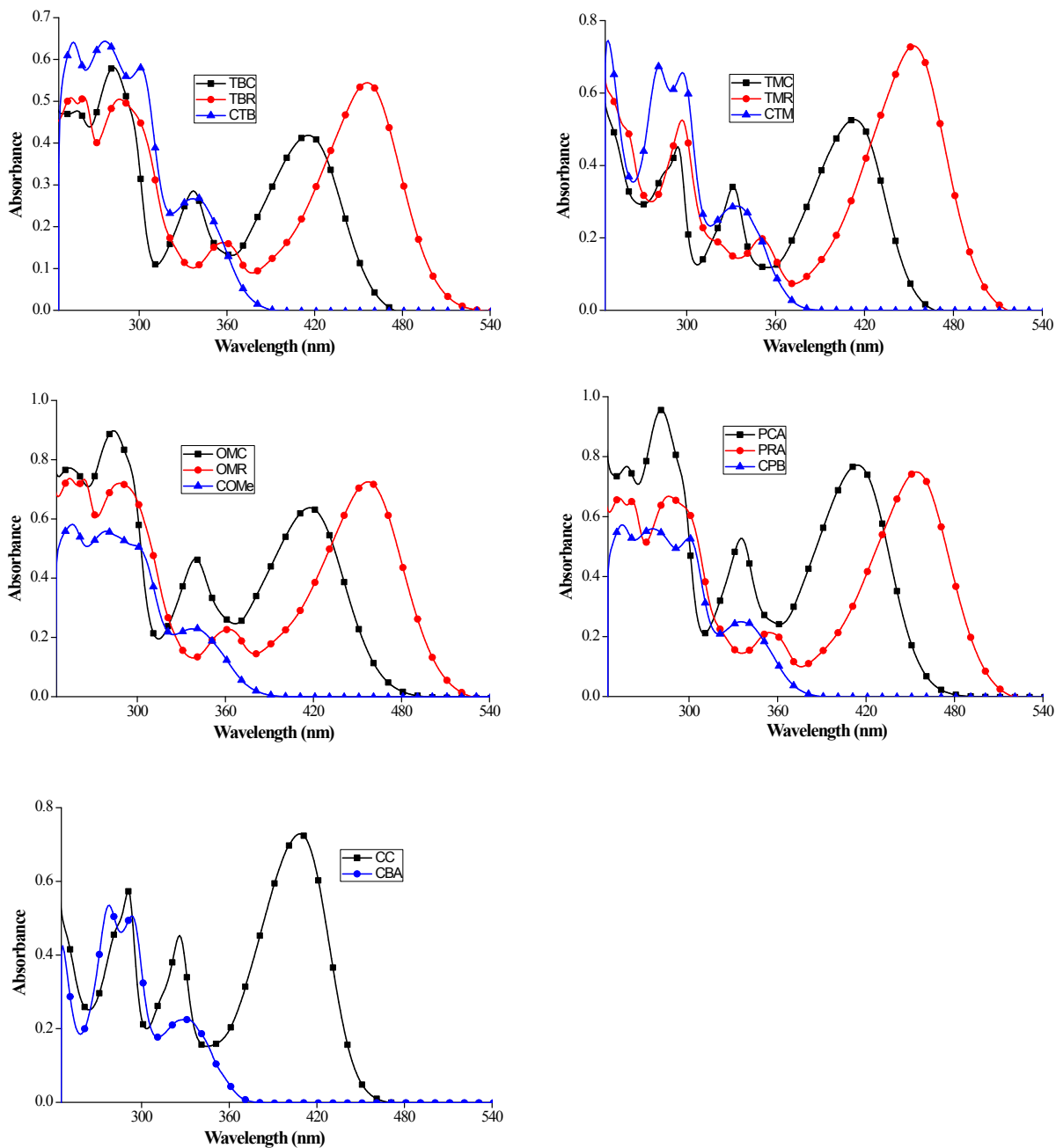


# Impact of strength and size of donors on the optoelectronic properties of D- $\pi$ -A sensitizers

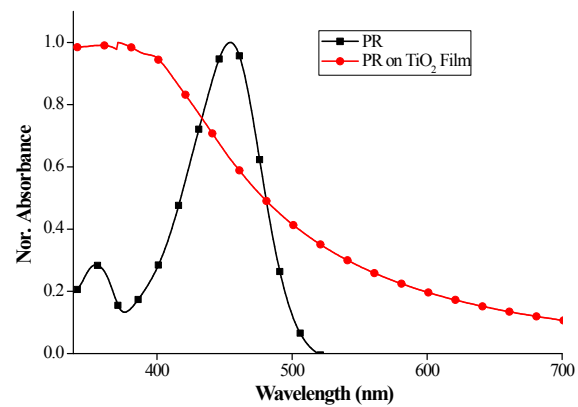
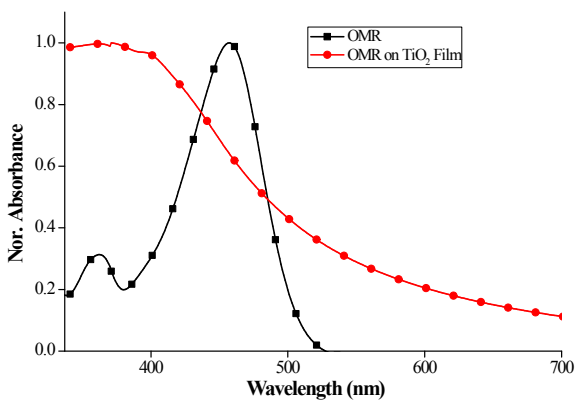
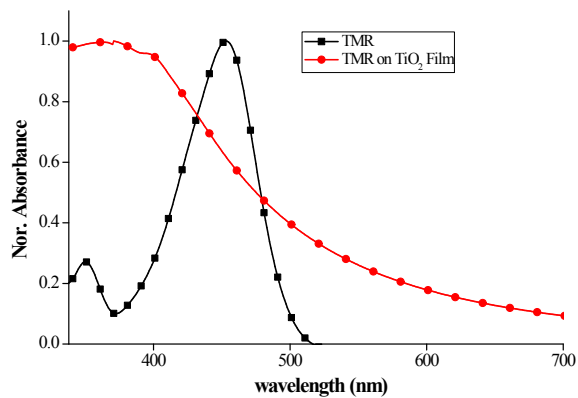
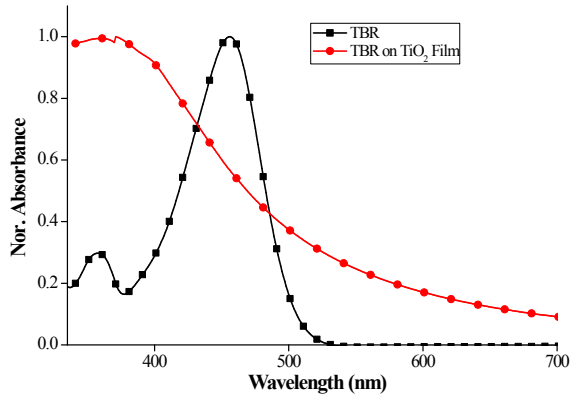
*S. Jagadeeswari<sup>a</sup>, G. Paramaguru<sup>b</sup>, Peng Gao<sup>b\*</sup>, Md. K. Nazeeruddin<sup>b\*</sup>, Alexei Emeline<sup>c</sup>, Detlef*

*Bahnemann<sup>c</sup> and R. Renganathan<sup>a\*</sup>*

**Figure S1:** Comparison of carbazole aldehydes with phenyl donor based carbazole sensitizers by using absorption spectra.



**Figure S2:** Normalised absorption spectrum of TBR, TMR, OMR and PR dyes in  $\text{CHCl}_3$  solution and on  $\text{TiO}_2$  films



## Synthetic pathways for the preparation of intermediate compounds.

### 9-Octyl-9H-carbazole (CB)

Carbazole (1mol ratio) was added to a suspension of sodium hydroxide (1.2 mol ratio) in DMSO (13V) under nitrogen atmosphere. The mixture was stirred for 30 min and then 1- bromo octane (1.1 mol ratio) was added. After completion of the reaction, the mixture was extracted with  $\text{CHCl}_3$  and dried over sodium sulphate and evaporated to afford CB. Product: brown liquid. Yield: 90 %.  $^1\text{H}$  NMR, (400MHz,  $\text{CDCl}_3$ -d): $\delta$  = 8.10-8.07 (m, 2 H), 7.46-7.42 (m, 2 H), 7.38 (d,  $J = 8 \text{ Hz}$ , 2 H), 7.23-7.19 (m, 2 H), 4.26 (t,  $J = 7.2 \text{ Hz}$ , 2 H), 1.84 (p,  $J = 7.3 \text{ Hz}$ , 2 H), 1.39-1.23 (m, 10H), 0.85 (t,  $J = 7.2 \text{ Hz}$ , 3 H) ppm.  $^{13}\text{C}$  NMR, (100MHz,  $\text{CDCl}_3$ -d): $\delta$  = 140.52, 125.64, 122.90, 120.42, 118.77, 108.73, 43.13, 34.14, 31.90, 29.48, 29.28, 29.06, 27.41, 22.71, 14.18 ppm. HRMS (ESI)  $m/z$ : calculated for  $\text{C}_{20}\text{H}_{25}\text{N}$   $[\text{M}+\text{H}]^+$ : 279.20, Found : 280.17.

### 9-Octyl-9H-carbazole-3-carbaldehyde (CBA)

A round bottom flask was charged with a solution of DMF (2.01 mol ratio) and 1, 2-dichloroethane (3ml) at  $0^\circ\text{C}$ .  $\text{POCl}_3$  (1.25 mol ratio) was slowly added to the mixture. Then, CB (1 mol ratio) in 1, 2-dichloroethane (3ml) was added dropwise to the mixture. The mixture was stirred for 12h at  $90^\circ\text{C}$ . Next, it was poured into ice water and the compound was filtered and dried to give CBA. Product: yellow solid, Yield: 88 %.  $^1\text{H}$  NMR, (400MHz,  $\text{CDCl}_3$ -d): $\delta$  = 10.09 (s, 1 H), 8.62 (s, 1 H), 8.16 (d,  $J = 8 \text{ Hz}$ , 1 H), 8.01 (dd,  $J = 8.8, 1.2 \text{ Hz}$ , 1 H), 7.55-7.51 (m, 1 H), 7.47 (t,  $J = 8.4 \text{ Hz}$ , 2 H), 7.34-7.30 (m, 1 H), 4.34 (t,  $J = 7.2 \text{ Hz}$ , 2 H), 1.89 (p,  $J = 7.4 \text{ Hz}$ , 2 H), 1.41-1.23 (m, 10 H), 0.86 (t,  $J = 6.8 \text{ Hz}$ , 3 H) ppm.  $^{13}\text{C}$  NMR, (100MHz,  $\text{CDCl}_3$ -d): $\delta$  = 191.77, 144.08, 141.18, 128.50, 127.14, 126.70, 123.99, 123.07, 123.00, 120.74, 120.29, 109.40, 108.94, 43.44, 31.76, 29.32, 28.93, 27.26, 22.59, 14.06 ppm.

### **6-Iodo-9-octyl-9H-carbazole-3-carbaldehyde (CBAI)**

To a two neck RB flask, CBA (1mol ratio) was dissolved in glacial acetic acid (16V) and then KI (0.67 mol ratio) and KIO<sub>3</sub> (0.4 mol ratio) were added. The mixture was stirred at 80°C until iodine was fully consumed, then the mixture was cooled to room temperature, a pale brown colour solid appeared and filter the solid and then poured into 5% NaHSO<sub>3</sub> to remove KIO<sub>3</sub>. After 1 hr stirring, the mixture was filtered off and dried to get CBAI. Product: pale brown colour solid, yield: 68 %. <sup>1</sup>H NMR, (400MHz, CDCl<sub>3</sub>-d):δ = 10.08 (s, 1 H), 8.54 (s, 1 H), 8.46 (s, 1 H), 8.03 (dd, *J* = 8.4, 1.6 Hz, 1 H), 7.77 (dd, *J* = 8.8, 1.6 Hz, 1 H), 7.47 (d, *J* = 8.4 Hz, 1 H), 7.24 (d, *J* = 8.4 Hz, 1 H), 4.30 (t, *J* = 7.2 Hz, 2 H), 1.86 (p, *J* = 7.3 Hz, 2 H), 1.37-1.23 (m, 10 H), 0.86 (t, *J* = 6.8 Hz, 3 H) ppm. <sup>13</sup>C NMR, (100MHz, CDCl<sub>3</sub>-d):δ = 191.50, 143.87, 140.32, 134.94, 129.59, 128.94, 127.43, 125.38, 124.32, 121.72, 111.38, 109.22, 82.89, 43.53, 31.73, 29.27, 29.11, 28.87, 27.20, 22.57, 14.05 ppm.

### **6-(4-tert-Butyl-phenyl)-9-octyl-9H-carbazole-3-carbaldehyde (CTB)**

Tetrahydrofuran (50V) and water (10V) was charged with a dried 100 ml two neck RB flask under nitrogen atmosphere for 10 min. 4-tert-butyl phenyl boronic acid (1 mol ratio) and CBAI (1.2 mol ratio) and K<sub>2</sub>CO<sub>3</sub> (3 mol ratio) was added to the above mixture and stirred for 5 min. Then Pd(PPh<sub>3</sub>)<sub>4</sub> (0.05 mol ratio) was added and heat at 75°C for 12 hr. After completion of the reaction, the mixture was extracted with DCM and dried over anhydrous sodium sulphate. The residue was purified by column chromatography (100-200 mesh, silica gel) with hexane/ethylacetate as the eluent to afford CTB. Product: light yellow solid, yield: 91 %. <sup>1</sup>H NMR, (400MHz, CDCl<sub>3</sub>-d):δ = 10.11 (s, 1 H), 8.65 (s, 1 H), 8.36 (s, 1 H), 8.02 (dd, *J* = 8.8, 1.2 Hz, 1 H), 7.77 (dd, *J* = 8.4, 1.6 Hz, 1 H), 7.65 (d, *J* = 8.4 Hz, 2 H), 7.53-7.47 (m, 4 H), 4.35 (t, *J* = 7.2 Hz, 2 H), 1.91 (p, *J* = 7.3 Hz, 2 H), 1.39 (s, 9 H), 1.36-1.25 (m, 10 H), 0.86 (t, *J* = 6.4 Hz,

3 H) ppm.  $^{13}\text{C}$  NMR, (100MHz,  $\text{CDCl}_3$ -*d*):  $\delta$  = 191.77, 149.82, 144.47, 140.49, 138.67, 133.75, 128.91, 128.56, 127.33, 127.20, 126.94, 126.17, 125.87, 124.12, 123.51, 123.23, 119.00, 109.61, 109.09, 43.57, 34.56, 31.78, 31.45, 29.74, 29.34, 29.17, 29.00, 27.29, 22.62, 14.16, 14.09 ppm. HRMS (ESI-TOF) *m/z*: calculated for  $\text{C}_{31}\text{H}_{37}\text{NO}$   $[\text{M}+\text{H}]^+$ : 439.29, Found : 440.3097.

### **9-Octyl-6-(2,4,6-trimethyl-phenyl)-9H-carbazole-3-carbaldehyde (CTM)**

Product: pale brown colour, yield: 78 %.  $^1\text{H}$  NMR, (400MHz,  $\text{CDCl}_3$ -*d*):  $\delta$  = 10.08 (s, 1 H), 8.55 (s, 1 H), 8.02 (dd,  $J$  = 8.8, 1.6 Hz, 1 H), 7.92 (s, 1 H), 7.49 (d,  $J$  = 8 Hz, 2 H), 7.30 (dd,  $J$  = 8.4, 1.2 Hz, 1 H), 6.99 (s, 2 H), 4.36 (t,  $J$  = 7.2 Hz, 2 H), 2.36 (s, 3 H), 2.04 (s, 6 H), 1.94 (p,  $J$  = 7.4 Hz, 2 H), 1.46-1.20 (m, 10 H), 0.86 (t,  $J$  = 6.8 Hz, 3 H) ppm.  $^{13}\text{C}$  NMR, (100MHz,  $\text{CDCl}_3$ -*d*):  $\delta$  = 191.72, 144.35, 140.03, 139.18, 136.60, 136.54, 133.28, 128.50, 128.26, 128.15, 126.99, 124.26, 123.16, 123.09, 121.27, 109.33, 109.05, 43.62, 31.79, 29.35, 29.19, 29.04, 27.35, 22.63, 21.09, 21.00, 14.09 ppm. HRMS (ESI-TOF) *m/z*: calculated for  $\text{C}_{30}\text{H}_{35}\text{NO}$   $[\text{M}+\text{H}]^+$ : 425.27, Found : 426.2767.

### **6-(4-Methoxy-phenyl)-9-octyl-9H-carbazole-3-carbaldehyde (COMe)**

Product: yellow colour, yield: 68 %.  $^1\text{H}$  NMR, (400MHz,  $\text{CDCl}_3$ -*d*):  $\delta$  = 10.11 (s, 1 H), 8.65 (s, 1 H), 8.32 (s, 1 H), 8.02 (d,  $J$  = 8.4 Hz, 1 H), 7.73 (d,  $J$  = 8.4 Hz, 1 H), 7.64 (d,  $J$  = 8.4 Hz, 2 H), 7.49 (dd,  $J$  = 8.4, 3.6 Hz, 2 H), 7.04 (d,  $J$  = 8.4 Hz, 2 H), 4.35 (t,  $J$  = 7.2 Hz, 2 H), 3.88 (s, 3 H), 1.91 (p,  $J$  = 7.3 Hz, 2 H), 1.43-1.20 (m, 10 H), 0.86 (t,  $J$  = 6.4 Hz, 3 H) ppm.  $^{13}\text{C}$  NMR, (100MHz,  $\text{CDCl}_3$ -*d*):  $\delta$  = 191.70, 158.88, 144.43, 140.26, 134.18, 133.55, 128.54, 128.27, 127.13, 125.92, 124.11, 123.51, 123.17, 118.66, 114.37, 109.61, 109.06, 55.40, 43.51, 31.78, 29.74, 29.34, 29.17, 28.98, 27.27, 22.62, 14.09 ppm. HRMS (ESI-TOF) *m/z*: calculated for  $\text{C}_{28}\text{H}_{31}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 413.24, Found : 414.2444.

### **9-Octyl-6-phenyl-9H-carbazole-3-carbaldehyde (CPB)**

Product: yellow colour solid, yield: 47 % <sup>1</sup>H NMR, (400MHz, CDCl<sub>3</sub>-*d*): $\delta$  = 10.11 (s, 1 H), 8.66 (s, 1 H), 8.37 (s, 1 H), 8.03 (dd, *J* = 8.4, 1.2 Hz, 1 H), 7.78 (dd, *J* = 8.4, 1.6 Hz, 1 H), 7.71 (d, *J* = 7.6 Hz, 2 H), 7.52-7.47 (m, 4 H), 7.36 (t, *J* = 7.2 Hz, 1 H), 4.36 (t, *J* = 7.2 Hz, 2 H), 1.91 (p, *J* = 7.3 Hz, 2 H), 1.42-1.21 (m, 10 H), 0.86 (t, *J* = 6.4 Hz, 3 H) ppm. <sup>13</sup>C NMR, (100MHz, CDCl<sub>3</sub>-*d*): $\delta$  = 191.69, 144.44, 141.58, 140.61, 133.81, 128.93, 128.61, 127.30, 127.17, 126.84, 126.19, 124.11, 123.52, 123.18, 119.14, 109.67, 109.11, 43.51, 31.81, 29.35, 29.19, 28.99, 27.28, 22.65, 14.13 ppm.

### **General procedure for the preparation of amine donor aldehydes**

CBAI (0.0006 mol), amine donors (Bis-(4-methoxy-phenyl)-amine, Bis-(4-Hexyloxy-phenyl)-amine, Bis(2',4'-bis(hexyloxy)-[1,1'-biphenyl]-4-yl)amine) (0.0006 mol) and sodium tertiary butoxide (0.0008 mol) were dissolved in toluene (6 ml). This solution was degassed under nitrogen for 20 min and then Pd[P(t-Bu)<sub>3</sub>]<sub>2</sub> was added to the reaction mixture. The reaction was then brought to 80 °C and stirred for 12 hours. The reaction mixture was cooled to room temperature and plugged through a thin pad of NaSO<sub>4</sub> with DCM. The crude product was adsorbed in silica gel and purified by column chromatography to get the corresponding compounds.

### **6-[Bis-(4-methoxy-phenyl)-amino]-9-octyl-9H-carbazole-3-carbaldehyde (COMN)**

Yield: 35.7 %. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  10.04 (s, 1H), 8.45 (d, *J* = 1.3 Hz, 1H), 7.99 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.78 (d, *J* = 1.8 Hz, 1H), 7.45 (d, *J* = 8.6 Hz, 1H), 7.32 (s, 2H), 7.07 (d, *J* = 9.0 Hz, 4H), 6.84 (d, *J* = 9.0 Hz, 4H), 4.31 (s, 2H), 3.83 (s, 6H), 1.93 – 1.86 (m, 2H), 1.27 (s, 10H), 0.88 (d, *J* = 7.0 Hz, 3H).

**6-[Bis-(4-hexyloxy-phenyl)-amino]-9-octyl-9H-carbazole-3-carbaldehyde (CCN)**

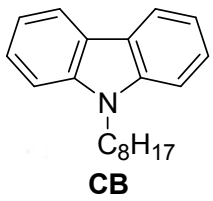
Yield: 25.7 %. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 10.04 (s, 1H), 8.45 (s, 1H), 7.99 (dd, *J* = 8.6, 1.2 Hz, 1H), 7.83 – 7.76 (m, 1H), 7.45 (s, 1H), 7.30 (dd, *J* = 5.5, 3.6 Hz, 2H), 7.05 (d, *J* = 8.9 Hz, 4H), 6.84 (d, *J* = 8.9 Hz, 4H), 4.31 (s, 2H), 3.96 (t, *J* = 6.6 Hz, 4H), 1.92 – 1.88 (m, 2H), 1.81 (s, 2H), 1.49 (s, 2H), 1.37 – 1.28 (m, 22H), 0.94 – 0.90 (m, 9H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ = 191.68, 154.67, 144.42, 143.34, 142.67, 142.07, 136.86, 135.22, 130.52, 128.98, 128.40, 128.16, 126.78, 125.41, 125.08, 124.54, 123.77, 123.74, 122.74, 115.21, 109.86, 108.95, 77.35, 77.23, 77.03, 76.71, 68.31, 59.53, 43.54, 38.16, 31.95, 31.86, 31.64, 31.26, 29.72, 29.68, 29.52, 29.49, 29.39, 29.37, 29.27, 29.04, 27.28, 25.80, 25.04, 24.90, 24.59, 22.72, 22.67, 22.64, 14.15, 14.13, 14.08.

**6-[Bis(20,40-bis(hexyloxy)-[1,10-biphenyl]-4-yl)amino]-9-octyl-9H-carbazole-3-carbaldehyde (CHN)**

Yield: 18.6 %. <sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 10.06 (s, 1H), 8.50 (d, *J* = 1.3 Hz, 1H), 8.03 (dd, *J* = 8.3, 1.7 Hz, 2H), 7.51 – 7.38 (m, 8H), 7.31 (s, 1H), 7.19 – 7.15 (m, 4H), 6.56 (dd, *J* = 6.1, 2.3 Hz, 4H), 4.35 (s, 2H), 4.02 – 3.97 (m, 8H), 1.97 – 1.91 (m, 2H), 1.84 – 1.76 (m, 8H), 1.48 – 1.28 (m, 34H), 0.96 – 0.85 (m, 15H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ = 191.64, 159.44, 156.96, 146.67, 144.46, 141.31, 137.91, 132.01, 130.82, 130.10, 128.42, 126.08, 123.94, 123.10, 122.74, 122.40, 118.34, 110.11, 109.13, 105.27, 100.41, 77.35, 77.24, 77.03, 76.72, 68.39, 68.12, 43.62, 31.87, 31.64, 31.46, 29.54, 29.51, 29.39, 29.34, 29.28, 29.08, 27.32, 25.79, 25.77, 22.67, 22.65, 22.57, 14.13, 14.08, 14.03.

