# Electronic Supplementary Information

## Chirality-induced supramolecular nanodishes: enantioselectivity and energy transfer

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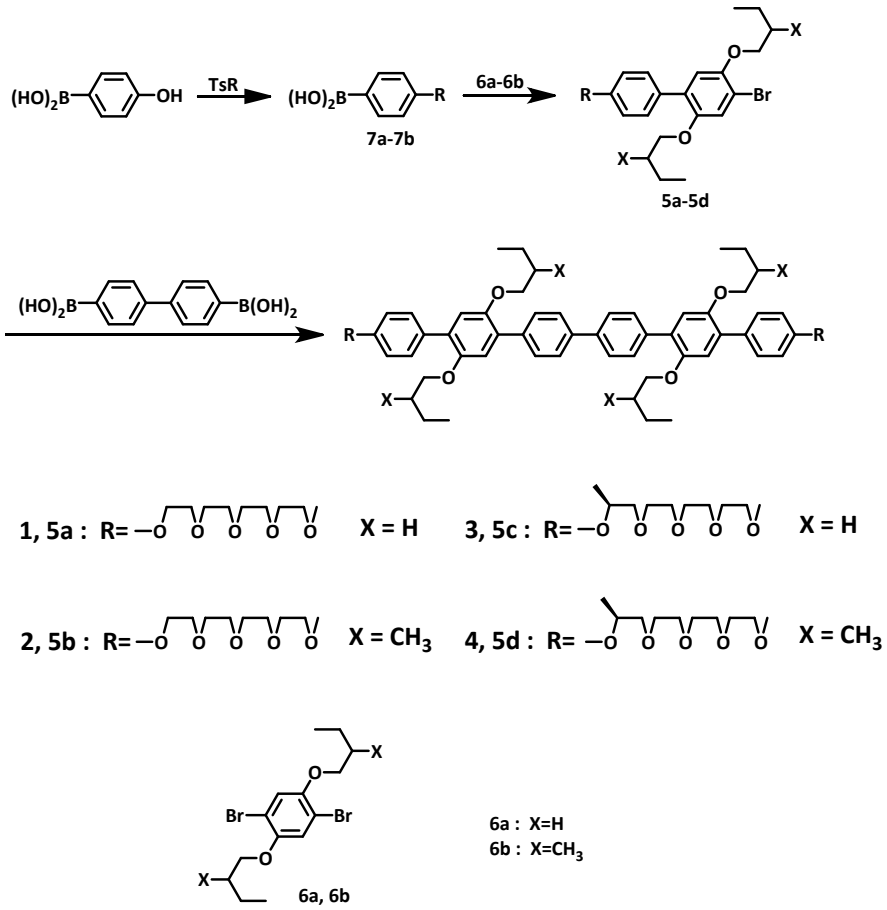
# 1. Materials and Methods

## 1.1 Synthetic route

**Scheme S1.** Synthesis route of molecules **1-4**.



## 1.2 Materials

Triethylene glycol monomethyl ether, Tetraethylene glycol, lithium aluminum hydride, (S)-(+)-1-Bromo-2-methylbutane, 3,4-Dihydro-2H-pyran, sodium hydride, 2,5-Dibromobenzene-1,4-diol, Sodium carbonate anhydrous, L-Lactic acid ethyl ester, 1-Bromobutane, 4,4'-Biphenyldiboronic, toluene-p-sulfonyl chloride (TsCl, 99%), pyridine, Sodium bicarbonate, Hydrochloric acid, 4-Hydroxybenzeneboronic acid, potassium carbonate, Calcium chloride, p-Toluenesulfonic acid monohydrate, tetrakis(triphenylphosphine) palladium (0), Iodomethane, Magnesium sulfate anhydrous, and conventional reagents were used as received. All manipulations involving air-sensitive reagents were performed under an atmosphere of dry nitrogen.

## 1.3 Synthetic process

**Synthesis of compounds 1-4.** All four compounds were synthesized by a similar procedure, herein we represent synthesis of compound **1**.

