Electronic Supplementary Information (ESI)

Binaphthanol-based Organic Fluorophores with Color Tunability and Their Optical Properties

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Contents

1. Crystal data and structure refinement for **DB-5**.

Table 1 Crystal data and structure refinement for DB-5.

Empirical formula	$C_{36}H_{32}N_6O_4$
Formula weight	612.67
Temperature/K	169.98(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.3936(3)
b/Å	13.3227(4)
c/Å	14.5610(4)
α/°	70.316(2)
β/°	88.607(2)
γ/°	80.167(2)
Volume/Å^3	1689.51(9)
Z	2
ρ_{calc}g/cm^3	1.204
μ/mm^{-1}	0.652
F(000)	644.0
Crystal size/mm^3	0.312 × 0.305 × 0.213
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.45 to 150.946
Index ranges	$-10 \leq h \leq 11$, $-16 \leq k \leq 16$, $-18 \leq l \leq 18$
Reflections collected	18961
Independent reflections	6677 [R_{int} = 0.0155, R_{sigma} = 0.0134]
Data/restraints/parameters	6677/0/421
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0455, wR_2 = 0.1253
Final R indexes [all data]	R_1 = 0.0488, wR_2 = 0.1311
Largest diff. peak/hole / e Å^{-3}	0.68/-0.27

2. Supplemental figures

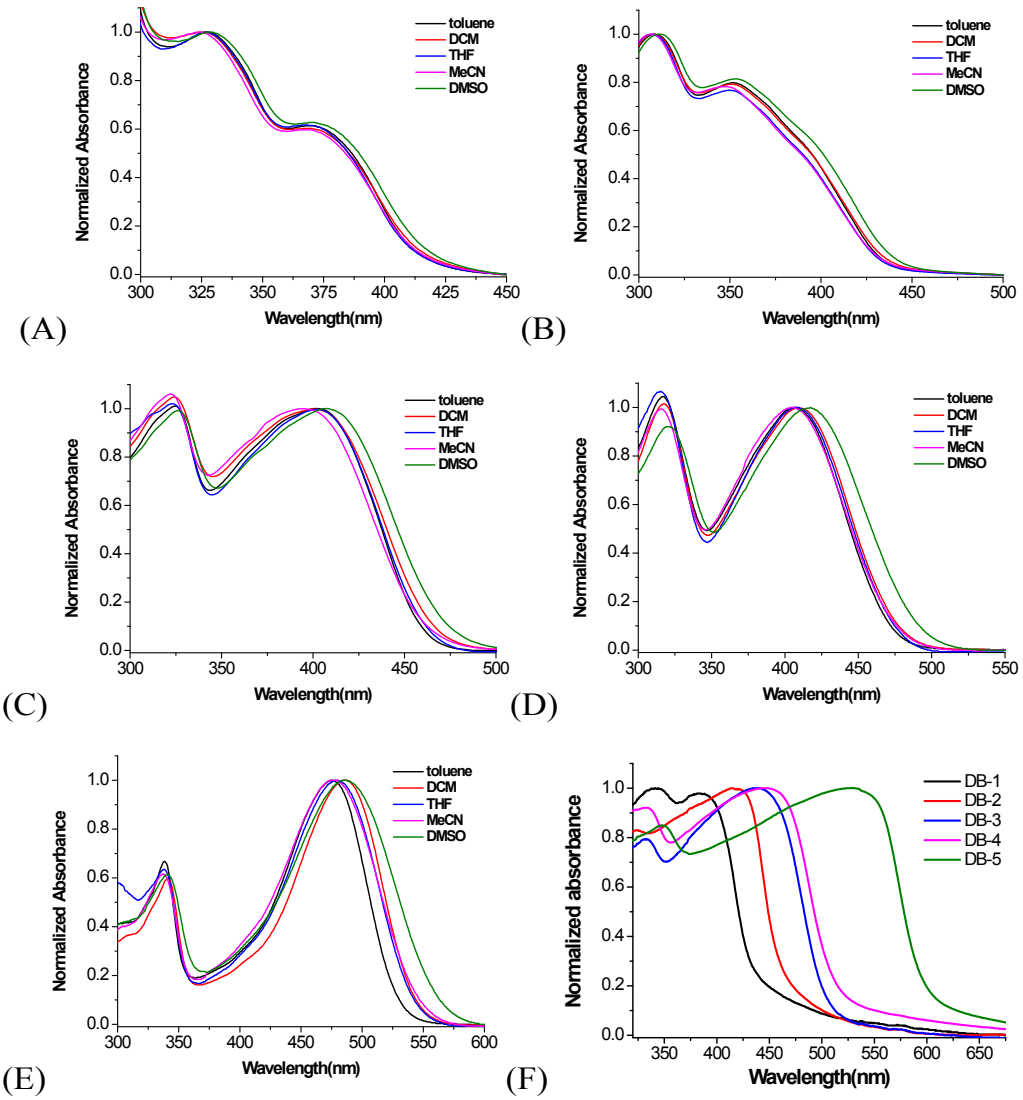
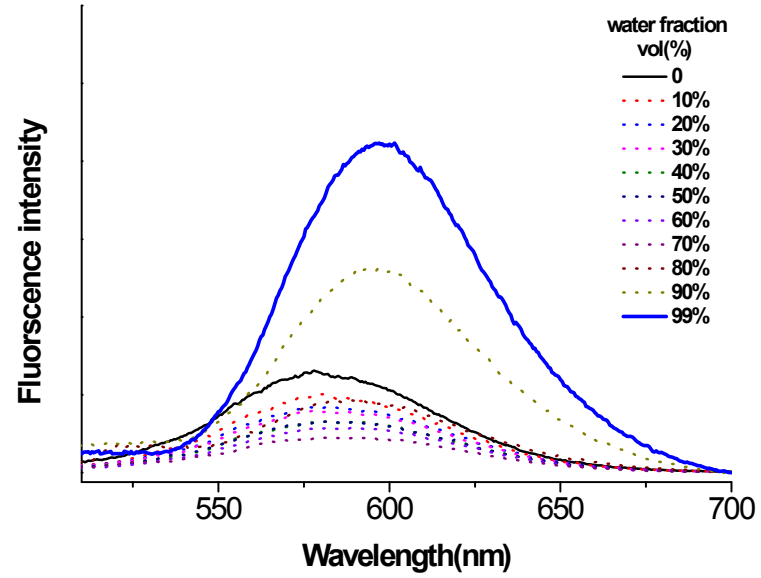
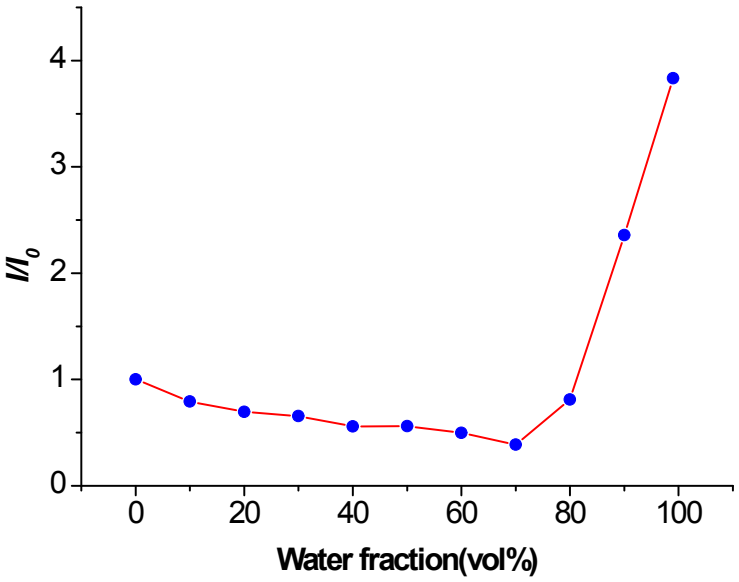


