Electronic Supplementary Material (ESI) for Materials Advances.

Seven-Member-Ring Based Electron-Transporting Materials for High-efficiency OLEDs

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Contents:

1. moecular design concept of novel ETMs

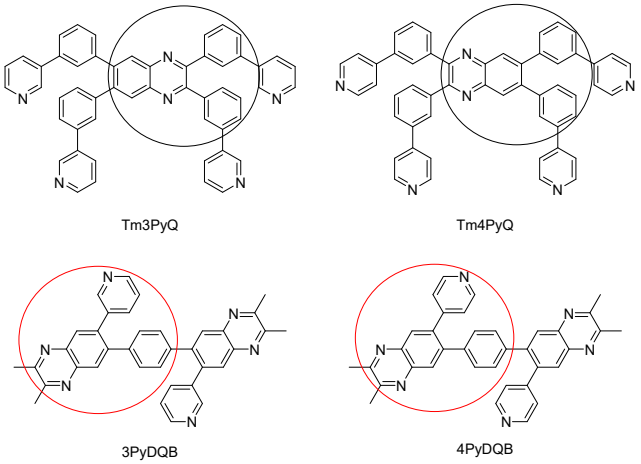


Figure S1. Molecular structures of Tm3PyQ, Tm4PyQ, 3PyDQB, and 4PyDQB.

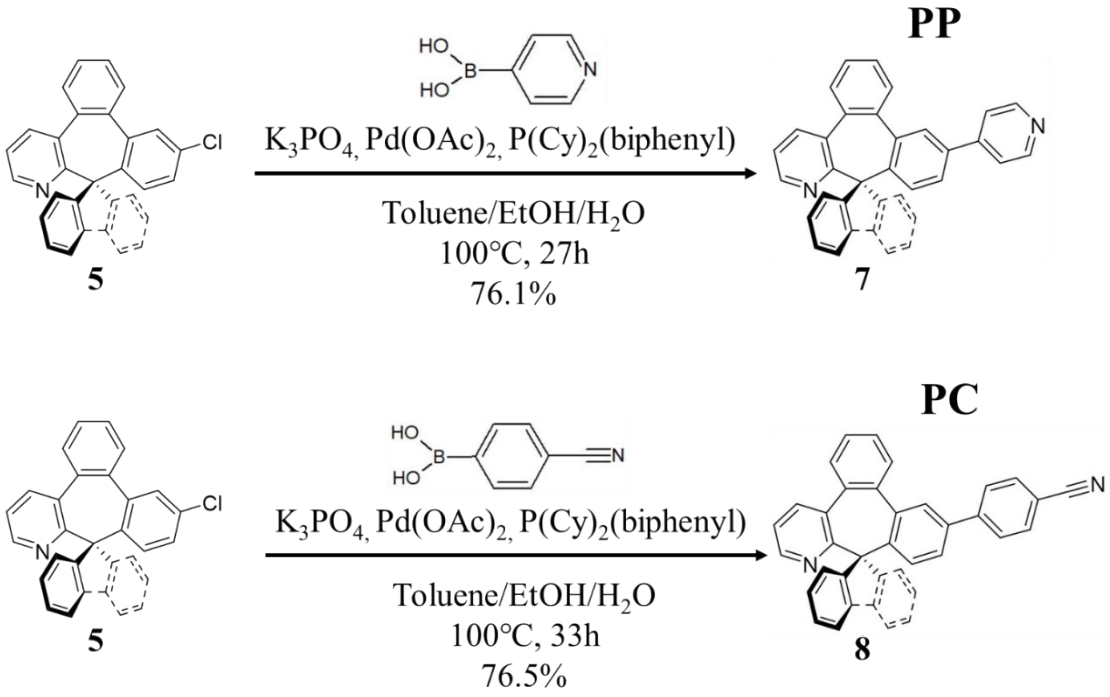
2. ETMs synthesis

Scheme 1 shows the synthesis of the electron transporting materials, namely, PP and PC. 12-Chlorospiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluorene](1922.9 mg, 4.5 mmol), 4-pyridineboronic acid(633.7 mg, 5.4 mmol), potassium phosphate(4776.9 mg, 22.5 mmol) were dissolved in Toluene/EtOH/H_2O. The reaction mixture was heated to 100 °C for 27 h. After cooling to room temperature, the organic layer was separated to remove the solvent. The residue was purified by column chromatography (Hexane/CH_2Cl_2/EtOAc, 1/1/1) to give a light yellow crystalline powder, PP (1.607 g, 76.%).
Spectral Data of PP: M.W.: 470.58; 1H NMR (400 MHz, CDCl3) δ 8.64 (d, J = 5.7 Hz, 2H), 8.34 (dd, J = 4.5, 1.7 Hz, 1H), 8.00 (dd, J = 7.7, 1.6 Hz, 1H), 7.92 (d, J = 2.0 Hz, 1H), 7.84 (d, J = 7.4 Hz, 1H), 7.72-7.67 (m, 4H), 7.63-7.58 (m, 3H), 7.55-7.48 (m, 3H), 7.35 (dd, J = 8.6, 2.0 Hz, 1H), 7.31-7.25 (m, 2H), 7.13 (t, J = 7.3 Hz, 1H), 6.62 (dt, J = 7.6, 1.0 Hz, 1H), 5.80 (d, J = 8.0 Hz, 1H); 13C NMR (125 MHz, CDCl3) δ 160.5, 149.5, 148.6, 148.5, 148.0, 146.7, 146.3, 140.6, 140.3, 140.2, 140.1, 138.3, 137.6, 136.9, 134.6, 133.0, 132.2, 131.7, 129.8, 129.2, 129.0, 127.8, 127.6, 127.1, 125.6, 125.62, 125.57, 122.7, 121.6, 119.8, 69.1; HR-MS Calcd for C35H22N2: 470.1778, found: 470.1776; TLC Rf 0.25 (Hexane/EtOAc, 2/1).

As to the PC, 12-Chlorospiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluorene](2066.4 mg, 4.8 mmol), 4-cyanophenylboronic acid (853 mg, 5.8 mmol), potassium phosphate(5011.6 mg, 24.0 mmol) were dissolved in Toluene/EtOH/H_2O. The reaction mixture was heated to 100 °C for 33 h. After cooling to room

temperature, the organic layer was separated to remove the solvent. The residue was purified by column chromatography (Hexane/CH_2Cl_2, 1/1) to give a light yellow crystalline powder, PC (1.816 g, 76.5%). The description regarding how the 12-Chlorospiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluorene], is synthesized can be referred to in the supplementary information.

Spectral Data of PC: M.W.: 494.60; 1H NMR (400 MHz, CDCl3) δ 8.45 (d, J = 3.3 Hz, 1H), 8.07 (d, J = 7.6 Hz, 1H), 7.87-7.85 (m, 2H), 7.71-7.50 (m, 12H), 7.34-7.25 (m, 3H), 7.14 (t, J = 7.4 Hz, 1H), 6.62 (d, J = 7.6 Hz, 1H), 5.79 (d, J = 8.1 Hz, 1H); 13C NMR (125 MHz, CDCl3) δ 160.1, 148.3, 147.9, 146.3, 145.3, 144.5, 140.5, 140.4, 140.1, 139.0, 138.4, 137.3, 135.1, 132.7, 132.7, 132.6, 132.6, 132.3, 131.8, 130.0, 129.2, 129.0, 128.0, 127.9, 127.5, 127.5, 127.5, 127.2, 126.0, 125.9, 125.2, 123.0, 120.1, 120.0, 118.8, 111.1, 68.7; HR-MS Calcd for C37H22N2: 494.1778, found: 494.1777; TLC Rf 0.36 (Hexane/EtOAc, 4/1).



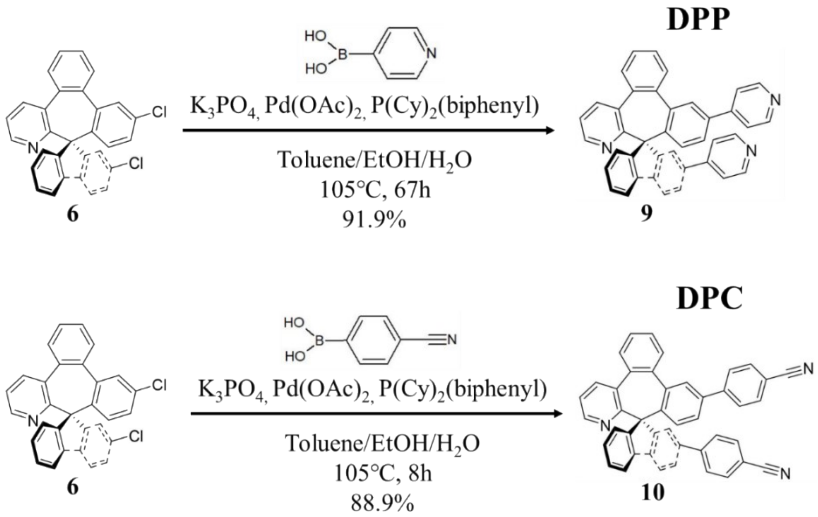
Scheme 1. Schematic illustration of the synthesis of compound 7 (PP) and compound 8 (PC), namely, 12-(Pyridin-4-yl)spiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluorene] and 4-(Spiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluoren]-12-yl)benzonitrile.

Scheme 2 shows the synthesis of the electron transporting materials, namely, DPP and DPC. 2',12-Dichlorospiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluorene] (1664.1 mg, 3.6 mmol), 4-pyridinylboronic acid (1348.7 mg, 10.8 mmol), potassium phosphate(4617.0 mg, 21.6 mmol) were dissolved in Toluene/EtOH/H_2O. The

