Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Palladium-Catalyzed Tandem N–H/C–H Arylation: Regioselective Synthesis of *N*-Heterocycle-Fused Phenanthridines as Versatile Blue-Emitting Luminophores

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I. Fluorescence lifetimes of compounds 3e, 3h, 3l and 4m

Table S1. Fluorescence lifetimes of compounds **3e**, **3h**, **3l** and **4m**.[a]

Compd	Lifetime in MeCN		Compd	Lifetime in MeCN	
3e	τ_1 = 16.38 ns	χ^2 = 1.06	**3l**	τ_1 = 3.22 ns (17.55%) τ_2 = 14.78 ns (82.45%)	χ^2 = 1.04
3h	τ_1 = 2.91 ns (3.33%) τ_2 = 18.35 ns (96.67%)	χ^2 = 1.05	**4m**	τ_1 = 4.08 ns (41.39%) τ_2 = 14.26 ns (58.61%)	χ^2 = 1.01

[a] Fluorescence lifetimes were determined on a HORIBA TEMPRO-01 instrument at room temperature.

II. Electrochemical properties of compounds 3e, 3h, 3l and 4m

Cyclic voltammetry (CV) measurements were performed on LK2005A using an Ag/Ag^+ (0.01 M of $AgNO_3$ in dry acetonitrile) reference electrode, a platinum wire counter electrode, and a platinum plate working electrode. CV measurements were carried out in dry acetonitrile using Fc/Fc^+ as reference at a scanning rate of 100 $mV \cdot s^{-1}$ with tetrabutylammonium hexafluorophosphate (NBu_4PF_6, 0.1 M) as supporting electrolyte.

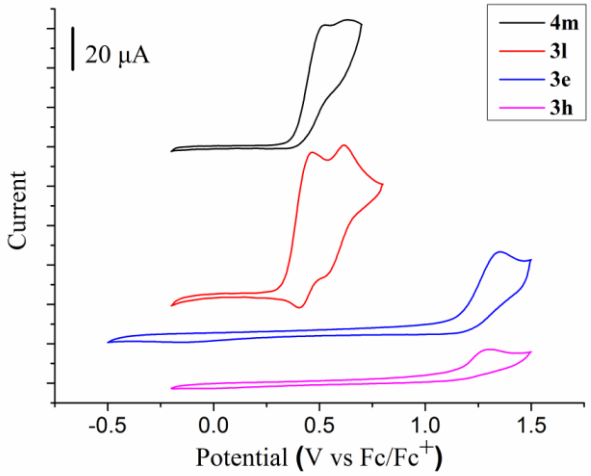


Figure S1 Electrochemical properties of compounds **3e**, **3h**, **3l** and **4m**.

III. Thermal properties of compounds 3e, 3h, 3l and 4m

Thermal decomposition temperatures were detected by thermogravimetry/differential thermal analysis (TG/DTA) on a NETZSCH-Leading Thermal Analysis in the temperature range of 30-500 °C at a heating rate of 10 °C/min under a nitrogen atmosphere.

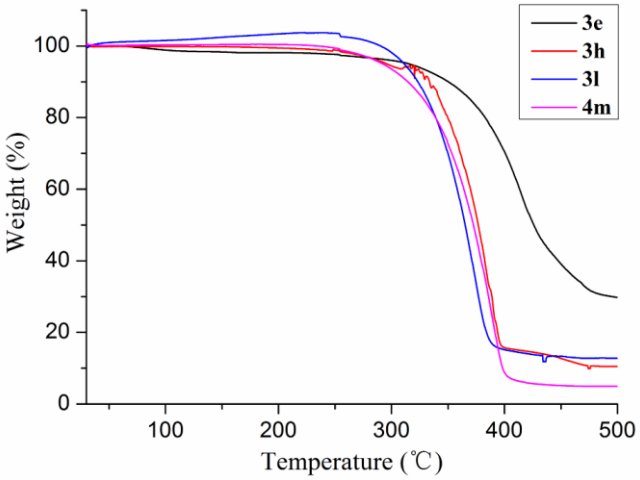
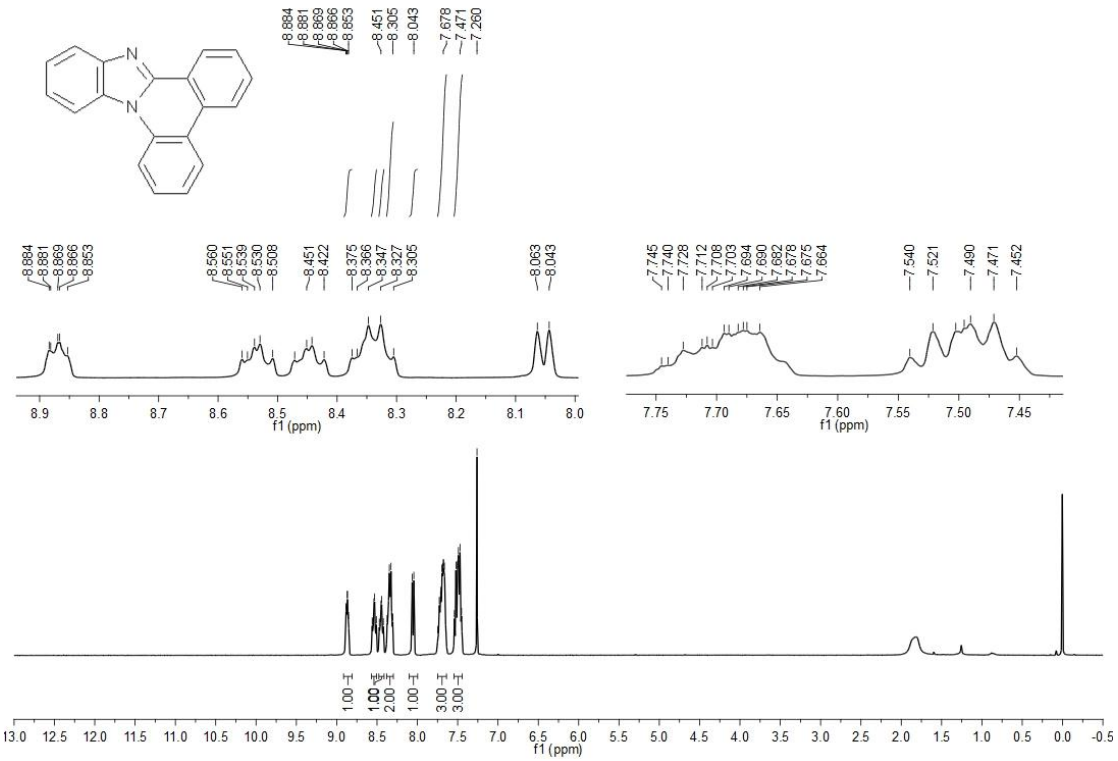
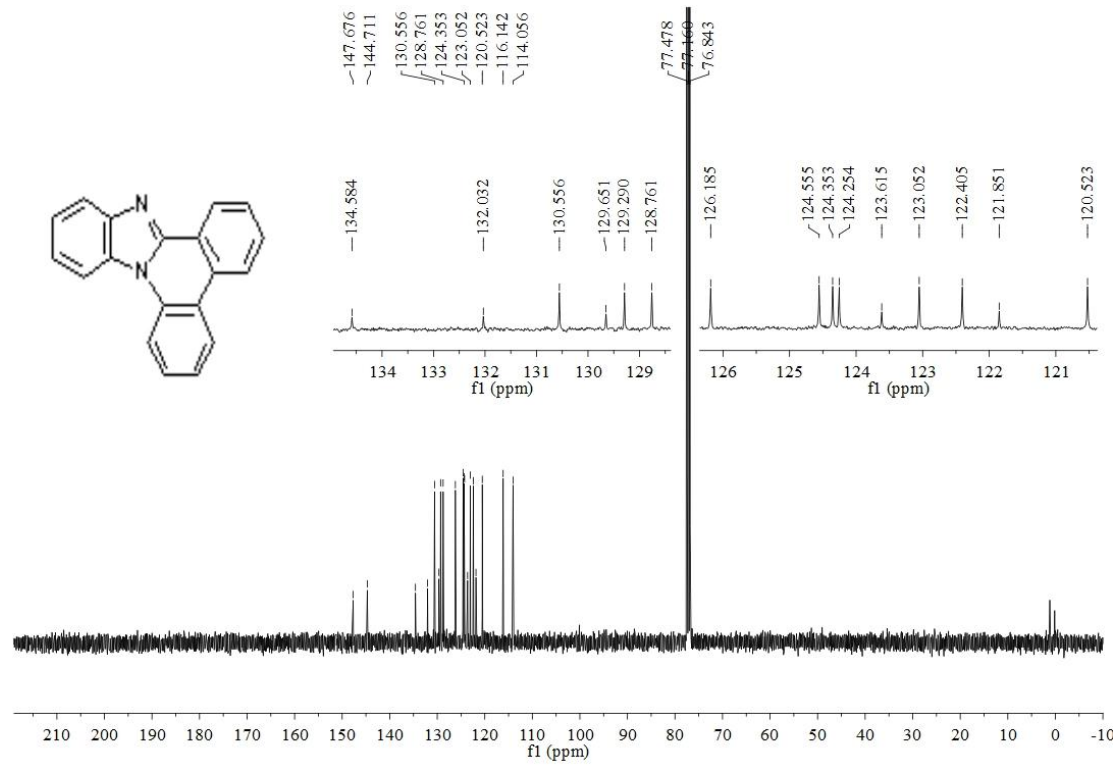
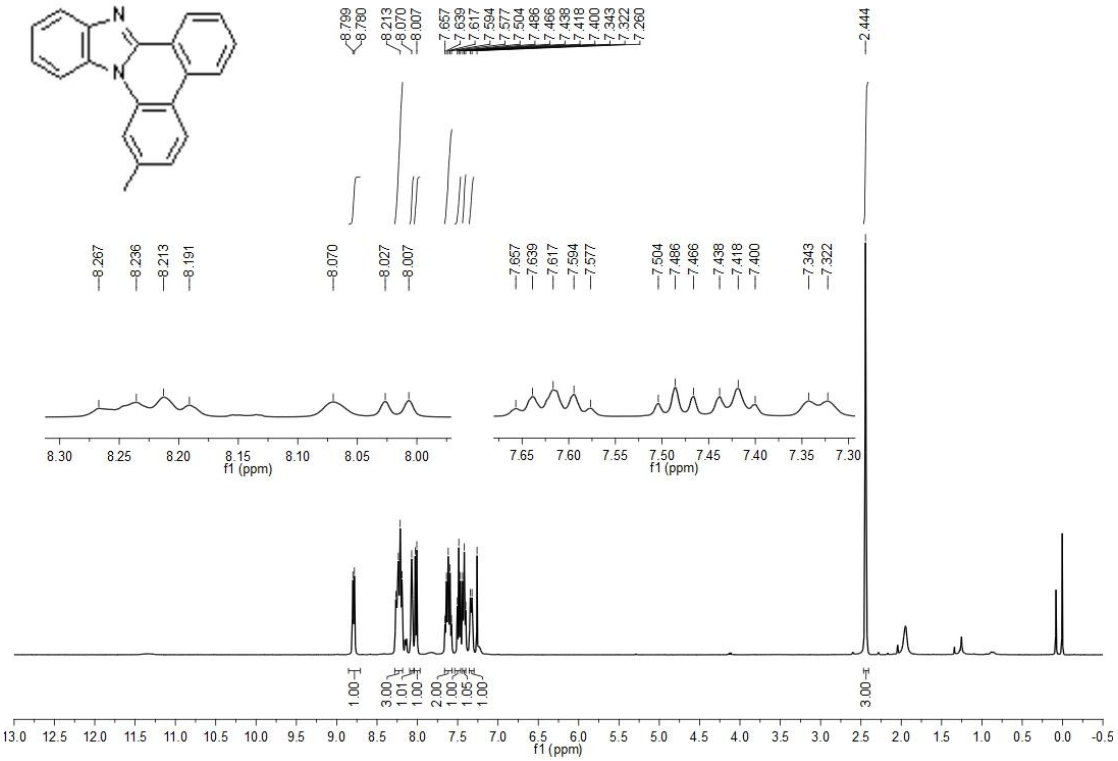


Figure S2 TGA curves of the compounds **3e**, **3h**, **3l** and **4m**.

IV. Copies of ^{1}H, ^{13}C and ^{1}H-^{1}H NOESY NMR spectra



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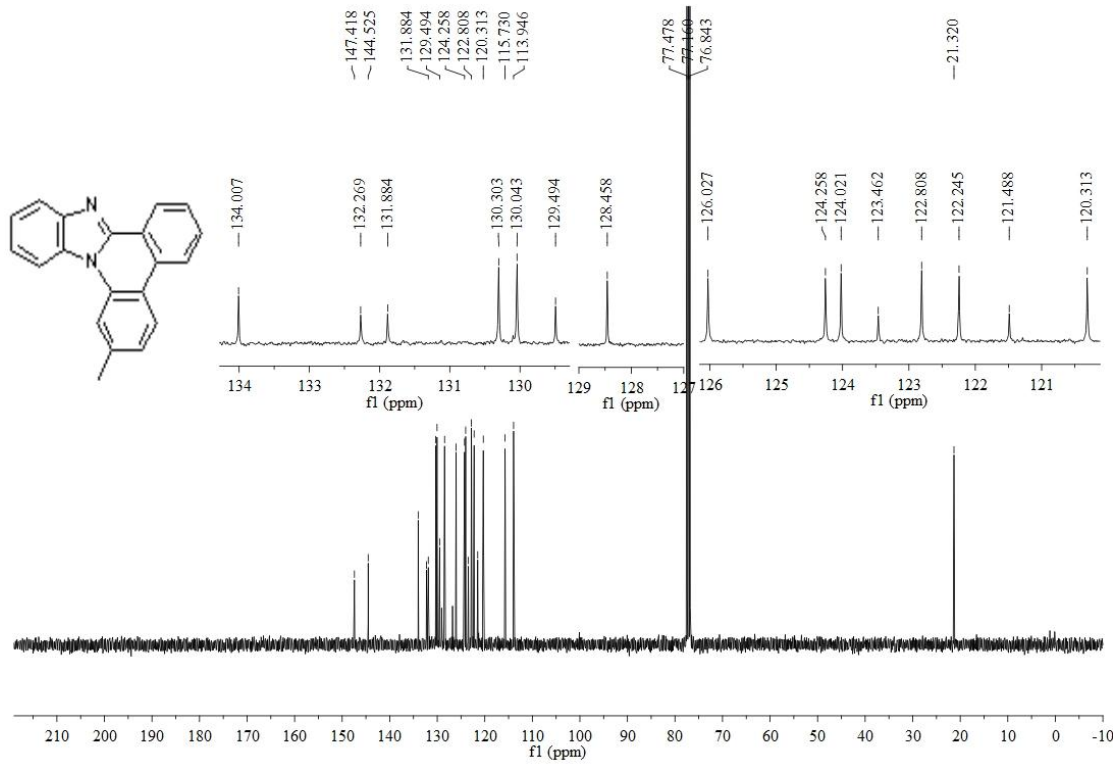
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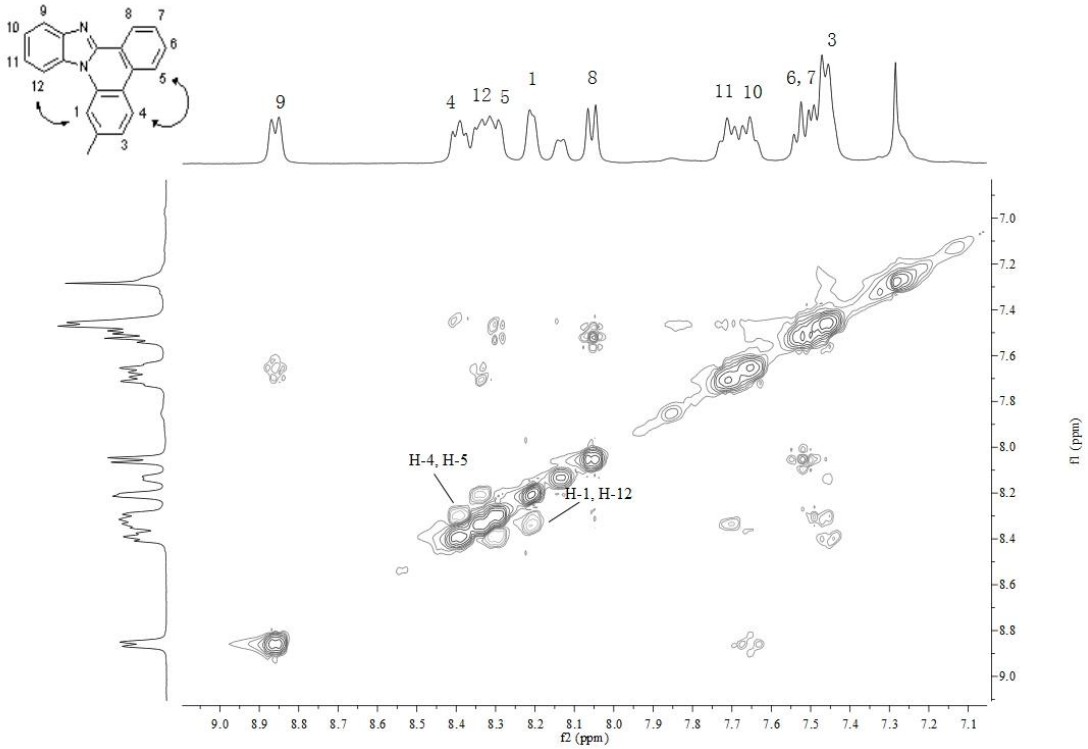