Fig. S1 Absorption spectra of **DB-1** (A), **DB-2** (B), **DB-3** (C), **DB-4** (D), **DB-5** (E) in different solvents (concentration = 10 μM). Absorption spectra (F) of **DB-1**-**DB-5** in solid states.

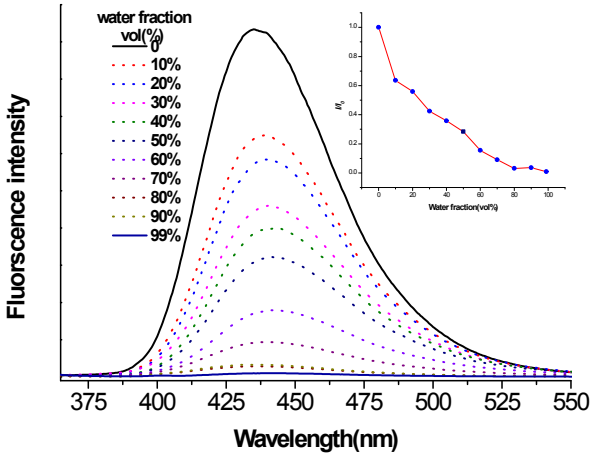


(A)

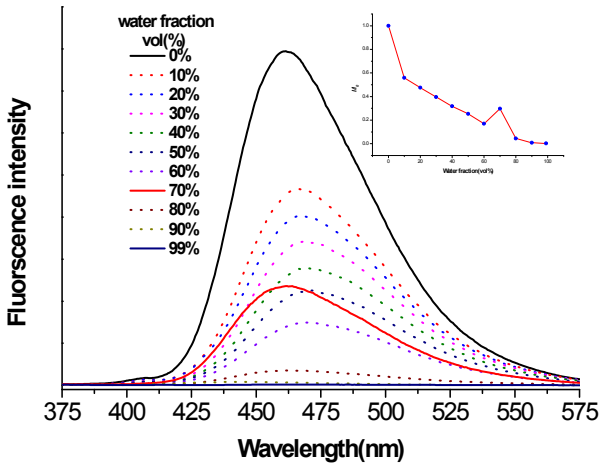


(B)

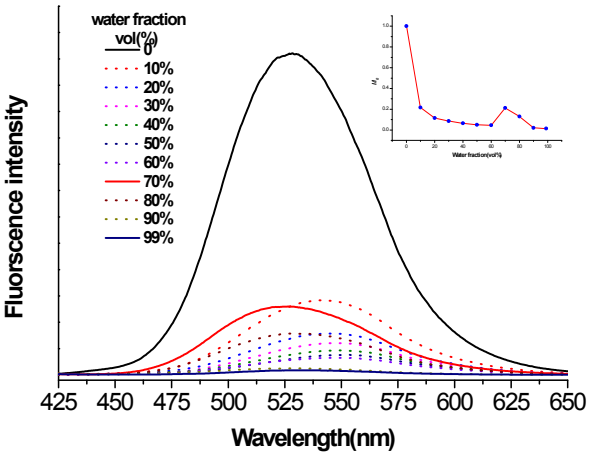
Fig. S2 (A) PL spectra of **DB-5** in MeCN-water mixtures with different water fractions; λ_{ex}: 480 nm, concentration: 10 μM. (B) Changes in the PL intensity of **DB-5** in MeCN-water mixtures with different water fractions.



(A)

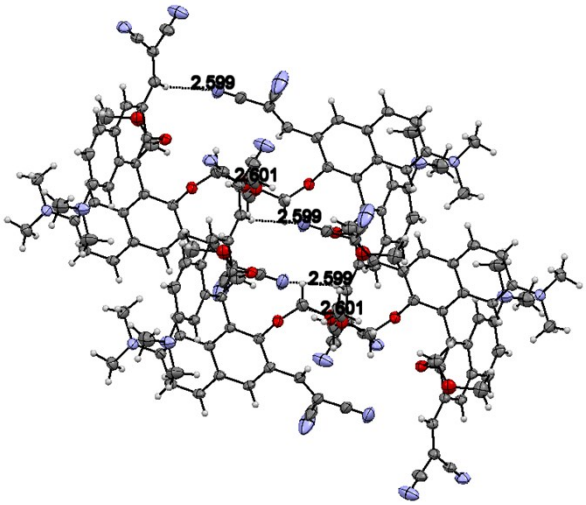


(B)

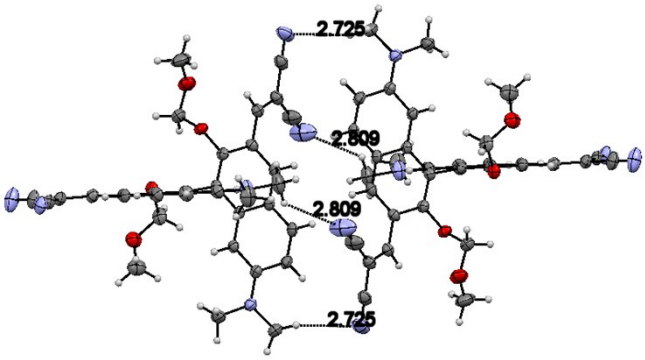


(C)

Fig. S3 PL spectra of **DB-1** (A)**, DB-2** (B)**, DB-3** (C) in MeCN-water mixtures with different water fractions; concentration: 10 μM. Inserted images are changes in the PL intensity in MeCN-water mixtures with different water fractions.