reaction mixture was heated to 105 °C for 67 h. After cooling to room temperature, the organic layer was separated to remove the solvent. The residue was purified by column chromatography (CH_2Cl_2/Acetone, 2/1) to give a yellow crystalline powder, DPP (1.811 g, 91.9%).
Spectral Data of DPP: M.W.: 547.66; 1H NMR (500 MHz, CDCl3) Conformer A: δ 8.64 (dd, J = 4.5, 1.2 Hz, 2H), 8.50 (d, J = 6.1 Hz, 2H), 8.35 (dd, J = 4.3, 1.8 Hz, 1H), 8.02 (dd, J = 7.9, 1.3 Hz, 1H), 7.95 (d, J = 1.8 Hz, 1H), 7.88 (d, J = 7.3 Hz, 1H), 7.72-7.68 (m, 3H), 7.67-7.65 (m, 2H), 7.61 (d, J = 7.3 Hz, 1H), 7.59-7.52 (m, 2H), 7.47 (d, J = 5.6 Hz, 2H), 7.43 (dd, J = 7.9, 1.2 Hz, 1H), 7.35 (d, J = 2.2 Hz, 1H), 7.31 (d, J = 8.6 Hz, 1H), 7.28 (dd, J = 7.7, 4.7 Hz, 1H), 6.96 (d, J = 6.1 Hz, 2H), 6.41 (d, J = 1.1 Hz, 1H); Conformer B: δ 8.68 (d, J = 6.1 Hz, 2H), 8.63 (dd, J = 4.5, 1.2 Hz, 2H), 8.33 (dd, J = 4.4, 1.4 Hz, 1H), 8.02 (dd, J = 7.9, 1.3 Hz, 1H), 7.96 (d, J = 1.8 Hz, 1H), 7.94 (d, J = 4.5 Hz, 1H), 7.93 (d, J = 1.8 Hz, 1H), 7.83 (dd, J = 8.1, 1.3 Hz, 1H), 7.77 (s, 1H), 7.76 (d, J = 2.2 Hz, 1H), 7.72-7.68 (m, 3H), 7.67-7.65 (m, 1H), 7.64-7.60 (m, 1H), 7.47 (d, J = 5.6 Hz, 2H), 7.38 (d, J = 2.0 Hz, 1H), 7.35 (d, J = 3.3 Hz, 1H), 7.30-7.27 (m, 1H), 7.16 (t, J = 7.3 Hz, 1H), 6.68 (dt, J = 7.7, 1.2 Hz, 1H), 5.84 (d, J = 8.2 Hz, 1H); 13C NMR (125 MHz, CDCl3) Conformer A: δ 160.19, 150.2, 149.7, 149.4, 149.0, 148.9, 148.1, 147.1, 146.8, 145.7, 141.6, 140.3, 139.7, 139.3. 138.5, 137.8, 137.5, 136.3, 135.1, 134.6, 134.4, 133.1, 132.3, 131.7, 130.0, 129.3, 129.3, 129.2, 127.8, 126.7, 126.6, 126.2, 125.8, 124.3, 122.9, 121.5, 121.3, 120.3, 120.2, 69.1; Conformer B: δ 160.15, 150.1, 149.5, 149.4, 149.0, 148.9, 148.1, 147.0, 146.6, 145.7, 141.3, 140.2, 140.0, 139.7, 139.3, 138.4, 137.4, 137.4, 136.3, 135.1, 134.6, 134.5, 133.1, 131.7, 131.6, 129.9, 129.1, 129.0, 128.8, 128.0, 127.7, 126.6, 125.7, 125.4, 122.9, 121.7, 121.5, 120.4, 120.3, 69.2; HR-MS Calcd for C40H25N3: 547.2043, found: 547.2045; TLC Rf 0.07 (Hexane/EtOAc, 2/1).

As to the DPC, 2',12-Dichlorospiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluorene] (1616.5 mg, 3.5 mmol), 4-cyanophenylboronic acid (1544.0 mg, 10.5 mmol), potassium phosphate(4501.0 mg, 21.0 mmol) were dissolved in Toluene/EtOH/H_2O. The reaction mixture was heated to 105 °C for 8 h. After cooling to room temperature, the organic layer was separated to remove the solvent. The residue was purified by column chromatography (Hexane/CH_2Cl_2, 1/2) to give a yellow crystalline powder, DPC (1.853 g, 88.9%). The description regarding how the 2',12-Dichlorospiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluorene], is synthesized can be referred to in the supplementary information.
Spectral Data of DPC: M.W.: 595.71; 1H NMR (500 MHz, CDCl3) Conformer A: δ 8.37 (dd, J = 4.6, 1.5 Hz, 1H), 8.04 (dd, J = 7.8, 1.5 Hz, 1H), 7.91 (s, 1H), 7.88 (s, 1H), 7.83 (d, J = 8.3 Hz, 1H), 7.75-7.65 (m, 9H), 7.61 (d, J = 7.5 Hz, 1H), 7.58-7.54 (m,

3H), 7.39 (dd, J = 7.9, 1.8 Hz, 1H), 7.34-7.29 (m, 3H), 7.13 (d, J = 8.0 Hz, 2H), 6.36 (d, J = 1.2 Hz, 1H); Conformer B: δ 8.36 (dd, J = 4.6, 1.5 Hz, 1H), 8.04 (dd, J = 7.8, 1.5 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.91 (s, 1H), 7.89 (s, 1H), 7.78 (dd, J = 8.0, 1.6 Hz, 1H), 7.77 (d, J = 1.8, 1H), 7.74-7.64 (m, 9H), 7.59-7.53 (m, 3H), 7.35-7.29 (m, 3H), 7.17 (t, J = 7.5 Hz, 1H), 6.68 (dt, J = 7.7, 1.2 Hz, 1H), 5.85 (d, J = 8.1 Hz, 1H);13C NMR (125 MHz, CDCl3) Conformer A: δ 160.2, 149.7, 149.2, 146.8, 146.1, 145.3, 145.2, 144.3, 141.2, 140.4, 140.0, 139,4, 138.6, 138.5, 137.8, 137.4, 134.5, 133.0, 132.6, 132.3, 131.9, 131.8, 130.2, 129.2, 129.2, 127.9, 127.8, 127.5, 126.9, 126.2, 126.0, 124.5, 122.9, 120.3, 120.2, 119.0, 118.7, 111.2, 110.3, 69.1; Conformer B: δ 160.1, 149.4, 148.9, 146.6, 146.1, 145.3, 145.2, 144.3, 140.9, 140.2, 139.7, 139.4, 138.6, 138.5, 137.4, 136.3, 134.7, 133.0, 132.5, 132.3, 131.9, 131.7, 130.1, 129.1, 128.8, 128.0, 127.7, 127.5, 126.9, 125.9, 125.4, 124.5, 122.9, 120.5, 120.2, 119.0, 118.7, 111.2, 110.6, 69.2; HR-MS Calcd for C44H25N3: 595.2043, found: 595.2045; TLC Rf 0.54 (Hexane/EtOAc, 2/1).



Scheme 2. Schematic illustration of the synthesis of compound 9 (DPP) and compound 10 (DPC), namely, 2',12-di(Pyridin-4-yl)spiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluorene] and 4,4'-(Spiro[dibenzo[3,4:5,6]cyclohepta[1,2-b]pyridine-9,9'-fluorene]-2',12-diyl)dibenzonitrile.

3. DSC data and graph of the four seven-member-ring based ETMs

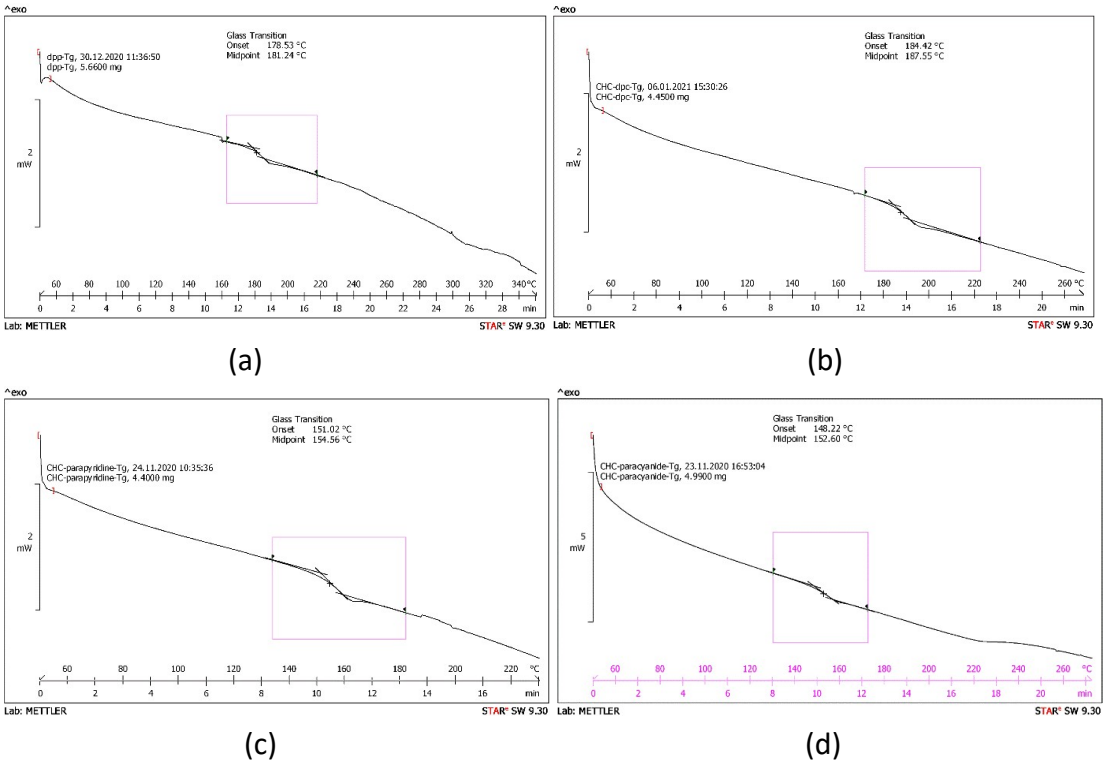
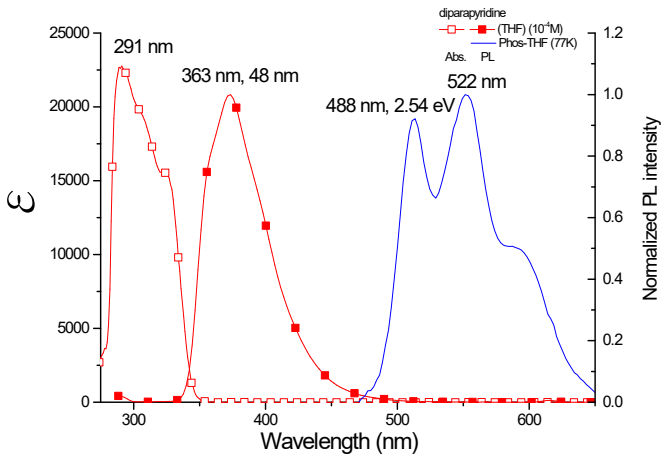
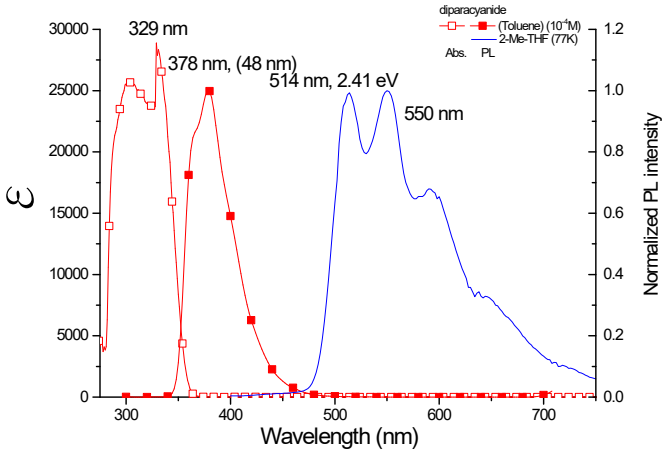


Figure S2. DSC data and graph of (a) 1-aza-DBdippy (DPP), (b) 1-aza-DBdipPhCN (DPC), (c) 1-aza-DBppy (PP), (d) 1-aza-DBpPhCN (PC).

