

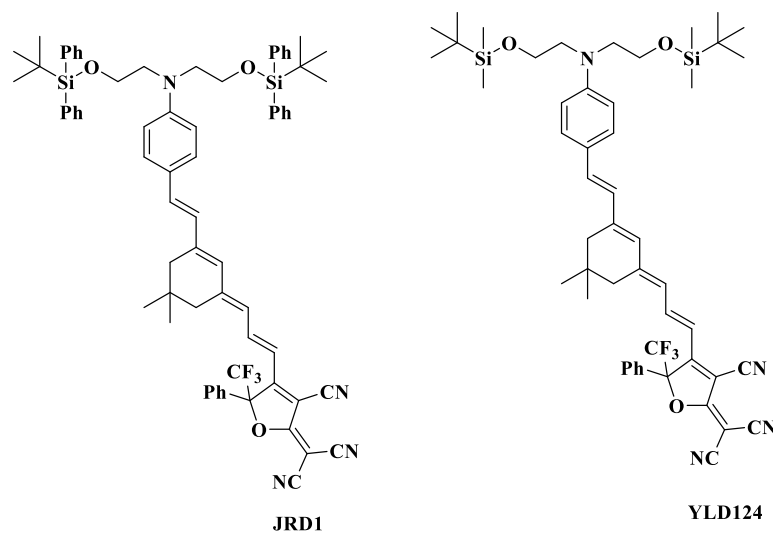
Modifiable Double donor based on Bis(N-Ethyl-N-hydroxyethyl)aniline for Organic optical nonlinear Chromophores

Qingzhu Zeng^a, Xunyu Chen^a, Abdul Rahman^{a*}, Ziying Zeng^a, Zhiwei Liang^a, Lei Shi^a, Zeling Huang^a, Shuhui Bo^b, Fenggang Liu^{a**} and Jiahai Wang^{a***}

^aSchool of Chemistry and Chemical Engineering, Guangzhou University, Guangzhou 510006, P. R. China. E-mail address: a.rahman.chemist@gmail.com, liufg6@gzhu.edu.cn ;
jjiahaiwang@gzhu.edu.cn

^b Optoelectronics Research Centre, School of Science, Minzu University of China, Beijing, 100081, PR China.

