

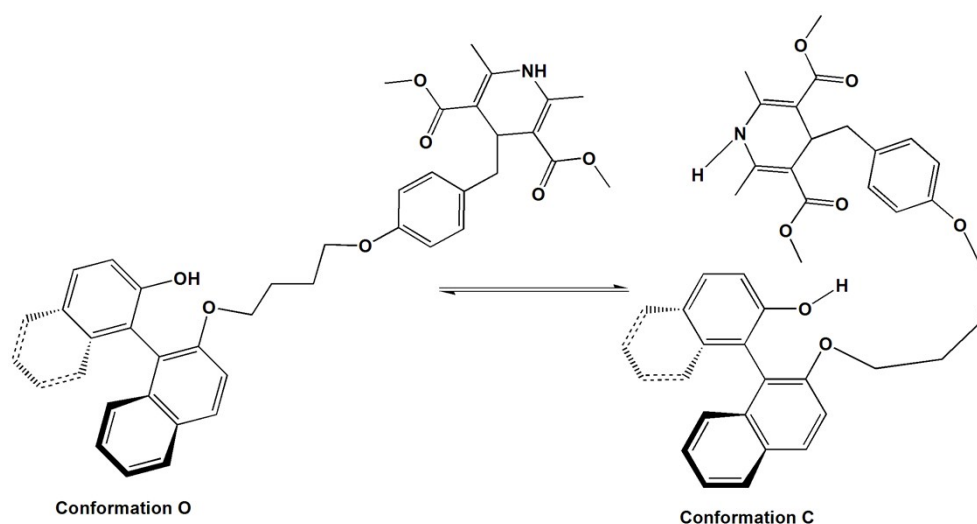
Supporting Information

For

Axially chiral 1,4-dihydropyridine derivatives: aggregation-induced emission and application as viscosity probe

Zeren Yang,^a Yanmin Huo,^a Yanke Liu,^a Guifen Du,^a Wenhao Zhang,^a Lijie Zhou,^a Lihui Zhan,^a Xuerui Ren,^a Wenzeng Duan,^{a, *} Shuwen Gong^{a, *}

^a Institute of Functional Organic Molecules and Materials, School of Chemistry and Chemical Engineering, Liaocheng University, No.1 Hunan Road, Liaocheng, People's Republic of China; E-mail: duanwenzeng@lcu.edu.cn; gongshw@lcu.edu.cn.



Scheme S1. Proposed conformation O (opened) in solvents and conformation C (closed) in glycol, THF-H₂O.

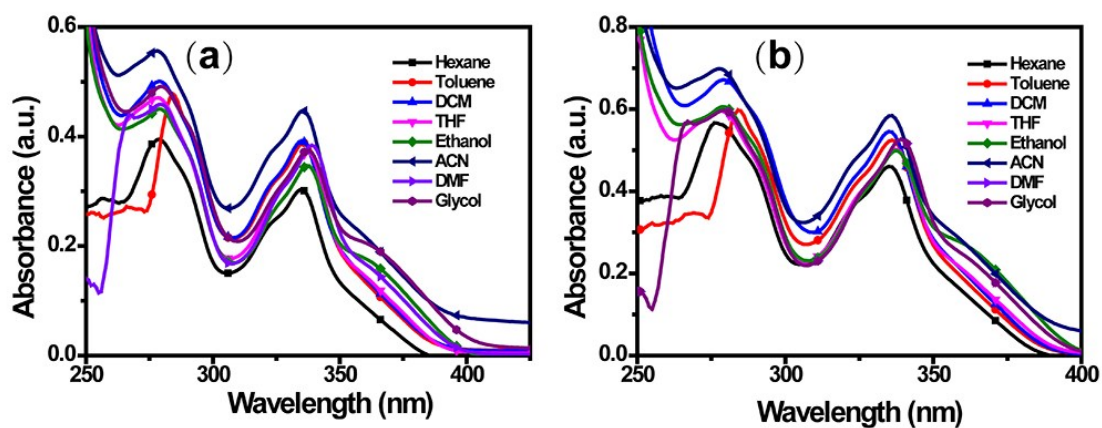


Figure S1. Absorption spectra of compounds (*R*)-2 (a) and (*S*)-2 (b) in various solvents (50 μ M) such as hexane, toluene, dichloromethane (DCM), tetrahydrofuran (THF), ethanol, acetonitrile (ACN), *N,N*-dimethylformamide (DMF), and glycol, respectively.