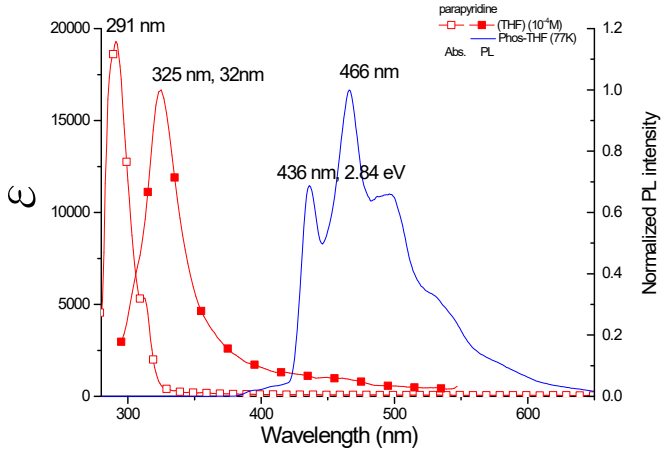
4. Photoluminescence (PL) spectra



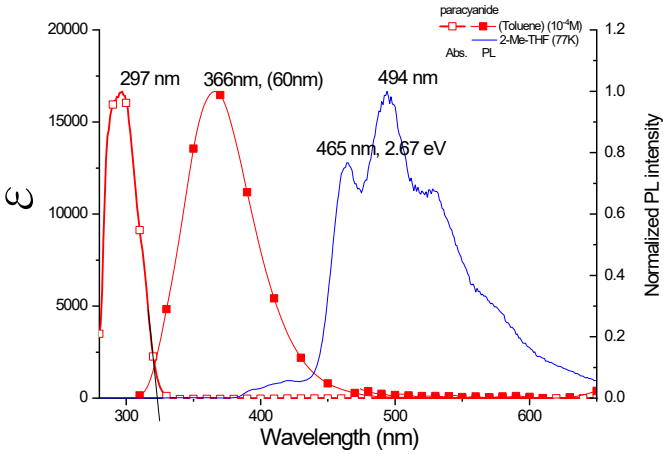
(a)



(b)



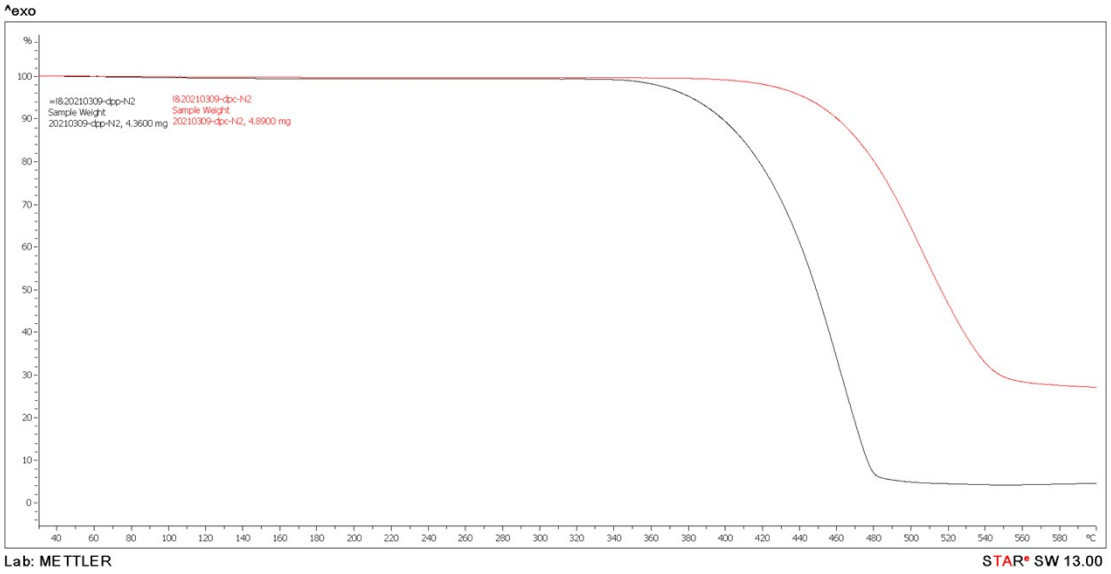
(c)



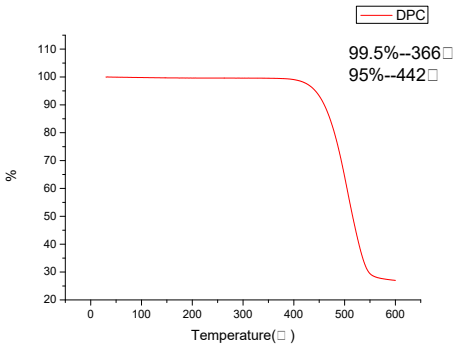
(d)

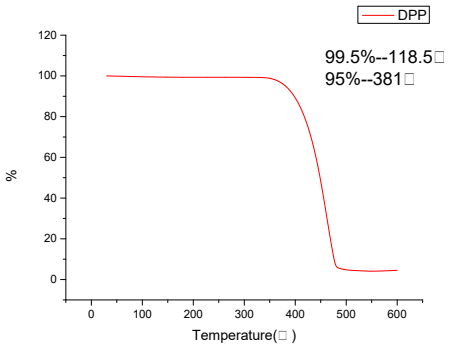
Figure S3. Photoluminescence (PL) spectra of (a) 1-aza-DBdippy (DPP), (b) 1-aza-DBdipPhCN (DPC), (c) 1-aza-DBppy (PP), (d) 1-aza-DBpPhCN (PC).

5. TGA:



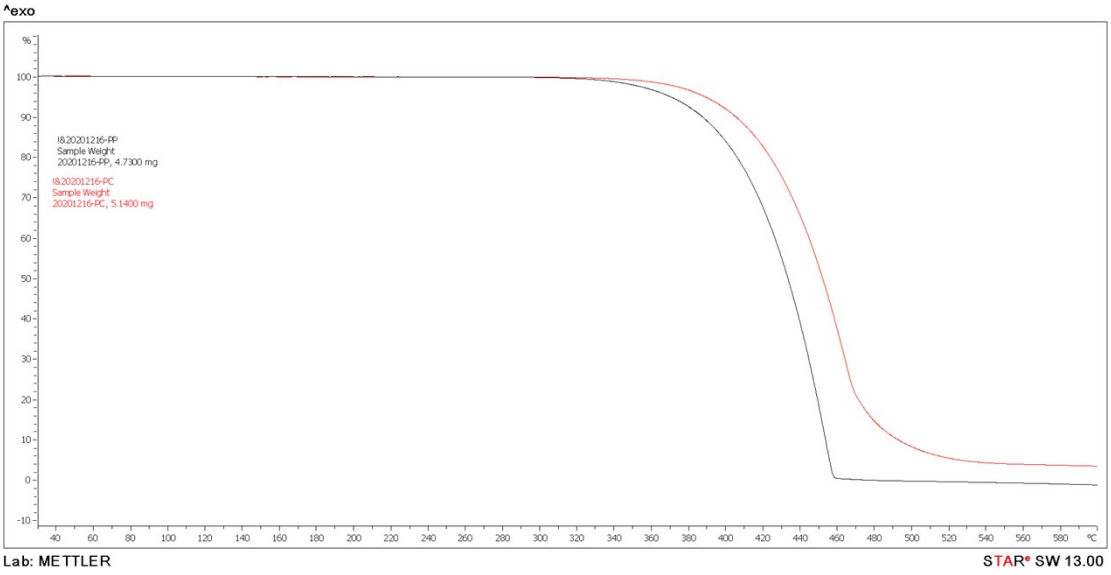
(a)



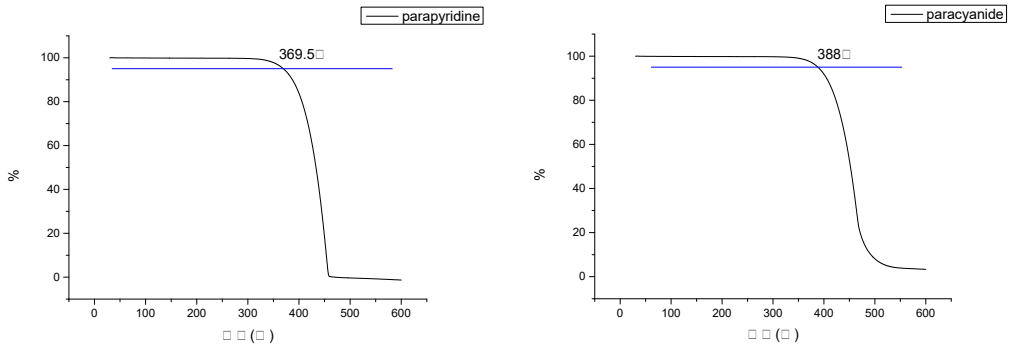


(b) (c)

Figure S4. (a)Effect of DPC and DPP on TGA. TGA curves of (b) DPC, (c) DPP.



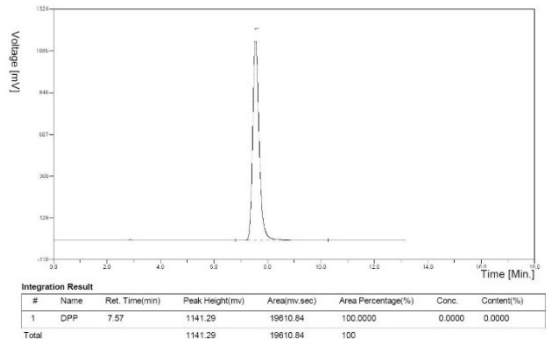
(a)



(b) (c)

Figure S5. (a)Effect of PP and PC on TGA. TGA curves of (b) PP, (c) PC.

