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Supporting Information

$FeCl_3$-Mediated selenylative benzannulation of aryl alkynones to 3-selenyl *β*-naphthols

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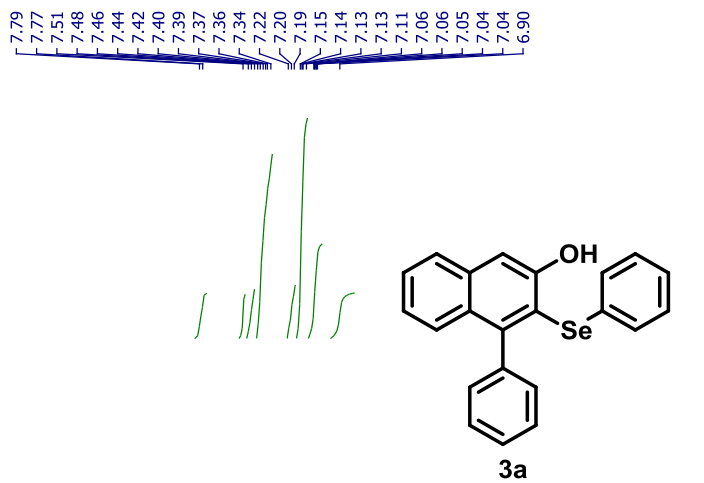
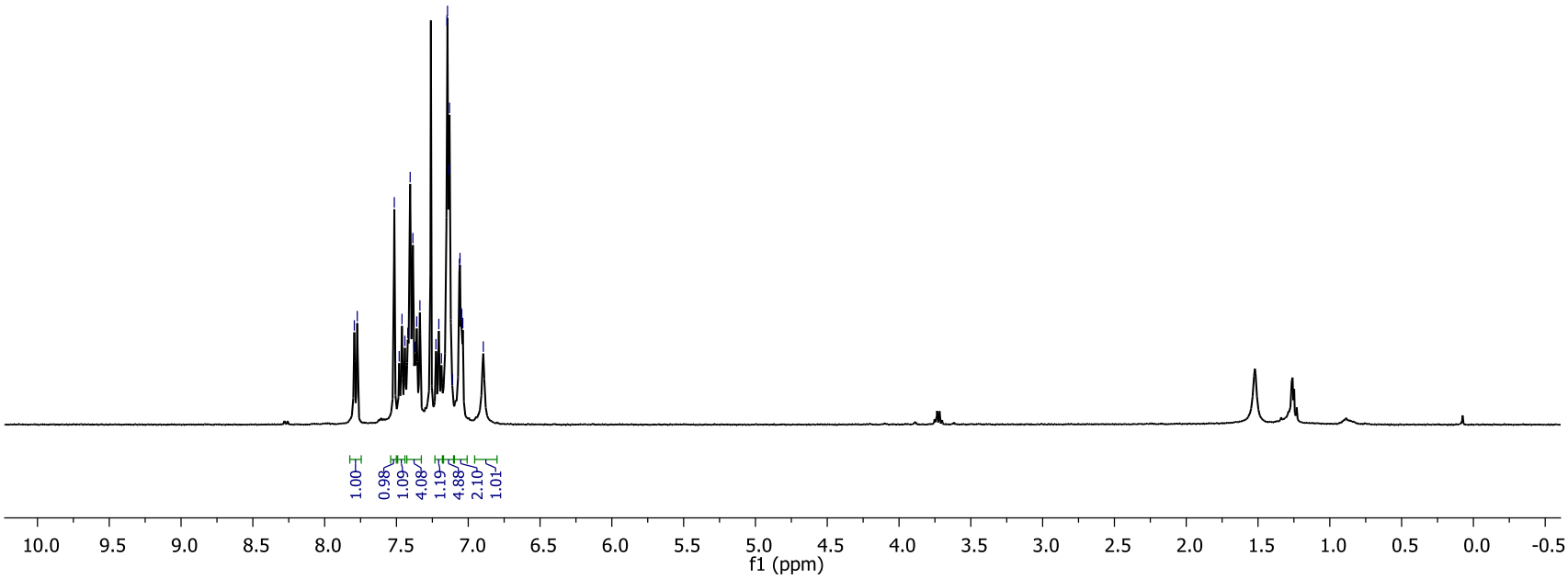
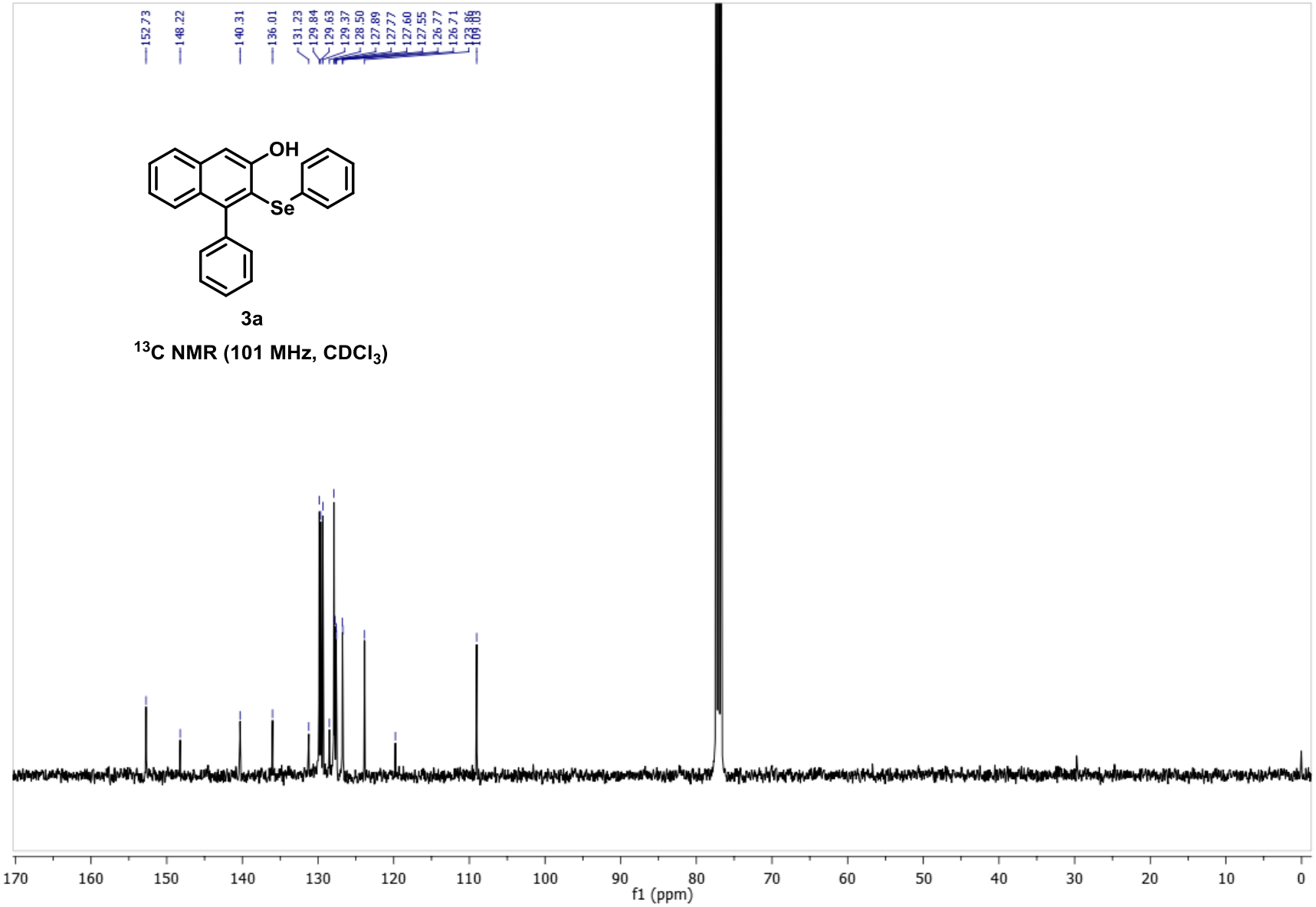


3a

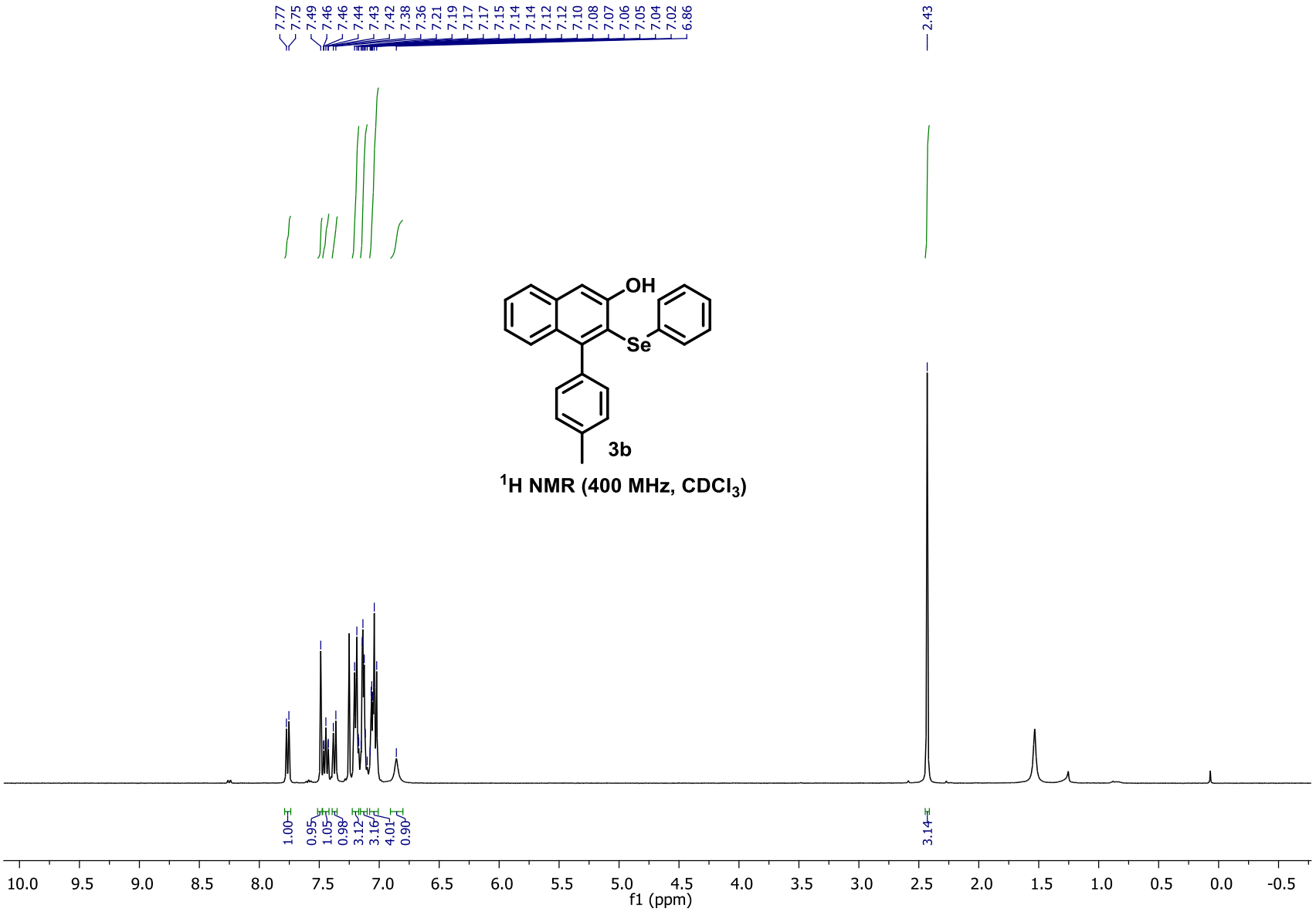
^{1}H NMR (400 MHz, $CDCl_3$)



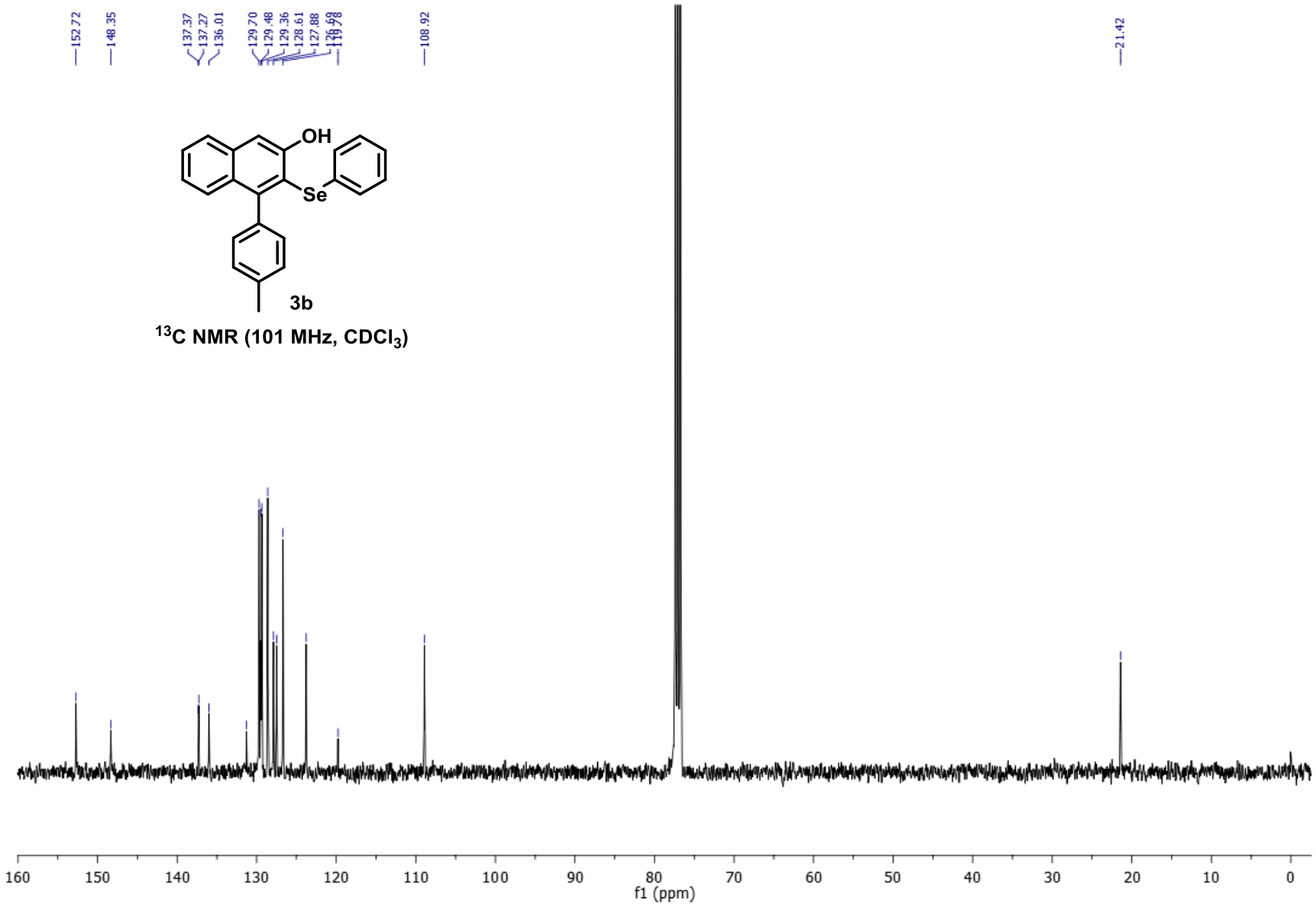


3a

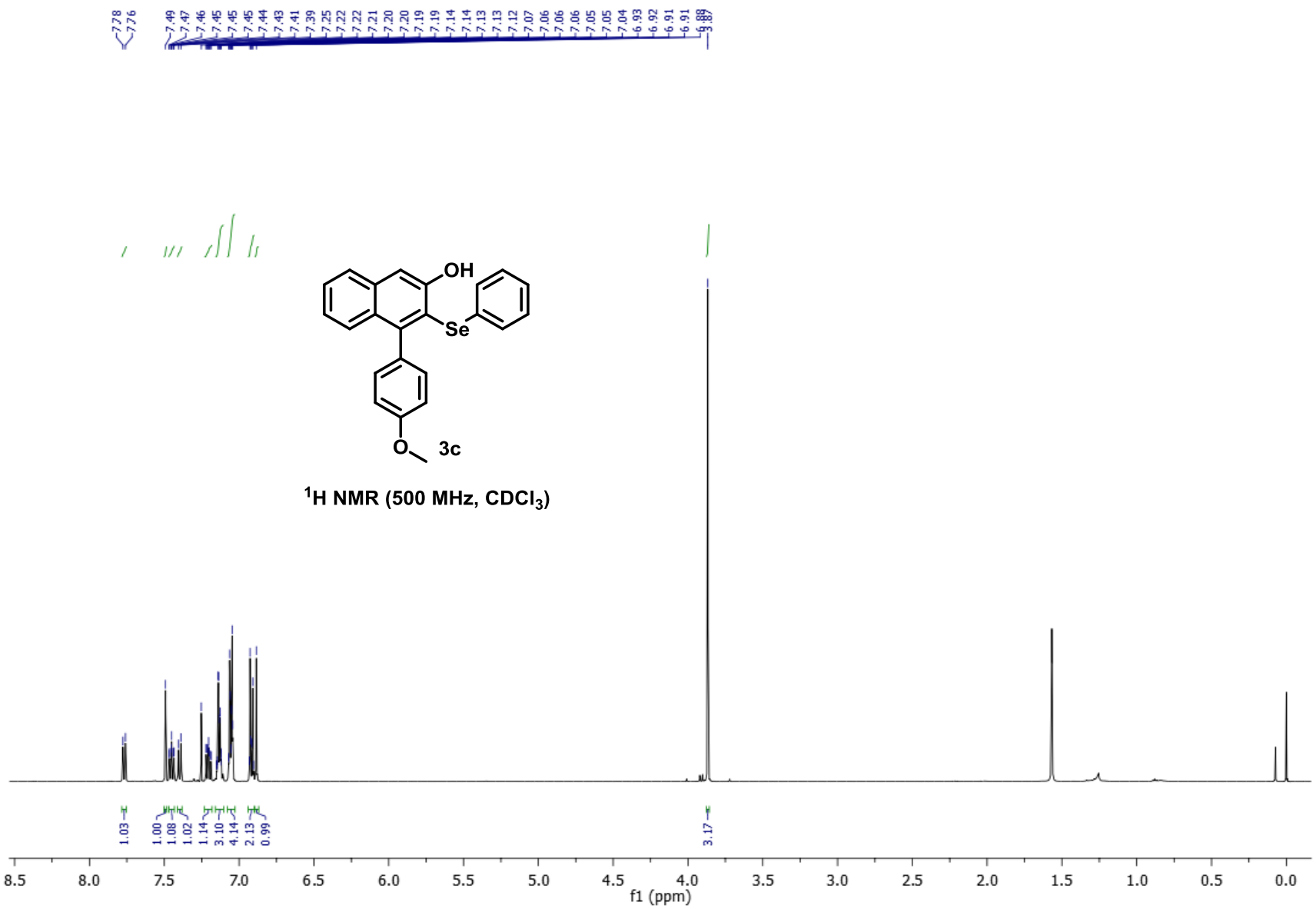
^{13}C NMR (101 MHz, $CDCl_3$)



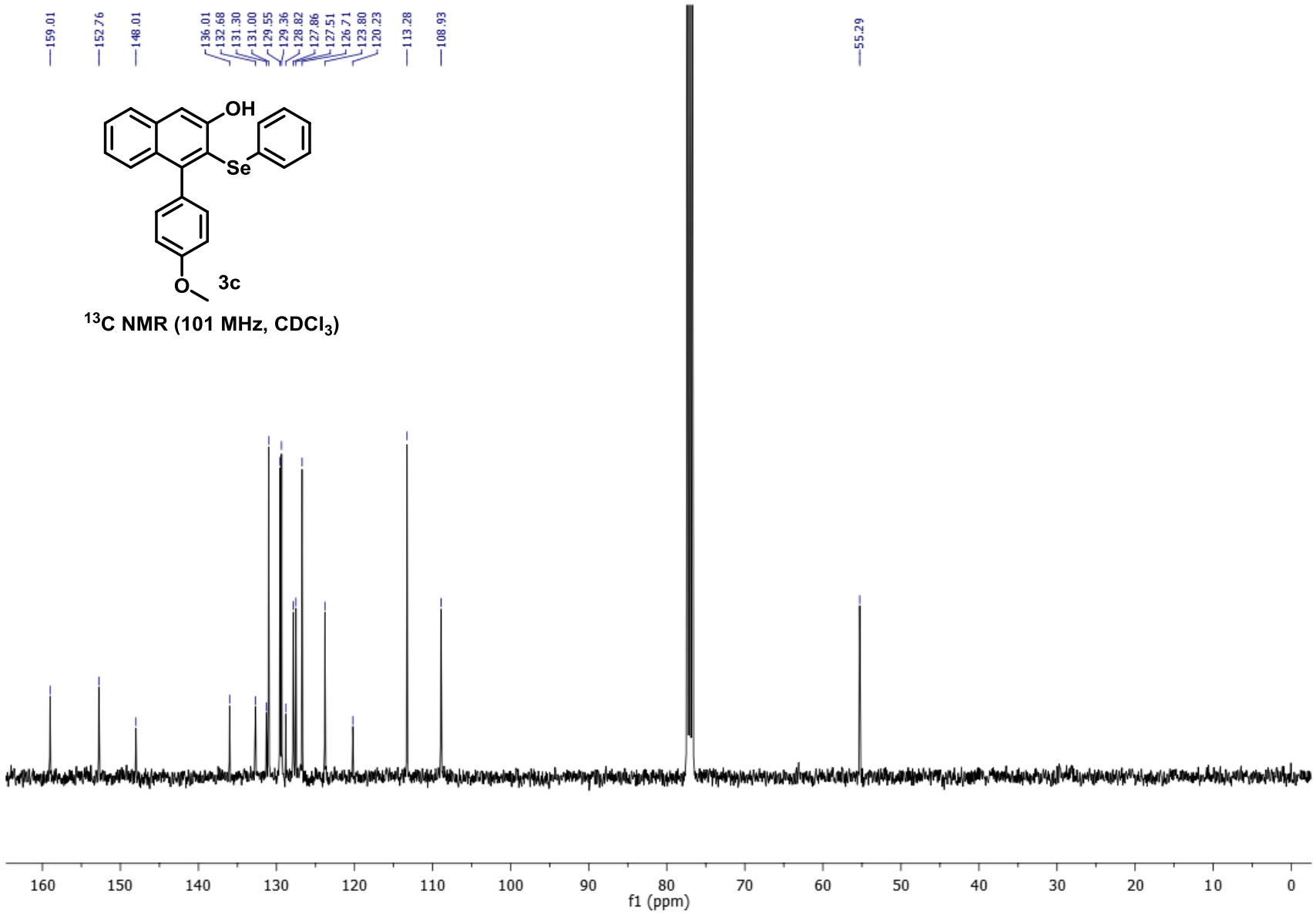
^{1}H NMR (400 MHz, $CDCl_3$)