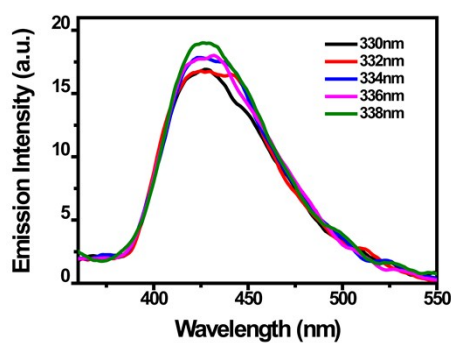


Figure S2. Emission spectra of (*R*)-2 in water/THF mixtures ($f_w = 90\%$, 50 μ M) with varied excitation wavelength.

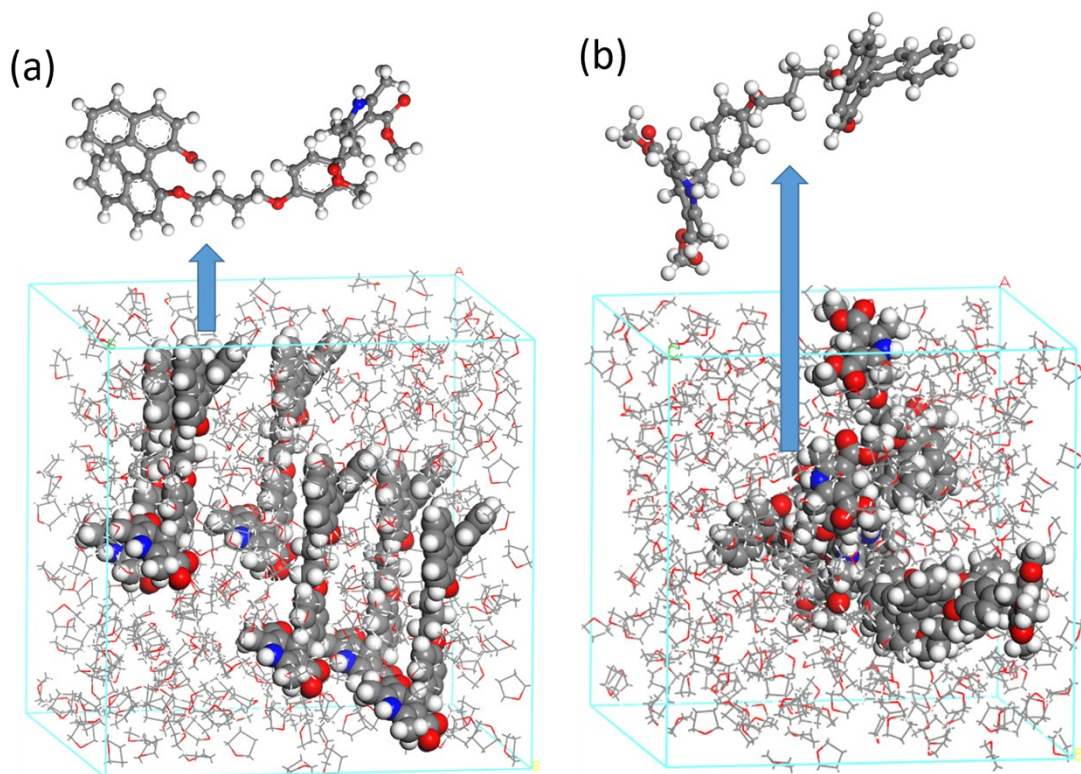


Figure S3. The molecular dynamic simulation of (*R*)-2 in THF solution: (a) 0 ns of the molecular conformation and (b) 1 ns of the molecular conformation.

