Supporting Information

Exploiting the σ-phylic properties of cationic gold(I) catalysts in the ring opening reactions of aziridines with indoles

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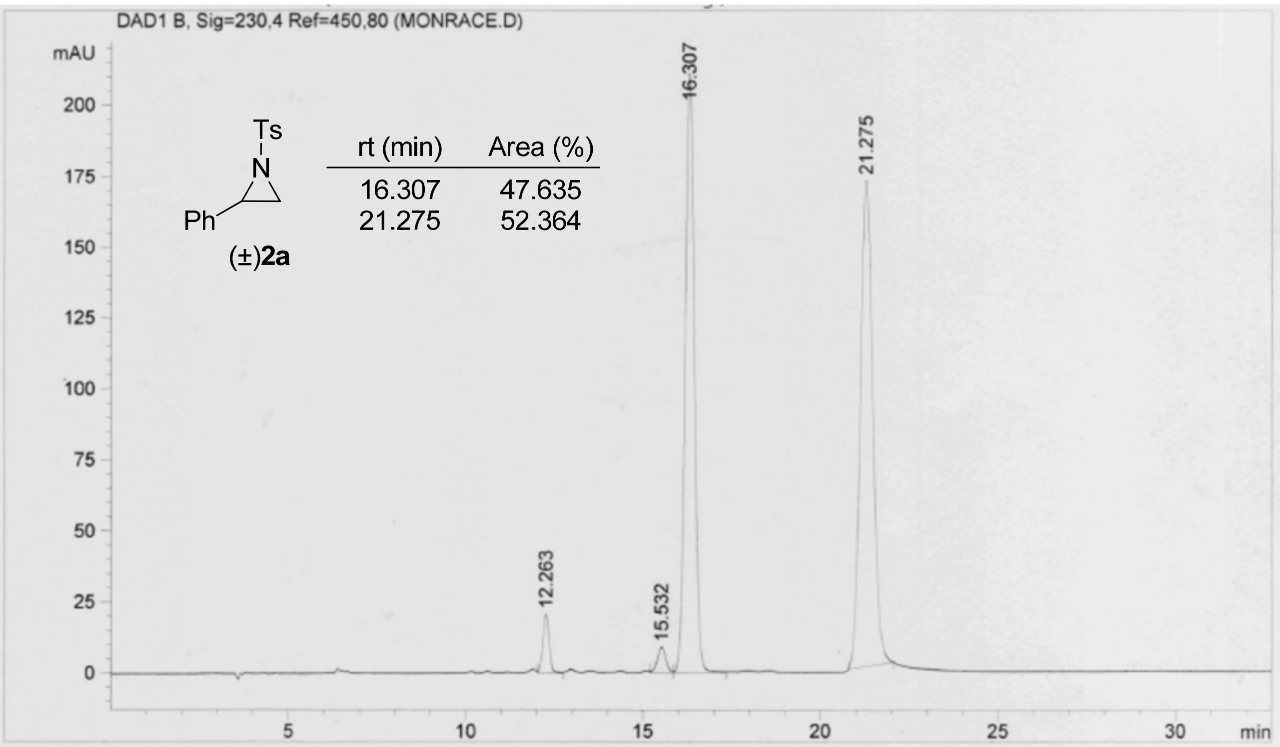
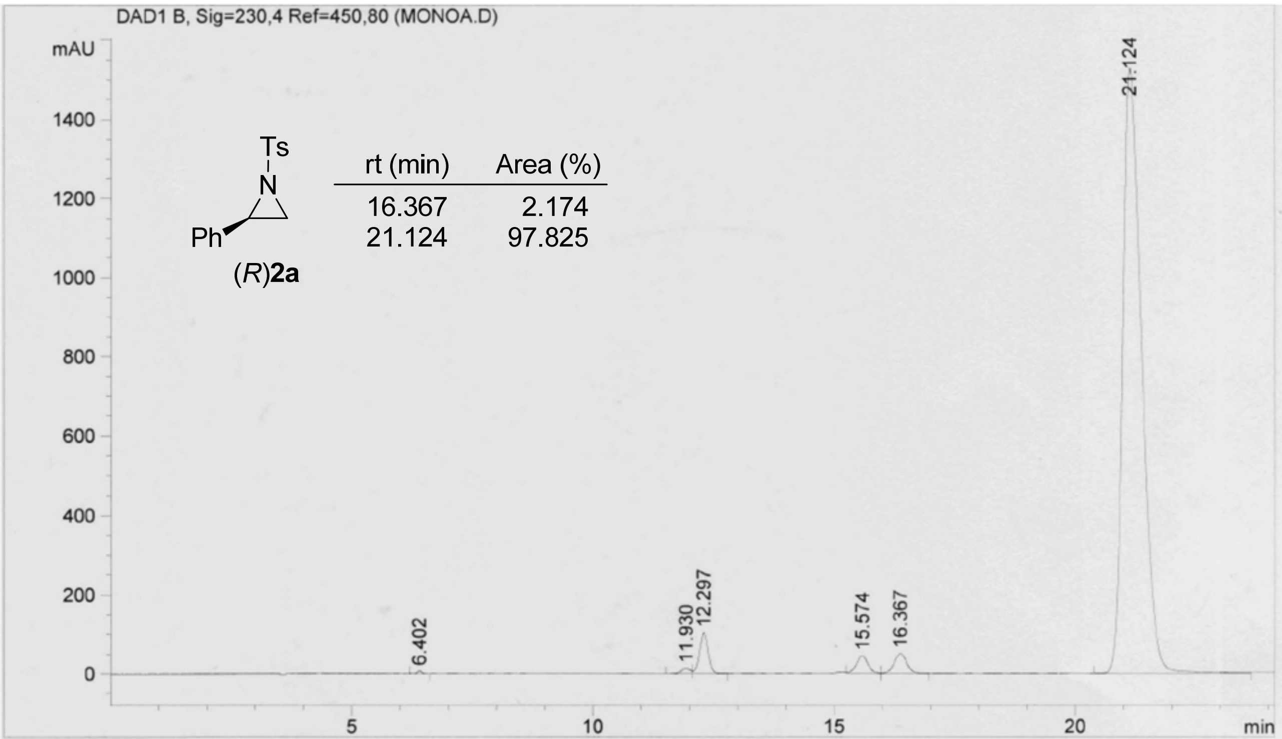
Contents

HPLC Traces

(±)2a and (*R*)2a

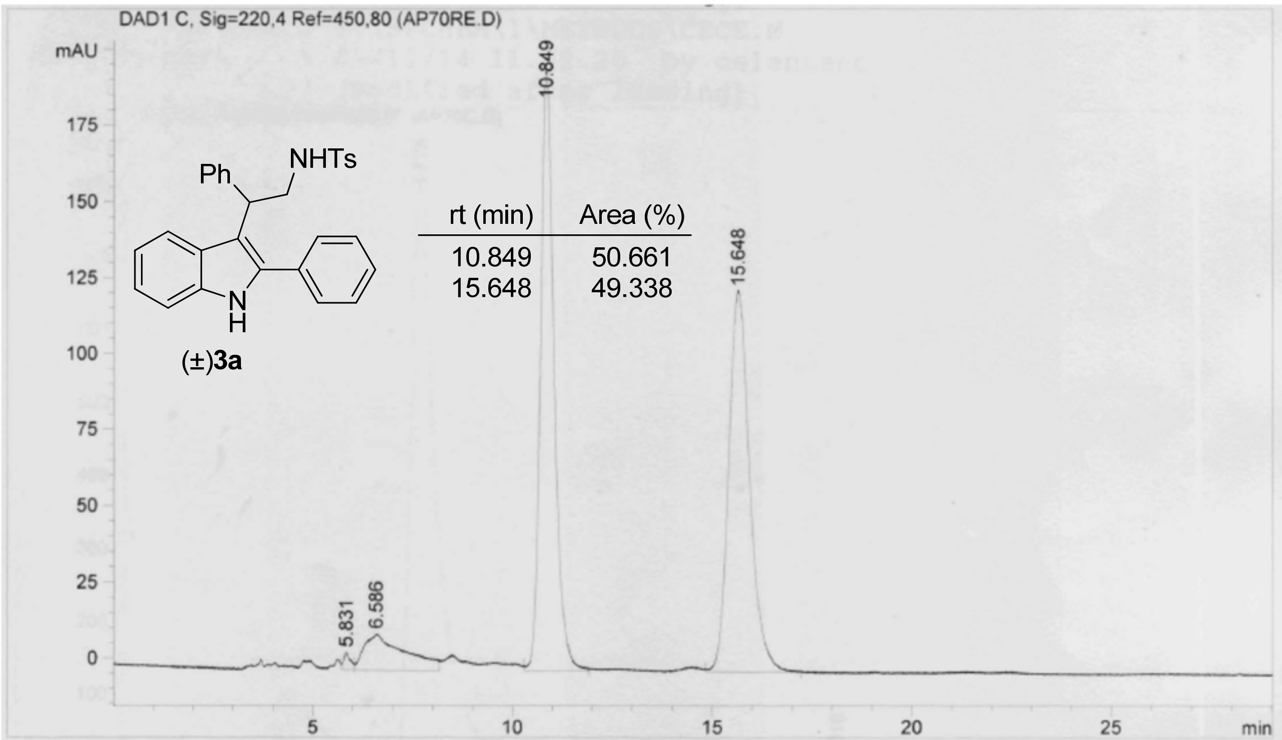
<u>Method:</u> Phenomenex Lux 3µ Cellulose-4 (250 x 4.60 mm); hexane/isopropanol 90:10 (0.8 mL/min); λ = 230.4 nm

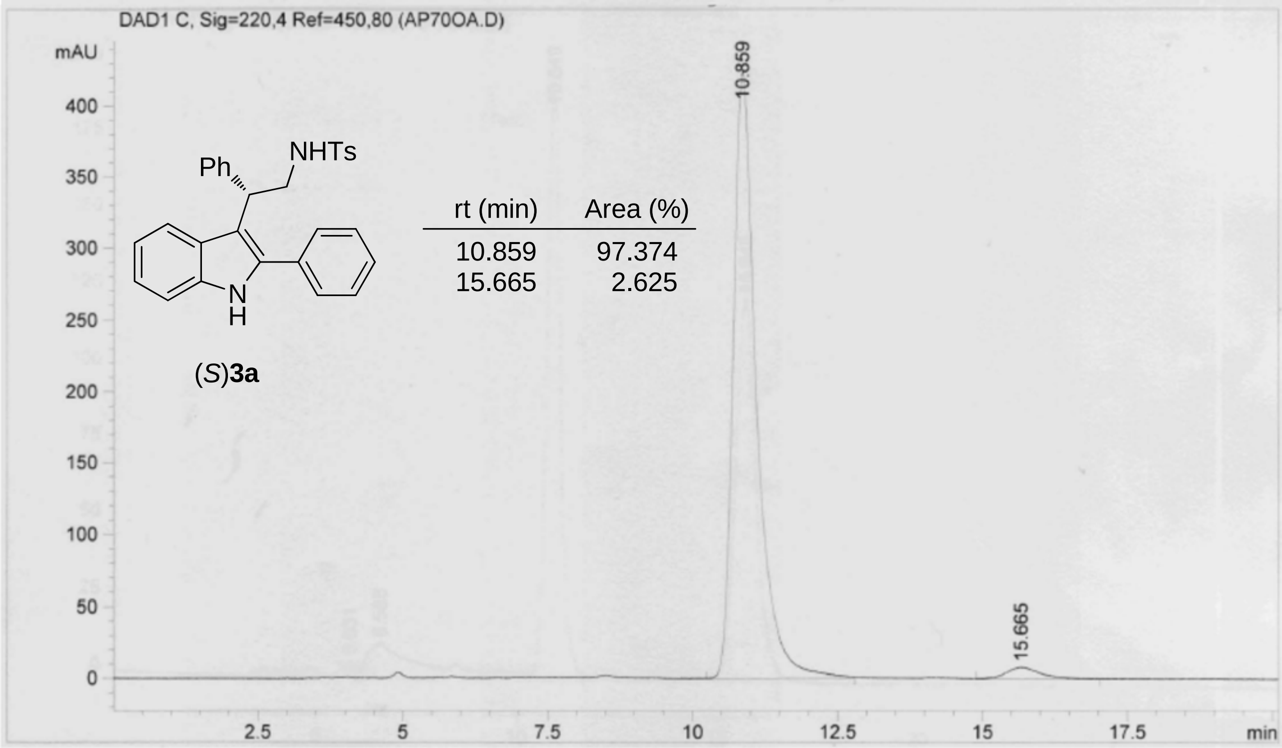




(±)3a and (*S*)3a

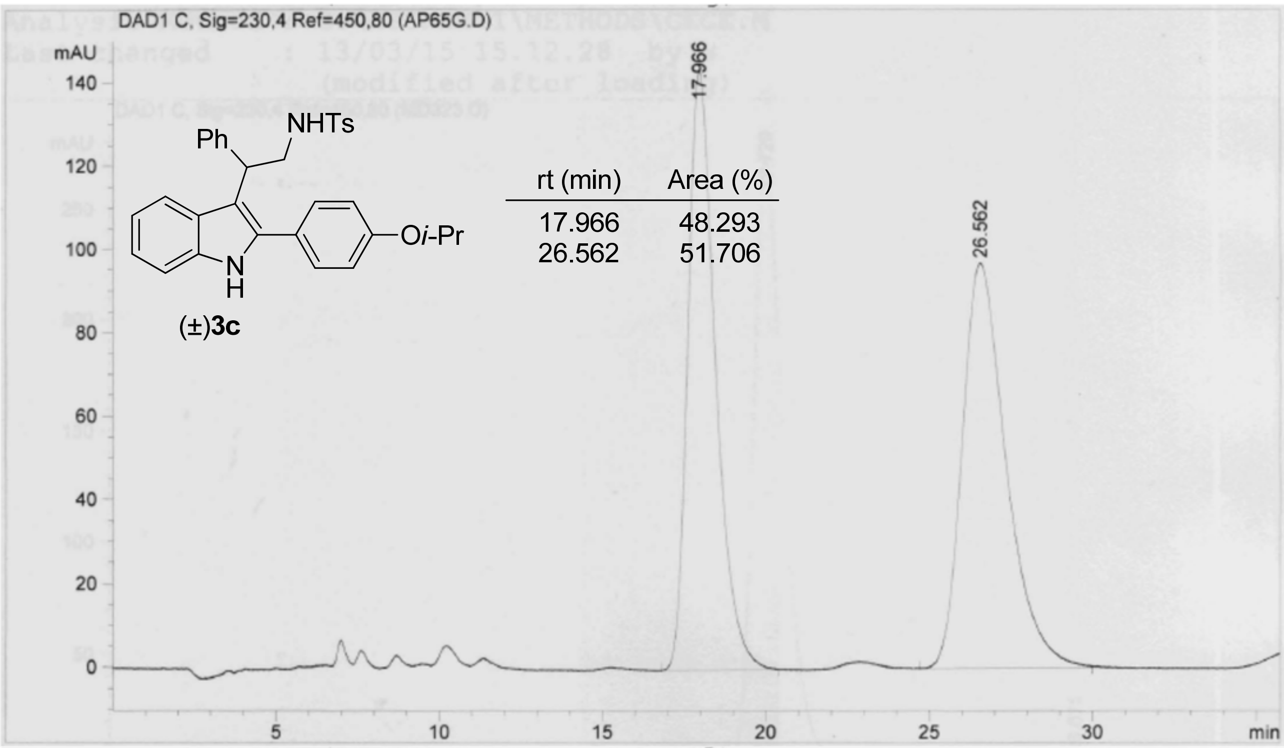
<u>Method:</u> Chiralpak AD 10μ (250 x 4.60 mm); hexane/isopropanol 60:40 (0.8 mL/min); λ = 230.4 nm

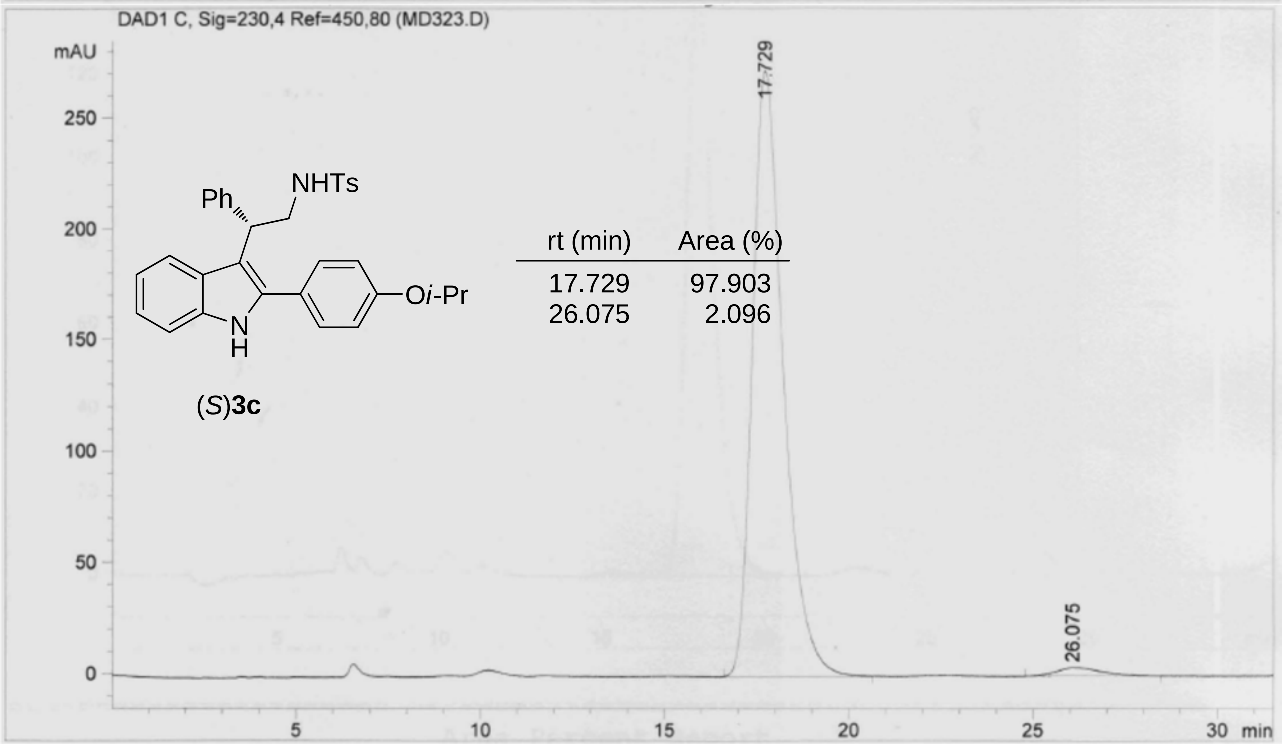




(±)3c and (*S*)3c

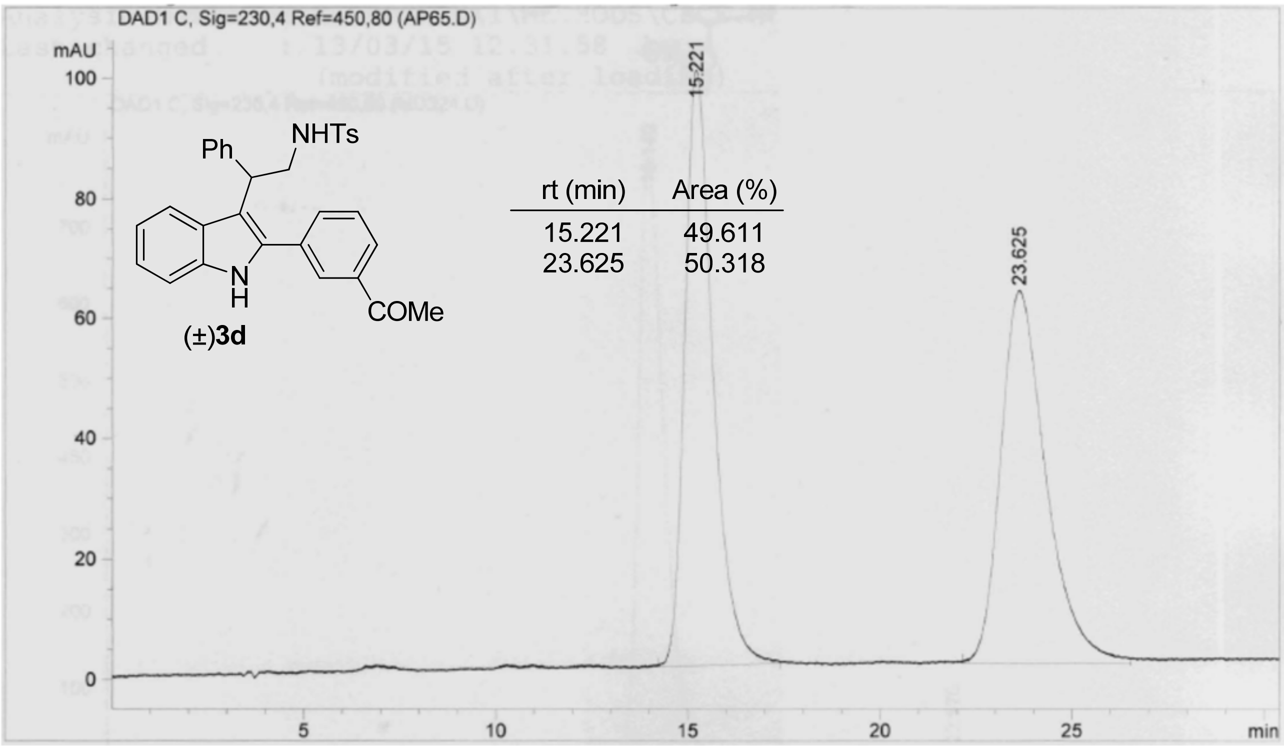
Method: Chiralpak AD 10μ (250 x 4.60 mm); hexane/isopropanol 70:30 (0.8 mL/min); λ = 230.4 nm



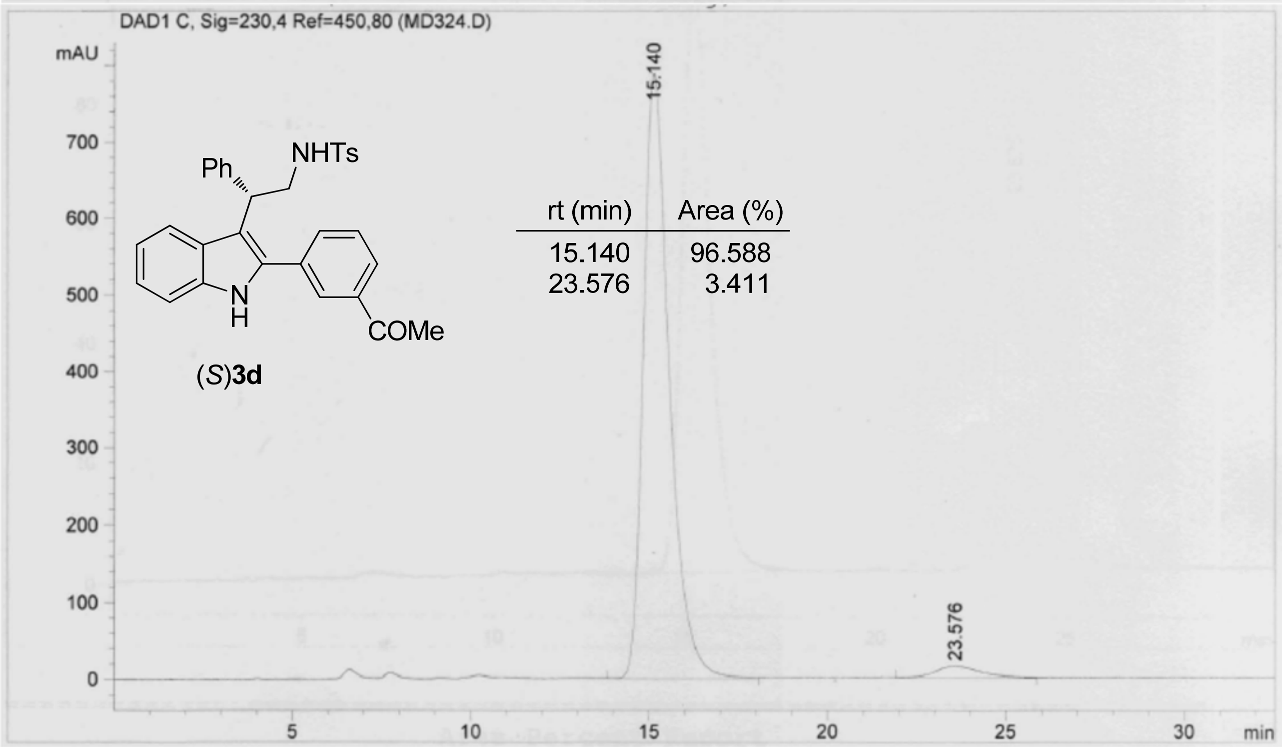


(±)3d and (*S*)3d

Method: Chiralpak AD 10µ (250 x 4.60 mm); hexane/isopropanol 70:30 (0.8 mL/min); λ = 230.4 nm



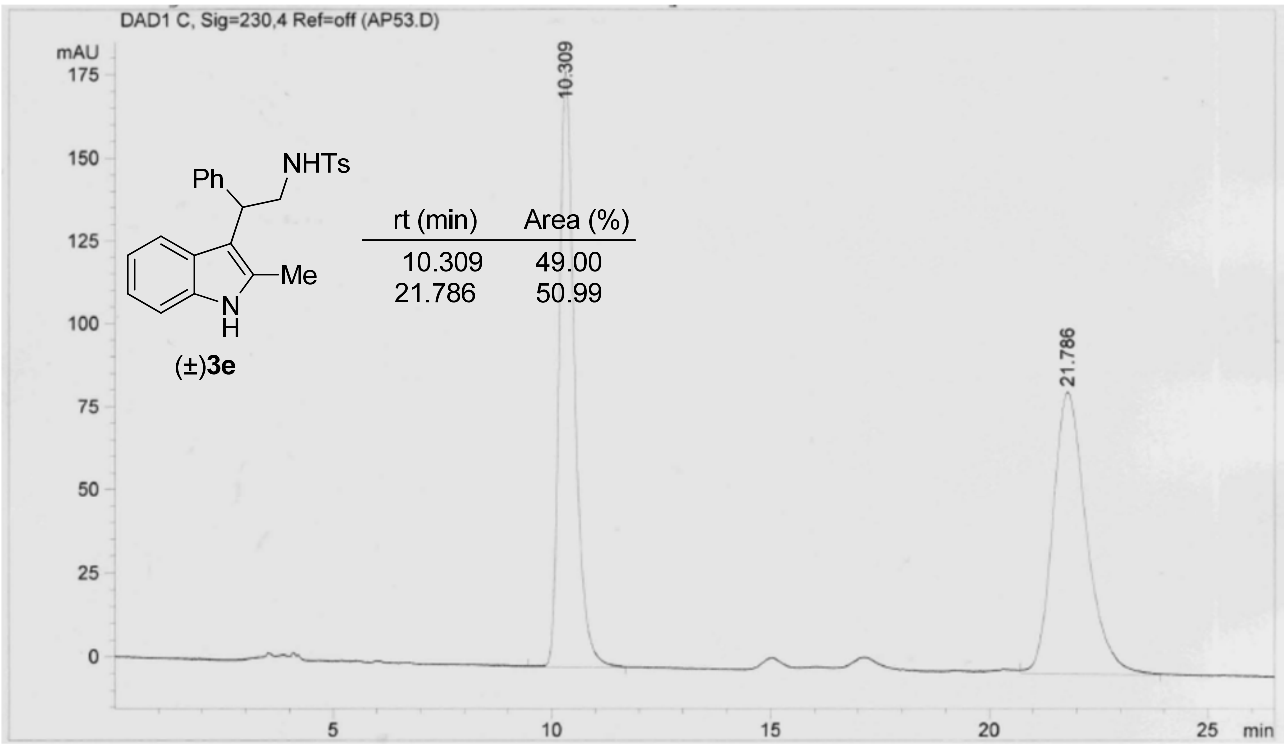
rt (min)	Area (%)
15.221	49.611
23.625	50.318

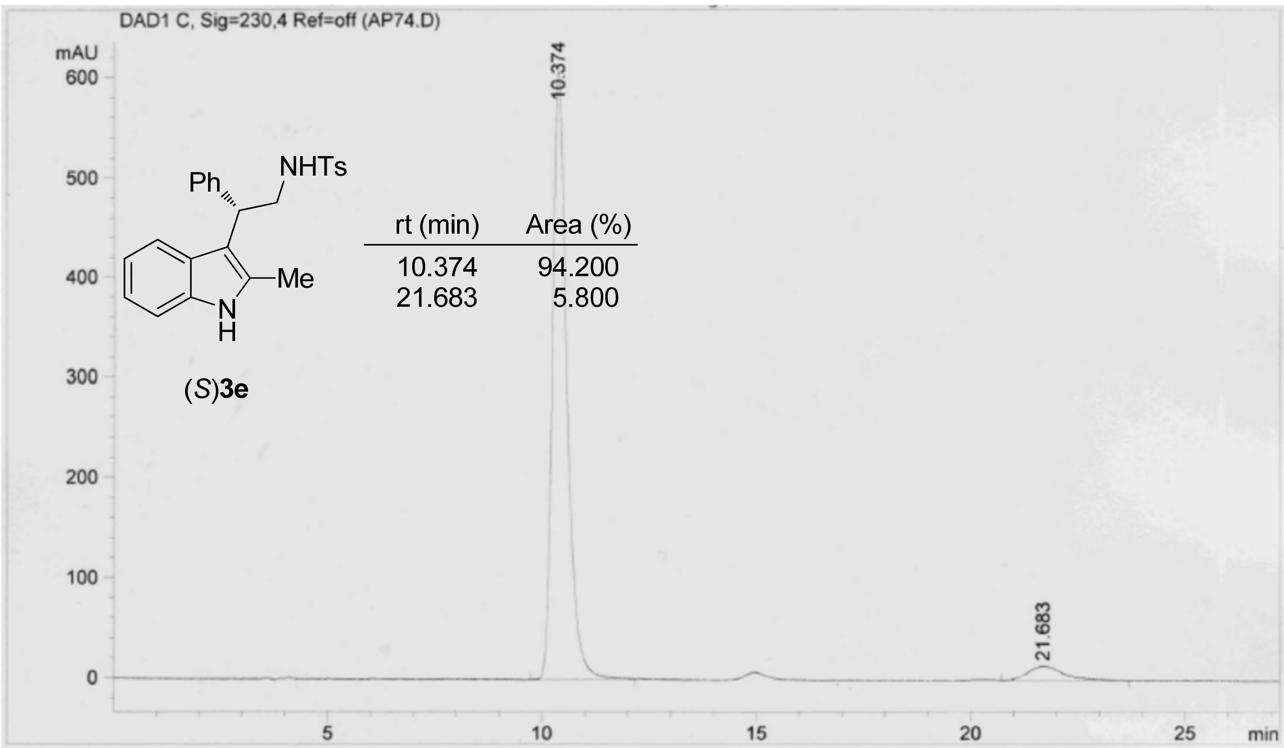


rt (min)	Area (%)
15.140	96.588
23.576	3.411

(±)3e and (*S*)3e

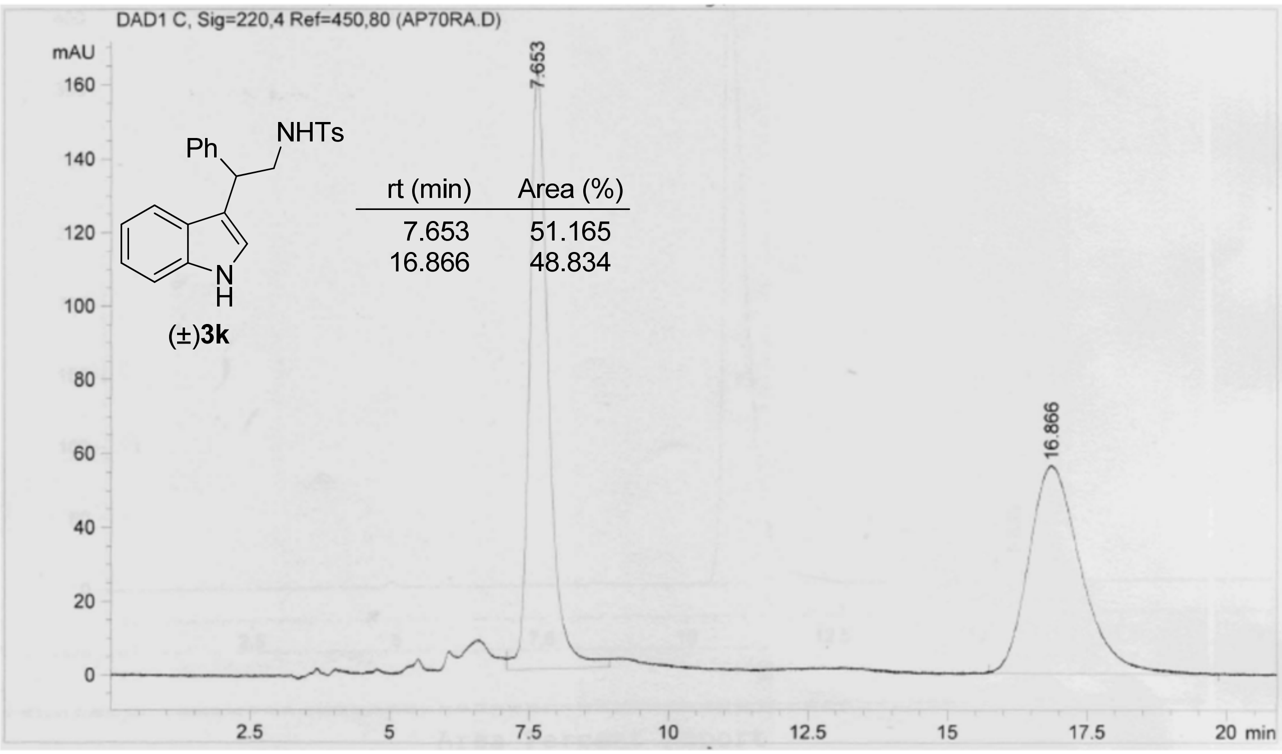
Method: Chiralpak AD 10μ (250 x 4.60 mm); hexane/isopropanol 70:30 (0.8 mL/min); λ = 270.4 nm

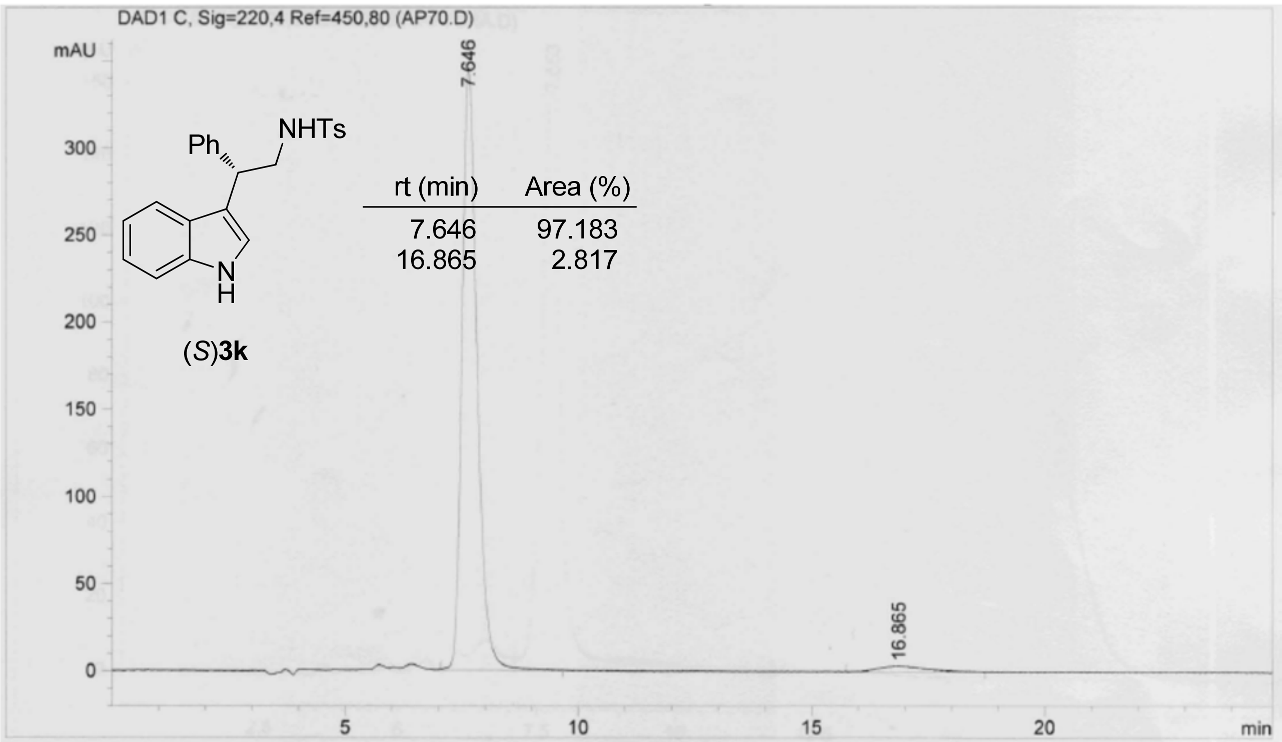




(±)3k and (*S*)3k

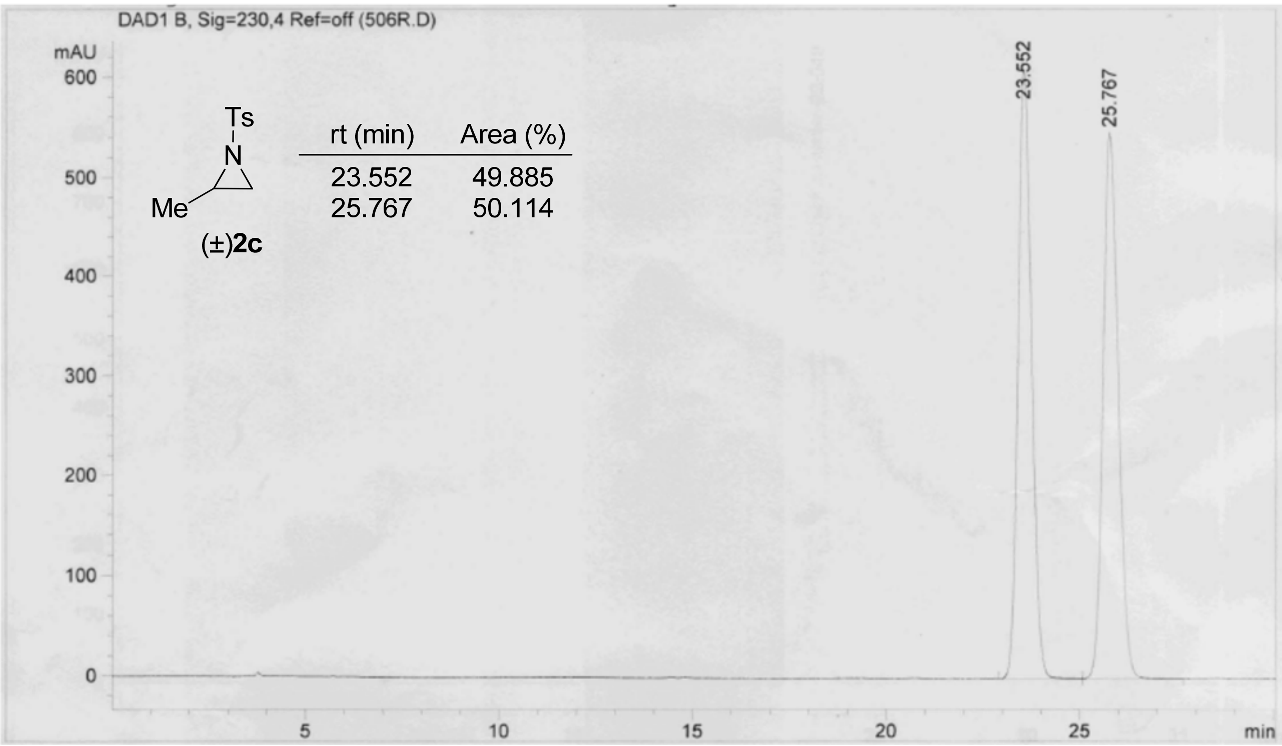
Method: Chiralcel OD-H 5μ (250 x 4.60 mm); hexane/isopropanol 70:30 (0.8 mL/min); λ = 280.4 nm

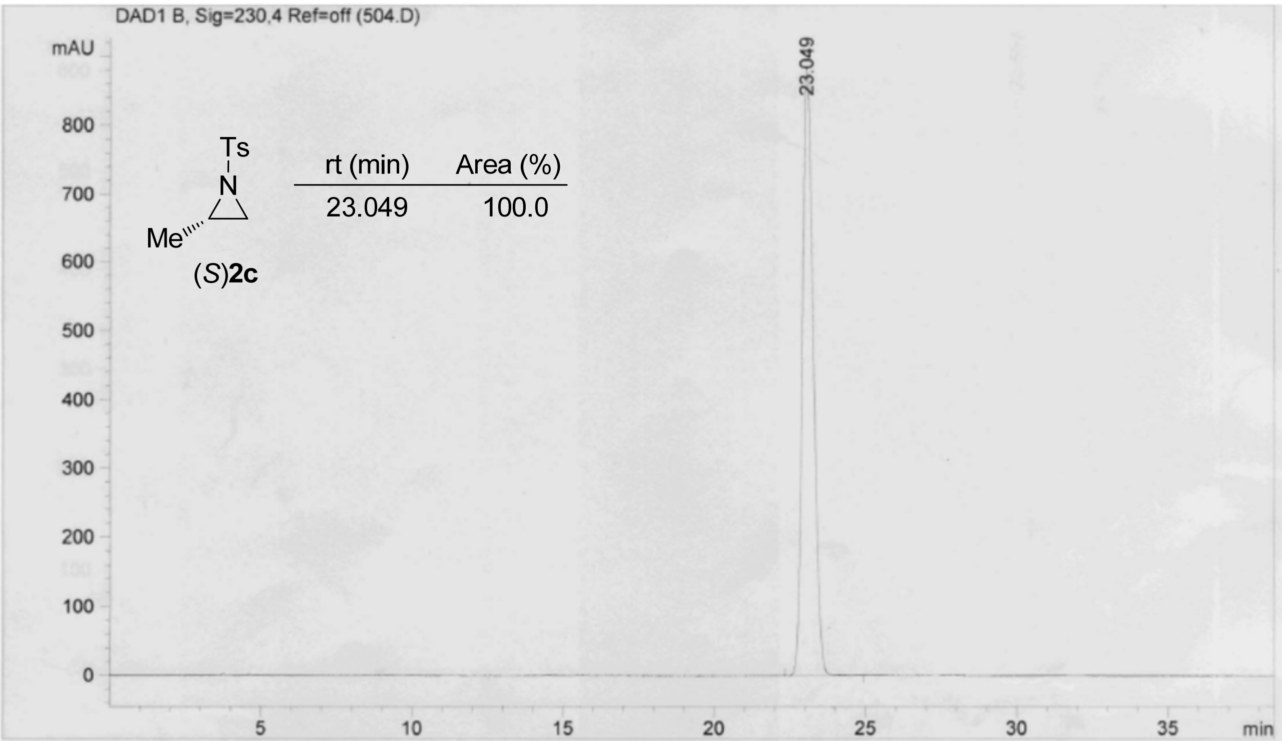




(±)2c and (*S*)2c

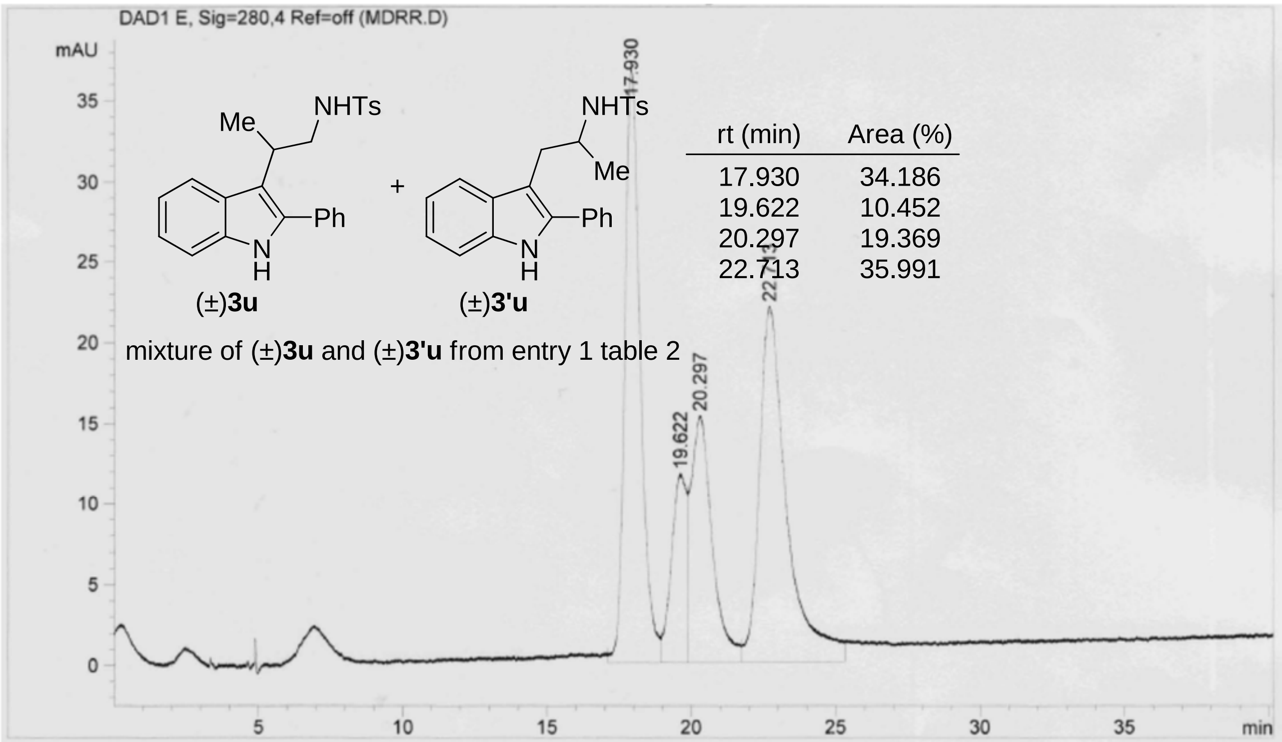
Method: Phenomenex Lux 3μ Cellulose-4 (250 x 4.60 mm); hexane/isopropanol 90:10 (0.8 mL/min); λ = 230.4 nm

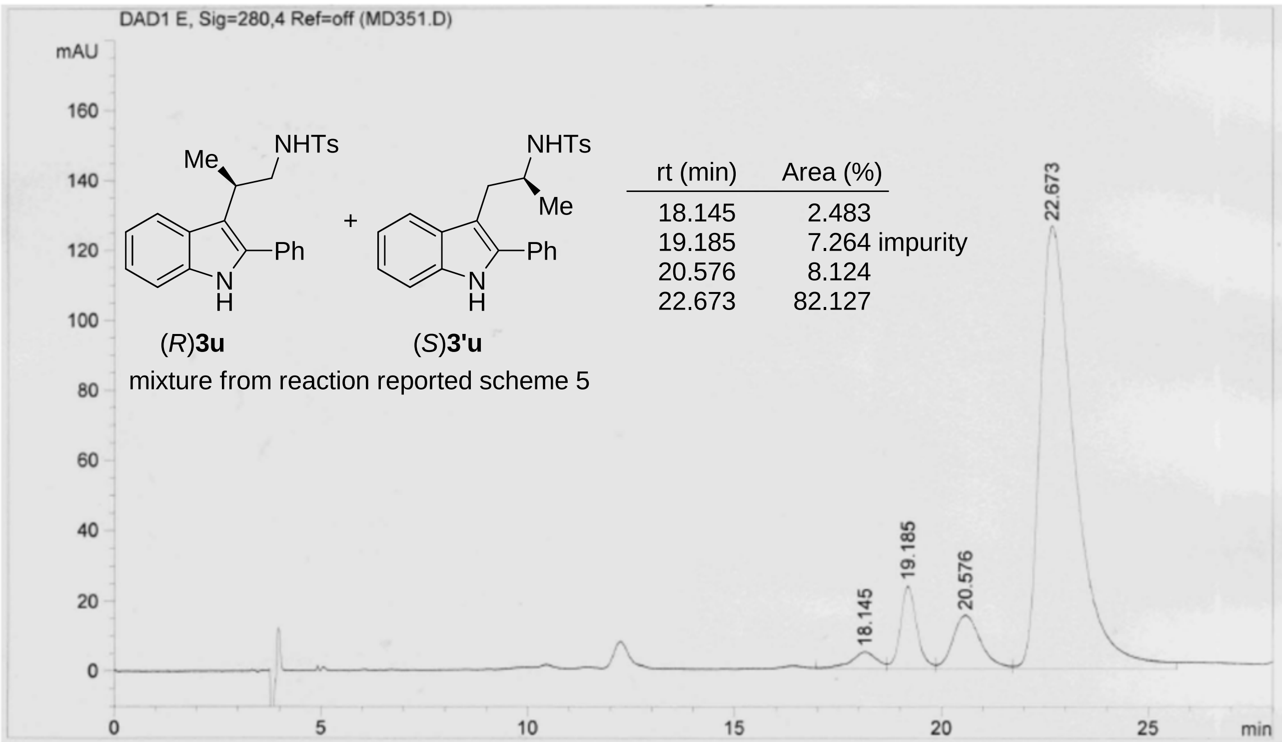




(±)3u/(±)3’u and (*R*)3u/3’u

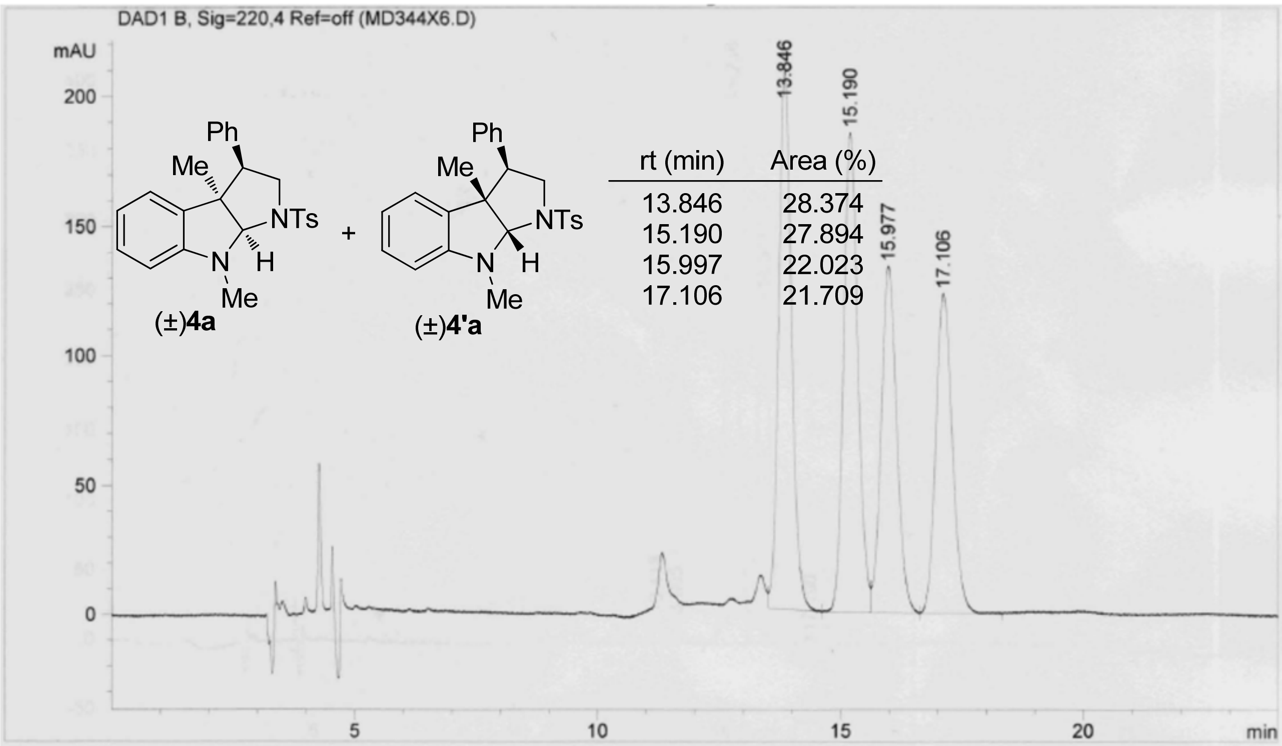
Method: Phenomenex Lux 3μ Cellulose-4 (250 x 4.60 mm); hexane/isopropanol 80:20 (0.8 mL/min); λ = 230.4 nm.