6. HPLC:



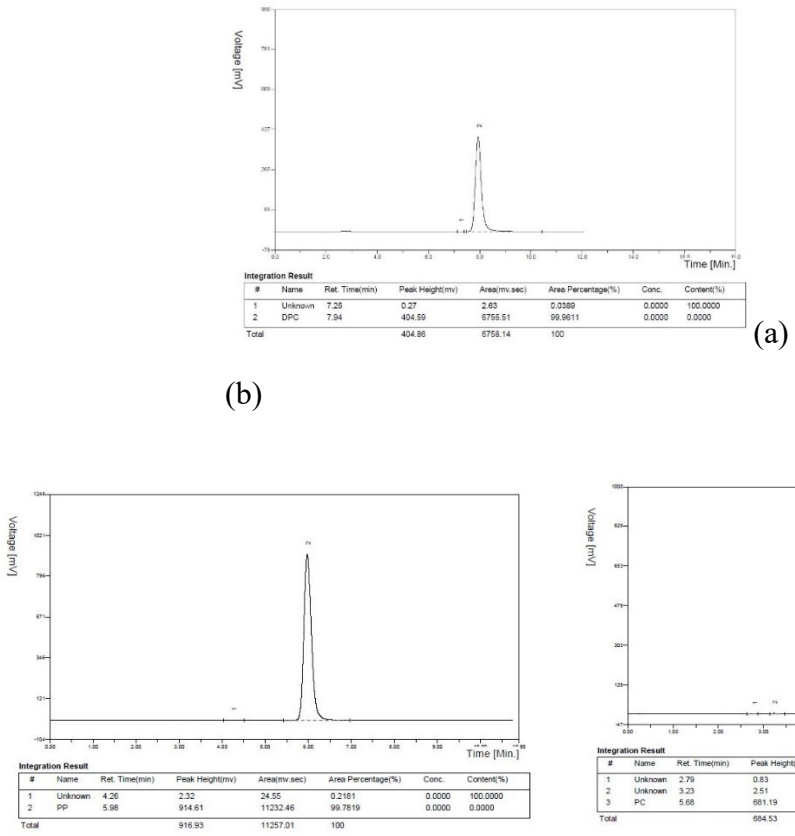
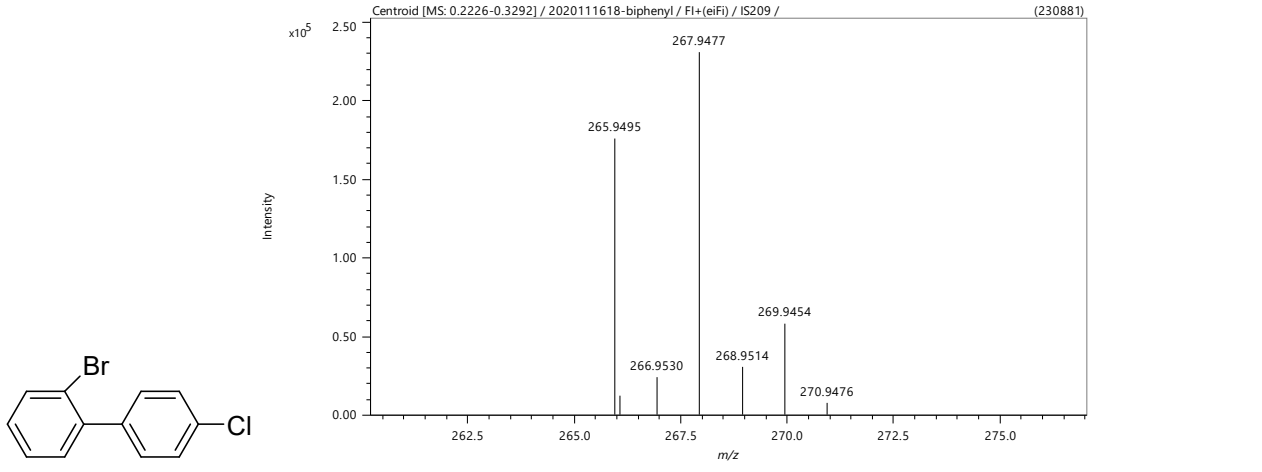


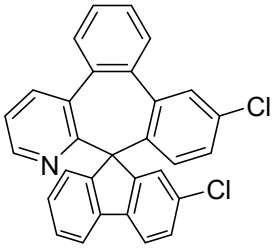
Figure S6. HPLC spectra of (a) DPP, (b) DPC, (c) PP, (d) PC.

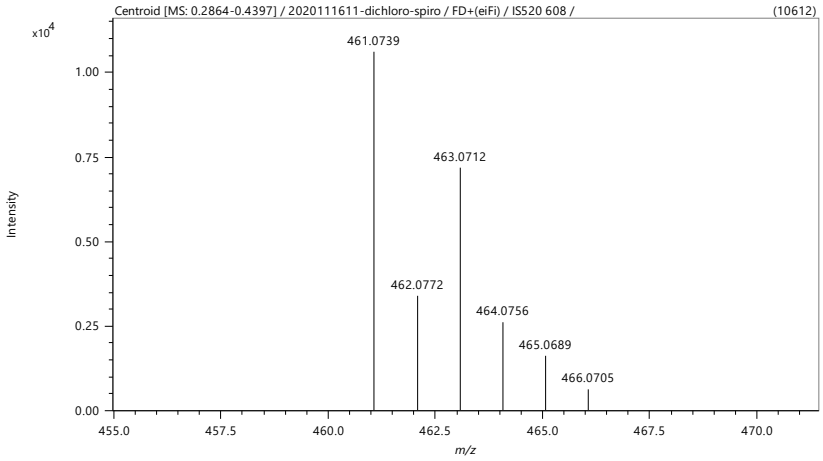
7. Mass spectra for all the intermediate and final compounds



	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▶	265.94952	175704.54	C12 H8 Cl Br	265.94924	0.28	1.05	8.0

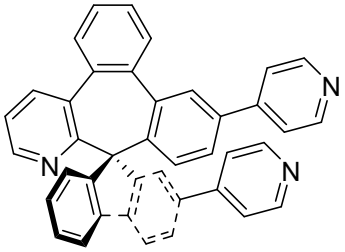
(a)

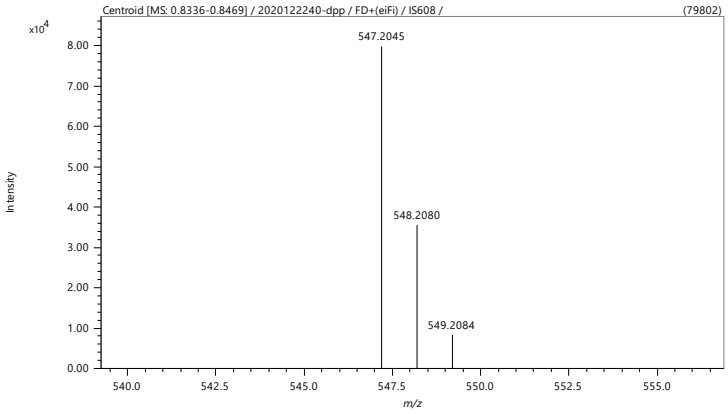




	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▶	461.07389	10611.86	C30 H17 N Cl2	461.07326	0.63	1.36	22.0

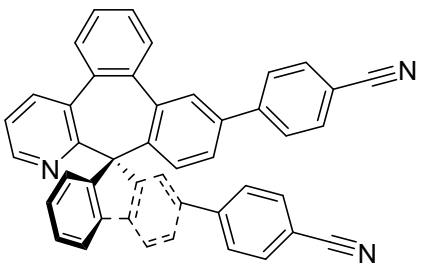
(b)

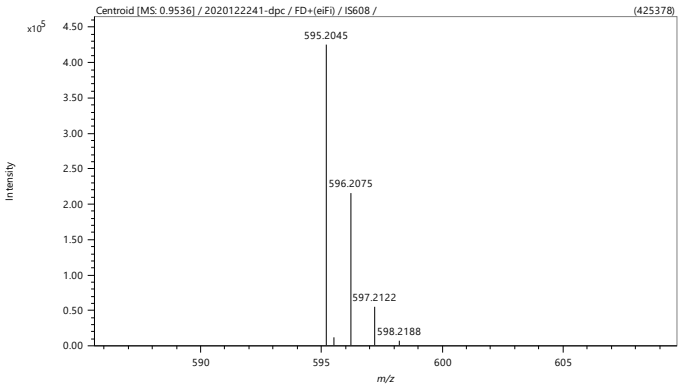




	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▶	547.20446	79801.73	C40 H25 N3	547.20430	0.16	0.29	30.0

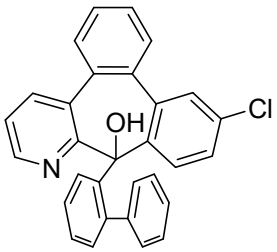
(c)

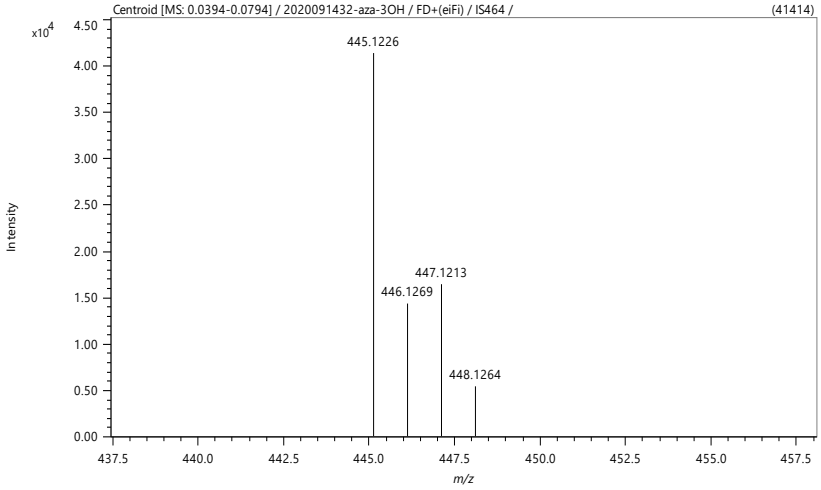




	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▶	595.20453	425378.00	C44 H25 N3	595.20430	0.23	0.38	34.0

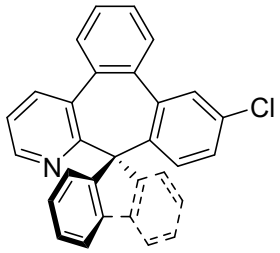
(d)

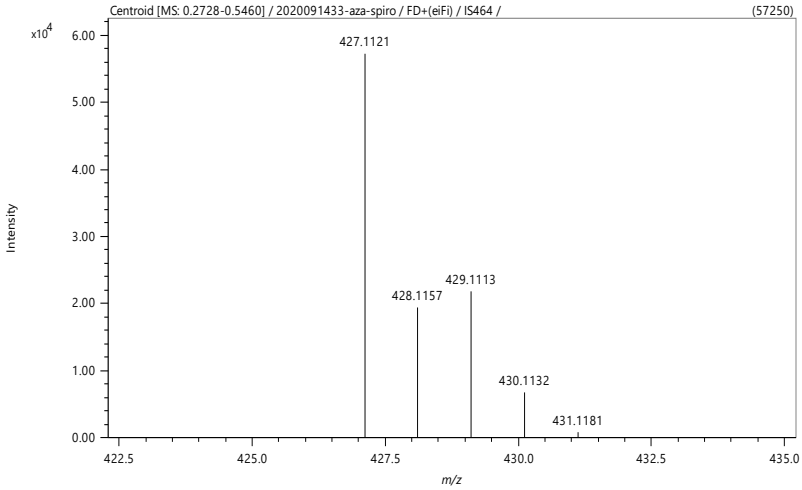




	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▶	445.12257	41413.68	C30 H20 N O Cl	445.12279	-0.22	-0.49	21.0

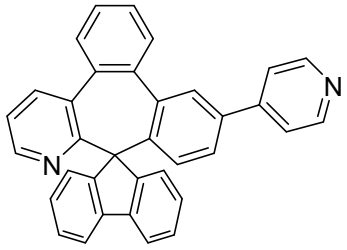
(e)

