Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

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Synthesis of novel nonlinear optical chromophores with enhanced electro-optic activity by introducing suitable isolation groups into the donor and bridge

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1. Solvatochromic behavior

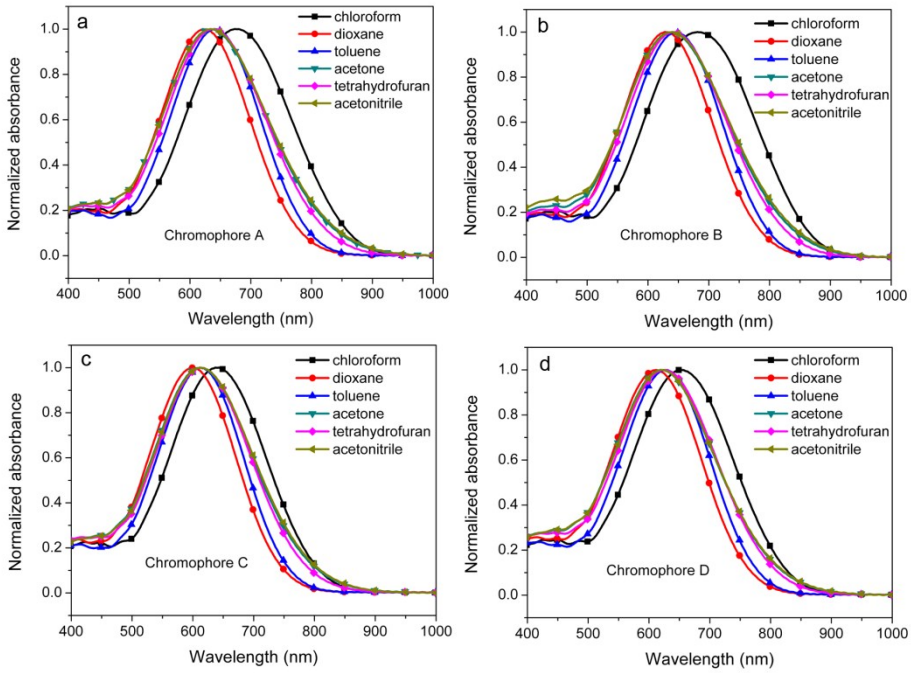

Fig. S1 UV-Vis absorption spectra of chromophores A-D in six kinds of aprotic solvents with varying dielectric constants.

2. Molecular orbital energy level diagram

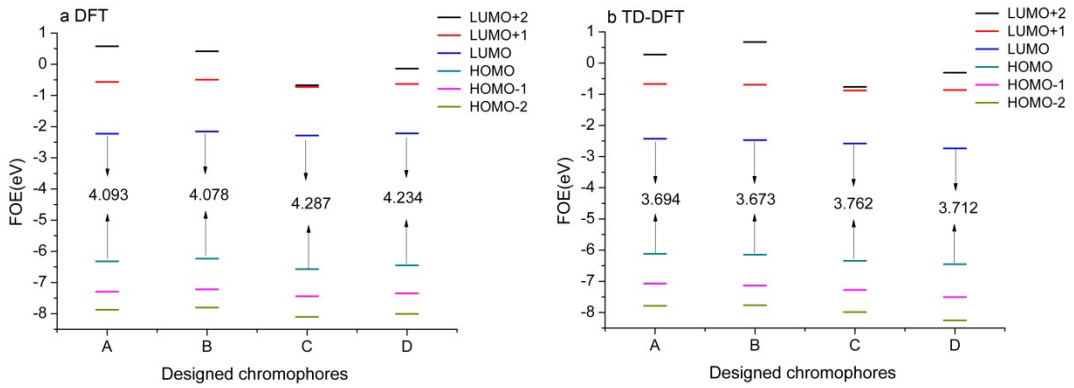

Fig. s2 Molecular orbital energy level diagram of the chromophores calculated from DFT and TD-DFT in vacuum.

