Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting information

An expedite synthesis of isoquinolinones by intramolecular coupling of amides and ketones

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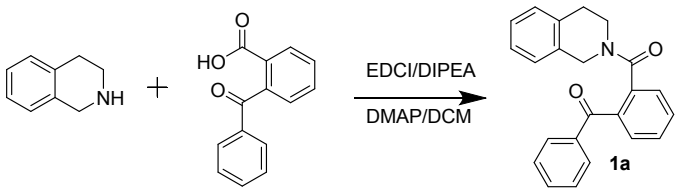
1. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AVANCE 400 spectrometer. Chemical shifts of protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CDCl_3$: δ 7.26). Chemical shifts of carbon are referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.0). Peaks are labeled as singlet (s), doublet (d), triplet (t), quartet (q) and multiplet (m). Melting points were measured on a WRS-2A melting point apparatus and are uncorrected. Infrared (IR) spectra were recorded on a Bruker Tensor 37 spectrophotometer. Data are represented as follows: frequency of absorption (cm^{-1}). All products were further characterized by HRMS (high resolution mass spectra). Copies of their ^{1}H NMR and ^{13}C NMR spectra were provided. KO*t*-Bu (99.99%) were purchased from Sigma-Aldrich and used without further purification.

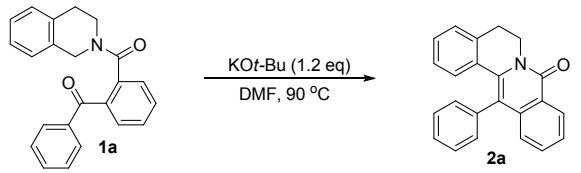
2. General Procedures

(I) Typical procedure for the preparation of substrates 1a-1w.



The compound was synthesized according to a known procedure.[1][2] A solution of 1,2,3,4-tetrahydroisoquinoline (0.67 g, 5.0 mmol) and 2-benzoylbenzoic acid (1.13 g, 5.0 mmol) in DCM (50 mL), was added EDCI (1.15 g, 6.0 mmol). The mixture was stirred for five minutes. DIPEA (774 mg, 6.0 mmol) and DMAP (61 mg, 0.5 mmol) were added successively. The reaction mixture was stirred for 15 h at room temperature. After the completion of the reaction as shown by TLC, water (30 mL) was used to dilute the reaction mixture. The organic layer was extracted with DCM（20 mL × 3). The combined organic layer was washed with saturated brine (30 mL), dried over anhydrous magnesium sulfate and concentrated under vacuum. The crude product was purified by flash chromatography (ethyl acetate/petroleum ether = 1:1) to give **1a** as a white solid (1.36 g, yield: 80%).

(II) Typical procedure for intramolecular coupling of 1a



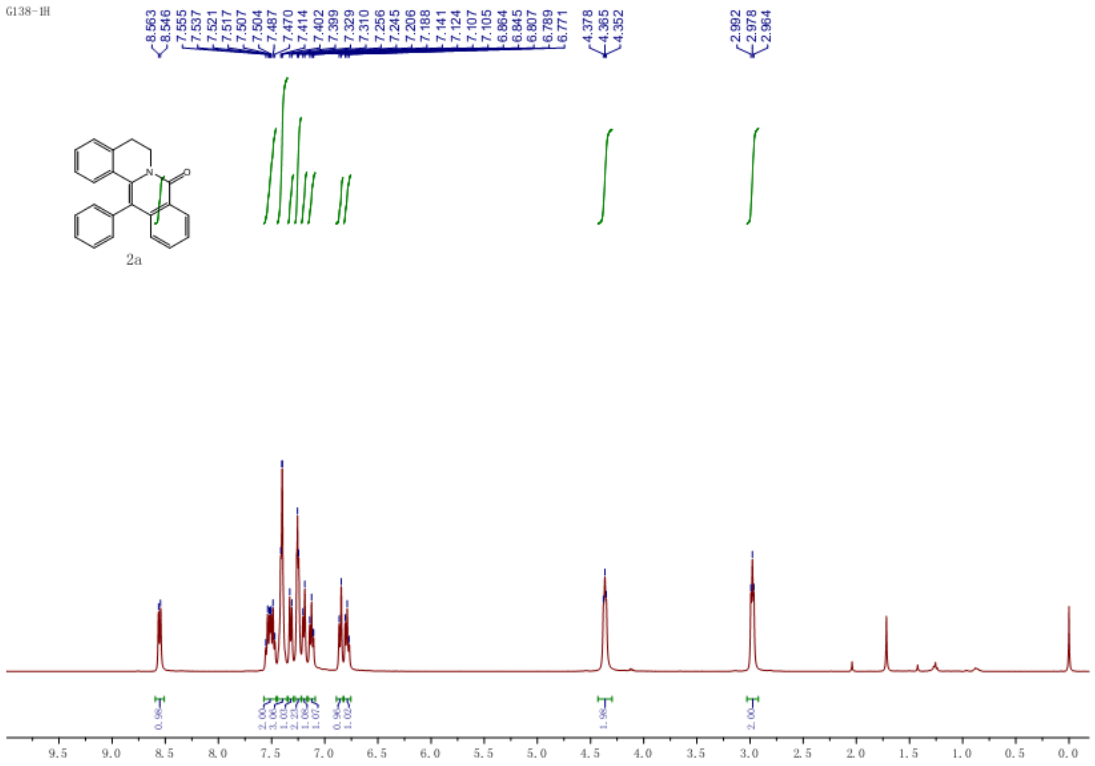
A solution of (2-benzoylphenyl)(3,4-dihydroisoquinolin-2(1H)-yl)methanone **1a** (68.4 mg, 0.2 mmol), KO*t*-Bu (27.0 mg, 0.24 mmol) in DMF (2 mL) was stirred at 90 °C under an argon atmosphere. After the completion of the reaction as shown by TLC, the solvent was removed under vacuum. The crude product was purified by flash chromatography (ethyl acetate/petroleum ether = 1:3) to give **2a** as a white solid (52.3 mg, yield: 81%).

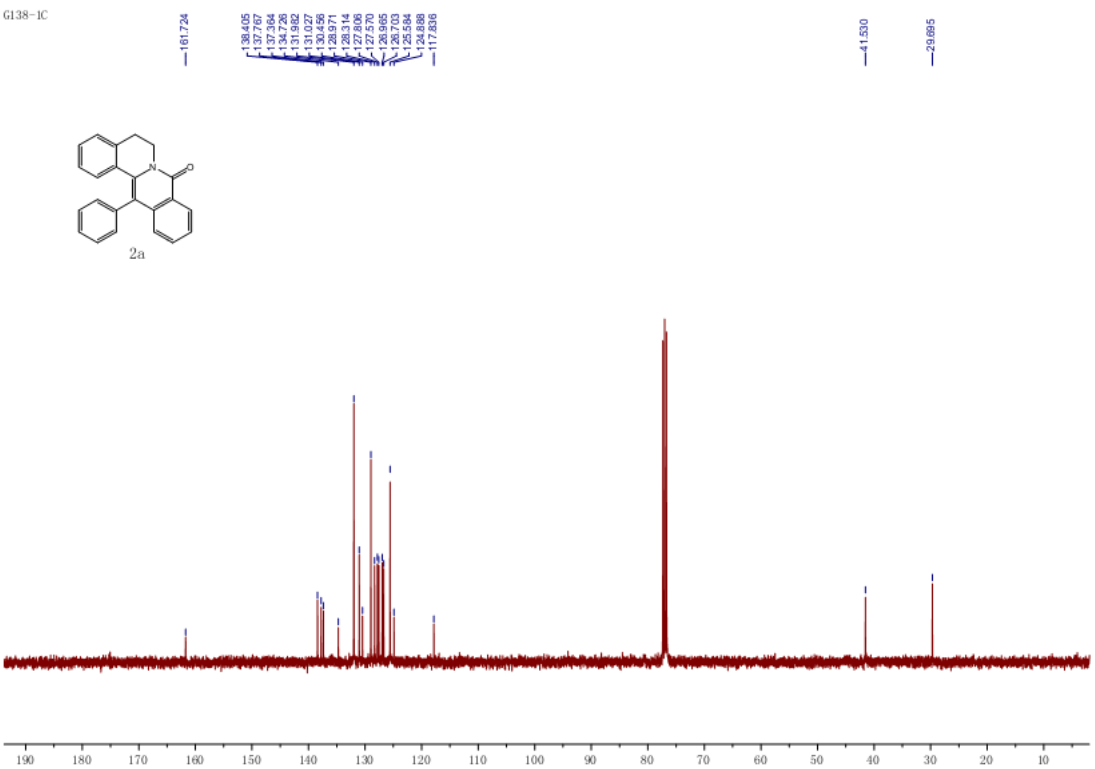
3. **References**

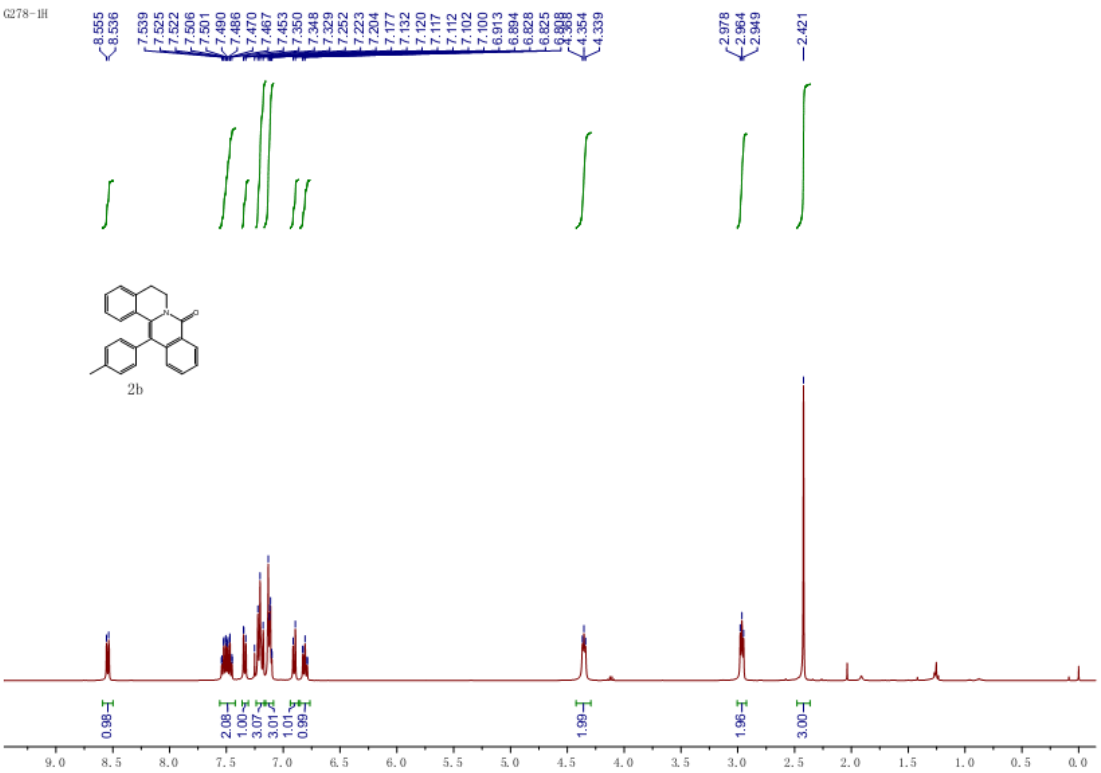
[1] F. M. Santangelo, K. K. Ogden, K. L. Strong, A. Khatri, K. M. Chepiga, H. S. Jensen, S. F. Traynelis and D. C. Liotta, *J. Med. Chem.* **2013,** *56*, 5351.

[2] G. Tang, C. Yang, Z. Nikolovska-Coleska, J. Guo and S. Qiu, *J. Med. Chem.* **2007**, *50*, 1723.