Synthesis of compound **7a**: Weigh the tetraethylene glycol(10.00g, 51.55mmol), Add tetrahydrofuran (150 ml) to 250 ml round-bottomed flask and was added sodium hydride (2.47 g, 60 % in kerosene) in ice bath. The iodomethane (1.65ml, 26.41mmol) was dissolved in a drip funnel with THF(20 mL), and then dropped into a round-bottomed flask (250 mL) under an ice bath, and stirred for 24 hrs at room temperature, the reaction solution changes from white to black. Then the solvent was removed and distilled water was added to the the residue, which was extracted with dichloromethane and ethyl acetate. It was condensed for purification through silica-gel column chromatography using petroleum ether and ethyl acetate as flowing phase, generating pale yellow oily liquid (3.45 g, productivity of 62.80%). Then we took a certain amount (3.45 g, 16.59 mmol) of it, and p-toluene sulfonyl chloride (5.06 g, 26.54 mmol) were dissolved in dichloromethane (100 mL), to which added pyridine (10 mL), and stirred for 10 hrs at room temperature. Subsequently distilled water (30 mL) was added to the mixture above and stirred for another 0.5 hrs, and then pH of the system was adjusted to acidic state with hydrochloric acid followed by continue stirring of 1.5 hrs. After that it was extracted with dichloromethane and ethyl acetate. It was condensed for purification through silica-gel column chromatography using petroleum ether and ethyl acetate as flowing phase, generating colorless oily liquid (4.04 g, productivity of 67.32 %). Then we took a certain amount (4.04 g, 11.15mmol) of it, dissolved in acetonitrile (150 mL) together with 4-Hydroxybenzeneboronic acid (1.28 g, 9.29 mmol) and potassium carbonate (5.13 g, 37.16 mmol), and refluxed for 24 hrs. After that the solvent was removed and distilled water was added to the the residue, which was extracted with dichloromethane and ethyl acetate. It was condensed for purification through silica-gel column chromatography using dichloromethane

and methanol as flowing phase, generating dark brown viscous liquid (0.93 g, productivity of 30.73 %).

Synthesis of compound **6a**: Compounds **6a-6b** were prepared by a similar procedure, here we represent synthesis of compound **6a** as an example. 2, 5-dibromo-1, 4-phenyldiol (5.00 g, 18.66 mmol) and bromobutane (7.67 g, 55.98 mmol) was dissolved in acetonitrile (150 mL) and added potassium carbonate (12.80 g, 92.75 mmol), and refluxed for 48 hrs. After that the solvent was removed and distilled water was added to the the residue, which was extracted with dichloromethane and ethyl acetate. It was condensed for purification through silica-gel column chromatography using dichloromethane and methanol as flowing phase, generating dark brown viscous liquid (1.65 g, productivity of 22.57 %).

Synthesis of compound **5a**: Compound **7a** (0.93 g, 2.83 mmol) was dissolved in THF (20 mL) into a drip funnel, while compound **6a** (1.40 g, 3.68 mmol) was dissolved in THF (30 mL) together with tetrakis(triphenylphosphine)palladium (0) (0.72 g, 0.62 mmol) and sodium carbonate (2.0 M, 20 mL) into a two-necked flask, and added dropwise, then refluxed for 24 hrs under $N_2$ atmosphere and dark. It was cooled to room temperature, and followed by solvent removal, adding distilled water, extraction by methylene chloride and ethyl acetate, and condensation for further purification through silica-gel column chromatography using petroleum ether and ethyl acetate as flowing phase, generating dark brown solid (0.96 g, productivity of 58.20 %).

Synthesis of molecule **1**: Compound **5a** (0.96 g, 1.65 mmol) was dissolved in THF (30 mL) together with Tetrakis(triphenylphosphine)palladium (0.19 g, 0.16mmol) and 4,4,-Biphenyldiboronic (0.18 g, 0.74 mmol) in a 100 mL one-neck flask. Subsequently sodium carbonate solution (2.0 M, 20 mL) was added to the mixture above and it was then refluxed for 24 hours under $N_2$ atmosphere and dark. After that THF was removed from the mixture, and the residue was added distilled water, extracted with dichloromethane and ethyl acetate, dried with anhydrous magnesium sulfate, filtered, and condensed. The obtained crude product was purified by silica-gel column chromatography to get molecule 1 (White snowflake solid, 0.36 g, productivity of 42.3%).

