

Supporting Information

Optimizing molecular structure of 1,1,7,7-tetramethyljulolidine fused furan based chromophores by introducing heterocycle ring to achieve a high electro-optic activity

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¹H and ¹³C NMR spectra of compound 2

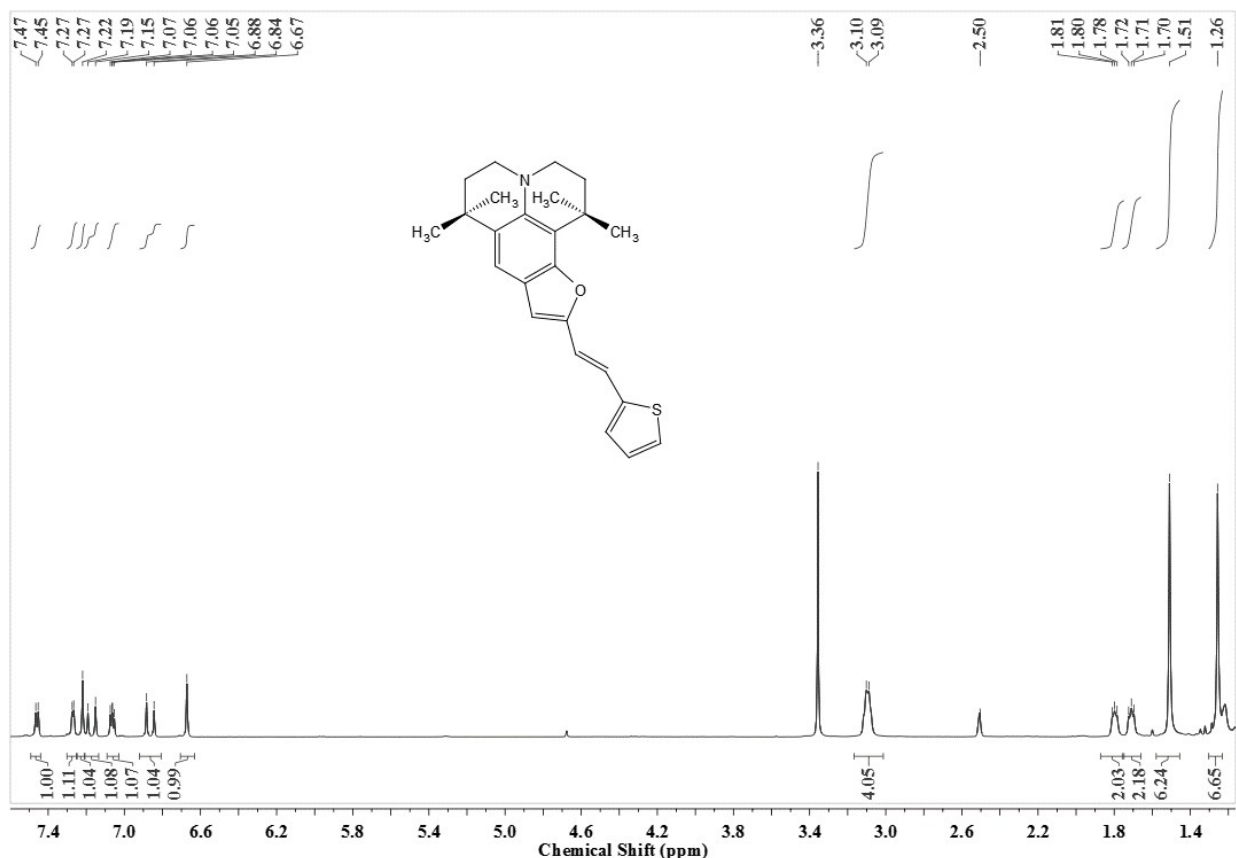


Fig. S1

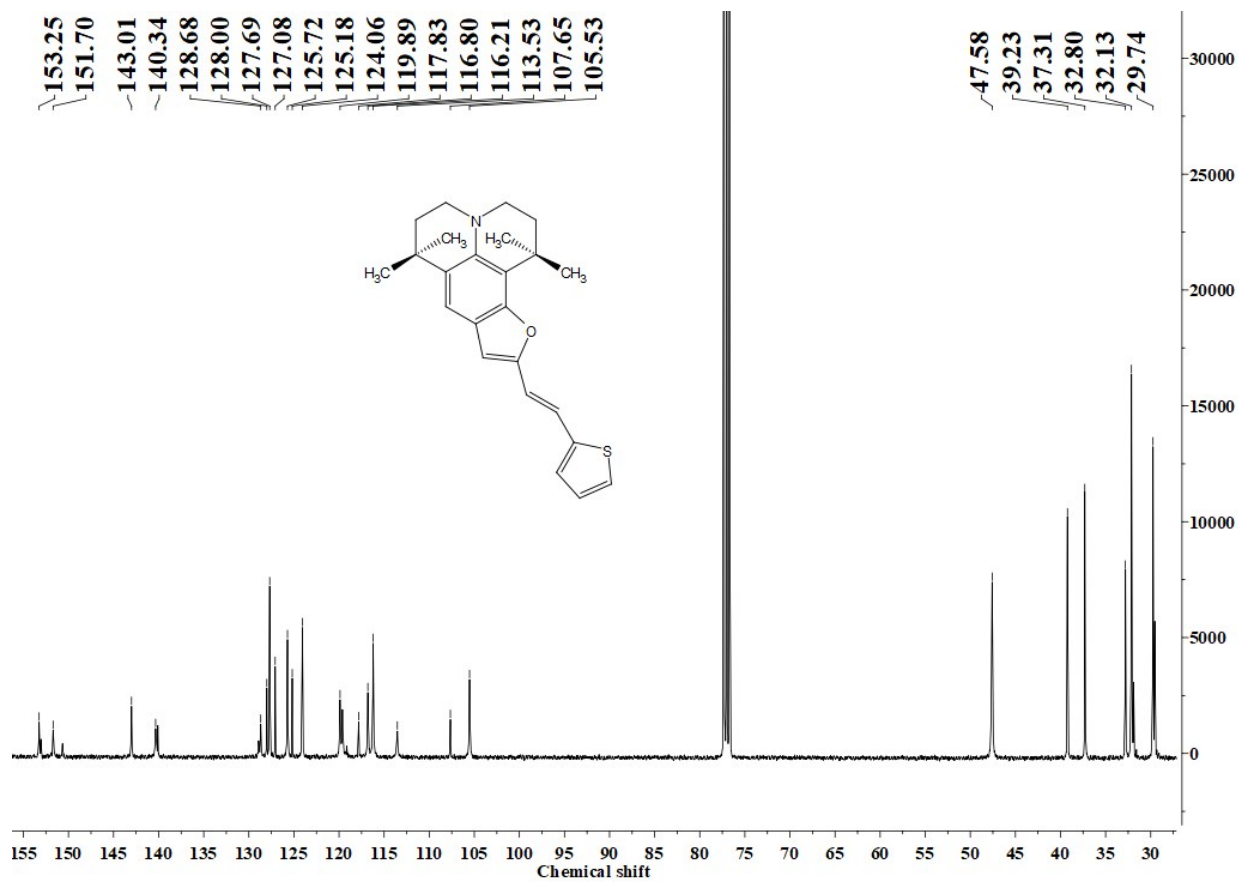


Fig. S2

¹H and ¹³C NMR spectra of compound 3

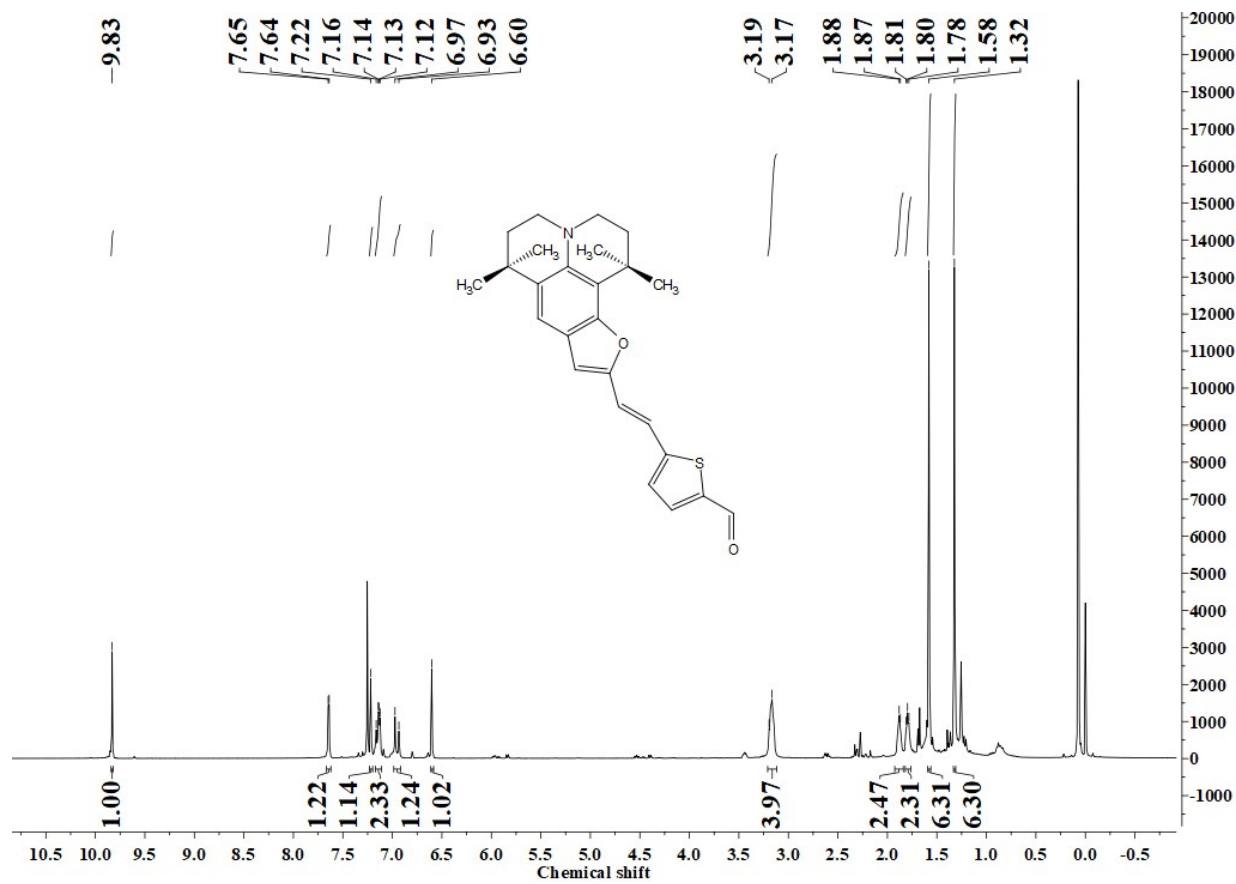


Fig. S3

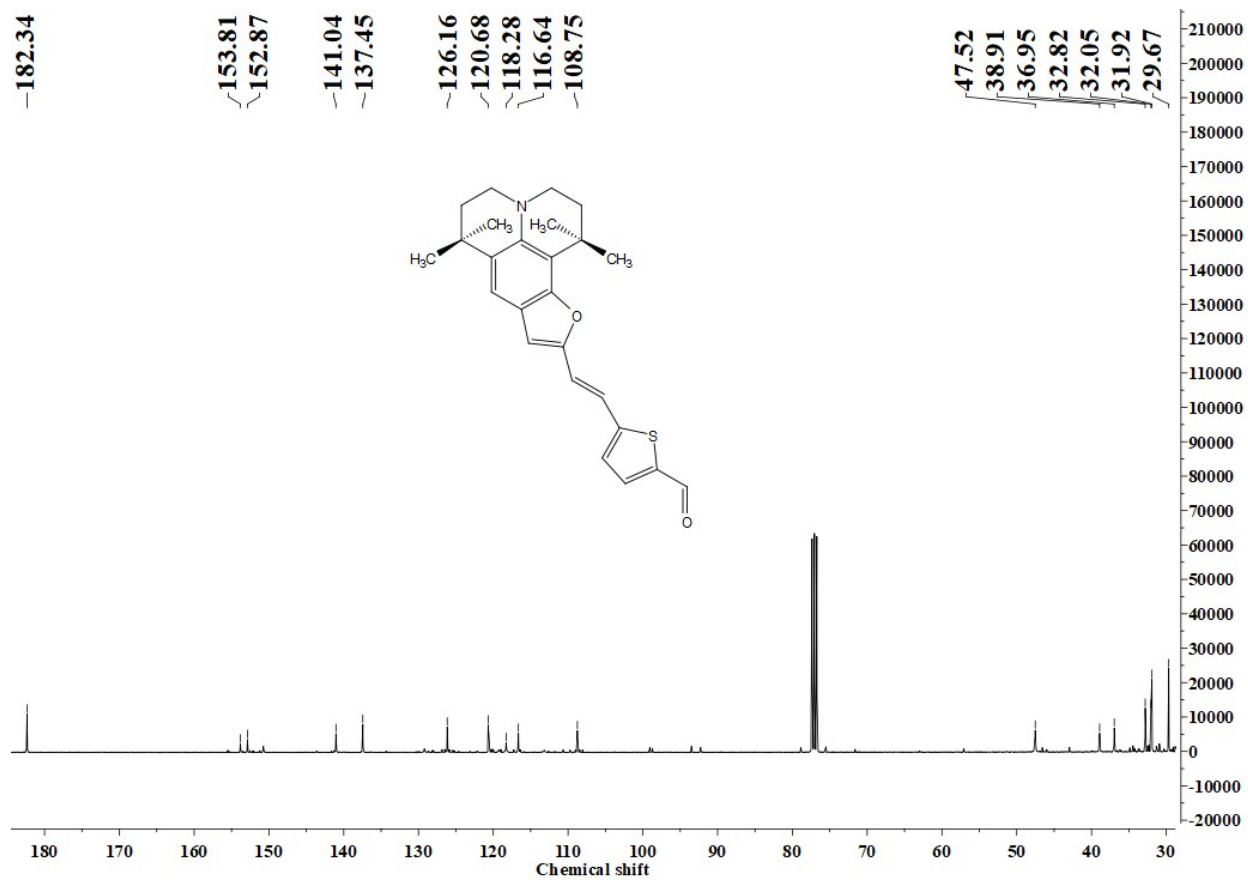


Fig. S4

^1H and ^{13}C NMR spectra of Chromophore 2