4. ^{1}H and ^{13}C NMR Spectra



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7.522
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7.350
7.348
7.329
7.252
7.223
7.204
7.177
7.132
7.120
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7.112
7.102
7.100
6.913
6.894
6.828
6.825
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2.964
2.949
2.421
2b
0.98
2.08
1.00
3.07
3.01
1.01
0.99
1.99
1.96
3.00
9.0
8.5
8.0
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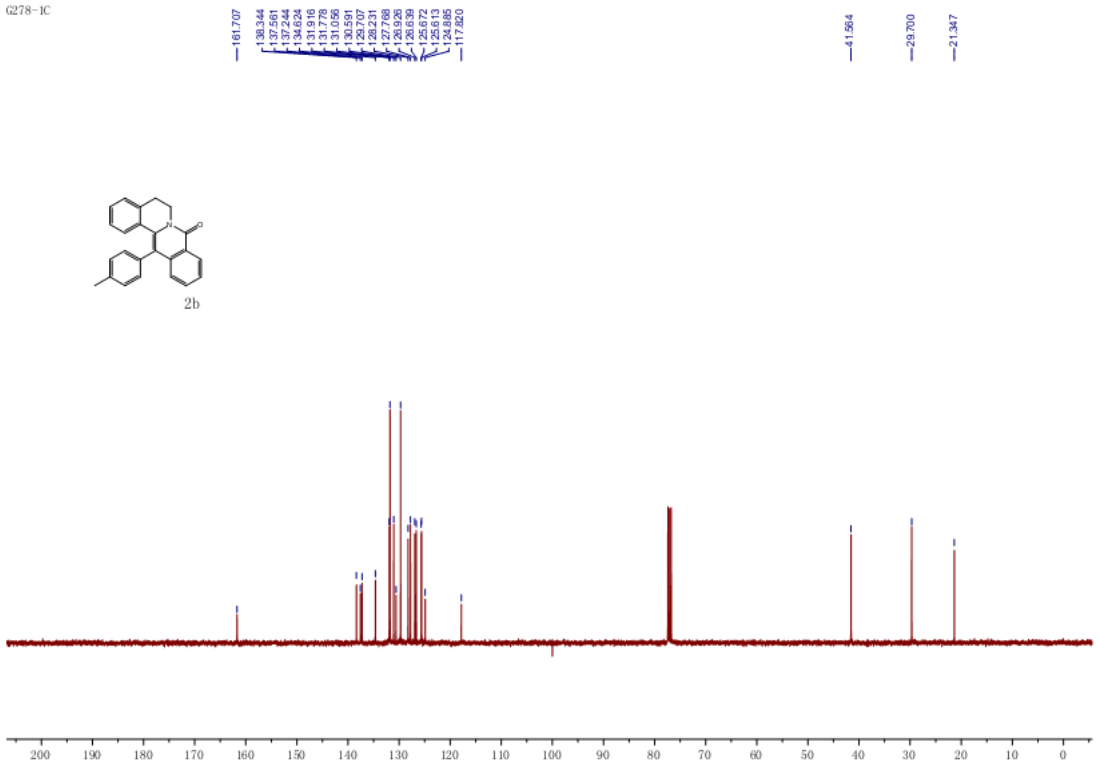
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127.768
126.926
126.359
125.672
125.613
124.885
117.820
41.564
29.700
21.347
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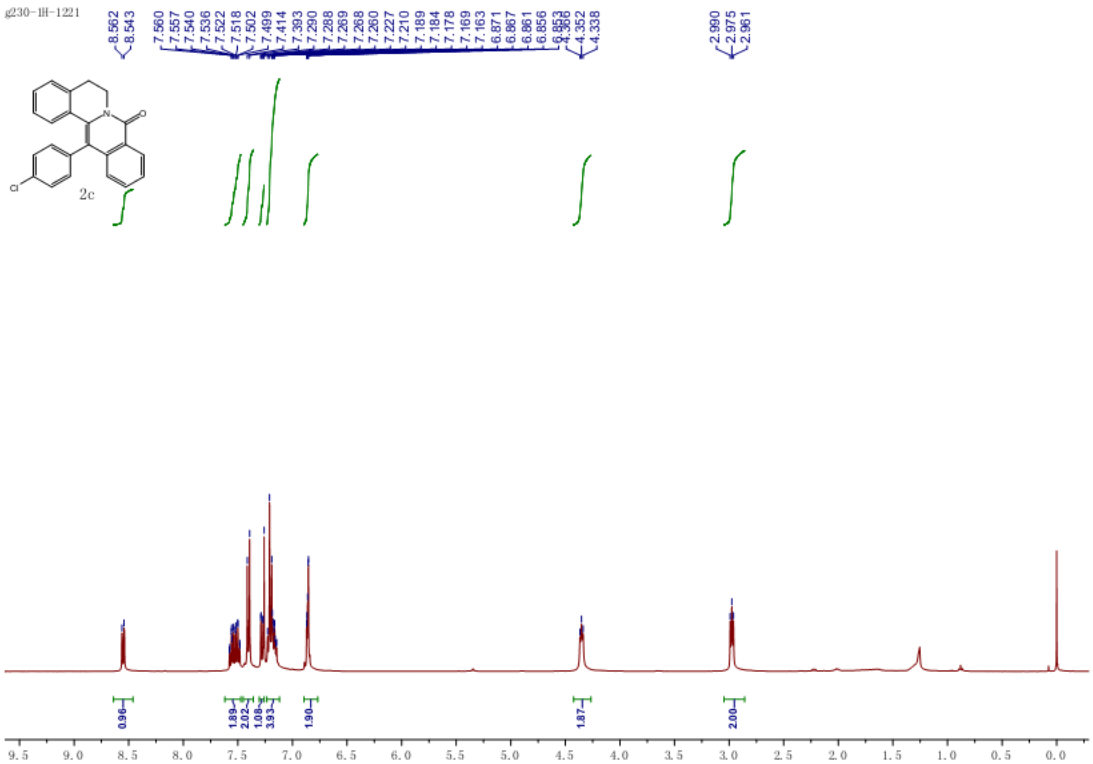
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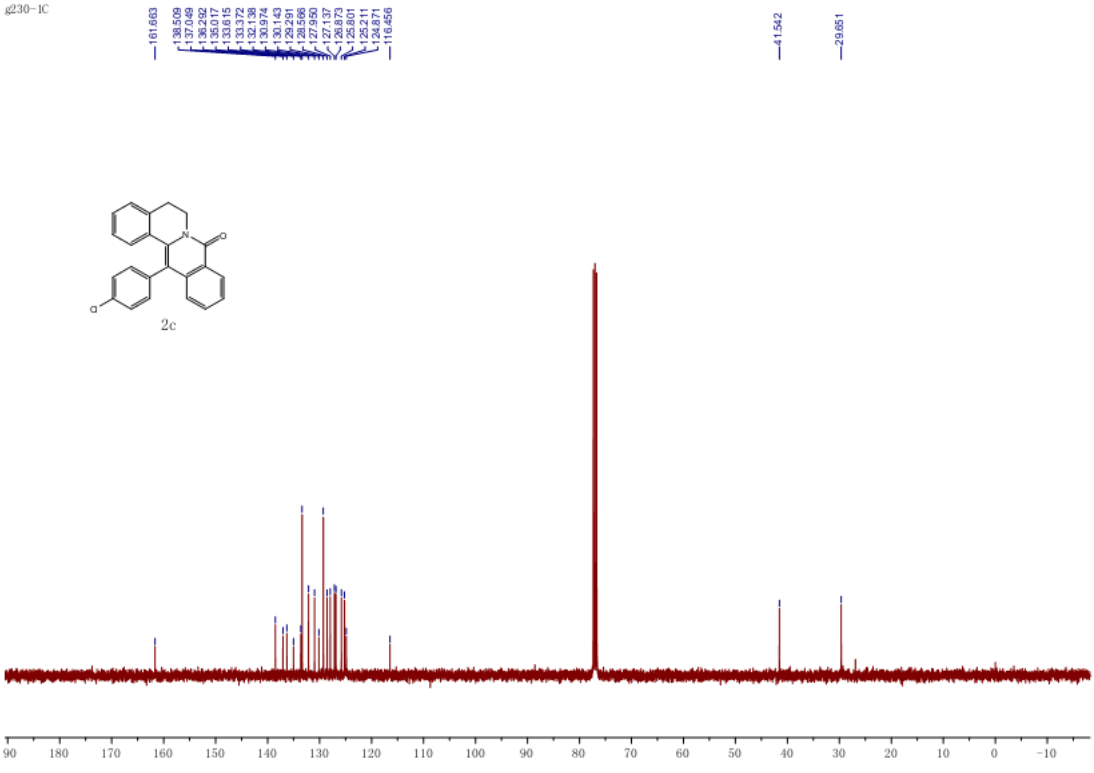
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29.651
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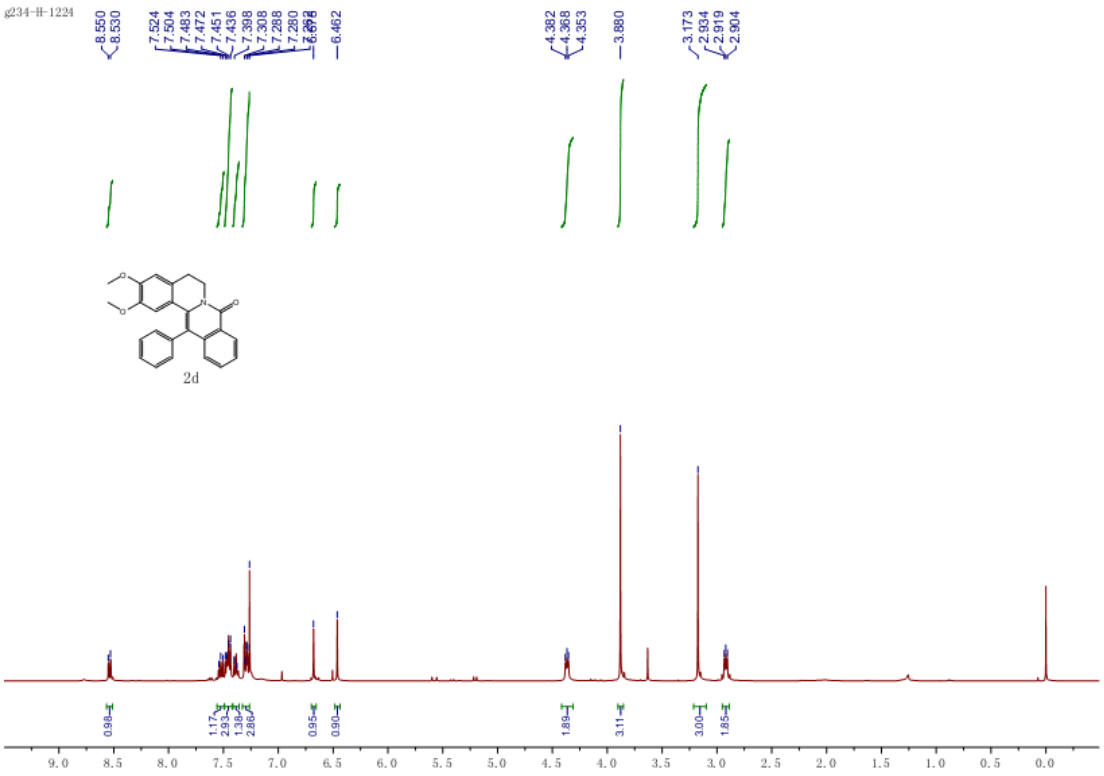
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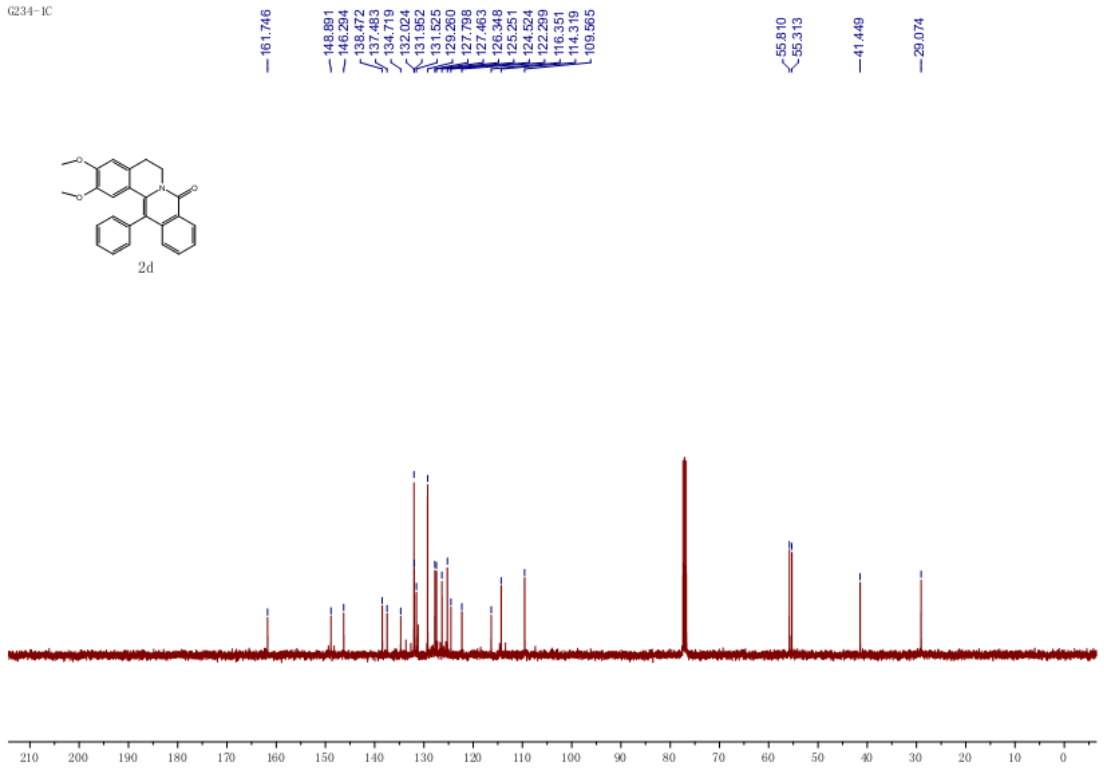
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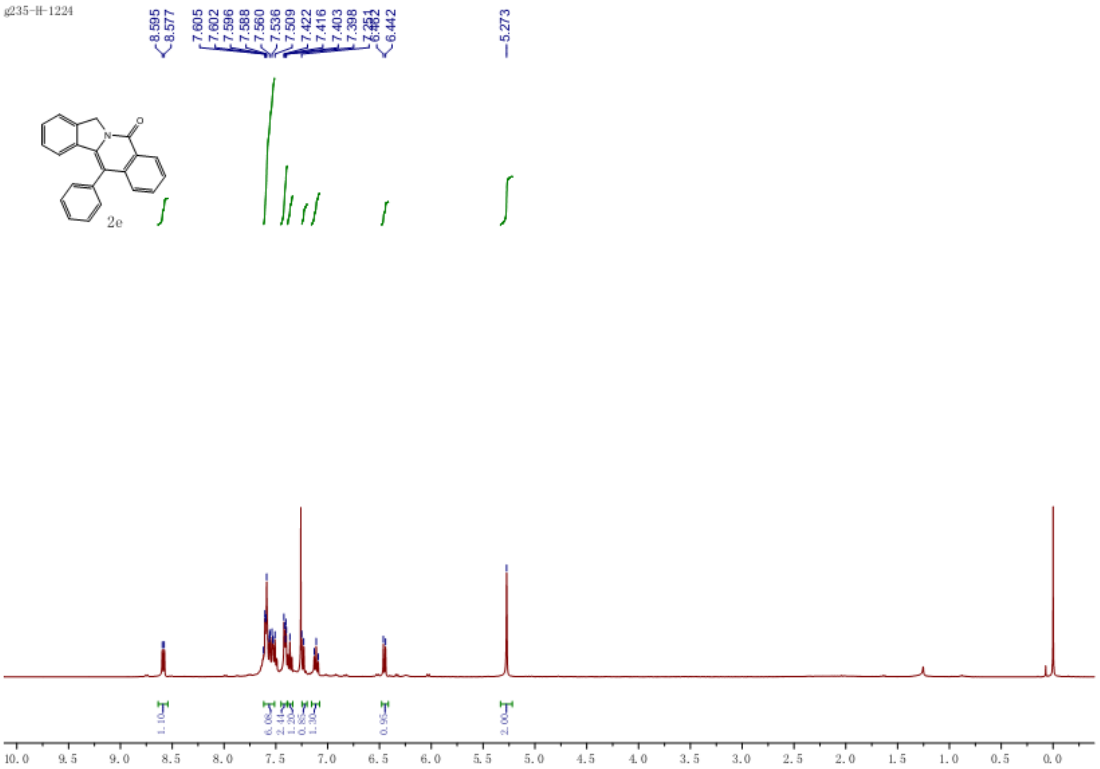
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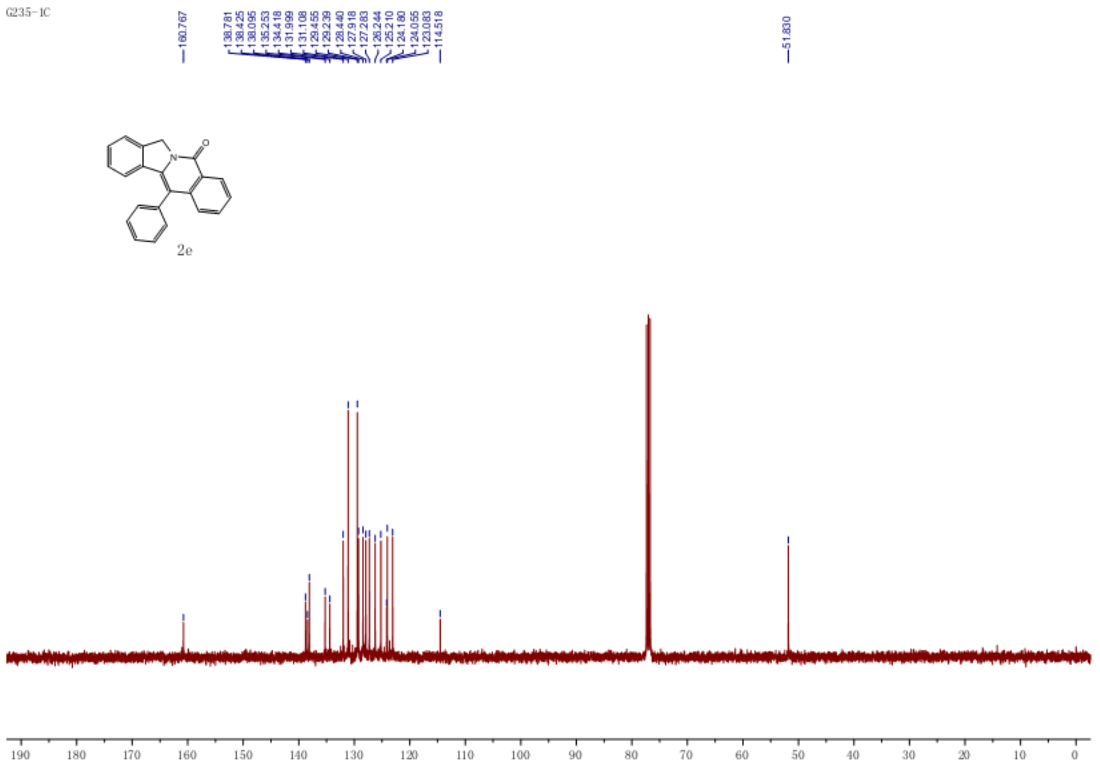
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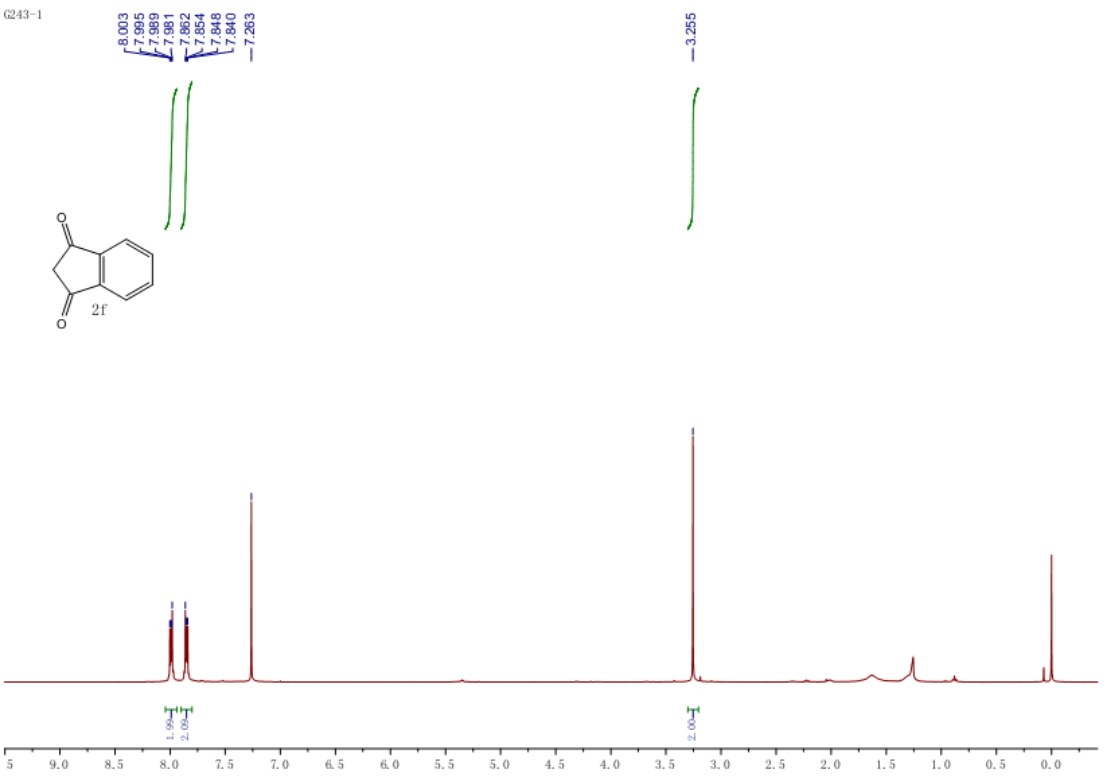
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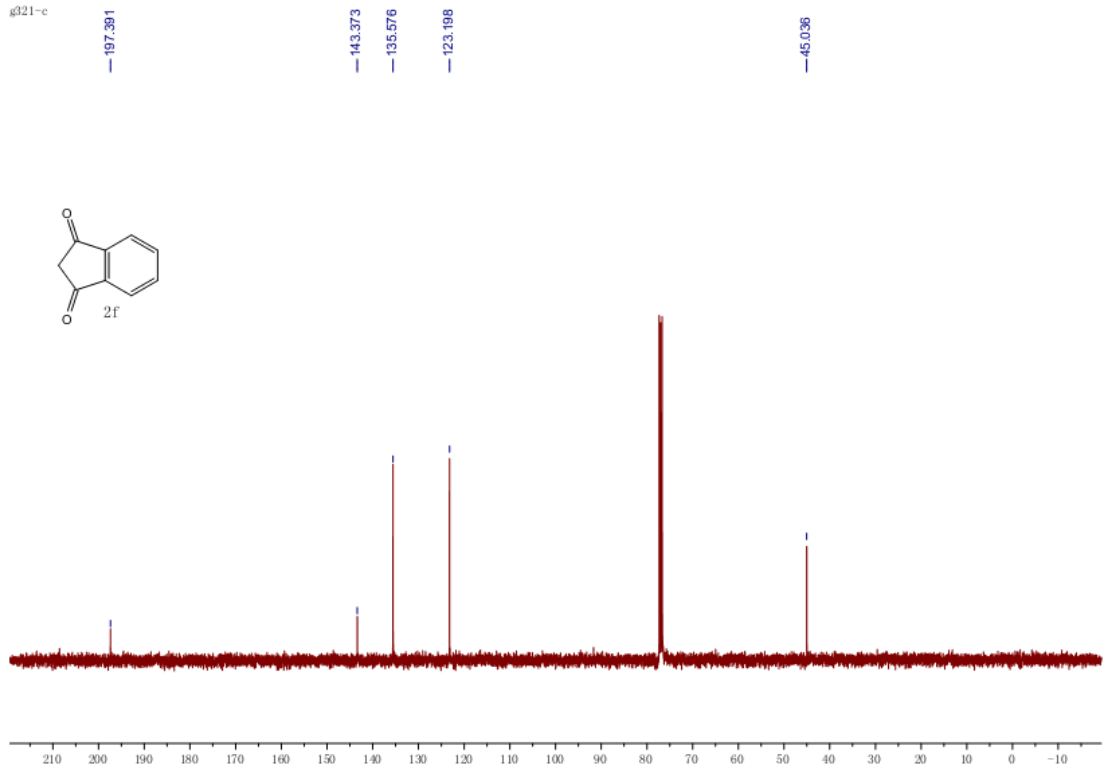
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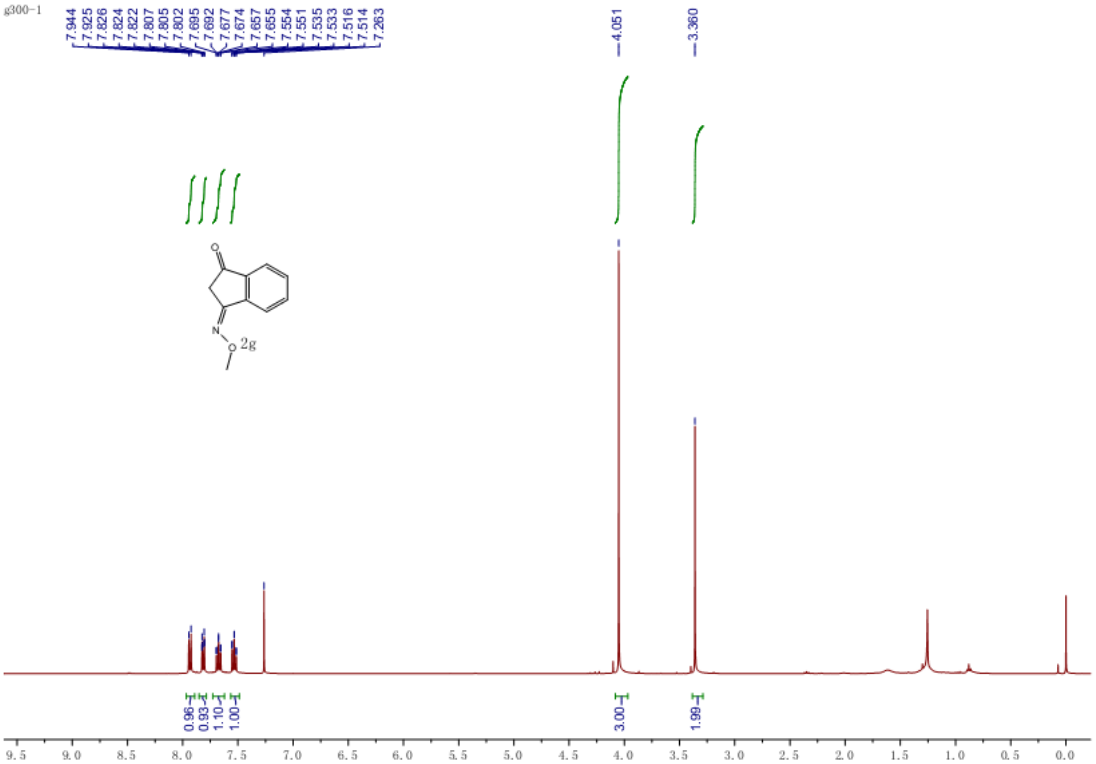
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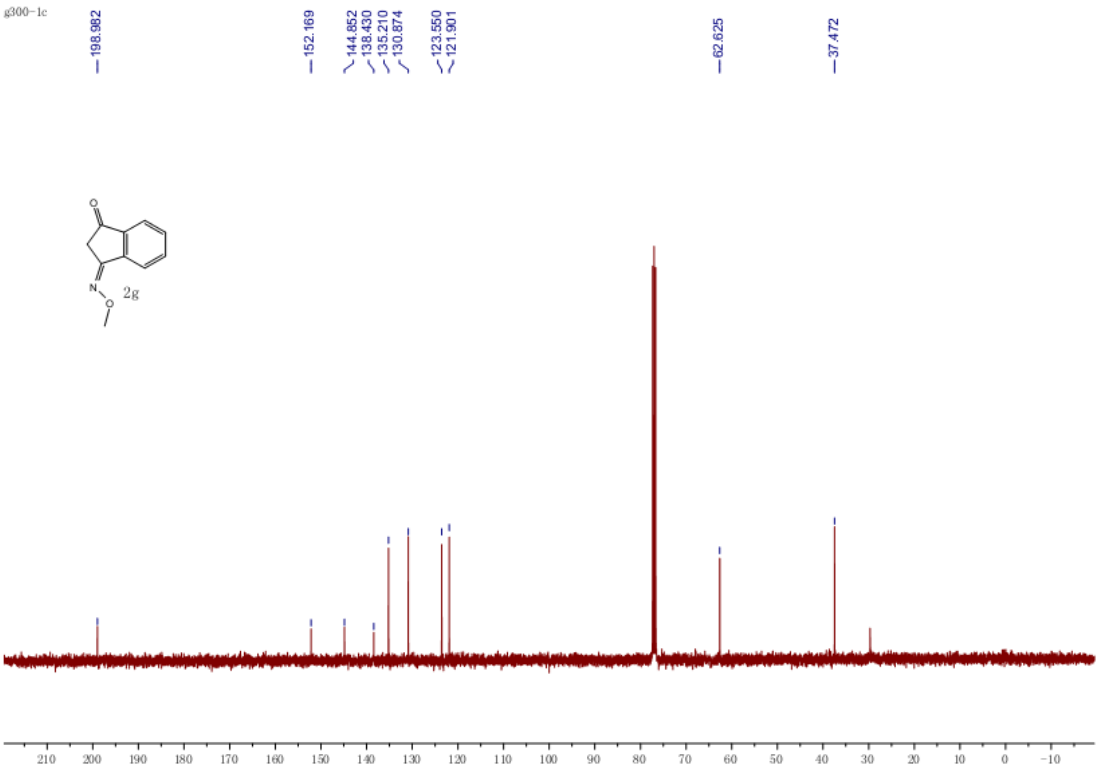
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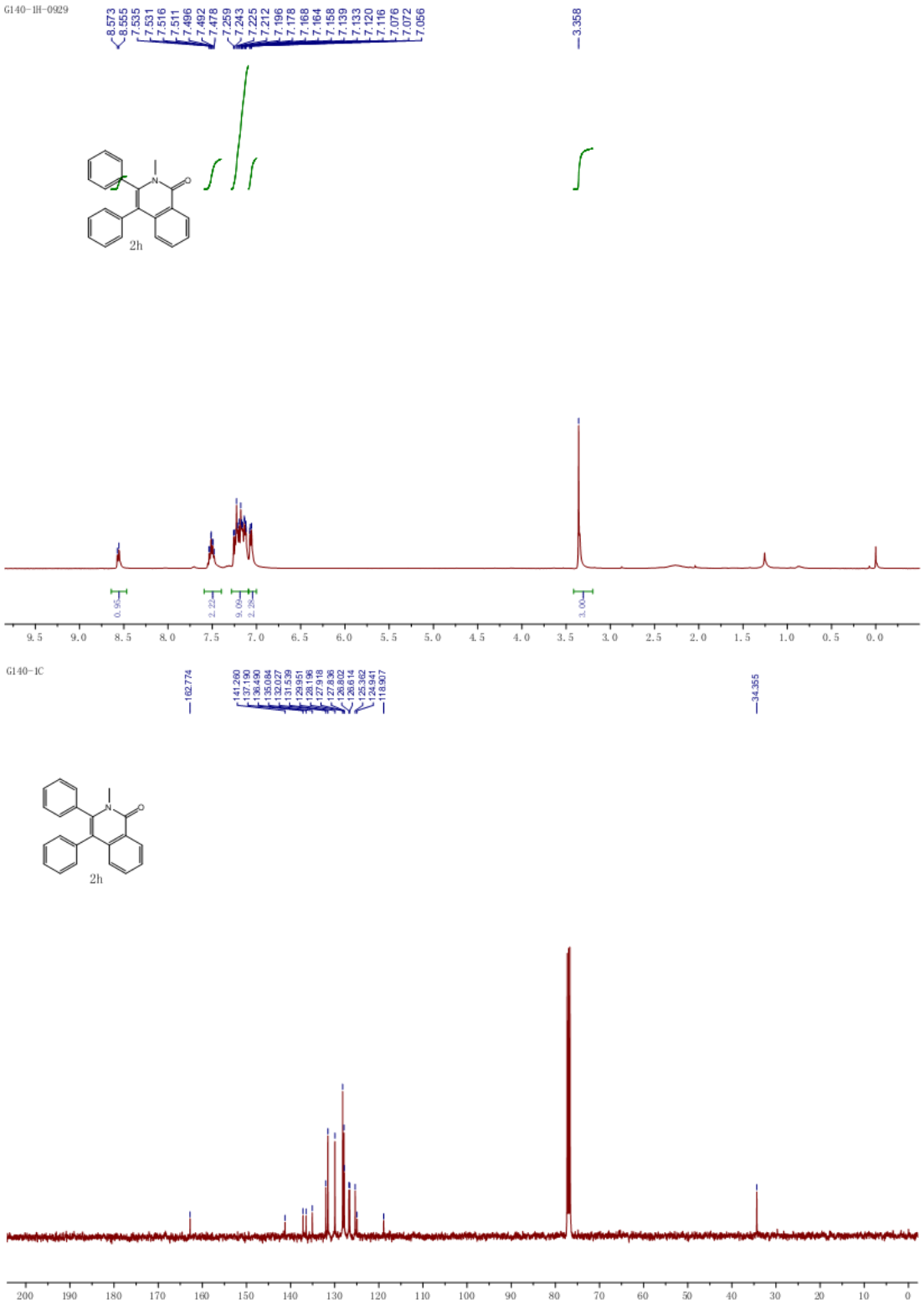
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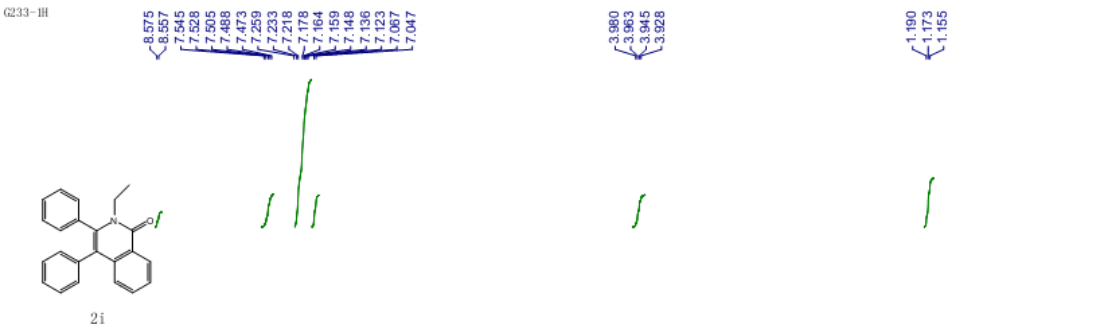
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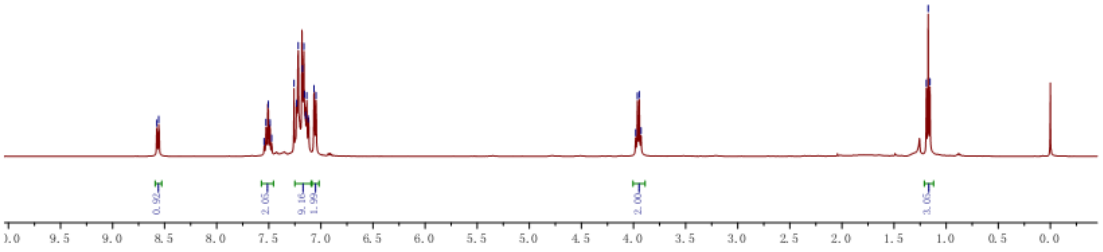
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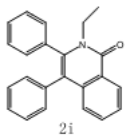

