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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Contents

1. X-ray crystallographic structure of **3a**……S2

2. Copies of NMR spectra……S3

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

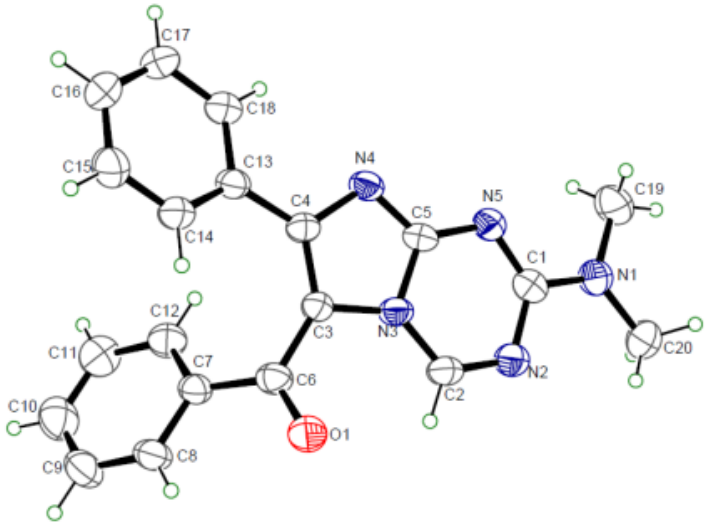

Figure S1 The crystal structure of **3a** with thermal ellipsoid contour at 30% probability level

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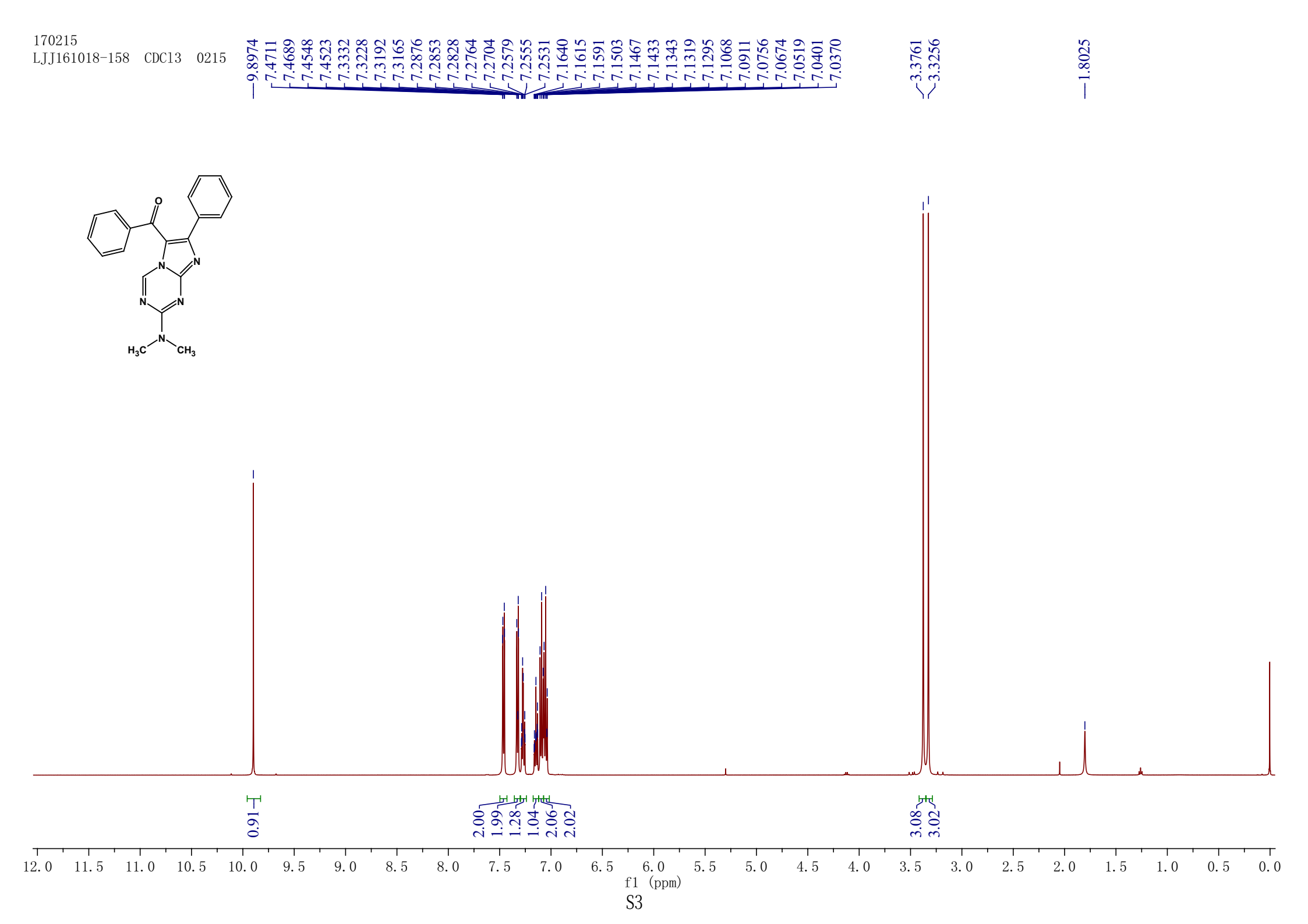

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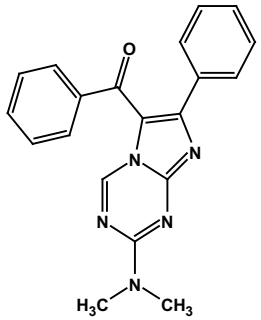

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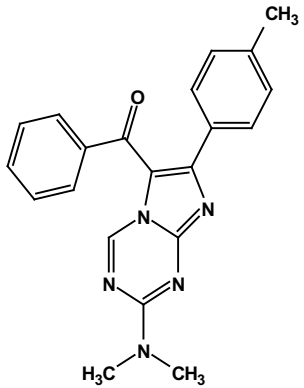

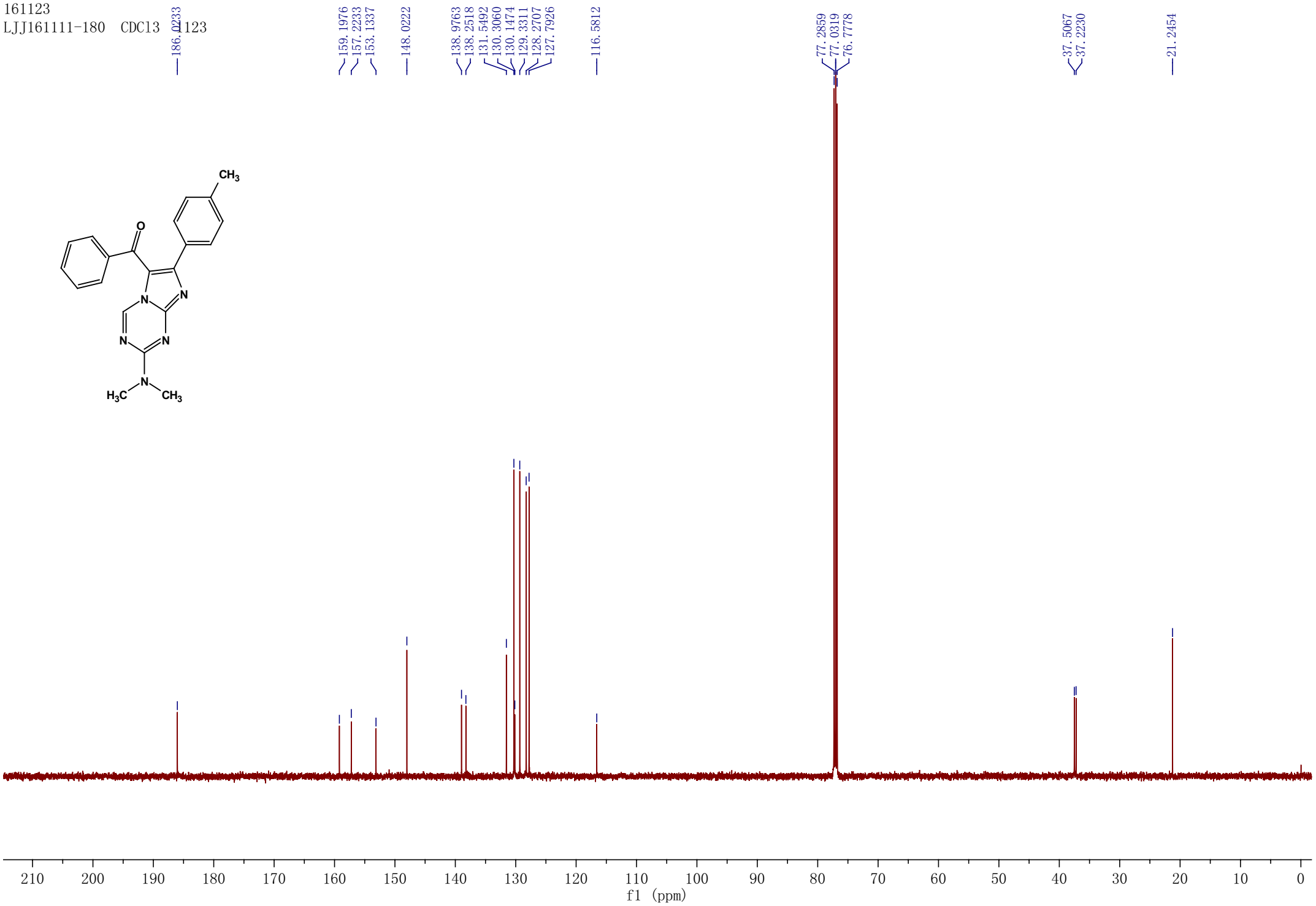
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157.2233
153.1337
148.0222
138.9763
138.2518
131.5492
130.3060
130.1474
129.3311
128.2707
127.7926
116.5812
77.2859
77.0319
76.7778
37.5067
37.2230
21.2454
CH3
O
N
N
N
N
H3C
N
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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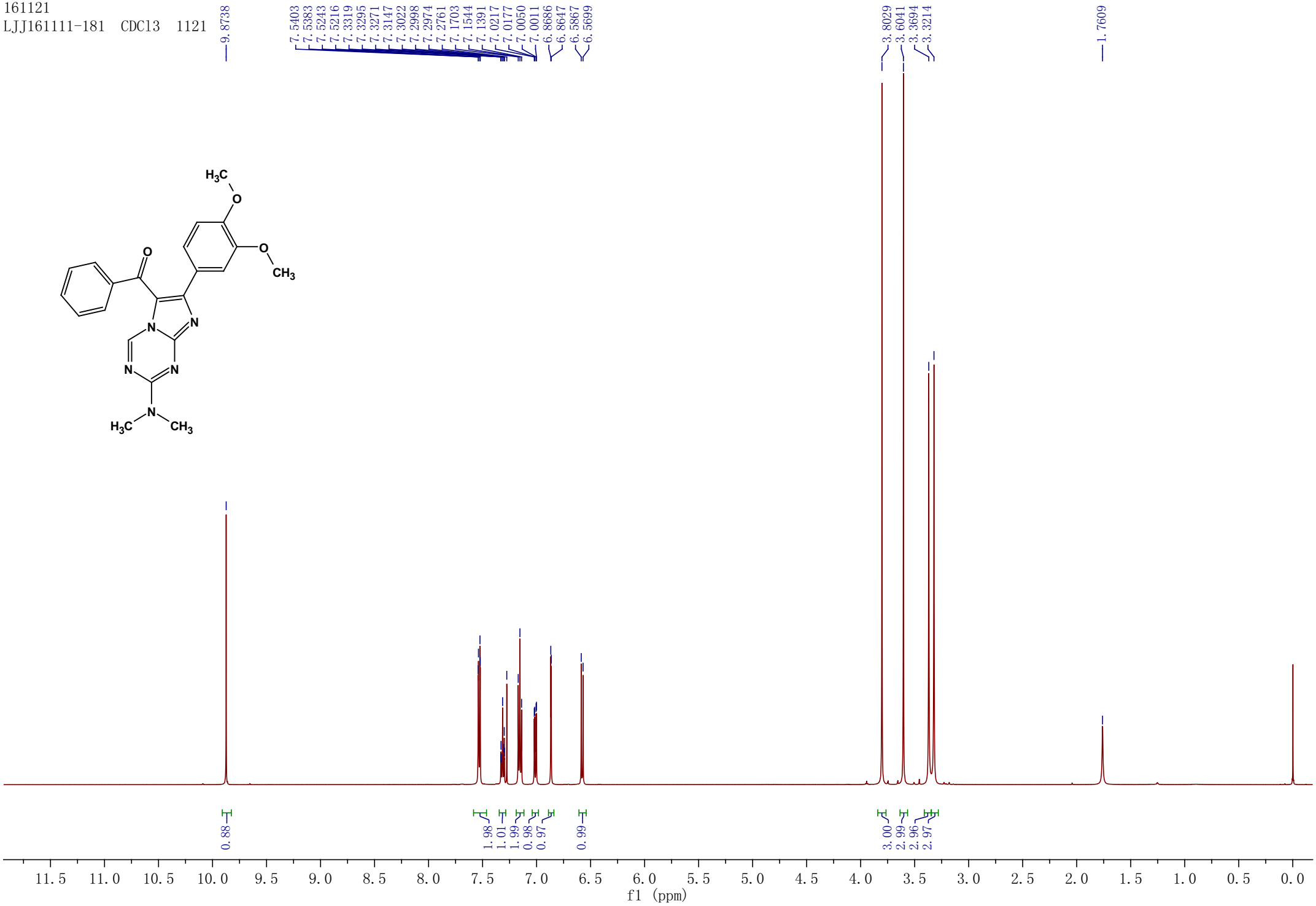
30
20
10
0
f1 (ppm)

