

Electronic Supplementary Information (ESI)

Metal-Free Organic Dyes Derived from Triphenylethylene for Dye-Sensitized Solar Cells: Tuning of the Performance by Phenothiazine and Carbazole

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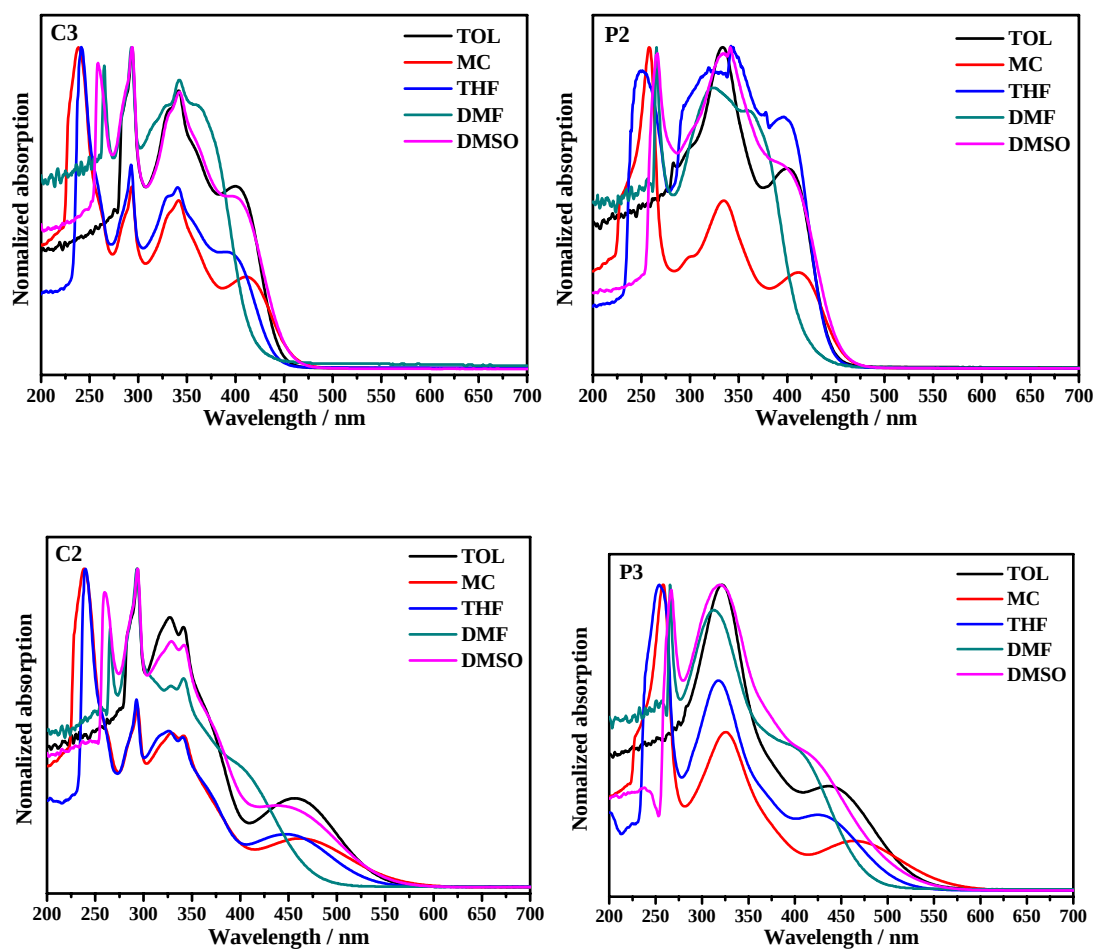


Fig. S1. UV-vis absorption spectra of **C3**, **P2**, **C2** and **P3** dyes in different solvents.

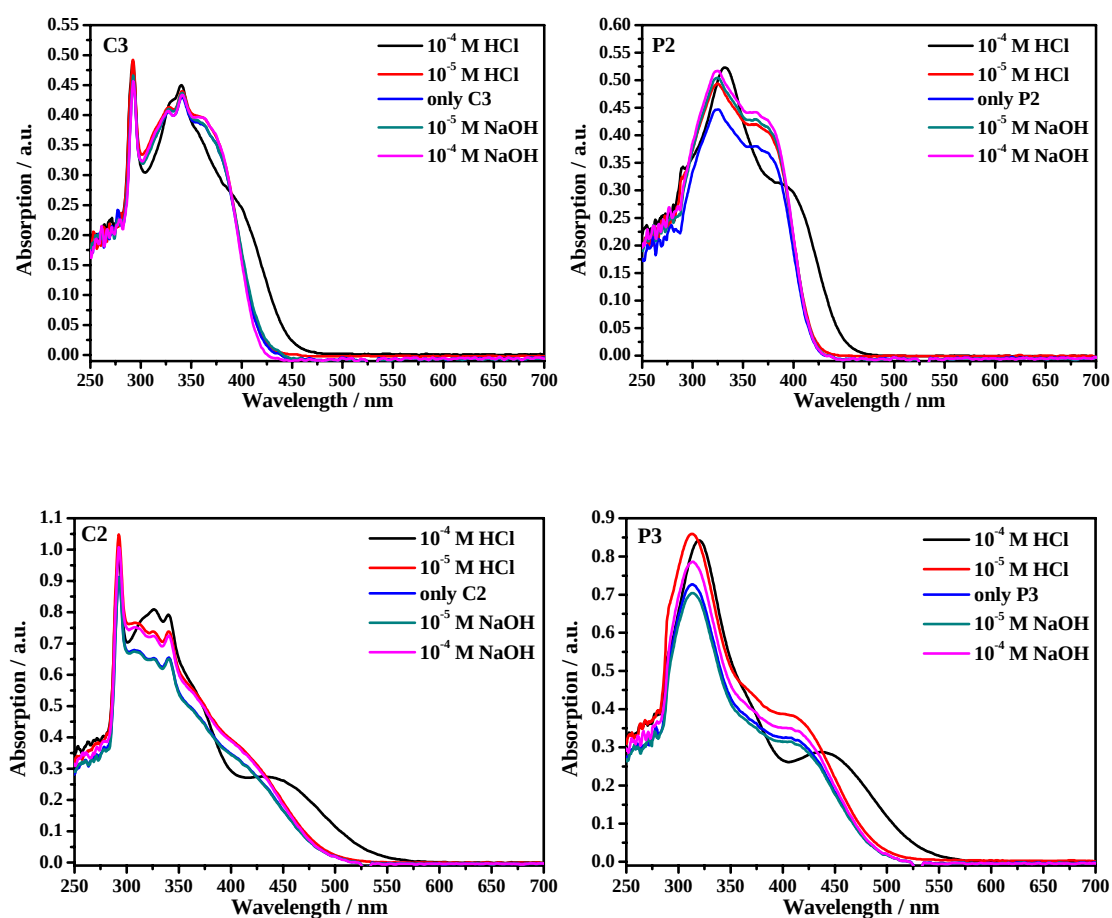


Fig. S2. UV-vis absorption spectra of 10^{-5} M C3, P2, C2 and P3 dyes in THF/H₂O (1:1) mixture with different acidity and alkalinity.

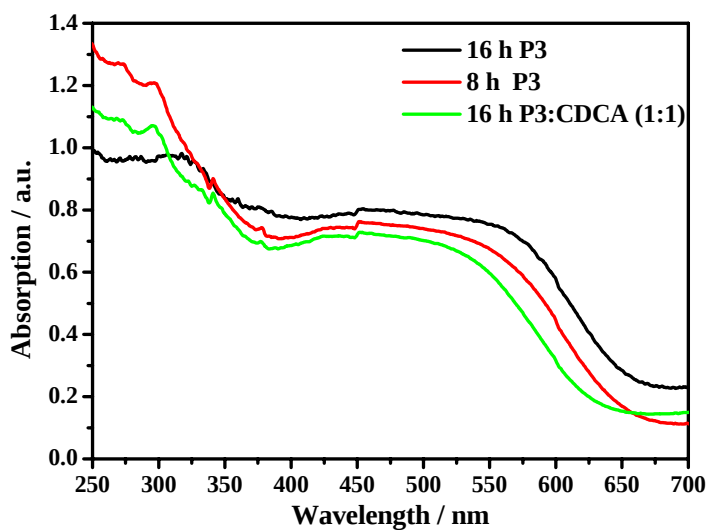


Fig. S3.UV-vis absorption spectra of **P3** on TiO₂ film.

Table S1 P3 amount vs time			
Dye	P3 (8 h)	P3 (16 h)	P3:CDCA (1:1, 16 h)
Amount / 10 ⁻⁷ mol cm ⁻²	4.1	4.1	3.7

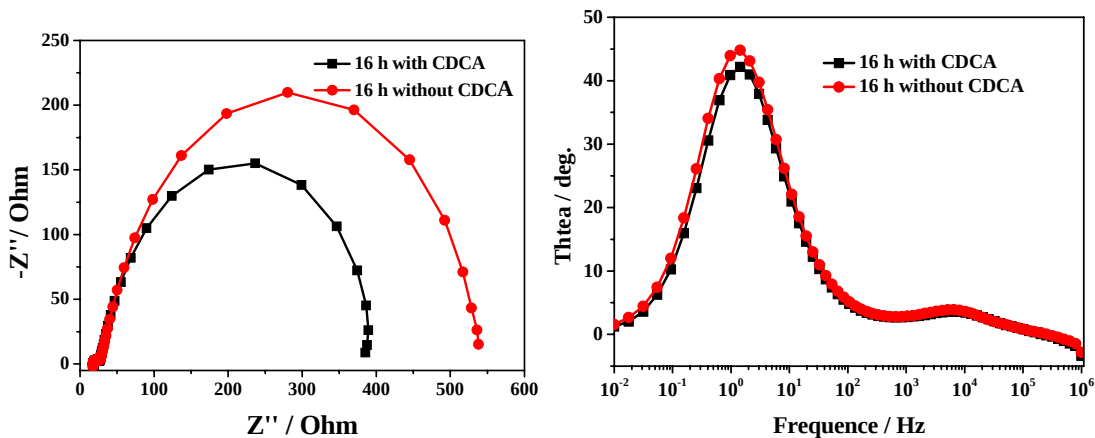


Fig. S4. EIS Nyquist and Bode plots of dye **P3** with coadsorbent (CDCA, 1:1) in the dark.

Lifetime:

With CDCA: 381.3 * 0.001072=408.8 ms

Without CDCA: 481.1 ms

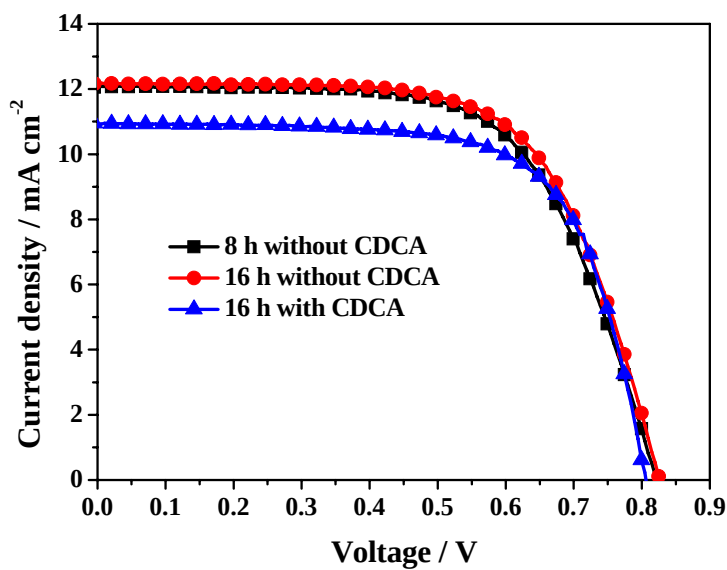


Fig. S5 Photocurrent density-photovoltage curves of **P3** in the dark.