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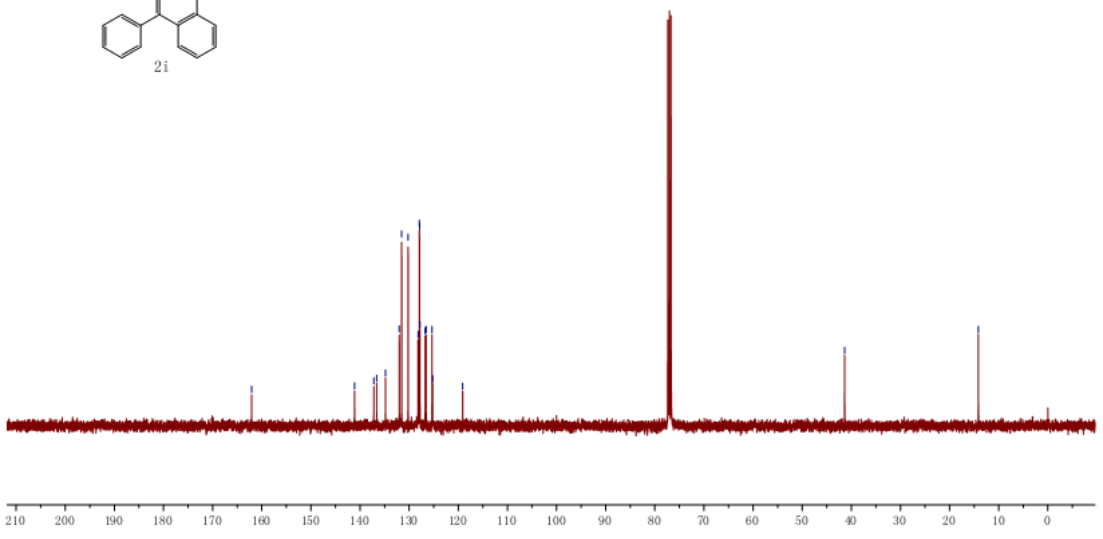

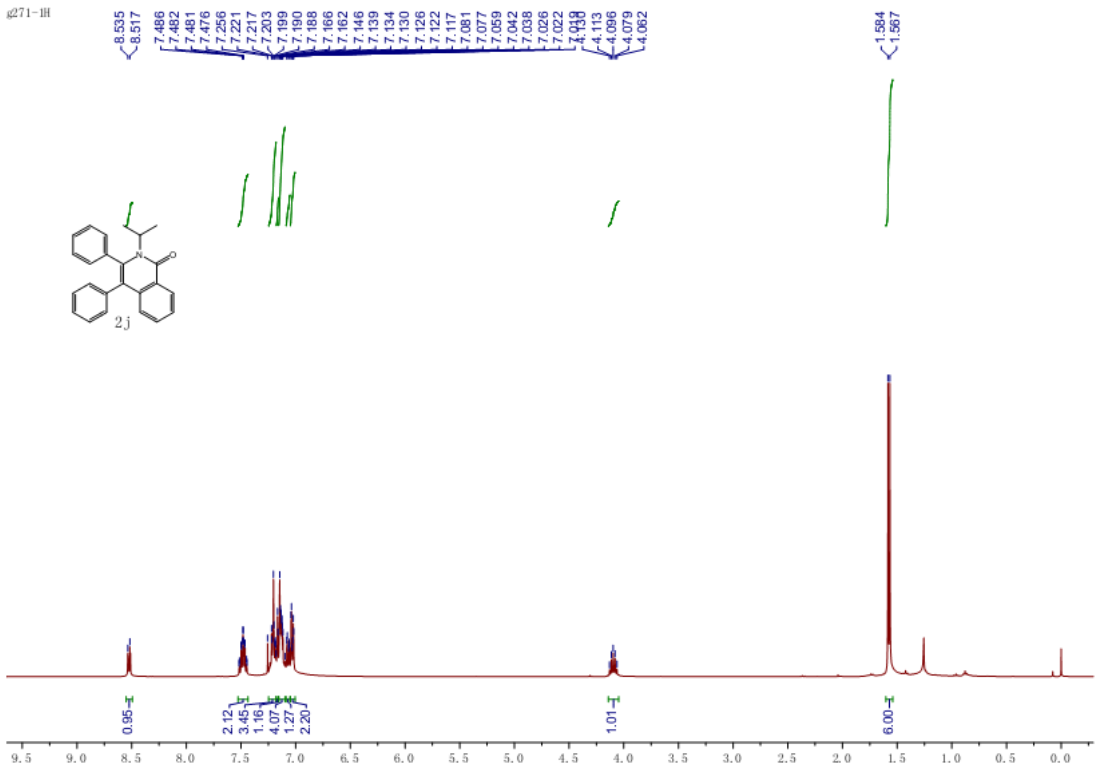
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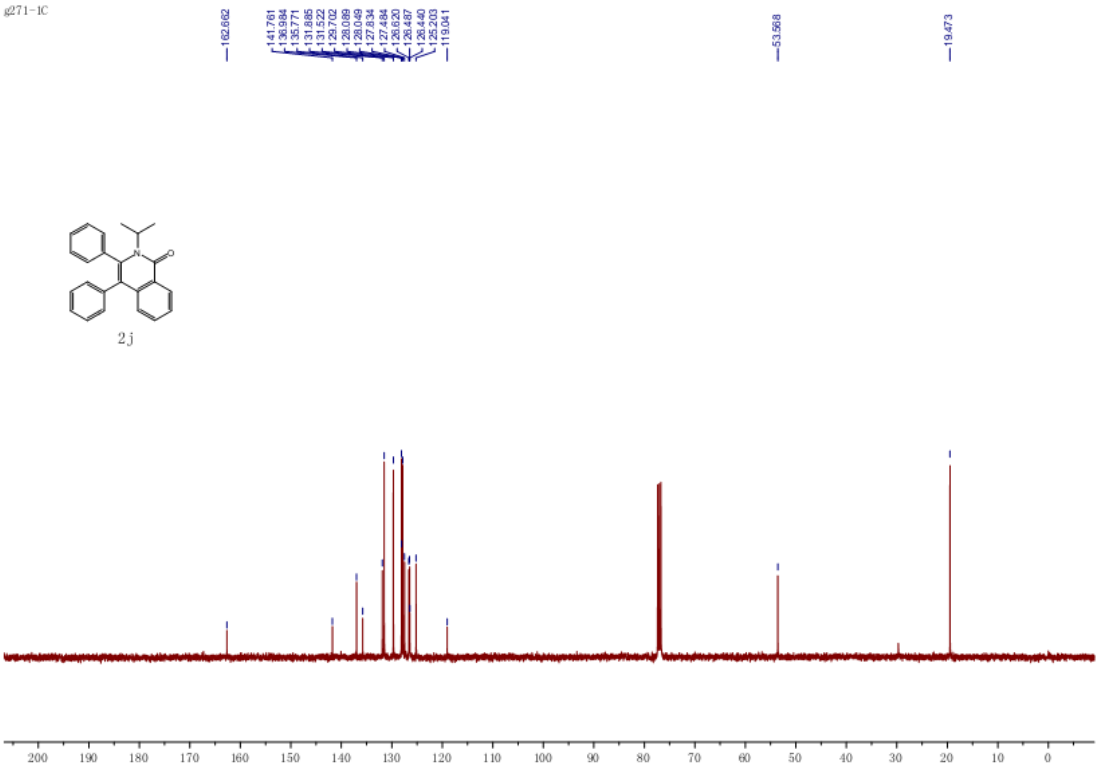
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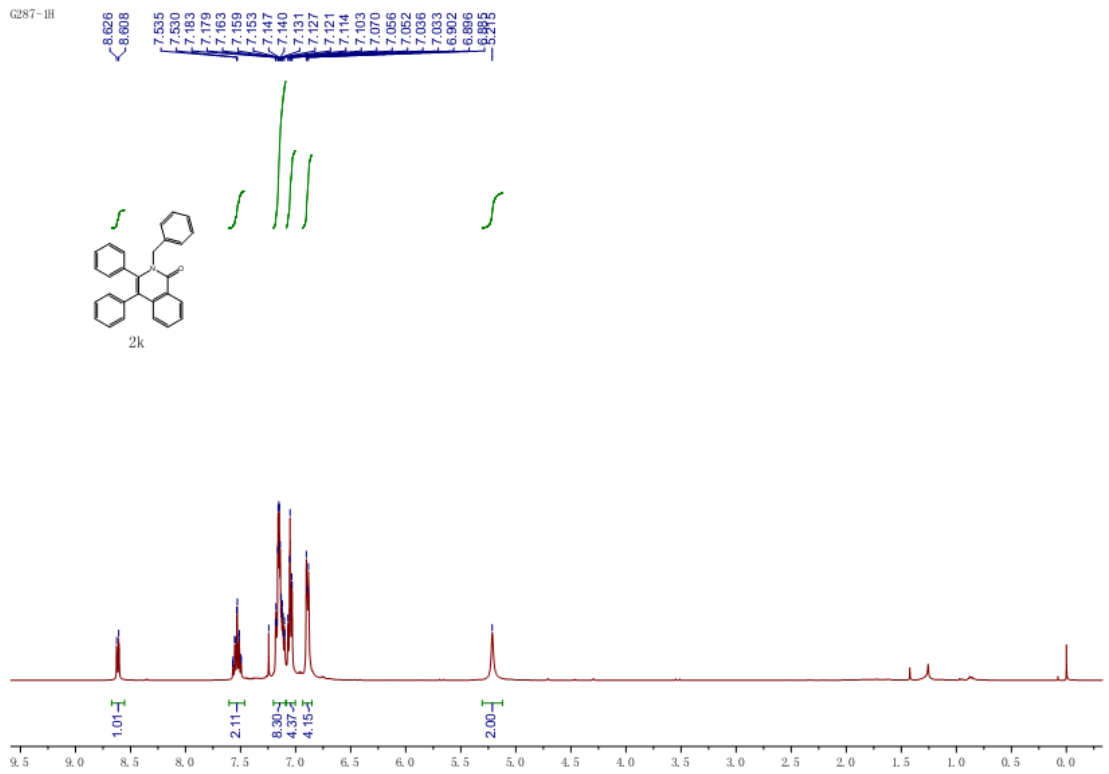
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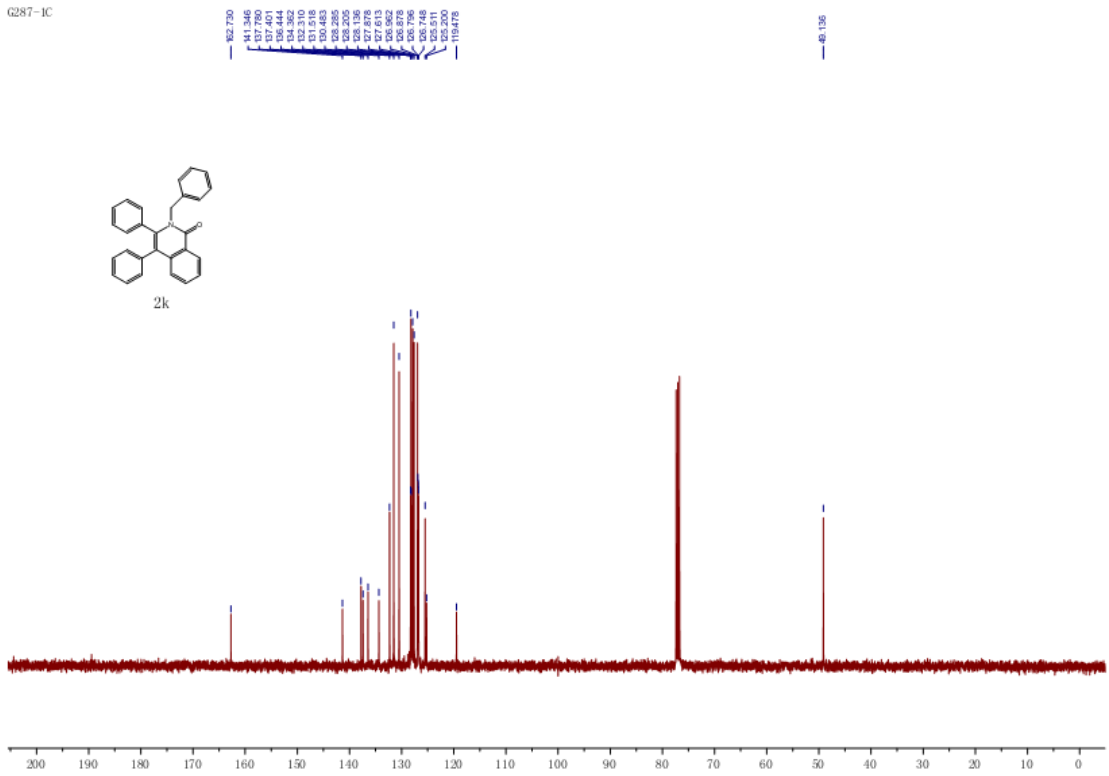
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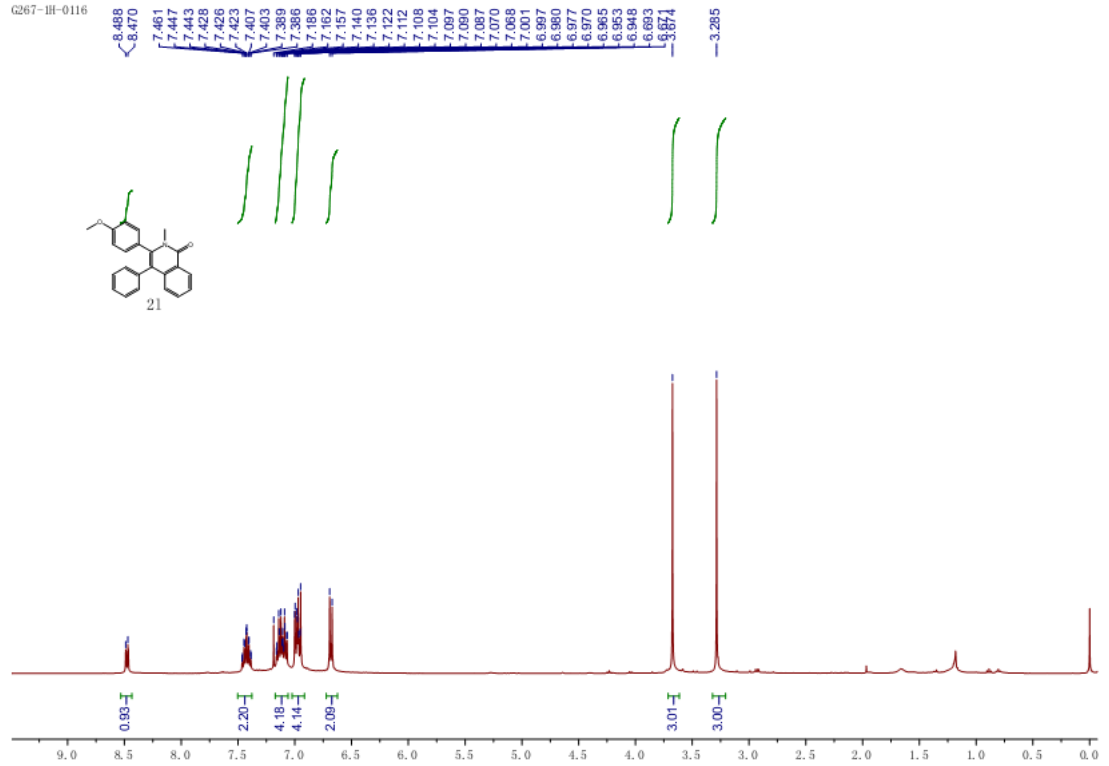
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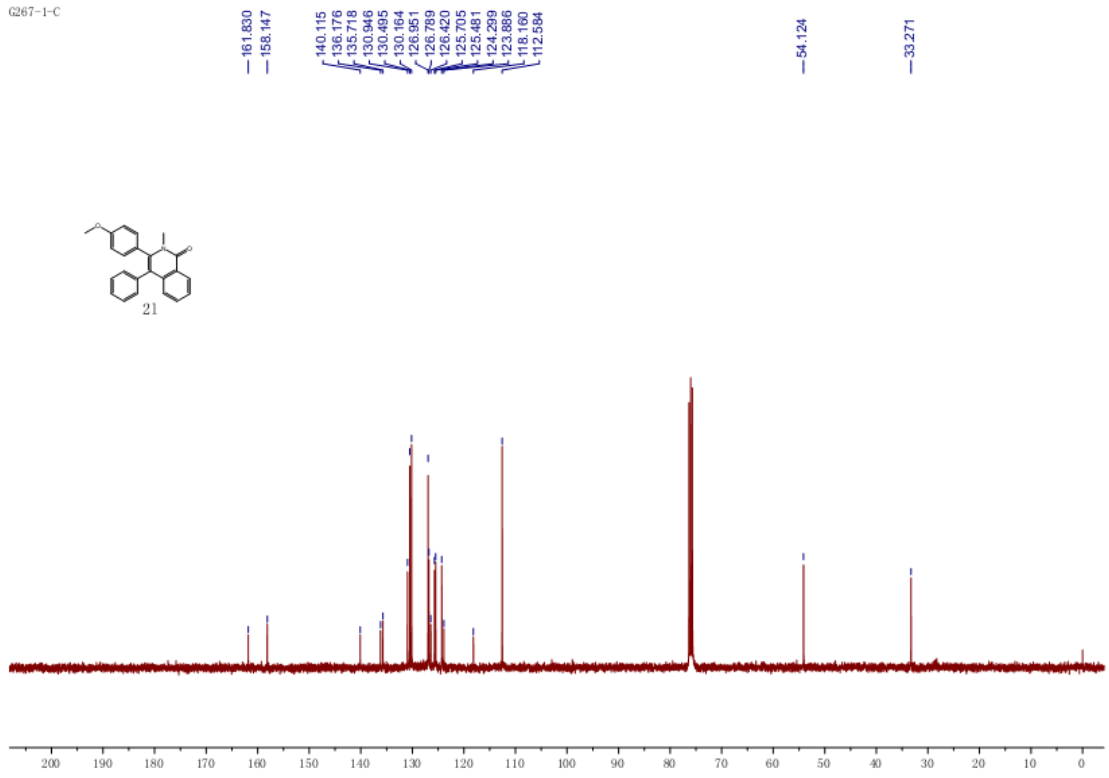
G267-1-C
161.830
158.147
140.115
136.176
135.718
130.946
130.495
130.164
126.951
126.789
126.420
125.705
125.481
124.299
123.886
118.160
112.584
54.124
33.271
21
200
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150
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110
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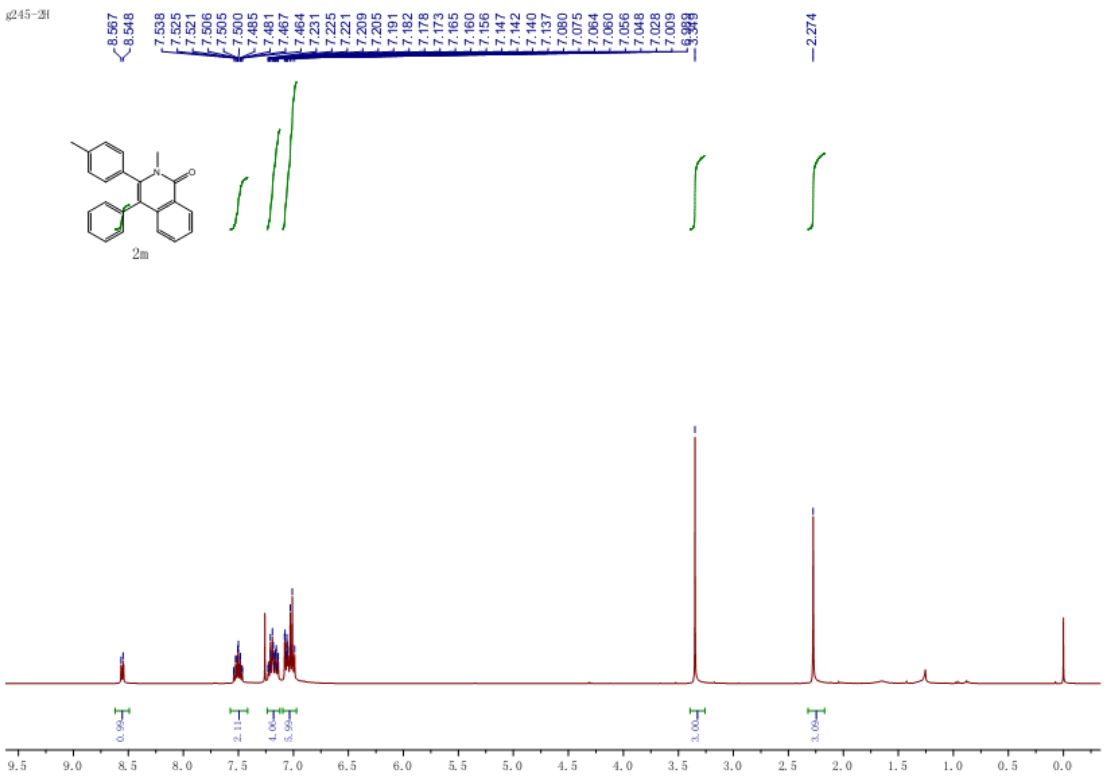
g245-2H
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8.548
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7.505
7.500
7.485
7.481
7.467
7.464
7.231
7.225
7.221
7.209
7.205
7.191
7.182
7.178
7.173
7.165
7.160
7.156
7.147
7.142
7.140
7.137
7.080
7.075
7.064
7.060
7.056
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7.028
7.009
3.349
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2m
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2.11
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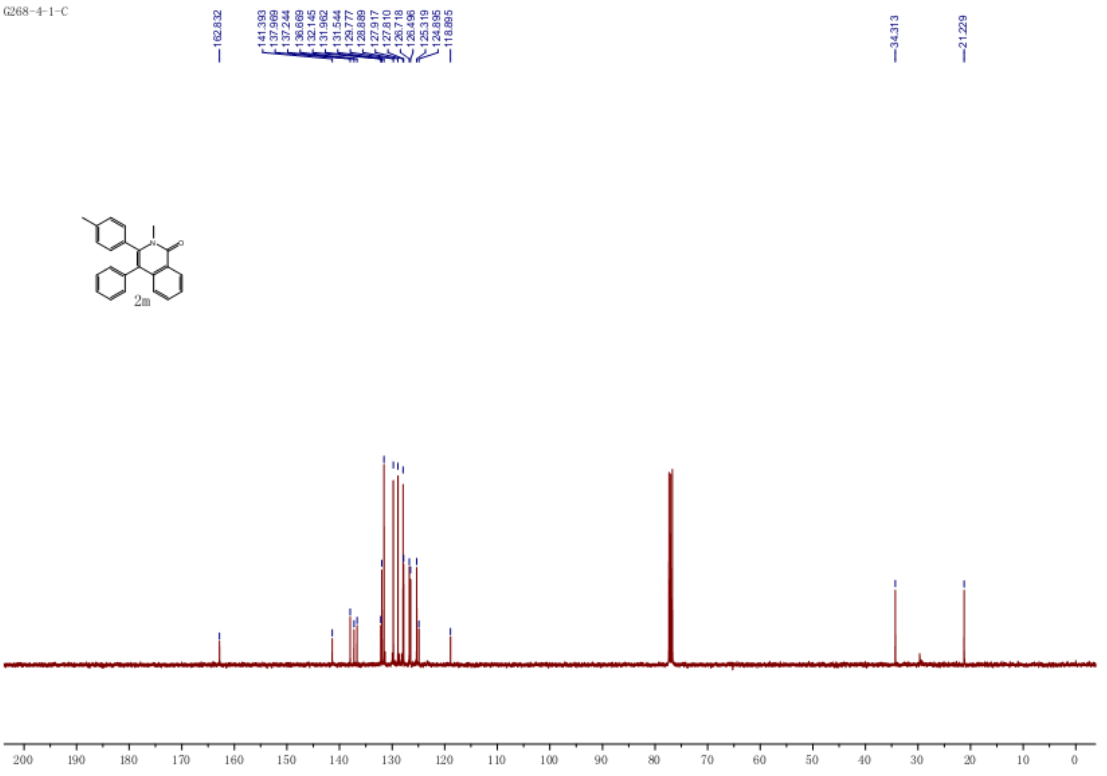
5.99
3.00
3.00