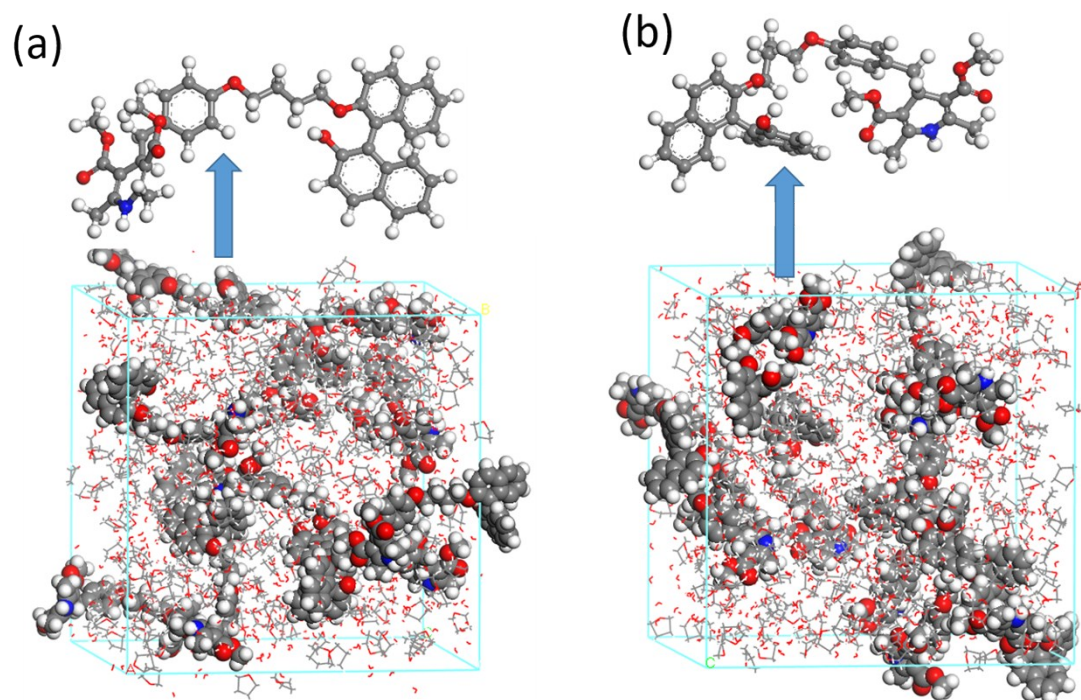


Figure S4. The molecular dynamic simulation of (*R*)-2 in THF/water mixtures: (a) 0 ns of the molecular conformation and (b) 1 ns of the molecular conformation.

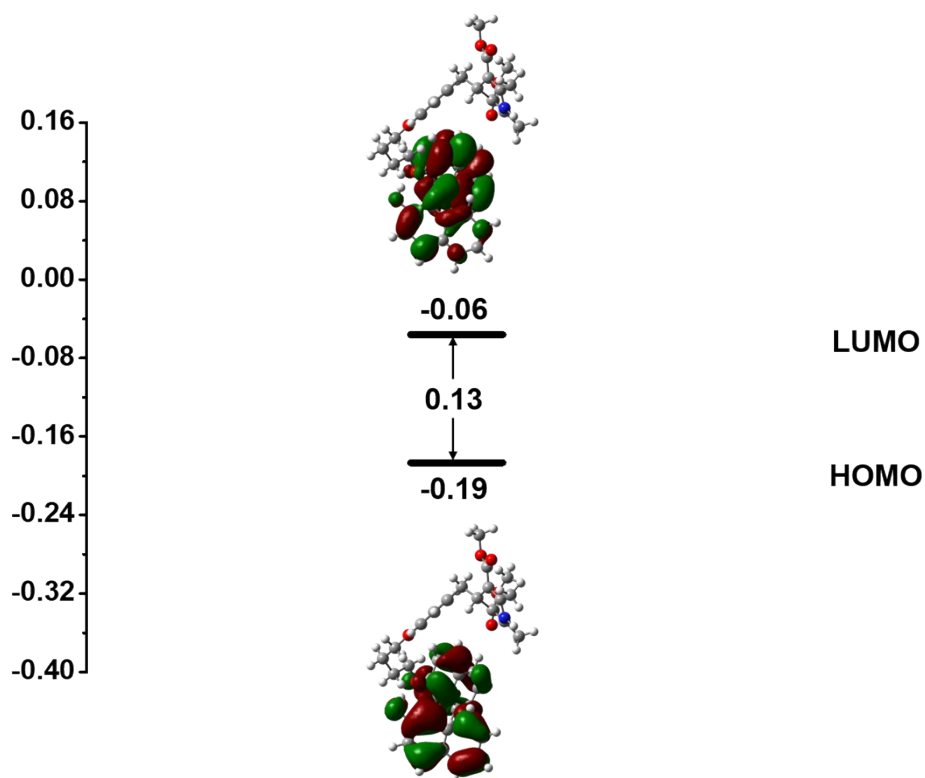


Figure S5. Calculated orbital energy levels, energy gaps and electron density contours of HOMOs and LUMOs for (R)-2 at their S_0 equilibrium geometries in solution.

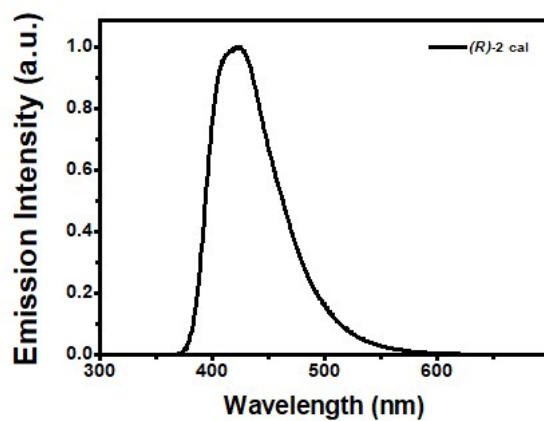


Figure S6. Calculated optical emission spectra for (R)-2 in conformation C.

