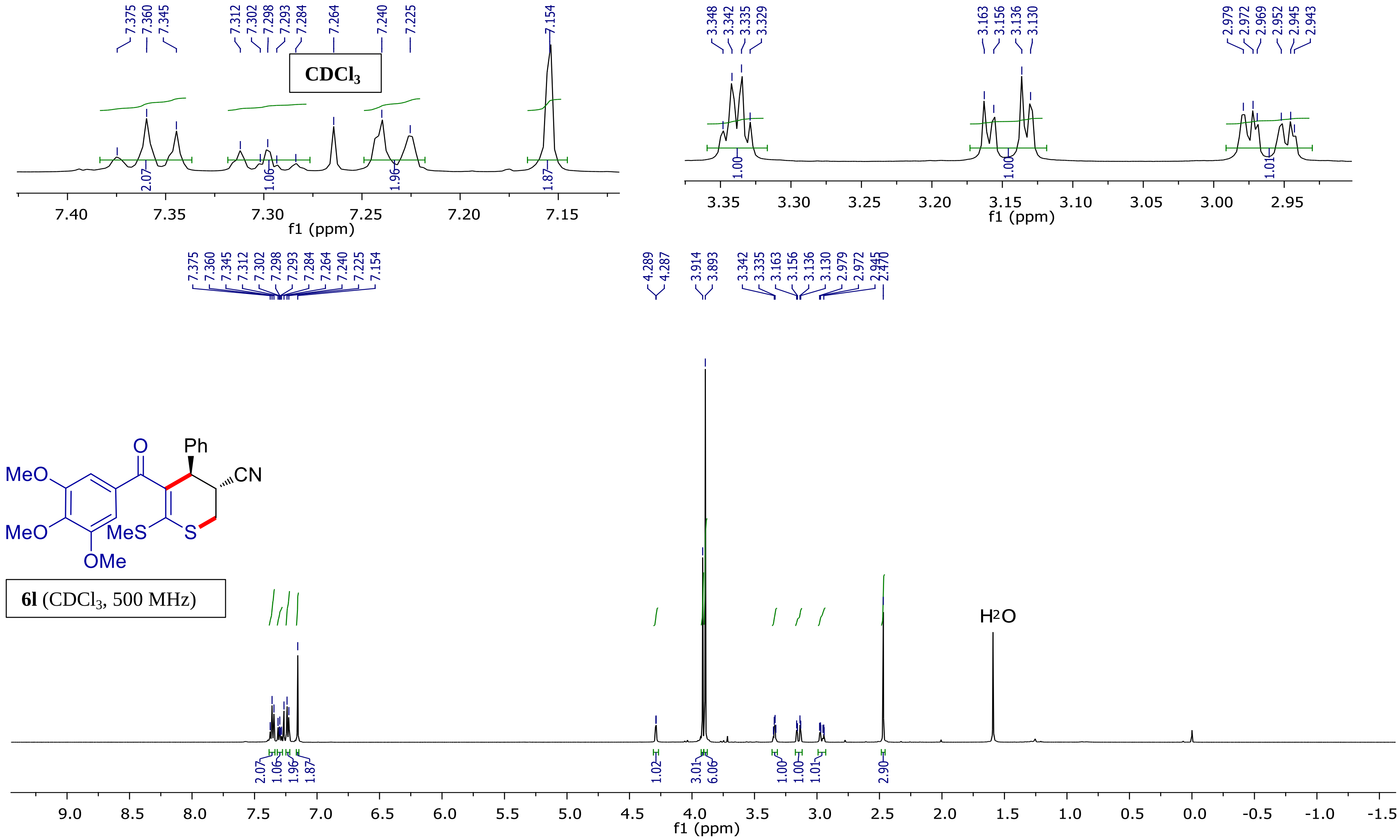


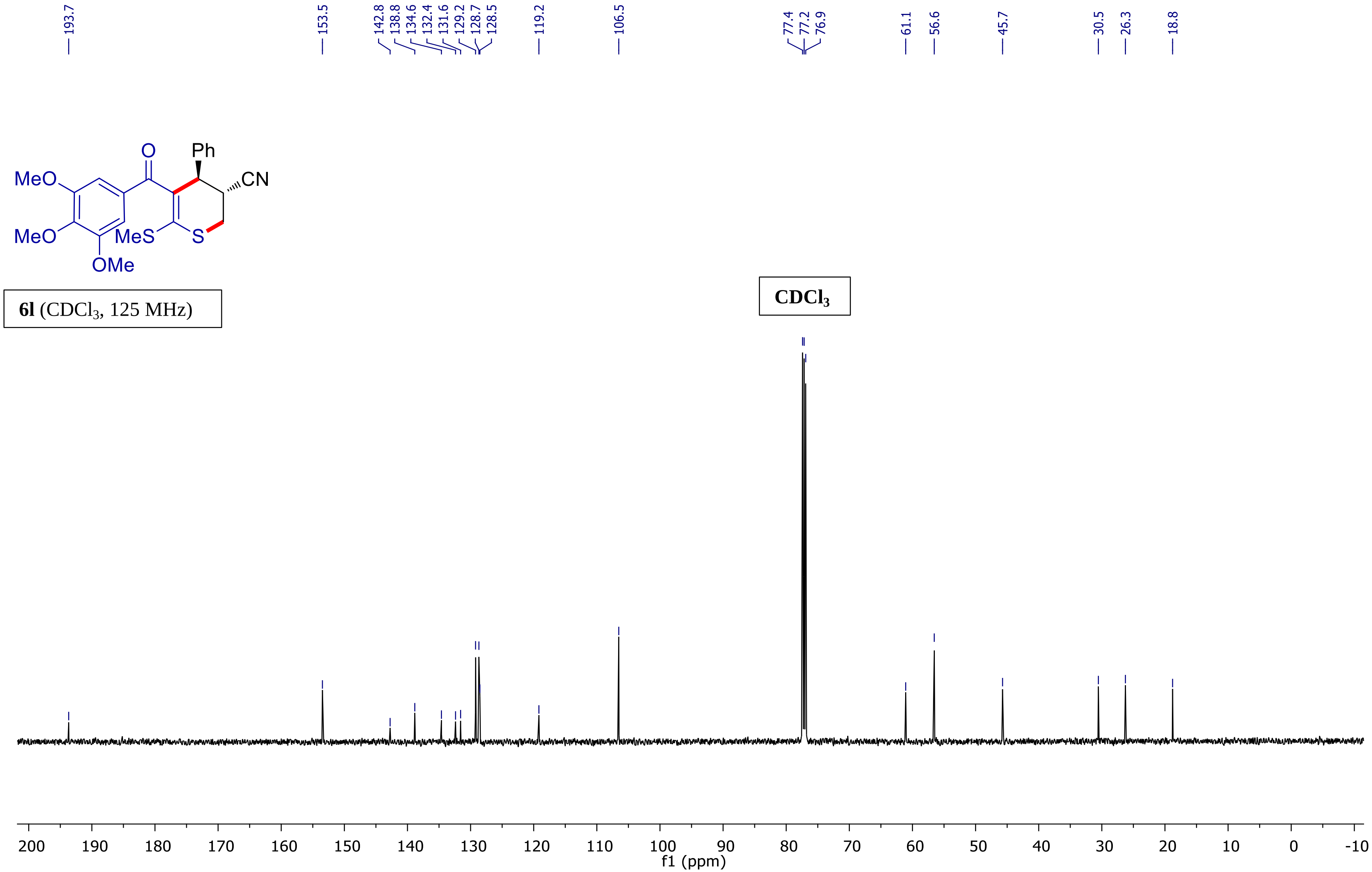


6k ($CDCl_3$, 125 MHz)

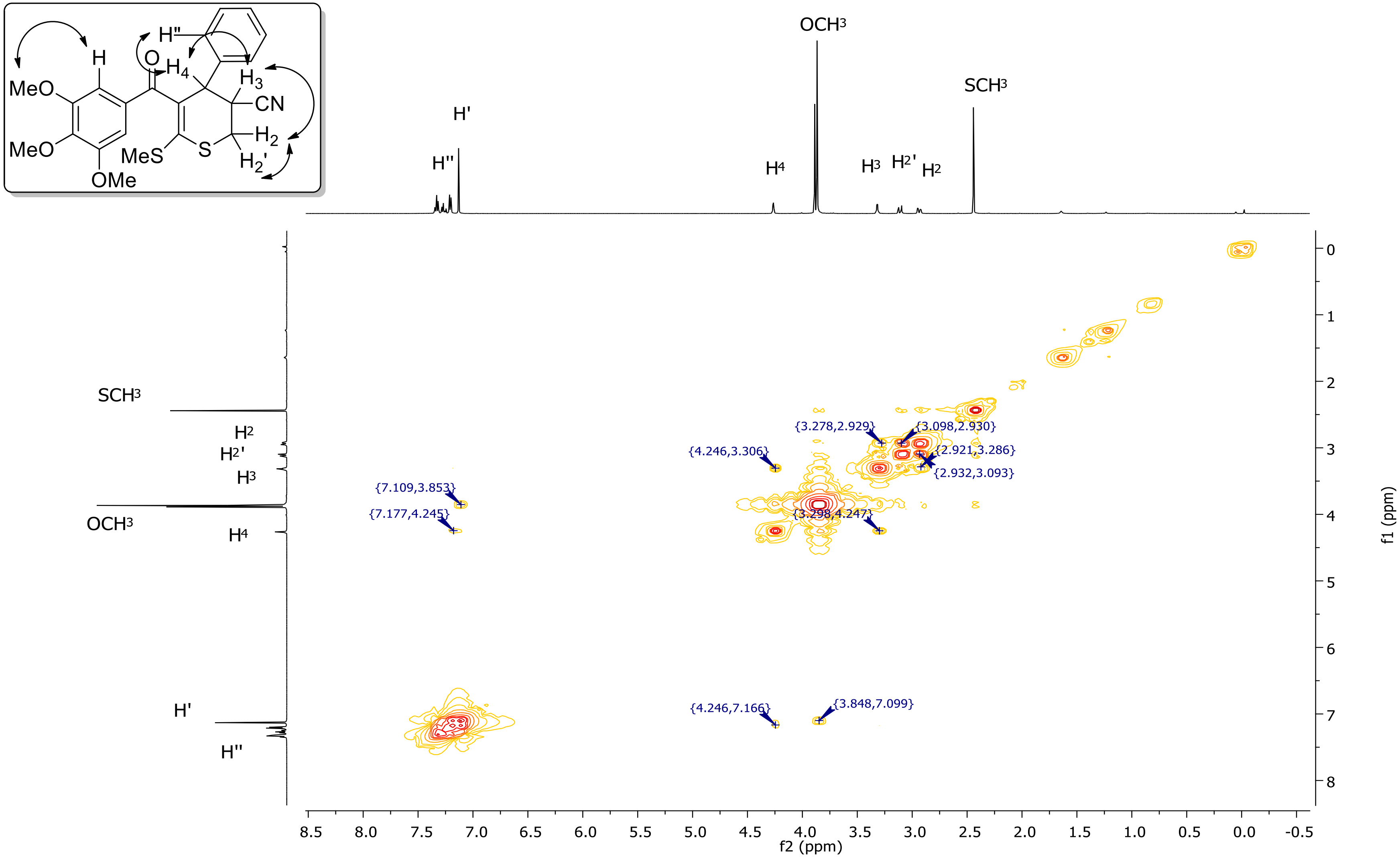


[1]H (500 MHz, $CDCl_3$) and [13]C([1]H) (125 MHz, $CDCl_3$) NMR of Compound 6l

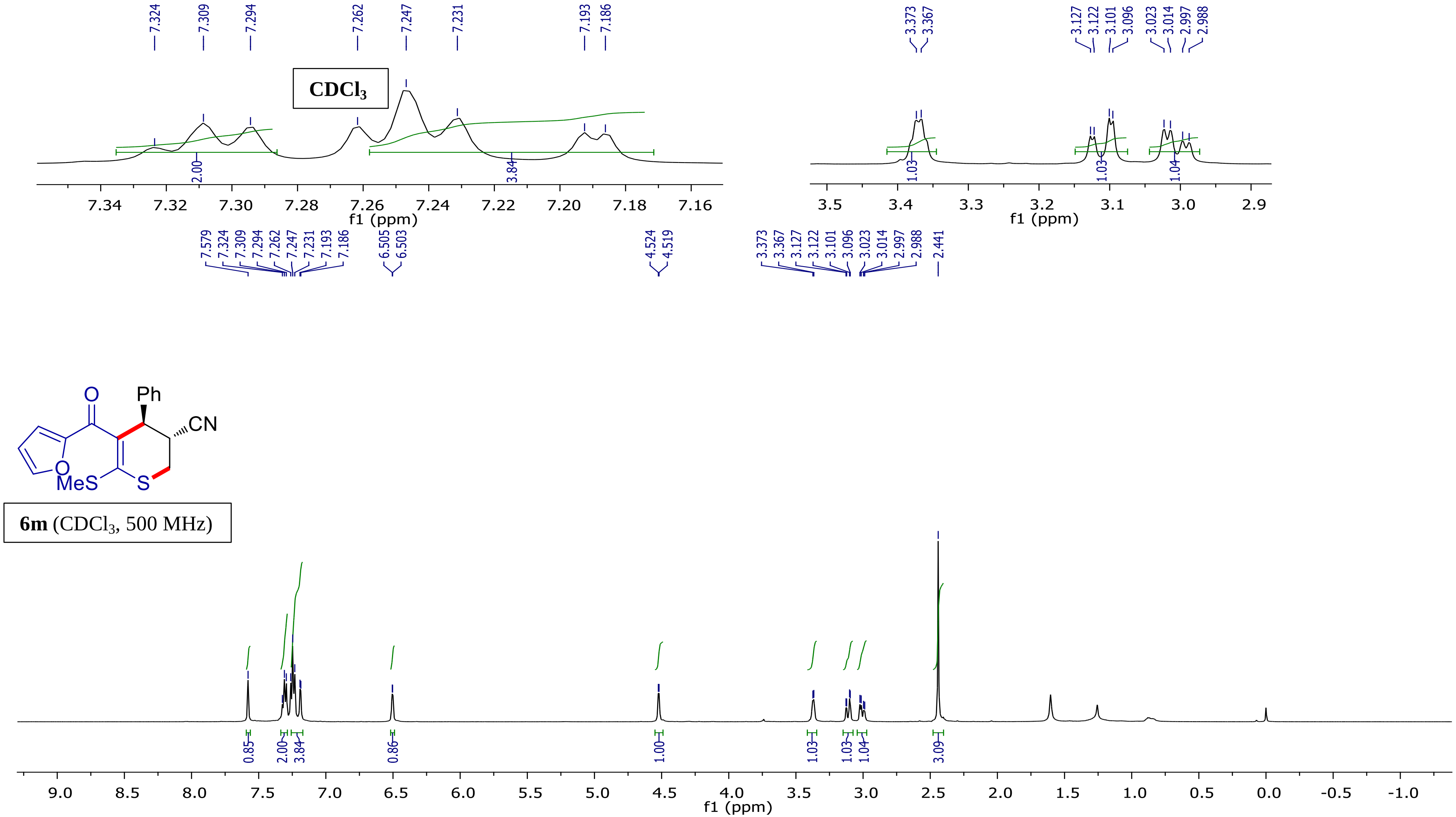


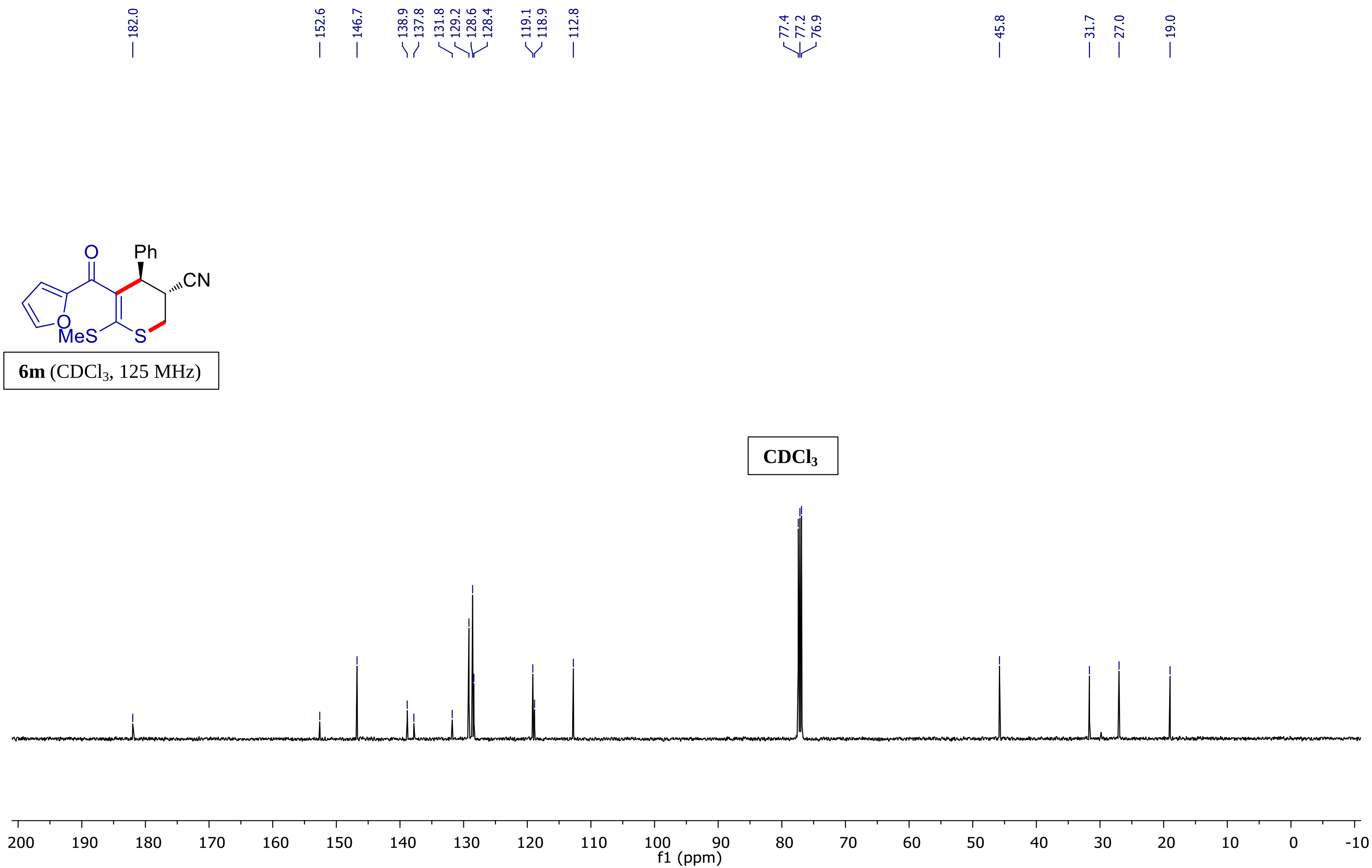

193.7
153.5
142.8
138.8
134.6
132.4
131.6
129.2
128.7
128.5
119.2
106.5
77.4
77.2
76.9
61.1
56.6
45.7
30.5
26.3
18.8
MeO
MeO
OMe
O
Ph
CN
MeS
S
6l (CDCl3, 125 MHz)
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

COSY NMR of Compound 6l

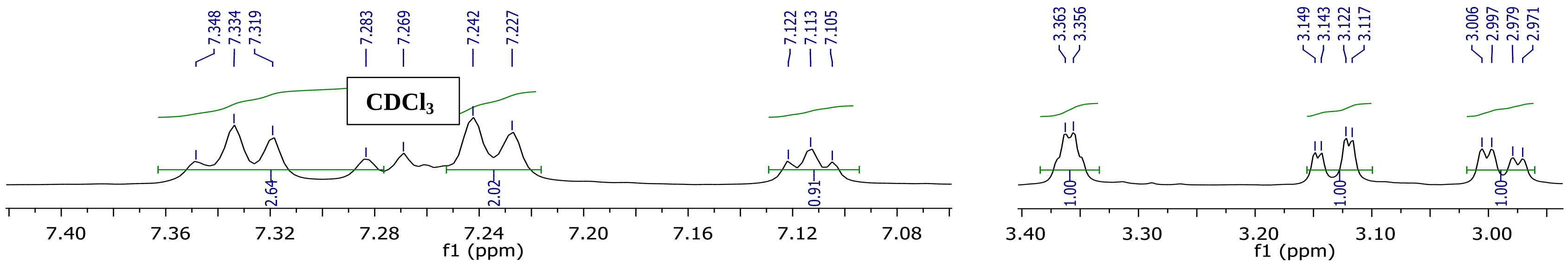


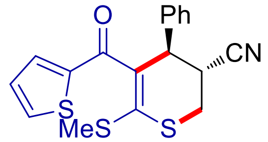
^{1}H (500 MHz, $CDCl_3$) and ^{13}C(^{1}H) (125 MHz, $CDCl_3$) NMR of Compound 6m



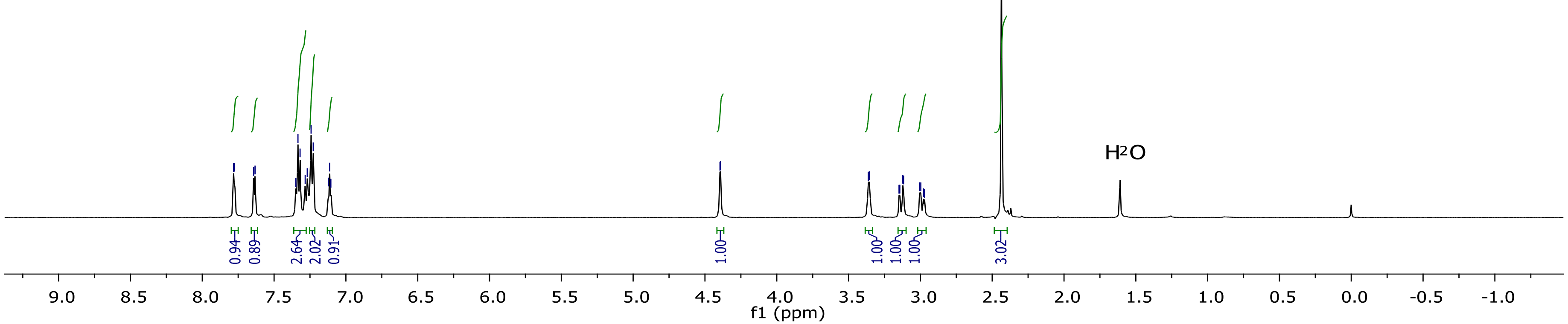

182.0
152.6
146.7
138.9
137.8
131.8
129.2
128.6
128.4
119.1
118.9
112.8
77.4
77.2
76.9
45.8
31.7
27.0
19.0
O
Ph
CN
O
MeS
S
6m ($CDCl_3$, 125 MHz)
$CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

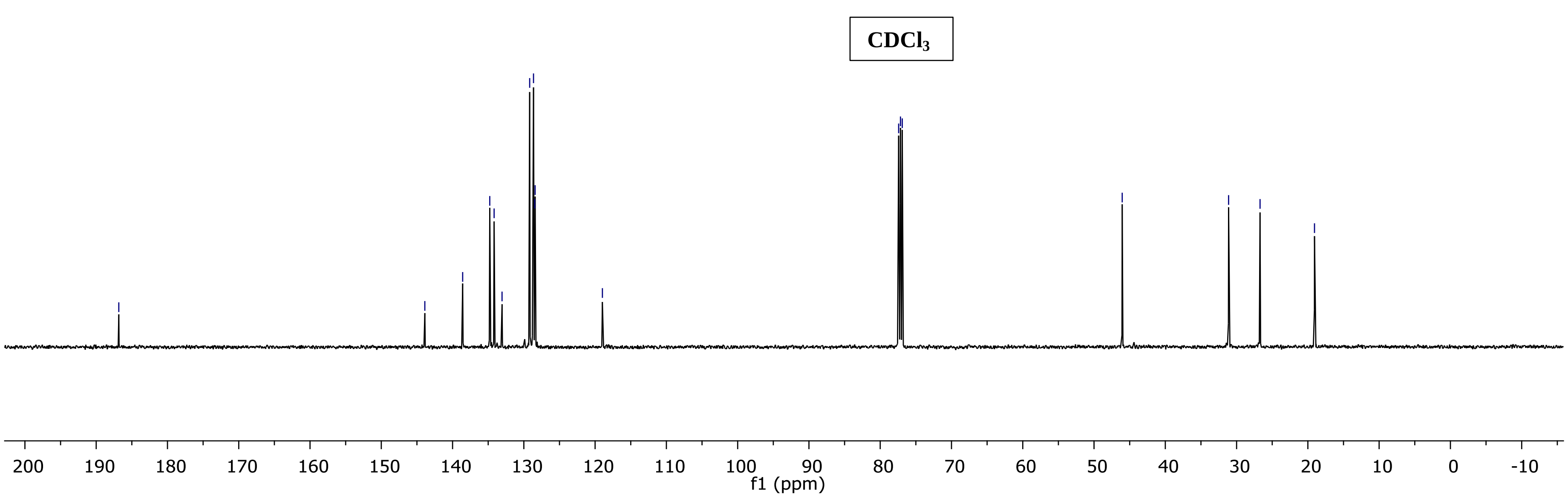
[1]H (500 MHz, $CDCl_3$) and [13]C([1]H) (125 MHz, $CDCl_3$) NMR of Compound 6n

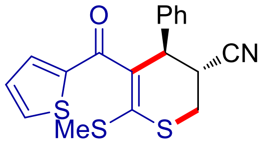




6n ($CDCl_3$, 500 MHz)

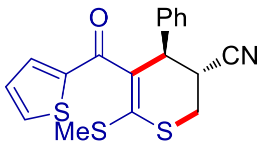




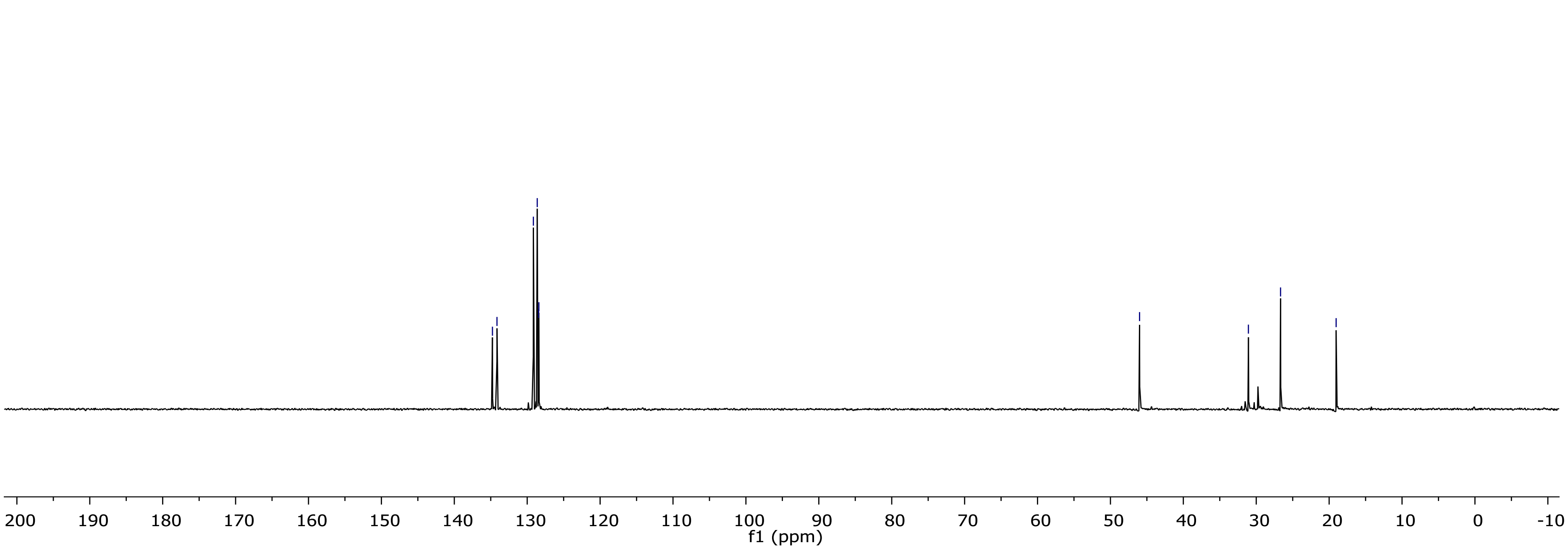


6n ($CDCl_3$, 125 MHz)

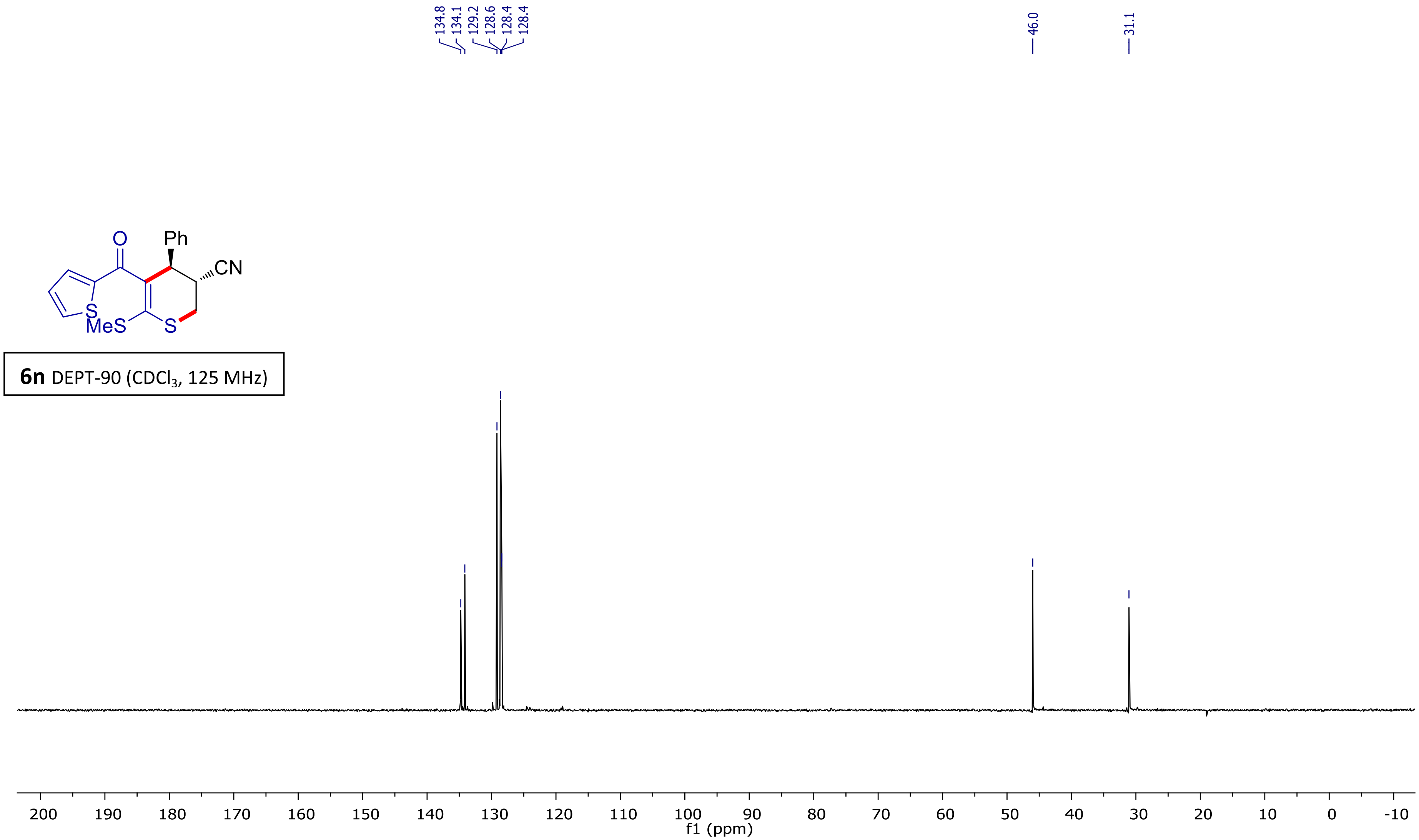
DEPT-45 NMR of Compound 6n



6n DEPT-45 ($CDCl_3$, 125 MHz)

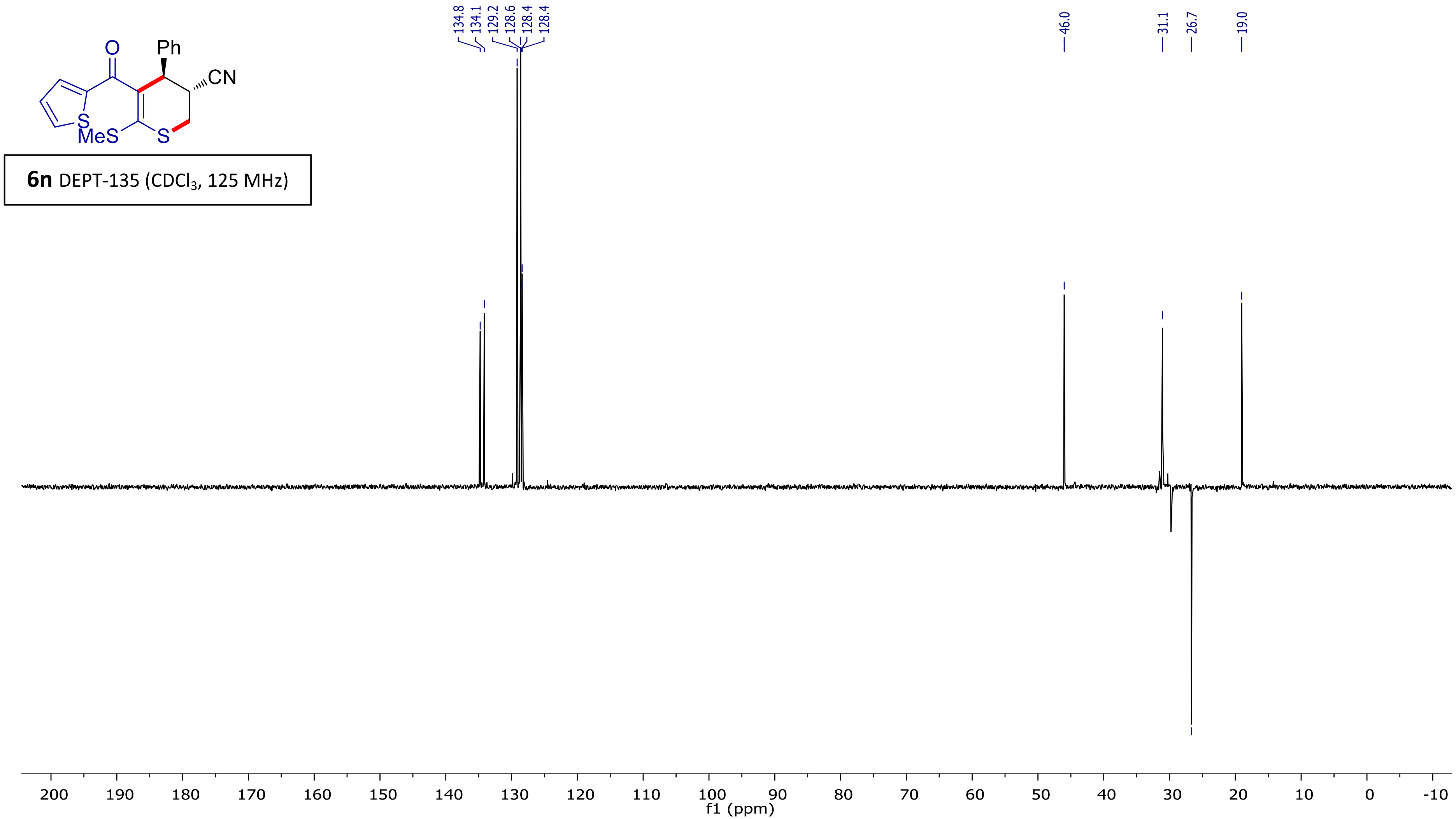


DEPT-90 NMR of Compound 6n

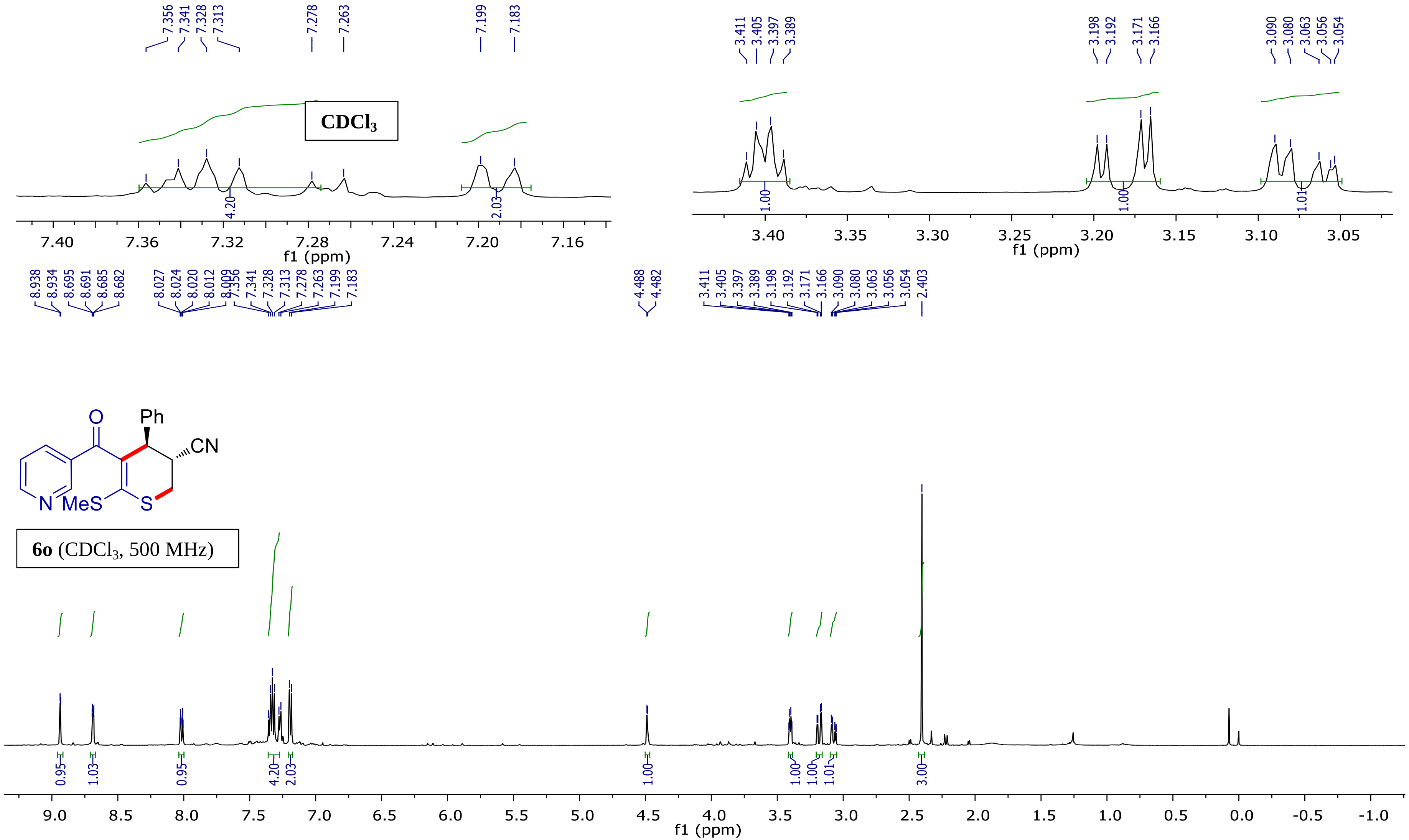


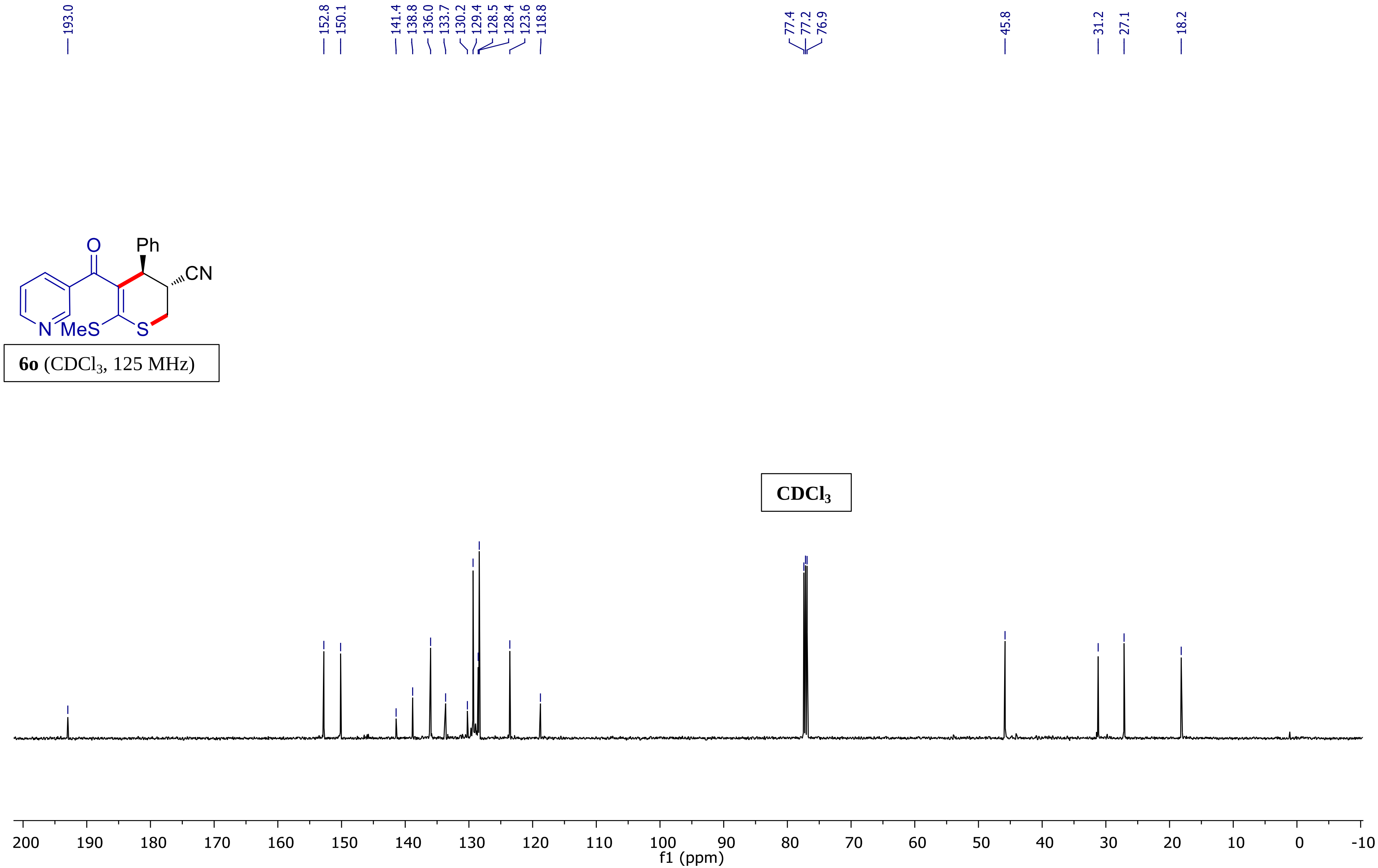
6n DEPT-90 ($CDCl_3$, 125 MHz)