G268-4-1-C
162.832
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137.244
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129.777
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127.810
126.718
126.496
125.319
124.895
118.895
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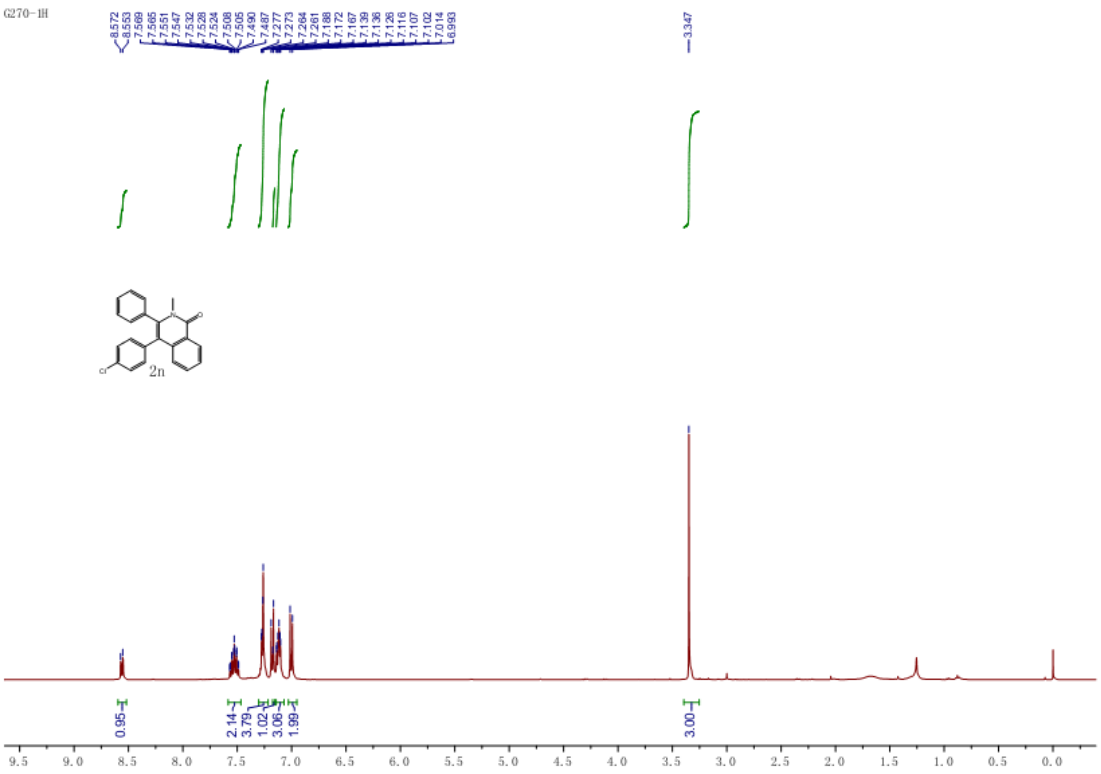
21.229
2m


G270-1H
8.572
8.553
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7.565
7.551
7.547
7.532
7.528
7.524
7.508
7.505
7.490
7.487
7.277
7.273
7.264
7.261
7.188
7.172
7.167
7.139
7.136
7.126
7.116
7.107
7.102
7.014
6.993
3.347
2n
0.95
2.14
3.79
1.02
3.06
1.99
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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2.0
1.5
1.0
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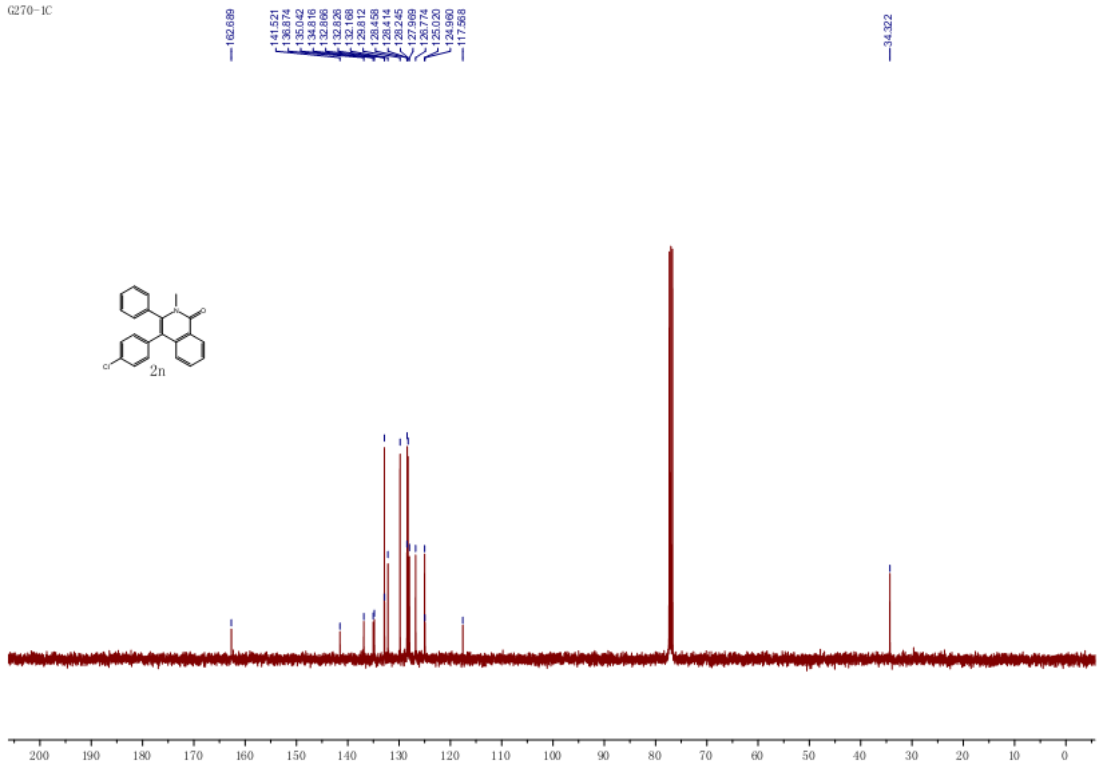
G270-1C
162.689
141.521
136.874
135.042
134.816
132.866
132.826
132.168
129.812
128.458
128.414
128.245
127.969
126.774
125.020
124.960
117.568
34.322
2n
200
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150
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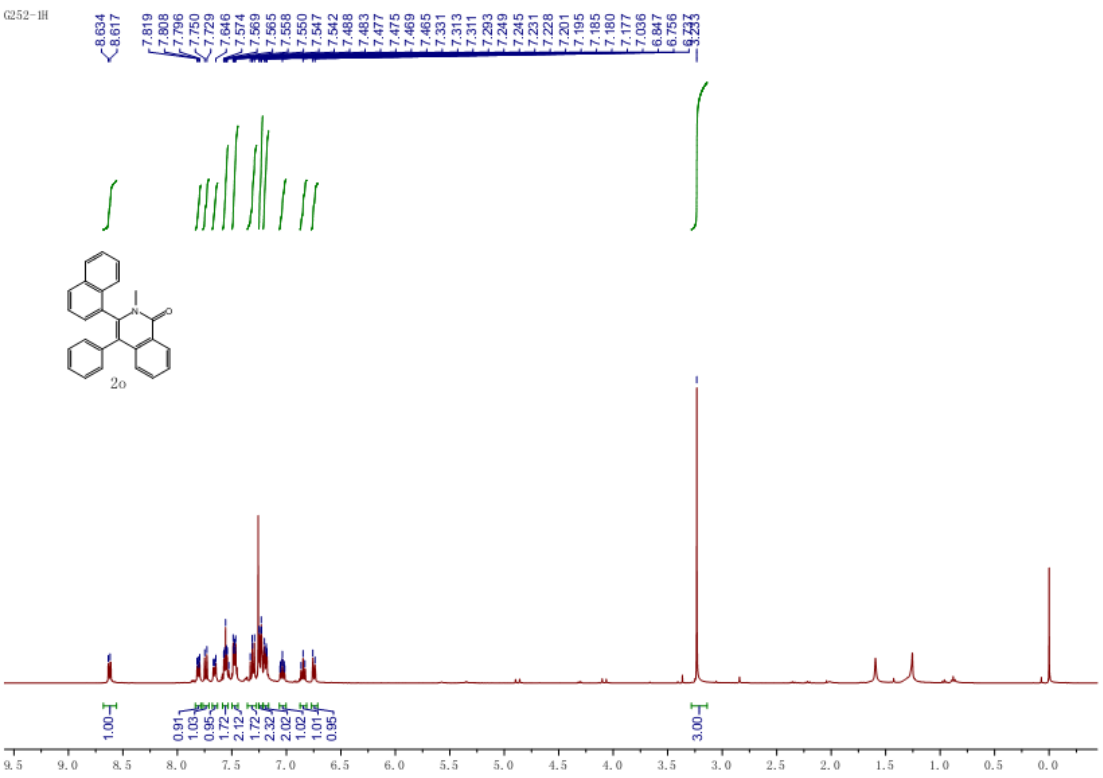
G252-1H
8.634
8.617
7.819
7.808
7.796
7.750
7.729
7.646
7.574
7.569
7.565
7.558
7.550
7.547
7.542
7.488
7.483
7.477
7.475
7.469
7.465
7.331
7.313
7.311
7.293
7.249
7.245
7.231
7.228
7.201
7.195
7.185
7.180
7.177
7.036
6.847
6.756
3.233
2o
1.00
0.91
1.03
0.95
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2.12
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2.02
1.02
1.01
0.95
3.00
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6.0
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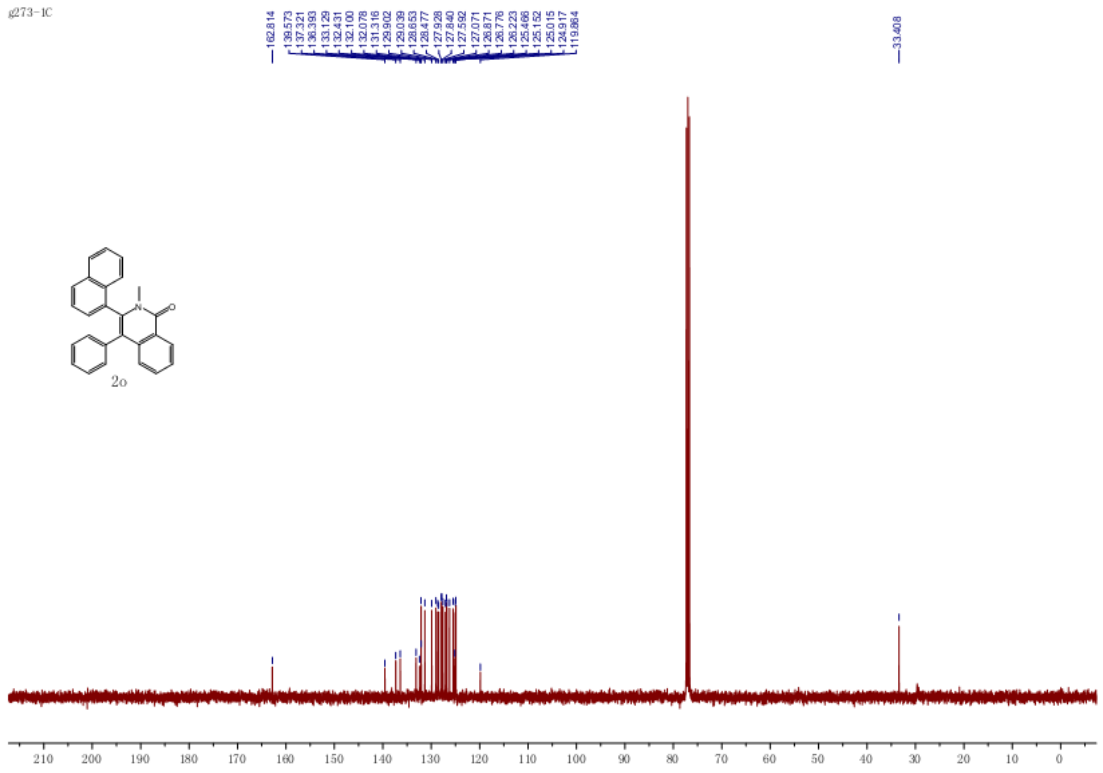
g273-1C
162.814
138.573
137.321
136.393
133.129
132.431
132.100
132.078
131.316
129.902
129.039
128.653
128.477
127.928
127.840
127.592
127.071
126.871
126.776
125.223
125.066
125.152
125.015
124.917
119.884
33.408
2o
210
200
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150
140
130
120
110
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70
60
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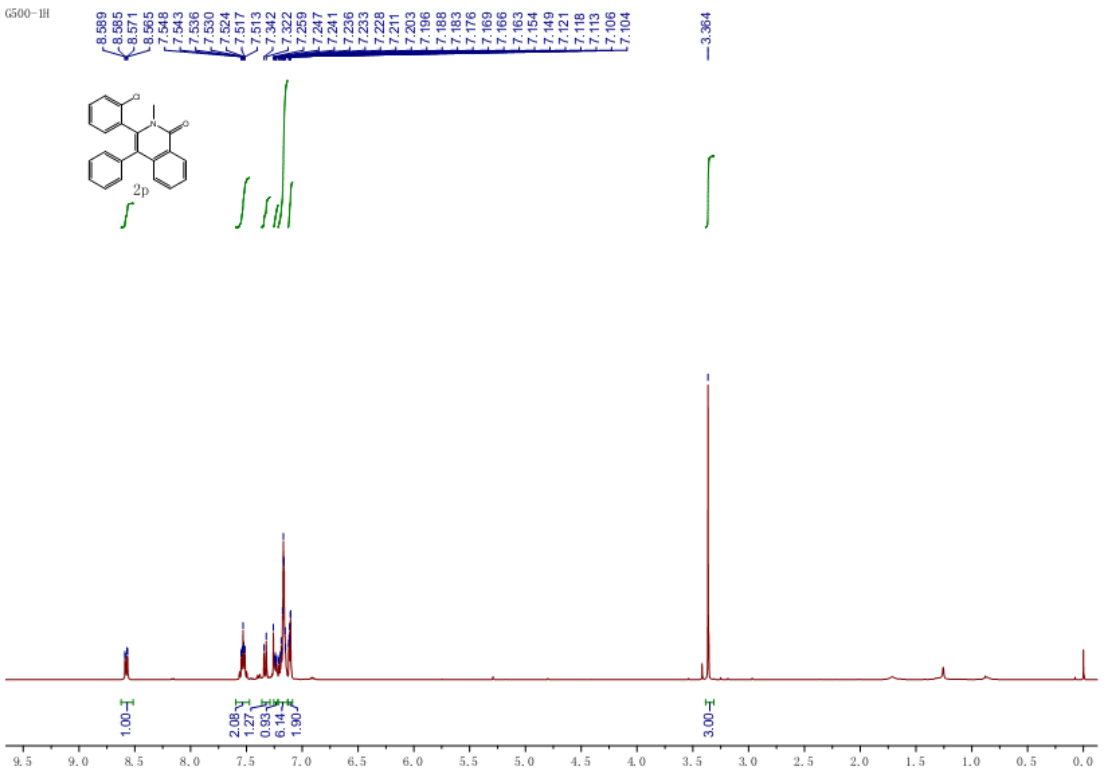
10
0


