Supporting Information

Synthesis of Tetrahydropyrrolo[1,2-*a*]quinolinone Analogues via $CoCl_2/AgSbF_6$-Catalyzed Cyclization of Unactivated *N,O*-Acetals with Olefins

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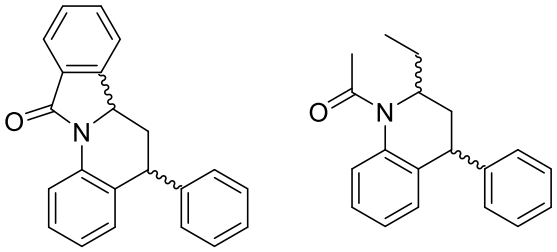
Table of Contents

1. Supplementary of Applicability for Various *N,O*-Acetal……S2

2.X-Ray Structure for Compounds **10c**/A and **10f**/B……S2

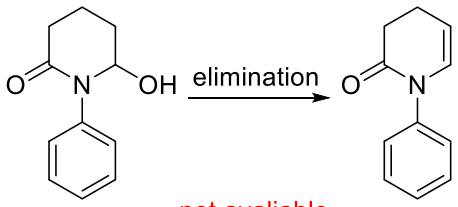
3. NMR Spectra of New Compounds……S7

1. Supplementary of Applicability for Various *N,O*-Acetal



11p, complex

11q, complex



8m **13**

2. X-Ray Structure for compounds 10c/A and 10f/B

The single crystal of compound **10c**/A and **10f**/B was prepared from its solution in petroleum ether/ethylacetate (5:1) by slow evaporation of the solvent. Crystal structure information has been deposited at the Cambridge Crystallographic Data Centre, CCDC: 2433902, 2433903.

a) X-ray data of Compound 10c/A:

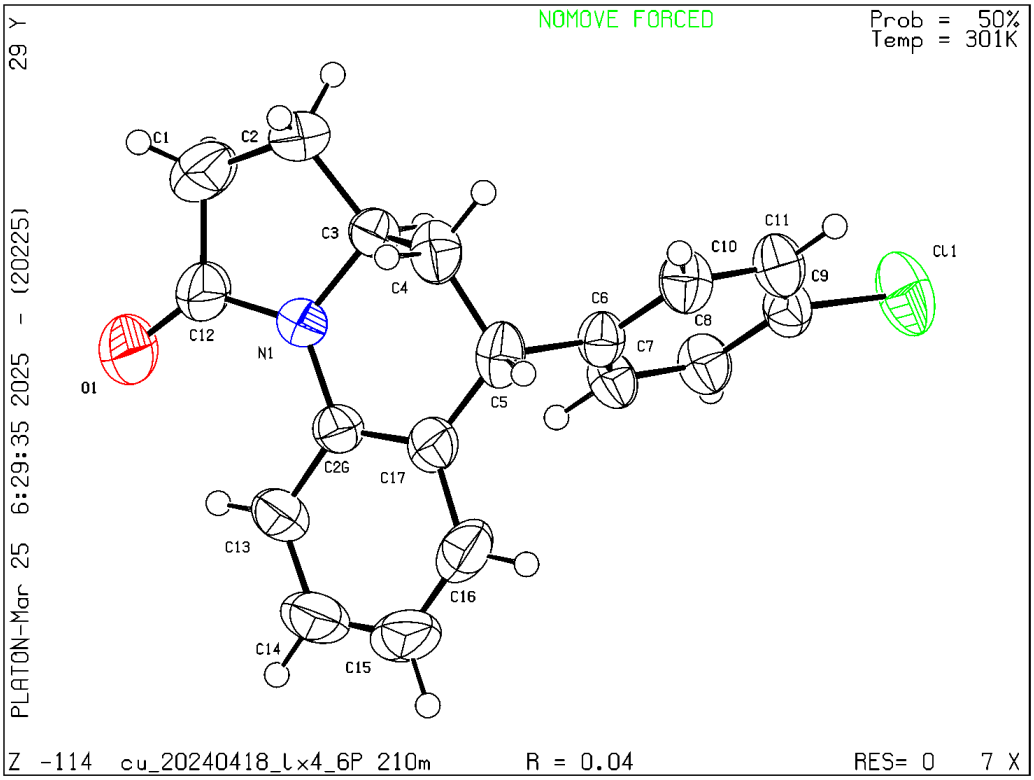


Figure S1. Ball and stick representation of compound **10c**/A (CCDC: 2433902) and thermal ellipsoids are drawn with 50% probability

Crystal data and structure refinement for 10c/A:

Identification code	20240418_lx4_64_1	
Chemical formula	$C_{18}H_{16}ClNO$	
Formula weight	297.77 g/mol	
Temperature	301(2) K	
Wavelength	1.54178 Å	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 7.1512(4) Å	α = 90°
	b = 11.1221(6) Å	β = 105.442(3)°
	c = 9.7789(5) Å	γ = 90°
Volume	749.70(7) $Å^3$	

Z	2	
Density (calculated)	1.319 g/cm^3	
Absorption coefficient	2.226 mm^{-1}	
F(000)	312	
Diffractometer	d8 venture	
Theta range for data collection	4.69 to 65.05°	
Index ranges	-8<=h<=8, -13<=k<=9, -11<=l<=11	
Reflections collected	9245	
Independent reflections	2246 [R(int) = 0.0565]	
Coverage of independent reflections	99.7%	
Absorption correction	Multi-Scan	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2018/2 (Sheldrick, 2018)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	2246 / 1 / 190	
Goodness-of-fit on F^2	1.054	
Final R indices	2023 data; I>2σ(I)	R1 = 0.0403, wR2 = 0.1021
	all data	R1 = 0.0458, wR2 = 0.1062

b) X-ray data of Compound 10f/B:

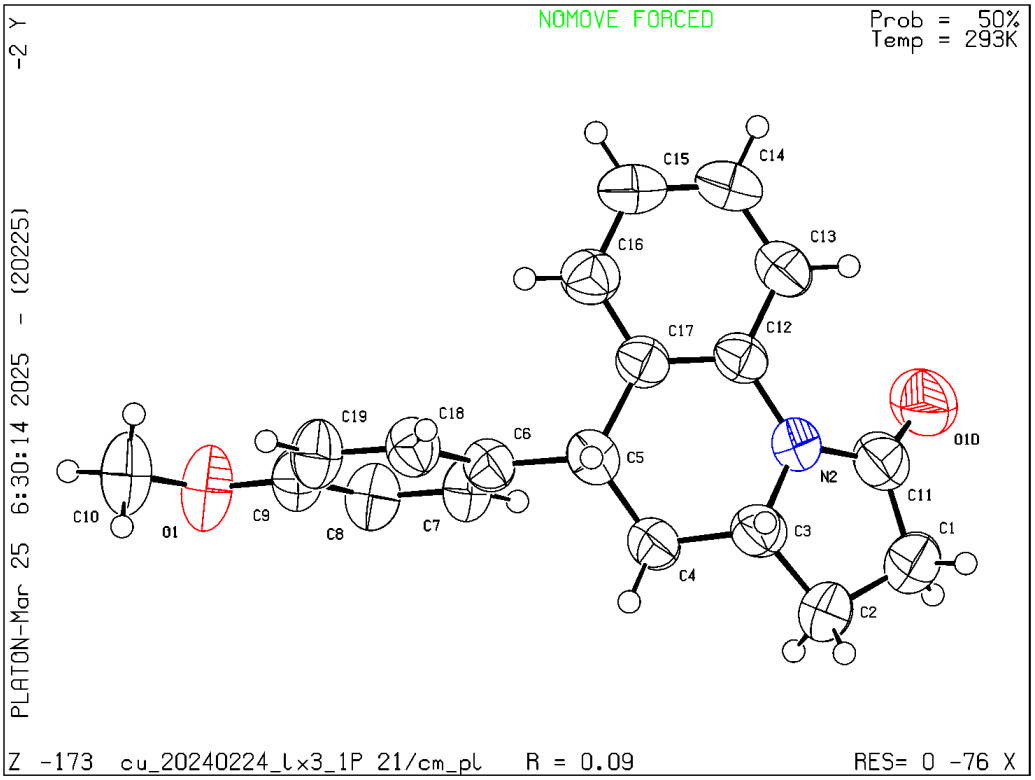


Figure S2. Ball and stick representation of compound **10f**/B (CCDC: 2433903) and thermal ellipsoids are drawn with 50% probability

Crystal data and structure refinement for 10f/B:

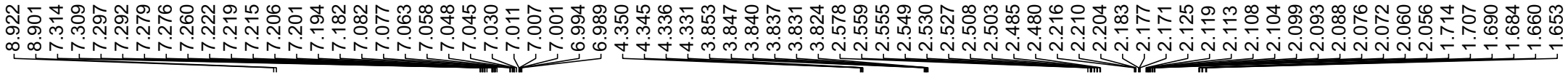
Identification code	20240224_LX3_151_2	
Chemical formula	$C_{19}H_{19}NO_2$	
Formula weight	293.35 g/mol	
Temperature	293(2) K	
Wavelength	1.54184 Å	
Crystal size	0.200 x 0.200 x 0.150 mm	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 21.821(9) Å	α = 90°
	b = 8.608(3) Å	β = 95.229(17)°
	c = 8.127(4) Å	γ = 90°

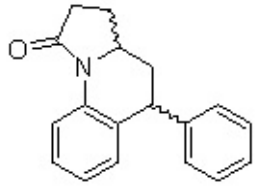
Volume	1520.2(11) $Å^3$
Z	4
Density (calculated)	1.282 g/cm^3
Absorption coefficient	0.658 mm^{-1}
F(000)	624
Diffractometer	d8_venture
Theta range for data collection	4.069 to 65.397°
Index ranges	-25<=h<=25, -10<=k<=10, -9<=l<=9
Reflections collected	28991
Independent reflections	2589 [R(int) = 0.1005]
Coverage of independent reflections	99.0%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7526 and 0.6550
Structure solution technique	direct methods
Structure solution program	SHELXT 2018/2 (Sheldrick, 2018)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2589 / 0 / 200
Goodness-of-fit on F^2	0.952

Final R indices	1914 data; I>2σ(I)	R1 = 0.0924, wR2 = 0.2725
	all data	R1 = 0.1160, wR2 = 0.2937

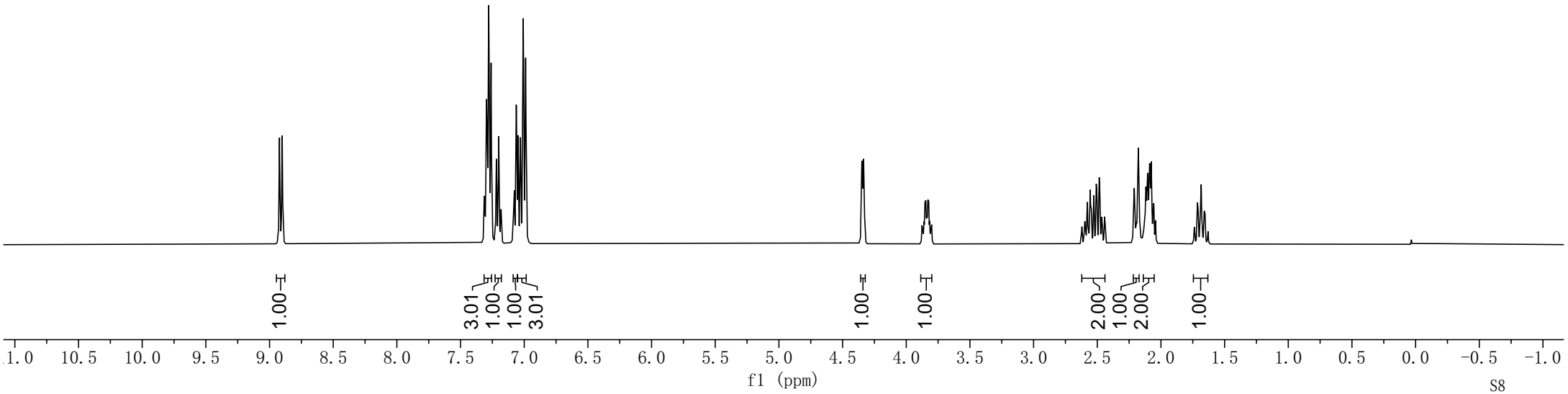
3. NMR Spectra of New Compounds

10a/A



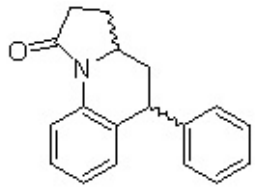


(^{1}H NMR, 400 MHz, $CDCl_3$)

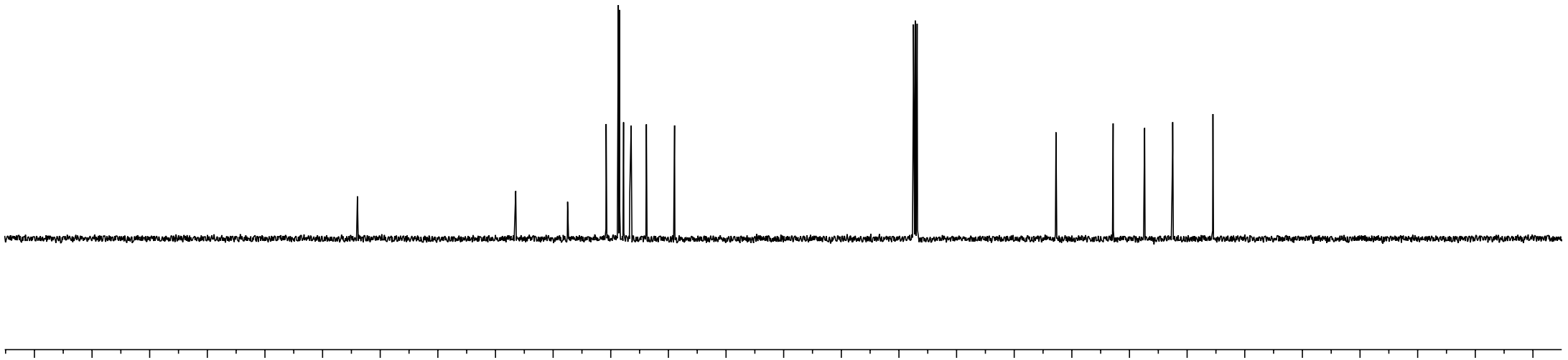


10a/A

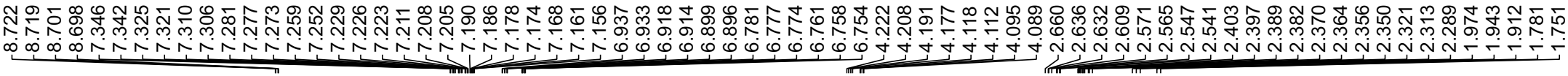
173.953
146.489
137.490
130.800
128.686
128.473
127.779
126.703
126.467
123.822
118.931
52.752
42.838
37.376
32.503
25.520

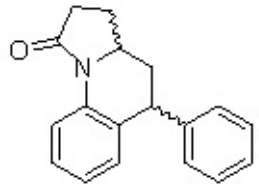


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

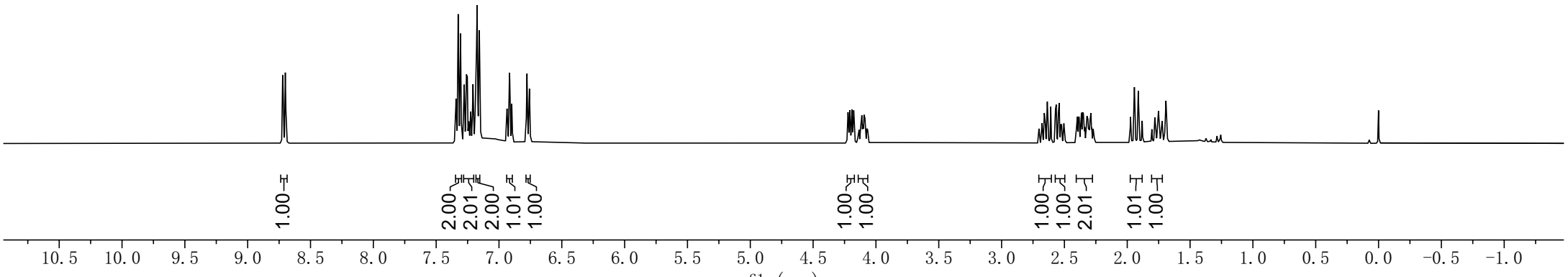


10a/B



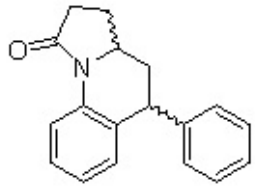


(^{1}H NMR, 400 MHz, $CDCl_3$)

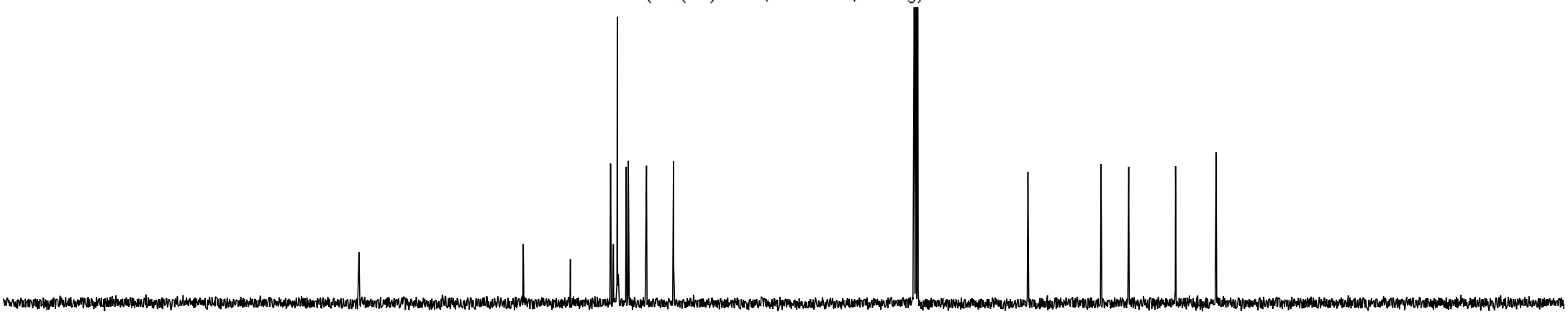


10a/B

173.575
145.137
136.992
130.025
129.539
128.867
128.719
127.316
126.953
123.805
119.135
57.777
45.124
40.329
32.229
25.202



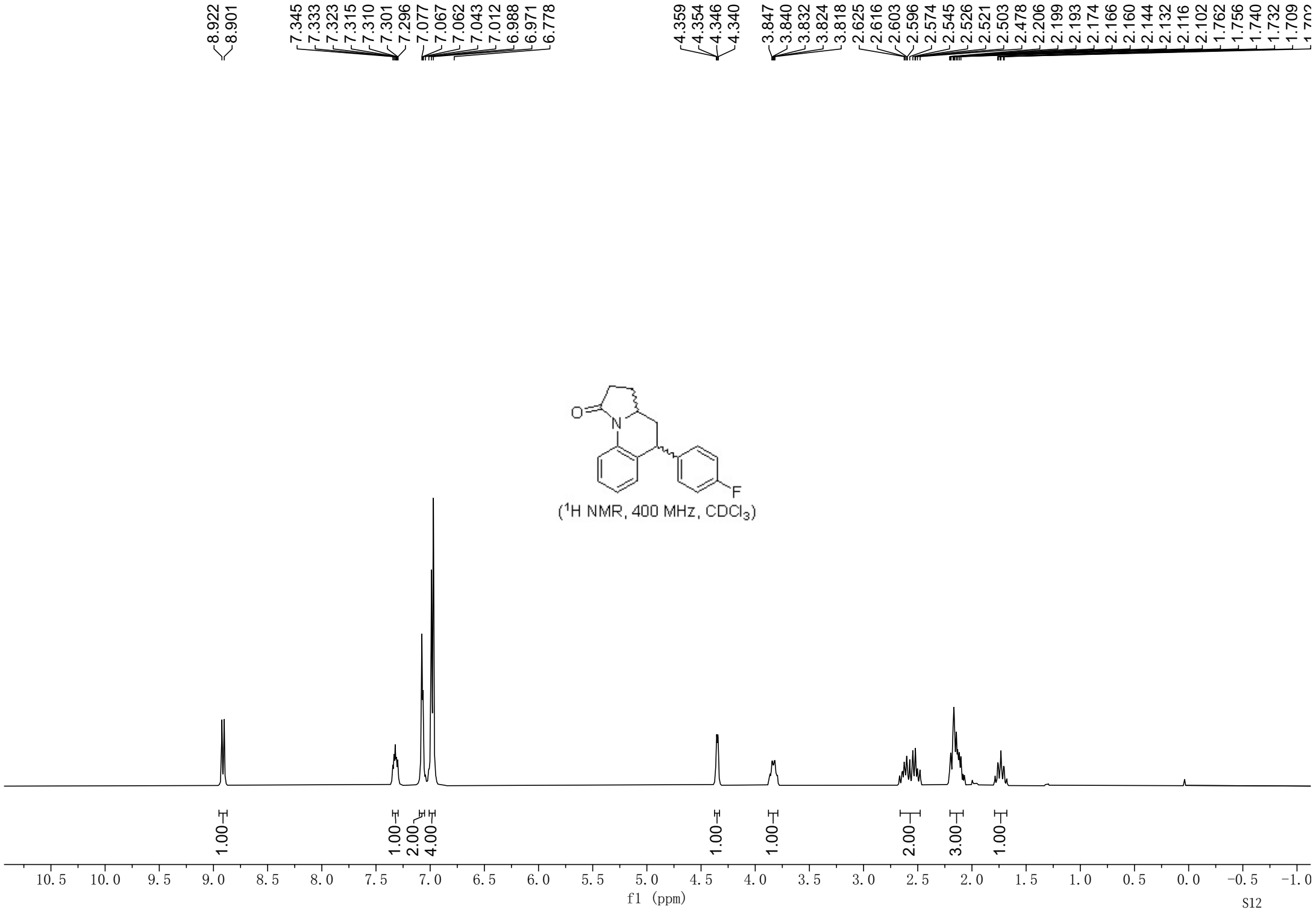
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30

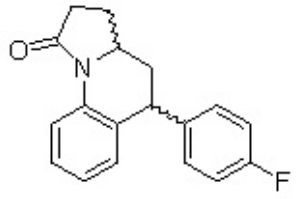
f1 (ppm)

10b/A

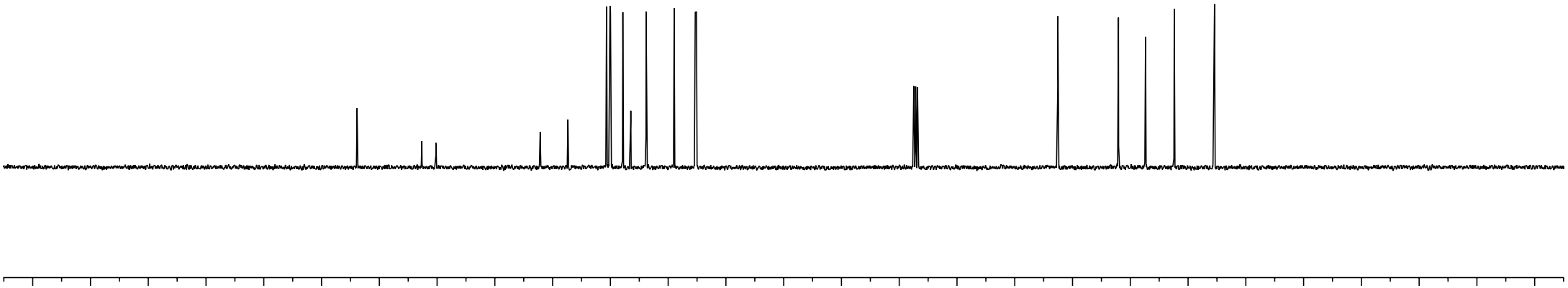

8.922
8.901
7.345
7.333
7.323
7.315
7.310
7.301
7.296
7.077
7.067
7.062
7.043
7.012
6.988
6.971
6.778
4.359
4.354
4.346
4.340
3.847
3.840
3.832
3.824
3.818
2.625
2.616
2.603
2.596
2.574
2.545
2.526
2.521
2.503
2.478
2.206
2.199
2.193
2.174
2.166
2.160
2.144
2.132
2.116
2.102
1.762
1.756
1.740
1.732
1.709
O
N
F
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
2.00
4.00
1.00
1.00
2.00
3.00
1.00
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 -0.5 -1.0
f1 (ppm)

10b/A

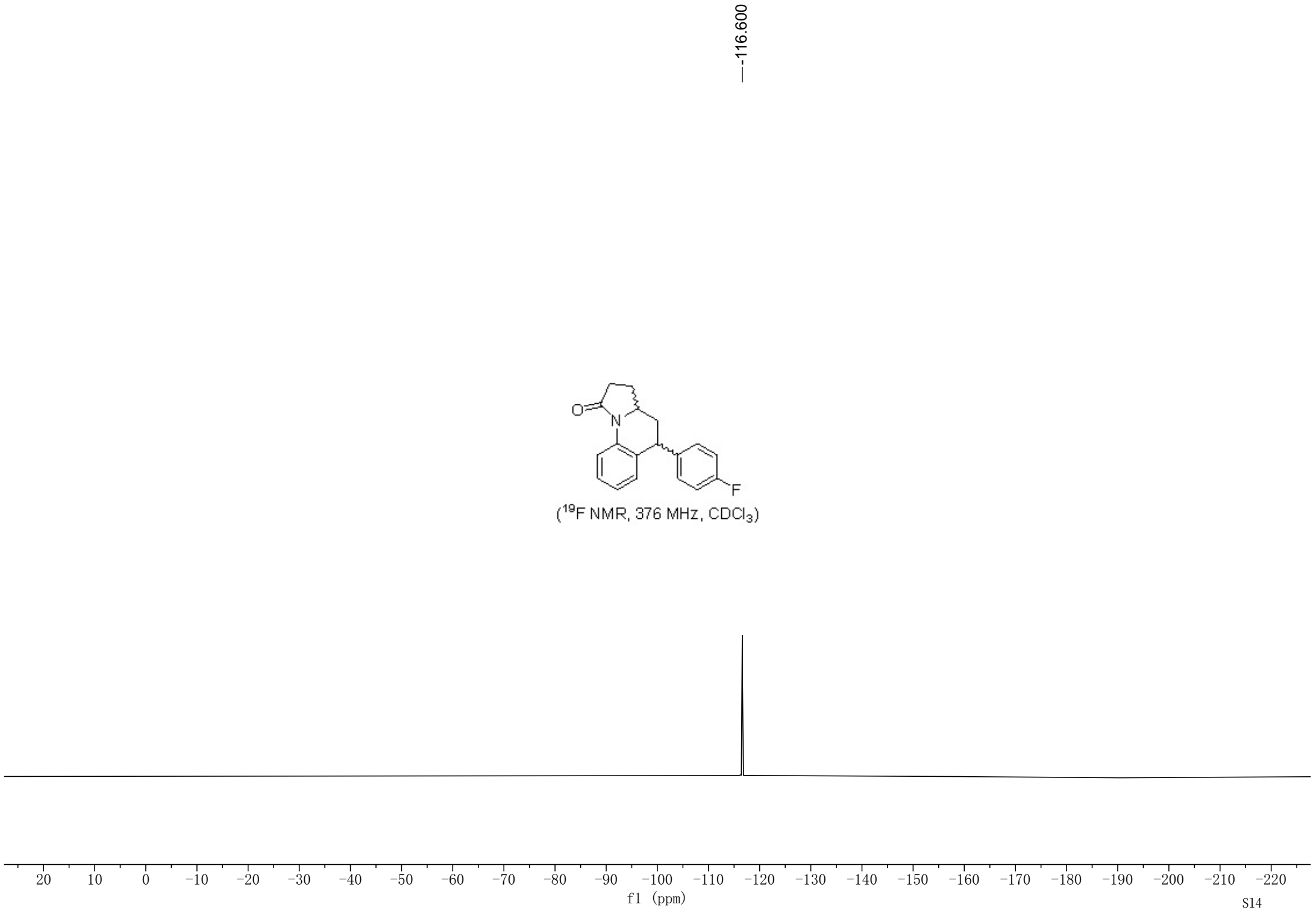
173.847
162.635
160.195
142.154
142.123
137.349
130.664
130.063
129.984
127.844
126.470
123.817
118.959
115.312
115.100
52.539
42.049
37.360
32.393
25.422



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

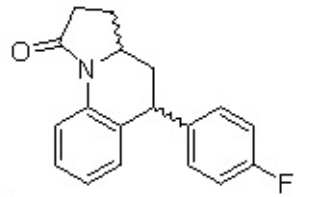


10b/A

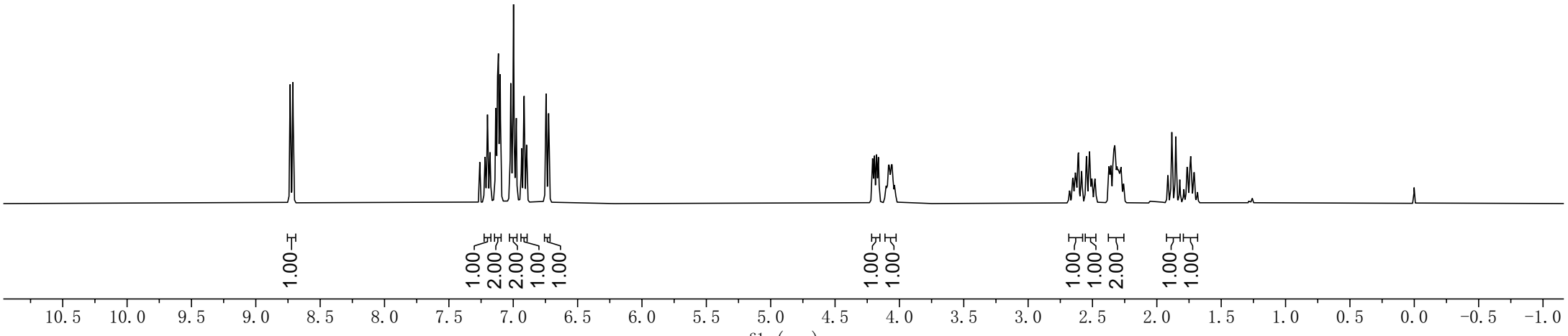

-116.600
O
N
F
(19F NMR, 376 MHz, CDCl3)
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −220
f1 (ppm)

10b/B

8.733 8.712 7.220 7.201 7.198 7.180 7.136 7.131 7.123 7.115 7.106 7.101 7.019 6.998 6.977 6.935 6.916 6.897 6.745 6.725 4.208 4.194 4.177 4.163 4.090 4.085 4.080 4.074 4.067 4.062 4.056 4.051 2.651 2.636 2.632 2.617 2.612 2.608 2.604 2.585 2.581 2.548 2.544 2.541 2.530 2.524 2.518 2.506 2.481 2.373 2.366 2.358 2.353 2.340 2.334 2.325 2.319 2.307 2.299 2.293 2.283 2.276 1.915 1.884 1.853 1.766 1.759 1.741 1.735 1.716 1.712 1.708

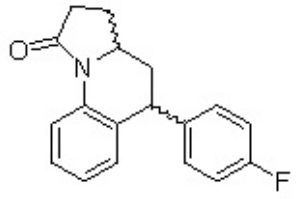


(^{1}H NMR, 400 MHz, $CDCl_3$)

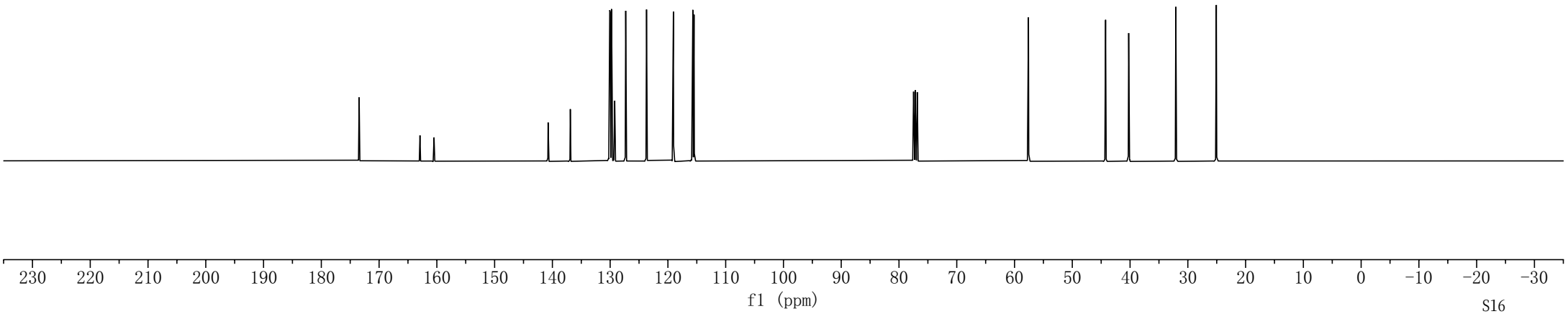


10b/B

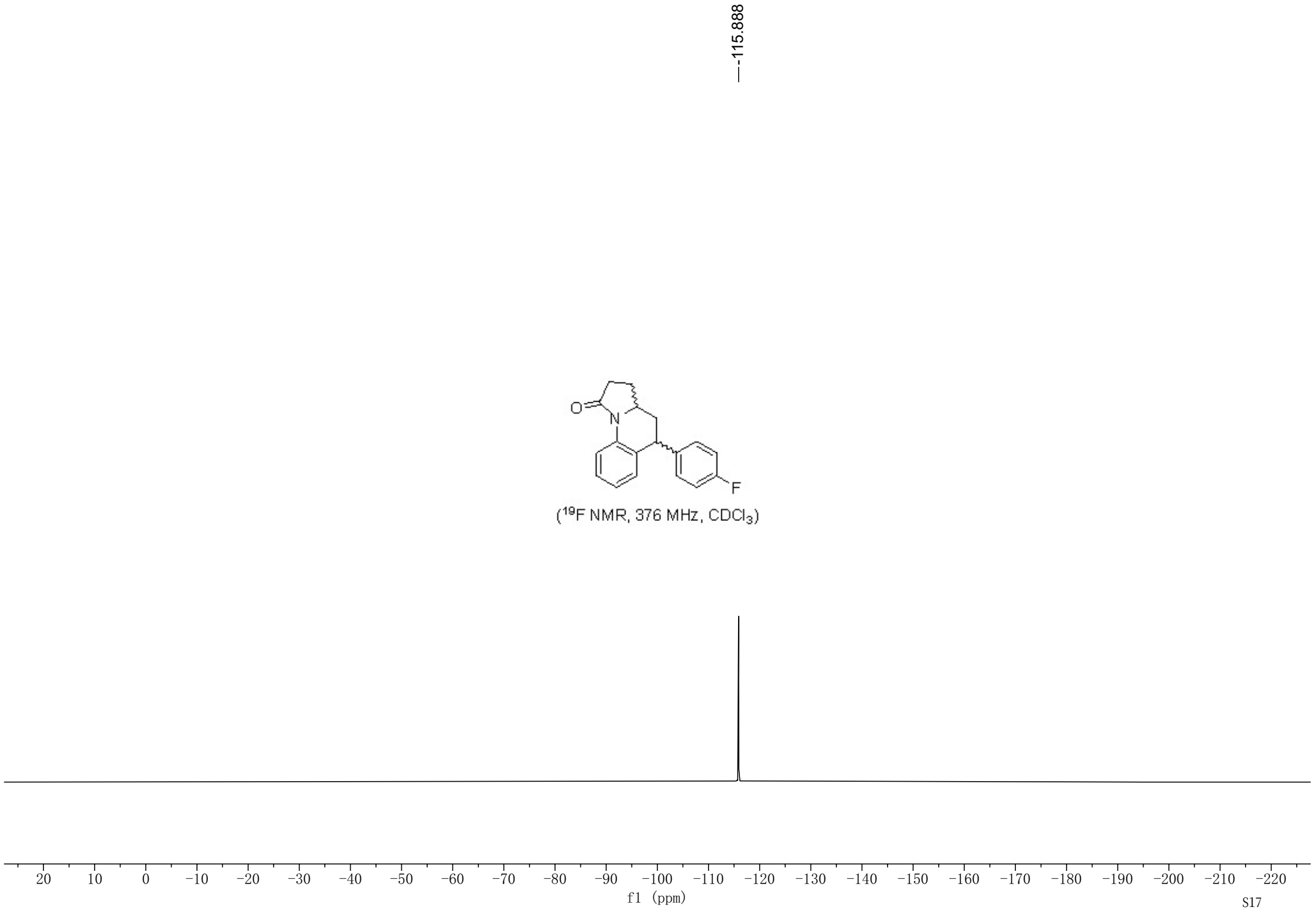
173.451
162.923
160.487
140.743
140.710
136.899
130.072
129.994
129.766
129.209
127.311
123.703
119.052
115.689
115.478
57.588
44.237
40.239
32.080
25.068



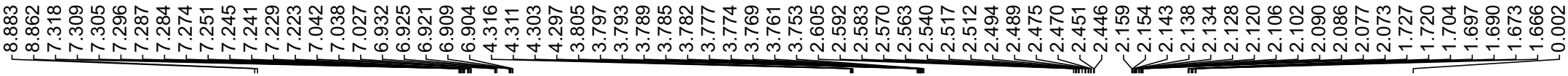
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

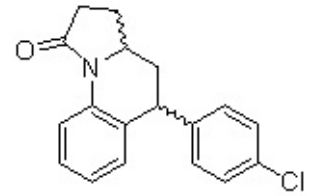


10b/B

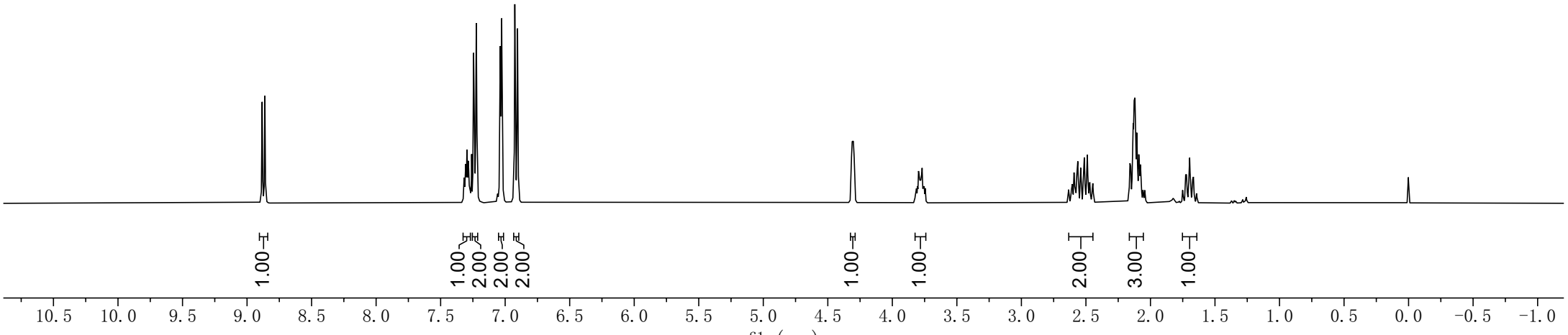

-115.888
O
N
F
(19F NMR, 376 MHz, CDCl3)
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
−220
f1 (ppm)

10c/A

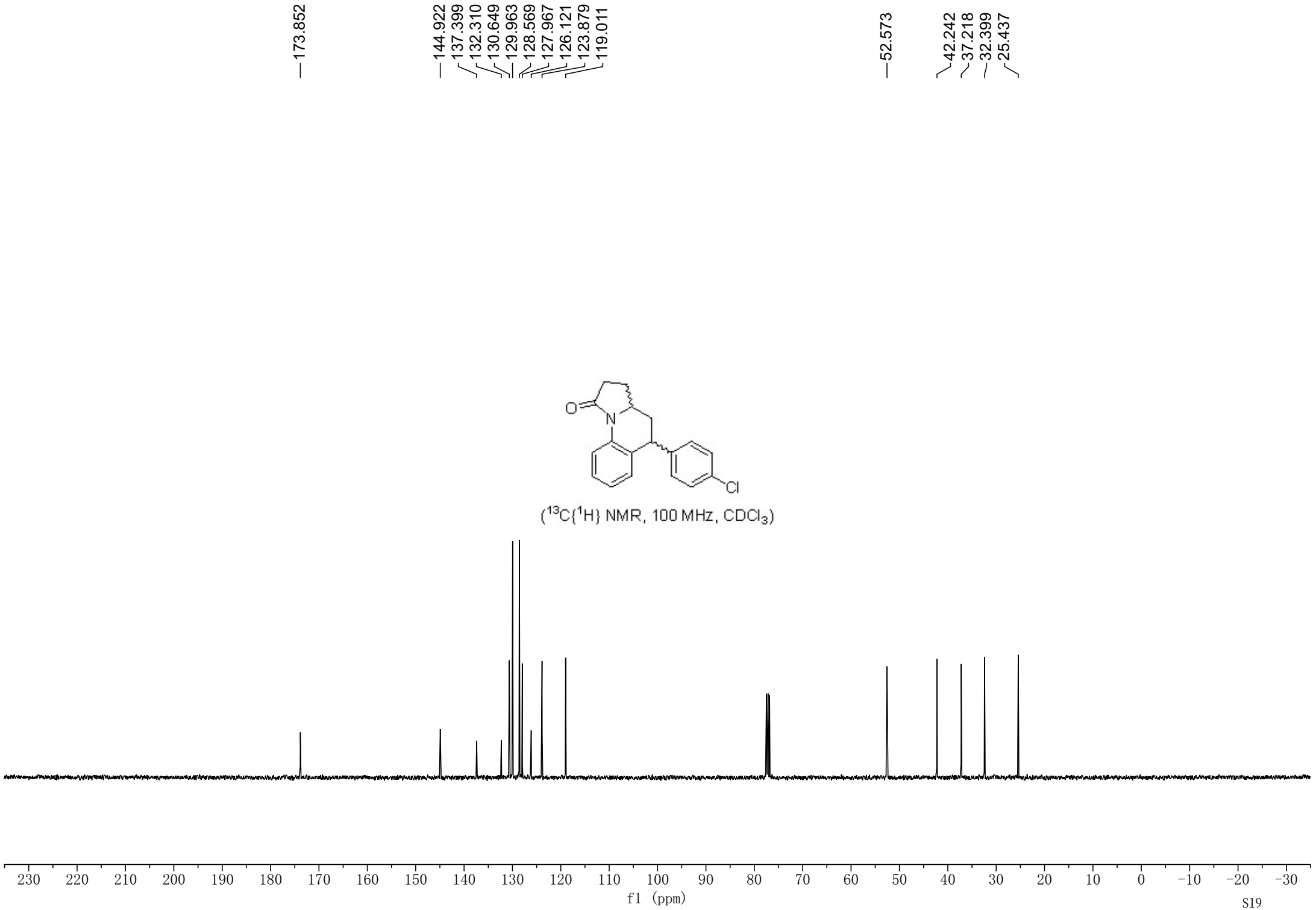




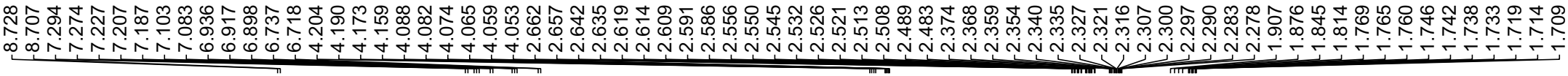
(^{1}H NMR, 400 MHz, $CDCl_3$)

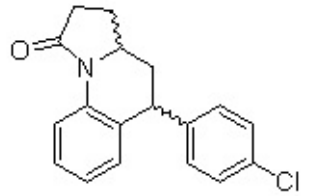


10c/A

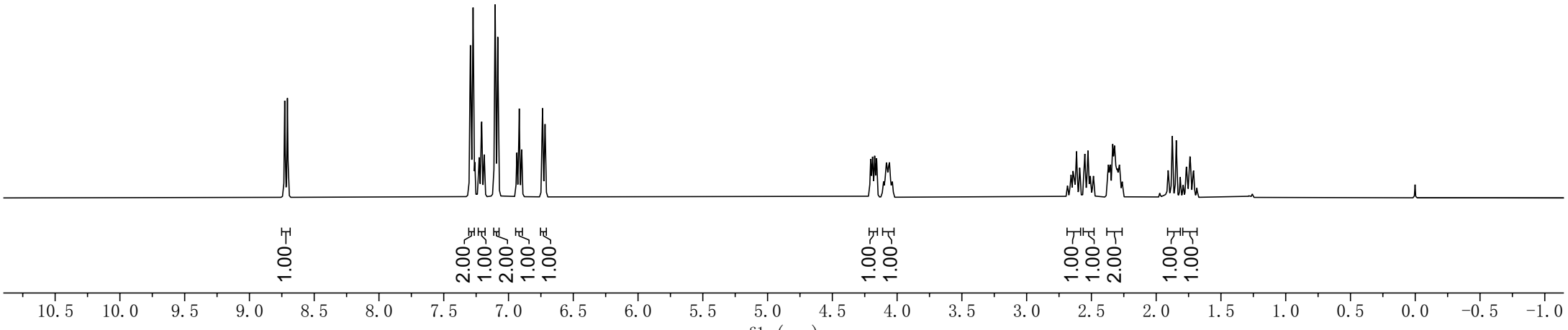

173.852
144.922
137.399
132.310
130.649
129.963
128.569
127.967
126.121
123.879
119.011
52.573
42.242
37.218
32.399
25.437
O
N
Cl
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

10c/B



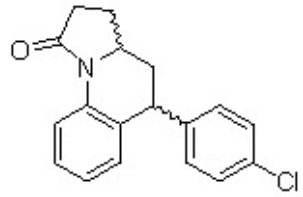


(^{1}H NMR, 400 MHz, $CDCl_3$)

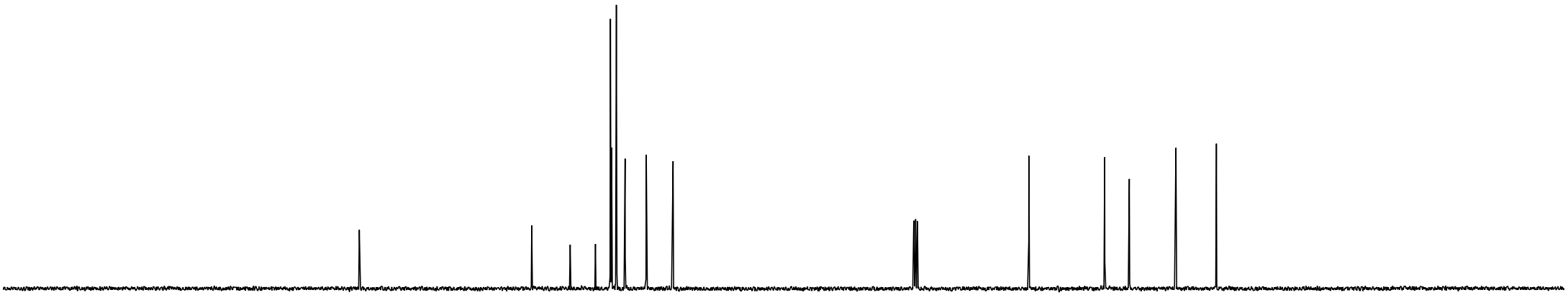


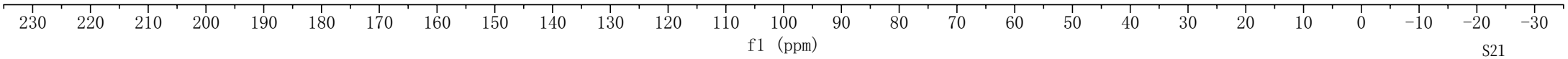
10c/B

173.455
143.607
136.949
132.583
129.984
129.786
128.958
128.876
127.445
123.780
119.141
57.551
44.428
40.165
32.096
25.088

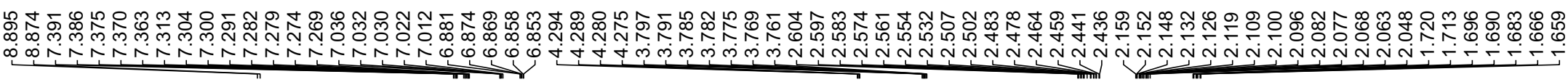


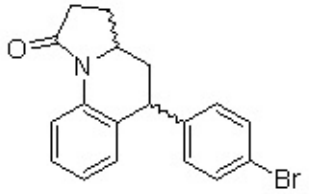
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



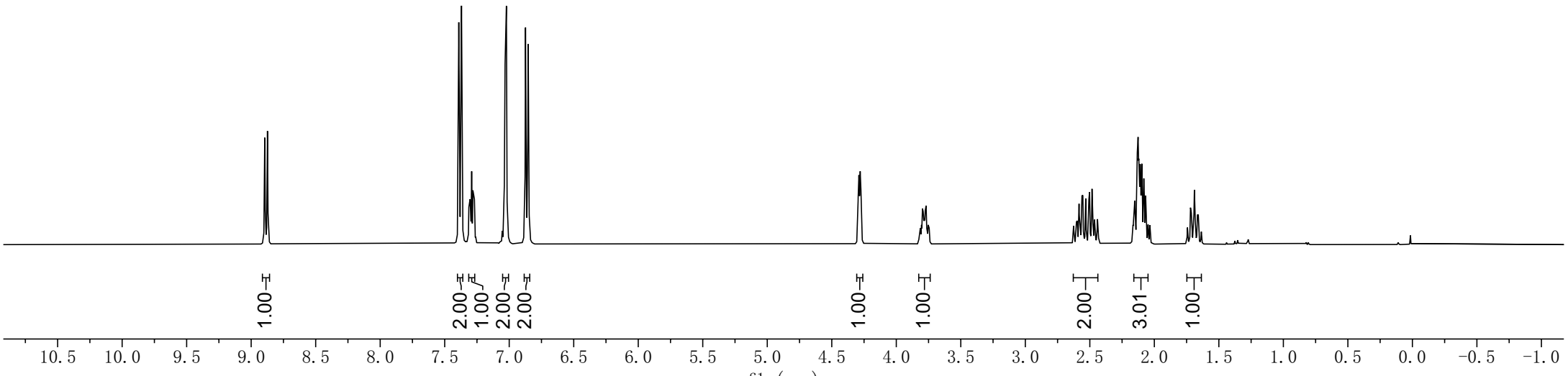


10d/A

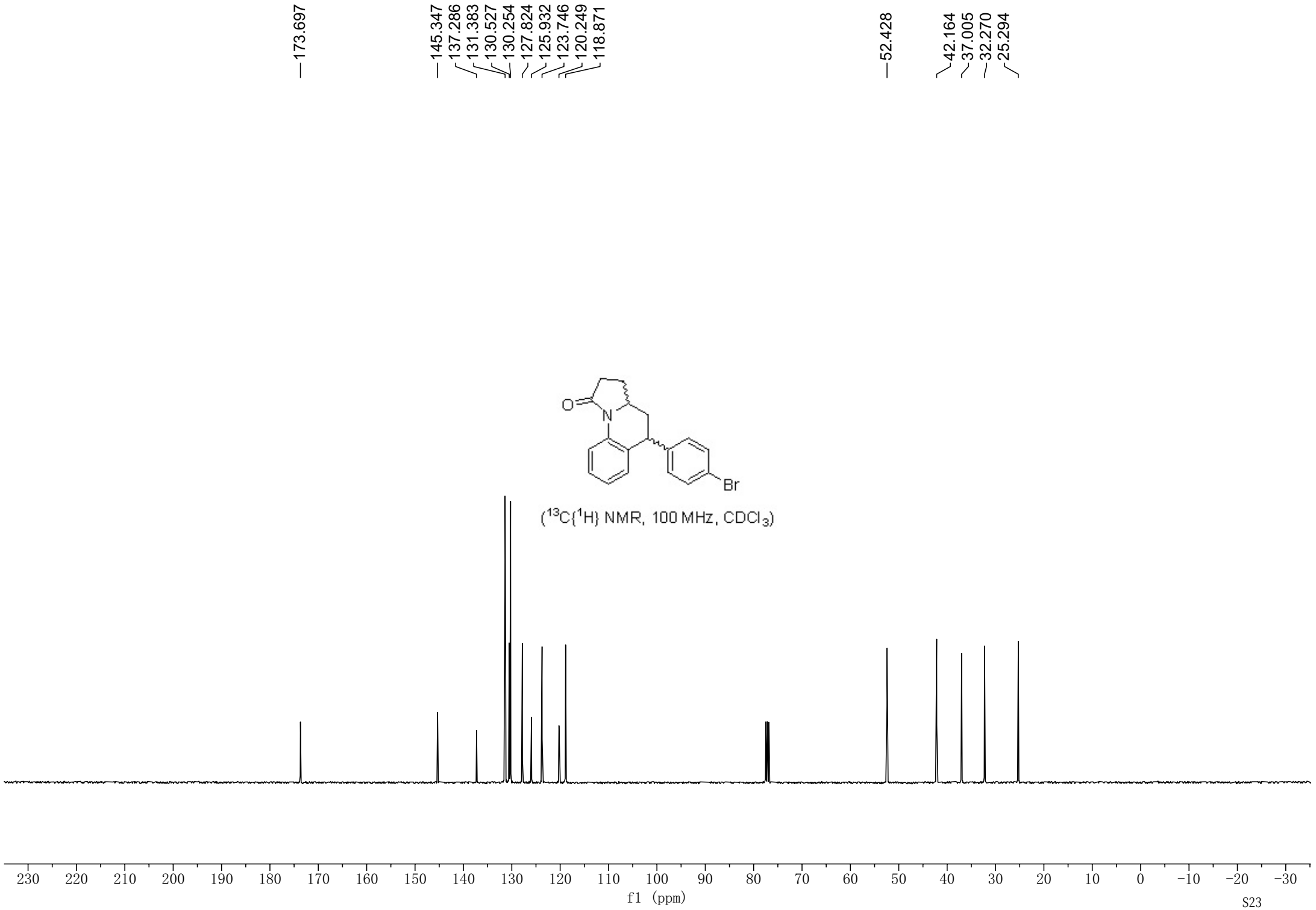




(^{1}H NMR, 400 MHz, $CDCl_3$)