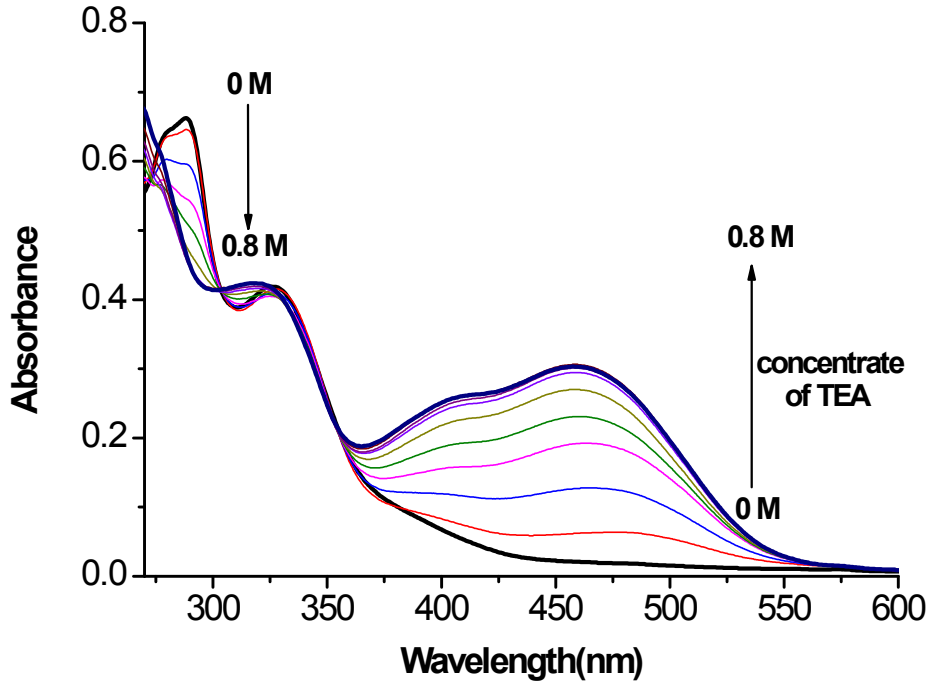


(A)

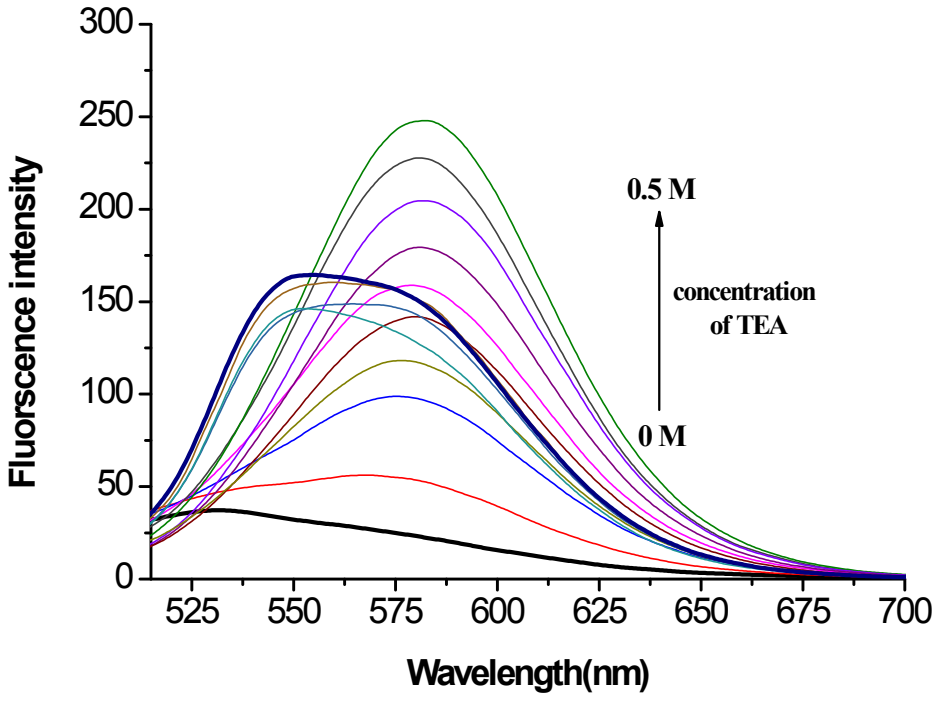


(B)

Fig. S4 The intermolecular hydrogen bonding interactions in crystal along *c*-axis (A) and *b*-axis (B).



(A)



(B)

Fig. S5 Absorption changes (A) and fluorescence changes (B) of **DB-5** on addition of Et_3N to the respective acidic solutions in DCM (conc. = 1×10^{-5} M, l = 10 mm, λ_{ex} = 480 nm).

