Supporting Information

A new series of pyrenyl-based triarylamines: syntheses, structures, optical properties, electrochemistry and electroluminescence

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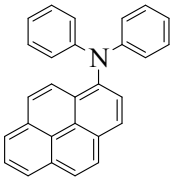
1. The structure of the compound *N*, *N*-diphenylpyren-1-amine



1py

Scheme S1. The structure of the compound *N*, *N*-diphenylpyren-1-amine (**1py**).

2. Absorption and emission parameters of compounds 2a–2d and 3py in different solvents

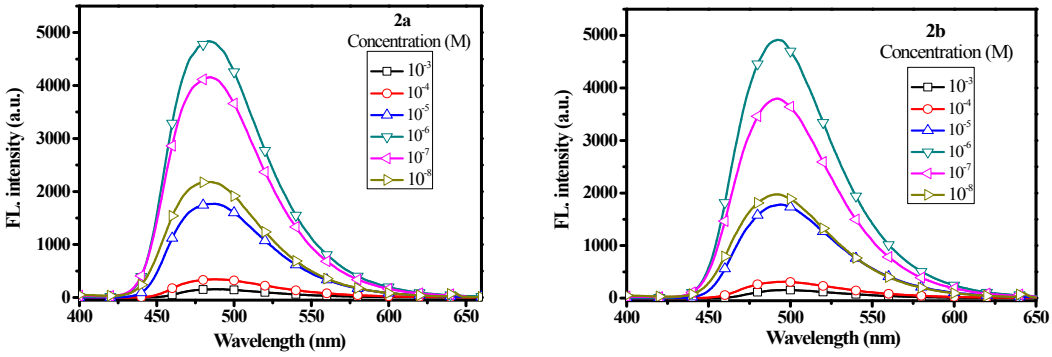
Table S1. Absorption properties of compounds **2a**–**2d** and **3py** in different solvents

	λ_{max} (nm)					
Com.	TOL	DCM	THF	MeOH	DMF	MeCN
2a	333 , 410	275, 333, 407	274, 331, 406	273, 316, 403	274, 331, 406	272, 330, 404
2b	334, 412	275, 333, 411	274, 332, 410	273 , 330, 407	275, 333, 410	273, 330, 408
2c	335, 416	275, 334, 413	274, 333, 414	273, 331, 409	275, 334, 413	273, 331, 410
2d	334, 409	275, 333, 407	274, 332, 406	272, 329, 403	275, 330, 406	274, 330, 403
3py	337,410	337,413	336, 409	334,406	337,409	334, 405

Table S2. Emission properties of compounds **2a**–**2d** and **3py** in different solvents

	λ_{em} (nm)/Stokes shift (cm^{-1})					
Com.	TOL	DCM	THF	MeOH	DMF	MeCN
2a	459/2604	486/3994	467/3217	478/3914	494/4387	496/4592
2b	467/2857	491/3964	476/3390	491/4200	499/4350	500/4510
2c	480/3207	506/4372	496/3879	505/4648	520/4982	521/5196
2d	460/2711	482/3823	471/3399	481/4024	496/4469	497/4693
3py	469/2891	494/4147	481/3660	495/4429	501/4490	504/4850

3. The emission spectra of compound 2a–2d and 3py in dichloromethane with different concentrations.



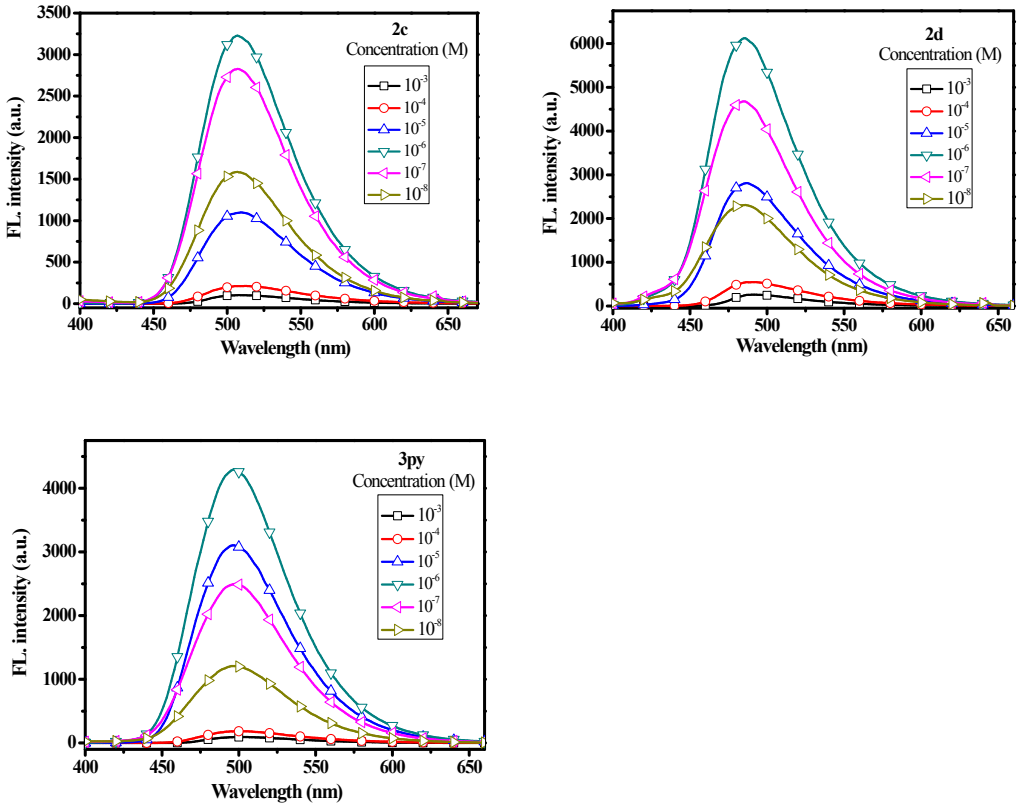
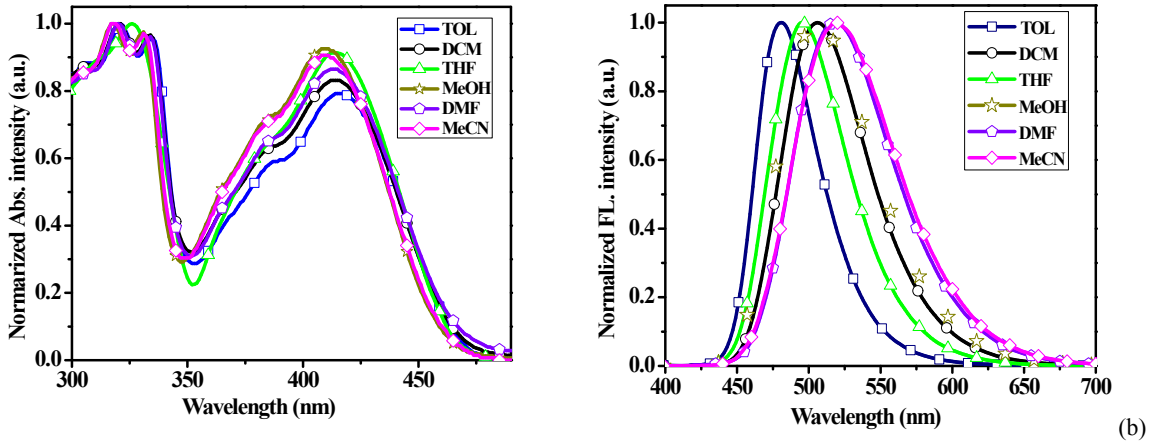


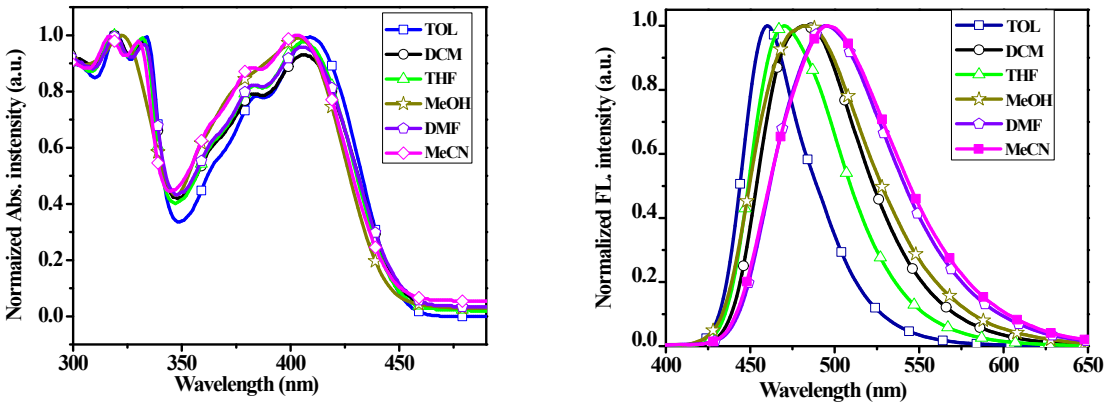
Figure S1. Emission spectra of compounds **2a–2d** and **3py** in dichloromethane with different concentrations.