Table S2 Performance of DSSC under different conditions				
Dye	$J_{sc}/\text{mA cm}^{-2}$	V_{oc}/mV	$\eta(\%)$	Fill factor (ff)
8 h without CDCA	12.09	822	6.36	0.64
16 h without CDCA	12.18	826	6.55	0.65
16h with CDCA	10.94	806	6.07	0.69

MS and NMR spectra

Instrument:DSQ(Thermo)

Ionization Method:EI

D:\DSQ\DATA-LR\11\O50518

5/5/2011 3:11:18 PM

Pe2CO

O50518 #186 RT: 3.03 AV: 1 NL: 5.95E5

T: + c Full ms [45.00-800.00]

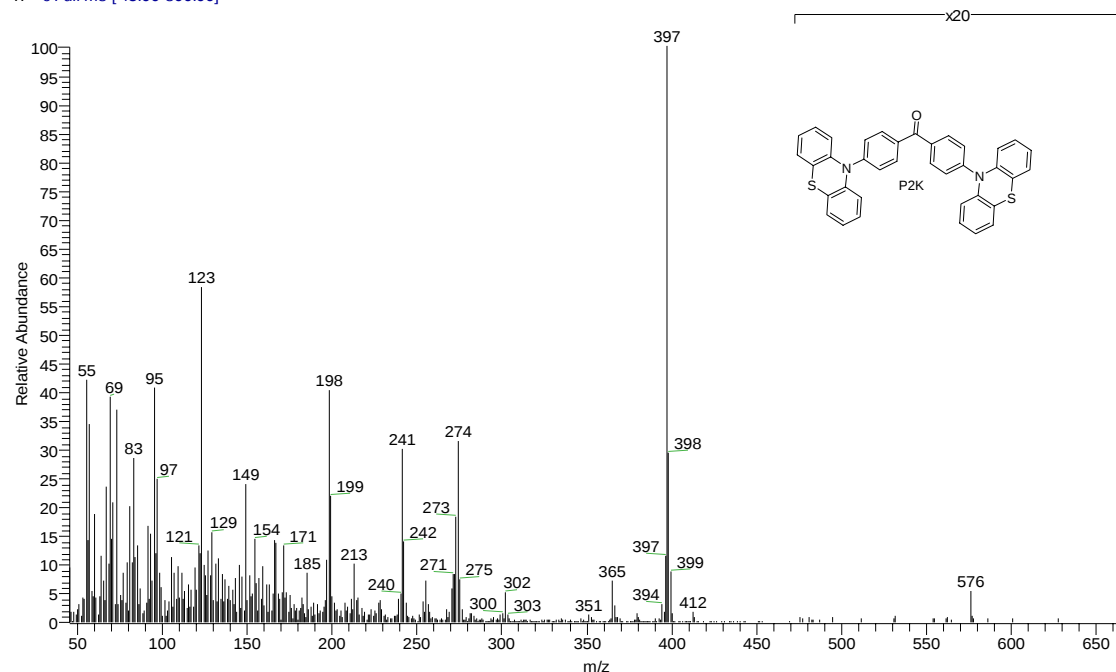


Fig. S6 MS spectrum of P2K.

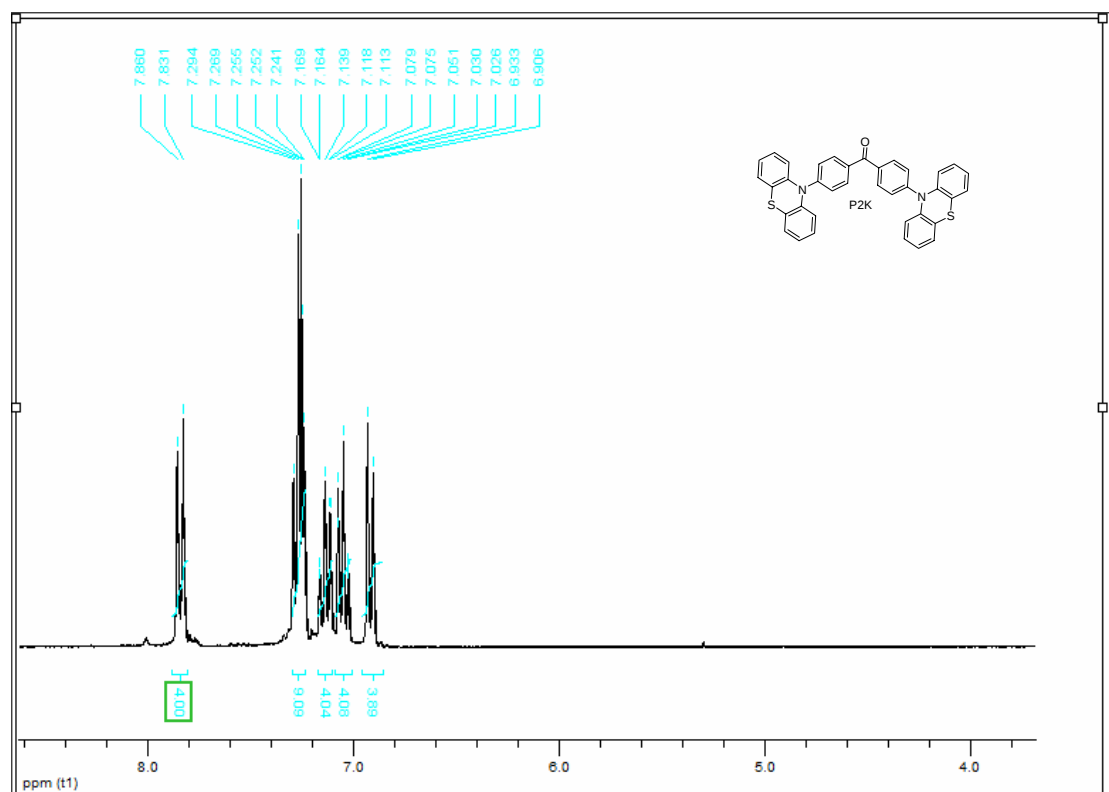


Fig. S7 ¹H NMR spectrum of P2K.

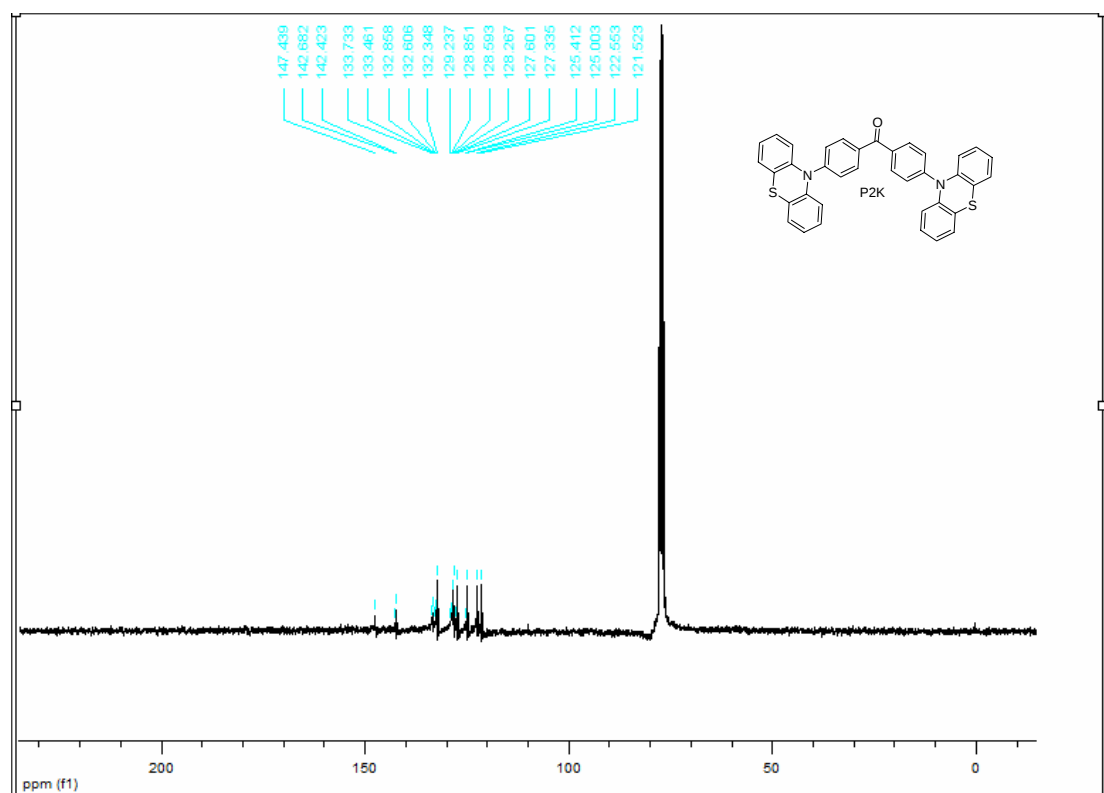


Fig. S8 ^{13}C NMR spectrum of P2K.

Instrument:DSQ(Thermo)

Ionization Method:EI

D:\DSQDATA-LR\11\O50521

5/5/2011 3:58:34 PM

Pe2P3Br

O50521 #180 RT: 2.93 AV: 1 NL: 2.67E6

T: + c Full ms [45.00-800.00]

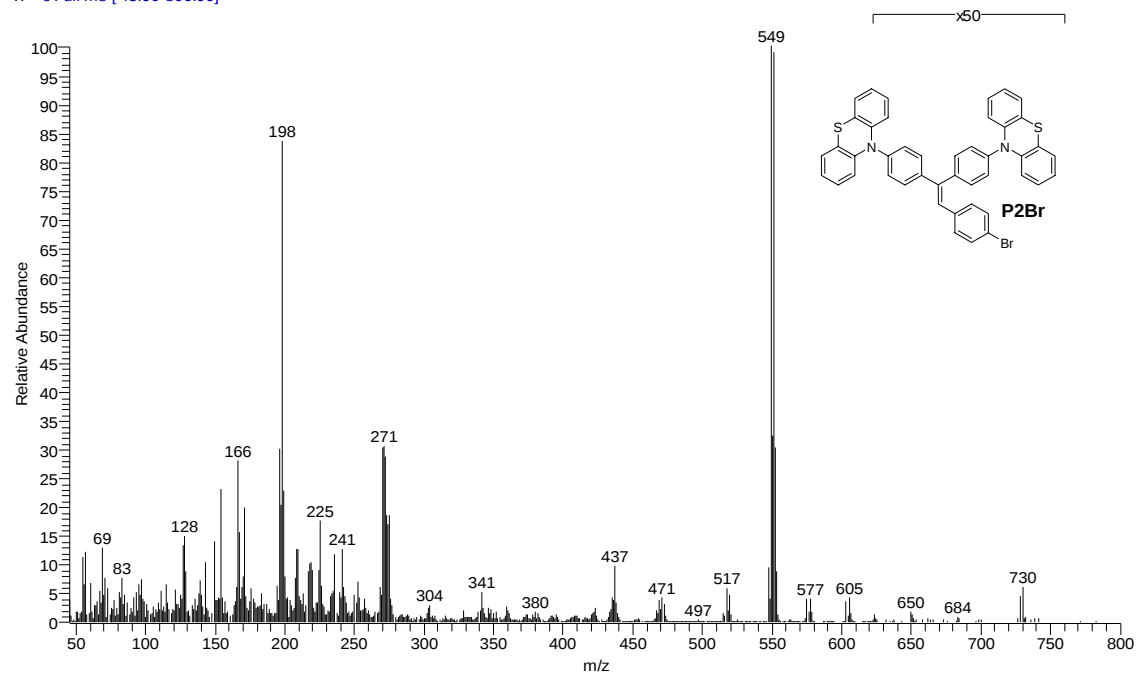


Fig. S9 MS spectrum of P2Br.

