

**Copper (II) catalyzed iodine-promoted oxidative cyclization of
2-amino-1,3,5-triazines and chalcones: synthesis of
aroylimidazo[1,2-a][1,3,5]triazines**

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X-ray crystallographic structure of **3a**

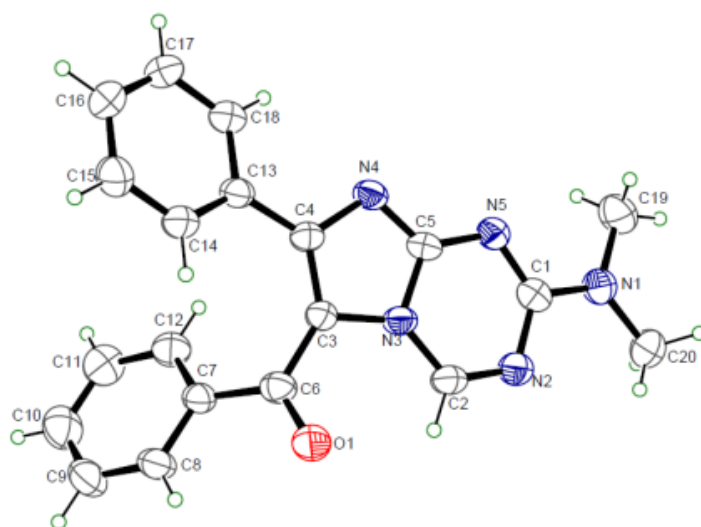
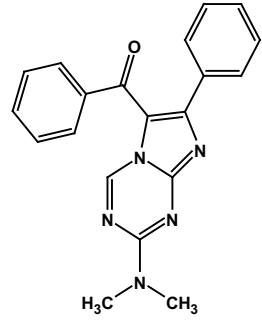


Figure S1 The crystal structure of **3a** with thermal ellipsoid contour at 30% probability level

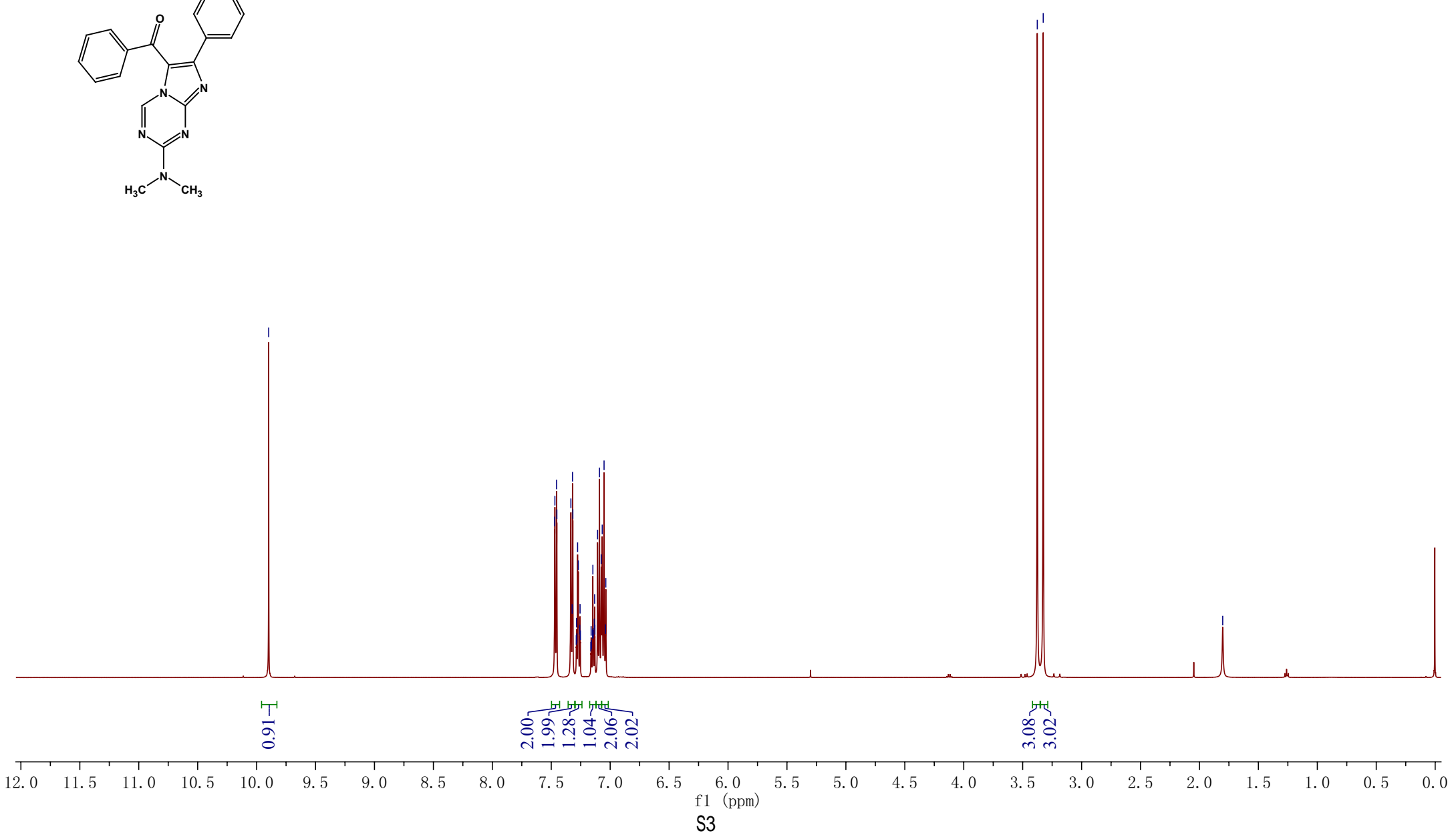
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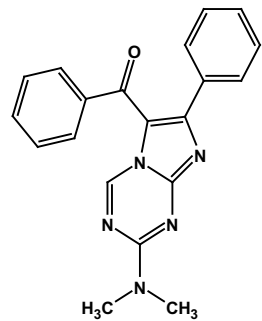
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1.8025



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—157.1266

—153.1621

—148.0787

—138.1691

—133.1225

—131.6791

—130.3554

—129.3168

—128.8835

—127.7963

—127.5681

—116.8025

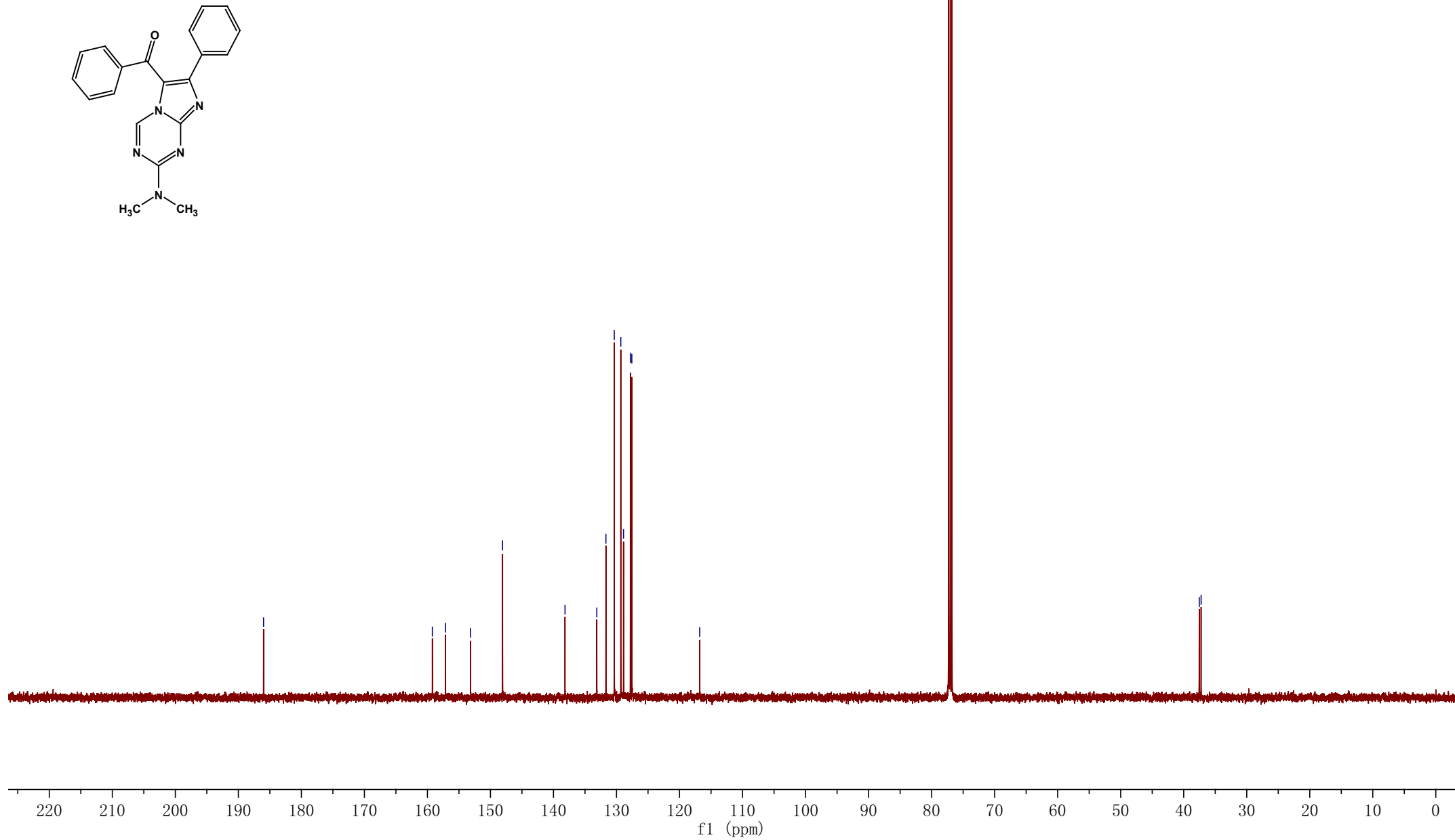
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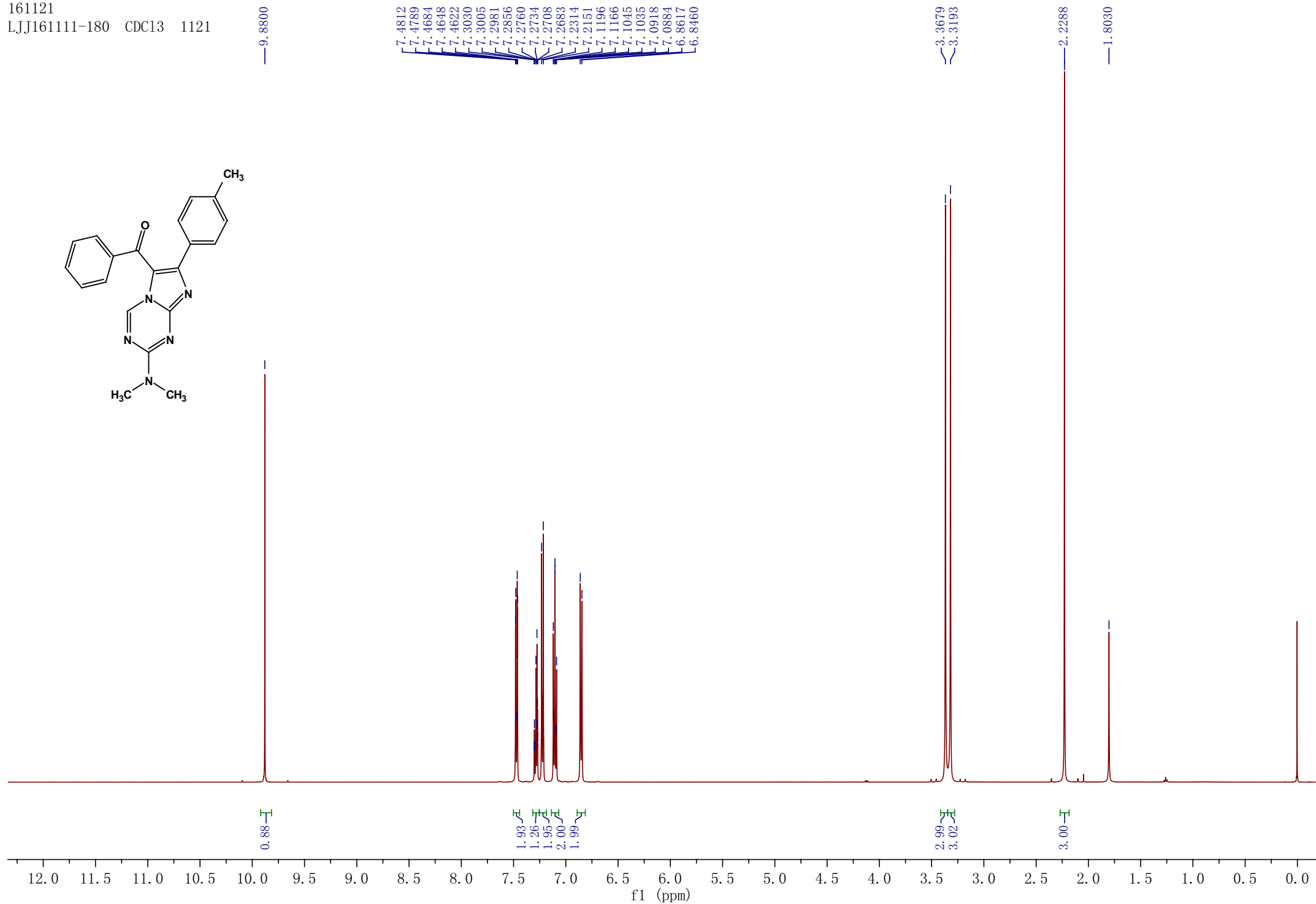
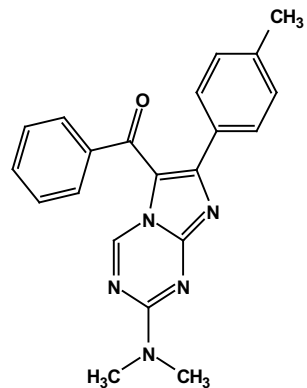
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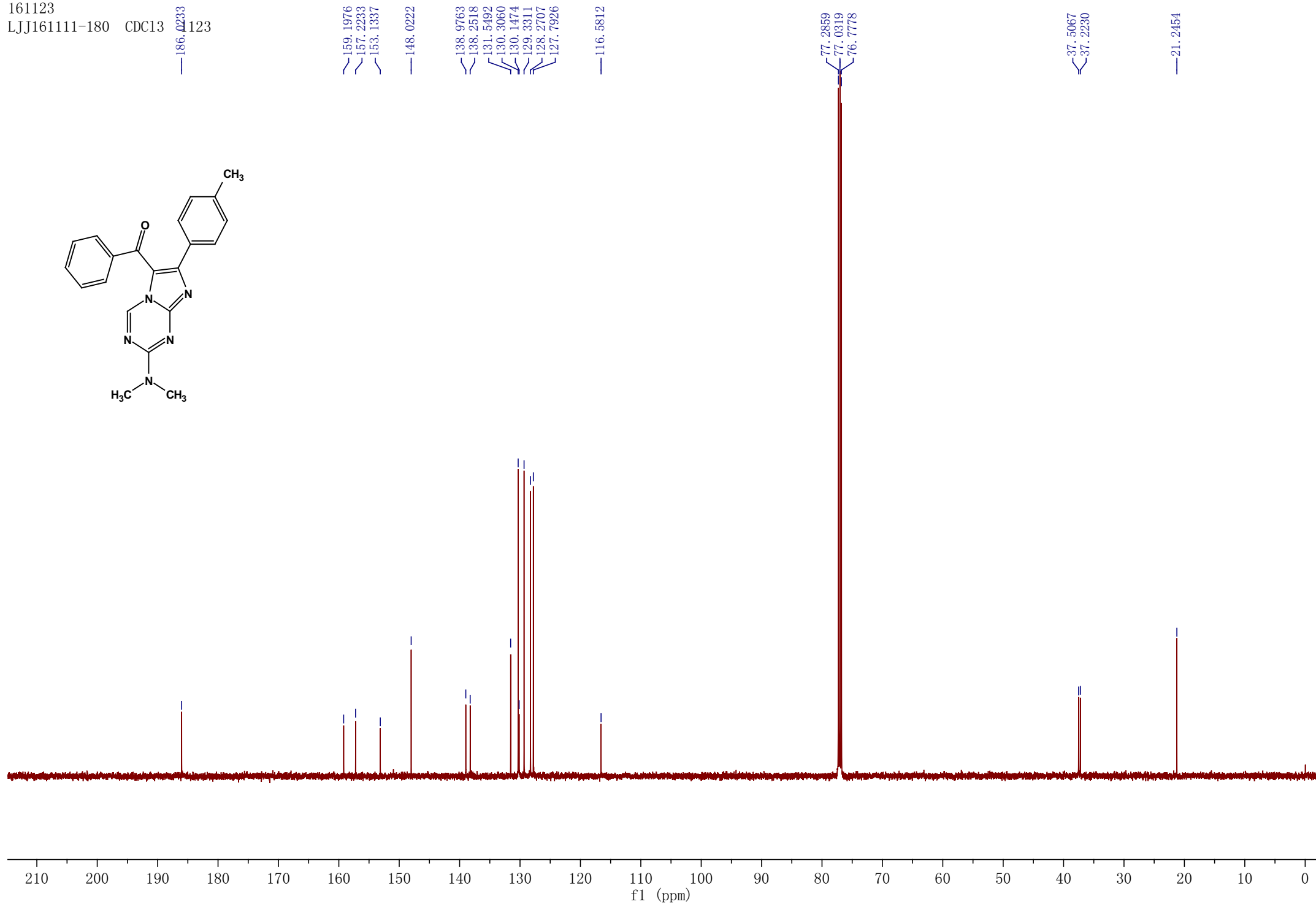
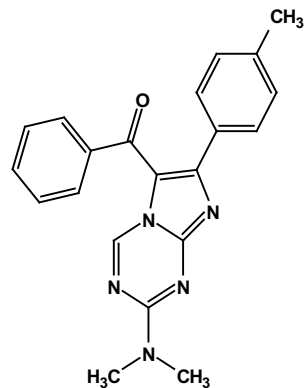


