Supplementary information

Dithienopyrrolobenzothiadiazole-Based Organic Dyes for Efficient Dye-Sensitized Solar Cells

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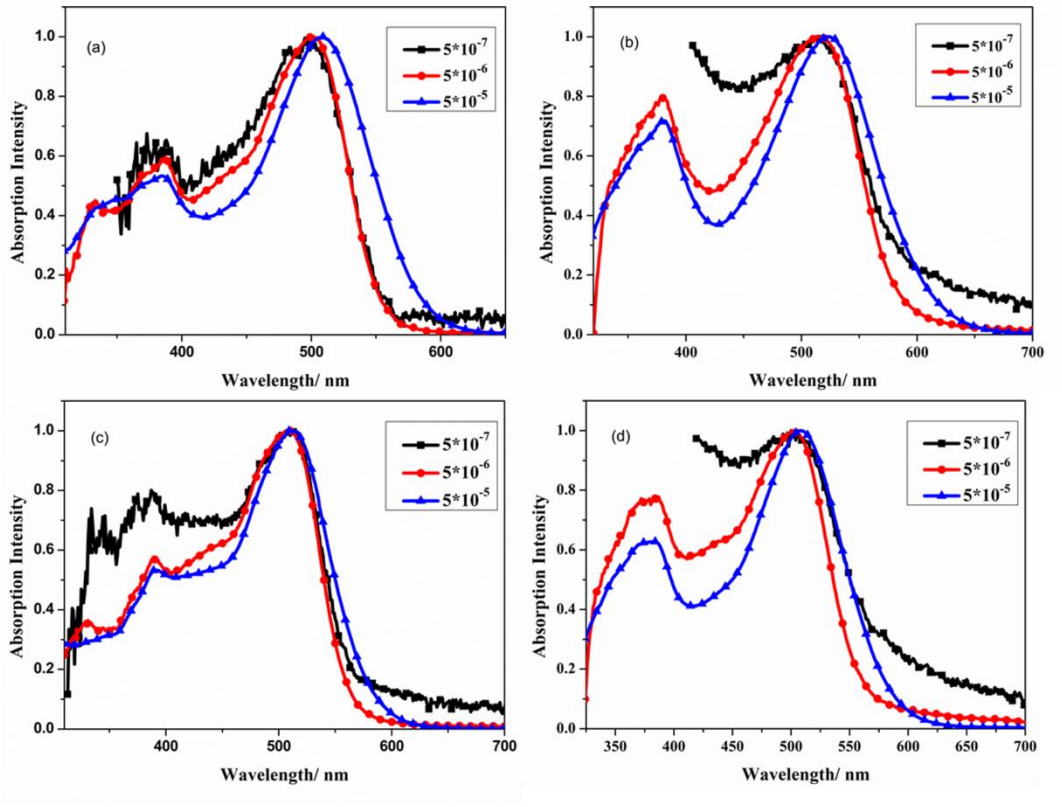

Figure S1. The absorption spectra of (a) **DTP1**, (b) **DTP2**, (c) **DTP3** and (d) **DTP4** in the solution with the concentration from 5×10^{-7} M to 5×10^{-5} M.

Computational detials:

The vertical excitation energies were calculated by TDDFT at MPW1K/6-31G** levels.[1] because the similar permittivity of acetone to DCM/MeOH (1/1), we selected acetone to consider the solvent effect. The solvent effect was simulated by the conductor-like polarizable continuum model (C-PCM).[2] All the calculations were carried out with the Gaussian 09 program package.

Table S1. Calculated TDDFT Wavelengths, Excitation energies (eV), Oscillator Strengths (*f*) and Composition in terms of Molecular Orbital Contributions of the dyes **DTP1-4**.

Dye	Wavelength	*E* (eV)	Composition [a]	*f*
DTP1	511.1	2.43	H→L: 77.7%, H-1→L: 15.8%	1.8270
	393.0	3.15	H-1→L: 9.8%, H-1→L+1: 16.9%, H→L+1：66.7%	0.1091
DTP2	549.8	2.25	H→L:76.8%, H-1→L: 14.6%	2.0428
	356.2	3.48	H-2→L:31.2%, H→L+2：39.3%	0.5189
DTP3	524.3	2.36	H→L:73.3%, H-1→L: 17.2%	2.2818
	378.0	3.28	H-1→L:9.7%, H→L:10.4%, H→L+2:68.7%	0.6832
DTP4	516.1	2.40	H→L:80.9%, H-1→L:12.6	1.8848
	361.1	3.43	H-2→L:88.4%	0.1928

[a] H = HOMO, L = LUMO, H-1 = HOMO-1, H-2 = HOMO-2, L = LUMO, L+1 = LUMO+1, L+2 = LUMO+2

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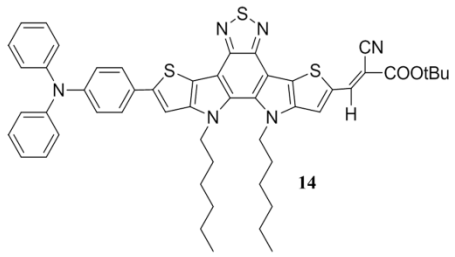
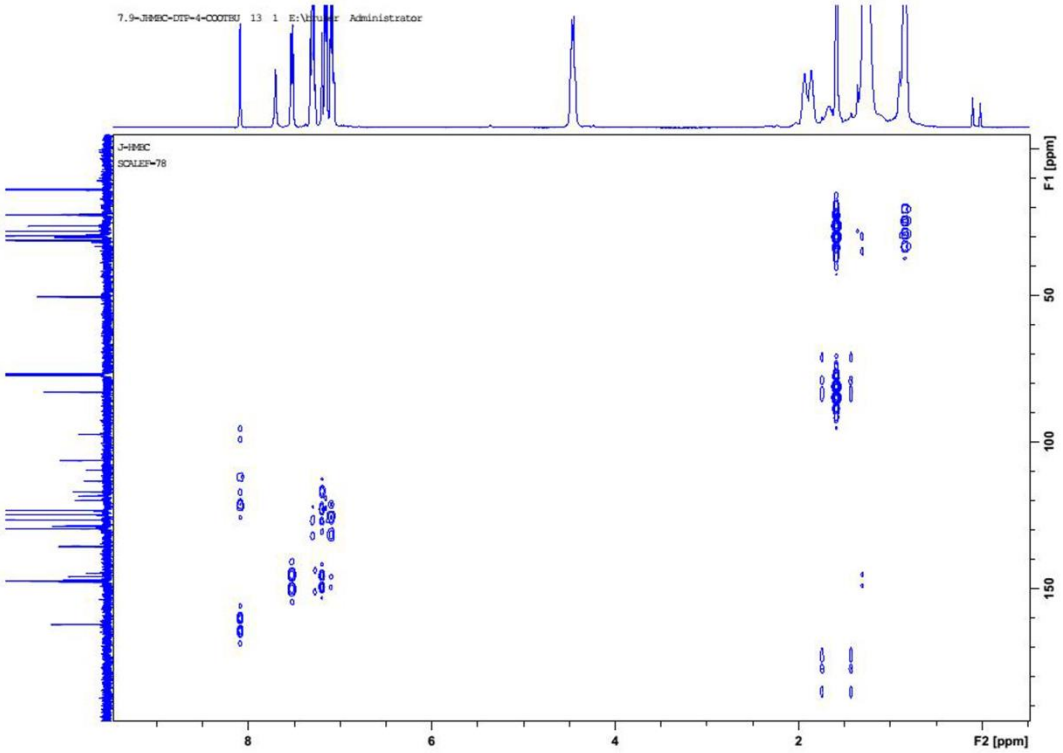


14

J-HMBC:

δ (H_3) = 8.08 ppm
δ (C_1) = 162.2 ppm
$^3J_{CH}$ = 5.5Hz



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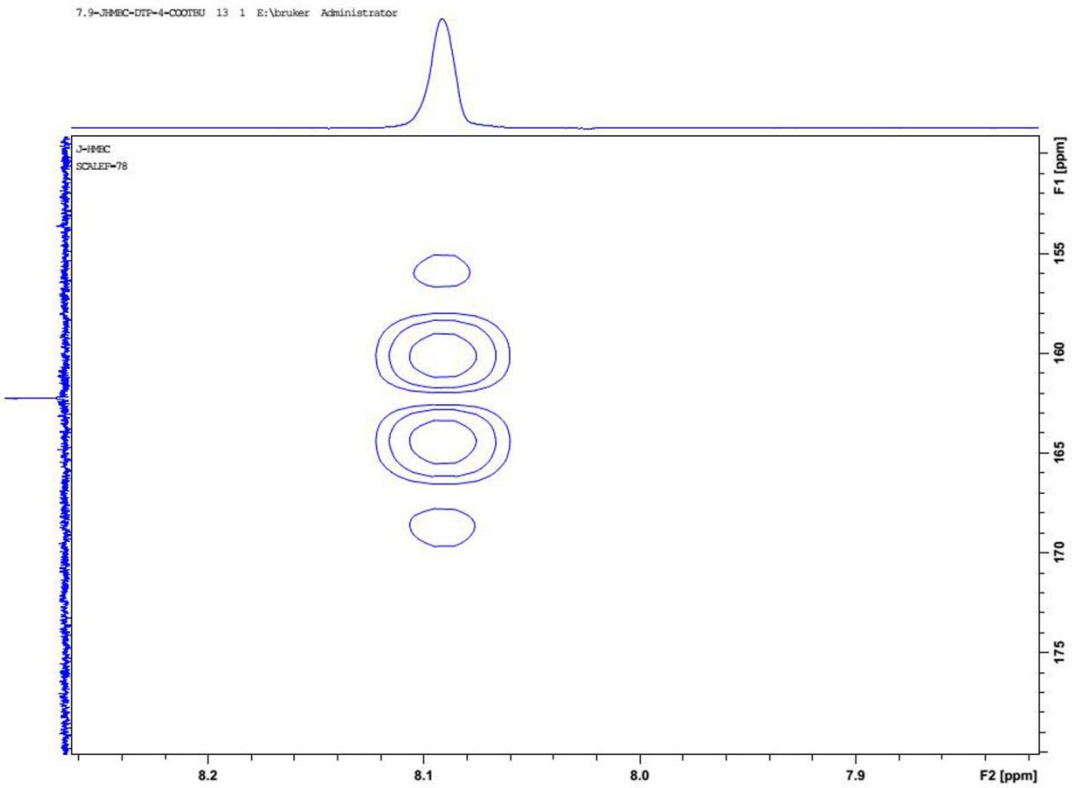

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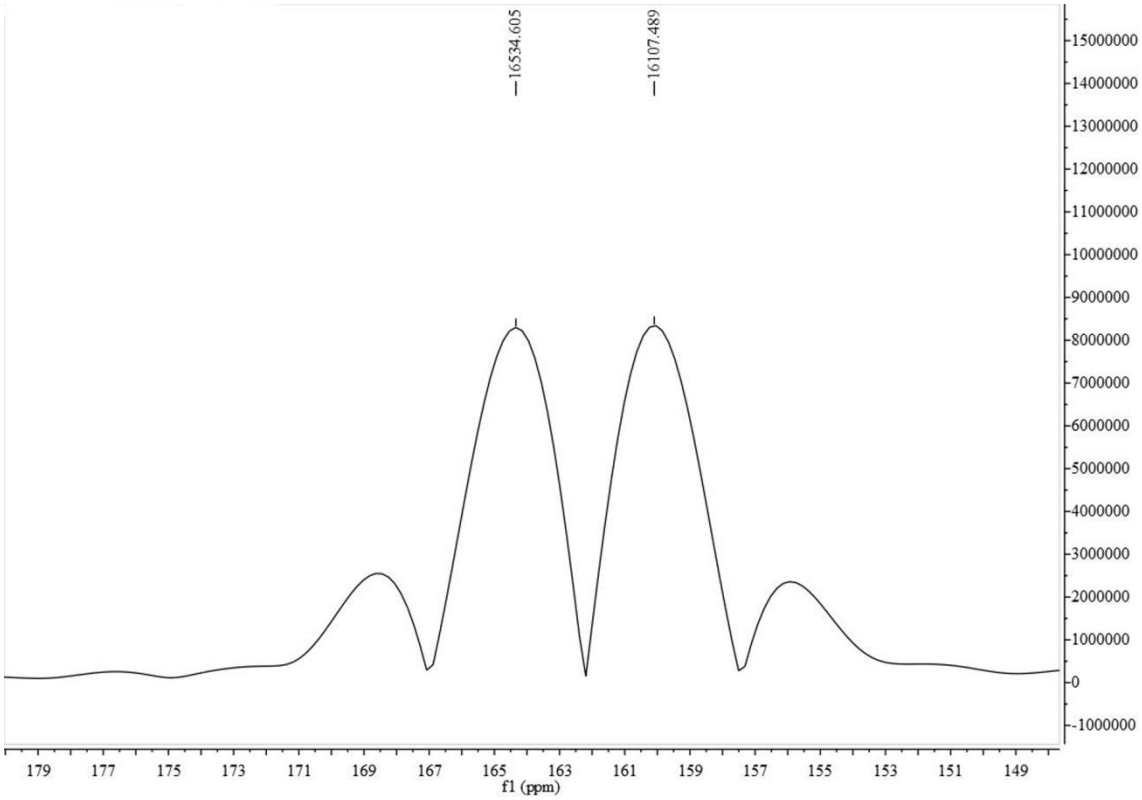