## 1.4 Techniques

Column chromatography filled silica gel (100-200 mesh) was proceeded for further purification. $^1$H-NMR (300 MHz) spectra were recorded in $CDCl_3$ (or DMSO-d6) on the Bruker AM-300 instrument; Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) was performed on the PerSeptive Biosystems Voyager-DESfTR instrument using 2-cyano-3-(4-hydroxyphenyl) acrylic acid (CHCA) as the matrix.

UV-vis and FL experiments were performed through the Shimadzu UV-1650PC spectrometer and the Hitachi F-4500 fluorescence spectrometer, respectively. CD spectra was obtained by a Biologic PMS450. TEM images were collected with the JEOL 2100 plus microscope. The ee% was estimated on a Shimadzu LC 20A high performance liquid chromatography (HPLC) equipped with a UV-Vis spectrometer and a Daicel CHIRALPAK® AYH0CE-VB023 column. The mobile phase is n-Hexane/EtOH/Diethylamine = 90/10/0.1 (v/v/v), and flow rate is 1.0 mL/min. It should be mentioned that after catakytic reaction, the whole reaction system was directly freeze-dried and absolutely dissolved for HPLC analysis. Atomic force microscope (AFM) images were produced by an Agilent 5500 Atomic Force Microscope.

## 1.5 Characterization

**TEM experiments.** A drop of each sample solution was placed on a carbon-coated copper grid and the solution was allowed to evaporate under ambient conditions. These samples were stained by uranyl acetate aqueous solution (0.2-0.4 wt%) on the surface of the sample-loaded grid. The dried specimen was observed by TEM at 120 or 200 KV.

**AFM experiments.** A drop of each sample solution was placed on mica surface and was prepared by evaporation of sample solutions. The dried specimen was observed by AFM.

## 1.6 Preparation of Supramolecular Co-Assemblies with DCCS.

1) Prepare a DCCS solution at a given concentration: 1.0 mg of DCCS was dissolved in 1 mL THF as stuck solution.

2) Prepare four initial assembly systems with molecule **1**-**4**, respectively. The concentration and total volume was fixed to be 100 μM and 10 mL, and they were separately transferred in vials for further use.

3) 100 μL of stuck solution from 1) was added to the four initial solutions and the vials were seal-capped. The mixture was sonicated for 30 minutes and stand for two hours to form supramolecular co-assembly.