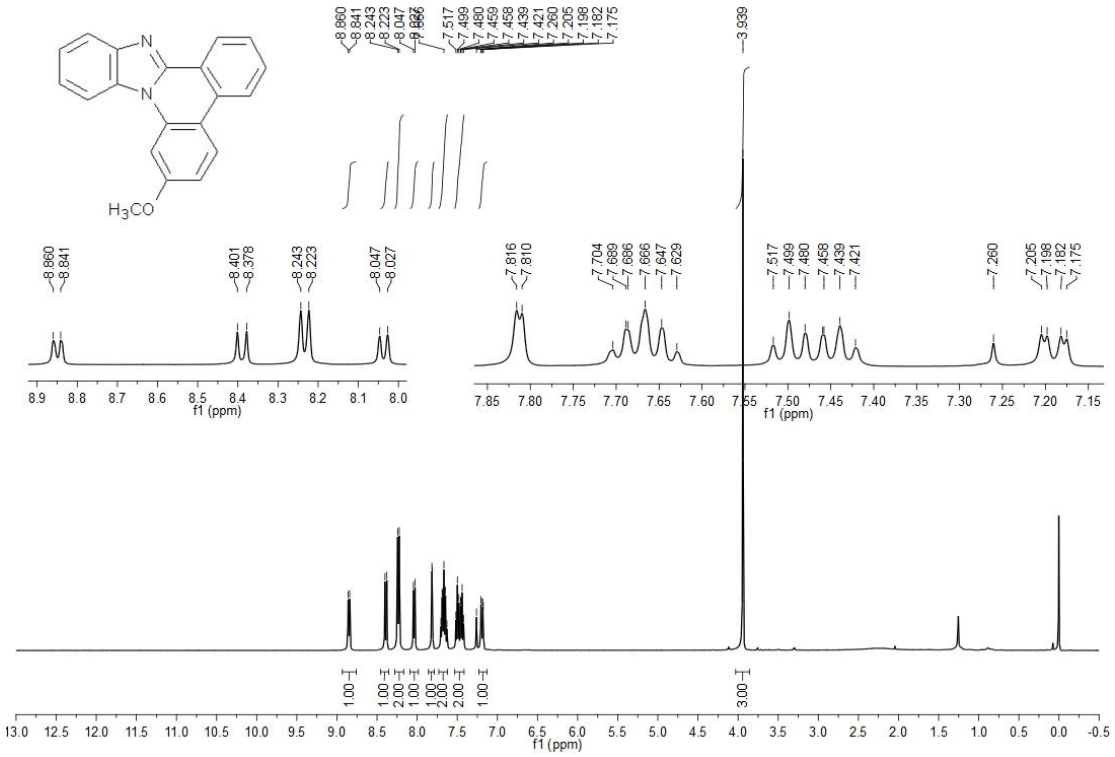

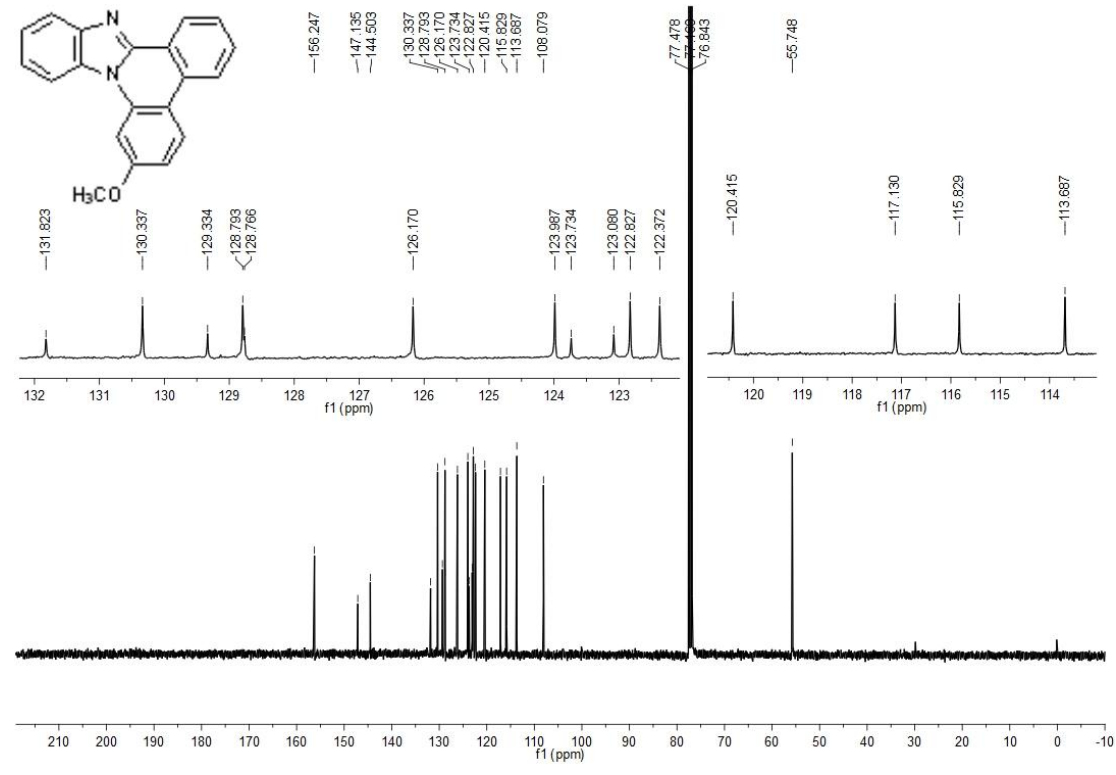

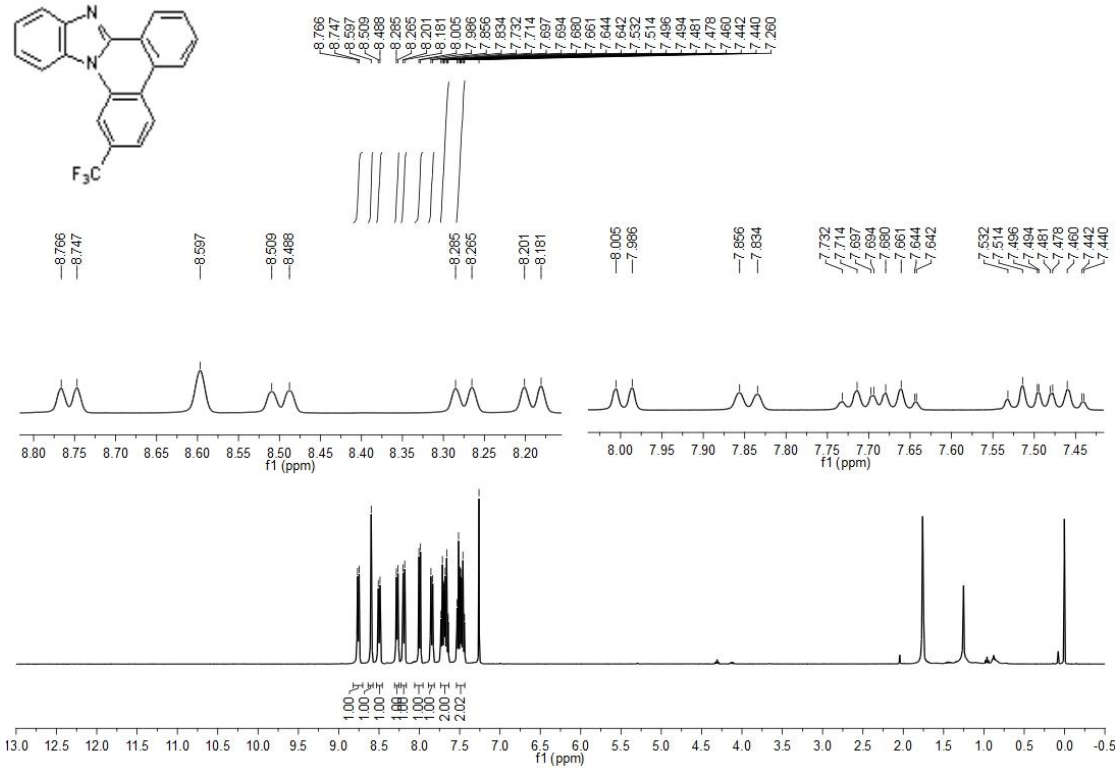
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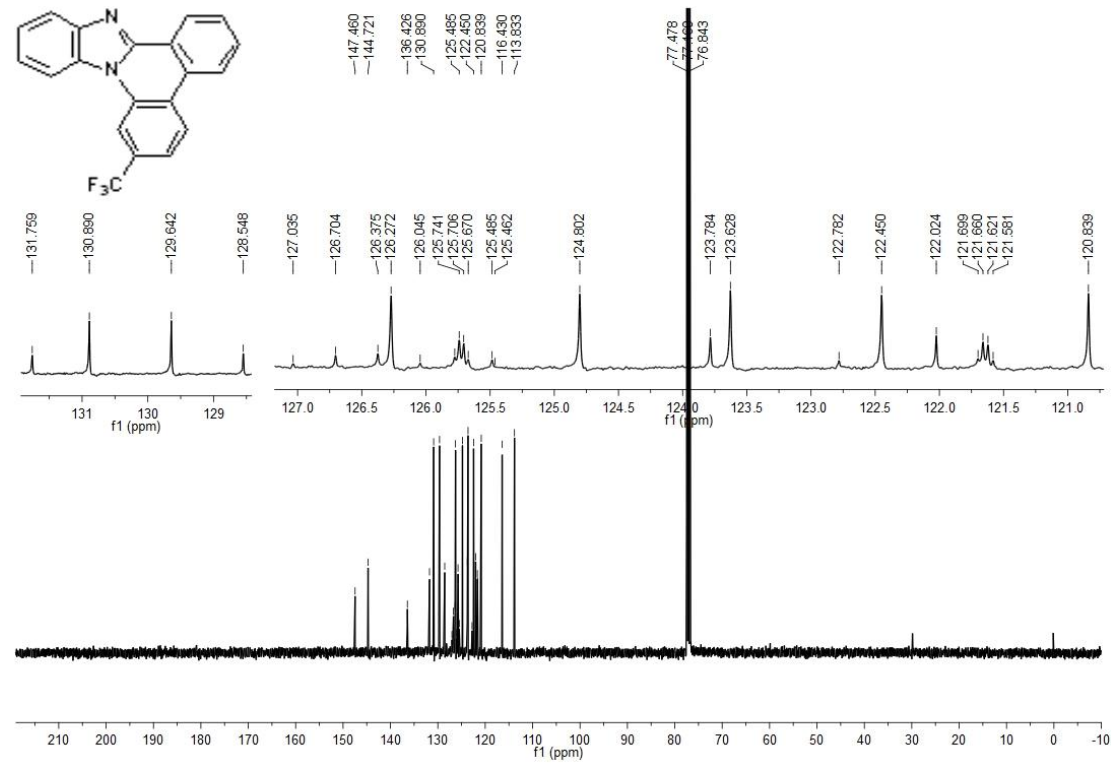
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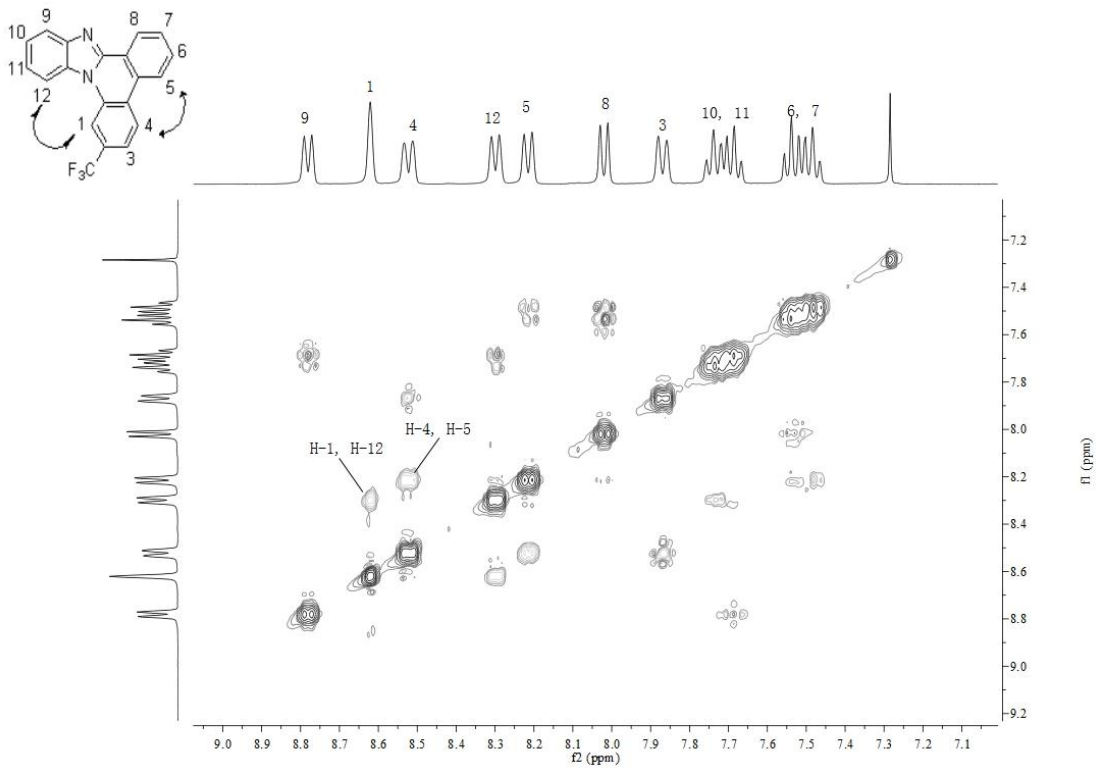
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6, 7
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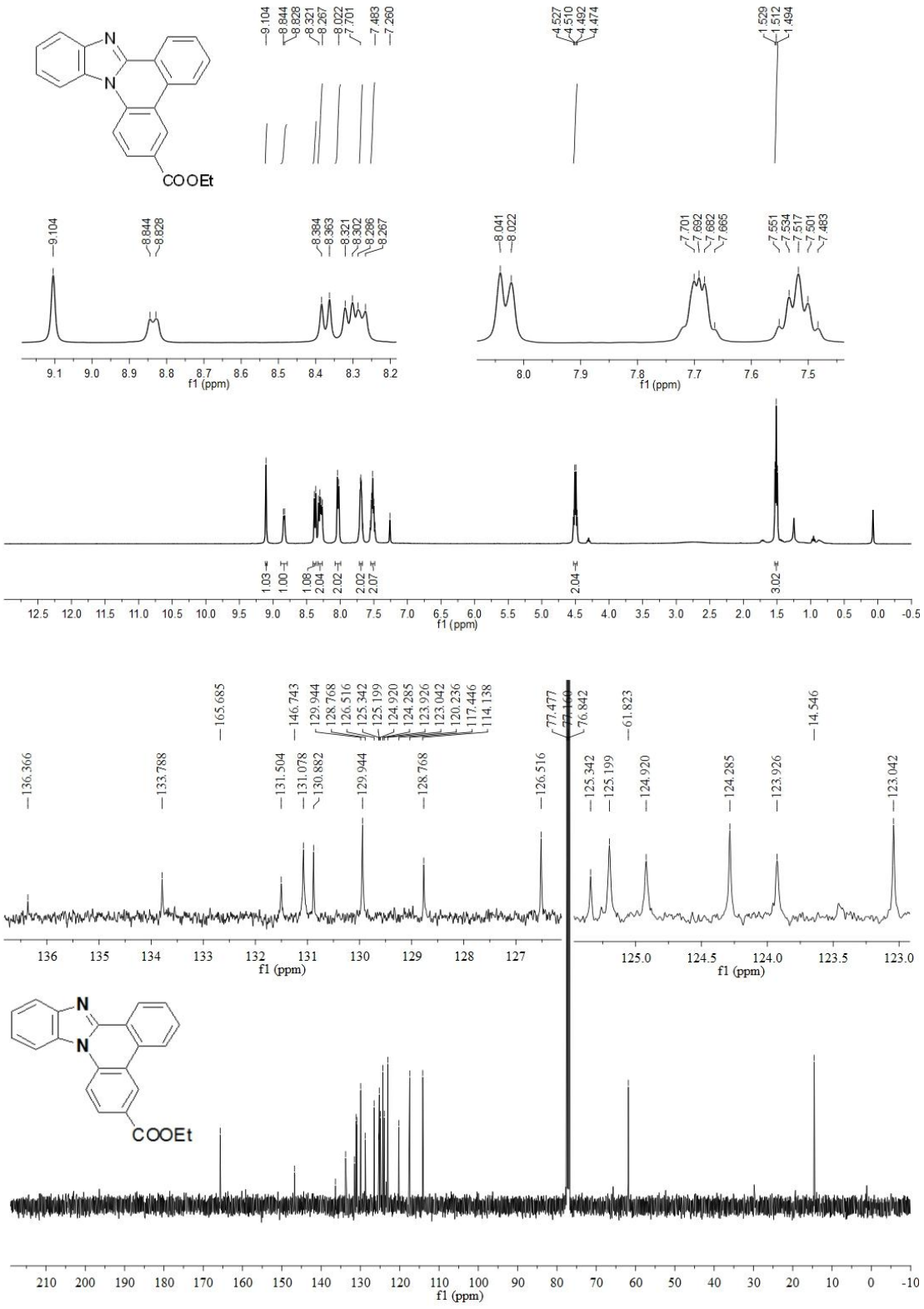
H-4, H-5
f2 (ppm)
f1 (ppm)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3.02
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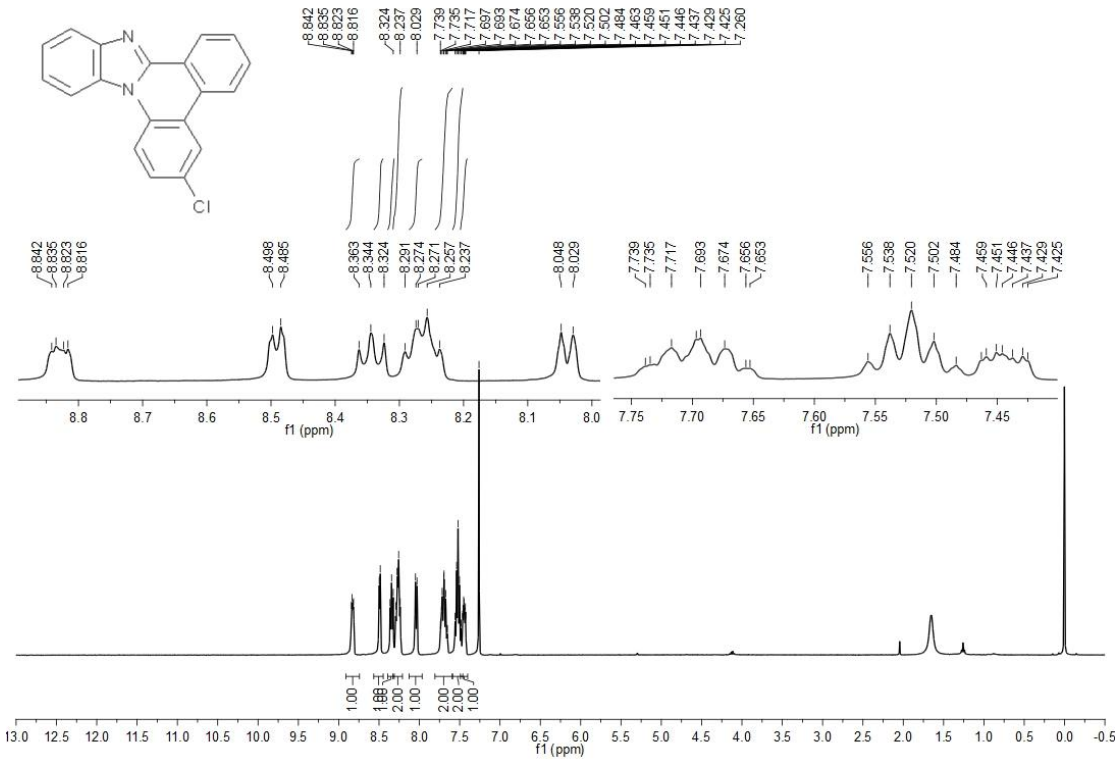

