Supporting Information for

"Multi-Carbazole Derivatives: New Dyes for Highly Efficient Dye-Sensitized Solar Cells"

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1. Detailed Characterization

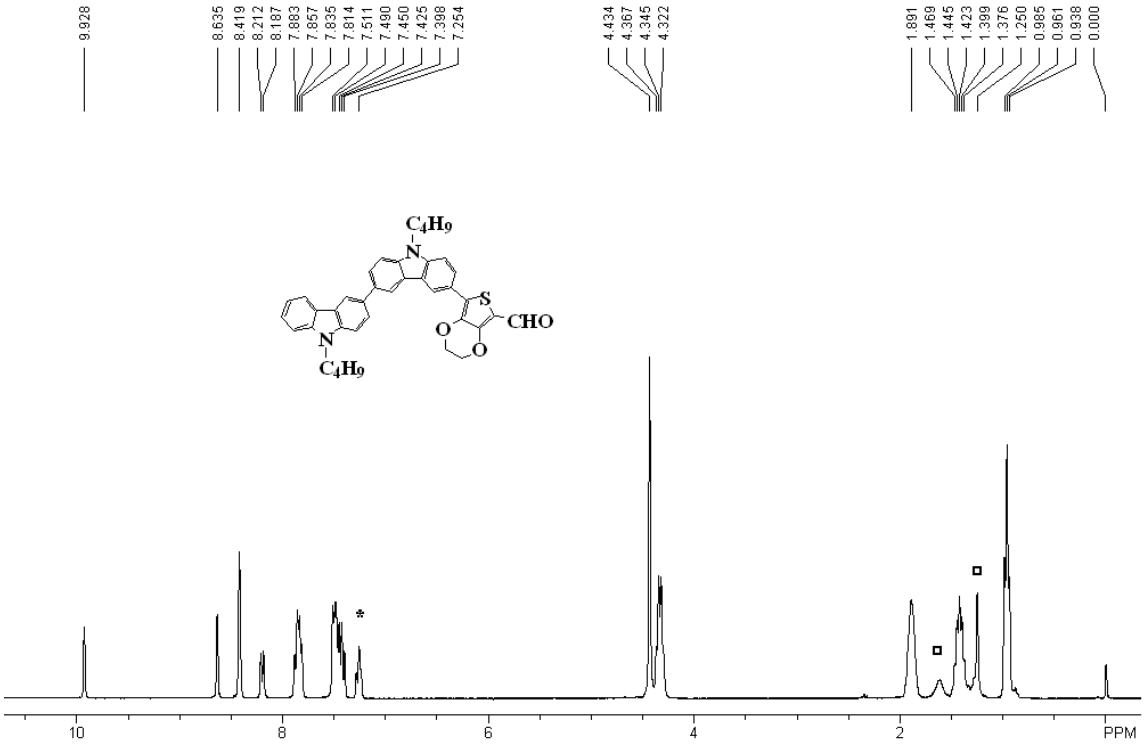


Figure S1. ^{1}H NMR spectrum of **6** (300 MHz, $CDCl_3$). The peak with asterisk is attributed to $CHCl_3$ and the peaks with square are attributed to H_2O or impurities, respectively.

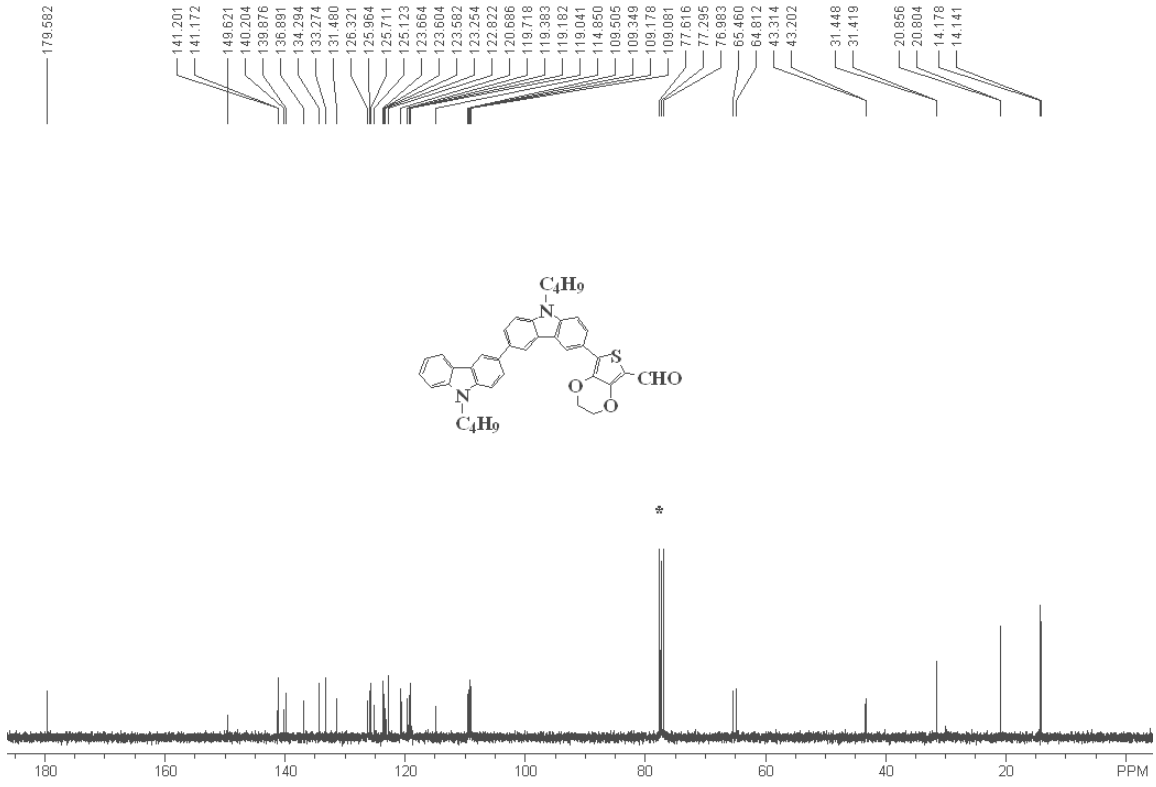


Figure S2. ^{13}C NMR spectrum of **6** (100 MHz, $CDCl_3$). The peak with asterisk is attributed to $CHCl_3$.