DEPT-135 NMR of Compound 6n



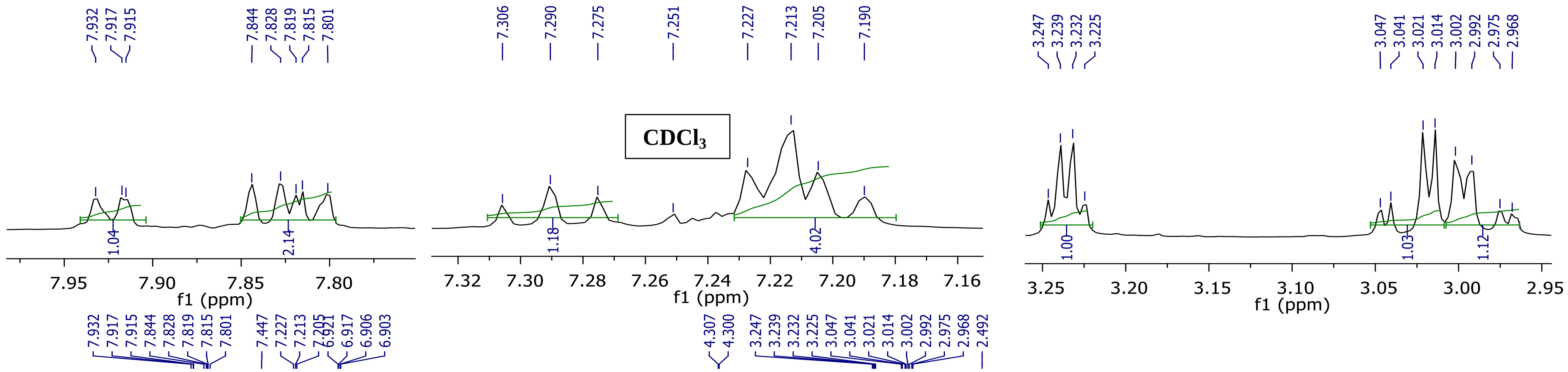
[1]H (500 MHz, $CDCl_3$) and [13]C([1]H) (125 MHz, $CDCl_3$) NMR of Compound 6o

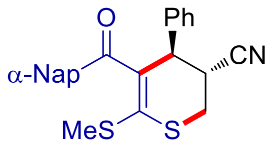




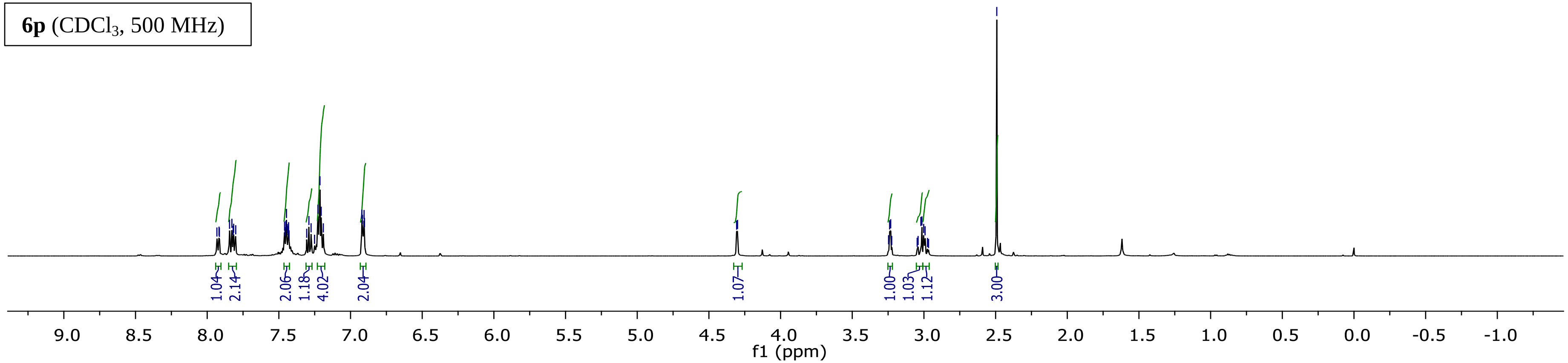
6o ($CDCl_3$, 125 MHz)

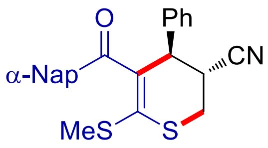
^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR of Compound 6p



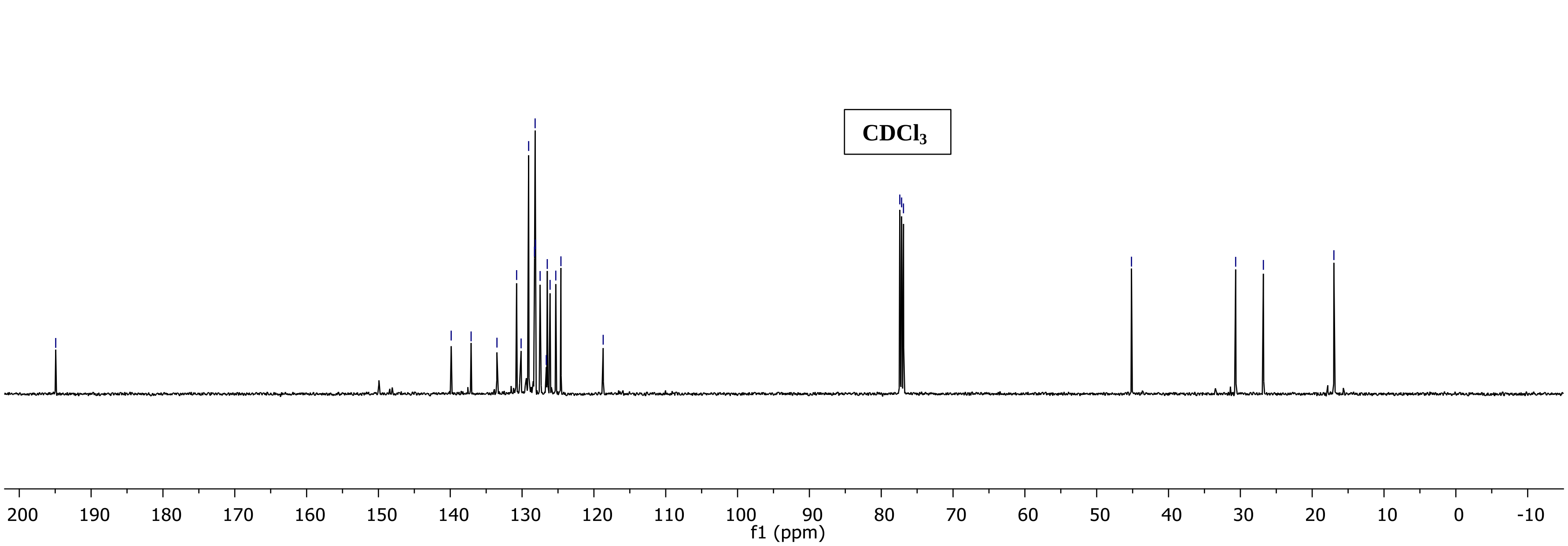


6p ($CDCl_3$, 500 MHz)

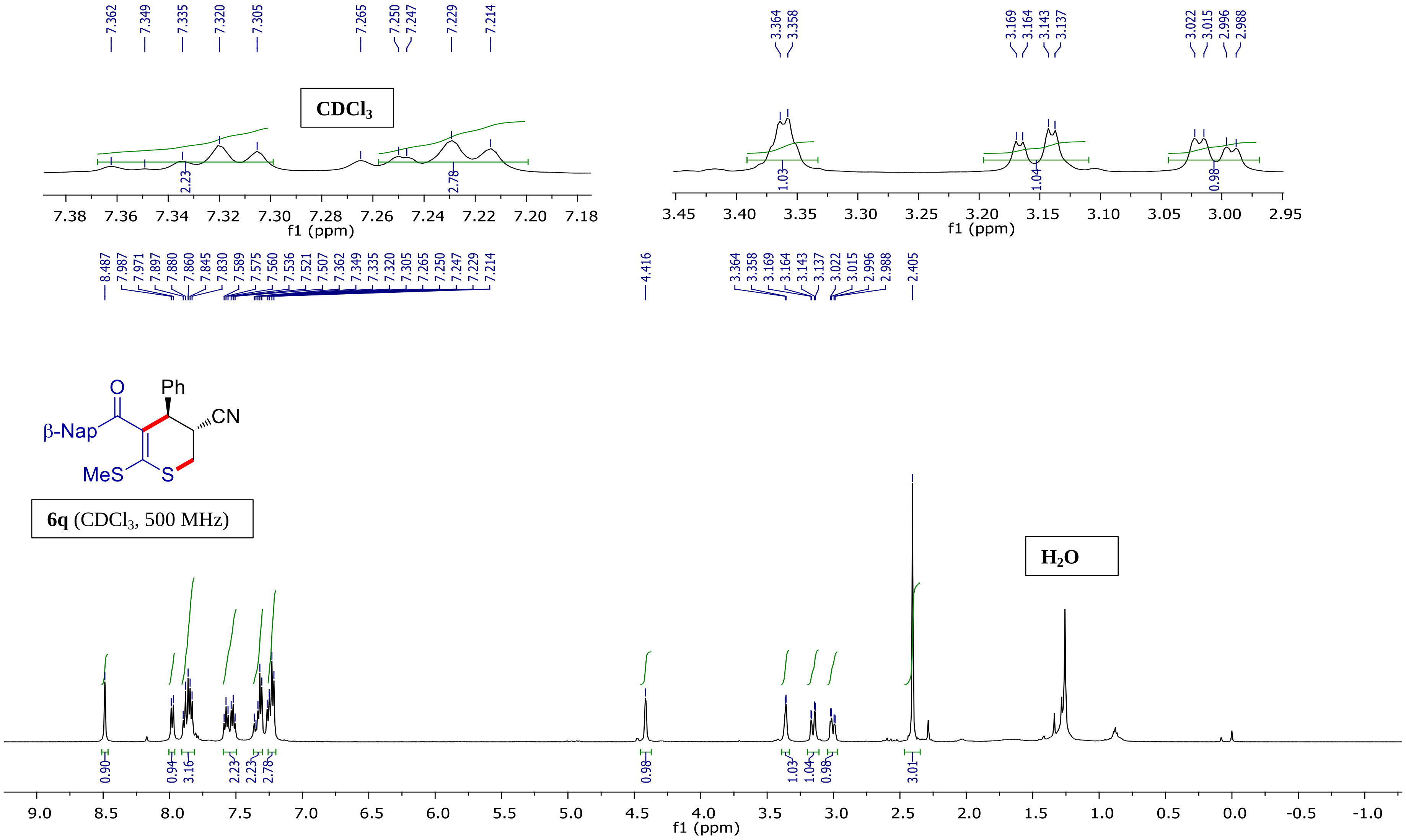


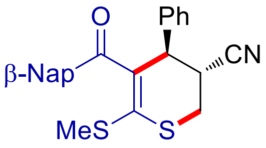


6p ($CDCl_3$, 125 MHz)

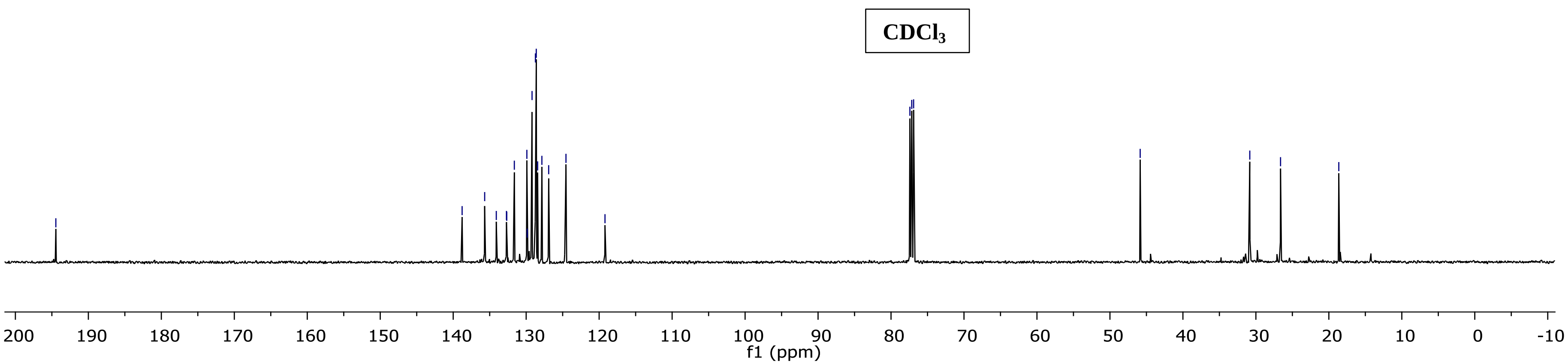


^{1}H - (500 MHz, $CDCl_3$) and $^{13}C(^{1}H)$ (125 MHz, $CDCl_3$) NMR of Compound 6q

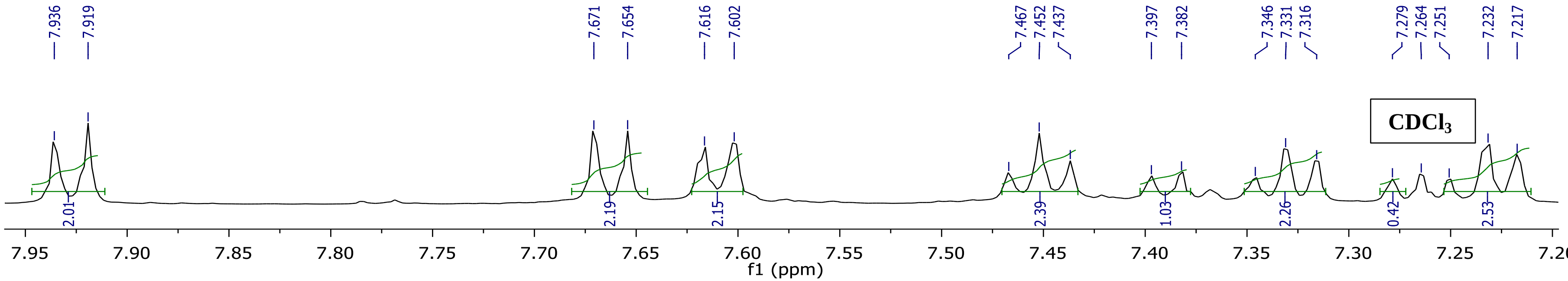


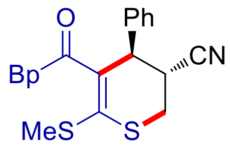


6q ($CDCl_3$, 125 MHz)

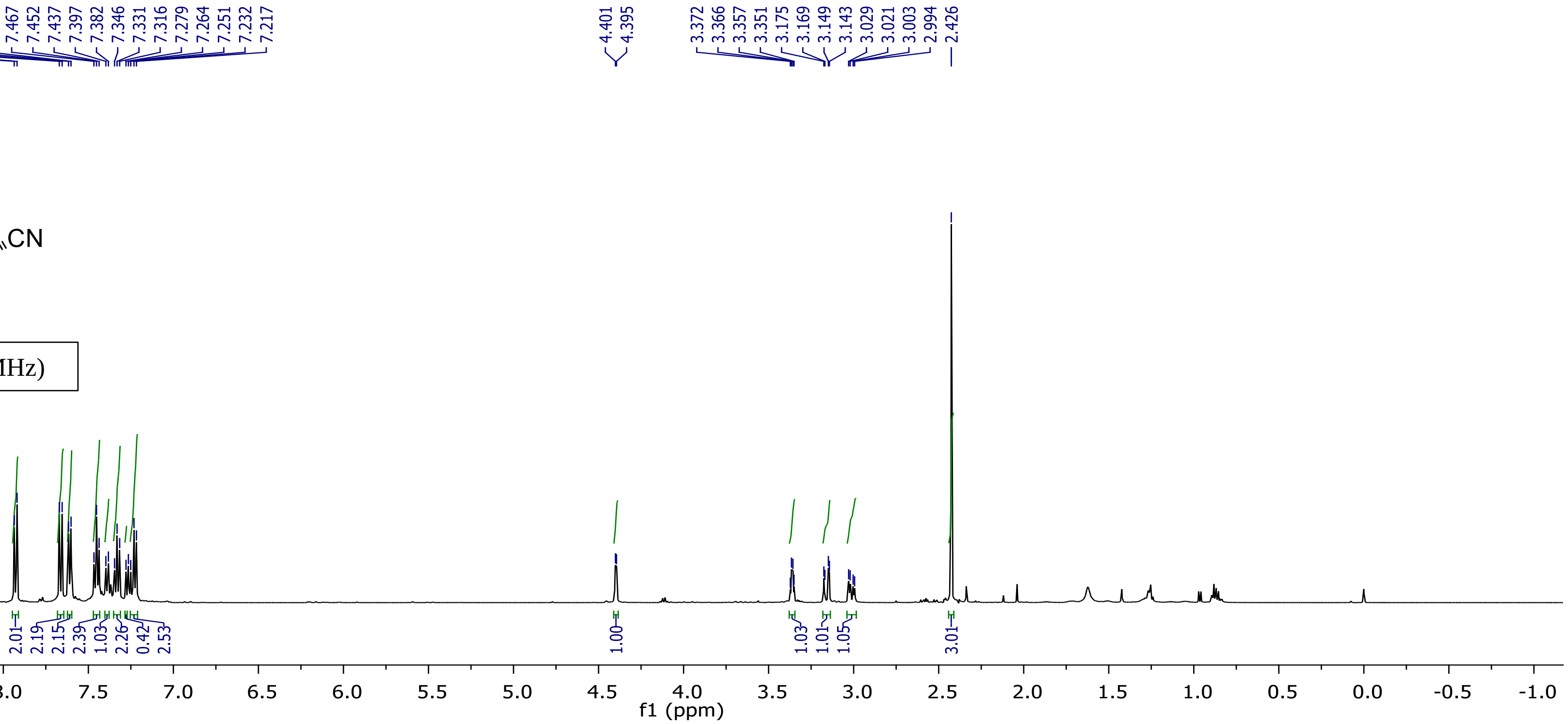


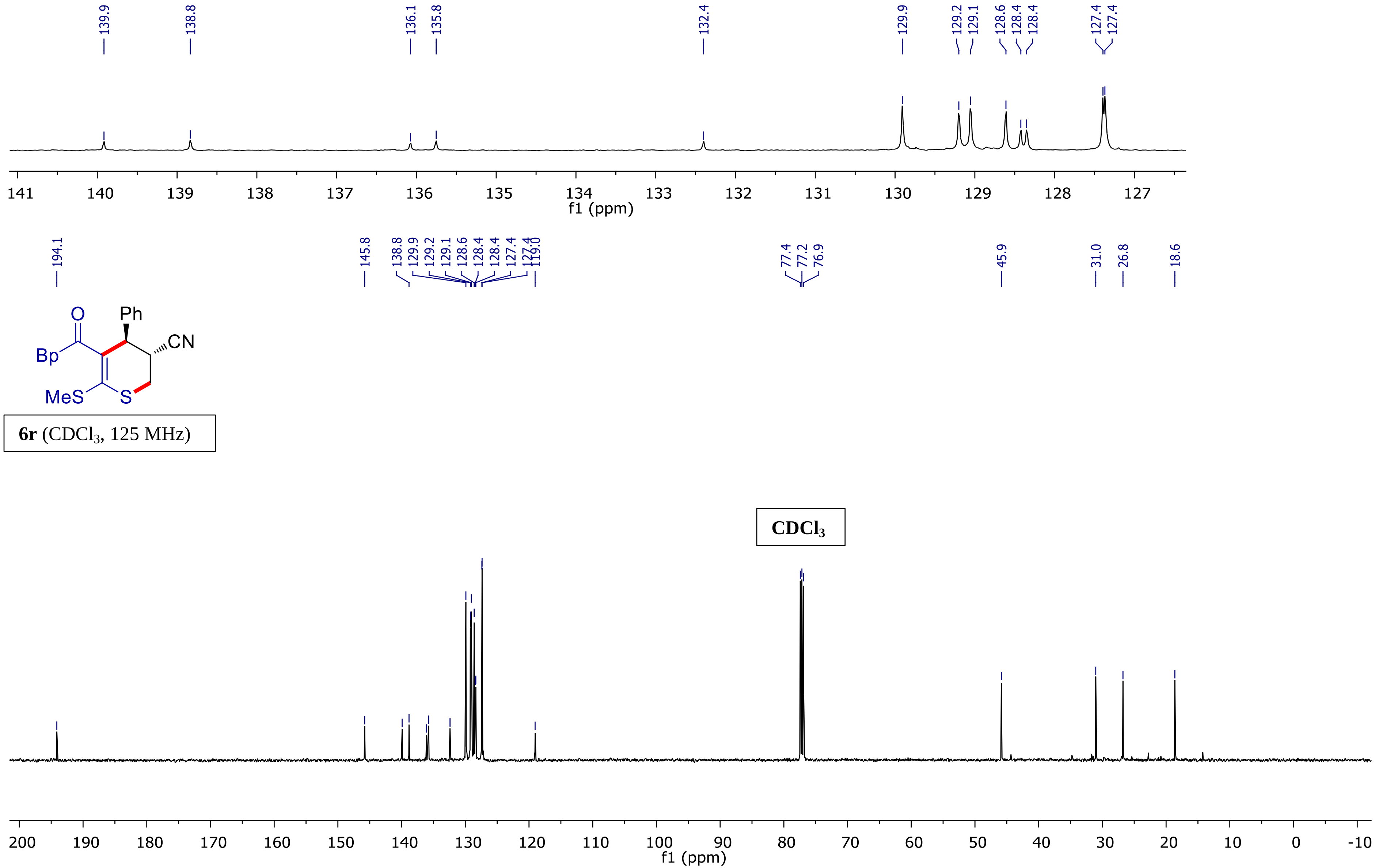
^{1}H (500 MHz, $CDCl_3$) and $^{13}C(^{1}H)$ (125 MHz, $CDCl_3$) NMR of Compound 6r





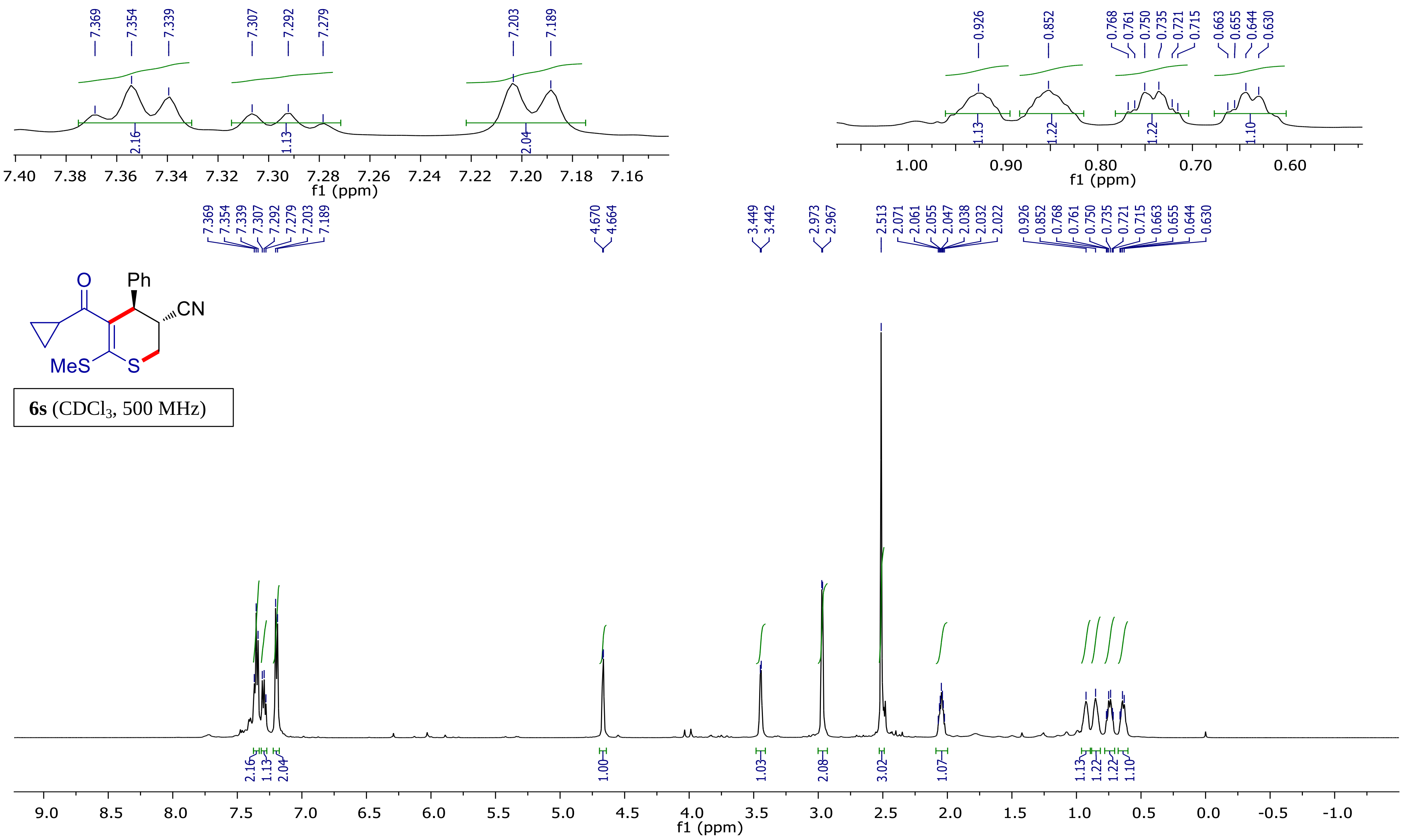
6r ($CDCl_3$, 500 MHz)

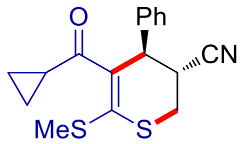




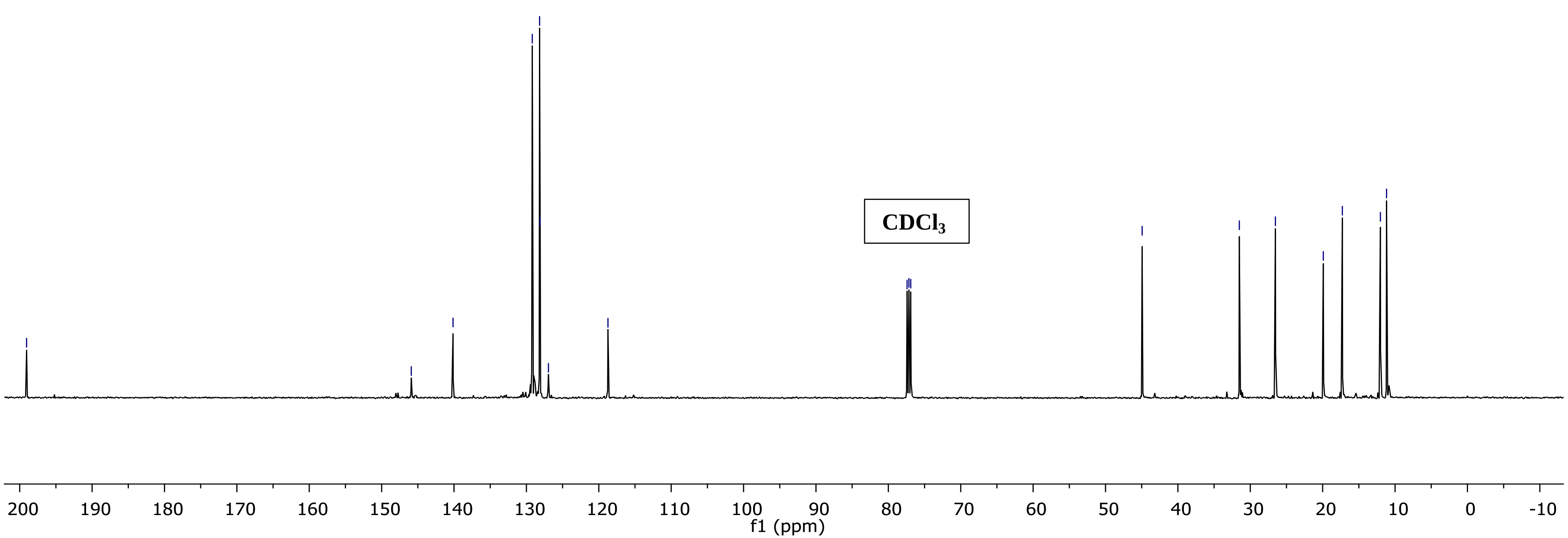
6r ($CDCl_3$, 125 MHz)

^{1}H (500 MHz, CDCl$_3$) and ^{13}C(^{1}H) (125 MHz, CDCl$_3$) NMR of Compound 6s

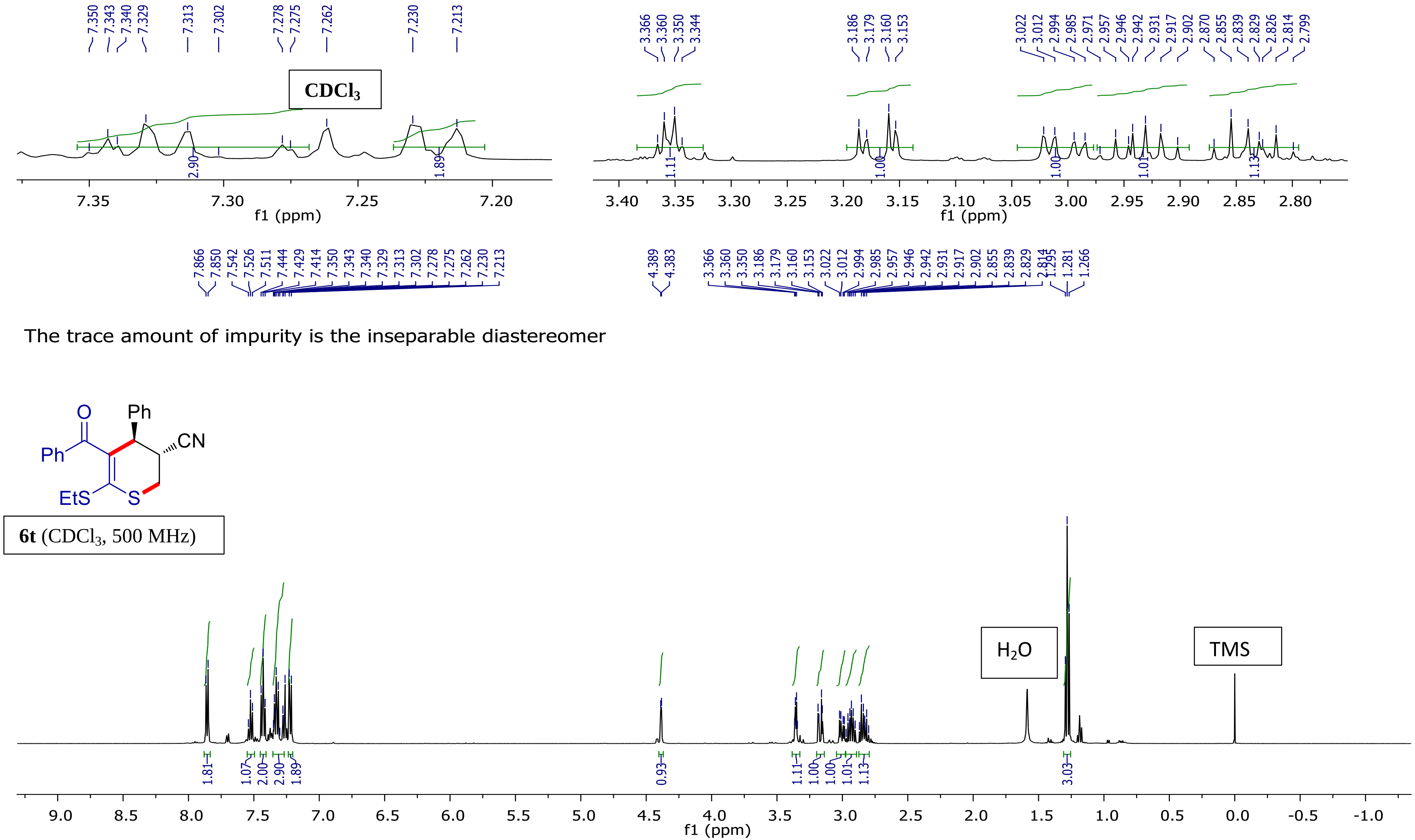




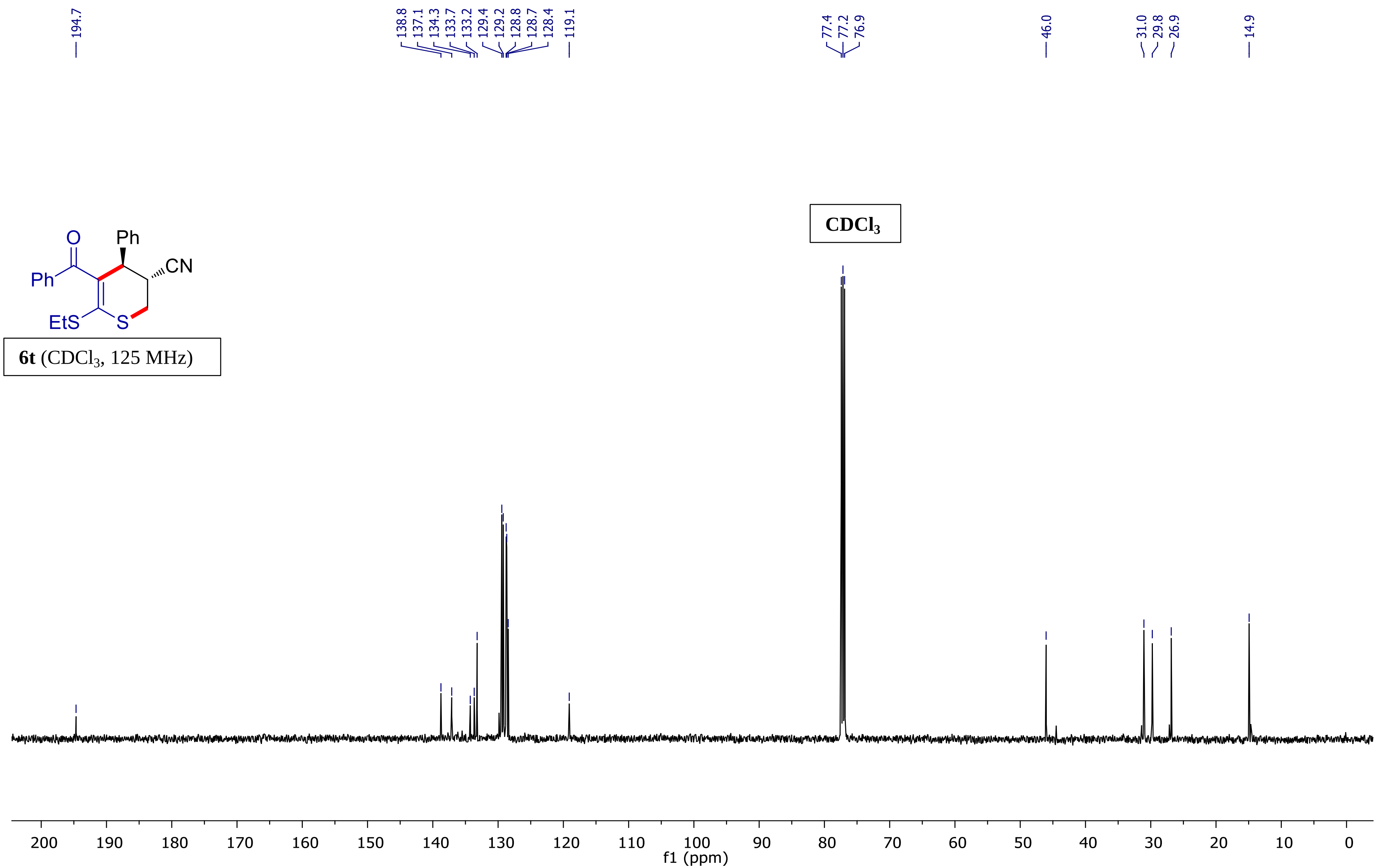
6s ($CDCl_3$, 125 MHz)



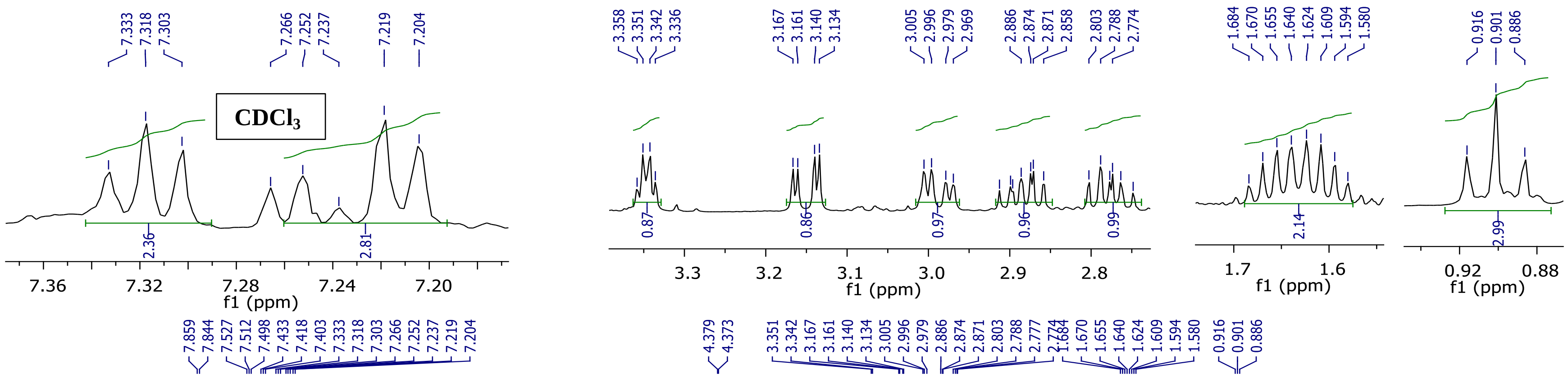
^{1}H (500 MHz, $CDCl_3$) and ^{13}C(^{1}H) (125 MHz, $CDCl_3$) NMR of Compound 6t

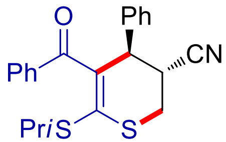


The trace amount of impurity is the inseparable diastereomer

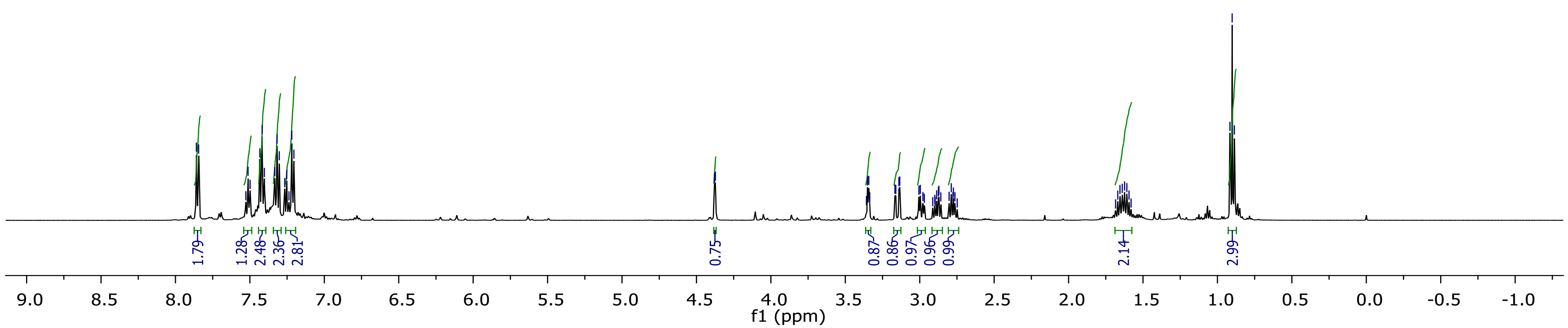

194.7
138.8
137.1
134.3
133.7
133.2
129.4
129.2
128.8
128.7
128.4
119.1
77.4
77.2
76.9
46.0
31.0
29.8
26.9
14.9
CDCl3
O
Ph
CN
Ph
EtS
S
6t (CDCl3, 125 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

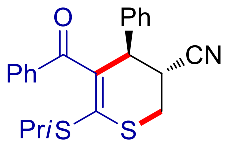
[1]H (500 MHz, $CDCl_3$) and [13]C([1]H) (125 MHz, $CDCl_3$) NMR of Compound 6u



