Tandem Halogenation/Michael-initiated Ring-closing Reaction of α,β-Unsaturated Nitriles and Activated Methylene Compounds: One-pot Diastereoselective Synthesis of Functionalized Cyclopropanes

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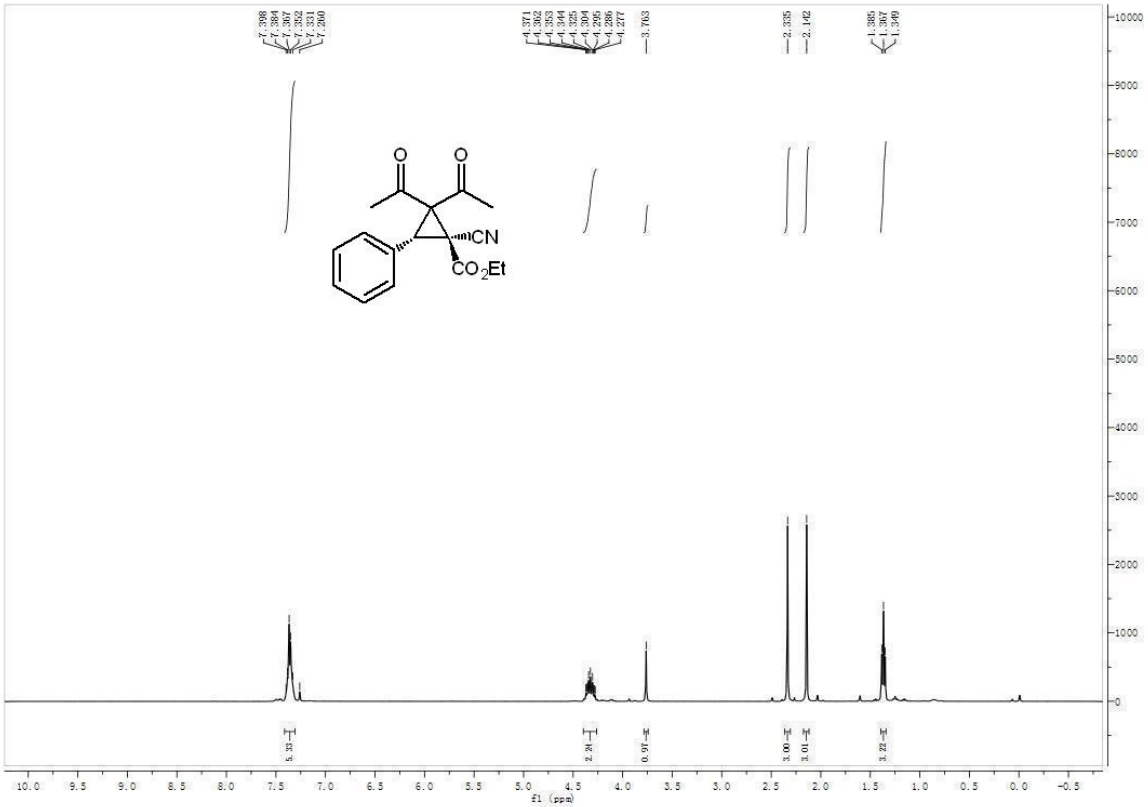
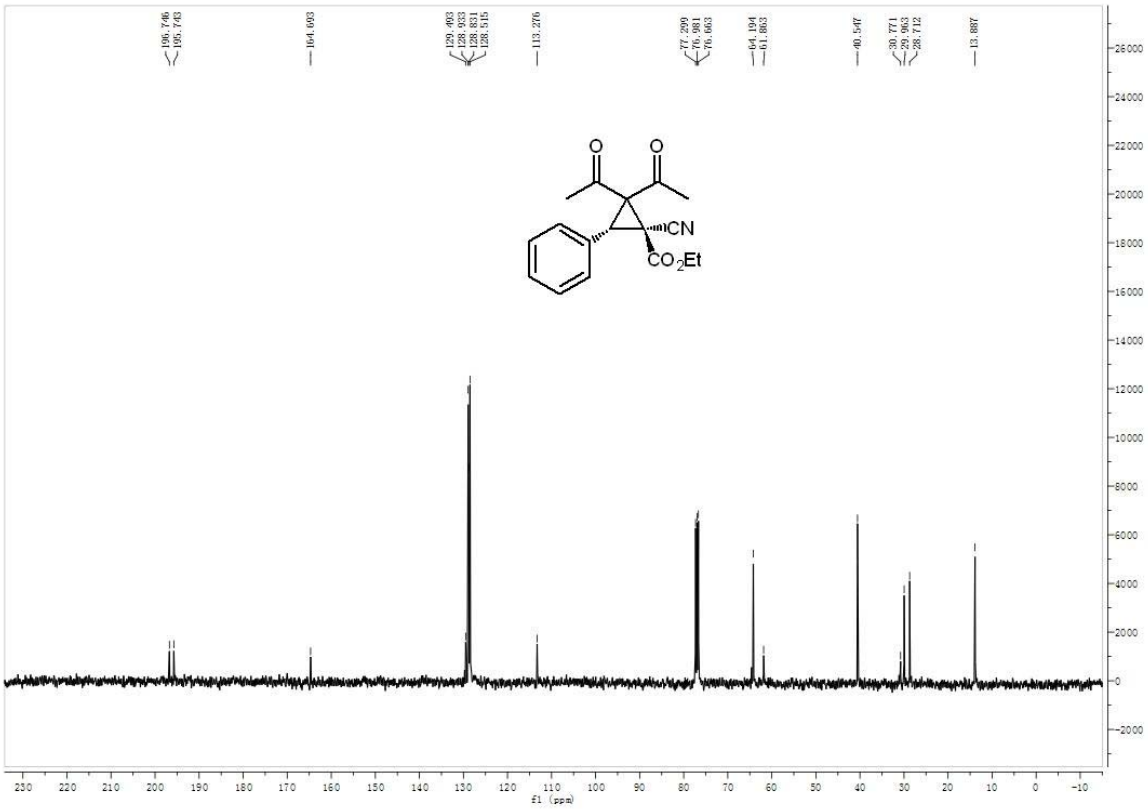
Electronic Supplementary Information

Copies of NMR spectra for compounds 3-7

3aa





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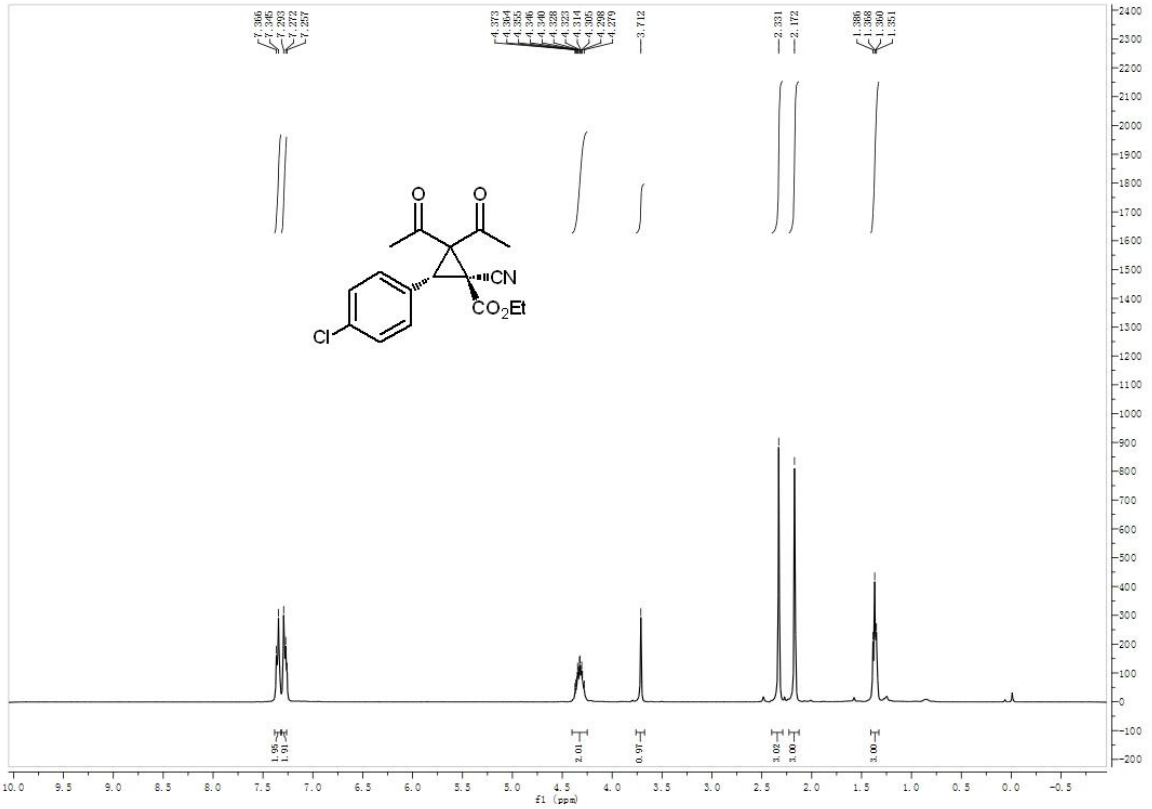
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CO2Et
Cl
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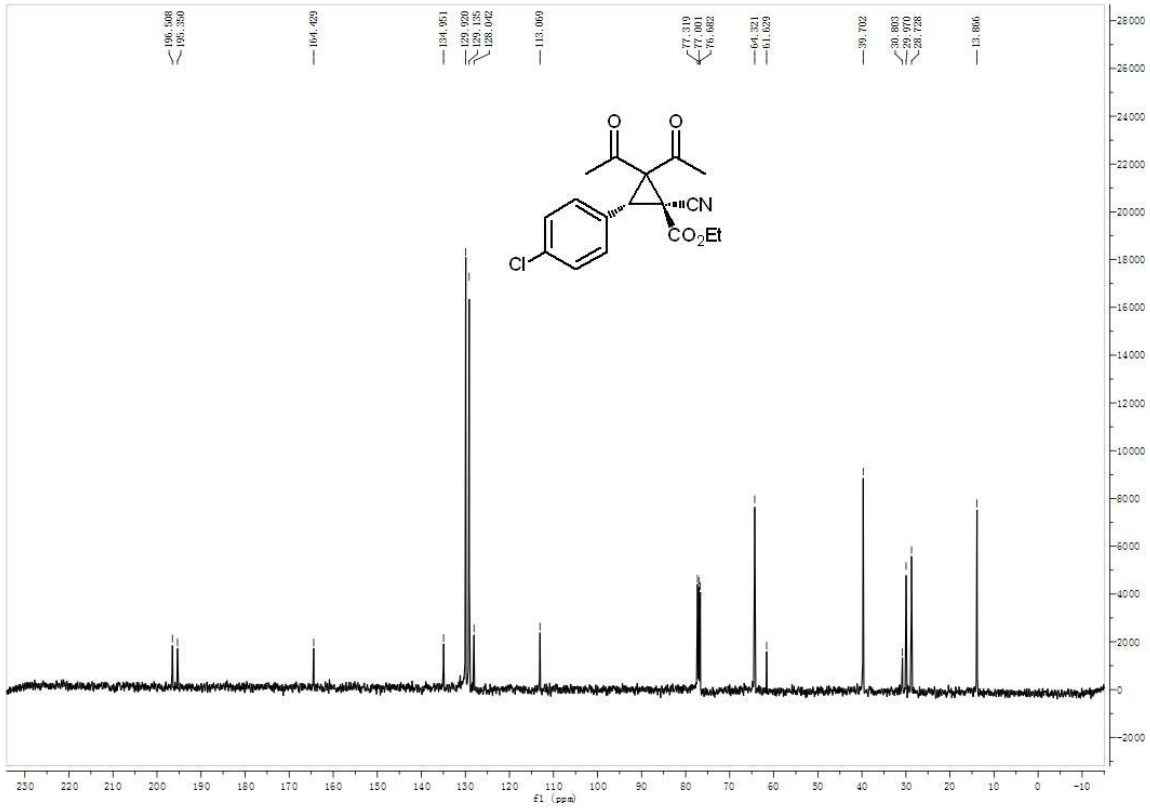
3.02
3.00
3.00
f1 (ppm)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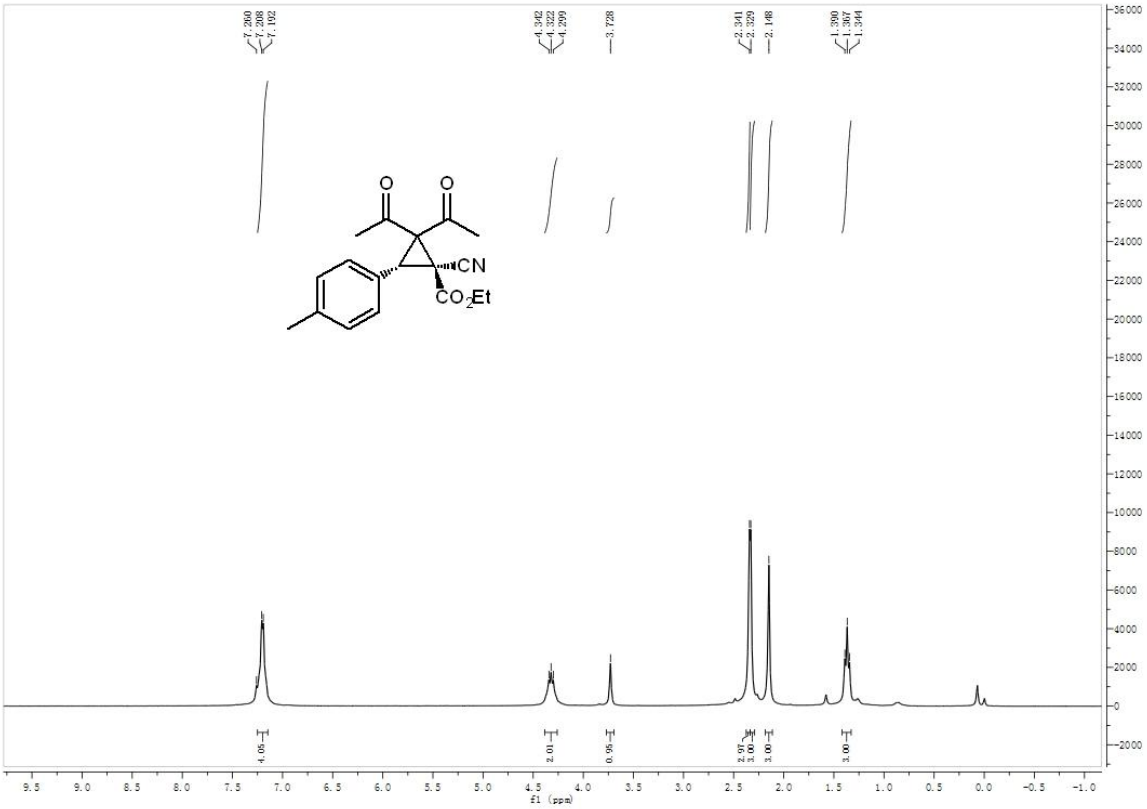
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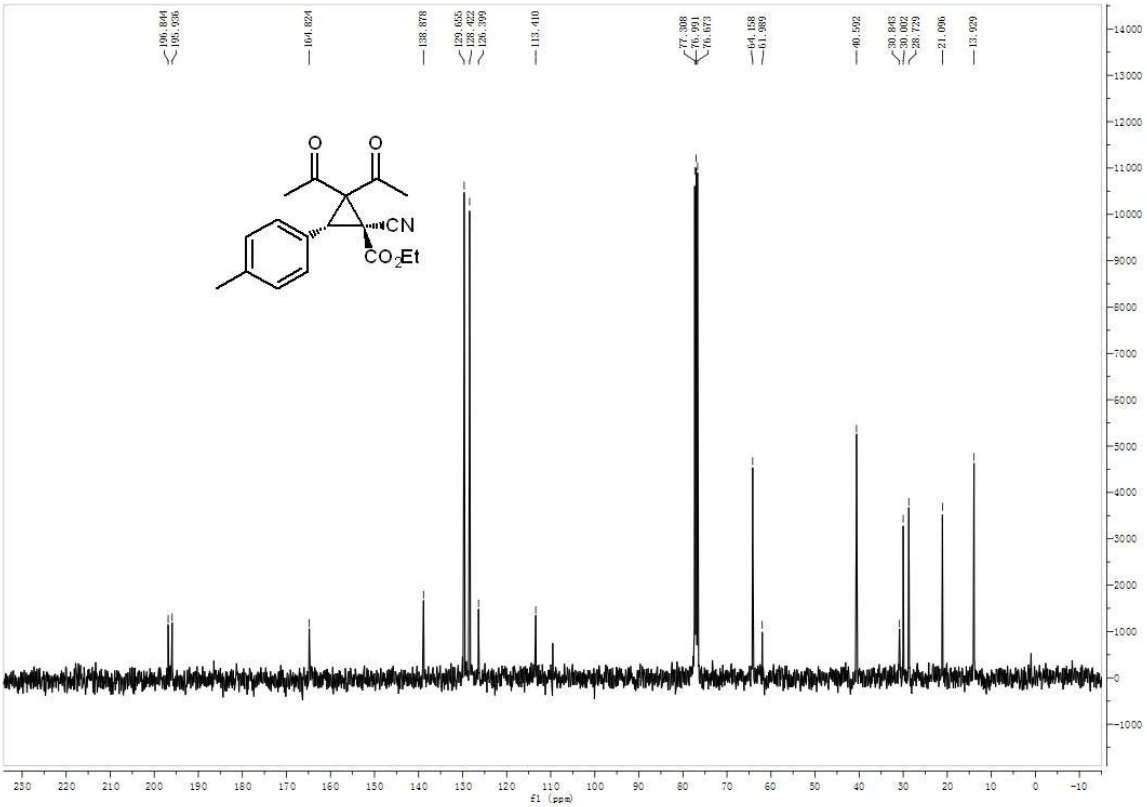
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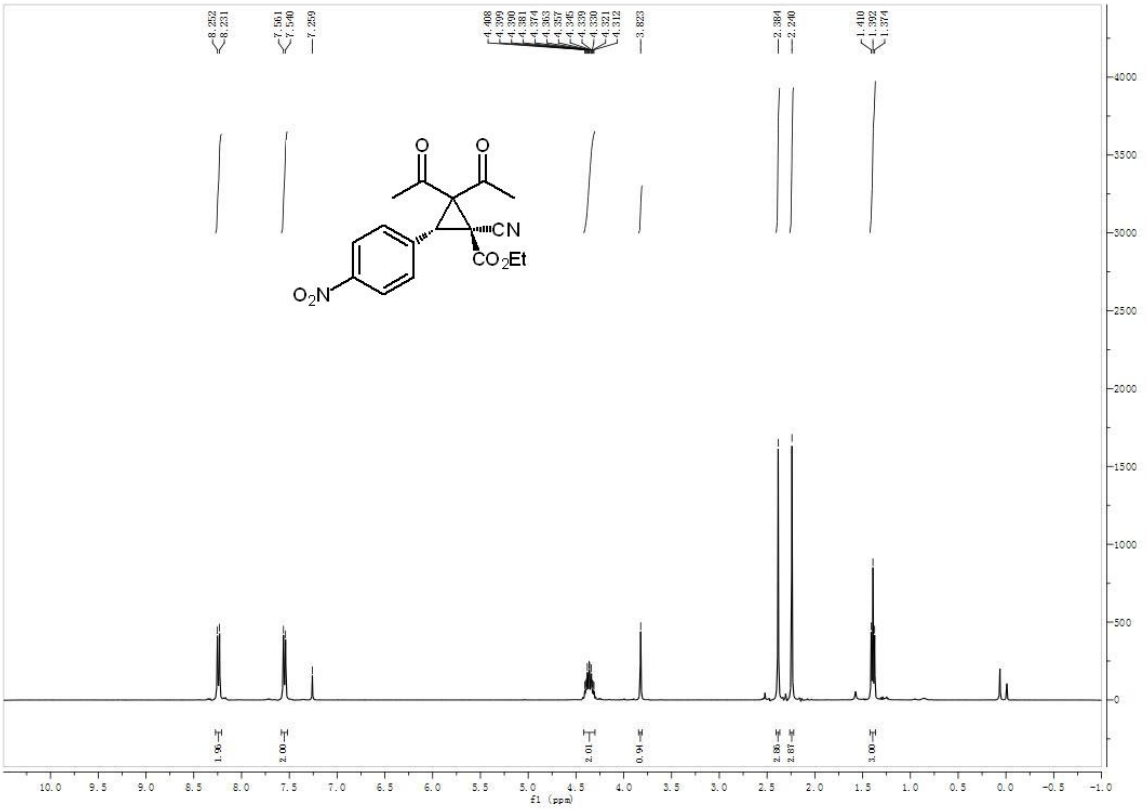
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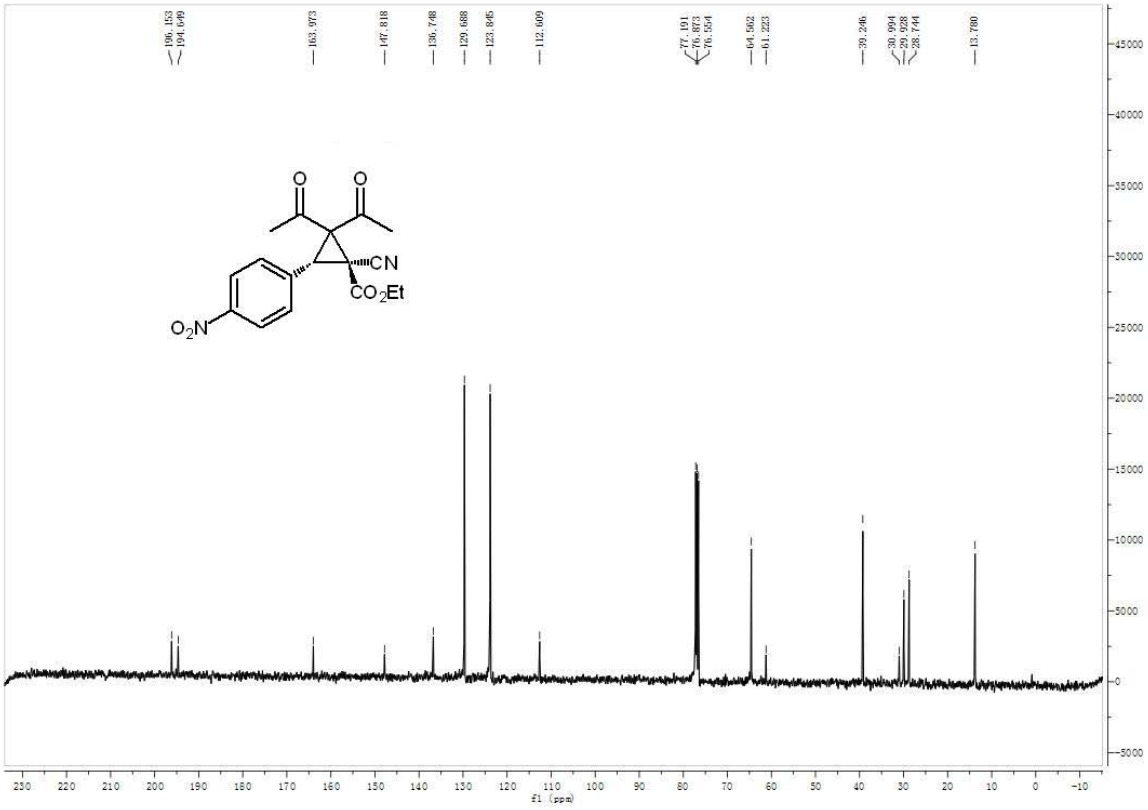
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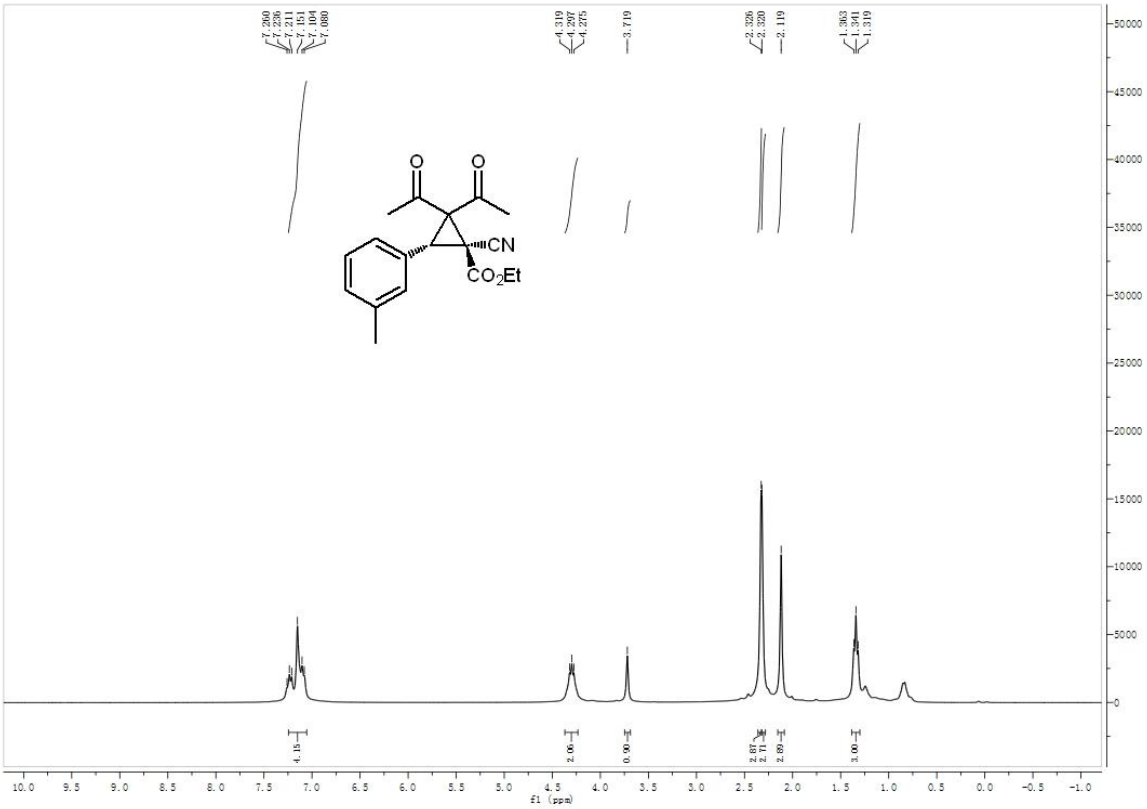
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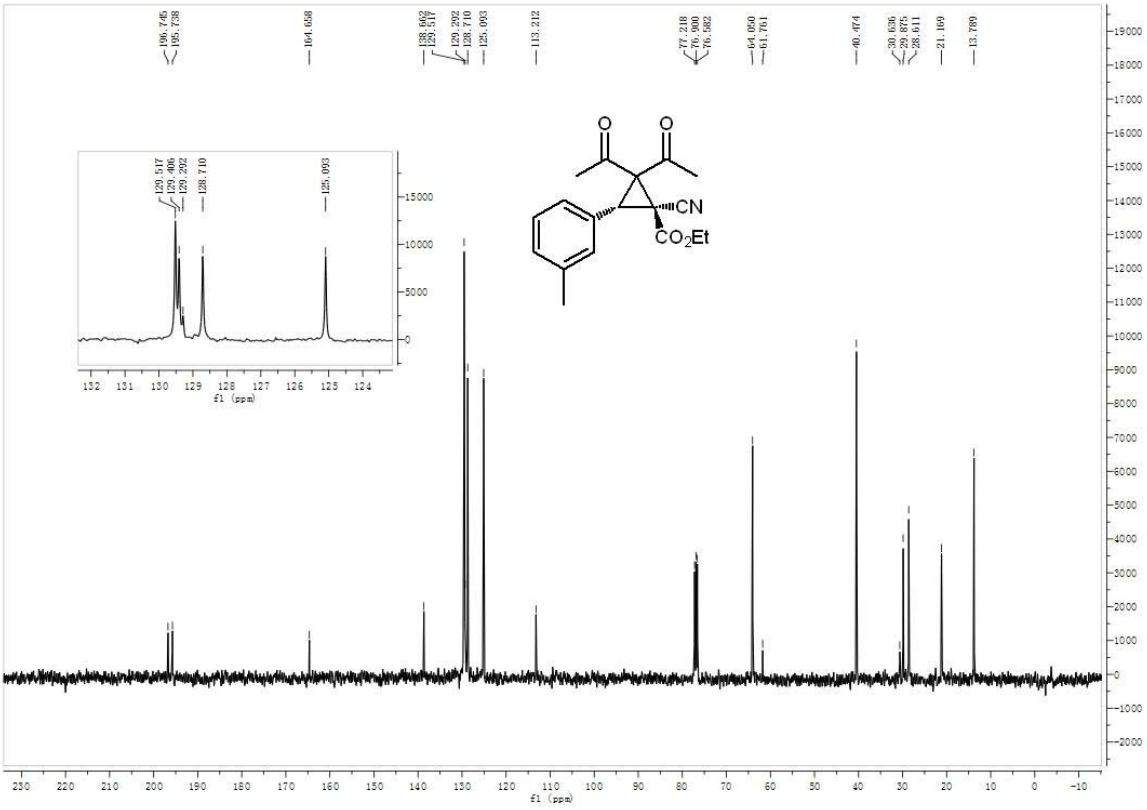
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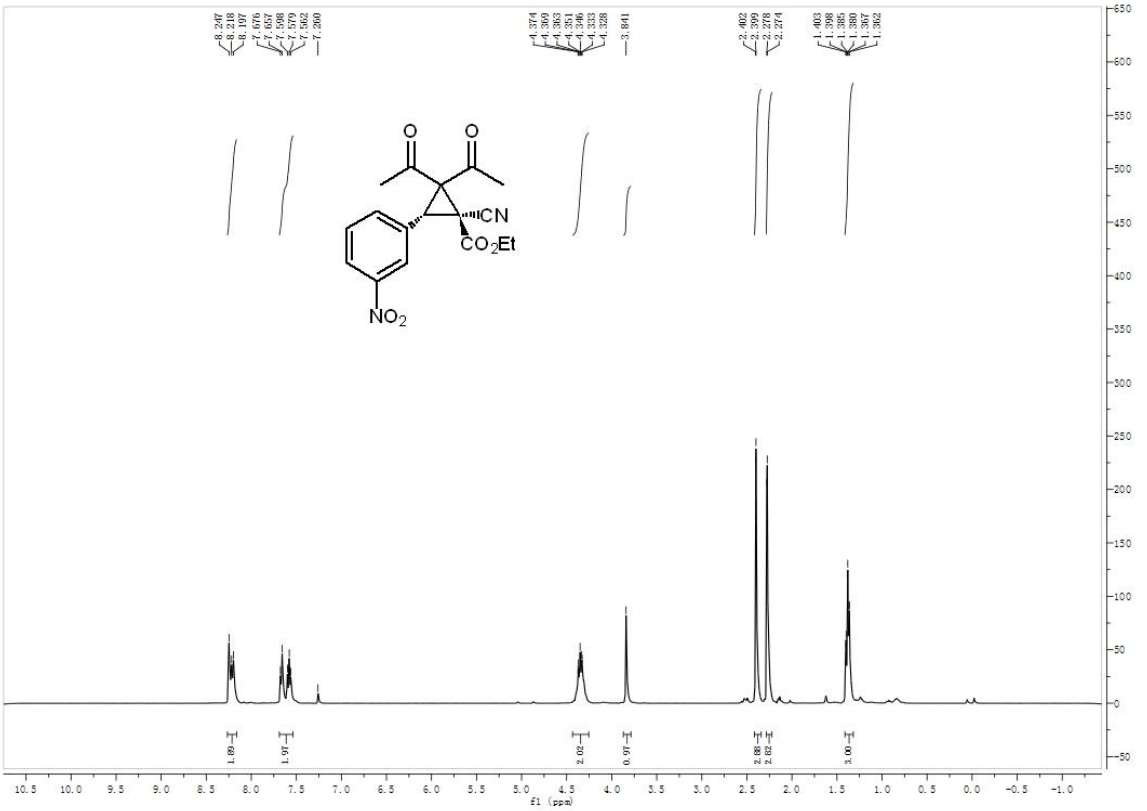
CO2Et
f1 (ppm)