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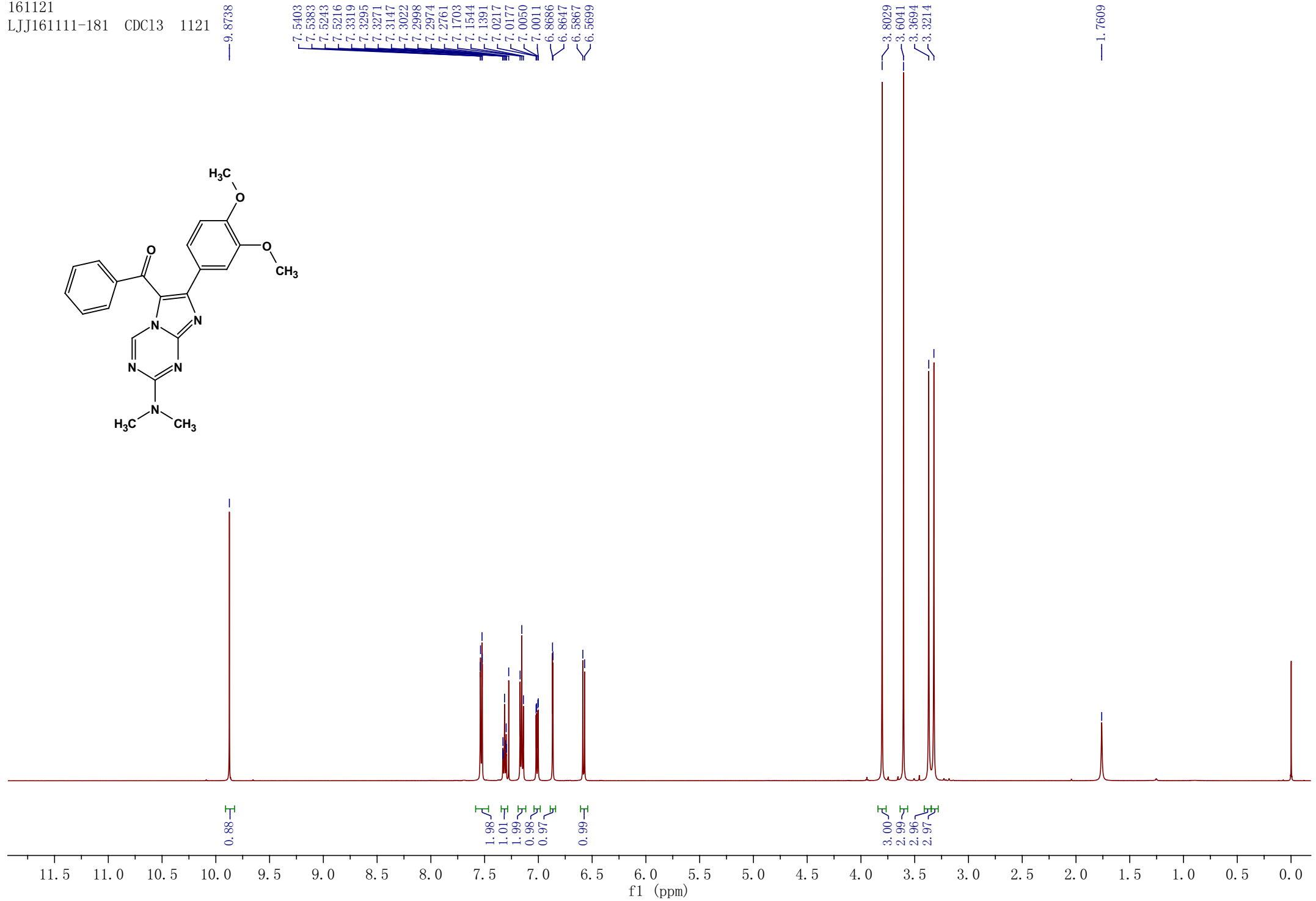
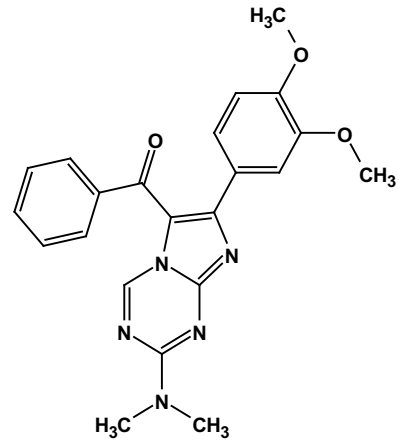
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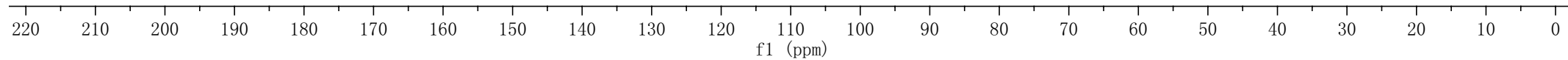
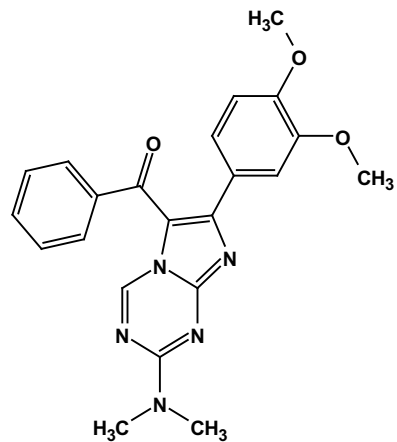
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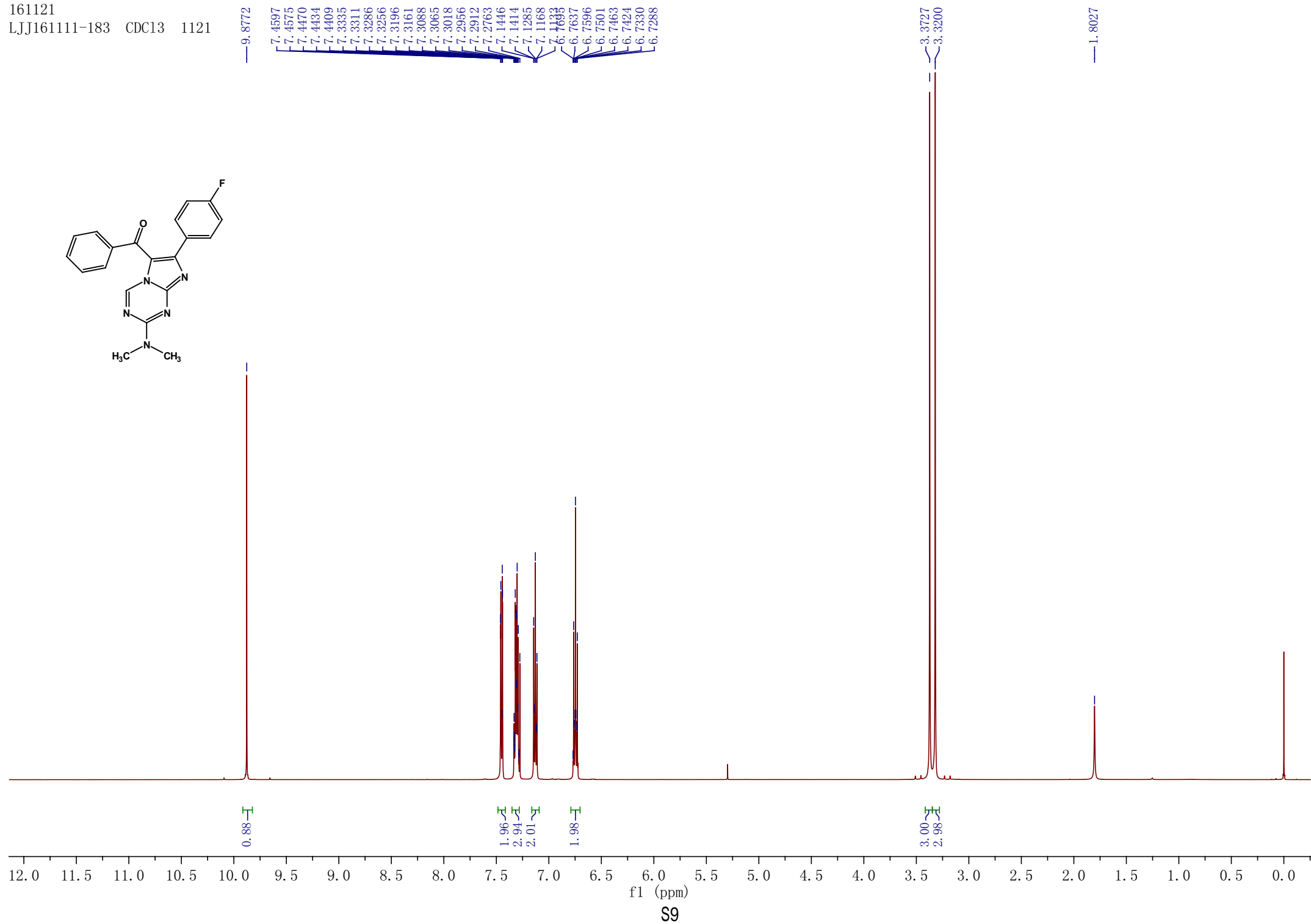
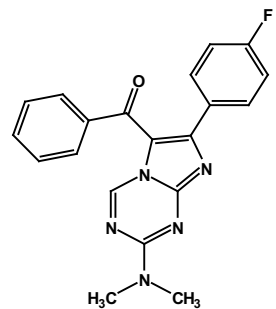
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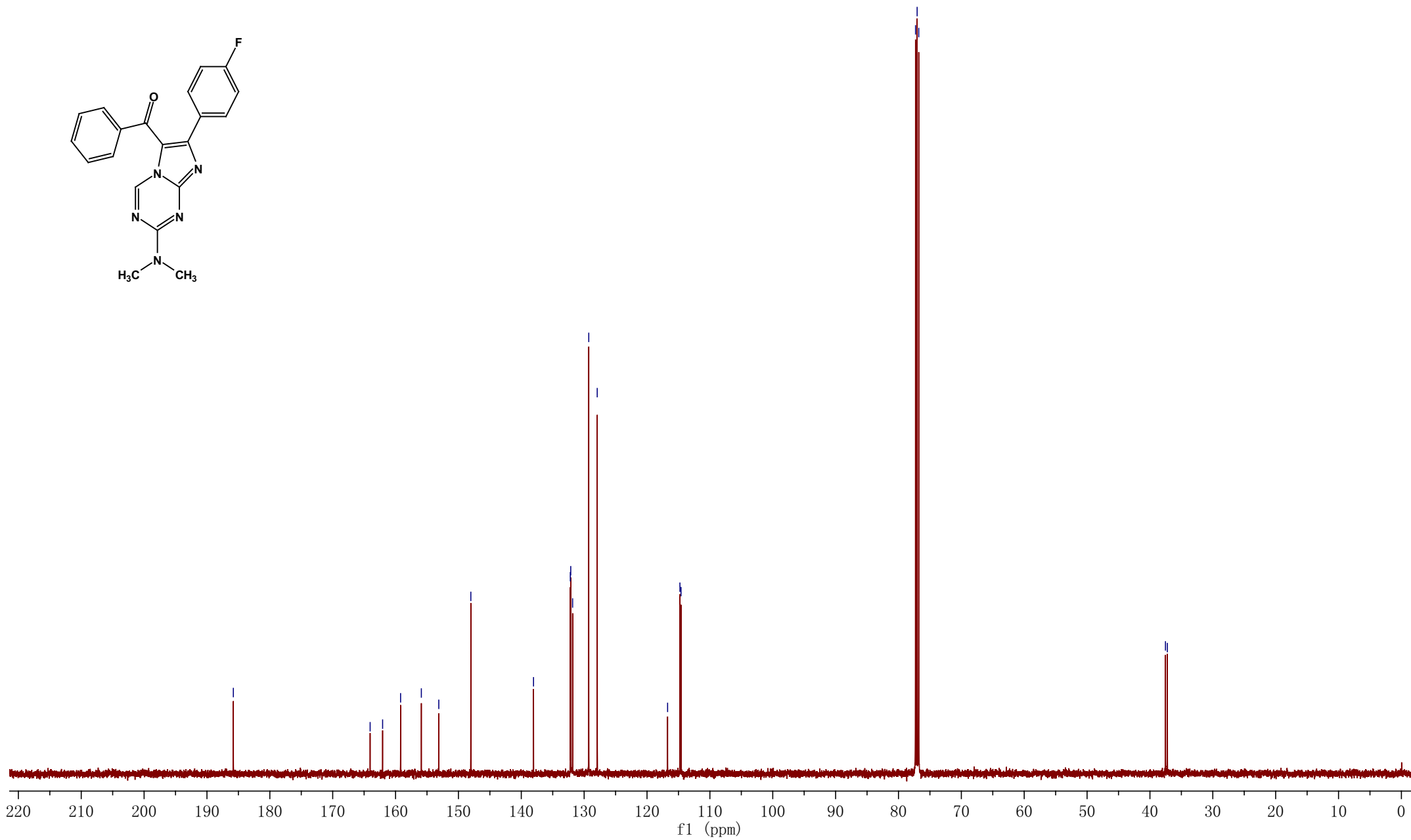
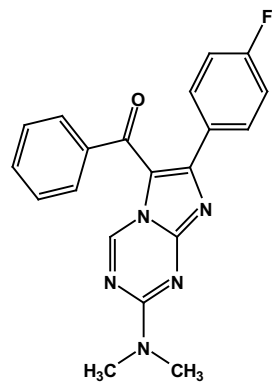
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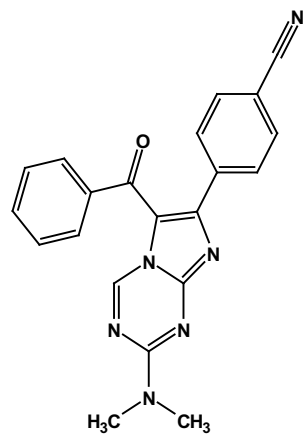
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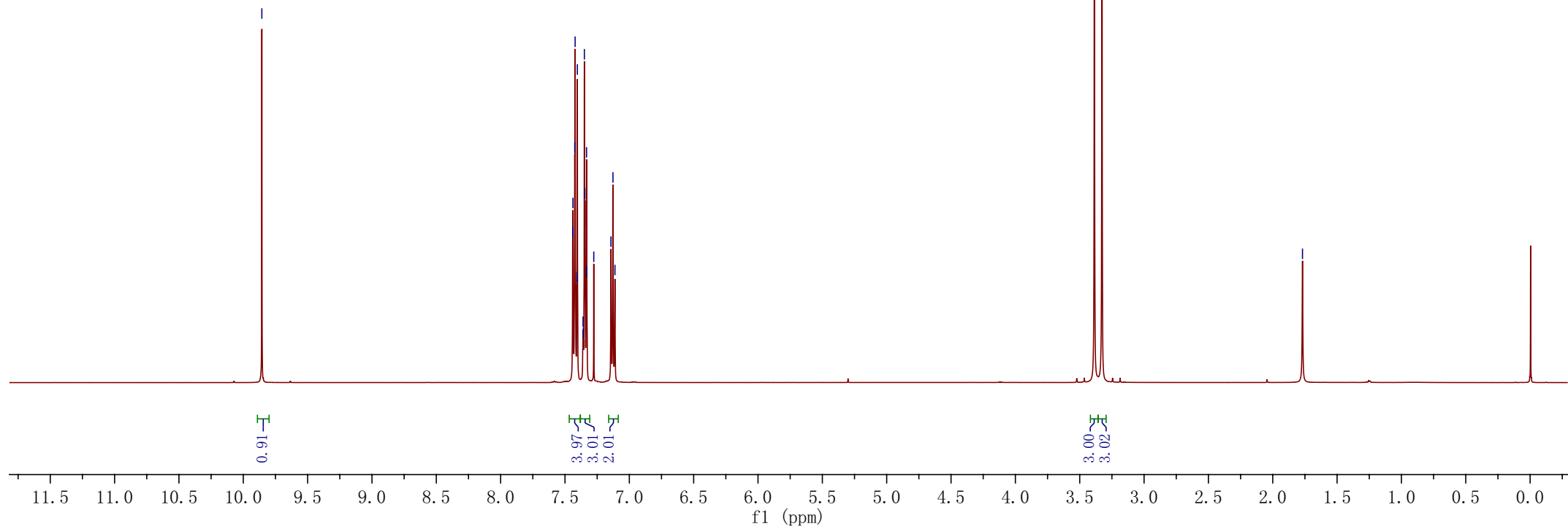
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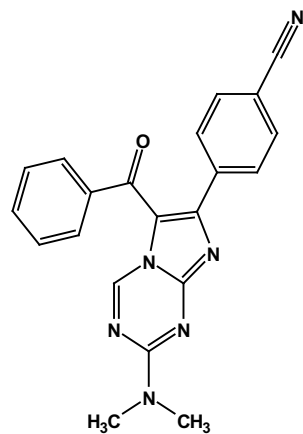
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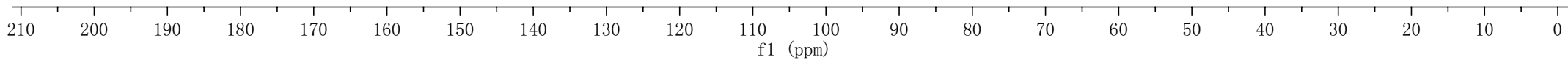
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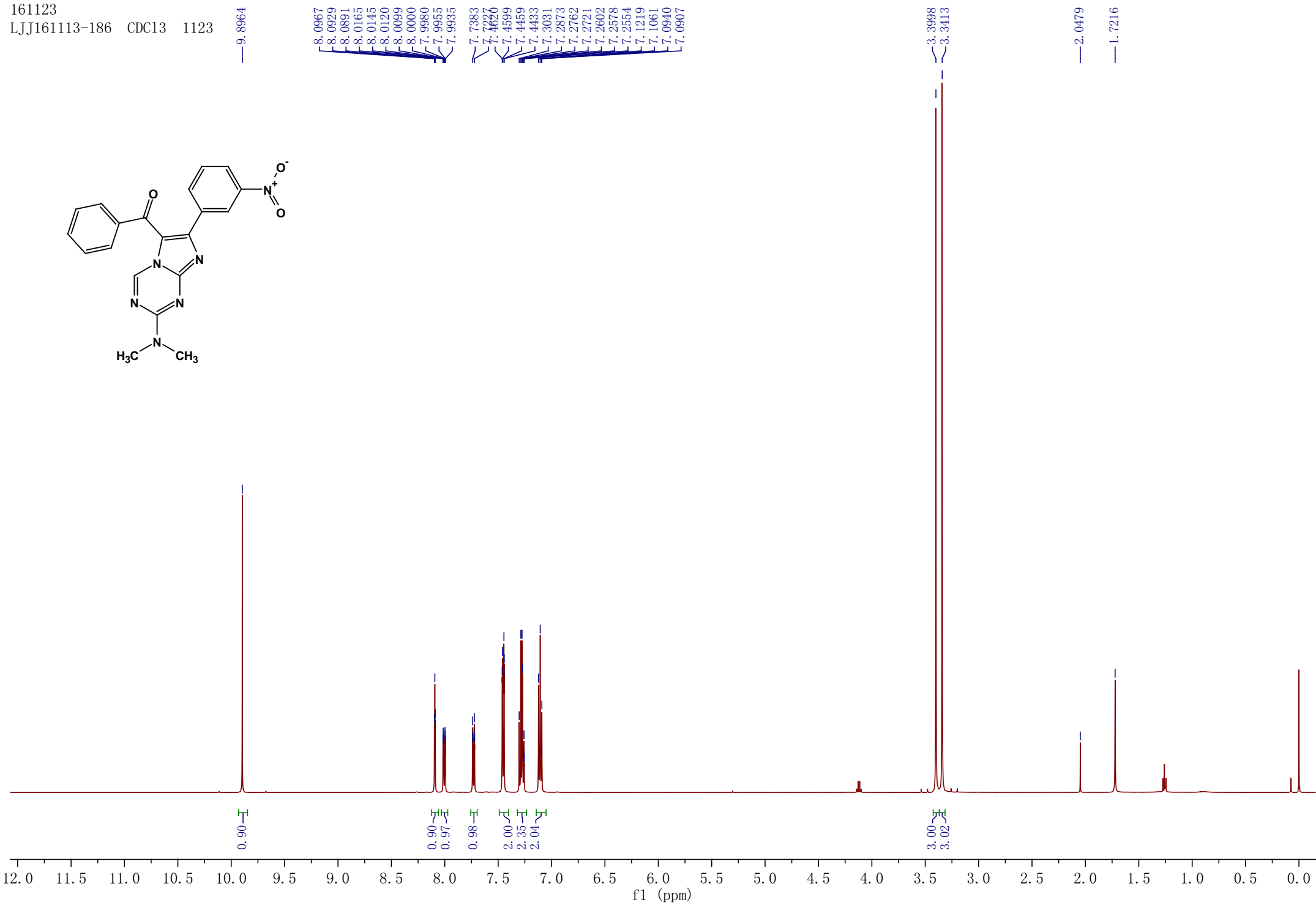
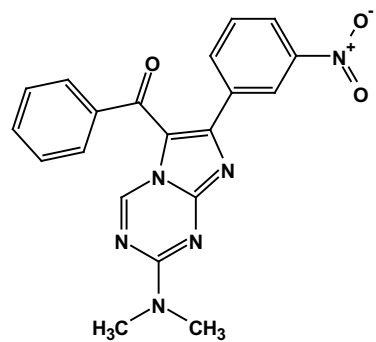
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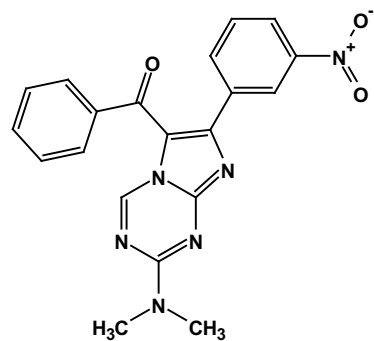


