

Supporting Information

Zn(OTf)₂-Catalyzed Hydroamination of Ynamides with Aromatic Amines

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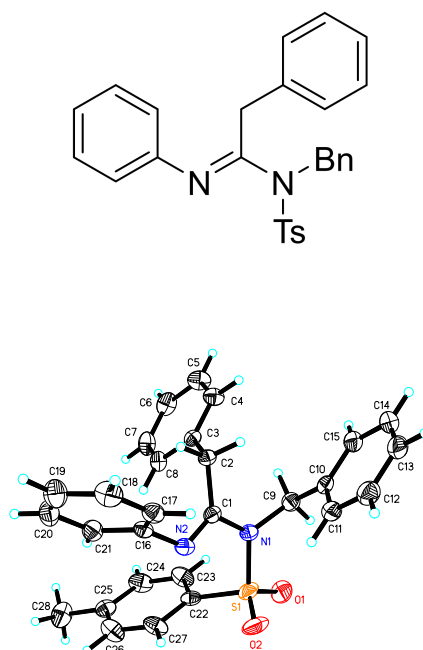
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I. X-Ray Structure for compound 3 aa

ORTEP drawing of the X-ray crystallographic structure of 3aa



CCDC- 2052690. 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 **3aa**.

Identification code	3aa	
Empirical formula	C ₂₈ H ₂₆ N ₂ O ₂ S	
Formula weight	454.57	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /n	
Unit cell dimensions	a = 10.0012(8) Å	α = 90°.
b = 22.074(2) Å	β = 90.349(3)°.	
c = 10.7284(10) Å	γ = 90°.	
Volume	2368.4(4) Å ³	
Z	4	
Density (calculated)	1.275 Mg/m ³	
Absorption coefficient	0.165 mm ⁻¹	
F(000)	960	
Crystal size	0.150 x 0.120 x 0.070 mm ³	

Theta range for data collection	2.748 to 25.497°.
Index ranges	-10<=h<=12, -26<=k<=26, -12<=l<=12
Reflections collected	22334
Independent reflections	4391 [R(int) = 0.0700]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6366
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4391 / 0 / 299
Goodness-of-fit on F ²	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0608, wR2 = 0.1143
R indices (all data)	R1 = 0.0994, wR2 = 0.1316
Extinction coefficient	n/a
Largest diff. peak and hole	0.203 and -0.405 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for mo_dd20113_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	8100(1)	7058(1)	4279(1)	51(1)
O(1)	7489(3)	7597(1)	4769(2)	75(1)
O(2)	9393(2)	6888(1)	4727(2)	69(1)
N(1)	6984(2)	6508(1)	4528(2)	41(1)
N(2)	8289(2)	5804(1)	3514(2)	41(1)
C(1)	7160(3)	5931(1)	3982(3)	36(1)
C(2)	5928(3)	5537(1)	3962(3)	34(1)
C(3)	4779(3)	5804(1)	3208(3)	34(1)
C(4)	3478(3)	5761(1)	3637(3)	46(1)
C(5)	2421(3)	5975(2)	2925(3)	56(1)
C(6)	2666(3)	6248(2)	1797(3)	57(1)
C(7)	3950(4)	6308(2)	1373(3)	53(1)
C(8)	5003(3)	6081(1)	2069(3)	44(1)
C(9)	5931(3)	6607(1)	5469(3)	45(1)
C(10)	6063(3)	6215(1)	6608(3)	42(1)
C(11)	7270(3)	5974(1)	7001(3)	49(1)
C(12)	7334(4)	5626(2)	8076(3)	64(1)
C(13)	6196(4)	5511(2)	8747(3)	67(1)

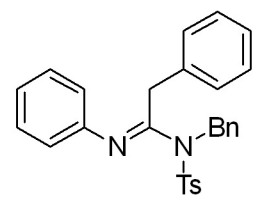
C(14)	4997(4)	5742(2)	8368(3)	68(1)
C(15)	4926(3)	6094(2)	7292(3)	55(1)
C(16)	8494(3)	5239(1)	2933(3)	37(1)
C(17)	8778(3)	4729(1)	3649(3)	45(1)
C(18)	8981(3)	4171(2)	3075(4)	60(1)
C(19)	8915(4)	4123(2)	1797(4)	70(1)
C(20)	8689(3)	4631(2)	1088(3)	62(1)
C(21)	8482(3)	5189(2)	1651(3)	49(1)
C(22)	8149(3)	7123(1)	2654(3)	40(1)
C(23)	7080(3)	7395(2)	2048(4)	59(1)
C(24)	7116(3)	7457(2)	769(4)	61(1)
C(25)	8175(3)	7256(1)	82(3)	49(1)
C(26)	9226(3)	6993(2)	716(4)	60(1)
C(27)	9223(3)	6922(1)	1991(3)	54(1)
C(28)	8213(4)	7340(2)	-1317(3)	75(1)

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

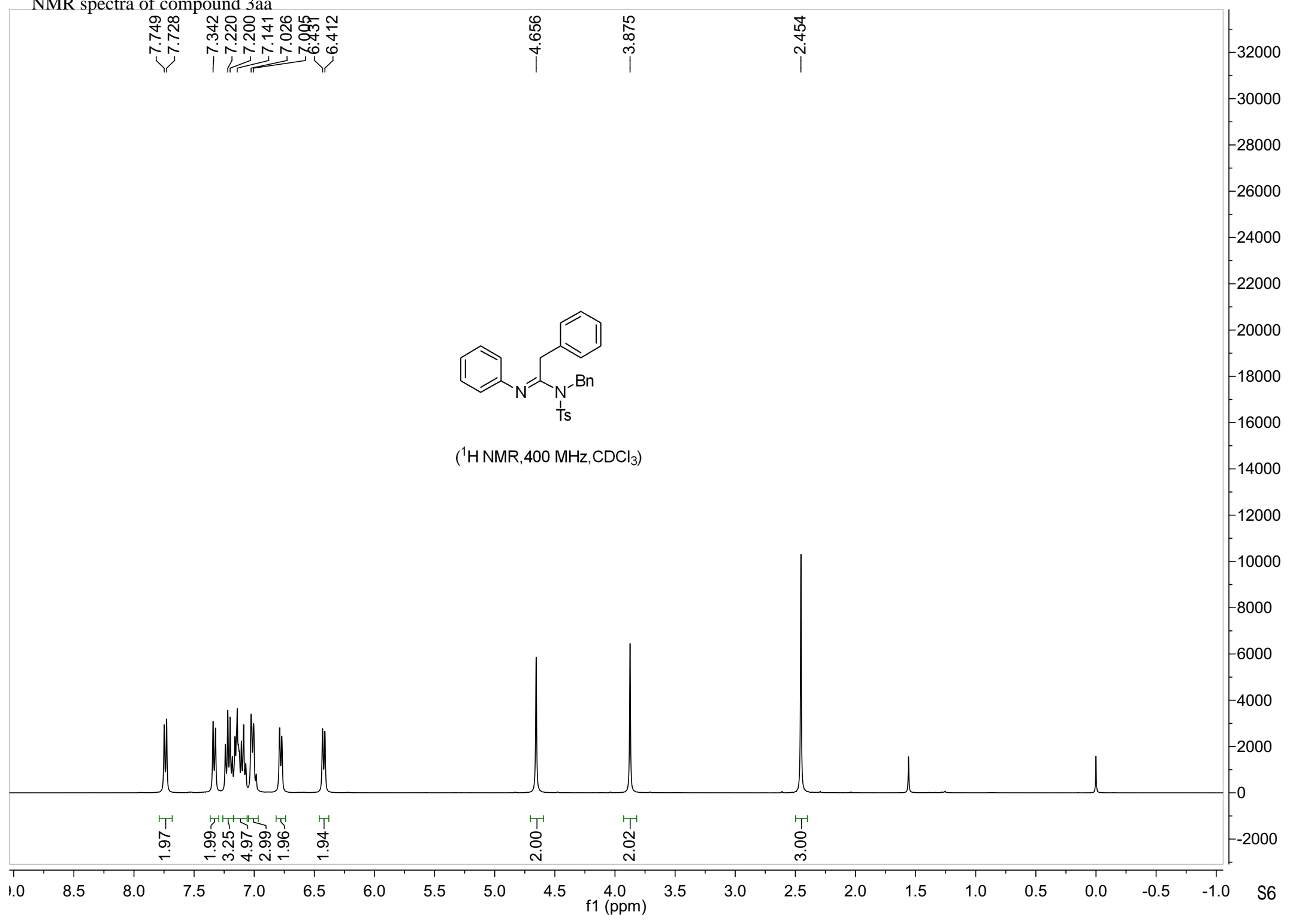
NMR spectra of compound 3aa

7.749
7.728
7.342
7.220
7.200
7.141
7.026
6.995
6.431
6.412

4.656
3.875
2.454



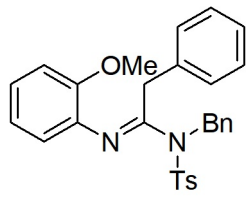
(¹H NMR, 400 MHz, CDCl₃)



NMR spectra of compound 3ba

7.838
7.818
7.327
7.307
7.119
7.046
7.026
6.782
6.764
6.330
6.327
6.311

4.621
3.851
3.750
2.435



(¹H NMR, 400 MHz, CDCl₃)

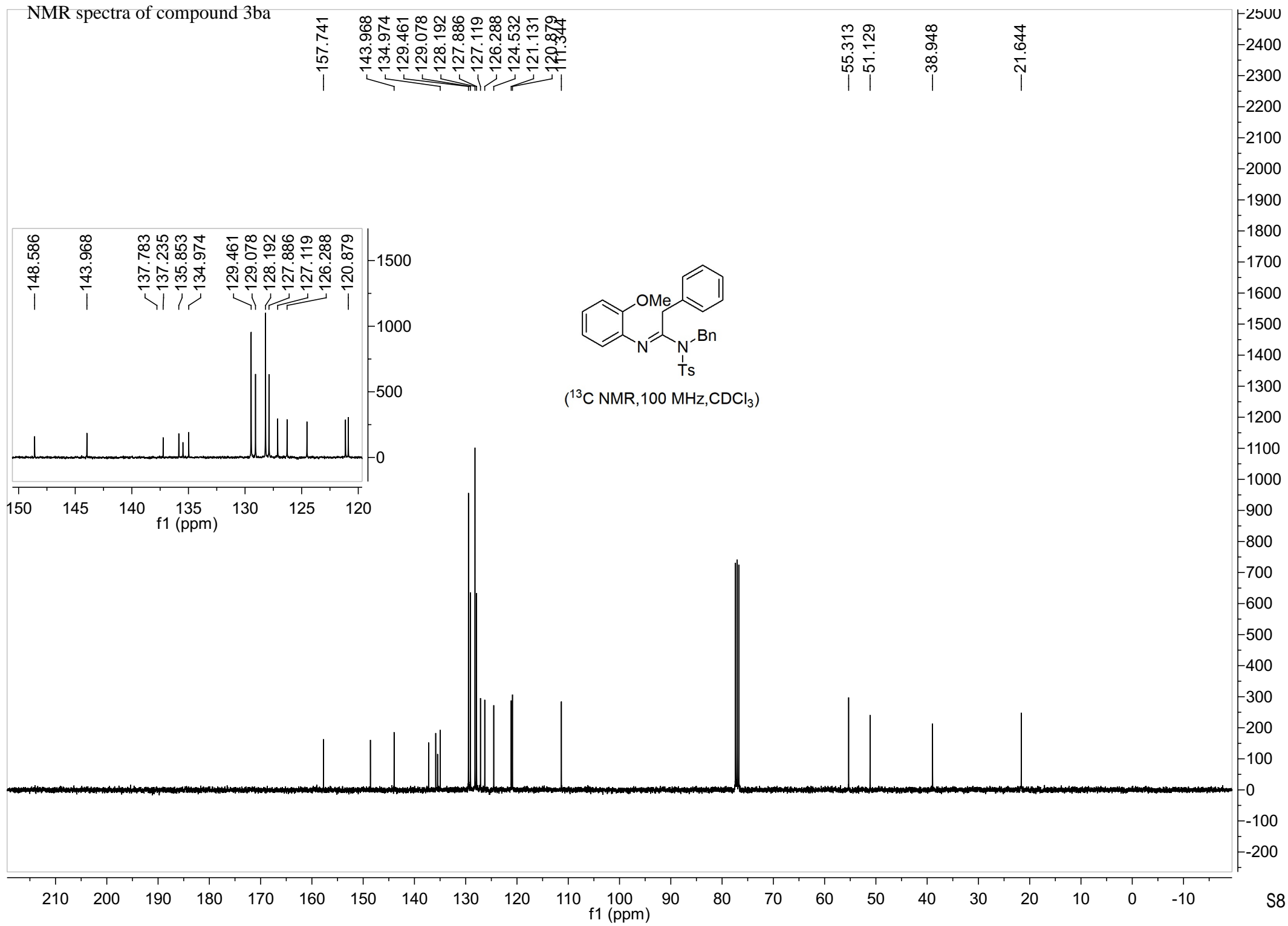
1.98
1.95
4.32
4.99
3.97
1.00

1.95
2.04
2.92
3.00

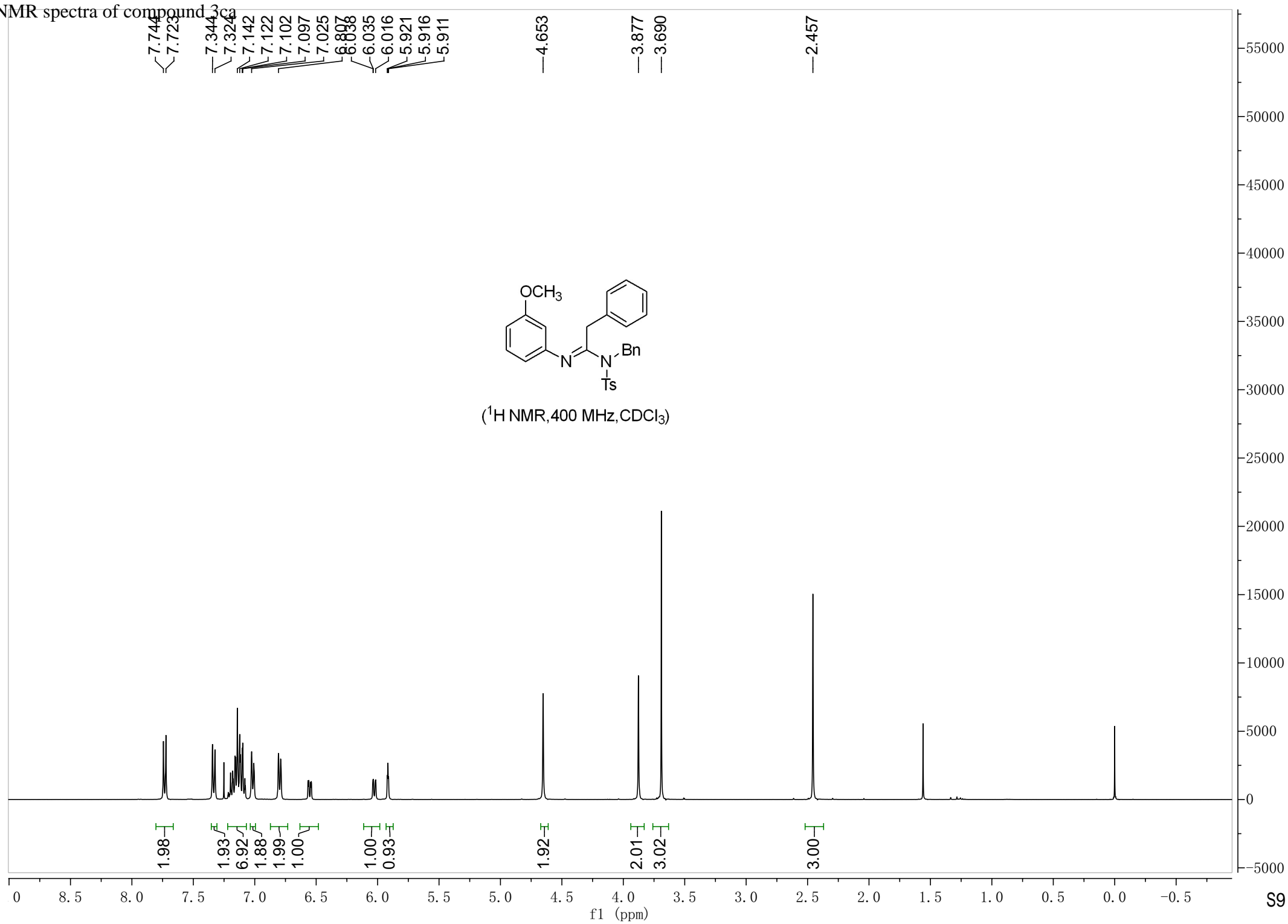
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 S7

36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000

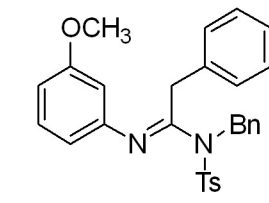
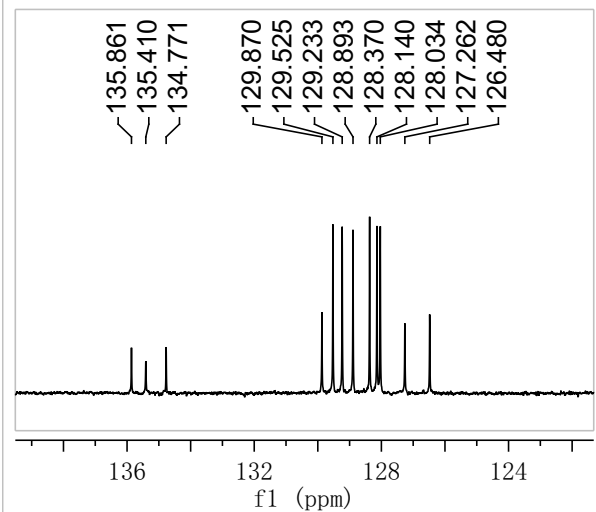
NMR spectra of compound 3ba



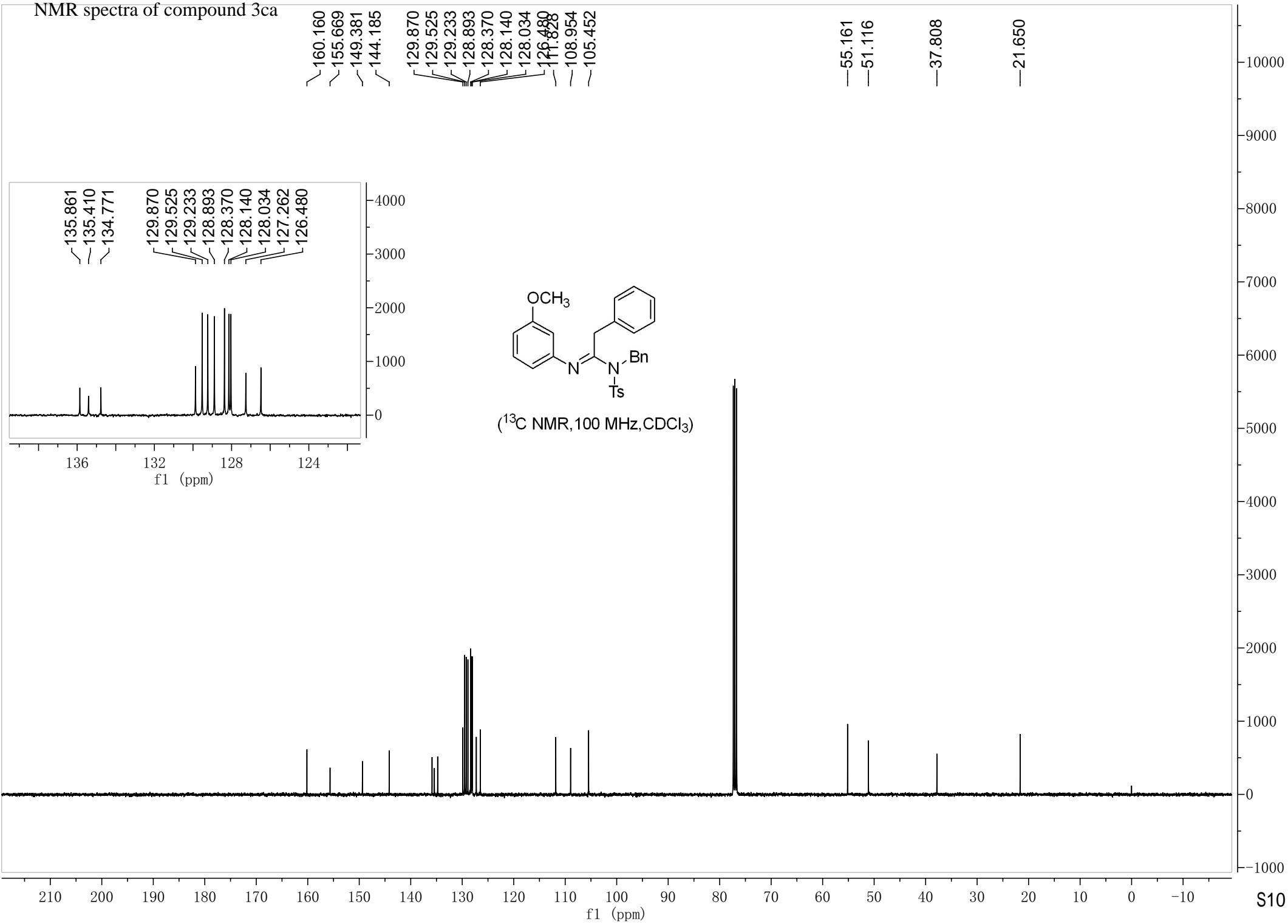
NMR spectra of compound 3ca



NMR spectra of compound 3ca



(¹³C NMR, 100 MHz, CDCl₃)



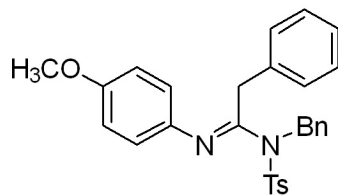
NMR spectra of compound 3da

7.741
7.721
7.337
7.131
7.083
6.792
6.776
6.368
6.368

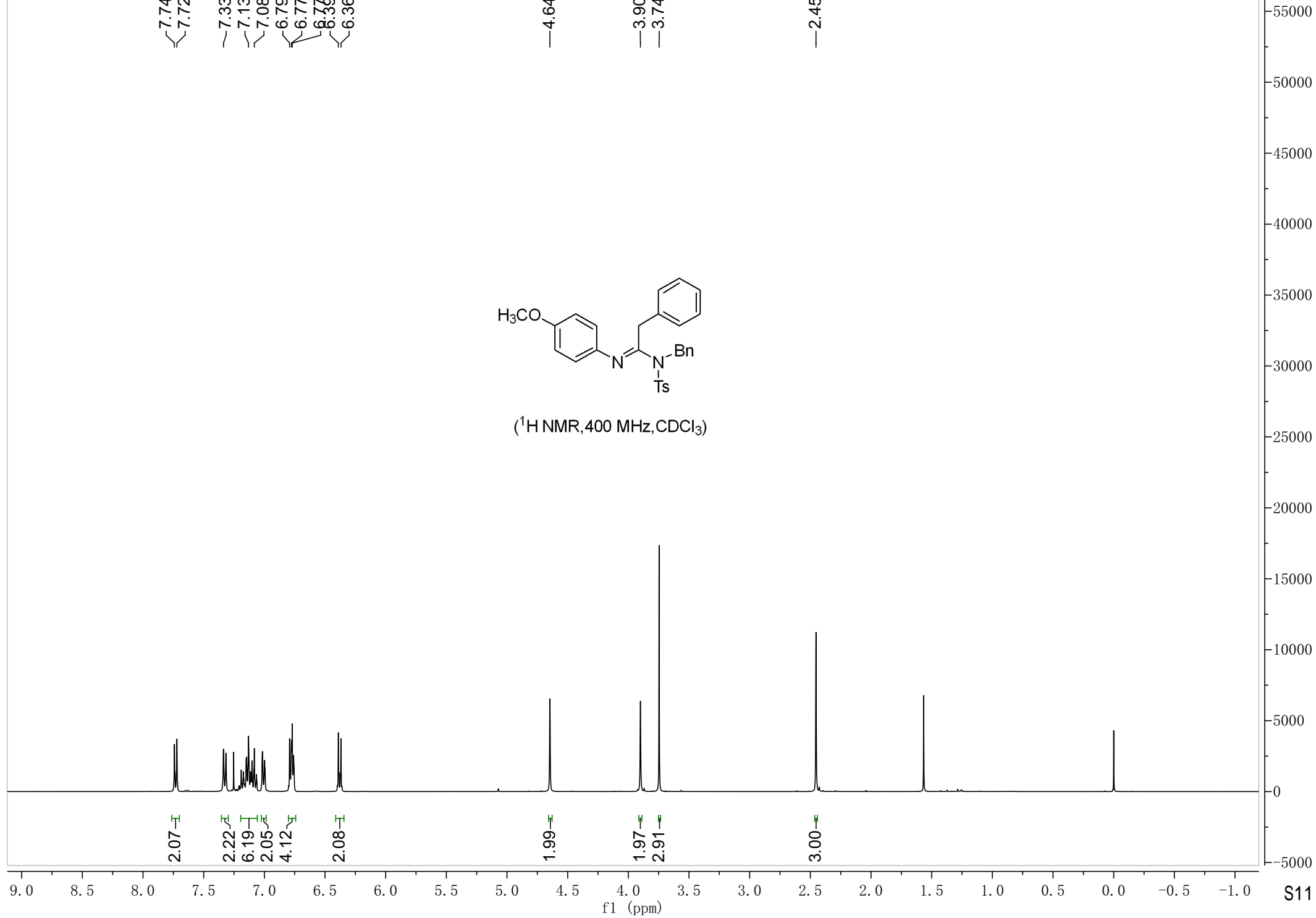
4.647

3.901
3.746

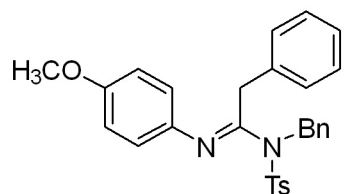
2.454



(¹H NMR, 400 MHz, CDCl₃)



NMR spectra of compound 3da



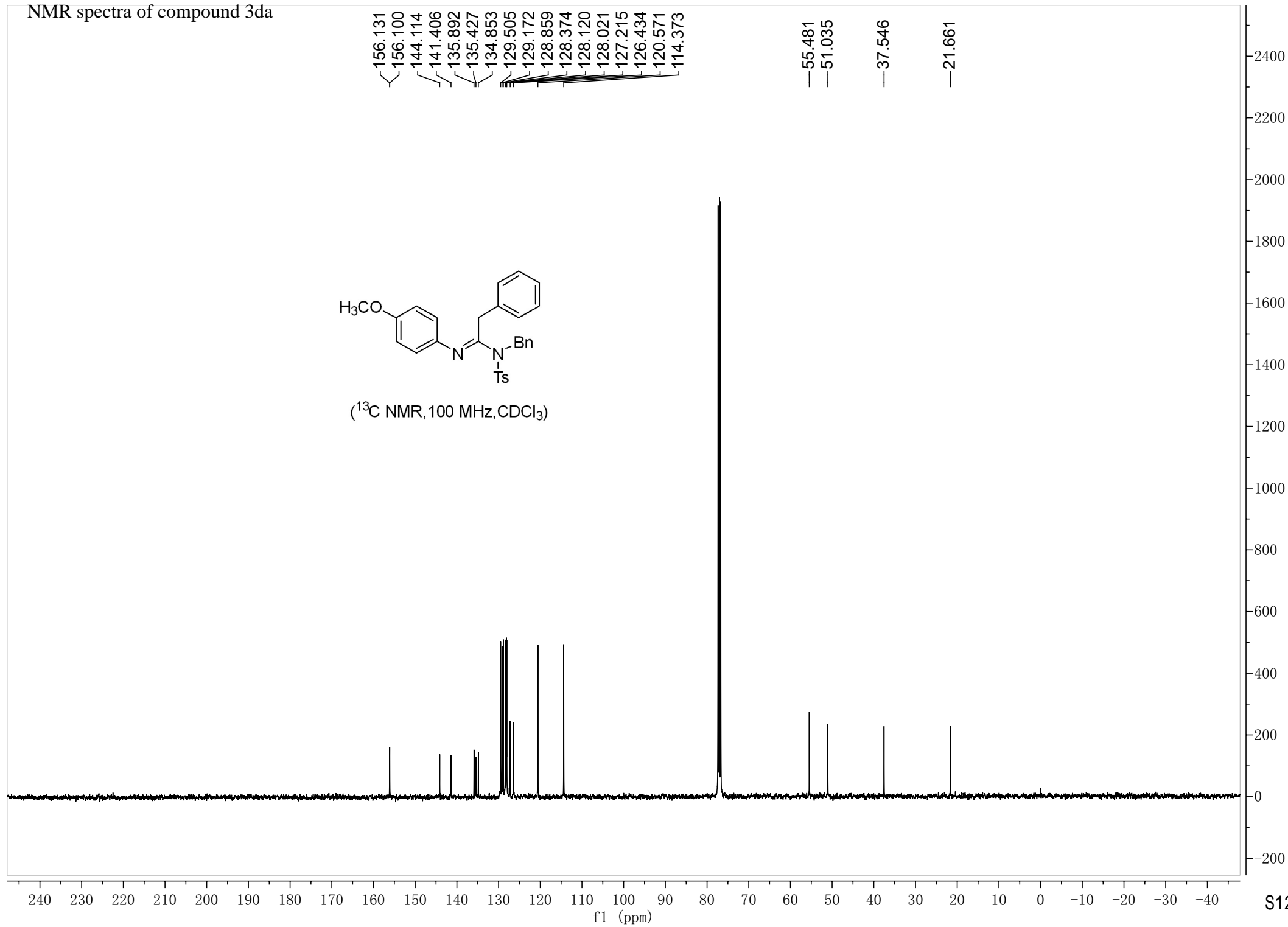
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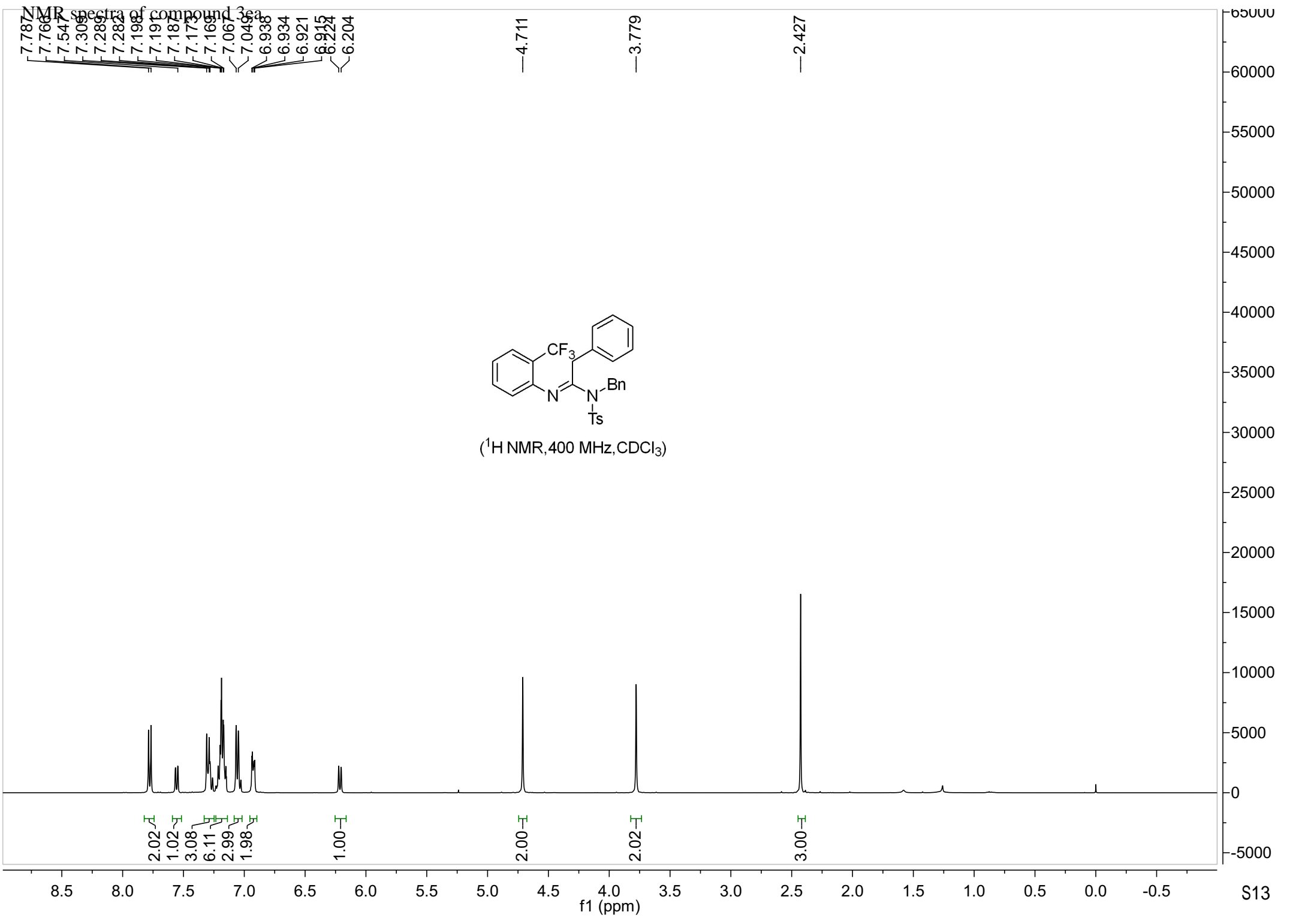
156.131
156.100
144.114
141.406
135.892
135.427
134.853
129.505
129.172
128.859
128.374
128.120
128.021
127.215
126.434
120.571
114.373