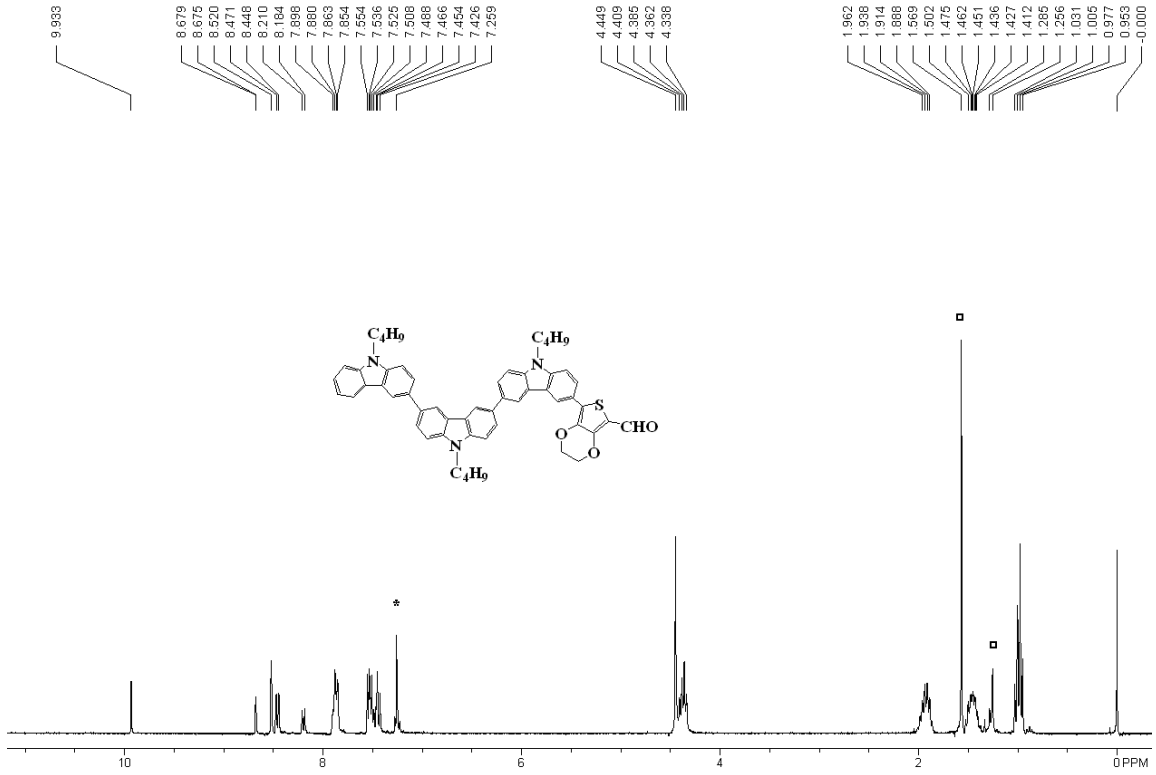


Figure S3. ^{1}H NMR spectrum of **8** (300 MHz, $CDCl_3$). The peak with asterisk is attributed to $CHCl_3$ and the peaks with square are attributed to H_2O or impurities, respectively.

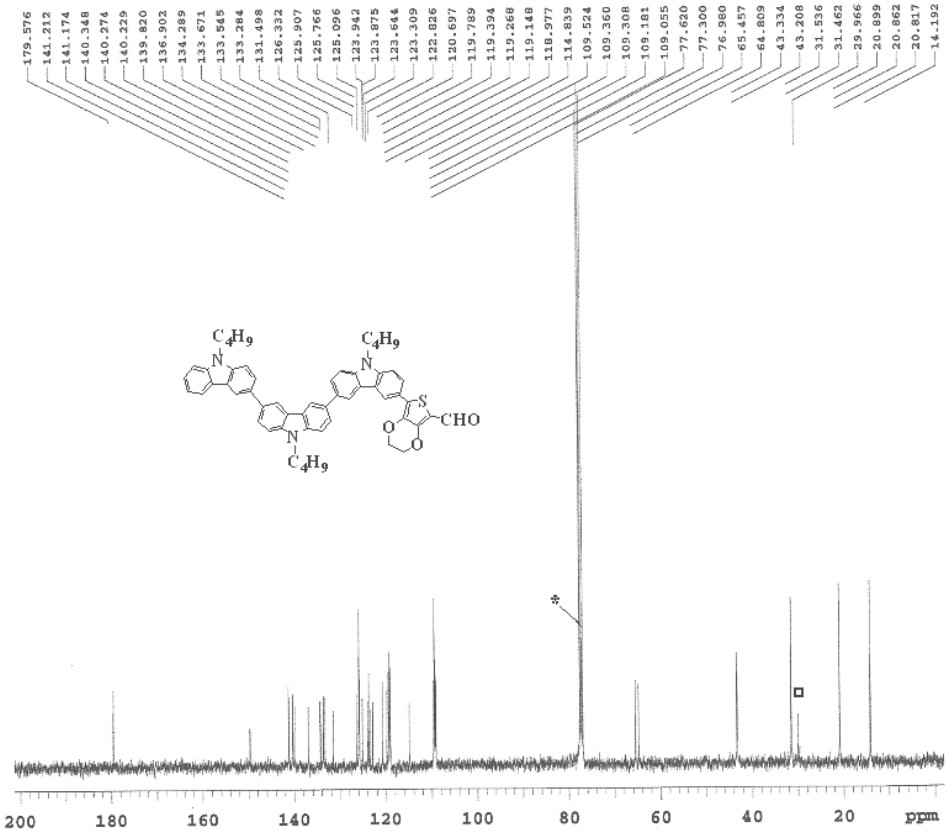


Figure S4. ^{13}C NMR spectrum of **8** (100 MHz, $CDCl_3$). The peak with asterisk is attributed to $CHCl_3$ and the peaks with square are attributed to impurities, respectively.

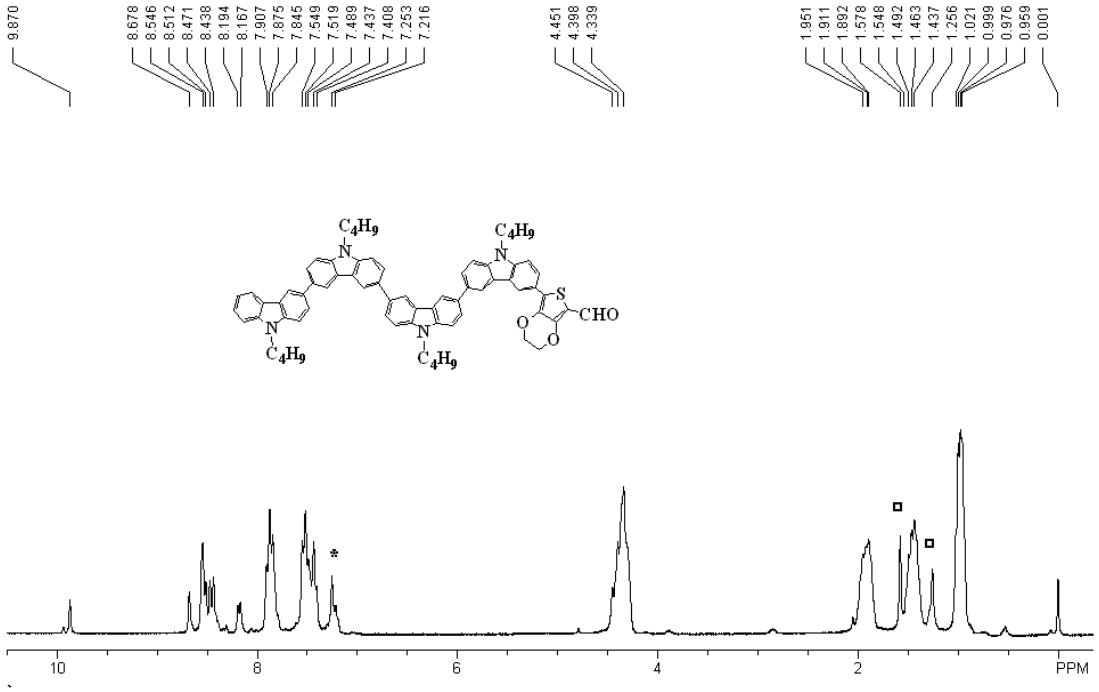


Figure S5. ^{1}H NMR spectrum of **9** (300 MHz, $CDCl_3$). The peak with asterisk is attributed to $CHCl_3$ and the peaks with square are attributed to H_2O or impurities,respectively.