## 2. Supporting data

### 2.1 $^{1}$H-NMR spectra of molecules 1-4 in $CDCl_3$

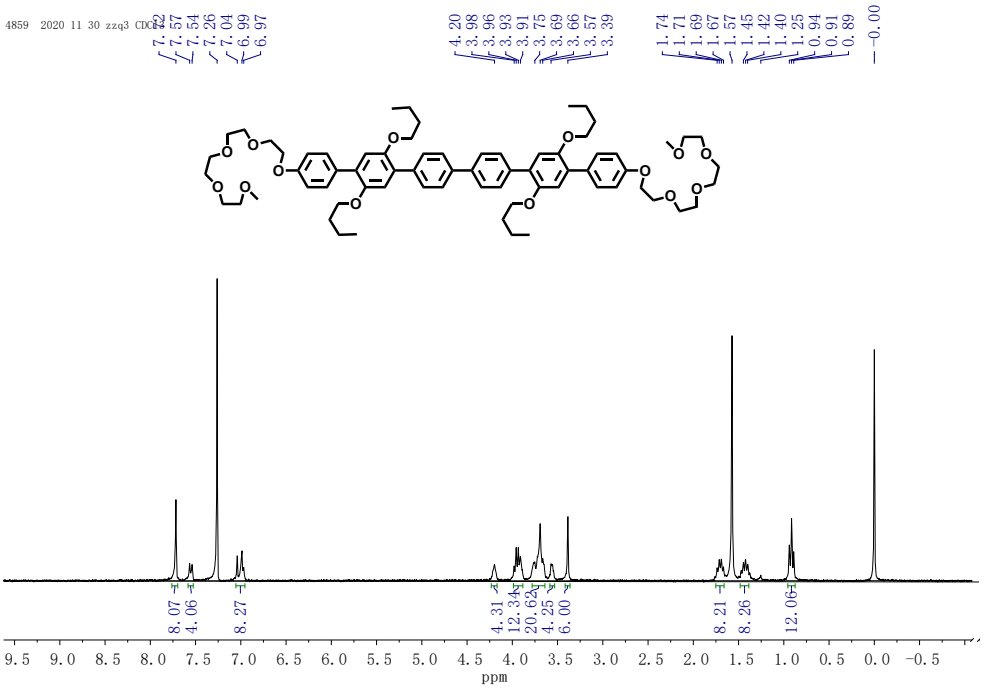



**Figure S1.** $^{1}$H-NMR spectrum of molecule **1** in $CDCl_3$.

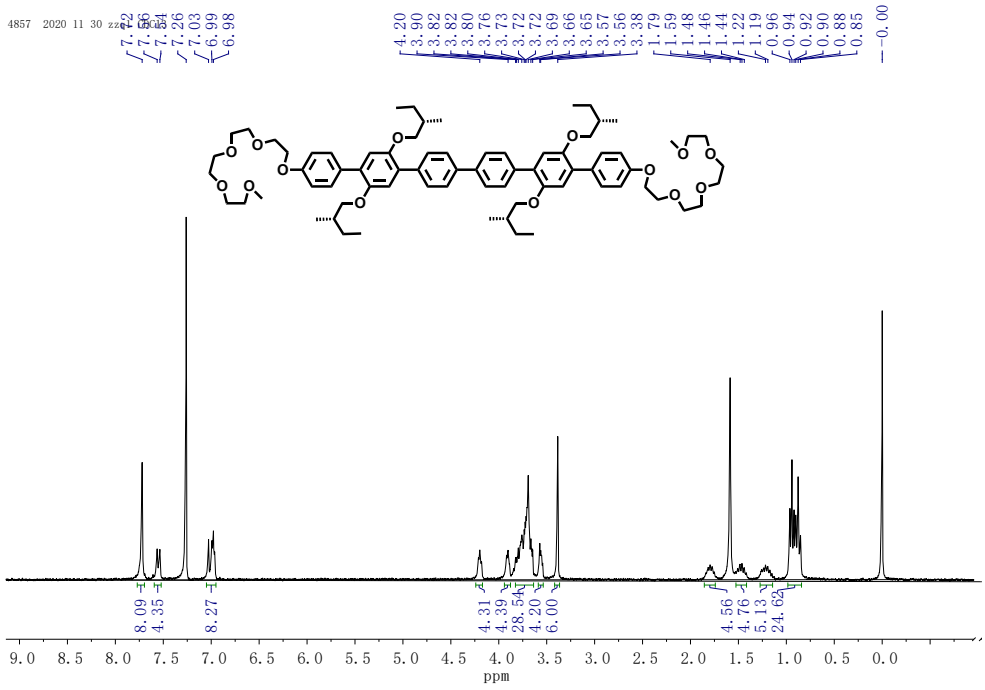



**Figure S2.** $^{1}$H-NMR spectrum of molecule **2** in $CDCl_3$.

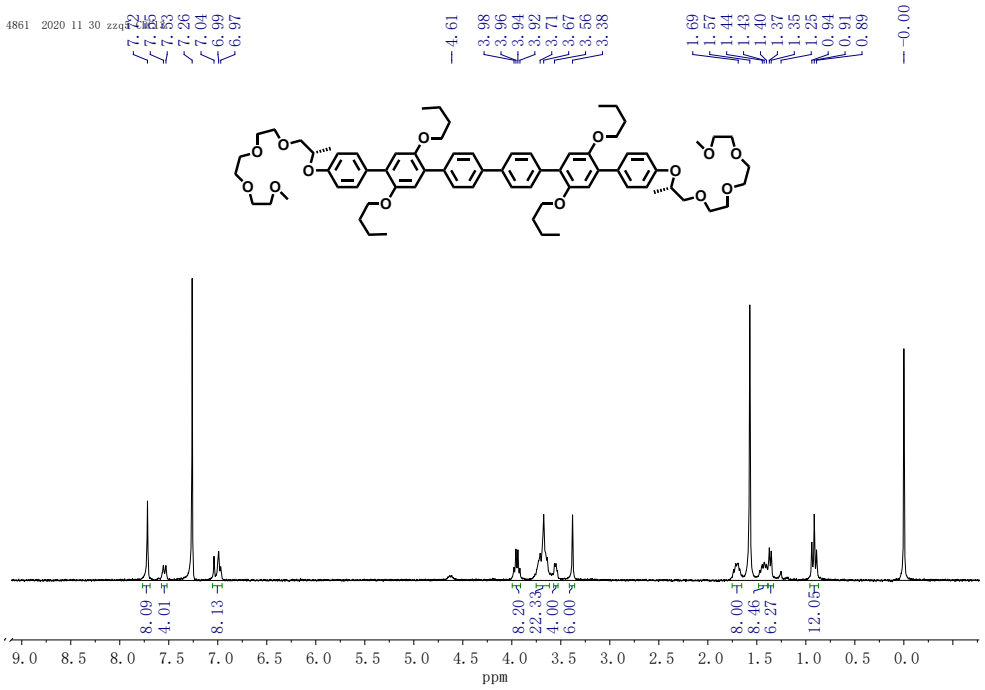