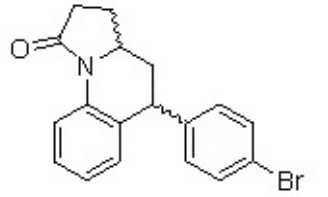


10d/A

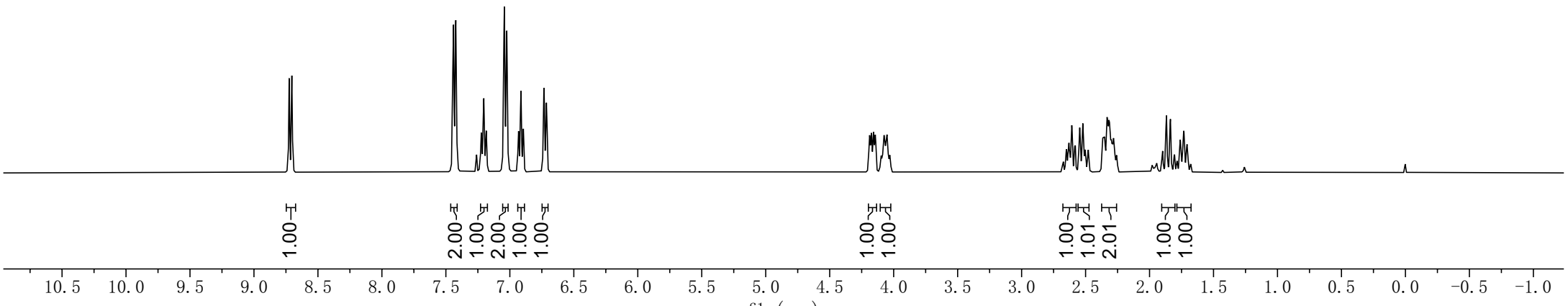

173.697
145.347
137.286
131.383
130.527
130.254
127.824
125.932
123.746
120.249
118.871
52.428
42.164
37.005
32.270
25.294
O
N
Br
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

10d/B

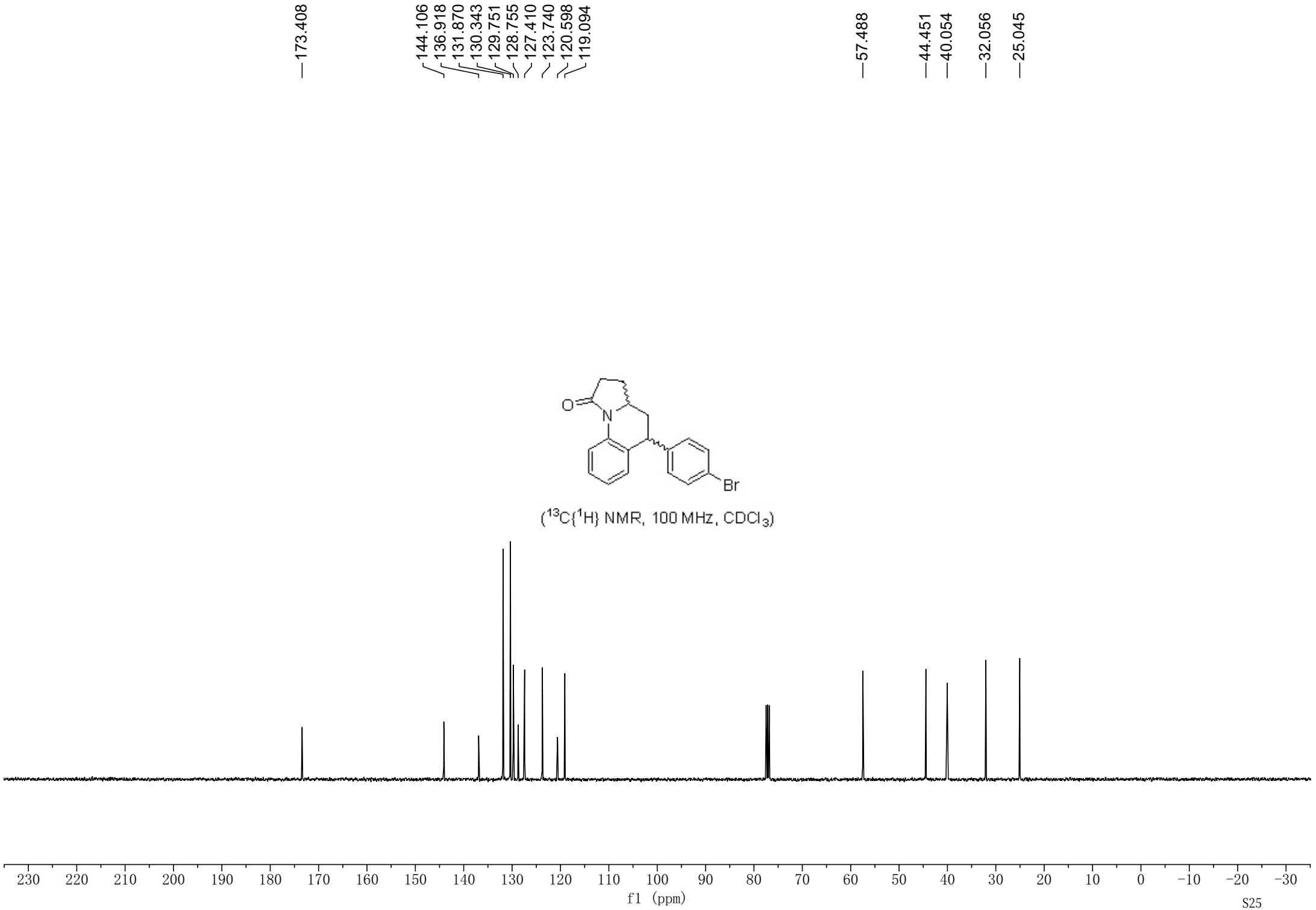
8.725 8.704 7.445 7.440 7.424 7.419 7.223 7.204 7.184 7.047 7.042 7.026 7.021 6.932 6.913 6.894 6.734 6.714 4.188 4.174 4.157 4.143 4.099 4.081 4.075 4.069 4.059 4.052 4.046 4.030 2.655 2.650 2.636 2.630 2.621 2.608 2.602 2.585 2.579 2.552 2.546 2.540 2.528 2.521 2.515 2.503 2.479 2.371 2.366 2.359 2.351 2.346 2.333 2.326 2.318 2.312 2.306 2.298 2.290 2.281 2.274 2.258 1.901 1.897 1.868 1.837 1.804 1.760 1.736 1.730 1.708 1.701



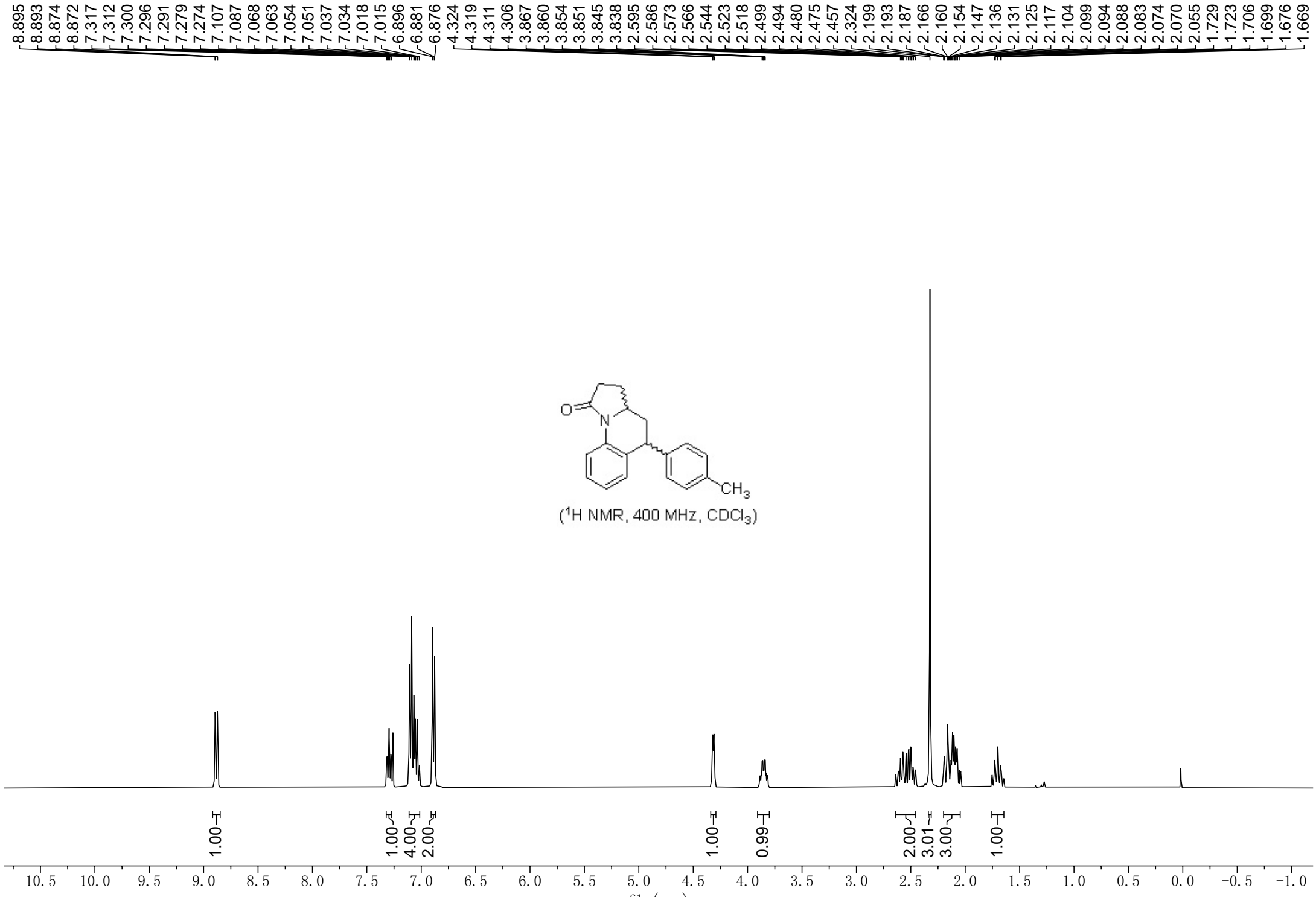
(^{1}H NMR, 400 MHz, $CDCl_3$)



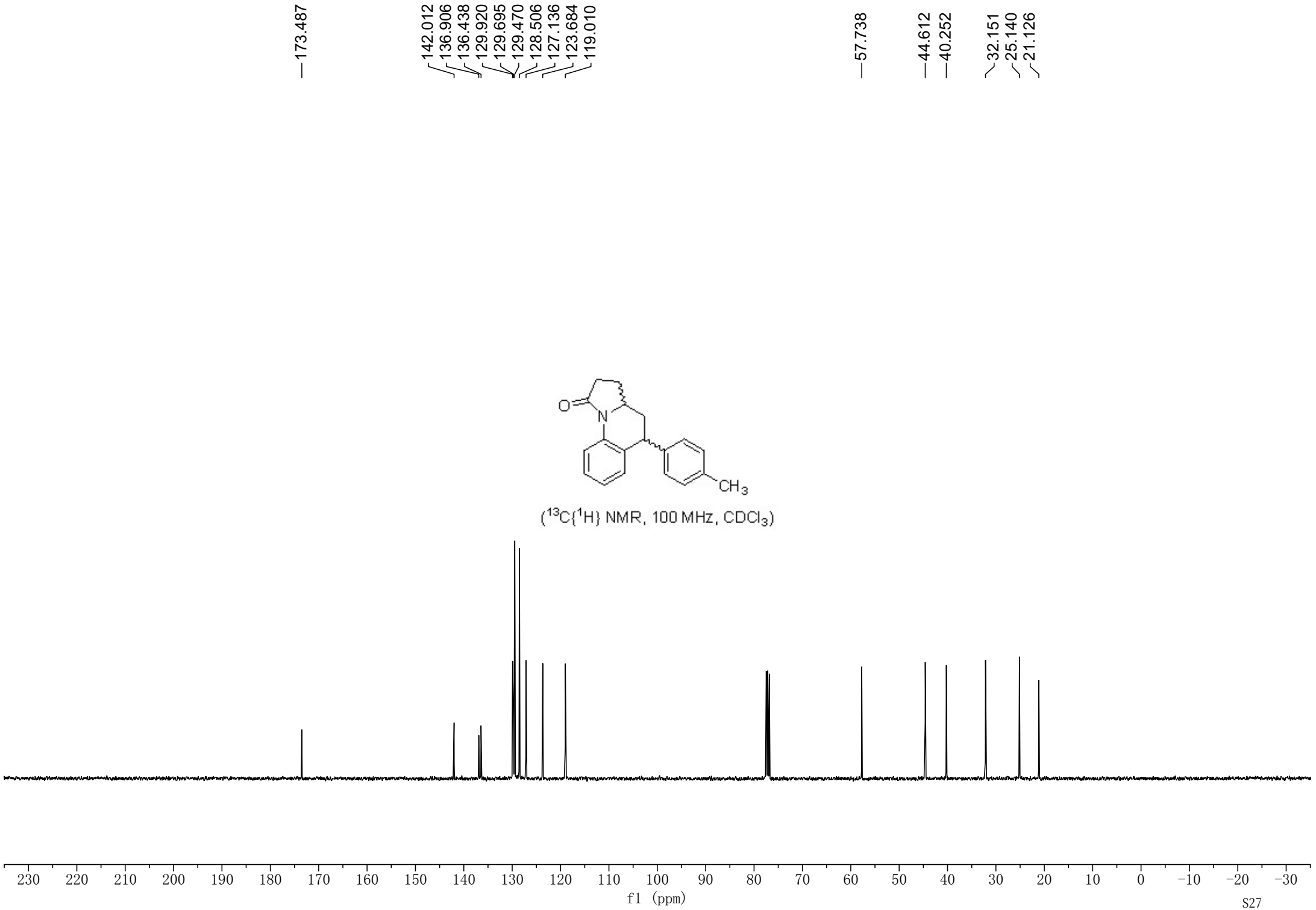
10d/B


173.408
144.106
136.918
131.870
130.343
129.751
128.755
127.410
123.740
120.598
119.094
57.488
44.451
40.054
32.056
25.045
O
N
Br
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

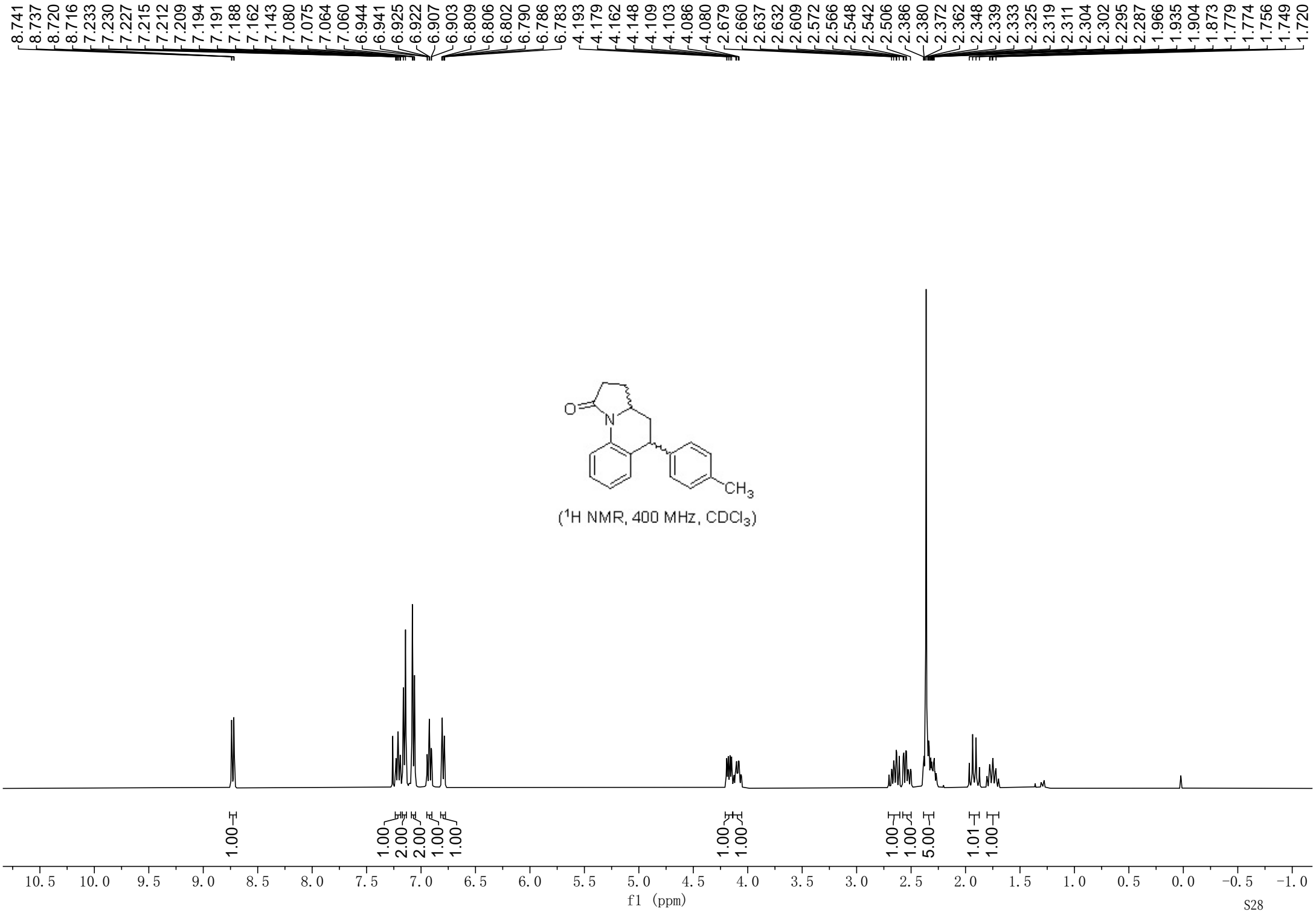
10e/A


8.895
8.893
8.874
8.872
7.317
7.312
7.300
7.296
7.291
7.279
7.274
7.107
7.087
7.068
7.063
7.054
7.051
7.037
7.034
7.018
7.015
6.896
6.881
6.876
4.324
4.319
4.311
4.306
3.867
3.860
3.854
3.851
3.845
3.838
2.595
2.586
2.573
2.566
2.544
2.523
2.518
2.499
2.494
2.480
2.475
2.457
2.324
2.199
2.193
2.187
2.166
2.160
2.154
2.147
2.136
2.131
2.125
2.117
2.104
2.099
2.094
2.088
2.083
2.074
2.070
2.055
1.729
1.723
1.706
1.699
1.676
1.669
O
N
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
4.00
2.00
1.00
0.99
2.00
3.01
3.00
1.00
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
-0.5
-1.0
f1 (ppm)

10e/A

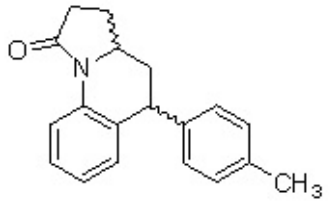

173.487
142.012
136.906
136.438
129.920
129.695
129.470
128.506
127.136
123.684
119.010
57.738
44.612
40.252
32.151
25.140
21.126
O
N
CH3
(13C{1H} NMR, 100 MHz, CDCl3)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
f1 (ppm)

10e/B

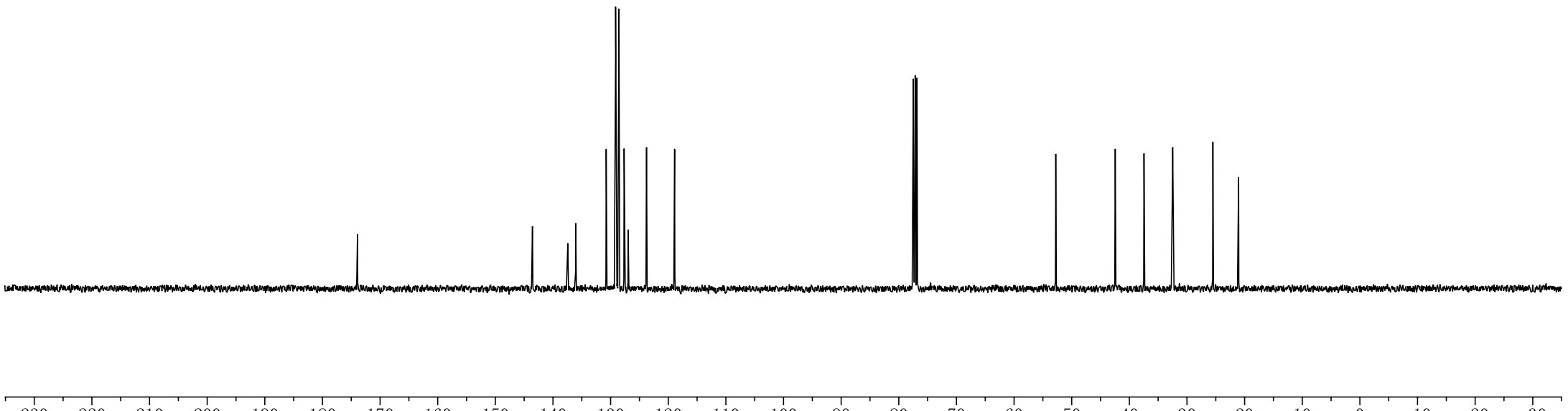

8.741
8.737
8.720
8.716
7.233
7.230
7.227
7.215
7.212
7.209
7.194
7.191
7.188
7.162
7.143
7.080
7.075
7.064
7.060
6.944
6.941
6.925
6.922
6.907
6.903
6.809
6.806
6.802
6.790
6.786
6.783
4.193
4.179
4.162
4.148
4.109
4.103
4.086
4.080
2.679
2.660
2.637
2.632
2.609
2.572
2.566
2.548
2.542
2.506
2.386
2.380
2.372
2.362
2.348
2.339
2.333
2.325
2.319
2.311
2.304
2.302
2.295
2.287
1.966
1.935
1.904
1.873
1.779
1.774
1.756
1.749
1.720
O
N
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
2.00
2.00
1.00
1.00
1.00
1.00
1.00
1.00
5.00
1.01
1.00
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
-0.5
-1.0
f1 (ppm)

10e/B

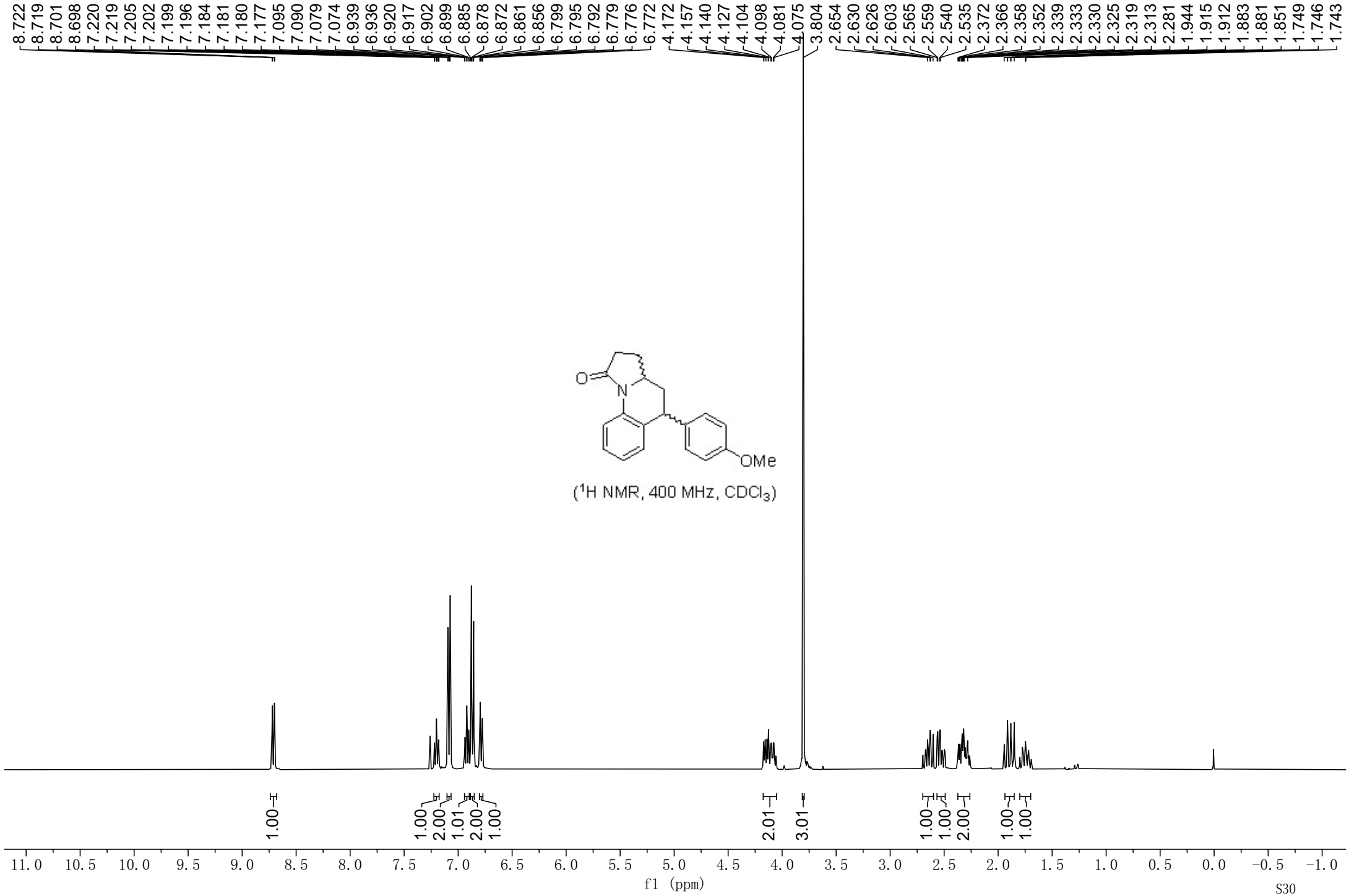
173.916
143.566
137.431
136.056
130.768
129.134
128.549
127.654
126.959
123.773
118.894
52.765
42.443
37.456
32.481
25.503
21.044



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

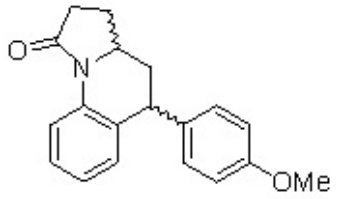


10f/B

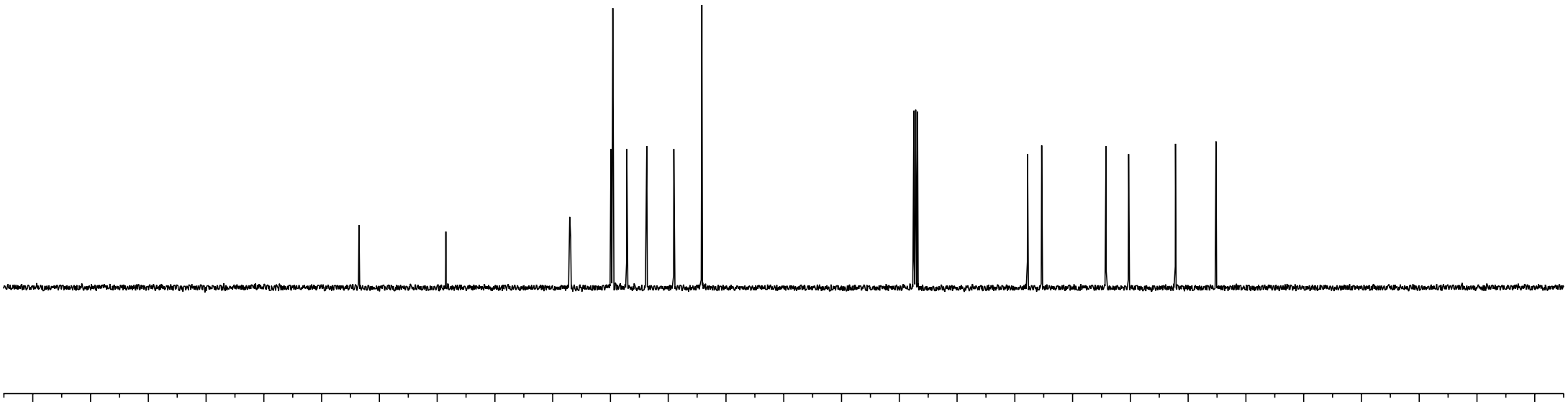

8.722
8.719
8.701
8.698
7.220
7.219
7.205
7.202
7.199
7.196
7.184
7.181
7.180
7.177
7.095
7.090
7.079
7.074
6.939
6.936
6.920
6.917
6.902
6.899
6.885
6.878
6.872
6.861
6.856
6.799
6.795
6.792
6.779
6.776
6.772
4.172
4.157
4.140
4.127
4.104
4.098
4.081
4.075
3.804
2.654
2.630
2.626
2.603
2.565
2.559
2.540
2.535
2.372
2.366
2.358
2.352
2.339
2.333
2.330
2.325
2.319
2.313
2.281
1.944
1.915
1.912
1.883
1.881
1.851
1.749
1.746
1.743
O
N
OMe
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
2.00
1.01
2.00
1.00
2.01
3.01
1.00
1.00
2.00
1.00
1.00
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
0.0
-0.5
-1.0
f1 (ppm)

10f/B

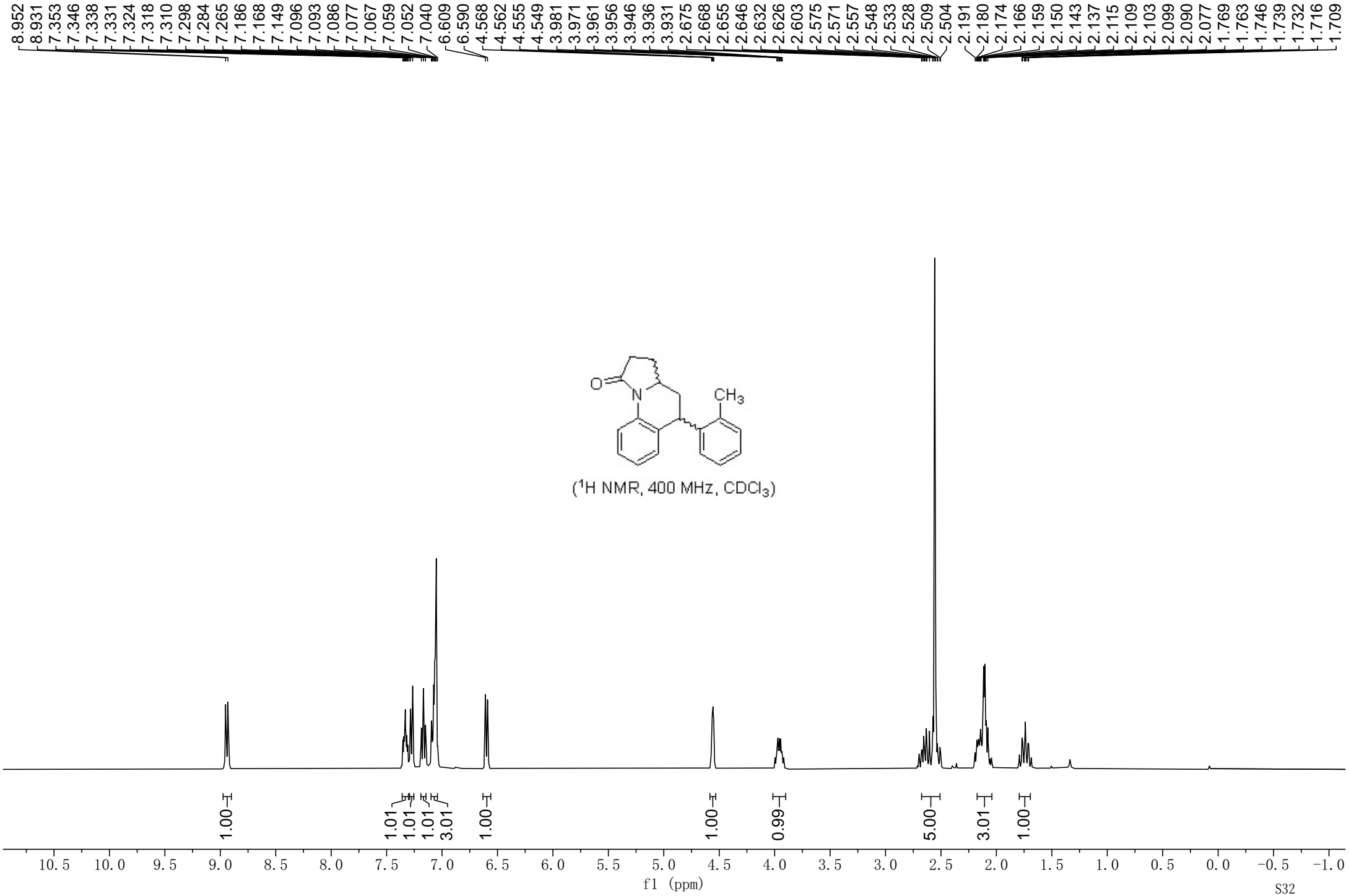
173.533
158.496
137.050
136.894
129.917
129.844
129.593
127.179
123.715
119.028
114.176
57.800
55.350
44.217
40.301
32.193
25.177



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

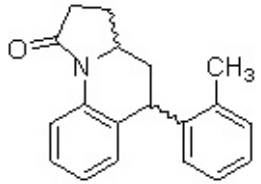


10g/A

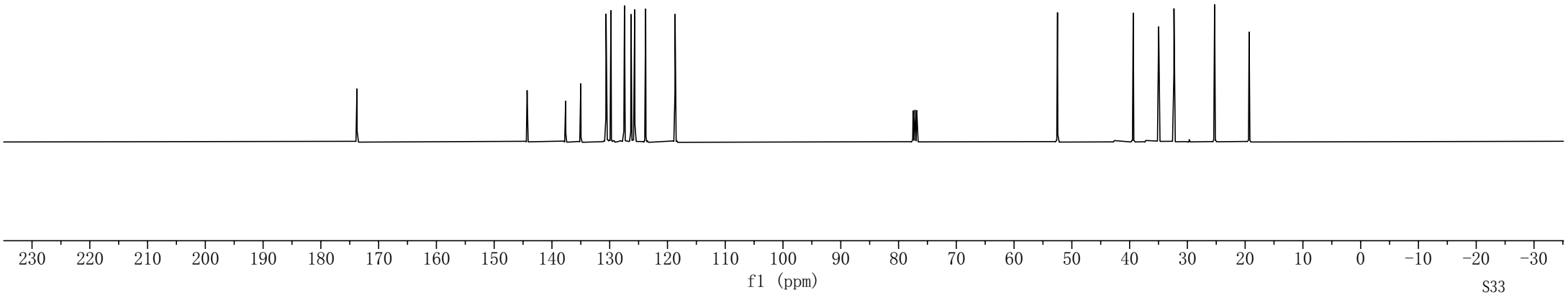

8.952
8.931
7.353
7.346
7.338
7.331
7.324
7.318
7.310
7.298
7.284
7.265
7.186
7.168
7.149
7.096
7.093
7.086
7.077
7.067
7.059
7.052
7.040
6.609
6.590
4.568
4.562
4.555
4.549
3.981
3.971
3.961
3.956
3.946
3.936
3.931
2.675
2.668
2.655
2.646
2.632
2.626
2.603
2.575
2.571
2.557
2.548
2.533
2.528
2.509
2.504
2.191
2.180
2.174
2.166
2.159
2.150
2.143
2.137
2.115
2.109
2.103
2.099
2.090
2.077
1.769
1.763
1.746
1.739
1.732
1.716
1.709
O
N
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
1.01
1.01
1.01
3.01
1.00
1.00
0.99
5.00
3.01
1.00
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
-0.5
-1.0
f1 (ppm)

10g/A

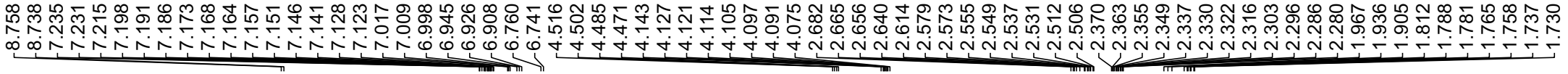
173.748
144.297
137.627
135.004
130.635
129.782
129.213
128.198
127.441
126.311
125.668
123.778
118.686
52.481
39.373
34.967
32.320
25.285
19.313

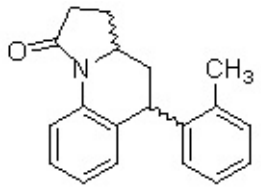


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

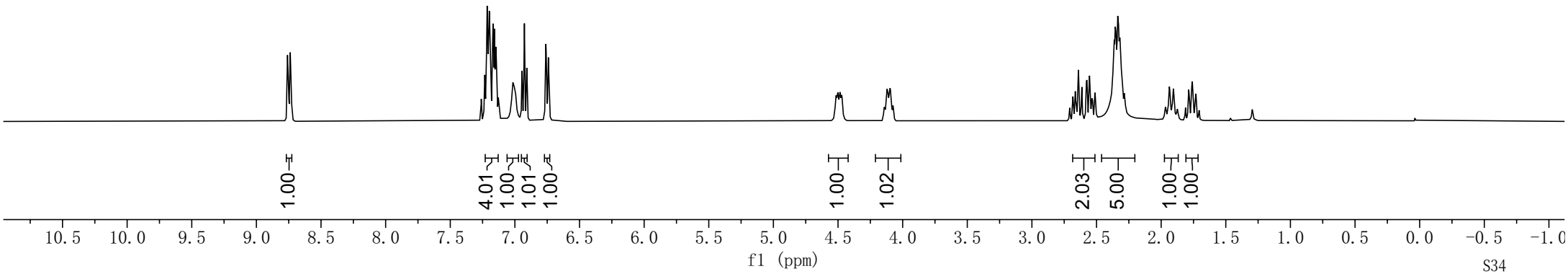


10g/B



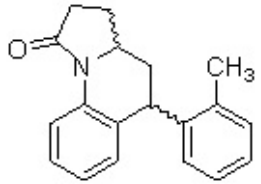


(^{1}H NMR, 400 MHz, $CDCl_3$)

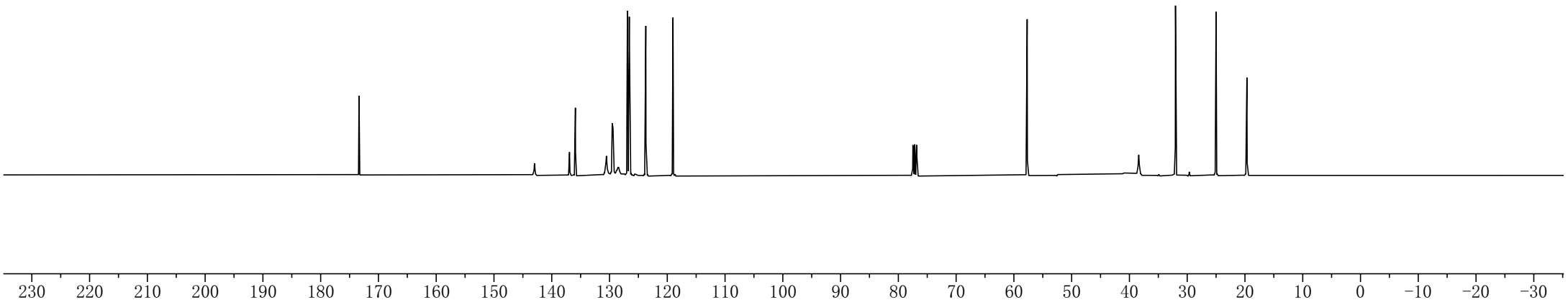


10g/B

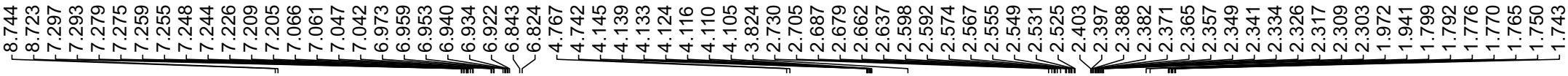
173.361
142.984
136.928
135.904
130.610
129.531
129.388
128.502
126.900
126.562
125.635
123.714
119.011
57.699
39.333
38.388
32.029
25.002
19.662

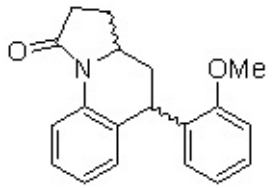


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

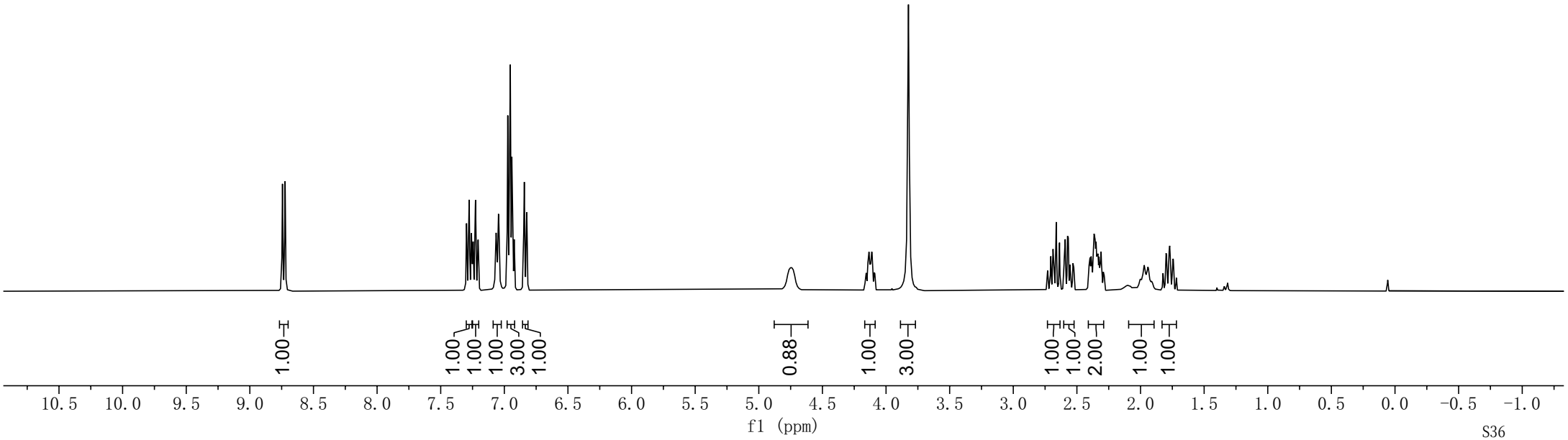


10h/B



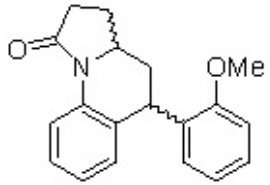


(^{1}H NMR, 400 MHz, $CDCl_3$)

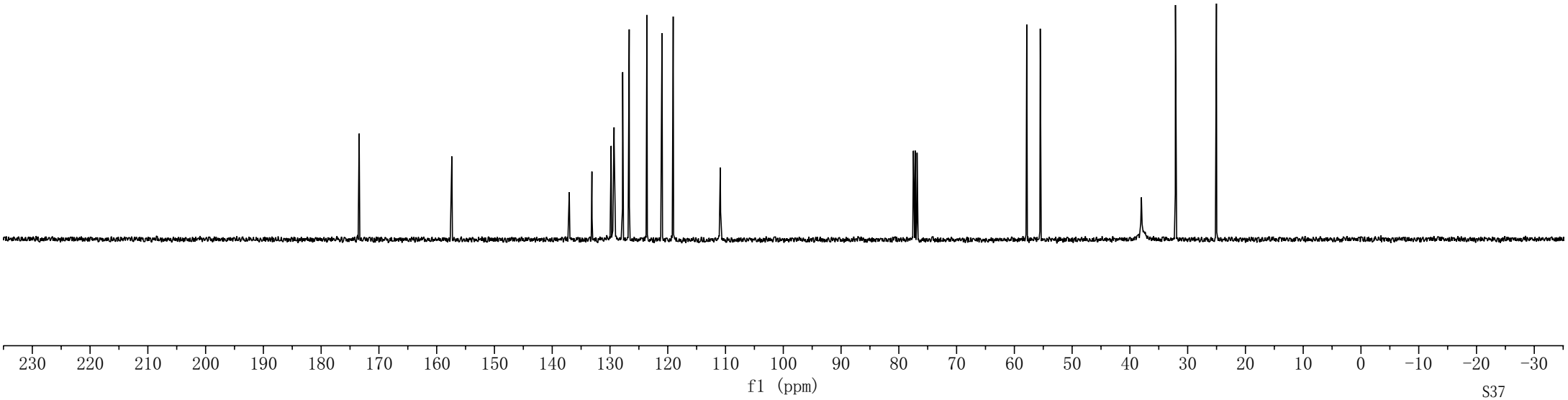


10h/B

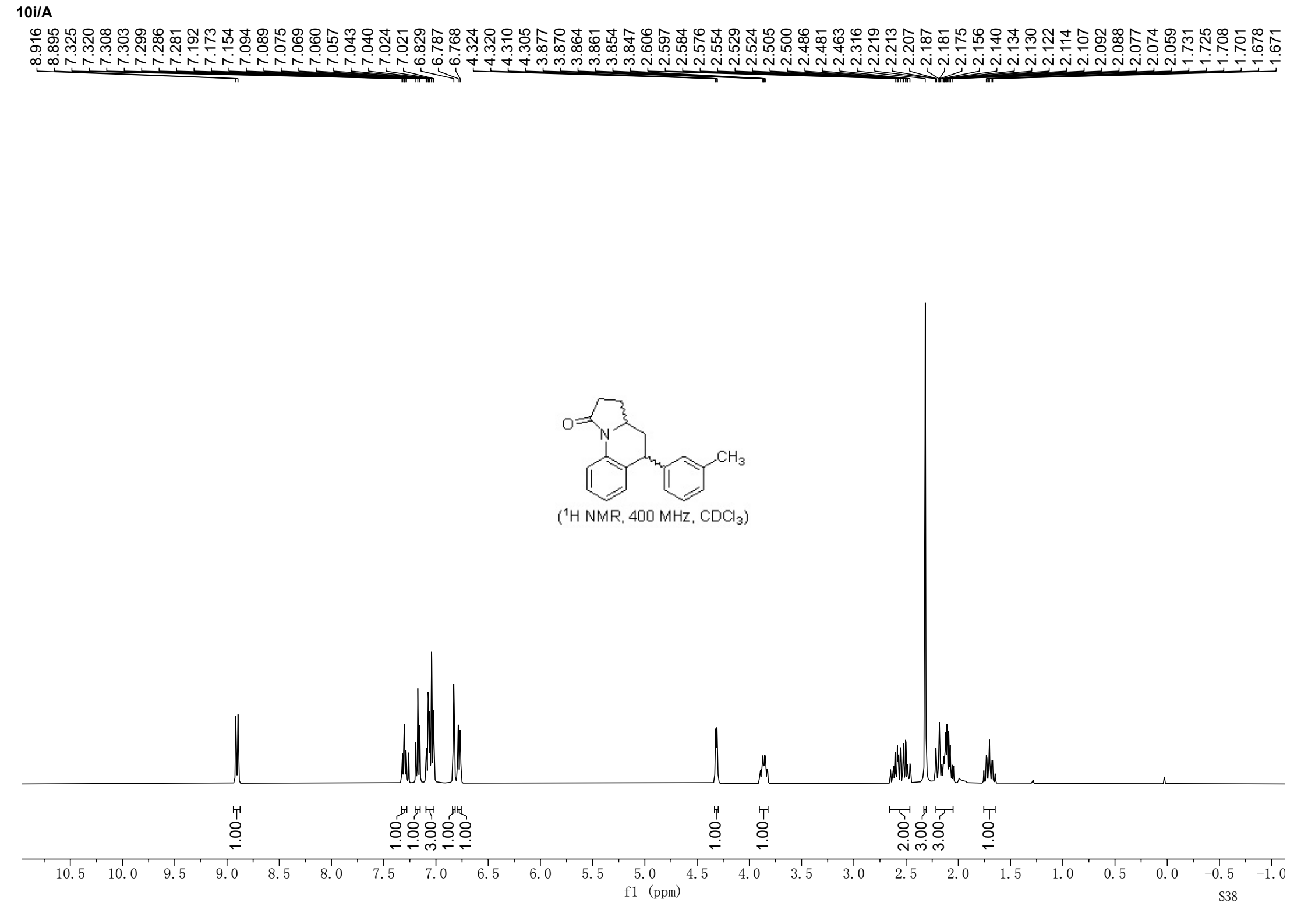
173.422
157.375
137.050
133.126
129.799
129.295
127.803
126.671
123.607
120.994
119.057
110.902
57.852
55.519
38.011
32.117
25.022



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

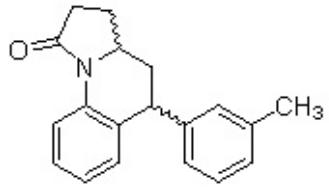


10i/A

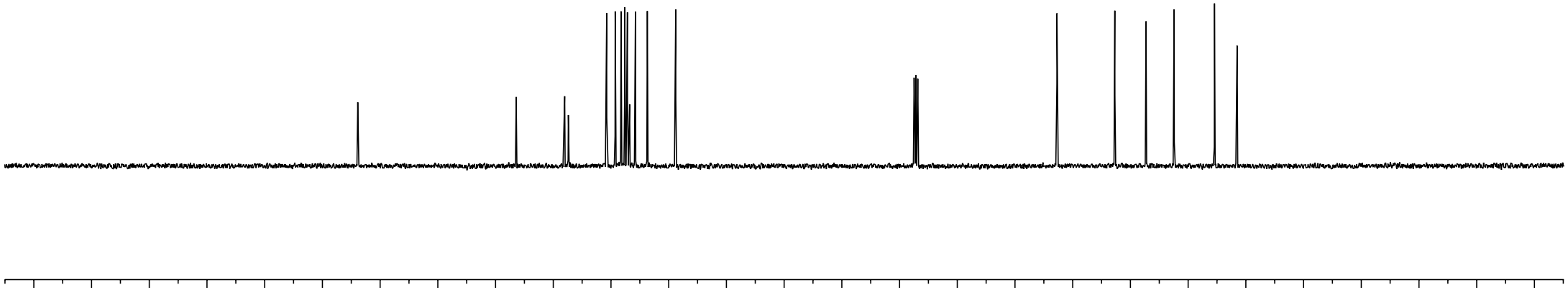

8.916
8.895
7.325
7.320
7.308
7.303
7.299
7.286
7.281
7.192
7.173
7.154
7.094
7.089
7.075
7.069
7.060
7.057
7.043
7.040
7.024
7.021
6.829
6.787
6.768
4.324
4.320
4.310
4.305
3.877
3.870
3.864
3.861
3.854
3.847
2.606
2.597
2.584
2.576
2.554
2.529
2.524
2.505
2.500
2.486
2.481
2.463
2.316
2.219
2.213
2.207
2.187
2.181
2.175
2.156
2.140
2.134
2.130
2.122
2.114
2.107
2.092
2.088
2.077
2.074
2.059
1.731
1.725
1.708
1.701
1.678
1.671
O
N
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
3.00
1.00
1.00
1.00
2.00
3.00
3.00
1.00
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
-0.5
-1.0
f1 (ppm)

10i/A

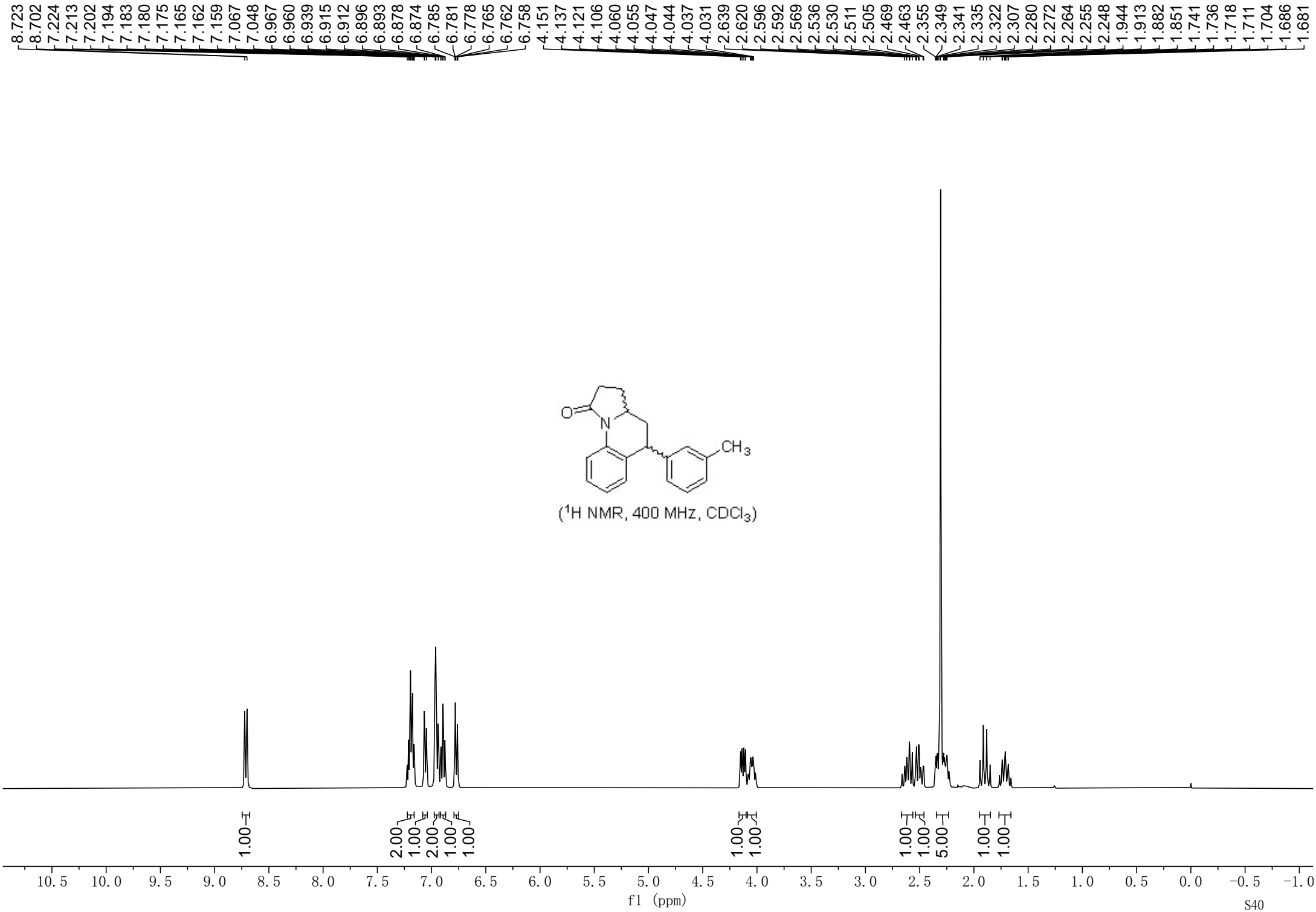
173.877
146.424
138.022
137.385
130.750
129.270
128.253
127.610
127.156
126.772
125.763
123.703
118.784
52.729
42.703
37.296
32.430
25.428
21.517