4. Absorption and emission spectra of compound 2b–2d and 3py recorded in different solvents.



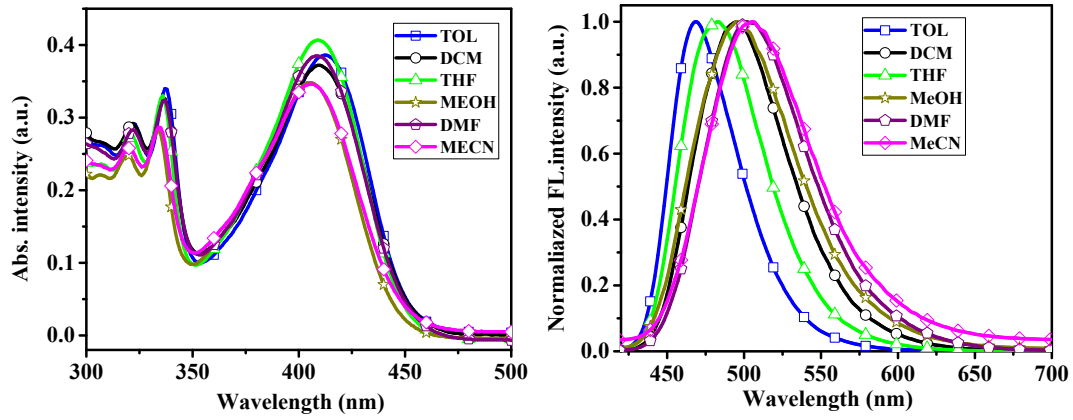
(a) (b)

Figure S2. Normalized UV-vis absorption spectra (a) and emission spectra (b) of compound **2c** recorded in different solvents at ~10^{-5} concentration.



(a) (b)

Figure S3. Normalized UV-vis absorption spectra (a) and emission spectra (b) of compound **2d** recorded in different solvents at ~10^{-5} concentration.



(a) (b)

Figure S4. Normalized UV-vis absorption spectra (a) and emission spectra (b) of compound **3py** recorded in different solvents at ~10^{-5} concentration.

5. The relationship between the stokes' shift and solvent parameter $E_T(30)$ for compounds 2a–2d and 3py

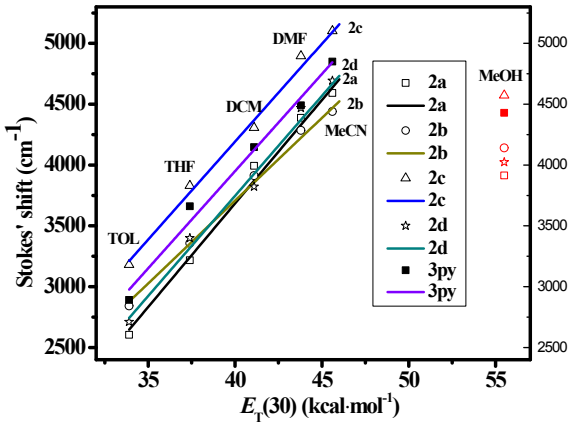
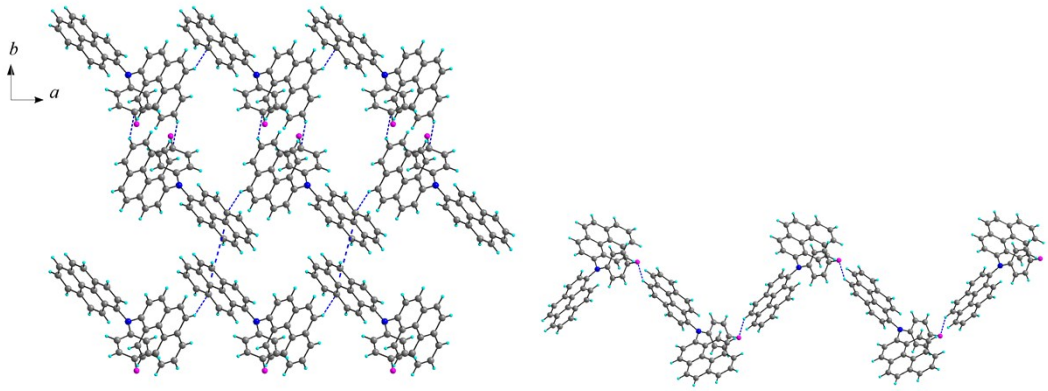


Figure S5. Correlation between the stokes' shift and solvent parameter $E_T(30)$ for compounds **2a–2d** and **3py**

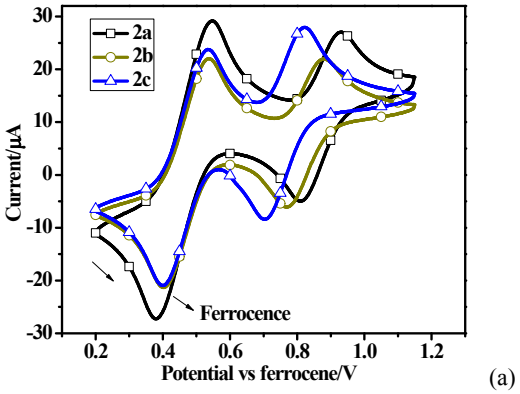
6. Supramolecular layer structure of compound 2d



(a) (b)

Figure S6 Two-dimensional supramolecular layer structure of compound **2d** linked by C–H···π interactions (a) and its one-dimensional structure linked by C–H···F hydrogen bonds (b).

7. Cyclic voltammograms for compounds 2a–2e and 3py.



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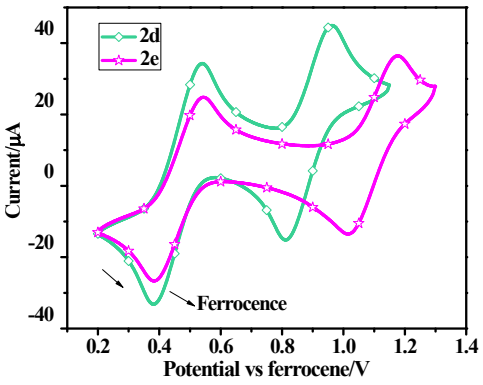

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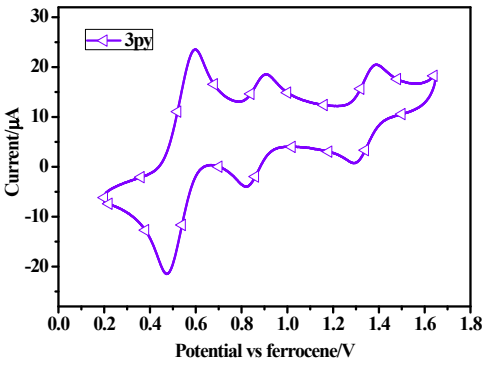
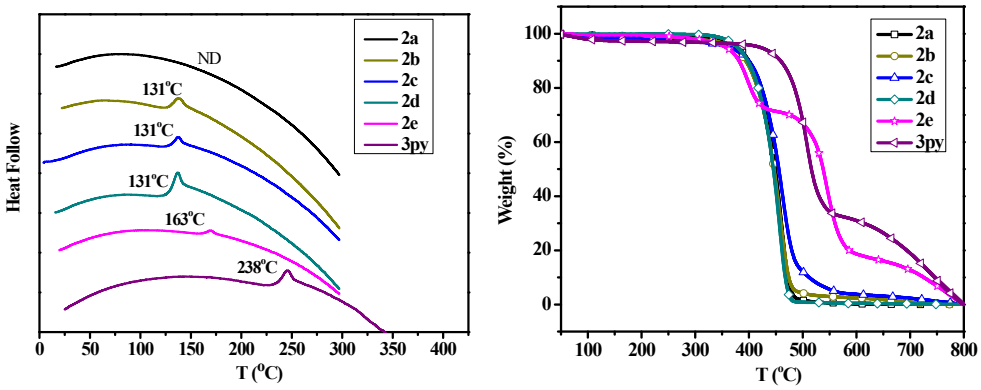


(c)

Figure S7. Cyclic voltammograms recorded in dry dichloromethane at the scan rate 50 mV/sec using ferrocene as an internal standard for compounds **2a**–**2c** (a), **2d**–**2e** (b) and **3py** (c).

8. DSC and TGA thermograms of 2a–2e and 3py



(a) (b)

Figure S8. DSC (a) and TGA (b) thermograms of **2a**–**2e** and **3py** recorded under N_2 at a heating rate of 10 °C min^{-1}.