3. Summary of DFT and TD-DFT data

Table s1 Summary of DFT and TD-DFT data

Cmpd	ΔE^a (eV)	$\beta_{tot}{}^b$ (10^{-30}esu)	ΔE^c (eV)	$\beta_{tot}{}^d$ (10^{-30}esu)	ΔE^e (eV)	$\beta_{tot}{}^f$ (10^{-30}esu)
A	4.093	668.04	3.694	985.19	3.531	2385.81
B	4.078	666.04	3.673	932.75	3.530	2240.70
C	4.287	548.49	3.762	808.51	3.566	1903.56
D	4.234	593.30	3.712	850.09	3.543	2177.63

[a,b] calculated from DFT calculations in vacuum. [c,d] calculated from TD-DFT calculations in vacuum [e,f] alculated from TD-DFT calculations in chloroform

4. Optimized structures of chromophores

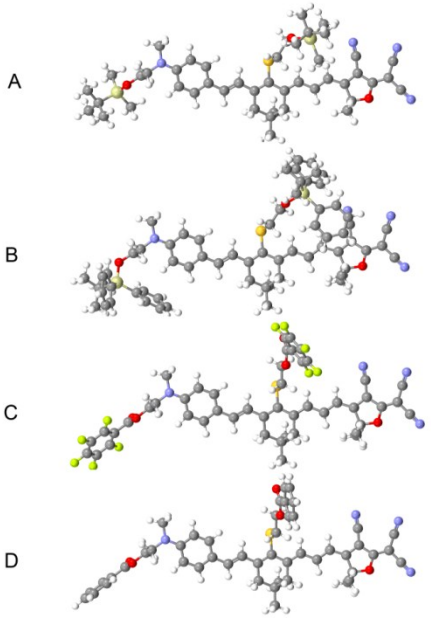

Fig. s3 Optimized structures of chromophores A-D.

5. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra

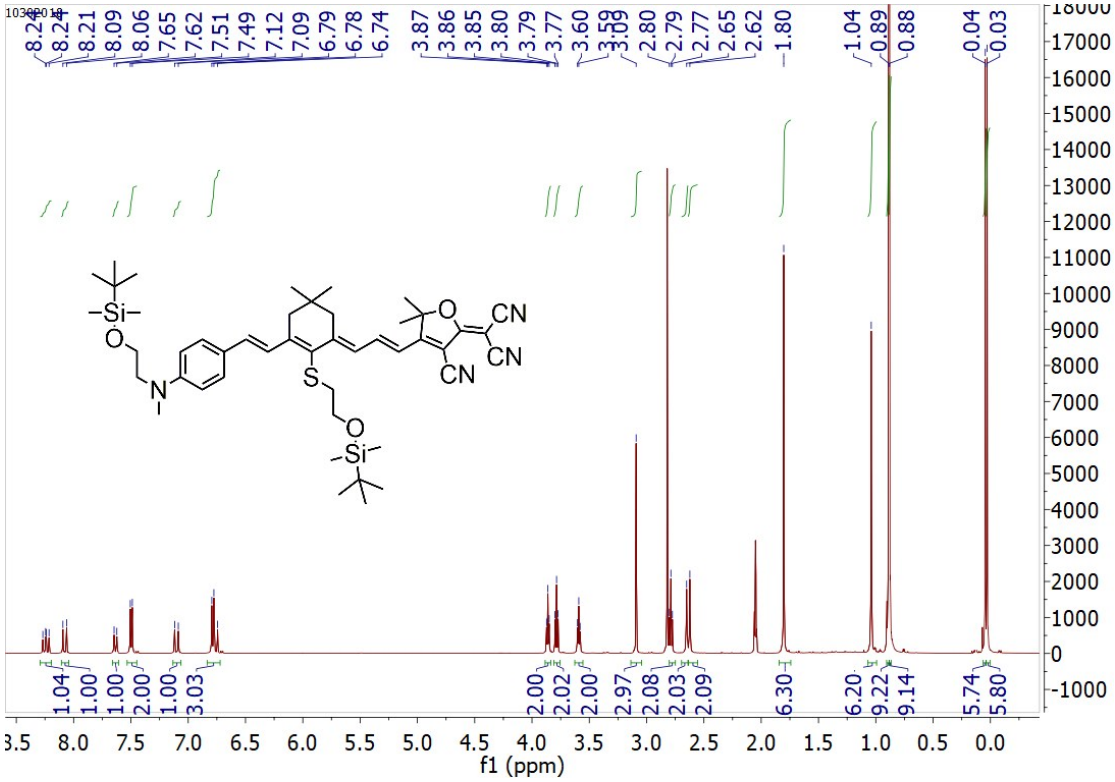

Figure S4 ^{1}H NMR spectra of Chromophore A

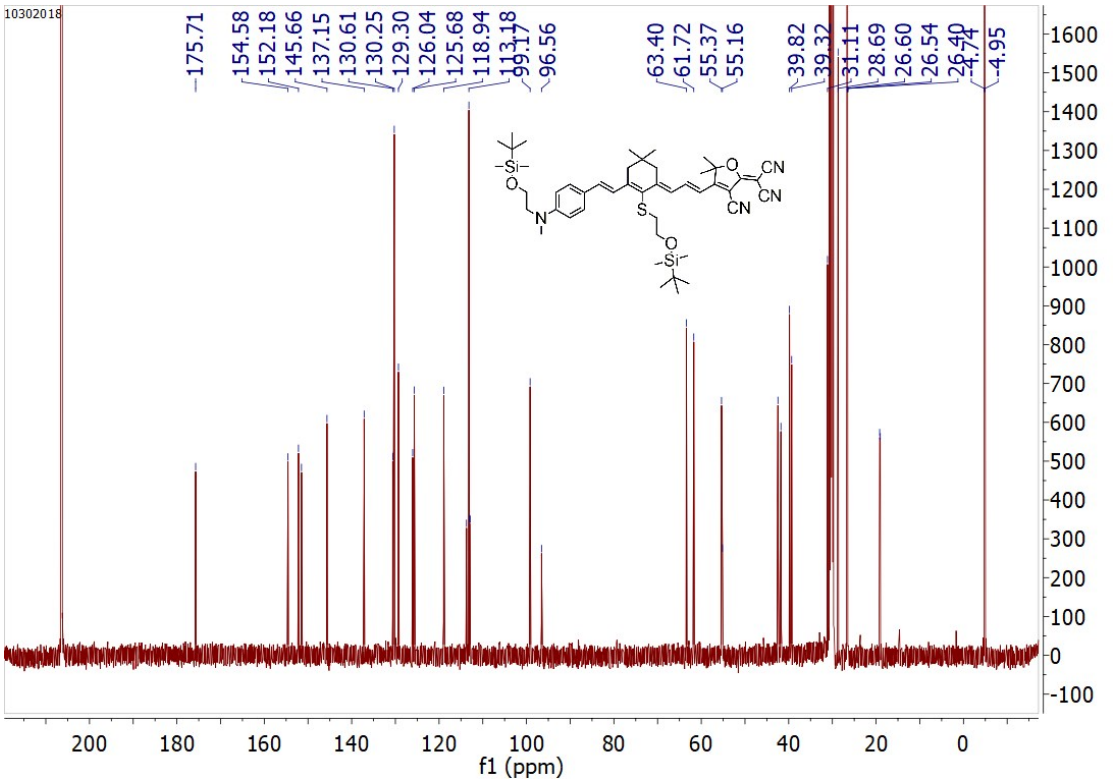