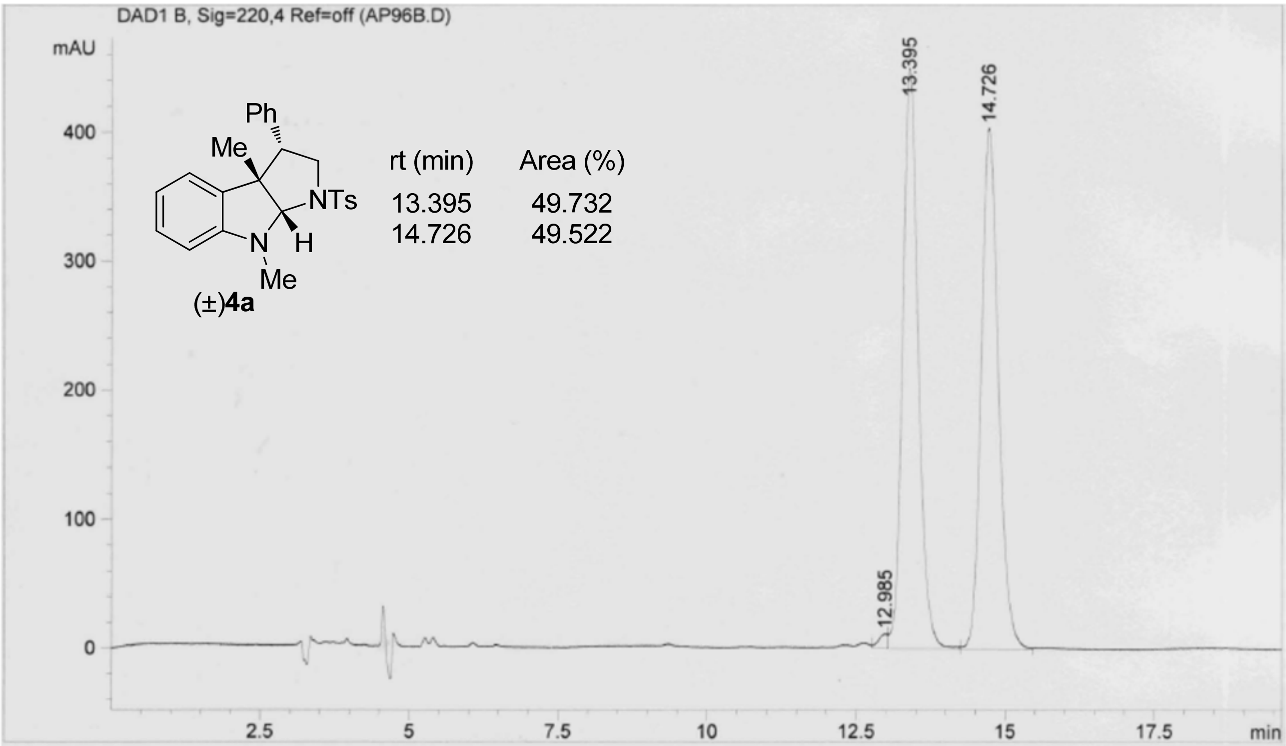


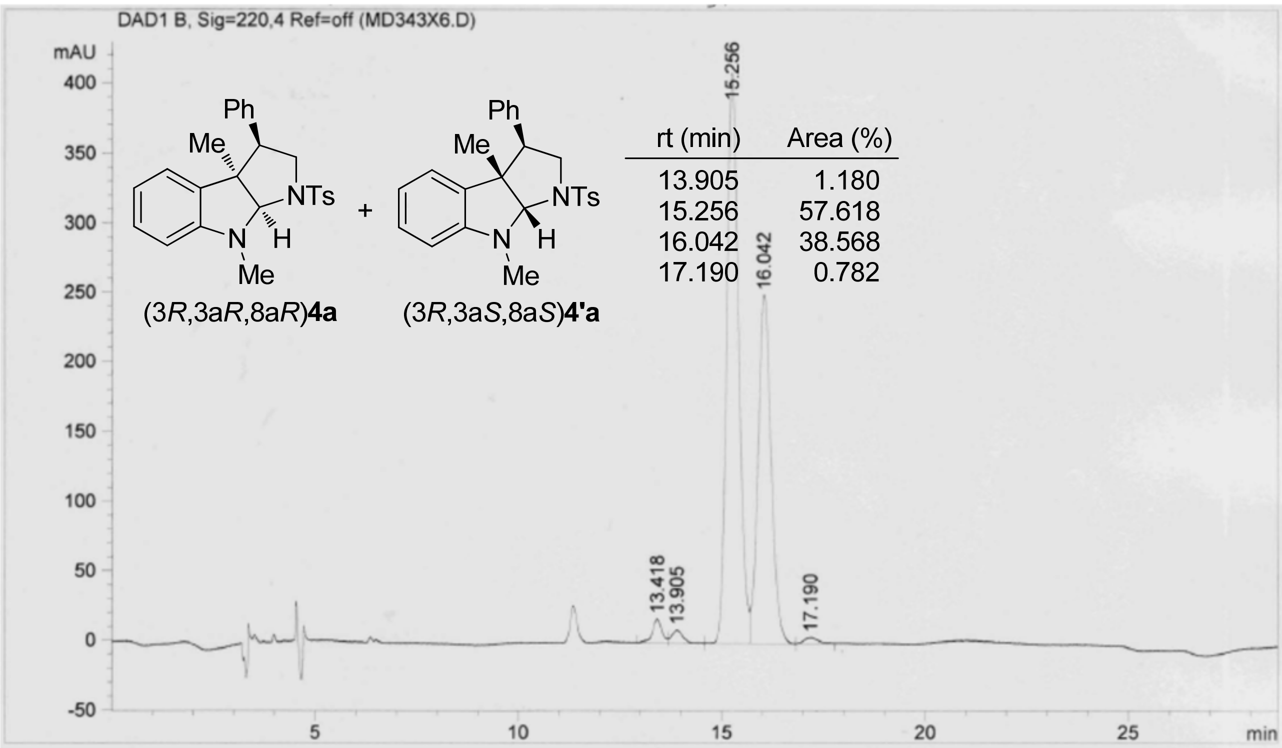


(±)4a/(±)4'a, (±)4a and (*R*,*R*,*R*)4a/(*R*,*S*,*S*)4'a

<u>Method:</u> Phenomenex Lux 3μ Cellulose-4 (250 x 4.60 mm); hexane/isopropanol/methanol 80:14:6 (0.8 mL/min); λ = 230.4 nm.

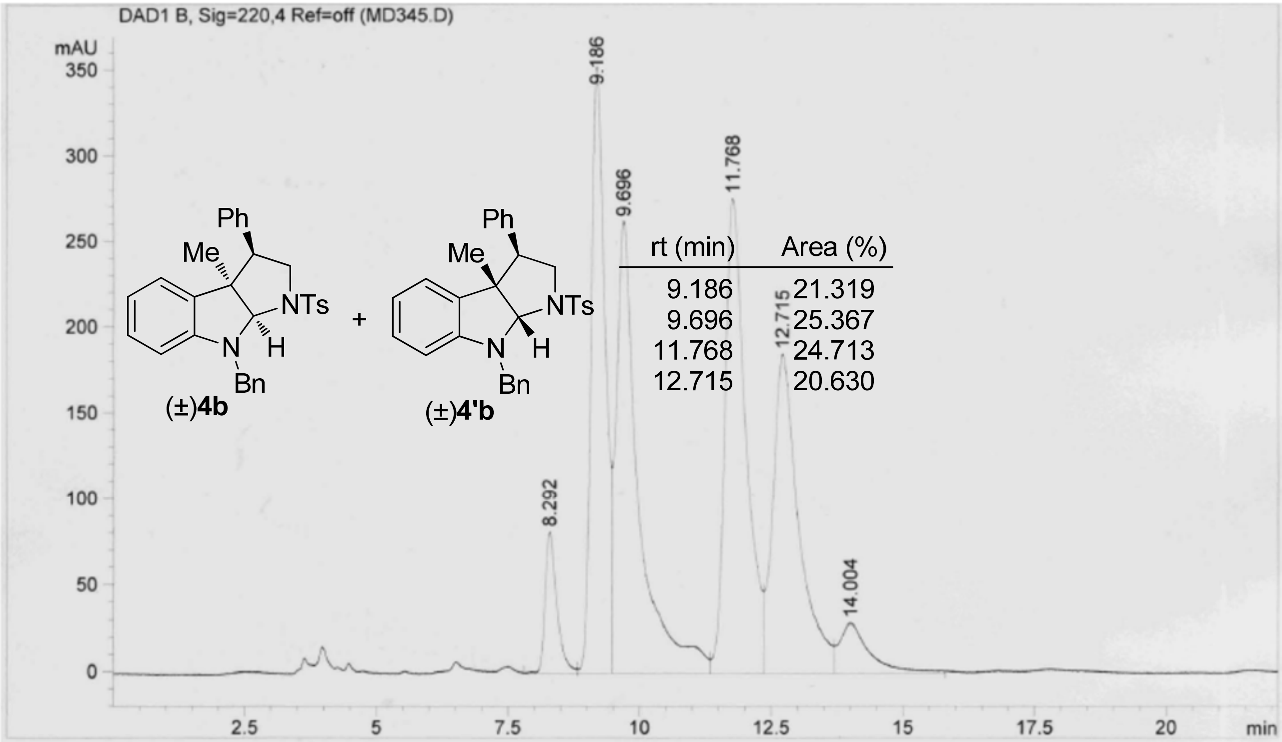


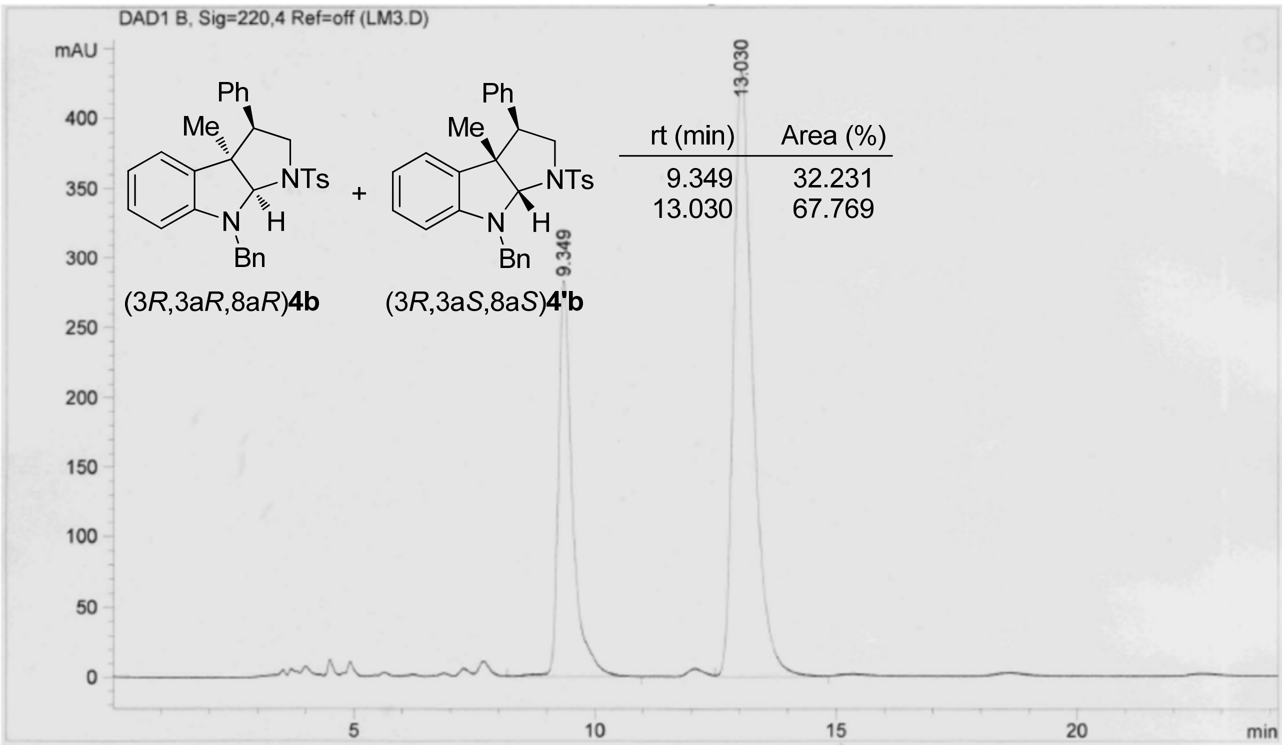



DAD1 B, Sig=220,4 Ref=off (MD343X6.D)
mAU
400
350
300
250
200
150
100
50
0
-50
5
10
15
20
25
min
15.256
16.042
13.418
13.905
17.190
Ph
Me
NTs
N
H
Me
(3R,3aR,8aR)4a
+
Ph
Me
NTs
N
H
Me
(3R,3aS,8aS)4'a
rt (min) Area (%)
13.905 1.180
15.256 57.618
16.042 38.568
17.190 0.782

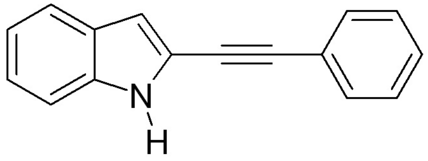
(±)4b/(±)4'b and (*R*,*R*,*R*)4b/(*R*,*S*,*S*)4'b

Method: Phenomenex Lux 3μ Cellulose-4 (250 x 4.60 mm); hexane/isopropanol/methanol 80:14:6 (0.8 mL/min); λ = 230.4 nm.

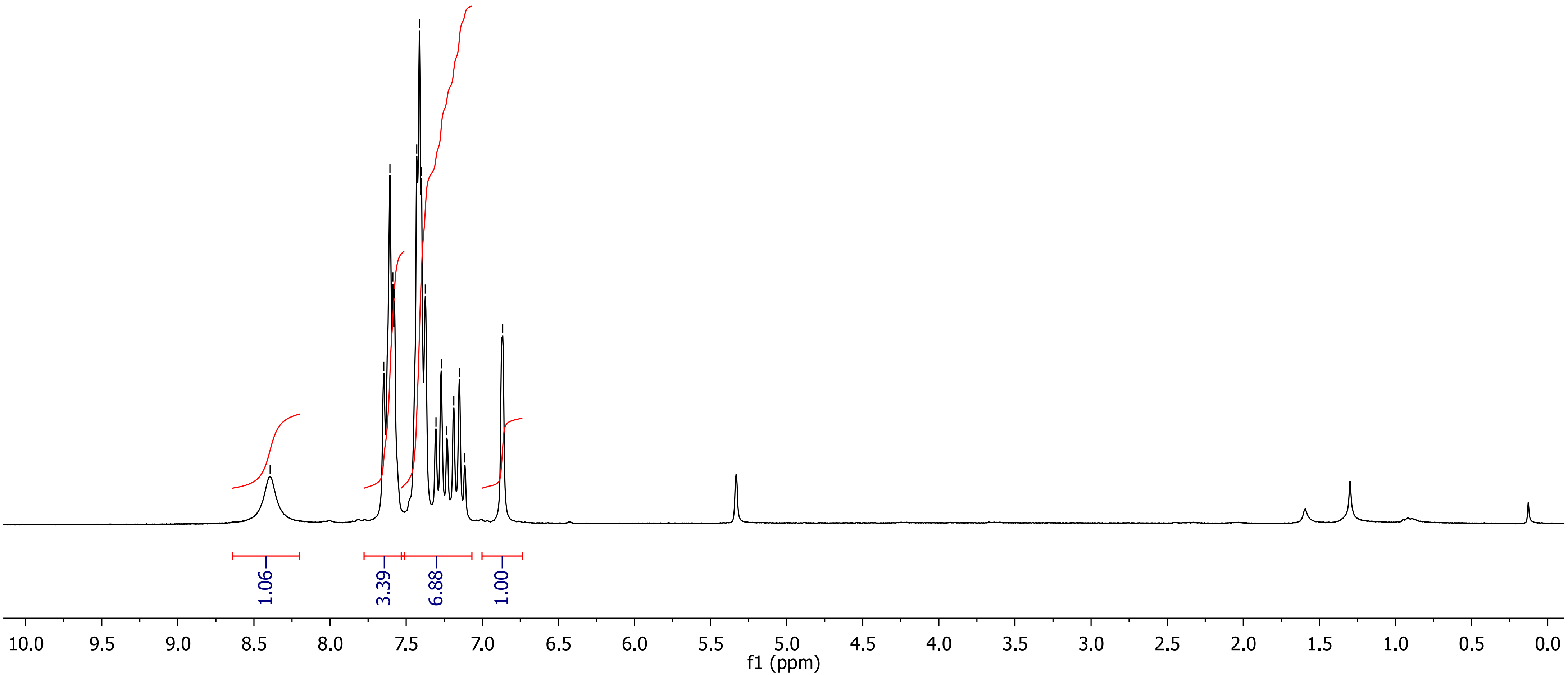


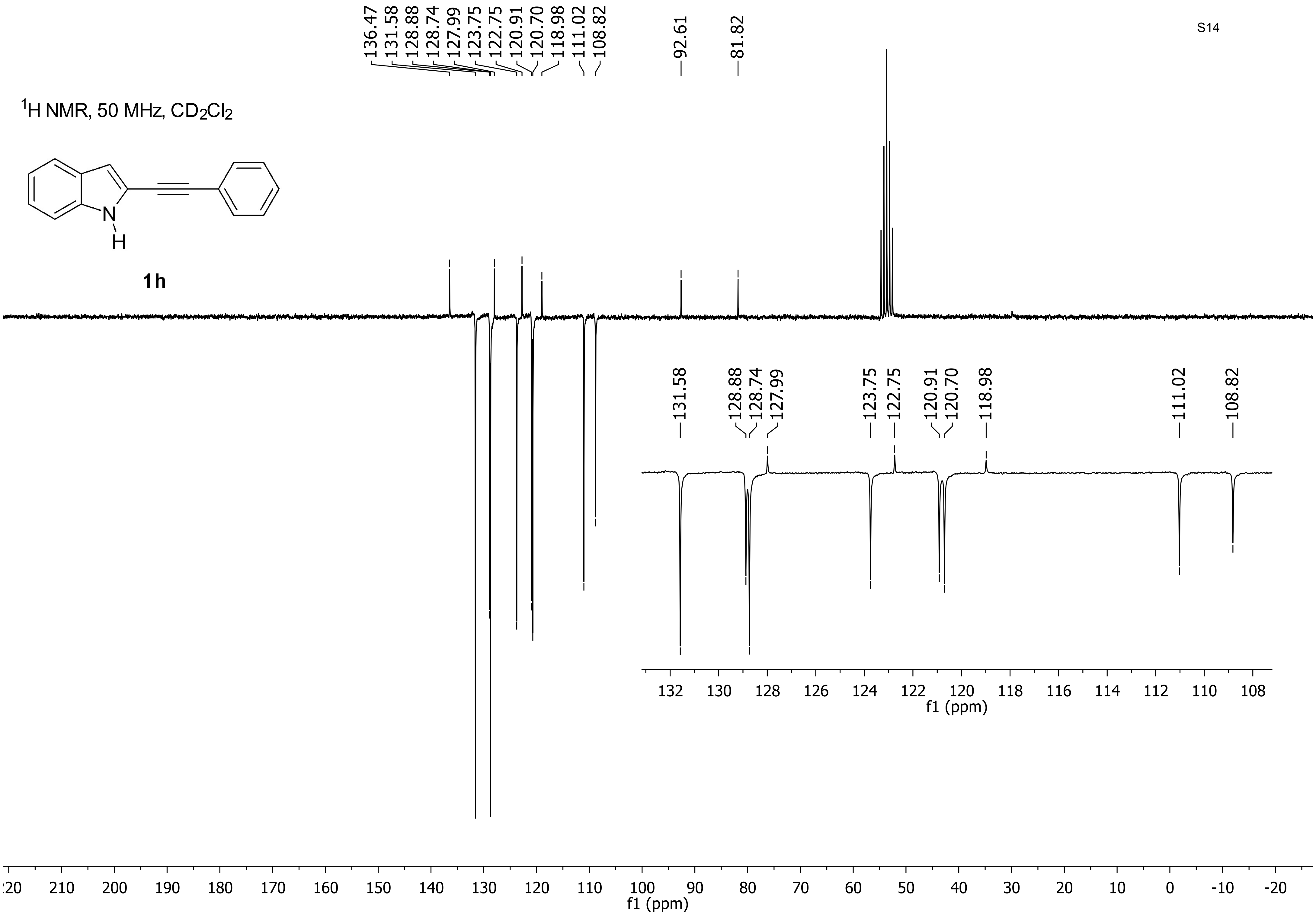


^{1}H NMR, 200 MHz, CD_2Cl_2

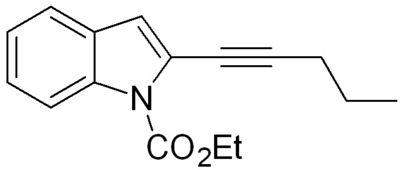


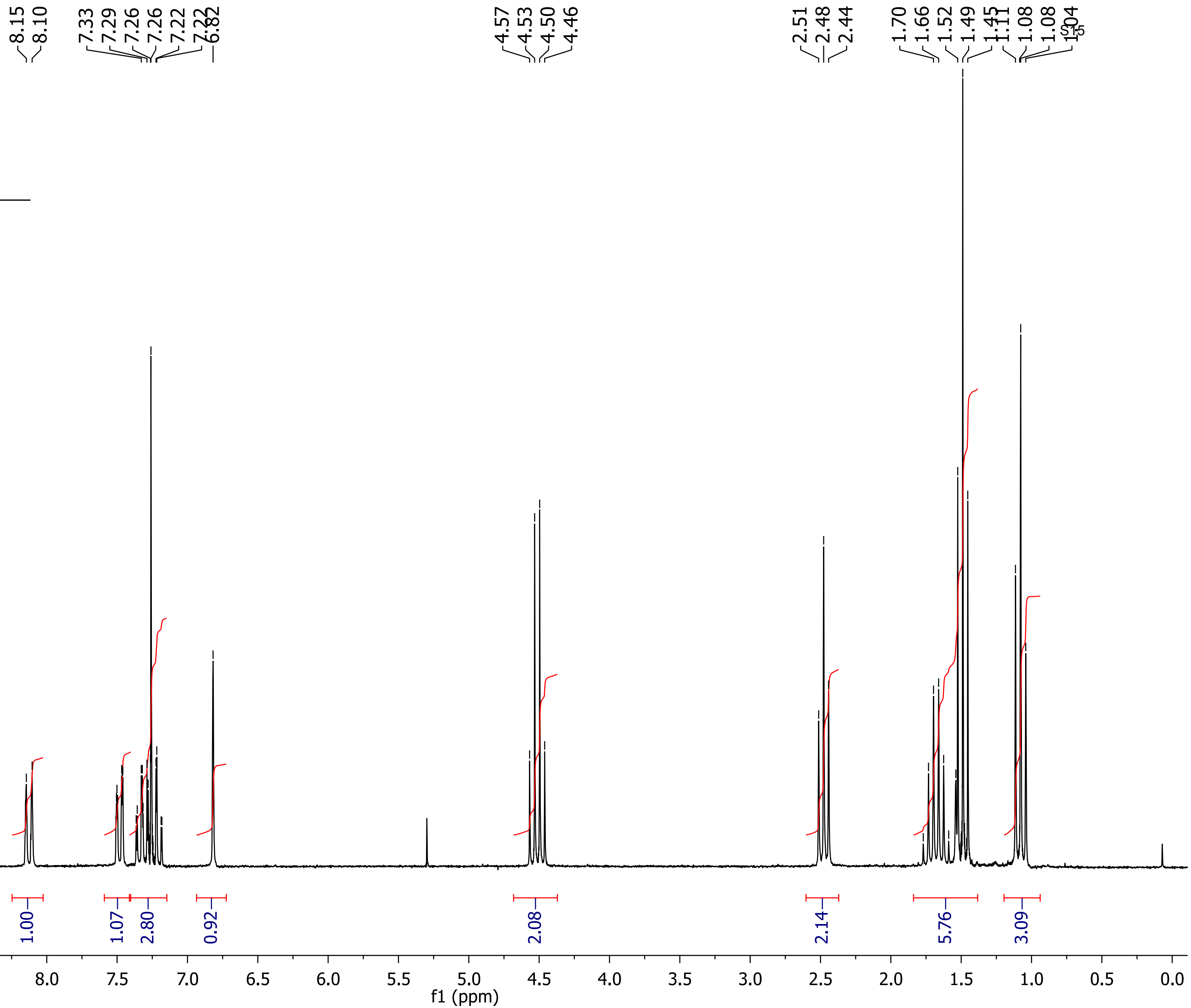
1h

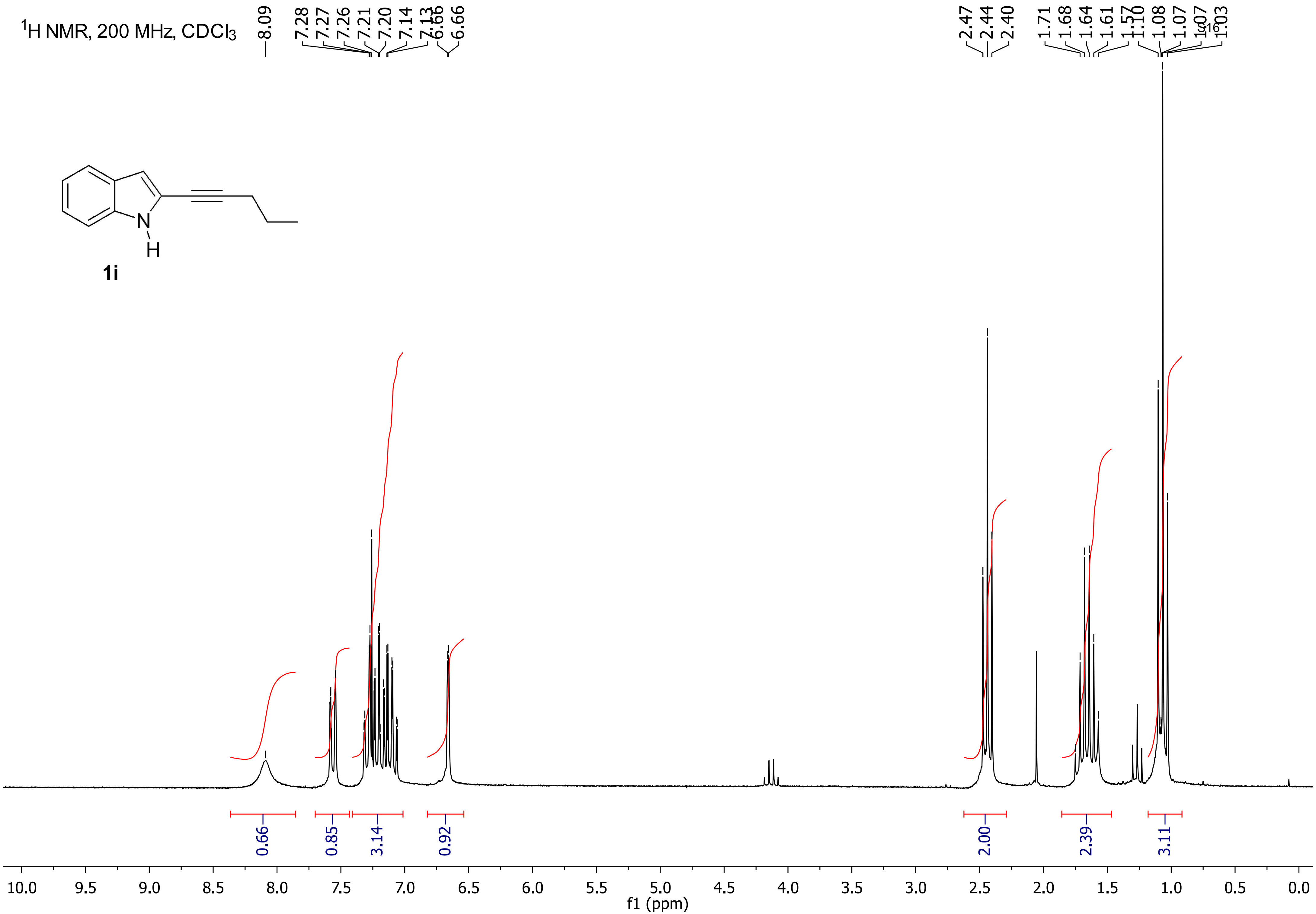



^{1}H NMR, 50 MHz, CD_2Cl_2
1h
136.47
131.58
128.88
128.74
127.99
123.75
122.75
120.91
120.70
118.98
111.02
108.82
92.61
81.82
f1 (ppm)

^1H NMR, 200 MHz, $CDCl_3$

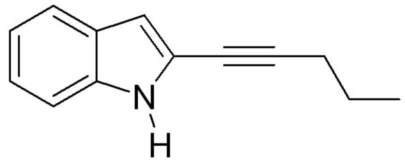




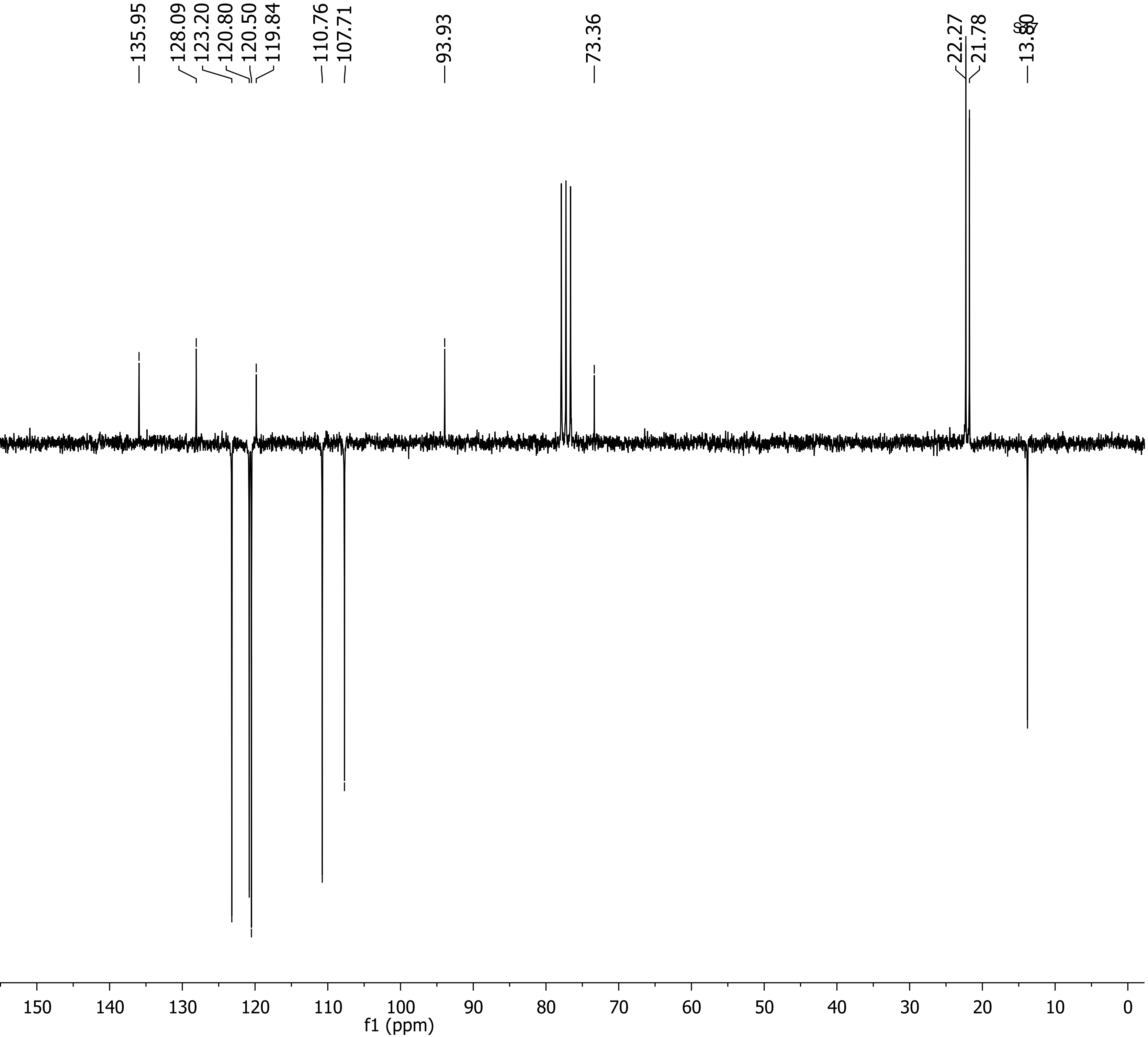

^{1}H NMR, 200 MHz, $CDCl_3$
8.09
7.28
7.27
7.26
7.21
7.20
7.14
7.13
6.66
6.66
2.47
2.44
2.40
1.71
1.68
1.64
1.61
1.57
1.10
1.08
1.07
1.07
1.03
0.66
0.85
3.14
0.92
2.00
2.39
3.11
f1 (ppm)

1i

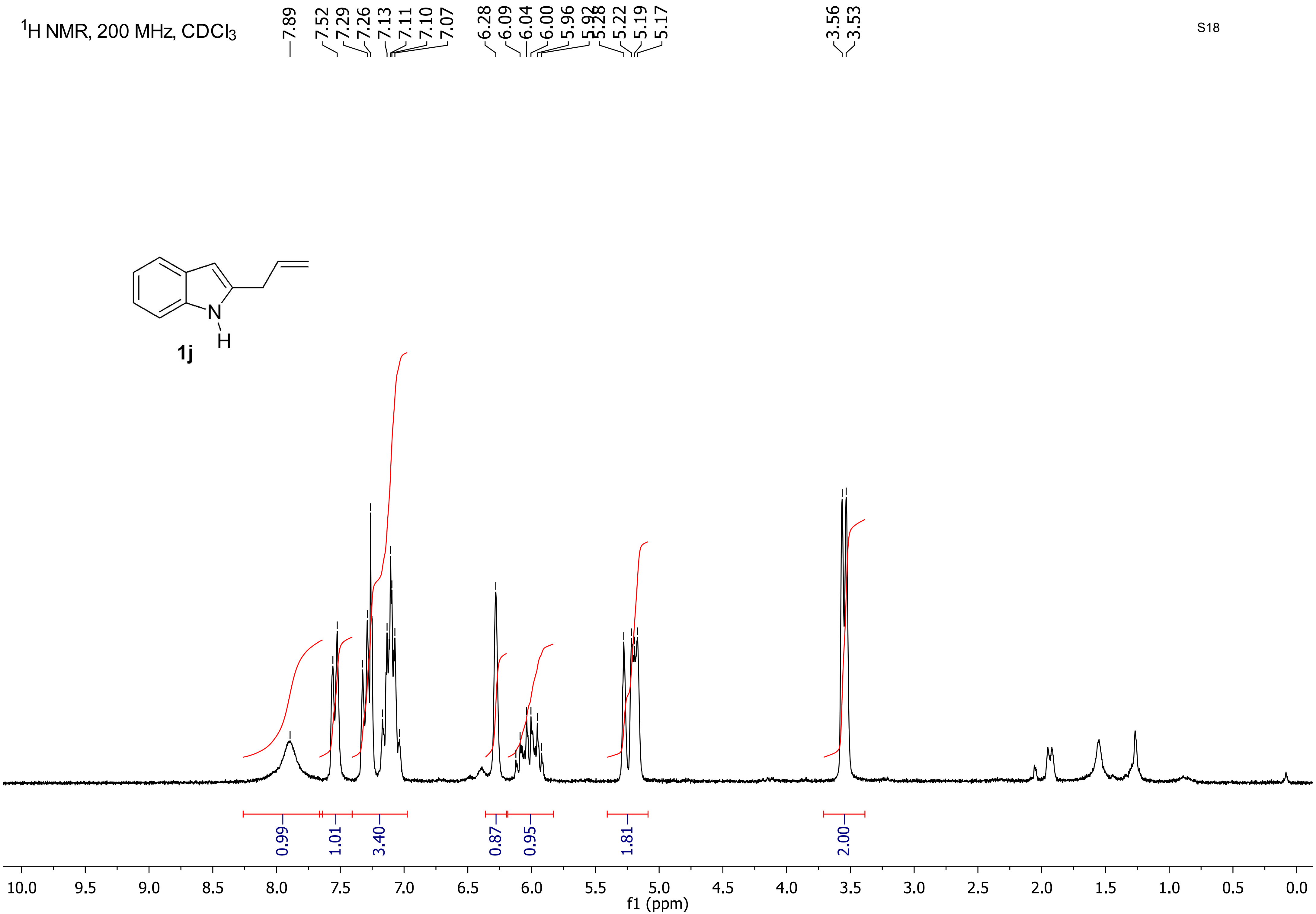
^{1}H NMR, 50 MHz, $CDCl_3$

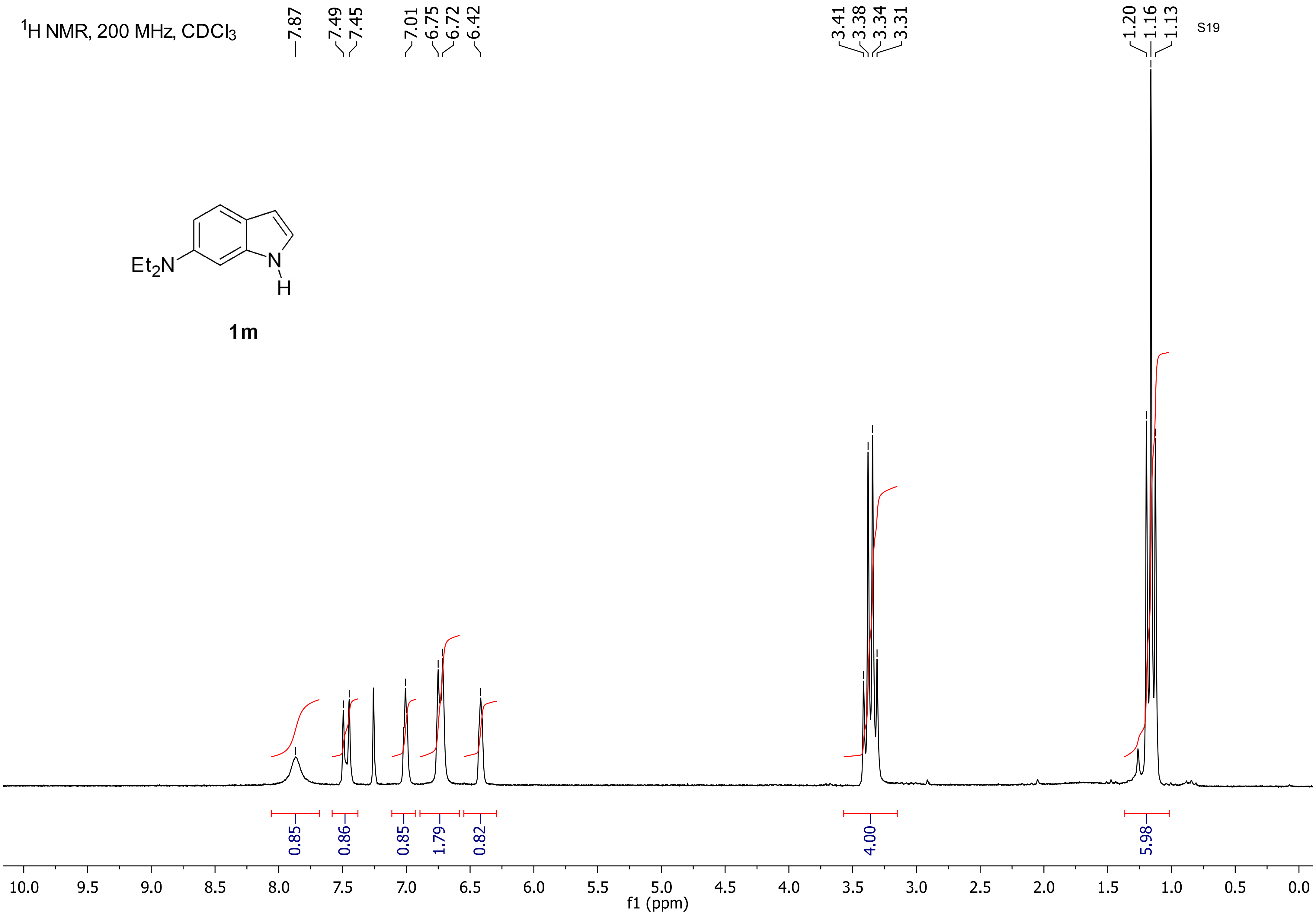


1i

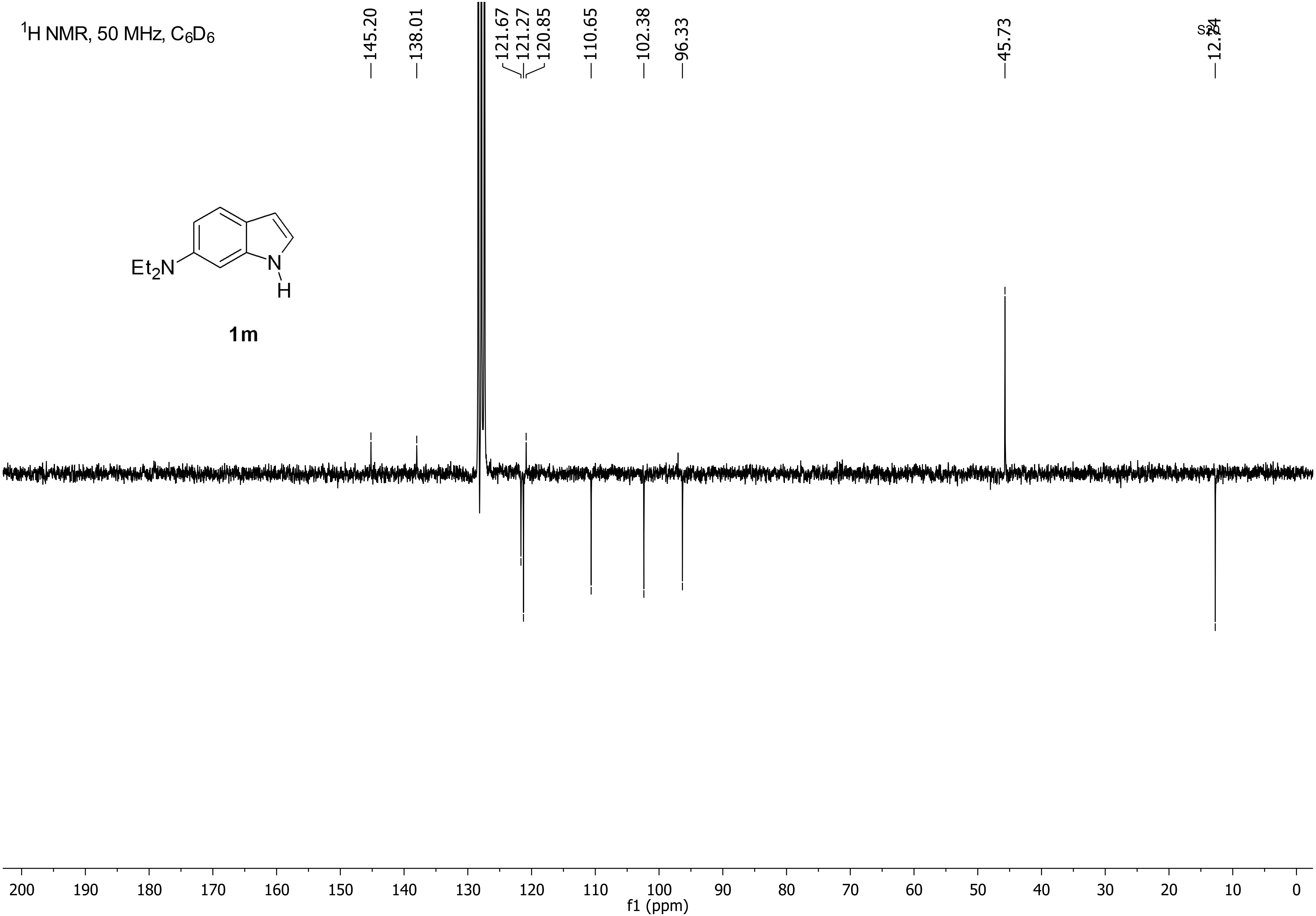


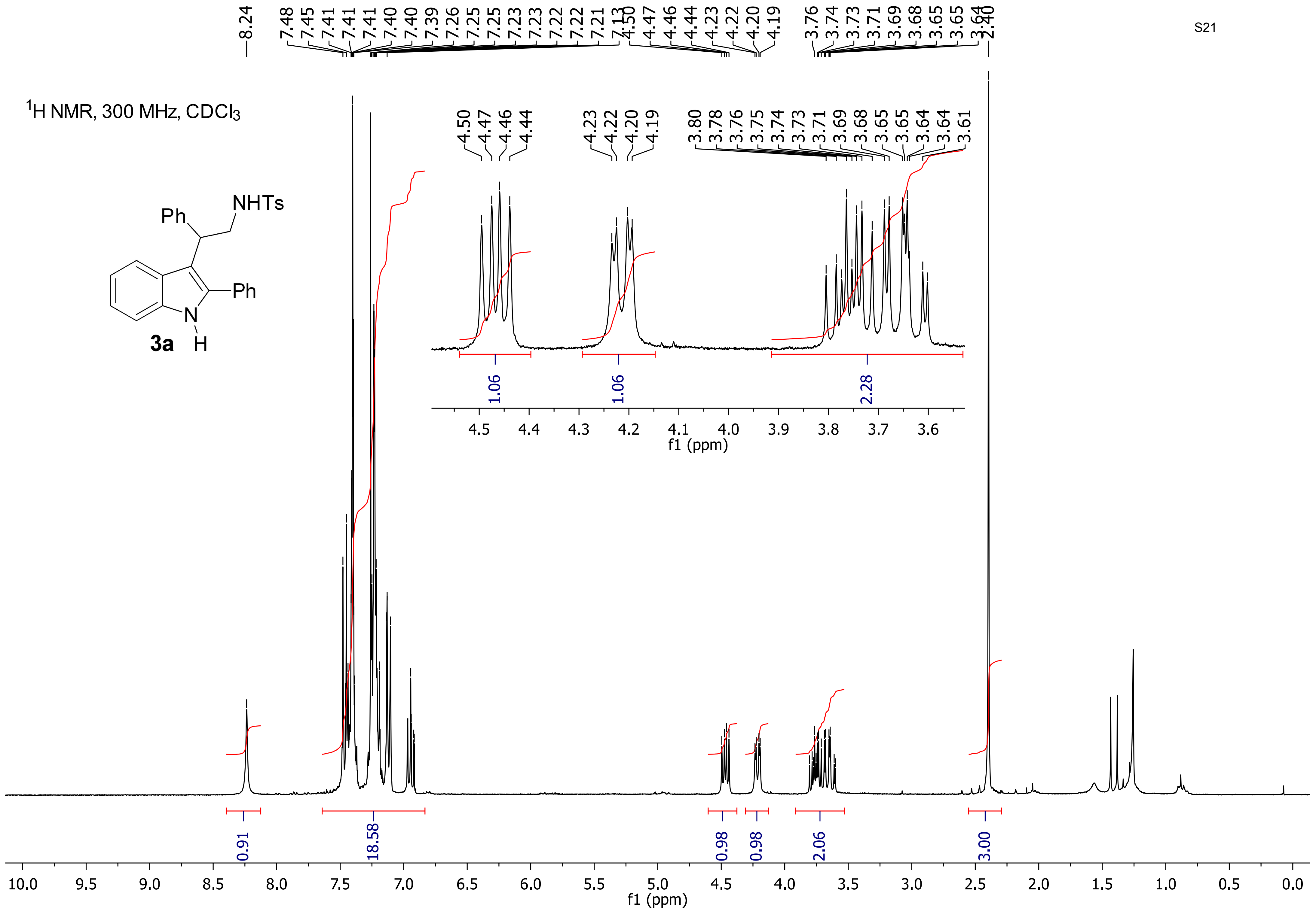
^{1}H NMR, 200 MHz, $CDCl_3$

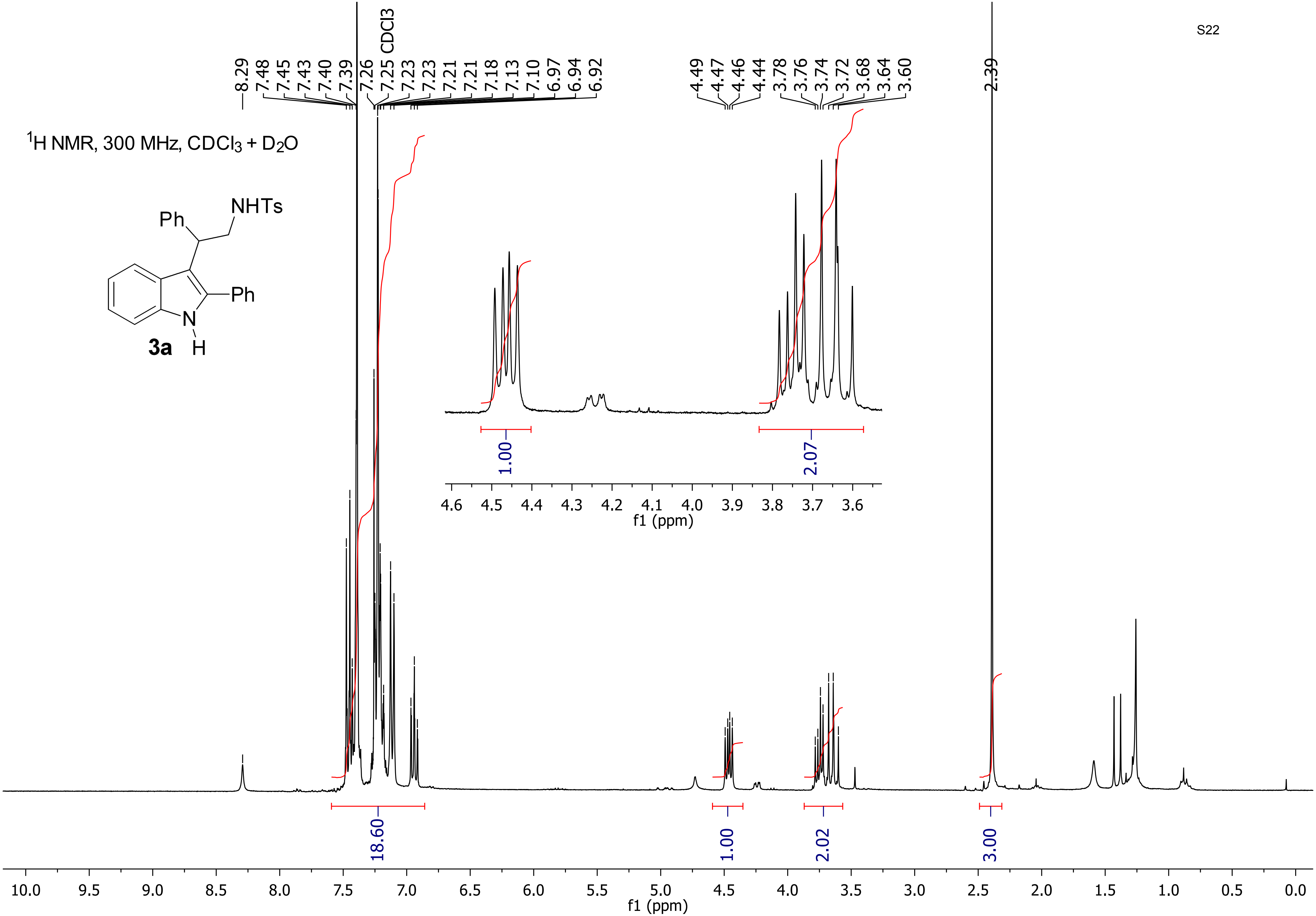



^{1}H NMR, 200 MHz, $CDCl_3$
7.87
7.49
7.45
7.01
6.75
6.72
6.42
3.41
3.38
3.34
3.31
1.20
1.16
1.13
Et_2N
N
H
1m
0.85
0.86
0.85
1.79
0.82
4.00
5.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