9. Structure of the non-doped devices and energy levels of materials 2c and 2d.

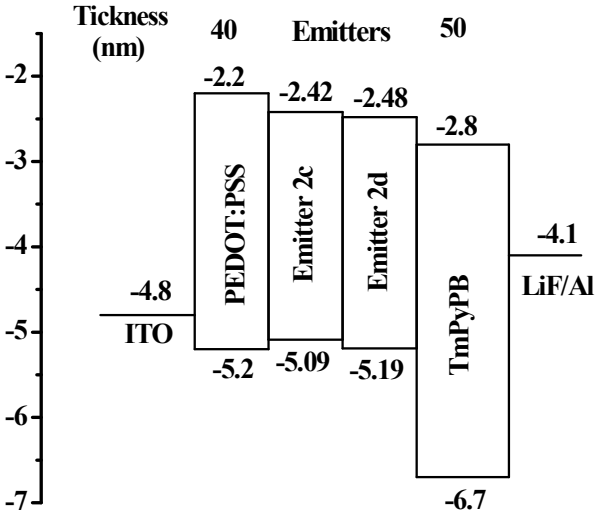
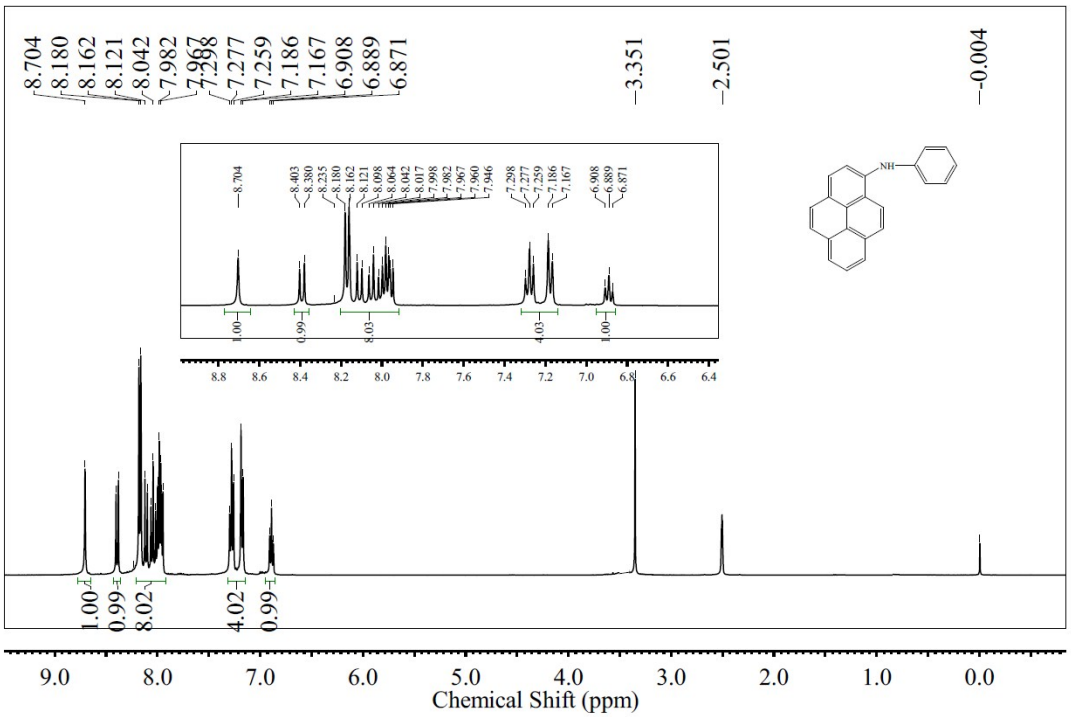


Figure S9 Structure of the non-doped devices and energy levels of materials **2c** and **2d**.