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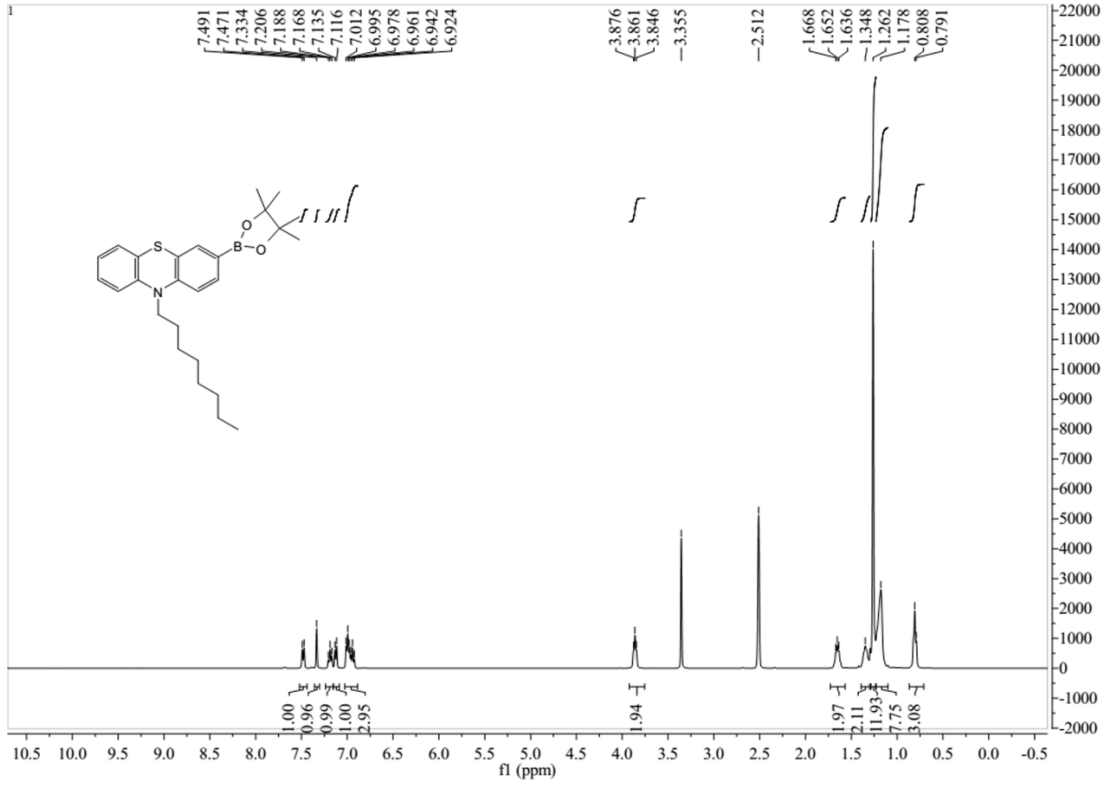
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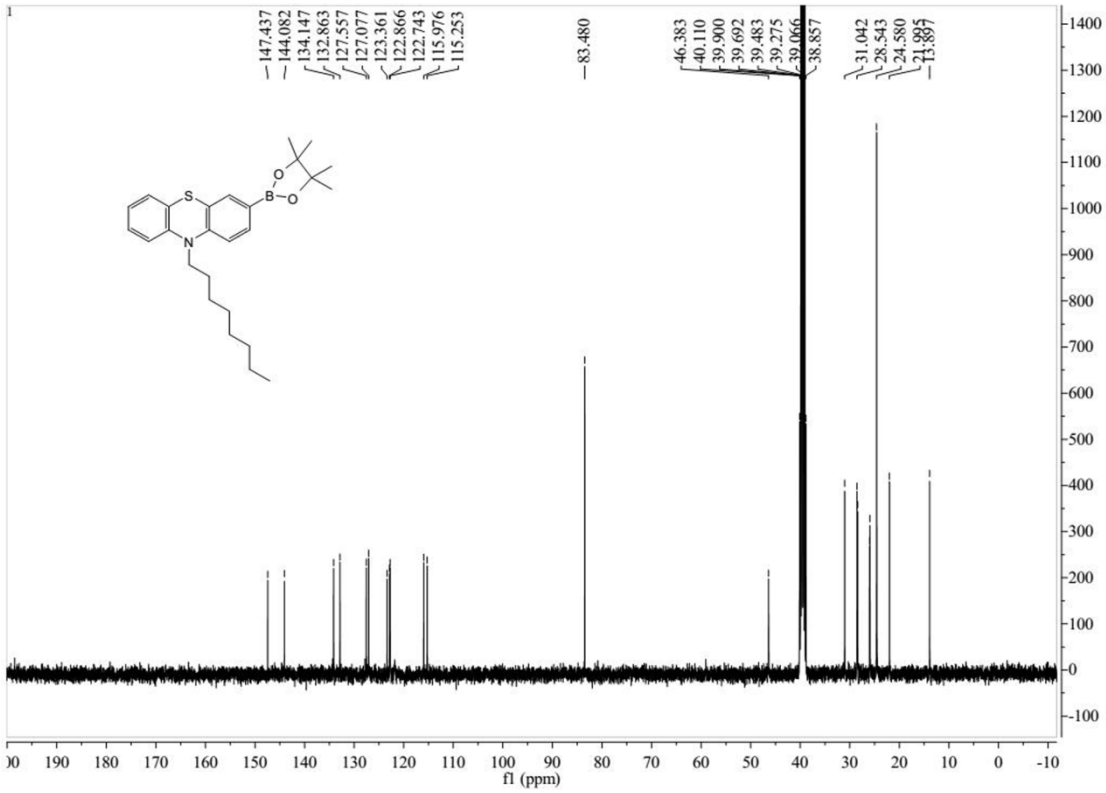
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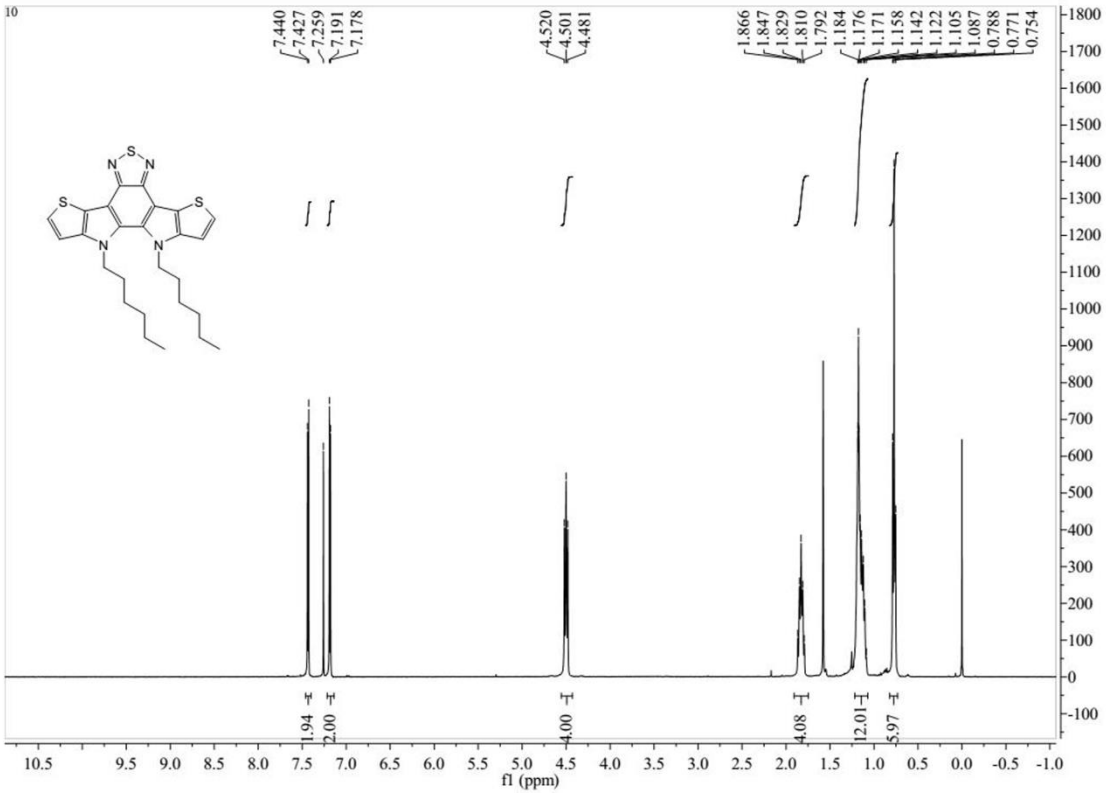
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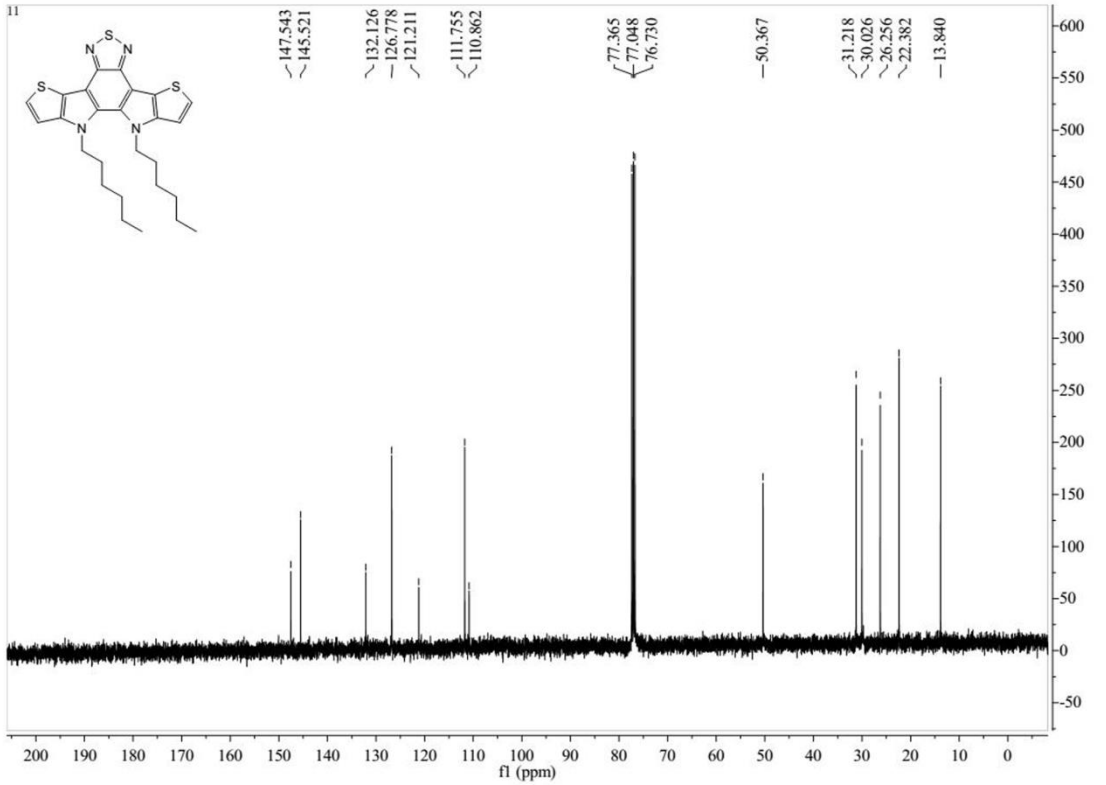
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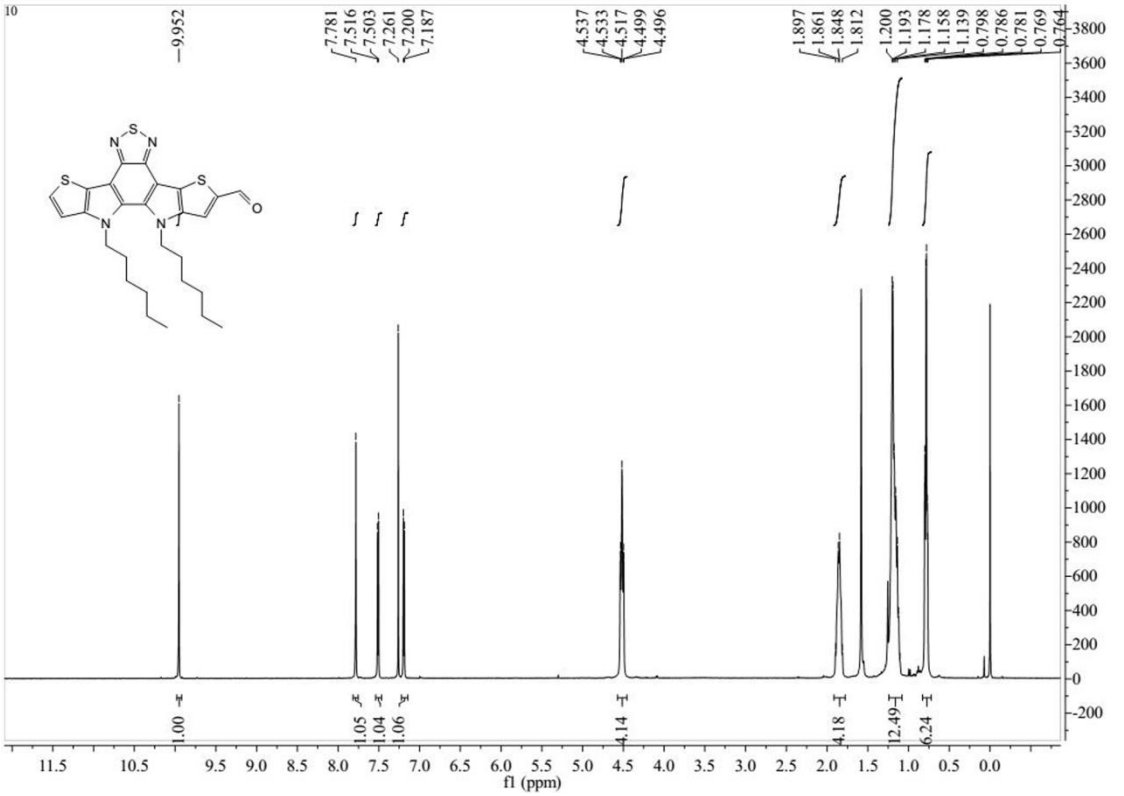
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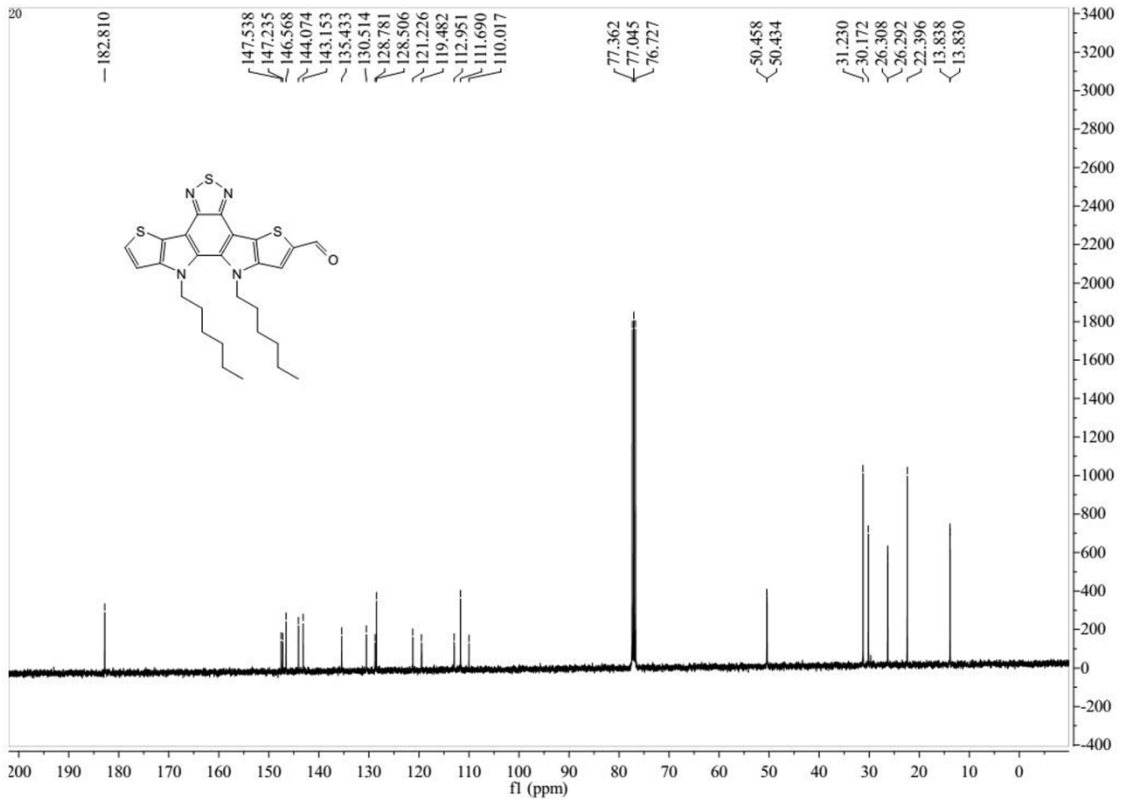
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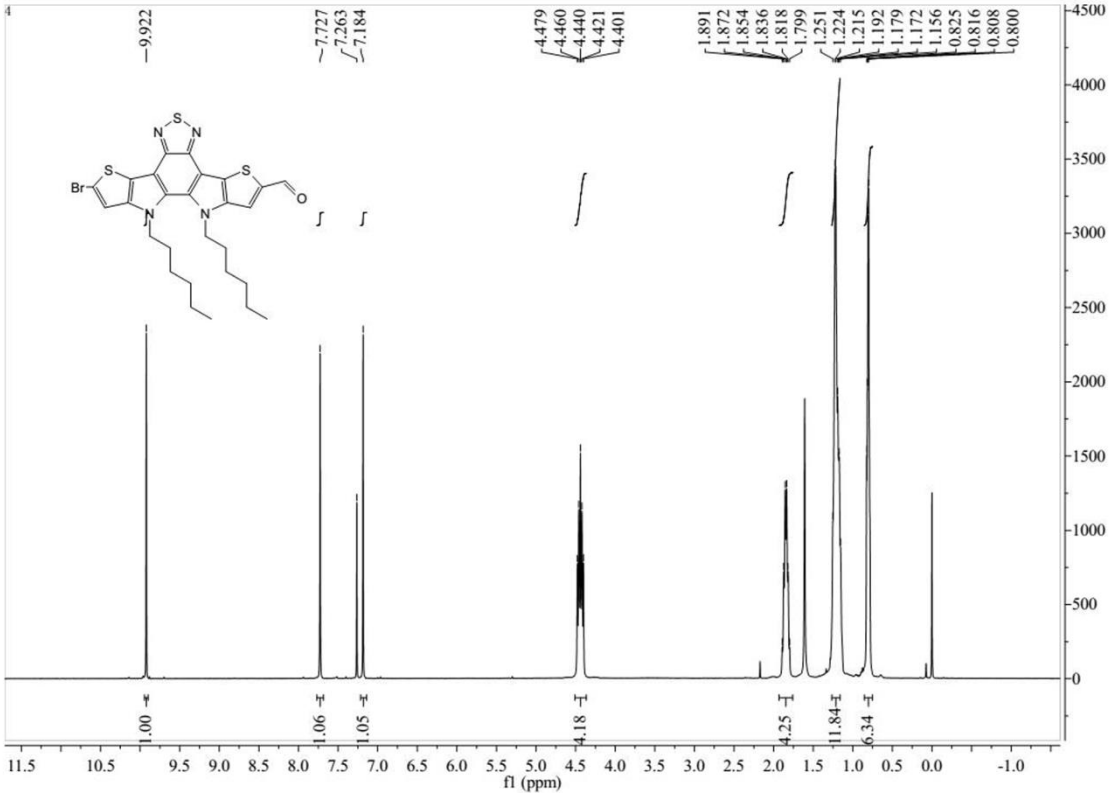