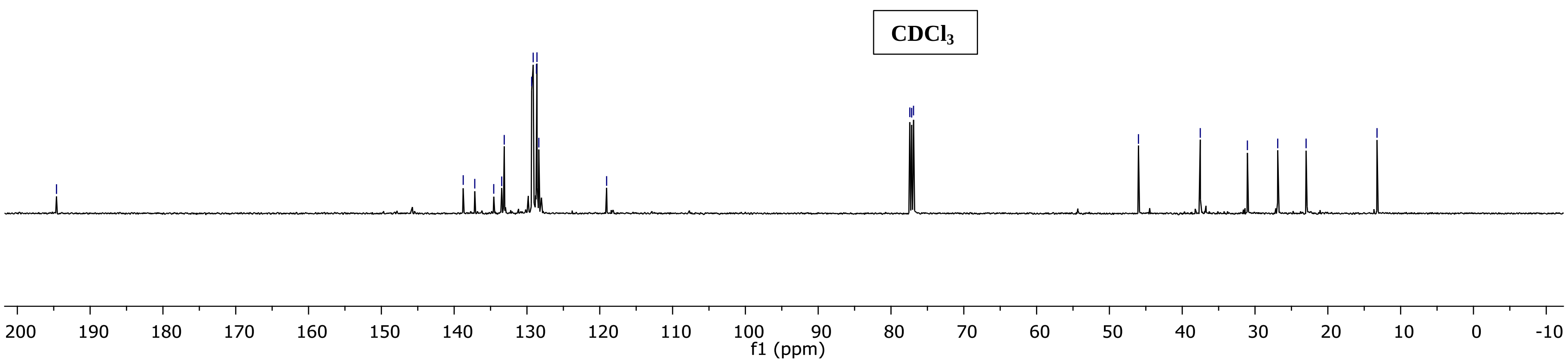


6u ($CDCl_3$, 500 MHz)

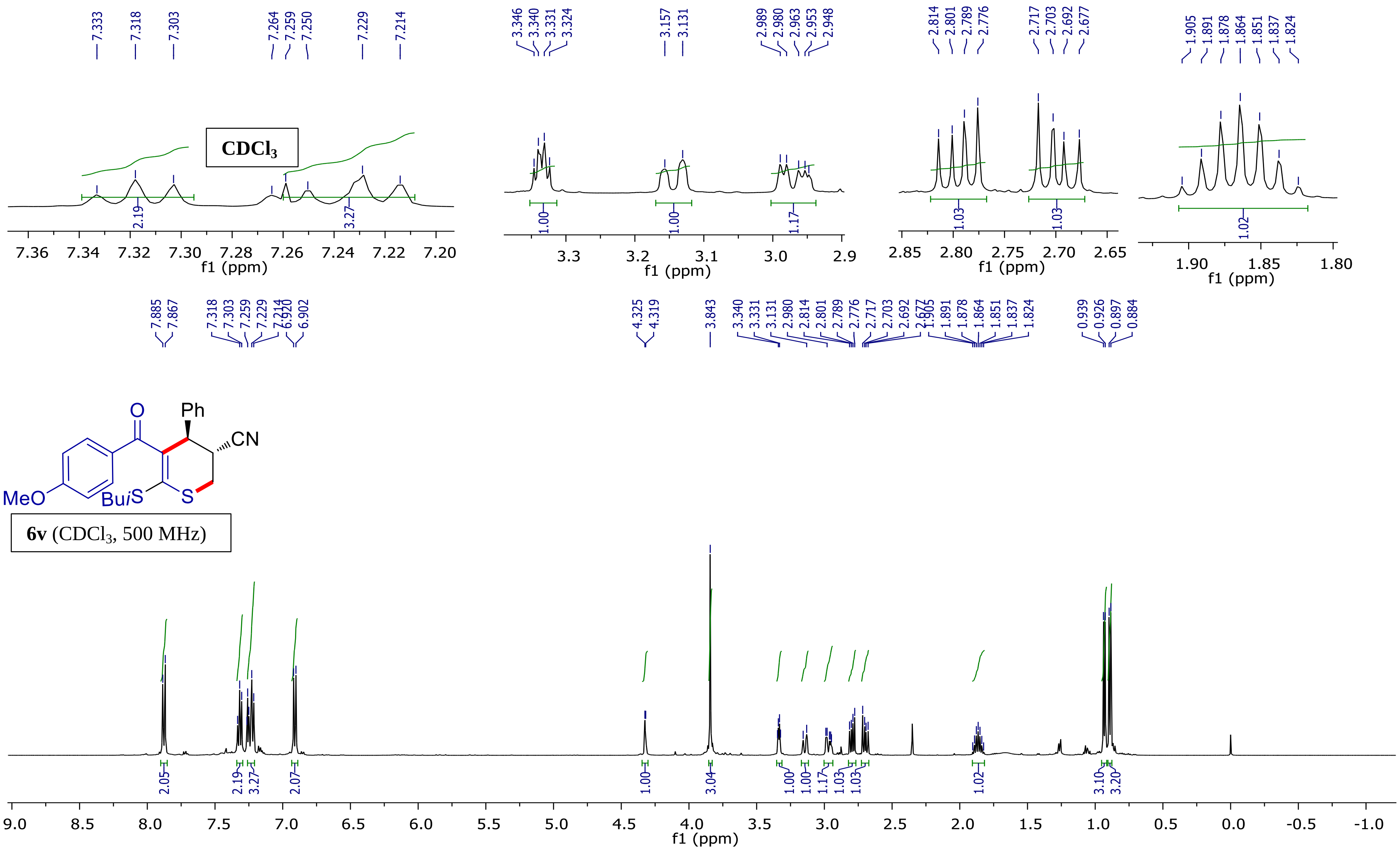


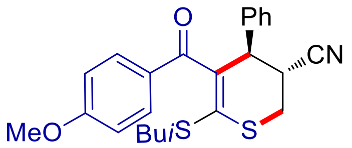


6u ($CDCl_3$, 125 MHz)

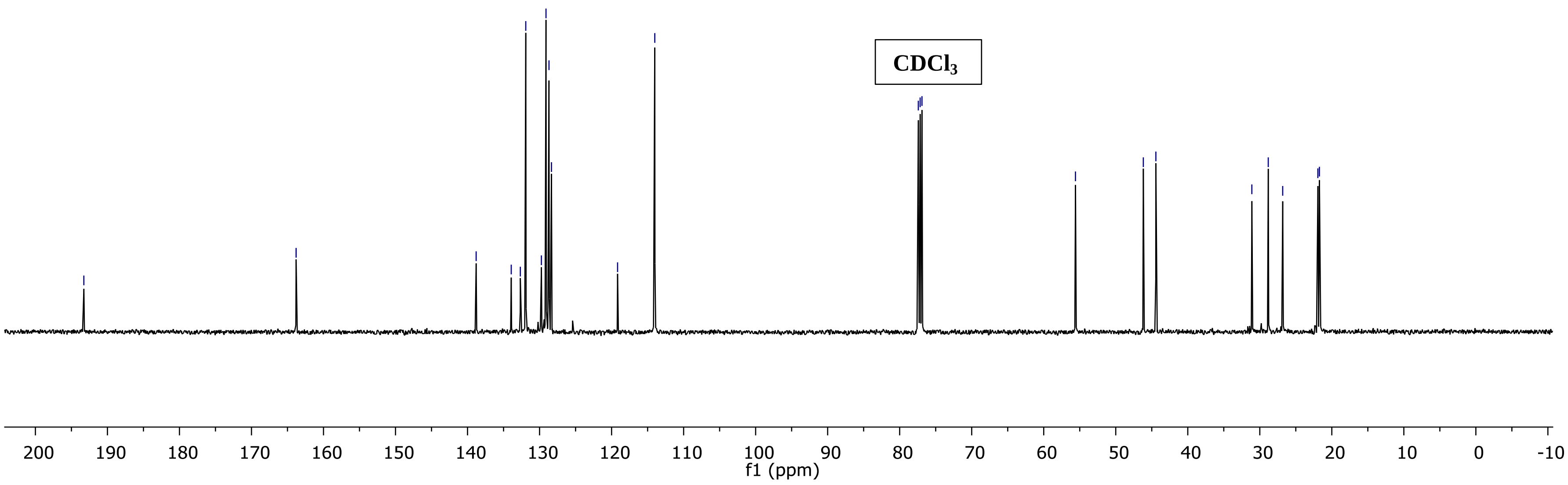


^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR of Compound 6v

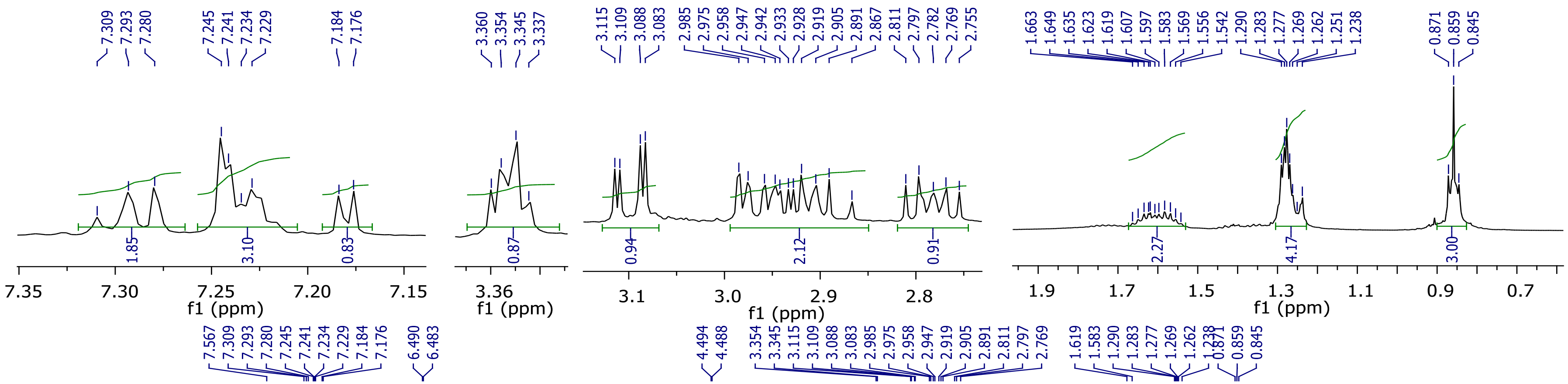


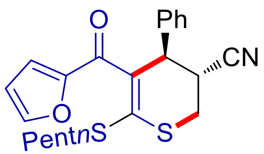


6v ($CDCl_3$, 125 MHz)

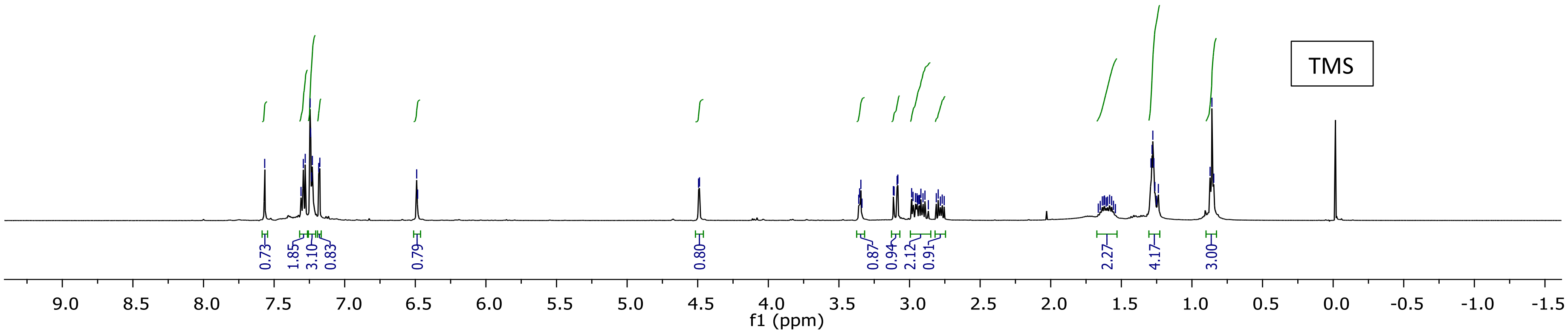


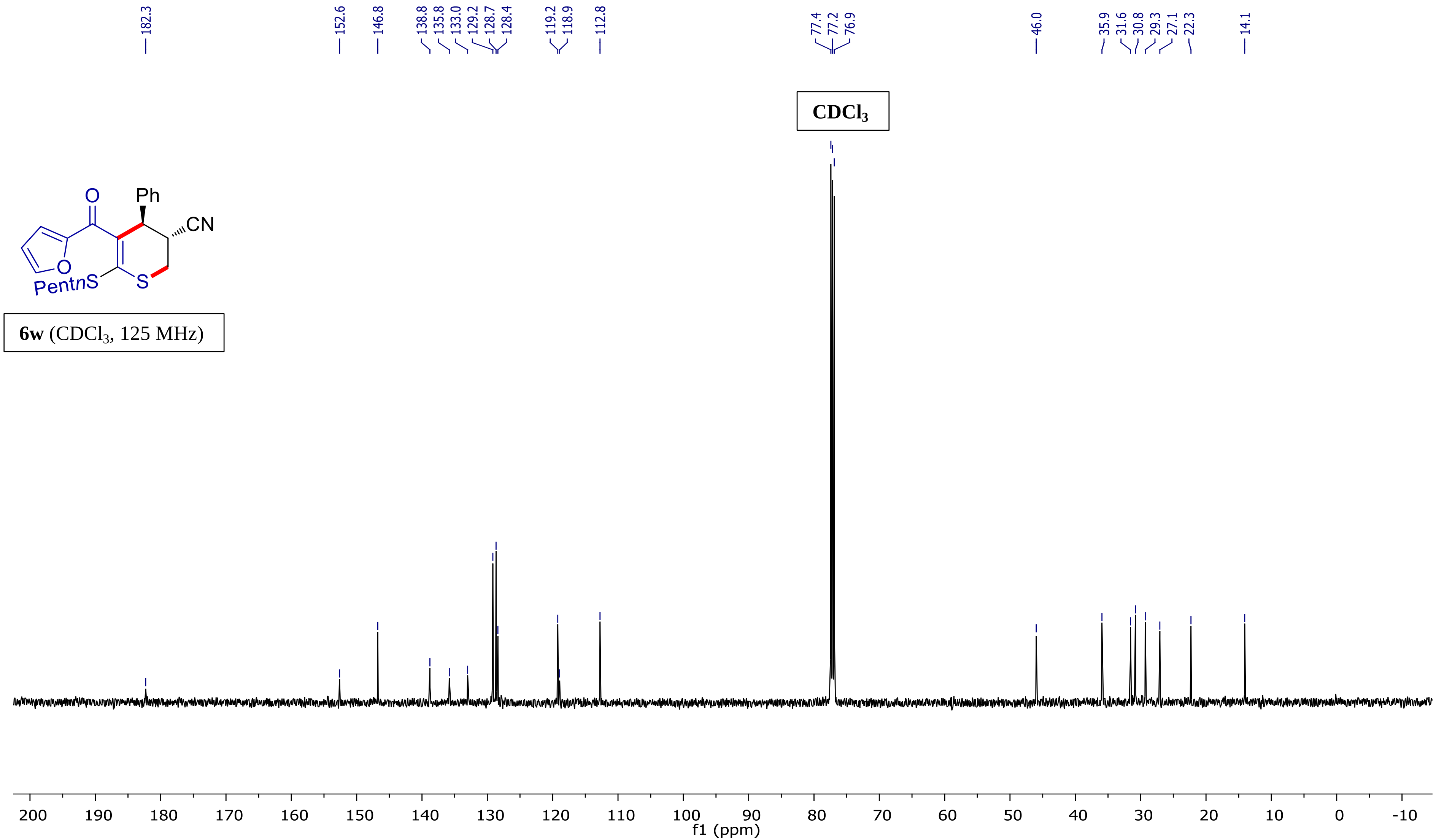
<u>**^{1}H (500 MHz, CDCl$_3$) and ^{13}C(^{1}H) (125 MHz, CDCl$_3$) NMR of Compound 6w**</u>





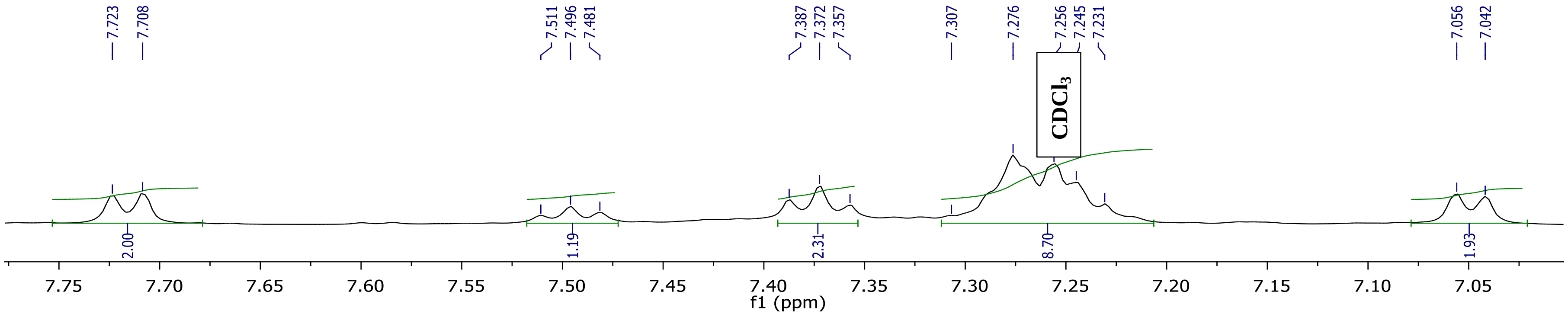
6w (CDCl$_3$, 500 MHz)

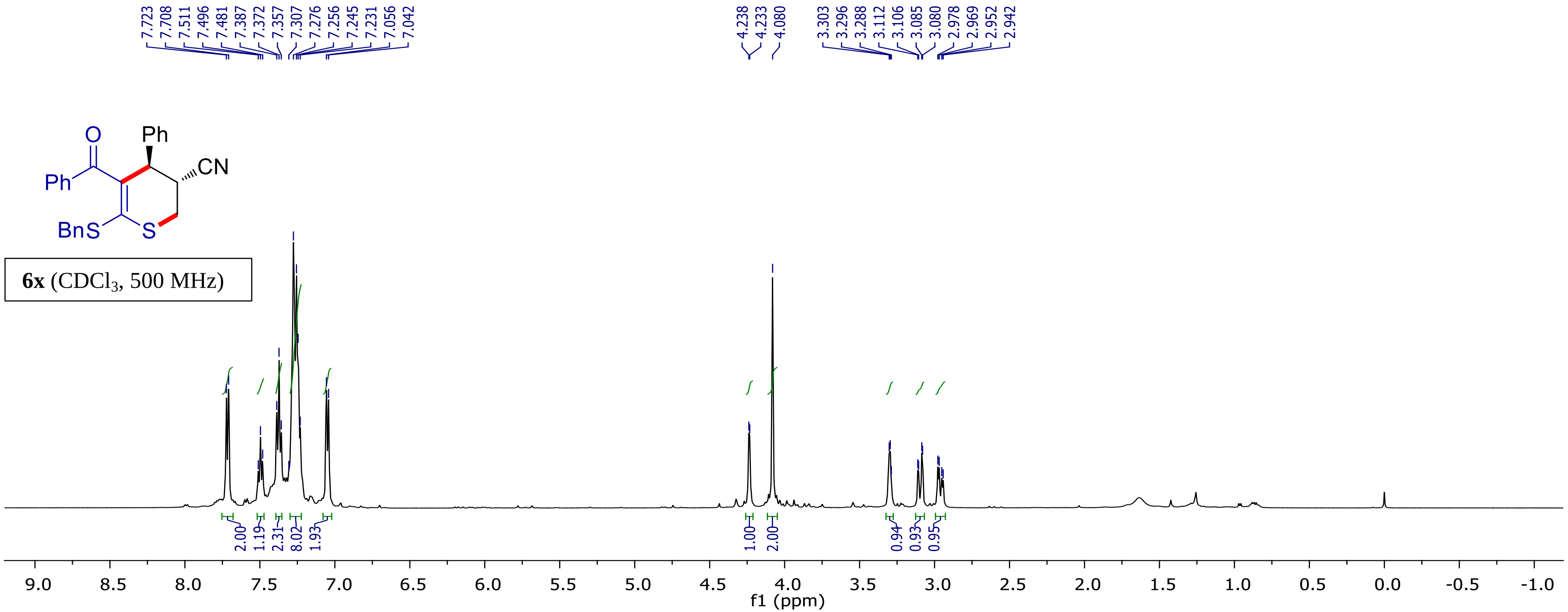


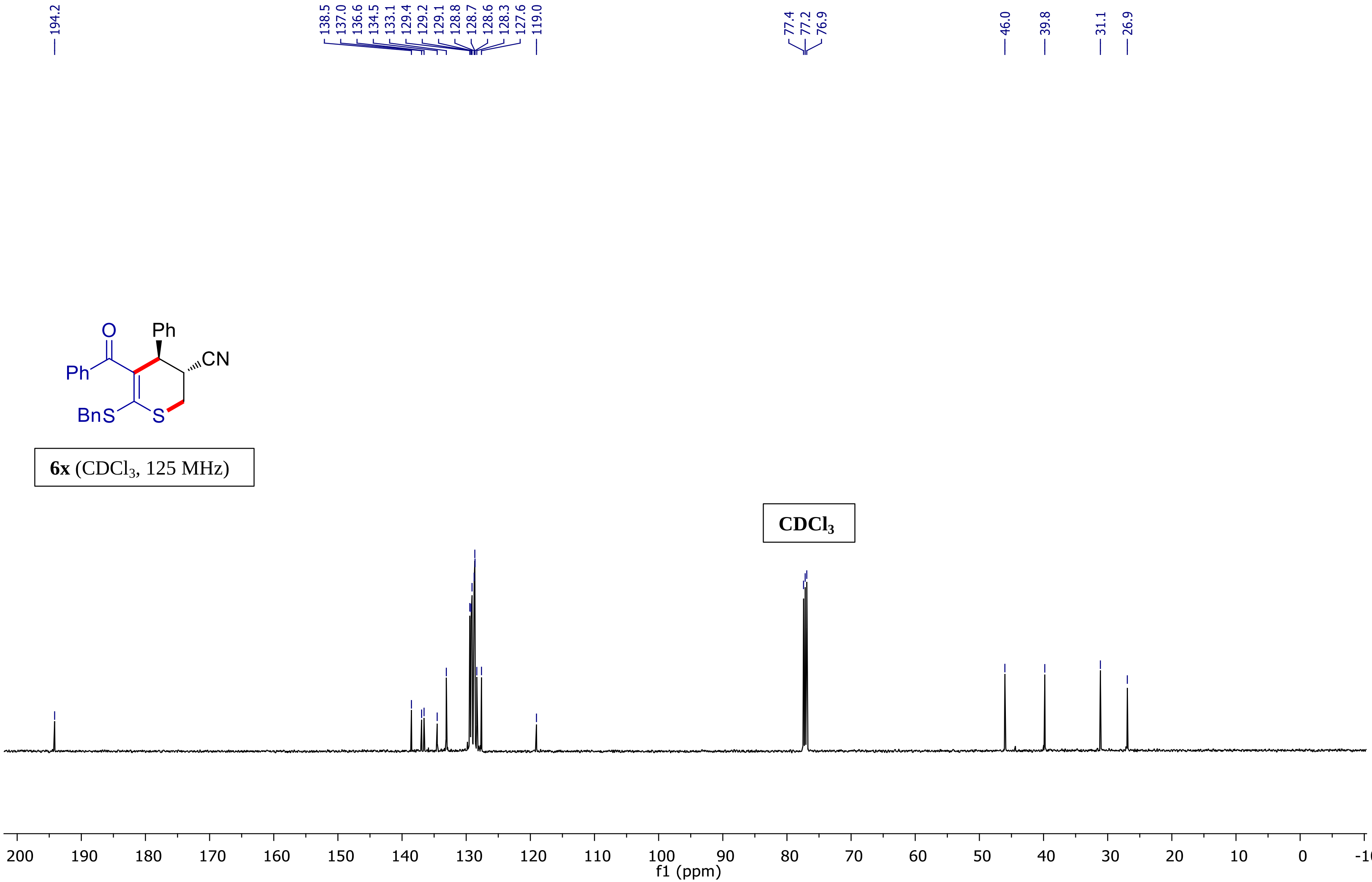


6w ($CDCl_3$, 125 MHz)

^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^1H\}$ (125 MHz, $CDCl_3$) NMR of Compound 6x

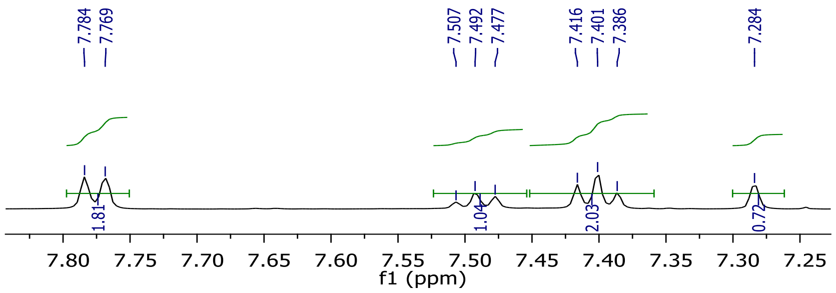


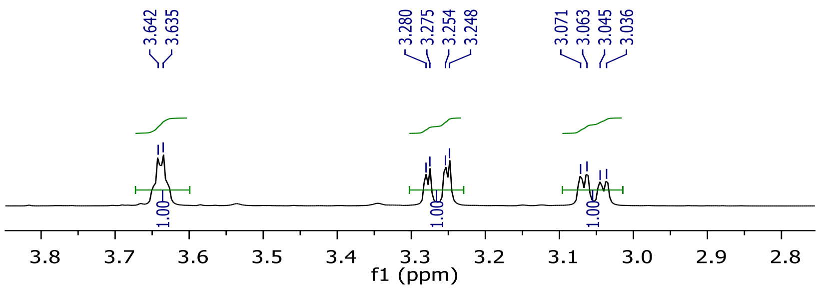




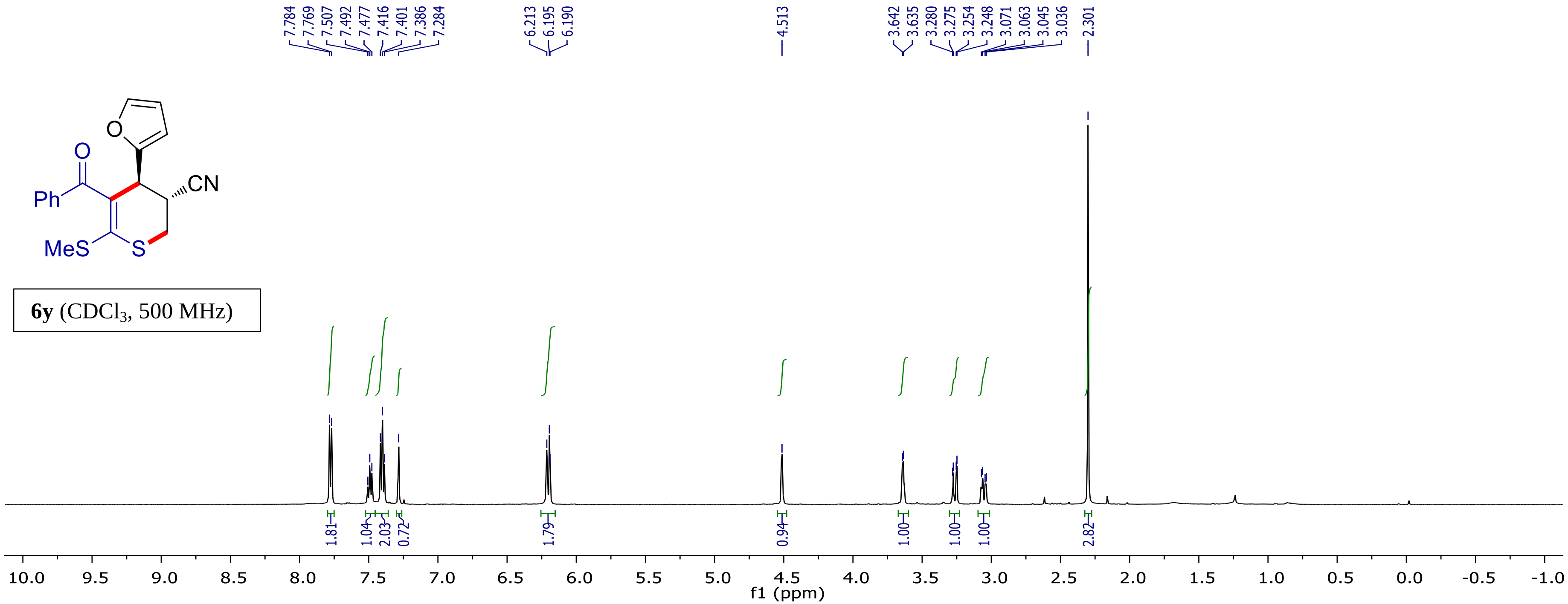
6x ($CDCl_3$, 125 MHz)

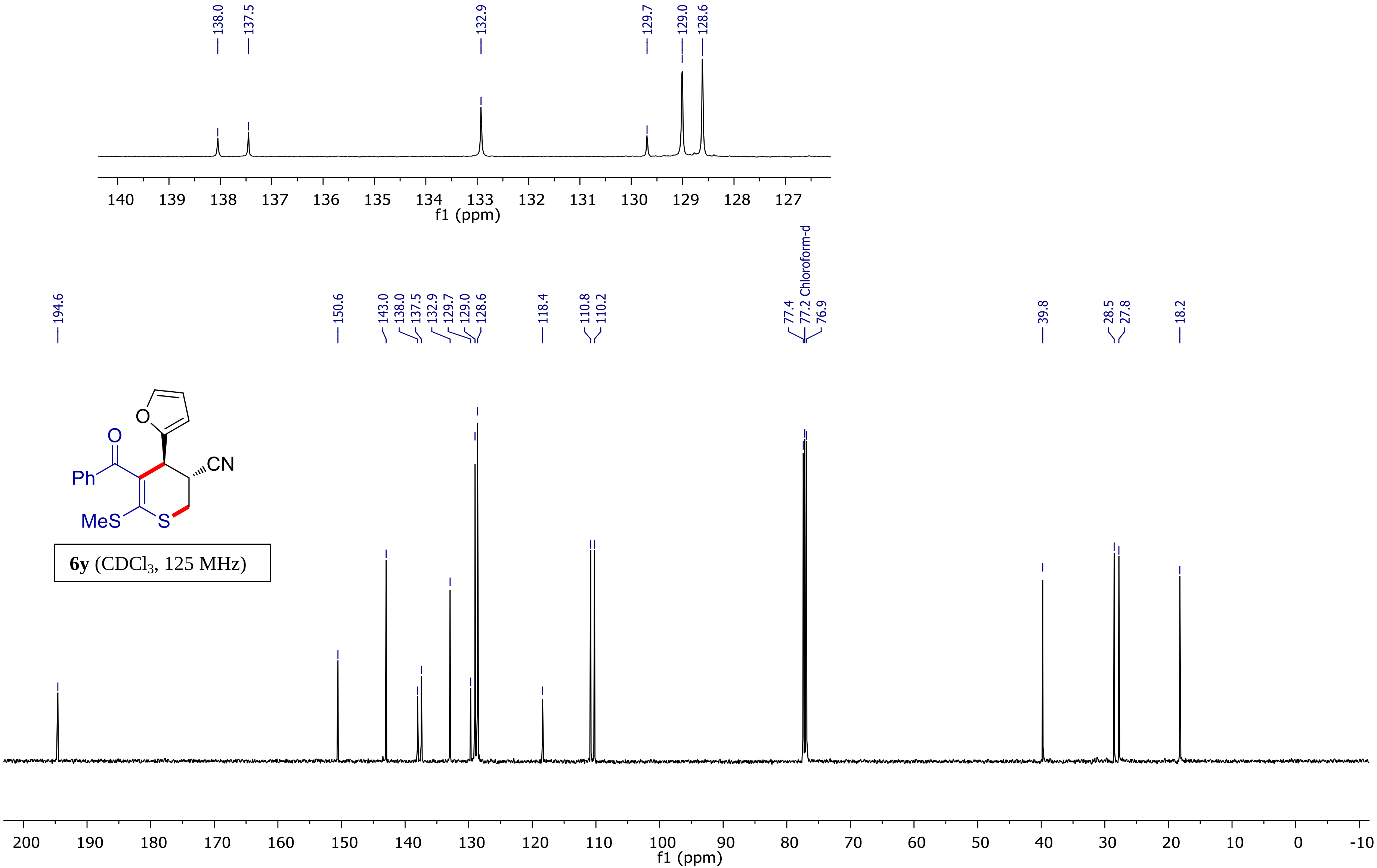
^{1}H (500 MHz, $CDCl_3$) and $^{13}C(^{1}H)$ (125 MHz, $CDCl_3$) NMR of Compound 6y



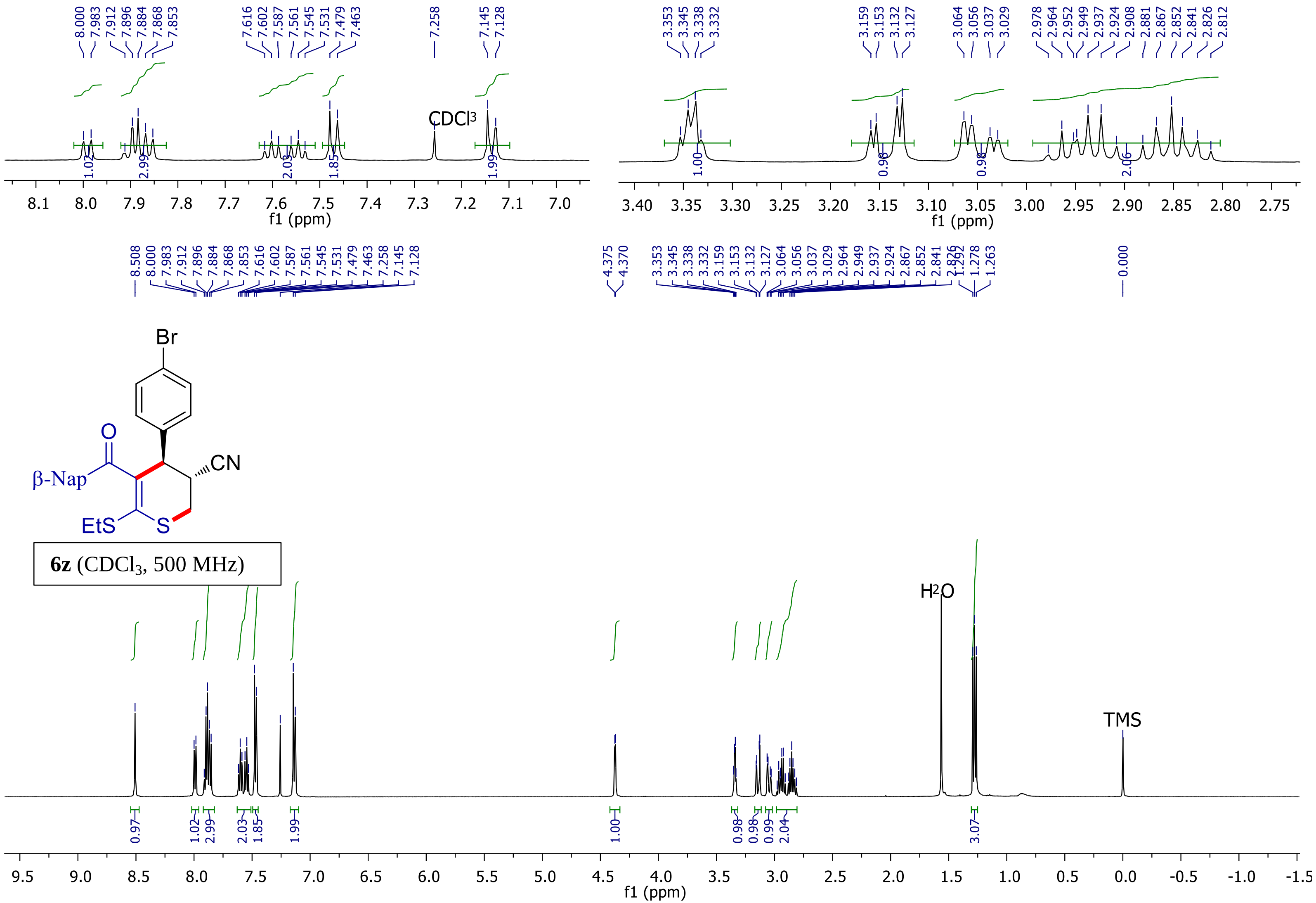


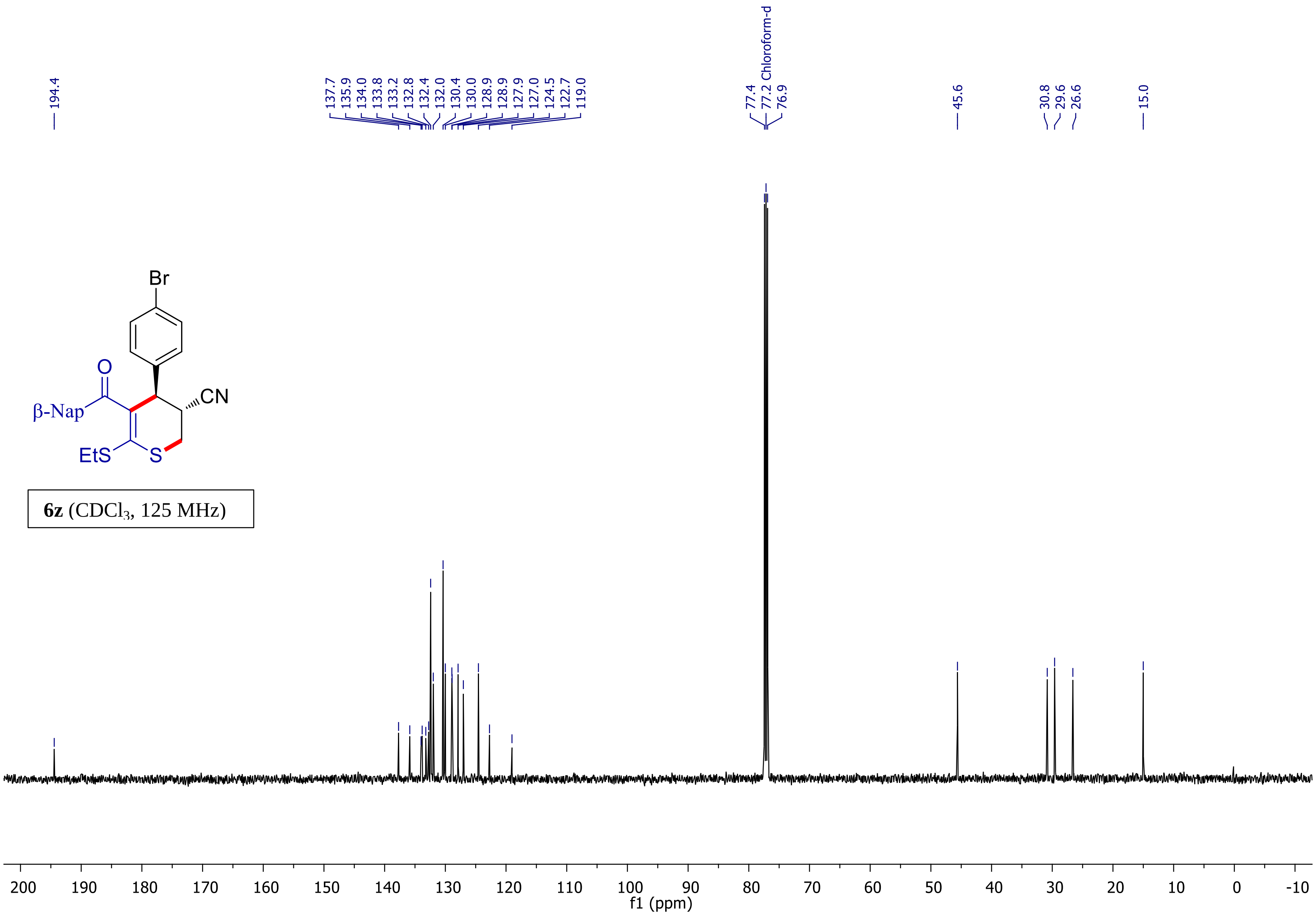
6y ($CDCl_3$, 500 MHz)



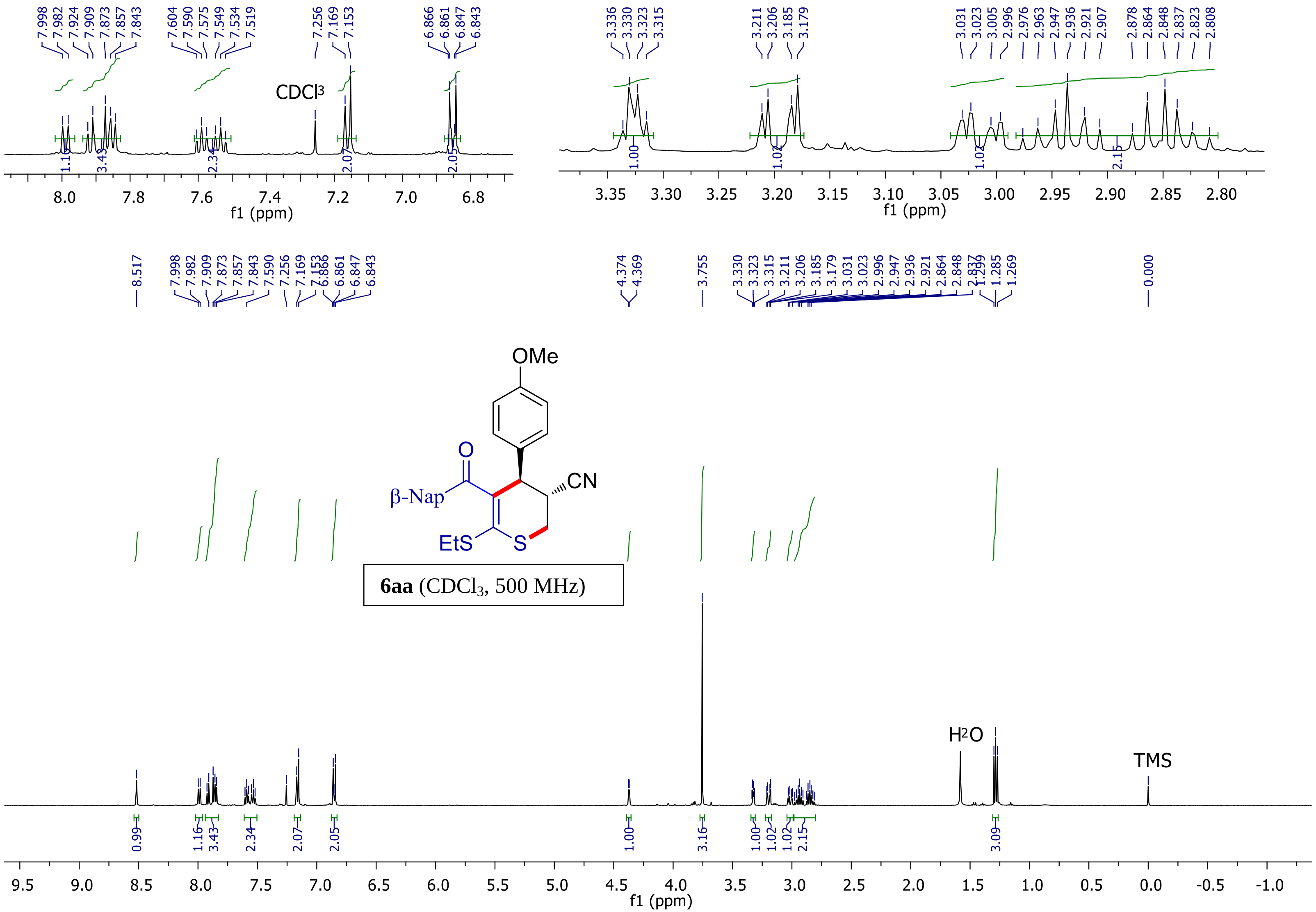

138.0
137.5
132.9
129.7
129.0
128.6
140 139 138 137 136 135 134 133 132 131 130 129 128 127
f1 (ppm)
194.6
150.6
143.0
138.0
137.5
132.9
129.7
129.0
128.6
118.4
110.8
110.2
77.4
77.2 Chloroform-d
76.9
39.8
28.5
27.8
18.2
O
Ph
CN
MeS
S
6y (CDCl3, 125 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