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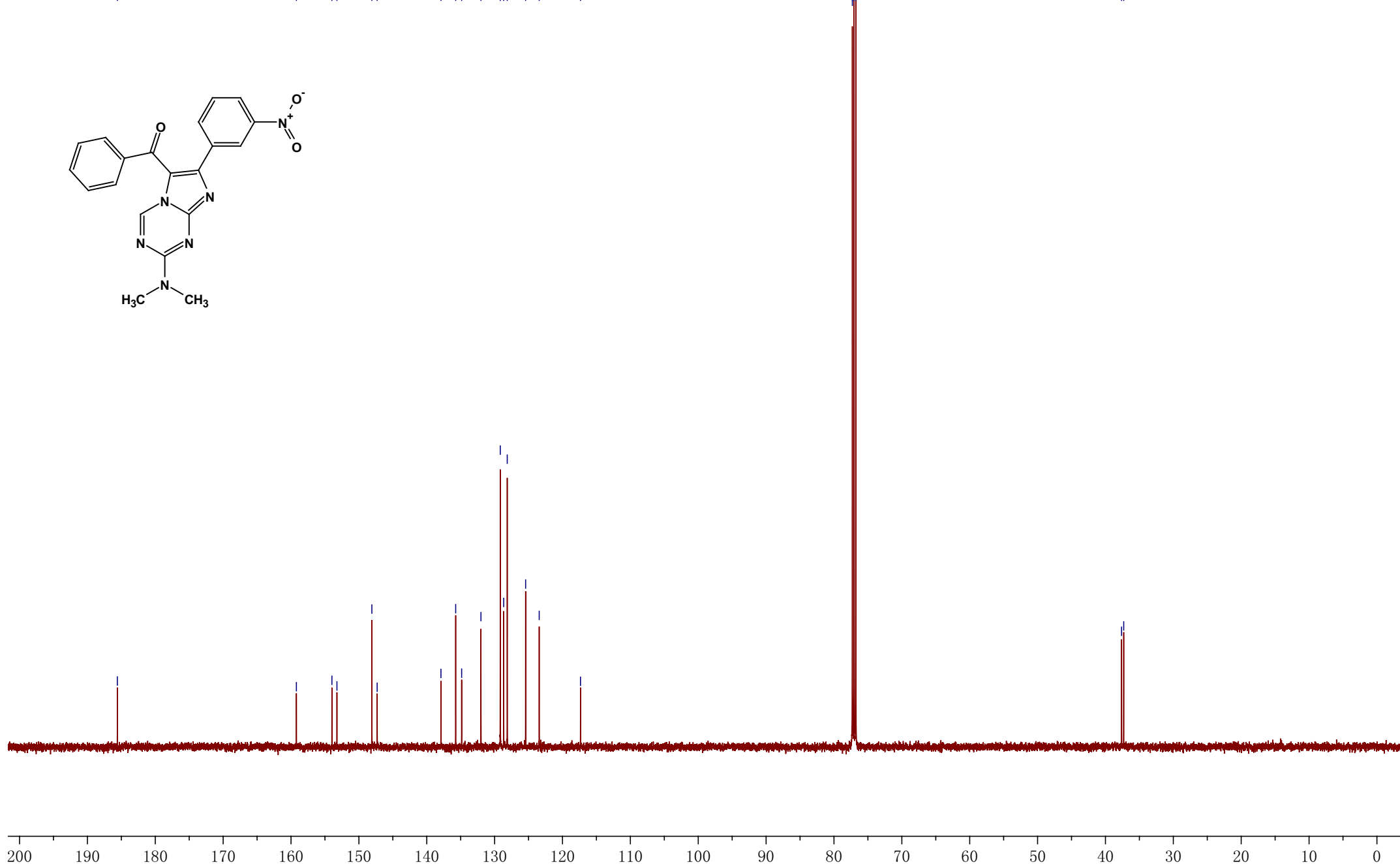
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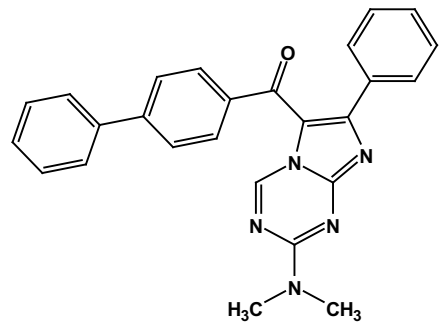
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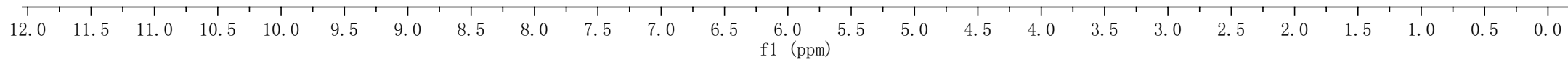
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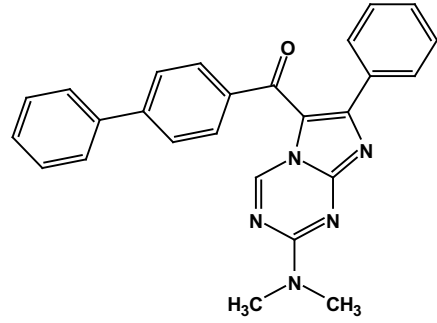
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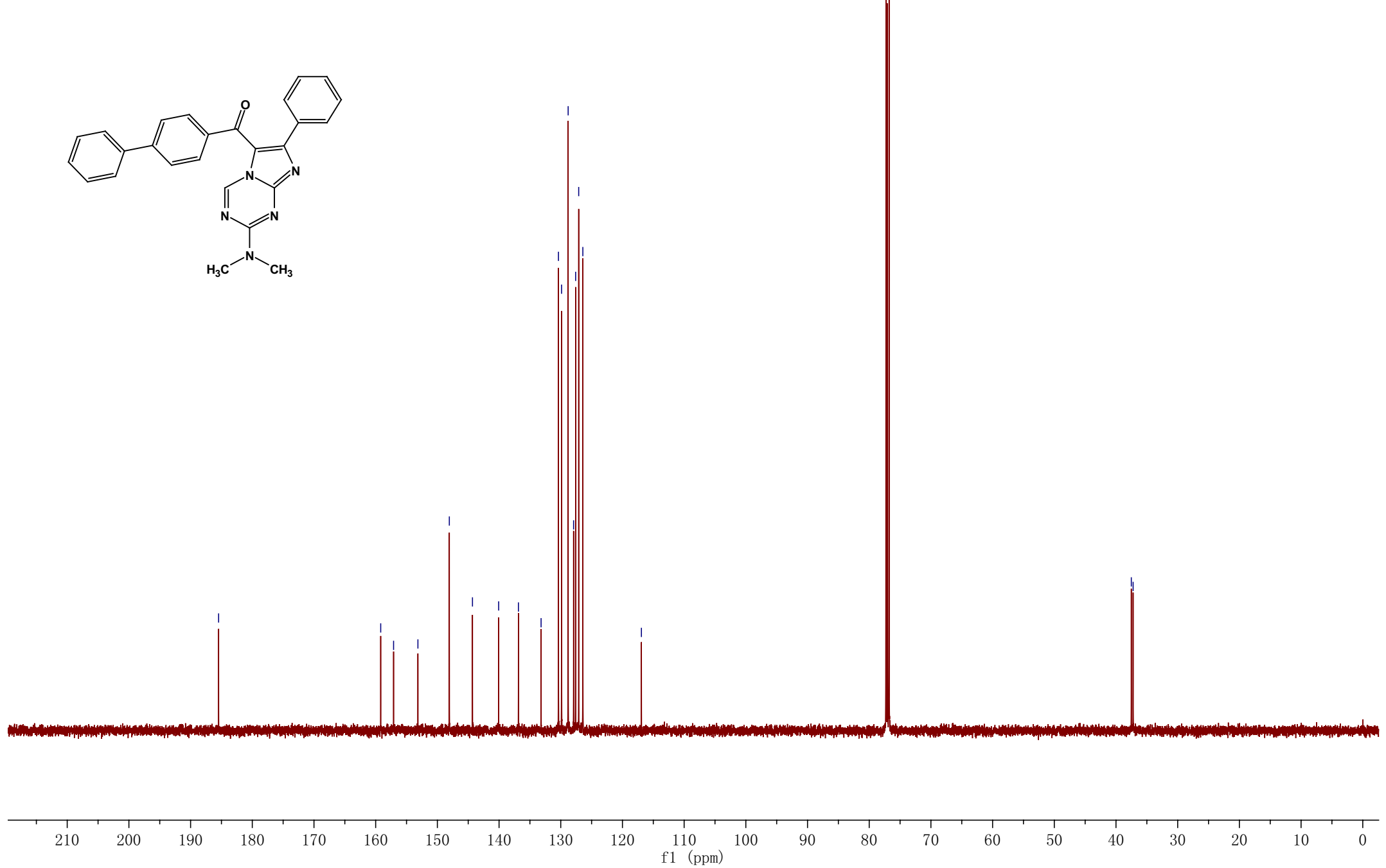
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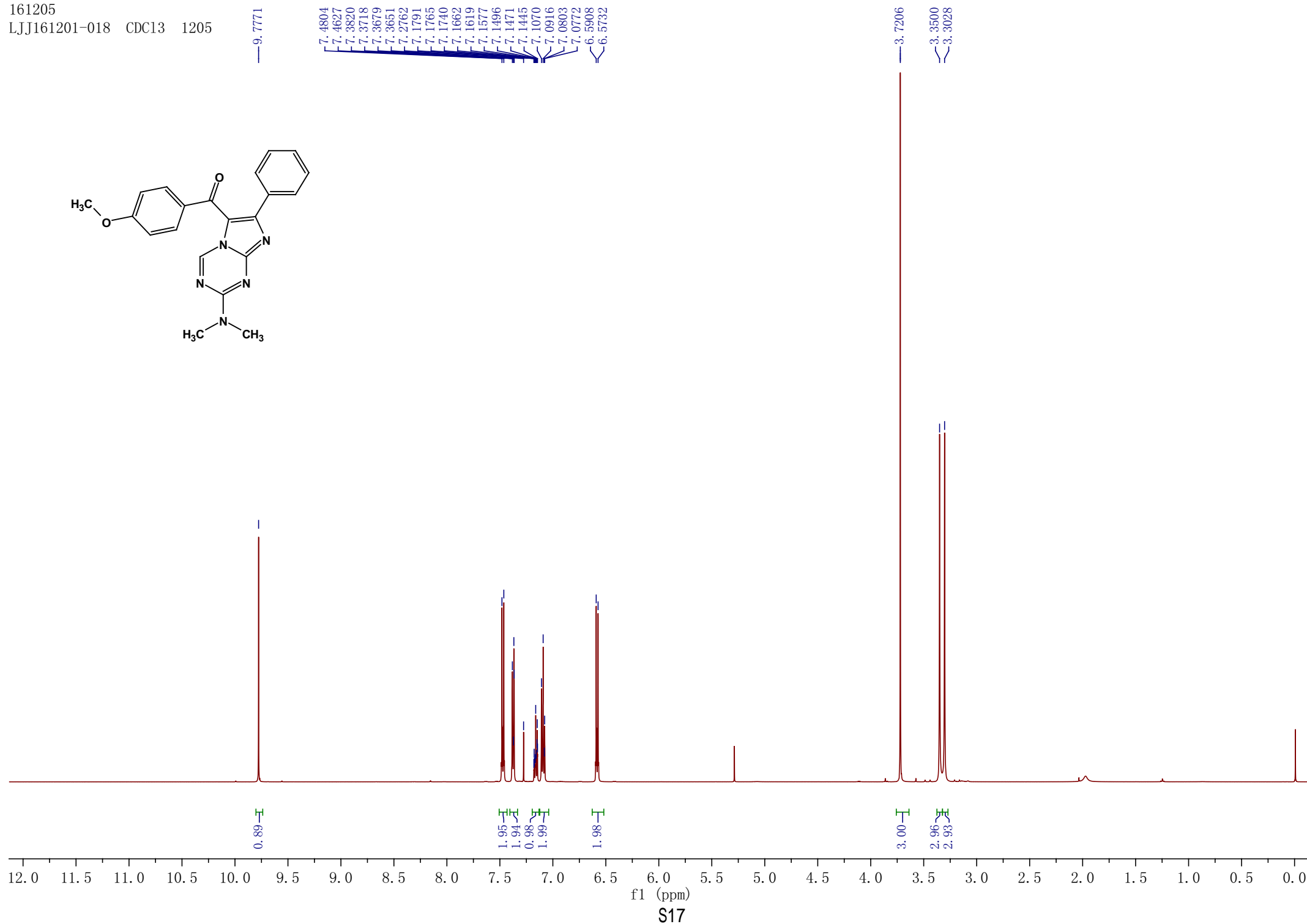
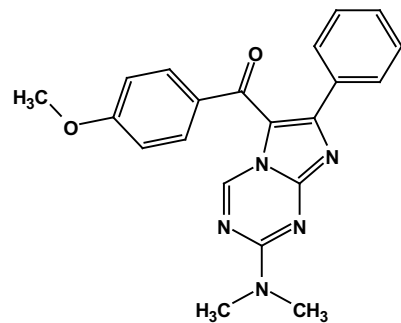
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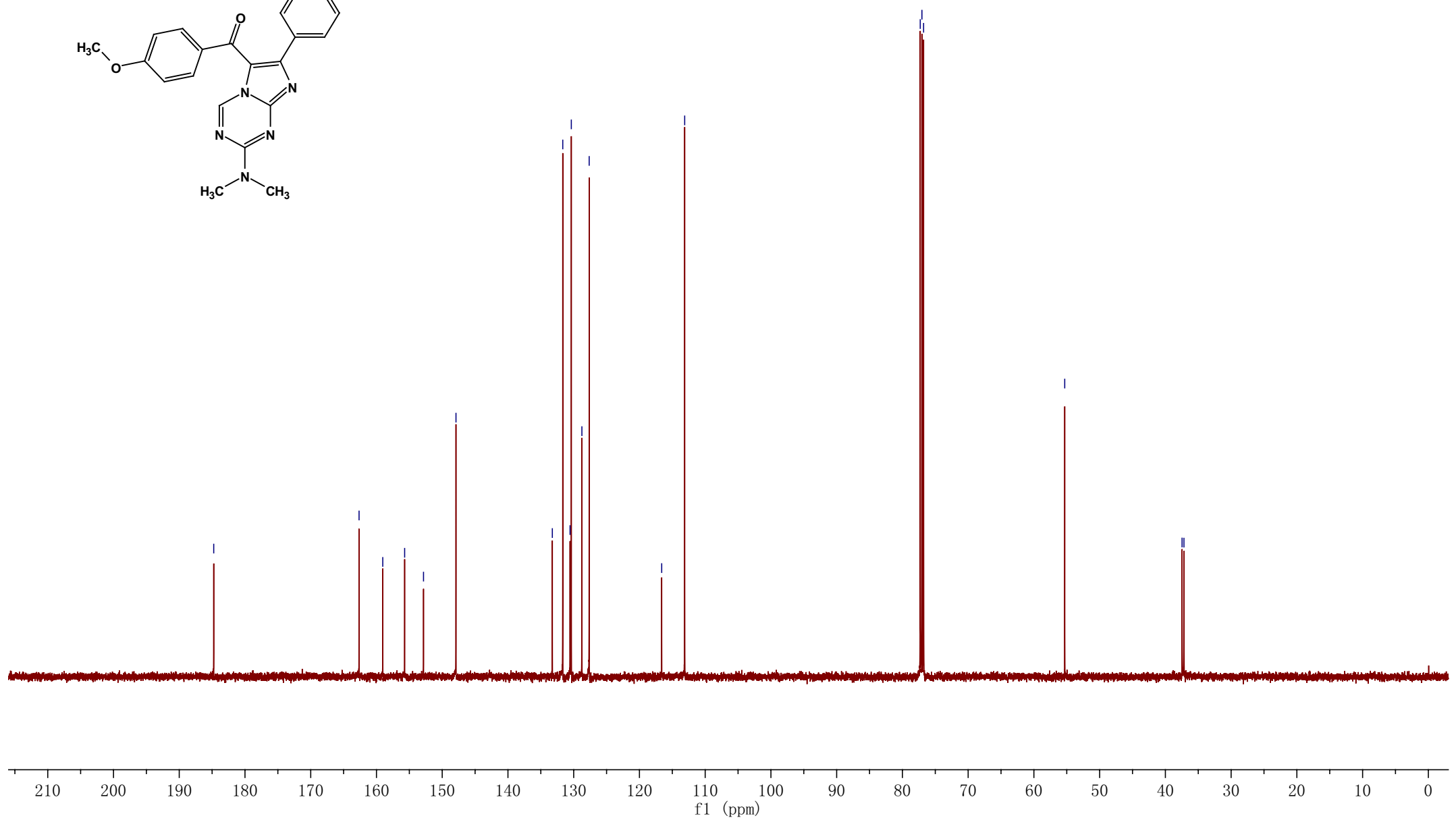
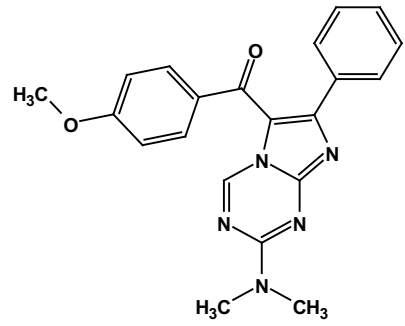
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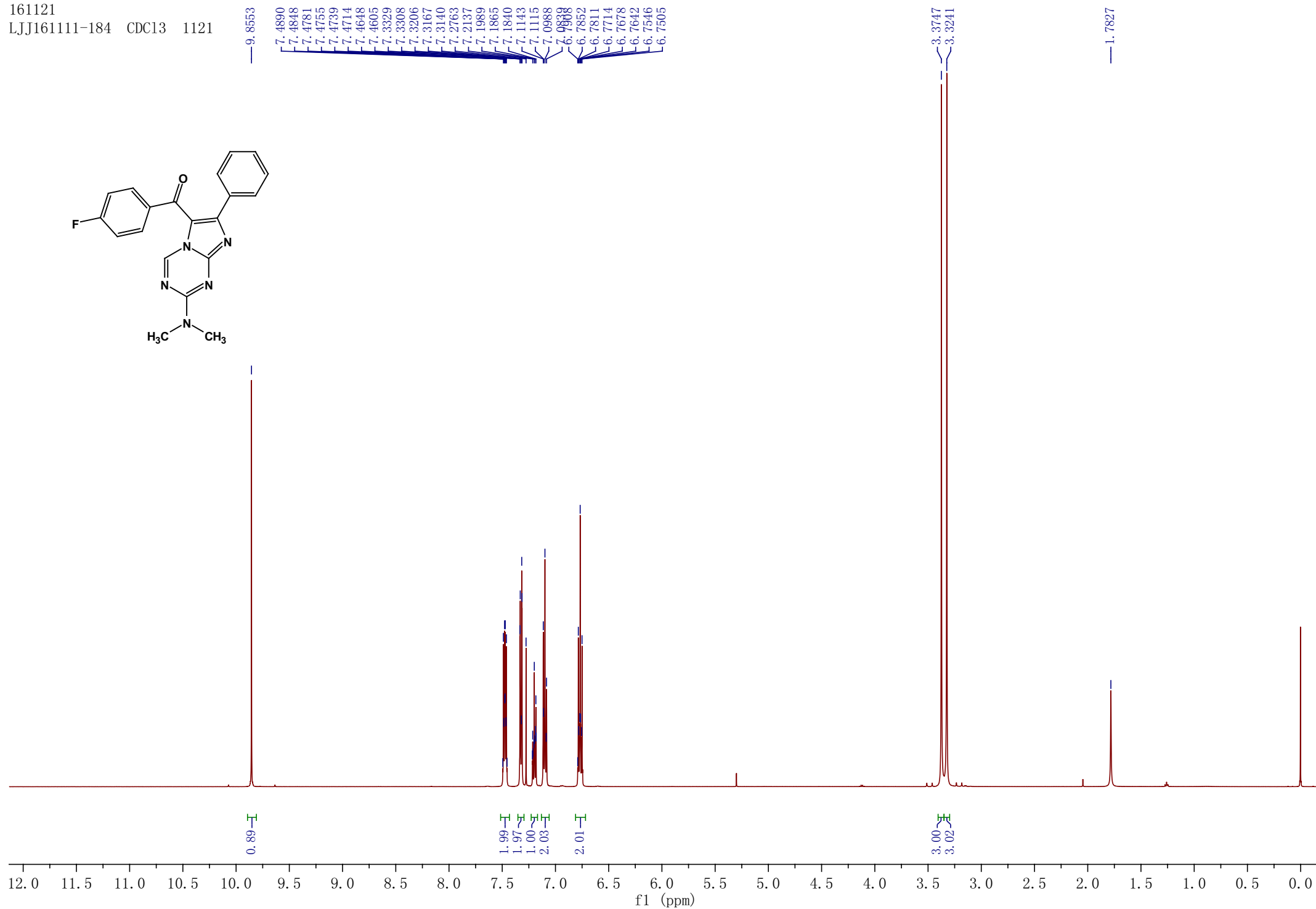
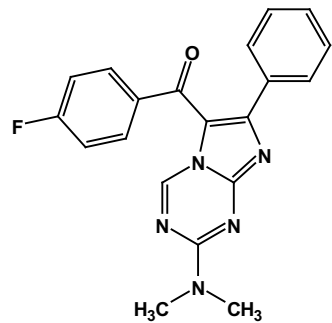
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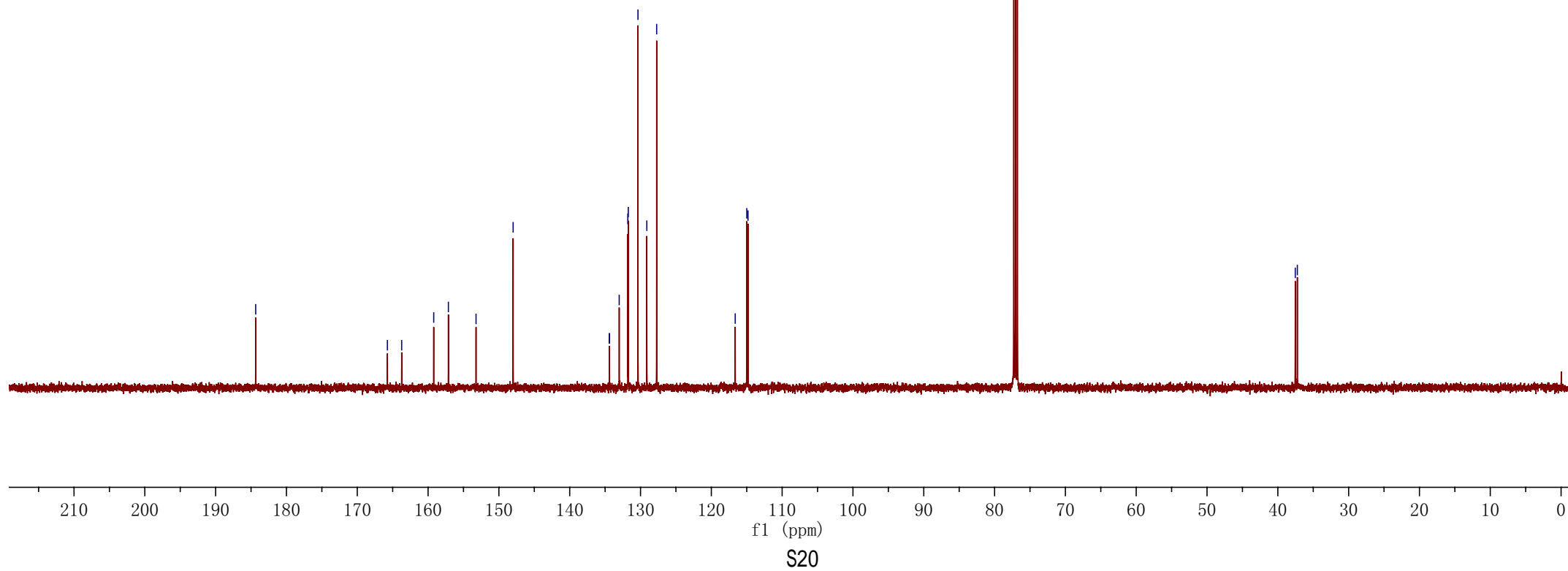
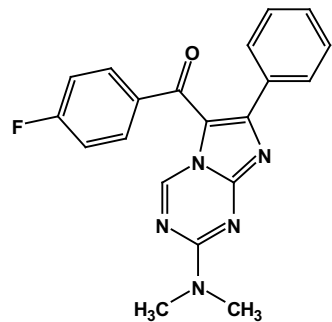
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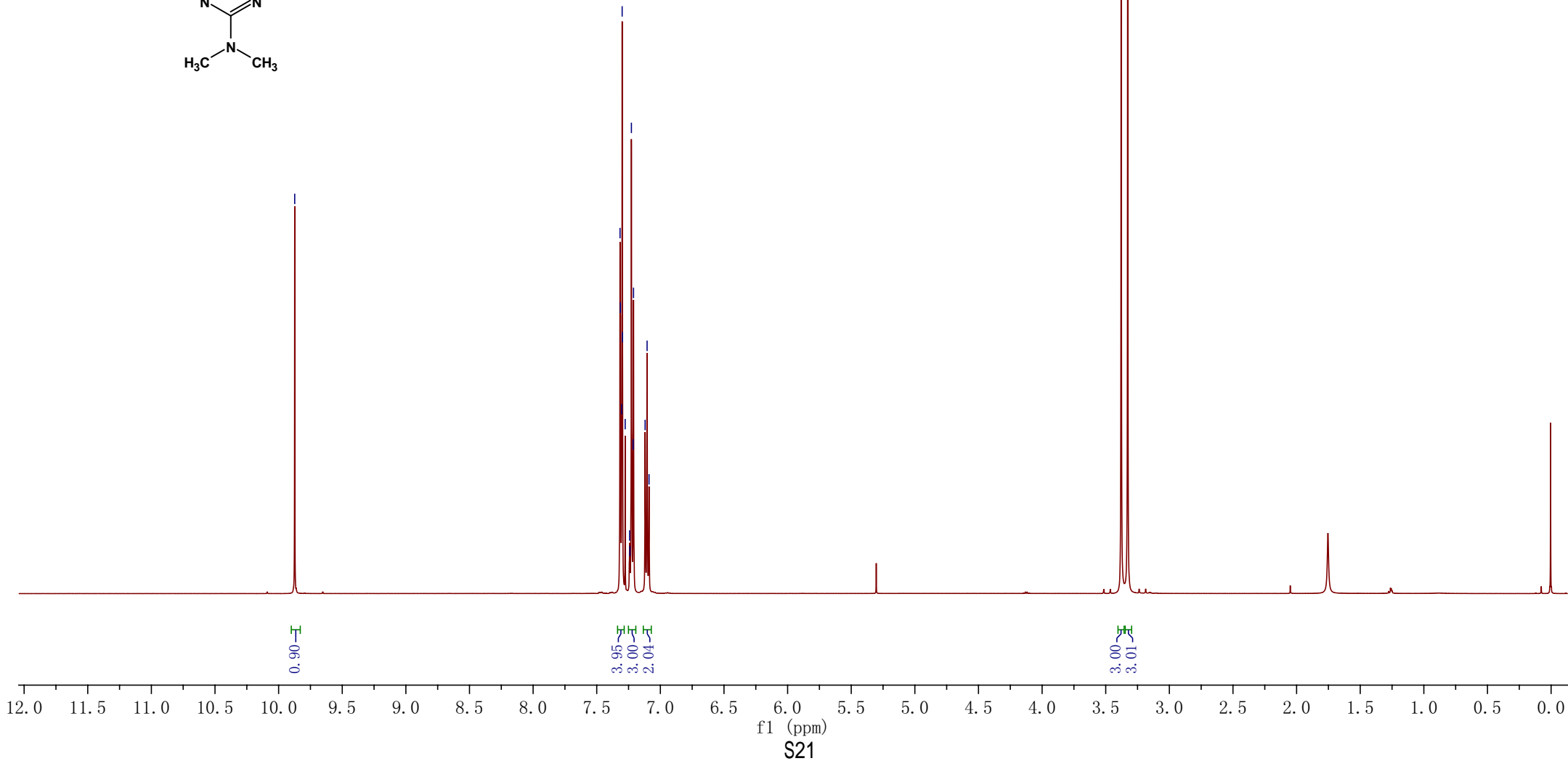
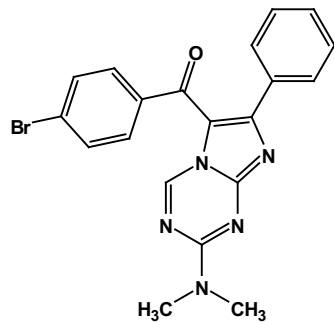


