

Supporting Information

Synthesis of 1-Benzylisoindoline and 1-Benzyl-Tetrahydroisoquinoline through Nucleophilic Addition of Organozinc Reagents to *N,O*-acetals

Rui-Jun Ma,^{a,b} Jian-Ting Sun,^a Chang-Hong Liu,^a Ling Chen,^a Chang-Mei Si^{a,*} and Bang-Guo Wei^{a,*}

^a Department of Natural Medicine, School of Pharmacy, Fudan University, 826 Zhangheng Road, Shanghai 201203, China

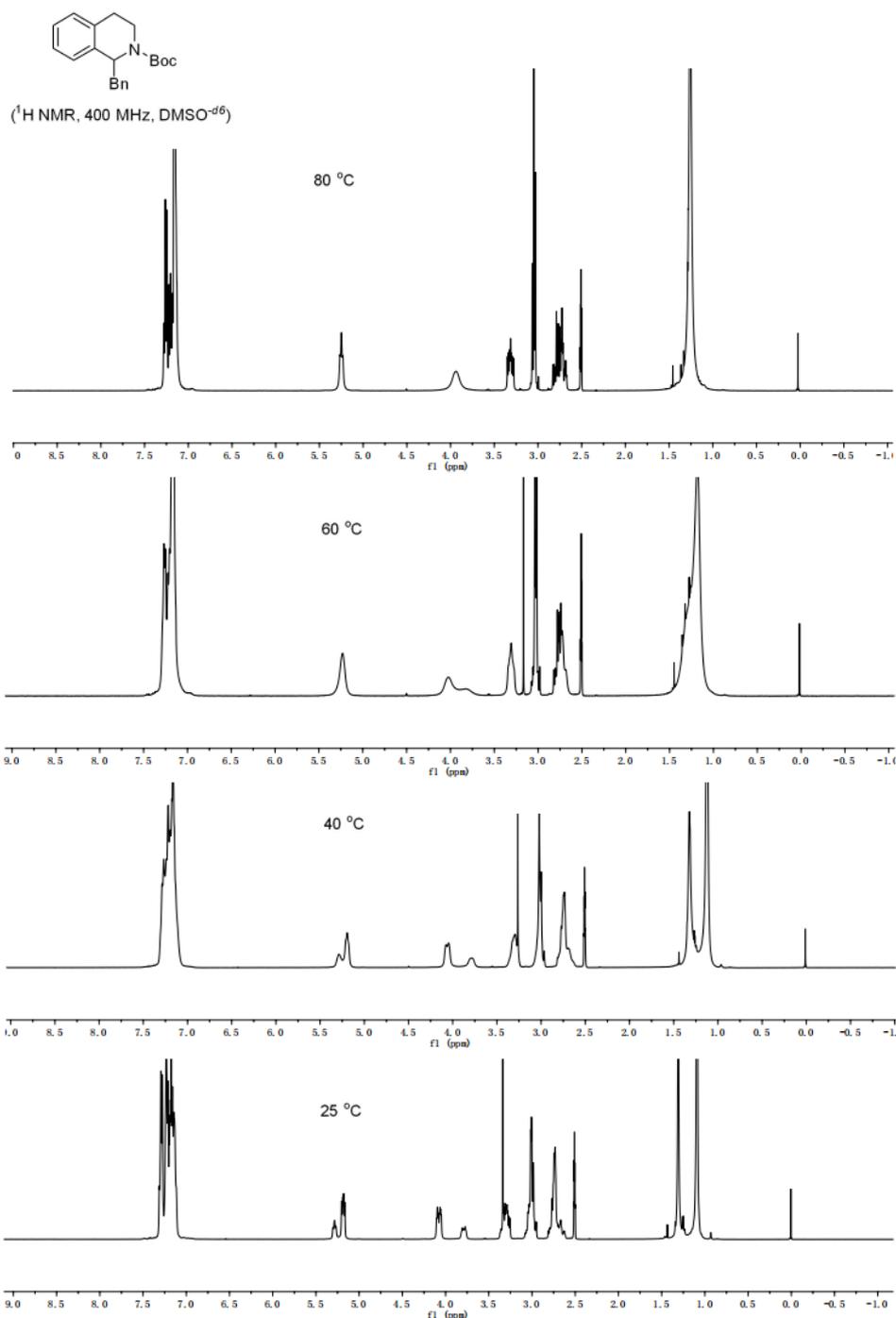
^b Center for Gastrointestinal Endoscopy, Shanxi Provincial People's Hospital, 29 ShuangTa Road, TaiYuan 030012, China

Email: sicm@fudan.edu.cn; bgwei1974@fudan.edu.cn

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I. NMR spectra of compound 9a at different temperatures



Rotational isomerism exist in the NMR spectrums of the compound **8** and **9**. For the existence of this rotation isomerism, we conducted a NMR spectrum test of the compound **9a** at different temperatures. According to the spectrums, it can be seen that when the temperature continues to rise, the fissures cause by the rotational isomerization continue to decrease. And when the temperature rises to 80 °C, the fissures on the ¹H NMR spectrum disappeared.

II. The synthetic details data for the substrates 12a-12f and 13.

General Procedure for the Synthesis of 12 and 13. To a solution of **10/11** (2.0 mmol) in dry THF (10 mL) was added DMAP (0.2 mmol) and Boc₂O (5.0 mmol). After being stirred at room temperature for 12 h, the mixture was quenched with NH₄Cl and extracted with EtOAc (30 mL×3). The combined organic layers were washed with brine, dried over MgSO₄, filtrated and concentrated. The residue was purified by flash chromatography on silica gel (PE/EA=5:1) to give the desired product **12/13**.

tert-Butyl 1-oxoisindoline-2-carboxylate 12a. Light-Yellow solid (457 mg, 98%); m.p. 121-123°C; IR (film): ν_{\max} 2979, 1780, 1743, 1393, 1300, 1276, 1151, 1102, 945, 843 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.94-7.85 (m, 1H), 7.67-7.59 (m, 1H), 7.52-7.46 (m, 2H), 4.76 (s, 2H), 1.61 (s, 9H) ppm; ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 166.7, 150.4, 140.7, 133.6, 131.5, 128.5, 125.0, 123.1, 83.2, 49.2, 28.2 ppm; HRMS (ESI-Orbitrap) m/z : [M + Na]⁺ Calcd for C₁₃H₁₅NO₃Na⁺: 256.0944, found: 256.0945.

tert-Butyl 4-bromo-1-oxoisindoline-2-carboxylate 12b. Colourless oil (618 mg, 99%); IR (film): ν_{\max} 2979, 1785, 1473, 1394, 1327, 1257, 1157, 954, 819, 726 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.98-7.85 (m, 1H), 7.84-7.75 (m, 1H), 7.45-7.38 (m, 1H), 4.67 (s, 2H), 1.62 (s, 9H) ppm; ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 165.7, 150.1, 141.1, 136.4, 133.5, 130.4, 124.0, 118.0, 83.6, 49.8, 28.2 ppm; HRMS (ESI-Orbitrap) m/z : [M + Na]⁺ Calcd for C₁₃H₁₄BrNO₃Na⁺: 334.0049, 336.0029, found: 334.0050, 336.0028.

tert-Butyl 6-bromo-1-oxoisindoline-2-carboxylate 12c. White solid (605 mg, 97%); m.p. 145-147°C; IR (film): ν_{\max} 2977, 1717, 1448, 1395, 1324, 1262, 1213, 1158, 778, 668 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.10-8.00 (m, 1H), 7.80-7.70 (m, 1H), 7.40-7.30 (m, 1H), 4.72 (s, 2H), 1.60 (s, 9H) ppm; ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 165.2, 150.2, 139.3, 136.7, 133.6, 128.1, 124.8, 122.7, 83.7, 49.0, 28.2 ppm; HRMS (ESI-Orbitrap) m/z : [M + Na]⁺ Calcd for C₁₃H₁₄BrNO₃Na⁺: 334.0049, 336.0029, found: 334.0048, 336.0027.

tert-Butyl 5-chloro-1-oxoisindoline-2-carboxylate 12d. White solid (519 mg, 97%); m.p. 118-120°C; IR (film): ν_{\max} 2976, 1730, 1477, 1363, 1305, 1204, 1182, 1154, 856, 792 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.86-7.80 (m, 1H), 7.50-7.42 (m, 2H), 4.75 (s, 2H), 1.60 (s, 9H) ppm; ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 165.6, 150.3, 142.2, 140.1, 130.1, 129.4, 126.3, 123.6, 83.6, 48.8, 28.2 ppm; HRMS (ESI-Orbitrap) m/z : [M + Na]⁺ Calcd for C₁₃H₁₄ClNO₃Na⁺: 290.0554, found: 290.0558.

tert-Butyl 4-methoxy-1-oxoisindoline-2-carboxylate 12e. White solid (484 mg, 92%); m.p. 128-130°C; IR (film): ν_{\max} 2970, 1779, 1713, 1497, 1364, 1290, 1154, 1073, 970, 774 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.55-7.45 (m, 1H), 7.43-7.38 (m, 1H), 7.11-7.05 (m, 1H), 4.68 (s, 2H), 3.93 (s, 3H), 1.60 (s, 9H) ppm; ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 166.9, 154.5, 150.5, 133.1, 130.2, 129.3, 116.8, 114.4, 83.2, 55.7, 47.2, 28.3 ppm; HRMS (ESI-Orbitrap) m/z : [M + H]⁺ Calcd for C₁₄H₁₈NO₄⁺: 264.1230, found: 264.1232.

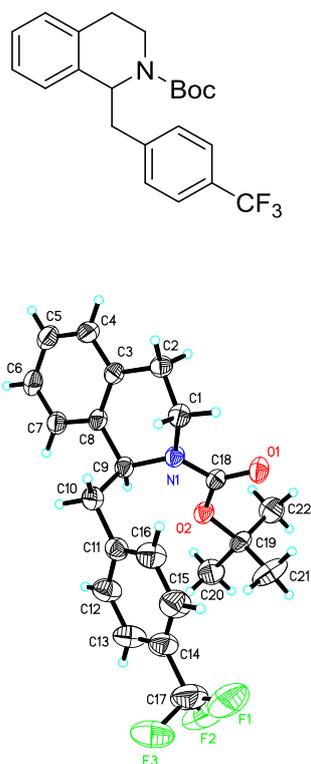
tert-Butyl 6-methoxy-1-oxoisindoline-2-carboxylate 12f. White solid (484 mg, 92%); m.p. 135-137°C; IR (film): ν_{\max} 2975, 1772, 1710, 1496, 1456, 1363, 1203, 1023, 981, 776 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.37-7.31 (m, 2H), 7.22-7.17 (m, 1H), 4.69 (s, 2H), 3.86 (s, 3H), 1.60 (s, 9H) ppm; ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 166.9, 160.2, 150.3, 133.0, 132.7, 123.9, 122.5, 106.9, 83.1, 55.7, 48.8, 28.1 ppm; HRMS (ESI-Orbitrap) m/z : [M + Na]⁺ Calcd for C₁₄H₁₇NO₄Na⁺: 286.1050, found: 286.1052.

tert-Butyl 1-oxo-3,4-dihydroisoquinoline-2(1H)-carboxylate 13. White solid (470 mg, 95%); m.p. 73-75 °C; IR (film): ν_{\max} 2978, 1783, 1390, 1327, 1267, 1155, 947, 853 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.20-8.12 (m, 1H), 7.50-7.45 (m, 1H), 7.39-7.31 (m, 1H), 7.24-7.18 (m, 1H), 4.03-3.96 (m, 2H), 3.04-2.97 (m, 2H), 1.59 (s, 9H) ppm; ¹³C{¹H} NMR

(100 MHz, CDCl₃) δ 164.1, 153.3, 139.6, 132.9, 129.7, 129.4, 127.3, 127.3, 83.3, 44.5, 28.4, 28.2 ppm; HRMS (ESI-Orbitrap) m/z : [M + Na]⁺ Calcd for C₁₄H₁₇NO₃Na⁺: 270.2832, found: 270.2832.

III. X-Ray Structure of **9i**

ORTEP drawing of the X-ray crystallographic structure of **9i**



CCDC 2011532. For detailed crystallographic data, please refer to the Cambridge Crystallographic Data Centre at <http://ccdc.cam.ac.uk>.

Table 1. Crystal data and structure refinement for **9i**.

Identification code	9i	
Empirical formula	C ₂₂ H ₂₄ F ₃ N O ₂	
Formula weight	391.42	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 18.7943(14) Å	$\alpha = 90^\circ$
	b = 11.2236(8) Å	$\beta = 95.655(2)^\circ$
	c = 9.8308(8) Å	$\gamma = 90^\circ$
Volume	2063.6(3) Å ³	

Z	4
Density (calculated)	1.260 Mg/m ³
Absorption coefficient	0.098 mm ⁻¹
F(000)	824
Crystal size	0.200 x 0.160 x 0.120 mm ³
Theta range for data collection	2.762 to 25.999 °.
Index ranges	-21<=h<=23, -13<=k<=13, -12<=l<=12
Reflections collected	30521
Independent reflections	4041 [R(int) = 0.0326]
Completeness to theta = 25.242 °	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6406
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4041 / 36 / 284
Goodness-of-fit on F ²	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0469, wR2 = 0.1159
R indices (all data)	R1 = 0.0670, wR2 = 0.1317
Extinction coefficient	0.037(4)
Largest diff. peak and hole	0.196 and -0.126 e.Å ⁻³

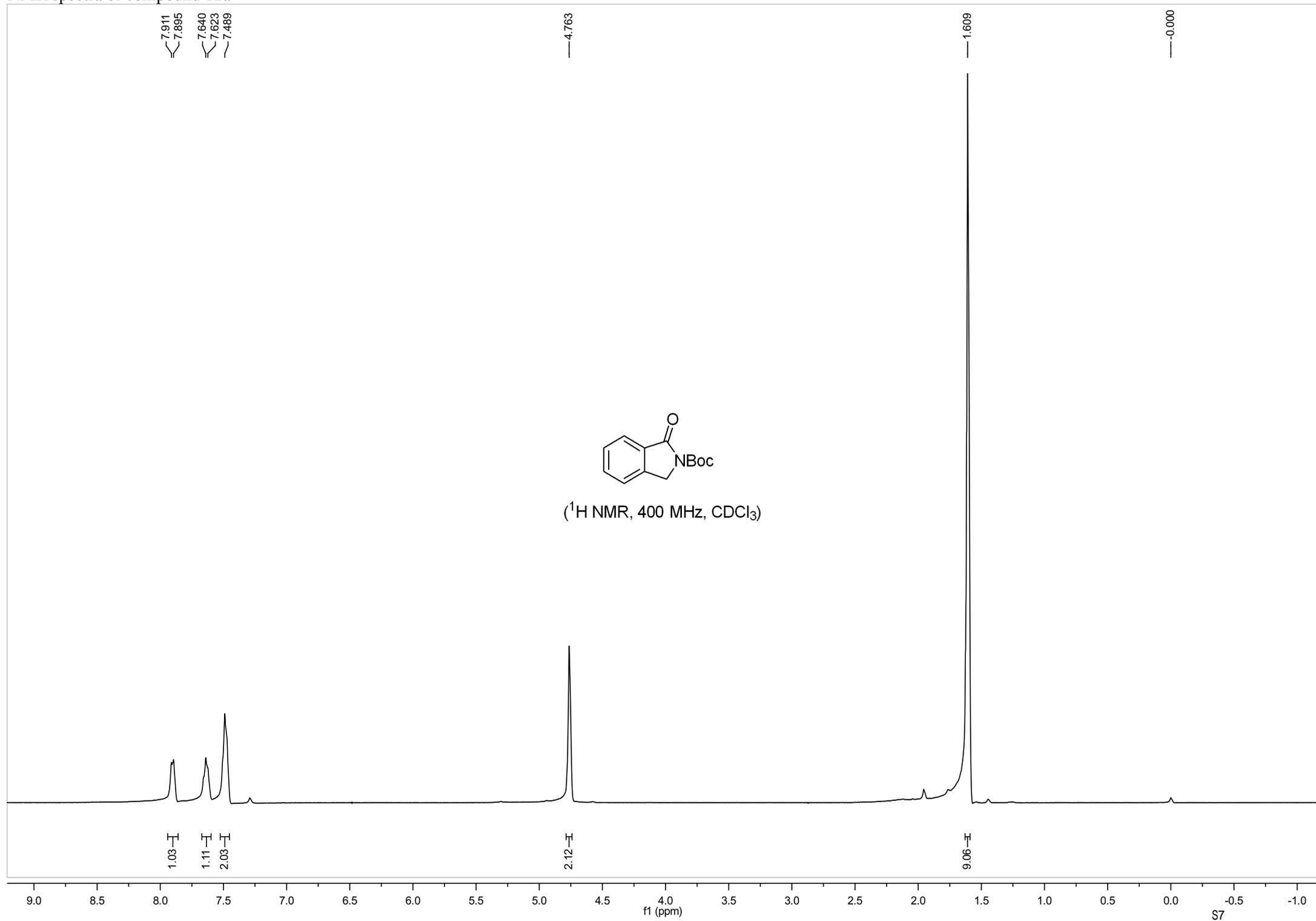
Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for dd20068. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1706(1)	4004(1)	8581(1)	68(1)
O(2)	2236(1)	5455(1)	7434(1)	61(1)
N(1)	1669(1)	3971(1)	6272(1)	52(1)
C(1)	1253(1)	2865(1)	6144(2)	60(1)
C(2)	530(1)	3096(2)	5382(2)	64(1)
C(3)	566(1)	3888(1)	4155(2)	55(1)
C(4)	-23(1)	3991(2)	3184(2)	68(1)
C(5)	-11(1)	4716(2)	2065(2)	74(1)
C(6)	592(1)	5358(2)	1884(2)	72(1)
C(7)	1180(1)	5275(2)	2828(2)	63(1)

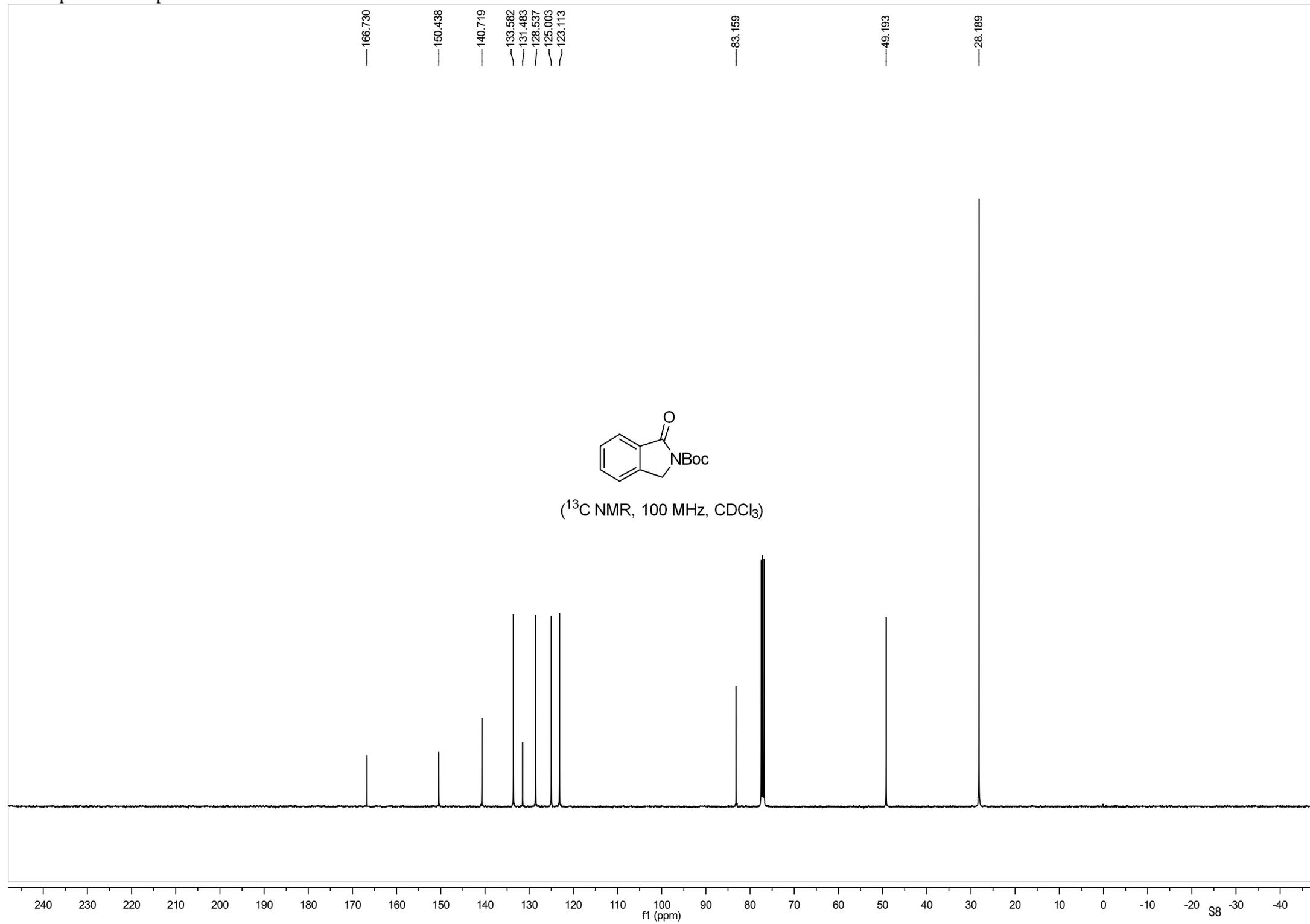
C(8)	1174(1)	4548(1)	3977(2)	52(1)
C(9)	1839(1)	4498(1)	4985(1)	52(1)
C(10)	2445(1)	3817(2)	4372(2)	67(1)
C(11)	3127(1)	3770(2)	5304(2)	63(1)
C(12)	3640(1)	4644(2)	5280(2)	83(1)
C(13)	4261(1)	4605(2)	6155(3)	96(1)
C(14)	4383(1)	3683(2)	7054(2)	88(1)
C(15)	3883(1)	2813(2)	7097(3)	96(1)
C(16)	3260(1)	2853(2)	6226(2)	82(1)
C(17)	5056(2)	3632(4)	7995(4)	132(1)
C(18)	1860(1)	4439(1)	7520(2)	51(1)
C(19)	2524(1)	6091(2)	8666(2)	64(1)
C(20)	2928(1)	7102(2)	8082(2)	101(1)
C(21)	3016(2)	5306(2)	9571(3)	120(1)
C(22)	1916(1)	6574(2)	9394(2)	90(1)
F(1)	5079(4)	2852(8)	8929(9)	185(2)
F(2)	5221(4)	4741(8)	8561(9)	185(2)
F(3)	5617(3)	3491(10)	7265(7)	184(2)
F(1')	5377(3)	2557(7)	7941(9)	189(2)
F(2')	4937(3)	3752(9)	9300(7)	174(2)
F(3')	5528(3)	4390(9)	7739(9)	185(2)

IV. Copies of ^1H NMR, ^{13}C NMR and ^{19}F NMR Spectrum

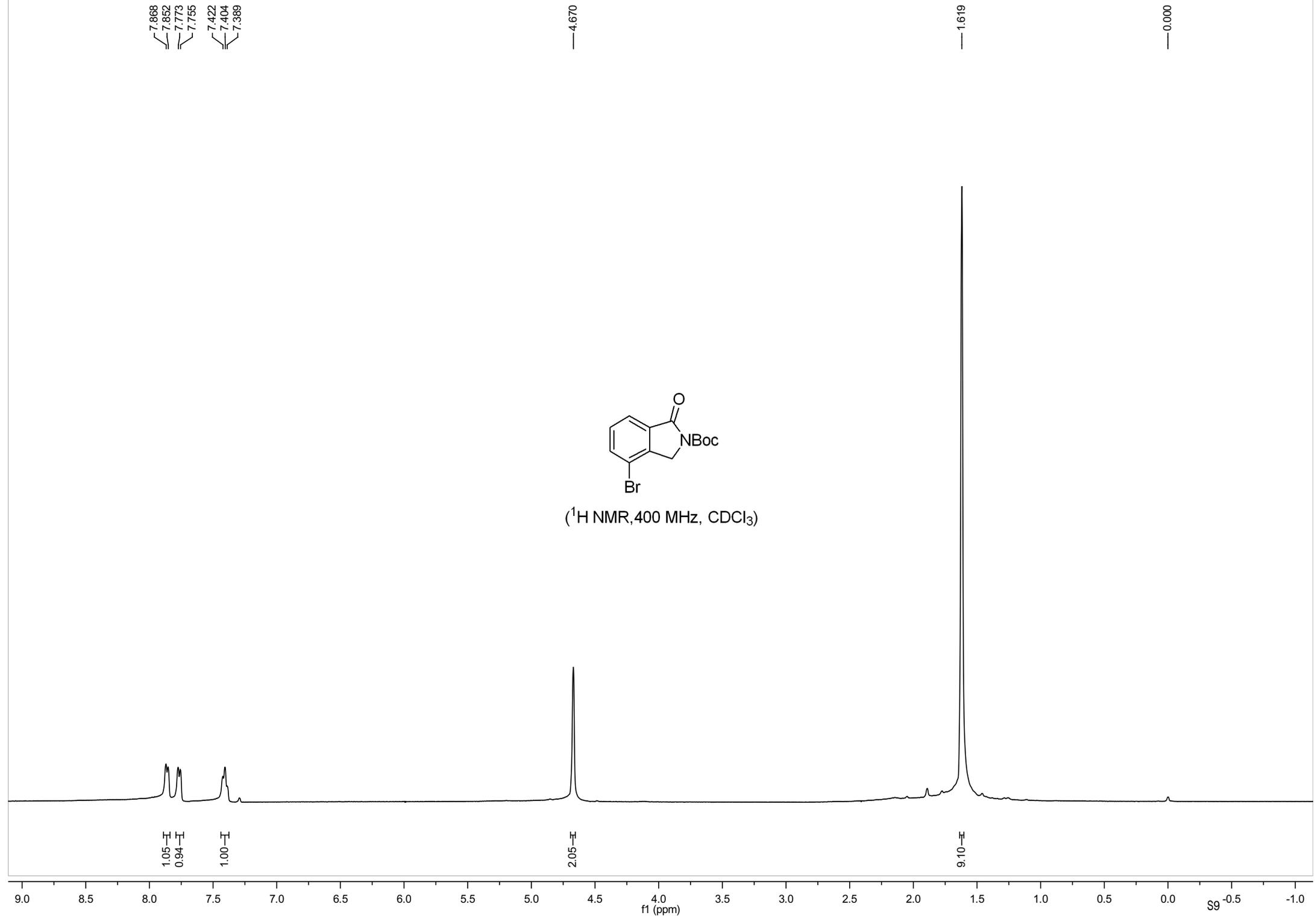
NMR spectra of compound 12a



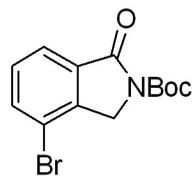
NMR spectra of compound 12a



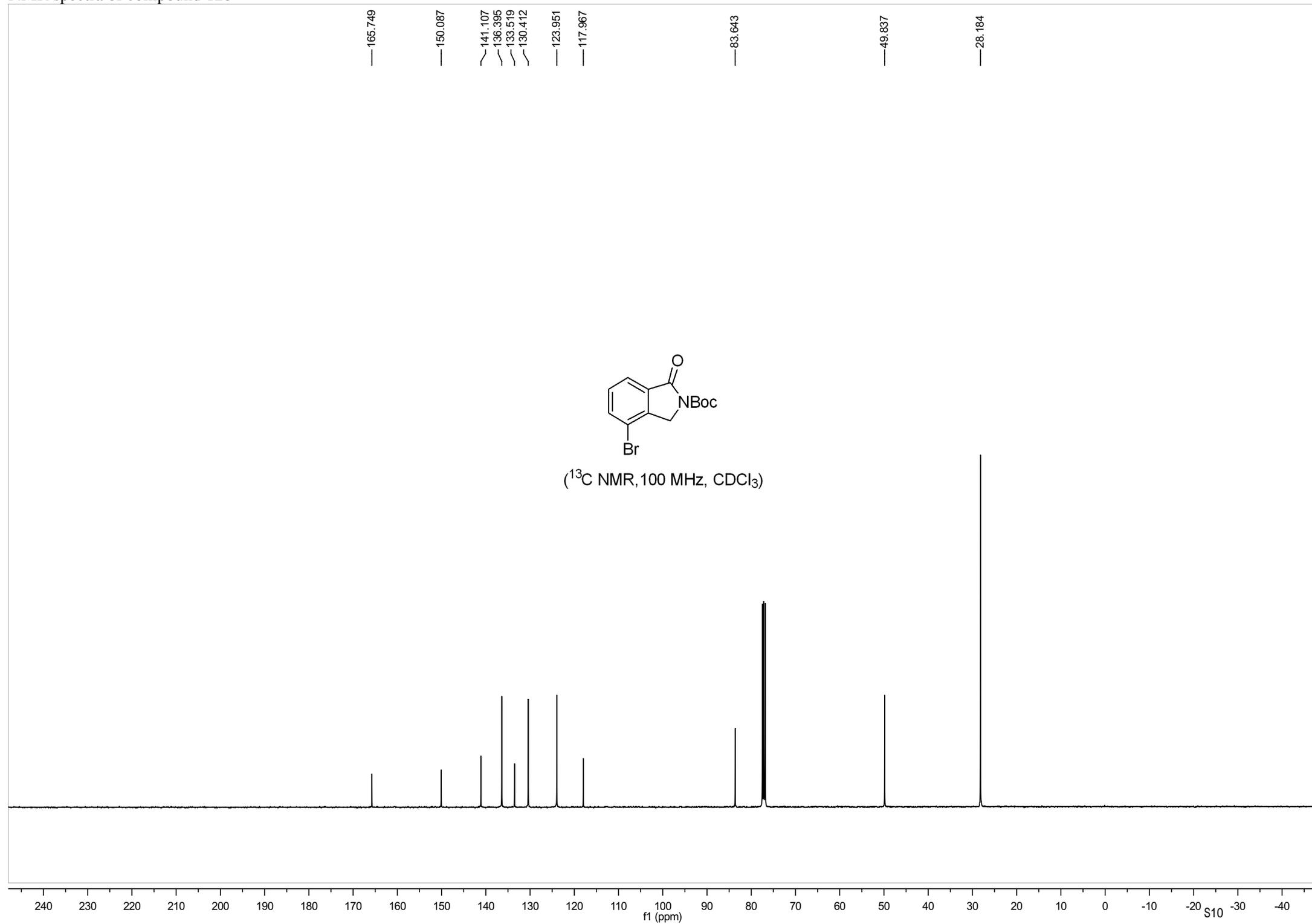
NMR spectra of compound 12b



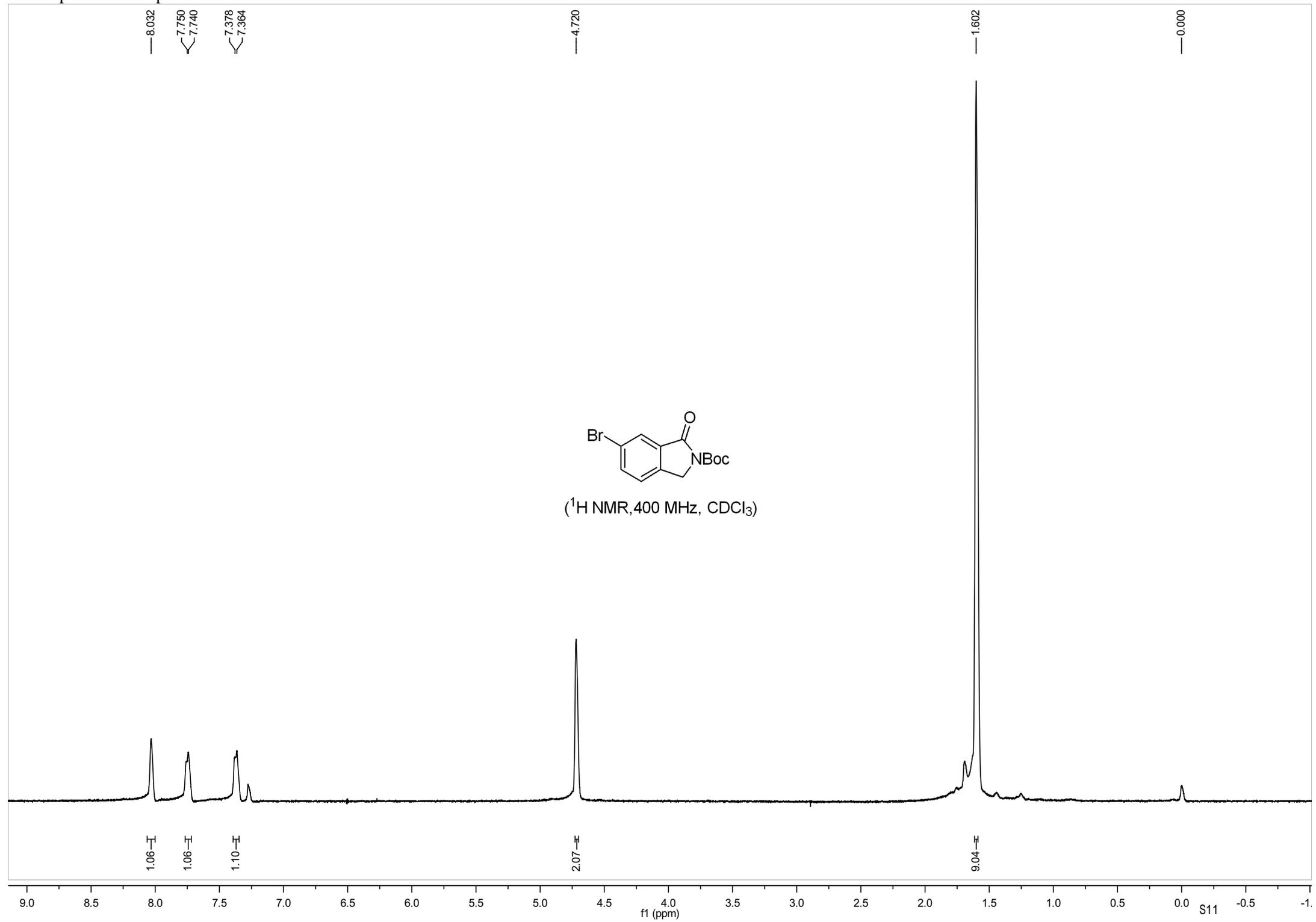
NMR spectra of compound 12b



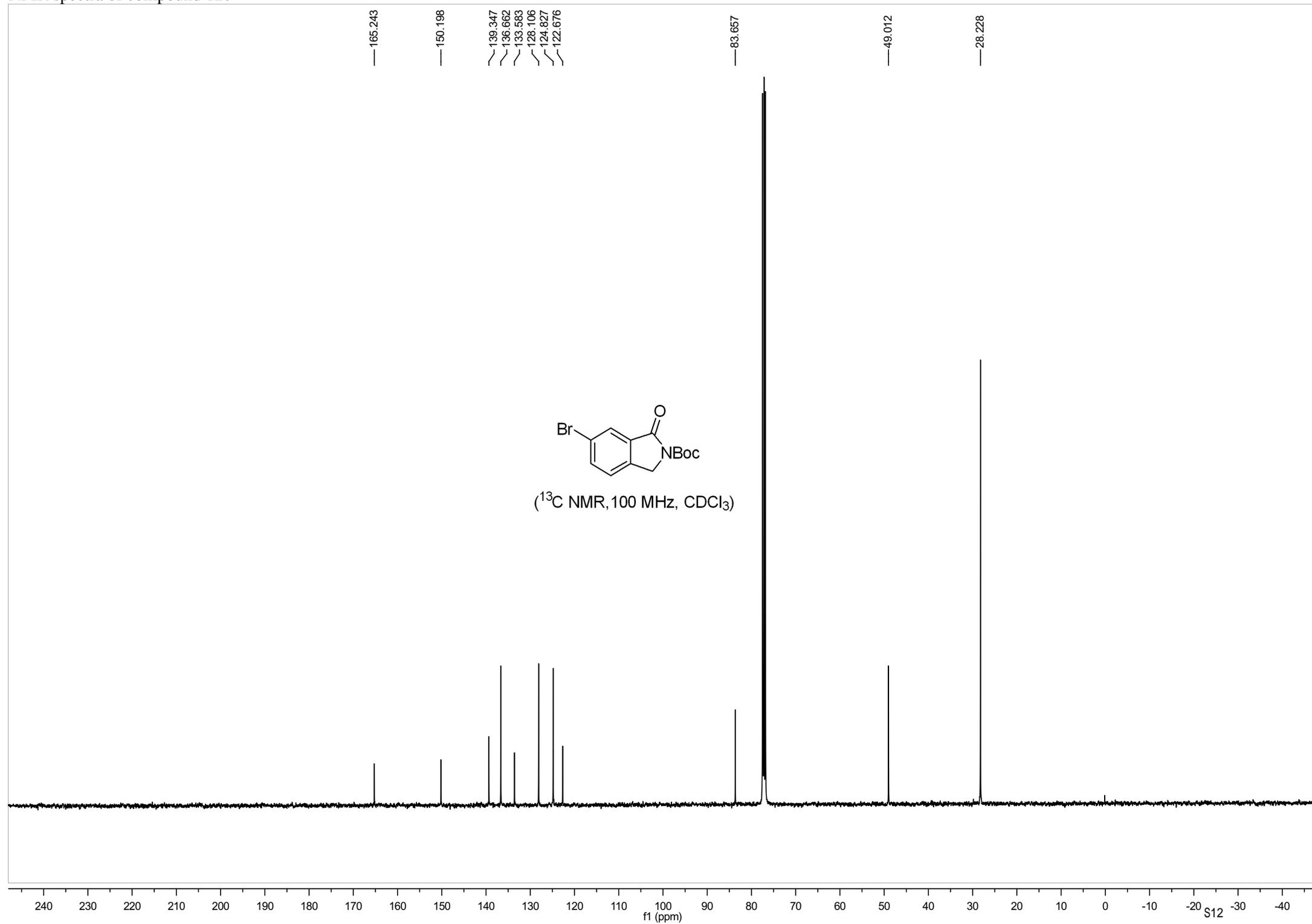
(¹³C NMR, 100 MHz, CDCl₃)



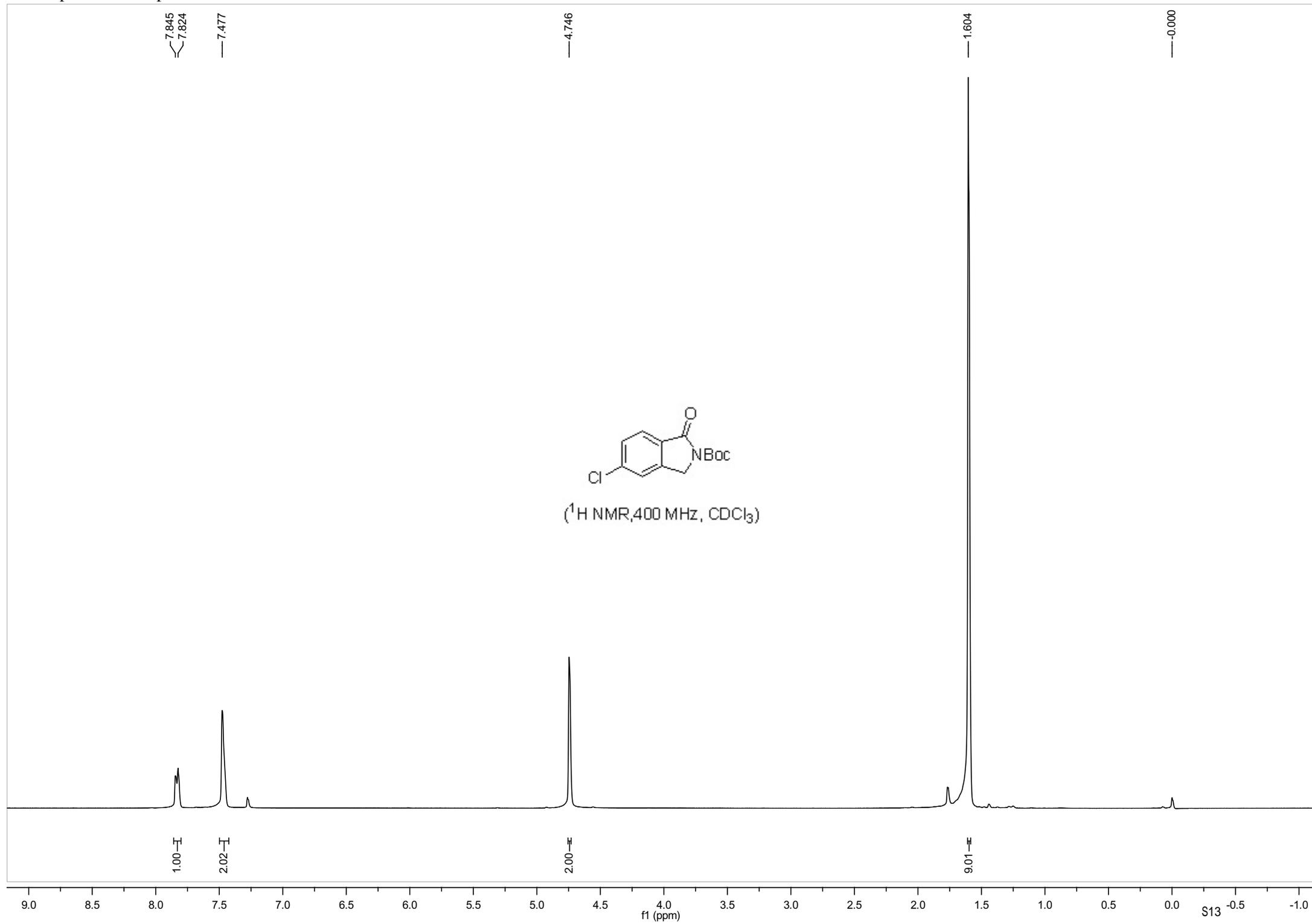
NMR spectra of compound 12c



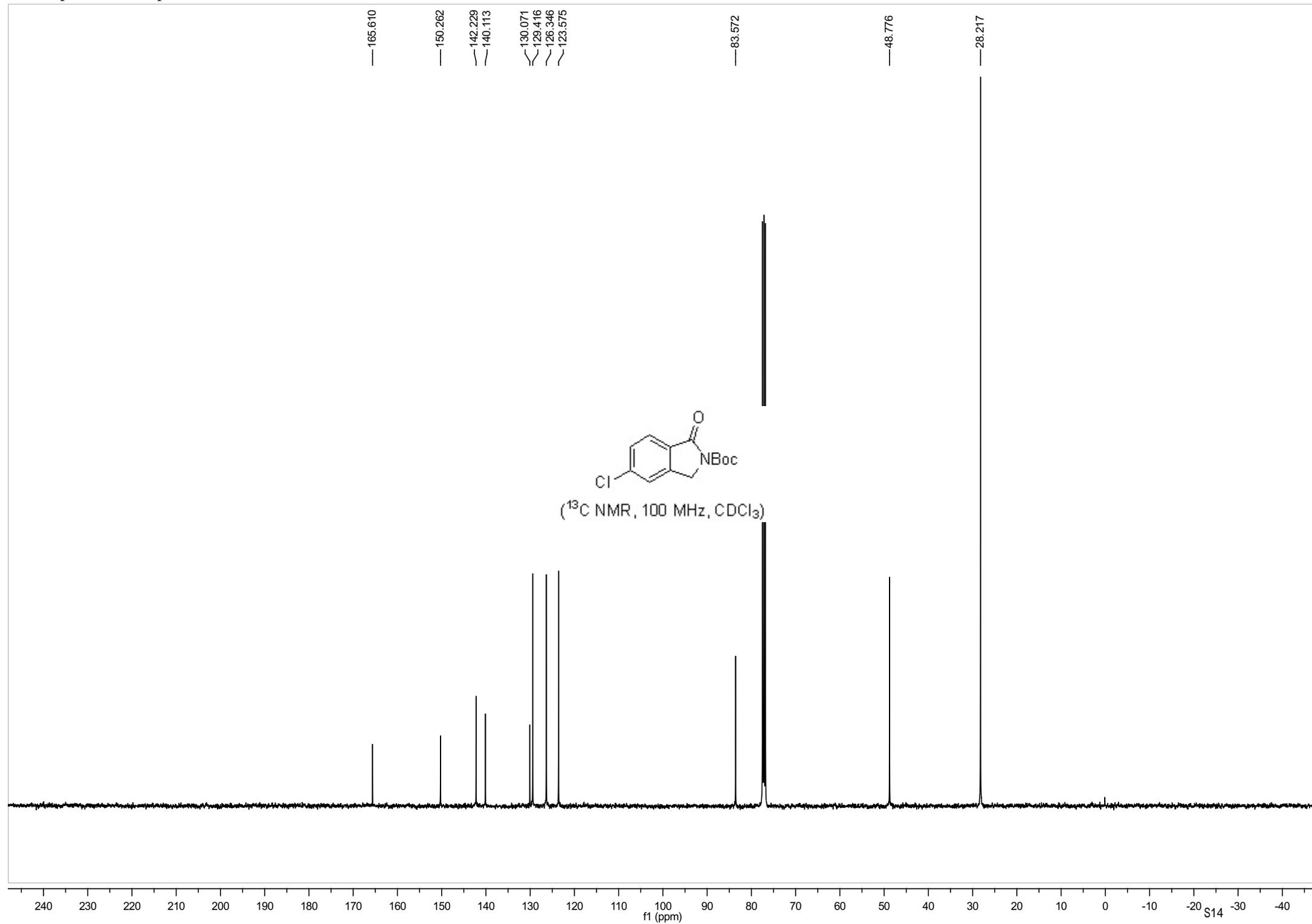
NMR spectra of compound 12c



NMR spectra of compound 12d



NMR spectra of compound 12d



NMR spectra of compound 12e

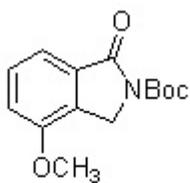
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7.464
7.445
7.426
7.085
7.066