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

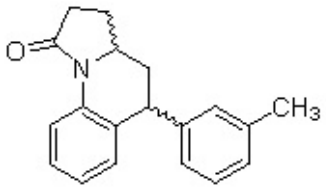


10i/B

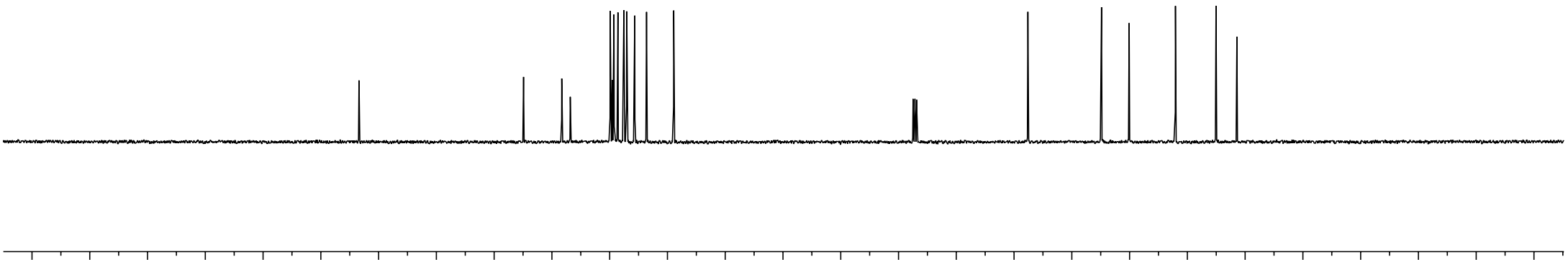

8.723
8.702
7.224
7.213
7.202
7.194
7.183
7.180
7.175
7.165
7.162
7.159
7.067
7.048
6.967
6.960
6.939
6.915
6.912
6.896
6.893
6.878
6.874
6.785
6.781
6.778
6.765
6.762
6.758
4.151
4.137
4.121
4.106
4.060
4.055
4.047
4.044
4.037
4.031
2.639
2.620
2.596
2.592
2.569
2.536
2.530
2.511
2.505
2.469
2.463
2.355
2.349
2.341
2.335
2.322
2.307
2.280
2.272
2.264
2.255
2.248
1.944
1.913
1.882
1.851
1.741
1.736
1.718
1.711
1.704
1.686
1.681
O
N
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
1.00
5.00
1.00
1.00
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
-0.5
-1.0
f1 (ppm)

10i/B

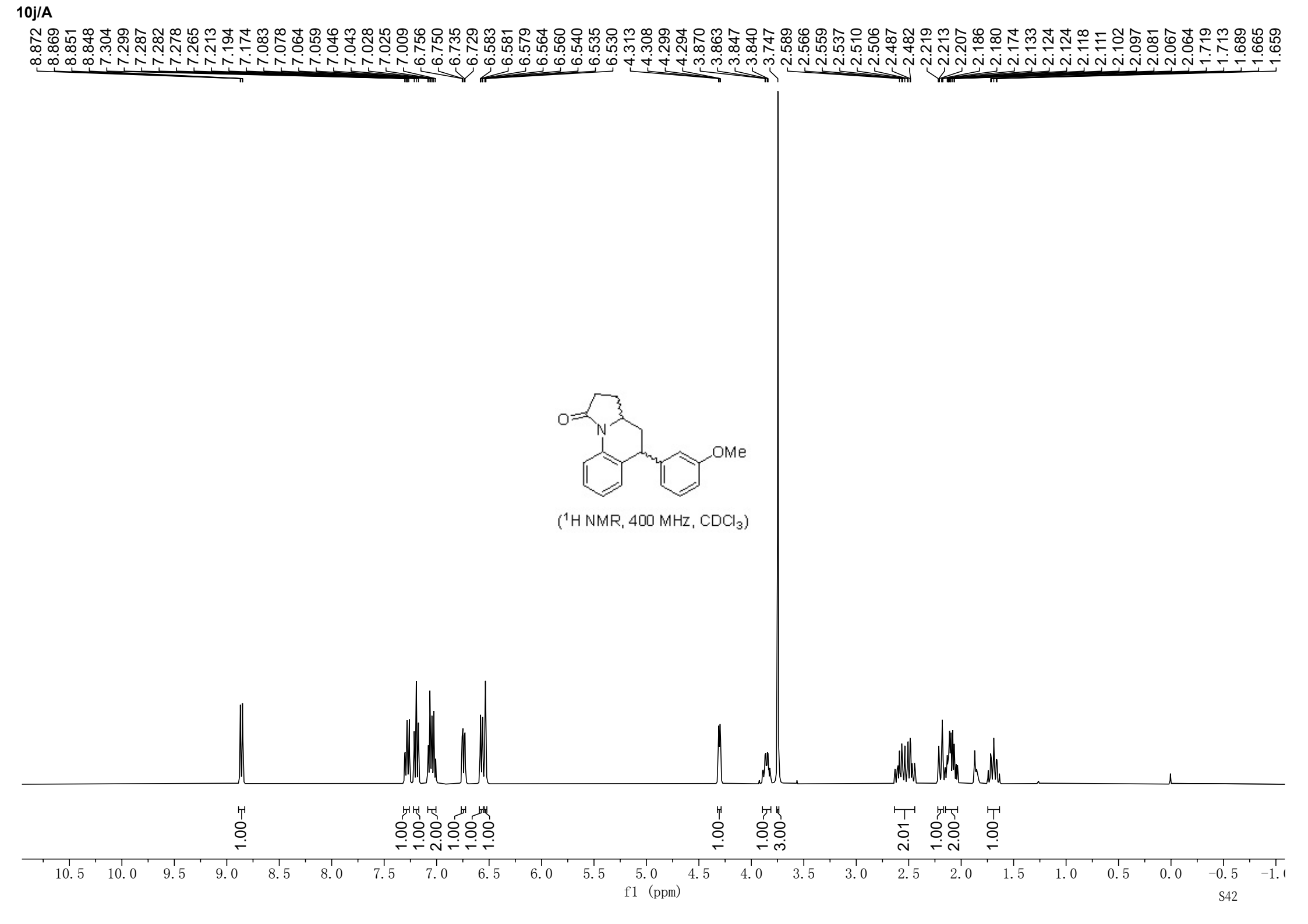
173.393
144.910
138.298
136.822
129.909
129.547
129.254
128.574
127.546
127.048
125.660
123.619
118.914
57.605
44.860
40.078
32.063
25.039
21.420



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

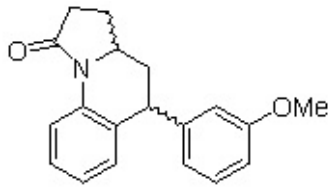


10j/A

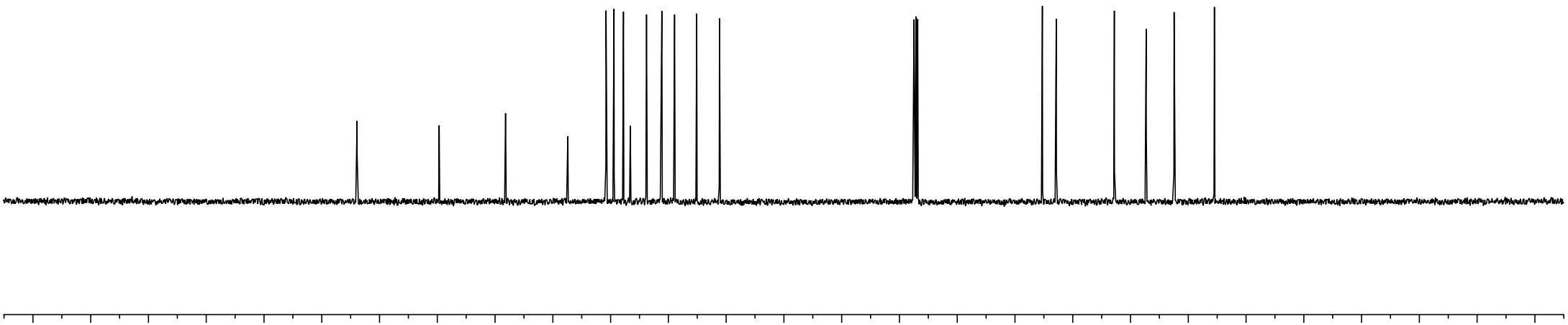

8.872
8.869
8.851
8.848
7.304
7.299
7.287
7.282
7.278
7.265
7.213
7.194
7.174
7.083
7.078
7.064
7.059
7.046
7.043
7.028
7.025
7.009
6.756
6.750
6.735
6.729
6.583
6.581
6.579
6.564
6.560
6.540
6.535
6.530
4.313
4.308
4.299
4.294
3.870
3.863
3.847
3.840
3.747
2.589
2.566
2.559
2.537
2.510
2.506
2.487
2.482
2.219
2.213
2.207
2.186
2.180
2.174
2.133
2.124
2.124
2.118
2.111
2.102
2.097
2.081
2.067
2.064
1.719
1.713
1.689
1.665
1.659
O
N
OMe
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
2.00
1.00
1.00
1.00
1.00
1.00
3.00
2.01
1.00
2.00
1.00
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
−0.5
f1 (ppm)

10j/A

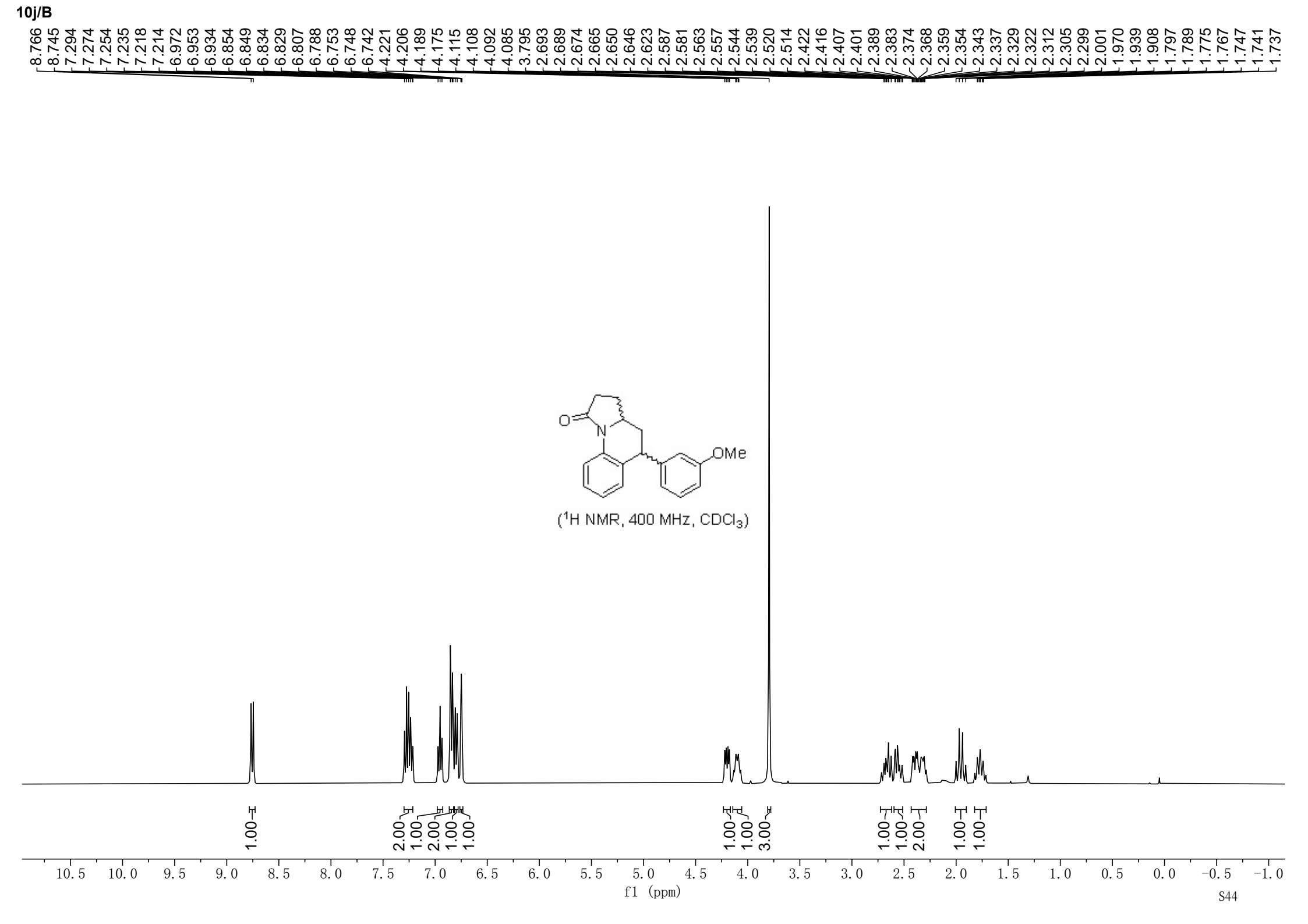
173.891
159.680
148.183
137.404
130.793
129.407
127.776
126.586
123.784
121.130
118.929
115.098
111.147
55.261
52.852
42.803
37.288
32.456
25.479



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

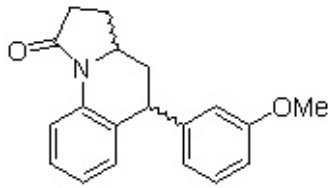


10j/B

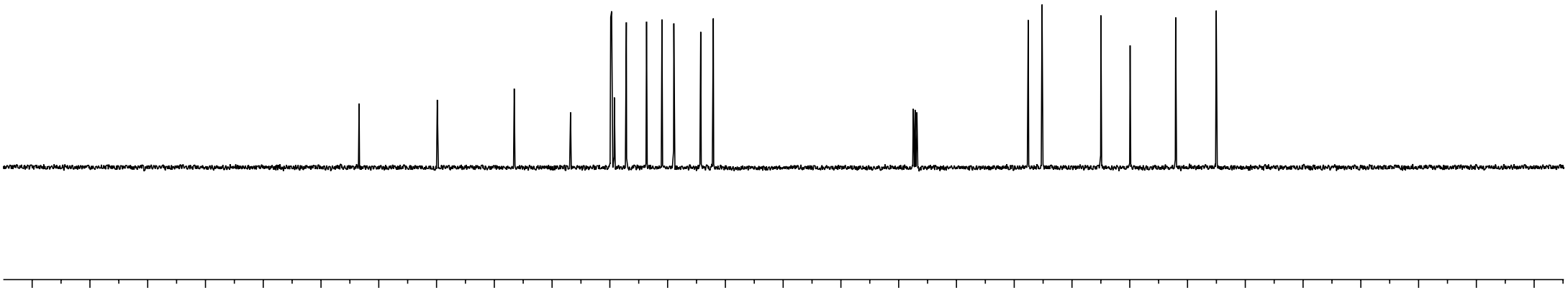

8.766
8.745
7.294
7.274
7.254
7.235
7.218
7.214
6.972
6.953
6.934
6.854
6.849
6.834
6.829
6.807
6.788
6.753
6.748
6.742
4.221
4.206
4.189
4.175
4.115
4.108
4.092
4.085
3.795
2.693
2.689
2.674
2.665
2.650
2.646
2.623
2.587
2.581
2.563
2.557
2.544
2.539
2.520
2.514
2.422
2.416
2.407
2.401
2.389
2.383
2.374
2.368
2.359
2.354
2.343
2.337
2.329
2.322
2.312
2.305
2.299
2.001
1.970
1.939
1.908
1.797
1.789
1.775
1.767
1.747
1.741
1.737
O
N
OMe
(1H NMR, 400 MHz, CDCl3)
1.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
1.00
2.00
1.00
1.00
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
-0.5
-1.0
f1 (ppm)

10j/B

173.408
159.873
146.552
136.803
129.852
129.692
129.222
127.146
123.648
120.980
118.920
114.272
112.092
57.577
55.186
44.993
39.937
32.055
25.033



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

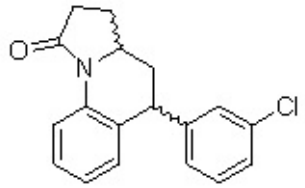


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30

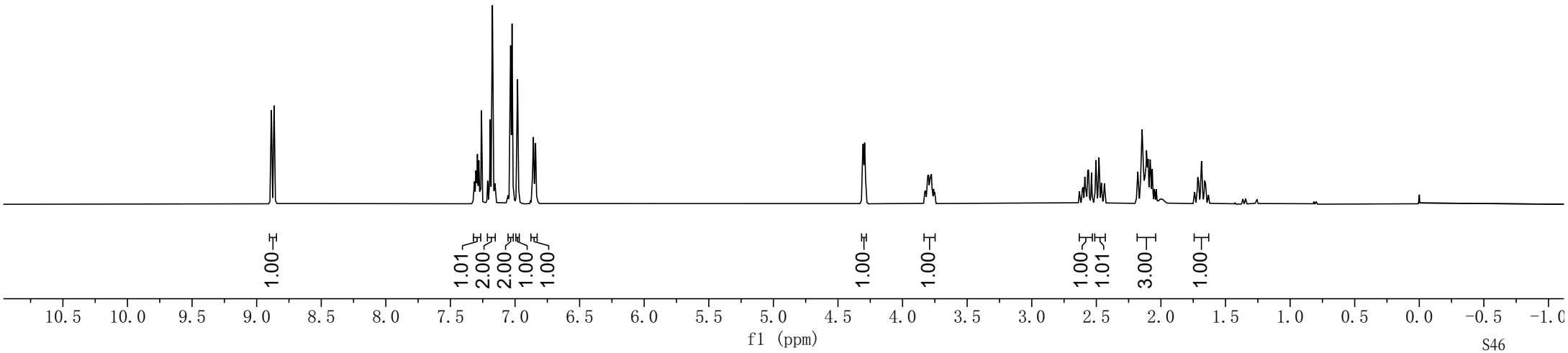
f1 (ppm)

10k/A

8.886 8.865 7.314 7.311 7.305 7.301 7.291 7.282 7.279 7.270 7.267 7.212 7.192 7.175 7.169 7.154 7.038 7.034 7.023 6.985 6.980 6.863 6.858 6.854 6.847 6.841 6.836 4.309 4.304 4.295 4.290 3.805 3.798 3.790 3.782 3.776 2.590 2.587 2.567 2.564 2.560 2.557 2.538 2.535 2.507 2.503 2.499 2.484 2.480 2.476 2.460 2.437 2.186 2.179 2.173 2.159 2.153 2.146 2.139 2.123 2.111 2.099 2.084 2.080 2.069 2.066 1.716 1.709 1.693 1.685 1.662 1.656

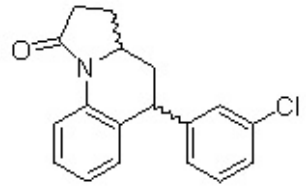


(^{1}H NMR, 400 MHz, $CDCl_3$)

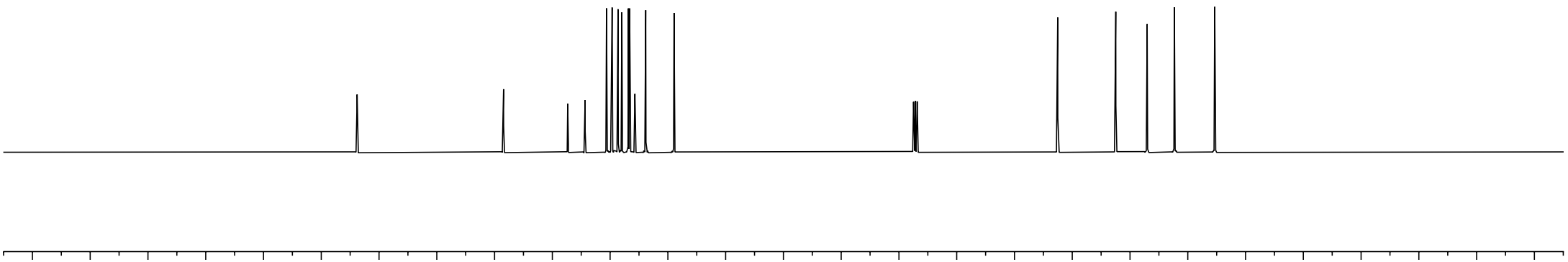


10k/A

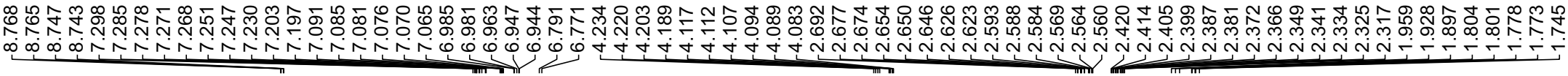
173.794
148.444
137.342
134.331
130.620
129.650
128.623
127.968
126.839
126.627
125.707
123.834
118.935
52.520
42.467
41.551
37.031
32.324
25.336

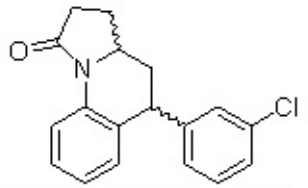


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

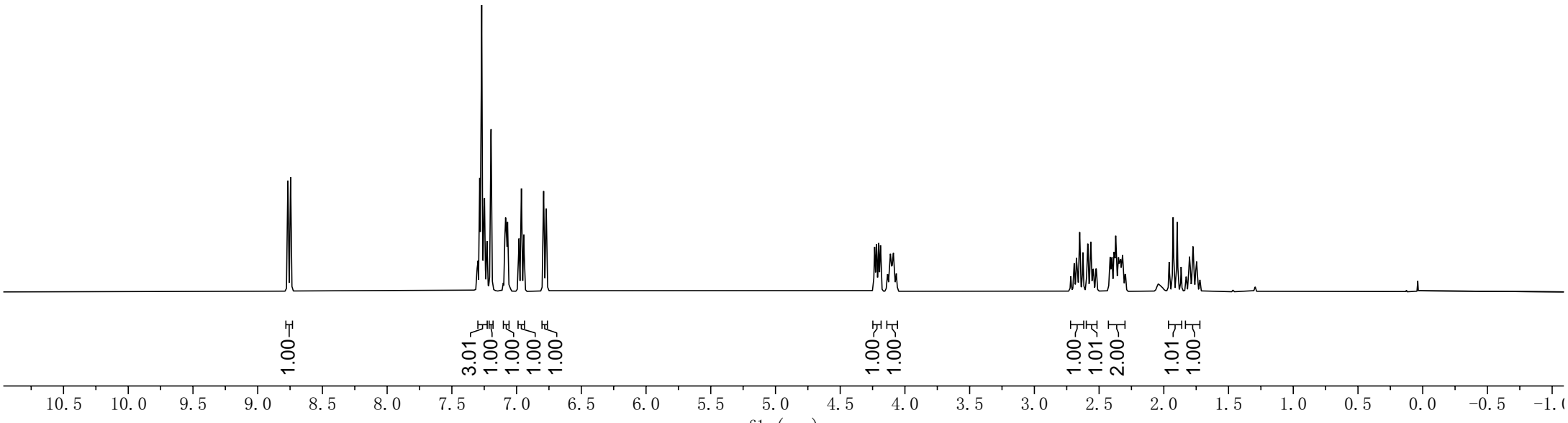


10k/B



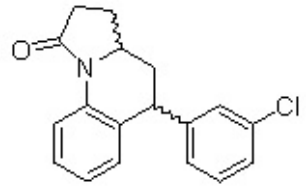


(^{1}H NMR, 400 MHz, $CDCl_3$)

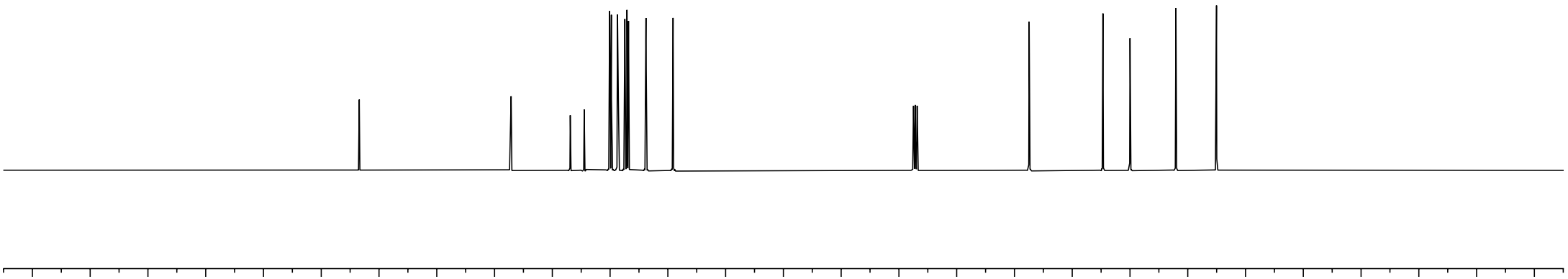


10k/B

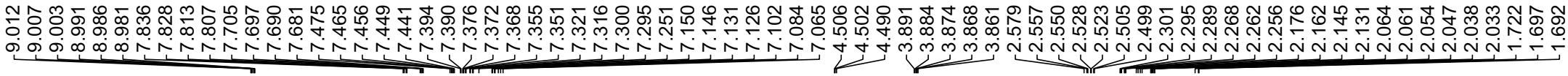
173.419
147.127
136.892
134.477
130.079
129.780
128.721
128.566
127.443
127.076
126.812
123.791
119.094
57.459
44.686
39.997
32.049
25.024

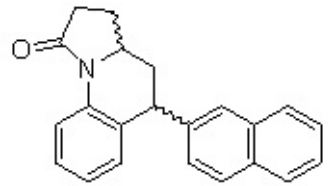


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

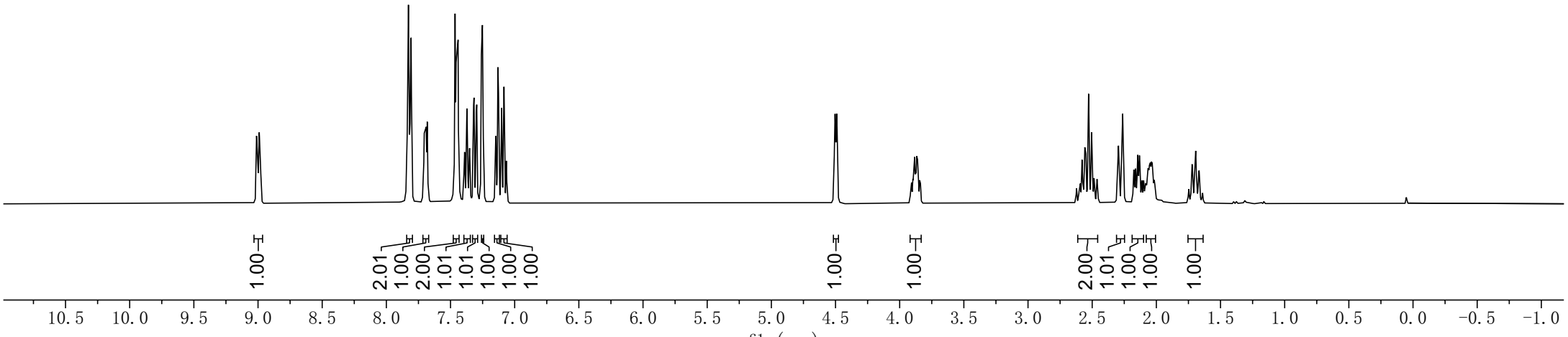


10l/A

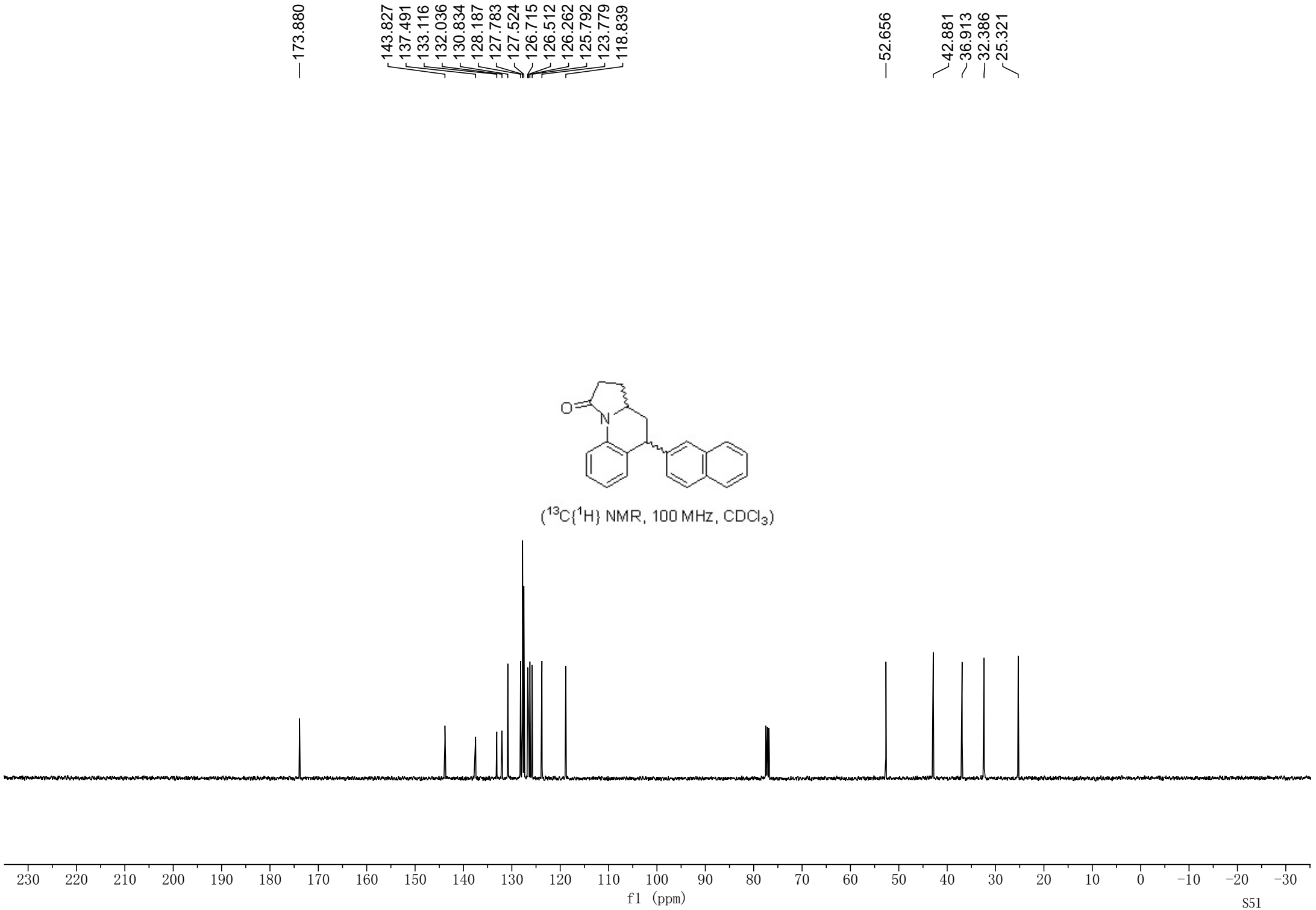




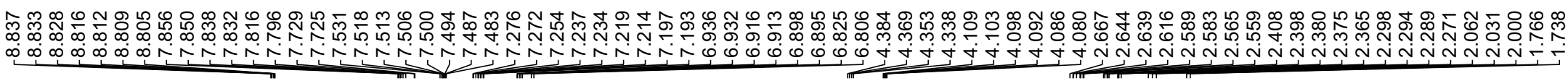
(^{1}H NMR, 400 MHz, $CDCl_3$)

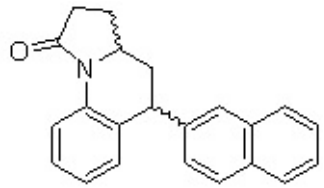


10l/A

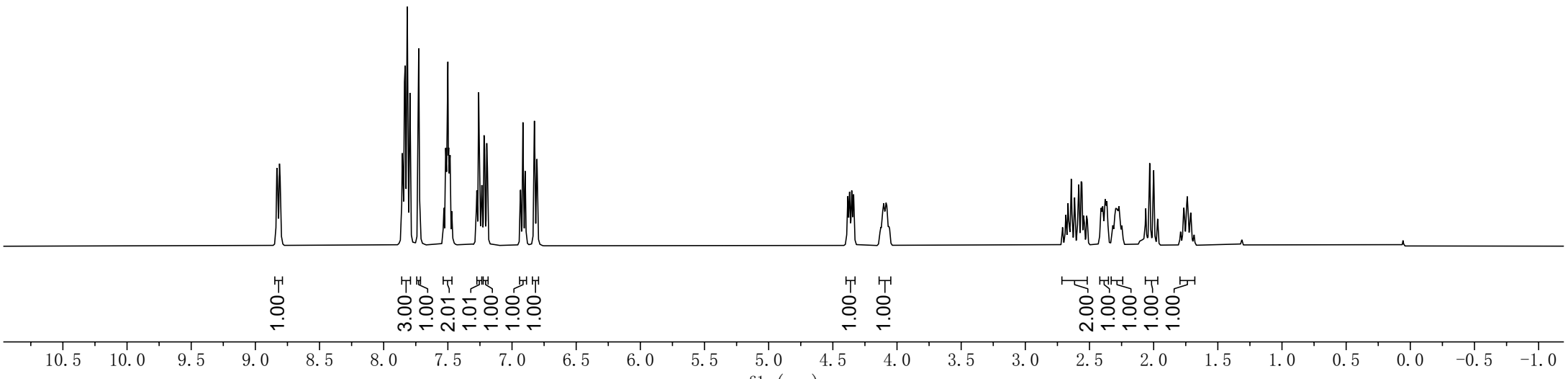

173.880
143.827
137.491
133.116
132.036
130.834
128.187
127.783
127.524
126.715
126.512
126.262
125.792
123.779
118.839
52.656
42.881
36.913
32.386
25.321
O
N
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

10l/B



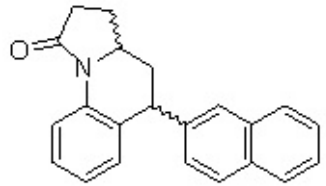


(^{1}H NMR, 400 MHz, $CDCl_3$)

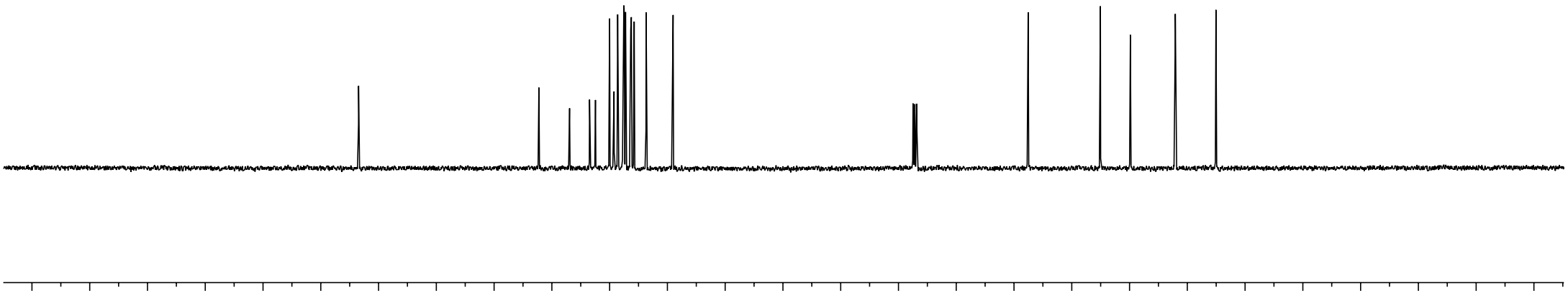


10l/B

173.460
142.243
136.934
133.475
132.453
130.005
129.234
128.610
127.700
127.546
127.487
127.244
126.341
126.243
125.747
123.686
119.011
57.553
45.045
39.854
32.077
25.040



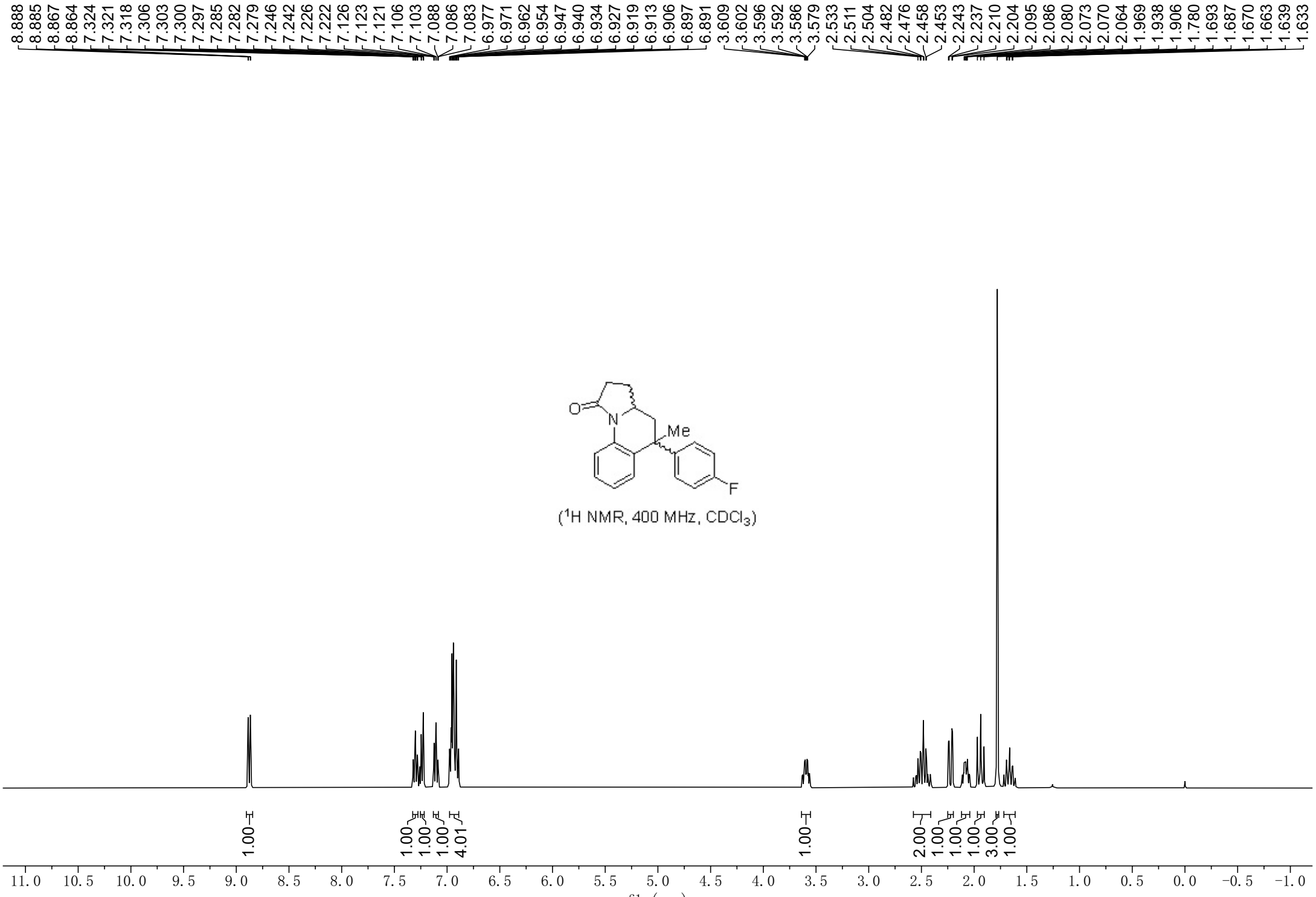
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30

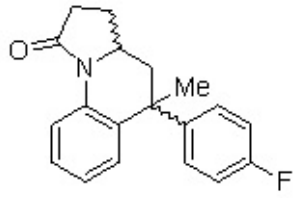
f1 (ppm)

10n/A

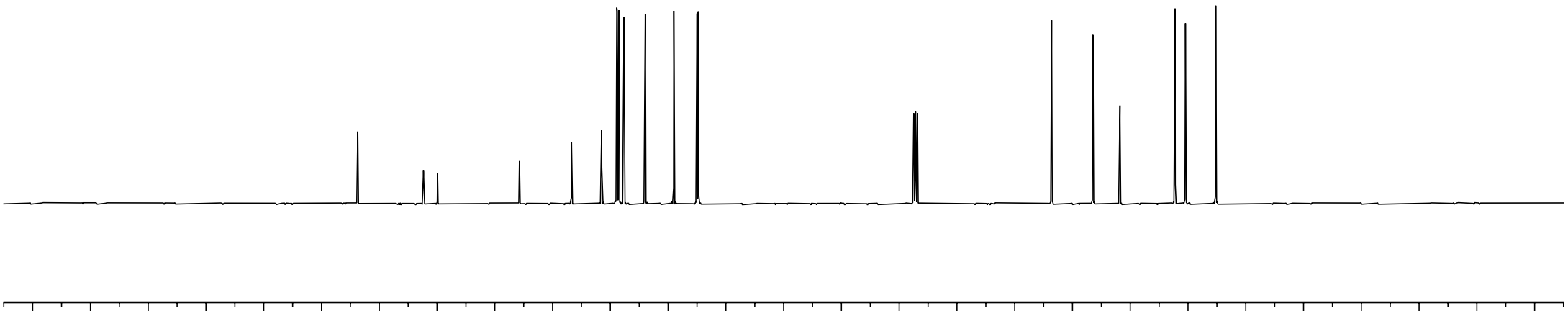

8.888
8.885
8.867
8.864
7.324
7.321
7.318
7.306
7.303
7.300
7.297
7.285
7.282
7.279
7.246
7.242
7.226
7.222
7.126
7.123
7.121
7.106
7.103
7.088
7.086
7.083
6.977
6.971
6.962
6.954
6.947
6.940
6.934
6.927
6.919
6.913
6.906
6.897
6.891
3.609
3.602
3.596
3.592
3.586
3.579
2.533
2.511
2.504
2.482
2.476
2.458
2.453
2.243
2.237
2.210
2.204
2.095
2.086
2.080
2.073
2.070
2.064
1.969
1.938
1.906
1.780
1.693
1.687
1.670
1.663
1.639
1.633
O
N
Me
F
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
1.00
4.01
1.00
2.00
1.00
1.00
1.00
3.00
1.00
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
0.0
-0.5
-1.0
f1 (ppm)

10n/A

173.722
162.351
159.910
145.764
145.733
136.719
131.501
128.884
128.807
128.528
127.658
123.948
119.011
114.999
114.790
53.610
46.463
41.778
32.239
30.441
25.200

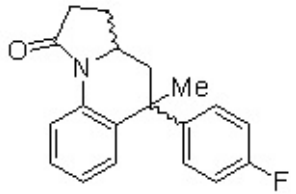


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

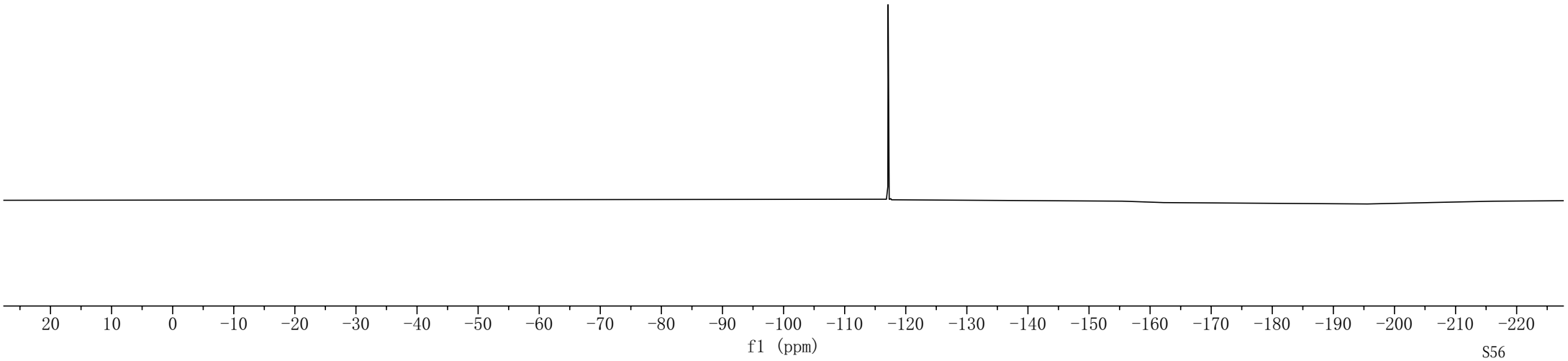


10n/A

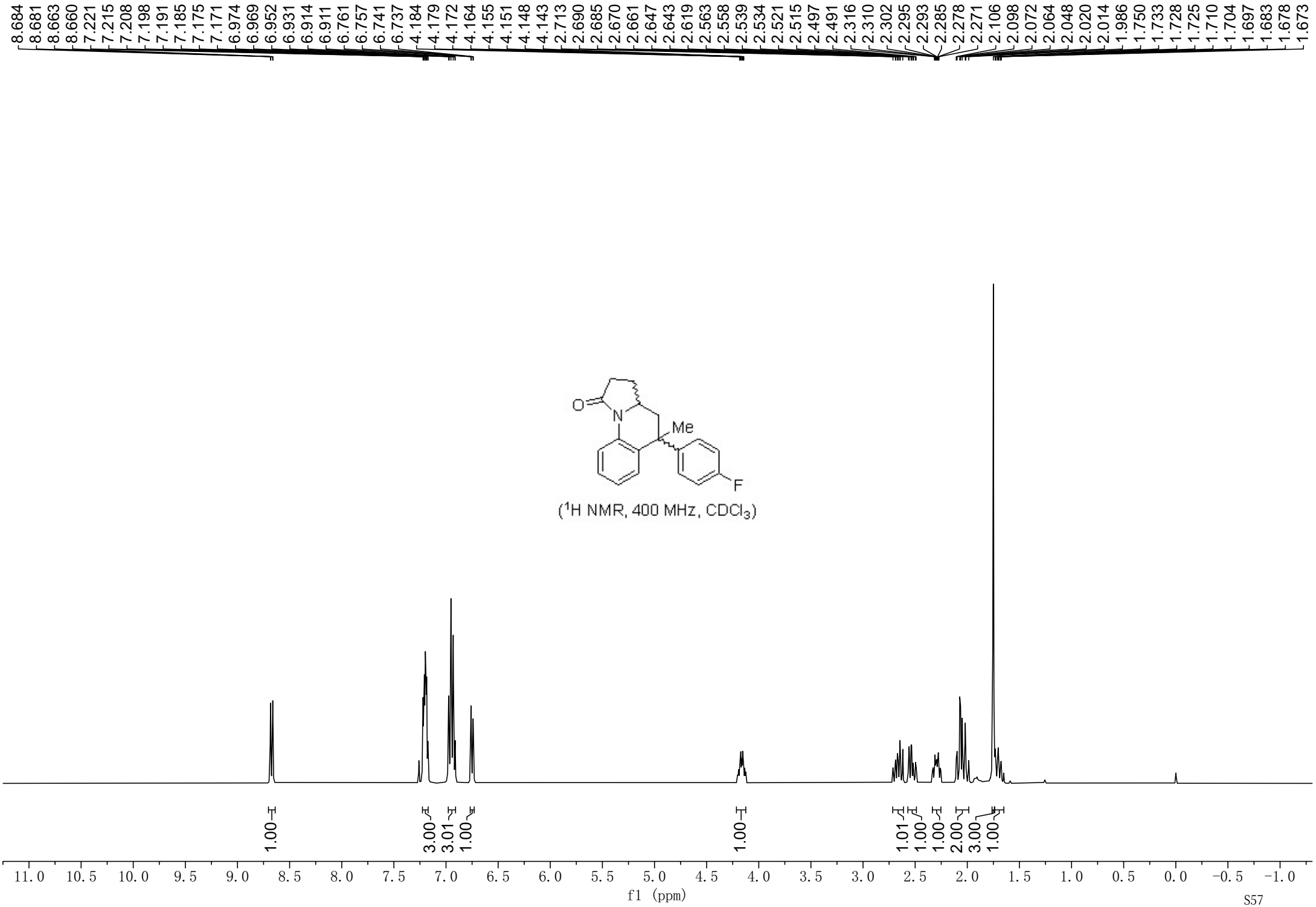
-117.116



(^{19}F NMR, 376 MHz, $CDCl_3$)

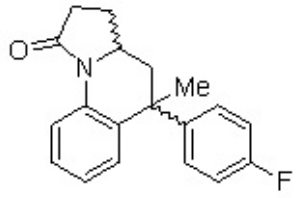


10n/B

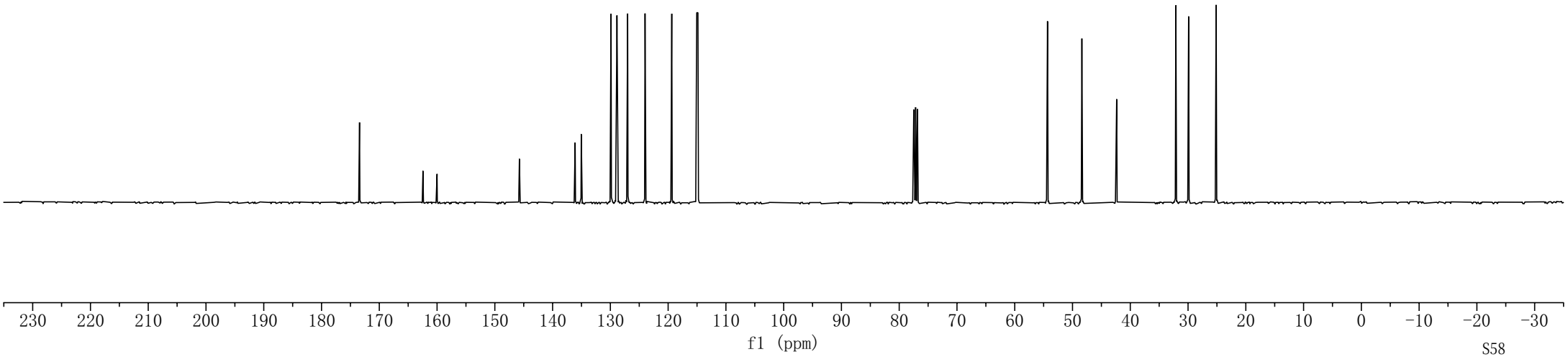

8.684
8.681
8.663
8.660
7.221
7.215
7.208
7.198
7.191
7.185
7.175
7.171
6.974
6.969
6.952
6.931
6.914
6.911
6.761
6.757
6.741
6.737
4.184
4.179
4.172
4.164
4.155
4.151
4.148
4.143
2.713
2.690
2.685
2.670
2.661
2.647
2.643
2.619
2.563
2.558
2.539
2.534
2.521
2.515
2.497
2.491
2.316
2.310
2.302
2.295
2.293
2.285
2.278
2.271
2.106
2.098
2.072
2.064
2.048
2.020
2.014
1.986
1.750
1.733
1.728
1.725
1.710
1.704
1.697
1.683
1.678
1.673
O
N
Me
F
(1H NMR, 400 MHz, CDCl3)
1.00
3.00
3.01
1.00
1.00
1.01
1.00
1.00
2.00
3.00
1.00
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
0.0
-0.5
-1.0
f1 (ppm)

10n/B

173.423
162.440
160.003
145.780
145.747
136.100
135.040
129.887
128.860
128.782
127.008
123.995
119.370
115.050
114.840
54.328
48.377
42.359
32.111
29.901
25.138

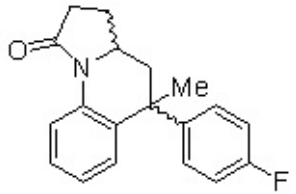


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

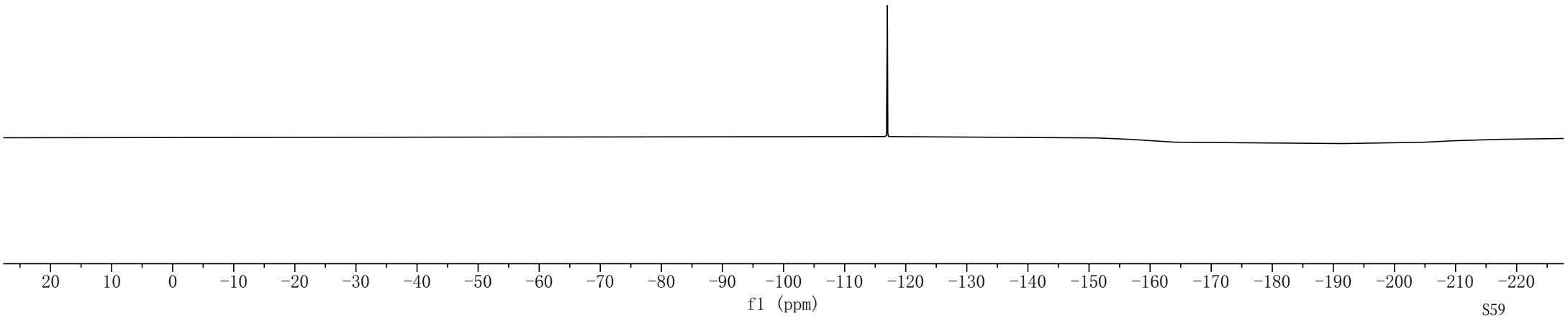


10n/B

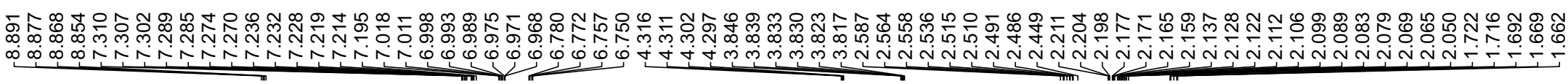
-116.998

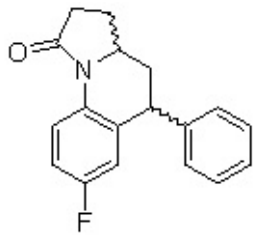


(^{19}F NMR, 376 MHz, $CDCl_3$)