Figure S5 $^{13}C\{^{1}H\}$ NMR spectra of Chromophore A

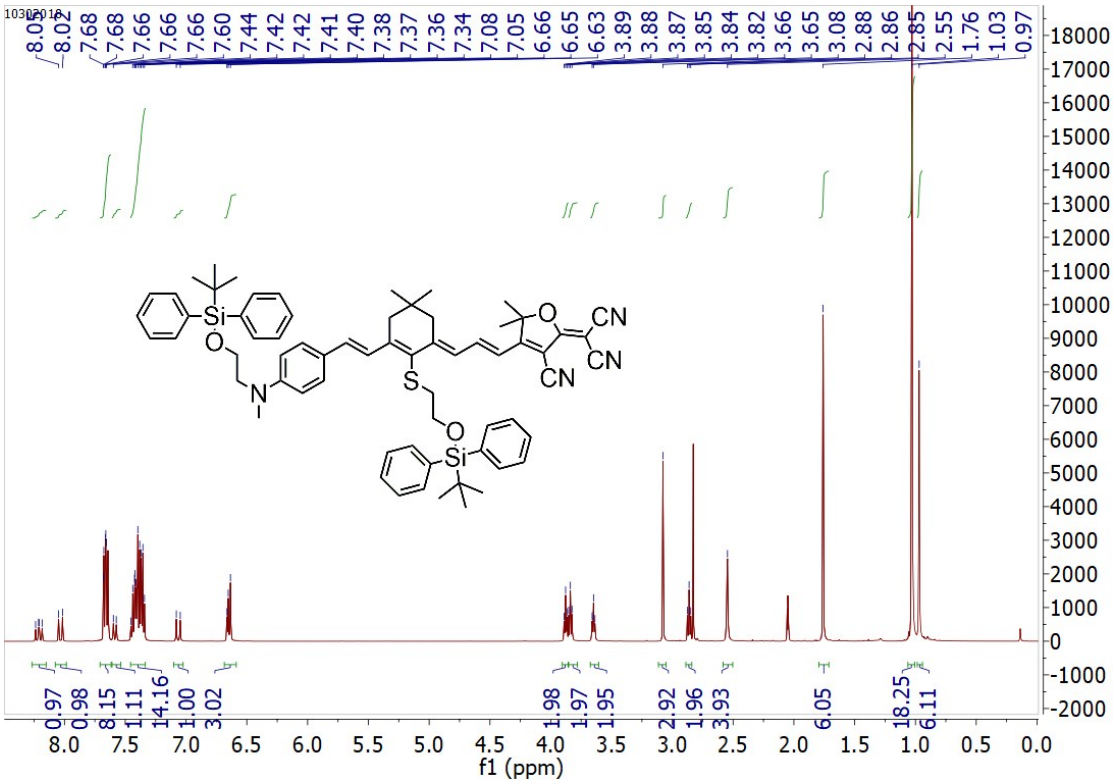

Figure S6 ^{1}H NMR spectra of Chromophore B

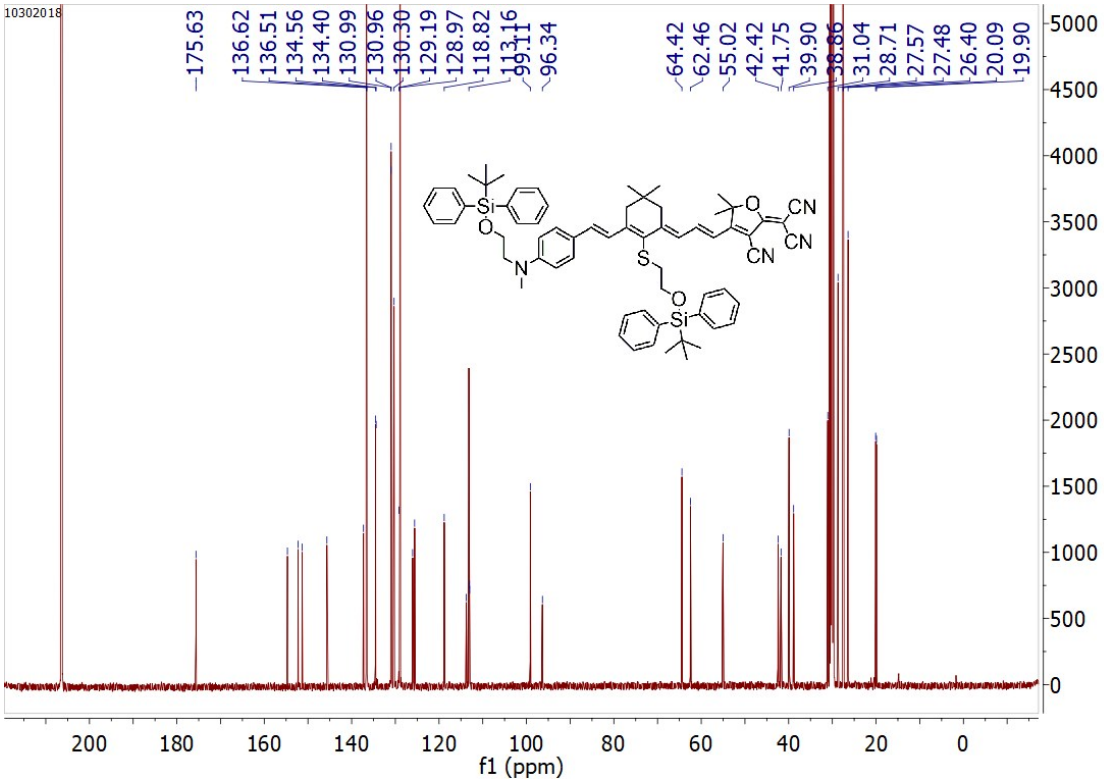