55.481
51.035

37.546

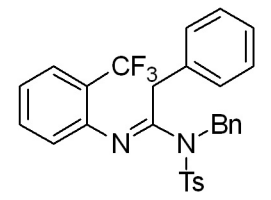
21.661



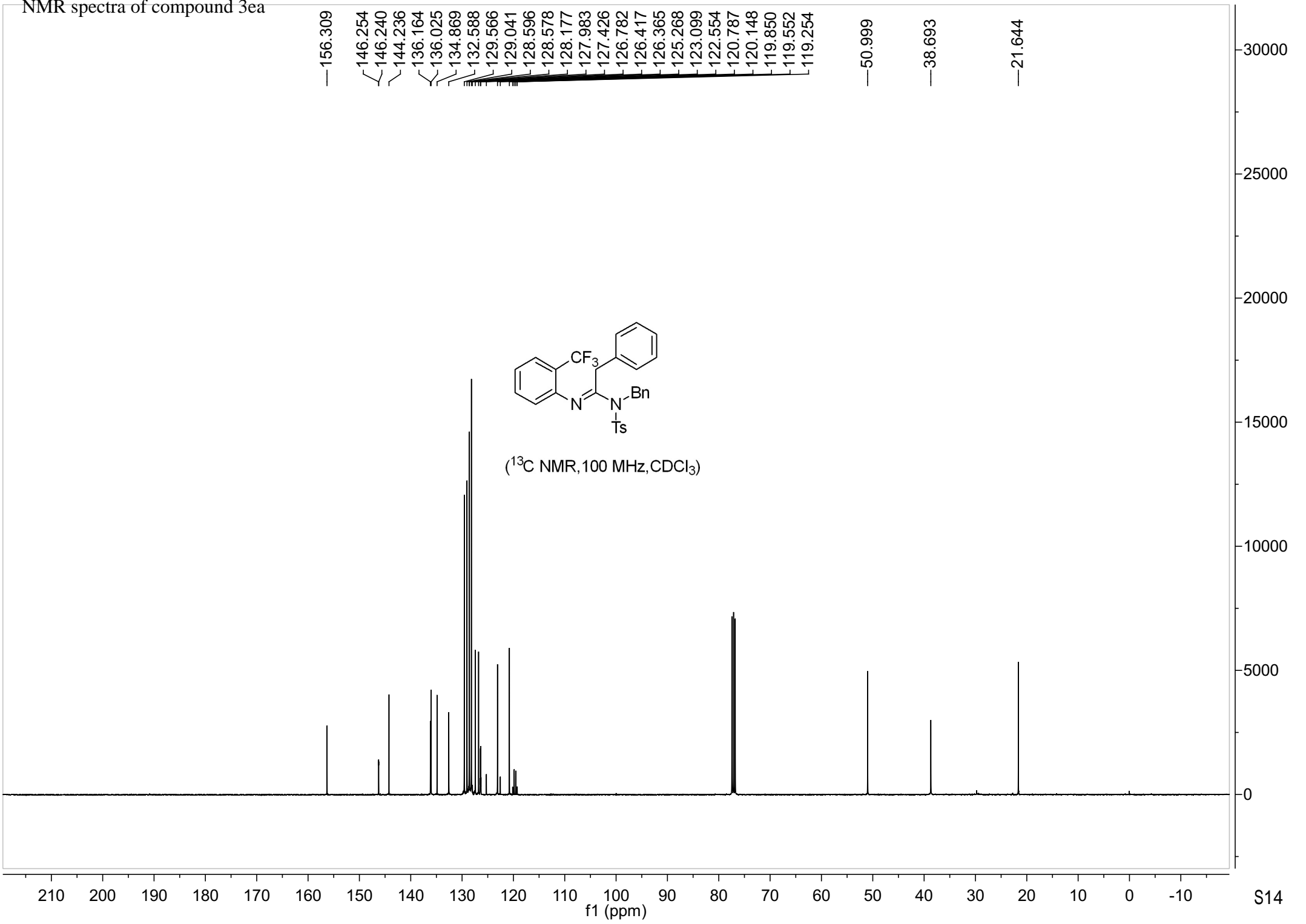


NMR spectra of compound 3ea

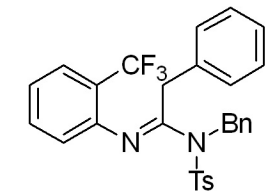
156.309
 146.254
 146.240
 144.236
 136.164
 136.025
 134.869
 132.588
 129.566
 129.041
 128.596
 128.578
 128.177
 127.983
 127.426
 126.782
 126.417
 126.365
 125.268
 123.099
 122.554
 120.787
 120.148
 119.850
 119.552
 119.254
 50.999
 38.693
 21.644



(¹³C NMR, 100 MHz, CDCl₃)

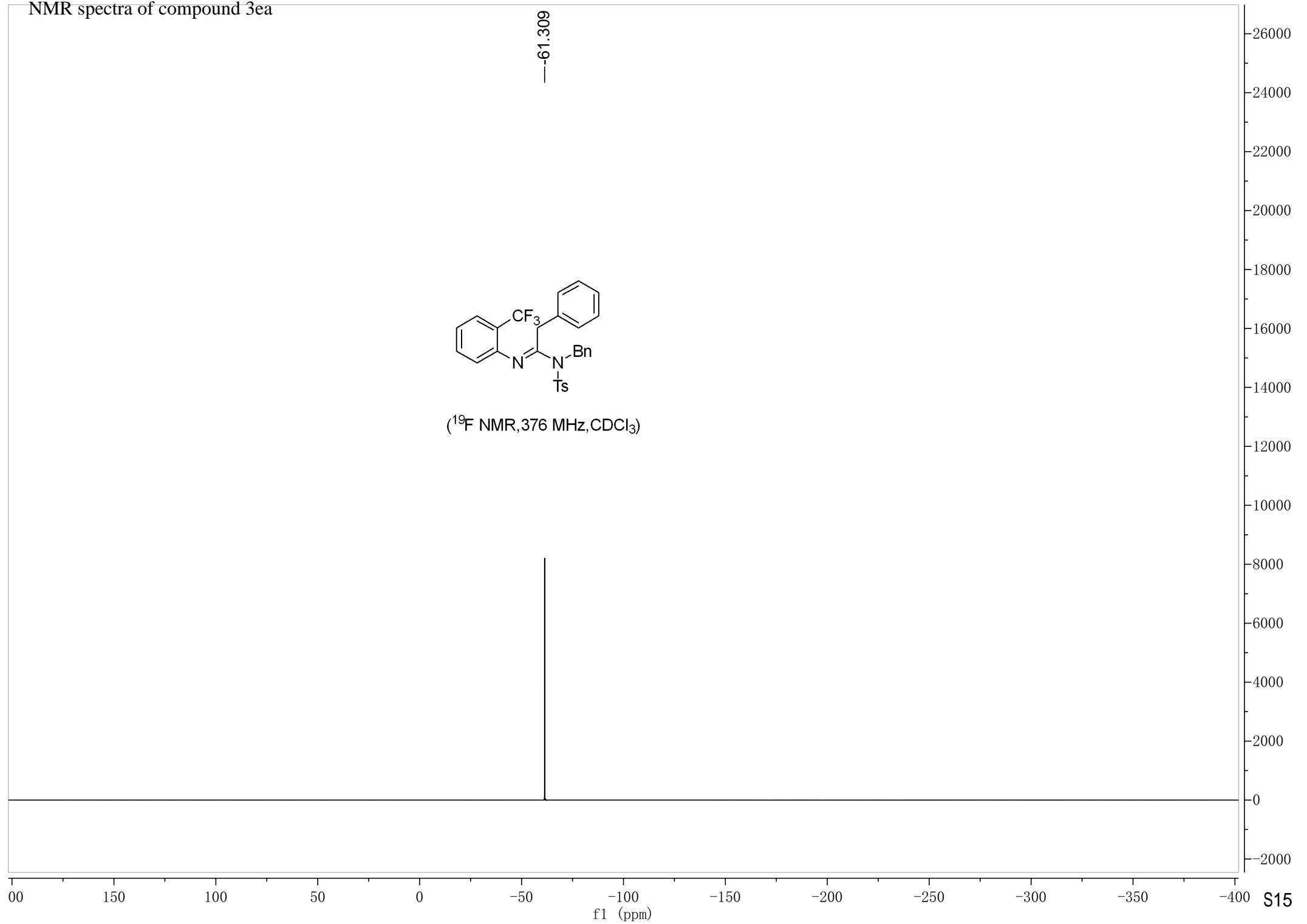


NMR spectra of compound 3ea



(¹⁹F NMR, 376 MHz, CDCl₃)

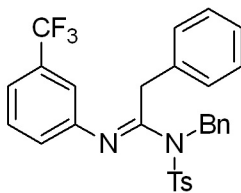
--61.309



NMR spectra of compound 3fa

7.750
7.730
7.357
7.196
7.106
6.986
6.753
6.540

4.732
3.825
2.473



(¹H NMR, 400 MHz, CDCl₃)

1.98

1.98

1.03

5.17

3.88

2.00

1.94

1.99

2.02

3.00

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 -0.5 -1.0 S16

f1 (ppm)

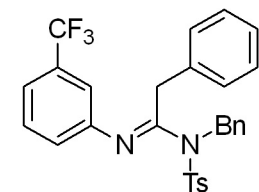
NMR spectra of compound 3fa

156.375
148.379
144.468
135.910
135.536
134.267
131.839
131.520
131.198
129.569
129.522
128.894
128.610
128.533
128.228
128.205
127.497
126.763
125.206
122.795
122.499
120.073
116.601
116.566

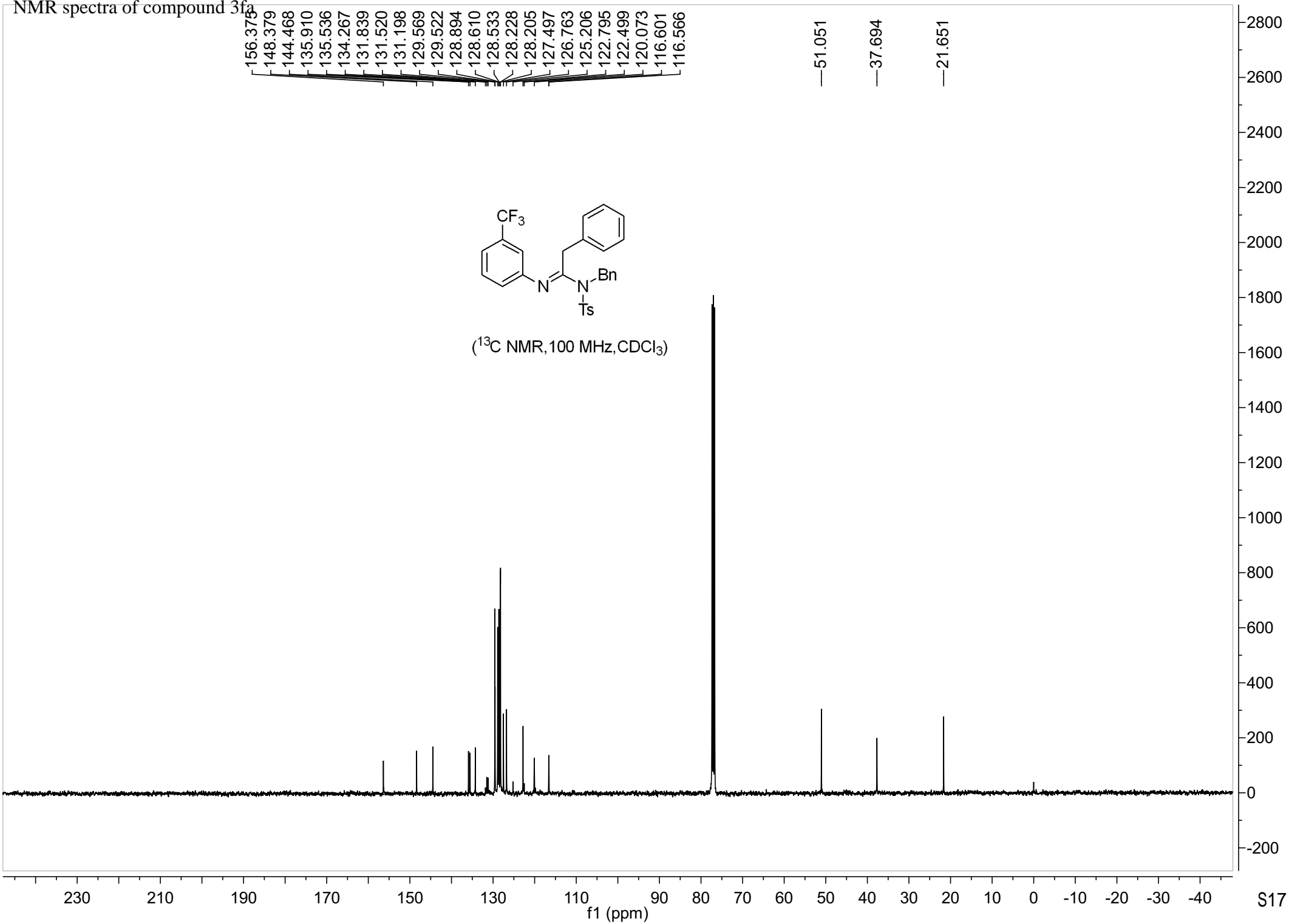
—51.051

—37.694

—21.651

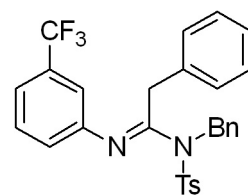


(¹³C NMR, 100 MHz, CDCl₃)

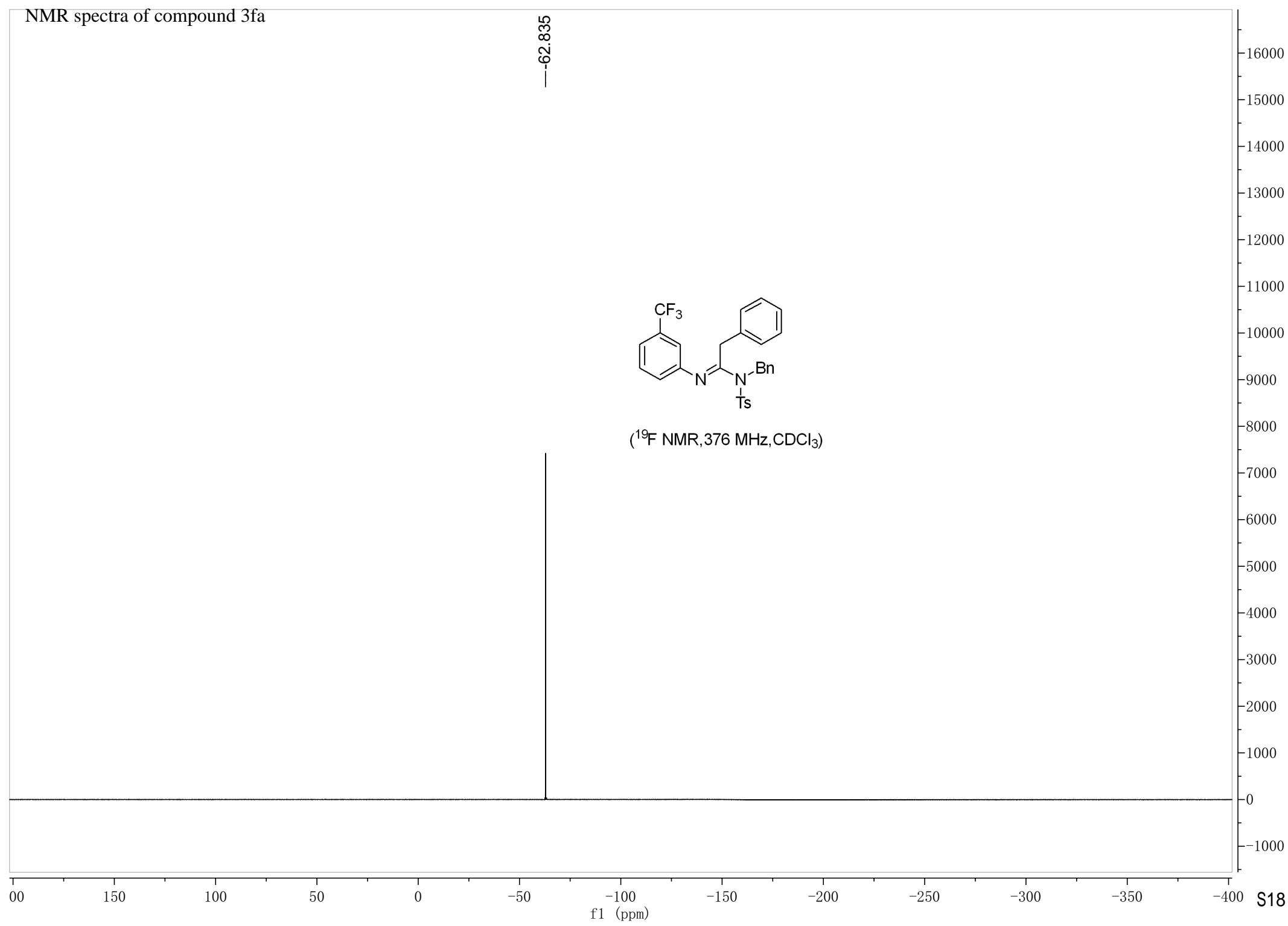


NMR spectra of compound 3fa

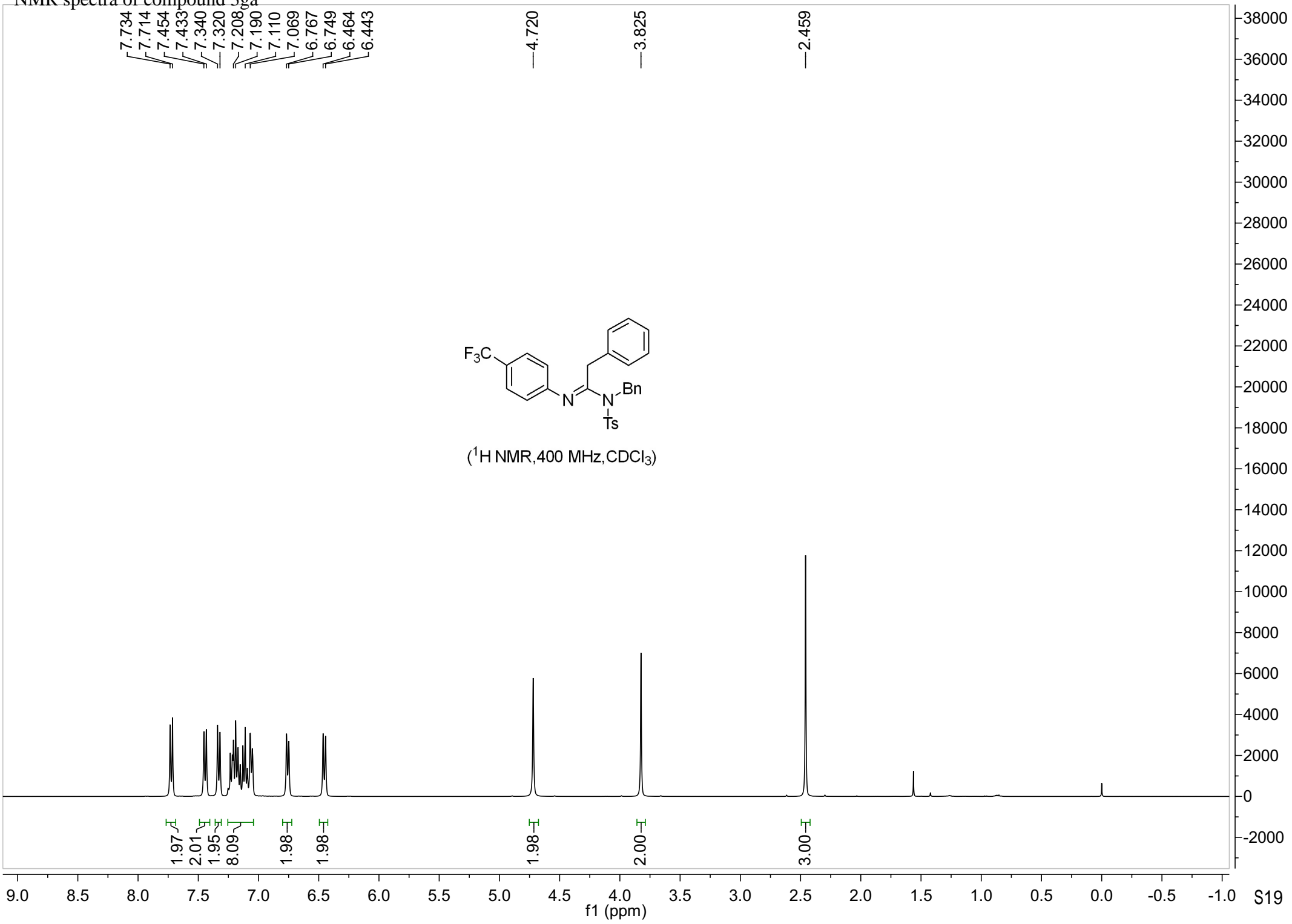
---62.835



(¹⁹F NMR, 376 MHz, CDCl₃)



NMR spectra of compound 3ga



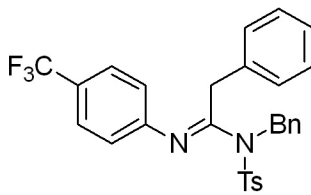
NMR spectra of compound 3ga

155.791
151.079
144.456
135.933
135.552
134.347
129.575
128.919
128.605
128.569
128.241
128.214
127.497
126.784
126.284
126.250
126.064
125.739
125.665
125.414
125.090
122.967
119.719

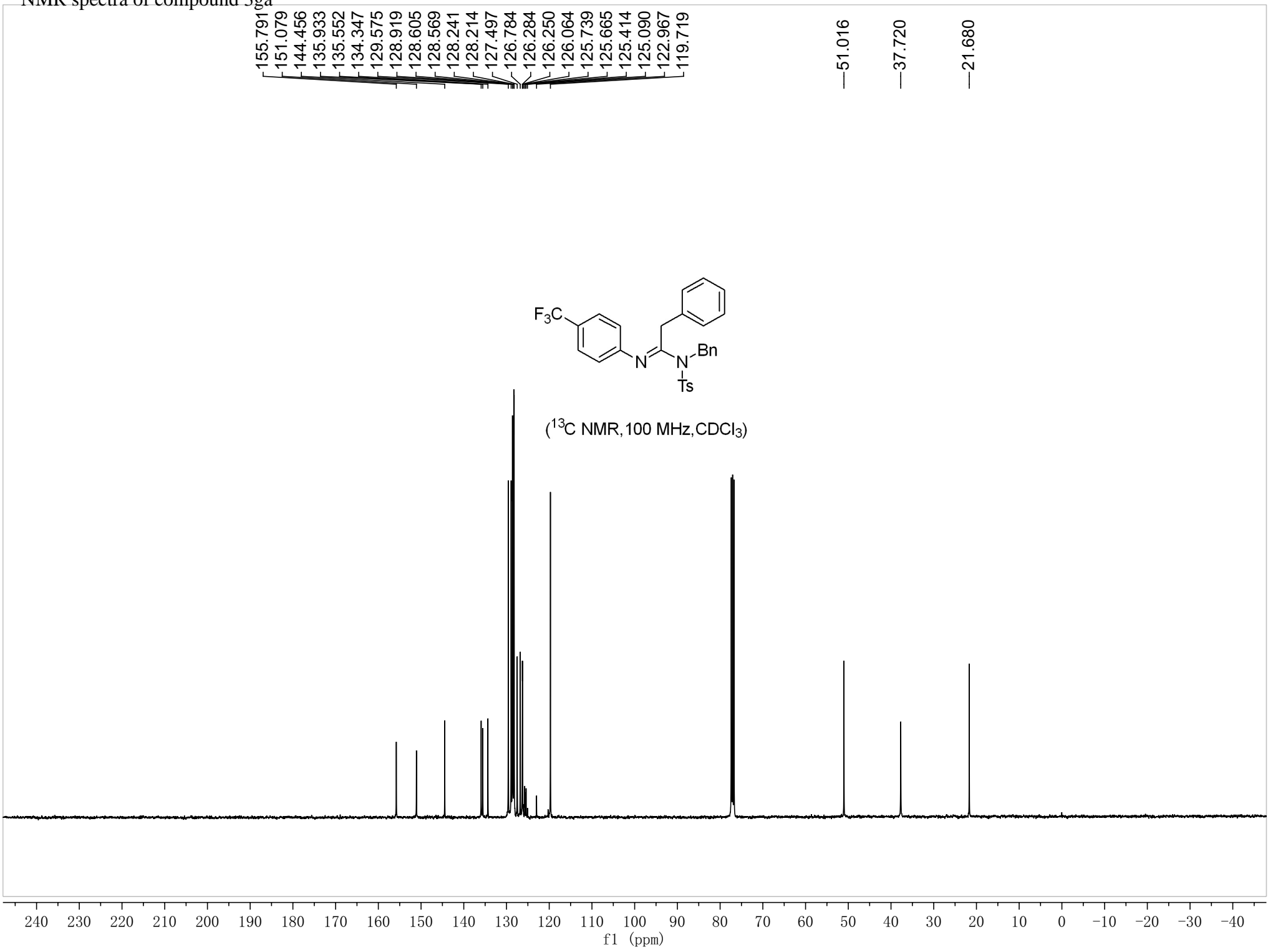
—51.016

—37.720

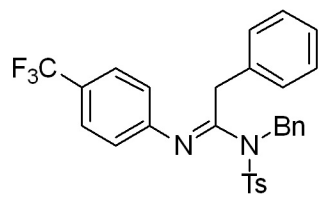
—21.680



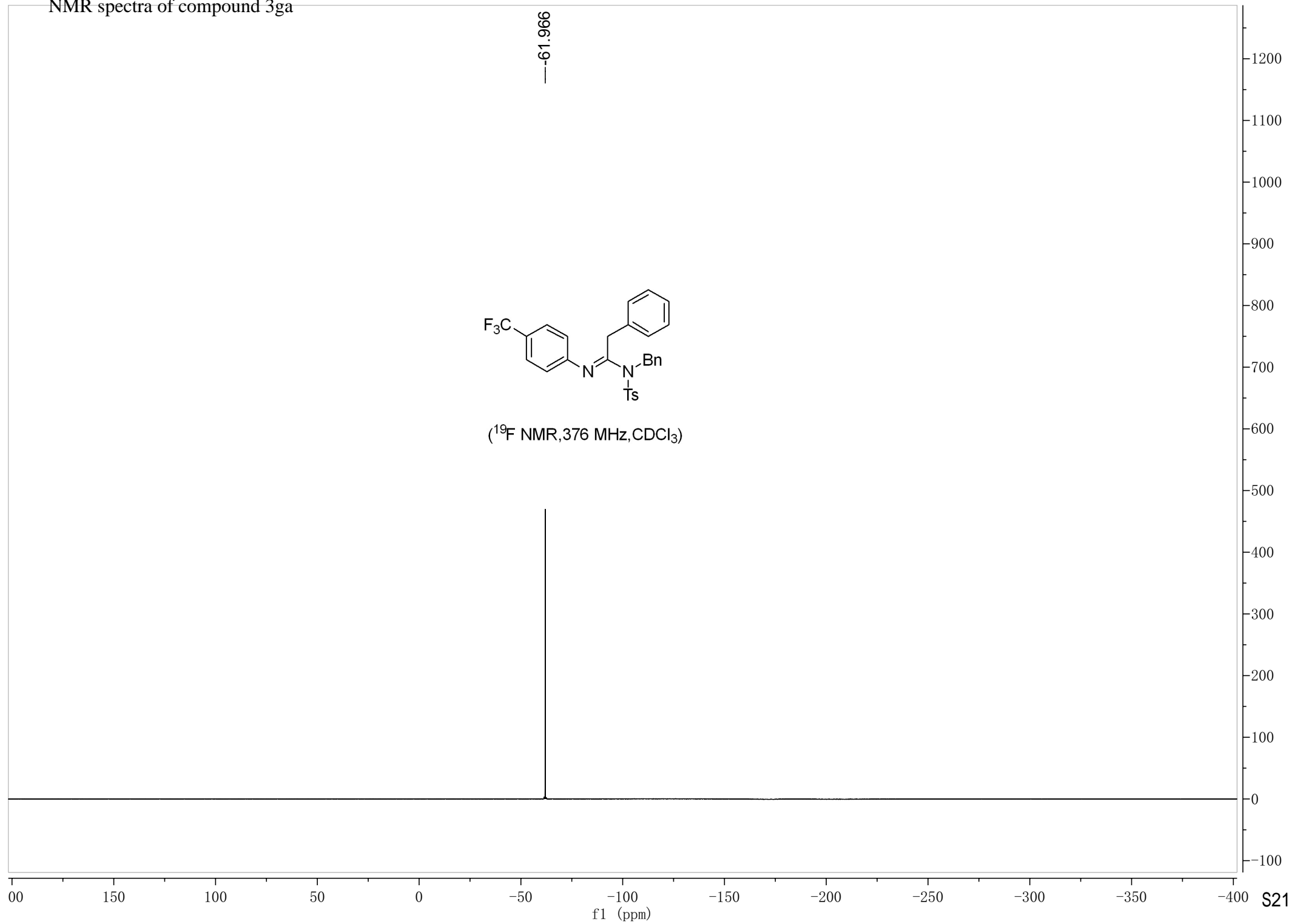
(¹³C NMR, 100 MHz, CDCl₃)



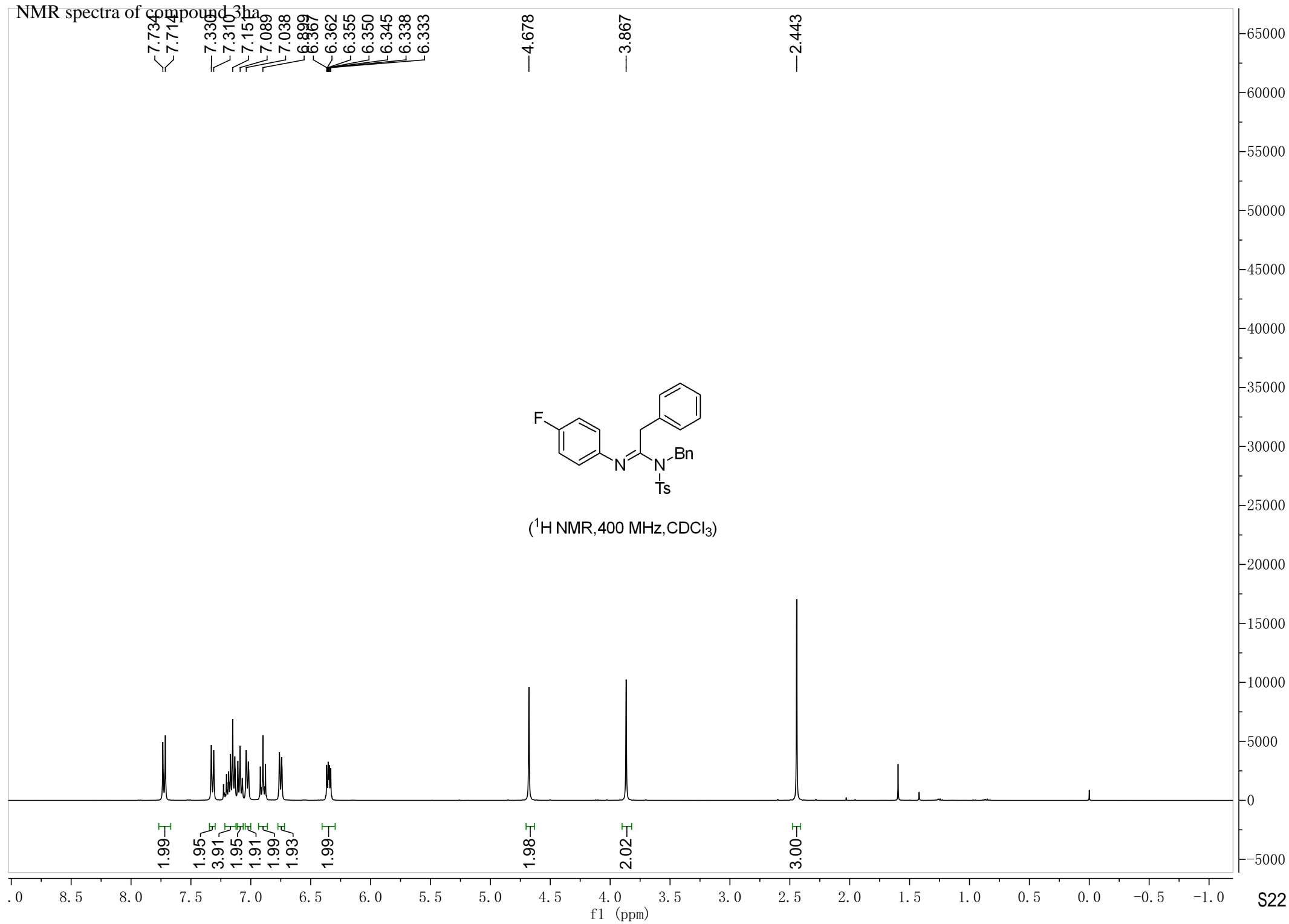
NMR spectra of compound 3ga



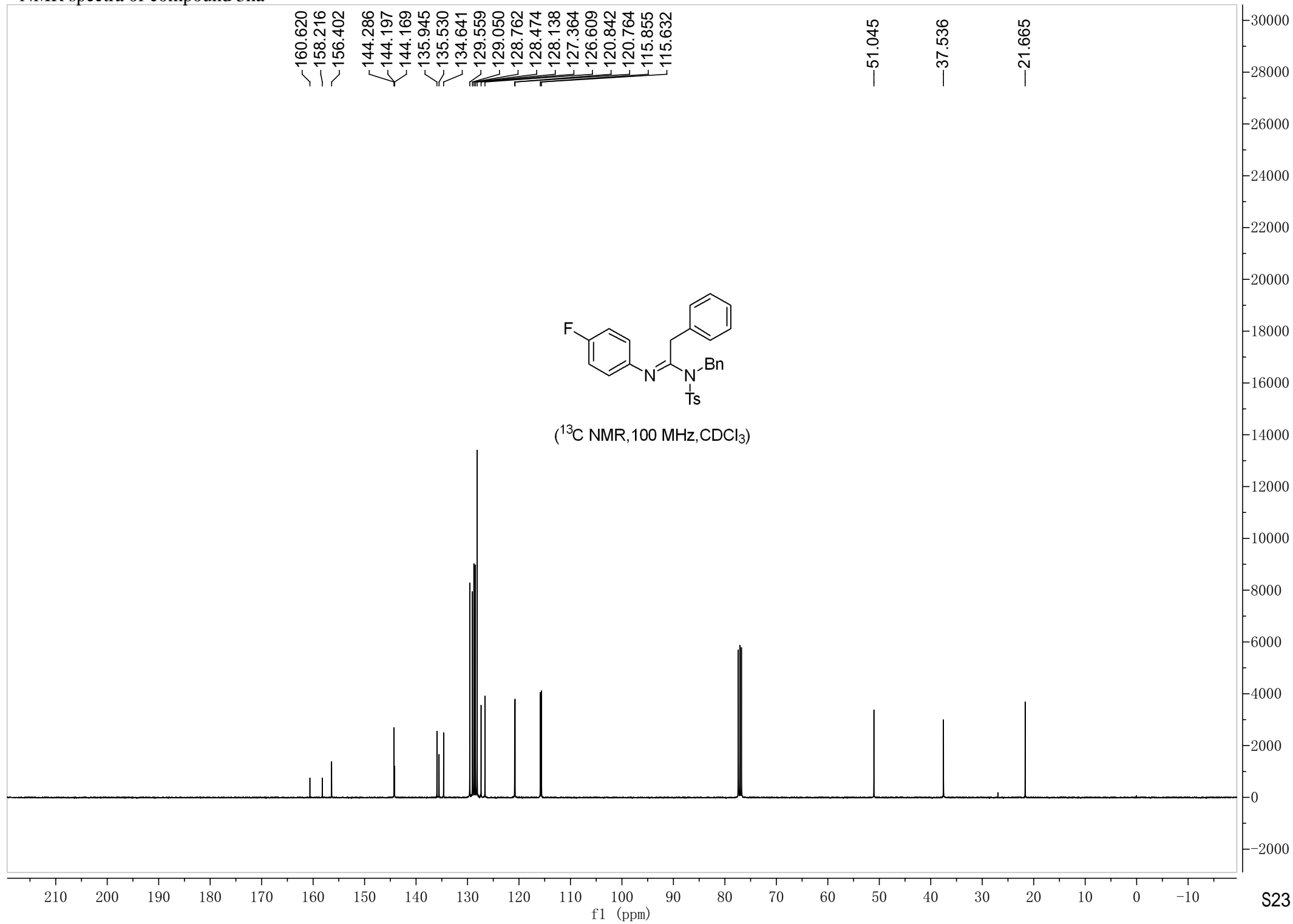
(¹⁹F NMR, 376 MHz, CDCl₃)