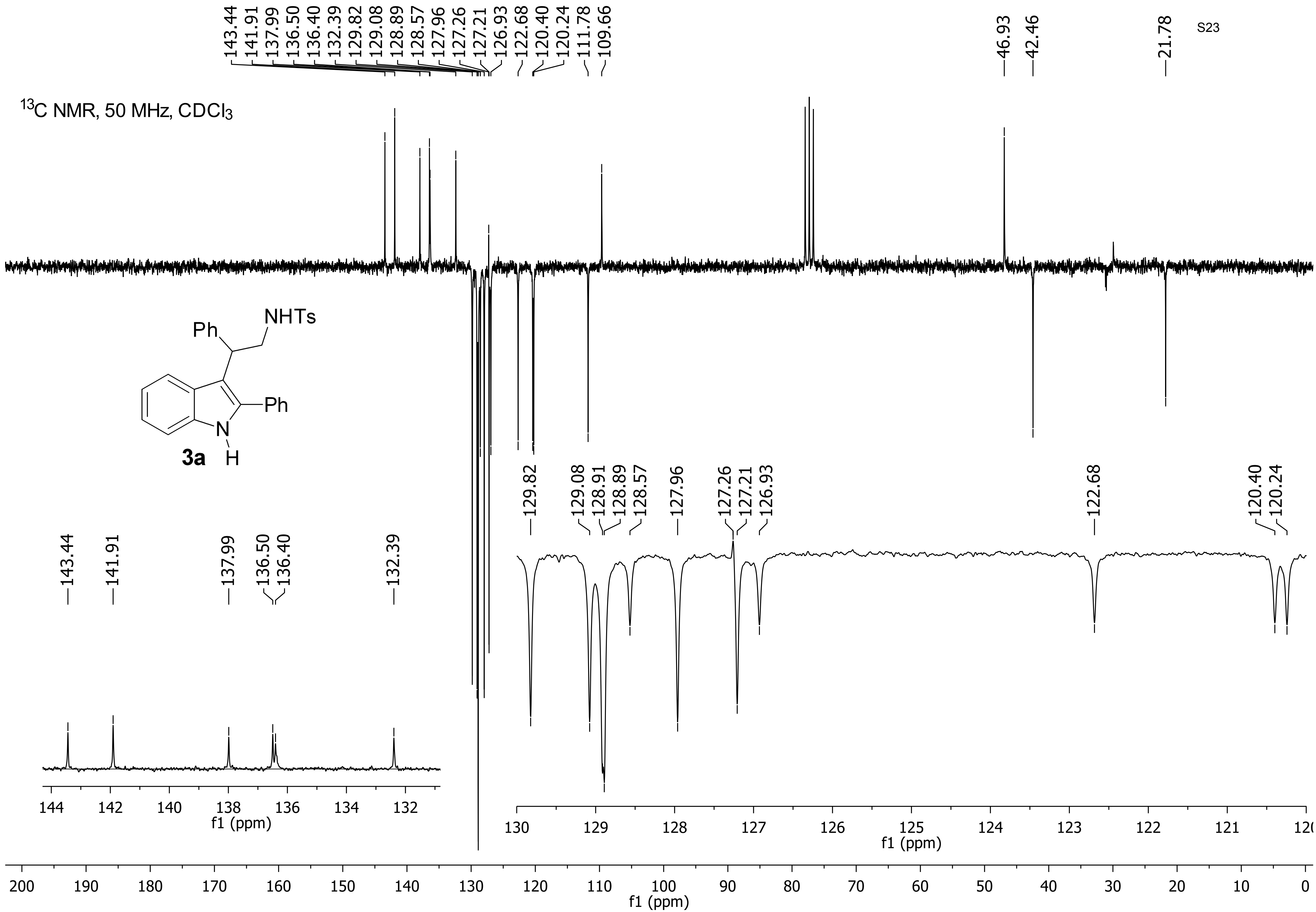
^1H NMR, 50 MHz, C_6D_6



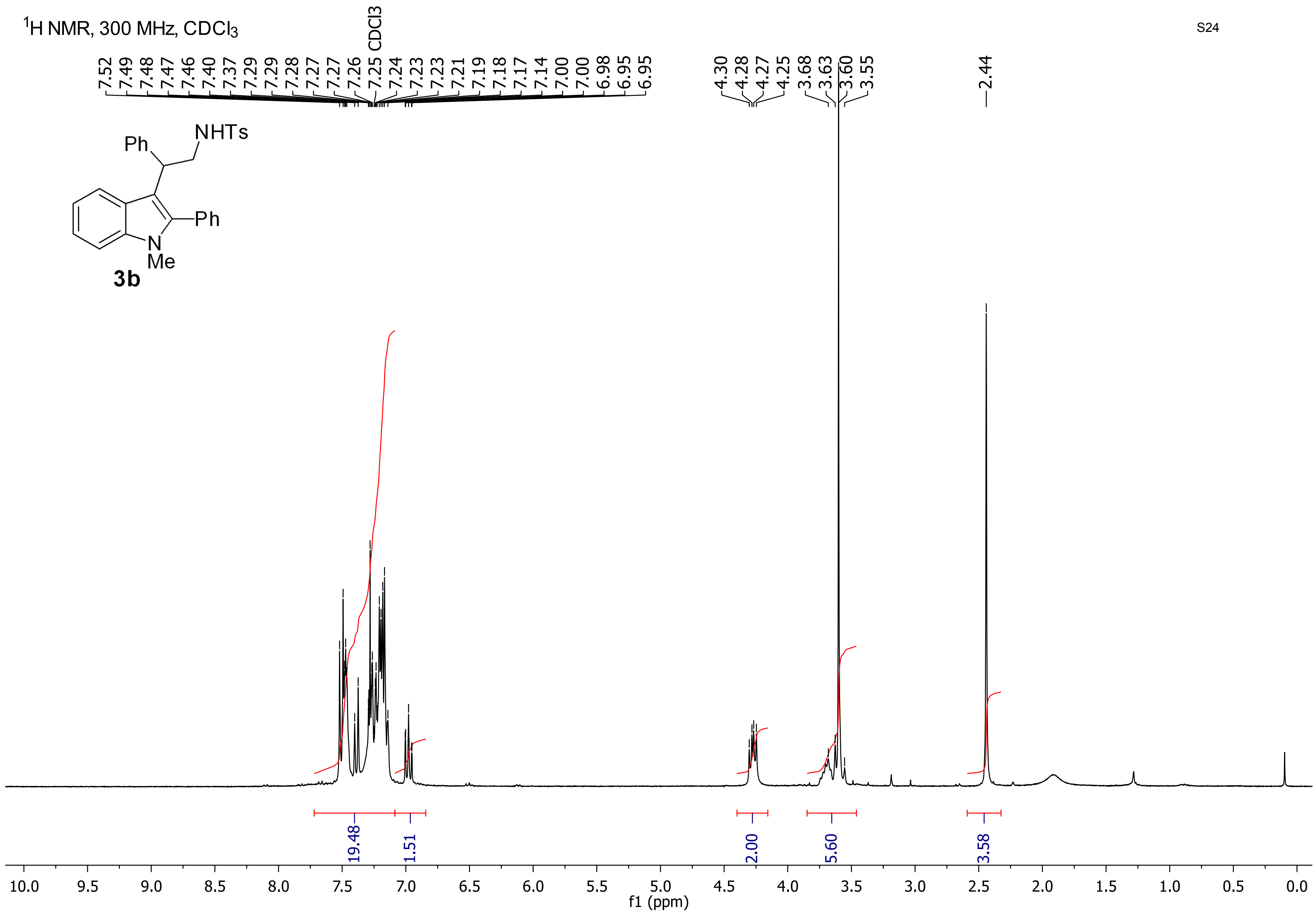

^{1}H NMR, 300 MHz, $CDCl_3$
NHTs
Ph
Ph
N
H
3a
0.91
18.58
0.98
0.98
2.06
3.00
1.06
1.06
2.28
f1 (ppm)
f1 (ppm)



8.29
7.48
7.45
7.43
7.40
7.39
7.26
7.25 CDCl3
7.23
7.23
7.21
7.21
7.18
7.13
7.10
6.97
6.94
6.92
4.49
4.47
4.46
4.44
3.78
3.76
3.74
3.72
3.68
3.64
3.60
2.39
1H NMR, 300 MHz, CDCl3 + D2O
NHTs
Ph
Ph
N
H
3a
1.00
2.07
4.6
4.5
4.4
4.3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
f1 (ppm)
18.60
1.00
2.02
3.00
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
0.0
f1 (ppm)

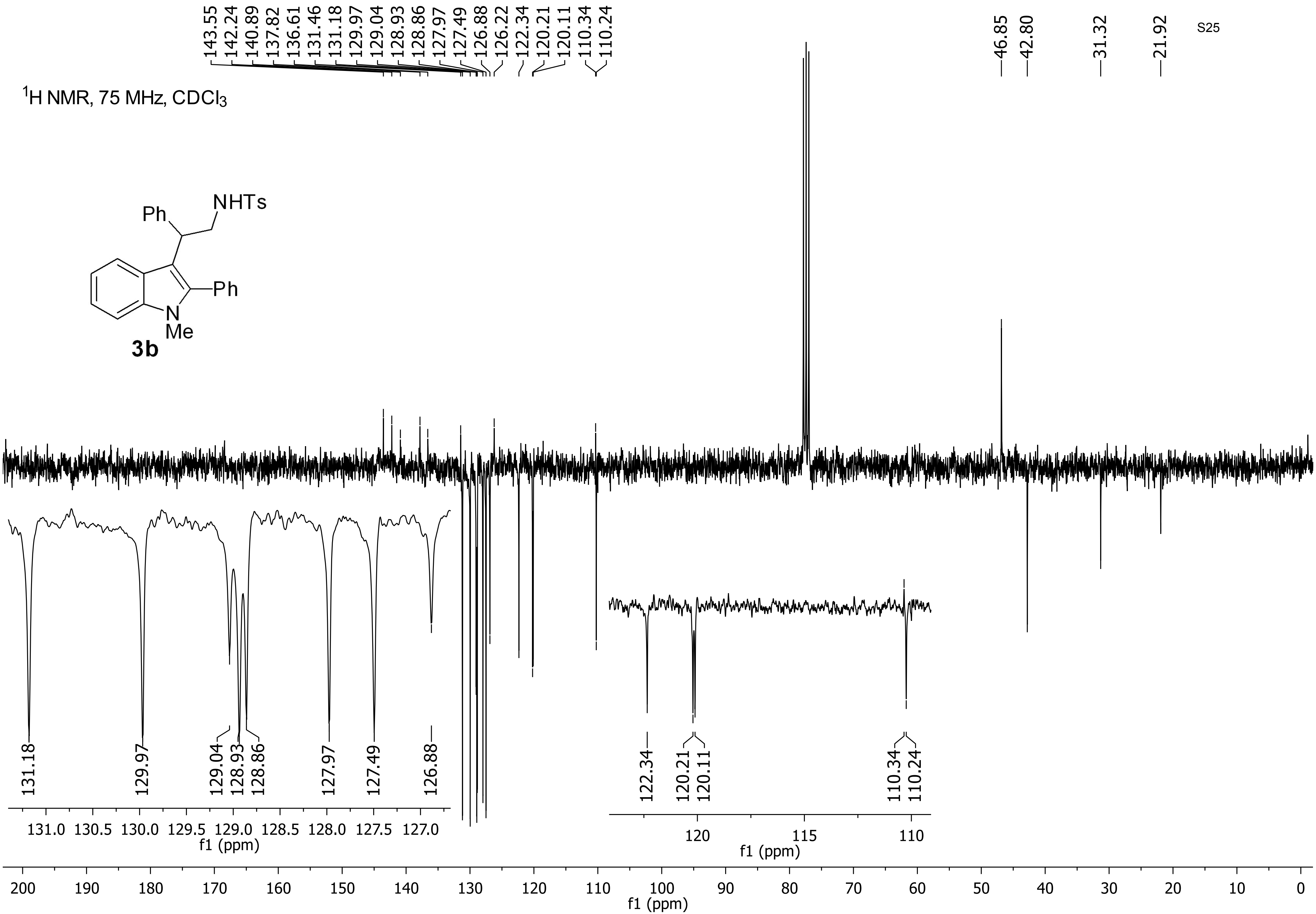


143.44
141.91
137.99
136.50
136.40
132.39
129.82
129.08
128.89
128.57
127.96
127.26
127.21
126.93
122.68
120.40
120.24
111.78
109.66
46.93
42.46
21.78
^{13}C NMR, 50 MHz, CDCl$_3$
NHTs
Ph
Ph
N
H
3a
129.82
129.08
128.91
128.89
128.57
127.96
127.26
127.21
126.93
122.68
120.40
120.24
143.44
141.91
137.99
136.50
136.40
132.39
144
142
140
138
136
134
132
f1 (ppm)
130
129
128
127
126
125
124
123
122
121
120
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

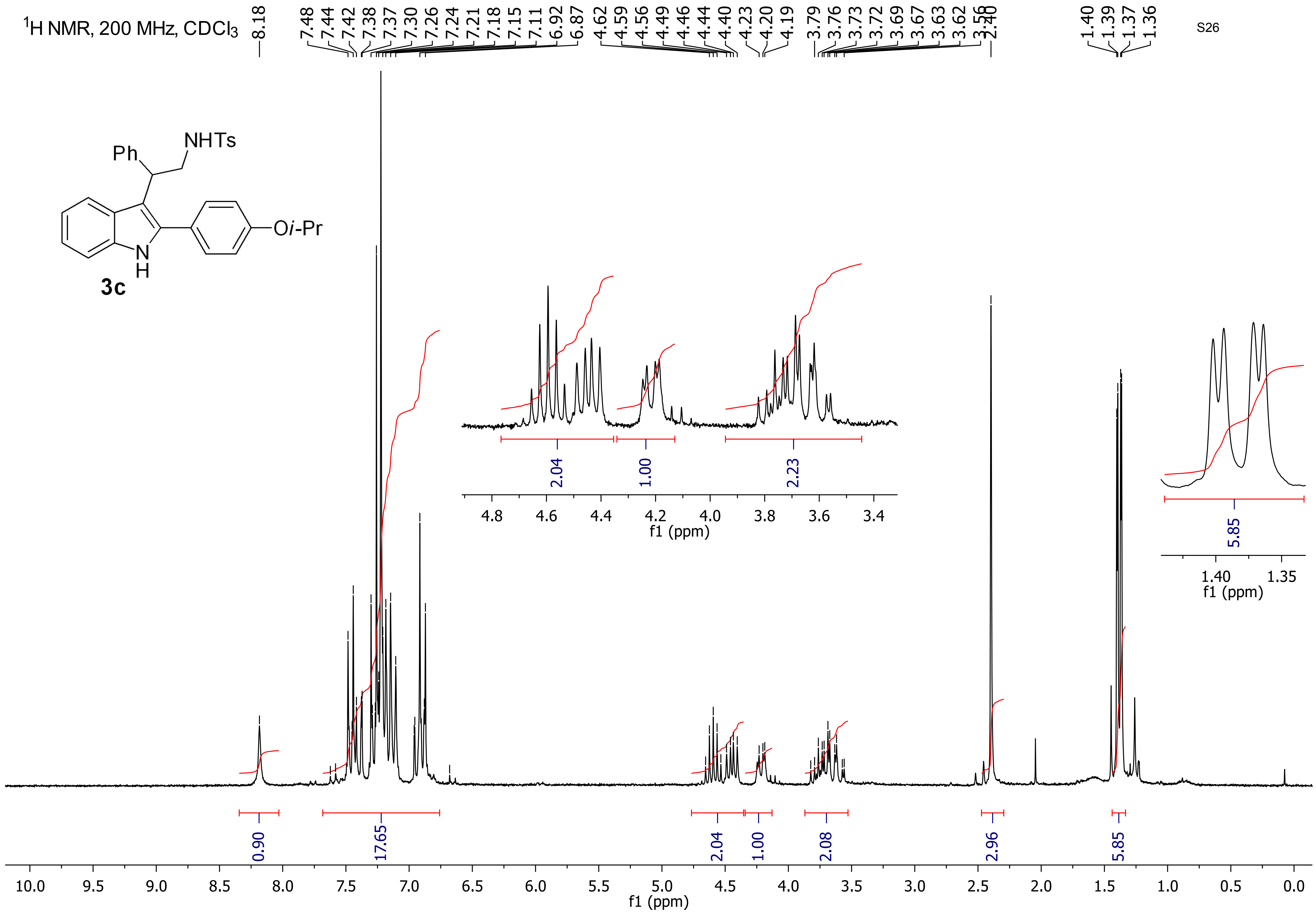


1H NMR, 300 MHz, CDCl3
CDCl3
7.52 7.49 7.48 7.47 7.46 7.40 7.37 7.29 7.29 7.28 7.27 7.27 7.26 7.25 7.24 7.23 7.23 7.21 7.19 7.18 7.17 7.14 7.00 7.00 6.98 6.95 6.95
4.30 4.28 4.27 4.25 3.68 3.63 3.60 3.55
2.44
NHTs
Ph
Ph
N
Me
3b
19.48
1.51
2.00
5.60
3.58
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

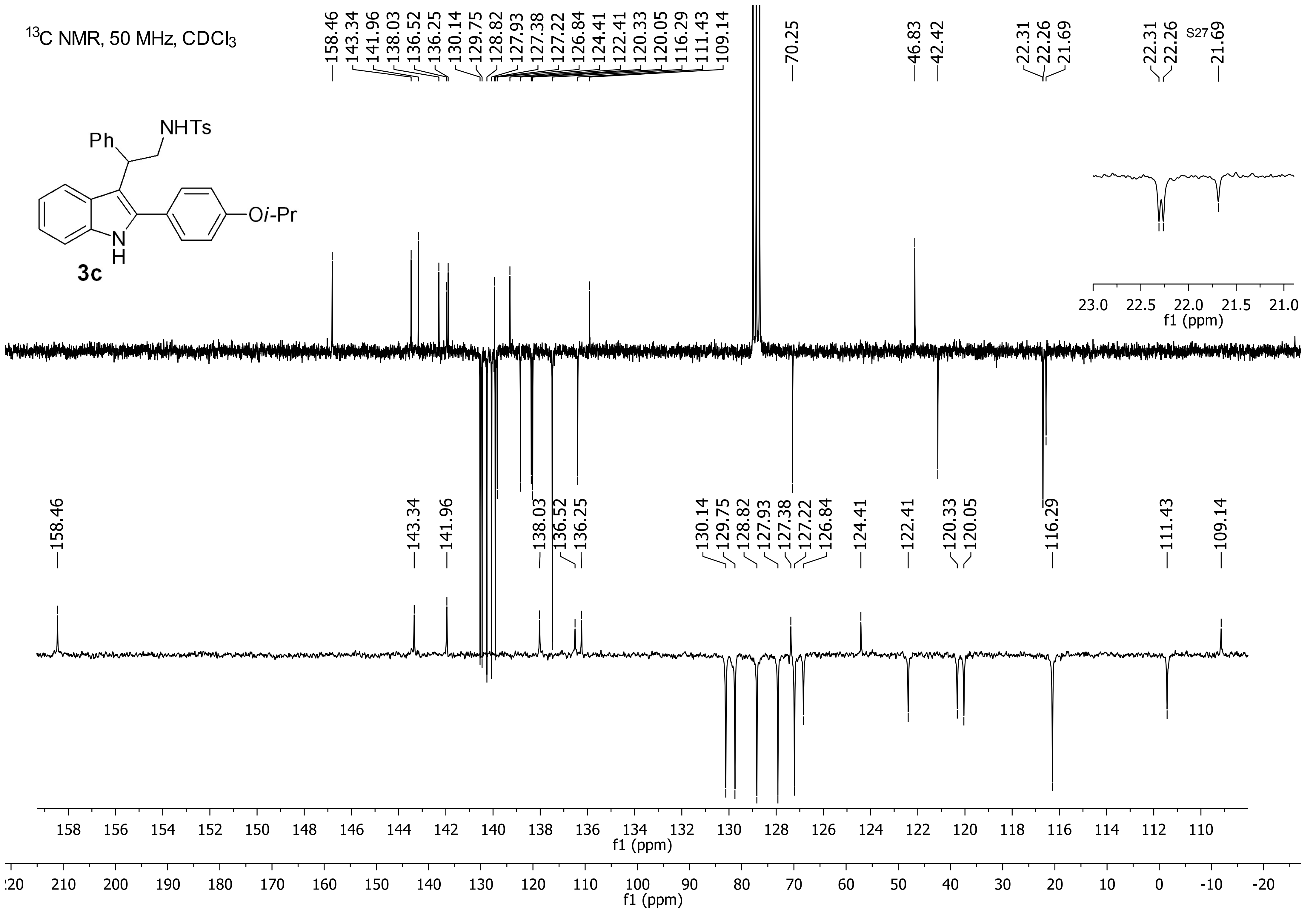
[1]H NMR, 75 MHz, $CDCl_3$



3b

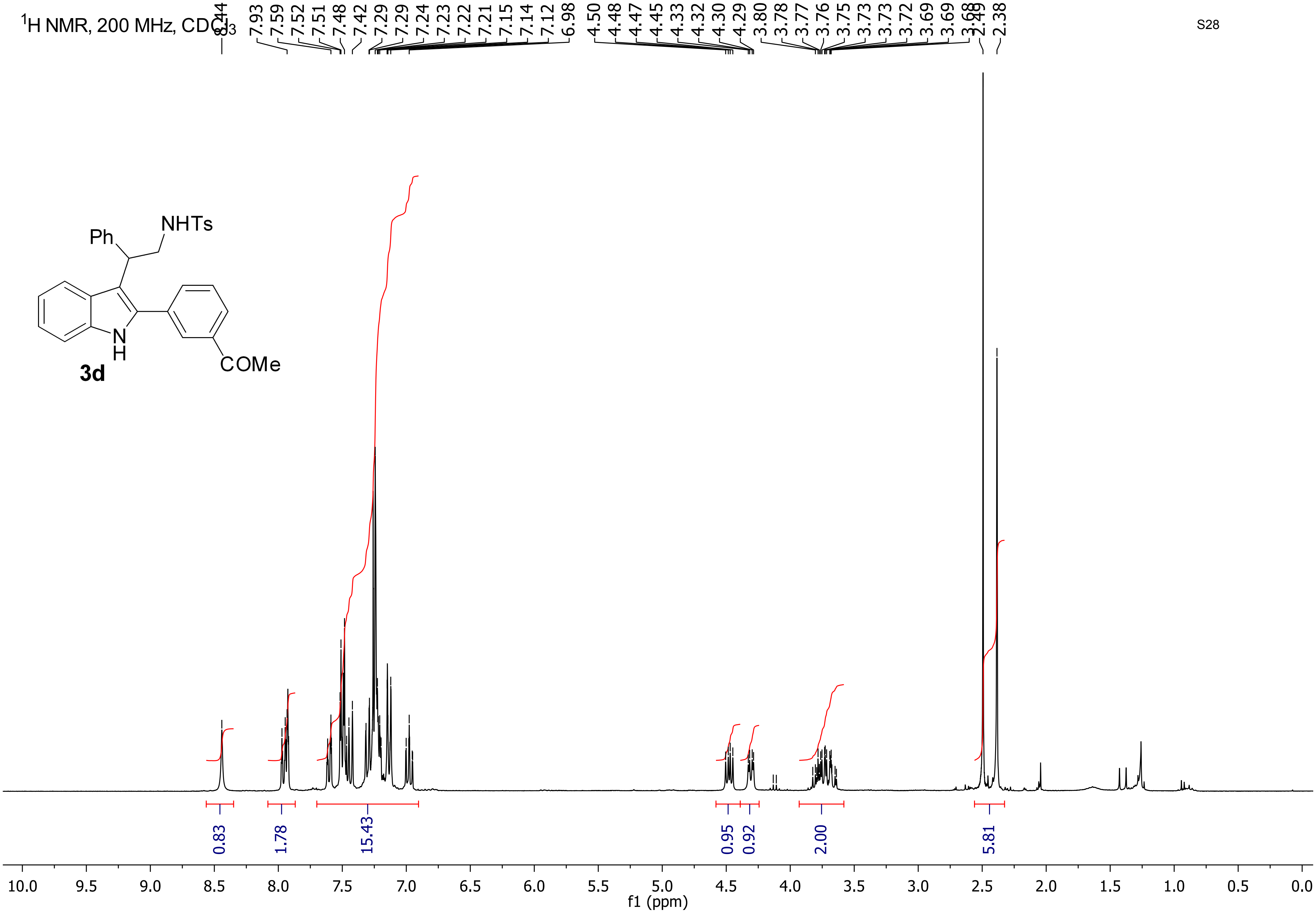


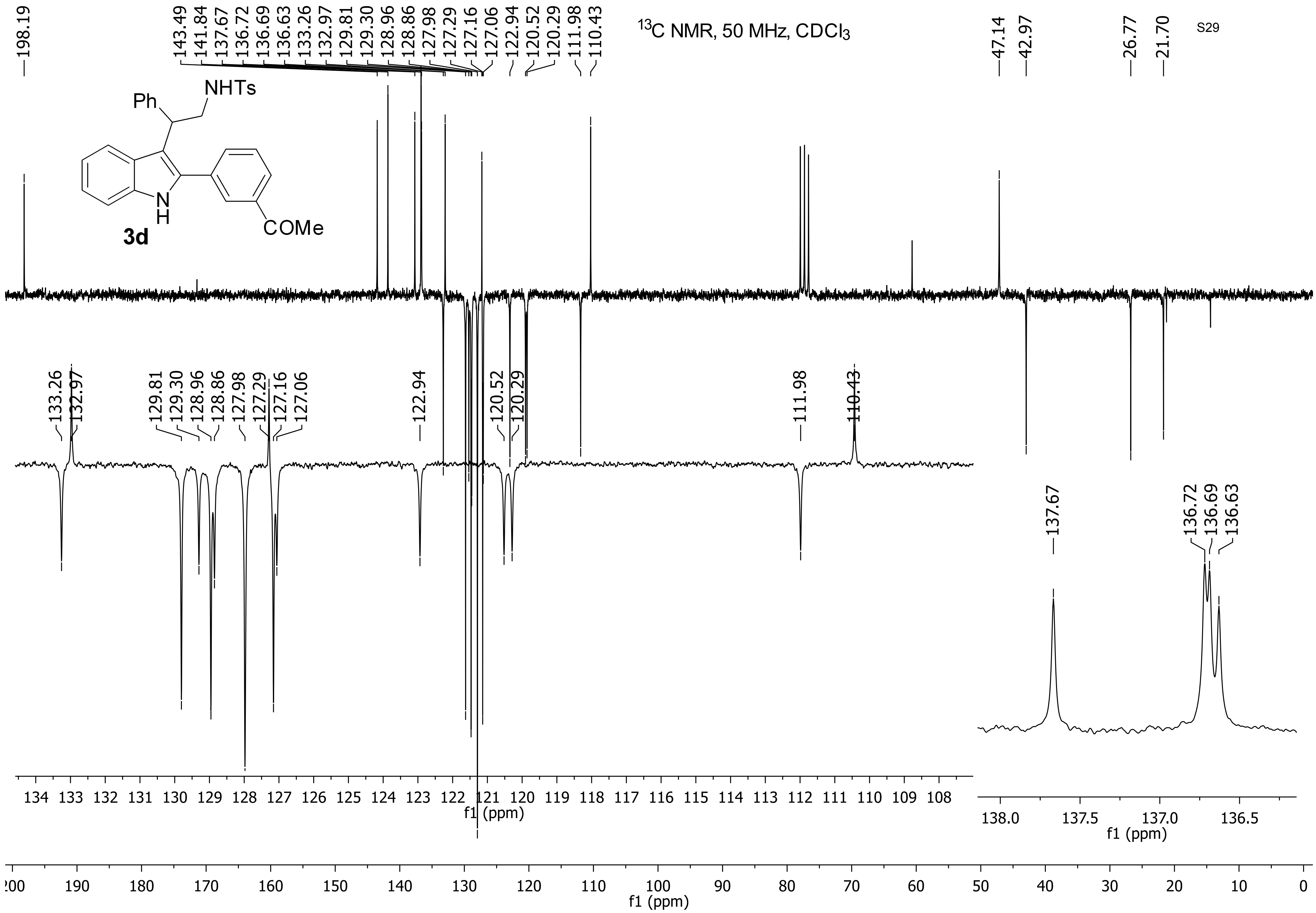
^{1}H NMR, 200 MHz, $CDCl_3$
S26
8.18
7.48
7.44
7.42
7.38
7.37
7.30
7.26
7.24
7.21
7.18
7.15
7.11
6.92
6.87
4.62
4.59
4.56
4.49
4.46
4.44
4.40
4.23
4.20
4.19
3.79
3.76
3.73
3.72
3.69
3.67
3.63
3.62
3.56
2.40
1.40
1.39
1.37
1.36
0.90
17.65
2.04
1.00
2.08
2.96
5.85
2.23
f1 (ppm)



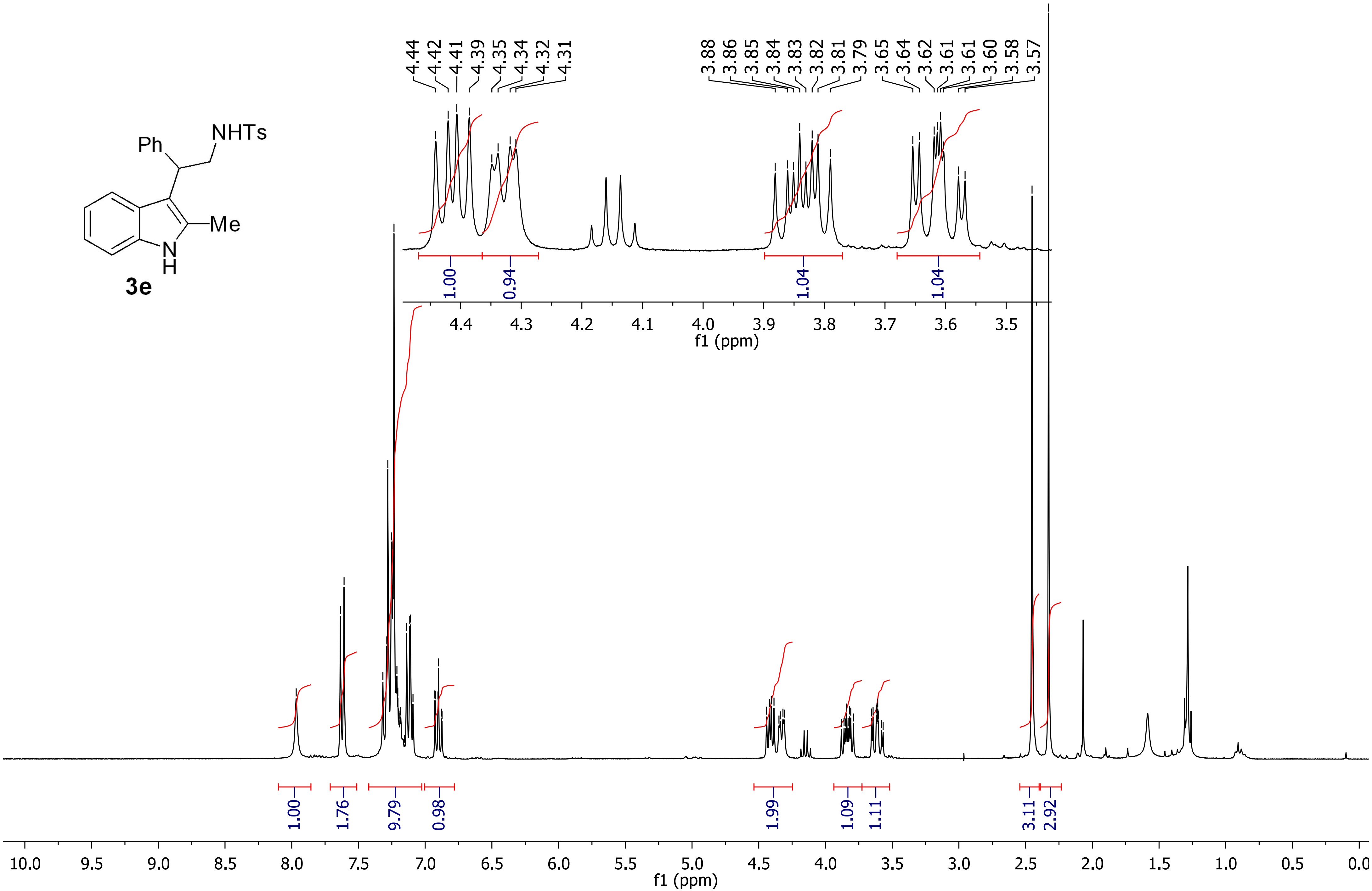
^{13}C NMR, 50 MHz, CDCl$_3$
NHTs
Ph
O*i*-Pr
N
H
3c
158.46 143.34 141.96 138.03 136.52 136.25 130.14 129.75 128.82 127.93 127.38 127.22 126.84 124.41 122.41 120.33 120.05 116.29 111.43 109.14
70.25
46.83
42.42
22.31 22.26 21.69
f1 (ppm)

^{1}H NMR, 200 MHz, $CDCl_3$

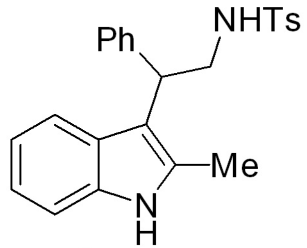



13C NMR, 50 MHz, CDCl3
198.19
143.49
141.84
137.67
136.72
136.69
136.63
133.26
132.97
129.81
129.30
128.96
128.86
127.98
127.29
127.16
127.06
122.94
120.52
120.29
111.98
110.43
47.14
42.97
26.77
21.70
Ph
NHTs
N
H
COMe
3d
f1 (ppm)