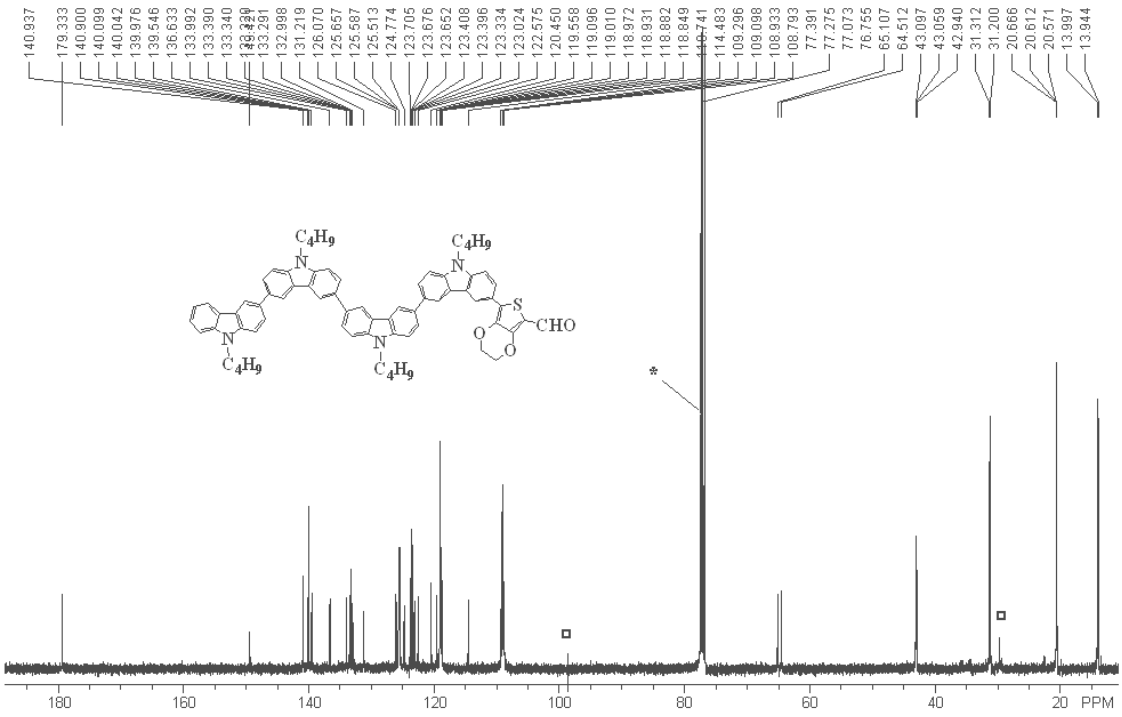


Figure S6. ^{13}C NMR spectrum of **9** (100 MHz, $CDCl_3$). The peak with asterisk is attributed to $CHCl_3$ and the peaks with square are attributed to impurities, respectively.

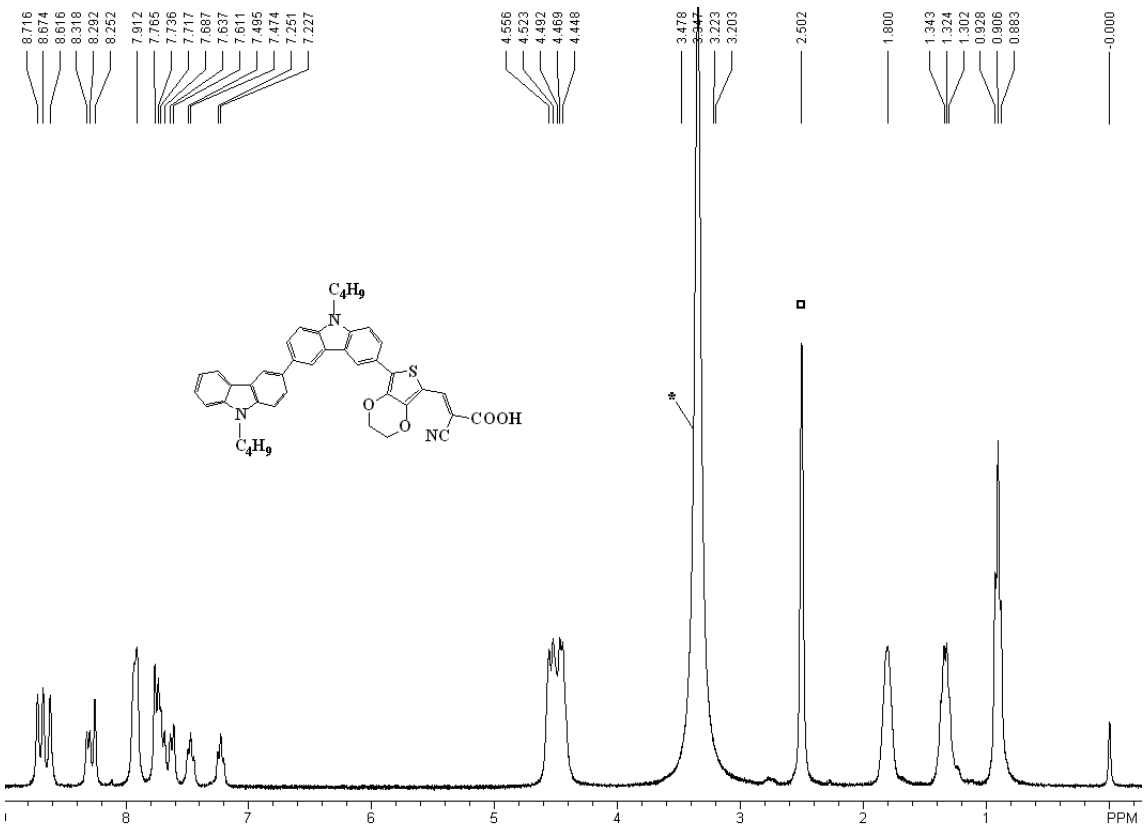


Figure S7. ^{1}H NMR spectrum of **2C** (300 MHz, DMSO-*d6*). The peak with asterisk is attributed to DMSO and the peak with square are attributed to H_2O, respectively.