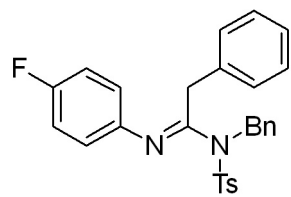
NMR spectra of compound 3ha



NMR spectra of compound 3ha

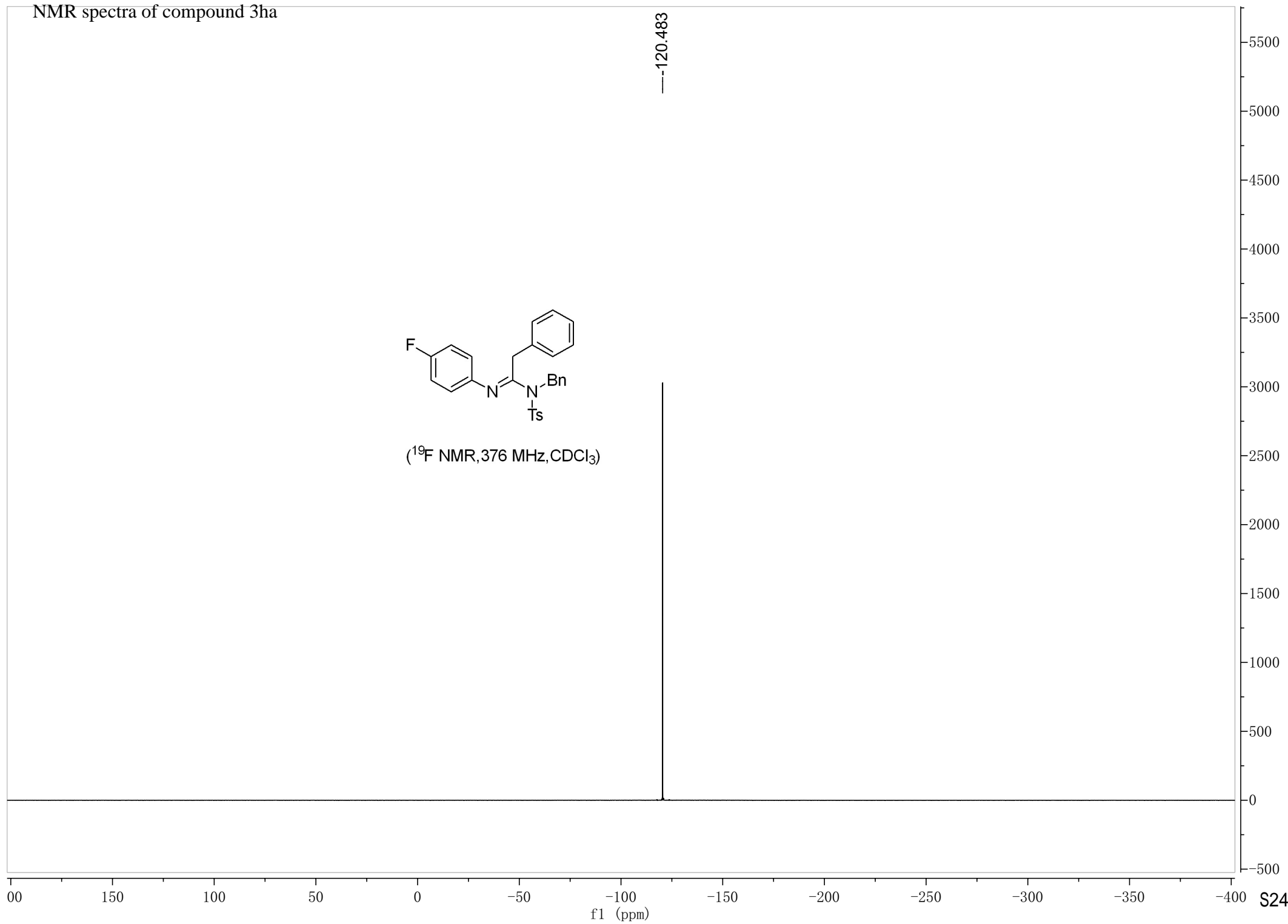


NMR spectra of compound 3ha



(¹⁹F NMR, 376 MHz, CDCl₃)

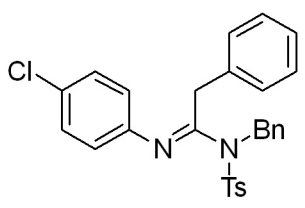
---120.483



NMR spectra of compound 3ia

7.729
7.708
7.338
7.318
7.181a
7.176
7.163
7.155
7.104
6.358
6.317

4.683
3.845
2.461



(¹H NMR, 400 MHz, CDCl₃)

1.94
1.93
5.84
1.98
1.88
1.95
1.93

1.95

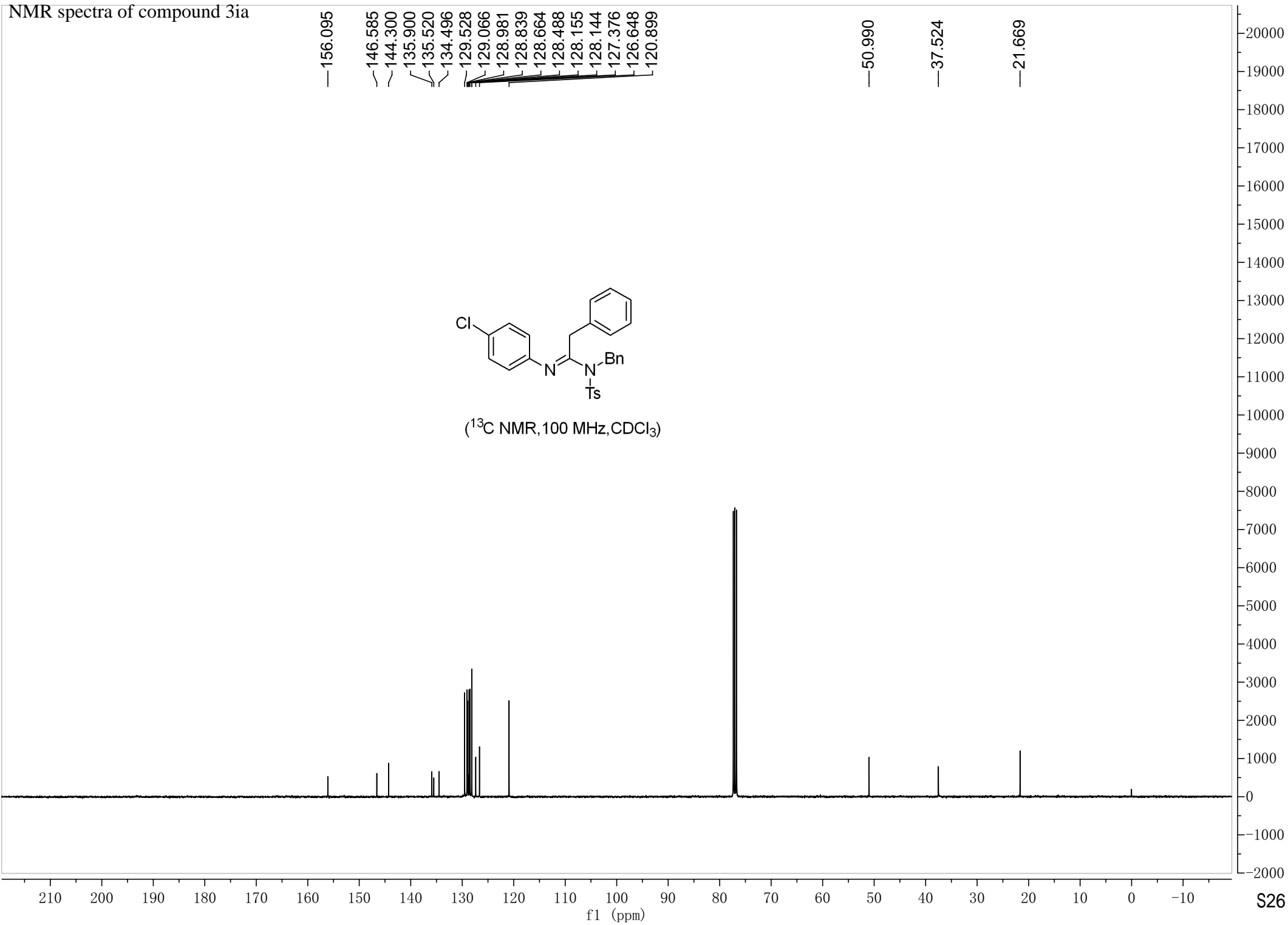
1.99

3.00

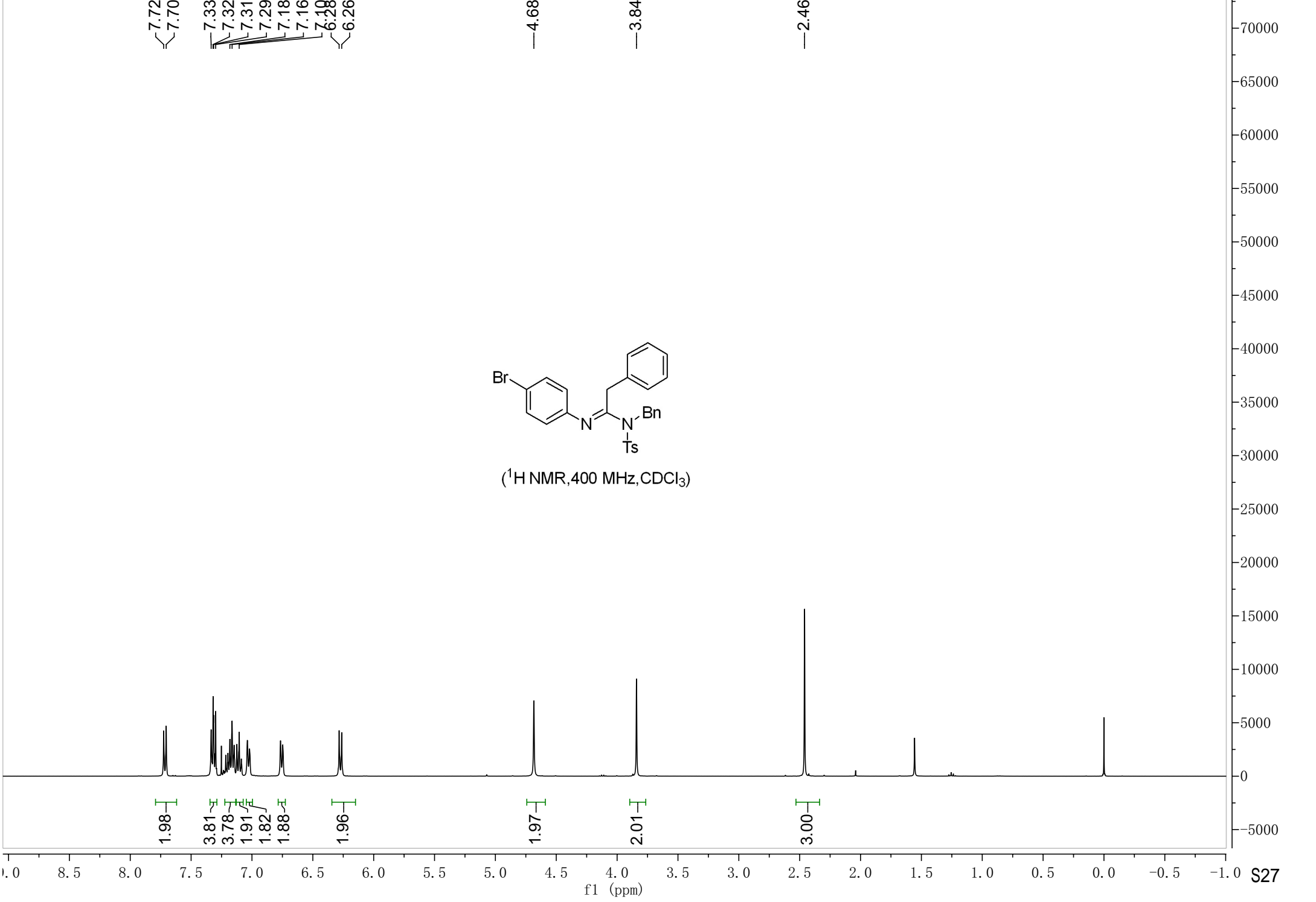
0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

f1 (ppm)

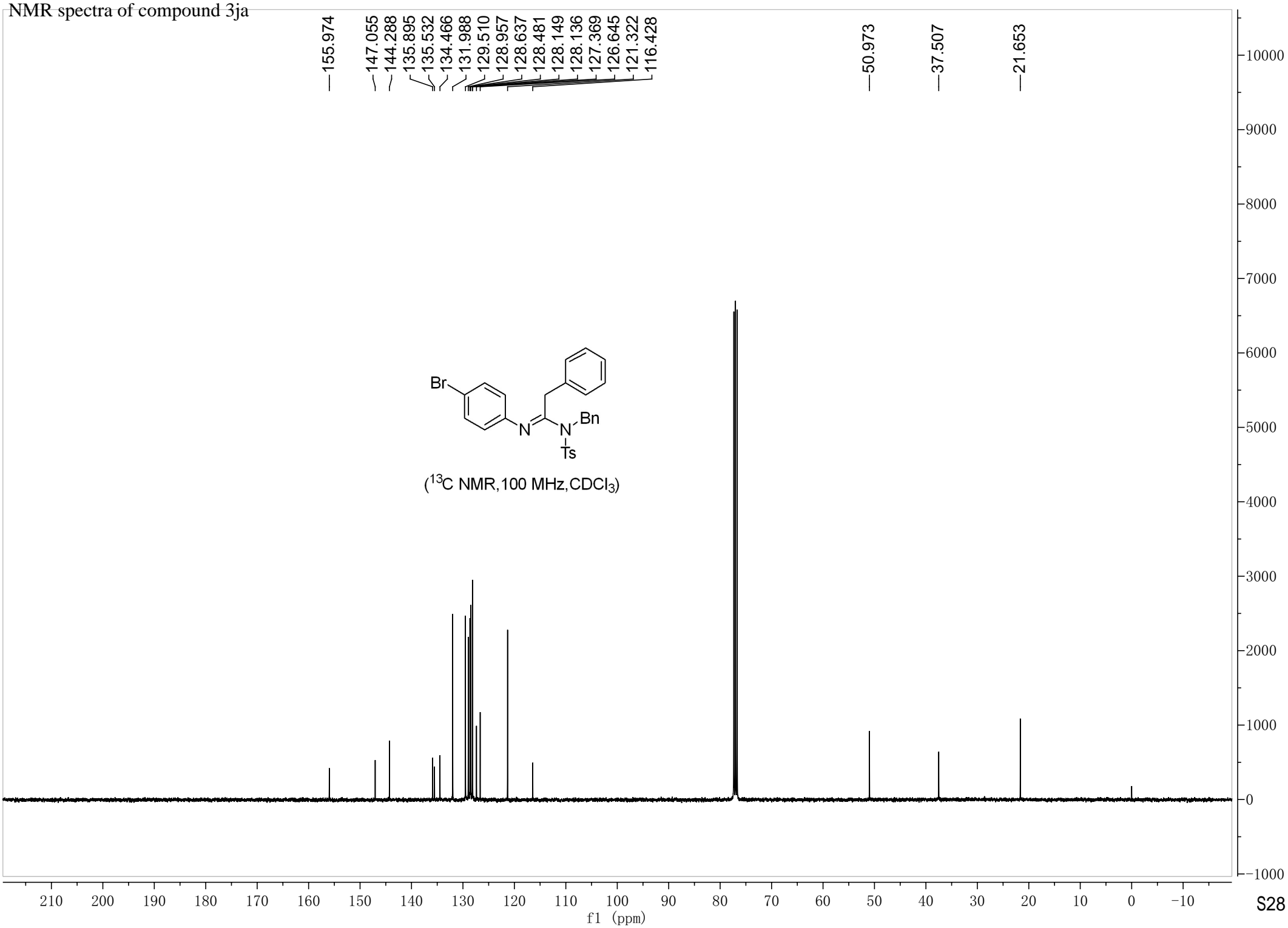
NMR spectra of compound 3ia



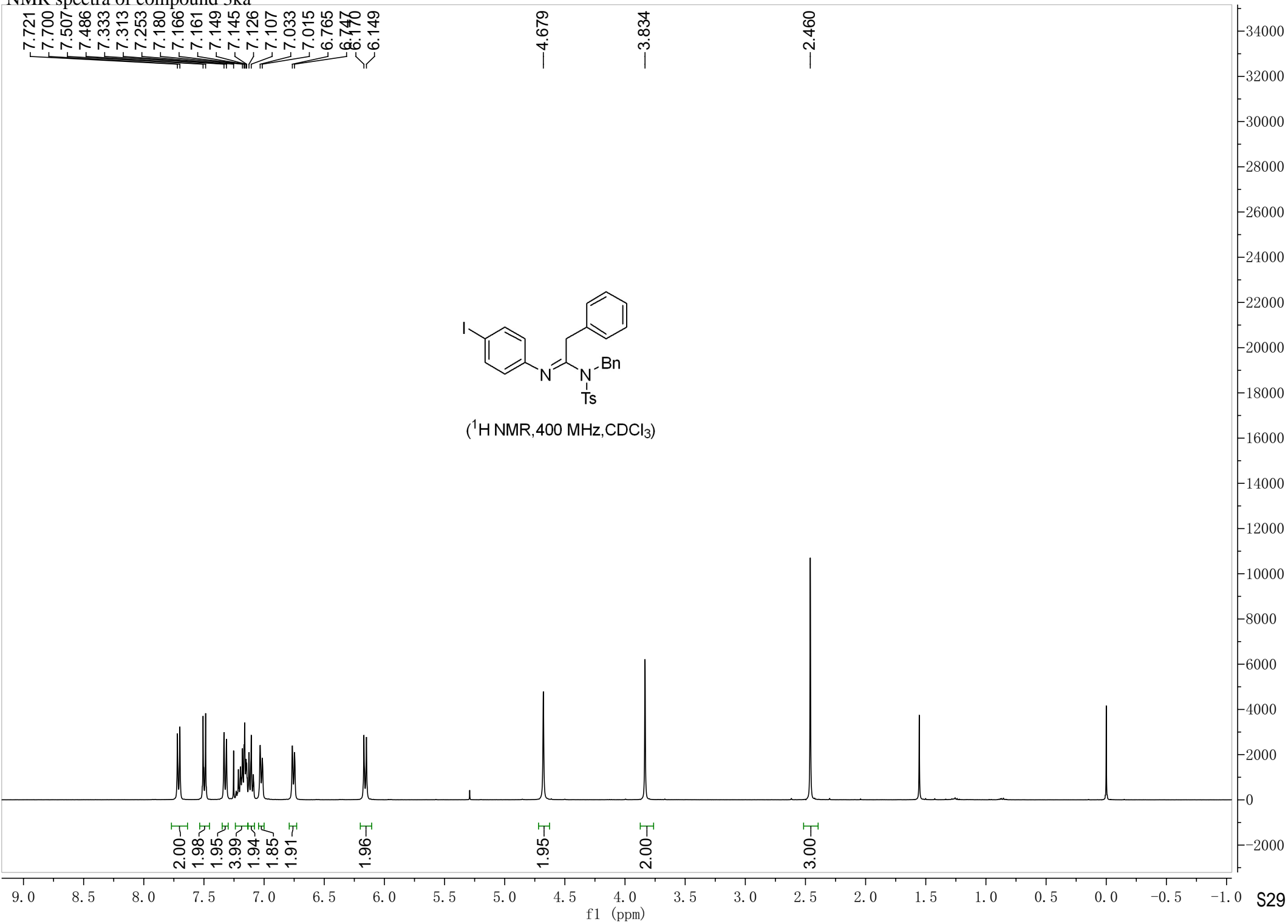
NMR spectra of compound



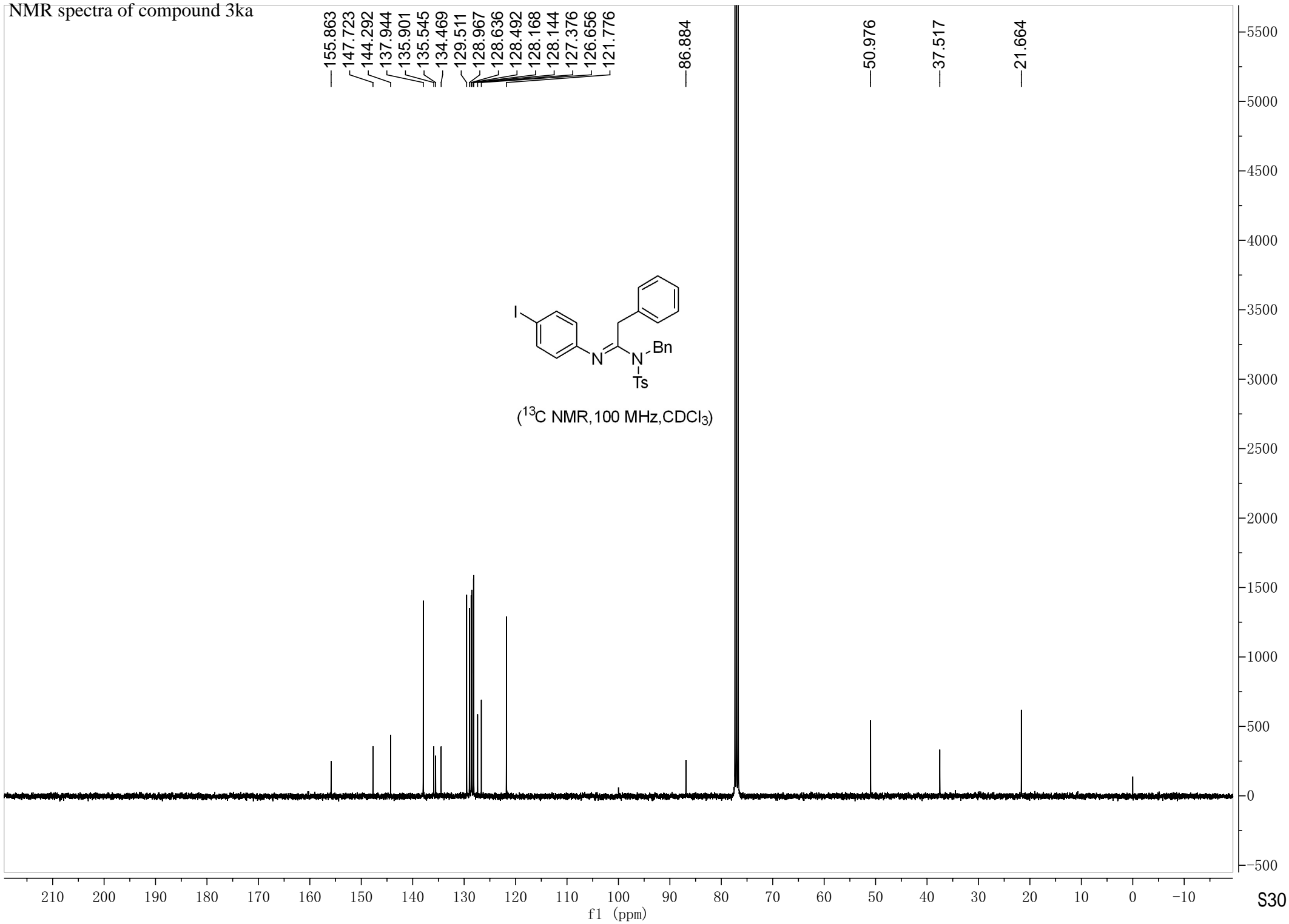
NMR spectra of compound 3ja



NMR spectra of compound 3ka



NMR spectra of compound 3ka



NMR spectra of compound 3la

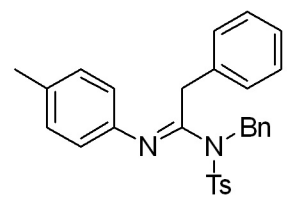
7.742
7.721
7.335
7.147
7.128
7.084
7.039
7.018
6.913
6.947
6.327

4.641

3.879

2.451

2.268



(¹H NMR, 400 MHz, CDCl₃)

1.97

1.95

5.83

3.91

1.95

1.97

1.92

2.00

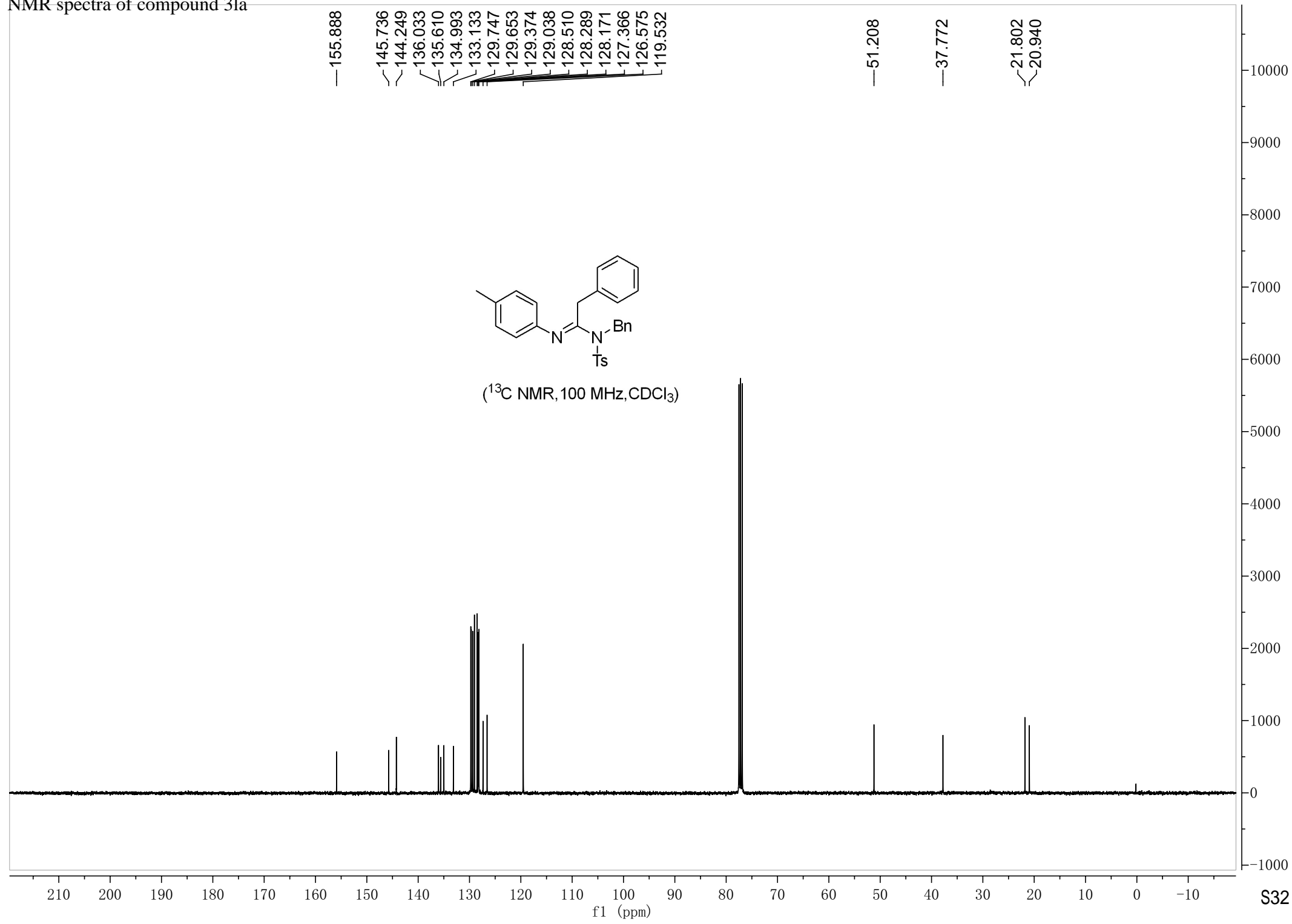
3.01

3.00

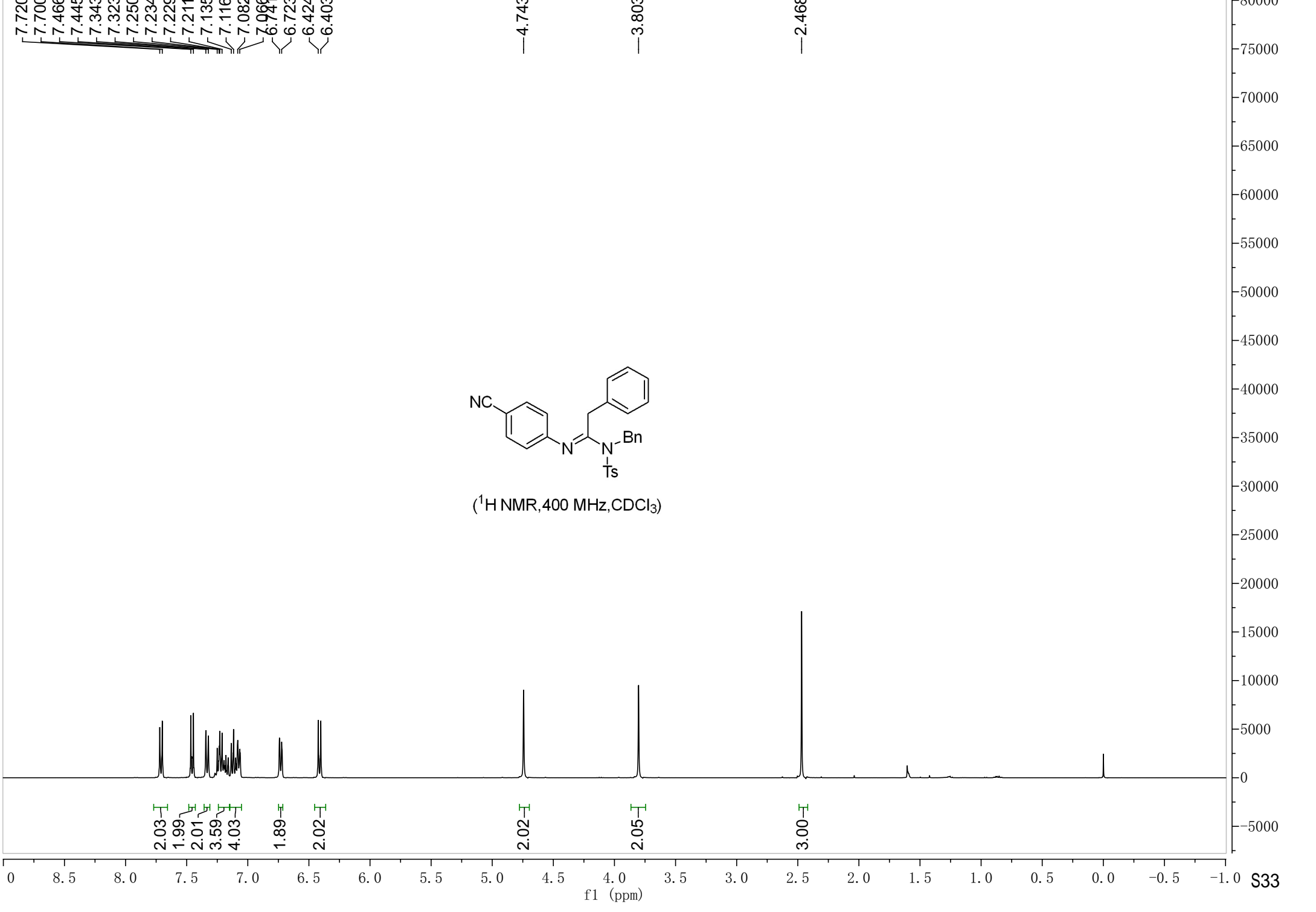
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

f1 (ppm)