G500-1H
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8.585
8.571
8.565
7.548
7.543
7.536
7.530
7.524
7.517
7.513
7.342
7.322
7.259
7.247
7.241
7.236
7.233
7.228
7.211
7.203
7.196
7.188
7.183
7.176
7.169
7.166
7.163
7.154
7.149
7.121
7.118
7.113
7.106
7.104
3.364
2p
1.00
2.08
1.27
0.93
6.14
1.90
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
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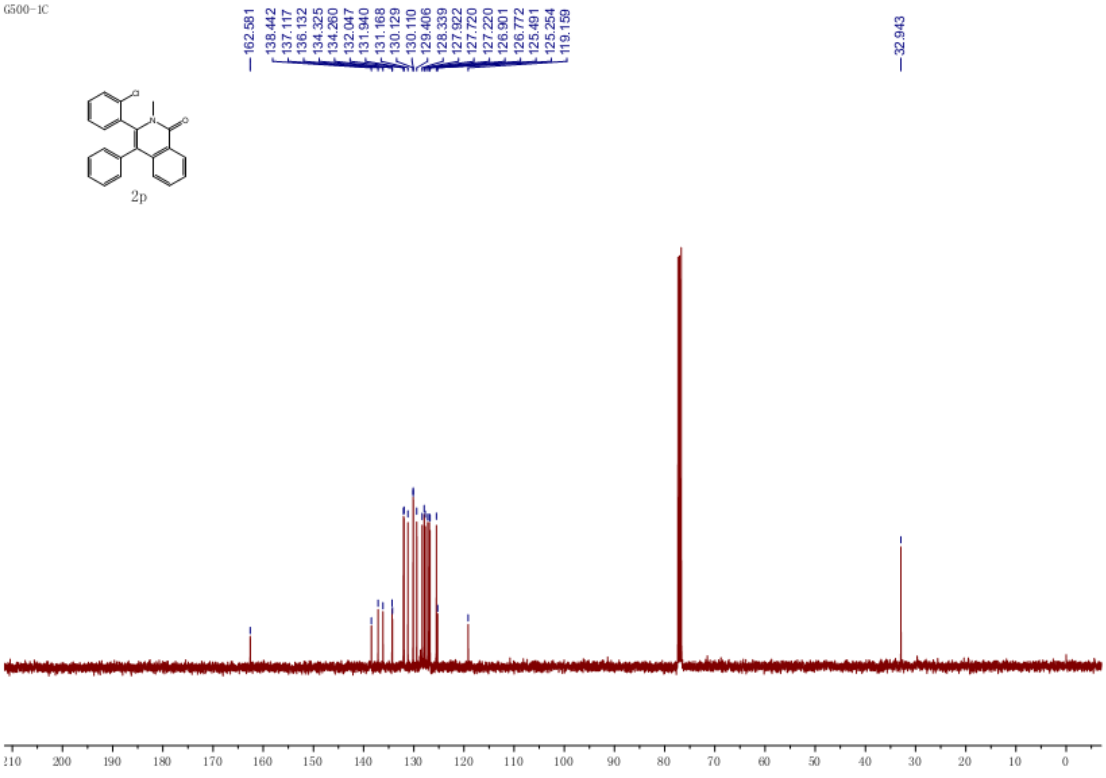
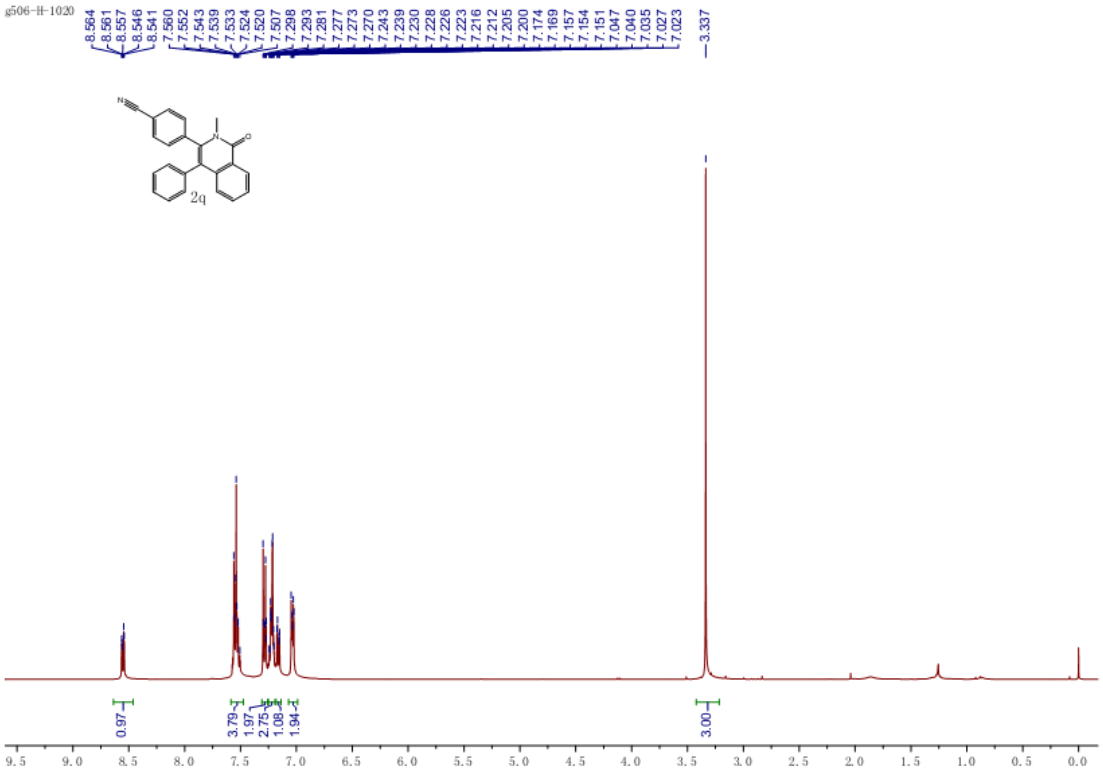
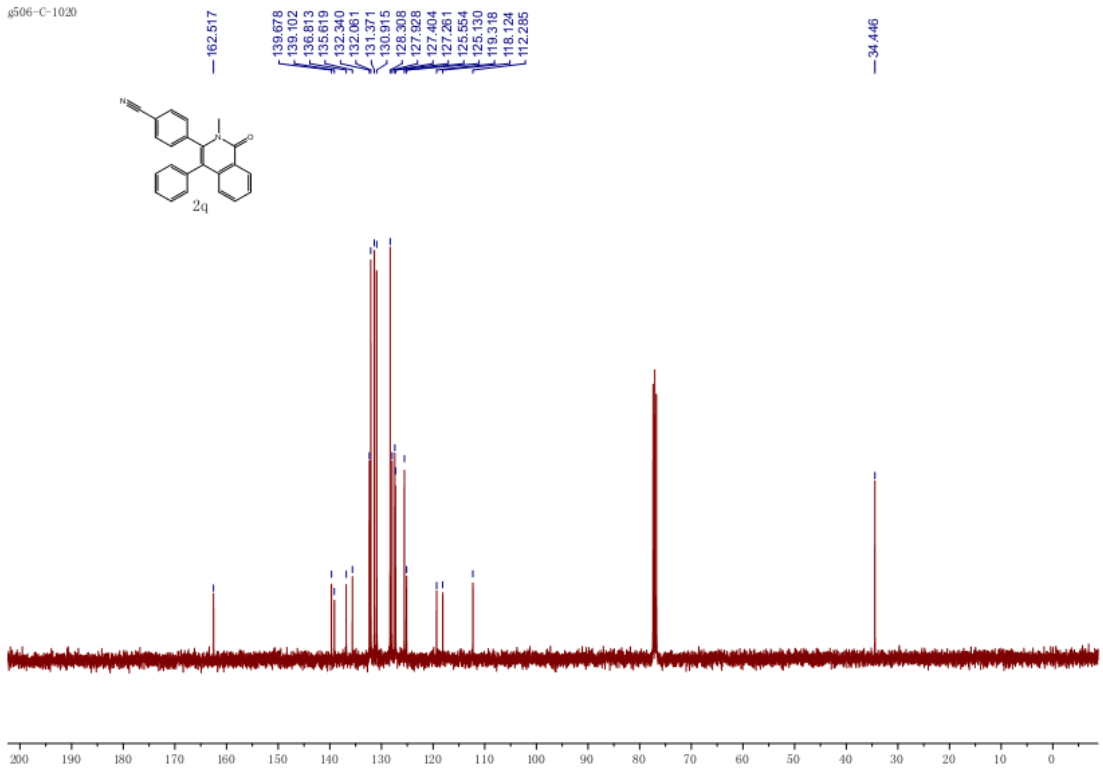
2.0
1.5
1.0
0.5
0.0


G500-1C
162.581
138.442
137.117
136.132
134.325
134.260
132.047
131.940
131.168
130.129
130.110
129.406
128.339
127.922
127.720
127.220
126.901
126.772
125.491
125.254
119.159
32.943
2p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


g506-H-1020
8.564
8.561
8.557
8.546
8.541
7.560
7.552
7.543
7.539
7.533
7.524
7.520
7.507
7.298
7.293
7.281
7.277
7.273
7.270
7.243
7.239
7.230
7.228
7.226
7.223
7.216
7.212
7.205
7.200
7.174
7.169
7.157
7.154
7.151
7.047
7.040
7.035
7.027
7.023
3.337
2q
0.97
3.79
1.97
2.75
1.08
1.94
3.00
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


g506-C-1020
162.517
139.678
139.102
136.813
135.619
132.340
132.061
131.371
130.915
128.308
127.928
127.404
127.261
125.554
125.130
119.318
118.124
112.285
34.446
2q
200
190
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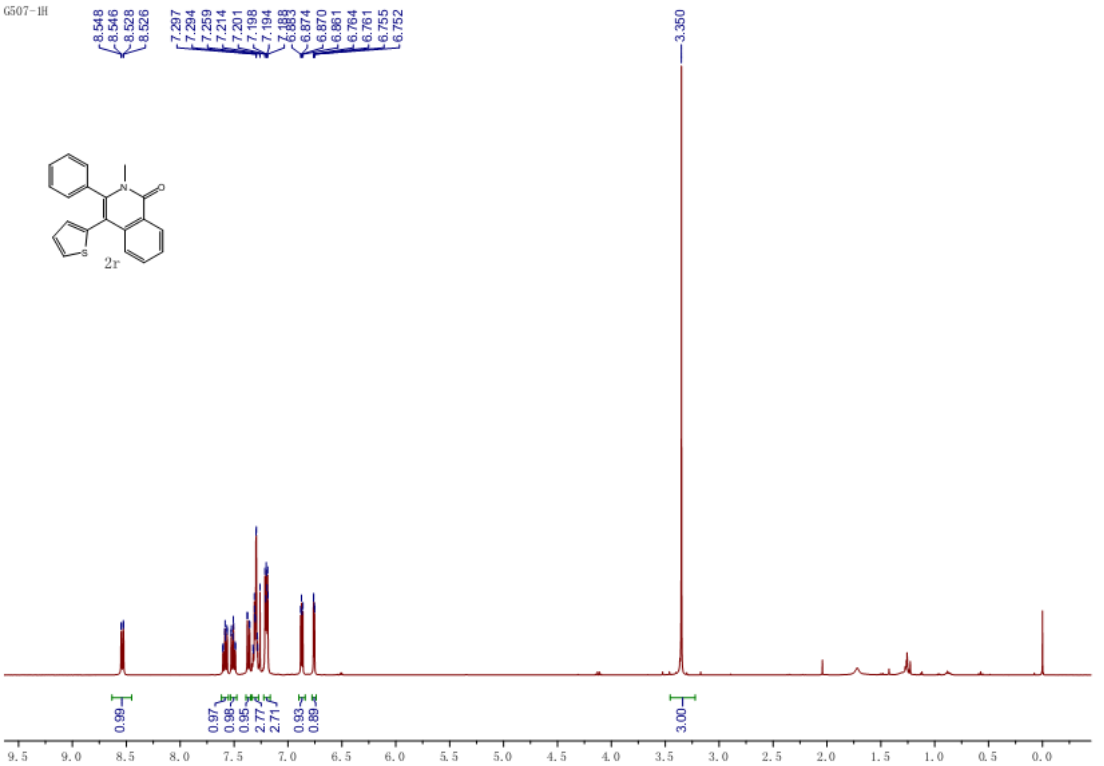
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


G507-1H
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8.528
8.526
7.297
7.294
7.259
7.214
7.201
7.198
7.194
6.883
6.874
6.870
6.861
6.764
6.761
6.755
6.752
3.350
2r
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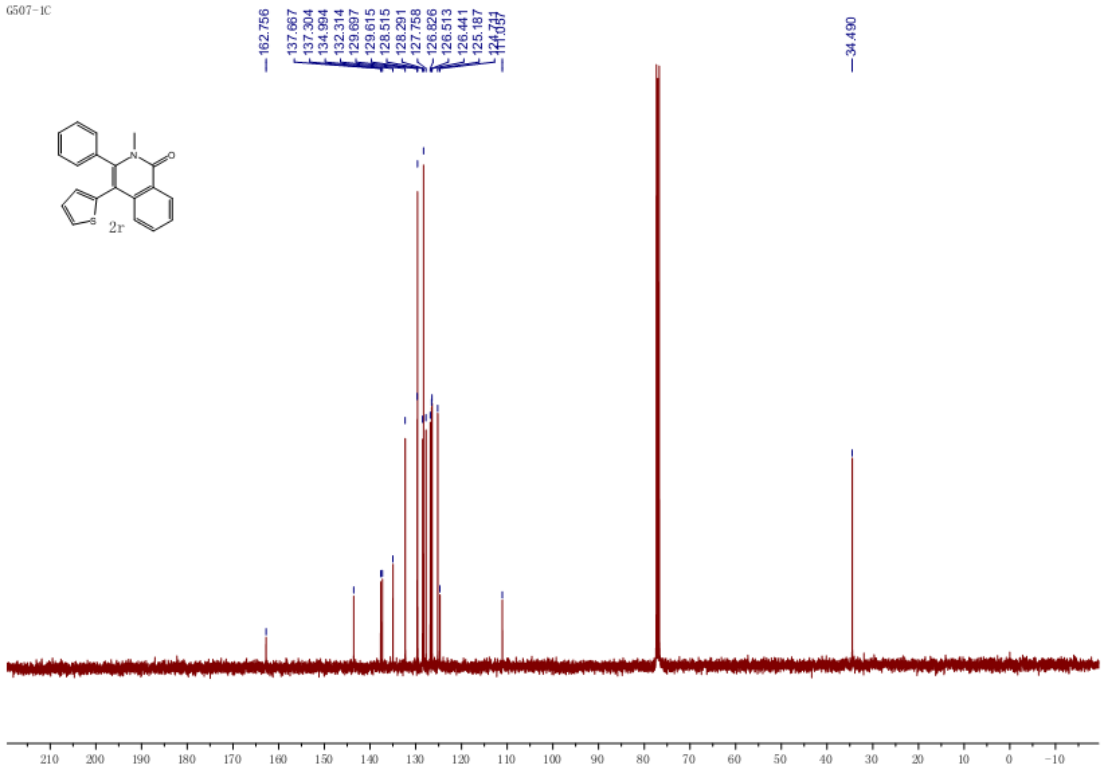
0.97
0.98
0.95
2.77
2.71
0.93
0.89
3.00


G507-1C
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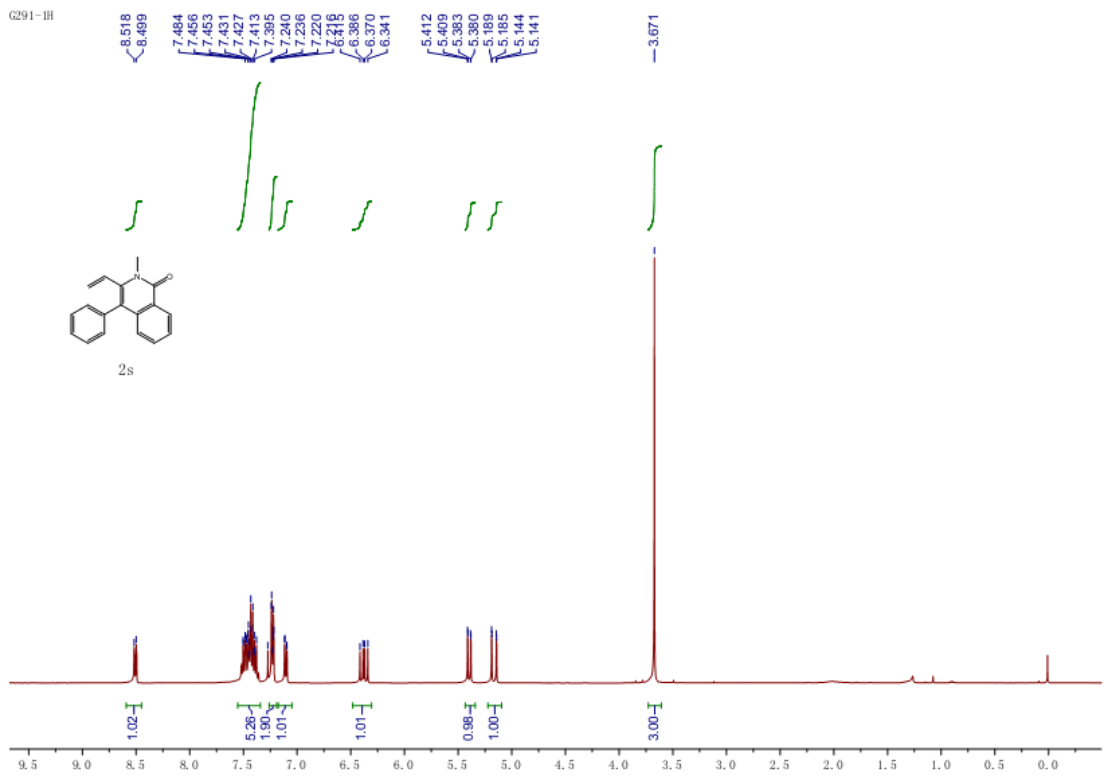
137.667
137.304
134.994
132.314
129.697
129.615
128.515
128.291
127.758
126.826
126.513
126.441
125.187
34.490
2r


G291-1H
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8.499
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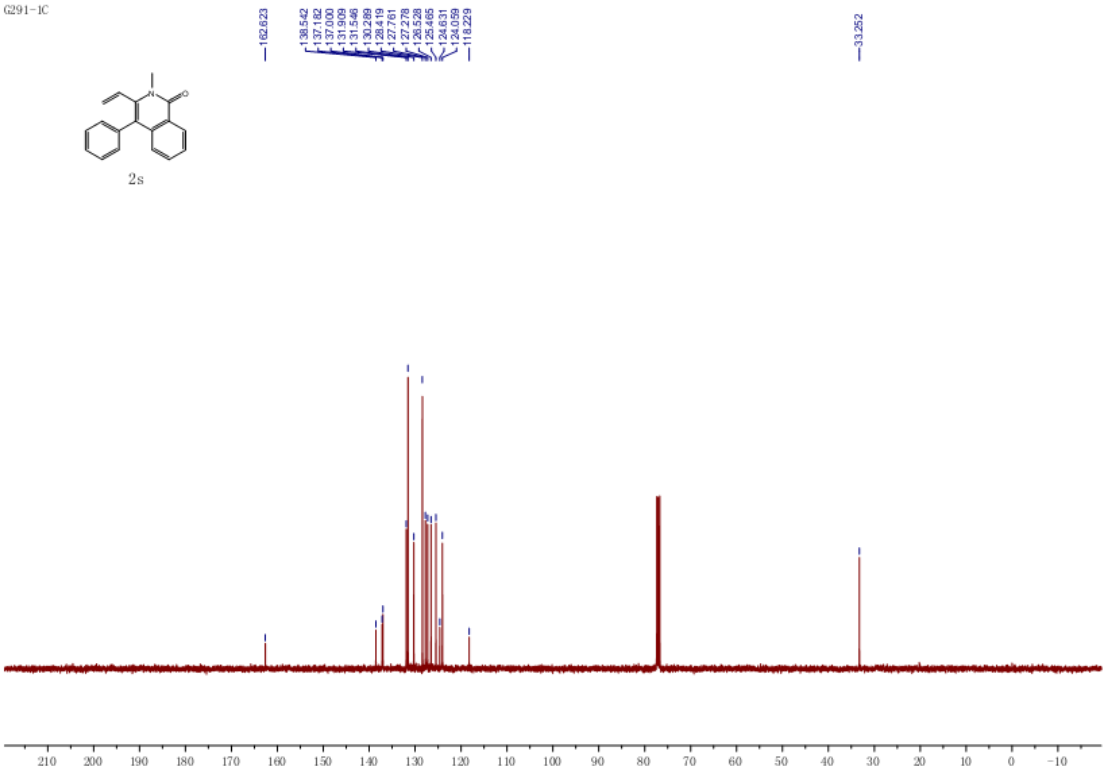
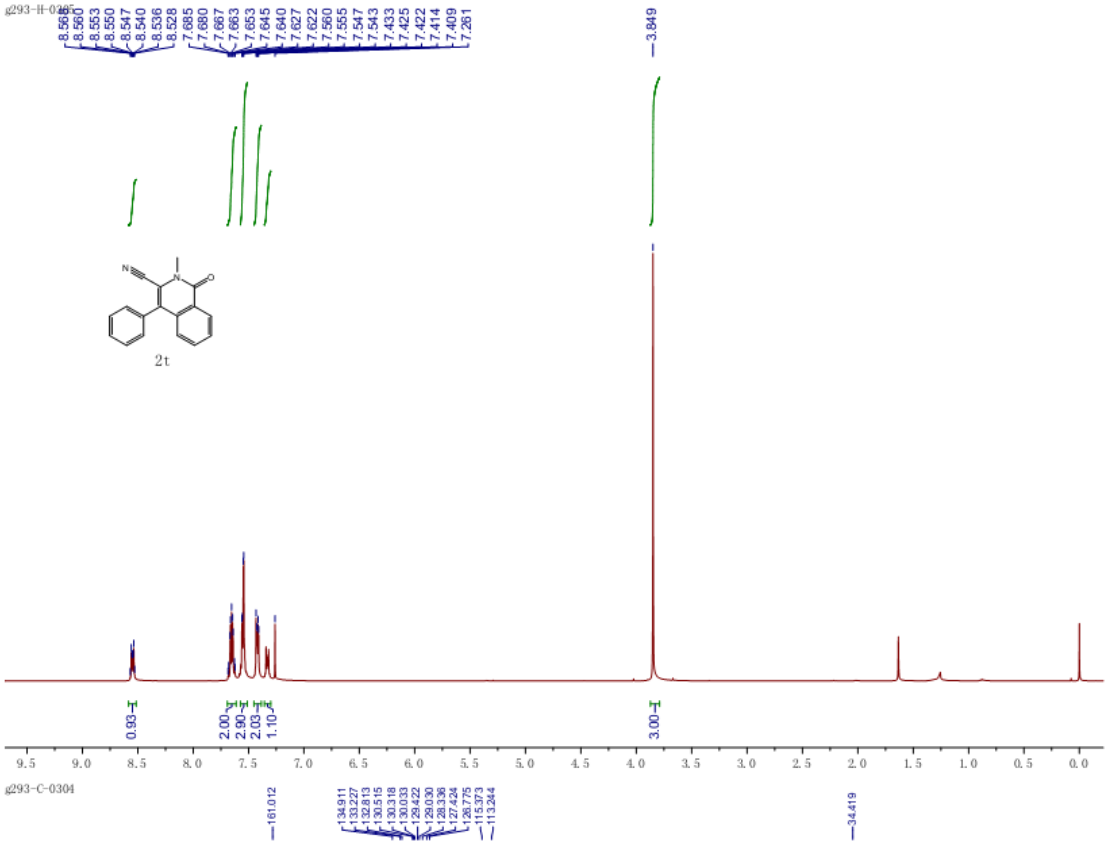
7.456
7.453
7.431
7.427
7.413
7.395
7.240
7.236
7.220
6.386
6.370
6.341
5.412
5.409
5.383
5.380
5.189
5.185
5.144
5.141
3.671
1.02
5.26
1.90
1.01
1.01
0.98
1.00
3.00
2s