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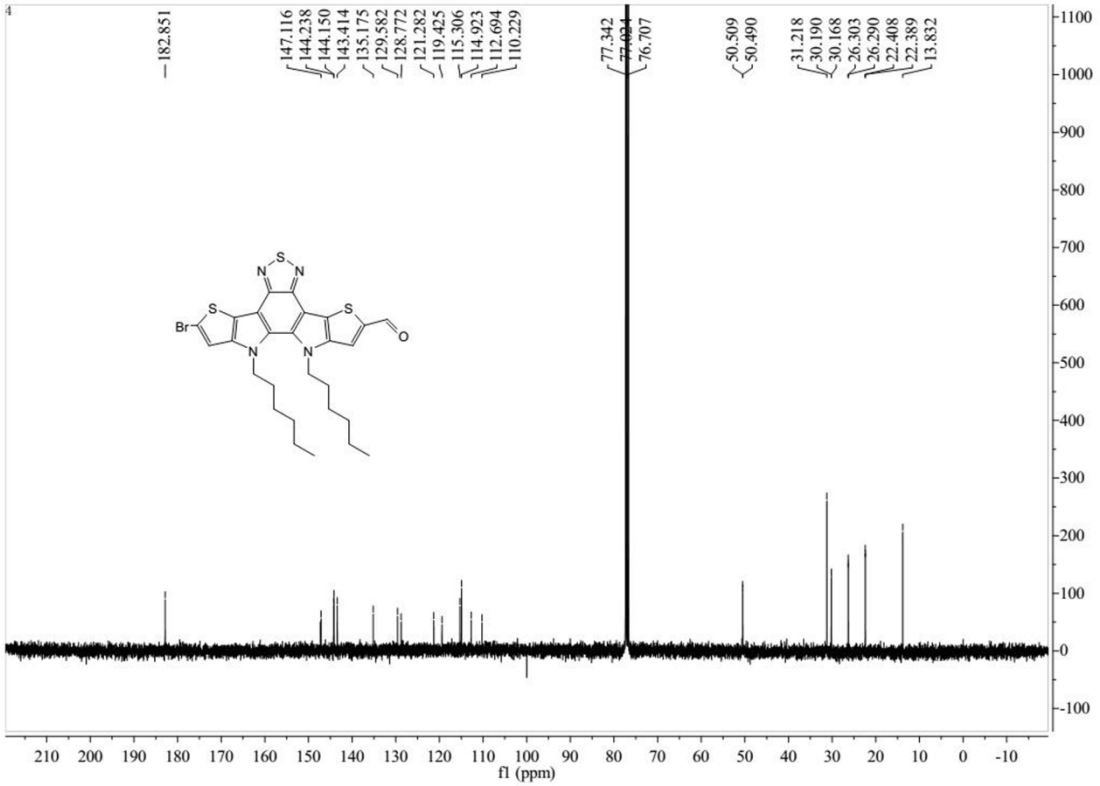
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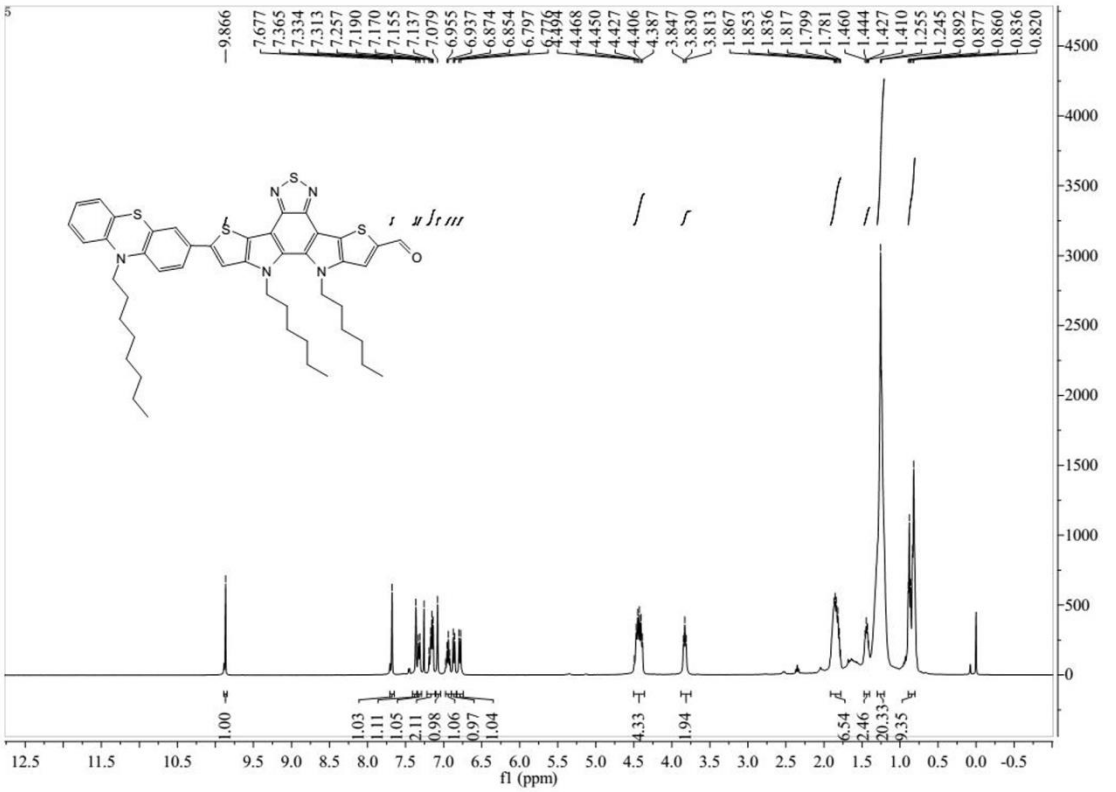
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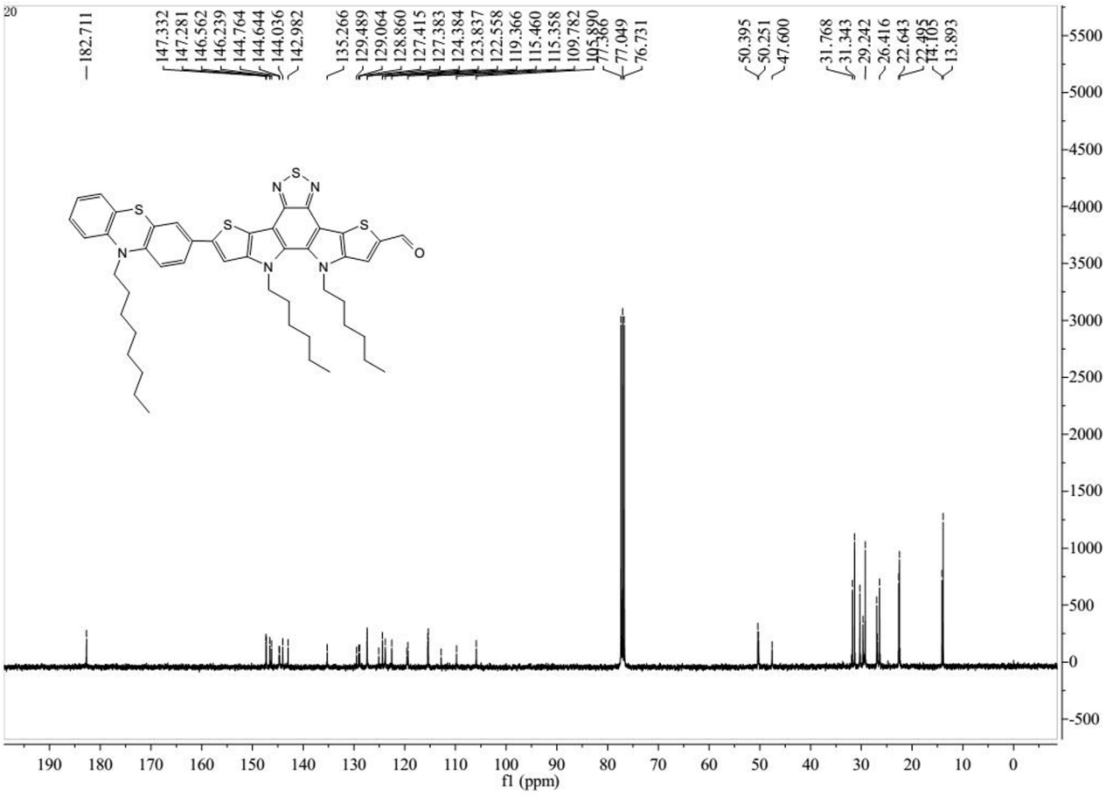
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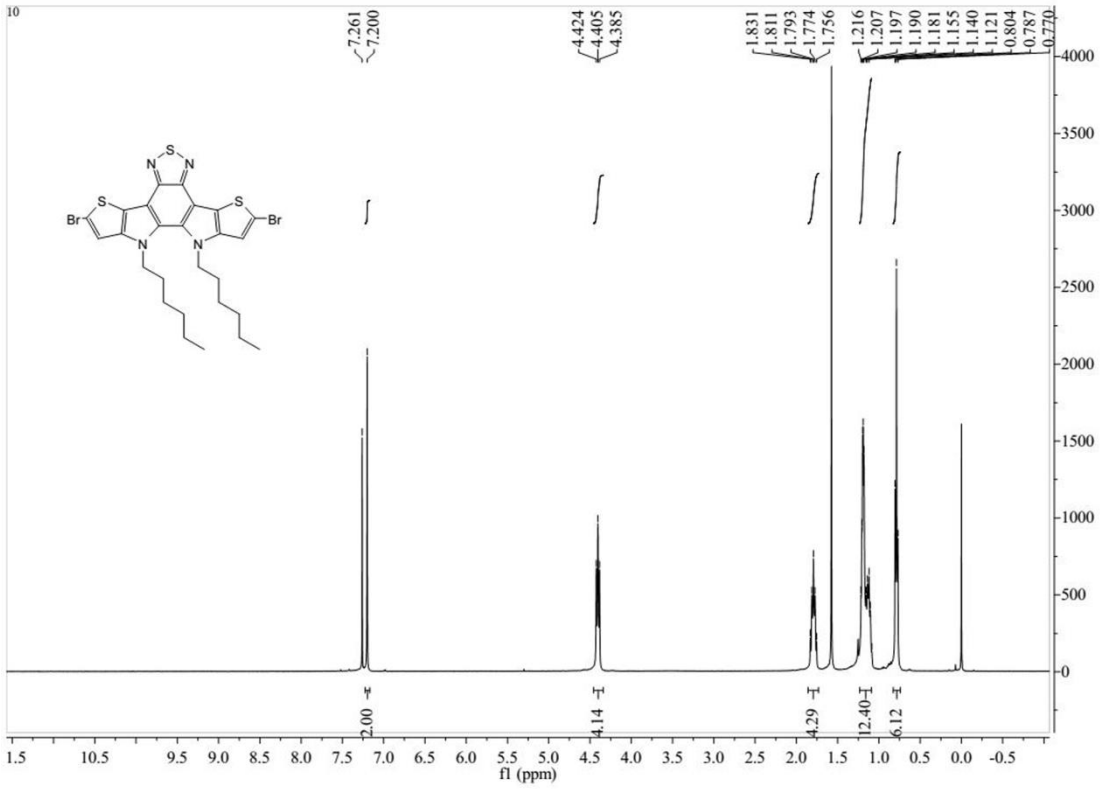
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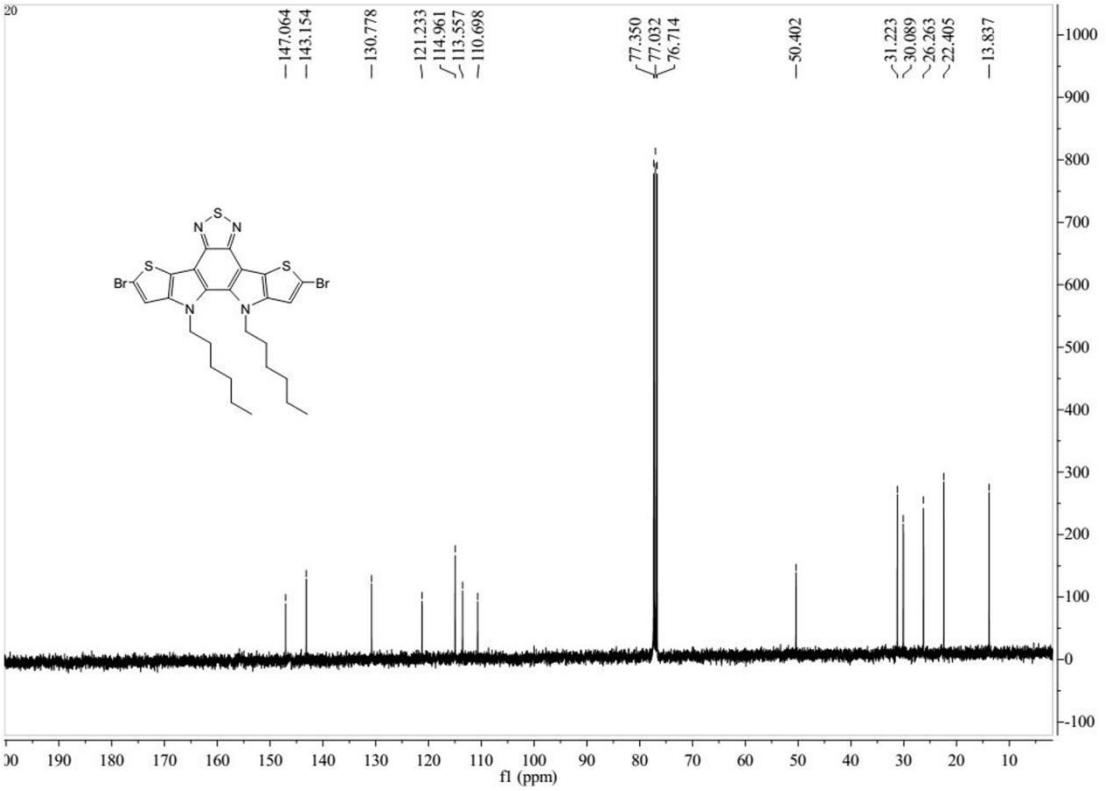
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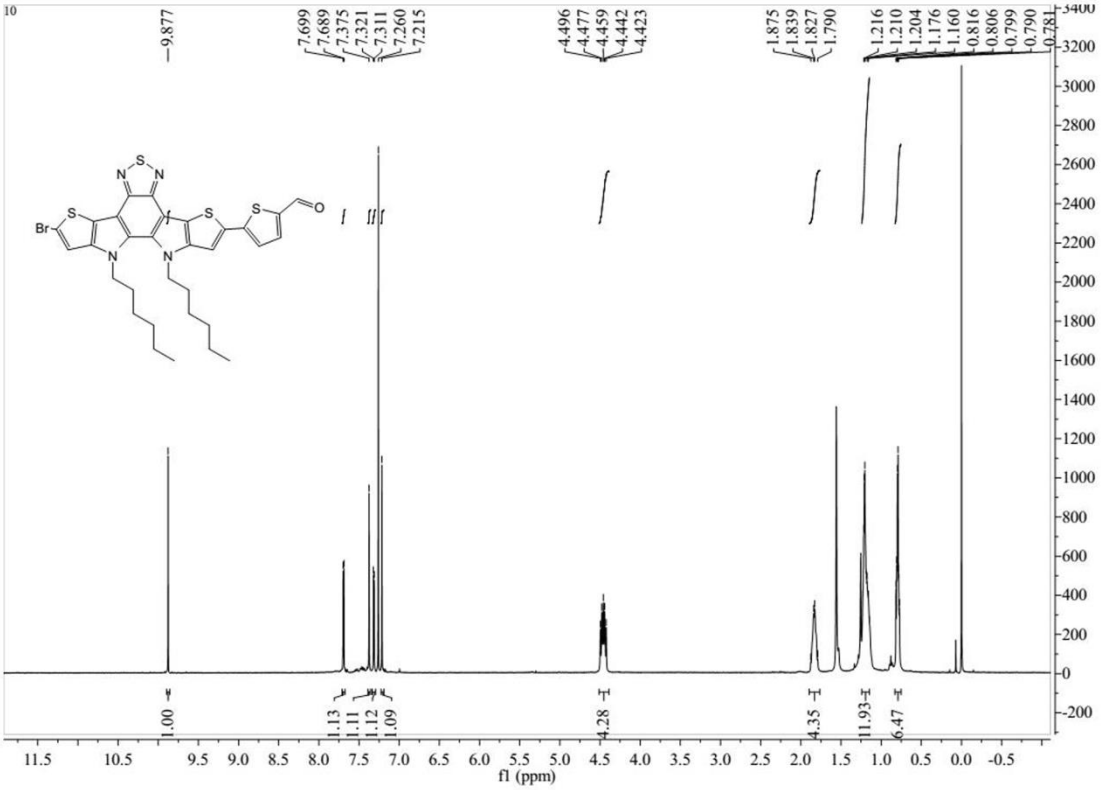