161121
LJJ161111-181 CDCl3 1121



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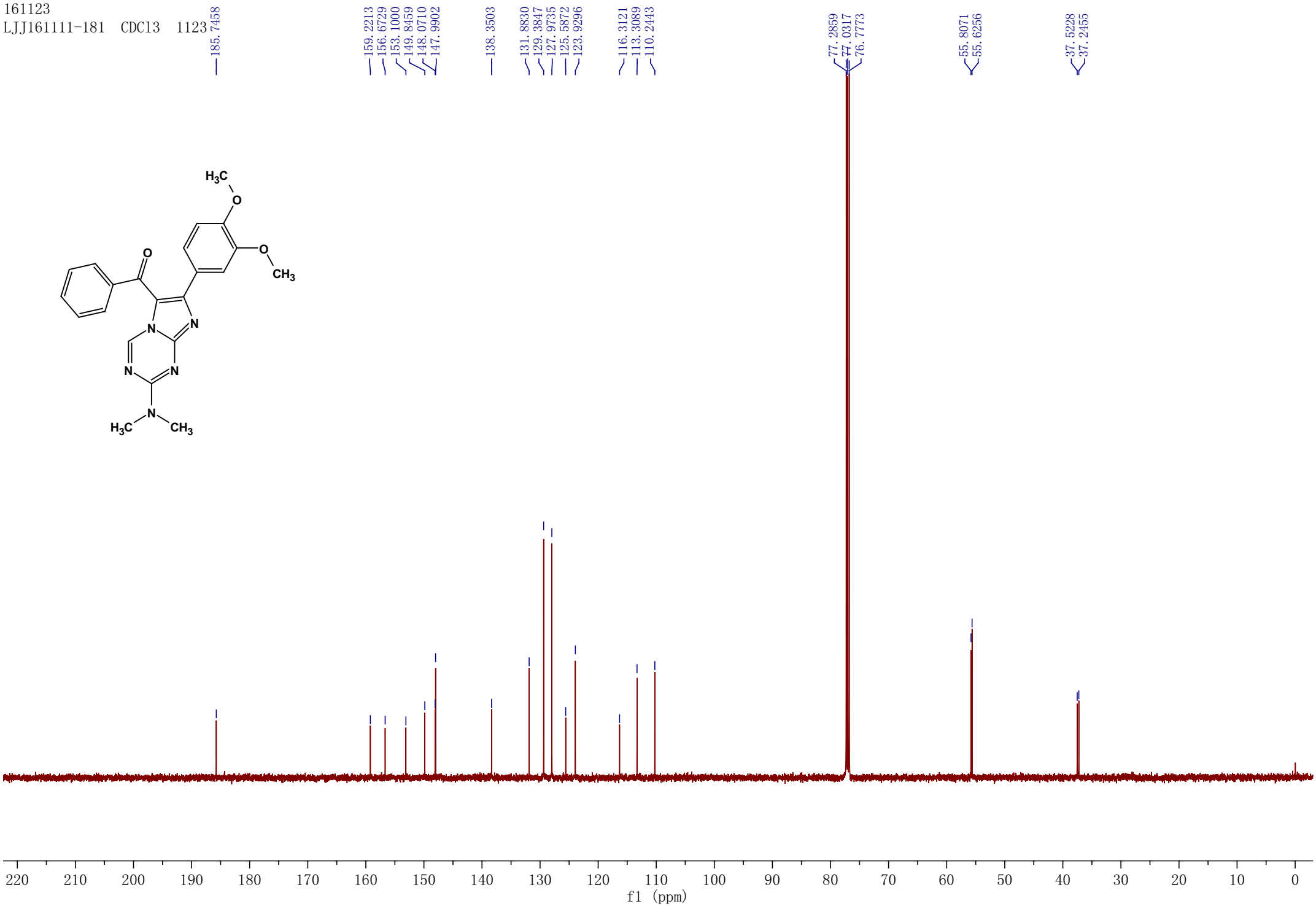

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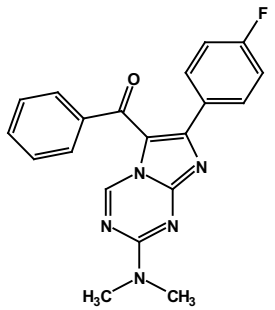

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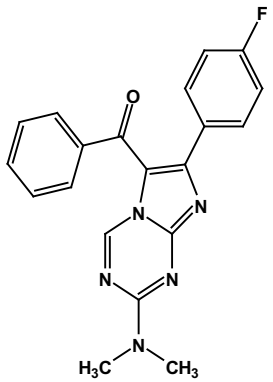

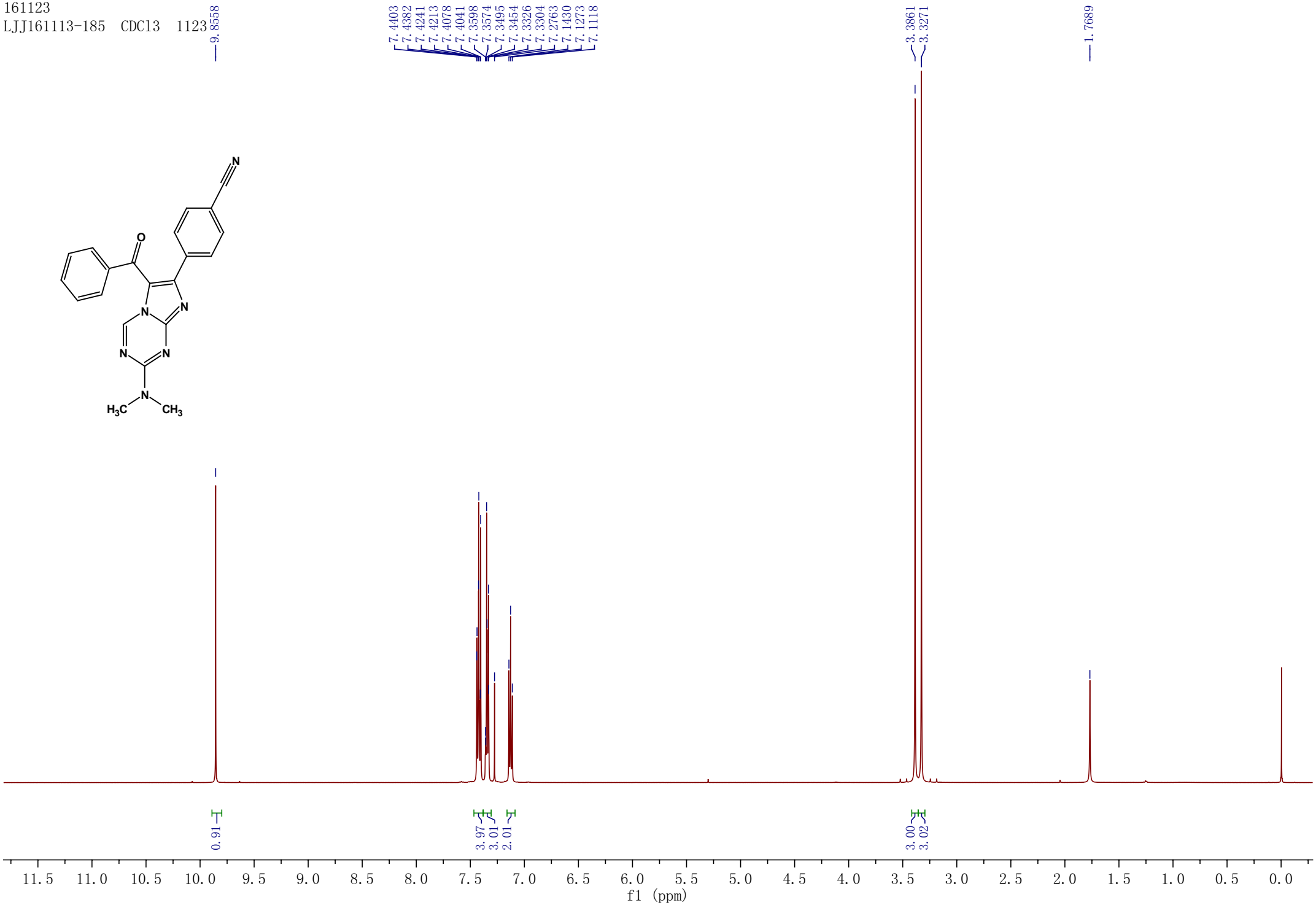
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7.4041
7.3598
7.3574
7.3495
7.3454
7.3326
7.3304
7.2763
7.1430
7.1273
7.1118
3.3861
3.3271
1.7689
O
N
N
N
N
N
N
H3C
CH3
0.91
3.97
3.01
2.01
3.00
3.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