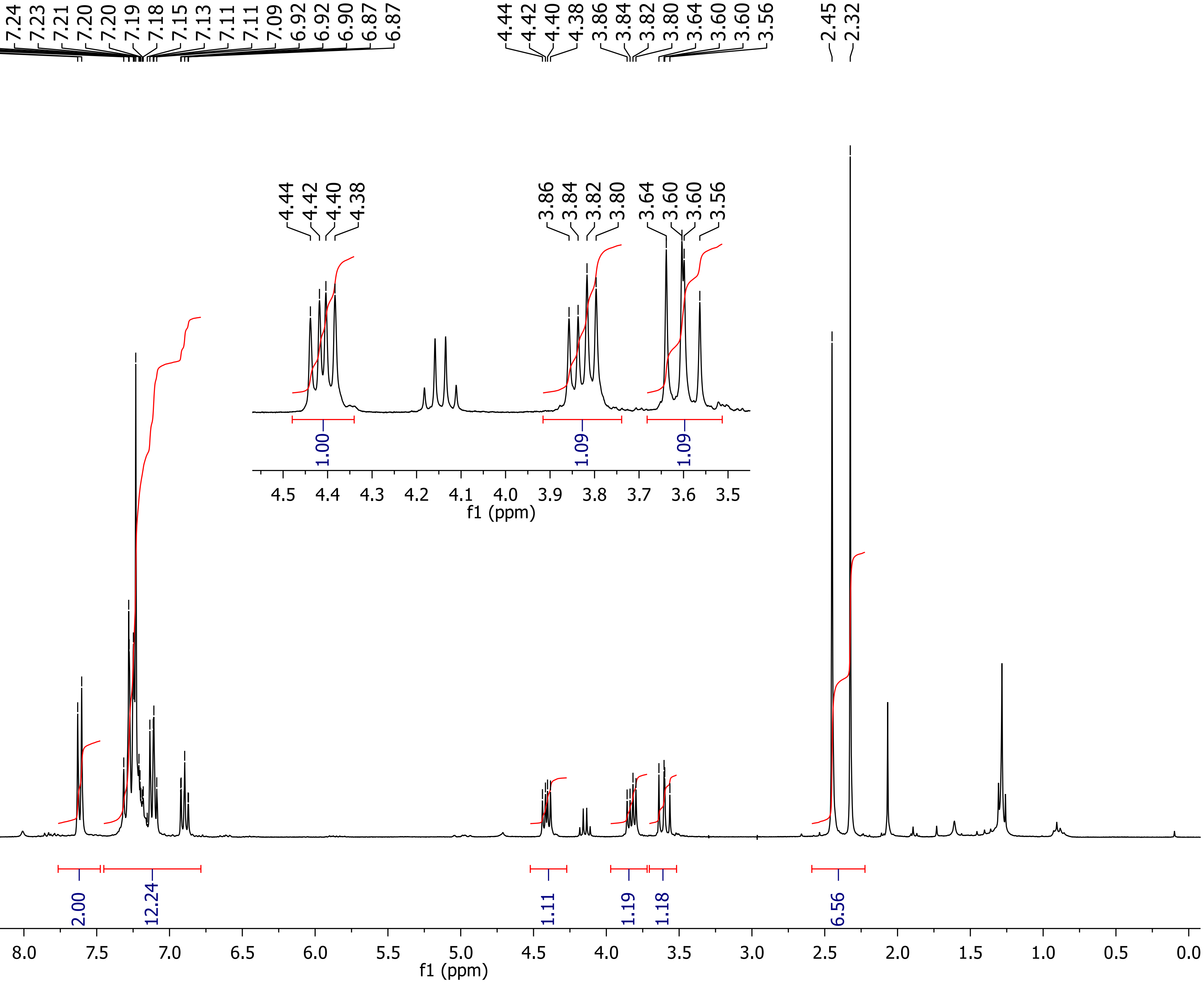
^{1}H NMR, 300 MHz, $CDCl_3$



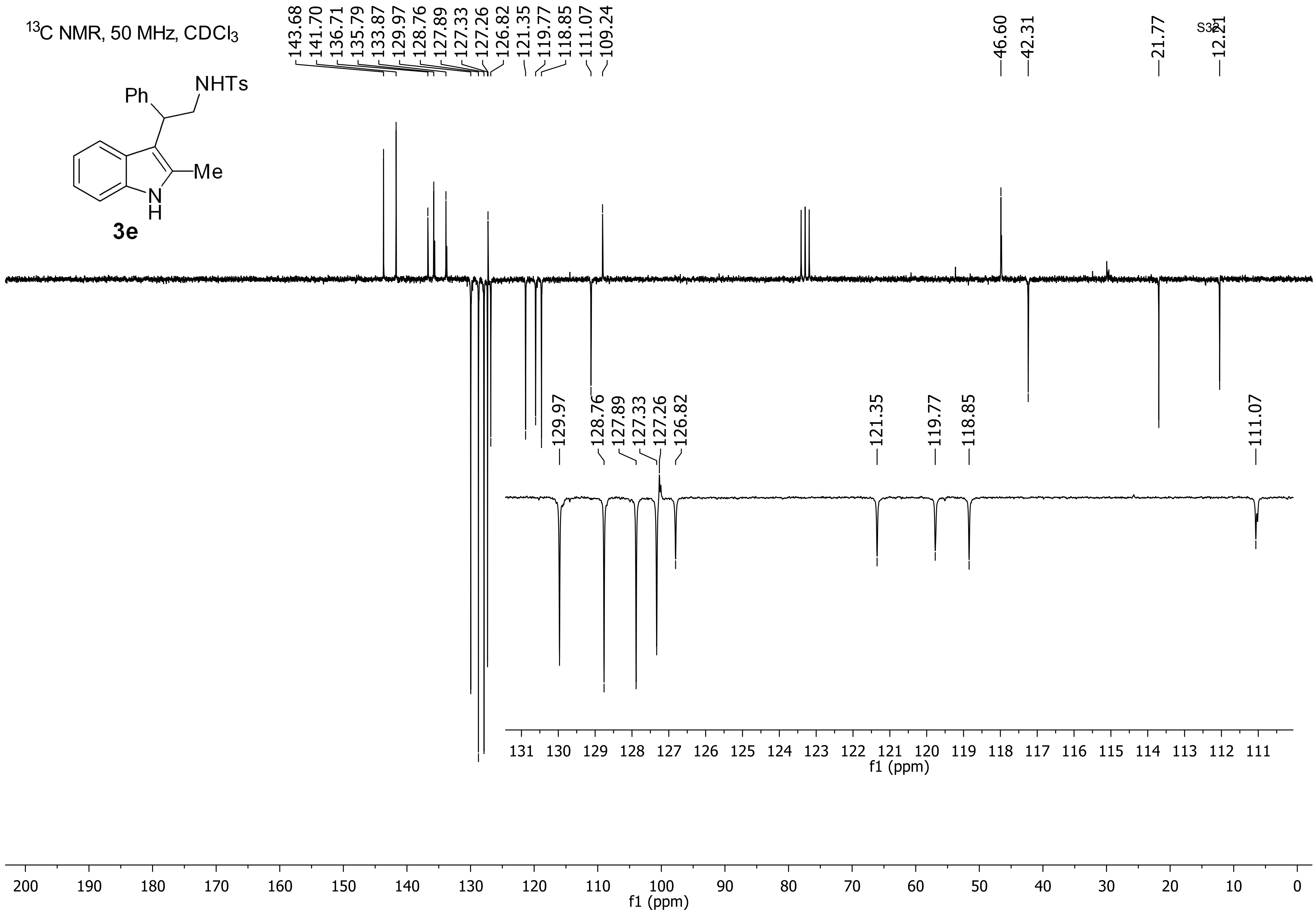
^{1}H NMR, 300 MHz, $CDCl_3$ + D_2O



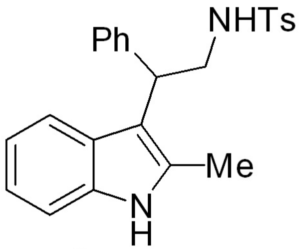
3e



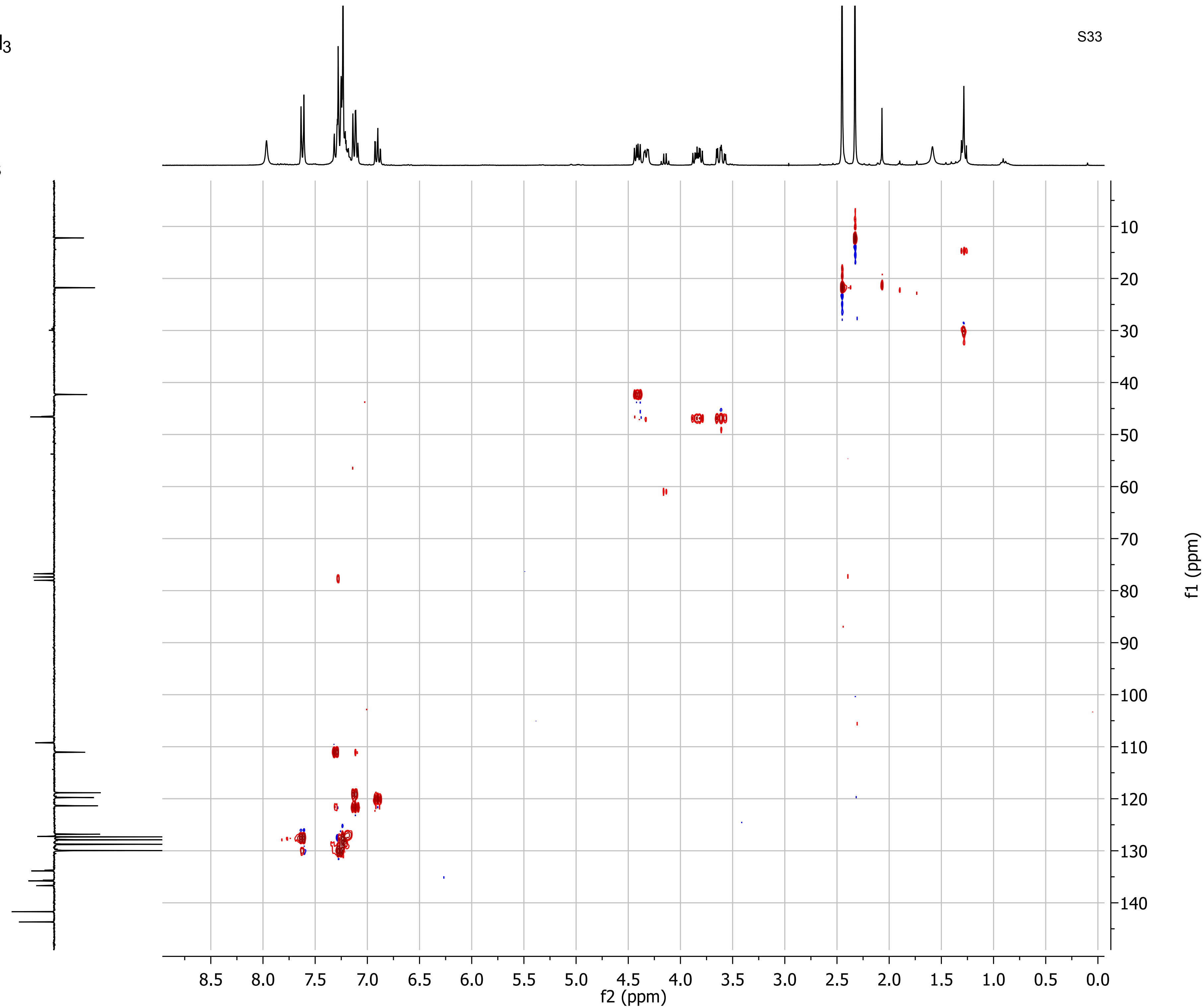
^{13}C NMR, 50 MHz, $CDCl_3$



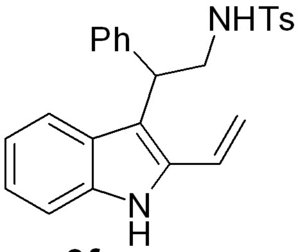
HSQC, 300 MHz, $CDCl_3$



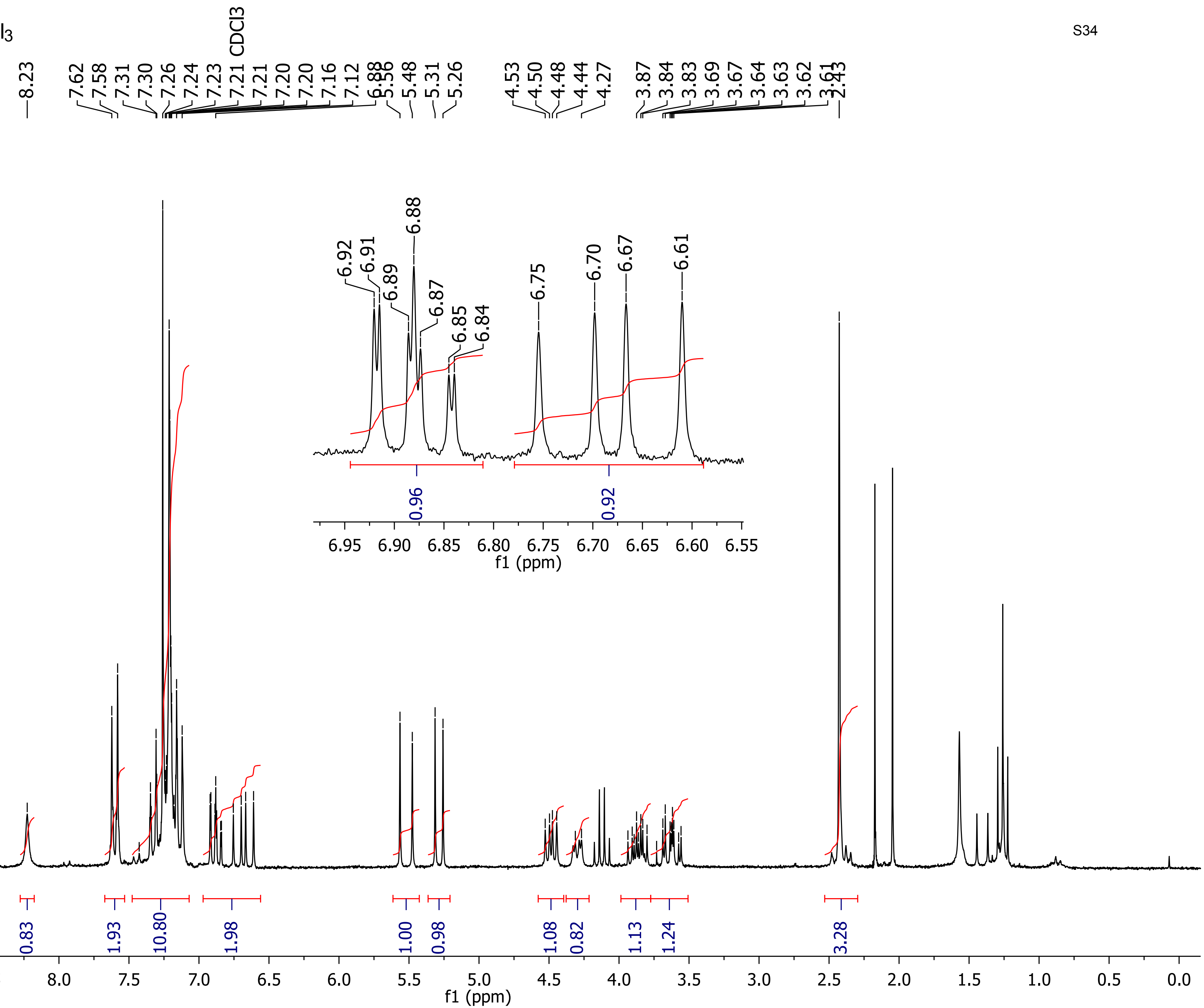
3e



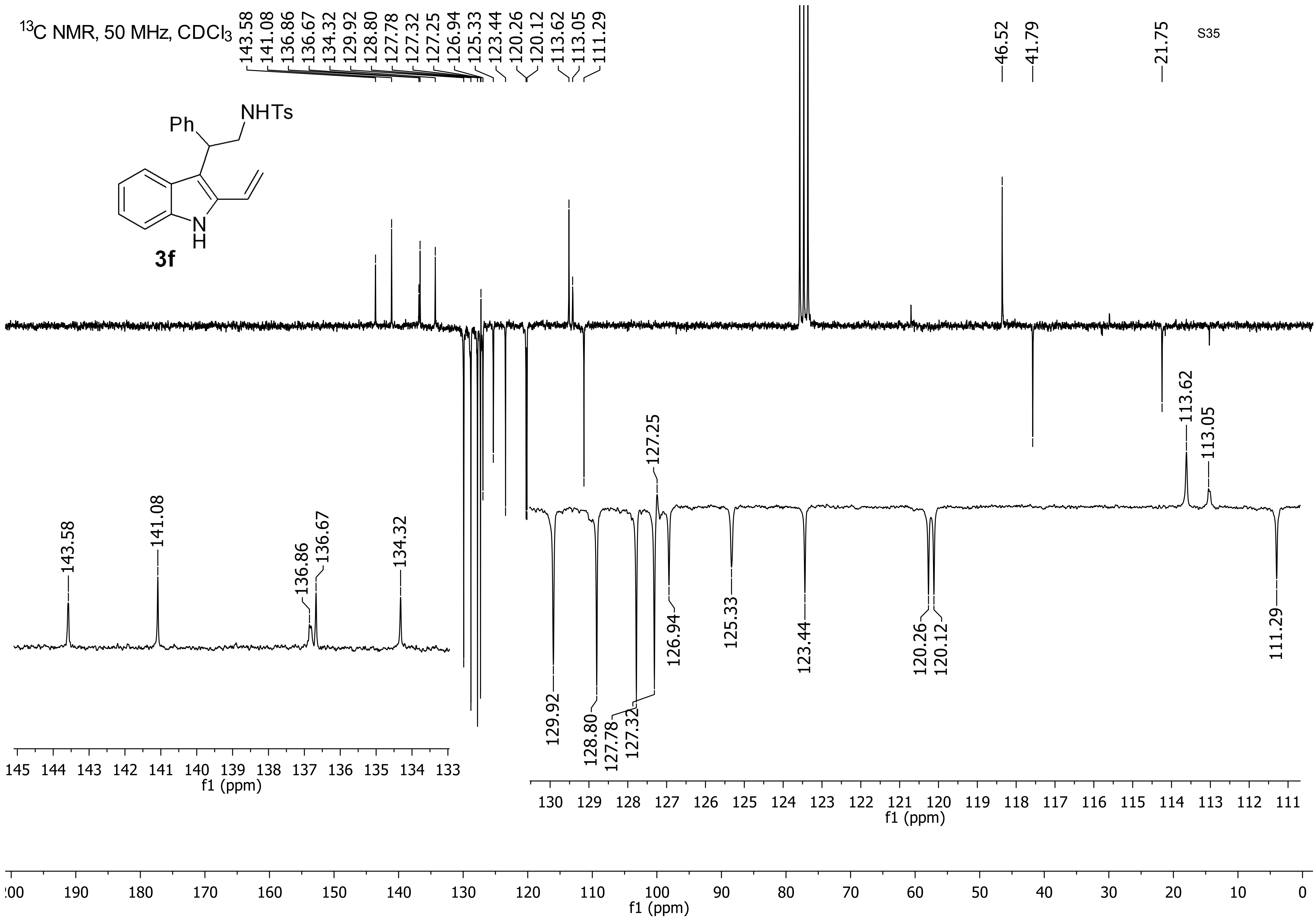
^{1}H NMR, 200 MHz, $CDCl_3$



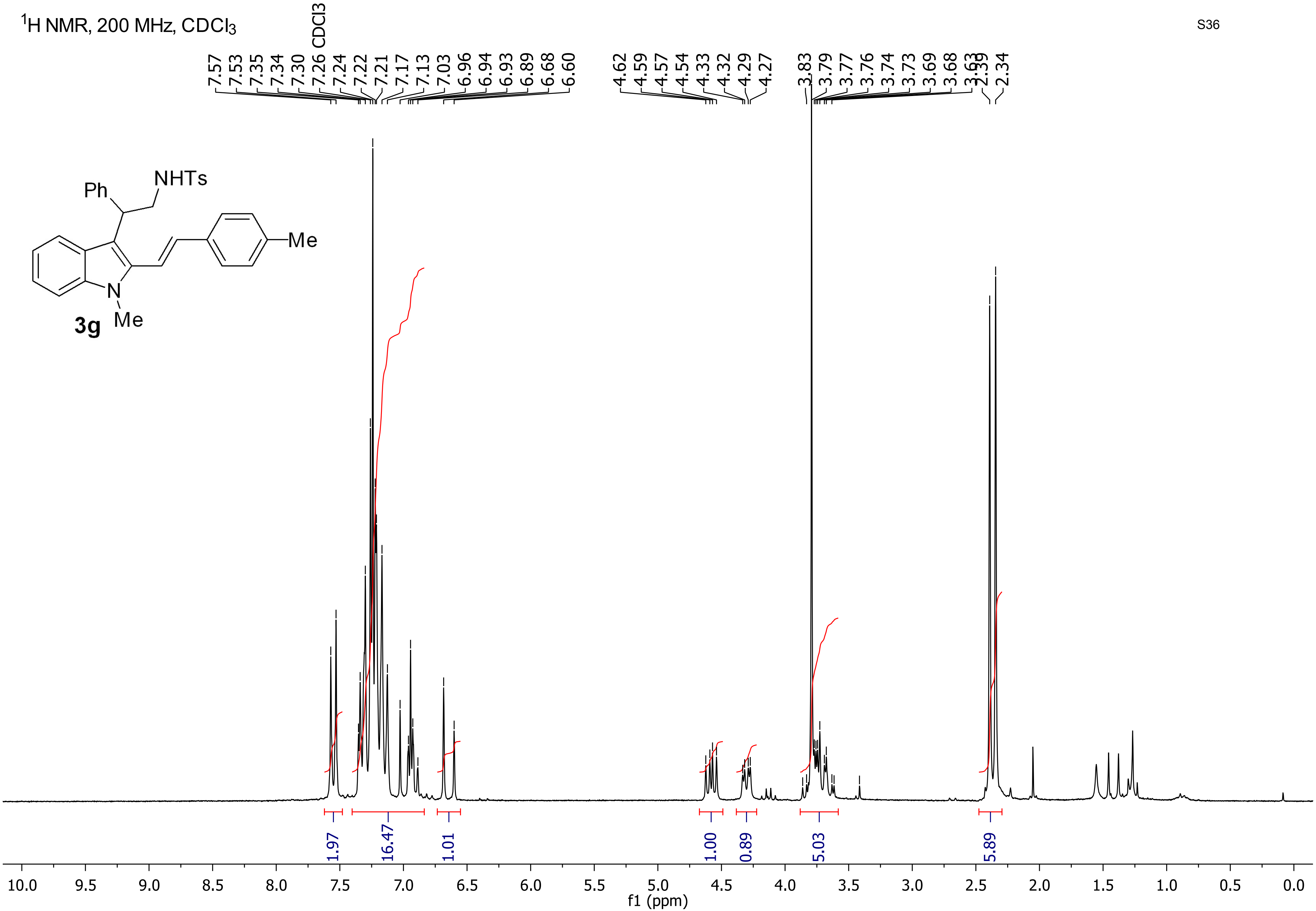
3f



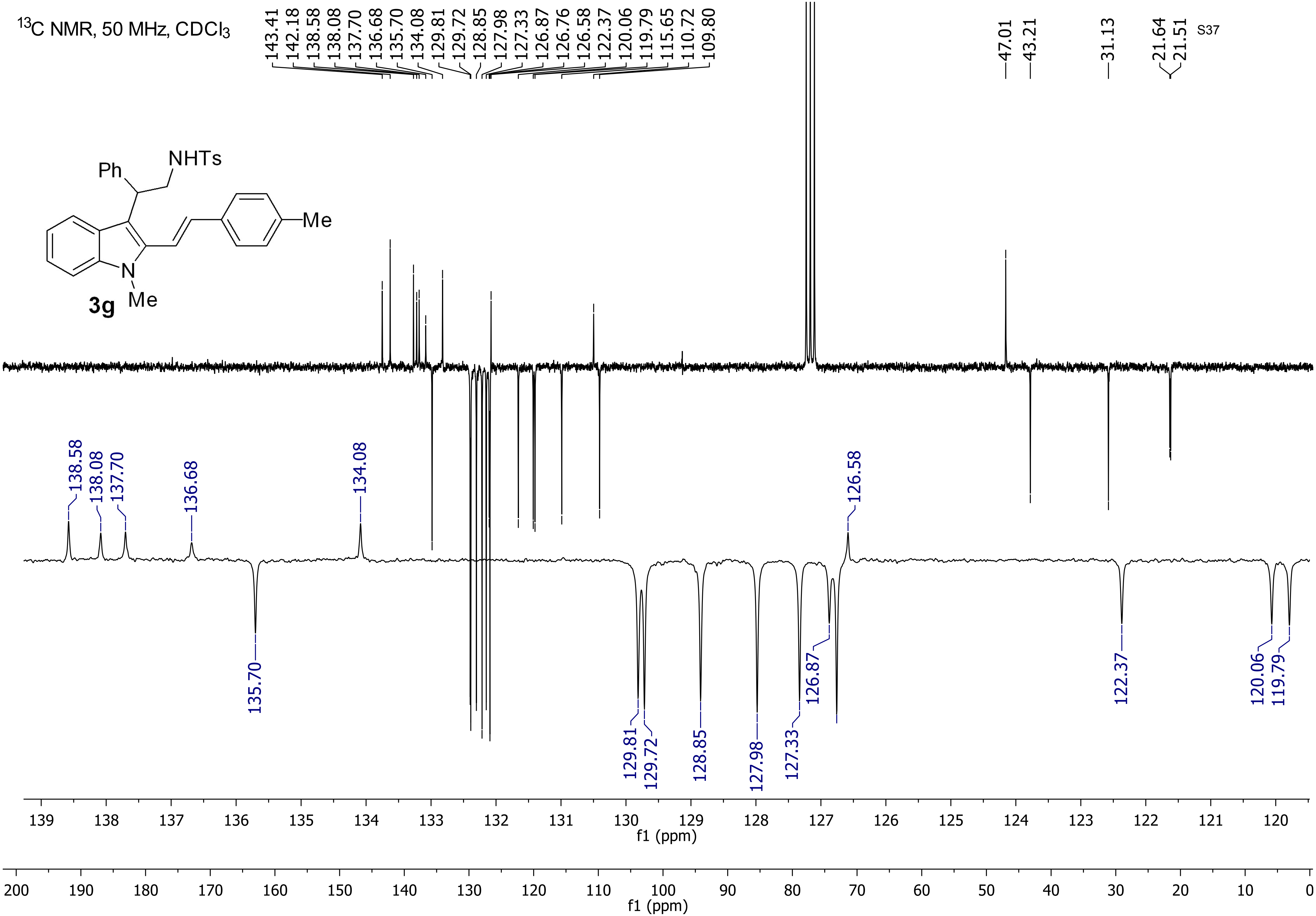
^{13}C NMR, 50 MHz, $CDCl_3$



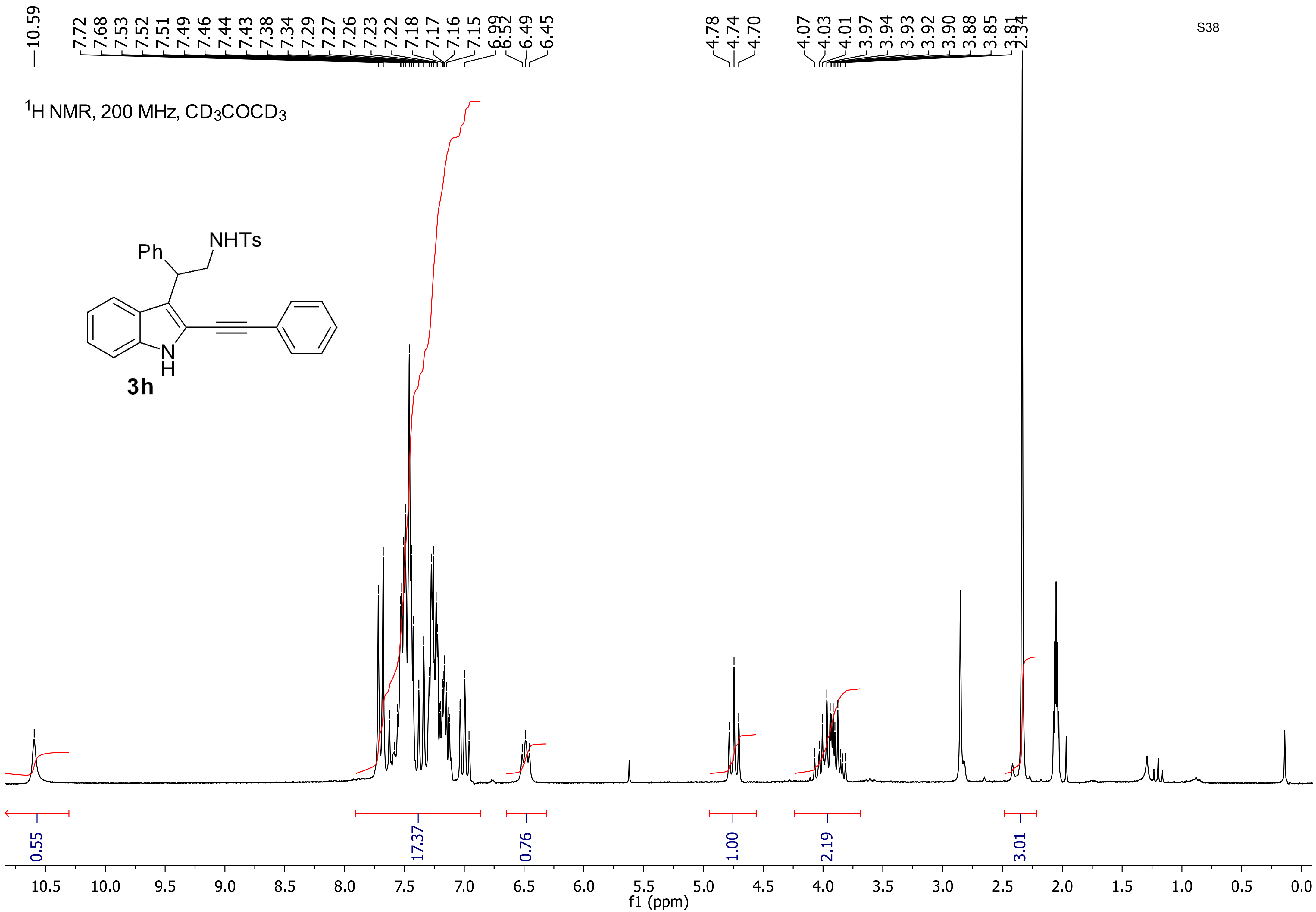
^{1}H NMR, 200 MHz, $CDCl_3$



^{13}C NMR, 50 MHz, $CDCl_3$

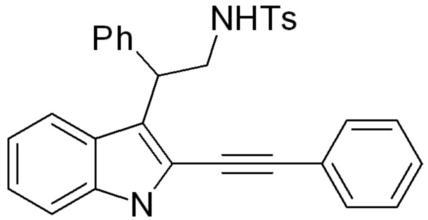


3g

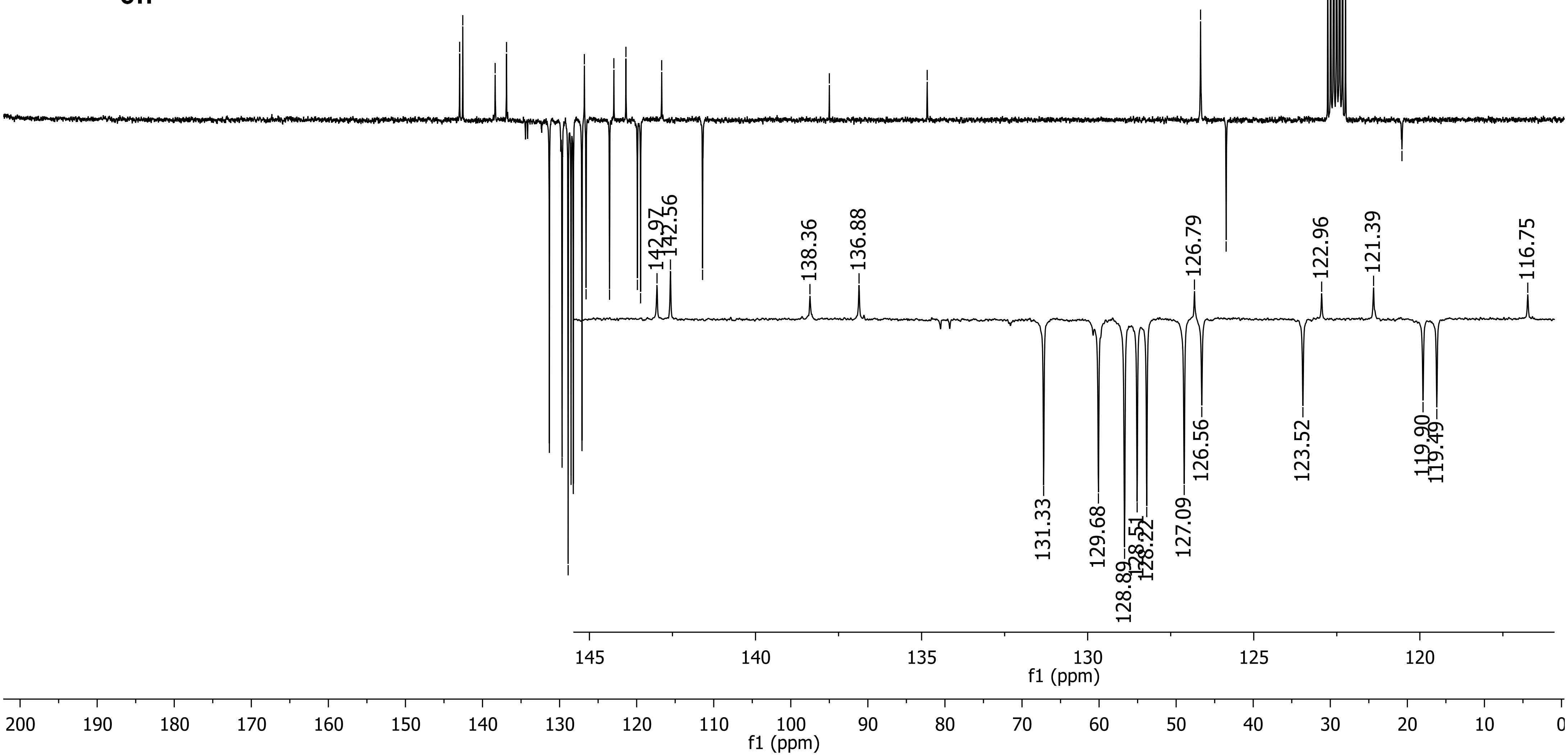


1H NMR, 200 MHz, CD3COCD3
NHTs
Ph
N
H
3h
10.59
7.72 7.68 7.53 7.52 7.51 7.49 7.46 7.44 7.43 7.38 7.34 7.29 7.27 7.26 7.23 7.22 7.18 7.17 7.16 7.15 6.99 6.52 6.49 6.45
4.78 4.74 4.70
4.07 4.03 4.01 3.97 3.94 3.93 3.92 3.90 3.88 3.85 3.81 2.34
0.55
17.37
0.76
1.00
2.19
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 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 0.0
f1 (ppm)

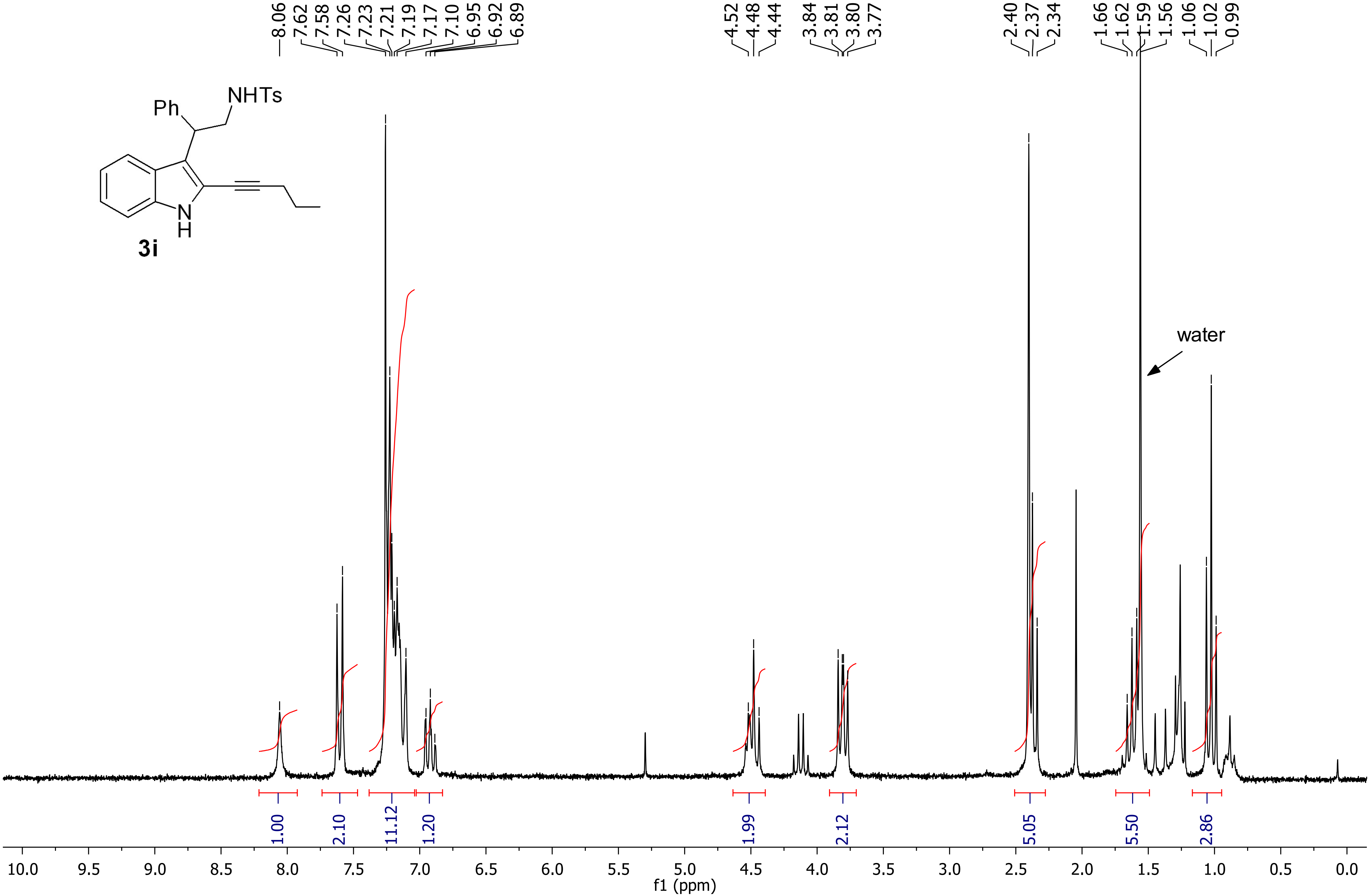
^{13}C NMR, 50 MHz, CD_3COCD_3



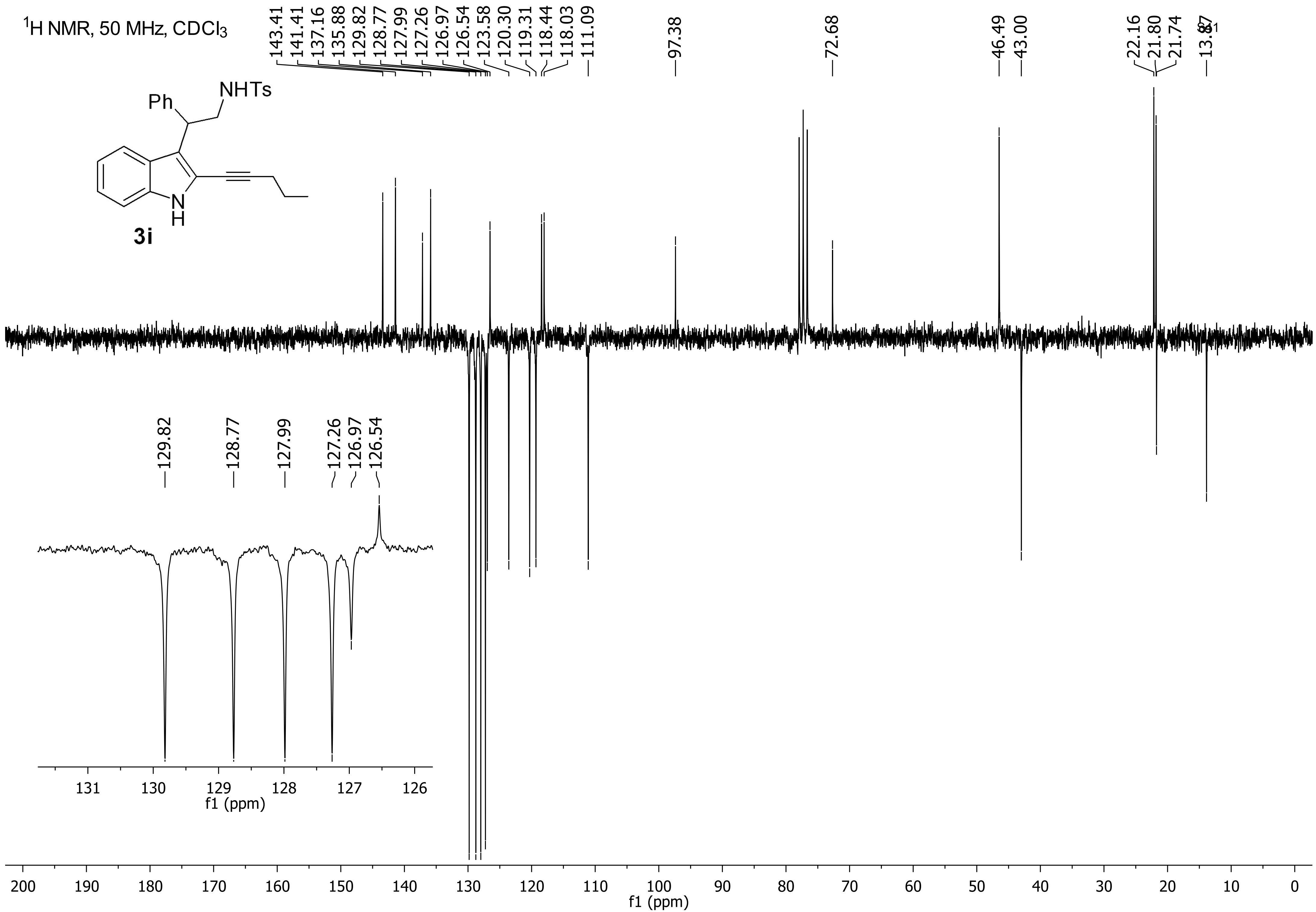
3h



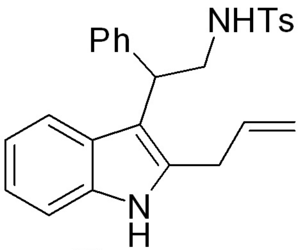
^{1}H NMR, 200 MHz, $CDCl_3$



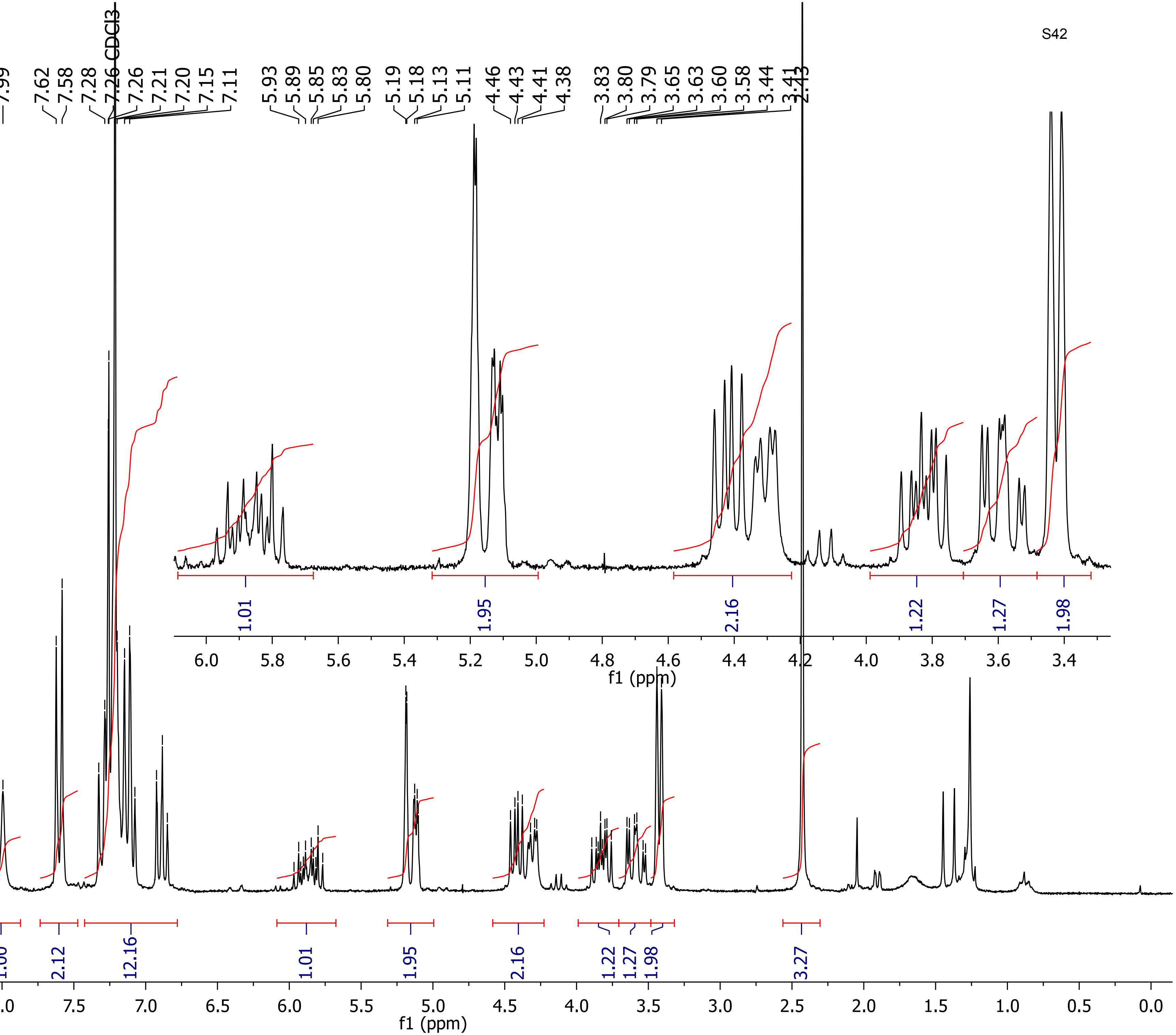
^{1}H NMR, 50 MHz, $CDCl_3$

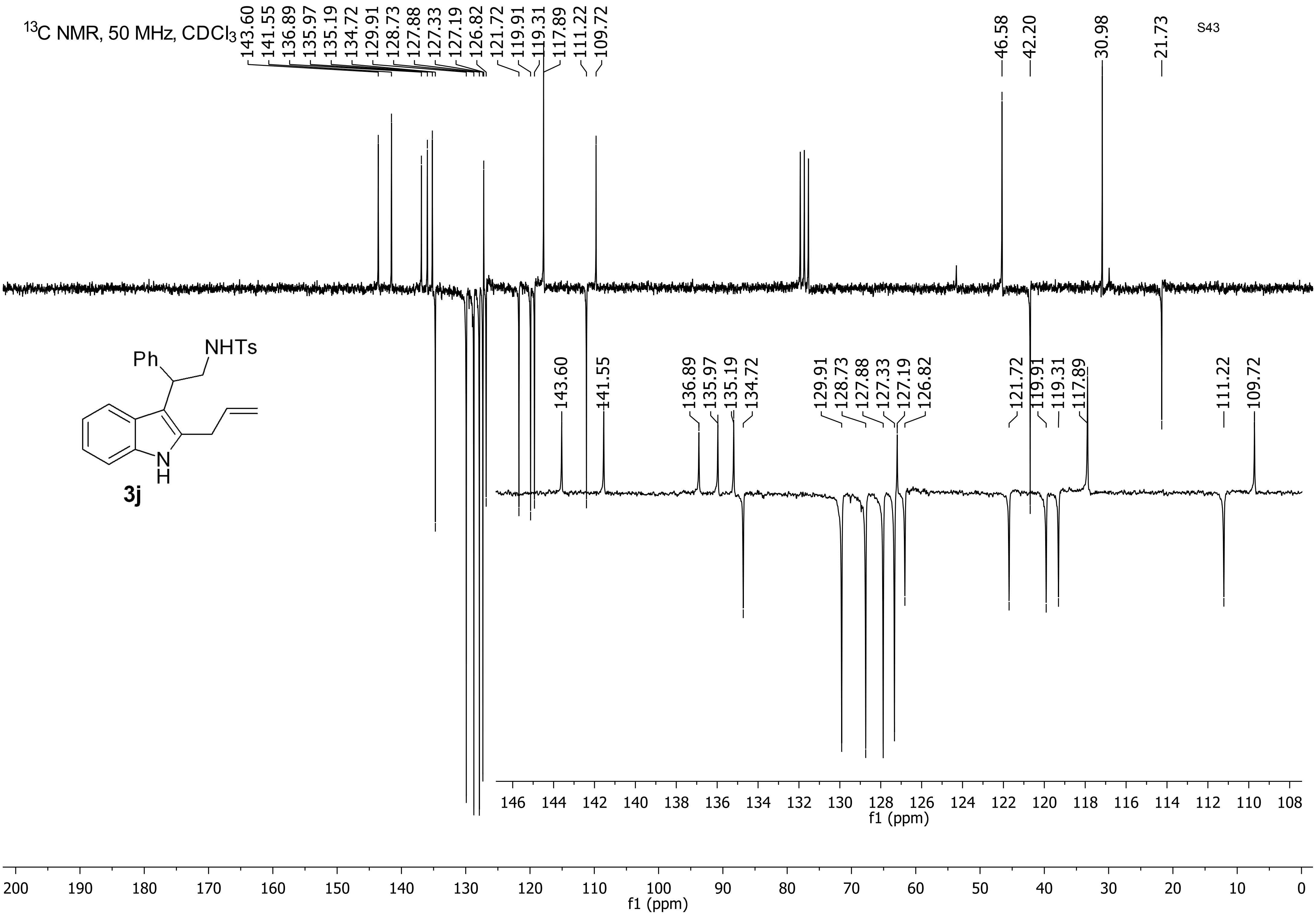


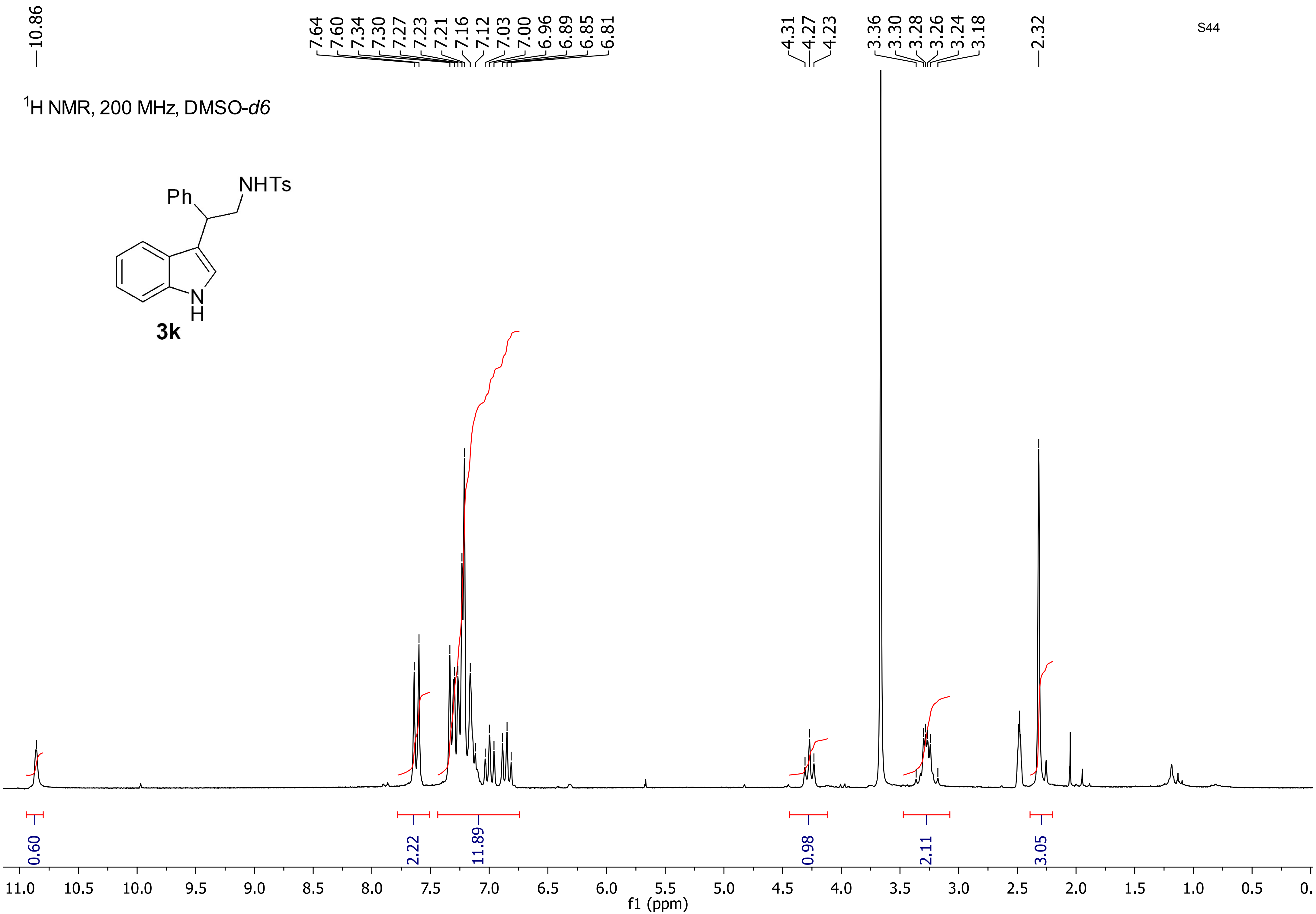
^{1}H NMR, 200 MHz, $CDCl_3$



3j



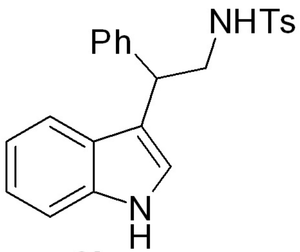

^{13}C NMR, 50 MHz, CDCl$_3$
143.60
141.55
136.89
135.97
135.19
134.72
129.91
128.73
127.88
127.33
127.19
126.82
121.72
119.91
119.31
117.89
111.22
109.72
46.58
42.20
30.98
21.73
Ph
NHTs
N
H
3j
f1 (ppm)
f1 (ppm)



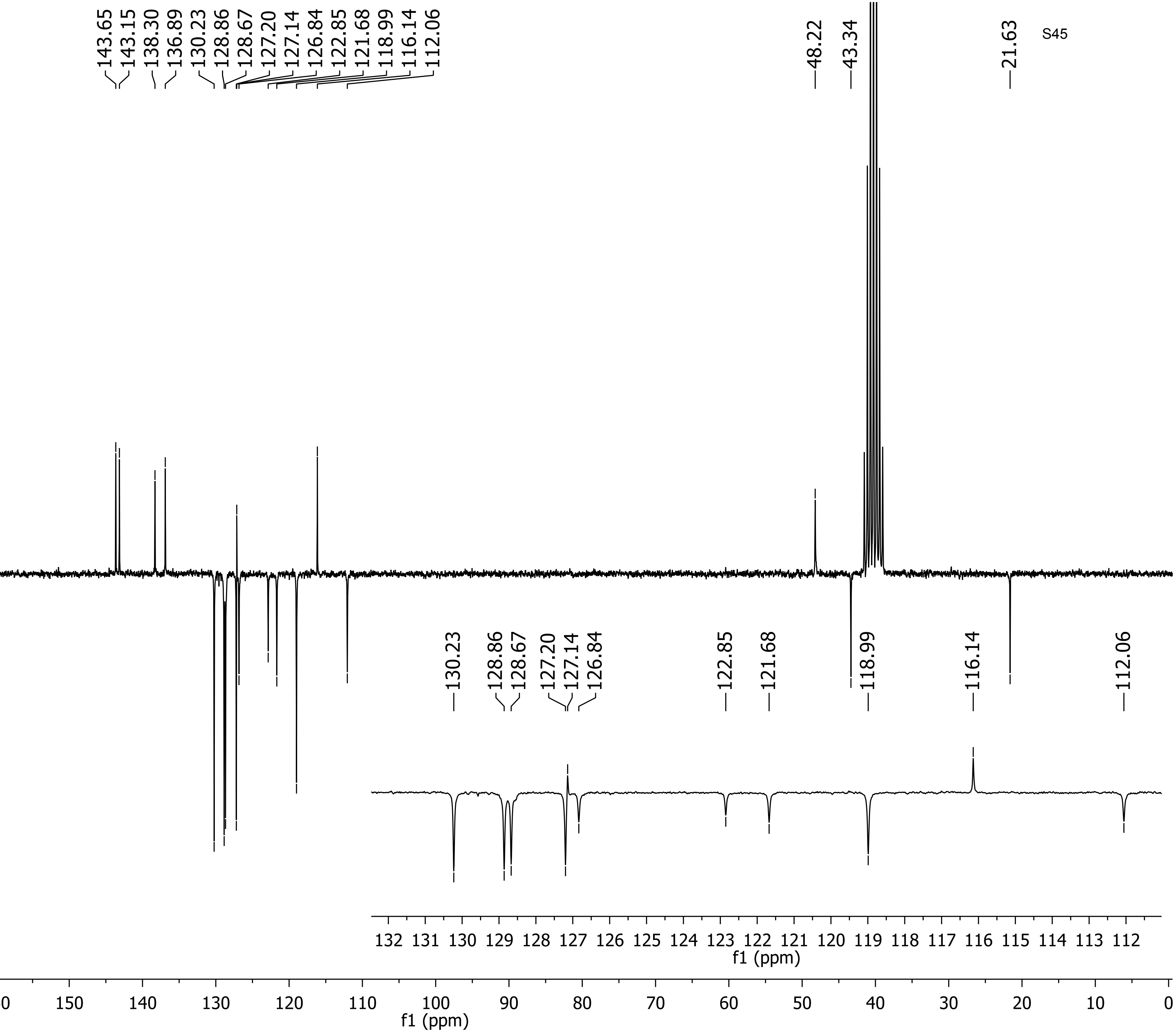
10.86
7.64
7.60
7.34
7.30
7.27
7.23
7.21
7.16
7.12
7.03
7.00
6.96
6.89
6.85
6.81
4.31
4.27
4.23
3.36
3.30
3.28
3.26
3.24
3.18
2.32
^{1}H NMR, 200 MHz, DMSO-*d6*
Ph
NHTs
N
H
3k
0.60
2.22
11.89
0.98
2.11
3.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

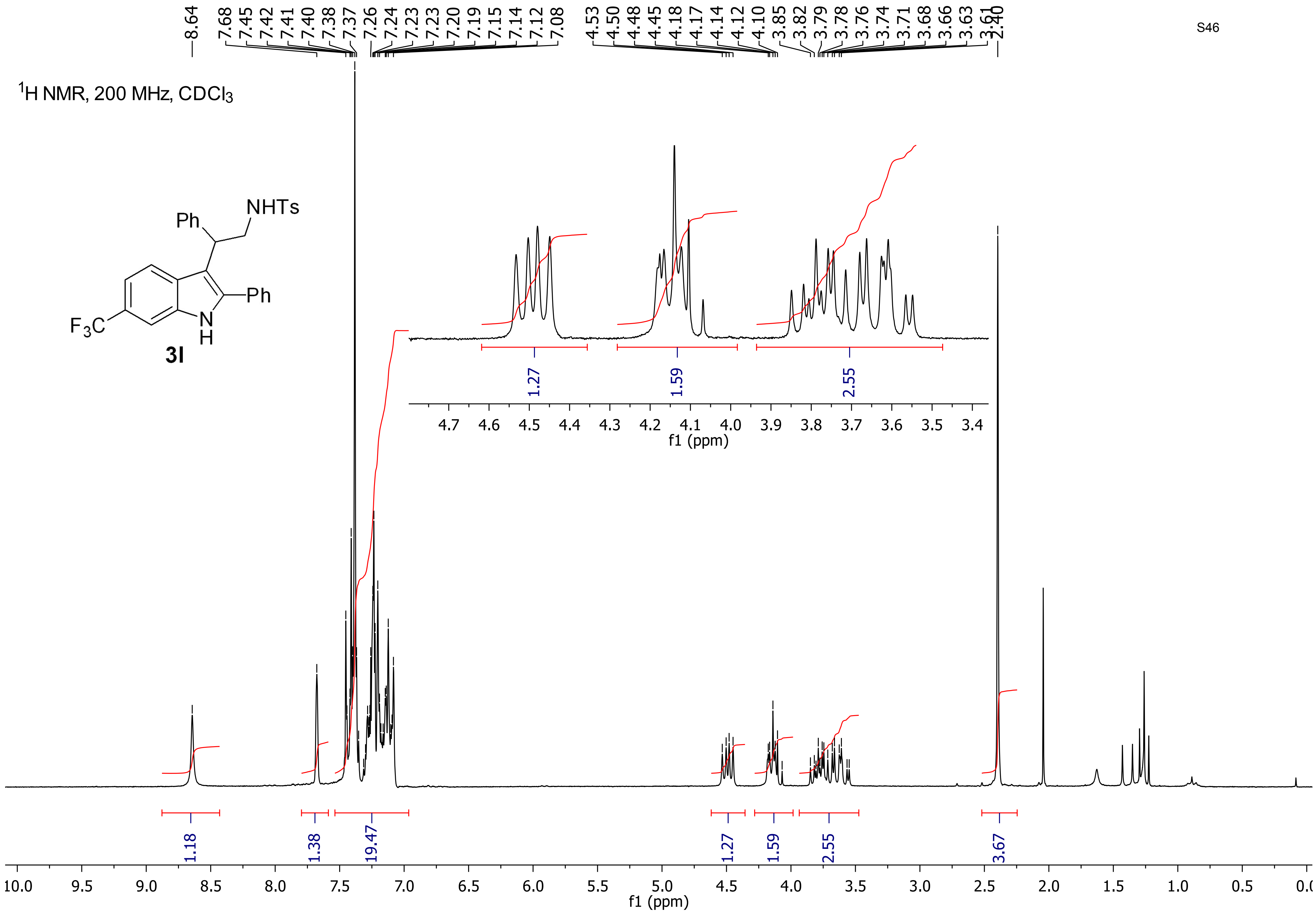
^{1}H NMR, 50 MHz, DMSO-*d6*

S45

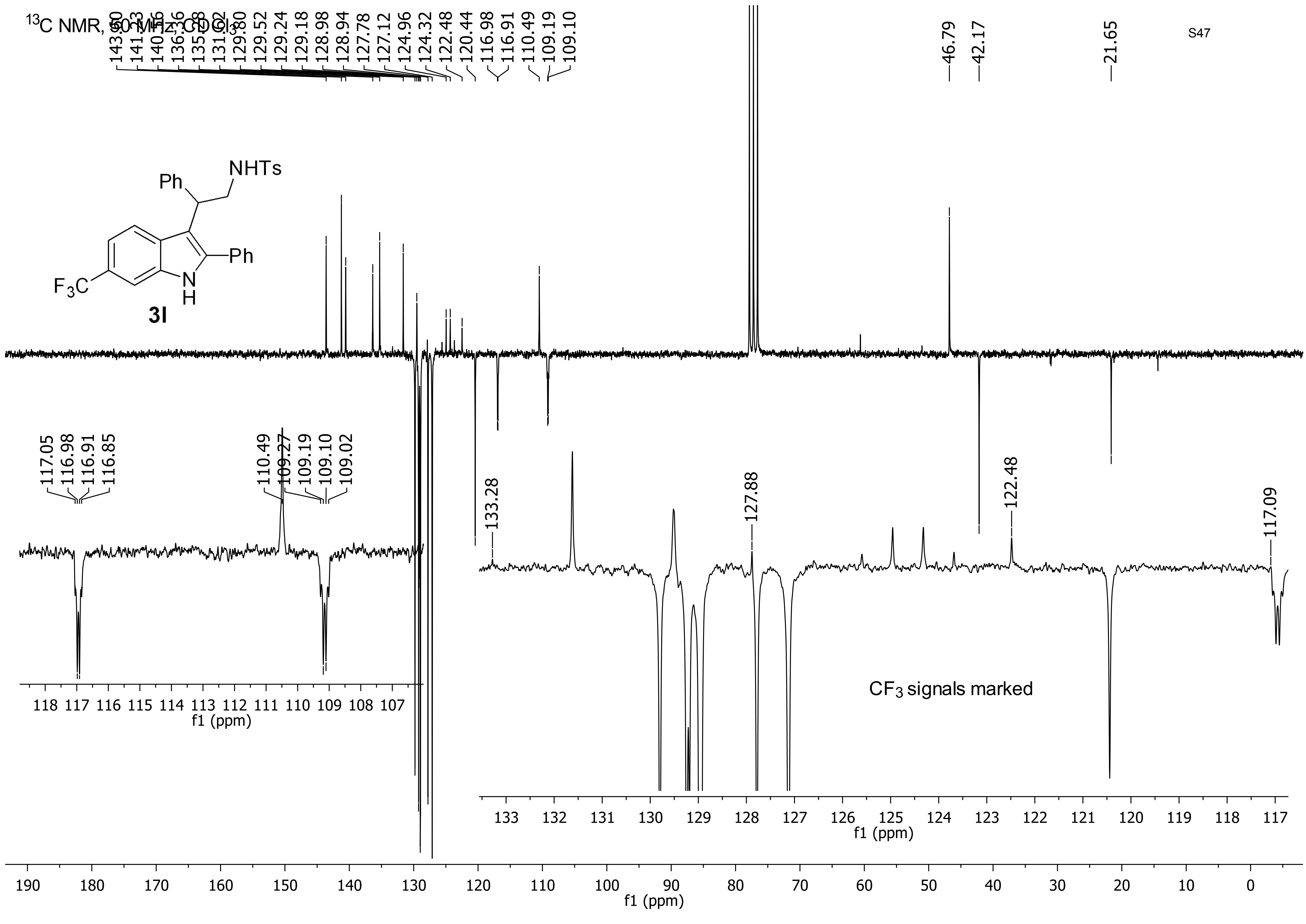


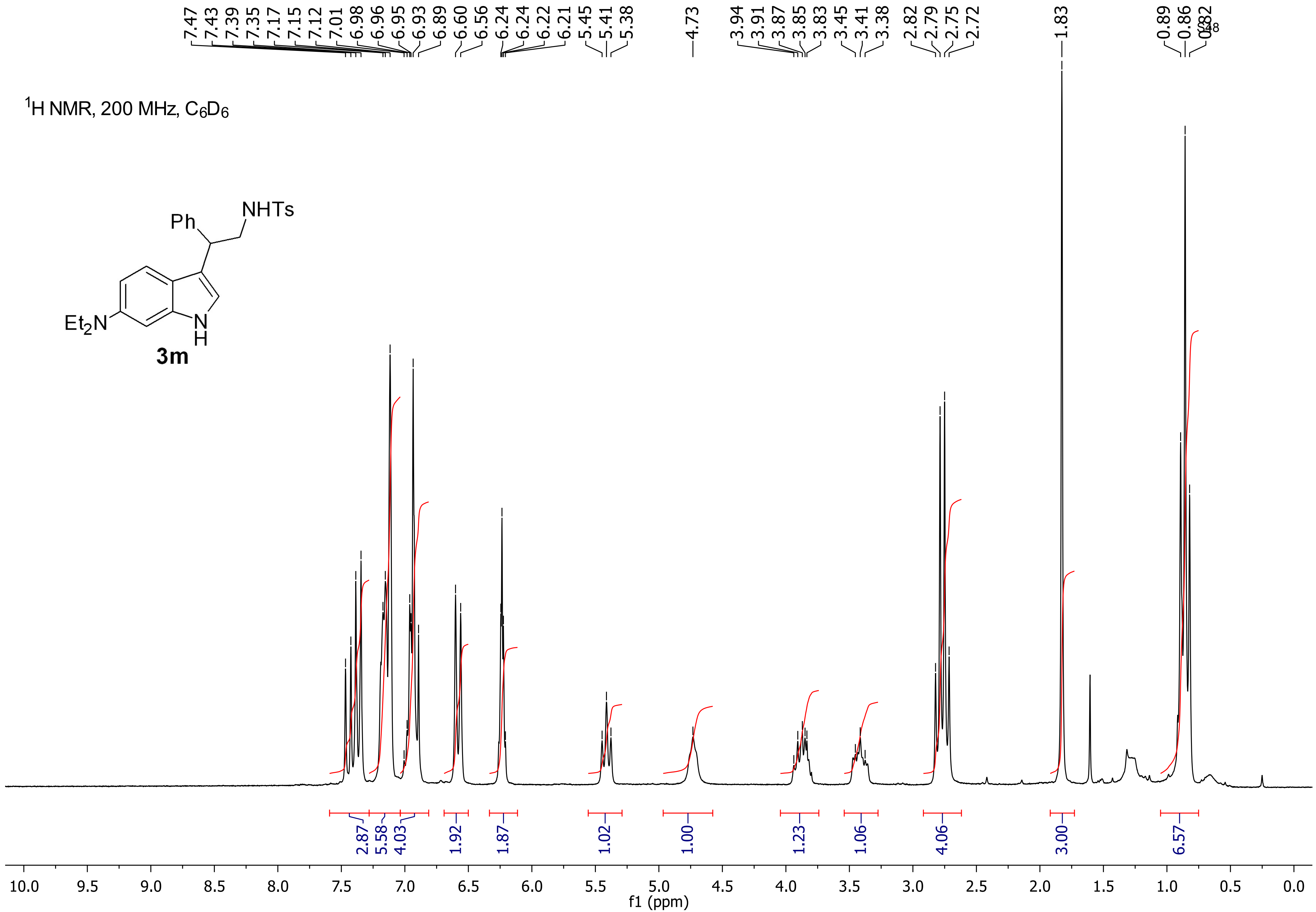
3k





1H NMR, 200 MHz, CDCl3
NHTs
Ph
Ph
F3C
N
H
3l
8.64
7.68
7.45
7.42
7.41
7.40
7.38
7.37
7.26
7.24
7.23
7.23
7.20
7.19
7.15
7.14
7.12
7.08
4.53
4.50
4.48
4.45
4.18
4.17
4.14
4.12
4.10
3.85
3.82
3.79
3.78
3.76
3.74
3.71
3.68
3.66
3.63
3.61
2.40
1.18
1.38
19.47
1.27
1.59
2.55
3.67
f1 (ppm)