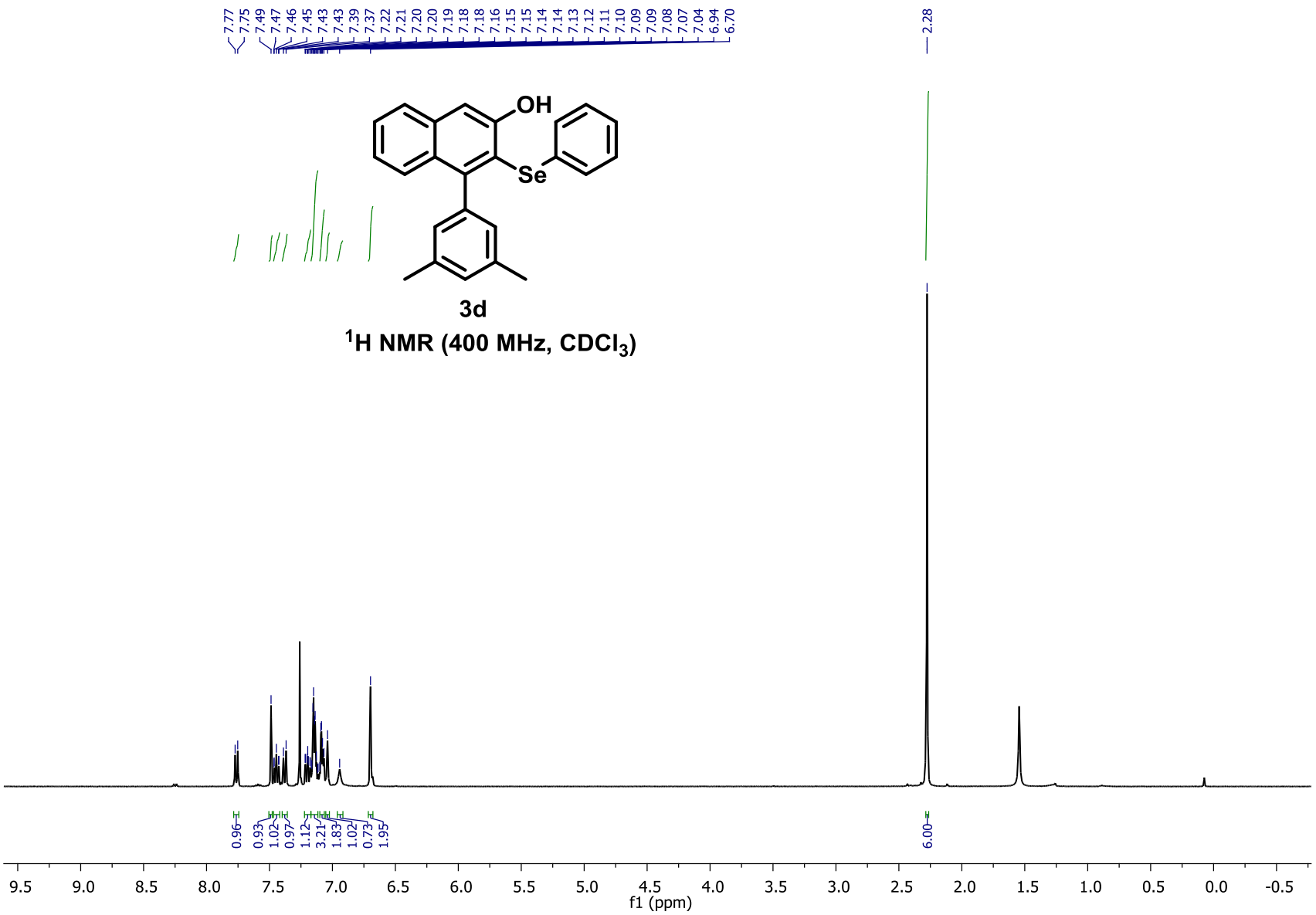
^{13}C NMR (101 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, $CDCl_3$)

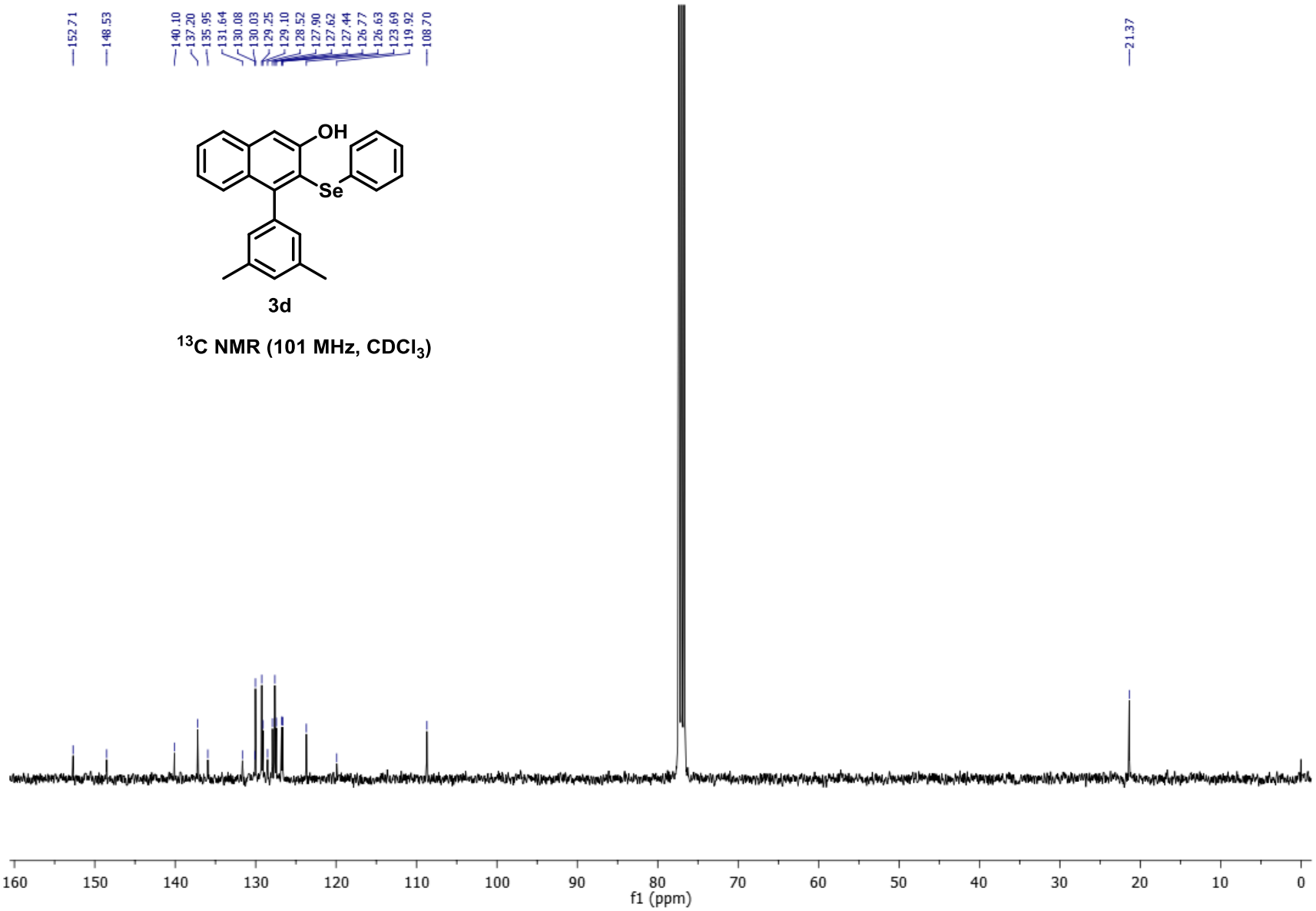


^{13}C NMR (101 MHz, $CDCl_3$)



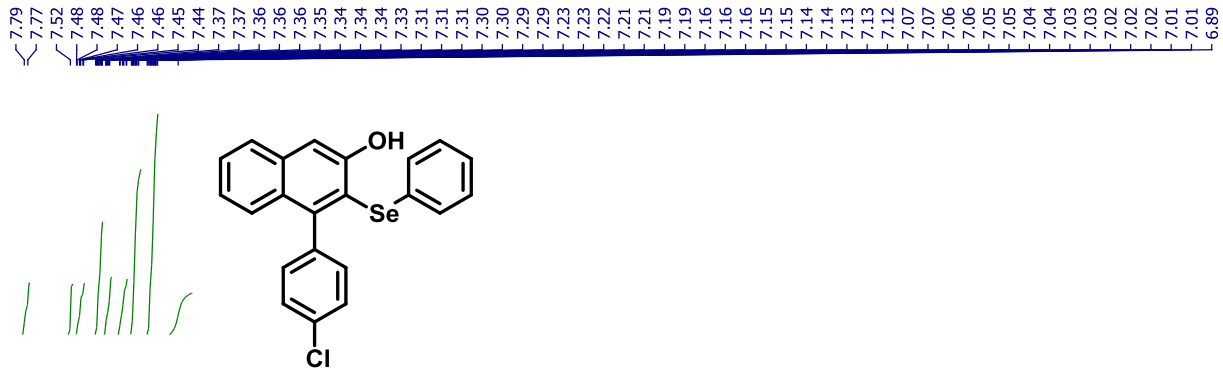
3d

^{1}H NMR (400 MHz, $CDCl_3$)



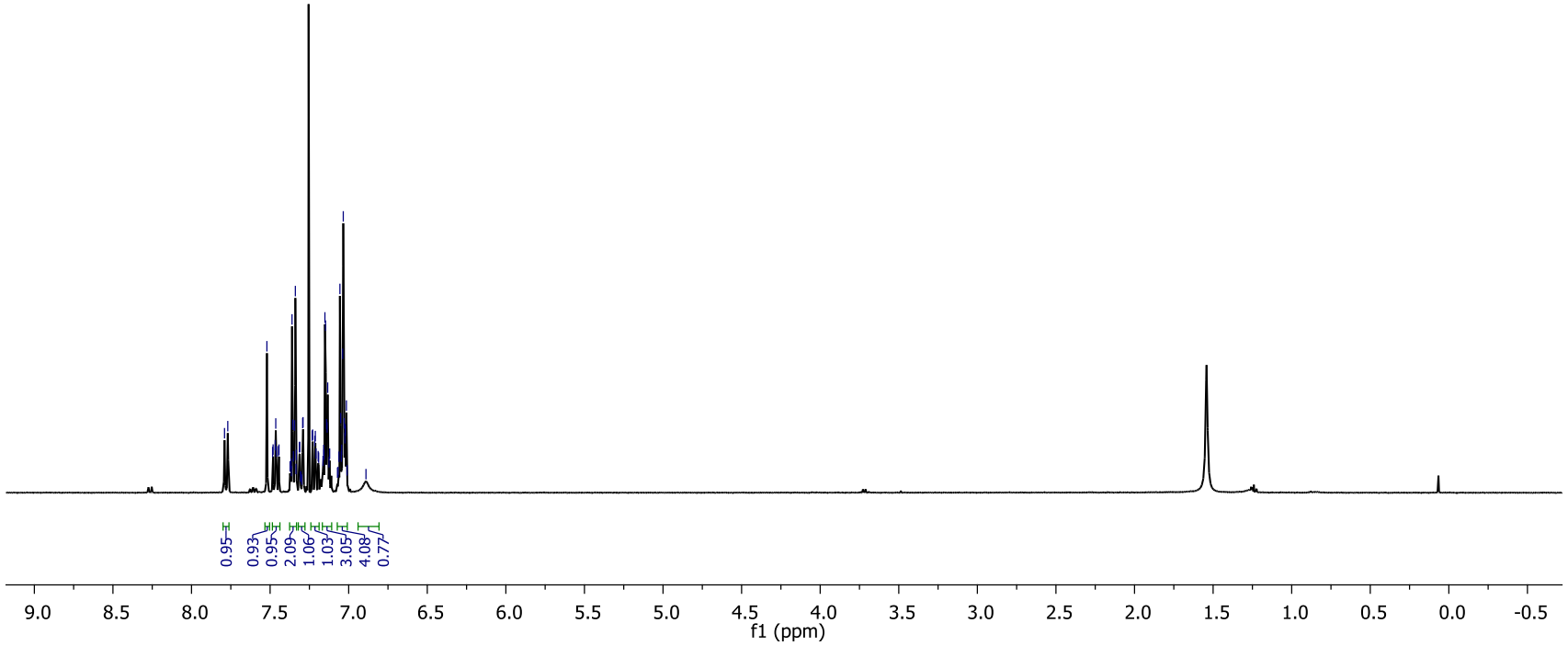
3d

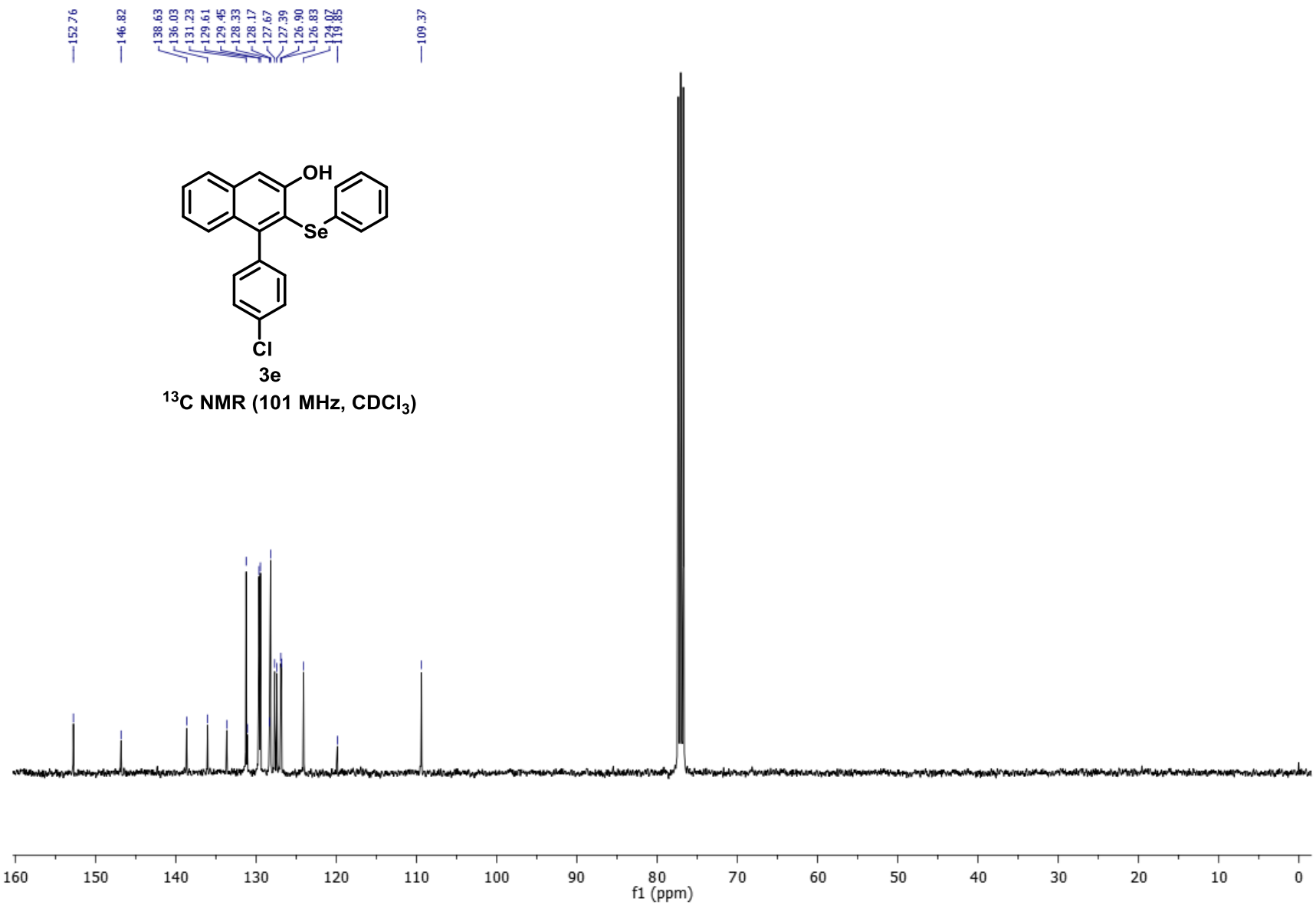
^{13}C NMR (101 MHz, $CDCl_3$)



3e

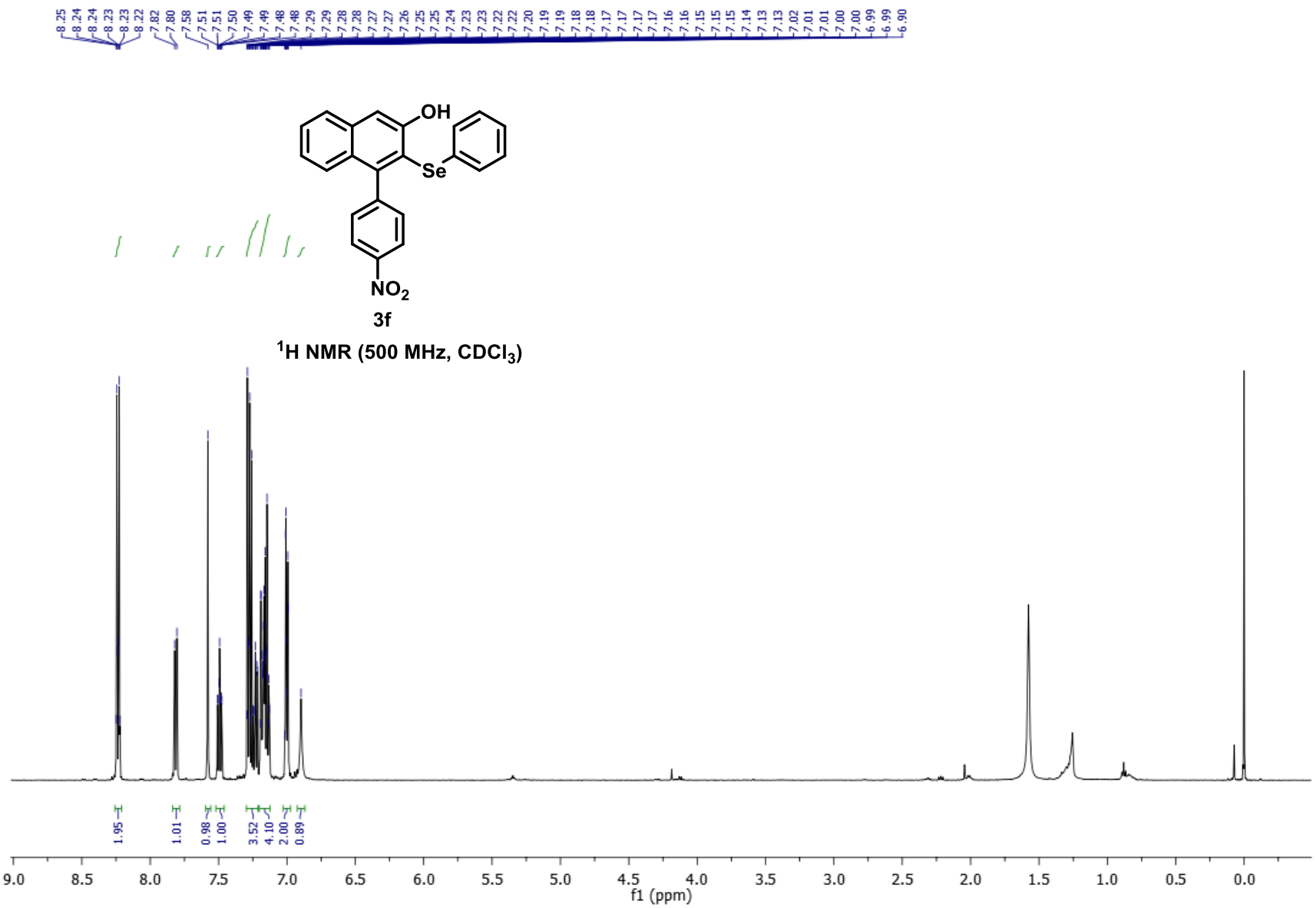
^{1}H NMR (400 MHz, $CDCl_3$)





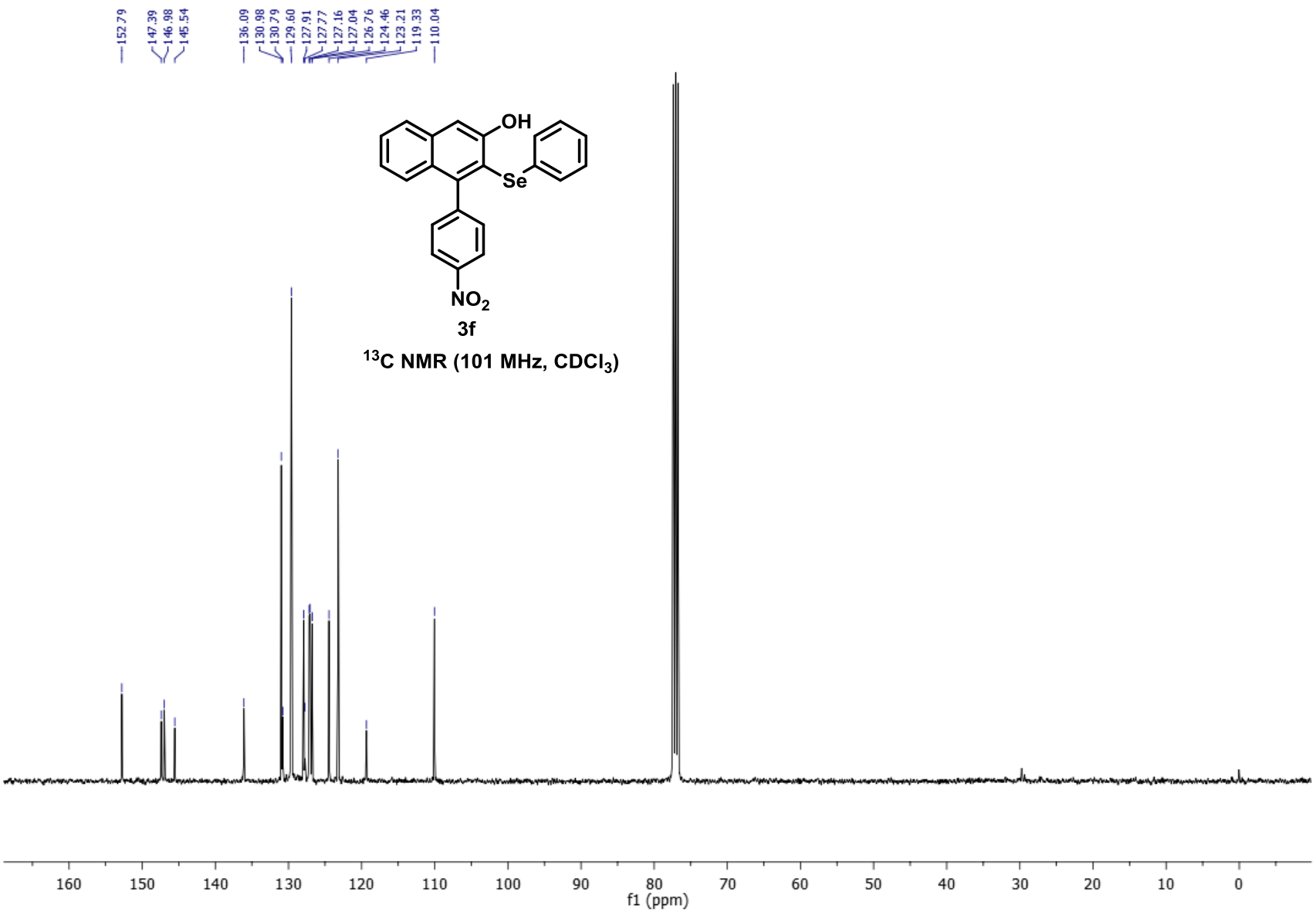
3e

^{13}C NMR (101 MHz, $CDCl_3$)