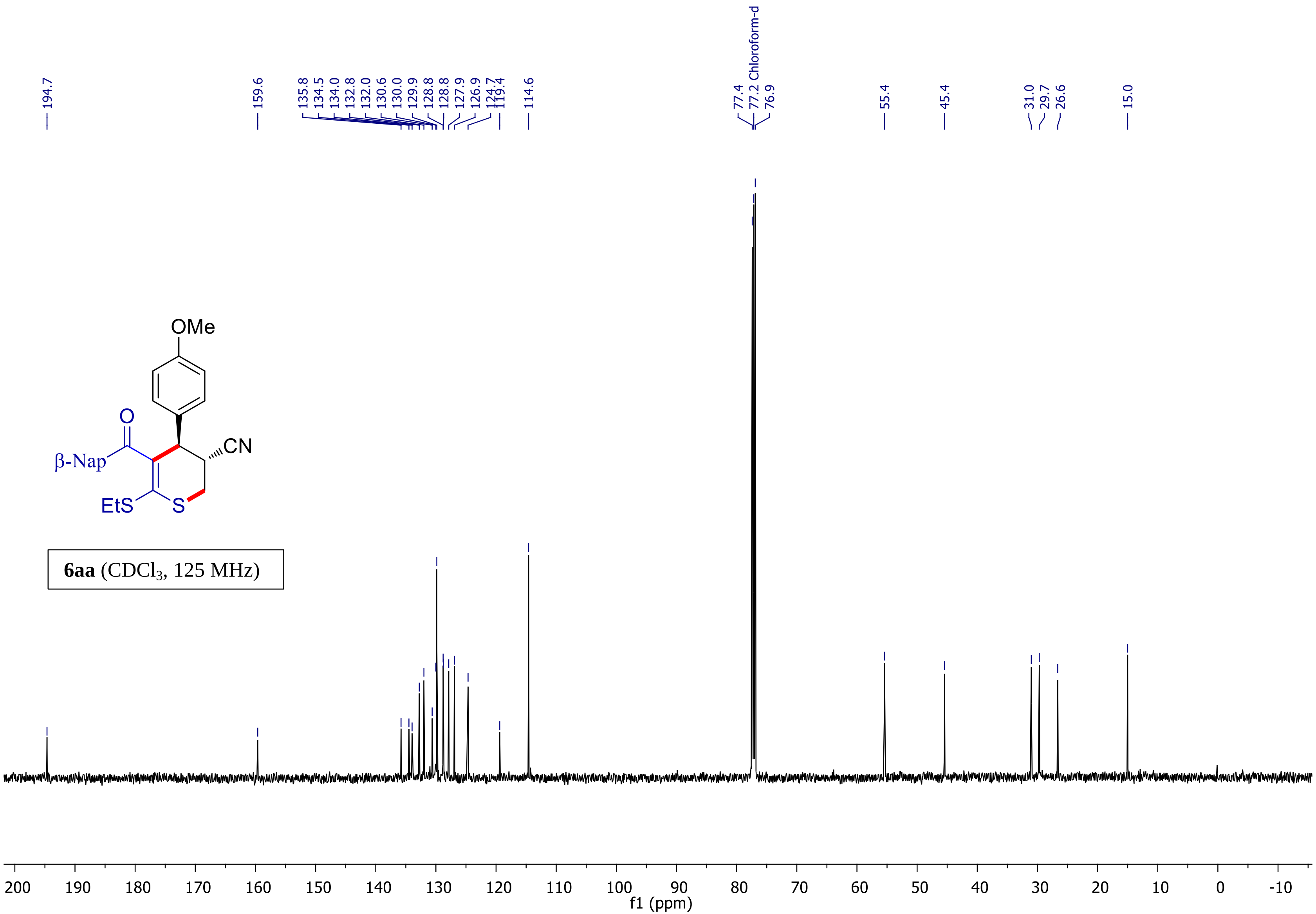
^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR of Compound 6z




194.4
137.7
135.9
134.0
133.8
133.2
132.8
132.4
132.0
130.4
130.0
128.9
128.9
127.9
127.0
124.5
122.7
119.0
77.4
77.2 Chloroform-d
76.9
45.6
30.8
29.6
26.6
15.0
Br
O
β-Nap
CN
EtS
S
6z ($CDCl_3$, 125 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

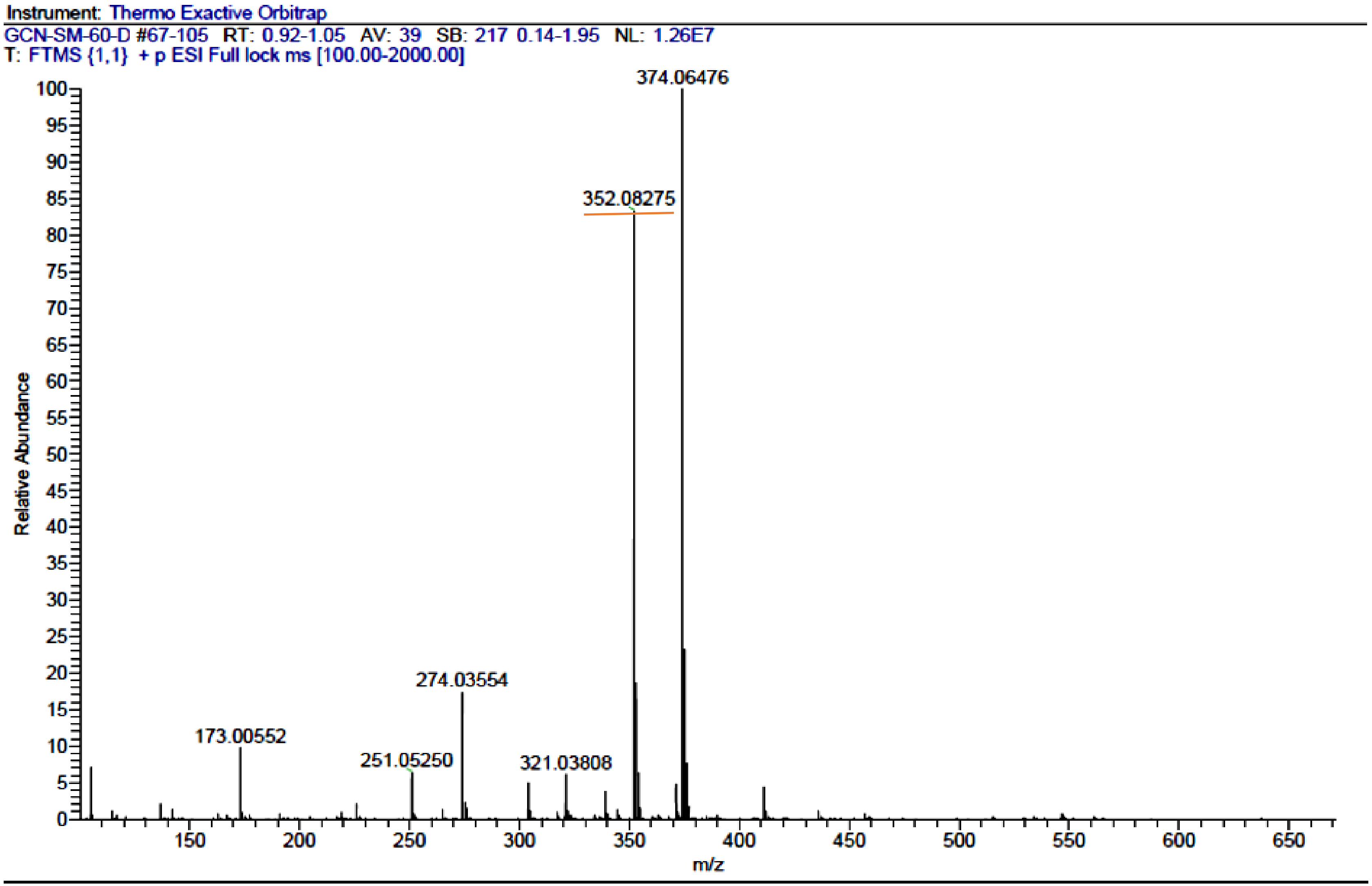
^{1}H (500 MHz, $CDCl_3$) and $^{13}C(^{1}H)$ (125 MHz, $CDCl_3$) NMR of Compound 6aa



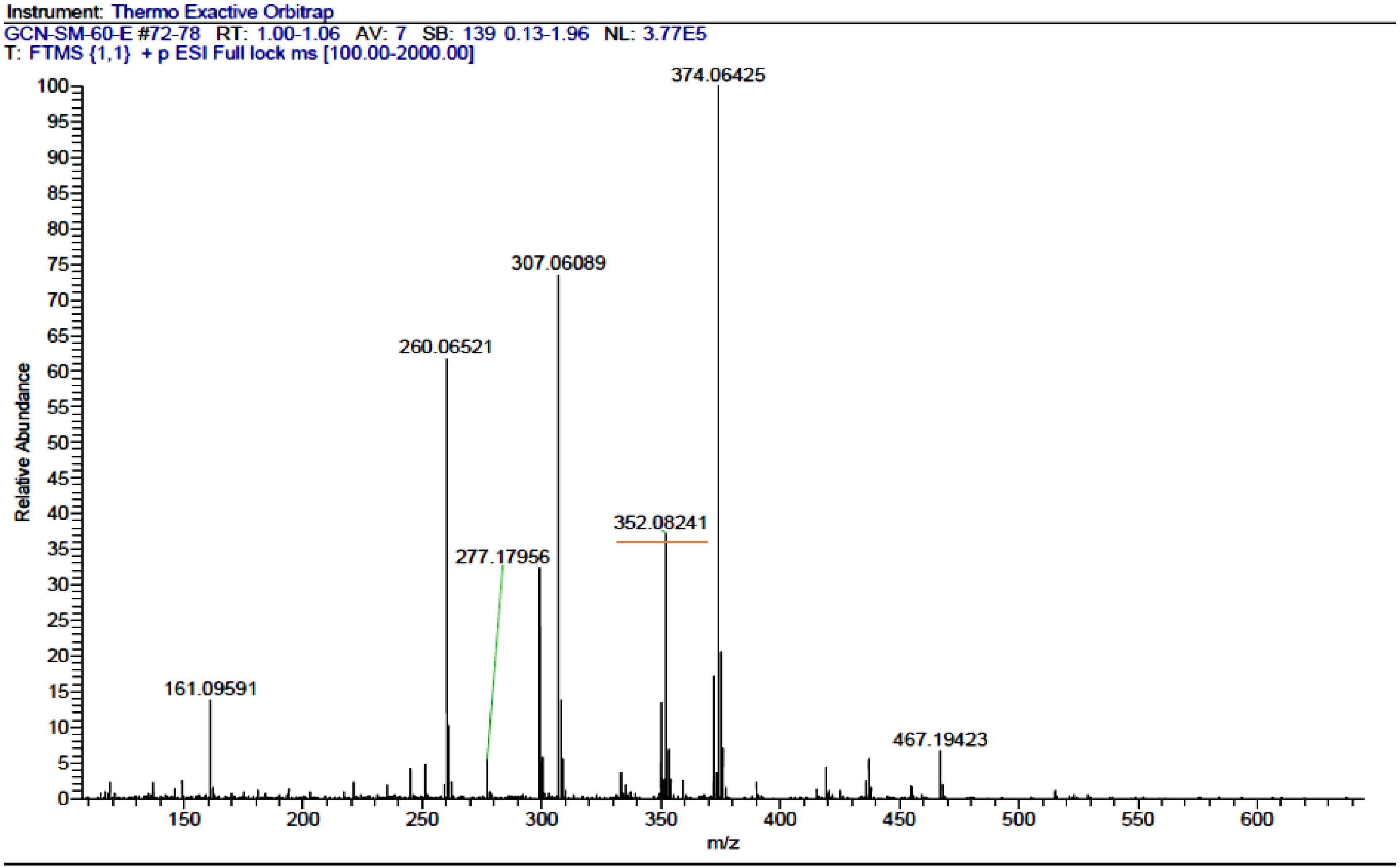


6aa ($CDCl_3$, 125 MHz)