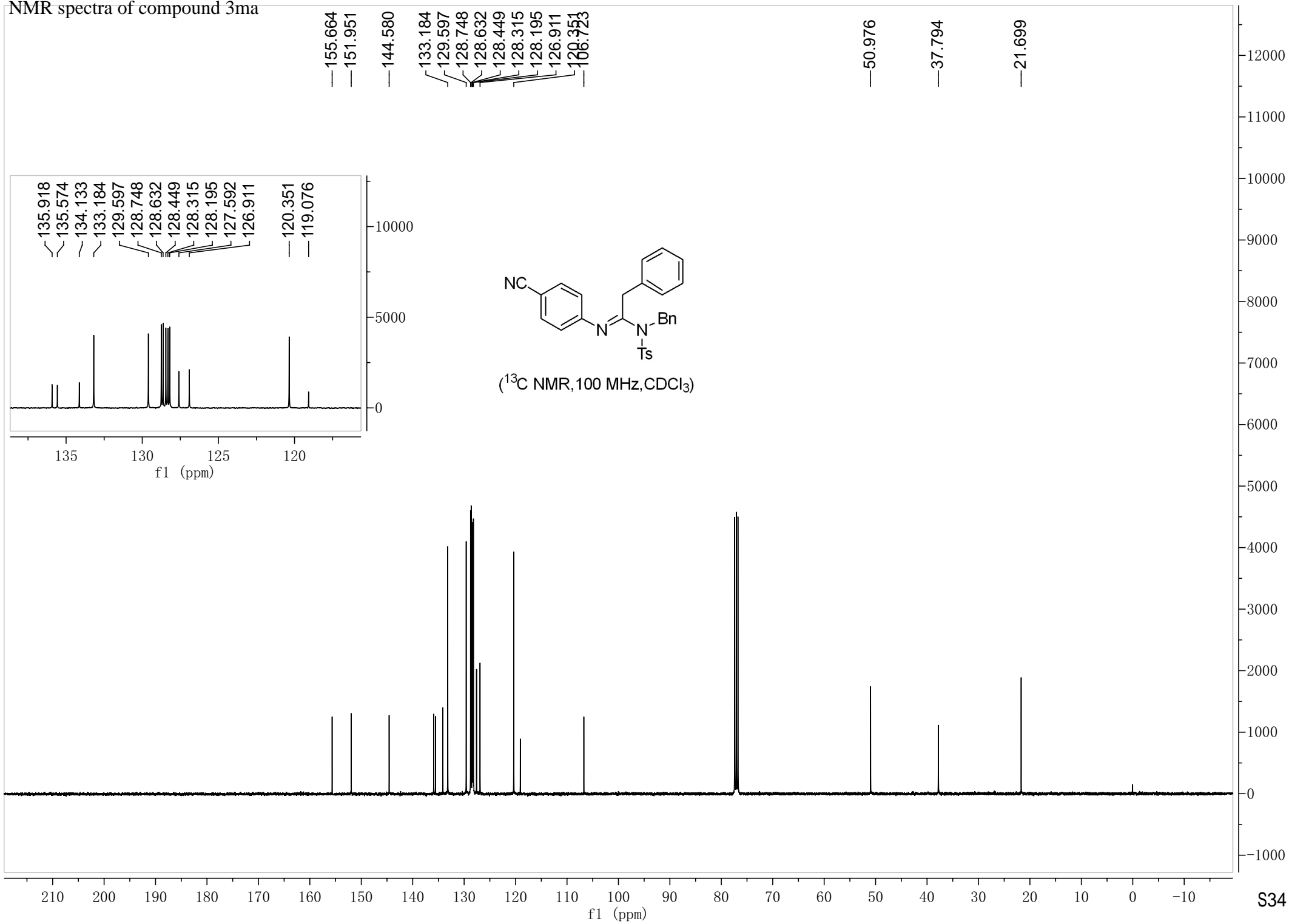
NMR spectra of compound 3la



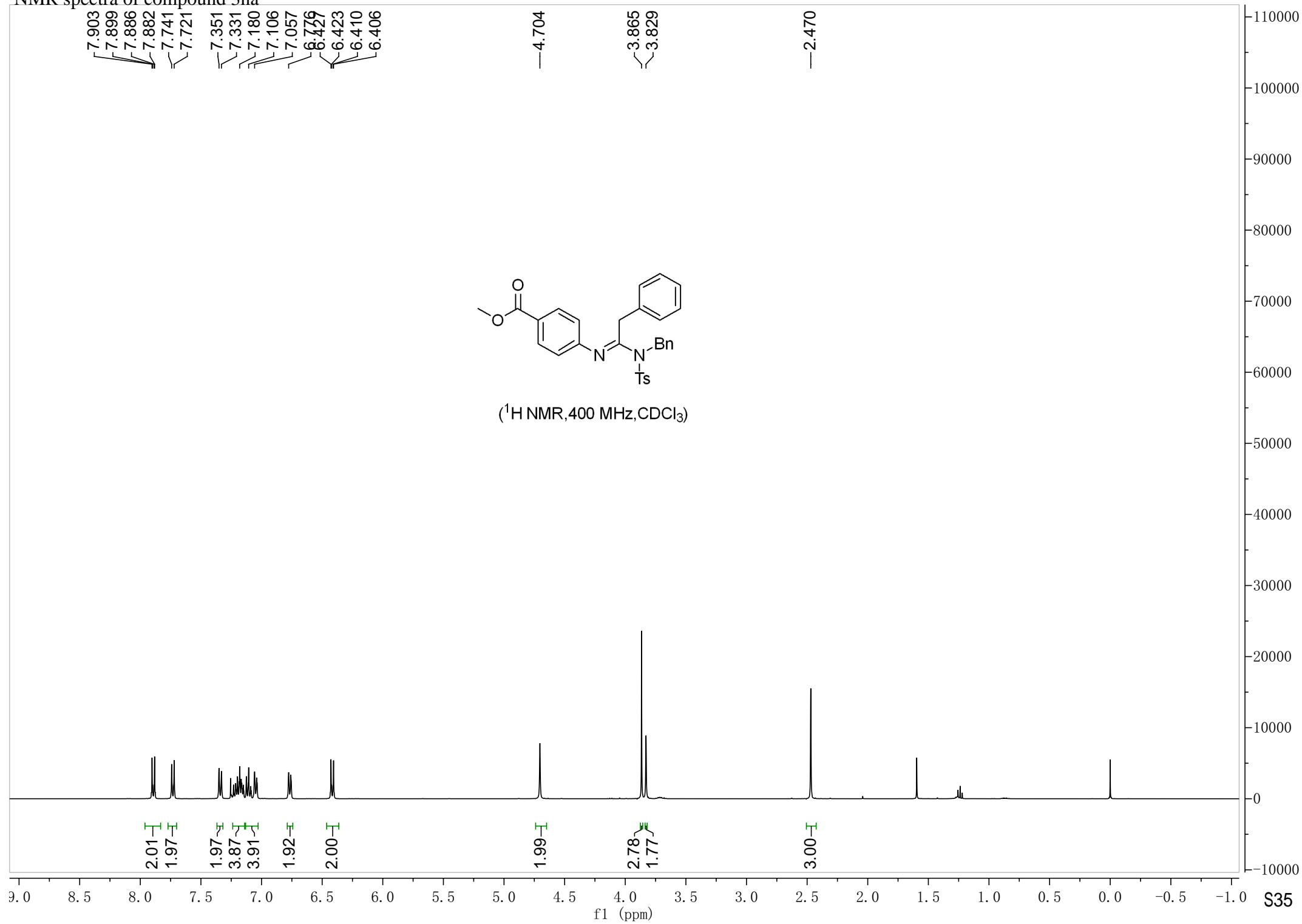
NMR spectra of compound 3ma



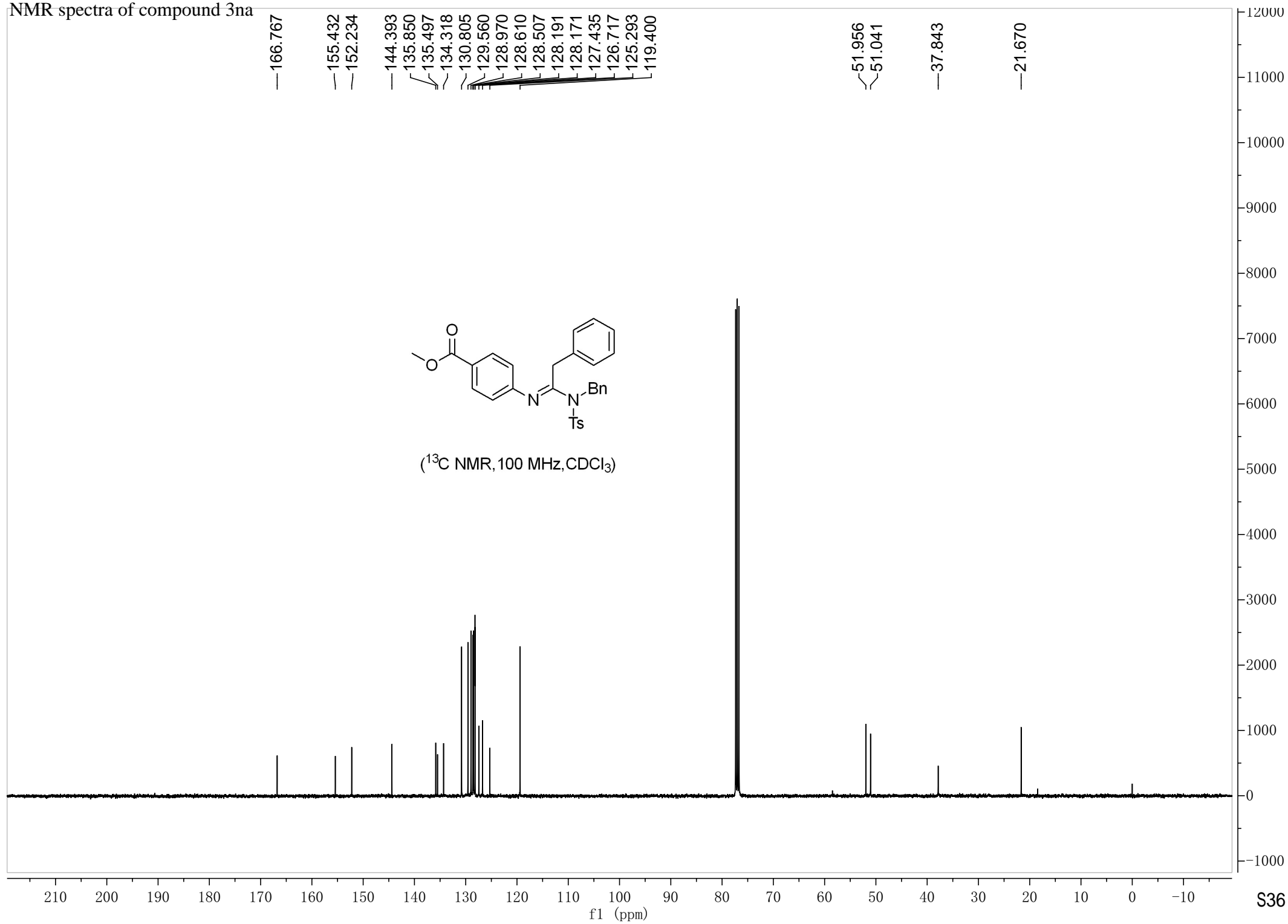
NMR spectra of compound 3ma



NMR spectra of compound 3na



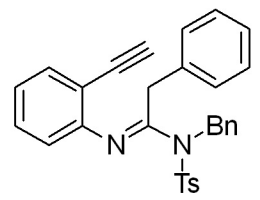
NMR spectra of compound 3na



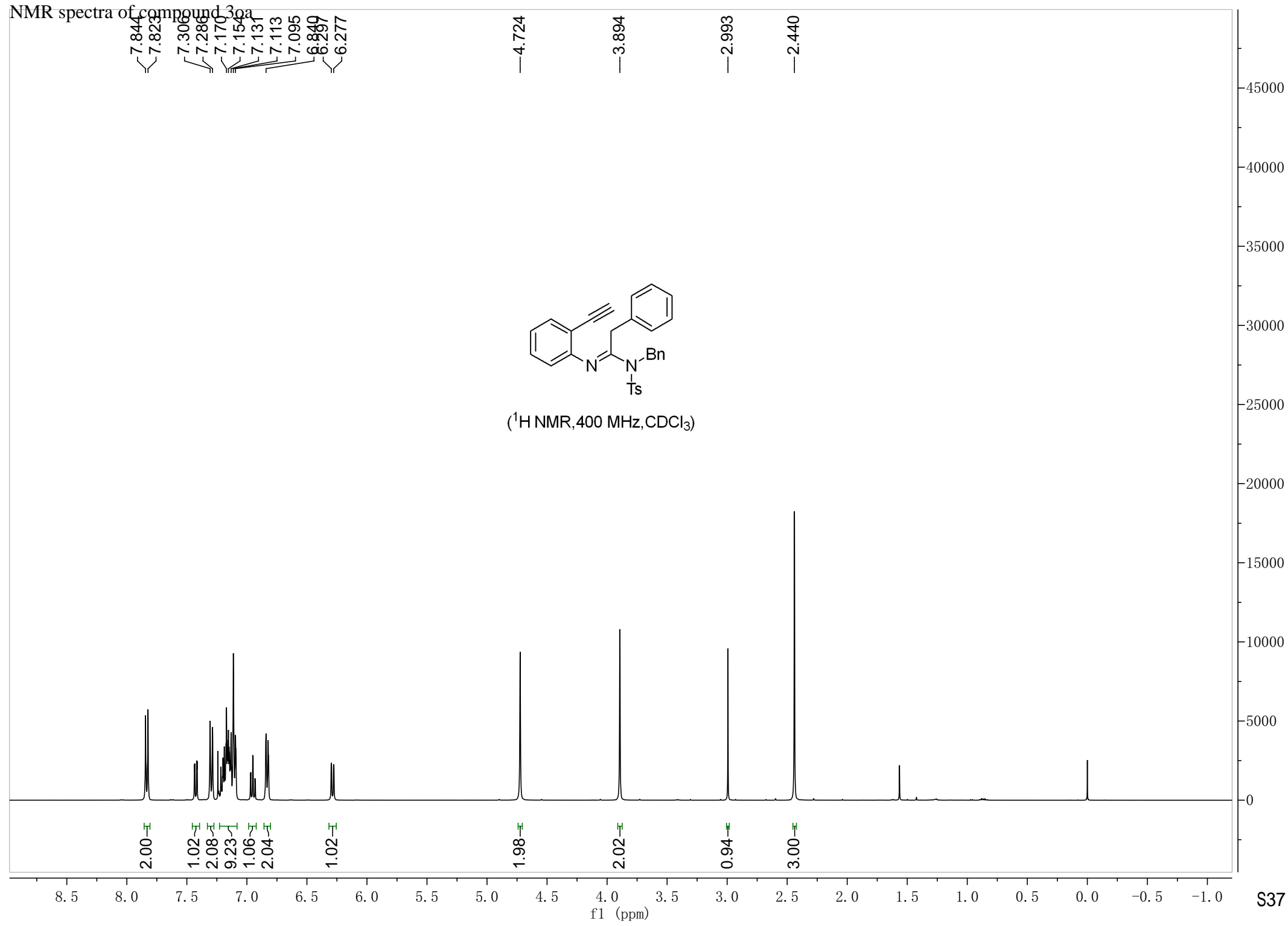
NMR spectra of compound 3oa

7.844
7.823
7.306
7.286
7.170
7.154
7.131
7.113
7.095
6.840
6.297
6.277

4.724
3.894
2.993
2.440



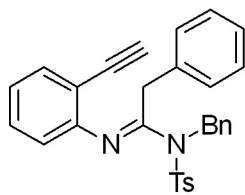
(¹H NMR, 400 MHz, CDCl₃)



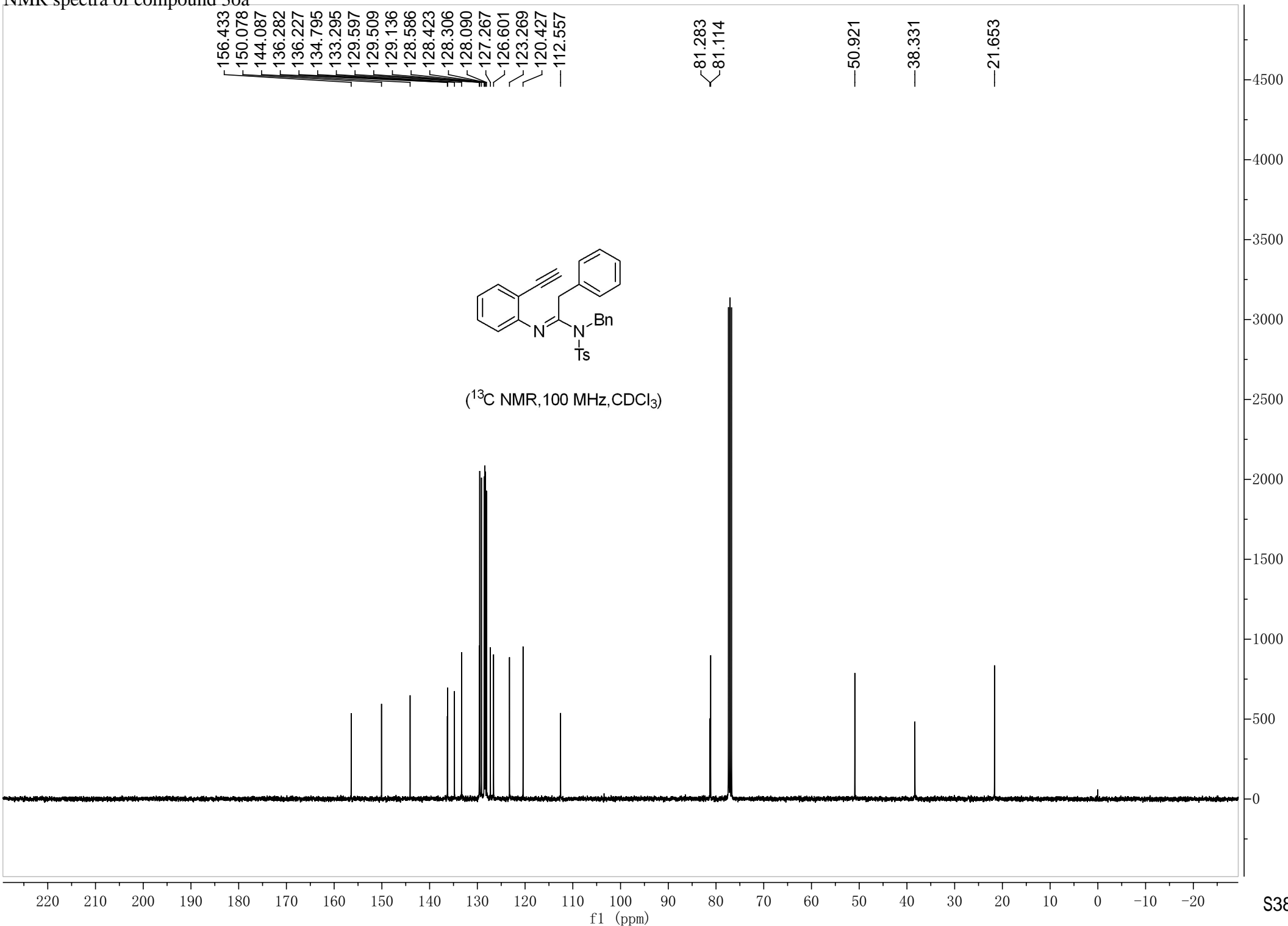
NMR spectra of compound 30a

156.433
 150.078
 144.087
 136.282
 136.227
 134.795
 133.295
 129.597
 129.509
 129.136
 128.586
 128.423
 128.306
 128.090
 127.267
 126.601
 123.269
 120.427
 112.557

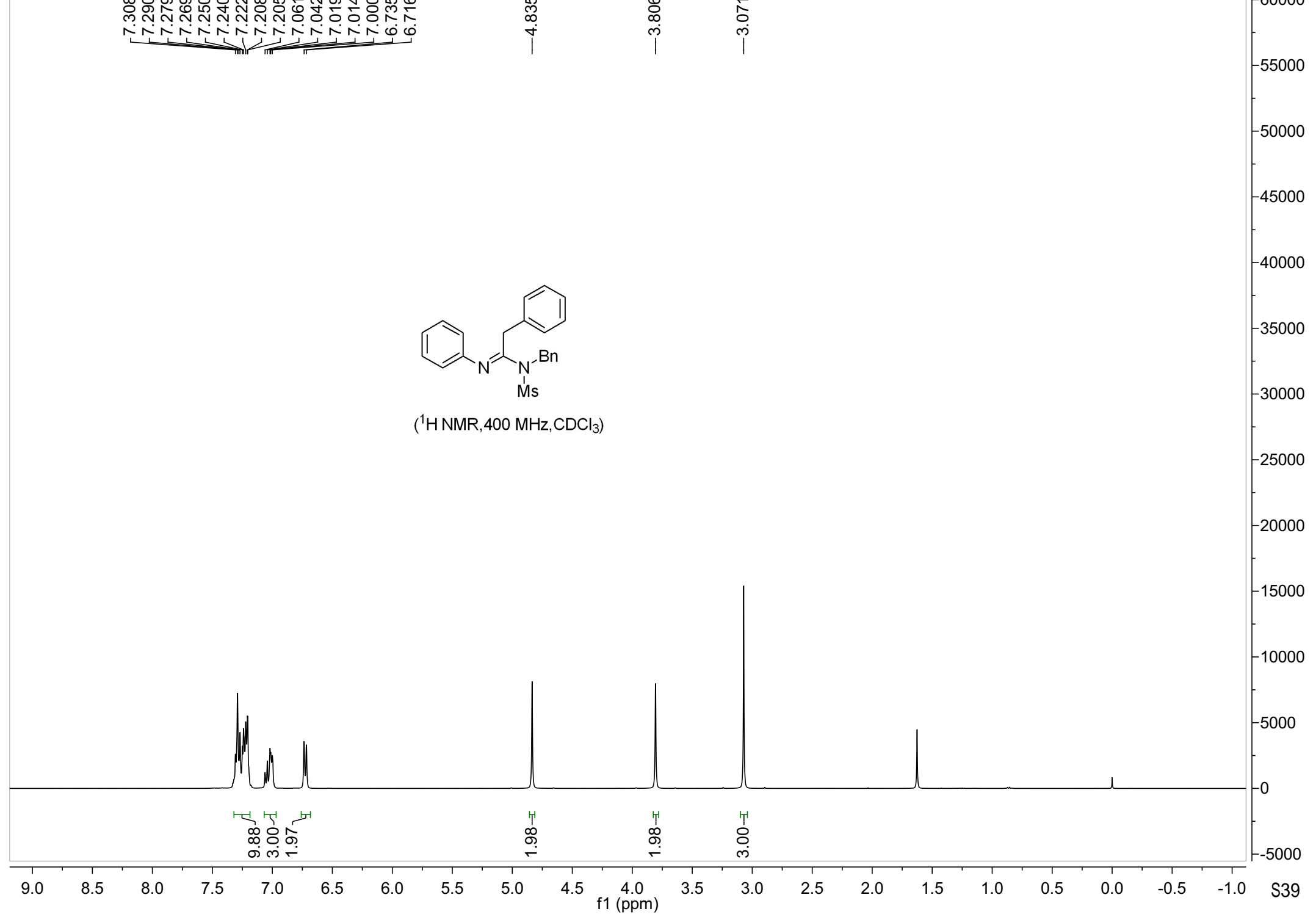
81.283
 81.114
 50.921
 38.331
 21.653



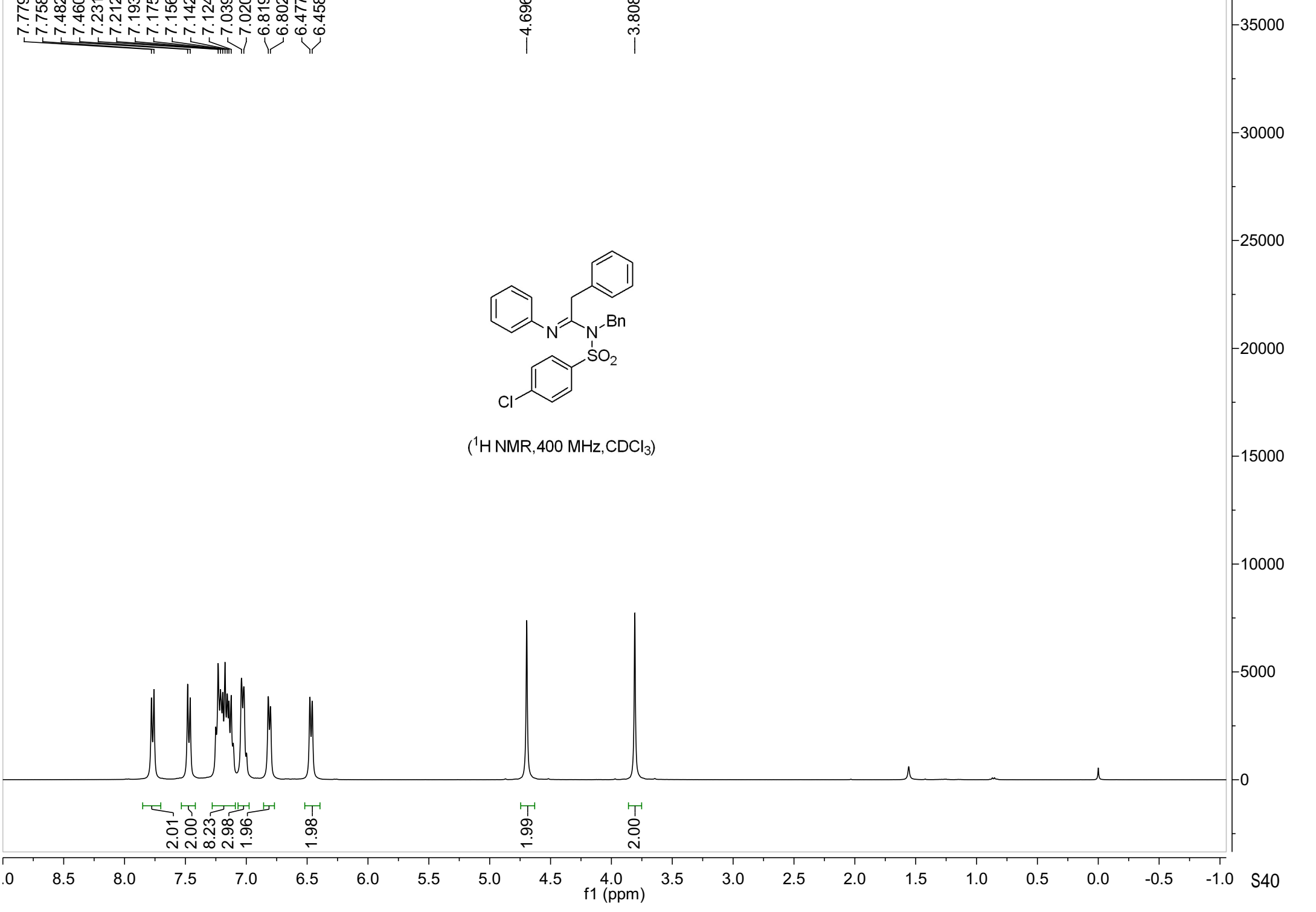
(¹³C NMR, 100 MHz, CDCl₃)