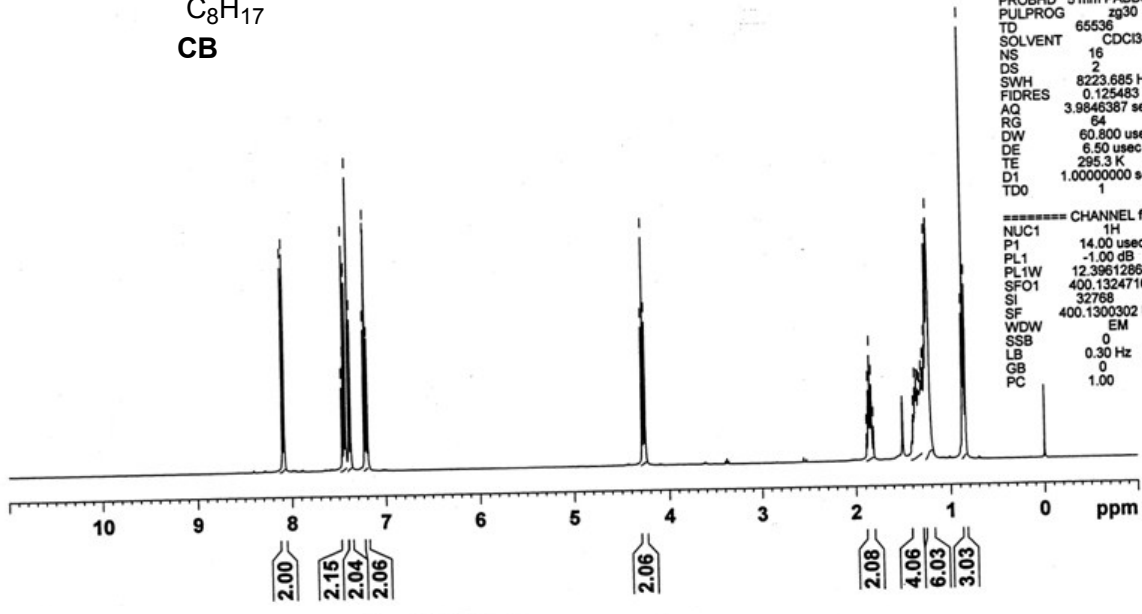


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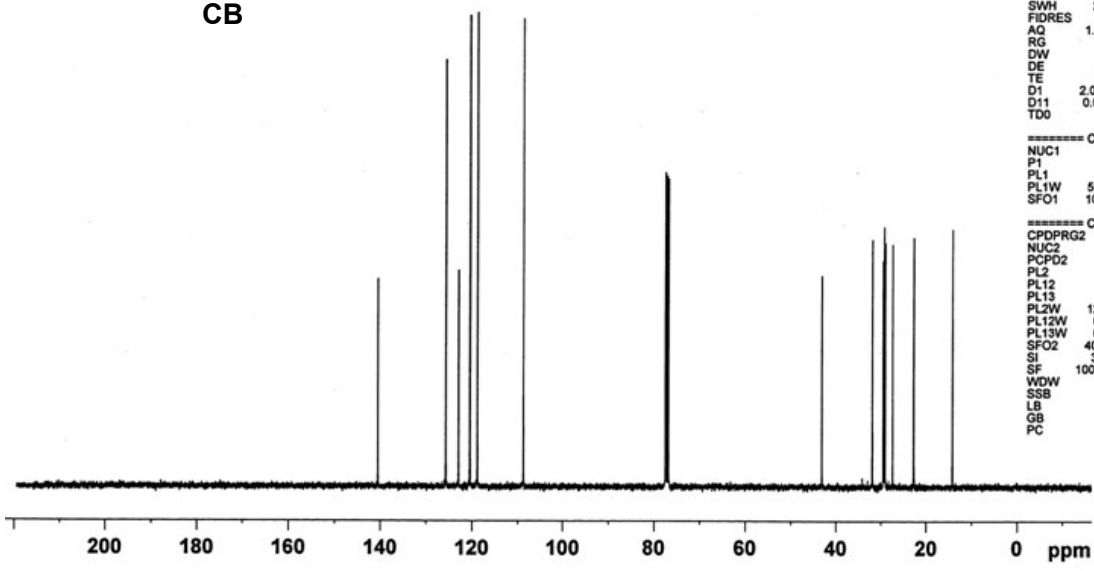
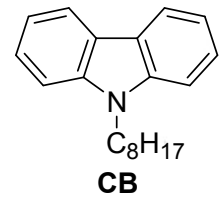
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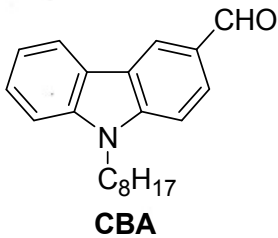
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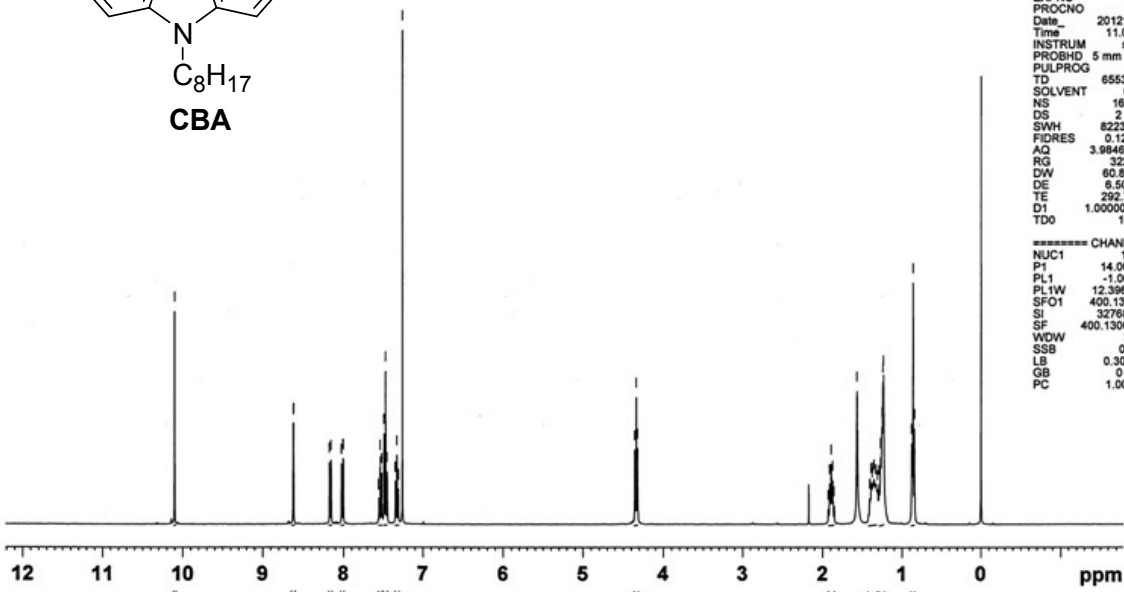


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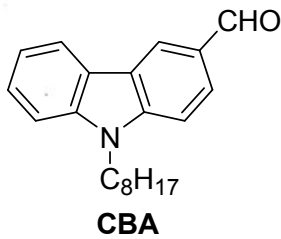


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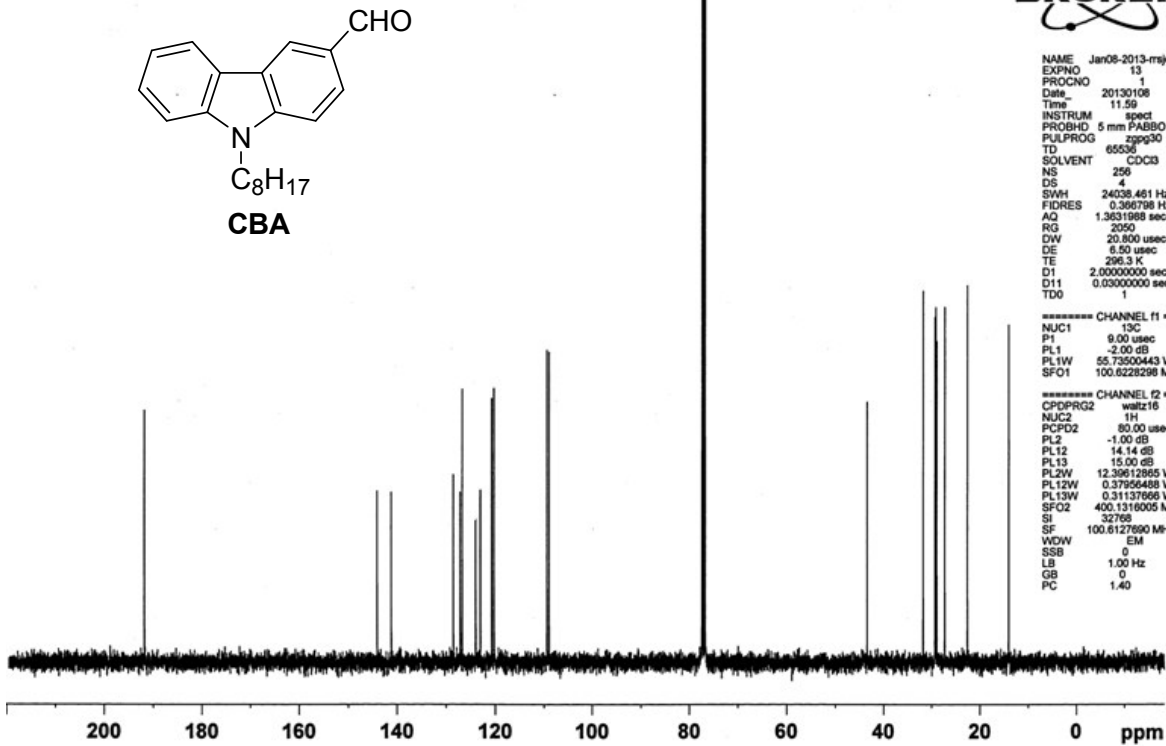
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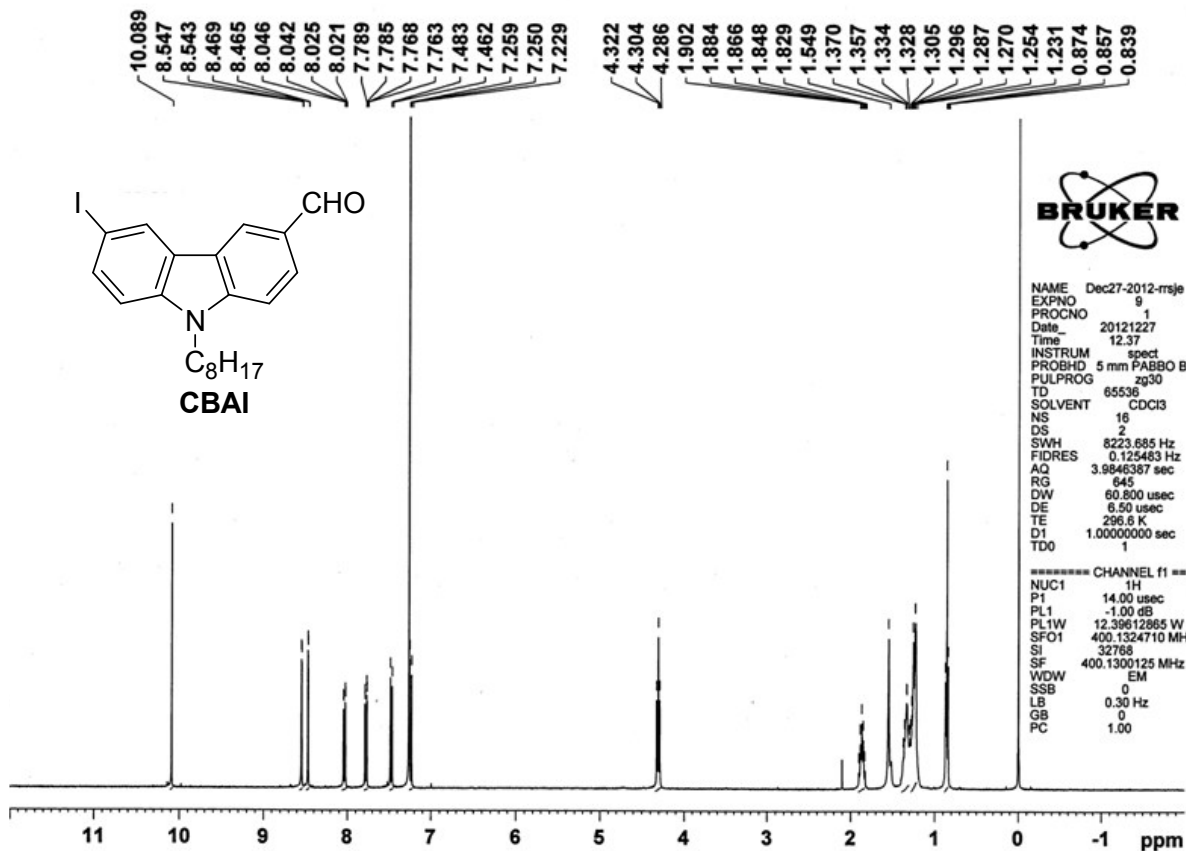


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NS 4  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631968 sec  
RG 2050  
DW 20.800 usec  
DE 6.50 usec  
TE 296.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PL1 -2.00 dB  
PL1W 55.73500443 W  
SFO1 100.6228298 MHz

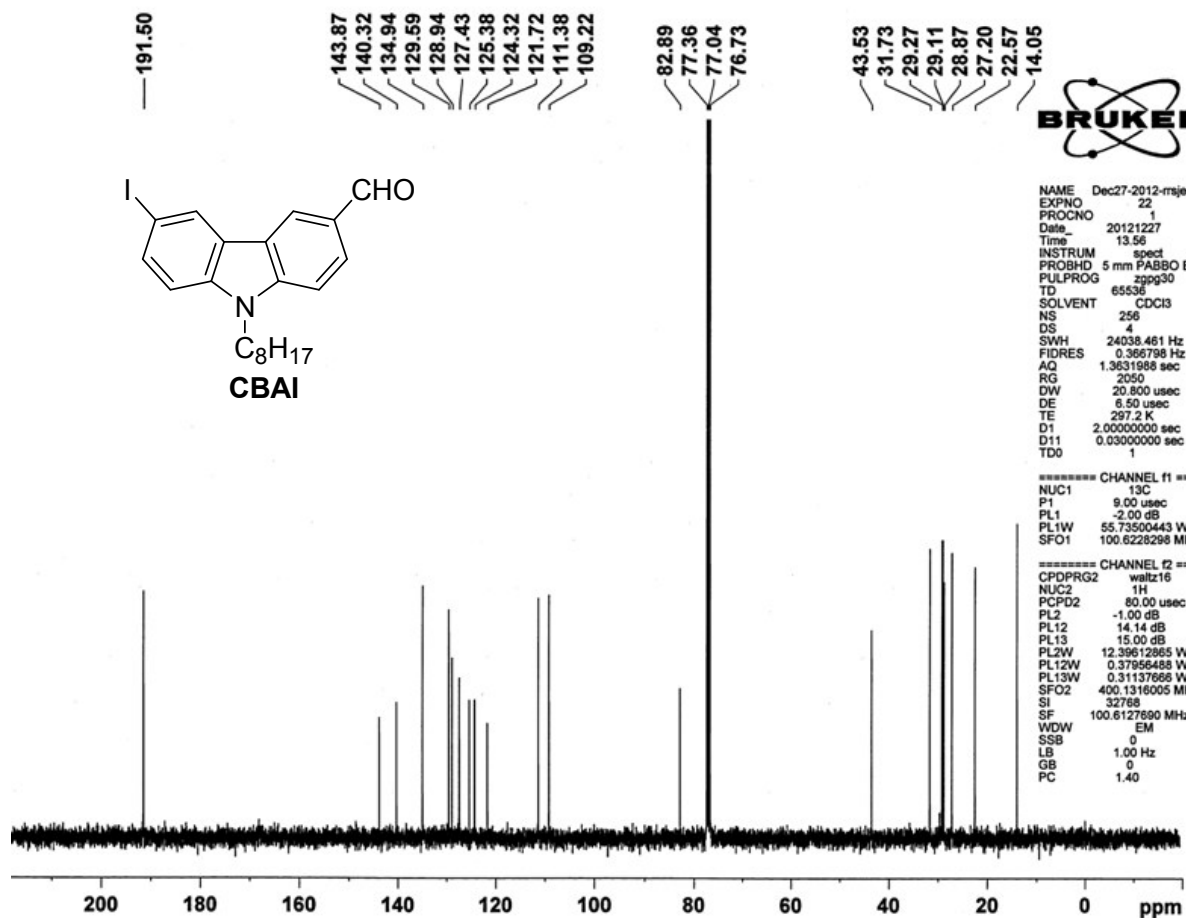
===== CHANNEL f2 =====  
CPOPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL2 14.14 dB  
PL13 15.00 dB  
PL2W 12.39612865 W  
PL12W 0.37956488 W  
PL13W 0.31137666 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





NAME Dec27-2012-rsje  
 EXPNO 9  
 PROCNO 1  
 Date\_ 20121227  
 Time 12.37  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 645  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.5 K  
 D1 1.00000000 sec  
 TD0 1

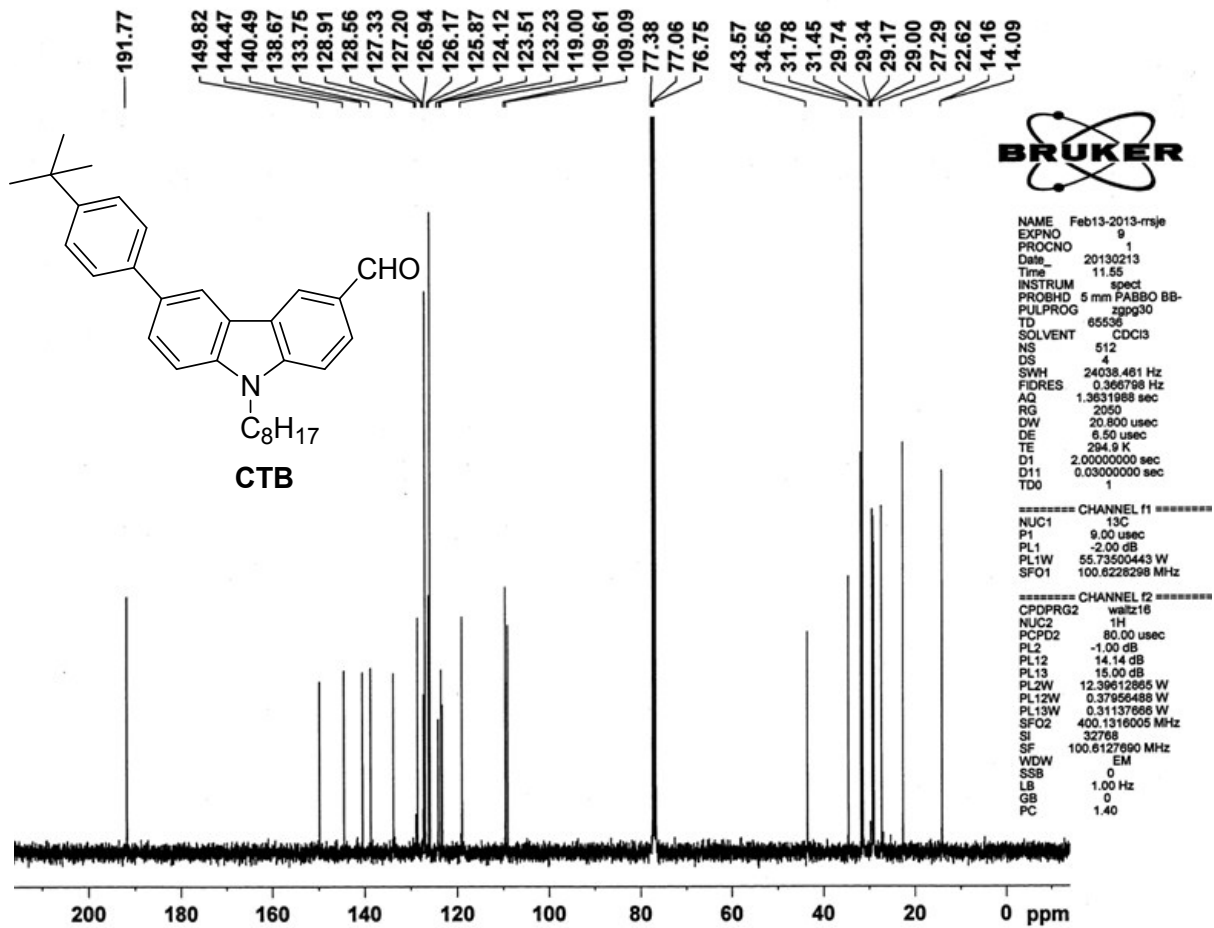
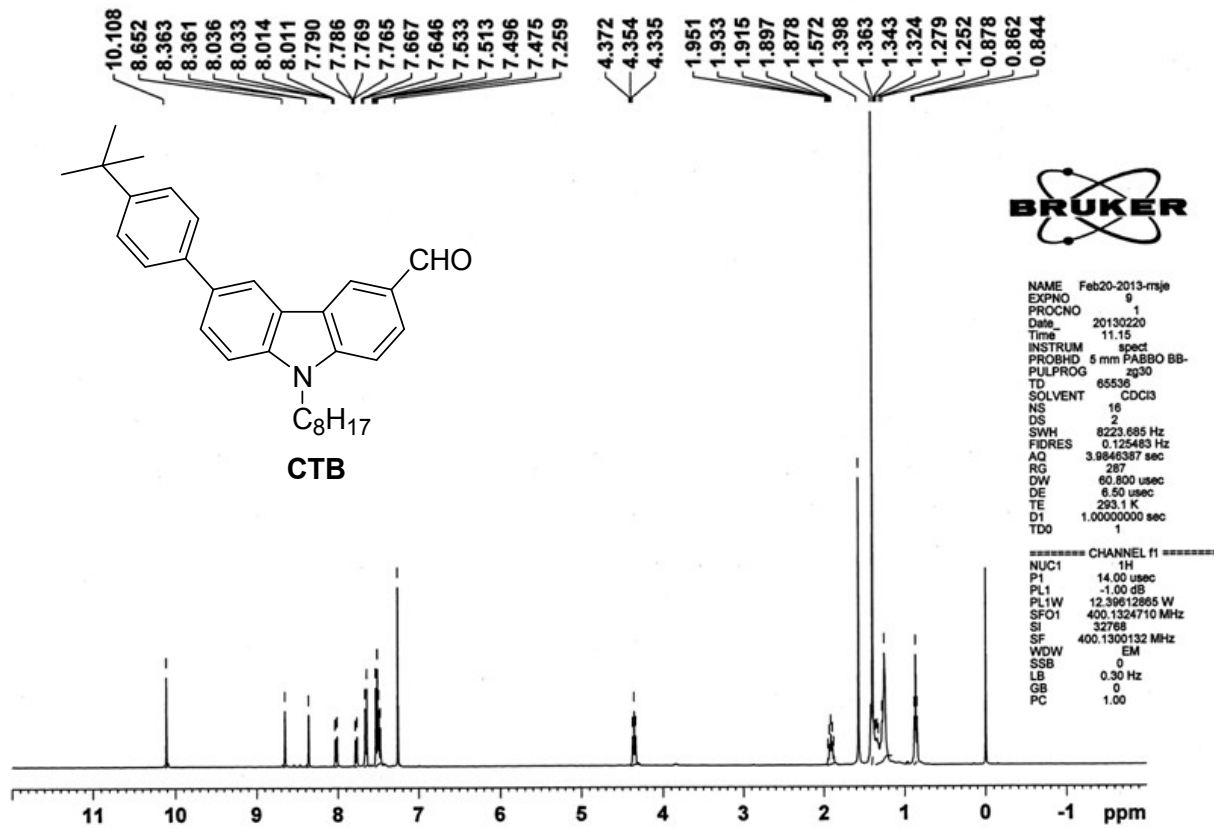
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -1.00 dB  
 PL1W 12.39612865 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300125 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

