

Electronic supplementary information (ESI)

Synthesis and characterization of Y-shaped optical nonlinear chromophores with strong acceptor

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1. Optical properties

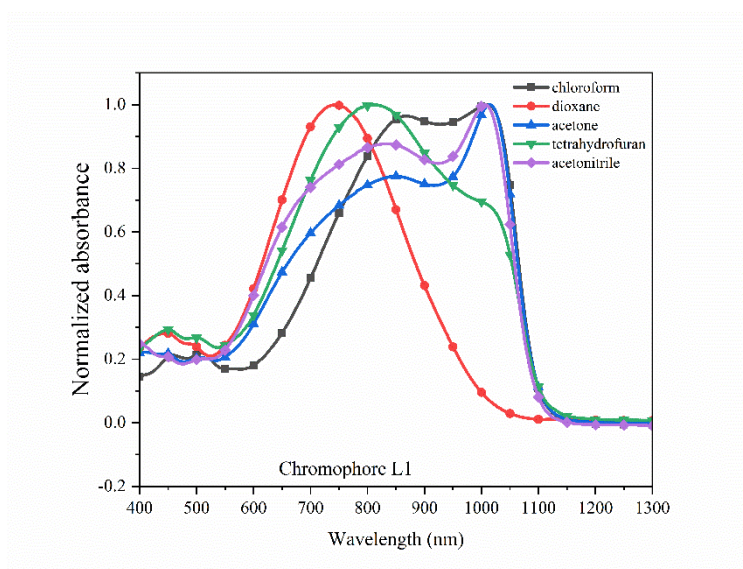


Figure S1 UV absorption spectra of chromophore L1 in solvents

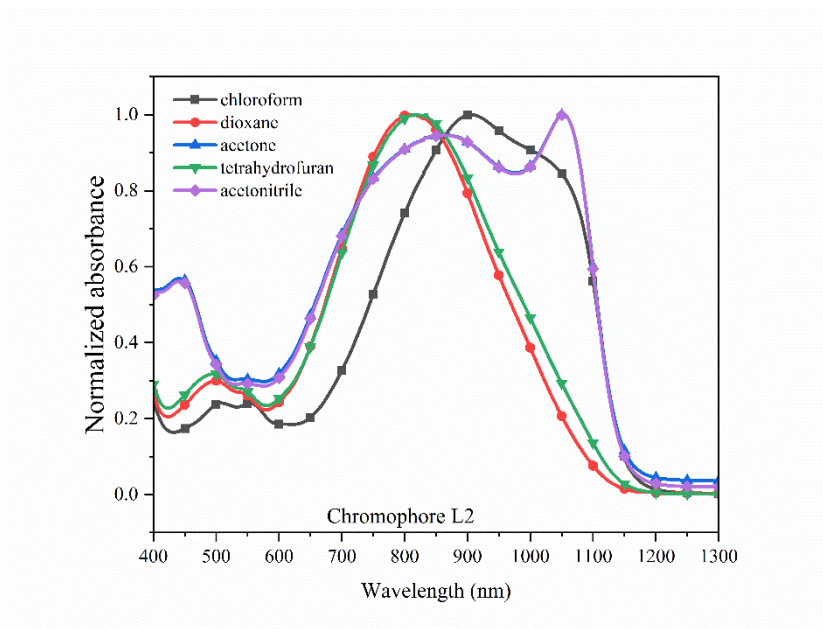


Figure S2 UV absorption spectra of chromophore L2 in solvents

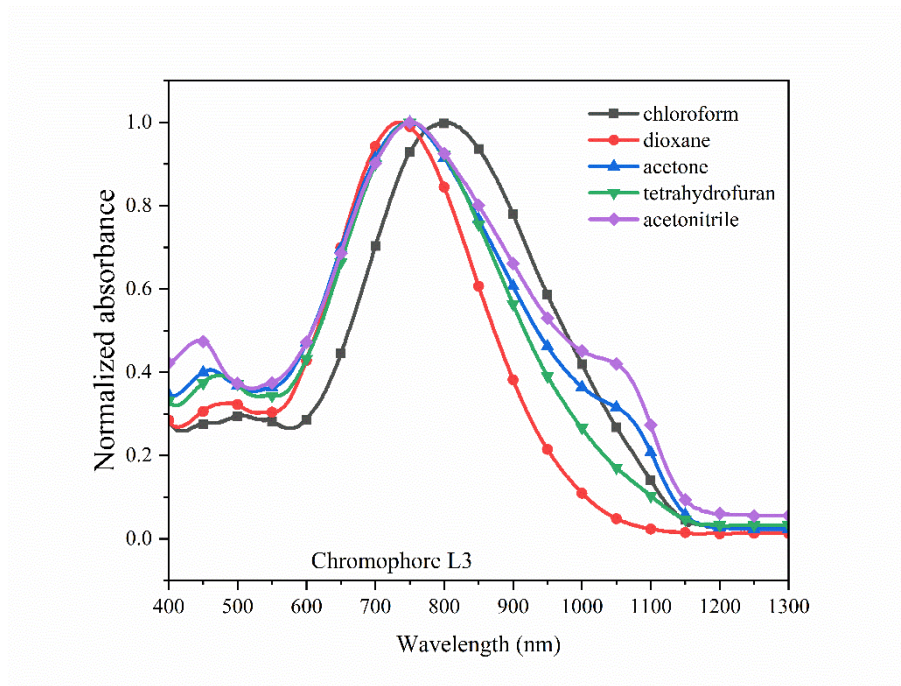


Figure S3 UV absorption spectra of chromophore L3 in solvents

2. Theoretical calculations

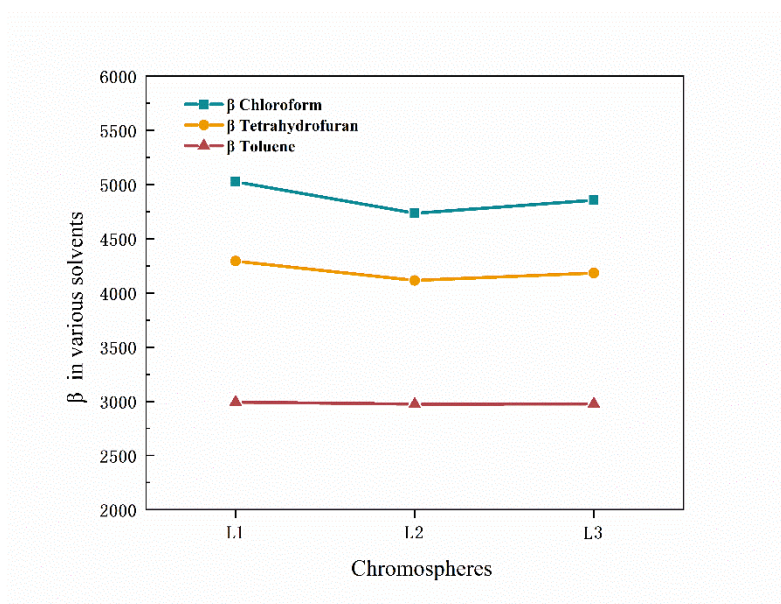


Figure S4. Hyperpolarizability in toluene, chloroform and tetrahydrofuran solution for chromophores L1-L3 calculated by DFT (M062X/6-31+G(d))