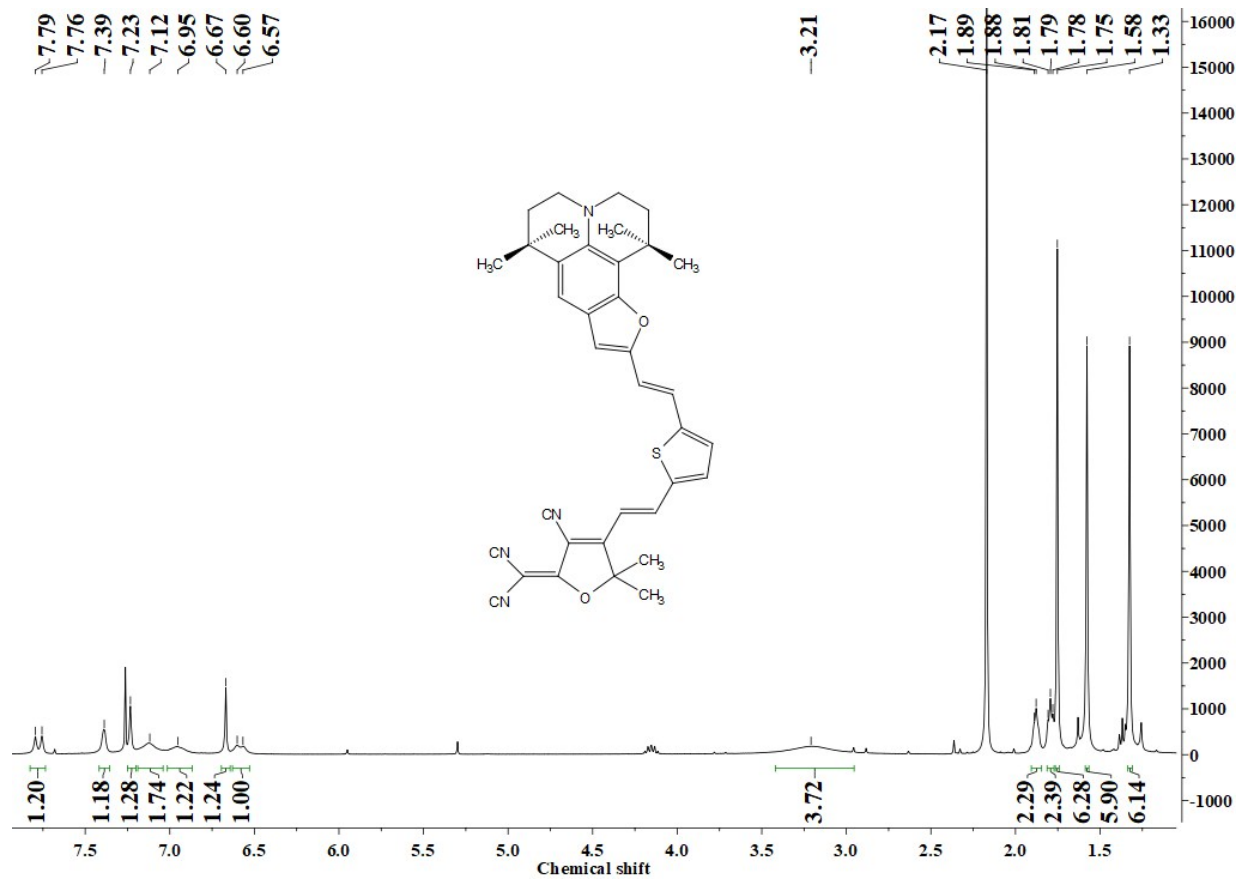


Fig. S5

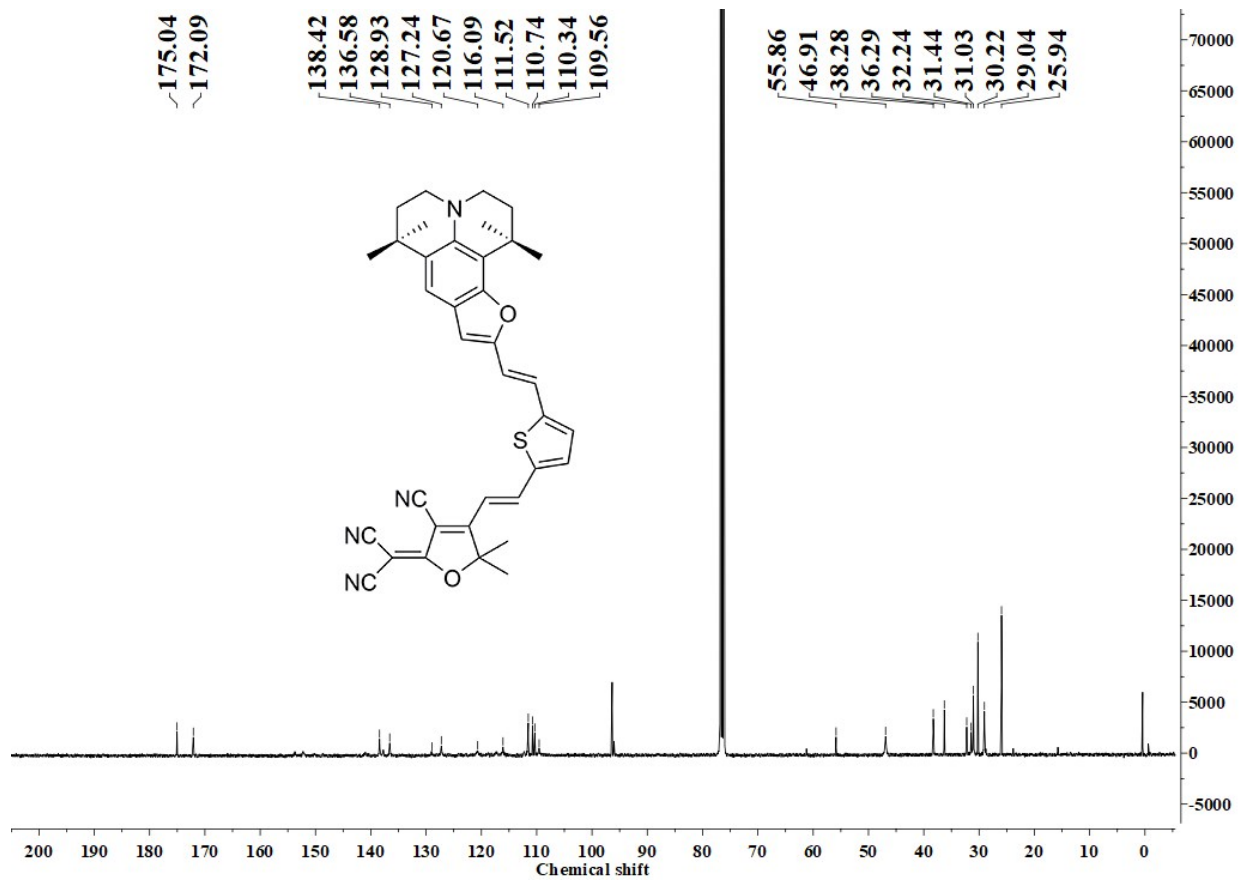


Fig. S6

^1H and ^{13}C NMR spectra of compound 4

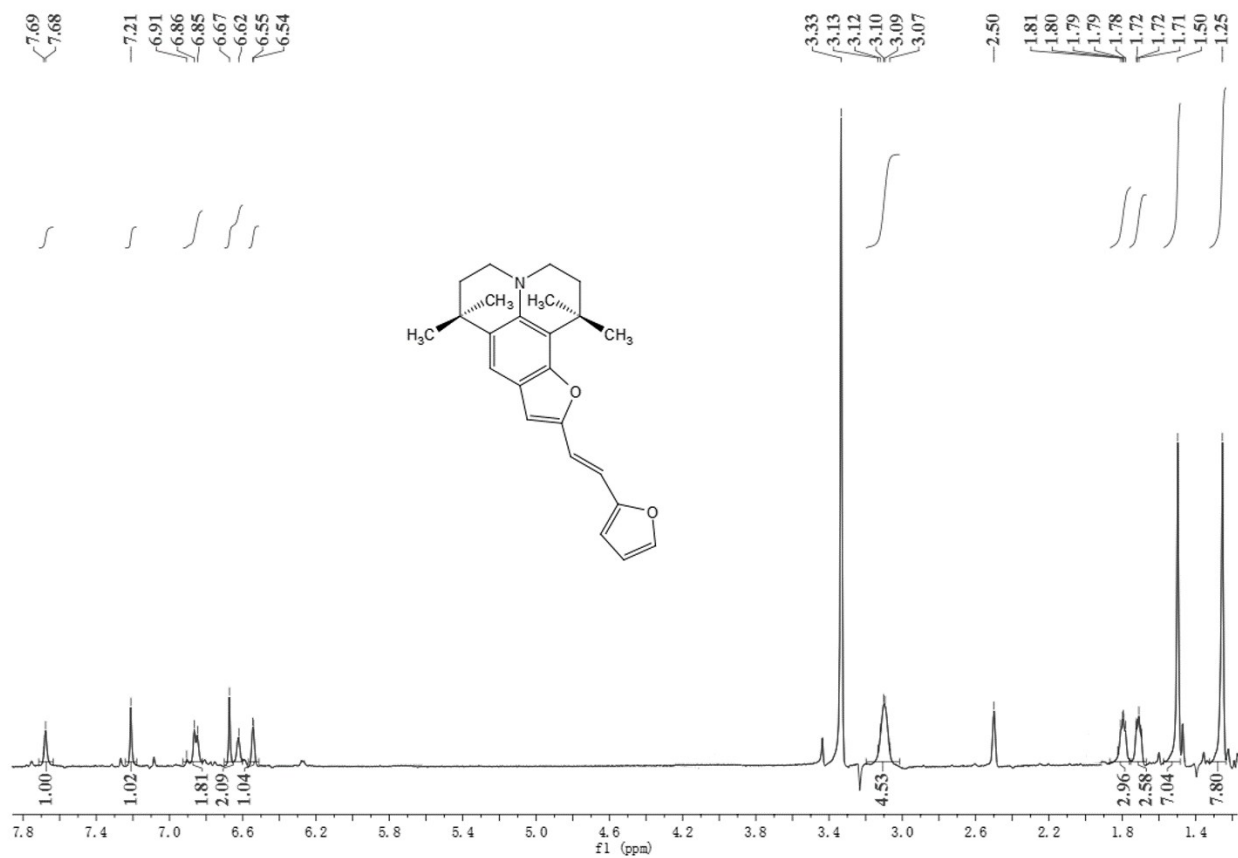


Fig. S7

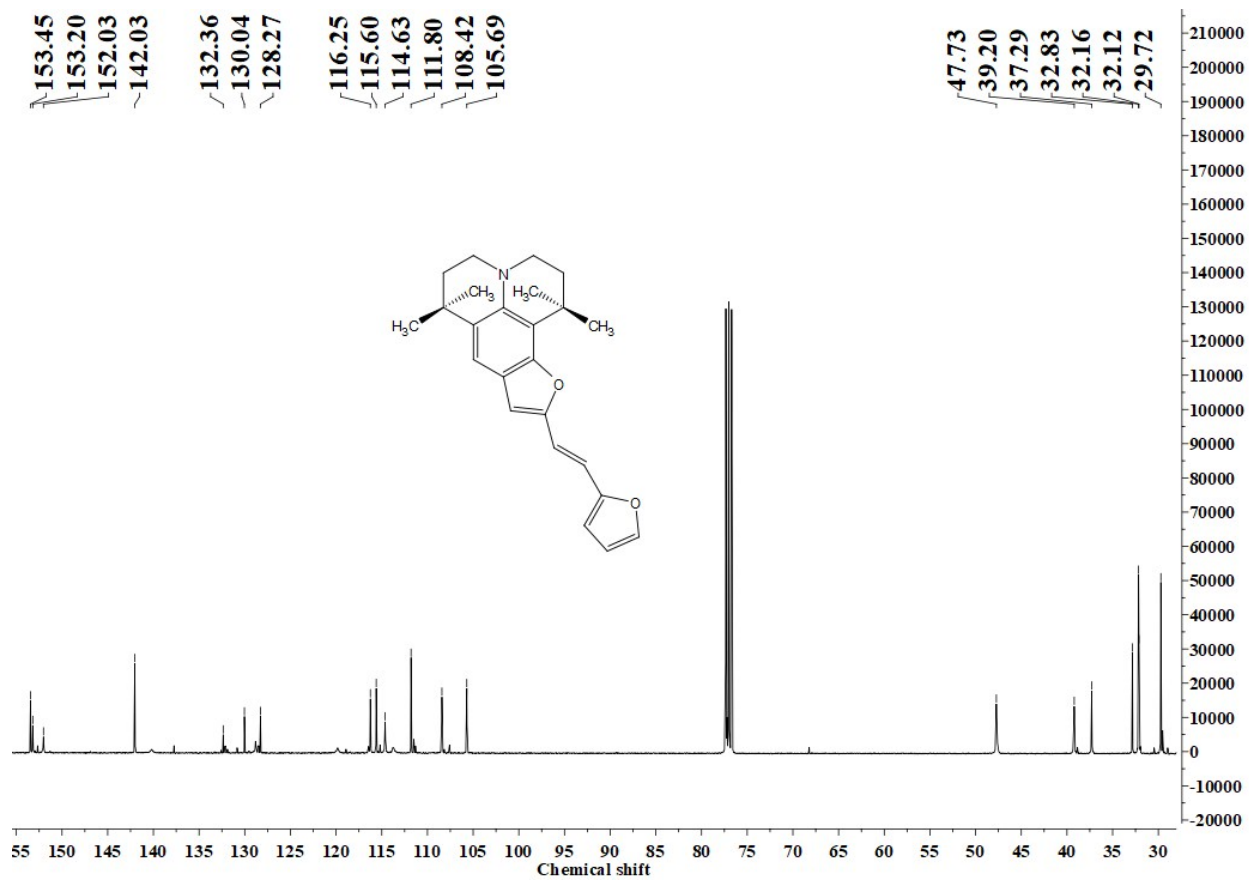


Fig. S8

^1H and ^{13}C NMR spectra of compound 5