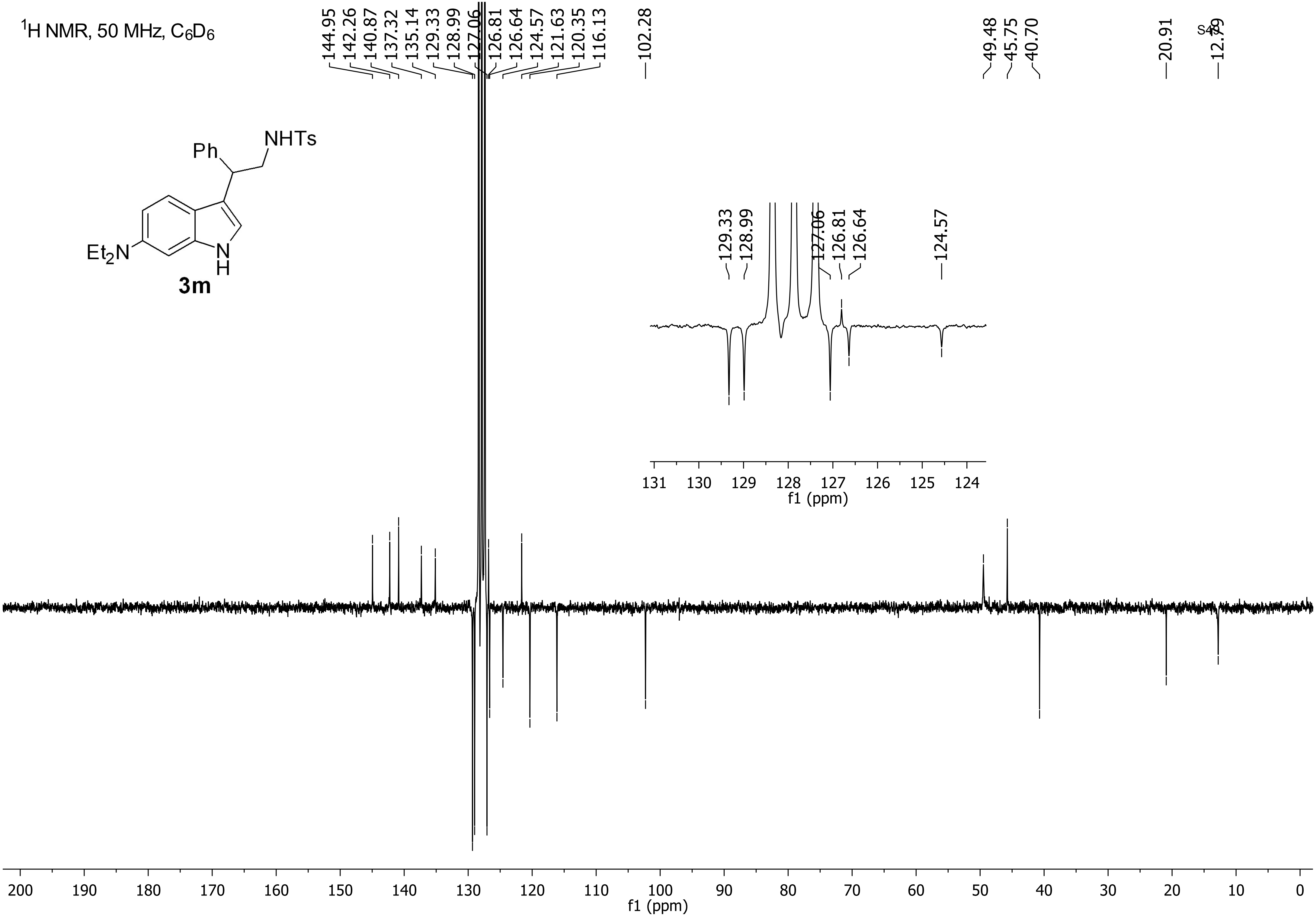

13C NMR, 50 MHz, CDCl3
143.50 141.33 140.56 136.36 135.08 131.62 129.80 129.52 129.24 129.18 128.98 128.94 127.78 127.12 124.96 124.32 122.48 120.44 116.98 116.91 110.49 109.19 109.10
46.79
42.17
21.65
NHTs
Ph
Ph
F3C
N
H
3l
117.05 116.98 116.91 116.85
110.49 109.27 109.19 109.10 109.02
118 117 116 115 114 113 112 111 110 109 108 107
f1 (ppm)
133.28
127.88
122.48
117.09
CF3 signals marked
133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



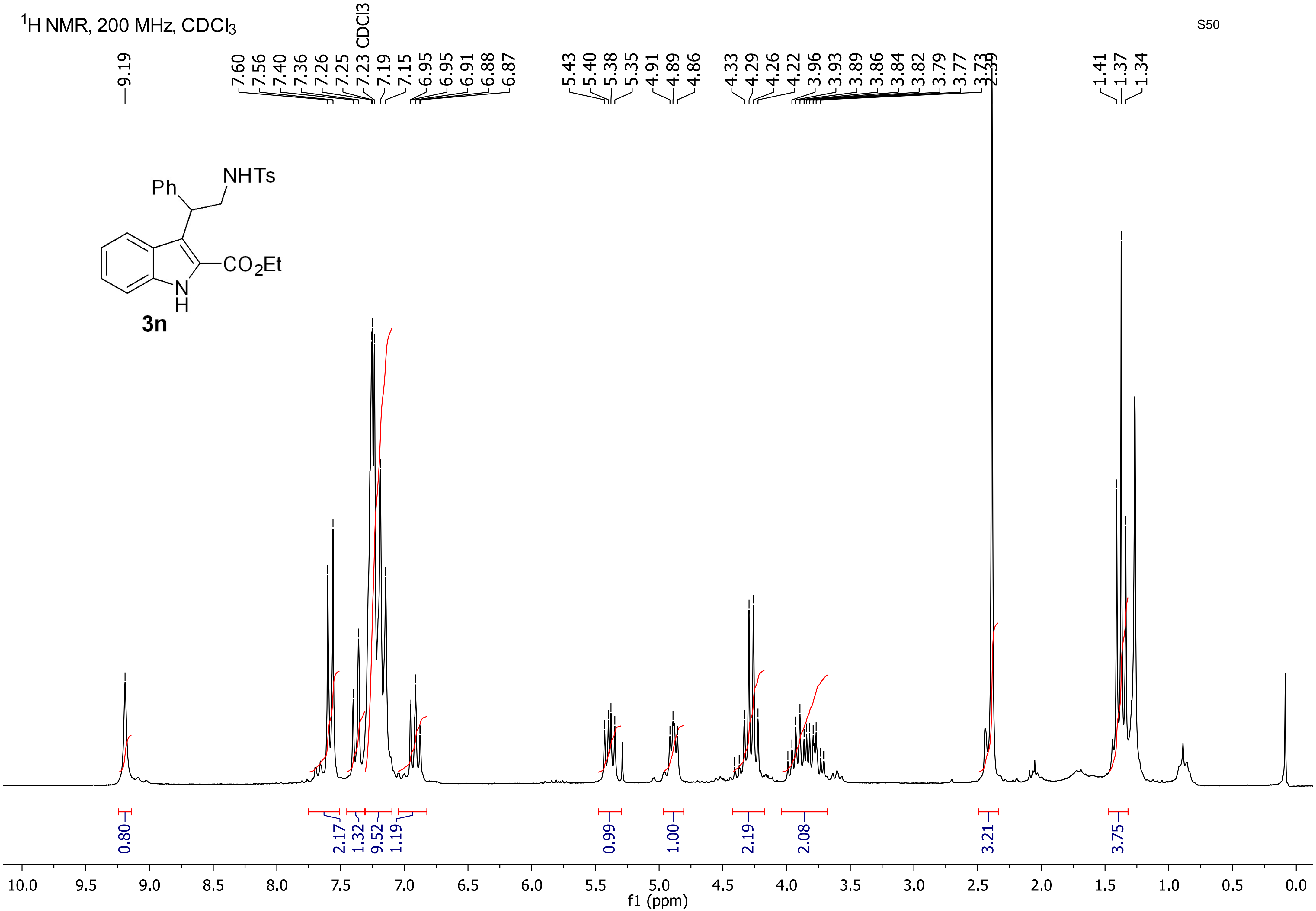
1H NMR, 200 MHz, C6D6
Ph
NHTs
Et2N
N
H
3m
7.47 7.43 7.39 7.35 7.17 7.15 7.12 7.01 6.98 6.96 6.95 6.93 6.89 6.60 6.56 6.24 6.24 6.22 6.21 5.45 5.41 5.38 4.73 3.94 3.91 3.87 3.85 3.83 3.45 3.41 3.38 2.82 2.79 2.75 2.72 1.83 0.89 0.86 0.82
2.87 5.58 4.03 1.92 1.87 1.02 1.00 1.23 1.06 4.06 3.00 6.57
10.0 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 0.0
f1 (ppm)

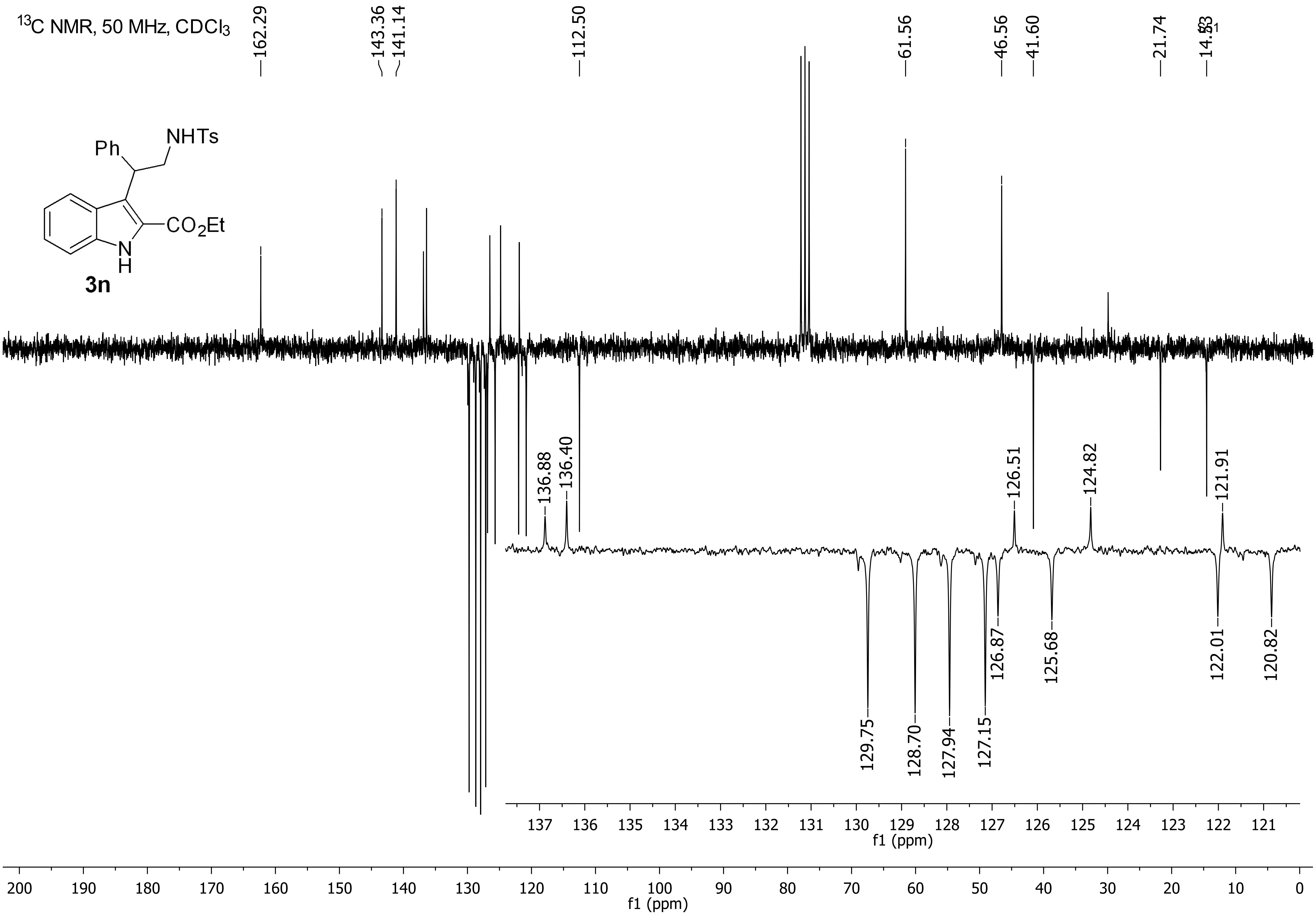
^{1}H NMR, 50 MHz, C_6D_6

3m

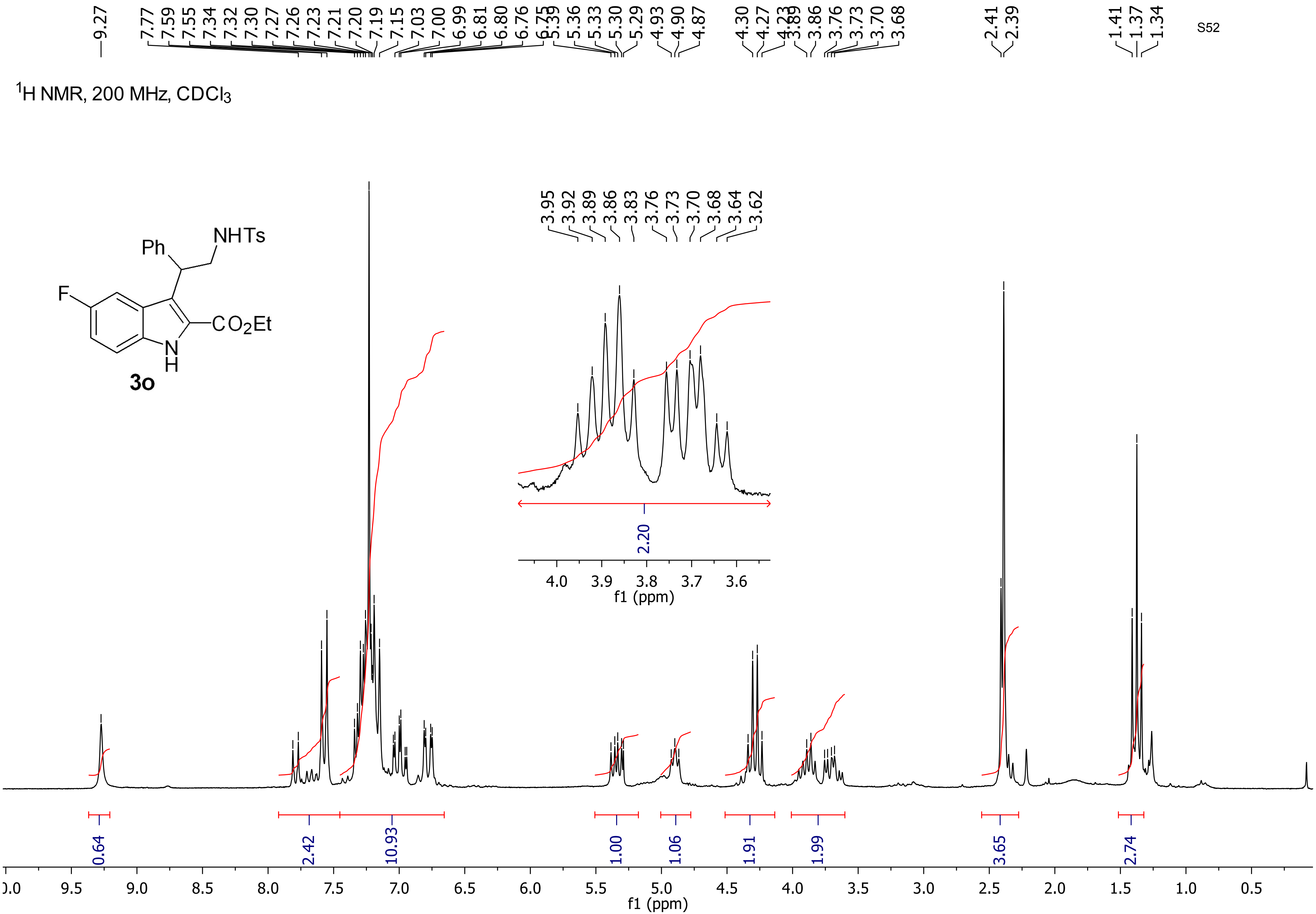


^{1}H NMR, 200 MHz, $CDCl_3$



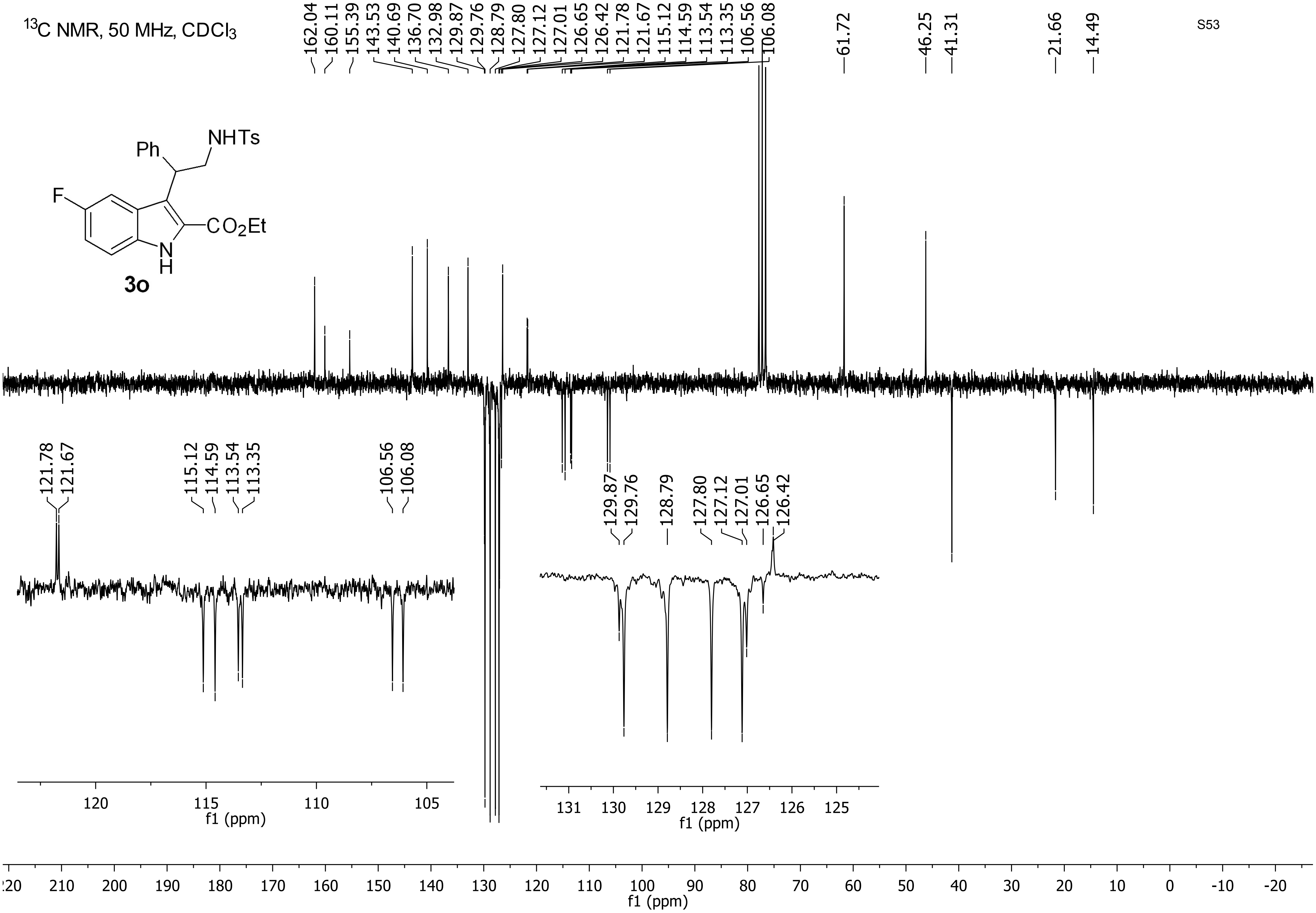


^{13}C NMR, 50 MHz, $CDCl_3$
162.29
143.36
141.14
112.50
61.56
46.56
41.60
21.74
Ph
NHTs
CO_2Et
N
H
3n
136.88
136.40
126.51
124.82
121.91
129.75
128.70
127.94
127.15
126.87
125.68
122.01
120.82
137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

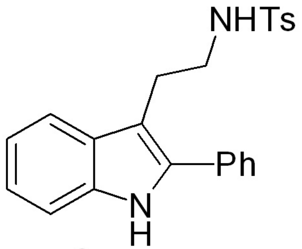


9.27
7.77 7.59 7.55 7.34 7.32 7.30 7.27 7.26 7.23 7.21 7.20 7.19 7.15 7.03 7.00 6.99 6.81 6.80 6.76 6.75 5.39 5.36 5.33 5.30 5.29 4.93 4.90 4.87
4.30 4.27 4.23 3.89 3.86 3.76 3.73 3.70 3.68
2.41 2.39
1.41 1.37 1.34
^{1}H NMR, 200 MHz, $CDCl_3$
Ph
NHTs
F
CO_2Et
N
H
3o
3.95 3.92 3.89 3.86 3.83 3.76 3.73 3.70 3.68 3.64 3.62
2.20
4.0 3.9 3.8 3.7 3.6
f1 (ppm)
0.64 2.42 10.93 1.00 1.06 1.91 1.99 3.65 2.74
0.0 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)

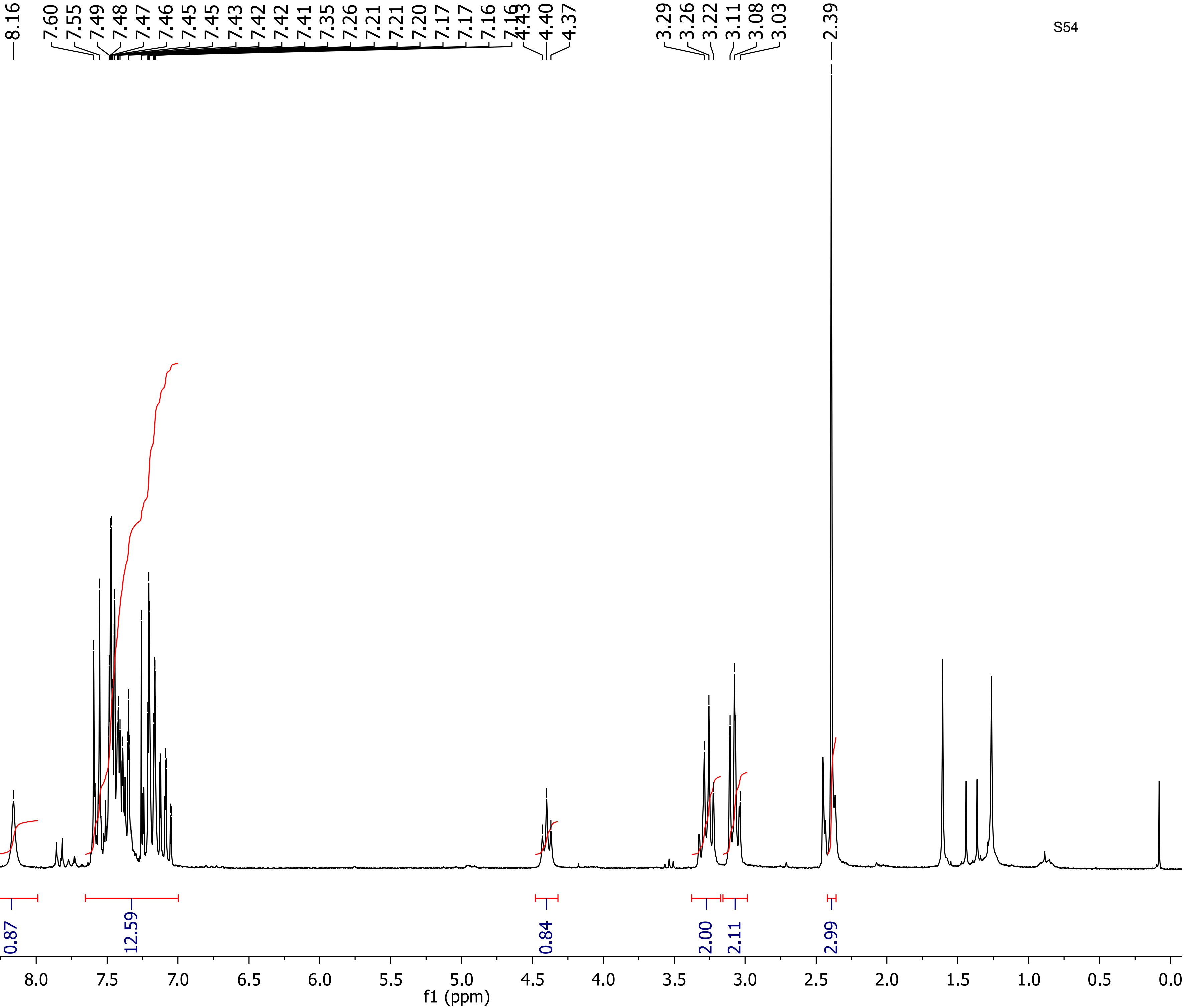
^{13}C NMR, 50 MHz, $CDCl_3$



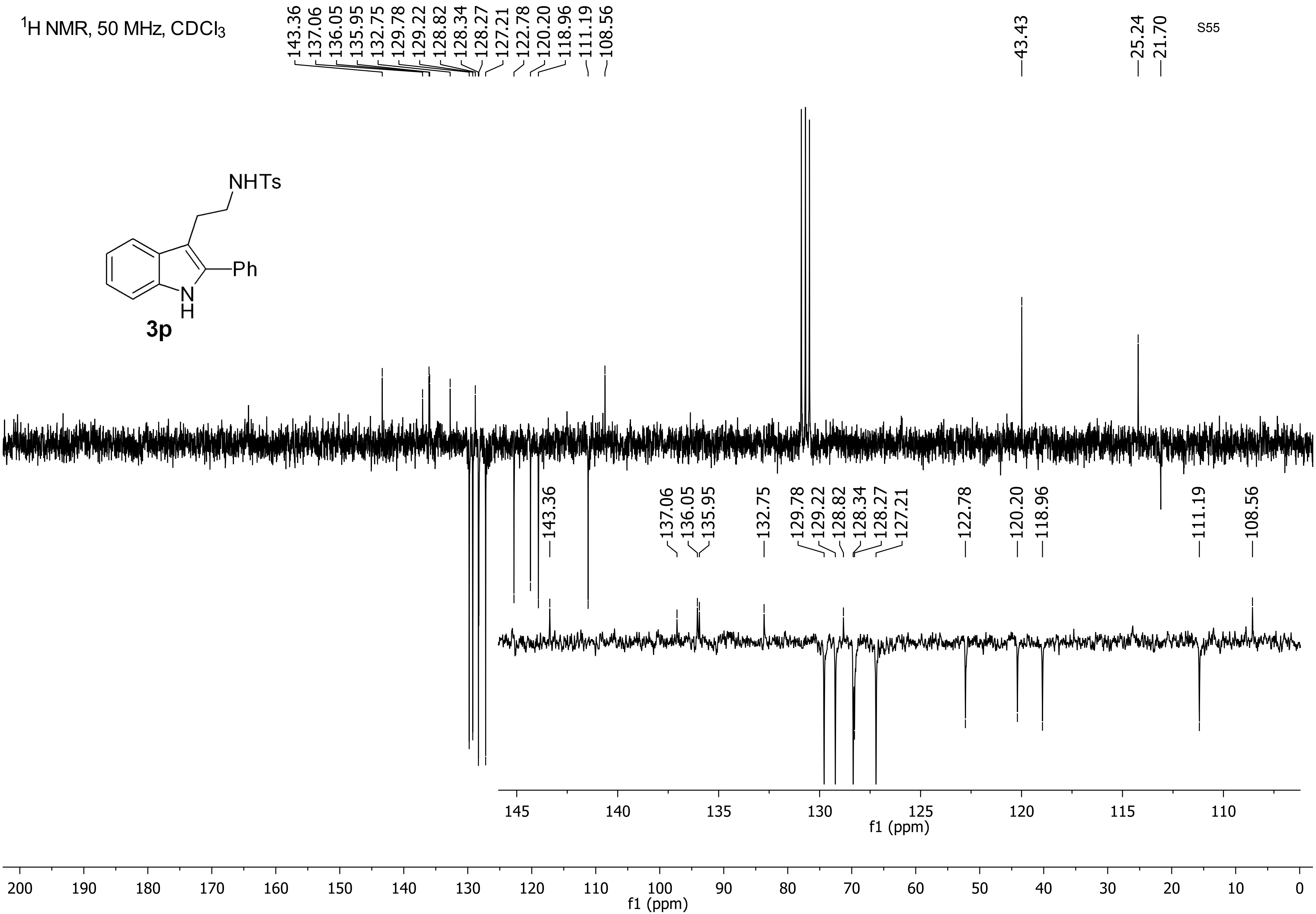
^{1}H NMR, 200 MHz, $CDCl_3$



3p

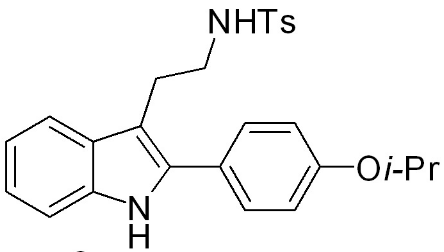


^1H NMR, 50 MHz, $CDCl_3$

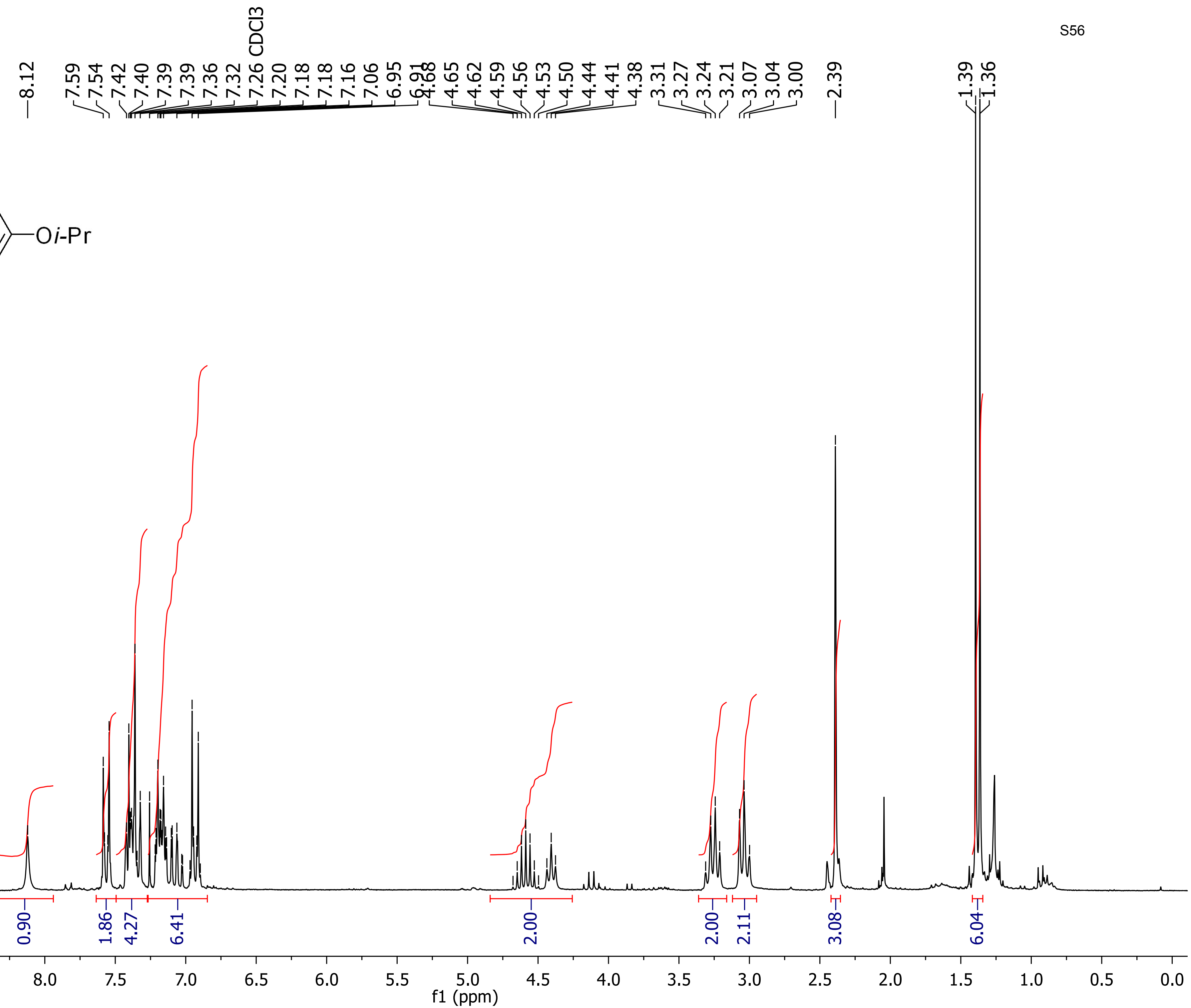


3p

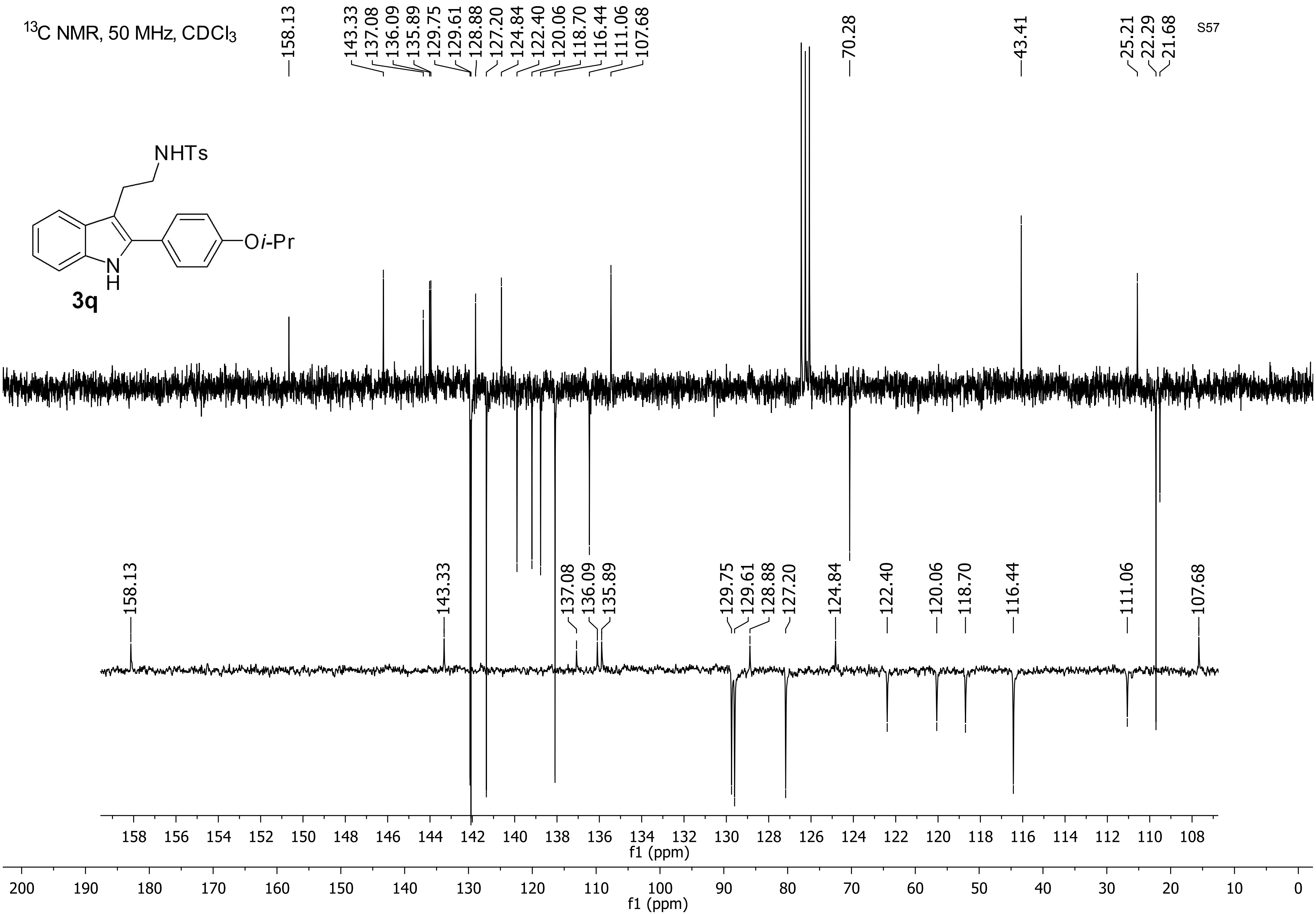
^{1}H NMR, 200 MHz, $CDCl_3$



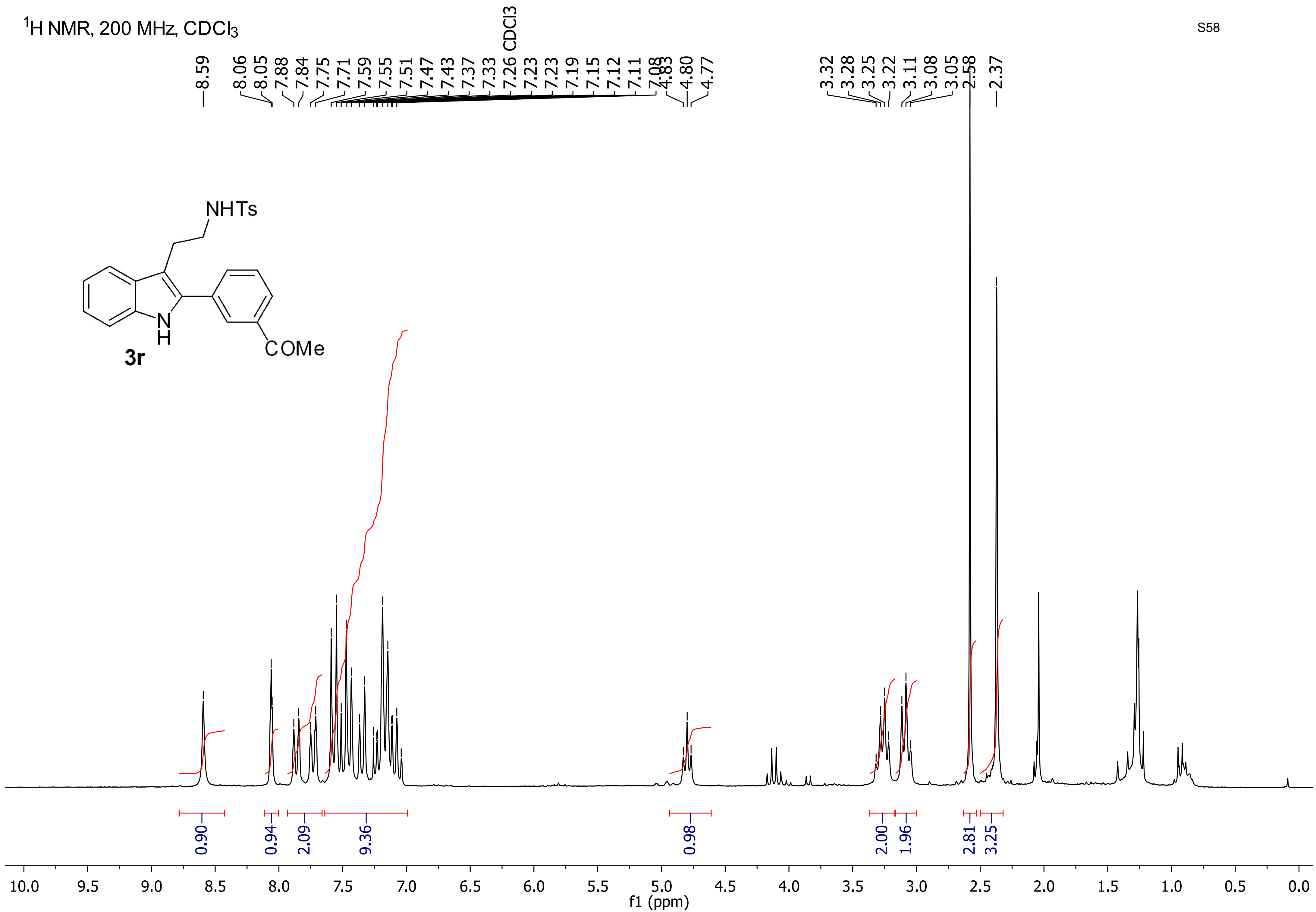
3q

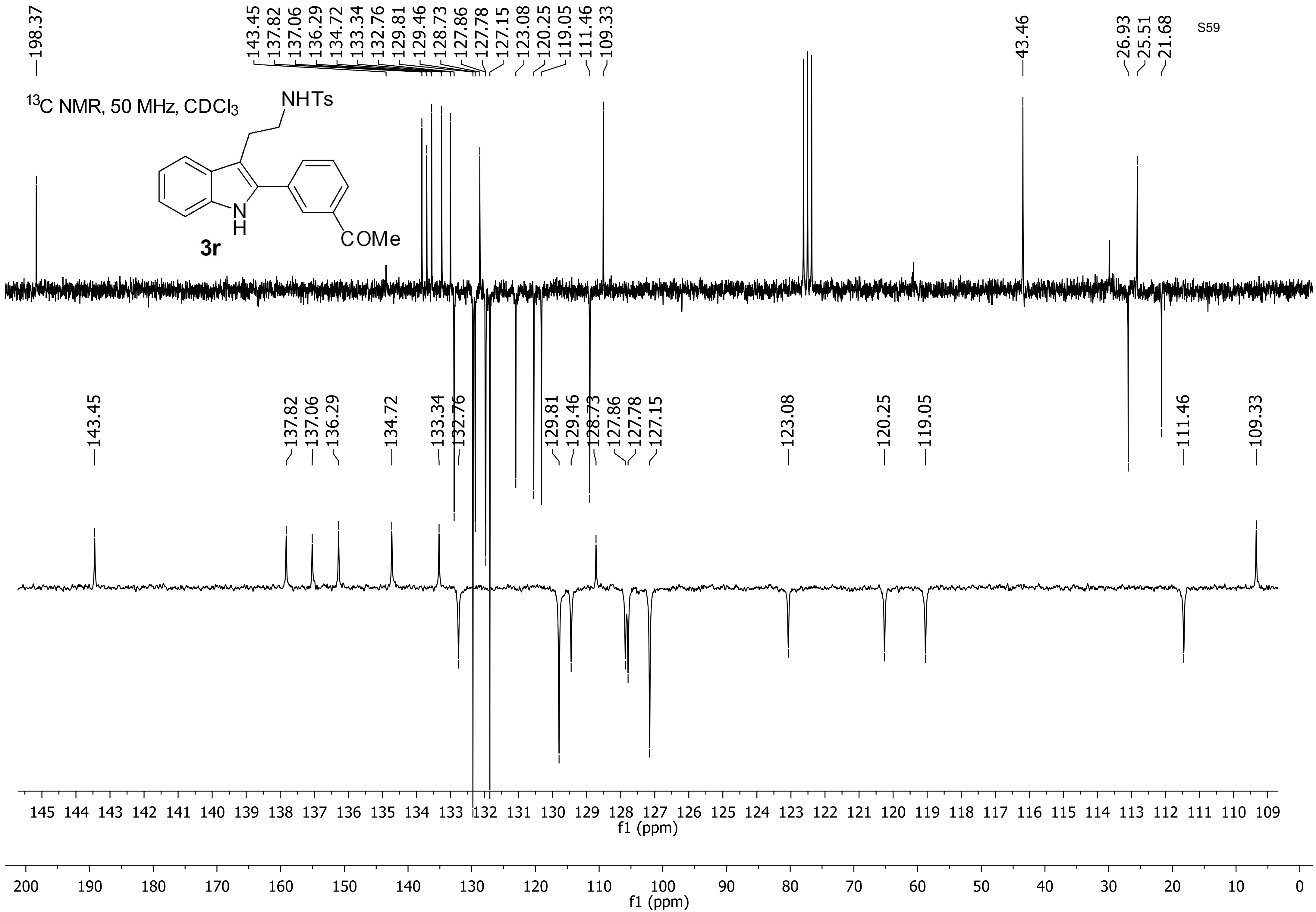


^{13}C NMR, 50 MHz, $CDCl_3$

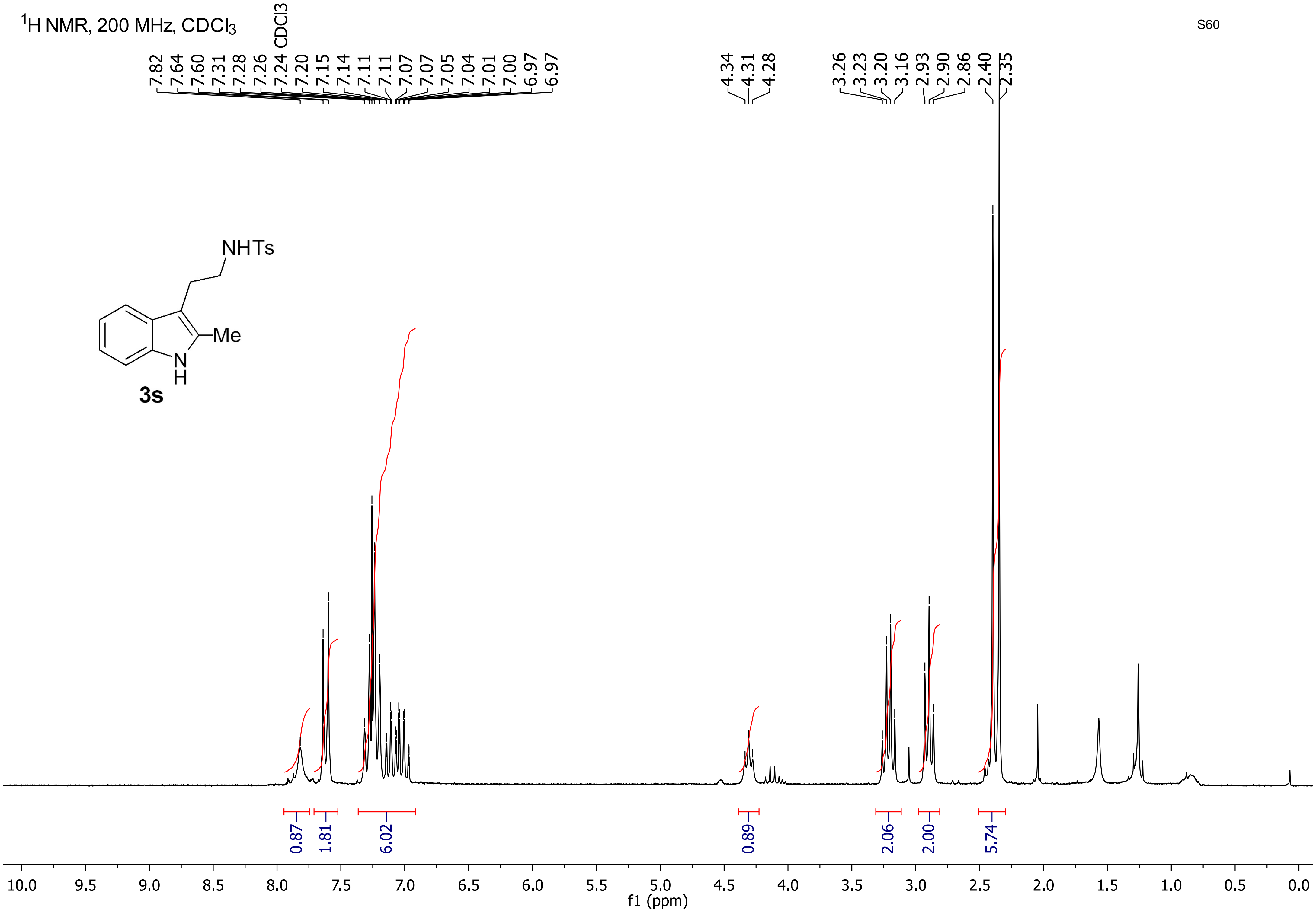


^{1}H NMR, 200 MHz, $CDCl_3$



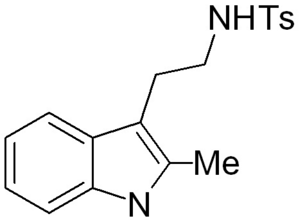


198.37
143.45
137.82
137.06
136.29
134.72
133.34
132.76
129.81
129.46
128.73
127.86
127.78
127.15
123.08
120.25
119.05
111.46
109.33
43.46
26.93
25.51
21.68
^{13}C NMR, 50 MHz, $CDCl_3$
NHTs
N
H
COMe
3r
f1 (ppm)
f1 (ppm)

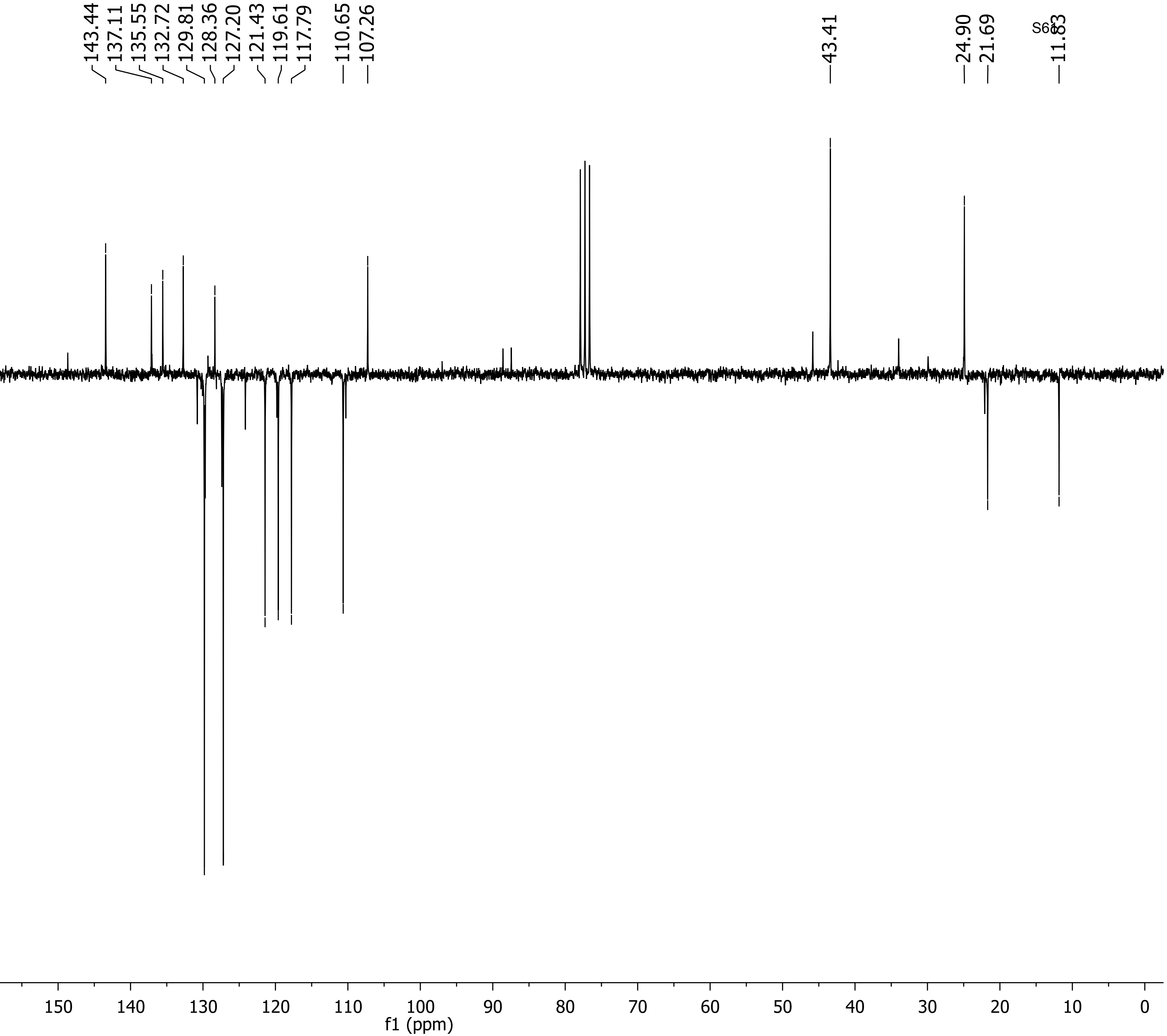


1H NMR, 200 MHz, CDCl3
CDCl3
7.82 7.64 7.60 7.31 7.28 7.26 7.24 7.20 7.15 7.14 7.11 7.11 7.07 7.07 7.05 7.04 7.01 7.00 6.97 6.97
4.34 4.31 4.28
3.26 3.23 3.20 3.16 2.93 2.90 2.86 2.40 2.35
NHTs
Me
N
H
3s
0.87 1.81 6.02 0.89 2.06 2.00 5.74
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