**Figure S3.** $^{1}$H-NMR spectrum of molecule **3** in $CDCl_3$.

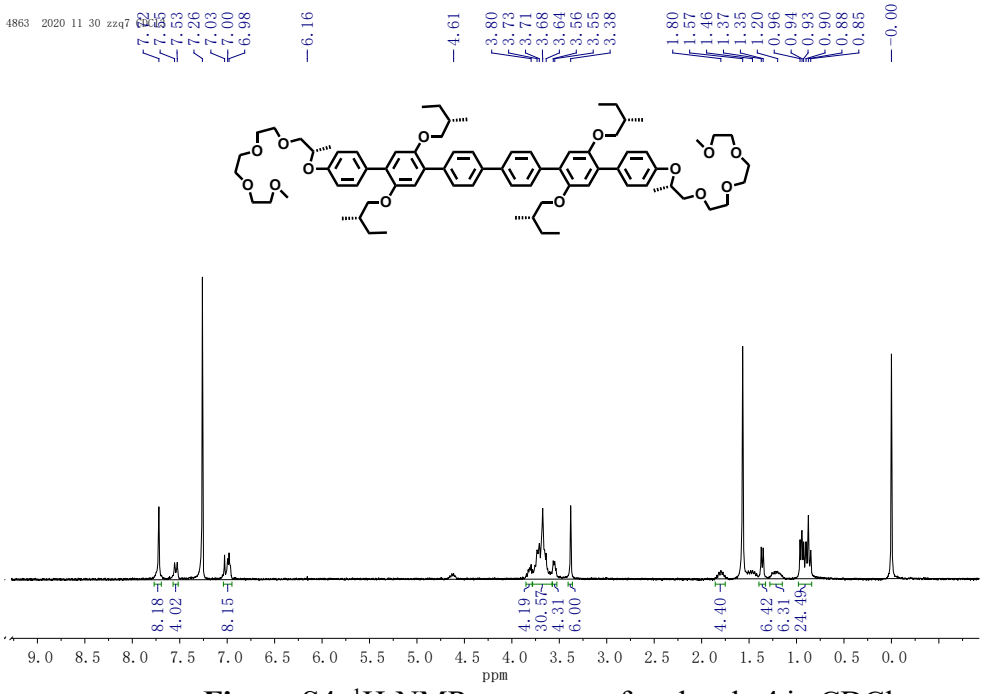


**Figure S4.** $^{1}$H-NMR spectrum of molecule **4** in $CDCl_3$.

## 2.2 MALDI-TOF-Mass spectra of molecules 1-4

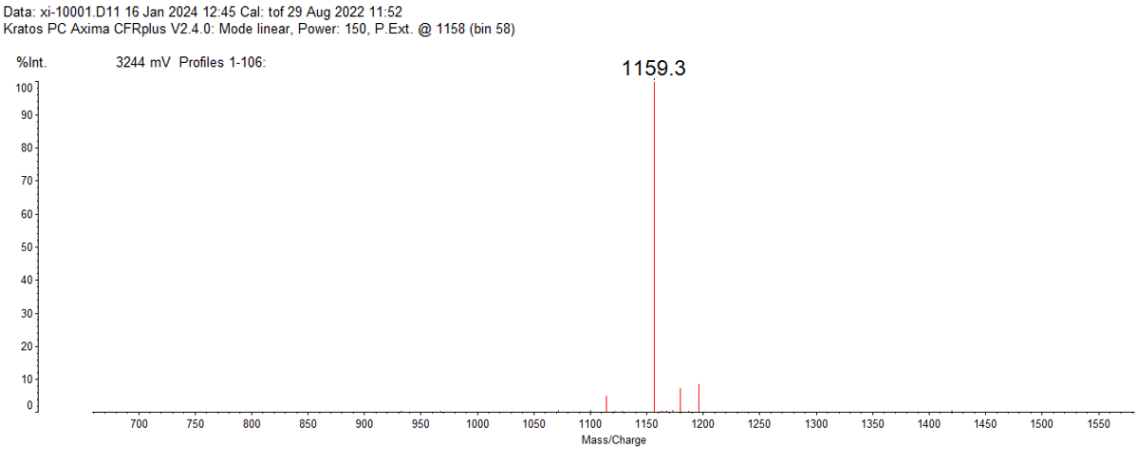



**Figure S5.** MALDI-TOF mass spectrum of molecule **1**.

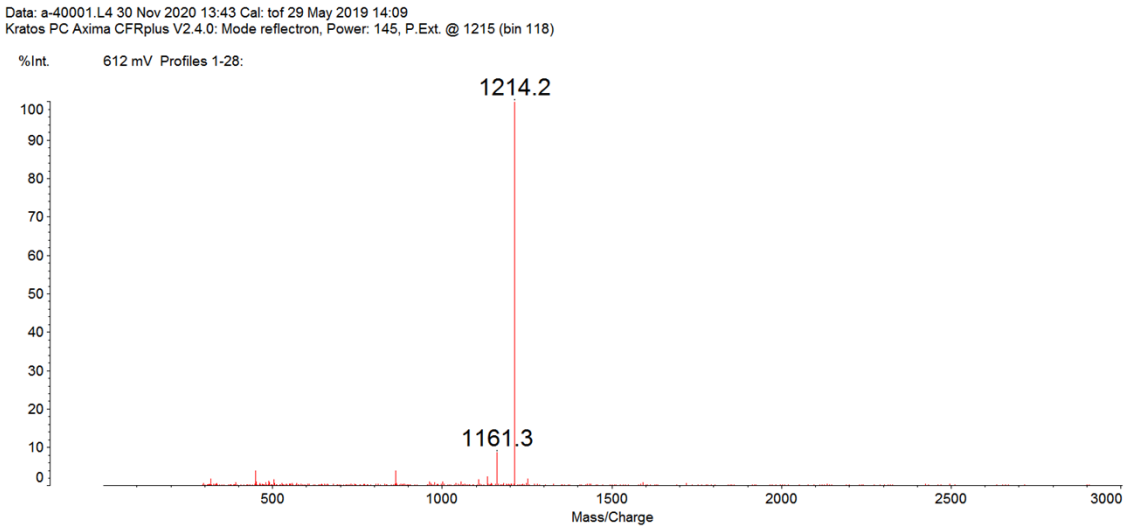