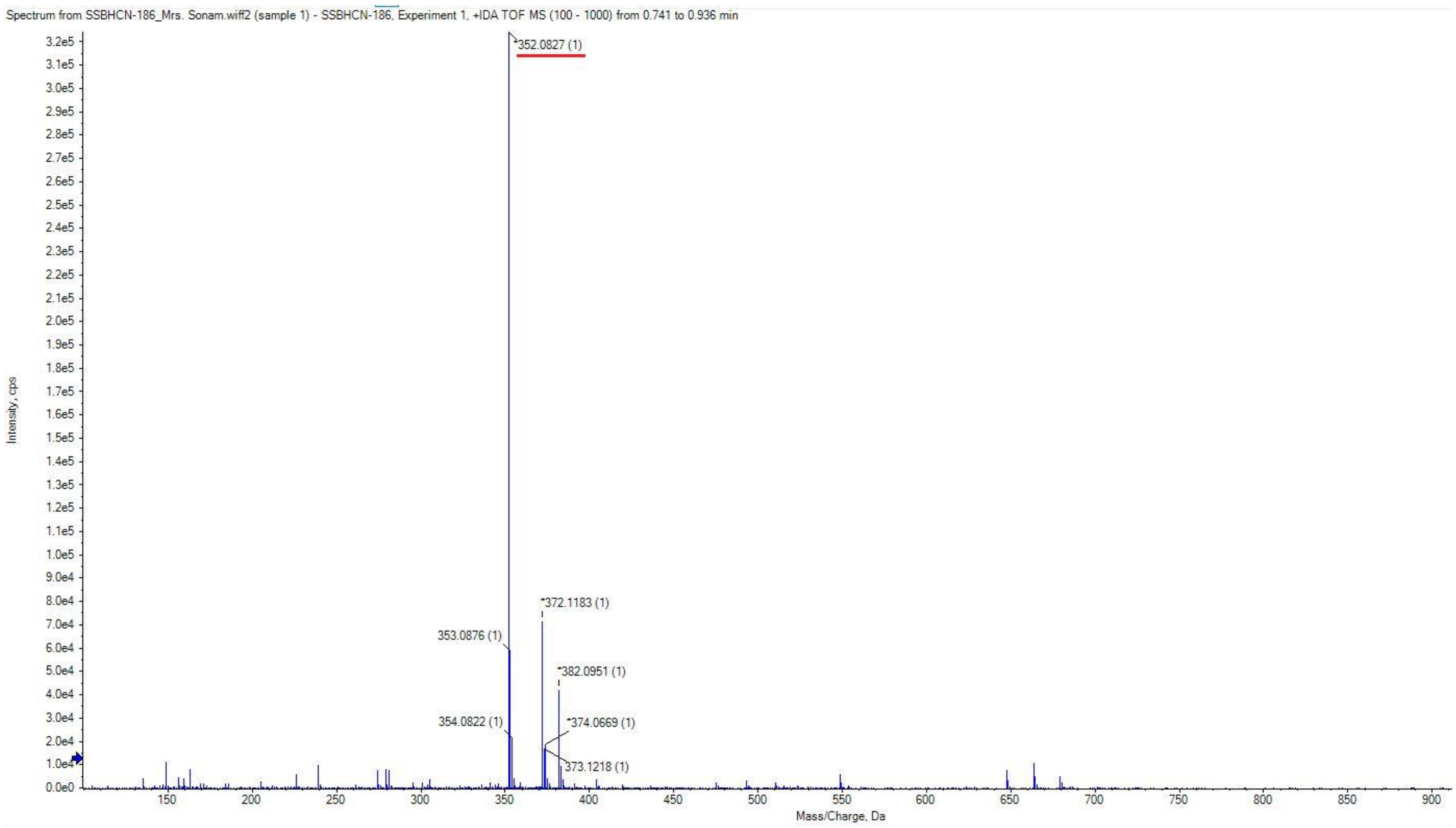
HRMS Spectra of Compound 3a



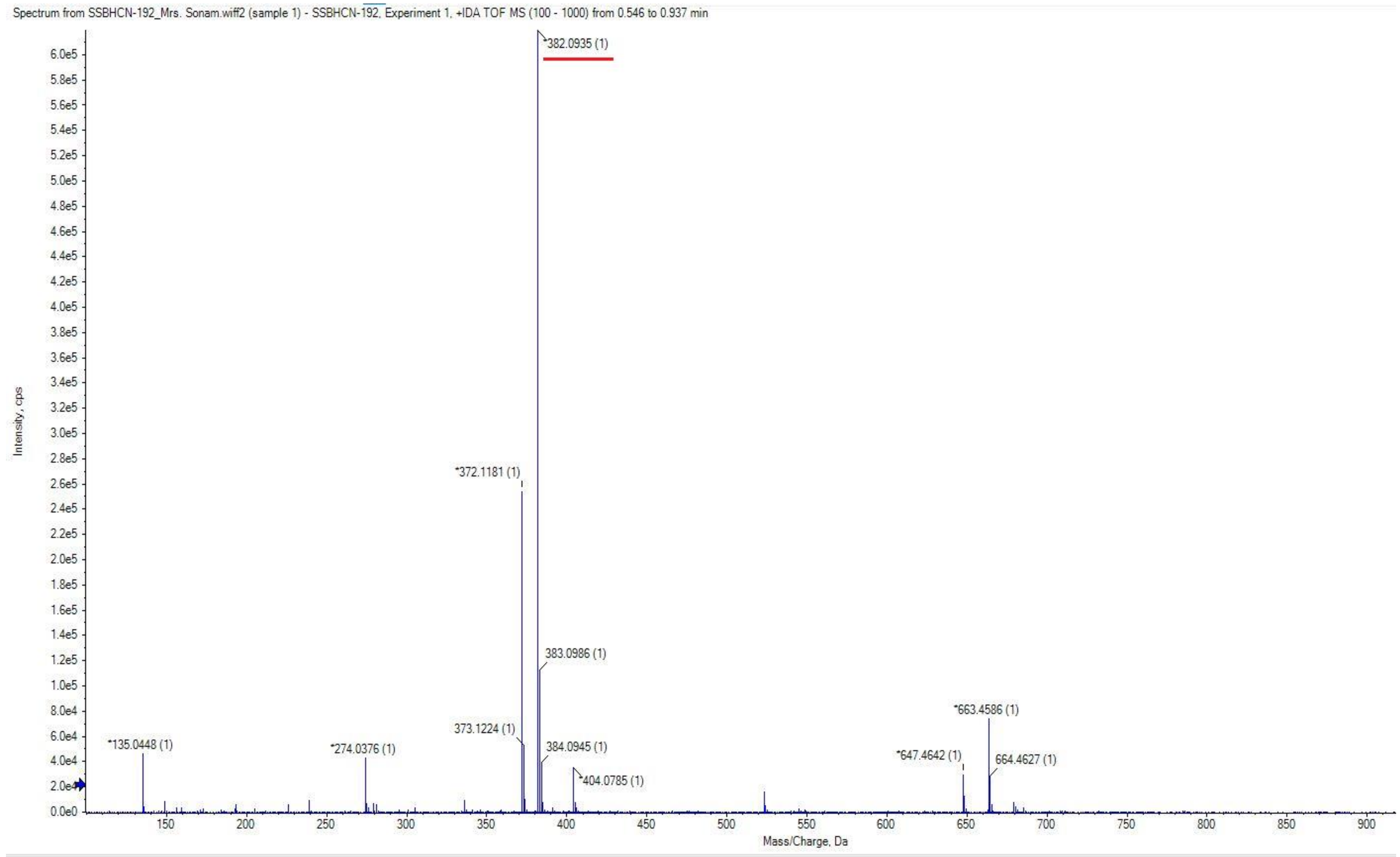
HRMS Spectra of Compound 5a



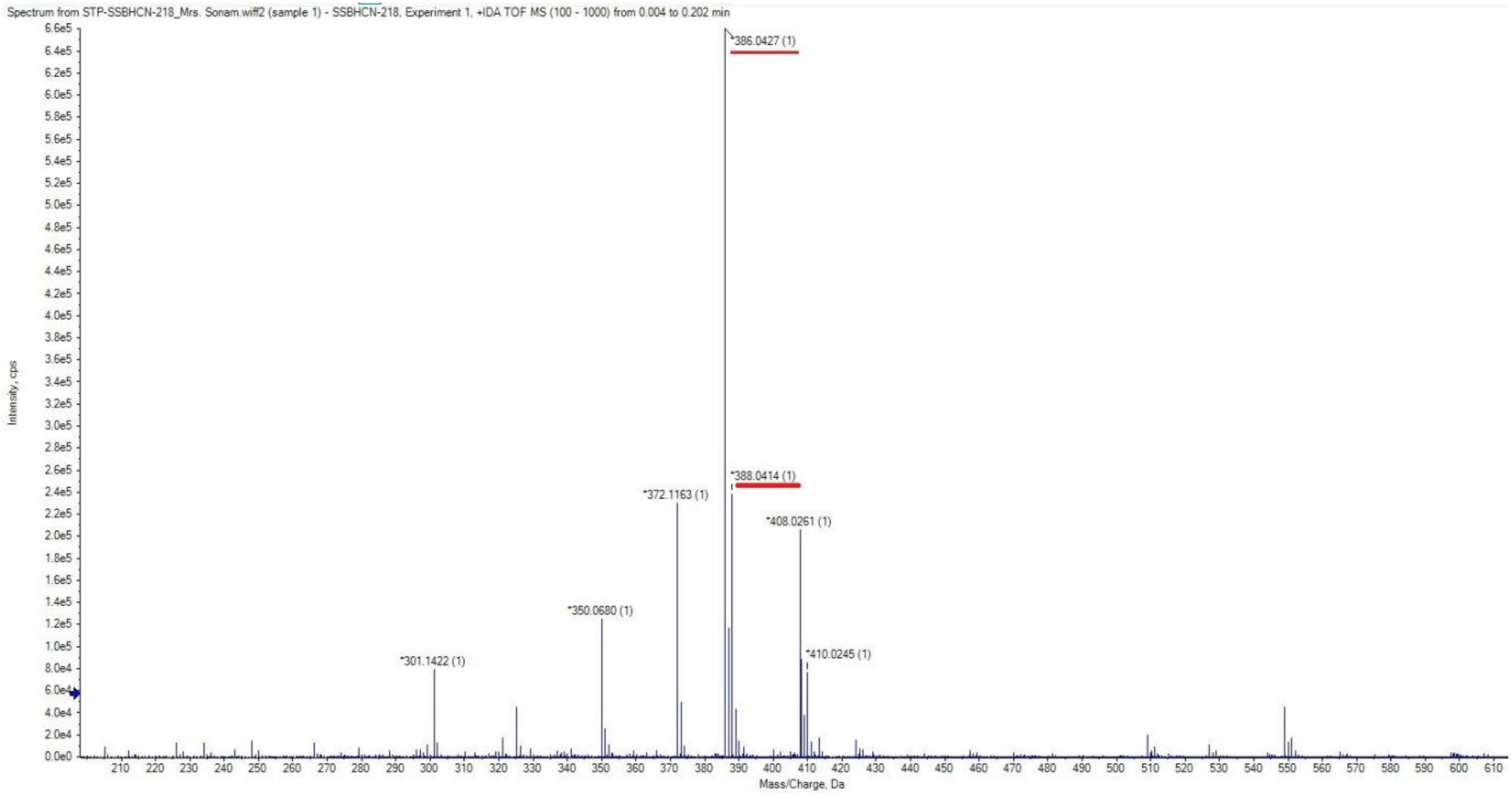
HRMS Spectra of Compound 6a



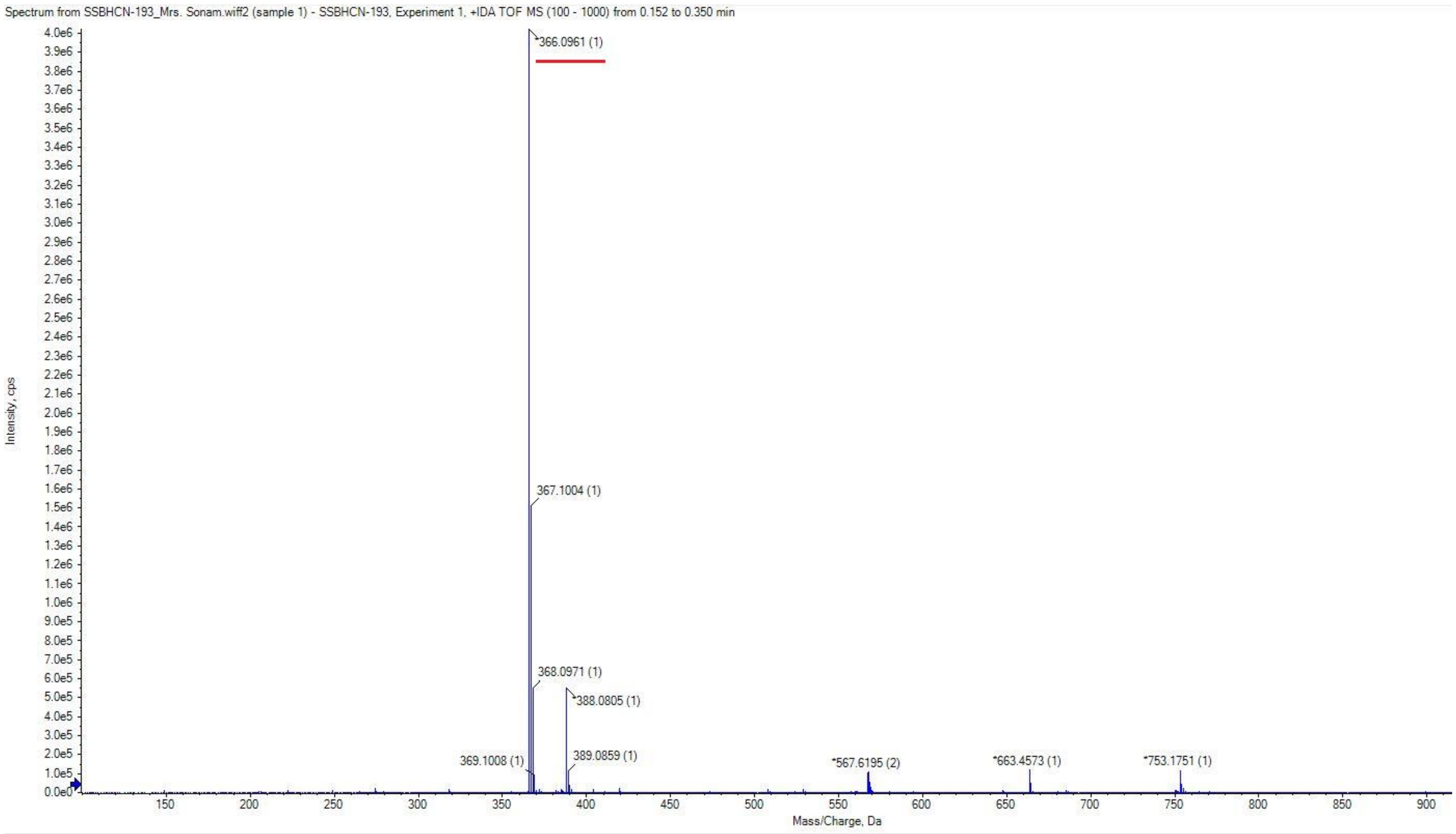
HRMS Spectra of Compound 6b



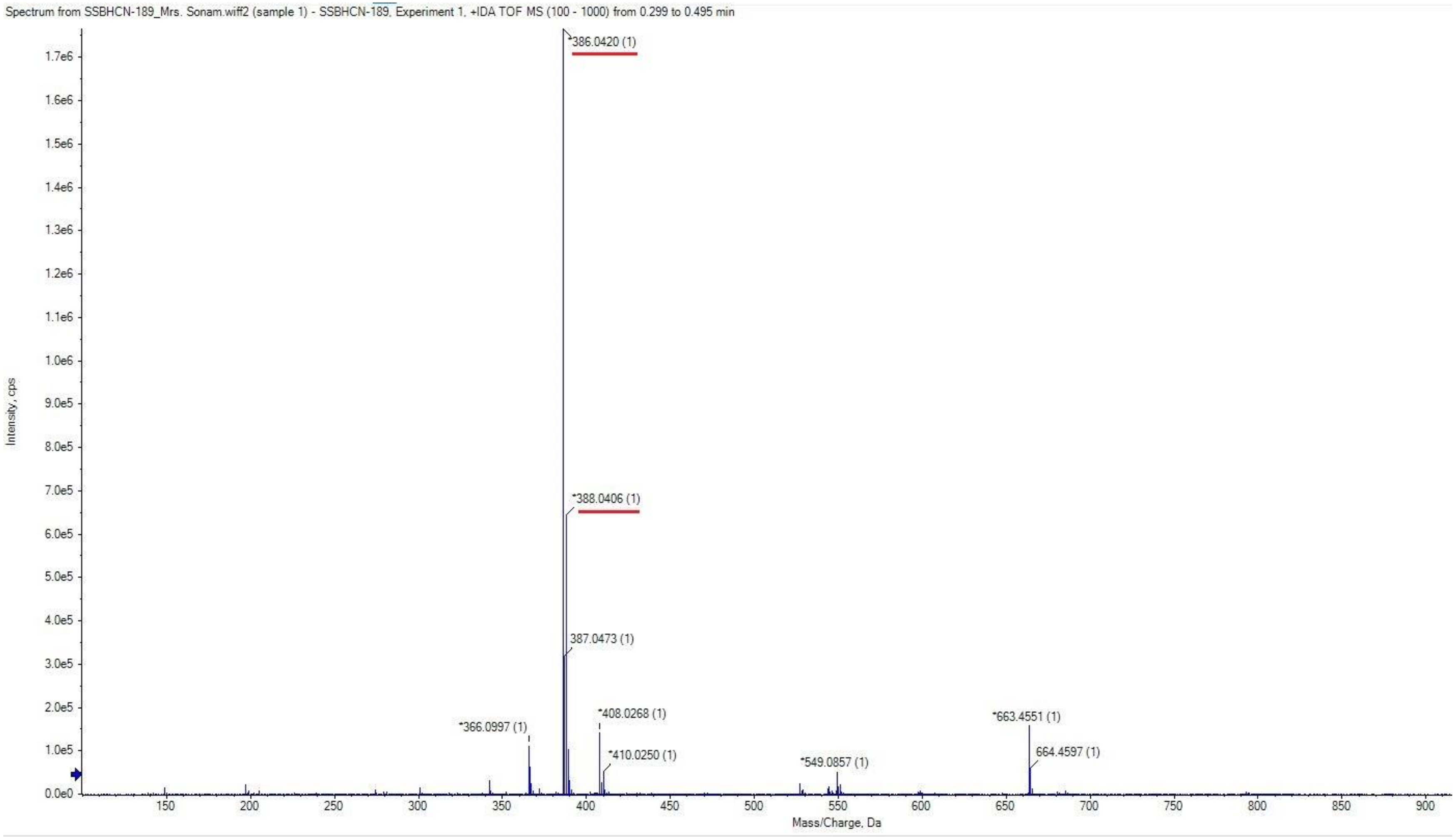
HRMS Spectra of Compound 6c



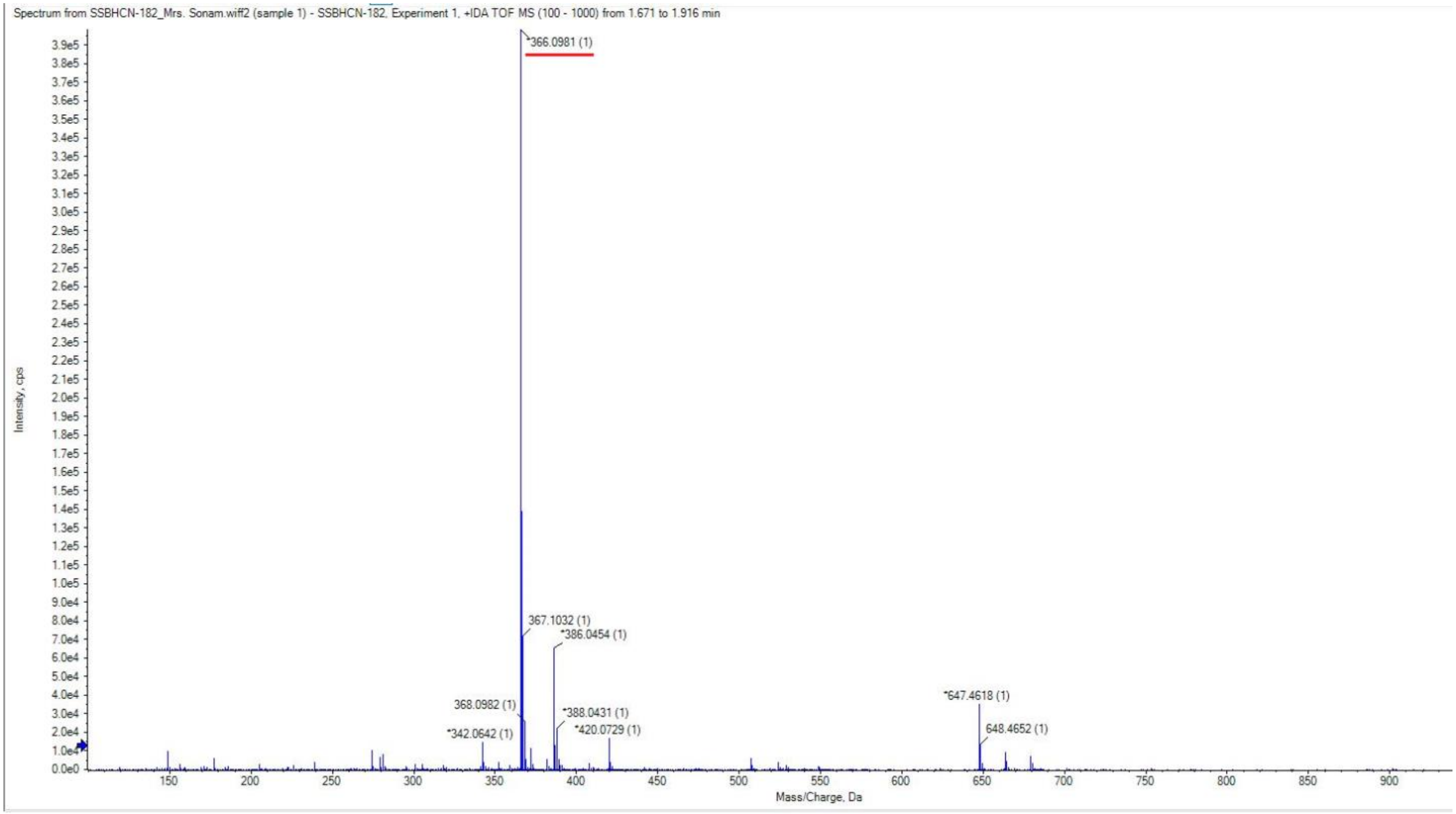
HRMS Spectra of Compound 6d



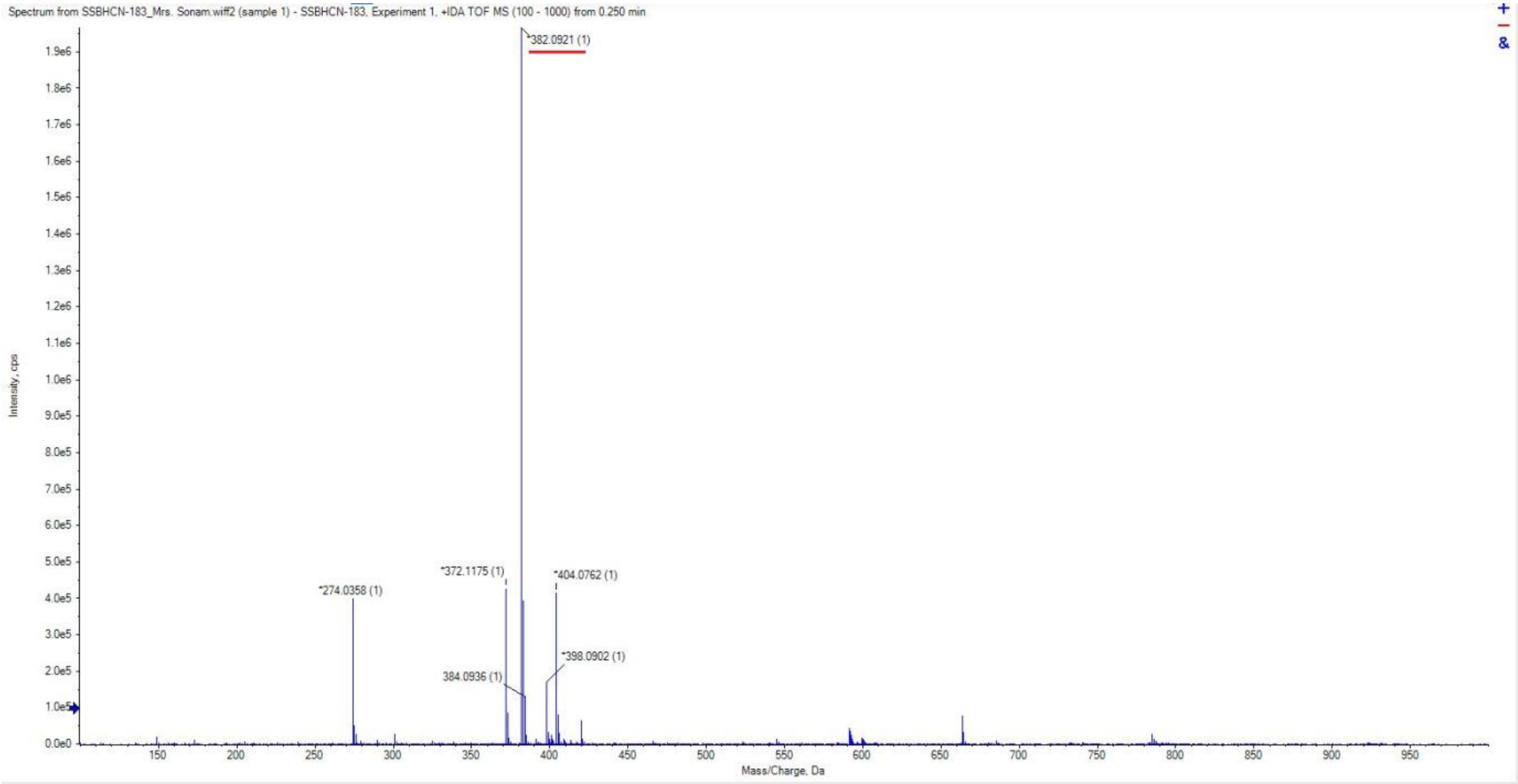
HRMS Spectra of Compound 6e



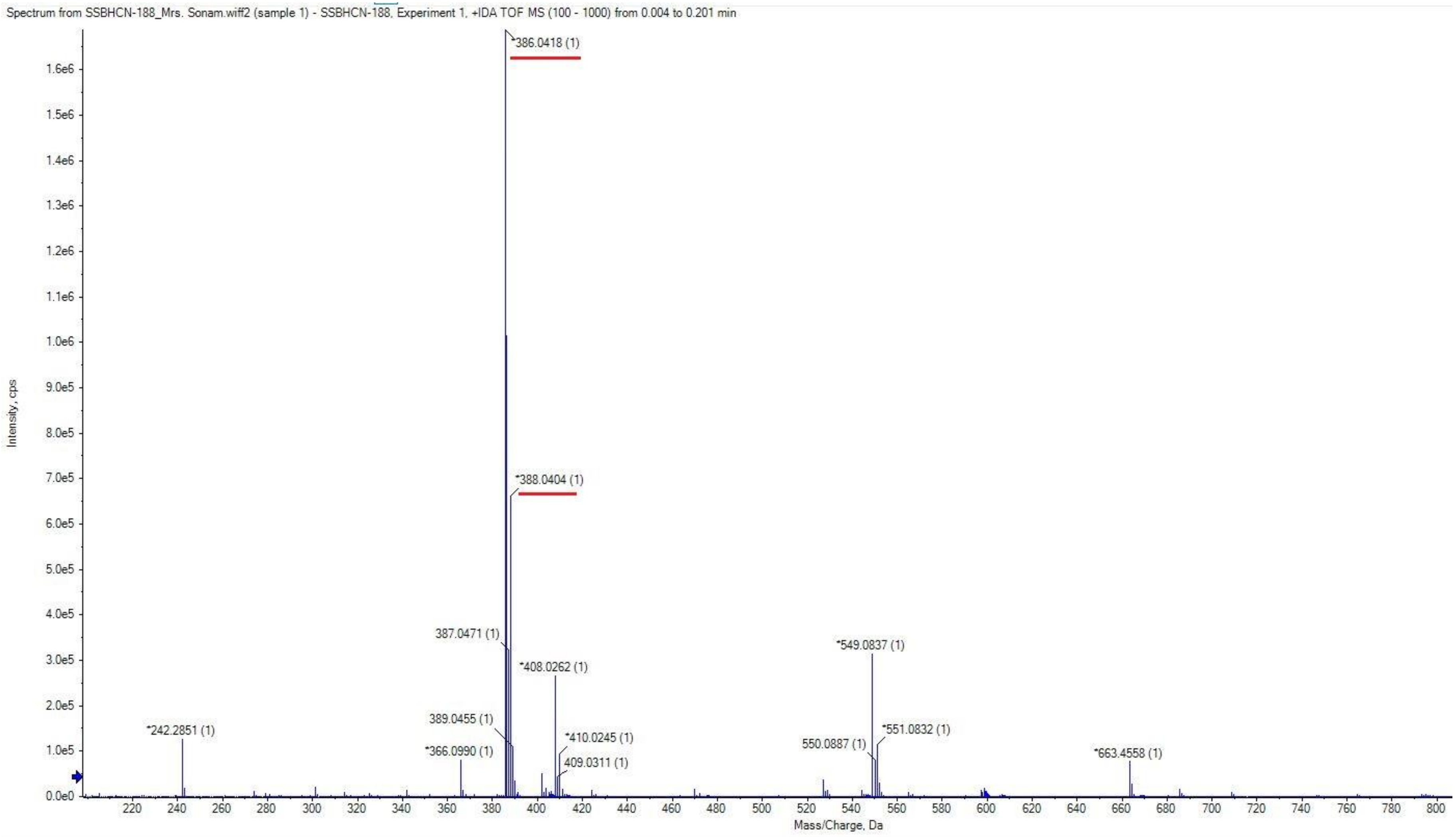
HRMS Spectra of Compound 6f



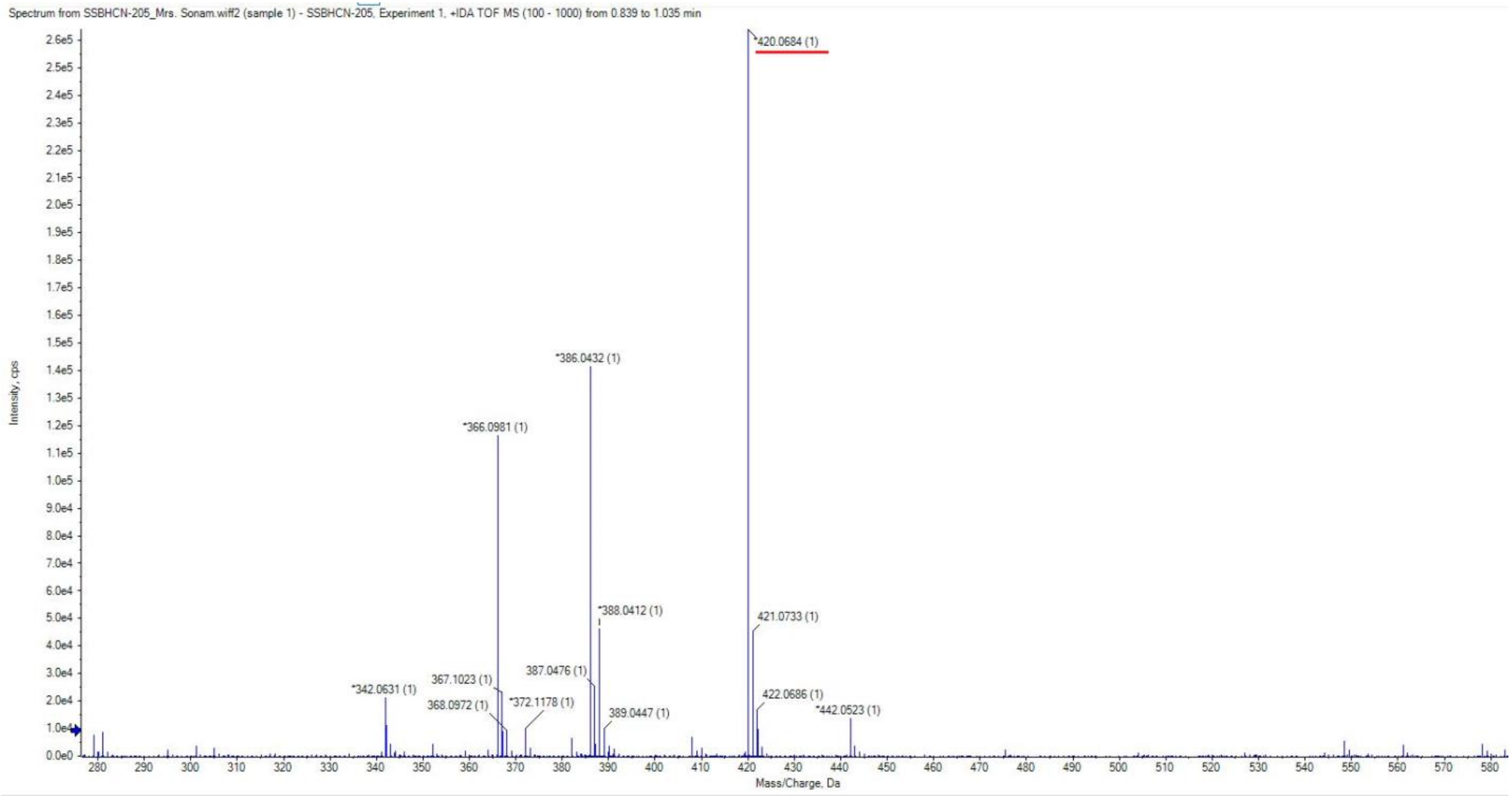
HRMS Spectra of Compound 6g



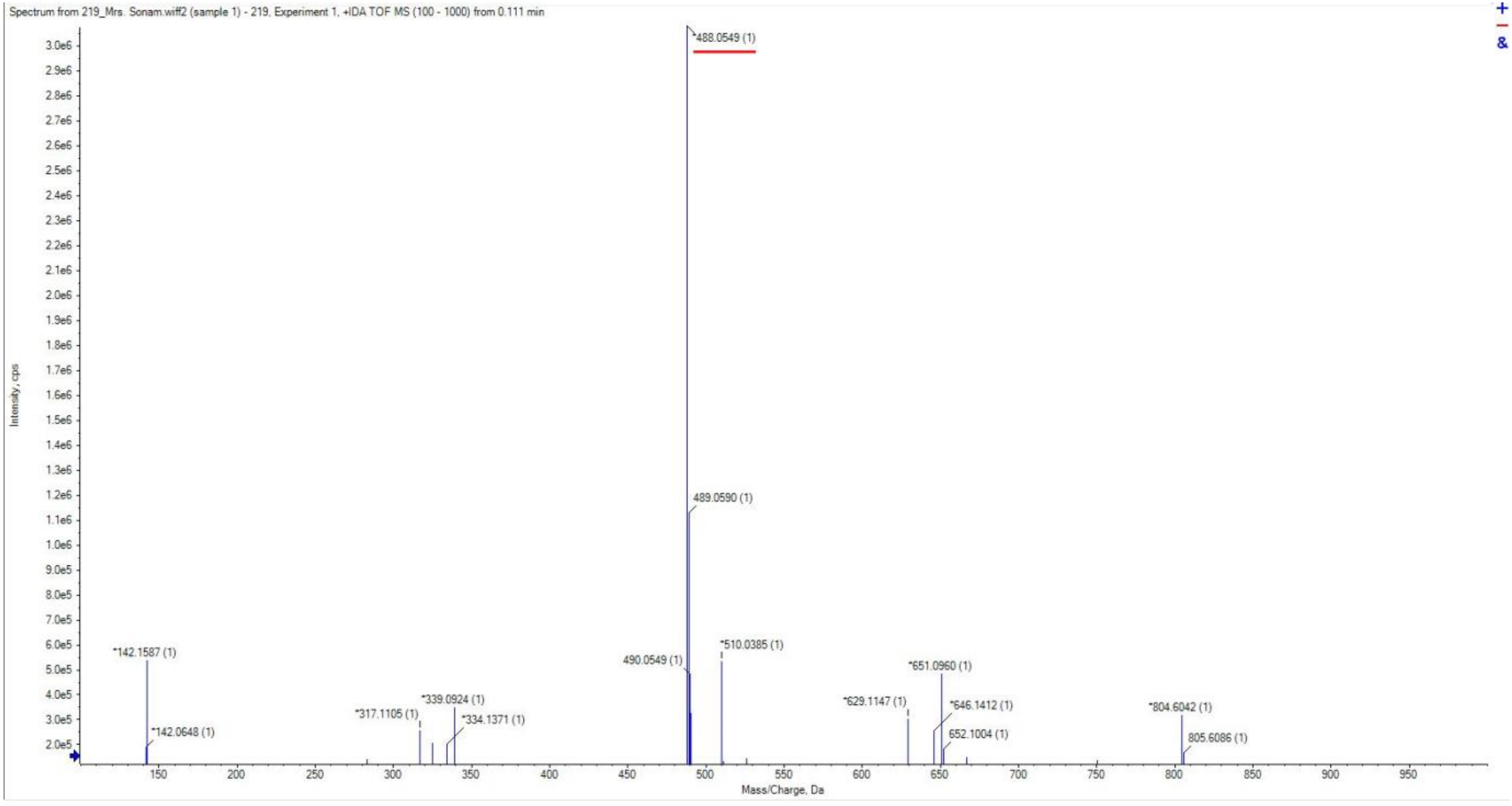
HRMS Spectra of Compound 6h



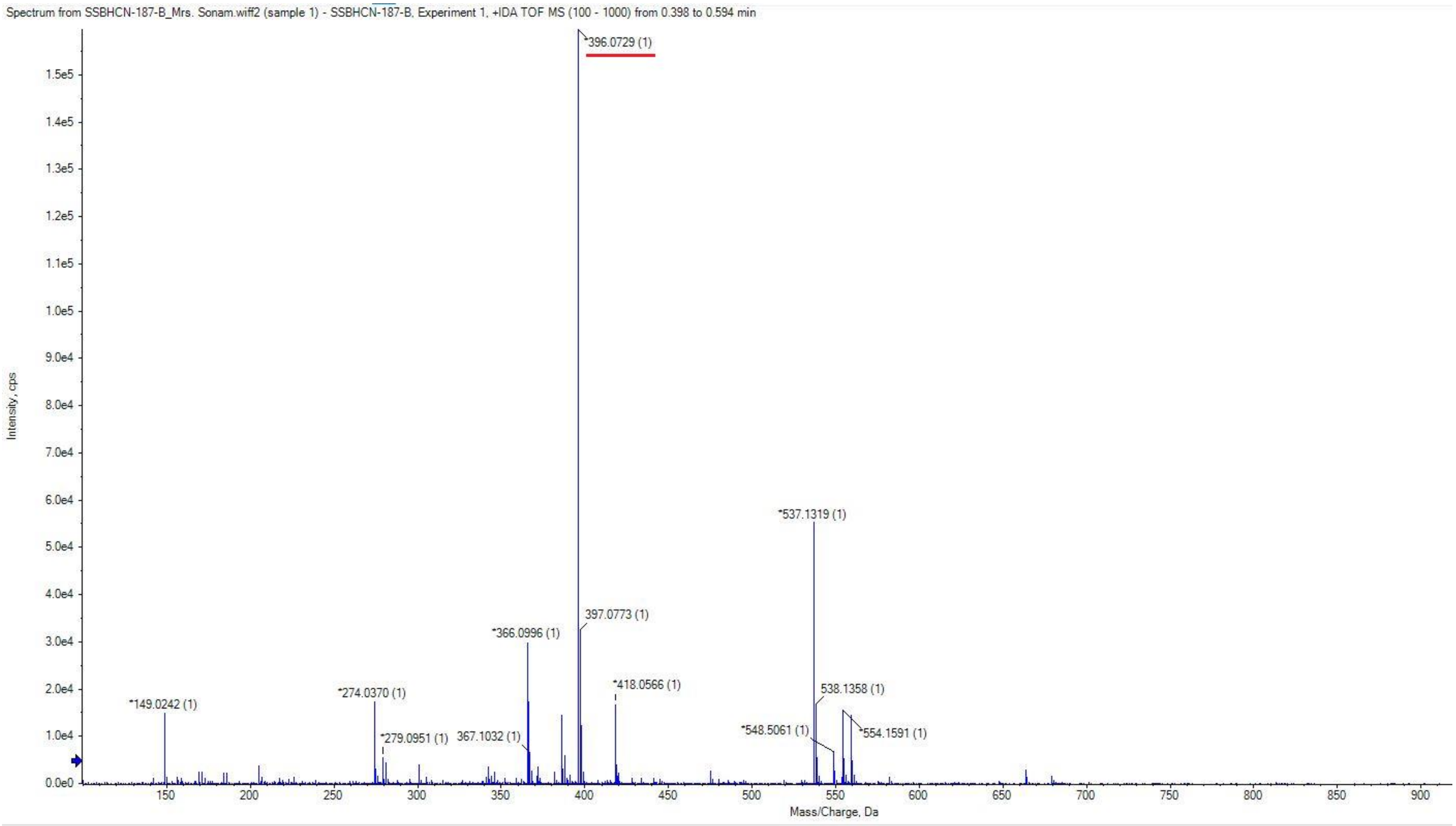
HRMS Spectra of Compound 6i



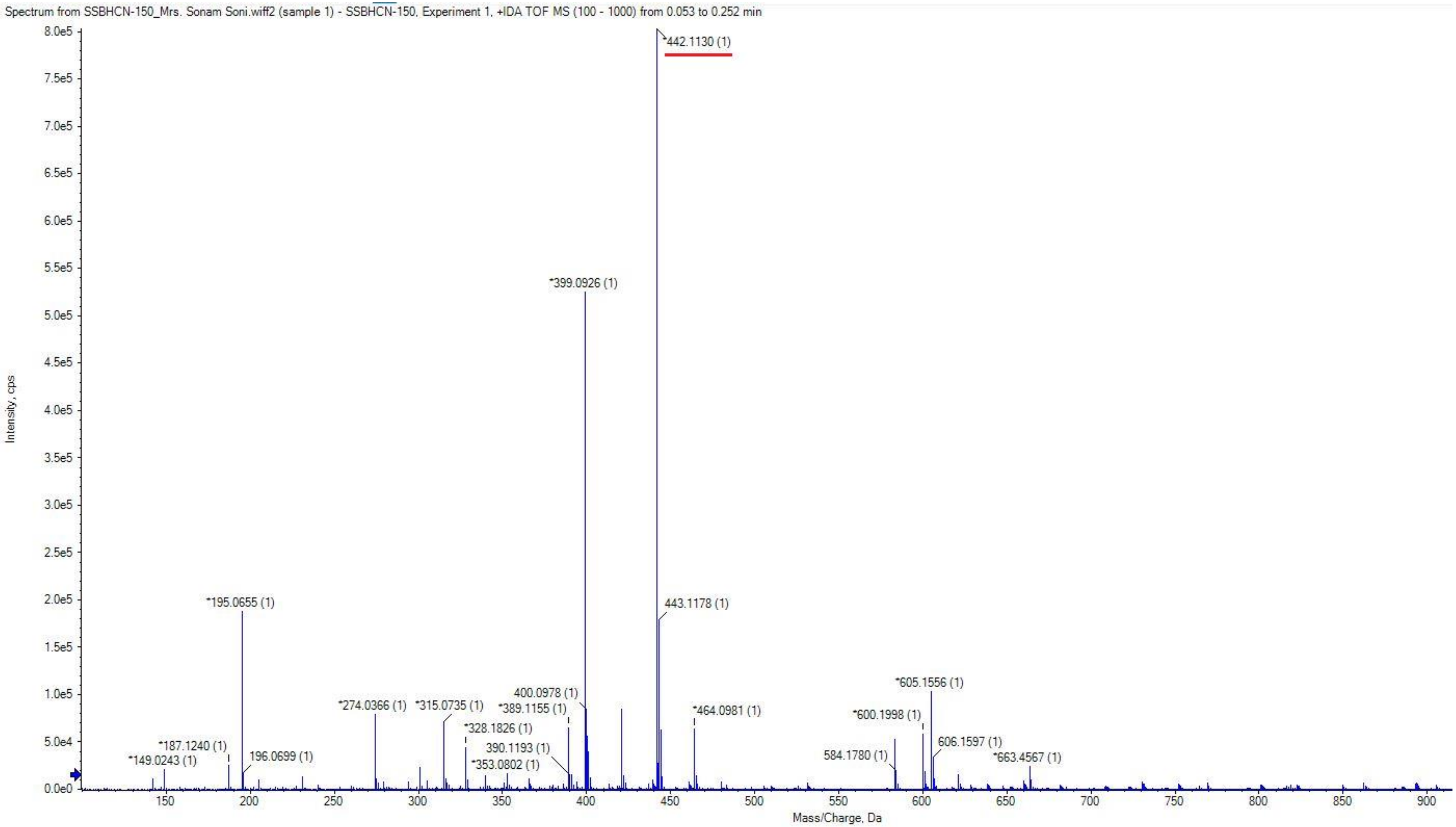
HRMS Spectra of Compound 6j



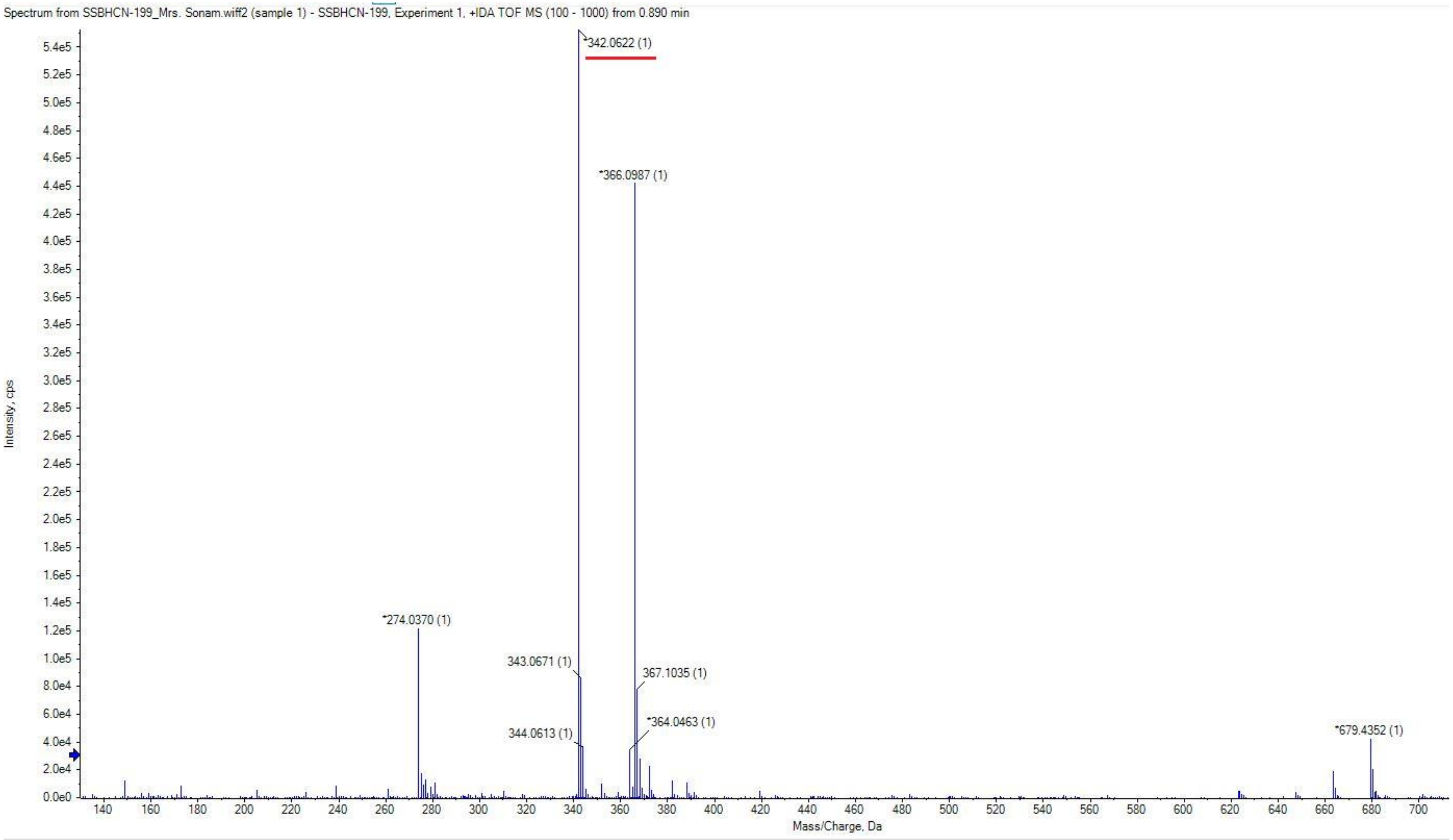
HRMS Spectra of Compound 6k



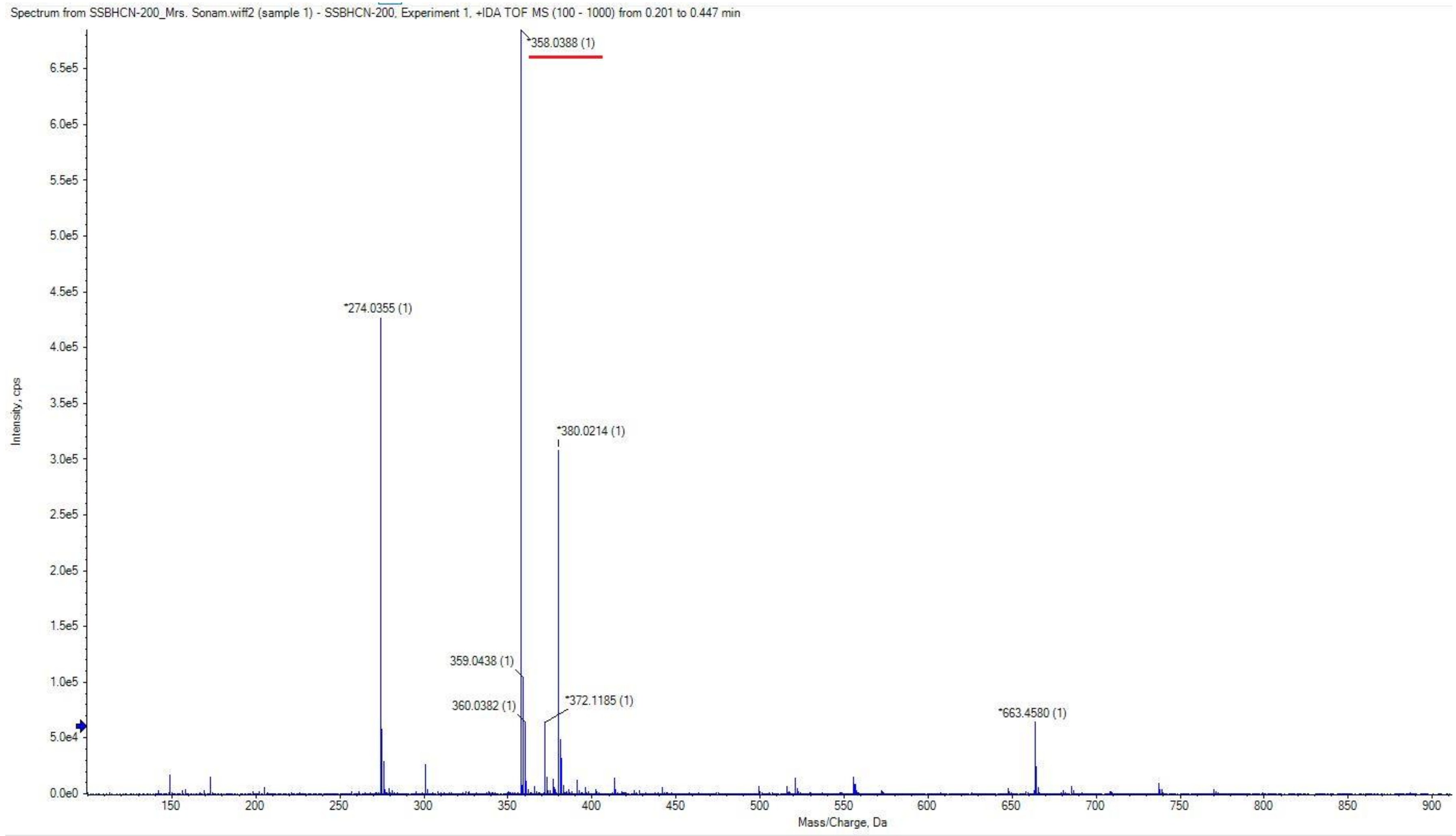
HRMS Spectra of Compound 6l



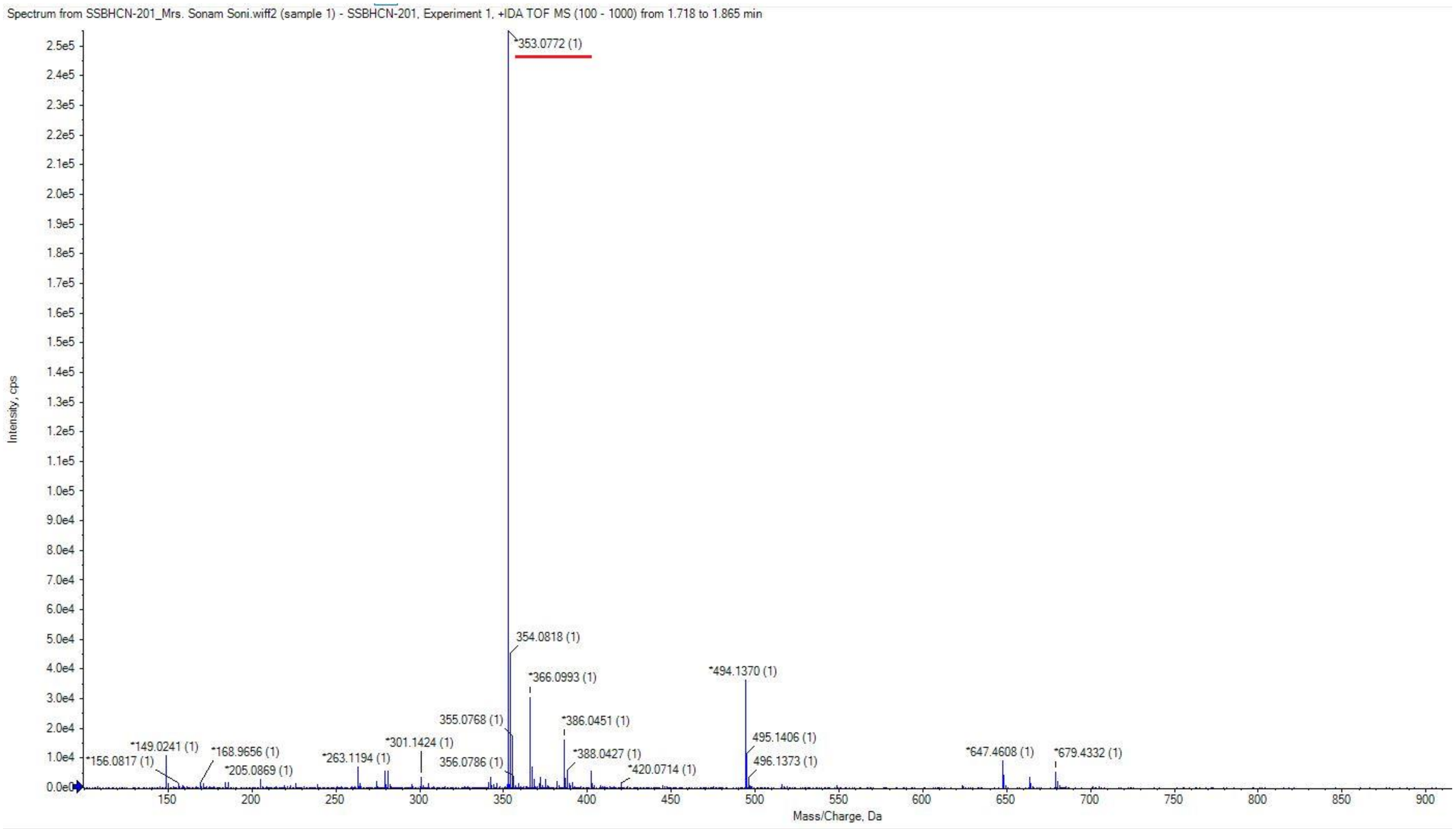
HRMS Spectra of Compound 6m



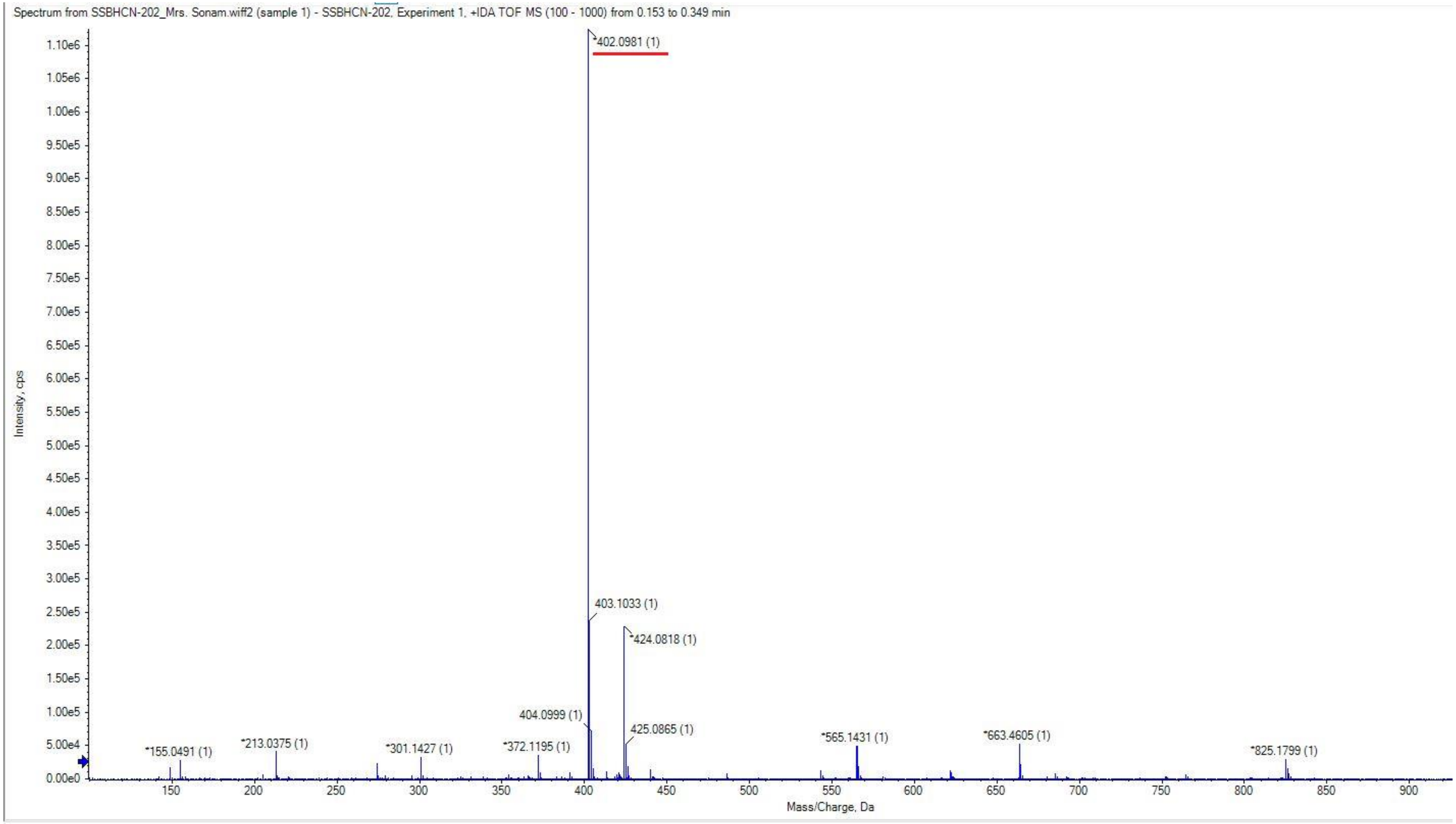
HRMS Spectra of Compound 6n



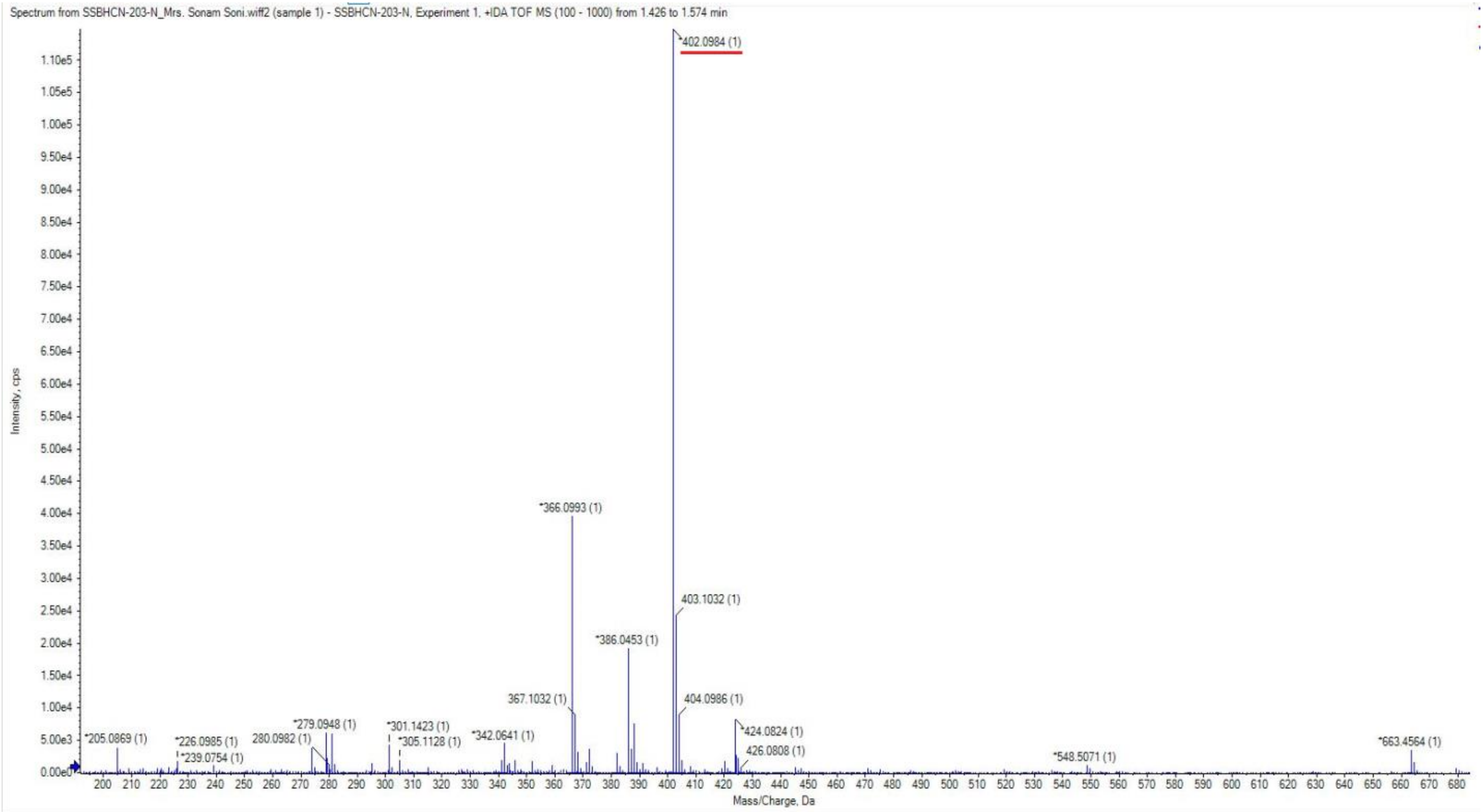
HRMS Spectra of Compound 6o



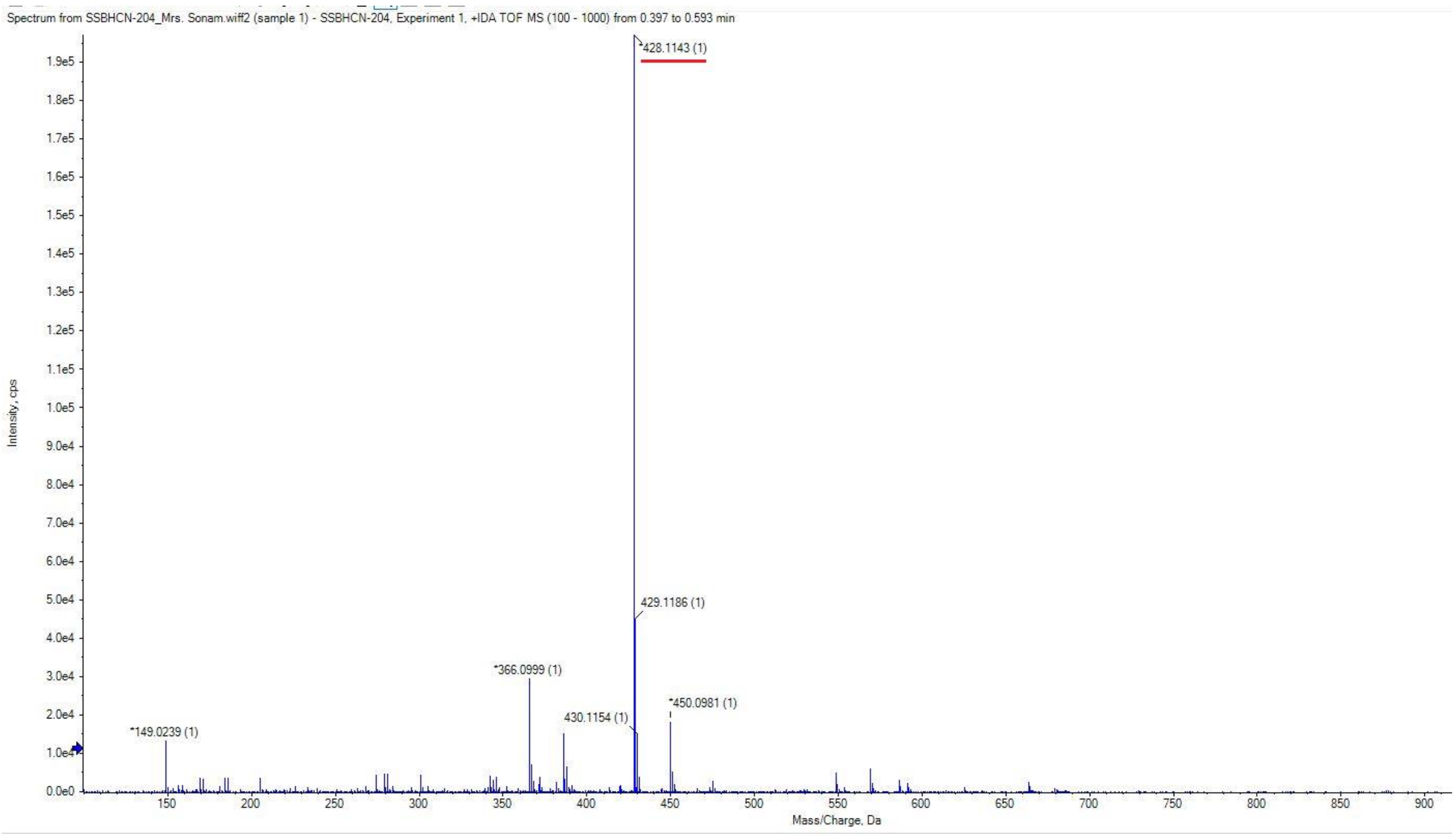
HRMS Spectra of Compound 6p



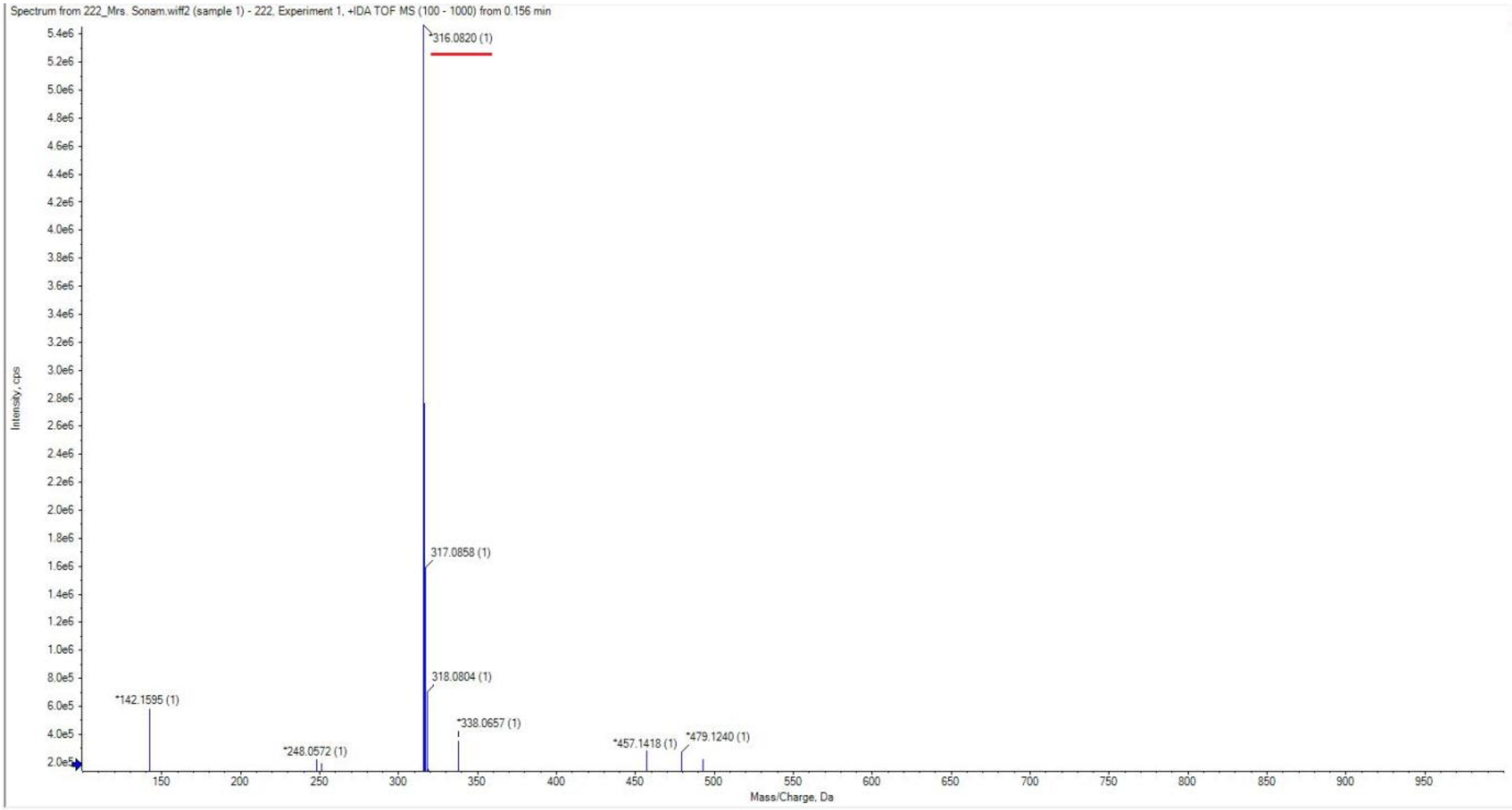
HRMS Spectra of Compound 6q



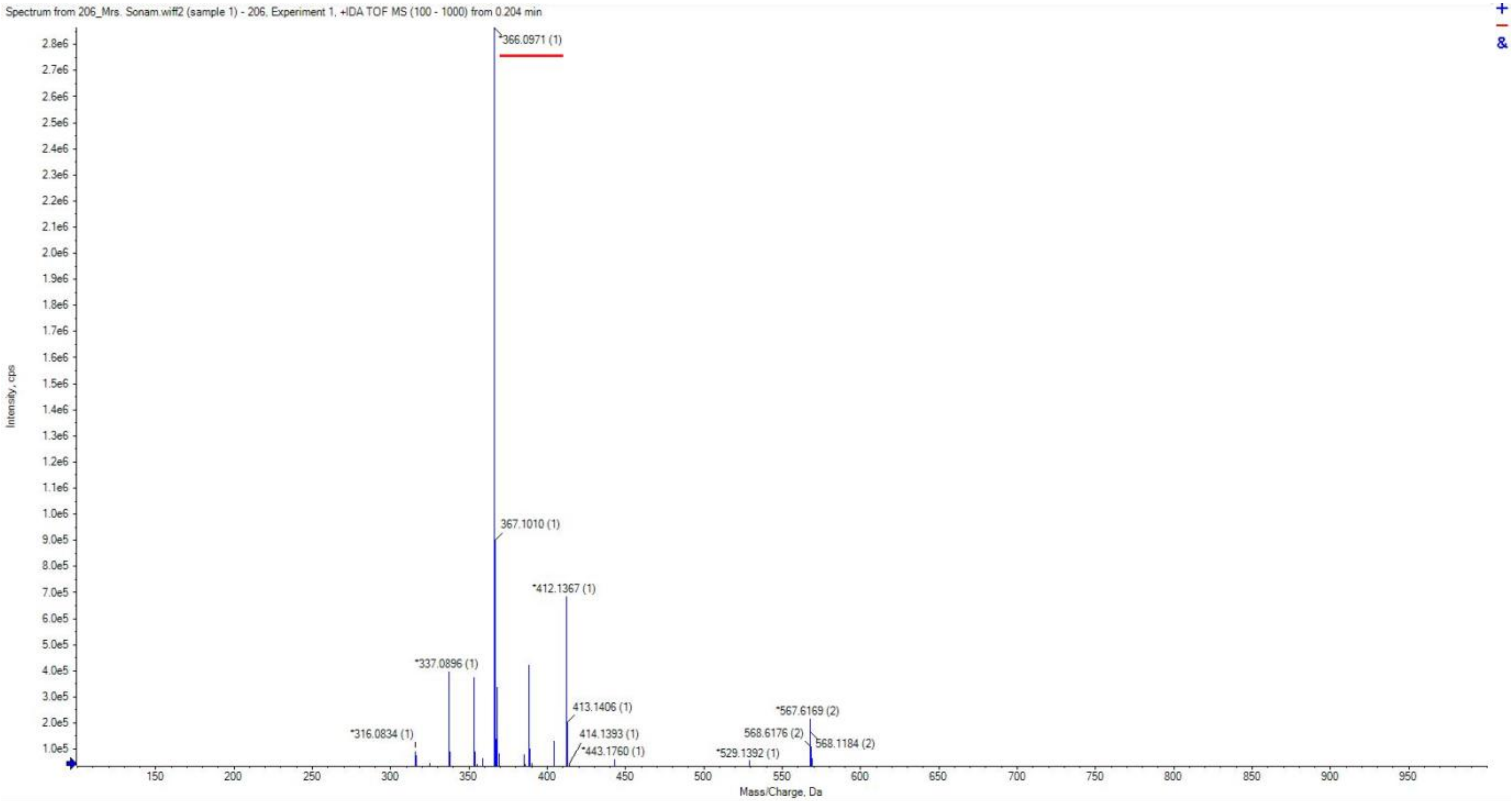
HRMS Spectra of Compound 6r



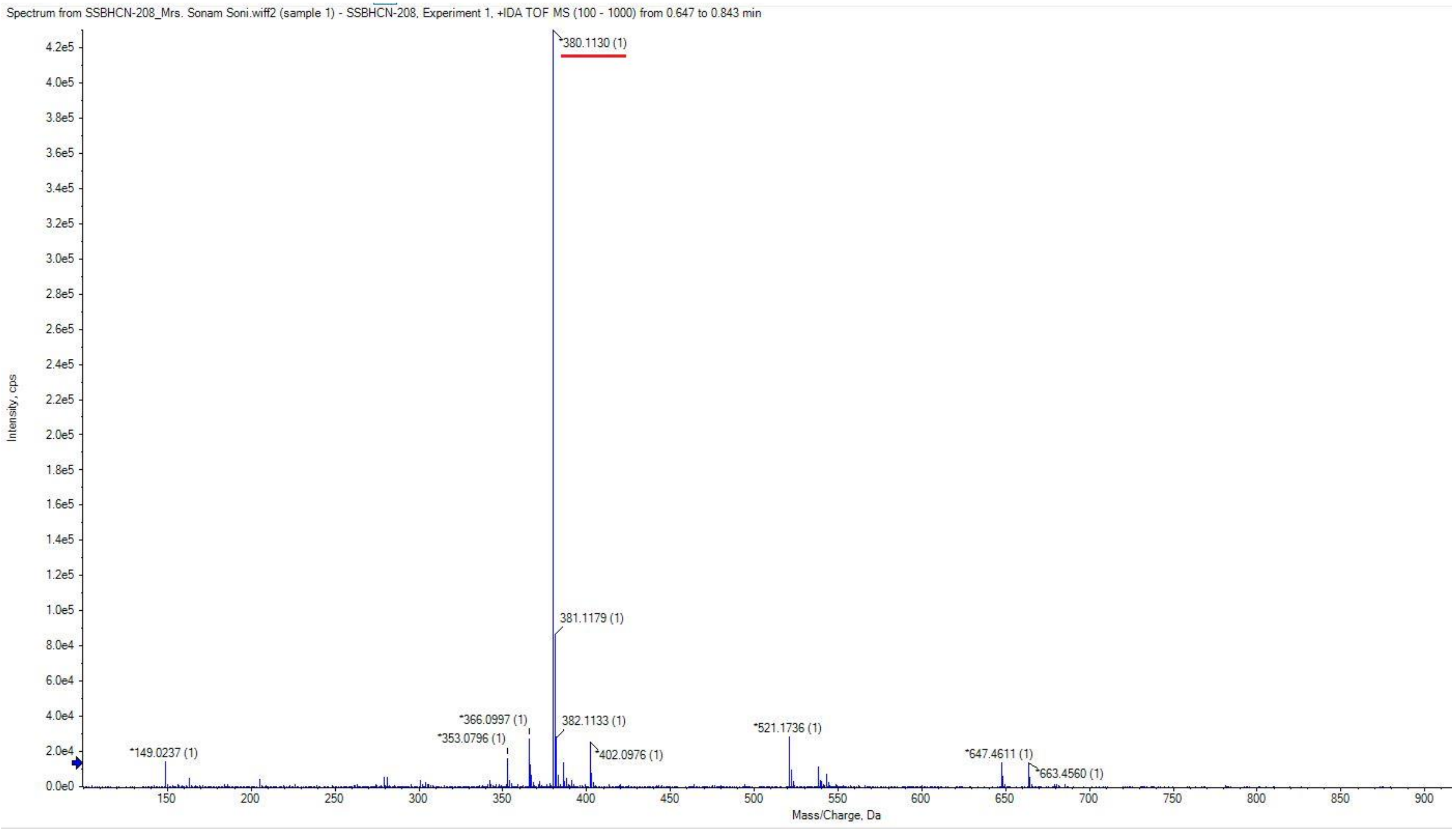
HRMS Spectra of Compound 6s



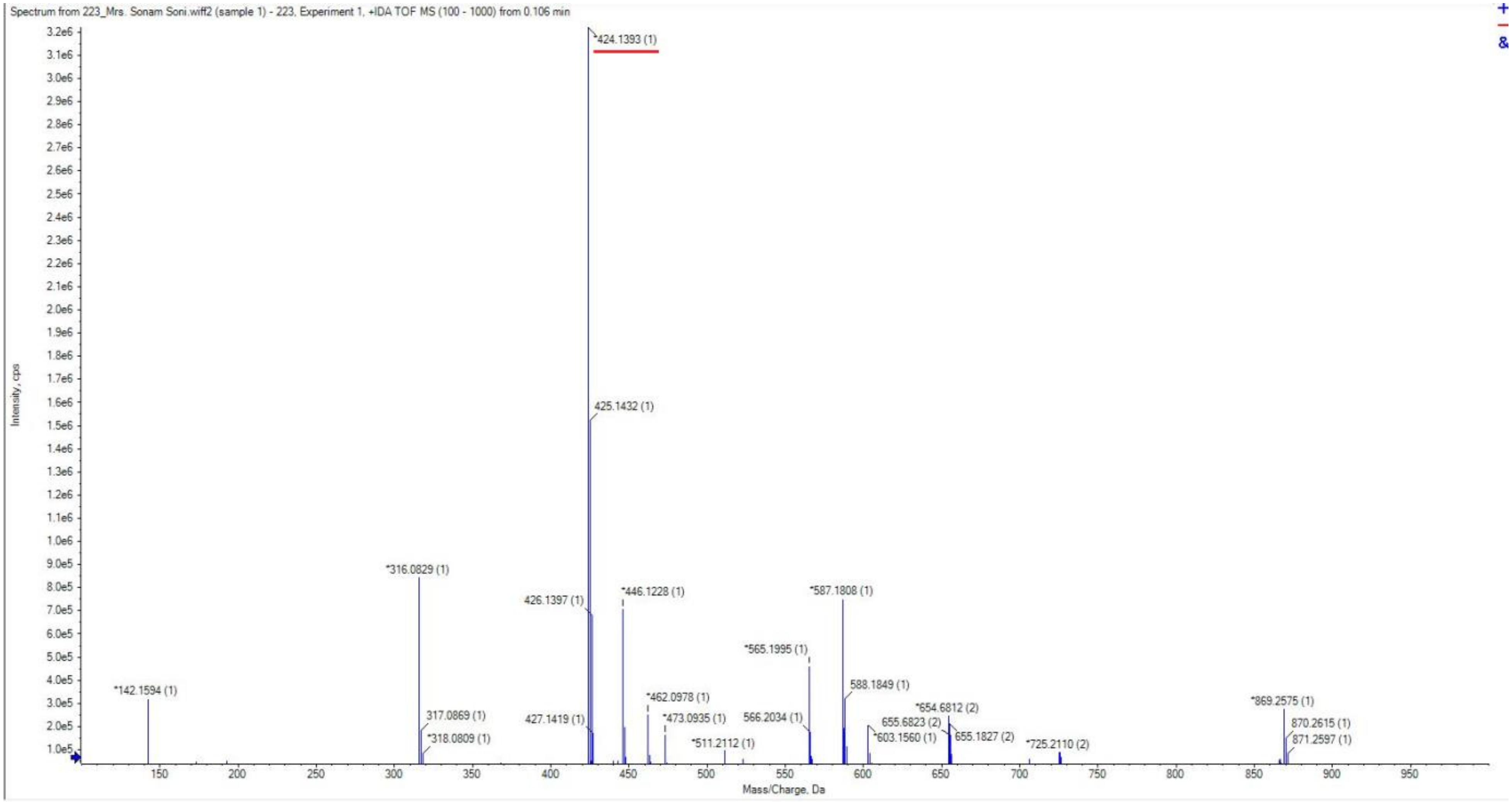
HRMS Spectra of Compound 6t



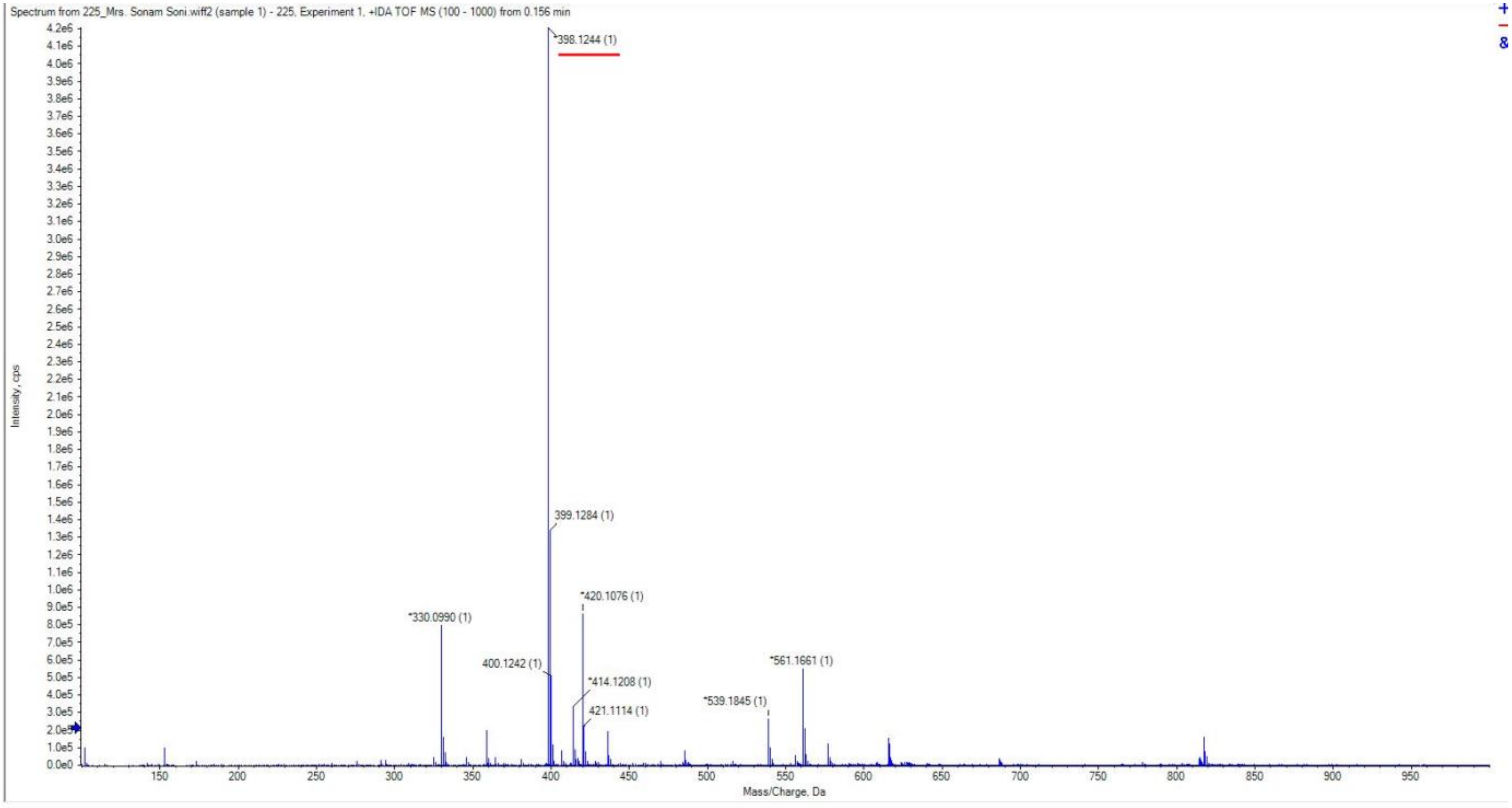
HRMS Spectra of Compound 6u



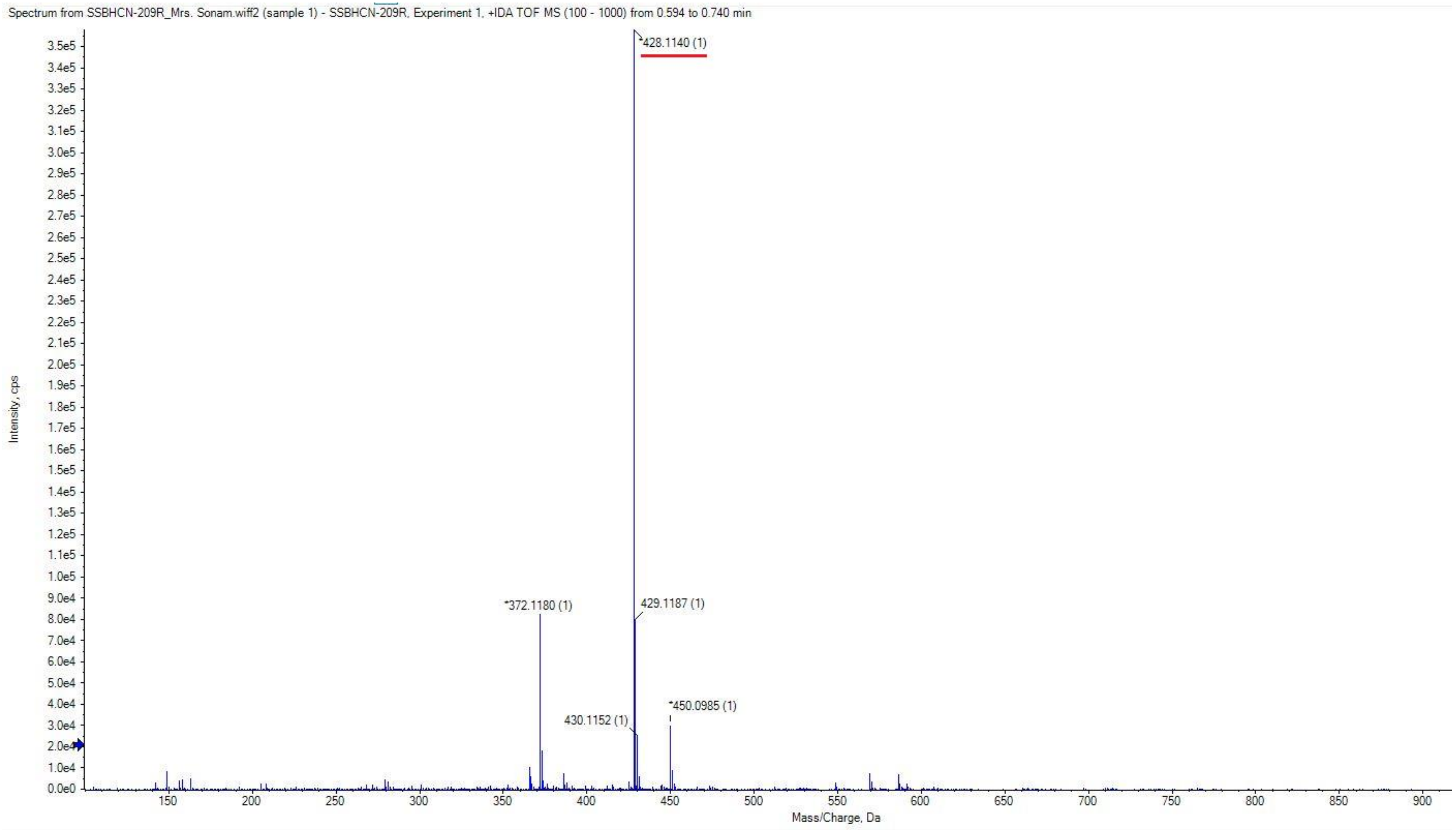
HRMS Spectra of Compound 6v



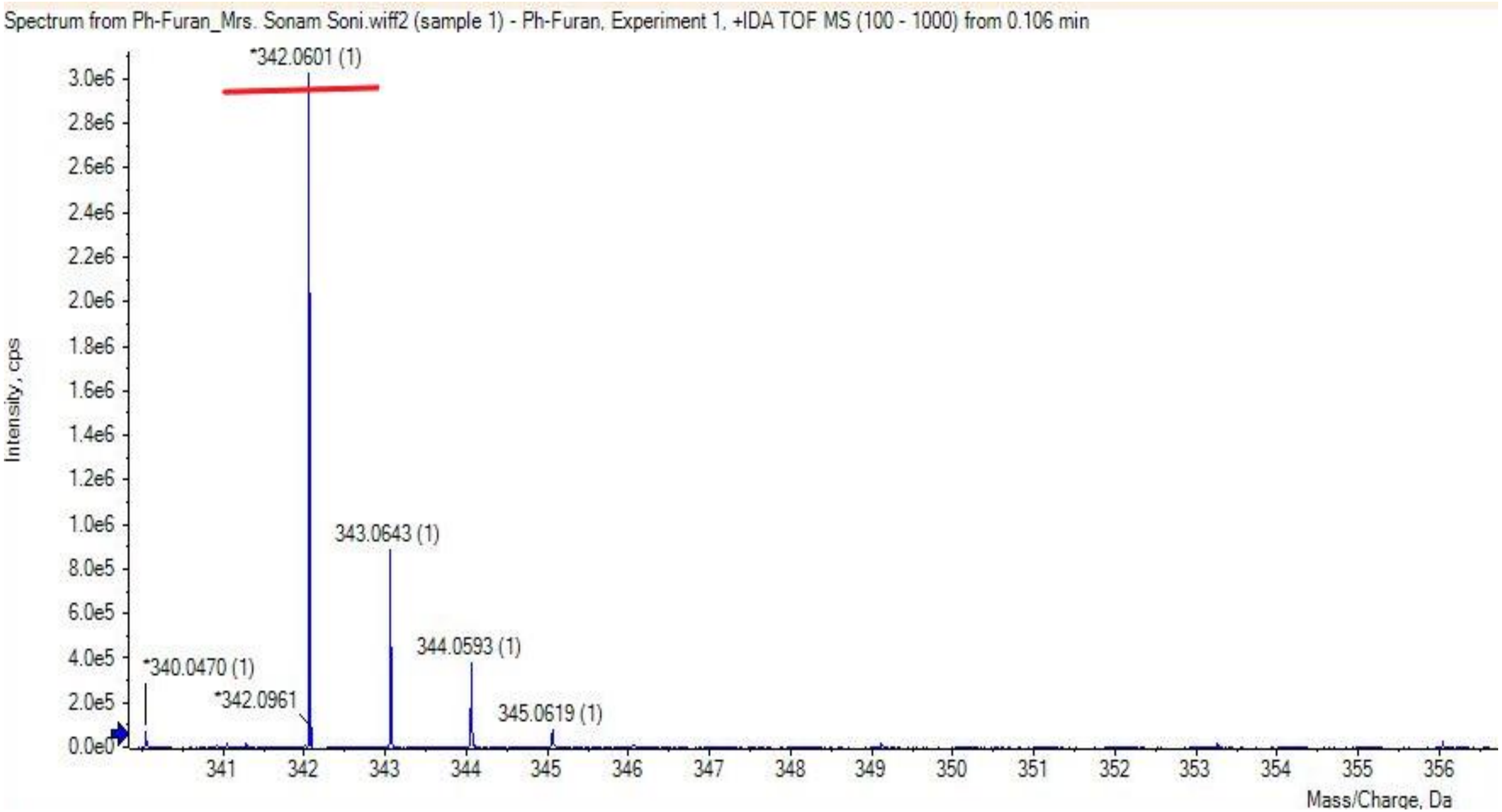
HRMS Spectra of Compound 6w



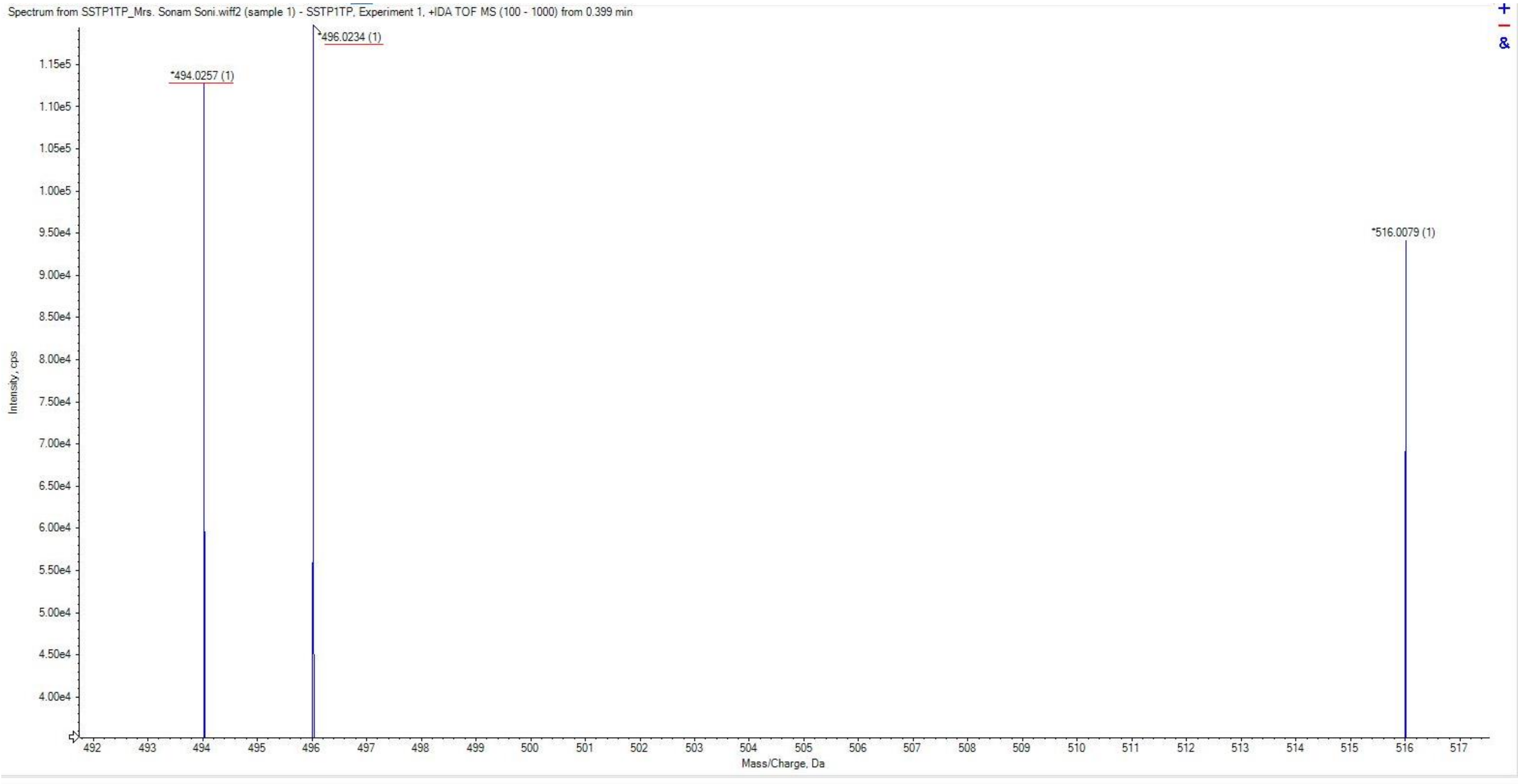
HRMS Spectra of Compound 6x



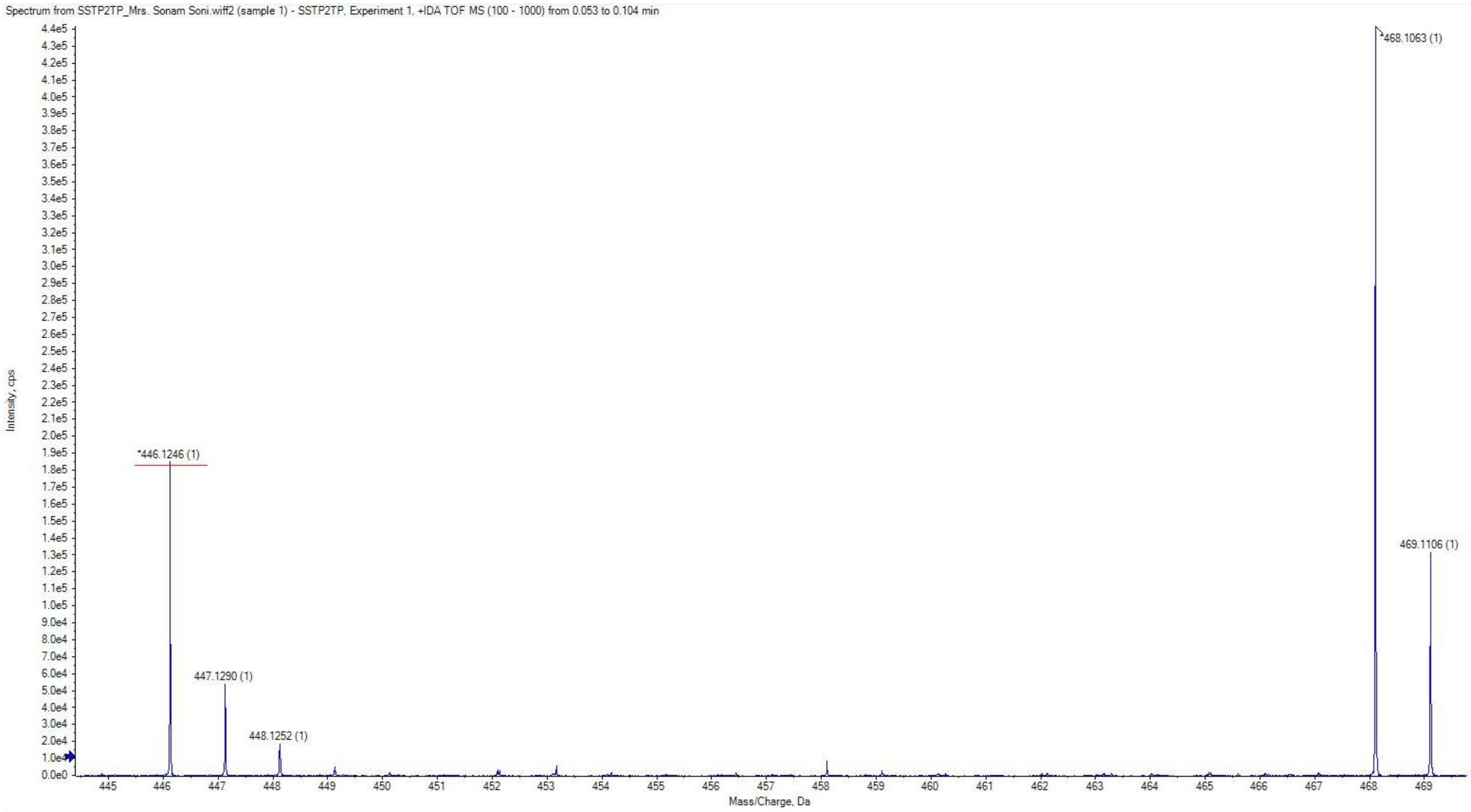
HRMS Spectra of Compound 6y



HRMS Spectra of Compound 6z

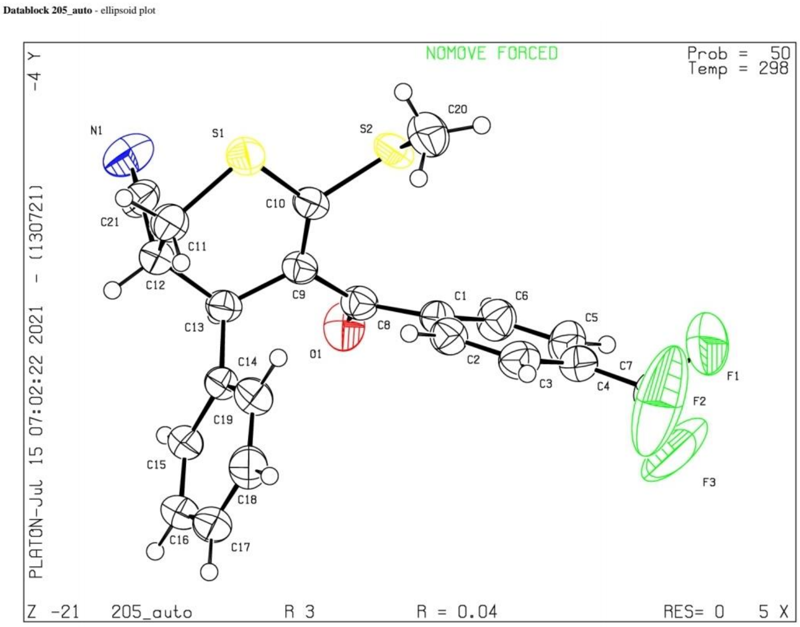


HRMS Spectra of Compound 6ab



Crystal Data[1] of 6i and 6l

ORTEP Diagram of Compound 6i (CCDC 2096630)



Crystallization Details For the crystallization of compound **6i**, vacuum dried pure sample of **6i** was taken in a vial and dissolved in 2 mL of acetonitrile. The vial was kept around 18-20 °C temperature for slow evaporation. After 5 days, we could find pale yellow needle shape crystal, which was picked up from the vial and performed single crystal XRD study.

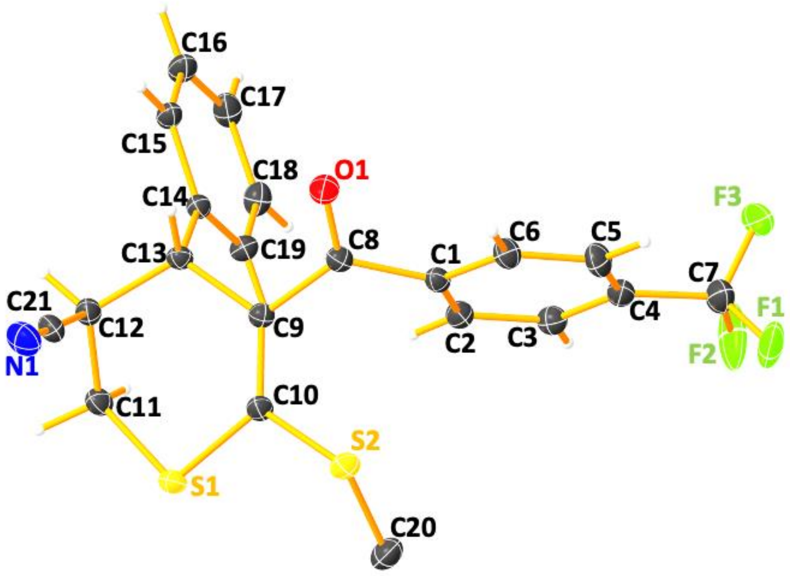


Figure S2: Thermal Ellipsoid Plot at 40% Probability Level

6i_auto

Table S1 Crystal data and structure refinement for 6i_auto.

Identification code	6i_auto
Empirical formula	$C_{21}H_{13}F_3NOS_2$
Formula weight	430.498
Temperature/K	N/A
Crystal system	trigonal
Space group	R3
a/Å	29.2329(6)
b/Å	29.2329(6)
c/Å	6.01889(12)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	4454.43(15)
Z	9
ρ_{calc}g/cm^3	1.444
μ/mm^{-1}	2.809
F(000)	2001.6
Crystal size/mm^3	N/A × N/A × N/A
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.04 to 136.12
Index ranges	$-33 \le h \le 35, -30 \le k \le 34, -7 \le l \le 3$
Reflections collected	4224
Independent reflections	2033 [R_{int} = 0.0237, R_{sigma} = 0.0257]

Data/restraints/parameters	2033/1/253
Goodness-of-fit on F^2	0.888
Final R indexes [I>=2σ (I)]	R_1 = 0.0463, wR_2 = 0.1374
Final R indexes [all data]	R_1 = 0.0468, wR_2 = 0.1387
Largest diff. peak/hole / e Å^{-3}	0.27/-0.18
Flack parameter	-0.00(2)

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6i_auto. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	-4708.2(4)	-3806.0(4)	-2519.4(19)	56.3(3)
O1	-5047.7(14)	-5035.3(14)	-8971(5)	59.2(8)
C8	-4899.2(14)	-4960.2(14)	-7034(6)	42.2(7)
C13	-5540.3(13)	-4659.9(14)	-6026(6)	41.0(7)
C1	-4657.9(14)	-5270.4(14)	-6126(6)	42.1(7)
C12	-5592.1(15)	-4190.3(15)	-5160(7)	45.7(8)
C9	-5004.4(14)	-4609.5(14)	-5602(5)	39.0(7)
C11	-5404.1(17)	-4048.8(17)	-2771(7)	51.3(9)
C10	-4634.4(14)	-4240.7(15)	-4250(6)	43.0(8)
C14	-5997.3(14)	-5180.7(14)	-5163(6)	39.6(7)
C21	-5300.6(19)	-3729.8(16)	-6653(7)	52.5(9)
C7	-4158(2)	-6350(2)	-4034(11)	72.5(13)
C2	-4766.1(15)	-5470.2(16)	-3981(7)	47.3(8)
N1	-5085(2)	-3389.5(17)	-7824(8)	73.0(12)
S2	-3974.5(3)	-4100.5(4)	-4435(2)	53.3(3)
C16	-6876.2(16)	-5915.5(18)	-5698(9)	58.4(11)
C15	-6450.5(15)	-5453.6(15)	-6460(7)	48.3(8)
C17	-6853.7(17)	-6121.4(17)	-3666(10)	61.1(11)