3fa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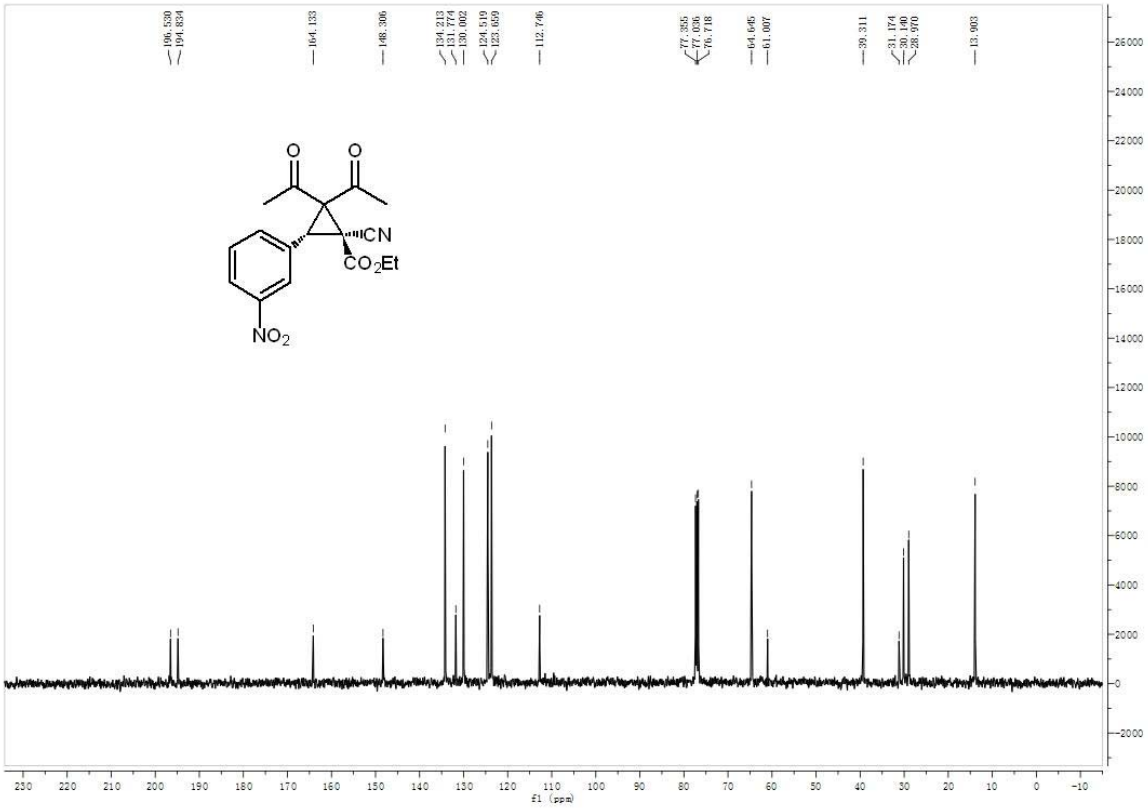
f1 (ppm)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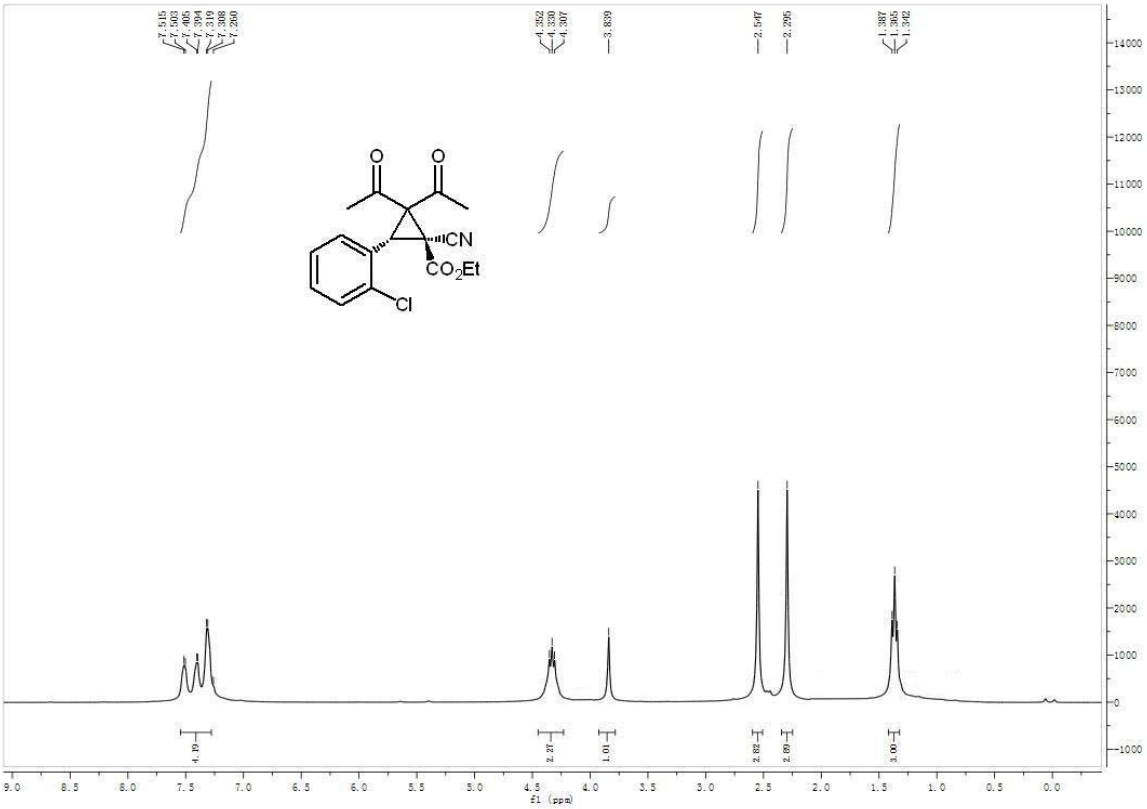
3ga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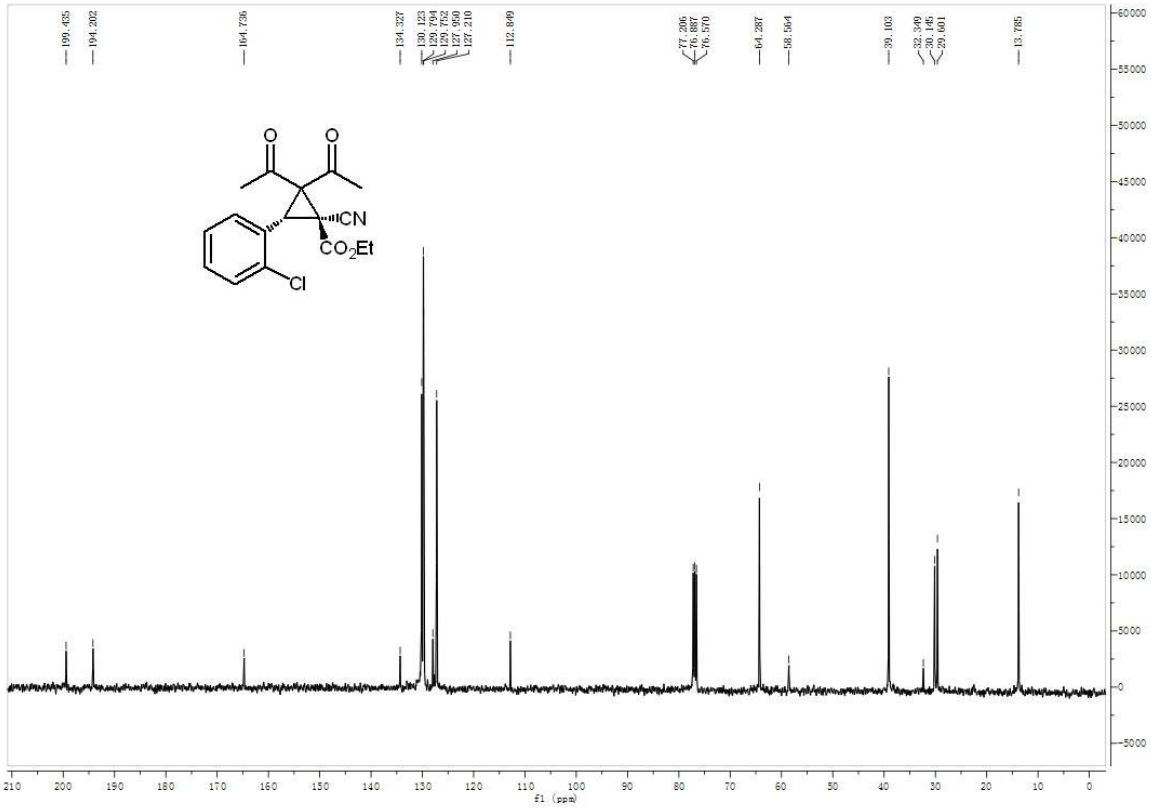
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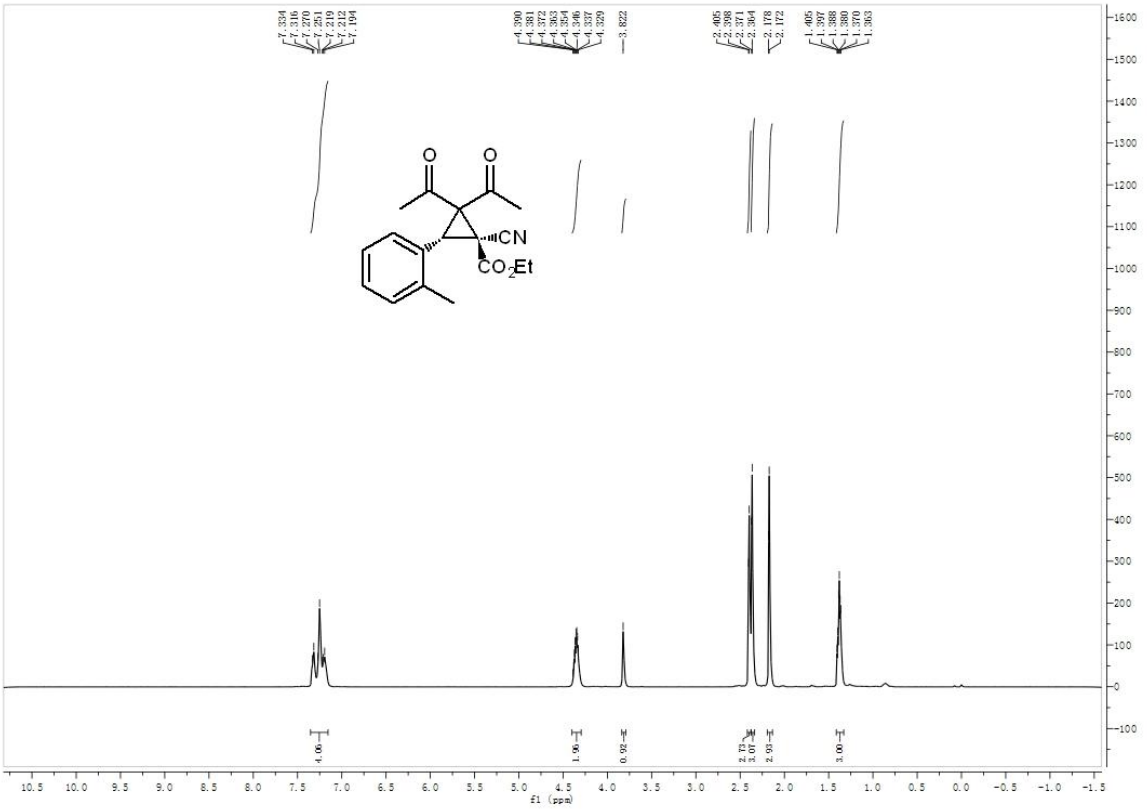
f1 (ppm)