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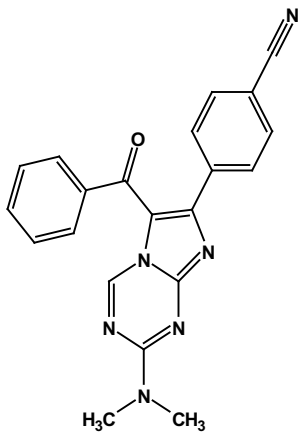

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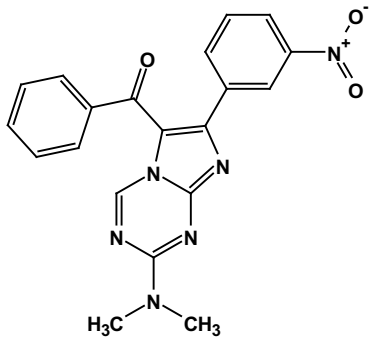

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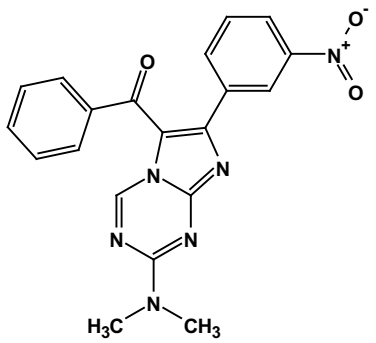

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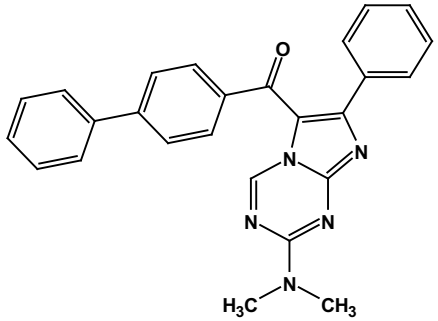

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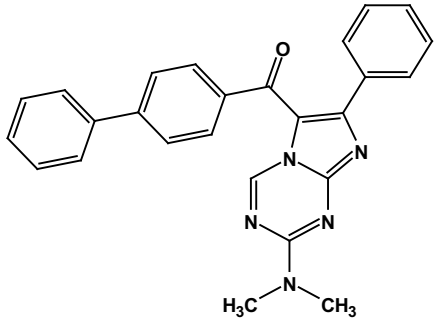

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153.1517
148.0594
144.3086
140.0657
136.8605
133.1878
130.3716
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128.7996
127.9165
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127.0903
126.4184
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f1 (ppm)

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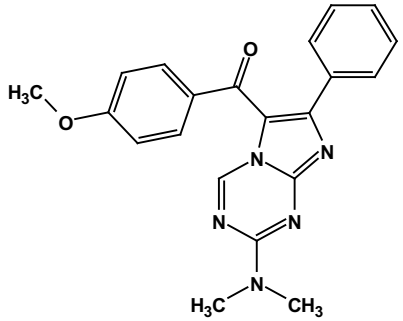

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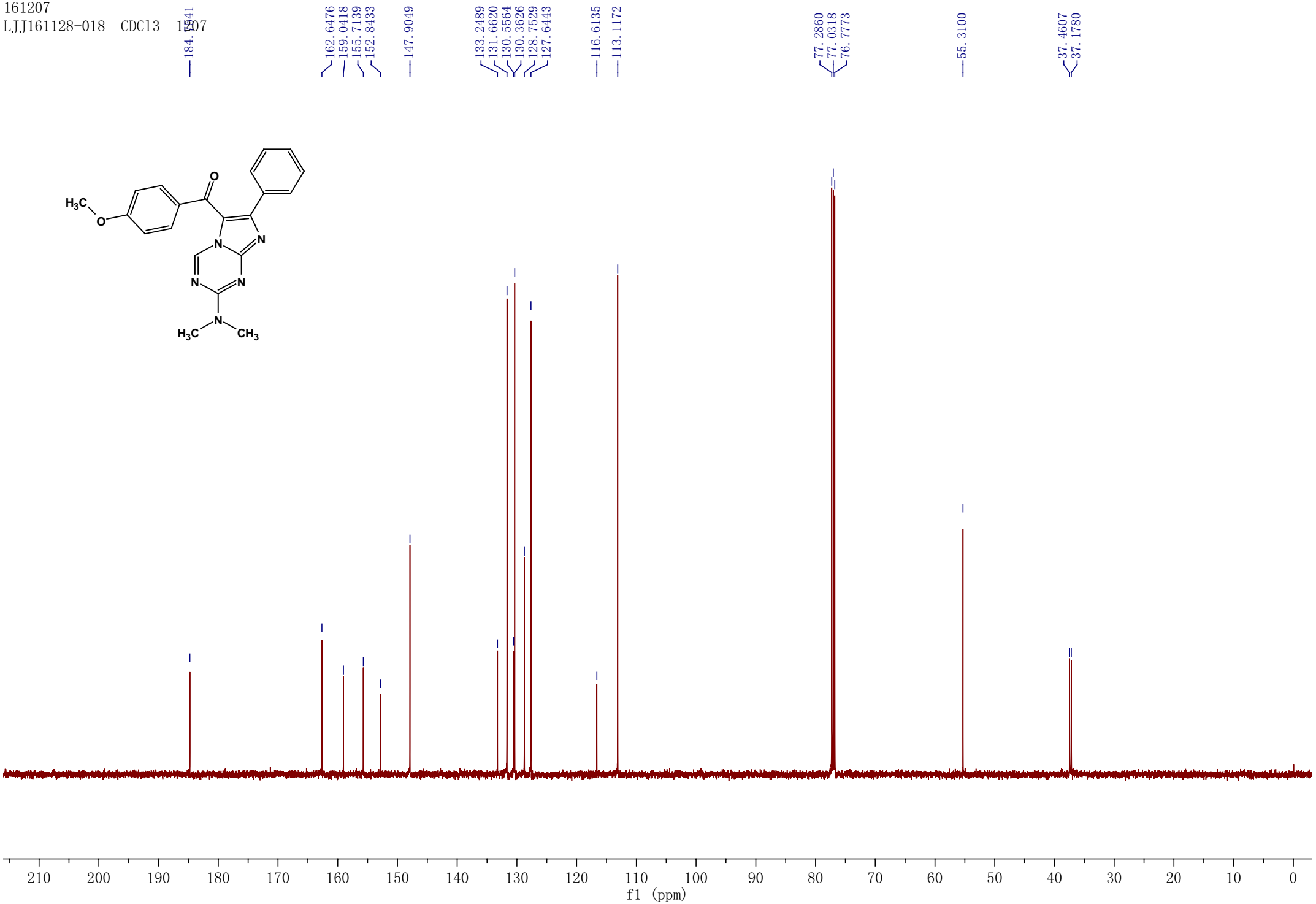

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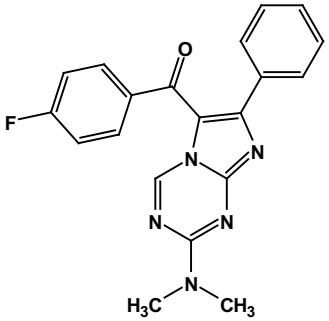

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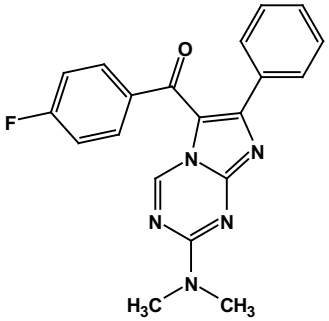

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159.2027
157.1318
153.2269
147.9878
134.4070
134.3830
133.0083
131.7967
131.7245
130.3595
129.1088
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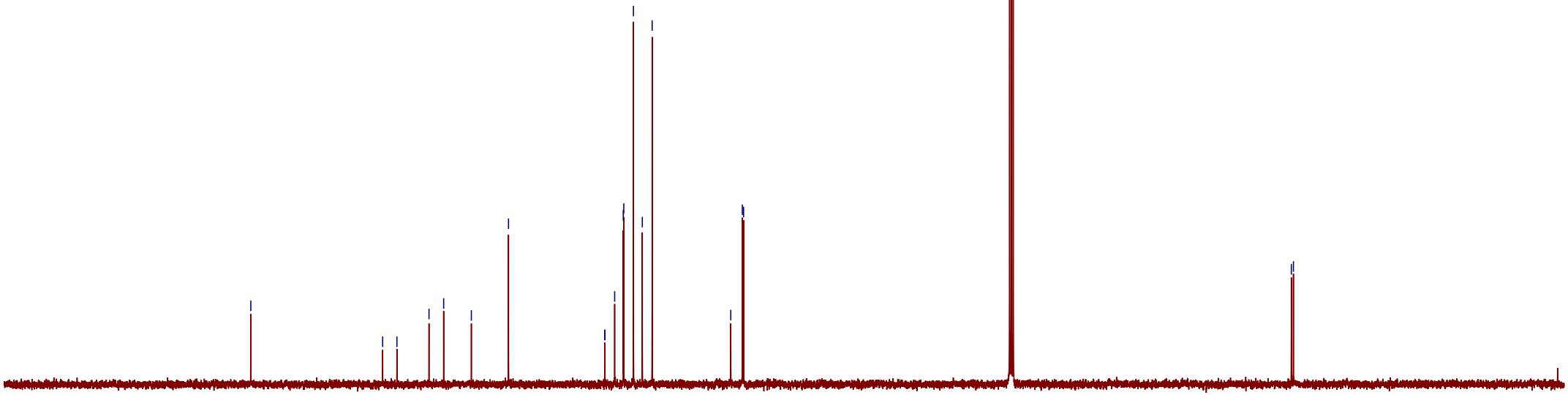
37.2441