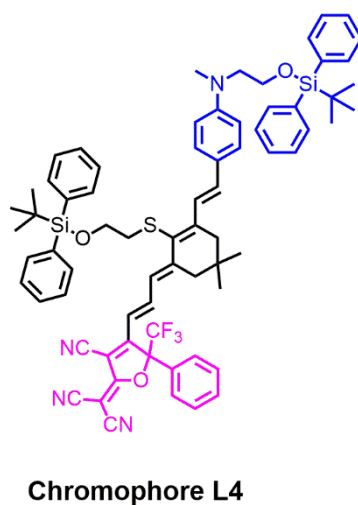


Figure S5. Chemical structure of monodonor chromophore L4

Table S1 Summary of DFT and EO coefficients of chromophores

| Cmpd | $\Delta E(\text{DFt})$ ^a (eV) | μ^b (D) | Cam ^c | Chl ^d | Thf ^e | Tol ^f | max.r ₃₃ (pm/V) |
|-----------|---|----------------|------------------|------------------|------------------|------------------|-------------------------------|
| L4 | 3.77 | 21.15 | 987 | 3077 | 2661 | 1911 | 173 |

^a calculated from DFT calculations. ^b the total dipole moment. ^{cdef} First order hyperpolarizability calculated in vacuum, Chloroform, Tetrahydrofuran and Toluene, respectively.