3ha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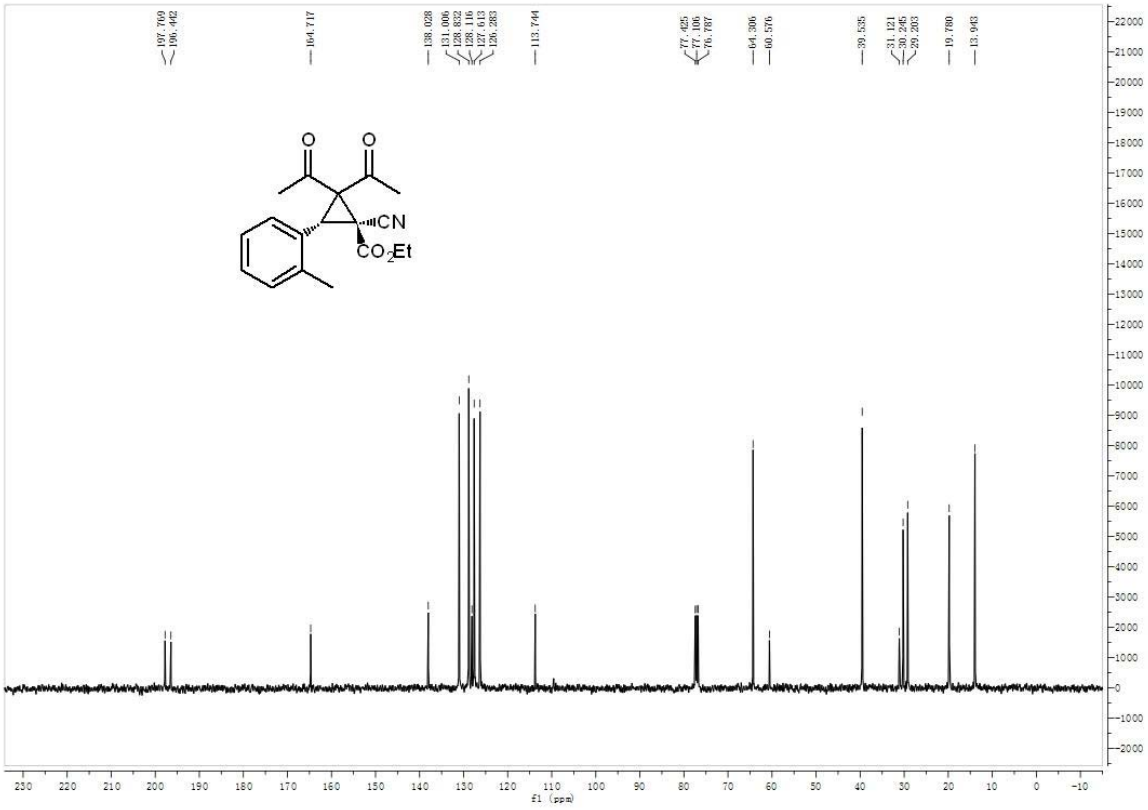
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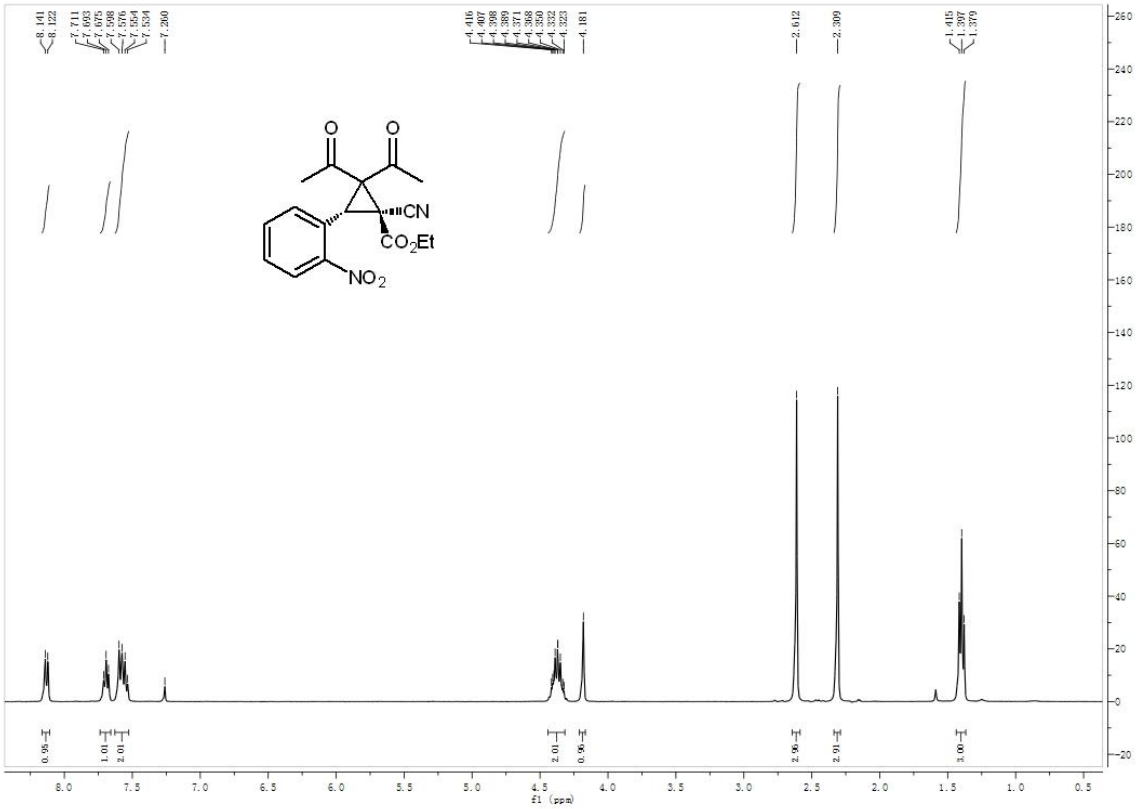
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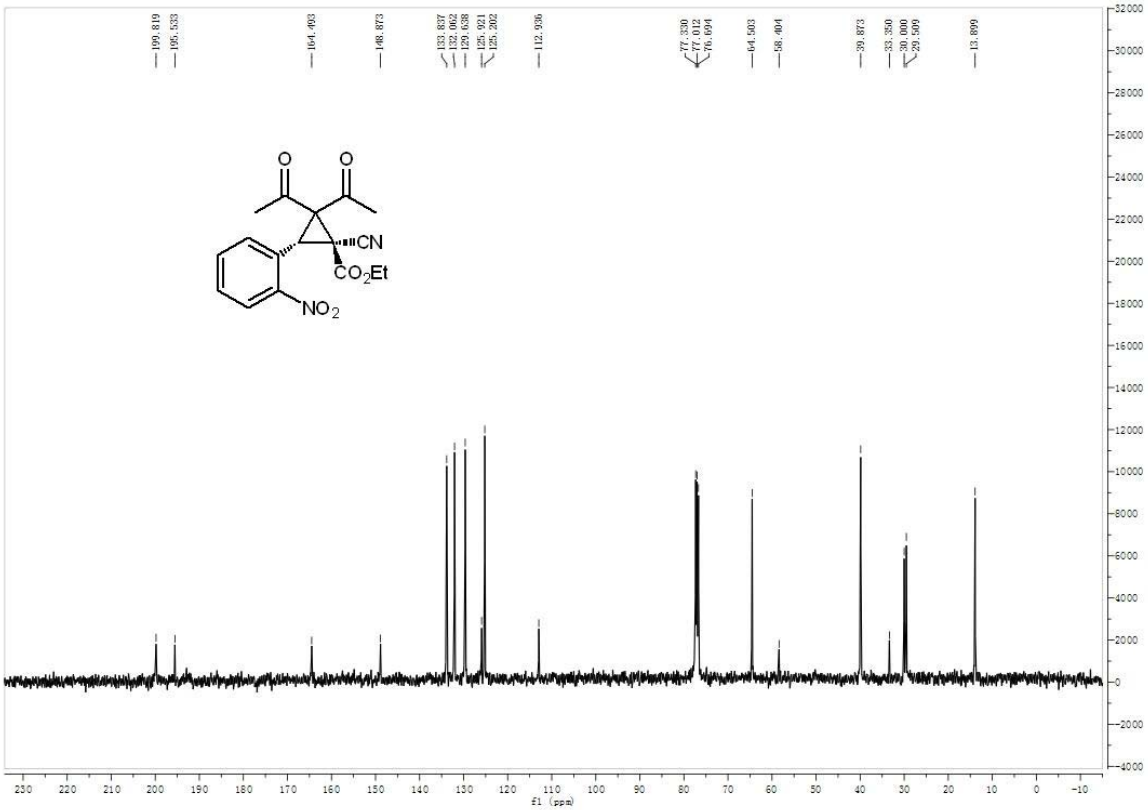
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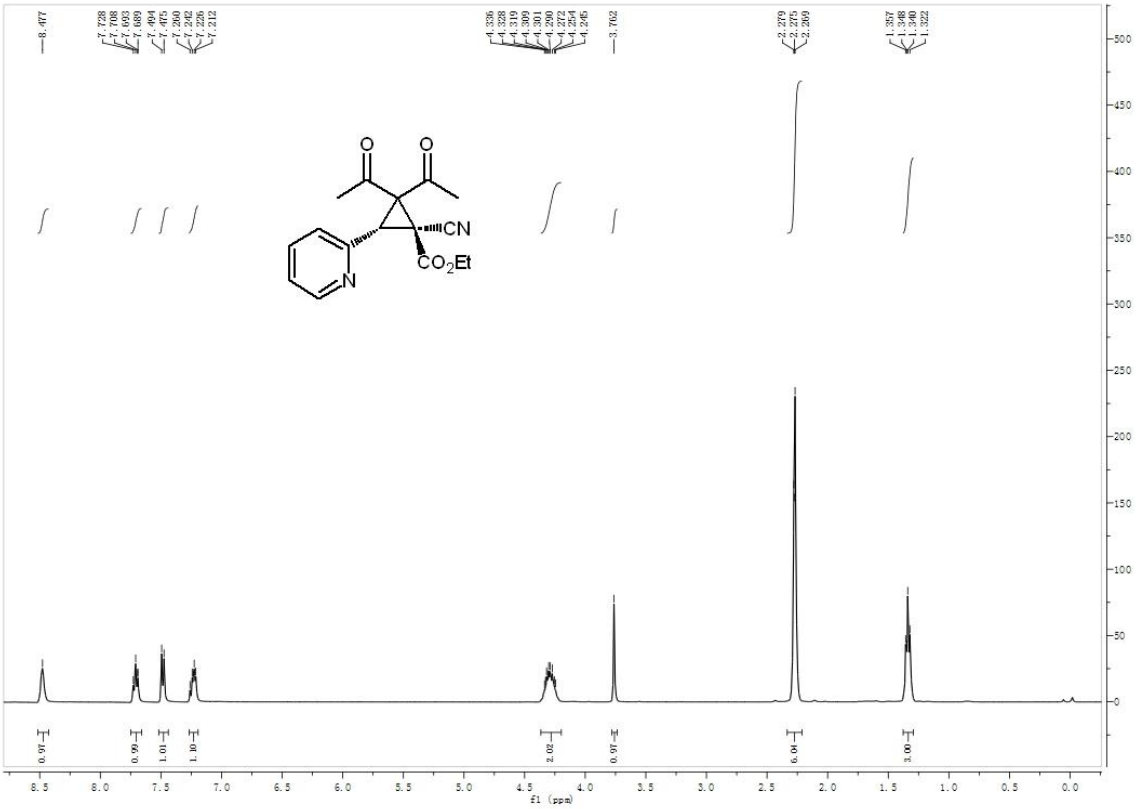
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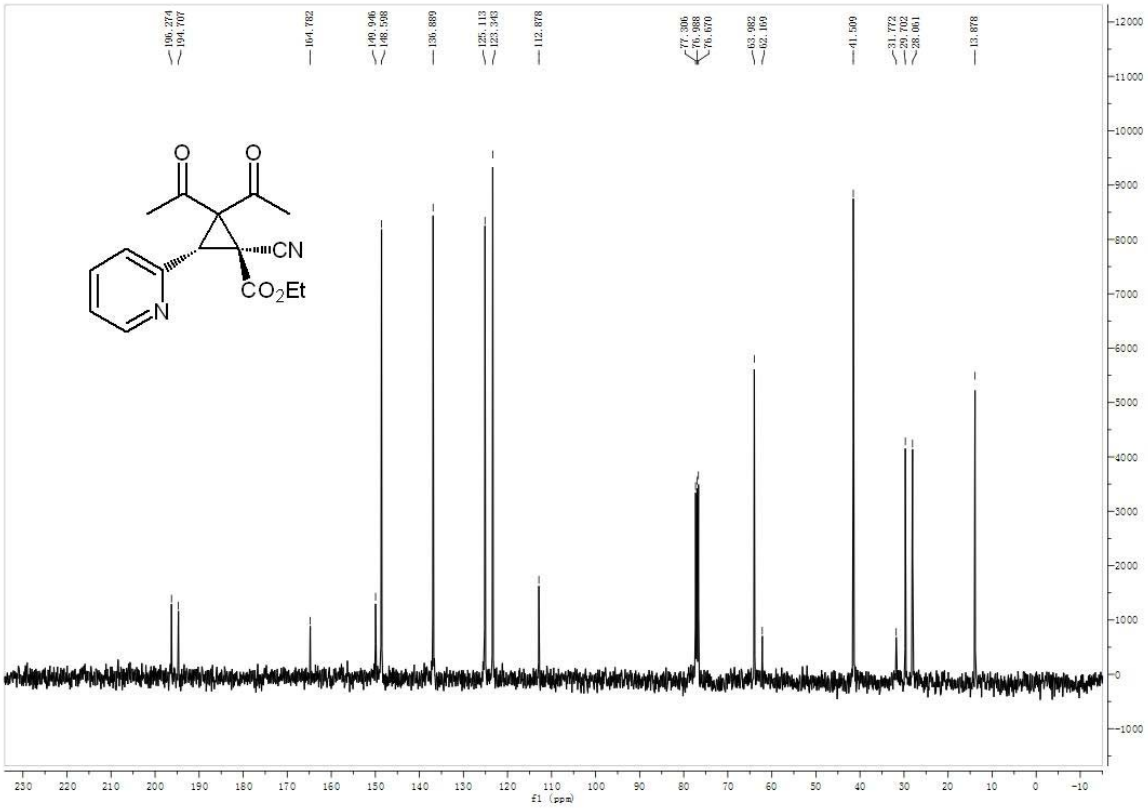
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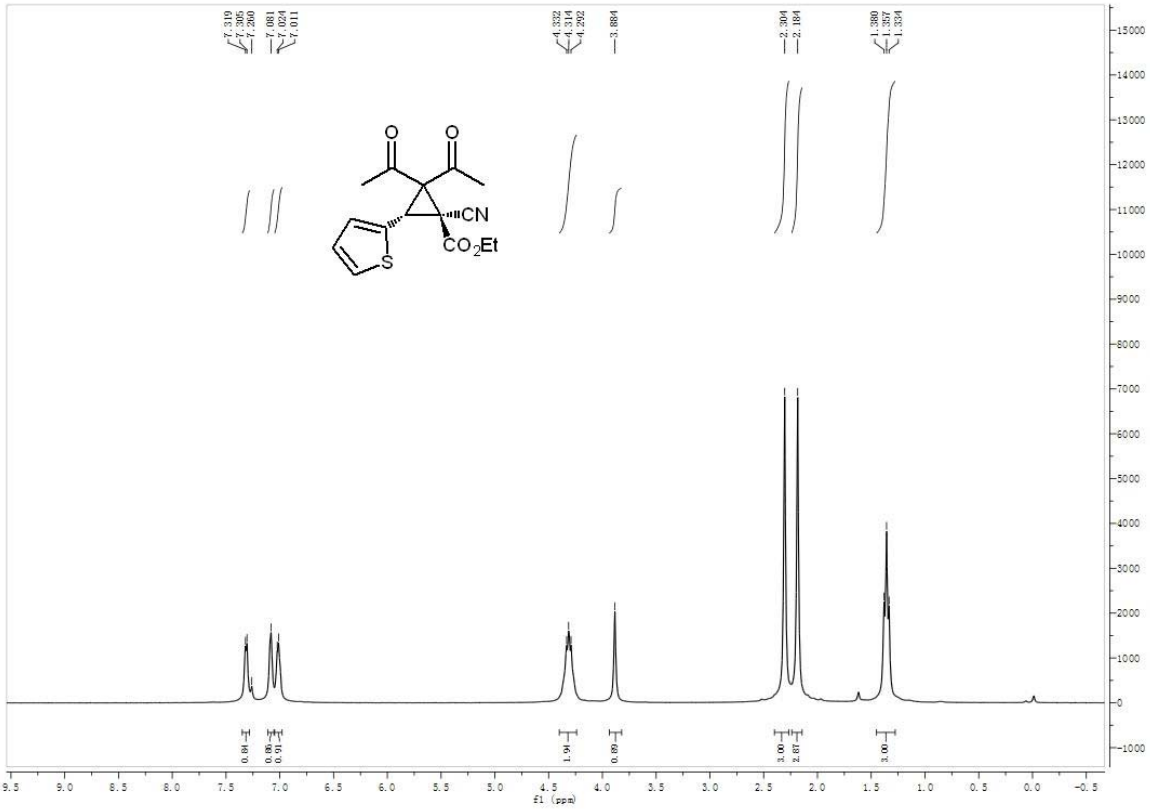
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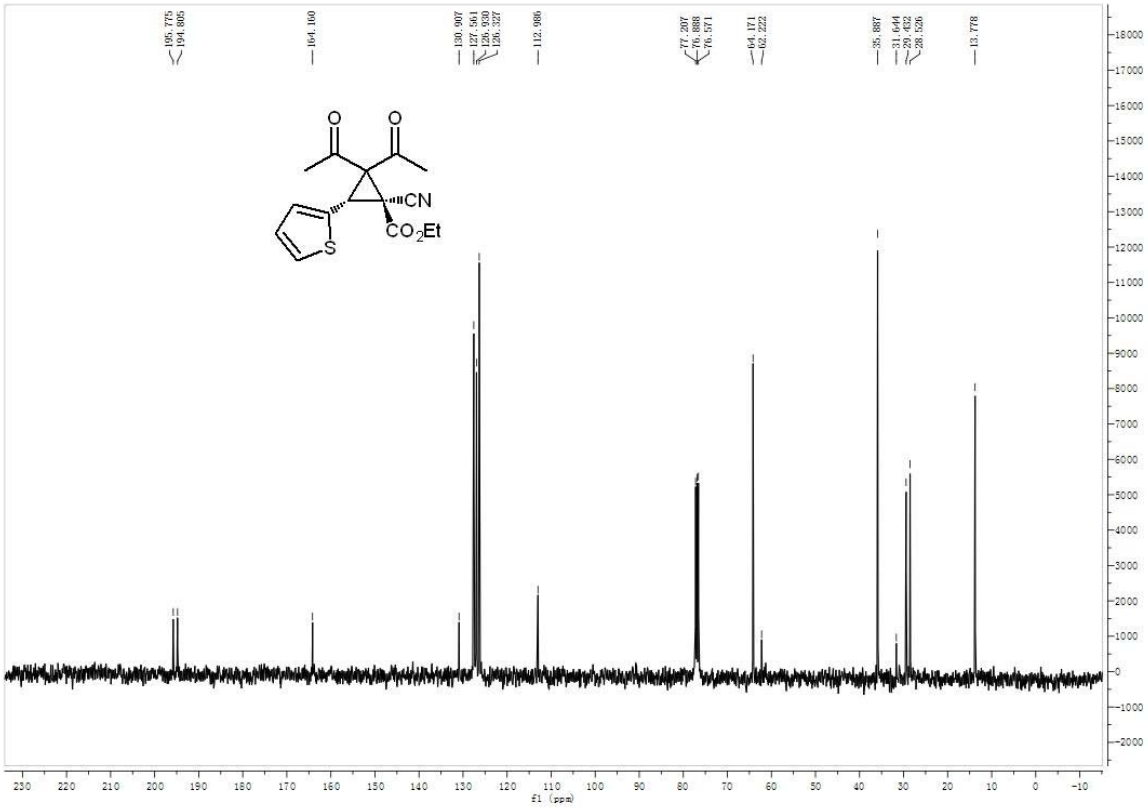
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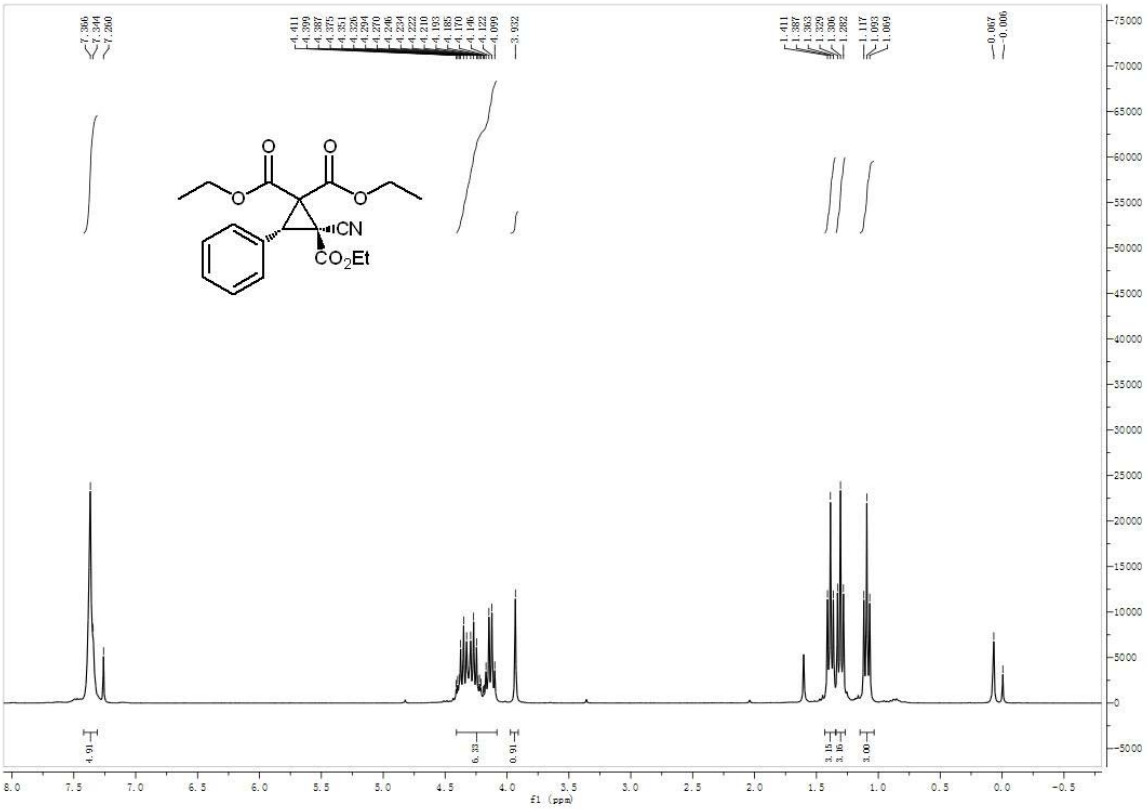
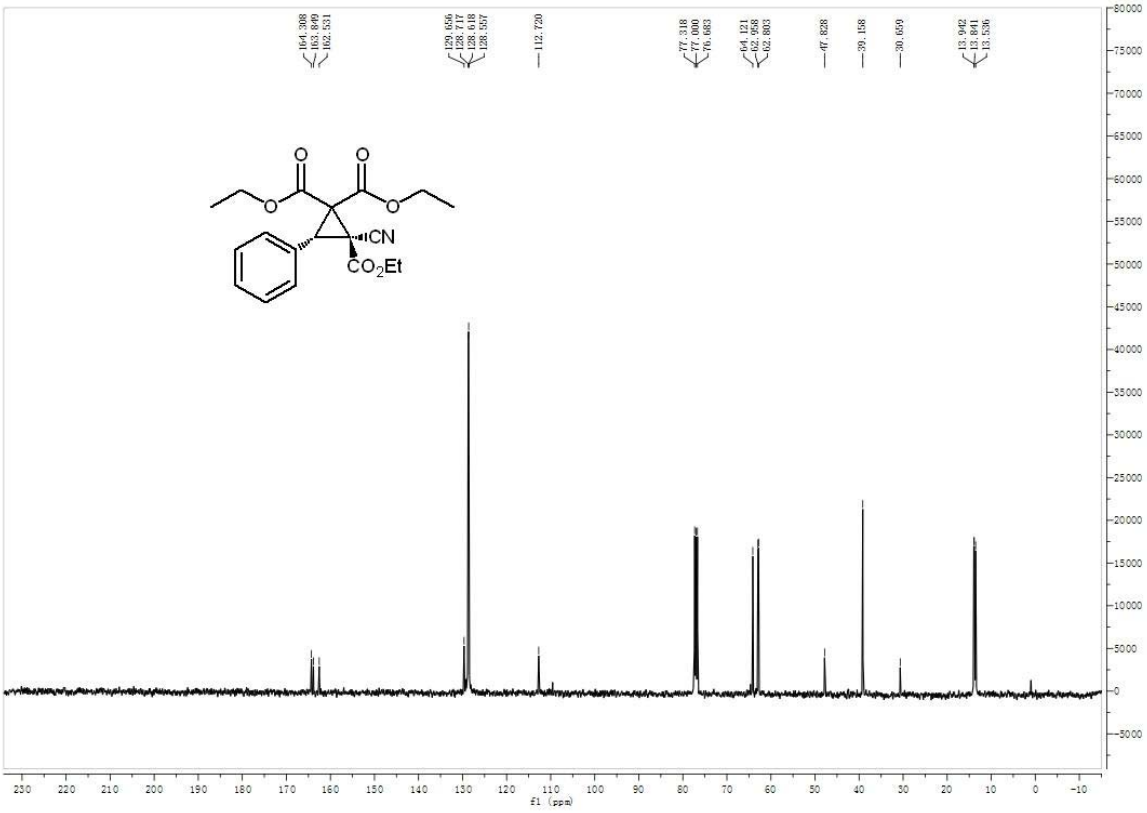
3ab