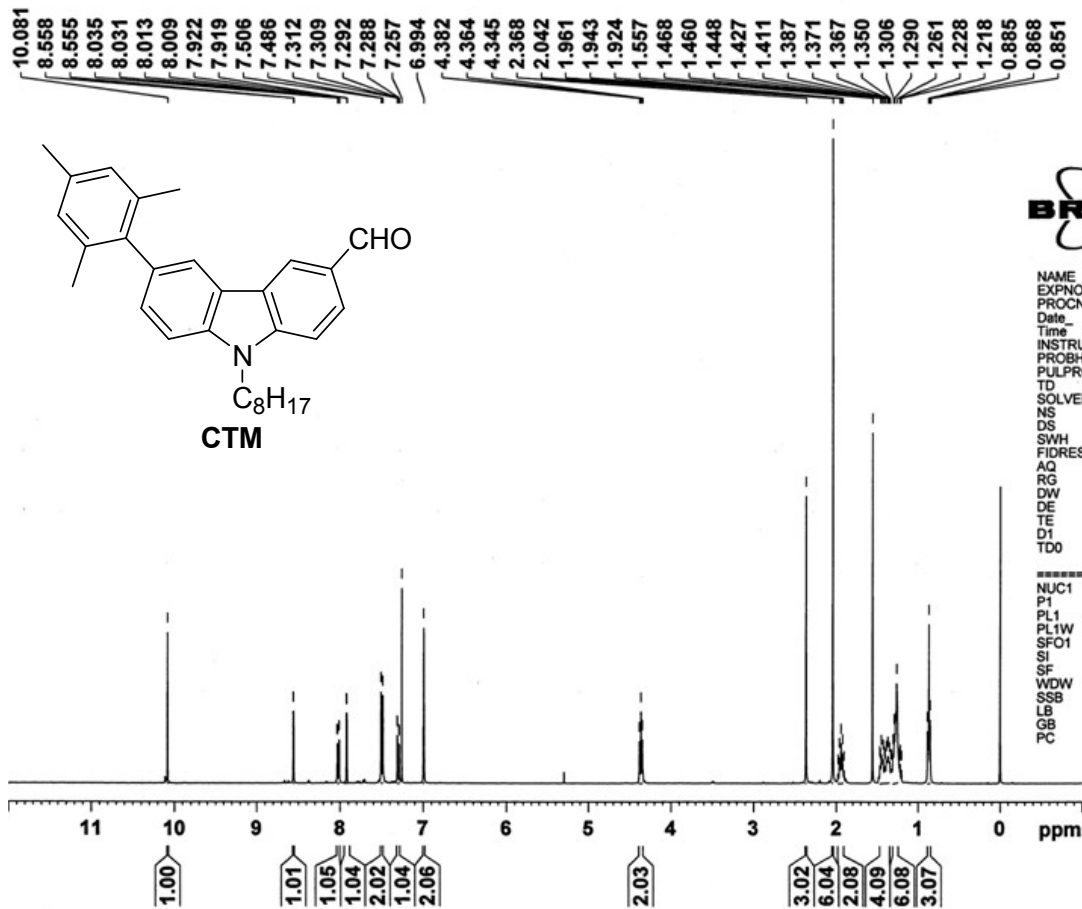


NAME Dec27-2012-rsje  
 EXPNO 22  
 PROCNO 1  
 Date\_ 20121227  
 Time 13.56  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 -2.00 dB  
 PL1W 55.73500443 W  
 SFO1 100.6228298 MHz

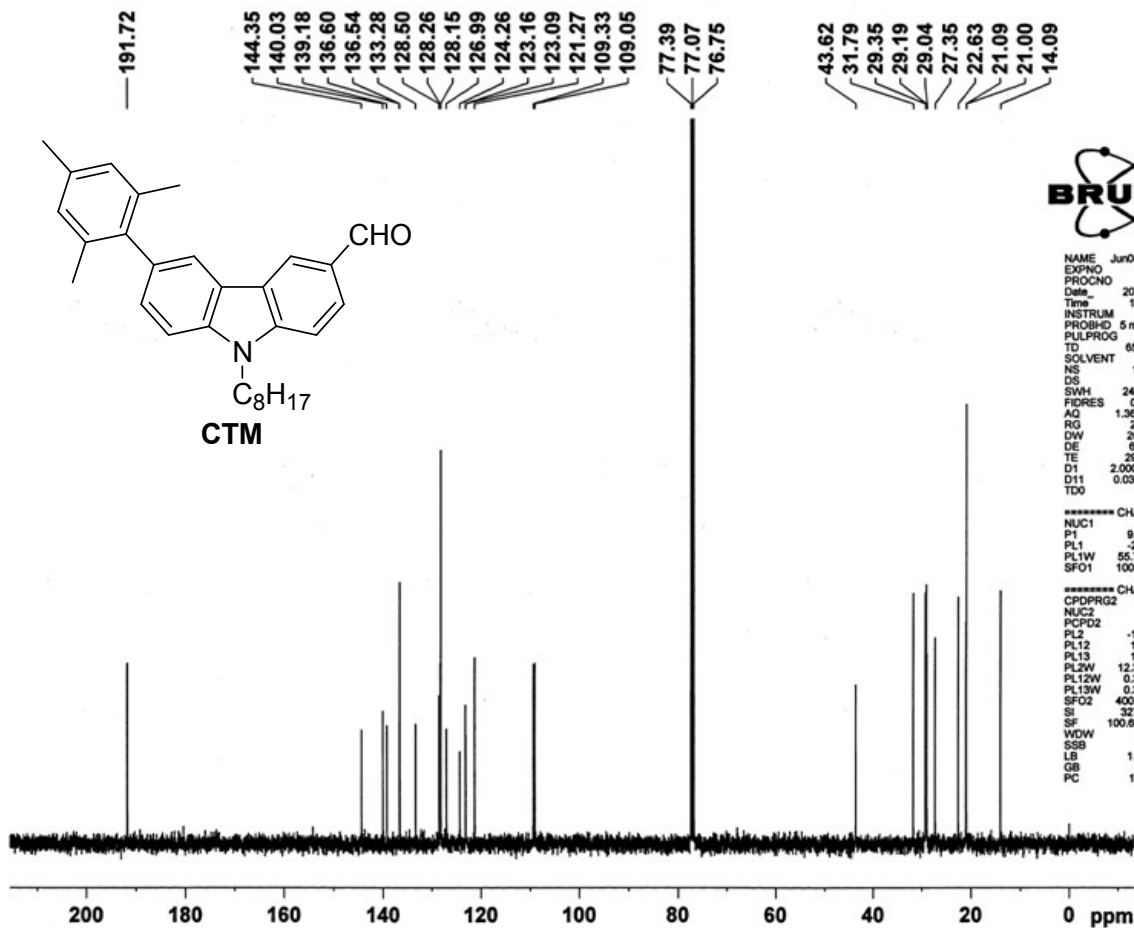
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.14 dB  
 PL13 15.00 dB  
 PL2W 12.39612865 W  
 PL12W 0.37956488 W  
 PL13W 0.31137666 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





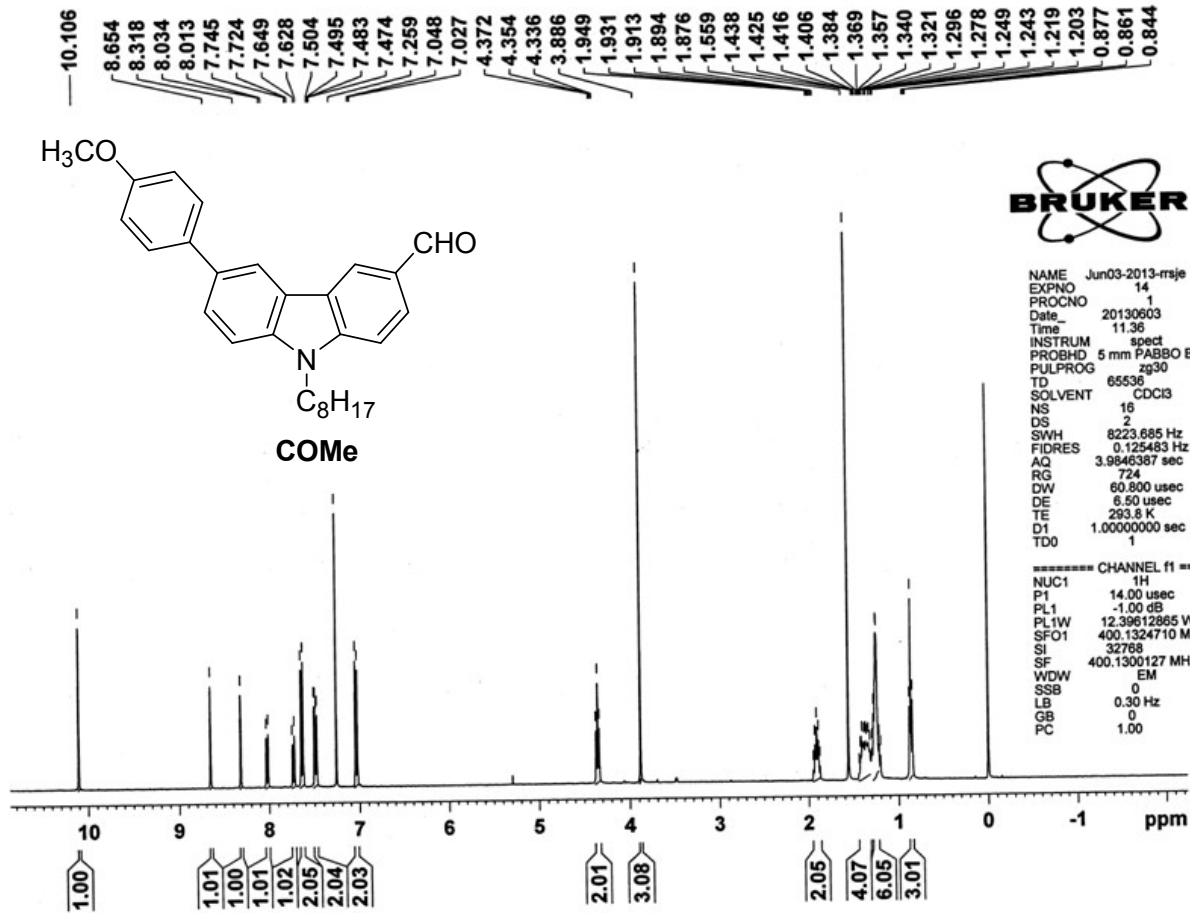
NAME Jun06-2013-rsje  
EXPNO 12  
PROCNO 1  
Date\_ 20130608  
Time 11.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 322  
DW 60.800 usec  
DE 6.50 usec  
TE 295.6 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.00 usec  
PL1 -1.00 dB  
PL1W 12.39612865 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300140 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



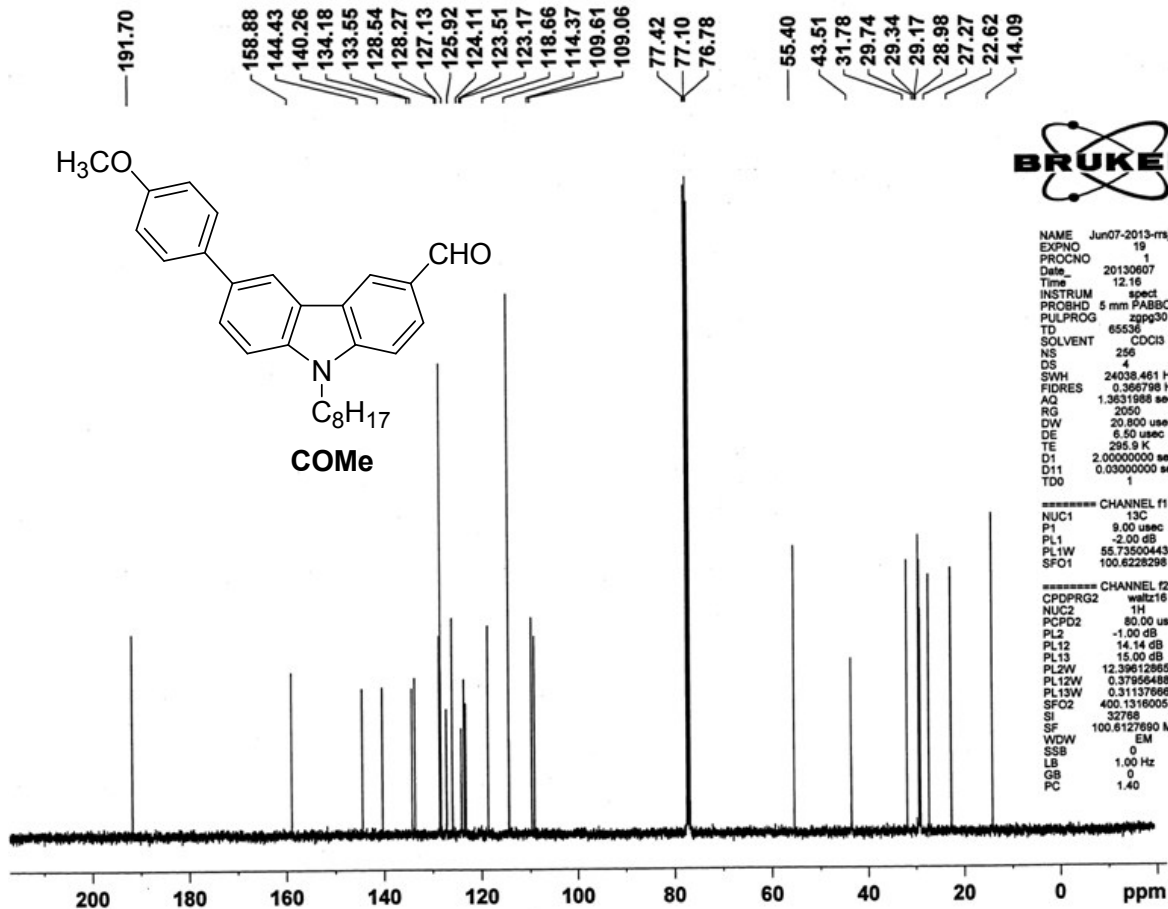
NAME Jun08-2013-rsje  
EXPNO 41  
PROCNO 1  
Date\_ 20130608  
Time 15.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 151  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 2050  
DW 20.800 usec  
DE 6.50 usec  
TE 297.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PL1 -2.00 dB  
PL1W 55.73500443 W  
SFO1 100.6228298 MHz  
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.14 dB  
PL13 15.00 dB  
PL12W 12.39612865 W  
PL13W 0.37956488 W  
PL13W 0.31137866 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6127890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



NAME Jun03-2013-rsje  
 EXPNO 14  
 PROCNO 1  
 Date\_ 20130603  
 Time 11.36  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.964387 sec  
 RG 724  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 293.8 K  
 D1 1.00000000 sec  
 TD0 1

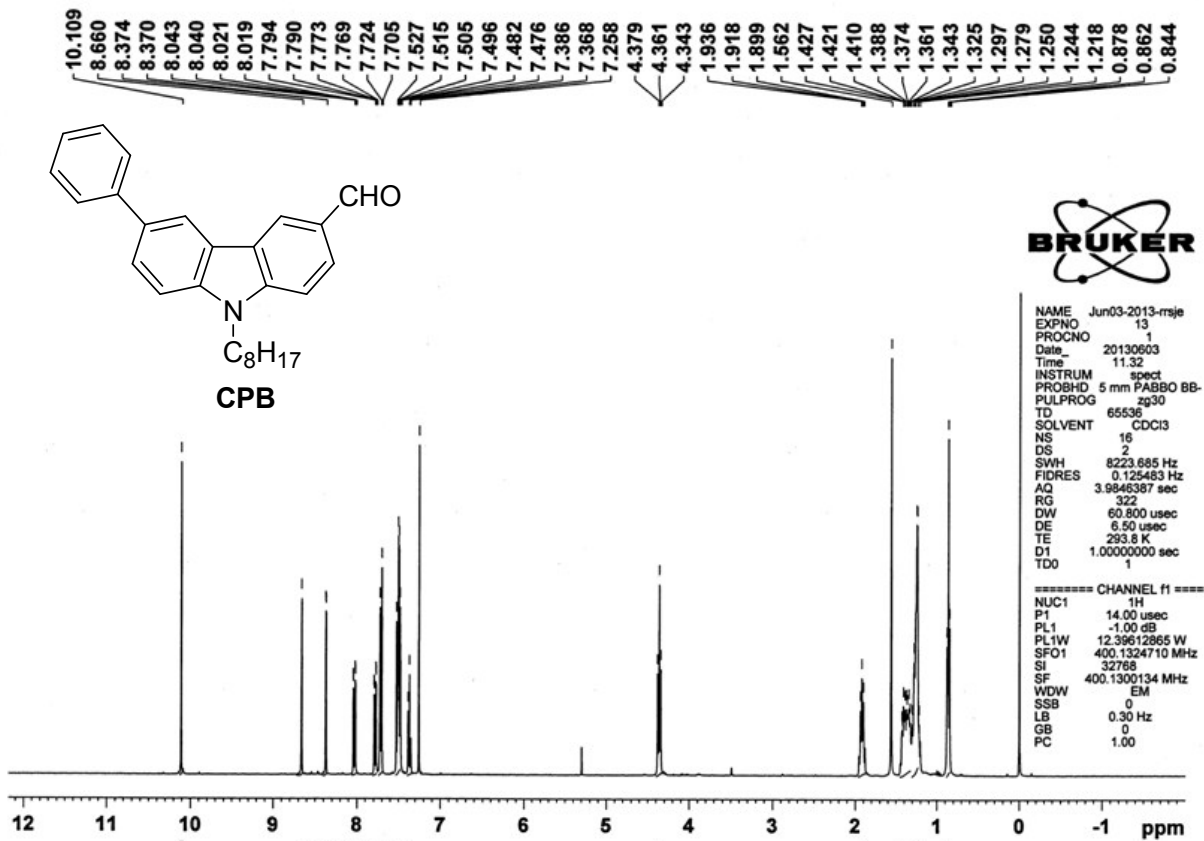
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -1.00 dB  
 PL1W 12.39612965 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300127 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME Jun07-2013-rsje  
 EXPNO 19  
 PROCNO 1  
 Date\_ 20130607  
 Time 12.16  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

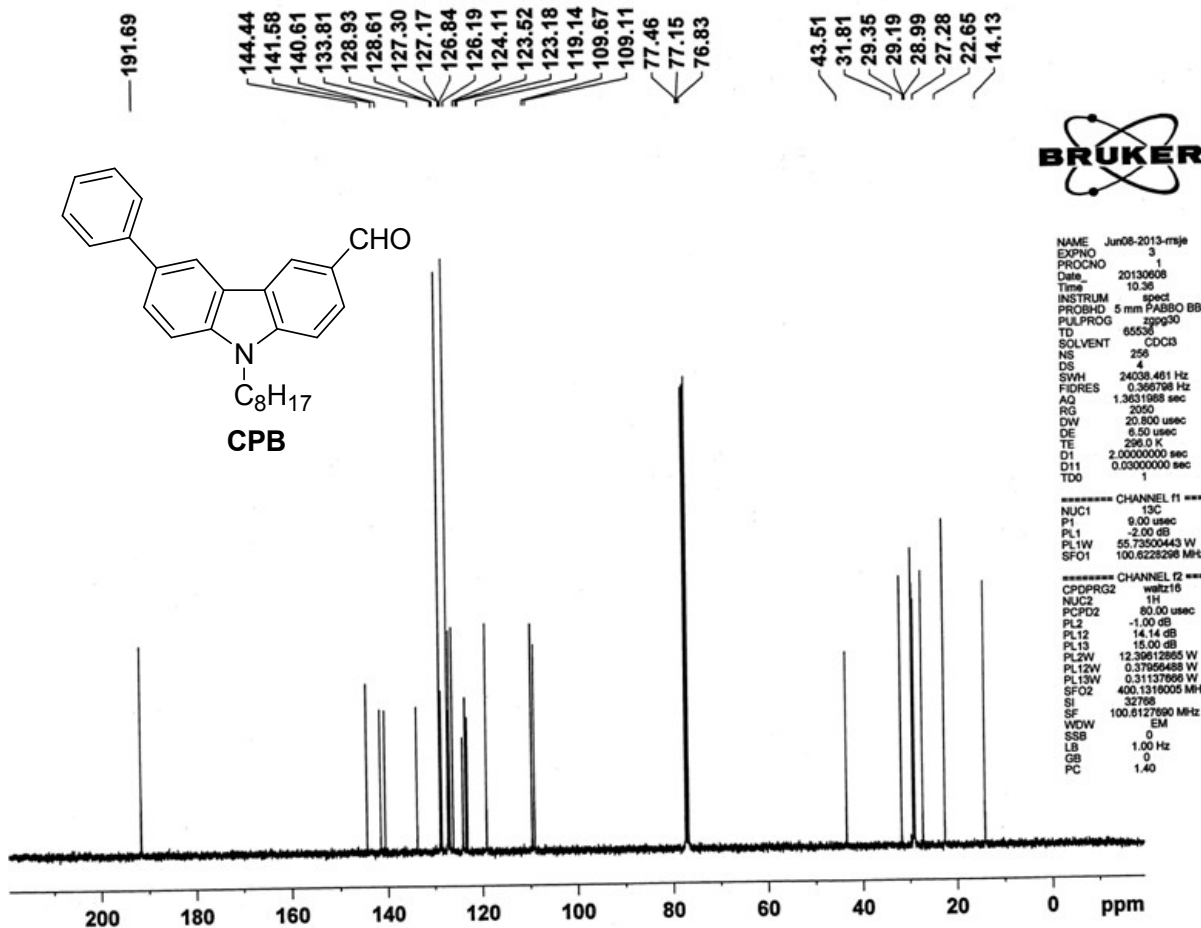
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 -2.00 dB  
 PL1W 55.73500443 W  
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.14 dB  
 PL13 15.00 dB  
 PL2W 12.39612965 W  
 PL12W 0.37956488 W  
 PL13W 0.31137666 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6127890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



NAME Jun03-2013-rsje  
 EXPNO 13  
 PROCNO 1  
 Date\_ 20130603  
 Time 11.32  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 322  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 293.8 K  
 D1 1.00000000 sec  
 TDO 1