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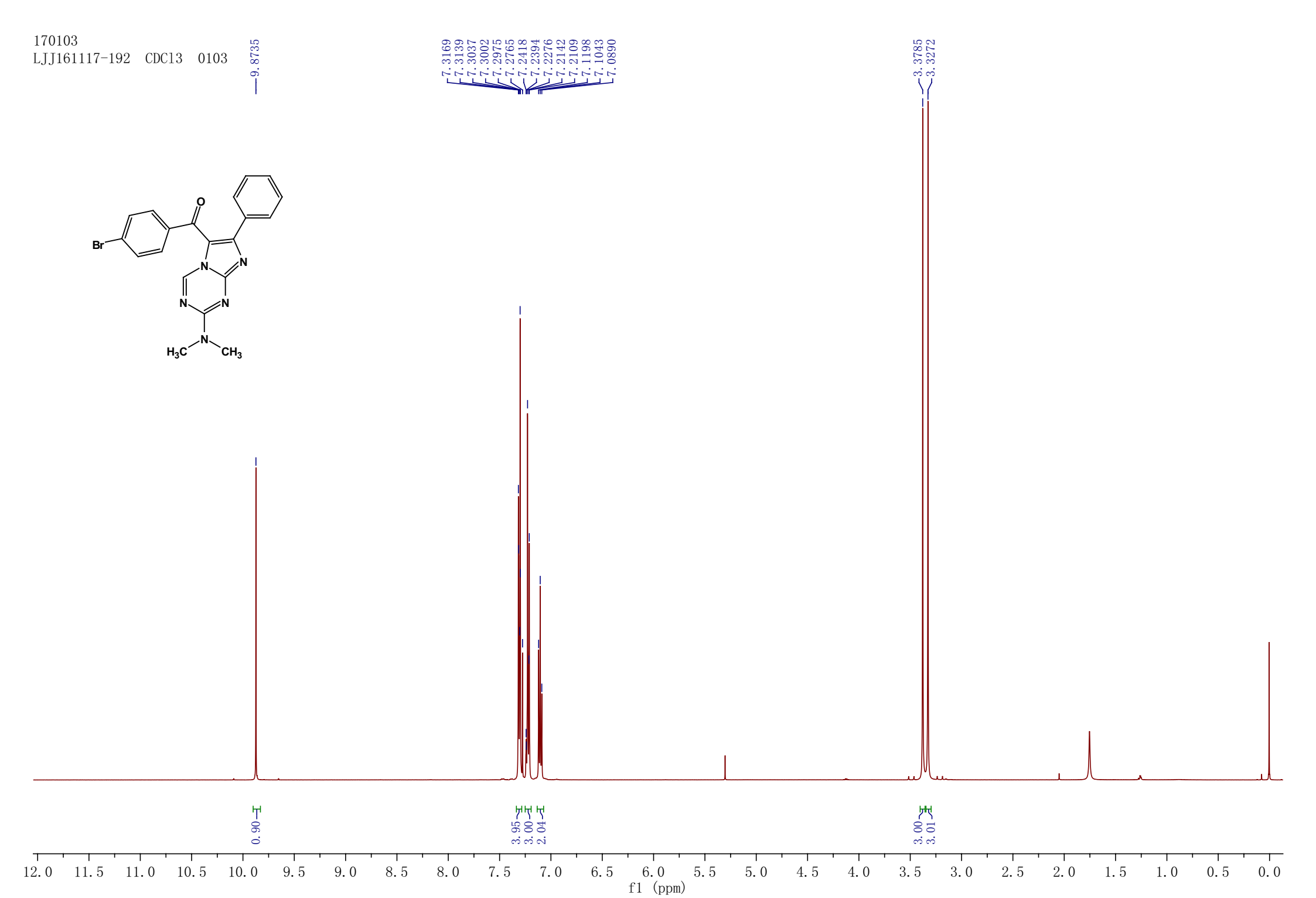
f1 (ppm)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7.2975
7.2765
7.2418
7.2394
7.2276
7.2142
7.2109
7.1198
7.1043
7.0890
3.3785
3.3272
Br
O
N
N
N
N
N
H3C
CH3
0.90
3.95
3.00
2.04
3.00
3.01
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

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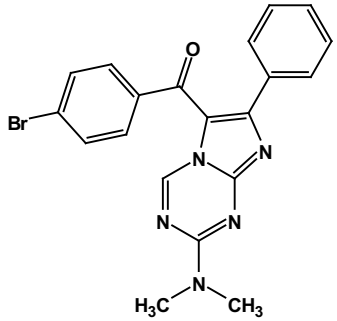
LJJ161117-192 CDCl3 0106



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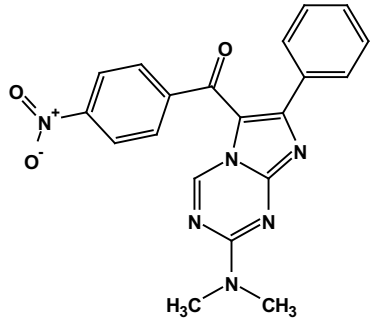

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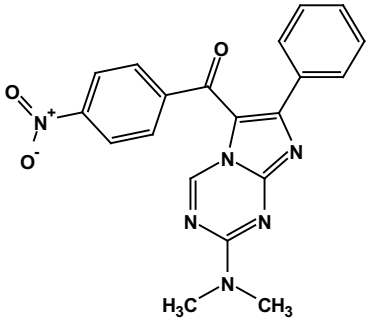
LJJ161115-188 CDCl3 1130



183.1224
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158.9353
153.7666
148.9448
148.0288
143.8205
132.6921
130.2662
129.9988
129.5874
127.8049
122.8538
116.7968
77.2872
77.0329
76.7788
37.6052
37.2922

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f1 (ppm)

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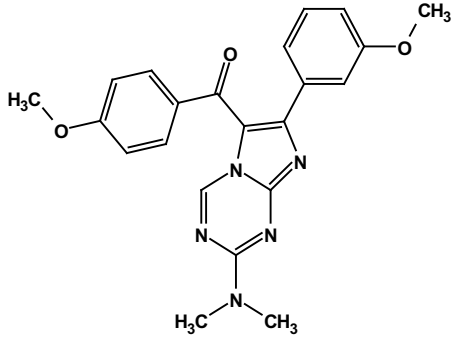
LJJ161111-182 CDCl3 1121



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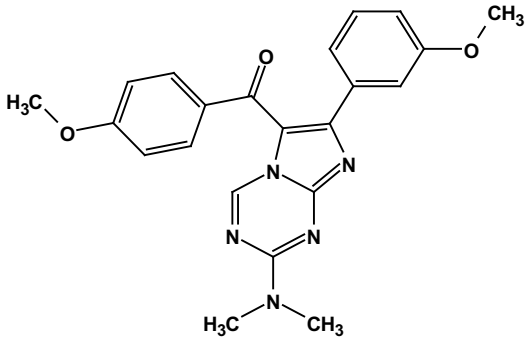

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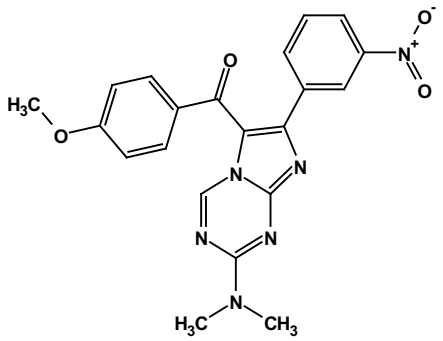

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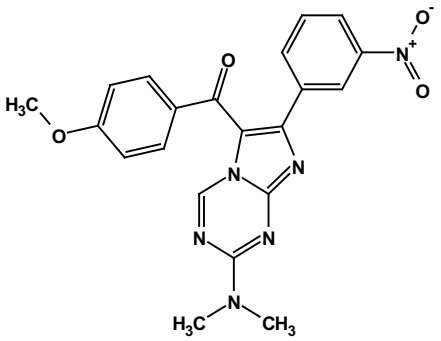

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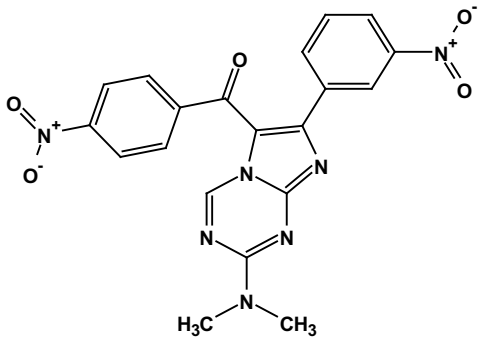

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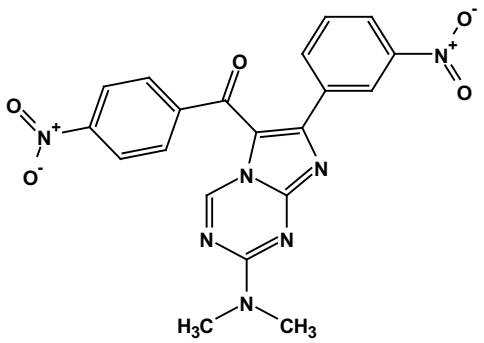

182.7372
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155.3690
153.8181
149.2621
148.0404
147.4534
143.4506
135.6887
134.4386
130.0719
129.0795
125.4332
124.0886
123.2398
117.1622
77.2855
77.0315
76.7772
37.7299
37.3964

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

f1 (ppm)

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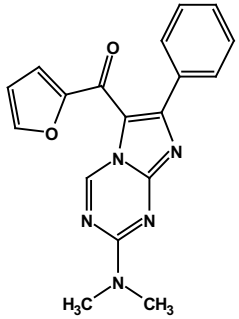
LJJ161128-012 CDCl3 1205



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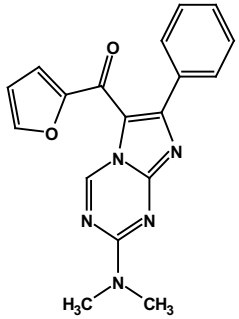

172.1025
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147.6077
145.5744
134.0225
129.6416
128.9429
128.0006
118.4553
116.1207
111.9830
77.2866
77.0324
76.7780
37.5066
37.2273