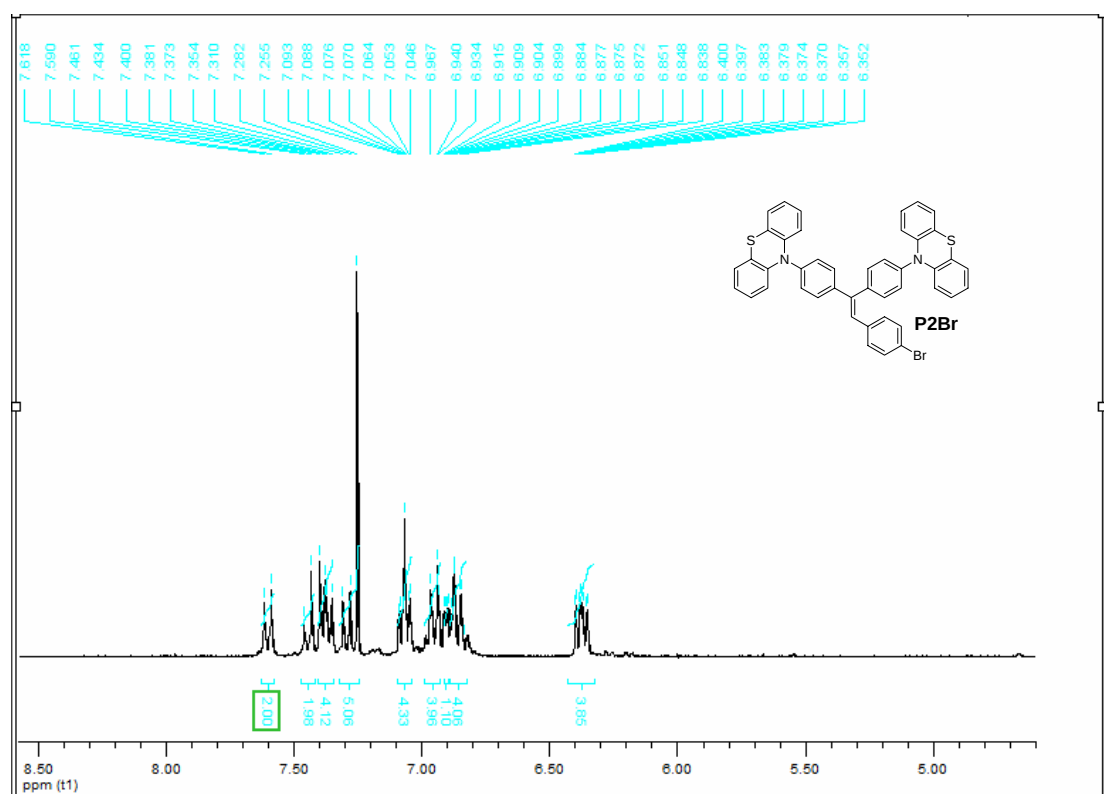


Fig. S10 ¹H NMR spectrum of **P2Br**

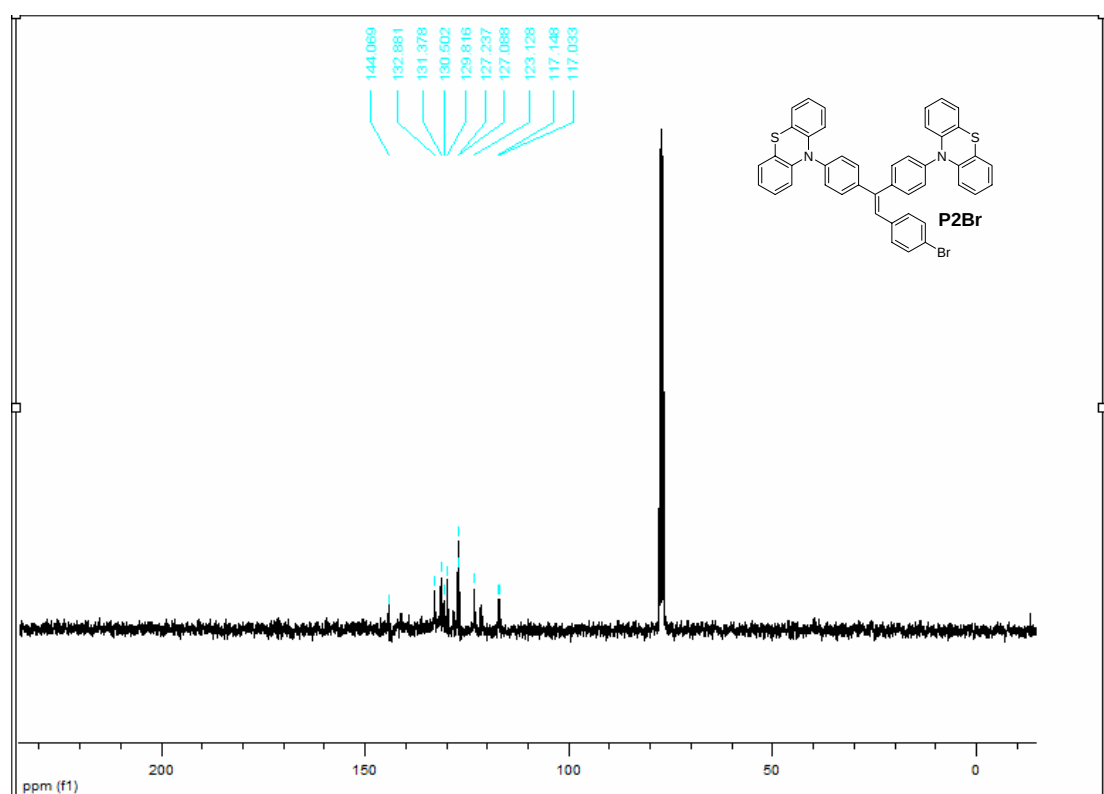


Fig. S11 ¹³C NMR spectrum of **P2Br**.

Instrument:DSQ(Thermo)

Ionization Method:EI

D:\DSQ\DATA-LR\11\050522

5/5/2011 4:07:09 PM

Pe2P3B

050522 #181 RT: 3.15 AV: 1 NL: 4.43E6

T: +c Full ms [50.00-860.00]

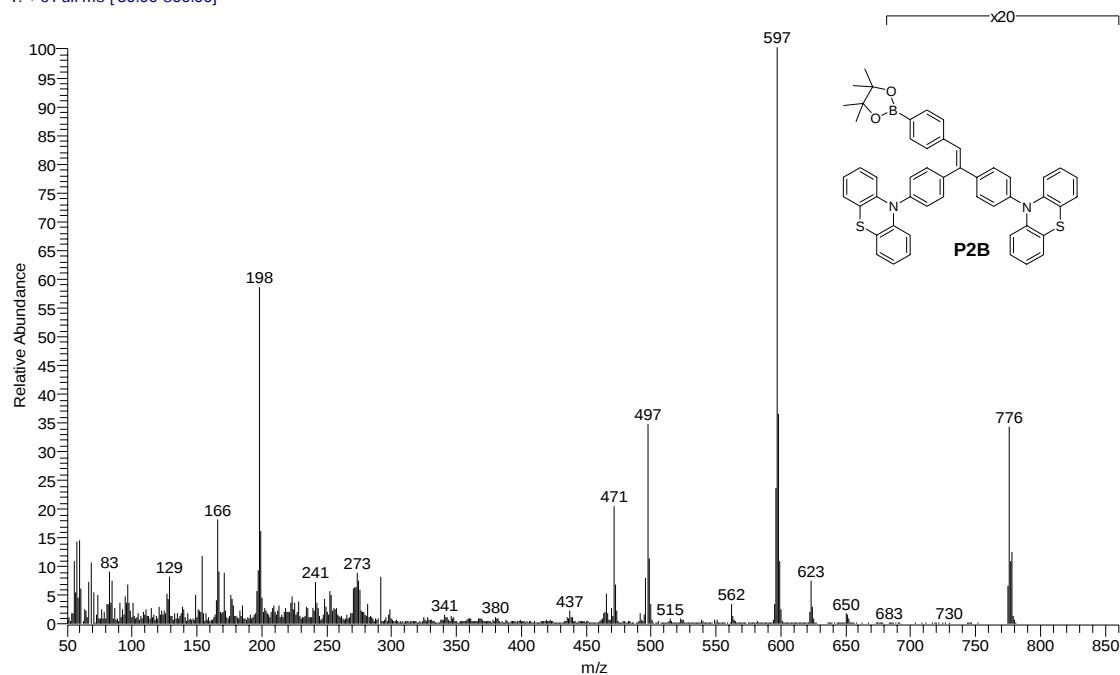


Fig. S12 MS spectrum of **P2B**.

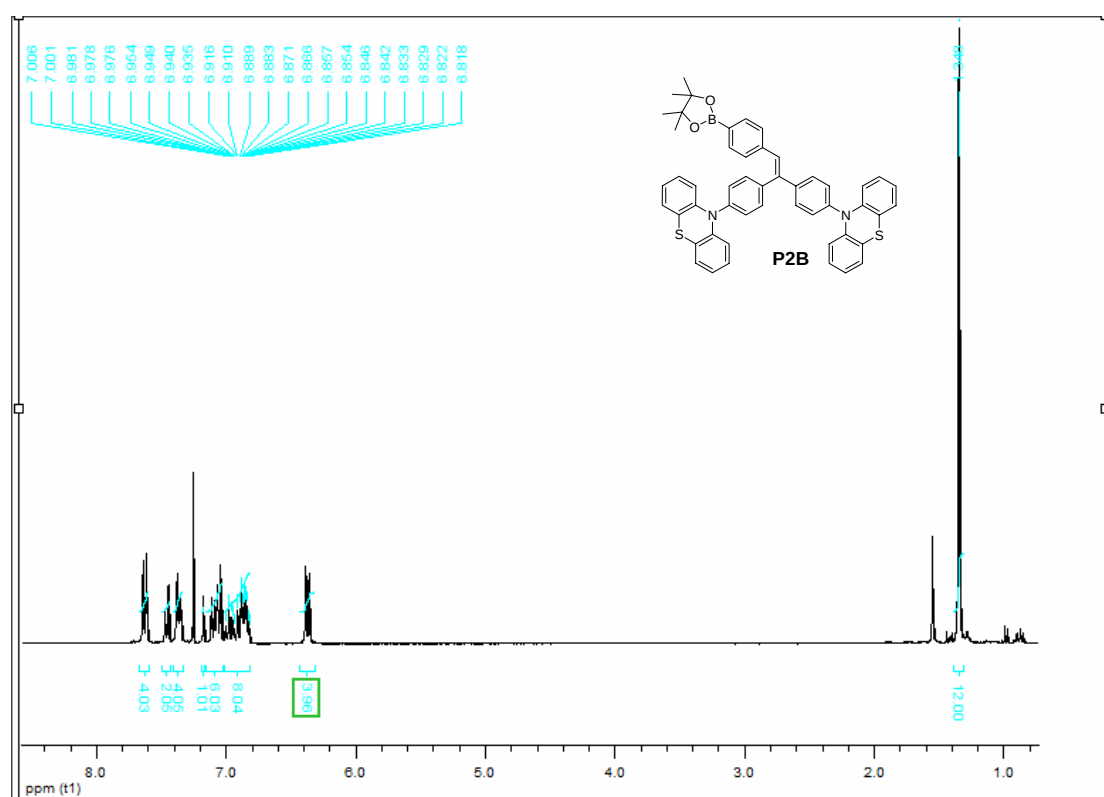


Fig. S13 ^1H NMR spectrum of **P2B**.

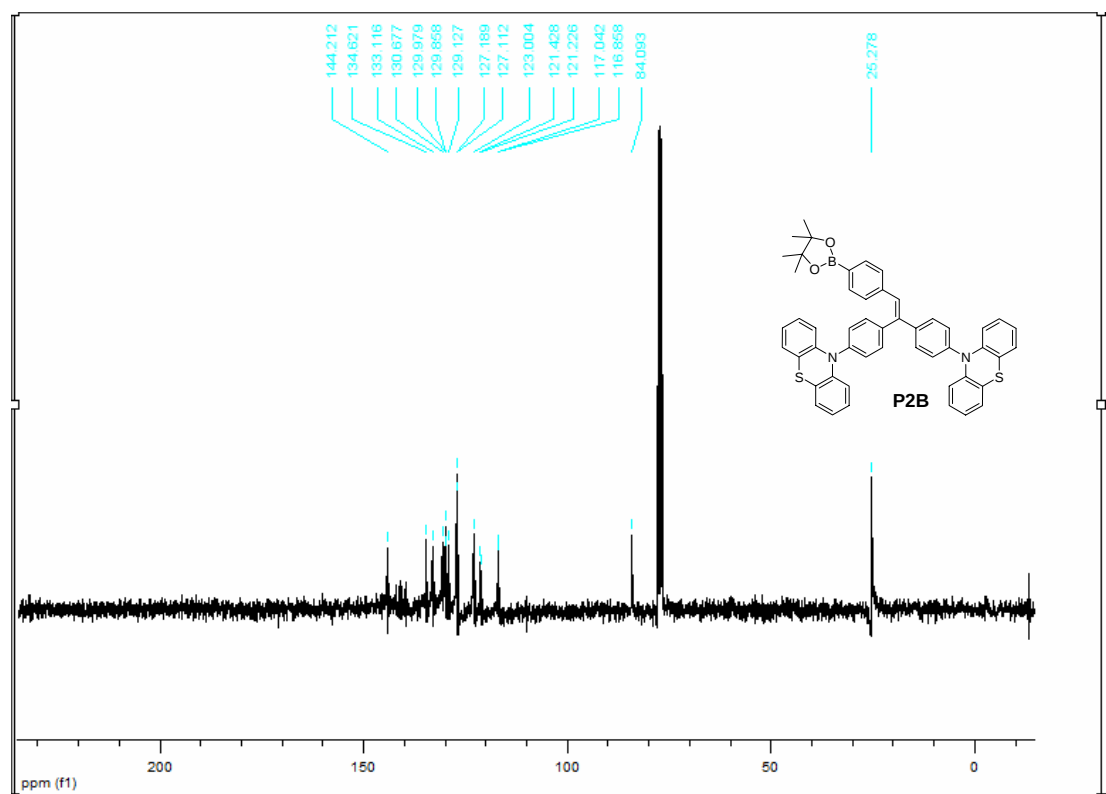


Fig. S14 ¹³C NMR spectrum of **P2B**.

Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\11\Q42707

4/27/2011 10:48:58 AM

Pe2CzCHO

O42707 #187 RT: 3.99 AV: 1 NL: 6.86E4
T: + c Full ms [50.00-1050.00]

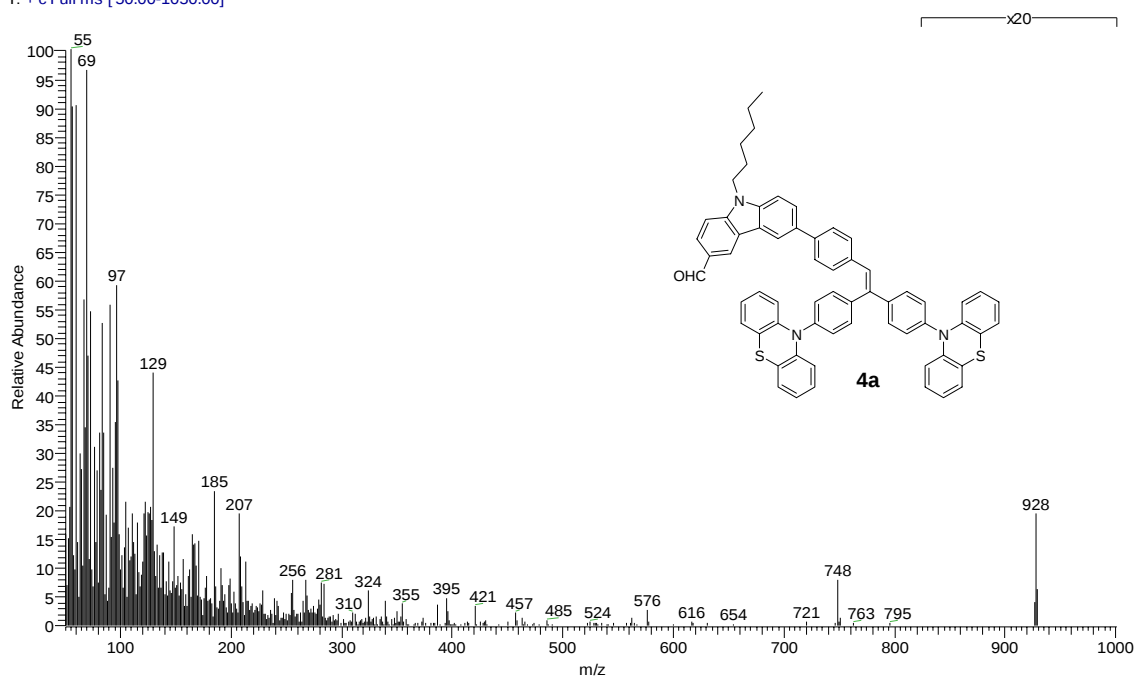


Fig. S15 MS spectrum of **4a**.

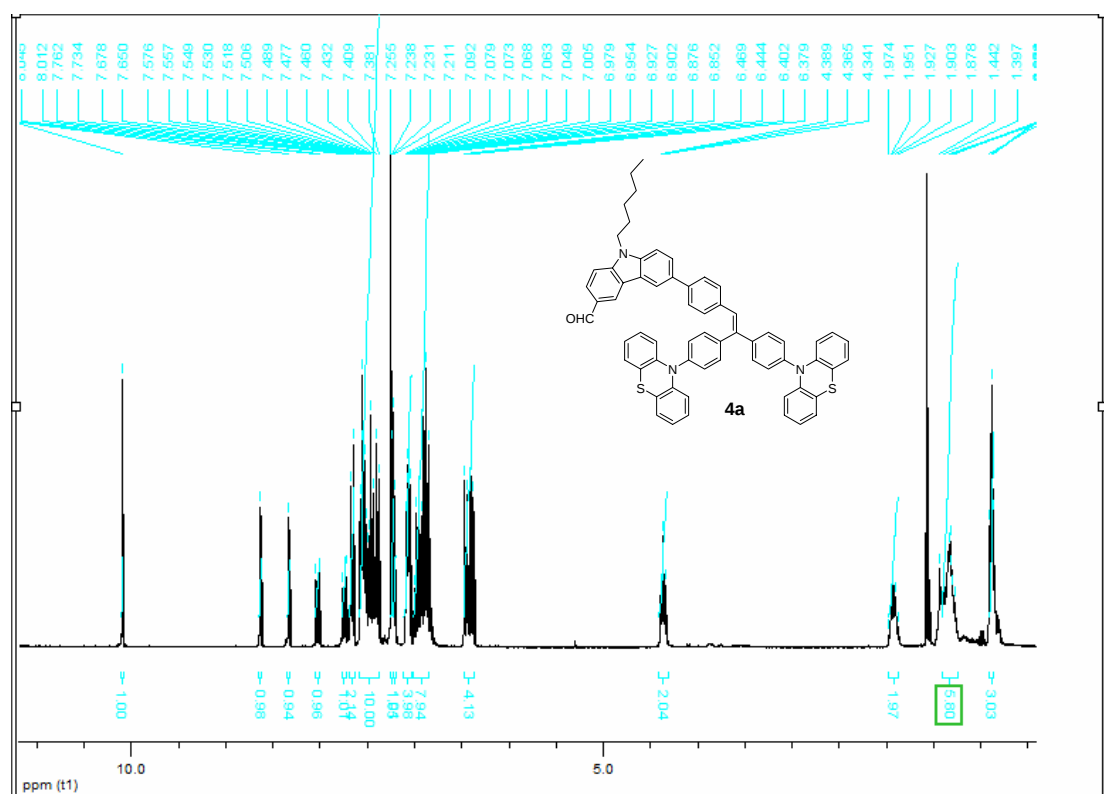


Fig. S16 ¹H NMR spectrum of 4a.

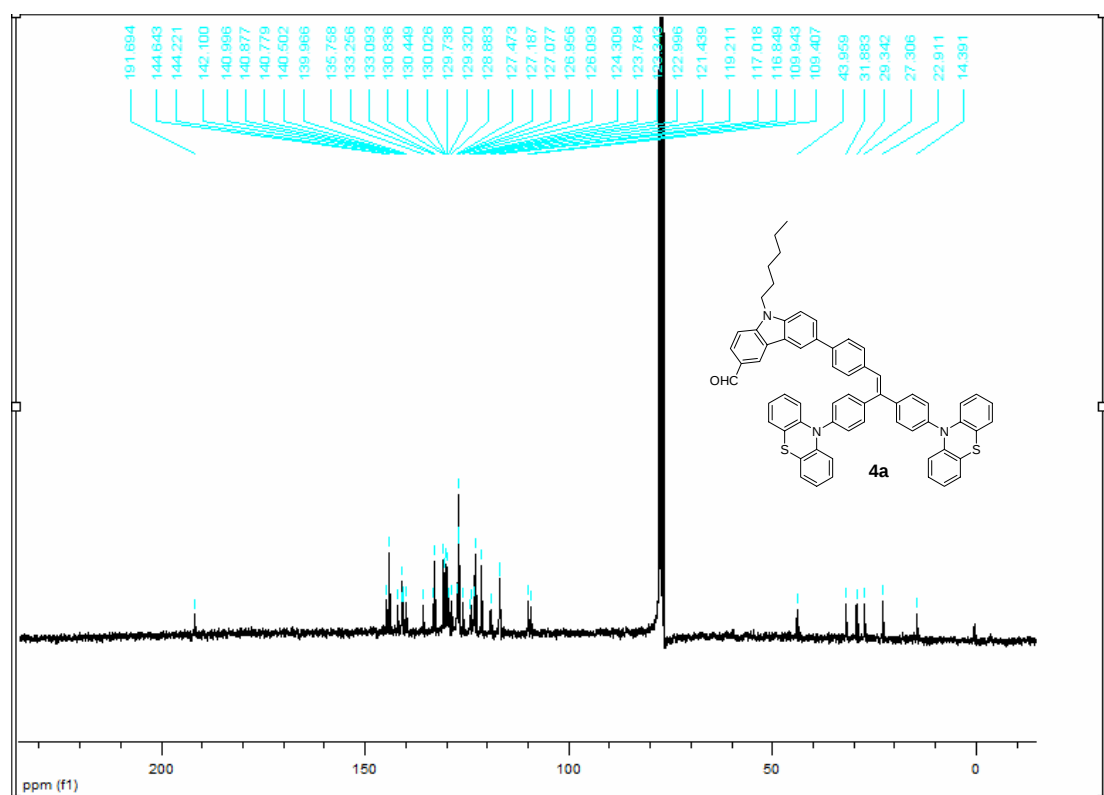


Fig. S17 ¹³C NMR spectrum of 4a.

Fig. S19 ^1H NMR spectrum of **4b**.

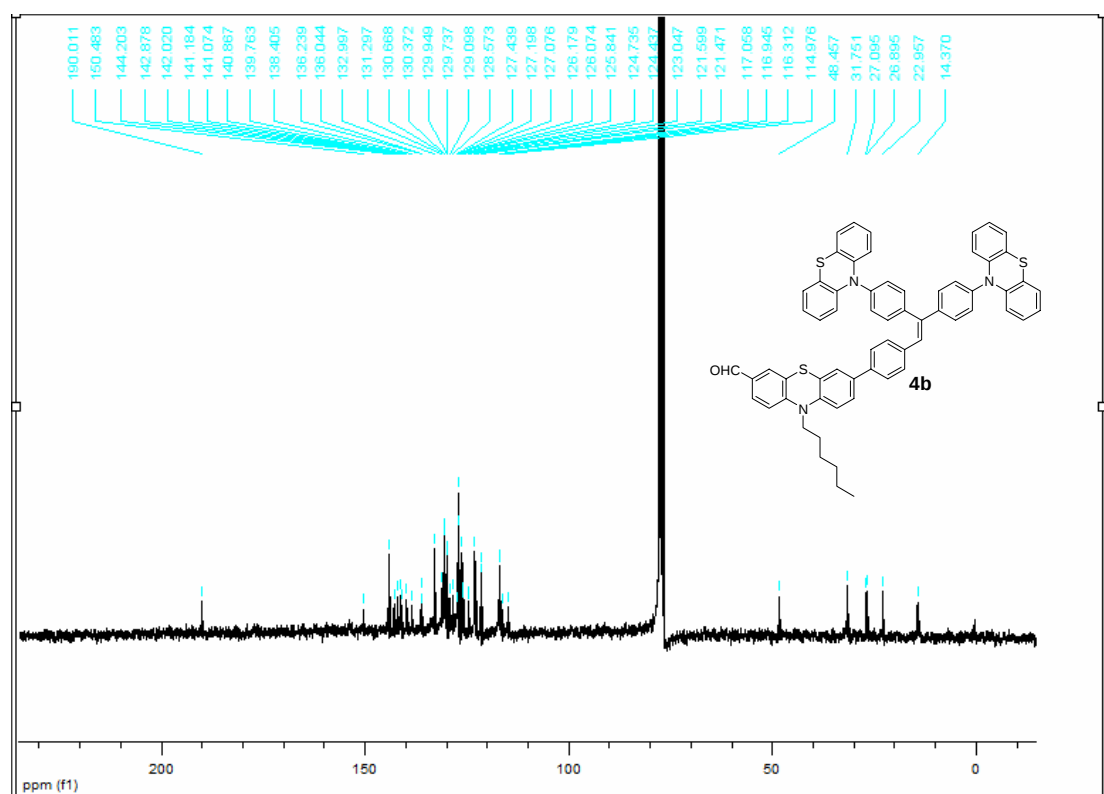


Fig. S20 ^{13}C NMR spectrum of **4b**.