1. Structure of YLD124, JRD1 and HLD1-2



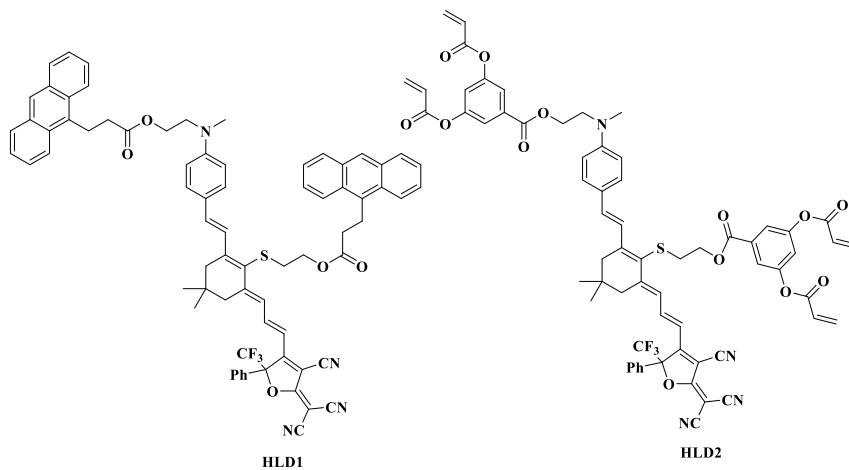


Figure S1. Structure of YLD124, JRD1 and HLD1-2

2. UV curves

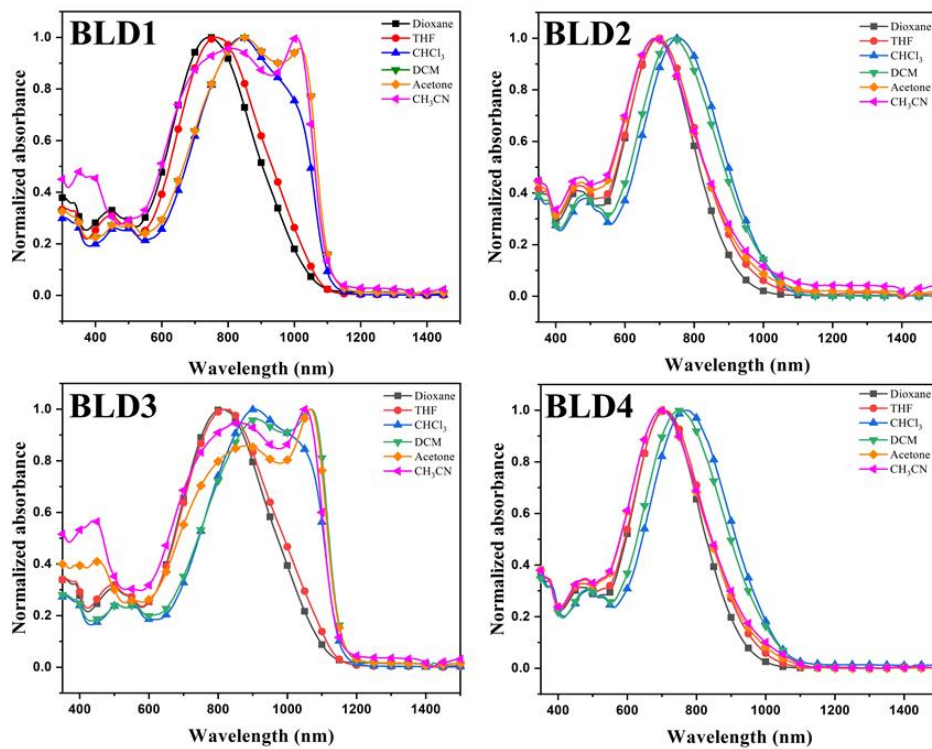


Figure S2. UV-Vis absorption spectra of chromophores BLD1-BLD4 in solvents

3. Optimized structures of chromophores

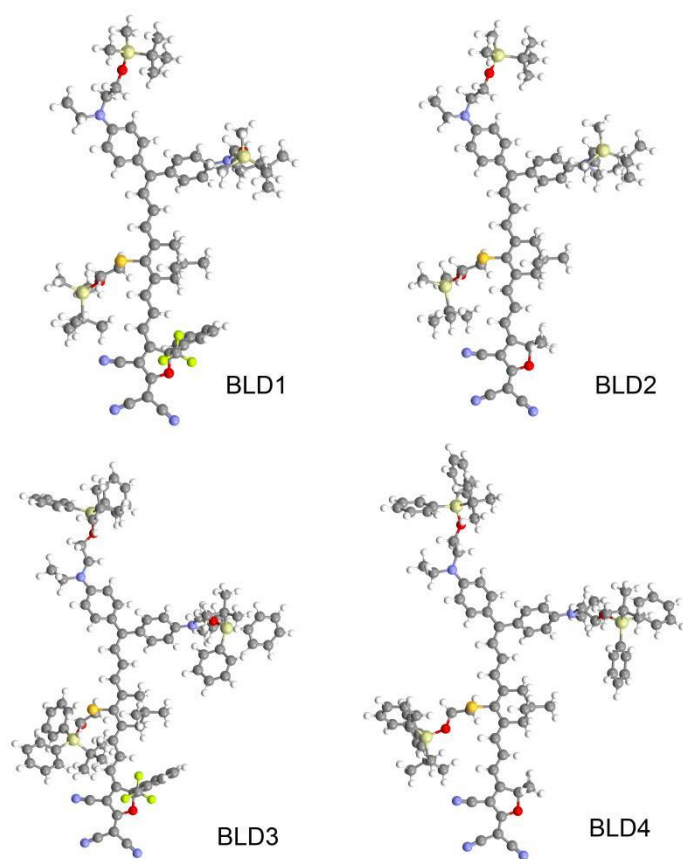


Fig. S3 Optimized structures of chromophores BLD1-BLD4.