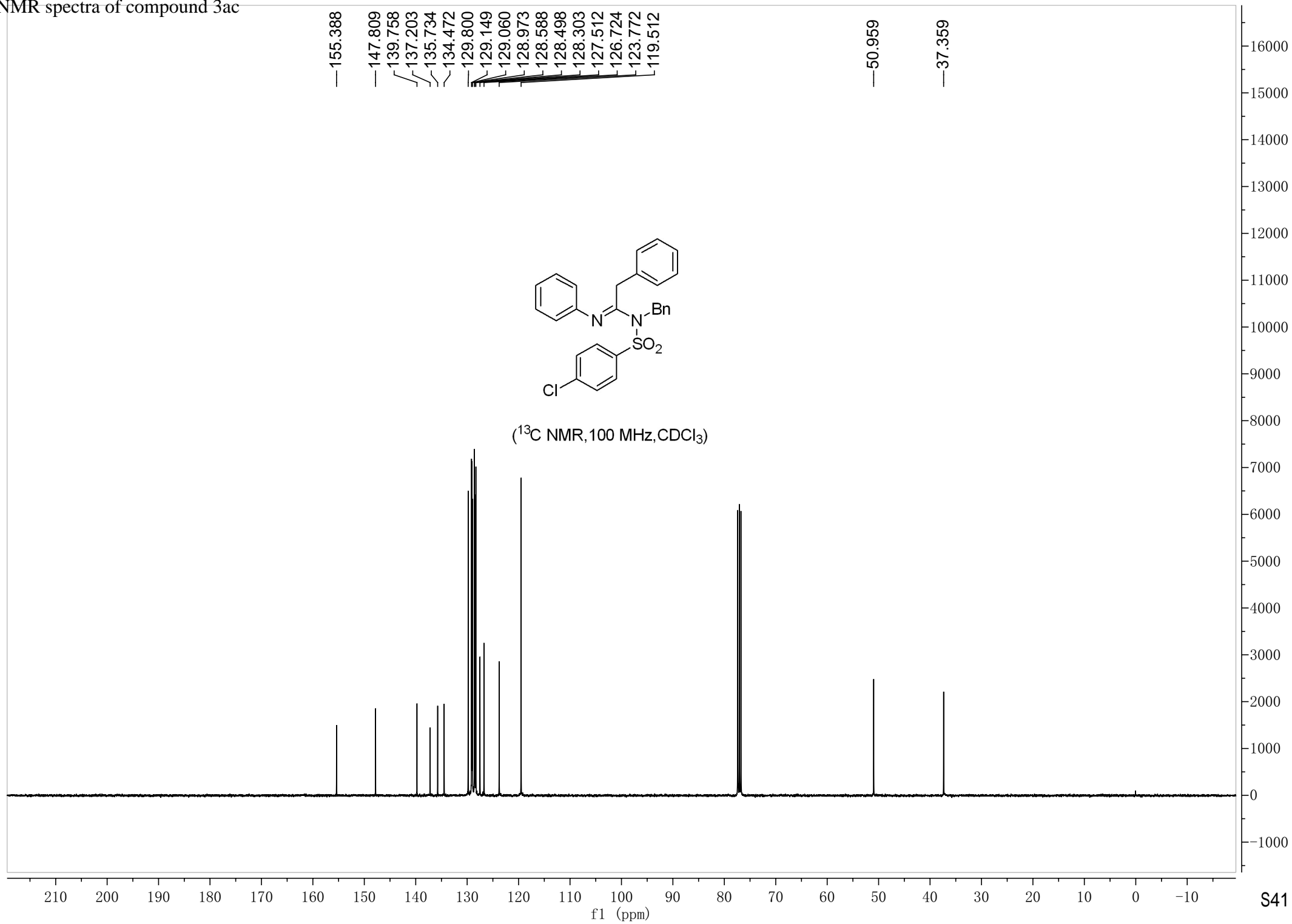
NMR spectra of compound 3ab



NMR spectra of compound 3ac

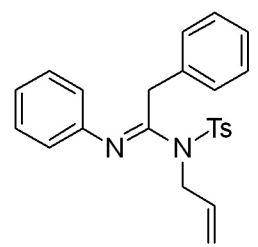


NMR spectra of compound 3ac

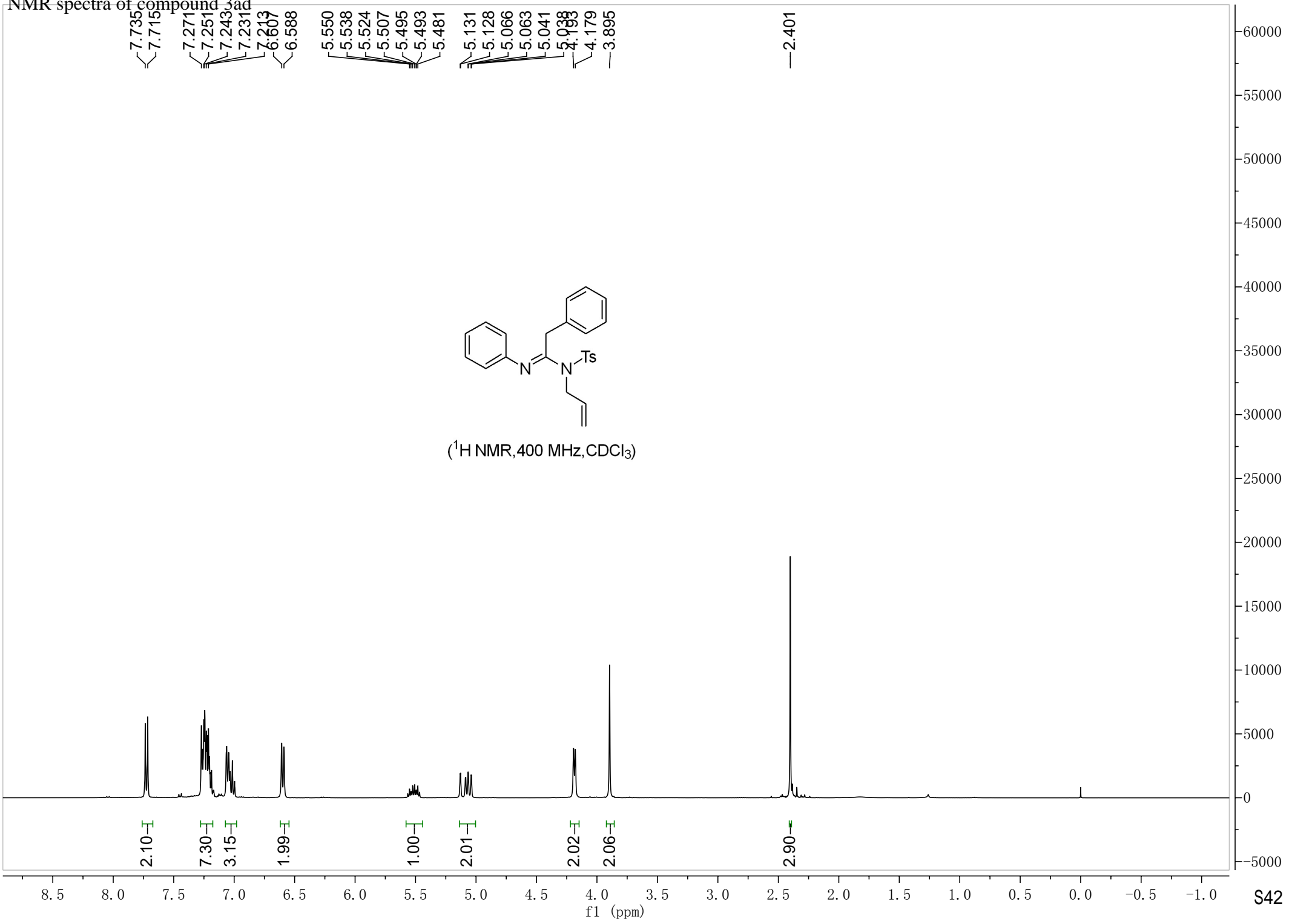


NMR spectra of compound 3ad

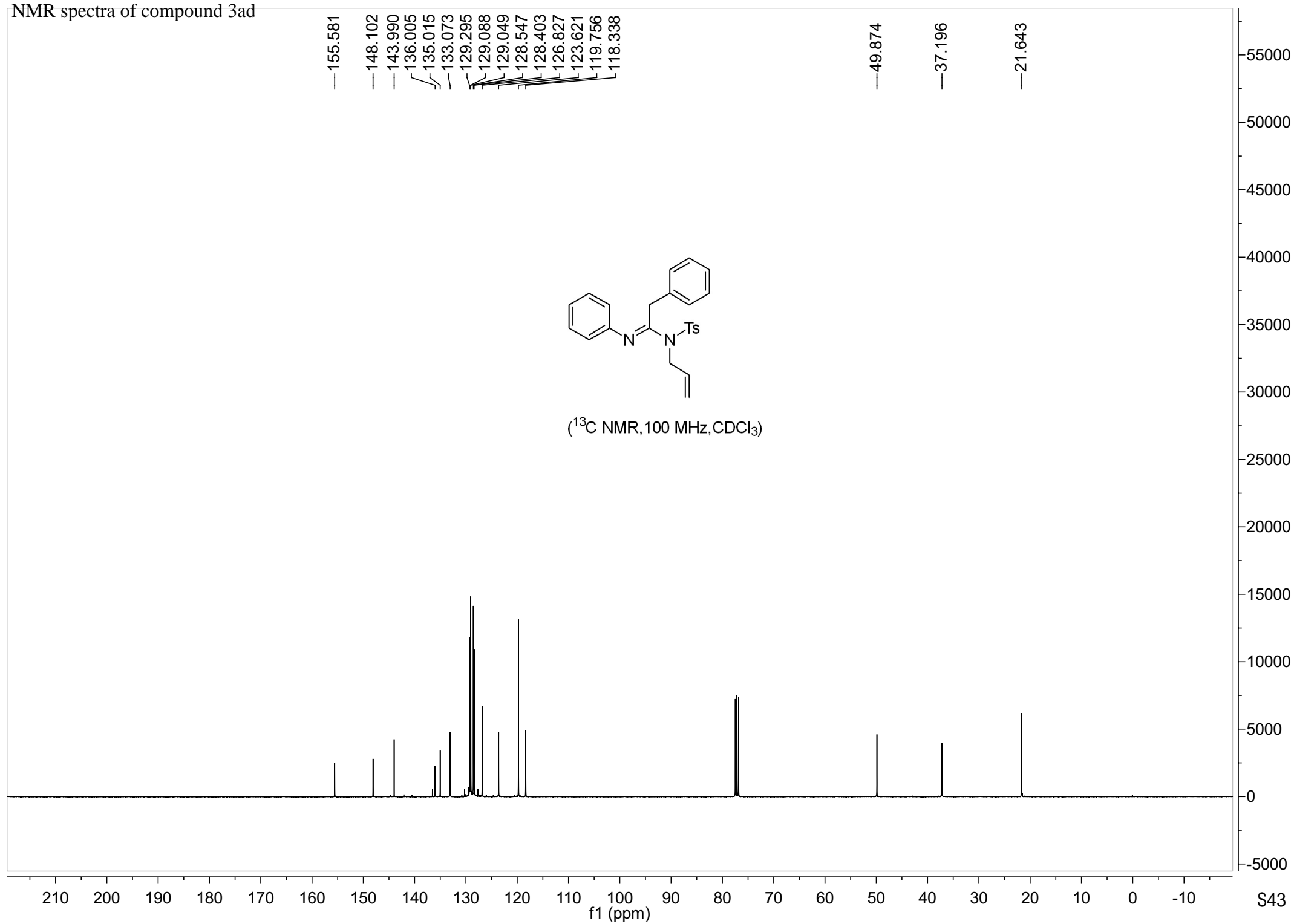
7.735
7.715
7.271
7.251
7.243
7.231
7.213
6.607
6.588
5.550
5.538
5.524
5.507
5.495
5.493
5.481
5.131
5.128
5.066
5.063
5.041
5.038
4.993
4.179
3.895
2.401



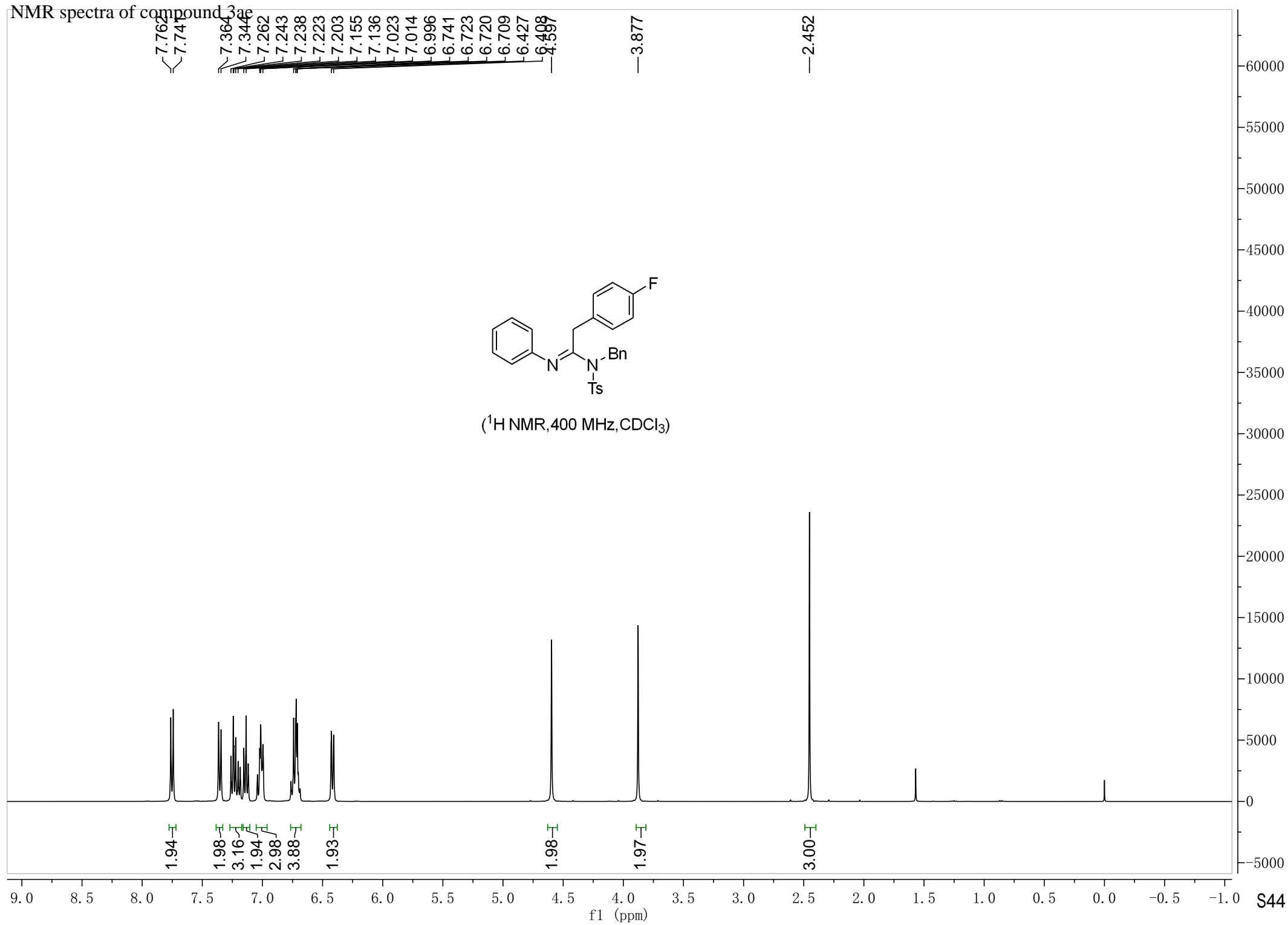
(¹H NMR, 400 MHz, CDCl₃)



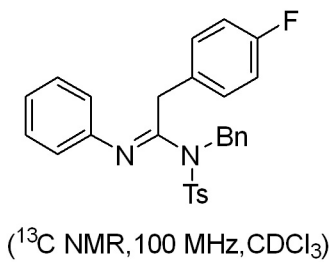
NMR spectra of compound 3ad



NMR spectra of compound 3ae



NMR spectra of compound 3ae

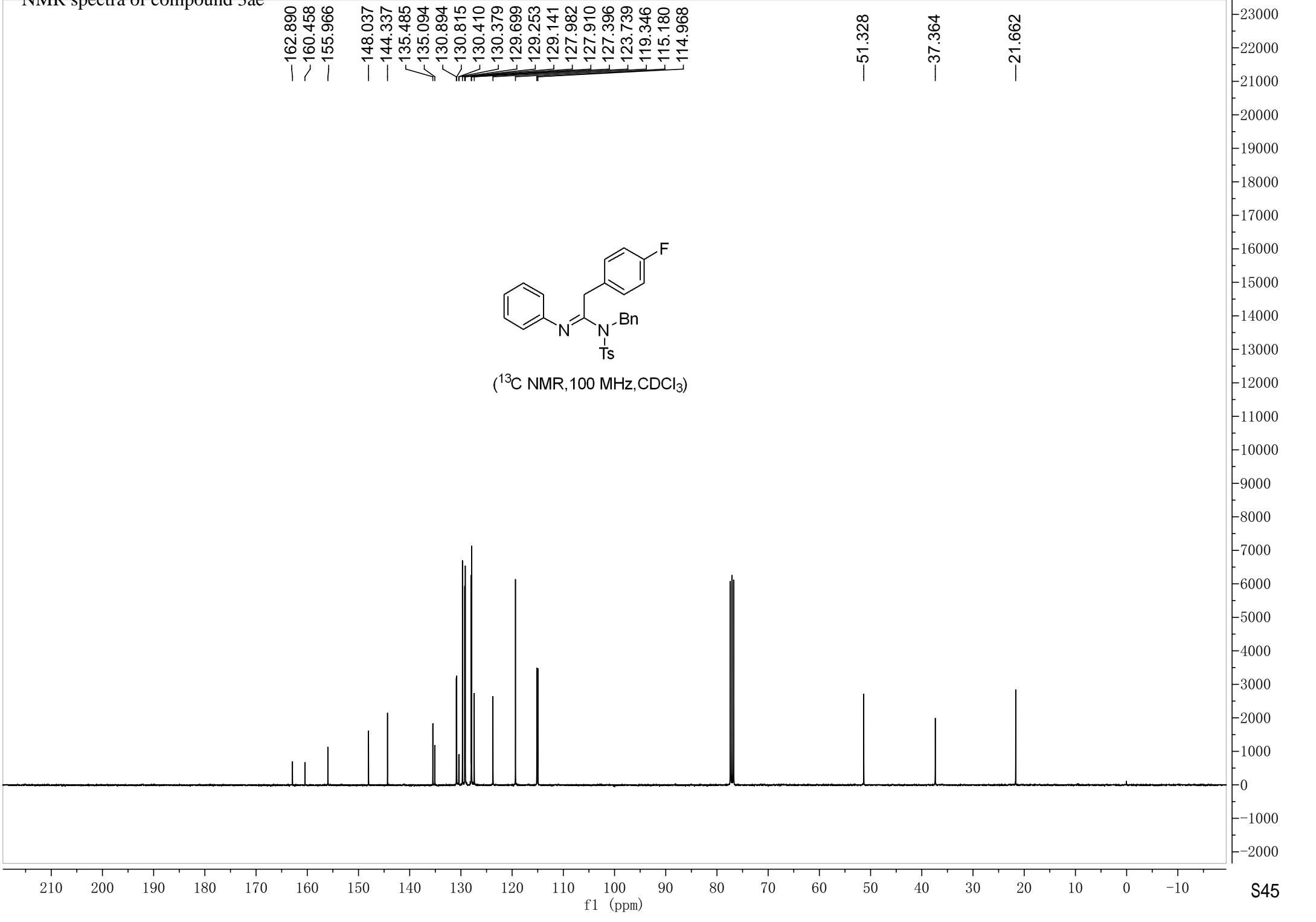


- 162.890
- 160.458
- 155.966
- 148.037
- 144.337
- 135.485
- 135.094
- 130.894
- 130.815
- 130.410
- 130.379
- 129.699
- 129.253
- 129.141
- 127.982
- 127.910
- 127.396
- 123.739
- 119.346
- 115.180
- 114.968

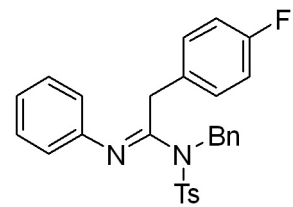
— 51.328

— 37.364

— 21.662

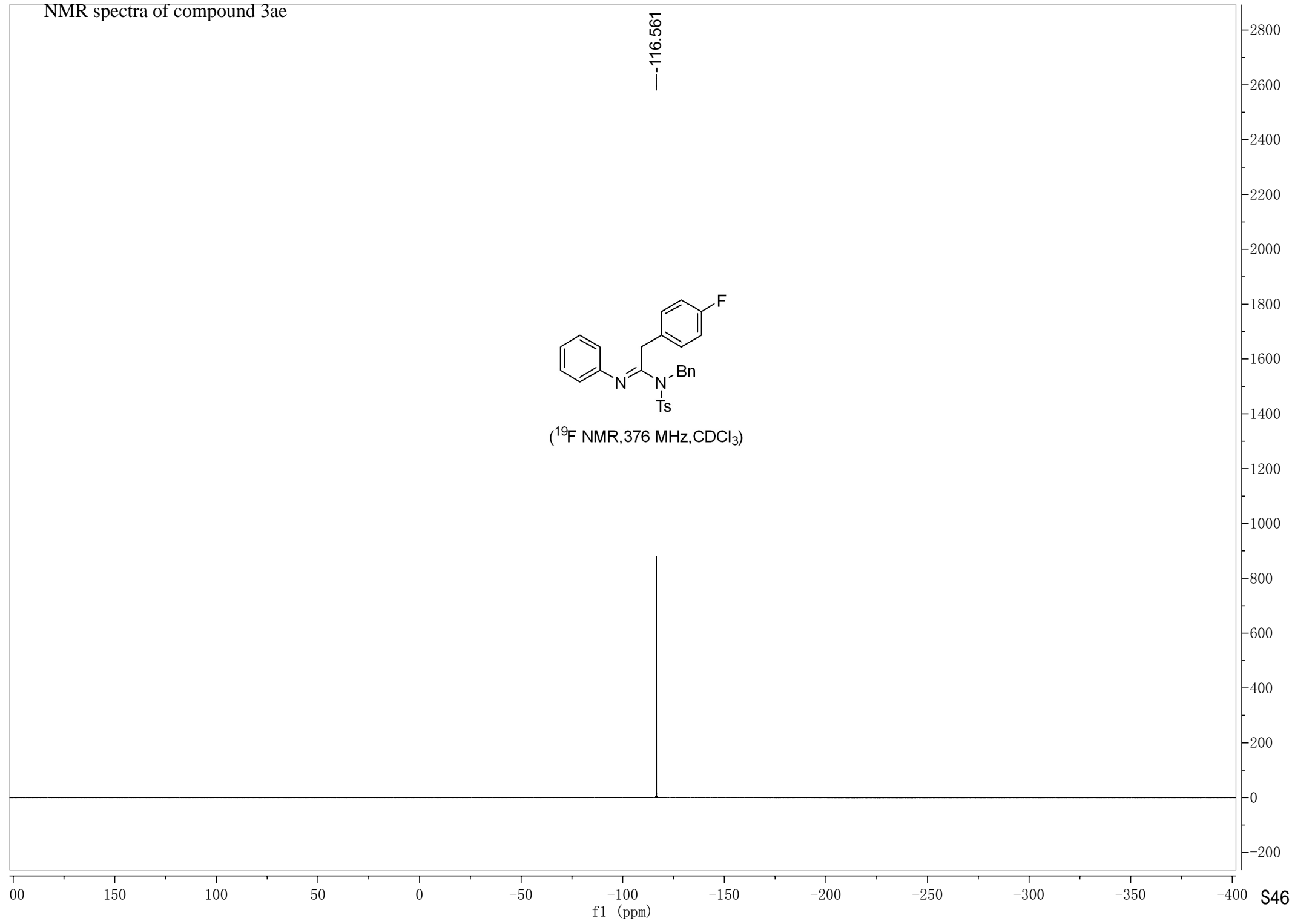


NMR spectra of compound 3ae



(¹⁹F NMR, 376 MHz, CDCl₃)

---116.561

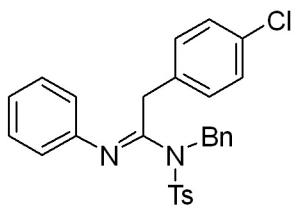


NMR spectra of compound 3af

7.762
7.741
7.364
7.344
7.261
7.242
7.241
7.238
7.222
7.154
7.135
7.022
7.014
6.996
6.740
6.723
6.719
6.709
6.429
6.426
6.408
6.396

3.876

2.452



(¹H NMR, 400 MHz, CDCl₃)

1.96

1.94

3.08

1.96

2.91

3.87

1.96

1.97

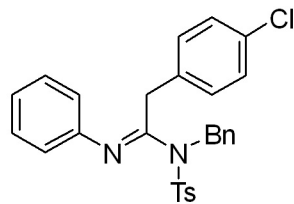
2.00

3.00

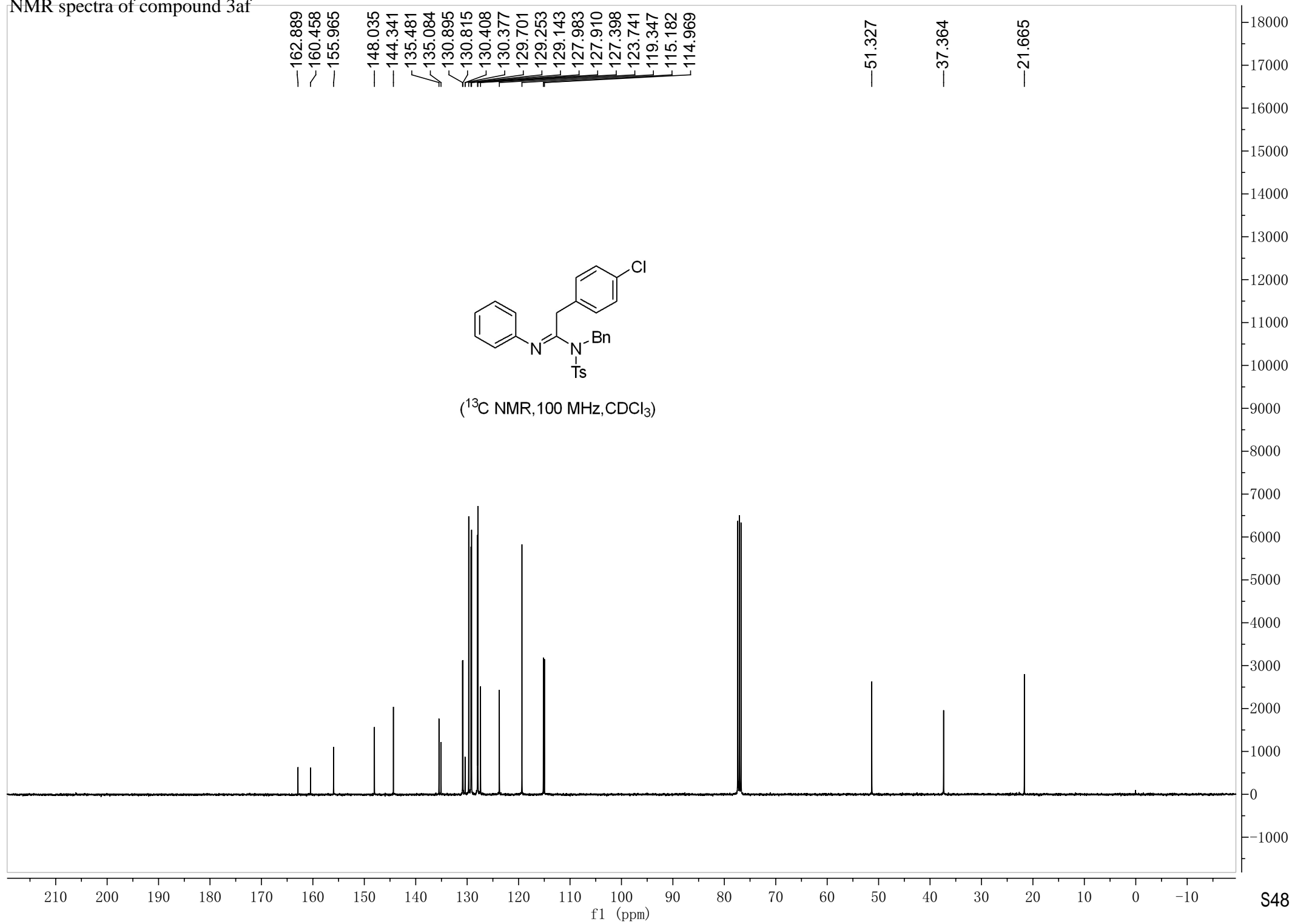
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

NMR spectra of compound 3af



(¹³C NMR, 100 MHz, CDCl₃)



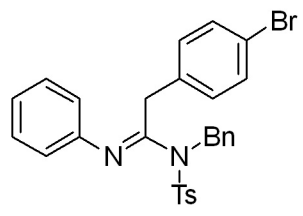
NMR spectra of compound 3a_g

7.754
7.733
7.370
7.251
7.167
7.147
6.625
6.604
6.436
6.434
6.416

4.589

3.860

2.462



(¹H NMR, 400 MHz, CDCl₃)

1.90

2.02

3.22

3.91

2.97

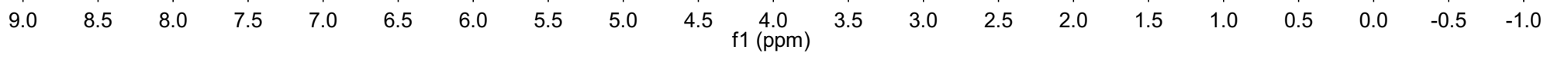
1.96

1.98

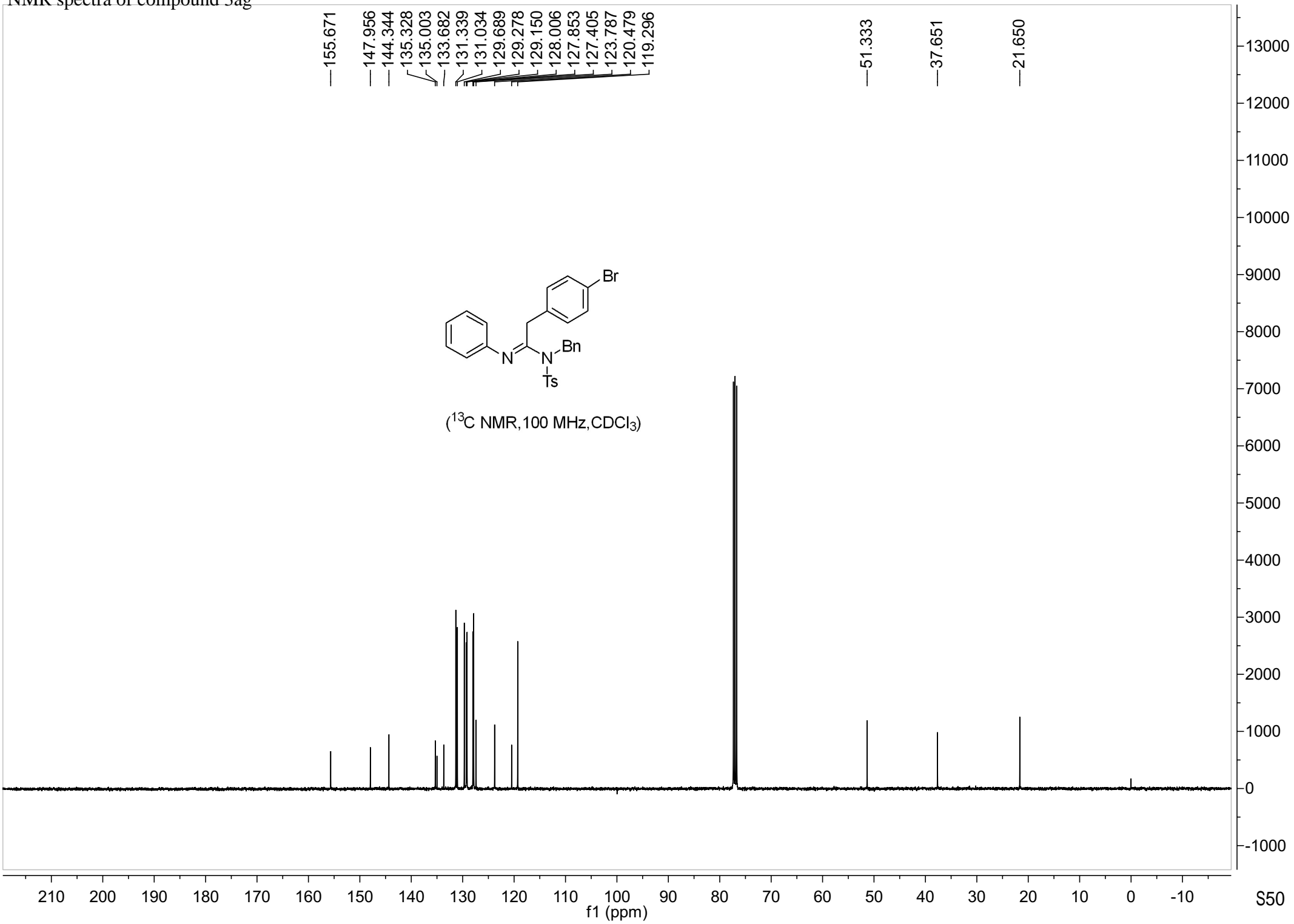
1.98

2.01

3.00



NMR spectra of compound 3ag

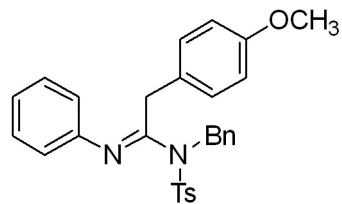


NMR spectra of compound 3ah

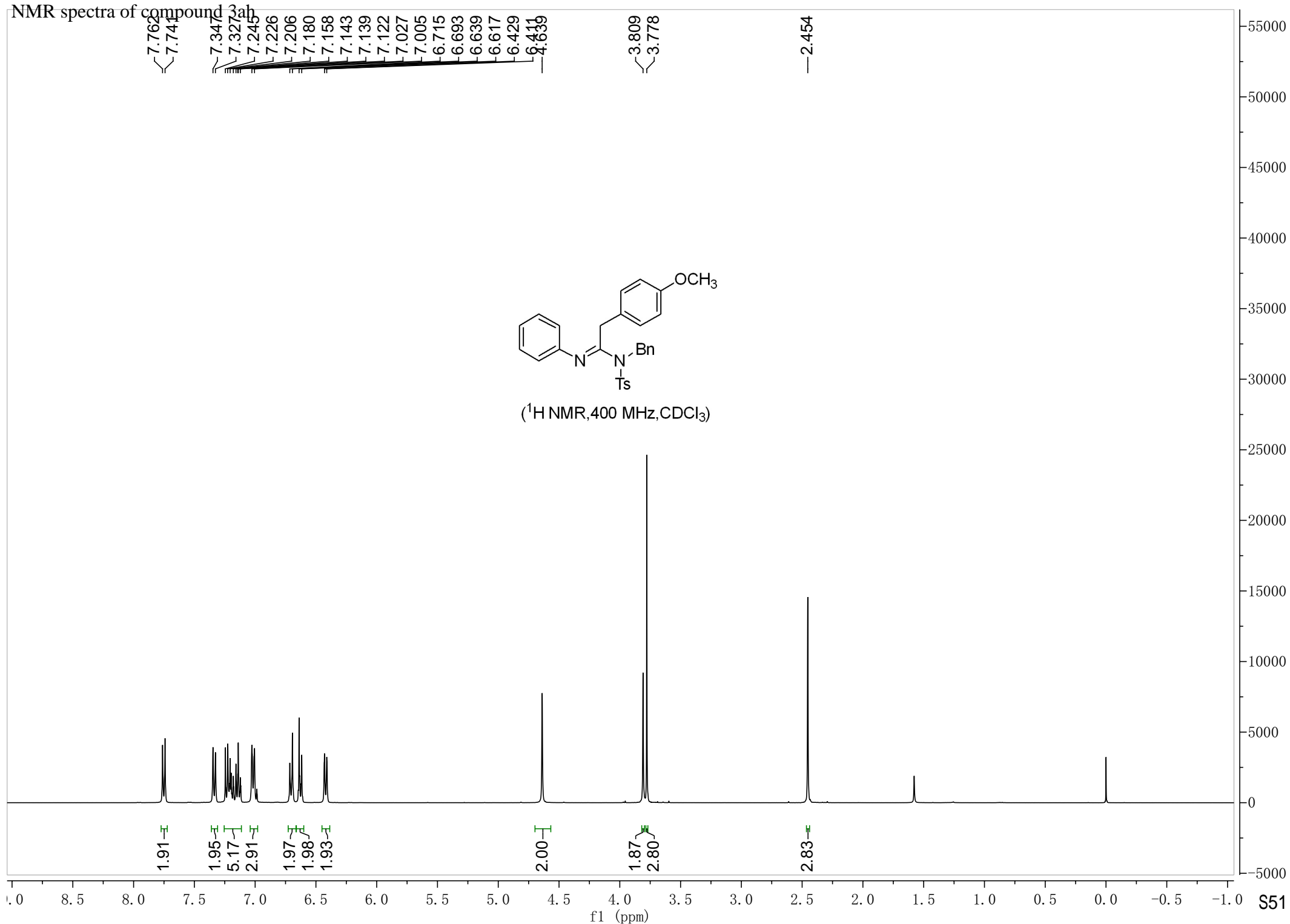
7.762
7.741
7.347
7.327
7.245
7.226
7.206
7.180
7.158
7.143
7.139
7.122
7.027
7.005
6.715
6.693
6.639
6.617
6.429
6.411
6.439

3.809
3.778

2.454



(¹H NMR, 400 MHz, CDCl₃)



NMR spectra of compound 3ah

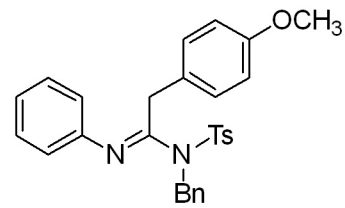
158.317
156.108
148.147
144.139
135.857
135.423
130.242
129.532
129.031
128.885
128.090
128.004
127.238
126.717
123.531
119.492
113.805