Instrument:DSQ(Thermo)

Ionization Method:EI

D:\DSQ\DATA-LR\11\Q42706

4/27/2011 10:33:06 AM

Cz3CHO

O42706 #197 RT: 3.80 AV: 1 NL: 1.44E5

T: + c Full ms [50.00-950.00]

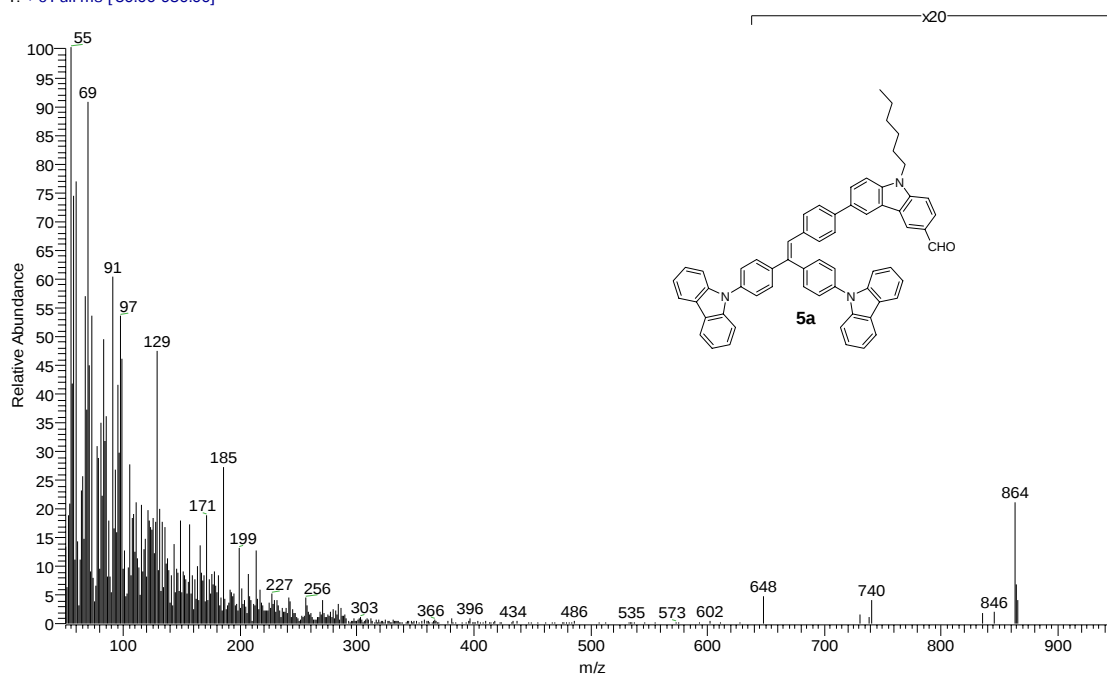


Fig. S21 MS spectrum of **5a**.

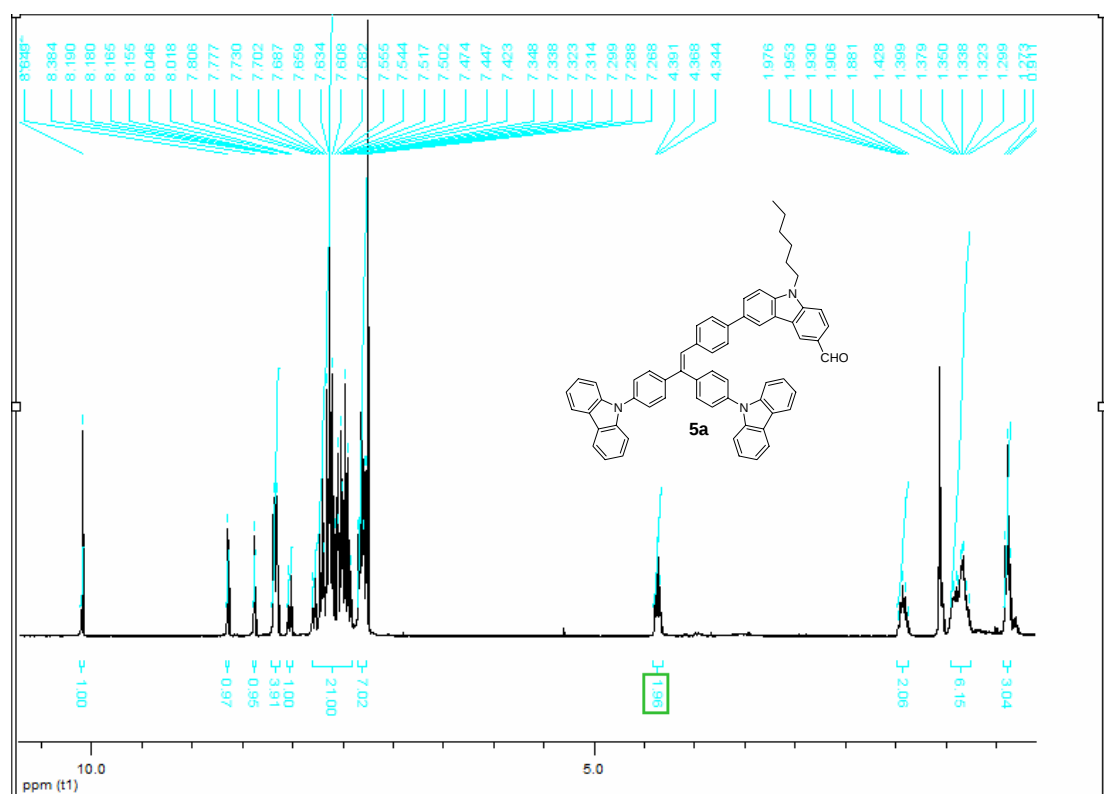


Fig. S22 ¹H NMR spectrum of 5a.

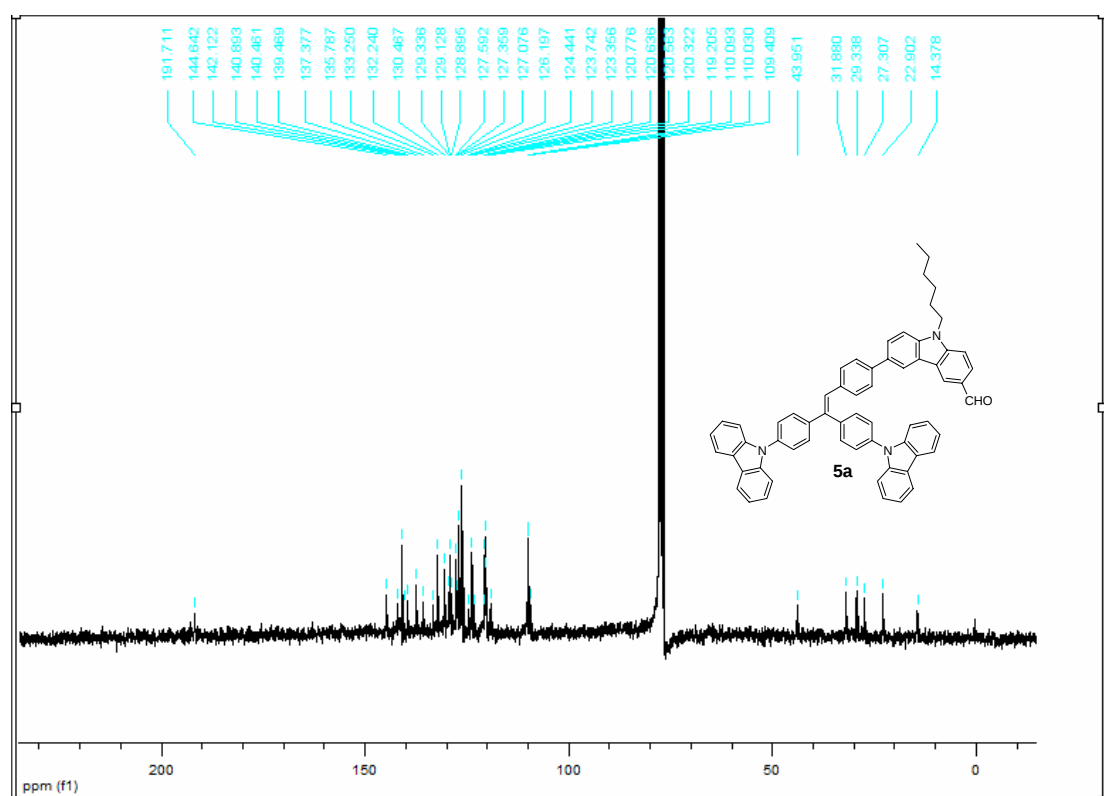


Fig. S23 ¹³C NMR spectrum of 5a.

Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\11\O41502

4/15/2011 3:05:36 PM

Cz2P3PeCHO

O41502 #239 RT: 4.87 AV: 1 NL: 7.51E4
T: +c Full ms [45.00-1000.00]

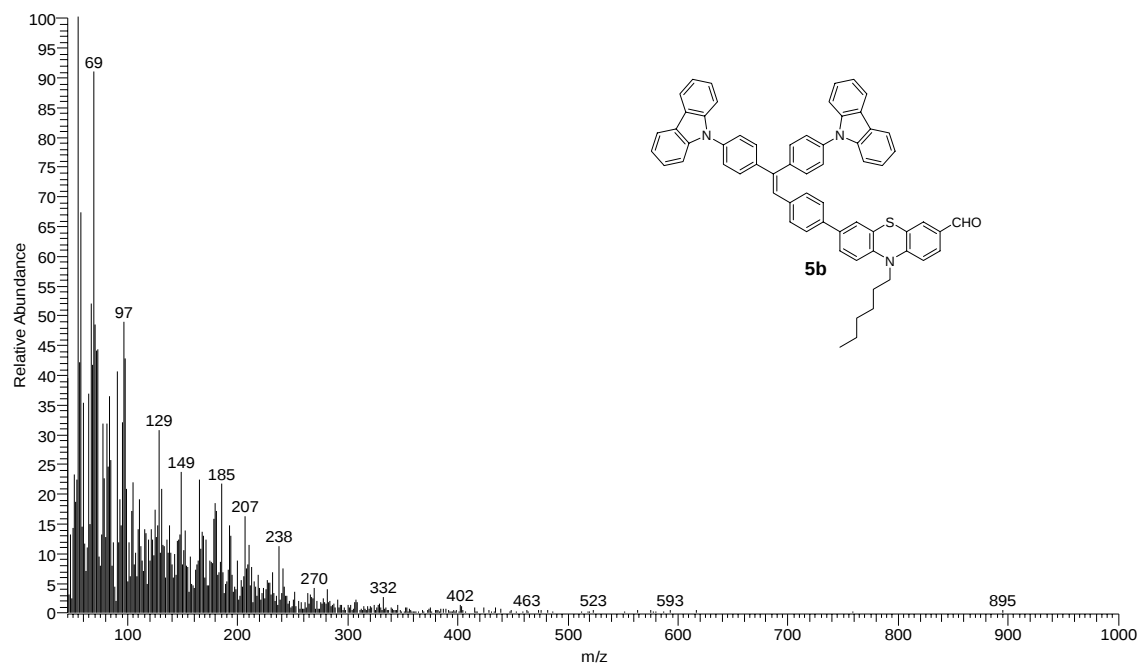


Fig. S24 MS spectrum of **5b**.

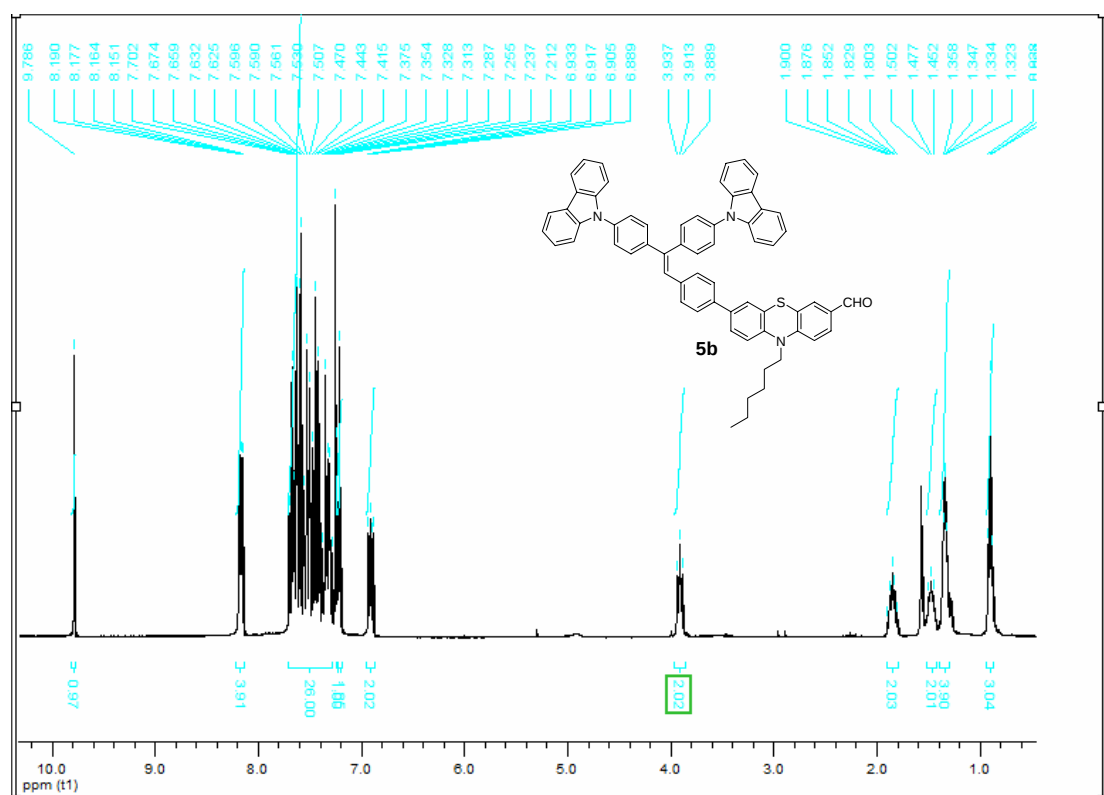


Fig. S25 ^1H NMR spectrum of **5b**.