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

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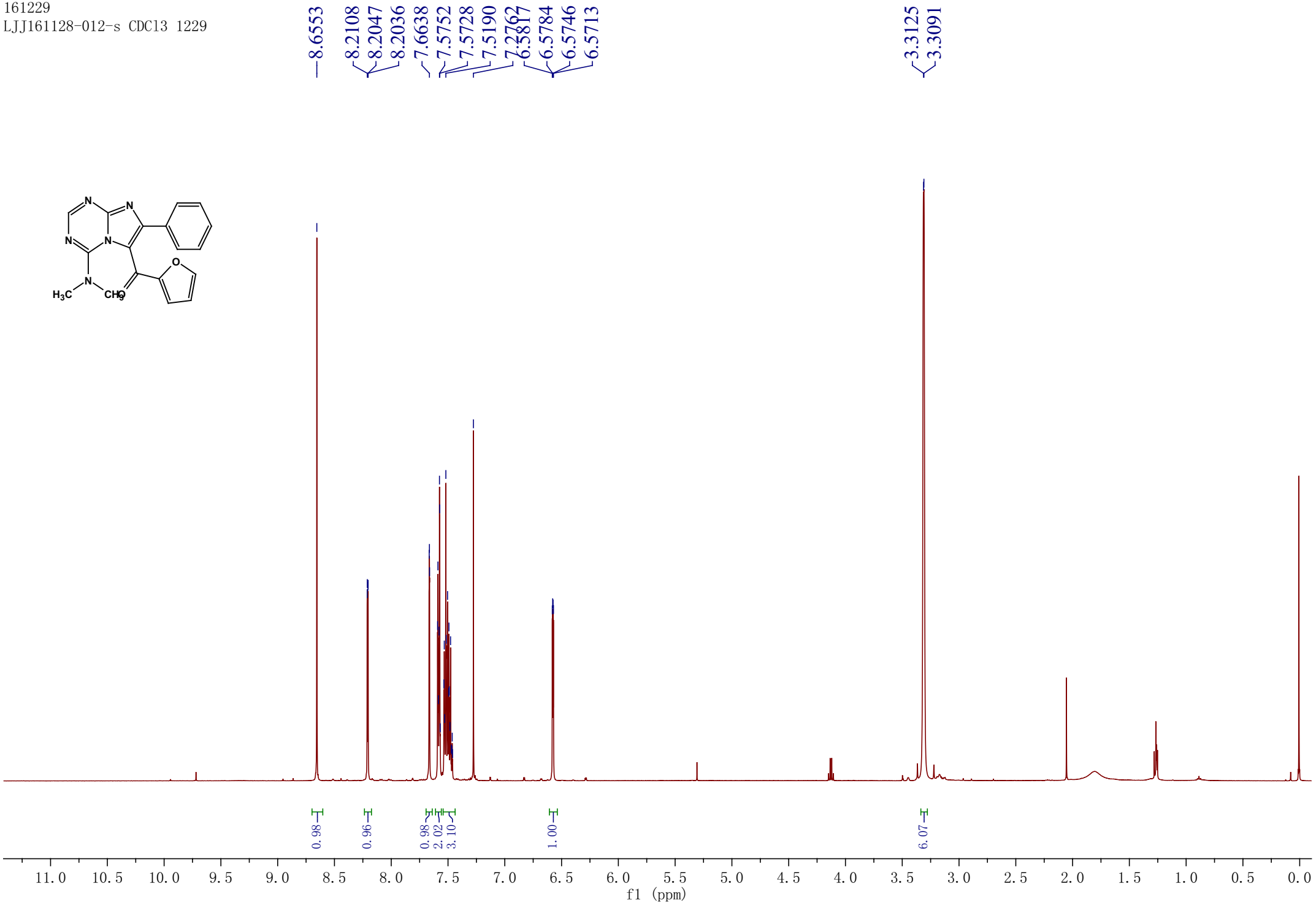

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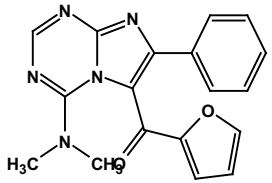

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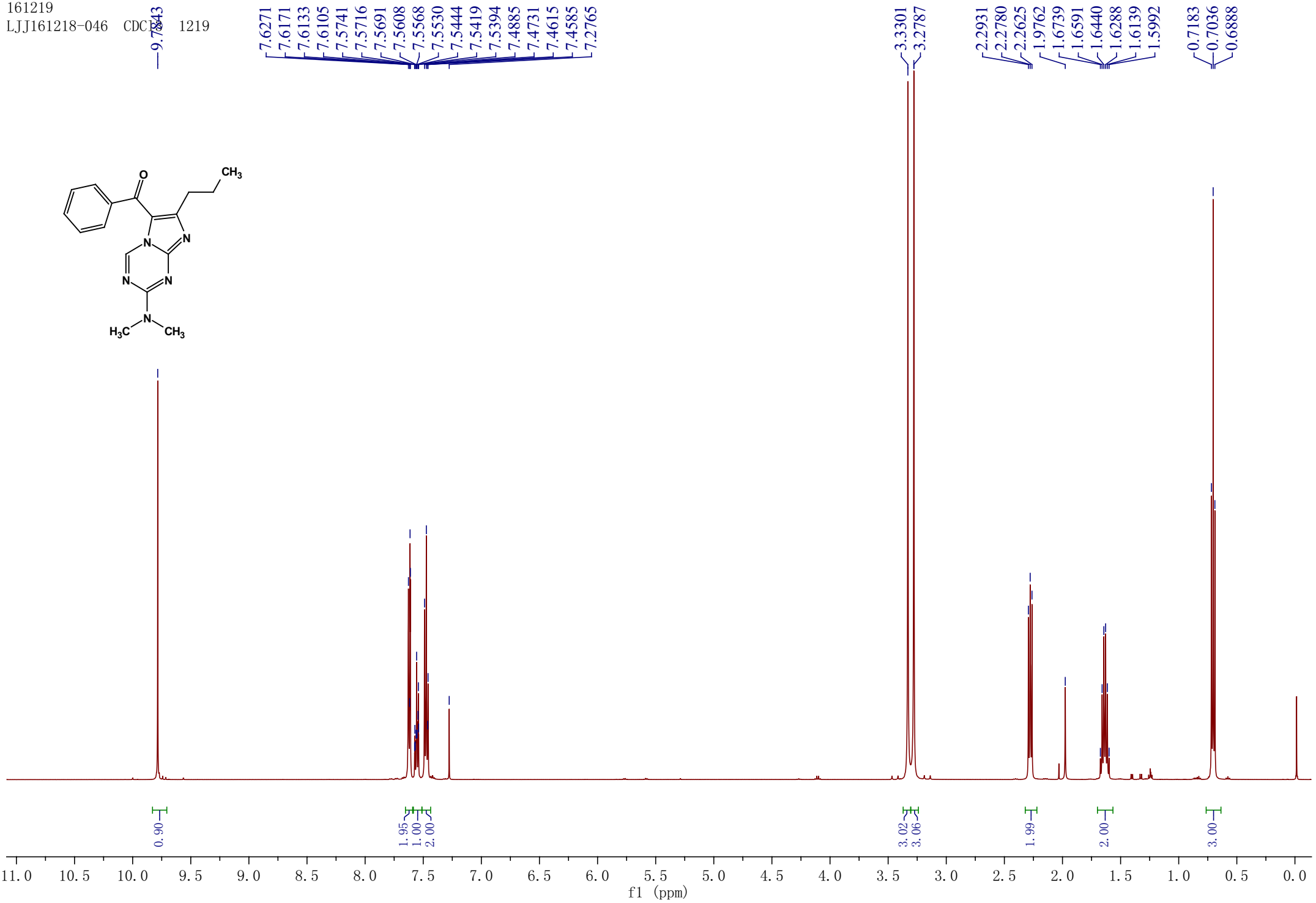