G291-1C
162.623
138.542
137.182
137.000
131.909
131.546
130.289
128.419
127.761
127.278
126.528
125.465
124.631
124.059
118.229
33.252
2s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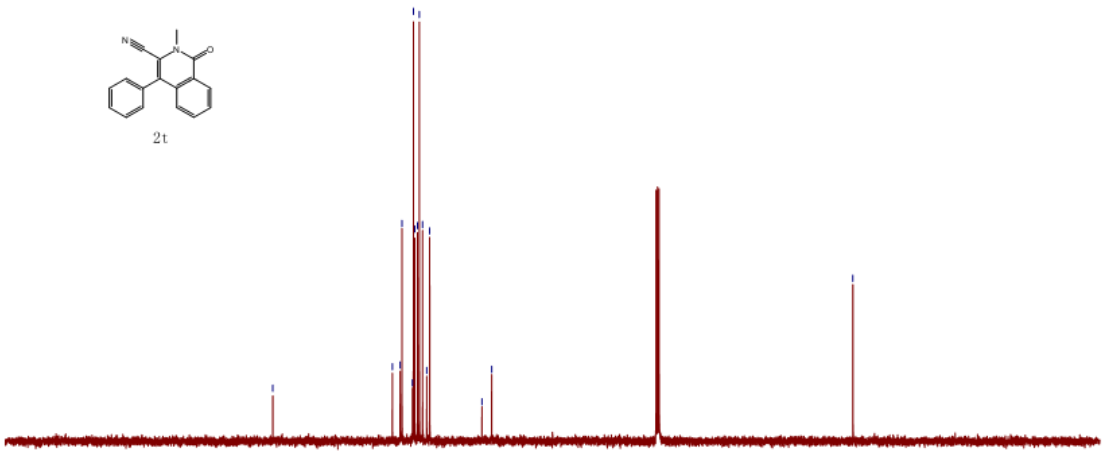
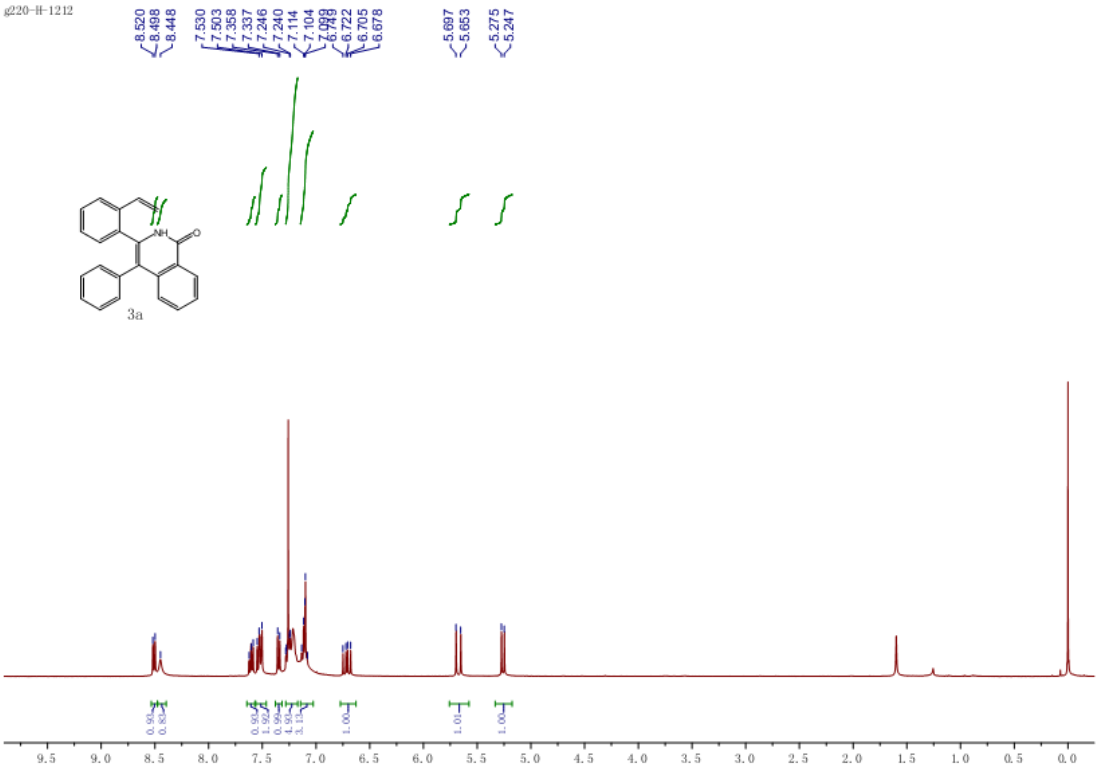
8.536
8.528
7.685
7.680
7.667
7.663
7.653
7.645
7.640
7.627
7.622
7.560
7.555
7.547
7.543
7.433
7.425
7.422
7.414
7.409
7.261
3.849
2t
0.93
2.00
2.90
2.03
1.10
3.00

g293-C-0304
161.012
134.911
133.227
132.813
130.515
130.318
130.033
129.922
129.030
128.336
127.424
126.775
115.373
113.244
34.419


2t


g220-H-1212
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7.114
7.104
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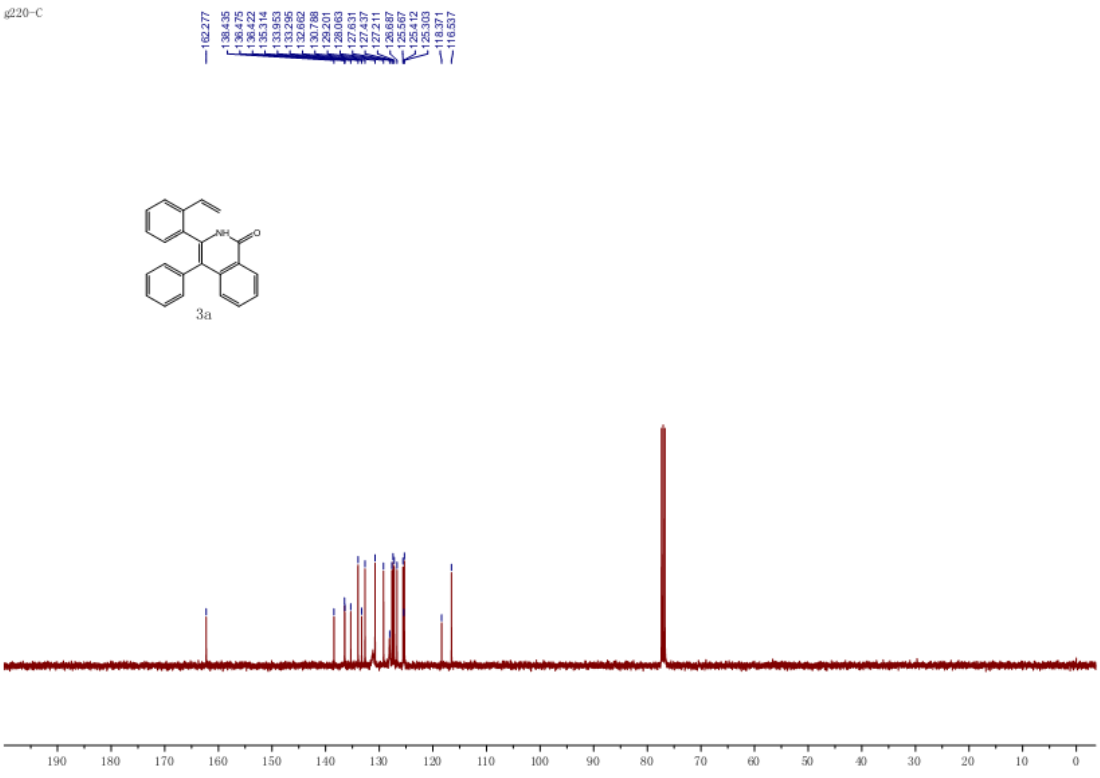
6.705
6.678
5.697
5.653
5.275
5.247
3a


g220-C
162.277
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136.422
135.314
133.953
133.295
132.662
130.788
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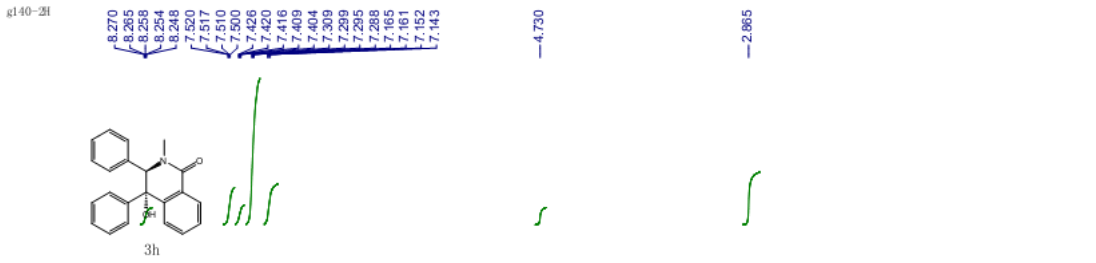
128.063
127.631
127.437
127.211
126.687
125.567
125.412
125.303
114.371
110.537
3a


g140-2H
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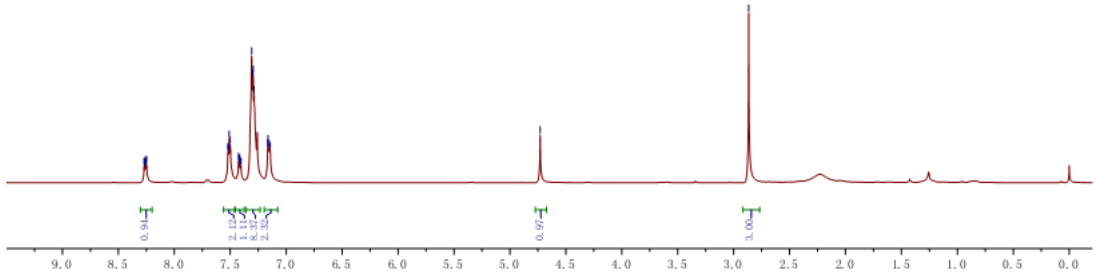
8.258
8.254
8.248
7.520
7.517
7.510
7.500
7.426
7.420
7.416
7.409
7.404
7.309
7.299
7.295
7.288
7.165
7.161
7.152
7.143
4.730
2.865
3h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1.14
4.15
2.35
0.97
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.5
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2.5
2.0
1.5
1.0
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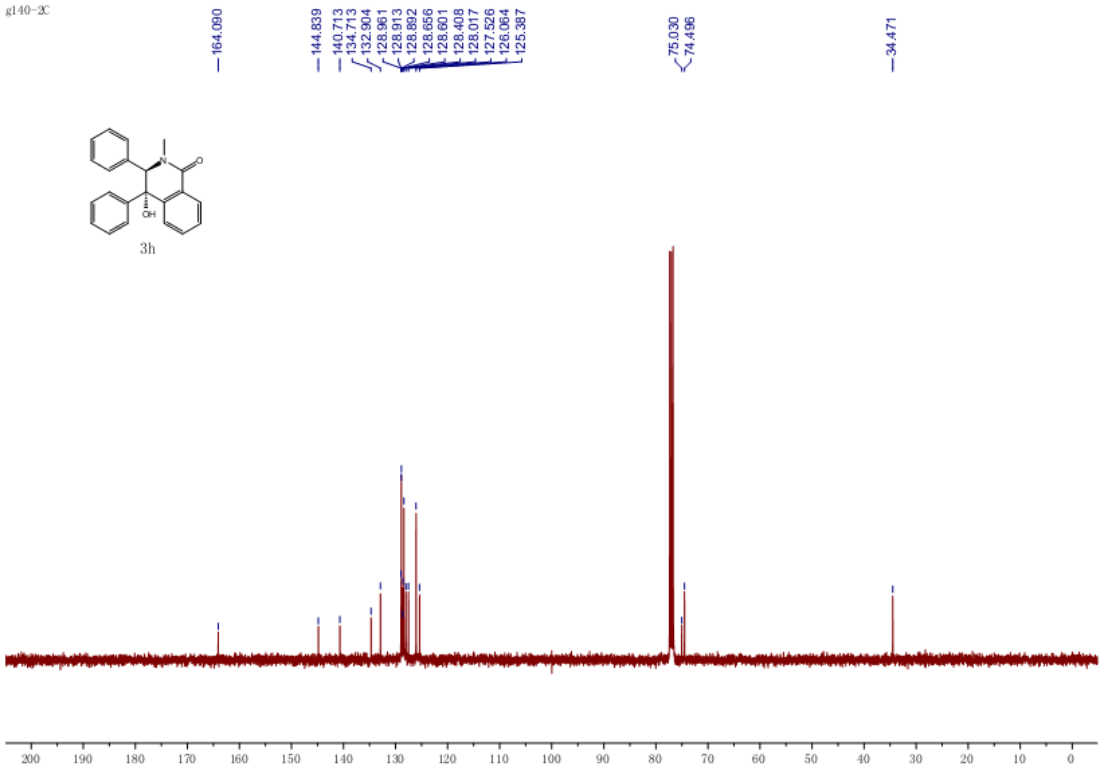
0.0


g140-2C
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144.839
140.713
134.713
132.904
128.961
128.913
128.892
128.656
128.601
128.408
128.017
127.526
126.064
125.387
75.030
74.496
34.471
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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30
20
10
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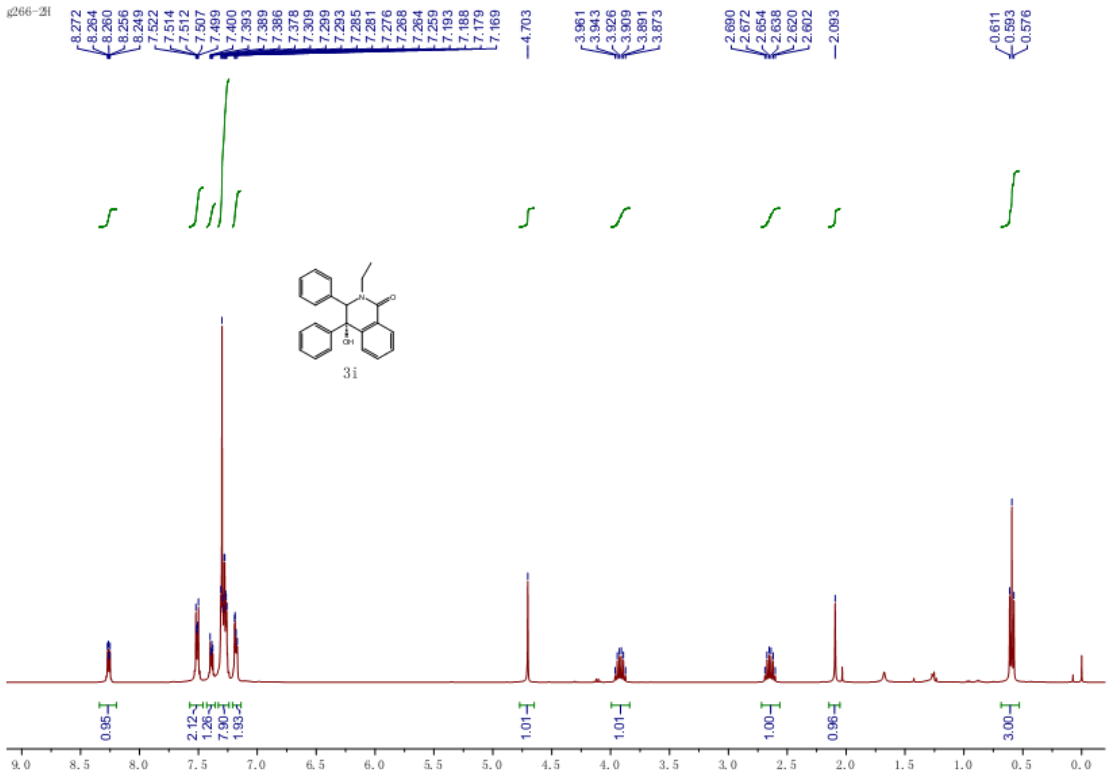
g266-2H
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8.260
8.256
8.249
7.522
7.514
7.512
7.507
7.499
7.400
7.393
7.389
7.386
7.378
7.309
7.299
7.293
7.285
7.281
7.276
7.268
7.264
7.259
7.193
7.188
7.179
7.169
4.703
3.961
3.943
3.926
3.909
3.891
3.873
2.690
2.672
2.654
2.638
2.620
2.602
2.093
0.611
0.593
0.576
0.95
2.12
1.26
7.90
1.93
1.01
1.01
1.00
0.96
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
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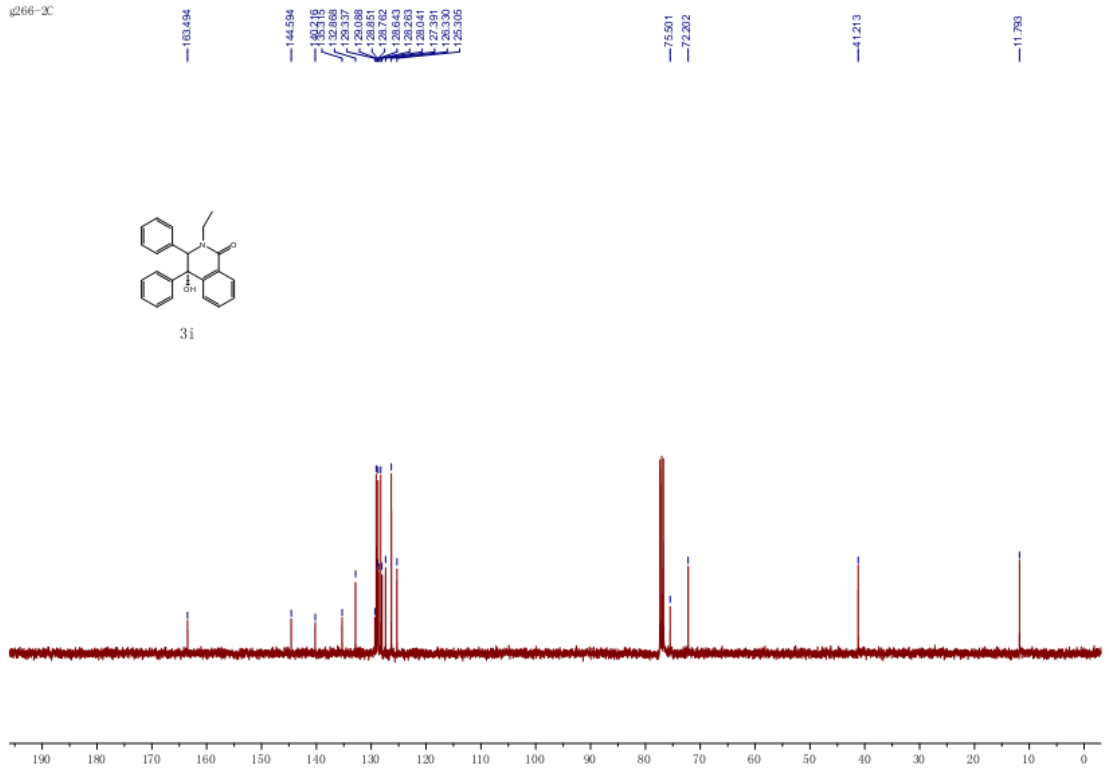
2.0
1.5
1.0
0.5
0.0

3i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132.868
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129.088
128.851
128.762
128.643
128.263
128.041
127.391
126.330
125.305
75.501
72.202
41.213
11.793
190
180
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100
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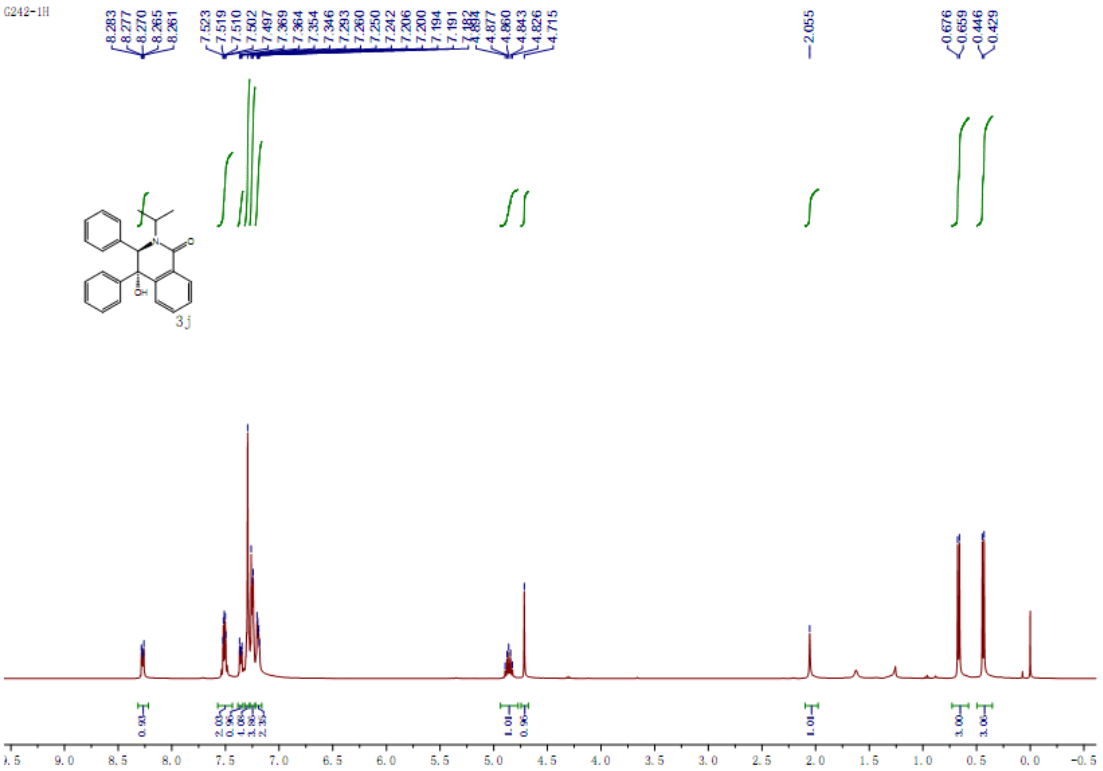
3i


G242-1H
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8.270
8.265
8.261
7.523
7.519
7.510
7.502
7.497
7.369
7.364
7.354
7.346
7.293
7.260
7.250
7.242
7.206
7.200
7.194
7.191
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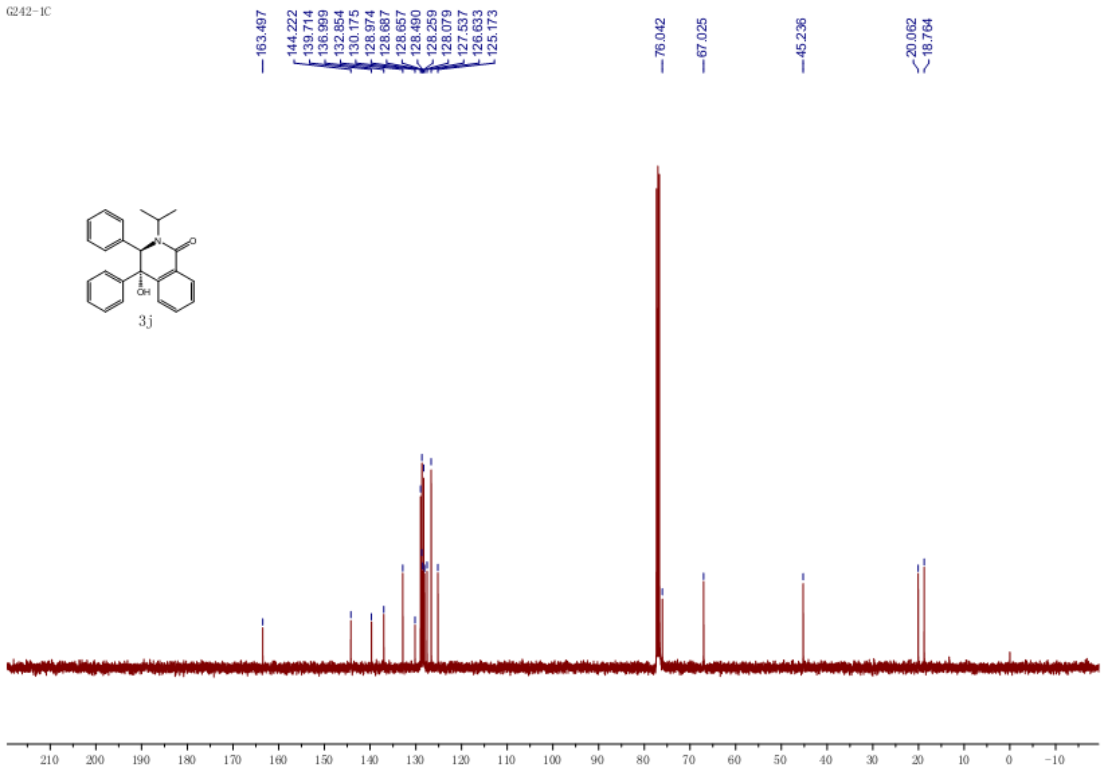
4.843
4.826
4.715
2.055
0.676
0.659
0.446
0.429
3j