4. ^1H and ^{13}C NMR spectra

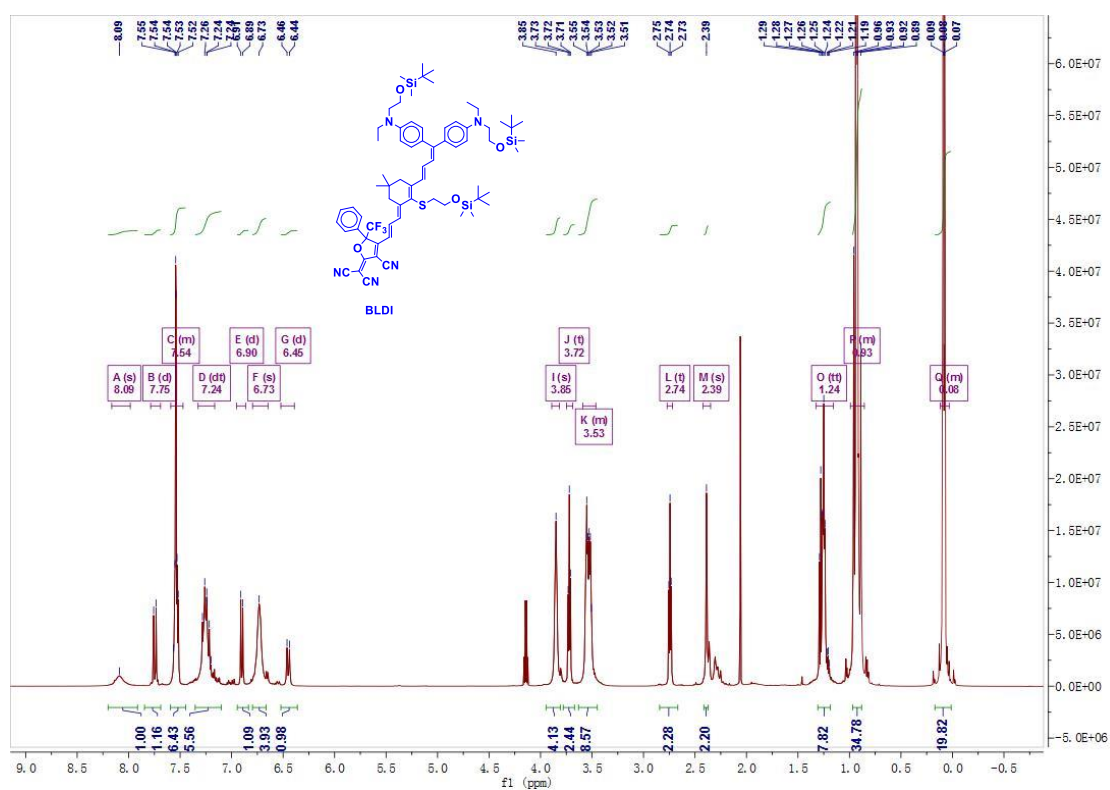


Figure S4 ^1H NMR spectra of Chromophore BLD1

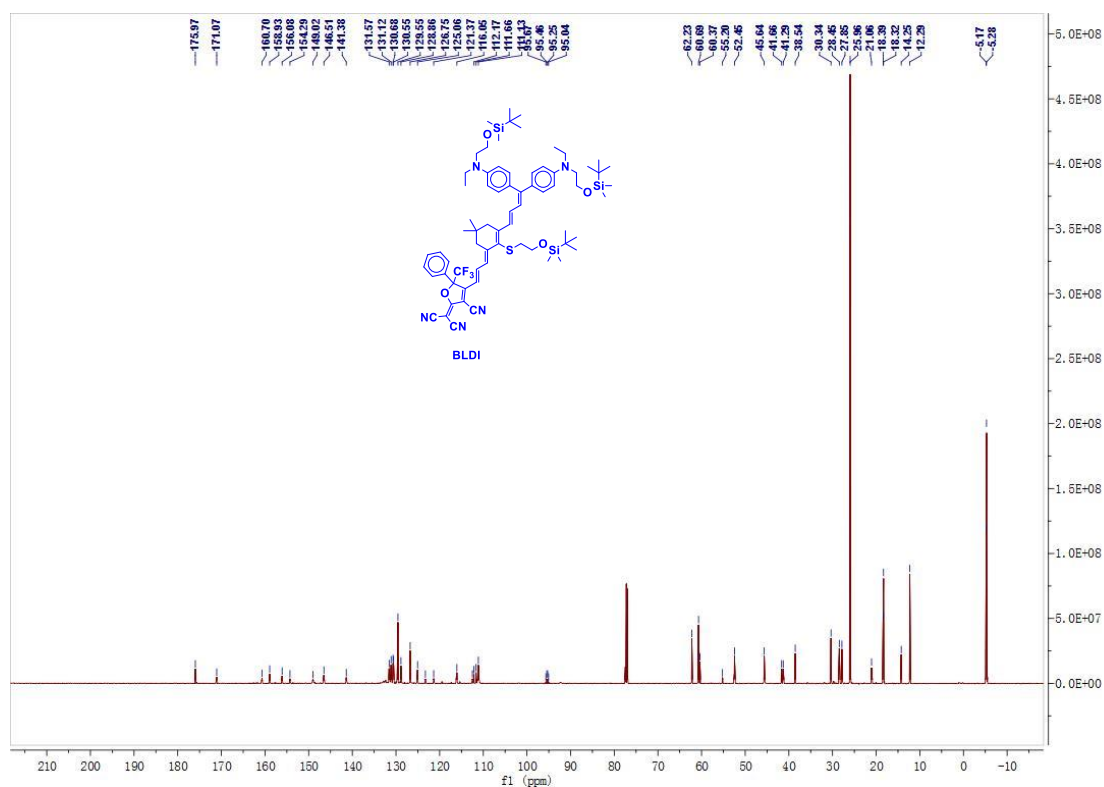


Figure S5 ^{13}C NMR spectra of Chromophore BLD1

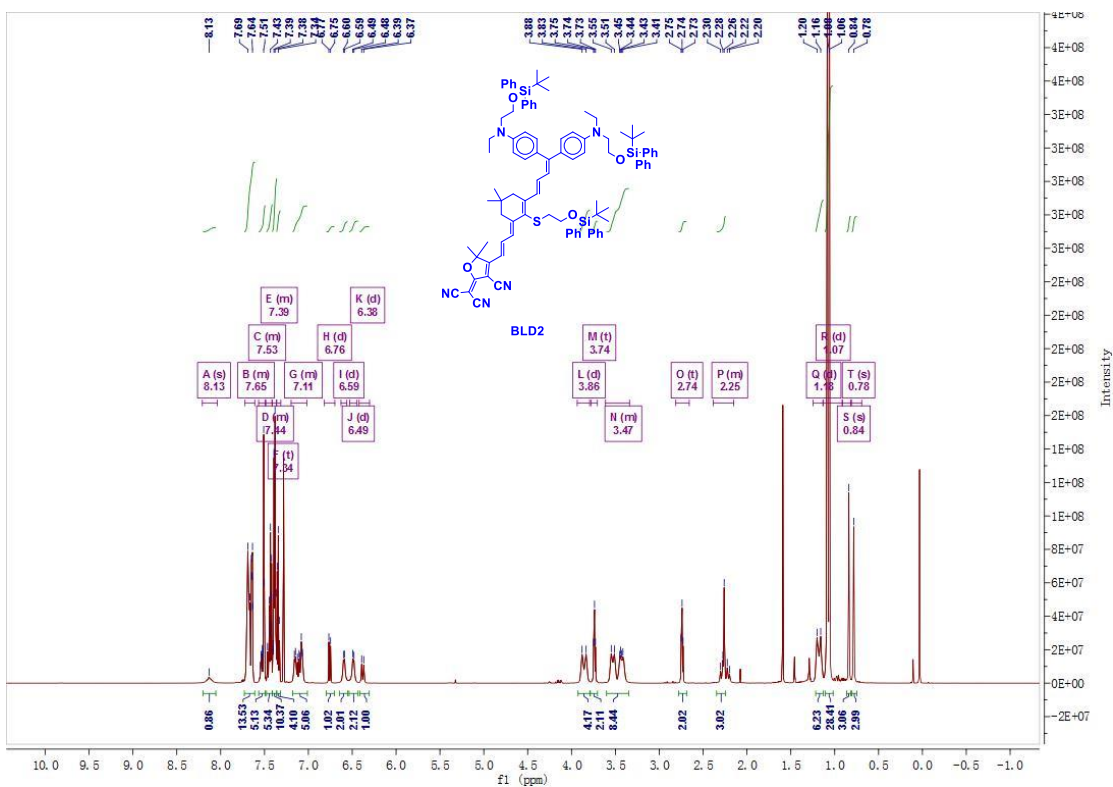


Figure S6 ^1H NMR spectra of Chromophore BLD2

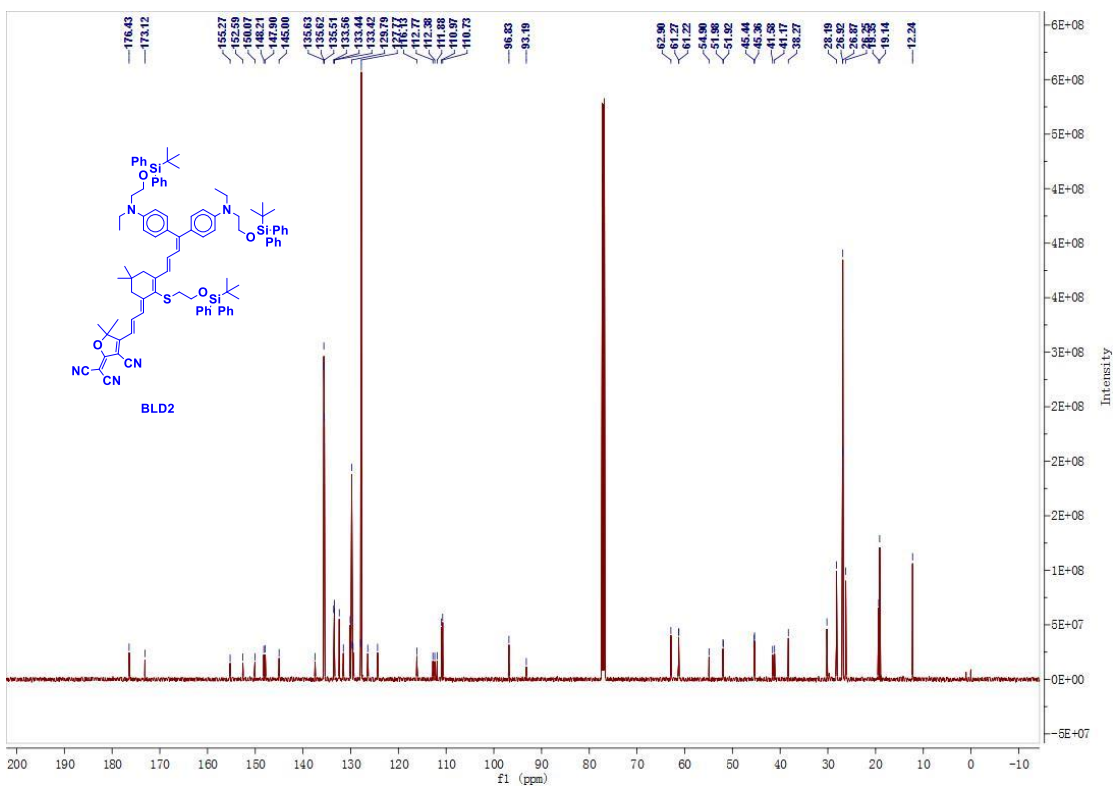


Figure S7 ^{13}C NMR spectra of Chromophore BLD2