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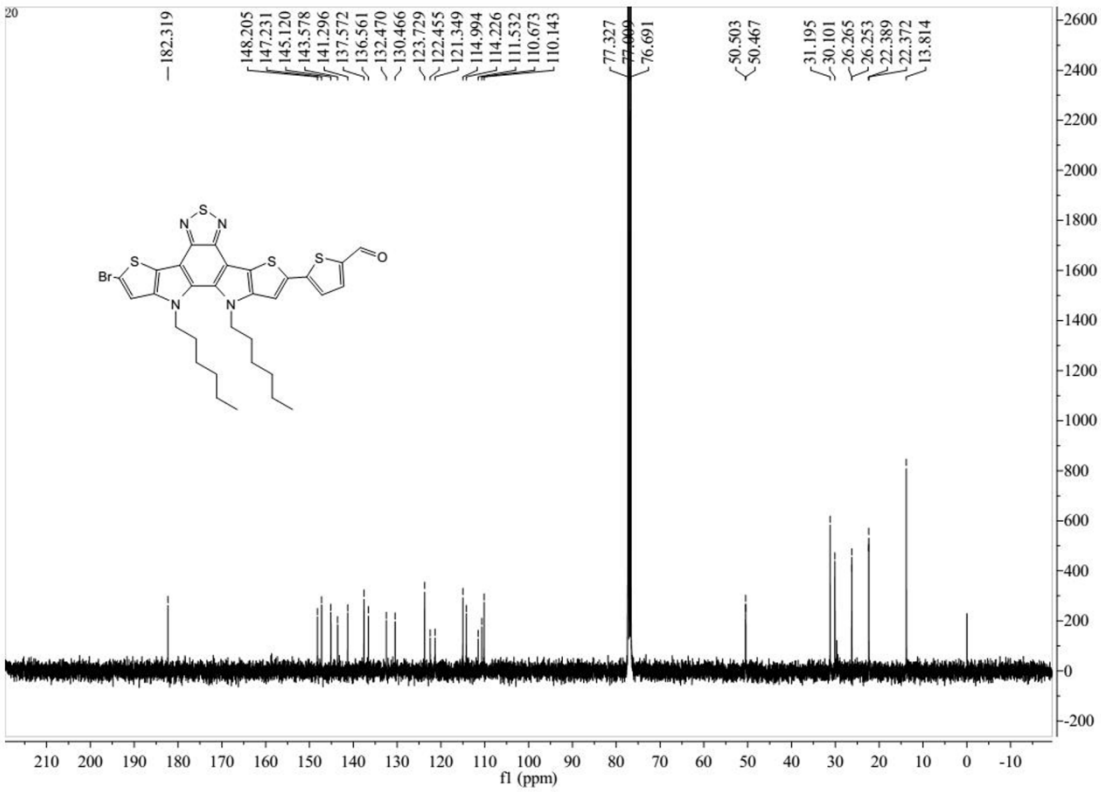
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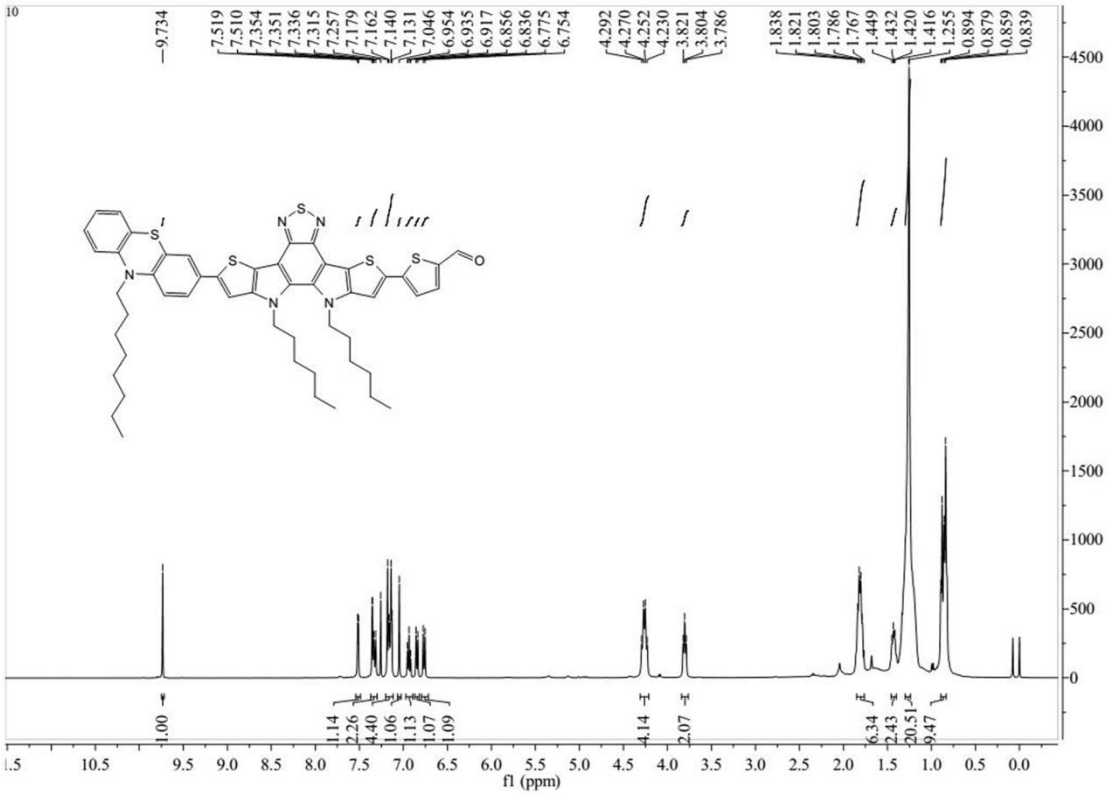
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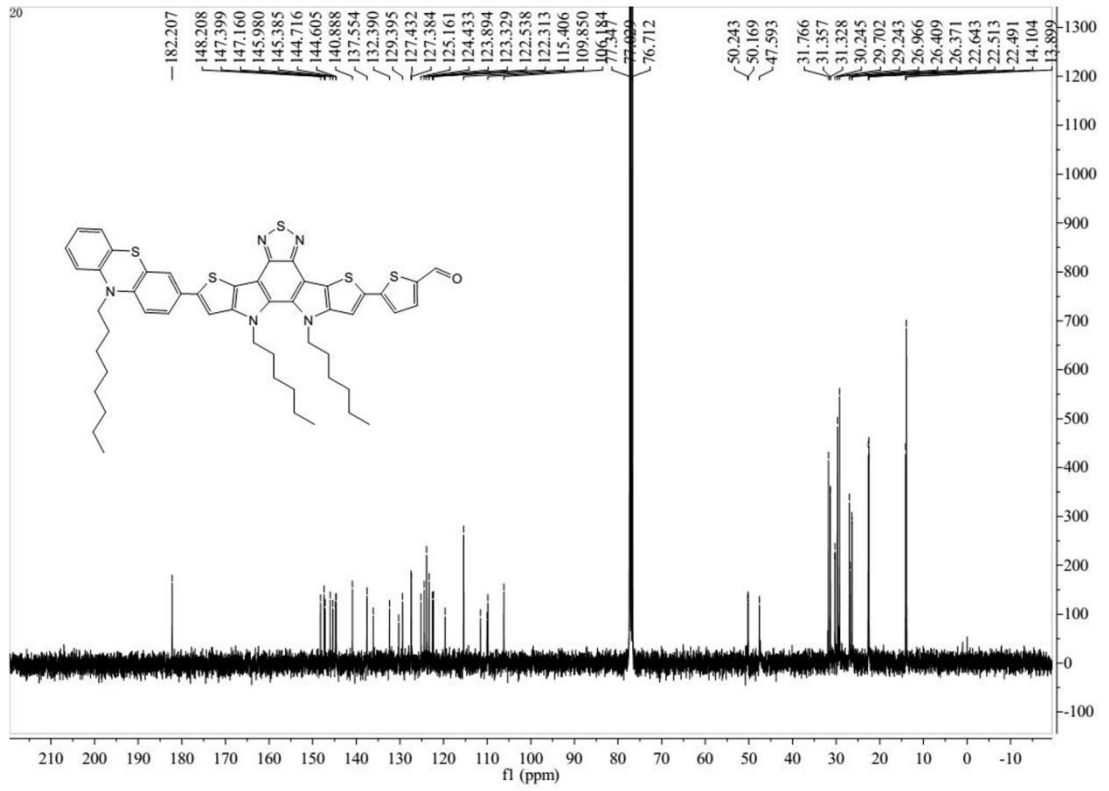
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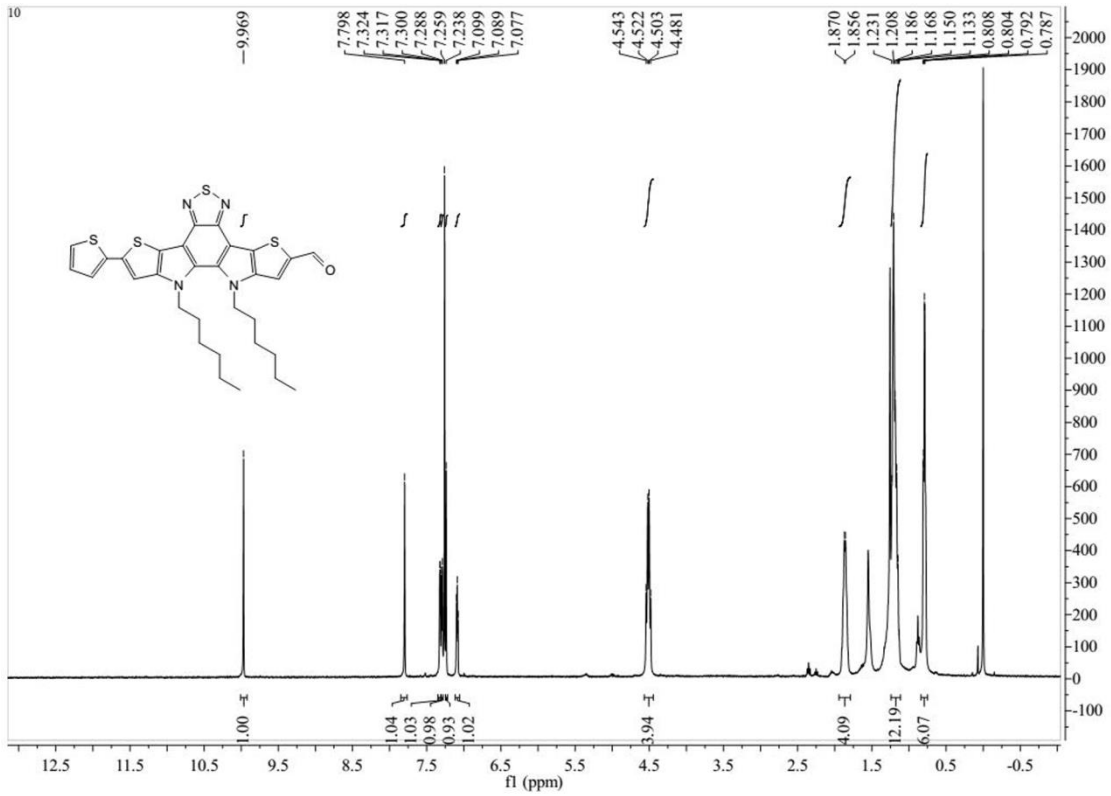
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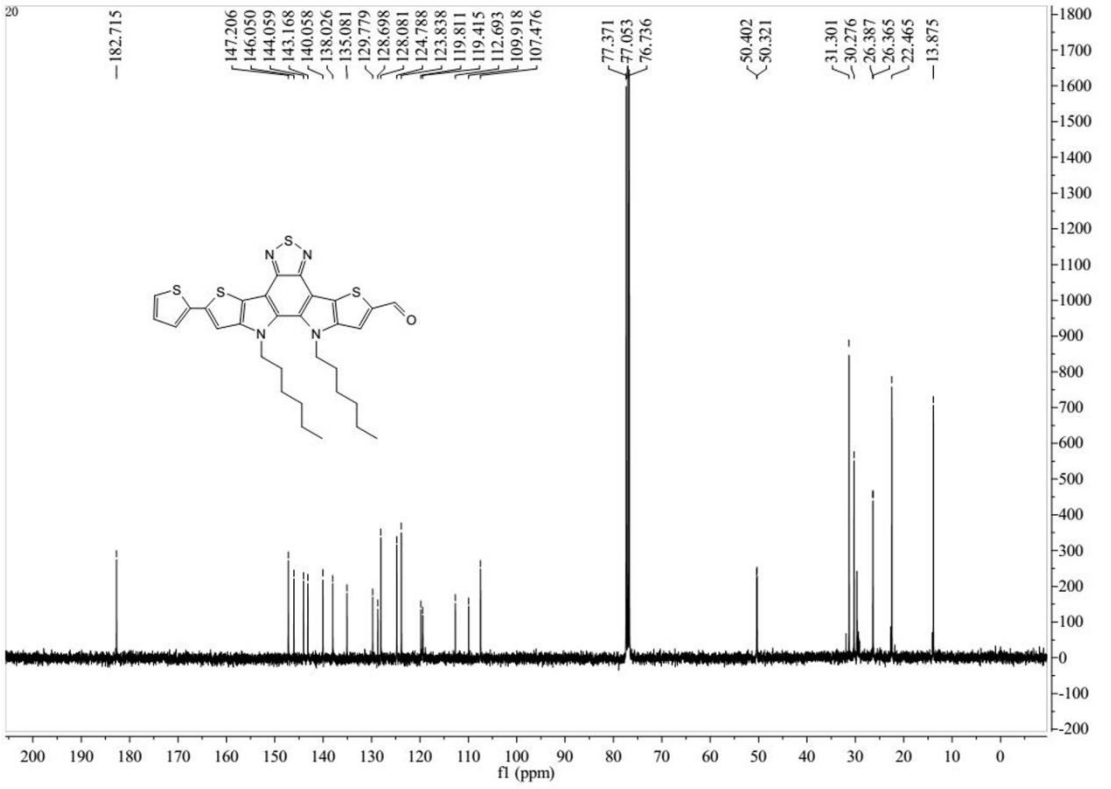
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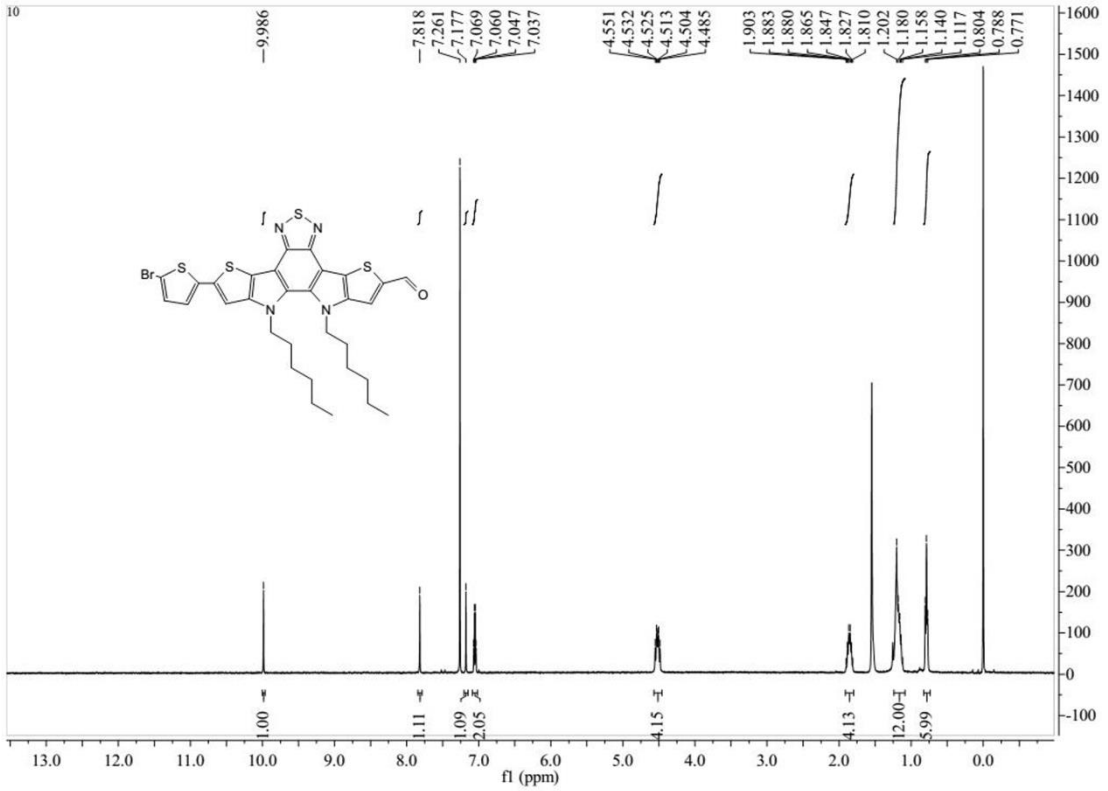
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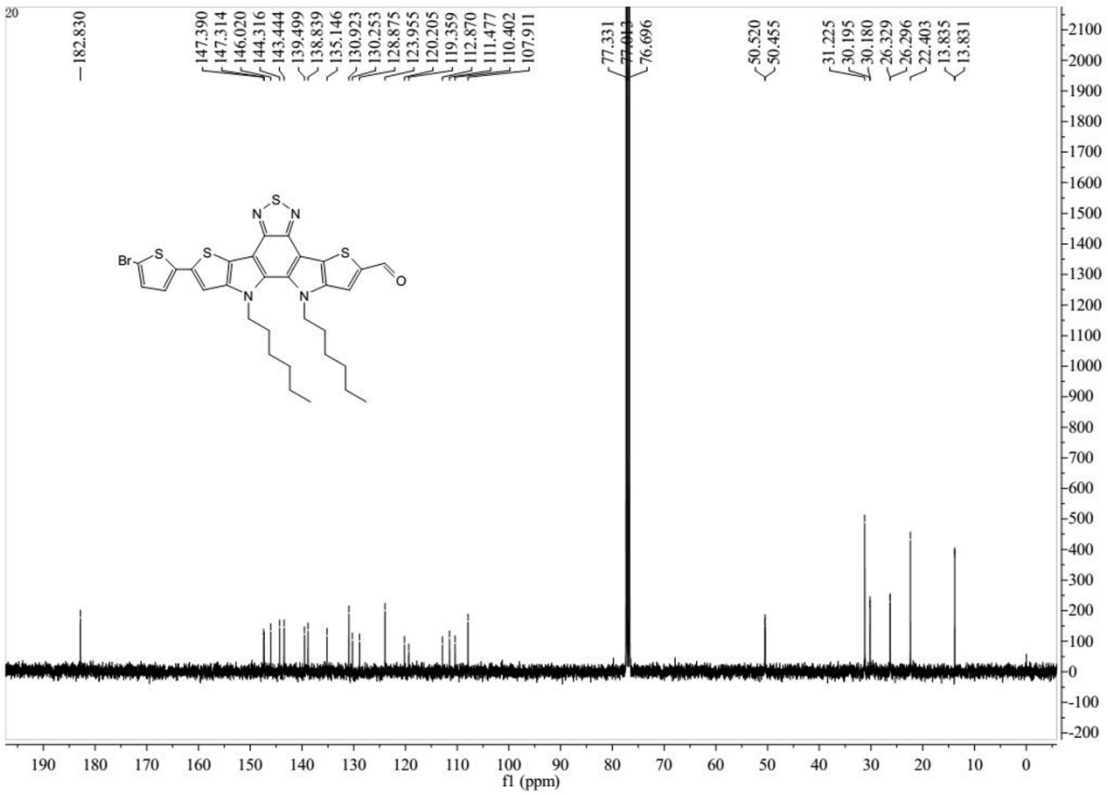