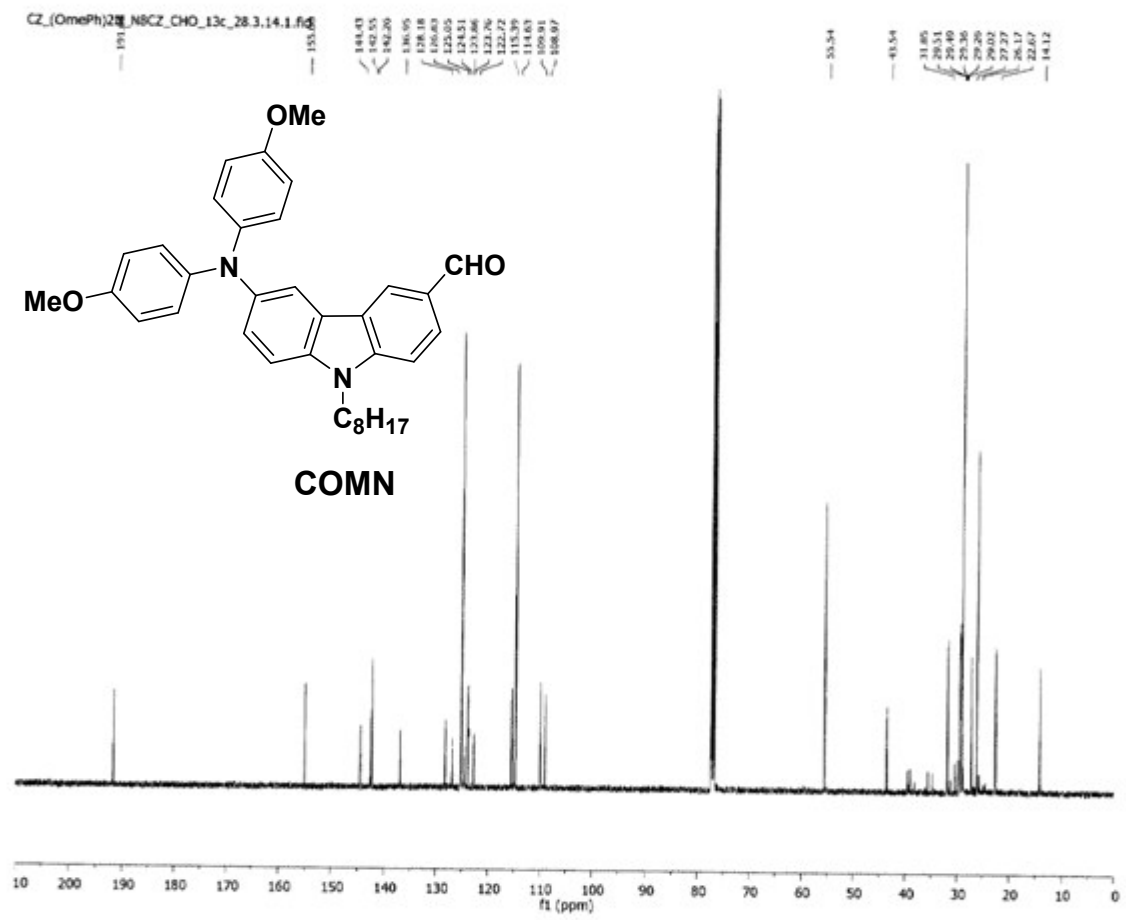
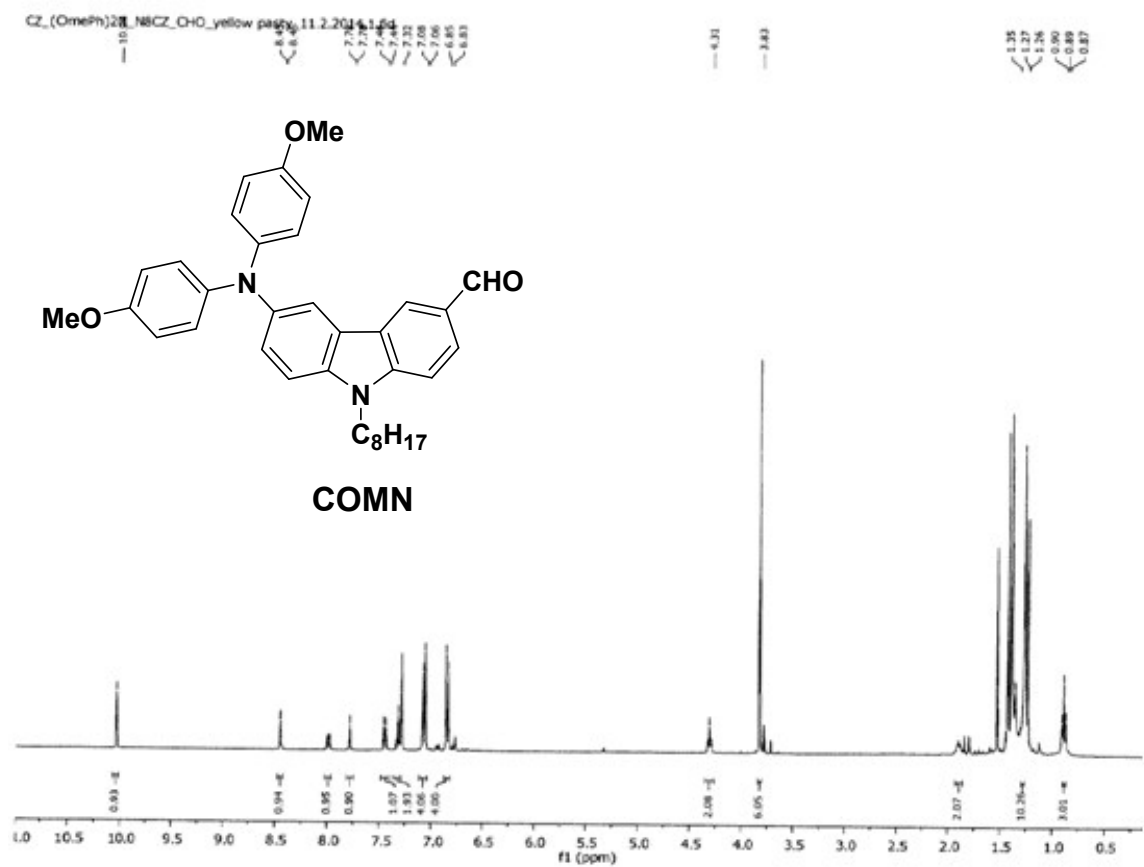
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -1.00 dB  
 PL1W 12.39612865 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300134 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



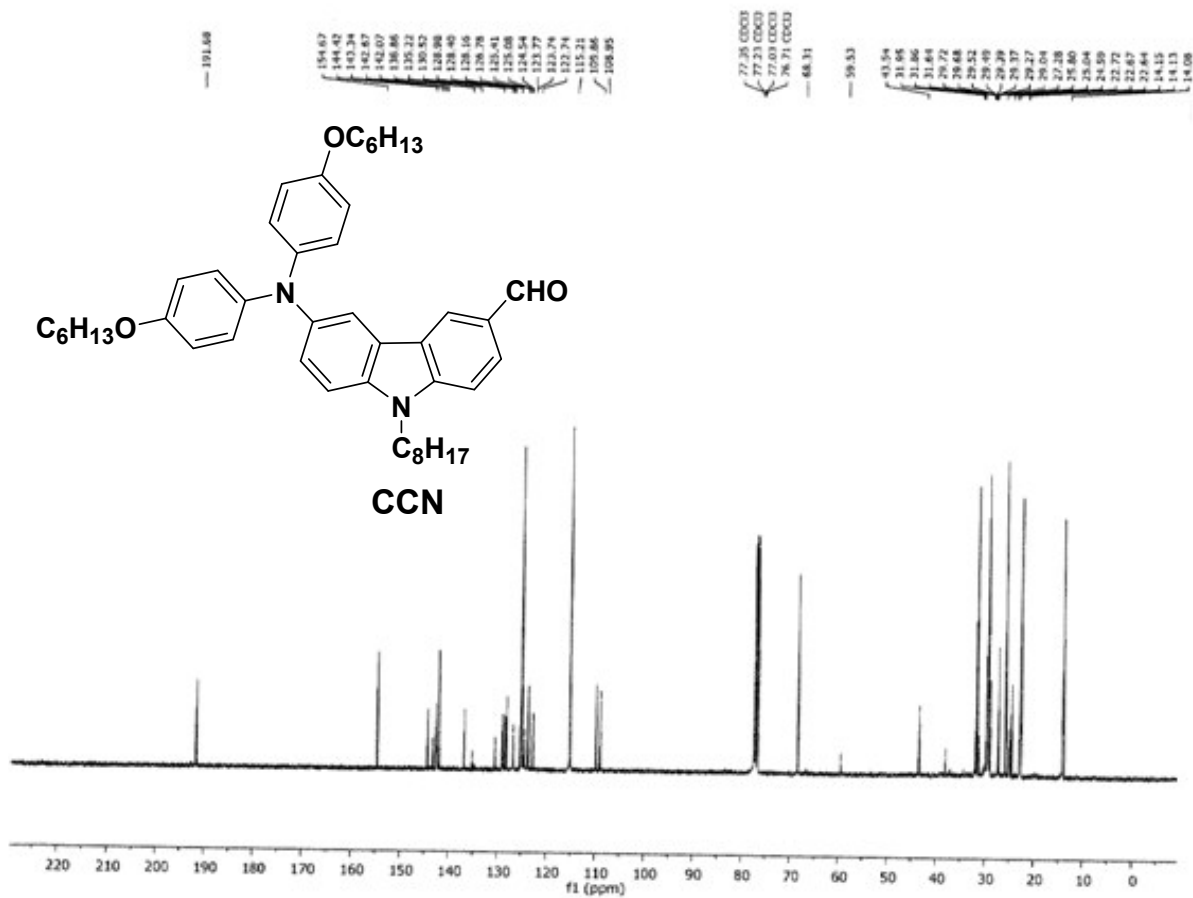
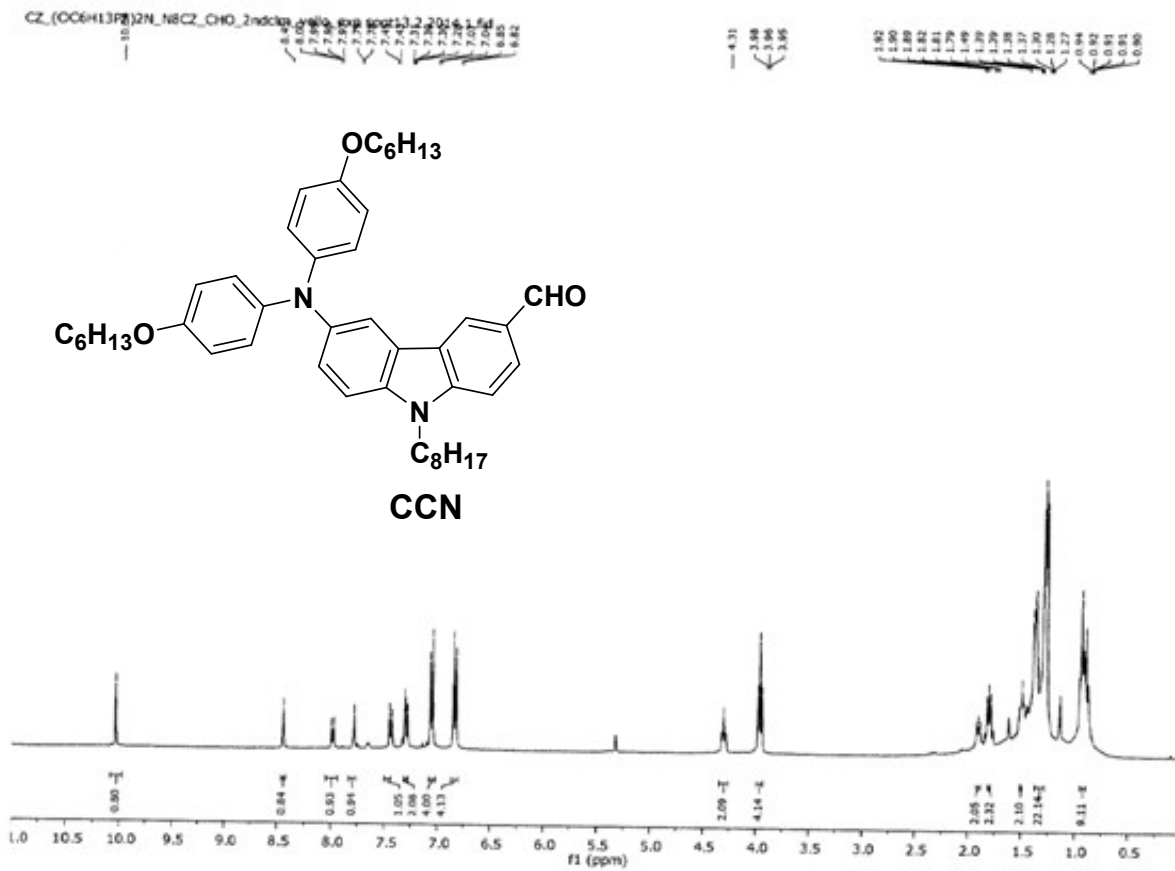
NAME Jun08-2013-rsje  
 EXPNO 3  
 PROCNO 1  
 Date\_ 20130608  
 Time 10.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631998 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

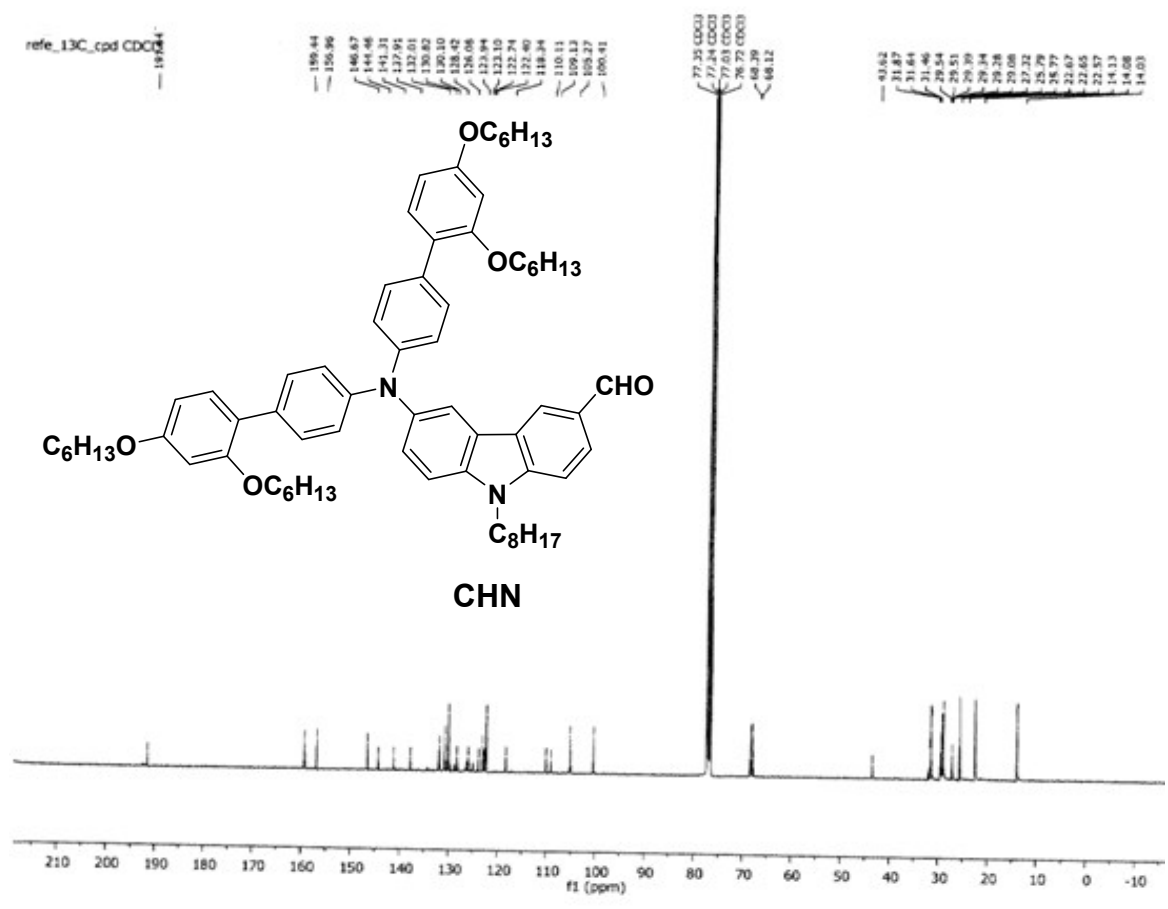
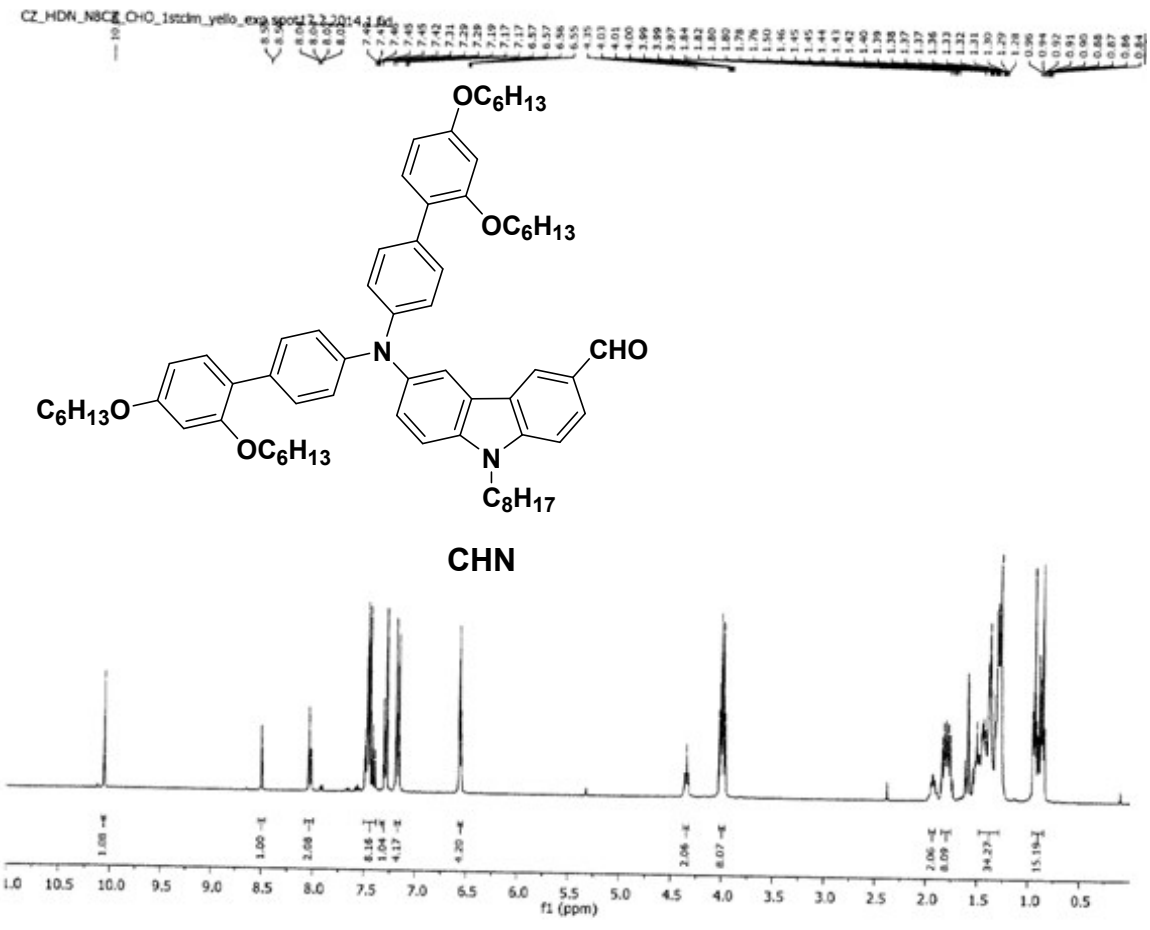
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 -2.00 dB  
 PL1W 55.73500443 W  
 SFO1 100.6225298 MHz

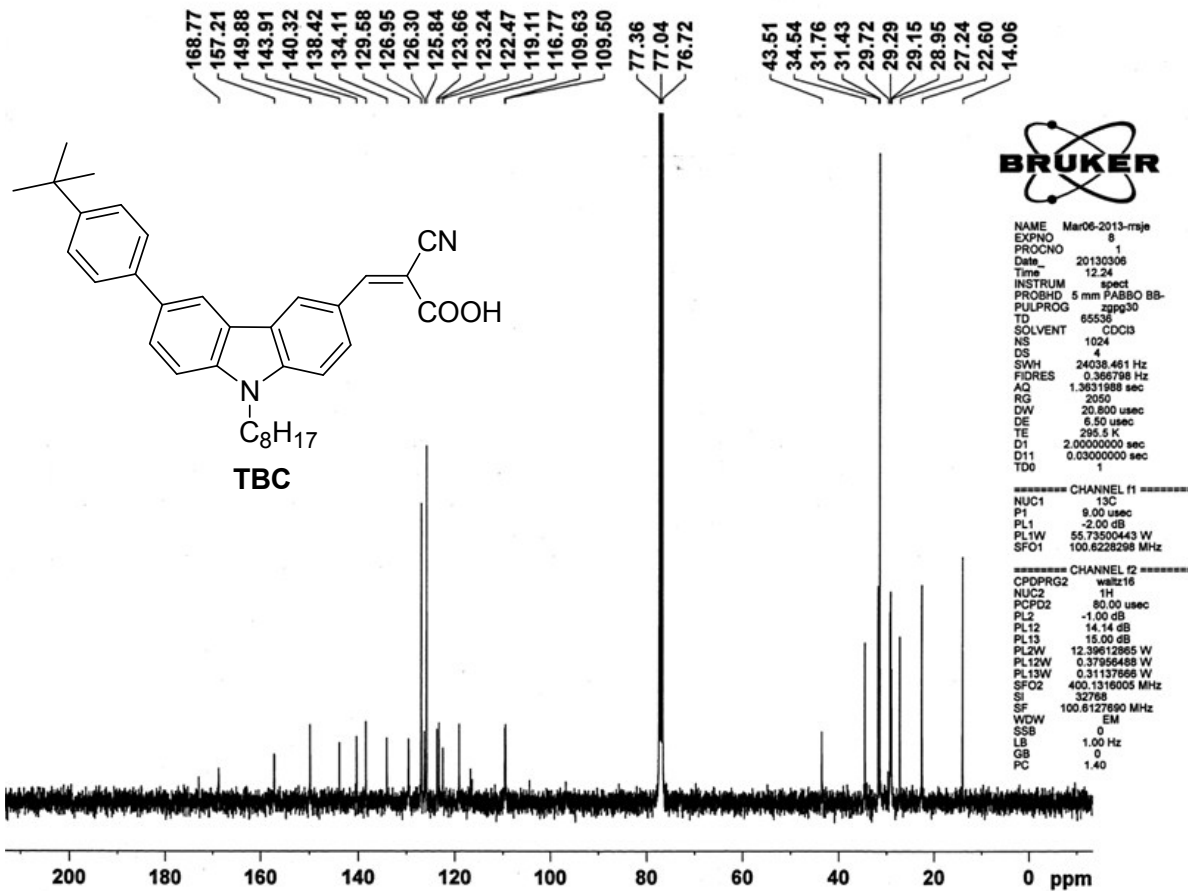
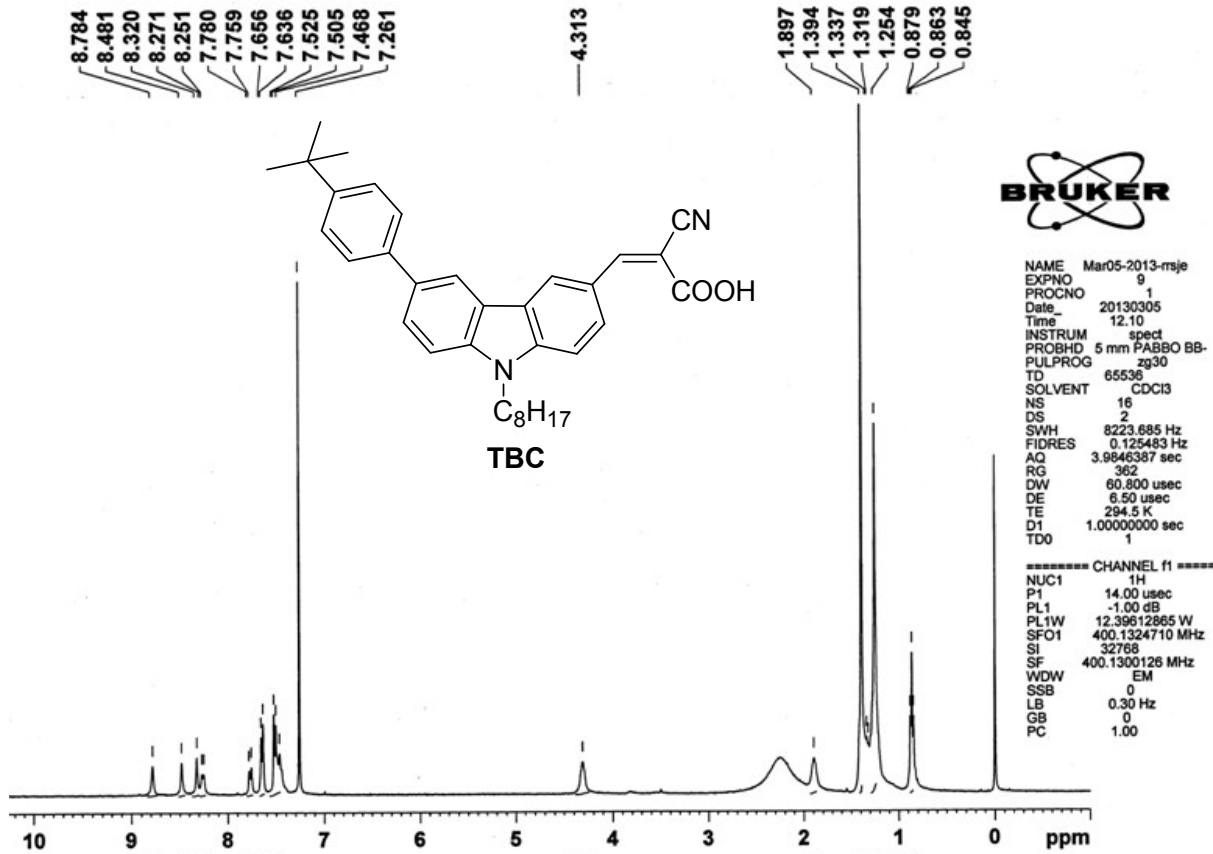
===== CHANNEL f2 =====  
 CPROG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.14 dB  
 PL13 15.00 dB  
 PL2W 12.39612865 W  
 PL12W 0.31769488 W  
 PL13W 0.31137696 W  
 SFO2 400.1319005 MHz  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