55.264

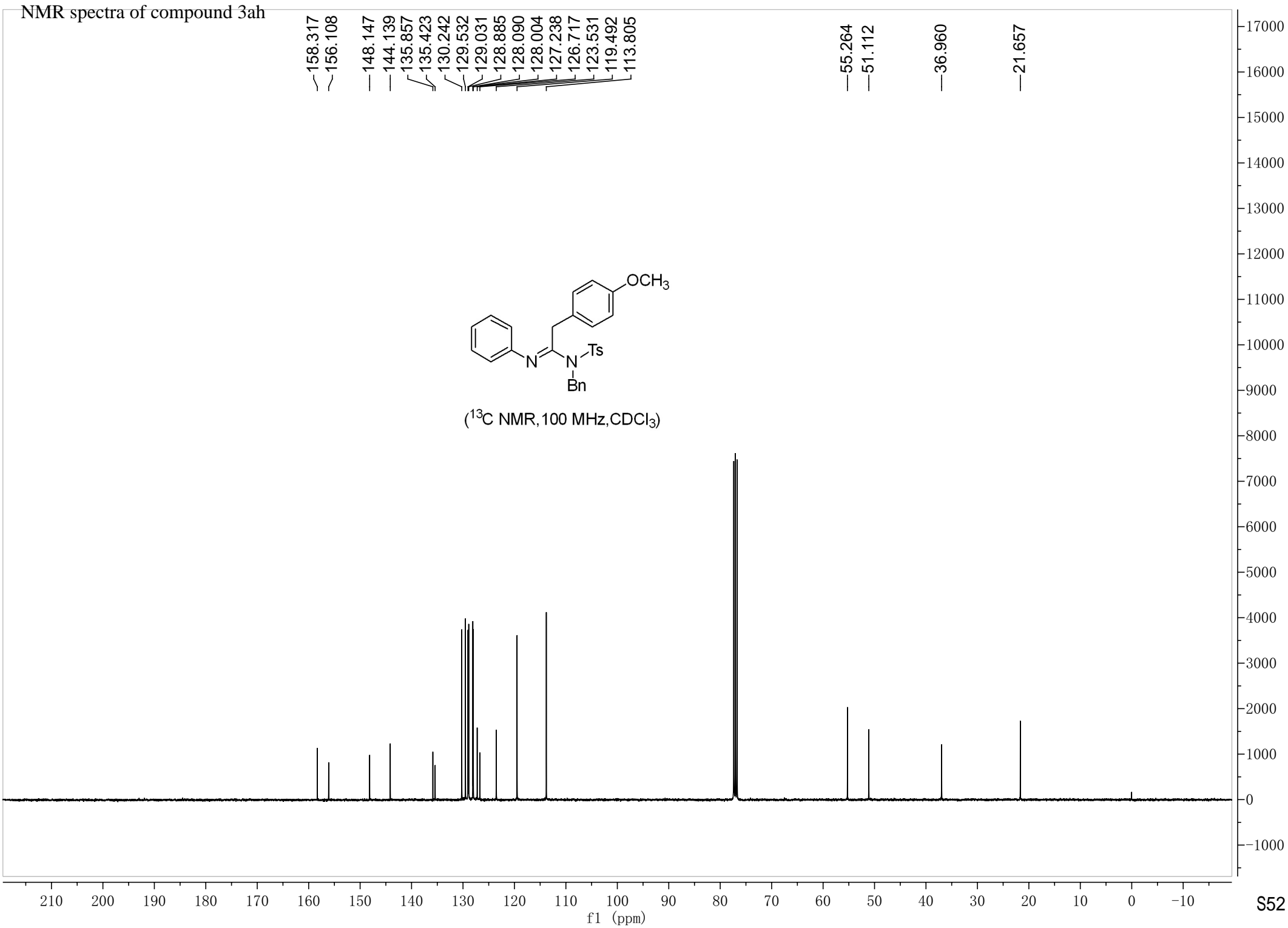
51.112

36.960

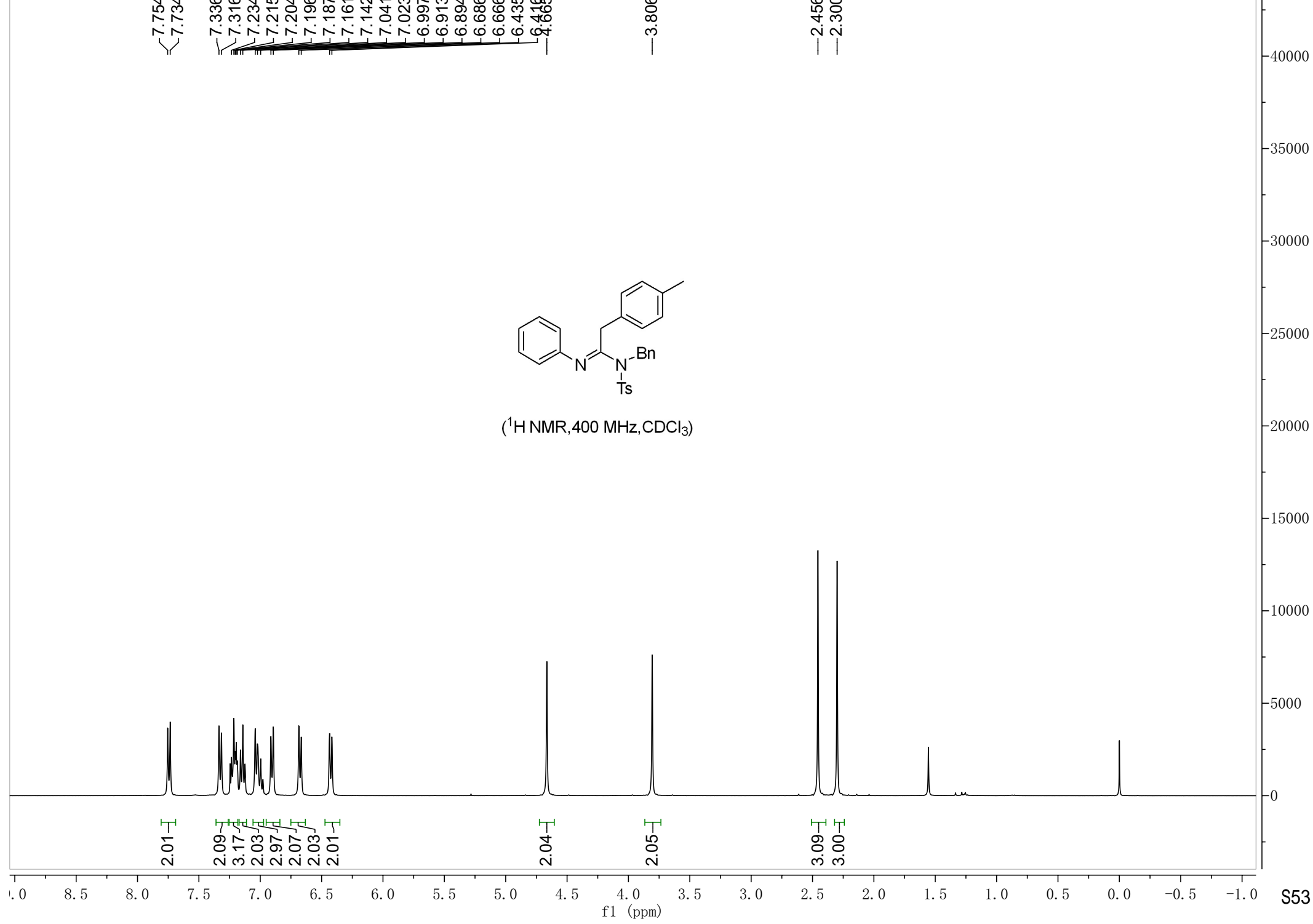
21.657



(¹³C NMR, 100 MHz, CDCl₃)



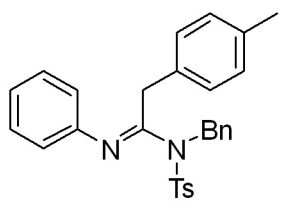
NMR spectra of compound 3ai



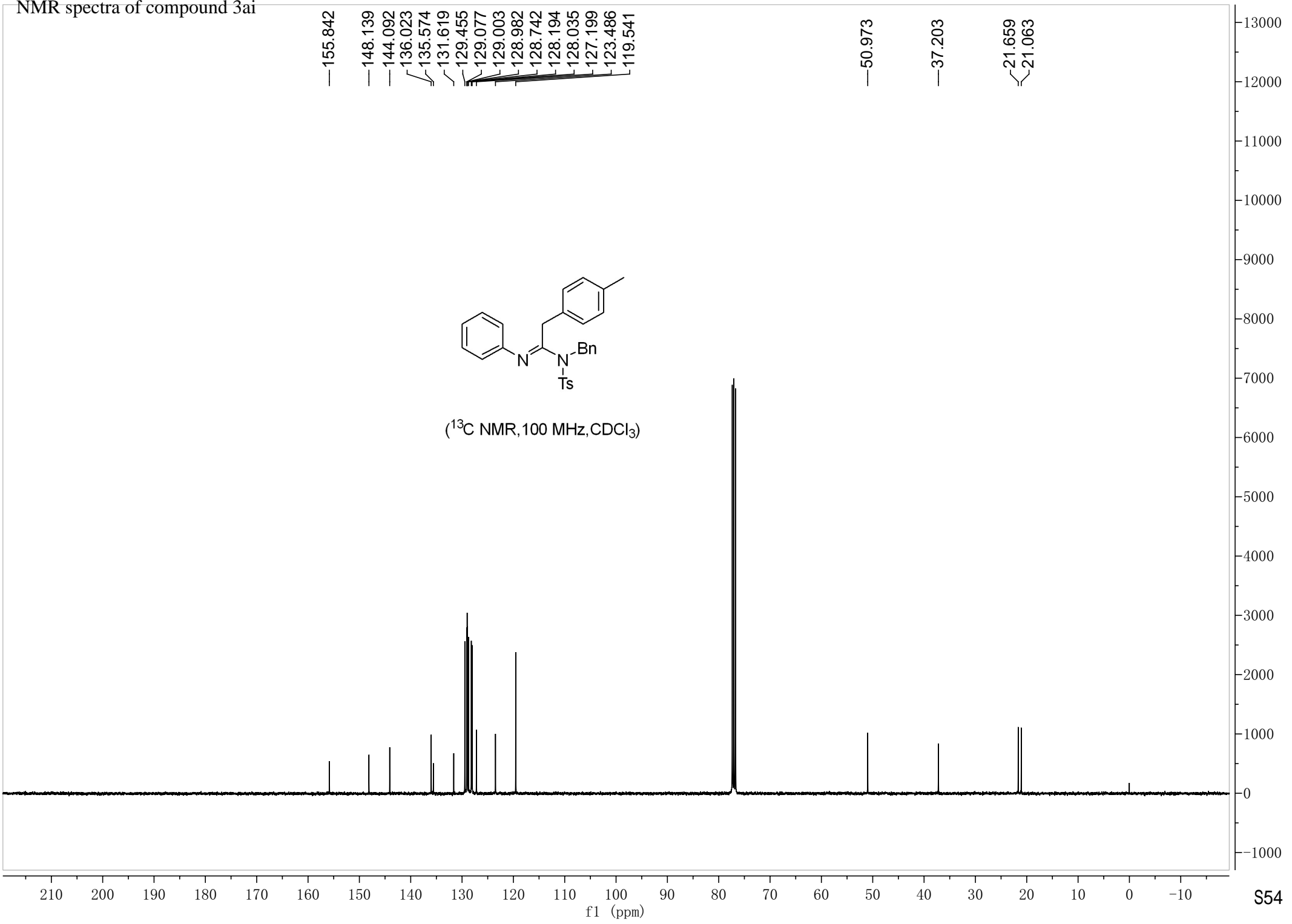
NMR spectra of compound 3ai

- 155.842
- 148.139
- 144.092
- 136.023
- 135.574
- 131.619
- 129.455
- 129.077
- 129.003
- 128.982
- 128.742
- 128.194
- 128.035
- 127.199
- 123.486
- 119.541

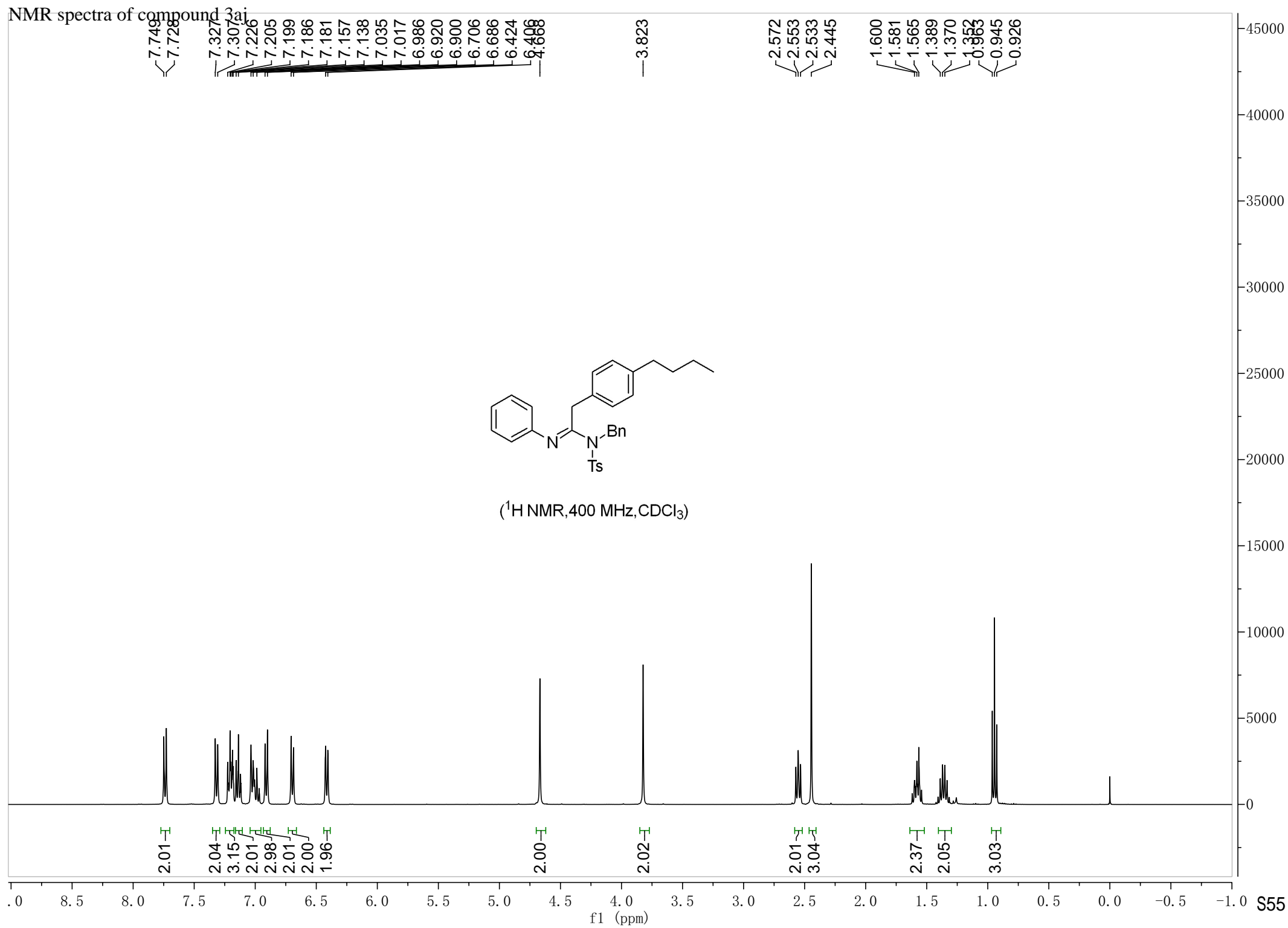
- 50.973
- 37.203
- 21.659
- 21.063



(¹³C NMR, 100 MHz, CDCl₃)



NMR spectra of compound 3aj



NMR spectra of compound 3aj

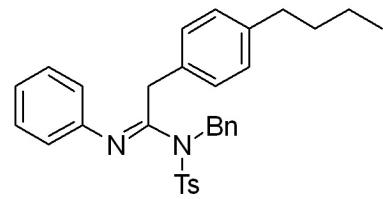
155.850
148.158
144.115
141.116
136.044
135.552
131.842
129.482
129.029
129.011
128.785
128.444
128.207
128.054
127.237
123.489
119.563

51.020

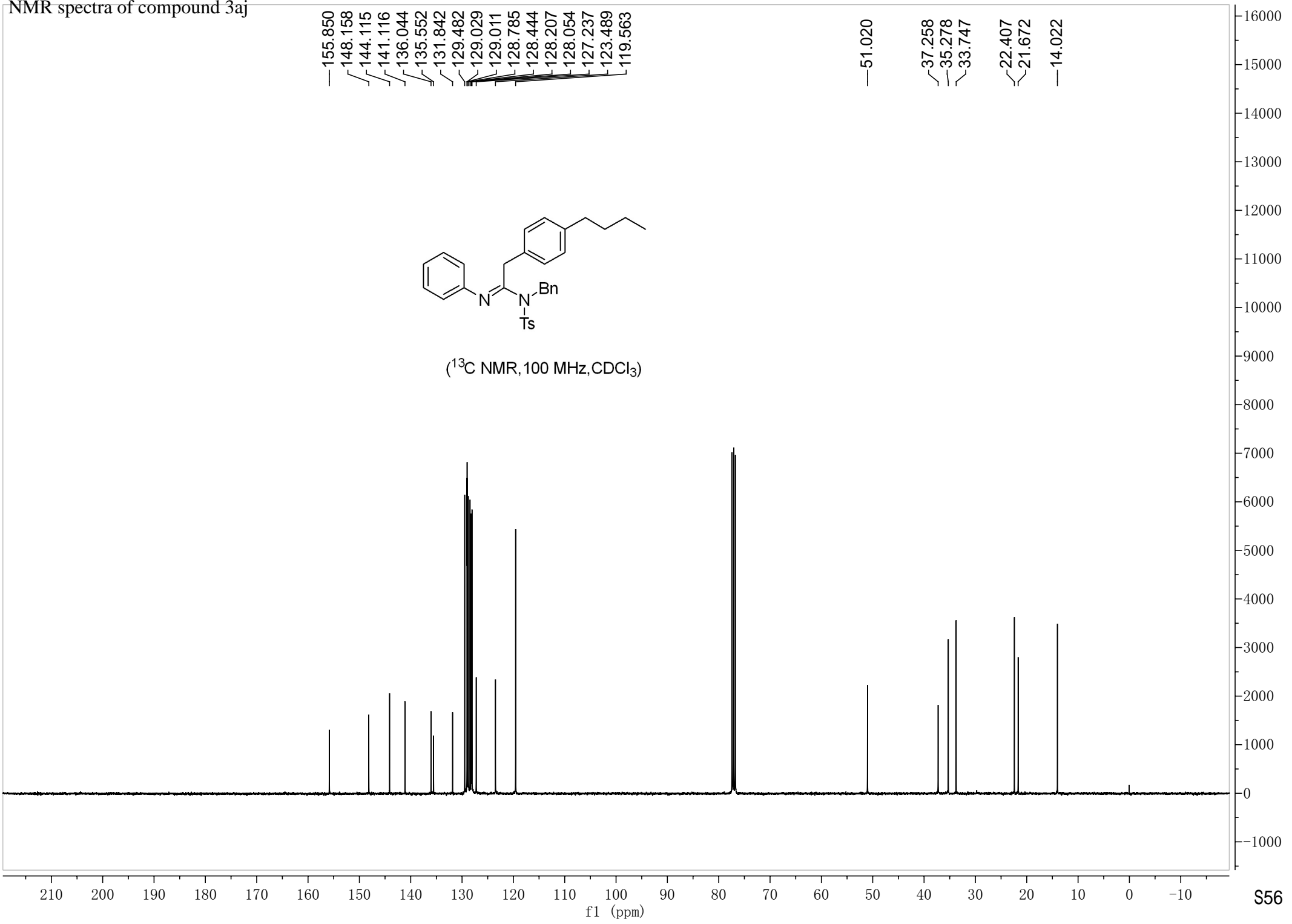
37.258
35.278
33.747

22.407
21.672

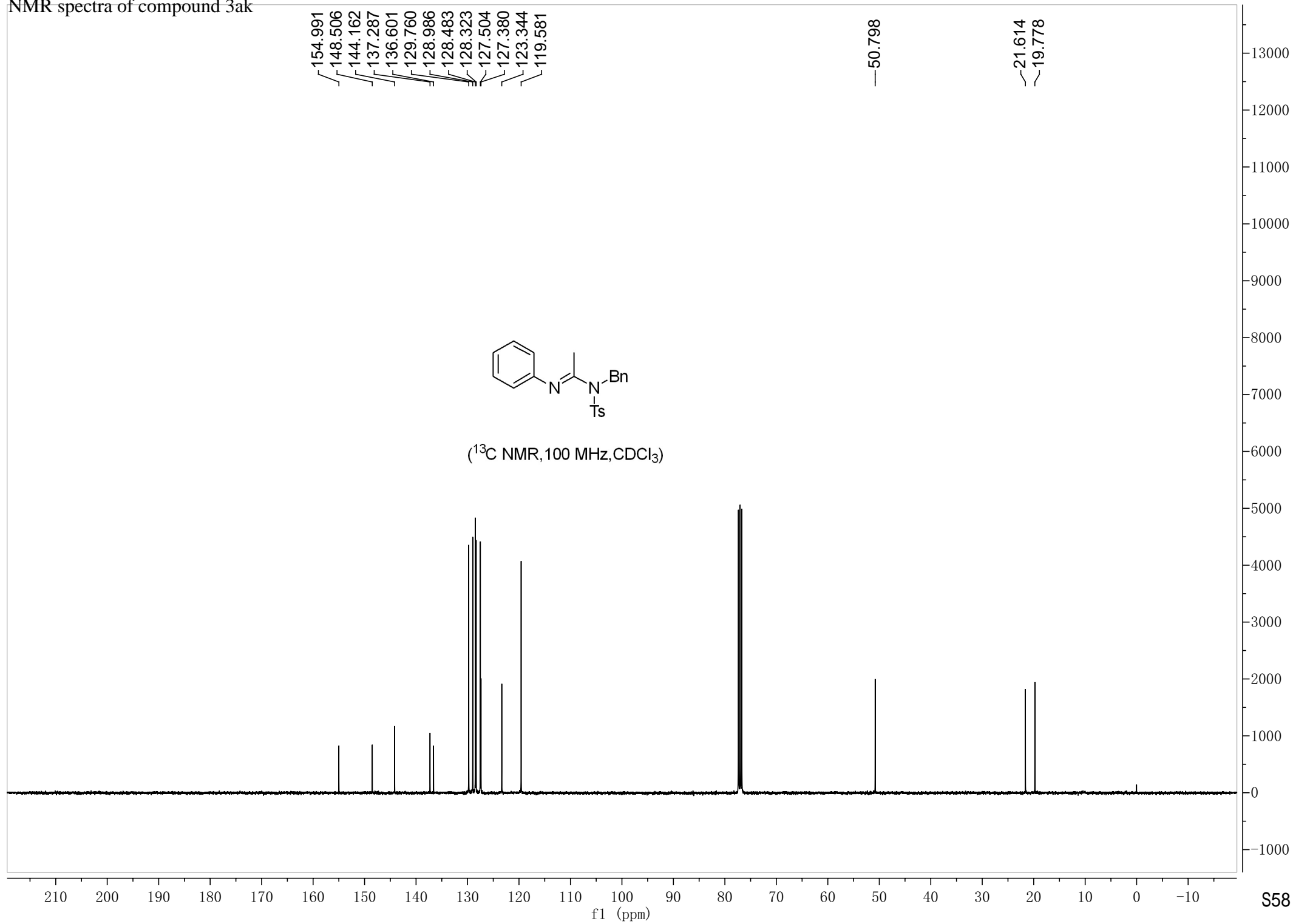
14.022



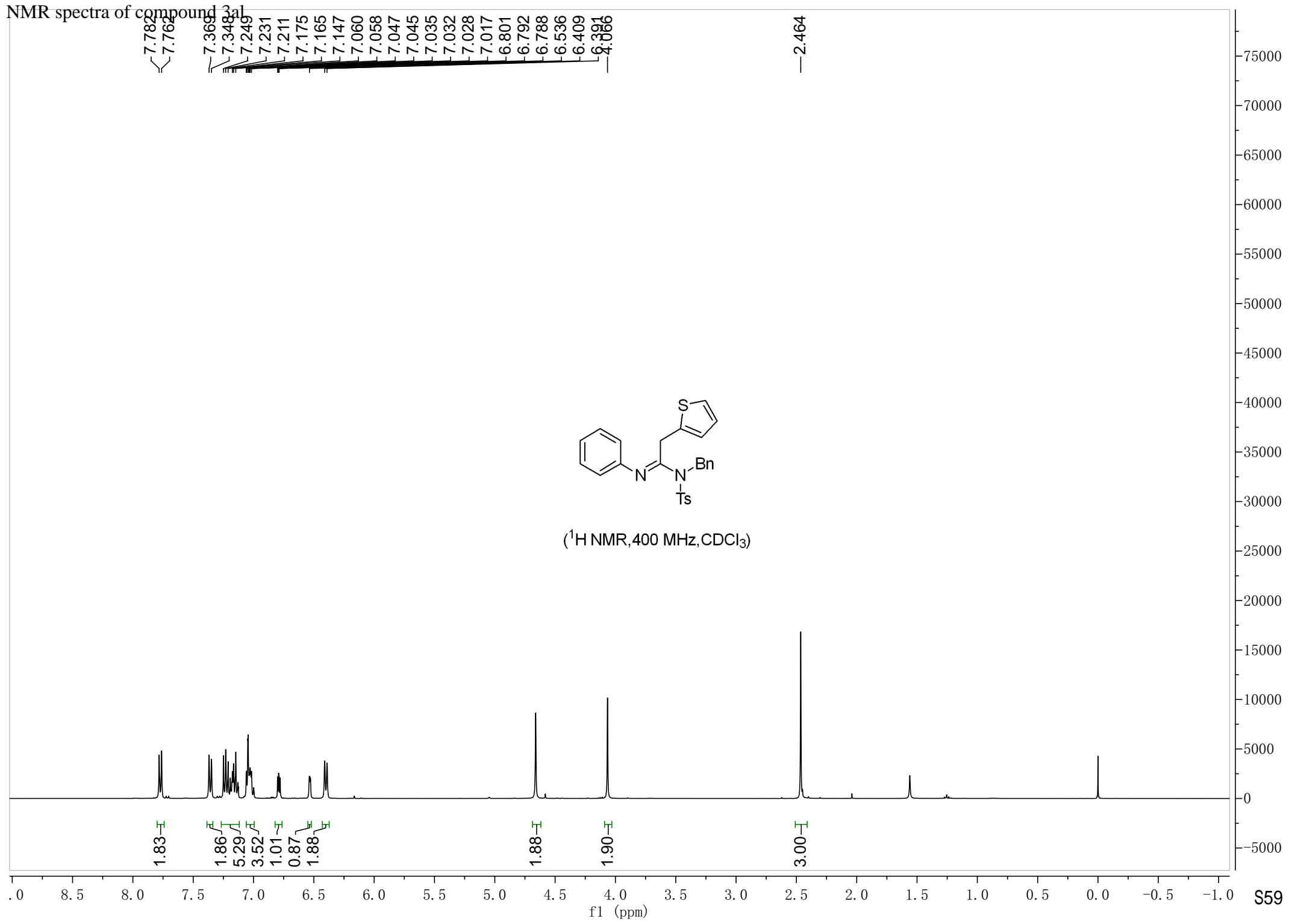
(¹³C NMR, 100 MHz, CDCl₃)



NMR spectra of compound 3ak



NMR spectra of compound 3al



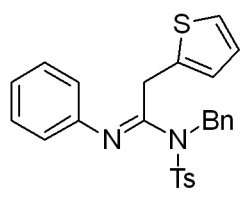
NMR spectra of compound 3al

154.874
147.859
144.255
135.793
135.239
129.644
129.073
128.747
128.041
127.971
127.284
127.241
126.687
124.541
123.664
119.303

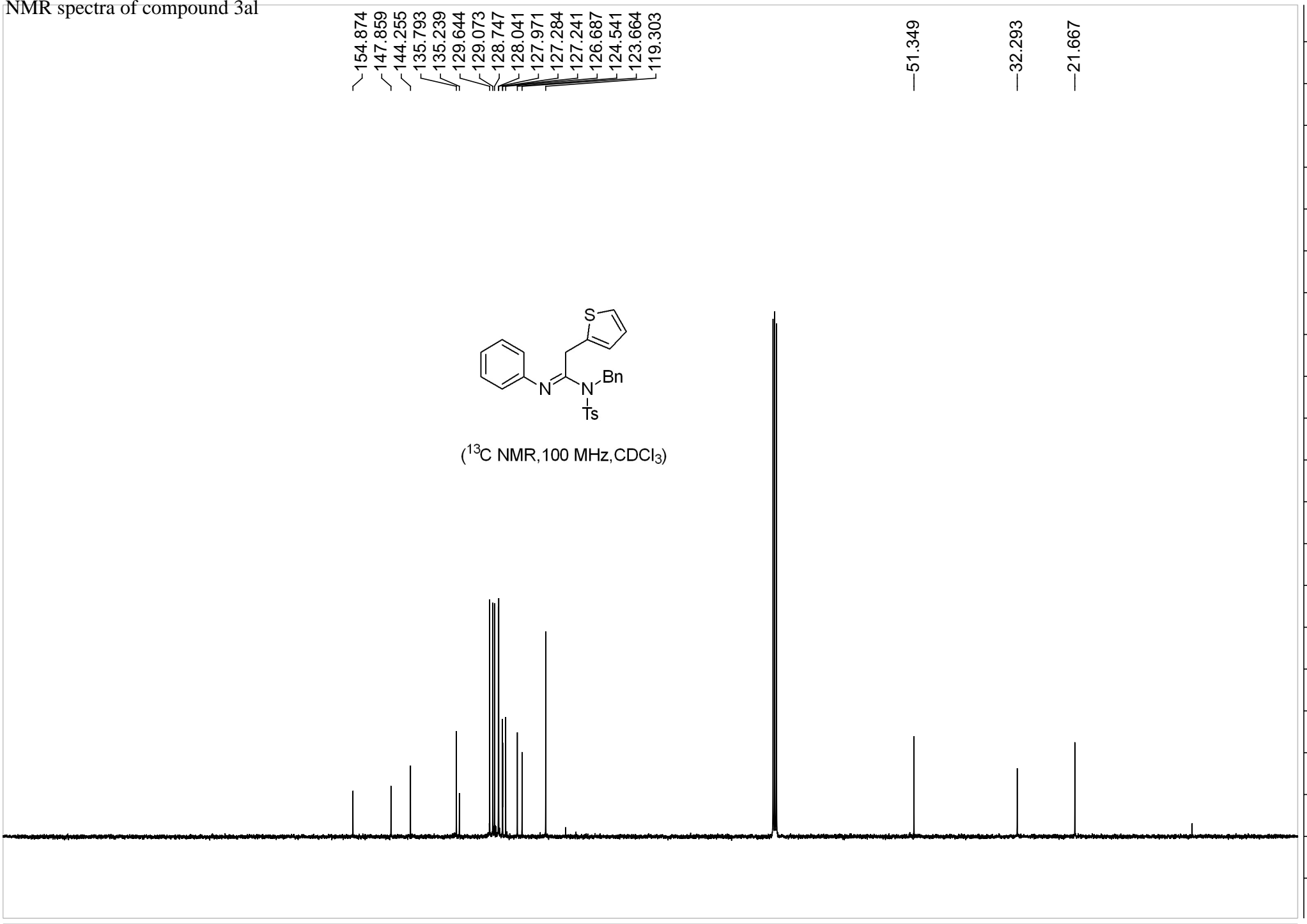
—51.349

—32.293

—21.667



(¹³C NMR, 100 MHz, CDCl₃)



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

NMR spectra of compound 3dk

7.773
7.752
7.424
7.371
7.354
7.350
6.820
6.798

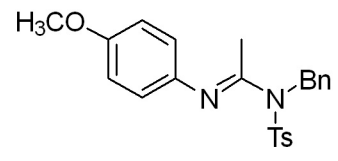
6.388
6.366

5.029

3.777

2.474

2.094



(¹H NMR, 400 MHz, CDCl₃)