3. ^1H and ^{13}C NMR spectra

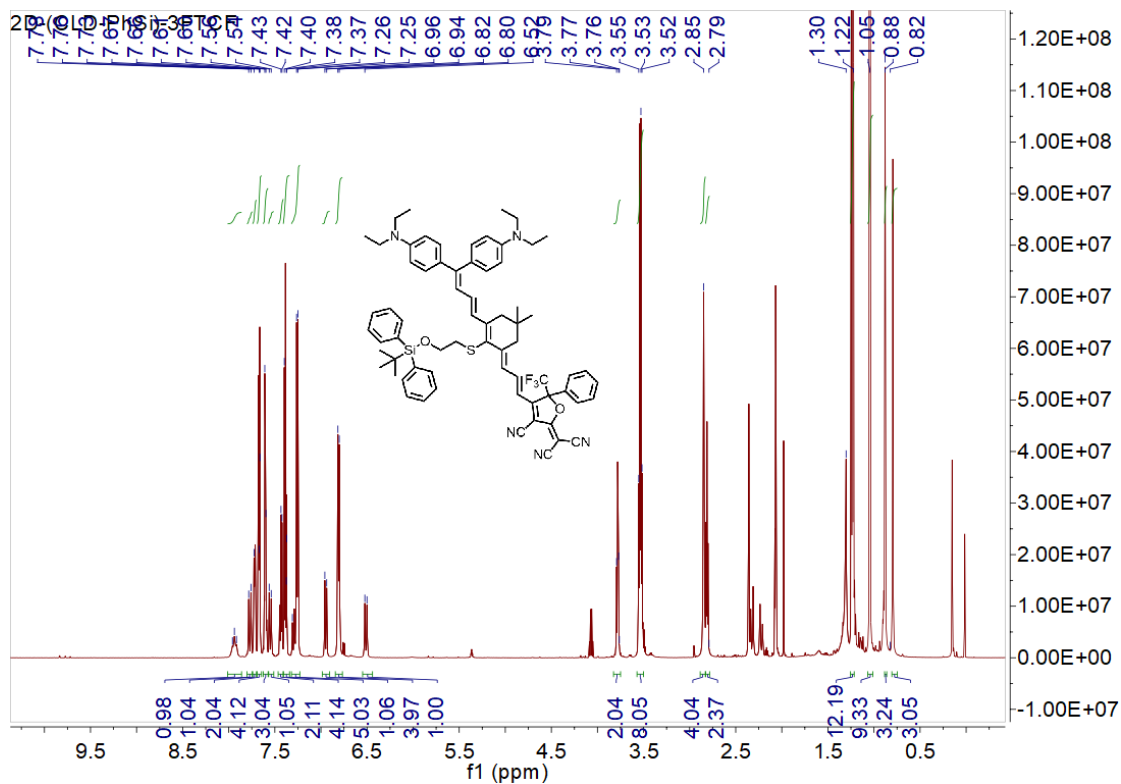


Figure S6. ^1H NMR spectra of chromophore L1

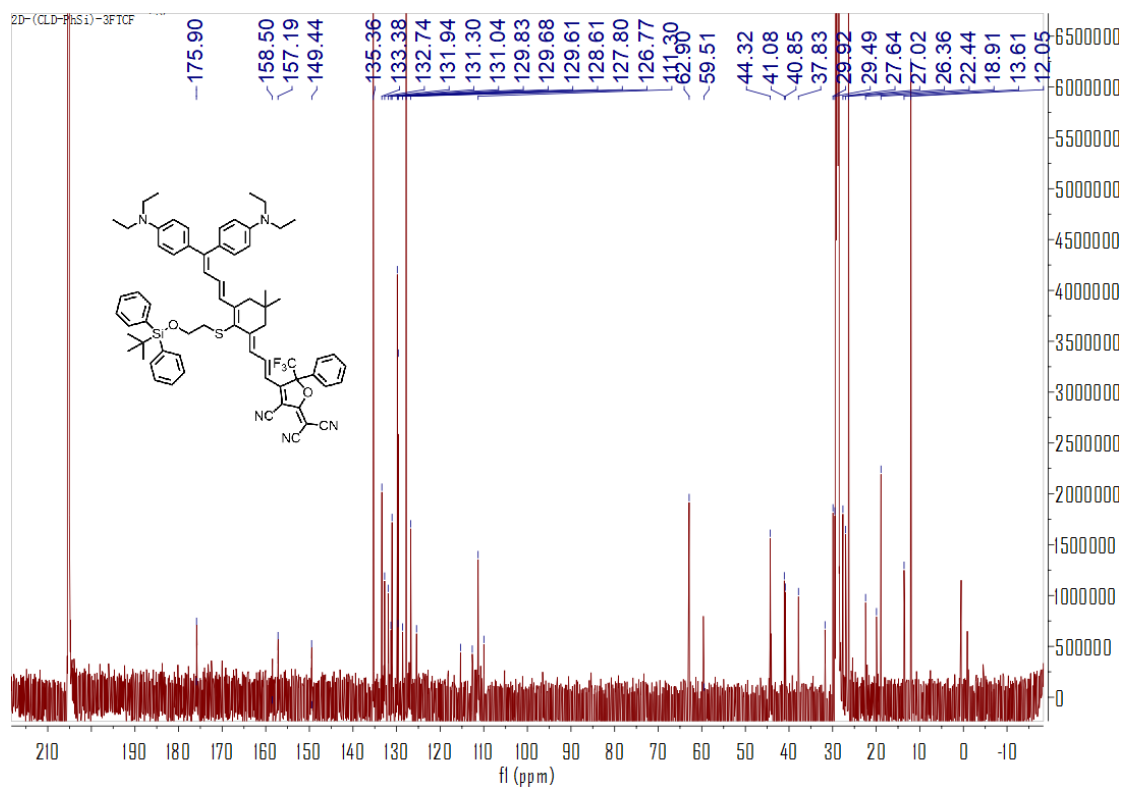