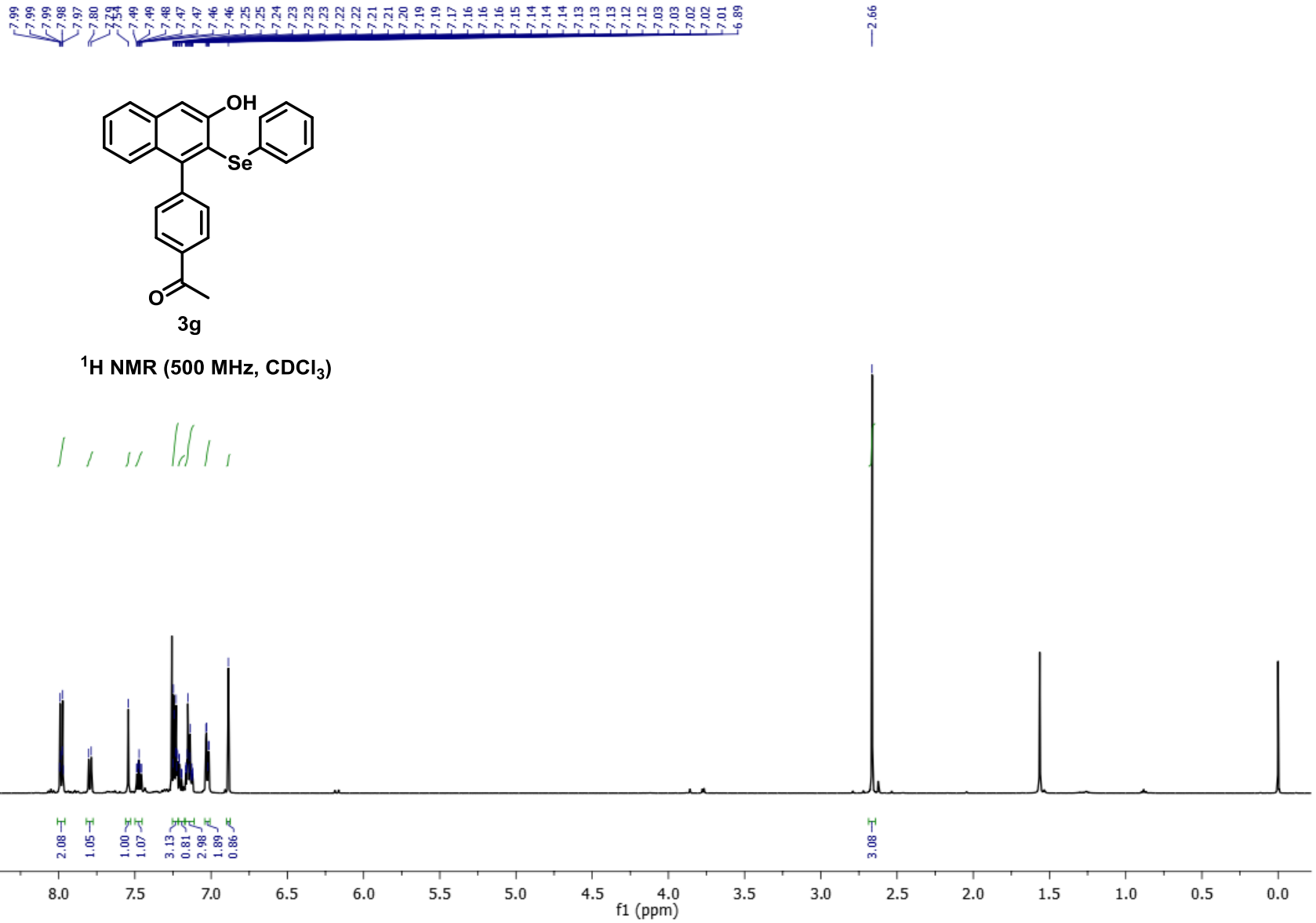
3f

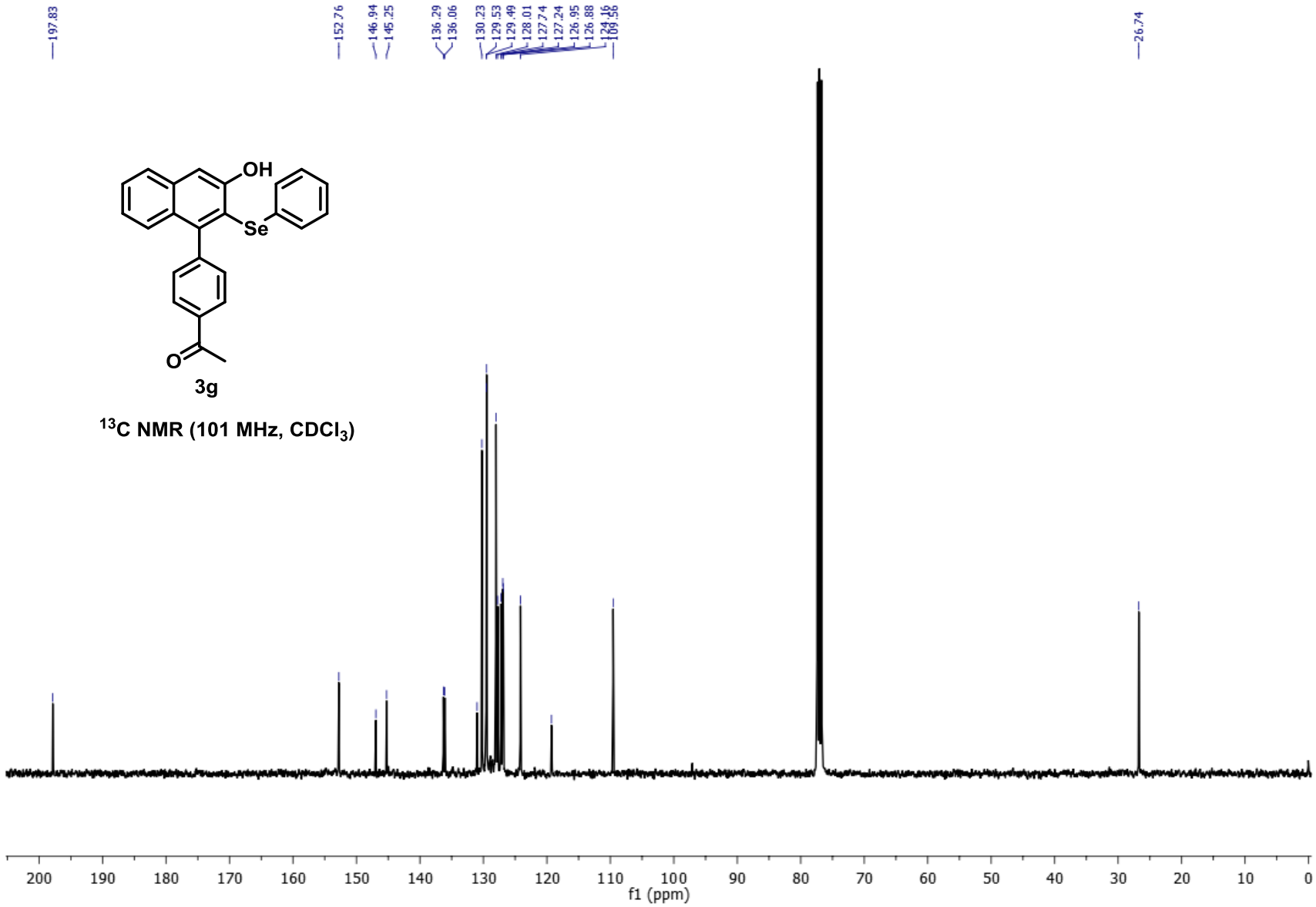
^{1}H NMR (500 MHz, $CDCl_3$)

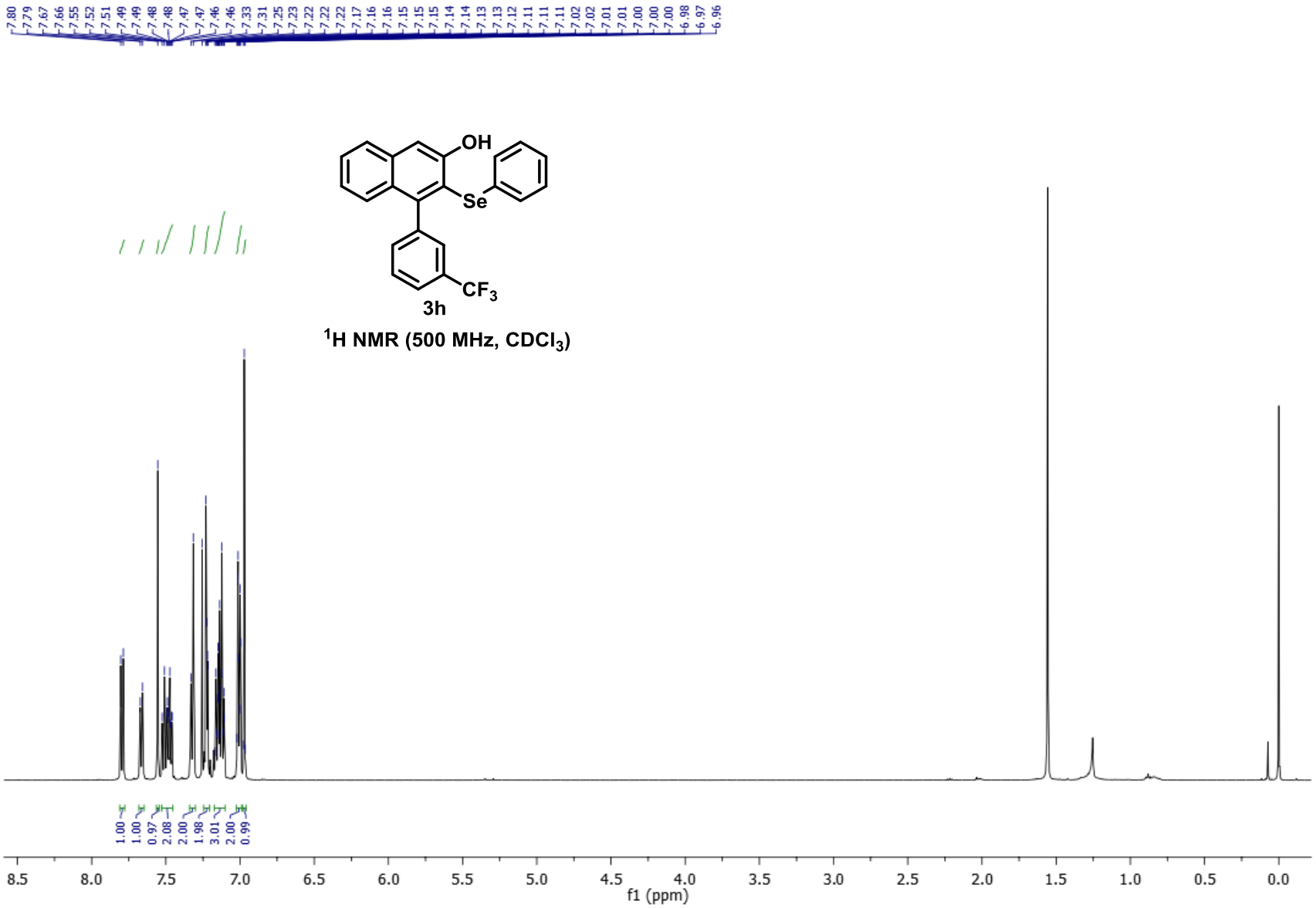


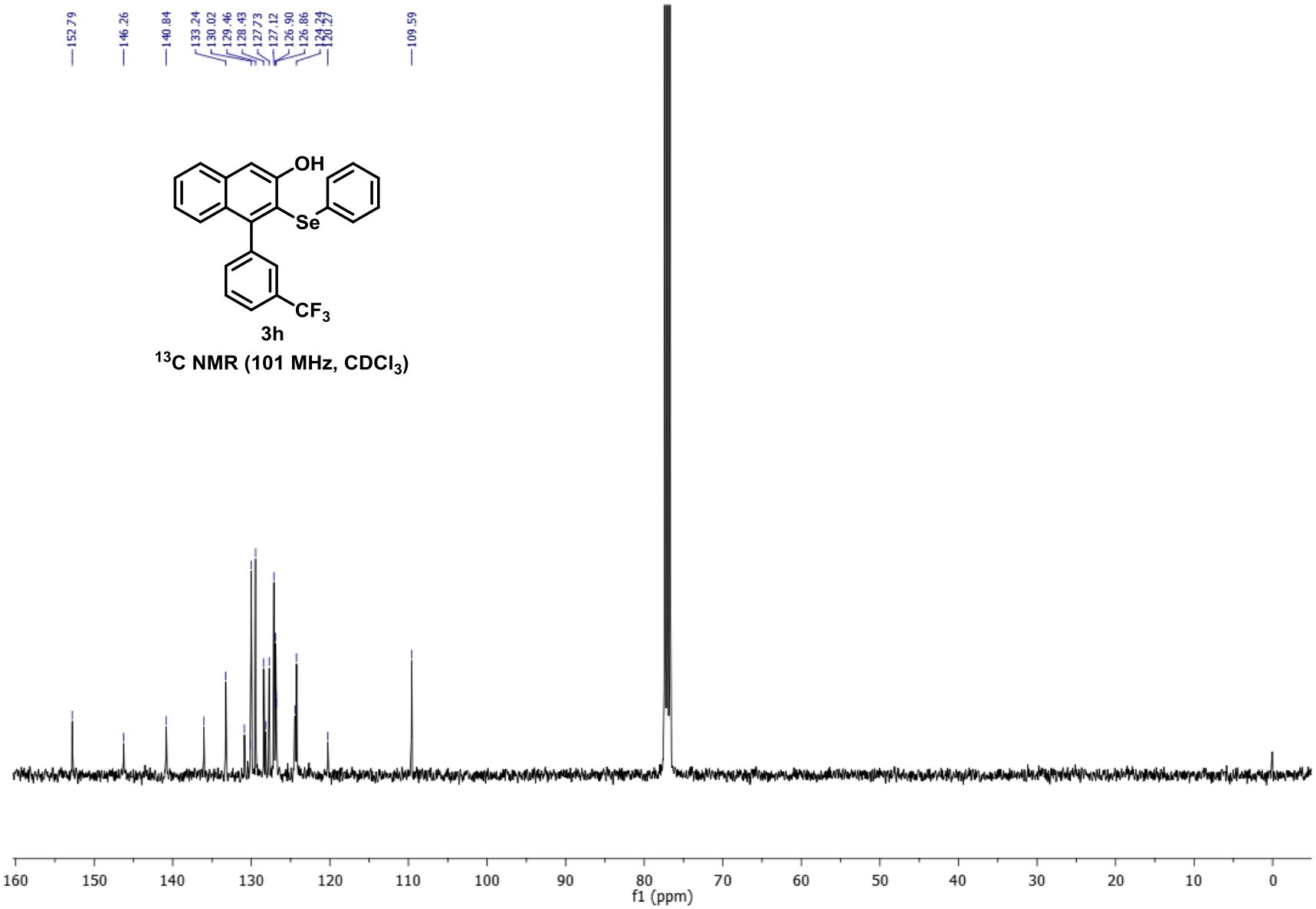
3f

^{13}C NMR (101 MHz, $CDCl_3$)


OH
Se
O
3g
^{1}H NMR (500 MHz, $CDCl_3$)
f1 (ppm)

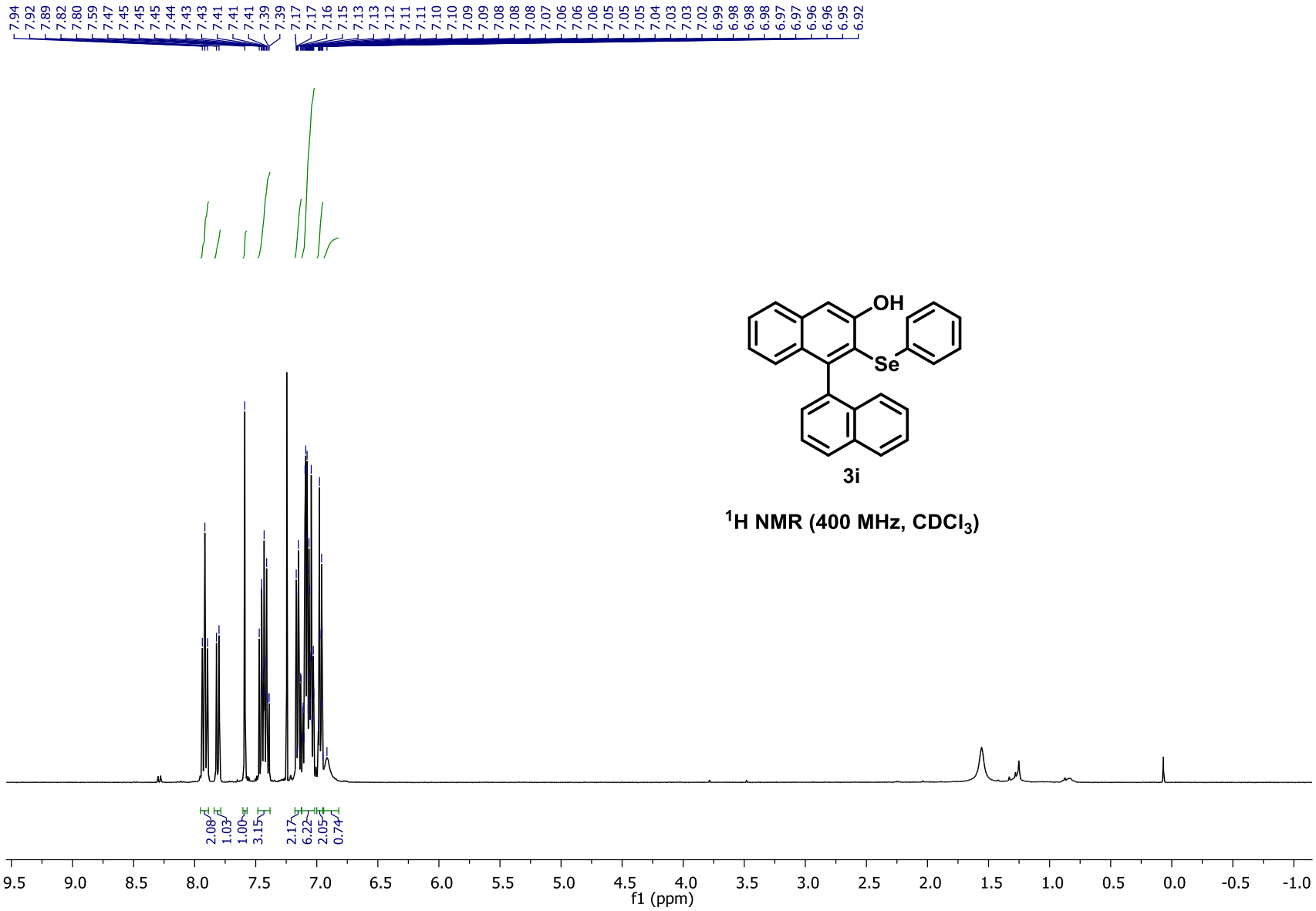

197.83
152.76
146.94
145.25
136.29
136.06
130.23
129.53
129.49
128.01
127.74
127.24
126.95
126.88
26.74
OH
Se
O
3g
^{13}C NMR (101 MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OH
Se
CF3
3h
1H NMR (500 MHz, CDCl3)
f1 (ppm)



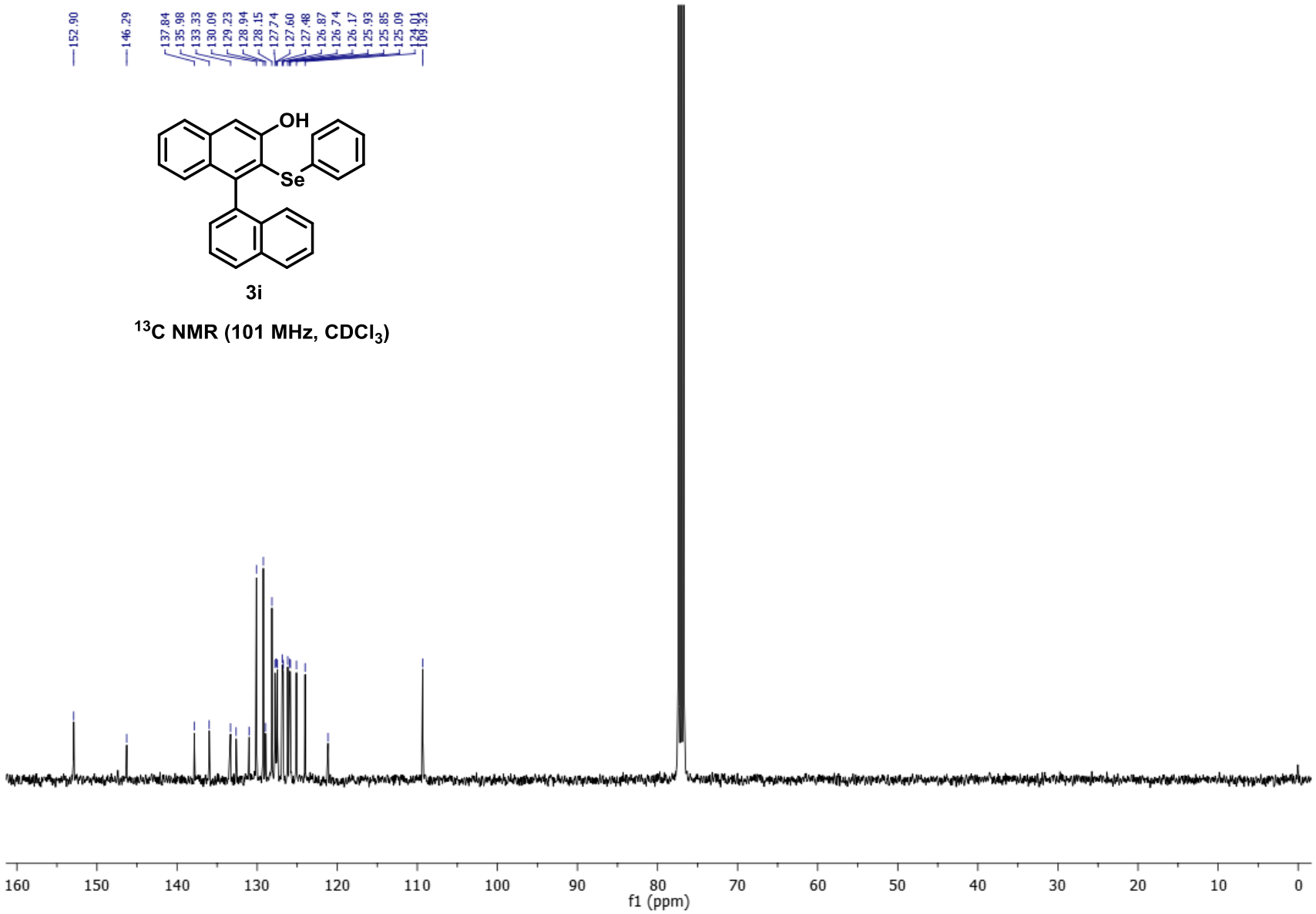
3h

^{13}C NMR (101 MHz, $CDCl_3$)



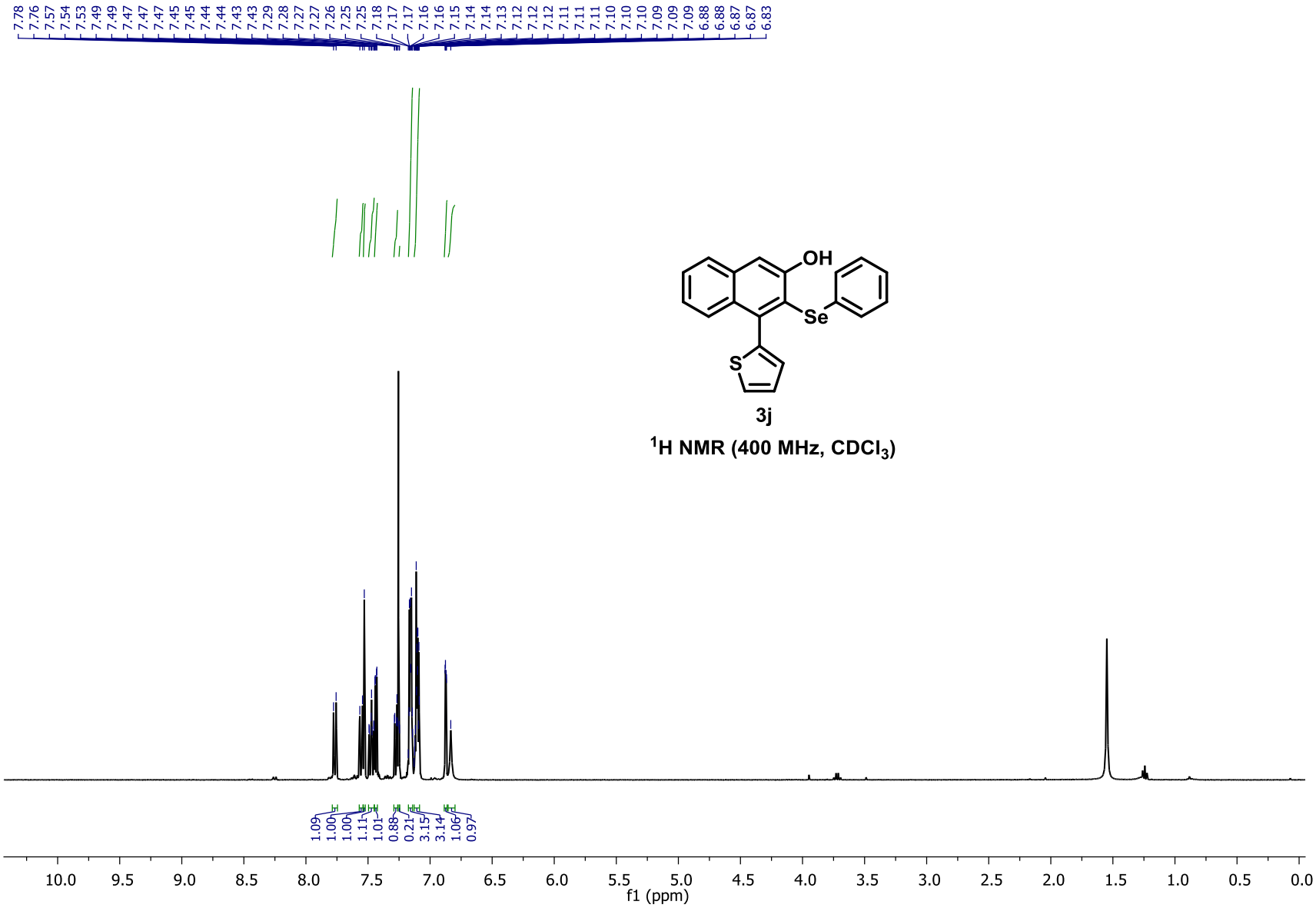
3i

^{1}H NMR (400 MHz, $CDCl_3$)