G242-1C
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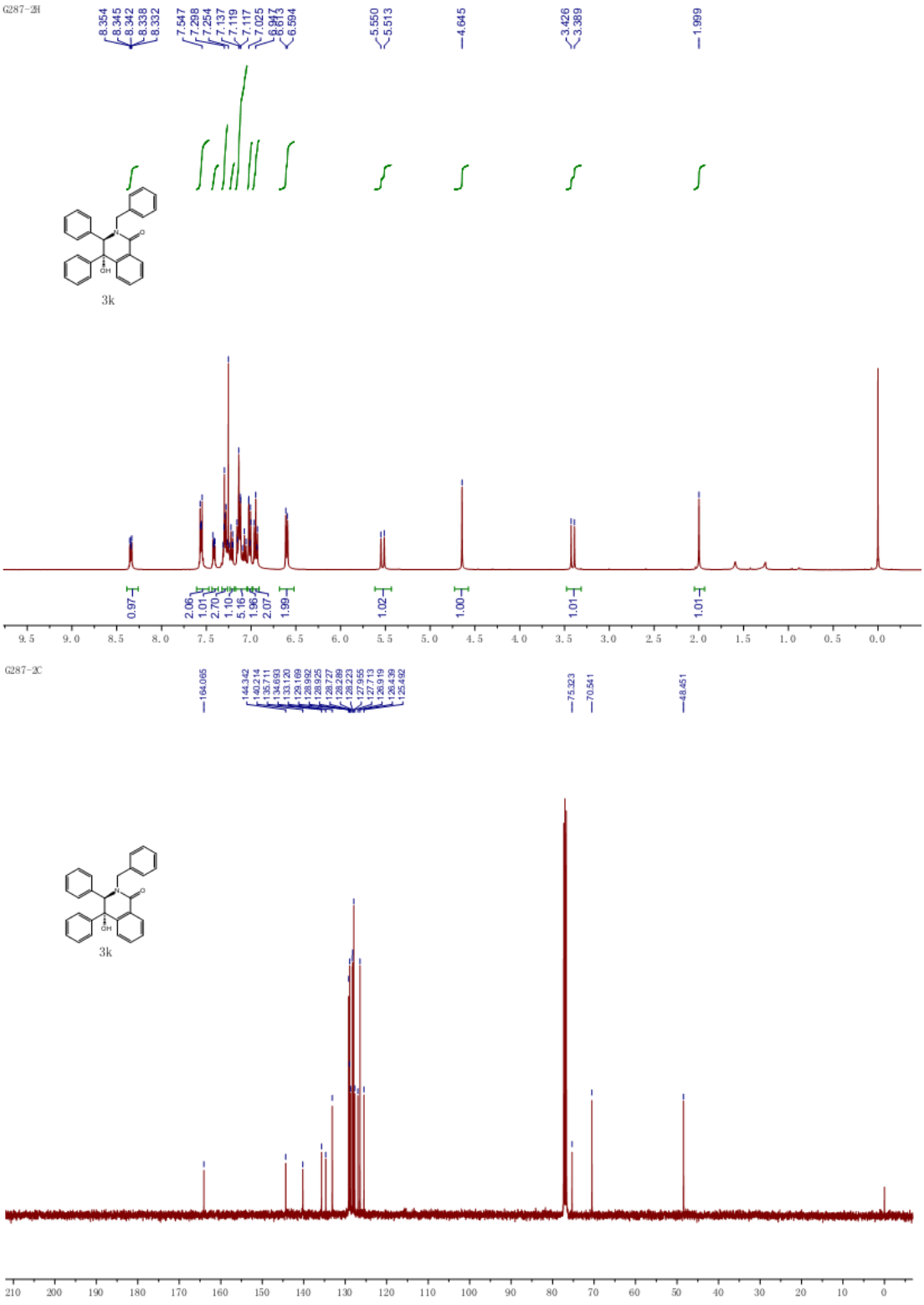
136.999
132.854
130.175
128.974
128.687
128.657
128.490
128.259
128.079
127.537
126.633
125.173
76.042
67.025
45.236
20.062
18.764
3j


G287-2H
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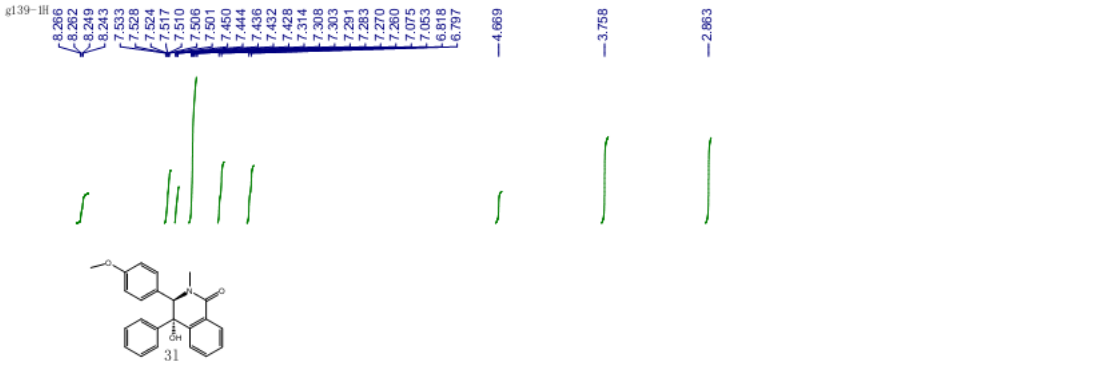
8.338
8.332
7.547
7.298
7.254
7.137
7.119
7.117
7.025
6.947
6.813
6.594
5.550
5.513
4.645
3.426
3.389
1.999
3k
0.97
2.06
1.01
2.70
1.10
5.16
1.96
2.07
1.99
1.02
1.00
1.01
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
G287-2C
164.065
144.342
140.214
135.711
134.693
133.120
129.169
128.992
128.925
128.727
128.289
128.223
127.955
127.713
126.919
126.439
125.482
75.323
70.541
48.451
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


g139-1H
8.266
8.262
8.249
8.243
7.533
7.528
7.524
7.517
7.510
7.506
7.501
7.450
7.444
7.436
7.432
7.428
7.314
7.308
7.303
7.291
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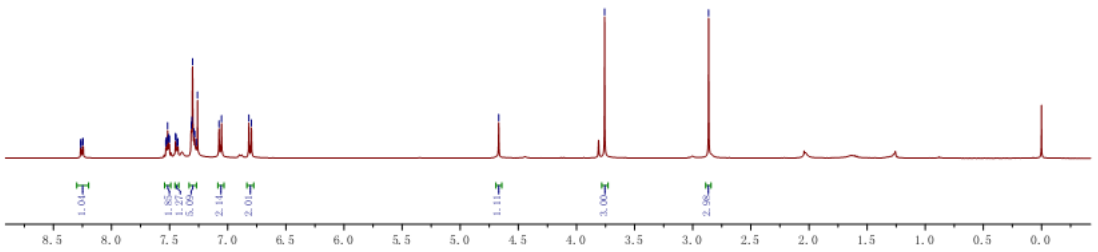
7.270
7.260
7.075
7.053
6.818
6.797
4.669
3.758
2.863

31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1.85
1.27
6.00
2.14
2.01
1.11
3.00
2.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
4.0
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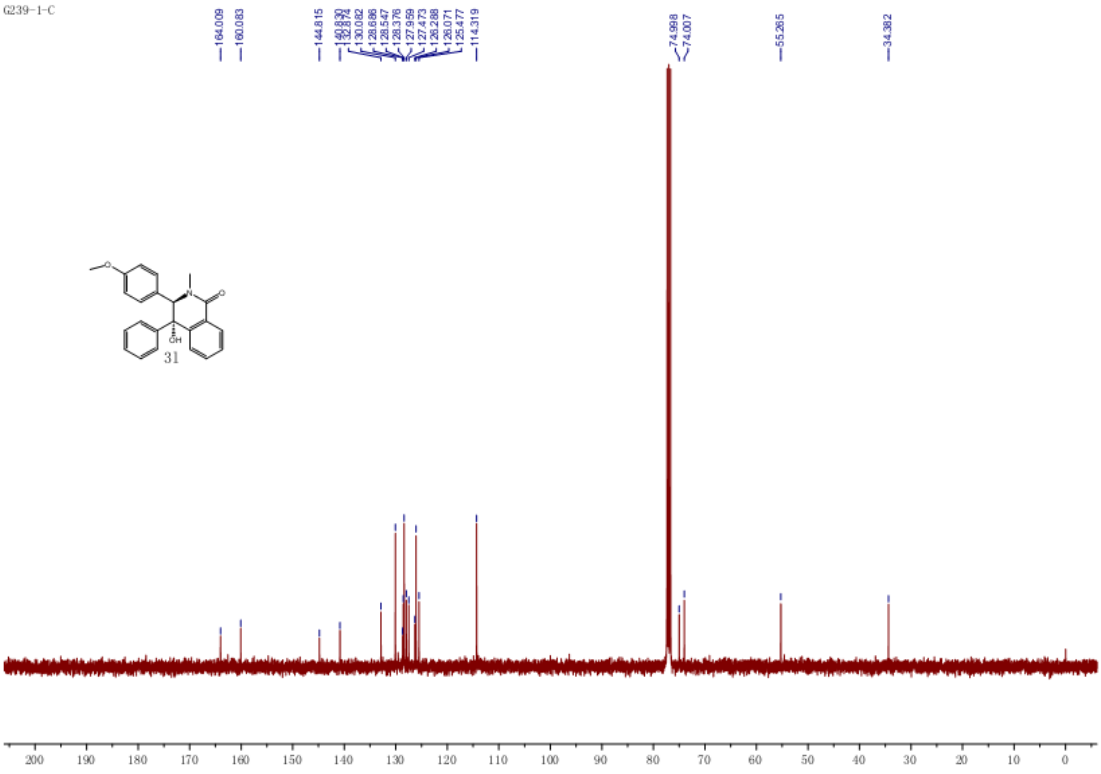
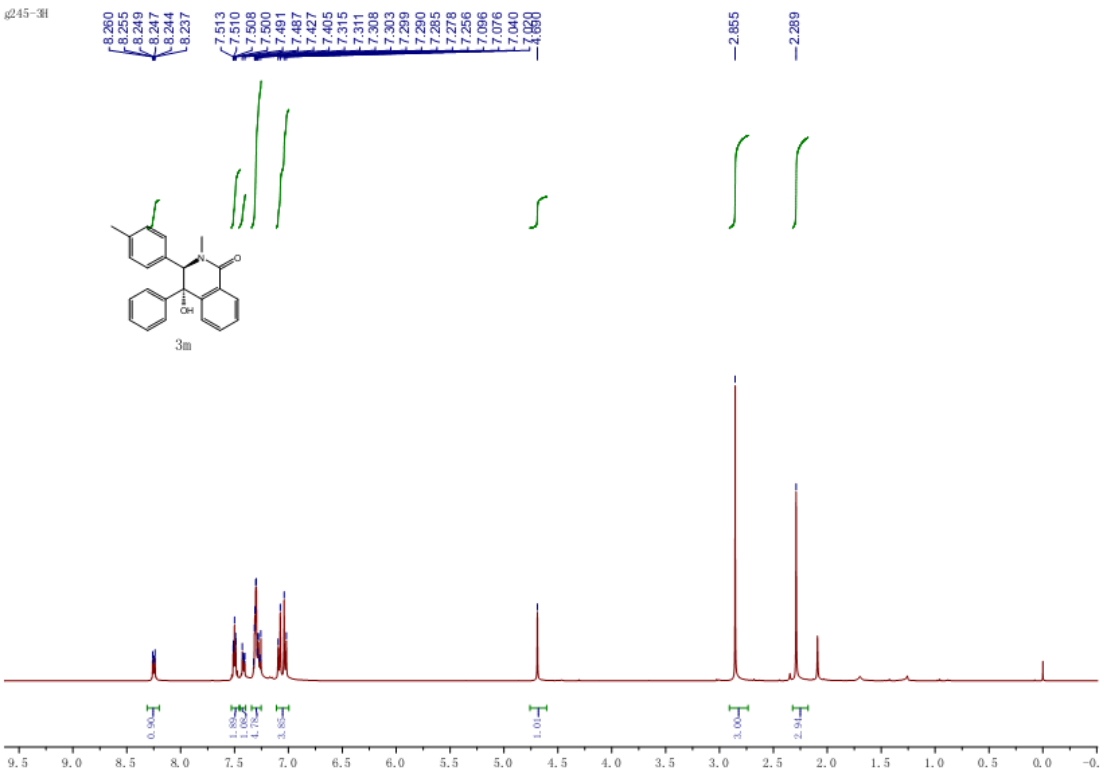
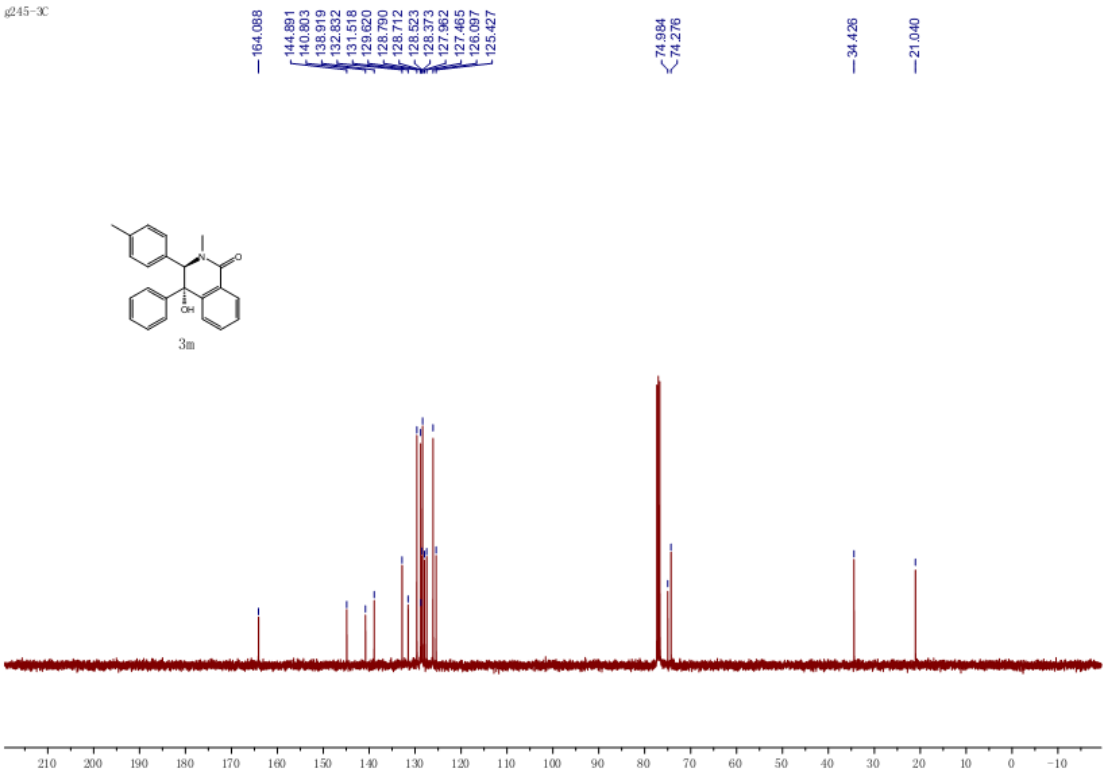
3.0
2.5
2.0
1.5
1.0
0.5
0.0


G239-1-C
164.009
160.083
144.815
140.830
132.974
130.082
128.686
128.547
128.376
127.959
127.473
126.288
126.071
125.477
114.319
74.998
74.007
55.265
34.382
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

31


g245-3H
8.260
8.255
8.249
8.247
8.244
8.237
7.513
7.510
7.508
7.500
7.491
7.487
7.427
7.405
7.315
7.311
7.308
7.303
7.299
7.290
7.285
7.278
7.256
7.096
7.076
7.040
4.690
2.855
2.289
3m
0.90
1.89
1.86
4.78
3.88
1.01
3.00
2.94
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.


g245-3C
164.088
144.891
140.803
138.919
132.832
131.518
129.620
128.790
128.712
128.523
128.373
127.962
127.465
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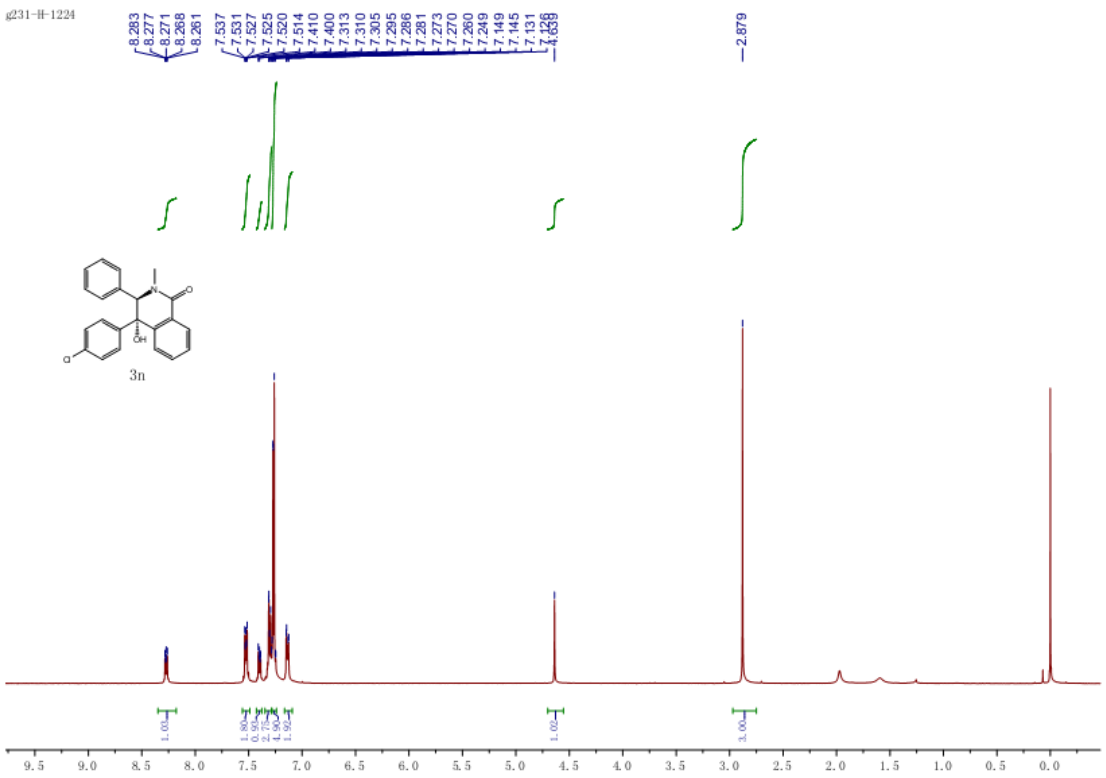
125.427
74.984
74.276
34.426
21.040
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