10. NMR spectra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8.042
7.982
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7.298
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7.259
7.186
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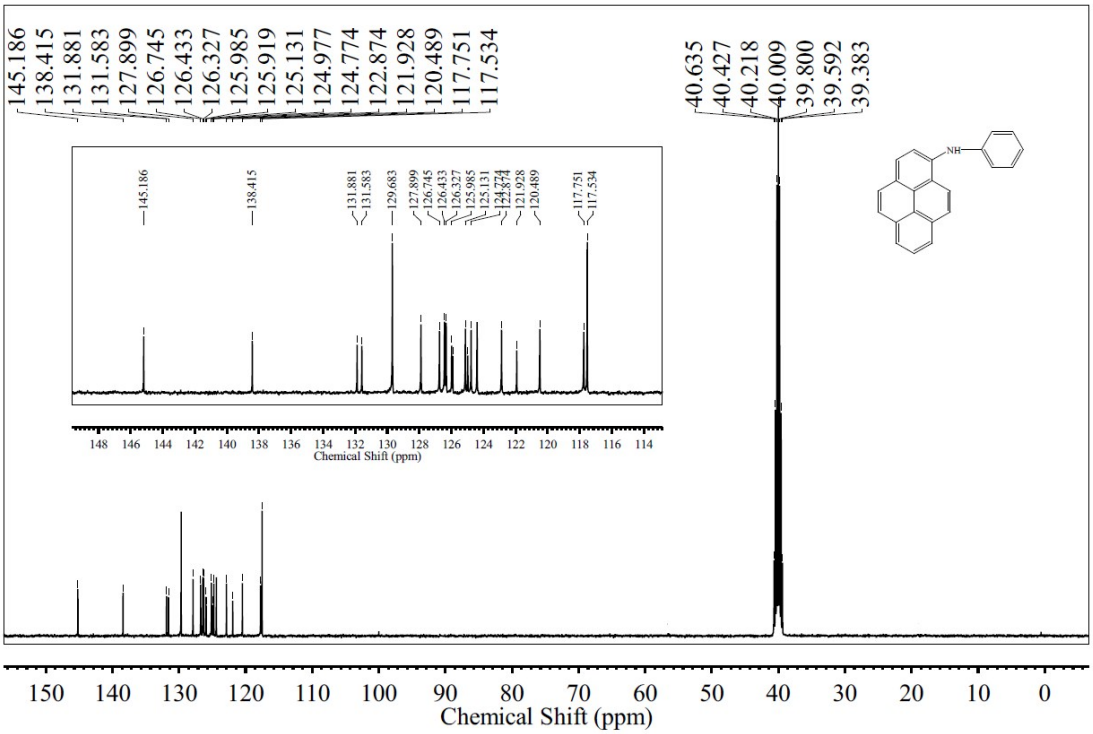
6.908
6.889
6.871
3.351
2.501
0.004
NH
1.00
0.99
8.02
4.02
0.99
Chemical Shift (ppm)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126.745
126.433
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124.774
122.874
121.928
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117.534
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40.218
40.009
39.800
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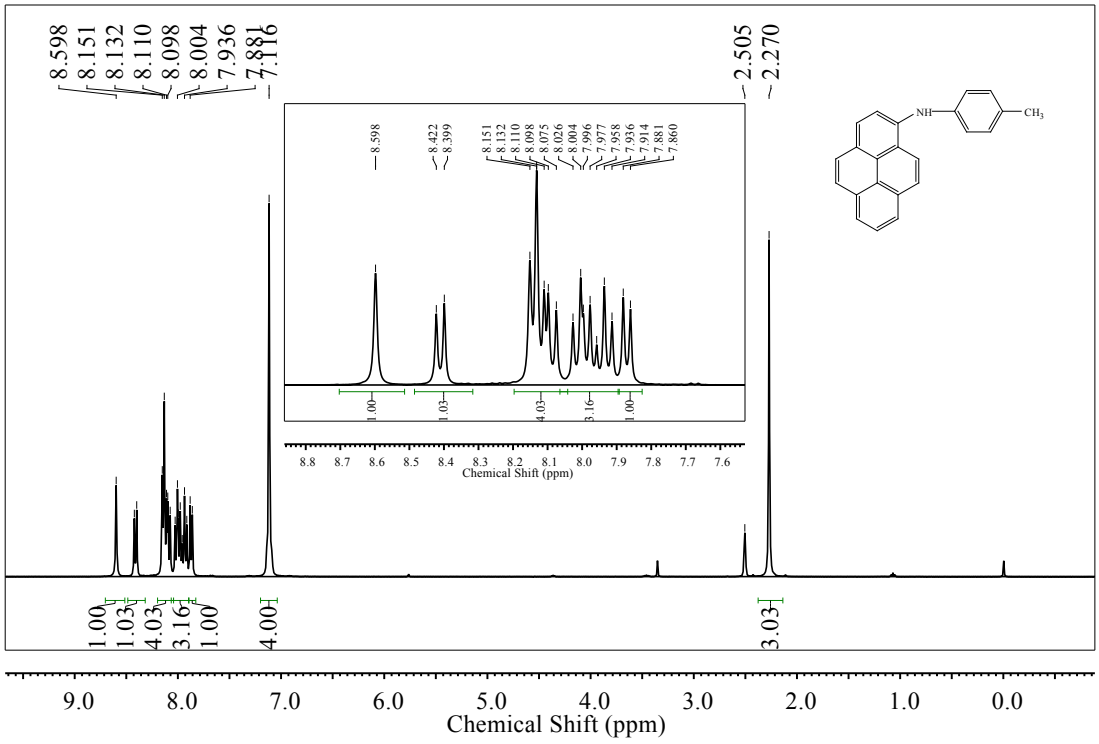
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8.098
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1.00