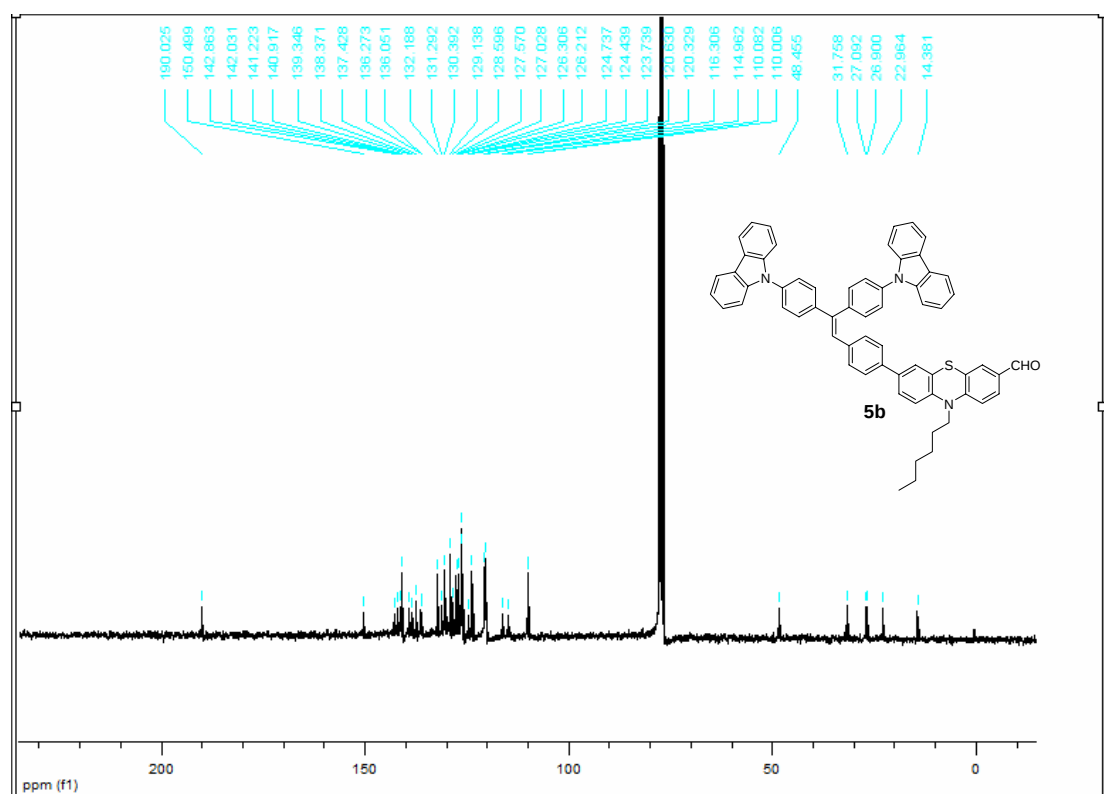


Fig. S26 ¹³C NMR spectrum of **5b**.

Instrument:DSQ(Thermo)

Ionization Method:EI

D:\DSQDATA-LR11\O50516

5/5/2011 12:13:41 PM

P2CCN

O50516 #201 RT: 4.30 AV: 1 NL: 3.12E5

T: + c Full ms [50.00-1050.00]

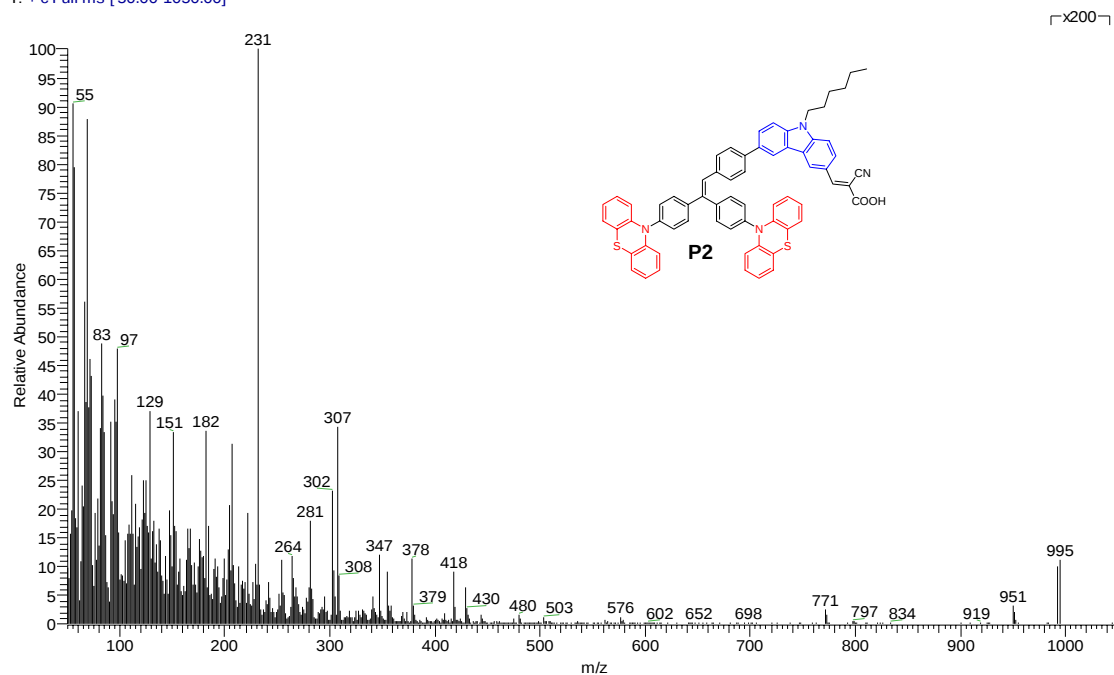


Fig. S27 MS spectrum of **P2**.

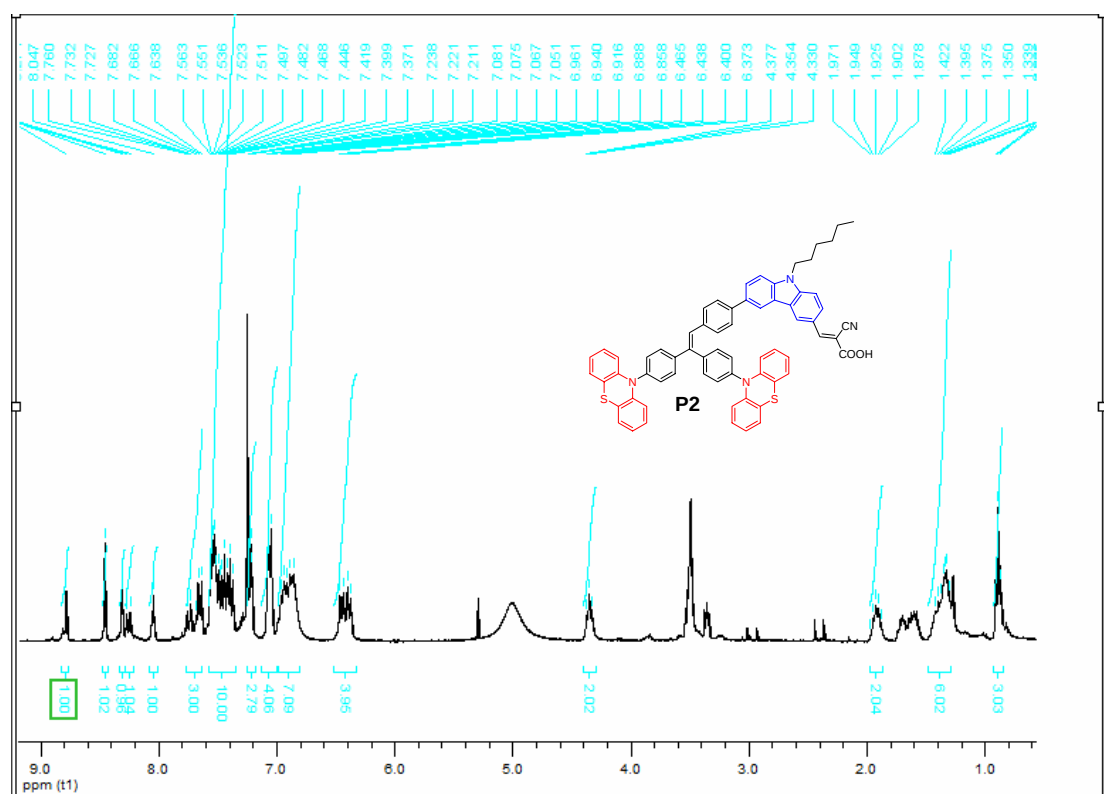


Fig. S28 ¹H NMR spectrum of P2.

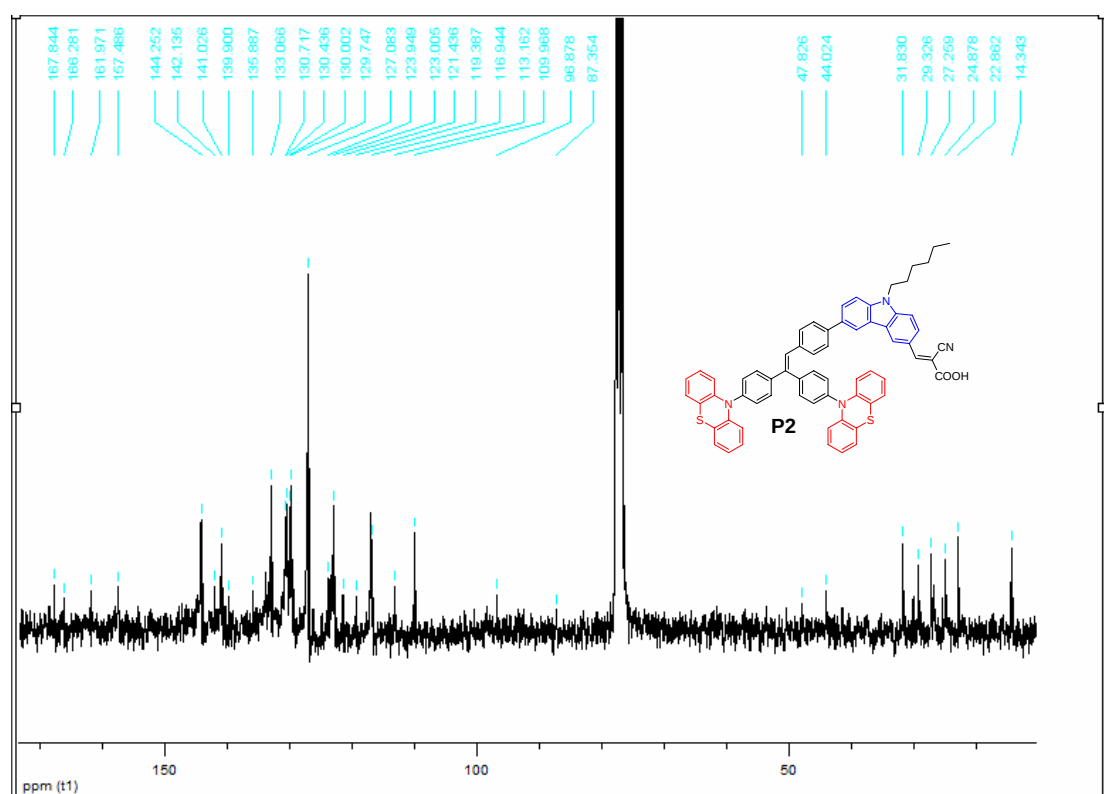


Fig. S29 ¹³C NMR spectrum of P2.

Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\11\050523

5/5/2011 4:37:06 PM

P3CN

O50523 #132-137 RT: 2.83-2.94 AV: 6 NL: 4.95E5
T: + c Full ms [50.00-1050.00]

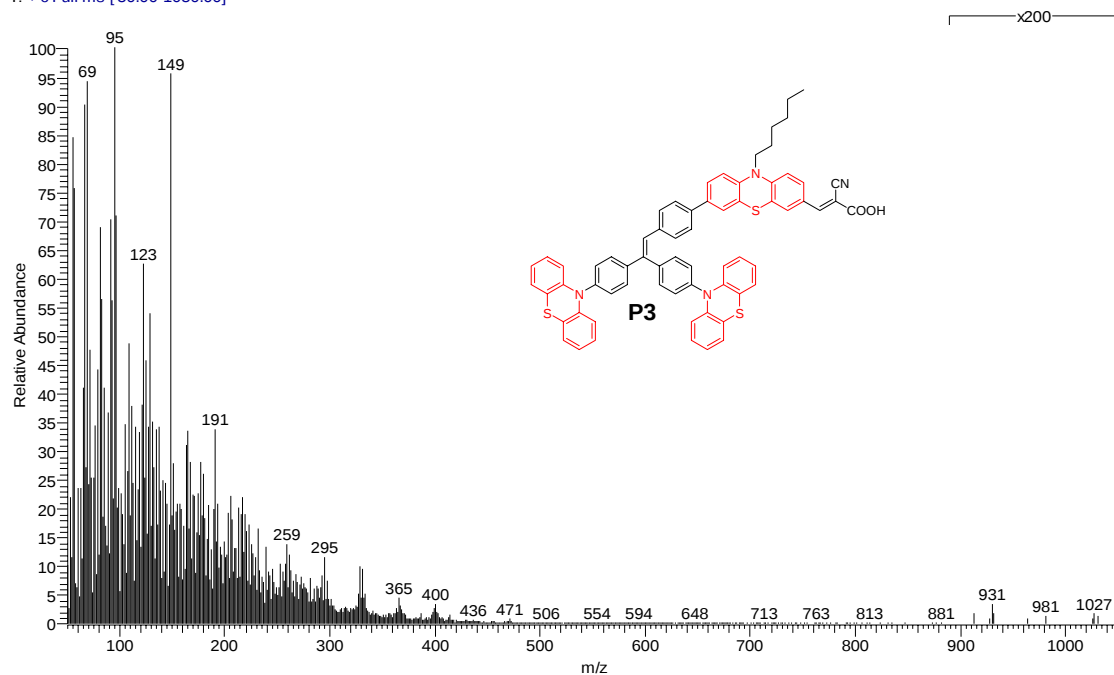


Fig. S30 MS spectrum of **P3**.

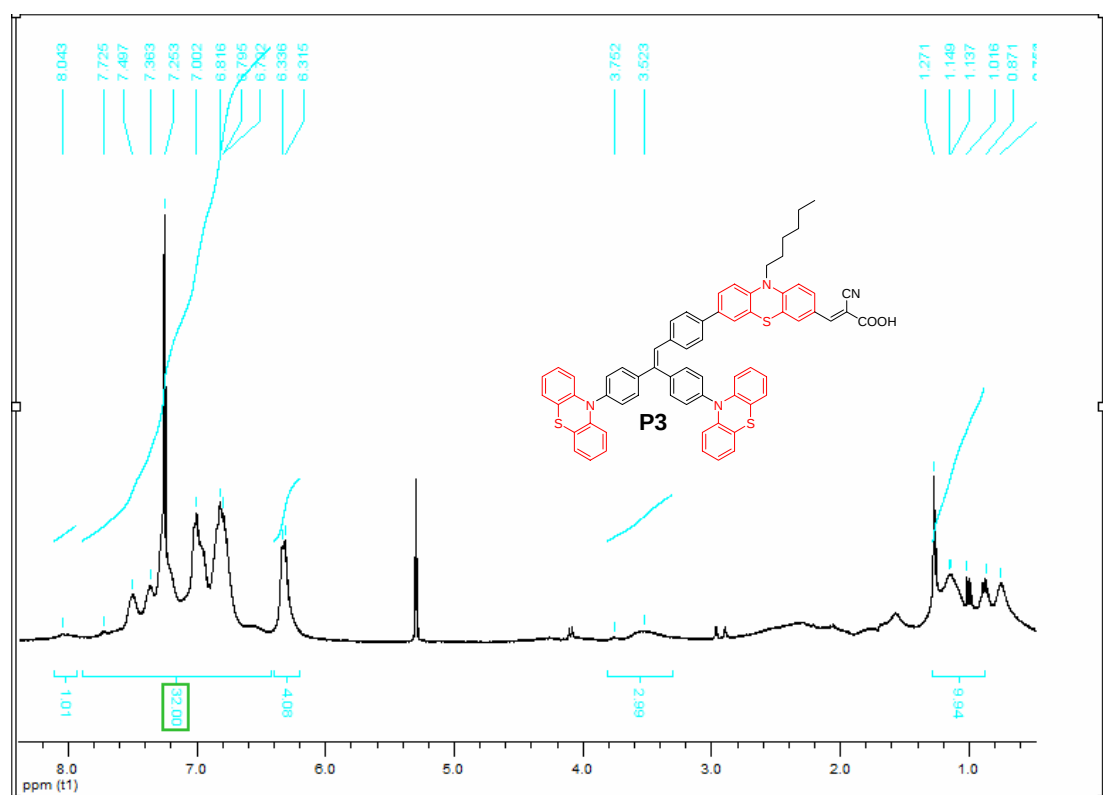


Fig. S31 ^1H NMR spectrum of **P3**.

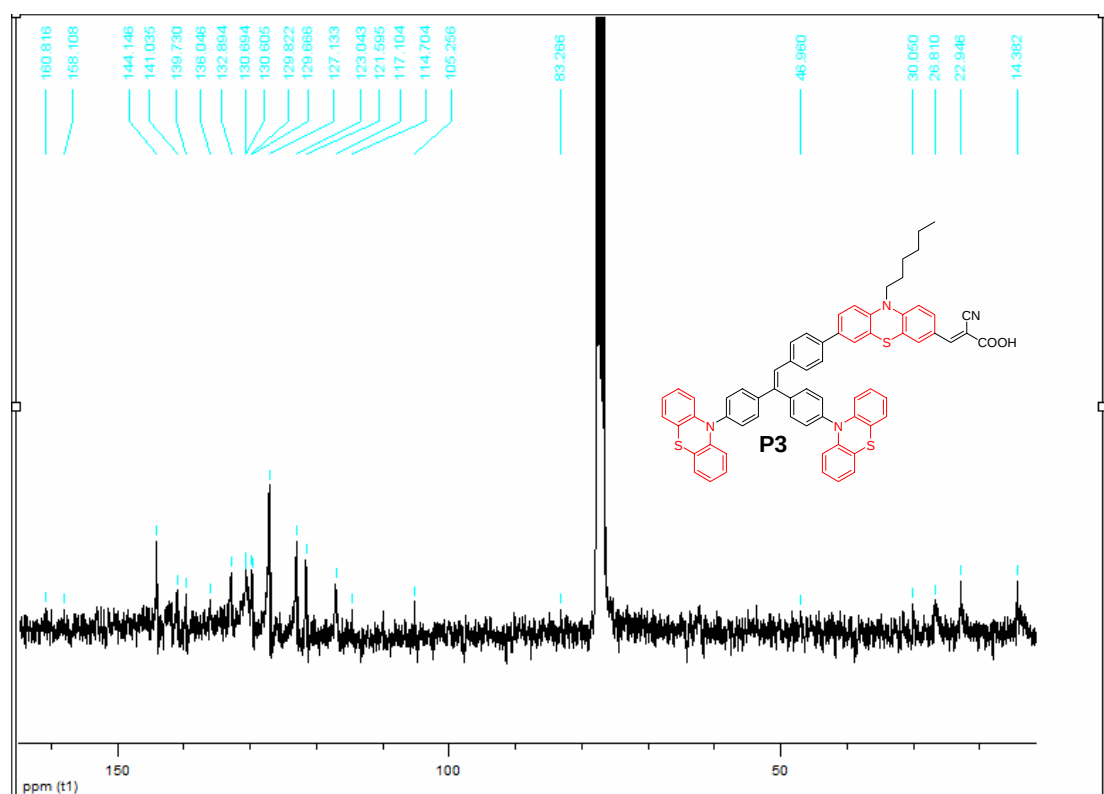


Fig. S32 ^{13}C NMR spectrum of **P3**.

Instrument:DSQ(Thermo)

Ionization Method:EI

D:\DSQ\DATA-LR\11\050514

5/5/2011 11:36:10 AM

C3CN

O50514 #115 RT: 2.46 AV: 1 NL: 2.62E6

T: + c Full ms [50.00-1050.00]

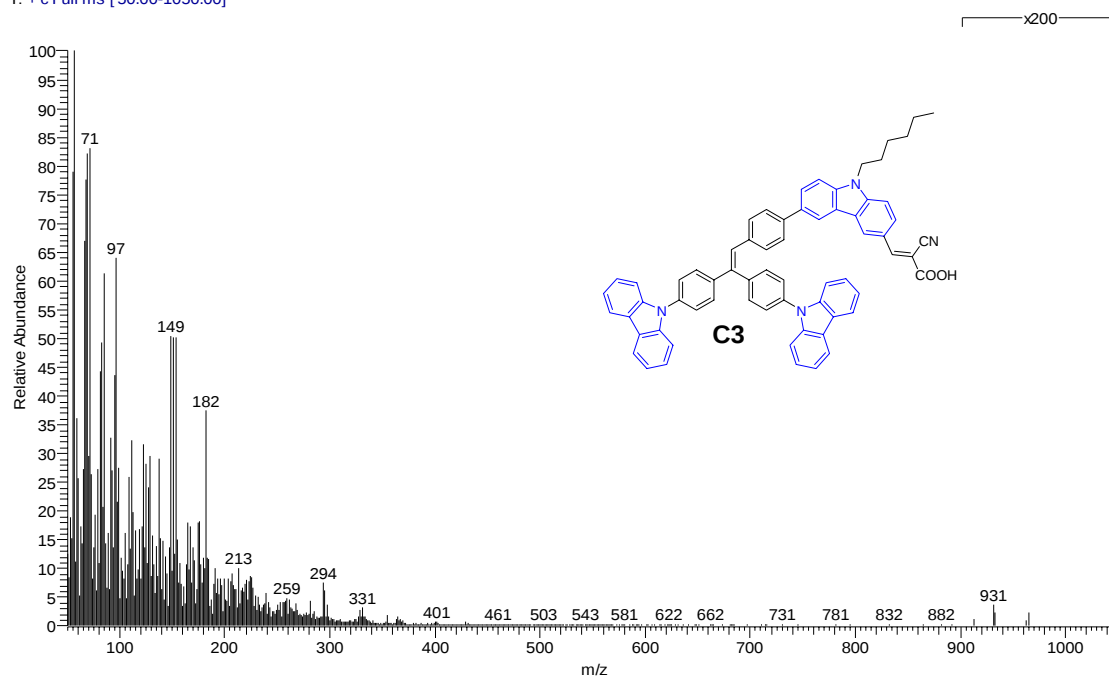


Fig. S33 MS spectrum of **C3**.

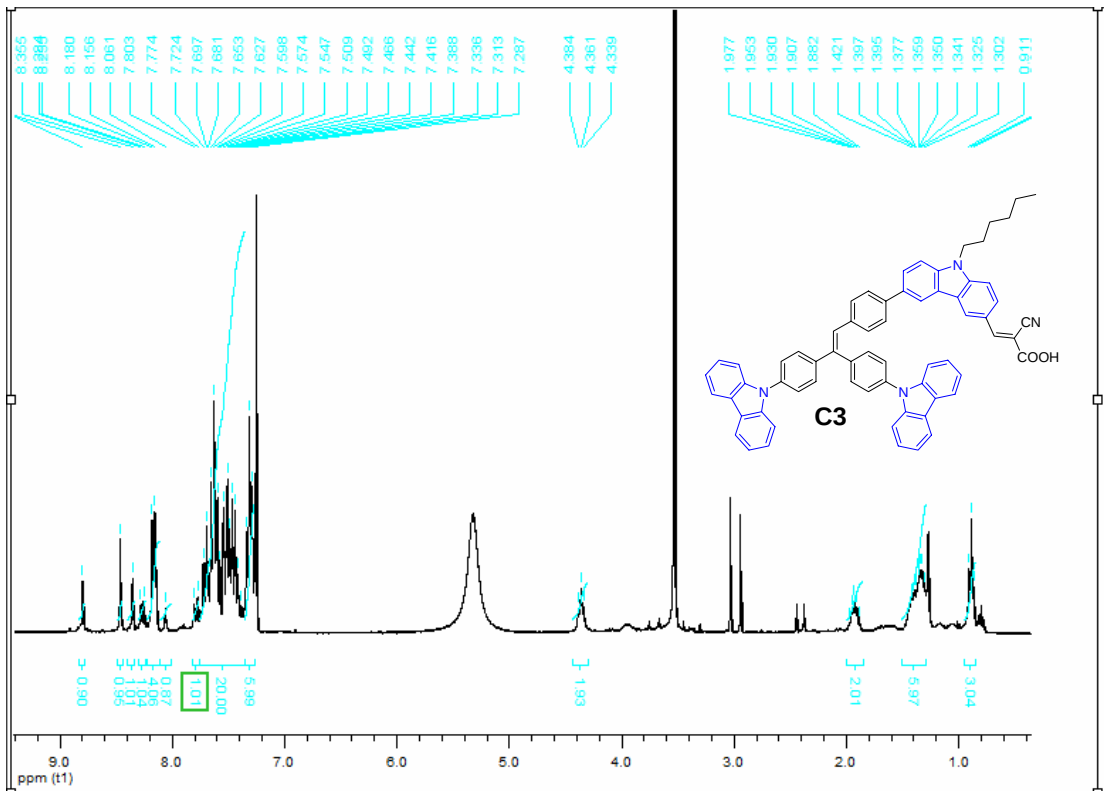


Fig. S34 ^1H NMR spectrum of **C3**.