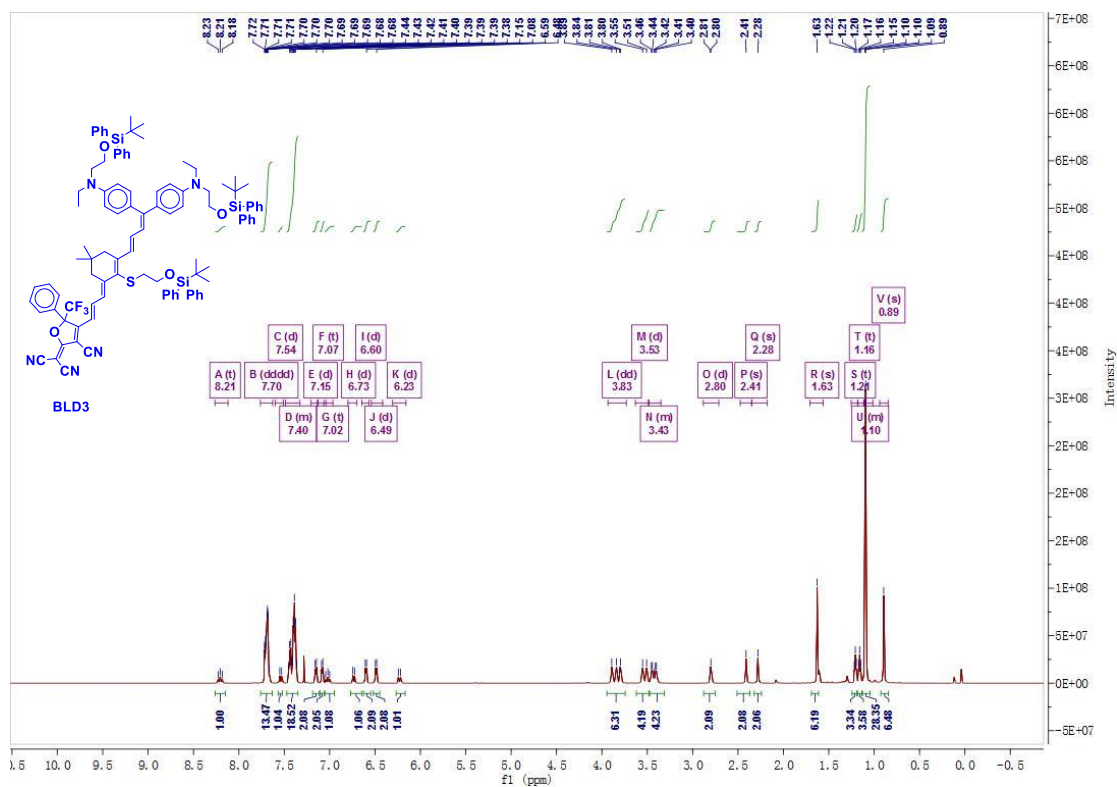


Figure S8 ^1H NMR spectra of Chromophore BLD3

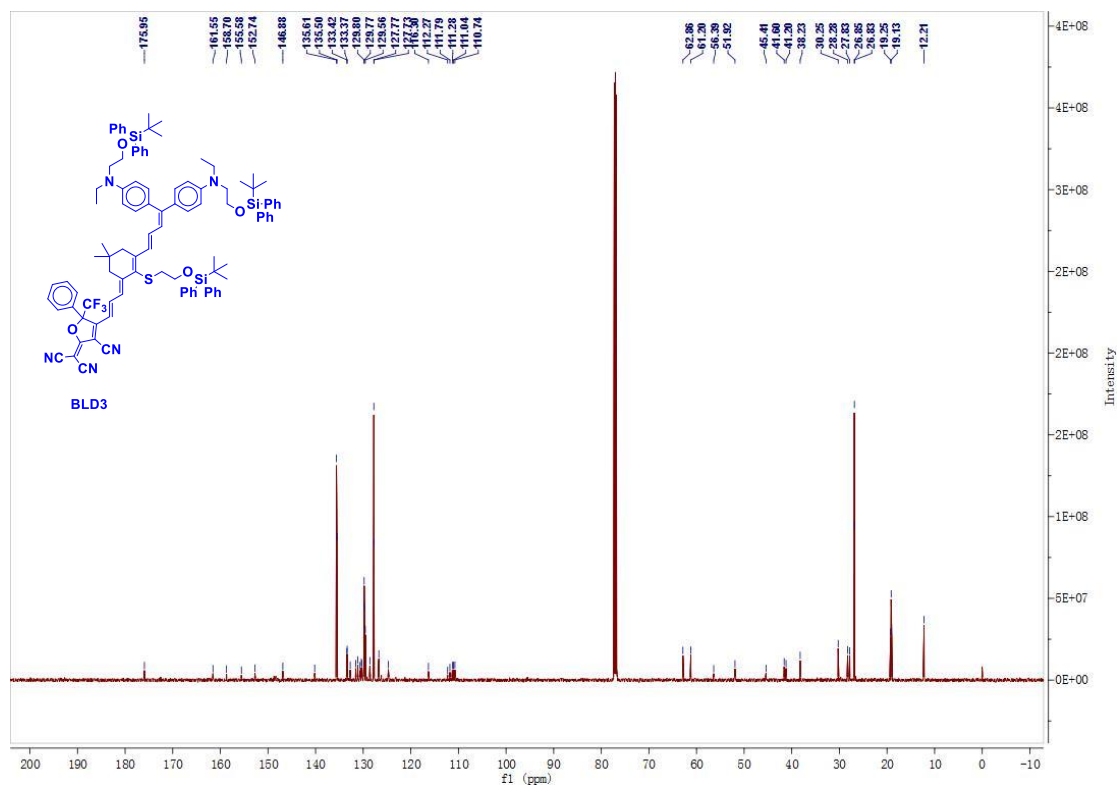


Figure S9 ^{13}C NMR spectra of Chromophore BLD3

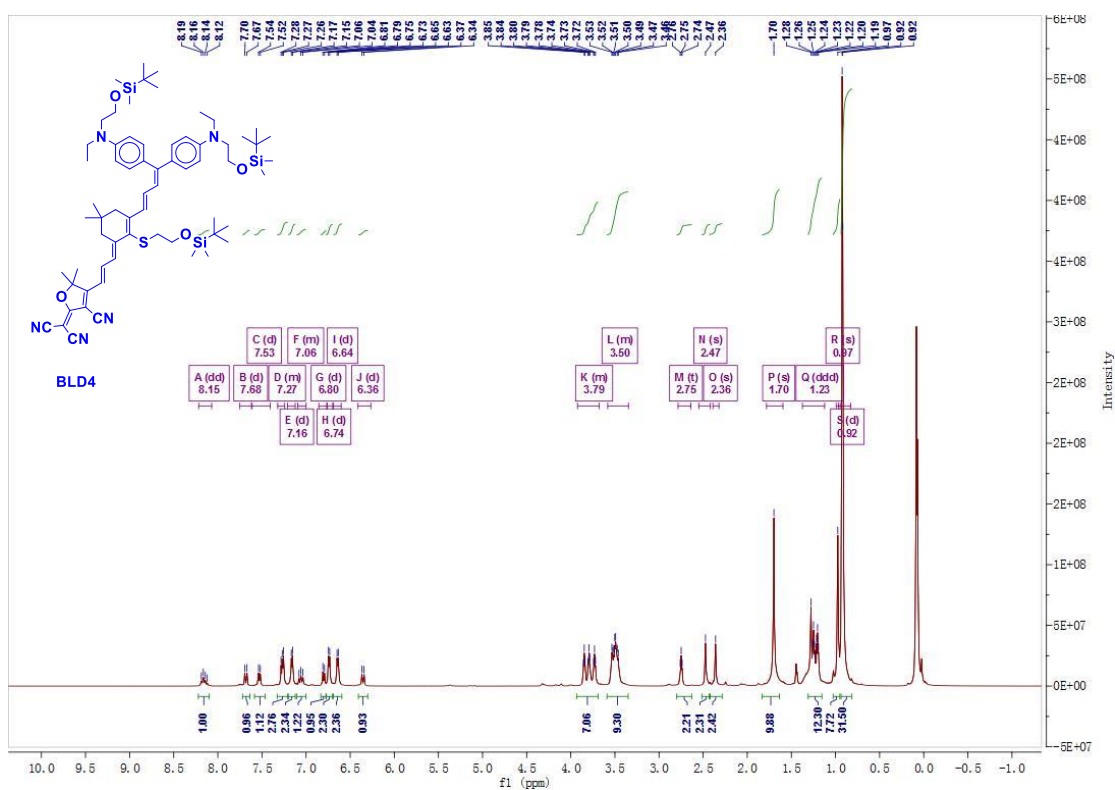


Figure S10 ^1H NMR spectra of Chromophore BLD4

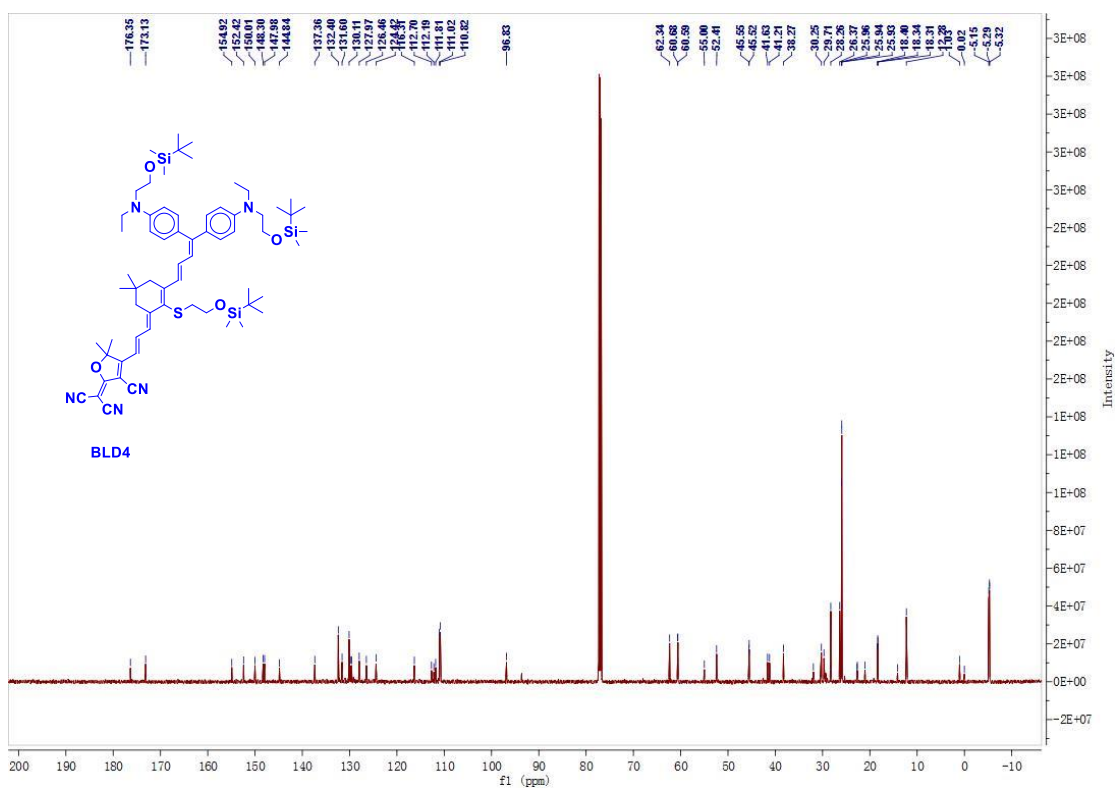


Figure S11 ^{13}C NMR spectra of Chromophore BLD4