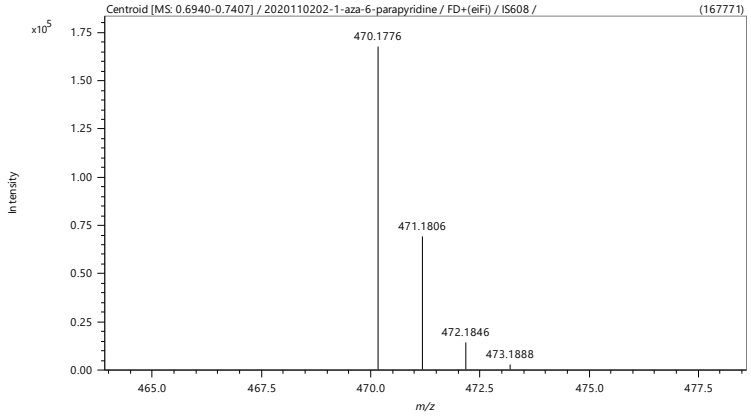




	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▶	427.11214	57250.15	C30 H18 N Cl	427.11223	-0.08	-0.20	22.0

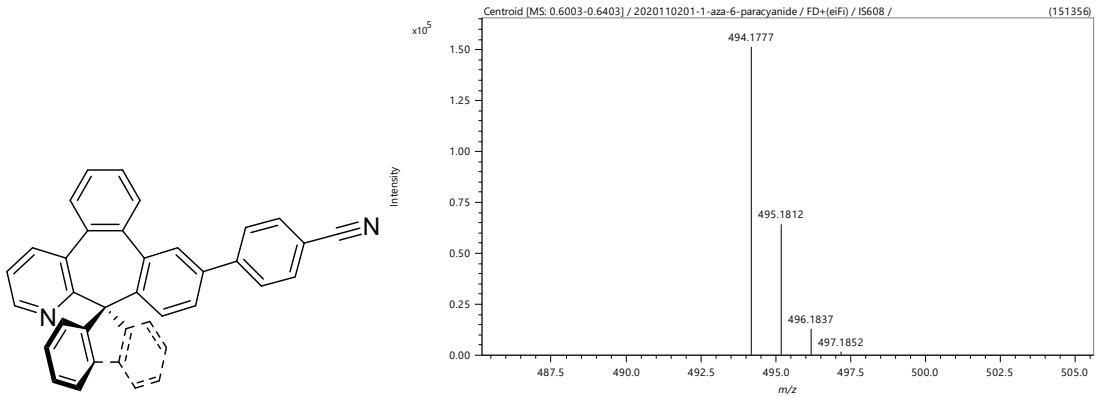
(f)





	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▶	470.17763	167770.92	C35 H22 N2	470.17775	-0.12	-0.25	26.0

(g)

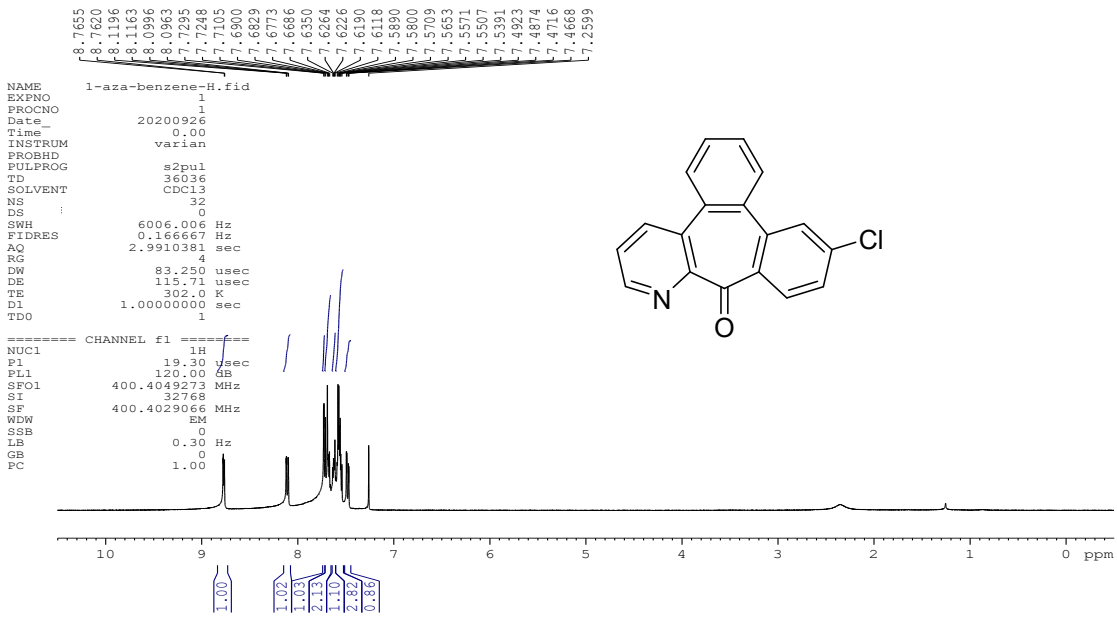


	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▶	494.17769	151356.24	C37 H22 N2	494.17775	-0.06	-0.13	28.0

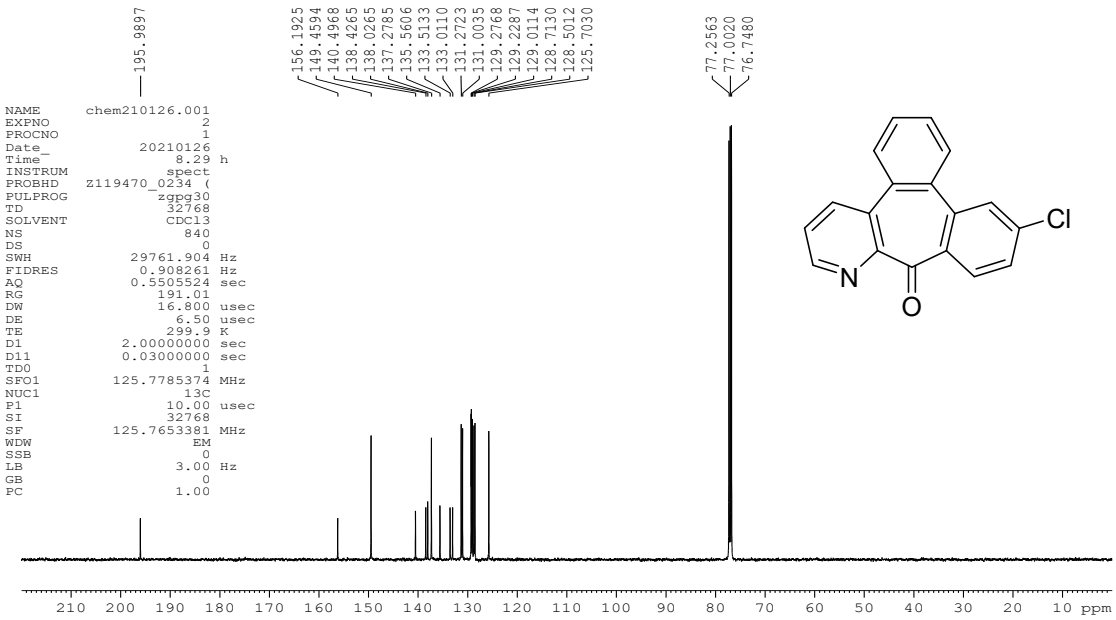
(h)

Figure S7. Mass spectra of (a) (b) intermediate compounds of DPP and DPC, (c) DPP, (d) DPC, (e) (f) intermediate compounds of PP and PC, (g) PP, (h) PC

9. NMR spectra for all the intermediate and final compounds



(a)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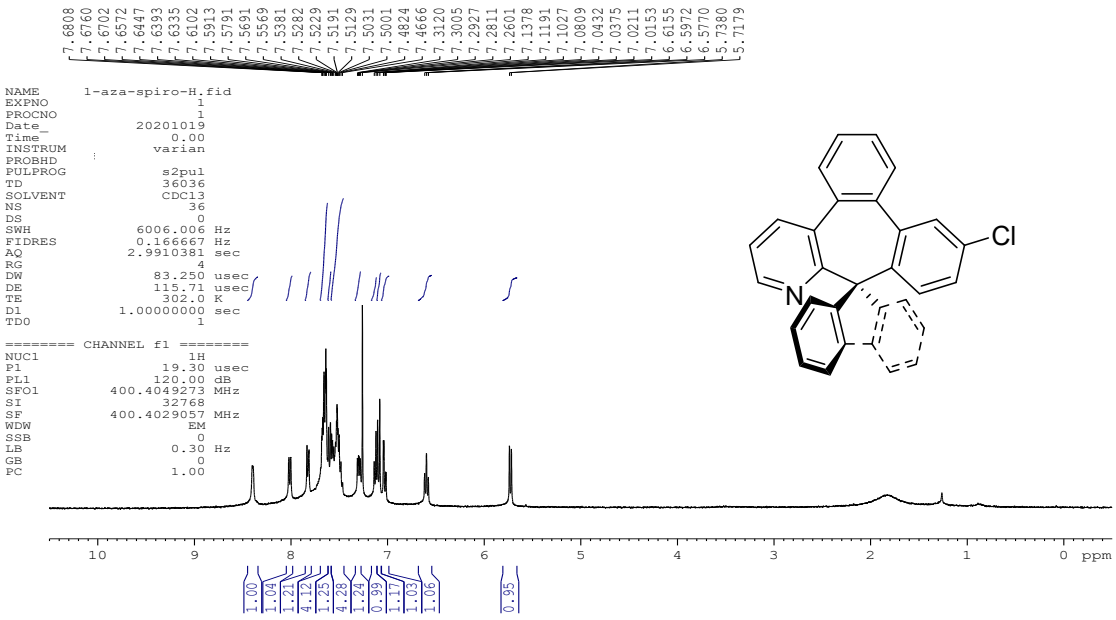
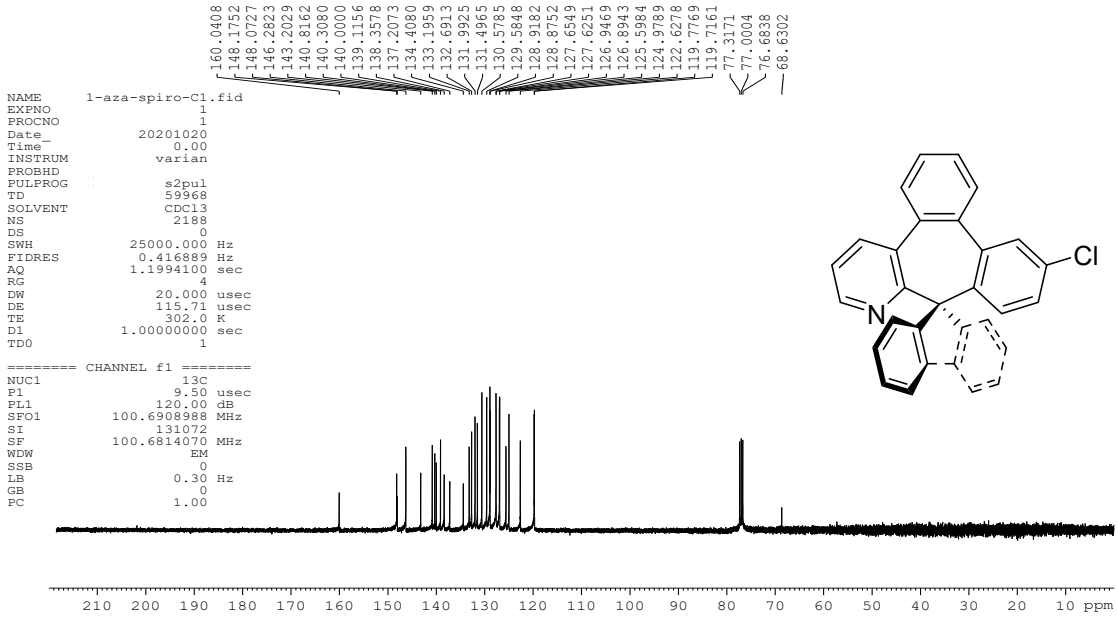
149.4594
140.4968
138.4265
138.0265
137.2785
135.5606
133.5133
133.0110
131.2723
131.0035
129.2768
129.2287
129.0114
128.7130
128.5012
125.7030
77.2563
77.0020
76.7480
NAME chem210126.001
EXPNO 2
PROCNO 1
Date_ 20210126
Time 8.29 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 840
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653381 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Cl
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