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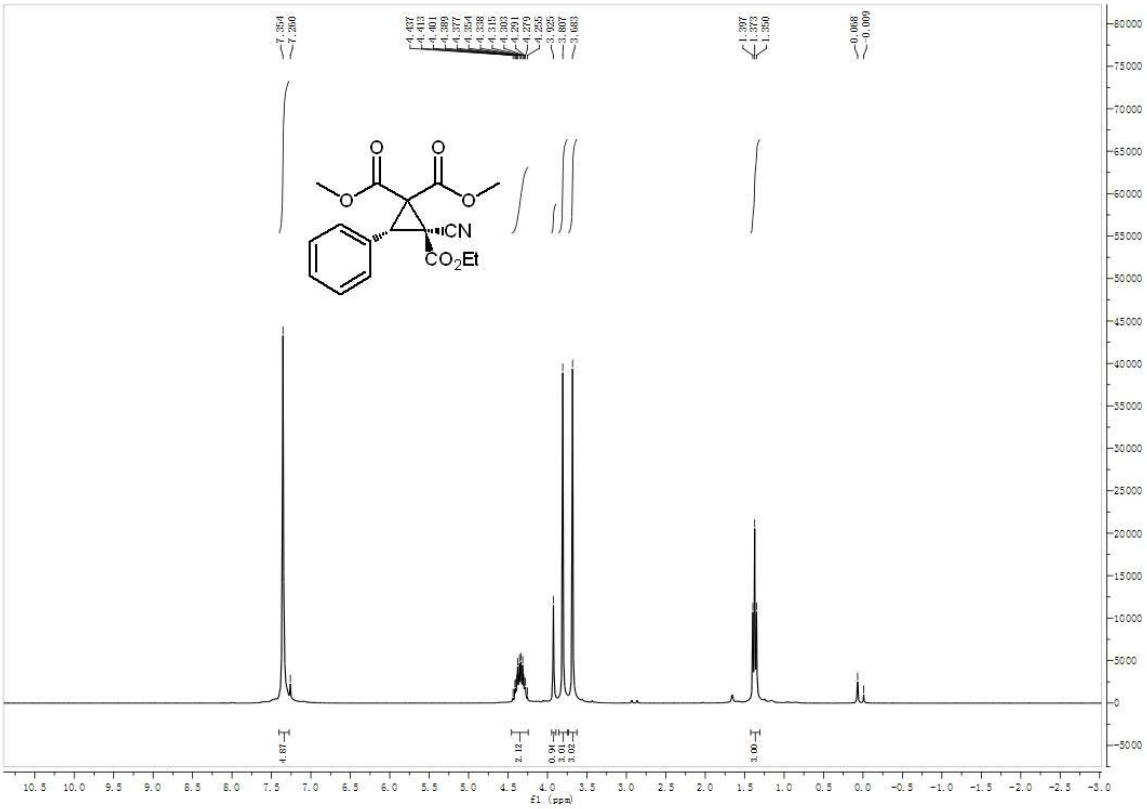
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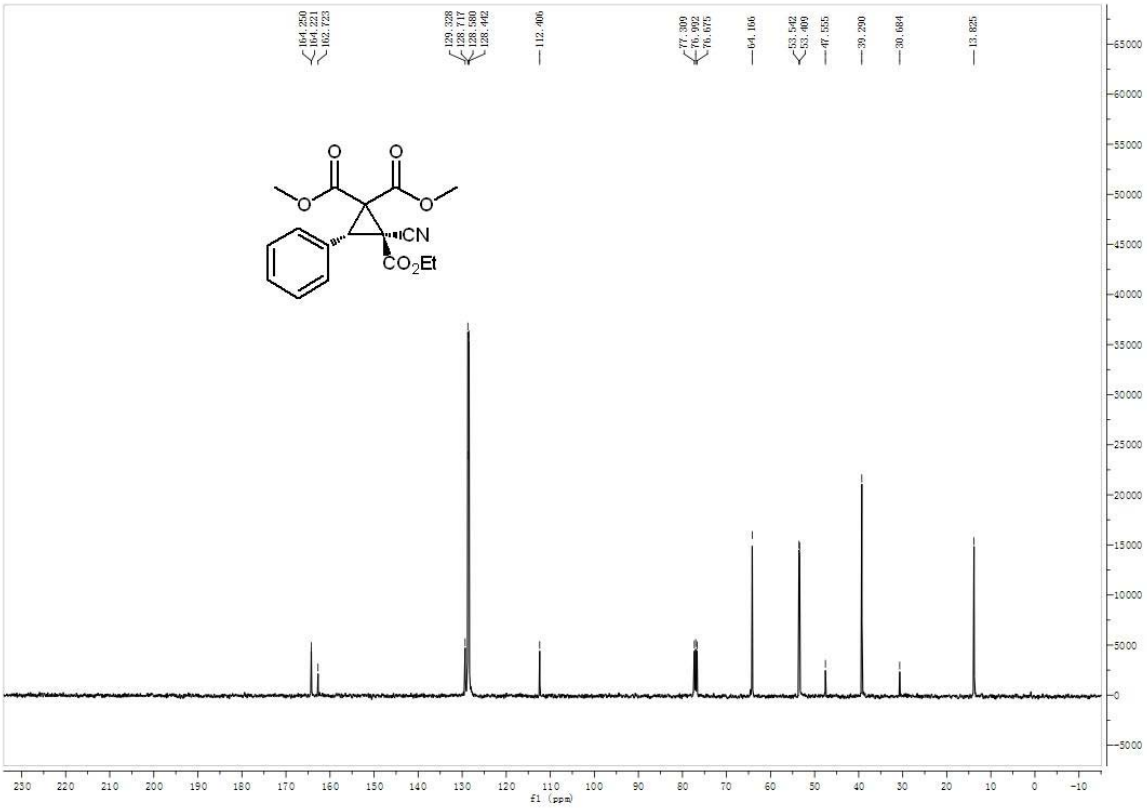
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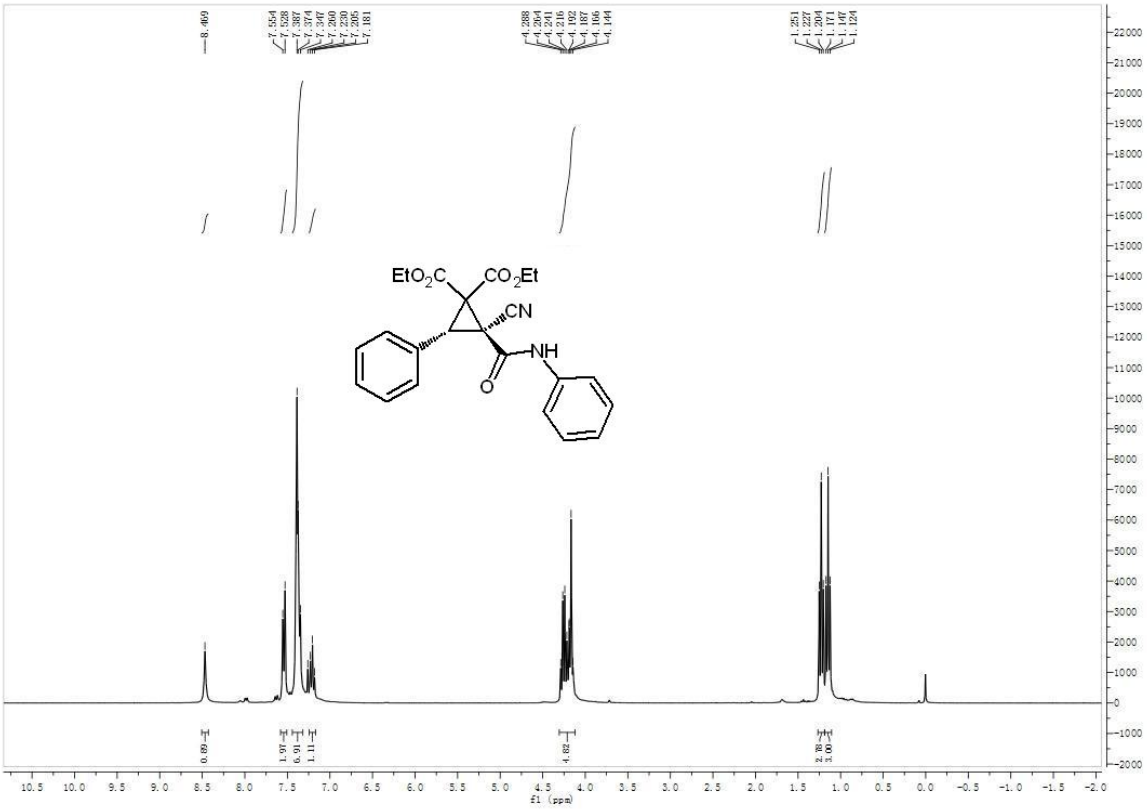
3lb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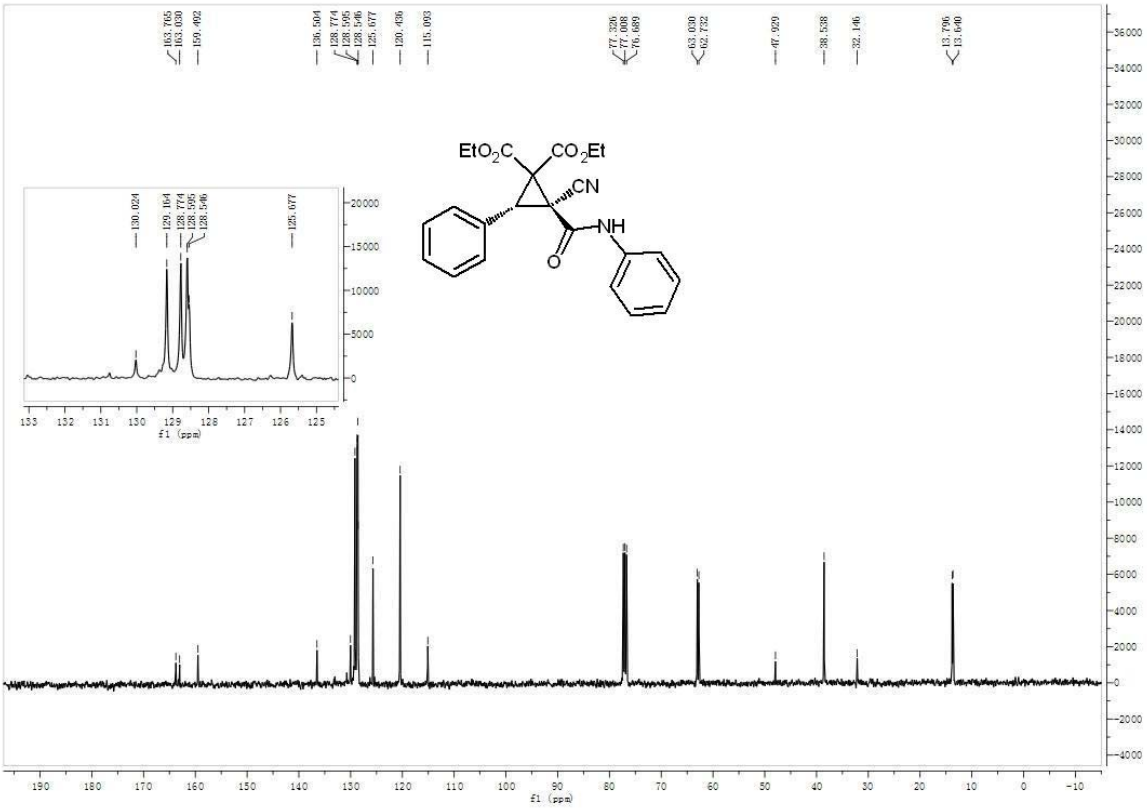
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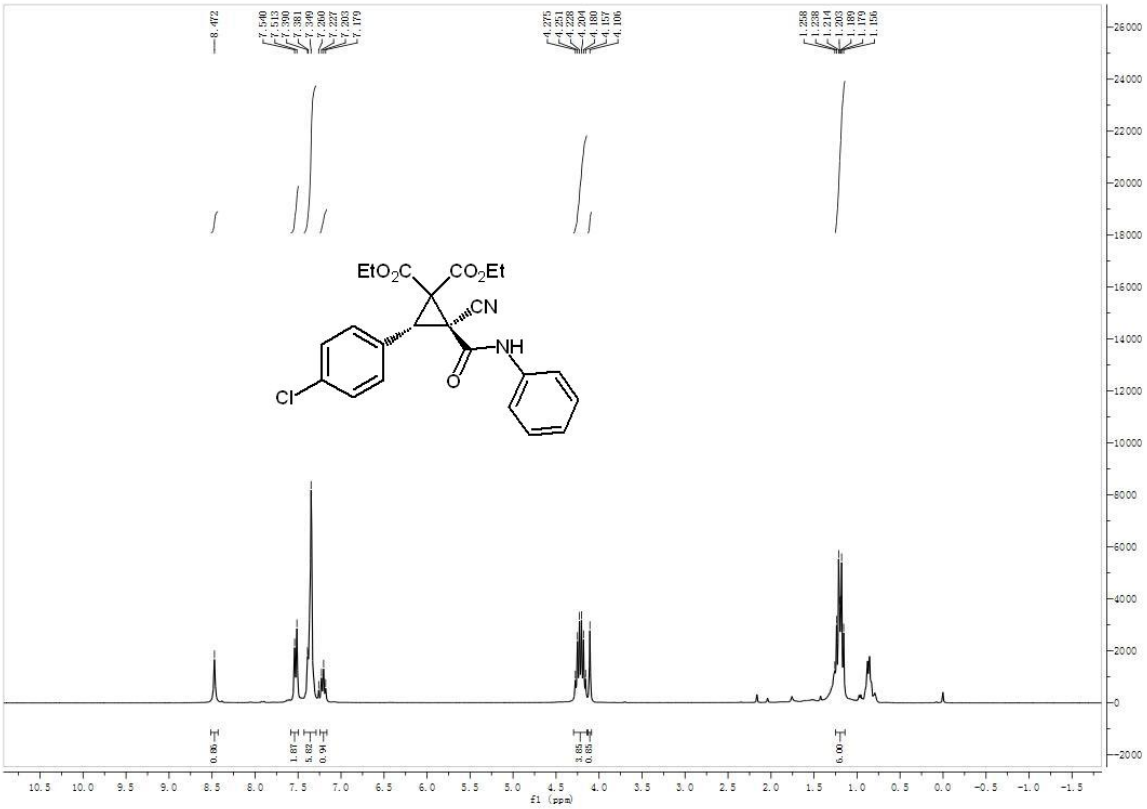
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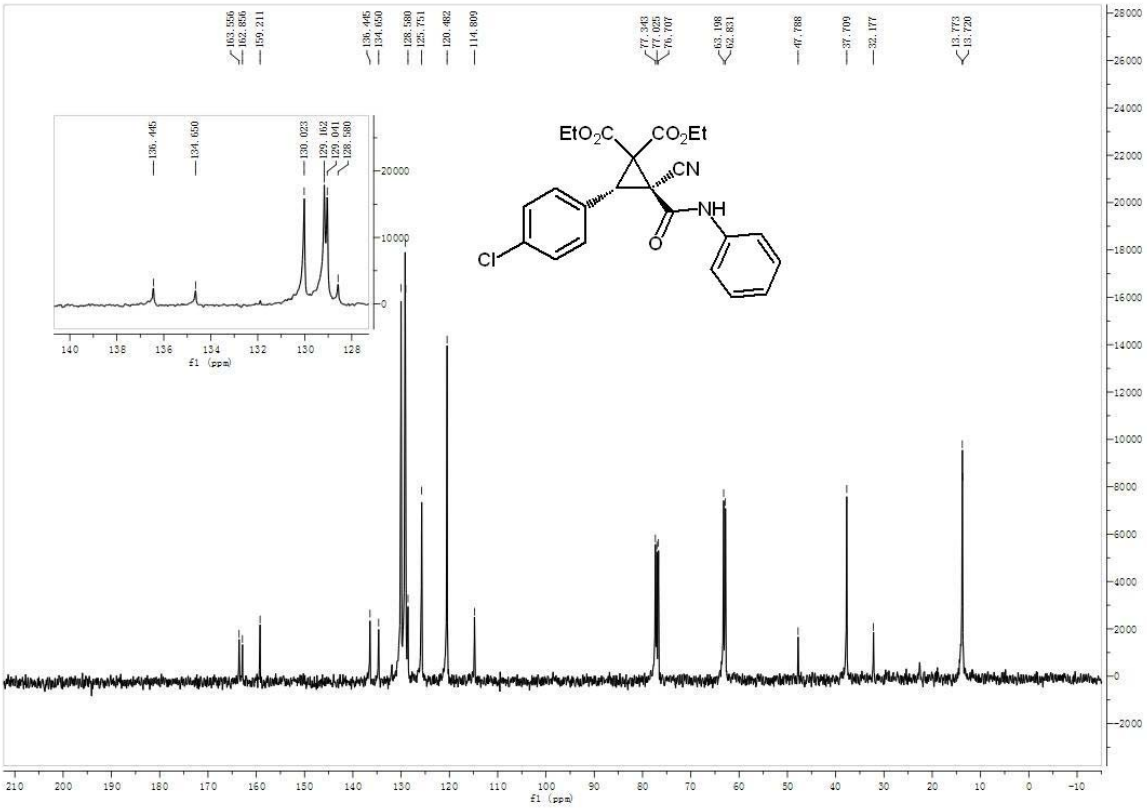
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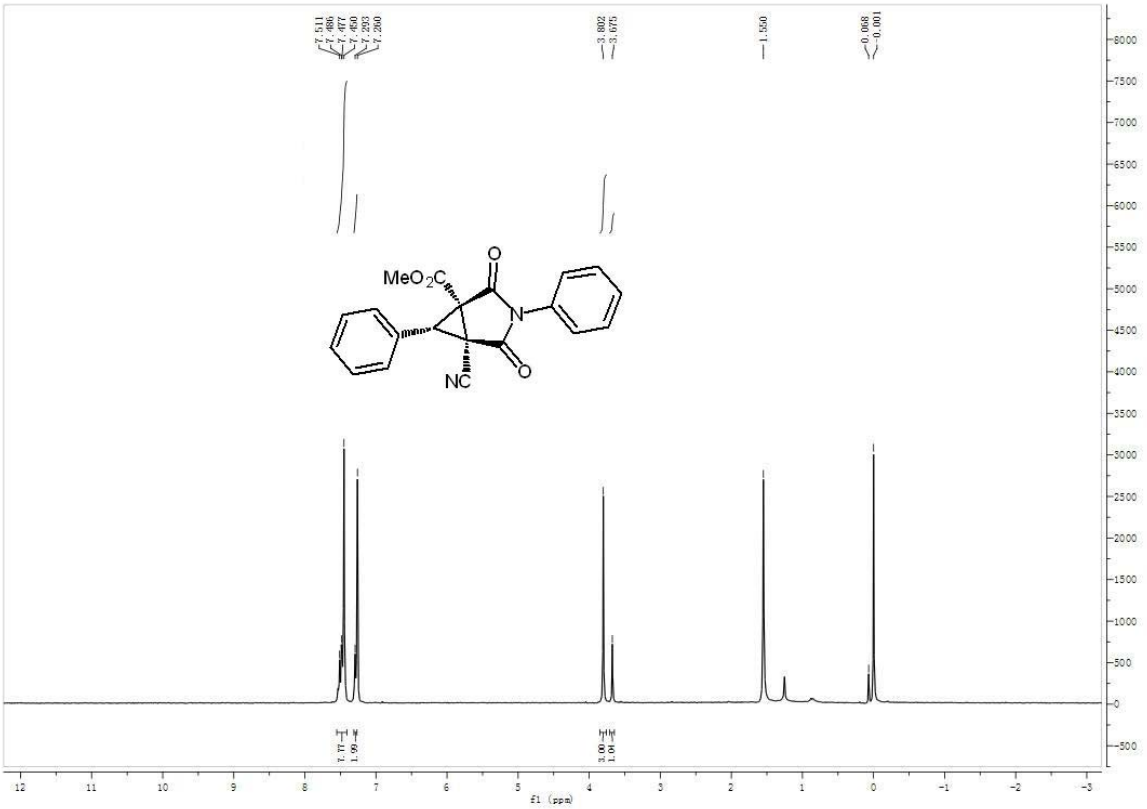
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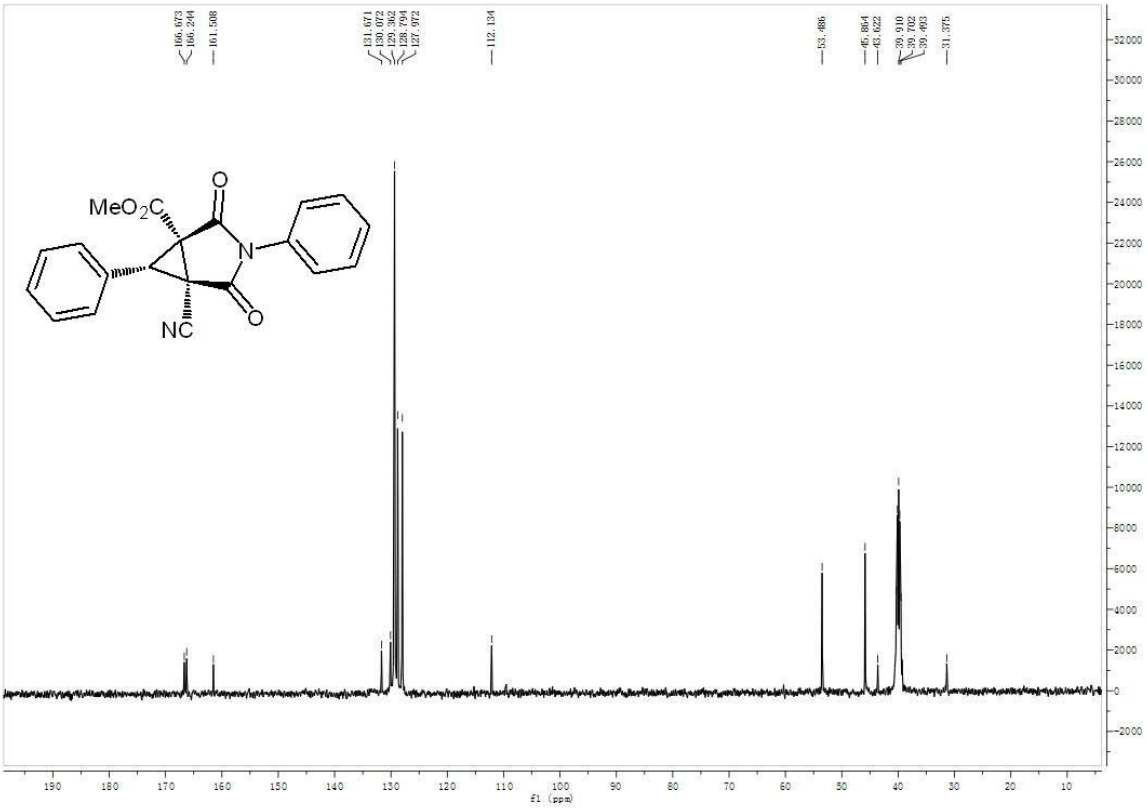
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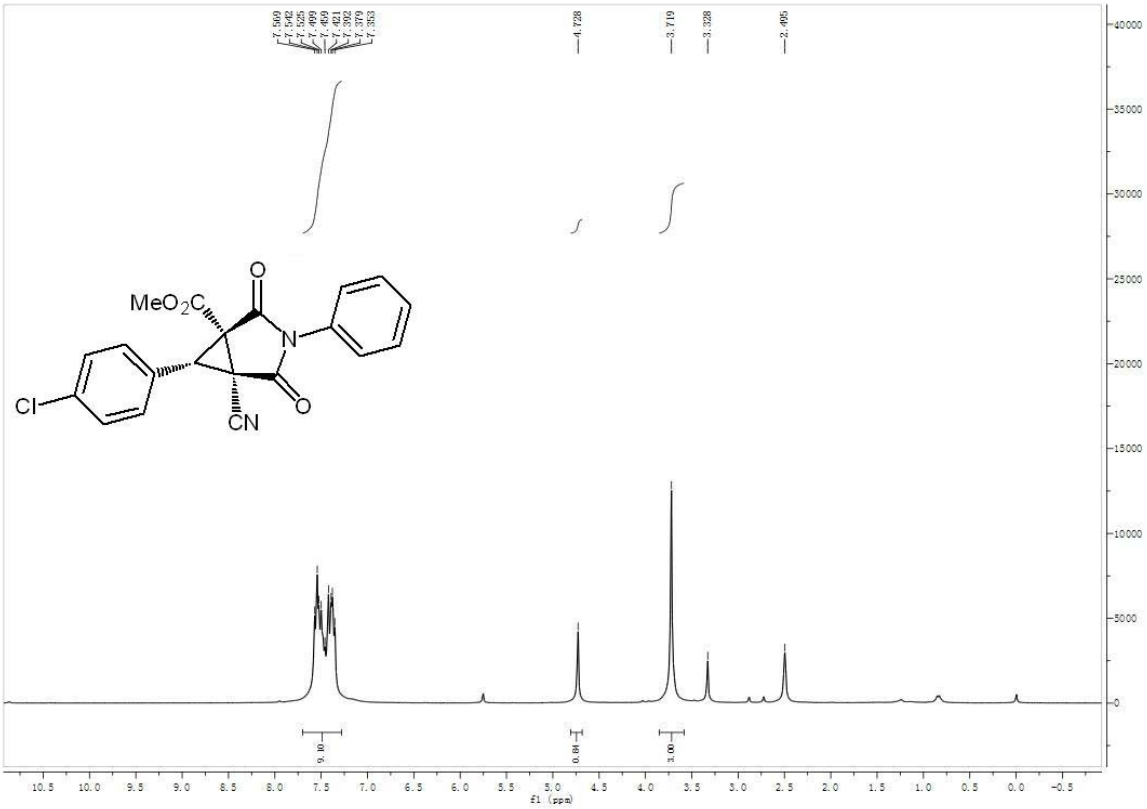
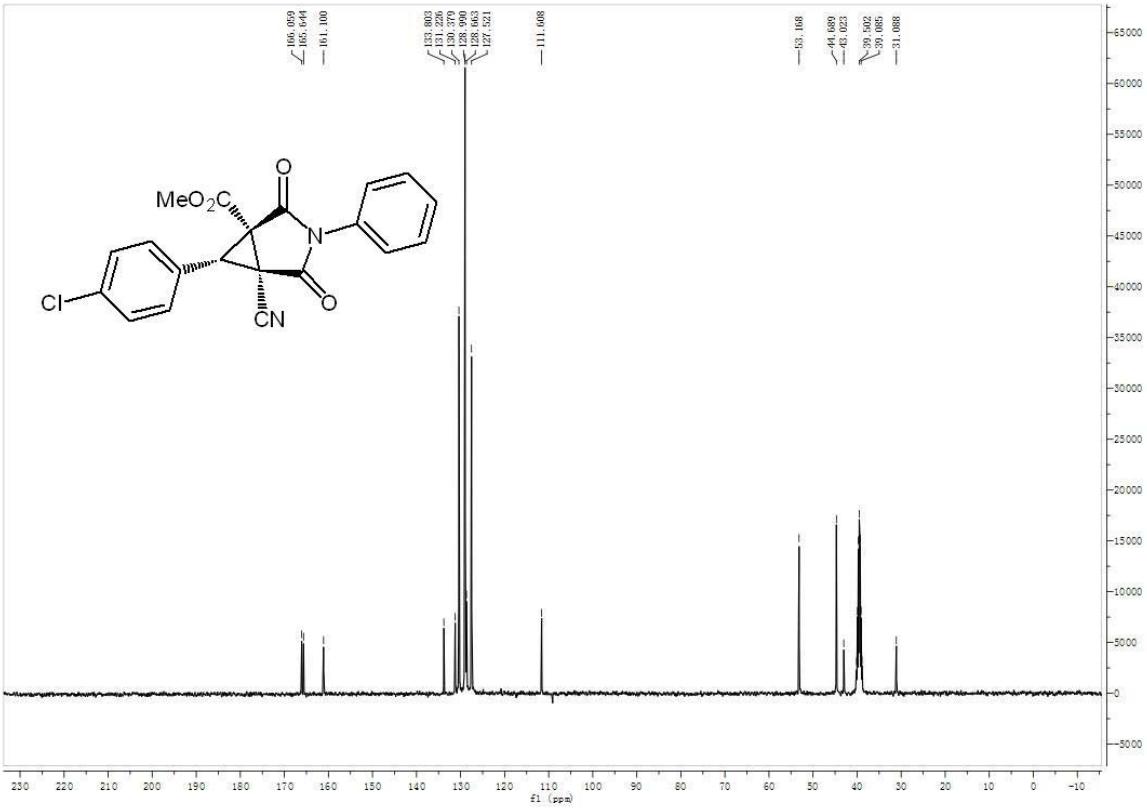
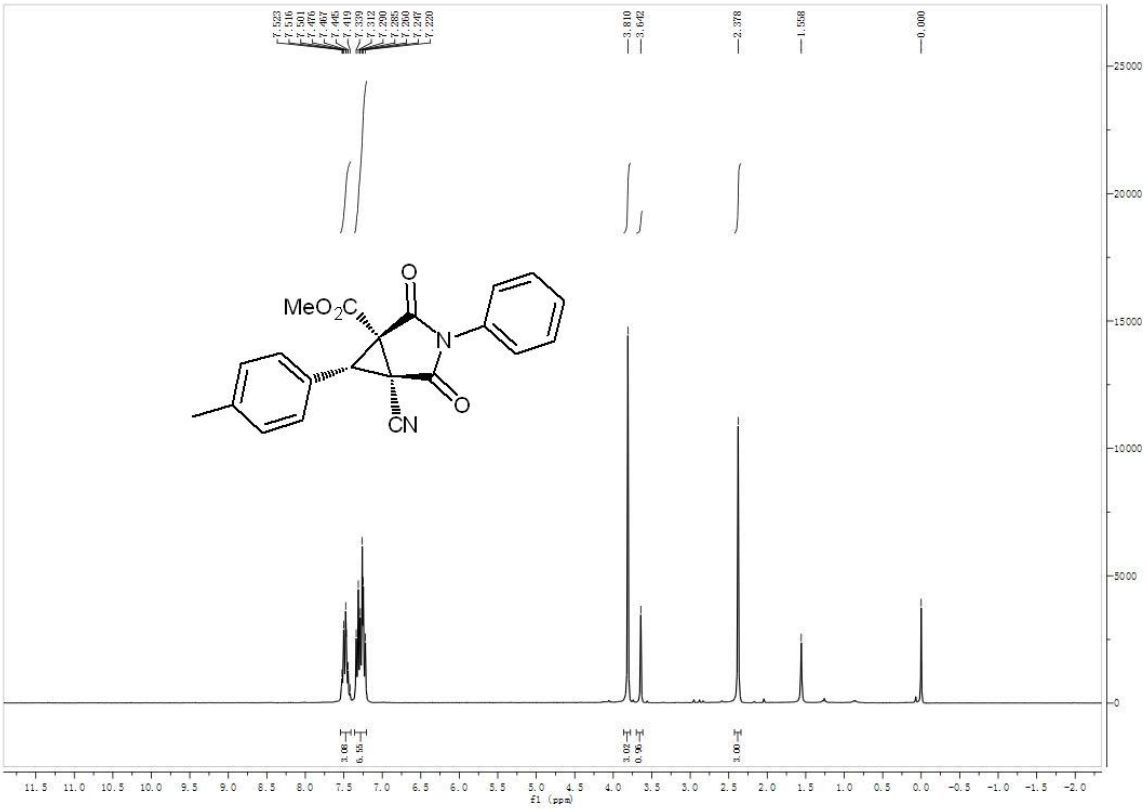
166.244
161.508
131.671
130.072
129.362
128.794
127.972
112.134
53.486
45.864
43.622
39.910
39.702
39.493
31.375
MeO2C
N
O
NC
f1 (ppm)