1.98

2.00
4.95

1.99

1.95

1.99

3.00

3.02

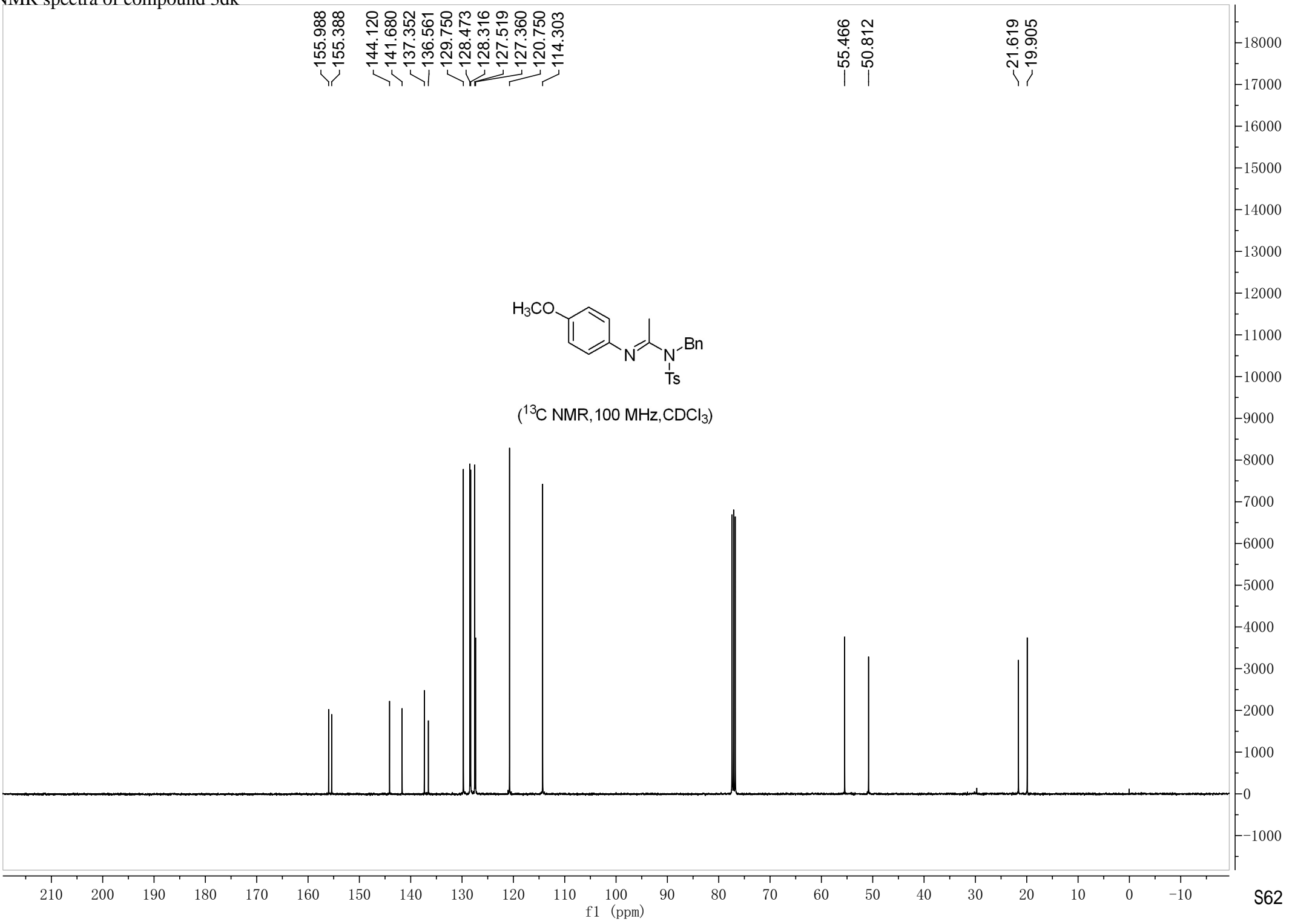
3.00

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 -0.5

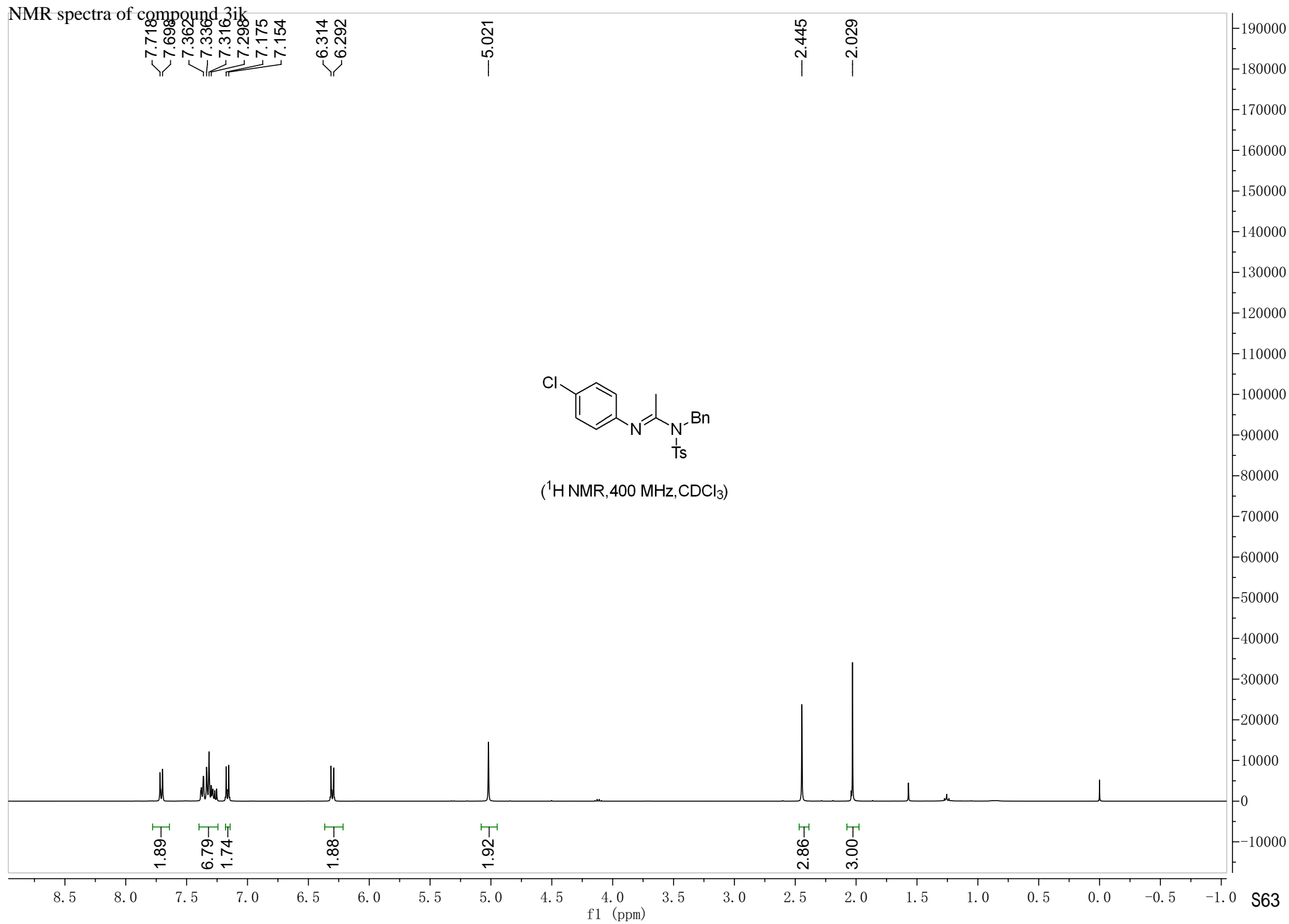
f1 (ppm)

S61

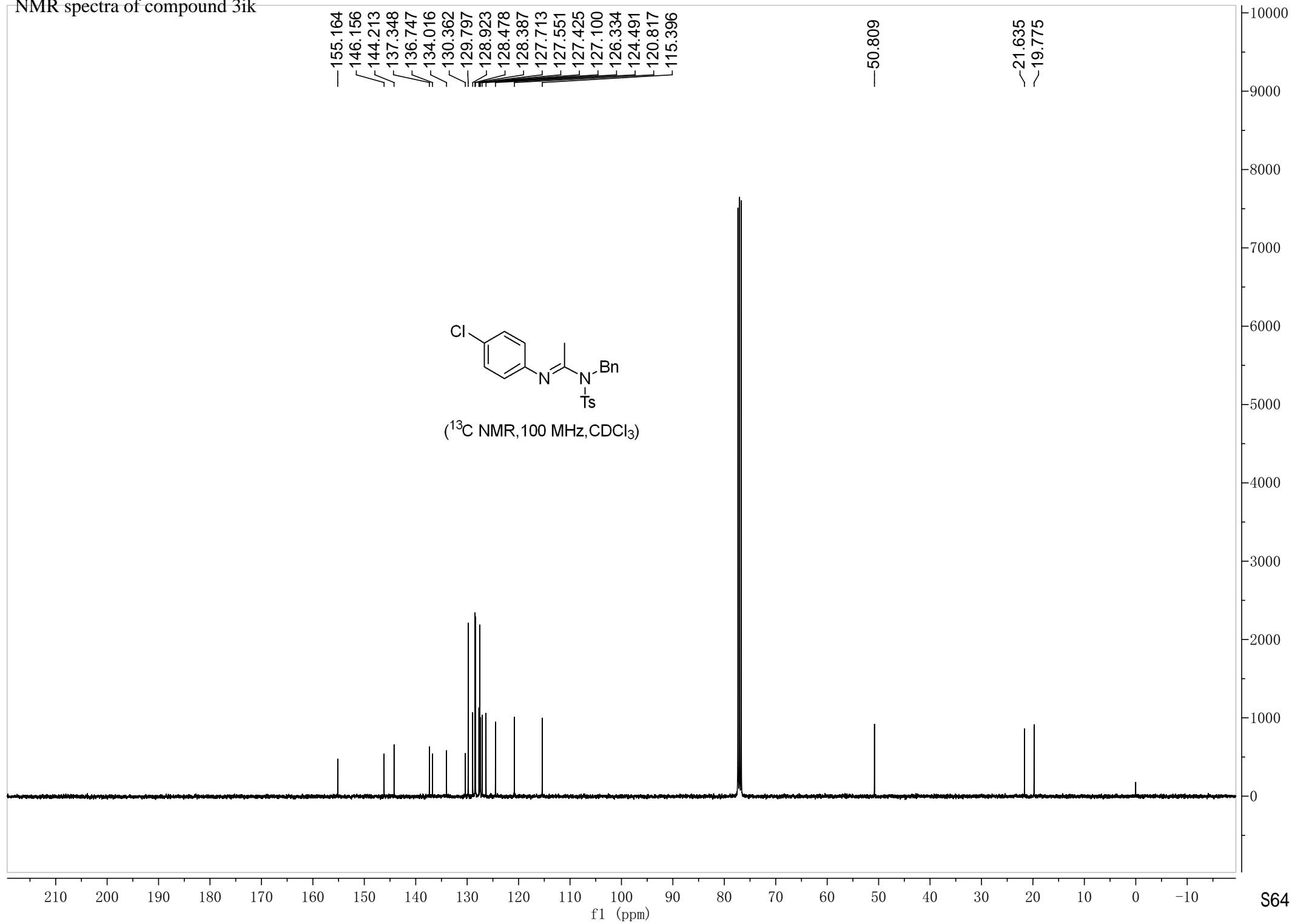
NMR spectra of compound 3dk



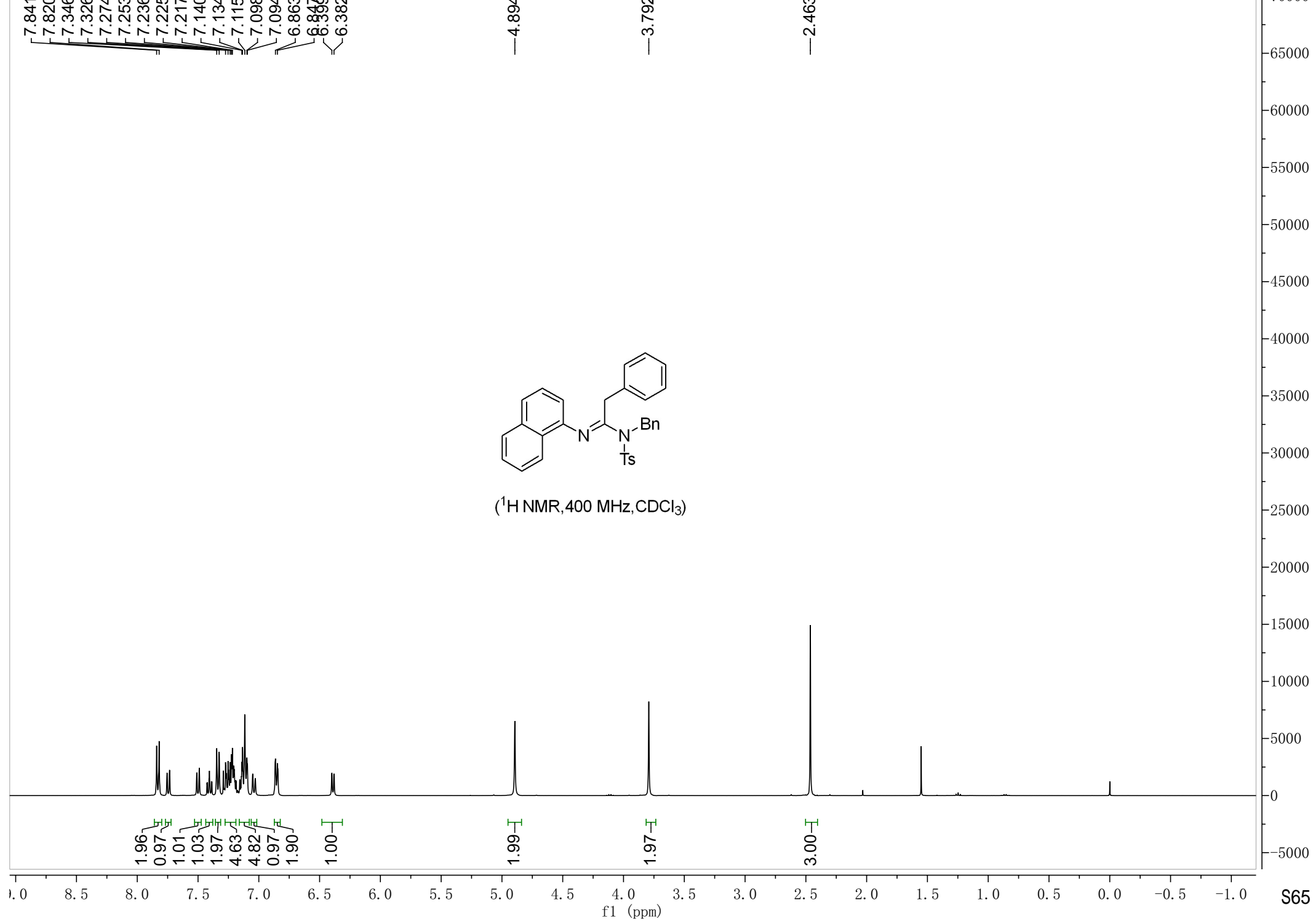
NMR spectra of compound 3ik



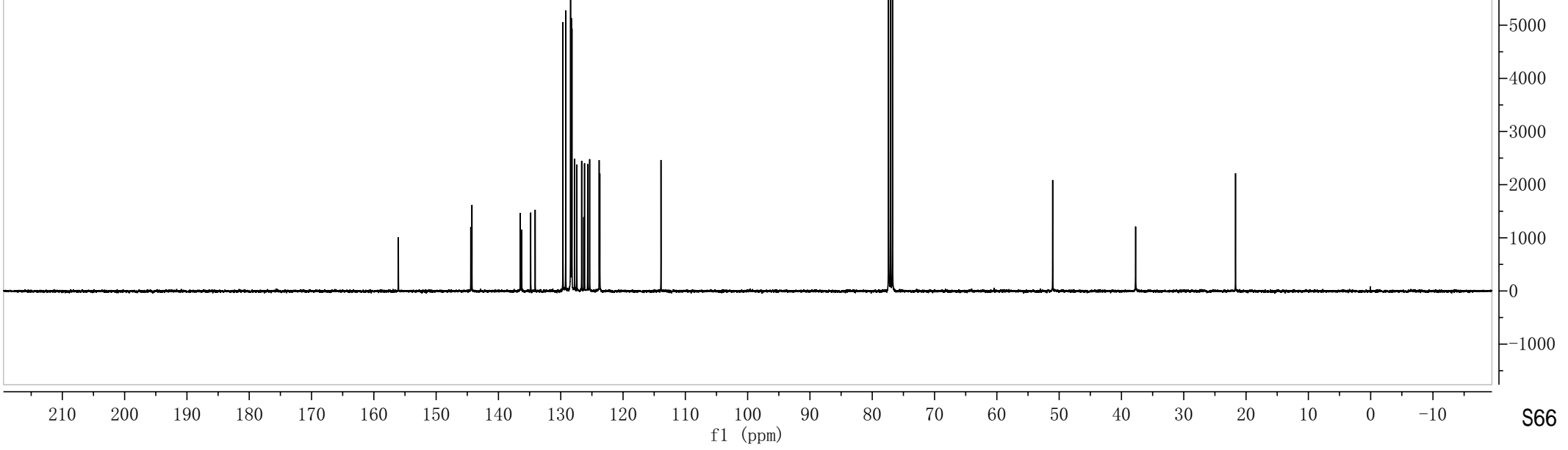
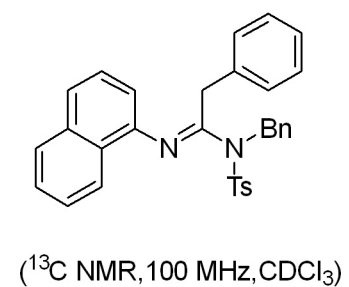
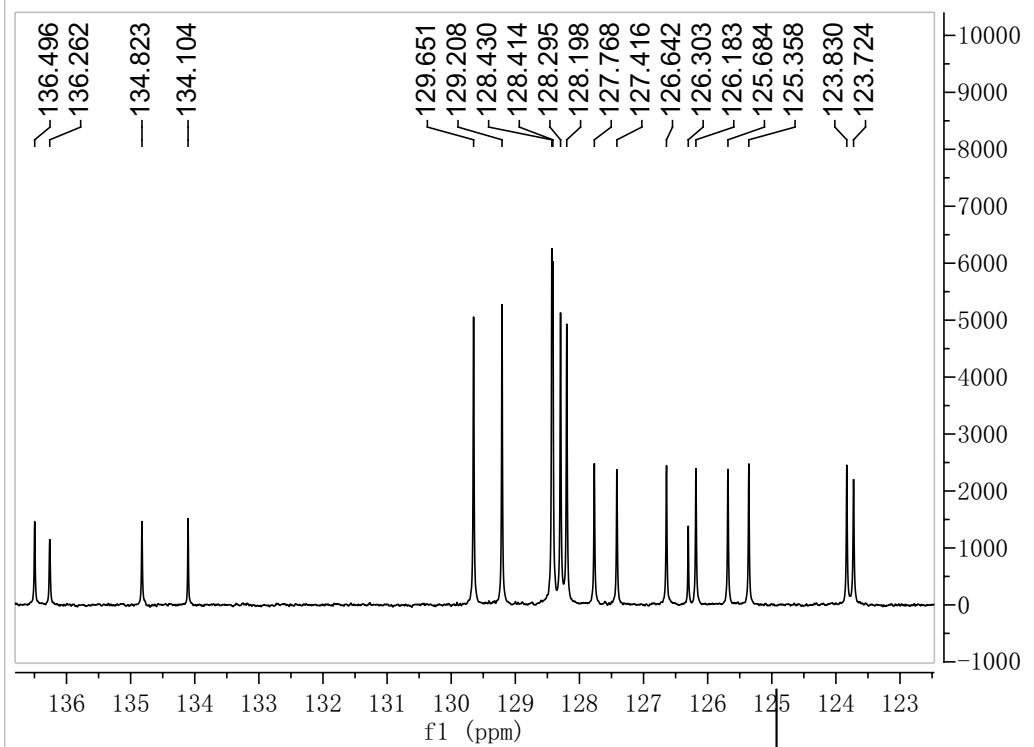
NMR spectra of compound 3ik