4.00
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CH3
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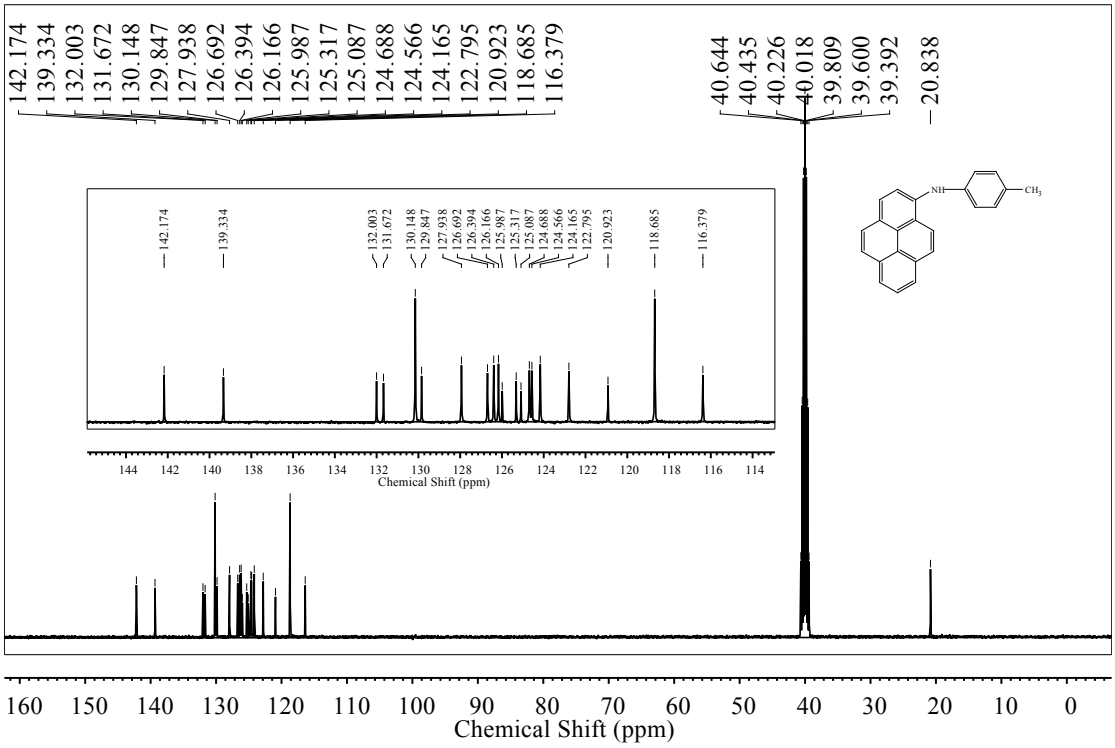
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124.688
124.566
124.165
122.795
120.923
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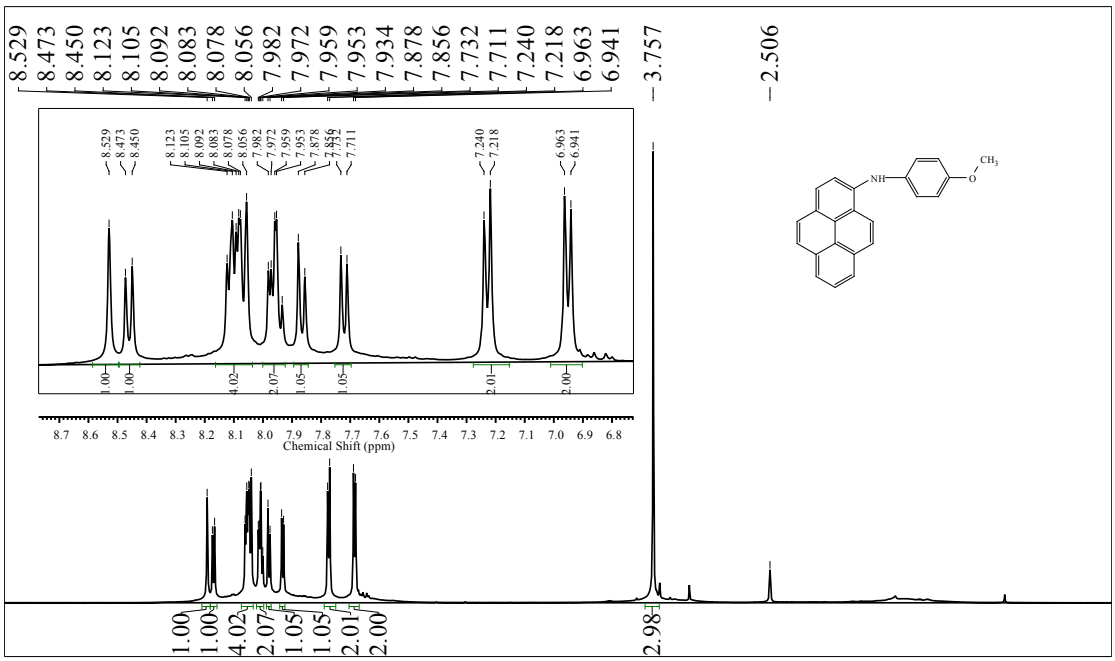
CH3
Chemical Shift (ppm)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7.953
7.934
7.878
7.856
7.732
7.711
7.240
7.218
6.963
6.941
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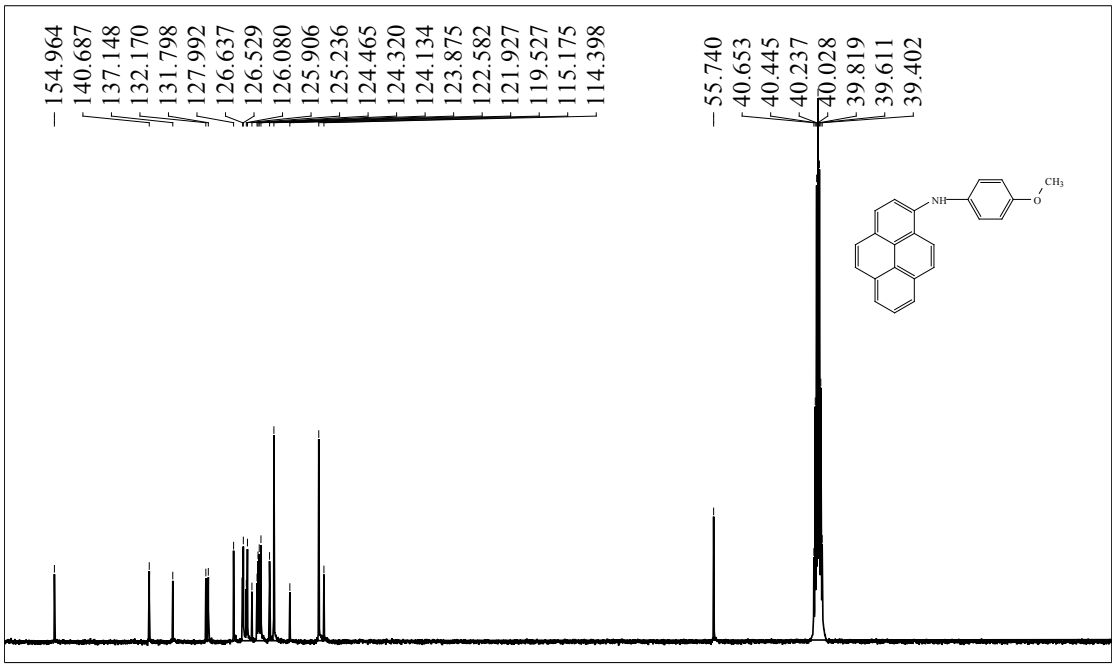
2.00
2.98
Chemical Shift (ppm)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124.134
123.875
122.582
121.927
119.527
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39.819
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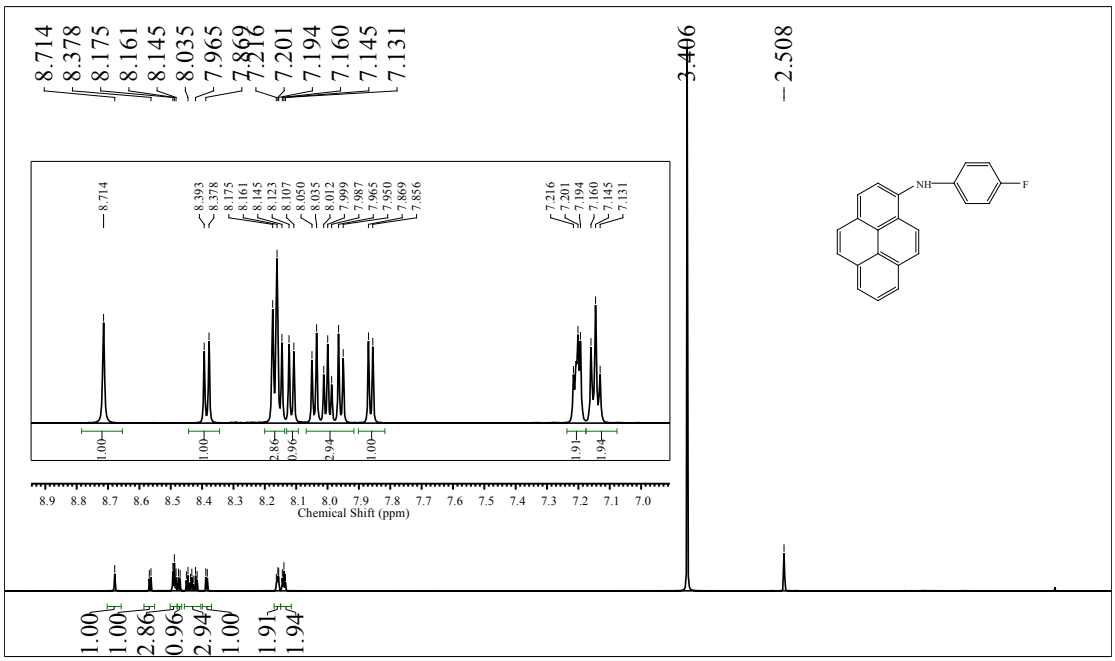