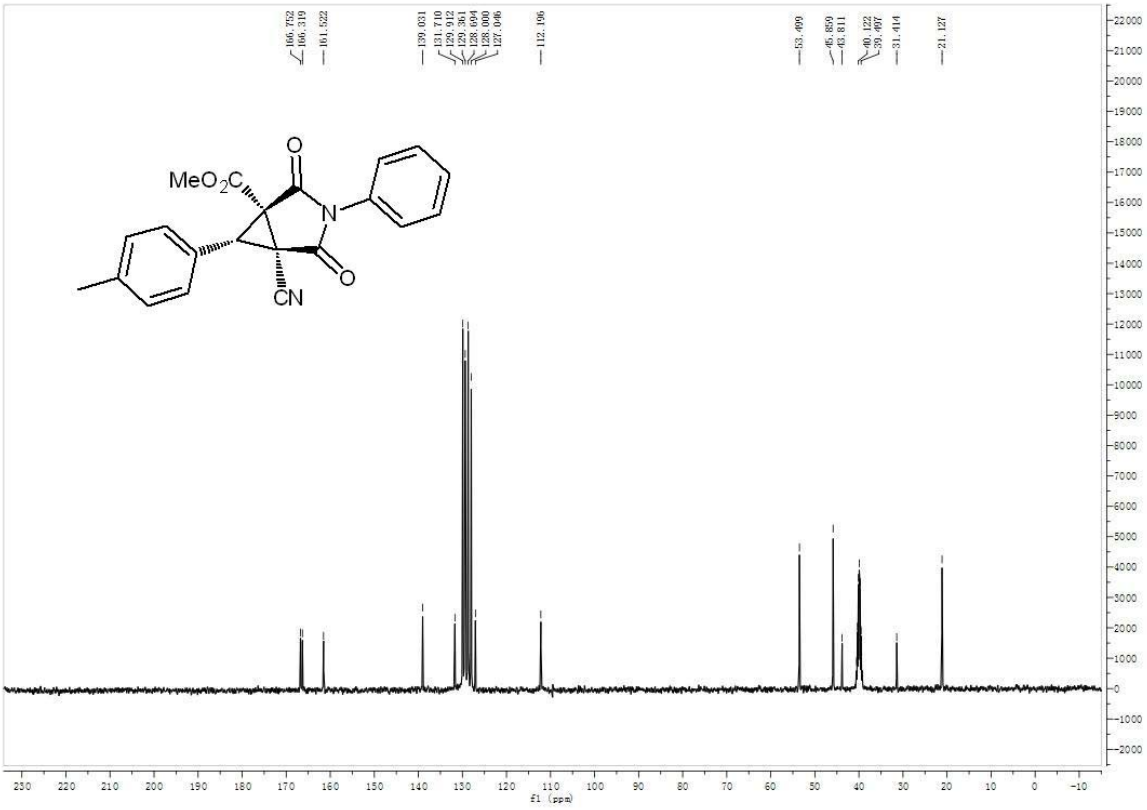
4mc


7.569
7.542
7.525
7.469
7.459
7.421
7.392
7.379
7.353
4.728
3.719
3.328
2.495
MeO2C
O
N
O
Cl
CN
9.10
0.89
3.00
f1 (ppm)

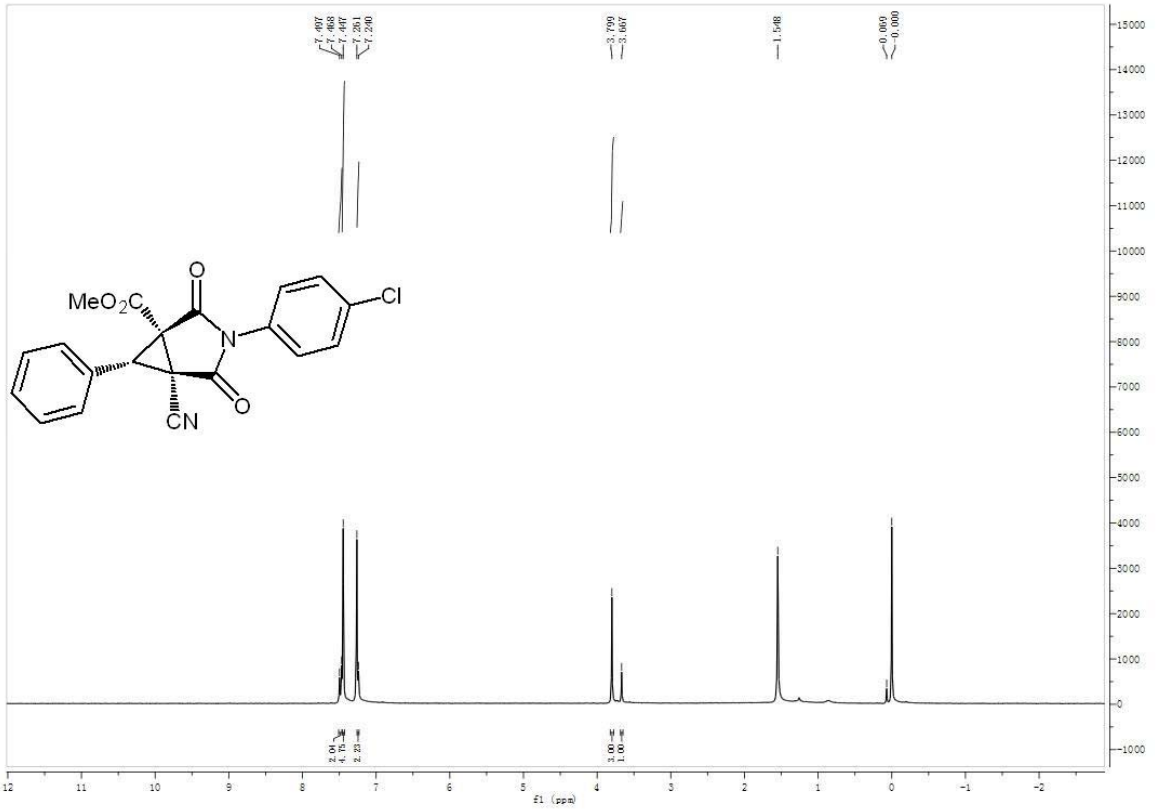

166.059
165.644
161.100
133.803
131.205
130.377
128.990
128.663
127.521
111.608
53.168
64.689
63.023
39.502
39.085
31.688
MeO2C
O
N
O
Cl
CN
f1 (ppm)

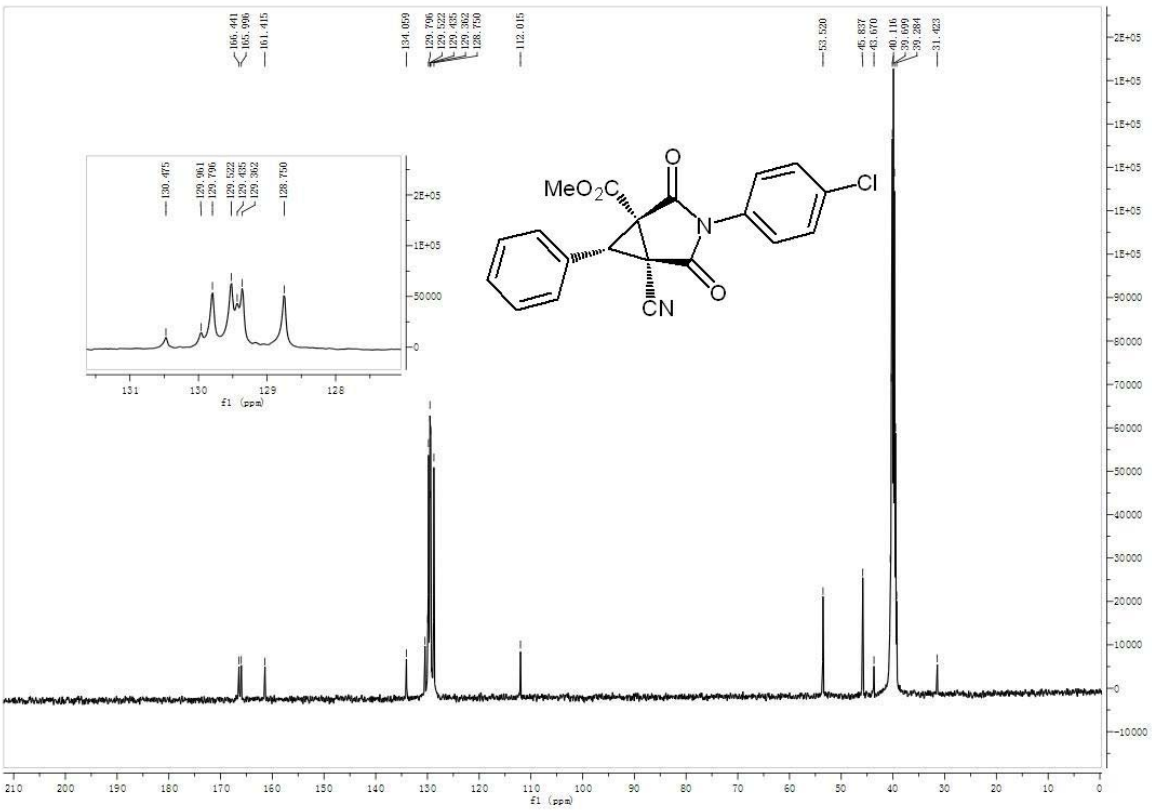
4nc


7.523
7.516
7.501
7.496
7.467
7.445
7.419
7.339
7.312
7.289
7.285
7.260
7.247
7.220
3.810
3.642
2.378
1.558
0.000
MeO2C
O
N
O
CN
f1 (ppm)