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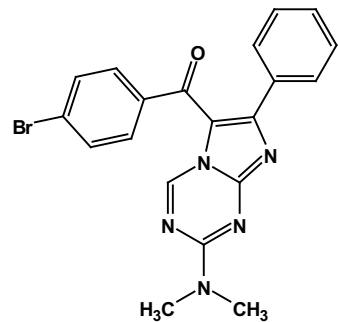
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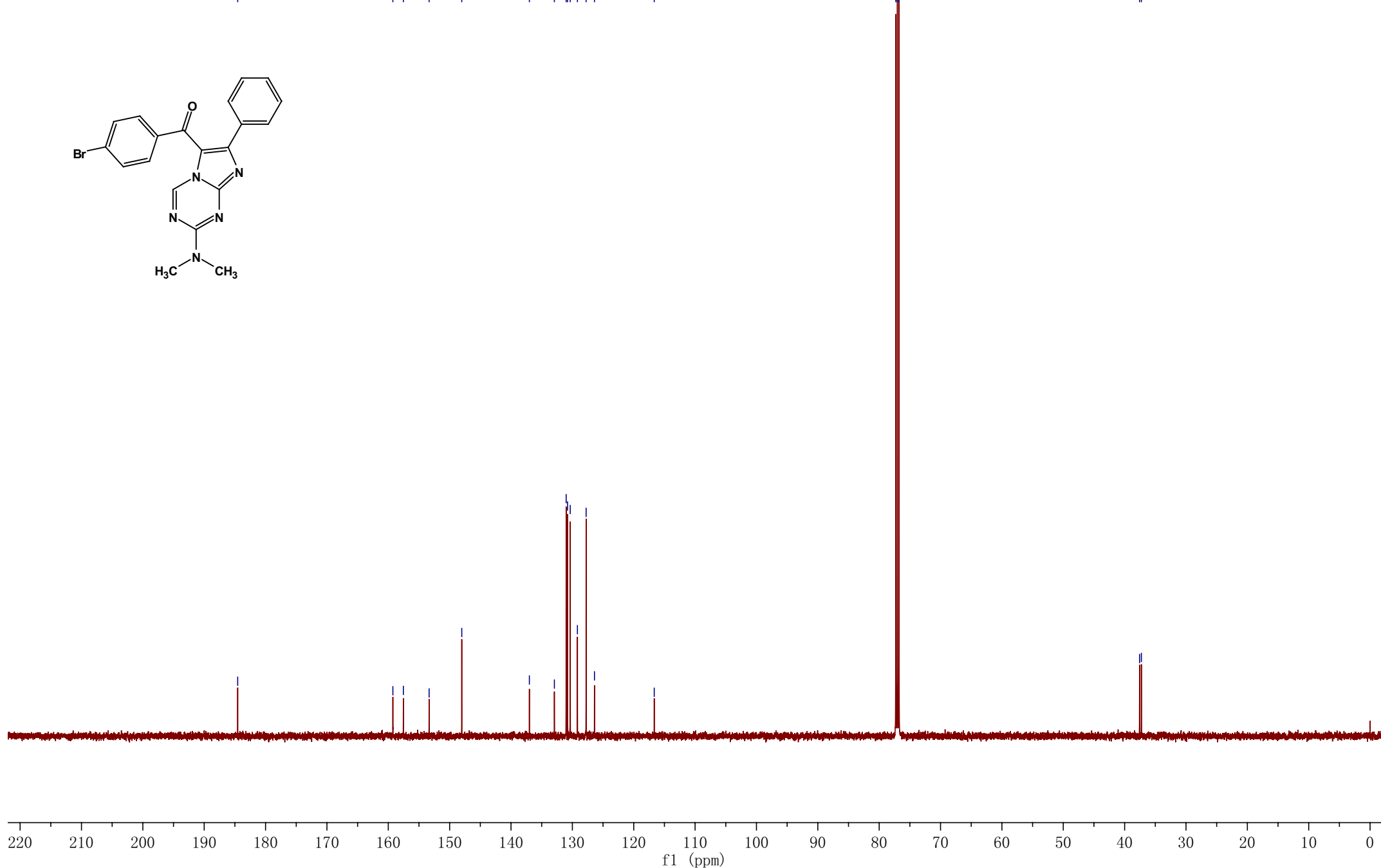
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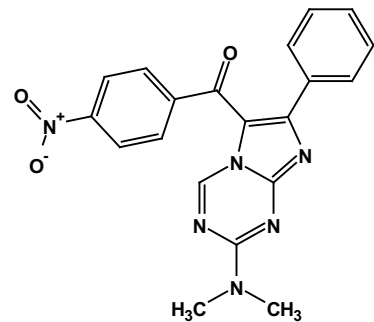
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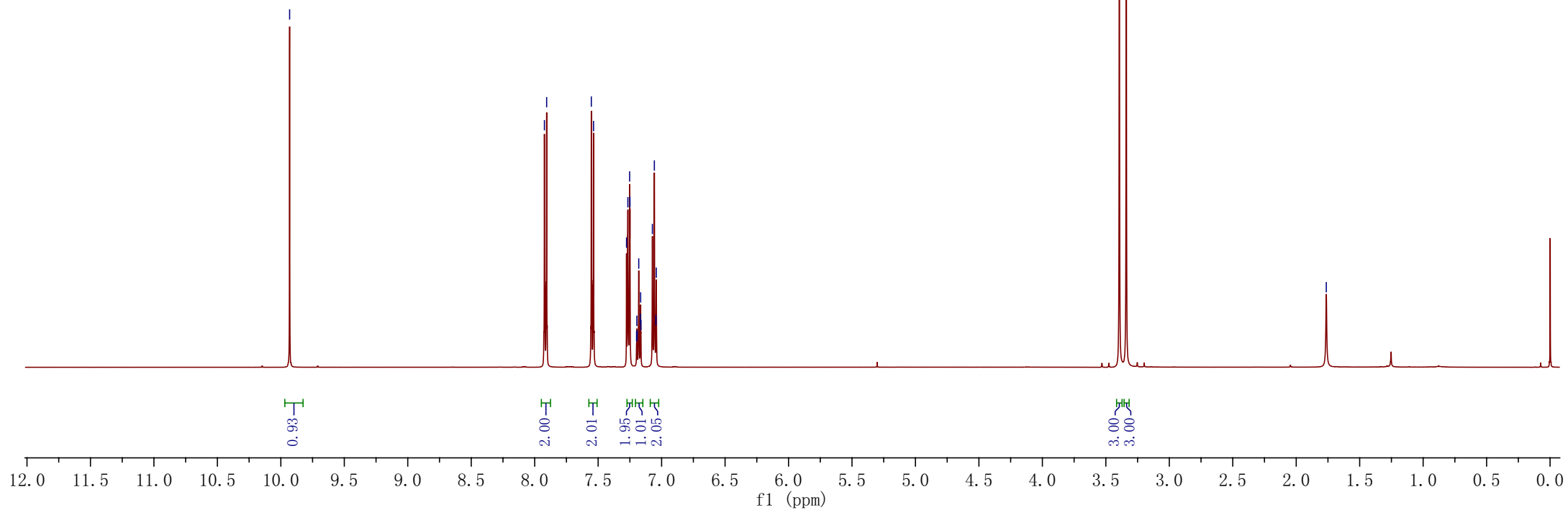


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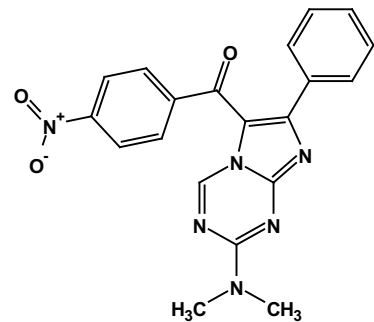
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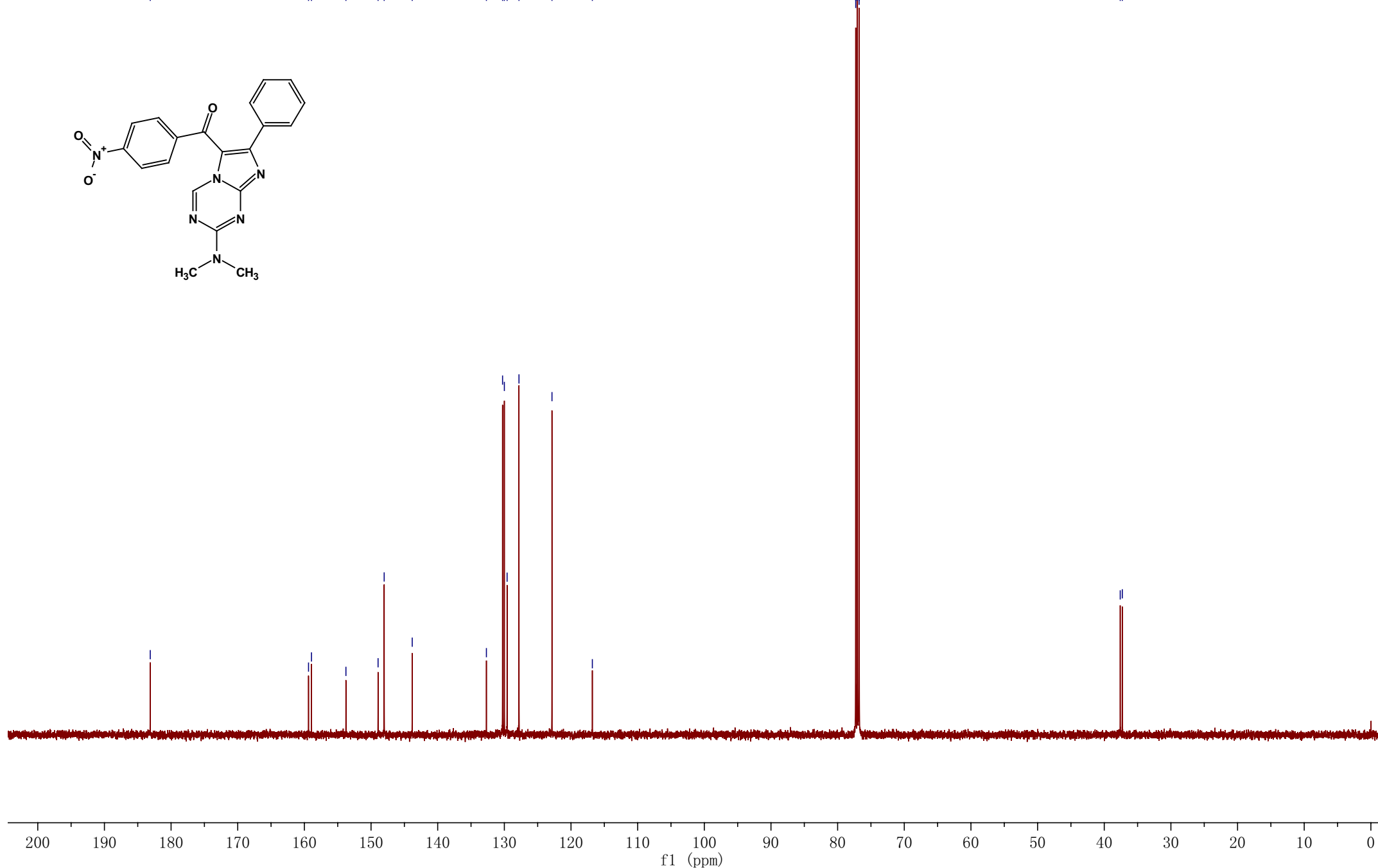
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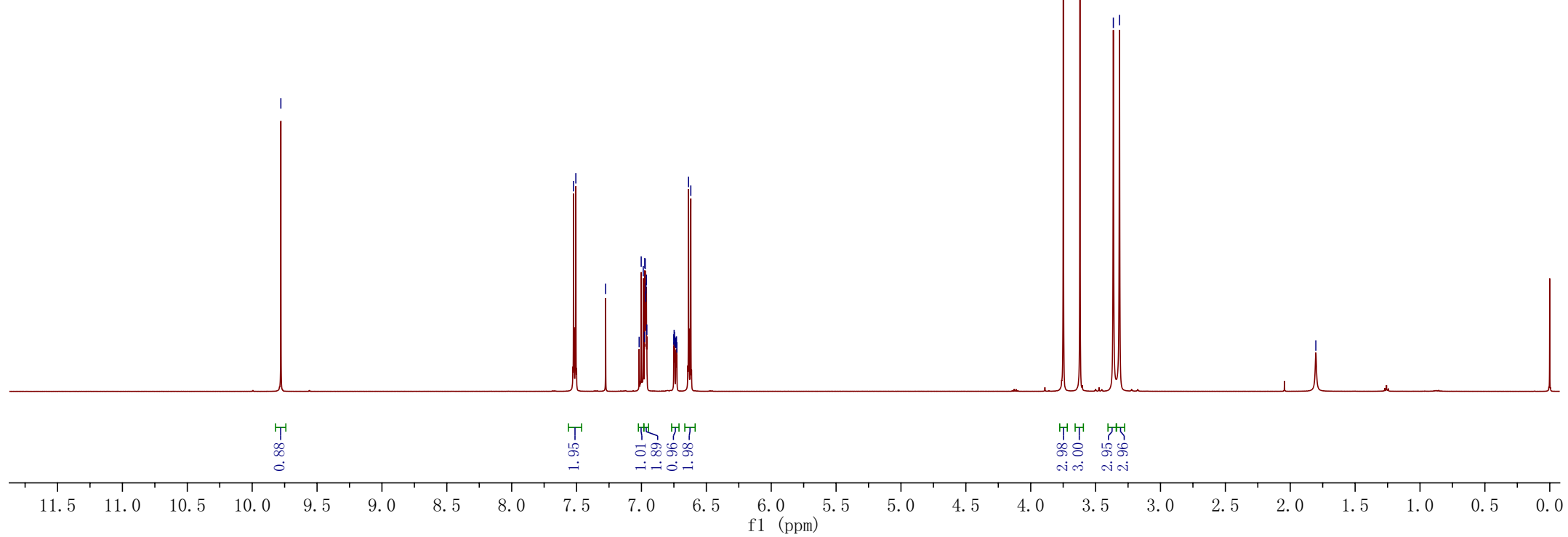
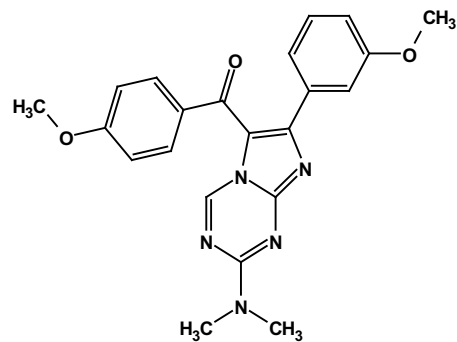
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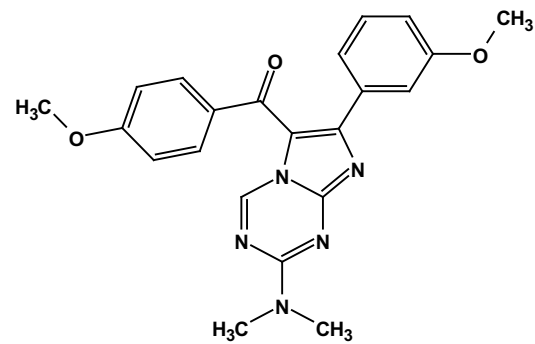
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S25