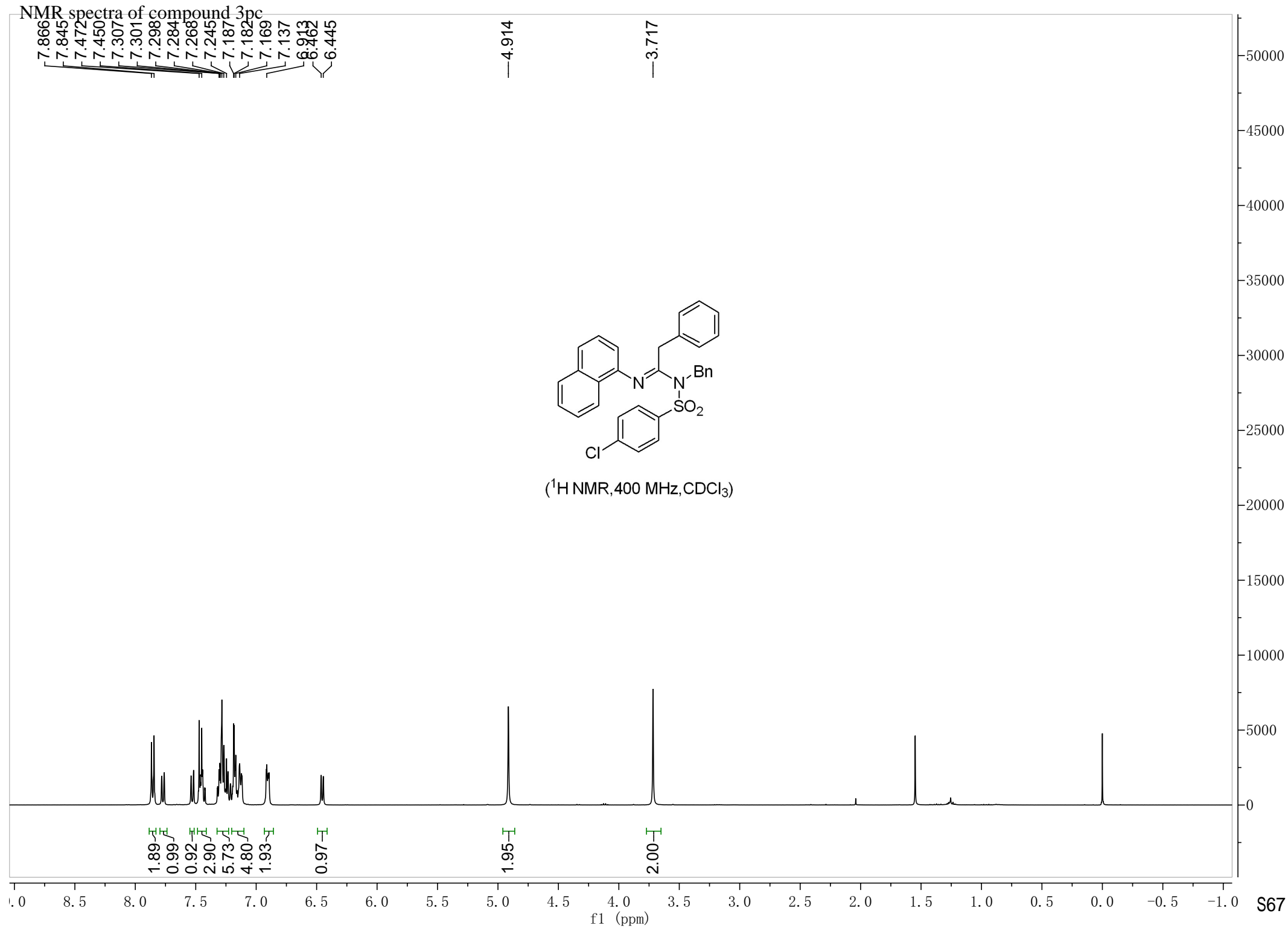
NMR spectra of compound 3pa



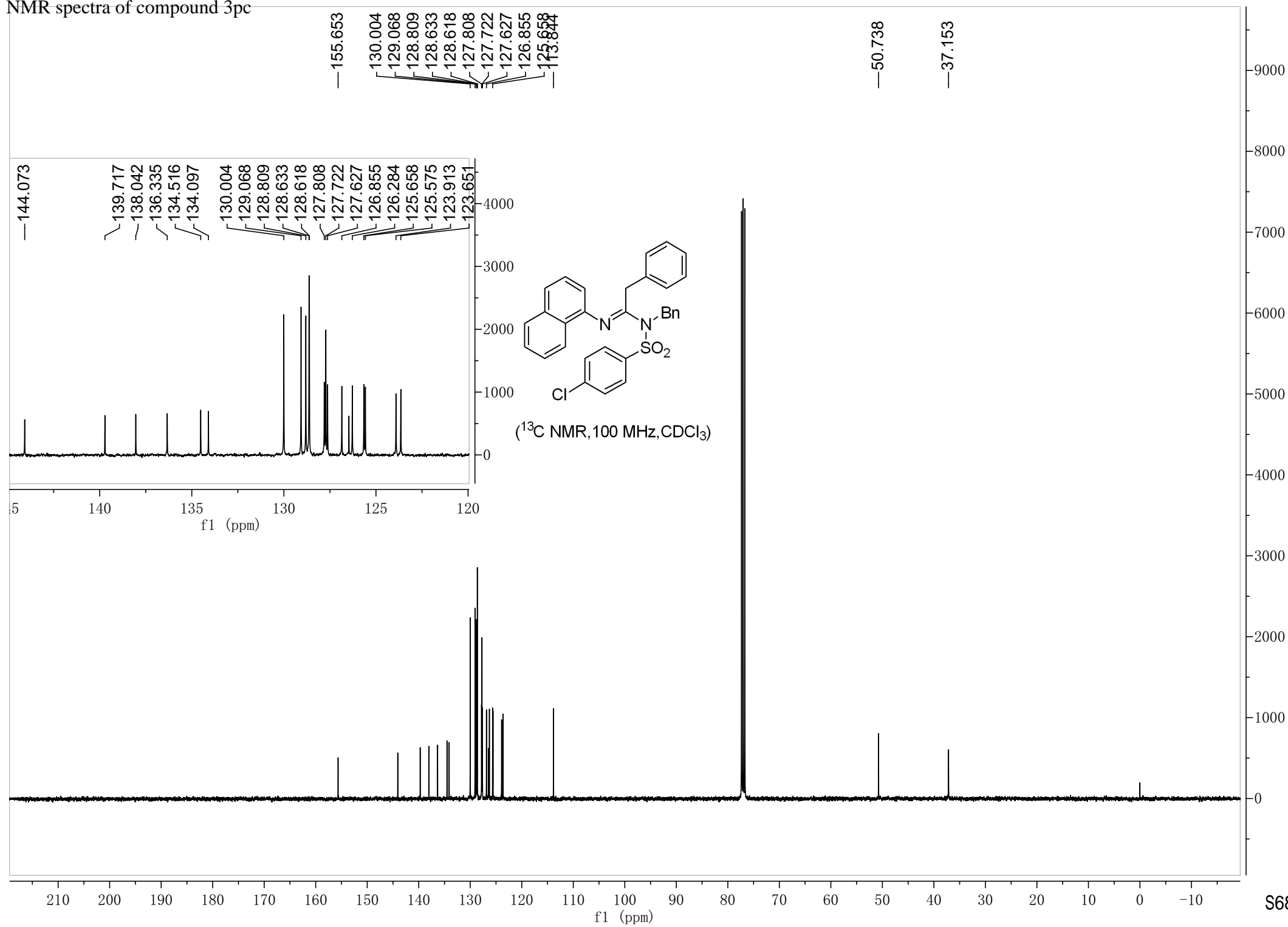
NMR spectra of compound 3pa



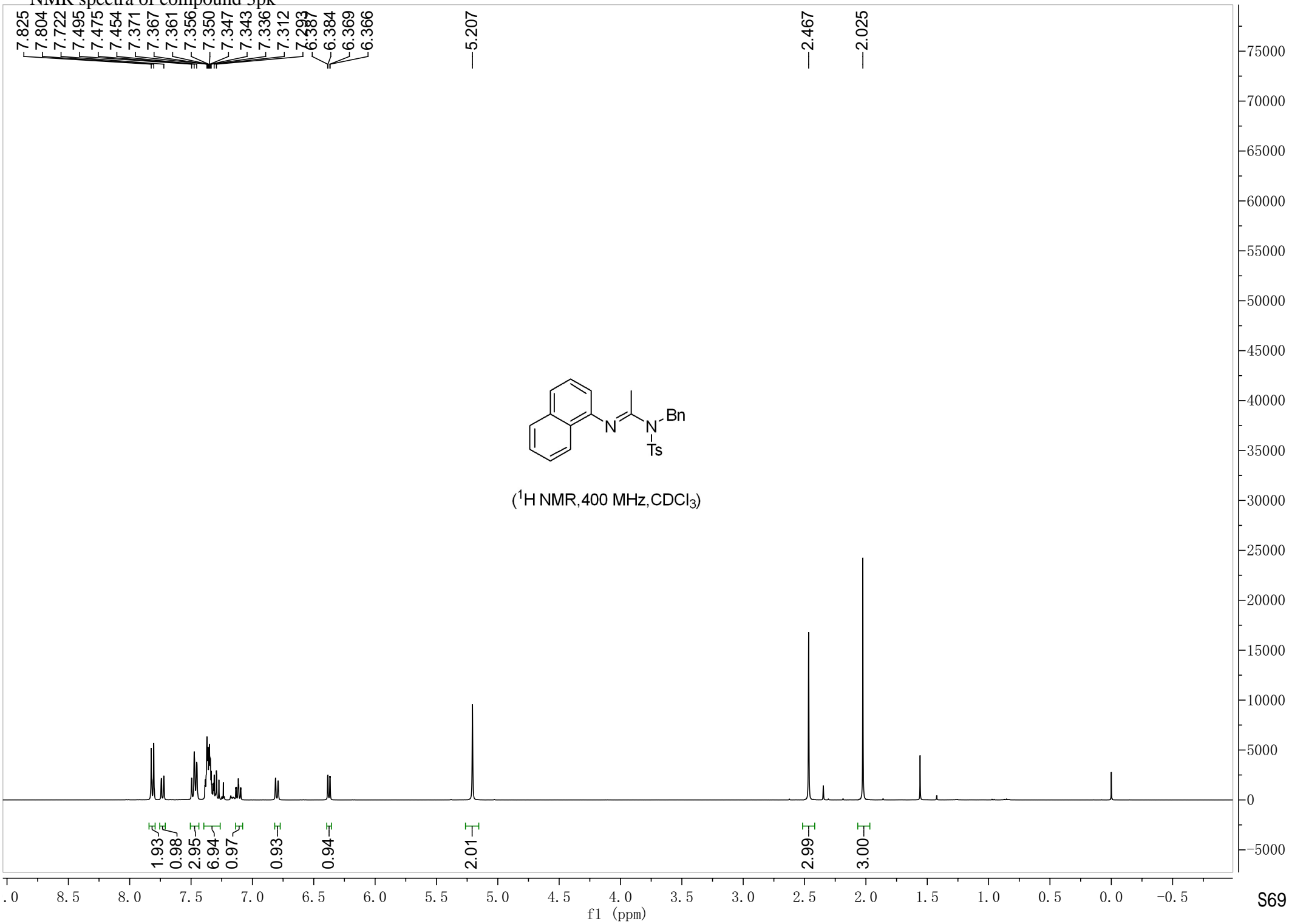
NMR spectra of compound 3pc



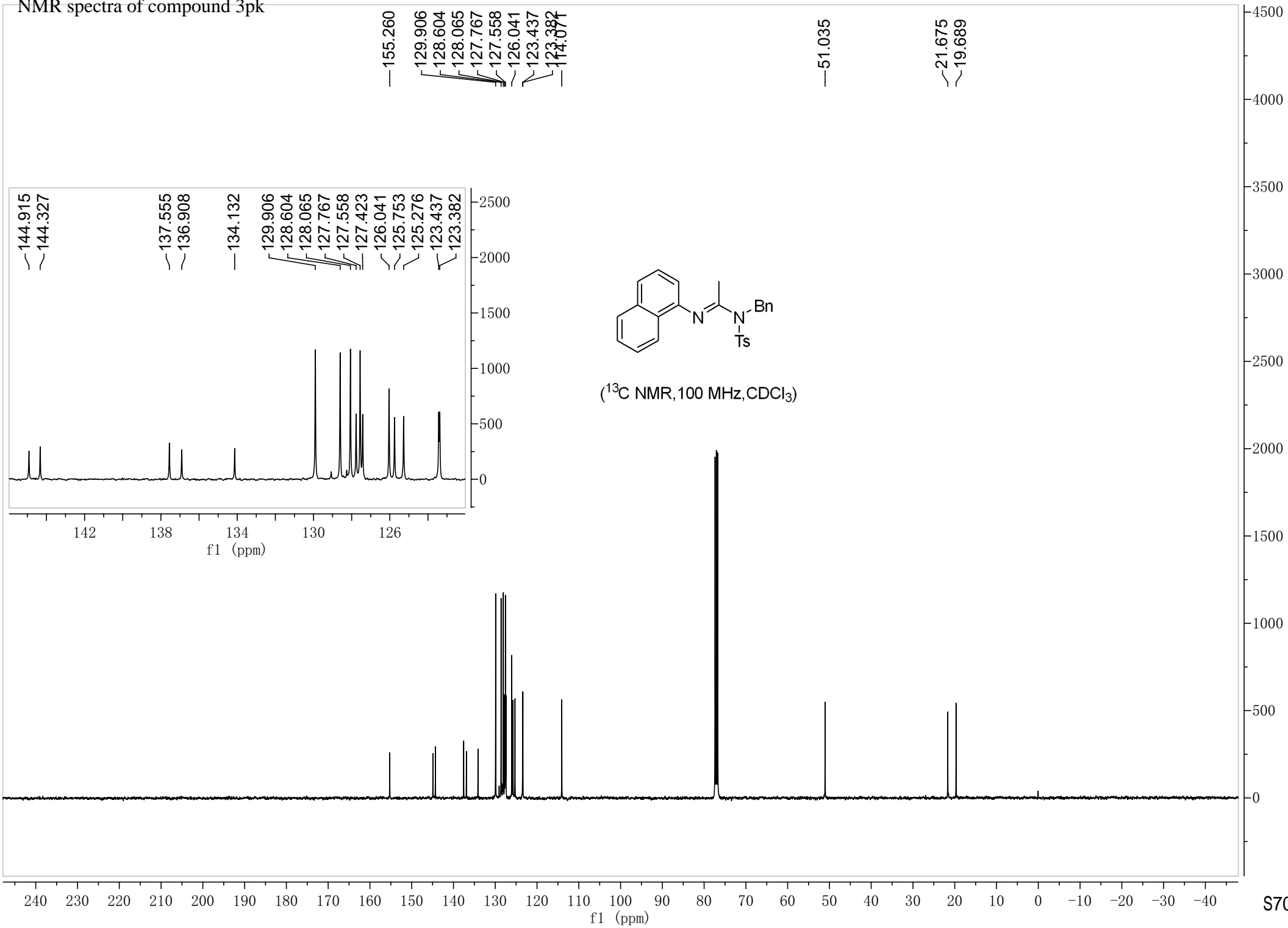
NMR spectra of compound 3pc

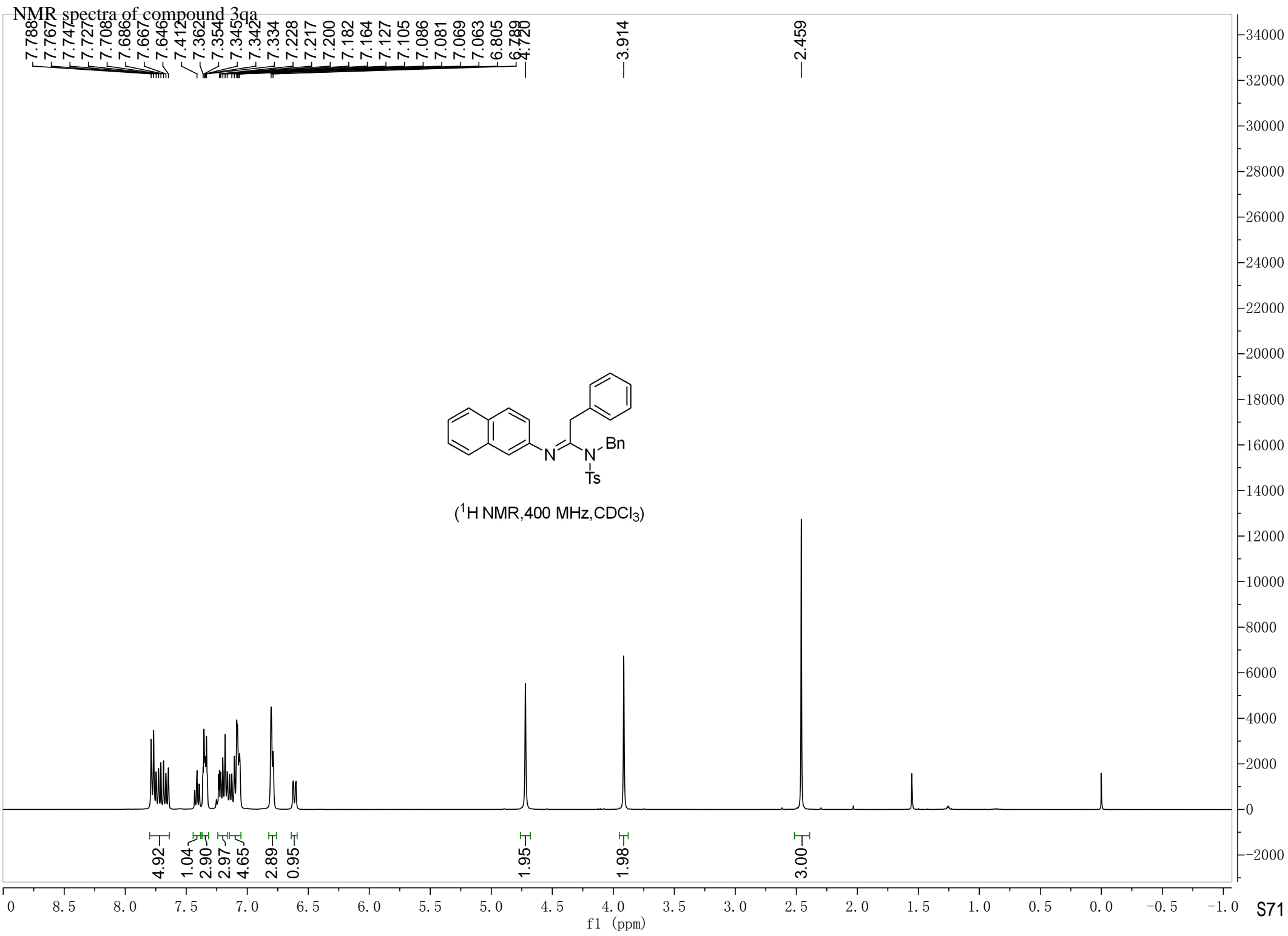


NMR spectra of compound 3pk

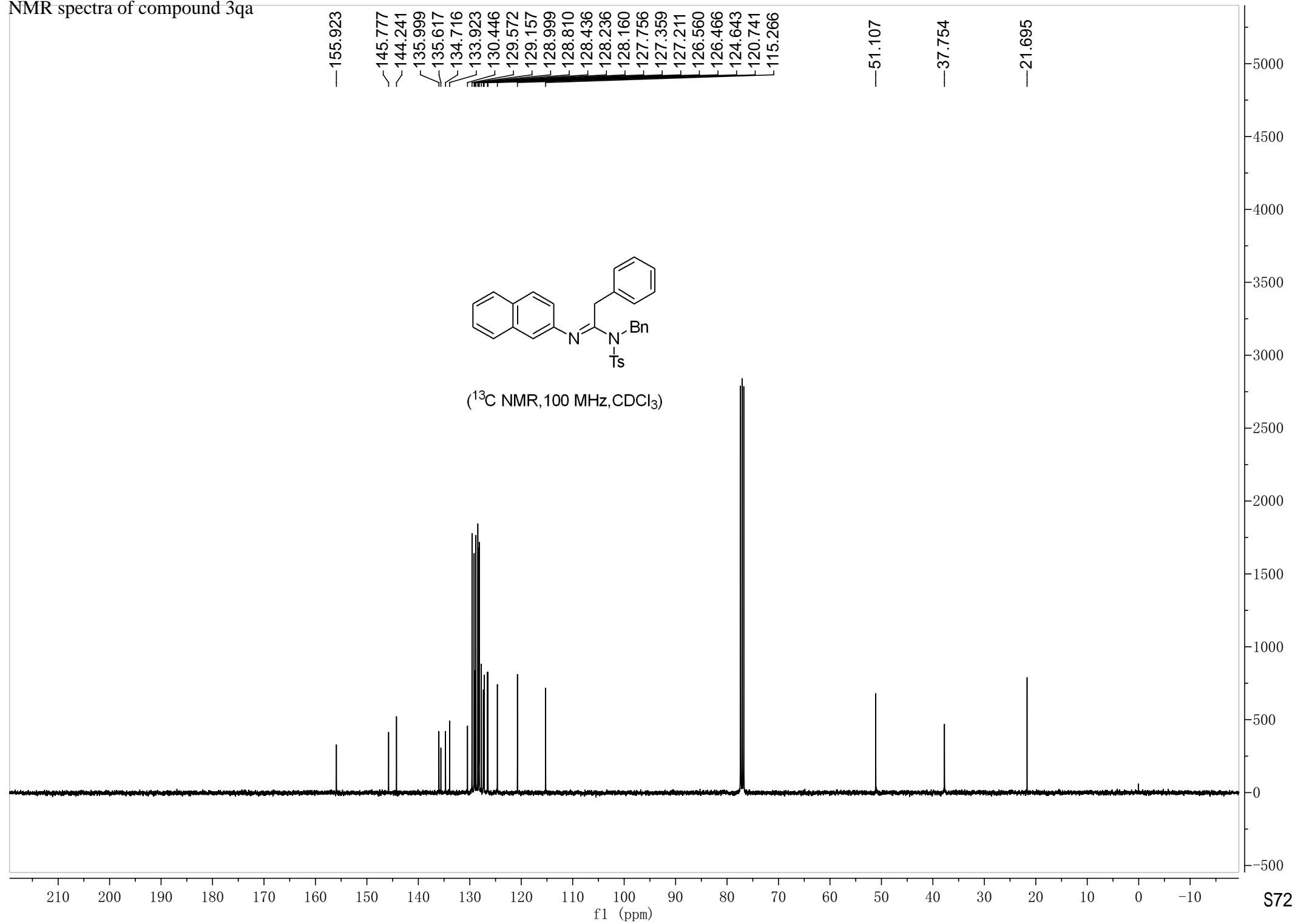


NMR spectra of compound 3pk



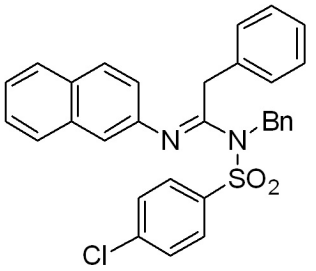


NMR spectra of compound 3qa



NMR spectra of compound 3gc

7.820
7.798
7.761
7.740
7.732
7.710
7.681
7.660
7.505
7.484
7.428
7.426
7.378
7.361
7.245
7.242
7.223
7.180
7.163
7.159
7.154
7.135
7.093
7.077
6.846
6.828
6.678
3.847



(¹H NMR, 400 MHz, CDCl₃)

1.93
1.98
0.98
1.95
0.98
1.02
8.03
2.96
1.00

2.01

2.00

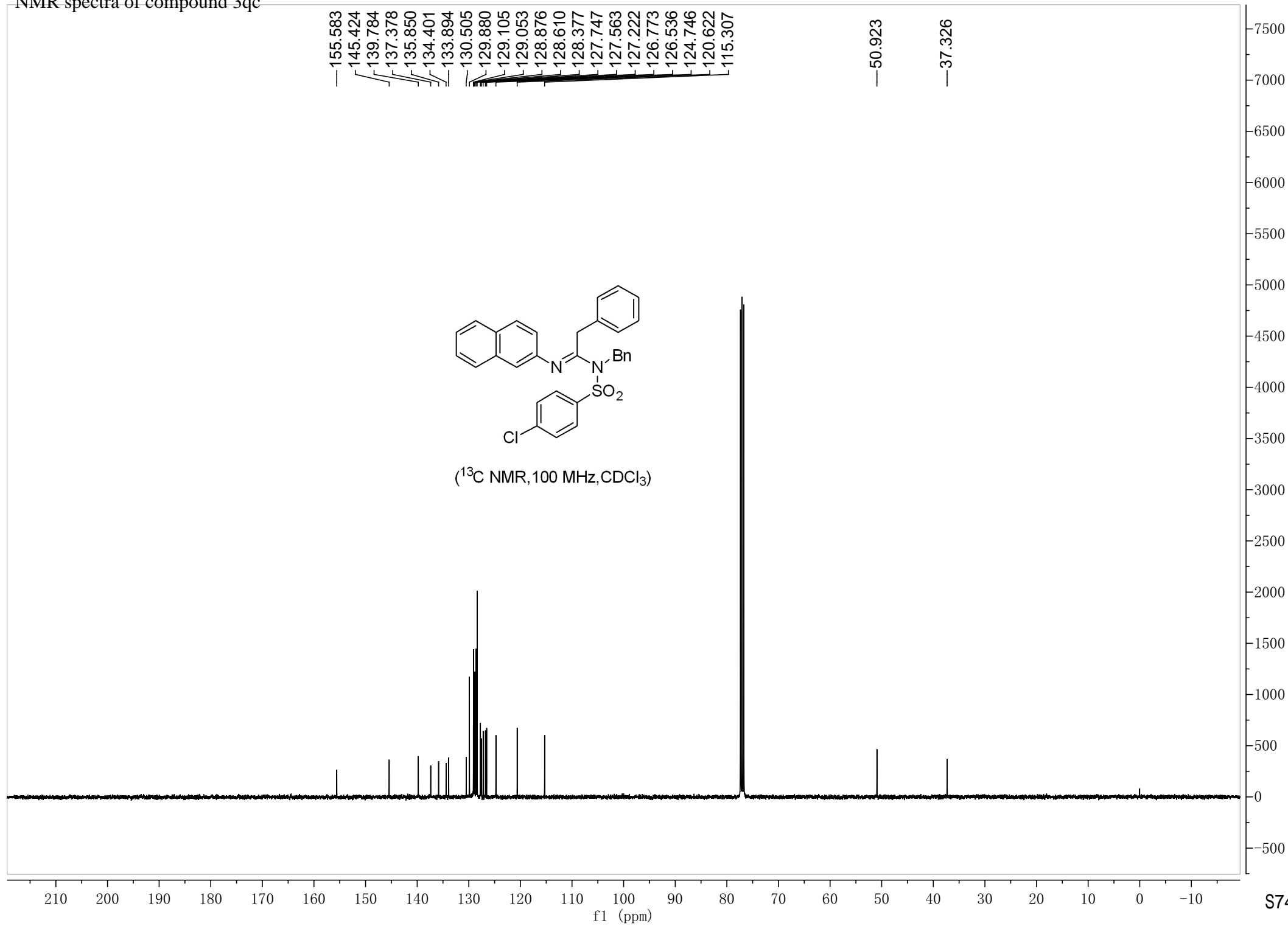
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

f1 (ppm)

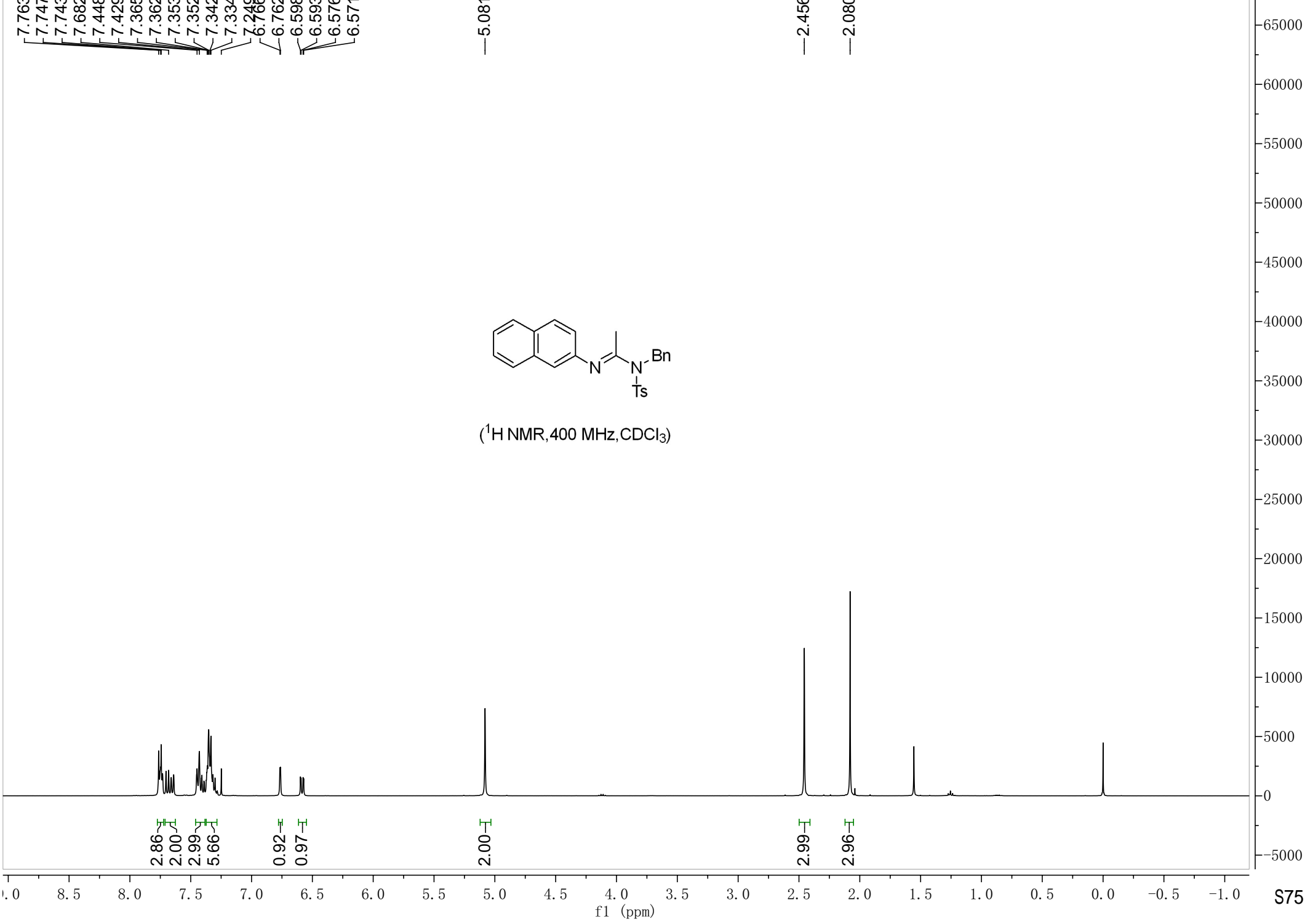
45000
40000
35000
30000
25000
20000
15000
10000
5000
0

S73

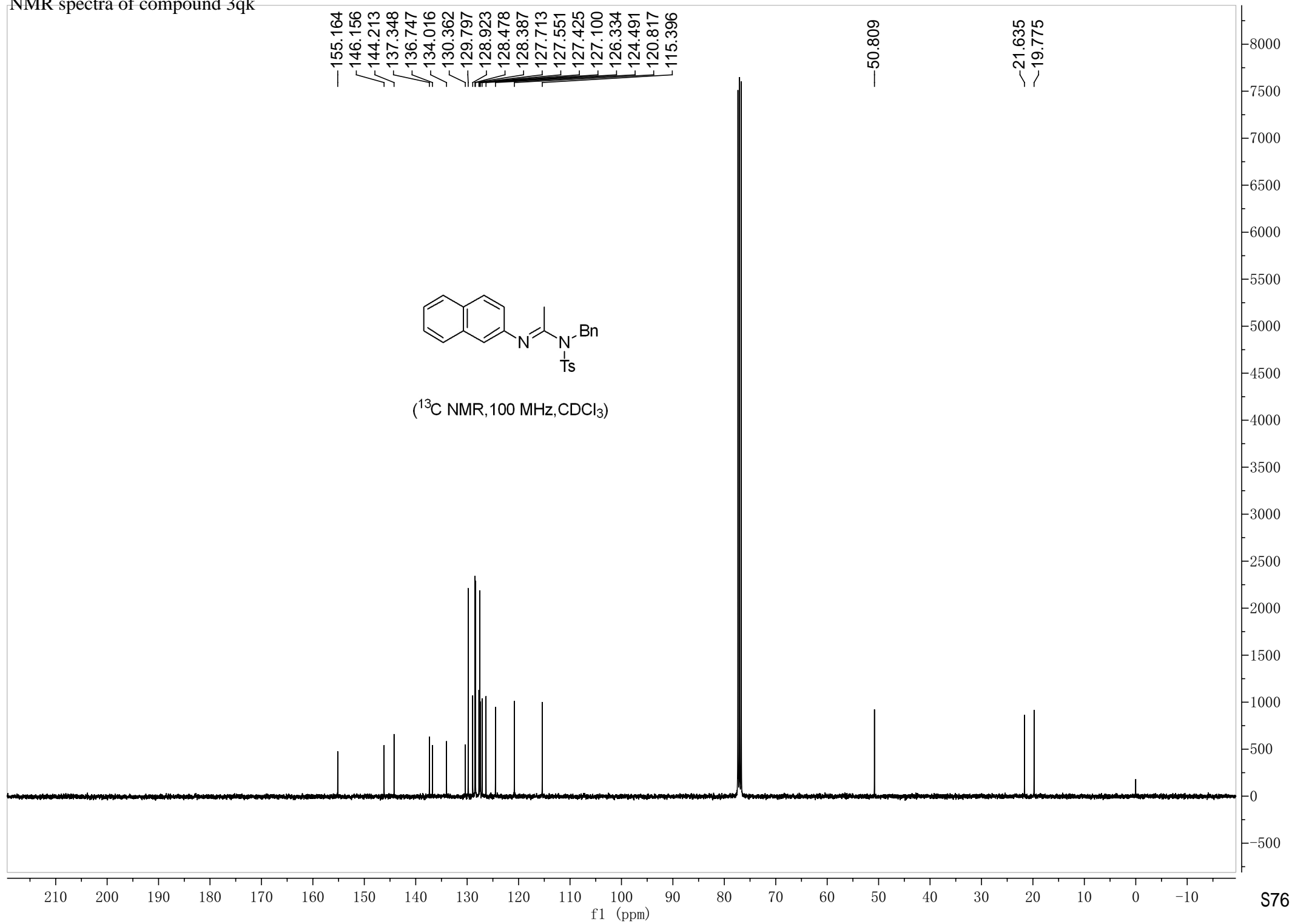
NMR spectra of compound 3qc



NMR spectra of compound 3qk



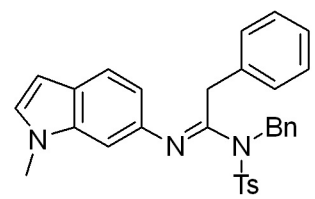
NMR spectra of compound 3qk



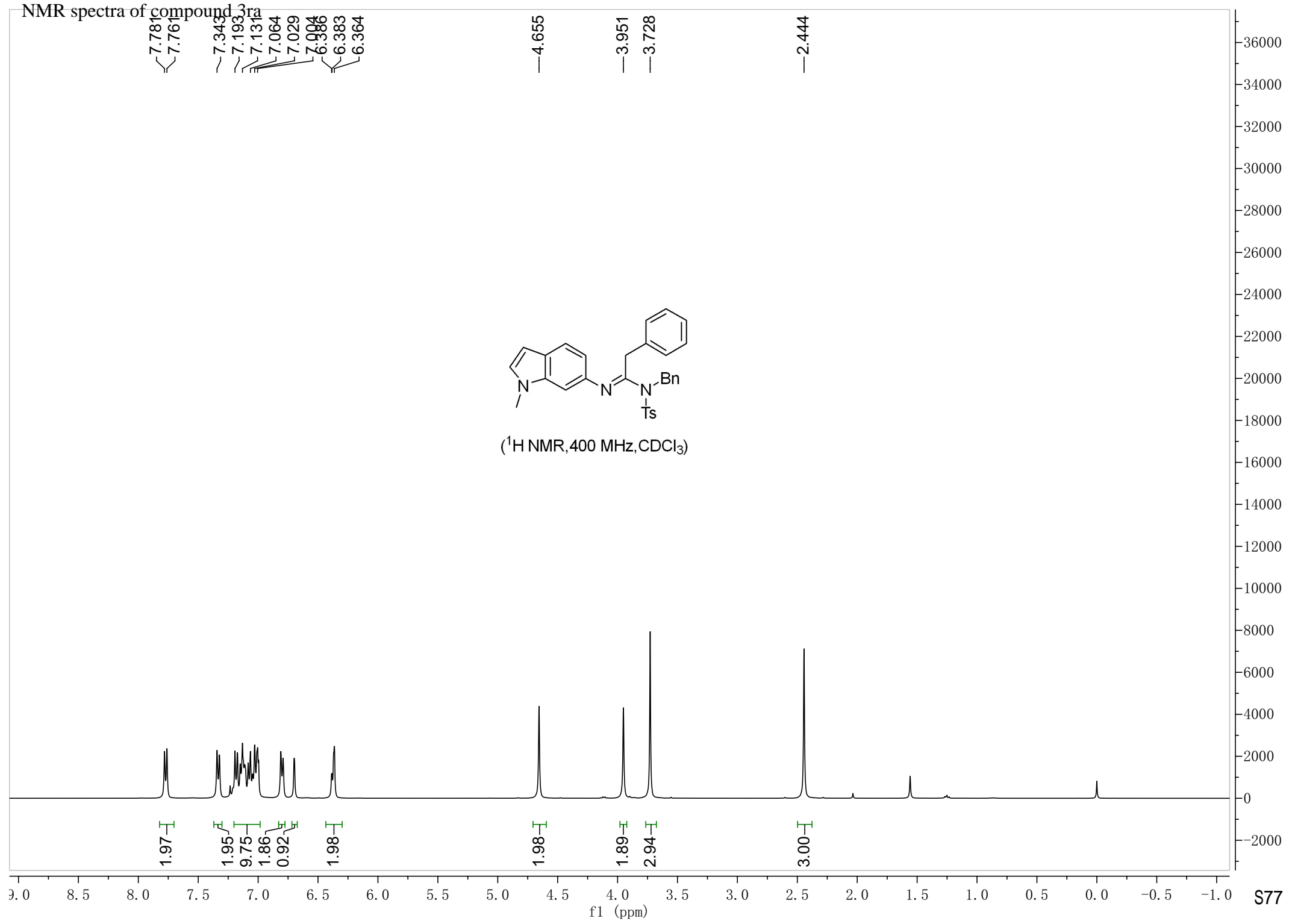
NMR spectra of compound 3ra

7.781
7.761
7.343
7.193
7.131
7.064
7.029
6.904
6.386
6.383
6.364

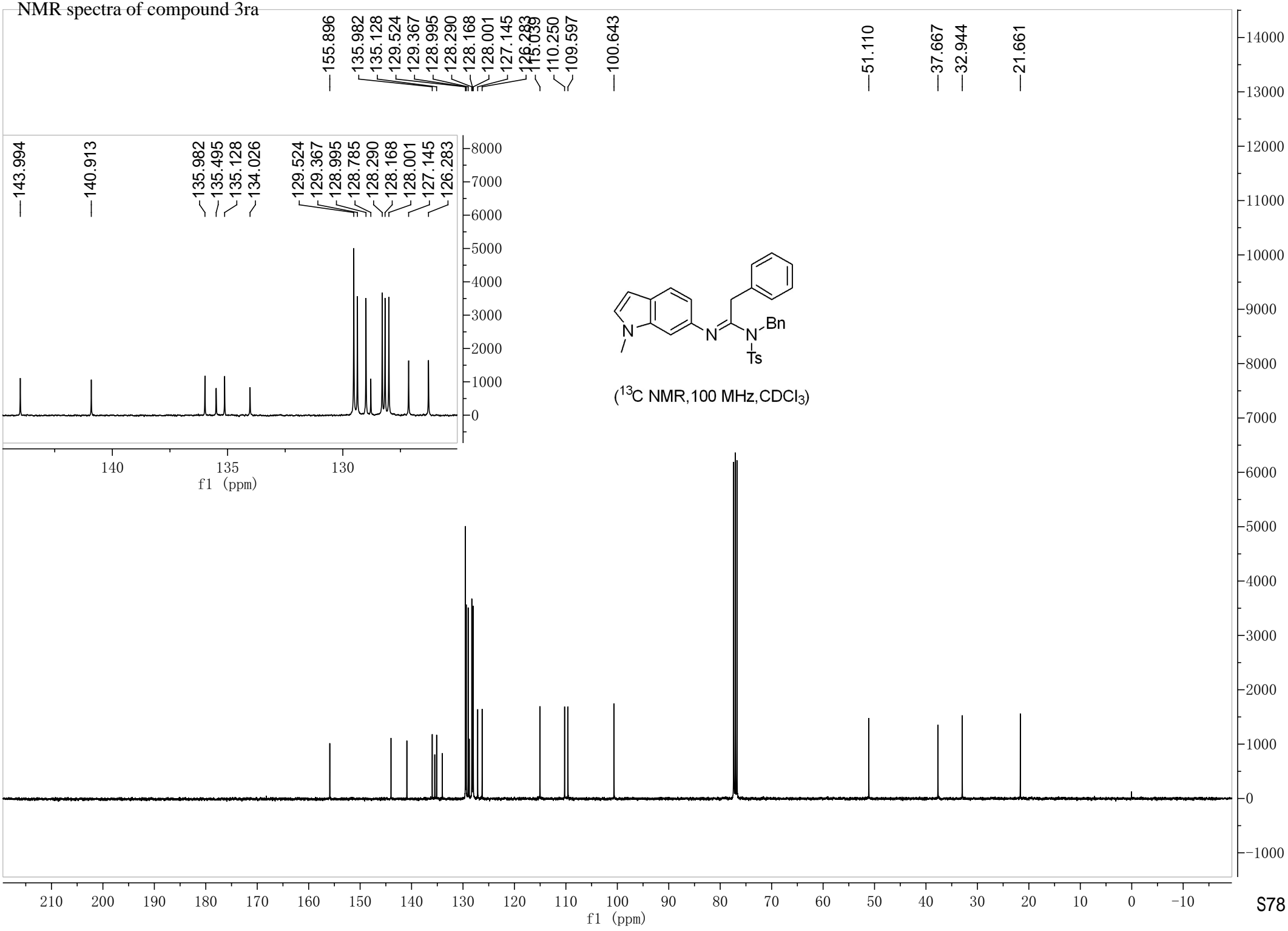
4.655
3.951
3.728
2.444



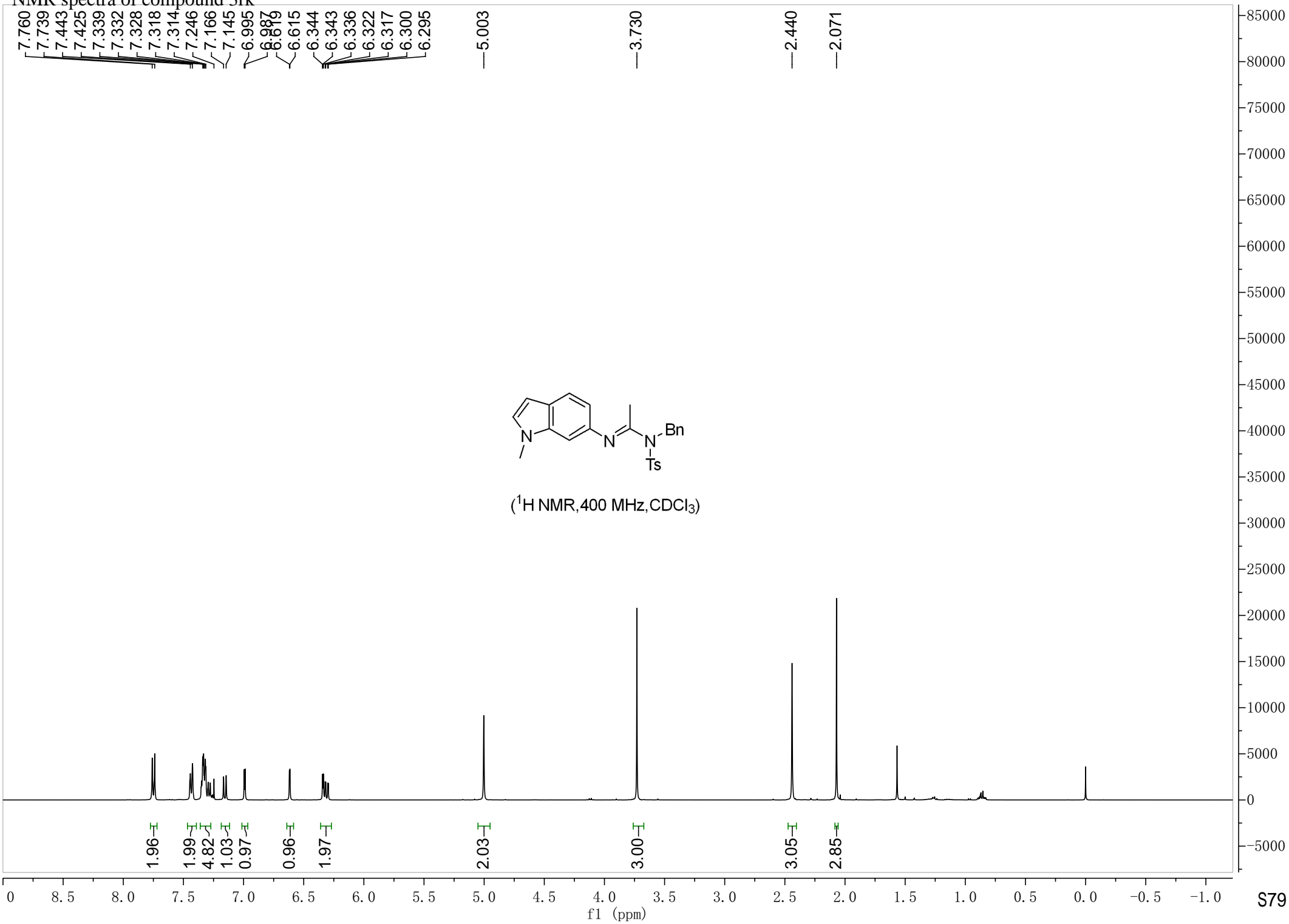
(¹H NMR, 400 MHz, CDCl₃)



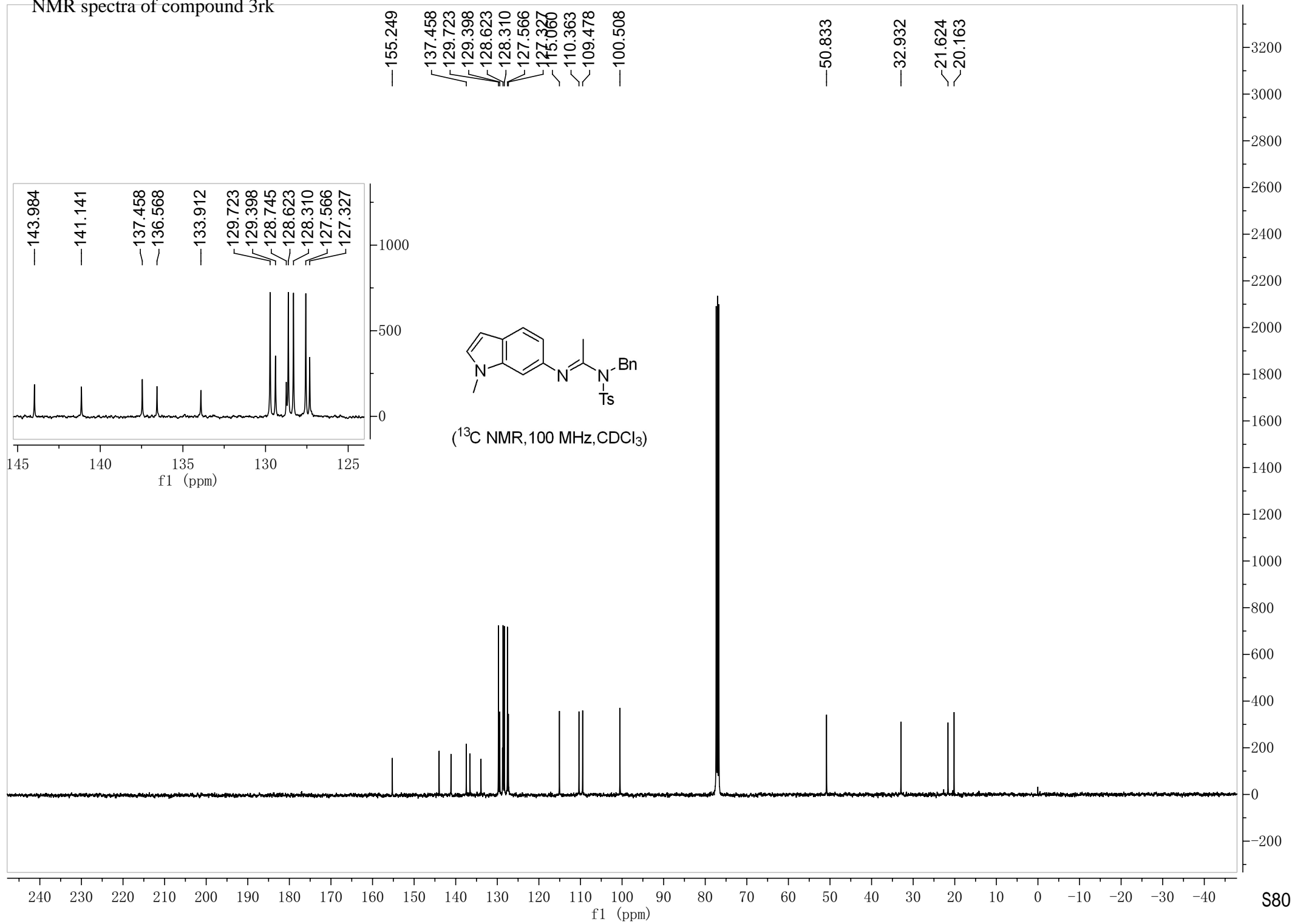
NMR spectra of compound 3ra



NMR spectra of compound 3rk



NMR spectra of compound 3rk

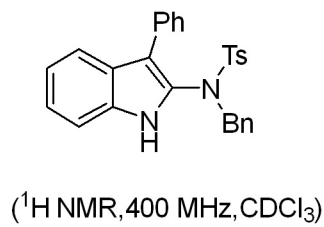


NMR spectra of compound 4

8.523
7.636
7.616
7.296
7.276
7.218
7.184
7.165
7.160
7.149
7.058
7.041
6.616
6.599

4.509

2.450



0.87

1.85

0.94

9.95

2.81

1.85

1.87

3.00

f1 (ppm)