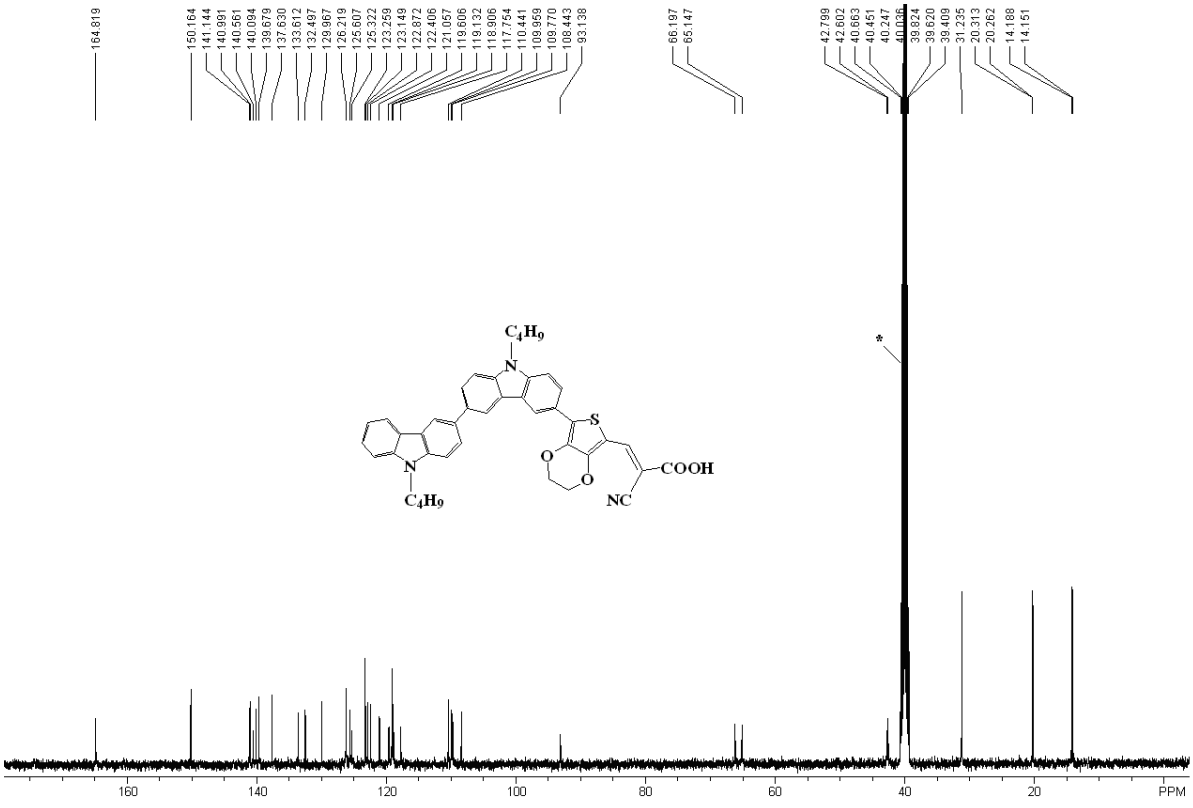


Figure S8. ^{13}C NMR spectrum of **2C** (100 MHz, DMSO-*d6*). The peak with asterisk is attributed to DMSO.

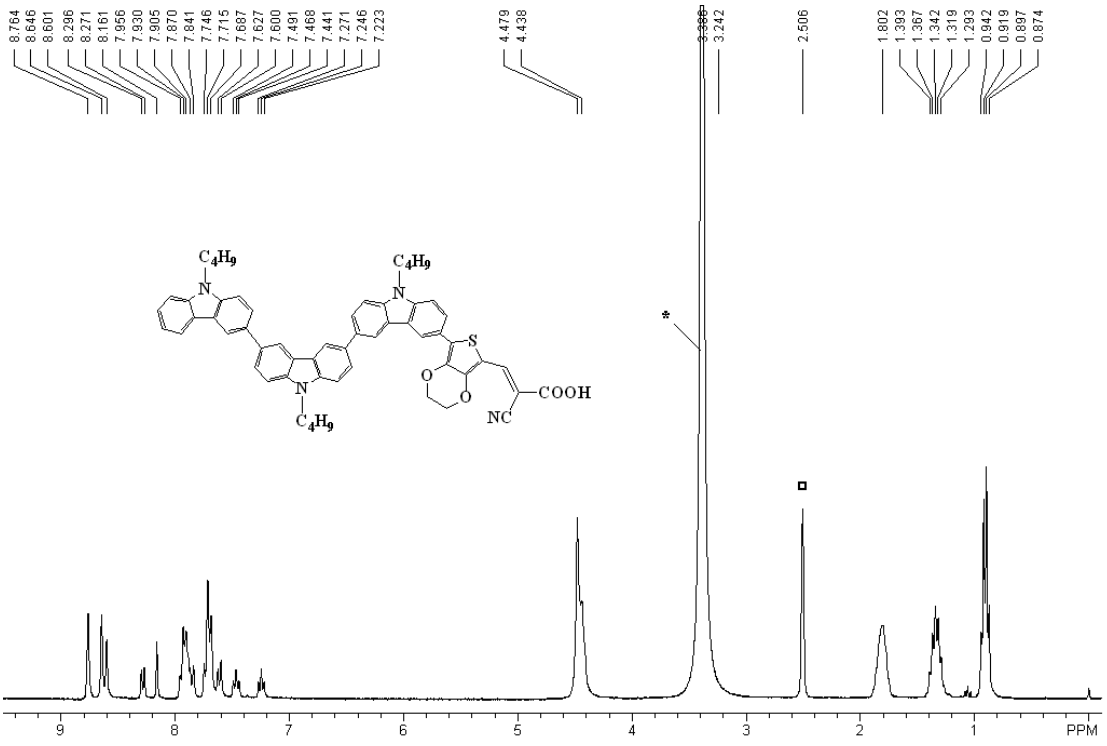


Figure S9. ^{1}H NMR spectrum of **3C** (300 MHz, DMSO-*d6*). The peak with asterisk is attributed to DMSO and the peak with square is attributed to H_2O, respectively.

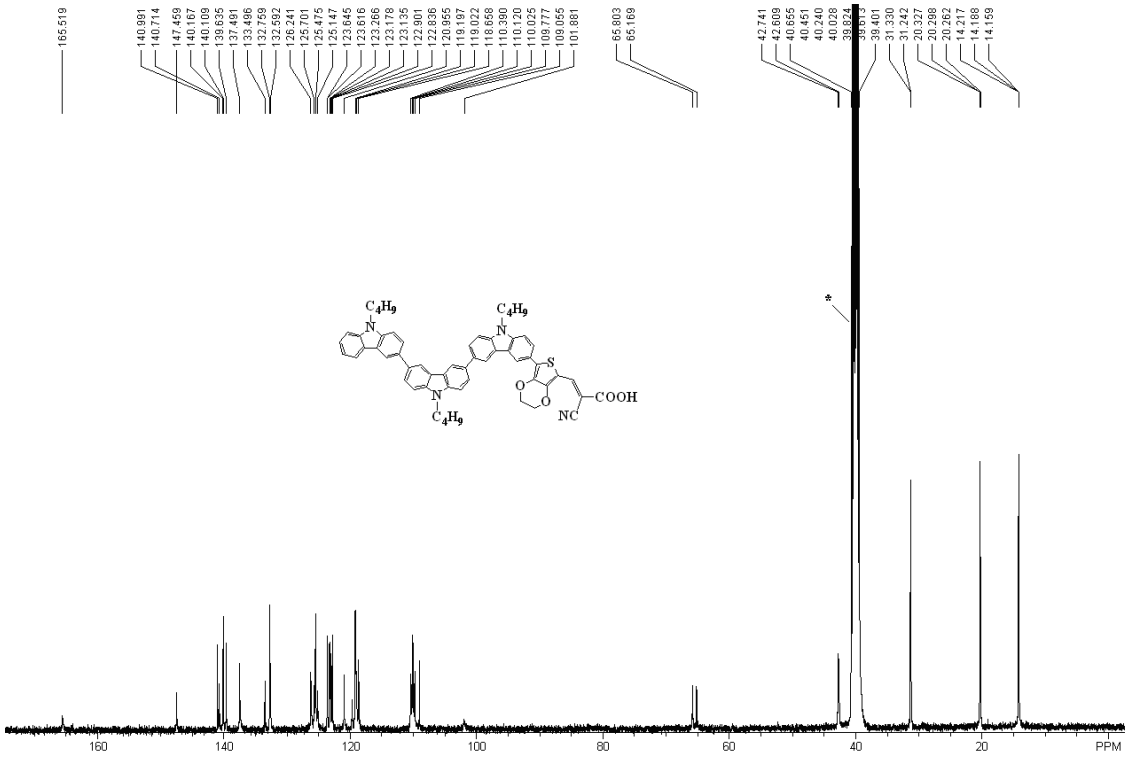


Figure S10. ^{13}C NMR spectrum of **3C** (100 MHz, DMSO-*d6*). The peak with asterisk is attributed DMSO.