C19	-5979.8(16)	-5393.0(17)	-3095(6)	48.1(8)
C6	-4373.8(18)	-5407.3(18)	-7558(7)	52.6(9)
C3	-4599.7(18)	-5821.3(17)	-3300(7)	53.4(9)
C5	-4207.2(19)	-5751(2)	-6868(8)	61.6(11)
C20	-3805(2)	-4143(2)	-1574(9)	69.0(13)
C4	-4322.4(17)	-5960.3(17)	-4742(8)	54.0(10)
C18	-6412.9(18)	-5863.6(19)	-2375(8)	56.6(10)
F1	-3658(2)	-6168(2)	-4206(11)	162(3)
F3	-4361(3)	-6760.2(19)	-5168(11)	217(5)
F2	-4244(5)	-6477(4)	-1975(10)	218(5)

Table S3 Anisotropic Displacement Parameters (Å^2×10^3) for 6i_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 6i_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S1	48.8(5)	53.7(6)	67.1(6)	26.1(4)	-15.1(4)	-24.6(4)
O1	73(2)	77(2)	40.9(14)	46.9(17)	-7.0(13)	-9.8(13)
C8	37.1(17)	41.3(18)	44.1(17)	16.5(14)	3.8(13)	-0.8(14)
C13	34.9(16)	36.6(17)	45.5(16)	13.3(14)	-1.9(13)	-3.6(13)
C1	36.9(17)	38.0(17)	49.5(18)	17.2(14)	0.2(14)	-5.1(14)
C12	37.8(17)	38.7(18)	58(2)	17.6(15)	0.5(15)	-1.4(15)
C9	34.9(16)	38.5(17)	39.7(16)	15.4(14)	2.4(13)	0.6(13)
C11	49(2)	51(2)	56(2)	25.9(18)	0.4(16)	-10.5(17)
C10	32.2(15)	38.1(17)	53(2)	13.0(14)	-0.2(14)	-2.7(14)
C14	35.6(16)	38.4(17)	44.4(16)	18.3(14)	-1.8(13)	-4.0(13)
C21	62(2)	41(2)	59(2)	28.8(18)	-6.0(18)	-7.2(18)
C7	75(3)	54(3)	95(4)	38(2)	-14(3)	-1(2)
C2	42.4(19)	47.1(19)	50.6(19)	21.0(17)	2.8(15)	0.3(15)
N1	91(3)	48(2)	74(3)	30(2)	-1(2)	3(2)
S2	30.2(4)	52.5(5)	67.0(6)	13.1(4)	-2.2(4)	-5.2(4)
C16	36.1(19)	46(2)	85(3)	14.2(17)	-9(2)	-2(2)
C15	38.5(18)	40.2(19)	64(2)	18.1(15)	-7.8(16)	-2.1(16)
C17	40(2)	42(2)	94(3)	15.6(17)	13(2)	7(2)
C19	43.0(19)	51(2)	48.3(19)	21.7(16)	-4.7(15)	-1.8(16)
C6	57(2)	55(2)	51.0(19)	32(2)	7.7(17)	-0.6(17)
C3	54(2)	47(2)	53(2)	20.7(17)	0.2(17)	4.6(17)
C5	64(3)	61(3)	72(3)	40(2)	11(2)	-4(2)
C20	57(3)	73(3)	77(3)	33(2)	-14(2)	4(2)
C4	48(2)	44(2)	68(3)	21.8(17)	-9.7(17)	-5.9(17)
C18	53(2)	59(2)	62(2)	31(2)	10.8(19)	13.5(19)
F1	99(3)	118(4)	299(10)	77(3)	-26(5)	23(5)
F3	270(9)	83(3)	340(11)	118(5)	-194(9)	-90(5)
F2	379(13)	287(10)	158(6)	294(11)	85(7)	110(7)

Table S4 Bond Lengths for 6i_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C11	1.795(4)	C14	C19	1.403(5)
S1	C10	1.738(4)	C21	N1	1.121(6)
O1	C8	1.225(5)	C7	C4	1.503(7)
C8	C1	1.503(5)	C7	F1	1.287(8)
C8	C9	1.485(5)	C7	F3	1.243(7)
C13	C12	1.545(5)	C7	F2	1.282(8)
C13	C9	1.520(5)	C2	C3	1.399(6)
C13	C14	1.529(5)	S2	C20	1.813(5)
C1	C2	1.387(6)	C16	C15	1.379(6)

Table S4 Bond Lengths for 6i_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C6	1.387(5)	C16	C17	1.379(8)
C12	C11	1.521(6)	C17	C18	1.364(7)
C12	C21	1.483(6)	C19	C18	1.393(6)
C9	C10	1.352(5)	C6	C5	1.382(7)
C10	S2	1.764(4)	C3	C4	1.380(6)
C14	C15	1.394(5)	C5	C4	1.385(7)

Table S5 Bond Angles for 6i_auto.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C10	S1	C11	100.99(18)	C19	C14	C15	118.6(3)
C1	C8	O1	118.0(3)	N1	C21	C12	178.3(5)
C9	C8	O1	119.9(4)	F1	C7	C4	113.1(5)
C9	C8	C1	121.8(3)	F3	C7	C4	113.4(5)
C9	C13	C12	114.3(3)	F3	C7	F1	104.5(7)
C14	C13	C12	110.2(3)	F2	C7	C4	113.8(5)
C14	C13	C9	112.6(3)	F2	C7	F1	102.4(7)
C2	C1	C8	121.0(3)	F2	C7	F3	108.8(7)
C6	C1	C8	118.5(4)	C3	C2	C1	119.5(4)
C6	C1	C2	120.0(4)	C20	S2	C10	103.2(2)
C11	C12	C13	112.2(3)	C17	C16	C15	120.4(4)
C21	C12	C13	109.6(3)	C16	C15	C14	120.5(4)
C21	C12	C11	111.1(3)	C18	C17	C16	120.1(4)
C13	C9	C8	113.3(3)	C18	C19	C14	119.8(4)
C10	C9	C8	122.7(3)	C5	C6	C1	120.2(4)
C10	C9	C13	123.6(3)	C4	C3	C2	120.2(4)
C12	C11	S1	111.8(3)	C4	C5	C6	120.1(4)
C9	C10	S1	127.0(3)	C3	C4	C7	120.2(5)
S2	C10	S1	112.9(2)	C5	C4	C7	119.8(5)
S2	C10	C9	119.6(3)	C5	C4	C3	120.0(4)
C15	C14	C13	119.1(3)	C19	C18	C17	120.6(4)
C19	C14	C13	122.3(3)				

Table S6 Torsion Angles for 6i_auto.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
S1	C11	C12	C13	65.6(3)	C13	C9	C10	S2	-163.2(3)
S1	C11	C12	C21	-57.5(3)	C13	C14	C15	C16	-177.9(4)
S1	C10	C9	C8	179.5(3)	C13	C14	C19	C18	178.6(4)
S1	C10	C9	C13	7.5(4)	C1	C2	C3	C4	1.1(5)
O1	C8	C1	C2	-140.4(4)	C1	C6	C5	C4	-0.1(5)

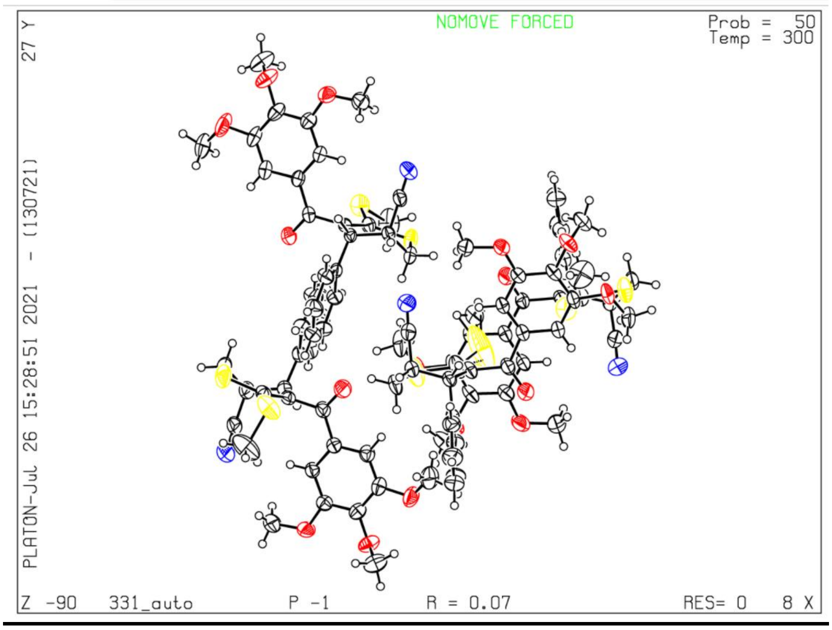
Table S6 Torsion Angles for 6i_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C8	C1	C6	32.1(4)	C14	C15	C16	C17	-1.8(5)
O1	C8	C9	C13	37.7(4)	C14	C19	C18	C17	0.2(5)
O1	C8	C9	C10	-135.1(4)	C7	C4	C3	C2	-178.1(4)
C8	C1	C2	C3	170.6(4)	C7	C4	C5	C6	177.6(5)
C8	C1	C6	C5	-171.2(4)	C2	C3	C4	C5	0.1(5)
C8	C9	C13	C12	-161.3(3)	C16	C17	C18	C19	-0.5(5)
C8	C9	C13	C14	71.9(3)	C6	C5	C4	C3	-0.6(6)
C8	C9	C10	S2	8.9(4)					

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6i_auto.