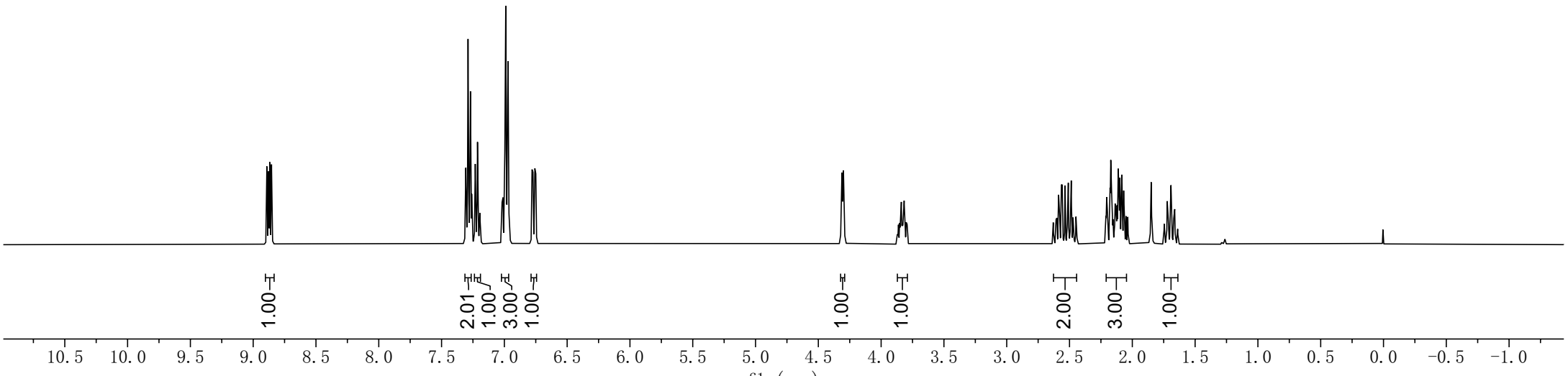


11a/A

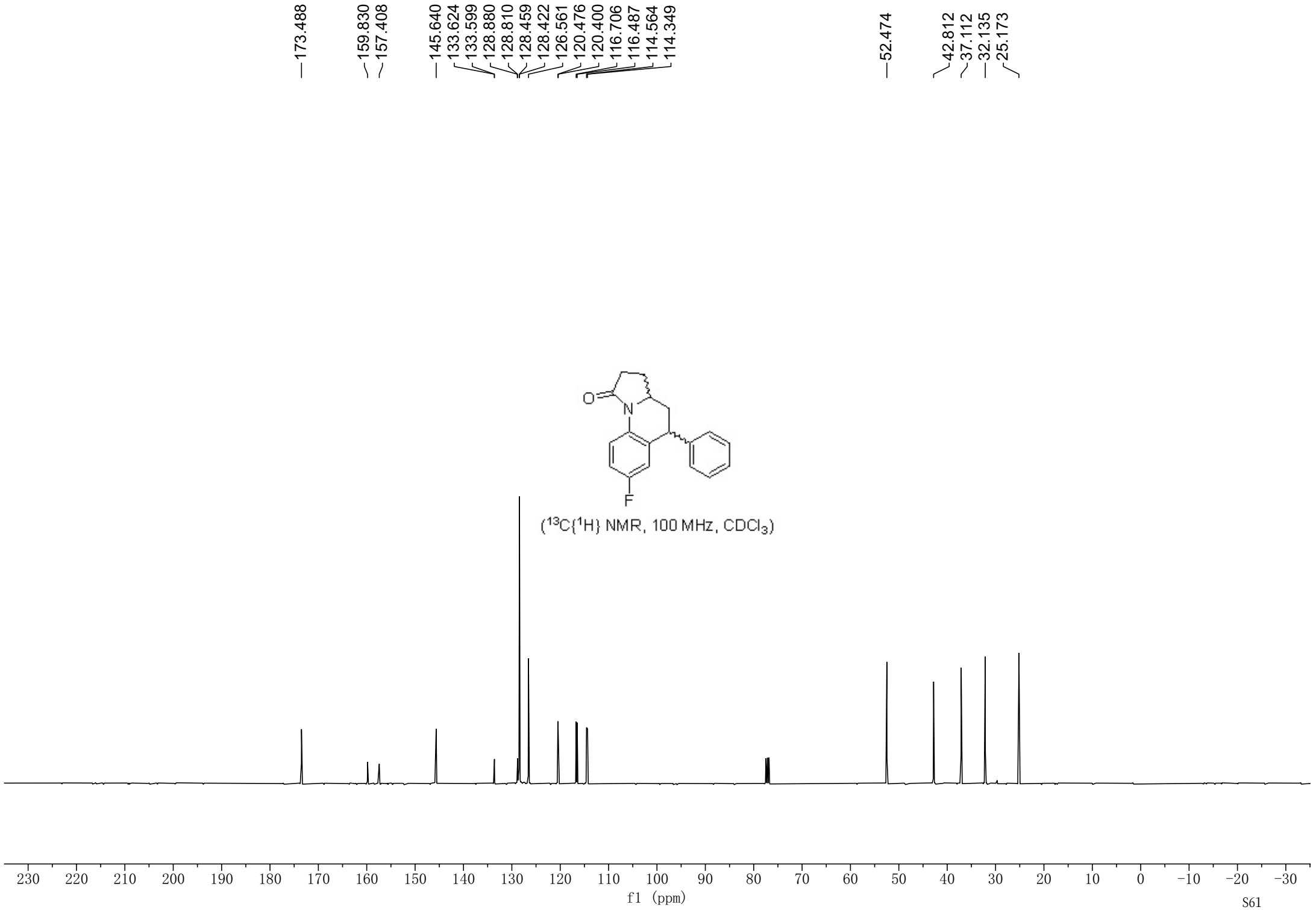




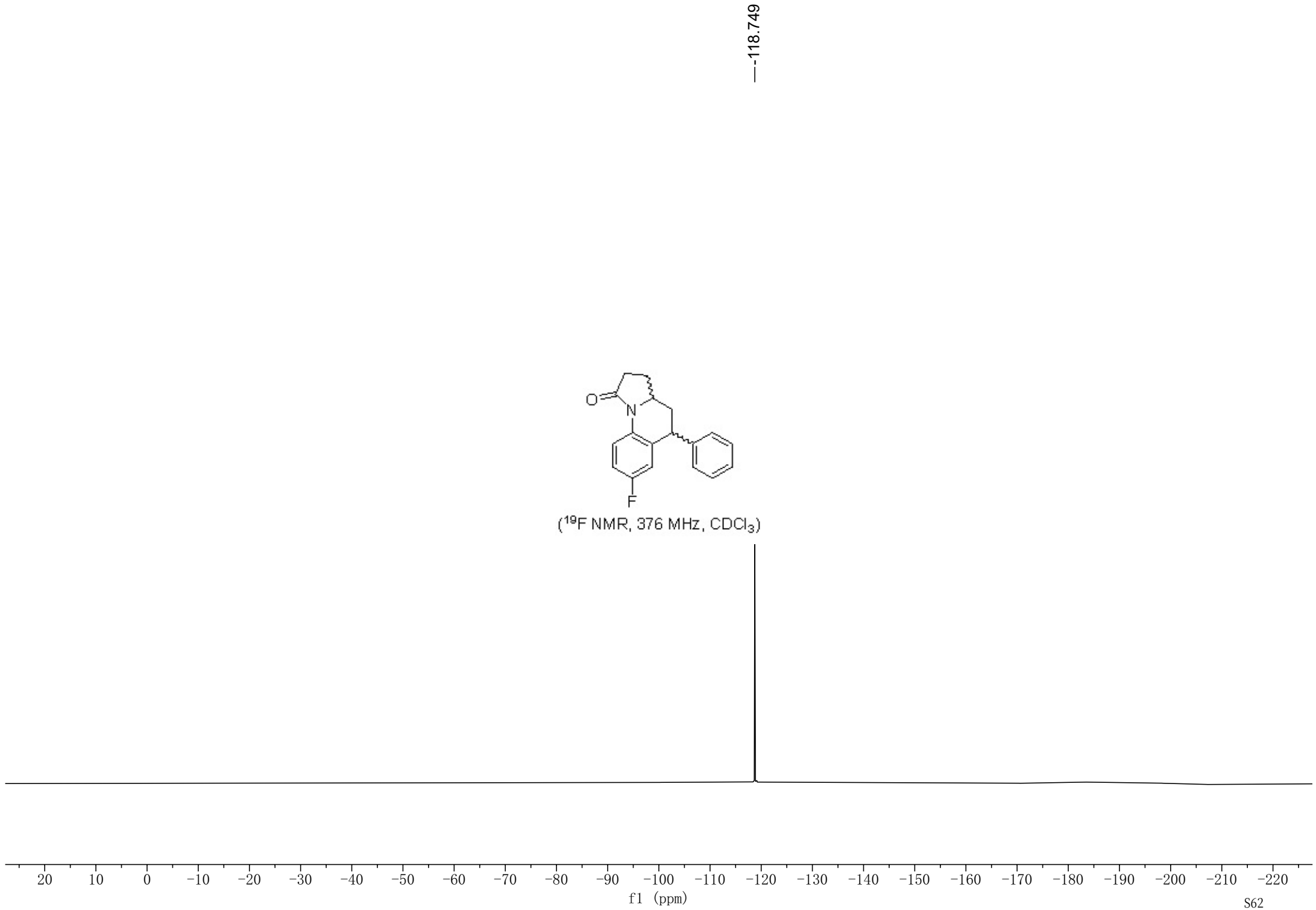
(^{1}H NMR, 400 MHz, $CDCl_3$)



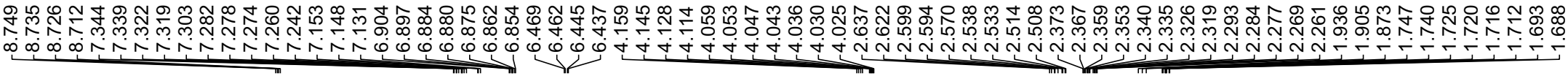
11a/A

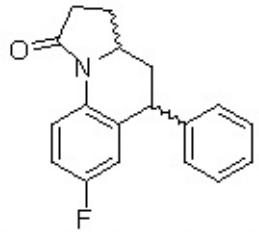

173.488
159.830
157.408
145.640
133.624
133.599
128.880
128.810
128.459
128.422
126.561
120.476
120.400
116.706
116.487
114.564
114.349
52.474
42.812
37.112
32.135
25.173
O
N
F
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11a/A

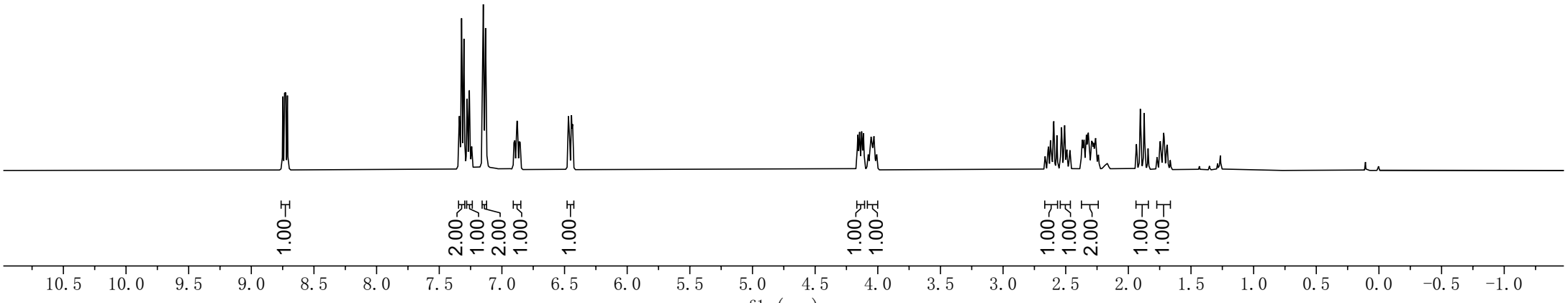

-118.749
O
N
F
(19F NMR, 376 MHz, CDCl3)
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
−220
f1 (ppm)

11a/B

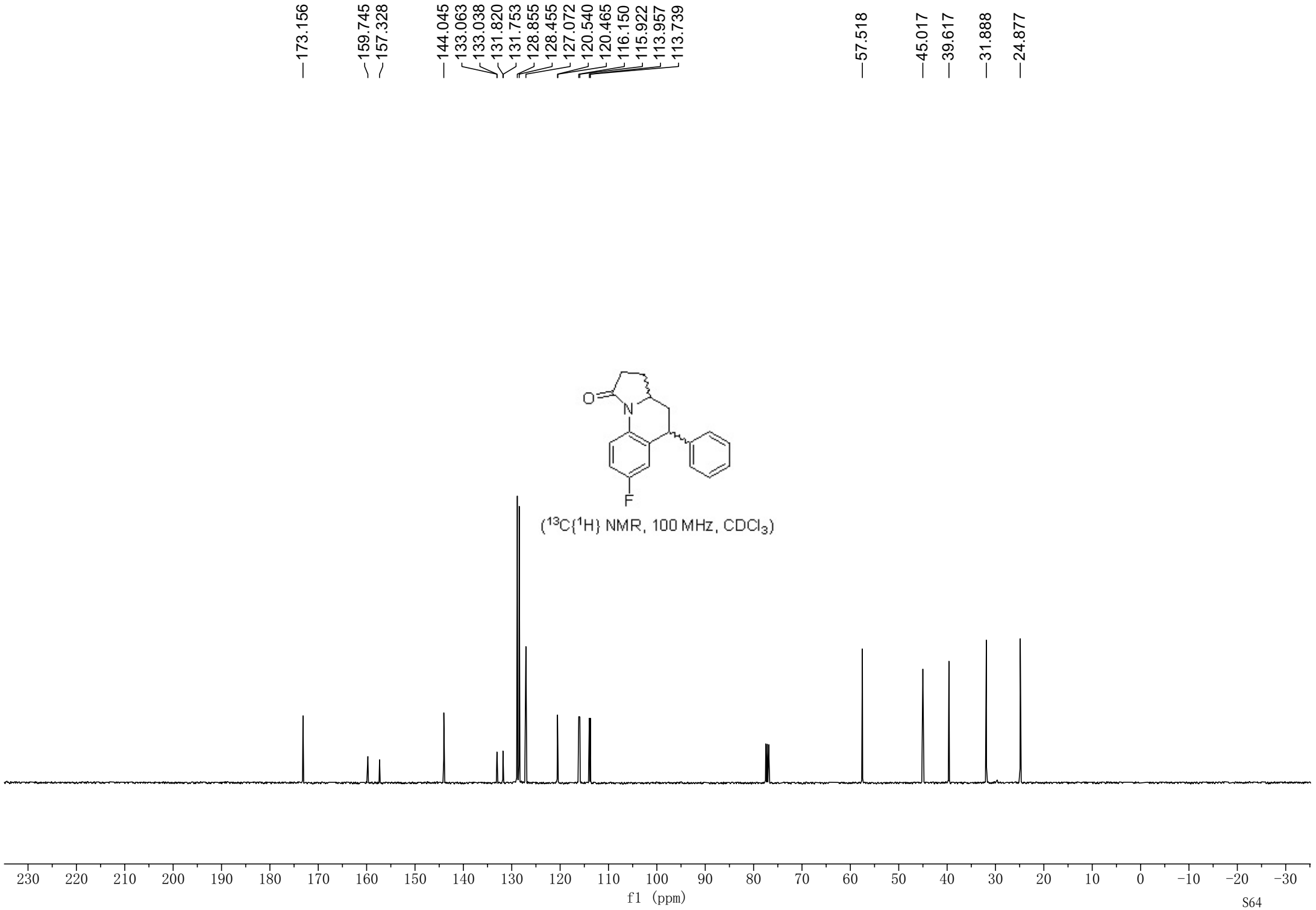




(^{1}H NMR, 400 MHz, $CDCl_3$)



11a/B

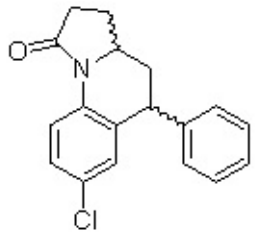

173.156
159.745
157.328
144.045
133.063
133.038
131.820
131.753
128.855
128.455
127.072
120.540
120.465
116.150
115.922
113.957
113.739
57.518
45.017
39.617
31.888
24.877
O
N
F
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11a/B

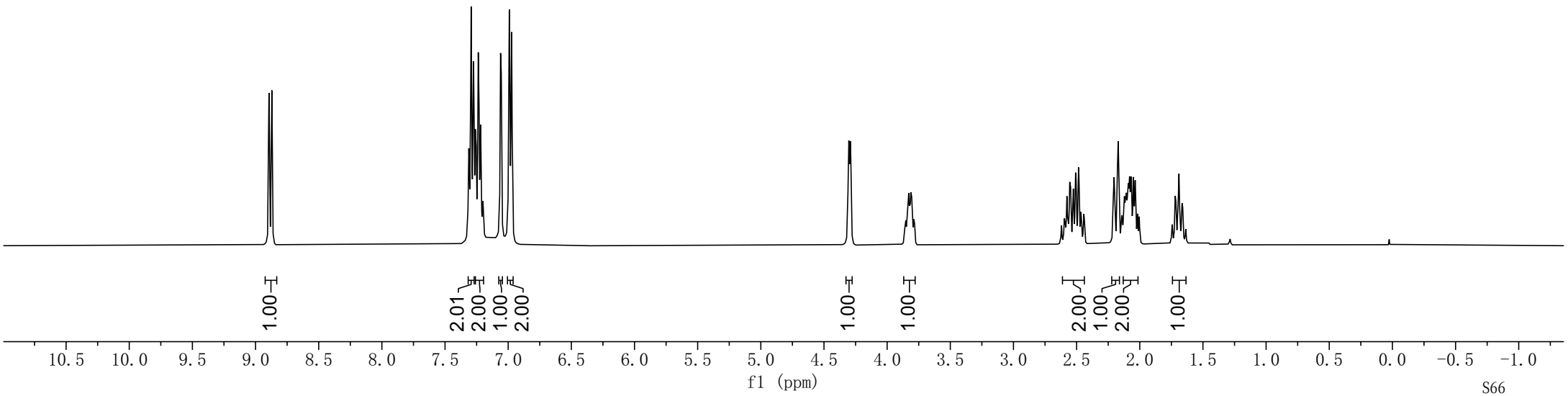

-117.953
O
N
F
(19F NMR, 376 MHz, CDCl3)
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
−220
f1 (ppm)

11b/A

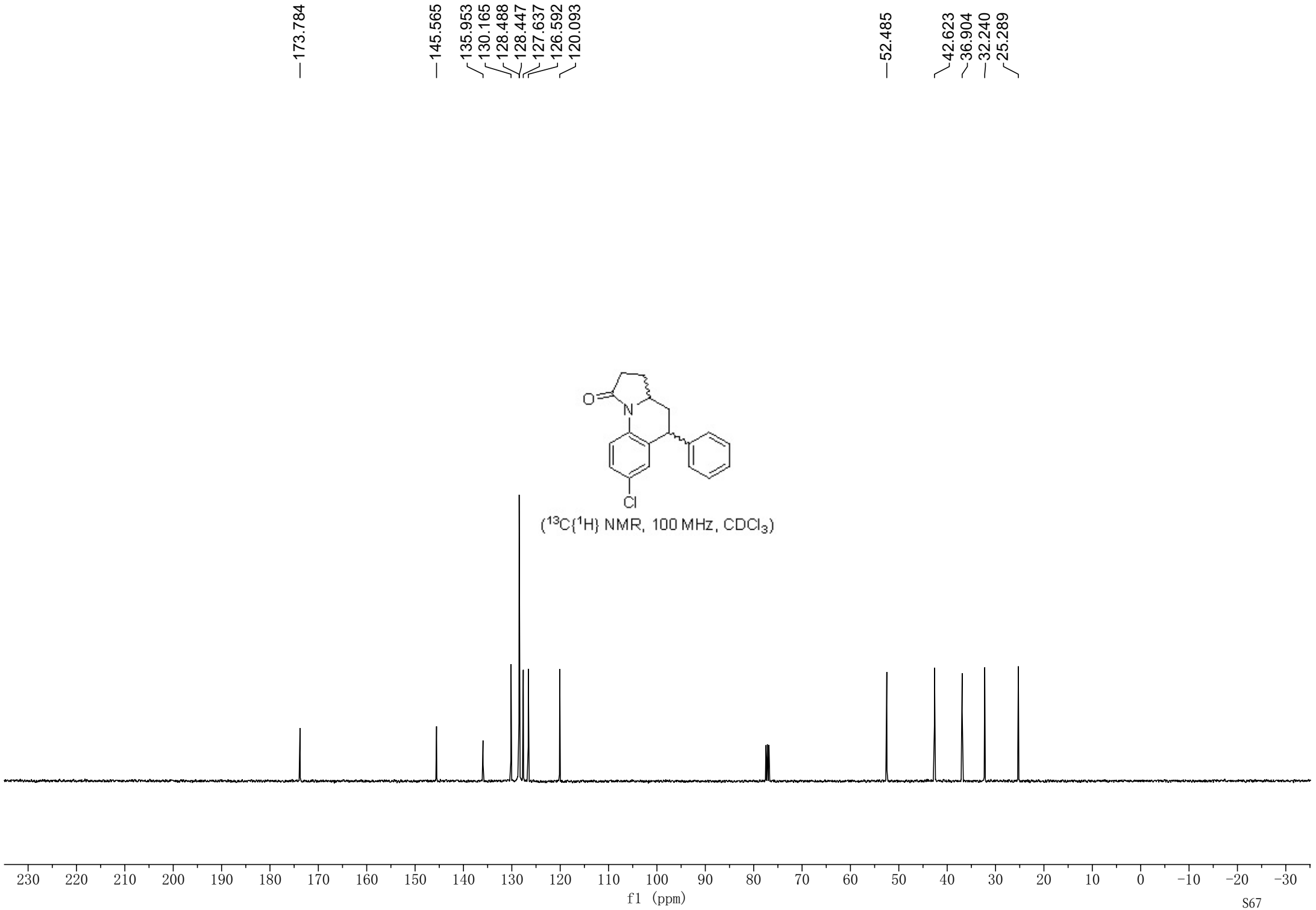
8.893 8.871 7.312 7.293 7.274 7.260 7.254 7.237 7.232 7.218 7.200 7.061 7.054 6.992 6.973 4.304 4.291 3.859 3.852 3.843 3.836 3.829 3.821 3.813 3.806 3.798 3.789 3.782 2.620 2.598 2.590 2.577 2.568 2.555 2.547 2.526 2.509 2.505 2.486 2.481 2.467 2.462 2.443 2.438 2.209 2.203 2.198 2.176 2.171 2.165 2.143 2.138 2.127 2.122 2.112 2.107 2.090 2.080 2.068 2.050 2.036 2.018 2.004 1.744 1.720 1.713 1.696 1.690 1.683 1.666 1.659 1.636



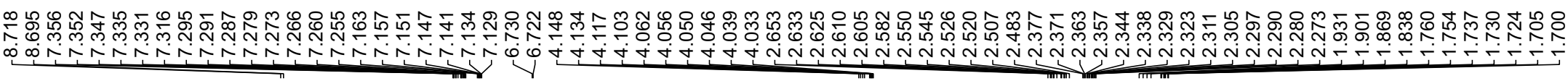
(^{1}H NMR, 400 MHz, $CDCl_3$)

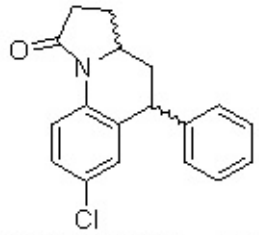


11b/A

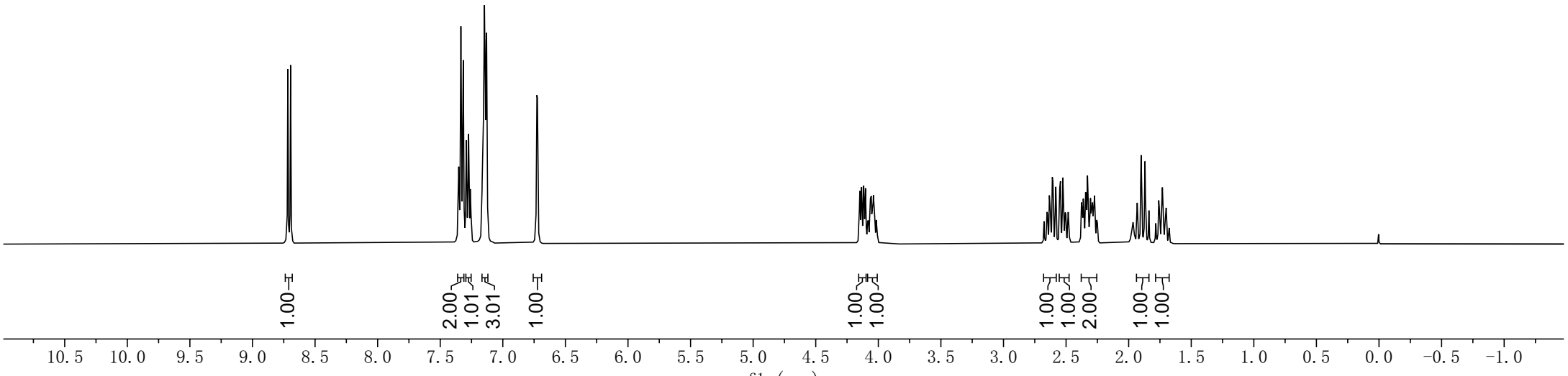

173.784
145.565
135.953
130.165
128.488
128.447
127.637
126.592
120.093
52.485
42.623
36.904
32.240
25.289
O
N
Cl
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11b/B

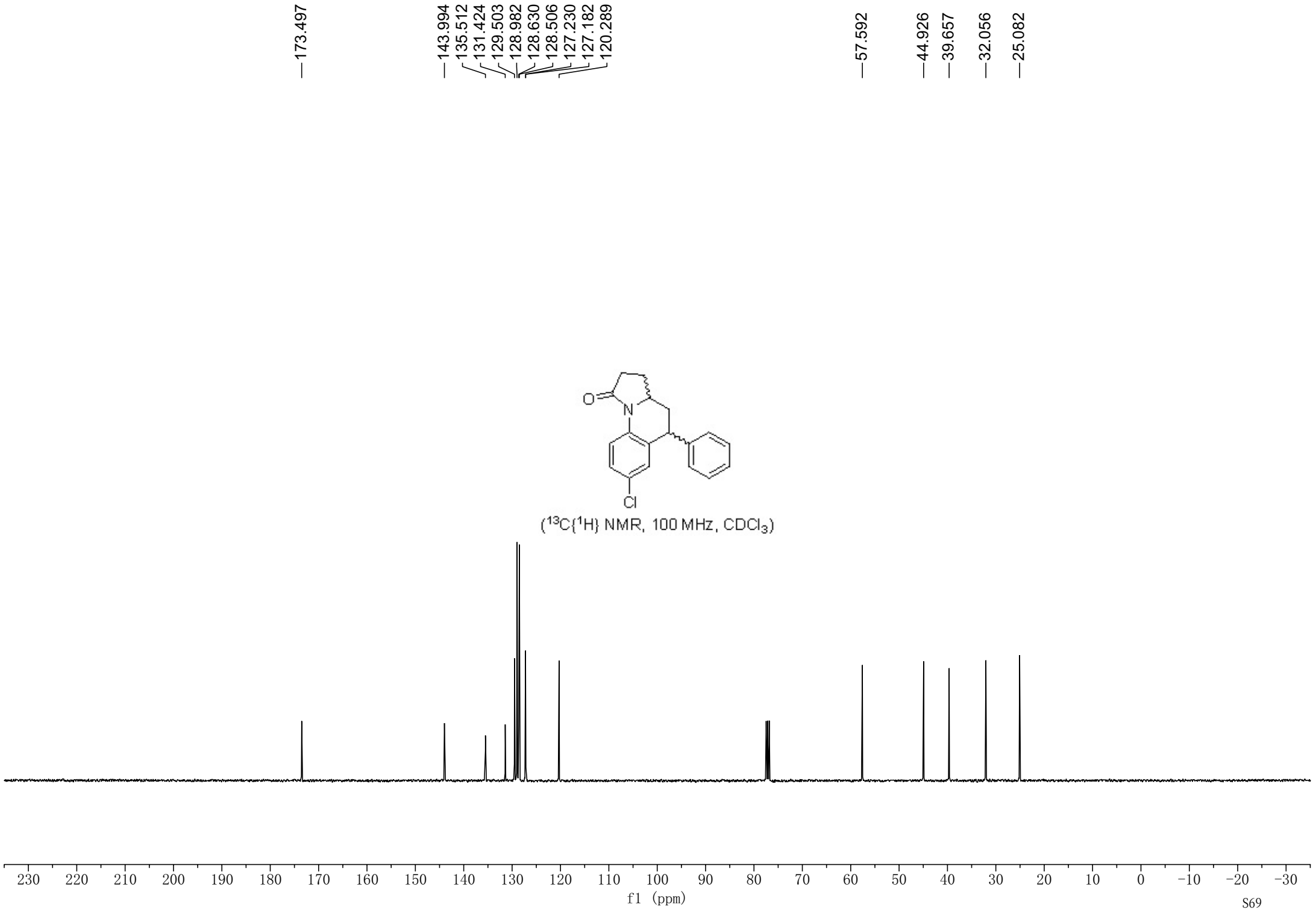




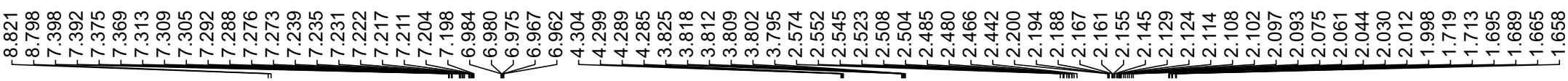
(^{1}H NMR, 400 MHz, $CDCl_3$)

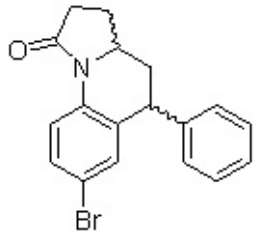


11b/B

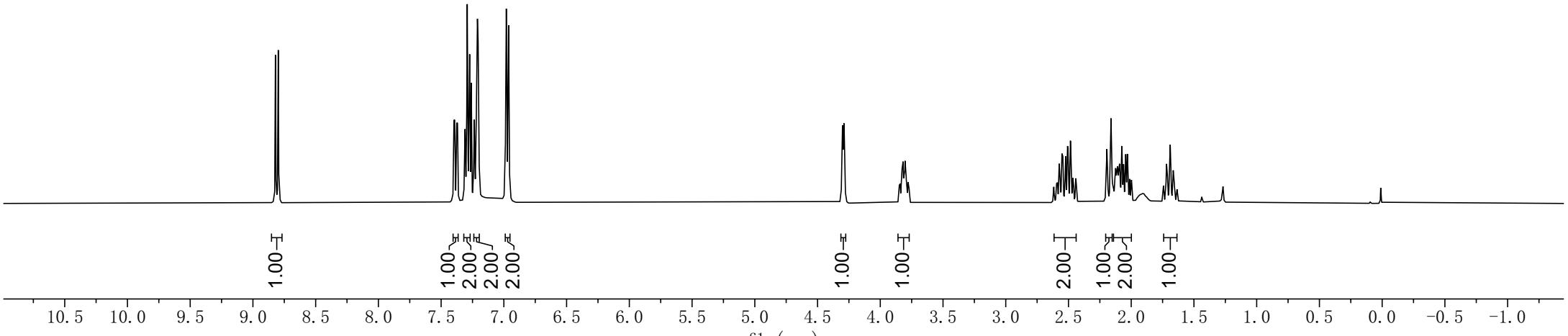

173.497
143.994
135.512
131.424
129.503
128.982
128.630
128.506
127.230
127.182
120.289
57.592
44.926
39.657
32.056
25.082
O
N
Cl
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11c/A

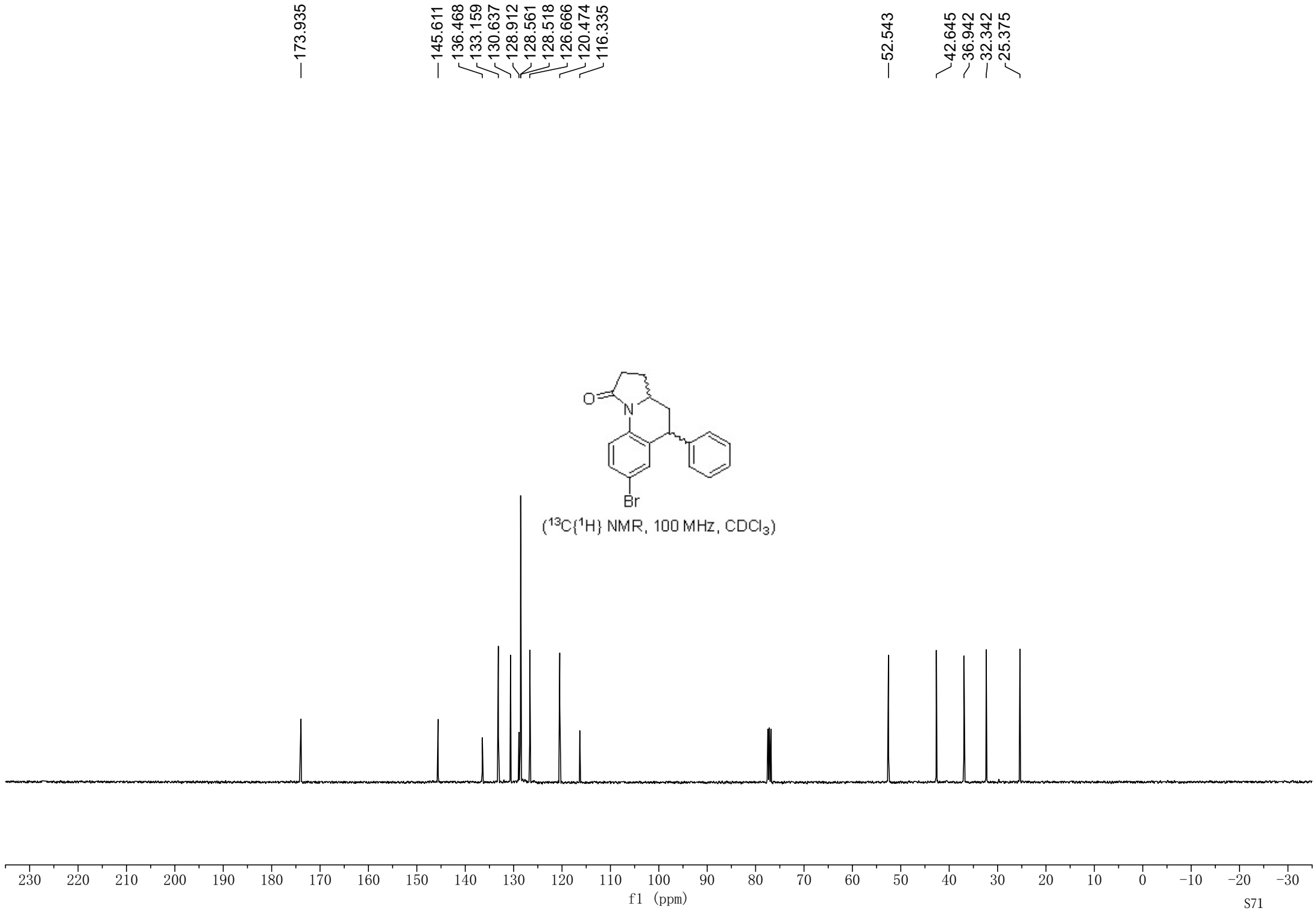




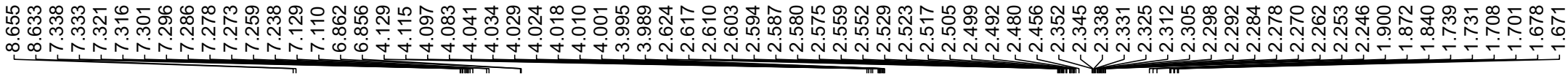
(^{1}H NMR, 400 MHz, $CDCl_3$)

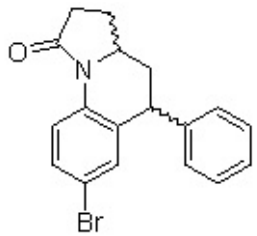


11c/A

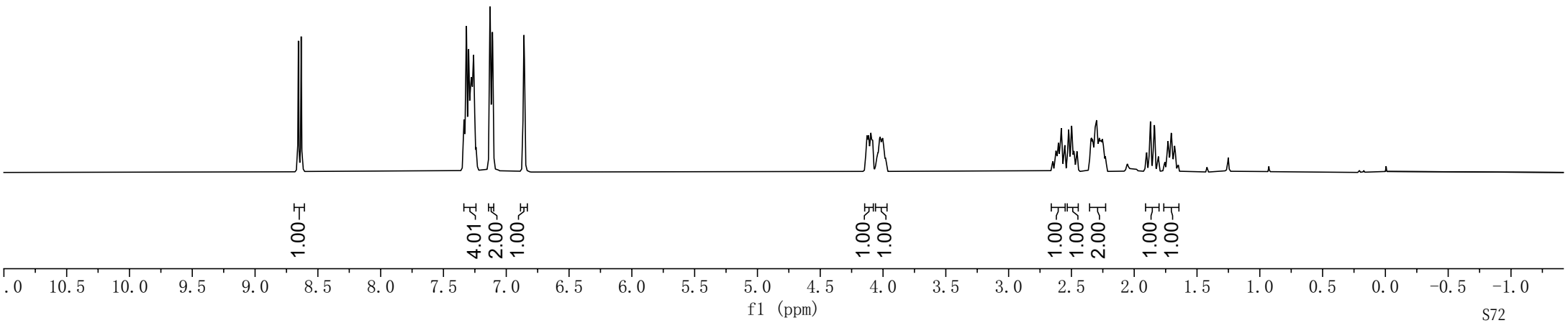

173.935
145.611
136.468
133.159
130.637
128.912
128.561
128.518
126.666
120.474
116.335
52.543
42.645
36.942
32.342
25.375
O
N
Br
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11c/B

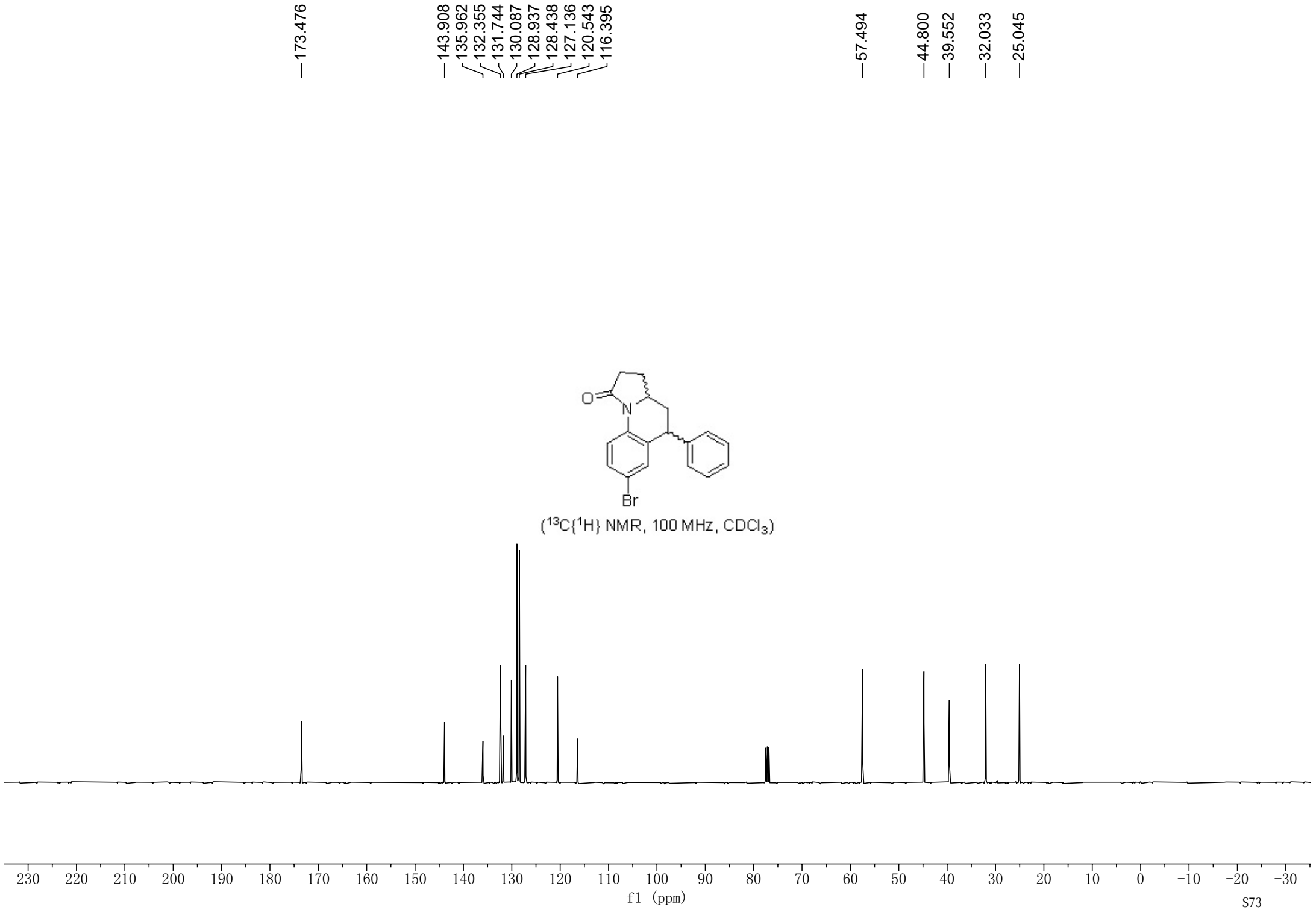




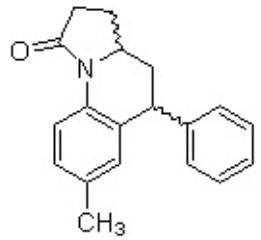
(^{1}H NMR, 400 MHz, $CDCl_3$)



11c/B


173.476
143.908
135.962
132.355
131.744
130.087
128.937
128.438
127.136
120.543
116.395
57.494
44.800
39.552
32.033
25.045
O
N
Br
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

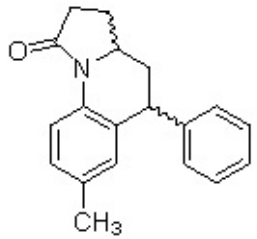
11d/A



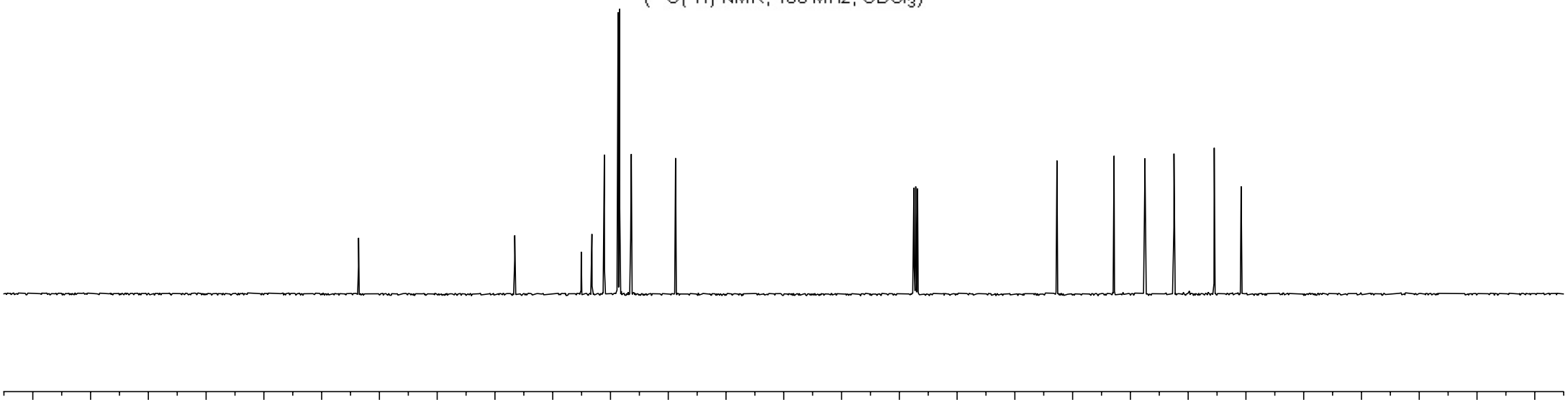
(^{1}H NMR, 400 MHz, $CDCl_3$)

11d/A

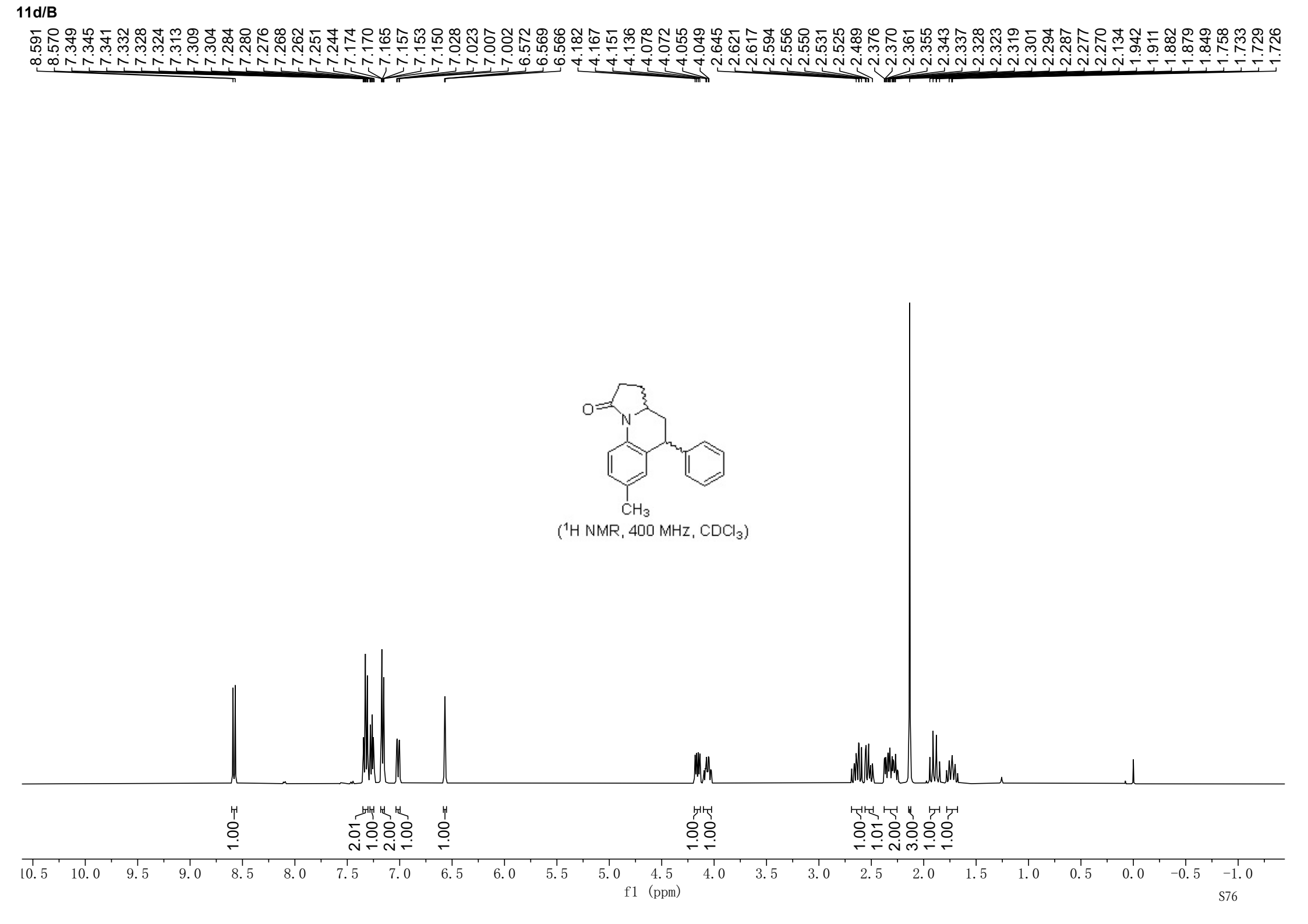
173.608
146.578
135.062
133.213
131.062
128.687
128.455
128.419
126.509
126.398
118.735
52.712
42.827
37.489
32.456
25.486
20.831



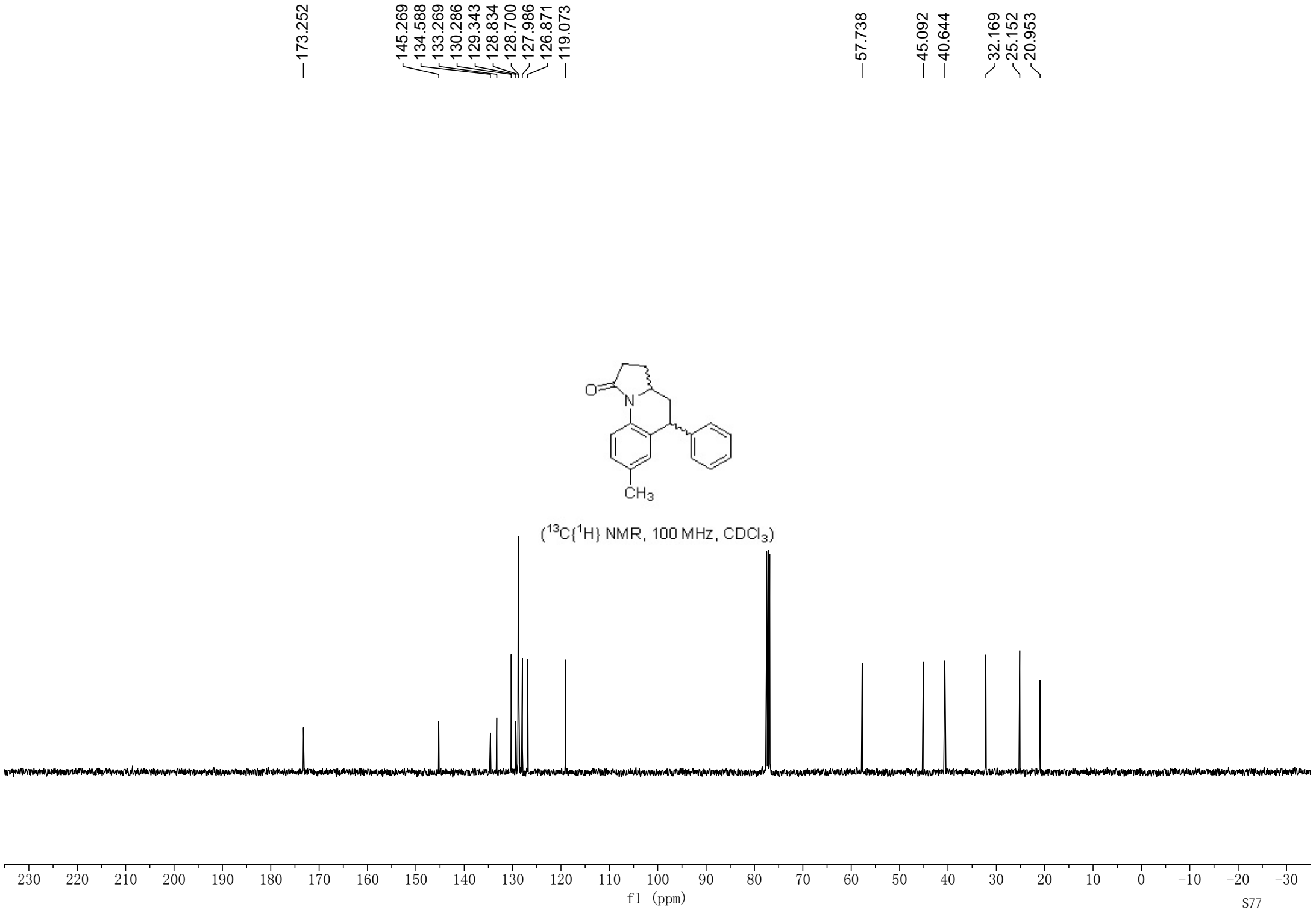
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



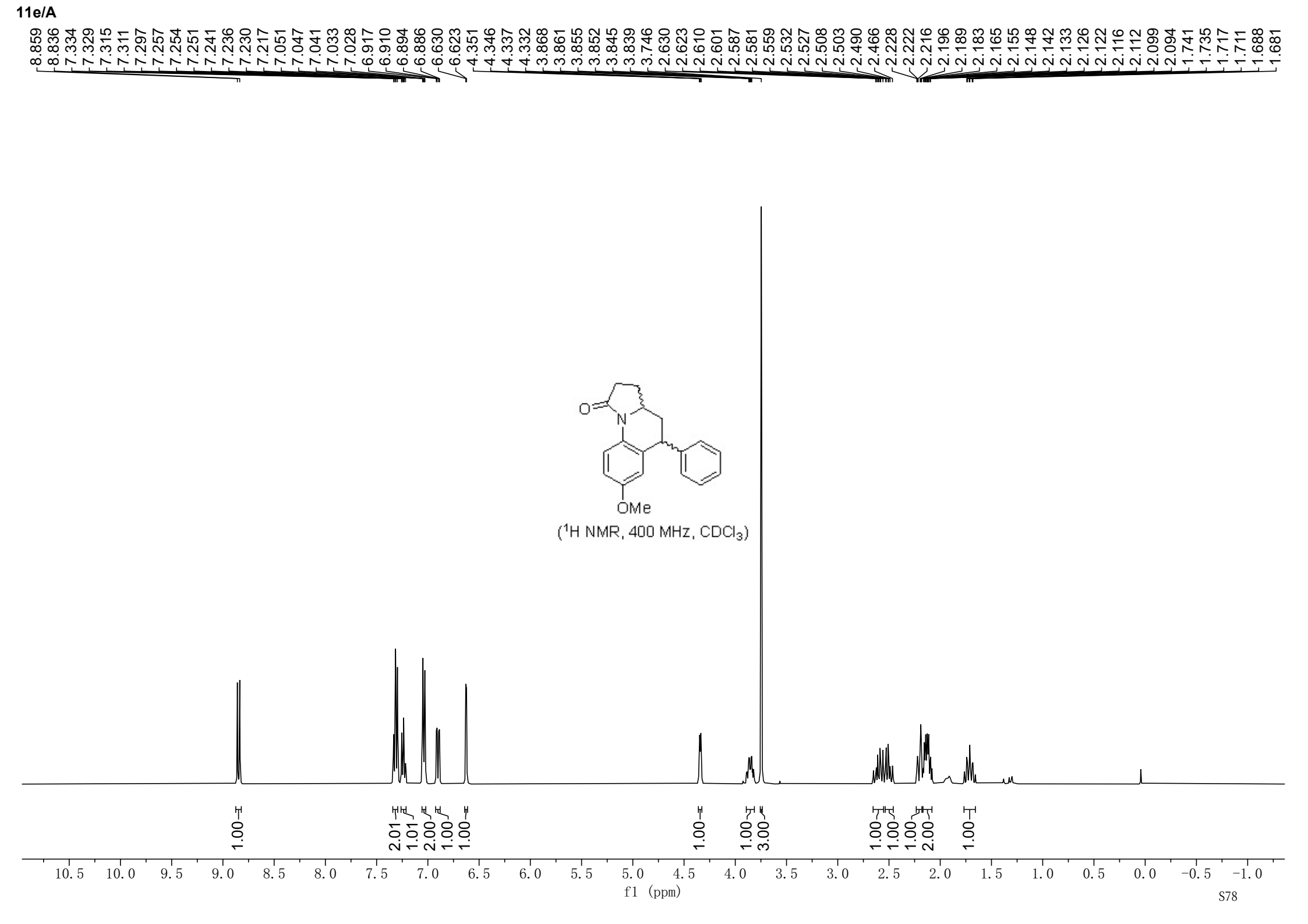
11d/B


8.591
8.570
7.349
7.345
7.341
7.332
7.328
7.324
7.313
7.309
7.304
7.284
7.280
7.276
7.268
7.262
7.251
7.244
7.174
7.170
7.165
7.157
7.153
7.150
7.028
7.023
7.007
7.002
6.572
6.569
6.566
4.182
4.167
4.151
4.136
4.078
4.072
4.055
4.049
2.645
2.621
2.617
2.594
2.556
2.550
2.531
2.525
2.489
2.376
2.370
2.361
2.355
2.343
2.337
2.328
2.323
2.319
2.301
2.294
2.287
2.277
2.270
2.134
1.942
1.911
1.882
1.879
1.849
1.758
1.733
1.729
1.726
O
N
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
2.01
1.00
2.00
1.00
1.00
1.00
1.00
1.01
2.00
3.00
1.00
1.00
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
-0.5
-1.0
f1 (ppm)