Figure S7. ^{13}C NMR spectra of chromophore L1

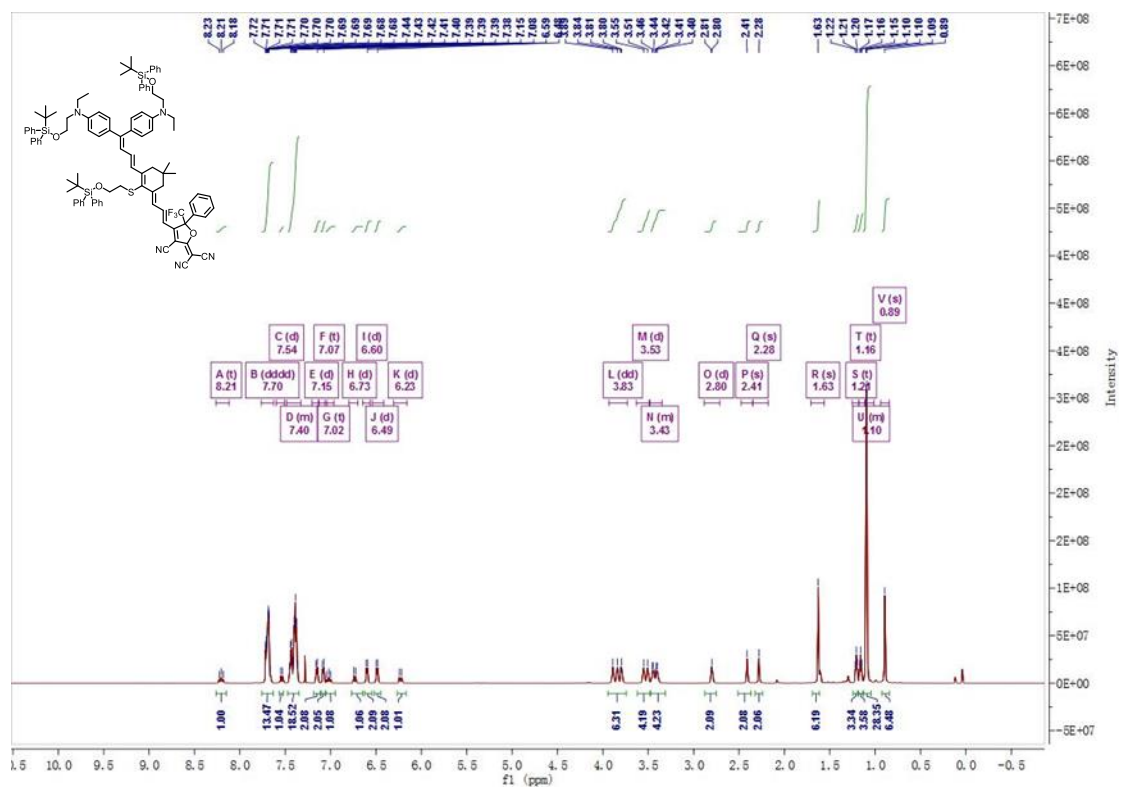


Figure S8. ¹H NMR spectra of chromophore L2