4.680

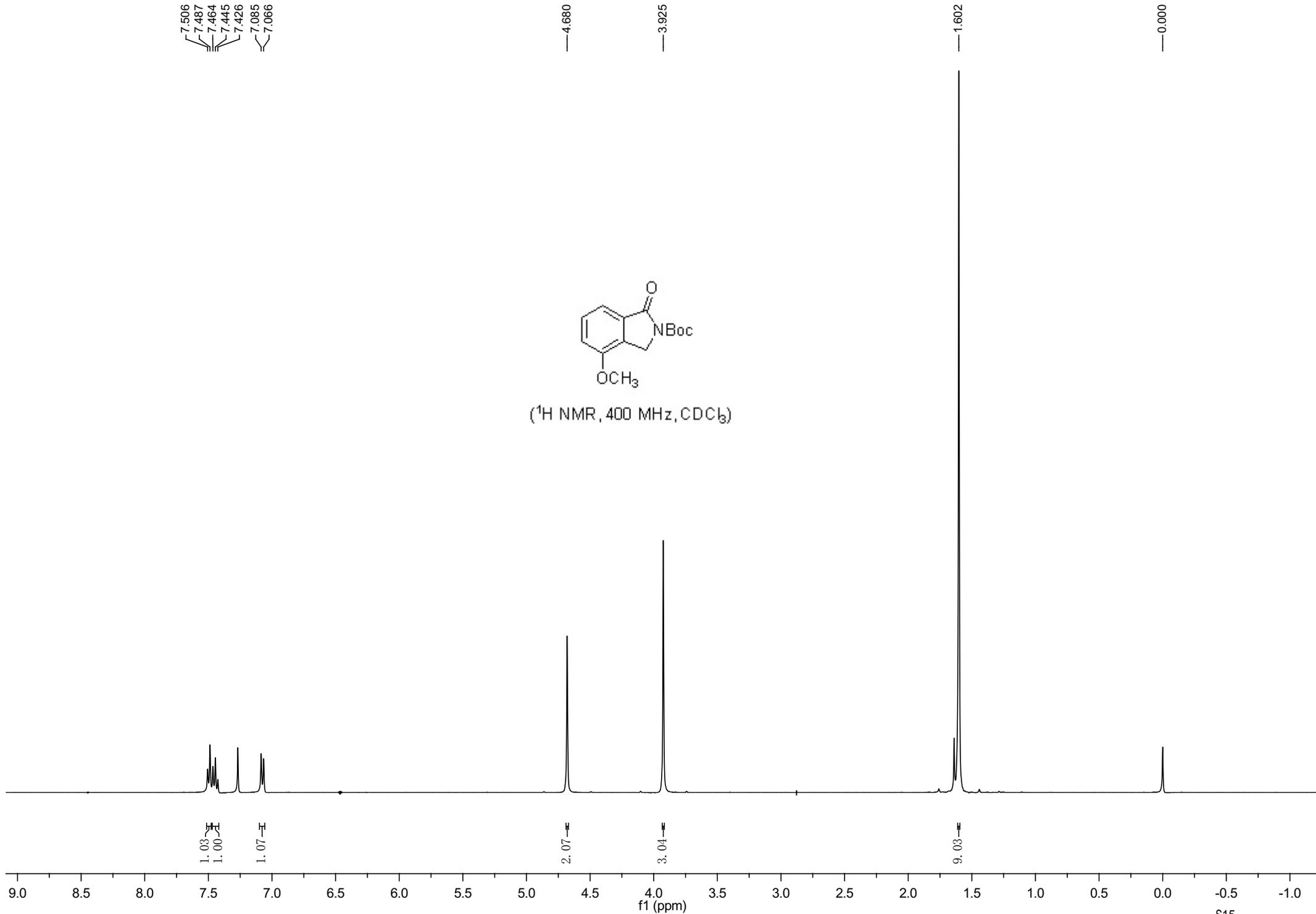
3.925

1.602

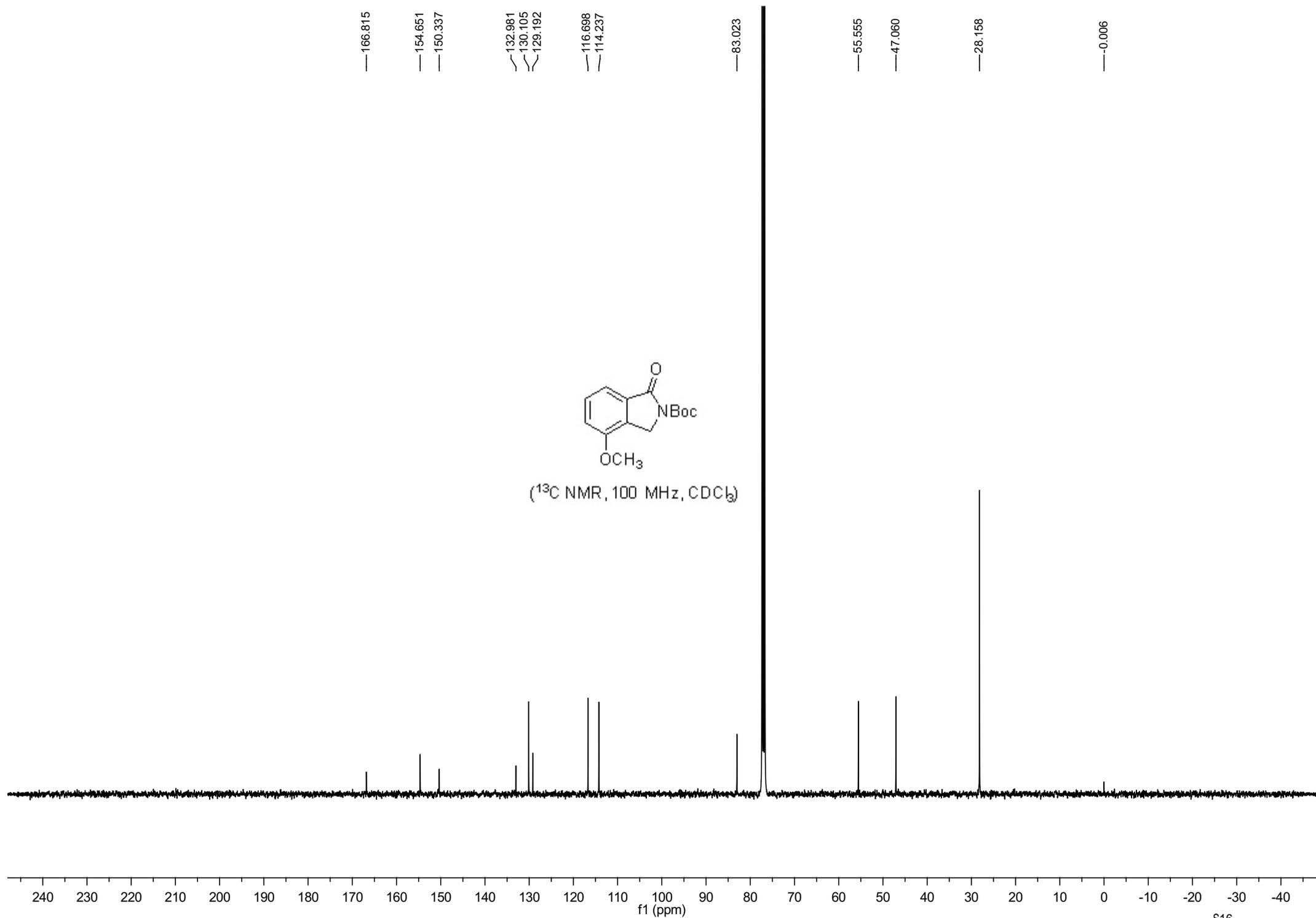
0.000



(¹H NMR, 400 MHz, CDCl₃)



NMR spectra of compound 12e



NMR spectra of compound 12f

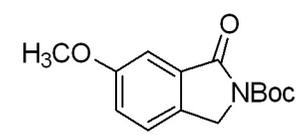
7.349
7.206
7.191

4.693

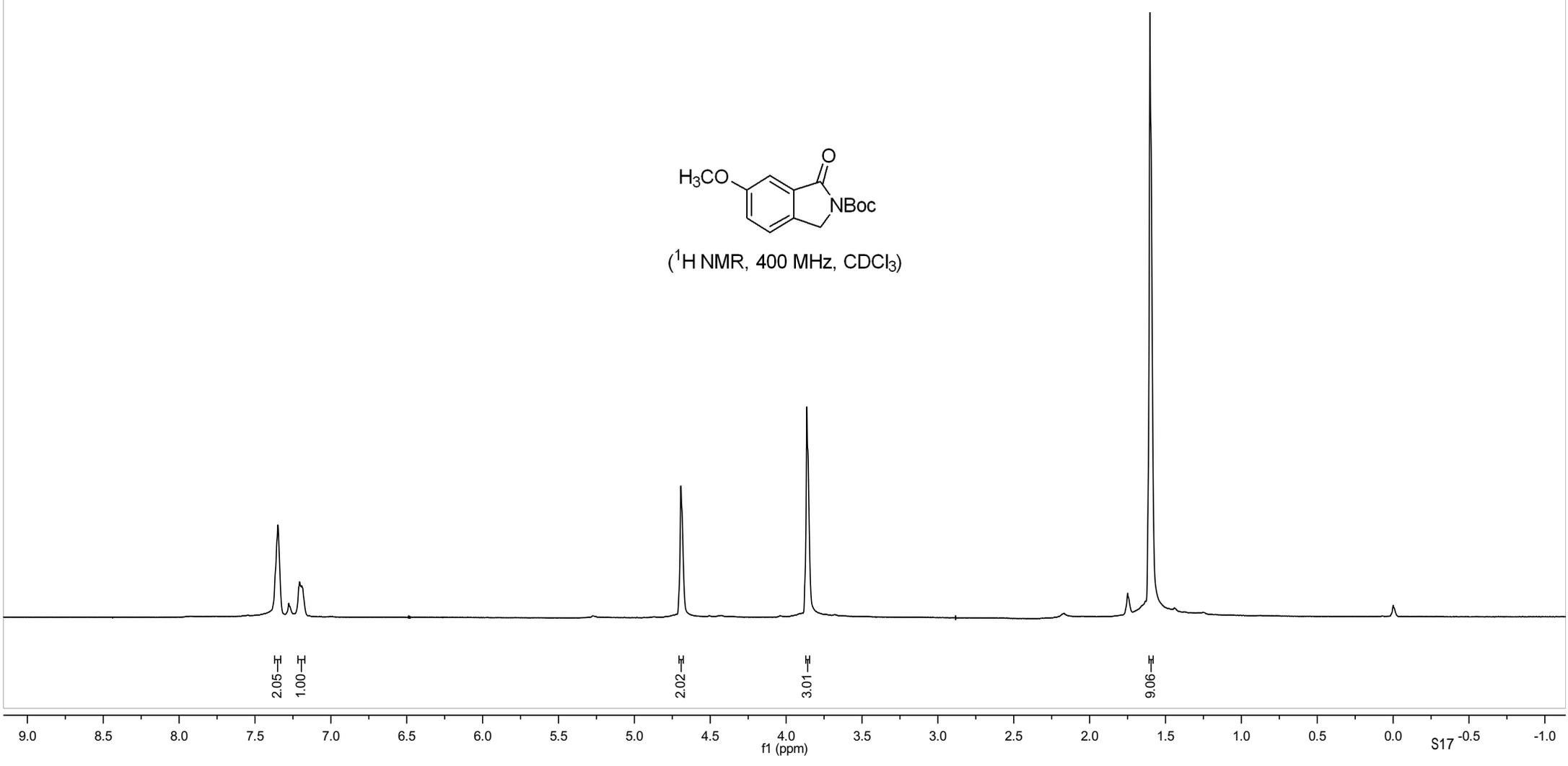
3.863

1.602

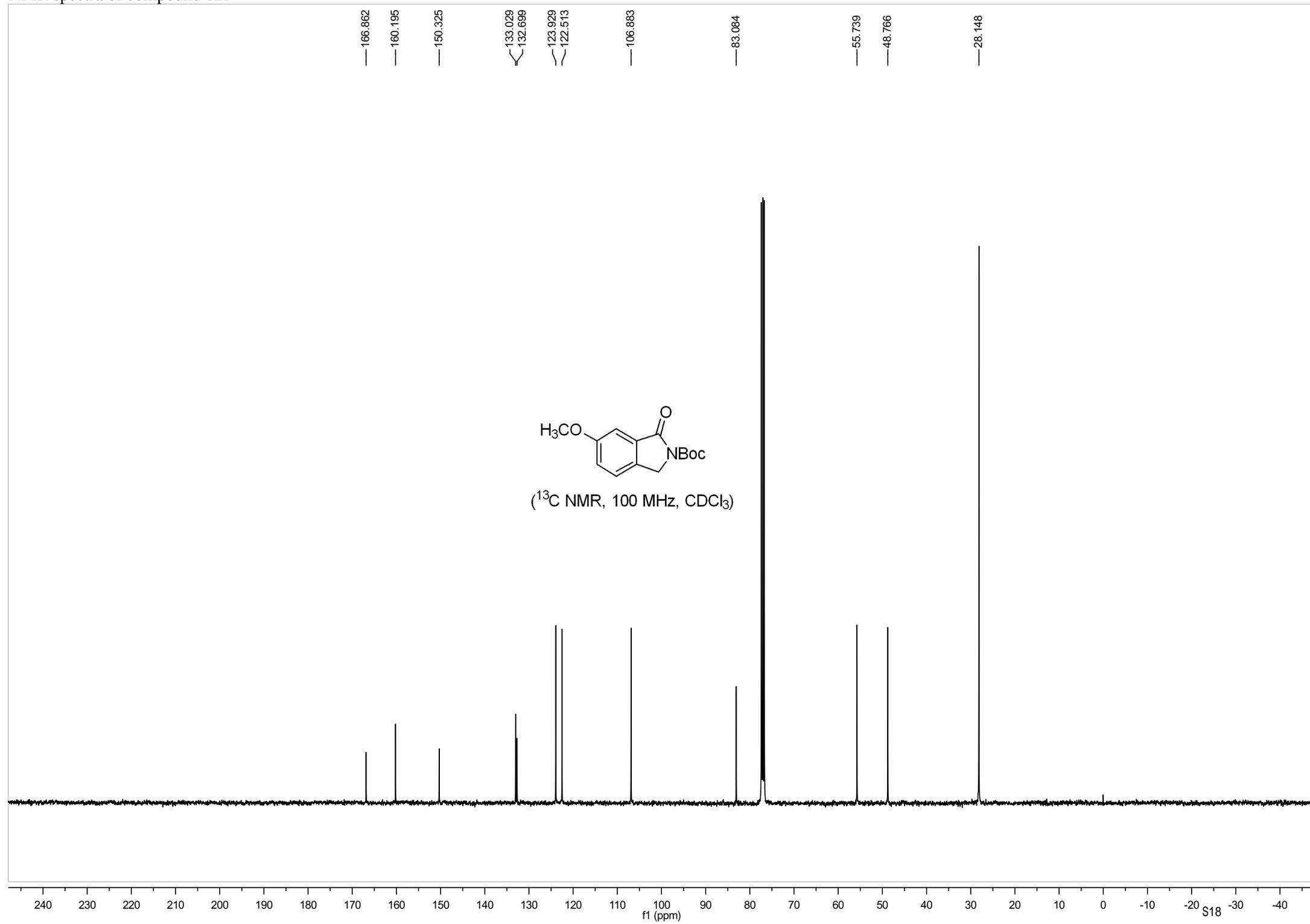
-0.000



(¹H NMR, 400 MHz, CDCl₃)



NMR spectra of compound 12f



NMR spectra of compound 13

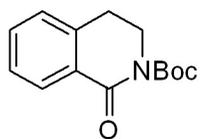
8.170
8.150
7.483
7.464
7.445
7.369
7.350
7.331
7.274
7.218
7.199

4.008
3.992
3.978

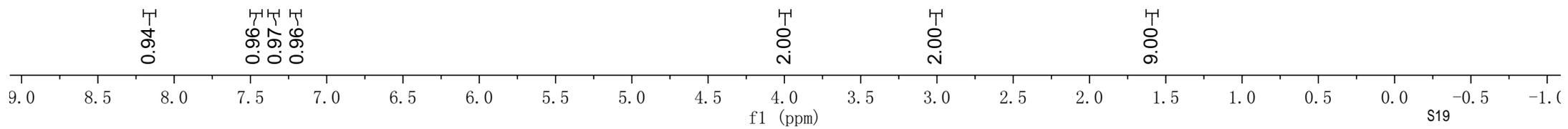
3.020
3.004
2.989

1.599

0.000



(¹H NMR, 400 MHz, CDCl₃)

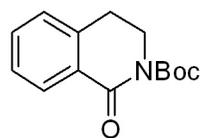


NMR spectra of compound 13

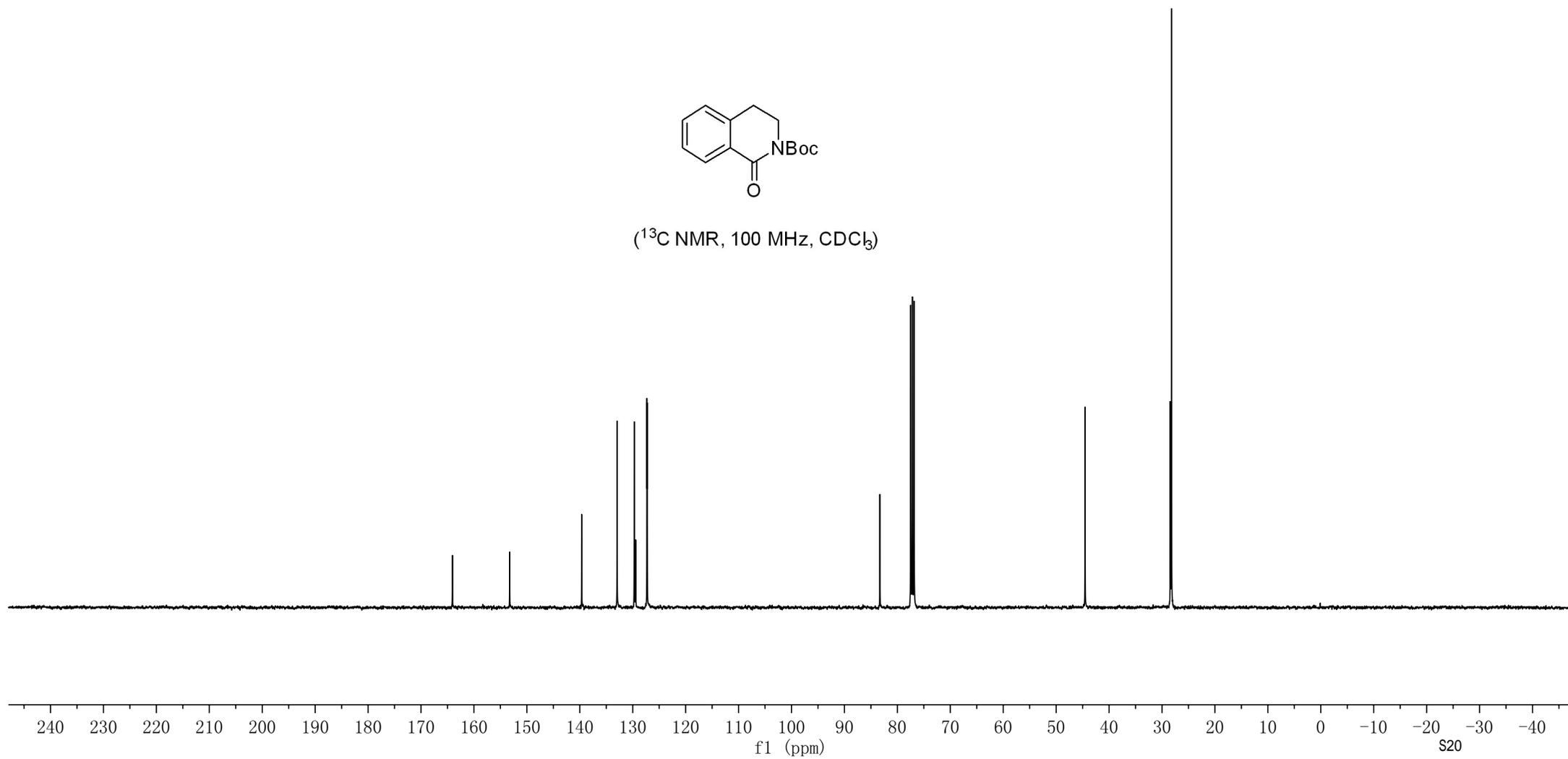
— 164.063
— 153.251
— 139.645
— 132.953
— 129.714
— 129.454
— 127.317
— 127.266

— 83.305

— 44.540
— 28.430
— 28.208



(¹³C NMR, 100 MHz, CDCl₃)



NMR spectra of compound 8a

7.205
7.190
7.164
7.126
7.047
7.038
6.990
6.929
6.899
6.888
6.869
6.850

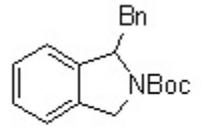
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5.327
5.254
5.238

4.652
4.615
4.507
4.471

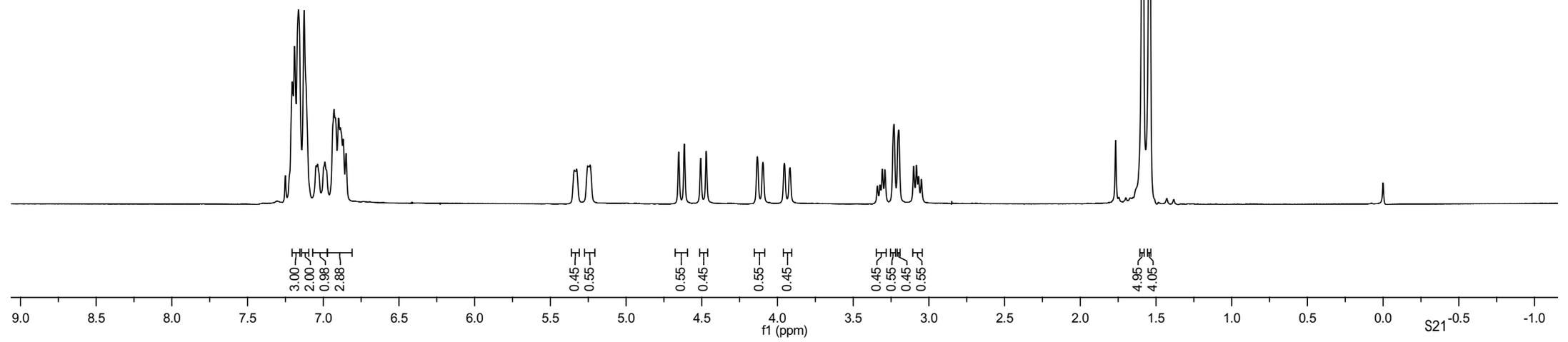
4.133
4.096
3.955
3.918

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3.323
3.308
3.290
3.231
3.200
3.100
3.082
3.068
3.050

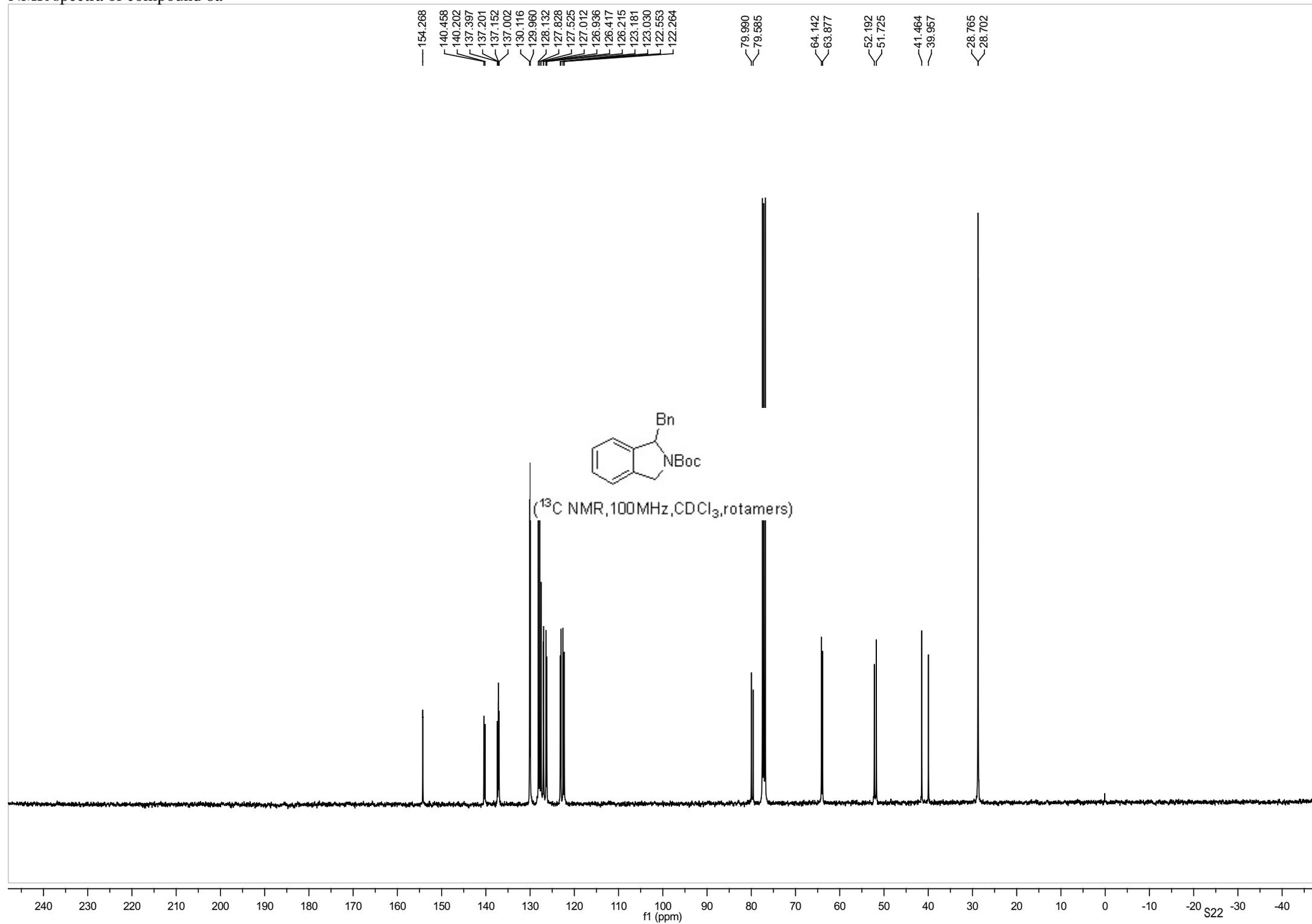
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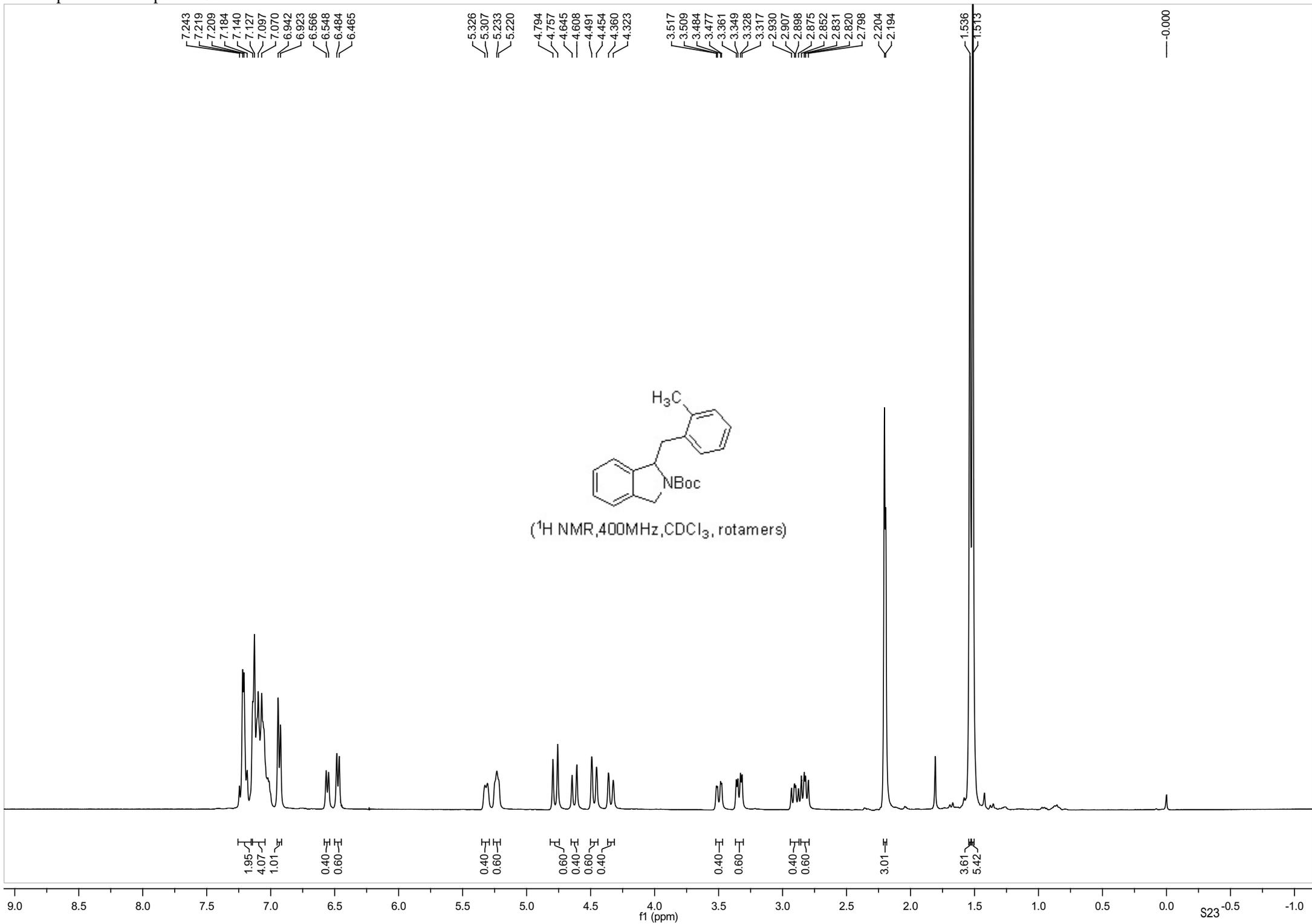
(¹H NMR, 400MHz, CDCl₃, rotamers)



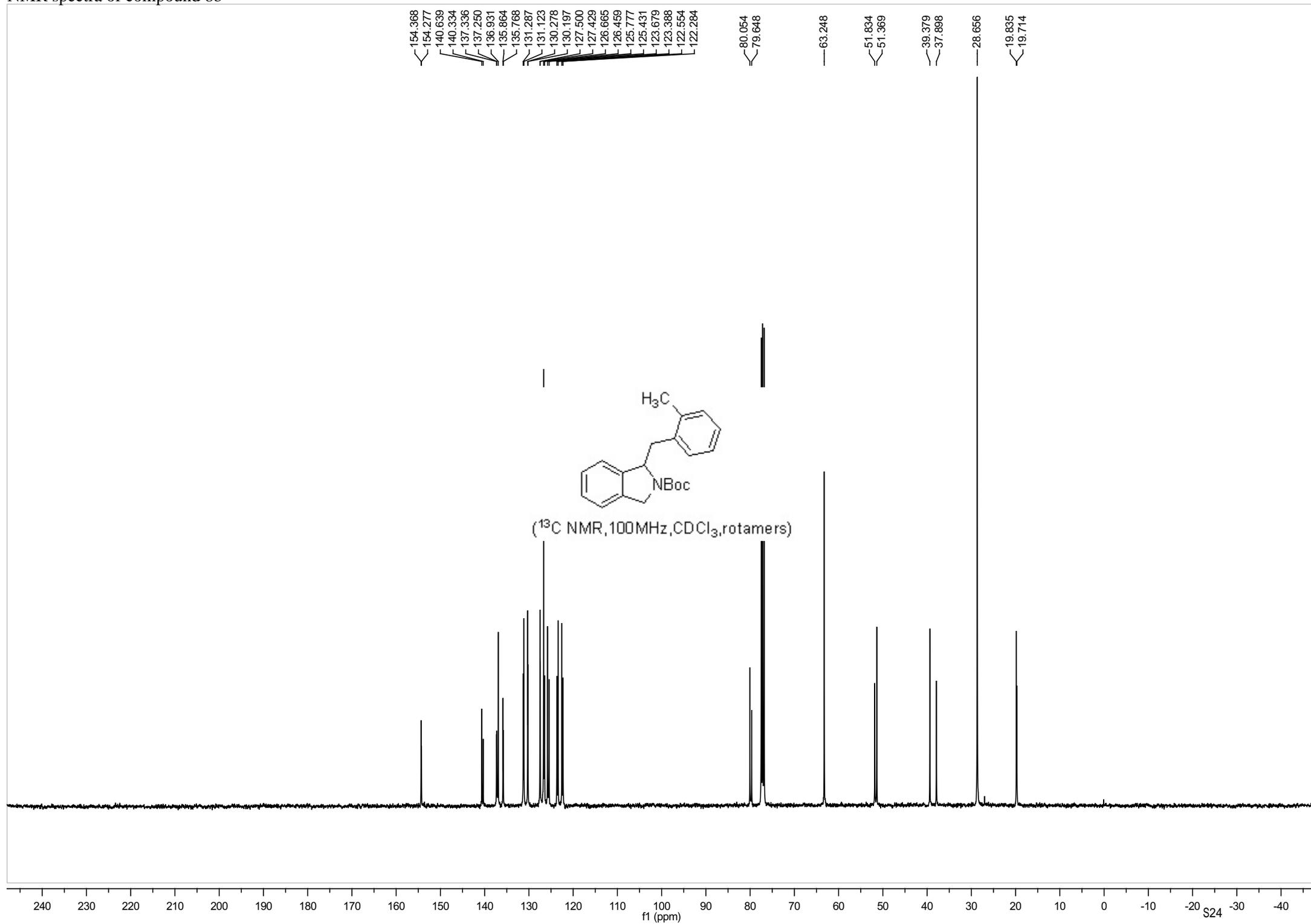
NMR spectra of compound 8a



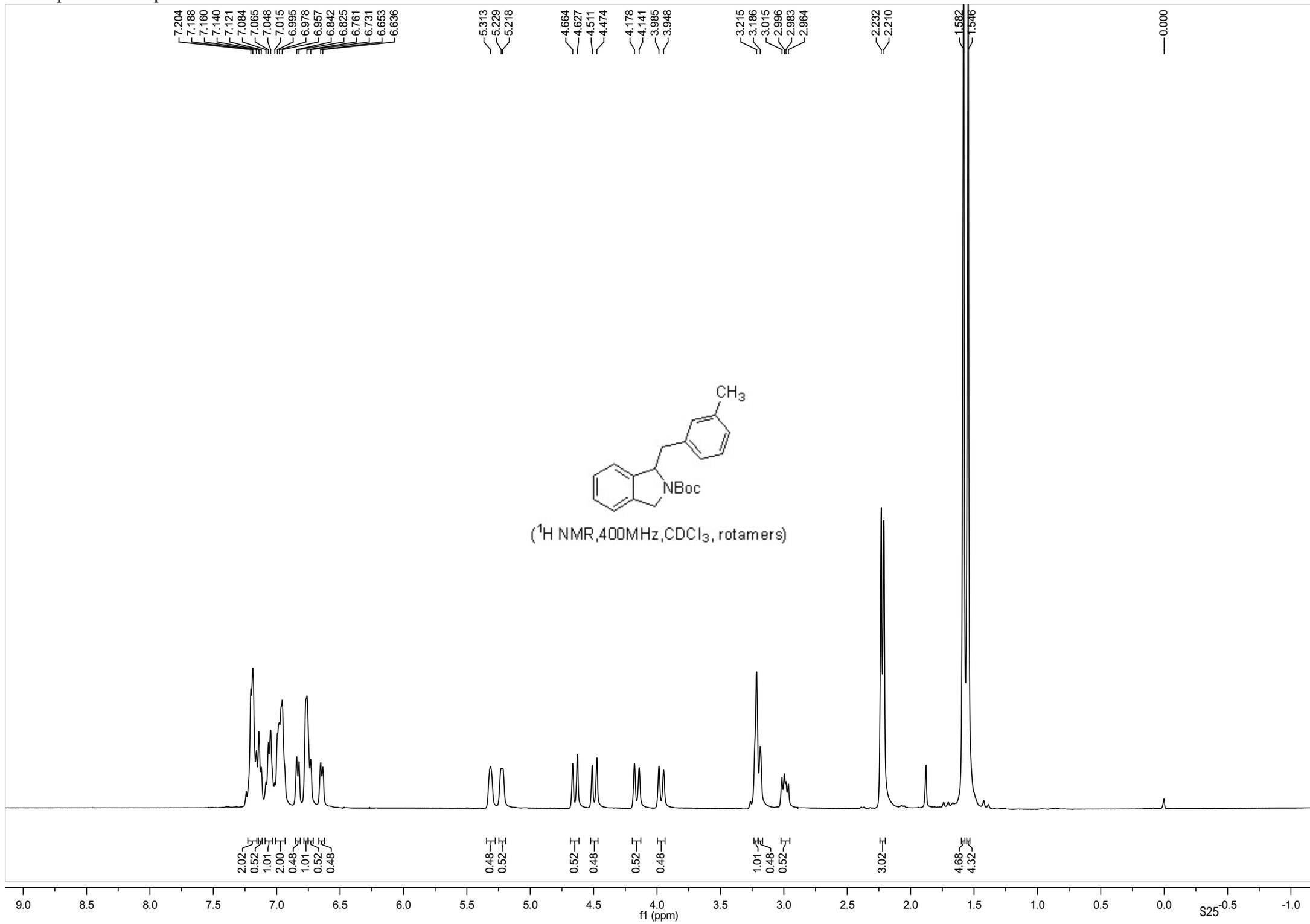
NMR spectra of compound 8b



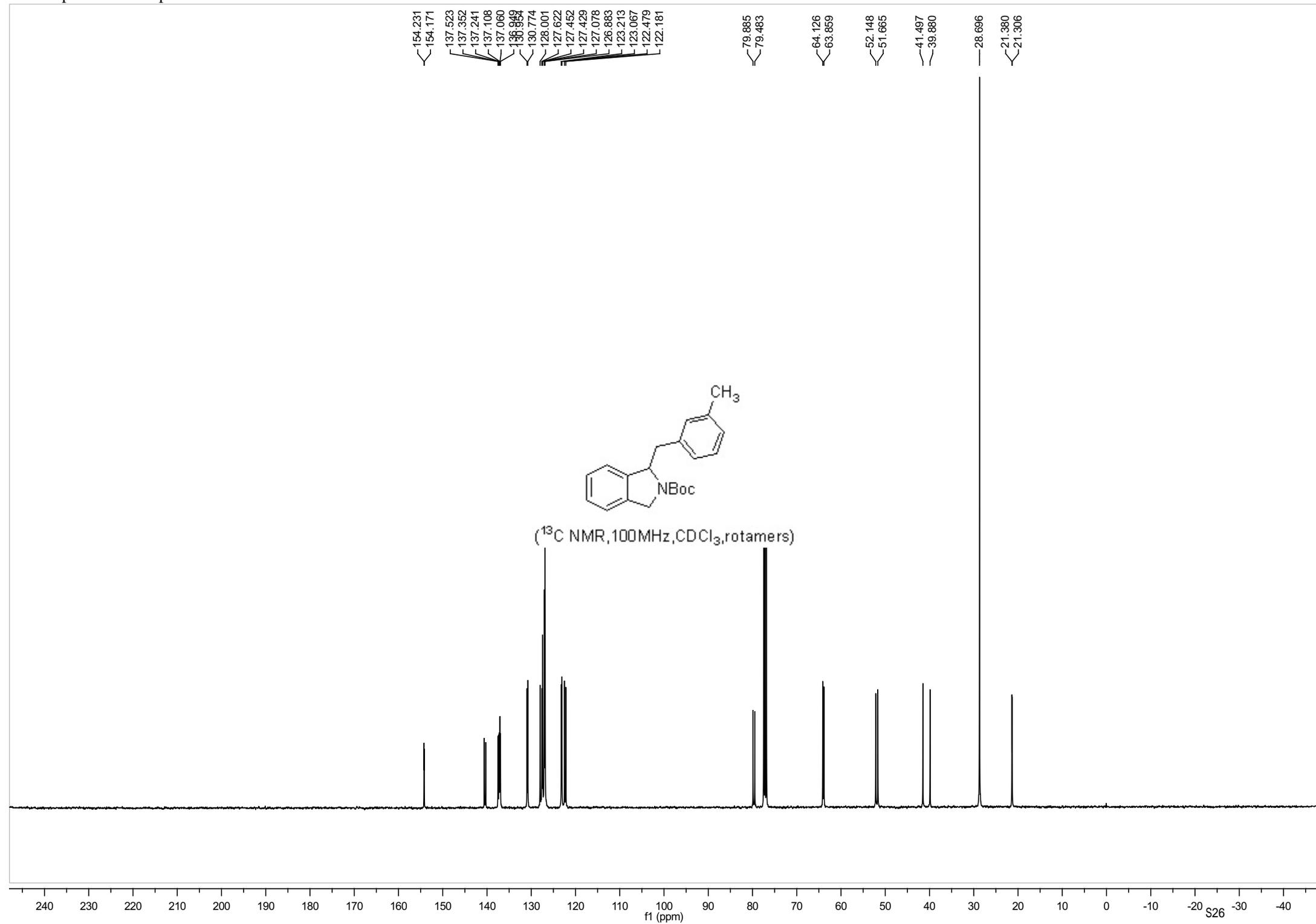
NMR spectra of compound 8b



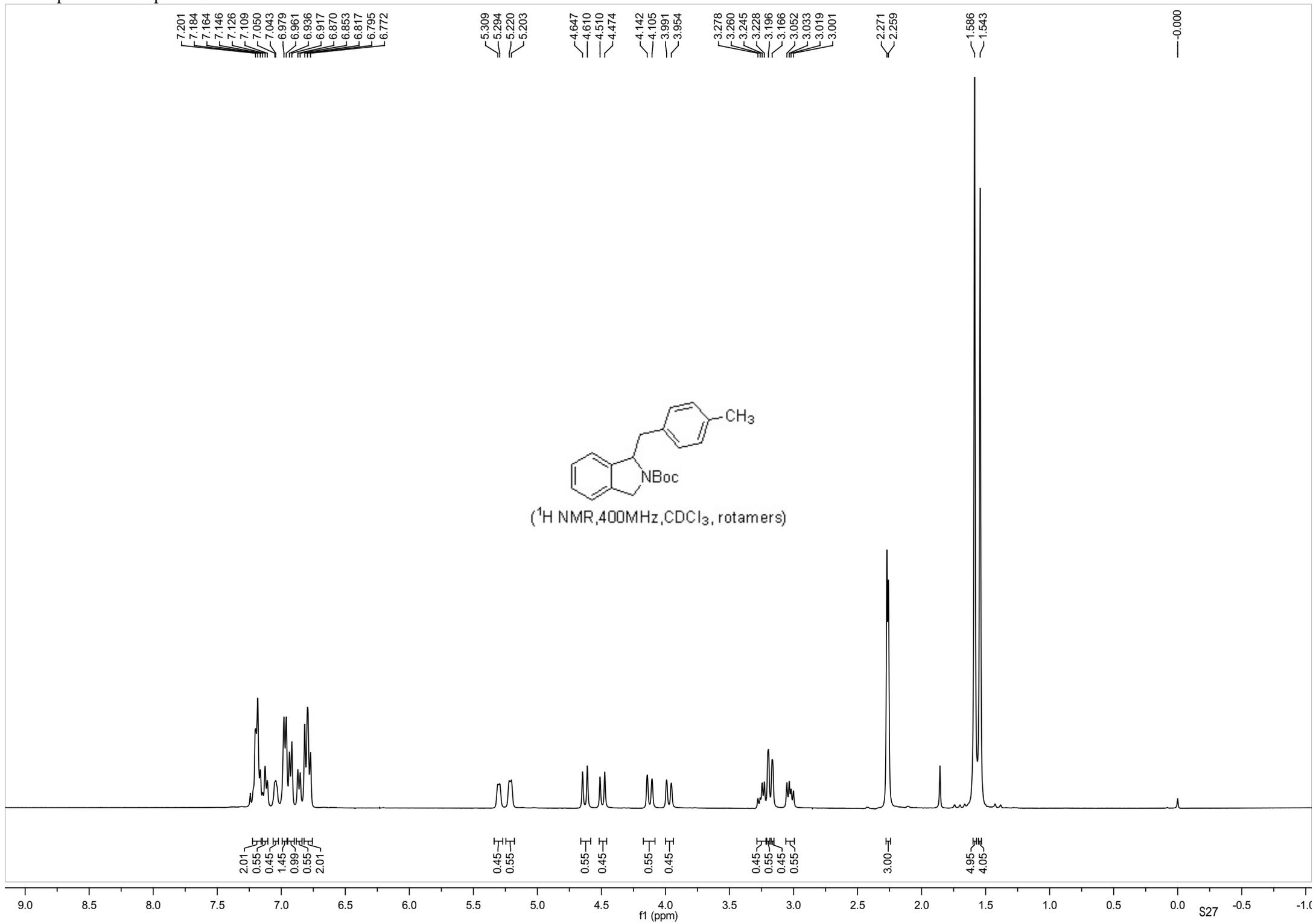
NMR spectra of compound 8c



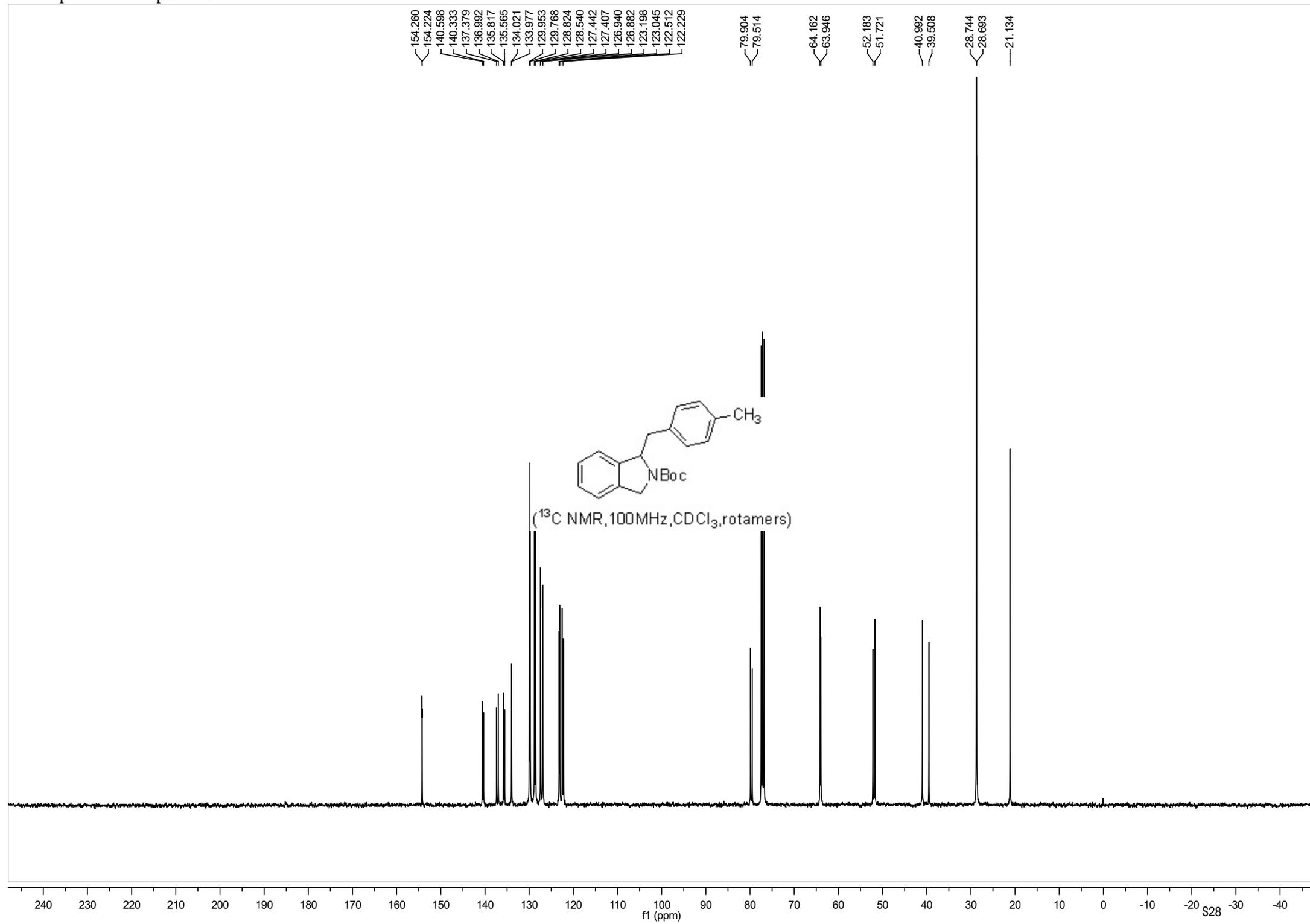
NMR spectra of compound 8c



NMR spectra of compound 8d



NMR spectra of compound 8d



NMR spectra of compound 8e

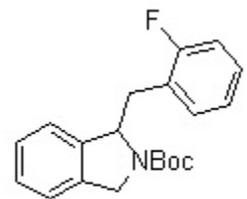
7.255
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7.164
7.148
6.965
6.943
6.924
6.868
6.850