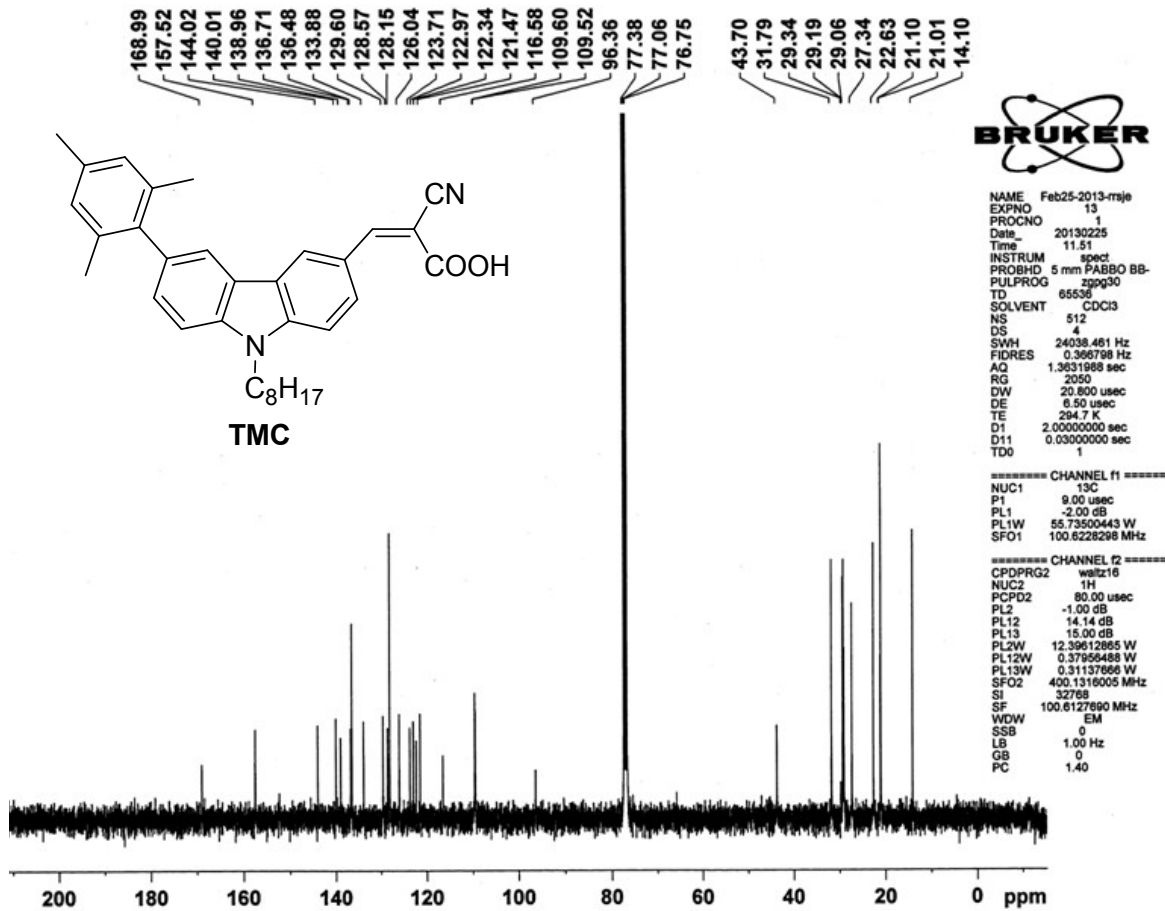
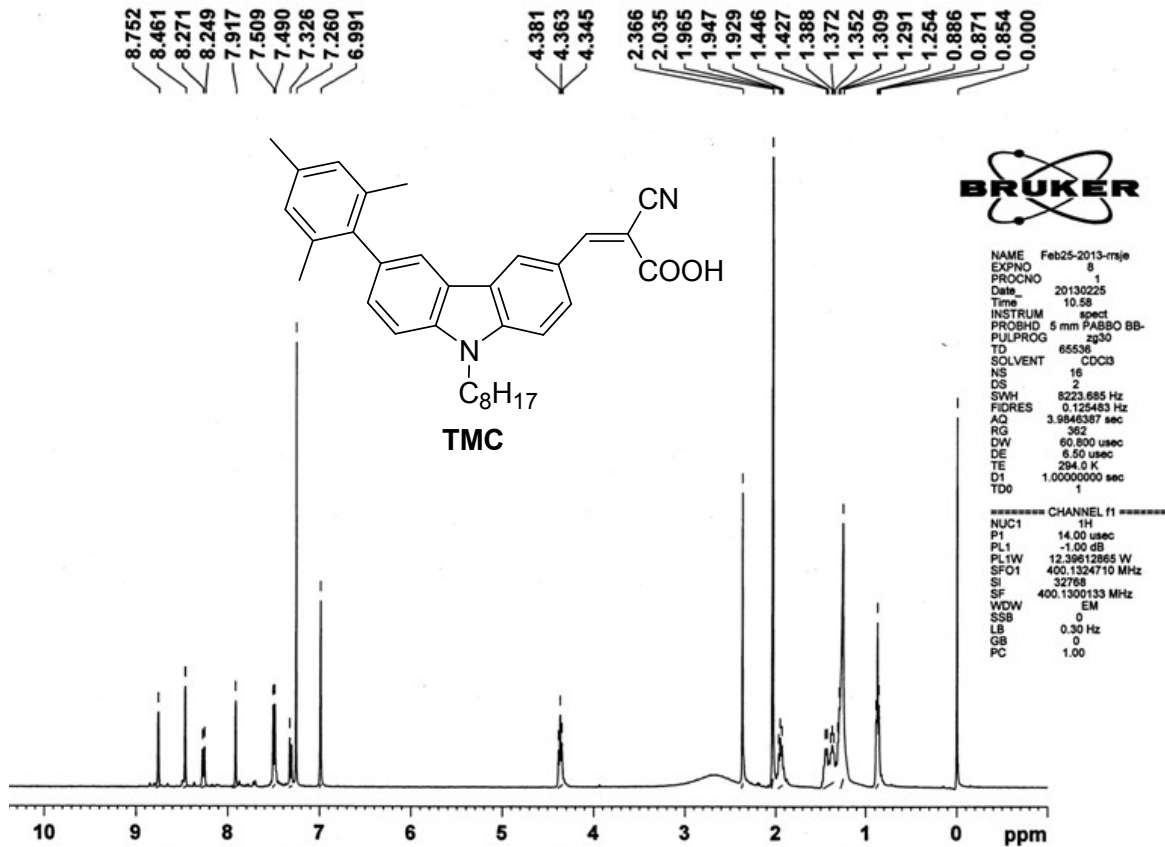


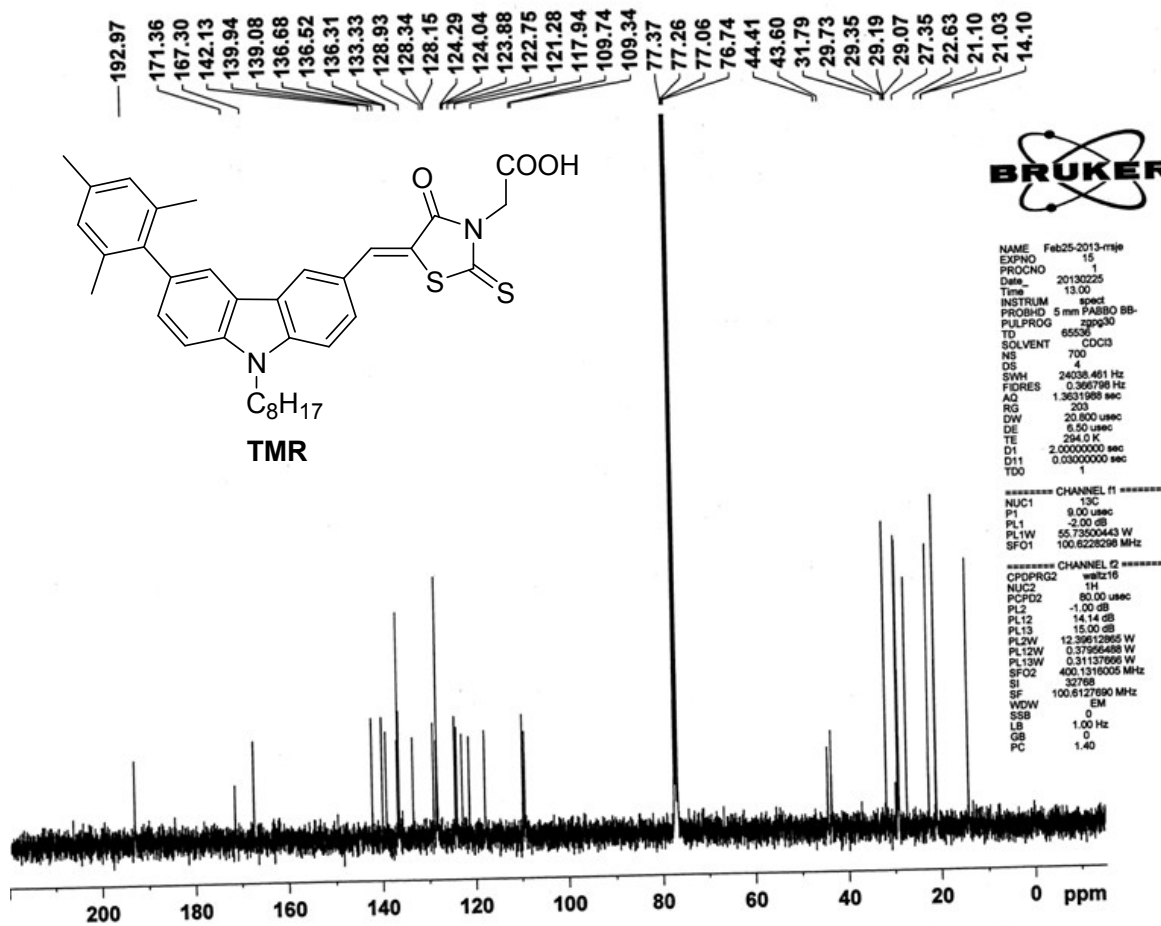
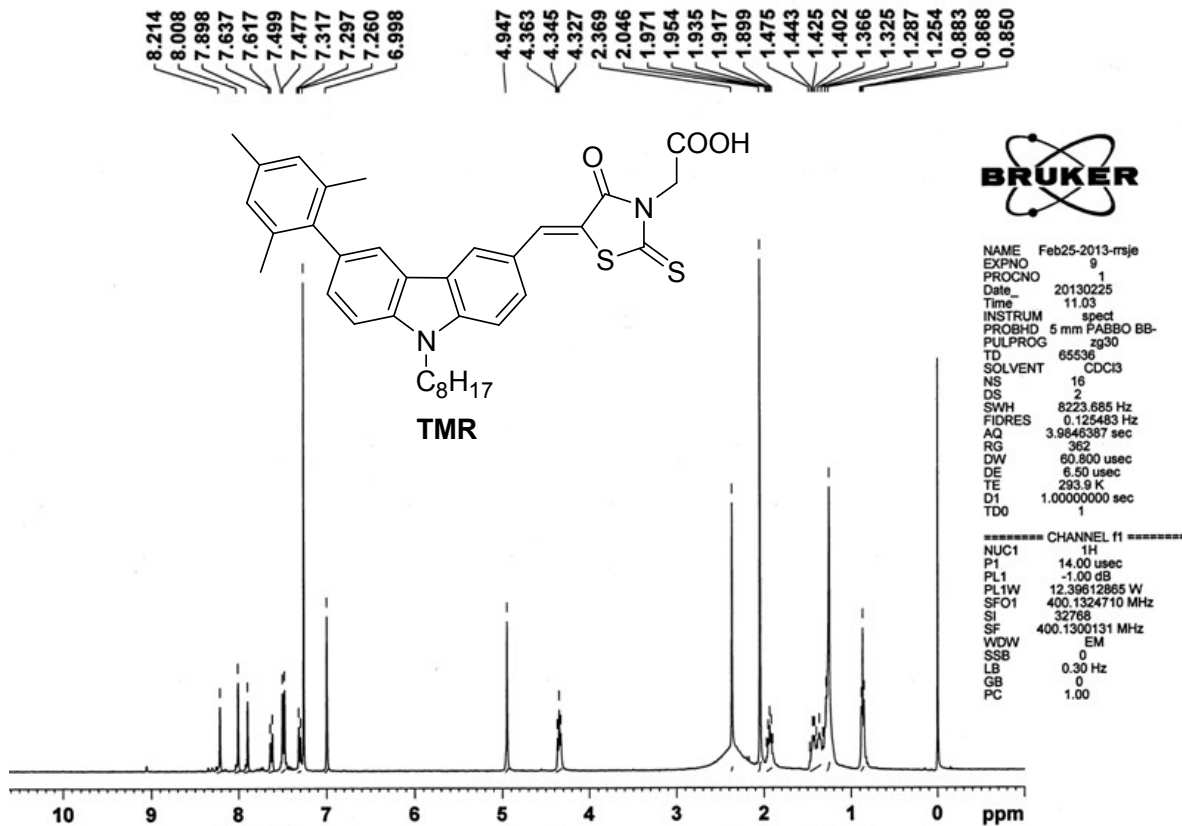






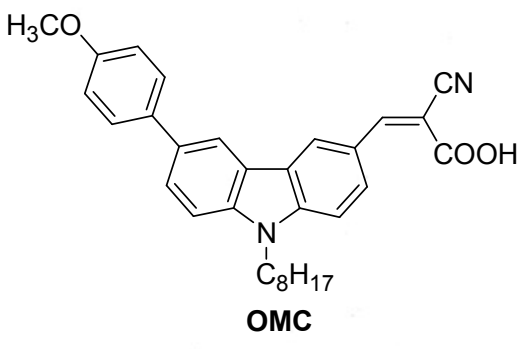






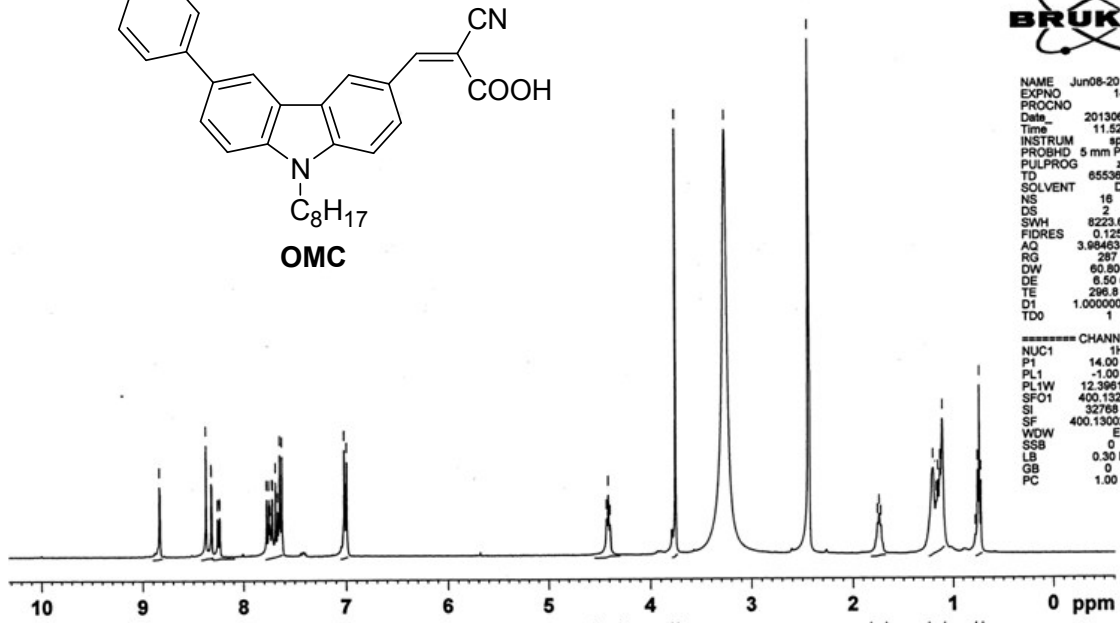
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8.323  
8.320  
8.261  
8.257  
8.239  
8.235  
7.776  
7.753  
7.744  
7.740  
7.722  
7.718  
7.688  
7.667  
7.647  
7.625  
7.019  
6.997

4.425  
4.409  
4.391  
3.755  
3.260  
2.441  
2.436  
1.757  
1.741  
1.724  
1.201  
1.167  
1.151  
1.131  
1.109  
0.777  
0.756  
0.740  
0.722

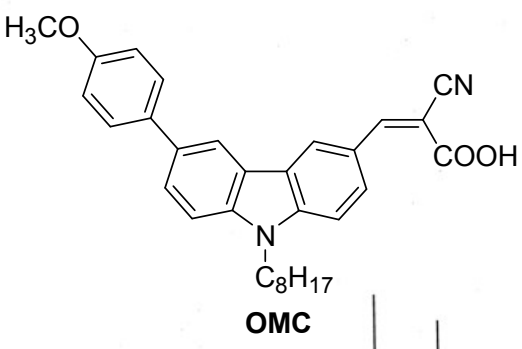


NAME Jun08-2013-rsje  
EXPNO 14  
PROCNO 1  
Date\_ 20130608  
Time 11.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 287  
DW 60.800 usec  
DE 6.50 usec  
TE 296.8 K  
D1 1.00000000 sec  
TD0

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.00 usec  
PL1 -1.00 dB  
PL1W 12.39612865 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300245 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



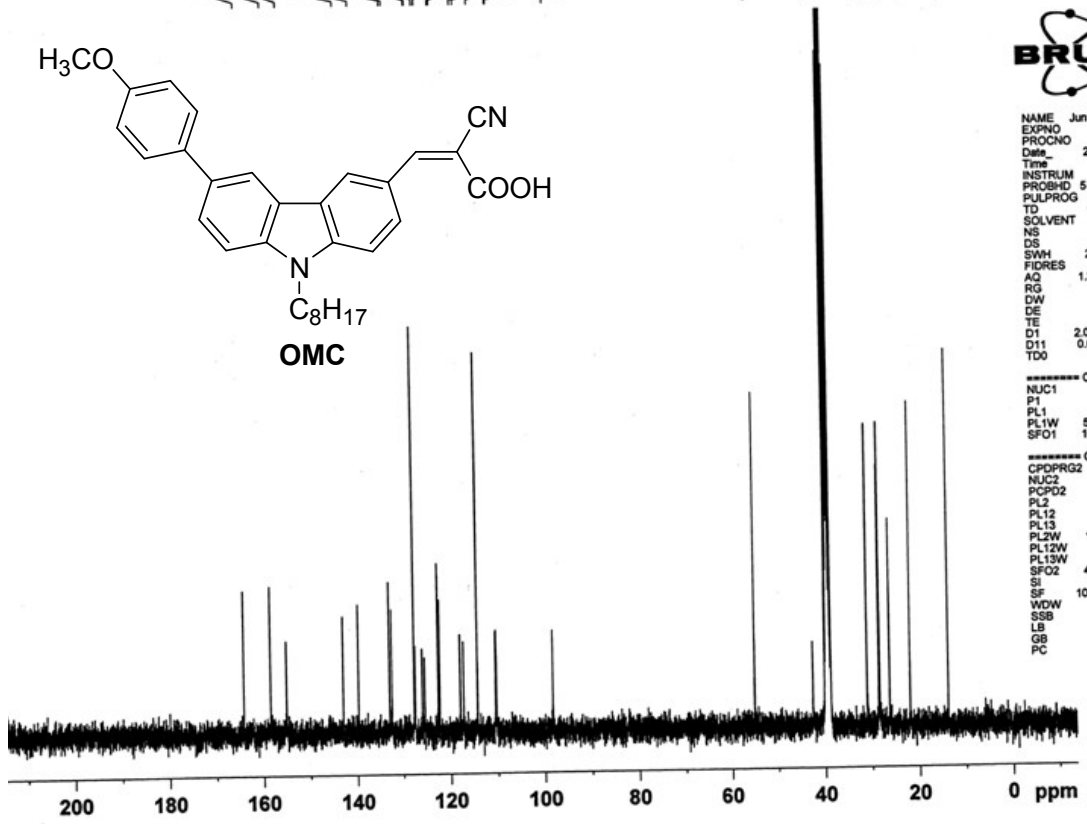
164.14  
158.43  
155.07  
143.03  
139.73  
133.05  
132.53  
127.74  
127.51  
125.99  
125.49  
122.61  
122.28  
117.93  
117.25  
114.33  
110.45  
110.31  
98.28  
55.09  
42.63  
40.09  
39.88  
39.67  
39.46  
39.25  
39.04  
38.84  
31.10  
28.63  
28.53  
28.46  
26.31  
21.95  
13.82