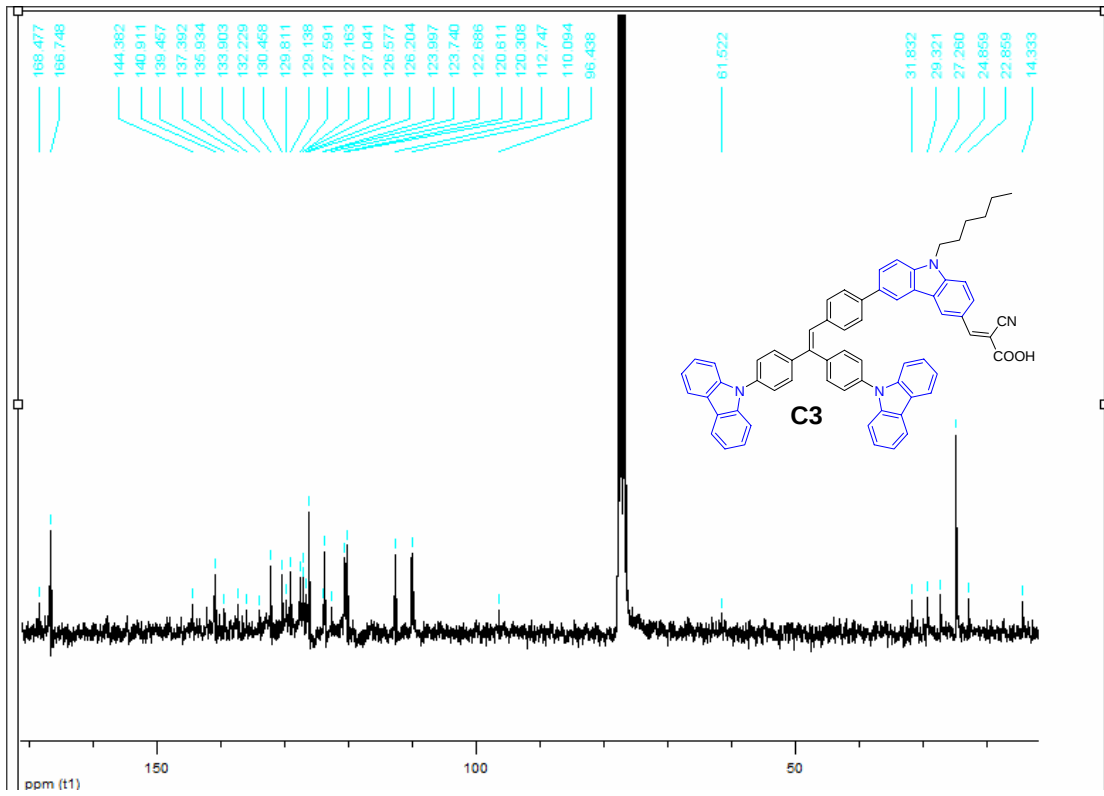


Fig. S35 ^{13}C NMR spectrum of **C3**.

Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\11\050515

5/5/2011 11:58:57 AM

C2PCN

O50515 #217 RT: 4.64 AV: 1 NL: 2.74E5
T: +c Full ms [50.00-1050.00]

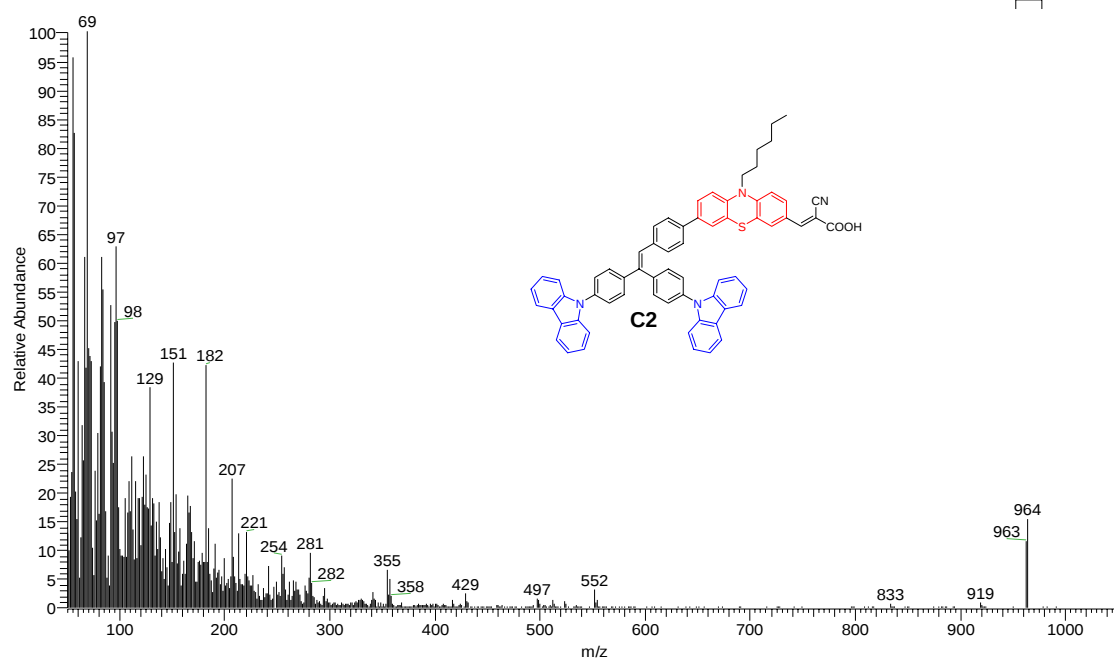


Fig. S36 MS spectrum of C2.

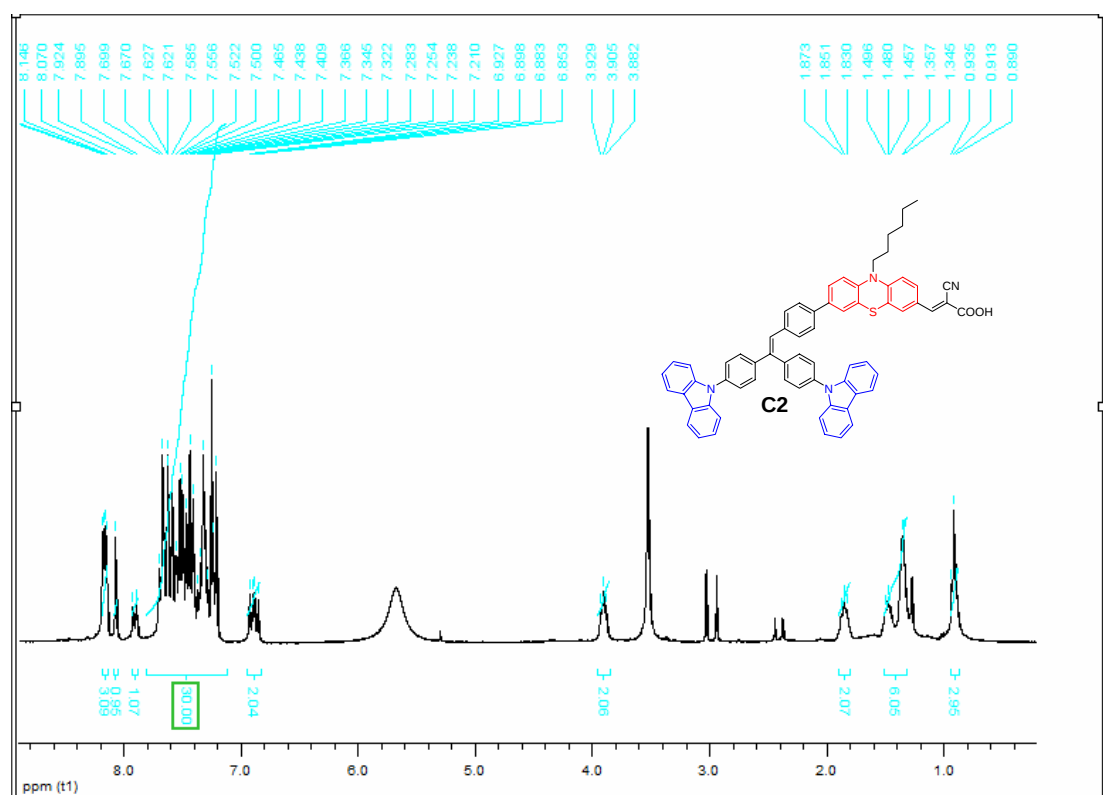


Fig. S37 ¹H NMR spectrum of C2.

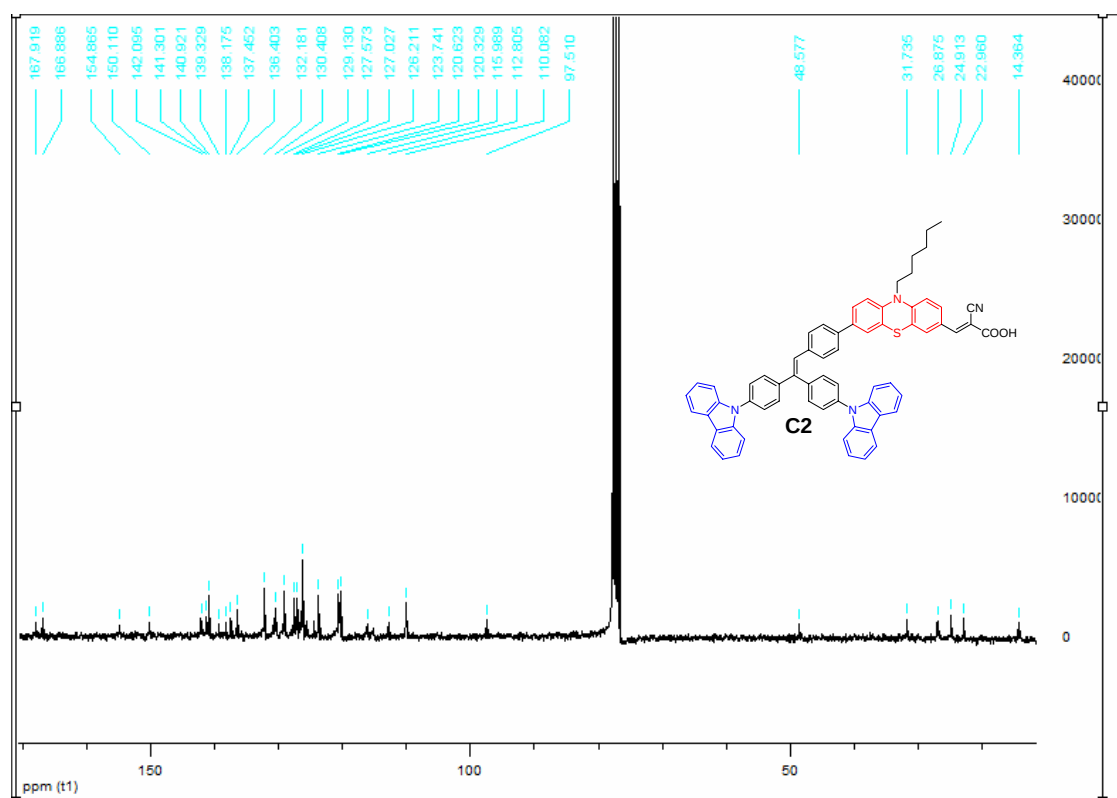


Fig. S38 ^{13}C NMR spectrum of **C2**.