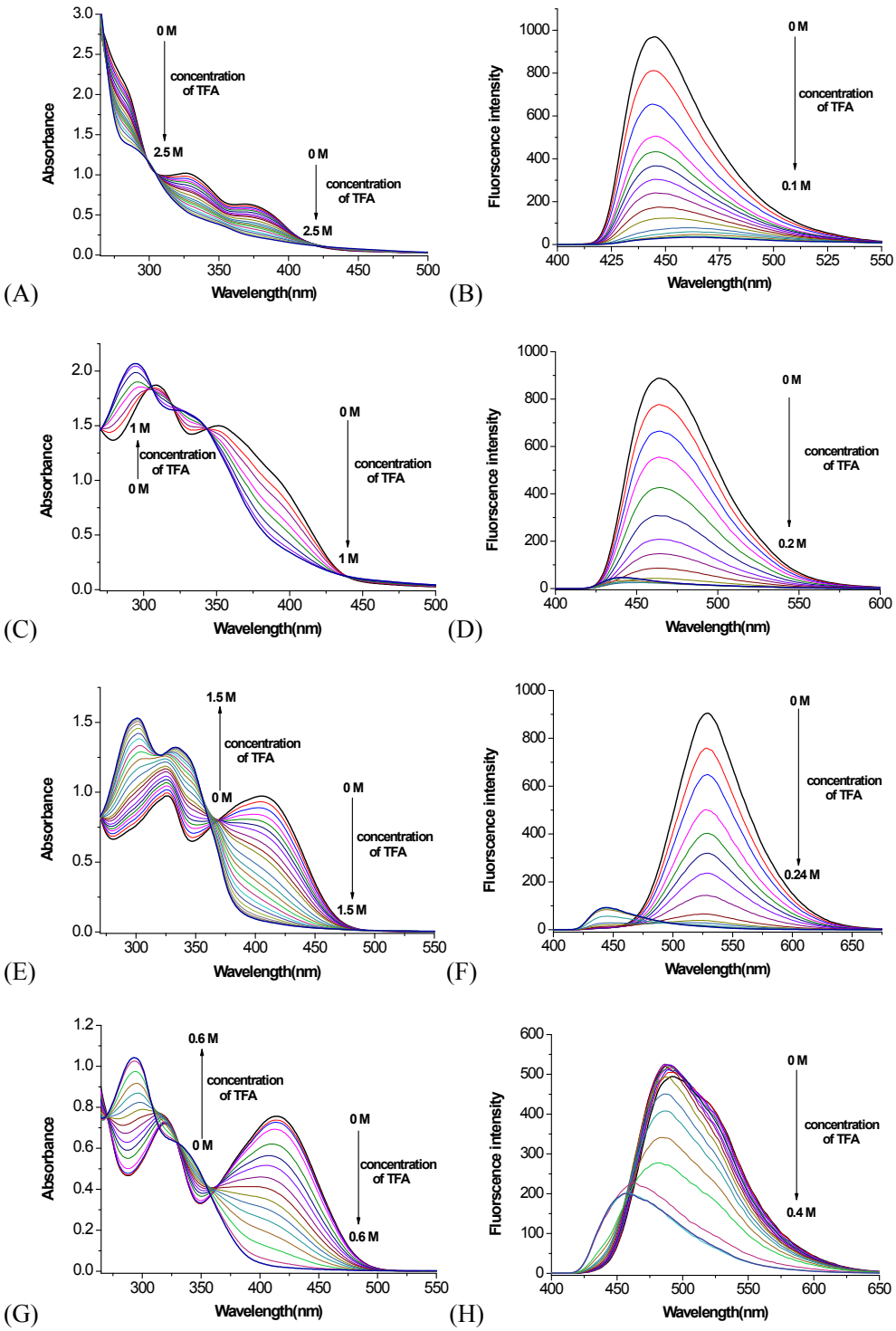
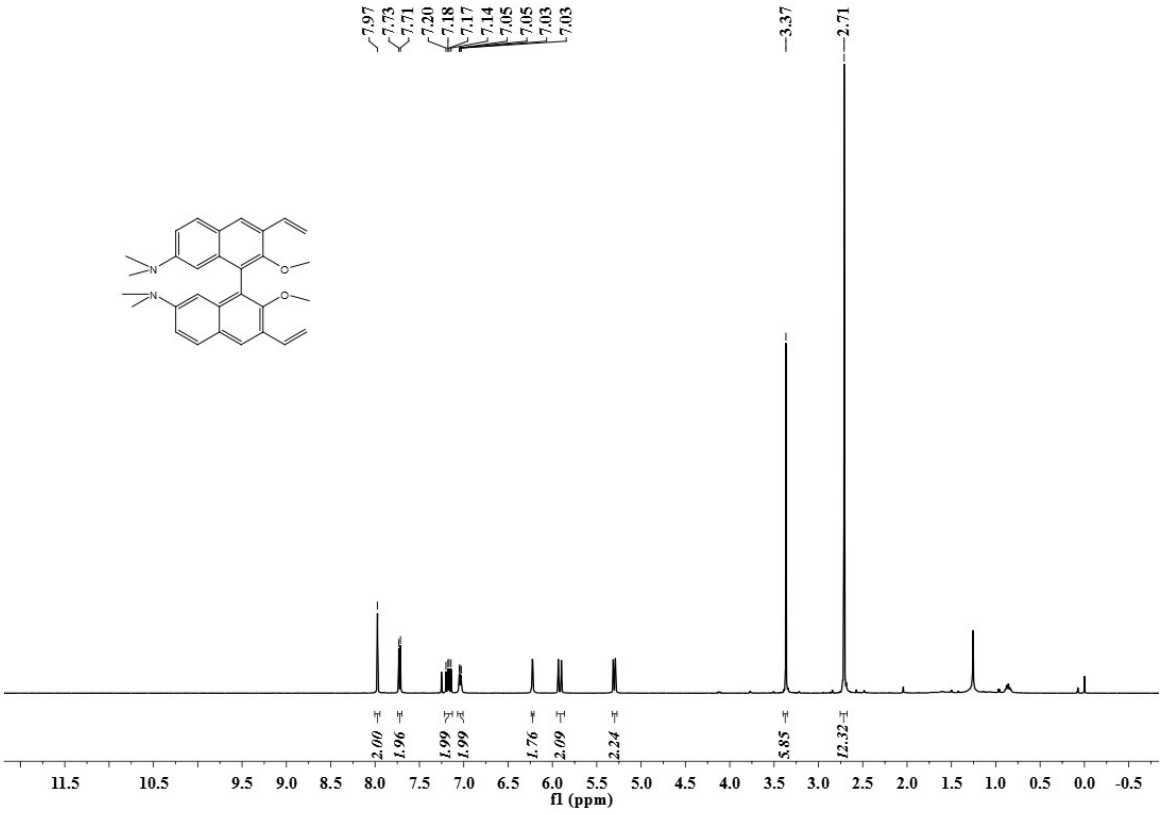
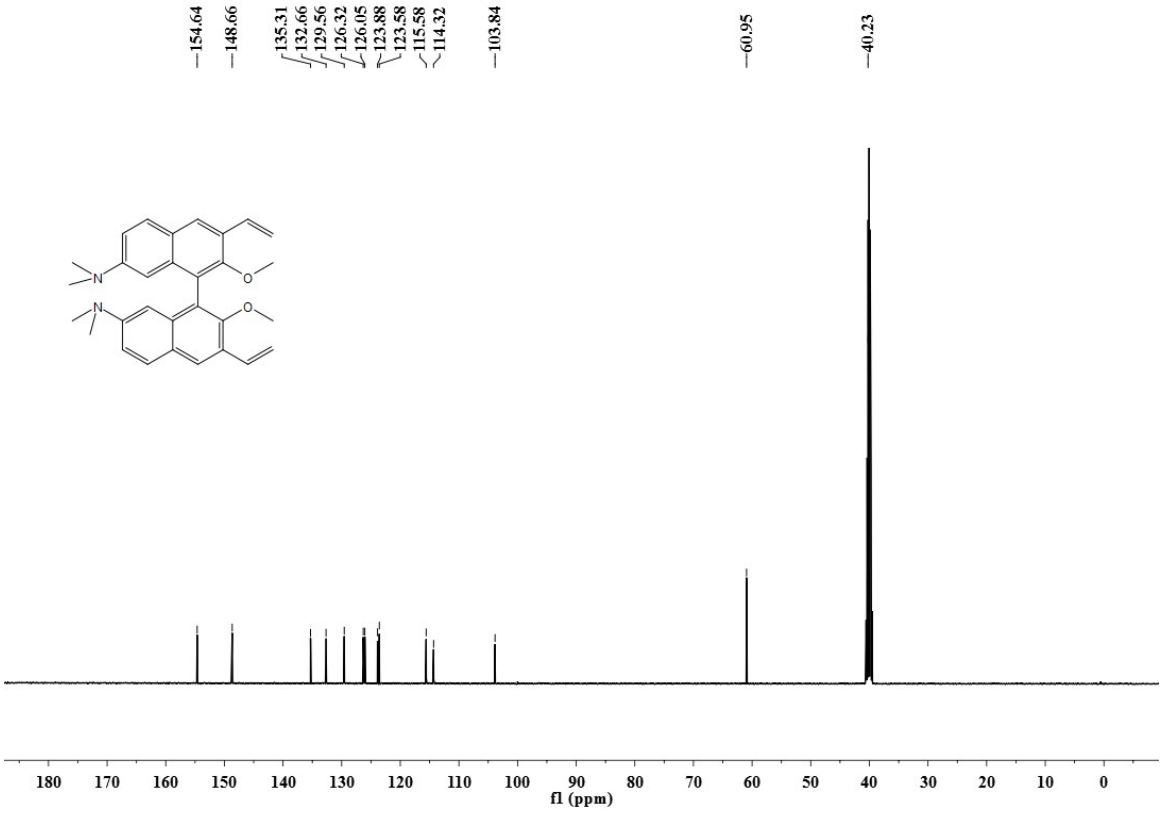