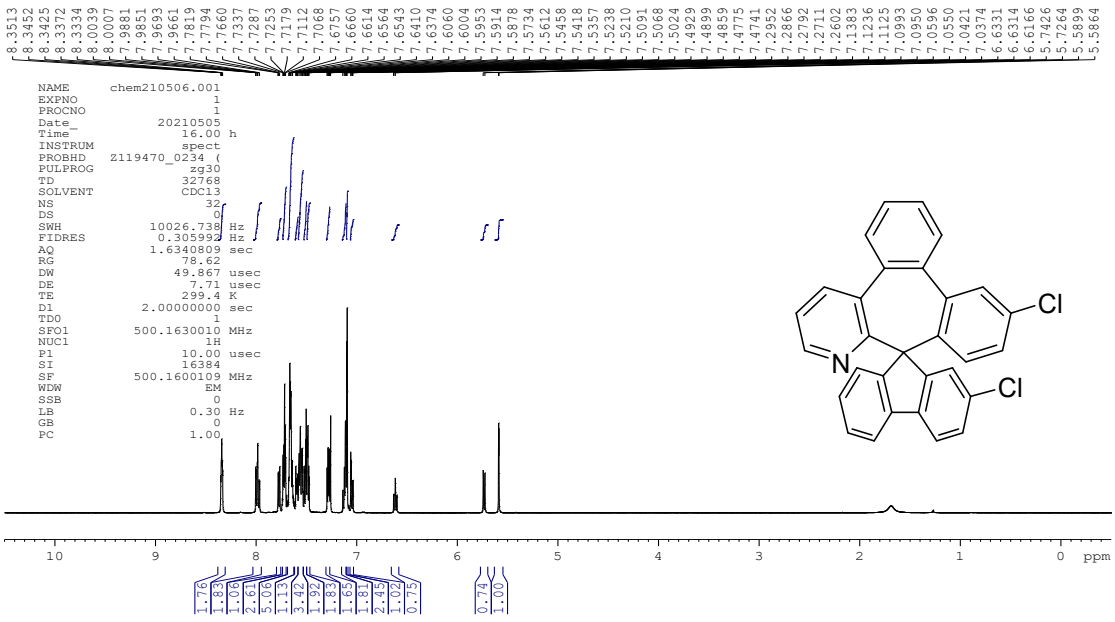
(b)


7.6808
7.6760
7.6702
7.6572
7.6447
7.6393
7.6335
7.6102
7.5913
7.5791
7.5691
7.5569
7.5381
7.5282
7.5229
7.5191
7.5129
7.5031
7.5001
7.4824
7.4666
7.3120
7.3005
7.2927
7.2811
7.2601
7.1378
7.1191
7.1027
7.0809
7.0432
7.0375
7.0211
7.0153
6.6155
6.5972
6.5770
5.7380
5.7179
NAME 1-aza-spiro-H.fid
EXPNO 1
PROCNO 1
Date_ 20201019
Time 0.00
INSTRUM varian
PROBHD
PULPROG s2pul
TD 36036
SOLVENT CDCl3
NS 36
DS 0
SWH 6006.006 Hz
FIDRES 0.166667 Hz
AQ 2.9910381 sec
RG 4
DW 83.250 usec
DE 115.71 usec
TE 302.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 19.30 usec
PL1 120.00 dB
SFO1 400.4049273 MHz
SI 32768
SF 400.4029057 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
N
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.04
1.21
4.12
1.25
4.28
1.24
0.99
1.17
1.03
1.06
0.95

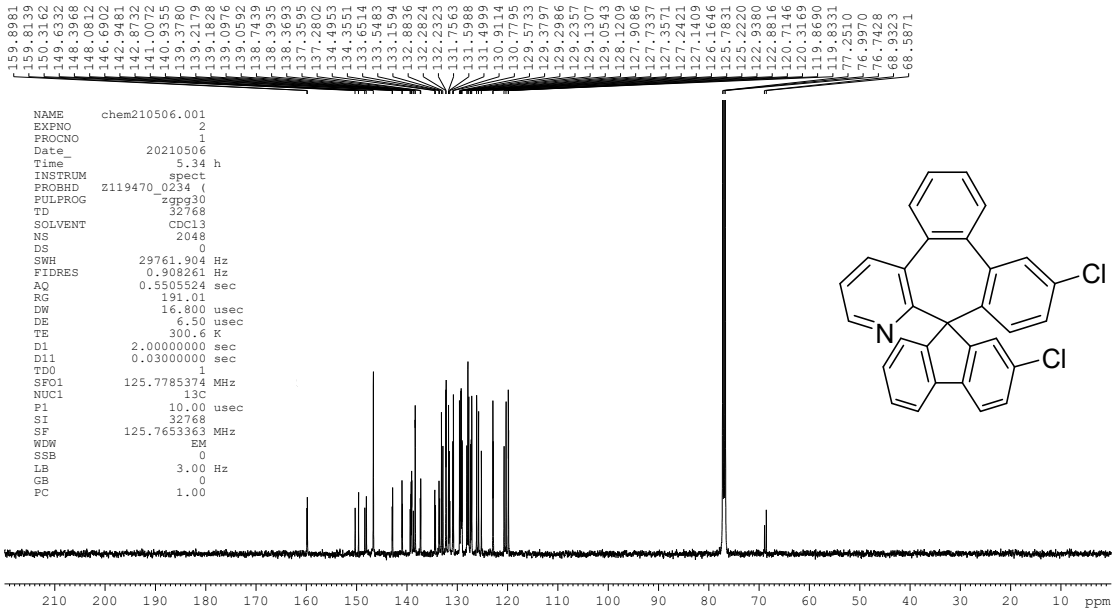
(c)


160.0408
148.1752
148.0727
146.2823
143.2029
140.8162
140.3080
140.0000
139.1156
138.3578
137.2073
134.4080
133.1959
132.6913
131.9925
131.4965
130.5785
129.5848
128.9182
128.8752
127.6549
127.6251
126.9469
126.8943
125.5984
124.9789
122.6278
119.7769
119.7161
77.3171
77.0004
76.6838
68.6302
NAME 1-aza-spiro-C1.fid
EXPNO 1
PROCNO 1
Date_ 20201020
Time 0.00
INSTRUM varian
PROBHD
PULPROG s2pul
TD 59968
SOLVENT CDCl3
NS 2188
DS 0
SWH 25000.000 Hz
FIDRES 0.416889 Hz
AQ 1.1994100 sec
RG 4
DW 20.000 usec
DE 115.71 usec
TE 302.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 120.00 dB
SFO1 100.6908988 MHz
SI 131072
SF 100.6814070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

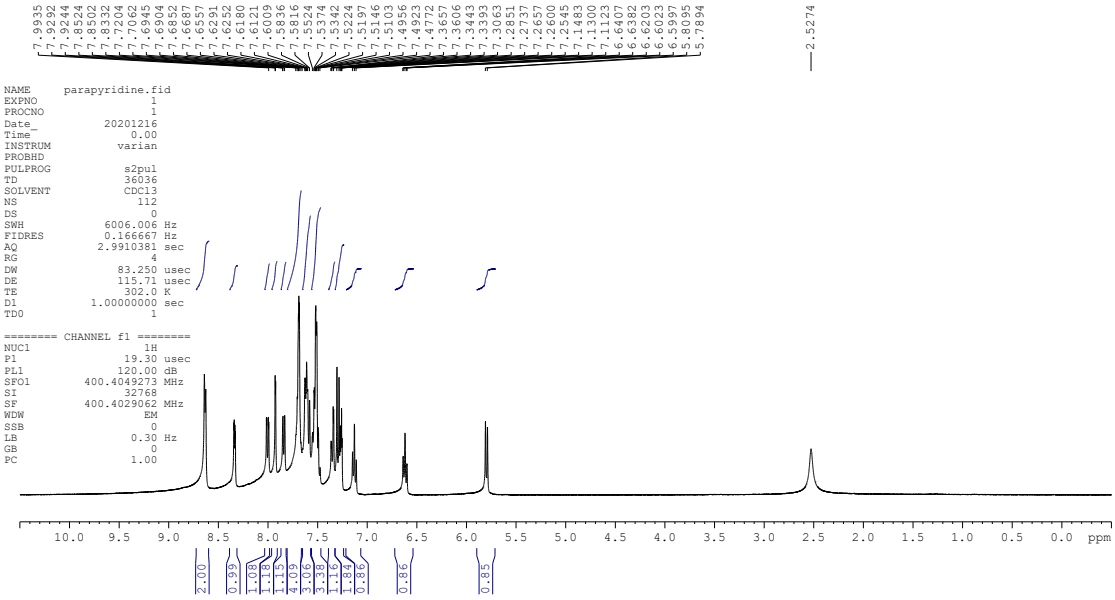
(d)


8.3513
8.3452
8.3425
8.3372
8.3334
8.0039
8.0007
7.9881
7.9851
7.9693
7.9661
7.7819
7.7794
7.7660
7.7337
7.7287
7.7253
7.7179
7.7112
7.7068
7.6757
7.6660
7.6614
7.6564
7.6543
7.6410
7.6374
7.6060
7.6004
7.5953
7.5914
7.5878
7.5734
7.5612
7.5458
7.5418
7.5357
7.5238
7.5210
7.5091
7.5068
7.5024
7.4929
7.4899
7.4859
7.4775
7.4741
7.2952
7.2866
7.2792
7.2711
7.2602
7.1383
7.1236
7.1125
7.0993
7.0950
7.0596
7.0550
7.0421
7.0374
6.6331
6.6314
6.6166
5.7426
5.7264
5.5899
5.5864
NAME chem210506.001
EXPNO 1
PROCNO 1
Date_ 20210505
Time 16.00 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
AQ 1.6340809 sec
RG 78.62
DW 49.867 usec
DE 7.71 usec
TE 299.4 K
D1 2.00000000 sec
TD0 1
SFO1 500.1630010 MHz
NUC1 1H
P1 10.00 usec
SI 16384
SF 500.1600109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
N
Cl
10 9 8 7 6 5 4 3 2 1 0 ppm
1.76
1.83
1.06
2.61
5.06
1.13
3.42
1.92
1.83
1.65
1.81
2.45
1.02
0.75
0.74
1.00