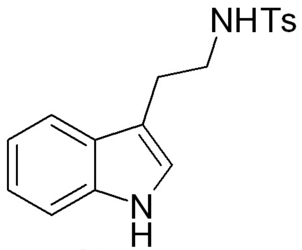
^{1}H NMR, 50 MHz, $CDCl_3$



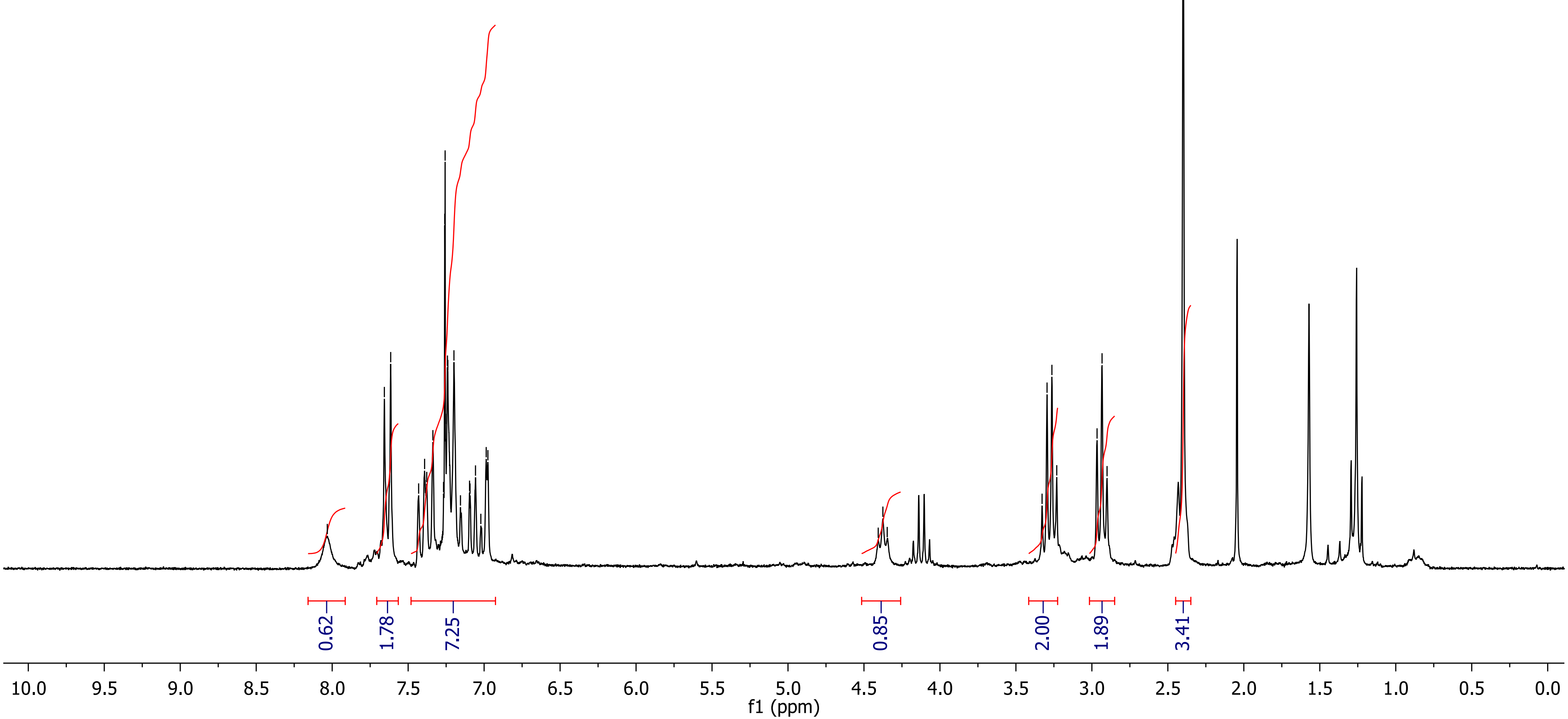
3s

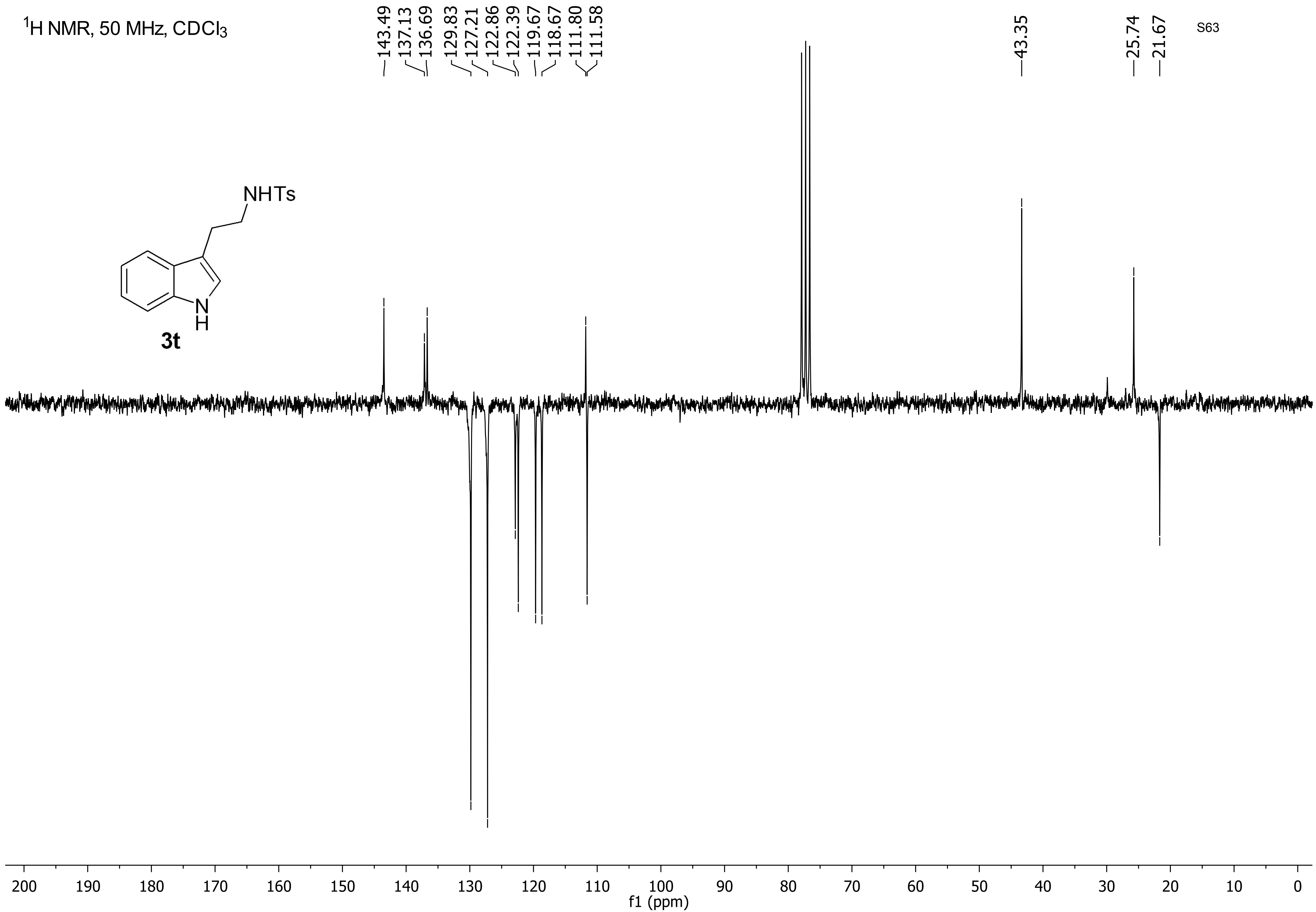


^{1}H NMR, 200 MHz, $CDCl_3$



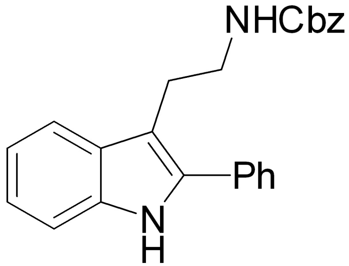
3t



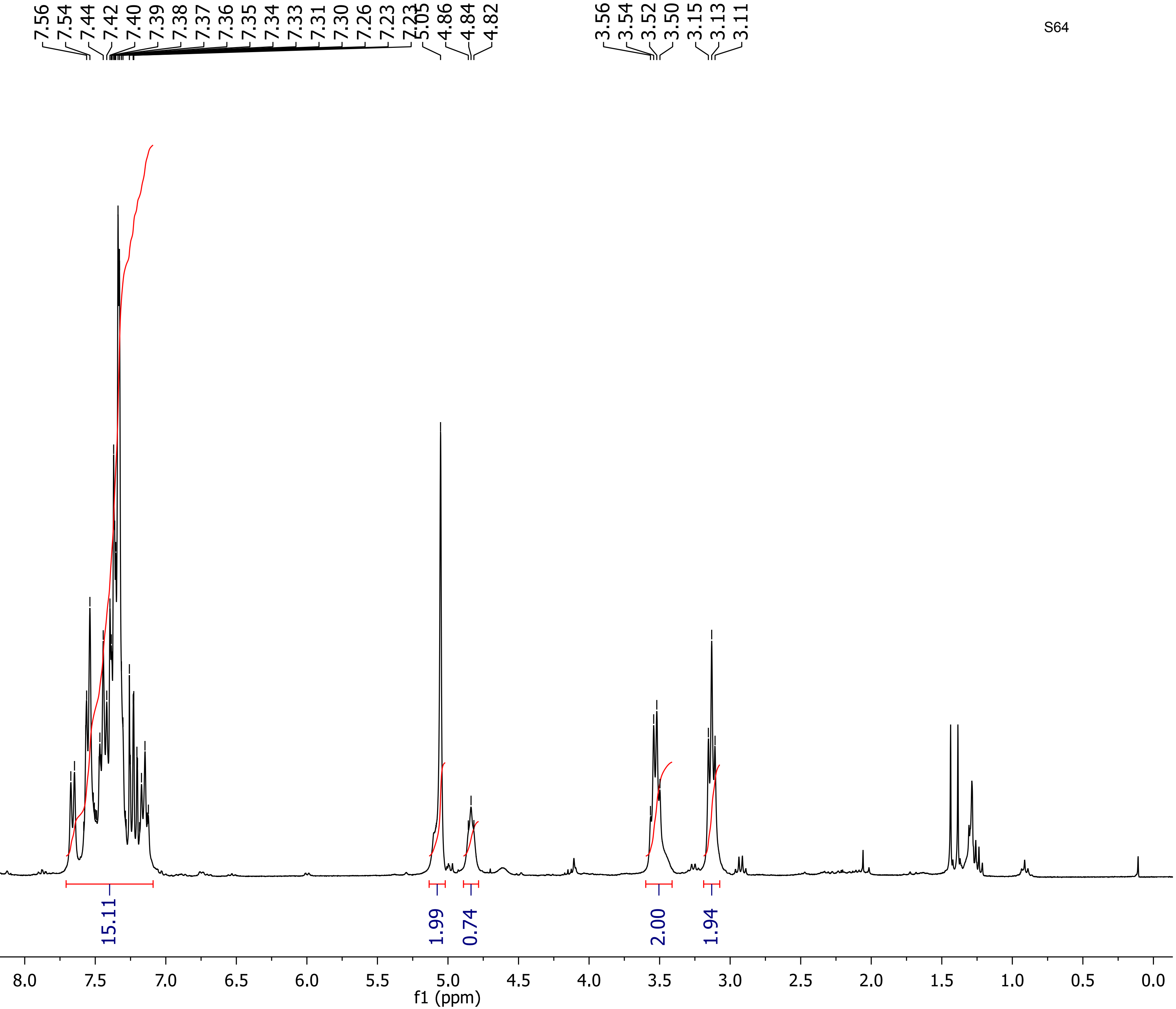


^{1}H NMR, 50 MHz, $CDCl_3$
143.49
137.13
136.69
129.83
127.21
122.86
122.39
119.67
118.67
111.80
111.58
43.35
25.74
21.67
NHTs
N
H
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR, 300 MHz, $CDCl_3$

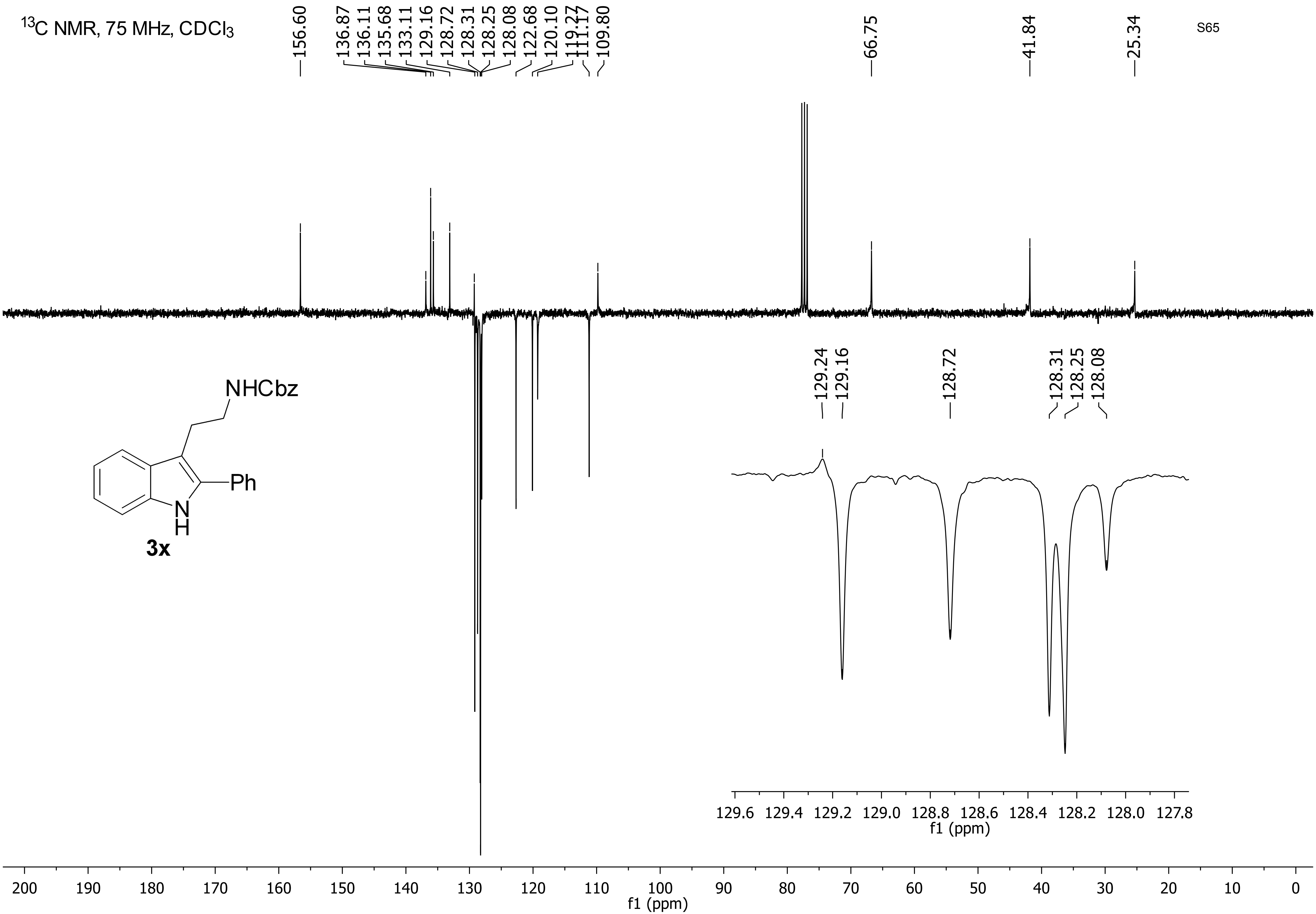


3x

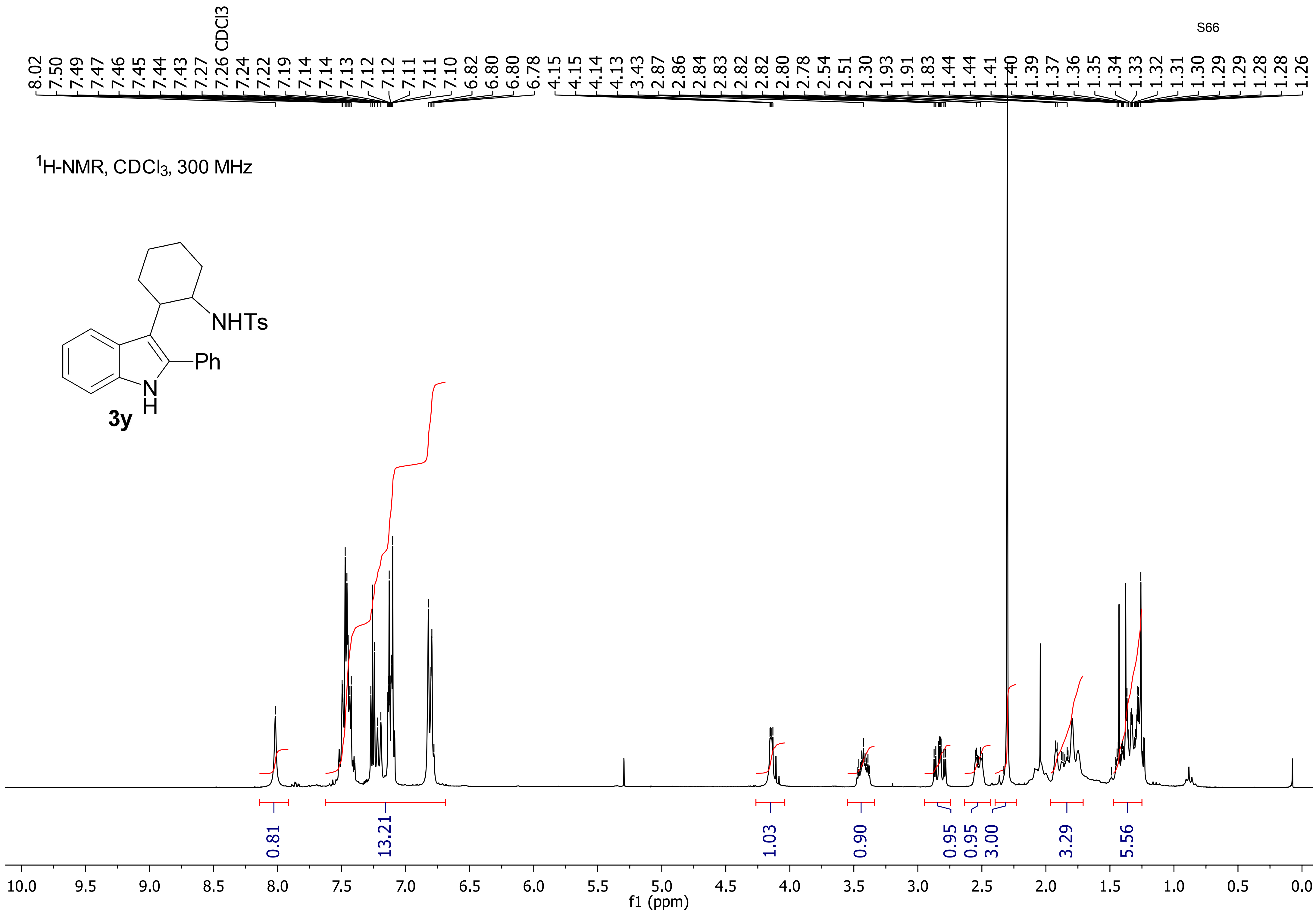


^{13}C NMR, 75 MHz, $CDCl_3$

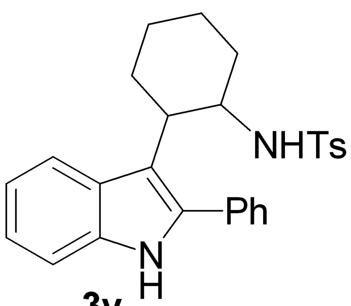
S65



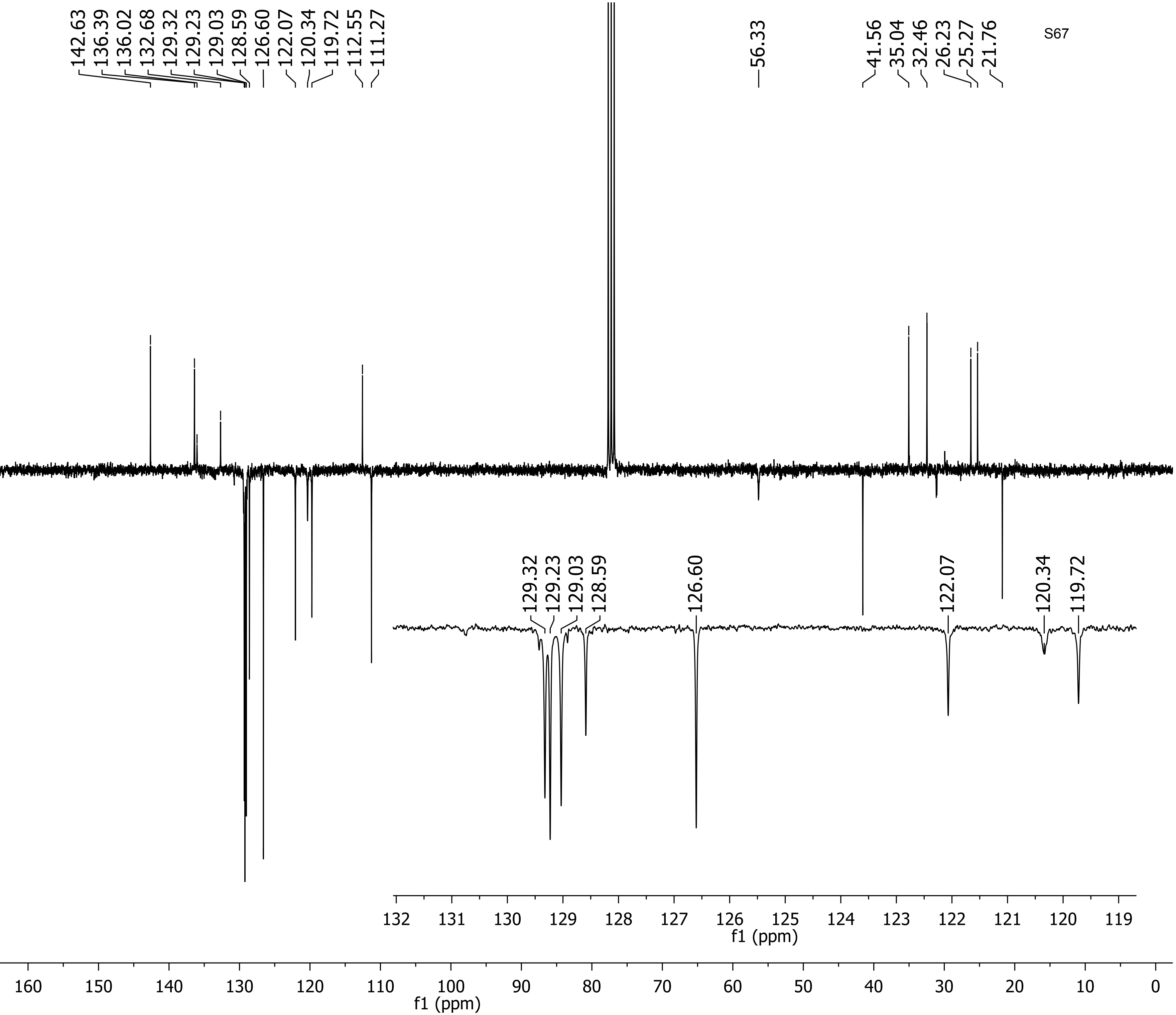
3x


8.02 7.50 7.49 7.47 7.46 7.45 7.44 7.43 7.27 7.26 CDCl3 7.24 7.22 7.19 7.14 7.14 7.13 7.12 7.12 7.11 7.11 7.10 6.82 6.80 6.80 6.78 4.15 4.15 4.14 4.13 3.43 2.87 2.86 2.84 2.83 2.82 2.82 2.80 2.78 2.54 2.51 2.30 1.93 1.91 1.83 1.44 1.44 1.41 1.40 1.39 1.37 1.36 1.35 1.34 1.33 1.32 1.31 1.30 1.29 1.29 1.28 1.28 1.26
^{1}H-NMR, $CDCl_3$, 300 MHz
NHTs
Ph
N
H
3y
0.81
13.21
1.03
0.90
0.95
0.95
3.00
3.29
5.56
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 0.0
f1 (ppm)

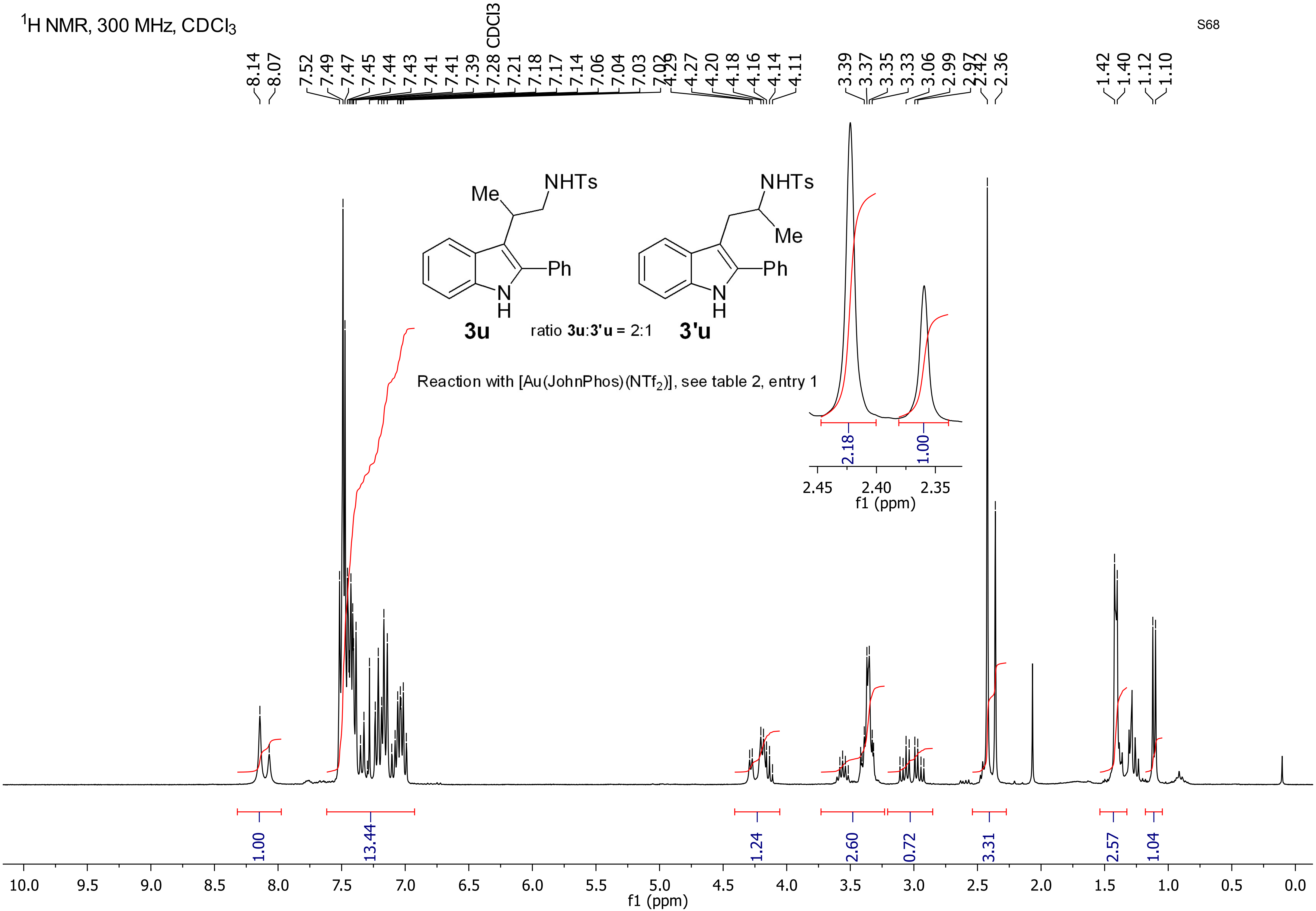
^{1}H-NMR, $CDCl_3$, 75 MHz



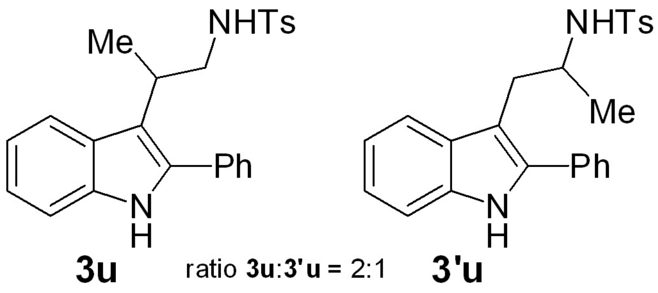
3y



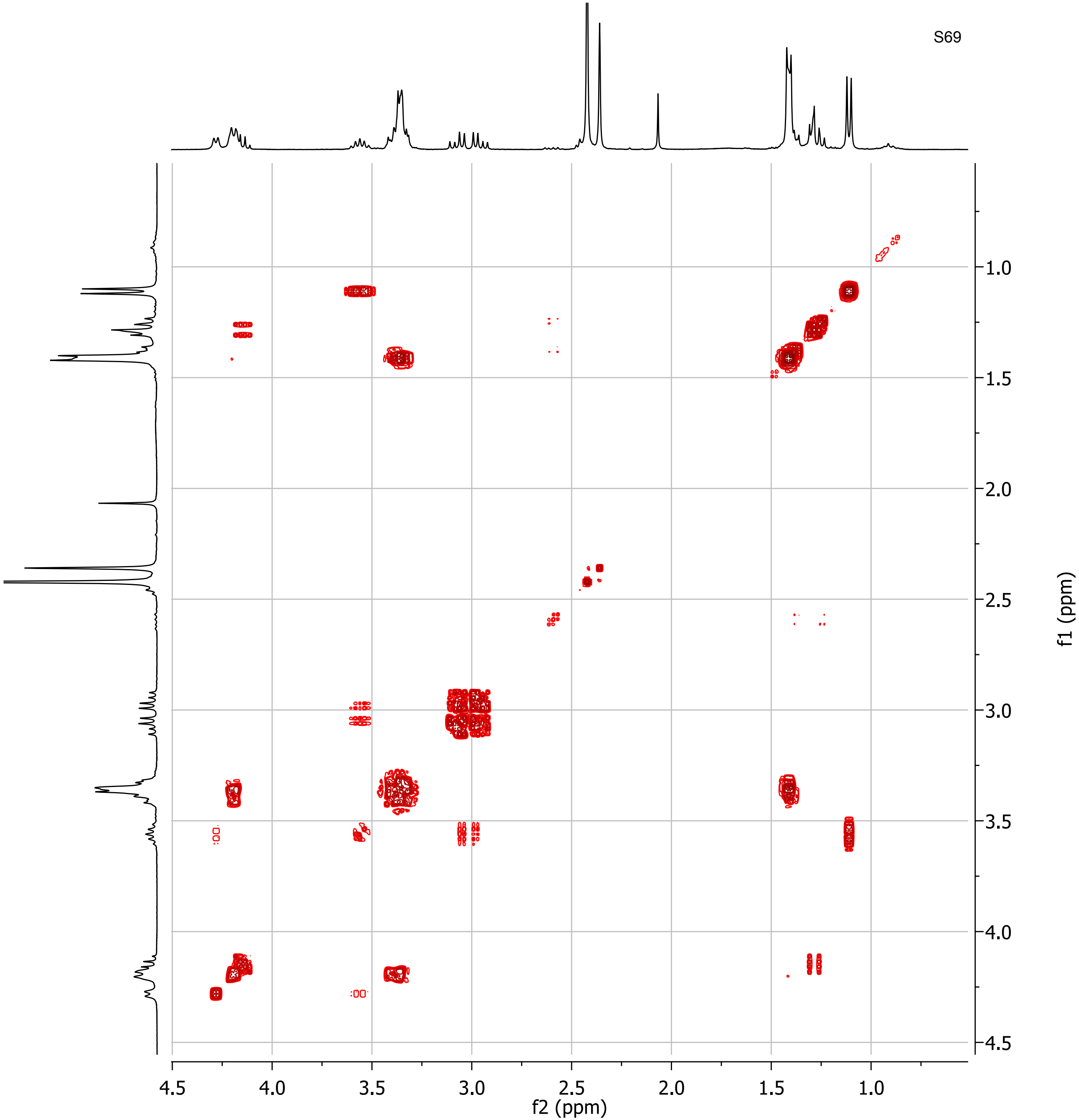
^{1}H NMR, 300 MHz, $CDCl_3$



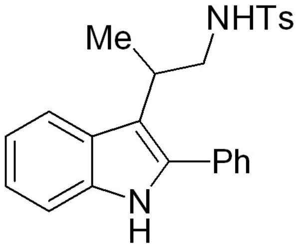
COSY, 300 MHz, $CDCl_3$



Reaction with [Au(JohnPhos)(NTf_2)], see table 2, entry 1

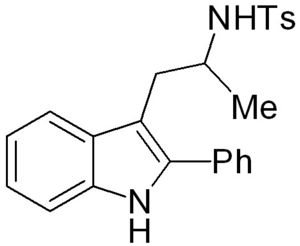


TOCSY, 300 MHz, $CDCl_3$



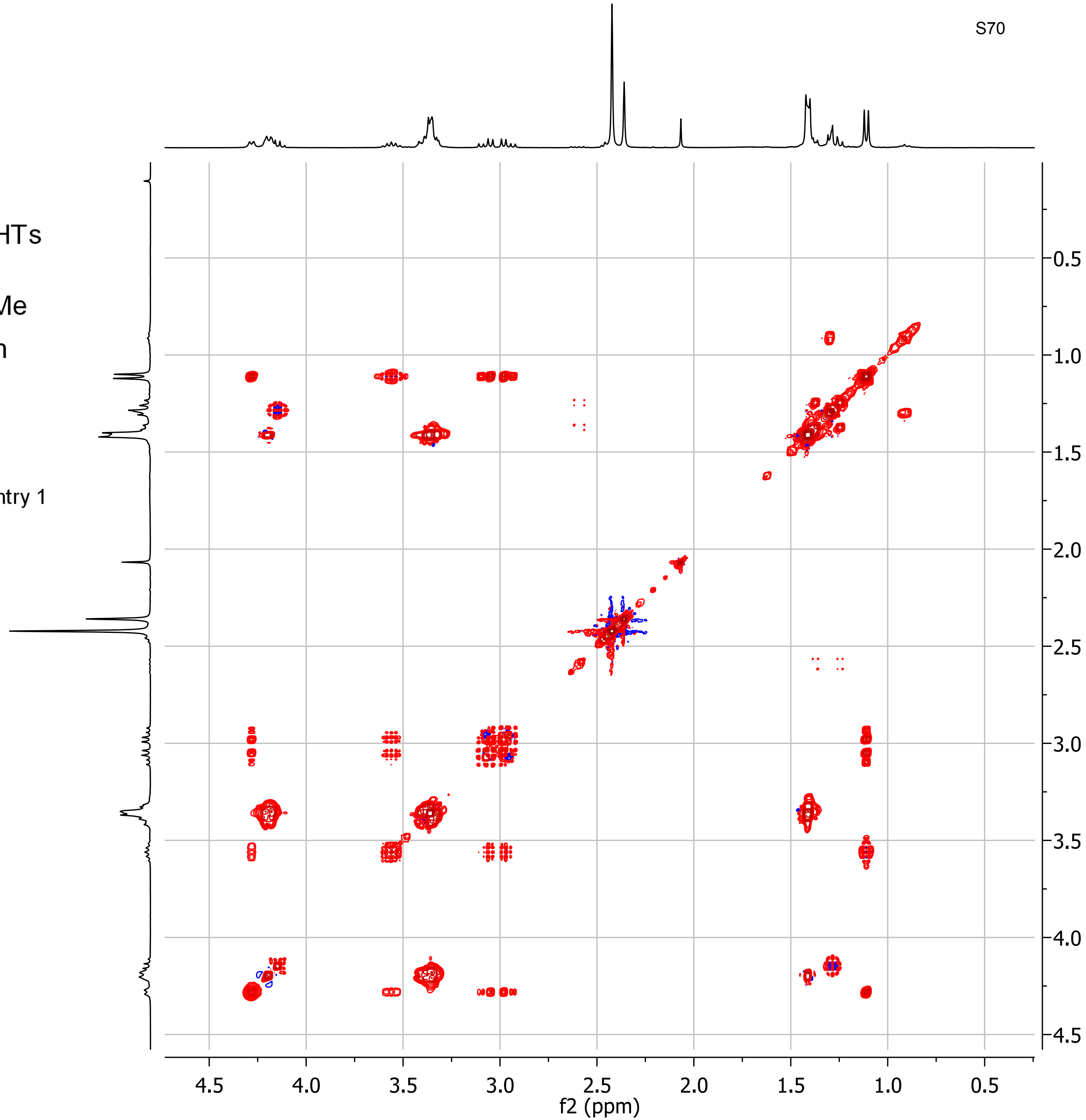
3u

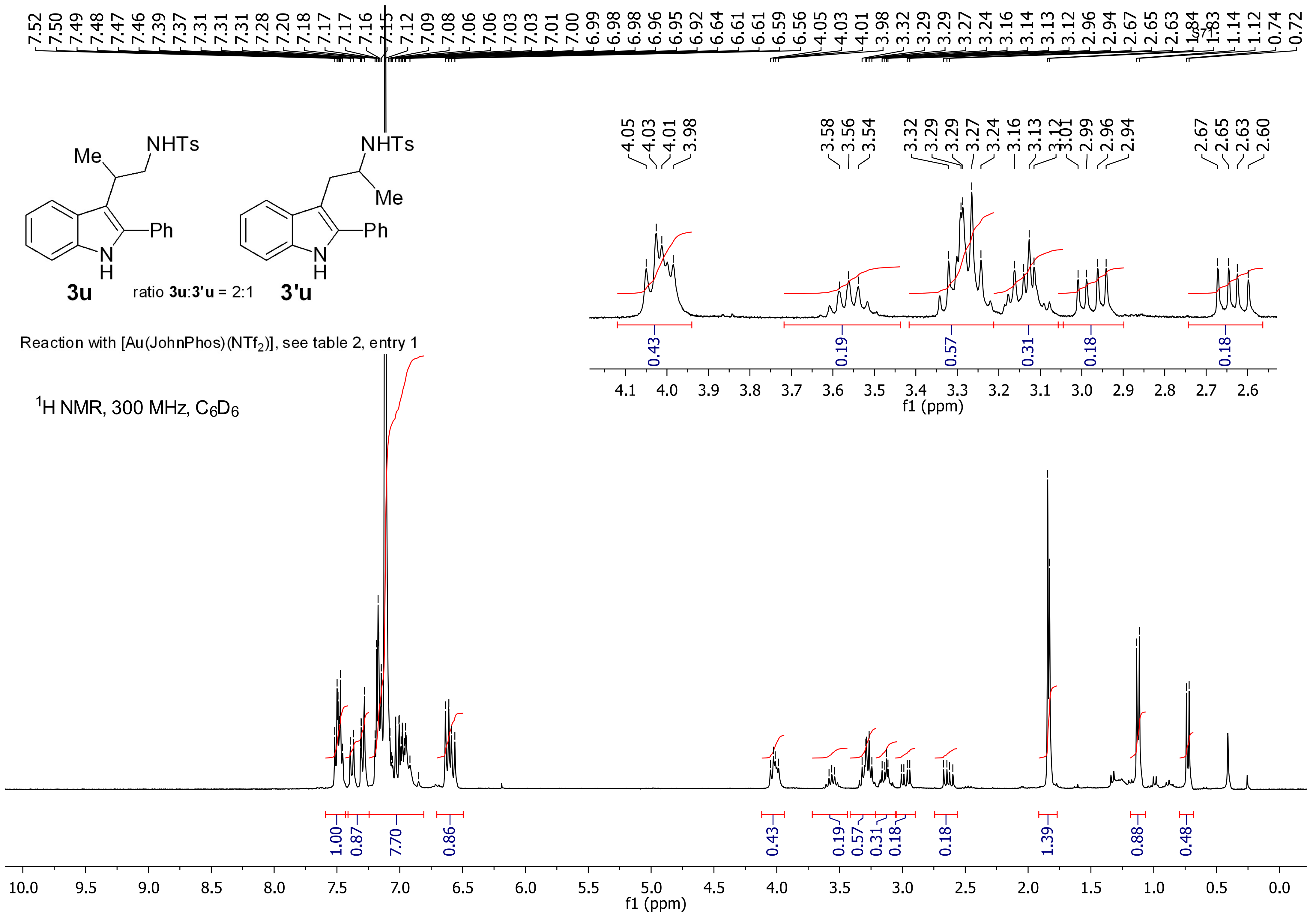
ratio **3u**:**3'u** = 2:1



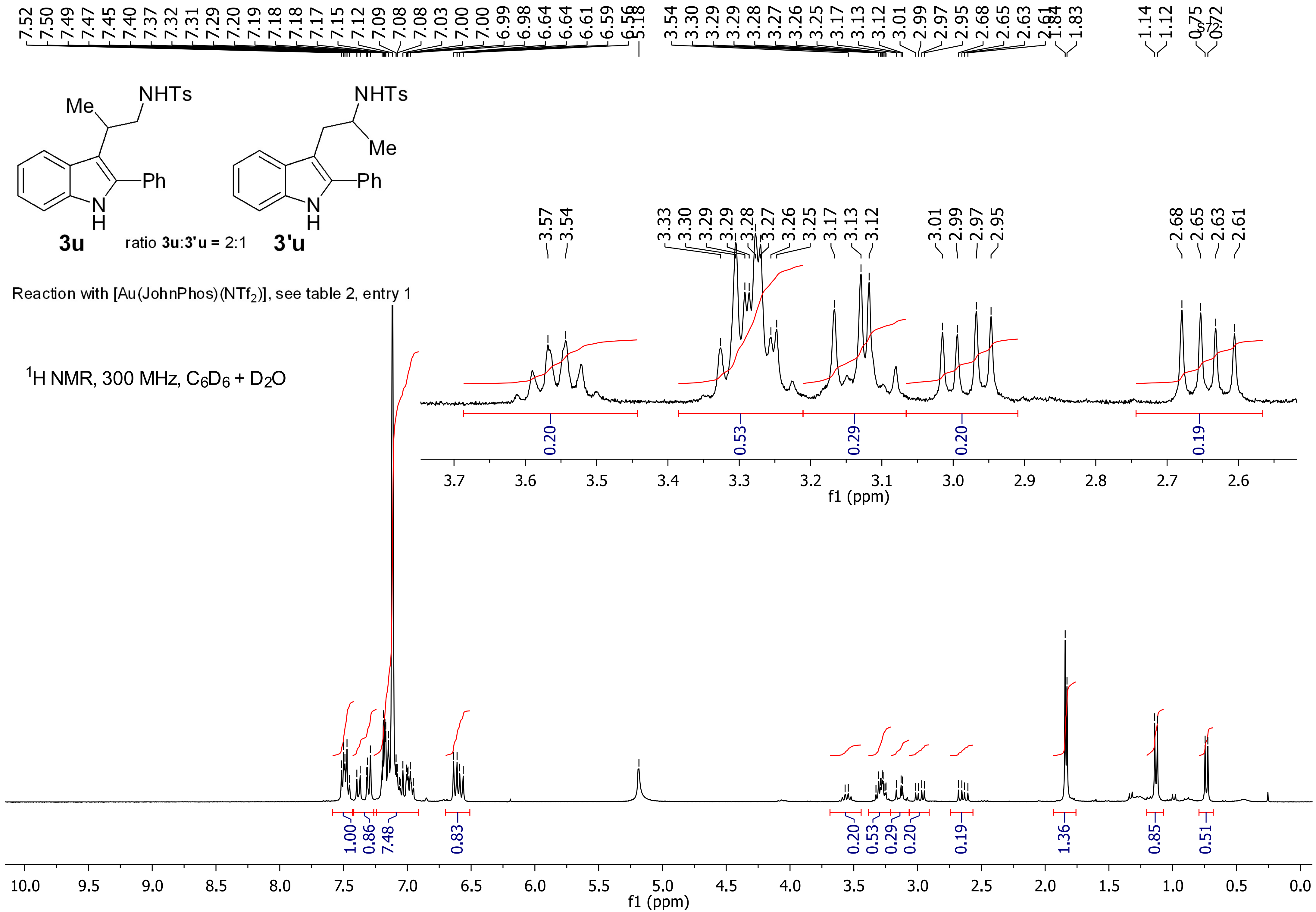
3'u

Reaction with [Au(JohnPhos)(NTf_2)], see table 2, entry 1



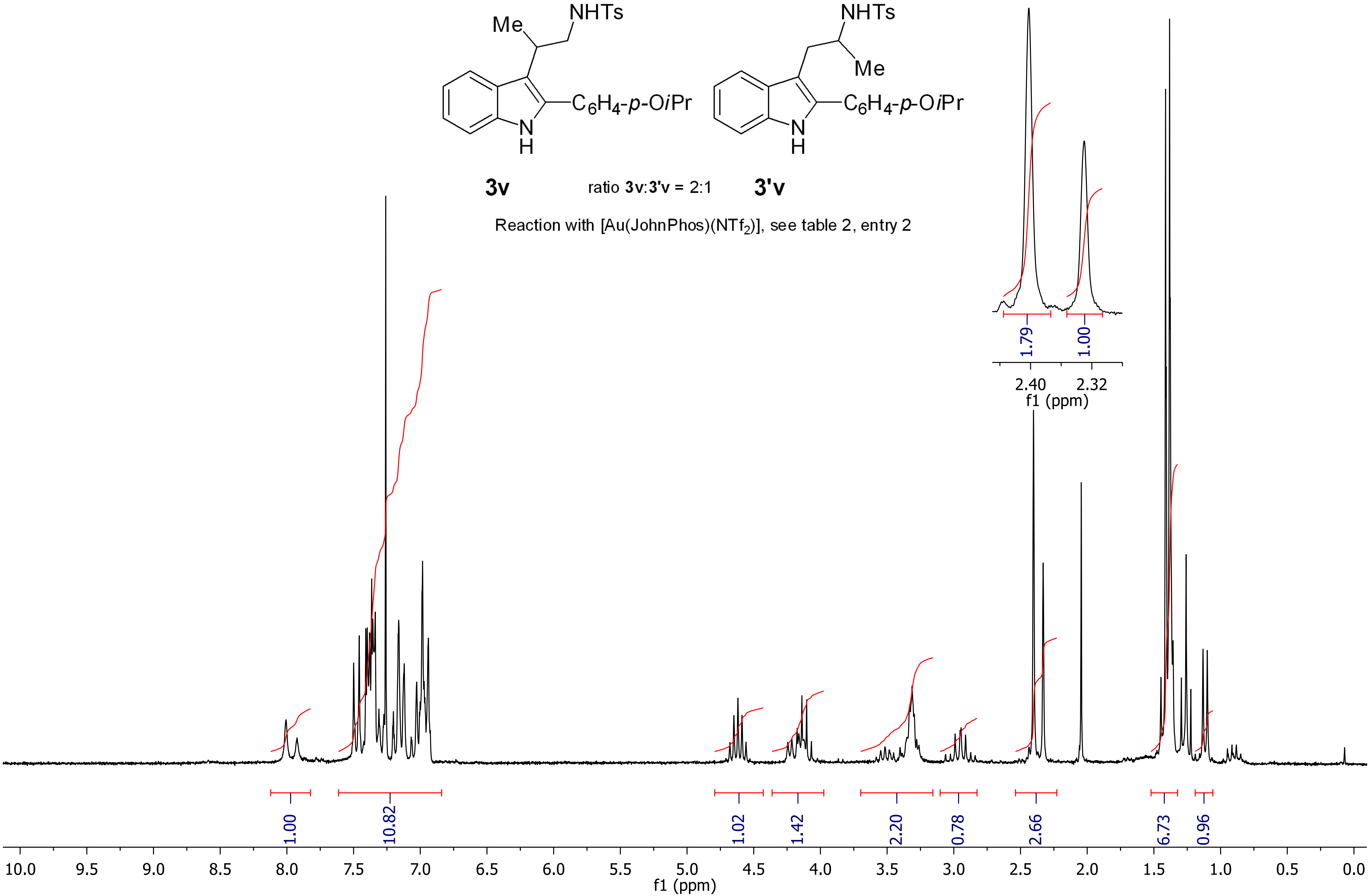


NHTs
Me
Ph
N
H
3u
ratio 3u:3'u = 2:1
3'u
Reaction with [Au(JohnPhos)(NTf2)], see table 2, entry 1
1H NMR, 300 MHz, C6D6
f1 (ppm)

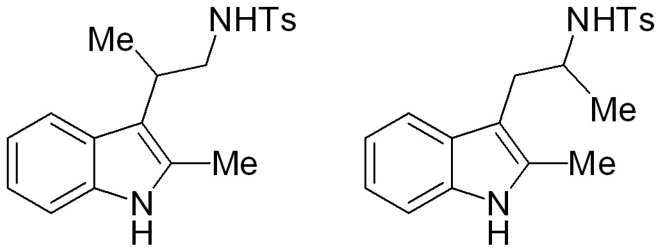


NHTs
Me
Ph
N
H
3u
ratio 3u:3'u = 2:1
3'u
Reaction with [Au(JohnPhos)(NTf2)], see table 2, entry 1
1H NMR, 300 MHz, C6D6 + D2O
f1 (ppm)