g231-H-1224
8.283
8.277
8.271
8.268
8.261
7.537
7.531
7.527
7.525
7.520
7.514
7.410
7.400
7.313
7.310
7.305
7.295
7.286
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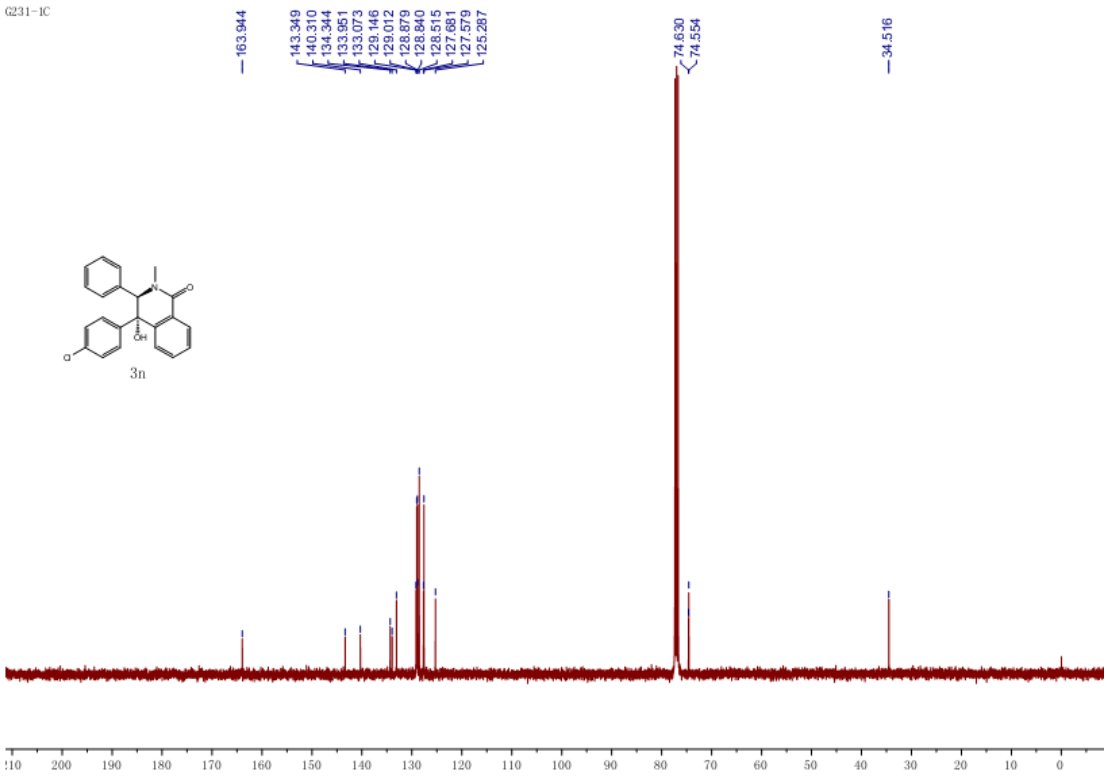
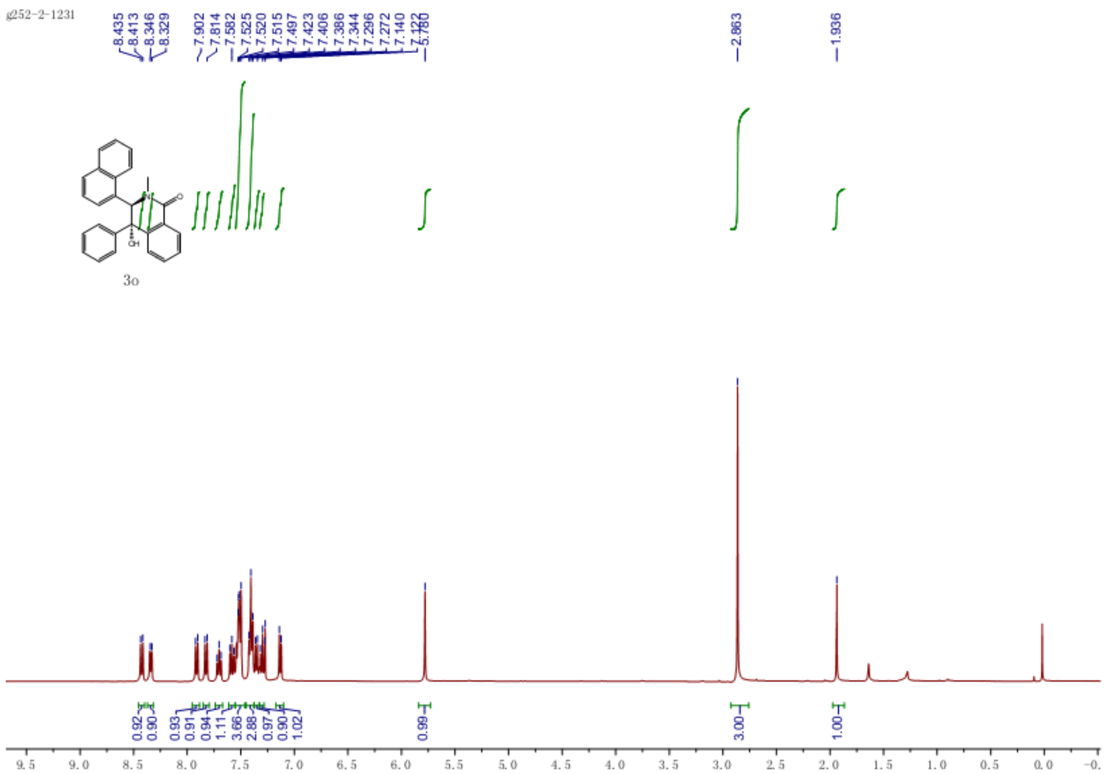
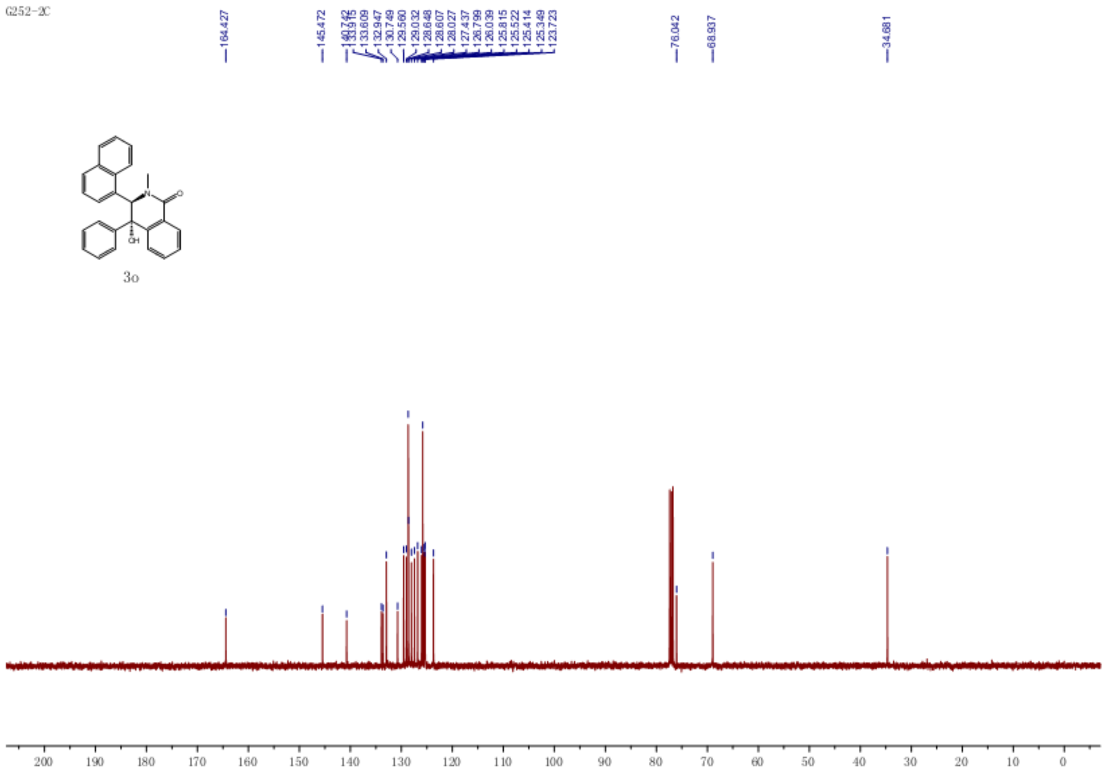
7.273
7.270
7.260
7.249
7.149
7.145
7.131
4.639
2.879
3n


G231-1C
163.944
143.349
140.310
134.344
133.951
133.073
129.146
129.012
128.879
128.840
128.515
127.681
127.579
125.287
74.630
74.554
34.516
3n


g252-2-1231
8.435
8.413
8.346
8.329
7.902
7.814
7.582
7.525
7.520
7.515
7.497
7.423
7.406
7.386
7.344
7.296
7.272
7.140
5.780
2.863
1.936
0.92
0.90
0.93
0.91
0.94
1.11
3.66
2.88
0.97
0.90
1.02
0.99
3.00
1.00
3o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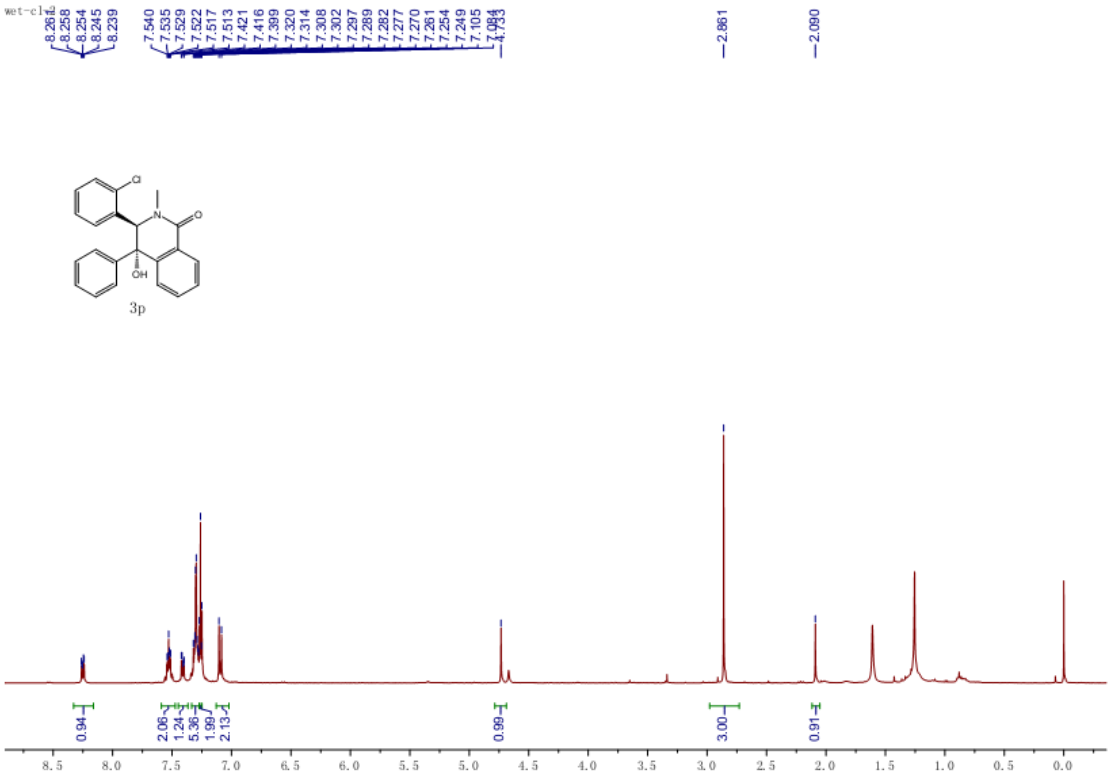
132.947
130.749
129.560
129.032
128.607
128.027
127.437
126.799
126.039
125.815
125.522
125.414
125.349
123.723
76.042
68.937
34.681
3o


wet-cl
8.264
8.258
8.254
8.245
8.239
7.540
7.535
7.529
7.522
7.517
7.513
7.421
7.416
7.399
7.320
7.314
7.308
7.302
7.297
7.289
7.282
7.277
7.270
7.261
7.254
7.249
7.105
7.094
4.193
2.861
2.090
Cl
N
O
OH
3p
0.94
2.06
1.24
5.36
1.99
2.13
0.99
3.00
0.91
8.5
8.0
7.5
7.0
6.5
6.0
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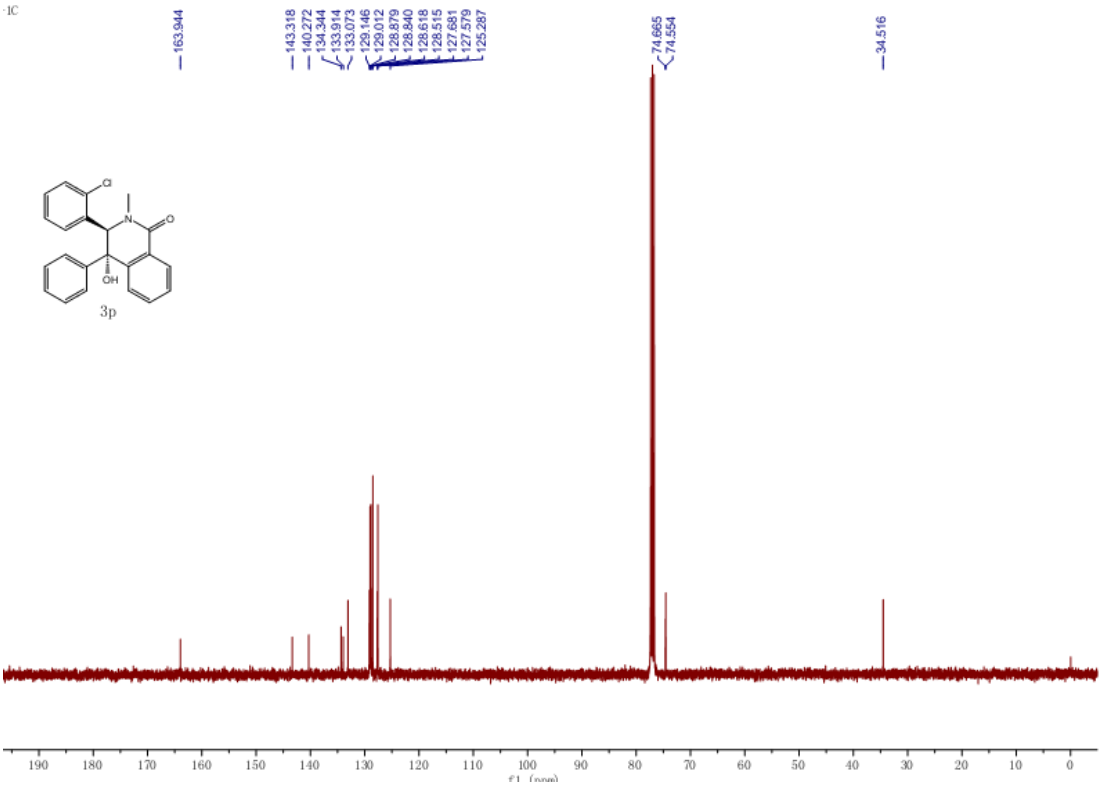
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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143.318
140.272
134.344
133.914
133.073
129.146
129.012
128.879
128.840
128.618
128.515
127.681
127.579
125.287
74.665
74.554
34.516
Cl
N
O
OH
3p
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180
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160
150
140
130
120
110
100
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70
60
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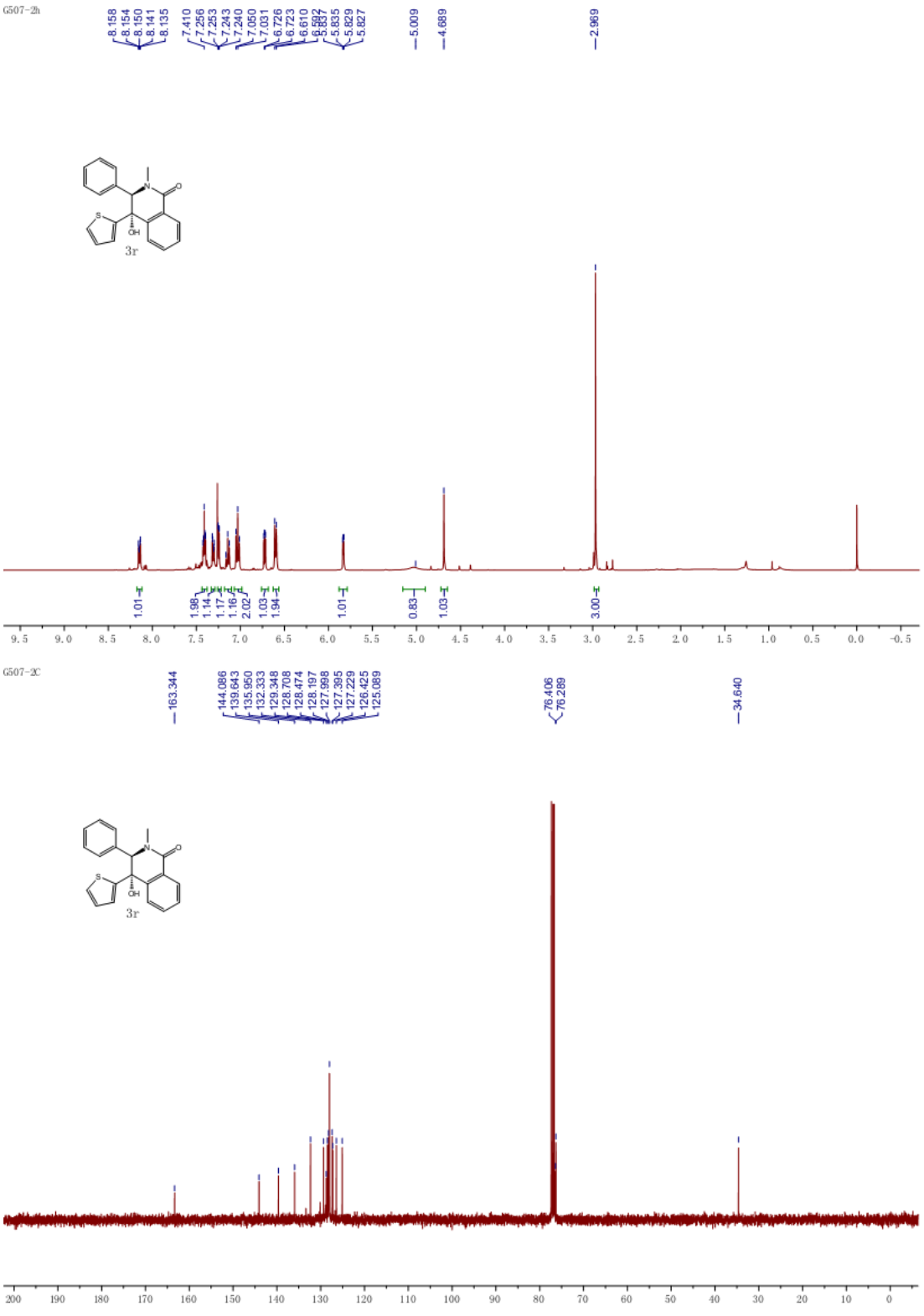
40
30
20
10
0


G507-2h
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8.135
7.410
7.256
7.253
7.243
7.240
7.050
7.031
6.726
6.723
6.610
6.607
5.835
5.829
5.827
5.009
4.689
2.969
3r
1.01
1.98
1.14
1.17
1.16
2.02
1.03
1.94
1.01
0.83
1.03
3.00
G507-2C
163.344
144.086
139.643
135.950
132.333
129.348
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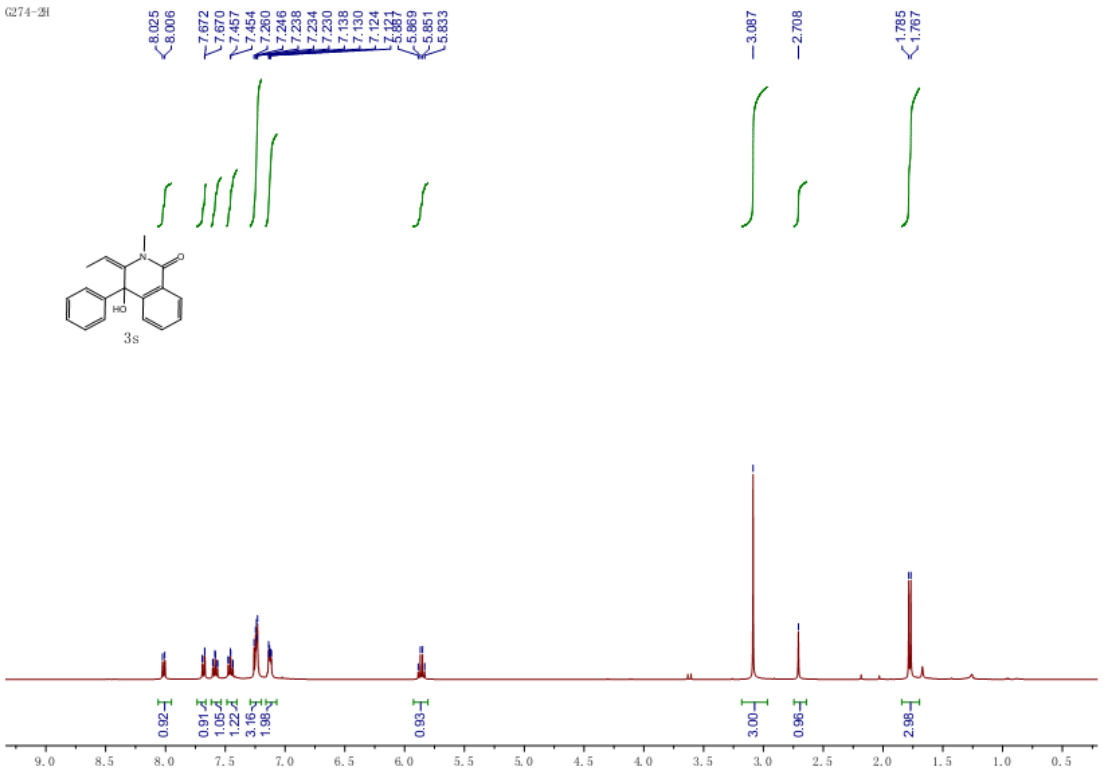
128.197
127.998
127.395
127.229
126.425
125.089
76.406
76.289
34.640
3r


G274-2H
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8.006
7.672
7.670
7.457
7.454
7.260
7.246
7.238
7.234
7.230
7.138
7.130
7.124
5.869
5.851
5.833
3.087
2.708
1.785
1.767
HO
3s
0.92
0.91
1.05
1.22
3.16
1.98
0.93
3.00
0.96
2.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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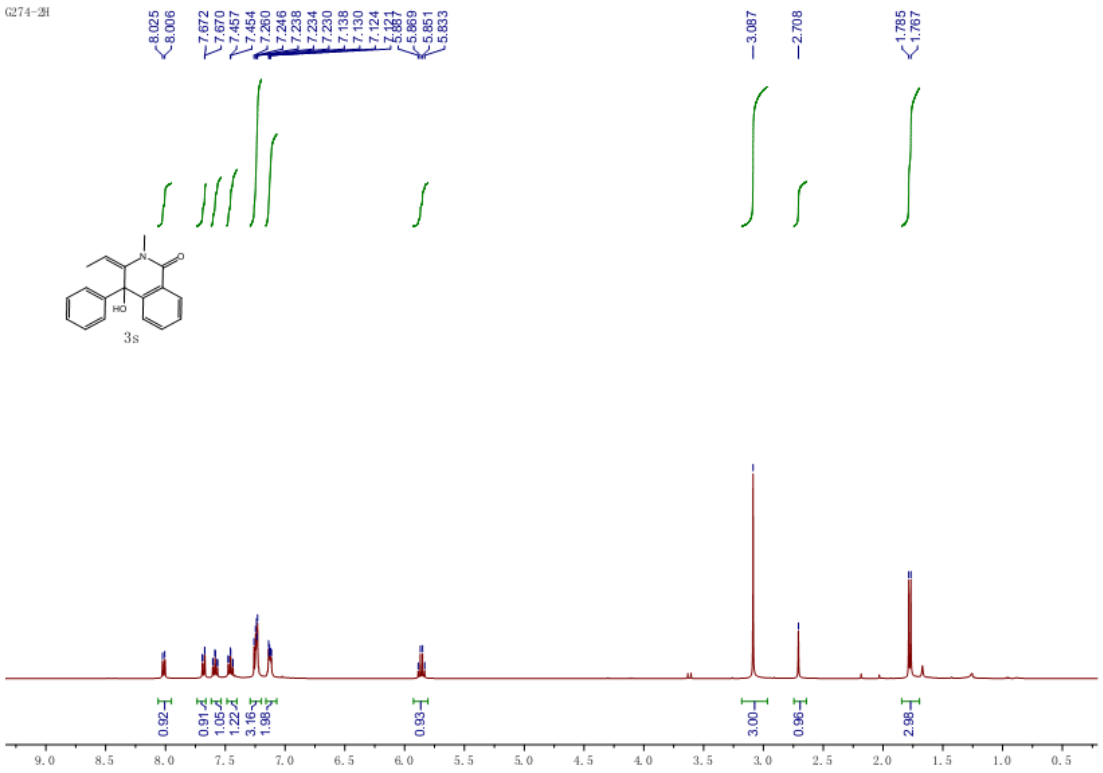
G274-2H
8.025
8.006
7.672
7.670
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7.238
7.234
7.230
7.138
7.130
7.124
5.869
5.851
5.833
3.087
2.708
1.785
1.767
HO
3s
0.92
0.91
1.05
1.22
3.16
1.98
0.93
3.00
0.96
2.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
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