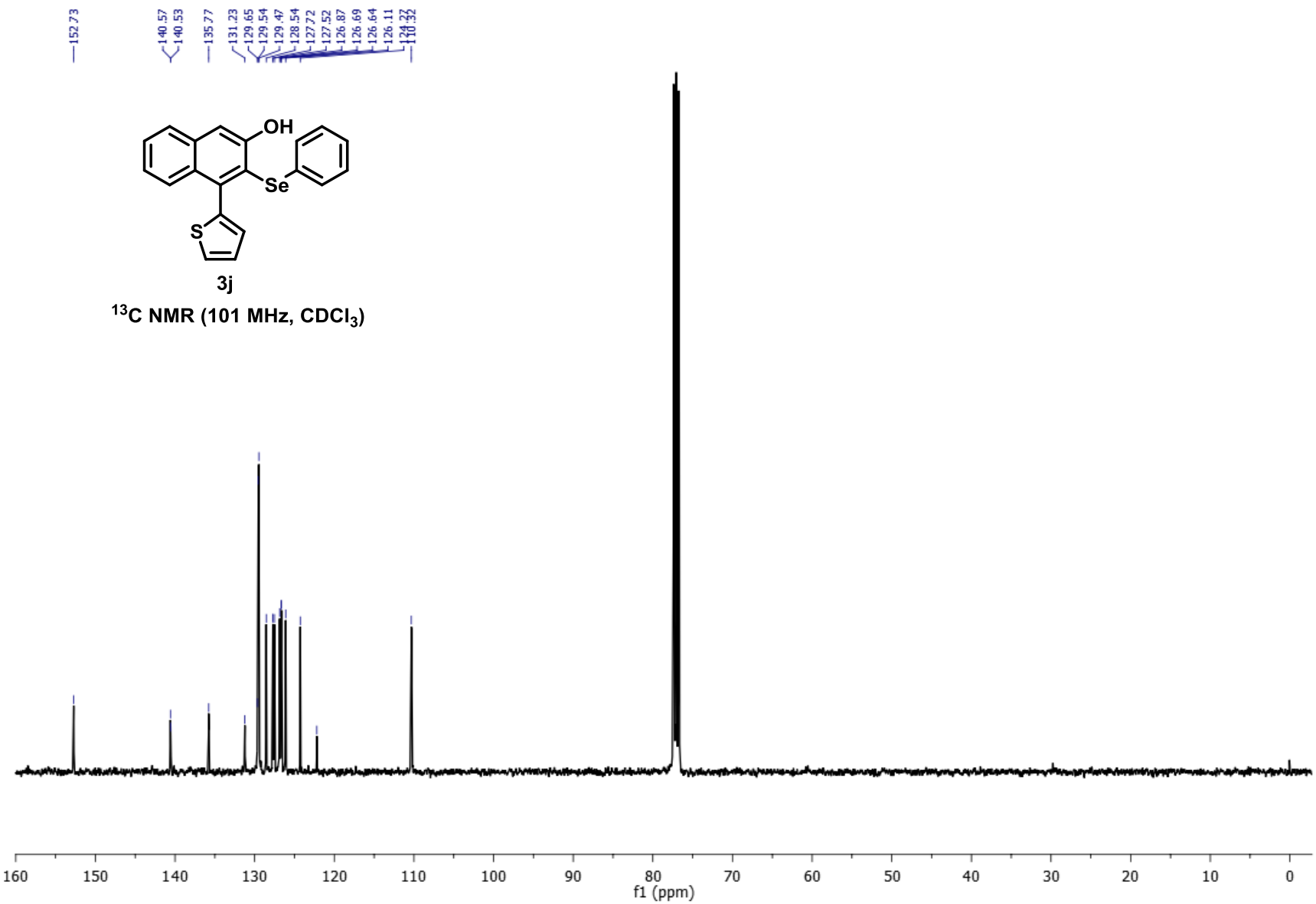
3i

^{13}C NMR (101 MHz, $CDCl_3$)



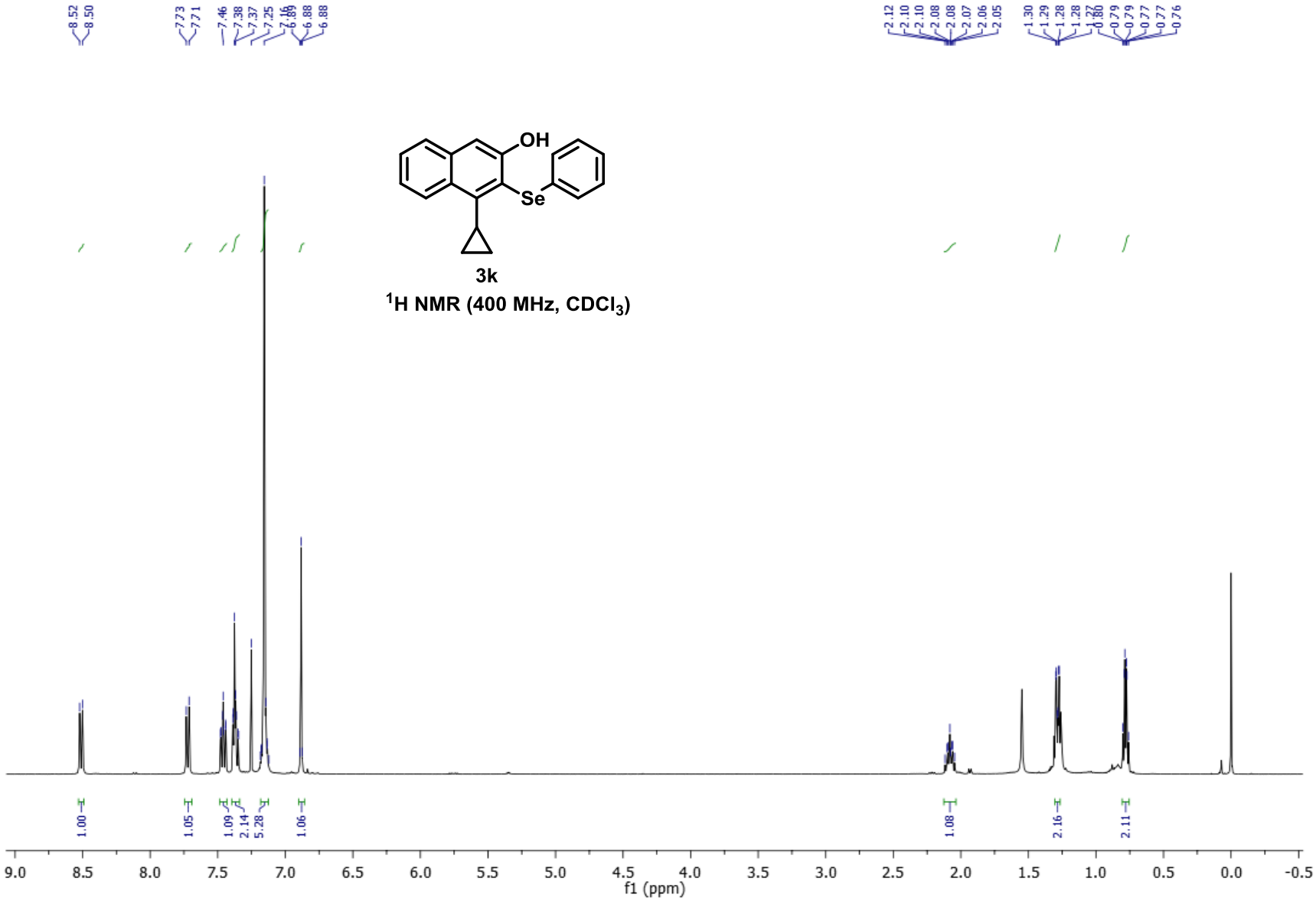
3j

^{1}H NMR (400 MHz, $CDCl_3$)



3j

^{13}C NMR (101 MHz, $CDCl_3$)

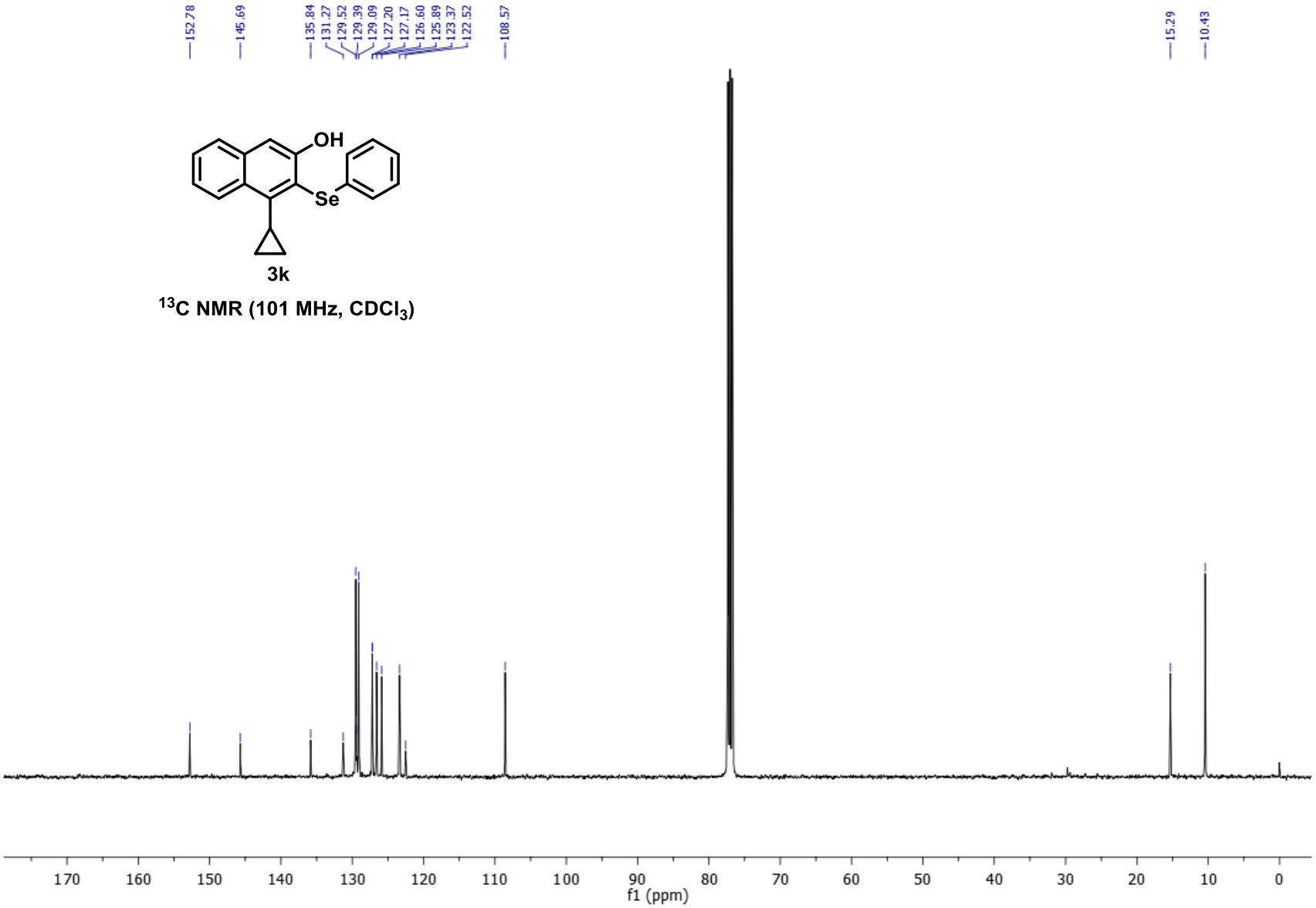


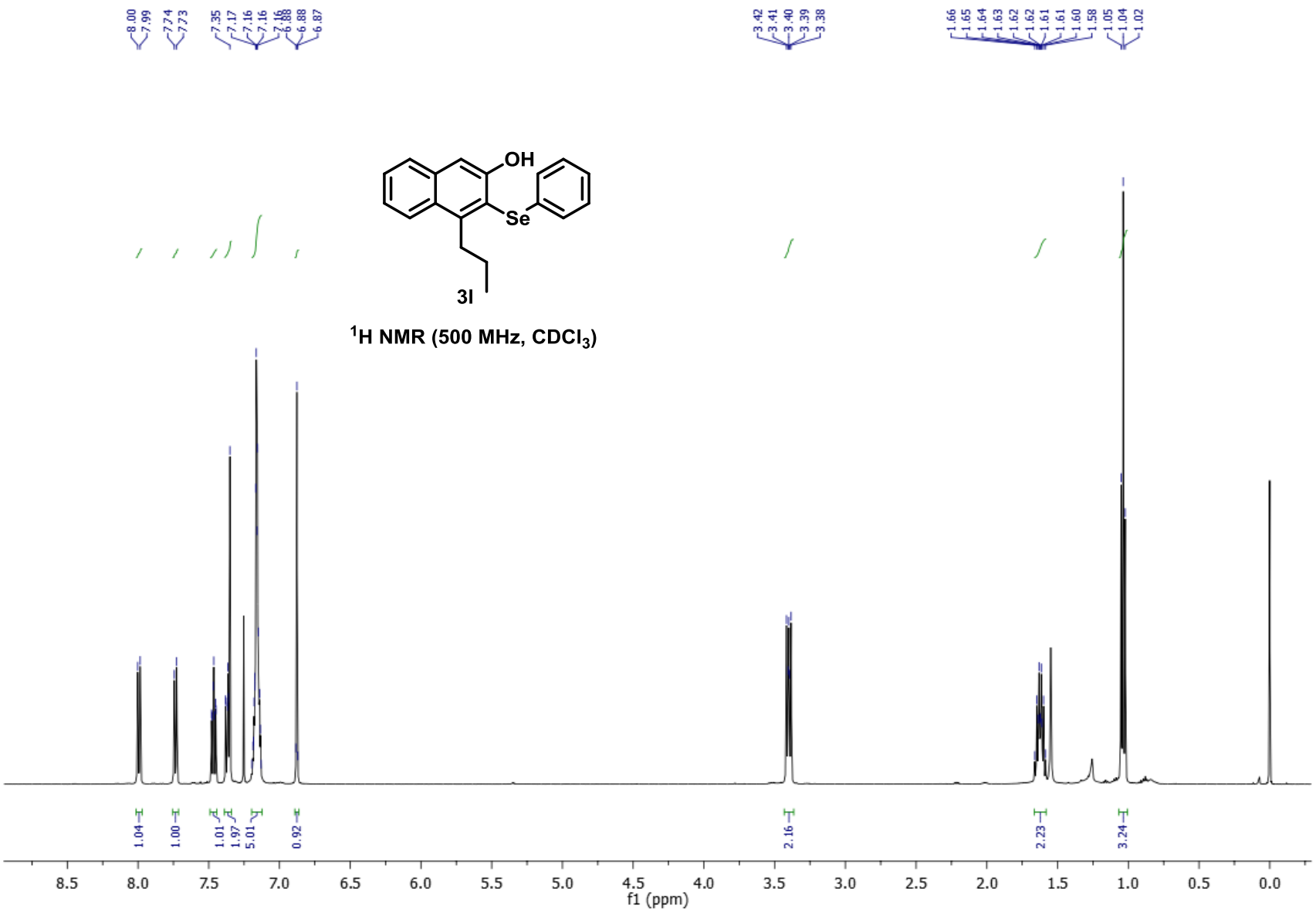
3k

^{1}H NMR (400 MHz, $CDCl_3$)

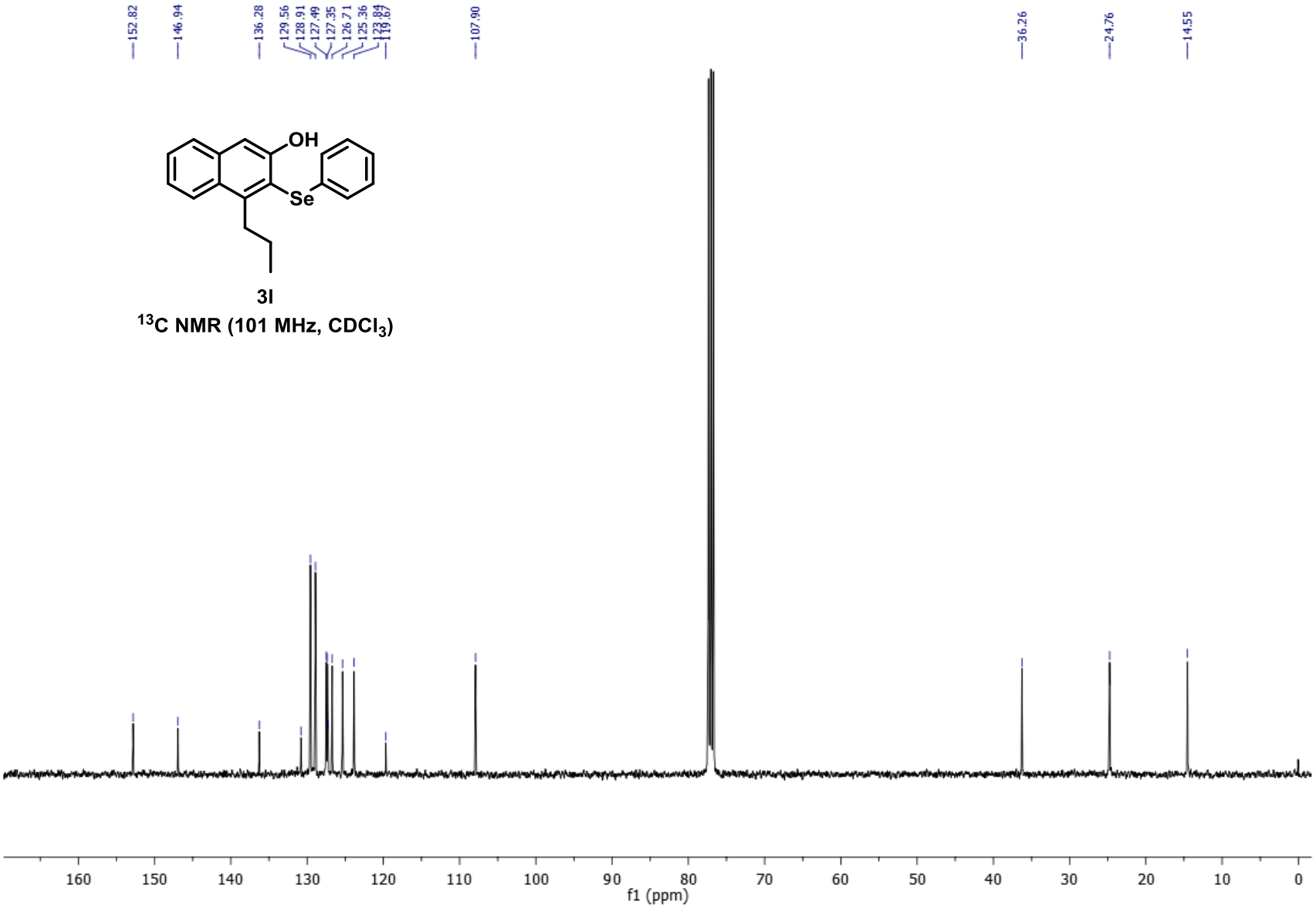
3k

^{13}C NMR (101 MHz, $CDCl_3$)



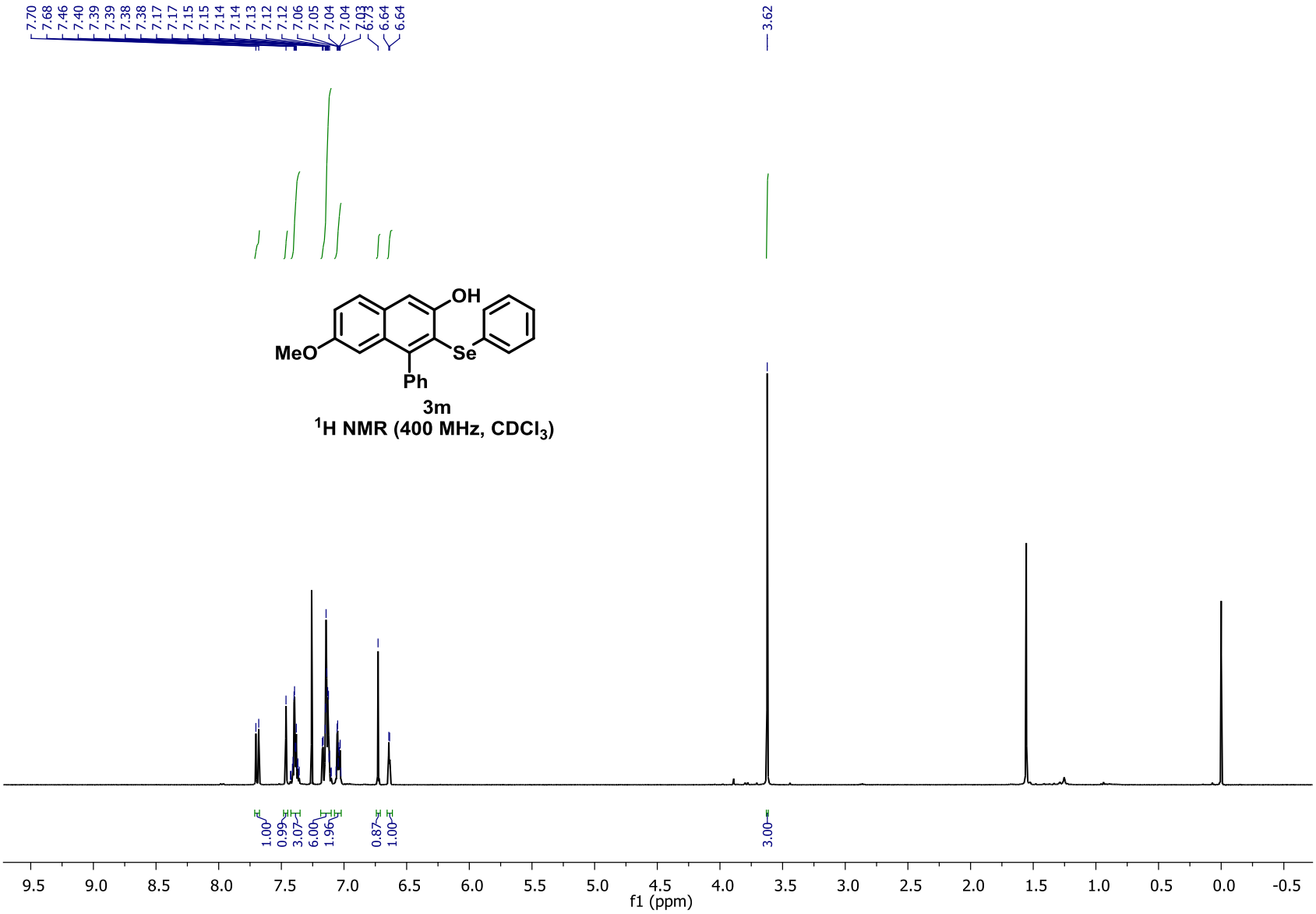


^{1}H NMR (500 MHz, $CDCl_3$)