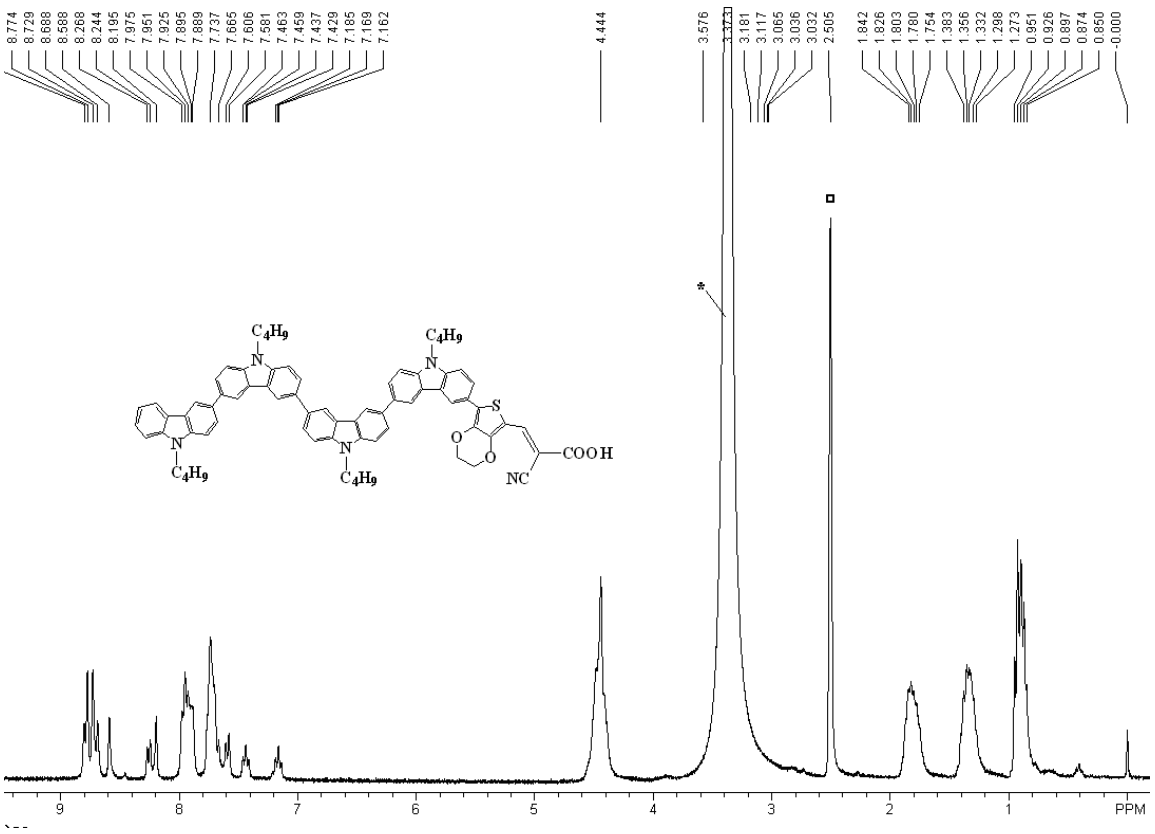


Figure S11. ^{1}H NMR spectrum of **4C** (300 MHz, DMSO-*d6*). The peak with asterisk is attributed to DMSO and the peak with square is attributed to H_2O, respectively.

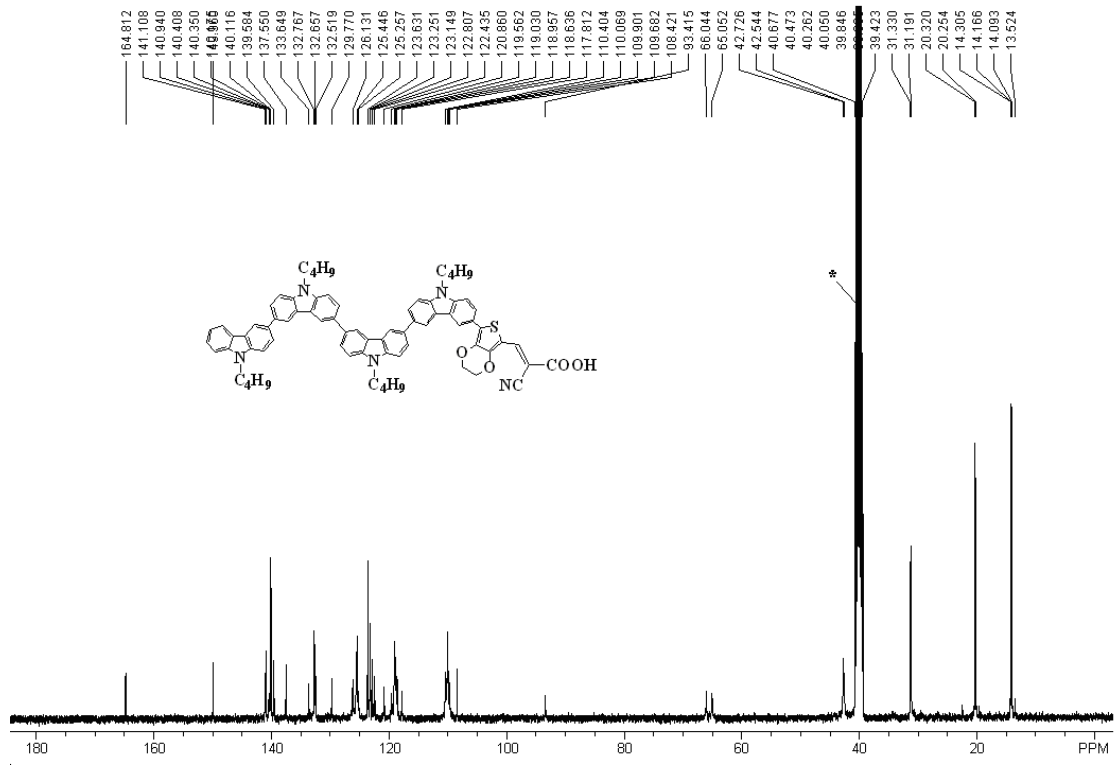


Figure S12. ^{13}C NMR spectrum of **4C** (100 MHz, DMSO-*d6*). The peak with asterisk is attributed

DMSO.