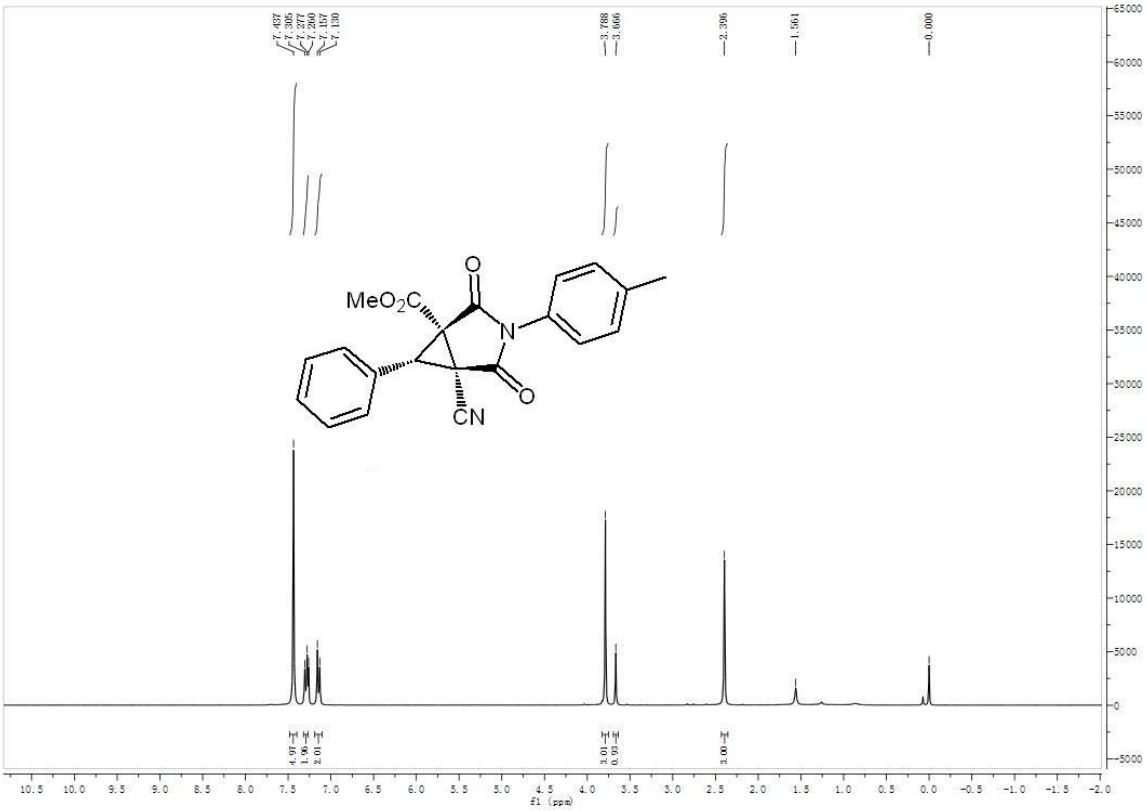

166.752
166.319
161.522
139.031
131.710
129.912
129.361
128.694
128.000
127.046
112.196
53.499
45.859
43.811
40.122
39.497
31.414
21.127
MeO2C
O
N
O
CN
f1 (ppm)

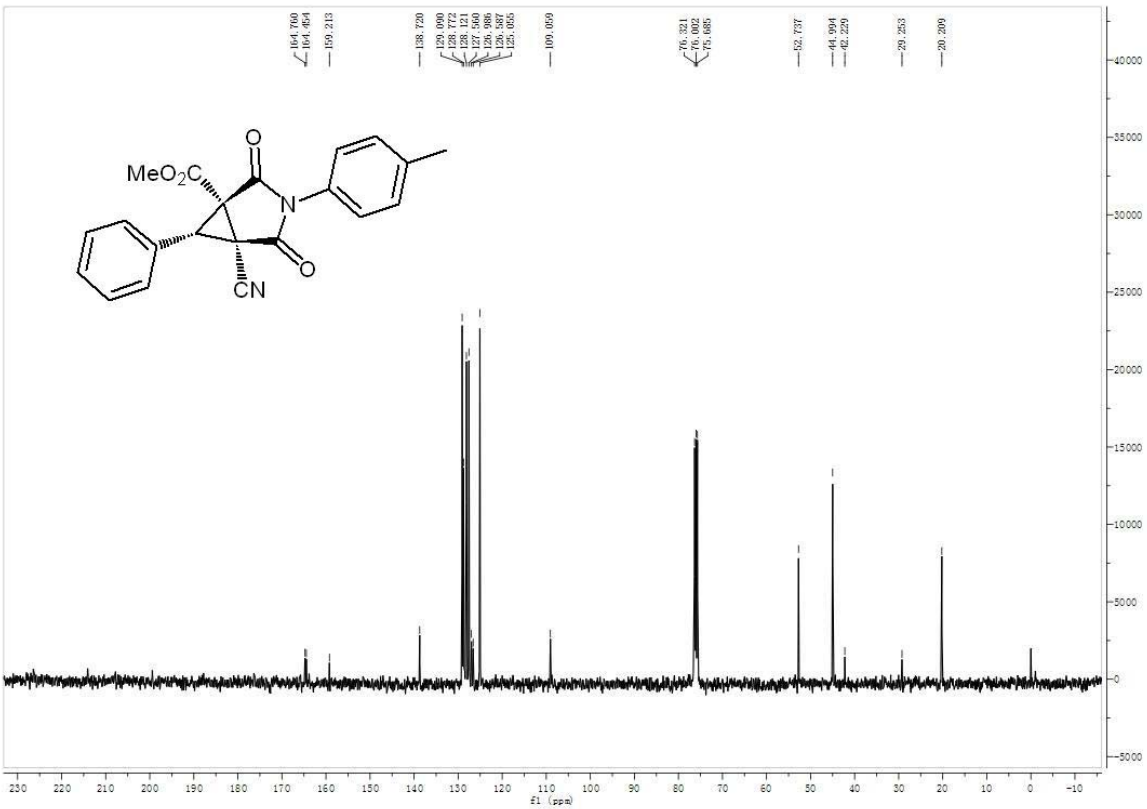
4oc


7.497
7.493
7.487
7.261
7.240
3.799
3.667
1.548
0.069
0.000
MeO2C
O
N
Cl
O
CN
f1 (ppm)


166.441
165.996
161.415
134.059
129.796
129.522
129.455
129.362
128.750
112.015
53.520
45.837
45.670
40.116
39.699
39.284
31.423
130.475
129.961
129.796
129.522
129.455
129.362
128.750
MeO2C
O
N
Cl
O
CN
f1 (ppm)

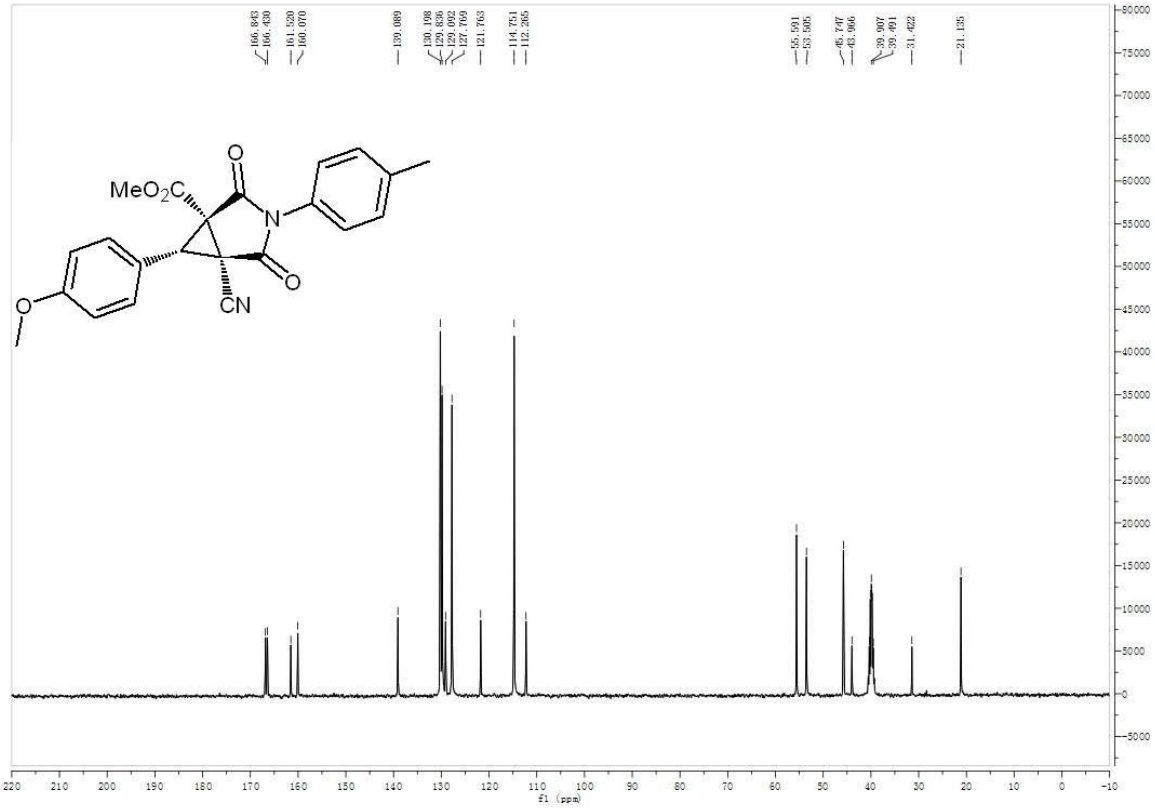
4pc


7.437
7.305
7.277
7.269
7.157
7.130
3.788
3.666
2.396
1.561
0.000
MeO2C
O
N
O
CN
4.97
1.98
2.01
3.01
0.93
3.00
f1 (ppm)

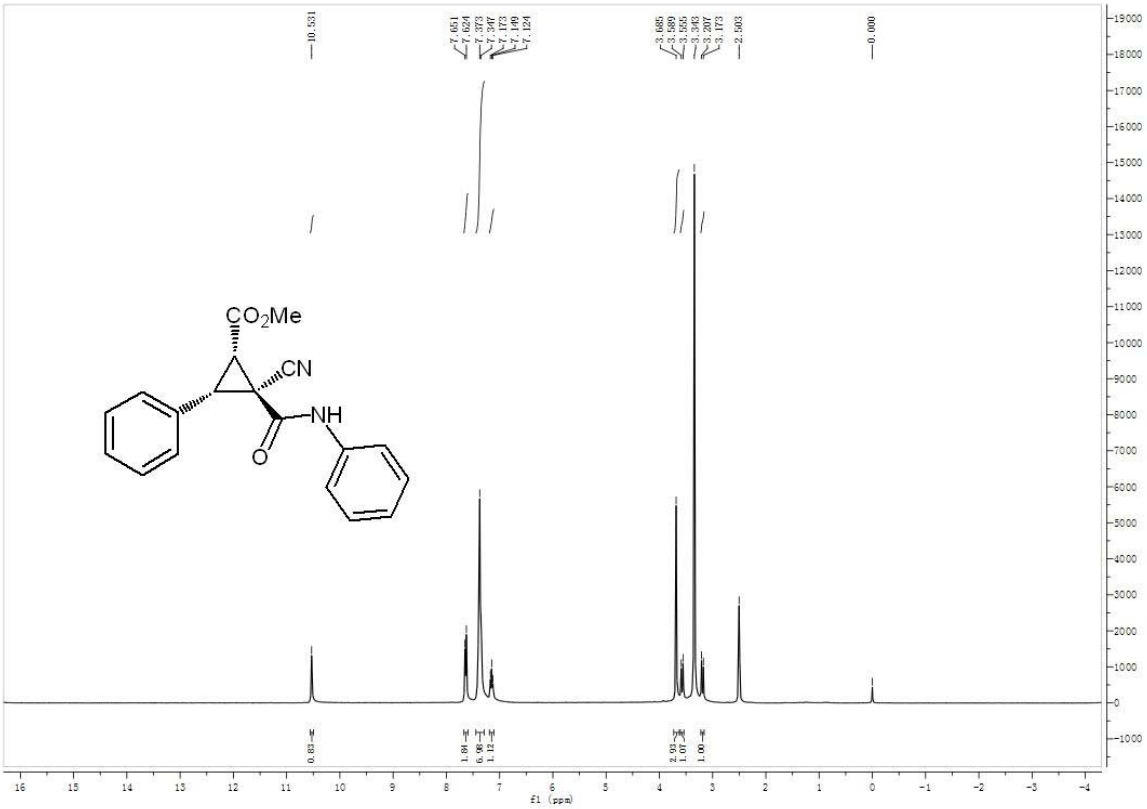

164.760
164.454
159.213
138.720
129.090
128.772
128.121
127.560
126.986
126.587
125.055
109.059
76.321
76.002
75.685
52.737
44.994
42.229
29.253
29.209
MeO2C
O
N
O
CN
f1 (ppm)

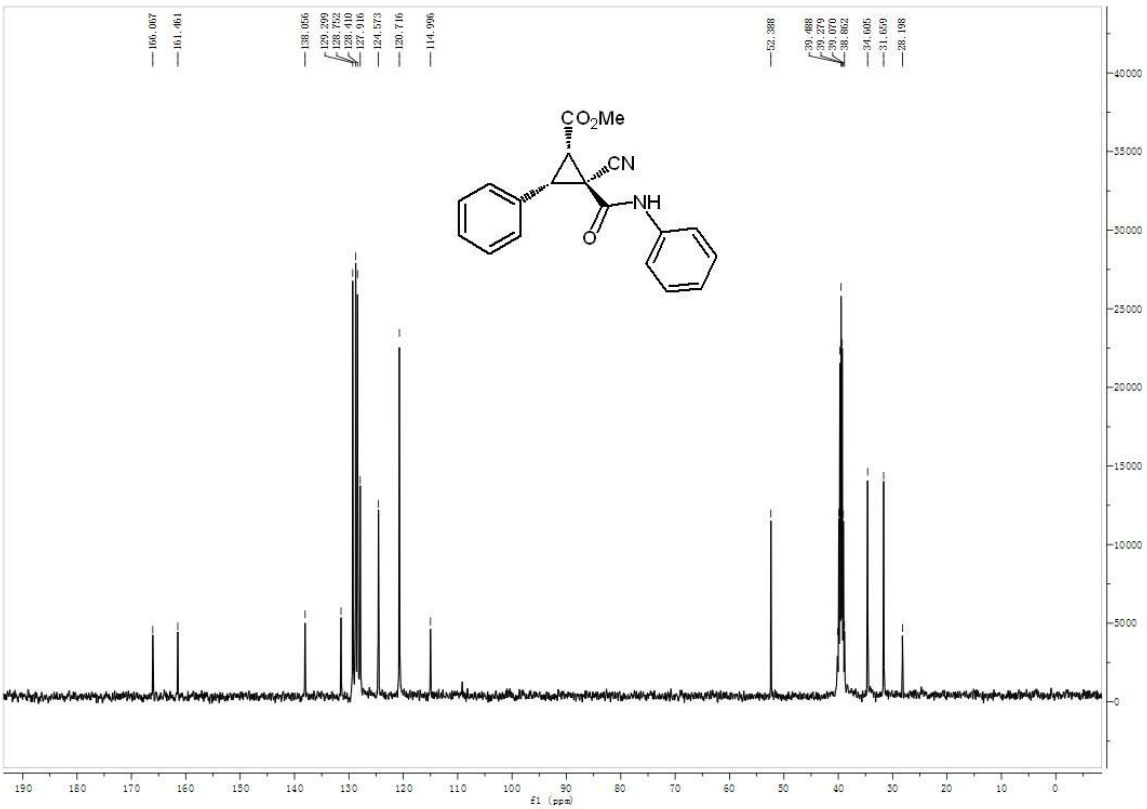
4qc


7.379
7.350
7.292
7.275
7.201
7.152
7.124
6.951
6.922
3.831
3.813
3.612
2.395
1.560
0.000
MeO2C
O
N
O
CN
O
f1 (ppm)

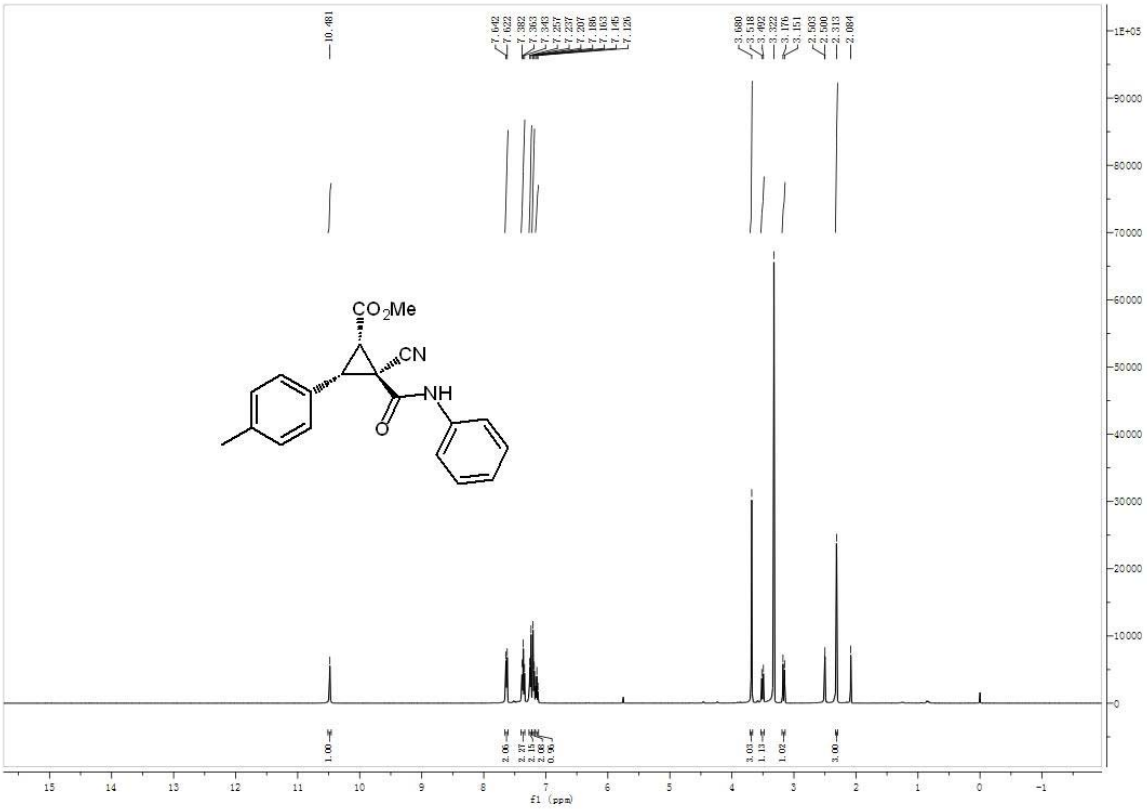

166.843
166.430
161.520
160.070
139.089
130.198
129.836
129.092
127.769
121.763
114.751
112.265
55.591
53.595
45.747
45.366
29.907
29.491
31.422
21.135
MeO2C
O
N
O
CN
O
f1 (ppm)

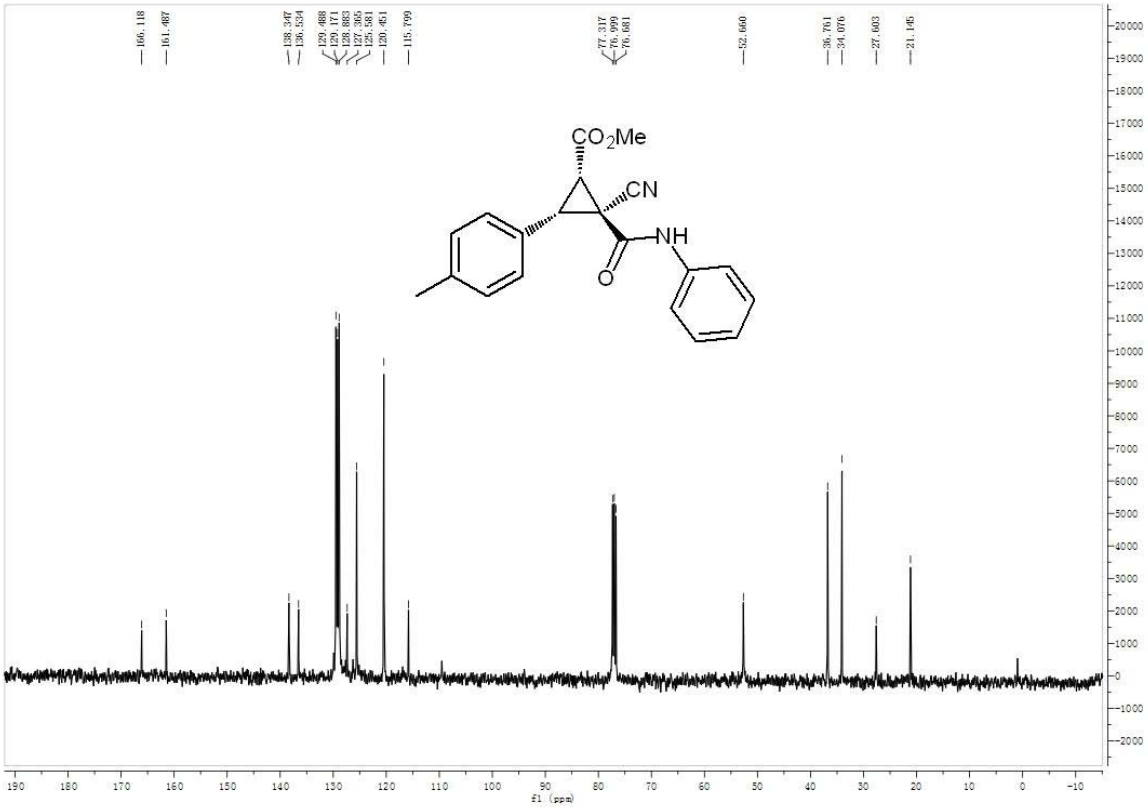
5lc


10.531
7.651
7.634
7.373
7.347
7.173
7.169
7.124
3.685
3.589
3.555
3.343
3.207
3.173
2.503
0.000
CO2Me
CN
NH
O
f1 (ppm)