5. DFT calculation and poling of the chromophore

Table S1 The M.O Composition (%) in the Ground State for Chromophores A-D

Cmpd	BLD1		BLD2		BLD3		BLD4	
	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO
donor	42.42%	14.48%	43.99%	14.40%	43.83%	14.41%	44.43%	15.41%
π bridge	39.67%	46.17%	40.14%	47.18%	37.86%	46.59%	38.47%	47.31%
acceptor	17.91%	39.35%	15.87%	38.42%	18.31%	38.99%	17.10%	37.28%

The molecular orbital composition was calculated using Multiwfn program with Ros-Schuit (SCPA) partition.

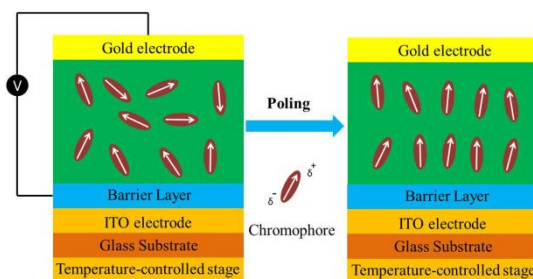


Figure S12 Artist's concept of poling process of EO chromophores BLD1-BLD4.

6. Future Directions.

Bis(*N-Ethyl-N-hydroxyethyl*)aniline-based group modified with two OH groups were