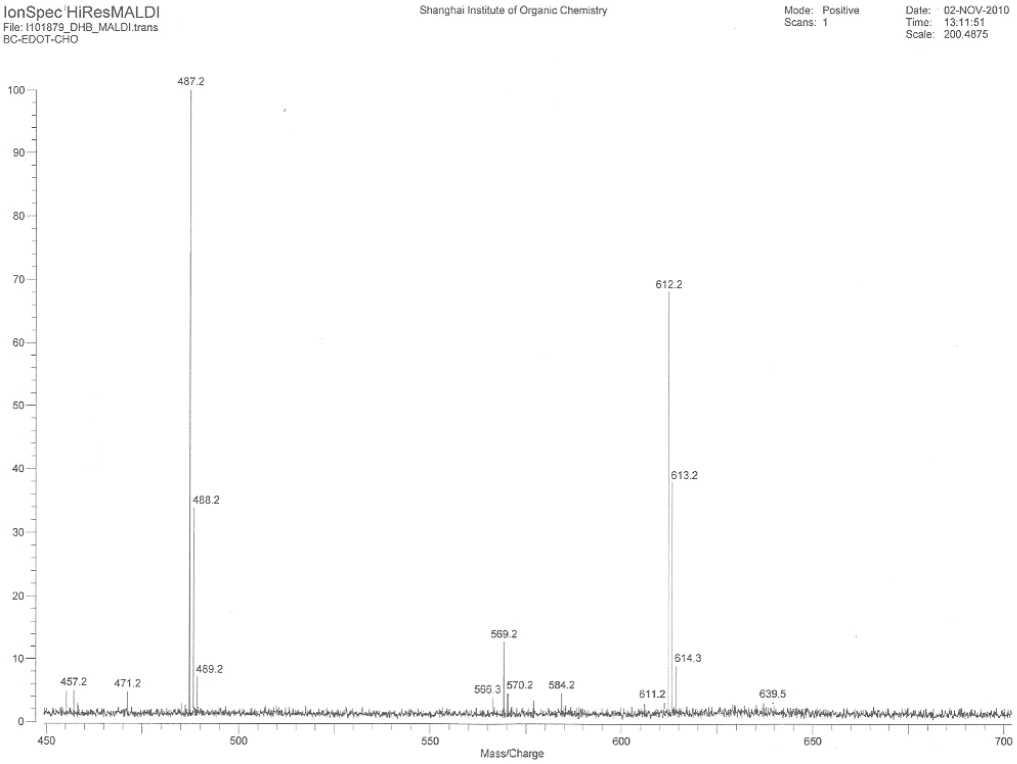


Figure S13. Mass spectrum of **6.**

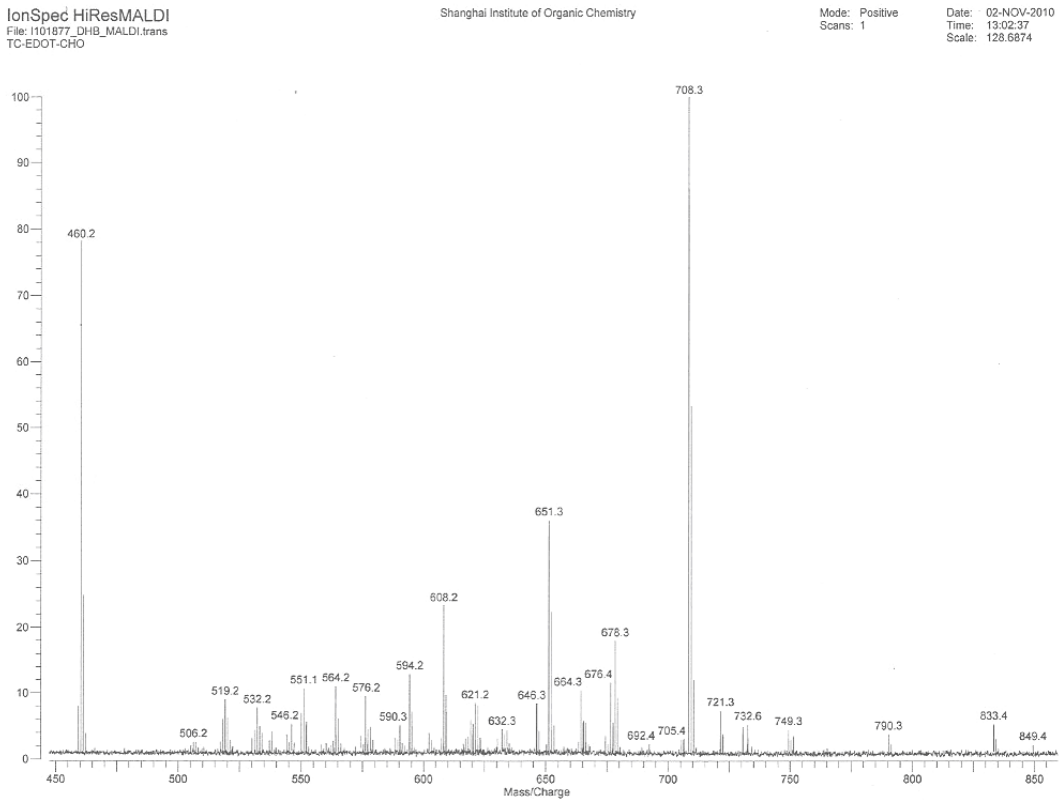


Figure S14. Mass spectrum of **8.**

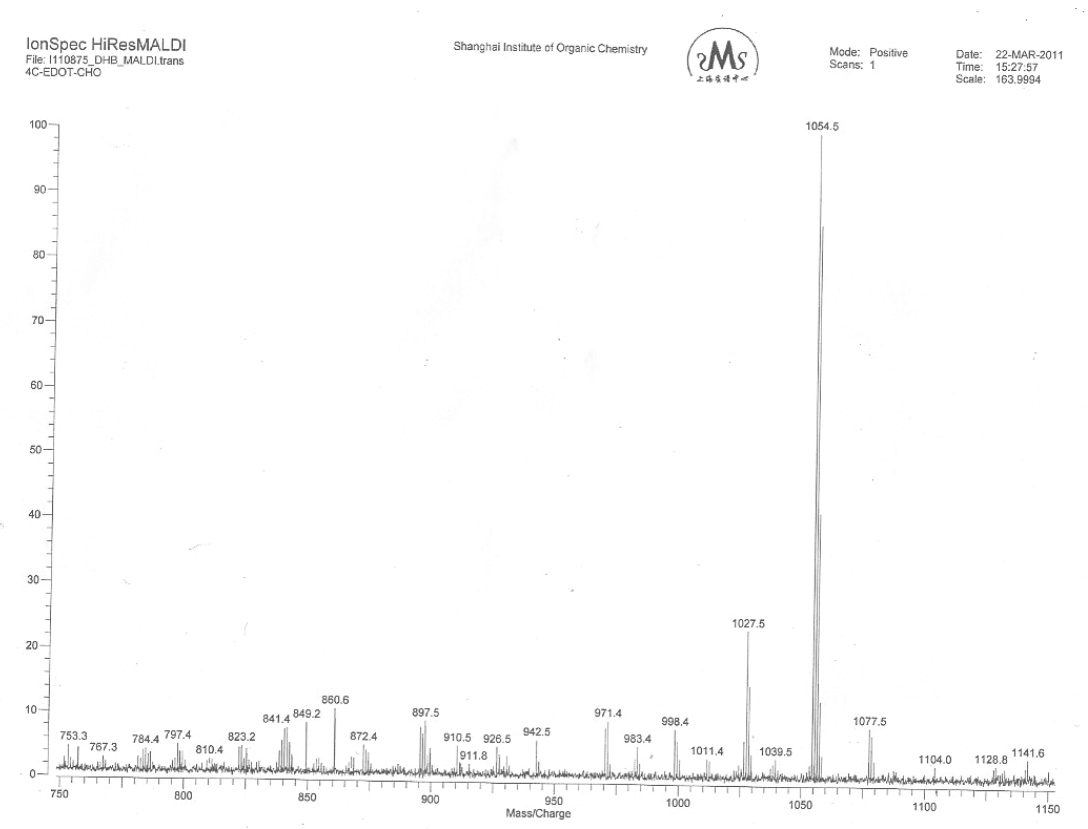


Figure S15. Mass spectrum of **9.**

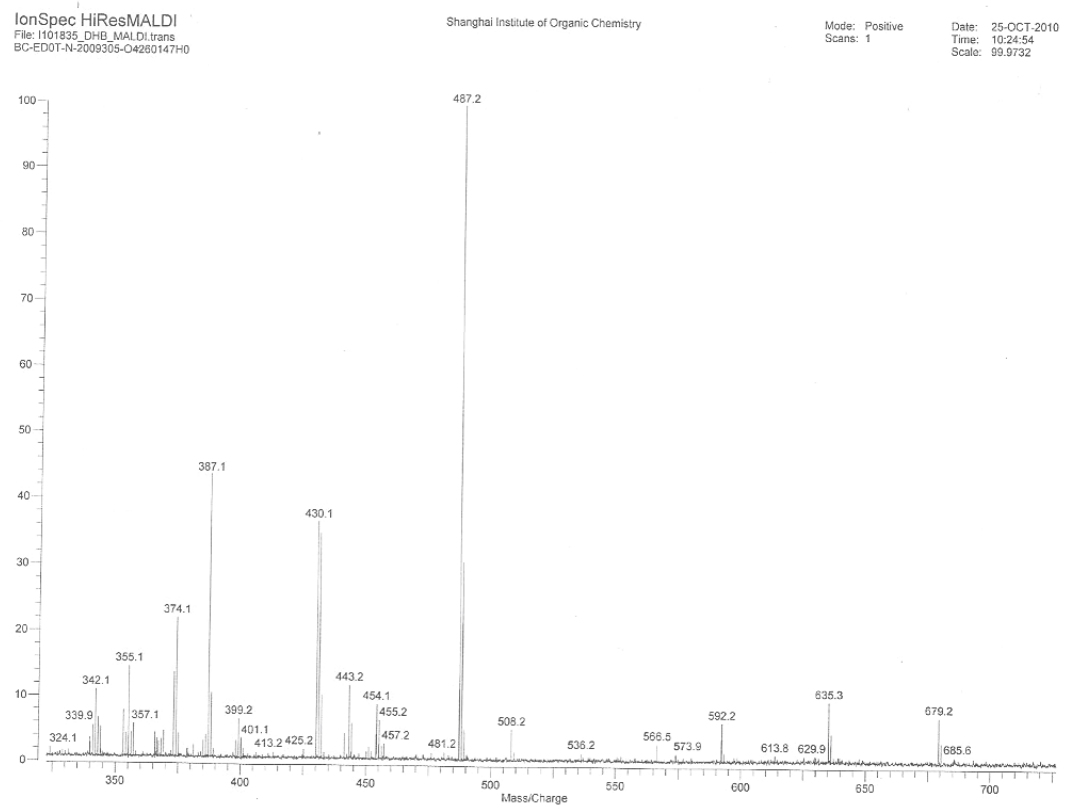


Figure S16. Mass spectrum of **2C.**

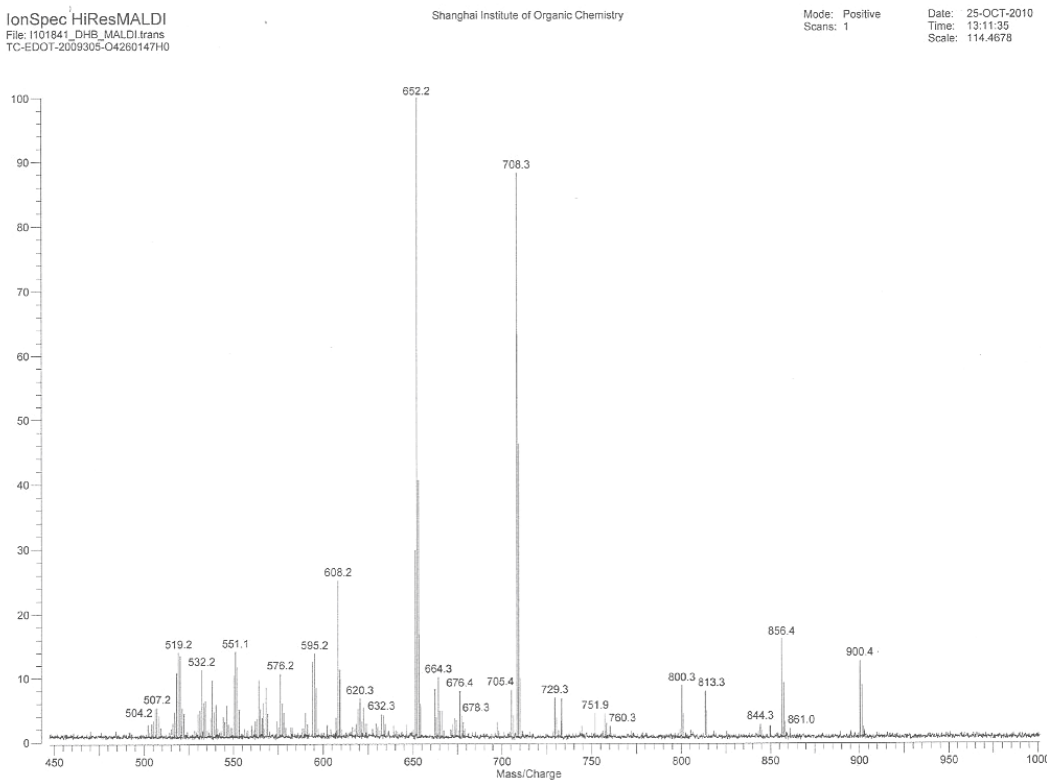


Figure S17. Mass spectrum of **3C.**

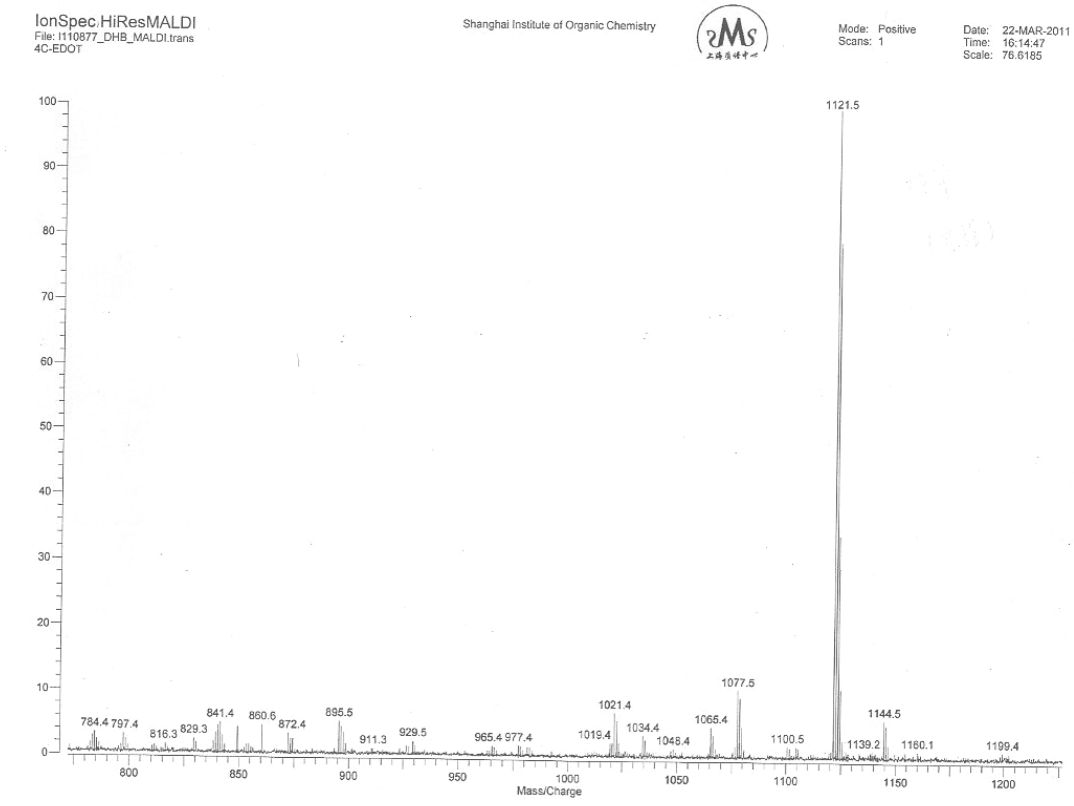


Figure S18. Mass spectrum of **4C.**

2. Optical properties of the dyes

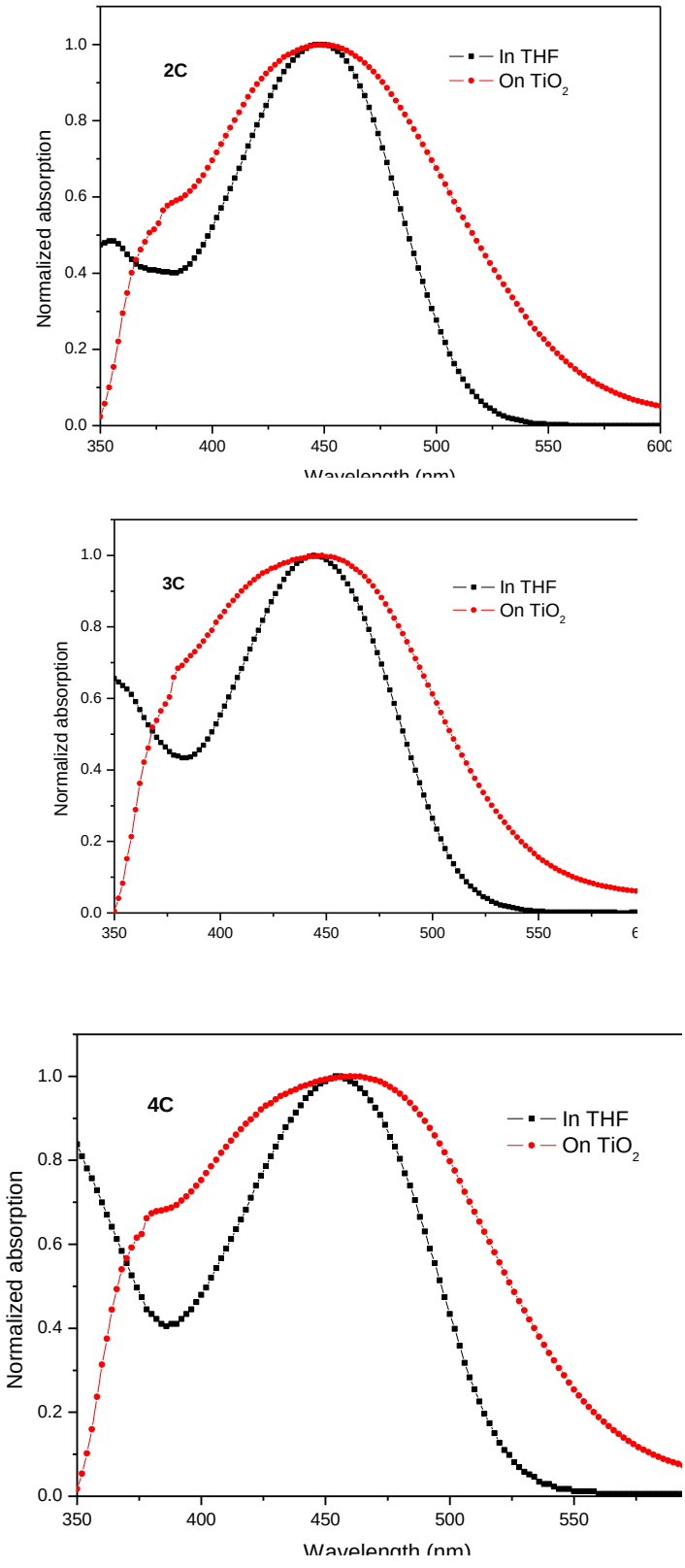