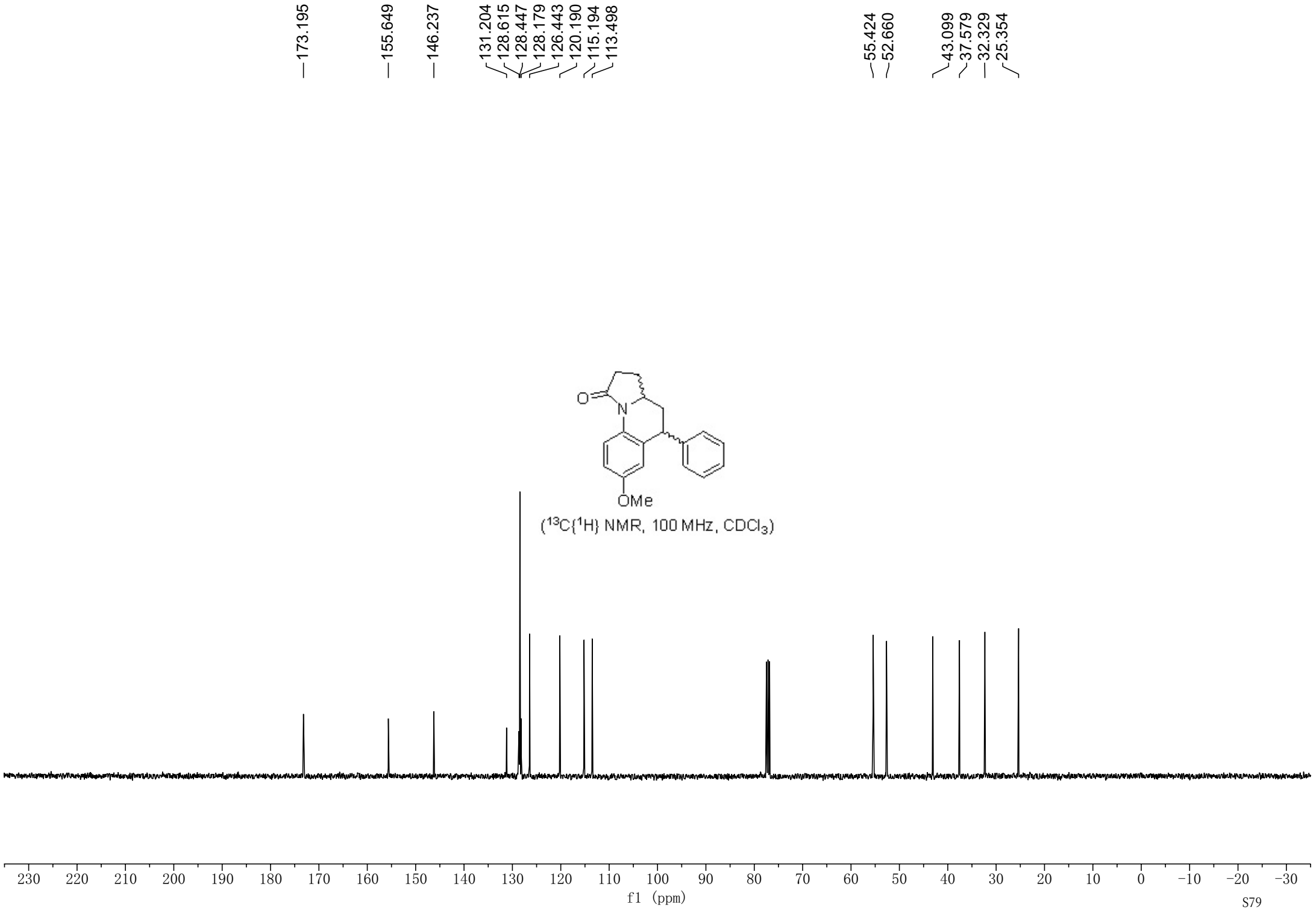
11d/B


173.252
145.269
134.588
133.269
130.286
129.343
128.834
128.700
127.986
126.871
119.073
57.738
45.092
40.644
32.169
25.152
20.953
O
N
CH3
(13C{1H} NMR, 100 MHz, CDCl3)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
f1 (ppm)

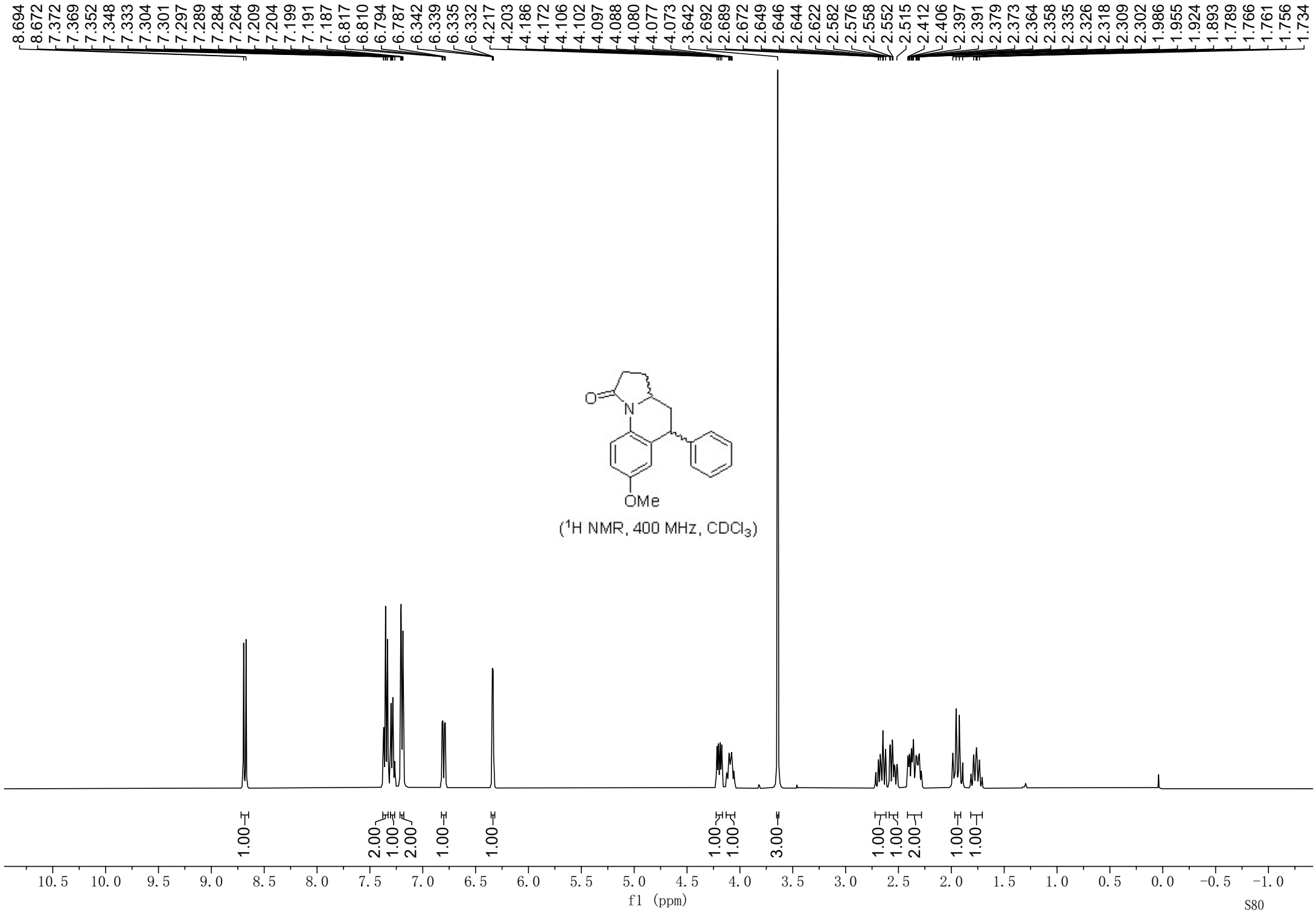
11e/A


8.859
8.836
7.334
7.329
7.315
7.311
7.297
7.257
7.254
7.251
7.241
7.236
7.230
7.217
7.051
7.047
7.041
7.033
7.028
6.917
6.910
6.894
6.886
6.630
6.623
4.351
4.346
4.337
4.332
3.868
3.861
3.855
3.852
3.845
3.839
3.746
2.630
2.623
2.610
2.601
2.587
2.581
2.559
2.532
2.527
2.508
2.503
2.490
2.466
2.228
2.222
2.216
2.196
2.189
2.183
2.165
2.155
2.148
2.142
2.133
2.126
2.122
2.116
2.112
2.099
2.094
1.741
1.735
1.717
1.711
1.688
1.681
O
N
OMe
(1H NMR, 400 MHz, CDCl3)
1.00
2.01
1.01
2.00
1.00
1.00
1.00
1.00
3.00
1.00
1.00
1.00
2.00
1.00
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
-0.5
-1.0
f1 (ppm)

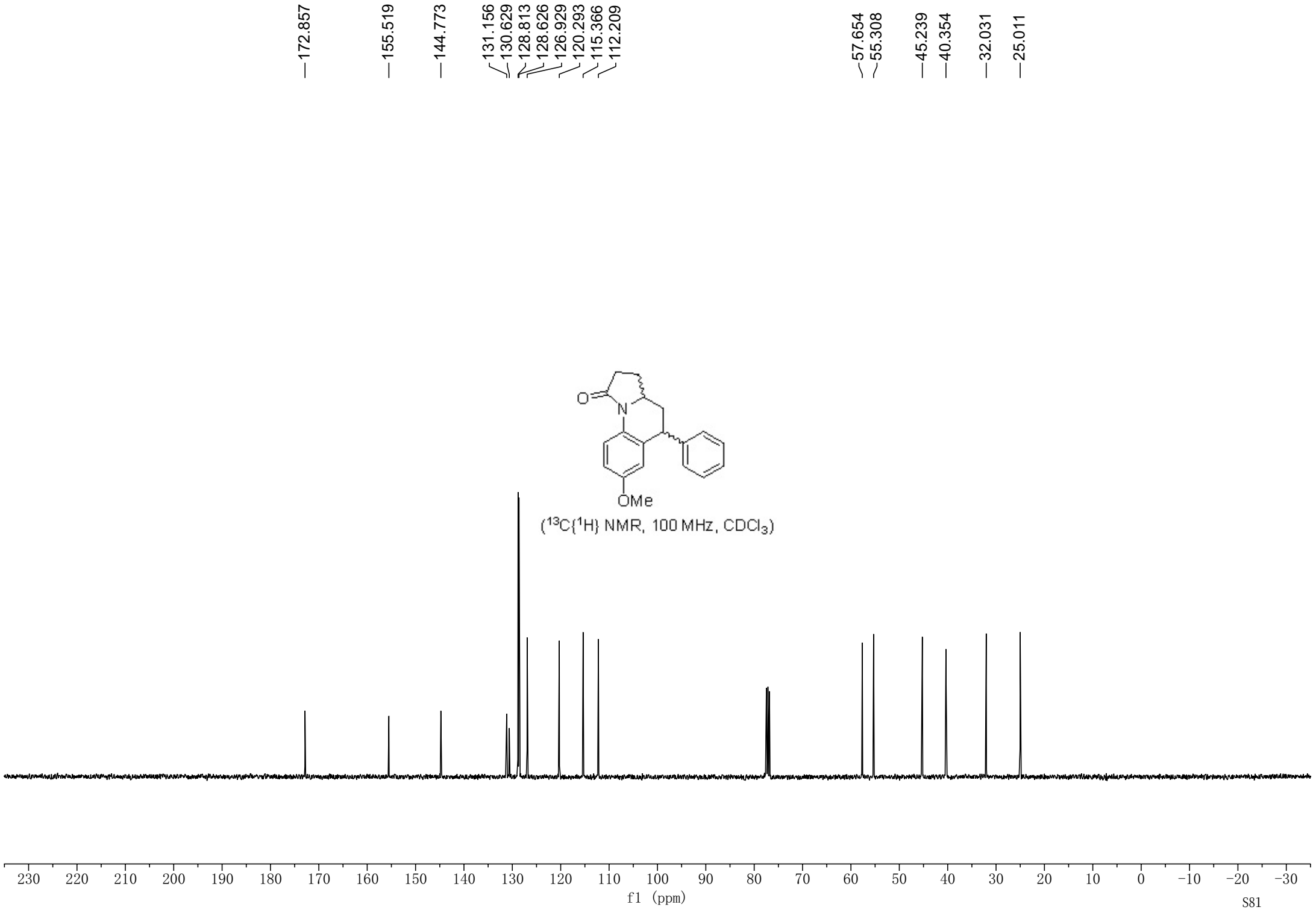
11e/A


173.195
155.649
146.237
131.204
128.615
128.447
128.179
126.443
120.190
115.194
113.498
55.424
52.660
43.099
37.579
32.329
25.354
O
N
OMe
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11e/B

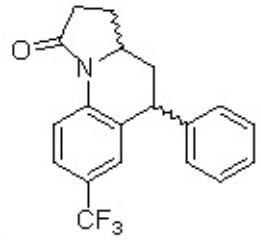

8.694
8.672
7.372
7.369
7.352
7.348
7.333
7.304
7.301
7.297
7.289
7.284
7.264
7.209
7.204
7.199
7.191
7.187
6.817
6.810
6.794
6.787
6.342
6.339
6.335
6.332
4.217
4.203
4.186
4.172
4.106
4.102
4.097
4.088
4.080
4.077
4.073
3.642
2.692
2.689
2.672
2.649
2.646
2.644
2.622
2.582
2.576
2.558
2.552
2.515
2.412
2.406
2.397
2.391
2.379
2.373
2.364
2.358
2.335
2.326
2.318
2.309
2.302
1.986
1.955
1.924
1.893
1.789
1.766
1.761
1.756
1.734
O
N
OMe
(1H NMR, 400 MHz, CDCl3)
1.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
1.00
2.00
1.00
1.00
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
-0.5
-1.0
f1 (ppm)

11e/B

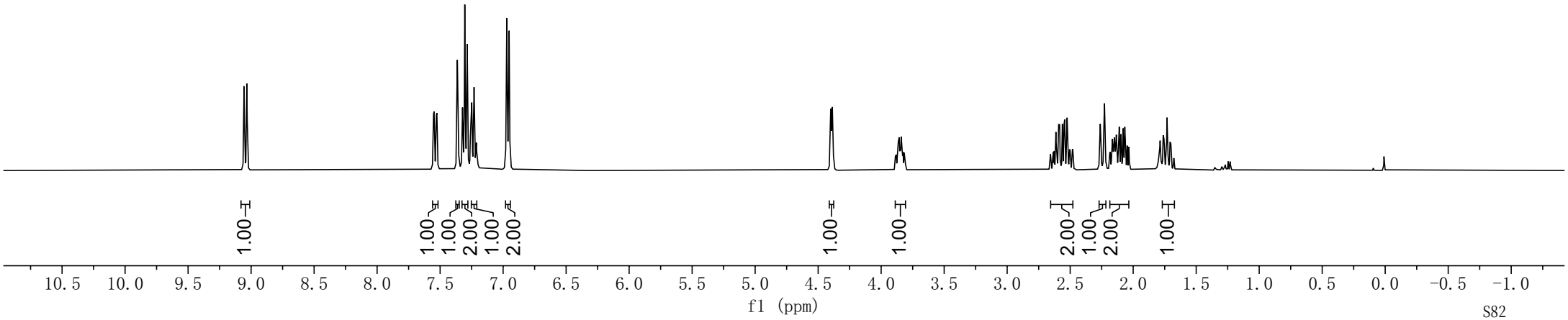

172.857
155.519
144.773
131.156
130.629
128.813
128.626
126.929
120.293
115.366
112.209
57.654
55.308
45.239
40.354
32.031
25.011
O
N
OMe
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11f/A

9.056 9.034 7.553 7.547 7.531 7.525 7.365 7.359 7.325 7.322 7.317 7.304 7.300 7.289 7.285 7.252 7.249 7.245 7.236 7.231 7.224 7.212 6.975 6.970 6.965 6.956 6.952 4.402 4.398 4.389 4.384 3.864 3.857 3.851 3.847 3.841 3.834 2.613 2.592 2.583 2.562 2.548 2.543 2.525 2.520 2.267 2.261 2.255 2.234 2.228 2.222 2.165 2.155 2.150 2.144 2.139 2.134 2.117 2.111 2.097 2.081 2.077 2.067 2.063 2.047 2.034 1.762 1.755 1.738 1.732 1.708 1.701

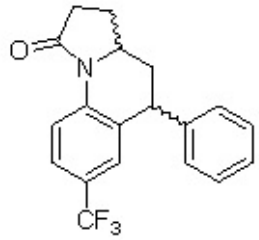


(^{1}H NMR, 400 MHz, $CDCl_3$)

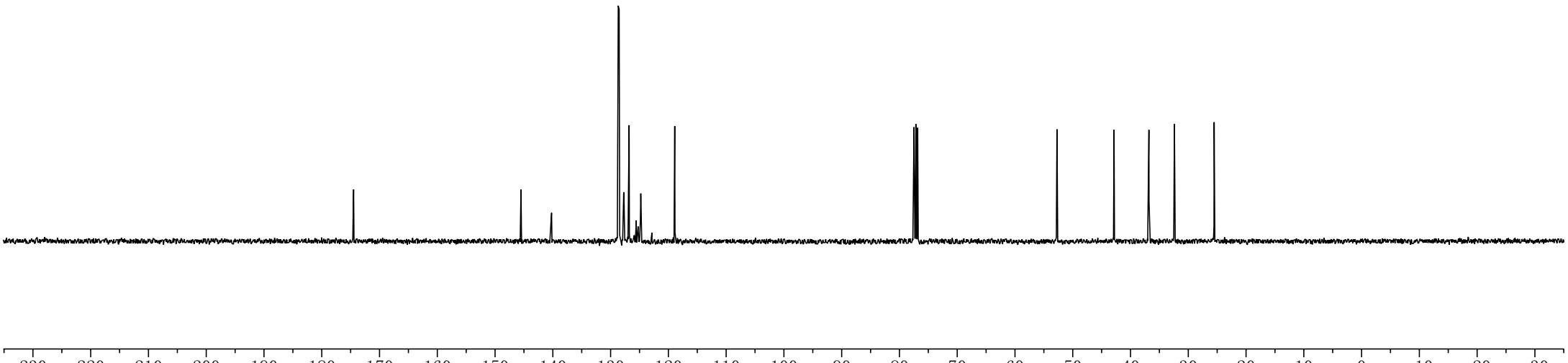


11f/A

174.491
145.511
140.219
128.678
128.522
127.779
127.739
127.701
127.663
126.914
126.794
125.569
125.249
124.811
124.774
124.737
122.862
118.900
52.733
42.852
36.813
32.399
25.519

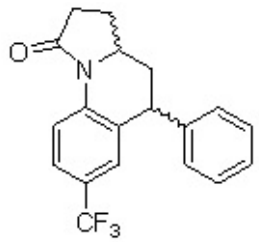


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

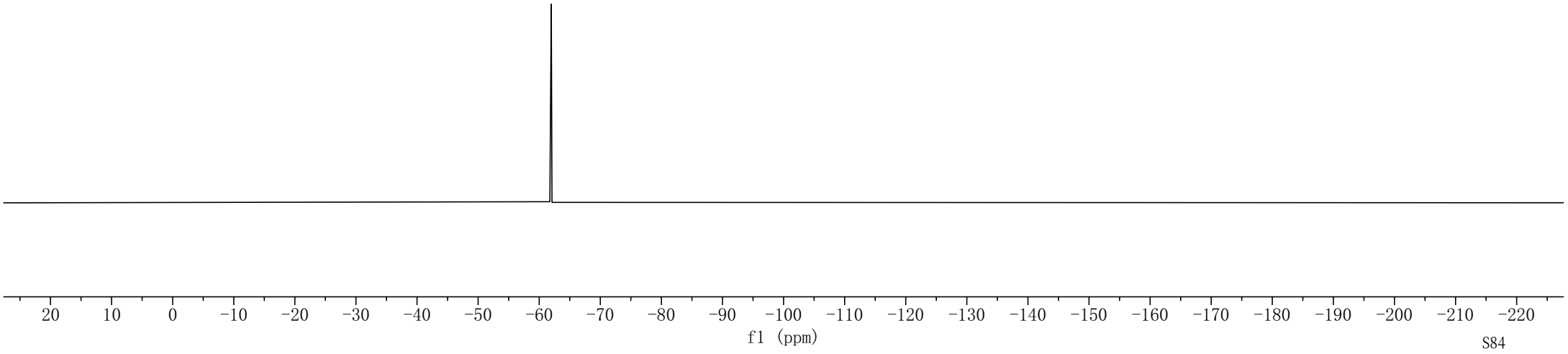


11f/A

-61.978

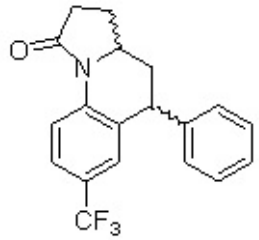


(^{19}F NMR, 376 MHz, $CDCl_3$)

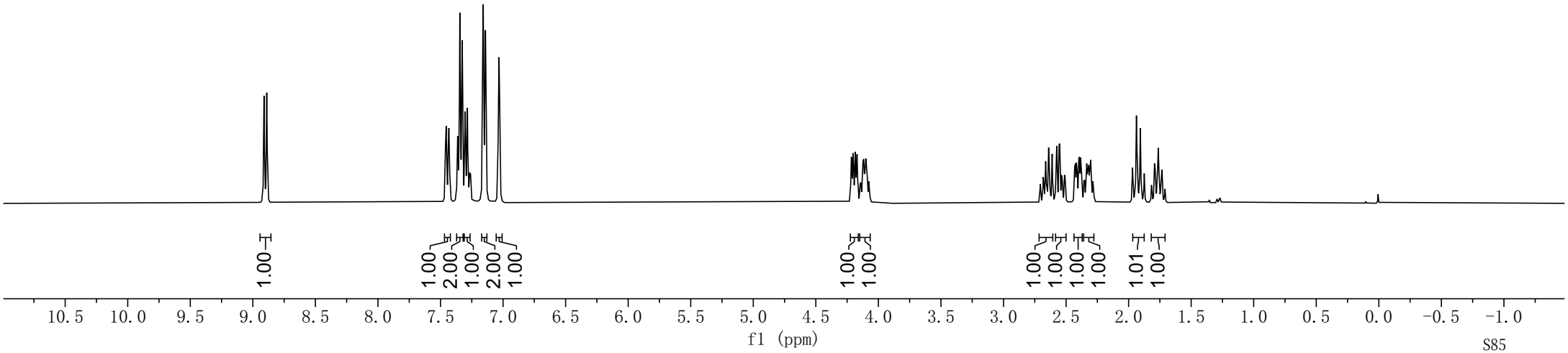


11f/B

8.911 8.889 7.458 7.452 7.436 7.430 7.367 7.363 7.346 7.341 7.327 7.307 7.303 7.299 7.291 7.285 7.277 7.267 7.163 7.158 7.141 7.035 7.029 4.216 4.202 4.185 4.171 4.123 4.117 4.111 4.107 4.100 4.094 2.682 2.677 2.663 2.654 2.640 2.634 2.611 2.579 2.574 2.556 2.550 2.537 2.531 2.513 2.507 2.431 2.425 2.417 2.411 2.398 2.392 2.384 2.378 2.335 2.326 2.319 2.310 2.303 1.968 1.937 1.906 1.875 1.793 1.786 1.770 1.763 1.756 1.740 1.733

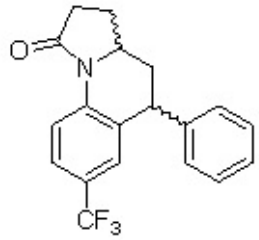


(^{1}H NMR, 400 MHz, $CDCl_3$)

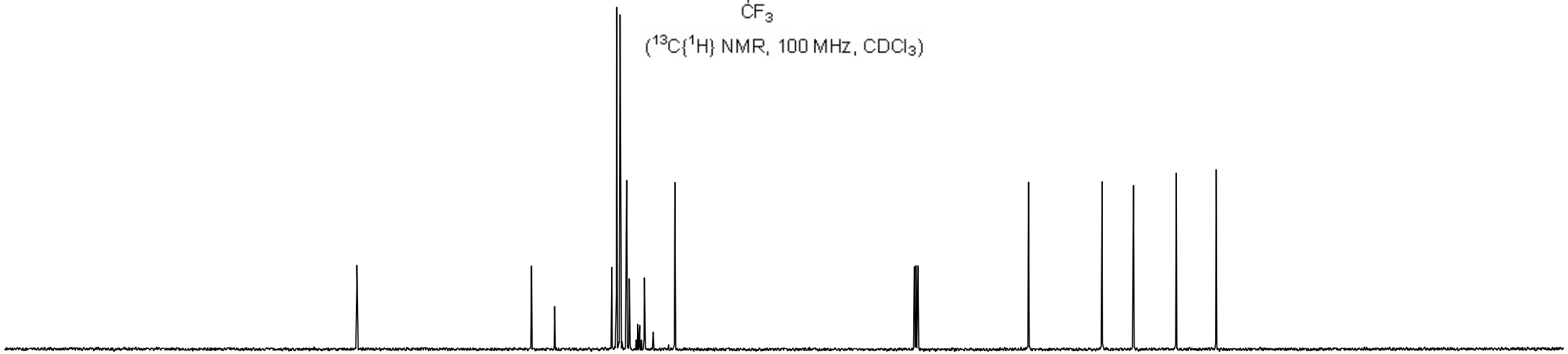


11f/B

174.066
143.807
139.803
129.882
129.063
128.467
128.133
127.316
126.901
126.863
126.822
126.784
125.711
125.430
125.387
125.063
124.741
124.280
124.242
124.205
124.168
122.729
120.027
118.969
57.691
44.944
39.511
32.095
25.189



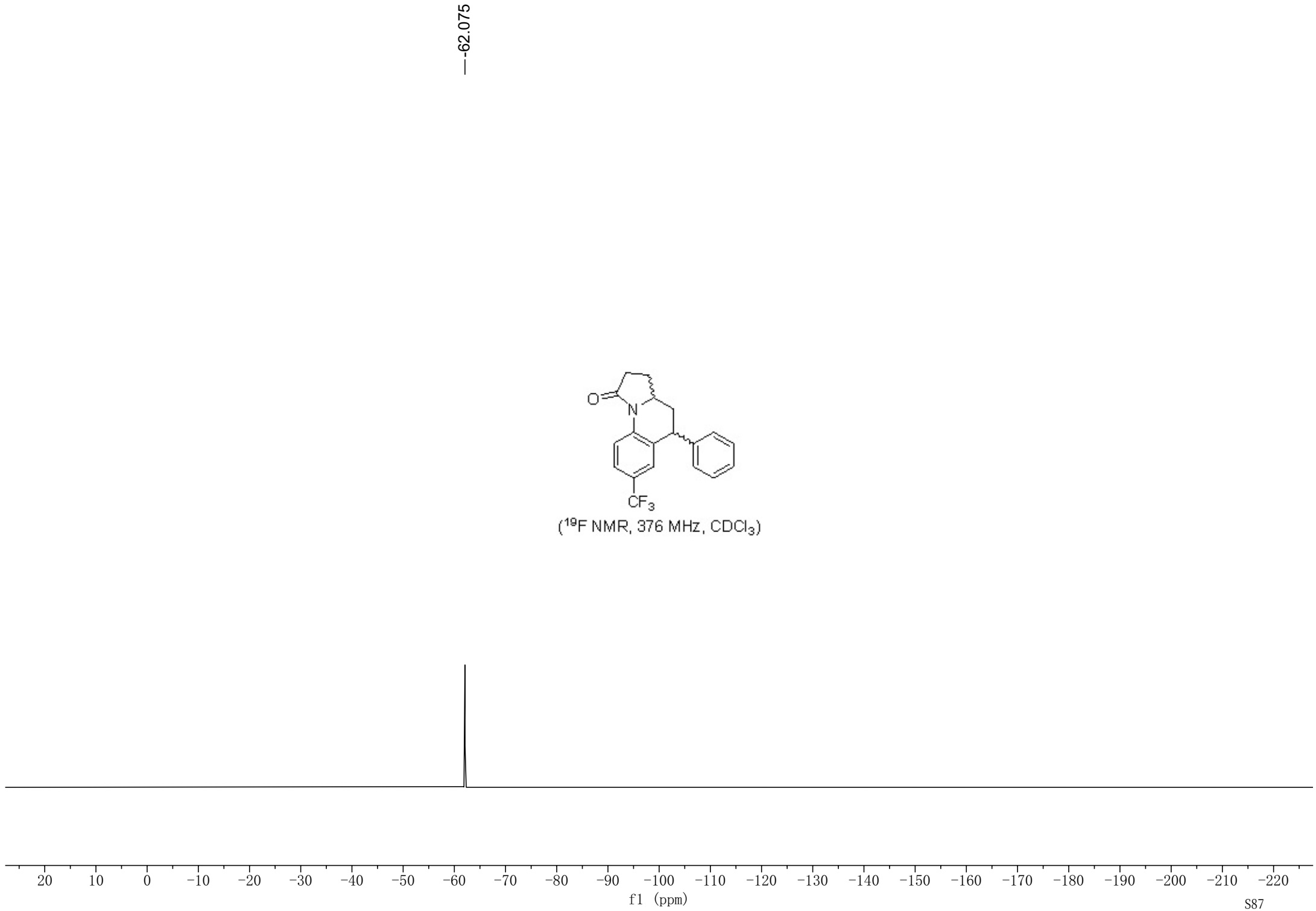
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



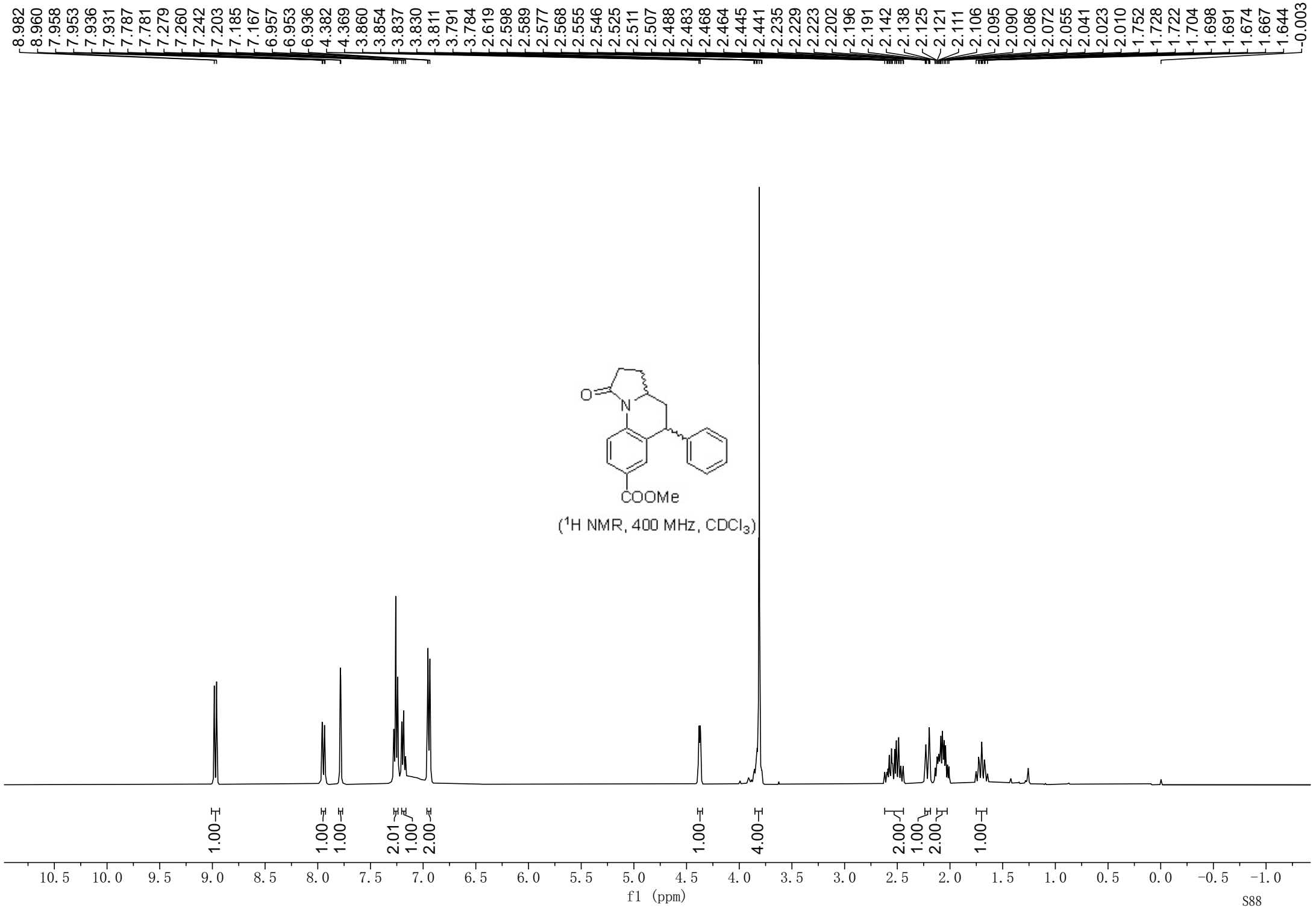
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30

f1 (ppm)

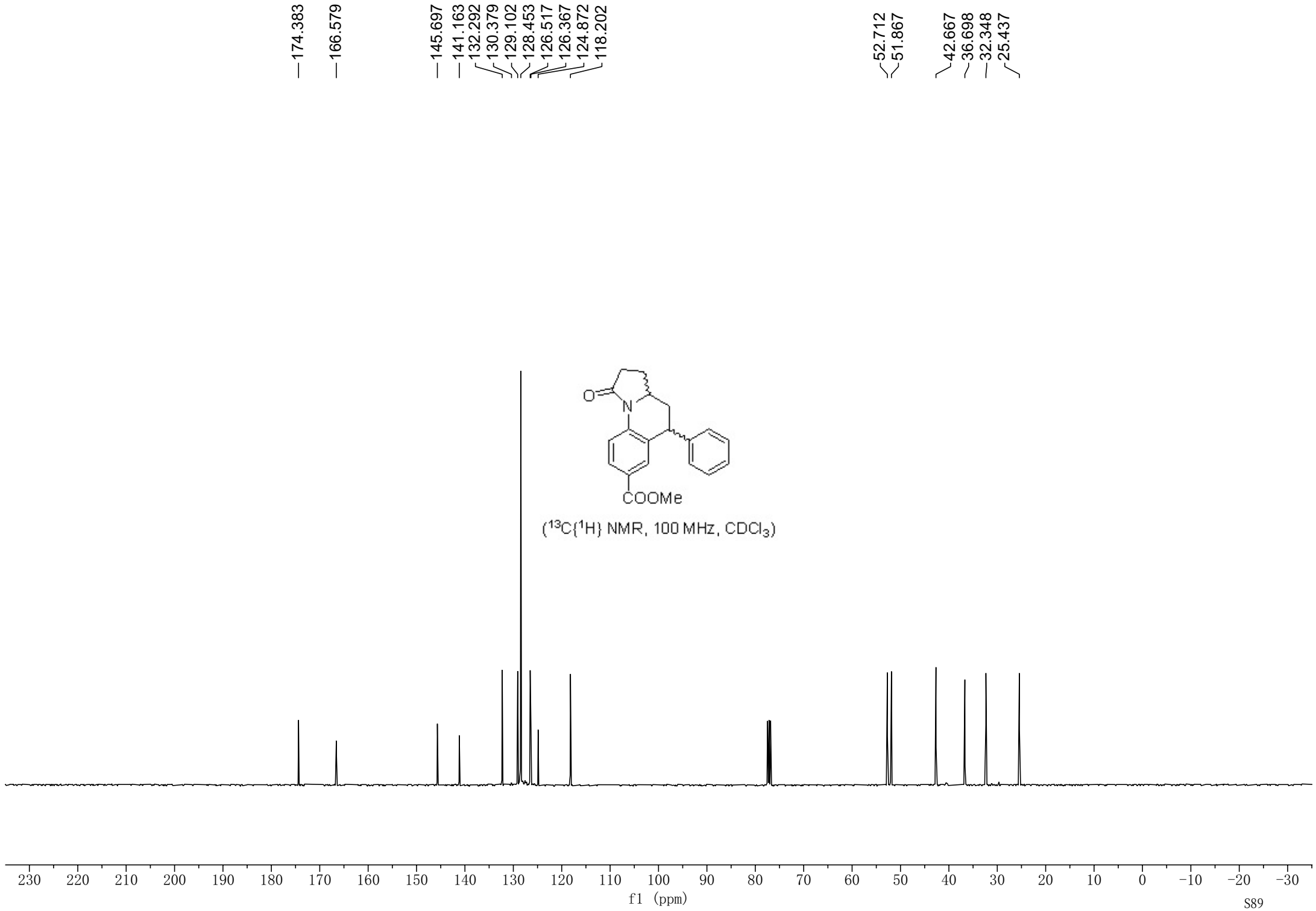
11f/B


-62.075
O
N
CF3
(19F NMR, 376 MHz, CDCl3)
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
f1 (ppm)

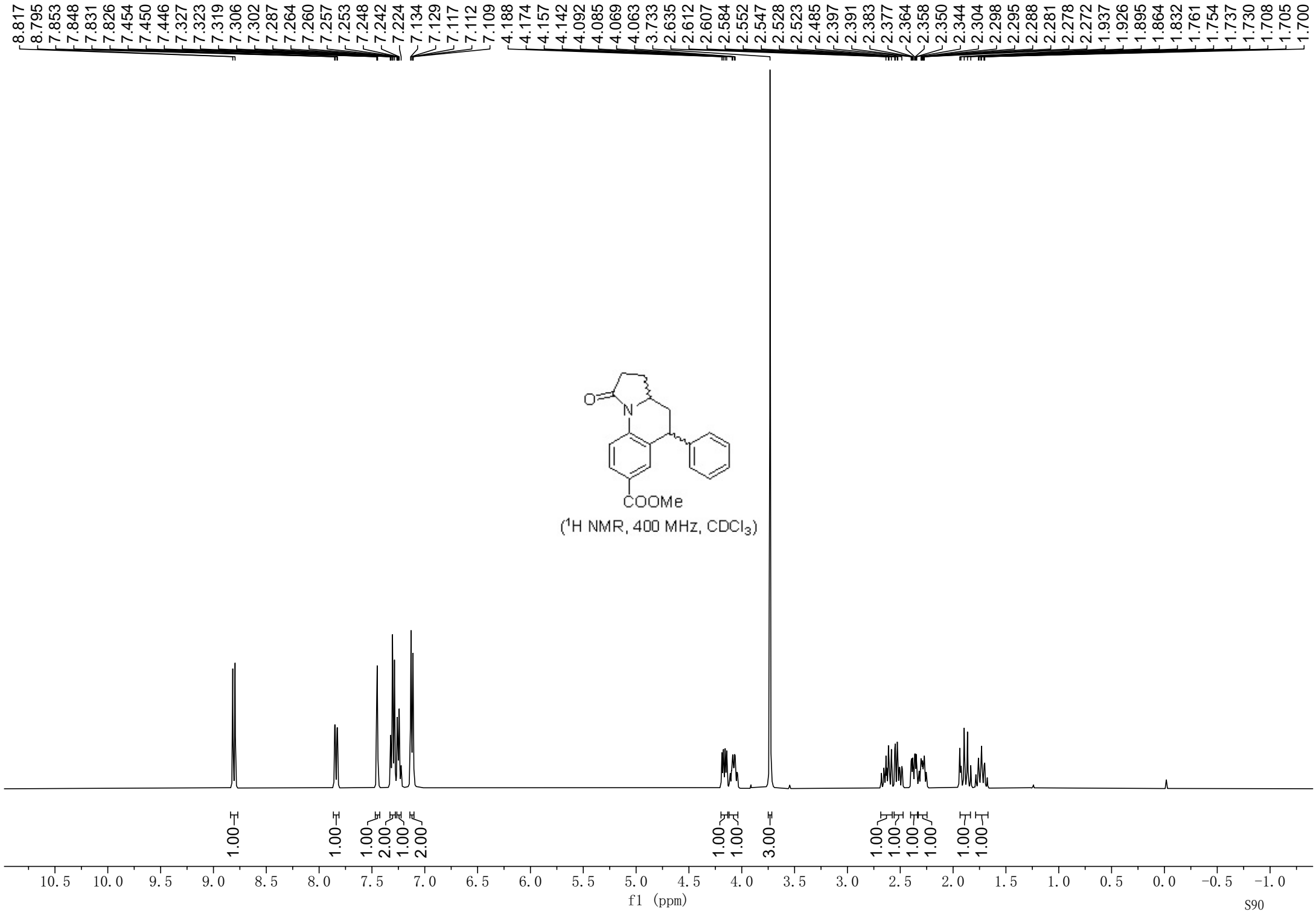
11g/A


8.982
8.960
7.958
7.953
7.936
7.931
7.787
7.781
7.279
7.260
7.242
7.203
7.185
7.167
6.957
6.953
6.936
4.382
4.369
3.860
3.854
3.837
3.830
3.811
3.791
3.784
2.619
2.598
2.589
2.577
2.568
2.555
2.546
2.525
2.511
2.507
2.488
2.483
2.468
2.464
2.445
2.441
2.235
2.229
2.223
2.202
2.196
2.191
2.142
2.138
2.125
2.121
2.111
2.106
2.095
2.090
2.086
2.072
2.055
2.041
2.023
2.010
1.752
1.728
1.722
1.704
1.698
1.691
1.674
1.667
1.644
-0.003
O
N
COOMe
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
2.01
1.00
2.00
1.00
4.00
2.00
1.00
2.00
1.00
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
-0.5
-1.0
f1 (ppm)

11g/A

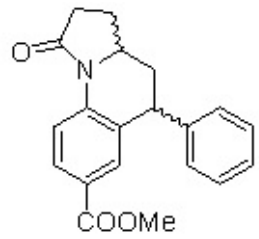

174.383
166.579
145.697
141.163
132.292
130.379
129.102
128.453
126.517
126.367
124.872
118.202
52.712
51.867
42.667
36.698
32.348
25.437
O
N
COOMe
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11g/B

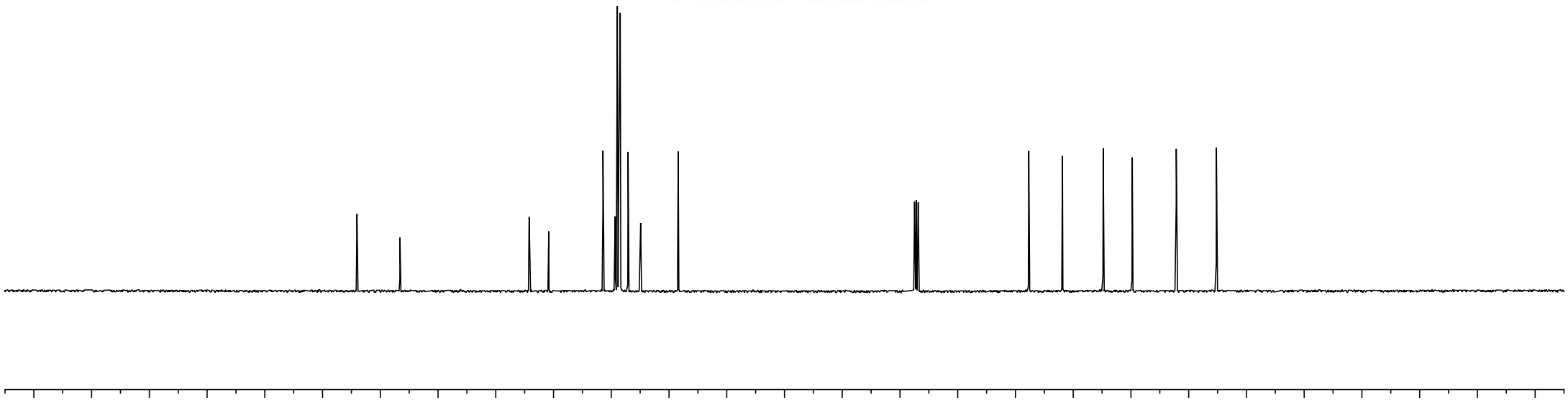

8.817
8.795
7.853
7.848
7.831
7.826
7.454
7.450
7.446
7.327
7.323
7.319
7.306
7.302
7.287
7.264
7.260
7.257
7.253
7.248
7.242
7.224
7.134
7.129
7.117
7.112
7.109
4.188
4.174
4.157
4.142
4.092
4.085
4.069
4.063
3.733
2.635
2.612
2.607
2.584
2.552
2.547
2.528
2.523
2.485
2.397
2.391
2.383
2.377
2.364
2.358
2.350
2.344
2.304
2.298
2.295
2.288
2.281
2.278
2.272
1.937
1.926
1.895
1.864
1.832
1.761
1.754
1.737
1.730
1.708
1.705
1.700
O
N
COOMe
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
2.00
1.00
2.00
1.00
1.00
3.00
1.00
1.00
1.00
1.00
1.00
1.00
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
-0.5
-1.0
f1 (ppm)

11g/B

174.036
166.596
144.223
140.826
131.440
129.316
128.946
128.684
128.448
127.085
124.910
118.405
57.692
51.862
44.809
39.769
32.153
25.197



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

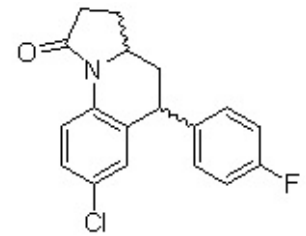


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30

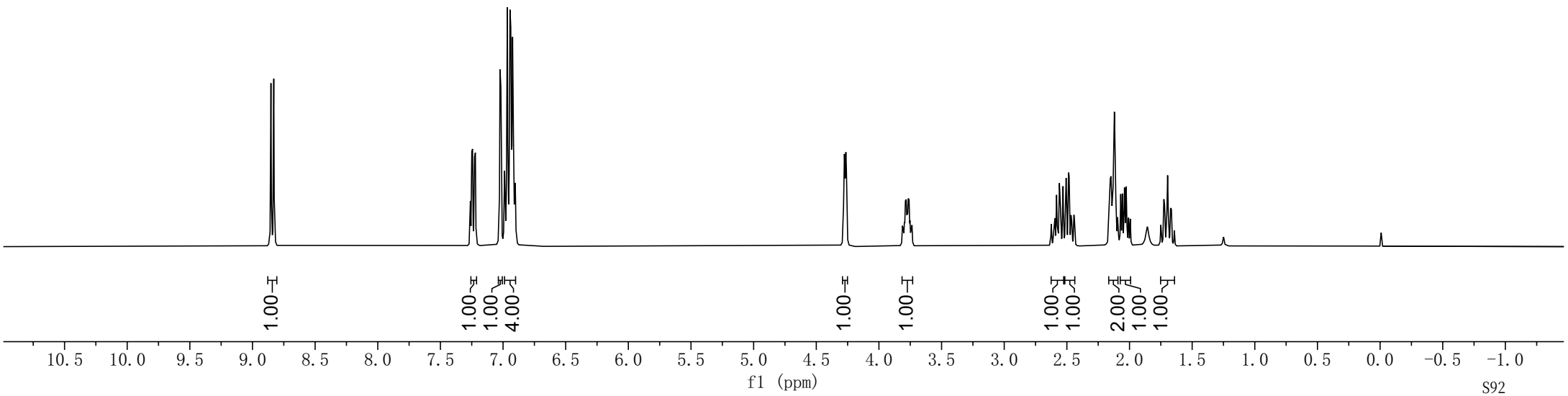
f1 (ppm)

11h/A

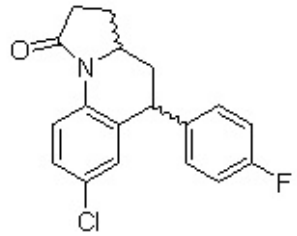
8.853 8.830 7.250 7.243 7.227 7.221 7.024 7.018 6.988 6.982 6.966 6.960 6.951 6.945 6.938 6.931 6.924 6.916 6.908 6.902 4.279 4.274 4.265 4.260 3.789 3.782 3.775 3.772 3.766 3.759 2.602 2.595 2.582 2.573 2.560 2.552 2.530 2.510 2.505 2.486 2.482 2.467 2.462 2.444 2.439 2.165 2.160 2.153 2.148 2.143 2.138 2.134 2.127 2.120 2.114 2.107 2.095 2.070 2.056 2.041 2.037 2.027 2.023 2.008 1.994 1.726 1.720 1.703 1.696 1.689 1.672 1.665



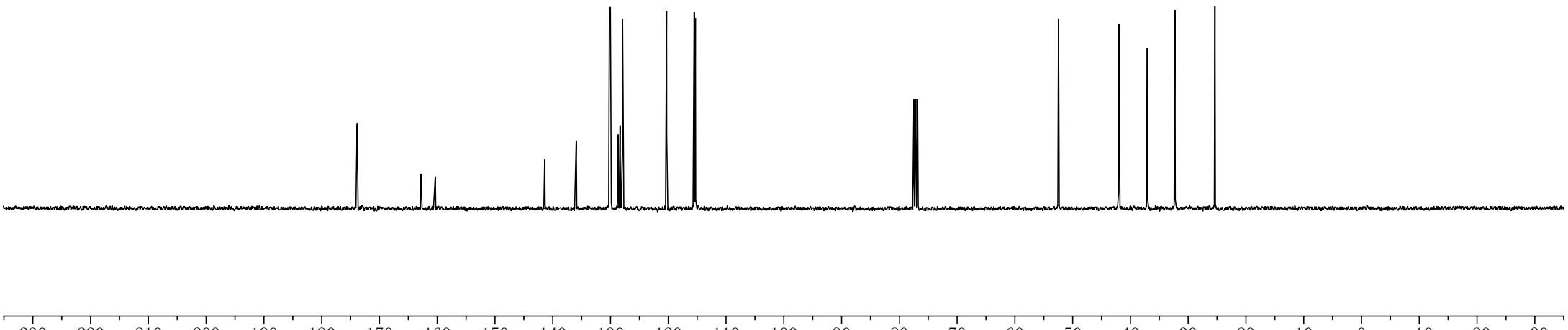
(^{1}H NMR, 400 MHz, $CDCl_3$)



11h/A

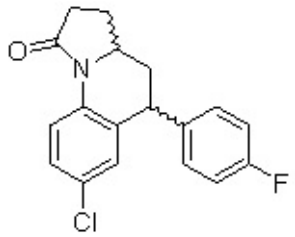


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

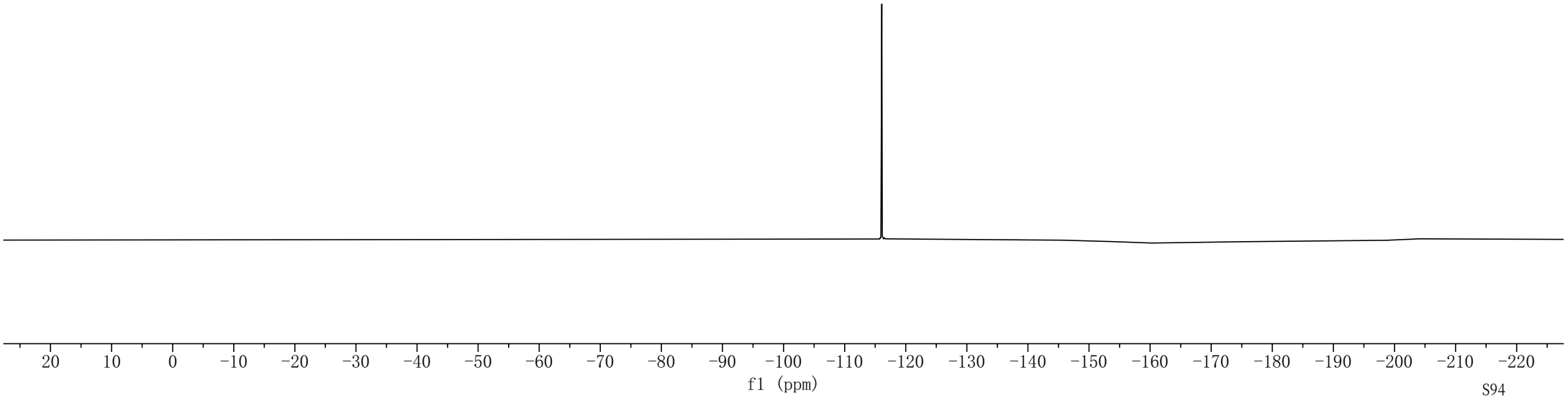


11h/A

-116.080

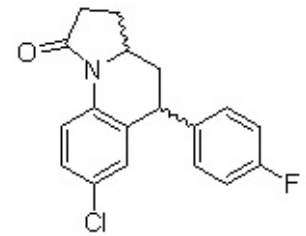


(^{19}F NMR, 376 MHz, $CDCl_3$)