Atom	*x*	*y*	*z*	U(eq)
H13	-5581.9(13)	-4665.0(14)	-7643(6)	49.2(9)
H12	-5966.6(15)	-4293.4(15)	-5208(7)	54.8(9)
H11a	-5595.1(17)	-4359.2(17)	-1842(7)	61.6(11)
H11b	-5481.9(17)	-3781.5(17)	-2244(7)	61.6(11)
H2	-4947.8(15)	-5371.5(16)	-3003(7)	56.8(10)
H16	-7180.2(16)	-6089.2(18)	-6559(9)	70.0(13)
H15	-6465.8(15)	-5323.1(15)	-7850(7)	58.0(10)
H17	-7139.6(17)	-6436.5(17)	-3174(10)	73.3(13)
H19	-5680.3(16)	-5220.1(17)	-2208(6)	57.7(10)
H6	-4295.3(18)	-5267.2(18)	-8985(7)	63.1(11)
H3	-4676.1(18)	-5961.3(17)	-1872(7)	64.0(11)
H5	-4017.3(19)	-5842(2)	-7834(8)	73.9(13)
H18	-6401.3(18)	-6003.3(19)	-1002(8)	68.0(12)

ORTEP Diagram of Compound 6l (CCDC 2099427)



Crystallization Details For the crystallization of compound **6l**, vacuum dried pure sample of **6l** was taken in a vial and dissolved in 2 mL of acetonitrile. The vial was kept around 18-20 °C temperature for slow evaporation. After 4 days, we could find pink cube shape crystal, which was picked up from the vial and performed single crystal XRD study.

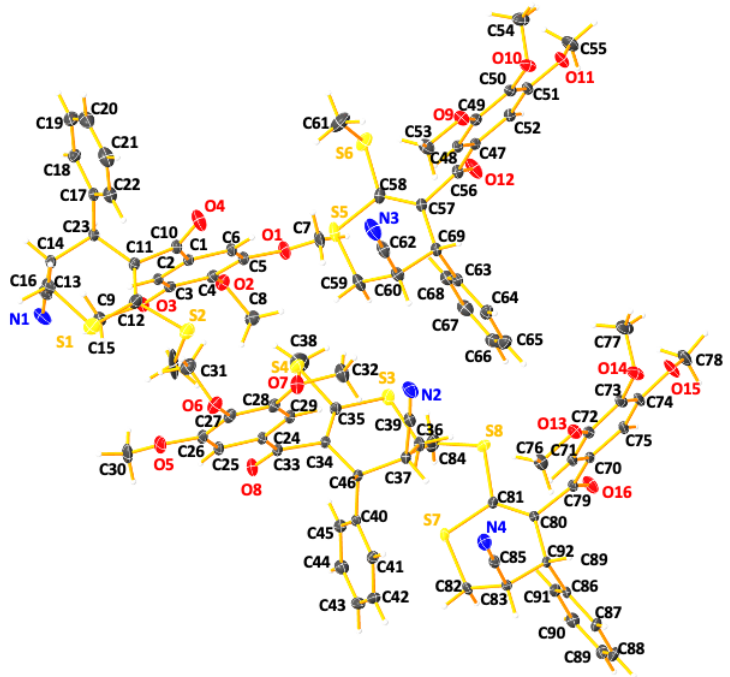


Figure S3: Thermal Ellipsoid Plot at 40% Probability Level

6l_auto

Table S8 Crystal data and structure refinement for 6l_auto.

Identification code	6l_auto
Empirical formula	$C_{92}H_{92}N_4O_{16}S_8$
Formula weight	1766.302
Temperature/K	300(2)
Crystal system	triclinic
Space group	P-1
a/Å	14.9969(2)
b/Å	15.45226(17)
c/Å	19.0015(2)
α/°	88.0358(9)
β/°	84.5699(10)
γ/°	88.8661(10)
Volume/Å^3	4380.40(9)
Z	2
ρ_{calc}g/cm^3	1.339
μ/mm^{-1}	2.450
F(000)	1866.8
Crystal size/mm^3	0.212 × 0.201 × 0.198
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.72 to 136.12
Index ranges	$-18 \le h \le 18$, $-18 \le k \le 18$, $-22 \le l \le 15$
Reflections collected	46312
Independent reflections	15812 [R_{int} = 0.0386, R_{sigma} = 0.0362]
Data/restraints/parameters	15812/0/1097
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0770, wR_2 = 0.1954
Final R indexes [all data]	R_1 = 0.0880, wR_2 = 0.2030
Largest diff. peak/hole / e Å^{-3}	1.45/-1.53

Table S9 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6l_auto. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O9	13674.7(17)	4897.8(17)	1362.9(15)	50.4(6)
O3	9622(2)	-2756.2(16)	3591.5(18)	65.2(8)
O10	13806.5(19)	6535(2)	971.1(16)	61.7(8)
C70	11307(2)	5585.2(19)	1678.7(16)	33.3(7)
C90	10342(2)	4013.1(18)	2805.0(15)	27.0(6)
O11	12392(2)	7631.1(18)	1069(2)	74.8(10)
C28	2848(2)	4536(2)	3616.9(17)	37.1(7)
C71	12050(2)	5034(2)	1644.7(16)	34.9(7)

Table S9 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6l_auto. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C29	3686(2)	4885(2)	3419.2(17)	36.0(7)
C79	10386(2)	5265.4(19)	1899.5(17)	35.1(7)
C83	10512(2)	3022.1(18)	2865.0(16)	32.3(6)
C24	4440(2)	4334(2)	3380.5(16)	34.0(7)
C27	2764(2)	3652(2)	3777.5(17)	39.6(7)
C2	8625(2)	-1547(2)	3914.3(18)	40.1(8)
C72	12891(2)	5366(2)	1418.9(17)	38.9(7)
C81	10018(2)	3808.2(19)	1536.6(16)	33.7(7)
C80	10238(2)	4310.5(18)	2049.9(15)	29.2(6)
C74	12227(3)	6788(2)	1265(2)	47.4(9)
C17	6720(2)	819(2)	5582.3(18)	37.3(7)
C3	9466(3)	-1914(2)	3763.1(19)	43.0(8)
C25	4356(2)	3453(2)	3538.6(18)	39.3(7)
O4	7017(2)	-823.7(19)	4459(2)	77.5(10)
C75	11390(3)	6466(2)	1500.1(18)	40.9(8)
C10	7626(2)	-332(2)	4285.9(19)	41.6(8)
C46	5383(2)	5851(2)	2205.3(18)	37.4(7)
C1	8543(2)	-669.4(19)	4071.8(16)	34.9(7)
C73	12974(3)	6237(2)	1211.8(19)	44.9(8)
C45	5959(3)	5468(3)	974(2)	54.6(10)
C26	3521(2)	3109(2)	3737.4(18)	41.5(8)
C41	7024(3)	5478(2)	1832(2)	49.8(9)
C40	6147(2)	5579(2)	1665.9(19)	39.9(7)
C76	13648(3)	3998(3)	1555(2)	55.8(10)
C18	5849(3)	797(3)	5396(2)	52.9(9)
C22	6859(3)	700(2)	6287.9(19)	48.1(9)
C77	13909(3)	6801(4)	239(3)	75.5(14)
C42	7702(3)	5282(3)	1311(3)	64.2(12)
C19	5145(3)	672(3)	5914(3)	71.8(14)
C44	6643(4)	5281(3)	460(2)	68.7(13)
C43	7506(4)	5193(3)	623(3)	71.5(14)
C20	5300(4)	571(3)	6610(3)	75.3(15)
C9	8883(3)	-3260(3)	3442(3)	70.0(13)
C21	6156(3)	576(3)	6796(2)	67.3(12)
C78	11663(4)	8187(3)	954(3)	72.7(14)
S1	6946.9(11)	2178.0(8)	3704.3(7)	82.7(4)
C92	11390(2)	2800(2)	2494.5(18)	40.1(8)
O5	4368.7(18)	-3.2(19)	1189.4(17)	60.3(7)
O8	8345.6(18)	478.5(17)	602.7(16)	55.8(7)
C89	8688(2)	4347(2)	3159.1(18)	38.1(7)
O13	2063.5(16)	4998.2(17)	3682.6(15)	51.4(6)

Table S9 Fractional Atomic Coordinates (×10[4]) and Equivalent Isotropic Displacement Parameters (Å[2]×10[3]) for 6l_auto. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C63	8166(2)	-705.2(19)	-927.7(16)	32.4(6)
O6	4352.3(19)	1648.3(19)	1488.6(15)	60.0(7)
C34	5518(2)	5596(2)	2964.3(18)	35.9(7)
C51	5950(3)	1727(2)	1237.7(19)	45.4(8)
C68	9059(2)	-637(2)	-830.2(19)	43.0(8)
O15	3367.7(19)	2254.0(16)	3888.1(17)	58.3(7)
C82	9774(2)	2524(2)	2571.3(18)	39.9(7)
C14	7704(2)	1987(2)	4989.5(19)	42.7(8)
C65	8507(3)	-290(2)	-2155.0(19)	53.0(10)
C37	5198(2)	6838(2)	2113(2)	47.3(9)
C85	9729(2)	4391(2)	4029.5(17)	39.6(7)
C87	8173(3)	4662(2)	4354(2)	50.2(9)
N4	12053(2)	2640(2)	2187(2)	58.8(9)
O14	1920.7(17)	3330.4(18)	3948.8(14)	52.7(7)
C62	6426(3)	-2192(2)	11(2)	48.3(9)
C58	7238(2)	-1964(2)	-448.1(18)	37.5(7)
C69	7660(2)	60(2)	621.7(16)	35.7(7)
C50	5162(2)	1261(2)	1284.4(18)	44.6(8)
C6	9294(2)	-158.9(19)	4072.0(16)	34.5(7)
C35	5815(2)	6130(2)	3422(2)	45.7(8)
N2	5822(3)	-2342(2)	397(2)	71.0(11)
C54	4195(3)	1752(3)	2230(2)	65.9(12)
S7	9740.4(7)	2710.2(5)	1631.1(5)	47.1(2)
C84	9563(2)	4268.9(18)	3334.9(16)	29.4(6)
O7	5860(2)	2572.7(16)	1423.7(17)	64.6(8)
O12	9750.6(19)	5769.1(16)	1967.7(19)	65.2(8)
C86	9039(3)	4584(3)	4536.3(19)	49.0(9)
C47	6774(2)	459(2)	841.9(16)	35.0(7)
C36	5965(3)	7371(2)	2330(3)	58.1(11)
C49	5178(2)	385(2)	1114.9(19)	43.1(8)
C66	9395(3)	-228(3)	-2054(2)	55.2(10)
C39	4349(3)	7073(2)	2515(3)	54.9(10)
C56	7716(2)	-868.6(19)	393.6(16)	32.2(6)
C52	6758(3)	1330(2)	1009.4(18)	42.3(8)
S5	6153.3(8)	7202.1(7)	3250.6(7)	68.6(3)
C88	7997(2)	4541(2)	3671(2)	47.6(9)
C60	8015(2)	-1493(2)	822.1(18)	41.7(8)
C23	7525(2)	1007(2)	5050.8(17)	34.9(7)
C48	5992(2)	-17(2)	895.8(18)	38.5(7)
C55	6632(4)	3005(3)	1587(3)	76.1(14)
C59	8013(3)	-2570(2)	-298(2)	46.7(8)

Table S9 Fractional Atomic Coordinates (×10[4]) and Equivalent Isotropic Displacement Parameters (Å[2]×10[3]) for 6l_auto. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C33	5359(2)	4658(2)	3171.9(19)	40.6(7)
O1	10928.7(16)	-108.5(15)	3929.0(13)	45.0(6)
C11	7456(2)	632(2)	4332.3(18)	39.4(7)
S8	10122.6(8)	4217.9(7)	655.1(5)	54.7(3)
C31	1738(3)	3019(3)	4658(2)	68.4(13)
C16	8604(3)	2143(2)	4642(2)	53.8(10)
C5	10143(2)	-536(2)	3934.1(16)	34.2(7)
O2	11071.0(17)	-1773.2(17)	3678.8(14)	51.4(6)
C57	7463(2)	-1007.0(19)	-343.3(16)	30.9(6)
C7	10894(3)	799(2)	4033(2)	49.7(9)
C13	6995(3)	2493(2)	4604(2)	58.0(11)
C91	9421(4)	3565(3)	199(3)	82.5(17)
C67	9675(3)	-404(3)	-1391(2)	53.7(10)
C38	4880(4)	6319(4)	4705(3)	95.2(19)
O16	5995.1(19)	4155.6(18)	3144(2)	76.1(10)
N1	9301(3)	2240(2)	4369(3)	76.0(12)
C64	7890(3)	-522(2)	-1601.4(18)	42.2(8)
C4	10231(2)	-1412(2)	3781.1(17)	40.0(8)
S6	5897.1(9)	5808.5(9)	4319.9(6)	71.8(4)
C30	4083(3)	1728(3)	4112(3)	69.9(13)
C8	11357(3)	-1991(3)	2968(2)	57.4(10)
C32	2090(3)	5901(3)	3529(3)	60.7(11)
N3	3694(3)	7234(3)	2832(3)	86.5(14)
C53	4337(3)	-894(3)	1029(3)	69.5(13)
C12	7223(3)	1075(3)	3767(2)	57.7(11)
S3	8209.9(9)	-2582.8(6)	622.5(6)	61.9(3)
S4	8106.5(9)	-1301.3(8)	1723.2(5)	62.7(3)
C61	9201(4)	-1706(4)	1835(3)	95.3(19)
S2	7118.3(10)	530.7(9)	2956.0(6)	75.1(4)
C15	7951(4)	868(3)	2636(4)	119(3)

Table S10 Anisotropic Displacement Parameters (Å[2]×10[3]) for 6l_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O9	36.5(14)	49.1(14)	65.7(16)	-4.0(11)	-7.2(12)	3.8(12)
O3	66.1(19)	29.4(13)	99(2)	14.0(12)	1.2(16)	-18.0(13)
O10	46.3(16)	69.5(18)	71.1(18)	-27.9(14)	-18.0(13)	21.8(14)
C70	40.3(18)	28.9(15)	32.0(15)	-4.9(13)	-8.6(13)	-2.8(12)
C90	26.1(15)	24.8(13)	31.4(14)	-1.0(11)	-7.6(11)	-4.8(11)
O11	75(2)	33.5(14)	117(3)	-17.9(14)	-22.7(19)	22.8(15)

Table S10 Anisotropic Displacement Parameters (Å^2×10^3) for 6l_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C28	32.0(17)	41.3(17)	38.7(16)	1.3(13)	-8.0(13)	-1.4(13)
C71	40.7(18)	28.4(15)	36.1(16)	-3.4(13)	-6.8(13)	0.0(12)
C29	36.4(18)	32.1(16)	40.3(17)	1.2(13)	-7.3(14)	-2.1(13)
C79	39.8(18)	25.8(15)	39.9(16)	2.7(13)	-4.5(14)	-4.2(12)
C83	35.4(17)	26.5(14)	34.8(15)	3.9(12)	-2.7(13)	-0.9(12)
C24	33.0(17)	35.1(16)	35.0(15)	0.3(13)	-7.7(13)	-4.1(12)
C27	38.6(19)	43.8(18)	37.7(17)	-7.4(14)	-11.1(14)	3.2(14)
C2	43(2)	28.9(15)	48.0(19)	2.8(13)	-0.3(15)	-7.6(13)
C72	38.5(19)	40.8(17)	38.7(17)	-6.5(14)	-10.0(14)	-0.8(13)
C81	37.8(18)	31.1(15)	33.1(15)	1.5(13)	-7.2(13)	-3.8(12)
C80	28.3(16)	26.5(14)	33.2(15)	-0.5(11)	-4.1(12)	-1.6(11)
C74	61(2)	30.7(16)	54(2)	-16.7(16)	-20.3(18)	6.6(15)
C17	34.5(18)	30.1(15)	47.8(18)	3.3(13)	-4.5(14)	-9.0(13)
C3	53(2)	26.8(15)	48.0(19)	9.8(14)	-1.0(16)	-7.7(13)
C25	38.4(19)	35.2(16)	45.5(18)	2.8(14)	-11.1(14)	-1.2(14)
O4	42.1(17)	45.7(16)	143(3)	-0.9(13)	7.1(18)	-19.1(18)
C75	53(2)	27.3(15)	44.8(18)	-4.6(14)	-14.5(16)	-1.4(13)
C10	40(2)	34.5(17)	50.8(19)	6.7(15)	-6.8(15)	-9.8(14)
C46	31.1(17)	33.1(16)	49.2(19)	1.5(13)	-9.5(14)	-5.1(13)
C1	40.5(18)	28.5(15)	35.6(16)	7.2(13)	-3.1(13)	-4.1(12)
C73	46(2)	43.7(19)	47.3(19)	-16.9(16)	-15.9(16)	5.9(15)
C45	64(3)	50(2)	51(2)	7.6(18)	-10.9(19)	-6.7(17)
C26	50(2)	32.5(16)	43.8(18)	-3.5(14)	-12.4(15)	2.1(13)
C41	42(2)	47(2)	60(2)	2.5(16)	-5.8(17)	-1.4(17)
C40	39.7(19)	30.9(15)	49.4(19)	2.3(13)	-5.4(15)	-3.6(14)
C76	46(2)	47(2)	76(3)	2.9(17)	-10.2(19)	0.4(19)
C18	37(2)	50(2)	72(3)	2.9(16)	-11.5(18)	-5.5(18)
C22	46(2)	52(2)	47(2)	-3.7(16)	-1.7(16)	-6.7(16)
C77	68(3)	86(3)	73(3)	-37(3)	-8(2)	17(3)
C42	45(2)	55(2)	89(3)	7.7(18)	10(2)	3(2)
C19	30(2)	63(3)	121(4)	1.2(18)	1(2)	-13(3)
C44	98(4)	57(2)	50(2)	14(2)	2(2)	-5.1(19)
C43	84(4)	54(2)	69(3)	13(2)	26(3)	3(2)
C20	64(3)	65(3)	90(4)	-5(2)	34(3)	-11(3)
C9	87(3)	35(2)	86(3)	-8(2)	12(3)	-22(2)
C21	73(3)	69(3)	57(3)	-10(2)	13(2)	-10(2)
C78	100(4)	31.8(19)	87(3)	-8(2)	-16(3)	11(2)
S1	127.1(12)	53.2(6)	68.8(7)	43.2(7)	-26.3(7)	4.2(5)
C92	44(2)	29.2(15)	47.1(18)	6.6(14)	-6.7(16)	-4.1(13)
O5	35.5(15)	59.7(17)	87(2)	6.3(12)	-4.3(13)	-23.9(15)
O8	42.4(15)	43.7(14)	83(2)	-3.6(12)	-6.5(13)	-20.6(13)
C89	32.6(18)	41.2(17)	41.7(17)	0.3(14)	-9.8(14)	-5.1(14)

Table S10 Anisotropic Displacement Parameters (Å^2×10^3) for 6l_auto. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O13	31.7(13)	48.7(14)	72.5(17)	4.7(11)	-1.8(12)	6.0(12)
C63	37.2(18)	25.9(14)	34.2(15)	3.7(12)	-3.5(13)	-4.9(11)
O6	51.8(17)	69.9(18)	59.5(16)	33.1(14)	-12.2(13)	-20.6(14)
C34	26.7(16)	34.7(16)	46.8(18)	2.6(12)	-4.2(13)	-7.3(13)
C51	62(2)	30.3(16)	44.9(19)	13.5(16)	-8.3(16)	-10.7(14)
C68	41(2)	43.7(18)	44.9(19)	1.5(15)	-7.6(15)	-1.0(15)
O15	56.4(17)	34.3(13)	85(2)	-6.3(11)	-13.5(14)	10.9(13)
C82	48(2)	24.1(14)	48.3(19)	-3.5(13)	-8.2(15)	-0.7(13)
C14	46(2)	32.8(16)	48.5(19)	0.1(14)	4.8(15)	-9.8(14)
C65	74(3)	48(2)	35.5(18)	-0.3(19)	-2.1(18)	2.1(15)
C37	40(2)	35.4(17)	66(2)	4.0(14)	-8.1(17)	2.1(16)
C85	35.4(18)	45.7(18)	39.8(17)	1.3(14)	-9.3(14)	-15.0(14)
C87	46(2)	47(2)	55(2)	-2.3(16)	12.0(17)	-14.7(16)
N4	49(2)	49.7(19)	76(2)	10.1(15)	3.9(18)	-11.7(16)
O14	39.1(14)	63.8(17)	55.9(15)	-13.8(12)	-12.2(12)	15.8(12)
C62	47(2)	37.0(18)	61(2)	-4.3(16)	-3.6(19)	-5.2(16)
C58	39.2(18)	33.3(16)	40.7(17)	-1.6(13)	-4.8(14)	-8.7(13)
C69	40.6(19)	31.9(16)	35.4(16)	3.2(14)	-6.3(13)	-8.0(12)
C50	45(2)	46.8(19)	42.6(18)	22.5(16)	-8.0(15)	-13.1(15)
C6	40.0(18)	27.5(14)	35.8(16)	6.0(13)	-3.0(13)	-3.2(12)
C35	35.5(19)	45.1(19)	59(2)	7.6(15)	-12.8(16)	-18.9(16)
N2	56(2)	58(2)	95(3)	-12.4(18)	14(2)	-2(2)
C54	63(3)	72(3)	61(3)	23(2)	2(2)	-15(2)
S7	65.8(6)	32.6(4)	45.8(5)	-10.2(4)	-15.6(4)	-9.9(3)
C84	30.0(16)	22.7(13)	36.1(15)	-1.6(11)	-5.2(12)	-5.0(11)
O7	80(2)	32.3(13)	82(2)	18.1(13)	-4.5(16)	-17.7(13)
O12	49.5(16)	31.3(13)	111(2)	9.4(11)	7.9(16)	5.2(14)
C86	53(2)	55(2)	40.1(19)	-1.3(17)	-2.9(16)	-18.2(16)
C47	37.4(18)	31.5(15)	36.7(16)	7.1(13)	-6.5(13)	-8.9(12)
C36	46(2)	33.7(18)	95(3)	-4.5(16)	-7(2)	-2.5(19)
C49	39(2)	46.7(19)	44.4(18)	9.8(15)	-6.2(15)	-12.0(15)
C66	66(3)	49(2)	47(2)	-2.3(18)	15.6(19)	1.5(16)
C39	40(2)	34.5(18)	90(3)	6.4(15)	-8(2)	-5.1(18)
C56	30.8(16)	30.9(15)	35.1(15)	3.4(12)	-3.0(12)	-7.5(12)
C52	51(2)	29.5(16)	47.4(19)	4.7(14)	-4.8(16)	-9.1(14)
S5	64.6(7)	43.6(5)	103.4(9)	-6.9(5)	-30.6(6)	-23.2(5)
C88	28.0(18)	50(2)	65(2)	2.0(15)	-3.9(16)	-4.6(17)
C60	49(2)	37.1(17)	40.3(17)	4.3(15)	-13.3(15)	-3.9(14)
C23	33.0(17)	30.9(15)	41.3(17)	4.5(12)	-5.7(13)	-4.0(13)
C48	38.1(19)	33.6(16)	44.5(18)	8.3(13)	-6.1(14)	-12.1(13)
C55	105(4)	37(2)	91(4)	4(2)	-25(3)	-24(2)
C59	53(2)	30.3(16)	57(2)	6.1(15)	-4.2(17)	-12.2(15)

Table S10 Anisotropic Displacement Parameters ($Å^2×10^3$) for 6l_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C33	35.1(18)	34.8(17)	53(2)	3.4(14)	-8.1(15)	-4.6(14)
O1	34.5(13)	42.0(13)	58.6(15)	5.0(10)	-4.4(11)	-6.4(11)
C11	40.2(19)	34.9(17)	43.8(18)	11.0(14)	-7.2(14)	-8.0(14)
S8	77.9(7)	55.0(5)	32.1(4)	-0.2(5)	-10.8(4)	0.3(4)
C31	63(3)	82(3)	59(3)	-19(2)	0(2)	13(2)
C16	56(3)	33.0(18)	69(3)	0.6(16)	10(2)	1.2(17)
C5	35.5(18)	35.5(16)	31.4(15)	6.0(13)	-3.6(13)	-3.0(12)
O2	43.2(15)	54.0(15)	57.6(15)	24.8(12)	-8.3(12)	-13.0(12)
C57	29.8(16)	29.5(14)	34.4(15)	4.7(12)	-7.5(12)	-6.2(12)
C7	48(2)	41.4(19)	60(2)	-2.7(16)	-5.7(18)	-4.0(16)
C13	66(3)	29.8(17)	76(3)	16.8(17)	4(2)	-4.3(17)
C91	126(5)	70(3)	61(3)	2(3)	-50(3)	-10(2)
C67	38(2)	56(2)	65(2)	-3.8(17)	3.3(18)	-2.8(19)
C38	100(4)	128(5)	59(3)	40(4)	-11(3)	-29(3)
O16	38.0(15)	39.6(15)	148(3)	8.0(12)	-1.8(17)	7.6(17)
N1	63(2)	47(2)	111(3)	1.3(17)	25(2)	10(2)
C64	48(2)	41.1(18)	39.1(17)	2.9(15)	-10.8(15)	-4.4(14)
C4	42(2)	38.6(17)	38.7(17)	15.5(14)	-3.0(14)	-6.4(13)
S6	74.5(8)	87.4(8)	56.8(6)	32.7(6)	-23.5(5)	-21.4(6)
C30	79(3)	43(2)	86(3)	5(2)	-10(3)	23(2)
C8	57(3)	54(2)	59(2)	19.8(19)	4.8(19)	-9.7(18)
C32	51(2)	46(2)	83(3)	11.8(18)	1(2)	5(2)
N3	51(2)	52(2)	153(4)	8.7(18)	12(3)	-13(2)
C53	49(3)	55(2)	104(4)	-1.7(19)	-3(2)	-14(2)
C12	79(3)	49(2)	46(2)	22(2)	-14(2)	-6.0(17)
S3	88.8(8)	34.9(5)	65.5(6)	19.1(5)	-28.8(6)	-3.6(4)
S4	81.8(8)	67.5(7)	41.4(5)	-1.3(6)	-18.6(5)	-4.8(4)
C61	96(4)	107(5)	91(4)	-11(3)	-57(3)	8(3)
S2	83.4(9)	85.9(9)	58.6(6)	-13.3(7)	-14.6(6)	-13.6(6)
C15	133(5)	52(3)	201(7)	18(3)	-149(5)	-50(3)

Table S11 Bond Lengths for 6l_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O9	C72	1.365(4)	C89	C84	1.386(4)
O9	C76	1.425(4)	C89	C88	1.388(5)
O3	C3	1.363(4)	O13	C32	1.417(5)
O3	C9	1.422(5)	C63	C68	1.376(5)
O10	C73	1.372(4)	C63	C57	1.525(4)
O10	C77	1.432(5)	C63	C64	1.400(4)
C70	C71	1.387(5)	O6	C50	1.371(4)

Table S11 Bond Lengths for 6l_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C70	C79	1.493(5)	O6	C54	1.420(5)
C70	C75	1.397(4)	C34	C35	1.332(5)
C90	C83	1.549(4)	C34	C33	1.505(4)
C90	C80	1.513(4)	C51	C50	1.391(6)
C90	C84	1.524(4)	C51	O7	1.366(4)
O11	C74	1.363(4)	C51	C52	1.387(5)
O11	C78	1.405(6)	C68	C67	1.385(5)
C28	C29	1.390(5)	O15	C30	1.422(5)
C28	C27	1.394(5)	C82	S7	1.805(3)
C28	O13	1.363(4)	C14	C23	1.541(4)
C71	C72	1.394(5)	C14	C16	1.467(5)
C29	C24	1.399(4)	C14	C13	1.534(6)
C79	C80	1.510(4)	C65	C66	1.370(6)
C79	O12	1.219(4)	C65	C64	1.376(5)
C83	C92	1.474(5)	C37	C36	1.524(5)
C83	C82	1.519(5)	C37	C39	1.468(6)
C24	C25	1.390(4)	C85	C84	1.386(4)
C24	C33	1.489(5)	C85	C86	1.381(5)
C27	C26	1.396(5)	C87	C86	1.376(6)
C27	O14	1.374(4)	C87	C88	1.369(6)
C2	C3	1.381(5)	O14	C31	1.420(5)
C2	C1	1.400(4)	C62	C58	1.470(5)
C72	C73	1.394(5)	C62	N2	1.133(5)
C81	C80	1.336(4)	C58	C59	1.520(5)
C81	S7	1.754(3)	C58	C57	1.547(4)
C81	S8	1.764(3)	C69	C47	1.484(4)
C74	C75	1.388(5)	C69	C56	1.512(4)
C74	C73	1.392(6)	C50	C49	1.401(5)
C17	C18	1.387(5)	C6	C5	1.395(4)
C17	C22	1.382(5)	C35	S5	1.753(4)
C17	C23	1.525(5)	C35	S6	1.775(4)
C3	C4	1.401(5)	O7	C55	1.413(6)
C25	C26	1.385(5)	C47	C52	1.392(4)
O4	C10	1.214(5)	C47	C48	1.391(5)
C10	C1	1.485(5)	C36	S5	1.807(5)
C10	C11	1.510(4)	C49	C48	1.394(5)
C46	C40	1.525(5)	C66	C67	1.381(6)
C46	C34	1.513(5)	C39	N3	1.130(5)
C46	C37	1.552(4)	C56	C60	1.339(5)
C1	C6	1.389(5)	C56	C57	1.508(4)
C45	C40	1.387(5)	C60	S3	1.752(3)
C45	C44	1.381(6)	C60	S4	1.766(3)
C26	O15	1.361(4)	C23	C11	1.515(5)

Table S11 Bond Lengths for 6l_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C41	C40	1.387(5)	C59	S3	1.800(4)
C41	C42	1.387(6)	C33	O16	1.217(4)
C18	C19	1.385(6)	O1	C5	1.362(4)
C22	C21	1.373(6)	O1	C7	1.422(4)
C42	C43	1.378(7)	C11	C12	1.325(5)
C19	C20	1.367(8)	S8	C91	1.774(5)
C44	C43	1.363(7)	C16	N1	1.132(5)
C20	C21	1.364(8)	C5	C4	1.396(4)
S1	C13	1.801(5)	O2	C4	1.367(4)
S1	C12	1.749(4)	O2	C8	1.428(5)
C92	N4	1.131(5)	C38	S6	1.806(5)
O5	C49	1.358(5)	C12	S2	1.802(4)
O5	C53	1.423(5)	S4	C61	1.774(6)
O8	C69	1.222(4)	S2	C15	1.436(8)

Table S12 Bond Angles for 6l_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C76	O9	C72	118.4(3)	O7	C51	C50	115.7(3)
C9	O3	C3	118.4(3)	C52	C51	C50	120.0(3)
C77	O10	C73	115.0(3)	C52	C51	O7	124.3(4)
C79	C70	C71	121.8(3)	C67	C68	C63	120.5(3)
C75	C70	C71	121.1(3)	C30	O15	C26	118.3(3)
C75	C70	C79	117.1(3)	S7	C82	C83	112.7(2)
C80	C90	C83	111.5(2)	C16	C14	C23	110.2(3)
C84	C90	C83	109.5(2)	C13	C14	C23	112.6(3)
C84	C90	C80	114.4(2)	C13	C14	C16	110.7(3)
C78	O11	C74	118.7(3)	C64	C65	C66	120.6(4)
C27	C28	C29	120.4(3)	C36	C37	C46	111.9(3)
O13	C28	C29	124.9(3)	C39	C37	C46	109.8(3)
O13	C28	C27	114.7(3)	C39	C37	C36	111.1(3)
C72	C71	C70	119.2(3)	C86	C85	C84	120.8(3)
C24	C29	C28	118.9(3)	C88	C87	C86	119.9(3)
C80	C79	C70	120.0(3)	C31	O14	C27	115.5(3)
O12	C79	C70	120.7(3)	N2	C62	C58	175.7(4)
O12	C79	C80	119.4(3)	C59	C58	C62	110.7(3)
C92	C83	C90	109.7(2)	C57	C58	C62	109.3(3)
C82	C83	C90	111.6(2)	C57	C58	C59	111.7(3)
C82	C83	C92	110.5(3)	C47	C69	O8	121.0(3)
C25	C24	C29	120.7(3)	C56	C69	O8	119.3(3)
C33	C24	C29	122.1(3)	C56	C69	C47	119.7(3)
C33	C24	C25	117.2(3)	C51	C50	O6	120.9(3)

Table S12 Bond Angles for 6l_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C26	C27	C28	120.2(3)	C49	C50	O6	118.6(4)
O14	C27	C28	118.4(3)	C49	C50	C51	120.5(3)
O14	C27	C26	121.3(3)	C5	C6	C1	119.3(3)
C1	C2	C3	119.6(3)	S5	C35	C34	126.9(3)
C71	C72	O9	125.3(3)	S6	C35	C34	121.7(3)
C73	C72	O9	114.7(3)	S6	C35	S5	111.4(2)
C73	C72	C71	120.0(3)	C82	S7	C81	101.16(14)
S7	C81	C80	126.1(2)	C89	C84	C90	122.8(3)
S8	C81	C80	119.1(2)	C85	C84	C90	118.7(3)
S8	C81	S7	114.43(17)	C85	C84	C89	118.5(3)
C79	C80	C90	114.5(2)	C55	O7	C51	118.2(3)
C81	C80	C90	125.6(3)	C87	C86	C85	120.1(3)
C81	C80	C79	119.9(3)	C52	C47	C69	117.2(3)
C75	C74	O11	124.8(4)	C48	C47	C69	121.7(3)
C73	C74	O11	115.1(3)	C48	C47	C52	121.1(3)
C73	C74	C75	120.1(3)	S5	C36	C37	113.0(3)
C22	C17	C18	118.3(3)	C50	C49	O5	115.1(3)
C23	C17	C18	123.1(3)	C48	C49	O5	125.5(3)
C23	C17	C22	118.5(3)	C48	C49	C50	119.5(3)
C2	C3	O3	124.4(3)	C67	C66	C65	119.7(3)
C4	C3	O3	115.5(3)	N3	C39	C37	178.3(4)
C4	C3	C2	120.0(3)	C60	C56	C69	120.1(3)
C26	C25	C24	120.2(3)	C57	C56	C69	115.2(3)
C74	C75	C70	119.3(3)	C57	C56	C60	124.6(3)
C1	C10	O4	120.8(3)	C47	C52	C51	119.5(3)
C11	C10	O4	119.1(3)	C36	S5	C35	102.30(18)
C11	C10	C1	120.0(3)	C87	C88	C89	120.3(3)
C34	C46	C40	114.6(3)	S3	C60	C56	126.6(3)
C37	C46	C40	109.3(3)	S4	C60	C56	120.7(3)
C37	C46	C34	111.6(3)	S4	C60	S3	112.23(19)
C10	C1	C2	116.9(3)	C14	C23	C17	110.6(3)
C6	C1	C2	120.9(3)	C11	C23	C17	113.7(3)
C6	C1	C10	122.0(3)	C11	C23	C14	111.5(3)
C72	C73	O10	118.5(3)	C49	C48	C47	119.5(3)
C74	C73	O10	121.3(3)	S3	C59	C58	111.4(2)
C74	C73	C72	120.2(3)	C34	C33	C24	121.3(3)
C44	C45	C40	120.1(4)	O16	C33	C24	119.9(3)
C25	C26	C27	119.6(3)	O16	C33	C34	118.8(3)
O15	C26	C27	115.9(3)	C7	O1	C5	118.4(3)
O15	C26	C25	124.5(3)	C23	C11	C10	115.8(3)
C42	C41	C40	120.4(4)	C12	C11	C10	119.0(3)
C45	C40	C46	118.3(3)	C12	C11	C23	125.1(3)
C41	C40	C46	122.7(3)	C91	S8	C81	105.3(2)

Table S12 Bond Angles for 6l_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C41	C40	C45	118.9(4)	N1	C16	C14	178.0(4)
C19	C18	C17	119.9(4)	O1	C5	C6	124.8(3)
C21	C22	C17	121.3(4)	C4	C5	C6	120.2(3)
C43	C42	C41	120.0(4)	C4	C5	O1	115.0(3)
C20	C19	C18	120.6(4)	C8	O2	C4	115.4(3)
C43	C44	C45	120.9(4)	C58	C57	C63	109.6(2)
C44	C43	C42	119.8(4)	C56	C57	C63	114.0(3)
C21	C20	C19	119.8(4)	C56	C57	C58	111.6(2)
C20	C21	C22	120.1(5)	C14	C13	S1	113.5(2)
C12	S1	C13	101.42(18)	C66	C67	C68	120.2(4)
N4	C92	C83	177.5(4)	C65	C64	C63	120.3(4)
C53	O5	C49	118.1(3)	C5	C4	C3	120.0(3)
C88	C89	C84	120.4(3)	O2	C4	C3	121.1(3)
C32	O13	C28	118.3(3)	O2	C4	C5	118.8(3)
C57	C63	C68	123.1(3)	C38	S6	C35	98.6(2)
C64	C63	C68	118.8(3)	C11	C12	S1	127.3(3)
C64	C63	C57	118.1(3)	S2	C12	S1	112.5(2)
C54	O6	C50	113.7(3)	S2	C12	C11	120.2(3)
C35	C34	C46	123.9(3)	C59	S3	C60	101.25(16)
C33	C34	C46	115.6(3)	C61	S4	C60	101.9(2)
C33	C34	C35	120.3(3)	C15	S2	C12	92.1(3)

Table S13 Torsion Angles for 6l_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O9	C72	C71	C70	179.8(3)	C10	C11	C23	C14	158.1(3)
O9	C72	C73	O10	0.6(3)	C10	C11	C12	S1	177.0(3)
O9	C72	C73	C74	-178.0(3)	C10	C11	C12	S2	-0.2(4)
O3	C3	C2	C1	-178.8(4)	C46	C40	C45	C44	175.5(3)
O3	C3	C4	C5	178.4(3)	C46	C40	C41	C42	-176.0(3)
O3	C3	C4	O2	-4.2(4)	C46	C34	C35	S5	-2.9(4)
O10	C73	C72	C71	-177.9(3)	C46	C34	C35	S6	176.3(3)
O10	C73	C74	O11	-0.5(4)	C46	C34	C33	O16	94.7(4)
O10	C73	C74	C75	179.0(3)	C46	C37	C36	S5	-61.6(3)
C70	C71	C72	C73	-1.8(4)	C1	C6	C5	O1	-179.0(3)
C70	C79	C80	C90	88.2(3)	C1	C6	C5	C4	1.5(4)
C70	C79	C80	C81	-92.9(3)	C45	C40	C41	C42	0.9(4)
C70	C75	C74	O11	179.2(3)	C45	C44	C43	C42	0.7(5)
C70	C75	C74	C73	-0.2(4)	C41	C42	C43	C44	-1.3(5)
C90	C83	C82	S7	65.4(2)	C18	C19	C20	C21	-1.2(5)
C90	C80	C79	O12	-91.0(3)	C22	C21	C20	C19	1.3(5)
C90	C80	C81	S7	3.9(4)	S1	C13	C14	C23	-61.6(3)

Table S13 Torsion Angles for 6l_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C90	C80	C81	S8	-168.7(3)	S1	C13	C14	C16	62.2(3)
C90	C84	C89	C88	176.8(3)	S1	C12	C11	C23	0.1(5)
C90	C84	C85	C86	-176.9(3)	O5	C49	C50	O6	-1.5(4)
O11	C74	C73	C72	178.1(3)	O5	C49	C50	C51	179.2(3)
C28	C29	C24	C25	-0.2(4)	O5	C49	C48	C47	180.0(4)
C28	C29	C24	C33	179.9(3)	O8	C69	C47	C52	1.3(4)
C28	C27	C26	C25	0.2(4)	O8	C69	C47	C48	-177.2(3)
C28	C27	C26	O15	-178.5(3)	O8	C69	C56	C60	76.2(4)
C28	C27	O14	C31	-113.0(4)	O8	C69	C56	C57	-100.6(3)
C71	C72	C73	C74	3.5(4)	C89	C84	C85	C86	0.3(4)
C29	C24	C25	C26	-0.0(4)	C89	C88	C87	C86	-0.5(4)
C29	C24	C33	C34	-2.4(4)	C63	C68	C67	C66	0.7(4)
C29	C24	C33	O16	-179.8(4)	C63	C57	C58	C62	-167.3(3)
C79	C80	C81	S7	-174.9(2)	C63	C57	C58	C59	70.0(3)
C79	C80	C81	S8	12.5(3)	C63	C57	C56	C69	73.8(3)
C24	C25	C26	C27	0.0(4)	C63	C57	C56	C60	-102.9(3)
C24	C25	C26	O15	178.6(3)	C63	C64	C65	C66	-0.6(4)
C24	C33	C34	C46	-82.8(3)	O6	C50	C51	O7	1.6(4)
C24	C33	C34	C35	101.4(3)	O6	C50	C51	C52	-178.0(3)
C27	C26	O15	C30	-157.1(4)	O6	C50	C49	C48	179.0(3)
C2	C3	C4	C5	-1.6(4)	C51	C50	C49	C48	-0.2(4)
C2	C3	C4	O2	175.7(3)	C51	C52	C47	C69	-178.2(3)
C2	C1	C10	O4	15.0(4)	C51	C52	C47	C48	0.4(4)
C2	C1	C10	C11	-168.6(3)	C68	C67	C66	C65	-0.5(5)
C2	C1	C6	C5	-2.0(4)	C14	C23	C11	C12	-25.0(4)
C72	C73	C74	C75	-2.5(4)	C85	C86	C87	C88	0.6(4)
C17	C18	C19	C20	0.0(5)	C62	C58	C59	S3	-55.3(3)
C17	C22	C21	C20	-0.2(5)	C62	C58	C57	C56	65.6(3)
C17	C23	C14	C16	164.1(3)	C58	C57	C56	C69	-161.4(3)
C17	C23	C14	C13	-71.7(3)	C58	C57	C56	C60	21.9(3)
C17	C23	C11	C10	-76.1(3)	C69	C47	C48	C49	179.1(3)
C17	C23	C11	C12	100.9(4)	C69	C56	C60	S3	-174.5(2)
C3	C4	C5	C6	0.3(4)	C69	C56	C60	S4	14.5(3)
C3	C4	C5	O1	-179.2(3)	C50	C49	C48	C47	-0.7(4)
C3	C4	O2	C8	73.4(4)	C6	C5	O1	C7	-3.6(4)
C25	C26	O15	C30	24.3(5)	C6	C5	C4	O2	-177.2(3)
O4	C10	C1	C6	-160.7(4)	C23	C11	C12	S2	-177.1(3)
O4	C10	C11	C23	84.2(4)	O1	C5	C4	O2	3.4(3)
O4	C10	C11	C12	-93.0(5)	C5	C4	O2	C8	-109.2(3)
C10	C1	C6	C5	173.6(3)					

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6l_auto.