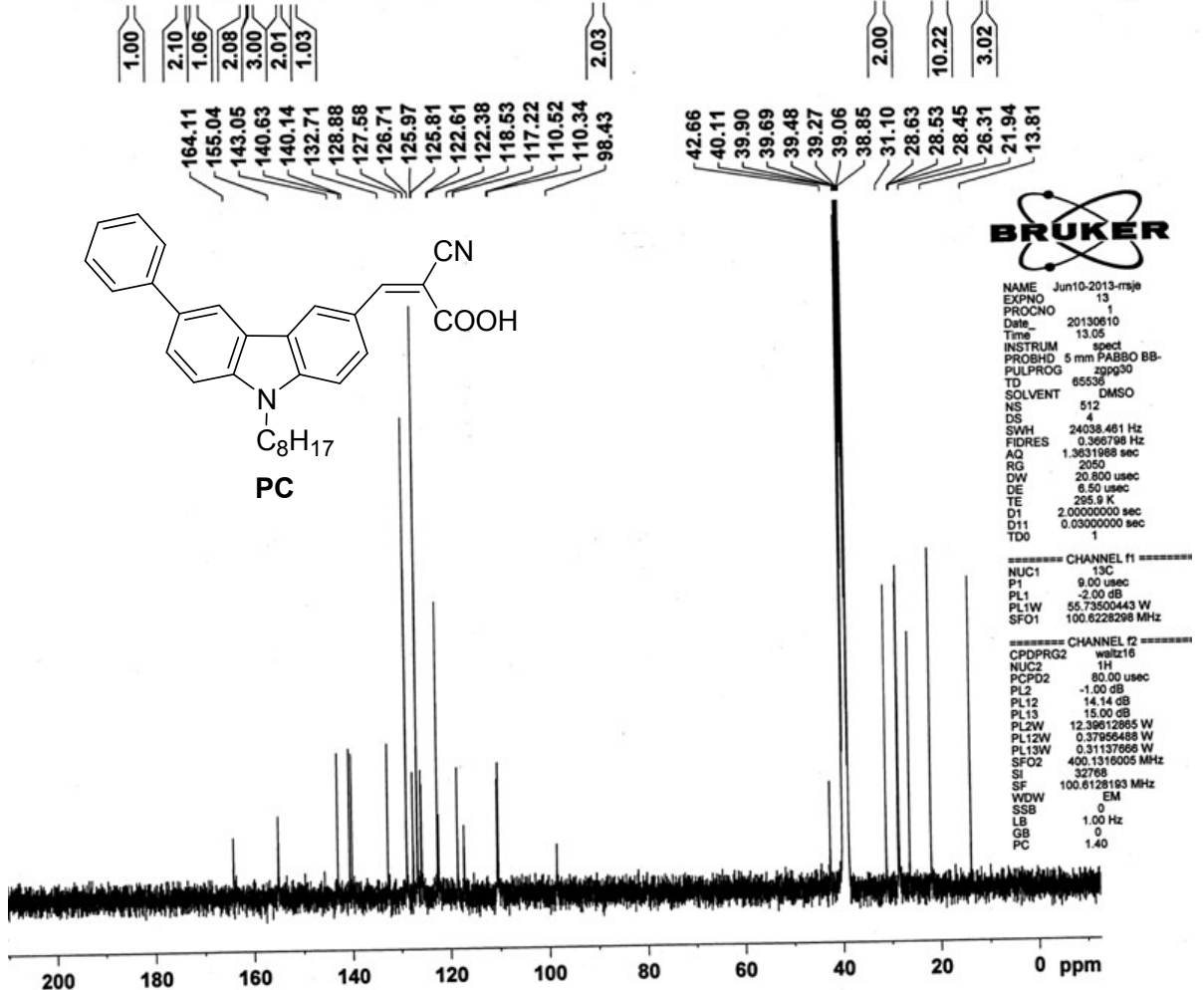
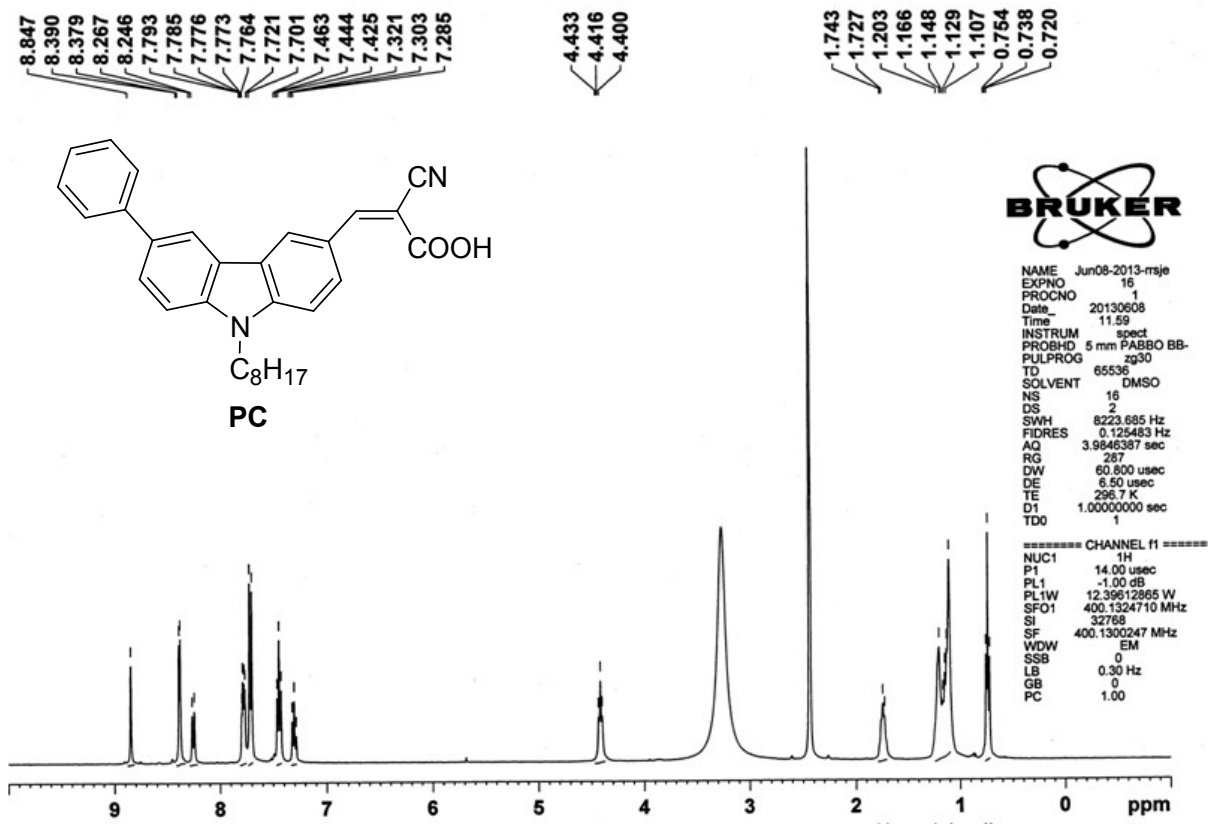


NAME Jun10-2013-rsje  
EXPNO 8  
PROCNO 1  
Date\_ 20130610  
Time 12.05  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 2050  
DW 20.800 usec  
DE 6.50 usec  
TE 294.8 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 13C  
P1 9.00 usec  
PL1 -2.00 dB  
PL1W 55.73500443 W  
SFO1 100.6228296 MHz

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.14 dB  
PL13 15.00 dB  
PL2W 12.39612865 W  
PL12W 0.37956488 W  
PL13W 0.31137686 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6128193 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





NAME Jun08-2013-rsje  
 EXPNO 16  
 PROCNO 1  
 Date\_ 20130608  
 Time 11.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8223.665 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 287  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 1.00000000 sec  
 TDO 1

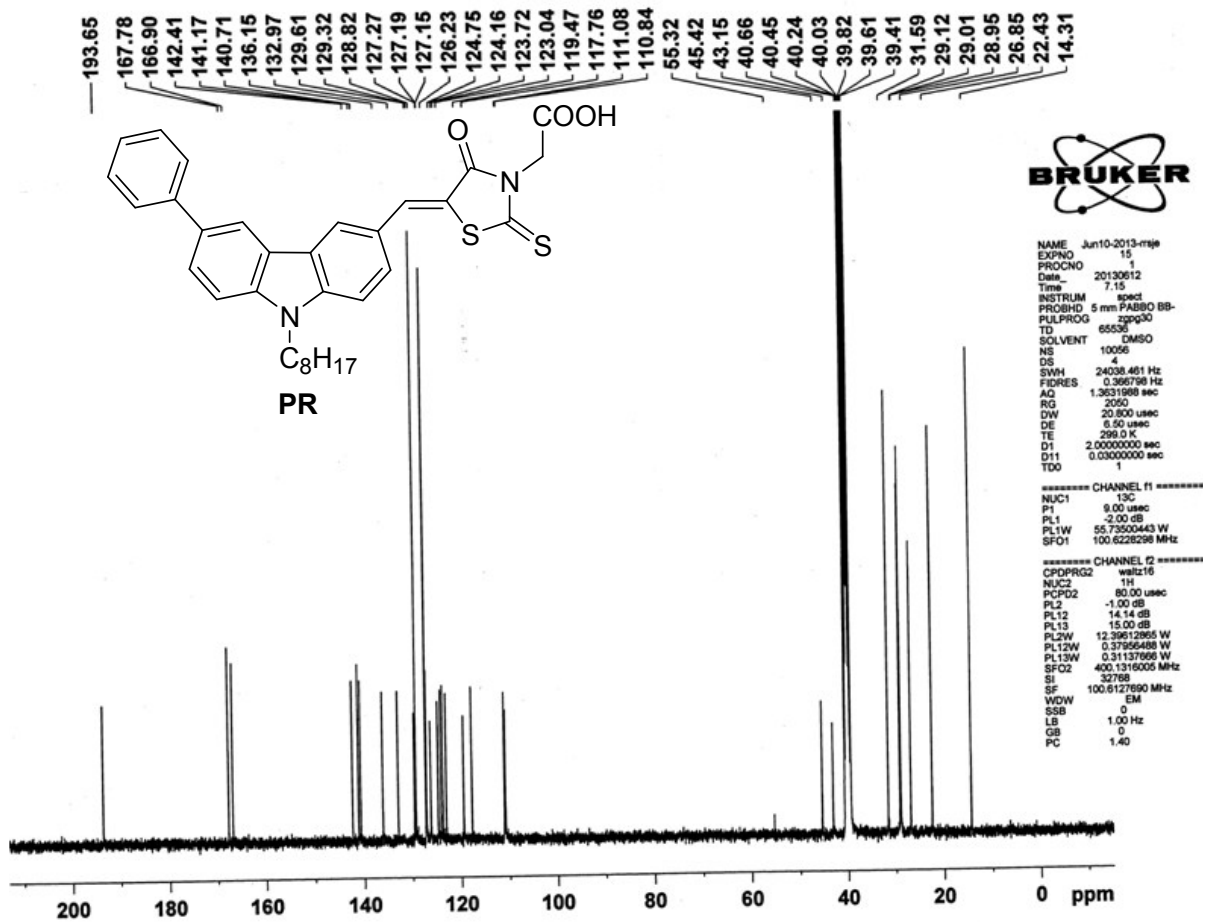
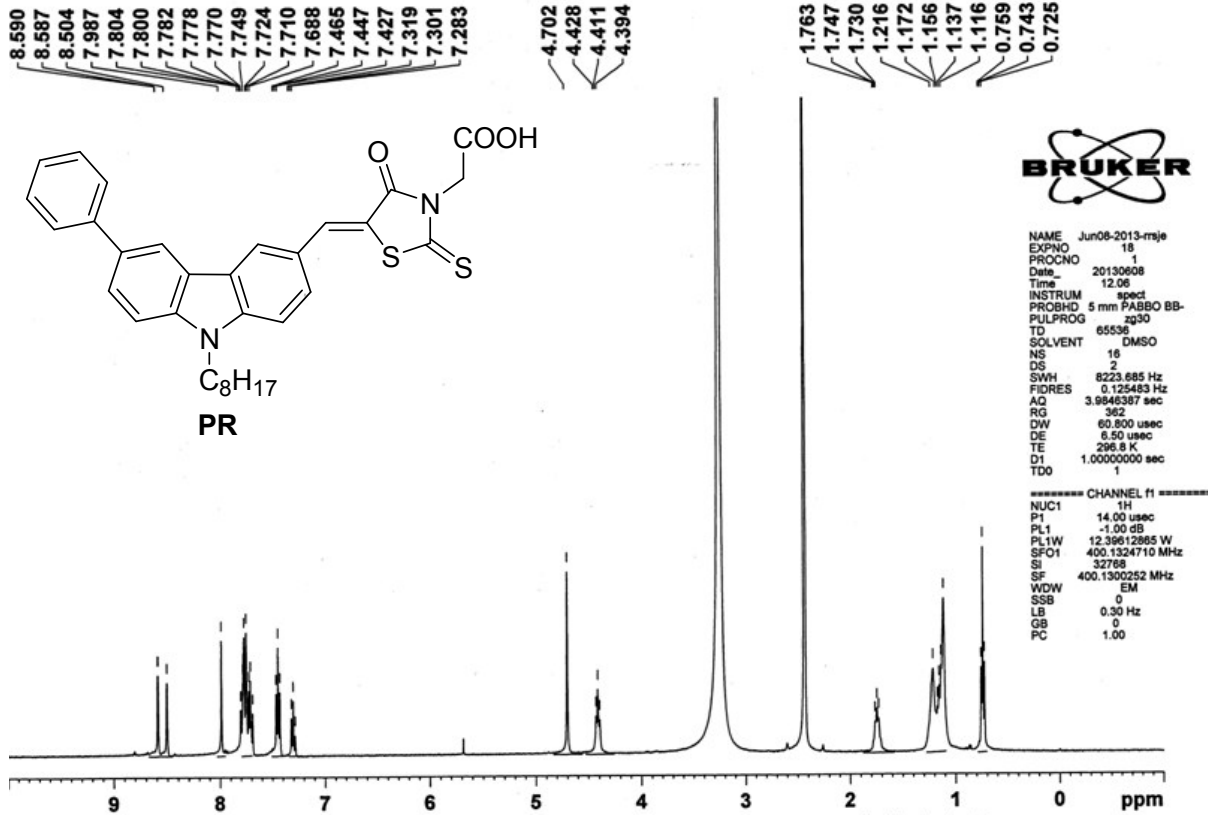
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -1.00 dB  
 PL1W 12.39612865 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300247 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME Jun10-2013-rsje  
 EXPNO 13  
 PROCNO 1  
 Date\_ 20130610  
 Time 13.55  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 512  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 -2.00 dB  
 PL1W 55.73500443 W  
 SFO1 100.6228298 MHz

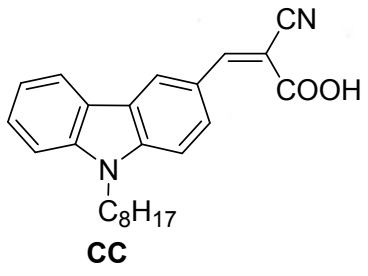
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.14 dB  
 PL13 15.00 dB  
 PL2W 12.39612865 W  
 PL12W 0.37956488 W  
 PL13W 0.31137666 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6128163 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



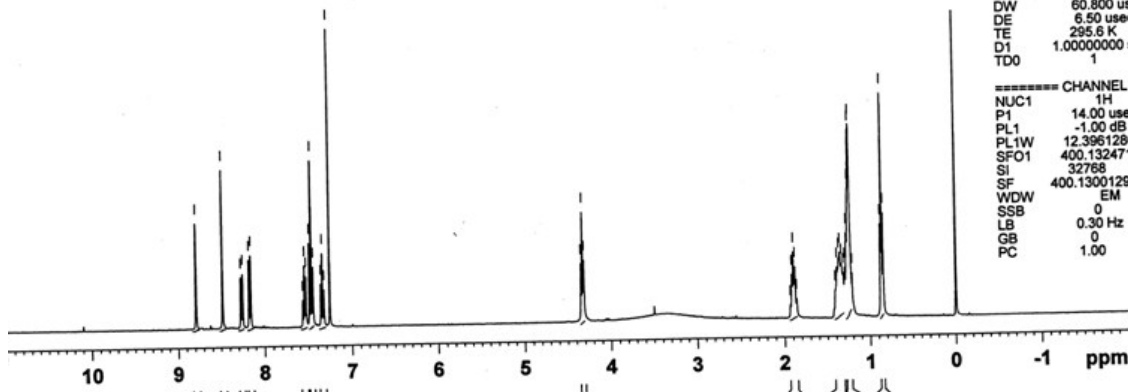


8.789  
8.481  
8.271  
8.250  
8.177  
8.158  
7.566  
7.546  
7.527  
7.489  
7.467  
7.447  
7.361  
7.342  
7.324  
7.259

4.350  
4.332  
4.314  
1.932  
1.914  
1.896  
1.878  
1.859  
1.410  
1.391  
1.368  
1.355  
1.337  
1.316  
1.297  
1.278  
1.260  
1.248  
1.242  
1.213  
0.879  
0.863  
0.846

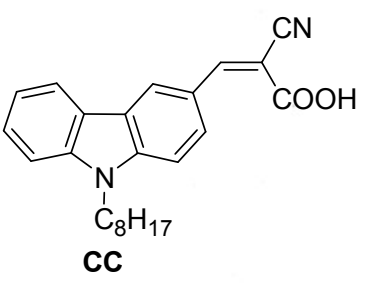


NAME Jun13-2013-rsje  
EXPNO 11  
PROCNO 1  
Date\_ 20130613  
Time 11.05  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCI3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 362  
DW 60.800 usec  
DE 6.50 usec  
TE 295.6 K  
D1 1.00000000 sec  
TD0 1

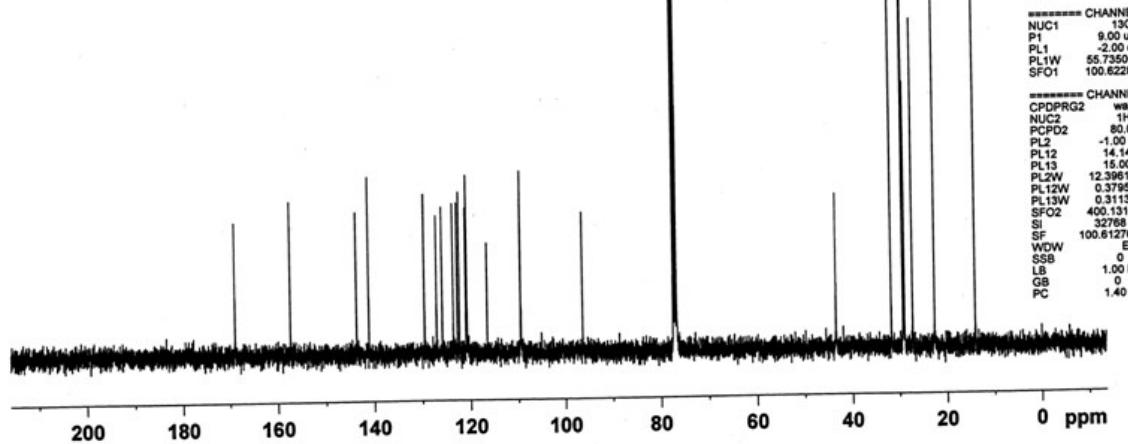


===== CHANNEL f1 =====  
NUC1 1H  
P1 14.00 usec  
PL1 -1.00 dB  
PL1W 12.39612865 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300129 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

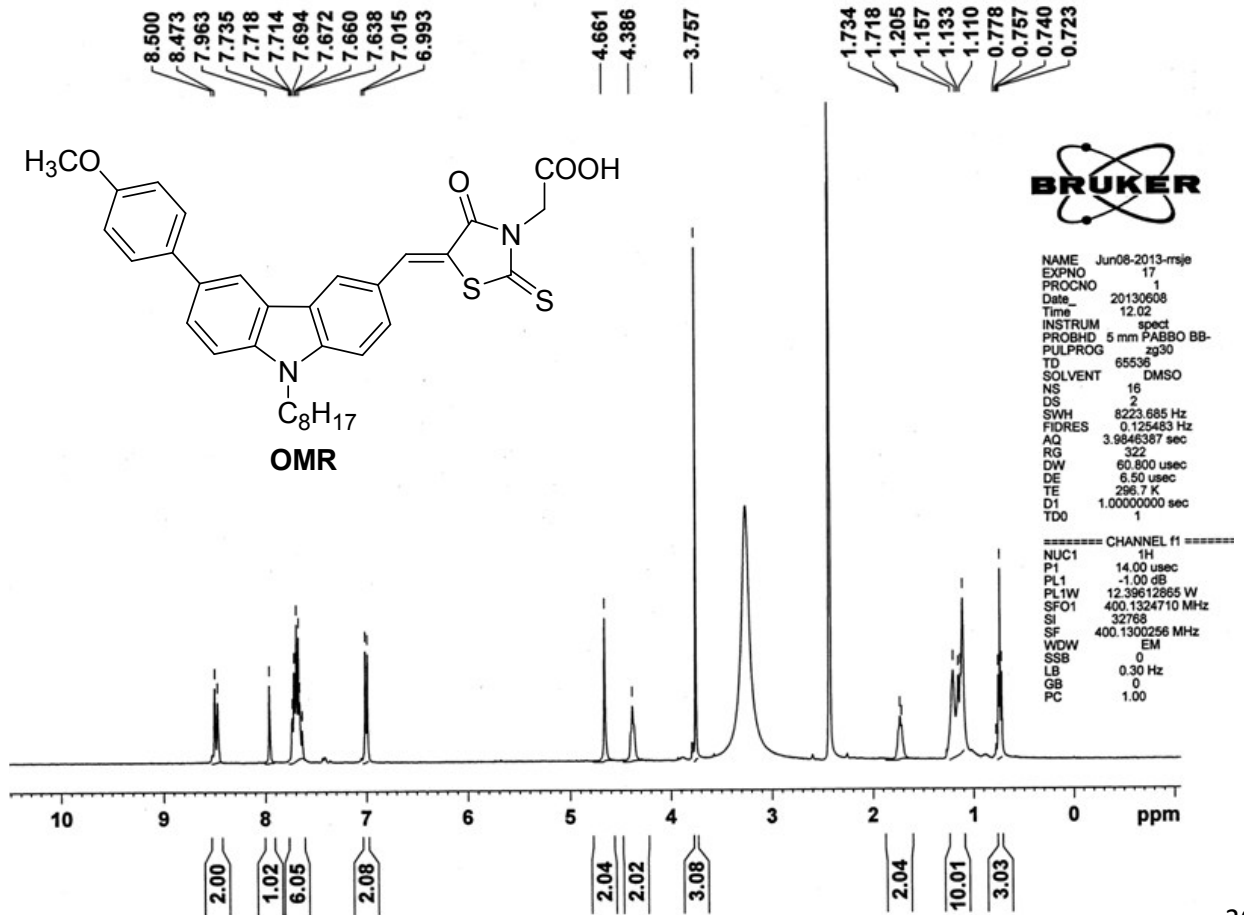
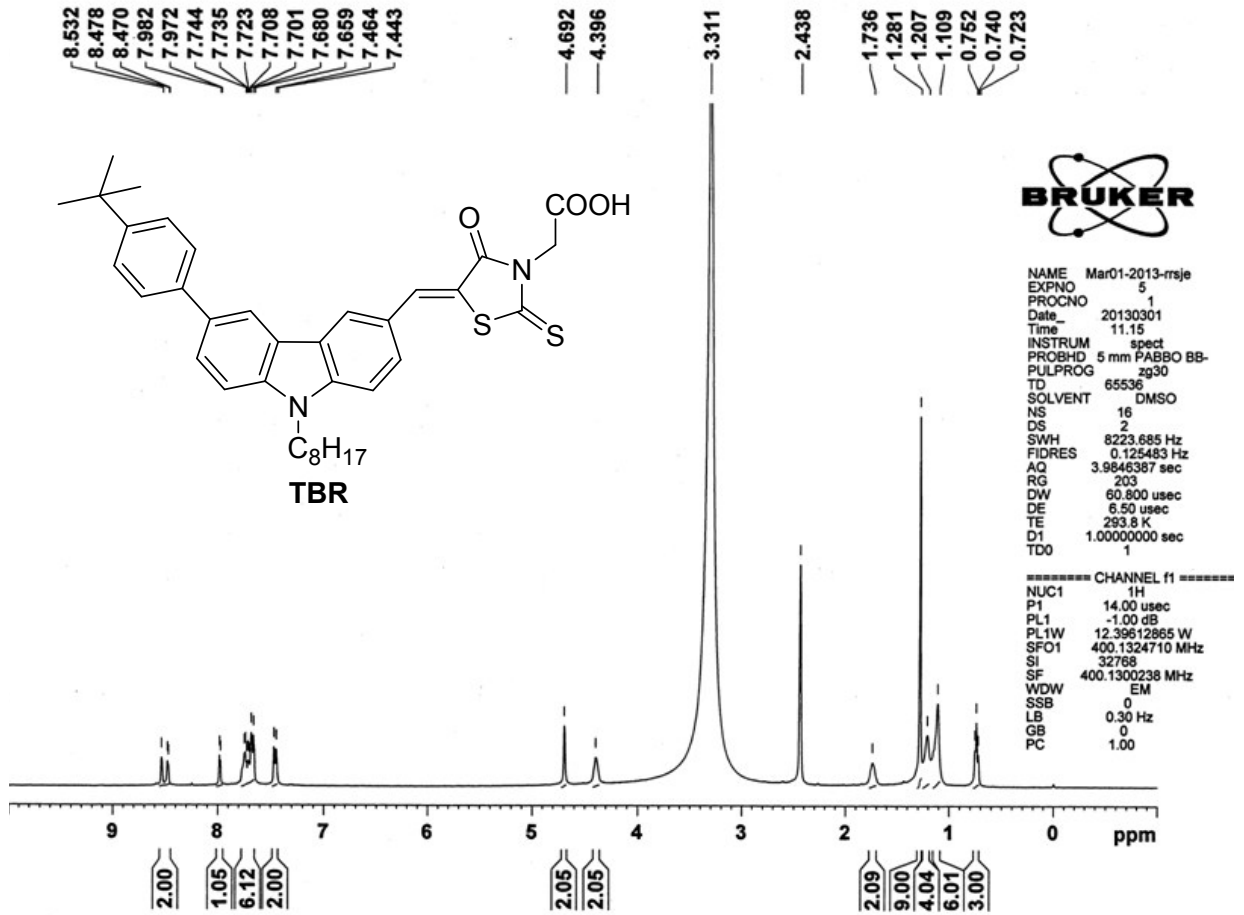
168.98  
157.42  
143.68  
141.11  
129.54  
127.04  
125.86  
123.59  
122.73  
122.32  
120.96  
120.75  
116.54  
109.53  
109.47  
96.34  
77.37  
77.05  
76.73  
43.47  
31.76  
29.30  
29.14  
28.94  
27.25  
22.60  
14.06