5.379
5.303

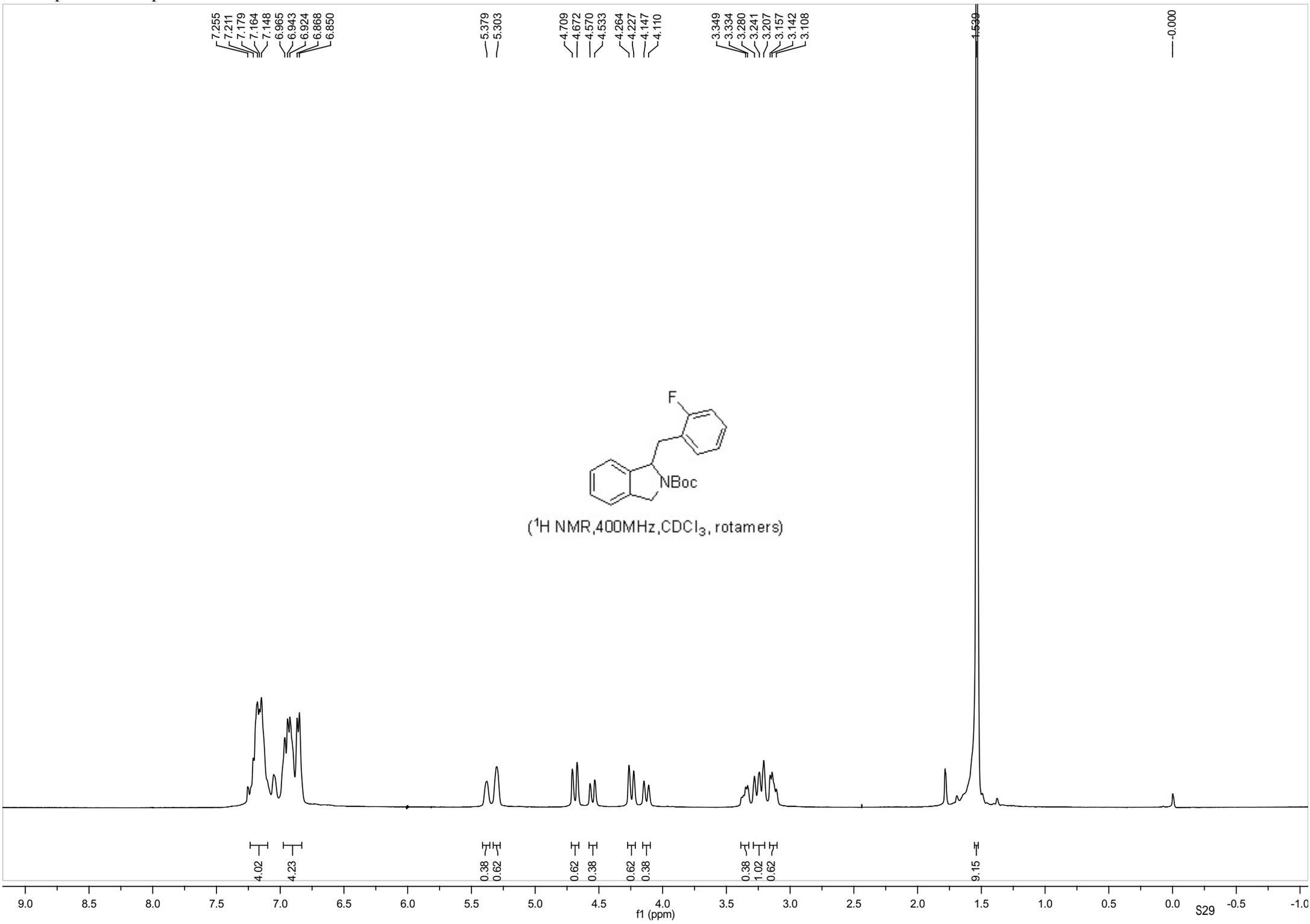
4.709
4.672
4.570
4.533
4.264
4.227
4.147
4.110

3.349
3.334
3.280
3.241
3.207
3.157
3.142
3.108

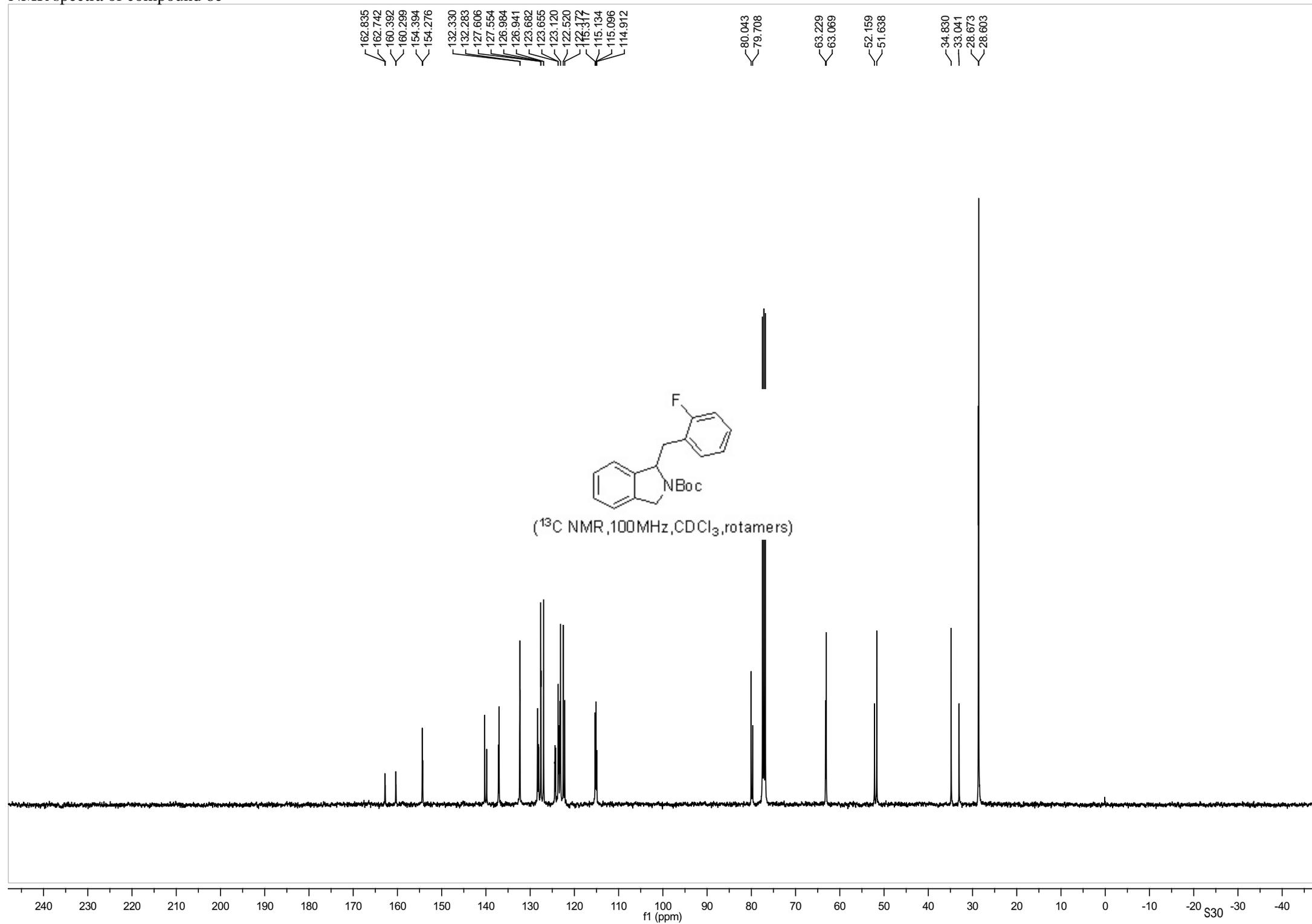
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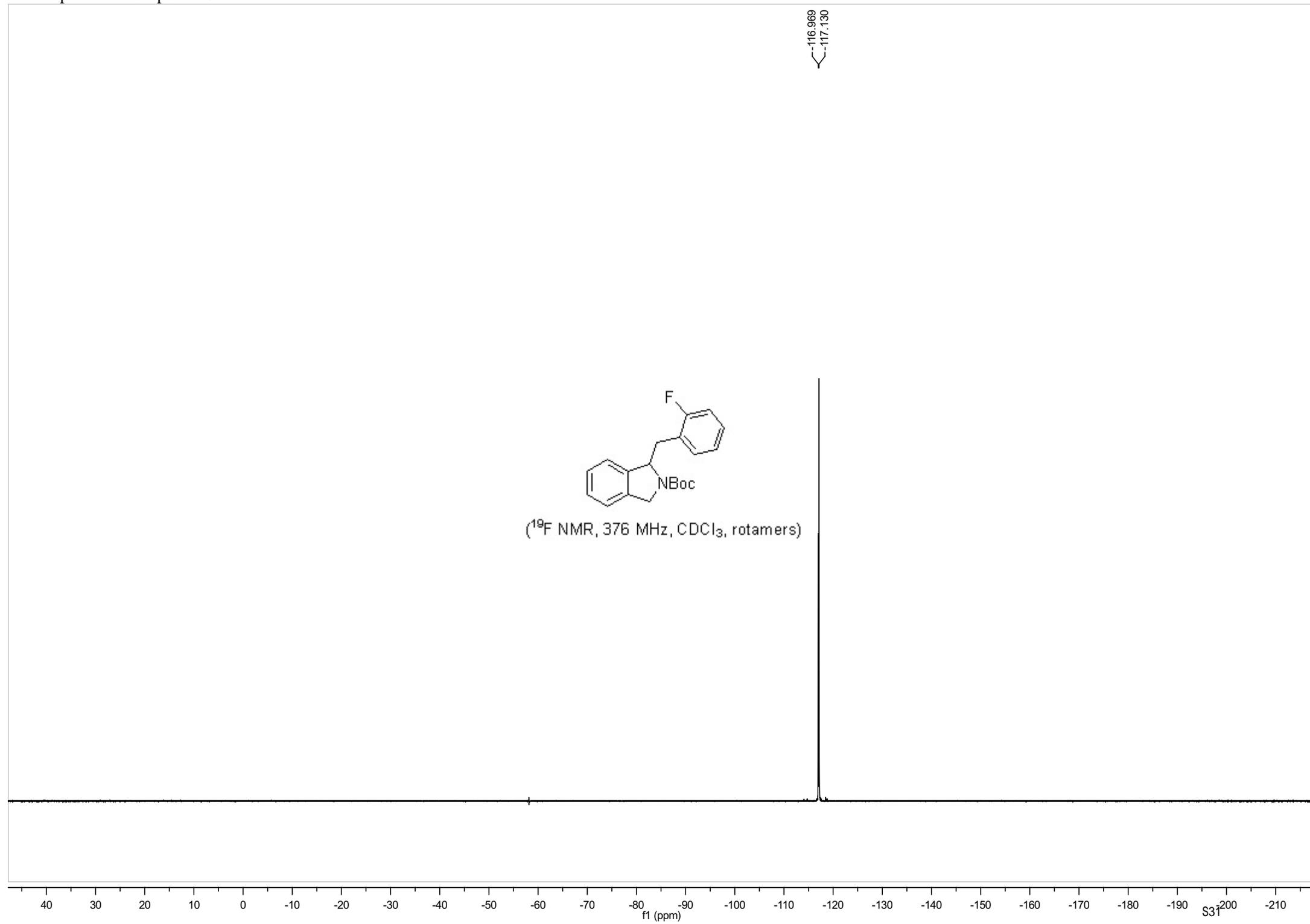
(¹H NMR, 400MHz, CDCl₃, rotamers)