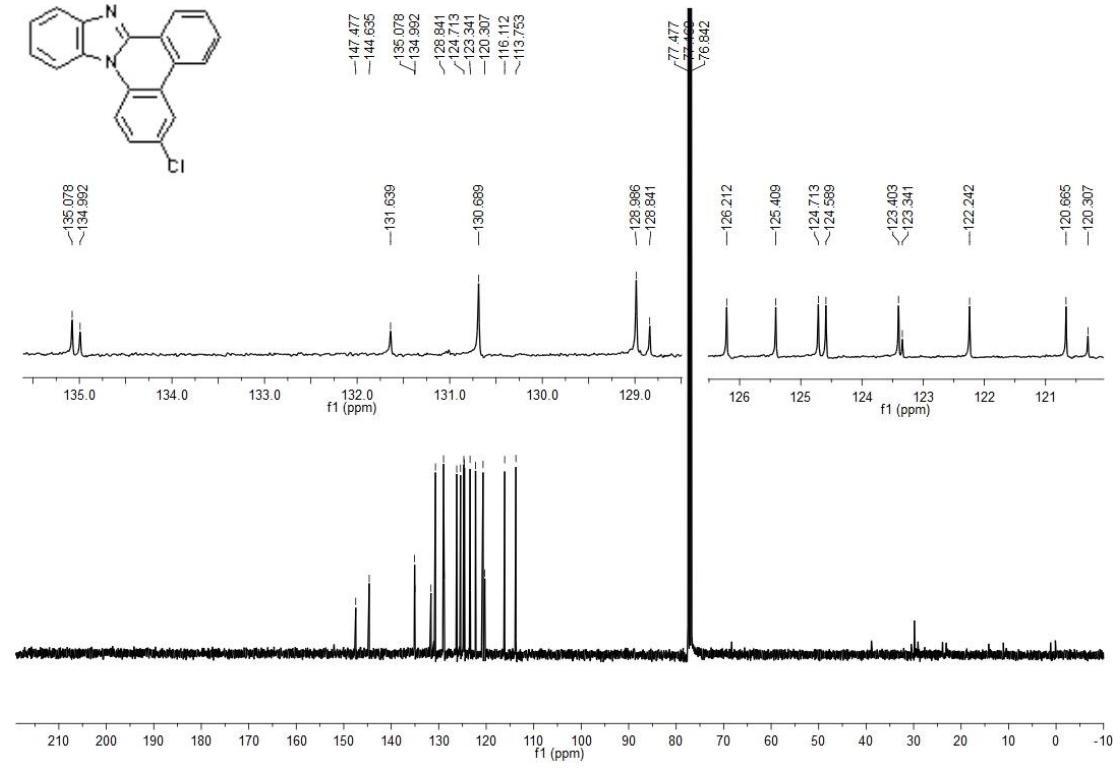

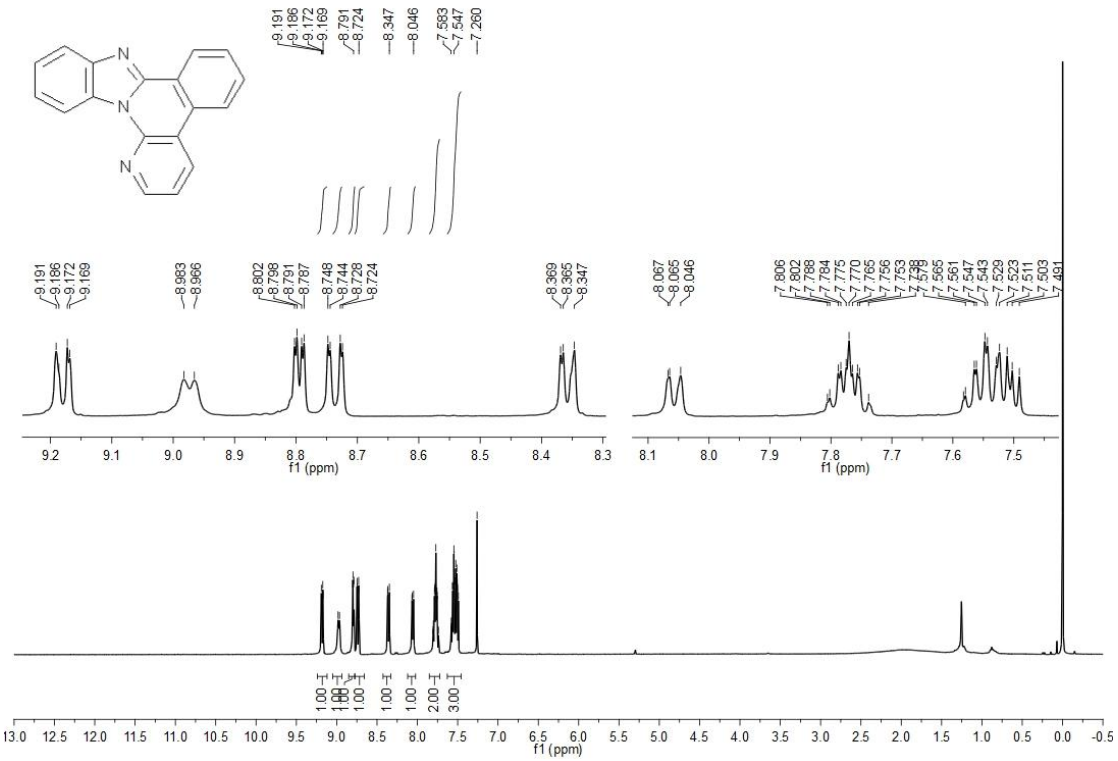
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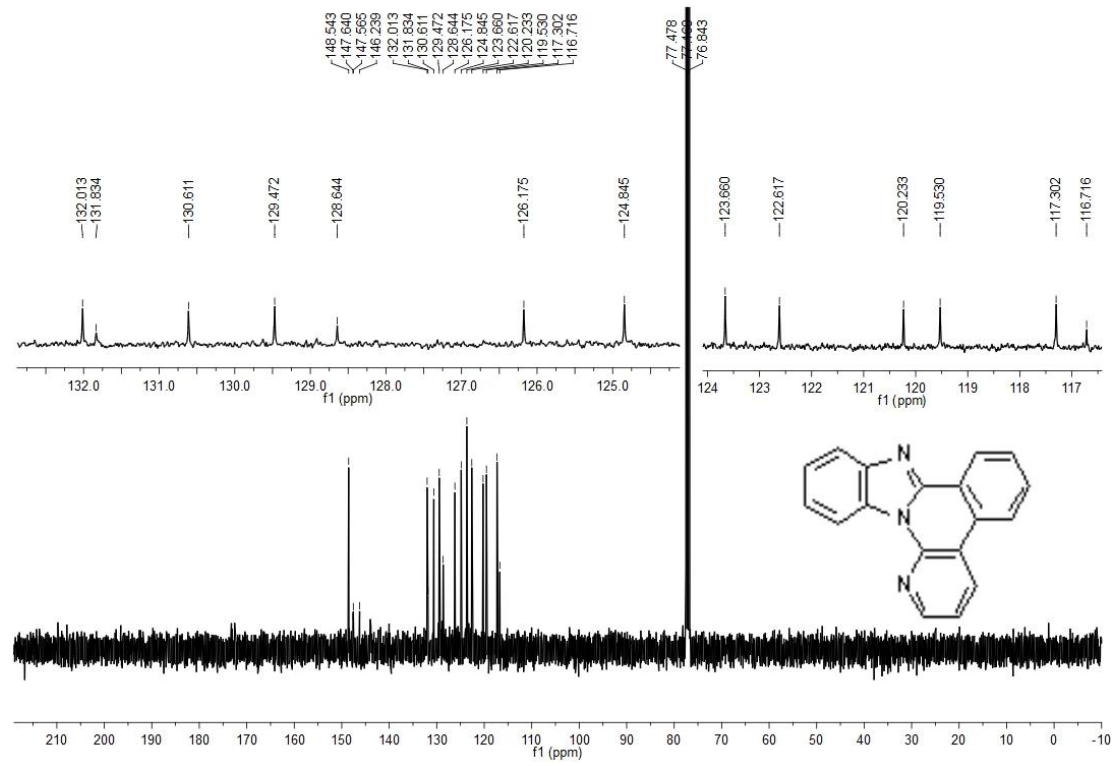
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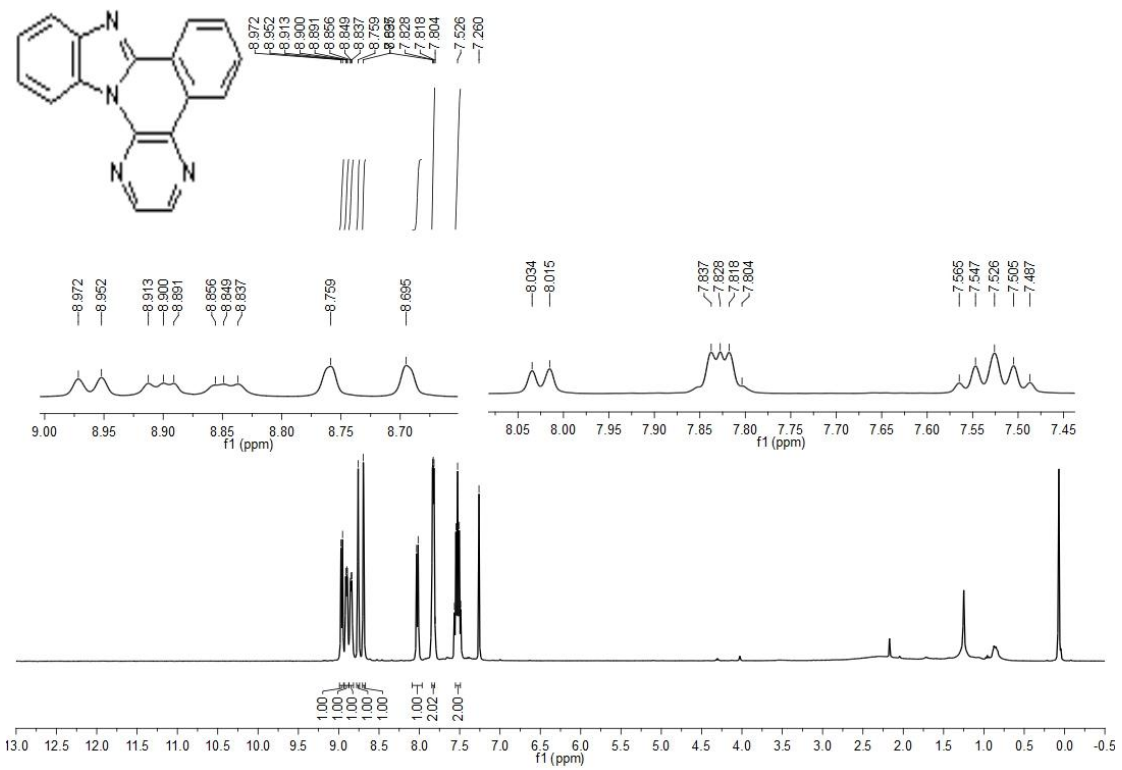