Chemical Shift (ppm)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7.131
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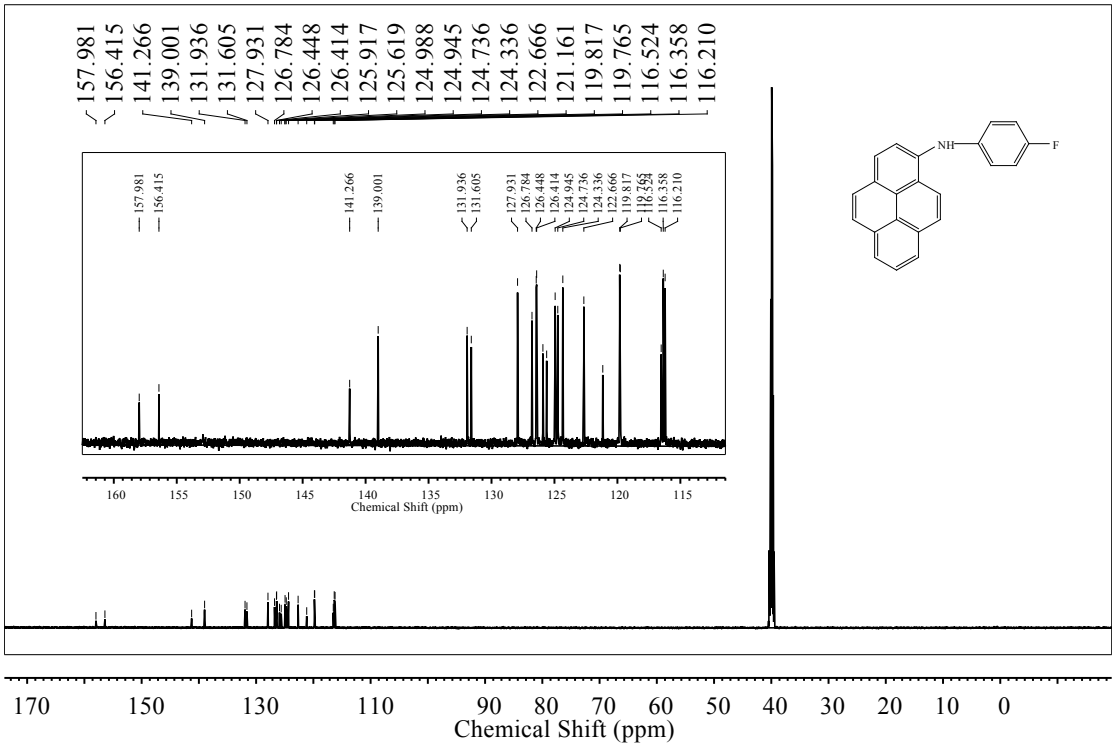
Chemical Shift (ppm)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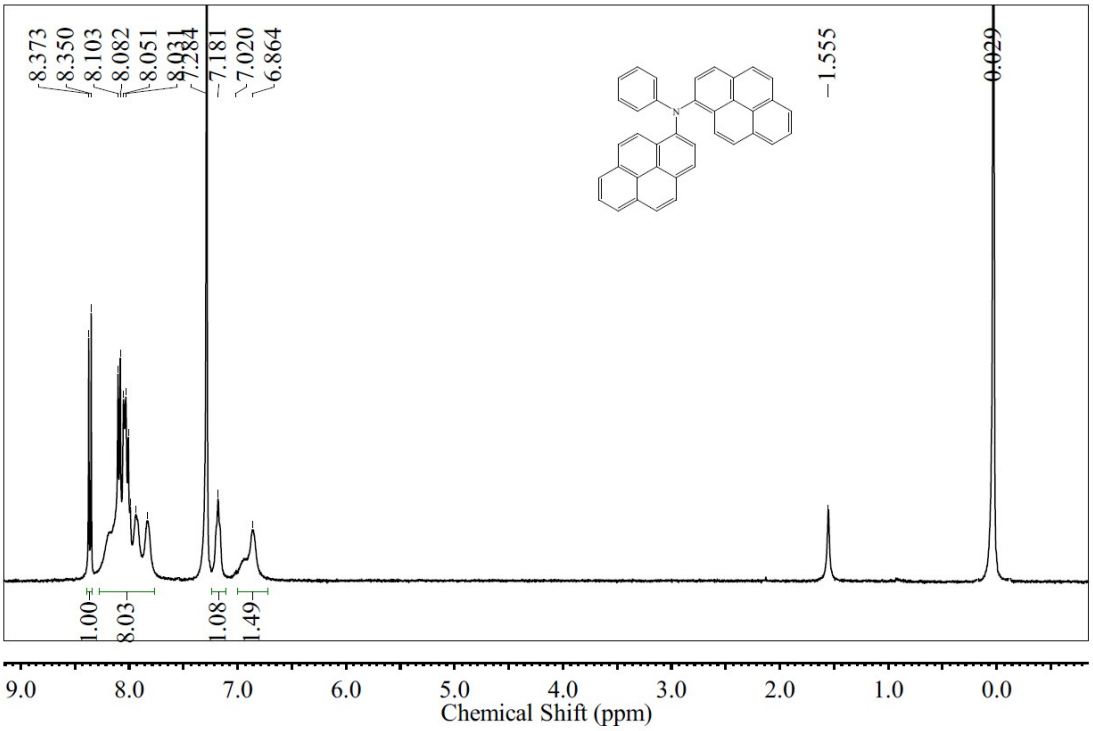
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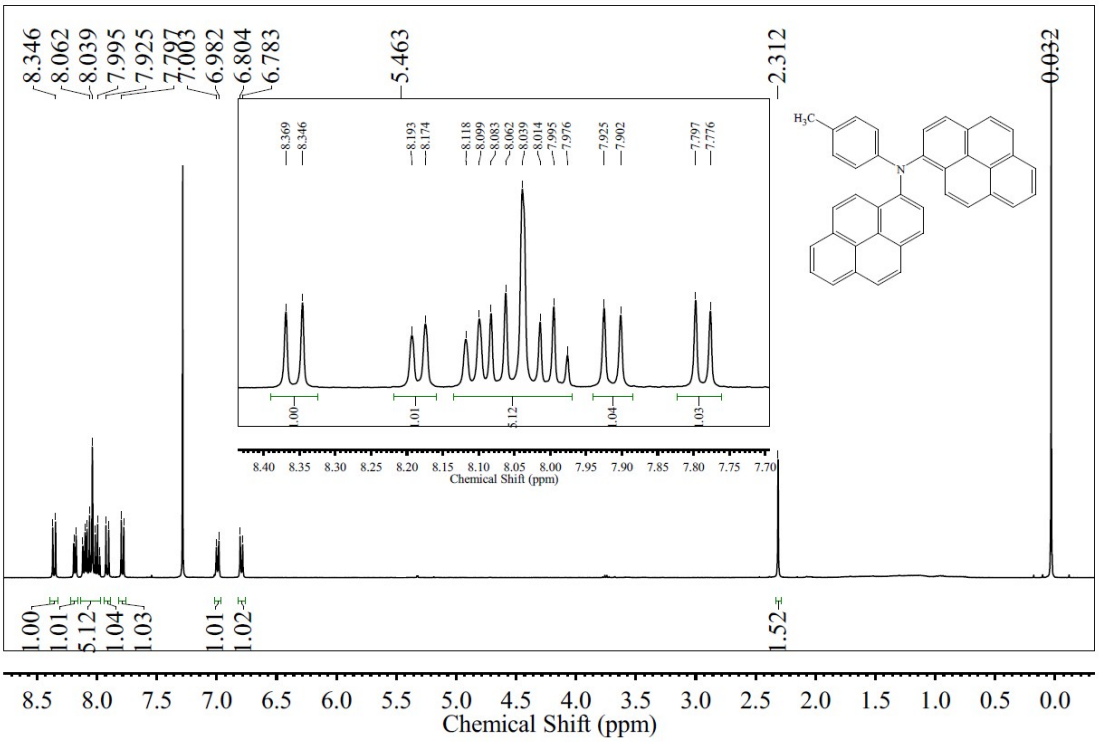
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8.193
8.174
8.118
8.099
8.083
8.062
8.039
8.014
7.995
7.976
7.925
7.902
7.797
7.776
1.00
1.01
5.12
1.04
1.03
8.40 8.35 8.30 8.25 8.20 8.15 8.10 8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70
Chemical Shift (ppm)
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1.01
5.12
1.04
1.03
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1.02
1.52