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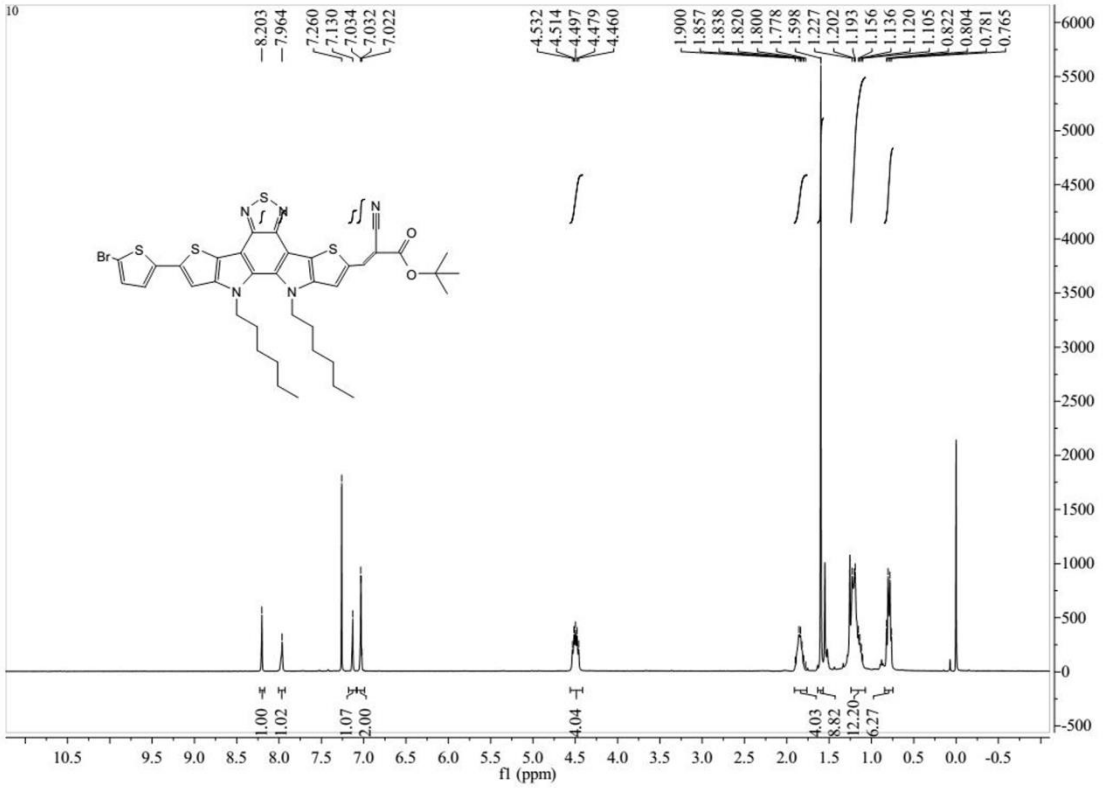
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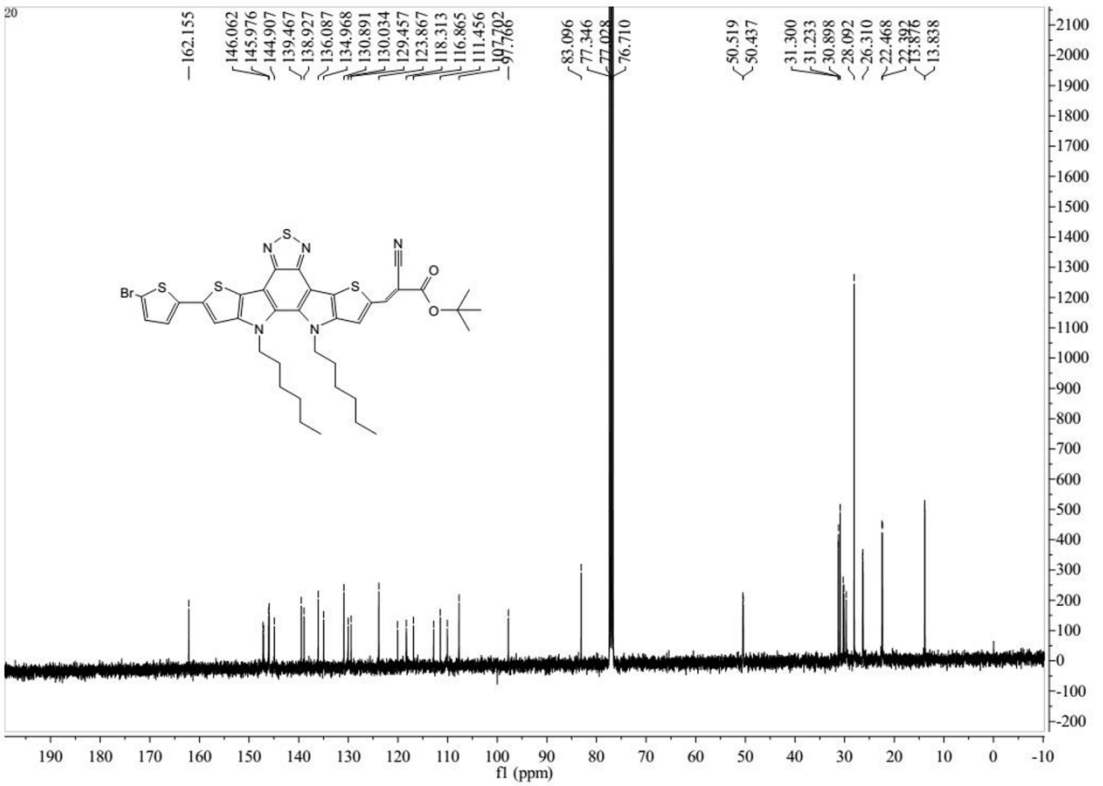
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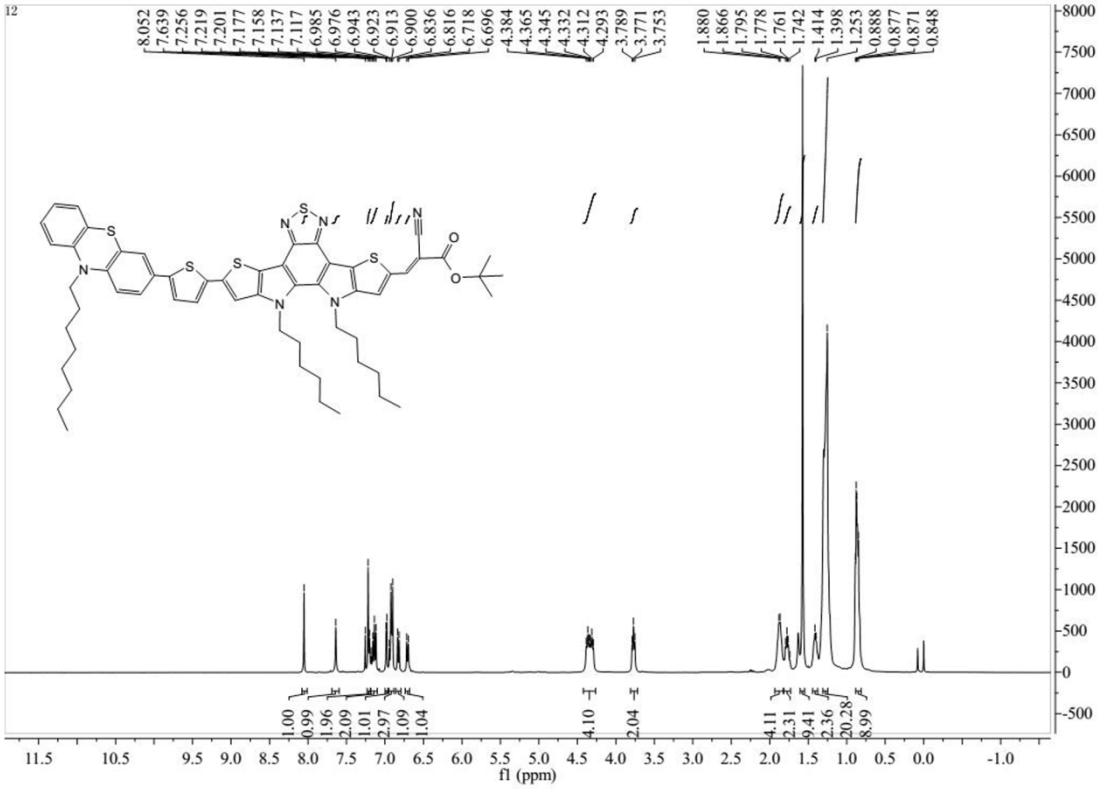
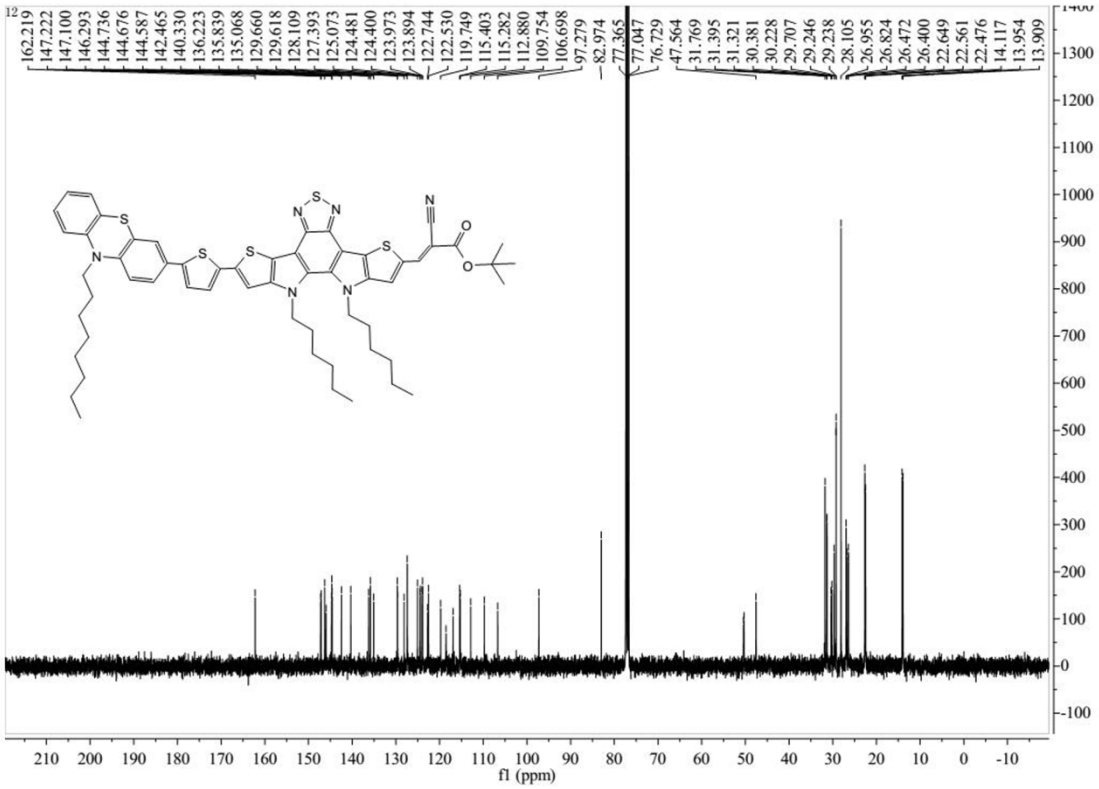
145.976
144.907
139.467
138.927
136.087
134.968
130.891
130.034
129.457
123.867
118.313
116.865
111.456
107.702
97.768
83.096
77.346
77.028
76.710
50.519
50.437
31.300
31.233
30.898
28.092
26.310
22.468
22.392
13.876
13.838
Br
S
N
O
f1 (ppm)