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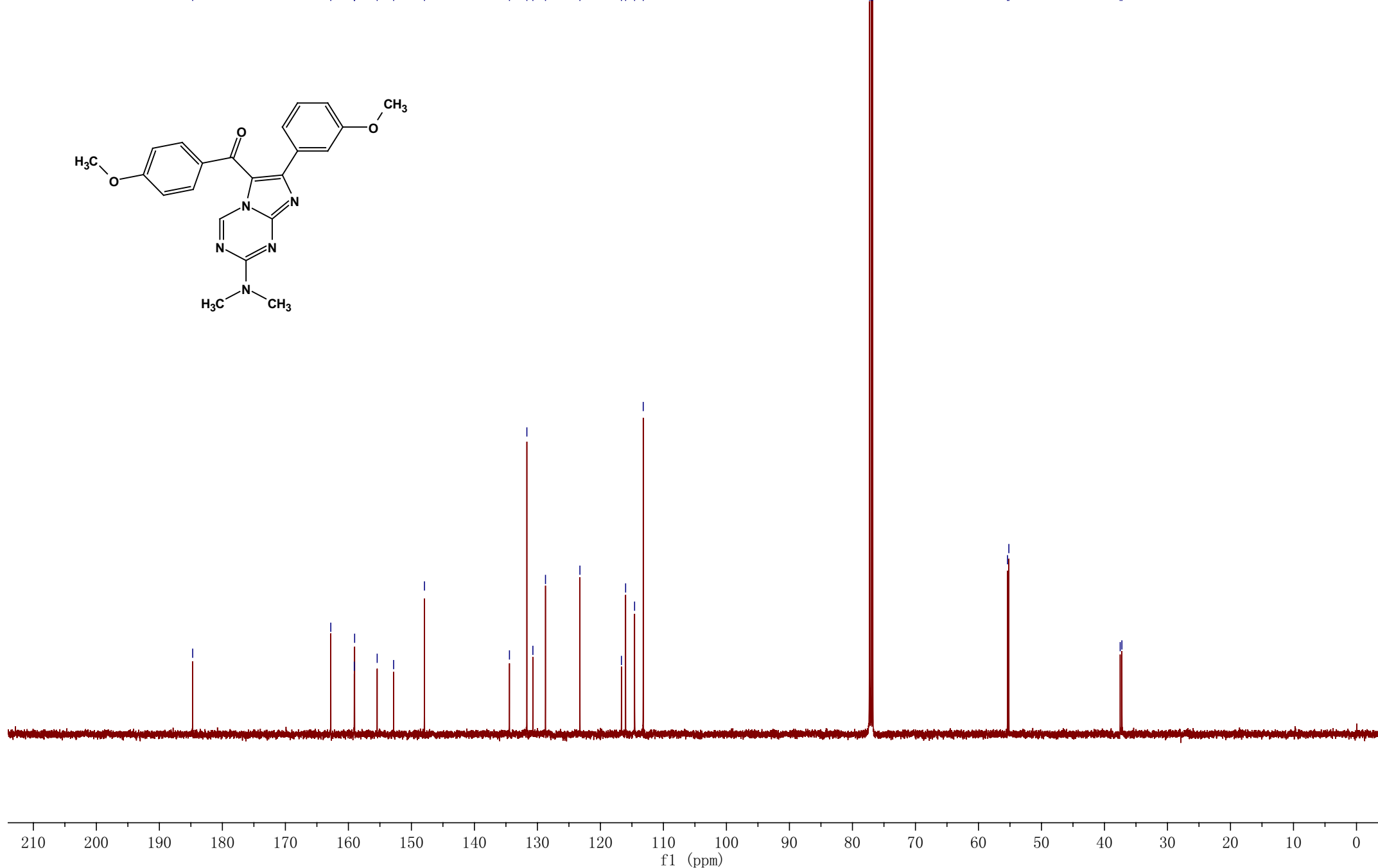
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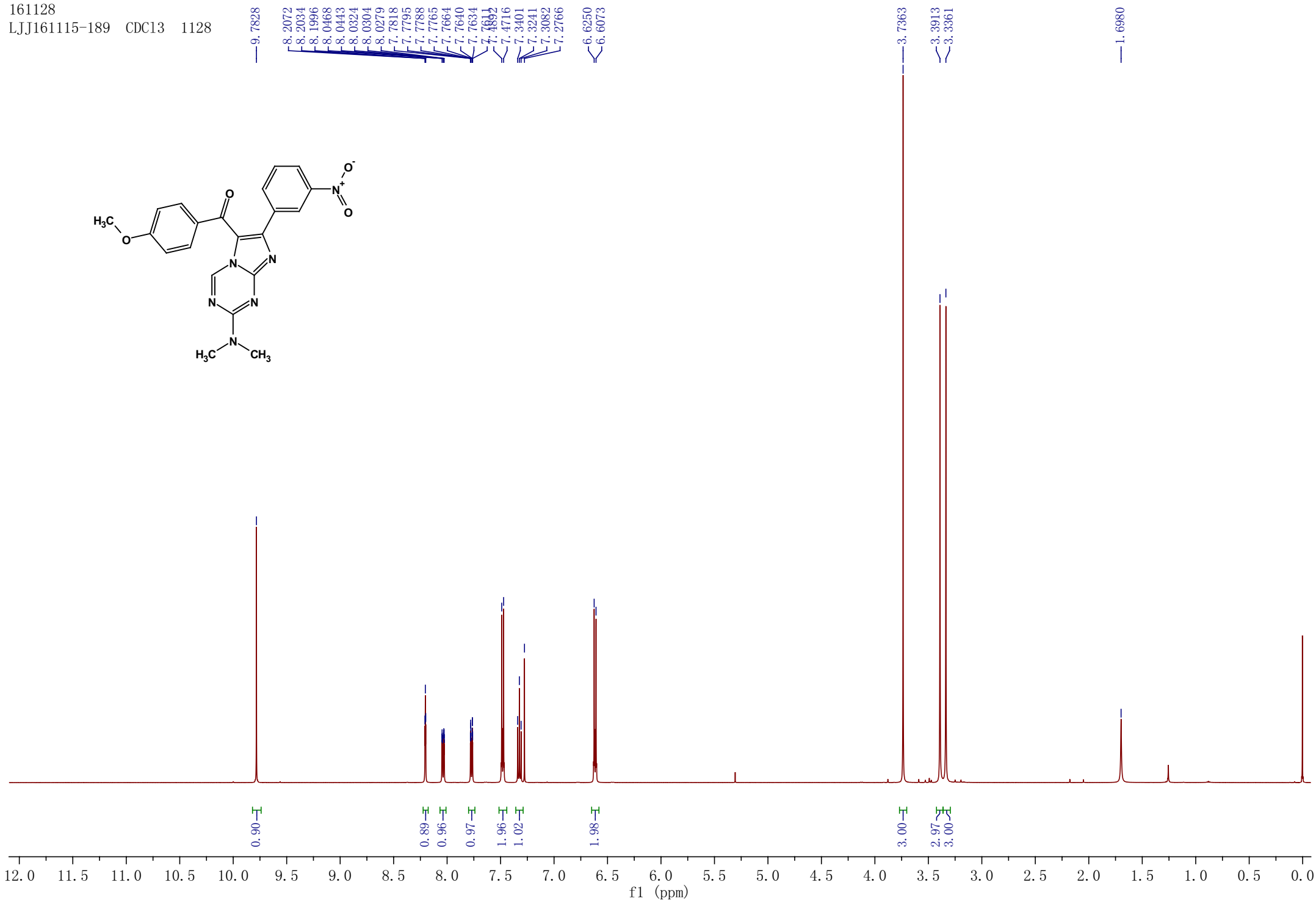
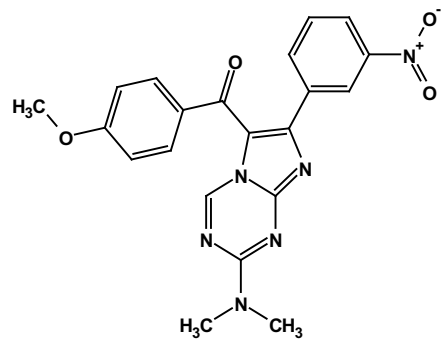
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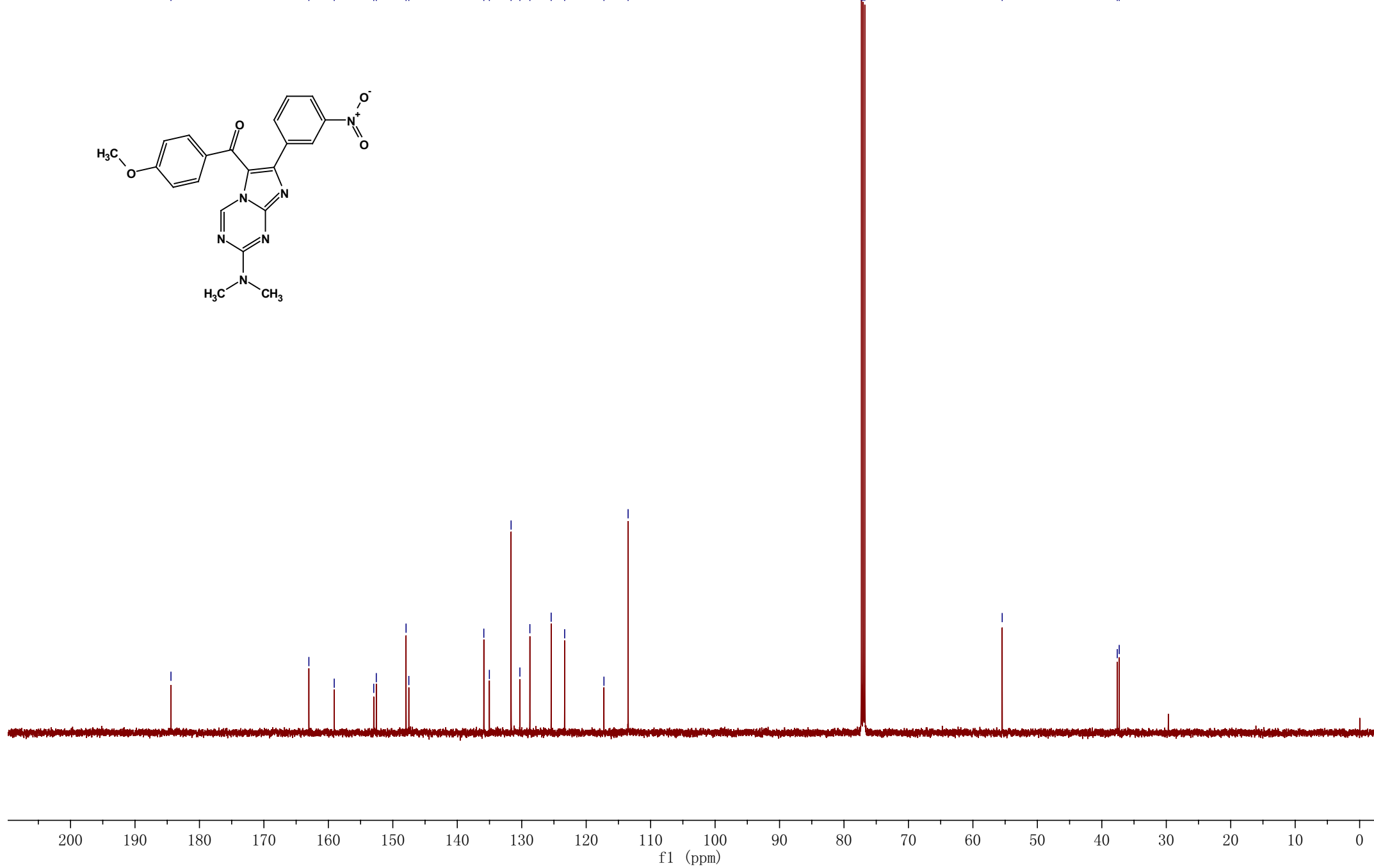
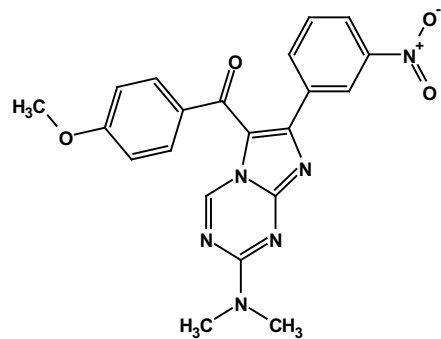
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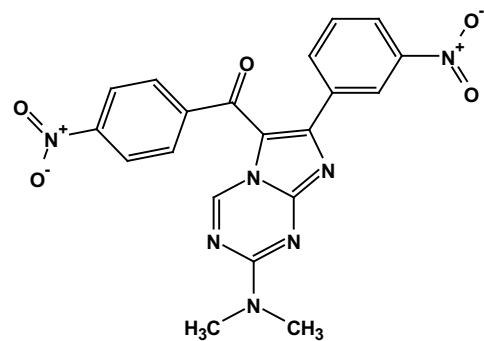
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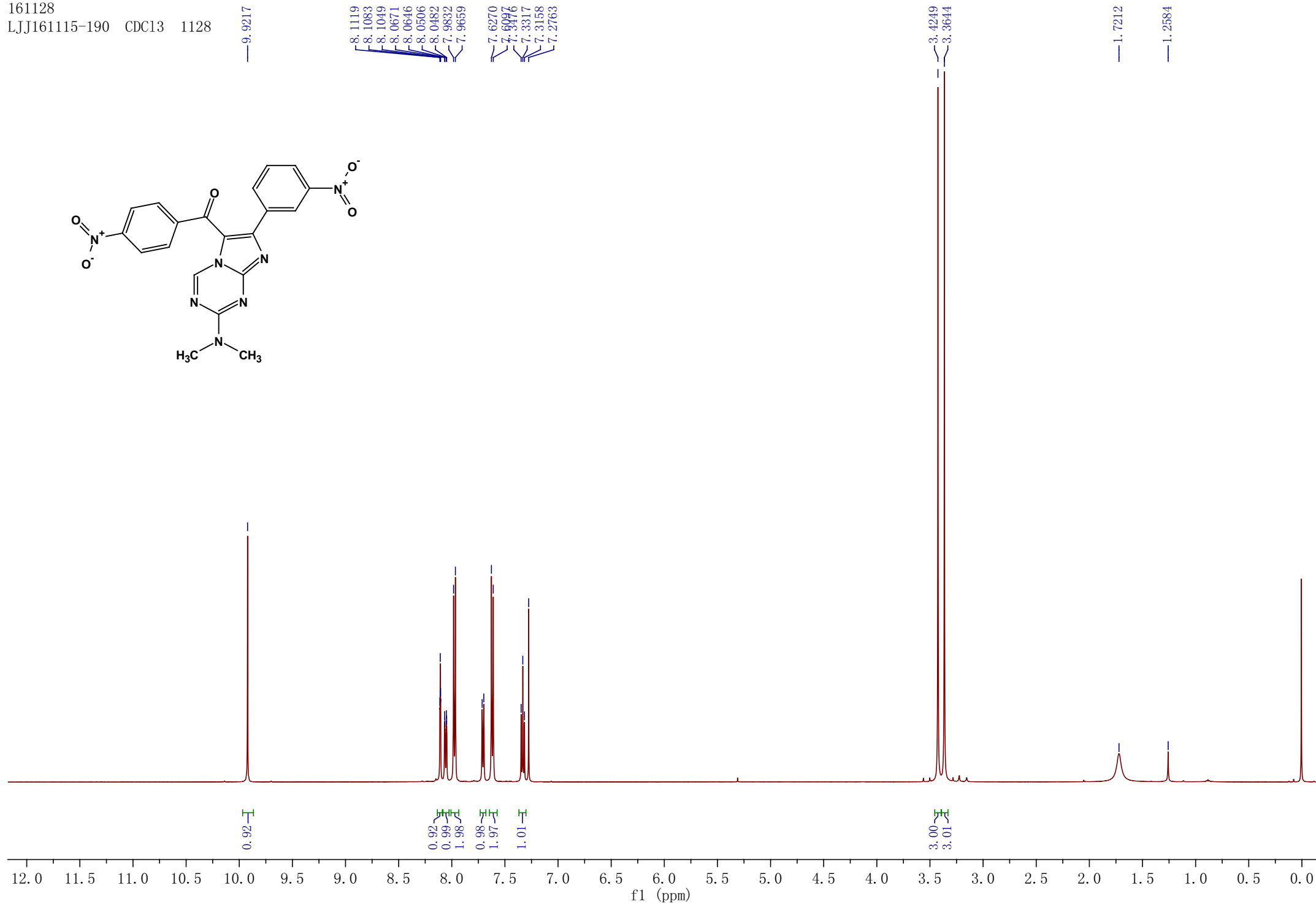


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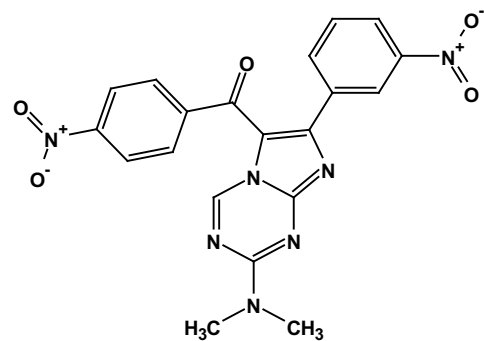
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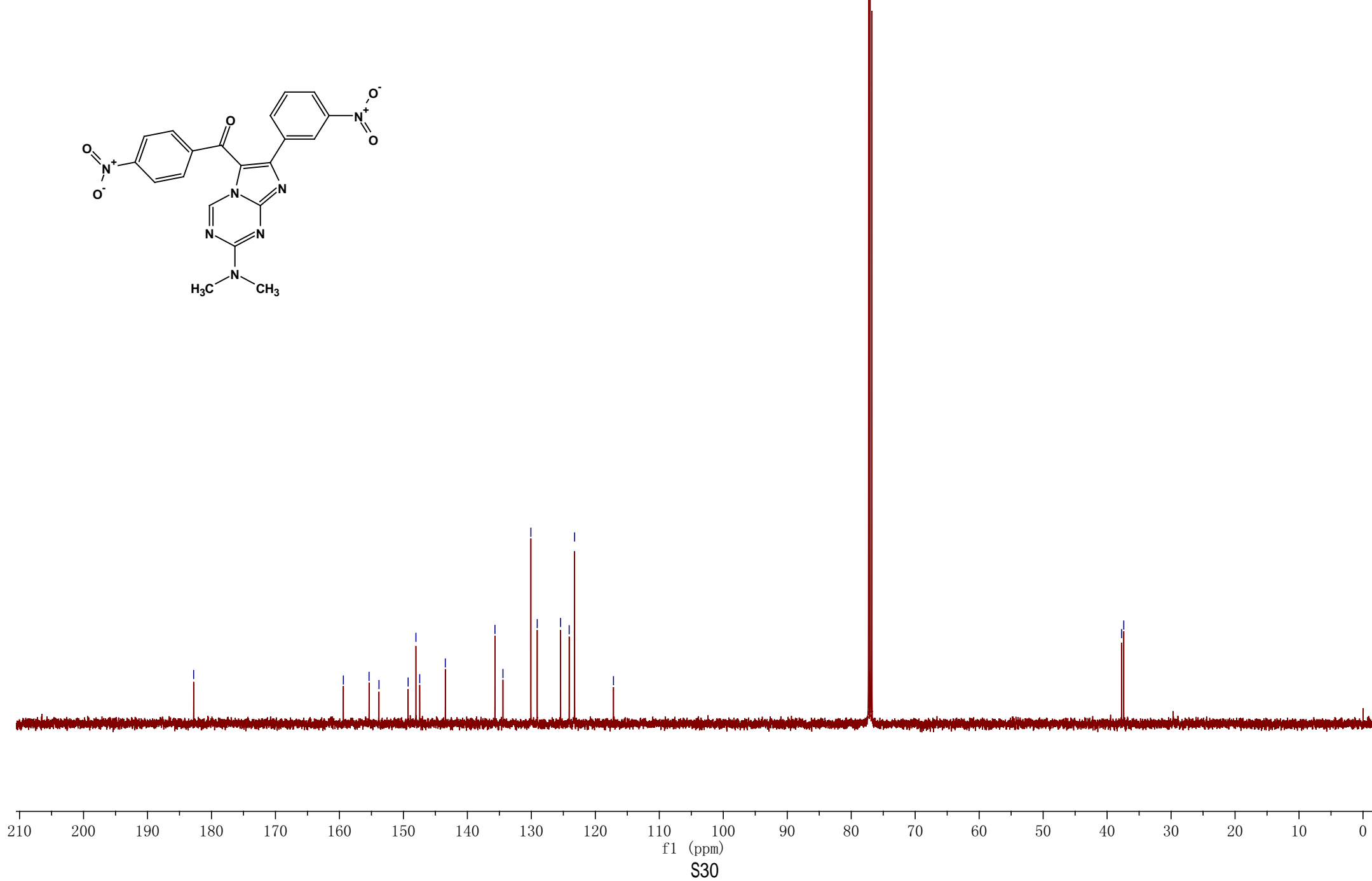
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LJJ161115-190 CDC13 1530



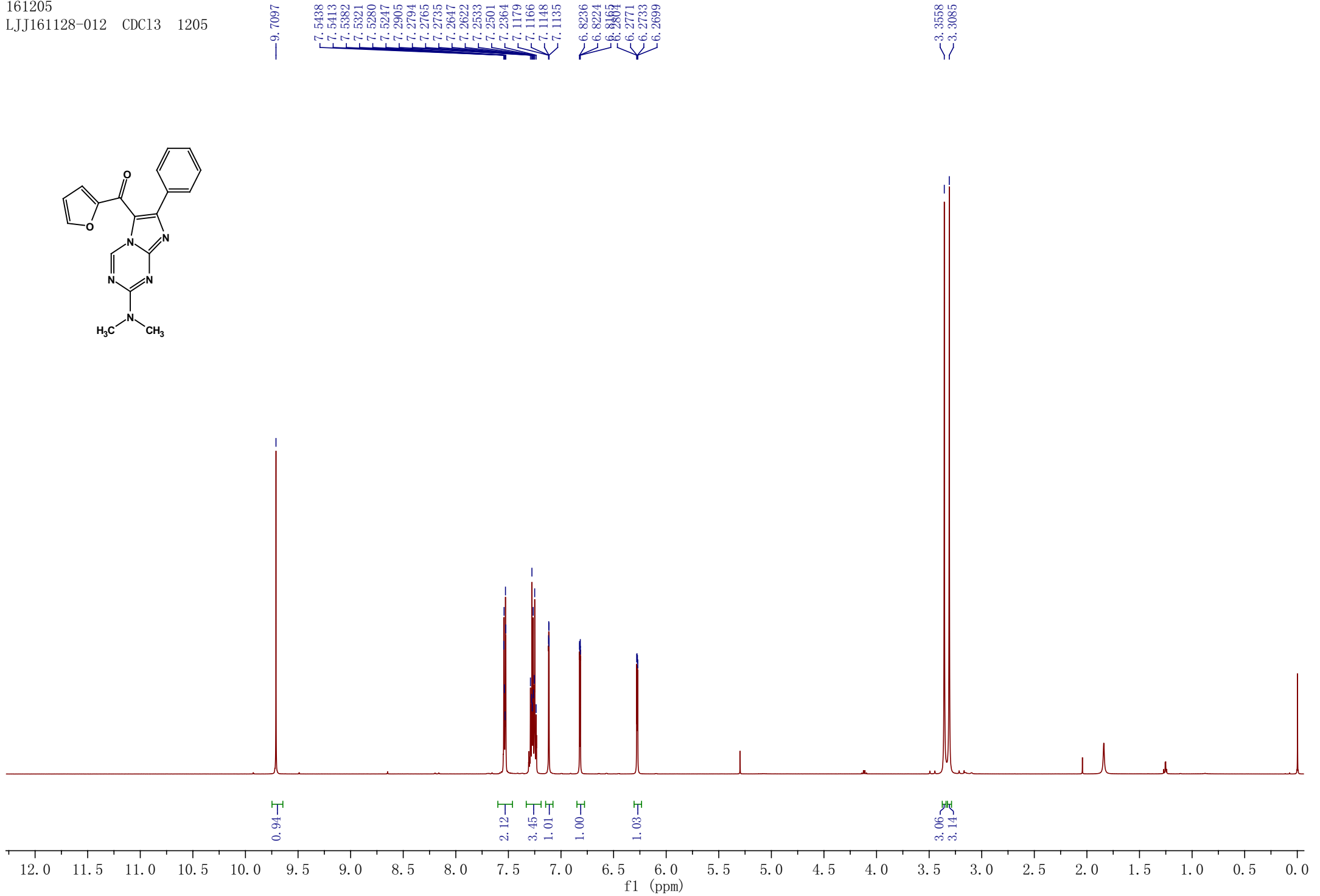
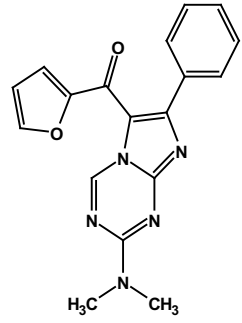
182.772
159.3859
155.3690
153.8181
149.2621
148.0404
147.4534
143.4506
135.6887
134.4386
130.0719
129.0795
125.4332
124.0886
123.2398
117.1622