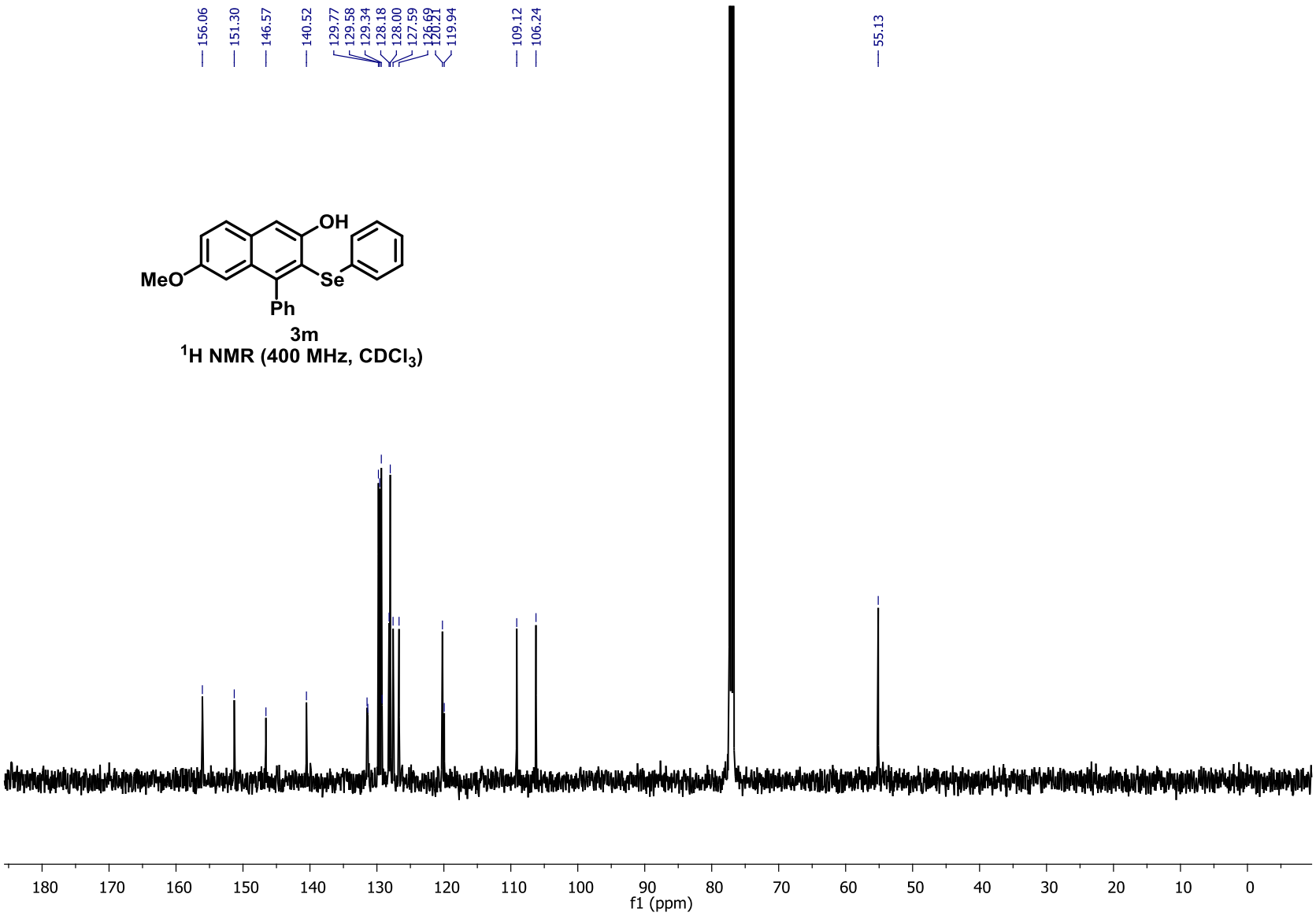
3l

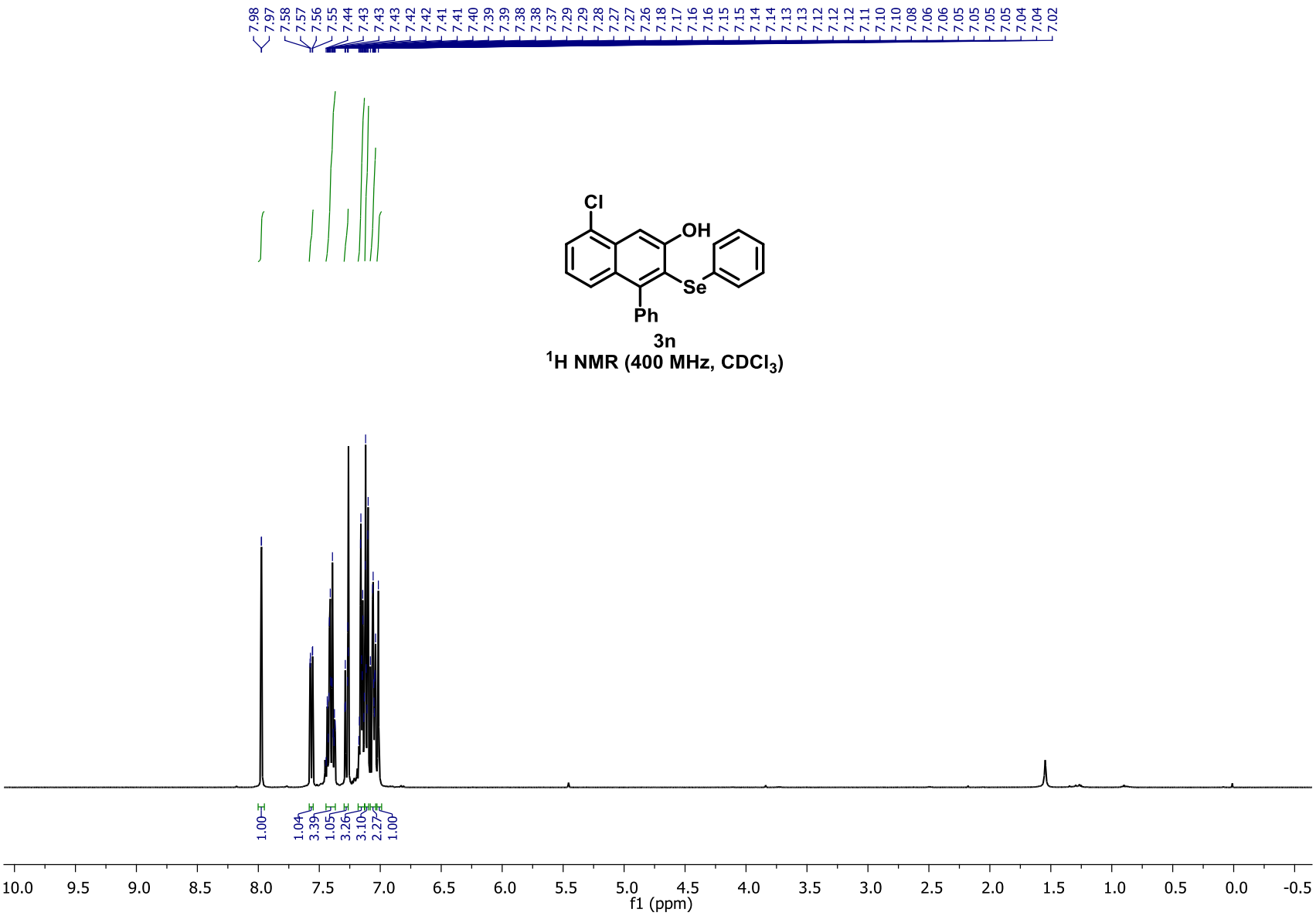
^{13}C NMR (101 MHz, $CDCl_3$)

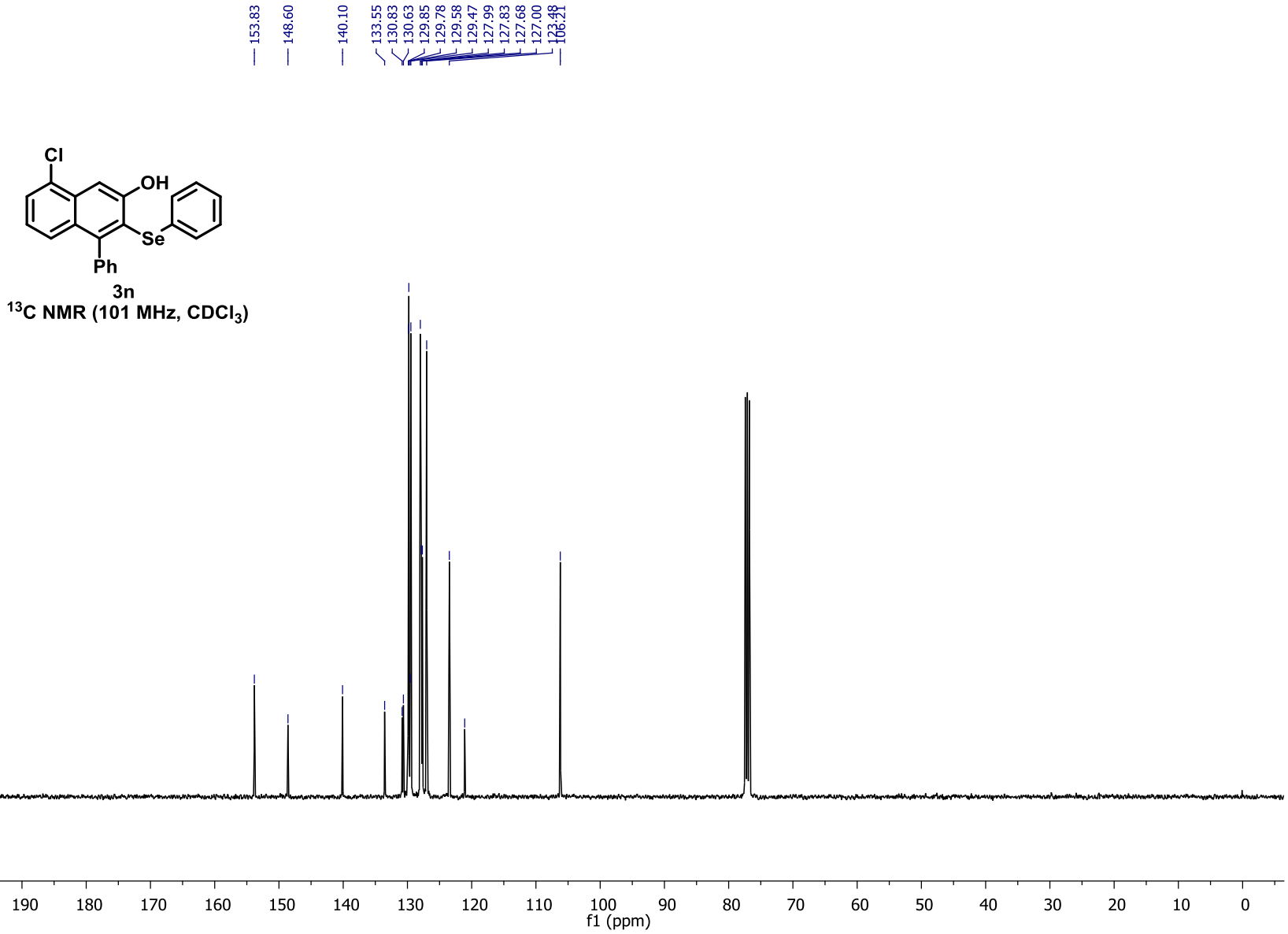


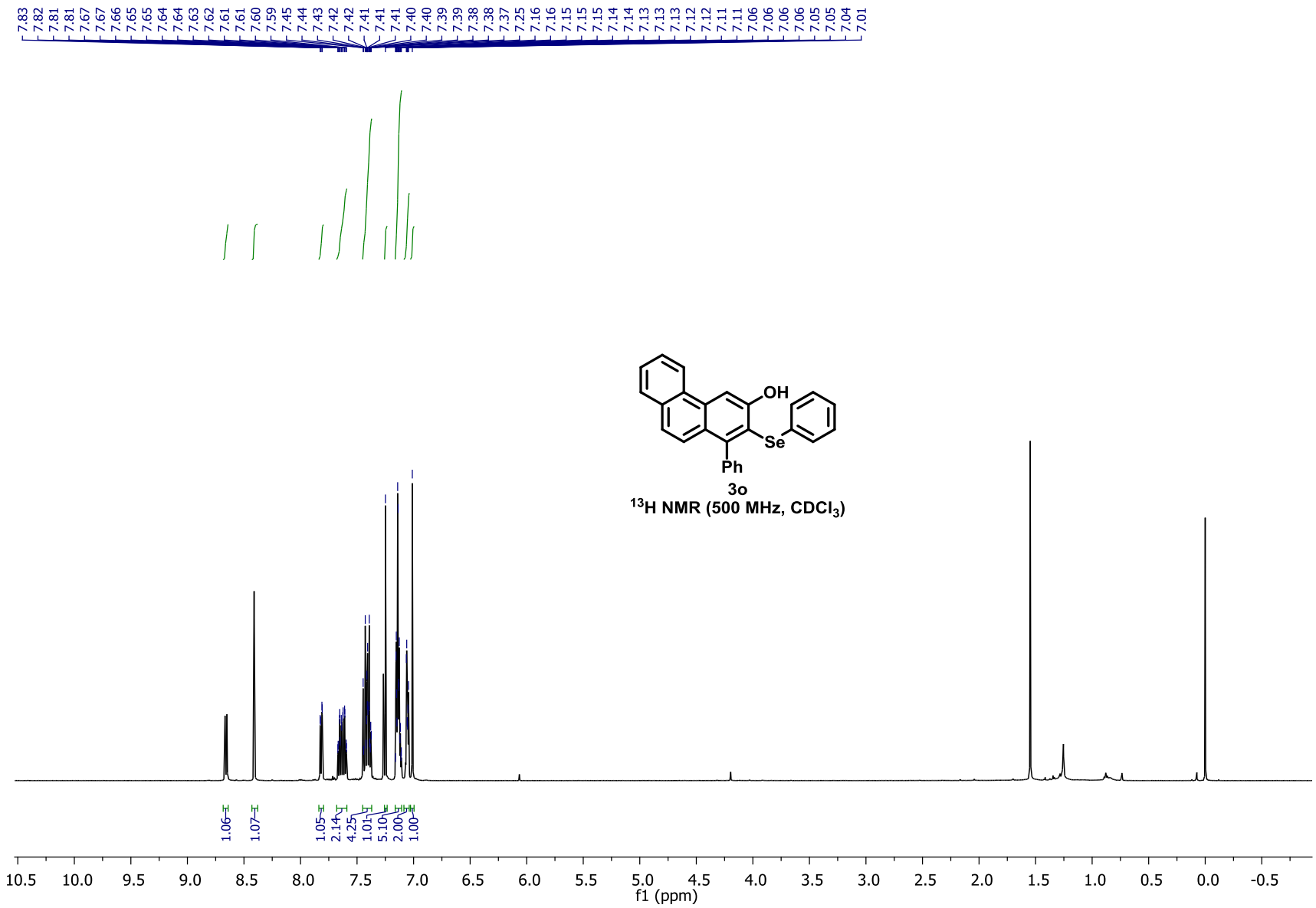
3m

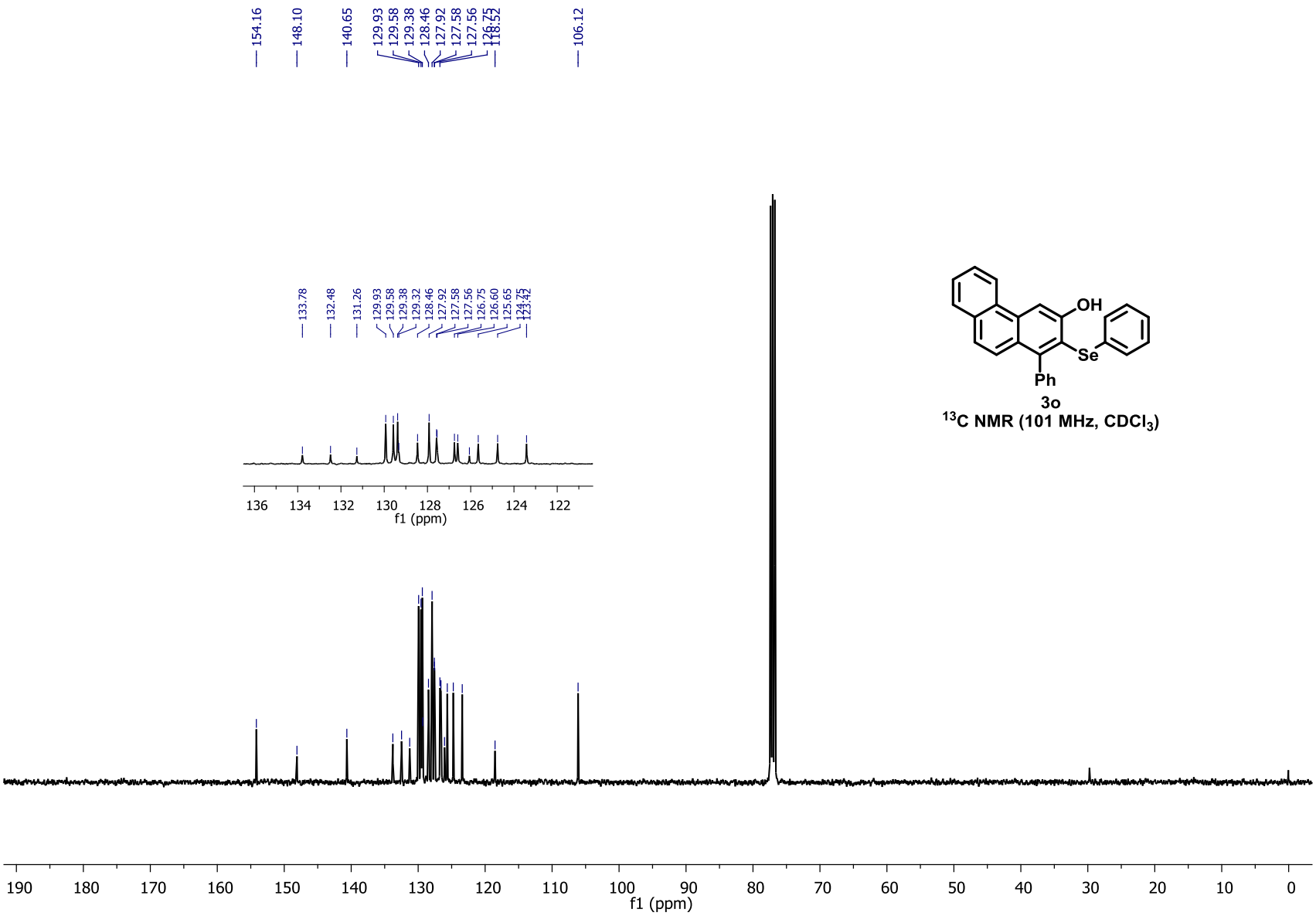
^{1}H NMR (400 MHz, $CDCl_3$)


156.06
151.30
146.57
140.52
129.77
129.58
129.34
128.18
128.00
127.59
126.69
120.21
119.94
109.12
106.24
55.13
OH
MeO
Se
Ph
3m
1H NMR (400 MHz, CDCl3)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Cl
OH
Se
Ph
3n
1H NMR (400 MHz, CDCl3)
f1 (ppm)

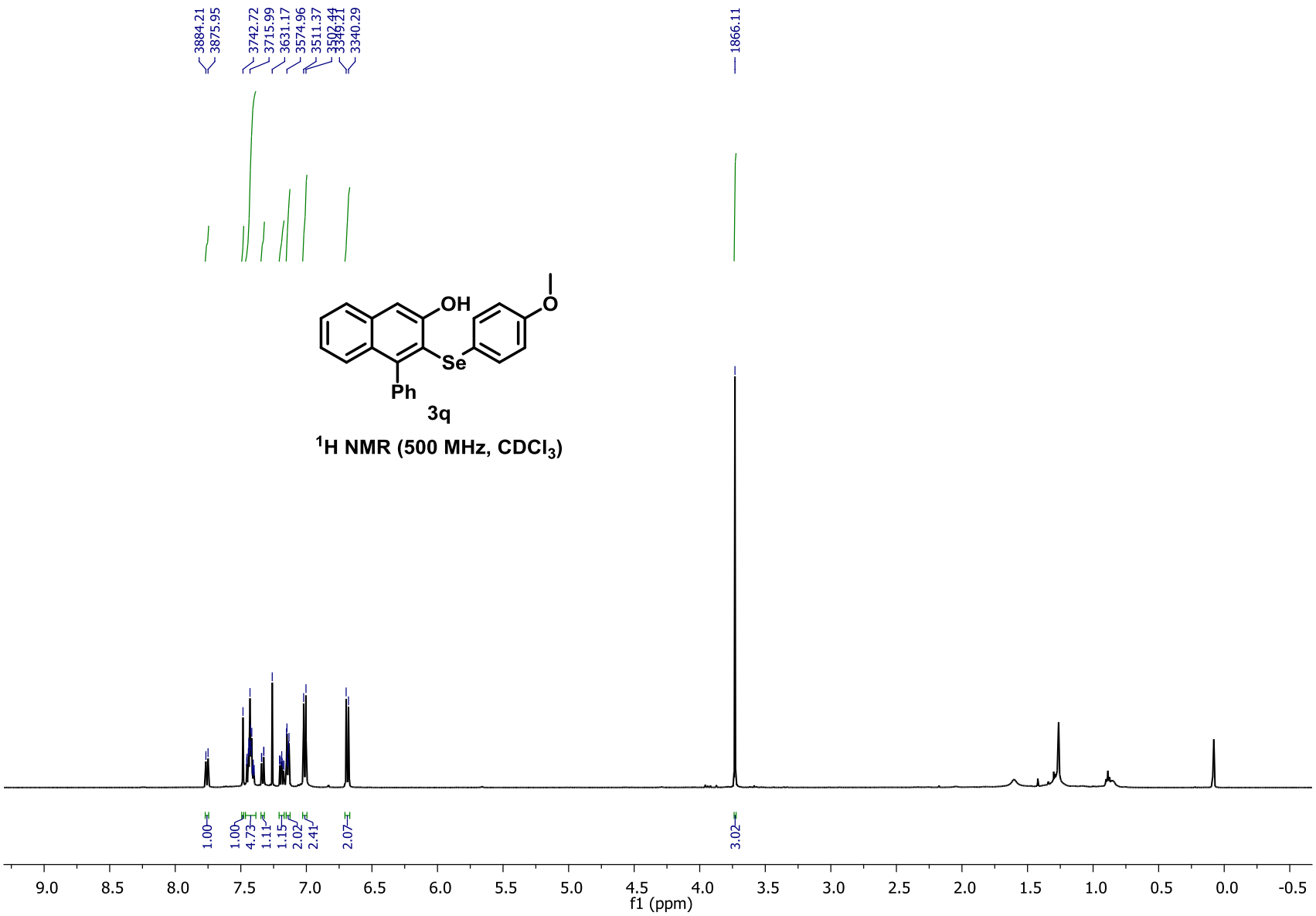

153.83
148.60
140.10
133.55
130.83
130.63
129.85
129.78
129.58
129.47
127.99
127.83
127.68
127.00
123.48
106.21
Cl
OH
Se
Ph
3n
^{13}C NMR (101 MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OH
Se
Ph
3o
13H NMR (500 MHz, CDCl3)
f1 (ppm)