Figure S19. Normalized UV-vis spectra of **2C**-**4C** in THF and on TiO_2.

Table S1. The maximum and onset absorption wavelength for **2C**-**4C** in THF and on TiO_2

Dyes	In THF[a]		On TiO_2[b]	
	λ_{max} (nm)	λ_{onset} (nm)	λ_{max} (nm)	λ_{onset} (nm)
2C	448	525	448	565
3C	444	525	448	555
4C	456	530	460	565

[a] In THF solution (10^{-5} M). [b] On TiO_2 (12 μm) films which were immersed into 1.5×10^{-4} M solution of these dyes in THF for 12 h.

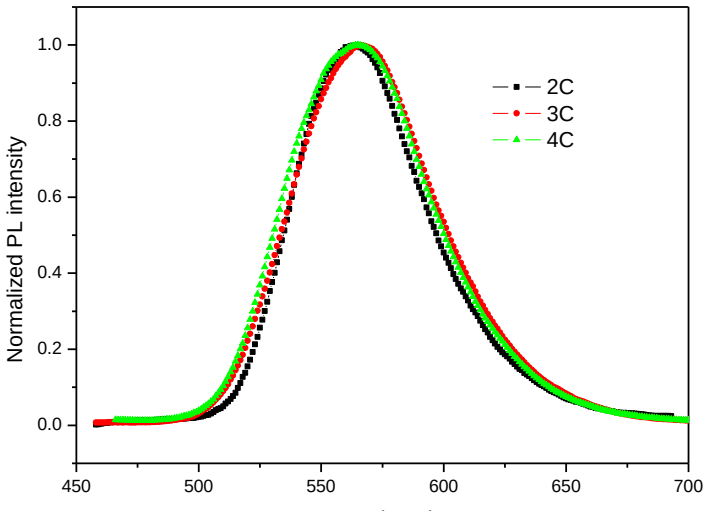


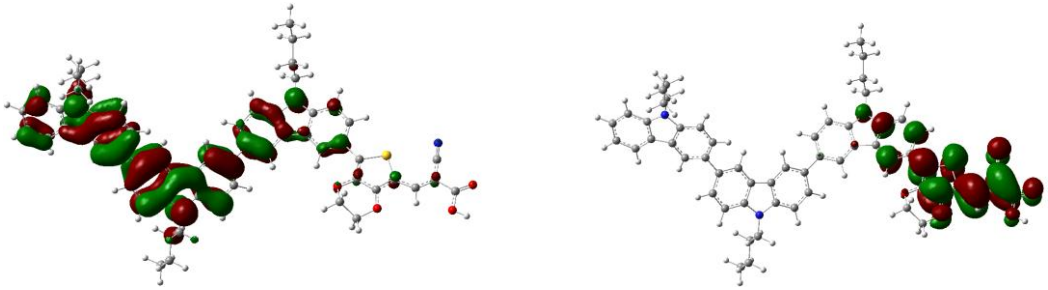
Figure S20. Normalized PL spectra of the dyes in THF.