Fig. S6 Absorption changes and fluorescence changes of **DB-1** (A, B)**, DB-2** (C, D), **DB-3** (E, F) and **DB-4** (G, H) on addition of TFA to the respective solutions in DCM (conc. = 1×10^{-5} M, l = 10 mm, λ_{ex} = 350 nm for **DB-1** and **DB-2**, 410 nm for **DB-3** and **DB-4**).

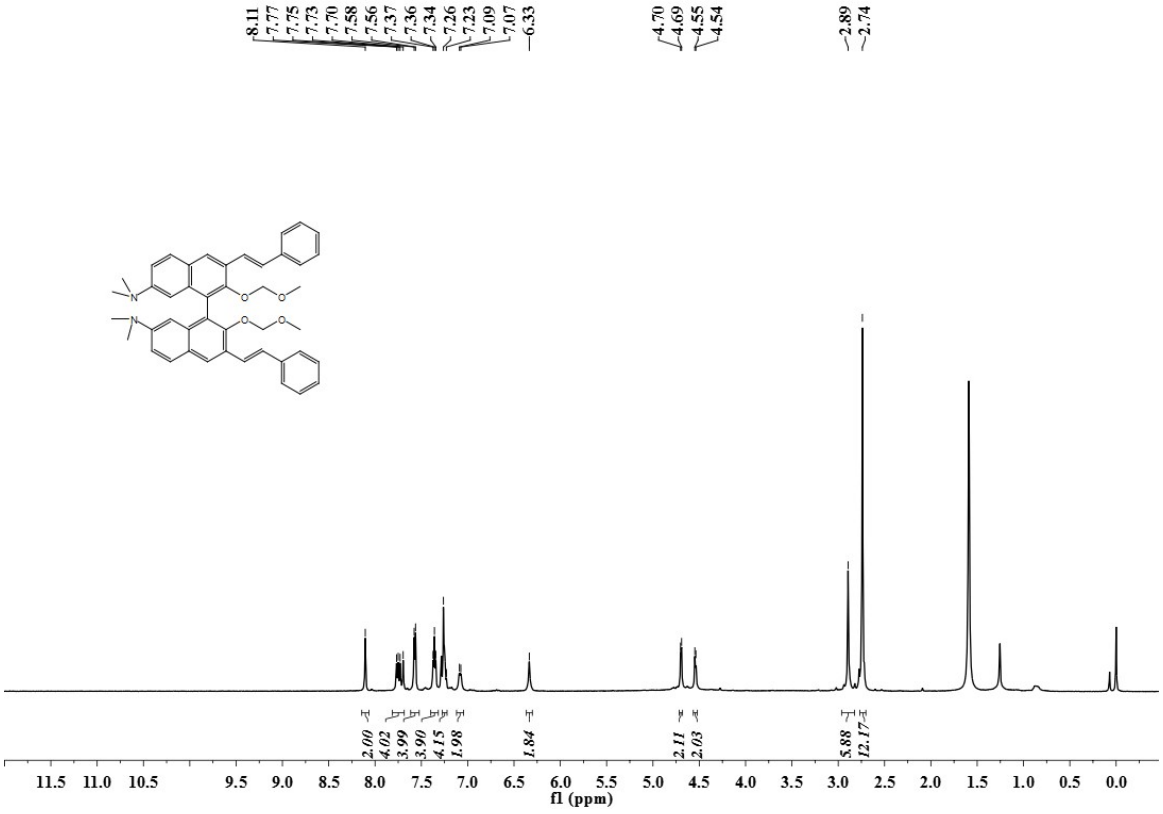
3. NMR spectra of products

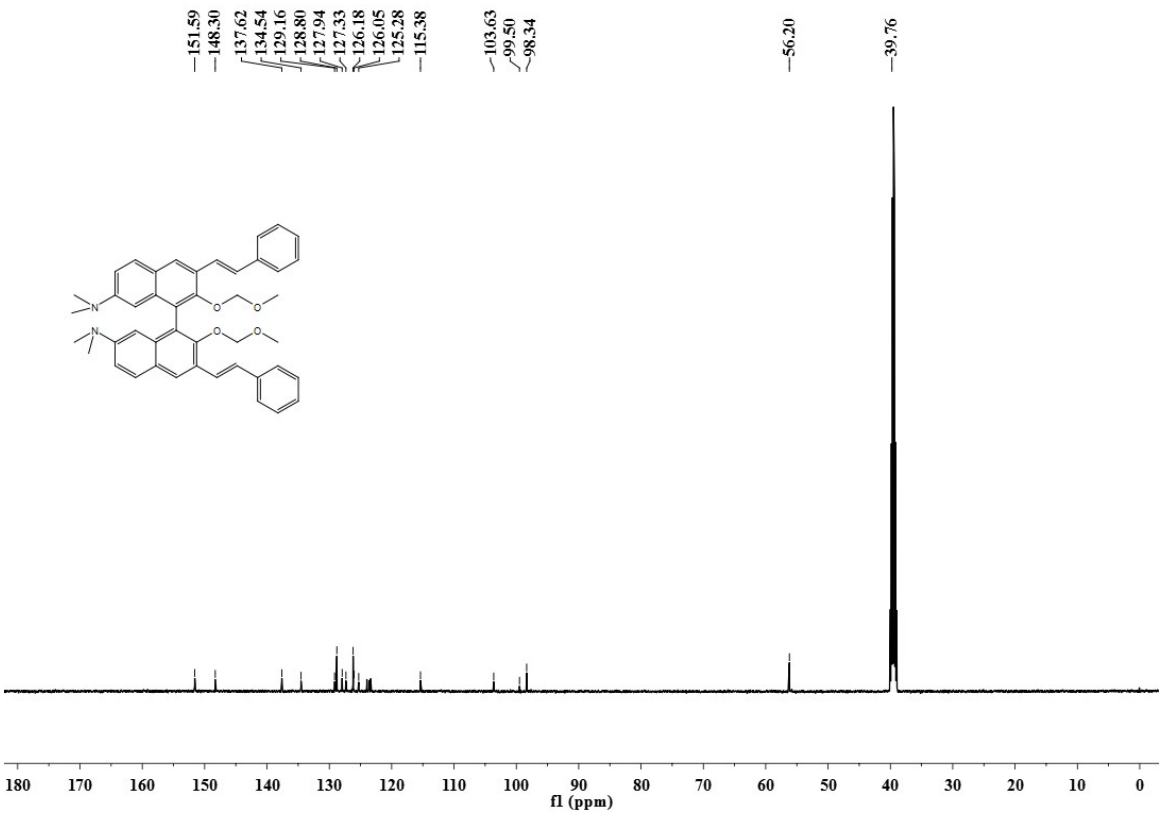
3.1 NMR spectra of **DB-1**