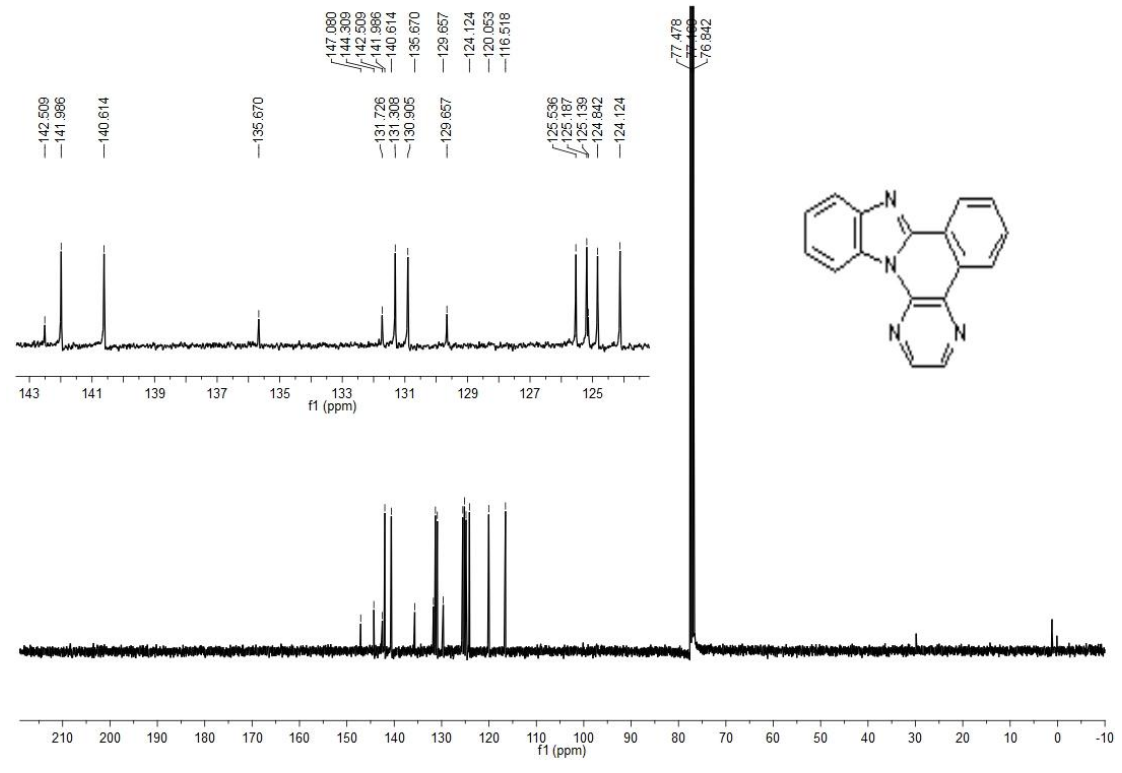

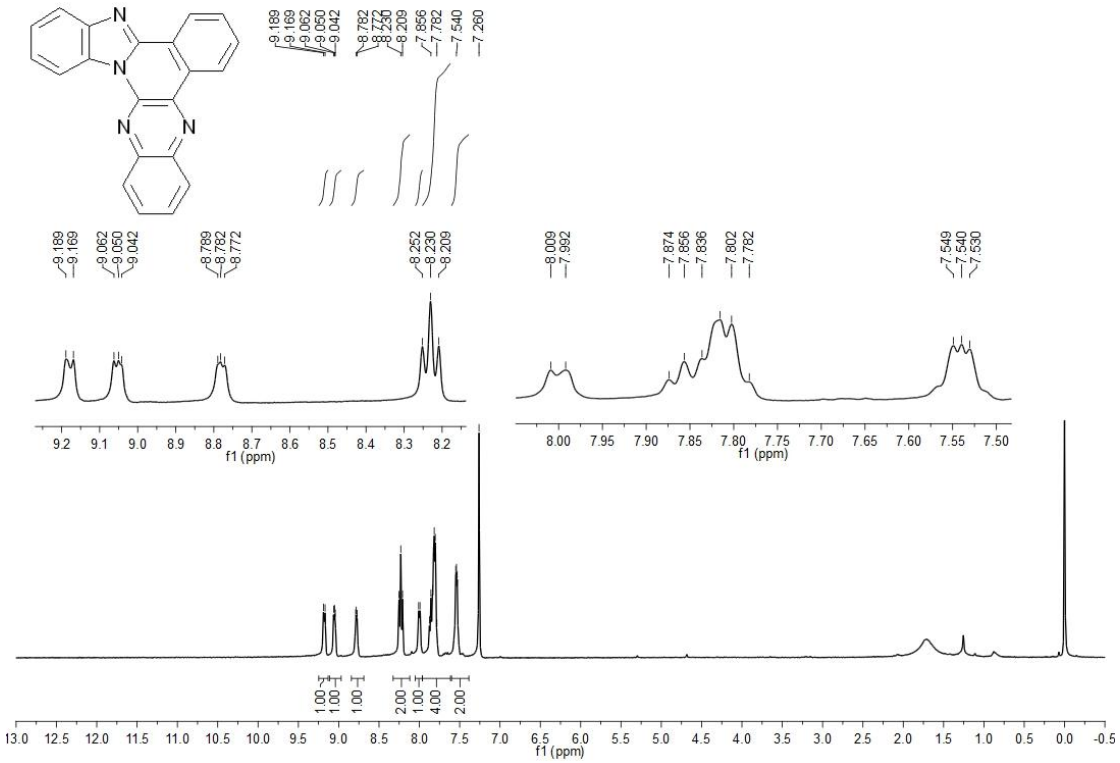

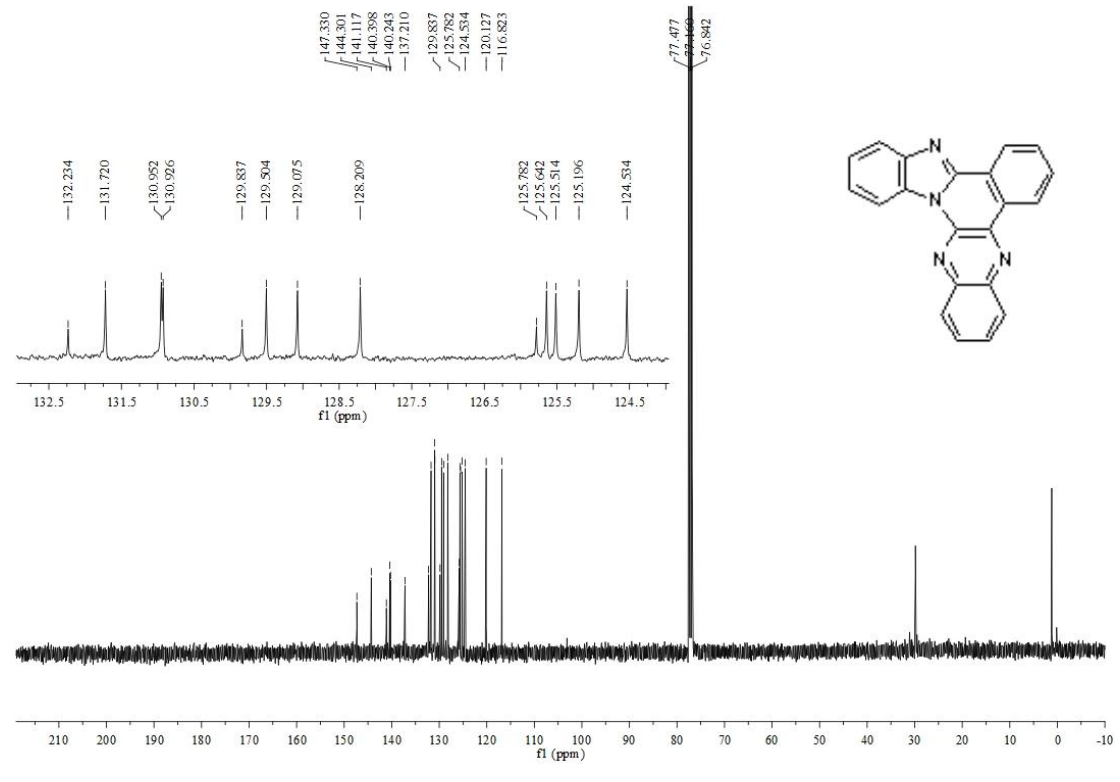

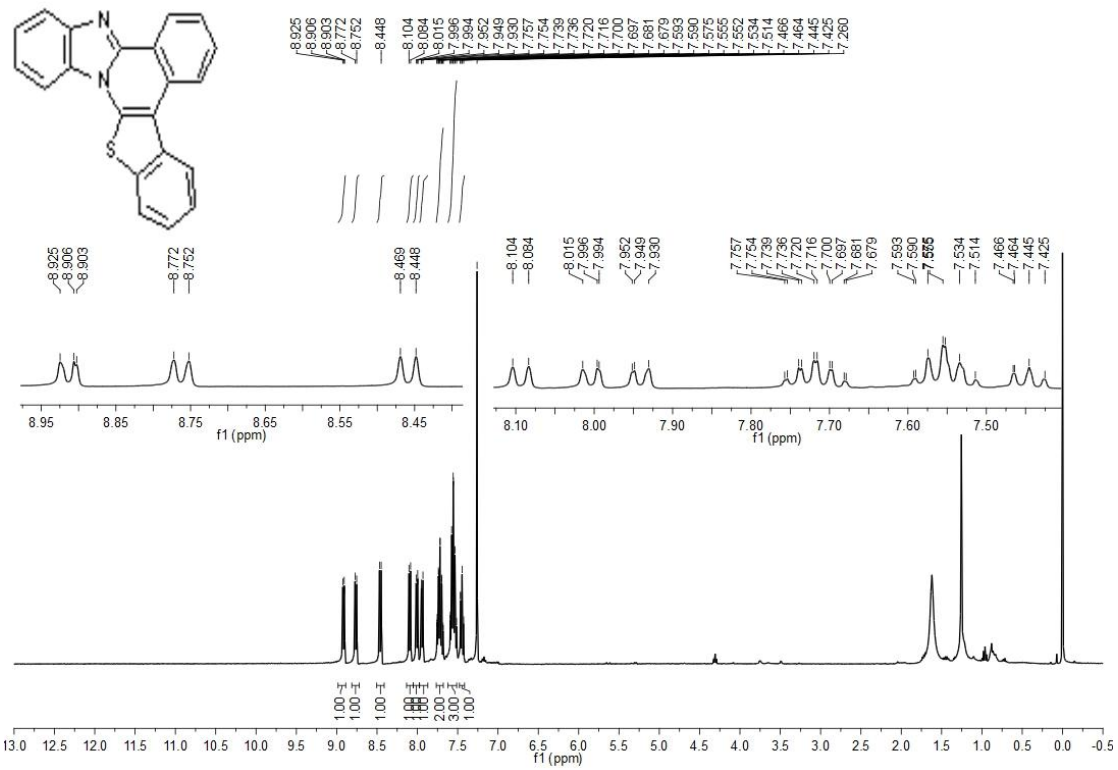
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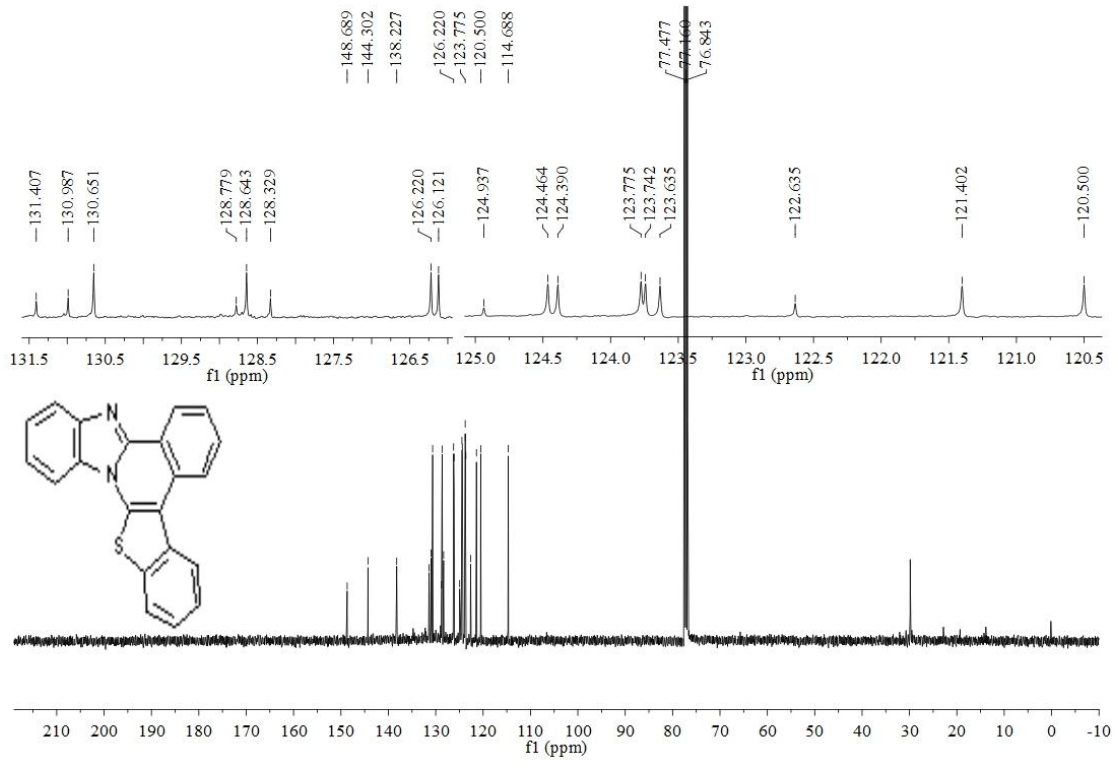
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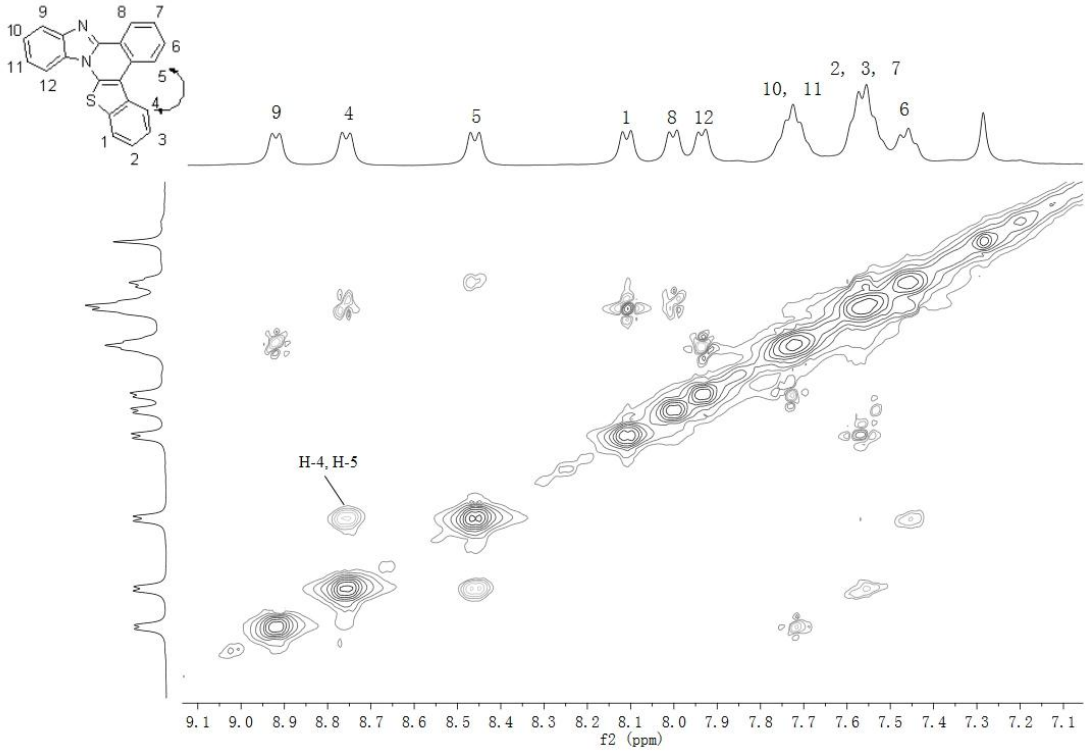

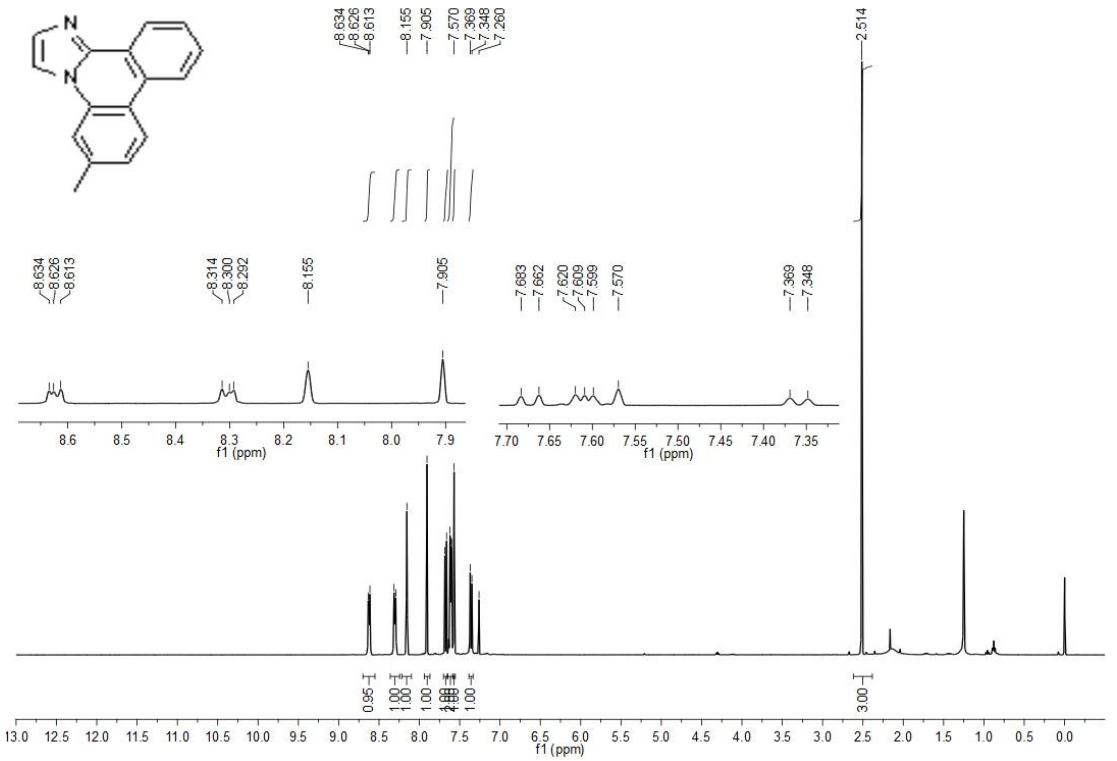
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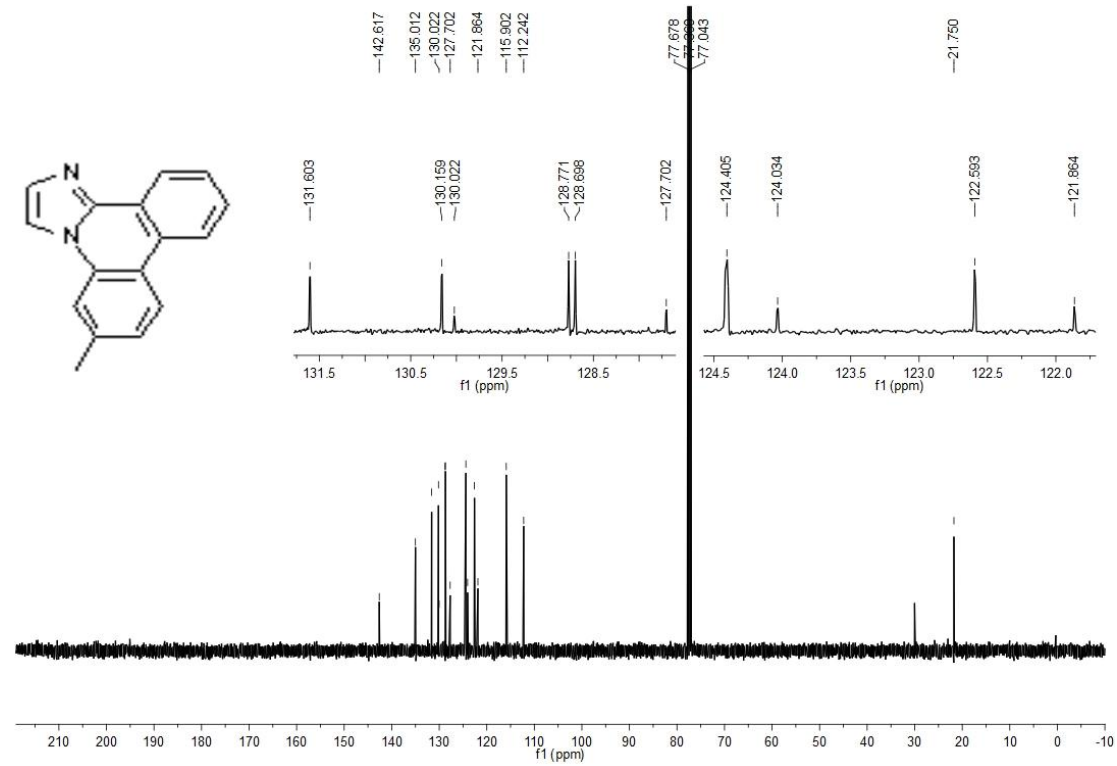
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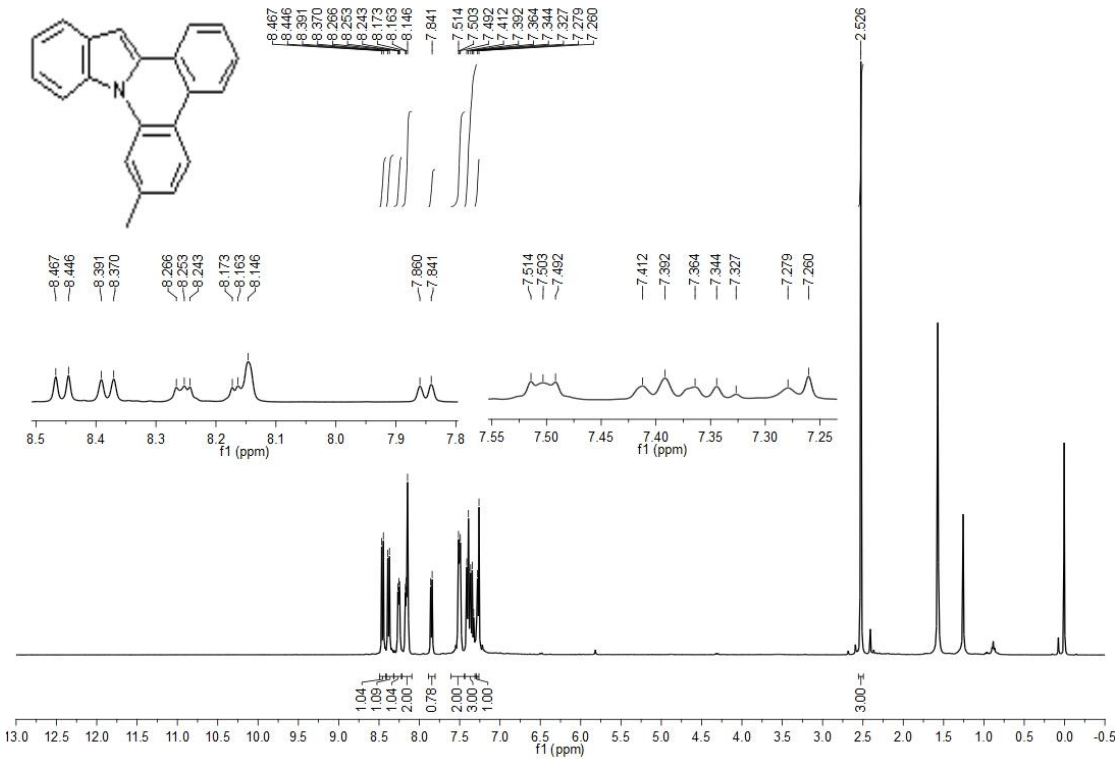