77.2855
77.0315
76.7772

37.7299
37.3964

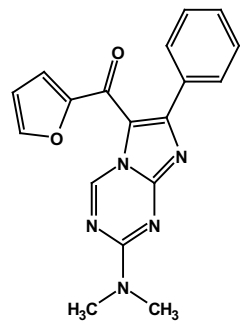


161205
LJJ161128-012 CDC13 1205

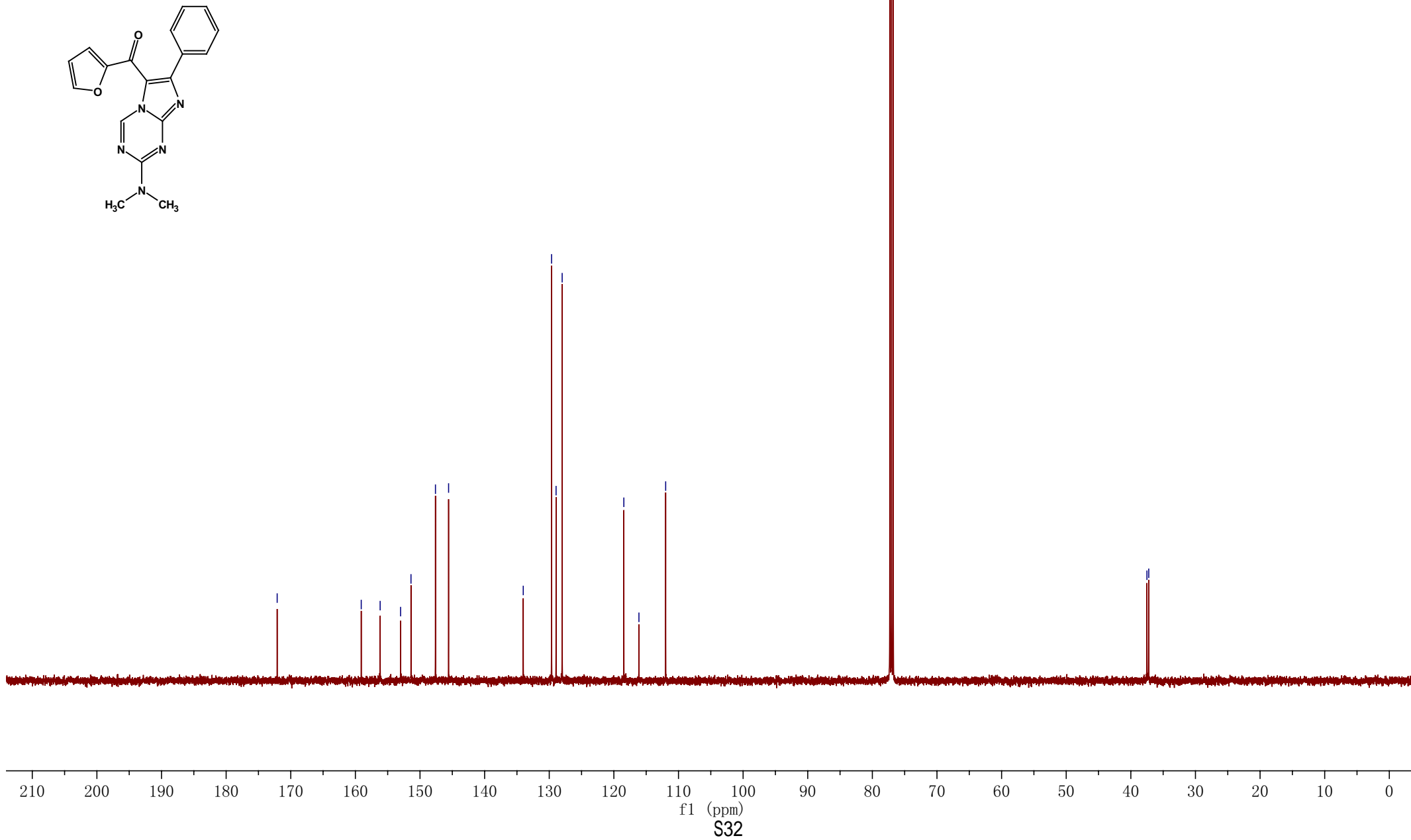


S31

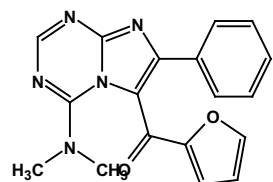
161207
LJJ161128-012 CDC13 1207



172.1025
159.0932
156.1674
153.0050
151.3944
147.6077
145.5744
134.0225
129.6416
128.9429
128.0006
118.4553
116.1207
111.9830
77.2866
77.0324
76.7780
37.5066
37.2273

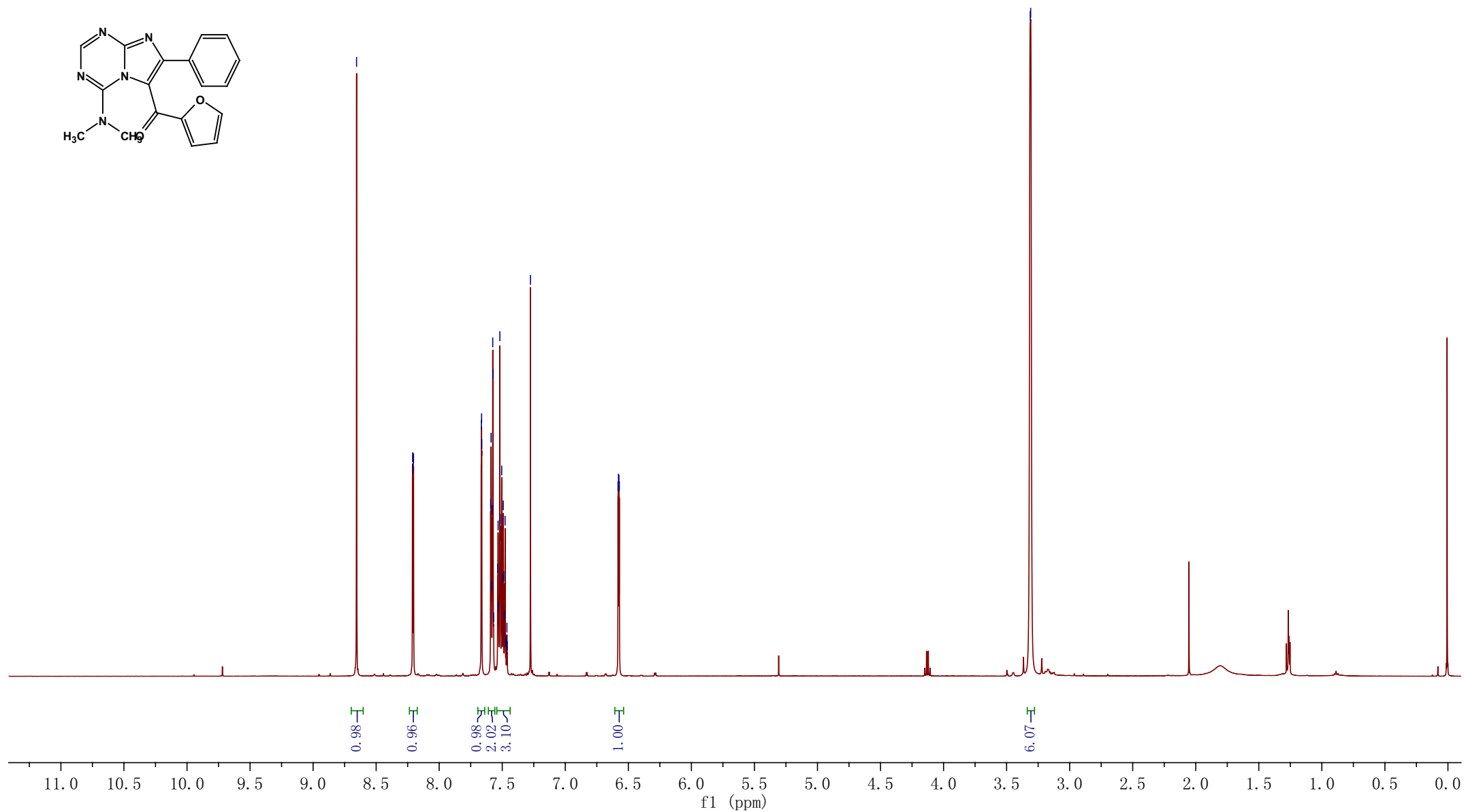


161229
LJJ161128-012-s CDC13 1229



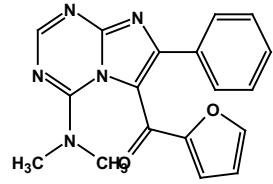
8.6553
8.2108
8.2047
8.2036
7.6638
7.5752
7.5728
7.5190
7.2767
6.5817
6.5784
6.5746
6.5713

3.3125
3.3091

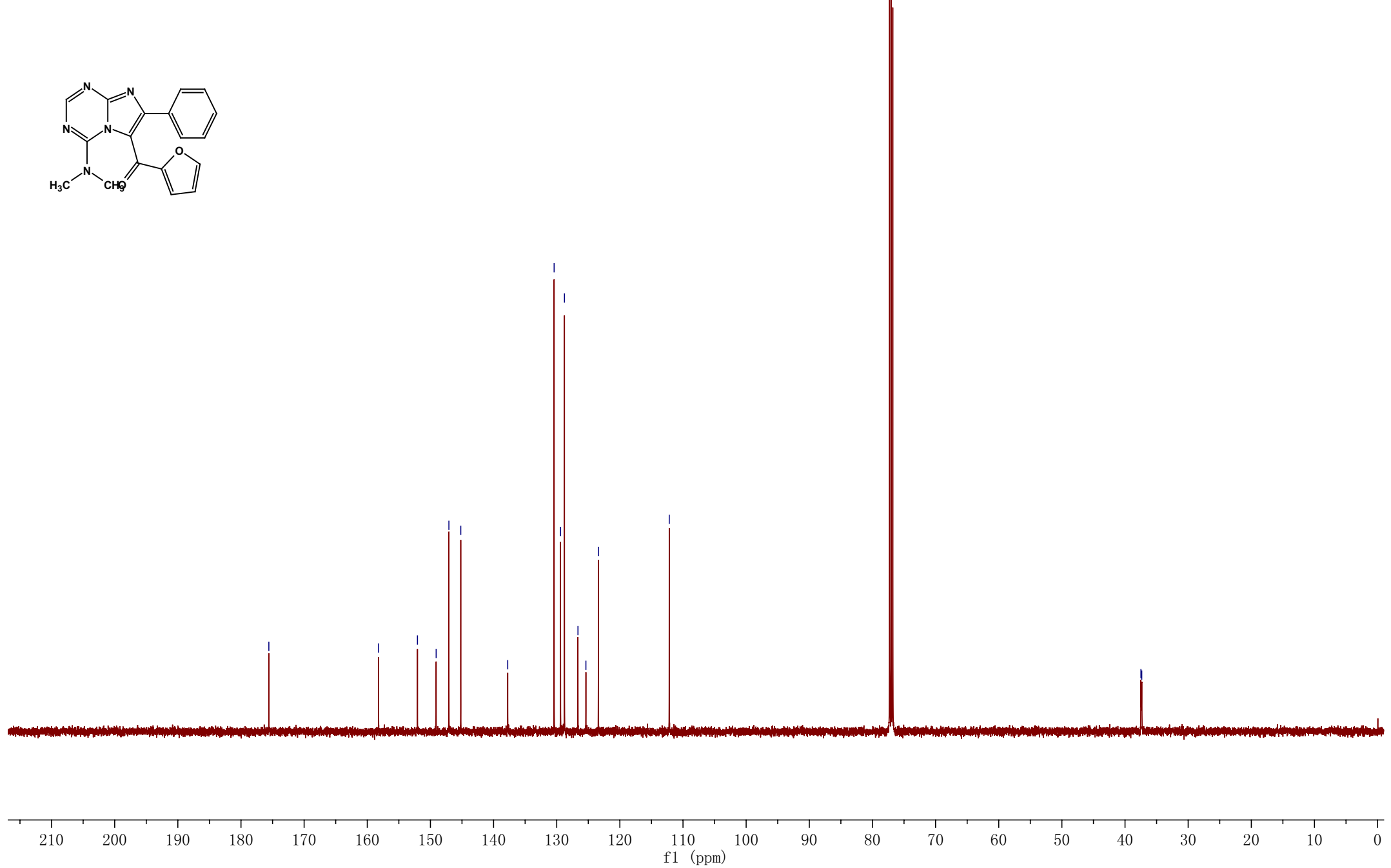


S33

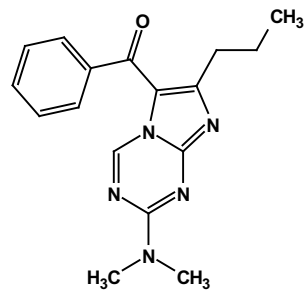
170306
LJJ161128-012-P2 CDC13 0306



175.5865
158.2121
152.0524
149.0923
147.0729
145.1922
137.7587
130.4087
129.3953
128.7748
126.6339
125.3761
123.3953
112.1787
77.2862
77.0321
76.7777
37.4801
37.3490



161219
LJJ161218-046 CDC-843 1219



9.7843

7.6271
7.6171
7.6133
7.6105
7.5741
7.5716
7.5691
7.5608
7.5568
7.5530
7.5444
7.5419
7.5394
7.4885
7.4731
7.4615
7.4585
7.2765

3.3301
3.2787

2.2931
2.2780
2.2625
1.9762
1.6739
1.6591
1.6440
1.6288
1.6139
1.5992
0.7183
0.7036
0.6888

0.90

1.95
1.00
2.00

3.02
3.06

1.99

2.00

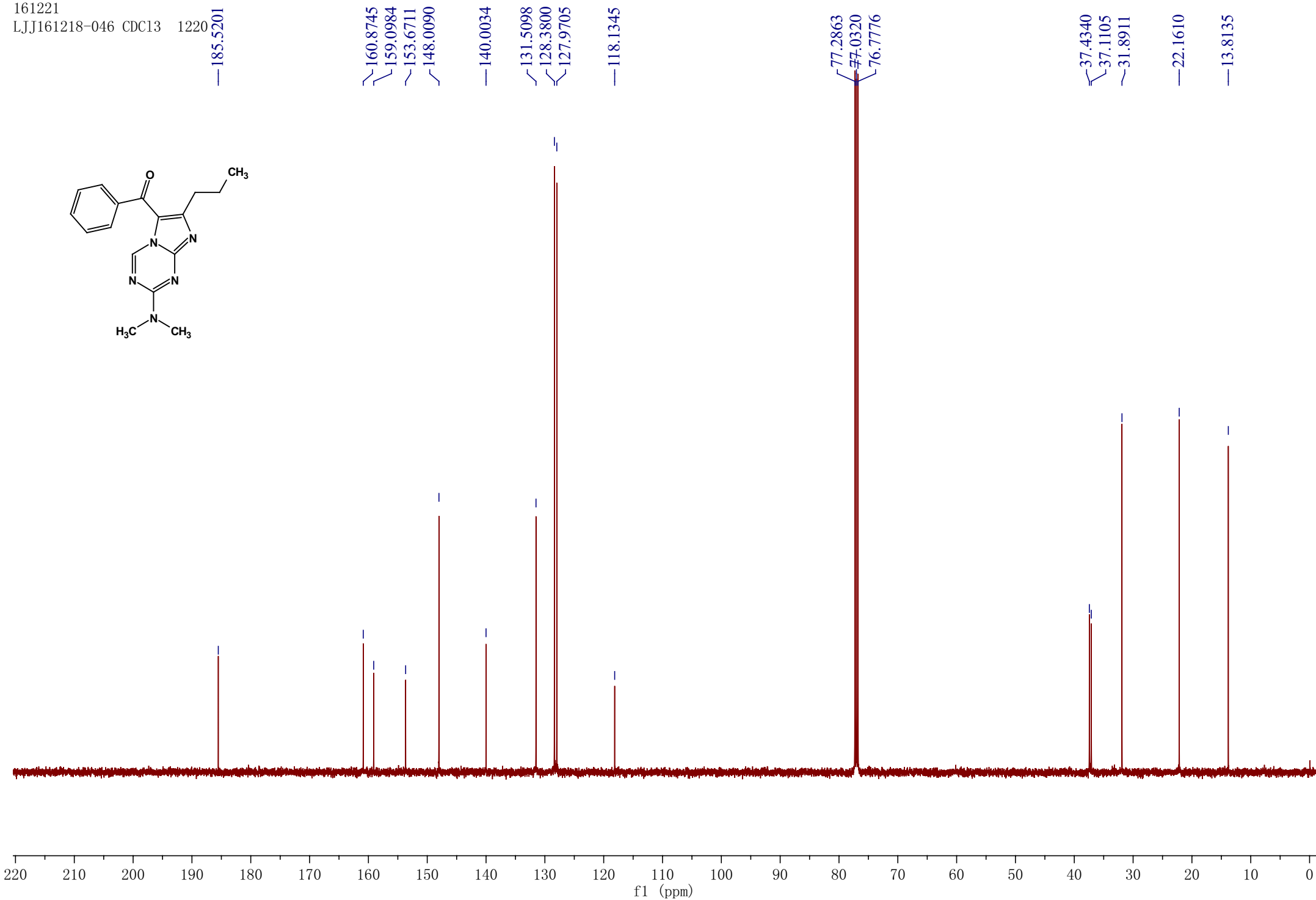
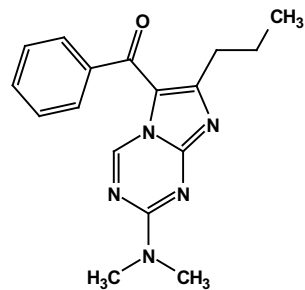
3.00

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

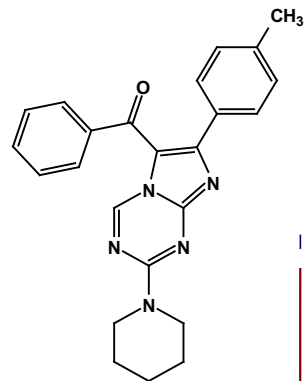
f1 (ppm)

S35

161221
LJJ161218-046 CDC13 1220



161201
LJJ161125-006 CDC13 1201

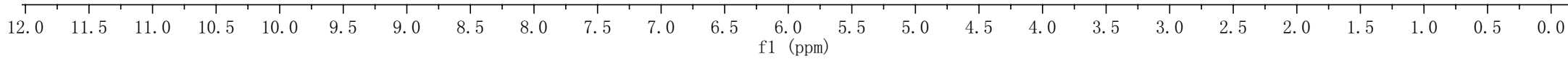


—9.8498

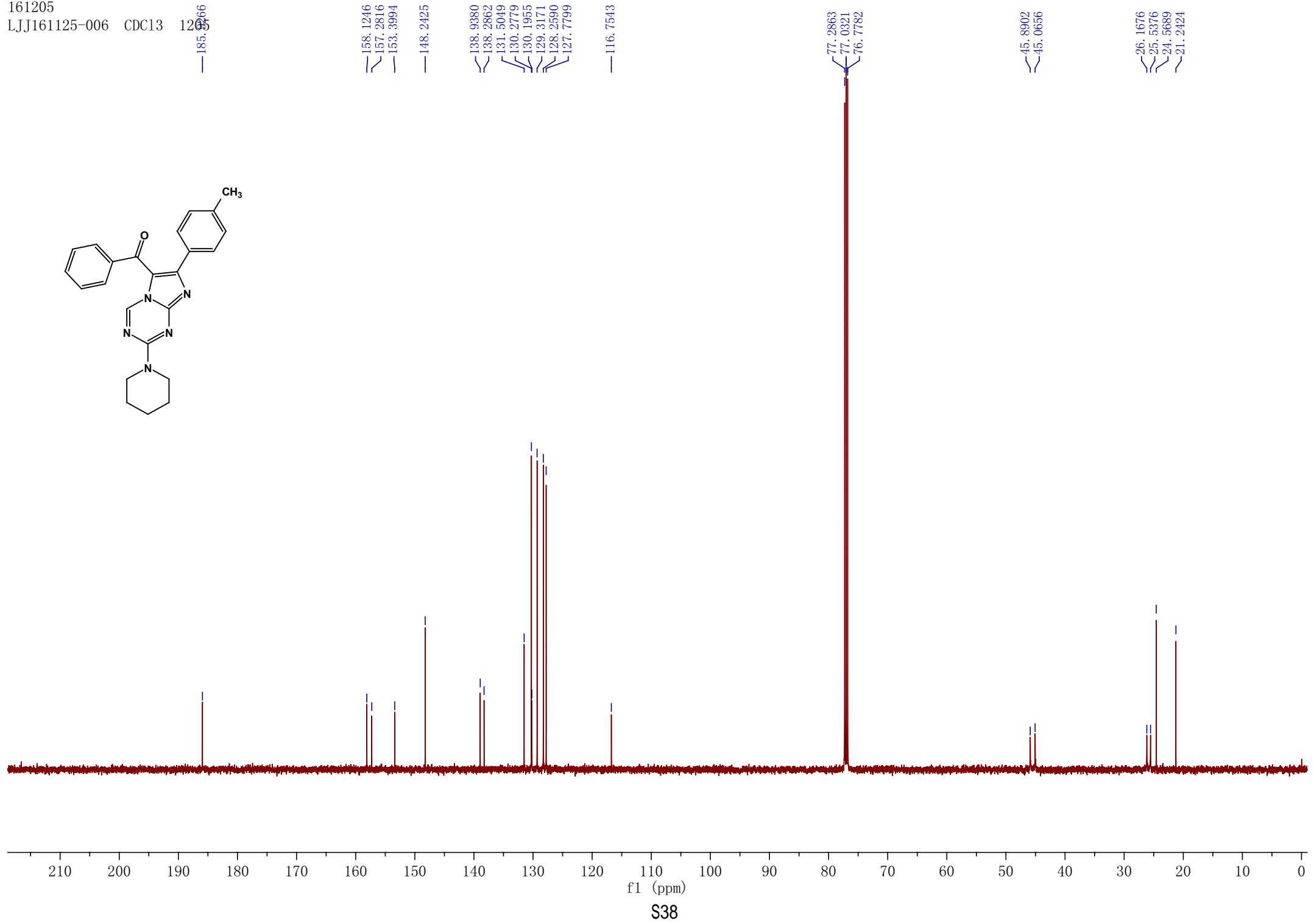
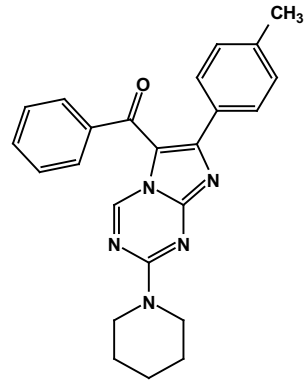
7.4754
7.4732
7.4625
7.4591
7.4566
7.3018
7.2993
7.2969
7.2844
7.2765
7.2721
7.2695
7.2671
7.2269
7.2107
7.1184
7.1154
7.1031
7.1024
7.0906
7.0872
6.8601
6.8443