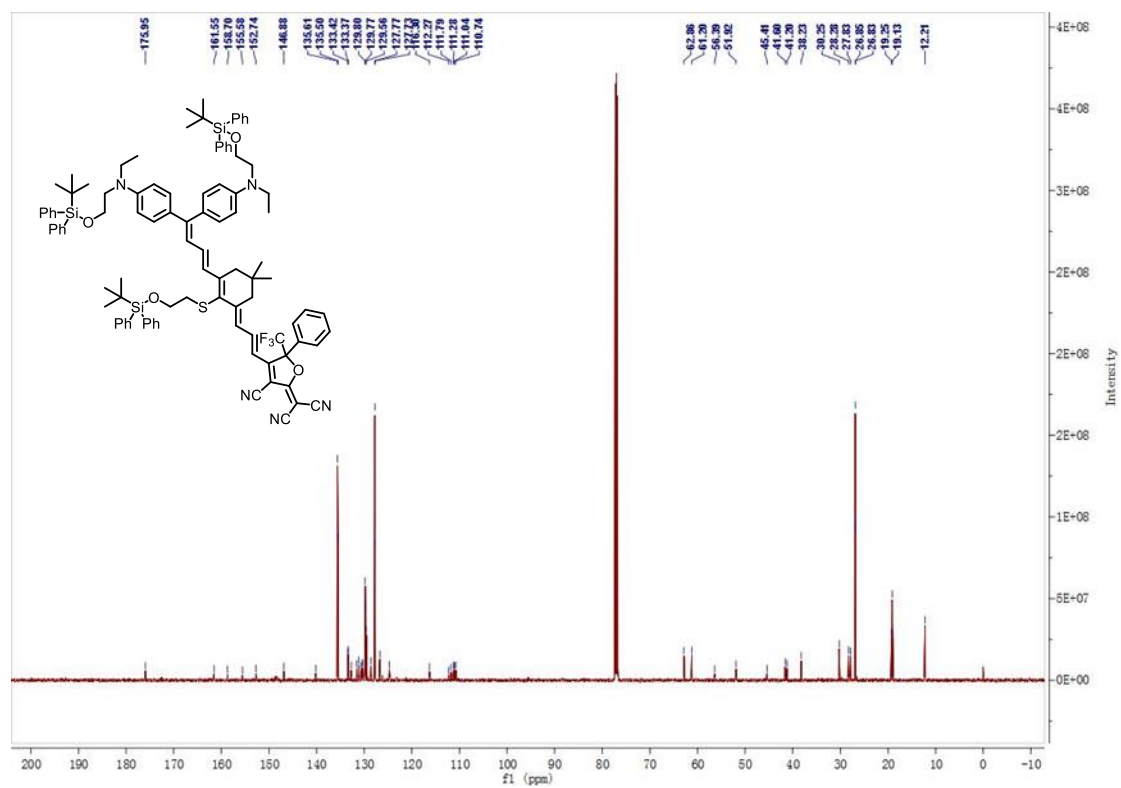


Figure S9. ¹³C NMR spectra of chromophore L2

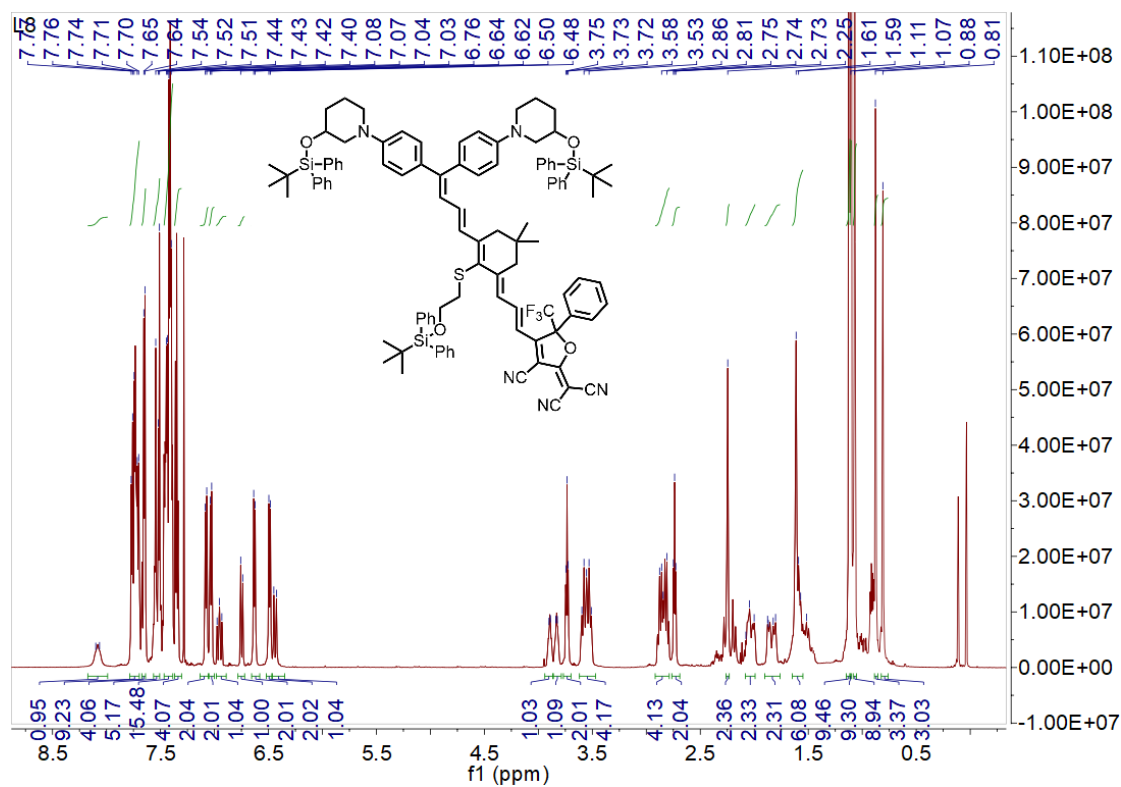


Figure S10. ^1H NMR spectra of chromophore L3