^{1}H NMR, 200 MHz, $CDCl_3$

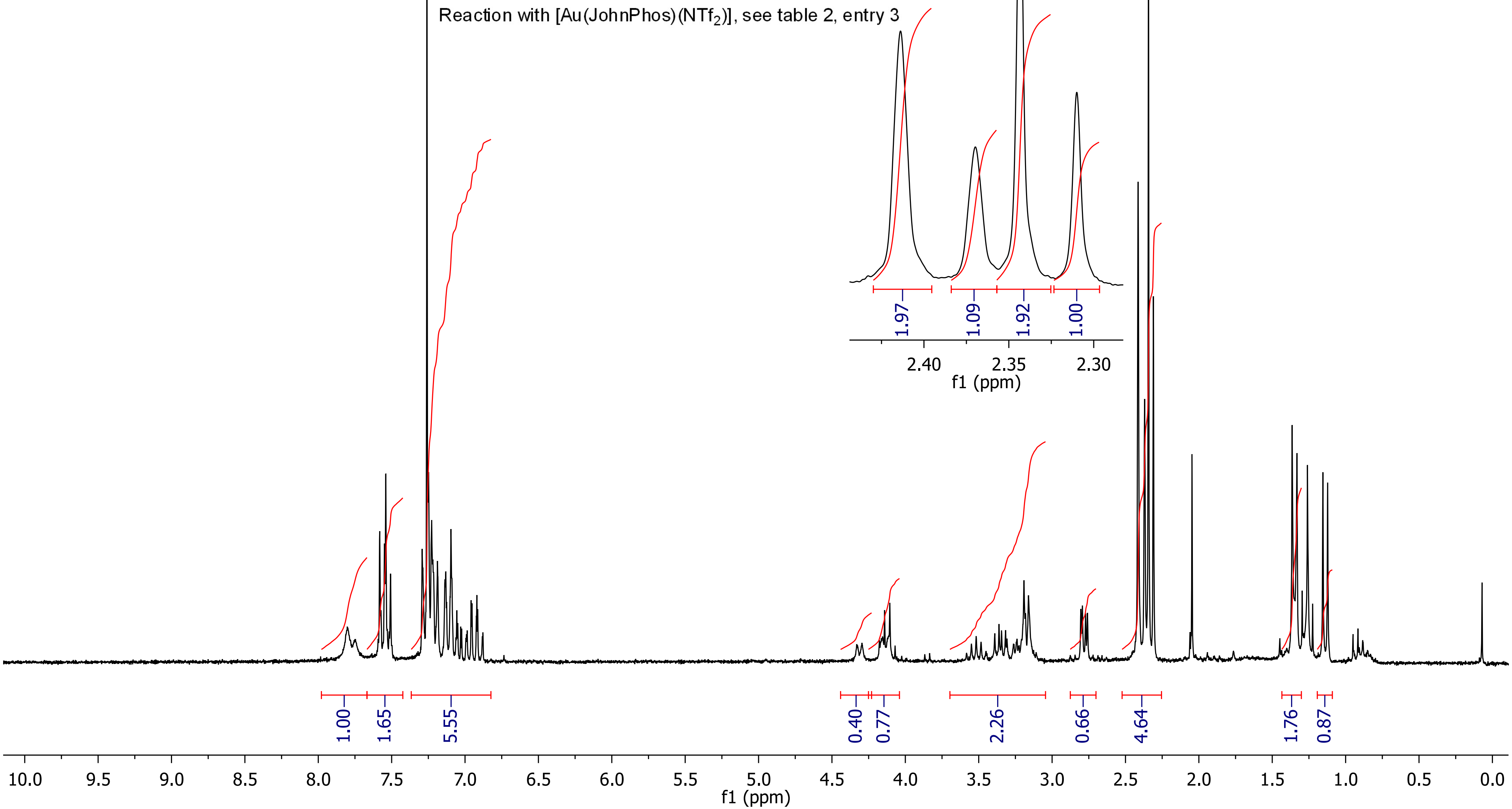


^{1}H NMR, 200 MHz, $CDCl_3$

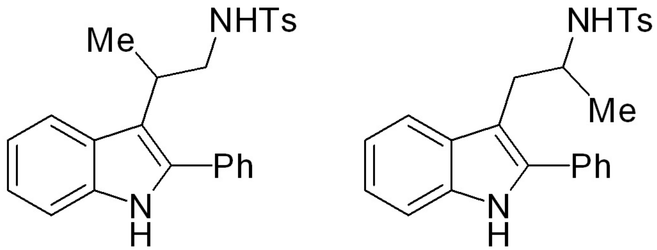


3w ratio **3w**:**3'w** = 2:1 **3'w**

Reaction with [Au(JohnPhos)(NTf_2)], see table 2, entry 3

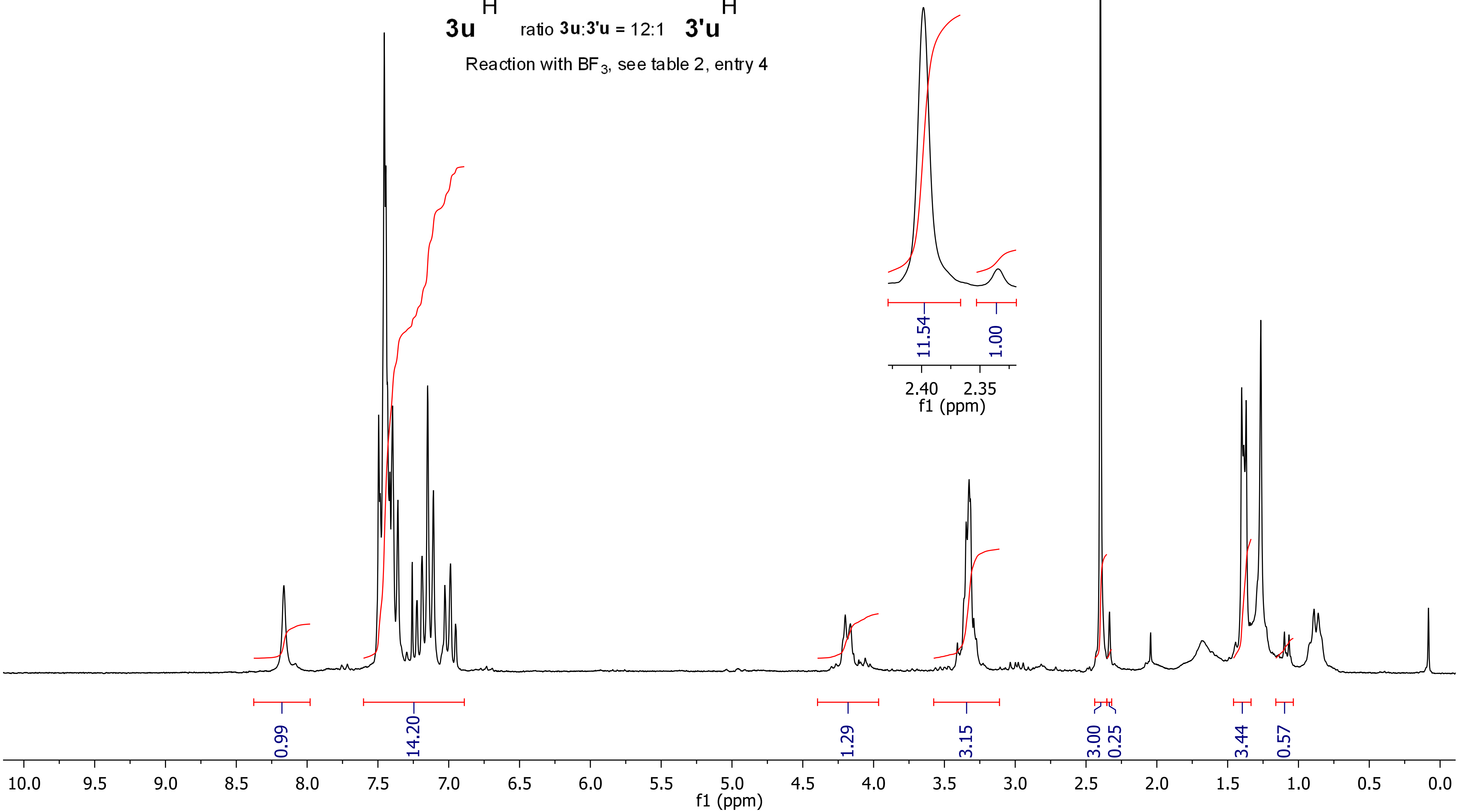


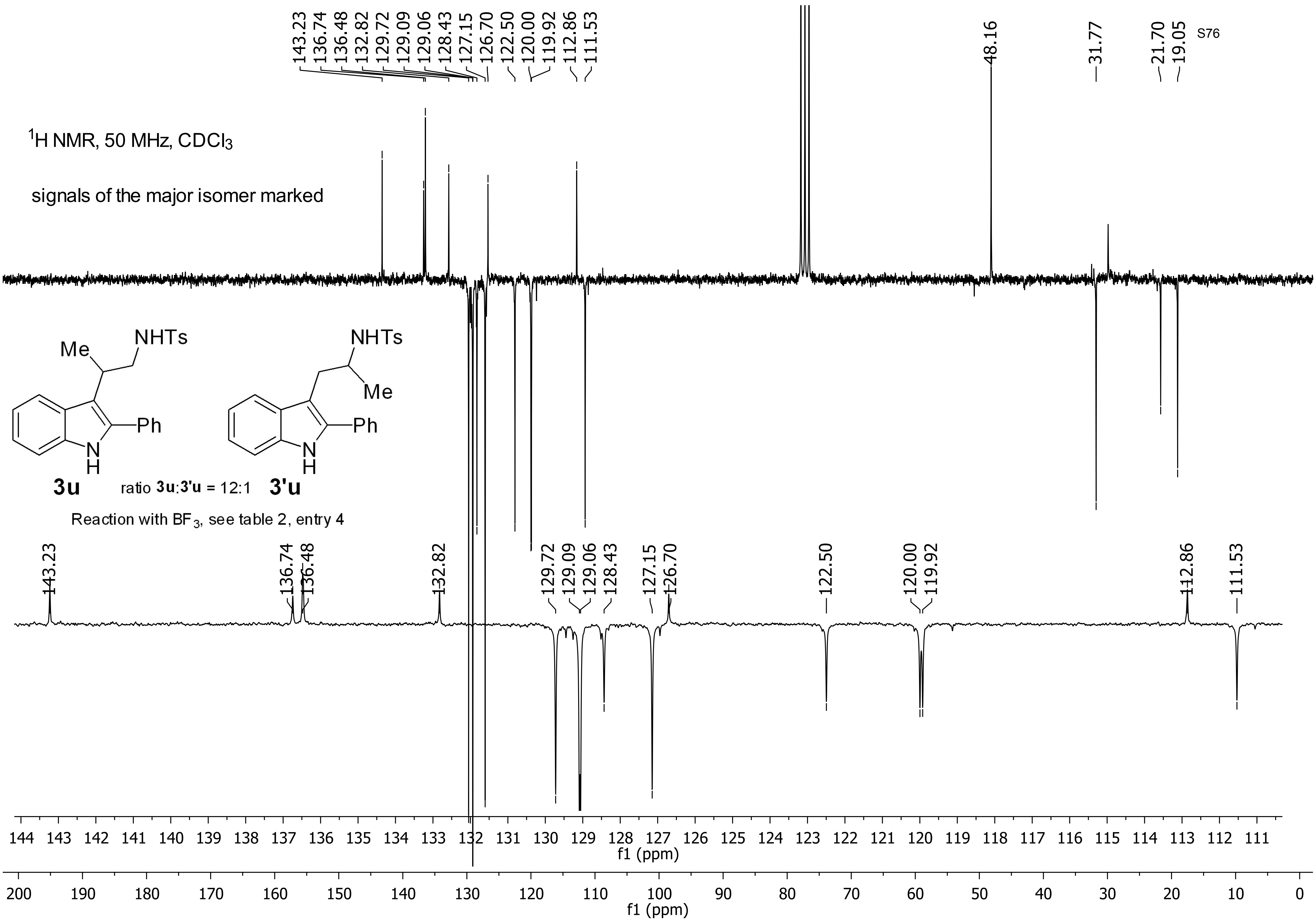
^1H NMR, 200 MHz, $CDCl_3$



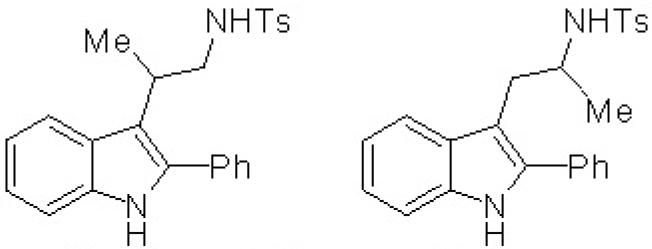
3u ratio **3u**:**3'u** = 12:1 **3'u**

Reaction with BF_3, see table 2, entry 4



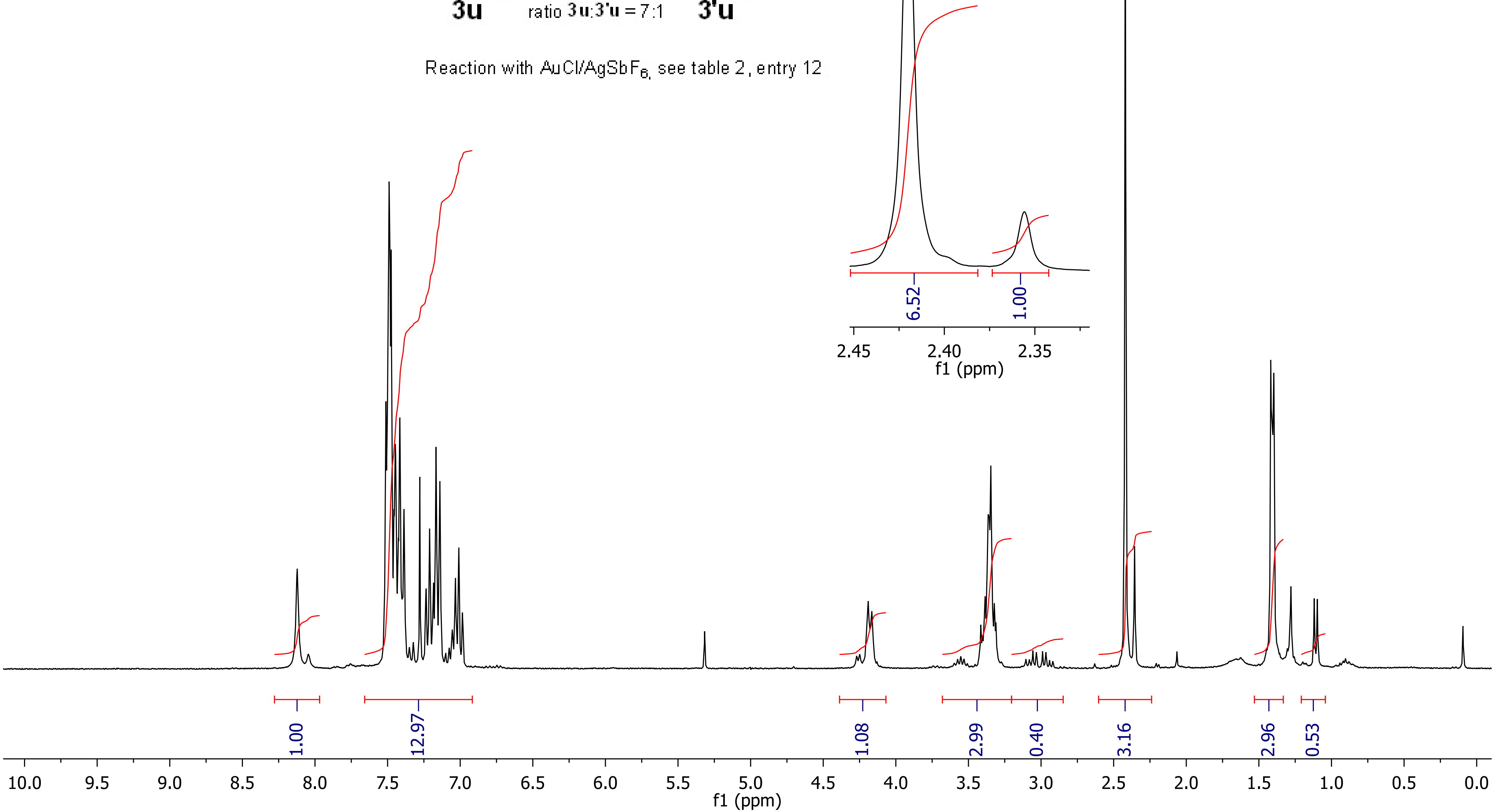

143.23
136.74
136.48
132.82
129.72
129.09
129.06
128.43
127.15
126.70
122.50
120.00
119.92
112.86
111.53
48.16
31.77
21.70
19.05
1H NMR, 50 MHz, CDCl3
signals of the major isomer marked
Me
NHTs
Ph
N
H
3u
NHTs
Me
Ph
N
H
3'u
ratio 3u:3'u = 12:1
Reaction with BF3, see table 2, entry 4
f1 (ppm)
f1 (ppm)

^{1}H NMR, 300 MHz, $CDCl_3$

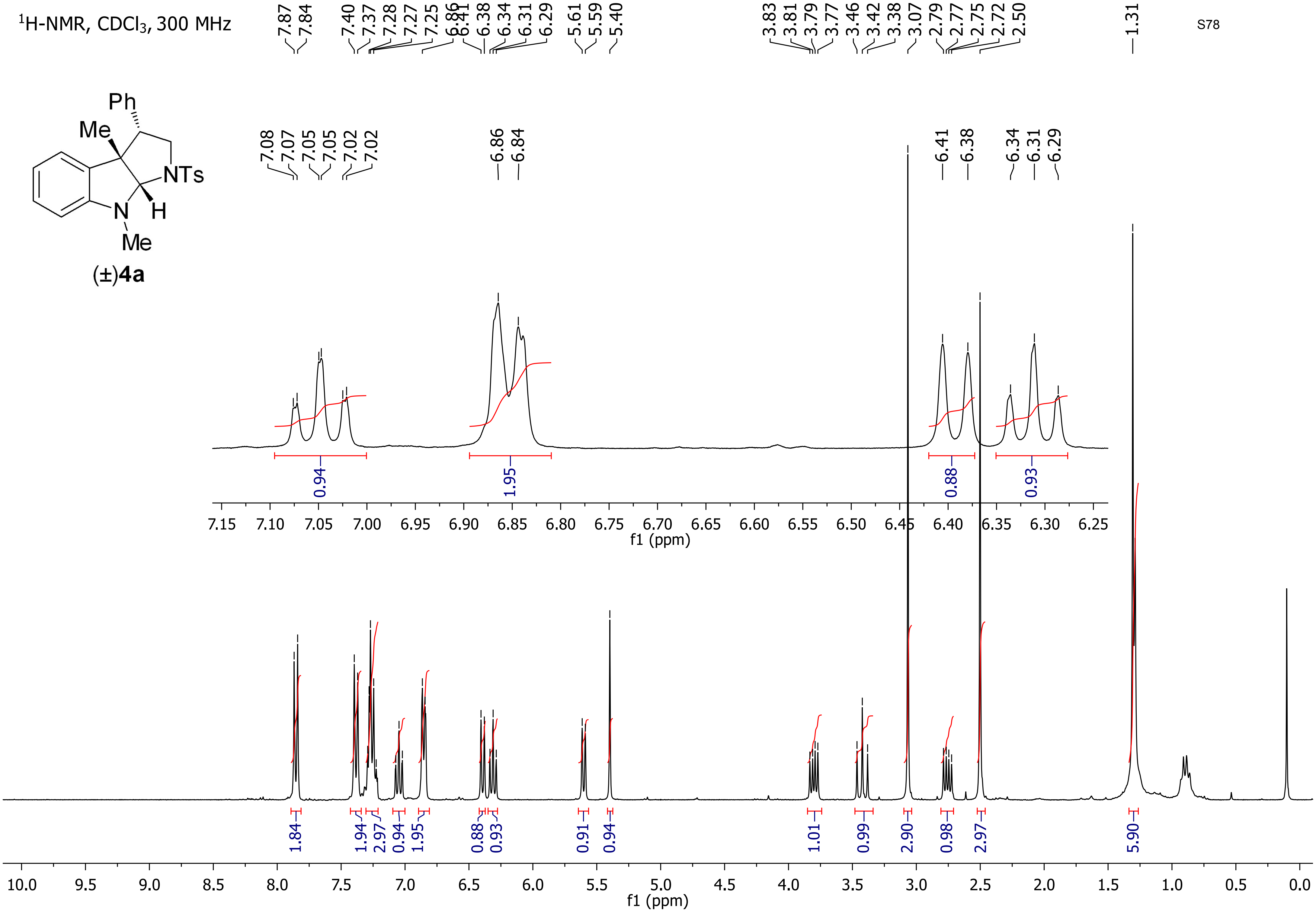


3u ratio **3u**:**3'u** = 7:1 **3'u**

Reaction with AuCl/AgSbF$_6$, see table 2, entry 12

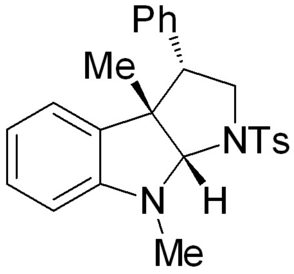


^{1}H-NMR, $CDCl_3$, 300 MHz

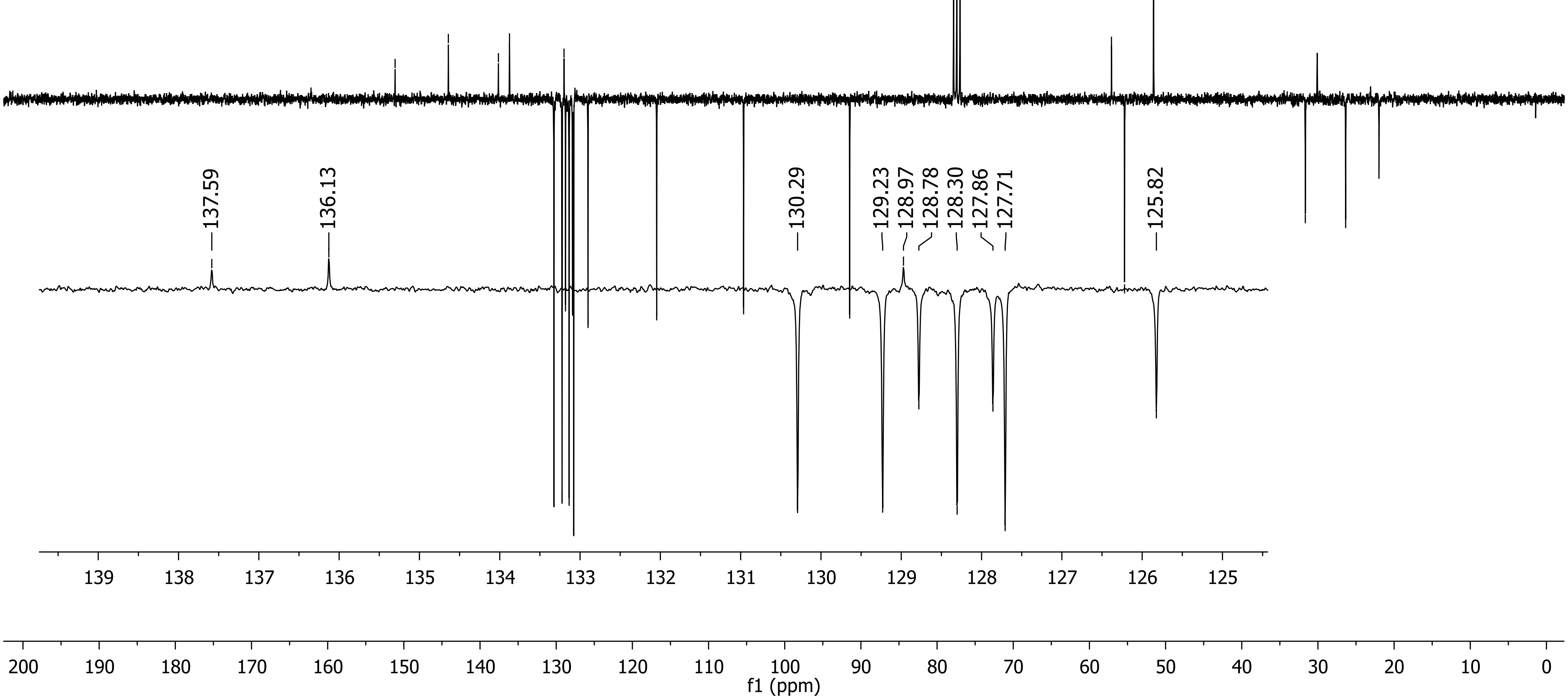


(±)**4a**

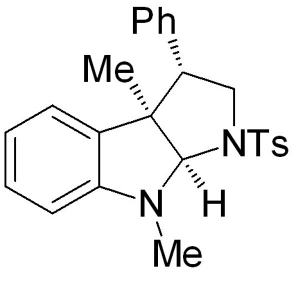
^{13}C-NMR, $CDCl_3$, 75 MHz



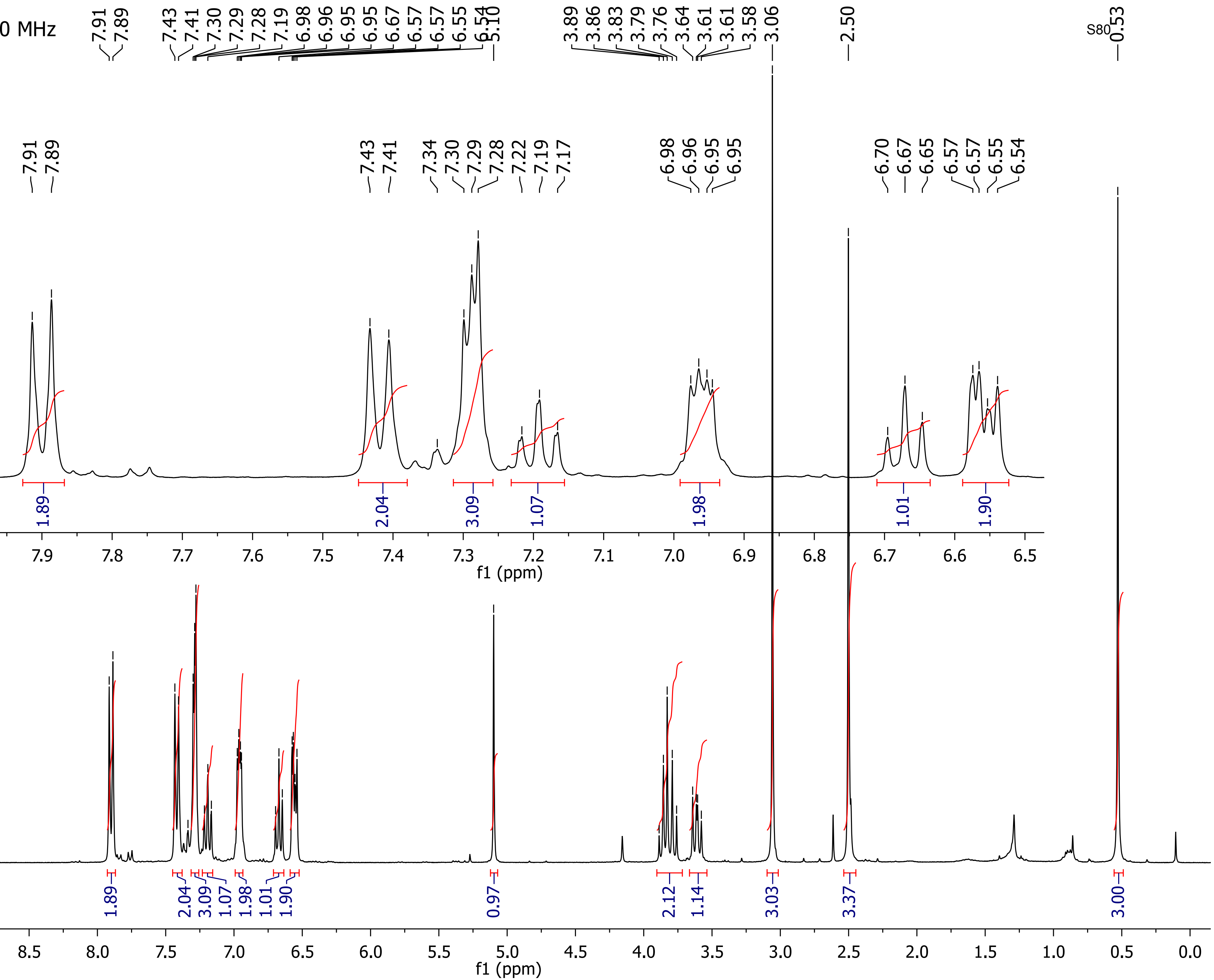
(±)**4a**



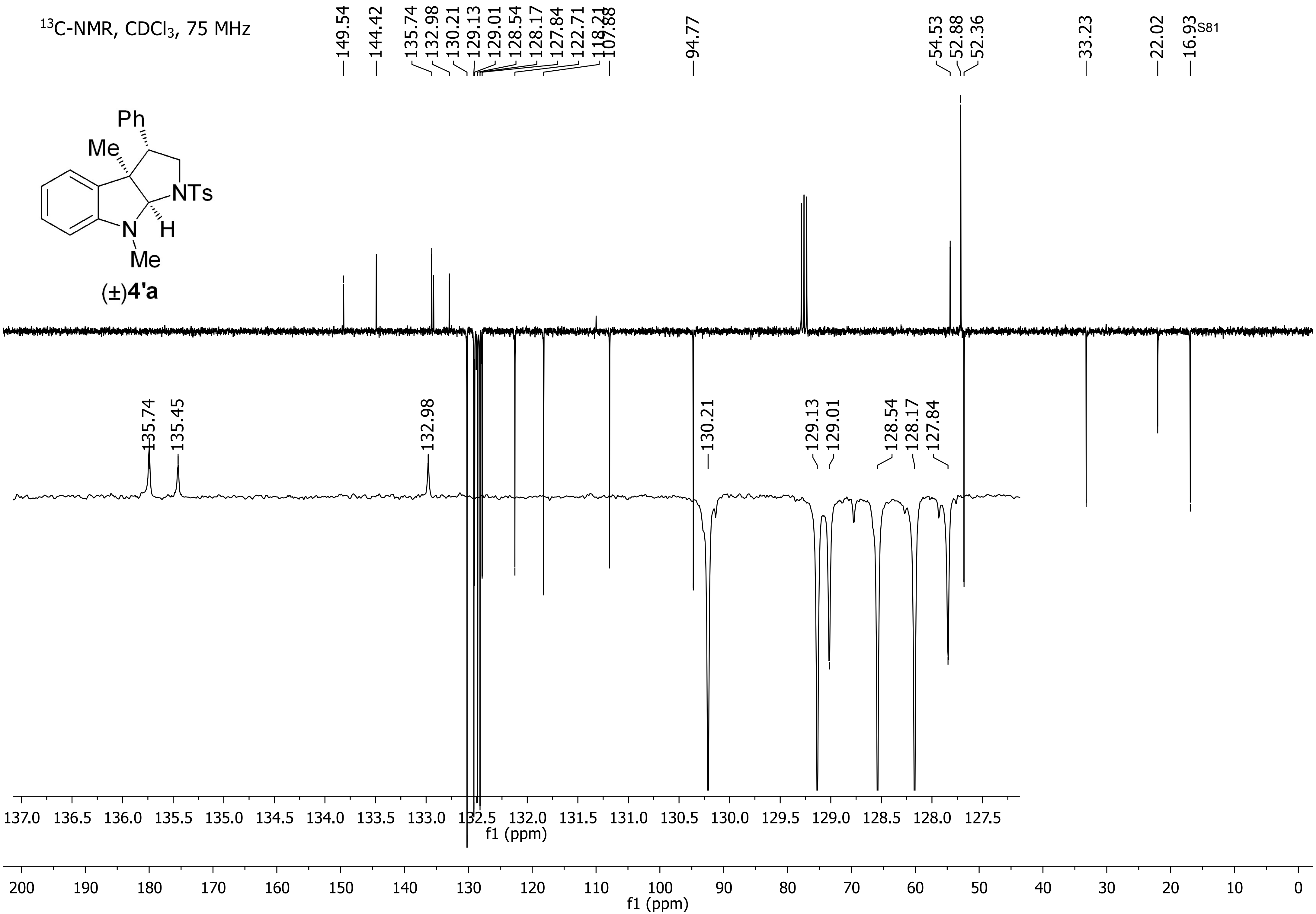
^{1}H-NMR, $CDCl_3$, 300 MHz

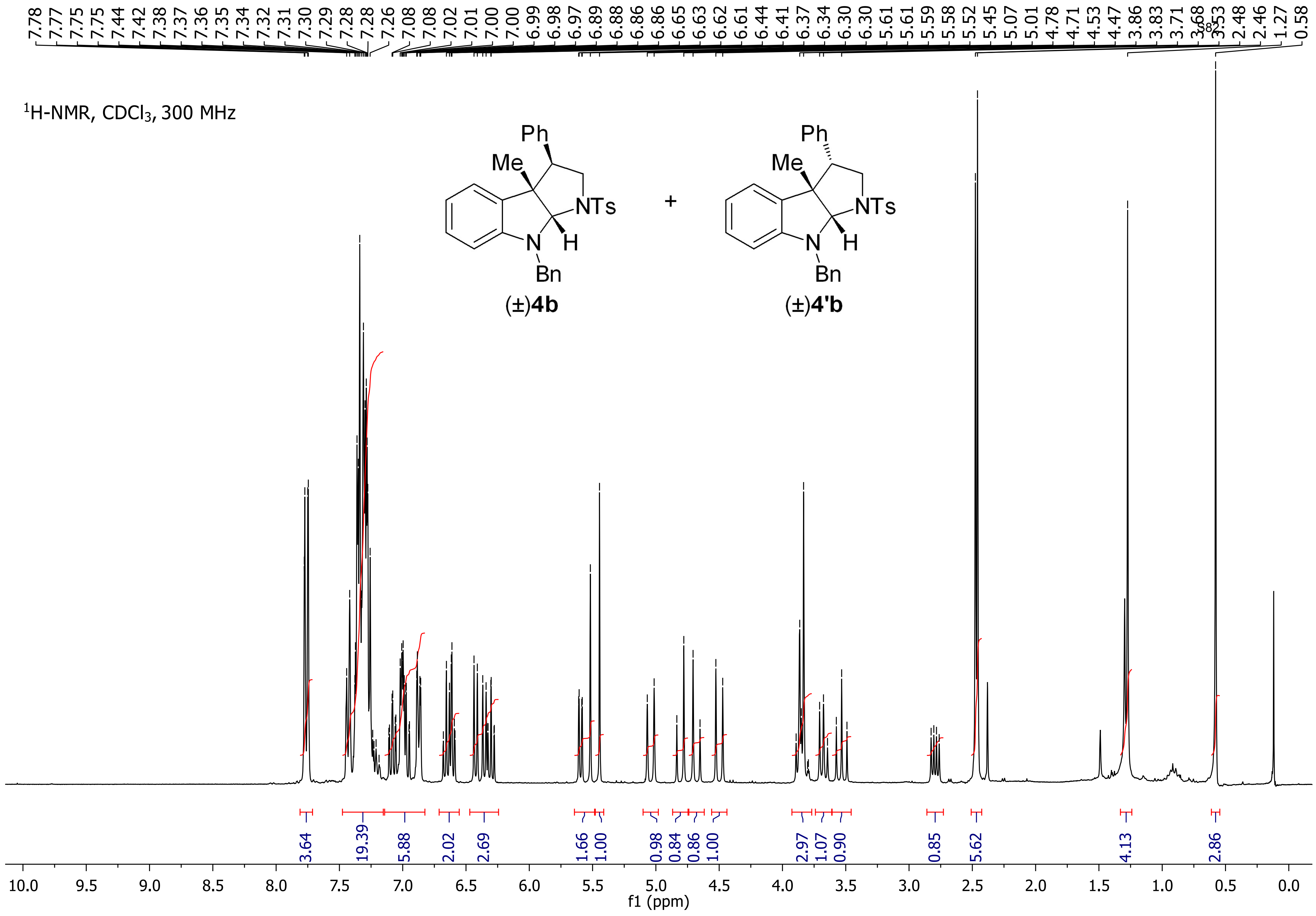


(±)**4'a**

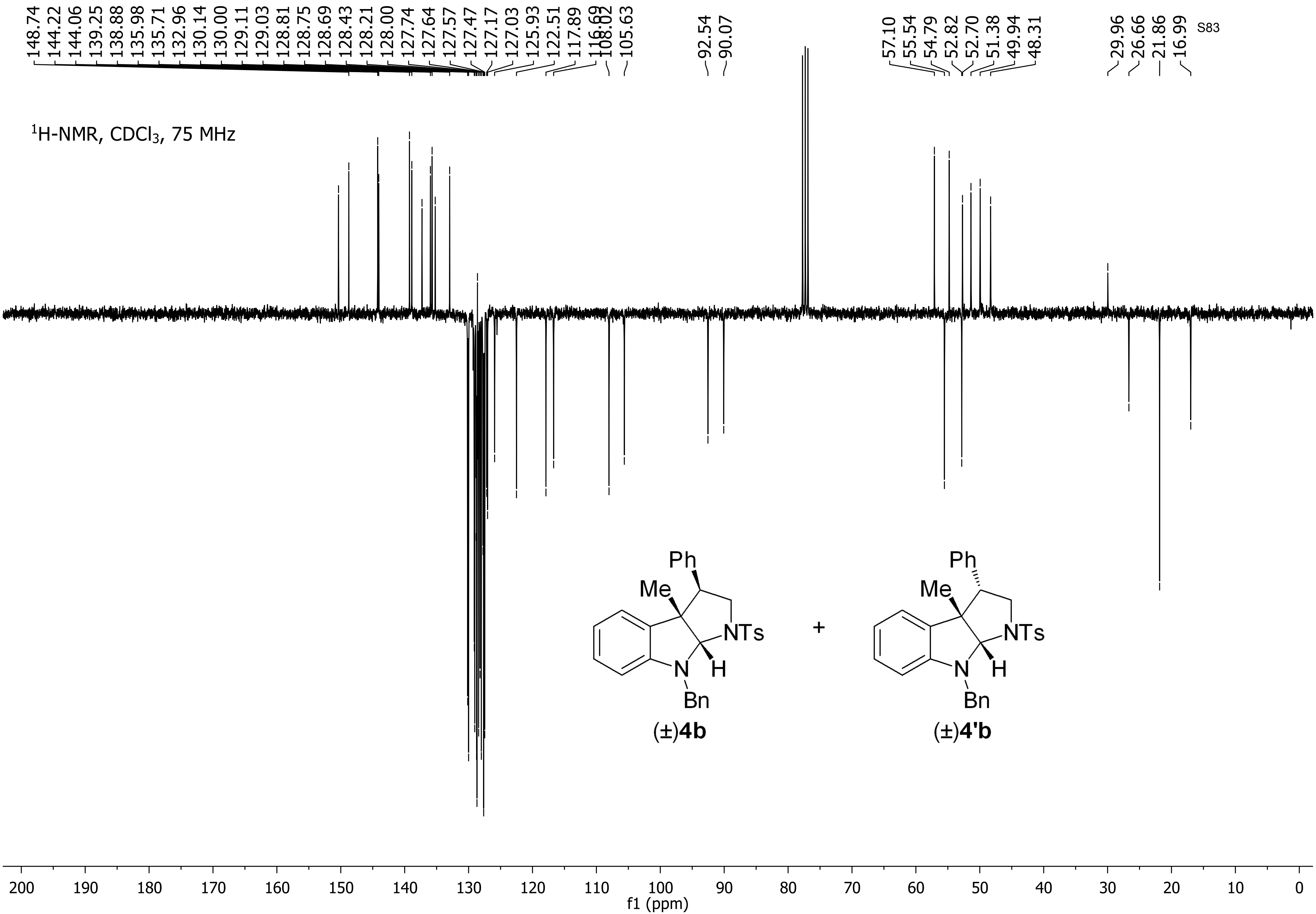


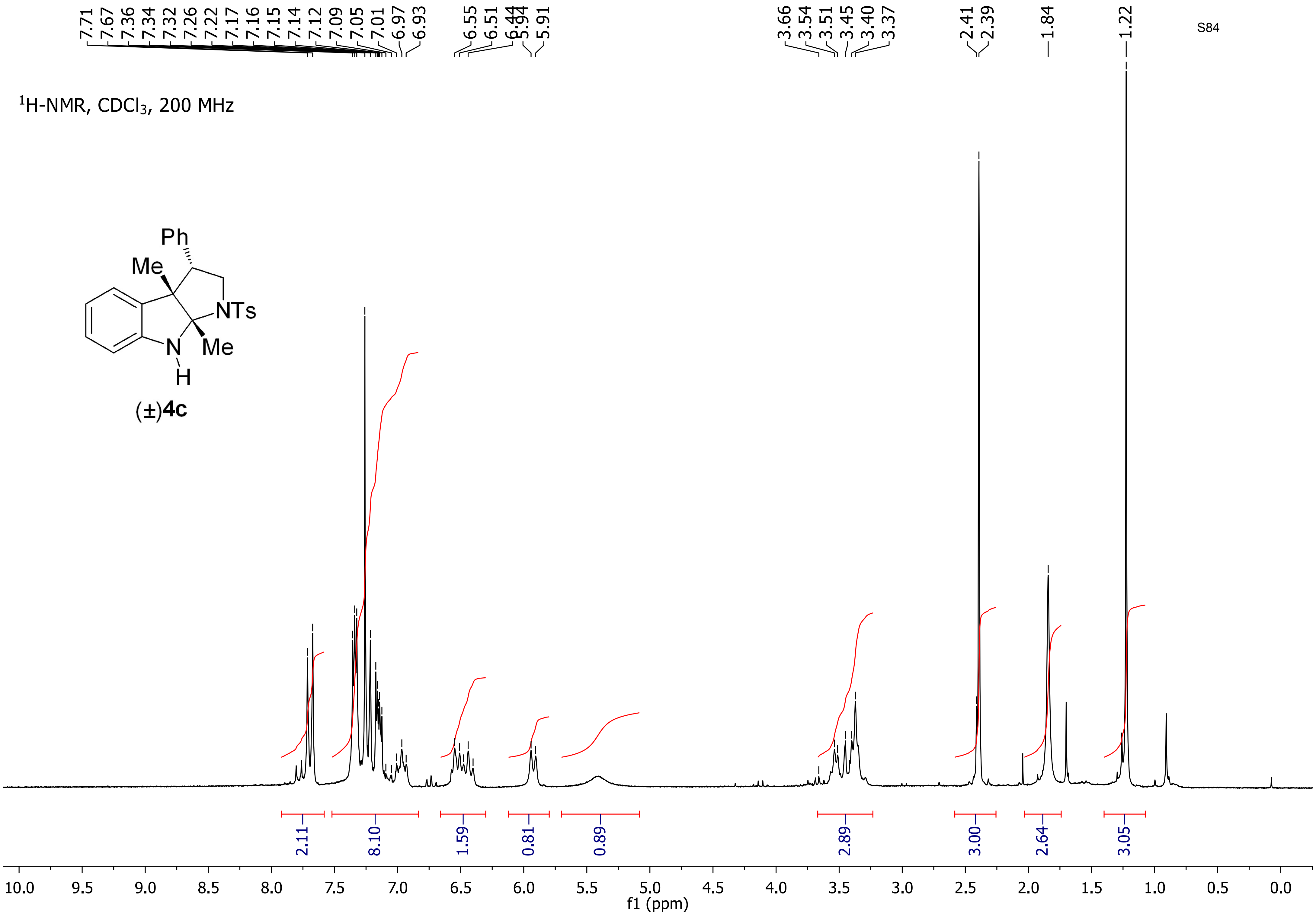
^{13}C-NMR, $CDCl_3$, 75 MHz



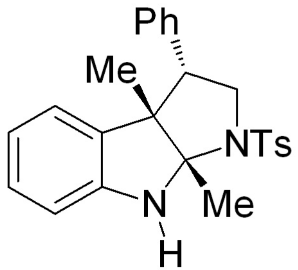


^{1}H-NMR, CDCl$_3$, 300 MHz
Ph
Me
NTs
N
H
Bn
(±)**4b**
+
Ph
Me
NTs
N
H
Bn
(±)**4'b**
3.64
19.39
5.88
2.02
2.69
1.66
1.00
0.98
0.84
0.86
1.00
2.97
1.07
0.90
0.85
5.62
4.13
2.86
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.74
144.22
144.06
139.25
138.88
135.98
135.71
132.96
130.14
130.00
129.11
129.03
128.81
128.75
128.69
128.43
128.21
128.00
127.74
127.64
127.57
127.47
127.17
127.03
125.93
122.51
117.89
116.69
108.02
105.63
92.54
90.07
57.10
55.54
54.79
52.82
52.70
51.38
49.94
48.31
29.96
26.66
21.86
16.99
^{1}H-NMR, $CDCl_3$, 75 MHz
Ph
Me
NTs
H
N
Bn
(±)4b
+
(±)4'b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.71
7.67
7.36
7.34
7.32
7.26
7.22
7.17
7.16
7.15
7.14
7.12
7.09
7.05
7.01
6.97
6.93
6.55
6.51
6.44
5.94
5.91
3.66
3.54
3.51
3.45
3.40
3.37
2.41
2.39
1.84
1.22
¹H-NMR, CDCl₃, 200 MHz
Ph
Me
NTs
N
Me
H
(±)4c
2.11
8.10
1.59
0.81
0.89
2.89
3.00
2.64
3.05
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
0.0
f1 (ppm)

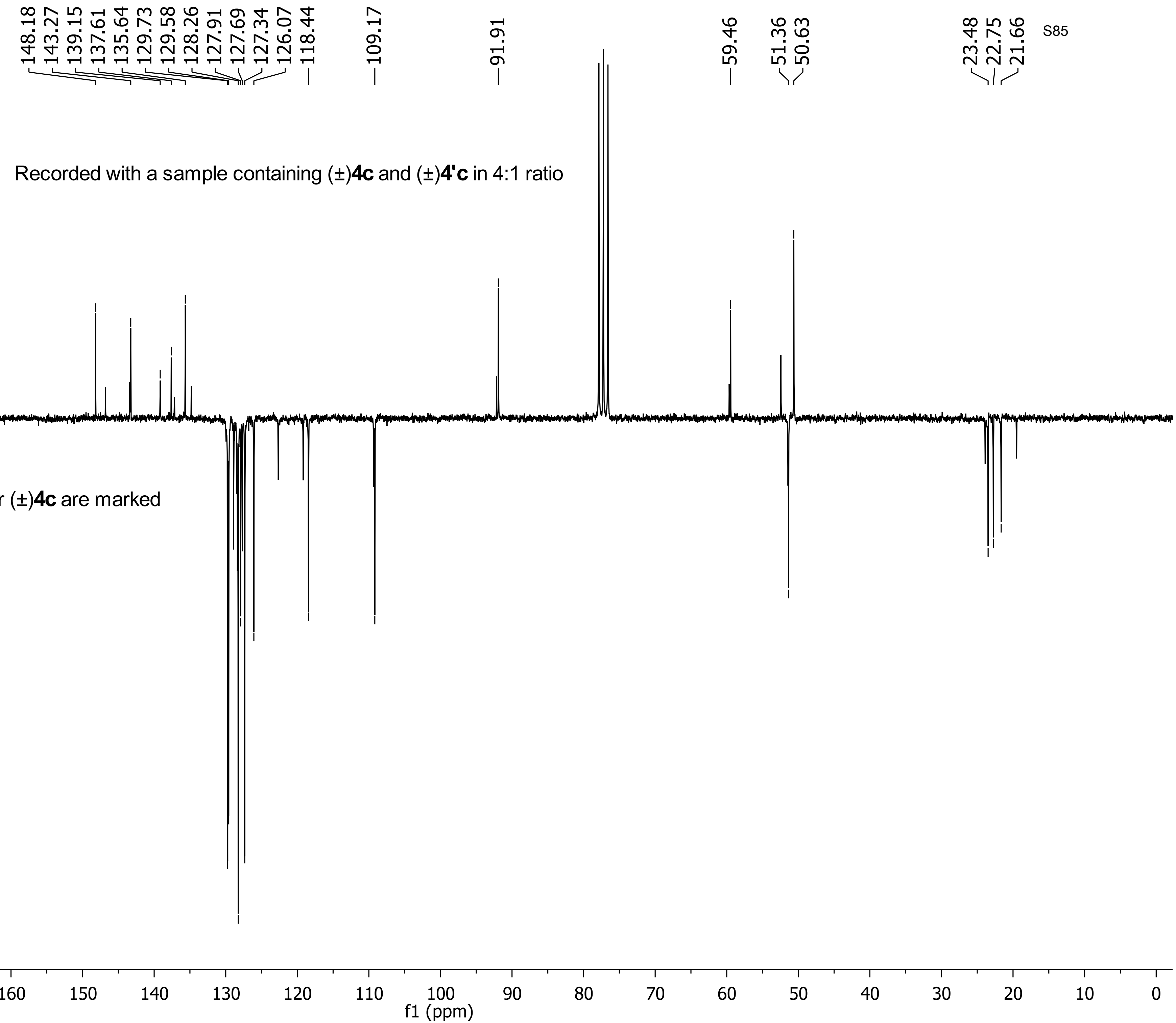
^{13}C-NMR, $CDCl_3$, 50 MHz



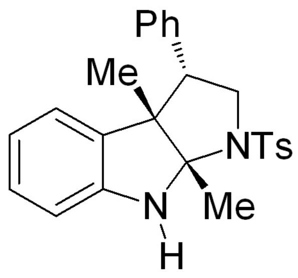
(±)**4c**

Recorded with a sample containing (±)**4c** and (±)**4'c** in 4:1 ratio

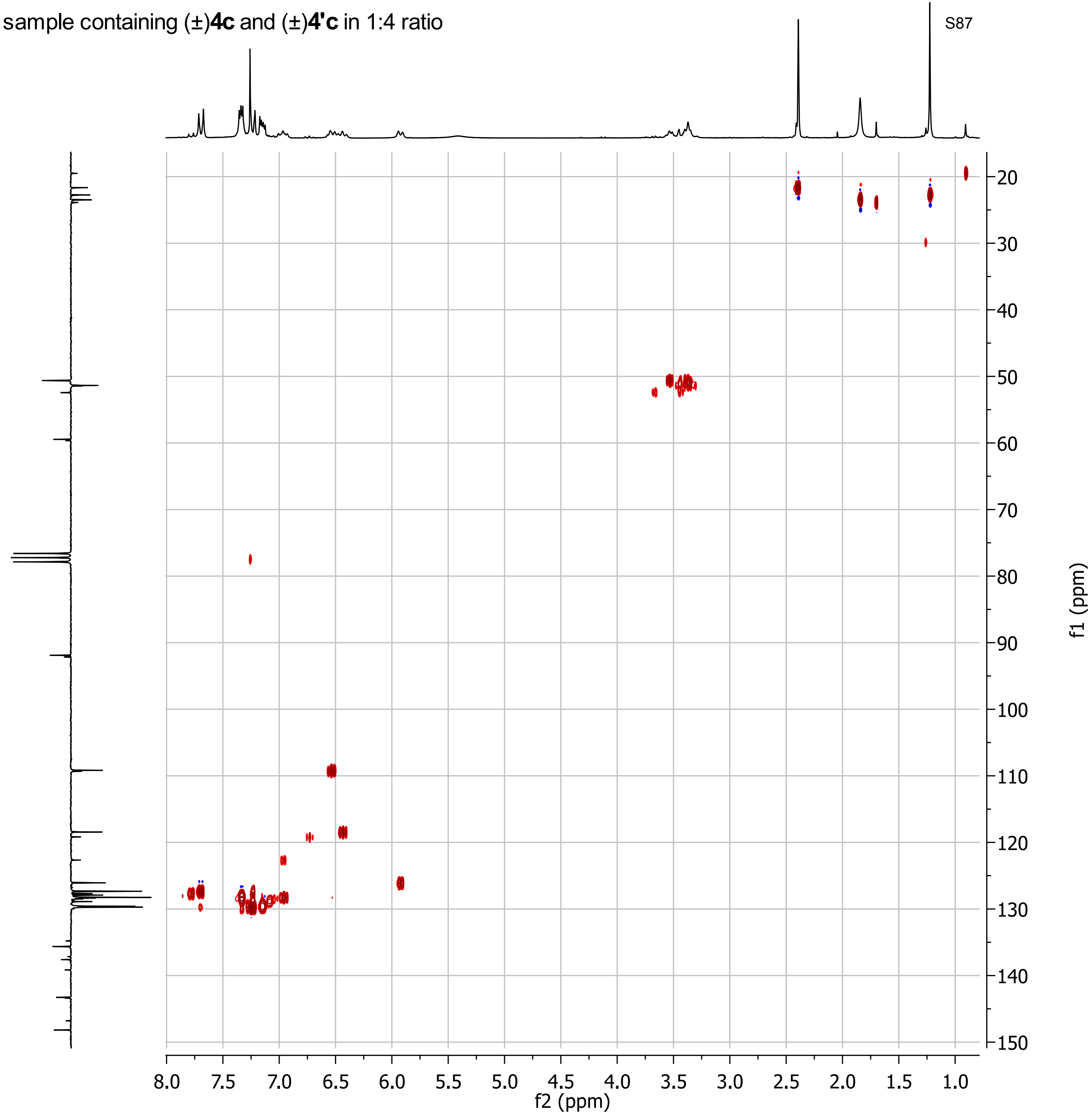
Peaks of the major isomer (±)**4c** are marked



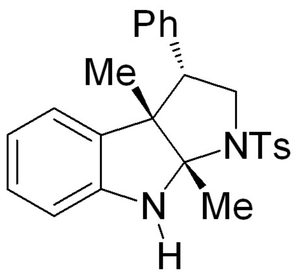
HSQC-NMR, $CDCl_3$, 300 MHz Recorded with a sample containing (±)**4c** and (±)**4'c** in 1:4 ratio