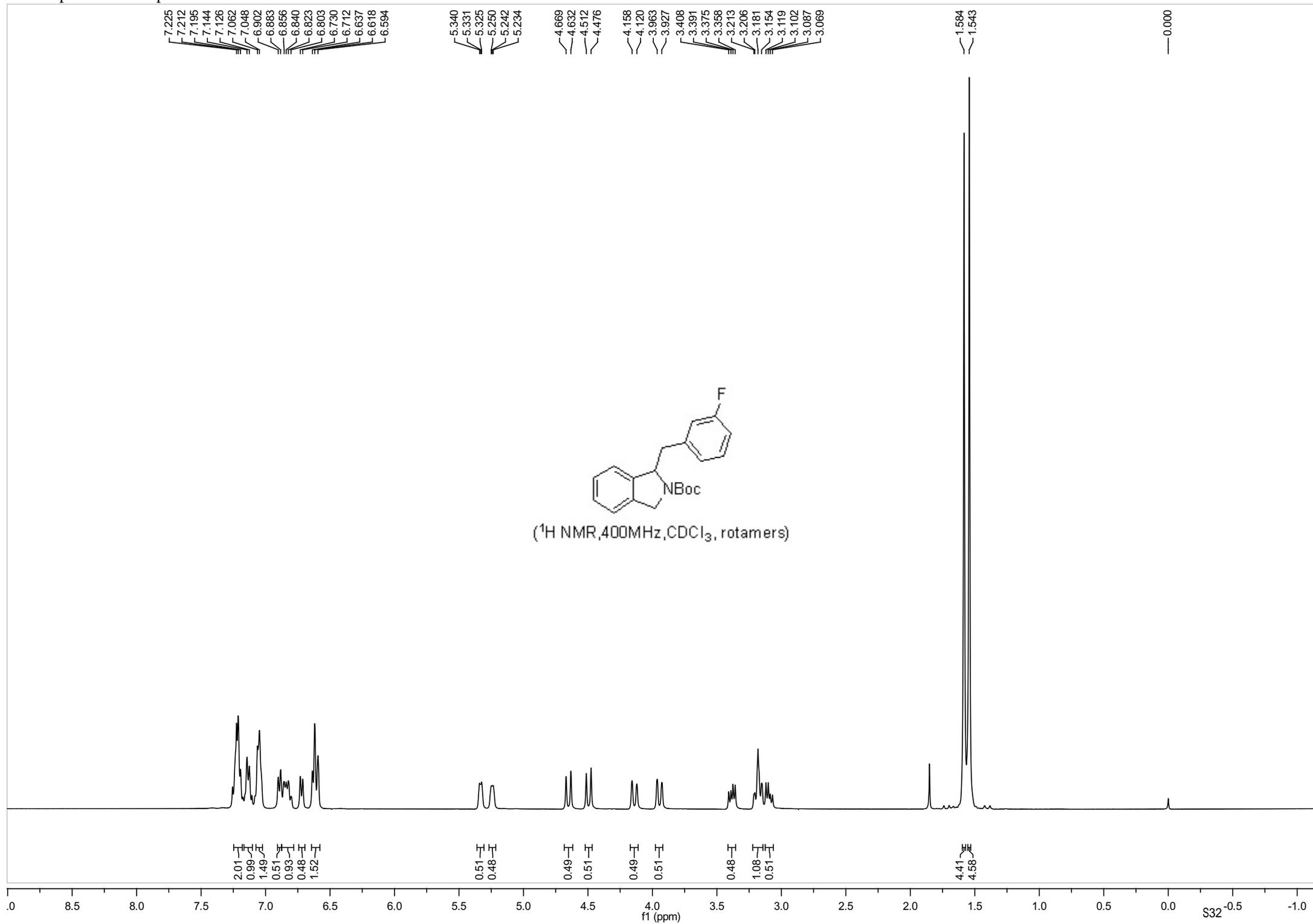
NMR spectra of compound 8e



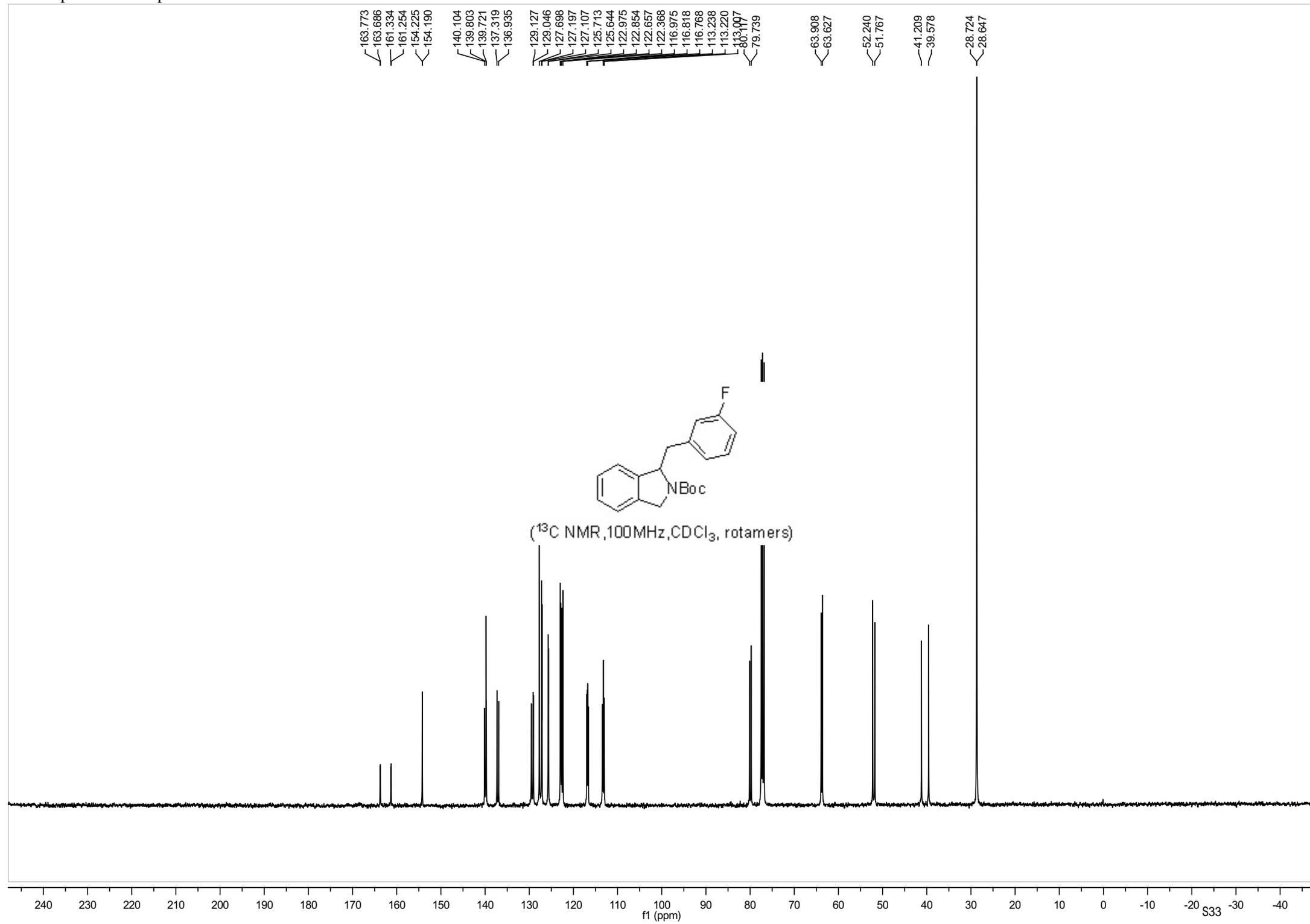
NMR spectra of compound 8e



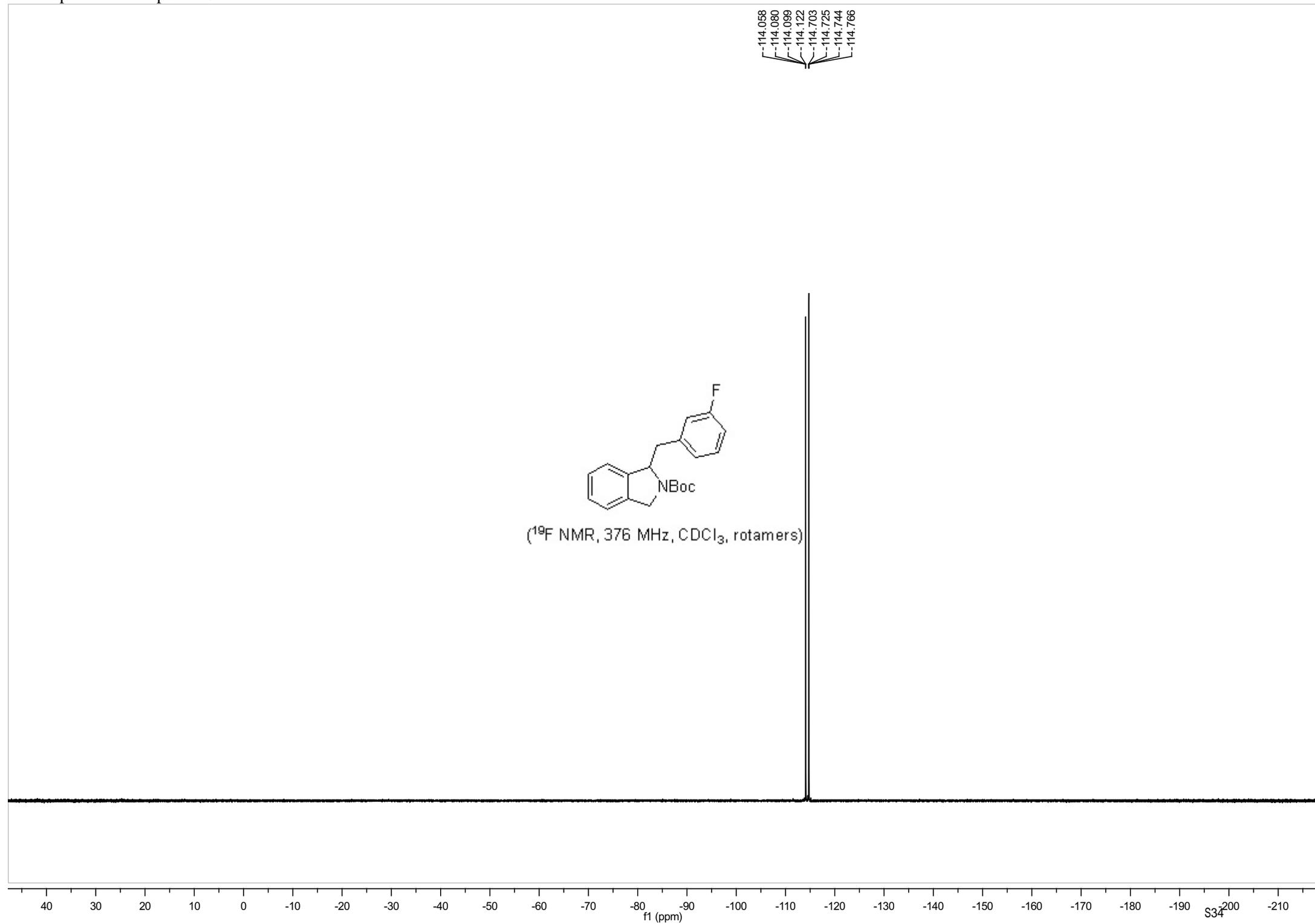
NMR spectra of compound 8f



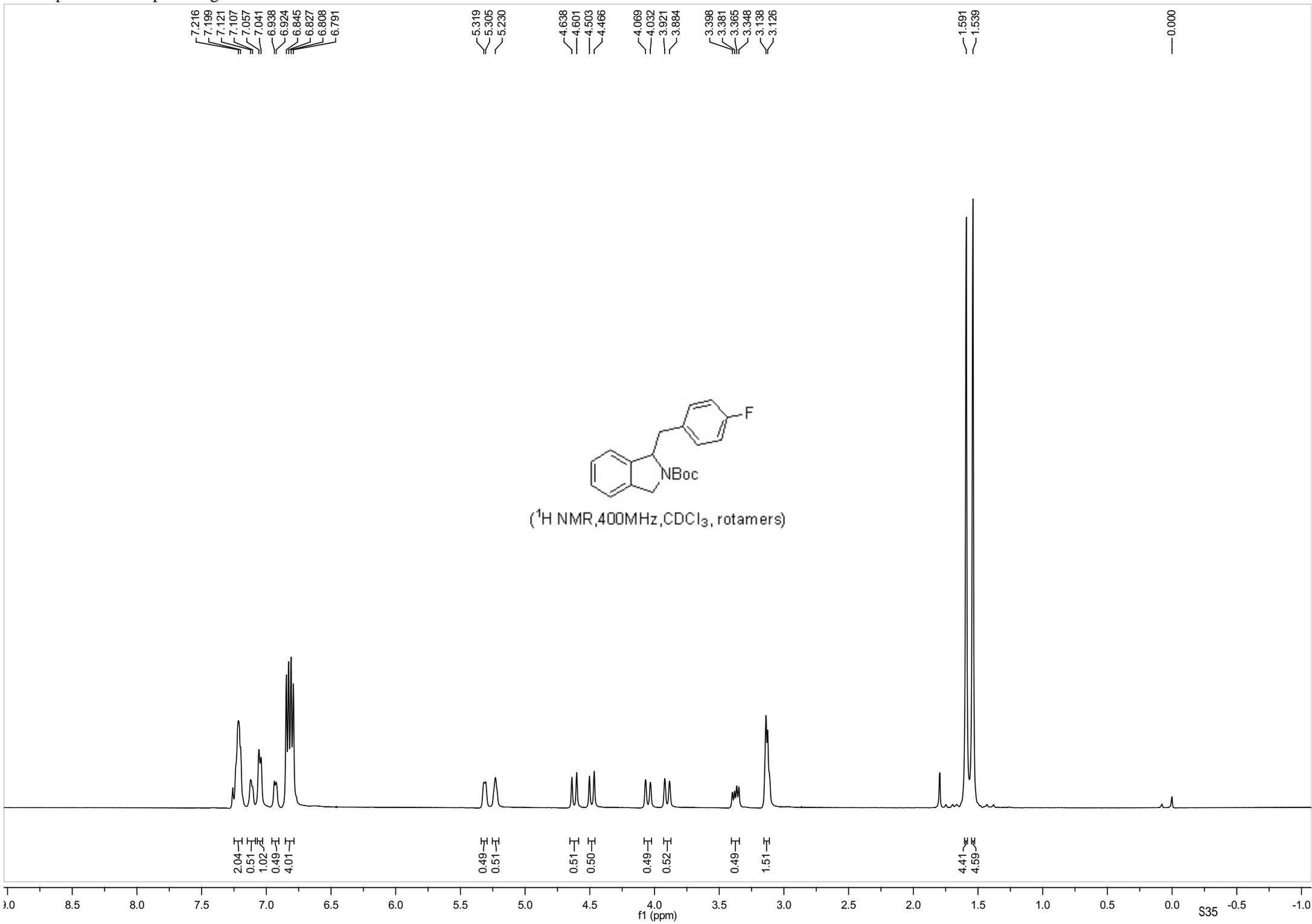
NMR spectra of compound 8f



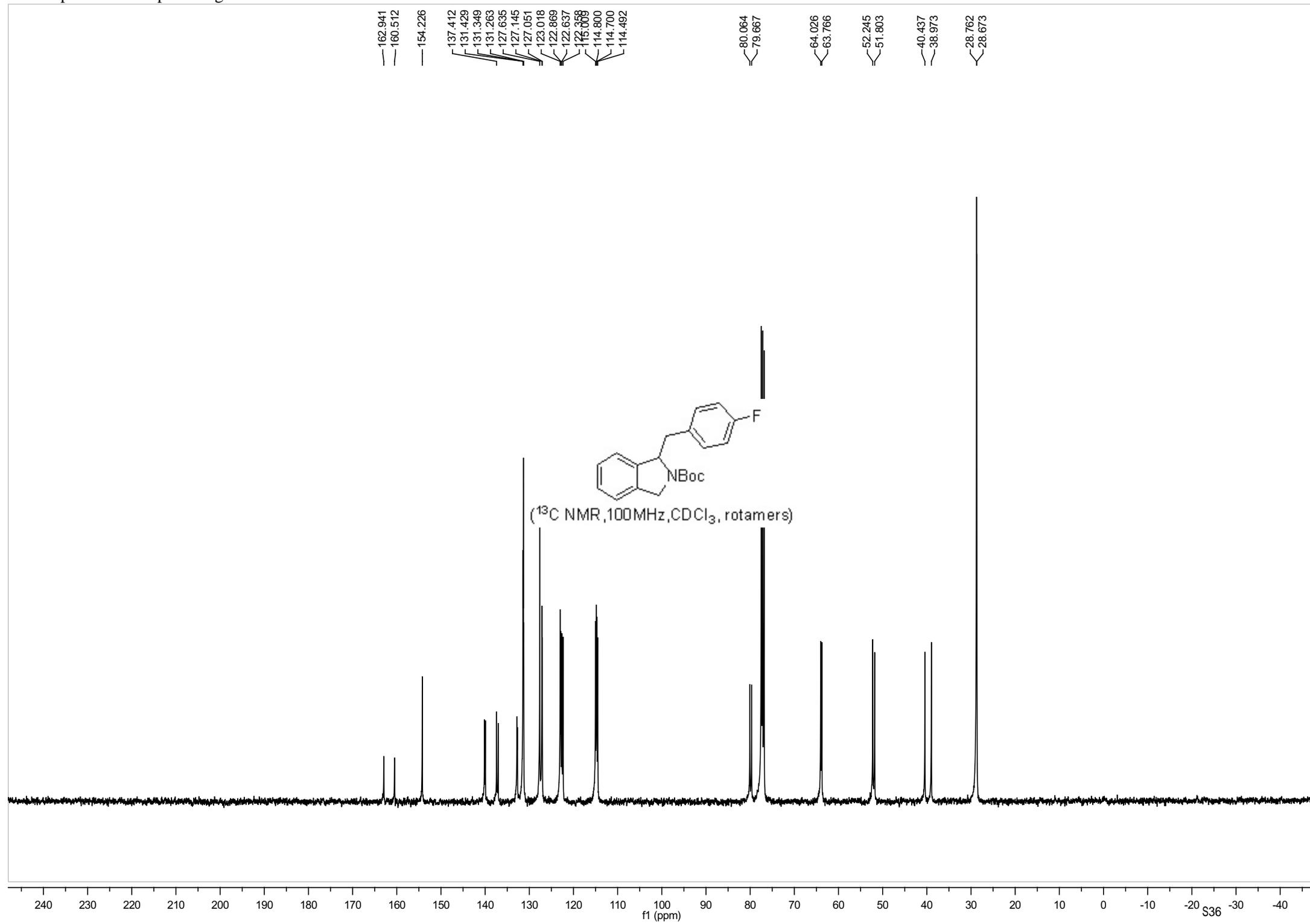
NMR spectra of compound 8f



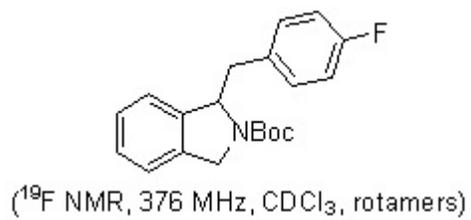
NMR spectra of compound 8g



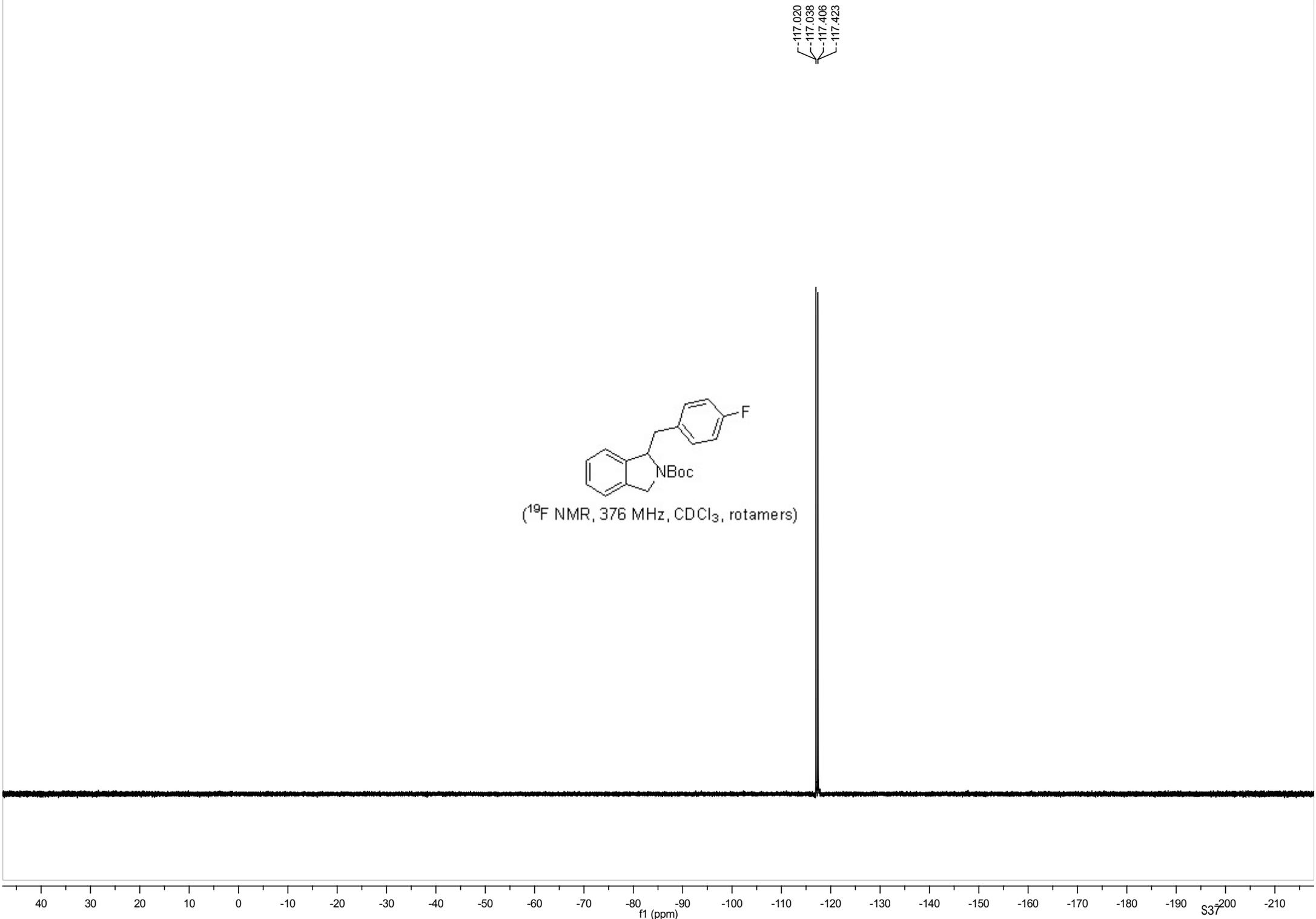
NMR spectra of compound 8g



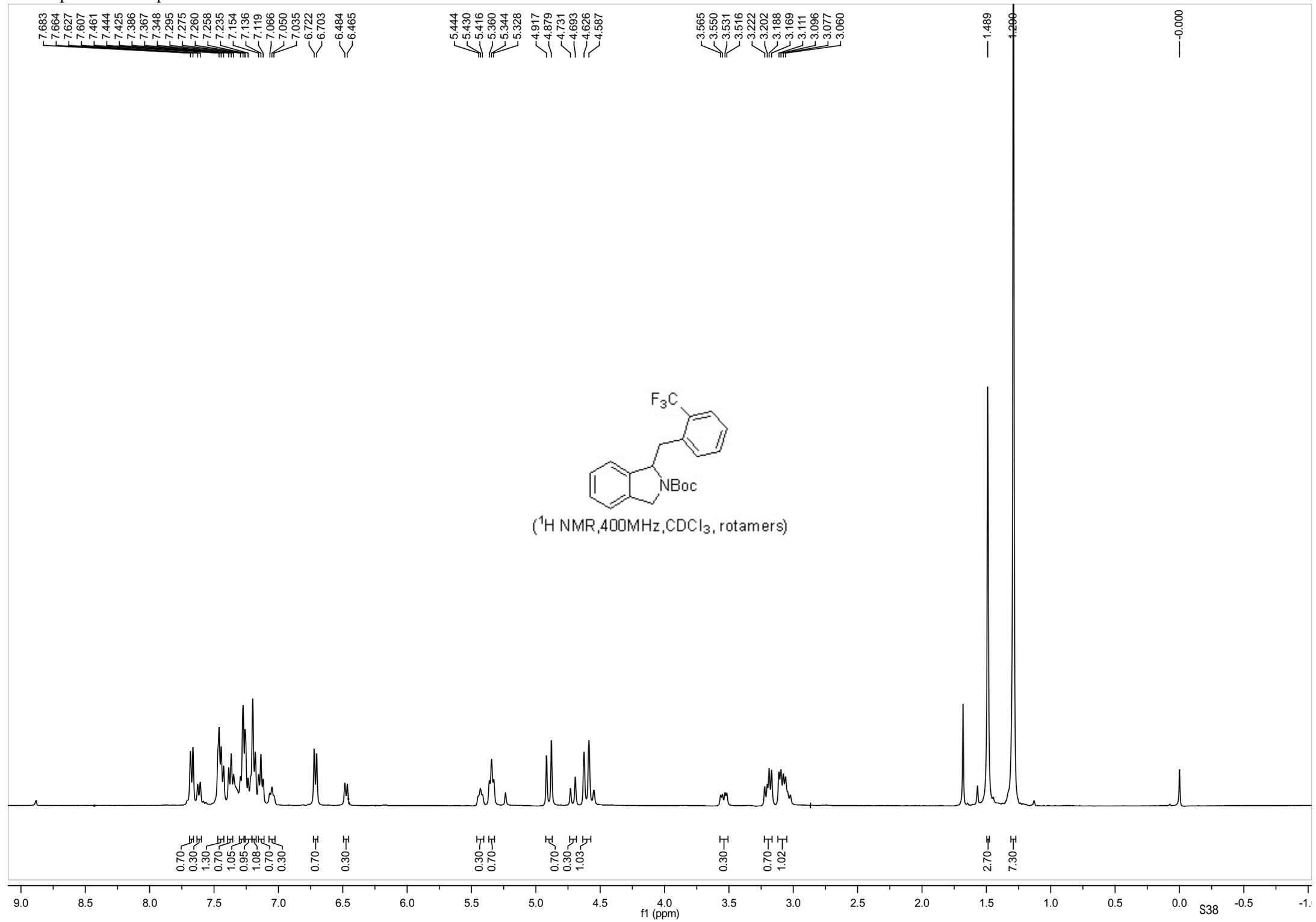
NMR spectra of compound 8g



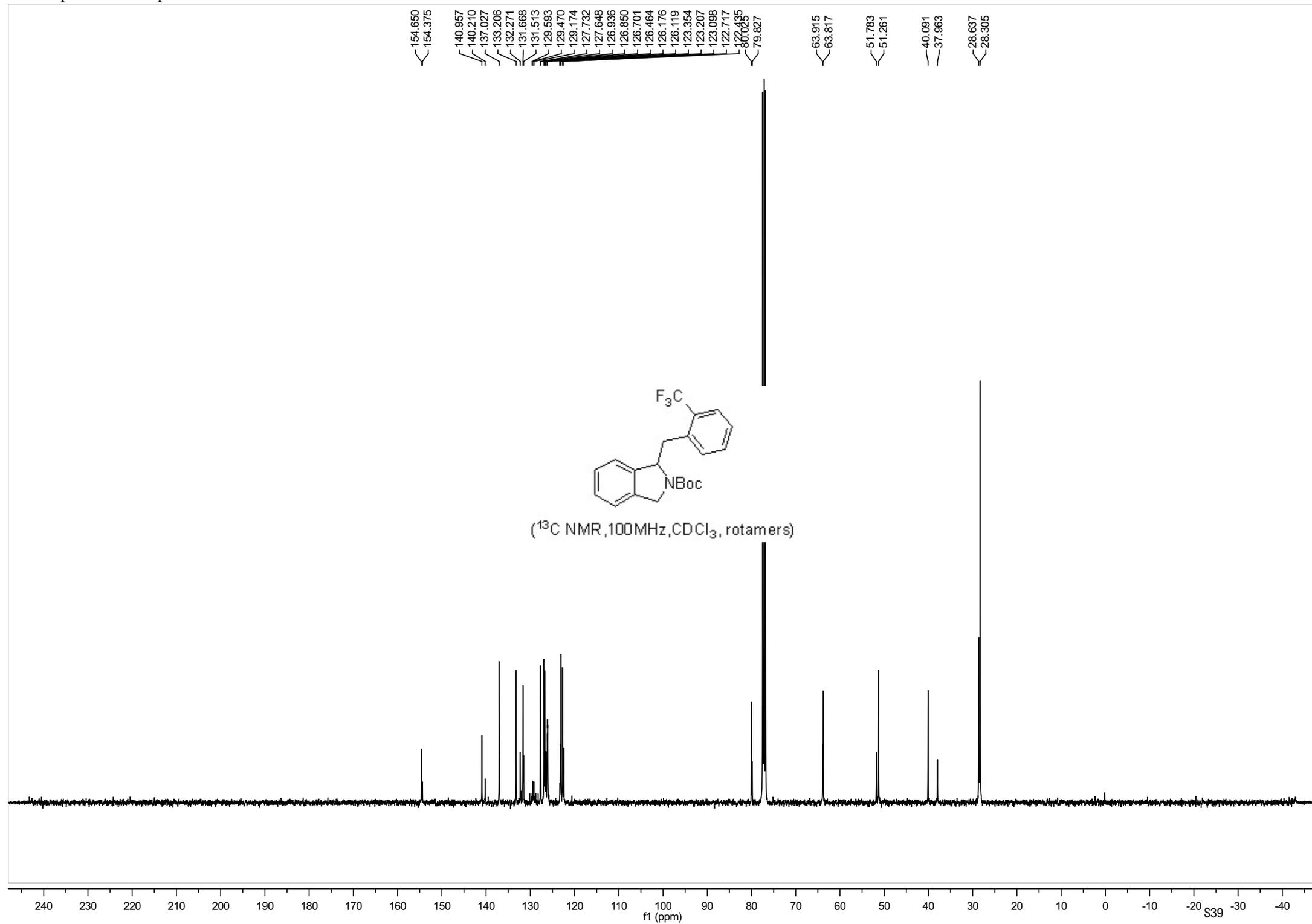
-117.020
-117.038
-117.406
-117.423



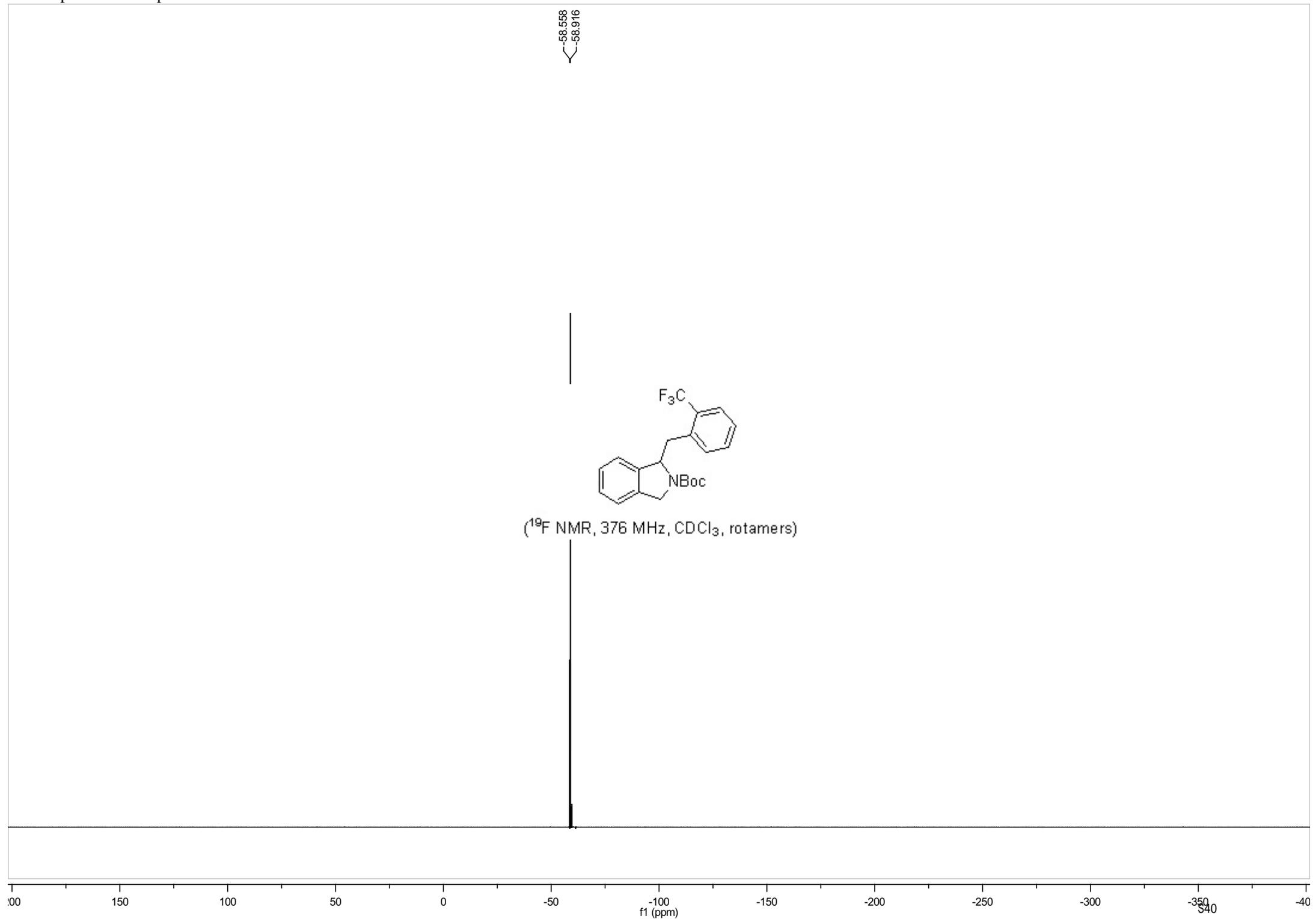
NMR spectra of compound 8h



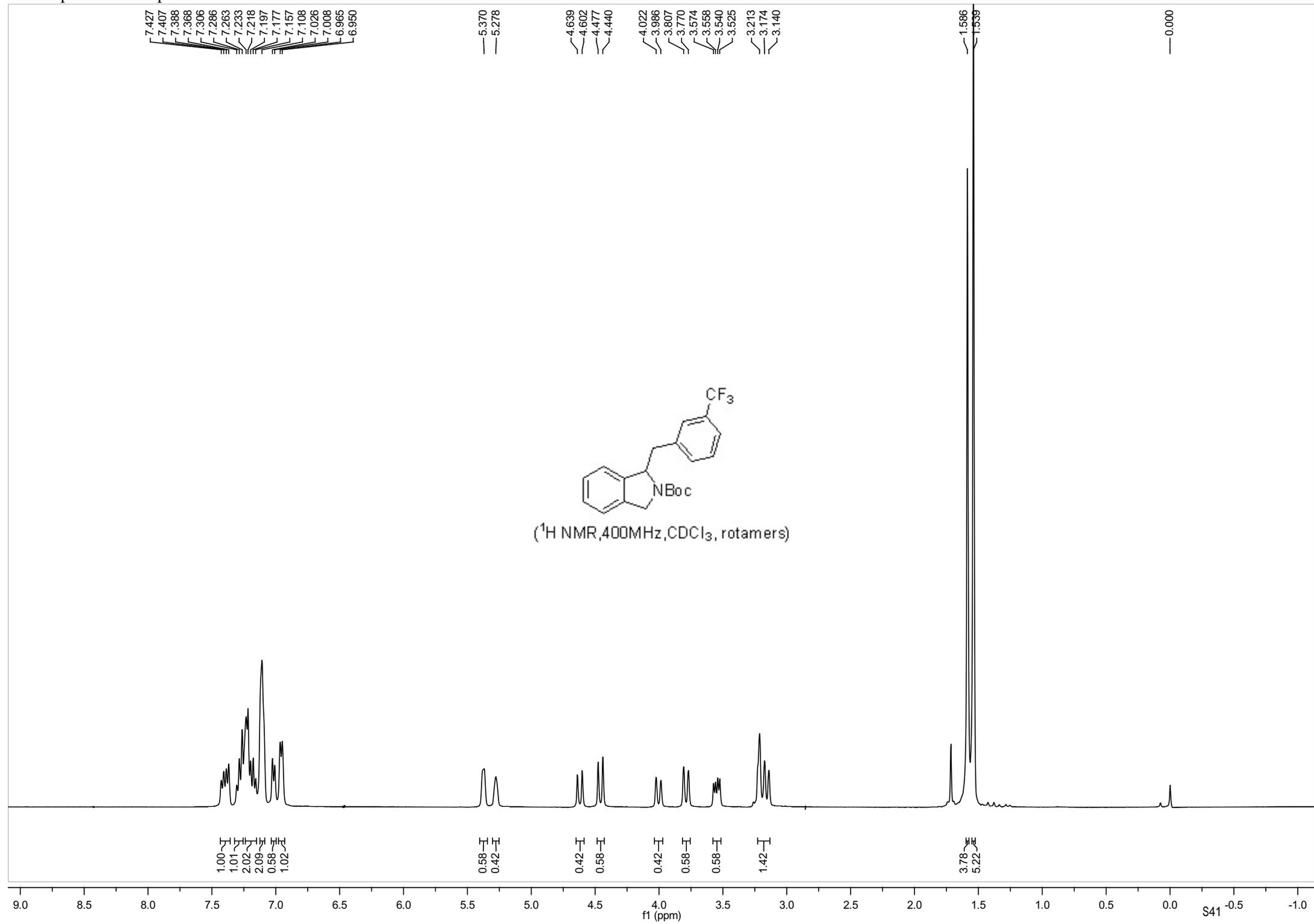
NMR spectra of compound 8h



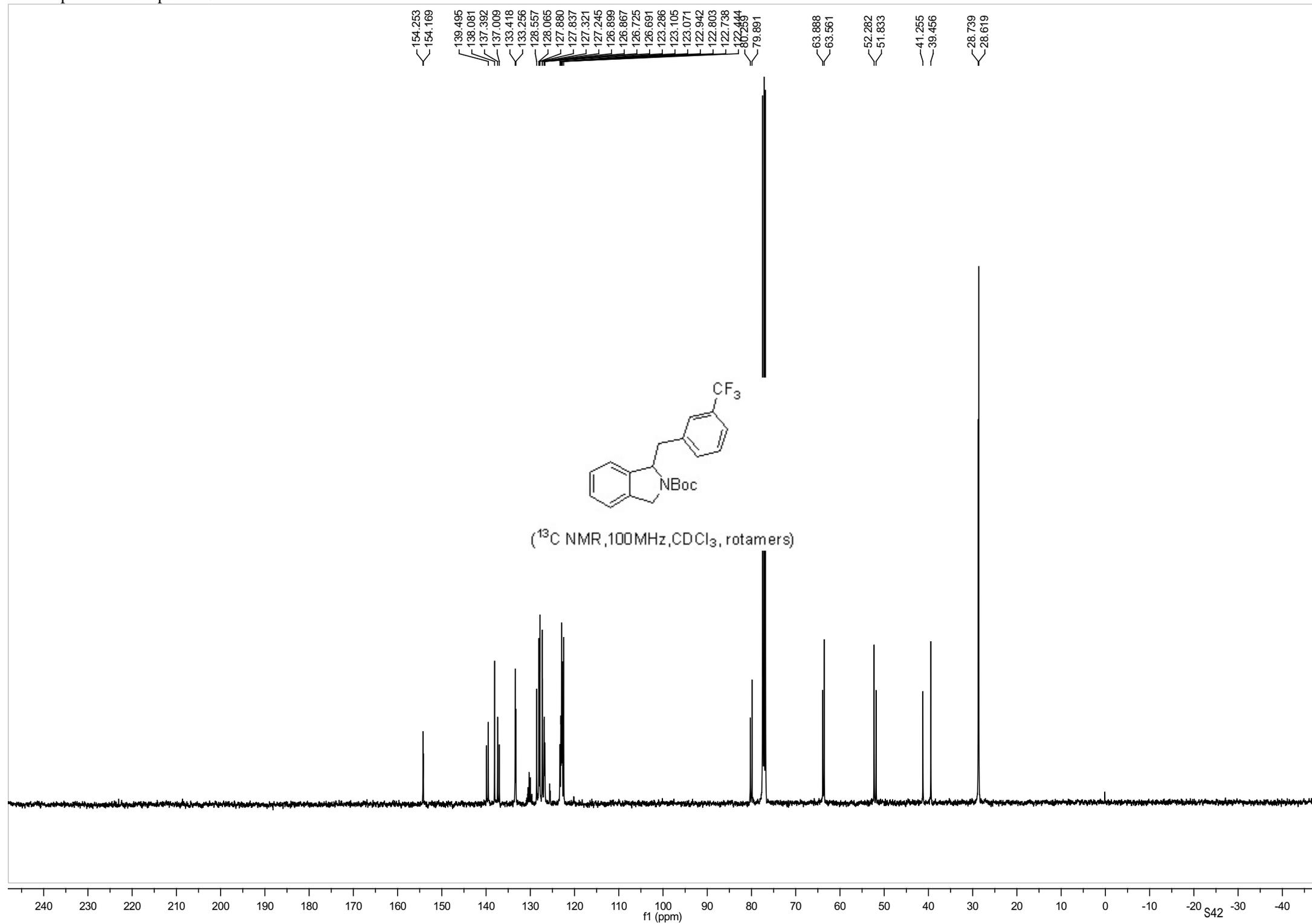
NMR spectra of compound 8h



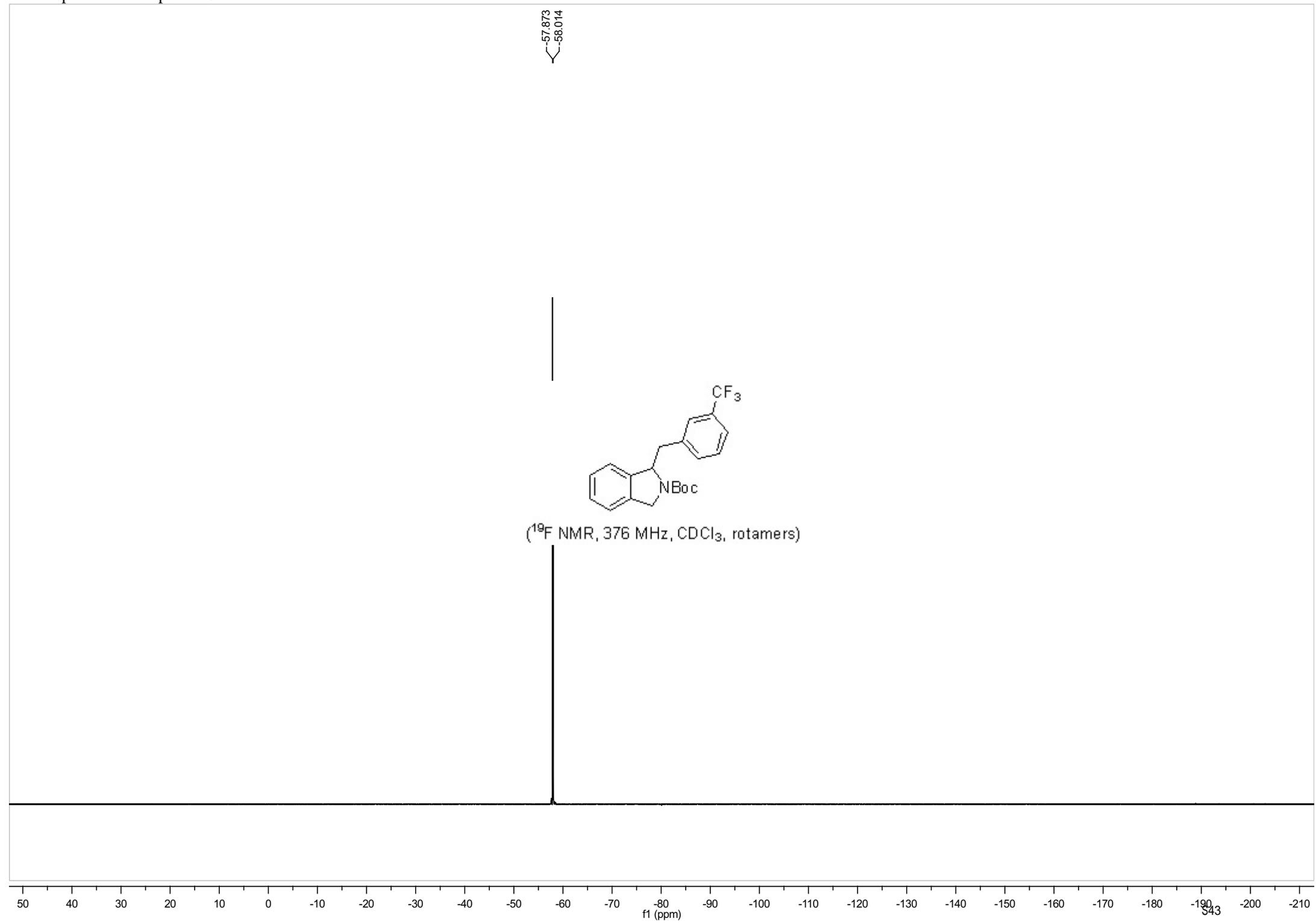
NMR spectra of compound 8i



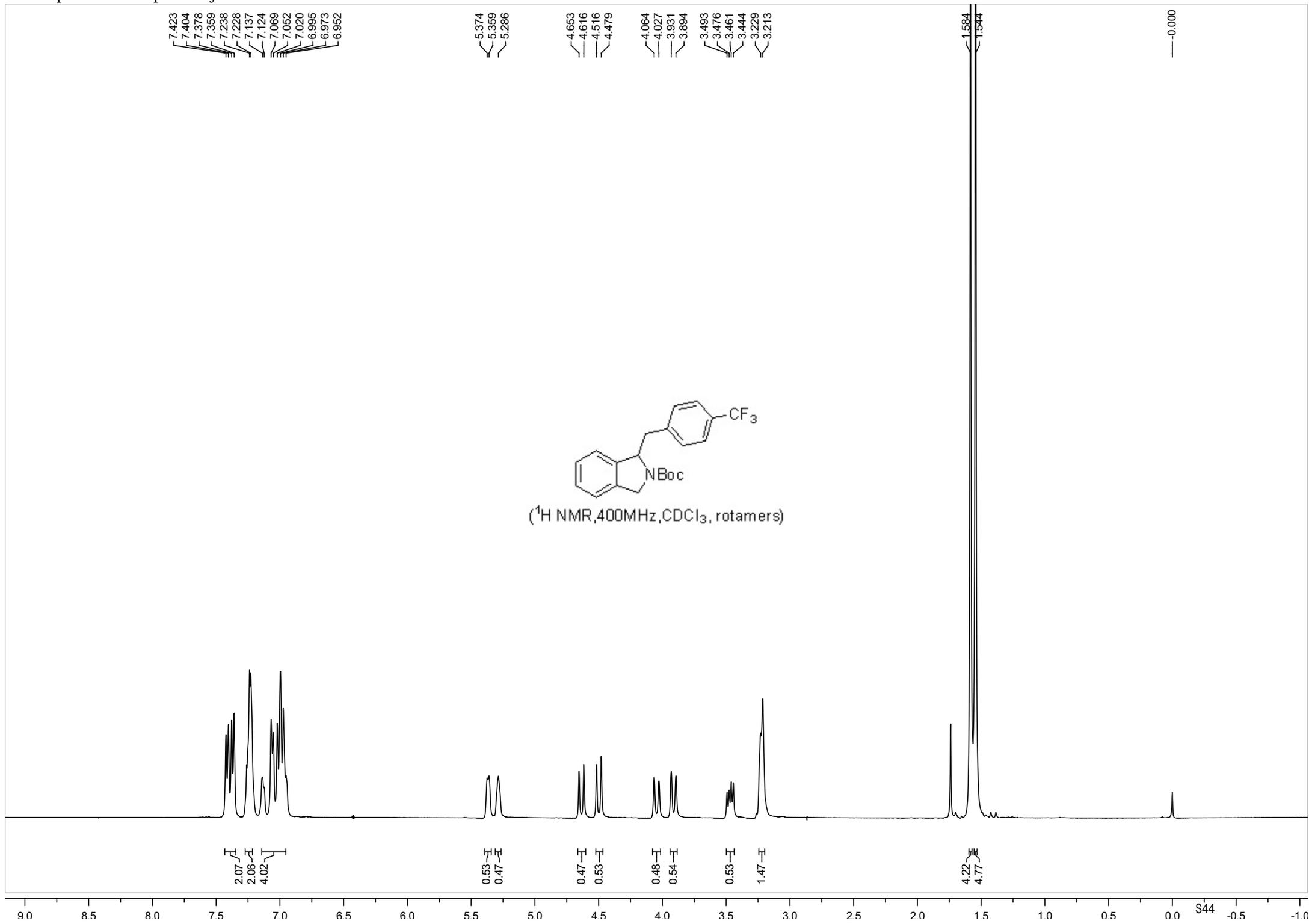
NMR spectra of compound 8i



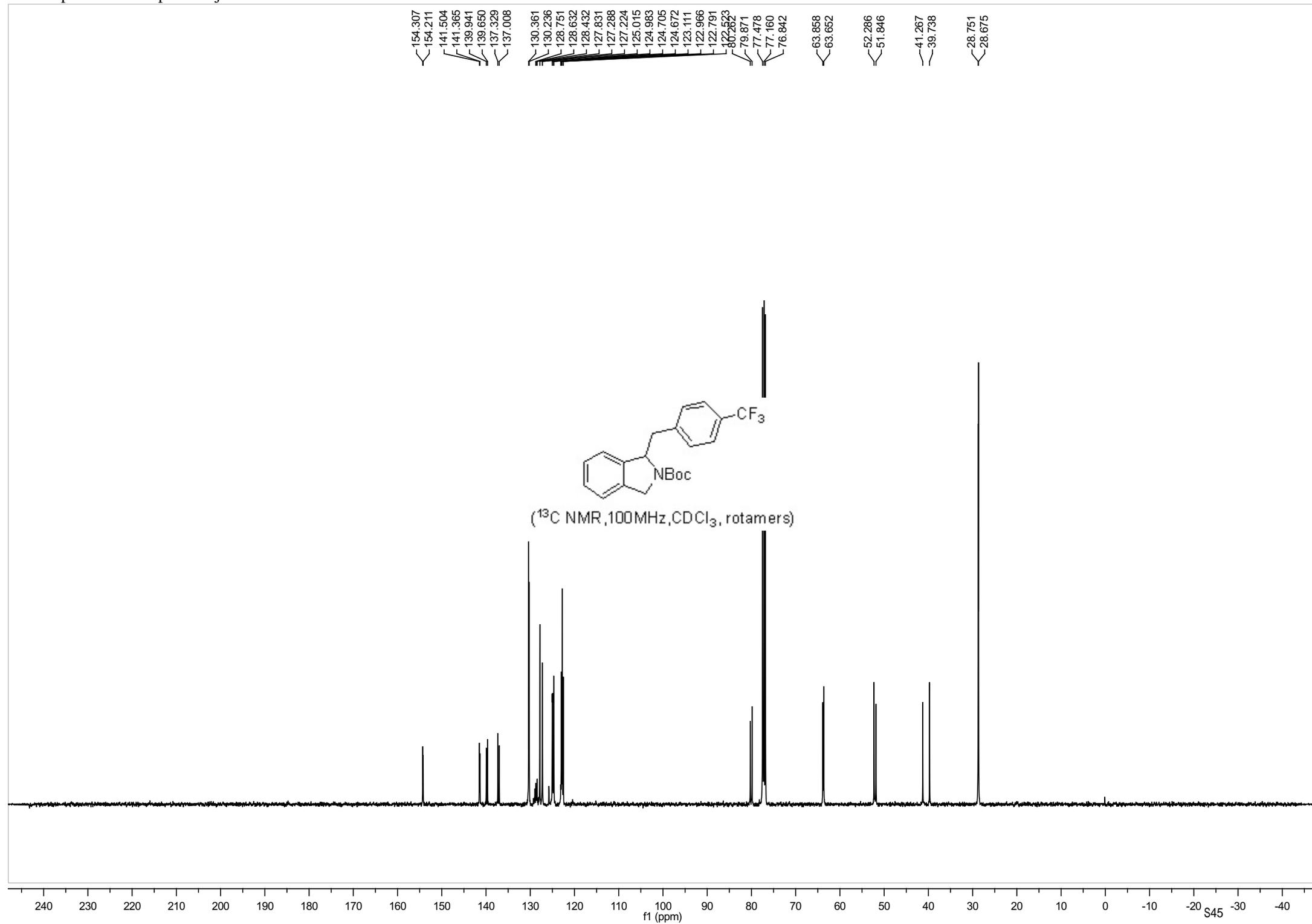
NMR spectra of compound 8i



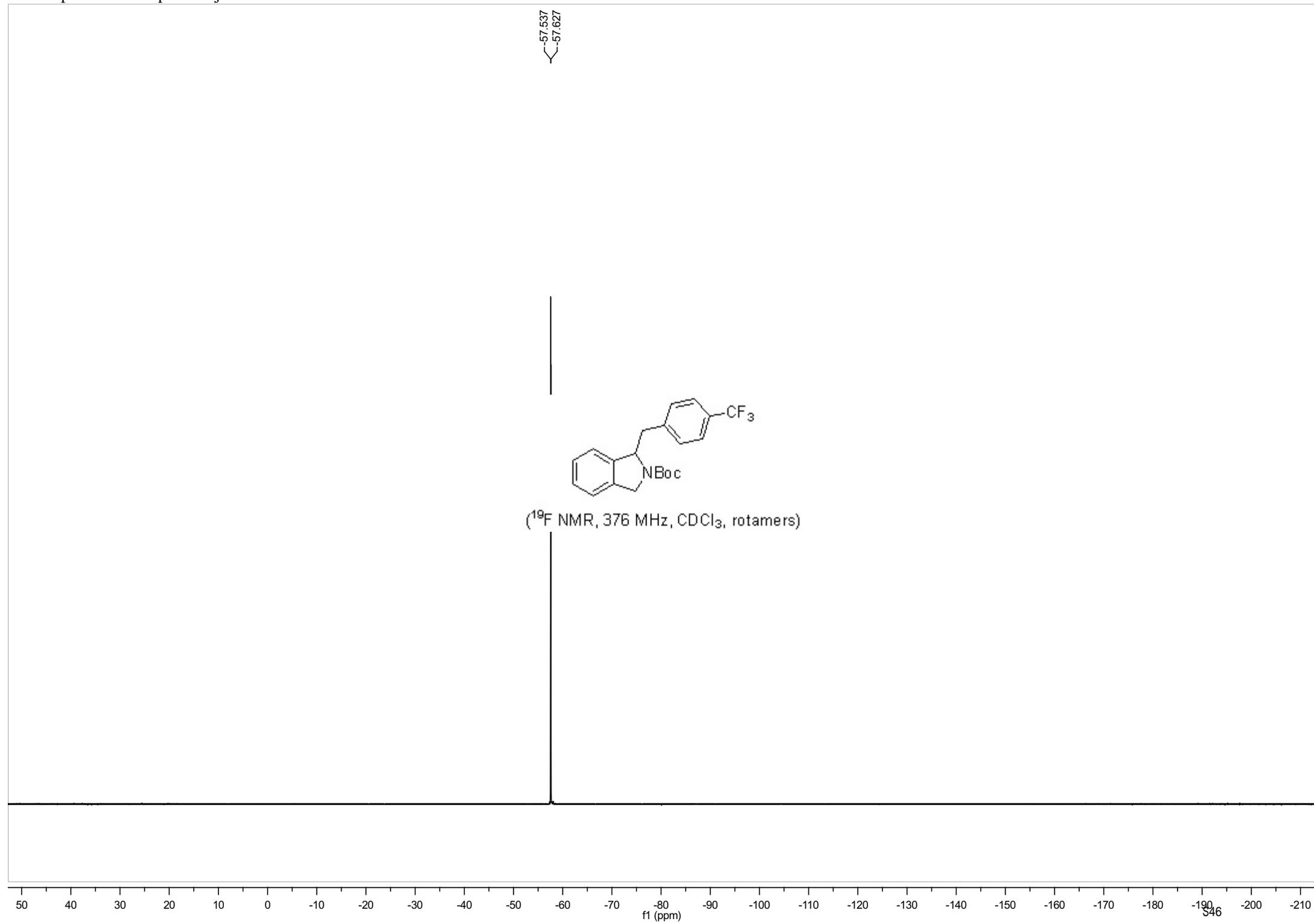
NMR spectra of compound 8j



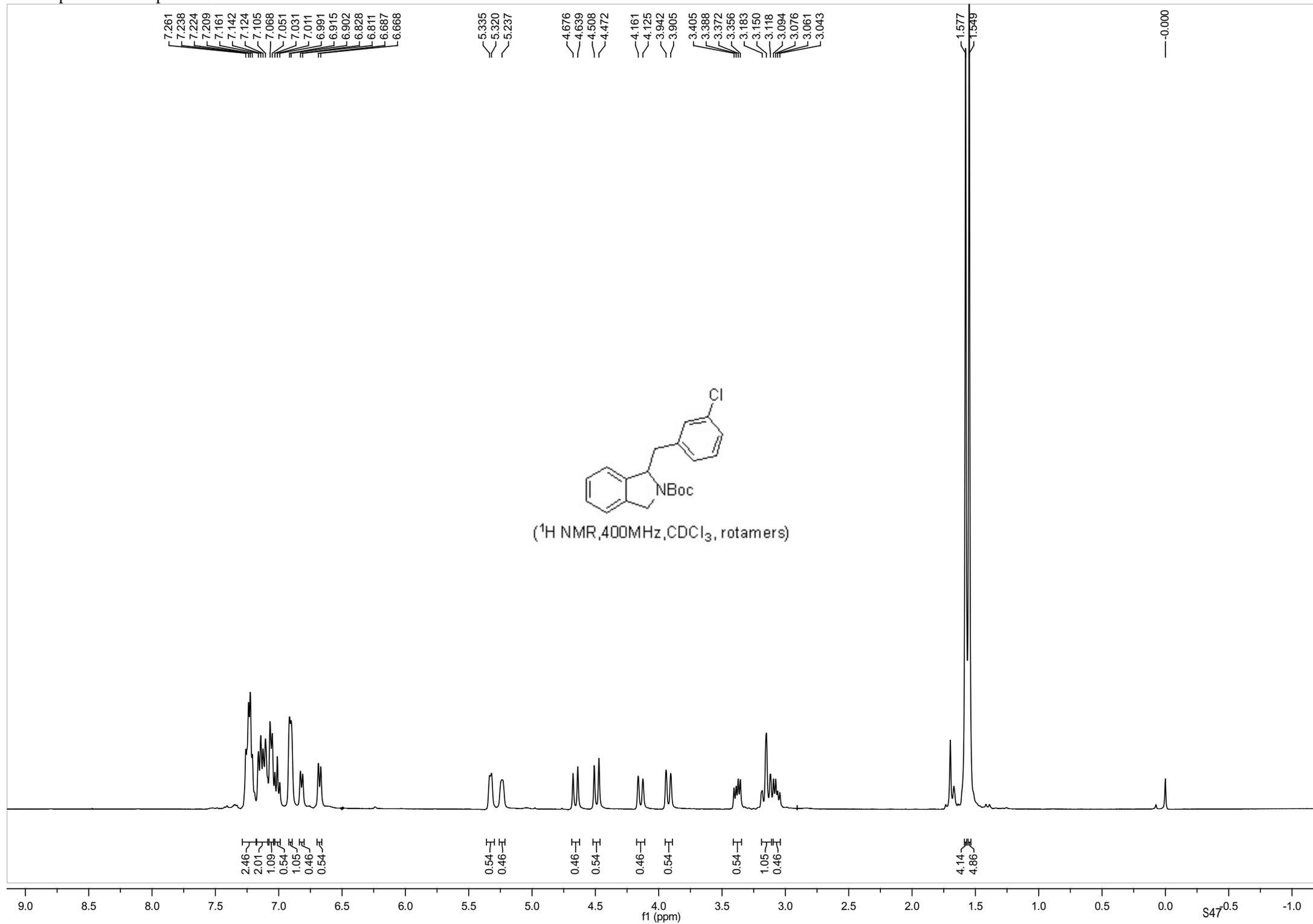
NMR spectra of compound 8j



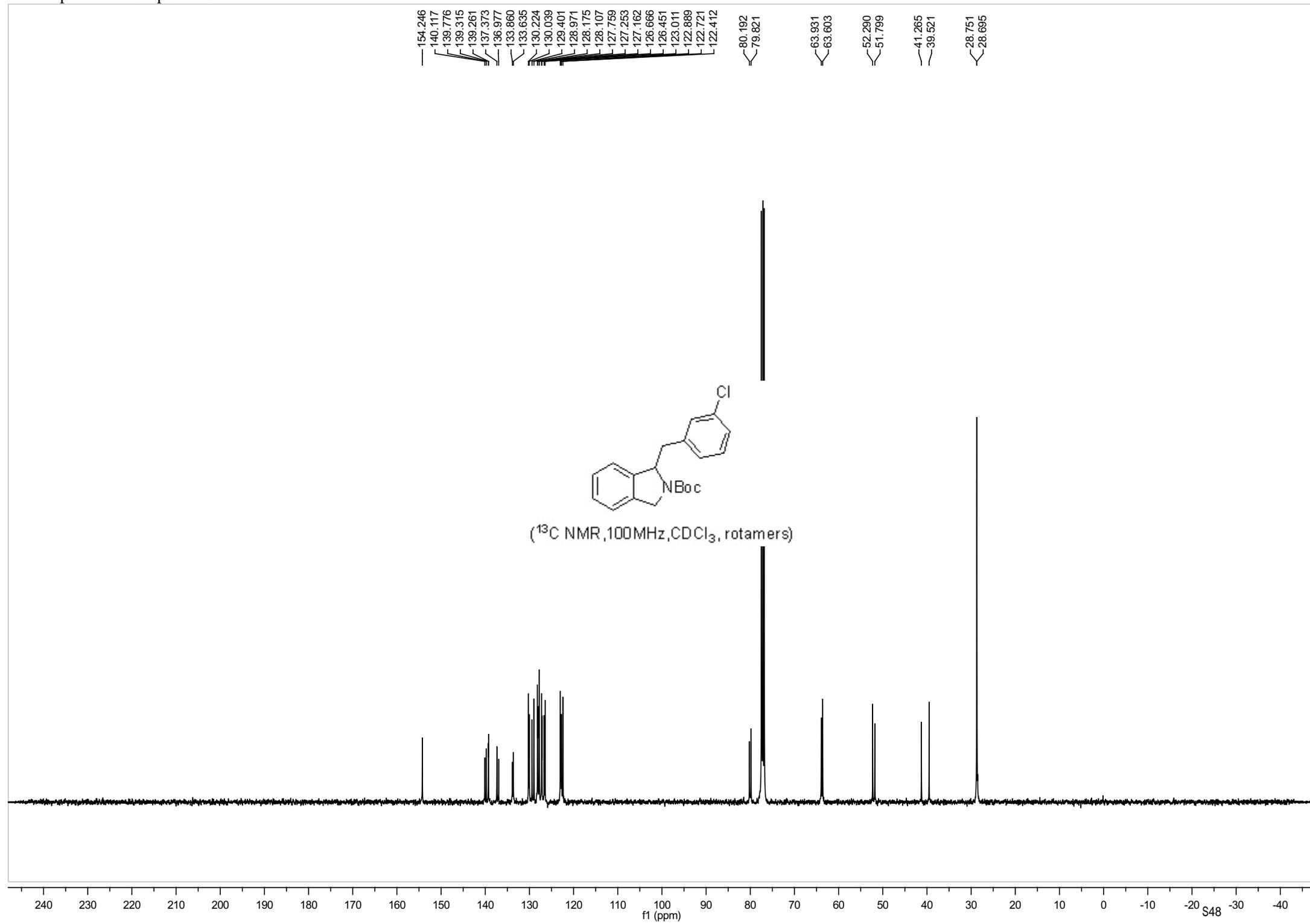
NMR spectra of compound 8j



NMR spectra of compound 8k



NMR spectra of compound 8k



NMR spectra of compound 81

7.246
7.217
7.197
7.178
7.162
7.151
7.144
7.070
7.054
6.932
6.913
6.898
6.878
6.865
6.847

5.307
5.292
5.226
5.208

4.674
4.637
4.534
4.497

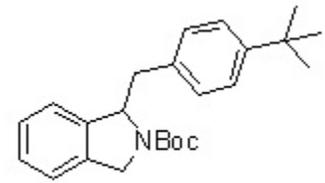
4.180
4.143
4.036
3.999

3.252
3.219
3.202
3.176
3.169
3.152
3.028
3.009
2.995
2.977

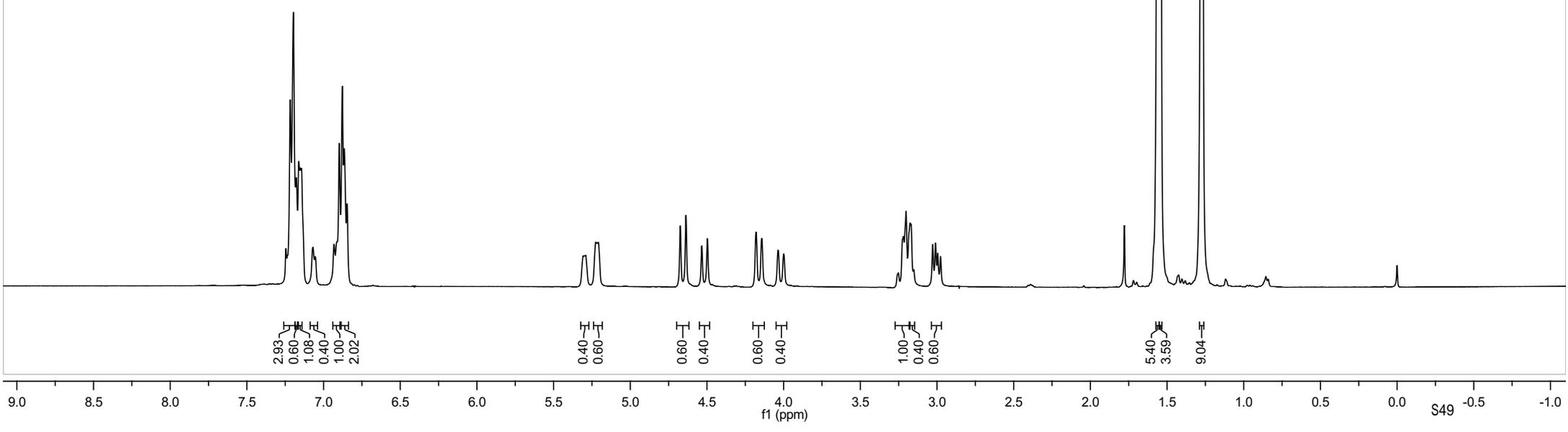
1.563
1.542

1.277

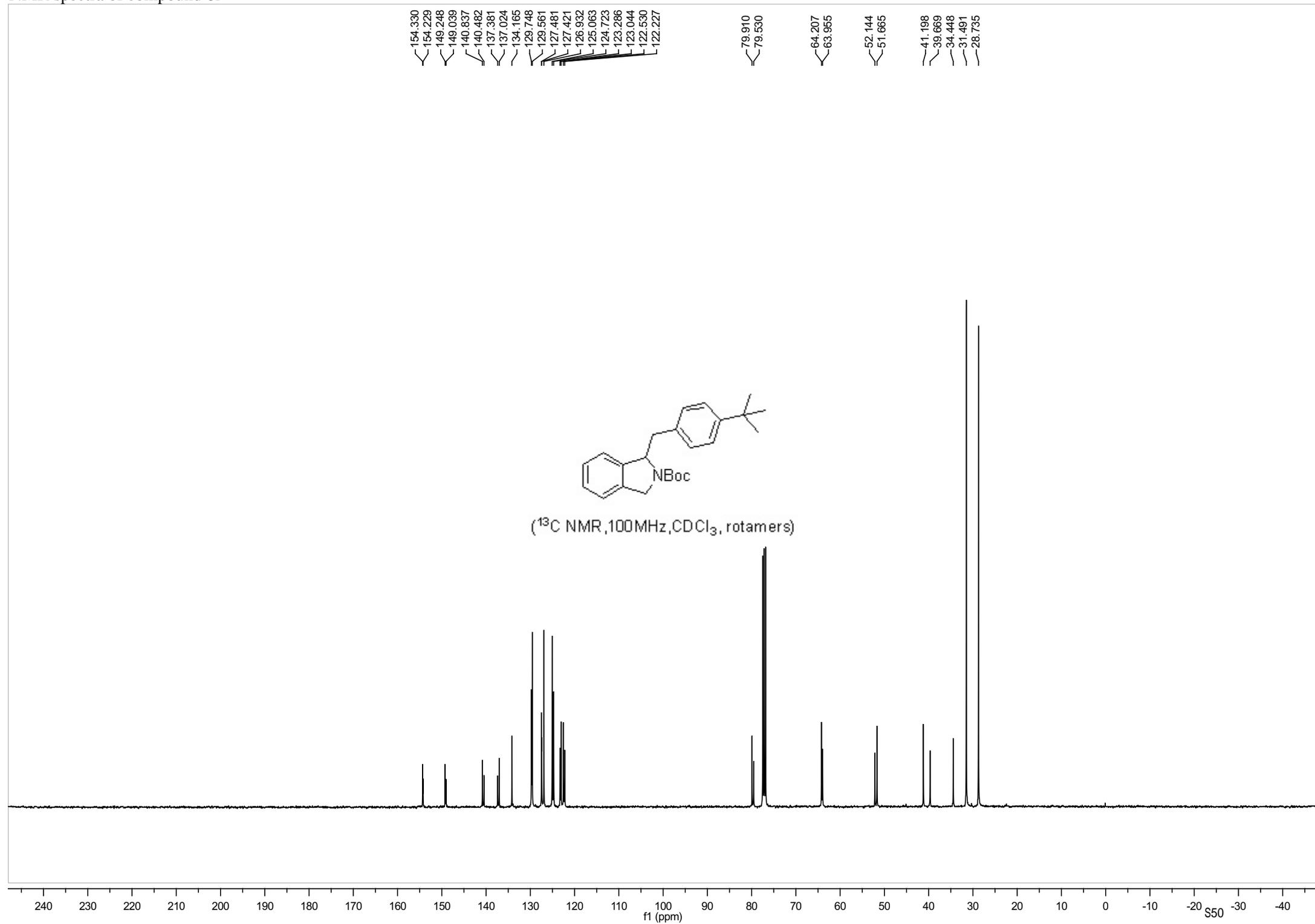
0.000



(¹H NMR, 400MHz, CDCl₃, rotamers)



NMR spectra of compound 81



NMR spectra of compound 8m

7.431
7.401
7.379
7.242
7.231
7.105
7.062
7.047
6.985
6.965
6.947

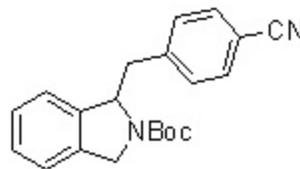
5.361
5.302

4.626
4.588
4.503
4.467

3.999
3.962
3.885
3.849
3.551
3.539
3.522
3.507
3.316
3.307
3.288
3.274
3.197
3.166

1.592
1.541

-0.000



(¹H NMR, 400MHz, CDCl₃, rotamers)

2.04
2.05
2.05
2.02

1.07

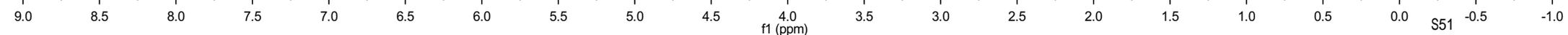
0.46
0.62

0.45
0.61

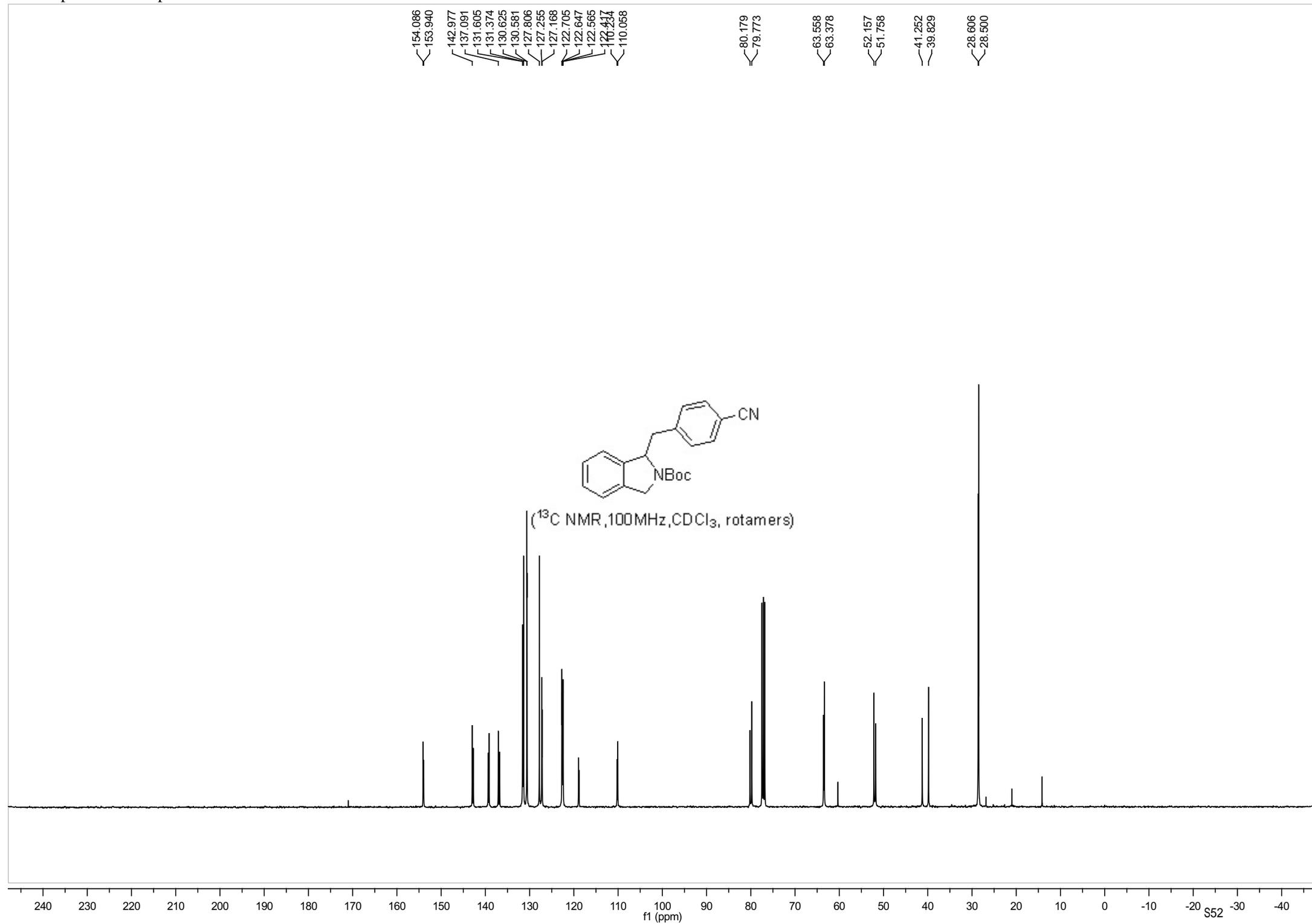
0.62

0.45
1.06

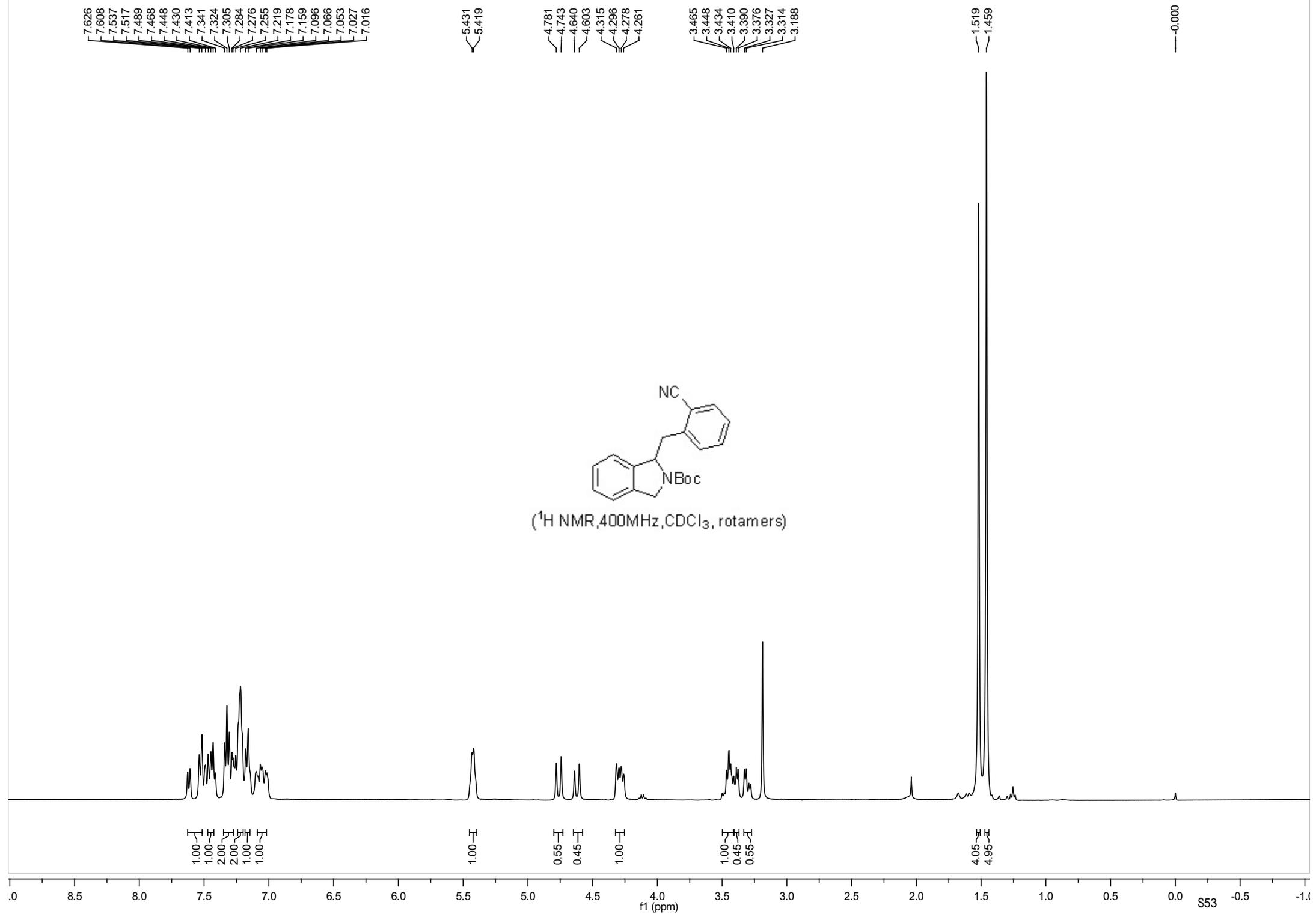
3.82
5.26



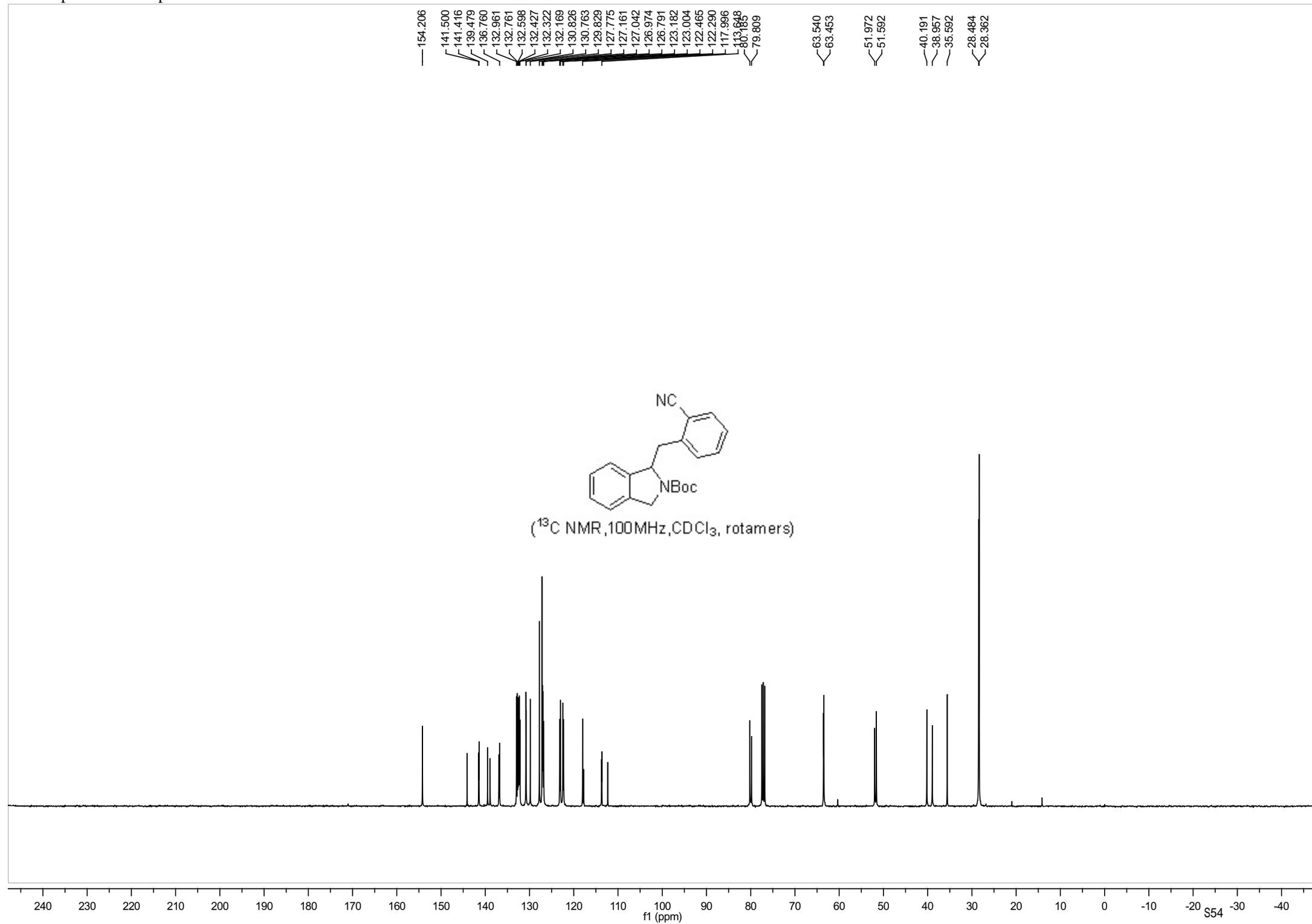
NMR spectra of compound 8m



NMR spectra of compound 8n



NMR spectra of compound 8n



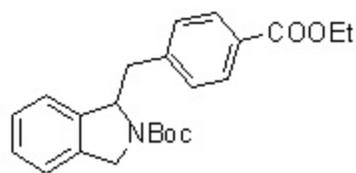
NMR spectra of compound 8o

7.853
7.833
7.802
7.782
7.235
7.222
7.209
7.194
7.121
7.105
7.060
7.043
7.027
6.983
6.963
6.948
6.928
6.915
6.897