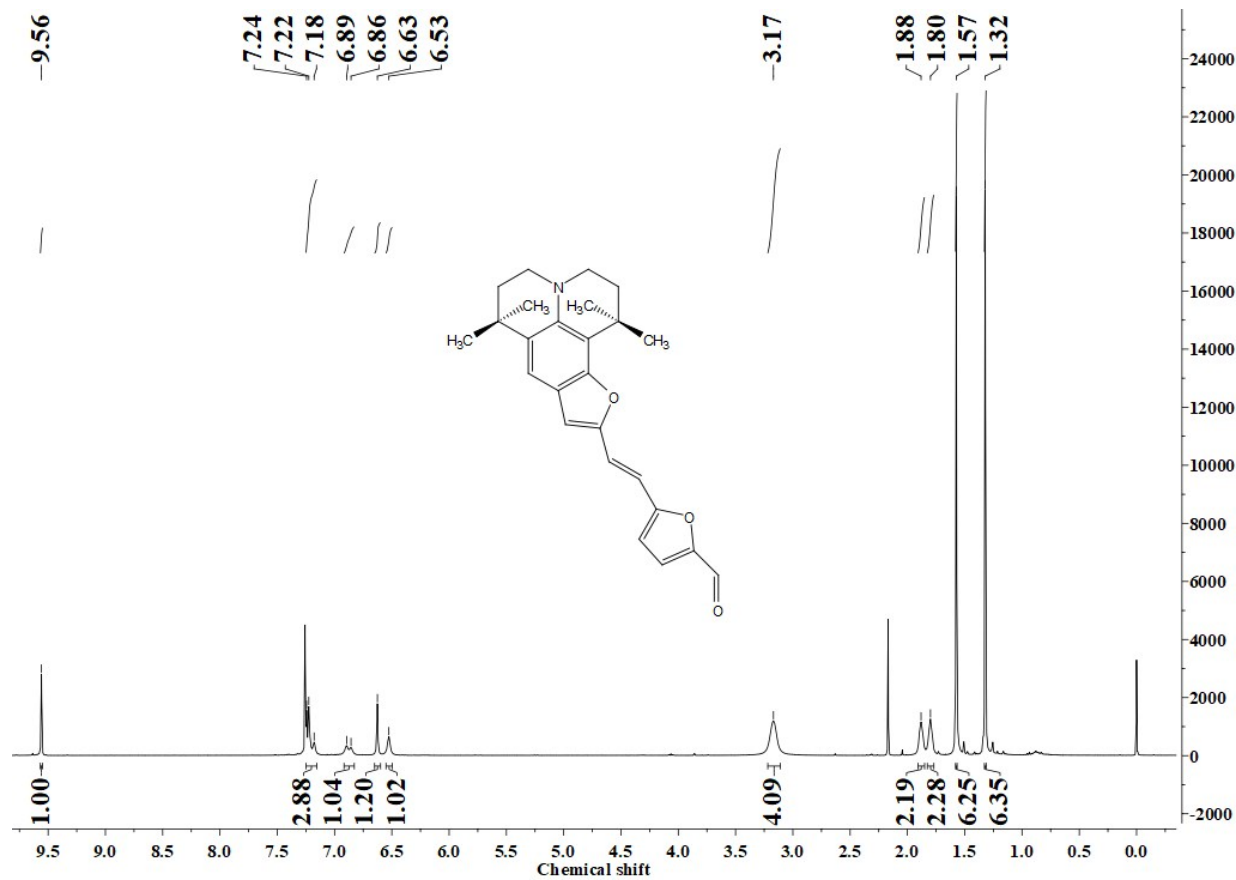


Fig. S9

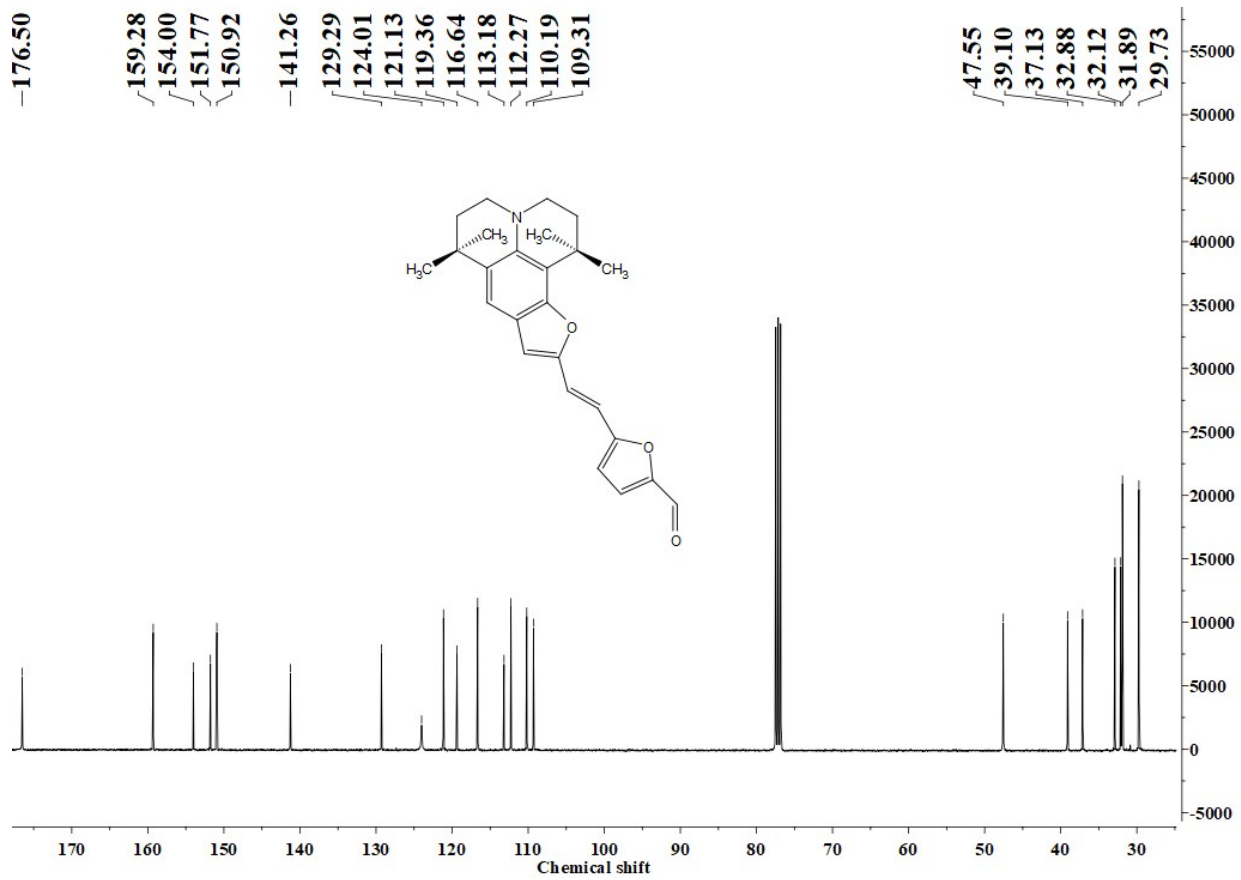


Fig. S10

¹H and ¹³C NMR spectra of Chromophore 1

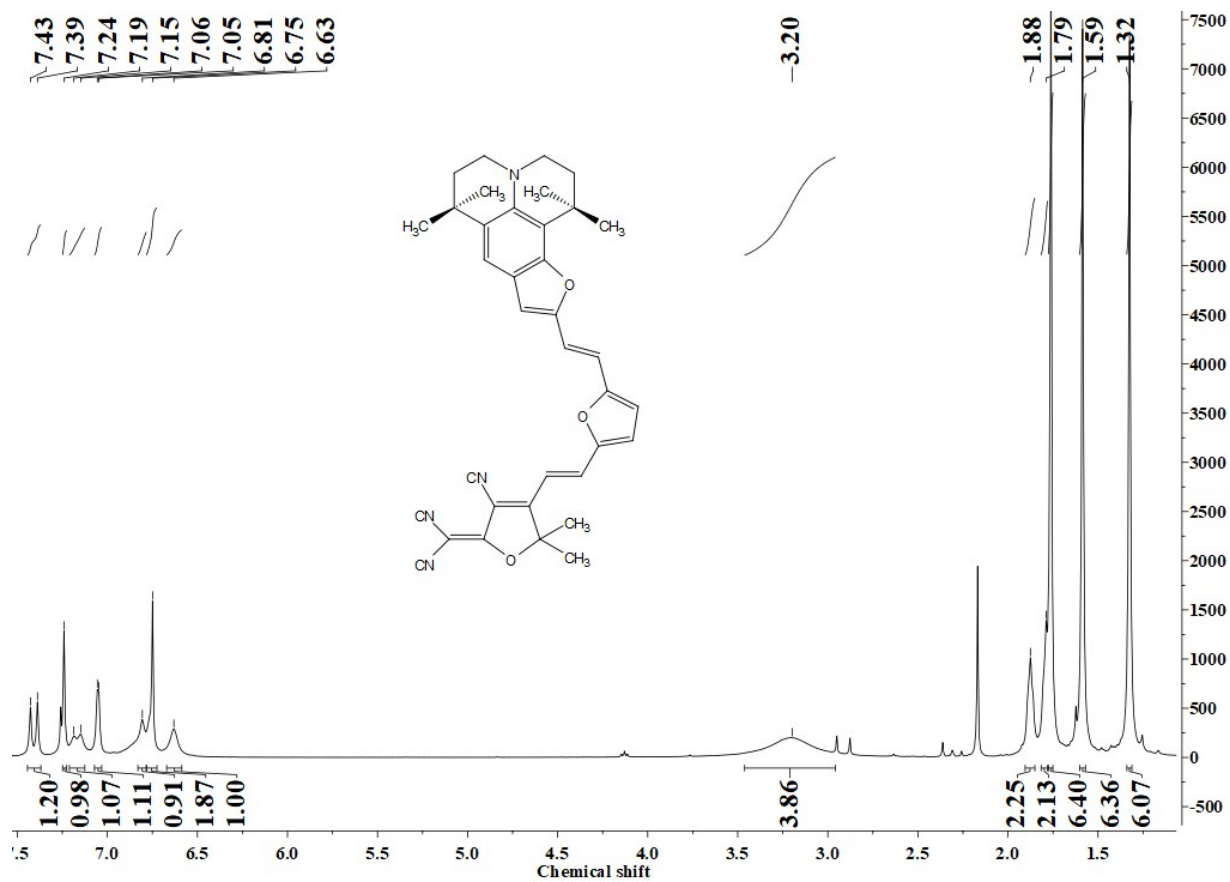


Fig. S11

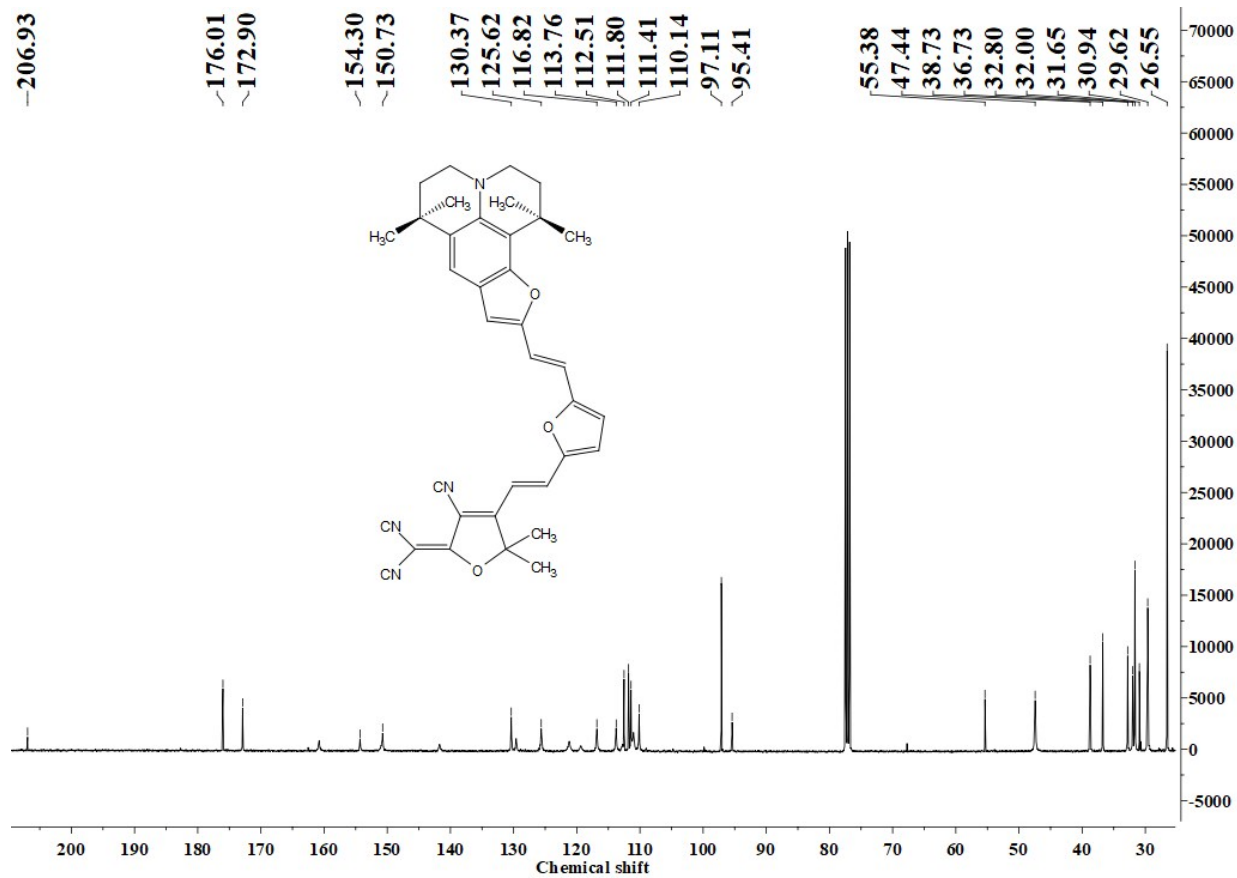


Fig. S12

Theoretical calculations