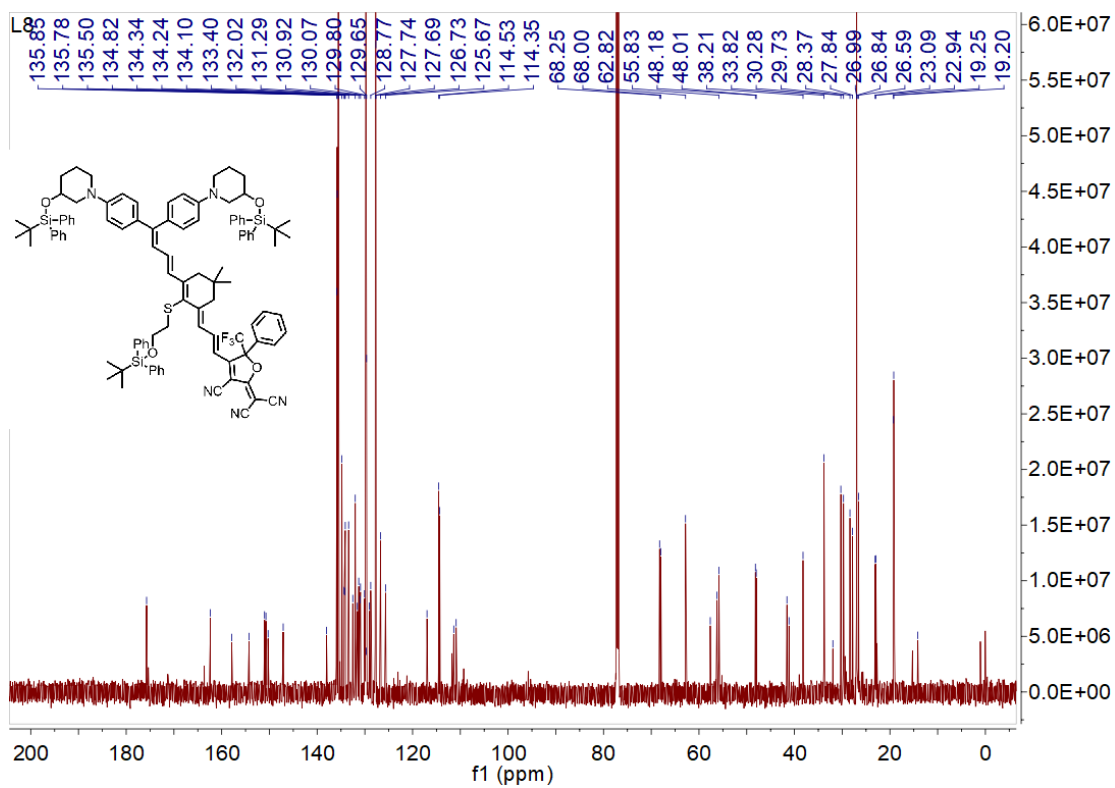


Figure S11. ^{13}C NMR spectra of chromophore L3

4. Poling and electro-optical coefficient parameters of chromophores