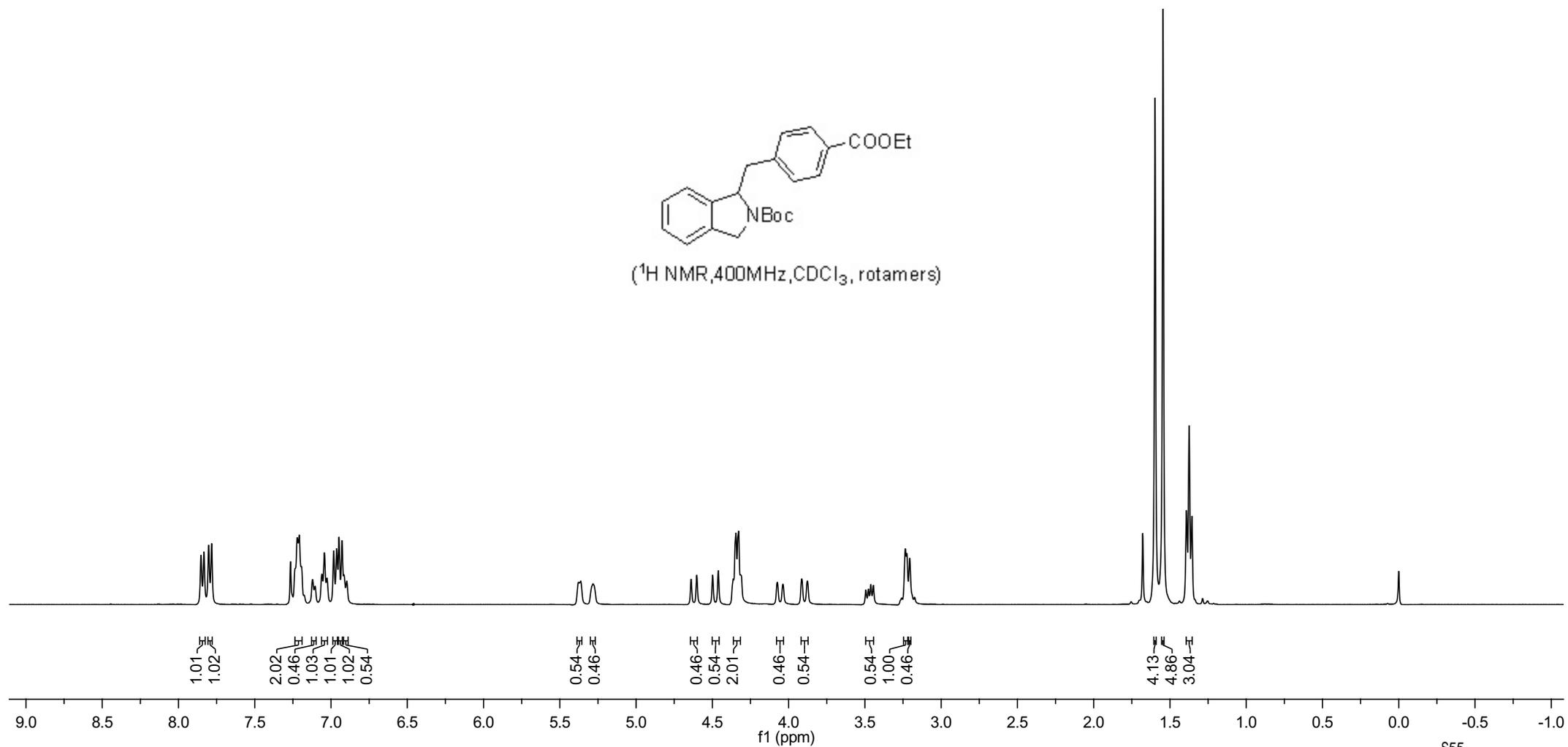
5.378
5.363
5.283

4.639
4.602
4.498
4.461
4.362
4.345
4.328
4.316
4.074
4.037
3.914
3.877
3.494
3.477
3.462
3.445
3.259
3.235
3.225
3.206
3.174

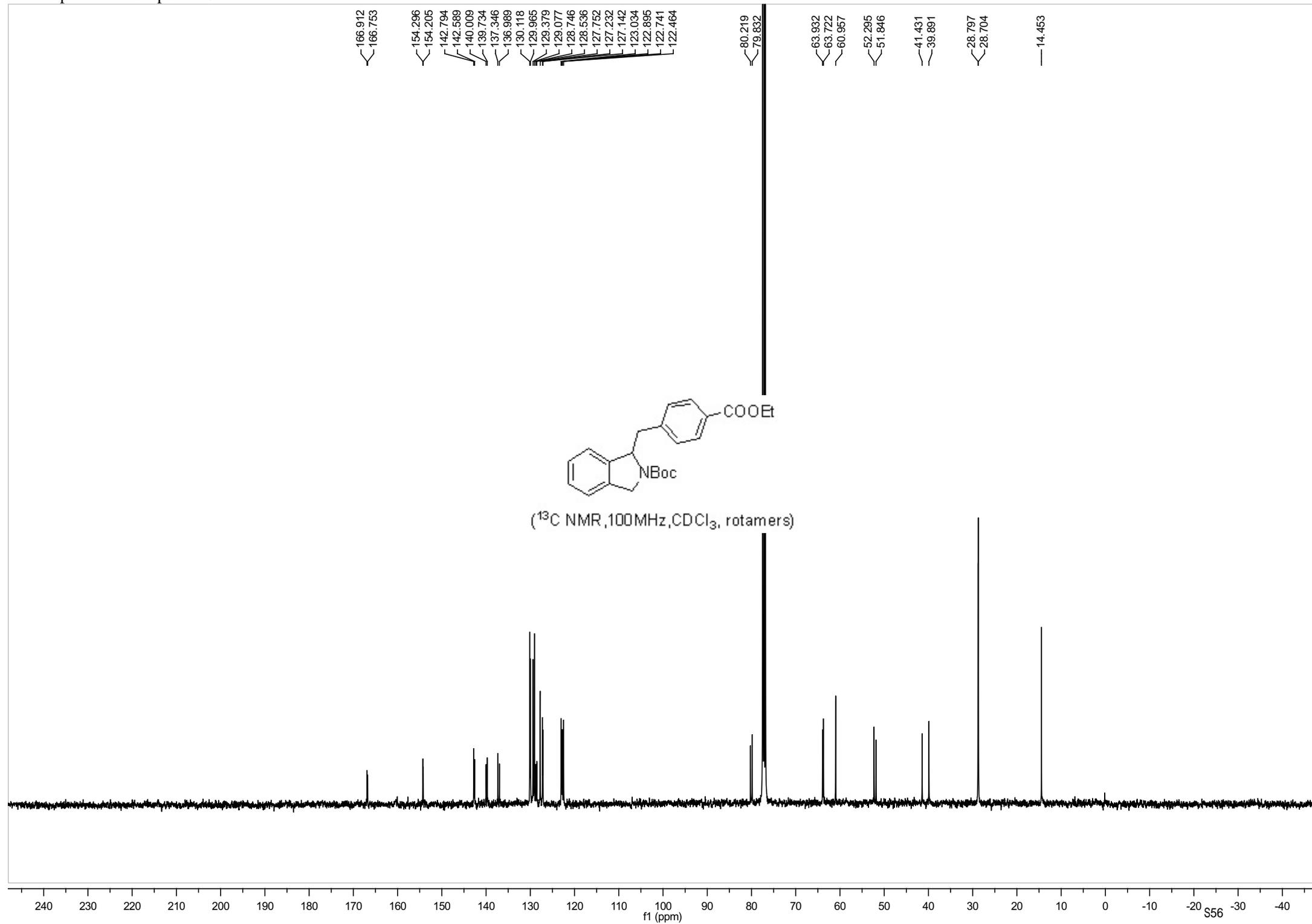
1.598
1.545
1.392
1.374
1.357



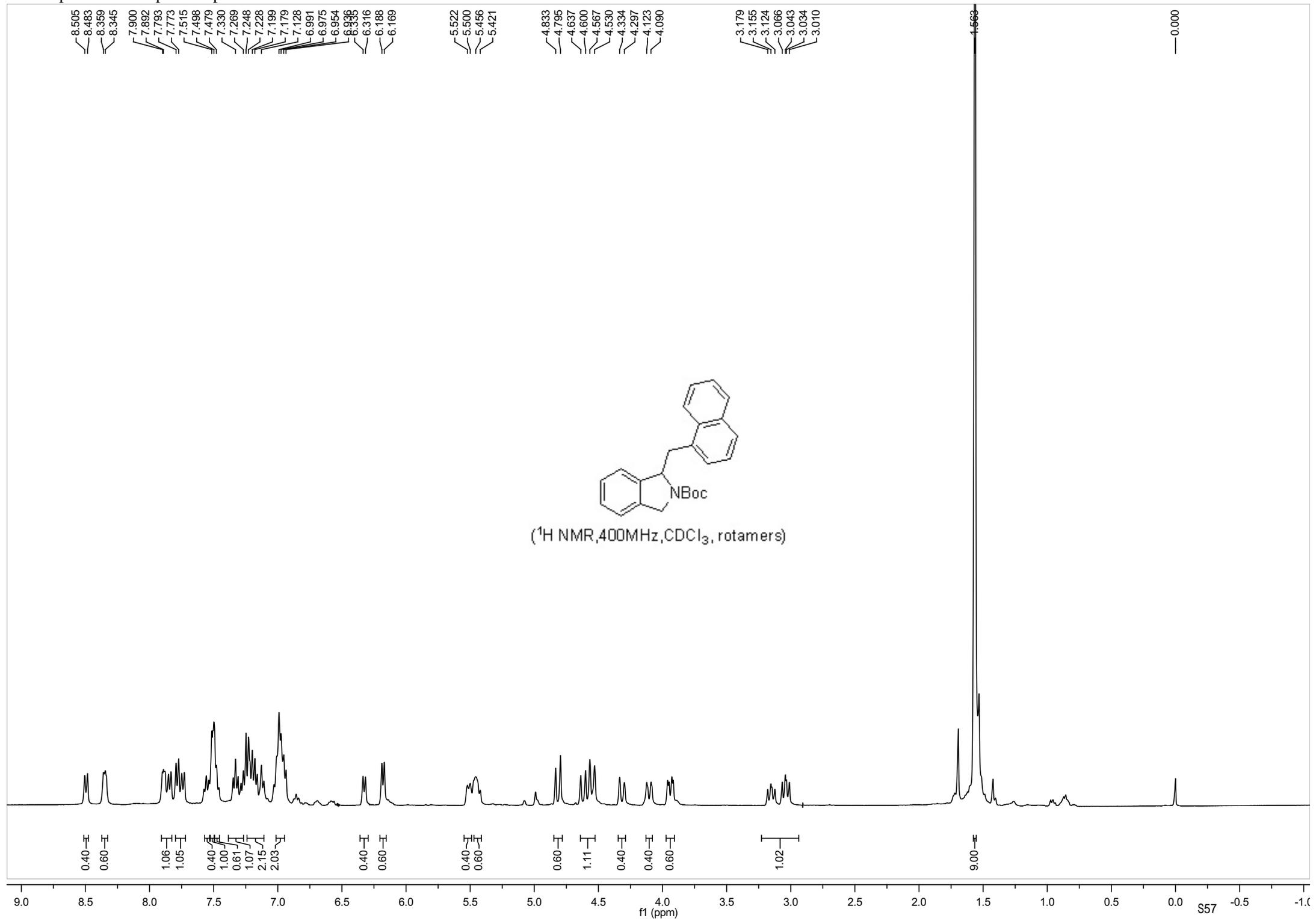
(¹H NMR, 400MHz, CDCl₃, rotamers)



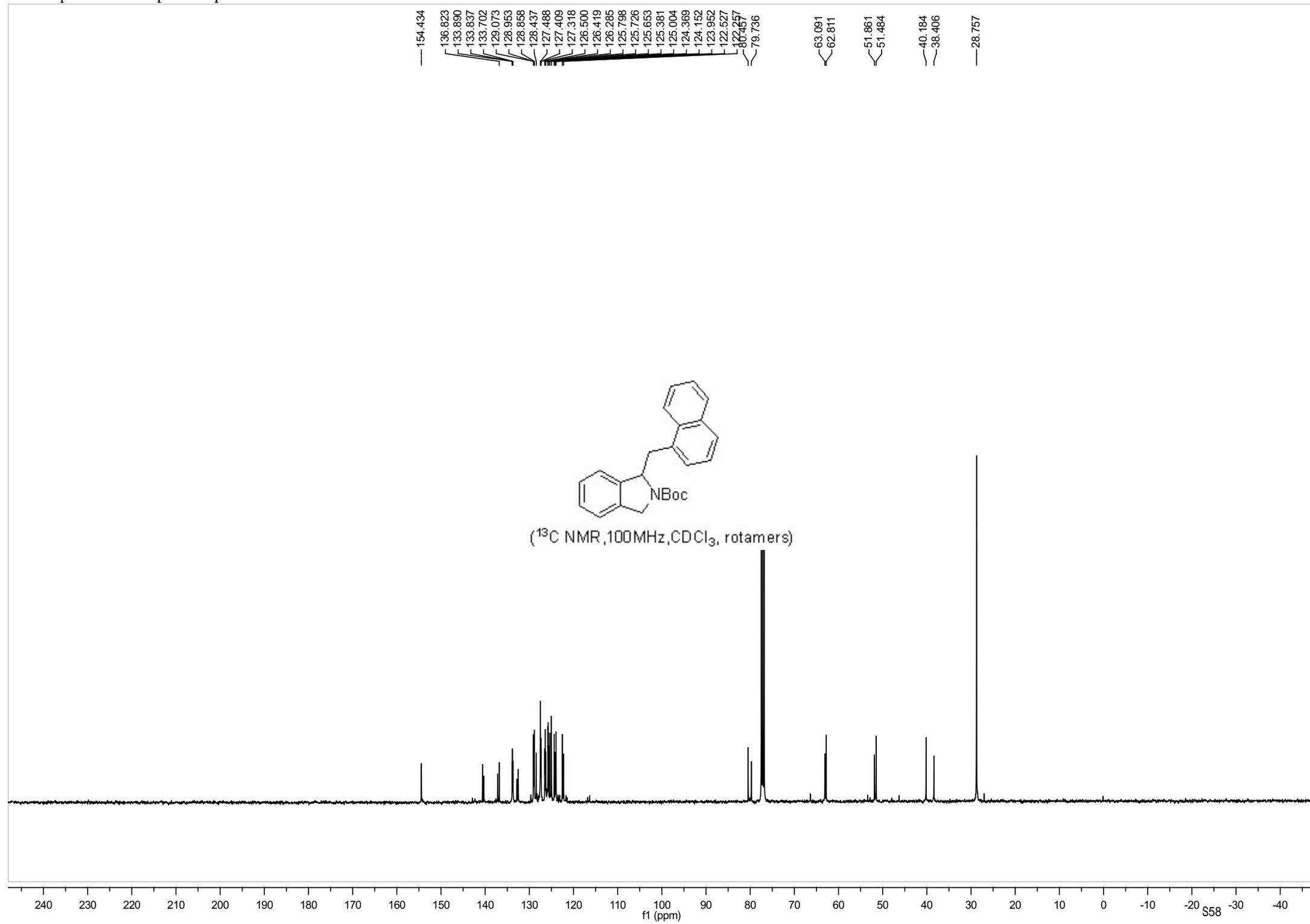
NMR spectra of compound 8o



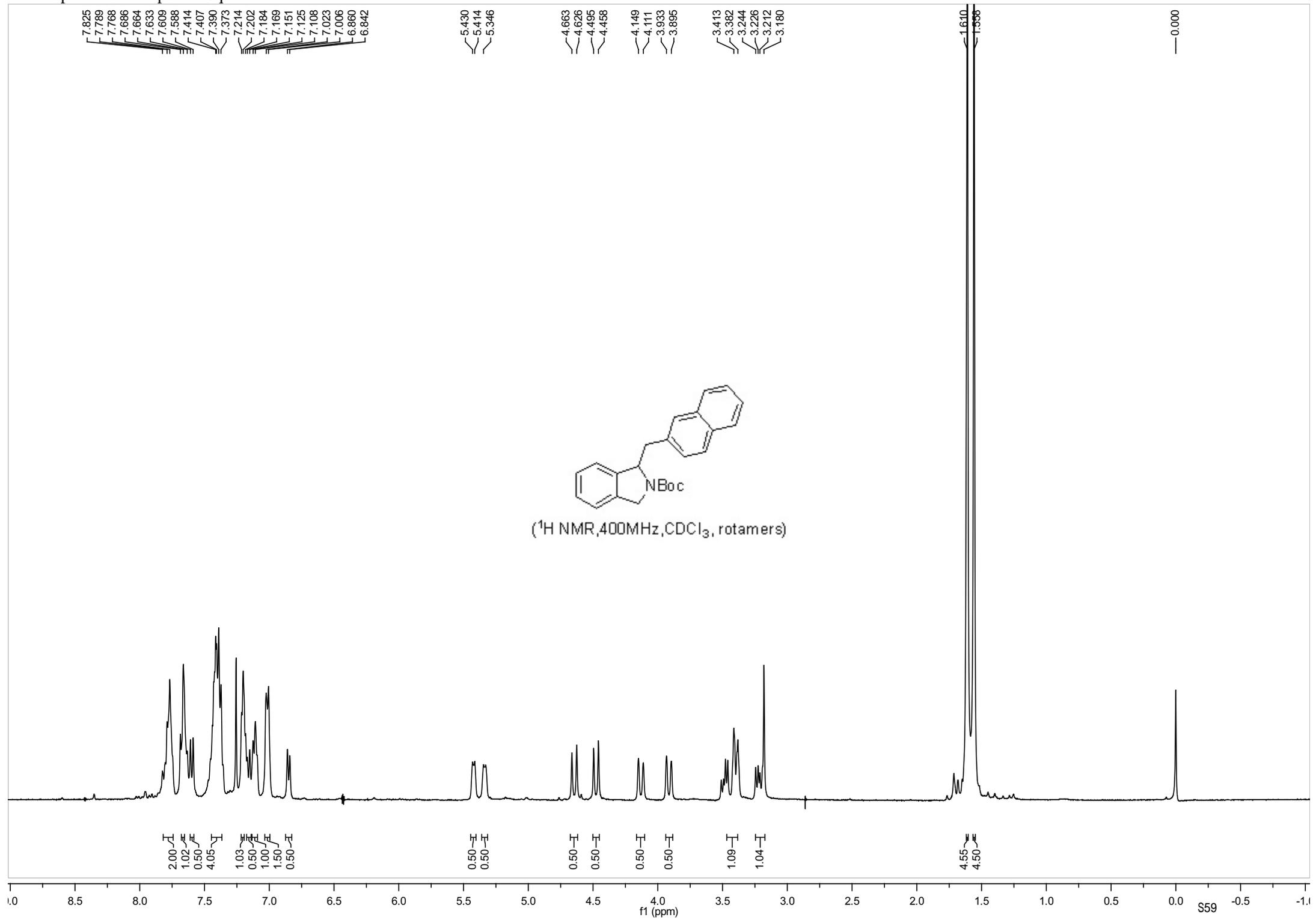
NMR spectra of compound 8p



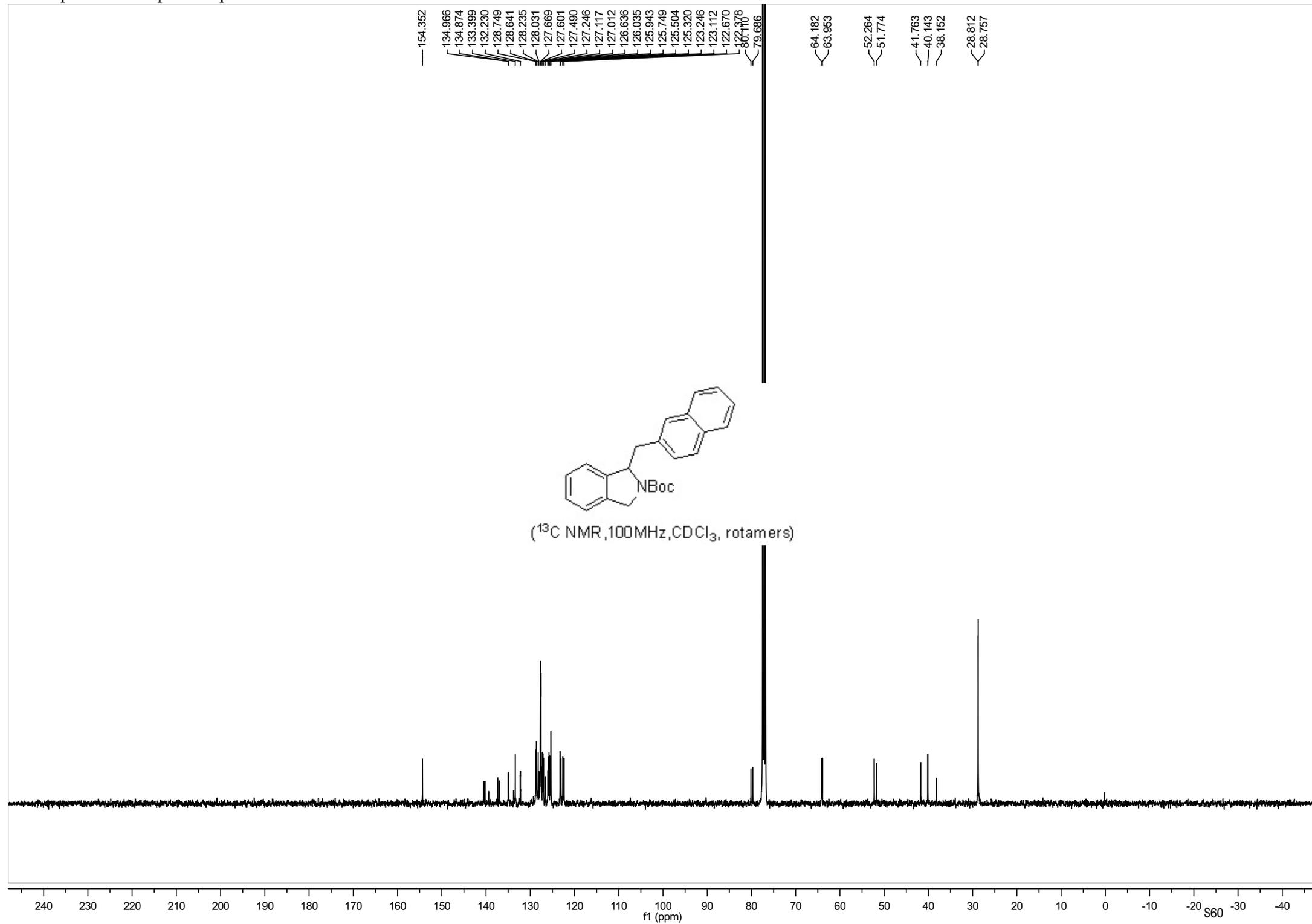
NMR spectra of compound 8p



NMR spectra of compound 8q



NMR spectra of compound 8q



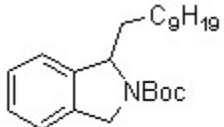
NMR spectra of compound 8r

7.261
7.218
7.179

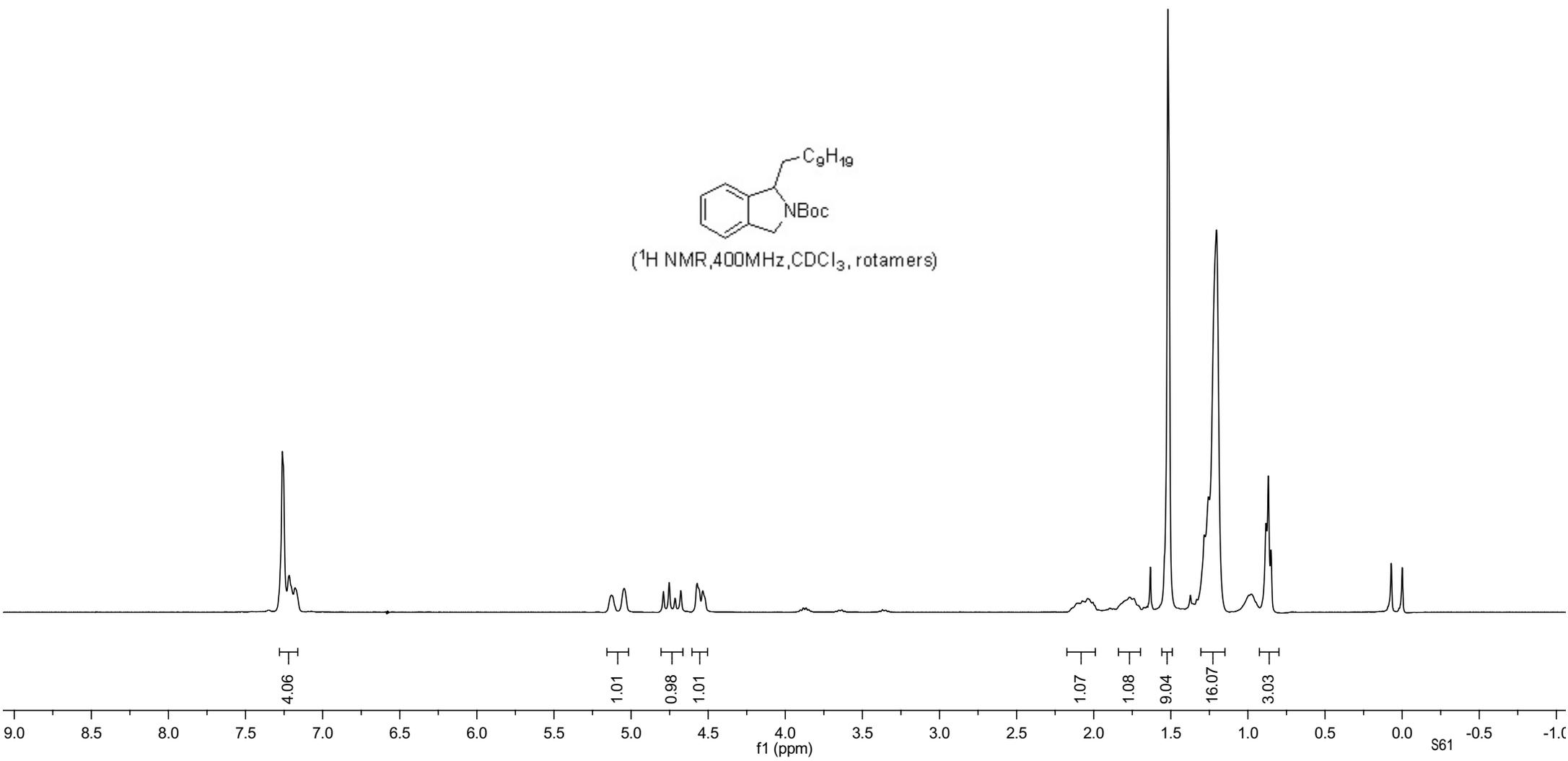
5.127
5.046
4.790
4.753
4.714
4.677
4.572
4.534

2.073
2.040
2.007
2.002
1.789
1.764
1.740
1.710
1.519
1.283
1.256
1.204
0.883
0.868
0.850

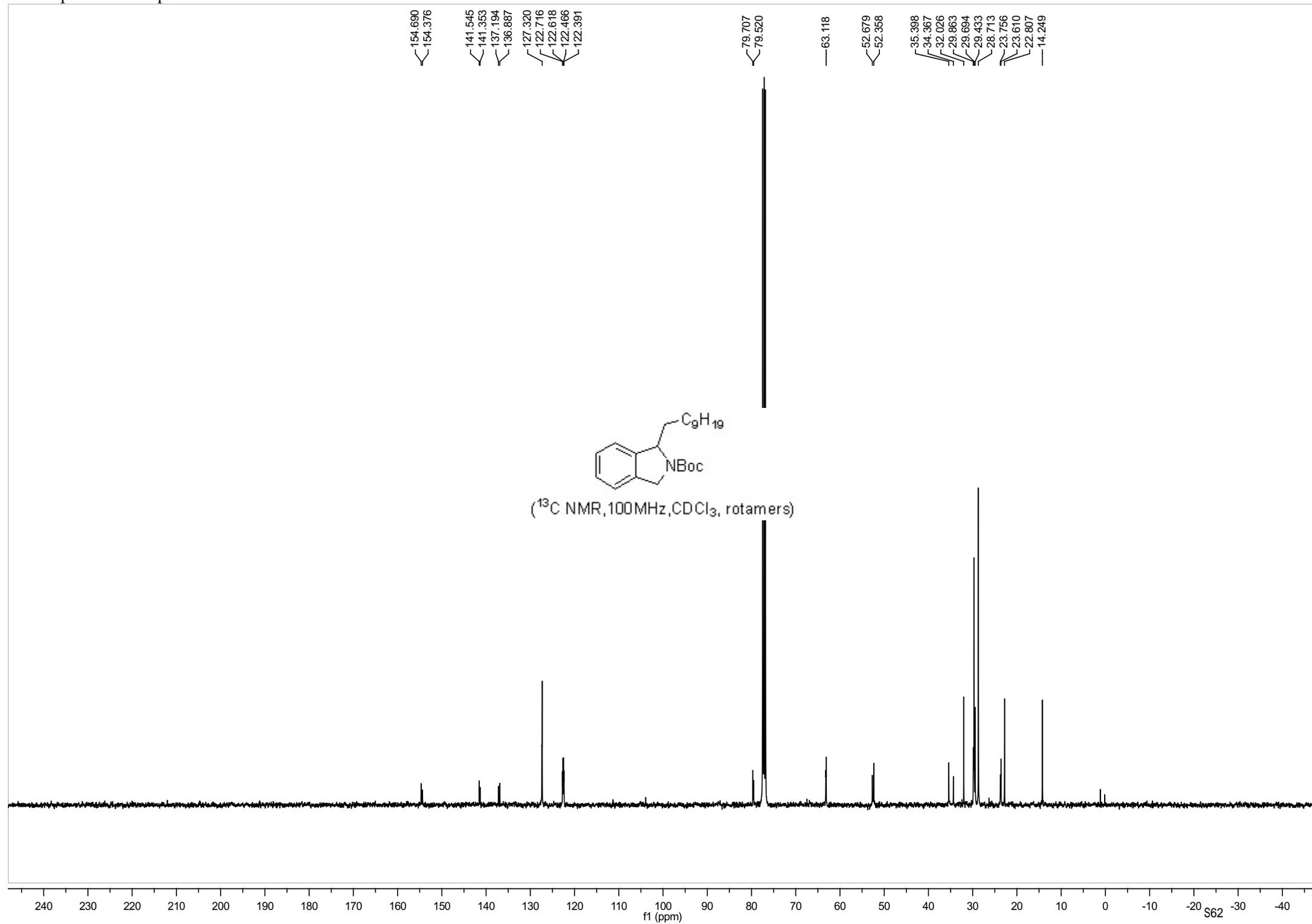
0.000



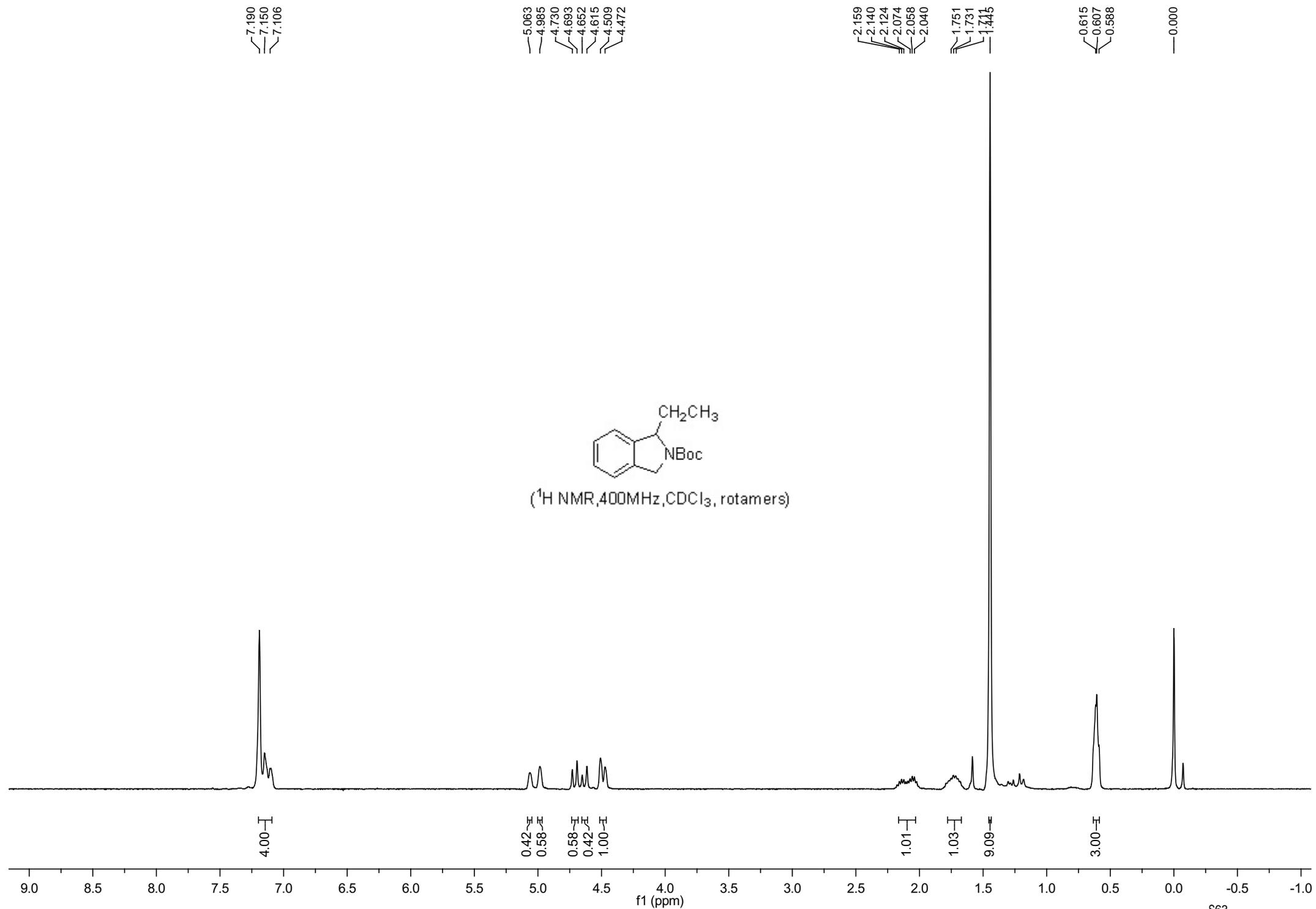
(¹H NMR, 400MHz, CDCl₃, rotamers)