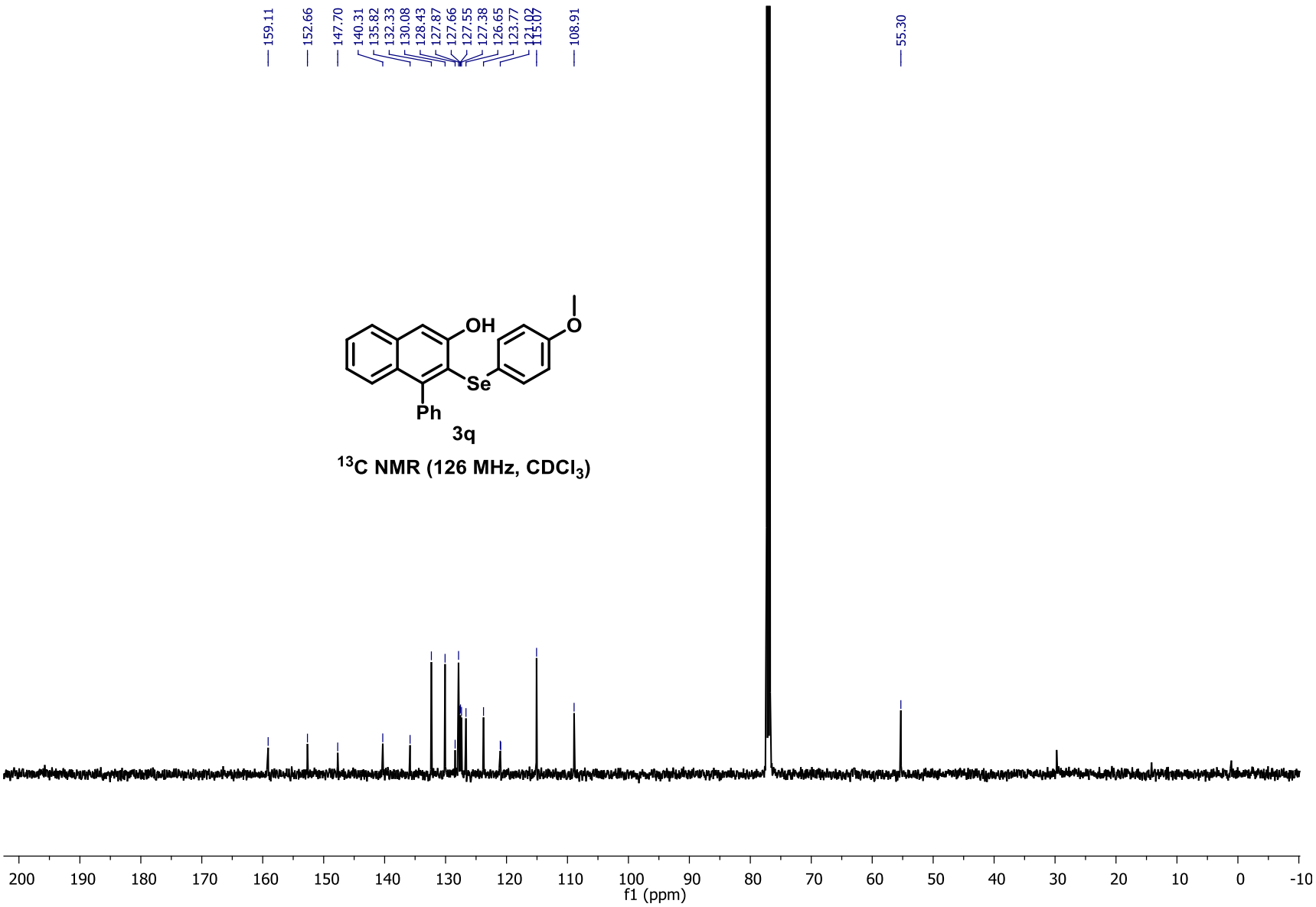


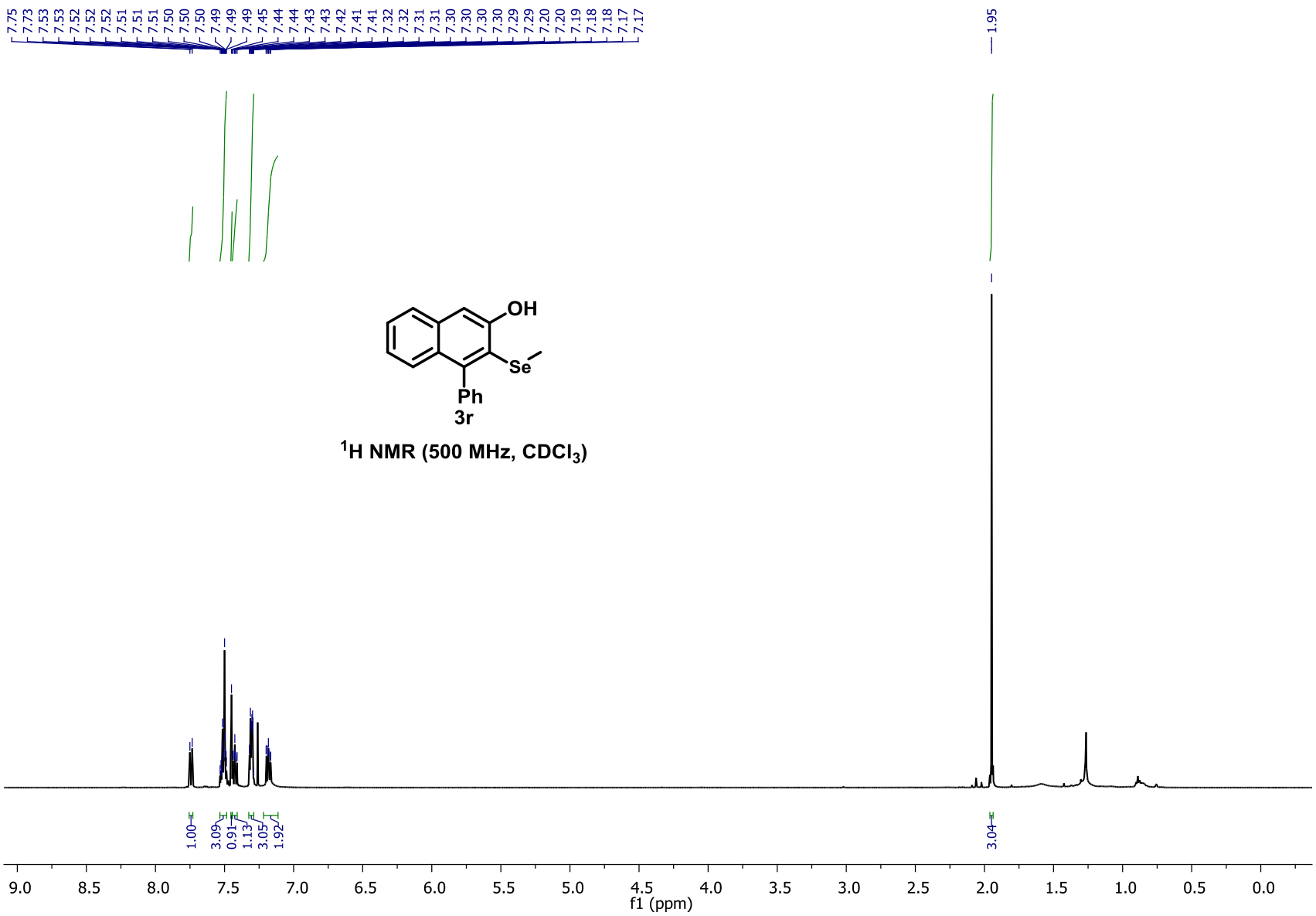
3o

^{13}C NMR (101 MHz, $CDCl_3$)

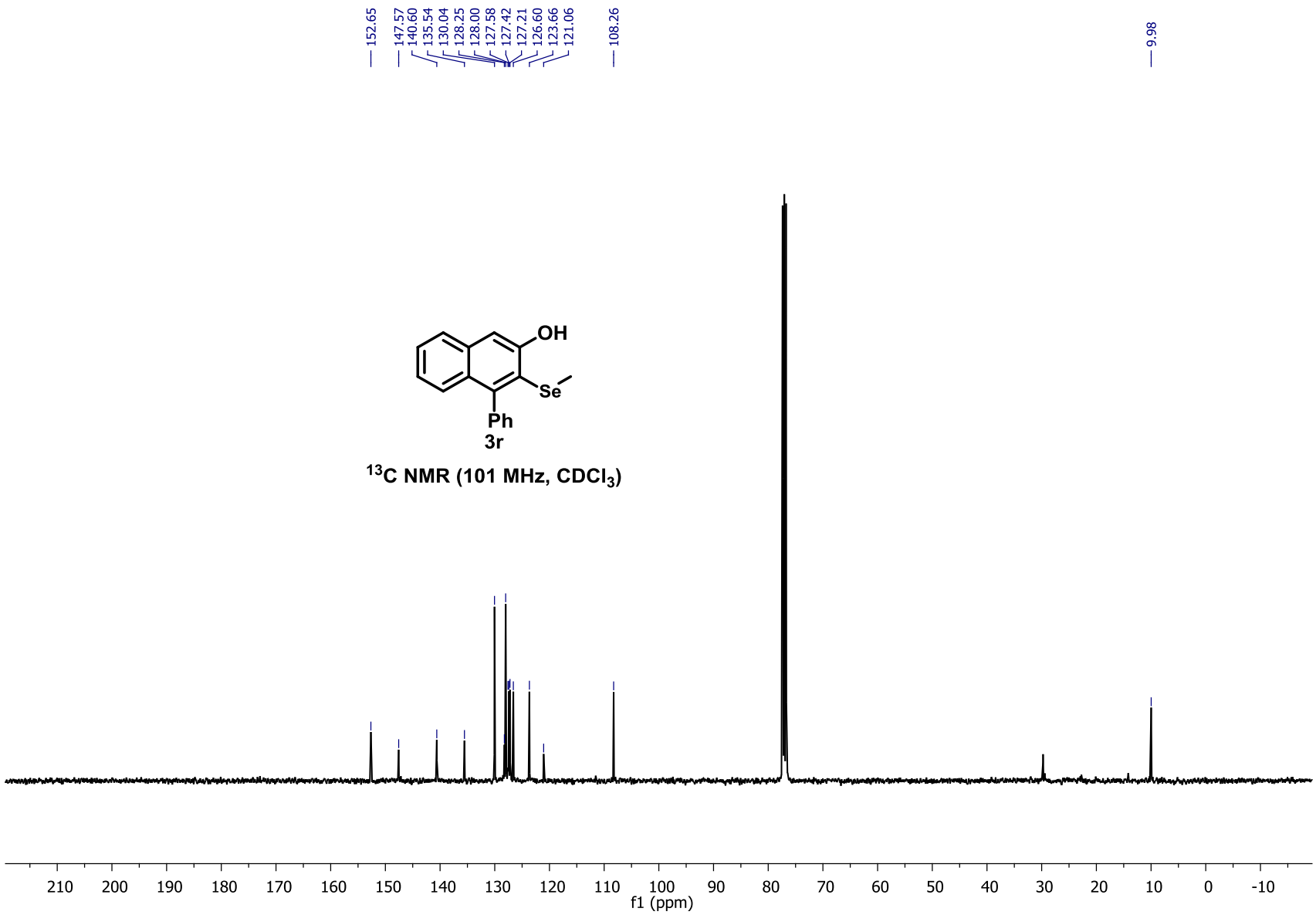


^{1}H NMR (500 MHz, $CDCl_3$)

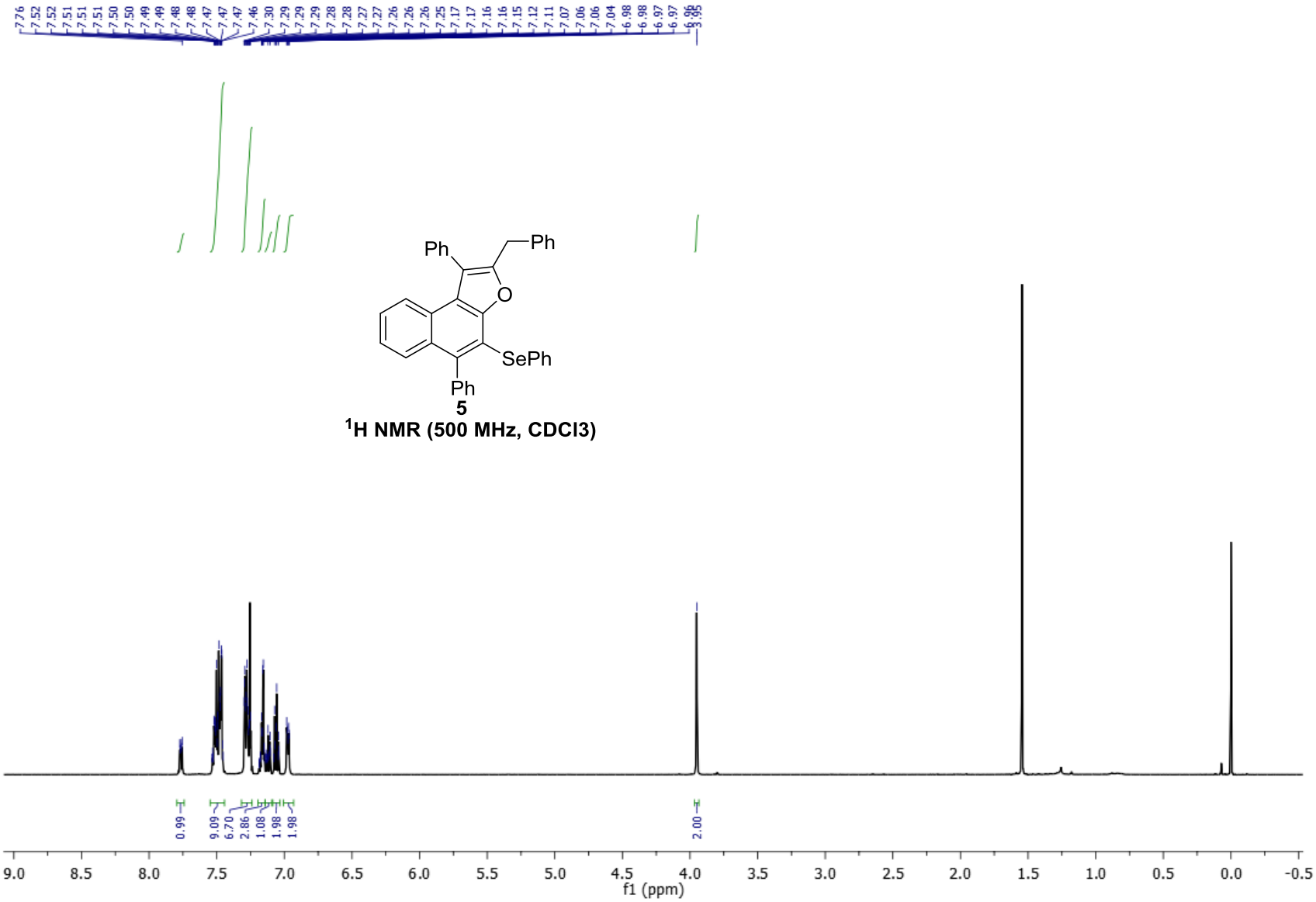

159.11
152.66
147.70
140.31
135.82
132.33
130.08
128.43
127.87
127.66
127.55
127.38
126.65
123.77
121.02
115.07
108.91
55.30
OH
O
Se
Ph
3q
^{13}C NMR (126 MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



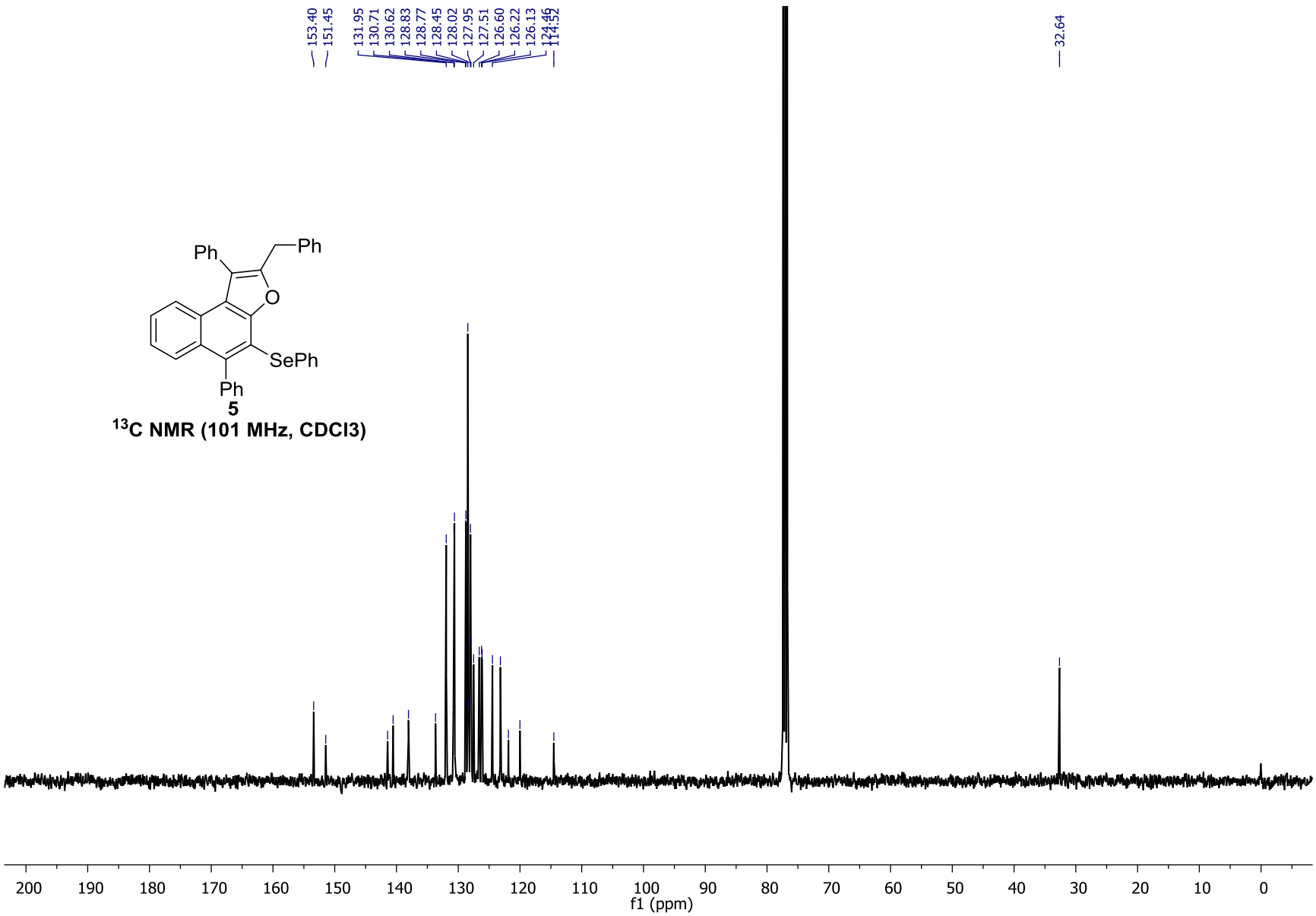
^{1}H NMR (500 MHz, $CDCl_3$)

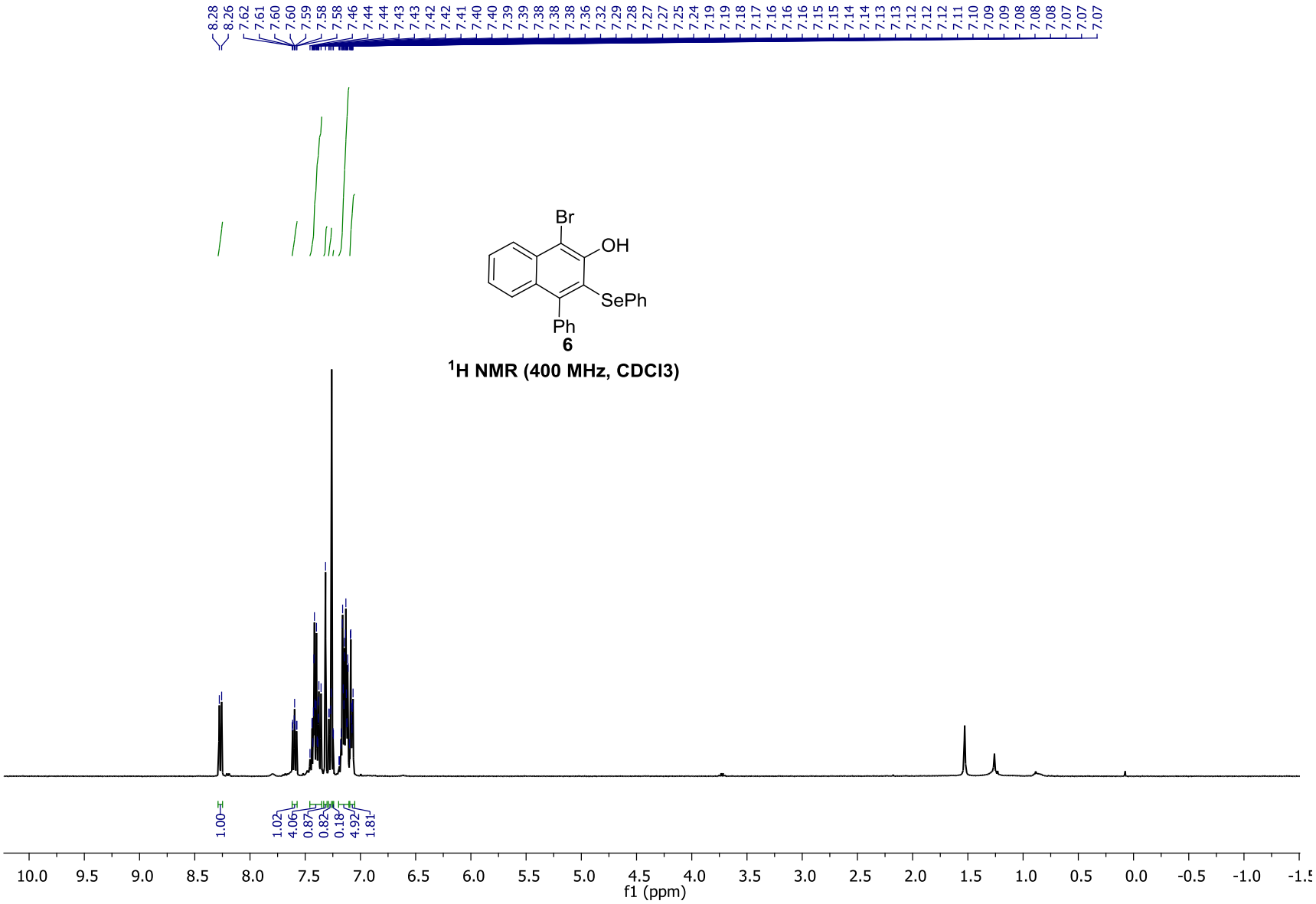


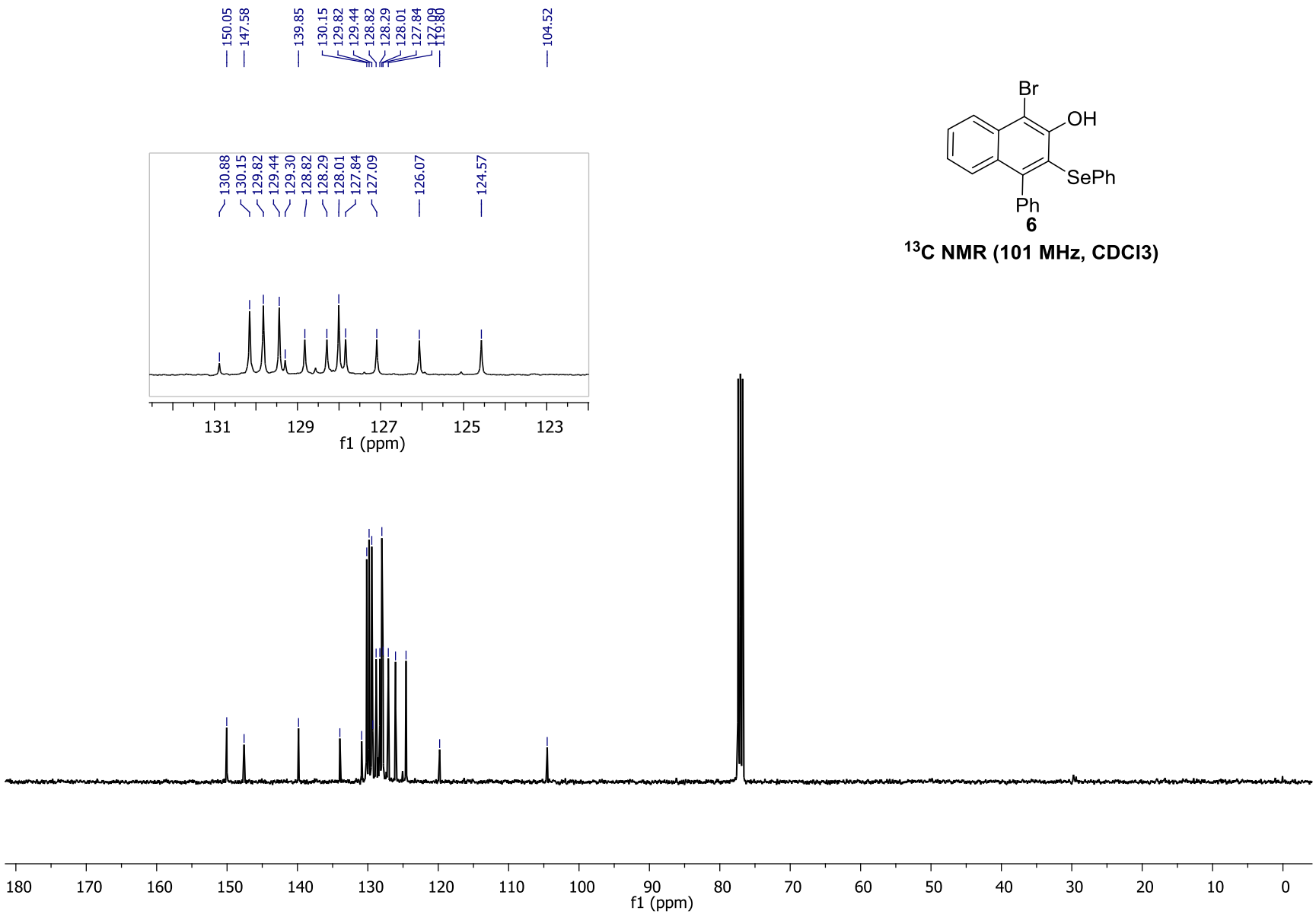
^{13}C NMR (101 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, CDCl3)