(e)


159.8981
159.8139
150.3162
149.6332
148.3968
148.0812
146.6902
142.9481
142.8732
141.0072
140.9355
139.3780
139.2179
139.1828
139.0976
139.0592
138.7439
138.3935
138.3693
137.3595
137.2802
134.4953
134.3551
133.6514
133.5483
133.1594
132.8836
132.2824
132.2323
131.7563
131.5988
131.4999
130.9114
130.7795
129.5733
129.3797
129.2986
129.2357
129.1307
129.0543
128.1209
127.9086
127.7337
127.3571
127.2421
127.1409
126.1646
125.7831
125.2220
122.9380
122.8816
120.7146
120.3169
119.8690
119.8331
77.2510
76.9970
76.7428
68.9323
68.5871
NAME chem210506.001
EXPNO 2
PROCNO 1
Date_ 20210506
Time 5.34 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2048
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653363 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Cl
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

(f)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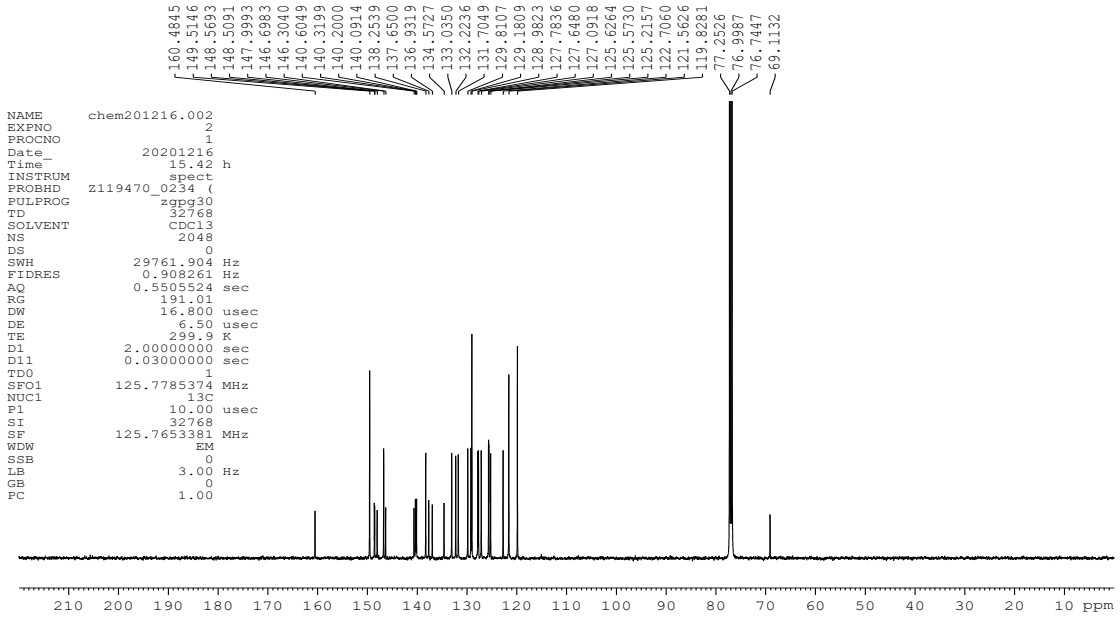
7.9244
7.8524
7.8502
7.8332
7.7204
7.7062
7.6945
7.6904
7.6852
7.6687
7.6557
7.6291
7.6252
7.6180
7.6021
7.5809
7.5836
7.5816
7.5524
7.5374
7.5342
7.5224
7.5197
7.5146
7.5103
7.4956
7.4923
7.4772
7.3657
7.3606
7.3443
7.3393
7.3063
7.2851
7.2737
7.2657
7.2600
7.2545
7.1483
7.1300
7.1123
6.6407
6.6382
6.6223
6.5997
5.8095
5.7894
2.5274
NAME parapyridine.fid
EXPNO 1
PROCNO 1
Date_ 20201216
Time 0.00
INSTRUM varian
PROBHD
PULPROG s2pul
TD 36036
SOLVENT CDCl3
NS 112
DS 0
SWH 6006.006 Hz
FIDRES 0.166667 Hz
AQ 2.9910381 sec
RG 4
DW 83.250 usec
DE 115.71 usec
TE 302.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 19.30 usec
PL1 120.00 dB
SFO1 400.4049273 MHz
SI 32768
SF 400.4029062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
2.00
0.99
1.08
1.16
1.15
4.09
3.06
3.38
1.15
1.84
0.86
0.86
0.85

(g)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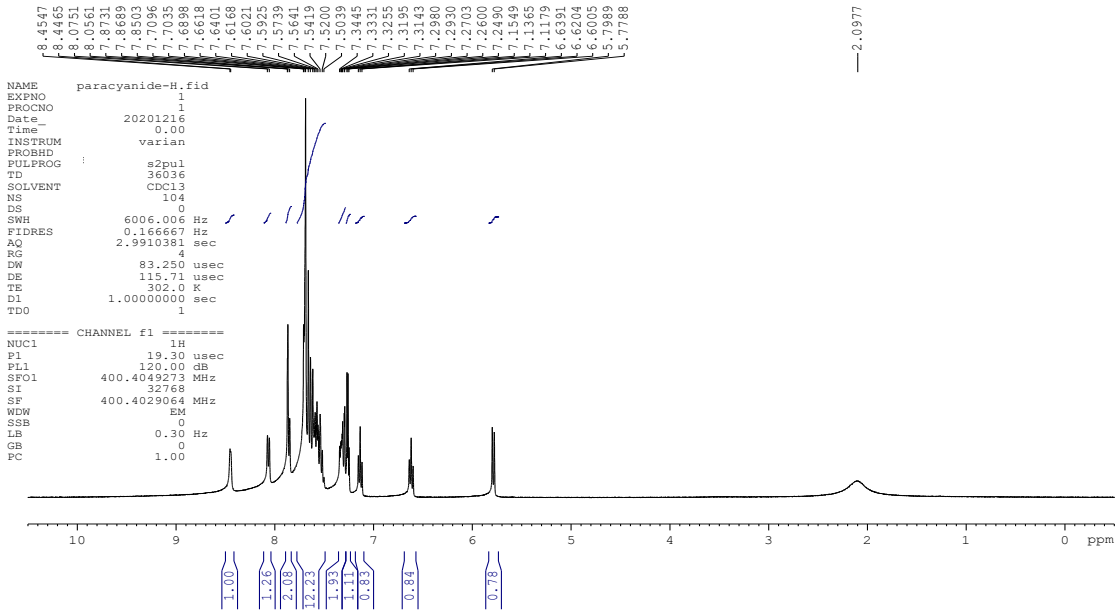
148.5091
147.9993
146.6983
146.3040
140.6049
140.3199
140.2000
140.0914
138.2539
137.6500
136.9319
134.5727
133.0350
132.2236
131.7049
129.8107
129.1809
128.9823
127.7836
127.6480
127.0918
125.6264
125.5730
125.2157
122.7060
121.5626
119.8281
77.2526
76.9987
76.7447
69.1132
NAME chem201216.002
EXPNO 2
PROCNO 1
Date_ 20201216
Time_ 15.42 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2048
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653381 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

(h)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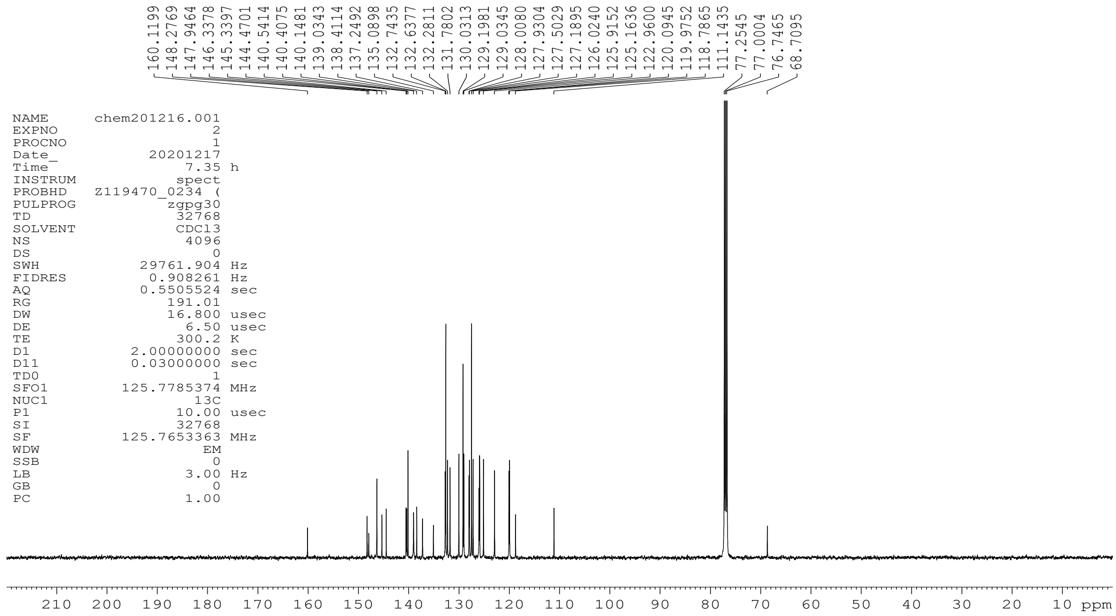
8.4465
8.0751
8.0561
7.8731
7.8689
7.8503
7.7096
7.7035
7.6898
7.6618
7.6401
7.6168
7.6021
7.5925
7.5739
7.5641
7.5419
7.5200
7.5039
7.3445
7.3331
7.3255
7.3195
7.3143
7.2980
7.2930
7.2703
7.2600
7.2490
7.1549
7.1365
7.1179
6.6391
6.6204
6.6005
5.7989
5.7788
2.0977
NAME paracyanide-H.fid
EXPNO 1
PROCNO 1
Date_ 20201216
Time 0.00
INSTRUM varian
PROBHD
PULPROG s2pul
TD 36036
SOLVENT CDCl3
NS 104
DS 0
SWH 6006.006 Hz
FIDRES 0.166667 Hz
AQ 2.9910381 sec
RG 4
DW 83.250 usec
DE 115.71 usec
TE 302.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 19.30 usec
PL1 120.00 dB
SFO1 400.4049273 MHz
SI 32768
SF 400.4029064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.26
2.08
12.23
1.93
1.11
0.83
0.84
0.78