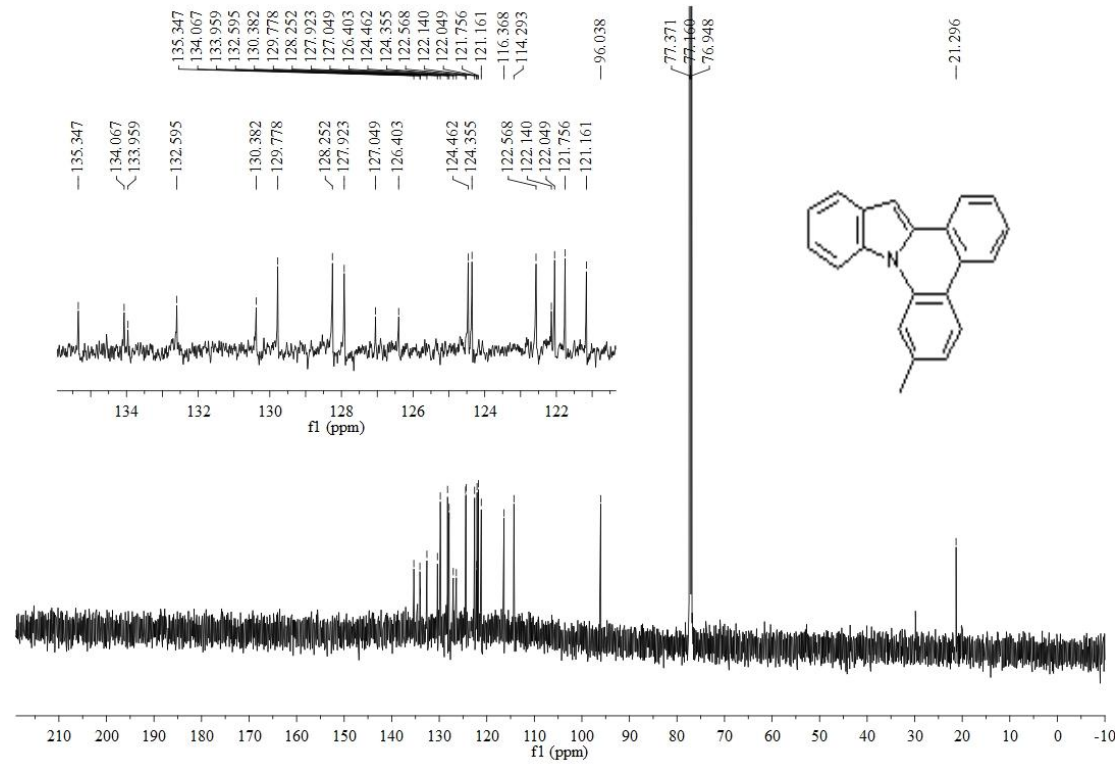

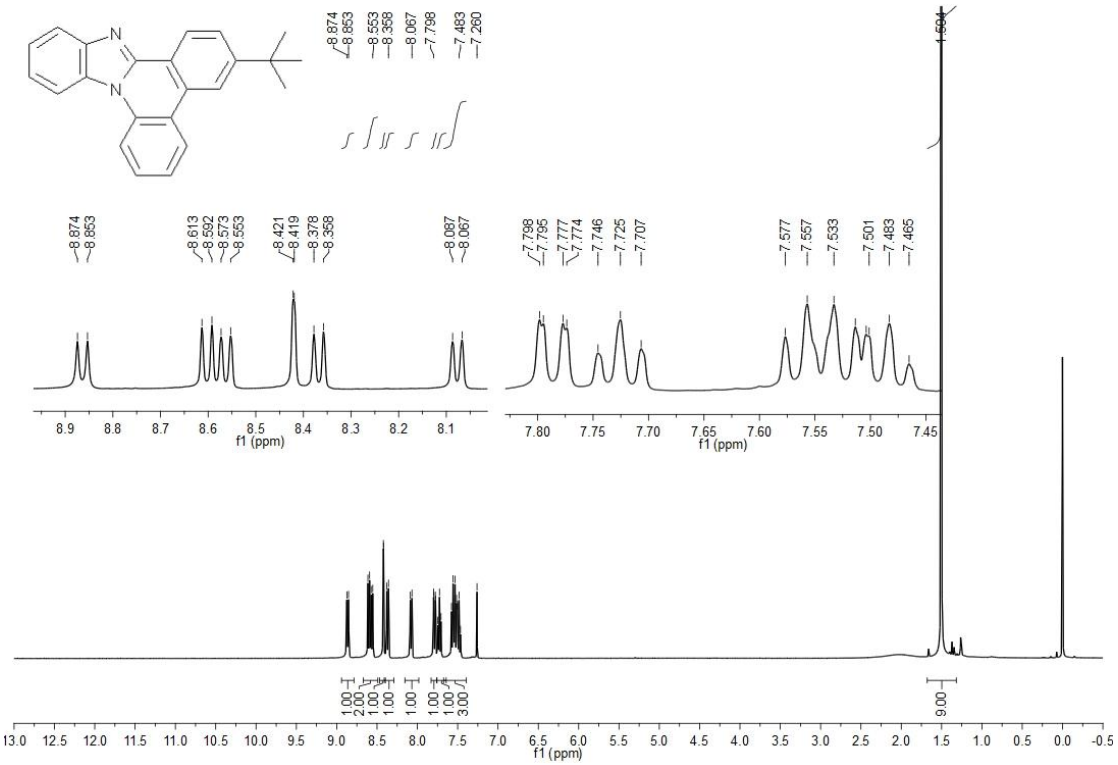
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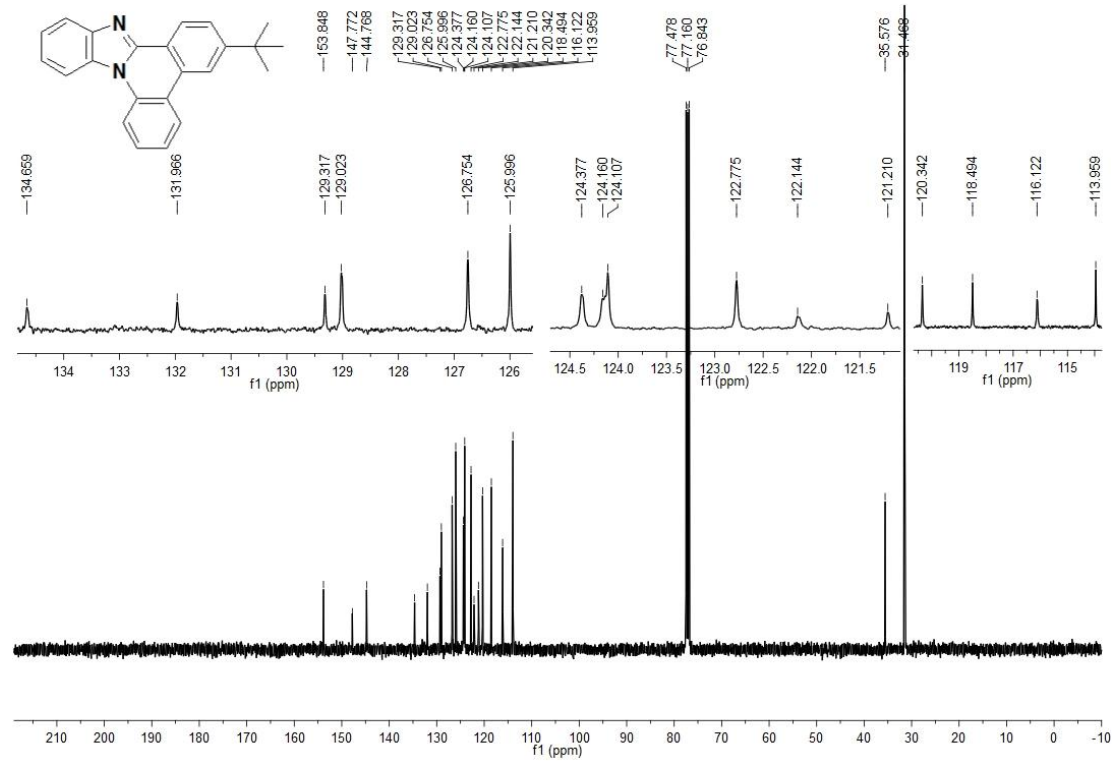
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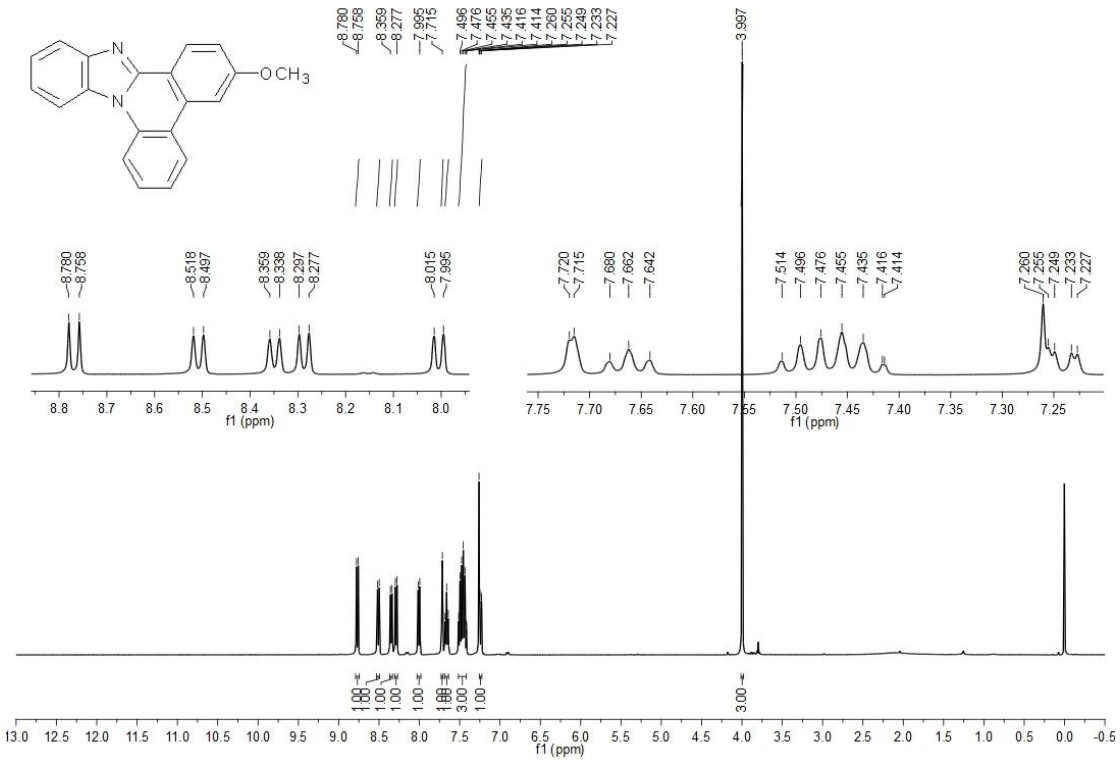