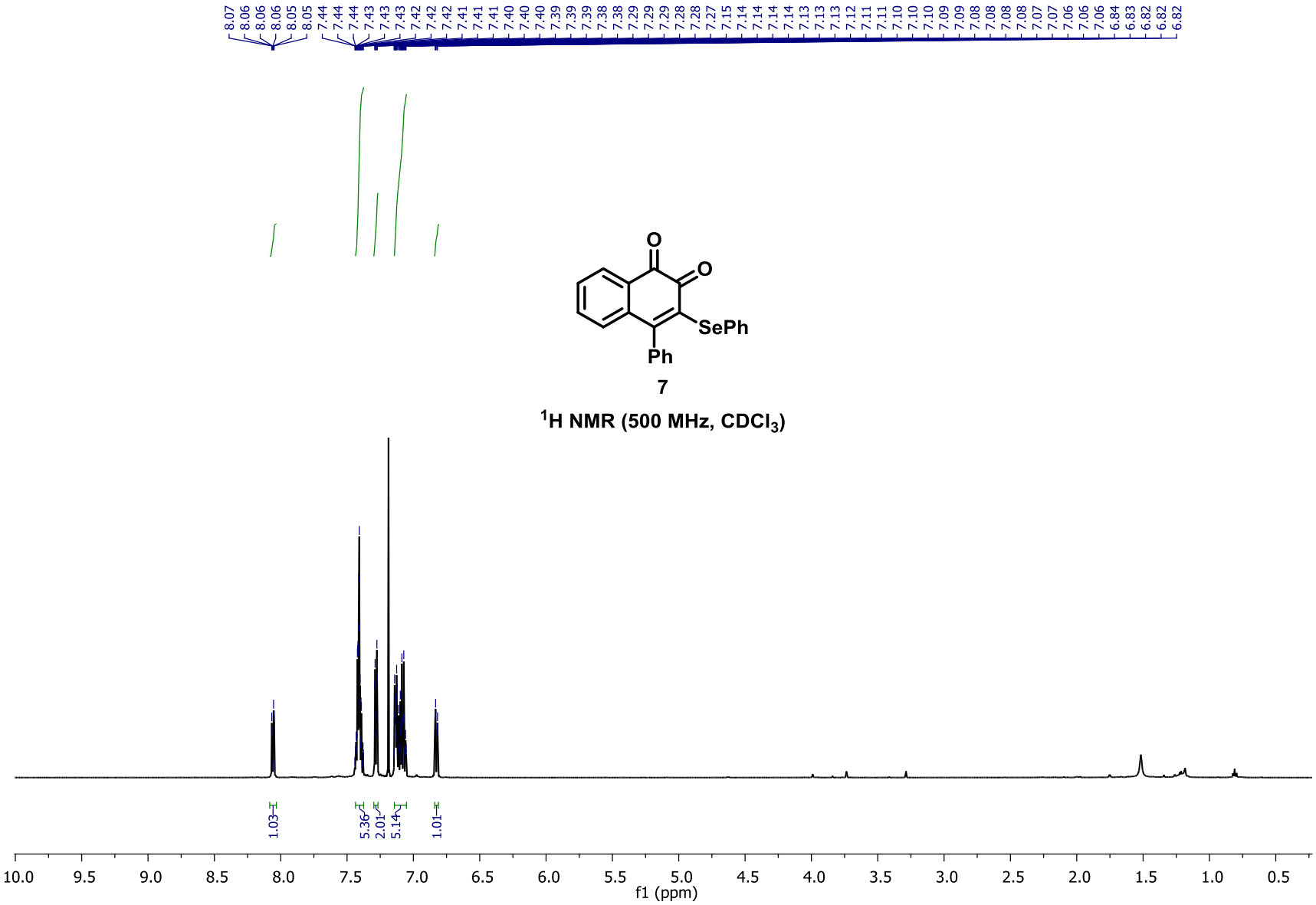

153.40
151.45
131.95
130.71
130.62
128.83
128.77
128.45
128.02
127.95
127.51
126.60
126.22
126.13
124.46
114.52
32.64
Ph
Ph
O
SePh
Ph
5
^{13}C NMR (101 MHz, CDCl3)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

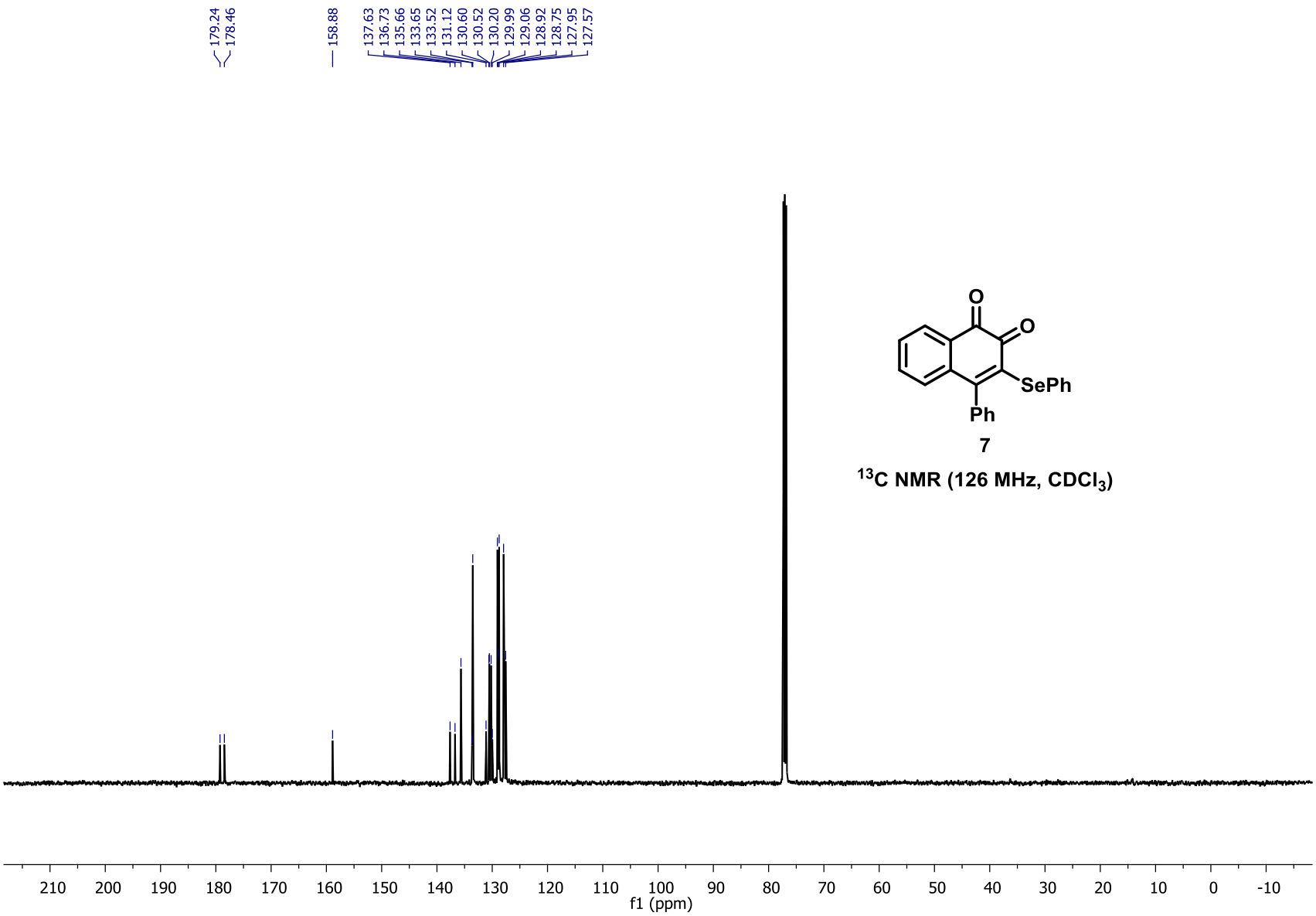

Br
OH
SePh
Ph
6
1H NMR (400 MHz, CDCl3)
f1 (ppm)



6

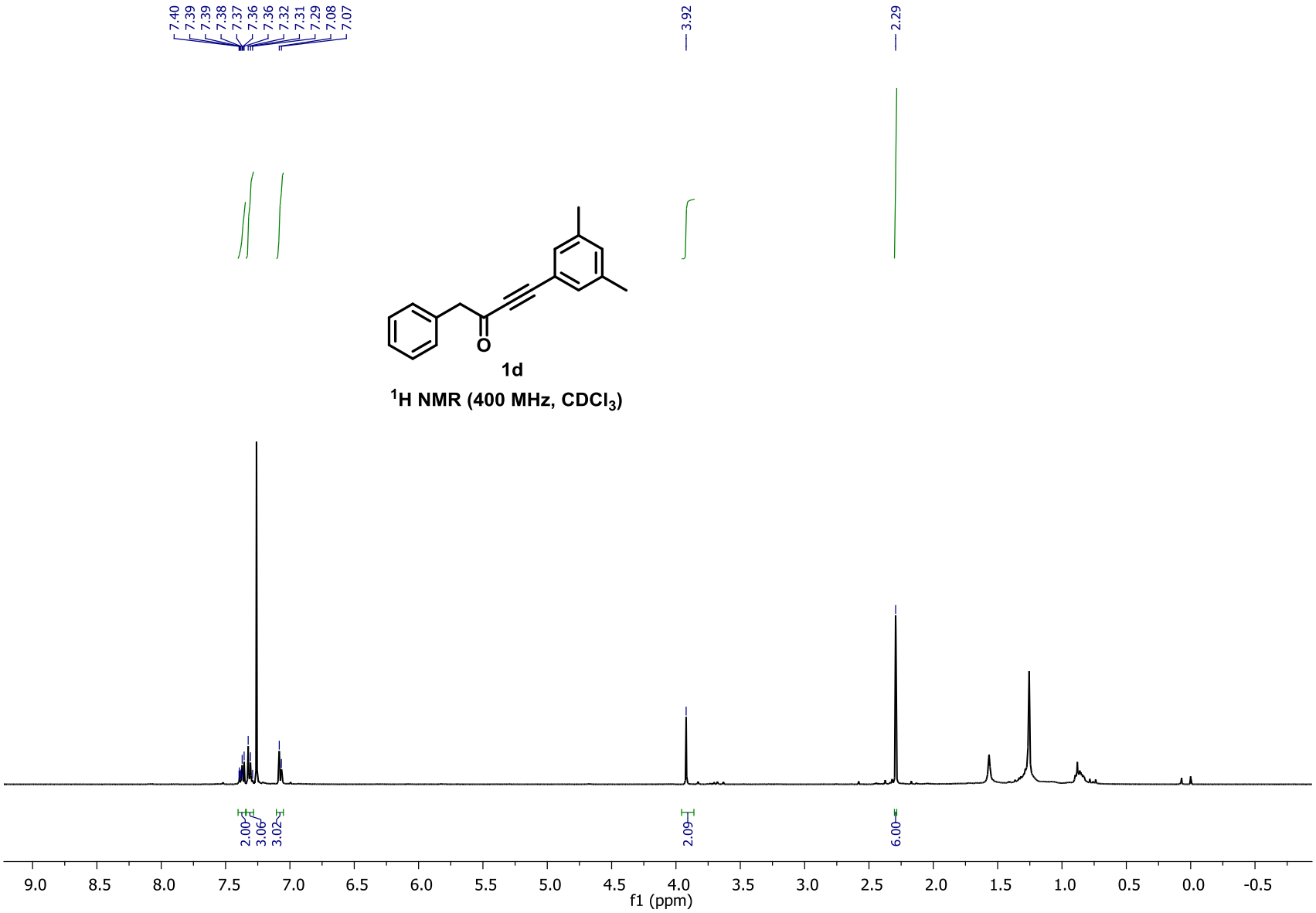
^{13}C NMR (101 MHz, CDCl3)


8.07 8.06 8.06 8.06 8.05 8.05 7.44 7.44 7.44 7.43 7.43 7.43 7.42 7.42 7.42 7.41 7.41 7.41 7.40 7.40 7.40 7.39 7.39 7.39 7.38 7.38 7.29 7.29 7.29 7.28 7.28 7.27 7.15 7.14 7.14 7.14 7.14 7.13 7.13 7.13 7.12 7.11 7.11 7.10 7.10 7.10 7.09 7.09 7.08 7.08 7.08 7.08 7.07 7.07 7.06 7.06 7.06 6.84 6.83 6.82 6.82 6.82
O
O
SePh
Ph
7
1H NMR (500 MHz, CDCl3)
1.03
5.36
2.01
5.14
1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)



7

^{13}C NMR (126 MHz, $CDCl_3$)

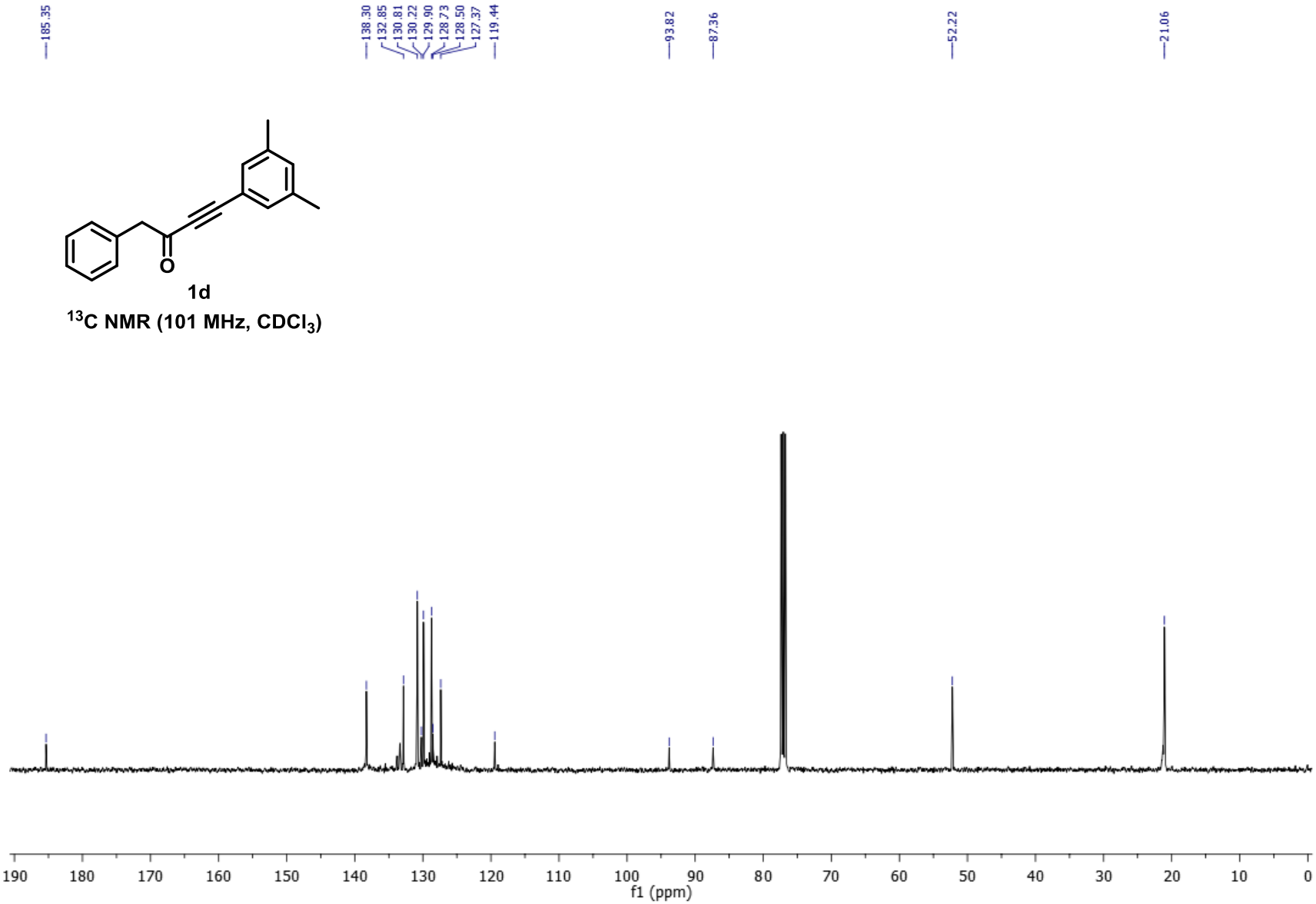


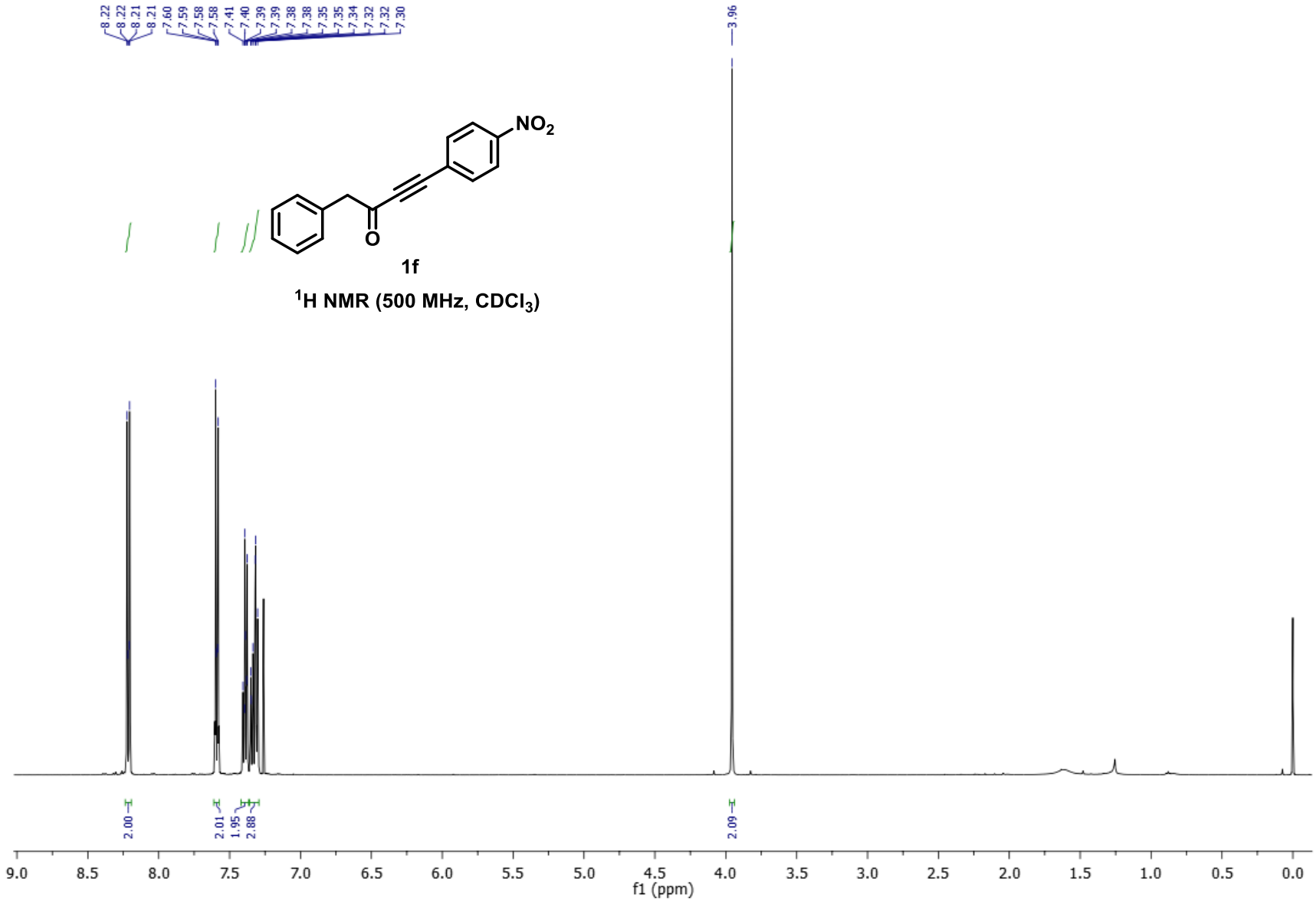
1d

^{1}H NMR (400 MHz, $CDCl_3$)

1d

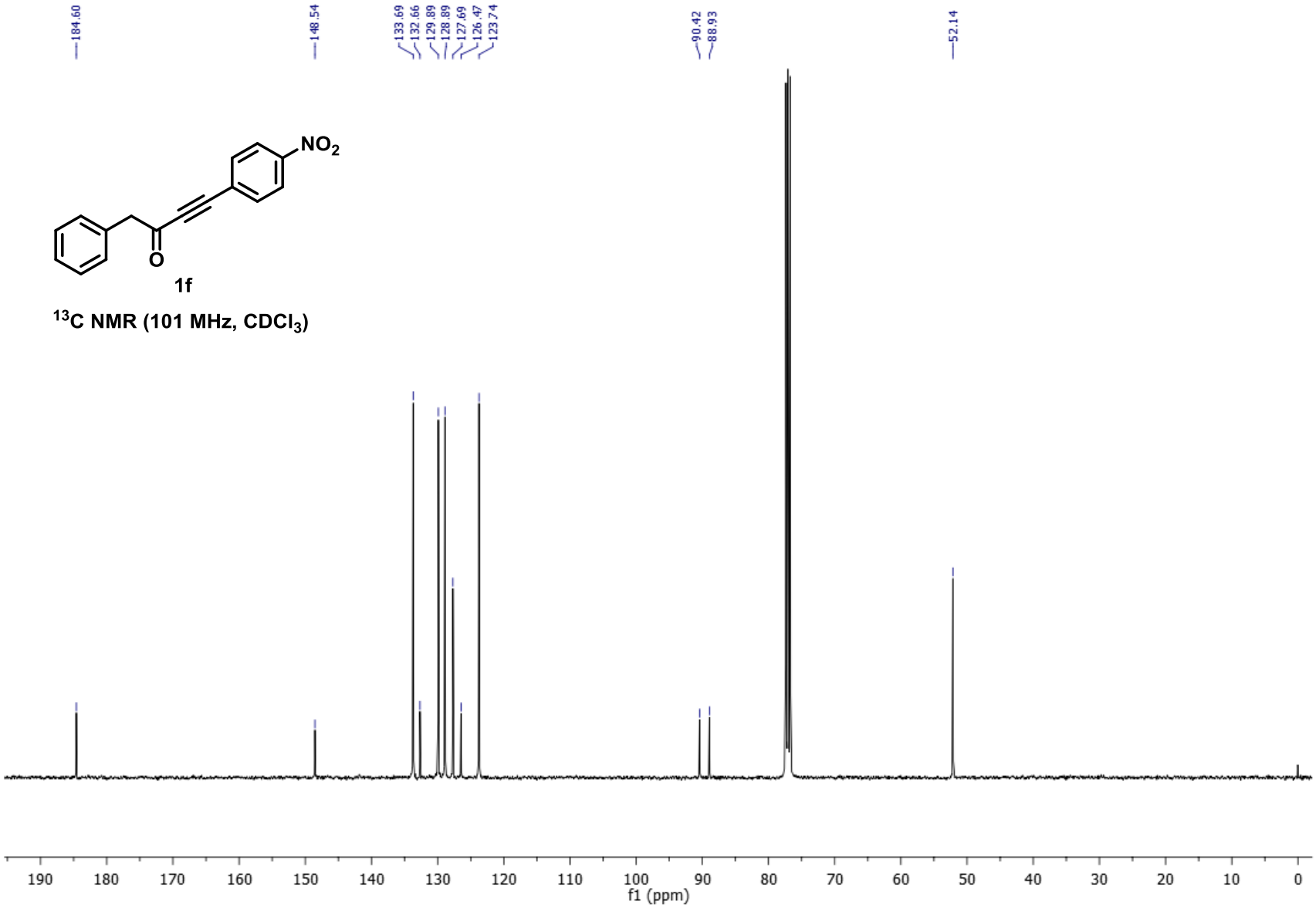
^{13}C NMR (101 MHz, $CDCl_3$)