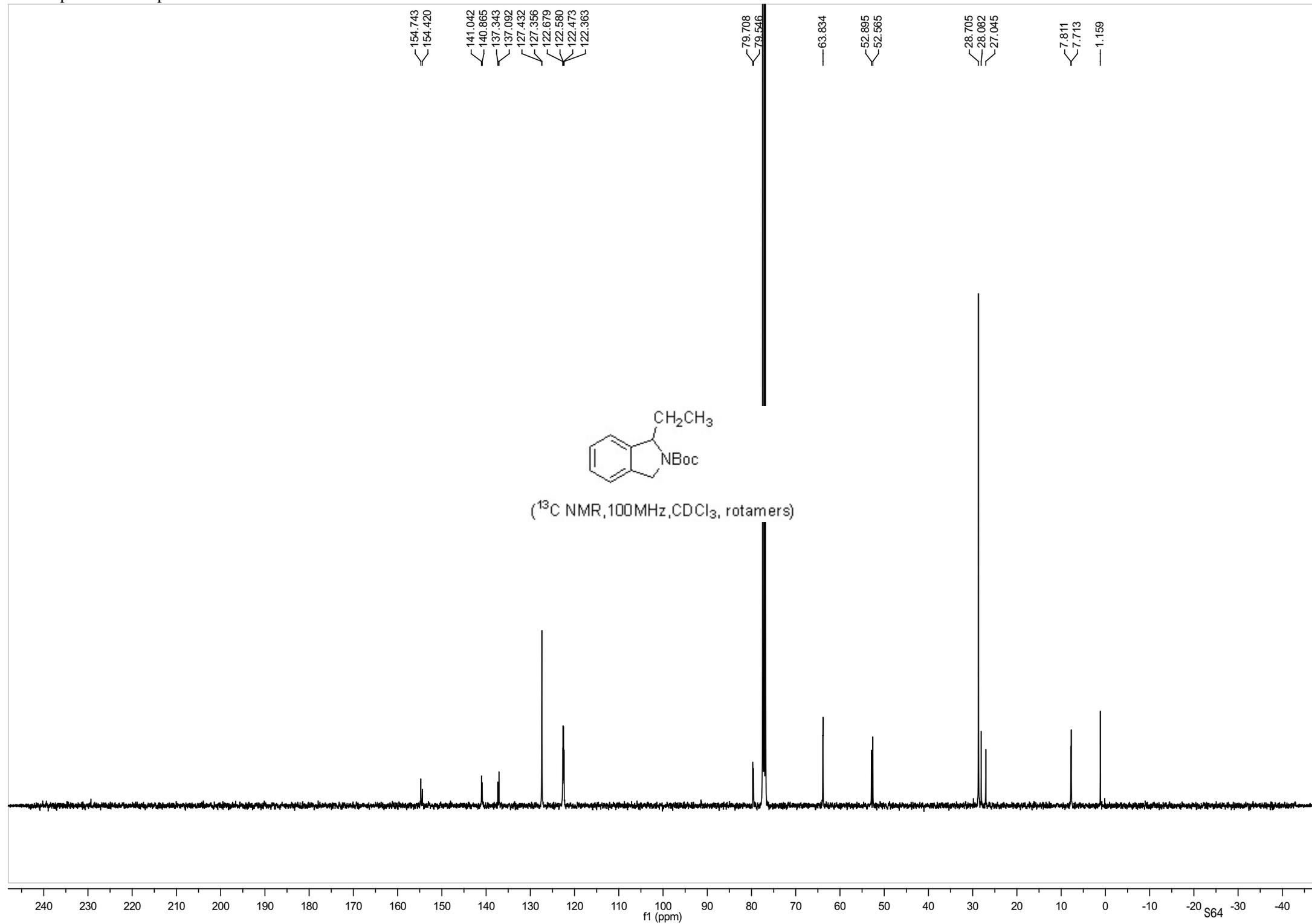
NMR spectra of compound 8r



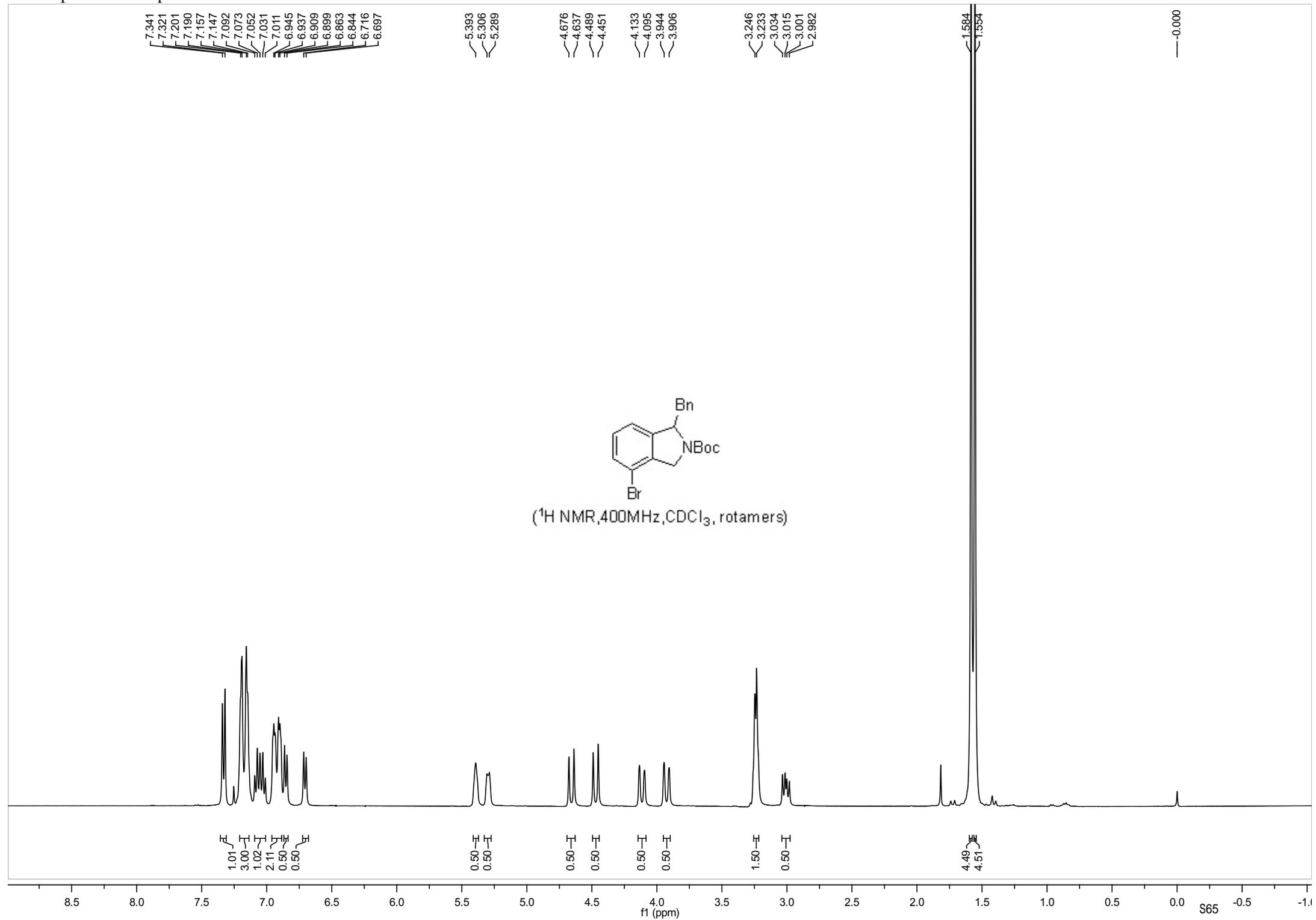
NMR spectra of compound 8s



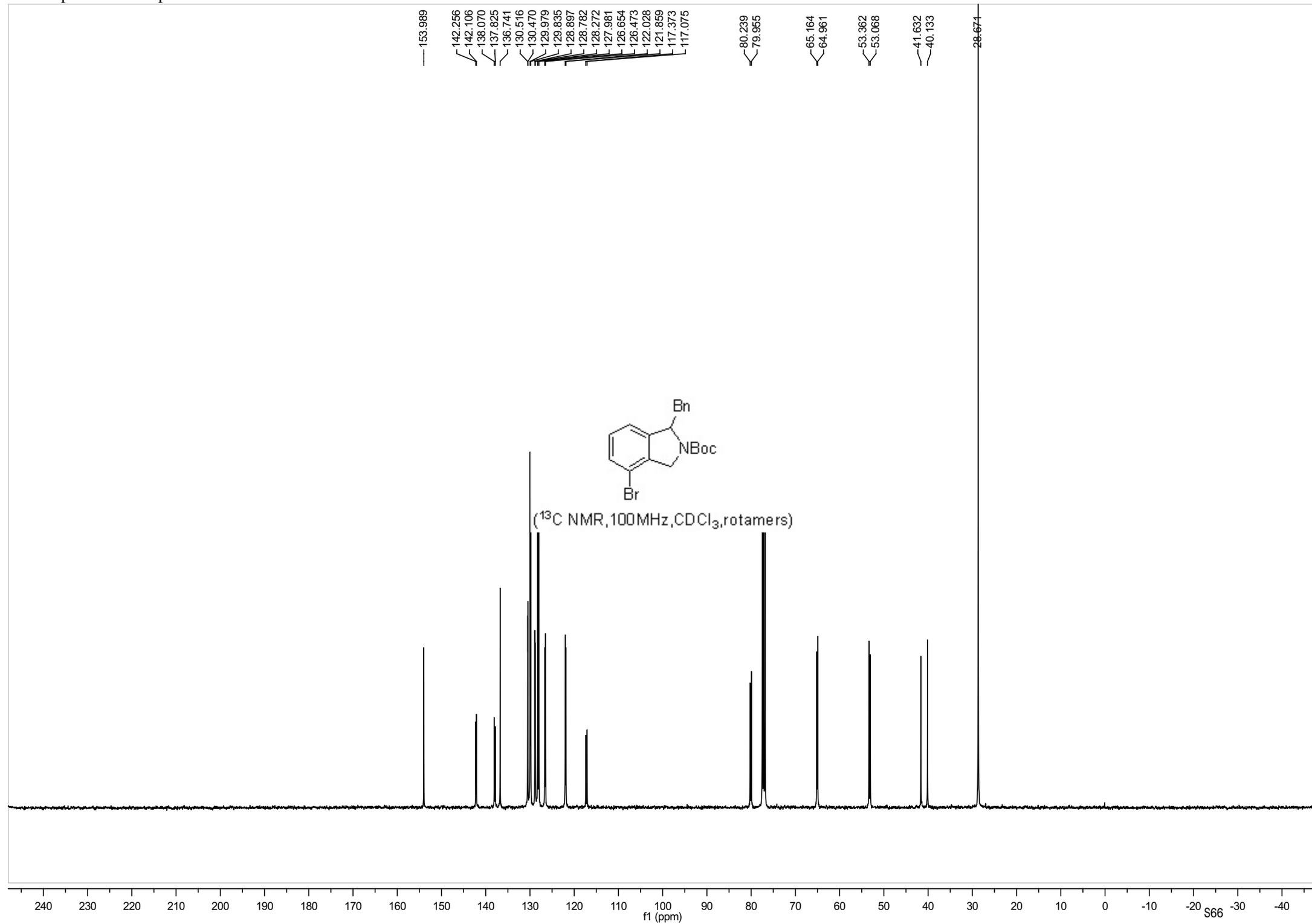
NMR spectra of compound 8s



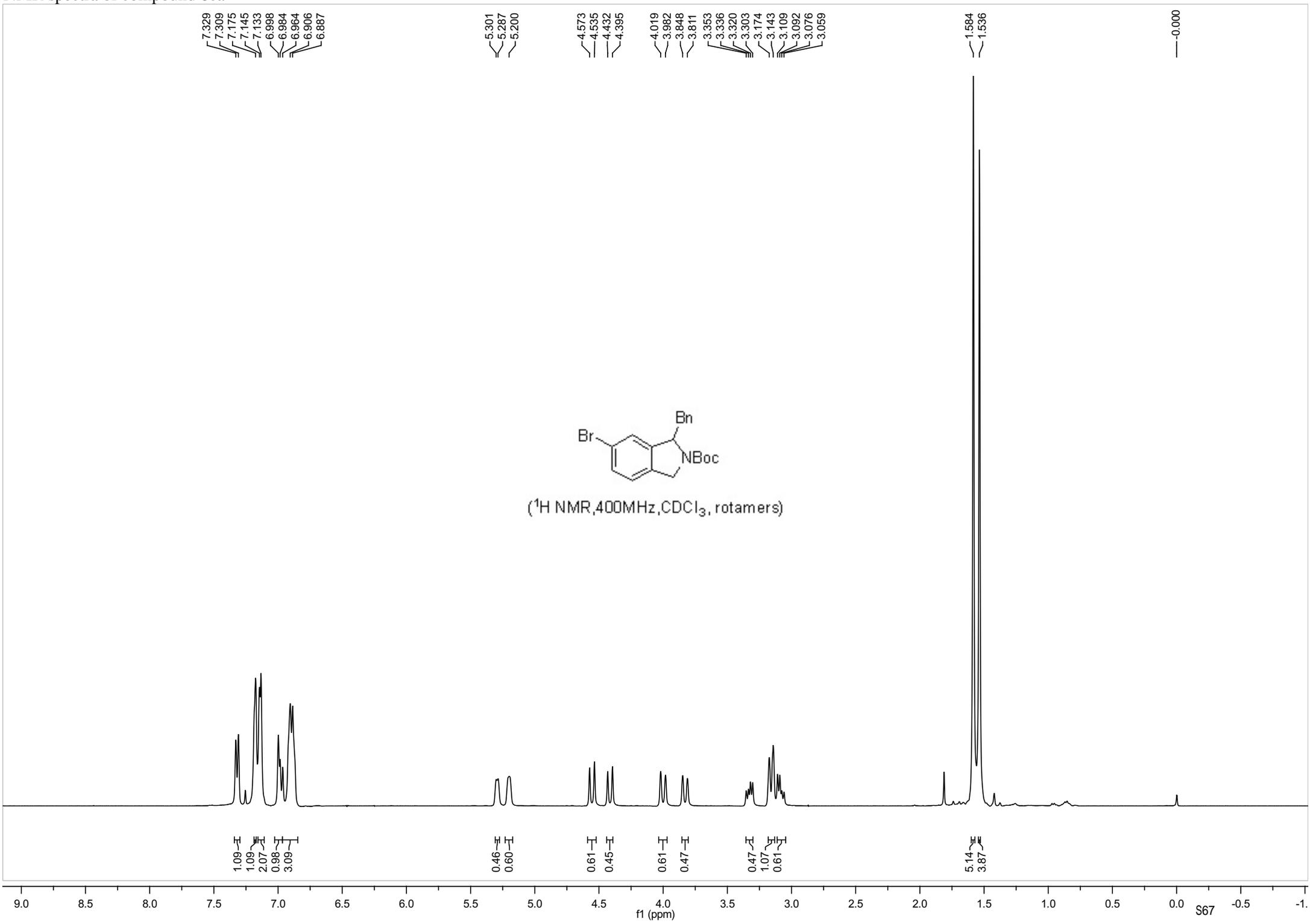
NMR spectra of compound 8ba



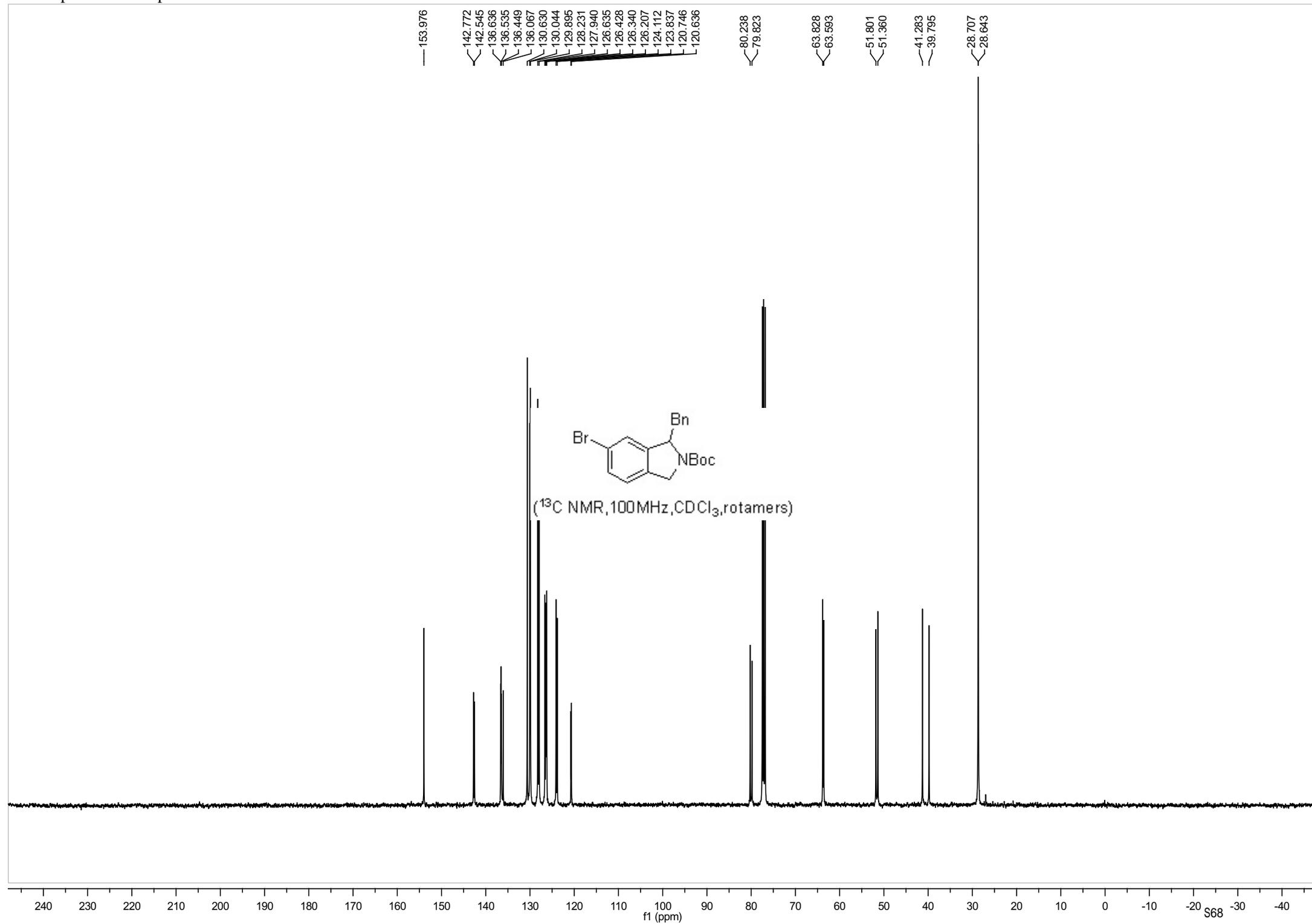
NMR spectra of compound 8ba



NMR spectra of compound 8ca



NMR spectra of compound 8ca



NMR spectra of compound 8da

7.176
7.143
7.096
7.011
6.920
6.911
6.896
6.880
6.859
6.745
6.725

5.286
5.279
5.271
5.202
5.185

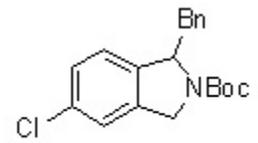
4.617
4.580
4.473
4.436

4.104
4.067
3.931
3.894

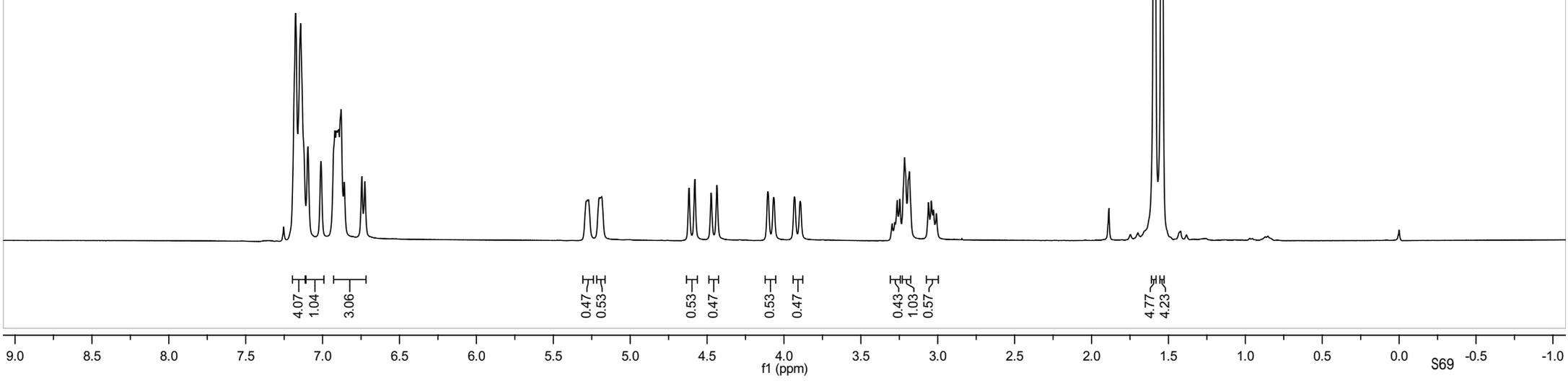
3.297
3.279
3.264
3.247
3.216
3.185
3.060
3.041
3.027
3.009

1.581
1.542

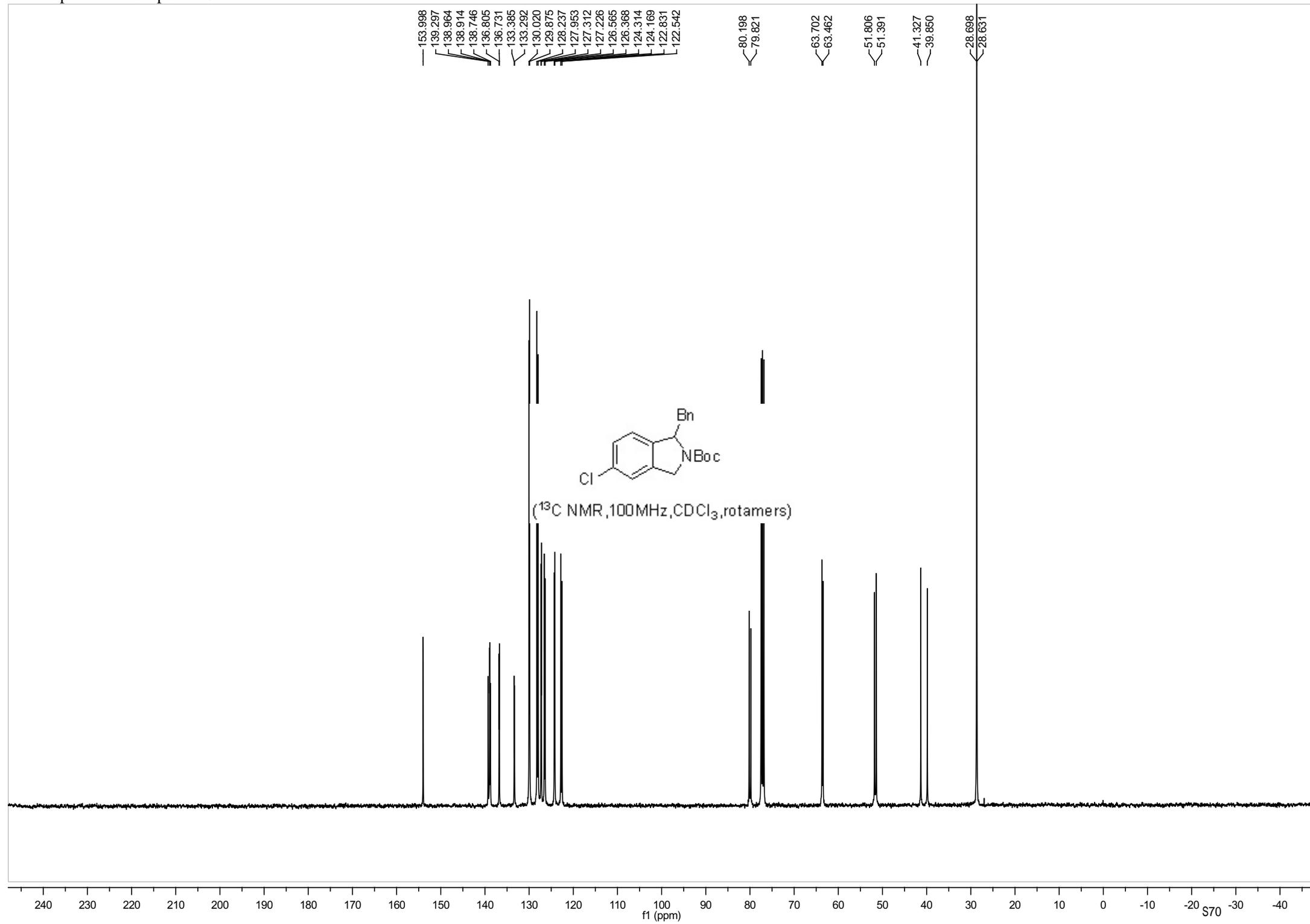
0.000



(¹H NMR, 400MHz, CDCl₃, rotamers)



NMR spectra of compound 8da



NMR spectra of compound 8ea

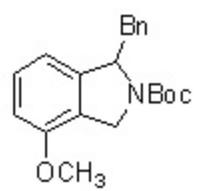
7.175
7.142
7.141
6.966
6.954
6.935
6.926
6.698
6.678
6.579
6.560
6.440
6.420

5.318
5.216

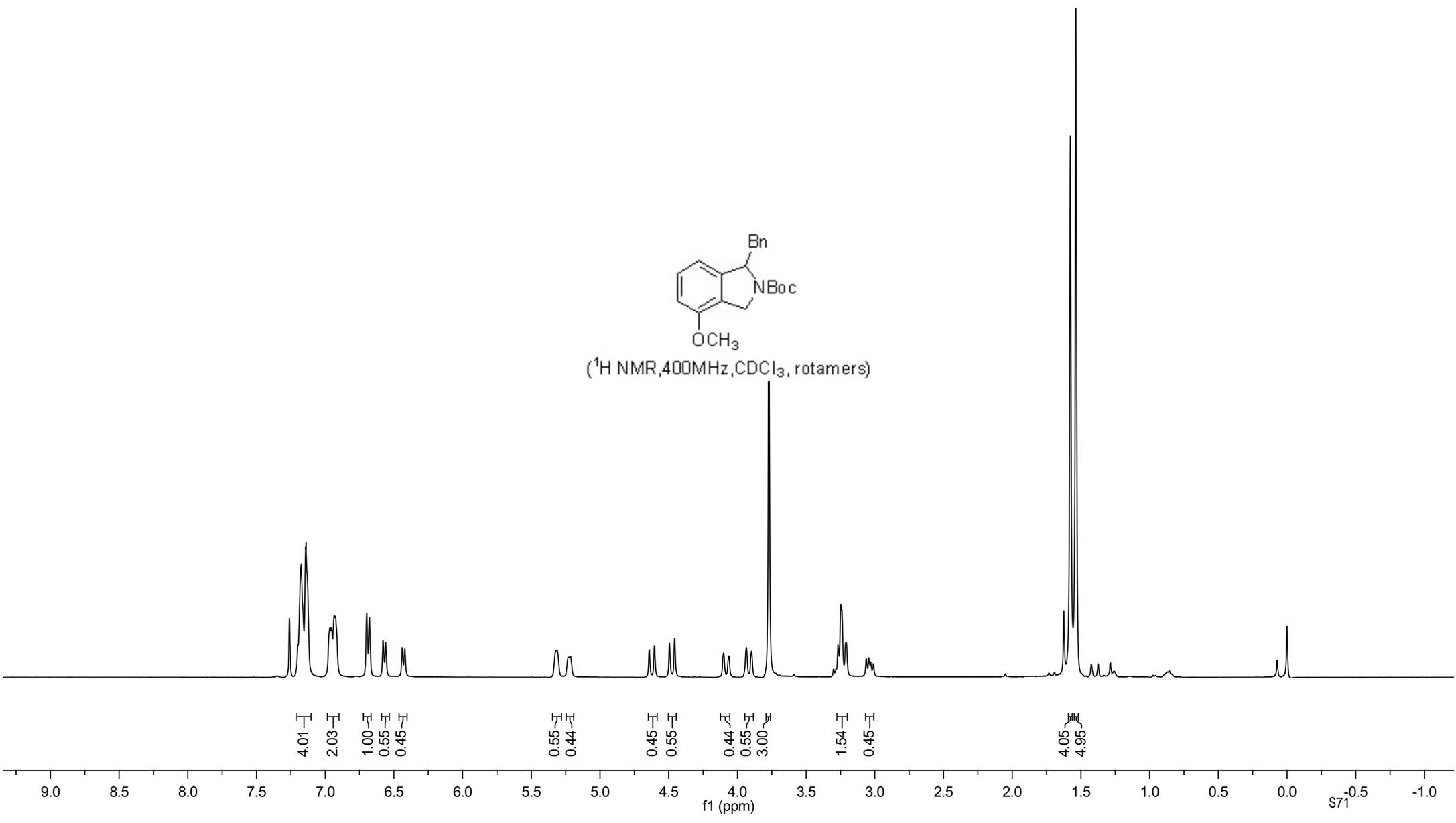
4.641
4.604
4.494
4.457
4.100
4.063
3.935
3.898
3.771
3.300
3.267
3.247
3.212
3.062
3.043
3.030
3.011

1.577
1.536

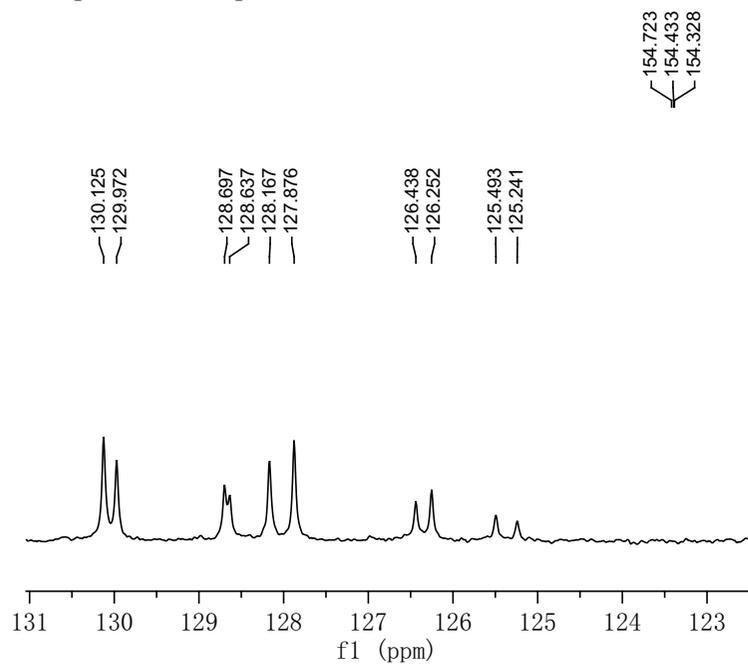
0.000



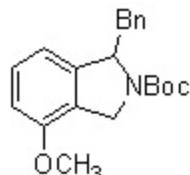
(¹H NMR, 400MHz, CDCl₃, rotamers)



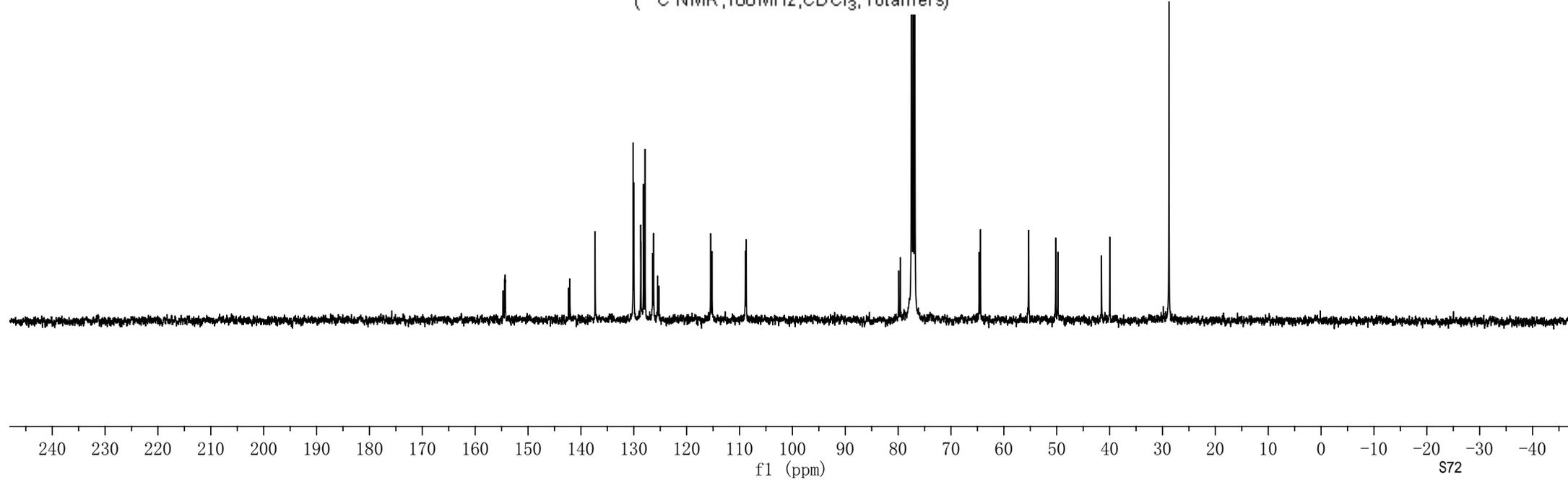
NMR spectra of compound 8ea



154.723
154.433
154.328
142.334
142.087
137.310
130.125
129.972
128.697
128.167
127.876
115.211
108.892
108.723
79.912
79.589
64.666
64.412
55.351
55.291
50.199
49.789
41.535
39.978
28.793
28.748



(¹³C NMR, 100MHz, CDCl₃, rotamers)



NMR spectra of compound 8fa

7.180
7.146
7.031
7.010
6.979
6.954
6.934
6.768
6.748
— 6.430
— 6.308

5.275
5.193
5.176

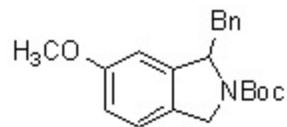
4.588
4.552
4.449
4.414

4.108
4.073
3.936
3.901
3.707
3.679

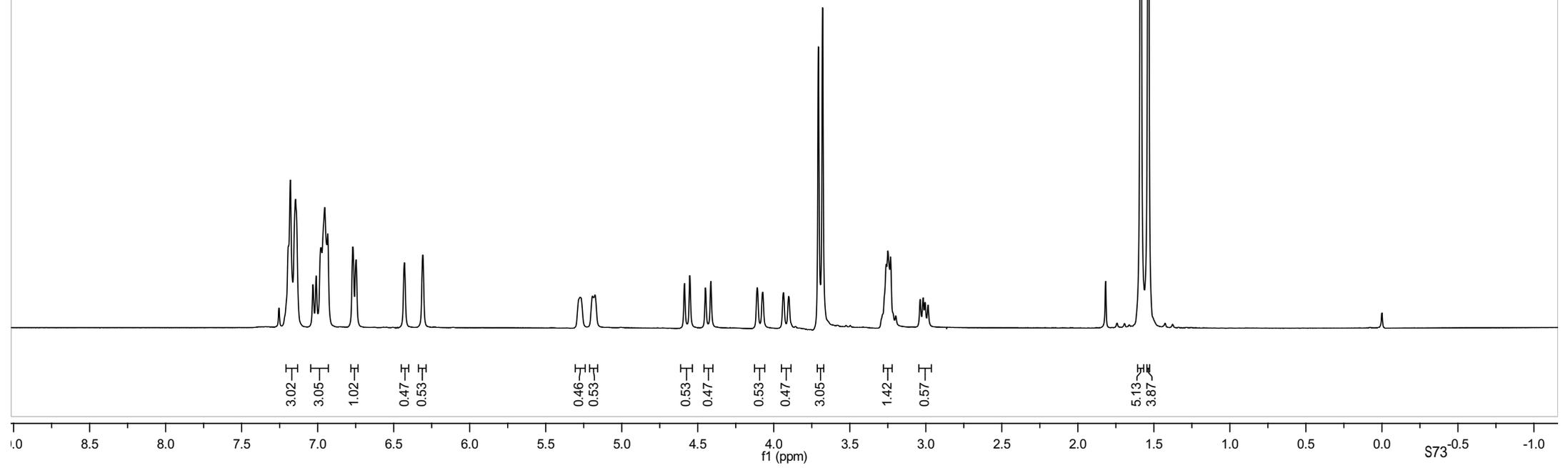
3.261
3.249
3.232
3.198
3.037
3.018
3.005
2.986

1.586
1.537

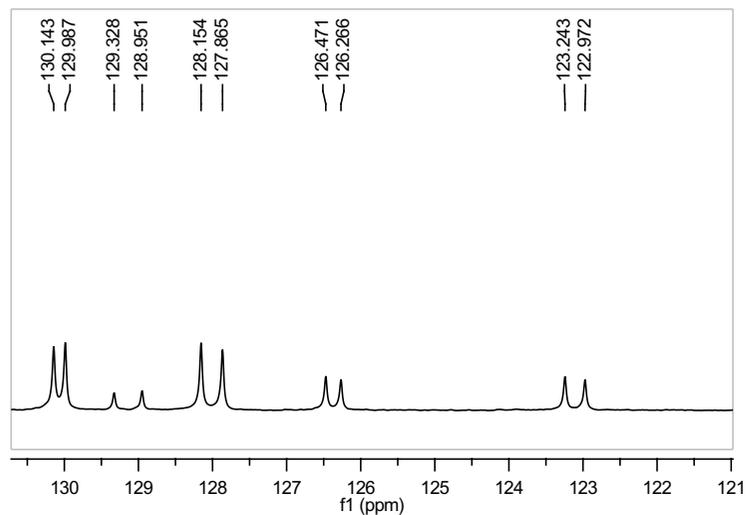
— 0.000



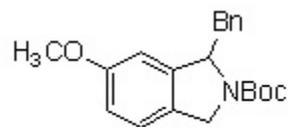
(¹H NMR, 400MHz, CDCl₃, rotamers)



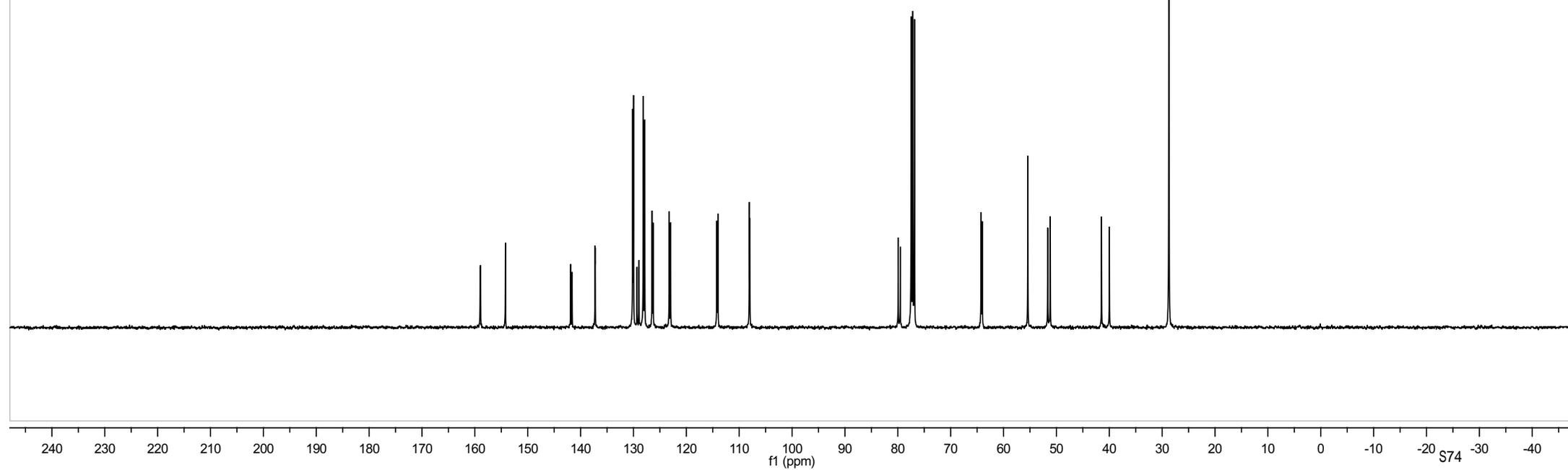
NMR spectra of compound 8fa



- 158.996
- 158.909
- 154.212
- 141.868
- 141.606
- 137.269
- 137.225
- 130.143
- 129.987
- 128.154
- 127.865
- 122.972
- 122.972
- 114.018
- 108.074
- 107.978
- 79.932
- 79.533
- 64.254
- 64.017
- 55.406
- 51.641
- 51.161
- 41.470
- 39.981
- 28.745
- 28.680



(¹³C NMR, 100MHz, CDCl₃, rotamers)



NMR spectra of compound 9a

7.280
7.263
7.244
7.221
7.203
7.182
7.167
7.160
7.151
7.131

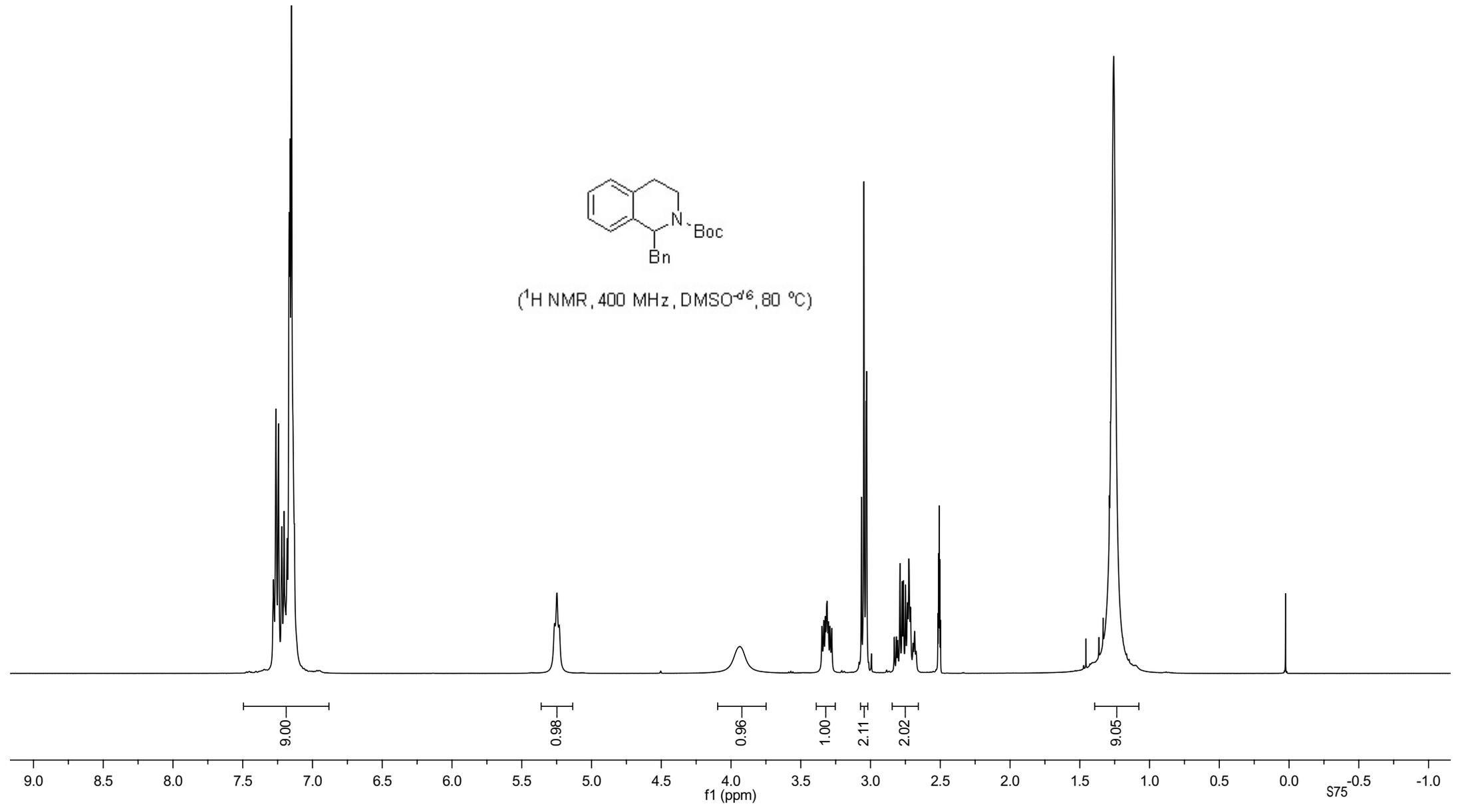
5.265
5.248
5.232

3.939

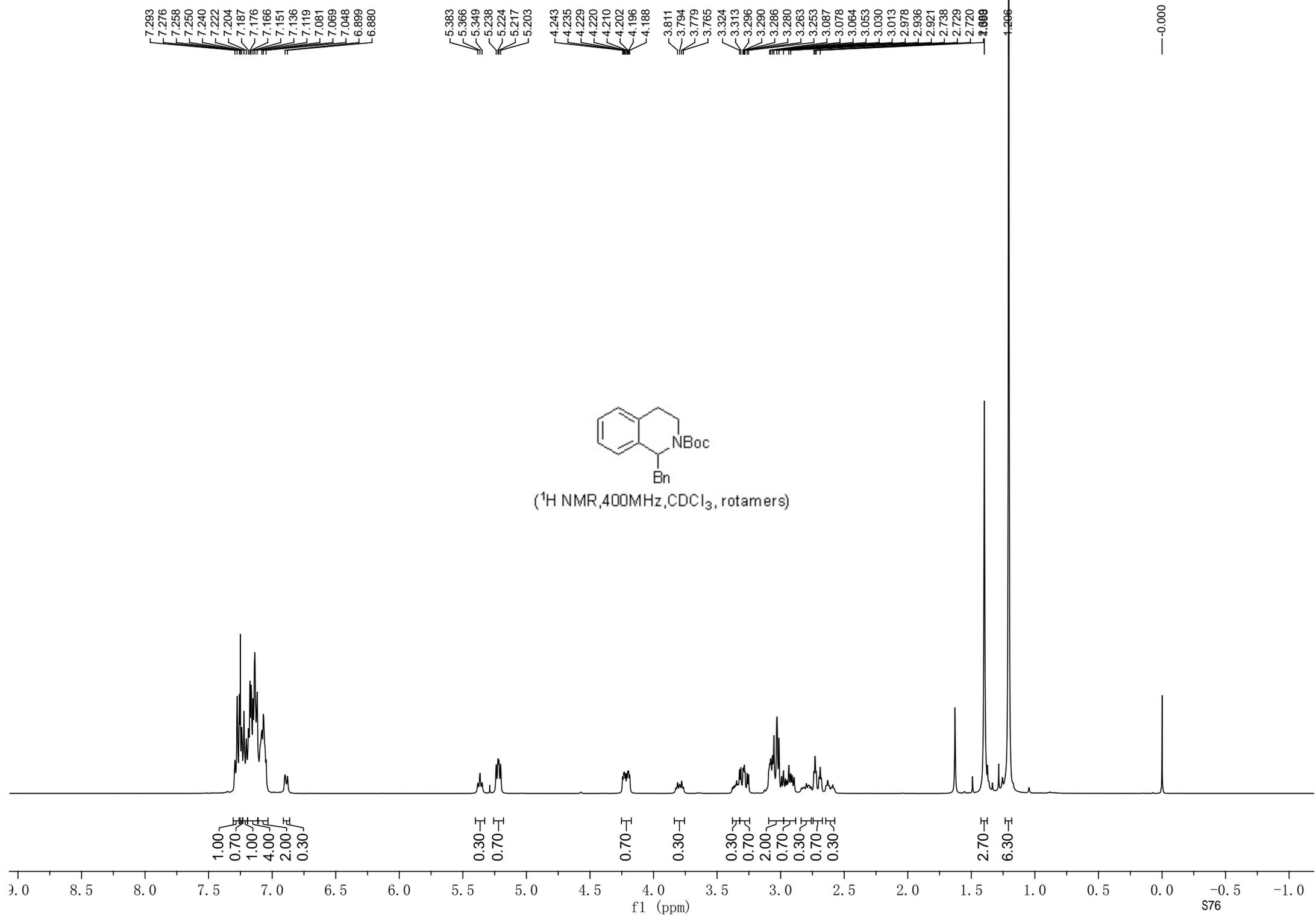
3.348
3.336
3.324
3.312
3.303
3.291
3.065
3.048
3.032
3.028
2.994
2.829
2.814
2.805
2.789
2.774
2.764
2.749
2.736
2.725
2.714
2.695
2.684
2.673
1.257



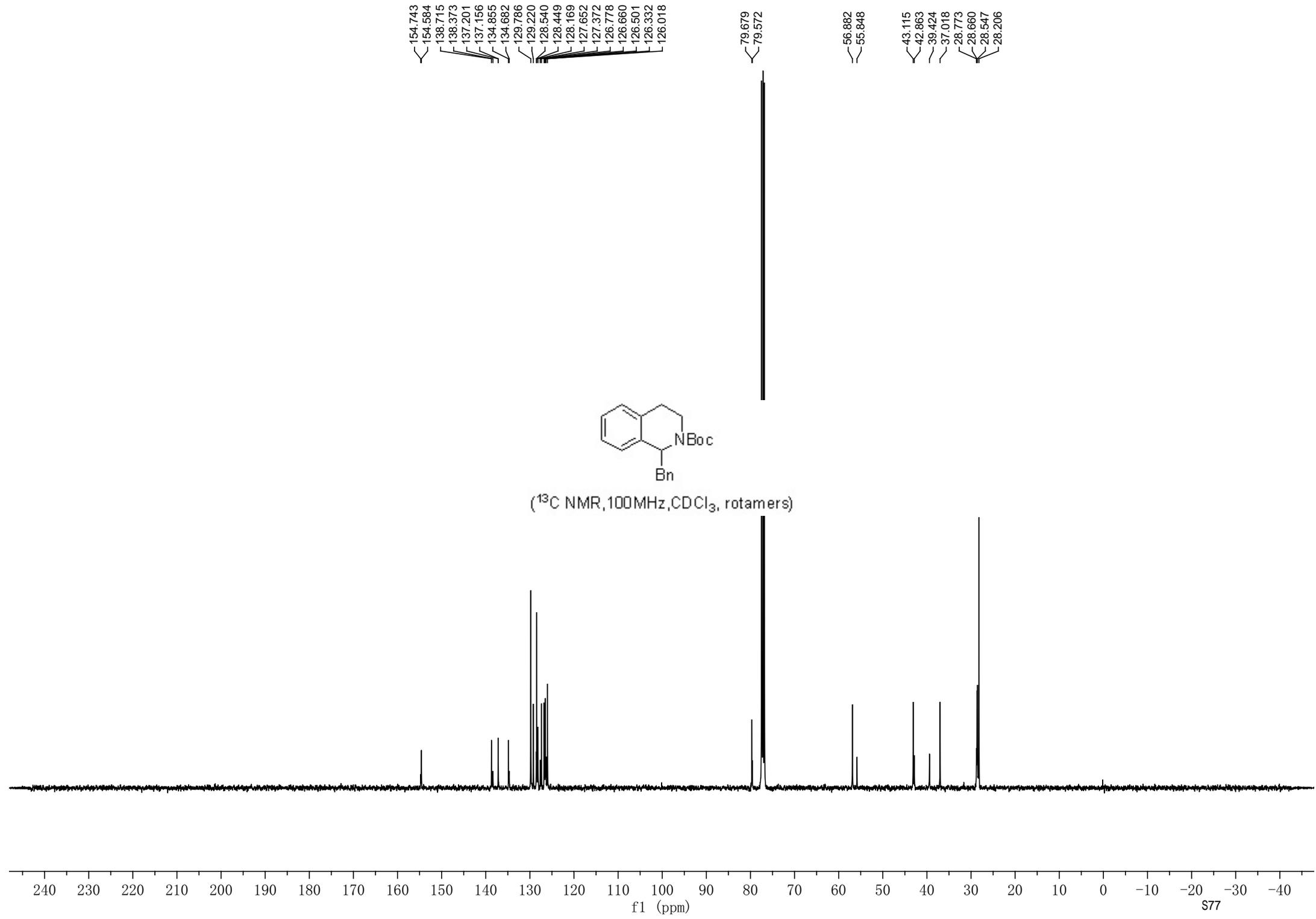
(¹H NMR, 400 MHz, DMSO-d₆, 80 °C)