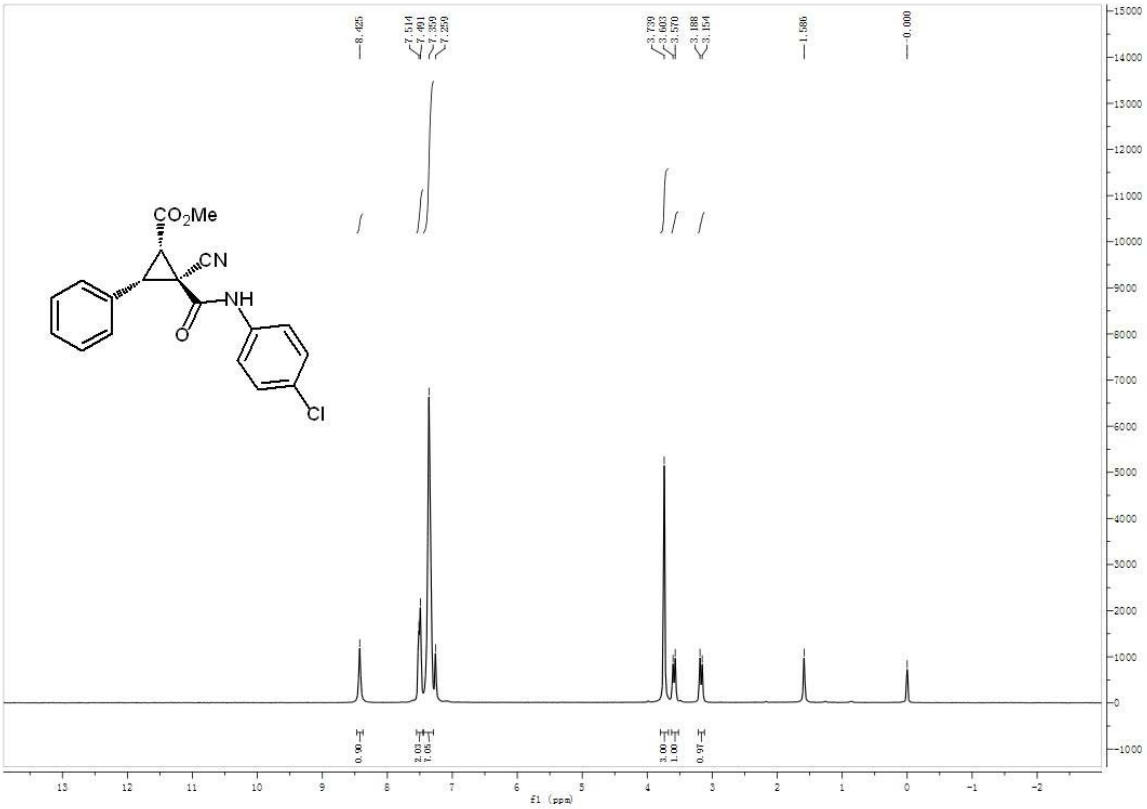

166.067
161.461
138.056
129.299
128.732
128.410
127.916
124.573
120.716
114.996
52.388
39.488
39.279
39.070
38.862
34.605
31.659
28.198
CO2Me
CN
NH
O
f1 (ppm)

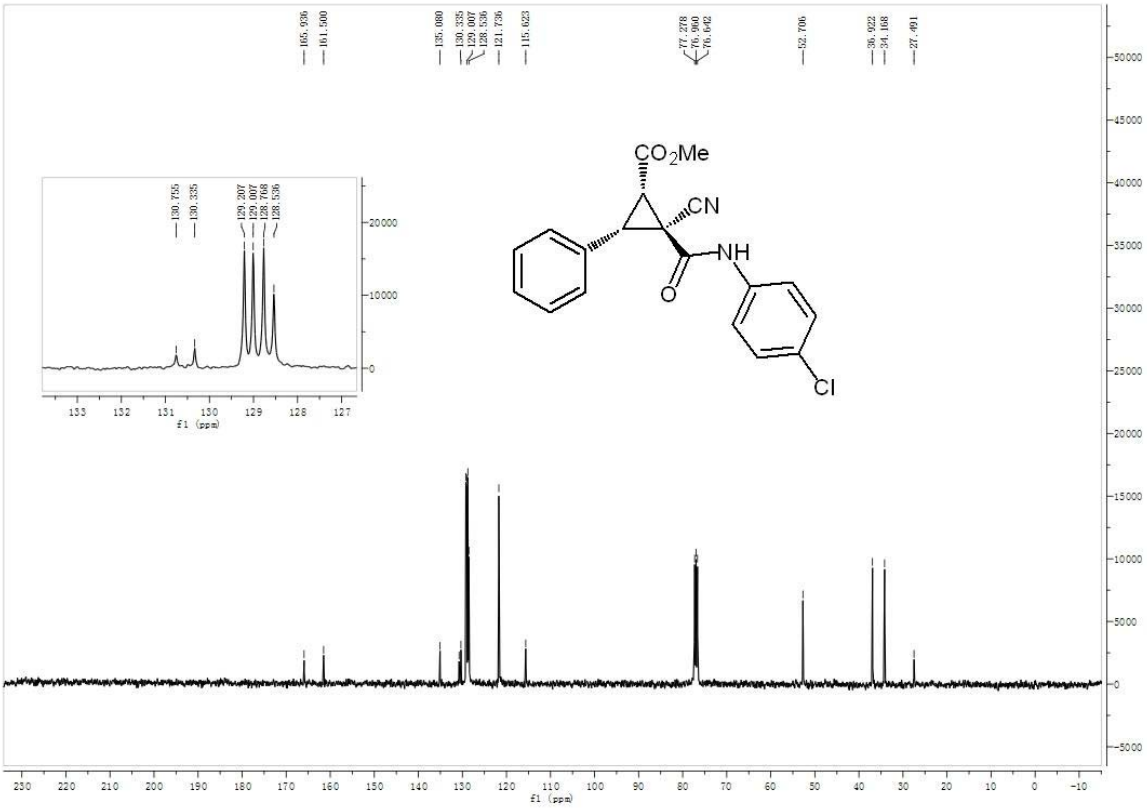
5nc



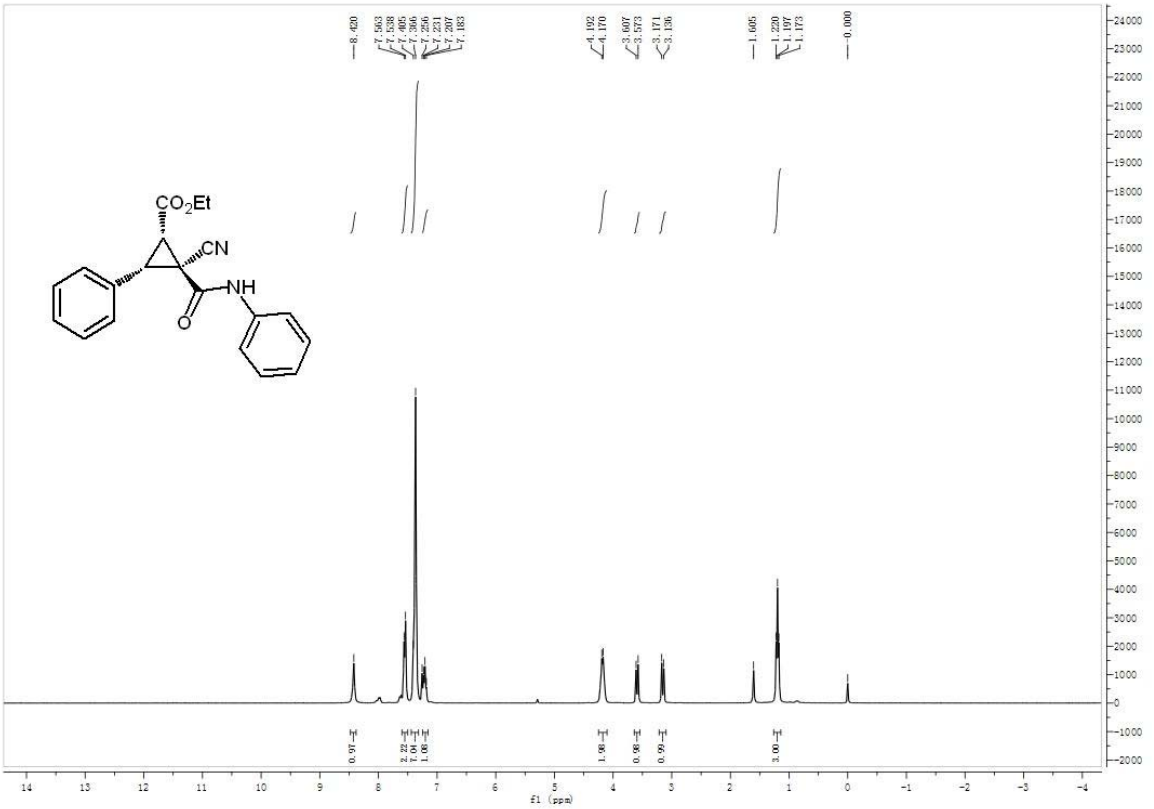


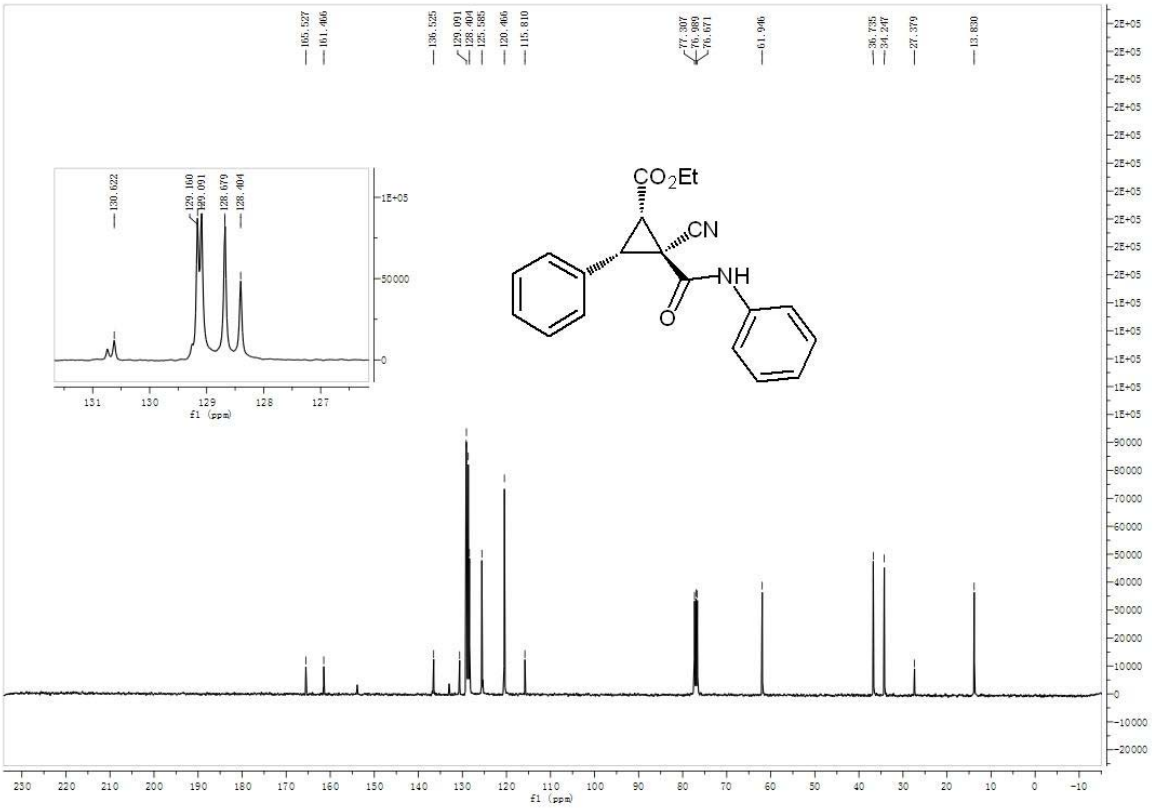
5oc


8.425
7.514
7.491
7.359
7.259
3.739
3.695
3.570
3.188
3.154
1.586
0.000
CO2Me
CN
NH
O
Cl
f1 (ppm)

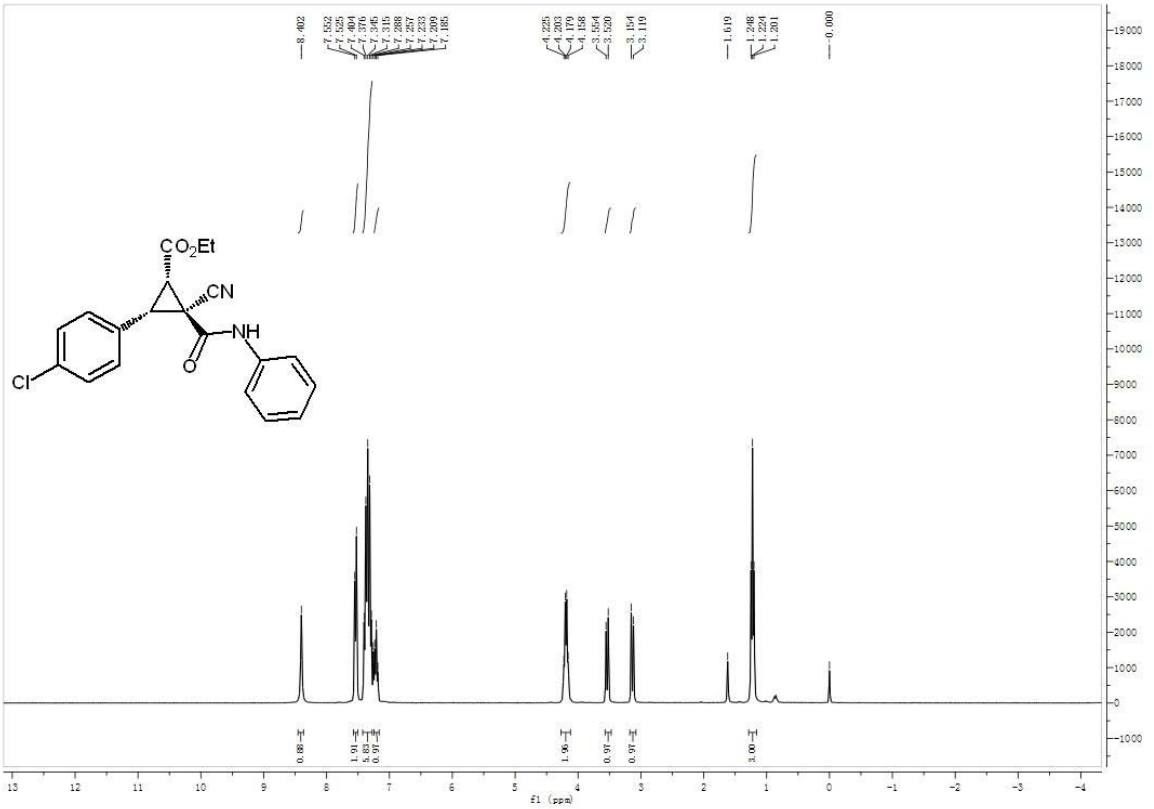

165.936
161.500
135.080
130.335
129.007
128.536
121.736
115.623
77.278
76.960
76.642
52.706
36.922
34.168
27.491
130.755
130.335
129.207
129.007
128.768
128.536
CO2Me
CN
NH
O
Cl
f1 (ppm)

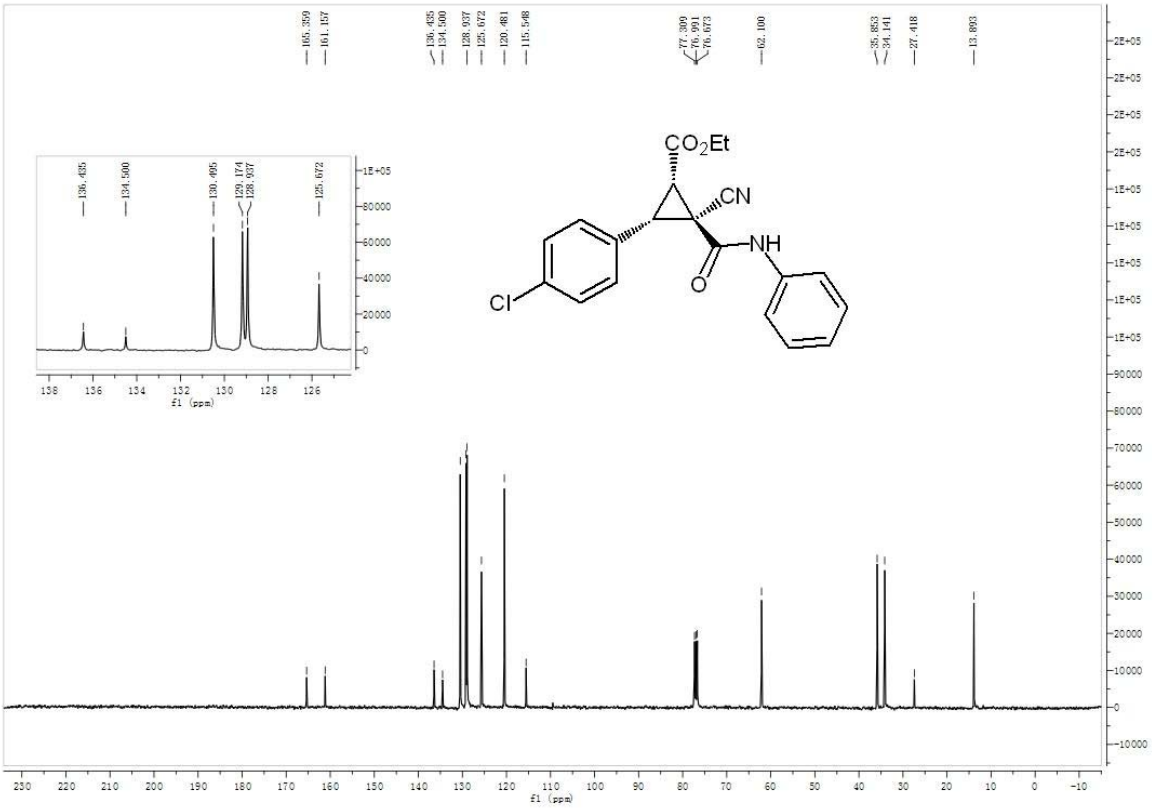
5lb


8.420
7.563
7.538
7.405
7.396
7.256
7.231
7.227
7.207
7.183
4.192
4.170
3.607
3.573
3.171
3.136
1.665
1.220
1.197
1.173
0.000
CO2Et
CN
NH
O
f1 (ppm)

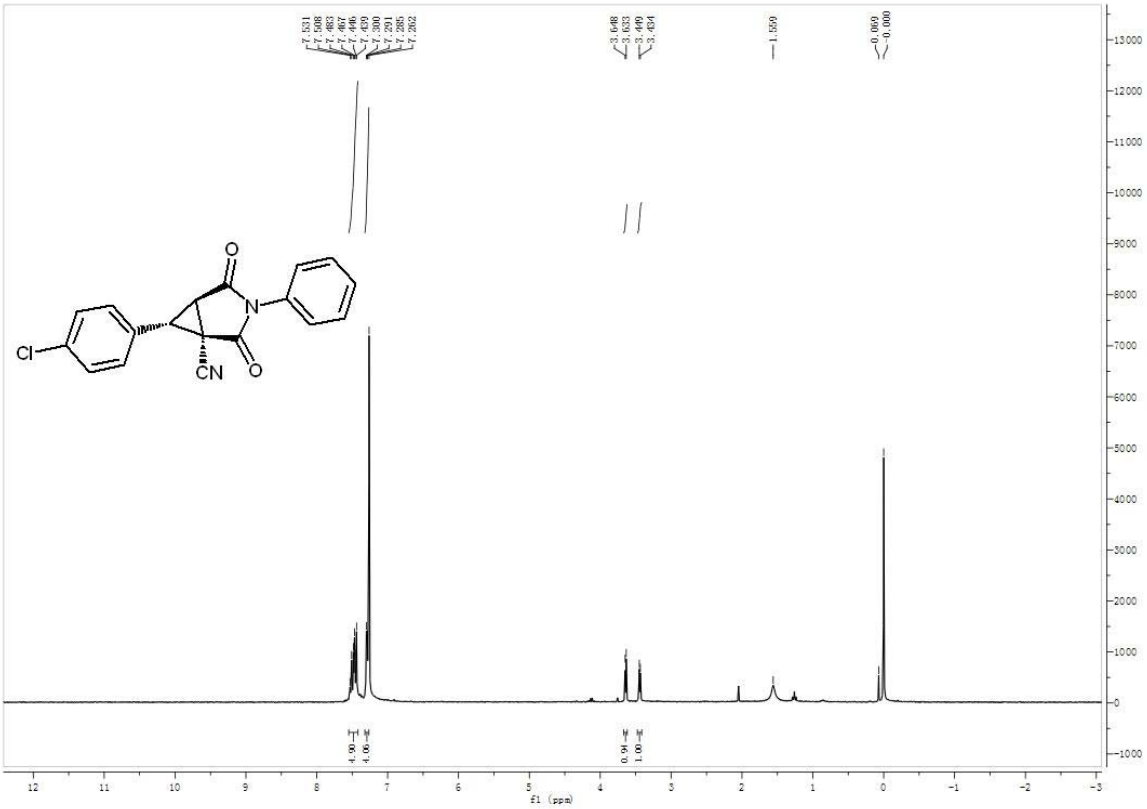

165.527
161.466
136.525
129.091
128.404
125.365
120.466
115.810
77.307
76.989
76.671
61.946
26.735
24.247
27.379
13.830
130.622
129.160
129.091
128.679
128.404
CO2Et
CN
NH
O
f1 (ppm)