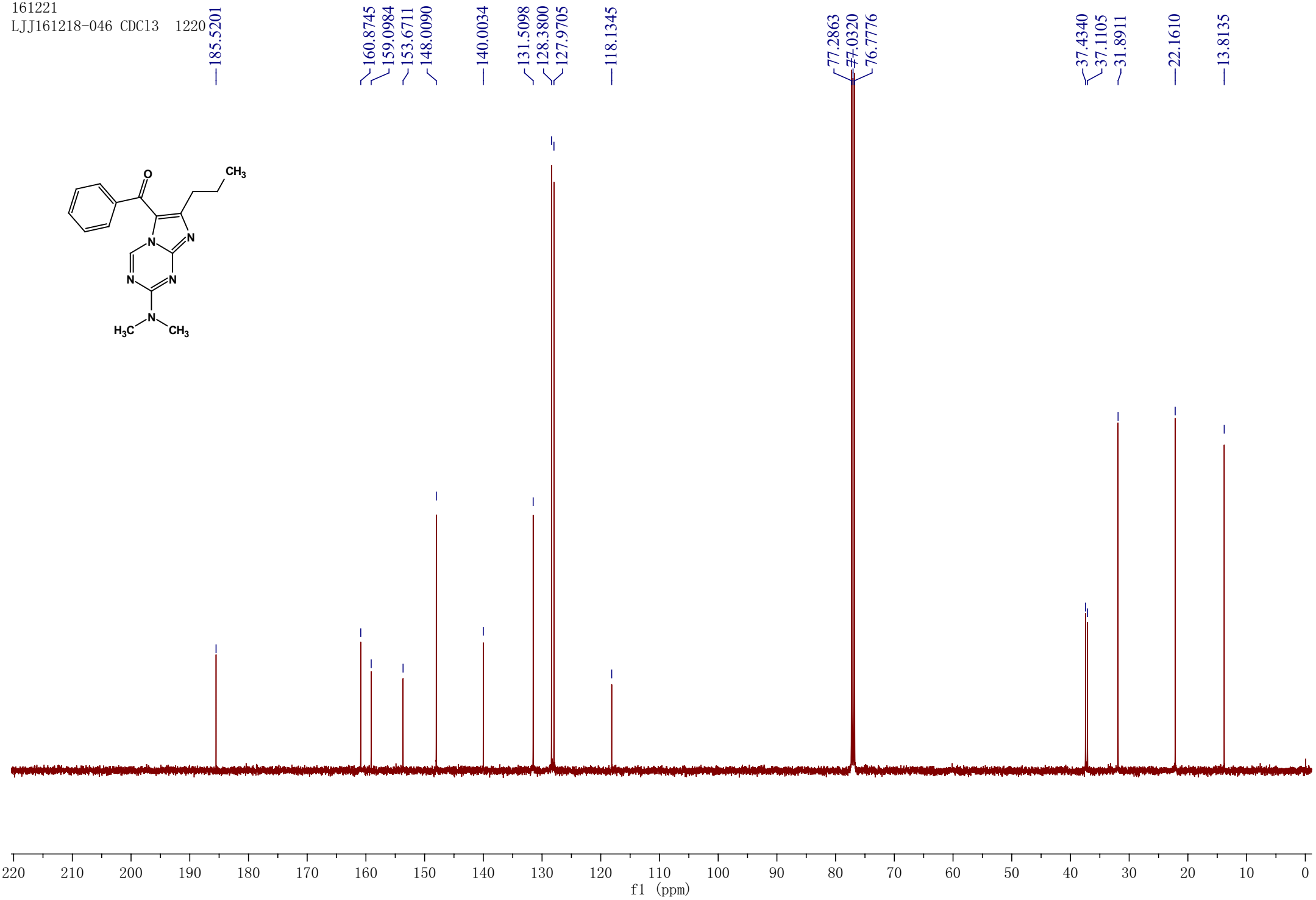
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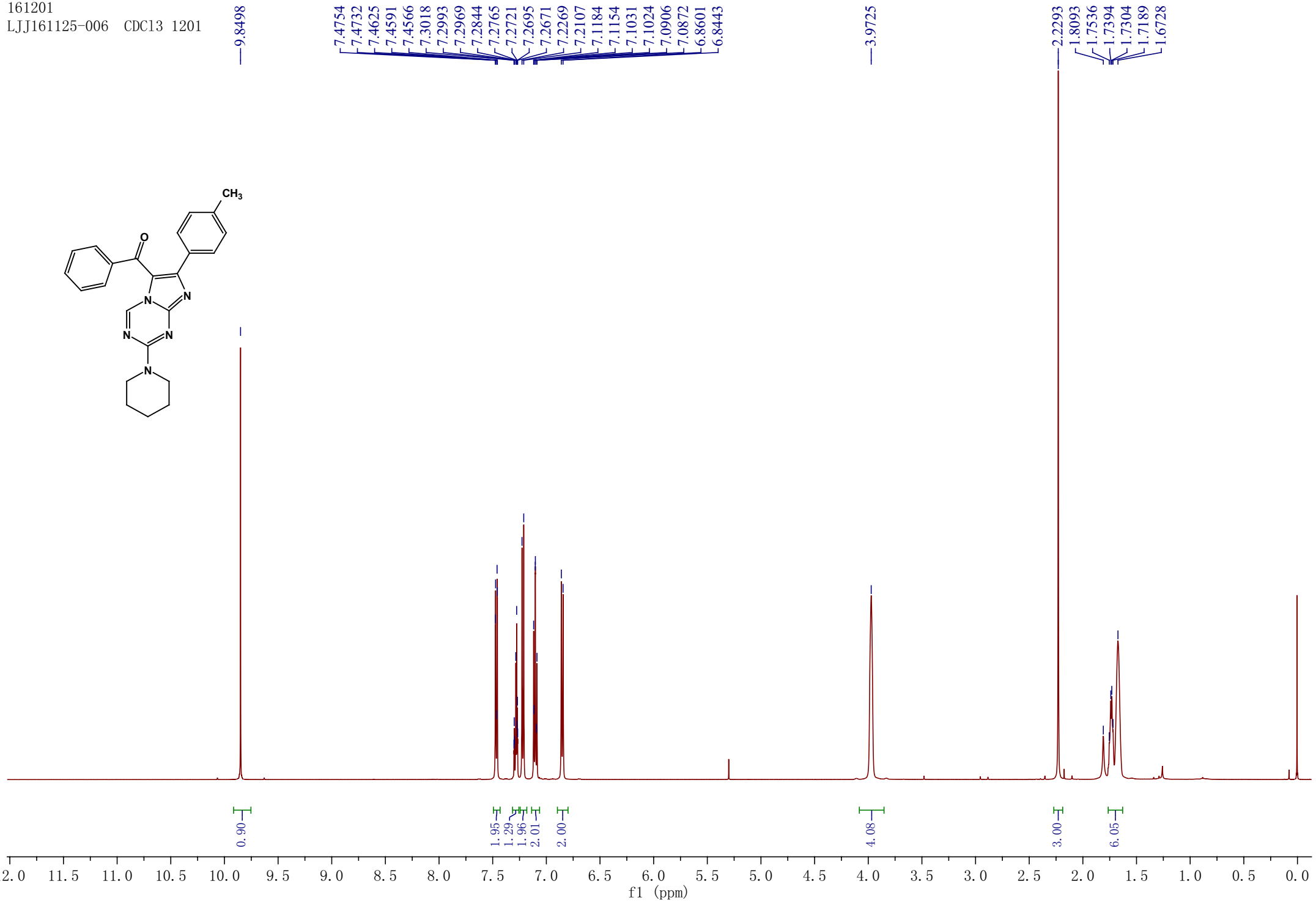
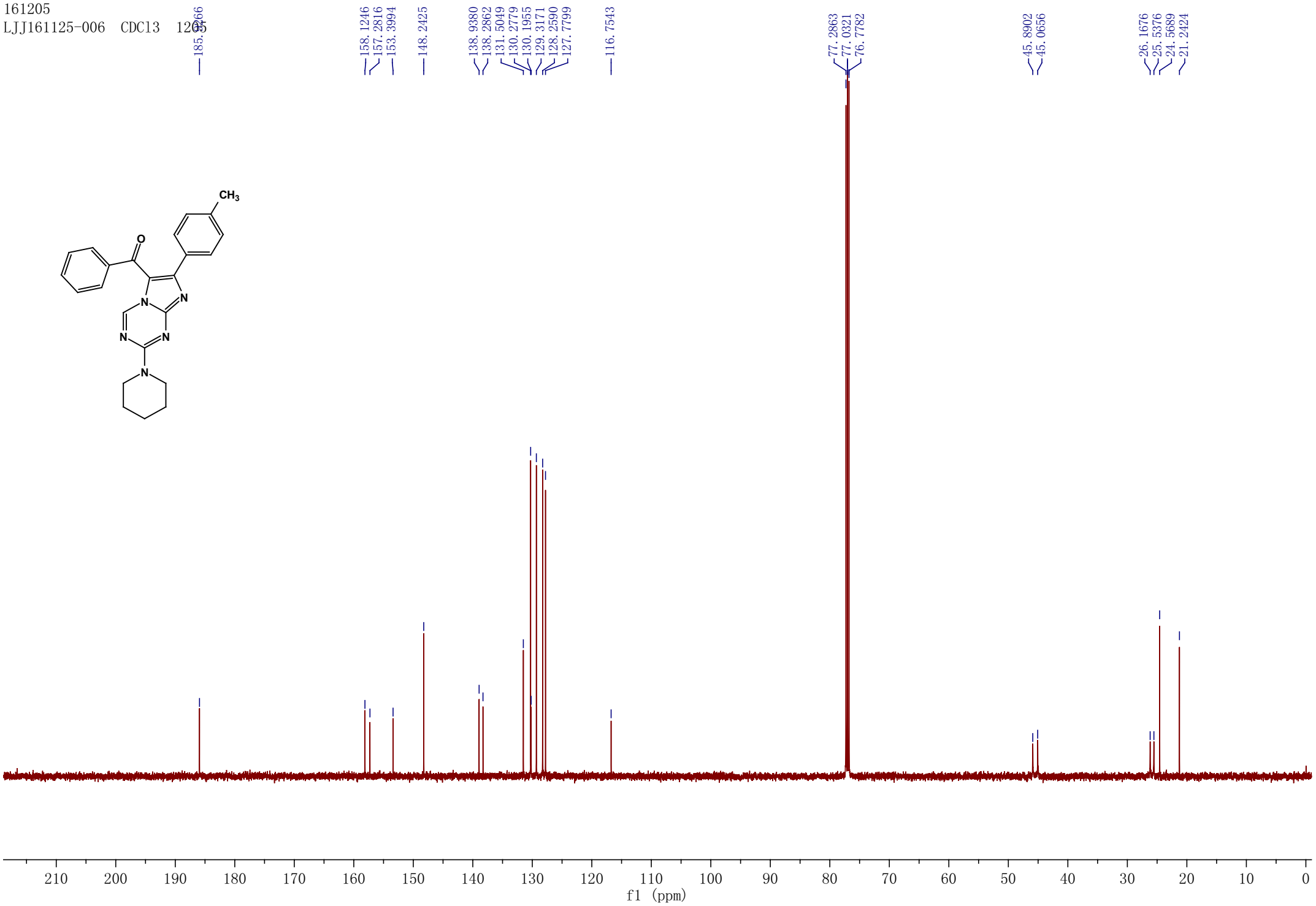
159.0984
153.6711
148.0090
140.0034
131.5098
128.3800
127.9705
118.1345
77.2863
77.0320
76.7776
37.4340
37.1105
31.8911
22.1610
13.8135
O
CH3
N
N
N
N
N
H3C
CH3
f1 (ppm)

161201
LJJ161125-006 CDCl3 1201

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131.5049
130.2779
130.1955
129.3171
128.2590
127.7799
116.7543
77.2863
77.0321
76.7782
45.8902
45.0656
26.1676
25.5376
24.5689
21.2424
CH3
O
N
N
N
N
N
210
200
190
180
170
160
150
140
130
120
110
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f1 (ppm)

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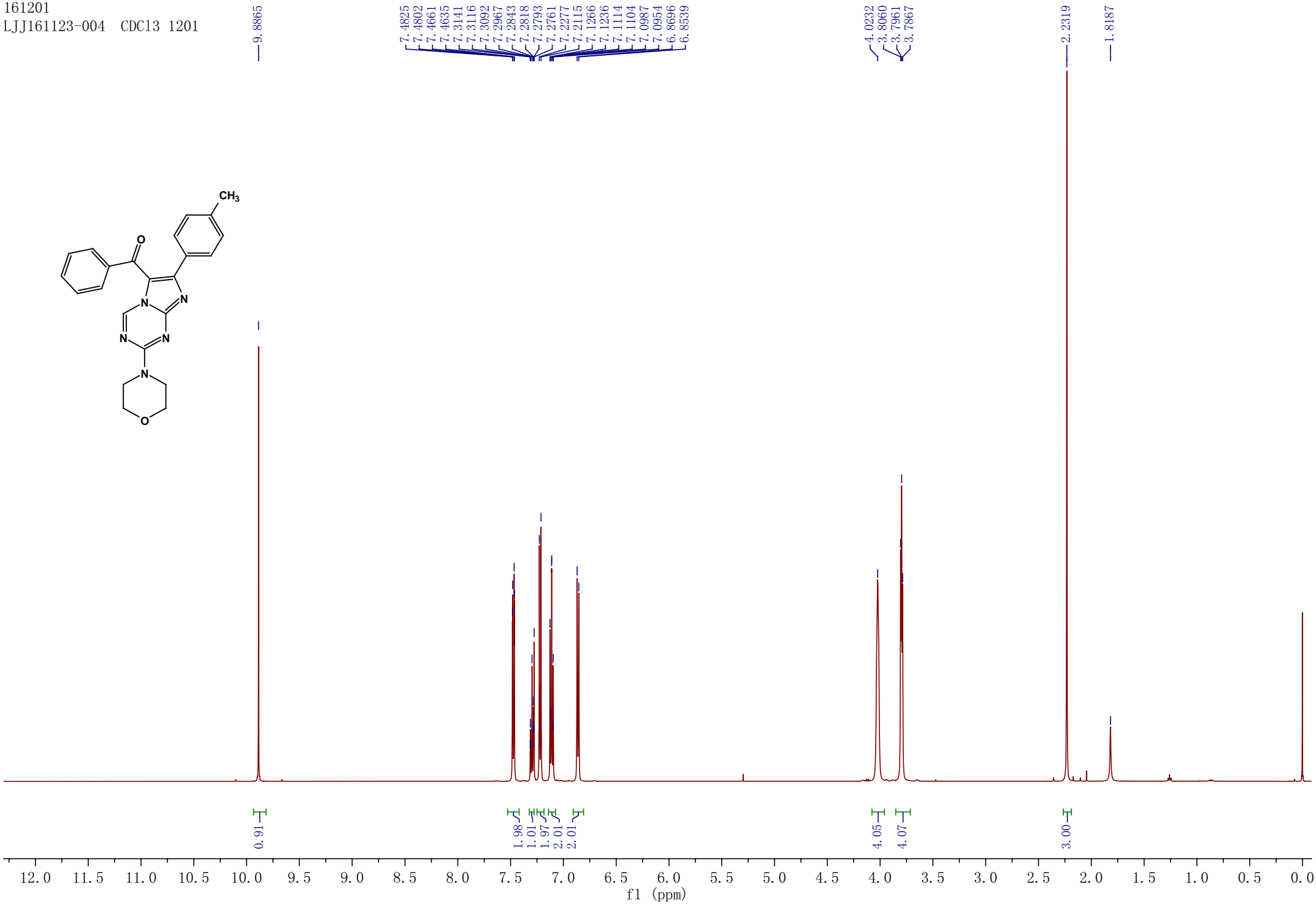
LJJ161123-004 CDCl3 1201