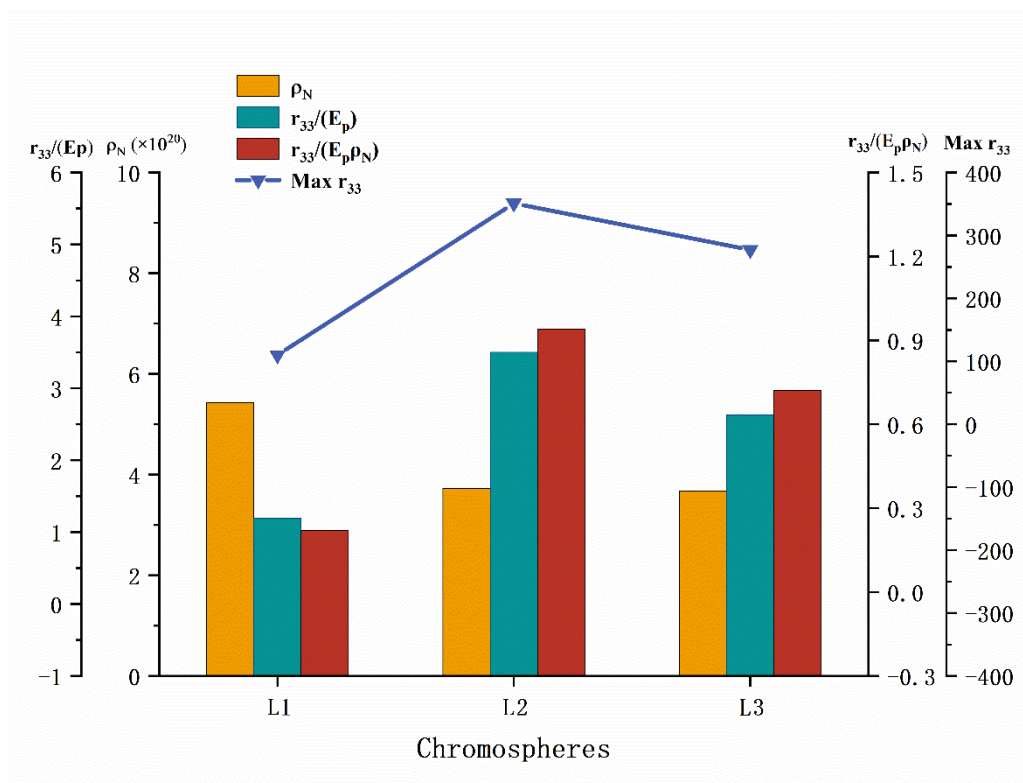


Figure S12. The Number density, Poling efficiency and Maximum electro-optic coefficient of chromophores L1-L3.