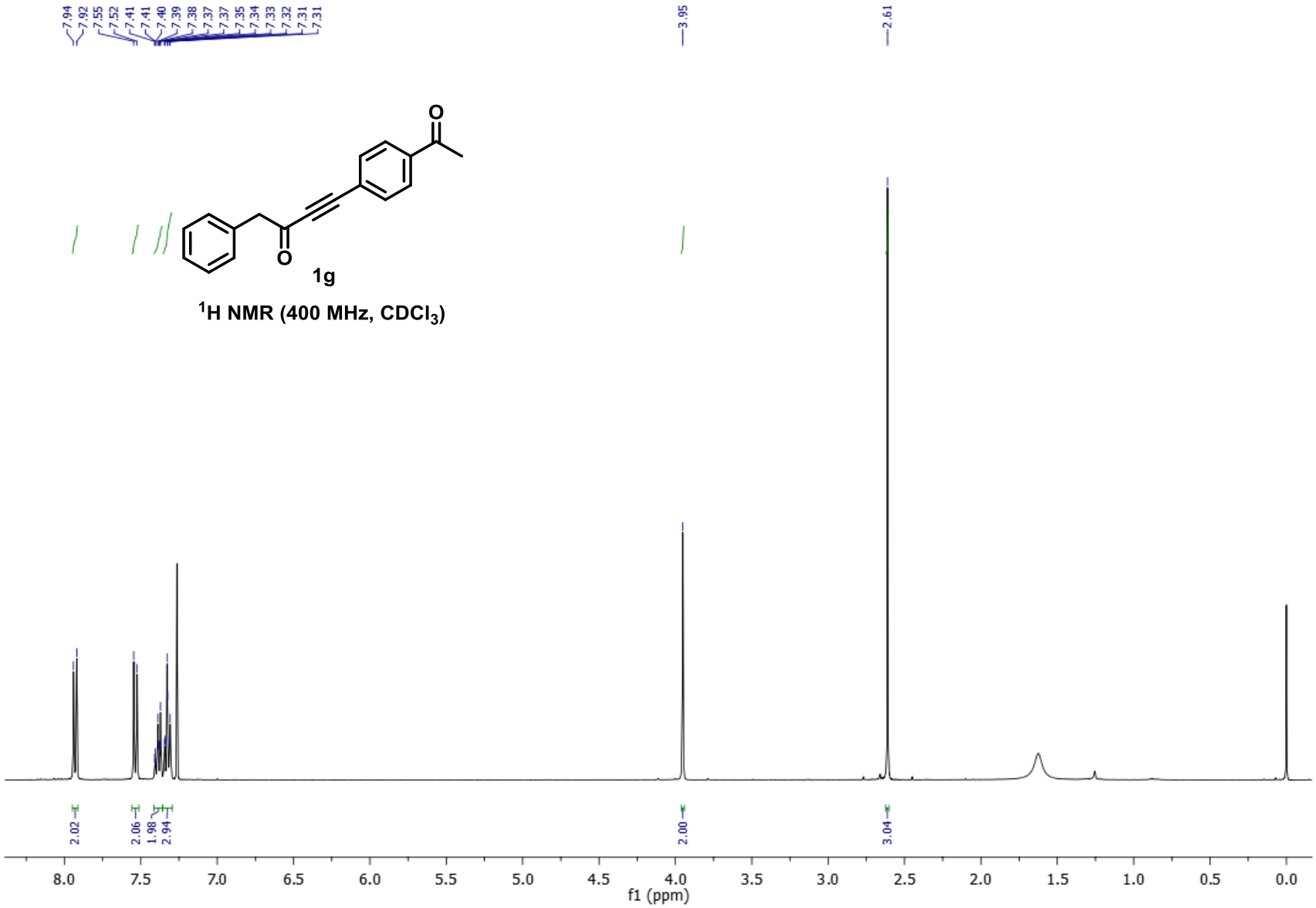




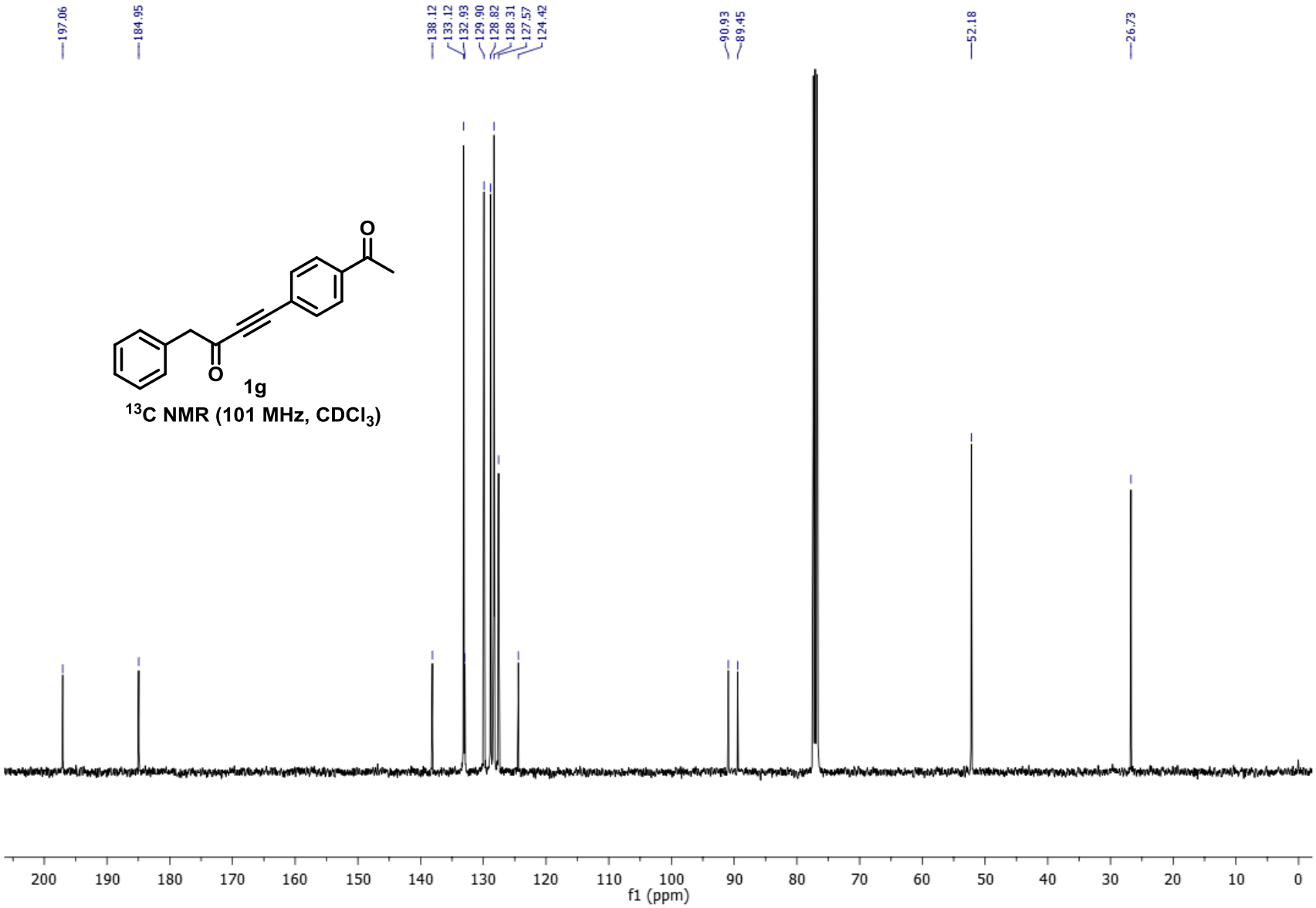
1f

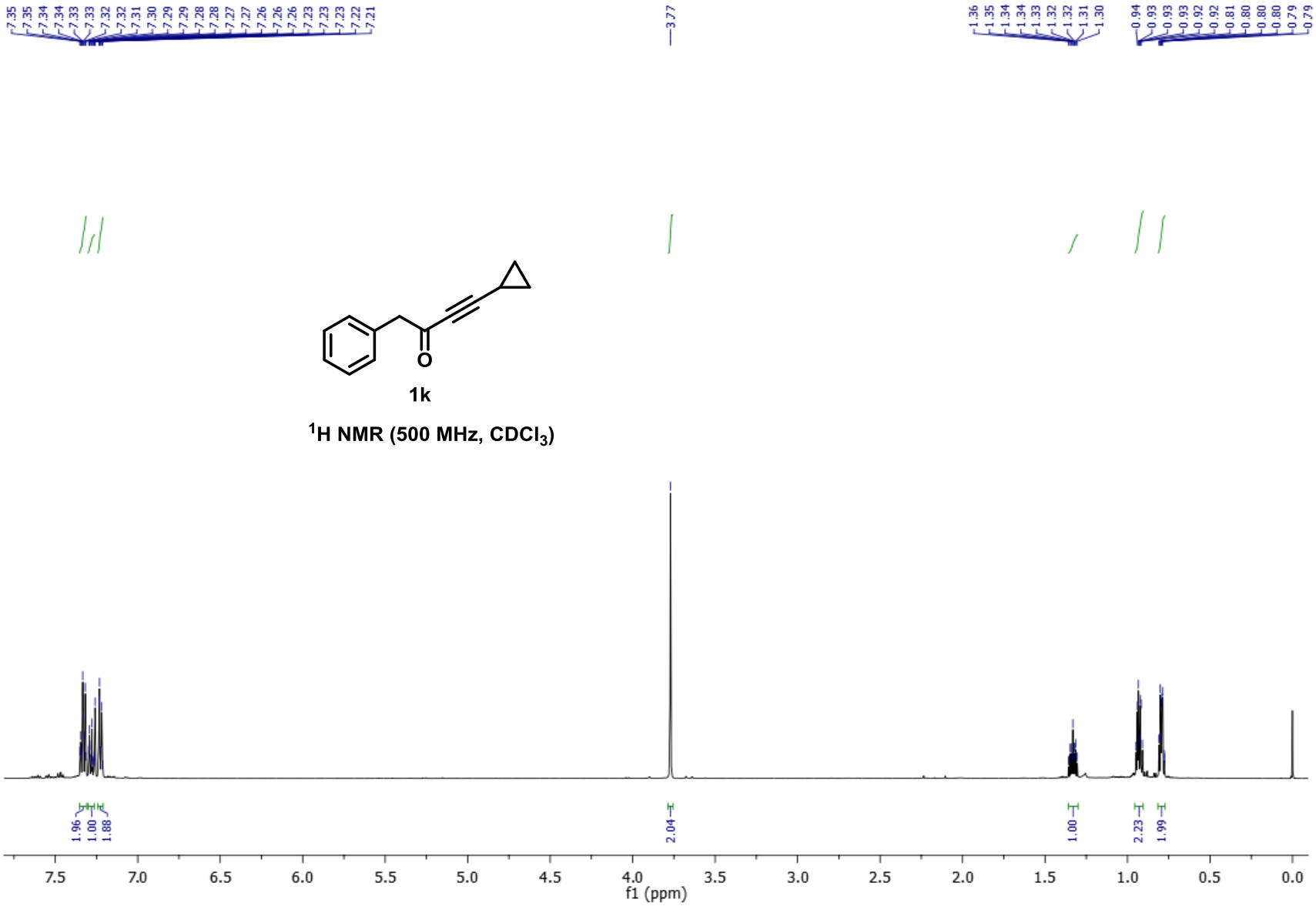
^{1}H NMR (500 MHz, $CDCl_3$)


184.60
148.54
133.69
132.66
129.89
128.89
127.69
126.47
123.74
90.42
88.93
52.14
NO2
O
1f
13C NMR (101 MHz, CDCl3)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



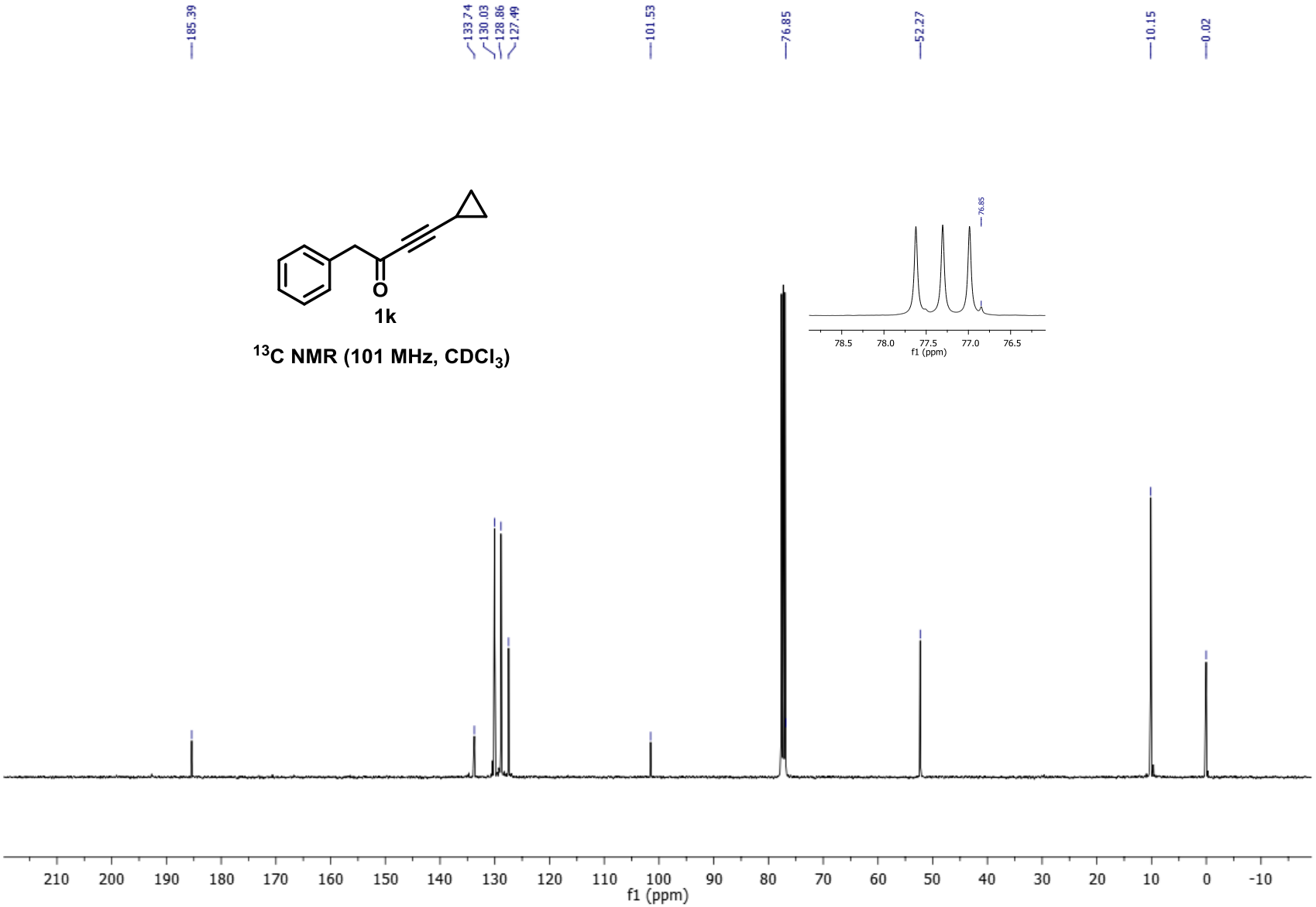
^{1}H NMR (400 MHz, $CDCl_3$)


197.06
184.95
138.12
133.12
132.93
129.90
128.82
128.31
127.57
124.42
90.93
89.45
52.18
26.73
O
O
1g
^{13}C NMR (101 MHz, $CDCl_3$)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



1k

^{1}H NMR (500 MHz, $CDCl_3$)


185.39
133.74
130.03
128.86
127.49
101.53
76.85
52.27
10.15
0.02
O
1k
^{13}C NMR (101 MHz, $CDCl_3$)
78.5
78.0
77.5
77.0
76.5
f1 (ppm)
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)

3. HRMS files of 1d, 1f, 1k, 1g and 7

Created by: Administrator, UNIFI

Created on: Sep 22, 2020

Item name: 20200728_Elemental Compostion Sep 22, 2020 09:29:05 India Standard Time

Created time: 09:42:45 India Standard Time

Item name: CRR_352_173_248

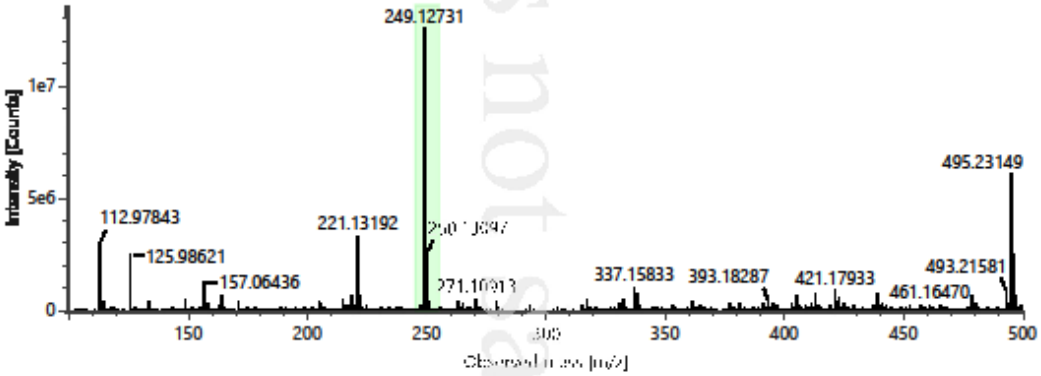
Item name: CRR_352_173_248, Sample position: 1 A,7, Replicate number: 1

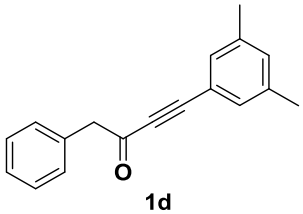
.	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C18H16O	248.1200	248.12012	249.1273	-0.3	+H

Component name: C18H16O

Item name: CRR_352_173_248
Item description:

Channel name: Low energy, Time 0.3118 +/- 0.0637 minutes





1d

UNIFI page 1 of 1

Results not saved

Created by: Administrator, UNIFI

Created on: Sep 14, 2020

Item name: 20200728_Elemental Compostion Sep 14, 2020 18:11:25 India Standard Time

Created time: 18:44:23 India Standard Time

Item name: CRR_352_169_265

Item name: CRR_352_169_265, Sample position: 1:1,5, Replication number: 1

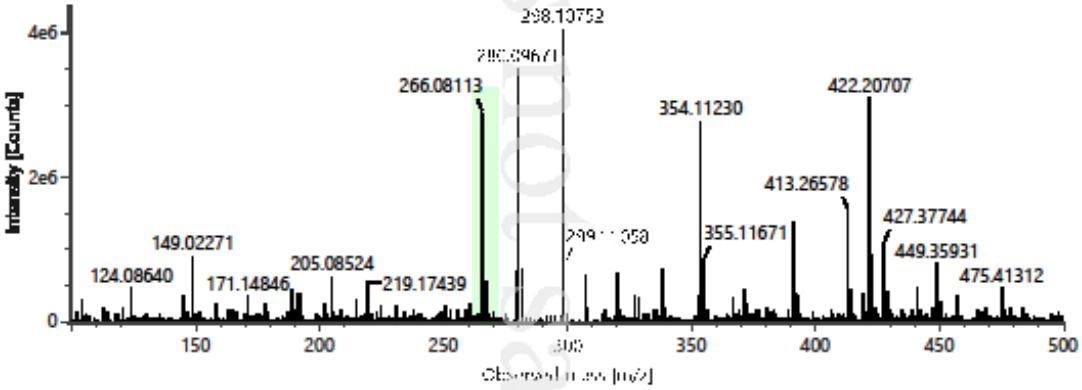
.	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C16H11NO3	265.0739	265.07389	266.0811	-0.2	+H

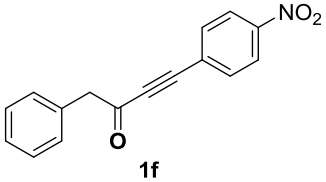
Component name: C16H11NO3

Item name: CRR_352_169_265

Item description:

Channel name: Low energy, Time 0.3676 +/- 0.0587 minutes





1f

Results not saved

Created by: Administrator, UNIFI

Created on: Nov 11, 2020

Item name: 20200728_Elemental Compostion Nov 10, 2020 17:39:08 India Standard Time

Created time: 09:35:39 India Standard Time

Item name: CRR-352-155-262

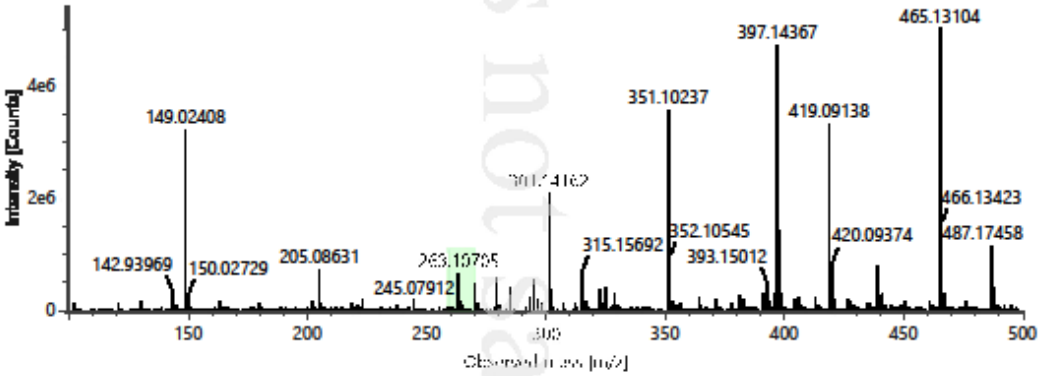
Item name: CRR-352-155-262, Sample position: 2:B,2, Replicate number: 1

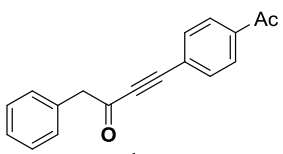
.	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C18H14O2	262.0998	262.09938	263.1070	1.5	+H

Component name: C18H14O2

Item name: CRR-352-155-262
Item description:

Channel name: Low energy, Time: 0.5357 +/- 0.0616 minutes





1g

Results not saved

Created by: Administrator, UNIFI

Created on: Sep 22, 2020

Item name: 20200728_Elemental Compostion Sep 22, 2020 09:29:05 India Standard Time

Created time: 09:36:20 India Standard Time

Item name: CRR_352_174_184

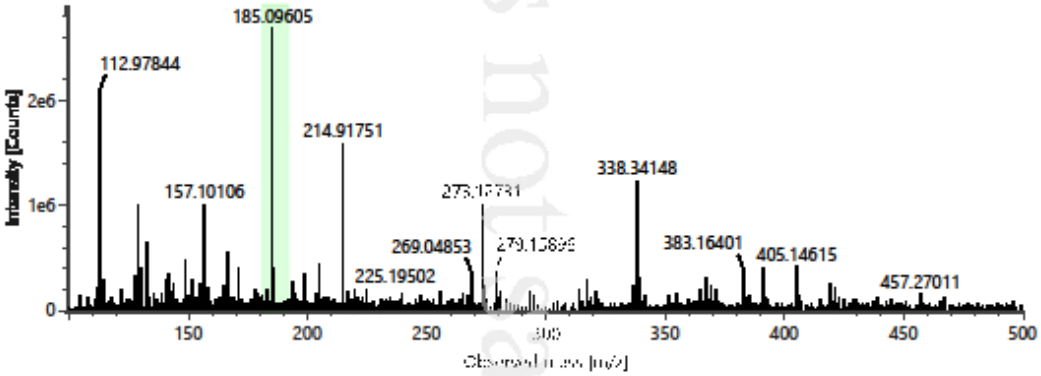
Item name: CRR_352_174_184, Sample position: 1 A2, Replicate number: 1

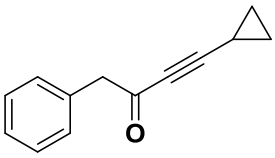
.	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C13H12O	184.0888	184.08882	185.0960	-0.2	+H

Component name: C13H12O

Item name: CRR_352_174_184
Item description:

Channel name: Low energy, Time 0.3122 +/- 0.0642 minutes





1k

Results not saved

Created by: Shekar, Dr.Anubala

Created on: Apr 22, 2022

Item name: HRMS Elemental composition Apr 22, 2022 14:31:16 India Standard Time

Created time: 15:00:45 India Standard Time

Item name: CRR-352-A-390

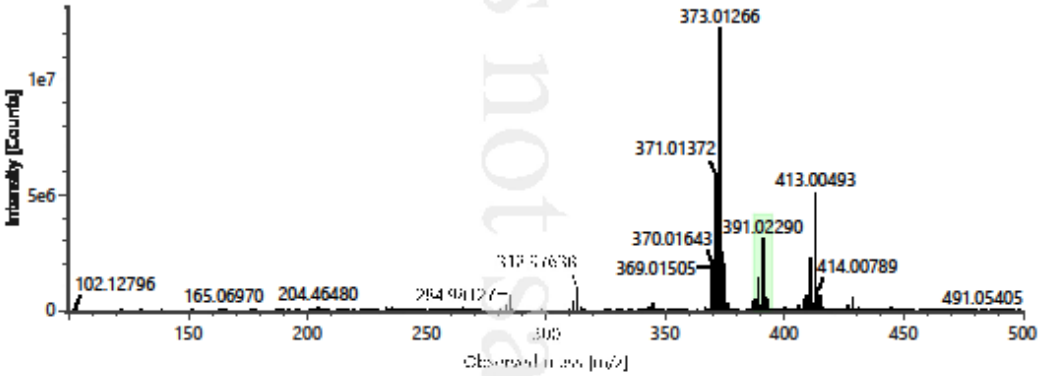
Item name: CRR-352-A-390, Sample position: 2:0,5, Replicate number: 1

.	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C22H14O2Se	390.0156	390.01590	391.0229	-0.7	+H

Component name: C22H14O2Se

Item name: CRR-352-A-390
Item description:

Channel name: Low energy, Time 0.3157 +/- 0.0703 minutes



Results not saved