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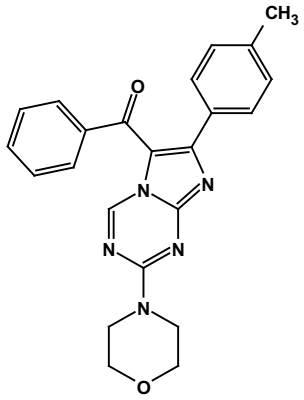

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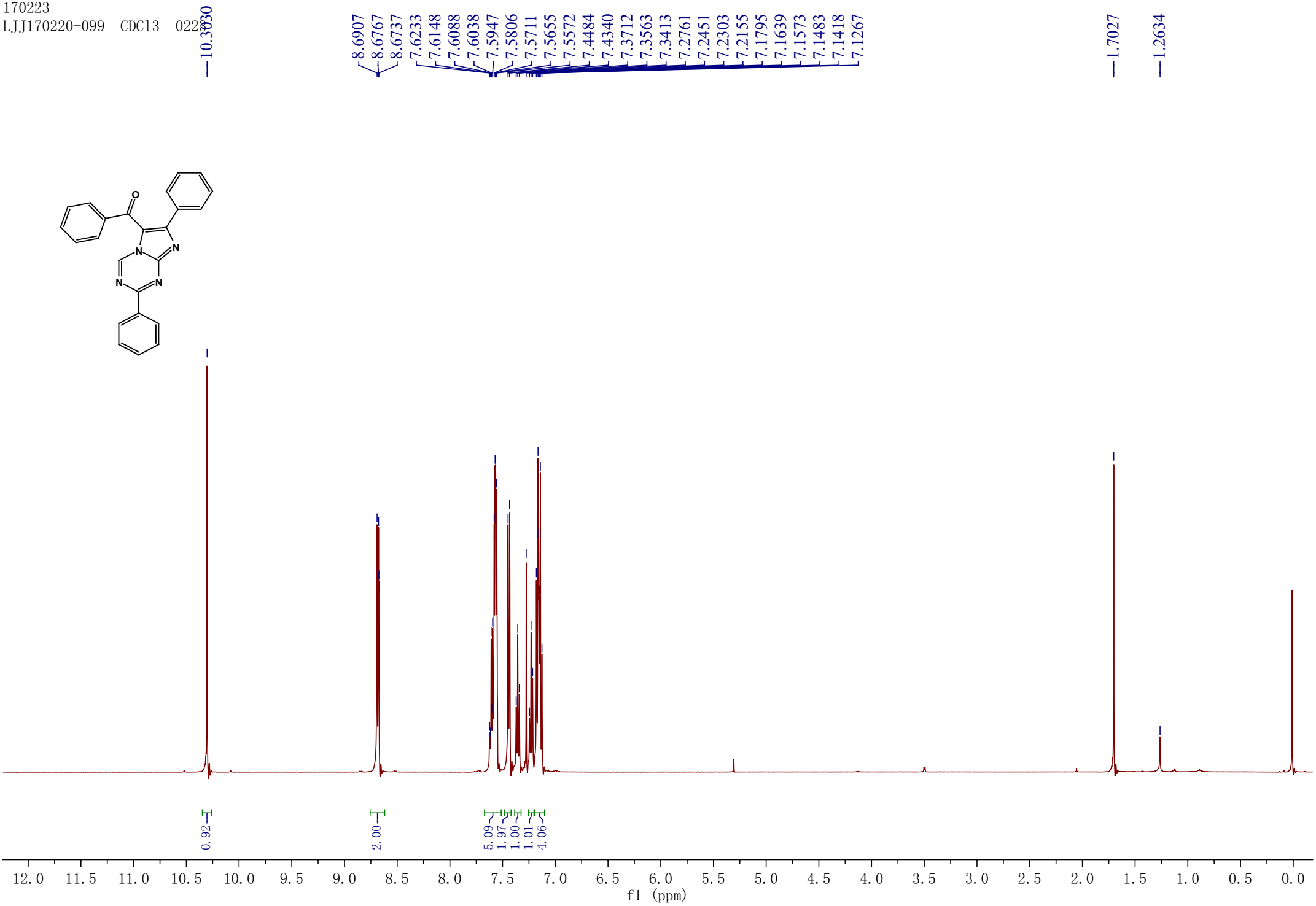

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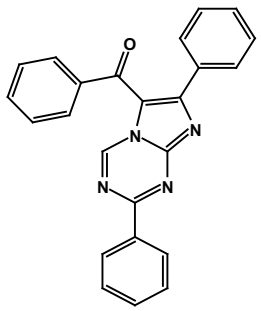
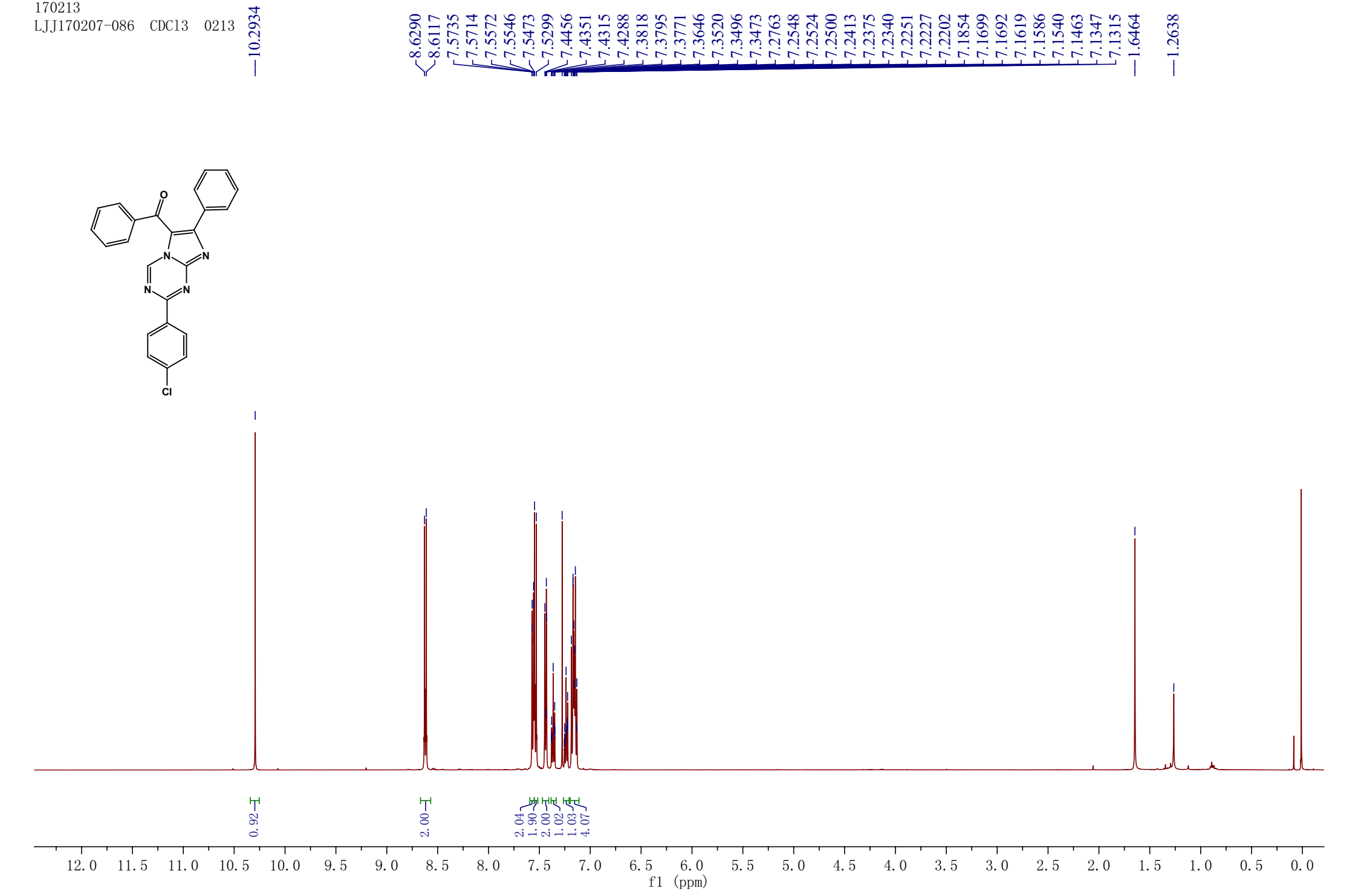
LJJ170220-099 CDCl3 C:\227



170213
LJJ170207-086 CDCl3 0213



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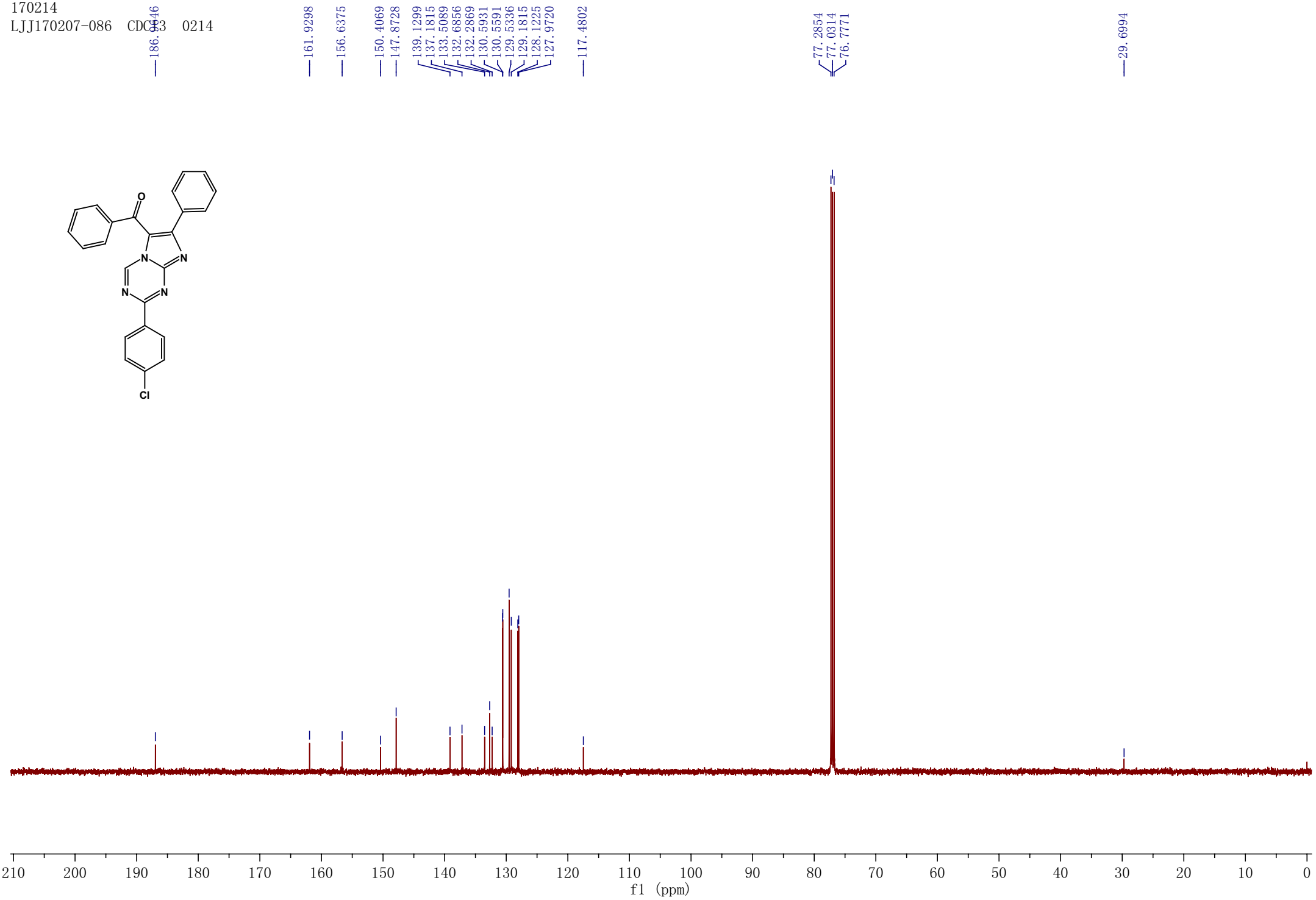
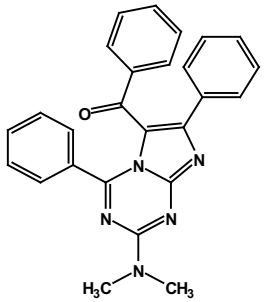