Figure S7 $^{13}C\{^{1}H\}$ NMR spectra of Chromophore B

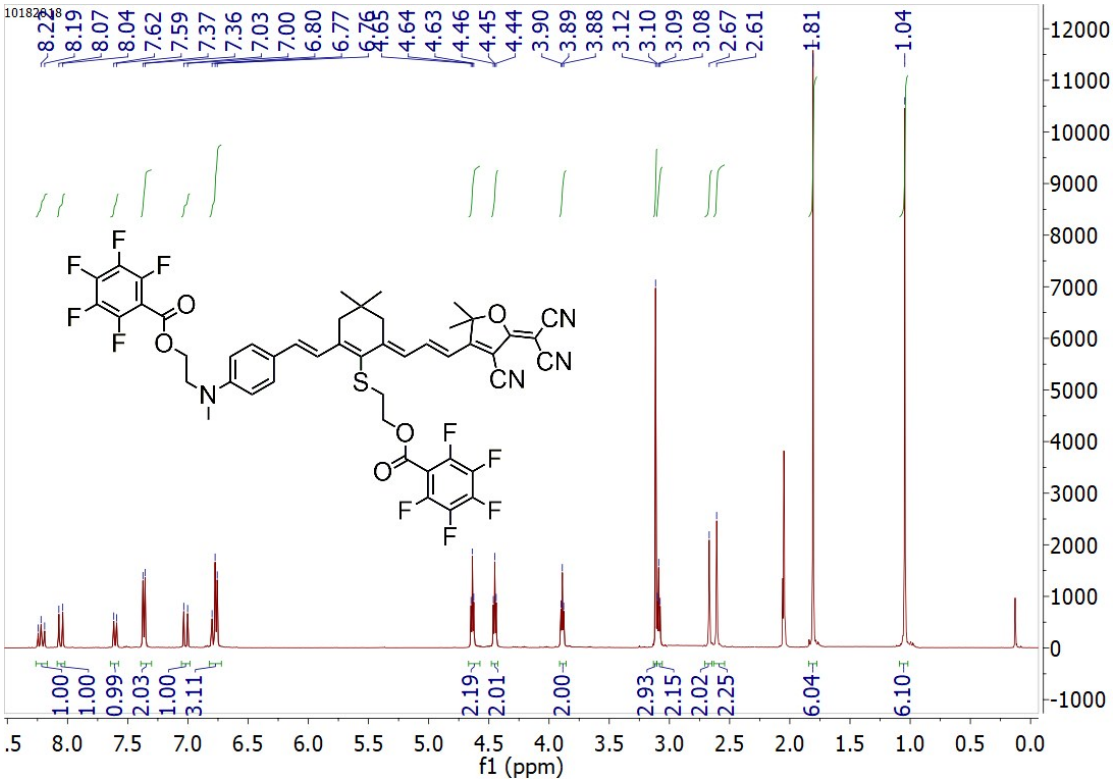

Figure S8 ^{1}H NMR spectra of Chromophore C

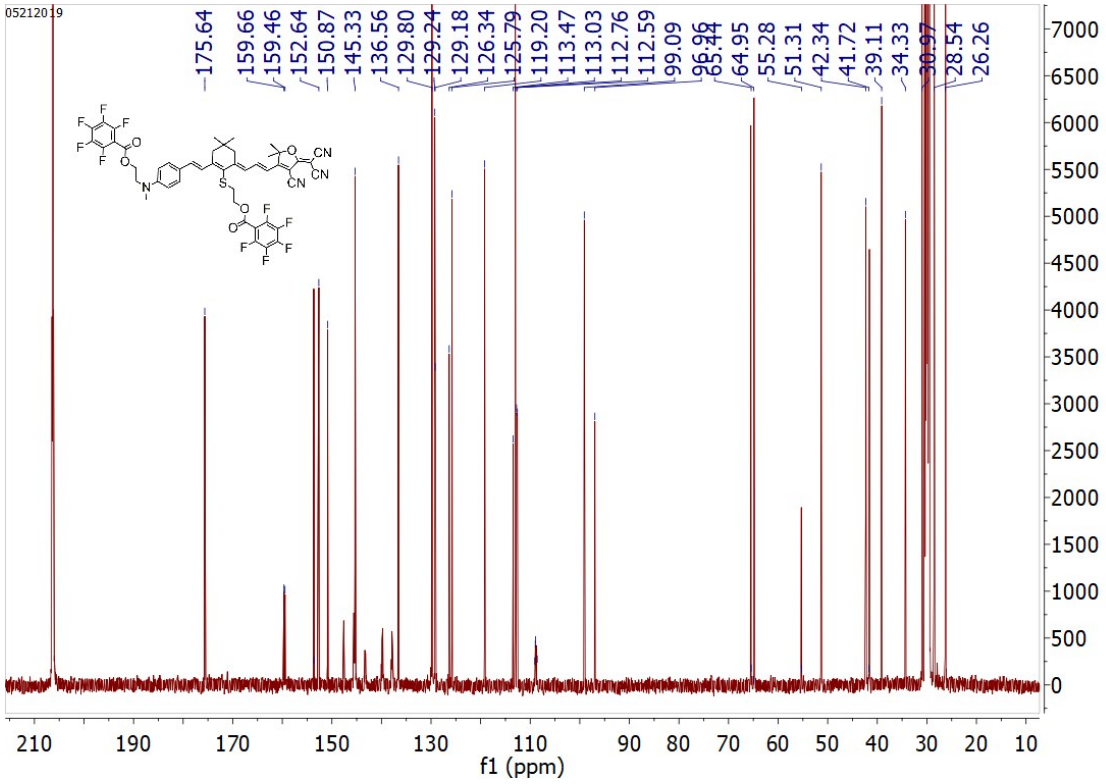