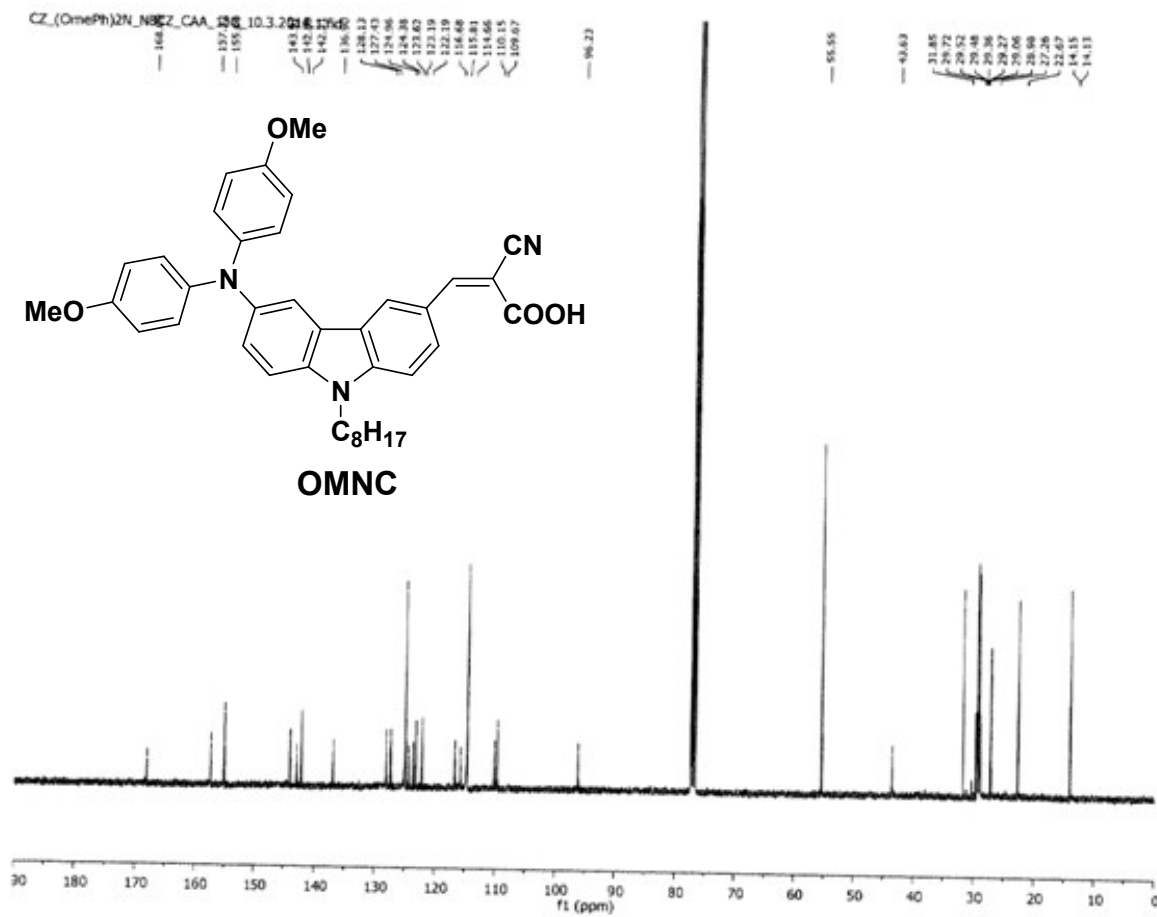
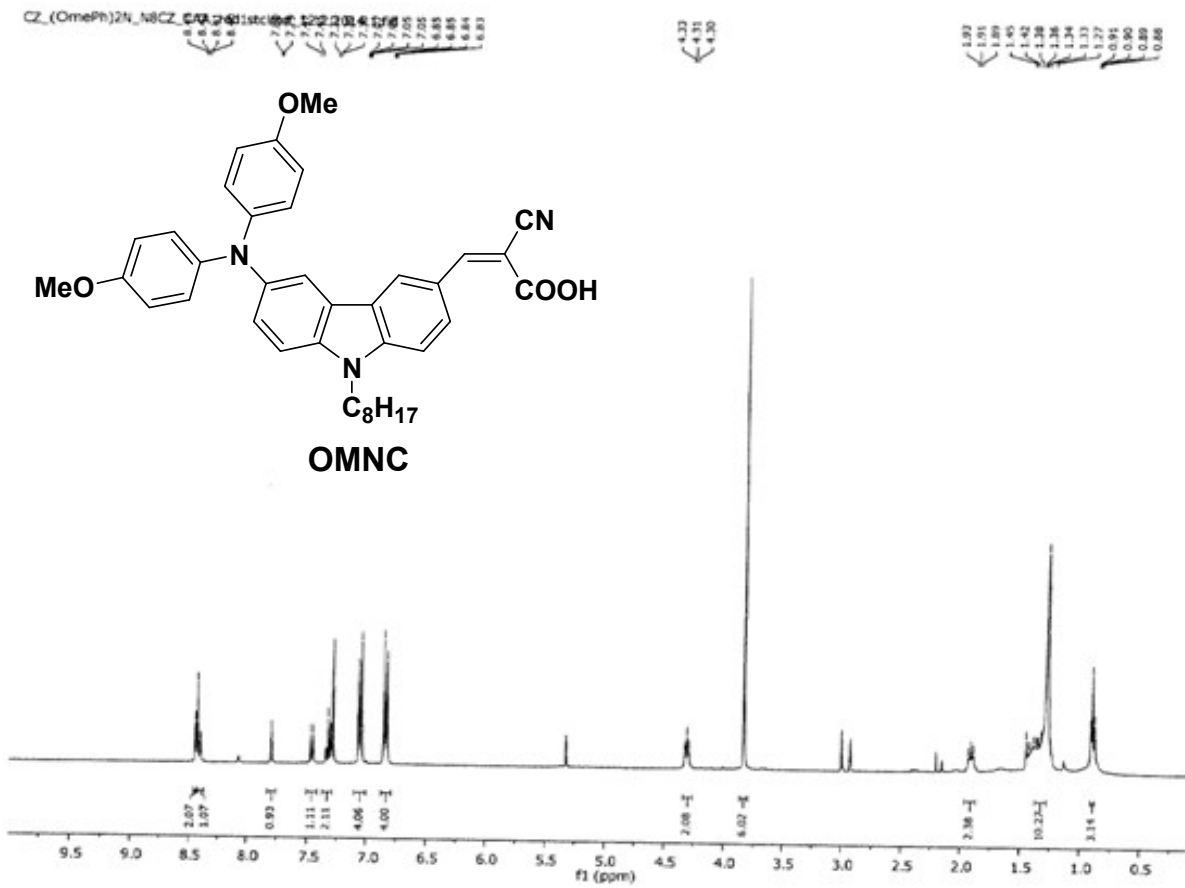


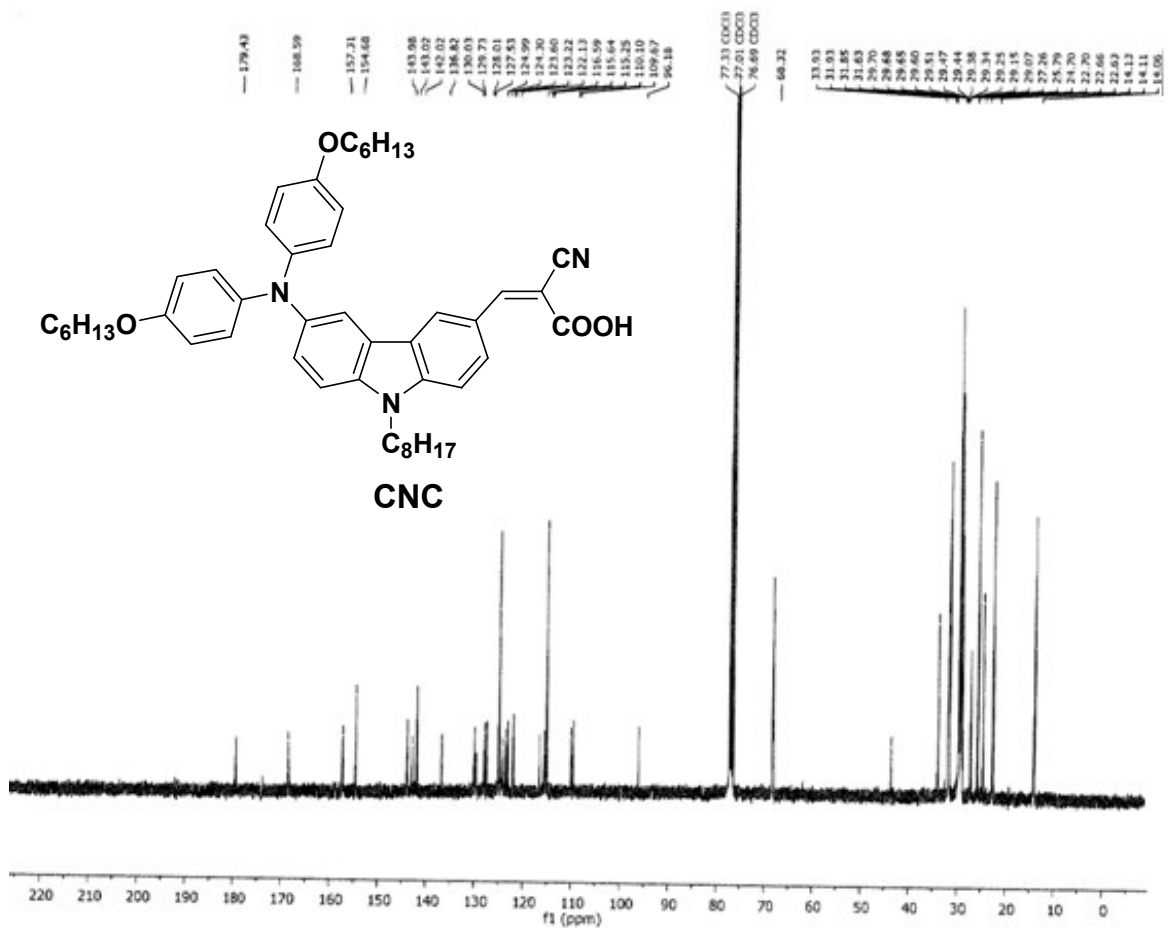
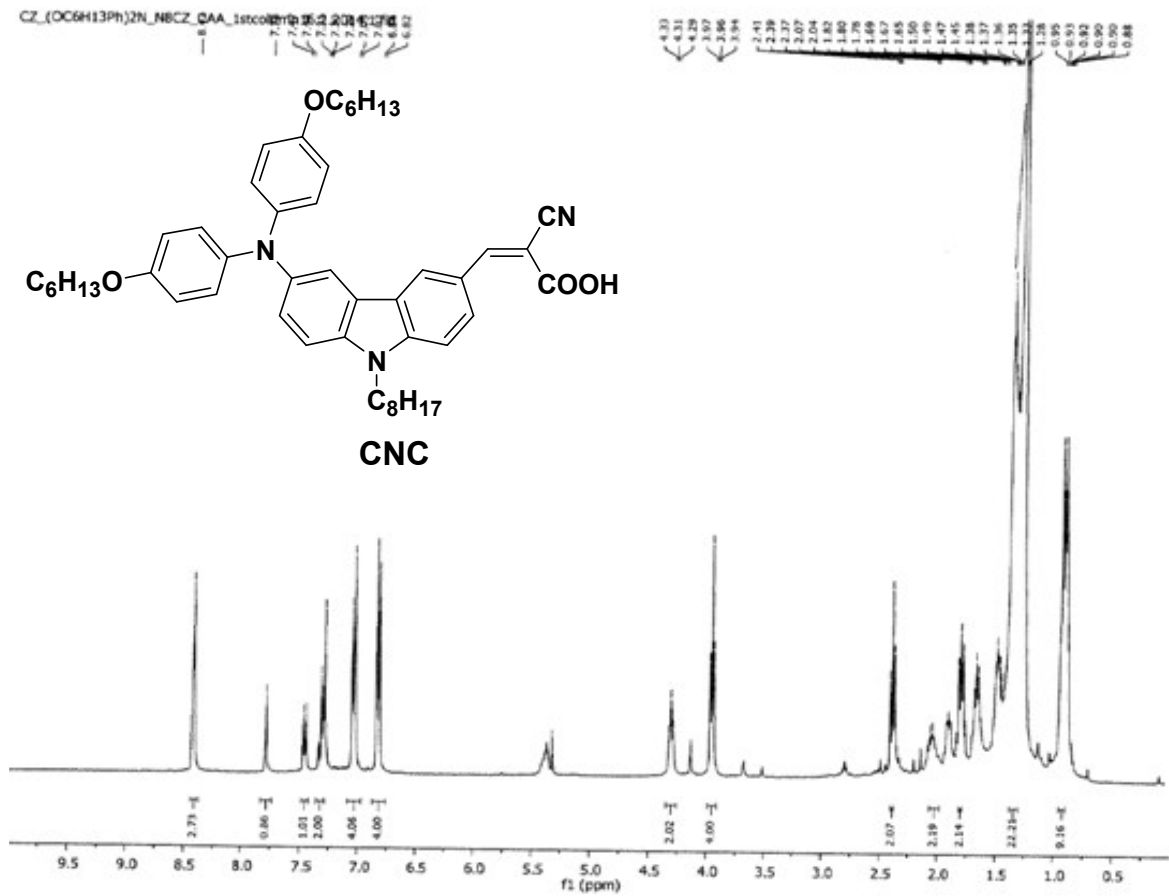
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EXPNO 20  
PROCNO 1  
Date\_ 20130613  
Time 12.40  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCI3  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 2050  
DW 20.800 usec  
DE 6.50 usec  
TE 297.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1



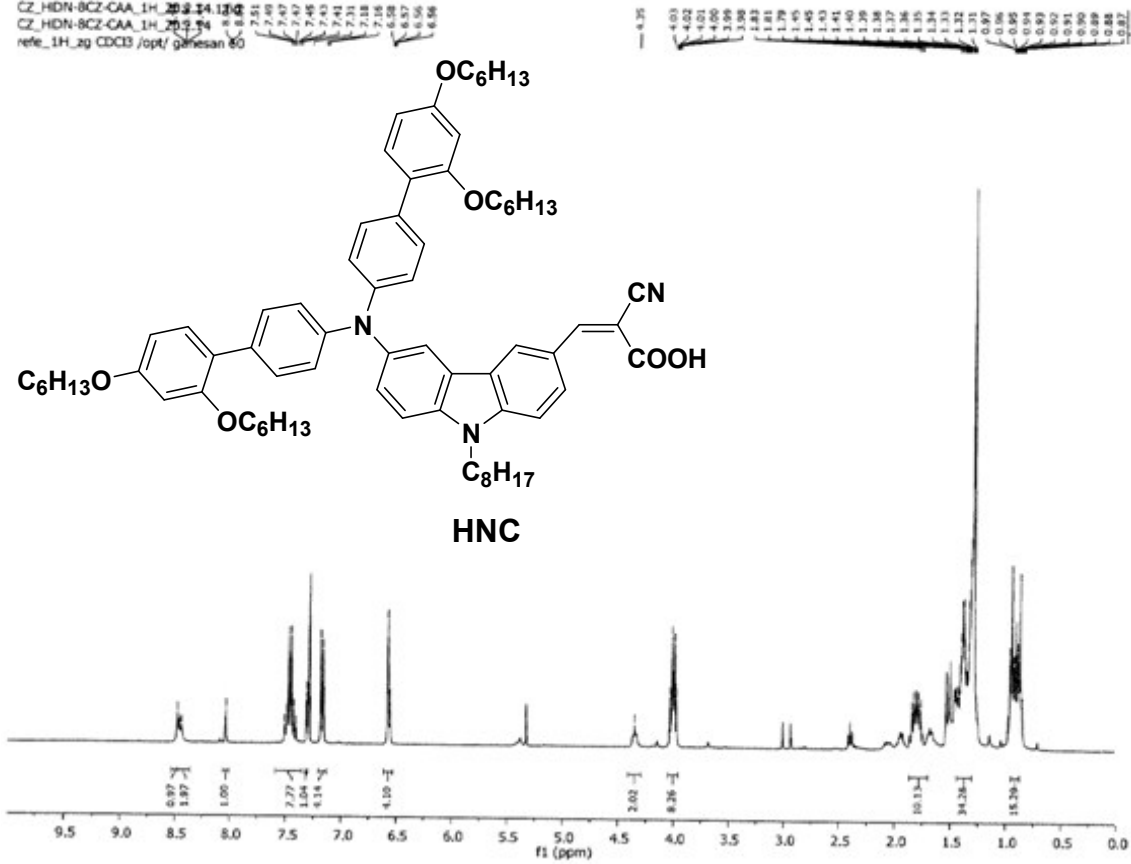
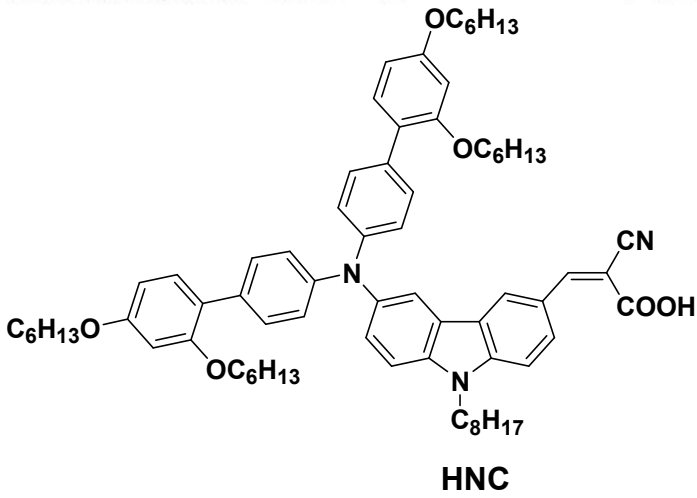
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NUC1 13C  
P1 9.00 usec  
PL1 -2.00 dB  
PL1W 56.73500443 W  
SFO1 100.6228298 MHz  
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.14 dB  
PL13 15.00 dB  
PL2W 12.39612865 W  
PL12W 0.37958488 W  
PL13W 0.31137686 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



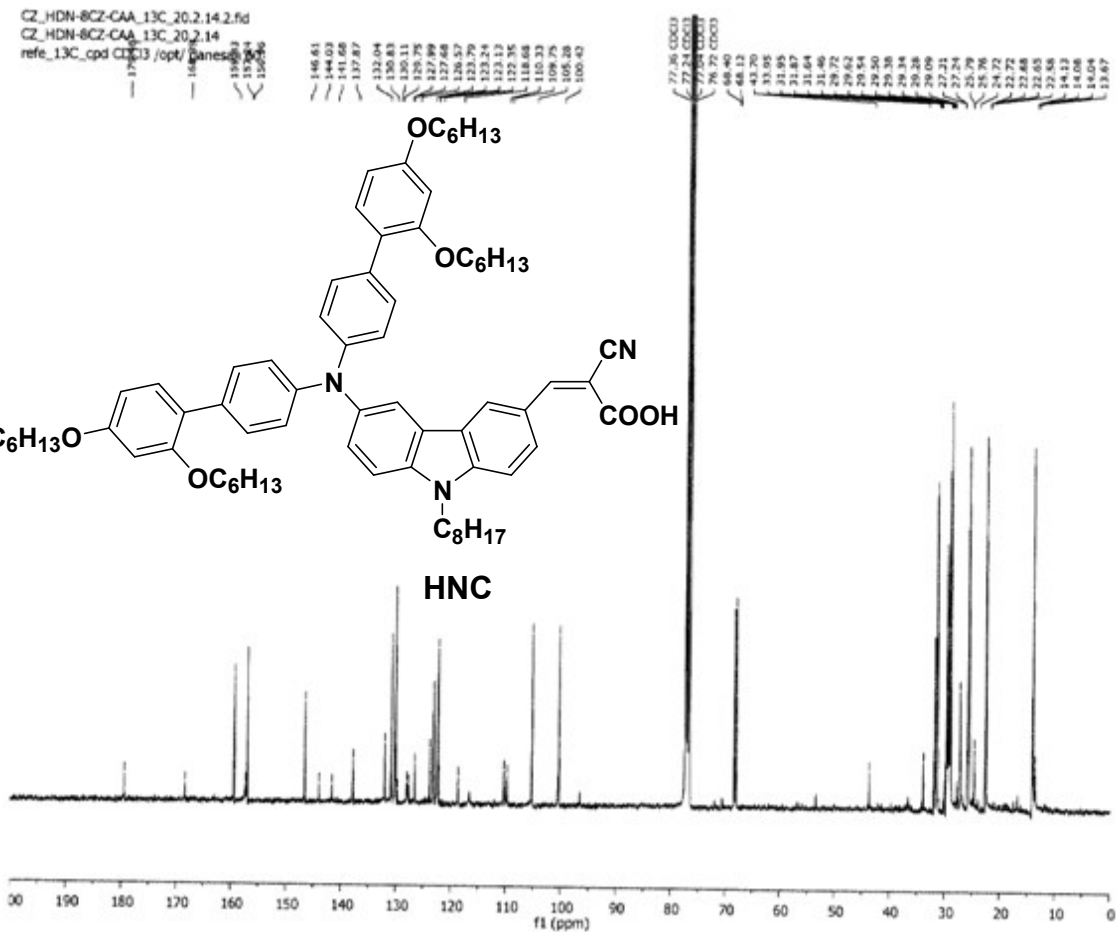
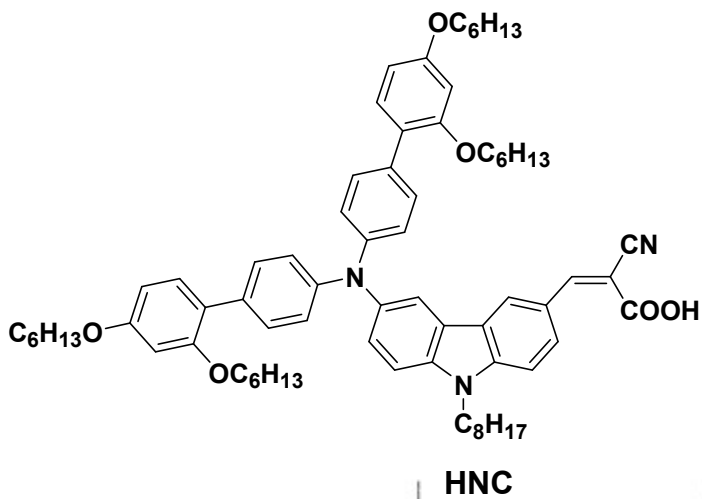