12
8.052
7.639
7.256
7.219
7.201
7.177
7.158
7.137
7.117
6.985
6.976
6.943
6.923
6.913
6.900
6.836
6.816
6.718
6.696
4.384
4.365
4.345
4.332
4.312
4.293
3.789
3.771
3.753
1.880
1.866
1.795
1.778
1.761
1.742
1.414
1.398
1.253
0.888
0.877
0.871
0.848
1.00
0.99
1.96
2.09
1.01
2.97
1.09
1.04
4.10
2.04
4.11
2.31
9.41
2.36
20.28
8.99
fl (ppm)


12
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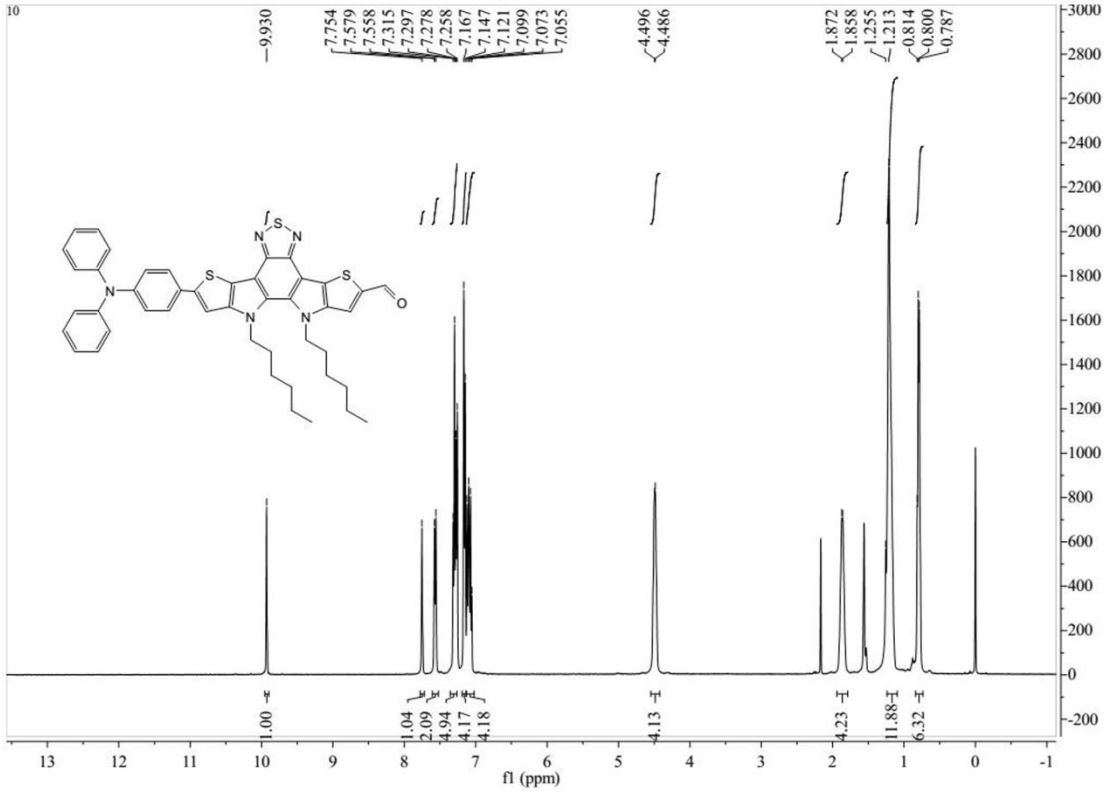
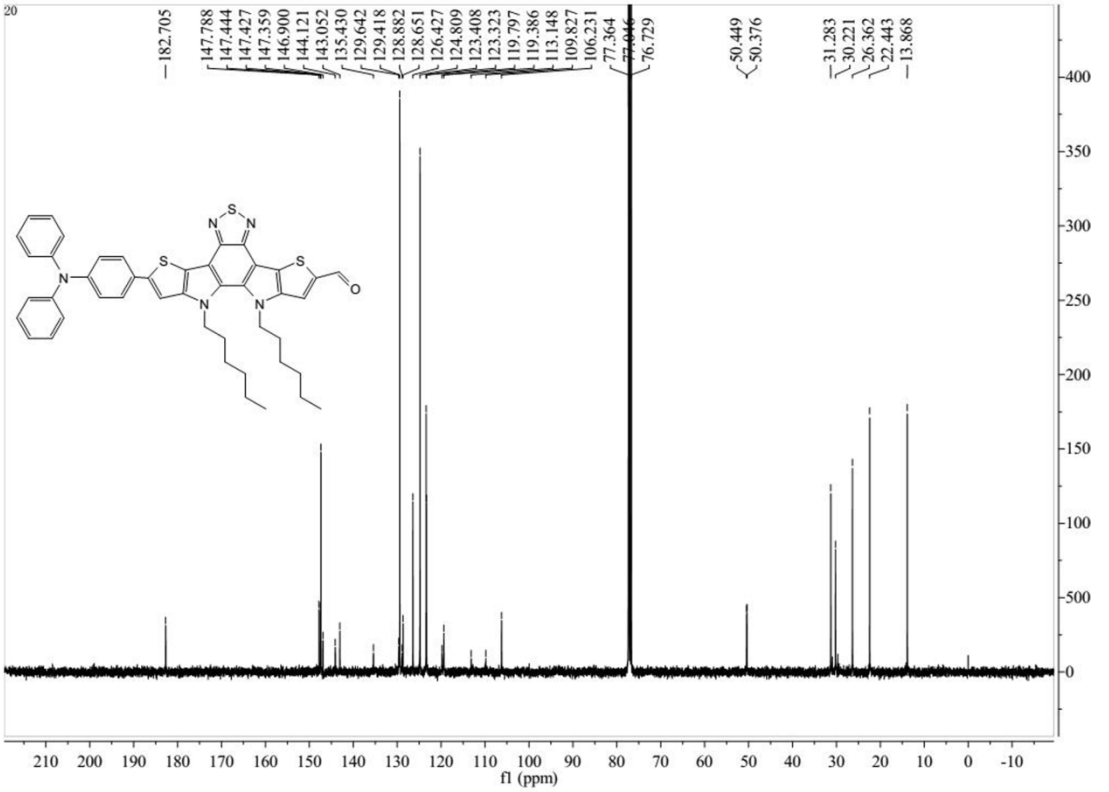
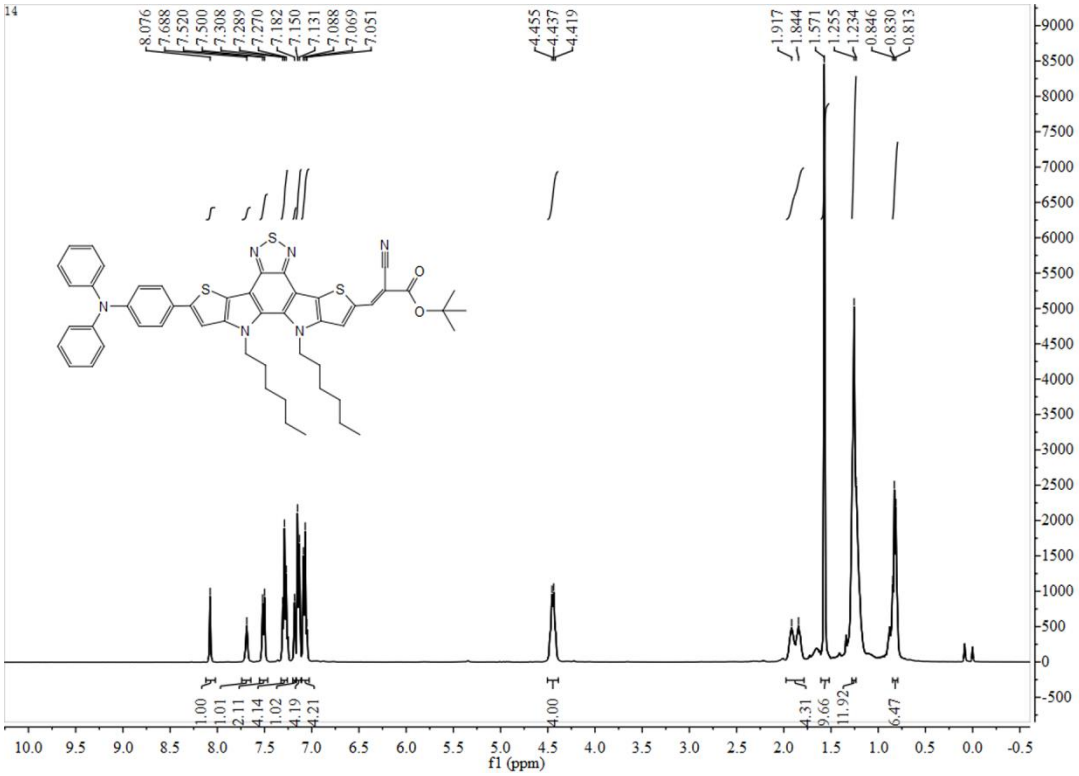
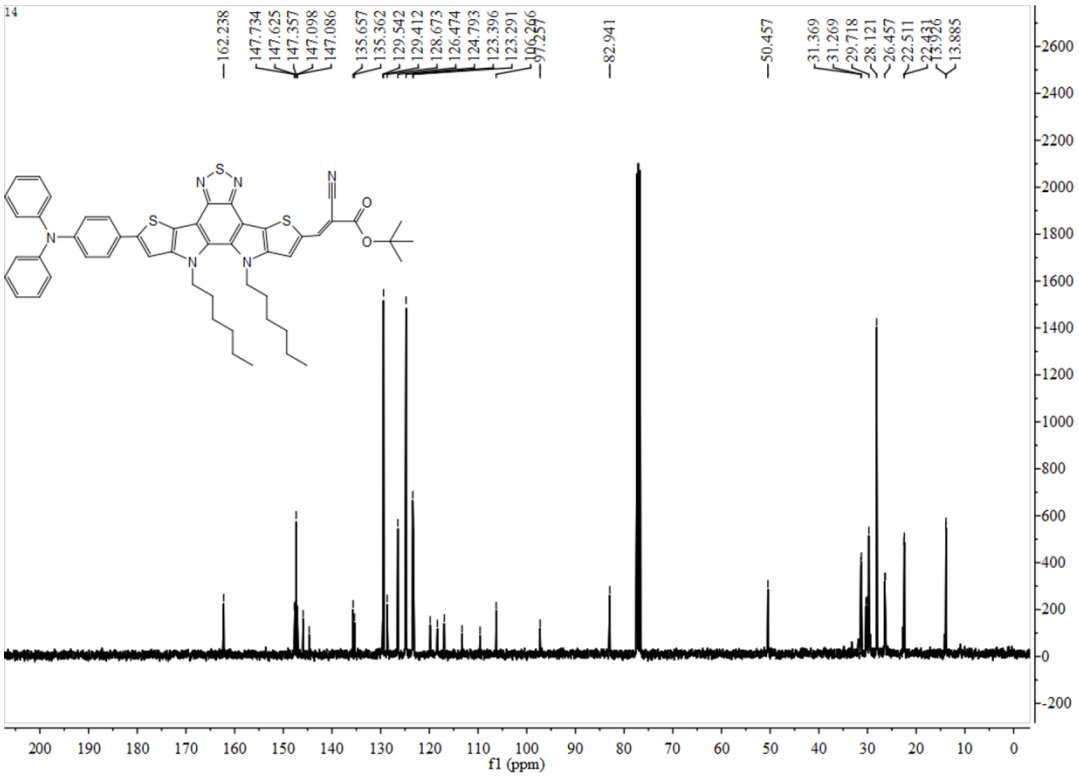
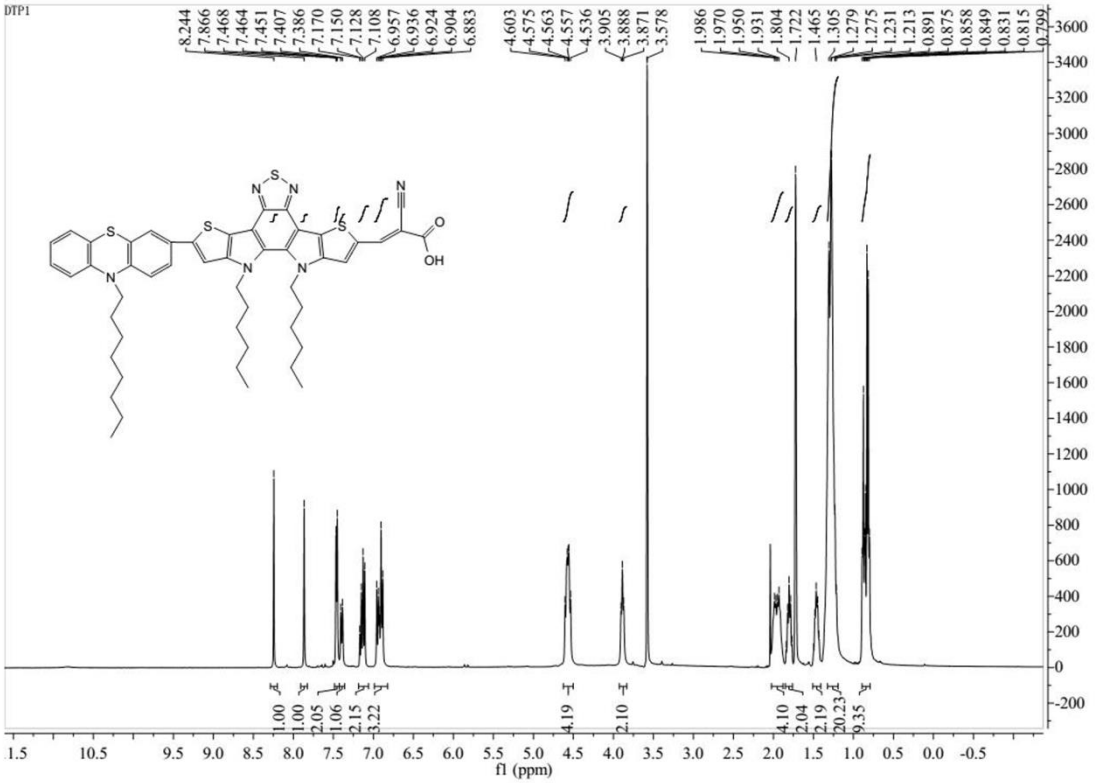
147.100
146.293
144.736
144.676
144.587
142.465
140.330
136.223
135.839
135.068
129.660
129.618
128.109
127.393
125.073
124.481
124.400
123.973
123.894
122.744
122.530
119.749
115.403
115.282
112.880
109.754
106.698
97.279
82.974
77.365
77.047
76.729
47.564
31.769
31.395
31.321
30.381
30.228
29.707
29.246
29.238
28.105
26.955
26.824
26.472
26.400
22.649
22.561
22.476
14.117
13.954
13.909
fl (ppm)