Figure S9 $^{13}C\{^{1}H\}$ NMR spectra of Chromophore C

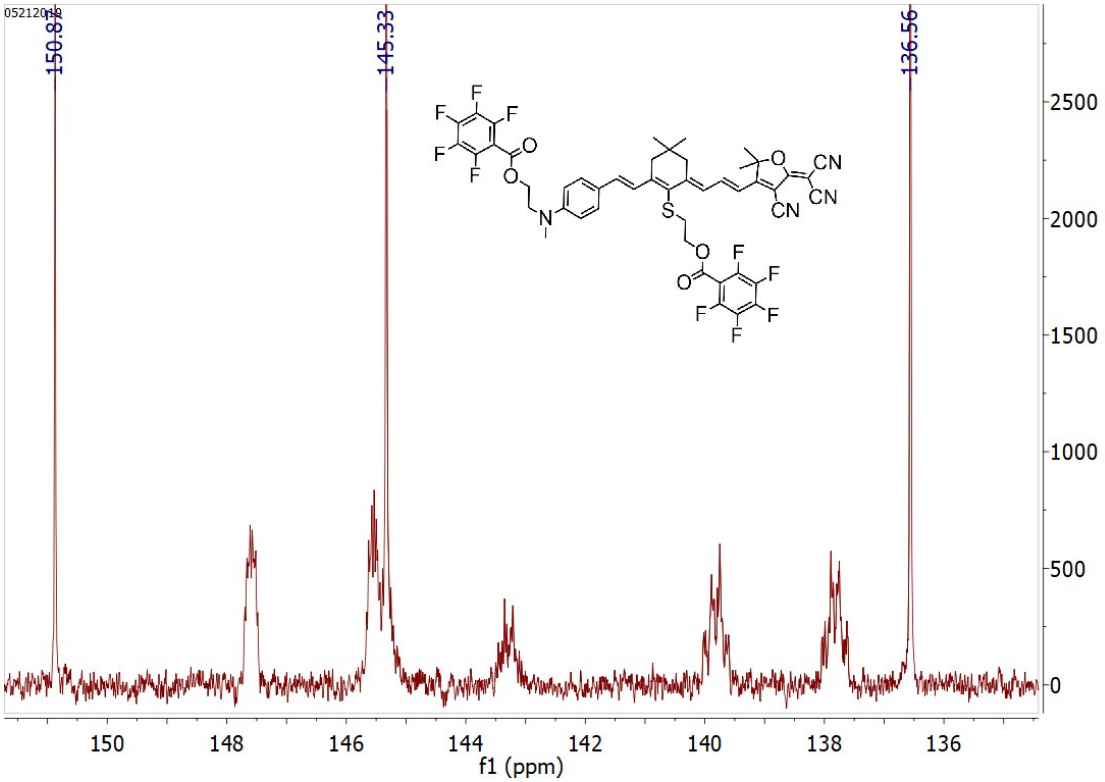

Figure S10 $^{13}C\{^{1}H\}$ NMR spectra of Chromophore C (Partial view)