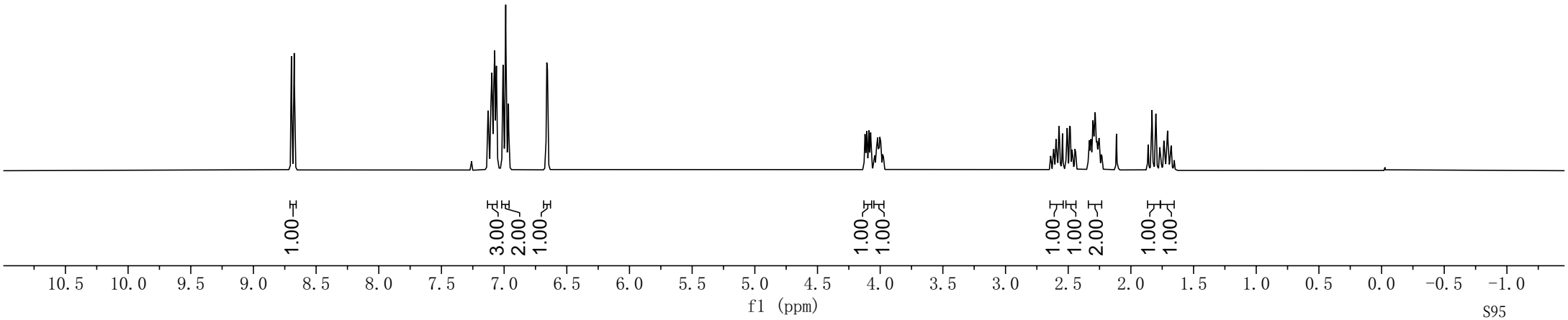


11h/B

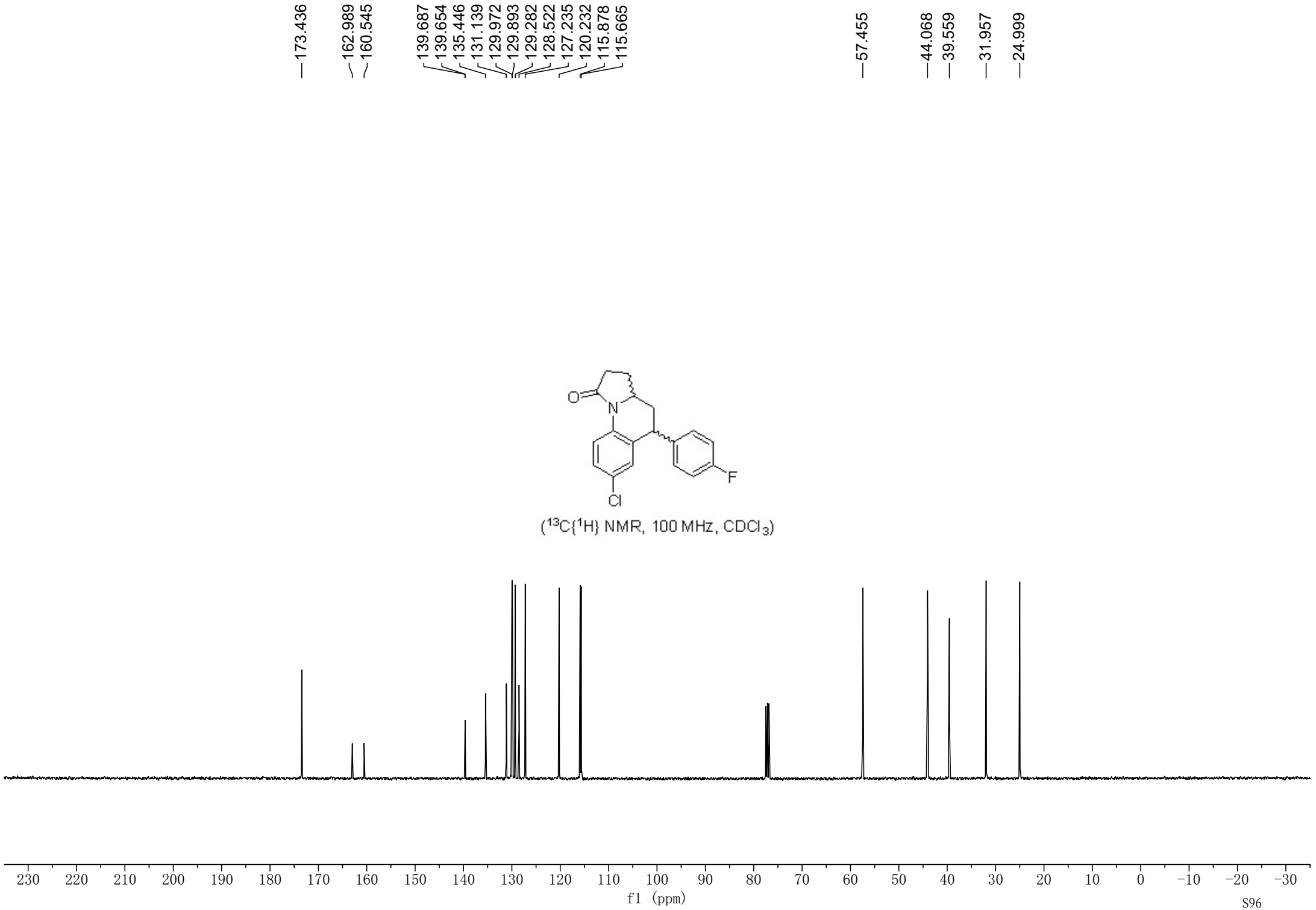
8.697 8.675 7.128 7.122 7.106 7.098 7.091 7.083 7.075 7.067 7.062 7.009 7.003 6.987 6.970 6.966 6.657 4.121 4.107 4.090 4.076 4.043 4.032 4.026 4.020 4.013 4.010 4.003 3.997 3.991 3.980 2.617 2.612 2.597 2.589 2.574 2.569 2.546 2.513 2.508 2.489 2.484 2.470 2.465 2.446 2.441 2.337 2.331 2.322 2.316 2.303 2.297 2.290 2.284 2.277 2.270 2.261 2.254 2.248 2.236 1.862 1.831 1.800 1.769 1.761 1.737 1.730 1.714 1.707 1.700 1.684 1.678



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

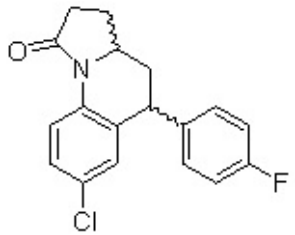


11h/B

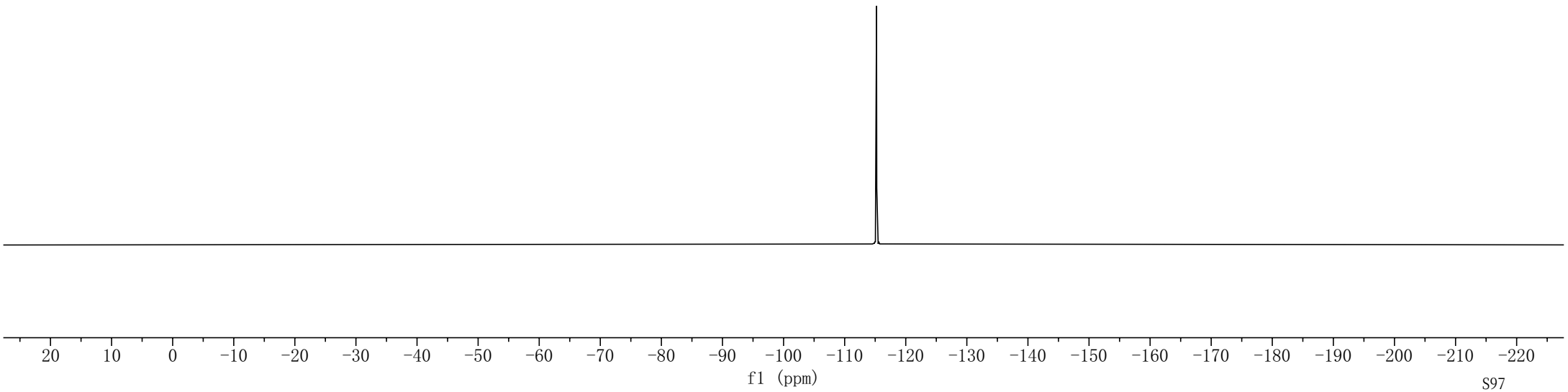

173.436
162.989
160.545
139.687
139.654
135.446
131.139
129.972
129.893
129.282
128.522
127.235
120.232
115.878
115.665
57.455
44.068
39.559
31.957
24.999
O
N
F
Cl
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11h/B

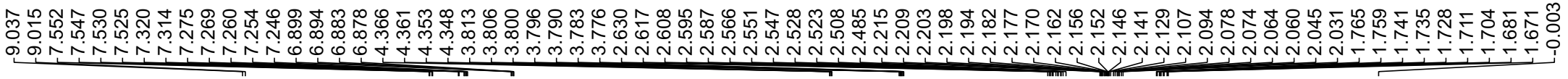
-115.221

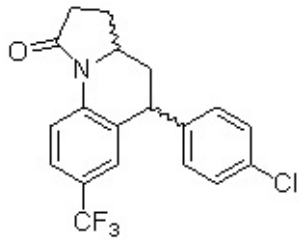


(^{19}F NMR, 376 MHz, $CDCl_3$)

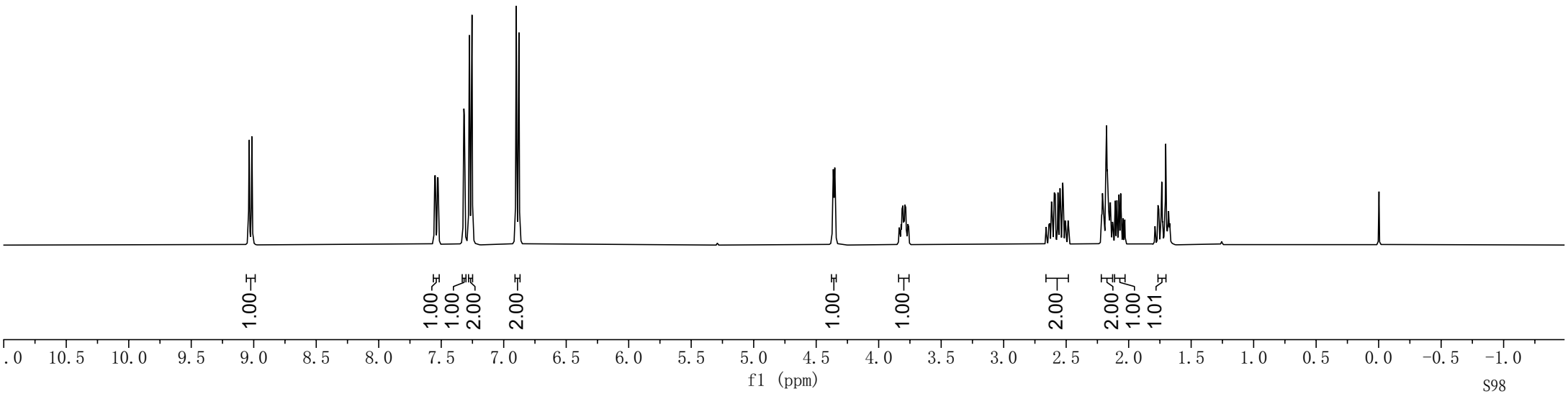


11i/A



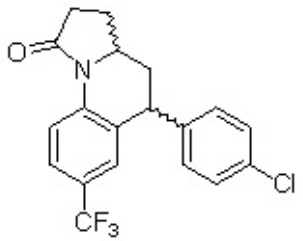


(^{1}H NMR, 400 MHz, $CDCl_3$)

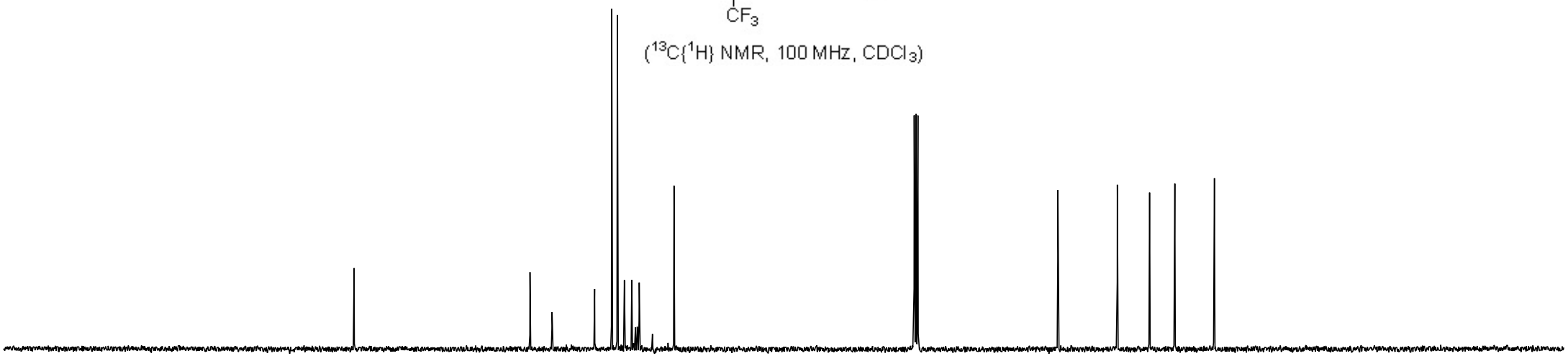


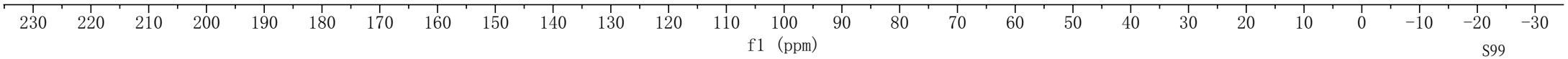
11i/A

174.442
143.993
140.171
132.801
129.851
128.871
127.690
127.653
127.615
127.578
126.371
125.747
125.497
125.422
125.083
125.043
122.797
120.070
119.062
52.617
42.322
36.737
32.367
25.517

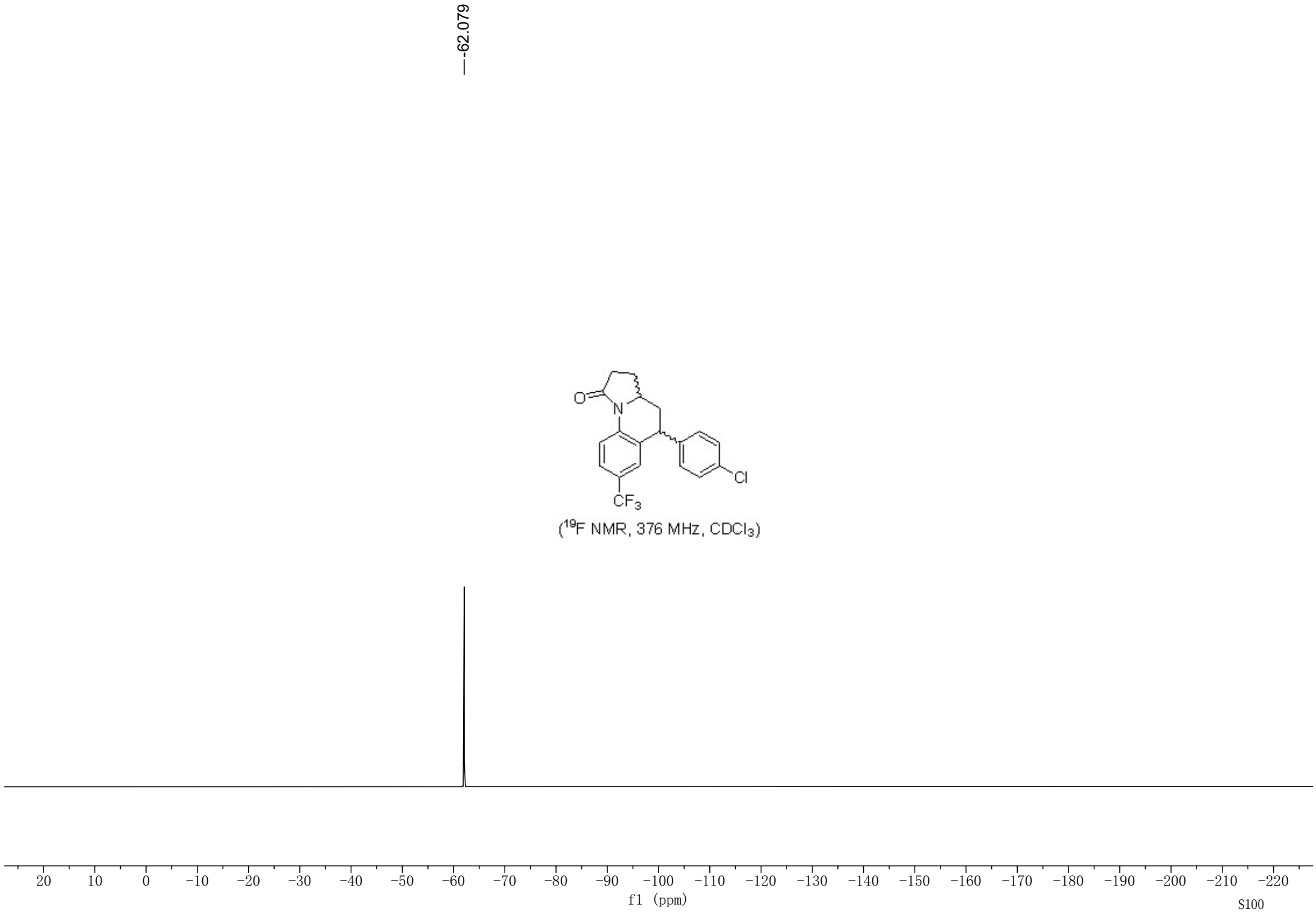


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

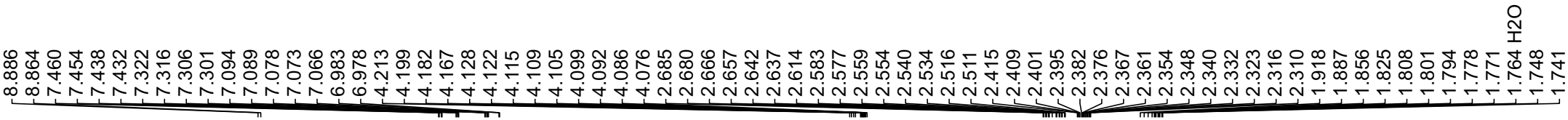


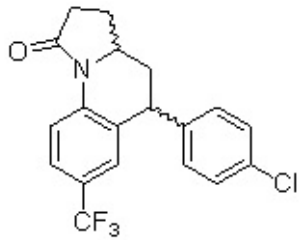


11i/A

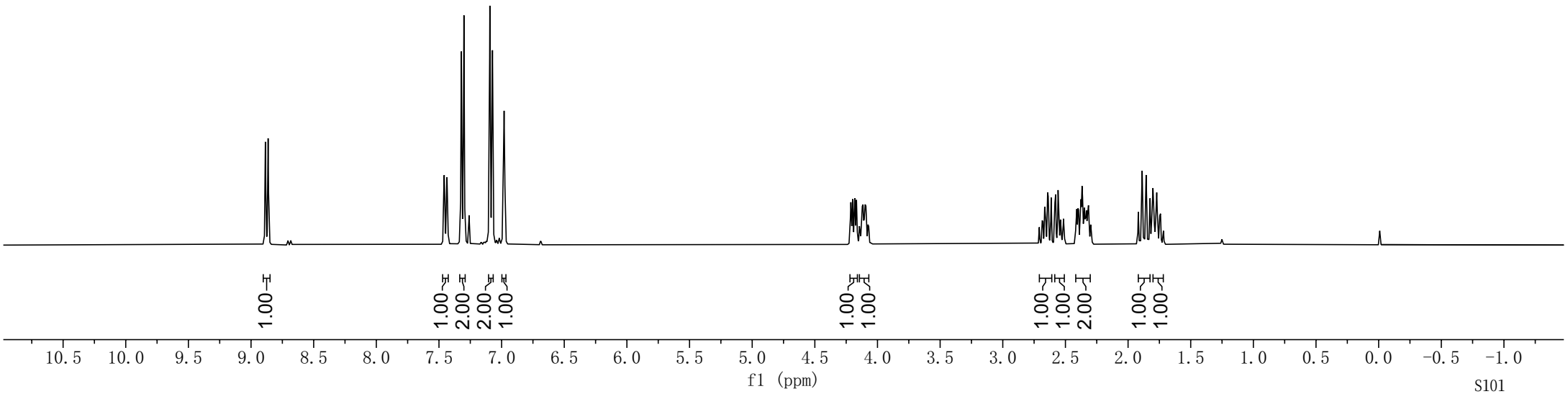

-62.079
O
N
Cl
CF_3
(^{19}F NMR, 376 MHz, $CDCl_3$)
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −220
f1 (ppm)

11i/B





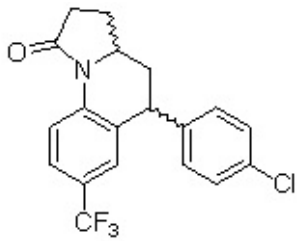
(^{1}H NMR, 400 MHz, $CDCl_3$)



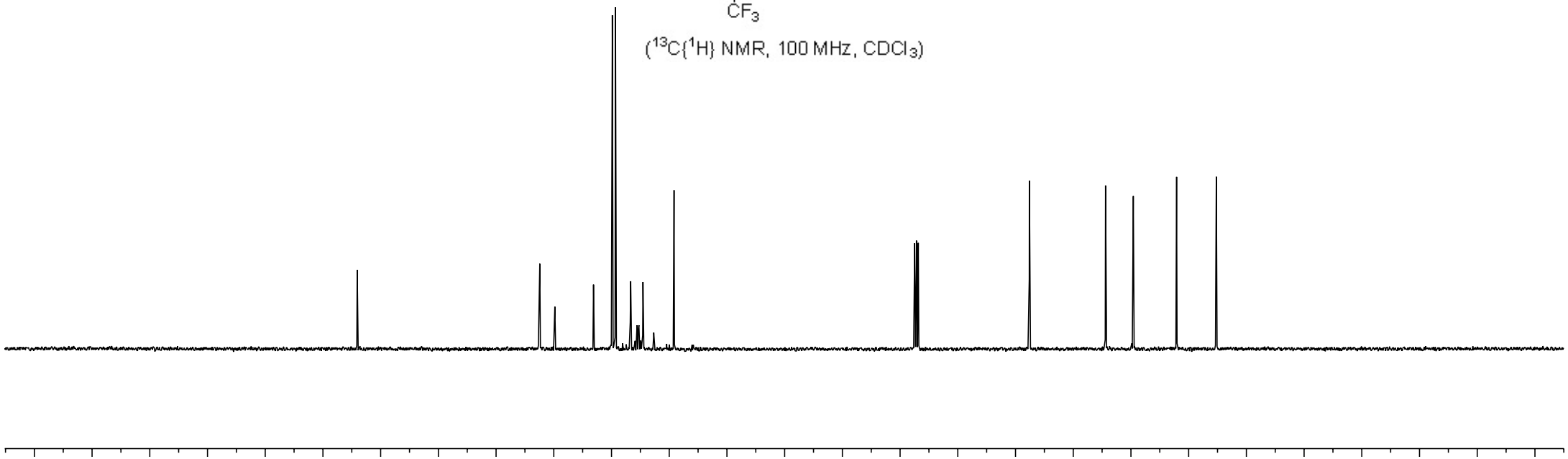
11i/B

174.064
142.425
139.823
133.119
129.861
129.316
129.256
126.756
126.715
126.678
126.641
125.907
125.582
125.385
125.257
124.934
124.585
124.547
124.510
124.473
122.684
119.993
119.166

57.602
44.402
39.588
32.090
25.206



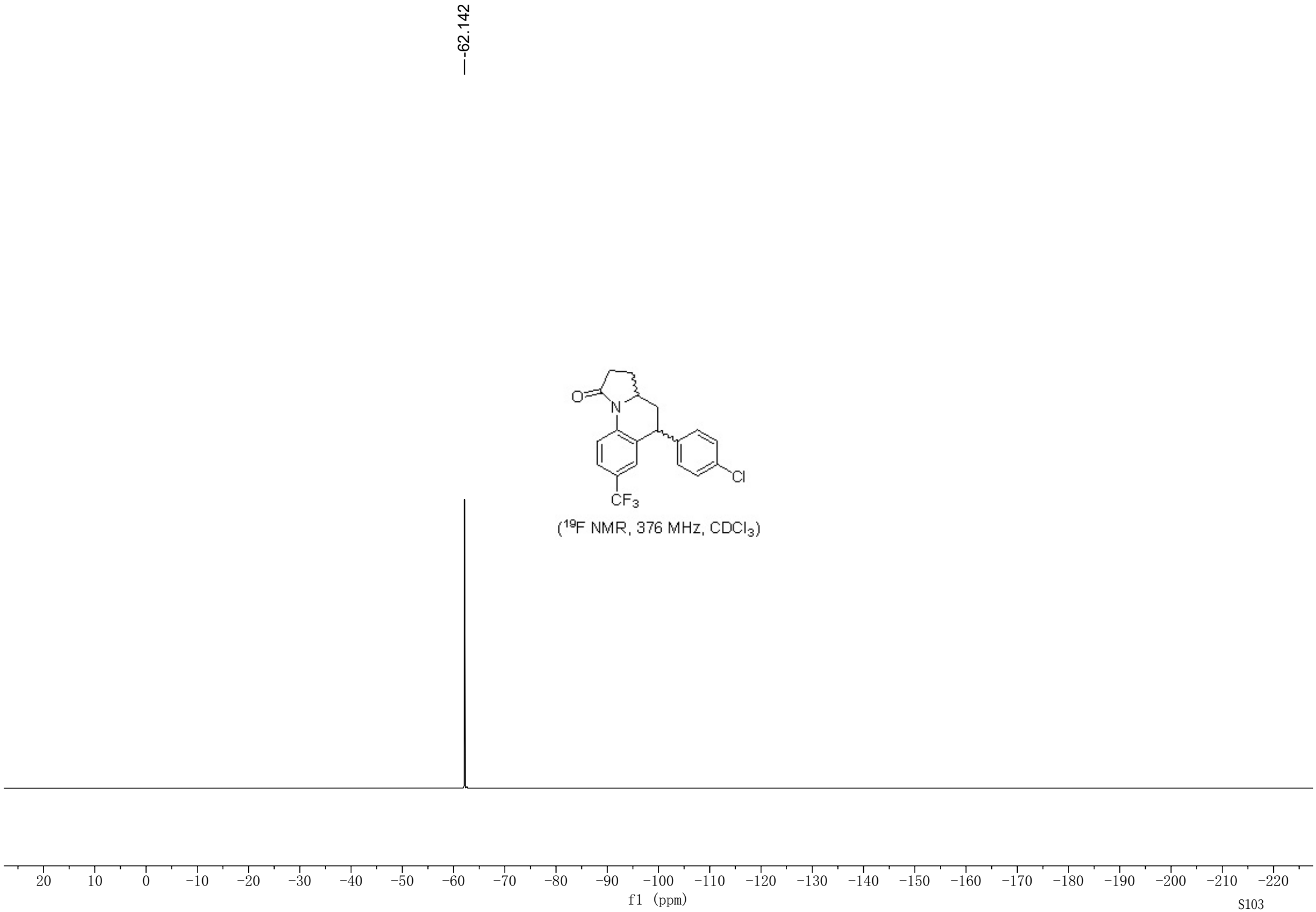
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



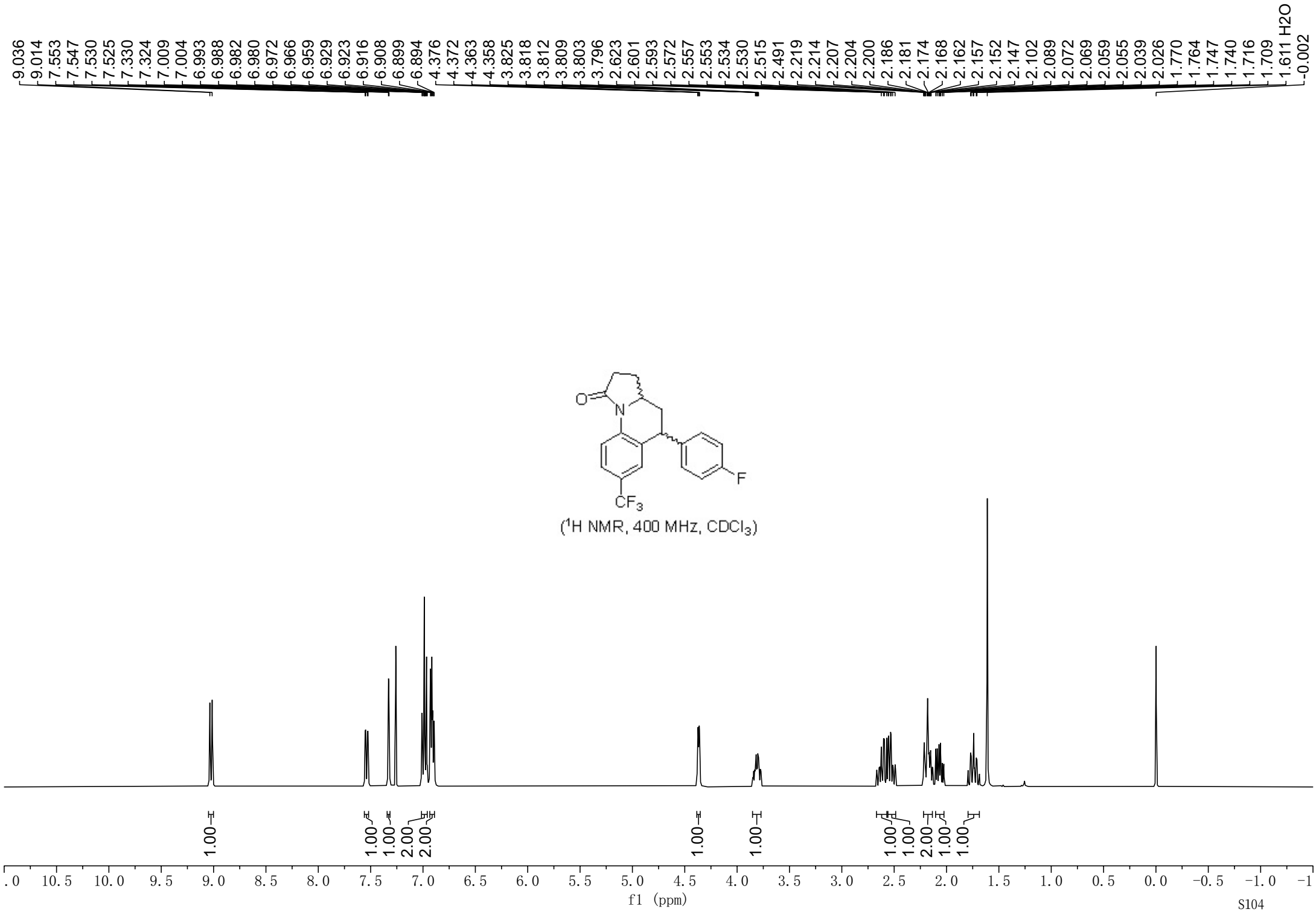
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30

f1 (ppm)

11i/B

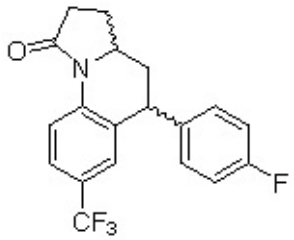

-62.142
O
N
Cl
CF3
(19F NMR, 376 MHz, CDCl3)
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
−220
f1 (ppm)

11j/A


9.036
9.014
7.553
7.547
7.530
7.525
7.330
7.324
7.009
7.004
6.993
6.988
6.982
6.980
6.972
6.966
6.959
6.929
6.923
6.916
6.908
6.899
6.894
4.376
4.372
4.363
4.358
3.825
3.818
3.812
3.809
3.803
3.796
2.623
2.601
2.593
2.572
2.557
2.553
2.534
2.530
2.515
2.491
2.219
2.214
2.207
2.204
2.200
2.186
2.181
2.174
2.168
2.162
2.157
2.152
2.147
2.102
2.089
2.072
2.069
2.059
2.055
2.039
2.026
1.770
1.764
1.747
1.740
1.716
1.709
1.611 H2O
-0.002
O
N
F
CF3
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
2.00
2.00
1.00
1.00
1.00
2.00
1.00
1.00
f1 (ppm)

11j/A

174.480
162.923
160.478
141.279
141.247
140.146
130.045
129.965
127.750
127.712
127.672
127.634
126.725
125.759
125.540
125.433
125.034
124.995
124.959
122.839
119.060
115.705
115.492
52.631
42.189
36.941
32.412
25.558

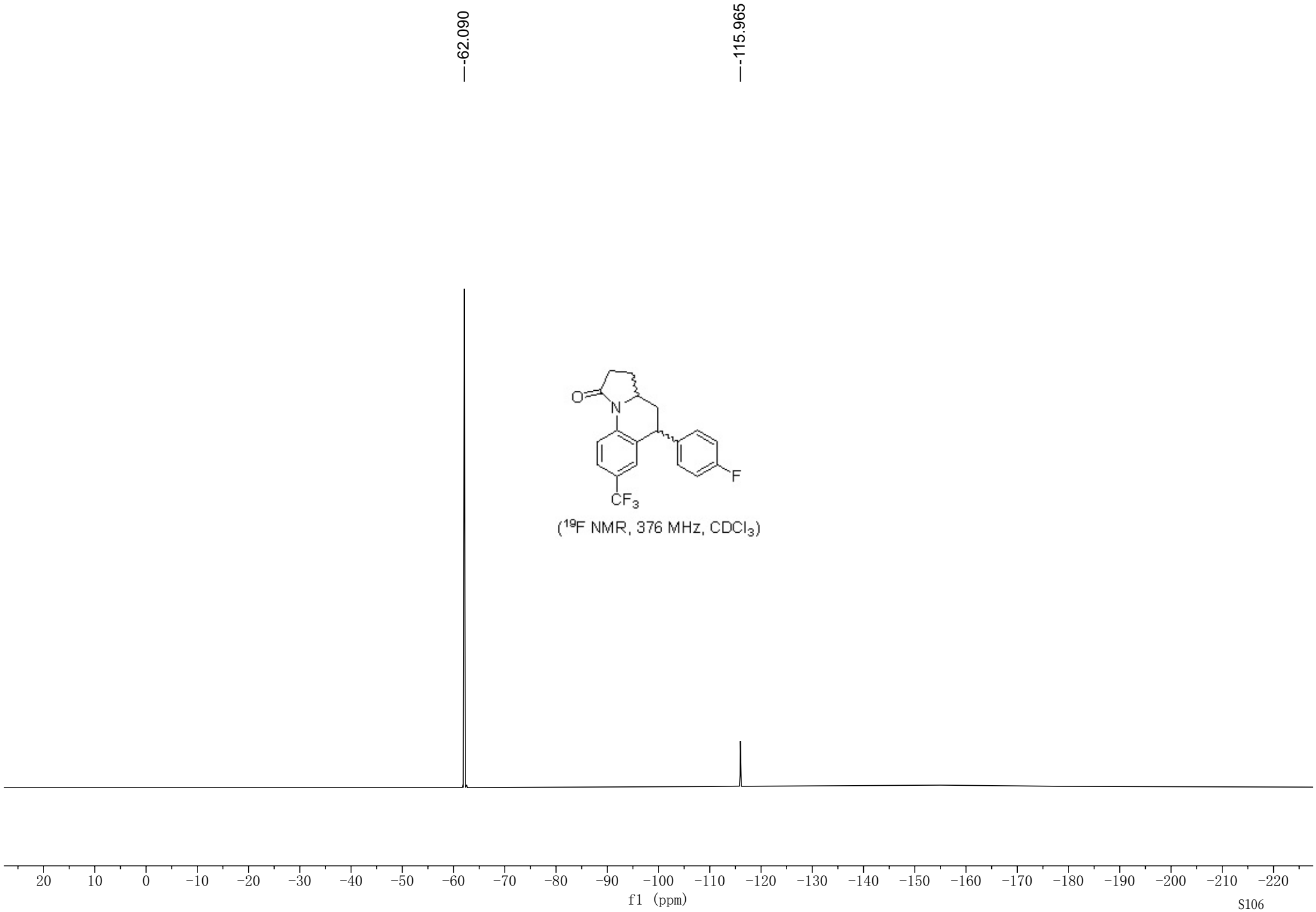


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30

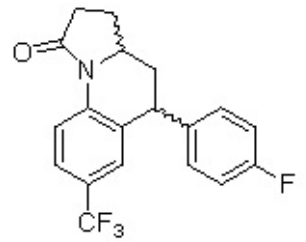
f1 (ppm)

11j/A

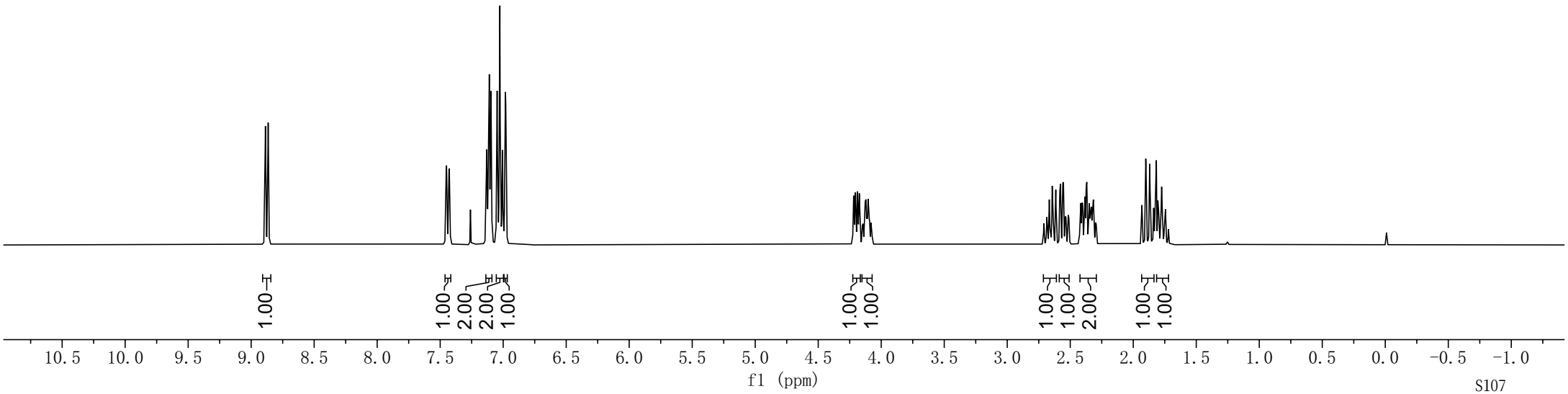

-62.090
-115.965
O
N
F
CF_3
(^{19}F NMR, 376 MHz, $CDCl_3$)
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −220
f1 (ppm)

11j/B

8.887 8.865 7.453 7.448 7.431 7.426 7.132 7.127 7.118 7.110 7.102 7.097 7.048 7.042 7.026 7.010 7.005 6.985 6.979 4.219 4.205 4.188 4.174 4.127 4.121 4.115 4.111 4.104 4.098 2.686 2.681 2.666 2.657 2.643 2.638 2.615 2.583 2.578 2.559 2.554 2.540 2.535 2.516 2.511 2.422 2.416 2.408 2.402 2.389 2.383 2.374 2.368 2.354 2.348 2.342 2.340 2.333 2.326 2.323 2.317 1.932 1.901 1.869 1.838 1.828 1.805 1.798 1.781 1.775 1.768 1.752 1.745

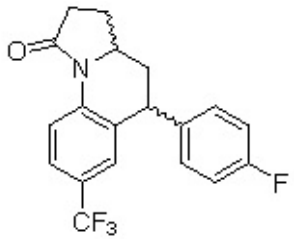


(^{1}H NMR, 400 MHz, $CDCl_3$)

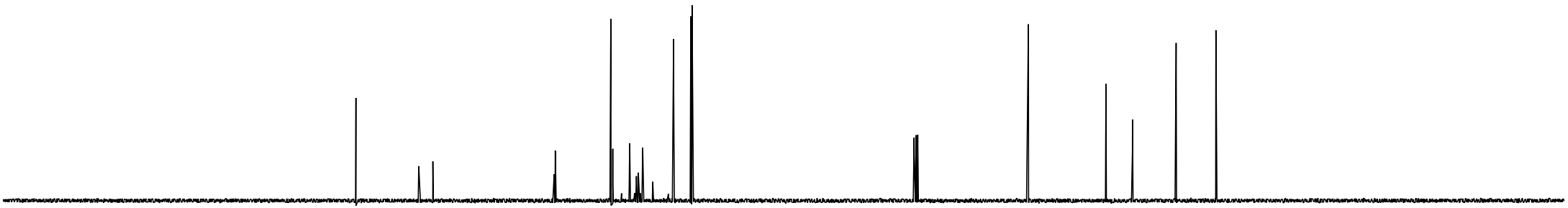


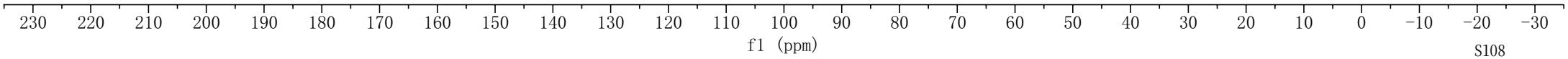
11j/B

174.094
163.220
160.776
139.795
139.782
139.617
139.584
130.046
129.972
129.634
128.116
126.784
126.744
126.707
126.669
125.863
125.541
125.215
124.890
124.493
124.456
124.419
124.381
122.713
120.013
119.106
116.121
115.907
101.975
57.683
44.257
39.663
32.112
25.230

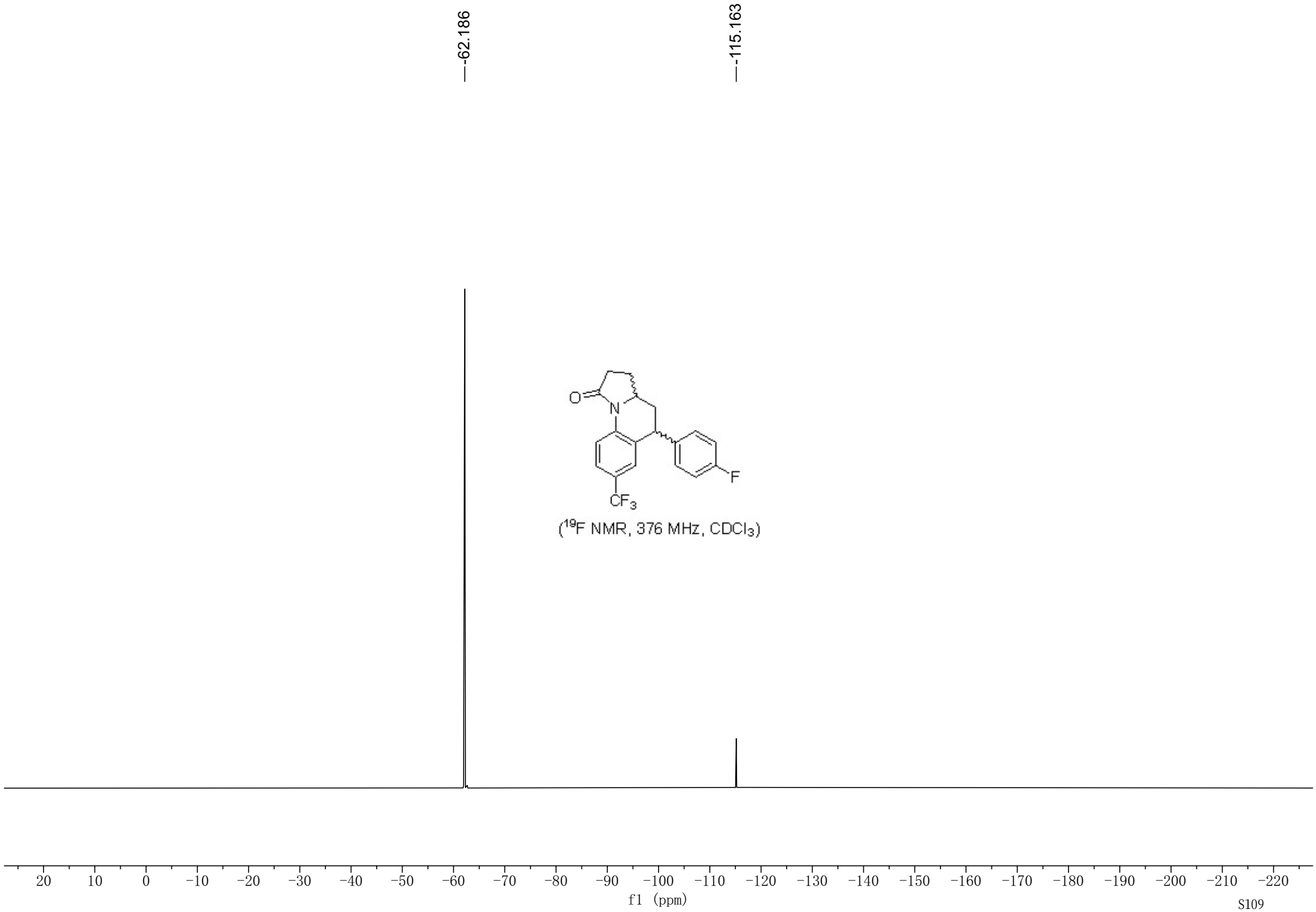


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



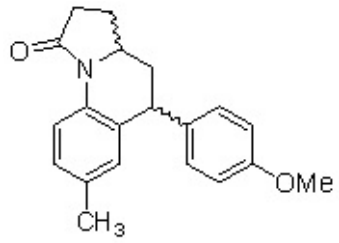


11j/B


-62.186
-115.163
O
N
F
CF_3
(^{19}F NMR, 376 MHz, $CDCl_3$)
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −220
f1 (ppm)

11k/B

8.579 8.557 7.098 7.090 7.085 7.074 7.068 7.061 7.022 7.018 7.016 7.001 6.995 6.887 6.880 6.874 6.863 6.858 6.585 6.582 6.579 4.133 4.119 4.102 4.094 4.088 4.077 4.072 4.066 4.049 4.043 3.813 2.659 2.655 2.640 2.632 2.617 2.612 2.589 2.549 2.543 2.525 2.519 2.507 2.483 2.348 2.342 2.334 2.328 2.321 2.316 2.309 2.301 2.298 2.295 2.290 2.283 2.280 2.274 2.266 2.143 1.917 1.886 1.855 1.824 1.758 1.753 1.735 1.728 1.721 1.703 1.699



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

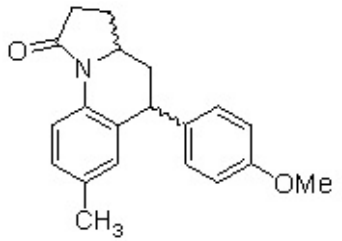
1.00 2.00 1.00 2.00 1.00 2.00 3.00 1.00 1.00 2.00 3.00 1.00 1.00

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 -0.5 -1.0

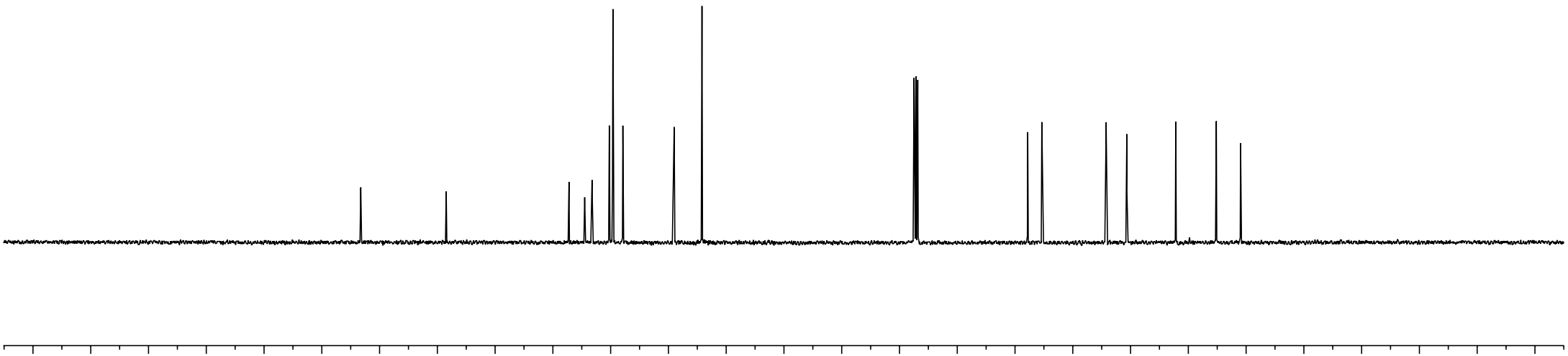
f1 (ppm)

11k/B

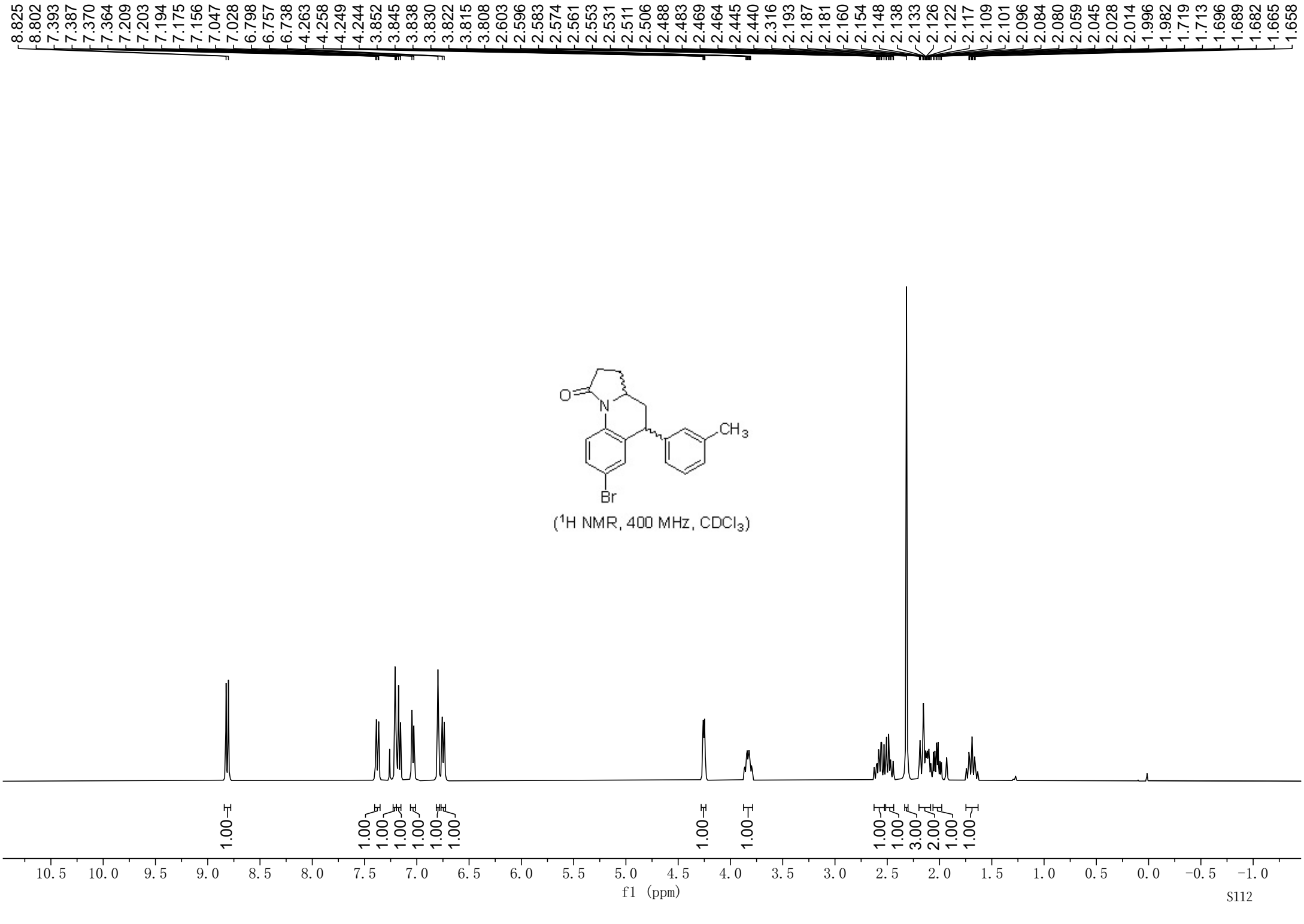
173.258
158.468
137.210
134.497
133.220
130.232
129.679
129.604
127.886
119.003
114.189
57.805
55.364
44.221
40.647
32.172
25.156
20.956