—3.9725

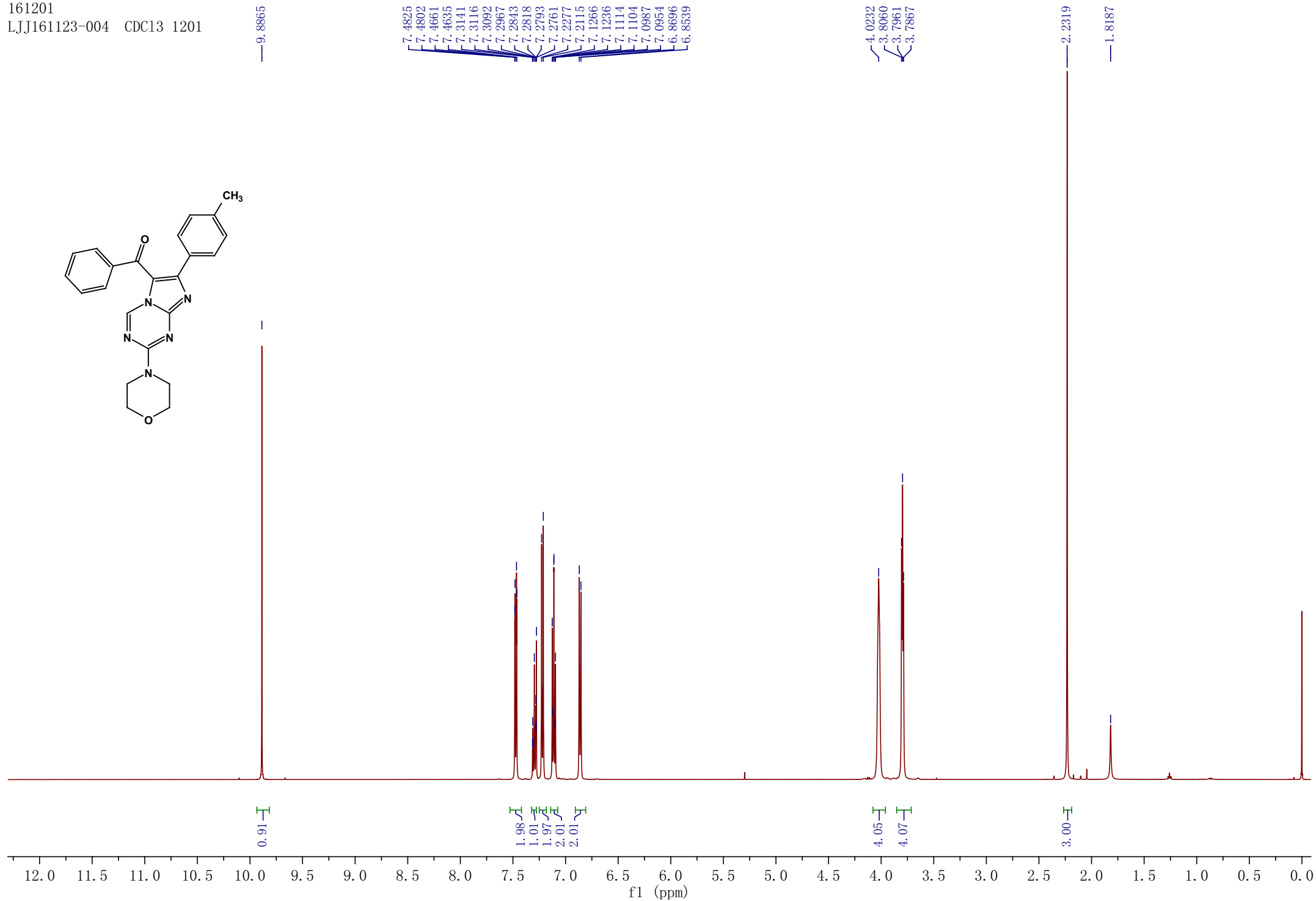
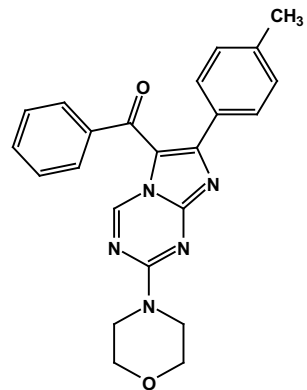
2.2293
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1.7536
1.7394
1.7304
1.7189
1.6728



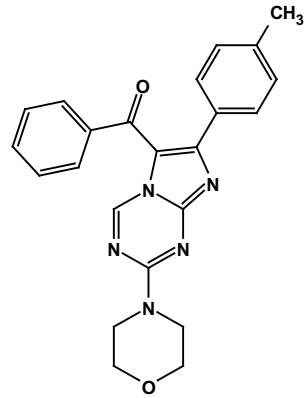
161205
LJJ161125-006 CDC13 128.95



161201
LJJ161123-004 CDC13 1201



161205
LJJ161123-004 CDC13 1205



186.1225

158.3588
157.1387
152.8843
148.5078

139.1244
138.0578
131.6956
130.2843
129.9740
129.3288
128.3323
127.8339

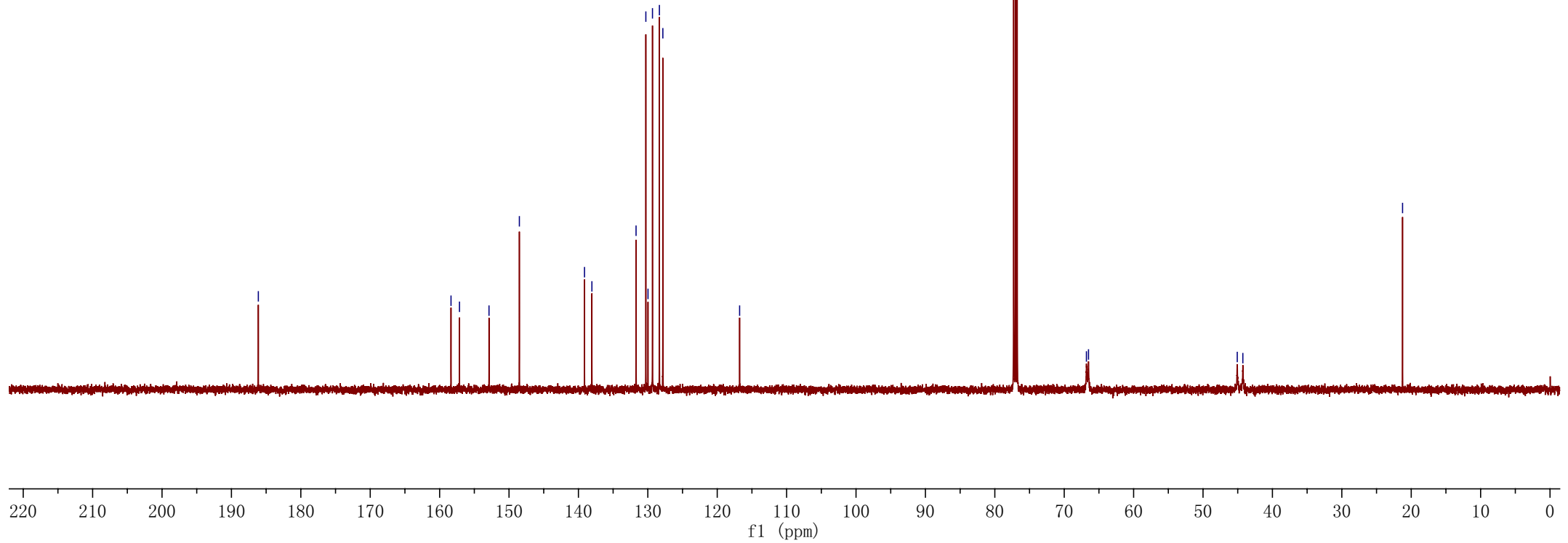
116.7730

77.2865
77.0321
76.7781

66.8018
66.5008

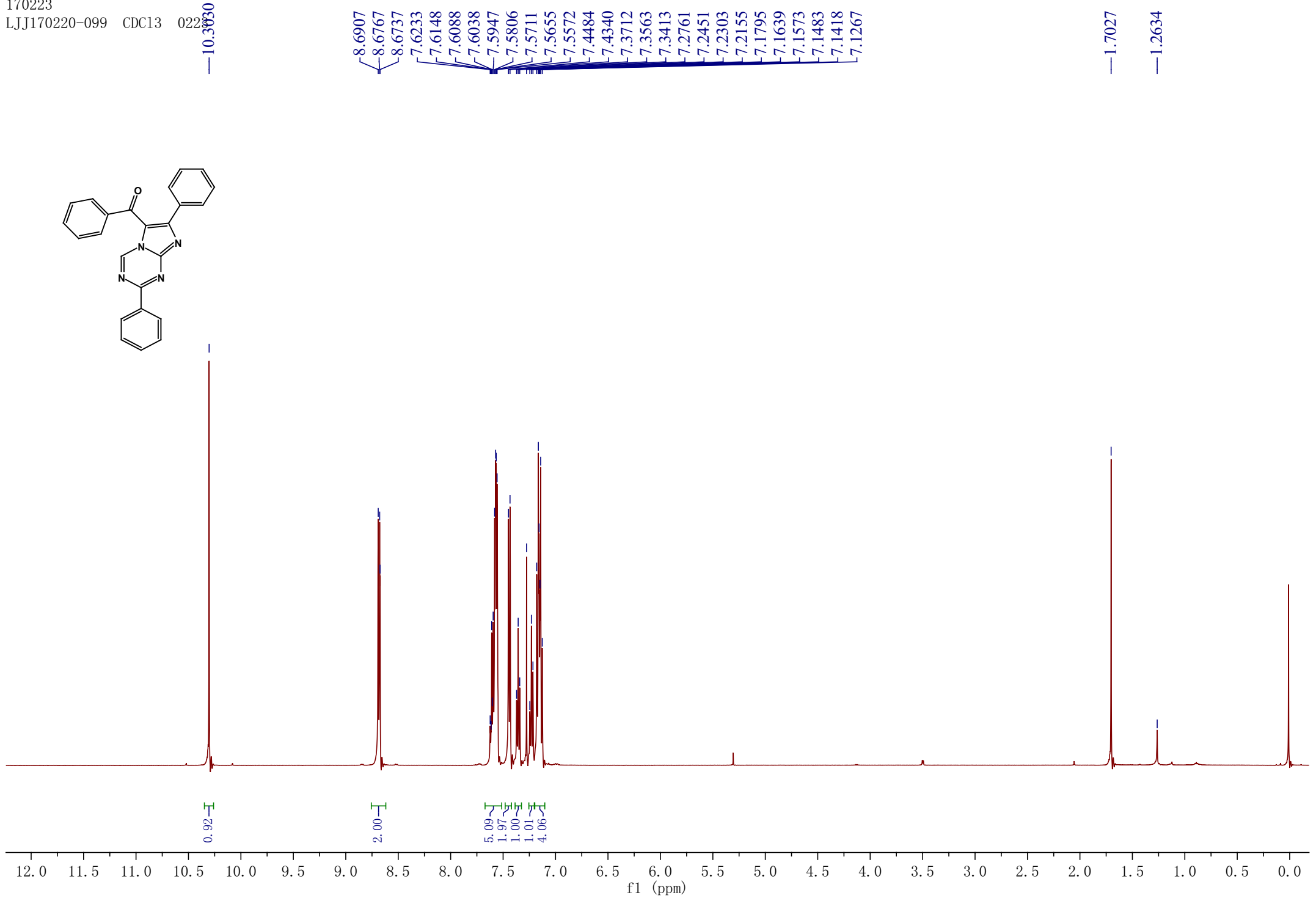
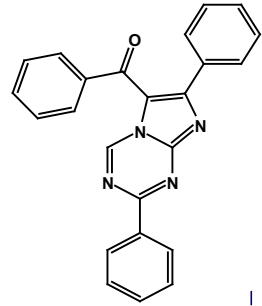
45.0673
44.2617

21.2474



f1 (ppm)
S40

170223
LJJ170220-099 CDC13 0223030



3t LJJ170220-099
LJJ170220-099 CDC13

186.2336
186.2327

162.9003

156.5514

150.5746

147.7649

137.2407

134.9790

132.6494

132.5834

132.3766

130.5450

129.5129

129.4235

129.3029

128.8311

128.0726

127.9190

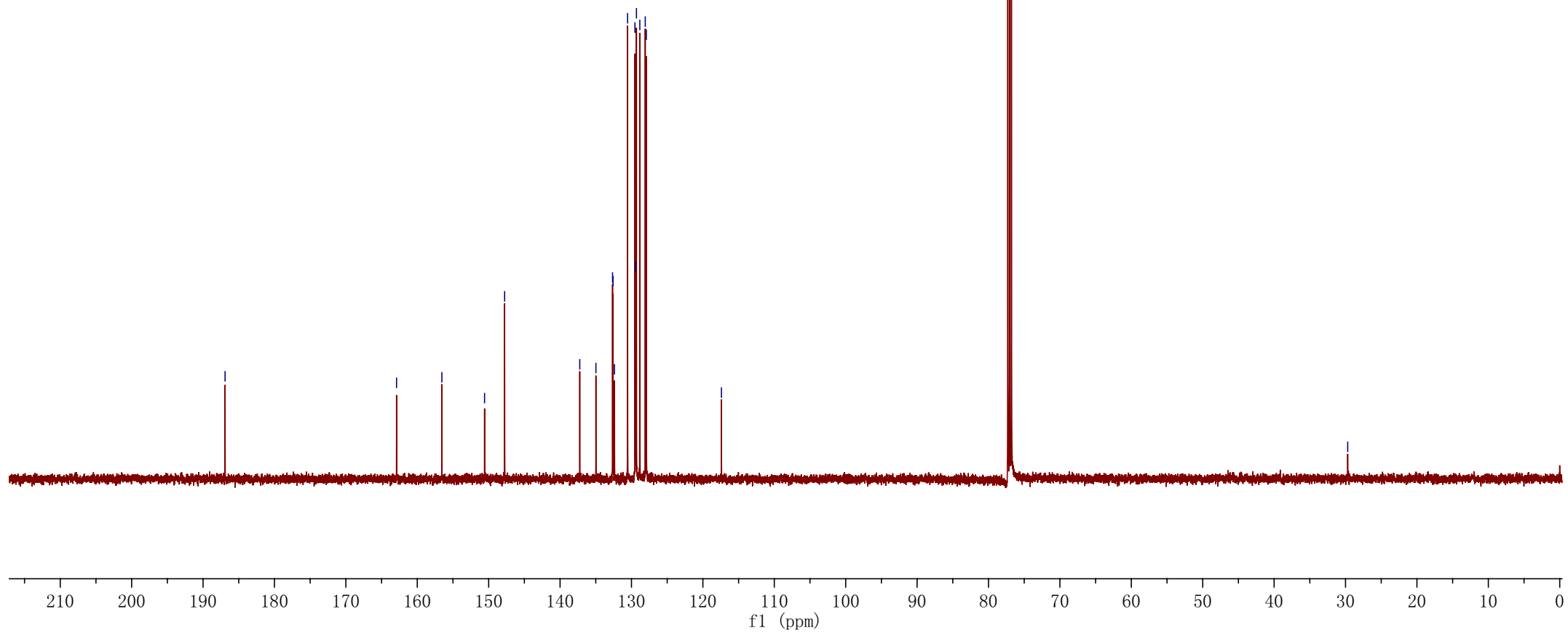
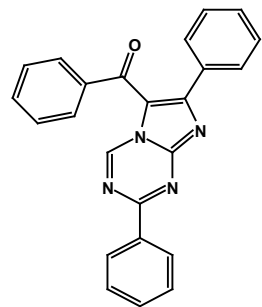
117.4015

77.2973

77.0431

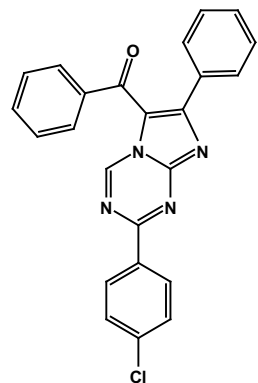
76.7891

29.6935



S42

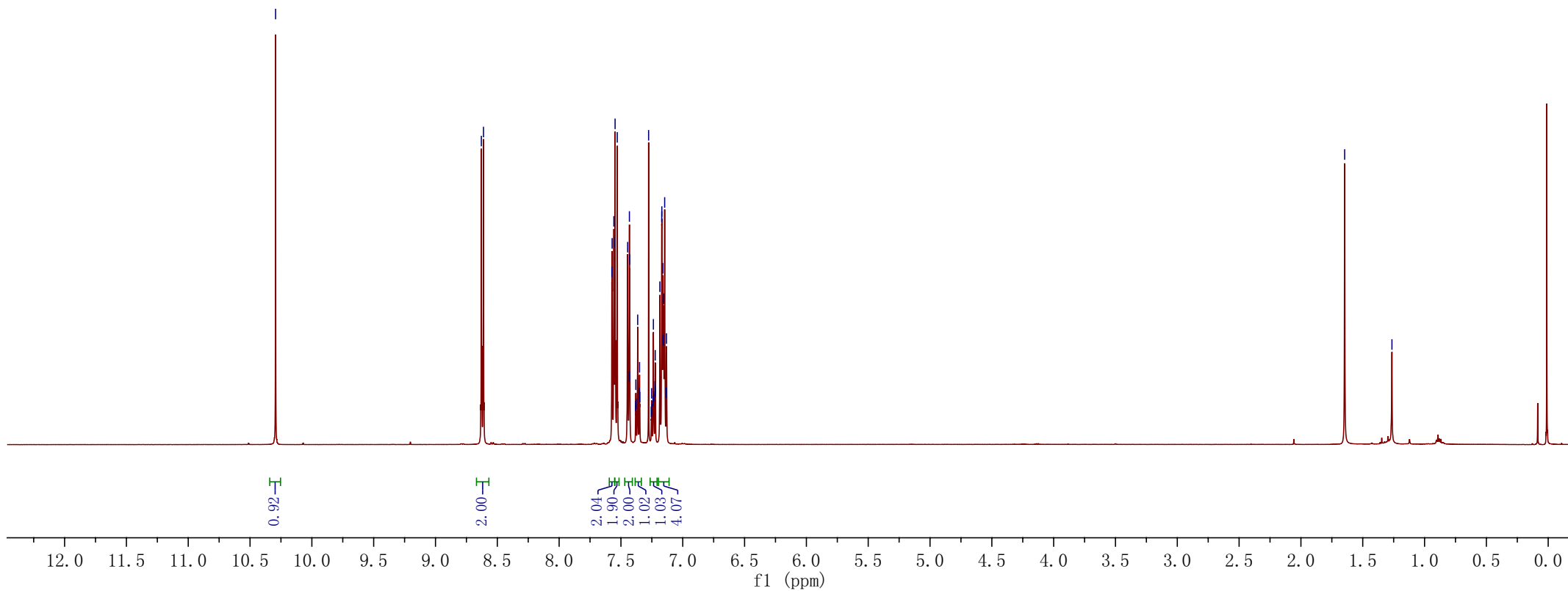
170213
LJJ170207-086 CDC13 0213



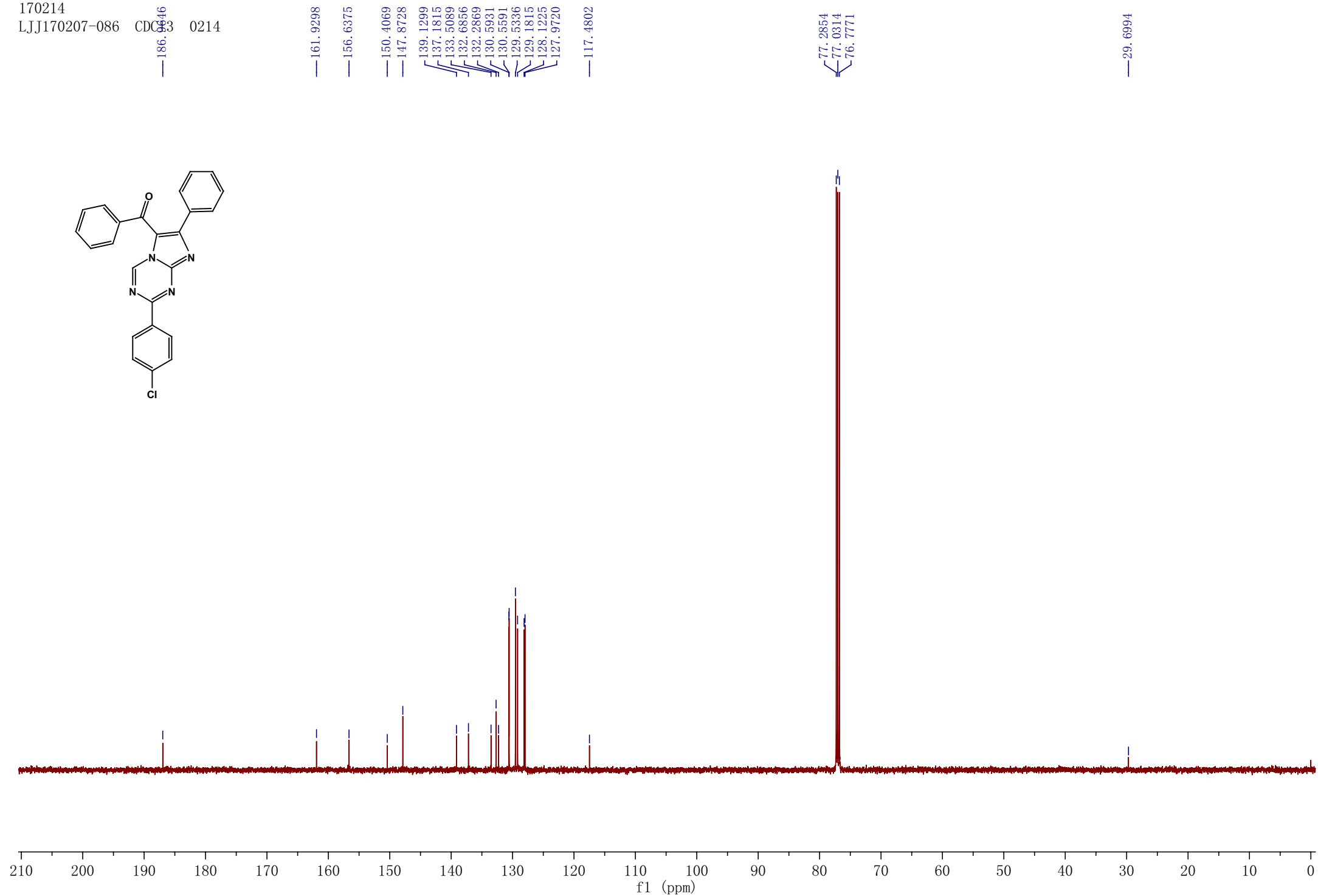
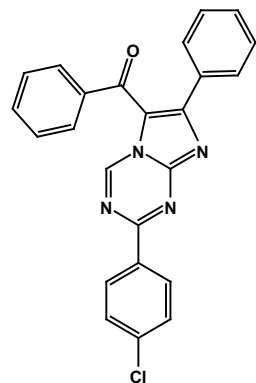
—10.2934