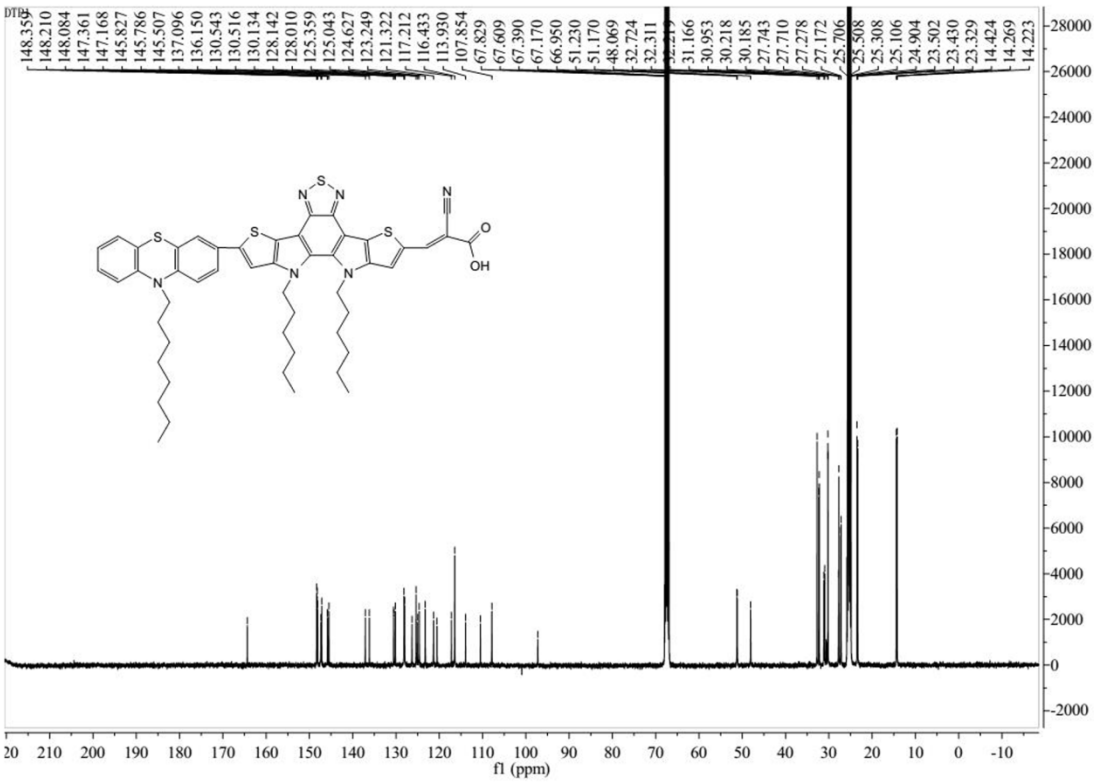

9.930
7.754
7.579
7.558
7.315
7.297
7.278
7.258
7.167
7.147
7.121
7.099
7.073
7.055
4.496
4.486
1.872
1.858
1.255
1.213
0.814
0.800
0.787
1.00
1.04
2.09
4.94
4.17
4.18
4.13
4.23
11.88
6.32
f1 (ppm)

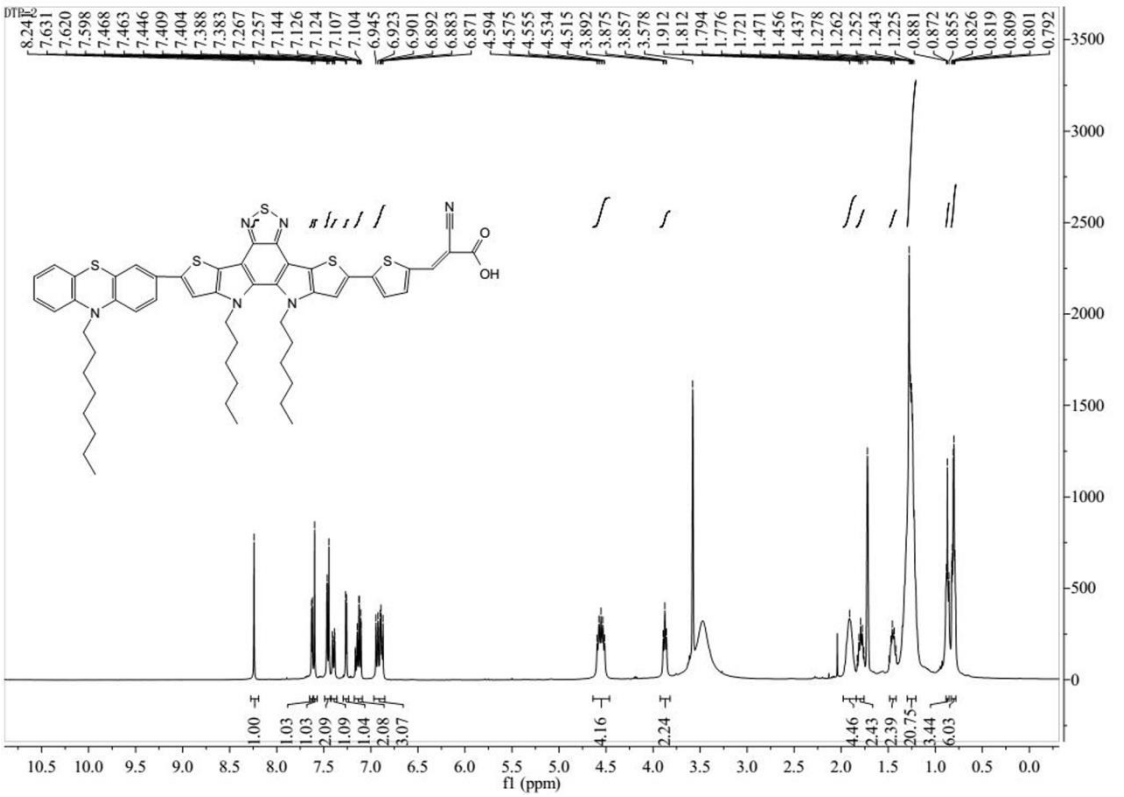

182.705
147.788
147.444
147.427
147.359
146.900
144.121
143.052
135.430
129.642
129.418
128.882
128.651
126.427
124.809
123.408
123.323
119.797
119.386
113.148
109.827
106.231
77.364
77.046
76.729
50.449
50.376
31.283
30.221
26.362
22.443
13.868
f1 (ppm)

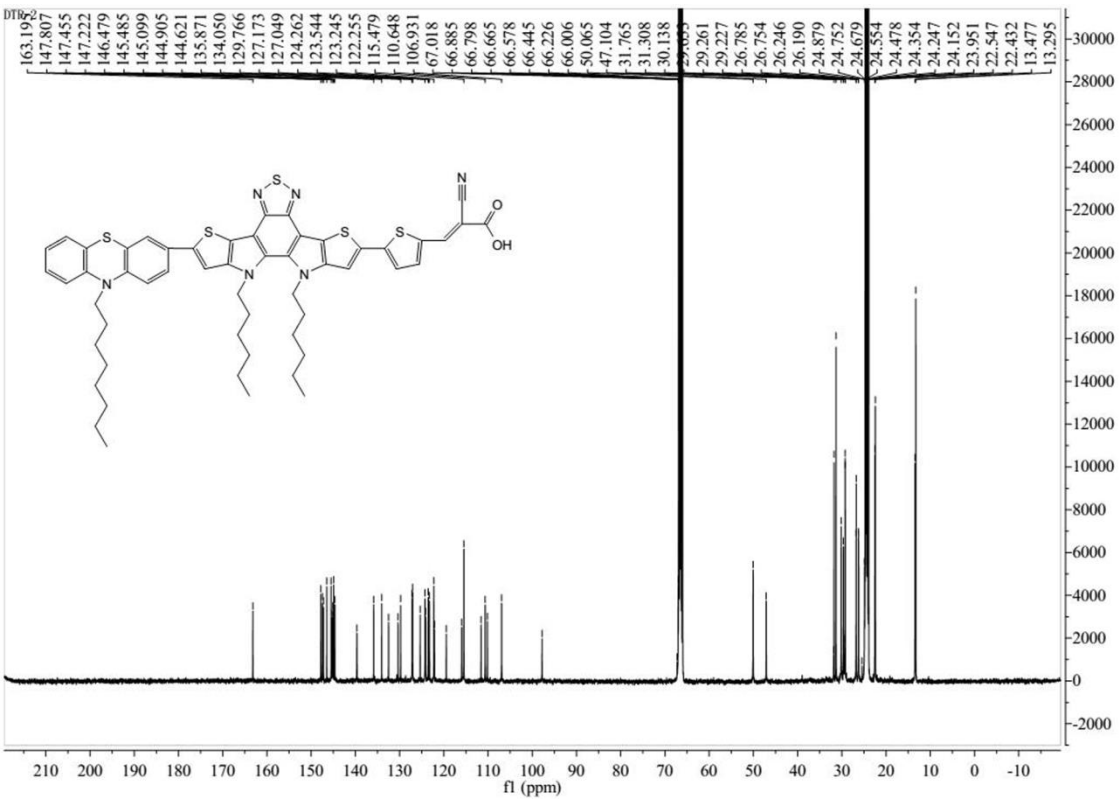

14
8.076
7.688
7.520
7.500
7.308
7.289
7.270
7.182
7.150
7.131
7.088
7.069
7.051
4.455
4.437
4.419
1.917
1.844
1.571
1.255
1.234
0.846
0.830
0.813
1.00
1.01
2.11
4.14
1.02
4.19
4.21
4.00
4.31
9.66
11.92
6.47
f1 (ppm)