**Figure S6.** MALDI-TOF mass spectrum of molecule **2**.

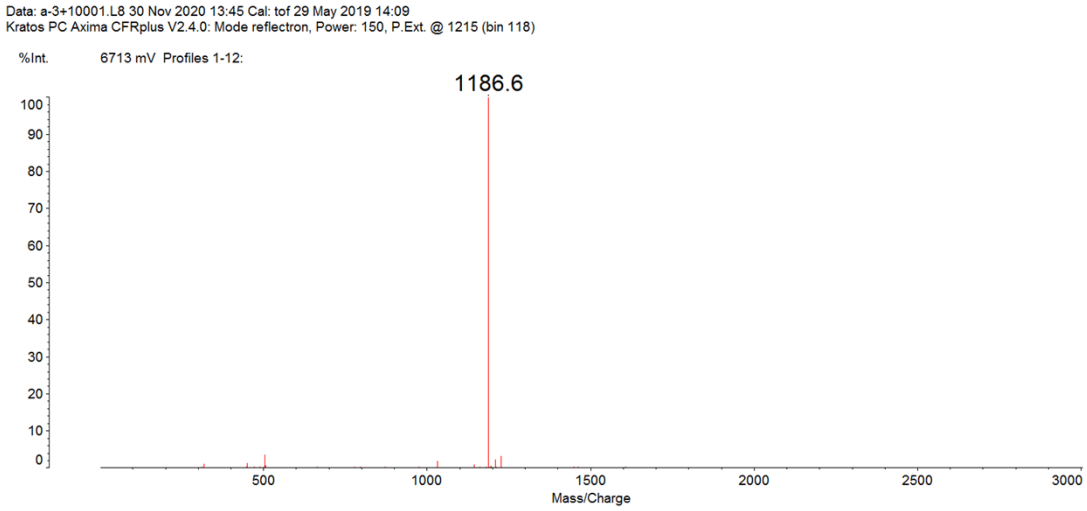



**Figure S7.** MALDI-TOF mass spectrum of molecule **3**.

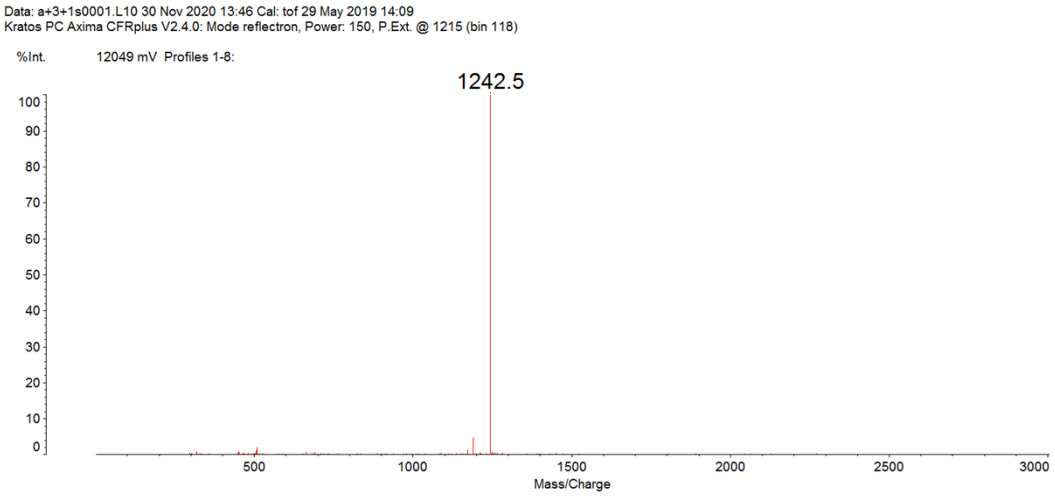



**Figure S8.** MALDI-TOF mass spectrum of molecule **4**.

## 2.3 Turbidity and Tyndall effect of molecule 4

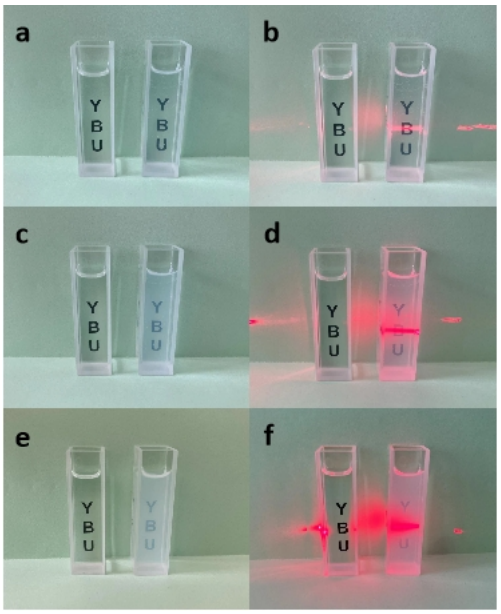