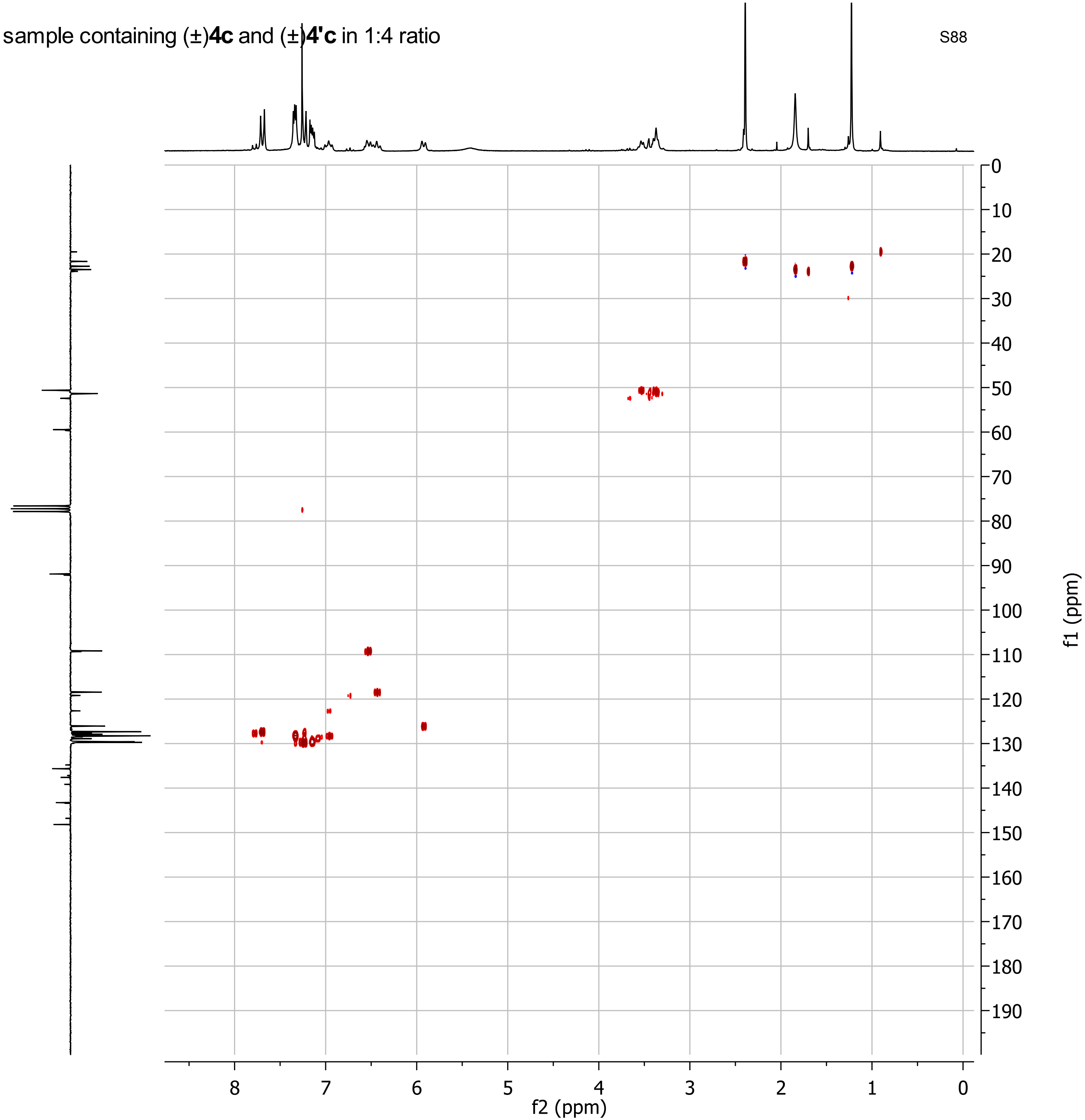
(±)**4c**



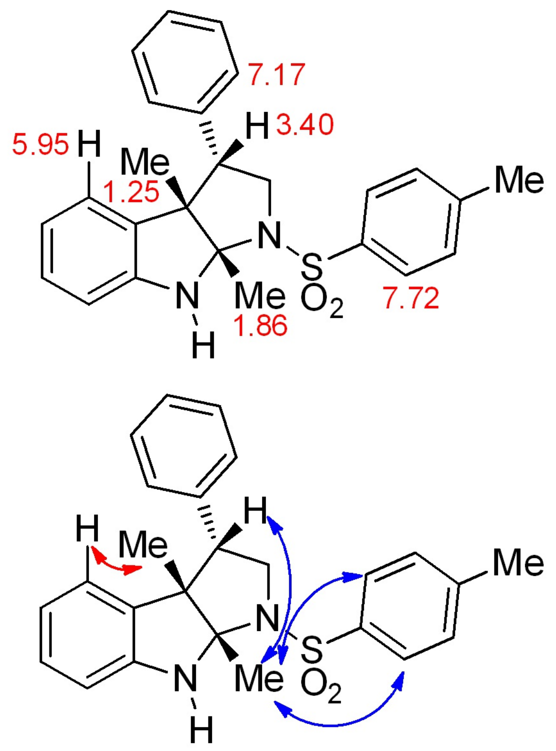
HSQC-NMR, $CDCl_3$, 300 MHz Recorded with a sample containing (±)**4c** and (±)**4'c** in 1:4 ratio



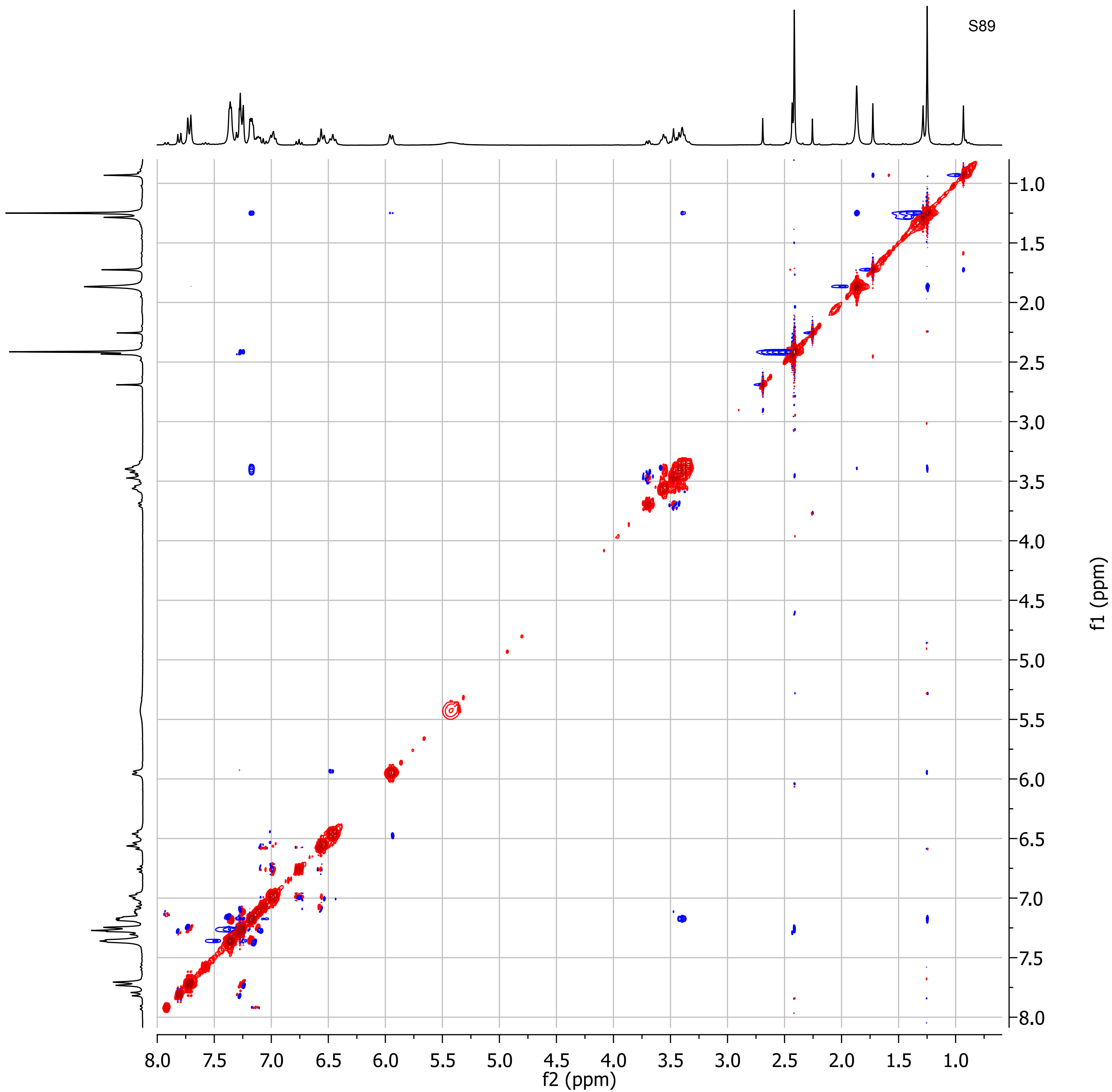
(±)**4c**



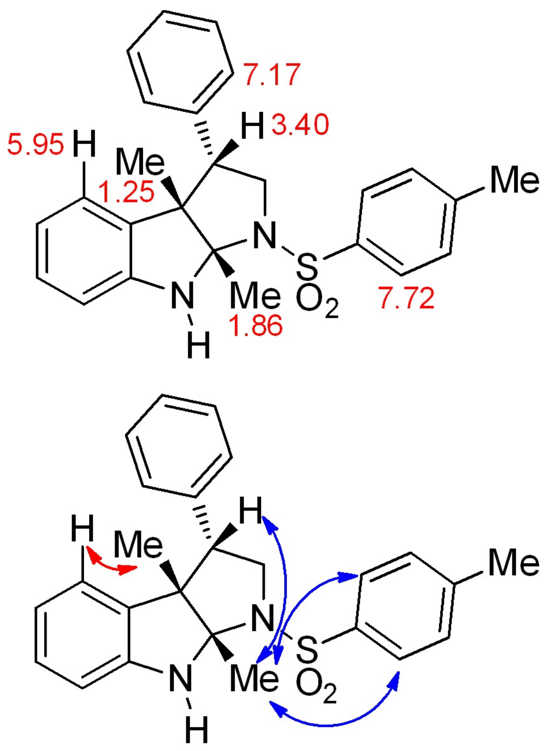
NOESY-NMR, $CDCl_3$, 300 MHz



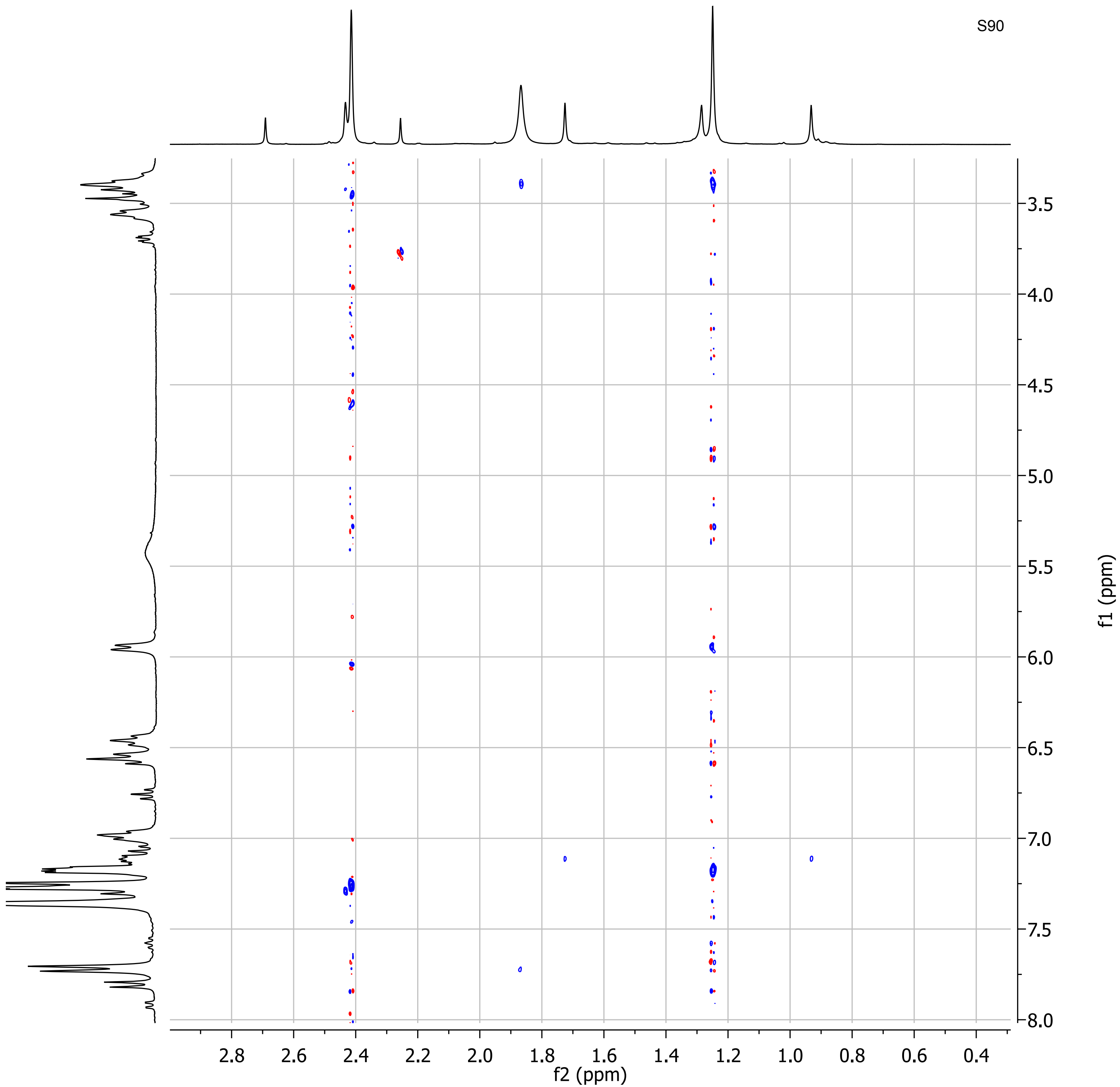
(±)**4c**

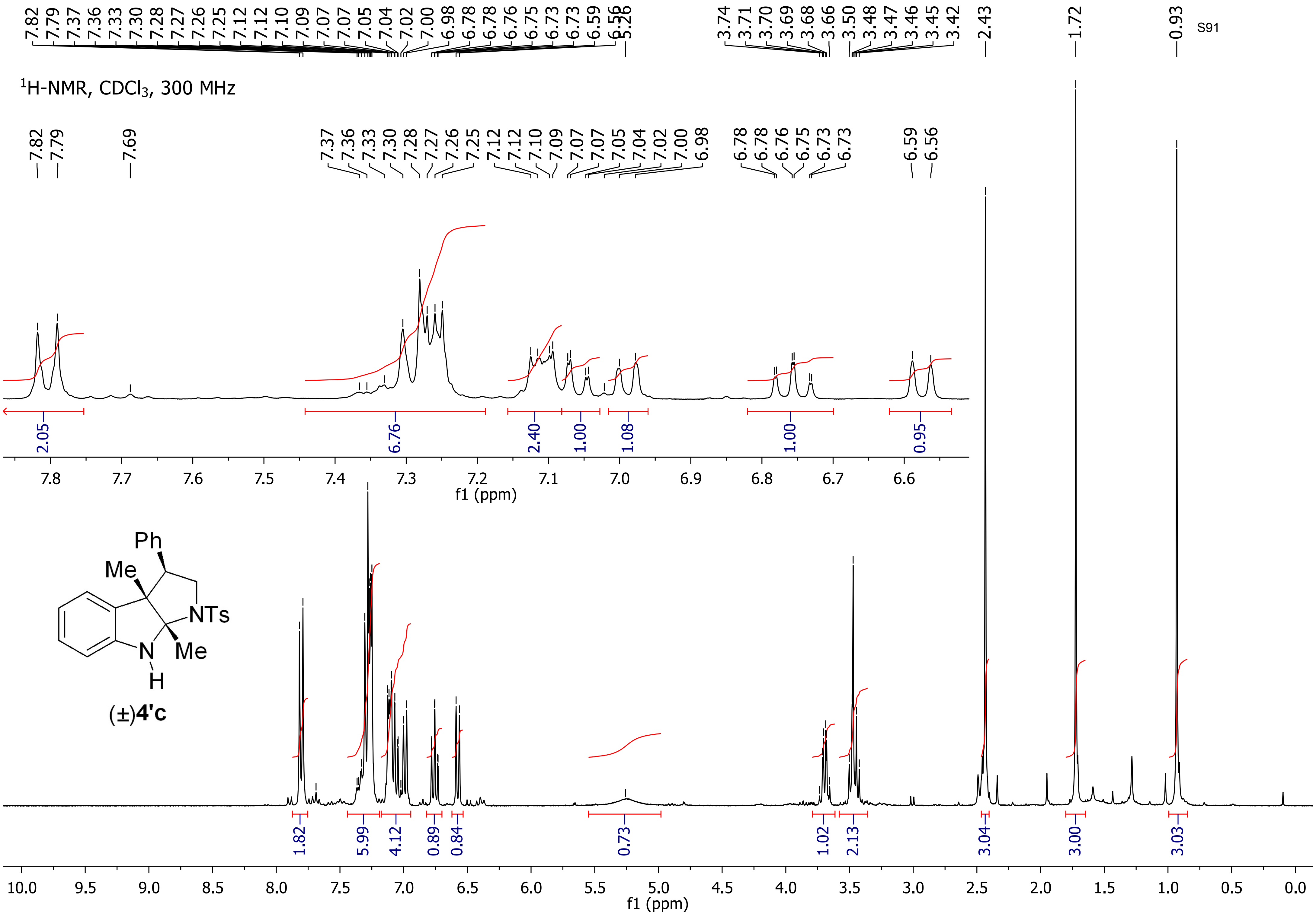


NOESY-NMR, $CDCl_3$, 300 MHz



(±)**4c**



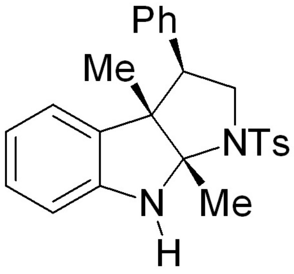


1H-NMR, CDCl3, 300 MHz
7.82 7.79 7.37 7.36 7.33 7.30 7.28 7.27 7.26 7.25 7.12 7.12 7.10 7.09 7.07 7.07 7.05 7.04 7.02 7.00 6.98 6.78 6.78 6.76 6.75 6.73 6.73 6.59 6.56 5.26
3.74 3.71 3.70 3.69 3.68 3.66 3.50 3.48 3.47 3.46 3.45 3.42
2.43
1.72
0.93
7.82 7.79 7.69
7.37 7.36 7.33 7.30 7.28 7.27 7.26 7.25 7.12 7.12 7.10 7.09 7.07 7.07 7.05 7.04 7.02 7.00 6.98
6.78 6.78 6.76 6.75 6.73 6.73
6.59 6.56
2.05 6.76 2.40 1.00 1.08 1.00 0.95
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6
f1 (ppm)
1.82 5.99 4.12 0.89 0.84 0.73 1.02 2.13 3.04 3.00 3.03
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 0.0
f1 (ppm)
Ph
Me
NTs
N
H
Me

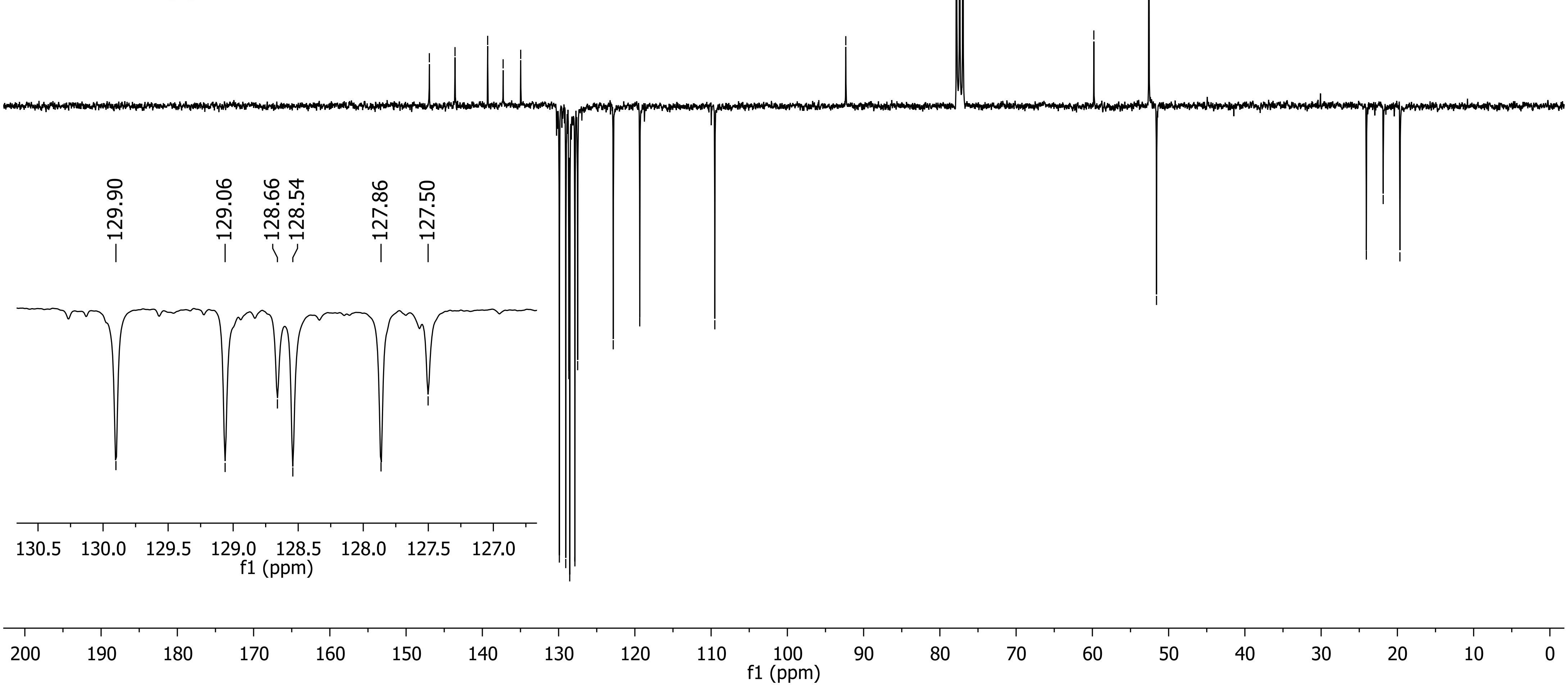
(±)**4'c**

^{13}C-NMR, $CDCl_3$, 75 MHz

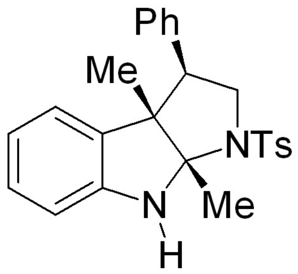
S92



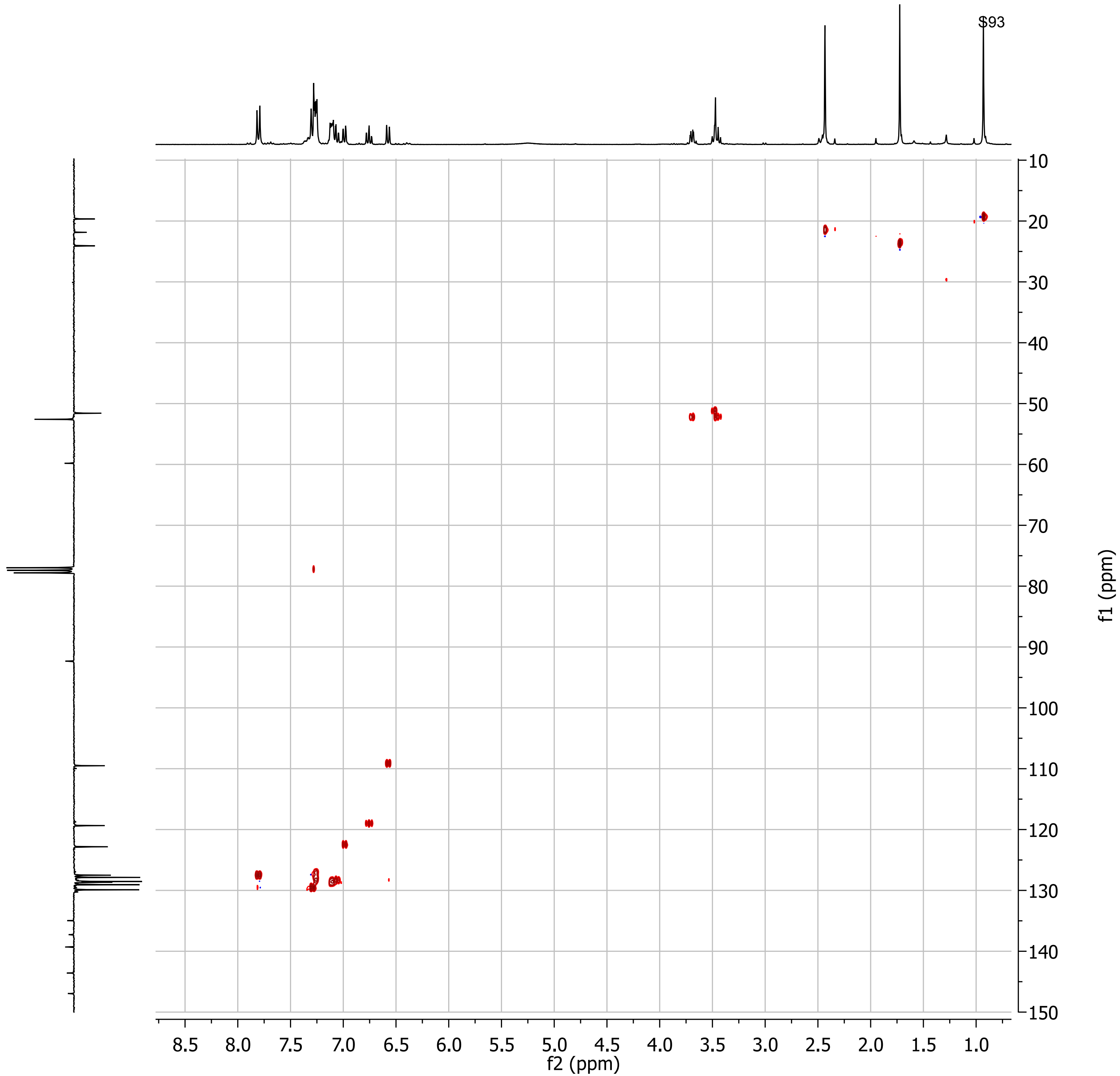
(±)**4'c**



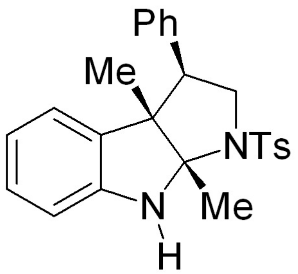
HSQC-NMR, CDCl$_3$, 300 MHz



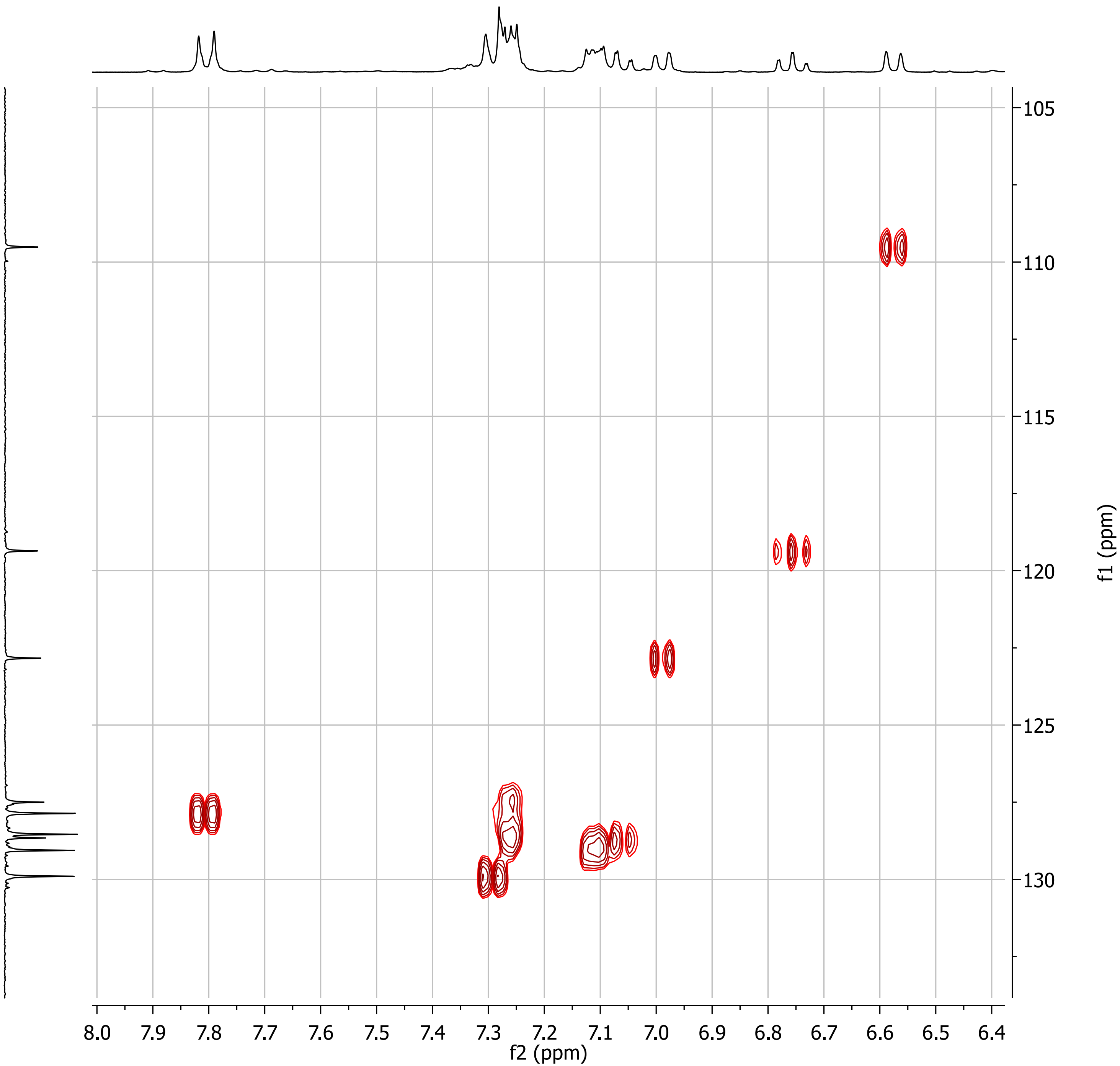
(±)**4'c**



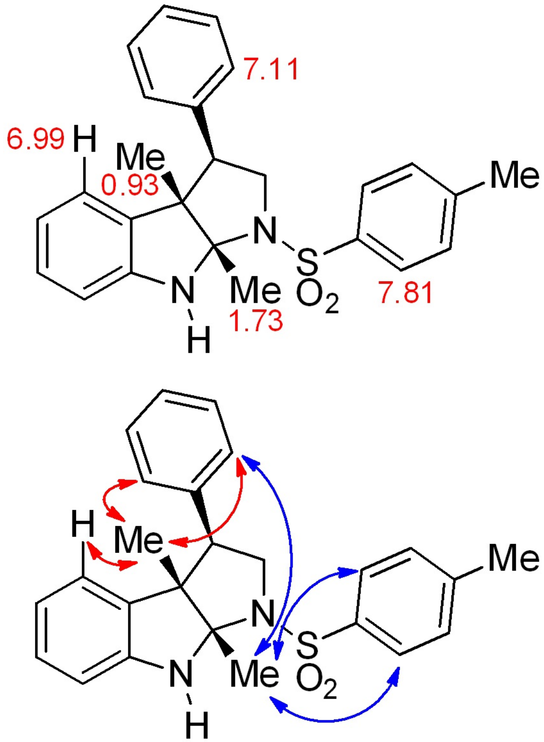
HSQC-NMR, $CDCl_3$, 300 MHz



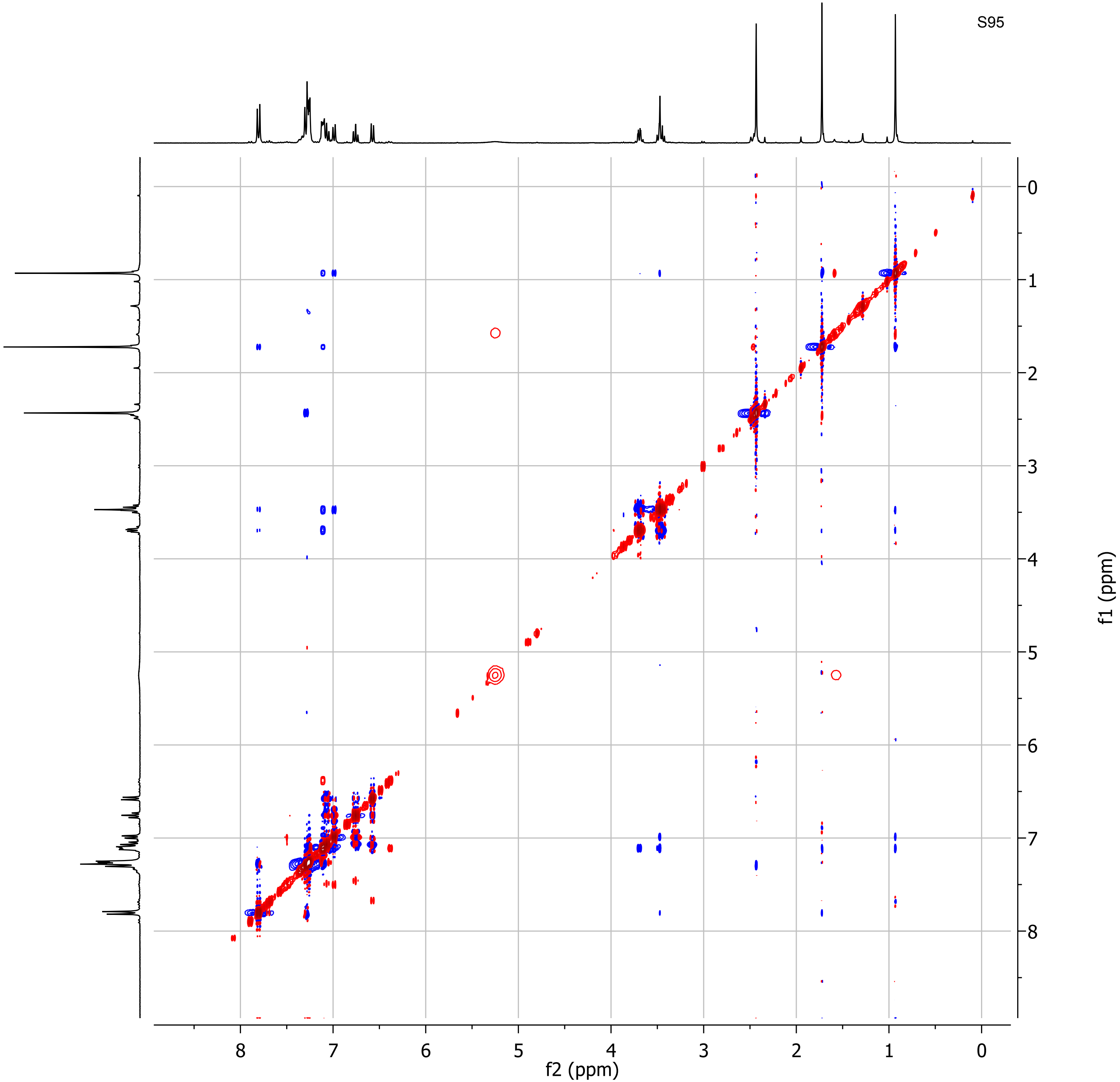
(±)**4'c**



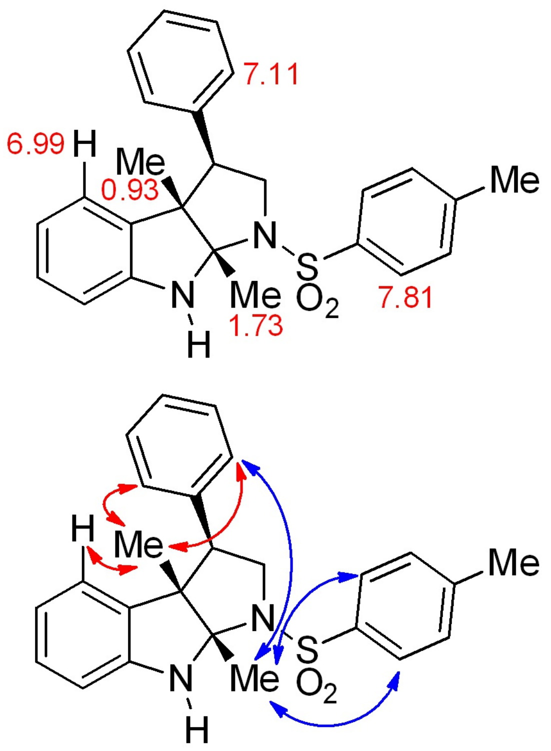
NOESY-NMR, $CDCl_3$, 300 MHz



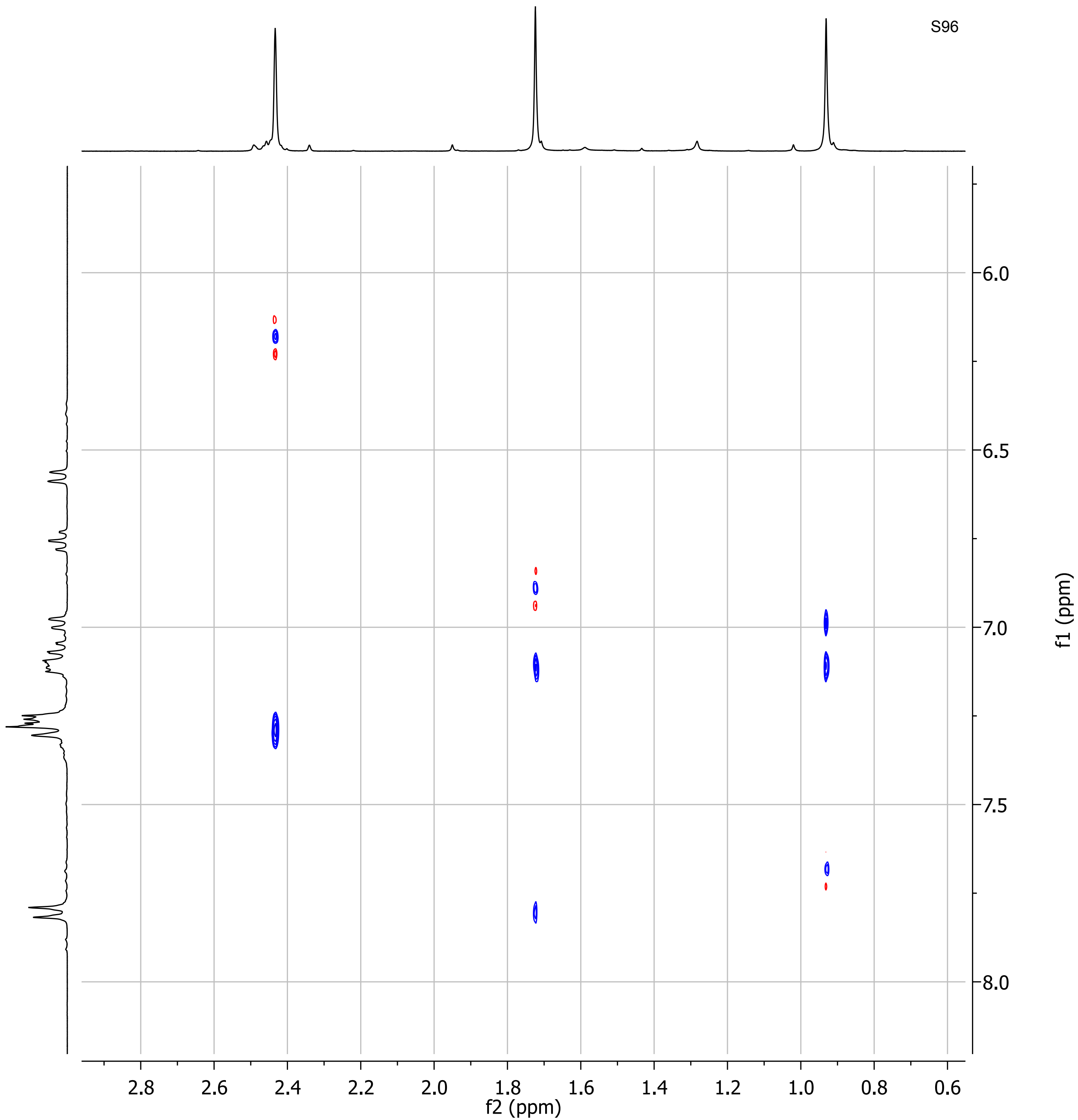
(±)**4'c**

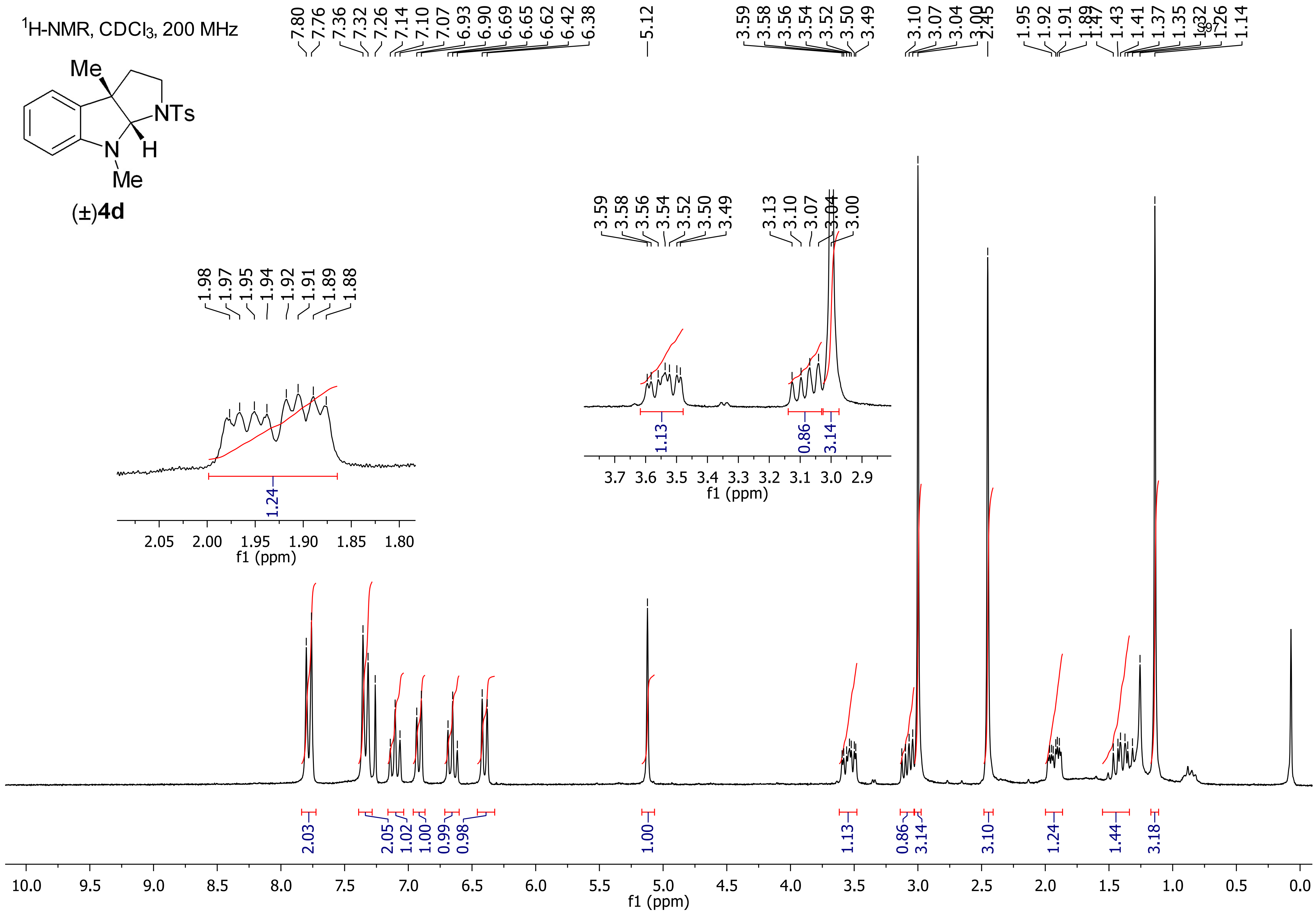


NOESY-NMR, $CDCl_3$, 300 MHz



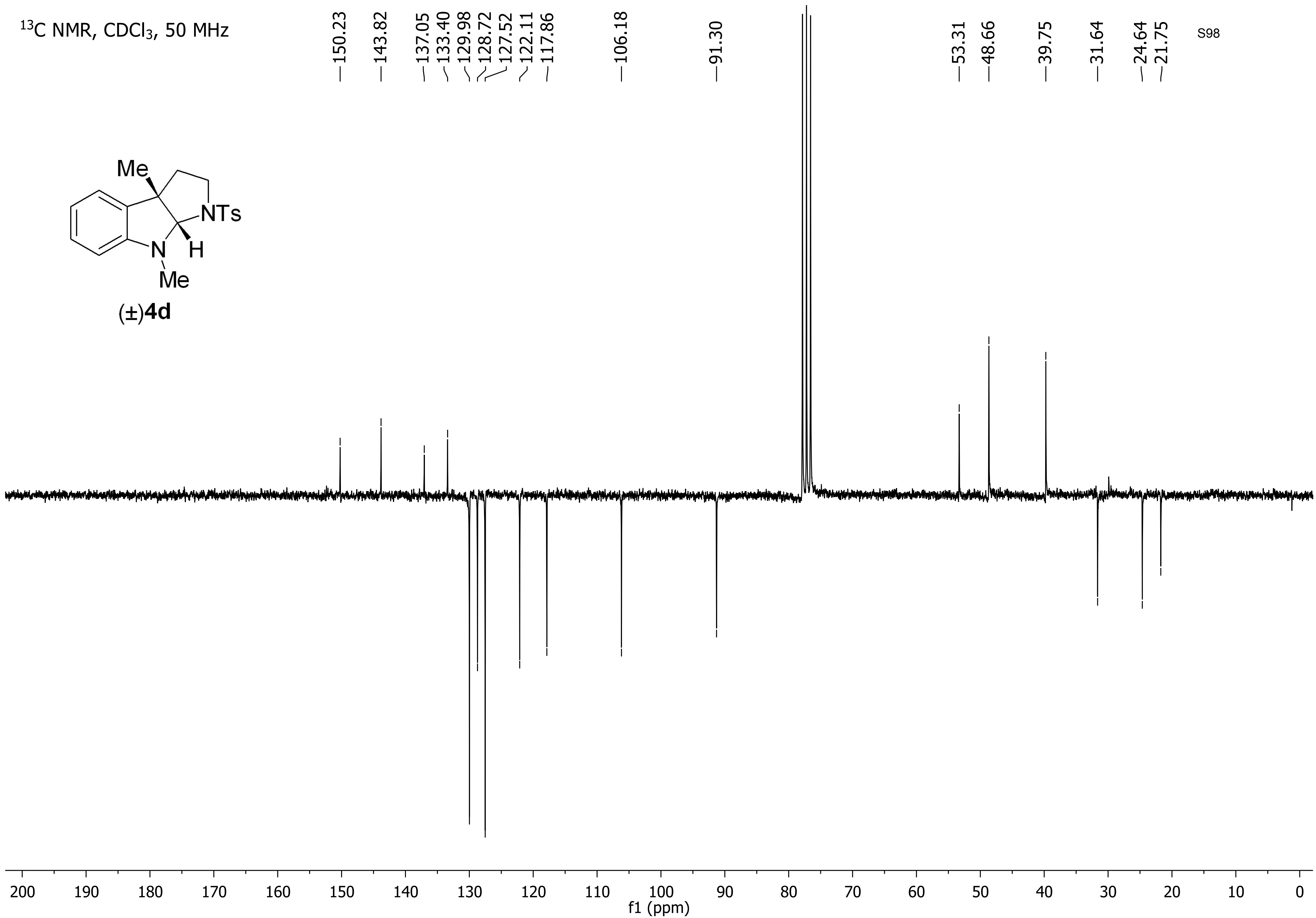
(±)**4'c**



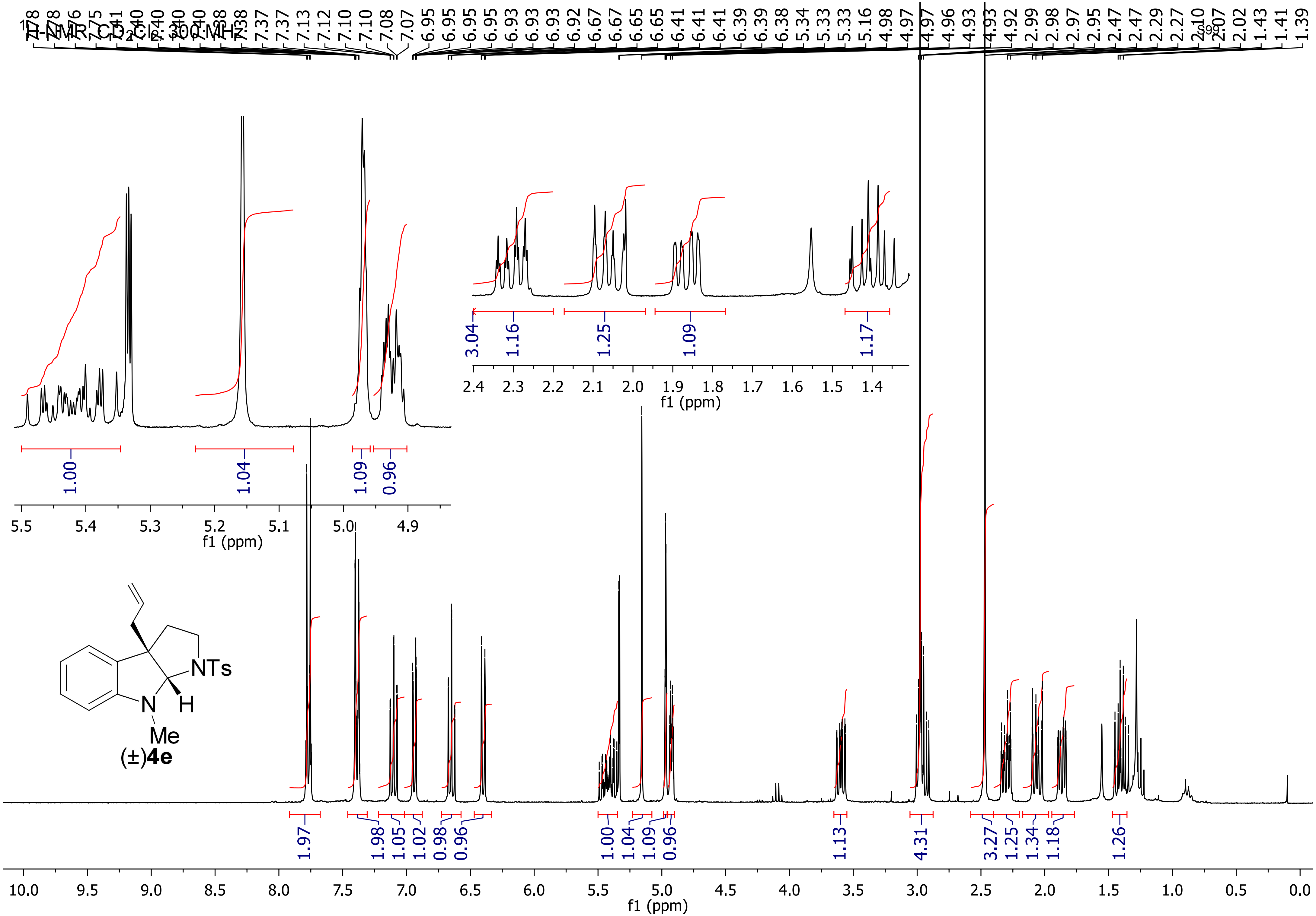


1H-NMR, CDCl3, 200 MHz
Me
NTs
N
H
Me
(±)4d
f1 (ppm)

^{13}C NMR, $CDCl_3$, 50 MHz

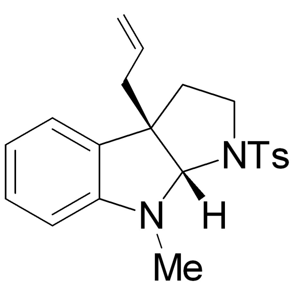


(±)**4d**



(±)**4e**

^{13}C-NMR, CD_2Cl_2, 75 MHz



(±)**4e**