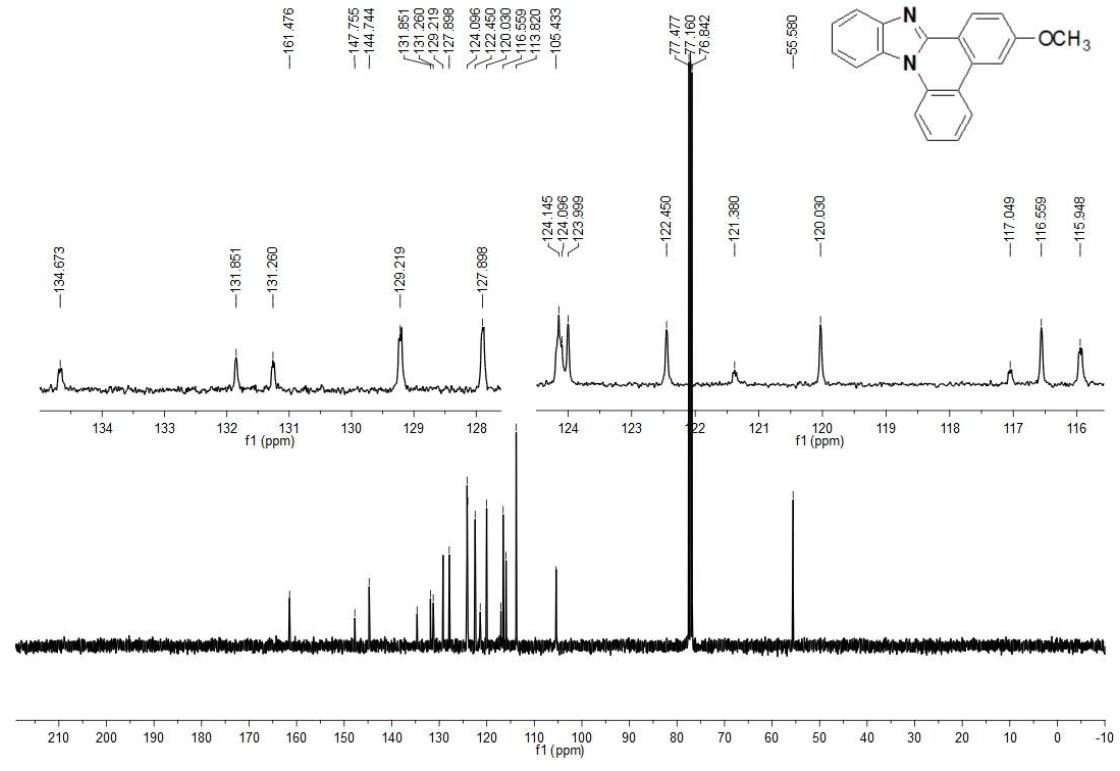

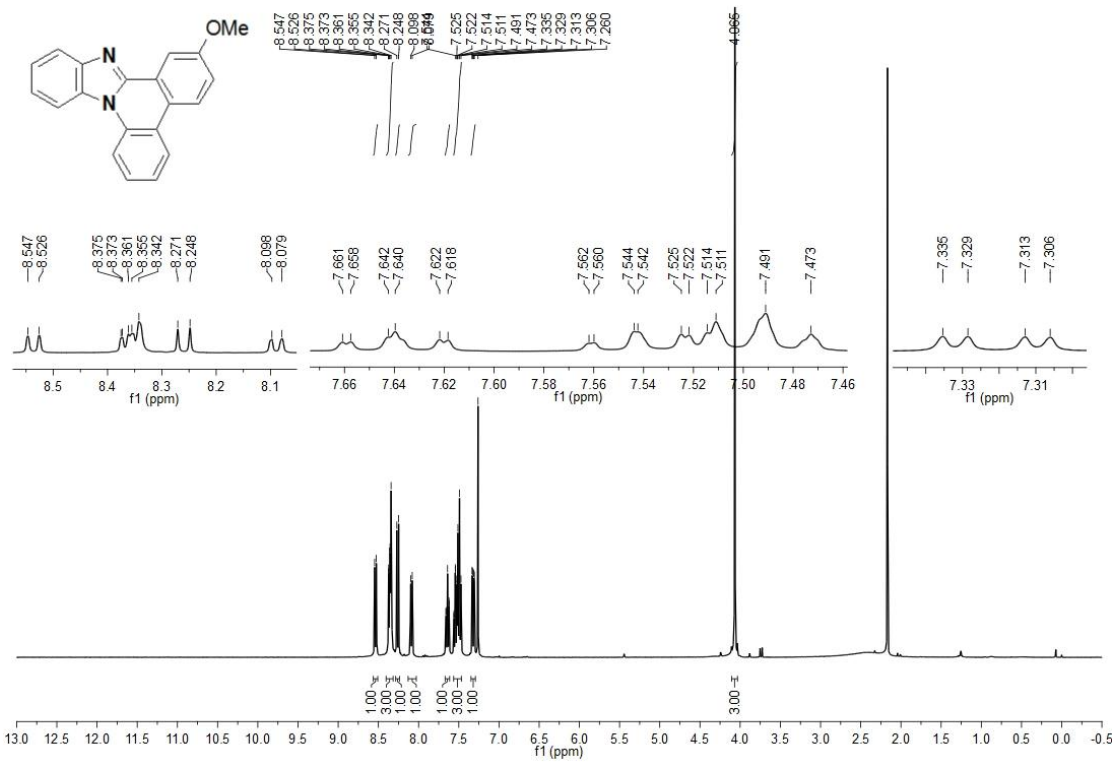

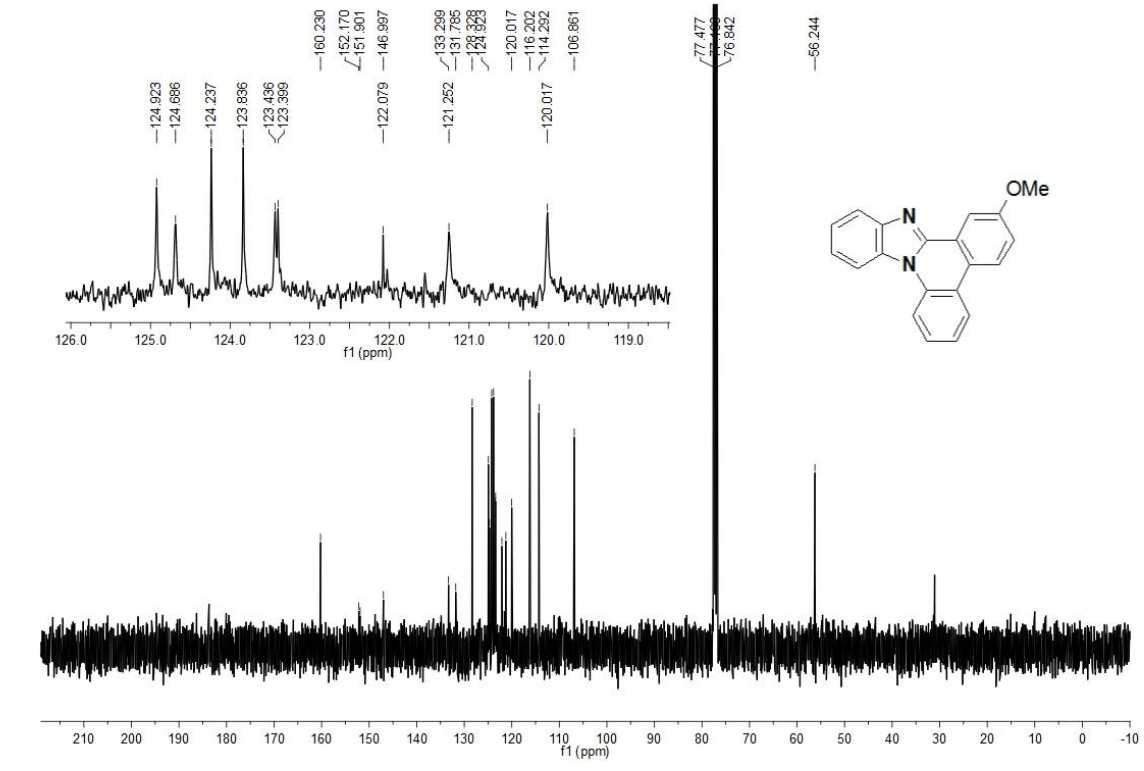

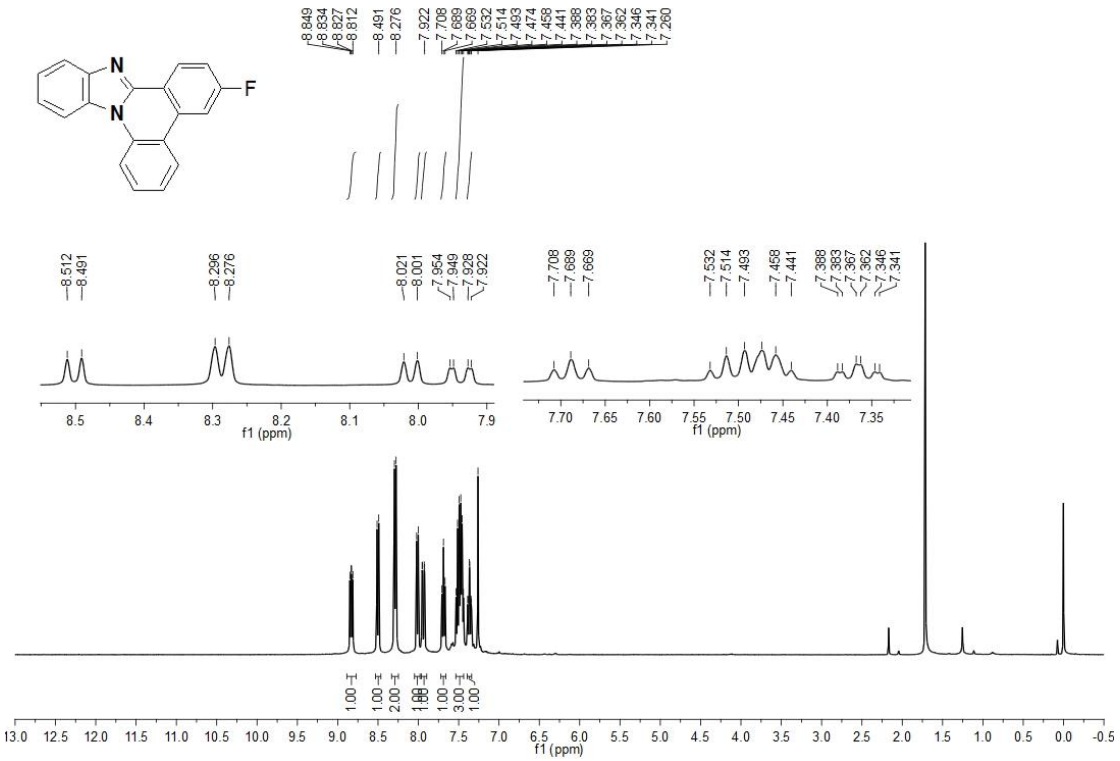
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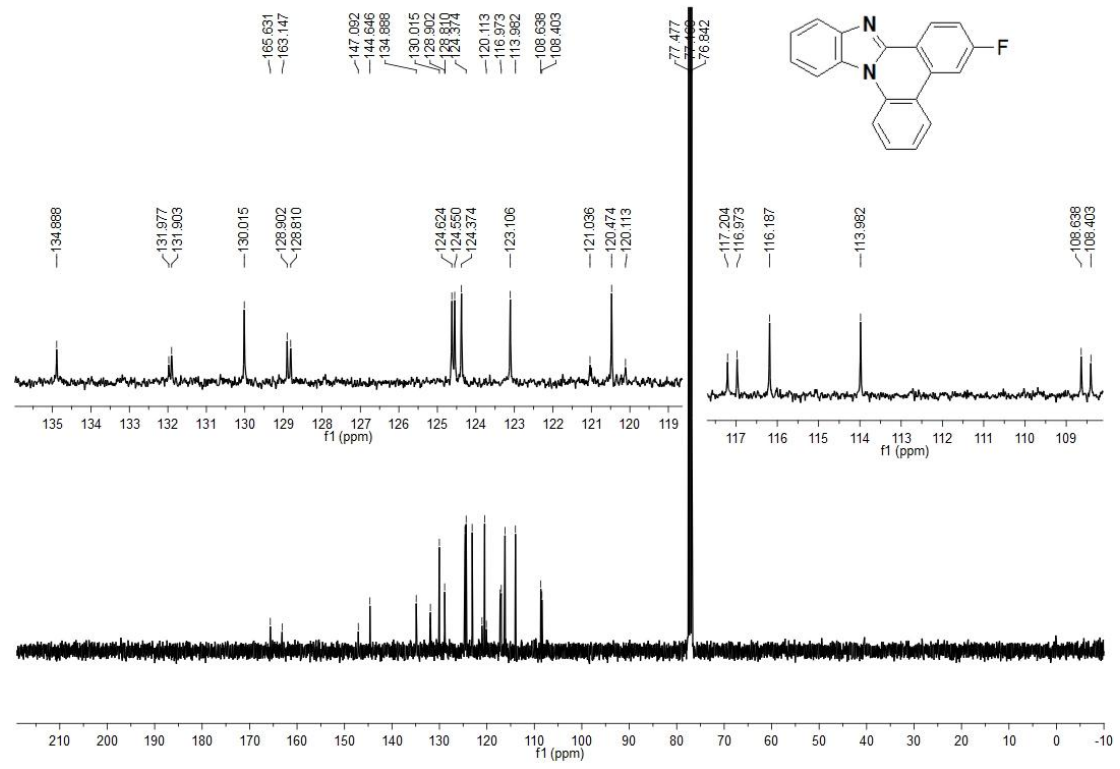
7.260
f1 (ppm)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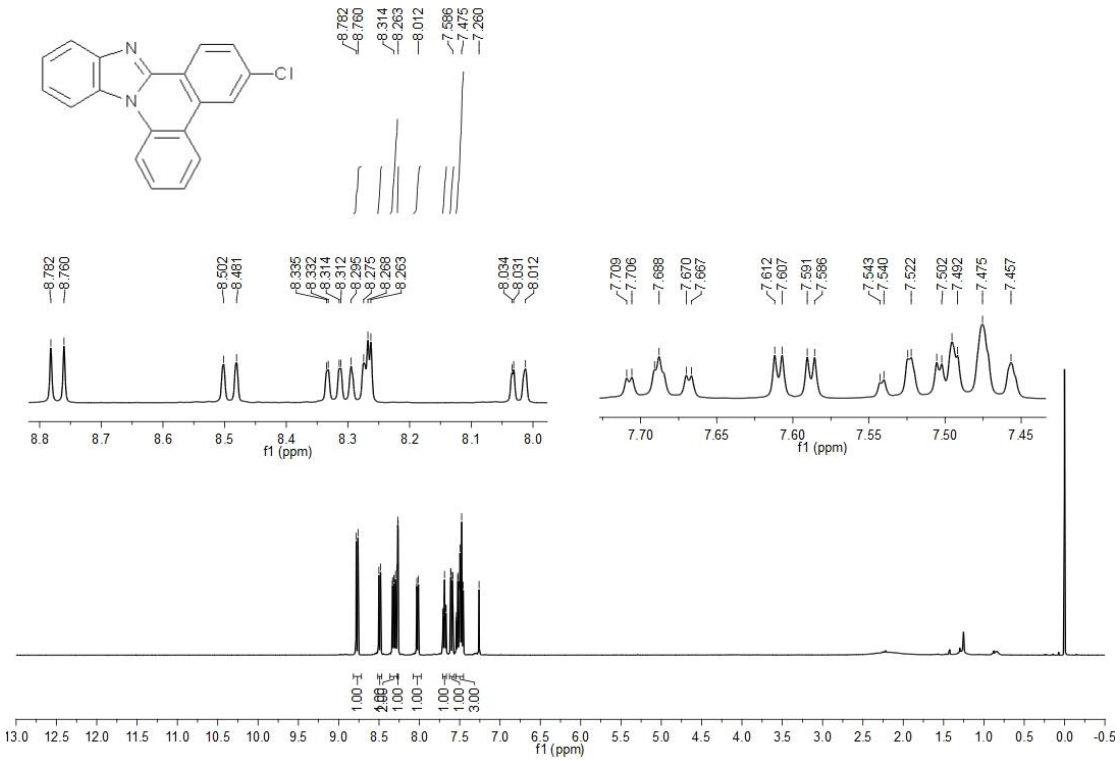
f1 (ppm)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N
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7.586
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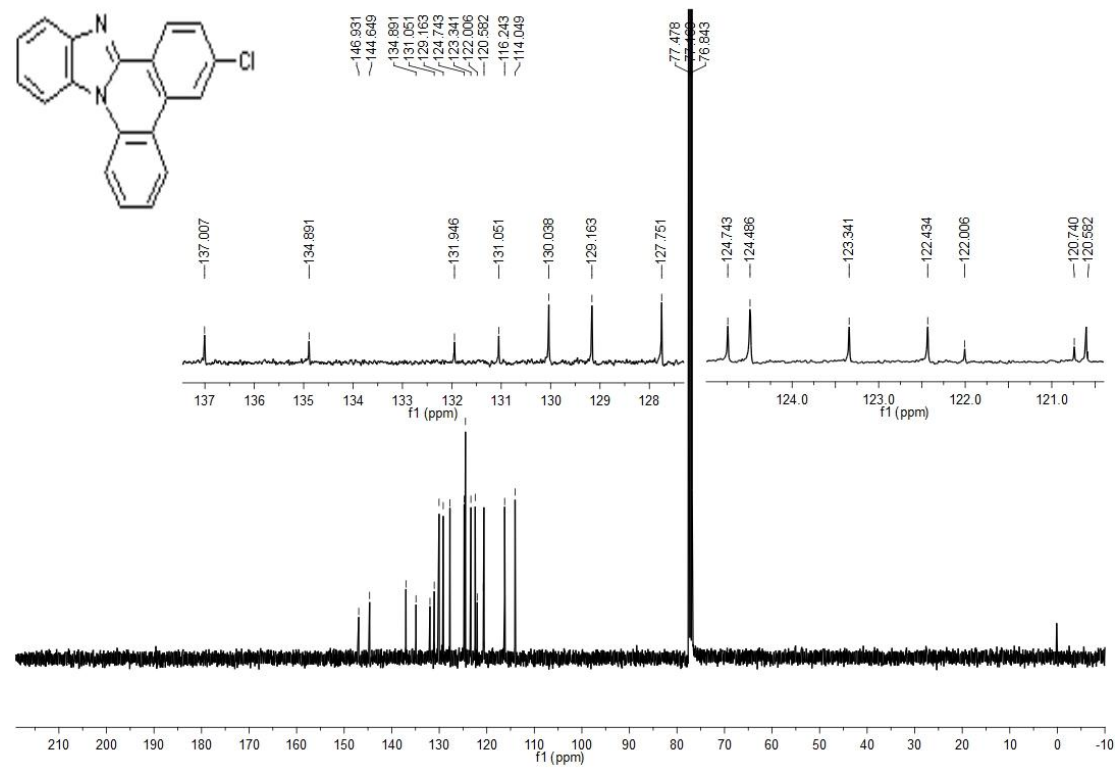
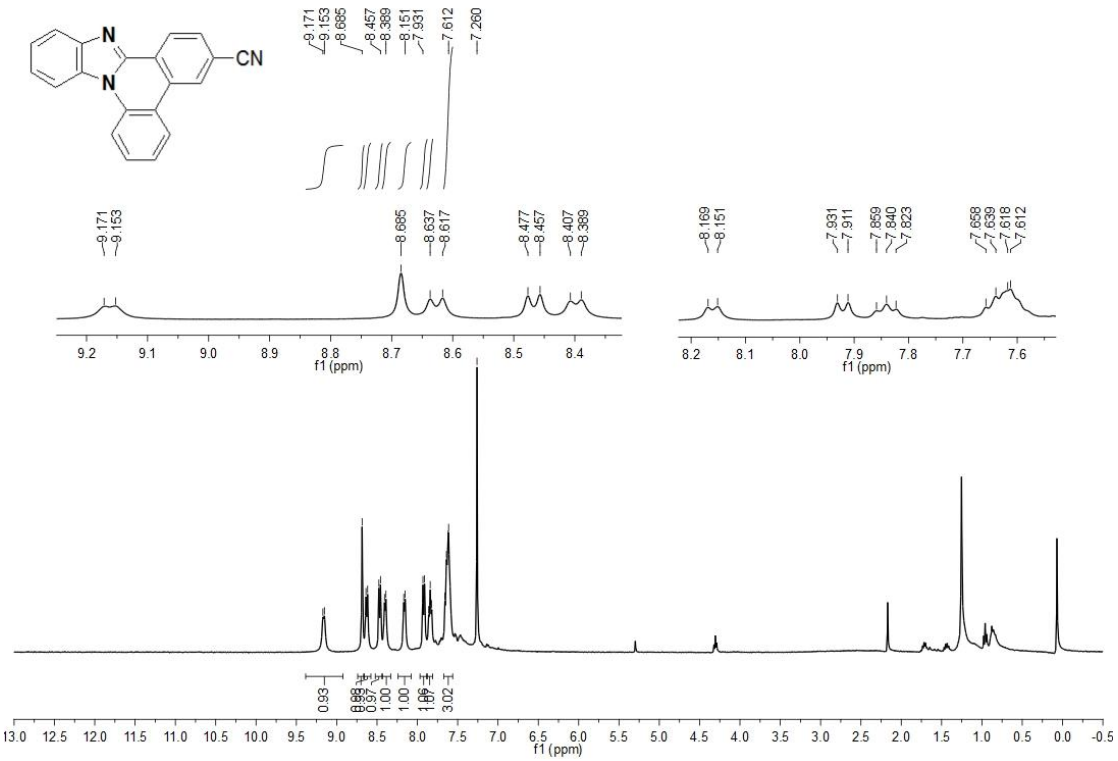
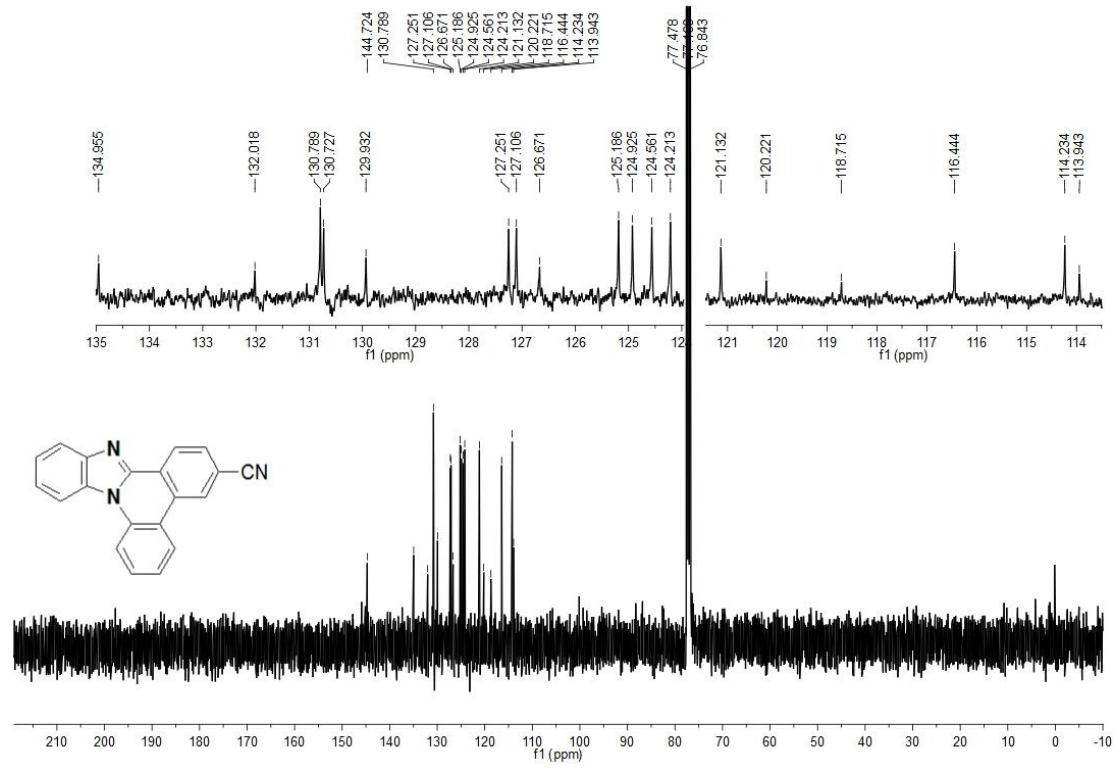
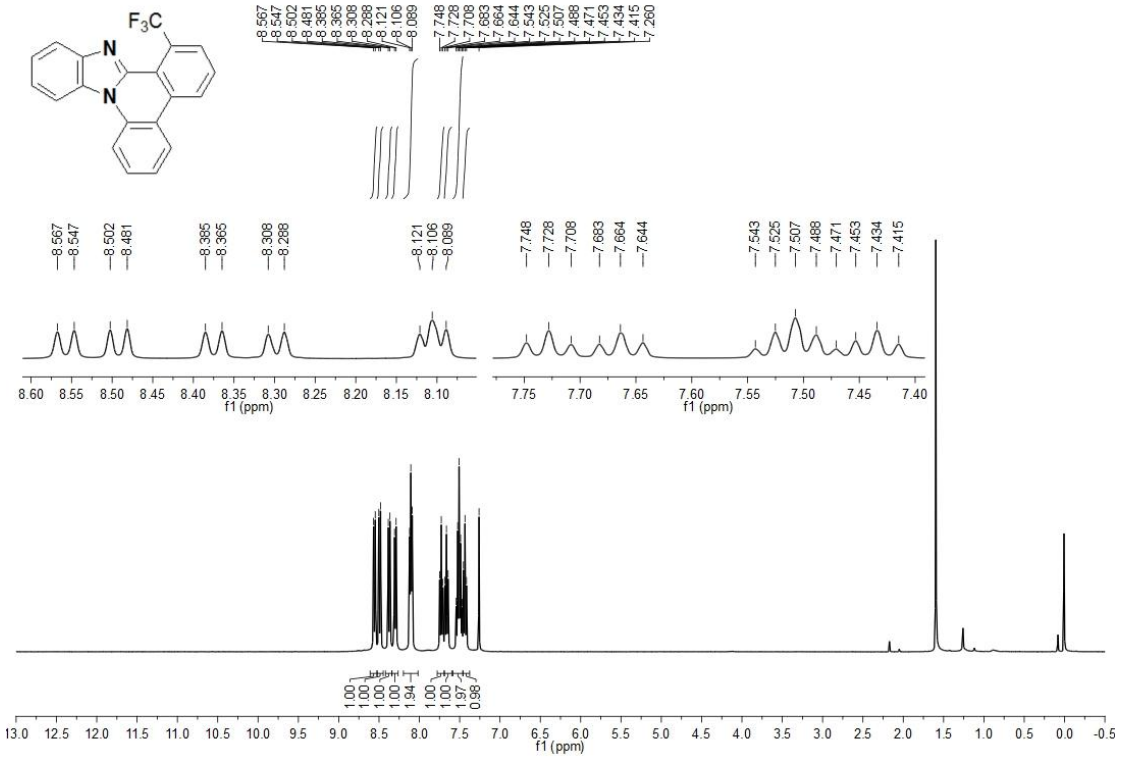
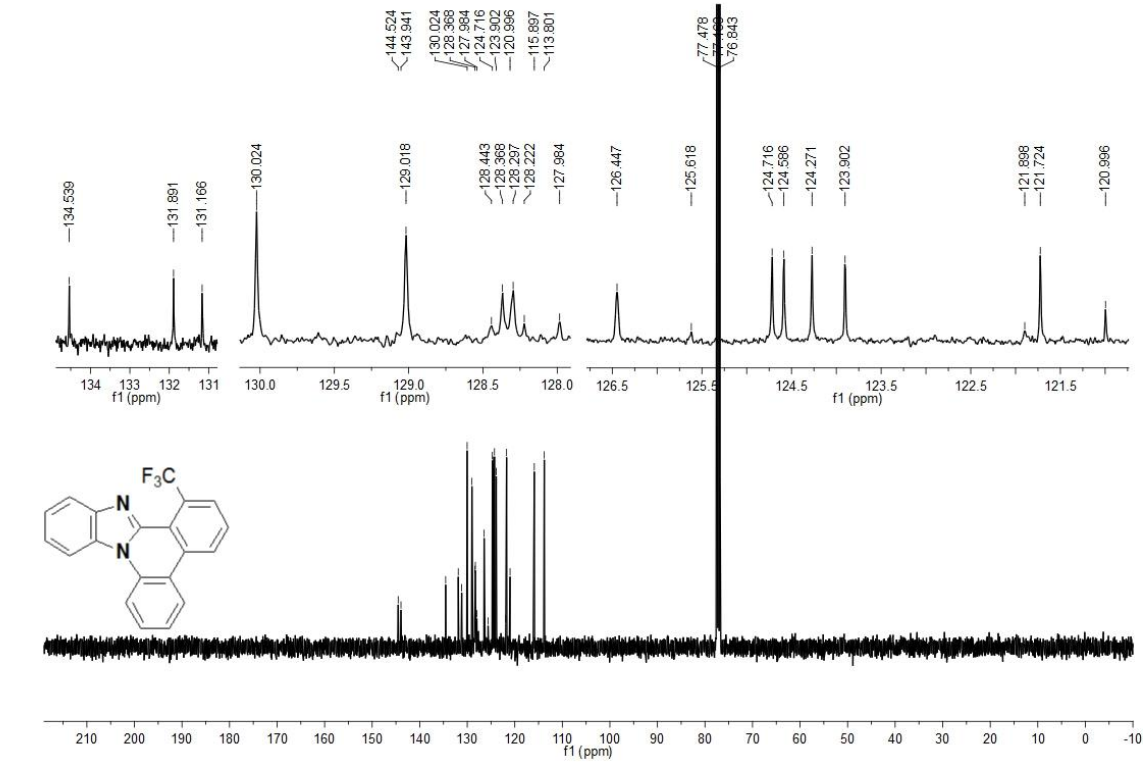
7.260
f1 (ppm)