LJJ170224-101-P1



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7.4008
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7.2914
7.2767
7.2623
7.2540
7.2457
7.2305
7.2147
7.1849
7.1705
7.1543
7.1390
7.1210
7.1116
7.0966
7.0808

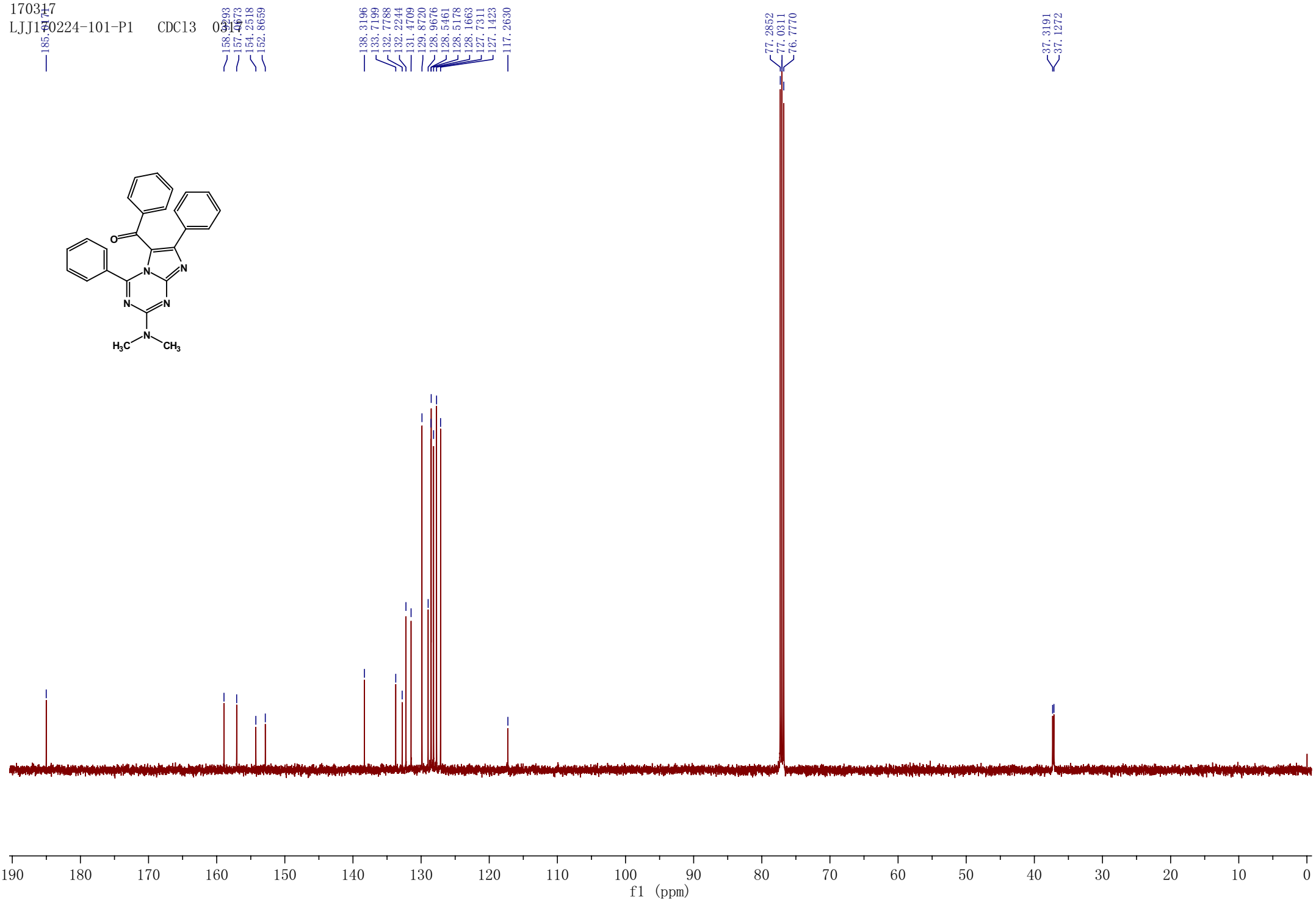
3.3482
3.3396

2.0401
1.7558
1.4112
1.2668
1.2494
1.1067
0.8882
0.8747
0.8607

1.79
1.79
1.22
6.08
1.99
2.03
6.00

12.0 11.5 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)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LJJ170224-101-P1 CDCl3 03
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152.8659
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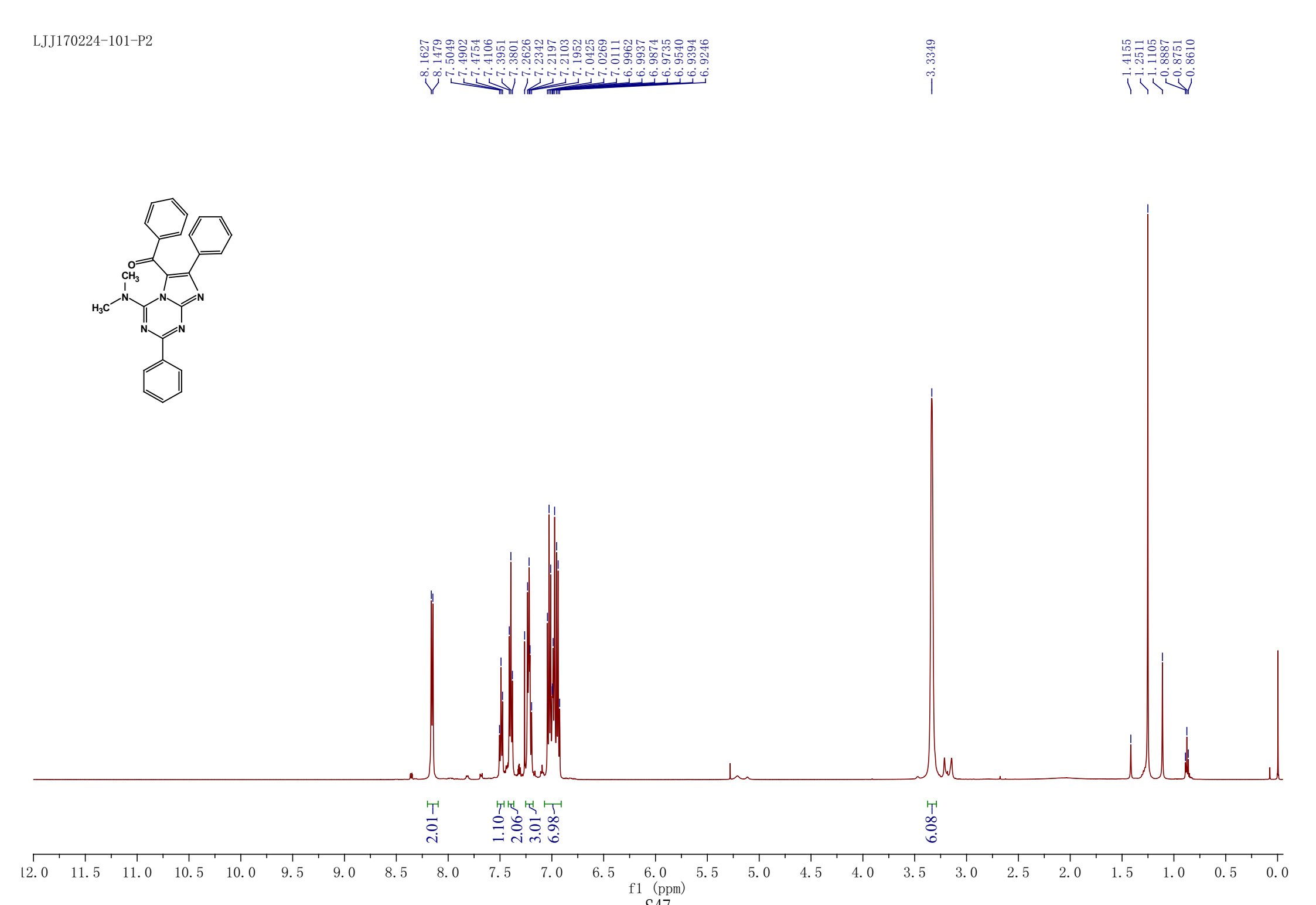
133.7199
132.7788
132.2244
131.4709
129.8720
128.9676
128.5461
128.5178
128.1663
127.7311
127.1423
117.2630
77.2852
77.0311
76.7770
37.3191
37.1272
O
N
N
N
N
N
H3C
CH3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

LJJ170224-101-P2



170310
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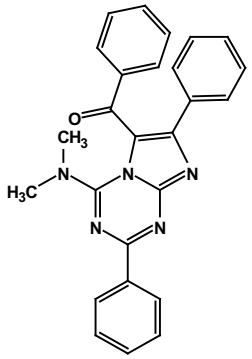

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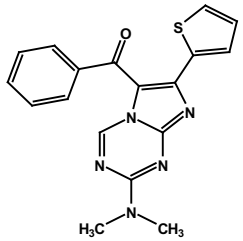

LJJ161114-187-P2 H
LJJ161114-187-P2 CDC13 0605

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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