Atom	*x*	*y*	*z*	U(eq)
H90	10877(2)	4291.4(18)	2945.1(15)	32.4(7)
H71	11988(2)	4450(2)	1771.1(16)	41.8(8)
H29	3744(2)	5474(2)	3314.4(17)	43.3(8)
H83	10523(2)	2855.5(18)	3366.4(16)	38.8(8)
H2	8117(2)	-1882(2)	3911.4(18)	48.1(9)
H25	4862(2)	3094(2)	3510.9(18)	47.2(9)
H75	10889(3)	6833(2)	1538.0(18)	49.1(9)
H46	4846(2)	5557(2)	2088.8(18)	44.8(8)
H45	5372(3)	5519(3)	857(2)	65.5(12)
H41	7159(3)	5542(2)	2294(2)	59.7(11)
H76a	13275(17)	3709(4)	1256(11)	83.8(15)
H76b	14243(4)	3755(5)	1498(16)	83.8(15)
H76c	13410(20)	3925(3)	2039(5)	83.8(15)
H18	5737(3)	865(3)	4924(2)	63.4(11)
H22	7440(3)	704(2)	6420.7(19)	57.7(10)
H77a	13670(20)	6367(12)	-37(3)	113(2)
H77b	13590(20)	7340(13)	174(4)	113(2)
H77c	14533(4)	6870(30)	89(6)	113(2)
H42	8289(3)	5211(3)	1425(3)	77.0(14)
H19	4562(3)	658(3)	5787(3)	86.1(17)
H44	6512(4)	5214(3)	-4(2)	82.4(15)
H43	7961(4)	5073(3)	271(3)	85.8(16)
H20	4822(4)	499(3)	6955(3)	90.3(18)
H9a	8592(15)	-2984(13)	3063(13)	105(2)
H9b	9093(5)	-3827(8)	3306(19)	105(2)
H9c	8465(13)	-3310(20)	3856(6)	105(2)
H21	6264(3)	495(3)	7268(2)	80.8(15)
H78a	11306(15)	7936(12)	623(15)	109(2)
H78b	11305(14)	8270(20)	1393(4)	109(2)
H78c	11881(4)	8736(9)	767(19)	109(2)
H89	8564(2)	4270(2)	2695.4(18)	45.7(9)
H68	9251(2)	-748(2)	-384.1(19)	51.6(9)
H82a	9865(2)	1910(2)	2668.4(18)	47.8(9)
H82b	9201(2)	2694(2)	2811.9(18)	47.8(9)
H14	7683(2)	2202(2)	5470.0(19)	51.2(9)
H65	8319(3)	-175(2)	-2601.8(19)	63.6(12)
H37	5138(2)	6968(2)	1611(2)	56.8(10)
H85	10313(2)	4344(2)	4155.8(17)	47.5(9)
H87	7709(3)	4796(2)	4695(2)	60.2(11)
H58	7115(2)	-2026(2)	-941.2(18)	45.0(8)
H6	9233(2)	427.8(19)	4163.1(16)	41.4(8)
H54a	4280(20)	1206(6)	2472(2)	98.9(18)

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6l_auto.

Atom	*x*	*y*	*z*	U(eq)
H54b	4605(16)	2164(18)	2376(4)	98.9(18)
H54c	3591(8)	1960(20)	2343(3)	98.9(18)
H86	9159(3)	4661(3)	5001.1(19)	58.8(11)
H36a	5835(3)	7980(2)	2241(3)	69.7(13)
H36b	6510(3)	7221(2)	2040(3)	69.7(13)
H66	9808(3)	-68(3)	-2429(2)	66.2(12)
H52	7285(3)	1643(2)	968.6(18)	50.8(9)
H88	7412(2)	4589(2)	3549(2)	57.1(10)
H23	8048(2)	730(2)	5242.5(17)	41.9(8)
H48	6013(2)	-600(2)	786.5(18)	46.2(9)
H55a	6925(15)	2667(13)	1934(16)	114(2)
H55b	7034(12)	3080(20)	1167(5)	114(2)
H55c	6462(5)	3561(11)	1770(20)	114(2)
H59a	8550(3)	-2385(2)	-583(2)	56.0(10)
H59b	7880(3)	-3151(2)	-430(2)	56.0(10)
H31a	1119(6)	2870(20)	4742(6)	102.6(19)
H31b	2107(18)	2517(14)	4738(6)	102.6(19)
H31c	1870(20)	3462(9)	4975(2)	102.6(19)
H57	6917(2)	-663.3(19)	-399.8(16)	37.1(8)
H7a	10575(17)	1083(3)	3673(9)	74.6(13)
H7b	10591(17)	911(3)	4490(7)	74.6(13)
H7c	11492(3)	1016(4)	4007(15)	74.6(13)
H13a	7124(3)	3106(2)	4604(2)	69.6(13)
H13b	6413(3)	2407(2)	4862(2)	69.6(13)
H91a	9410(20)	3787(17)	-278(7)	124(2)
H91b	9651(16)	2981(7)	190(20)	124(2)
H91c	8826(8)	3570(20)	435(13)	124(2)
H67	10278(3)	-366(3)	-1321(2)	64.4(11)
H38a	4373(4)	6070(20)	4520(20)	143(3)
H38b	4835(17)	6230(30)	5209(4)	143(3)
H38c	4893(15)	6929(6)	4590(20)	143(3)
H64	7288(3)	-557(2)	-1675.0(18)	50.6(9)
H30a	4561(11)	1709(19)	3739(7)	104.8(19)
H30b	4298(16)	1968(13)	4523(12)	104.8(19)
H30c	3874(7)	1152(7)	4226(19)	104.8(19)
H8a	11280(20)	-1496(7)	2658(3)	86.1(16)
H8b	11978(6)	-2160(20)	2934(4)	86.1(16)
H8c	11006(15)	-2460(14)	2832(6)	86.1(16)
H32a	2340(20)	6004(3)	3050(6)	91.0(17)
H32b	1493(4)	6141(4)	3585(18)	91.0(17)
H32c	2452(19)	6171(4)	3846(12)	91.0(17)
H53a	4710(20)	-1226(4)	1322(14)	104.3(19)

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6l_auto.

Atom	*x*	*y*	*z*	U(eq)
H53b	3732(5)	-1090(7)	1117(19)	104.3(19)
H53c	4540(20)	-967(4)	541(5)	104.3(19)
H61a	9610(7)	-1500(30)	1451(14)	143(3)
H61b	9384(13)	-1510(30)	2274(12)	143(3)
H61c	9202(8)	-2327(4)	1840(30)	143(3)
H15a	8080(20)	640(30)	2174(14)	179(4)
H15b	7907(14)	1488(4)	2600(30)	179(4)
H15c	8424(8)	700(30)	2924(17)	179(4)

Note: The atom No. C15 is showing high thermal parameter values with high anisotropicity. This is probably due to the receding of SCXRD data at room temperature. The atom needs splitting which tried to be performed by using the free variable method and with fixing thermal ellipsoid at 50-50 % but the atom is not refined properly thus atom C15 is kept as Isotropic.

3. Quantum Chemical Calculations

DFT calculations were employed to calculate the optimized energies and to compute the geometries for different possible conformers of intermediates and final product. DFT calculations with a hybrid functional B3LYP (Becke's three parameter hybrid functional using the LYP correlation functional) at 6-311++g(d,p) basis set were performed with the Gaussian 09W software package.[2] In every case, the optimized structures finally converged into the minima of the potential surface, which was confirmed from the absence of negative (imaginary) wavenumbers for any normal mode.

Optimized Coordinate_ 3

```
# opt b3lyp/6-311g geom=connectivity

Int-CC_Opt

0 1
 C                  3.44301900   -1.52550700   -1.23455400
 C                  3.66212400   -2.72234200   -0.53729600
 C                  2.88618100   -3.03436600    0.58863600
 C                  1.90074600   -2.14552900    1.00438500
 C                  1.66684100   -0.93941100    0.32048400
 C                  2.45827000   -0.64591800   -0.80988300
 C                  0.59836700   -0.05105500    0.82318100
 C                  0.33411300    1.30368000    0.12500700
```

O	-0.10933400	-0.38259900	1.79447700
C	-1.05055000	1.88392700	0.55583000
C	1.42485400	2.31582600	0.43639000
S	2.04404300	2.59459300	1.96964200
C	-2.22743200	1.16148000	-0.08695400
C	-3.00857400	0.31390000	0.62829700
C	-4.18739200	-0.47431600	0.26180600
C	-4.69846300	-1.35296600	1.24266400
C	-5.81466500	-2.14763900	0.99194400
C	-6.45424100	-2.08001100	-0.24852400
C	-5.96665600	-1.21147100	-1.23044600
C	-4.84871200	-0.41680700	-0.98407300
S	1.90005200	3.23840300	-1.05425100
C	3.16397200	4.47761200	-0.41220500
C	-2.41161100	1.44960100	-1.47398000
N	-2.49680600	1.72249400	-2.60900800
O	4.66805200	-3.52842800	-1.03956600
C	4.97511300	-4.78898500	-0.37945300
H	4.05544200	-1.31454700	-2.09846400
H	3.04227000	-3.95097600	1.13684100
H	1.29260500	-2.36702600	1.86938100
H	2.31596200	0.27097800	-1.36227600
H	0.31026700	1.13506400	-0.95512400
H	-1.12034000	1.81188800	1.63814600
H	-1.07964800	2.93965700	0.28083400
H	-2.69164800	0.17432800	1.65518800
H	-4.20496700	-1.40886100	2.20467800
H	-6.18423100	-2.81444200	1.75934400
H	-7.32242400	-2.69377200	-0.44790500
H	-6.45934500	-1.15119300	-2.19155100
H	-4.49903300	0.24474200	-1.76053400
H	3.47954300	5.03955900	-1.28626400
H	2.69519800	5.12604000	0.31965700
H	3.99778200	3.94559300	0.03244600
H	5.78774300	-5.21603400	-0.95647600
H	5.29935800	-4.62434100	0.64966300
H	4.11601500	-5.46204800	-0.39761800

1 2 1.5 6 1.5 27 1.0
2 3 1.5 25 1.0
3 4 1.5 28 1.0
4 5 1.5 29 1.0
5 6 1.5 7 1.0
6 30 1.0
7 8 1.0 9 2.0
8 10 1.0 11 1.0 31 1.0
9
10 13 1.0 32 1.0 33 1.0
11 12 1.0 21 1.0
12
13 14 2.0 23 1.5
14 15 1.0 34 1.0
15 16 1.5 20 1.5
16 17 1.5 35 1.0
17 18 1.5 36 1.0
18 19 1.5 37 1.0

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 19 20 1.5 38 1.0
 20 39 1.0
 21 22 1.0
 22 40 1.0 41 1.0 42 1.0
 23 24 3.0
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 25 26 1.0
 26 43 1.0 44 1.0 45 1.0
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Optimized Coordinate_7

```
# opt b3lyp/6-311g geom=connectivity

Pdt-CCN

0 1
 C                  5.27632500    0.25560700    0.84964800
 C                  5.16571800    1.16565800   -0.21612700
 C                  3.93735500    1.35149300   -0.86328200
 C                  2.82425800    0.62837100   -0.43500600
 C                  2.91712200   -0.28081600    0.62959500
 C                  4.16627600   -0.45841300    1.26320900
 C                  1.75782400   -1.06176300    1.09657900
 C                  0.37341000   -0.71751700    0.58330300
 O                  1.86895800   -1.95405400    1.96645300
 C                 -0.29086700    0.40980000    1.35178700
 C                 -0.20635700   -1.45053100   -0.37165500
 S                 -1.93624900   -1.25067300   -0.96163000
 C                 -1.56889600    1.00375000    0.70179800
 C                 -2.63794000   -0.08219400    0.40368900
 C                 -3.97422800    0.43307000   -0.06965400
 C                 -5.13824800    0.08502200    0.63042300
 C                 -6.38565000    0.56050200    0.22052500
 C                 -6.48481500    1.38853700   -0.89908300
 C                 -5.33112600    1.73622300   -1.60830200
 C                 -4.08559900    1.25975400   -1.19958400
 S                  0.69225800   -2.78990700   -1.27445900
```

C	0.26373500	-4.24539300	-0.12142600
C	-2.11397000	2.04186700	1.58623700
N	-2.52684800	2.85658800	2.31005300
O	6.33208500	1.82905300	-0.55150900
C	6.32352400	2.79075700	-1.64415800
H	6.23956000	0.13610000	1.32310900
H	3.84124500	2.03836700	-1.69004900
H	1.88054500	0.75803400	-0.94720600
H	4.23291300	-1.16547300	2.07741400
H	0.43029400	1.21952300	1.49045800
H	-0.53462400	0.05295600	2.35813300
H	-1.29838500	1.48110300	-0.24379100
H	-2.76995200	-0.70070000	1.28886900
H	-5.06620100	-0.55332000	1.50181700
H	-7.27337100	0.28629100	0.77424500
H	-7.44984700	1.75898700	-1.21740400
H	-5.40215100	2.37379200	-2.47919900
H	-3.20189800	1.51987000	-1.76697300
H	0.71961500	-5.12275400	-0.57109300
H	0.68749500	-4.04178000	0.85581700
H	-0.81430500	-4.35943000	-0.07683400
H	7.34119200	3.16074600	-1.69923100
H	6.05309300	2.31151200	-2.58679200
H	5.64112800	3.61666100	-1.43489600

1 2 1.5 6 2.0 27 1.0
2 3 1.5 25 1.0
3 4 1.5 28 1.0
4 5 1.5 29 1.0
5 6 1.5 7 1.0
6 30 1.0
7 8 1.0 9 2.0
8 10 1.0 11 2.0
9
10 13 1.0 31 1.0 32 1.0
11 12 1.0 21 1.0
12
13 14 1.0 23 1.0 33 1.0
14 15 1.0 34 1.0
15 16 1.5 20 1.5
16 17 1.5 35 1.0
17 18 1.5 36 1.0
18 19 1.5 37 1.0
19 20 1.5 38 1.0
20 39 1.0
21
22 40 1.0 41 1.0 42 1.0
23 24 3.0
24
25 26 1.0
26 43 1.0 44 1.0 45 1.0
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Optimized Coordinate_3'

```
# opt b3lyp/6-311g geom=connectivity

Int-CE_Opt

0 1
 C                  4.87686400   -0.74375800    0.95208200
 C                  5.96222500   -0.03528800    0.41760900
 C                  5.74245900    0.99866800   -0.50379900
 C                  4.44018000    1.31420700   -0.87671500
 C                  3.33784900    0.61626200   -0.35152100
 C                  3.58337200   -0.42133200    0.56925200
 C                  1.98713900    1.03178300   -0.79237700
 C                  0.71084800    0.32392100   -0.24785100
 O                  1.84829600    1.99865700   -1.56598100
 C                 -0.54063400    1.03404000   -0.86793400
 C                  0.68395000   -1.15467800   -0.57358600
 S                  0.89248600   -1.73500000   -2.14301600
 C                 -1.88385500    0.64695700   -0.27637000
 C                 -2.69376000   -0.24685100   -0.87897200
 C                 -4.00550600   -0.76336800   -0.45452400
 C                 -4.87886300   -1.25822100   -1.44528700
 C                 -6.14175300   -1.74599400   -1.11354600
 C                 -6.55621700   -1.76474600    0.22139000
 C                 -5.69273100   -1.30259000    1.21884300
 C                 -4.42935500   -0.81190300    0.88901200
 S                  0.32945600   -2.38672100    0.71127100
 C                  0.27545700   -1.49698700    2.39534100
 C                 -2.19735400    1.33394100    1.01363400
 O                 -1.55142900    1.12481300    2.04962200
 O                 -3.18412800    2.28572900    1.05586100
 C                 -4.71446700    3.95953100    0.27664700
 C                 -3.92542500    2.73845300   -0.14984200
 O                  7.21058800   -0.43406000    0.86193300
 C                  8.40040700    0.23043200    0.35071400
 H                  5.07735800   -1.54032400    1.65285800
 H                  6.56650900    1.55132800   -0.92864200
 H                  4.25051100    2.10819400   -1.58410600
 H                  2.76800100   -0.99500200    0.97894100
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H	0.69168500	0.47682300	0.83229400
H	-0.37207100	2.10585700	-0.76005000
H	-0.53667900	0.82507000	-1.93626600
H	-2.33830600	-0.64983200	-1.82245000
H	-4.55898300	-1.25423700	-2.47976000
H	-6.79673100	-2.11602800	-1.89091700
H	-7.53346000	-2.14774900	0.48264000
H	-5.99695100	-1.33538800	2.25638400
H	-3.76586500	-0.49847700	1.68159700
H	-0.09508700	-2.26081900	3.07374500
H	1.27612000	-1.19832100	2.69358200
H	-0.40406300	-0.65193400	2.37127800
H	-5.29289700	4.34232700	-0.56674300
H	-5.40377500	3.70821000	1.08187100
H	-4.04902900	4.74770100	0.62692500
H	-3.20921900	2.96994200	-0.93818100
H	-4.57437100	1.93011900	-0.48085200
H	9.23020300	-0.26281300	0.84459200
H	8.48652000	0.10485600	-0.73010500
H	8.39791900	1.29205700	0.60462700

1 2 1.5 6 1.5 30 1.0
2 3 1.5 28 1.0
3 4 1.5 31 1.0
4 5 1.5 32 1.0
5 6 1.5 7 1.0
6 33 1.0
7 8 1.0 9 2.0
8 10 1.0 11 1.0 34 1.0
9
10 13 1.0 35 1.0 36 1.0
11 12 1.0 21 1.0
12
13 14 2.0 23 1.0
14 15 1.0 37 1.0
15 16 1.5 20 1.5
16 17 1.5 38 1.0
17 18 1.5 39 1.0
18 19 1.5 40 1.0
19 20 1.5 41 1.0
20 42 1.0
21
22 43 1.0 44 1.0 45 1.0
23 24 2.0 25 1.0
24
25 27 1.0
26 27 1.0 46 1.0 47 1.0 48 1.0
27 49 1.0 50 1.0
28 29 1.0
29 51 1.0 52 1.0 53 1.0
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Optimized Coordinate_ 7′

```
# opt b3lyp/6-311g geom=connectivity

Pdt-CE

0 1
 C                  5.54914600    0.57445400    0.84438300
 C                  5.53408600    0.99243000   -0.49782500
 C                  4.36885800    0.86797500   -1.26515000
 C                  3.22298200    0.32726800   -0.68259000
 C                  3.22082800   -0.09235600    0.65652600
 C                  4.40695000    0.03872400    1.41114700
 C                  2.02470200   -0.66970200    1.29299800
 C                  0.70019700   -0.64331700    0.55680800
 O                  2.04600800   -1.11567300    2.46298200
 C                 -0.07036500    0.64999900    0.75885000
 C                  0.25414700   -1.72332300   -0.09236800
 S                 -1.40566900   -1.88545300   -0.86718200
 C                 -1.31209100    0.83143100   -0.14951600
 C                 -2.28801300   -0.35884800   -0.05100100
 C                 -3.62663200   -0.21161100   -0.72914900
 C                 -4.74806300   -0.85271400   -0.17571300
 C                 -5.99964600   -0.75941000   -0.78580400
 C                 -6.14890500   -0.02303800   -1.96378600
 C                 -5.03985300    0.61355800   -2.52634200
 C                 -3.78665500    0.51780100   -1.91851700
 C                 -1.90747300    2.22879800    0.06952500
 O                 -1.75145800    3.11020700   -0.77389700
 O                 -2.53824400    2.57748600    1.24664900
 C                 -3.50580200    2.54180900    3.43290300
 C                 -3.03067300    1.65964200    2.29481700
 S                  1.29353100   -3.23632100   -0.31701900
 C                  0.78268900   -4.16930300    1.26330700
 O                  6.72574000    1.51393000   -0.96828700
 C                  6.81432200    1.97391200   -2.34655400
 H                  6.46592200    0.68426100    1.40454200
```

```
H                  4.34530200    1.17931000   -2.29810800
H                  2.32850600    0.21658900   -1.28016500
H                  4.39989600   -0.29077800    2.44011300
H                  0.60528400    1.49128500    0.57792000
H                 -0.34857100    0.71651800    1.81530800
H                 -0.95897200    0.88025600   -1.17872700
H                 -2.42605800   -0.66447900    0.98221000
H                 -4.63483100   -1.43343100    0.73183200
H                 -6.85194700   -1.25898300   -0.34503700
H                 -7.11807200    0.05370400   -2.43780500
H                 -5.14781900    1.18638200   -3.43727000
H                 -2.94228700    1.01895000   -2.36920700
H                 -3.90782200    1.92769900    4.24146200
H                 -2.68334600    3.13826500    3.82592100
H                 -4.28643500    3.21830200    3.08813700
H                 -3.84722500    1.07013100    1.87983900
H                 -2.22889300    0.99657800    2.61971800
H                  1.30644200   -5.12027400    1.22863800
H                  1.09370700   -3.58350000    2.12149200
H                 -0.29071600   -4.32780600    1.25223200
H                  7.83277600    2.32875500   -2.45826300
H                  6.62893200    1.15649700   -3.04568600
H                  6.11563700    2.79146800   -2.53314900

1 2 1.5 6 2.0 30 1.0
2 3 1.5 28 1.0
3 4 1.5 31 1.0
4 5 1.5 32 1.0
5 6 1.5 7 1.0
6 33 1.0
7 8 1.0 9 2.0
8 10 1.0 11 2.0
9
10 13 1.0 34 1.0 35 1.0
11 12 1.0 26 1.0
12
13 14 1.0 21 1.0 36 1.0
14 15 1.0 37 1.0
15 16 1.5 20 1.5
16 17 1.5 38 1.0
17 18 1.5 39 1.0
18 19 1.5 40 1.0
19 20 1.5 41 1.0
20 42 1.0
21 22 2.0 23 1.0
22
23 25 1.0
24 25 1.0 43 1.0 44 1.0 45 1.0
25 46 1.0 47 1.0
26
27 48 1.0 49 1.0 50 1.0
28 29 1.0
29 51 1.0 52 1.0 53 1.0
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Optimized Coordinate_4

```
# opt b3lyp/6-311++g(d,p)

Int-SC1

0 1
 S                  1.08076000    0.34705400    0.67508200
 S                  0.67316300    2.27438200   -1.71705200
 O                 -1.30960000   -0.87851700    1.14407300
 C                 -2.01339200   -0.21161300    0.33444000
 C                 -0.07817700    1.08387700   -0.53946300
 C                 -3.48533300   -0.43039800    0.29060900
 C                 -4.01087200   -1.51940600    1.01831800
 H                 -3.32023700   -2.14156200    1.56826100
 C                  4.69318300    0.01873900    1.33052700
 H                  5.37009000   -0.04456300    2.17625100
 C                  3.71070400    0.95265700    1.42554600
 C                  5.02420000   -0.88495700    0.22354200
 C                 -1.39244200    0.75187700   -0.56718200
 H                 -2.01810800    1.20767000   -1.31727900
 C                  4.07076300   -1.43005600   -0.66104000
 H                  3.01988600   -1.22799600   -0.51646900
 C                  6.37621000   -1.25724300    0.06053000
 H                  7.11799700   -0.86734600    0.74605500
 C                 -6.24979100   -0.95190400    0.31998200
 C                 -5.37003800   -1.78195400    1.03200700
 C                 -4.38099300    0.39081200   -0.41029100
 H                 -4.02603900    1.25203000   -0.95858200
 C                  2.73199100    1.31983700    0.34747500
 H                  3.10237300    1.05058900   -0.63537600
 H                  2.49421000    2.37732500    0.38989900
 C                  4.46649400   -2.28693500   -1.68837200
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H                 3.71918000   -2.70463900   -2.34934200
C                 6.76811900   -2.10439500   -0.97313900
H                 7.81086300   -2.36870000   -1.08612000
C                 5.81341300   -2.61967100   -1.85548400
H                 6.11418100   -3.28469000   -2.65374200
C                -5.75530100    0.14090400   -0.40036700
H                -6.41856600    0.79666800   -0.94382000
C                -0.79788600    2.86165300   -2.74137300
H                -0.37332800    3.58959000   -3.42666000
H                -1.22782700    2.03607900   -3.29954500
H                -1.53417100    3.34087200   -2.10378800
H                -5.78200000   -2.61522100    1.58203800
C                 3.61095700    1.71197000    2.63851800
N                 3.52449500    2.34868400    3.61466900
C                -8.57704000   -0.49282500   -0.30451700
H                -9.52957600   -0.96445600   -0.08919800
H                -8.58262800    0.53427300    0.06608300
H                -8.39811400   -0.49900300   -1.38173200
O                -7.59052900   -1.29854600    0.39596600

1 5 1.0
2 5 1.0 34 1.0
3 4 2.0
4 6 1.0 13 1.0
5 13 2.0
6 7 1.5 21 1.5
7 8 1.0 20 2.0
8
9 10 1.0 11 2.0 12 1.0
10
11 23 1.0 39 1.5
12 15 1.5 17 1.5
13 14 1.0
14
15 16 1.0 26 1.5
16
17 18 1.0 28 1.5
18
19 20 1.5 32 1.5 45 1.0
20 38 1.0
21 22 1.0 32 1.5
22
23 24 1.0 25 1.0
24
25
26 27 1.0 30 1.5
27
28 29 1.0 30 1.5
29
30 31 1.0
31
32 33 1.0
33
34 35 1.0 36 1.0 37 1.0
35
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 37
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 39 40 3.0
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 41 42 1.0 43 1.0 44 1.0 45 1.0
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 43
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Optimized Coordinate_4'

```
# opt b3lyp/6-311++g(d,p)

Int-SE1_Opt

0 1
 S                 -0.80744200    0.16245700   -0.21903300
 S                 -0.31938700    0.33185900    2.83242100
 O                  1.63102300   -0.27481100   -1.40837700
 C                  2.34282900   -0.19696200   -0.36745800
 C                  0.39998600    0.13916700    1.15286400
 C                  3.82526900   -0.30390400   -0.48939400
 C                  4.35535600   -0.66762600   -1.74564600
 H                  3.66160800   -0.85164600   -2.55269200
 C                 -4.38504000   -0.24852500   -0.84743300
 H                 -5.13409900    0.11566900   -1.54369600
 C                 -3.54696000    0.70667300   -0.37164800
 C                 -4.48481500   -1.67541800   -0.53294600
 C                  1.73170900   -0.02234200    0.94316400
 H                  2.38258600   -0.04255200    1.80207100
 C                 -3.39897900   -2.47846300   -0.12492300
 H                 -2.40480400   -2.06075700   -0.07849500
 C                 -5.74832900   -2.28972500   -0.67944200
 H                 -6.58647100   -1.69373200   -1.01752900
 C                  6.60325500   -0.52795200   -0.87997700
 C                  5.72127500   -0.78254000   -1.94130100
 C                  4.72329800   -0.04915100    0.55740800
 H                  4.36475200    0.25552100    1.53033500
 C                 -2.49919400    0.51504000    0.67741000
 H                 -2.71849400   -0.33108800    1.31927100
 H                 -2.36357700    1.42198700    1.25181300
 C                 -3.58378600   -3.83249700    0.15447800
 H                 -2.73584900   -4.43417300    0.45298100
 C                 -5.93143500   -3.63902900   -0.38713900
 H                 -6.91050600   -4.08575400   -0.49694000
 C                 -4.84831500   -4.41584000    0.03579900
 H                 -4.98532300   -5.46632100    0.25484200
 C                  6.10417800   -0.15636100    0.37293900
 H                  6.76827100    0.05280000    1.19800300
 C                  1.18804200    0.25944000    3.96353200
 H                  0.77891400    0.37851200    4.96273700
 H                  1.68207100   -0.70348100    3.87963300
 H                  1.86737000    1.07720400    3.74371800
 H                  6.13630600   -1.06437700   -2.89786700
 C                  8.93872100   -0.42085000   -0.13911400
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H                  9.89746400   -0.59661100   -0.61469400
H                  8.88719100    0.61066800    0.21564500
H                  8.81191700   -1.10895900    0.69935700
O                  7.95169300   -0.66942800   -1.17635200
C                 -3.74592600    2.07330200   -0.92234400
O                 -4.54539400    2.37894800   -1.81948700
C                 -3.03056900    4.40229800   -0.80648700
C                 -2.04348100    5.21780600    0.00262200
H                 -2.79793000    4.39731200   -1.87077900
H                 -4.05842500    4.74285900   -0.68414500
H                 -2.06274100    6.25830600   -0.32832200
H                 -2.29297200    5.19122100    1.06343300
H                 -1.03083900    4.83582400   -0.12290400
O                 -2.94353200    3.00944800   -0.31200700

1 5 1.0
2 5 1.0 34 1.0
3 4 2.0
4 6 1.0 13 1.0
5 13 2.0
6 7 1.5 21 1.5
7 8 1.0 20 2.0
8
9 10 1.0 11 2.0 12 1.0
10
11 23 1.0 44 1.0
12 15 1.5 17 1.5
13 14 1.0
14
15 16 1.0 26 1.5
16
17 18 1.0 28 1.5
18
19 20 1.5 32 1.5 43 1.0
20 38 1.0
21 22 1.0 32 1.5
22
23 24 1.0 25 1.0
24
25
26 27 1.0 30 1.5
27
28 29 1.0 30 1.5
29
30 31 1.0
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32 33 1.0
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34 35 1.0 36 1.0 37 1.0
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39 40 1.0 41 1.0 42 1.0 43 1.0
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 42
 43
 44 45 2.0 53 1.0
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 46 47 1.0 48 1.0 49 1.0 53 1.0
 47 50 1.0 51 1.0 52 1.0
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Optimized Coordinate_6

```
# opt b3lyp/6-311++g(d,p)

Pdt-SCN

0 1
 C                  0.96556600    0.64407200    0.31731000
 C                  1.15993300    1.77652700   -0.37322400
 S                  2.69390000    2.14705900   -1.33227300
 C                  3.84602300    1.02635500   -0.33552200
 C                  3.28274600   -0.40355500   -0.35260600
 C                  1.93063000   -0.54751400    0.42445400
 C                 -0.18410100    0.50014900    1.30302400
 O                  0.12773800    0.47171700    2.51615300
 C                 -1.57719700    0.33491600    0.86131200
 C                 -2.59199900    0.26917800    1.84134000
 C                 -3.91671900    0.10482900    1.47999400
 C                 -4.26163200   -0.00626900    0.12221400
 C                 -3.27005100    0.04628000   -0.86535000
 C                 -1.93875200    0.21731400   -0.48867600
 S                 -0.06808800    3.15700900   -0.44191100
 C                 -6.07083000   -0.29065500   -1.51025000
 C                  4.26770200   -1.34409300    0.19809000
 N                  5.06600600   -2.06647500    0.64450100
 C                  1.24366800   -1.86322200    0.04548800
 C                  1.04584200   -2.86118700    1.00790400
 C                  0.43595300   -4.07111700    0.66414400
 C                  0.01665800   -4.29715400   -0.64780900
 C                  0.20682000   -3.30587100   -1.61567000
 C                  0.81412100   -2.09795200   -1.27029800
 O                 -5.61179300   -0.16831200   -0.13497600
 C                  0.86406900    4.46054100    0.58240700
 H                  4.81158900    1.08143300   -0.83019700
 H                  3.92313200    1.42243600    0.67363300
 H                  3.11909800   -0.67629000   -1.39727800
 H                  2.17183200   -0.60368300    1.48943600
 H                 -2.30796800    0.35213400    2.88027600
 H                 -4.70628200    0.05781300    2.21531700
 H                 -3.51962800   -0.04278400   -1.91146400
 H                 -1.17776700    0.25501400   -1.25392500
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H                  -7.14678800   -0.40406500   -1.43747000
H                  -5.83207000    0.60578000   -2.08551600
H                  -5.63881000   -1.16981800   -1.99203700
H                   1.36913400   -2.69111400    2.02640600
H                   0.29335600   -4.83267600    1.41892200
H                  -0.45221800   -5.23455600   -0.91519800
H                  -0.11660500   -3.47361900   -2.63451000
H                   0.95187000   -1.33500700   -2.02713300
H                   0.26256000    5.36275100    0.52003400
H                   0.93909000    4.12166300    1.60995800
H                   1.84318100    4.62815000    0.14710200

1 2 2.0 6 1.0 7 1.0
2 3 1.0 15 1.0
3
4 5 1.0 27 1.0 28 1.0
5 6 1.0 17 1.0 29 1.0
6 19 1.0 30 1.0
7 8 2.0 9 1.0
8
9 10 1.5 14 1.5
10 11 2.0 31 1.0
11 12 1.5 32 1.0
12 13 1.5 25 1.0
13 14 1.5 33 1.0
14 34 1.0
15
16 25 1.0 35 1.0 36 1.0 37 1.0
17 18 3.0
18
19 20 1.5 24 1.5
20 21 1.5 38 1.0
21 22 1.5 39 1.0
22 23 1.5 40 1.0
23 24 1.5 41 1.0
24 42 1.0
25
26 43 1.0 44 1.0 45 1.0
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Optimized Coordinate_6’

```
# opt b3lyp/6-311++g(d,p)

Pdt-SE_Opt

0 1
 C                  0.22639300    0.95991900    0.13201300
 C                  0.16207900    2.16833000   -0.44365700
 S                  1.47197300    2.88494900   -1.52376200
 C                  2.90052800    1.80461000   -0.90553900
 C                  2.50114900    0.32551700   -0.99240000
 C                  1.37739900   -0.05253000    0.01219500
 C                 -0.76869200    0.55221700    1.20569400
 O                 -0.34282300    0.52733800    2.38407600
 C                 -2.14192200    0.13780500    0.87446200
 C                 -3.01060800   -0.22563400    1.92637100
 C                 -4.30652000   -0.63397200    1.66712400
 C                 -4.76731600   -0.69323600    0.34113900
 C                 -3.92090000   -0.34198400   -0.71753500
 C                 -2.61766100    0.07054900   -0.44291800
 S                 -1.25158900    3.33701800   -0.19016300
 C                 -6.64795000   -1.20191600   -1.14902100
 C                  0.85953200   -1.46821400   -0.26746200
 C                  0.90590800   -2.44385200    0.73802500
 C                  0.44695500   -3.74185700    0.49683900
 C                 -0.06435300   -4.08262900   -0.75661900
 C                 -0.11832900   -3.11685100   -1.76596800
 C                  0.33729400   -1.82051800   -1.52179300
 O                 -6.07778300   -1.11442400    0.18640500
 C                 -0.41473600    4.55440200    1.00845400
 H                  3.73353800    2.03244700   -1.56622200
 H                  3.14050400    2.10161300    0.11125600
 H                  2.18037000    0.12275400   -2.01234200
 H                  1.83214200   -0.07201200    1.00576500
 H                 -2.63745700   -0.17619700    2.93896200
 H                 -4.98557400   -0.91292300    2.45930100
 H                 -4.26079900   -0.38446600   -1.74090100
 H                 -1.96813900    0.34151100   -1.26217000
 H                 -7.66527200   -1.54577200   -0.99792800
 H                 -6.65662700   -0.22570600   -1.63745400
 H                 -6.10251800   -1.92110600   -1.76314200
 H                  1.29289500   -2.18040000    1.71359700
 H                  0.48883200   -4.48131000    1.28562600
 H                 -0.41715600   -5.08757600   -0.94615800
 H                 -0.51255800   -3.37290600   -2.74056500
 H                  0.28797300   -1.08322000   -2.31308400
 H                 -1.13881600    5.34631100    1.17697200
 H                 -0.18733600    4.03905800    1.93544300
 H                  0.48189500    4.95274300    0.54576200
 C                  3.72914600   -0.54361100   -0.78265700
 O                  4.30975000   -1.17263500   -1.66889900
 C                  5.38335000   -1.29345800    0.85572600
```

C	5.68800500	-1.02869000	2.31518200
H	5.16902900	-2.34238800	0.65413300
H	6.18684500	-0.97462100	0.19268700
H	6.57583000	-1.58865900	2.61602400
H	5.87685600	0.03069700	2.48777100
H	4.85746800	-1.33687100	2.94975600
O	4.16953400	-0.50763500	0.51888900

1 2 2.0 6 1.0 7 1.0
2 3 1.0 15 1.0
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4 5 1.0 25 1.0 26 1.0
5 6 1.0 27 1.0 44 1.0
6 17 1.0 28 1.0
7 8 2.0 9 1.0
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9 10 1.5 14 1.5
10 11 2.0 29 1.0
11 12 1.5 30 1.0
12 13 1.5 23 1.0
13 14 1.5 31 1.0
14 32 1.0
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16 23 1.0 33 1.0 34 1.0 35 1.0
17 18 1.5 22 1.5
18 19 1.5 36 1.0
19 20 1.5 37 1.0
20 21 1.5 38 1.0
21 22 1.5 39 1.0
22 40 1.0
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24 41 1.0 42 1.0 43 1.0
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44 45 2.0 53 1.0
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46 47 1.0 48 1.0 49 1.0 53 1.0
47 50 1.0 51 1.0 52 1.0
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References

1. The crystallographic coordinates have been deposited with the Cambridge Crystallographic Data Centre; deposition nos. CCDC 2096630 (**6i**) and CCDC 2099427 (**6l**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.
2. Frisch et al. GAUSSIAN 09, REVISION D.02, Gaussian, Inc., Wallingford, CT, 2010.