To further disclose the role of the π -bridge on the properties of chromophores **C1** and **C2**, DFT calculations were conducted using hybrid B3LYP/6-31G* geometries by means of Gaussian 03 (G03). All C–C double bonds outside the aromatic rings were set to be in trans-configuration and their geometries were optimized in vacuum. The electronic structure of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of **C1** and **C2** were given after the calculation. As shown in Figure S13, both in the ground and excited states, the electron density was asymmetric along the dipolar direction due to the intramolecular charge transfer. Although both chromophores have the same electron distribution behaves, careful contrast their orbital's electron density shows up some differences, at the HOMO state, the electron density in the furyl-vinylene of **C1** is richer than in the thienyl-vinylene of **C2**, and these electrons of **C1** could effectively transfer to the π -bridge and acceptor moiety end at the LUMO state.

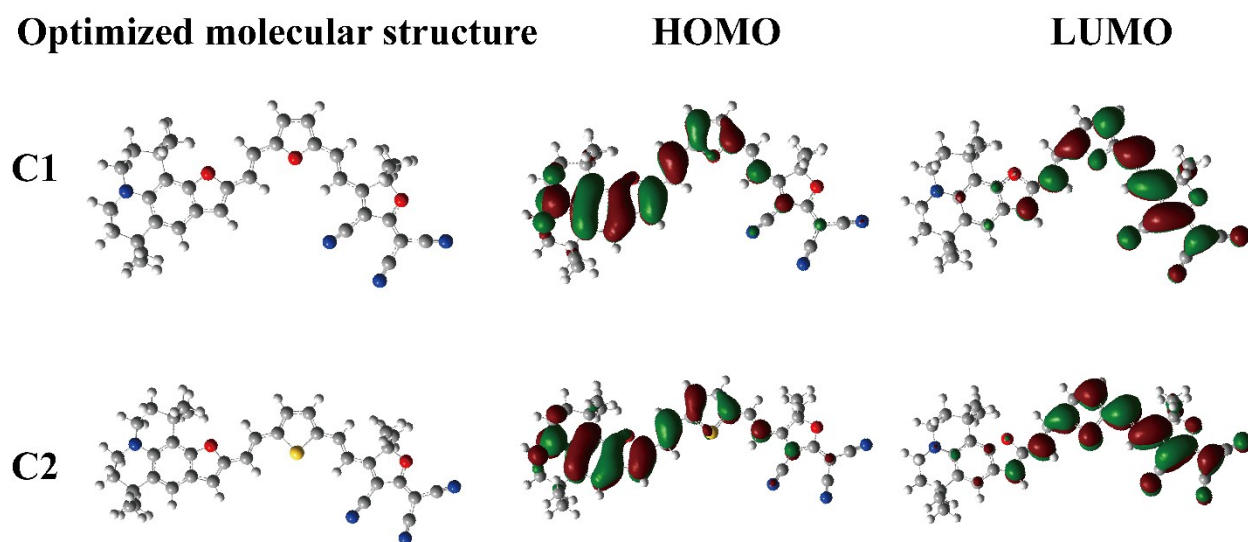


Fig. S13 The frontier HOMO and LUMO orbitals of the C1 (Top) and C2 (bottom) at the B3LYP/6-31G* level.