NMR spectra of compound 9a



NMR spectra of compound 9a



NMR spectra of compound 9b

7.181
7.171
7.161
7.147
7.143
7.124
7.096
7.076
7.069
7.055
7.046
7.025
6.997
6.979
6.952
6.935
6.916
6.903
6.857
6.839

5.362
5.345
5.328
5.229
5.216
5.207
5.194

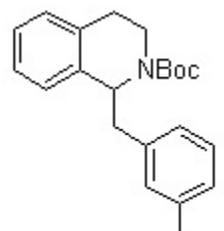
4.251
4.243
4.237
4.229
4.219
4.210
4.204
4.196

3.331
3.304
3.298
3.293
3.042
3.020
3.008
2.985
2.979
2.966
2.940
2.931
2.736
2.696
2.316
2.278

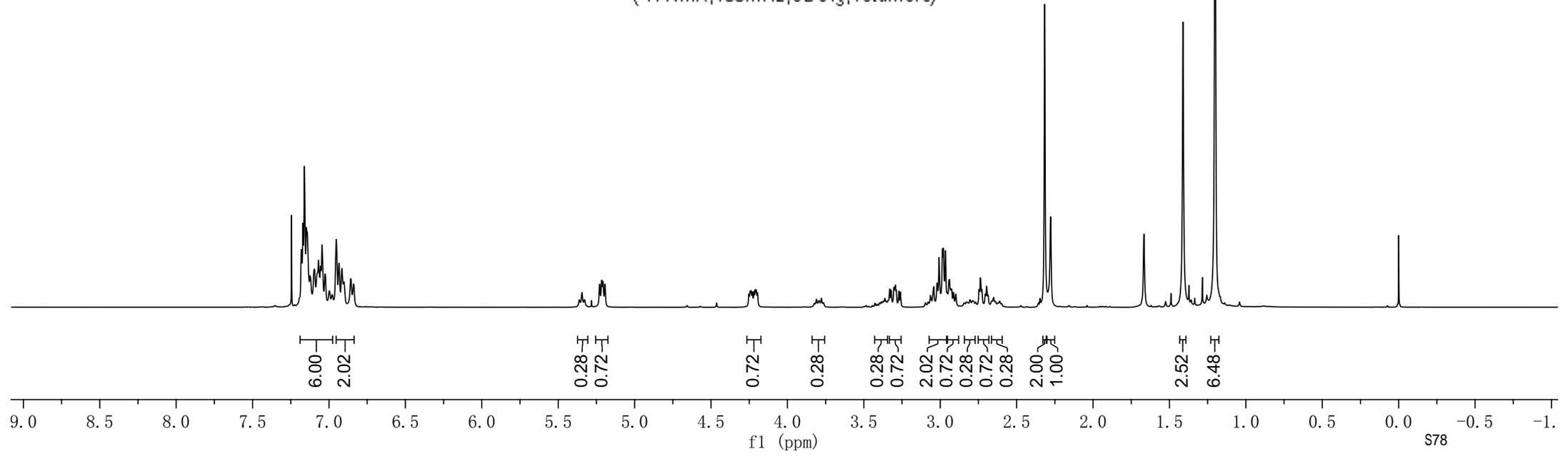
1.411

1.202

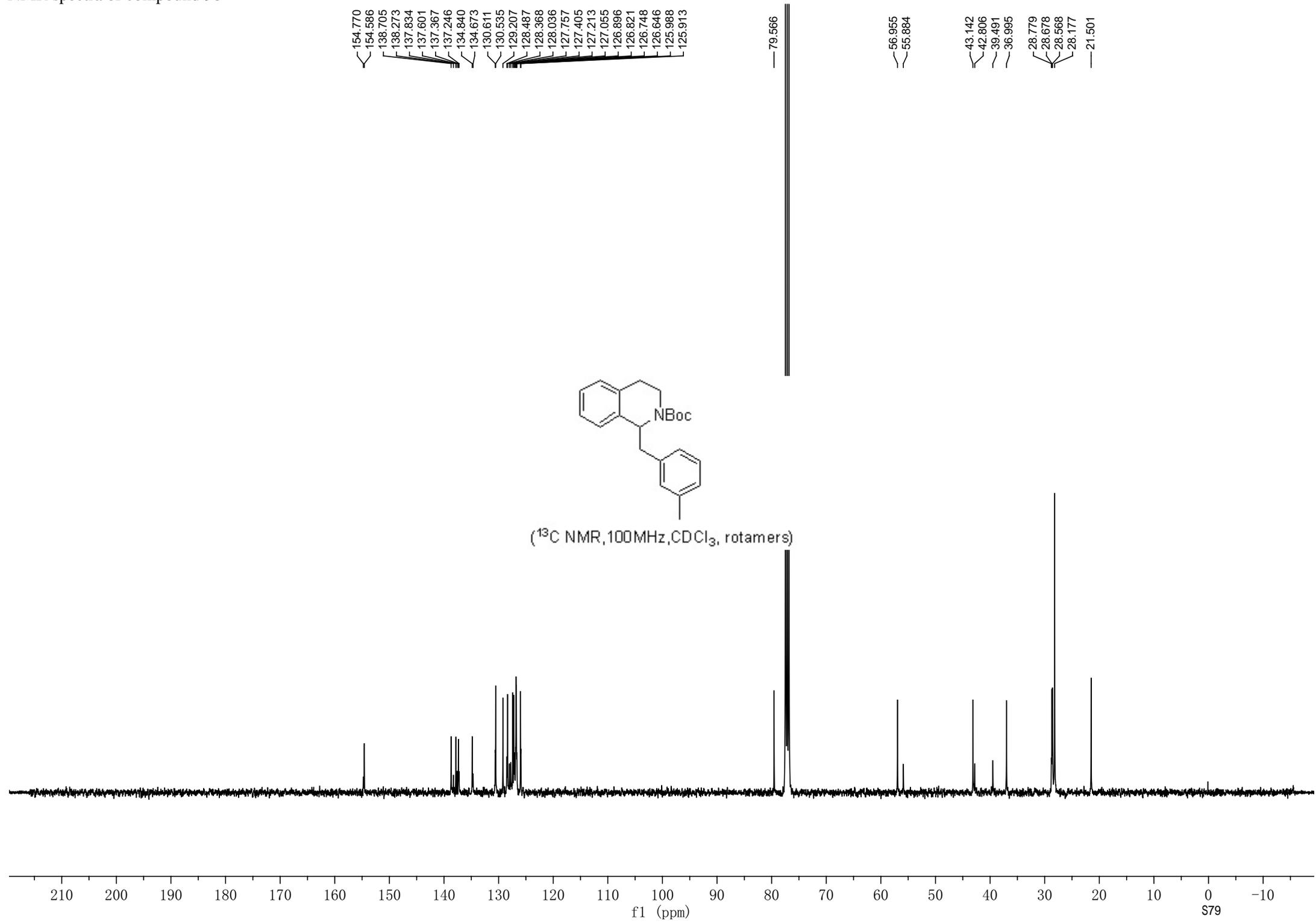
-0.000



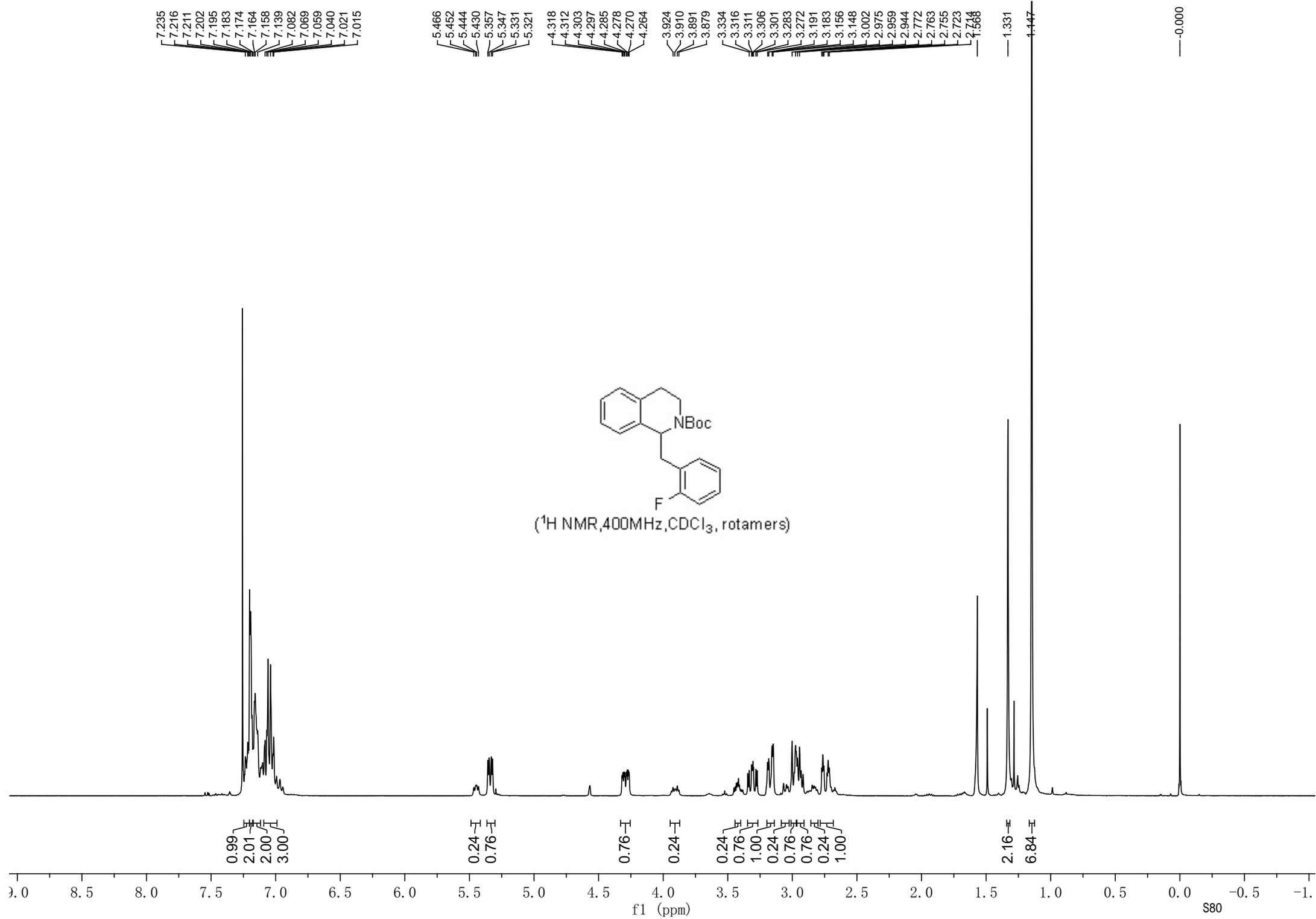
(¹H NMR, 400MHz, CDCl₃, rotamers)



NMR spectra of compound 9b



NMR spectra of compound 9c



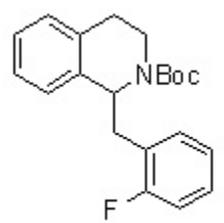
NMR spectra of compound 9c

163.119
162.961
160.685
160.546
154.589
154.478
137.270
134.788
132.144
132.098
129.319
128.420
128.341
127.485
127.390
126.872
126.771
126.187
126.056
124.119
123.367
115.145

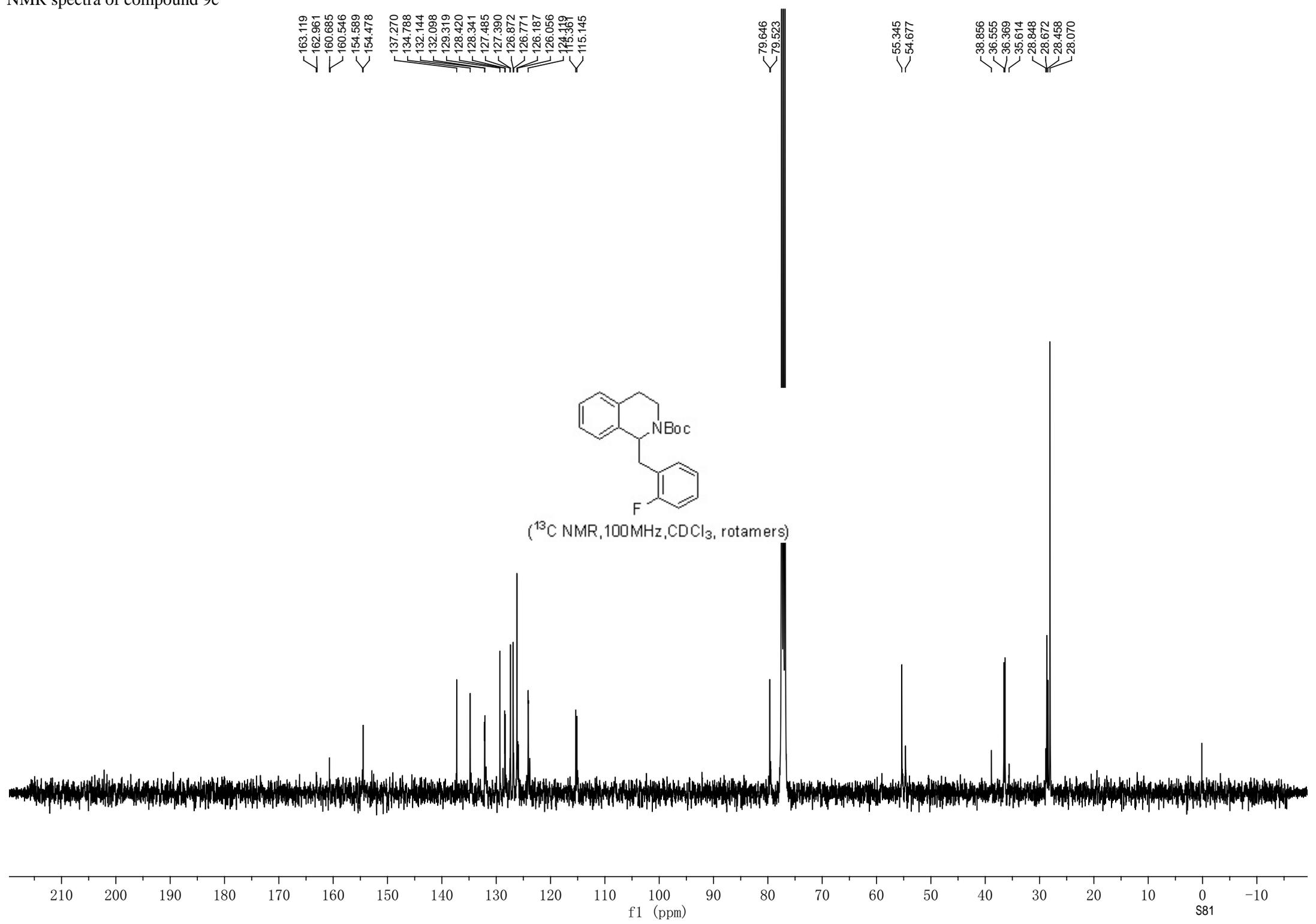
79.646
79.523

55.345
54.677

38.856
36.555
36.369
35.614
28.848
28.672
28.458
28.070



(¹³C NMR, 100MHz, CDCl₃, rotamers)

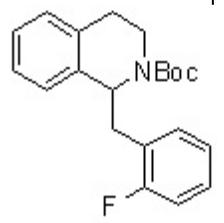


f1 (ppm)

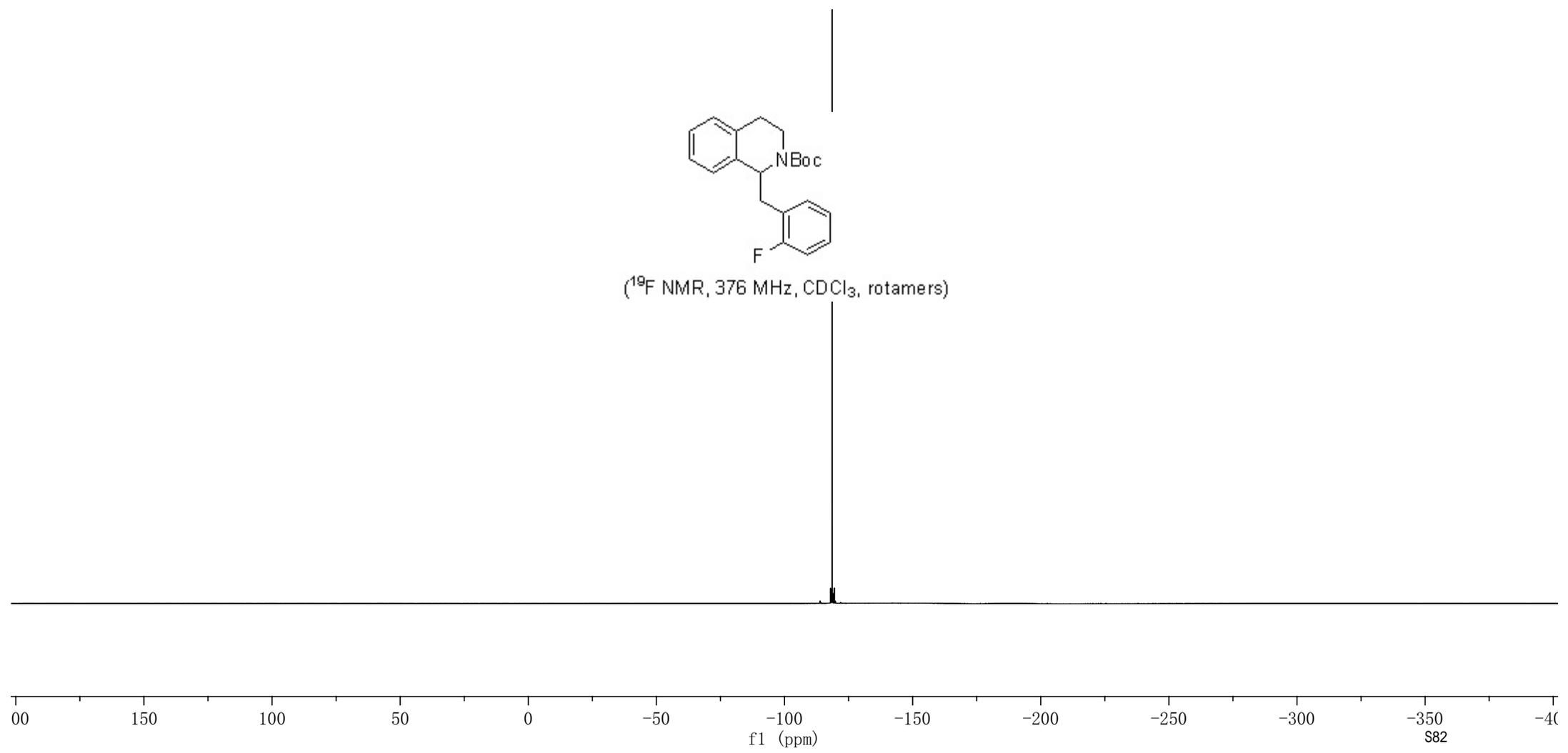
S81

NMR spectra of compound 9c

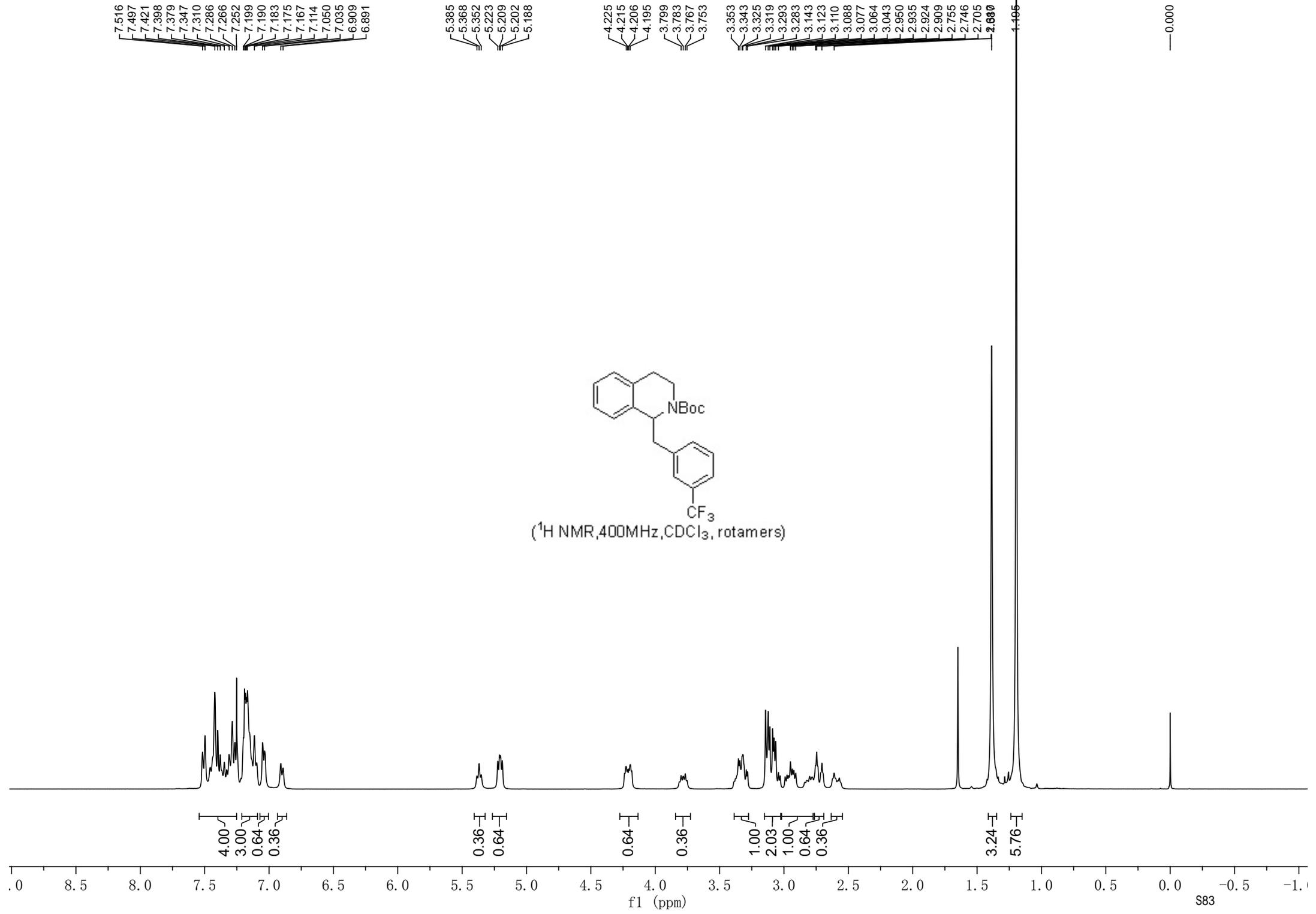
-118.540
-118.620



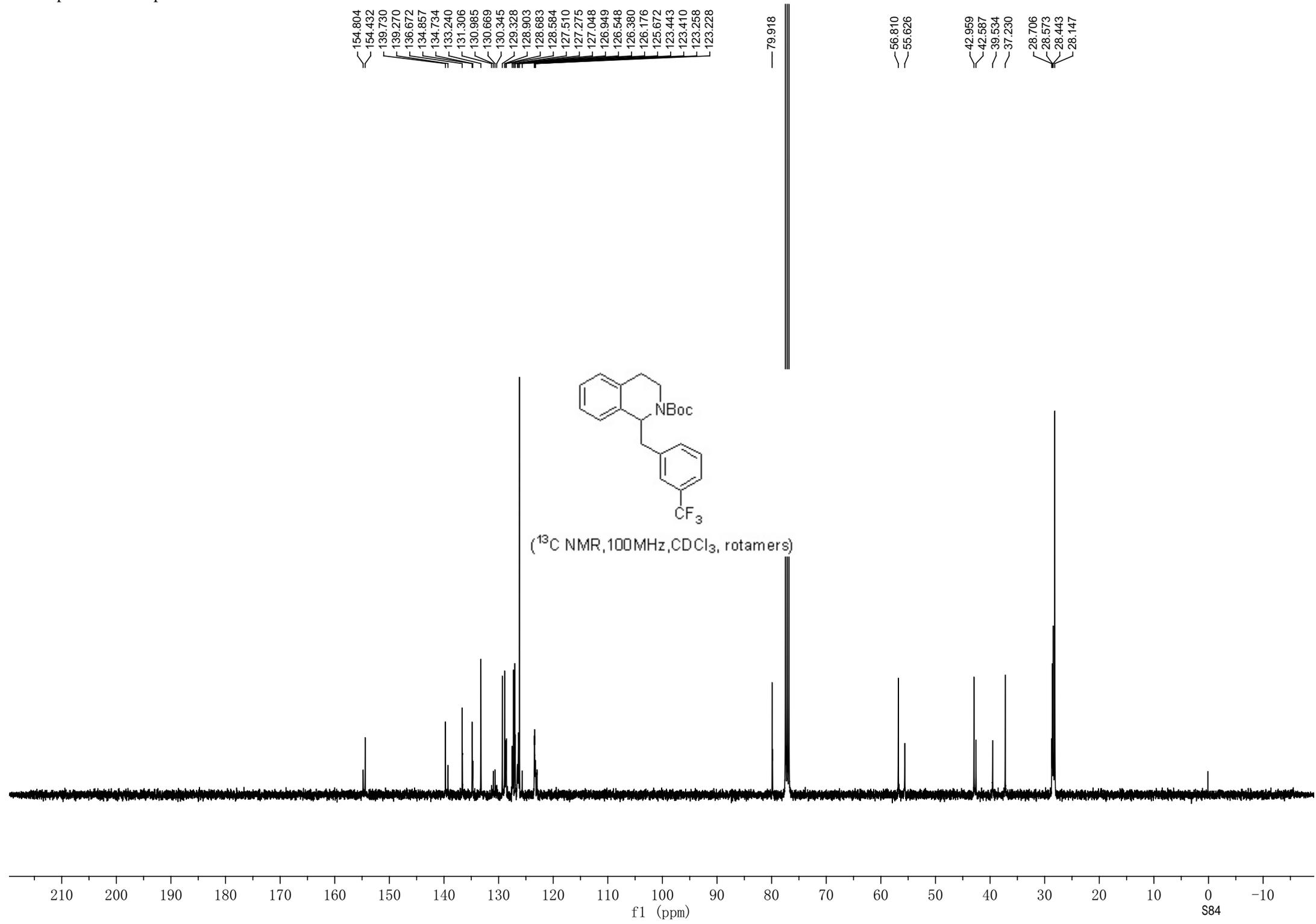
(¹⁹F NMR, 376 MHz, CDCl₃, rotamers)



NMR spectra of compound 9d

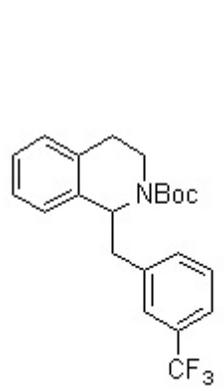


NMR spectra of compound 9d

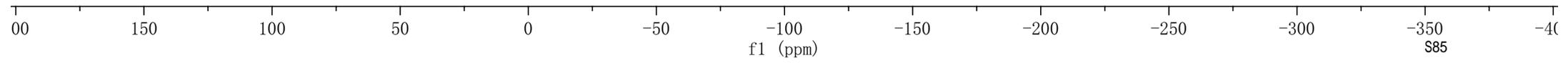


NMR spectra of compound 9d

---62.485



(¹⁹F NMR, 376 MHz, CDCl₃, rotamers)



NMR spectra of compound 9e

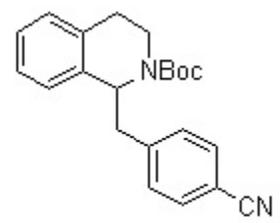
8.008
7.987
7.858
7.837
7.591
7.571
7.534
7.225
7.214
7.195
7.166
7.127
7.045
7.030
6.902
6.884

5.386
5.369
5.353
5.226
5.212
5.205
5.192

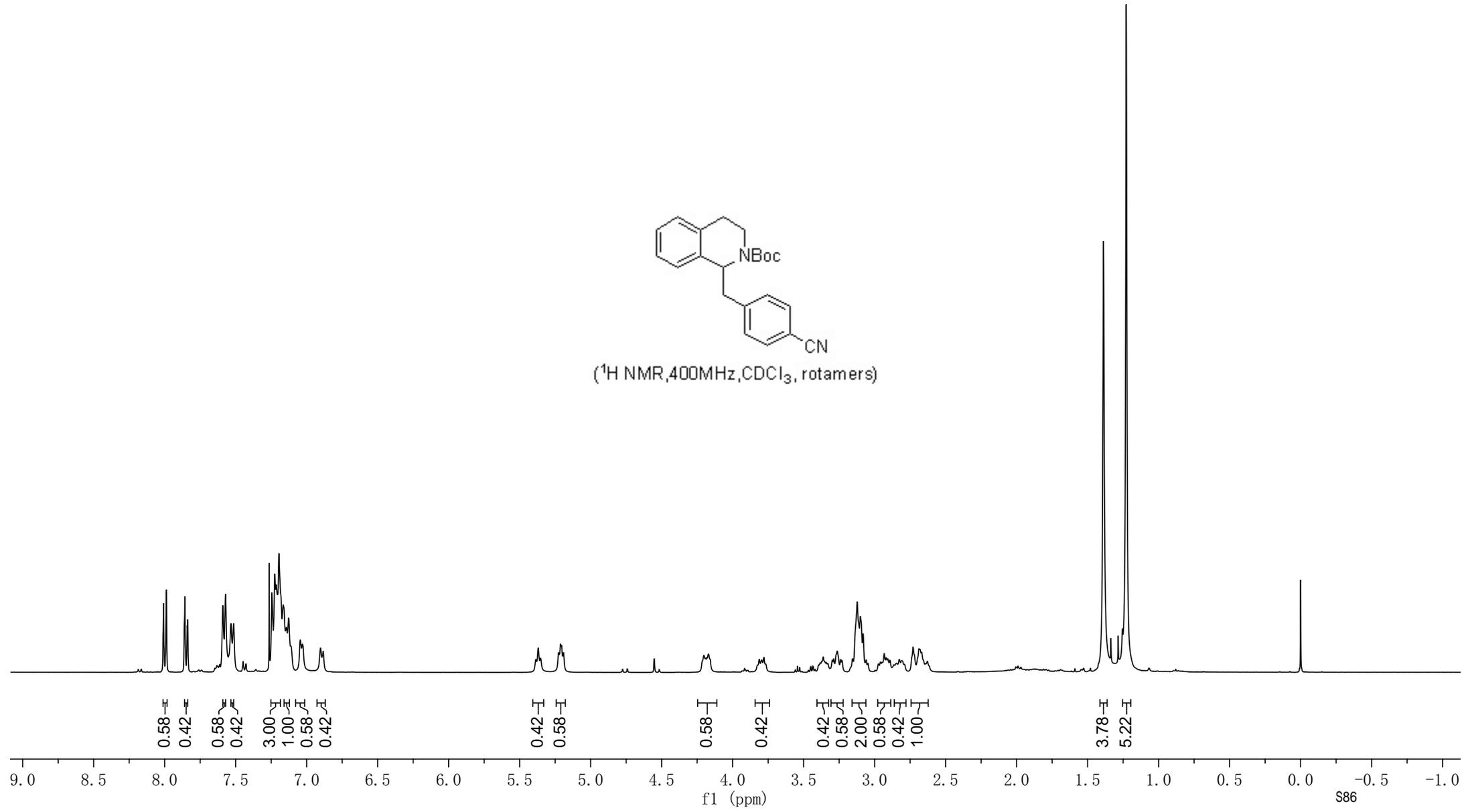
4.202
4.191
4.181
4.170
3.813
3.796
3.780
3.767

3.362
3.299
3.288
3.264
3.239
3.229
3.156
3.123
3.100
3.081
2.933
2.918
2.907
2.892
2.826
2.809
2.729
2.688
2.680
2.669
2.668
1.228

-0.000



(¹H NMR, 400MHz, CDCl₃, rotamers)



NMR spectra of compound 9e

190.698

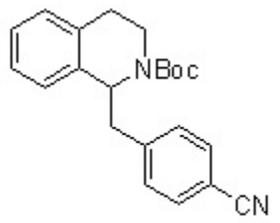
154.751
154.341
144.395
144.139
133.022
132.165
131.945
130.608
130.007
129.350
127.153
126.760
119.025
117.817
117.742
110.446
110.263

80.088
79.970

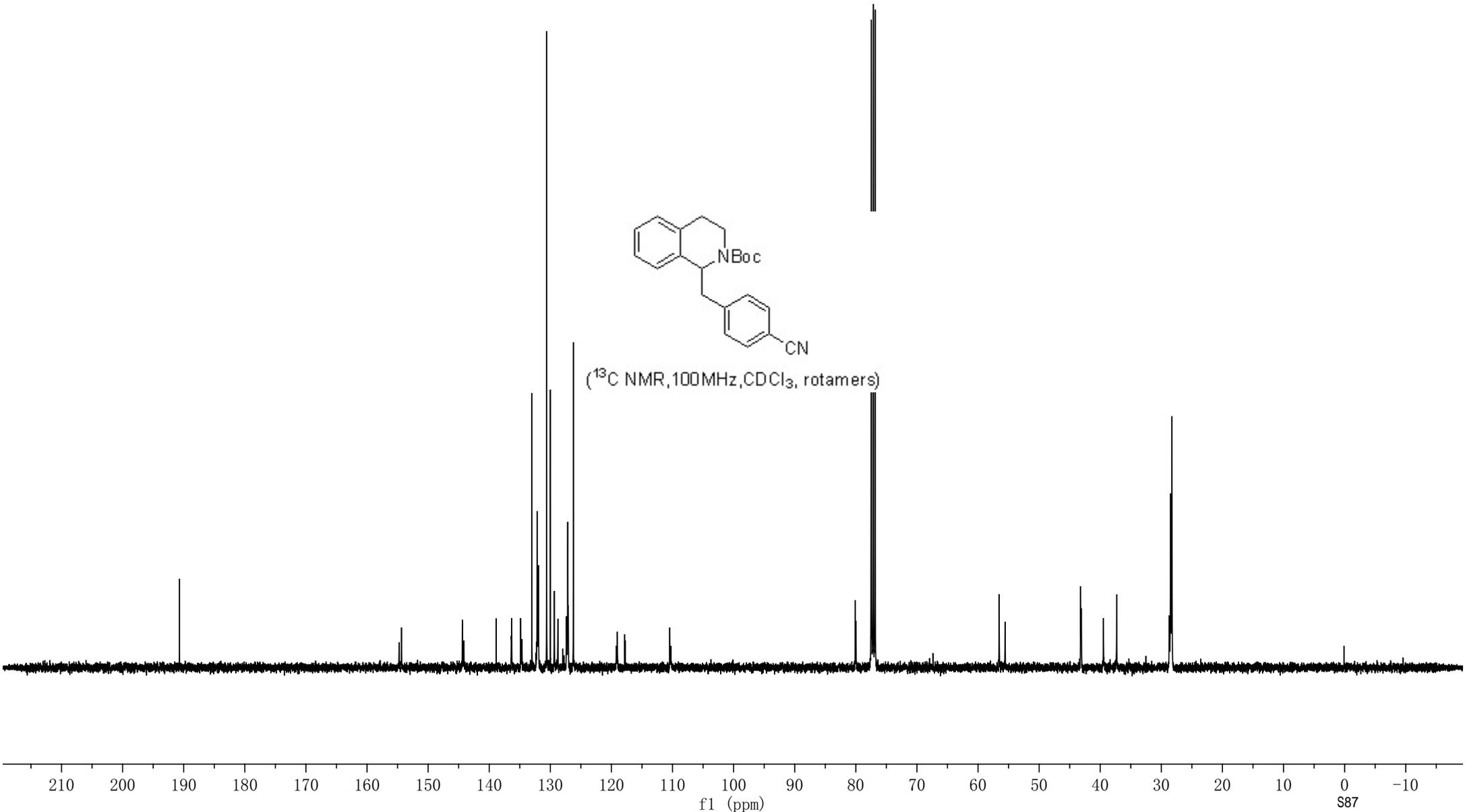
56.544
55.568

43.207
43.087
39.478
37.312

28.710
28.514
28.461
28.256



(¹³C NMR, 100MHz, CDCl₃, rotamers)



NMR spectra of compound 9f

8.269
8.248
7.891
7.871
7.764
7.743
7.572
7.494
7.353
7.350
7.332
7.203
7.194
7.179
7.130
6.608
6.589

5.555
5.538
5.521
5.506
5.496
5.481
5.470

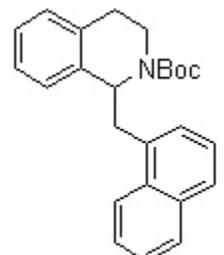
4.369
4.362
4.354
4.347
4.336
4.329
4.321
4.314

3.635
3.624
3.600
3.589
3.423
3.364
3.338
3.329

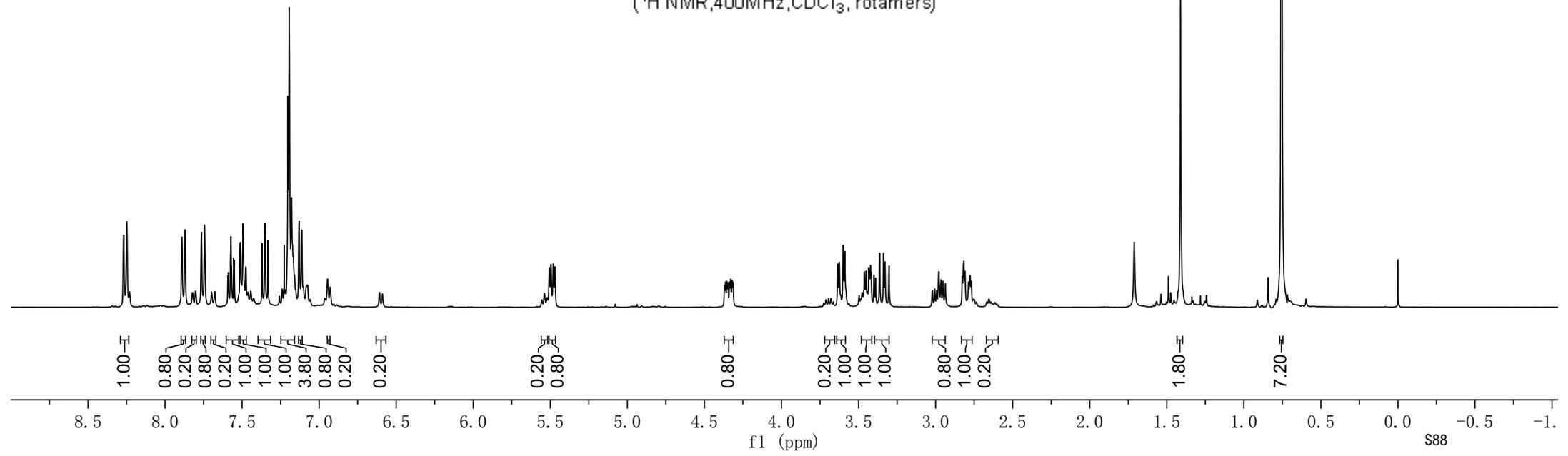
3.022
3.006
2.993
2.980
2.966
2.953
2.938
2.827
2.817
2.810
2.786
2.776
2.769
2.668
2.654
2.641
2.611

0.756

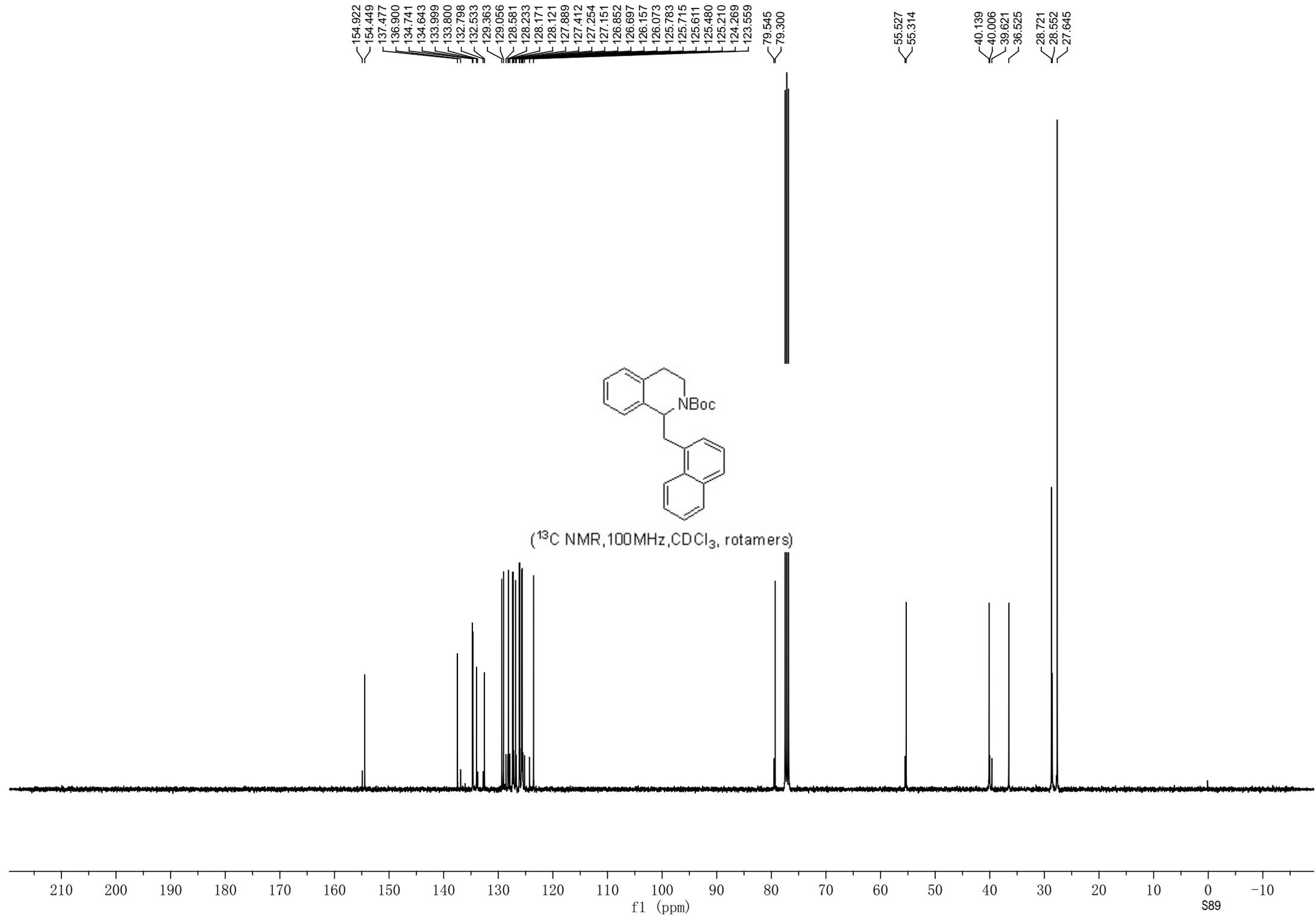
-0.000



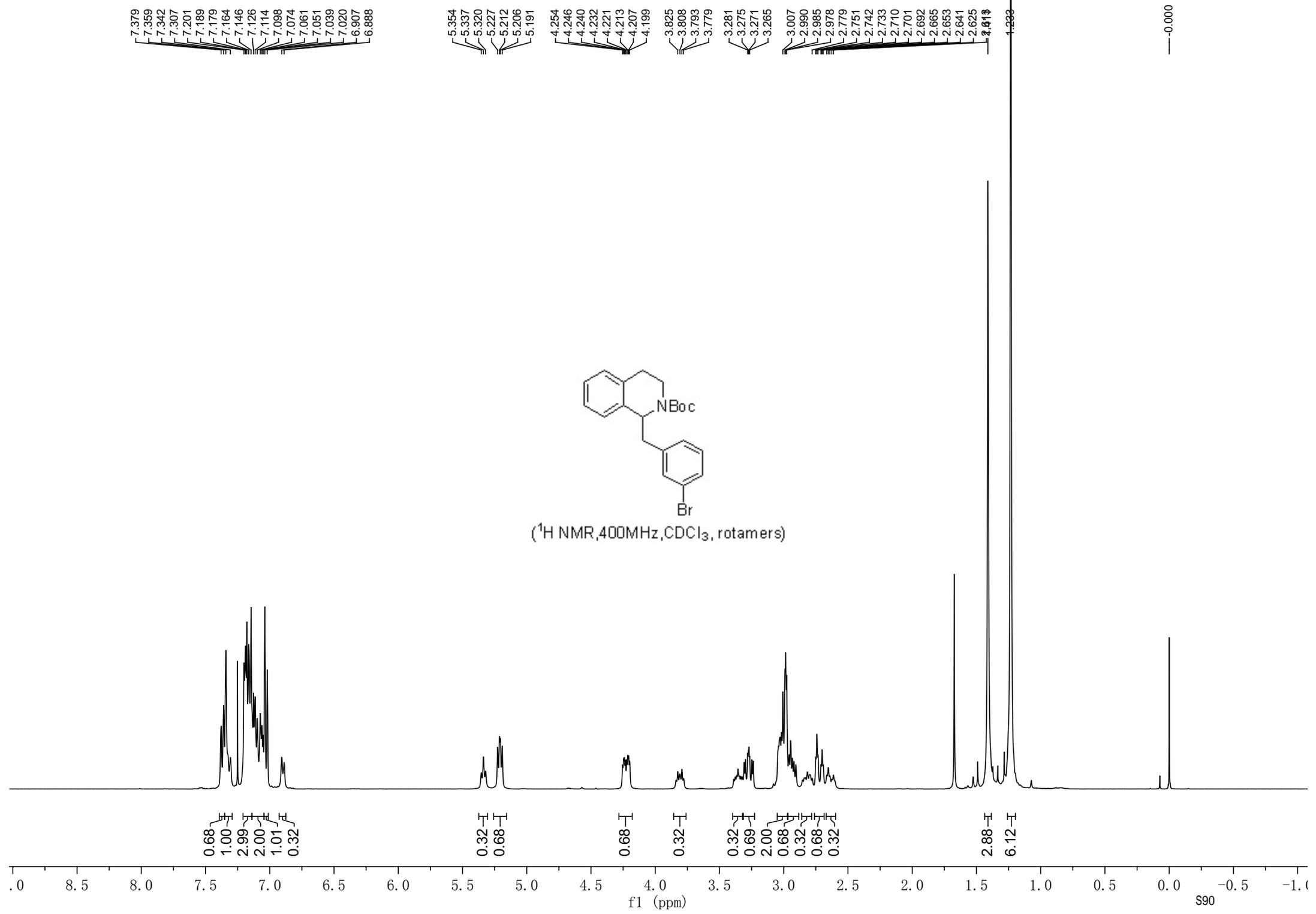
(¹H NMR, 400MHz, CDCl₃, rotamers)