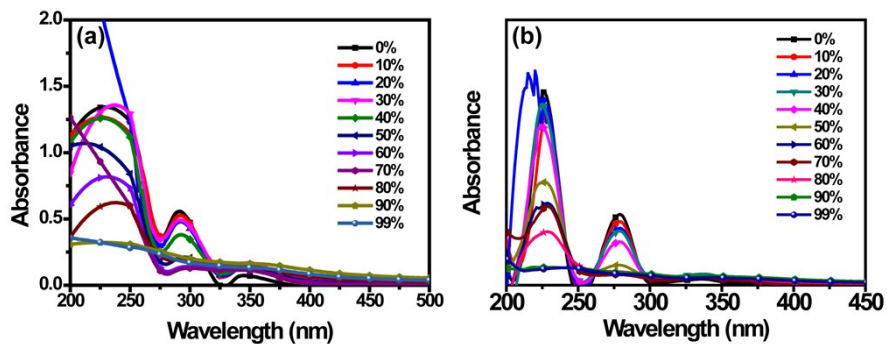


Figure S7. Absorption spectra of compounds (R)-2 (a) and (S)-2 (b) in THF/water mixtures (50 μ M) with varied volumetric fractions of water (f_w).

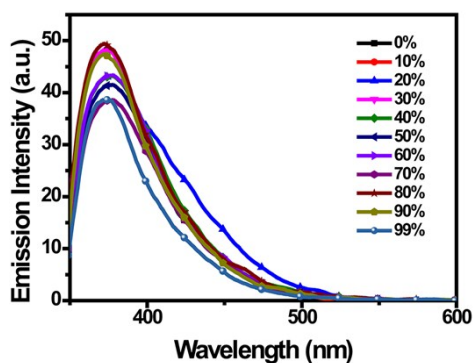


Figure S8. Fluorescence spectra of (R)-2 in THF/hexane mixtures (50 μ M) with varied volumetric fractions of hexane.

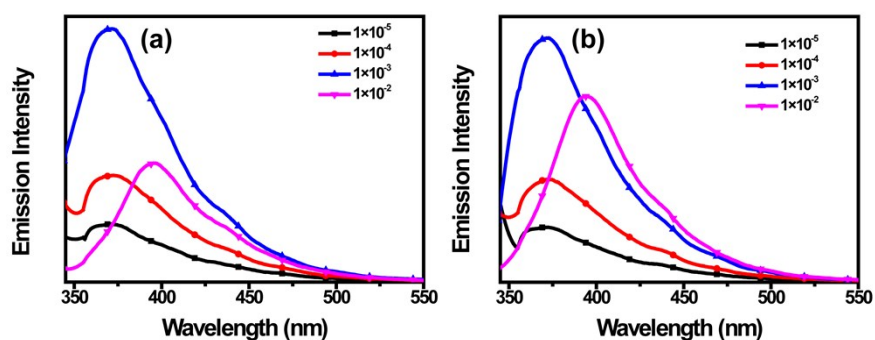


Figure S9. Effect of concentration on the fluorescence spectra of (R)-2 (a) and (S)-2 (b) in THF.

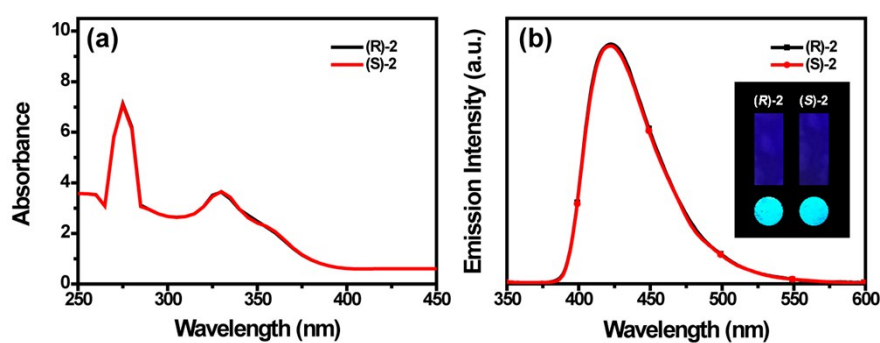


Figure S10. The absorption (a) and emission (b) spectra of (R)-/(S)-2 in solid-state; Inset in (b): the photo-pictures of (R)-/(S)-2 in the drop-cast film and powder state (λ_{ex} = 365 nm using a UV lamp).

NMR spectra