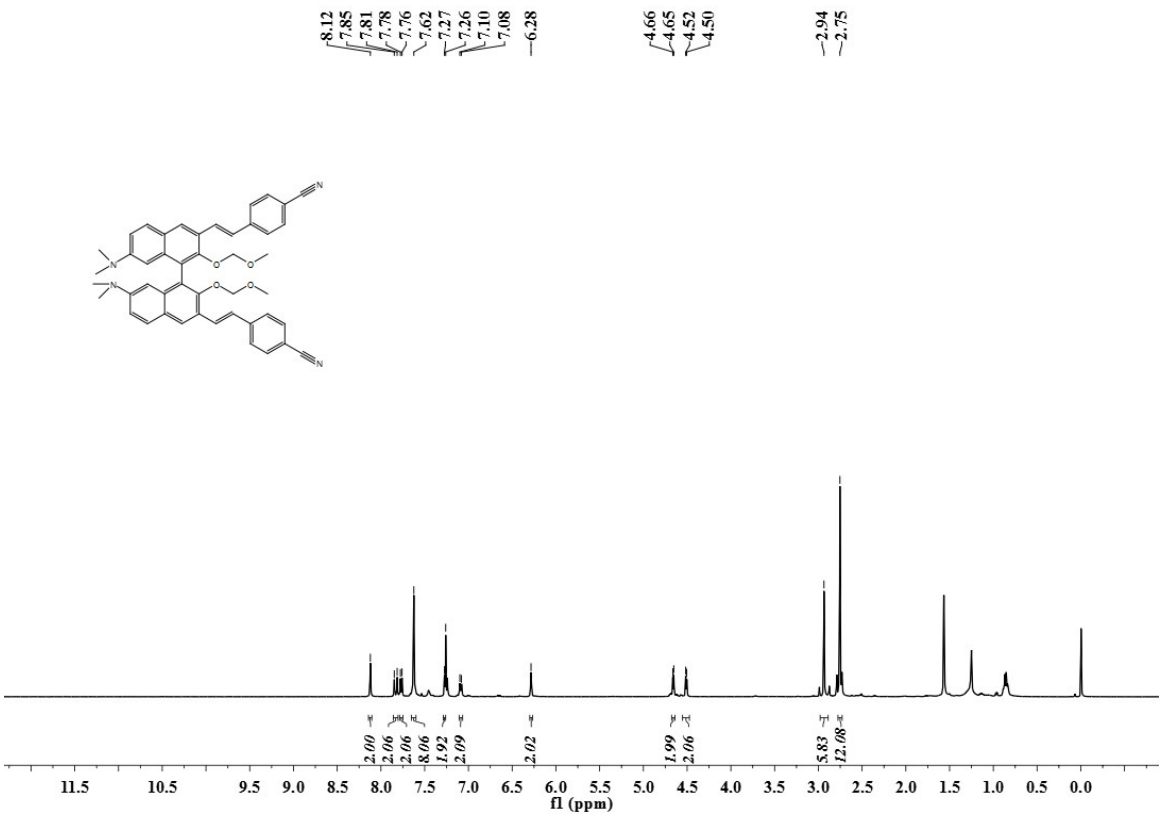


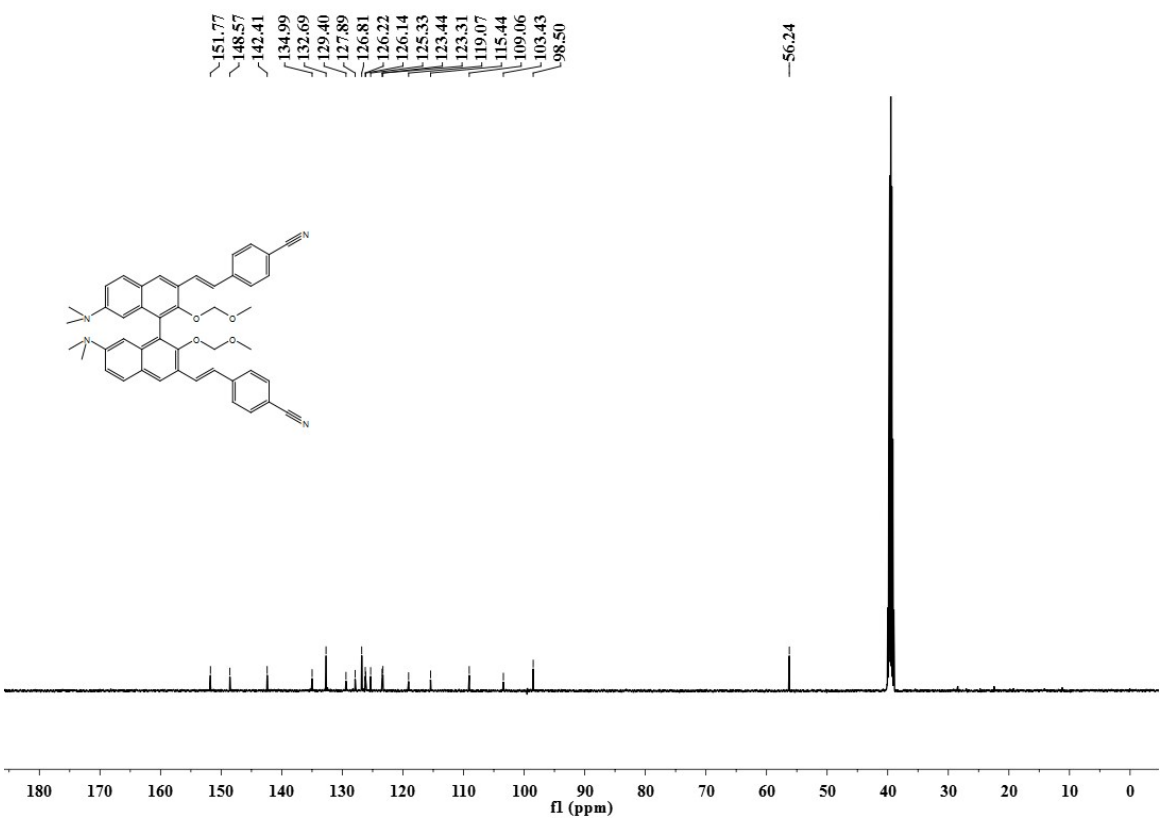
3.2 NMR spectra of **DB-2**



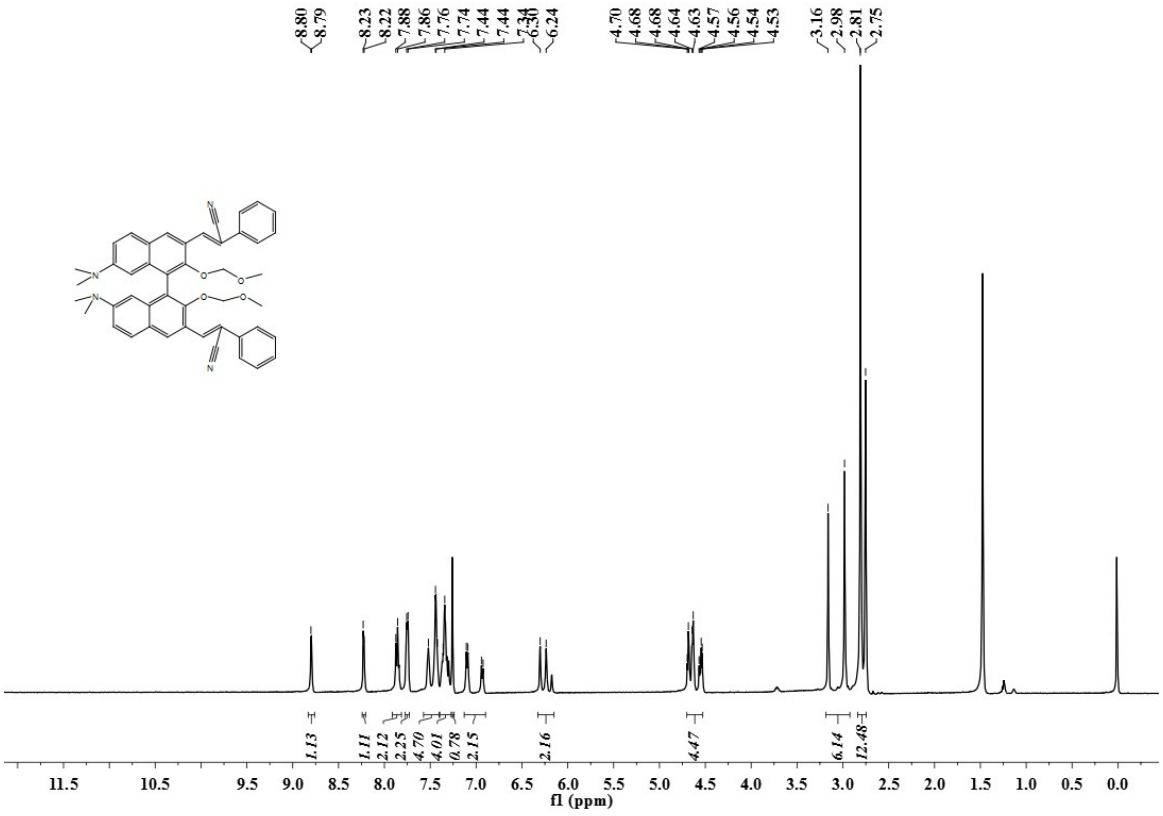


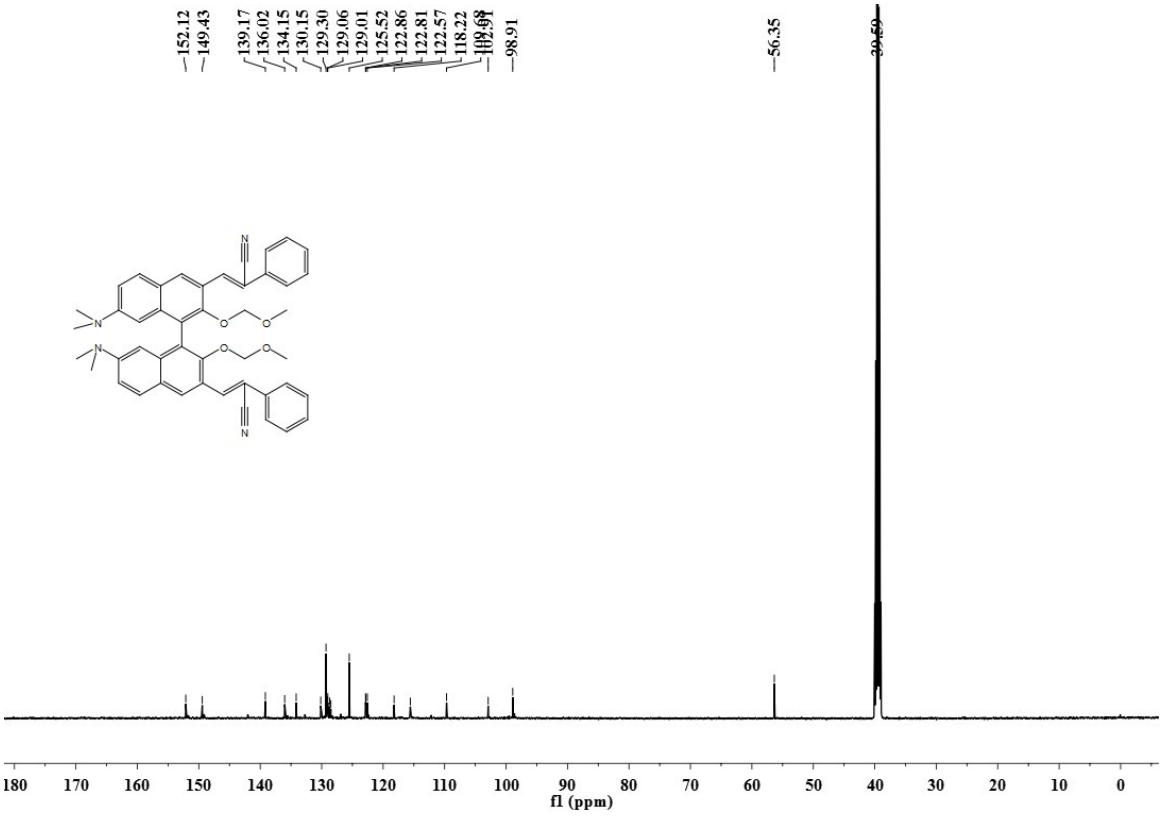
3.3 NMR spectra of **DB-3**