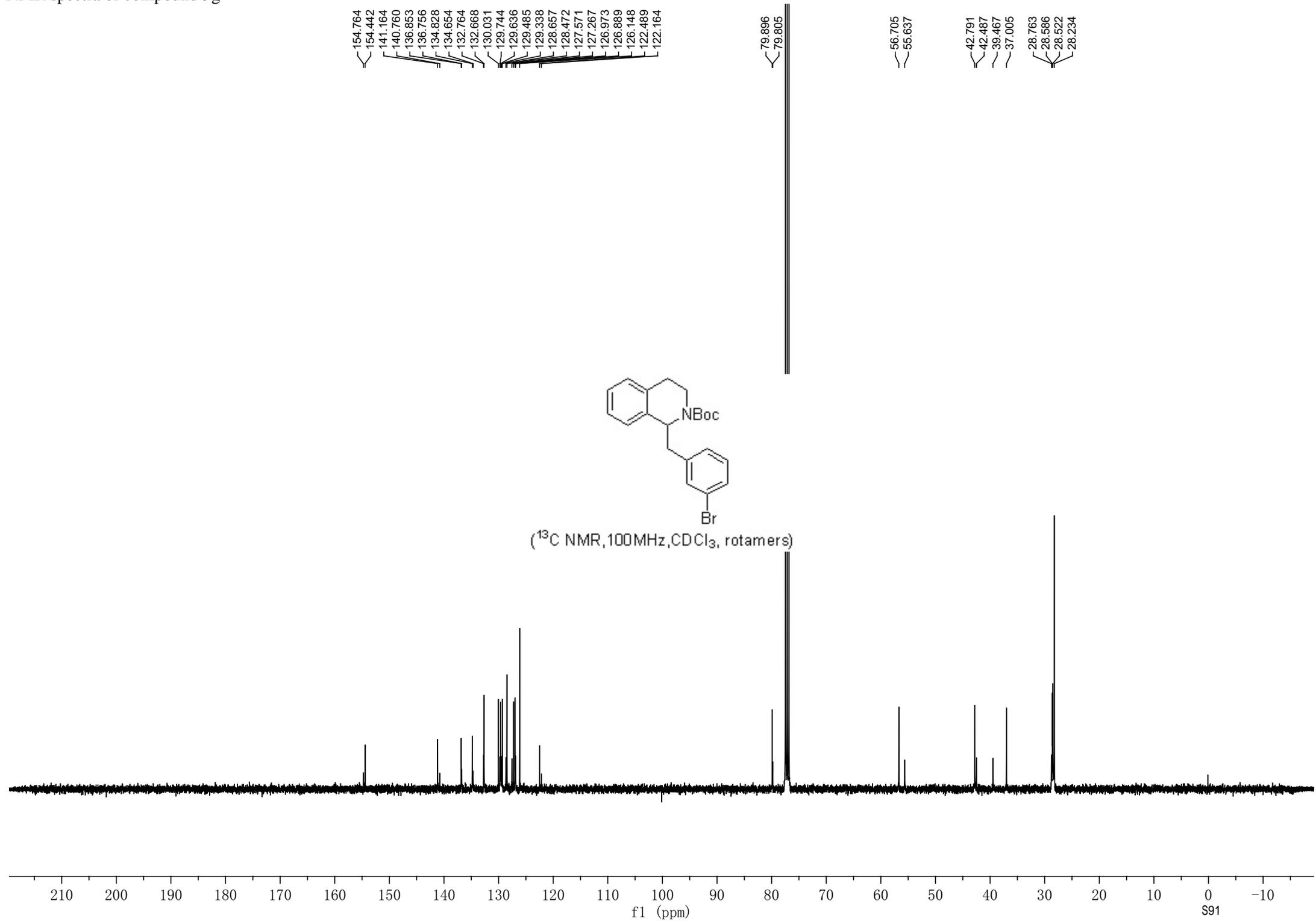
NMR spectra of compound 9f



NMR spectra of compound 9g



NMR spectra of compound 9g



NMR spectra of compound 9h

7.200
7.183
7.175
7.166
7.162
7.148
7.138
7.125
7.101
7.080
7.059
7.044
7.021
7.003
6.984
6.962
6.940
6.927
6.905
6.883

5.335
5.318
5.302
5.185
5.170
5.165
5.150

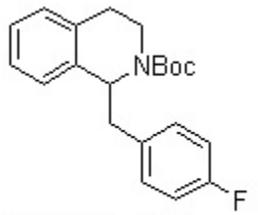
4.210
4.196
4.187
4.177
4.167
4.164
4.154

3.795
3.779
3.763
3.750

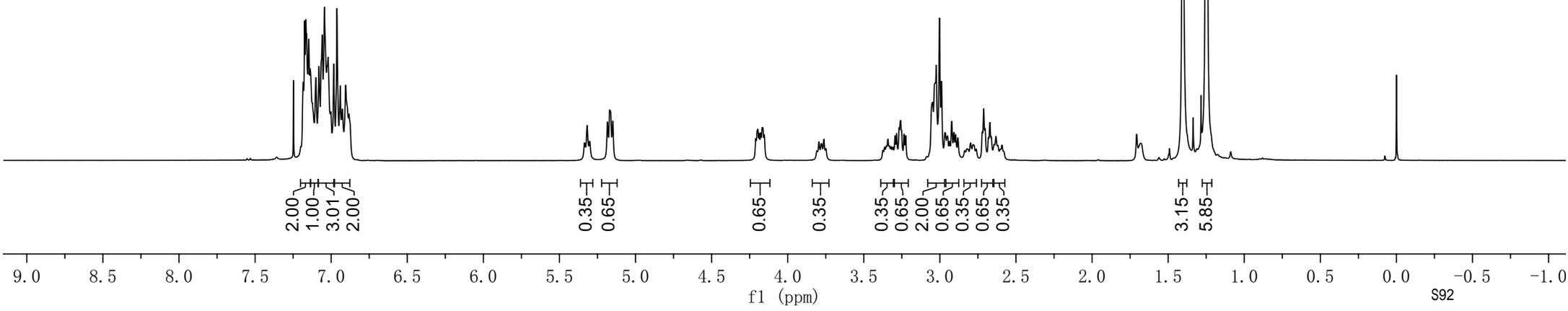
3.295
3.284
3.268
3.258
3.252
3.235
3.225
3.049
3.031
3.024
3.003
2.989
2.967
2.923
2.908
2.897
2.721
2.712
2.703

4.805
4.803
4.240

-0.000



(¹H NMR, 400MHz, CDCl₃, rotamers)



NMR spectra of compound 9h

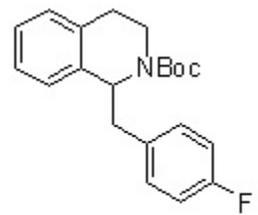
163.102
163.003
160.674
160.580
154.784
154.555
136.881
134.873
134.411
134.383
131.176
131.099
129.216
128.582
127.576
127.310
126.869
126.764
116.284
115.084
115.022
114.811

79.805
79.678

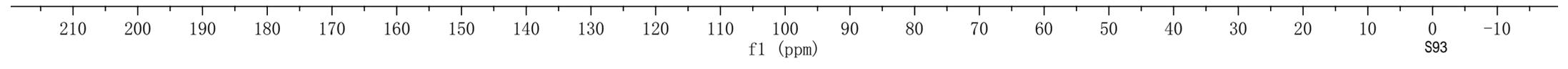
56.885
55.876

42.231
42.037
39.492
37.208

28.762
28.620
28.524
28.268

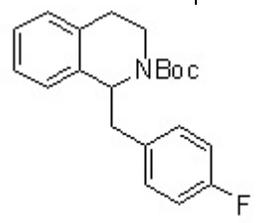


(¹³C NMR, 100MHz, CDCl₃, rotamers)

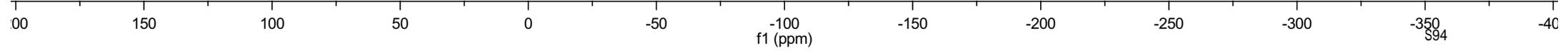


NMR spectra of compound 9h

116.916
117.146

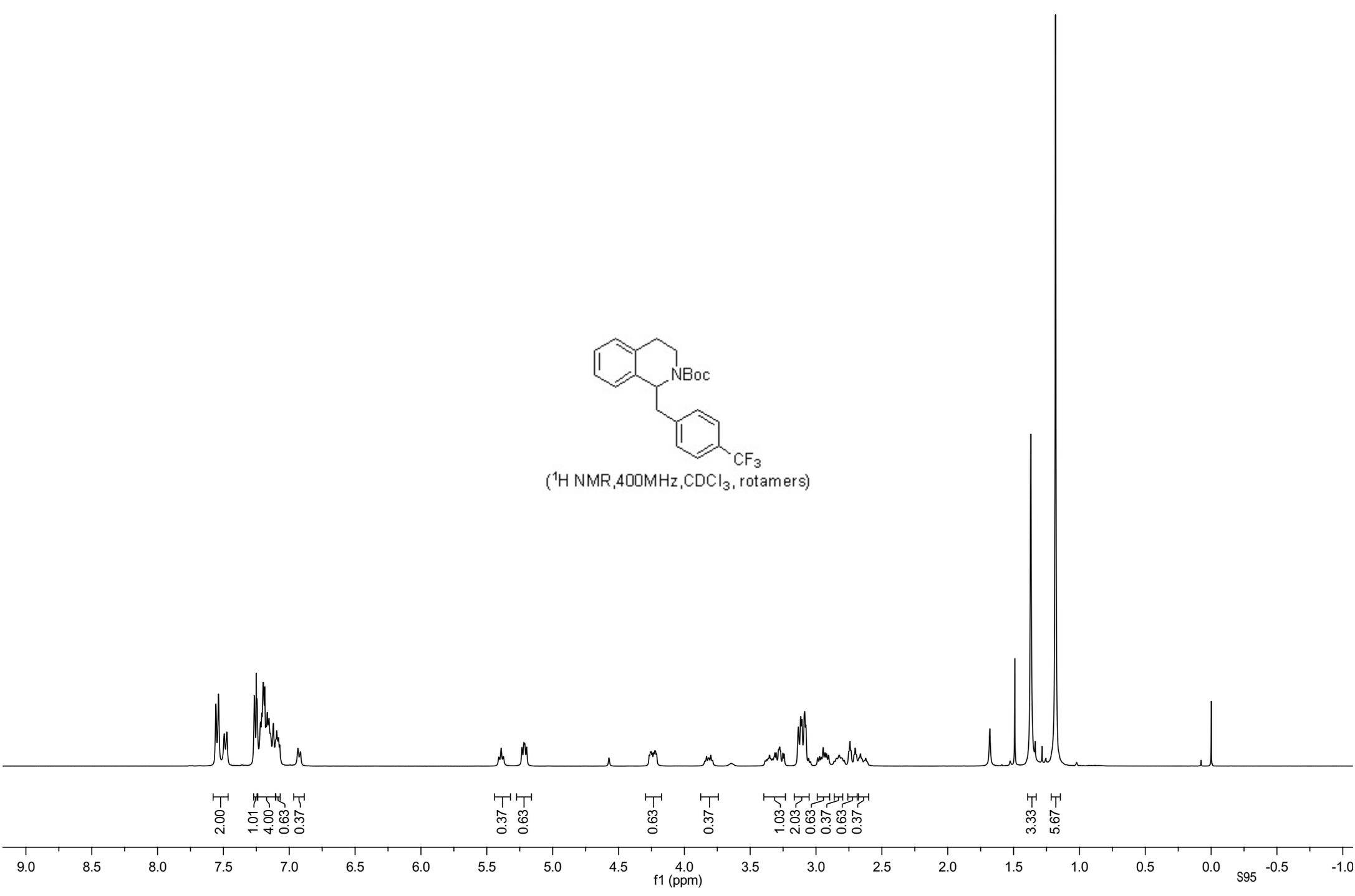
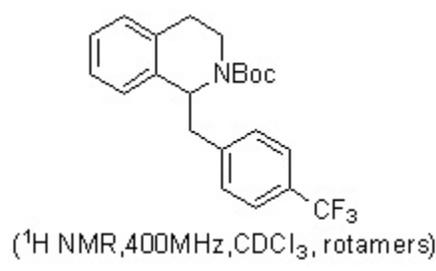


(¹⁹F NMR, 376 MHz, CDCl₃, rotamers)

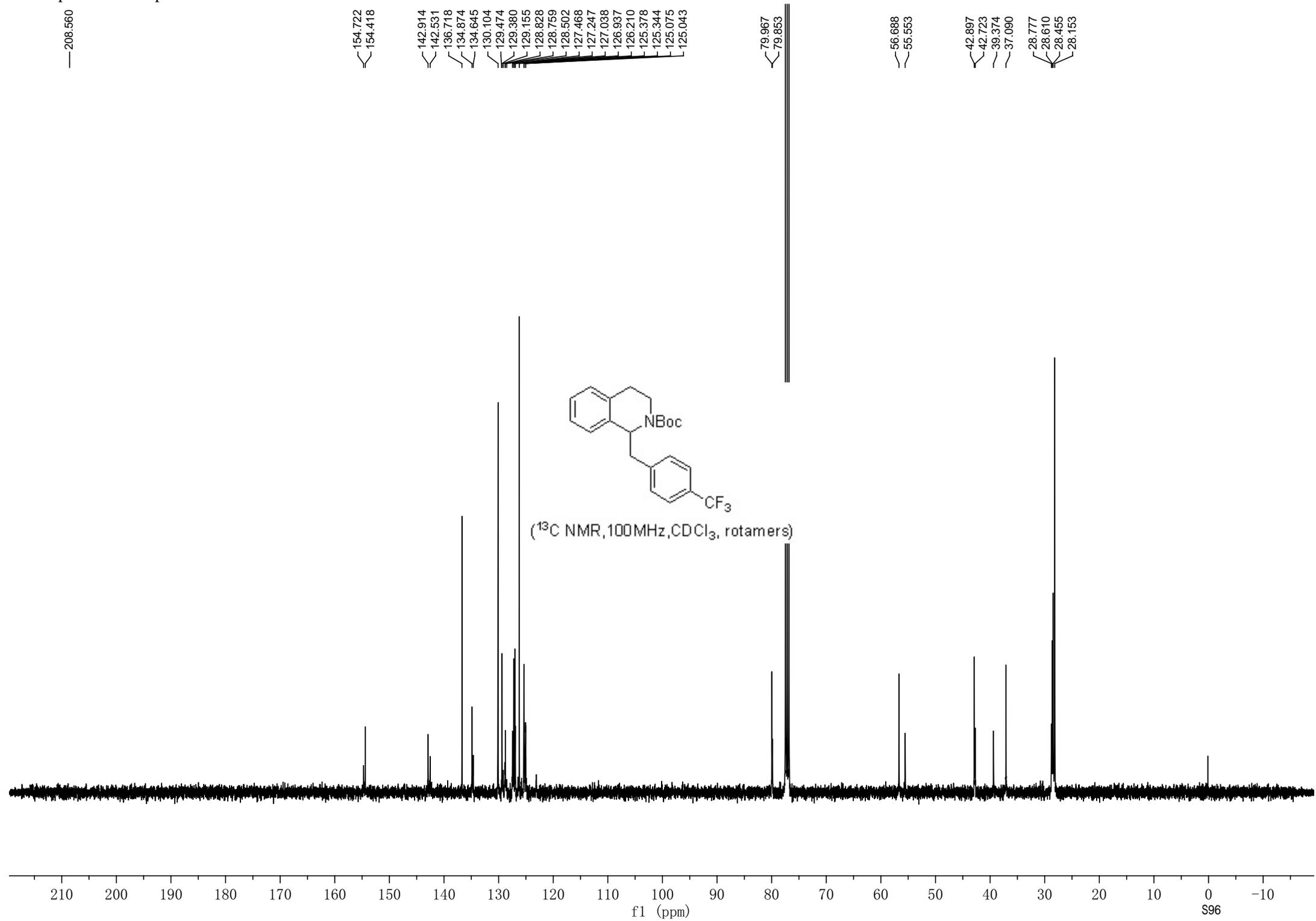


NMR spectra of compound 9i

7.557, 7.538, 7.494, 7.475, 7.265, 7.250, 7.245, 7.219, 7.209, 7.197, 7.187, 7.177, 7.168, 7.154, 7.143, 7.121, 7.103, 7.085, 7.083, 5.409, 5.392, 5.374, 5.233, 5.219, 5.212, 5.198, 4.266, 4.258, 4.252, 4.244, 4.233, 4.225, 4.219, 4.211, 3.882, 3.815, 3.800, 3.786, 3.313, 3.302, 3.285, 3.276, 3.253, 3.242, 3.135, 3.117, 3.107, 3.086, 3.077, 2.946, 2.932, 2.920, 2.751, 2.743, 2.734, 2.711, 2.702, 2.694, 2.690, 1.181, -0.000

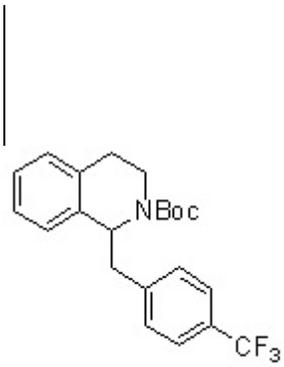


NMR spectra of compound 9i

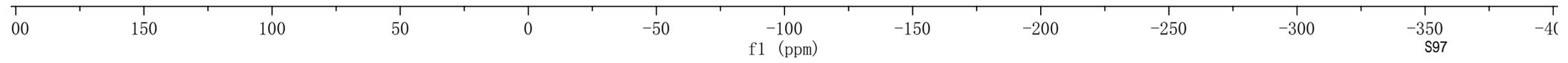


NMR spectra of compound 9i

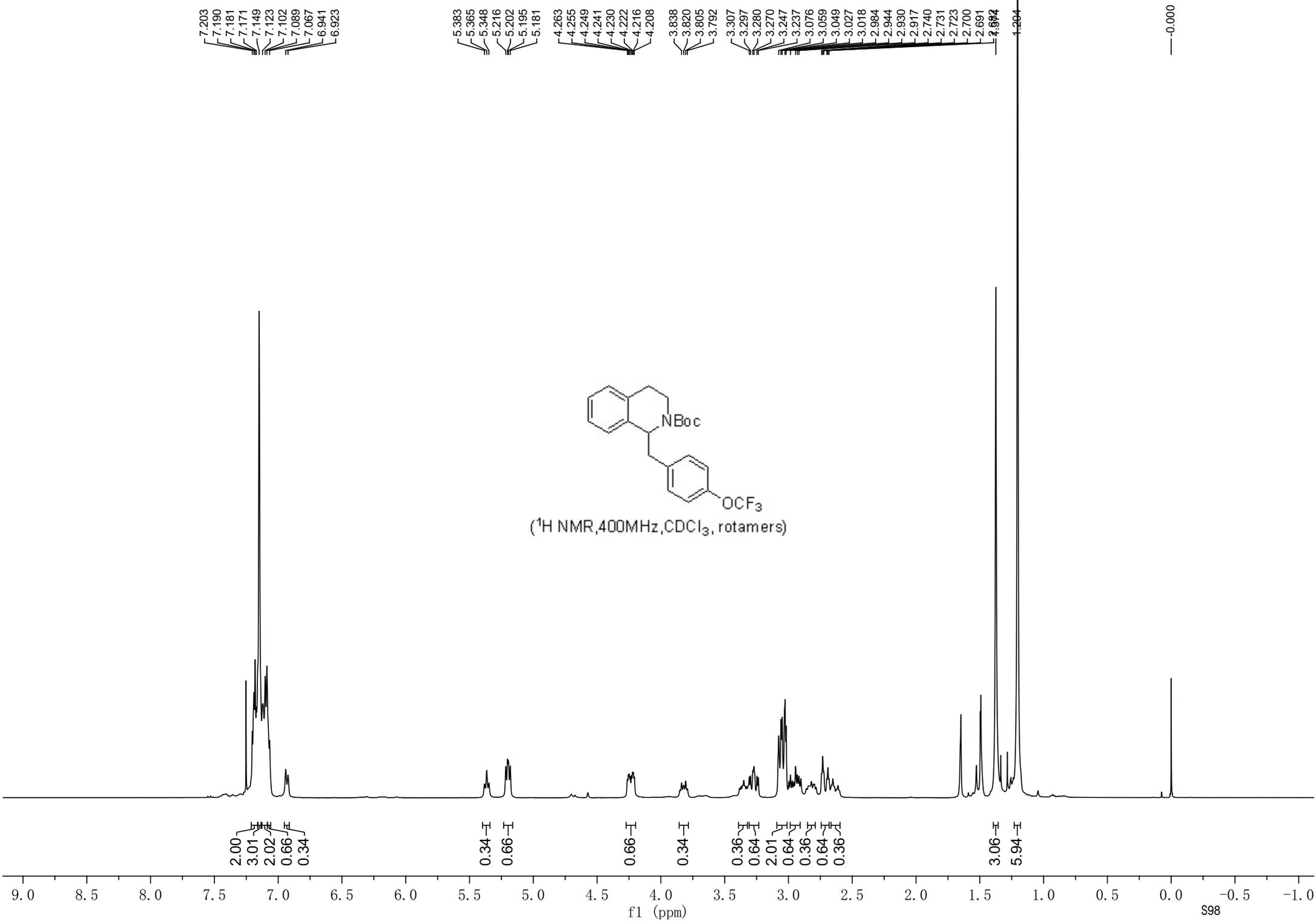
-62.338
-62.398



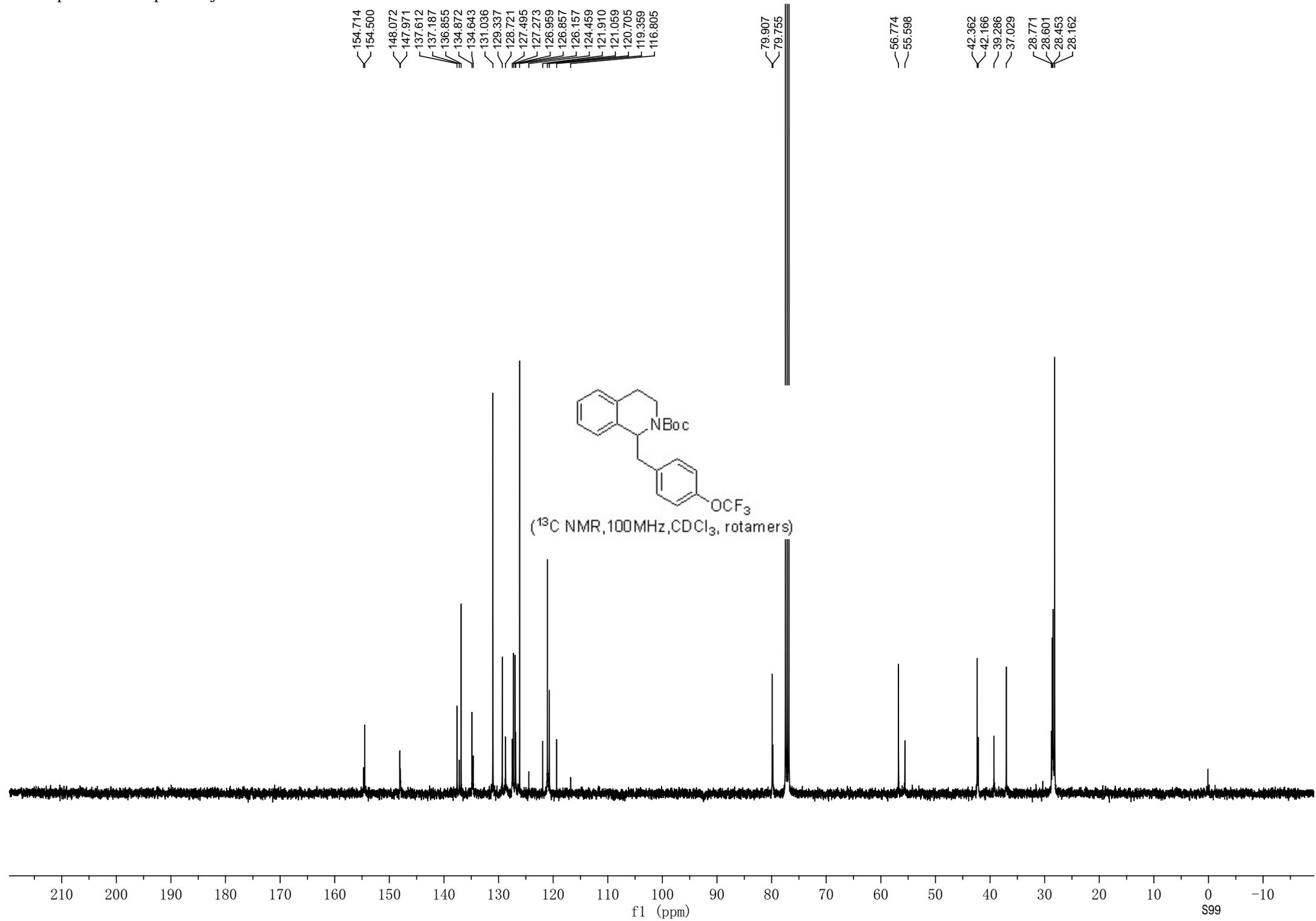
(¹⁹F NMR, 376 MHz, CDCl₃, rotamers)



NMR spectra of compound 9j

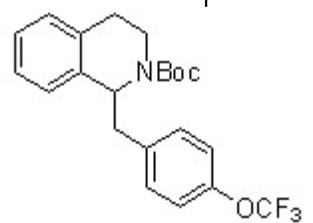


NMR spectra of compound 9j

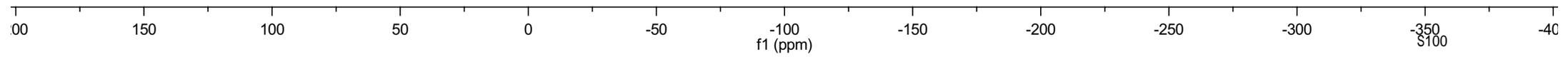


NMR spectra of compound 9j

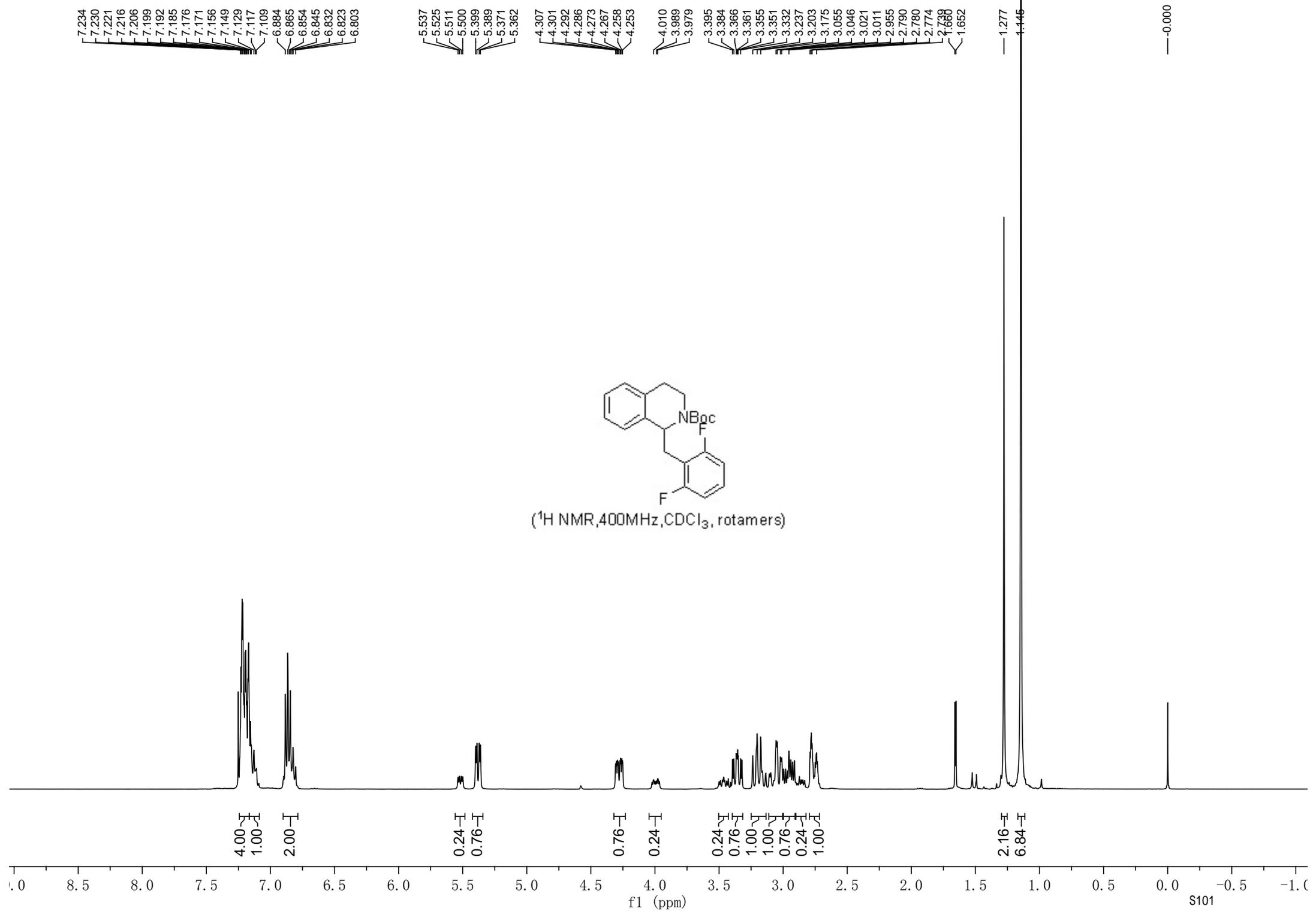
110.598
110.985



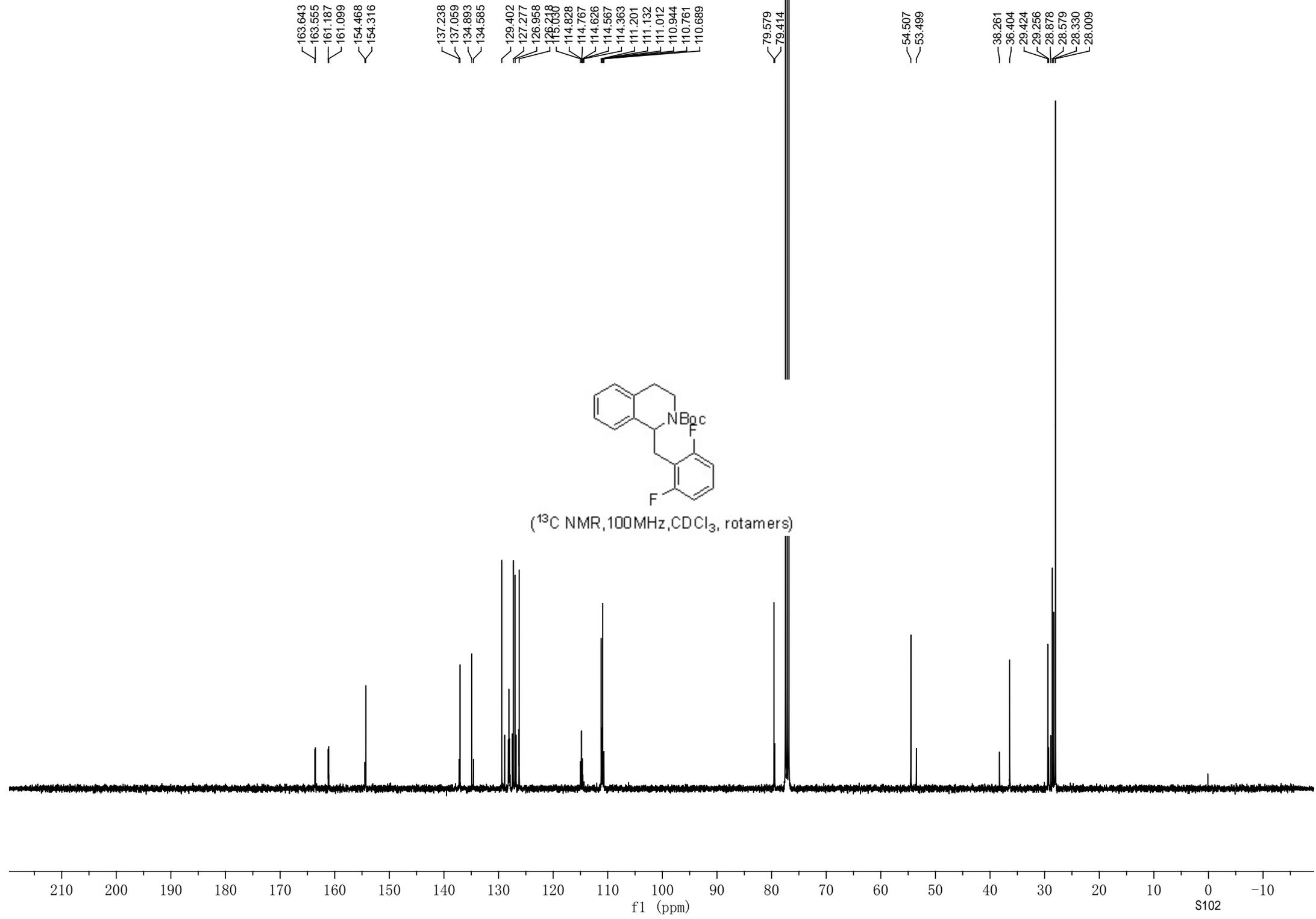
(¹⁹F NMR, 376 MHz, CDCl₃, rotamers)



NMR spectra of compound 9k

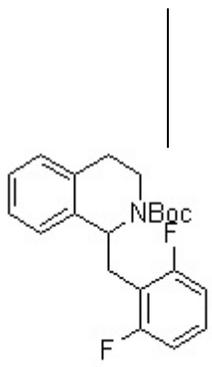


NMR spectra of compound 9k

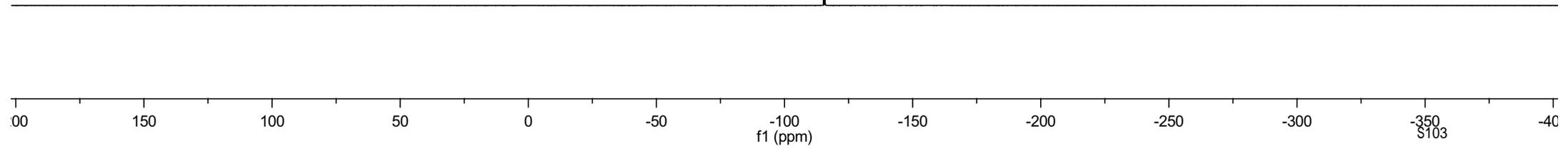


NMR spectra of compound 9k

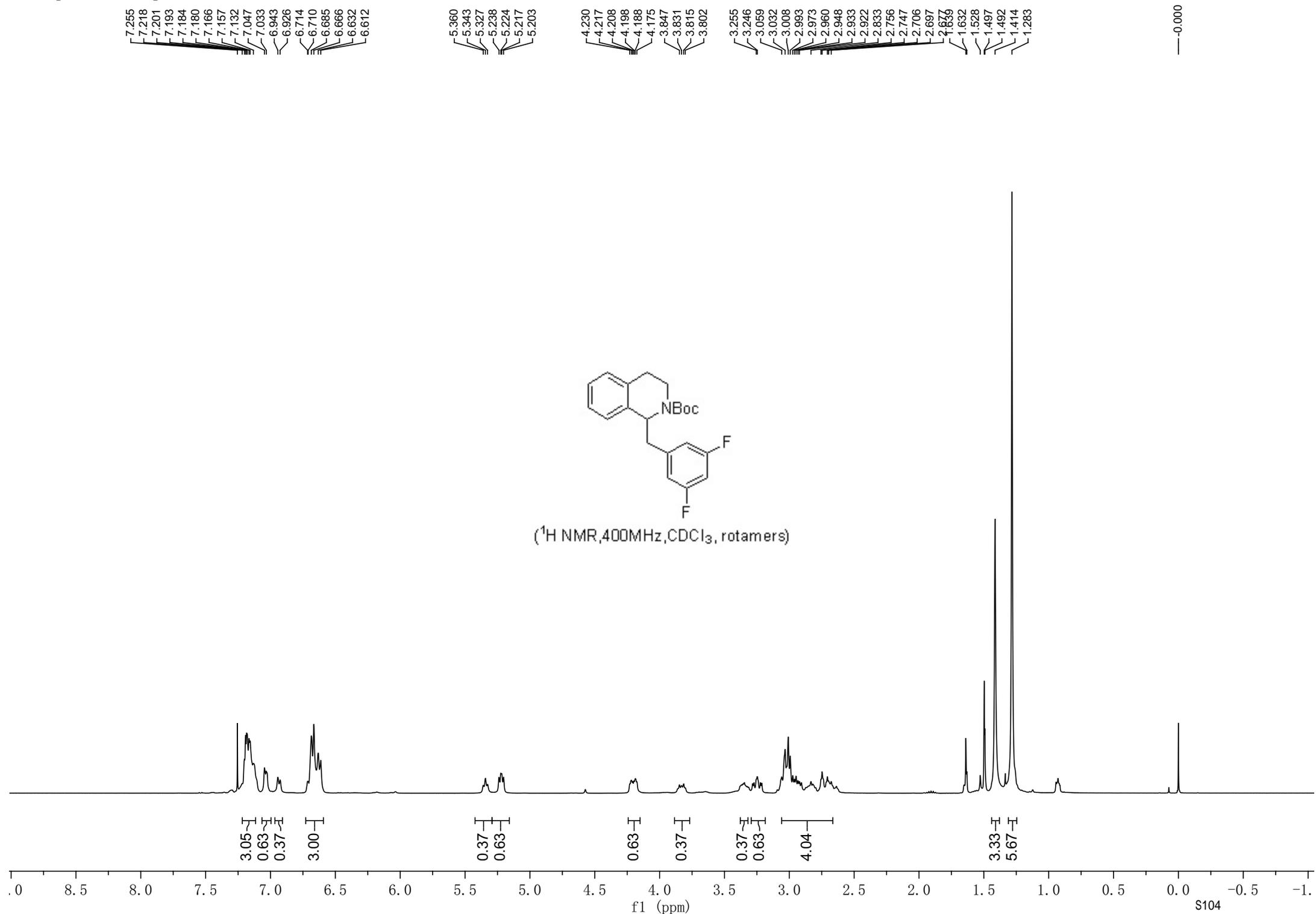
115.505
115.704



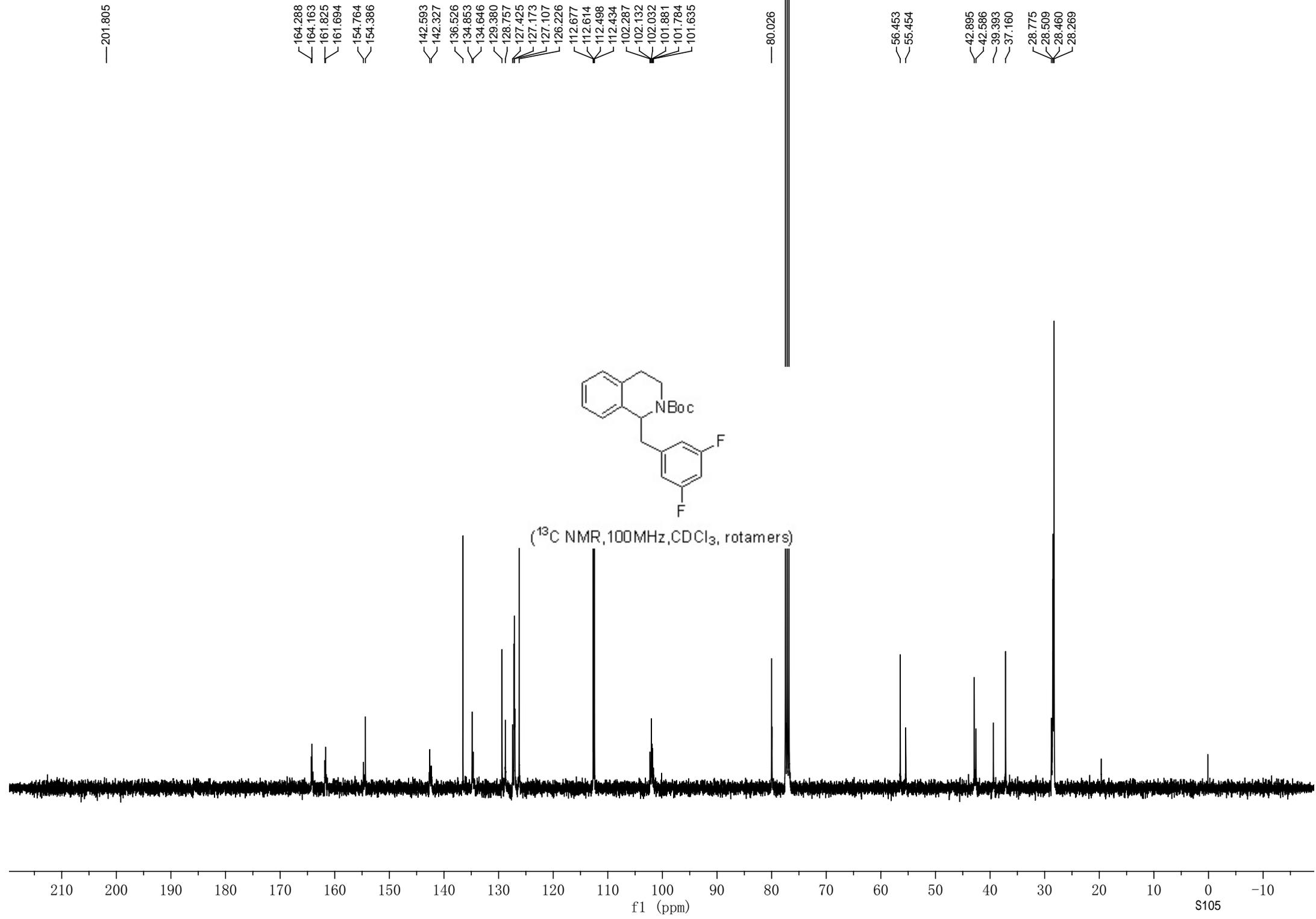
(¹⁹F NMR, 376 MHz, CDCl₃, rotamers)

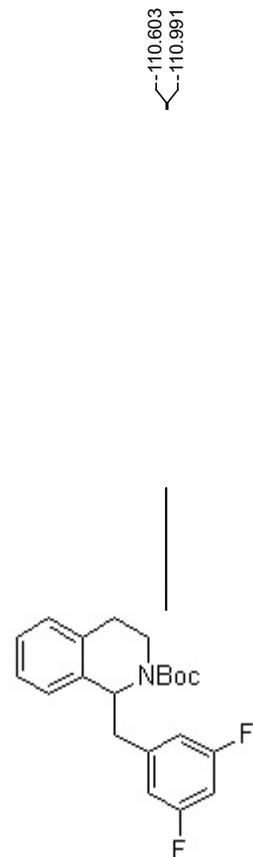


NMR spectra of compound 9l



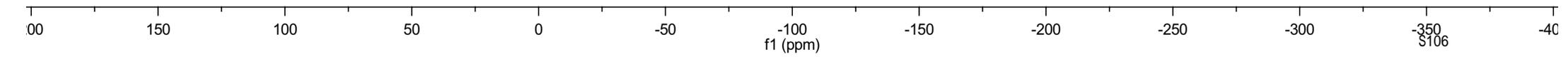
NMR spectra of compound 91





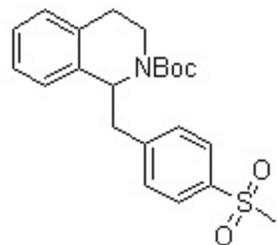
(¹⁹F NMR, 376 MHz, CDCl₃, rotamers)

110.603
110.991

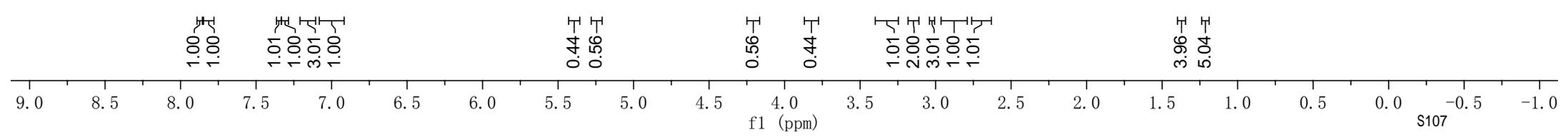


NMR spectra of compound 9m

7.882, 7.862, 7.822, 7.802, 7.360, 7.340, 7.318, 7.298, 7.270, 7.202, 7.194, 7.173, 7.165, 7.152, 7.134, 7.117, 7.078, 7.065, 6.945, 6.927, 5.412, 5.395, 5.379, 5.268, 5.253, 5.234, 4.224, 4.215, 4.204, 4.194, 3.837, 3.819, 3.804, 3.791, 3.365, 3.316, 3.306, 3.280, 3.256, 3.246, 3.173, 3.156, 3.137, 3.034, 3.015, 2.944, 2.930, 2.918, 2.904, 2.832, 2.815, 2.748, 2.708, 2.686, 2.674, 2.674, 1.246, 0.000

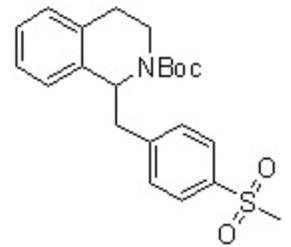


(¹H NMR, 400MHz, CDCl₃, rotamers)



NMR spectra of compound 9m

- 154.672
- 154.265
- 145.285
- 145.068
- 138.862
- 138.537
- 136.340
- 134.756
- 134.579
- 130.704
- 129.350
- 128.788
- 127.472
- 127.310
- 127.185
- 127.117
- 127.026
- 126.238
- 79.933
- 79.843
- 56.462
- 55.495
- 44.642
- 42.955
- 42.777
- 39.366
- 37.194
- 28.685
- 28.466
- 28.406
- 28.225



(¹³C NMR, 100MHz, CDCl₃, rotamers)