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

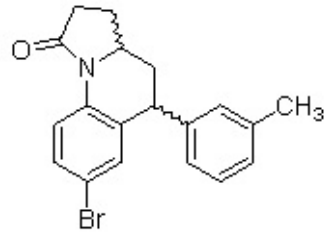


11l/A

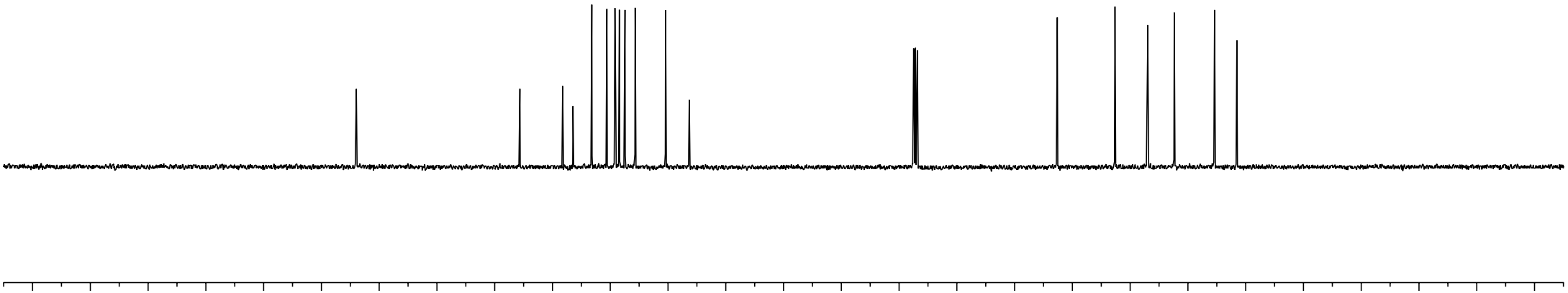

8.825
8.802
7.393
7.387
7.370
7.364
7.209
7.203
7.194
7.175
7.156
7.047
7.028
6.798
6.757
6.738
4.263
4.258
4.249
4.244
3.852
3.845
3.838
3.830
3.822
3.815
3.808
2.603
2.596
2.583
2.574
2.561
2.553
2.531
2.511
2.506
2.488
2.483
2.469
2.464
2.445
2.440
2.316
2.193
2.187
2.181
2.160
2.154
2.148
2.138
2.133
2.126
2.122
2.117
2.109
2.101
2.096
2.084
2.080
2.059
2.045
2.028
2.014
1.996
1.982
1.719
1.713
1.696
1.689
1.682
1.665
1.658
O
N
CH3
Br
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
3.00
2.00
1.00
1.00
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
-0.5
-1.0
f1 (ppm)

11l/A

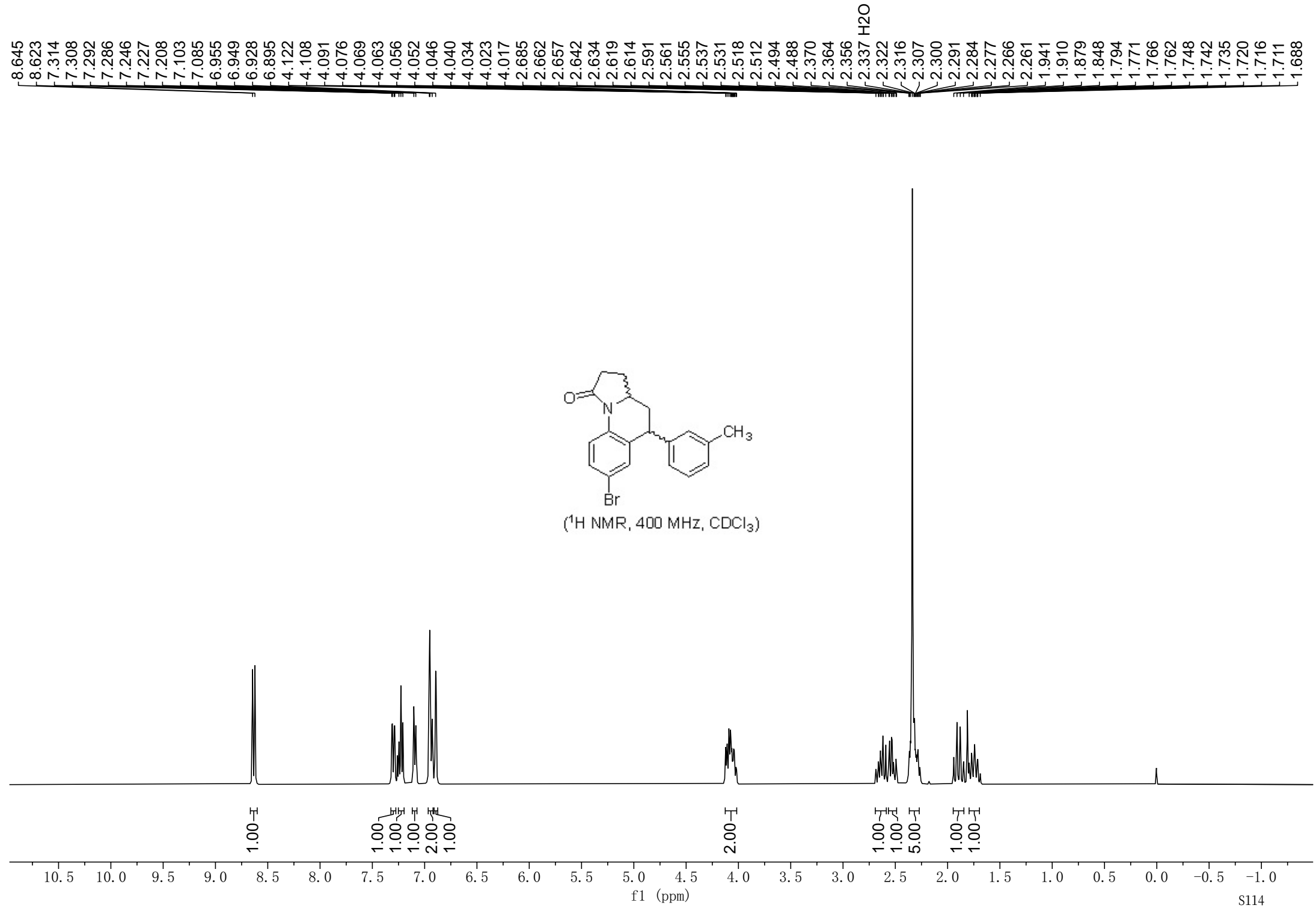
173.956
145.640
138.241
136.447
133.187
130.581
129.188
129.060
128.421
127.445
125.689
120.426
116.323
52.609
42.627
36.967
32.365
25.387
21.532



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

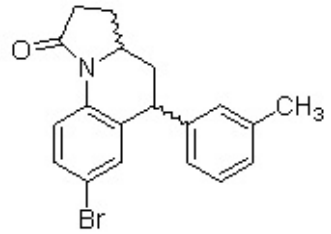


11l/B

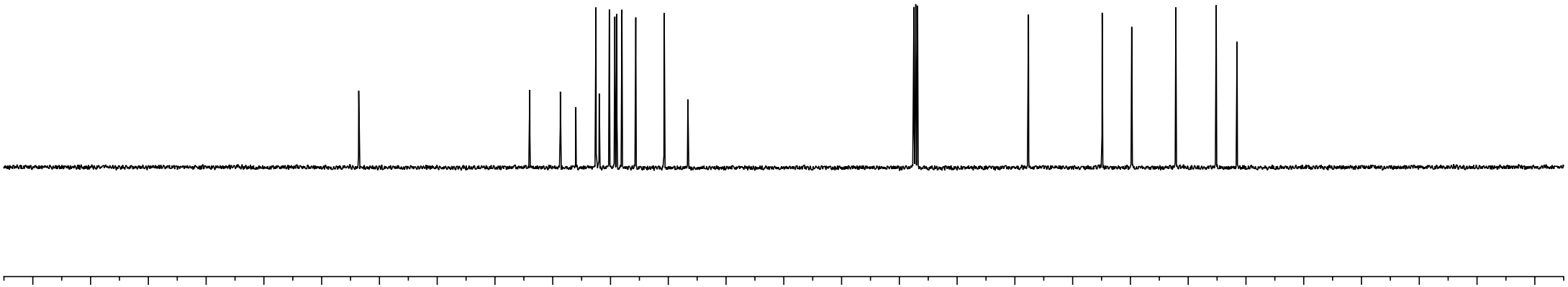

8.645
8.623
7.314
7.308
7.292
7.286
7.246
7.227
7.208
7.103
7.085
6.955
6.949
6.928
6.895
4.122
4.108
4.091
4.076
4.069
4.063
4.056
4.052
4.046
4.040
4.034
4.023
4.017
2.685
2.662
2.657
2.642
2.634
2.619
2.614
2.591
2.561
2.555
2.537
2.531
2.518
2.512
2.494
2.488
2.370
2.364
2.356
2.337 H2O
2.322
2.316
2.307
2.300
2.291
2.284
2.277
2.266
2.261
1.941
1.910
1.879
1.848
1.794
1.771
1.766
1.762
1.748
1.742
1.735
1.720
1.716
1.711
1.688
O
N
CH3
Br
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
1.00
2.00
1.00
2.00
1.00
1.00
5.00
1.00
1.00
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
-0.5
-1.0
f1 (ppm)

11l/B

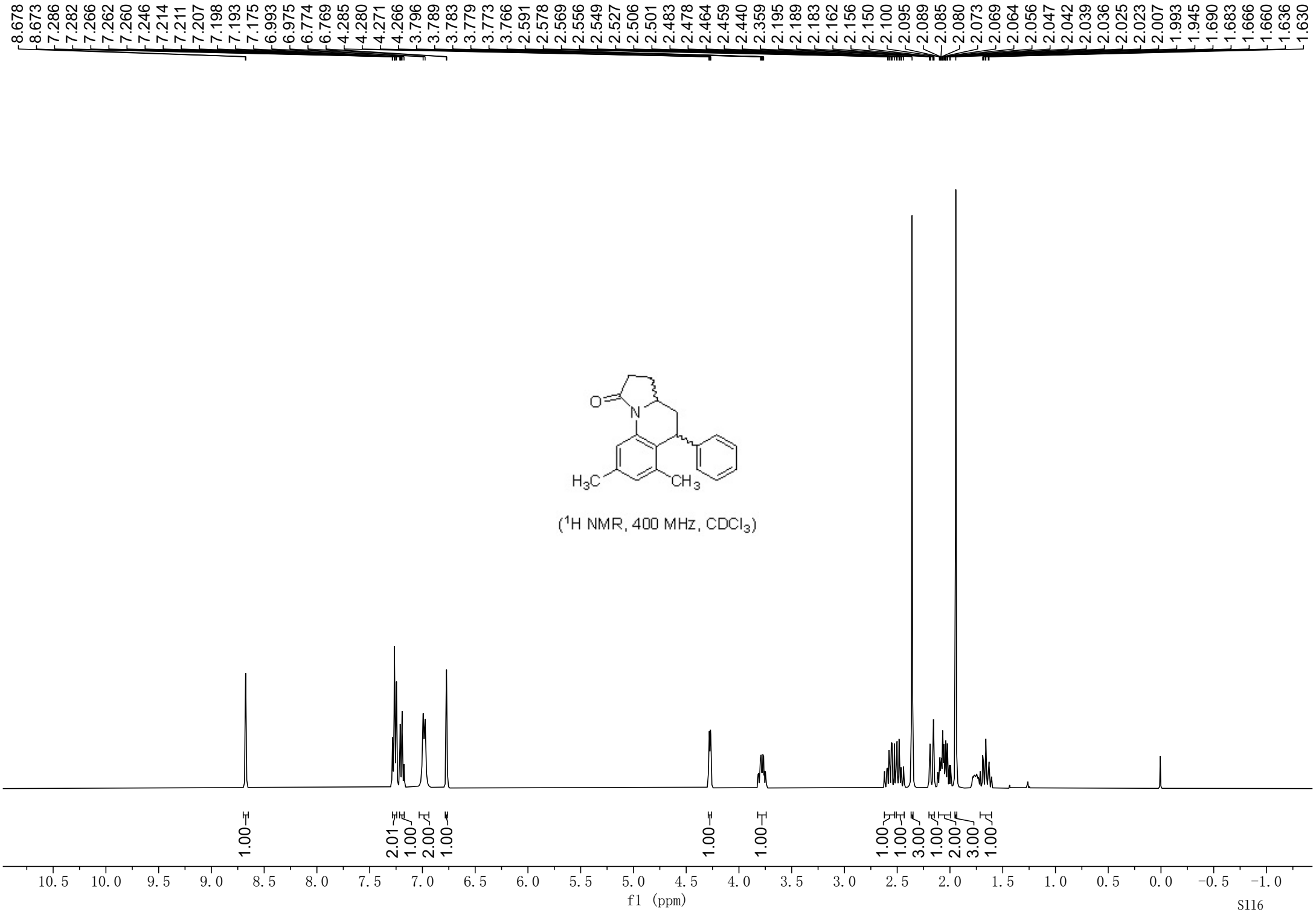
173.589
143.971
138.686
135.999
132.515
131.957
130.207
129.254
128.903
128.022
125.627
120.701
116.604
57.646
44.890
39.778
32.135
25.148
21.541



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

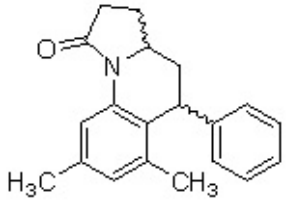


11m/A

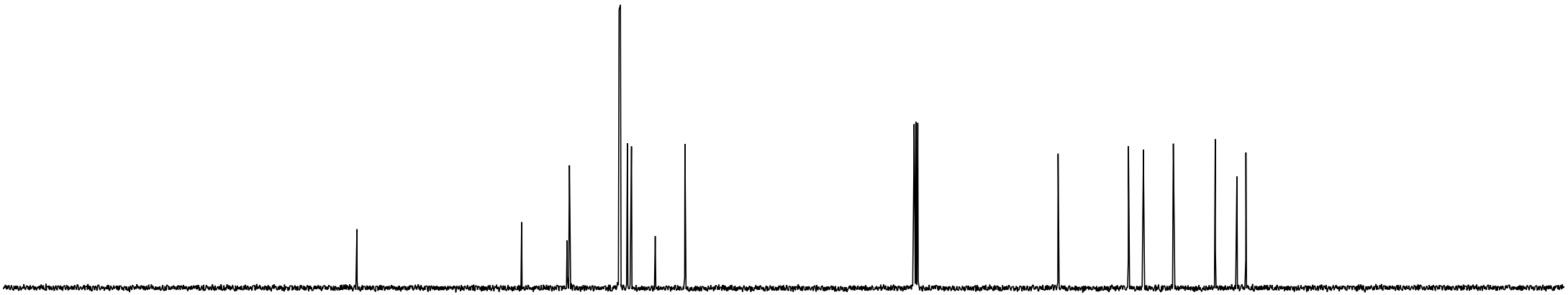

8.678
8.673
7.286
7.282
7.266
7.262
7.260
7.246
7.214
7.211
7.207
7.198
7.193
7.175
6.993
6.975
6.774
6.769
4.285
4.280
4.271
4.266
3.796
3.789
3.783
3.779
3.773
3.766
2.591
2.578
2.569
2.556
2.549
2.527
2.506
2.501
2.483
2.478
2.464
2.459
2.440
2.359
2.195
2.189
2.183
2.162
2.156
2.150
2.100
2.095
2.089
2.085
2.080
2.073
2.069
2.064
2.056
2.047
2.042
2.039
2.036
2.025
2.023
2.007
1.993
1.945
1.690
1.683
1.666
1.660
1.636
1.630
O
N
H3C
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
2.01
1.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
2.00
3.00
1.00
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
-0.5
-1.0
f1 (ppm)

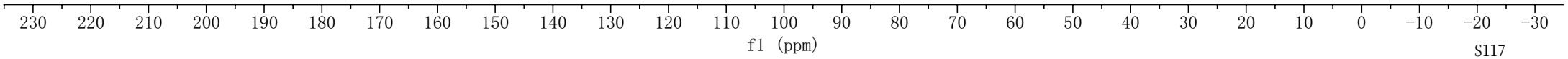
11m/A

173.927
145.425
137.553
137.144
128.550
128.315
127.107
126.401
122.293
117.150
52.555
40.378
37.772
32.606
25.347
21.594
20.042



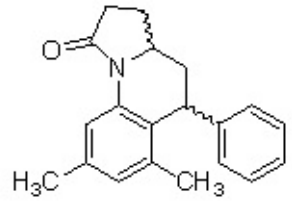
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)





11m/B

8.200 7.250 7.232 7.213 7.176 7.158 7.140 7.035 7.031 7.014 6.721 4.252 4.232 4.225 4.206 3.938 3.931 3.917 3.910 3.904 3.898 3.892 3.886 3.880 3.873 3.868 3.862 2.650 2.626 2.606 2.594 2.583 2.567 2.558 2.540 2.532 2.516 2.505 2.472 2.462 2.330 2.292 2.272 2.266 2.261 2.250 2.239 2.234 2.228 2.217 2.207 2.117 2.065 1.923 1.842 1.813 1.785 1.780 1.767 1.752 1.670 1.648 1.629 1.623 1.616 1.606 1.595 1.572



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

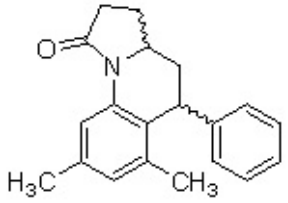
1.00 2.00 1.00 2.00 1.00 1.00 1.00 3.00 3.00 1.00 4.00 1.00

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

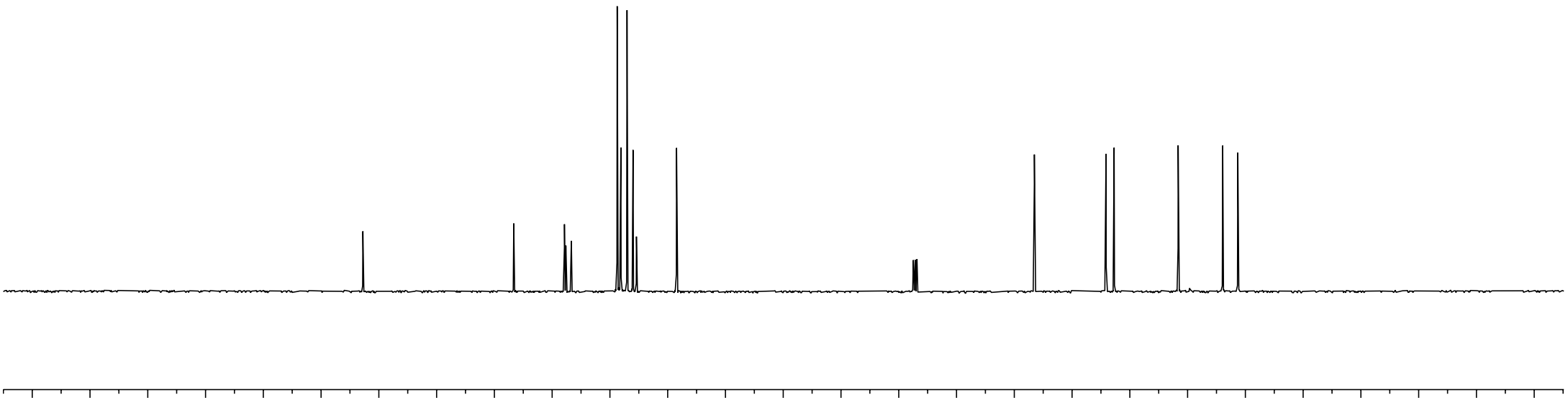
f1 (ppm)

11m/B

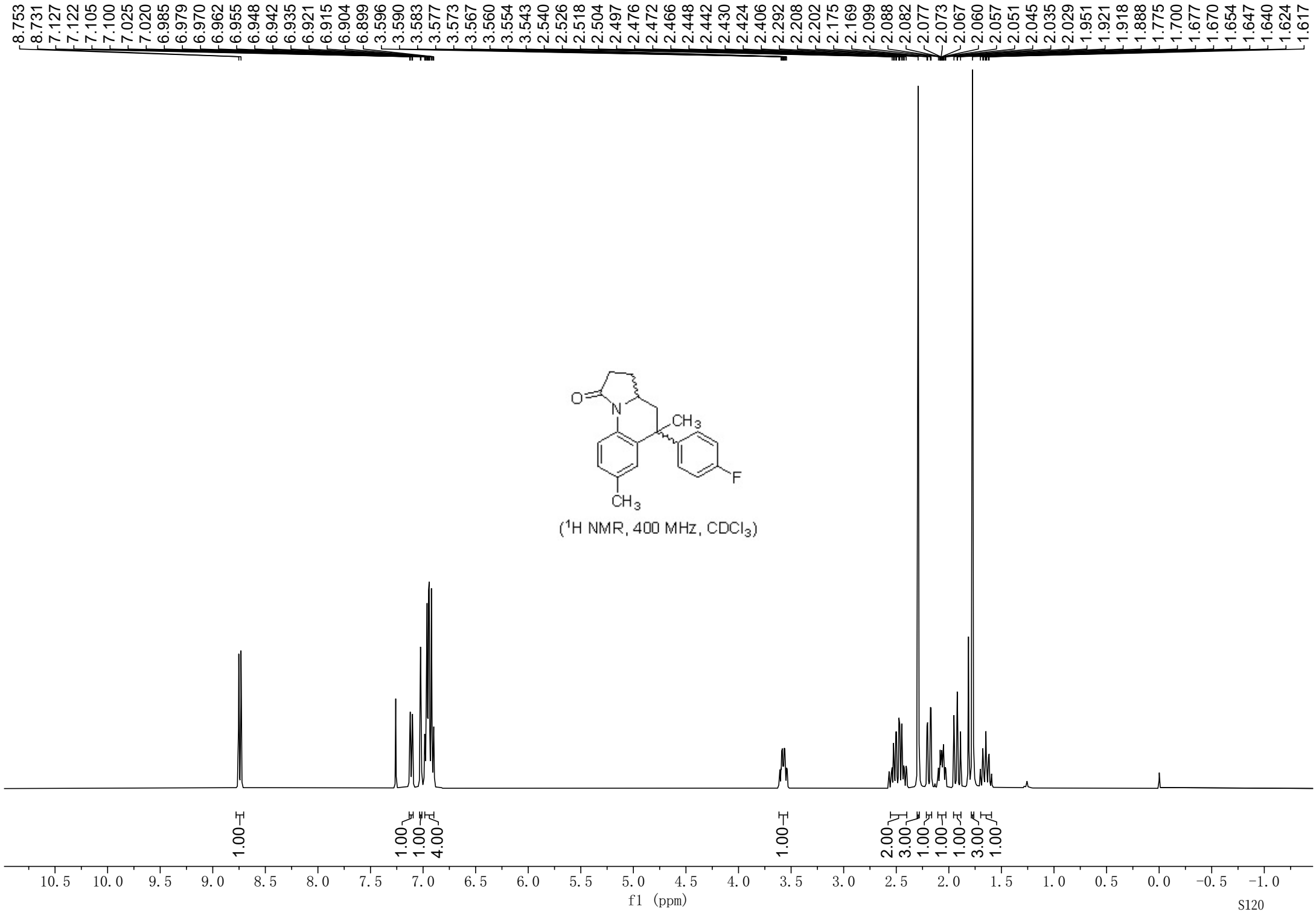
172.762
146.648
137.870
137.626
136.675
128.744
128.105
127.036
125.998
125.408
118.463
56.526
44.120
42.716
31.632
23.925
21.306
21.223



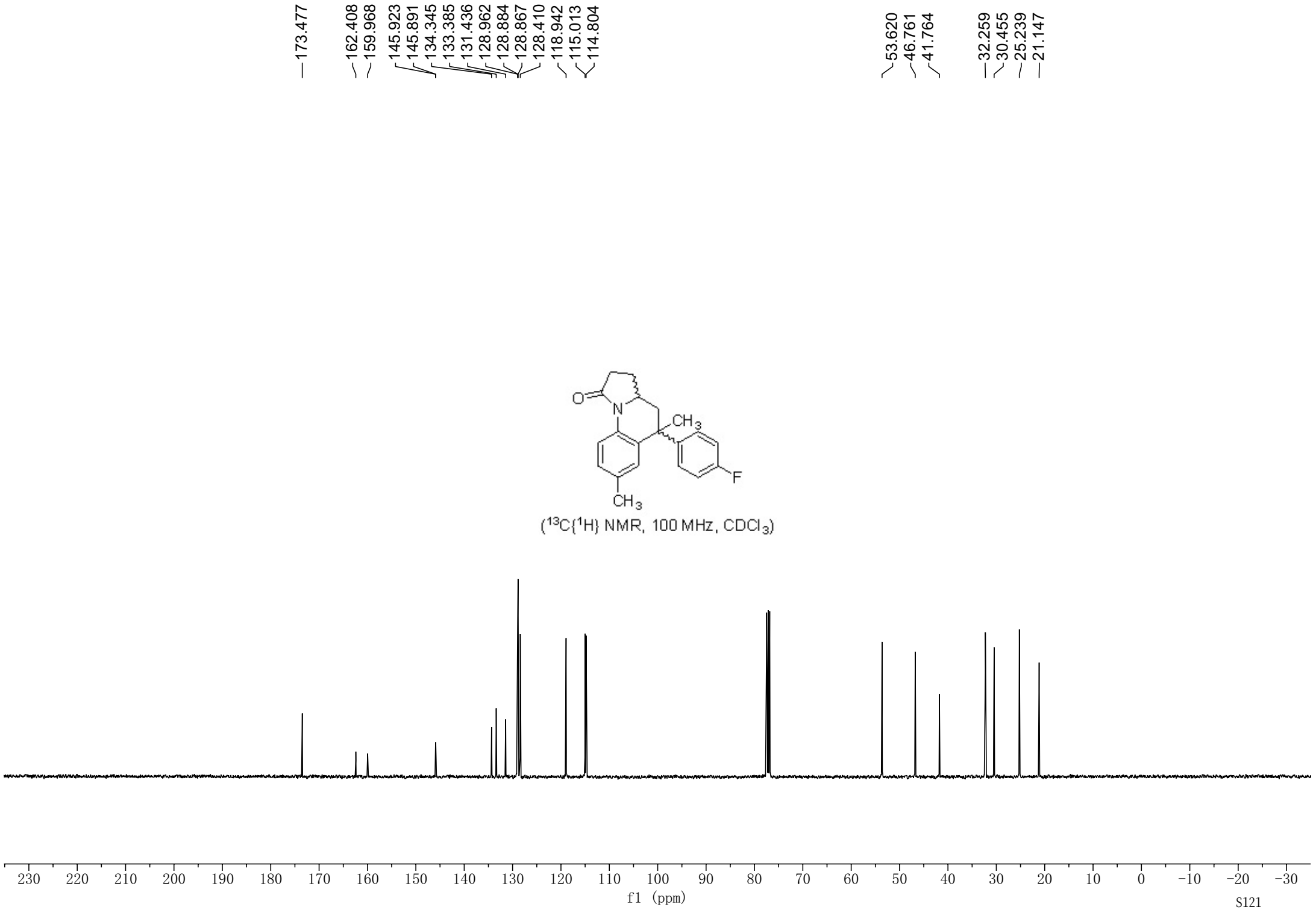
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



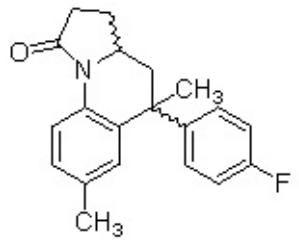
11n/A


8.753
8.731
7.127
7.122
7.105
7.100
7.025
7.020
6.985
6.979
6.970
6.962
6.955
6.948
6.942
6.935
6.921
6.915
6.904
6.899
3.596
3.590
3.583
3.577
3.573
3.567
3.560
3.554
3.543
2.540
2.526
2.518
2.504
2.497
2.476
2.472
2.466
2.448
2.442
2.430
2.424
2.406
2.292
2.208
2.202
2.175
2.169
2.099
2.088
2.082
2.077
2.073
2.067
2.060
2.057
2.051
2.045
2.035
2.029
1.951
1.921
1.918
1.888
1.775
1.700
1.677
1.670
1.654
1.647
1.640
1.624
1.617
O
N
CH3
F
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
4.00
1.00
2.00
3.00
1.00
1.00
1.00
3.00
1.00
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
-0.5
-1.0
f1 (ppm)

11n/A

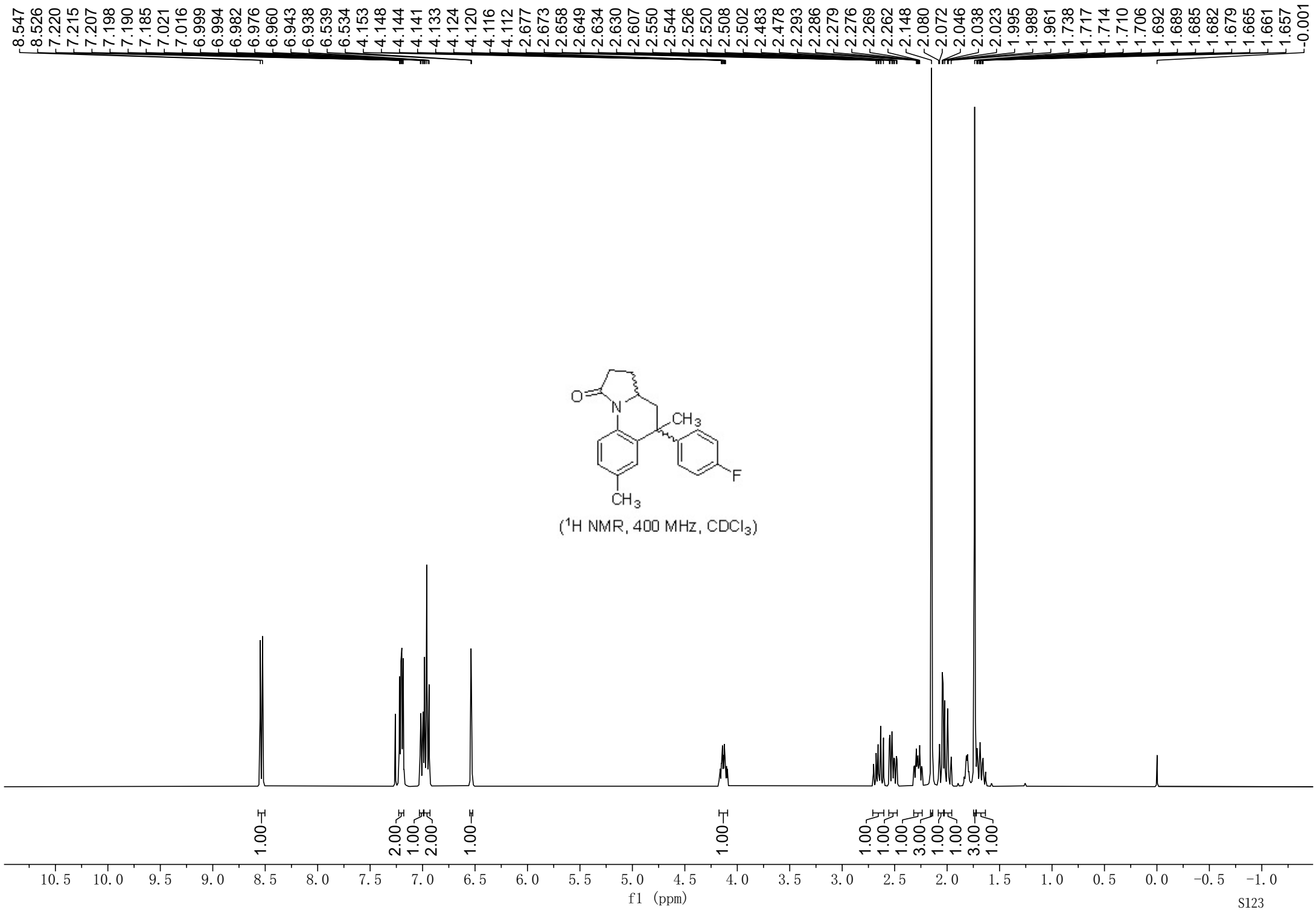

173.477
162.408
159.968
145.923
145.891
134.345
133.385
131.436
128.962
128.884
128.867
128.410
118.942
115.013
114.804
53.620
46.761
41.764
32.259
30.455
25.239
21.147
O
N
CH3
F
CH3
(13C{1H} NMR, 100 MHz, CDCl3)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11n/A



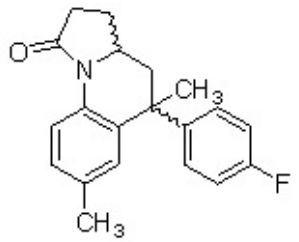
(^{19}F NMR, 376 MHz, $CDCl_3$)

11n/B

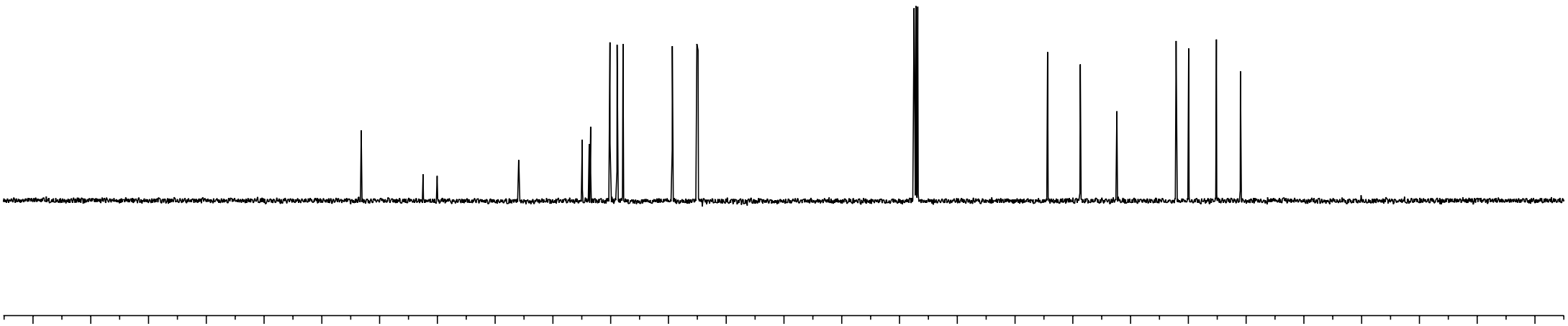

8.547
8.526
7.220
7.215
7.207
7.198
7.190
7.185
7.021
7.016
6.999
6.994
6.982
6.976
6.960
6.943
6.938
6.539
6.534
4.153
4.148
4.144
4.141
4.133
4.124
4.120
4.116
4.112
2.677
2.673
2.658
2.649
2.634
2.630
2.607
2.550
2.544
2.526
2.520
2.508
2.502
2.483
2.478
2.293
2.286
2.279
2.276
2.269
2.262
2.148
2.080
2.072
2.046
2.038
2.023
1.995
1.989
1.961
1.738
1.717
1.714
1.710
1.706
1.692
1.689
1.685
1.682
1.679
1.665
1.661
1.657
-0.001
O
N
CH3
F
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
1.00
3.00
1.00
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
-0.5
-1.0
f1 (ppm)

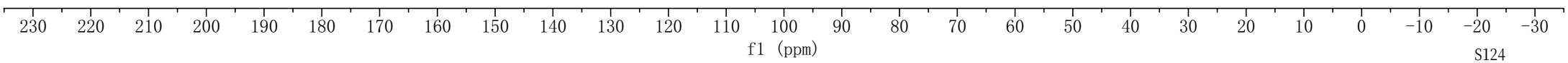
11n/B

173.175
162.478
160.042
145.931
145.899
134.918
133.715
133.475
130.124
128.888
128.809
127.868
119.330
115.080
114.871
54.370
48.706
42.378
32.119
29.948
25.146
20.985

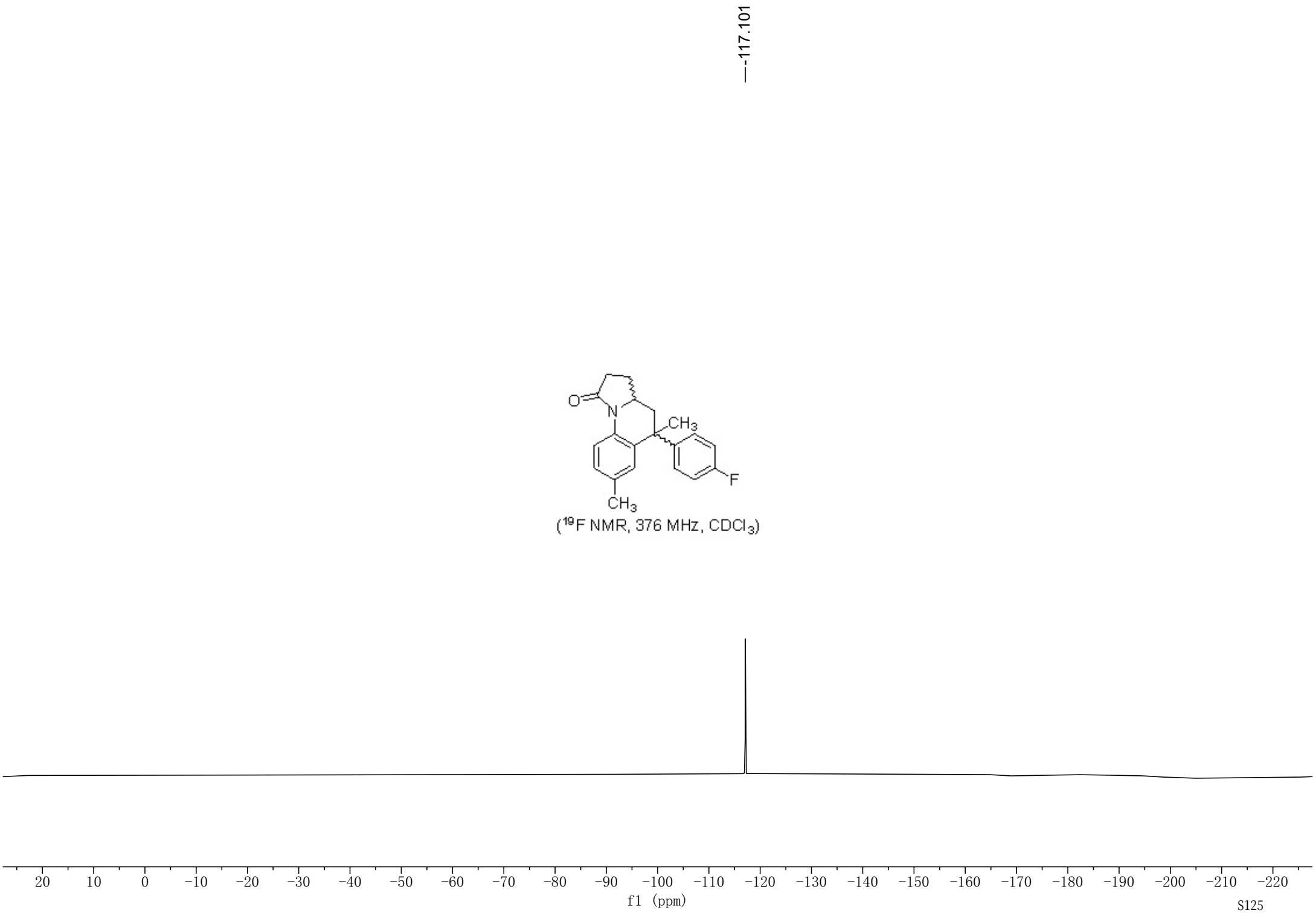


($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)

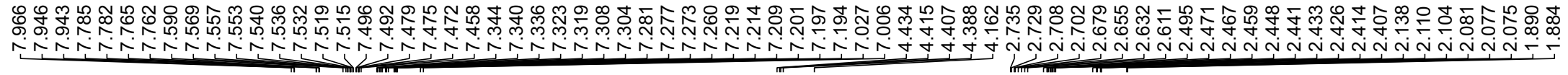


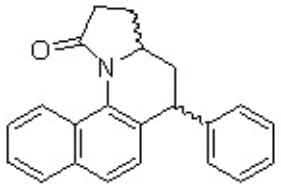


11n/B

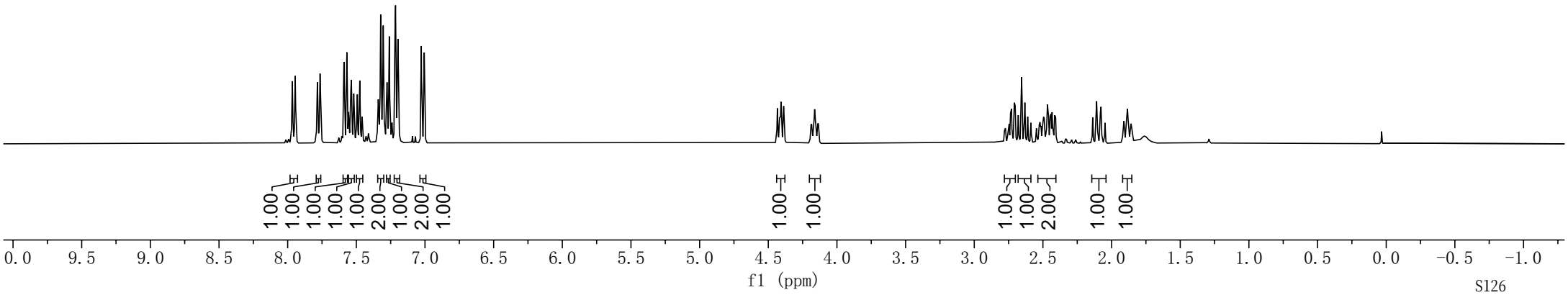

-117.101
O
N
CH3
F
CH3
(19F NMR, 376 MHz, CDCl3)
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
−220
f1 (ppm)

11o/A

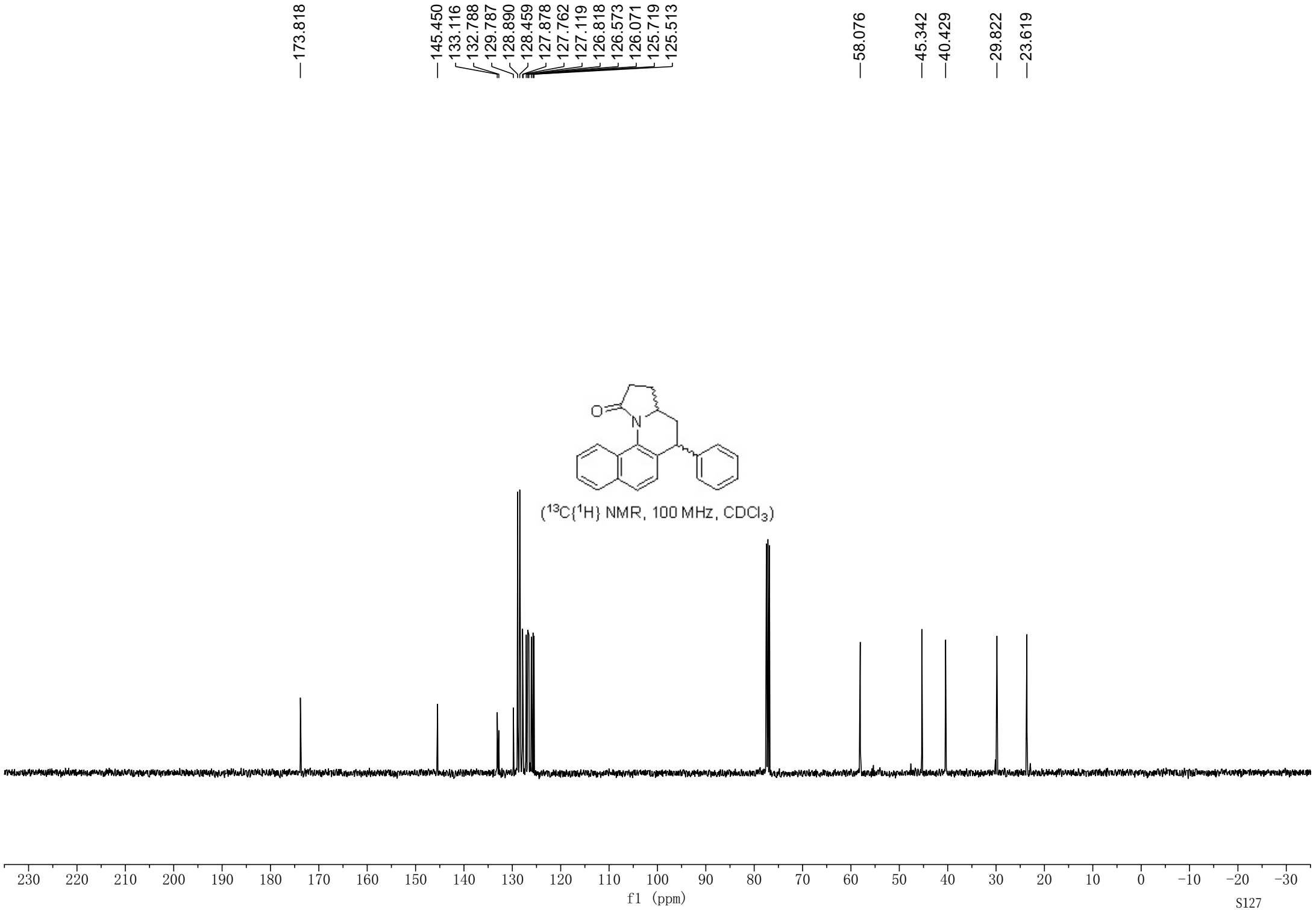




(^{1}H NMR, 400 MHz, $CDCl_3$)

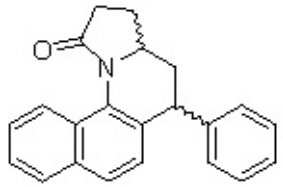


11o/A

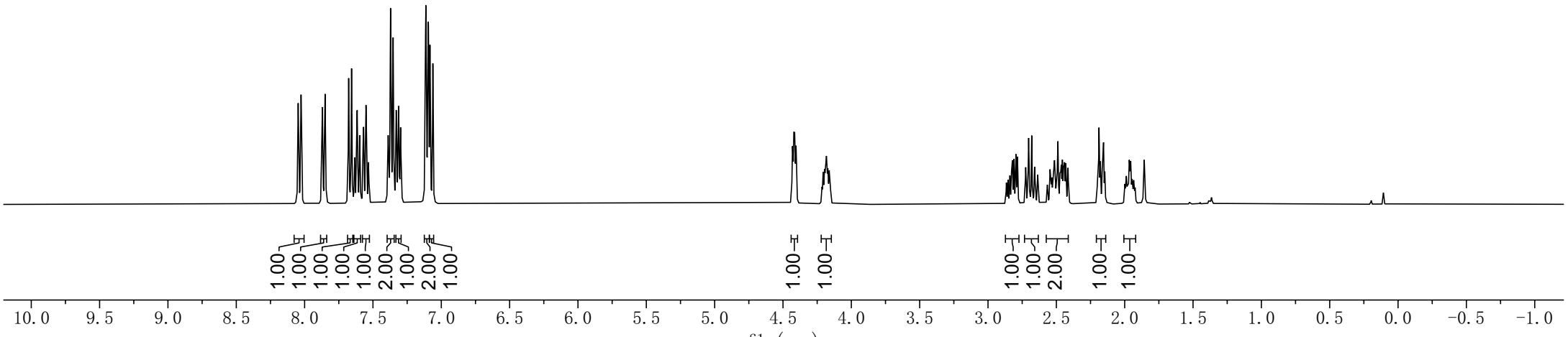

173.818
145.450
133.116
132.788
129.787
128.890
128.459
127.878
127.762
127.119
126.818
126.573
126.071
125.719
125.513
58.076
45.342
40.429
29.822
23.619
O
N
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

11o/B

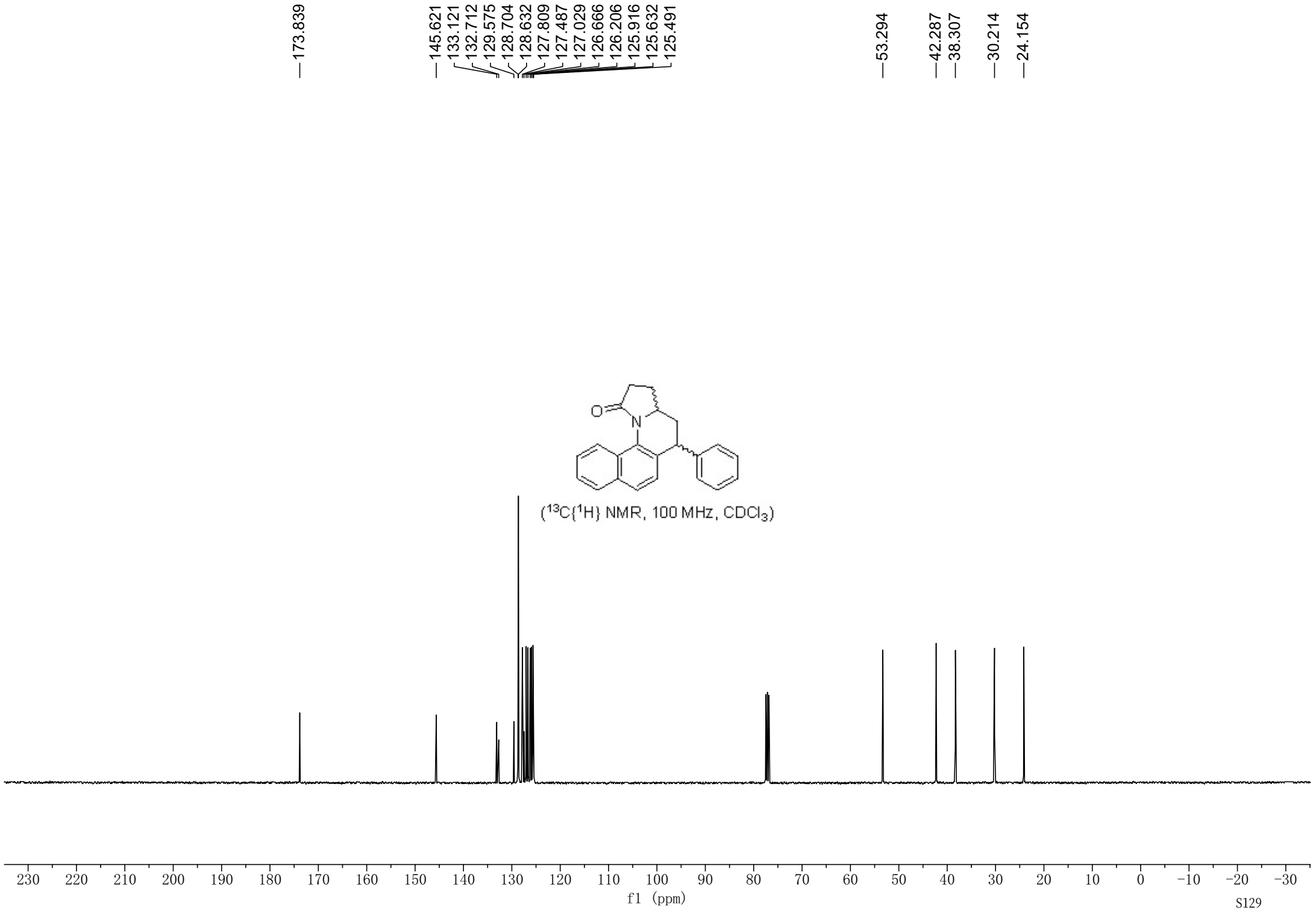
8.047 8.026 7.871 7.852 7.848 7.678 7.656 7.636 7.633 7.619 7.616 7.611 7.598 7.594 7.571 7.568 7.554 7.551 7.548 7.534 7.531 7.392 7.388 7.384 7.371 7.367 7.352 7.334 7.330 7.326 7.318 7.312 7.298 7.117 7.112 7.100 7.095 7.083 7.062 4.431 4.421 4.414 4.405 4.187 4.180 4.172 2.822 2.810 2.796 2.784 2.724 2.704 2.700 2.680 2.660 2.520 2.513 2.488 2.472 2.464 2.456 2.447 2.440 2.431 2.415 2.197 2.188 2.178 2.165 2.155 1.966 1.956



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

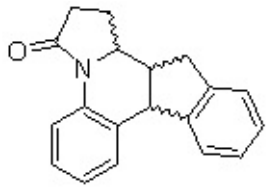


11o/B

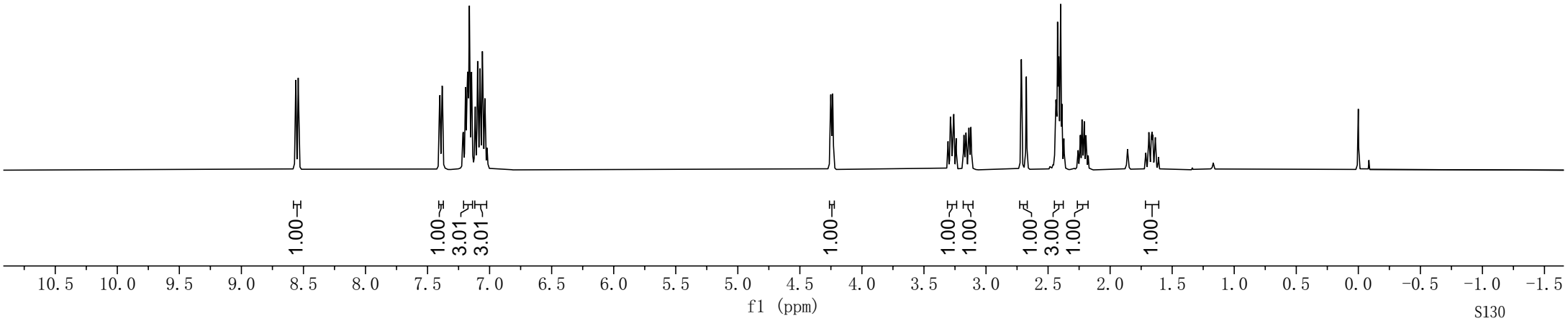

173.839
145.621
133.121
132.712
129.575
128.704
128.632
127.809
127.487
127.029
126.666
126.206
125.916
125.632
125.491
53.294
42.287
38.307
30.214
24.154
O
N
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

12a/A

8.564 8.561 8.543 8.540 7.403 7.399 7.384 7.380 7.216 7.211 7.197 7.193 7.181 7.177 7.172 7.163 7.146 7.142 7.118 7.115 7.100 7.096 7.090 7.081 7.077 7.074 7.072 7.059 7.054 7.038 7.022 7.018 4.251 4.236 3.306 3.287 3.279 3.268 3.260 3.241 3.178 3.162 3.138 3.122 2.715 2.675 2.442 2.436 2.431 2.423 2.416 2.412 2.404 2.398 2.388 2.373 2.245 2.240 2.226 2.221 2.213 2.208 2.195 2.190 1.693 1.688 1.681 1.667 1.662 1.656 1.642 1.636

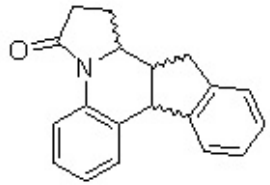


(^{1}H NMR, 400 MHz, $CDCl_3$)