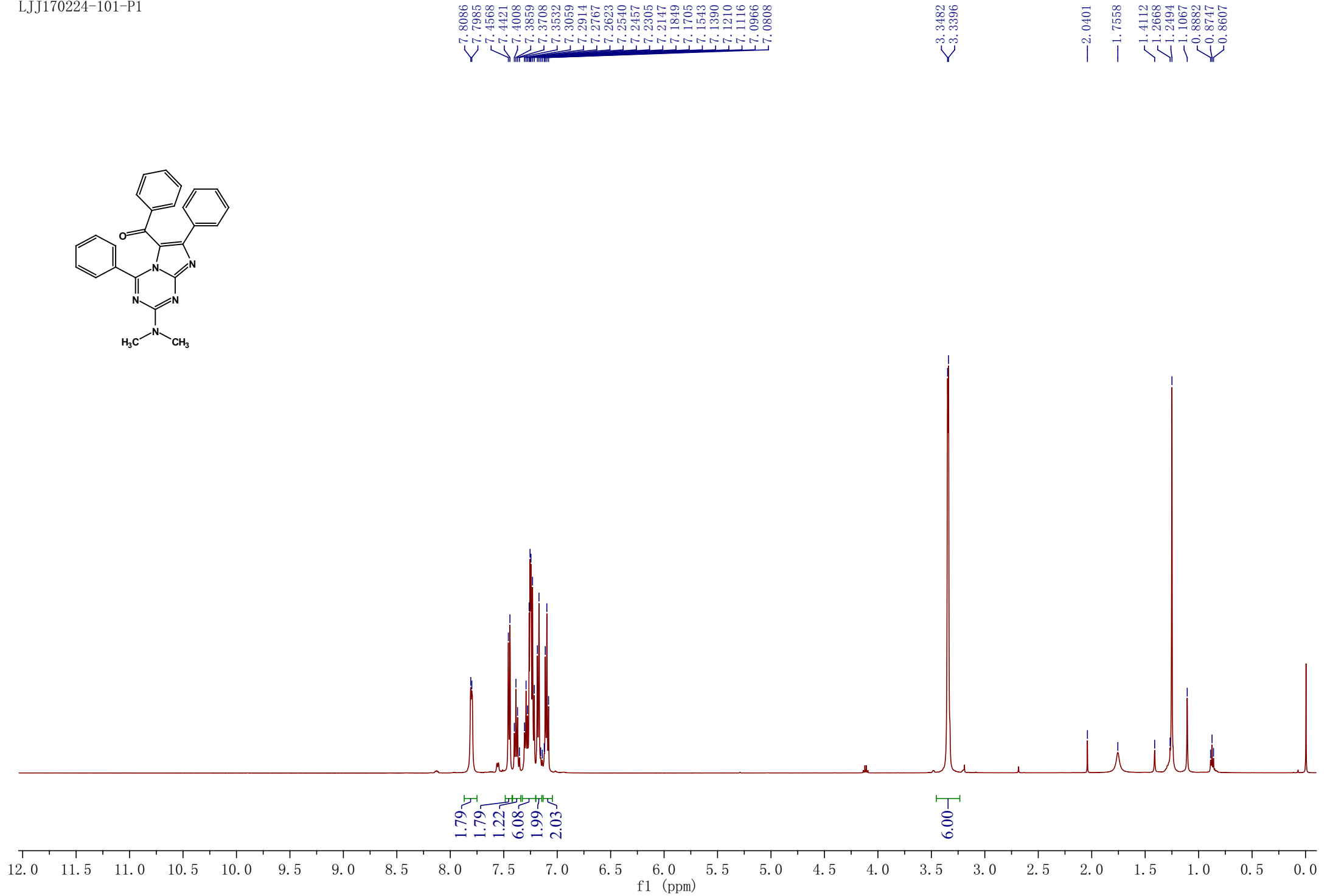
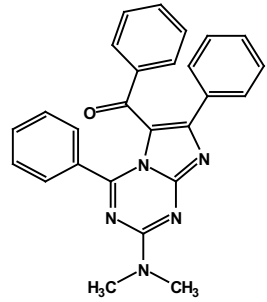
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7.5299
7.4456
7.4351
7.4315
7.4288
7.3818
7.3795
7.3771
7.3646
7.3520
7.3496
7.3473
7.2763
7.2548
7.2524
7.2500
7.2413
7.2375
7.2340
7.2251
7.2227
7.2202
7.1854
7.1699
7.1692
7.1619
7.1586
7.1540
7.1463
7.1347
7.1315
—1.6464

—1.2638



170214
LJJ170207-086 CDC-946 0214





170317

LJJ170224-101-P1

CDC13

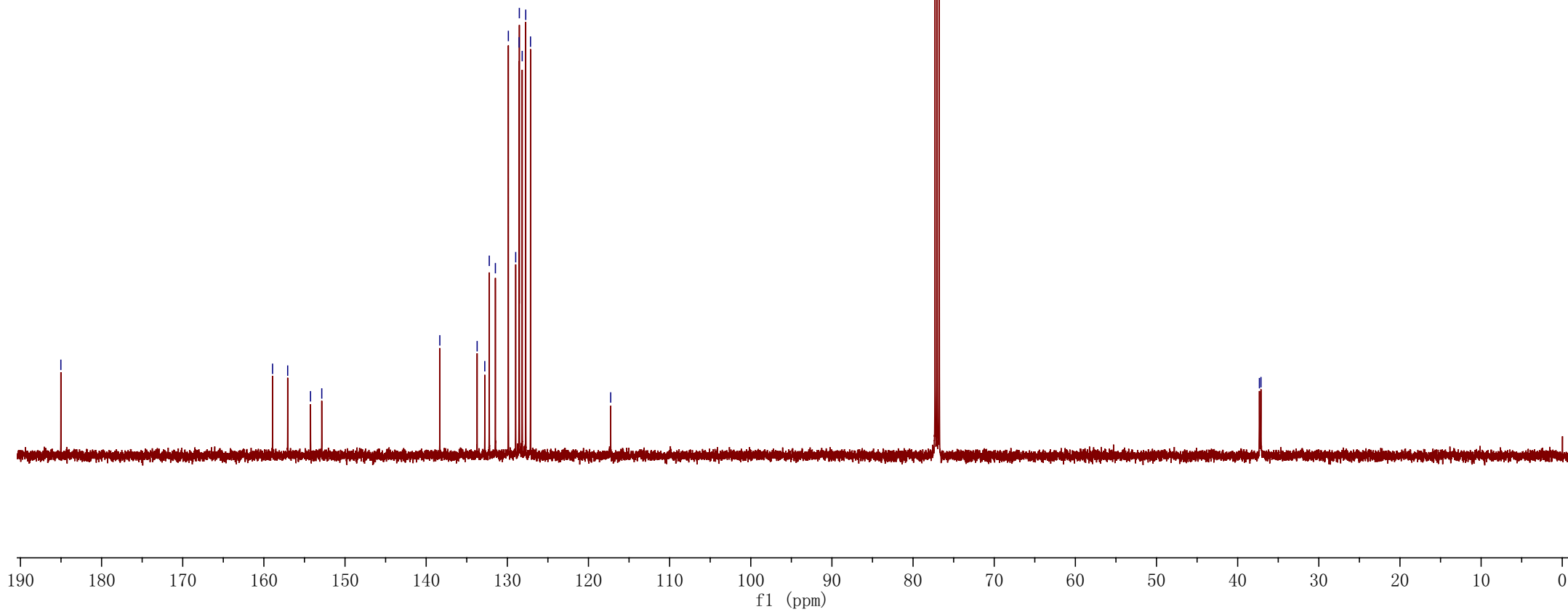
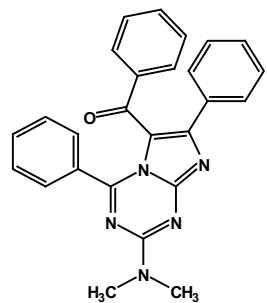
0914

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154.2518
152.8659

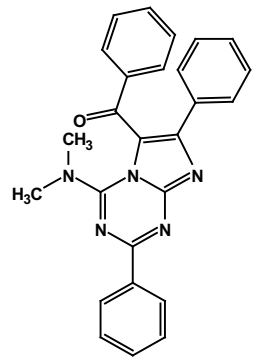
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132.7788
132.2244
131.4709
129.8720
128.9676
128.5461
128.5178
128.1663
127.7311
127.1423
117.2630

77.2852
77.0311
76.7770

37.3191
37.1272



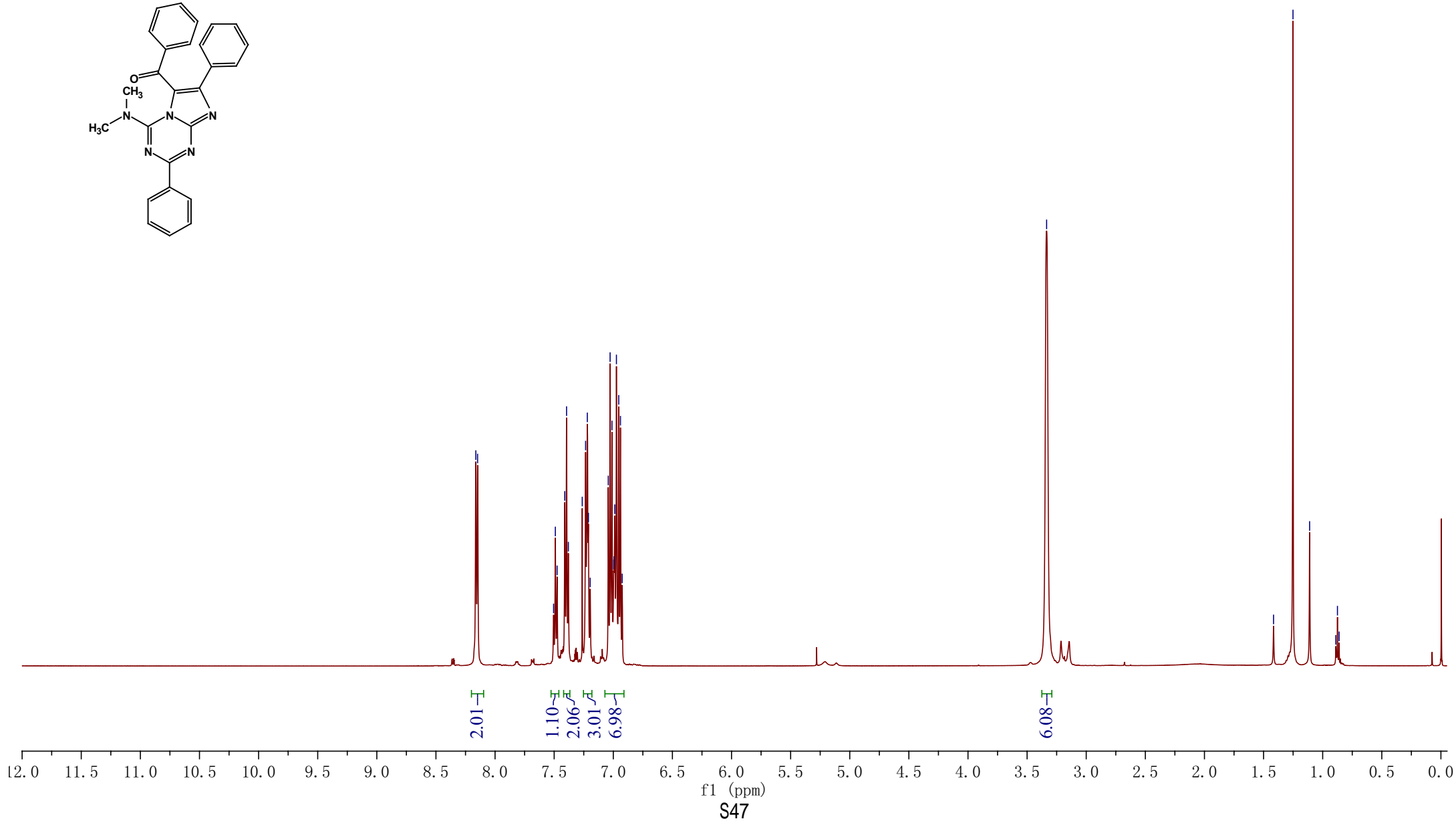
S46



8.1627
8.1479
7.5049
7.4902
7.4754
7.4106
7.3951
7.3801
7.2626
7.2342
7.2197
7.2103
7.1952
7.0425
7.0269
7.0111
6.9962
6.9937
6.9874
6.9735
6.9540
6.9394
6.9246

3.3349

1.4155
1.2511
1.1105
0.8887
0.8751
0.8610



170310
LJJ170224-101-P2 CDC13

190.2140

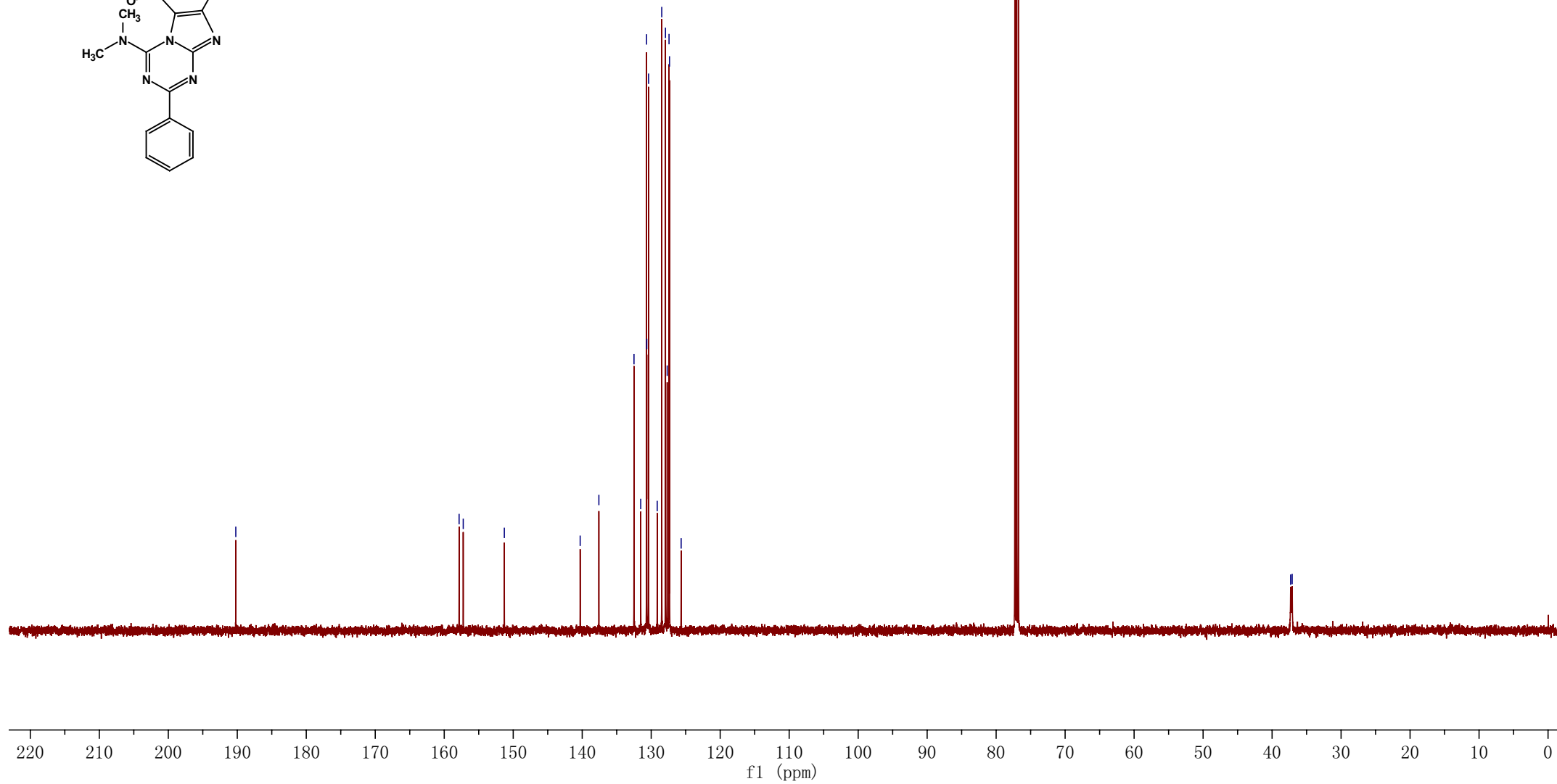
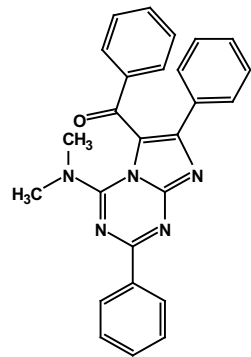
157.8442
157.2464

151.2891

140.2957
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131.5192
130.6737
130.6418
130.3829
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127.9336
127.6821
127.4158
127.3465
125.6590

77.2869
77.0325
76.7784

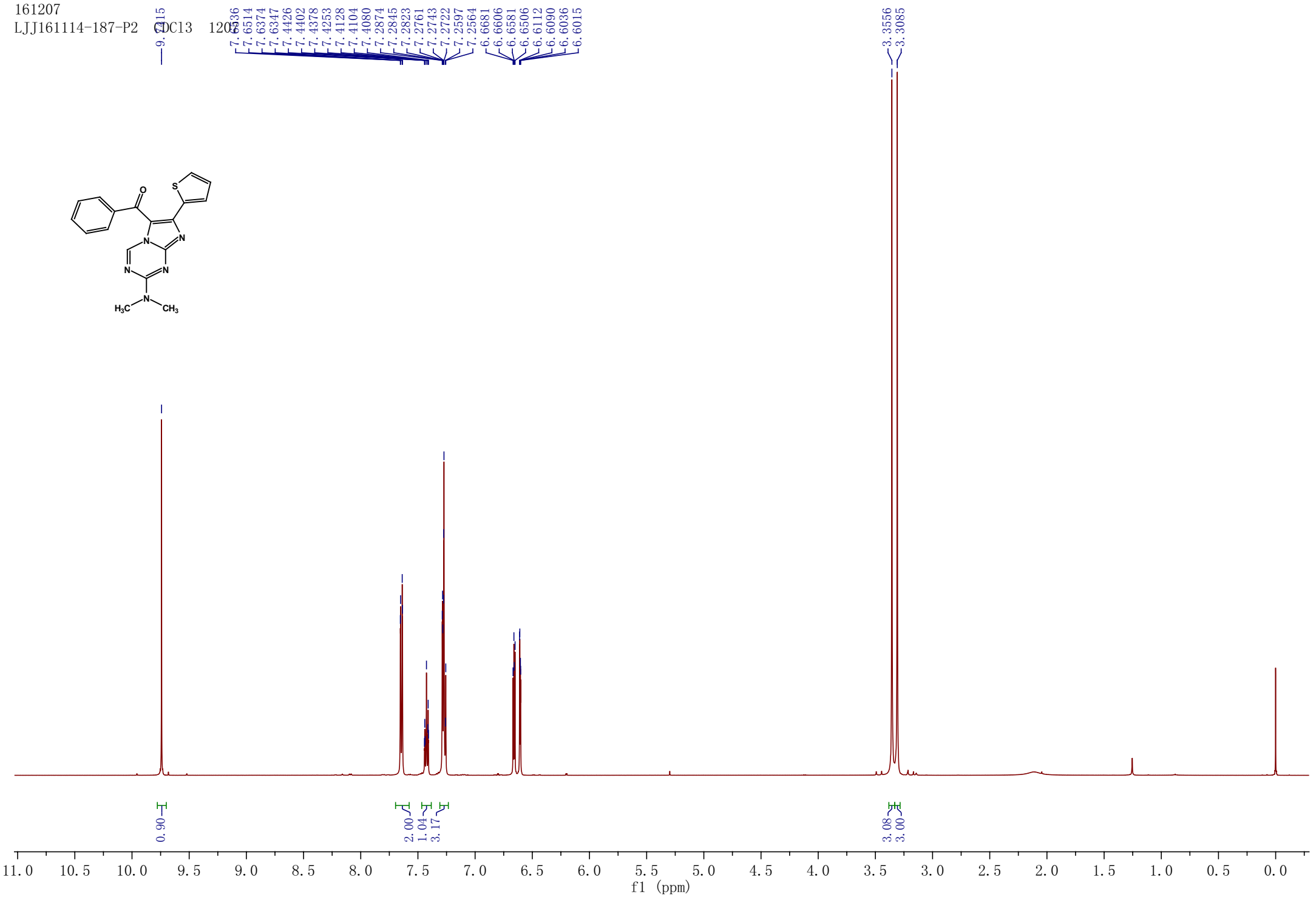
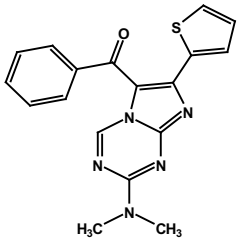
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37.0885



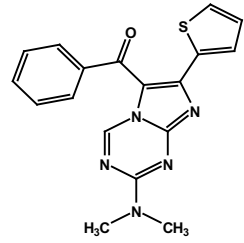
161207
LJJ161114-187-P2

CDCl₃

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7.4378
7.4253
7.4128
7.4104
7.4080
7.2874
7.2845
7.2823
7.2761
7.2743
7.2722
7.2597
7.2564
6.6681
6.6606
6.6581
6.6506
6.6112
6.6090
6.6036
6.6015



LJJ161114-187-P2 H
LJJ161114-187-P2 CDCl₃ 0605



185.6414

159.1886

152.9016

149.5473

147.7796

138.3115

135.3638

132.1891

130.9384

129.2333

129.0170

128.3298

127.0759

115.7982

77.2895

77.0354

76.7811

37.5328

37.2754