(i)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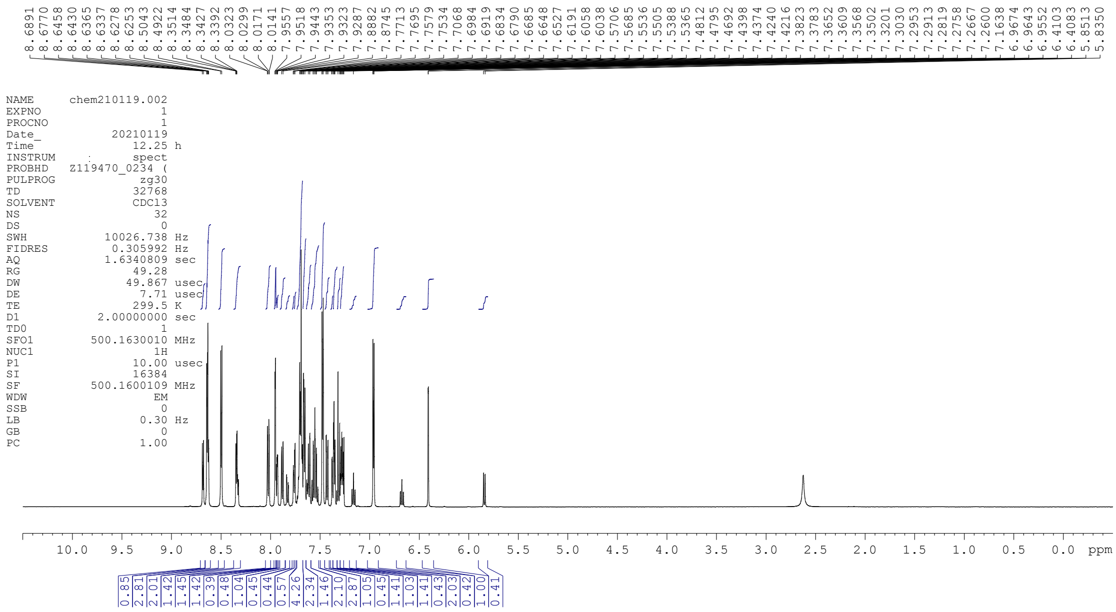
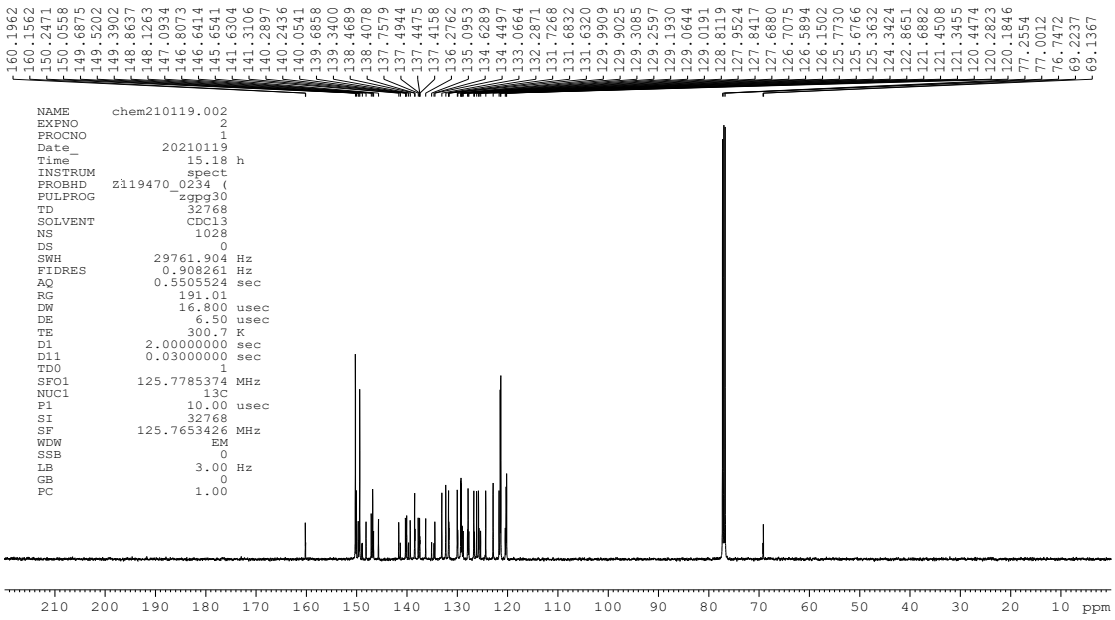
148.2769
147.9464
146.3378
145.3397
144.4701
140.5414
140.4075
140.1481
139.0343
138.4114
137.2492
135.0898
132.7435
132.6377
132.2811
131.7802
130.0313
129.1981
129.0345
128.0080
127.9304
127.5029
127.1895
126.0240
125.9152
125.1636
122.9600
120.0945
119.9752
118.7865
111.1435
77.2545
77.0004
76.7465
68.7095
NAME chem201216.001
EXPNO 2
PROCNO 1
Date_ 20201217
Time 7.35 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4096
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653363 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

(j)


8.6891
8.6770
8.6458
8.6430
8.6365
8.6337
8.6278
8.6253
8.5043
8.4922
8.3514
8.3484
8.3427
8.3392
8.0323
8.0299
8.0171
8.0141
7.9557
7.9518
7.9443
7.9353
7.9323
7.9287
7.9287
7.8882
7.8745
7.7713
7.7695
7.7579
7.7534
7.7068
7.6984
7.6919
7.6834
7.6790
7.6685
7.6648
7.6527
7.6191
7.6058
7.6038
7.5706
7.5685
7.5536
7.5505
7.5388
7.5365
7.4812
7.4795
7.4692
7.4398
7.4374
7.4240
7.4216
7.3823
7.3783
7.3652
7.3609
7.3568
7.3502
7.3201
7.3030
7.2953
7.2913
7.2819
7.2758
7.2667
7.2600
7.1638
6.9674
6.9643
6.9552
6.4103
6.4083
5.8513
5.8350
NAME chem210119.002
EXPNO 1
PROCNO 1
Date_ 20210119
Time 12.25 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
AQ 1.6340809 sec
RG 49.28
DW 49.867 usec
DE 7.71 usec
TE 299.5 K
D1 2.00000000 sec
TD0 1
SFO1 500.1630010 MHz
NUC1 1H
P1 10.00 usec
SI 16384
SF 500.1600109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm

(k)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NAME chem210119.002
EXPNO 2
PROCNO 1
Date_ 20210119
Time 15.18 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1028
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.7 K
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D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653426 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
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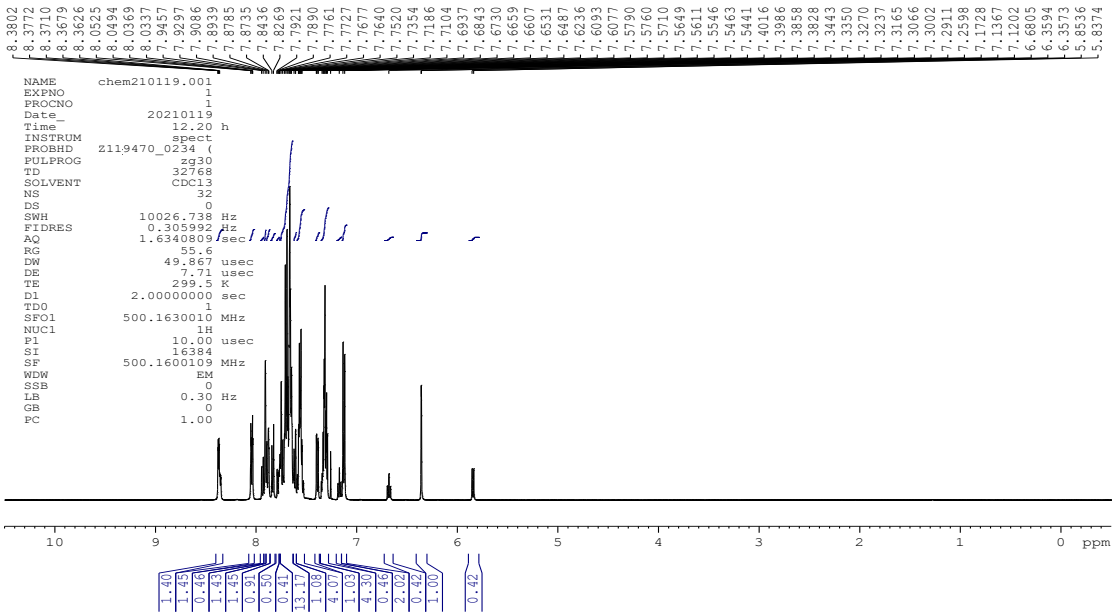
(l)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PROCNO 1
Date_ 20210119
Time 12.20 h
INSTRUM spect
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
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DE 7.71 usec
TE 299.5 K
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
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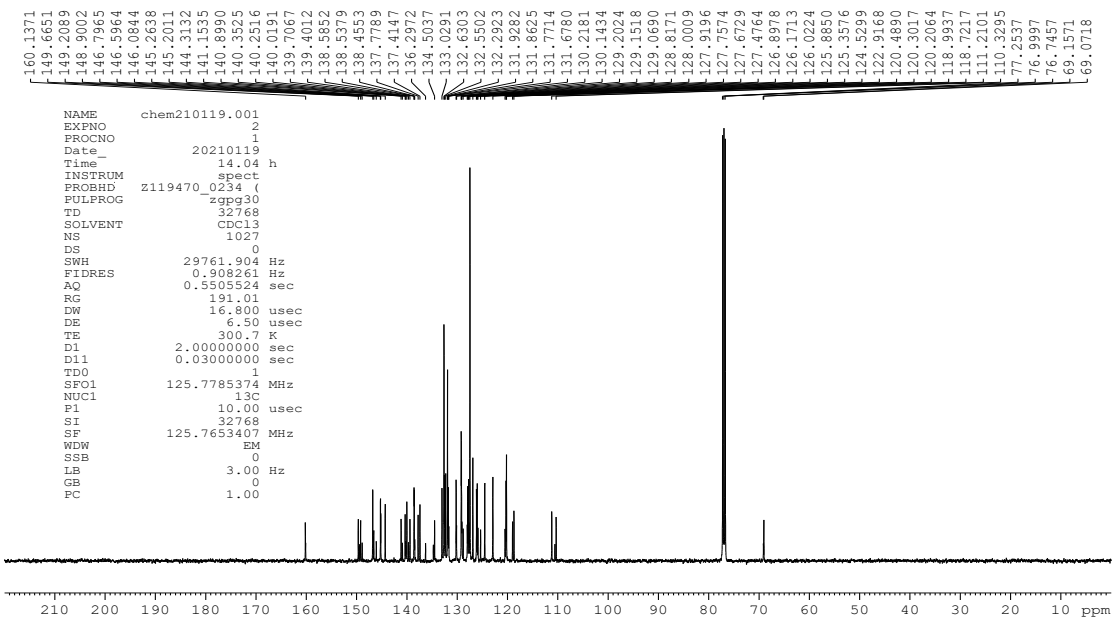
(m)



(n)

Figure S7. ^{1}H NMR spectrums of (a) (c) (e) intermediate compounds, (g) PP, (i) PC, (k)DPP, (m) DPC. ^{13}C NMR spectrums of(b) (d) (e)intermediate compounds, (h) PP, (j) PC, (l) DPP, (n) DPC.