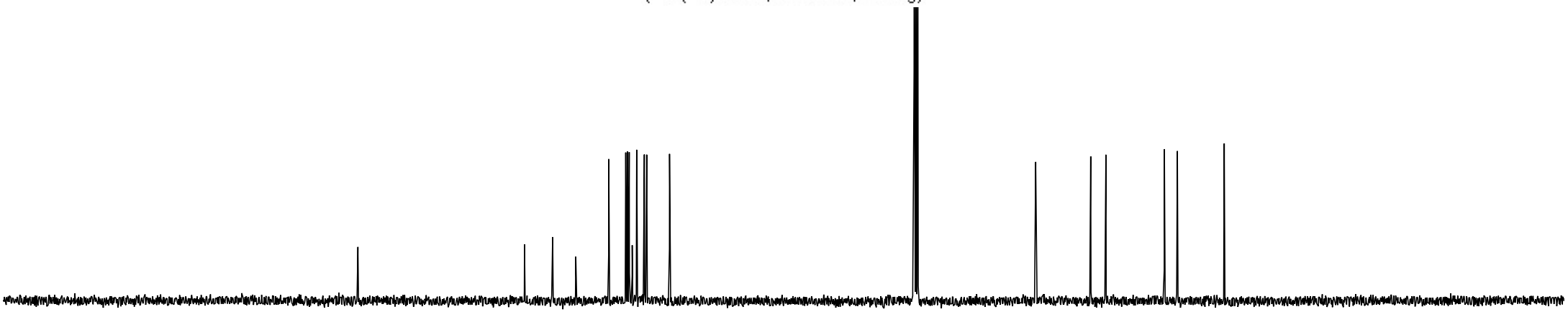


12a/A

173.768
144.931
140.058
136.057
130.346
127.408
127.115
126.800
126.287
125.512
124.188
123.776
119.823
56.438
46.916
44.281
34.165
31.917
23.800



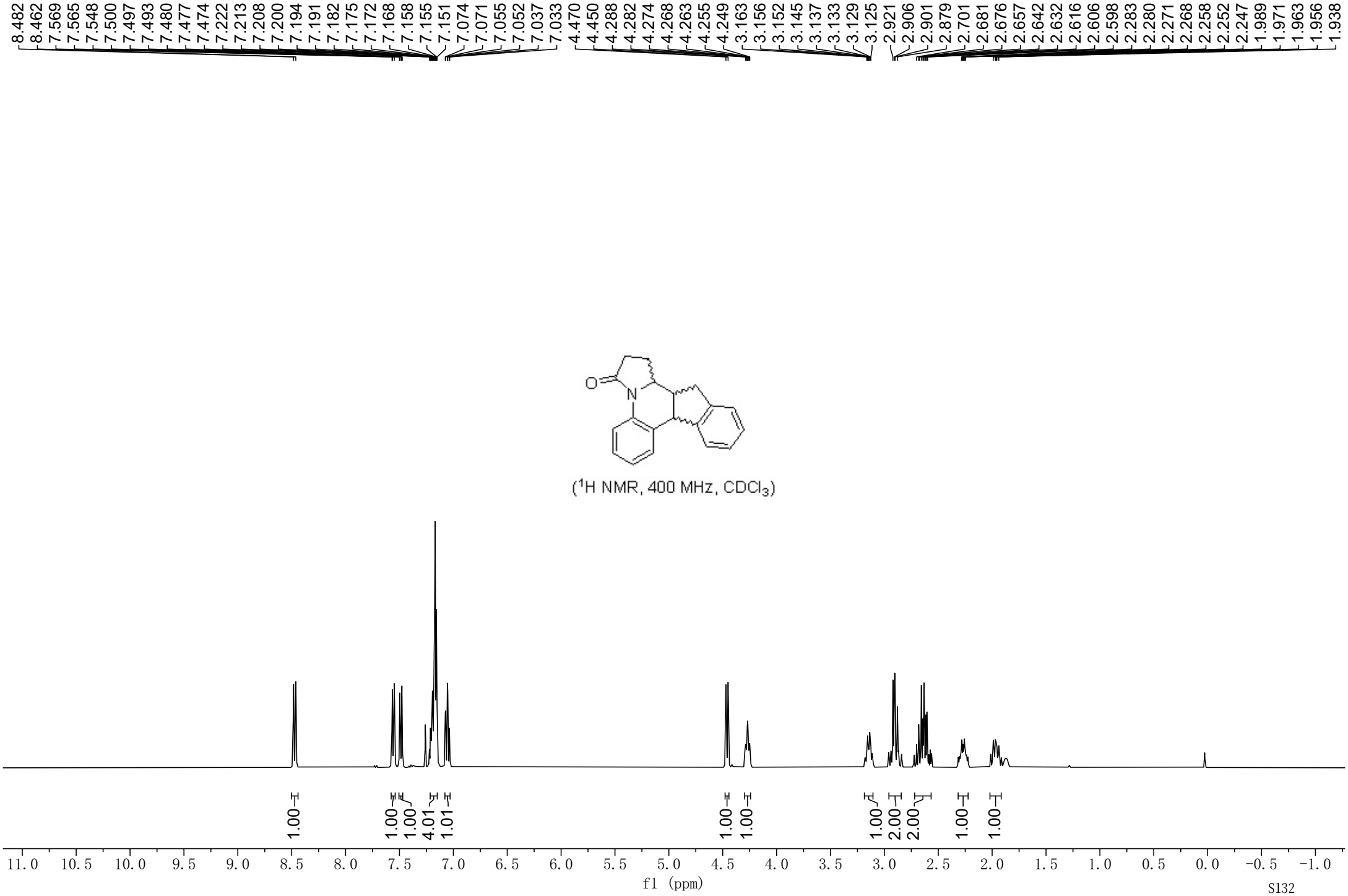
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



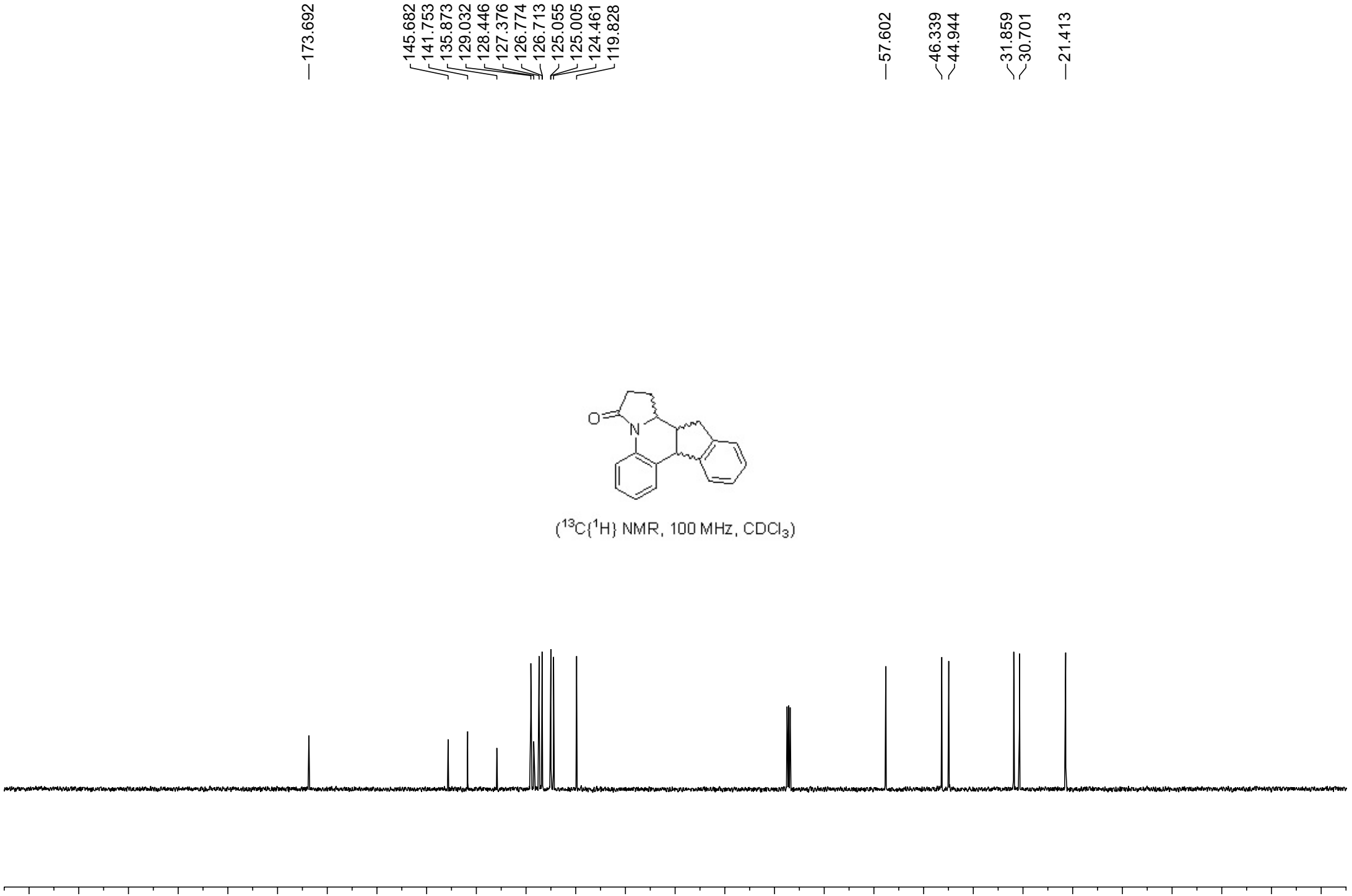
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30

f1 (ppm)

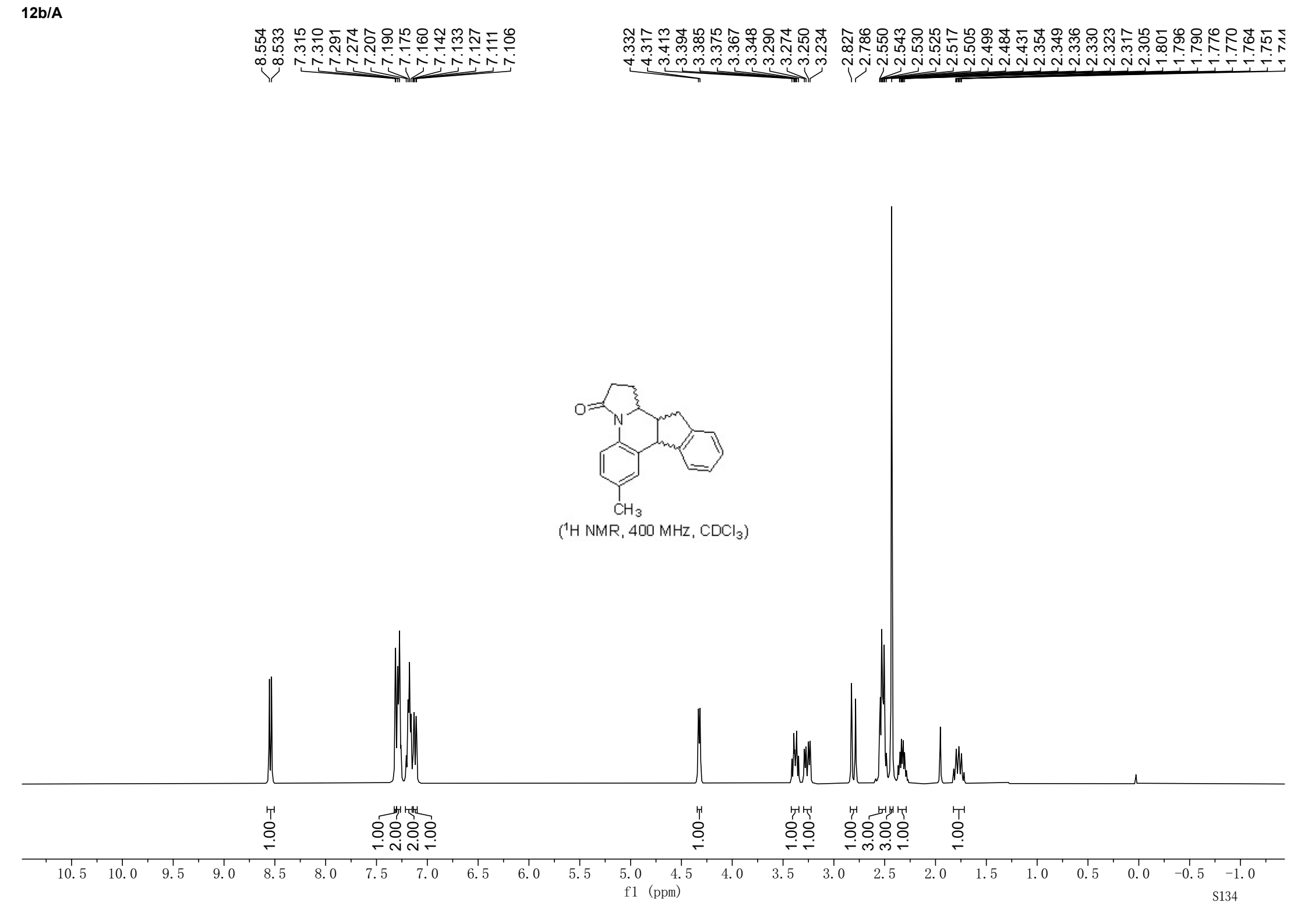
12a/B


8.482
8.462
7.569
7.565
7.548
7.500
7.497
7.493
7.480
7.477
7.474
7.222
7.213
7.208
7.200
7.194
7.191
7.182
7.175
7.172
7.168
7.158
7.155
7.151
7.074
7.071
7.055
7.052
7.037
7.033
4.470
4.450
4.288
4.282
4.274
4.268
4.263
4.255
4.249
3.163
3.156
3.152
3.145
3.137
3.133
3.129
3.125
2.921
2.906
2.901
2.879
2.701
2.681
2.676
2.657
2.642
2.632
2.616
2.606
2.598
2.283
2.280
2.271
2.268
2.258
2.252
2.247
1.989
1.971
1.963
1.956
1.938
O
N
(^{1}H NMR, 400 MHz, $CDCl_3$)
1.00
1.00
1.00
4.01
1.01
1.00
1.00
1.00
2.00
2.00
1.00
1.00
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
0.0
-0.5
-1.0
f1 (ppm)

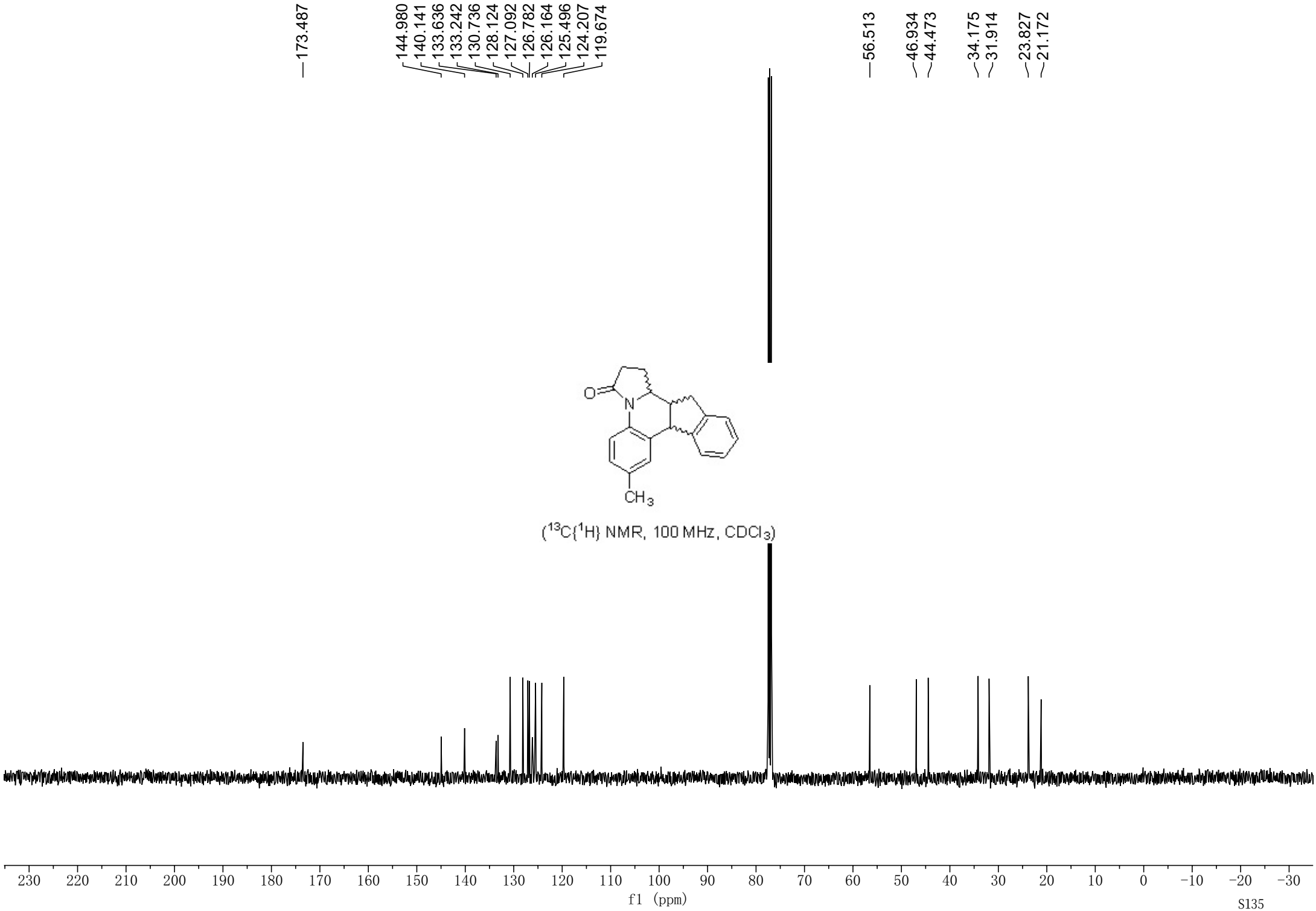
12a/B


173.692
145.682
141.753
135.873
129.032
128.446
127.376
126.774
126.713
125.055
125.005
124.461
119.828
57.602
46.339
44.944
31.859
30.701
21.413
O
N
($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

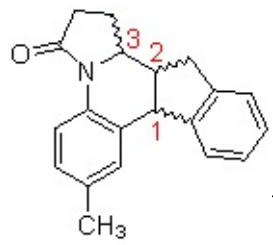
12b/A


8.554
8.533
7.315
7.310
7.291
7.274
7.207
7.190
7.175
7.160
7.142
7.133
7.127
7.111
7.106
4.332
4.317
3.413
3.394
3.385
3.375
3.367
3.348
3.290
3.274
3.250
3.234
2.827
2.786
2.550
2.543
2.530
2.525
2.517
2.505
2.499
2.484
2.431
2.354
2.349
2.336
2.330
2.323
2.317
2.305
1.801
1.796
1.790
1.776
1.770
1.764
1.751
O
N
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
2.00
2.00
1.00
1.00
1.00
1.00
1.00
1.00
3.00
3.00
1.00
1.00
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 -0.5 -1.0
f1 (ppm)

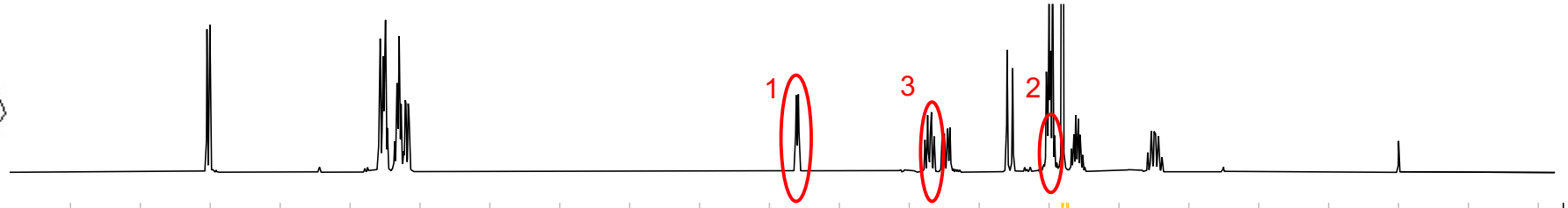
12b/A


173.487
144.980
140.141
133.636
133.242
130.736
128.124
127.092
126.782
126.164
125.496
124.207
119.674
56.513
46.934
44.473
34.175
31.914
23.827
21.172
O
N
CH3
(13C{1H} NMR, 100 MHz, CDCl3)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

12b/A

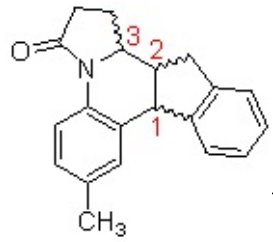

O
N
3
2
1
CH3

(H-H-COSY)

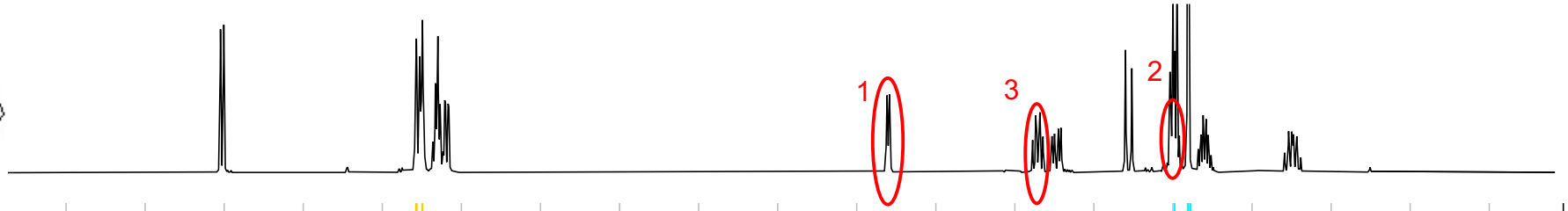

1
3
2

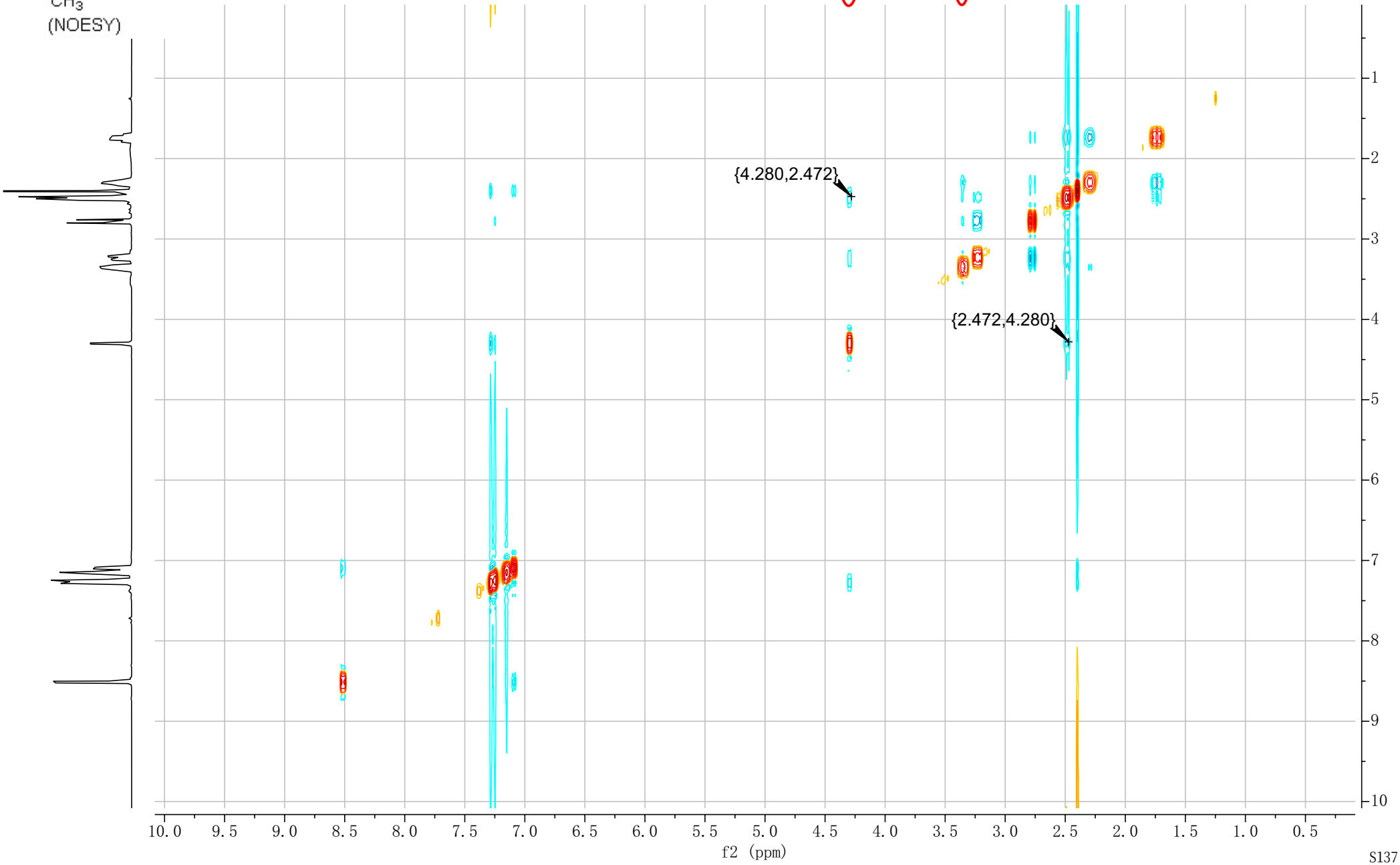

{4.280,2.472}
{3.346,2.472}
{2.472,3.346}
{2.482,4.280}
f2 (ppm)
f1 (ppm)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
-1 0 1 2 3 4 5 6 7 8 9 10

12b/A

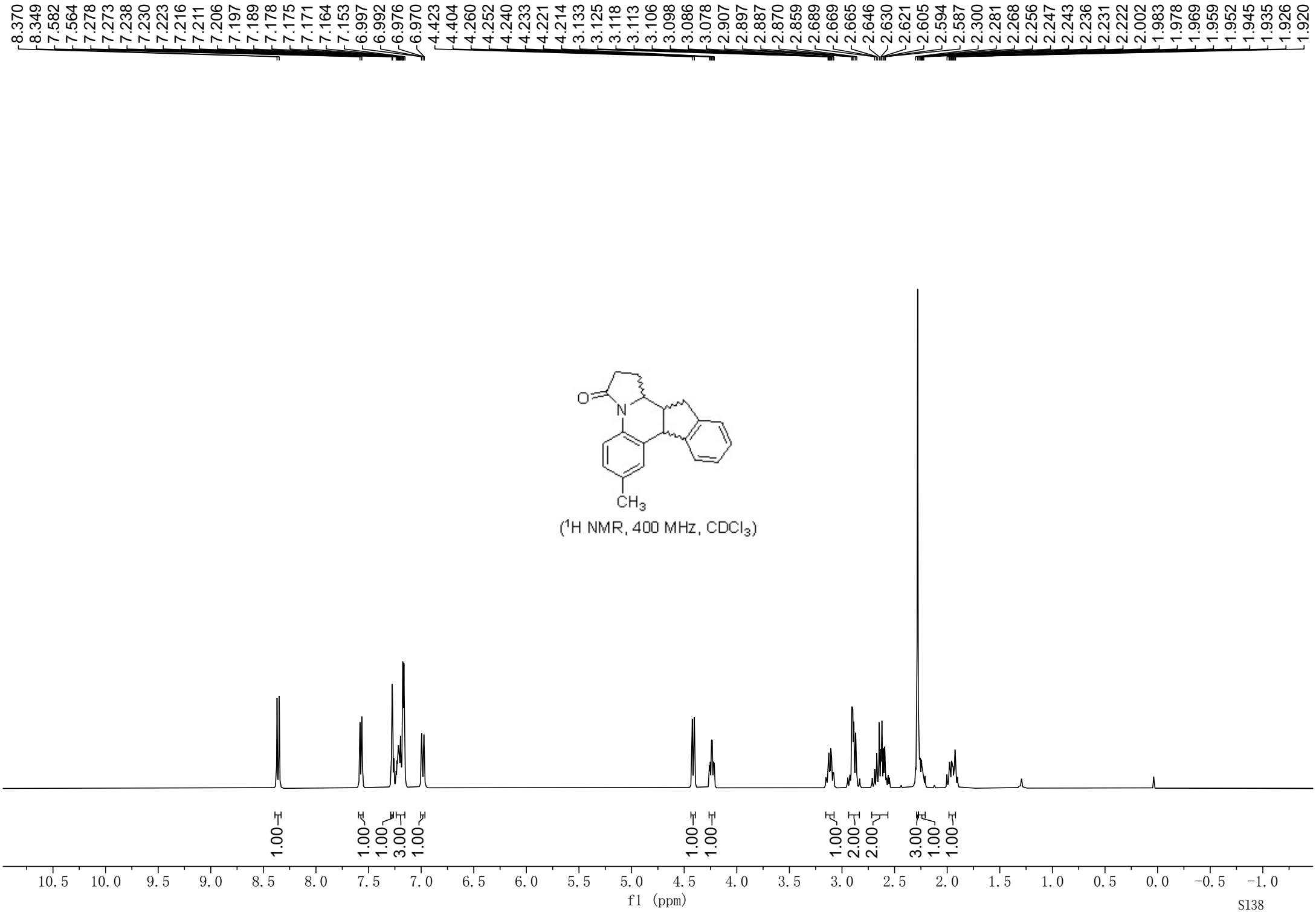

O
N
3
2
1
CH3

(NOESY)


1
3
2

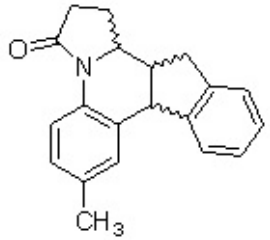

{4.280,2.472}
{2.472,4.280}
1
2
3
4
5
6
7
8
9
10
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)

12b/B

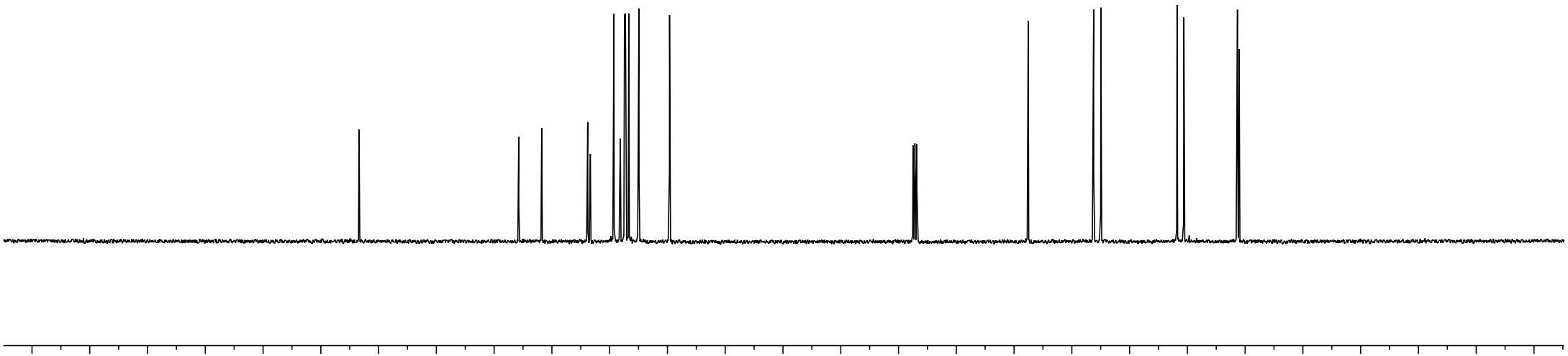

8.370
8.349
7.582
7.564
7.278
7.273
7.238
7.230
7.223
7.216
7.211
7.206
7.197
7.189
7.178
7.175
7.171
7.164
7.153
6.997
6.992
6.976
6.970
4.423
4.404
4.260
4.252
4.240
4.233
4.221
4.214
3.133
3.125
3.118
3.113
3.106
3.098
3.086
3.078
2.907
2.897
2.887
2.870
2.859
2.689
2.669
2.665
2.646
2.630
2.621
2.605
2.594
2.587
2.300
2.281
2.268
2.256
2.247
2.243
2.236
2.231
2.222
2.002
1.983
1.978
1.969
1.959
1.952
1.945
1.935
1.926
1.920
O
N
CH3
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.00
3.00
1.00
1.00
1.00
1.00
2.00
2.00
3.00
1.00
1.00
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
-0.5
-1.0
f1 (ppm)

12b/B

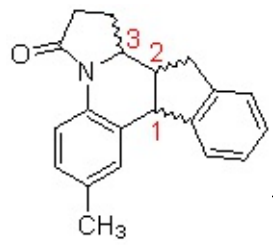
173.385
145.744
141.772
133.801
133.344
129.269
128.152
127.436
127.269
126.695
125.031
124.935
119.634
57.547
46.225
44.975
31.785
30.602
21.333
21.037



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



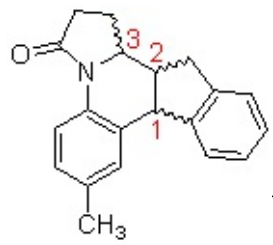
12b/B


O
N
3
2
1
CH3

(H-H-COSY)


1
3
2
{4.352,3.056}
{4.198,3.056}
{3.056,4.352}
{3.056,4.198}
f2 (ppm)
f1 (ppm)
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 -0.5 -1.0
-1 0 1 2 3 4 5 6 7 8 9 10

12b/B

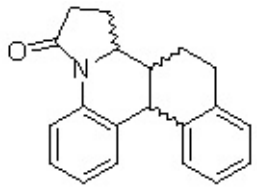

O
N
3
2
1
CH3

(NOESY)

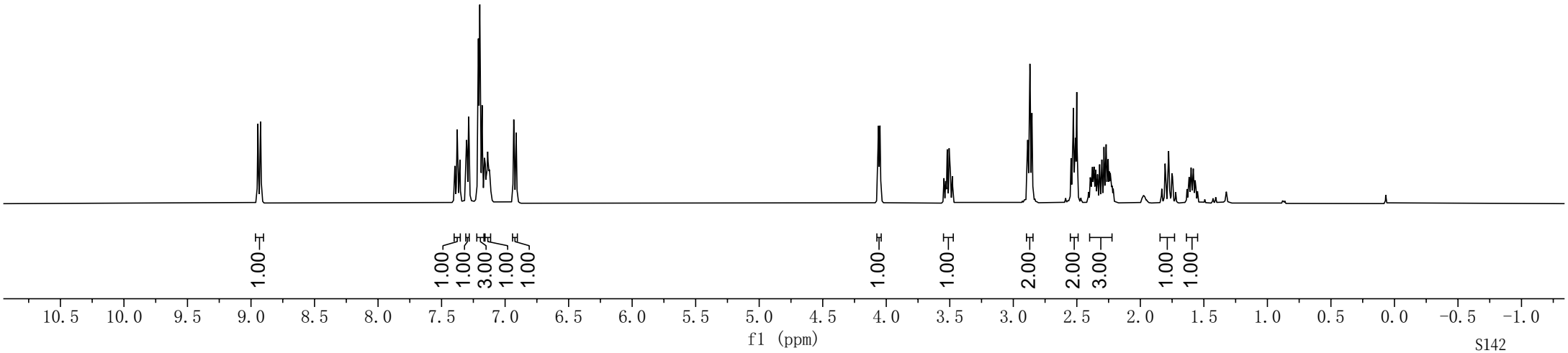
1
3
2
{4.352,3.056}
{4.198,3.056}
{3.056,4.352}
{3.056,4.198}
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)
1
2
3
4
5
6
7
8
9
f1 (ppm)

12c/A

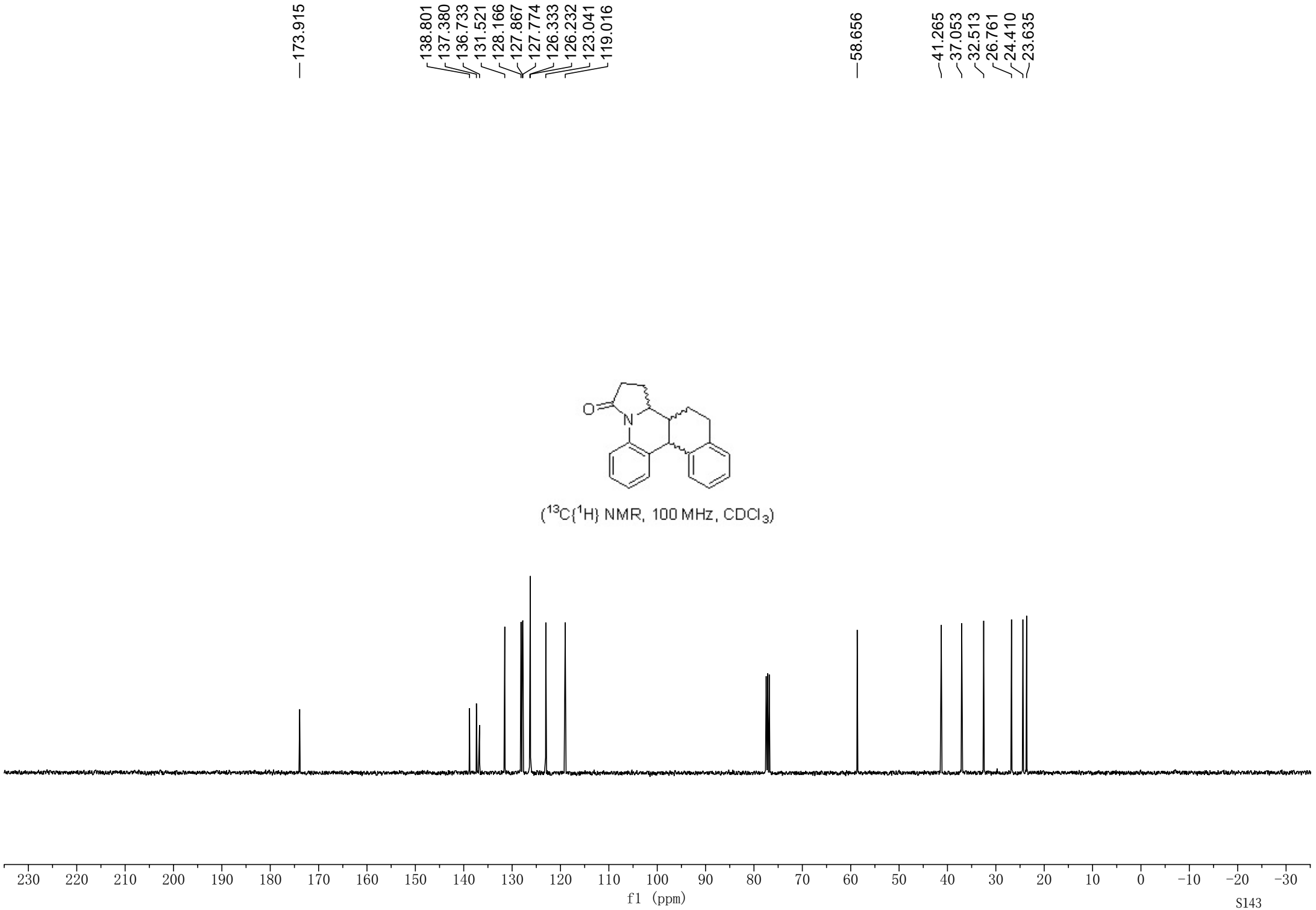
8.946 8.927 8.924 7.399 7.395 7.381 7.377 7.373 7.360 7.356 7.307 7.303 7.298 7.288 7.284 7.210 7.202 7.199 7.195 7.183 7.180 7.165 7.162 7.157 7.148 7.144 7.137 7.130 7.124 6.932 6.913 4.062 4.049 3.530 3.520 3.505 3.495 3.479 2.889 2.885 2.869 2.853 2.545 2.534 2.527 2.516 2.510 2.501 2.382 2.377 2.369 2.364 2.351 2.337 2.320 2.303 2.286 2.274 2.269 2.259 2.253 2.245 2.237 2.230 1.805 1.801 1.777 1.752 1.603 1.601 1.597 1.583



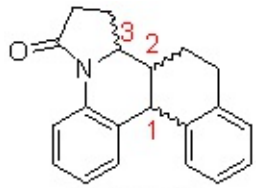
(^{1}H NMR, 400 MHz, $CDCl_3$)



12c/A


173.915
138.801
137.380
136.733
131.521
128.166
127.867
127.774
126.333
126.232
123.041
119.016
58.656
41.265
37.053
32.513
26.761
24.410
23.635
O
N
(13C{1H} NMR, 100 MHz, CDCl3)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30
f1 (ppm)

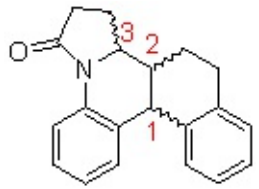
12c/A


O
N
3
2
1

(H-H-COSY)

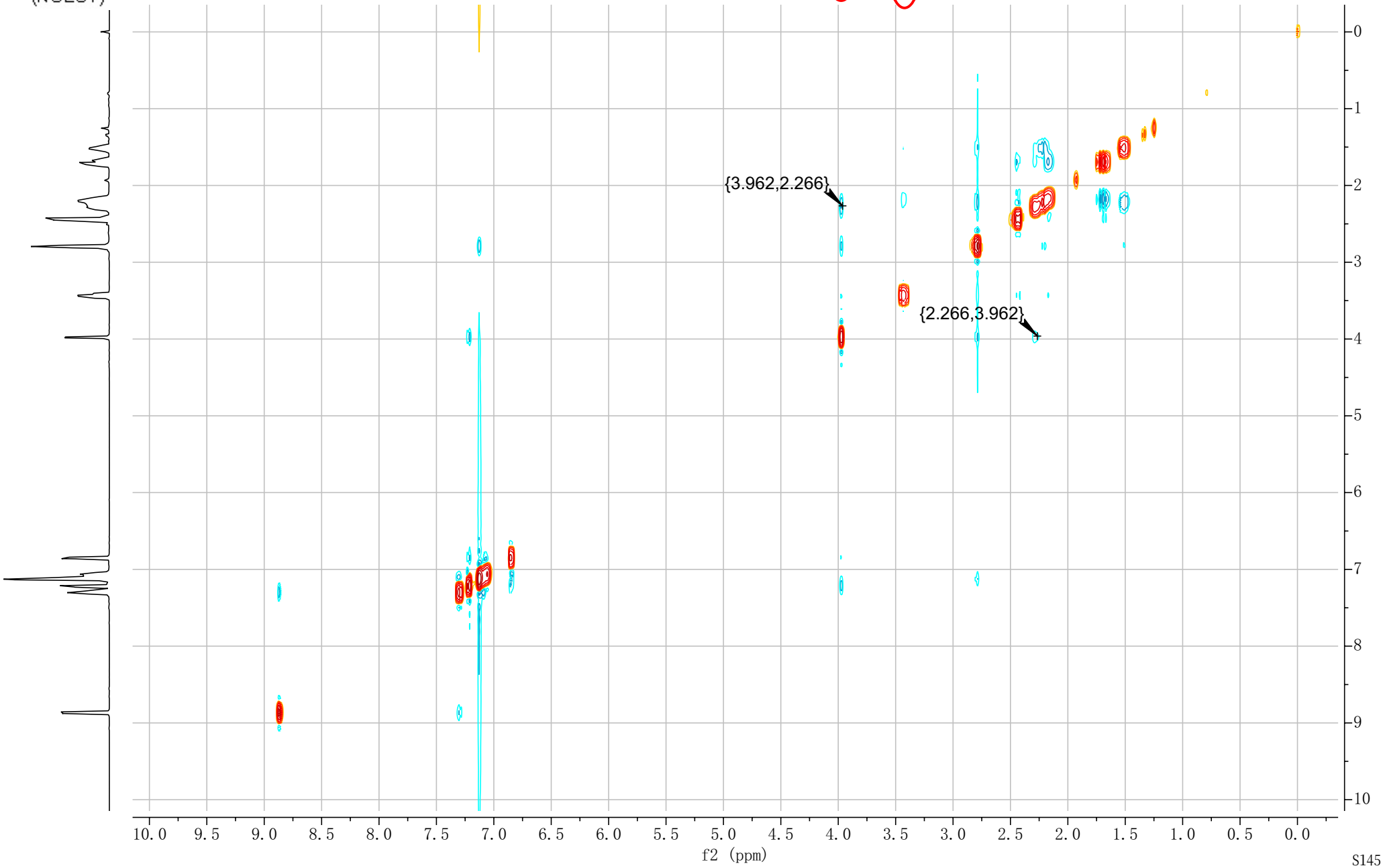
1
3
2
{3.962,2.266}
{3.420,2.266}
{2.266,3.420}
{2.266,3.962}
f2 (ppm)
f1 (ppm)

12c/A


O
N
3
2
1

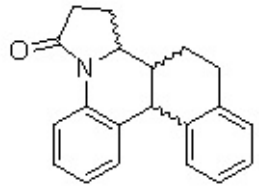
(NOESY)


1
3
2

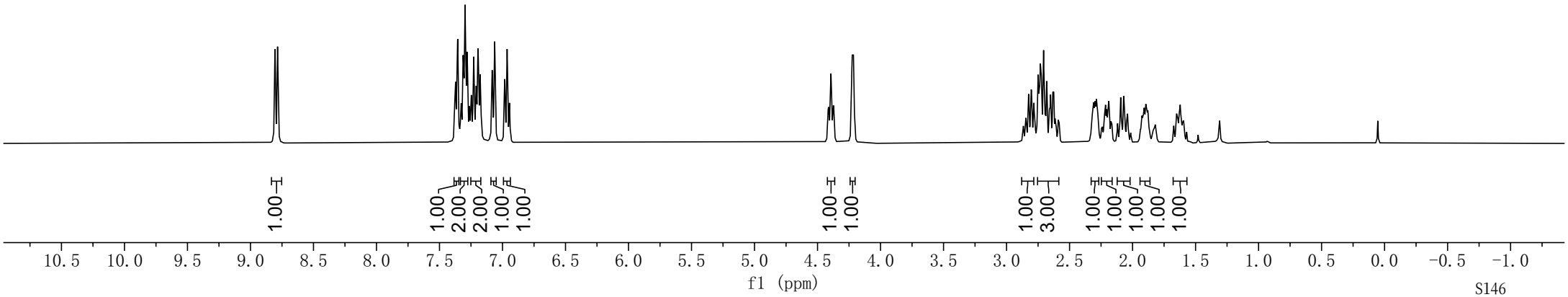

{3.962,2.266}
{2.266,3.962}
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)

12c/B

8.806 8.785 7.377 7.372 7.360 7.354 7.331 7.327 7.313 7.309 7.297 7.282 7.278 7.264 7.260 7.248 7.228 7.209 7.194 7.178 7.173 7.082 7.062 6.982 6.963 6.944 4.416 4.410 4.395 4.390 4.376 4.370 4.225 4.214 2.825 2.806 2.801 2.783 2.750 2.741 2.732 2.723 2.706 2.692 2.681 2.658 2.650 2.633 2.625 2.315 2.309 2.298 2.287 2.281 2.275 2.221 2.214 2.205 2.195 2.188 2.095 2.071 2.062 2.039 1.909 1.894 1.884 1.876 1.650 1.632 1.628 1.622

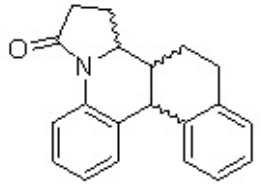


(^{1}H NMR, 400 MHz, $CDCl_3$)

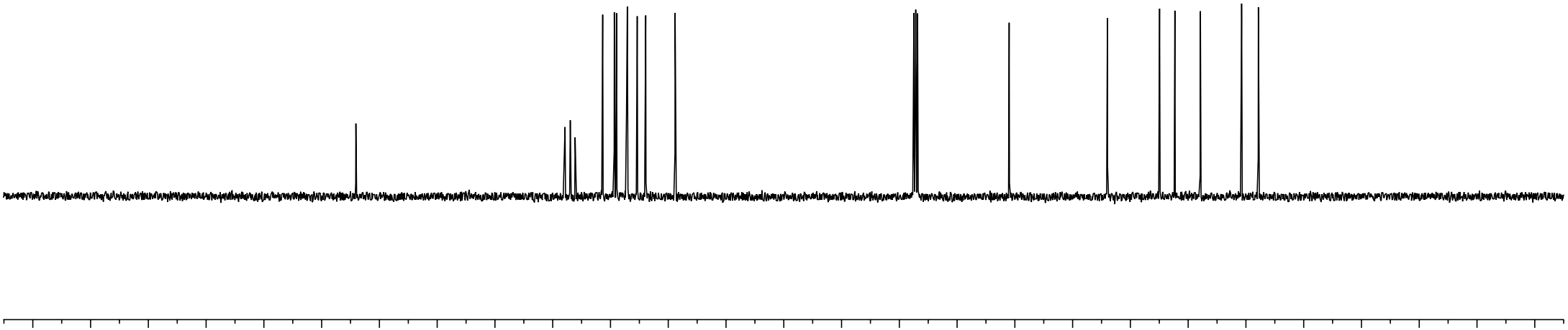


12c/B

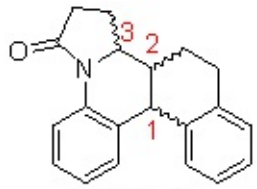
174.074
137.870
136.958
136.124
131.348
129.337
128.950
127.231
127.158
127.085
125.371
123.901
118.813
60.985
43.978
34.951
32.300
27.883
20.746
17.848



($^{13}C\{^{1}H\}$ NMR, 100 MHz, $CDCl_3$)



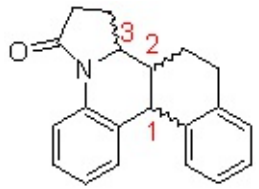
12c/B


O
N
3
2
1

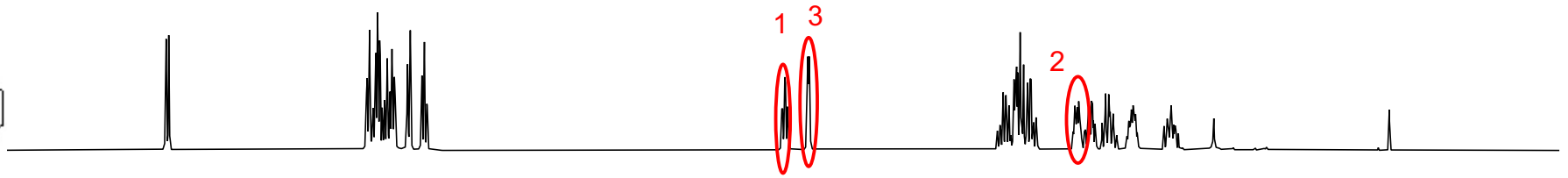
(H-H-COSY)

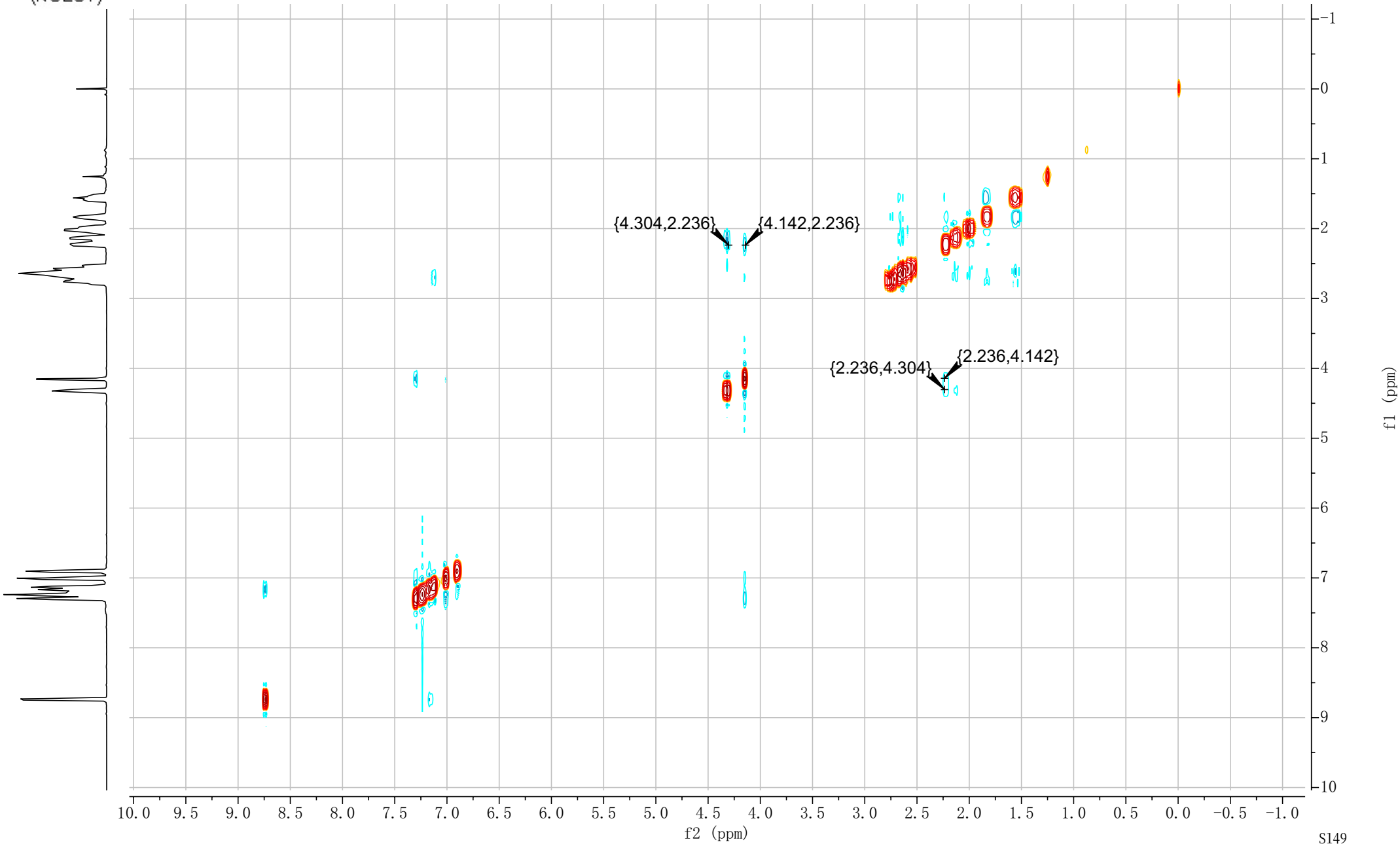
1
3
2
{4.304,2.236}
{4.142,2.236}
{2.236,4.304}
{2.236,4.142}
f2 (ppm)
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1
0
1
2
3
4
5
6
7
8
9
10

12c/B


O
N
3
2
1

(NOESY)


1
3
2


{4.304,2.236}
{4.142,2.236}
{2.236,4.304}
{2.236,4.142}
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 -0.5 -1.0
f2 (ppm)
-1 0 1 2 3 4 5 6 7 8 9 10
f1 (ppm)