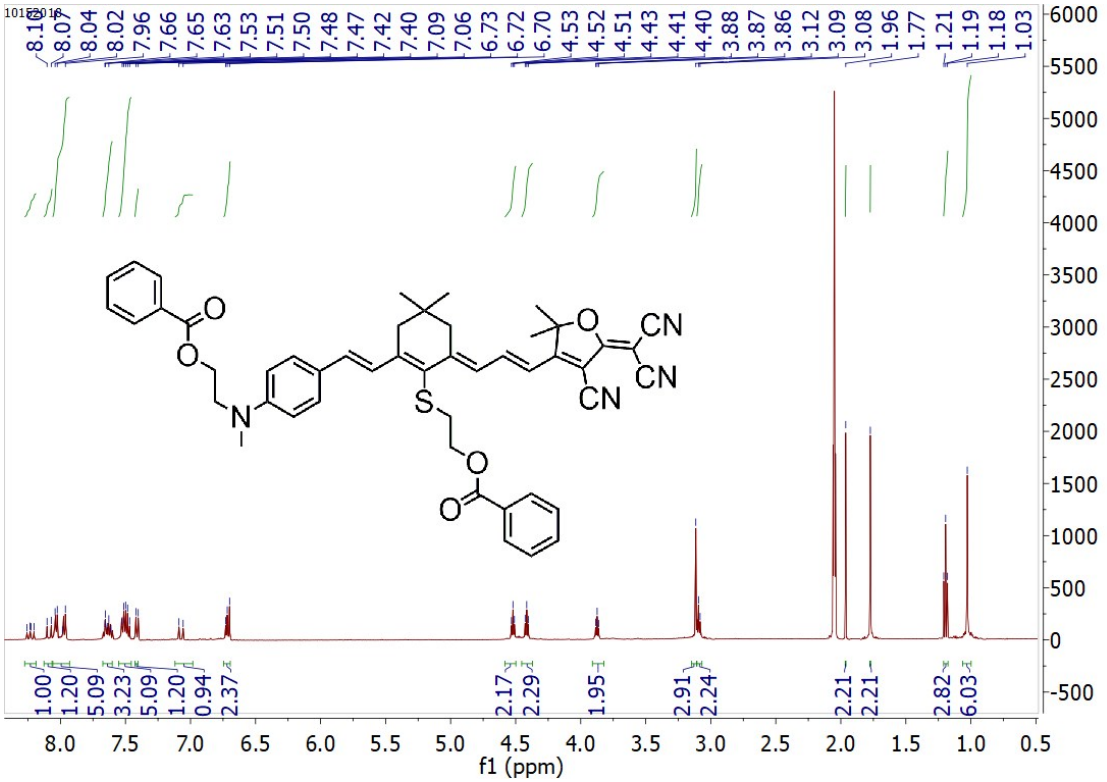

Figure S11 ^{1}H NMR spectra of Chromophore D

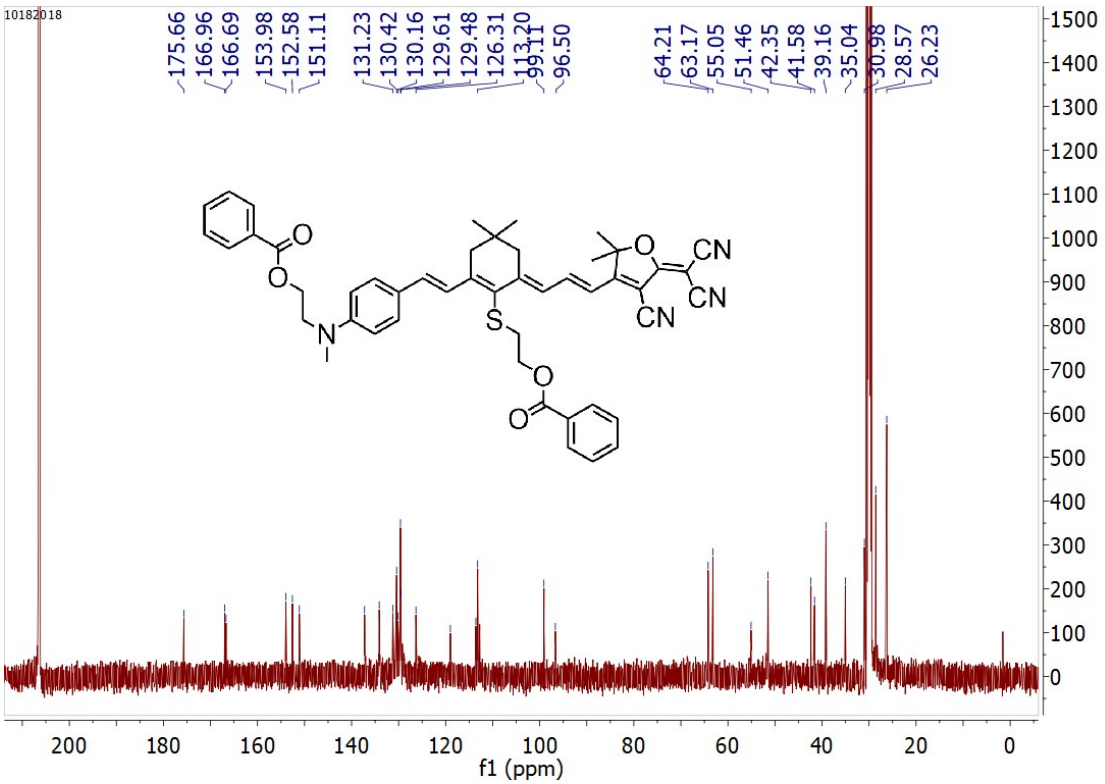

Figure S12 $^{13}C\{^{1}H\}$ NMR spectra of Chromophore D

6. Structure of chromophores CLD1, 2 and 5 and electro-optic coefficients

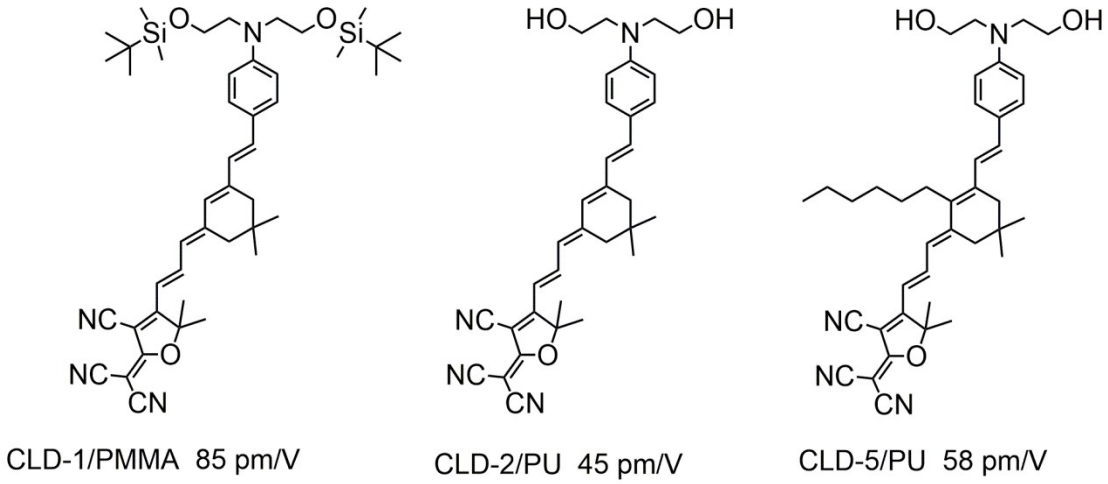

Figure S13 Structure of chromophores CLD1, 2 and 5 and electro-optic coefficients[1, 2]

1. C. Zhang, L. R. Dalton, M. C. Oh, H. Zhang and W. H. Steier, *Chemistry of Materials*, 2001, **13**, 3043-3050.
2. C. Zhang, C. G. Wang, J. L. Yang, L. R. Dalton, G. L. Sun, H. Zhang and W. H. Steier, *Macromolecules*, 2001, **34**, 235-243.