designed to enhance the electron-donating ability of chromophores and provide the linking sites for further modification of the donor for the first time. At present, there are few modification sites for donors with strong electron donor ability. As shown in Fig.S13, through esterification, groups that can be self-assembled, cross-linked or click chemical reaction can be introduced into the three OH groups on the donor and electron bridge of the chromophores. Cross-Linkable Molecular Glasses, Self-assembled dendrimers or click-type postfunctionalization of Nonlinear Optical Materials with large electro-optic coefficients are expected.

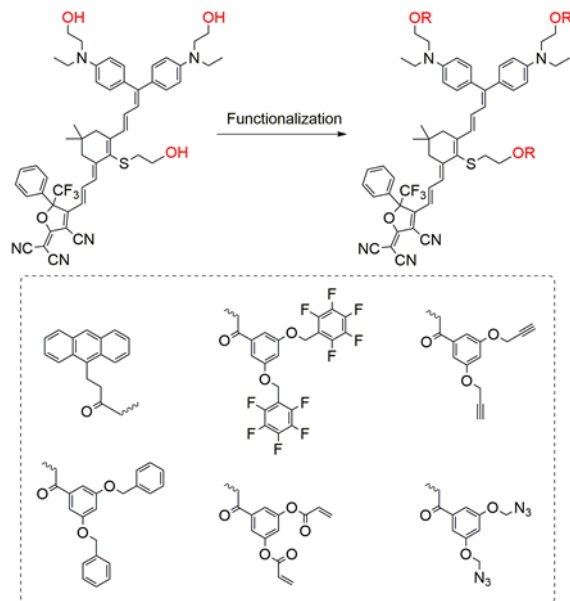


Figure S13 Functionalization of future BLD series chromophores