3. The theory estimation of HOMO and LUMO for the dyes

HOMO **LUMO**

2C

3C



4C

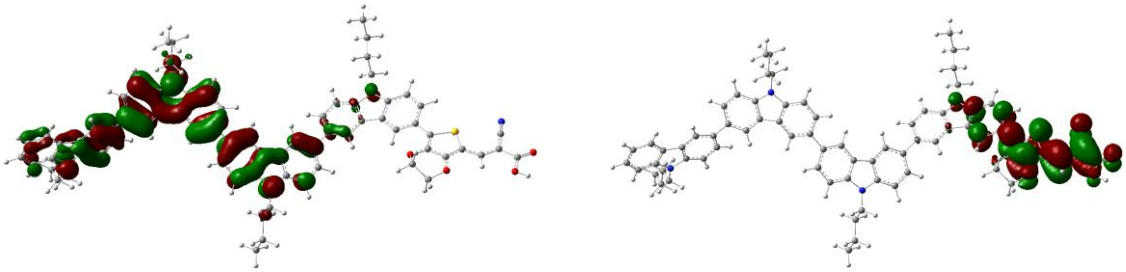


Figure S21. Frontier molecular orbital of the HOMO and LUMO calculated with DFT. (Density functional theory (DFT) calculations were conducted by using the B3LYP hybrid functional for the geometry optimizations. The molecular orbital levels of HOMO and LUMO were achieved with the 6-31G(d) basis set implemented in the Gaussian 03 package[1])

Reference

1 *(a)* A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648. (*b*) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.