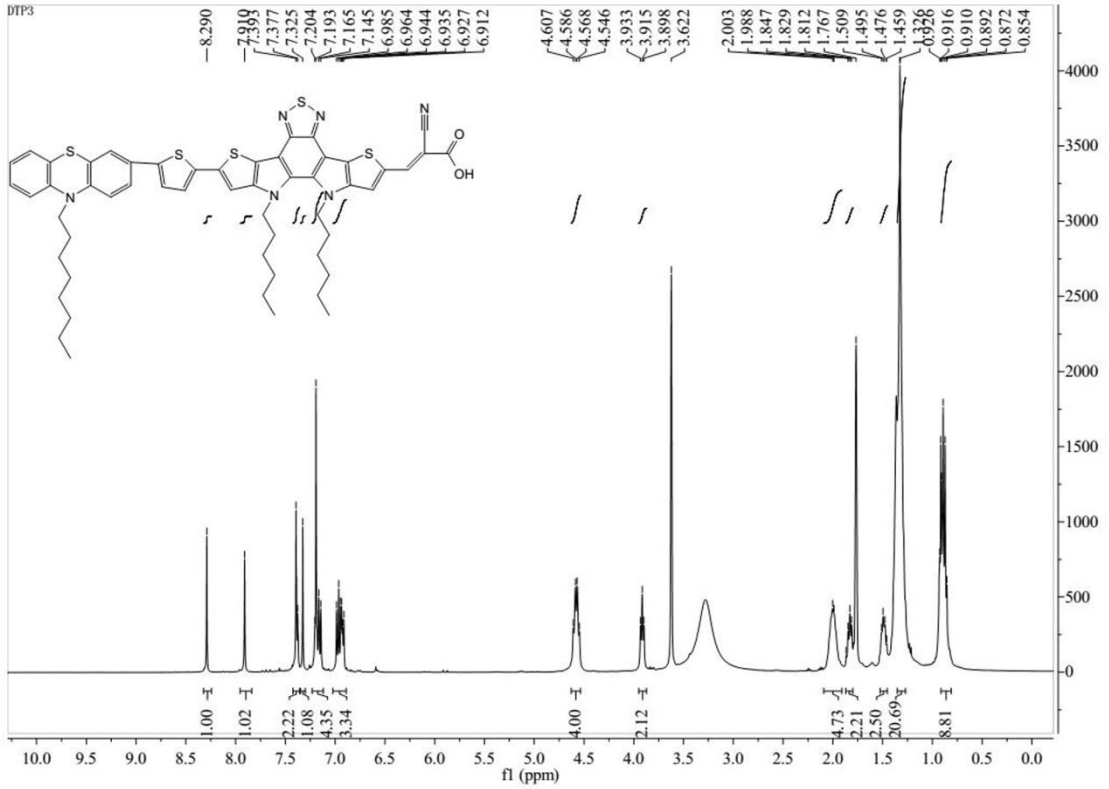

14
162.238
147.734
147.625
147.357
147.098
147.086
135.657
135.362
129.542
129.412
128.673
126.474
124.793
123.396
123.291
106.266
97.257
82.941
50.457
31.369
31.269
29.718
28.121
26.457
22.511
22.431
13.936
13.885
f1 (ppm)

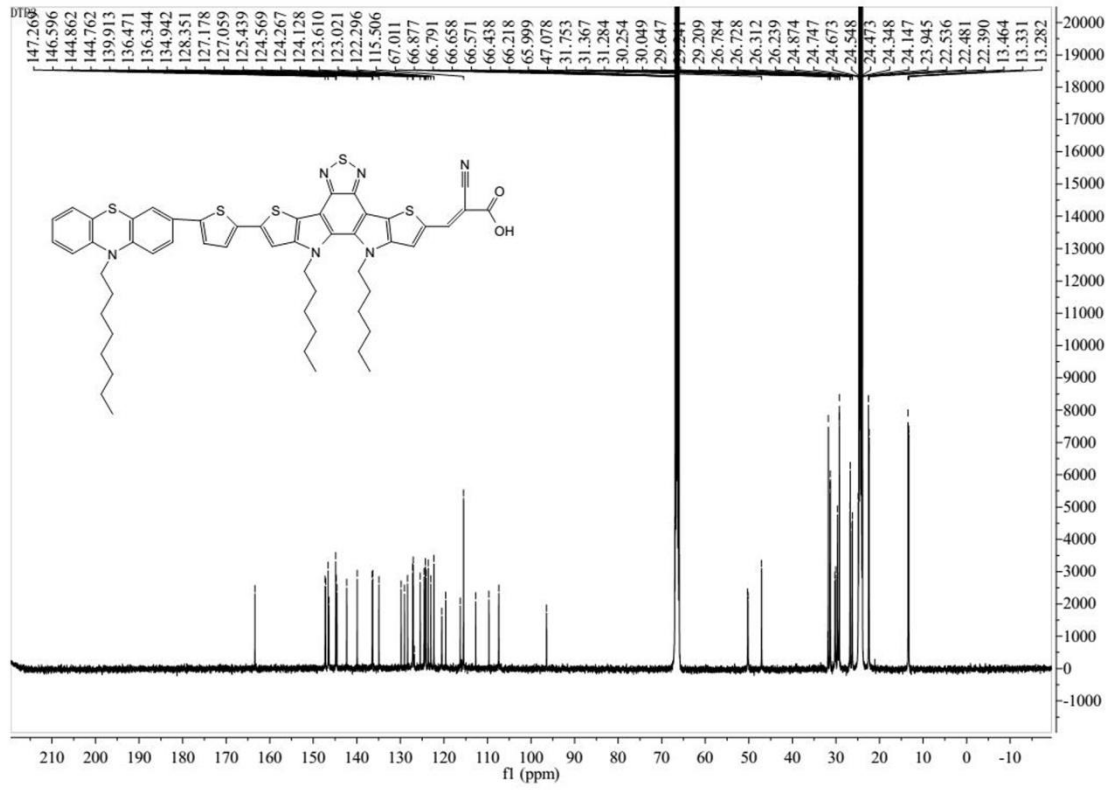

DTP1
8.244
7.866
7.468
7.464
7.451
7.407
7.386
7.170
7.150
7.128
7.108
6.957
6.936
6.924
6.904
6.883
4.603
4.575
4.563
4.557
4.536
3.905
3.888
3.871
3.578
1.986
1.970
1.950
1.931
1.804
1.722
1.465
1.305
1.279
1.275
1.231
1.213
0.891
0.875
0.858
0.849
0.831
0.815
0.799
1.00
1.00
2.05
1.06
2.15
3.22
4.19
2.10
4.10
2.04
2.19
20.23
9.35
f1 (ppm)

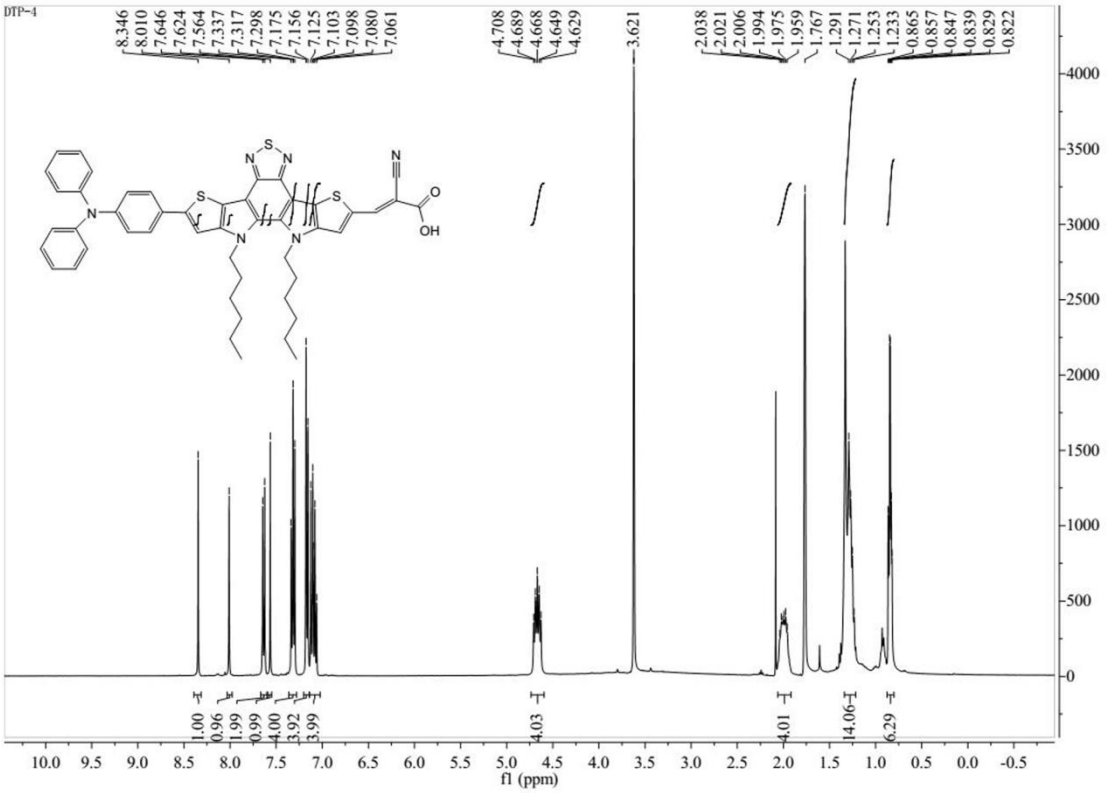

148.359
148.210
148.084
147.361
147.168
145.827
145.786
145.507
137.096
136.150
130.543
130.516
130.134
128.142
128.010
125.359
125.043
124.627
123.249
121.322
117.212
116.433
113.930
107.854
67.829
67.609
67.390
67.170
66.950
51.230
51.170
48.069
32.724
32.311
31.166
30.953
30.218
30.185
27.743
27.710
27.278
27.172
25.706
25.508
25.308
25.106
24.904
23.502
23.430
23.329
14.424
14.269
14.223
f1 (ppm)

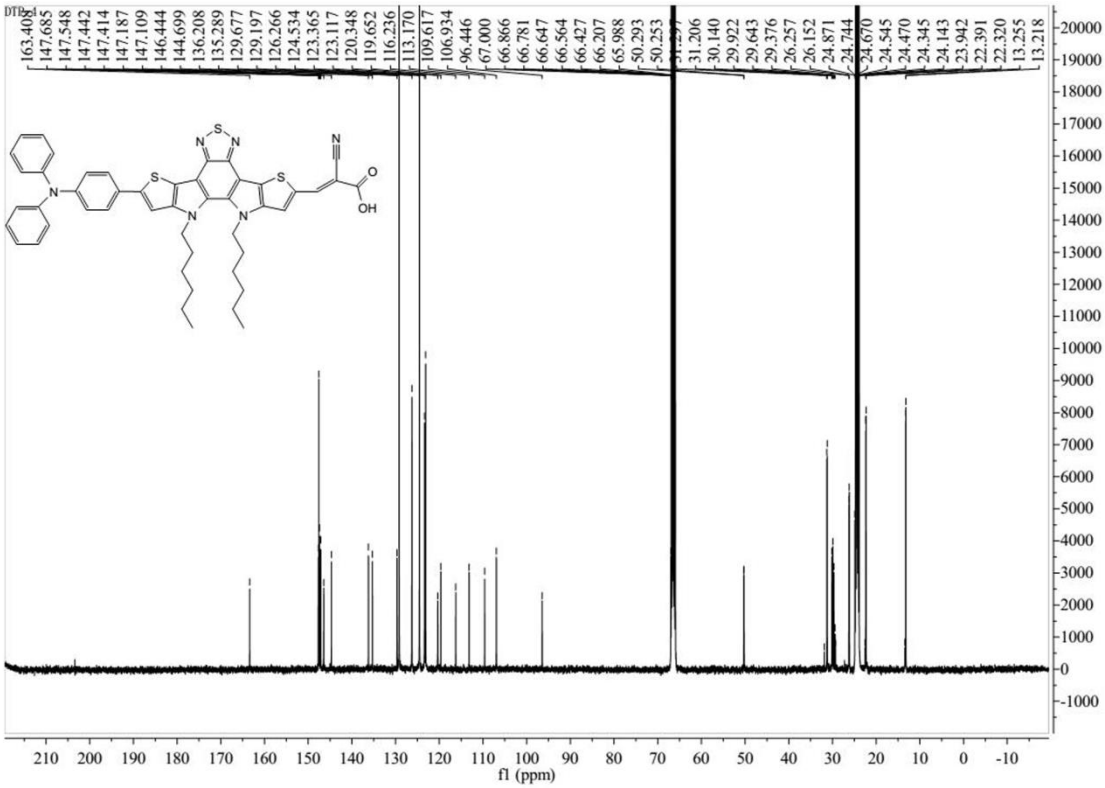

f1 (ppm)


f1 (ppm)


DTP3
fl (ppm)


fl (ppm)


DTP-4
8.346
8.010
7.646
7.624
7.564
7.337
7.317
7.298
7.175
7.156
7.125
7.103
7.098
7.080
7.061
4.708
4.689
4.668
4.649
4.629
3.621
2.038
2.021
2.006
1.994
1.975
1.959
1.767
1.291
1.271
1.253
1.233
0.865
0.857
0.847
0.839
0.829
0.822
1.00
0.96
1.99
0.99
4.00
3.92
3.99
4.03
4.01
14.06
6.29
fl (ppm)


163.408
147.685
147.548
147.442
147.414
147.187
147.109
146.444
144.699
136.208
135.289
129.677
129.197
126.266
124.534
123.365
123.117
120.348
119.652
116.236
113.170
109.617
106.934
96.446
67.000
66.866
66.781
66.647
66.564
66.427
66.207
65.988
50.293
50.253
31.206
30.140
29.922
29.643
29.376
26.257
26.152
24.871
24.744
24.670
24.545
24.470
24.345
24.143
23.942
22.391
22.320
13.255
13.218
fl (ppm)

References

1. H. Tan, C. Pan, G. Wang, Y. Wu, Y. Zhang, Y. Zou, G. Yu and M. Zhang, *Org. Electron.*, 2013, **14**, 2795-2801.
2. M. Zhang, Y. Wang, M. Xu, W. Ma, R. Li and P. Wang, *Energy Environ. Sci.*, 2013, **6**, 2944.