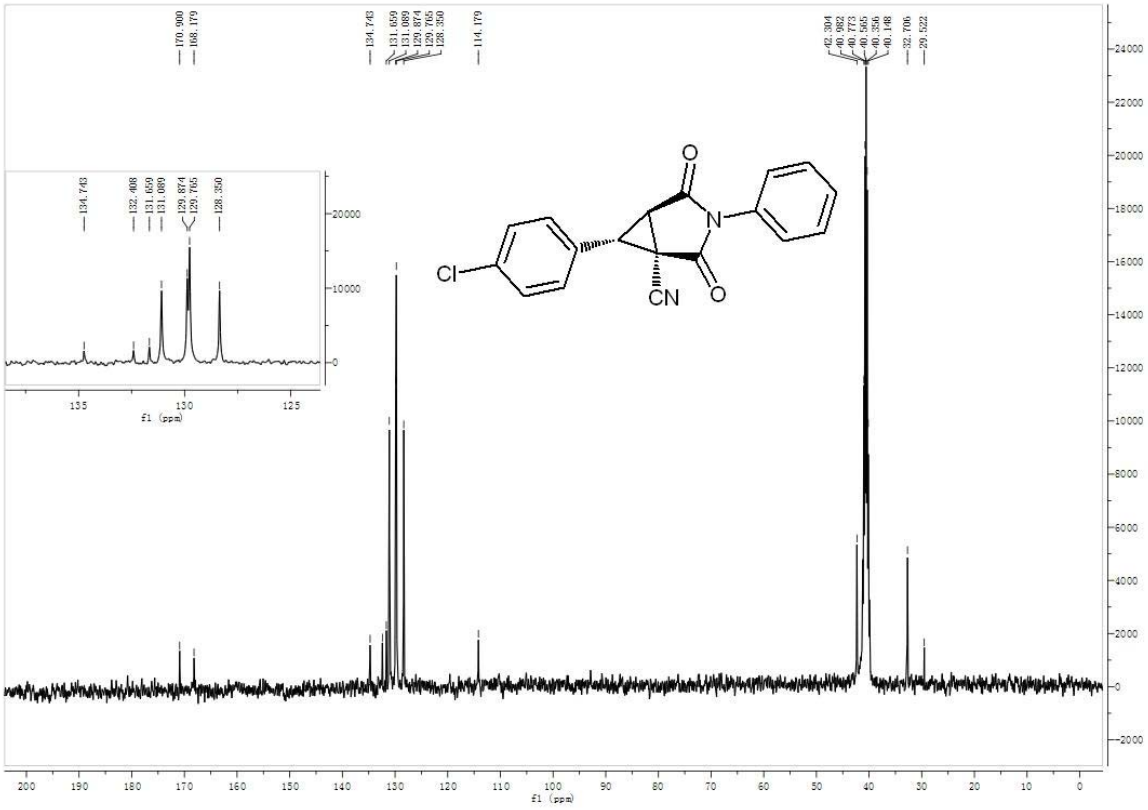
5mb



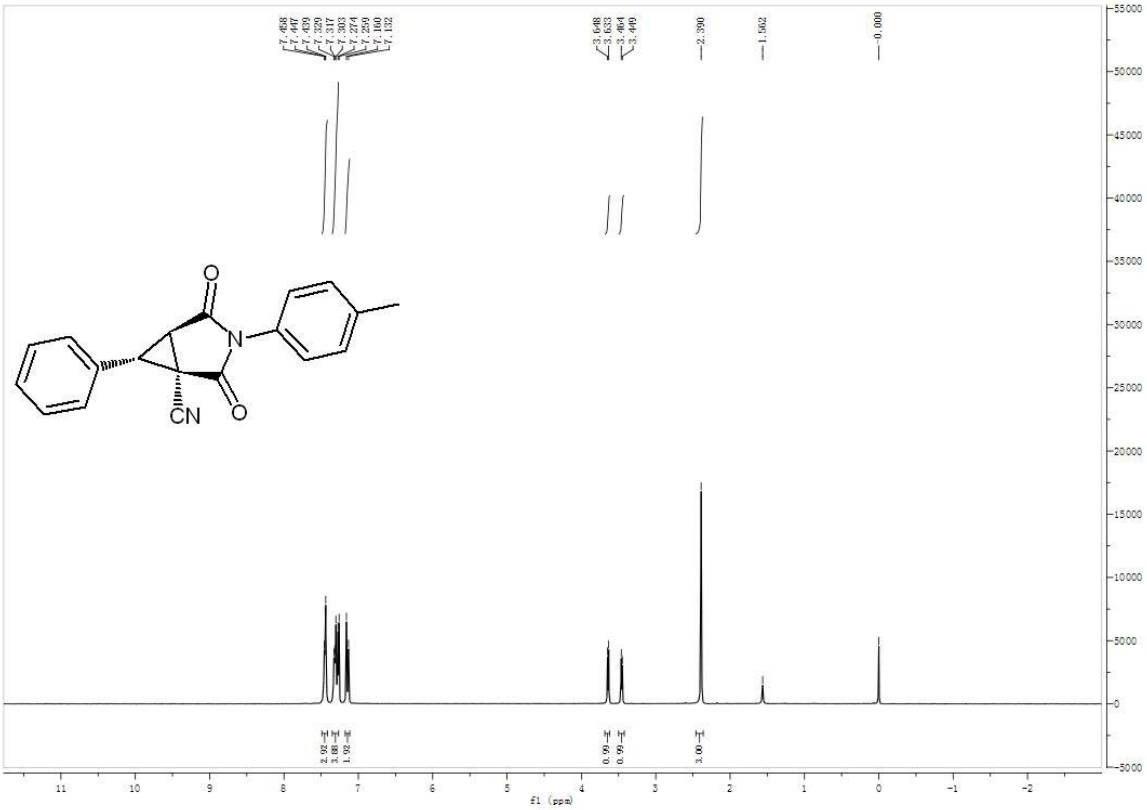


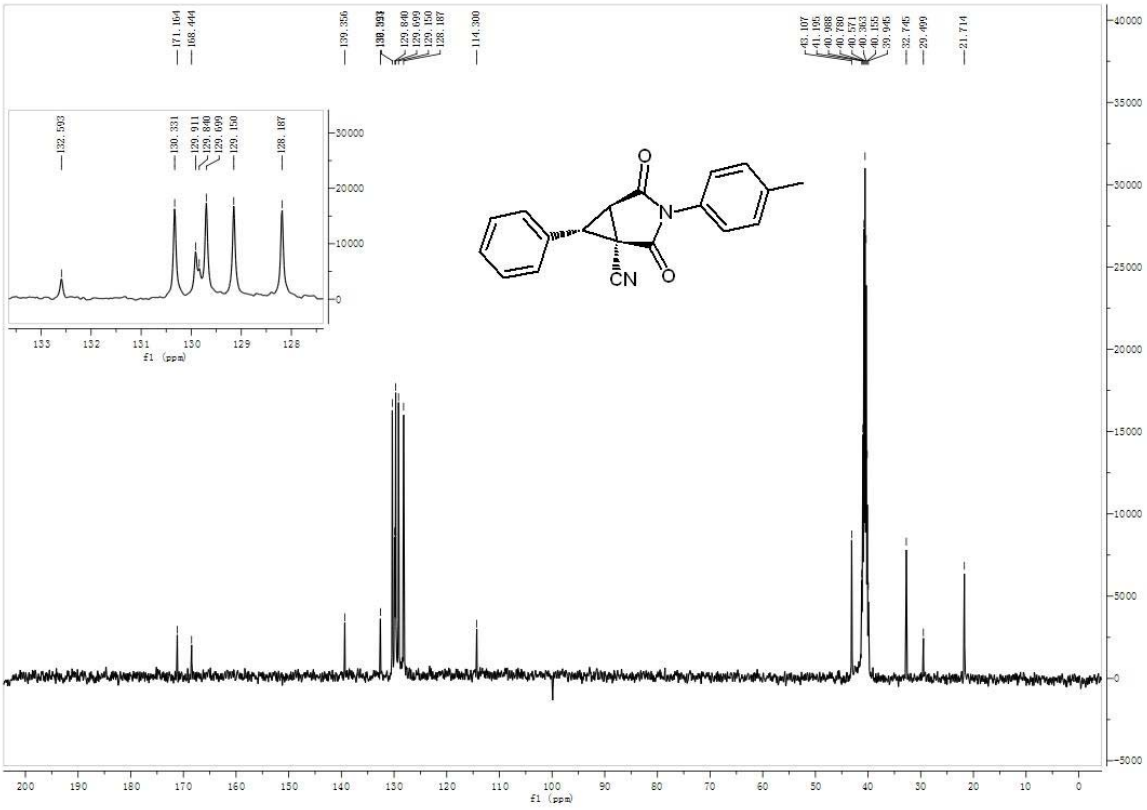
6mc


7.531
7.508
7.483
7.467
7.446
7.439
7.300
7.291
7.285
7.262
3.648
3.633
3.449
3.434
1.559
0.069
0.000
4.00
4.06
0.94
1.00
f1 (ppm)

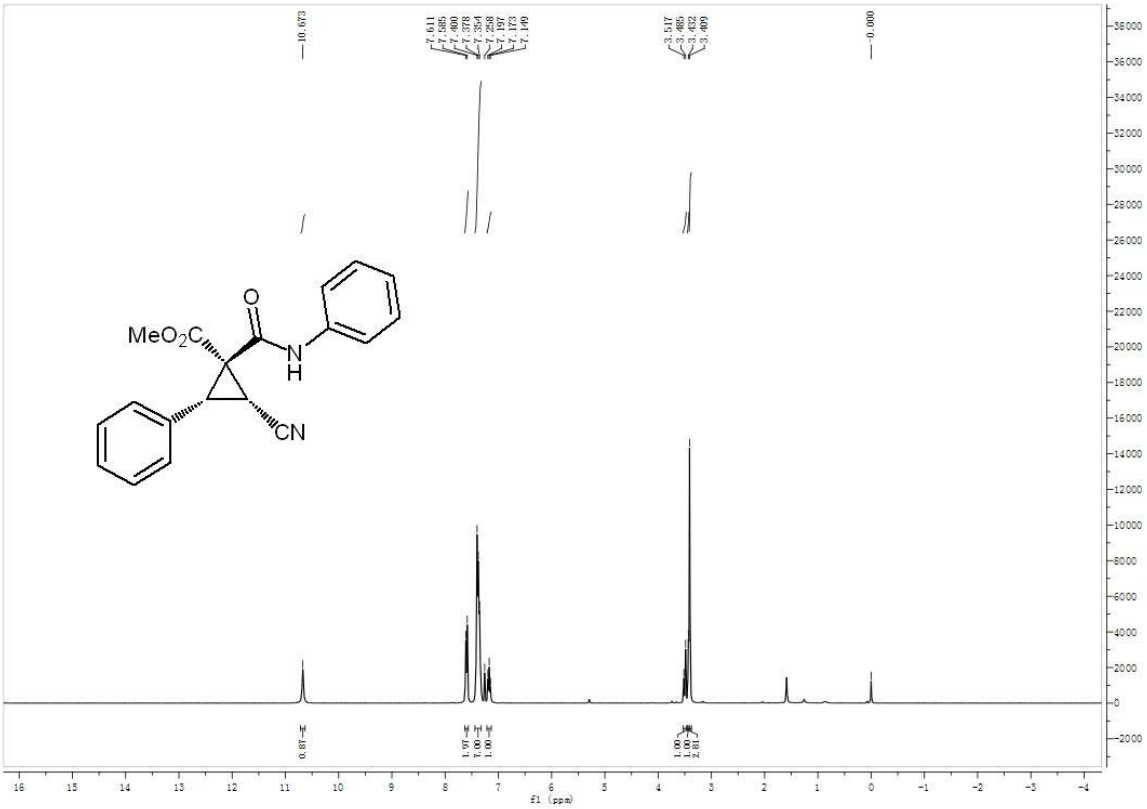

170.900
168.179
134.743
131.659
131.089
129.874
129.765
128.350
114.179
42.304
40.982
40.773
40.565
40.356
40.148
32.706
29.522
f1 (ppm)

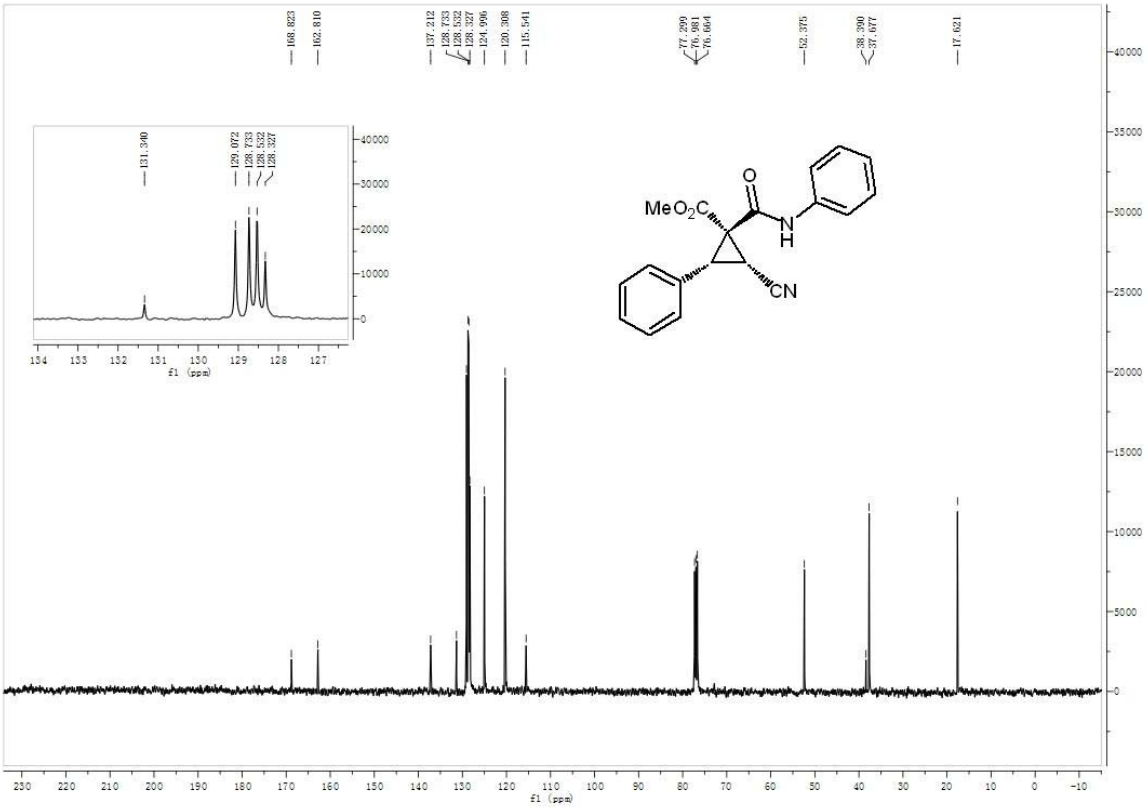
6pc


7.458
7.447
7.439
7.329
7.317
7.303
7.274
7.259
7.010
7.132
3.648
3.633
3.464
3.449
2.390
1.562
0.000
CN
O
N
f1 (ppm)

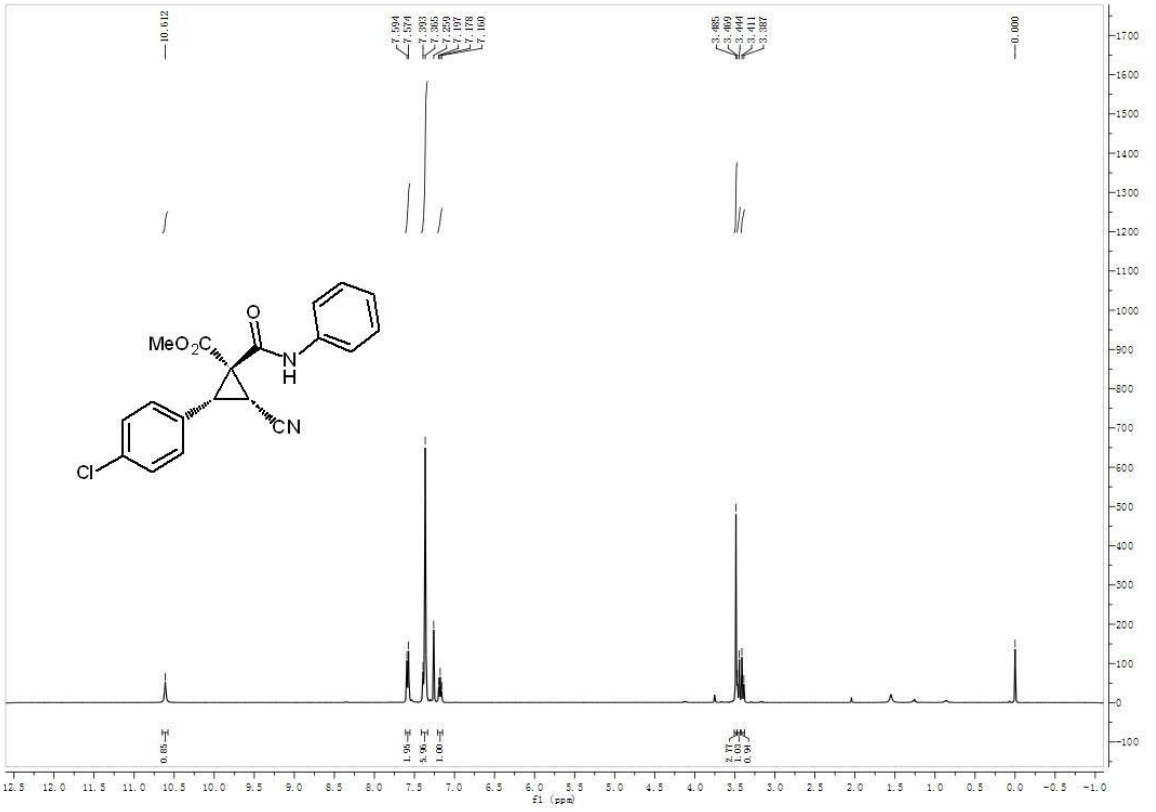

171.164
168.444
139.356
130.993
129.840
129.699
129.150
128.187
114.300
43.107
41.105
40.988
40.780
40.571
40.363
40.155
39.946
32.745
29.499
21.714
132.593
130.331
129.911
129.840
129.699
129.150
128.187
CN
O
N
f1 (ppm)

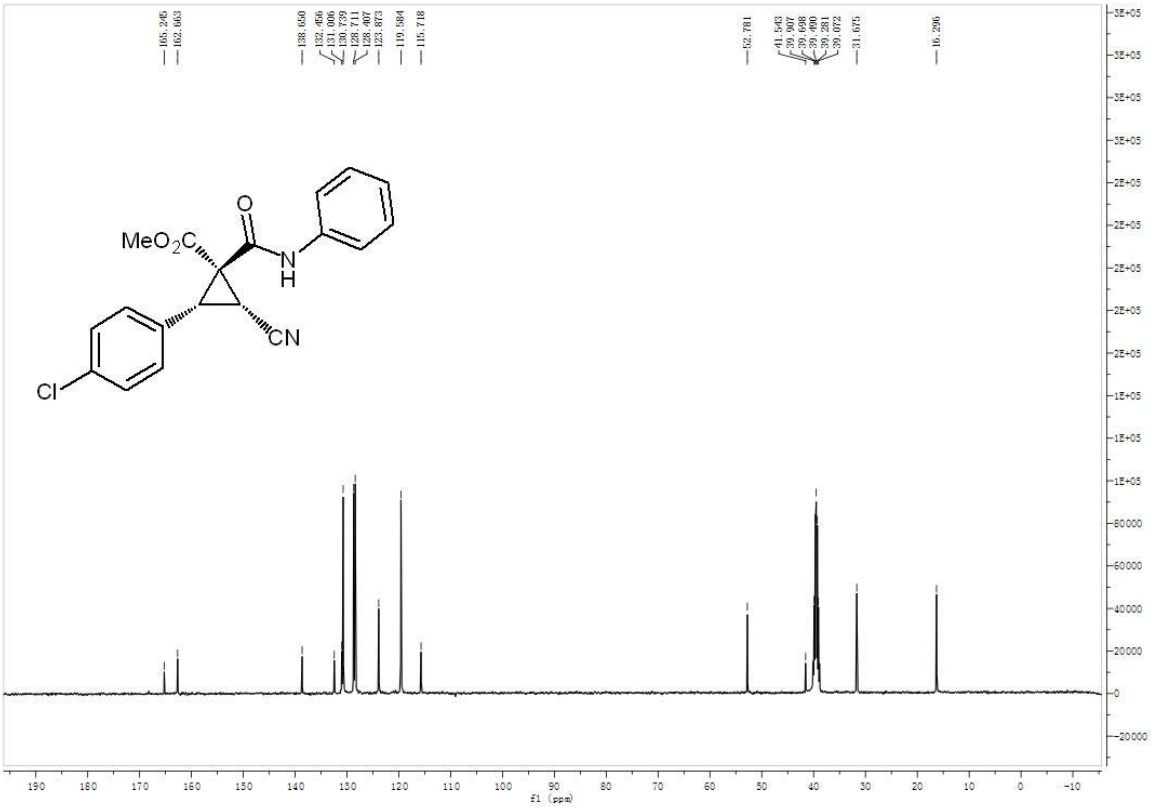
7lc





7mc


10.612
7.594
7.574
7.393
7.385
7.259
7.197
7.178
7.100
3.485
3.469
3.444
3.411
3.397
0.000
MeO2C
O
N
H
CN
Cl
0.65
1.95
5.96
1.00
2.17
1.02
0.94
f1 (ppm)


165.245
162.663
138.650
132.456
131.006
130.739
129.171
128.407
123.873
119.584
115.718
52.781
41.543
39.807
39.665
39.490
39.281
39.072
31.675
16.296
MeO2C
O
N
H
CN
Cl
f1 (ppm)