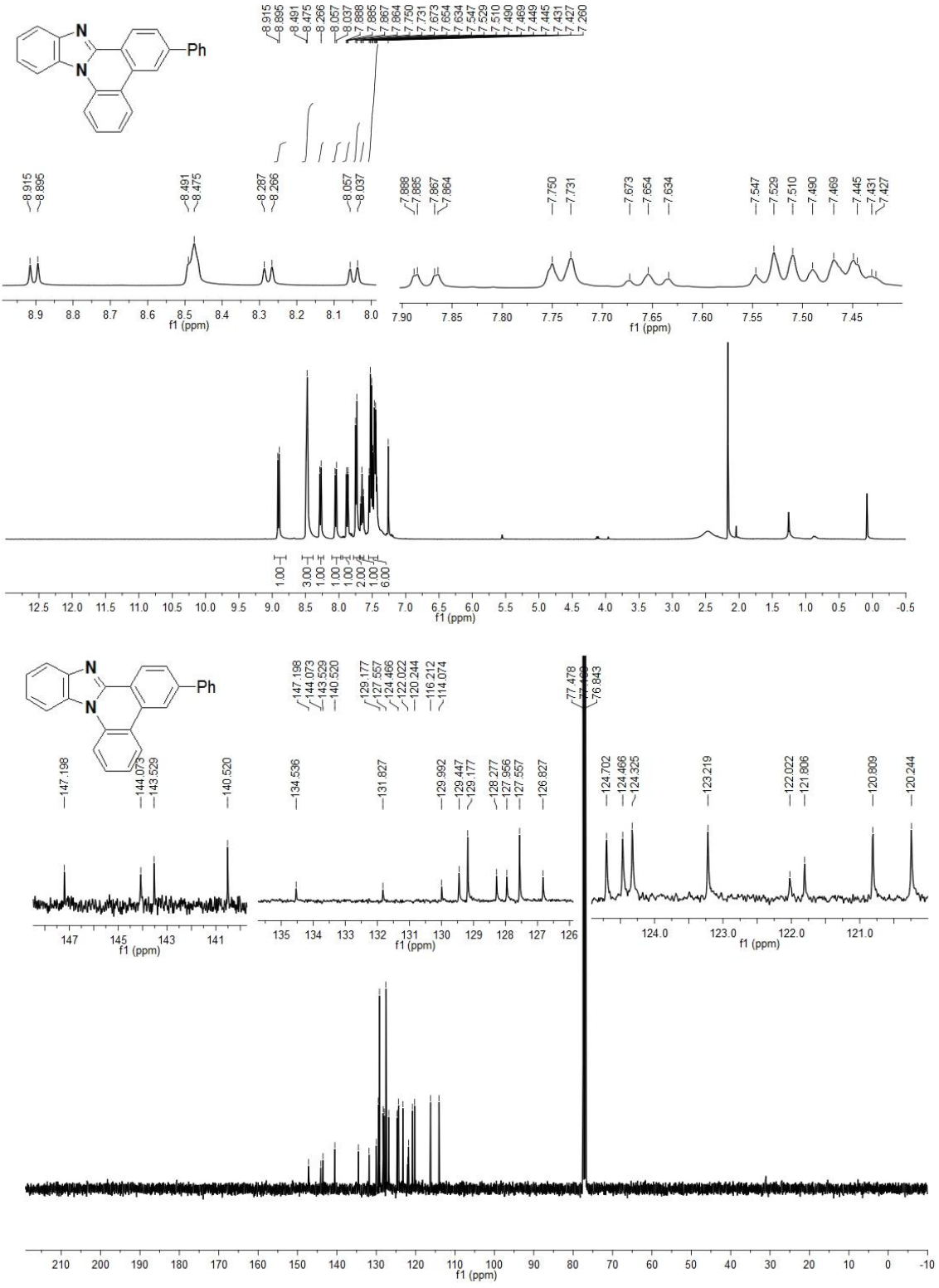

N
N
Cl
146.931
144.649
134.891
131.051
129.163
124.743
123.341
122.006
120.582
116.243
114.049
77.478
76.843
137.007
134.891
131.946
131.051
130.038
129.163
127.751
124.743
124.486
123.341
122.434
122.006
120.740
120.582
f1 (ppm)

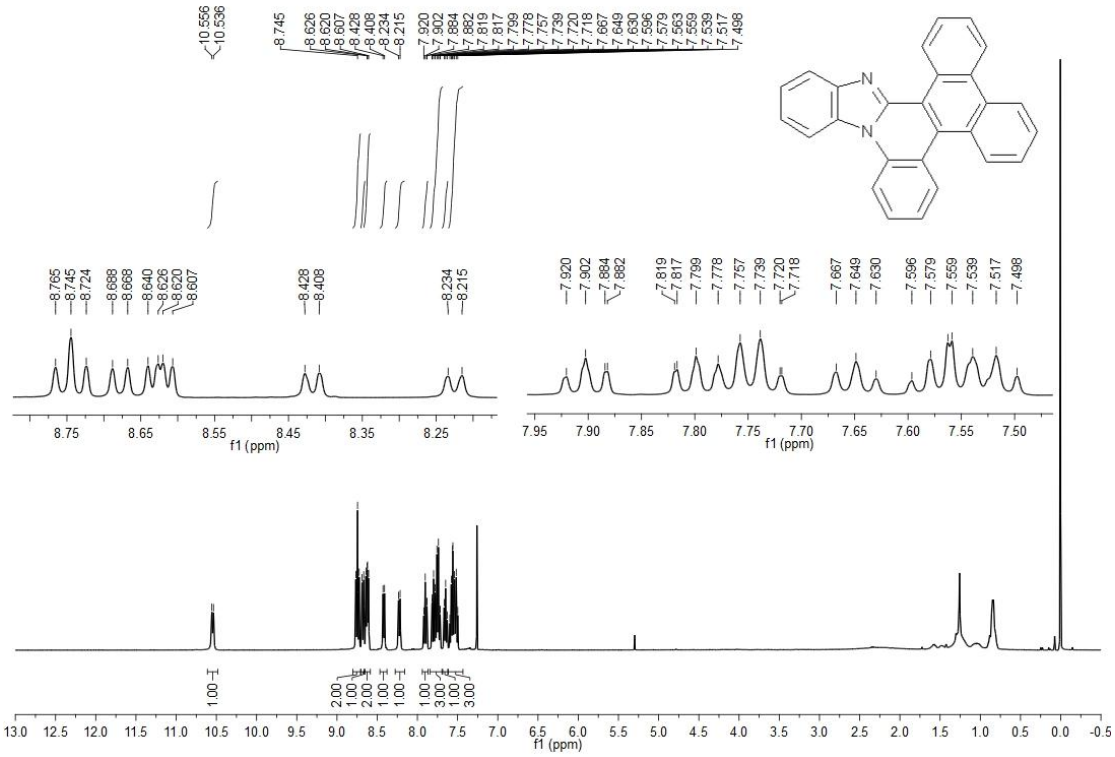

N
N
CN
9.171
9.153
8.885
8.457
8.389
8.151
7.931
7.612
7.260
8.637
8.617
8.477
8.457
8.407
8.389
8.169
8.151
7.931
7.911
7.859
7.840
7.823
7.658
7.639
7.618
7.612
f1 (ppm)
0.93
1.00
1.00
3.02

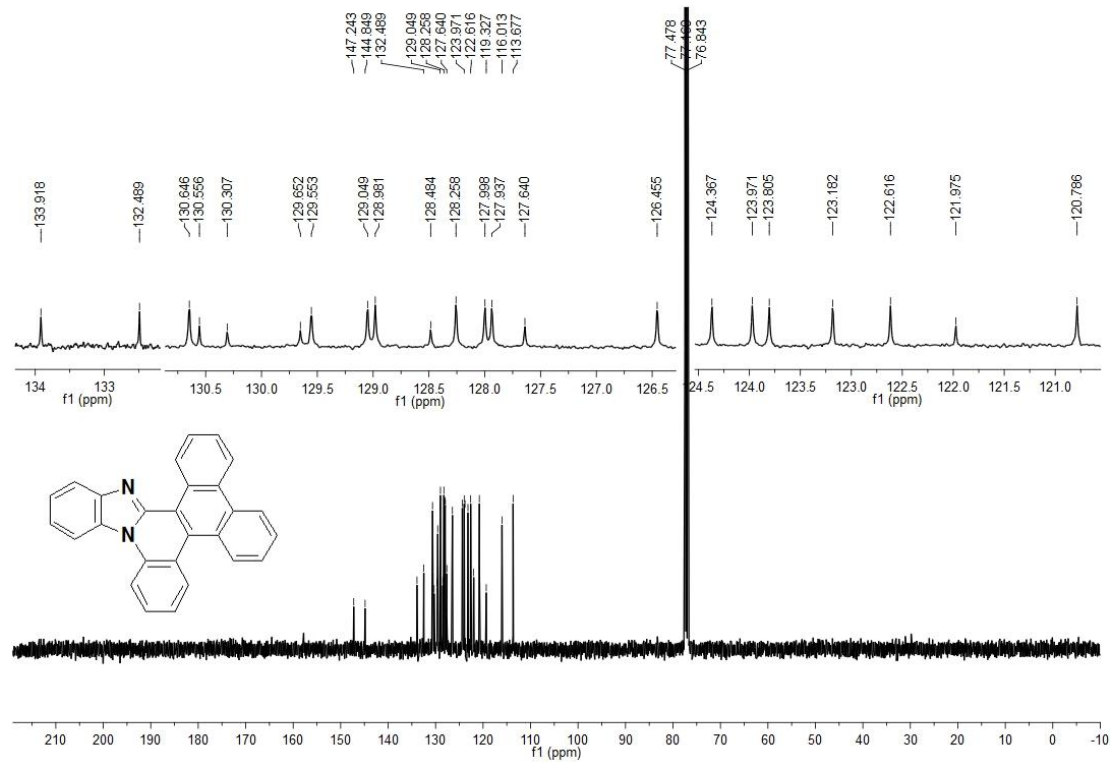

144.724
130.789
127.251
127.106
126.671
125.186
124.925
124.561
124.213
121.132
120.221
118.715
116.444
114.234
113.943
77.478
76.843
134.955
132.018
130.789
130.727
129.932
127.251
127.106
126.671
125.186
124.925
124.561
124.213
121.132
120.221
118.715
116.444
114.234
113.943
f1 (ppm)
N
N
CN

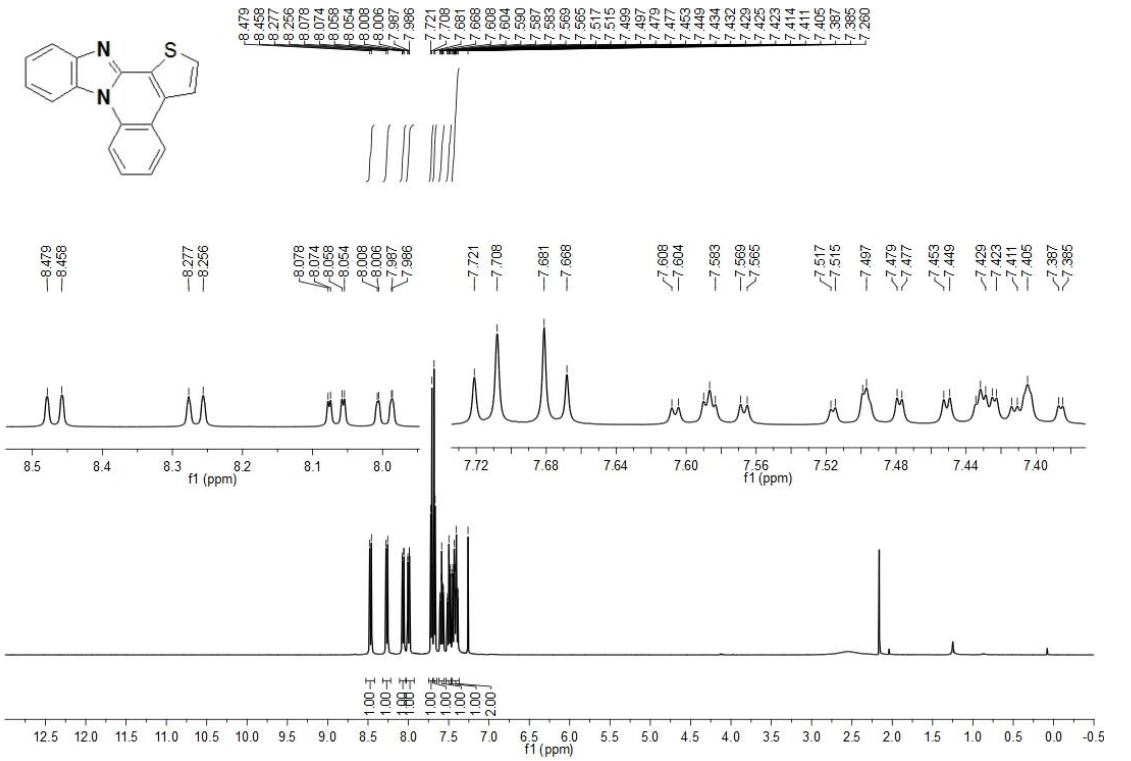

F3C
N
N
8.567
8.547
8.502
8.481
8.385
8.365
8.308
8.288
8.121
8.106
8.089
7.748
7.728
7.708
7.683
7.664
7.644
7.543
7.525
7.507
7.488
7.471
7.453
7.434
7.415
7.260
f1 (ppm)
1.00
1.00
1.00
1.00
1.94
1.00
1.00
1.97
0.98

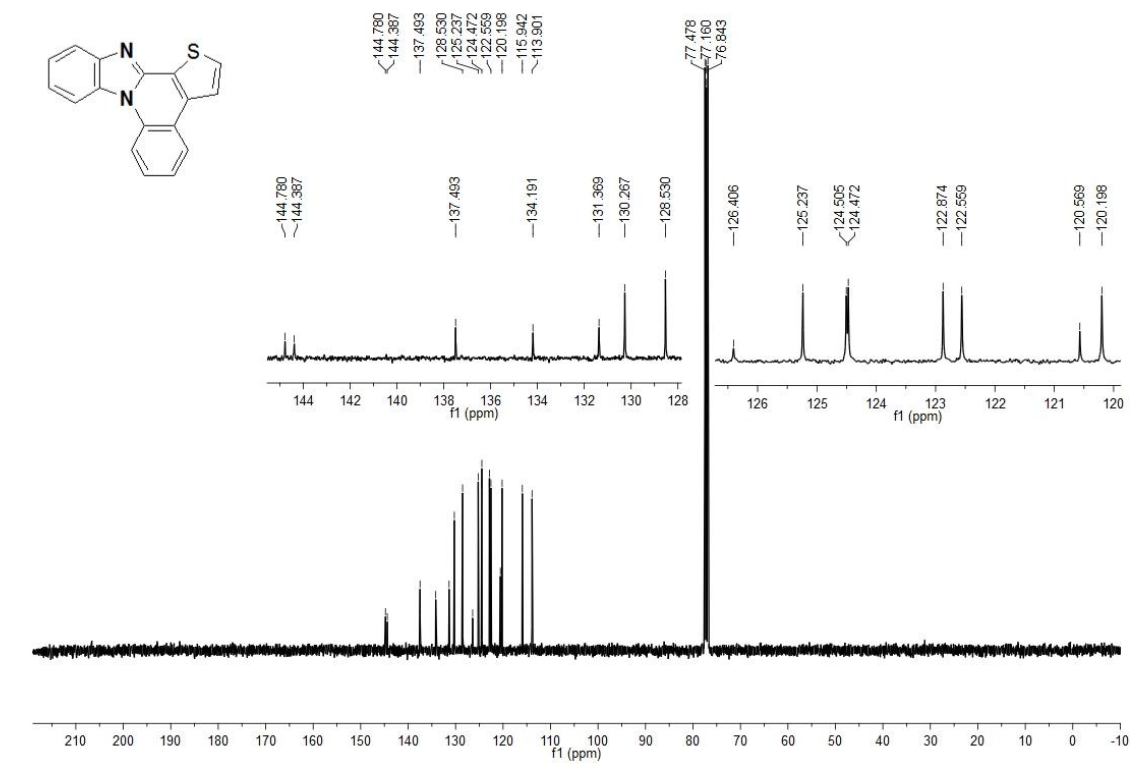

144.524
143.941
130.024
128.368
127.984
124.716
123.902
120.996
115.897
113.801
77.478
77.160
76.843
134.539
131.891
131.166
130.024
129.018
128.443
128.368
128.297
128.222
127.984
126.447
125.618
124.716
124.586
124.271
123.902
121.898
121.724
120.996
F3C
N
N
f1 (ppm)

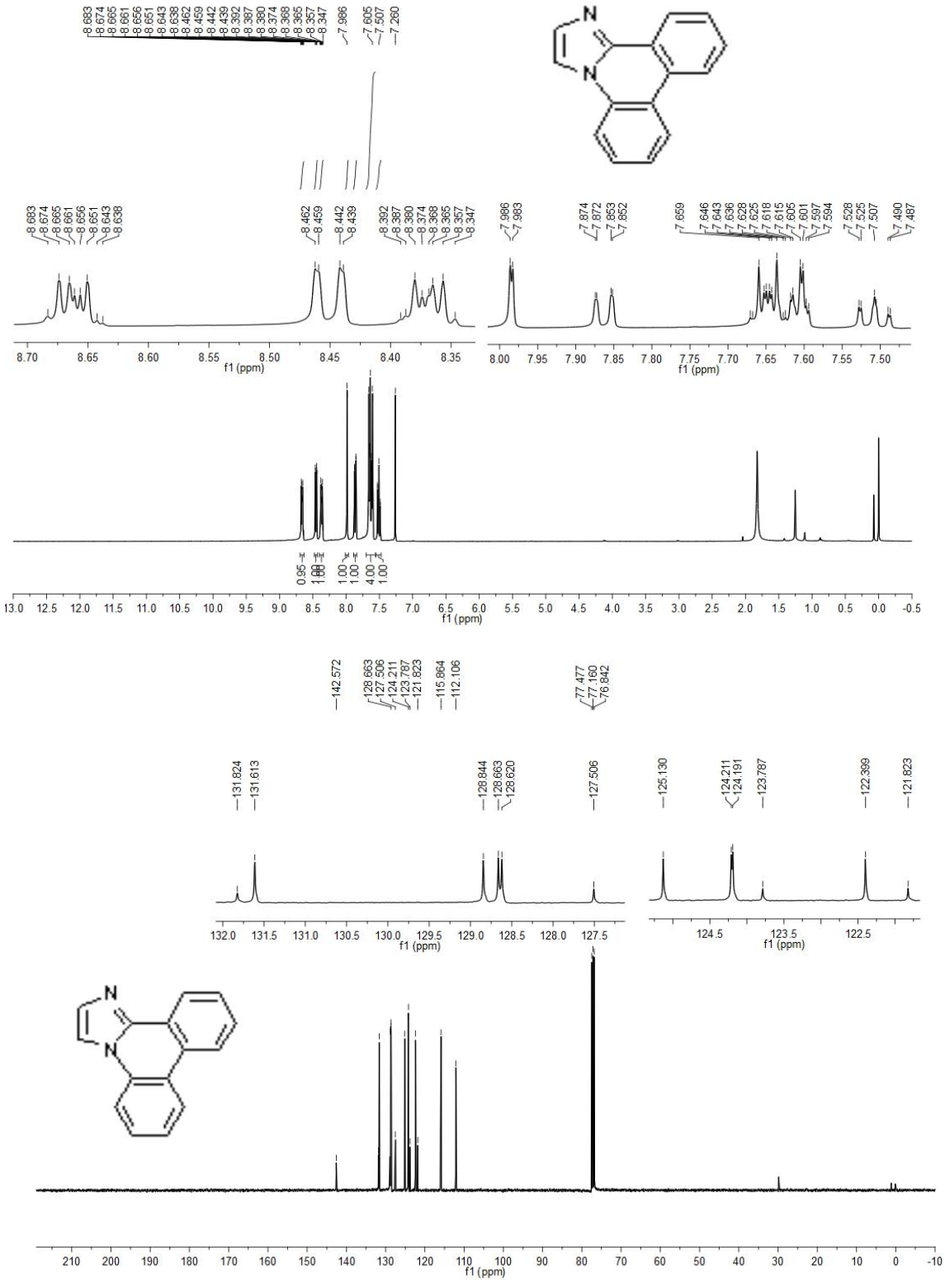

N
N
Ph
8.915
8.895
8.491
8.475
8.287
8.266
8.057
8.037
7.888
7.885
7.867
7.864
7.750
7.731
7.673
7.654
7.634
7.547
7.529
7.510
7.490
7.469
7.445
7.431
7.427
f1 (ppm)
1.00
3.00
1.00
1.00
1.00
2.00
1.00
6.00
147.198
144.073
143.529
140.520
134.536
131.827
129.992
129.447
129.177
128.277
127.956
127.557
126.827
124.702
124.466
124.325
123.219
122.022
121.806
120.809
120.244
77.478
77.160
76.843