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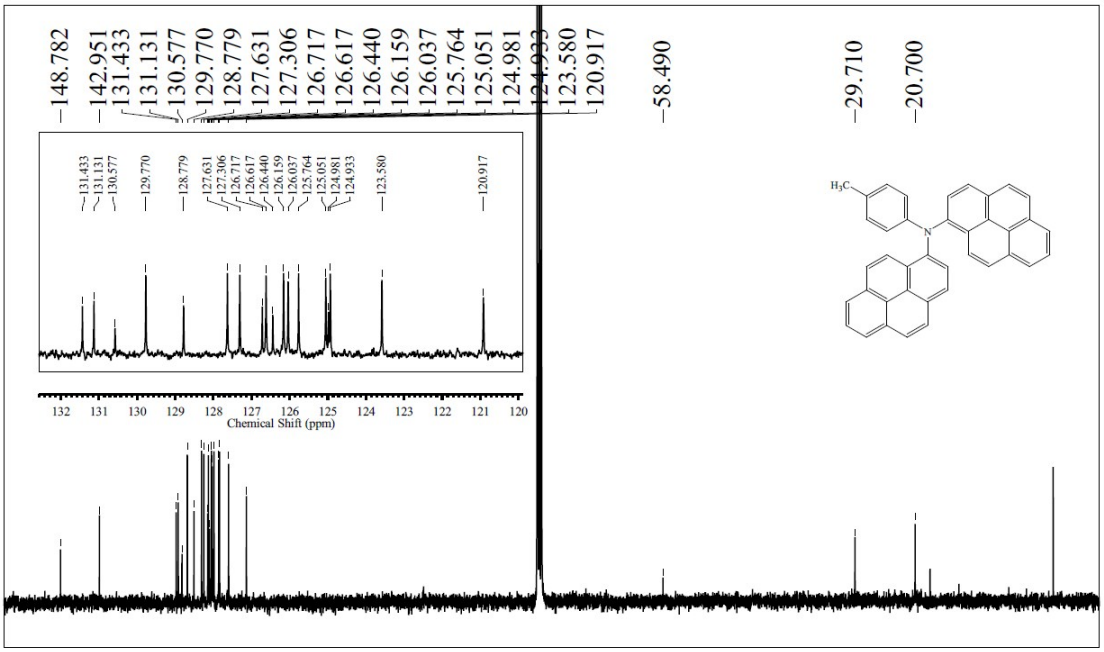
Chemical Shift (ppm)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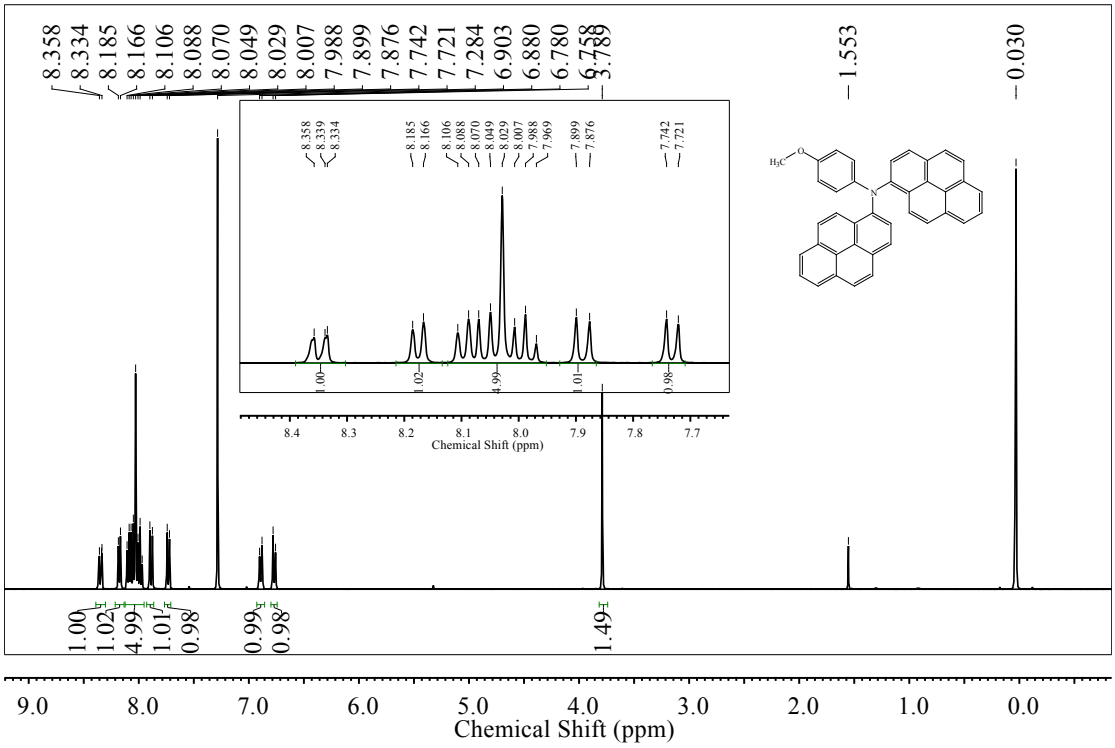
Chemical Shift (ppm)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7.742
7.721
7.284
6.903
6.880
6.780
6.758
3.789
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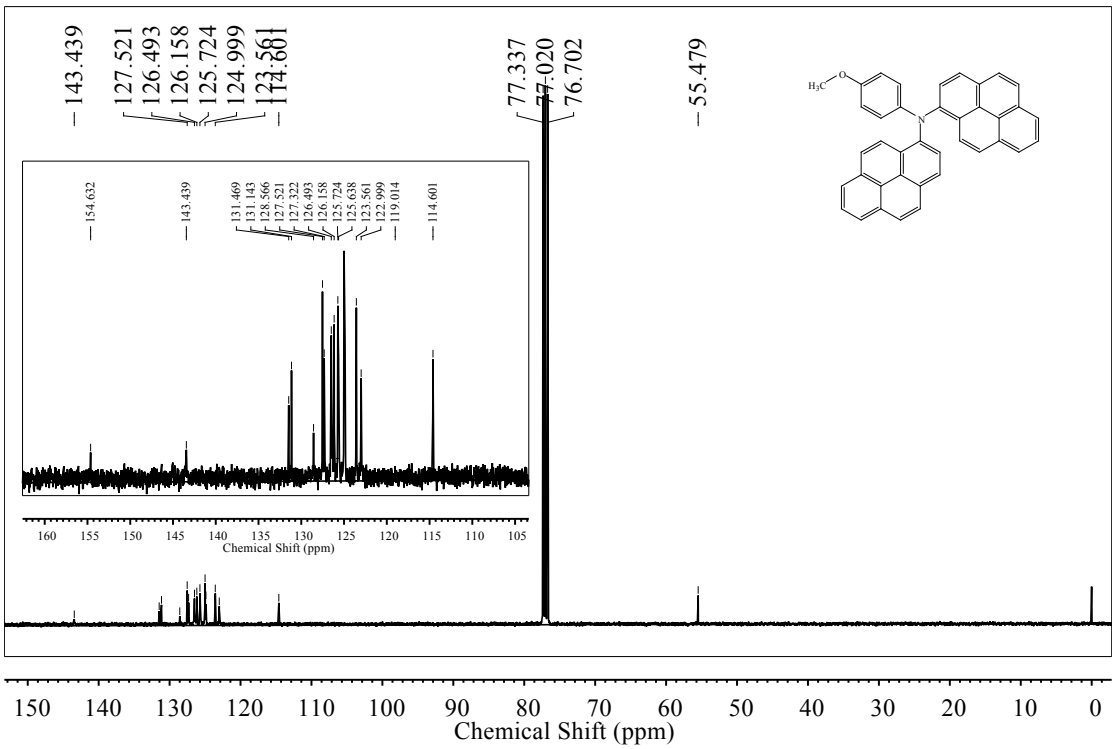
Chemical Shift (ppm)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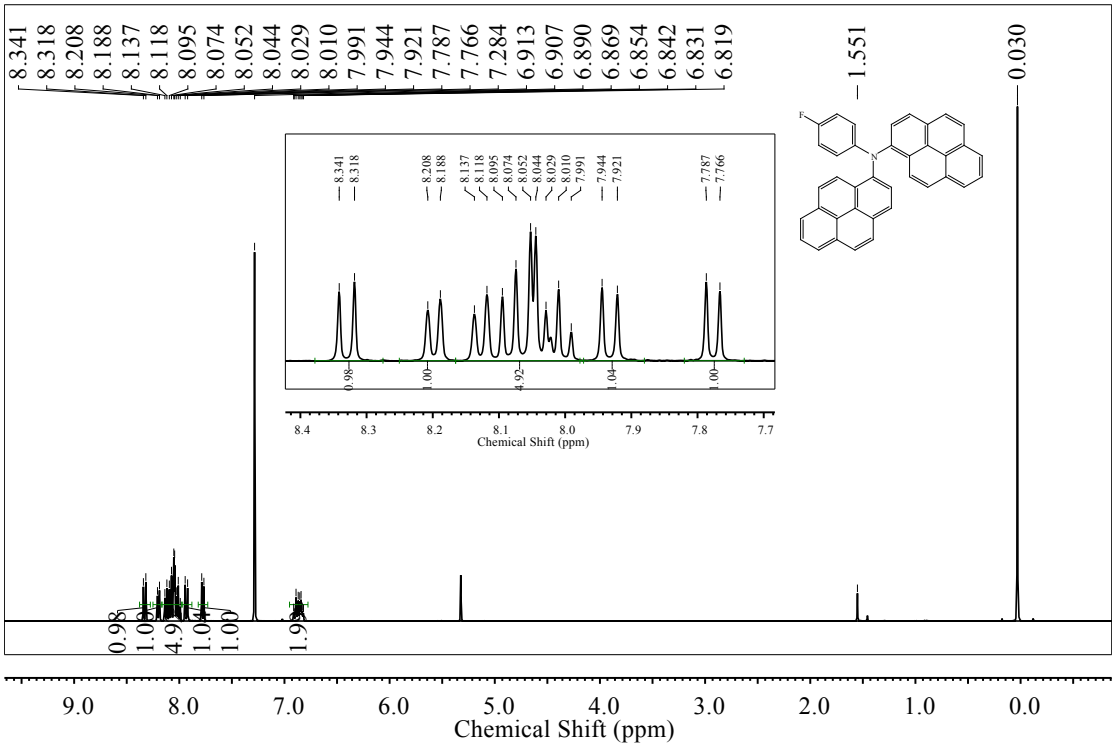
Chemical Shift (ppm)
Chemical Shift (ppm)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6.907
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6.831
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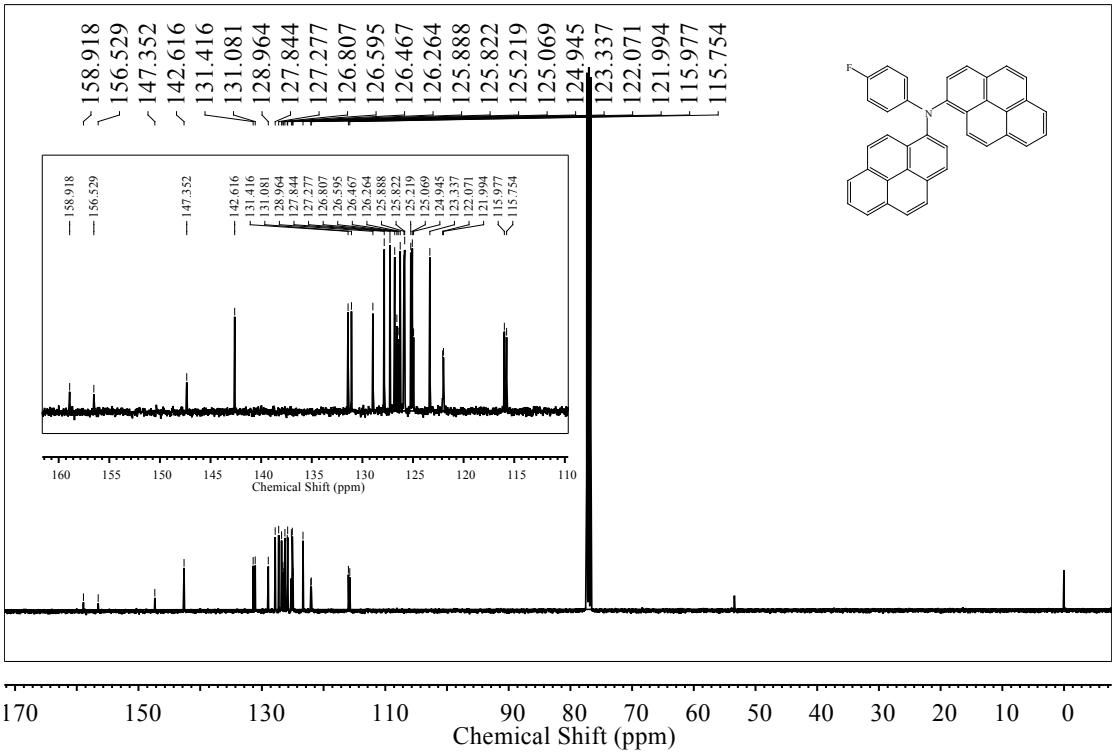
1.00
1.99
Chemical Shift (ppm)
Chemical Shift (ppm)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126.264