CZ\_HDN-8CZ-CAA\_1H\_20.2.14.2.fid  
CZ\_HDN-8CZ-CAA\_1H\_20.2.14  
refe\_1H\_zg CDCl3 /opt/ ganesan 60



CZ\_HDN-8CZ-CAA\_13C\_20.2.14.2.fid  
CZ\_HDN-8CZ-CAA\_13C\_20.2.14  
refe\_13C\_cp CDCl3 /opt/ ganesan 60



**Figure S3A:** Frontier molecular orbitals of carbazole based sensitizers

**HOMO**

**LUMO**

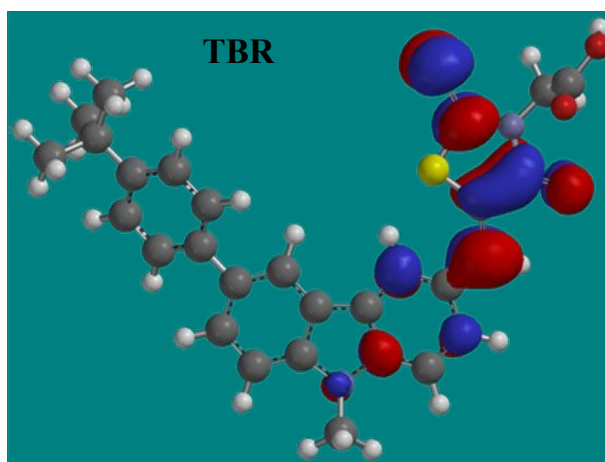
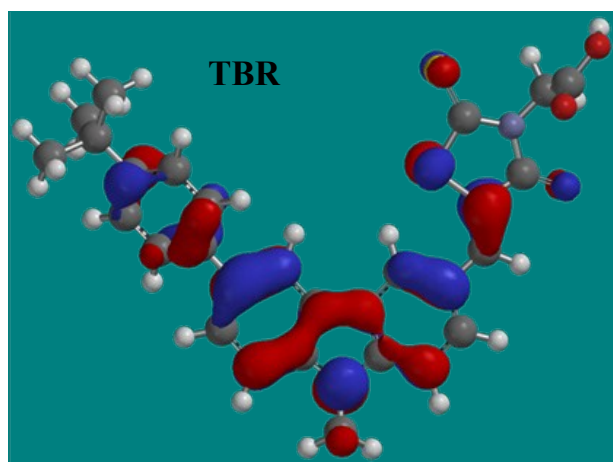
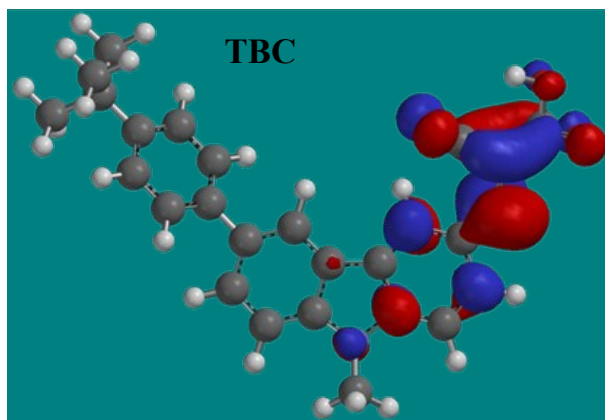
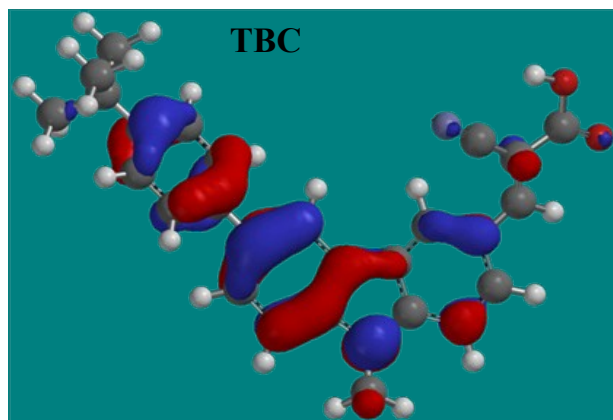


Figure S3B:

HOMO

LUMO

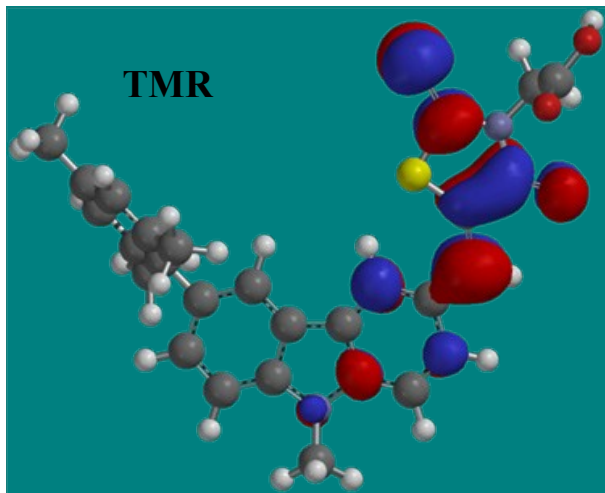
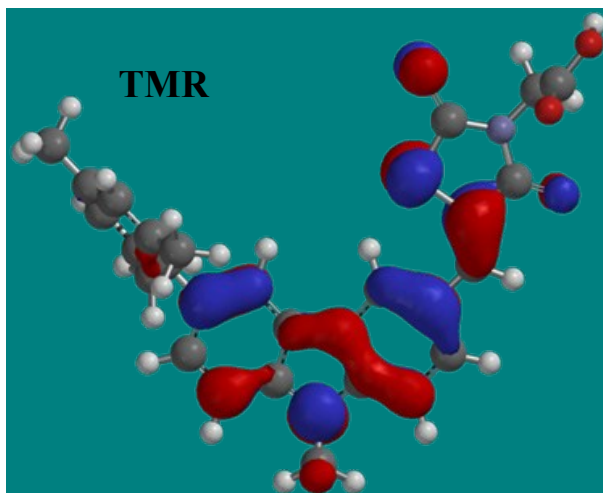
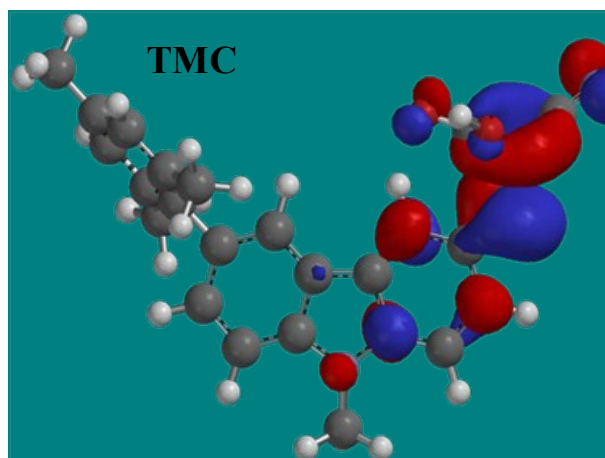
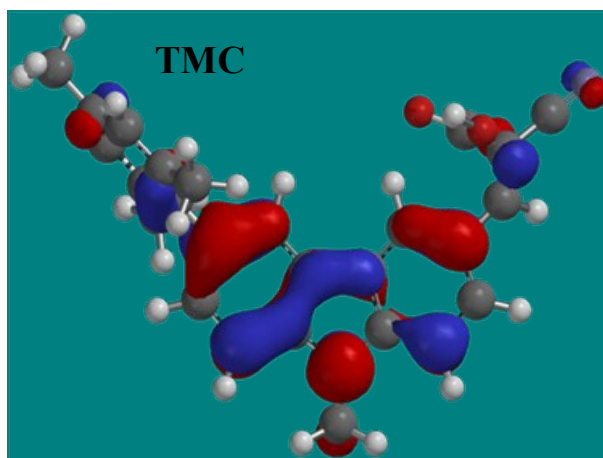
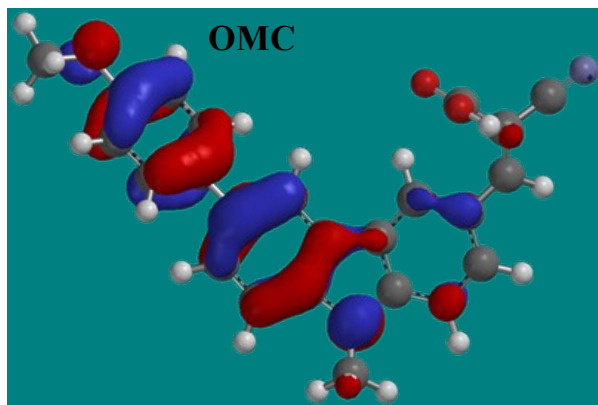


Figure S3C:

HOMO



LUMO

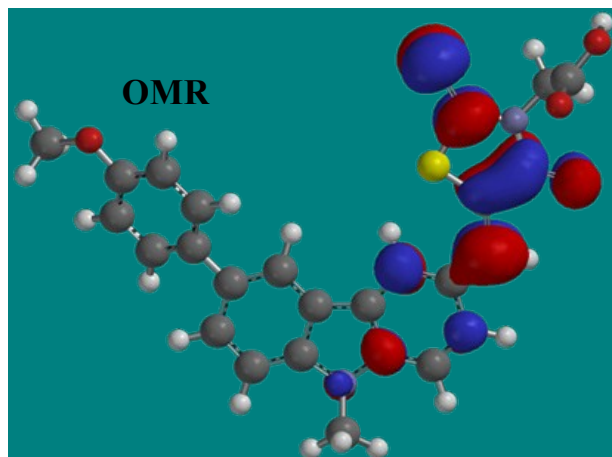
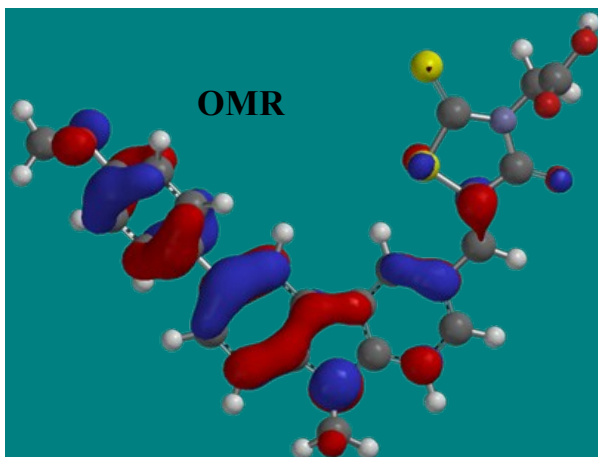
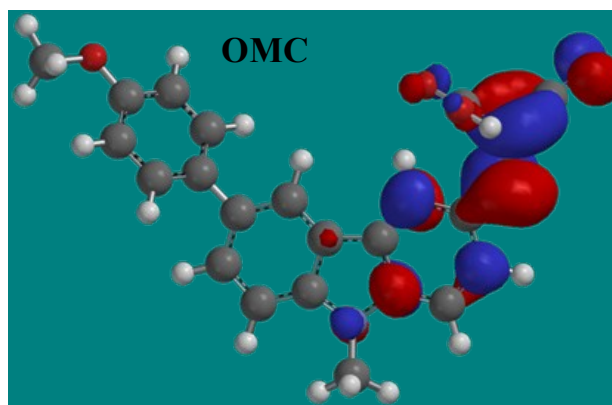
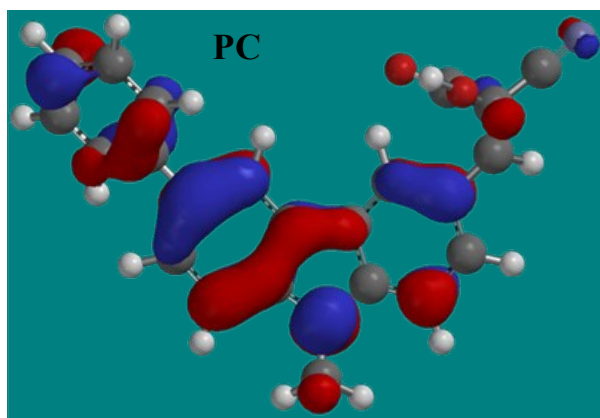




Figure S3D:

HOMO



LUMO

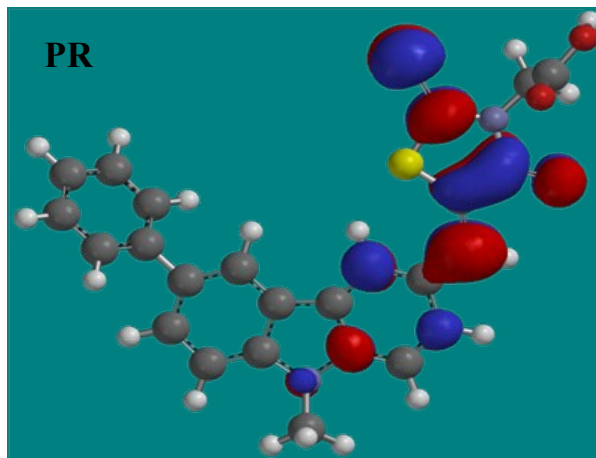
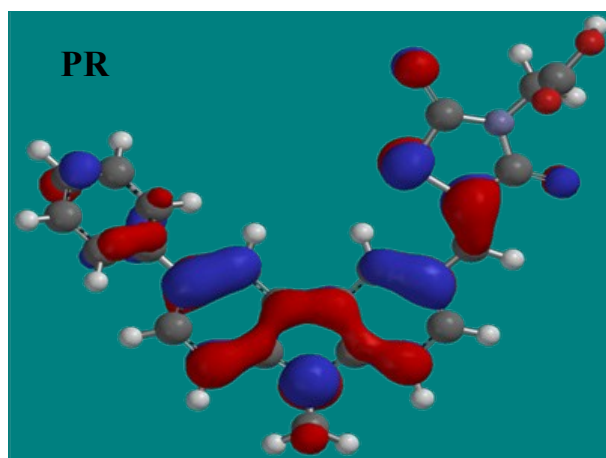
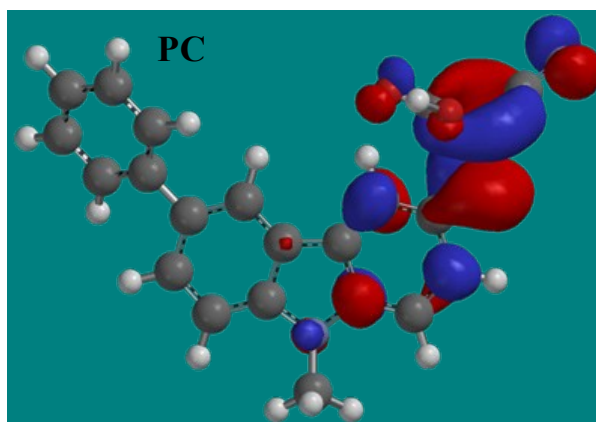


Figure S3E:

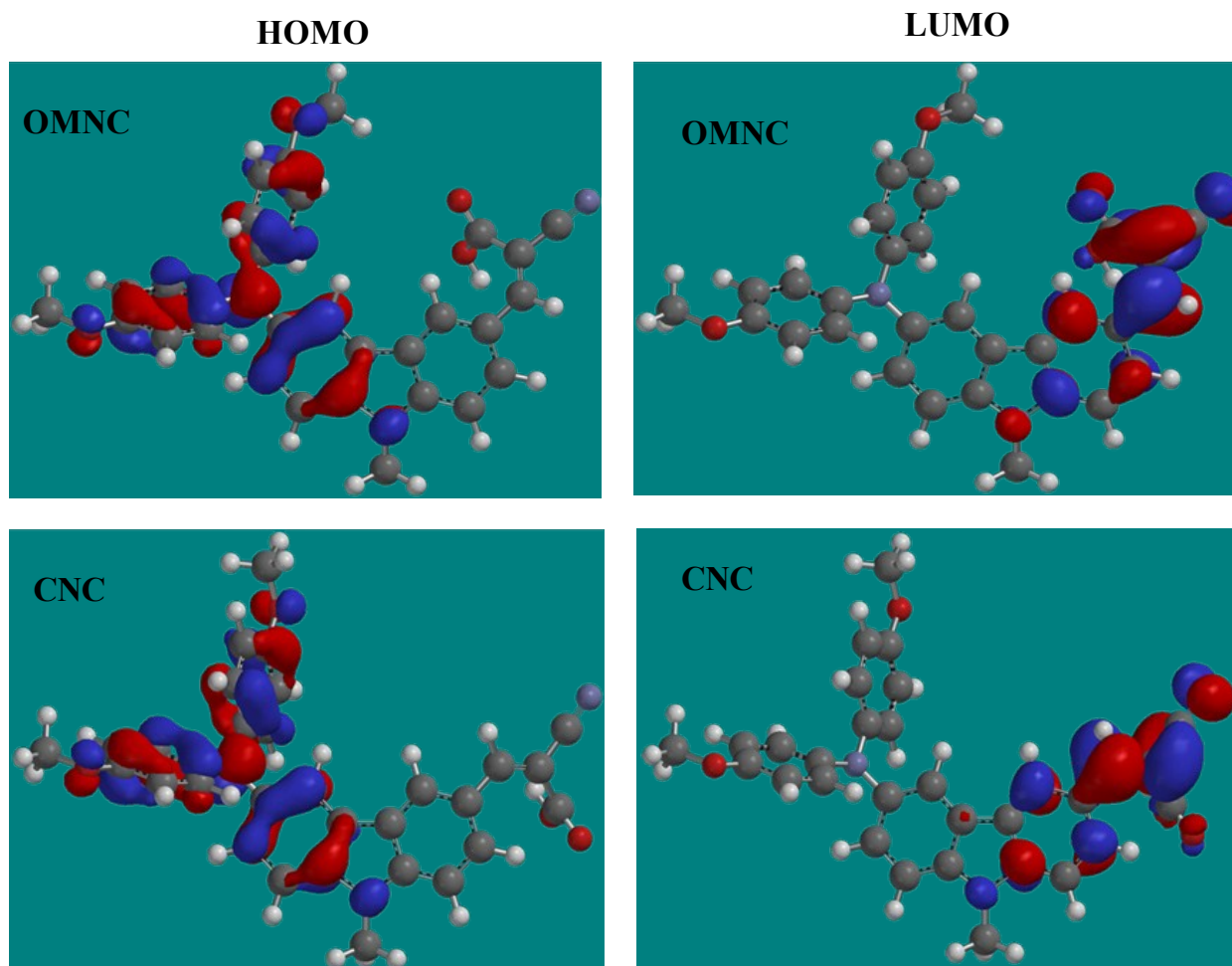
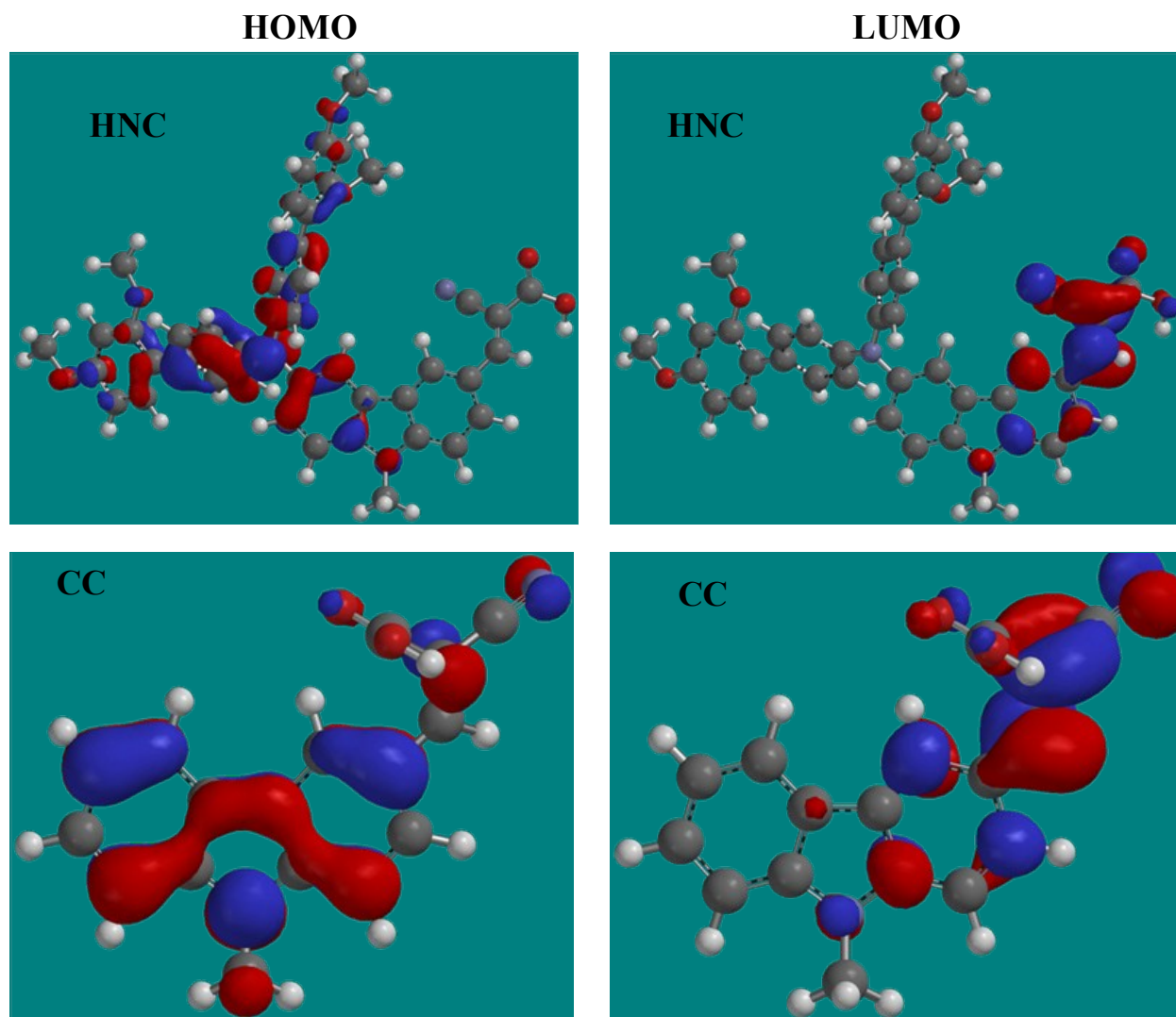


Figure S3F:



**Table S1:** HOMO and LUMO values of carbazole based sensitizers obtained from DFT calculations

	<b>HOMO (eV)</b>	<b>LUMO (eV)</b>
<b>TBC</b>	-5.6	-2.4
<b>TMC</b>	-5.7	-1.9
<b>OMC</b>	-5.4	-2
<b>PC</b>	-5.6	-1.9
<b>TBR</b>	-5.5	-2.4
<b>TMR</b>	-5.6	-2.4
<b>OMR</b>	-5.4	-2.3
<b>PR</b>	-5.5	-2.4
<b>CC</b>	-5.8	-2.1
<b>OMNC</b>	-4.7	-2.2
<b>CNC</b>	-4.7	-2
<b>HNC</b>	-4.5	-2.2