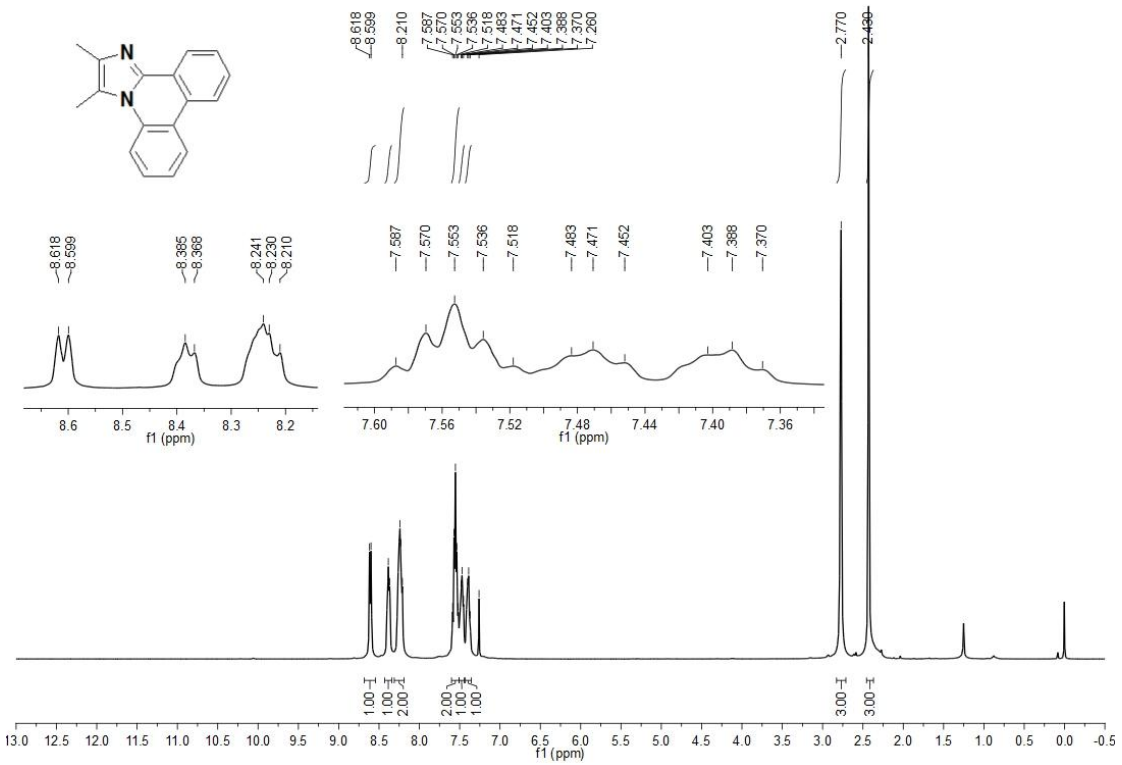

10.556
10.536
8.745
8.626
8.620
8.607
8.428
8.408
8.234
8.215
7.920
7.902
7.884
7.882
7.819
7.817
7.799
7.778
7.757
7.739
7.720
7.718
7.667
7.649
7.630
7.596
7.579
7.559
7.539
7.517
7.498
f1 (ppm)

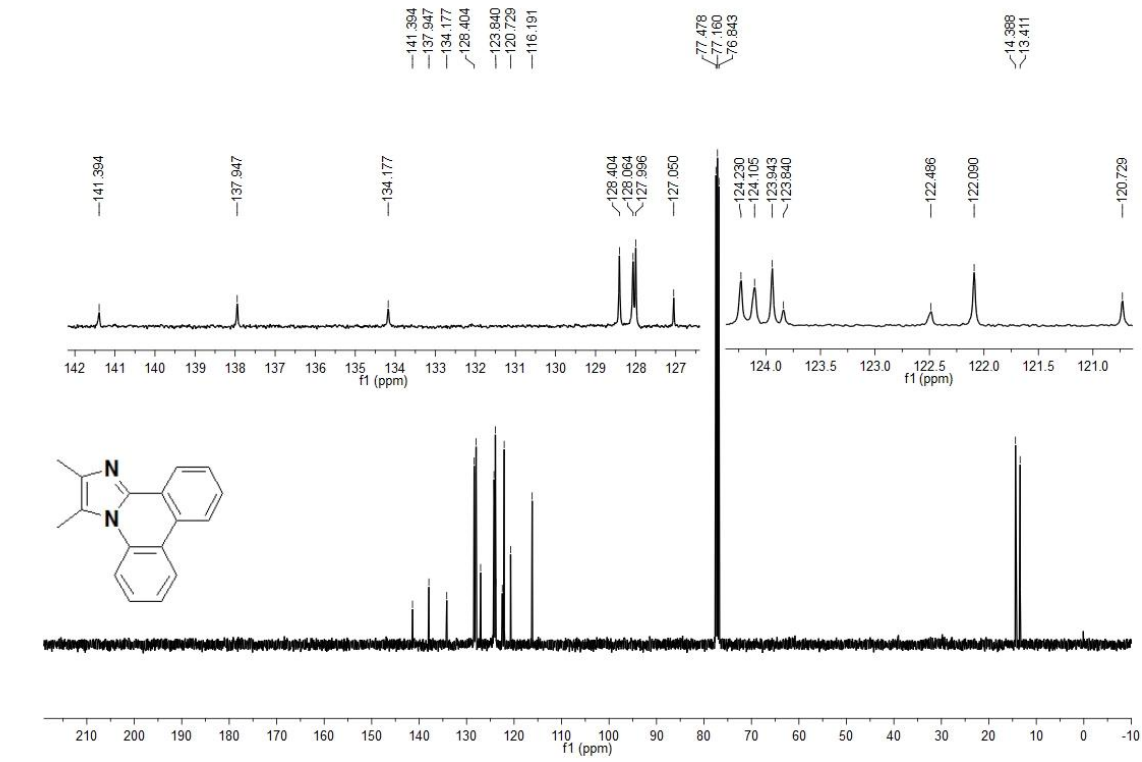

147.243
144.849
132.489
129.049
128.258
127.640
123.971
122.616
119.327
116.013
113.677
77.478
76.843
133.918
132.489
130.646
130.556
130.307
129.652
129.553
129.049
128.981
128.484
128.258
127.998
127.937
127.640
126.455
124.367
123.971
123.805
123.182
122.616
121.975
120.786
f1 (ppm)

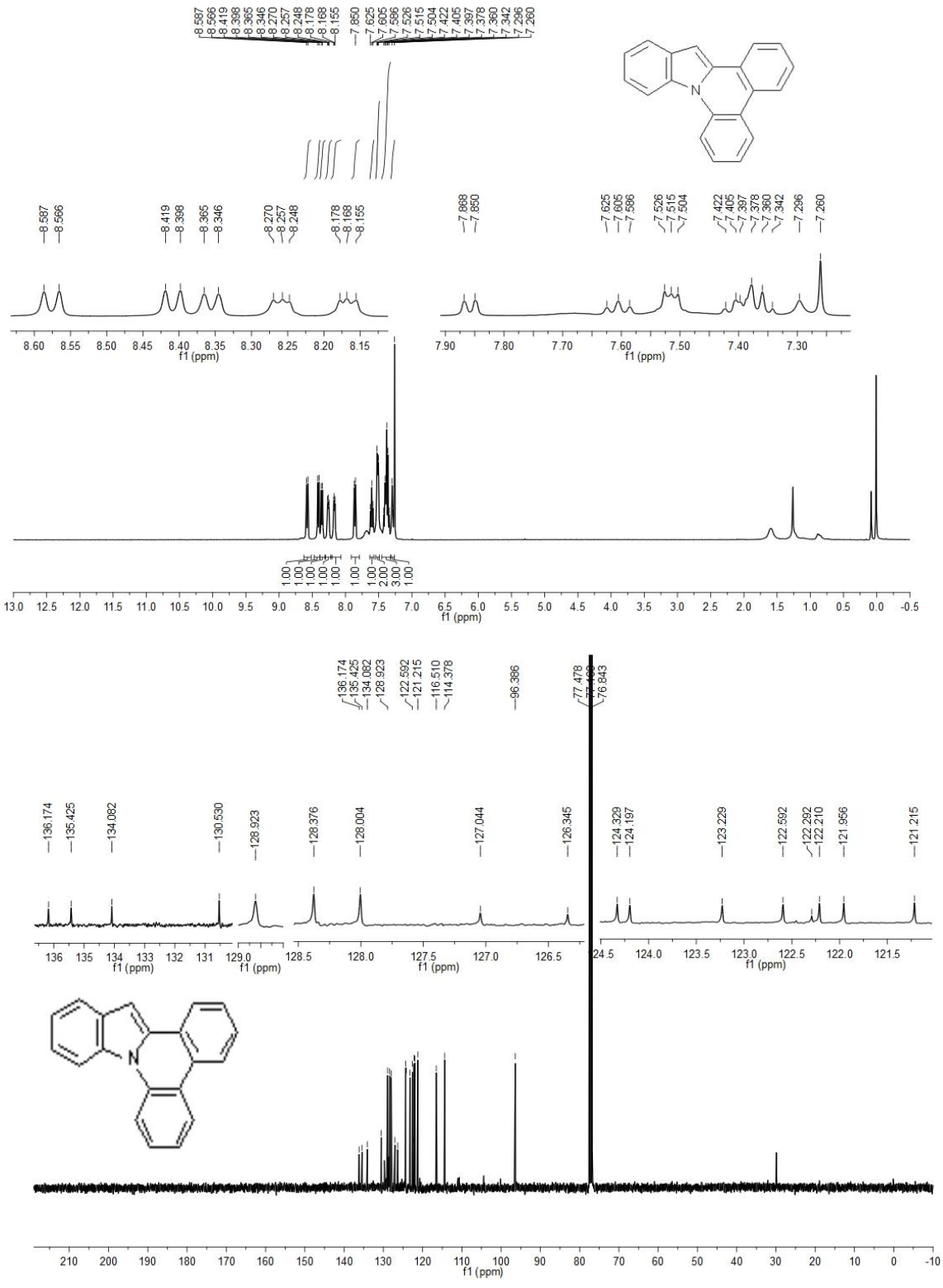

8.479
8.458
8.277
8.256
8.078
8.074
8.058
8.054
8.008
8.006
7.987
7.986
7.721
7.708
7.681
7.668
7.608
7.604
7.583
7.569
7.565
7.517
7.515
7.497
7.479
7.477
7.453
7.449
7.429
7.423
7.411
7.405
7.387
7.385
f1 (ppm)

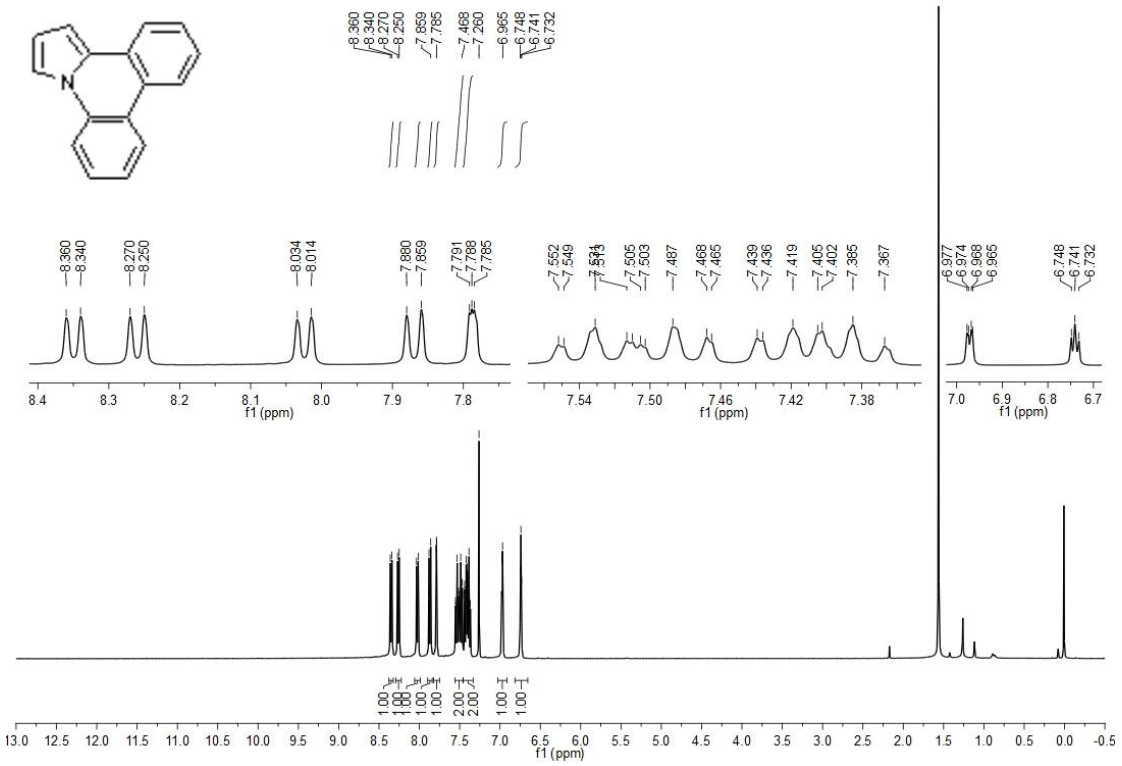

144.780
144.387
137.493
128.530
125.237
124.472
122.559
120.198
115.942
113.901
77.478
77.160
76.843
134.191
131.369
130.267
126.406
f1 (ppm)

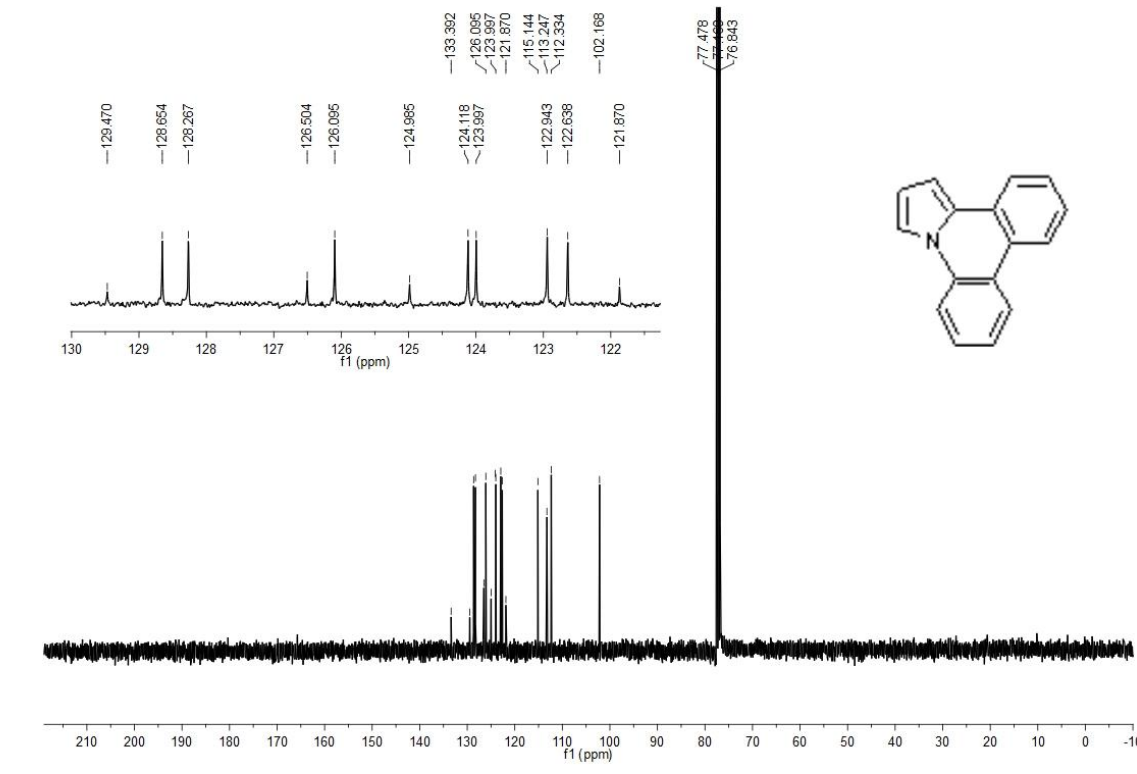



8.618
8.599
8.210
7.587
7.570
7.553
7.536
7.518
7.483
7.471
7.452
7.403
7.388
7.370
7.260
2.770
2.439
f1 (ppm)


141.394
137.947
134.177
128.404
123.840
120.729
116.191
77.478
77.160
76.843
14.388
13.411
128.064
127.996
127.050
124.230
124.105
123.943
123.840
122.486
122.090
f1 (ppm)




8.360
8.340
8.270
8.250
7.859
7.785
7.468
7.260
6.965
6.748
6.741
6.732
8.034
8.014
7.880
7.791
7.788
7.785
7.552
7.549
7.505
7.503
7.487
7.468
7.465
7.439
7.436
7.419
7.405
7.402
7.385
7.367
6.977
6.974
6.968
6.965
f1 (ppm)


133.392
126.095
123.997
121.870
115.144
113.247
112.334
102.168
77.478
77.160
76.843
129.470
128.654
128.267
126.504
126.095
124.985
124.118
123.997
122.943
122.638
121.870
f1 (ppm)