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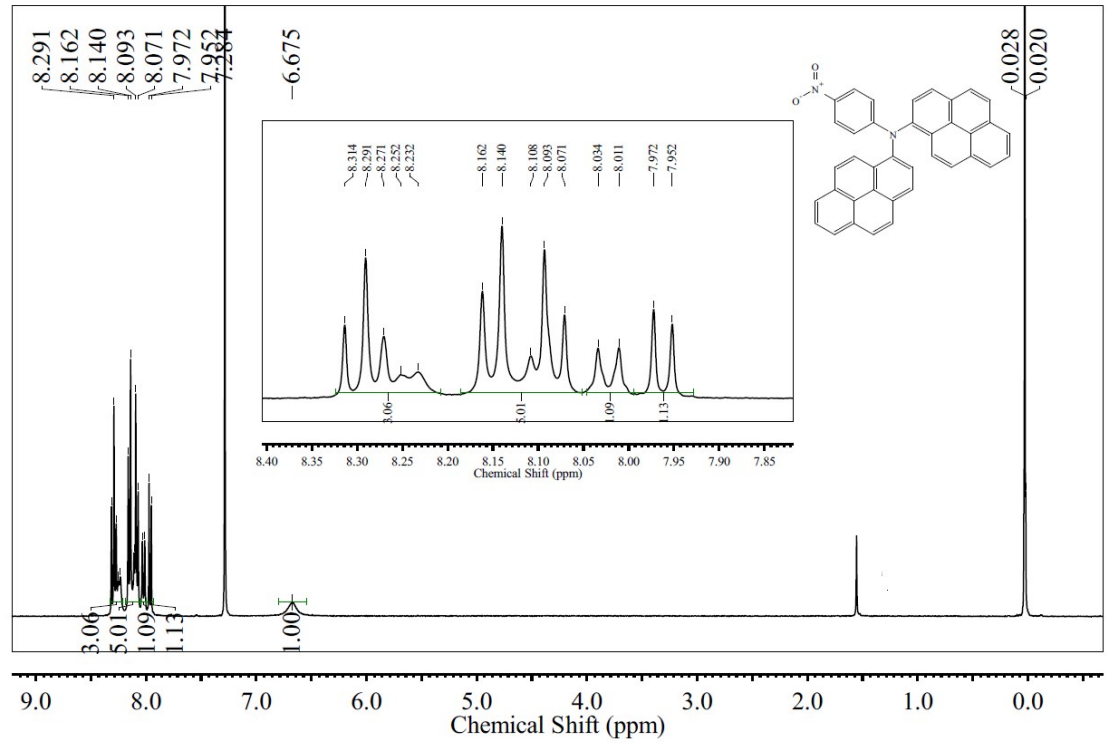
F
N
Chemical Shift (ppm)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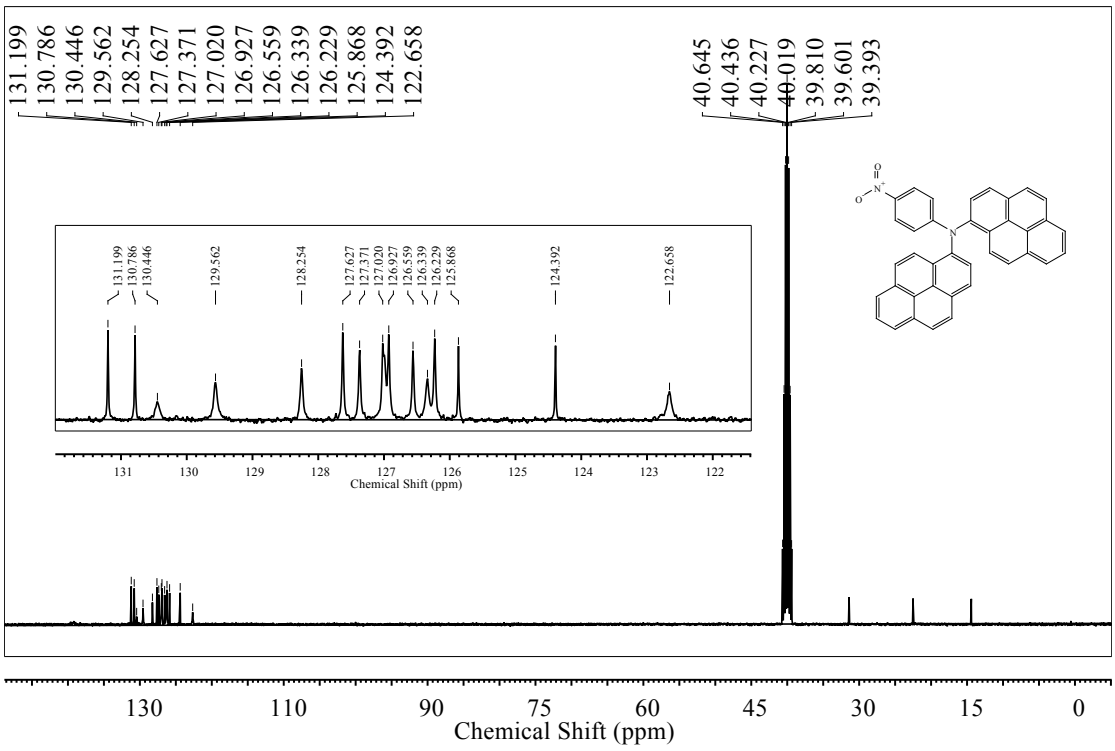
Chemical Shift (ppm)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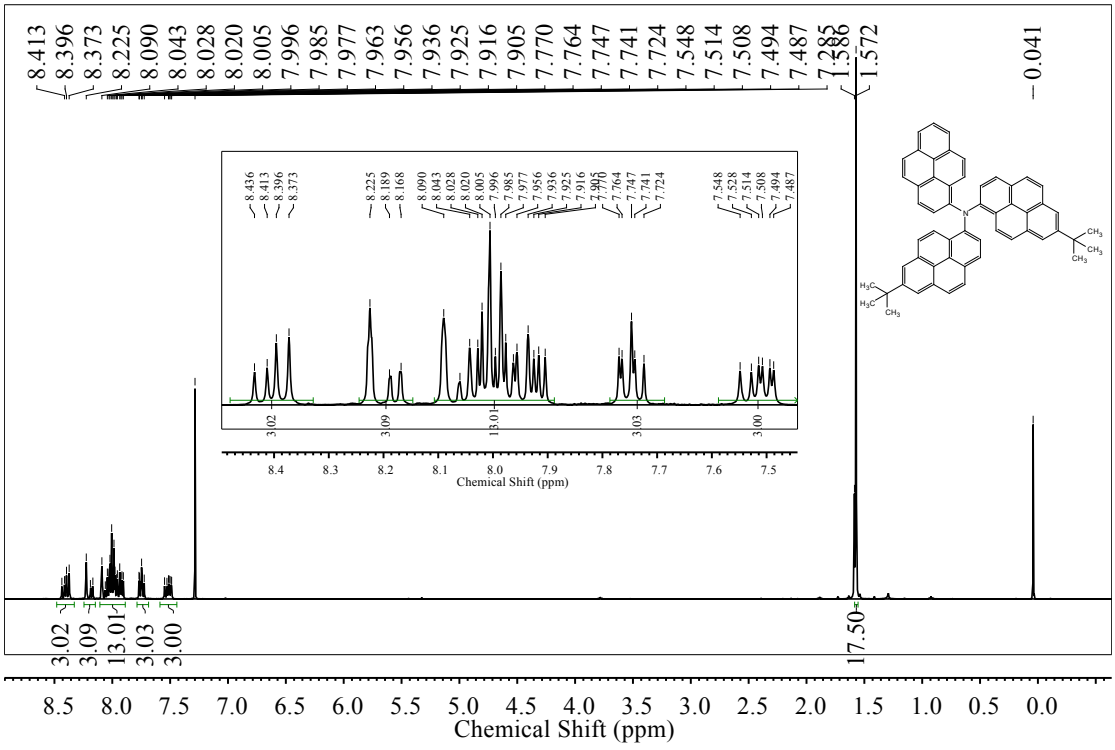
Chemical Shift (ppm)
Chemical Shift (ppm)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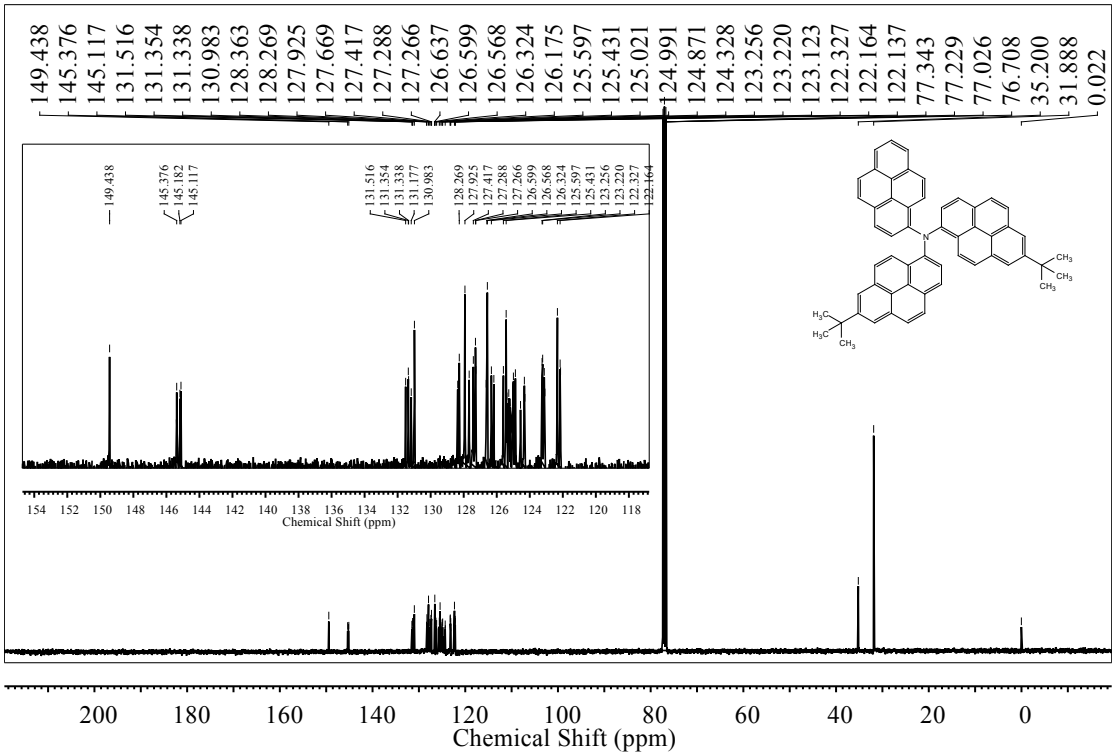
3.03
3.00
17.50
Chemical Shift (ppm)
Chemical Shift (ppm)


149.438
145.376
145.117
131.516
131.354
131.338
130.983
128.363
128.269
127.925
127.669
127.417
127.288
127.266
126.637
126.599
126.568
126.324
126.175
125.597
125.431
125.021
124.991
124.871
124.328
123.256
123.220
123.123
122.327
122.164
122.137
77.343
77.229
77.026
76.708
35.200
31.888
0.022
Chemical Shift (ppm)