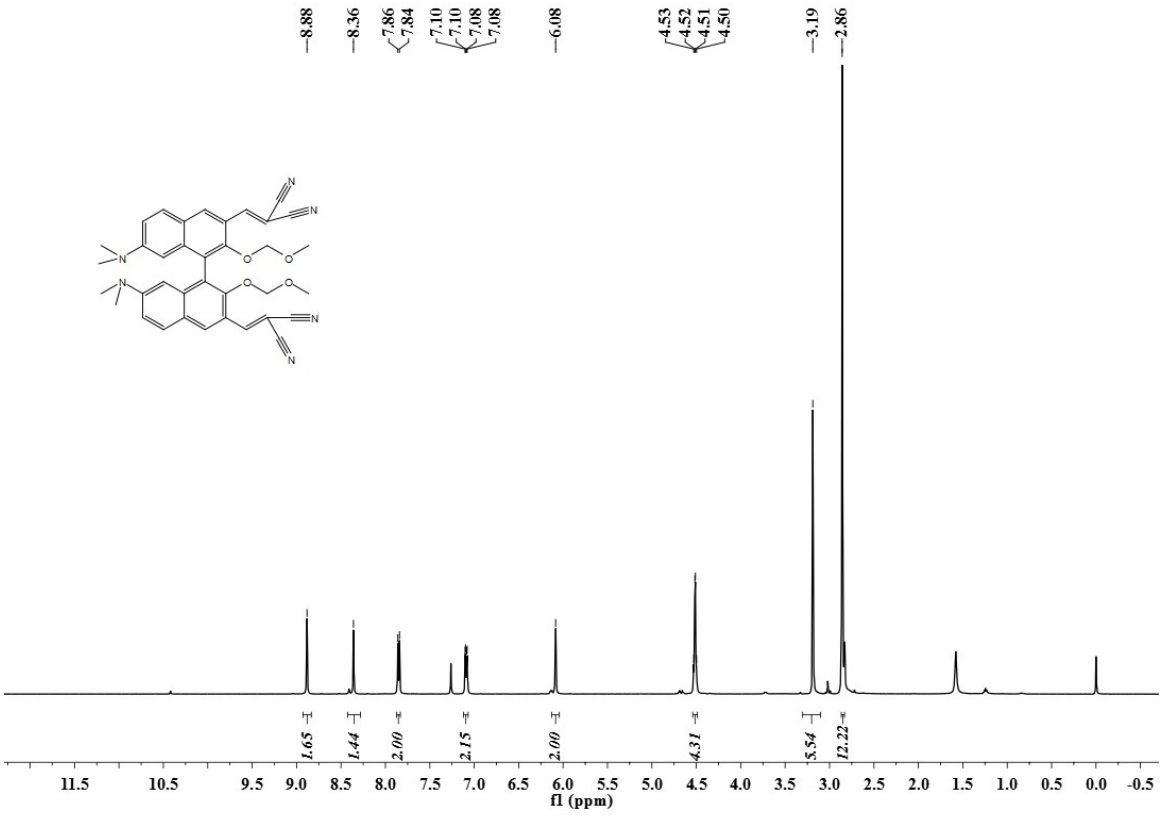


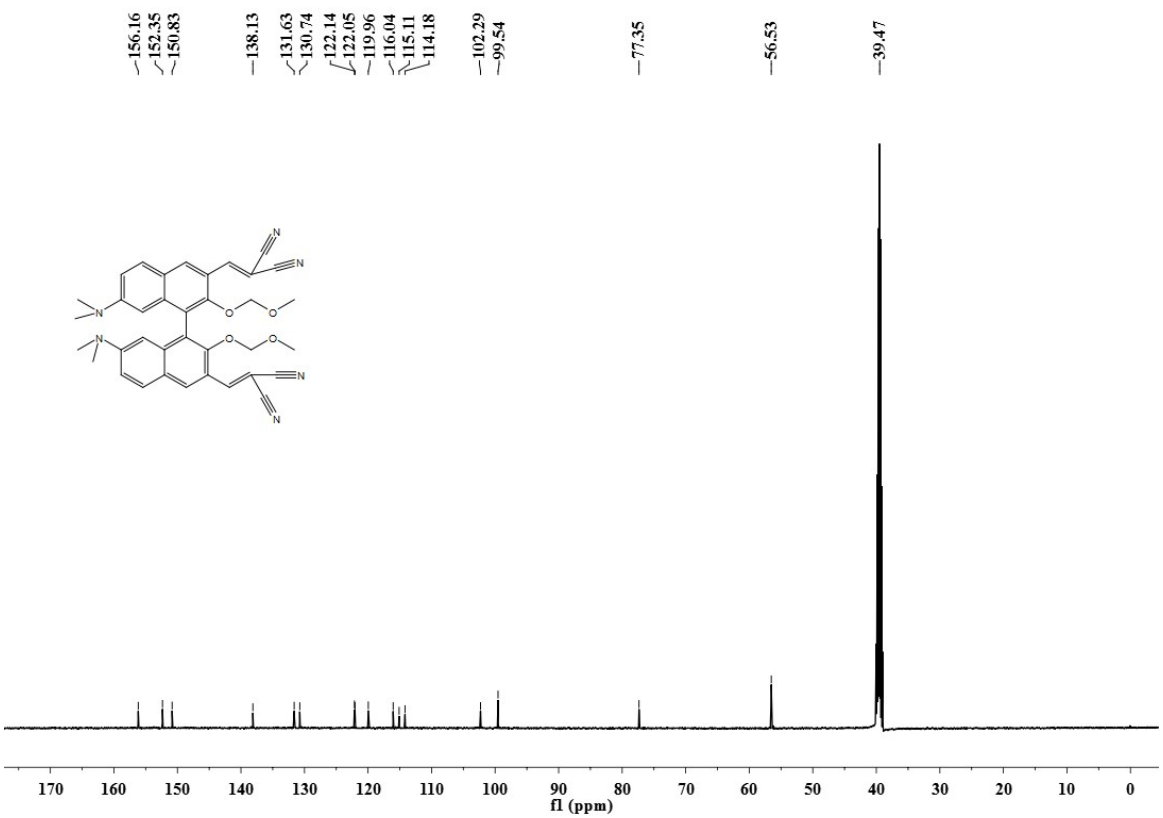
3.4 NMR spectra of **DB-4**





3.5 NMR spectra of **DB-5**





4. Full reference of Gaussian 09

Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.