**Figure S9.** Comparison of (a, c and e) the turbidity and (b, d and f) Tyndall effect at various concentrations of molecule **4** in THF solution (the left sample set in every picture) and in THF/$H_2O$ (v/v=1:9) solution (the right sample set in every picture). ([c] a, b=10 μM; [c] c, d=50 μM; [c] e, f=100 μM).

## 2.4 UV-Vis absorption spectra of molecules 1-4

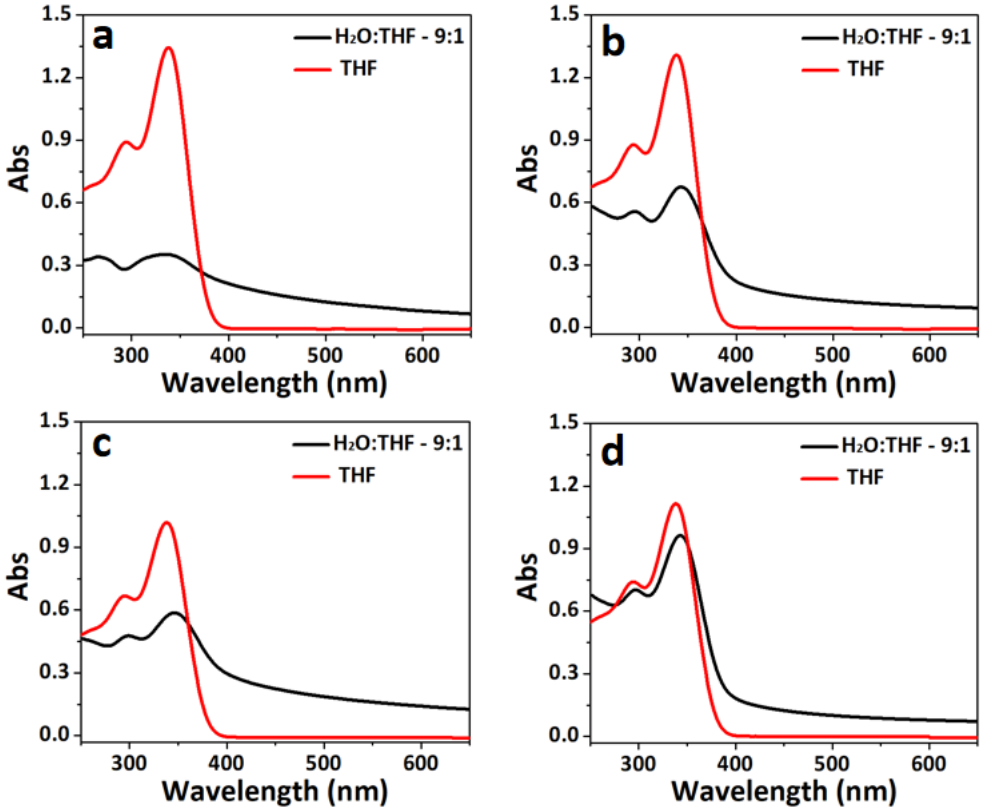



**Figure S10.** Normalized absorption spectra in THF and $H_2O$/THF (v/v = 9/1) mixed solvent under the concentration of 25 μM; (a) molecule **1**, (b) molecule **2**, (c) molecule **3**, and (d) molecule **4**.

## 2.5 TEM images of molecule 1-4

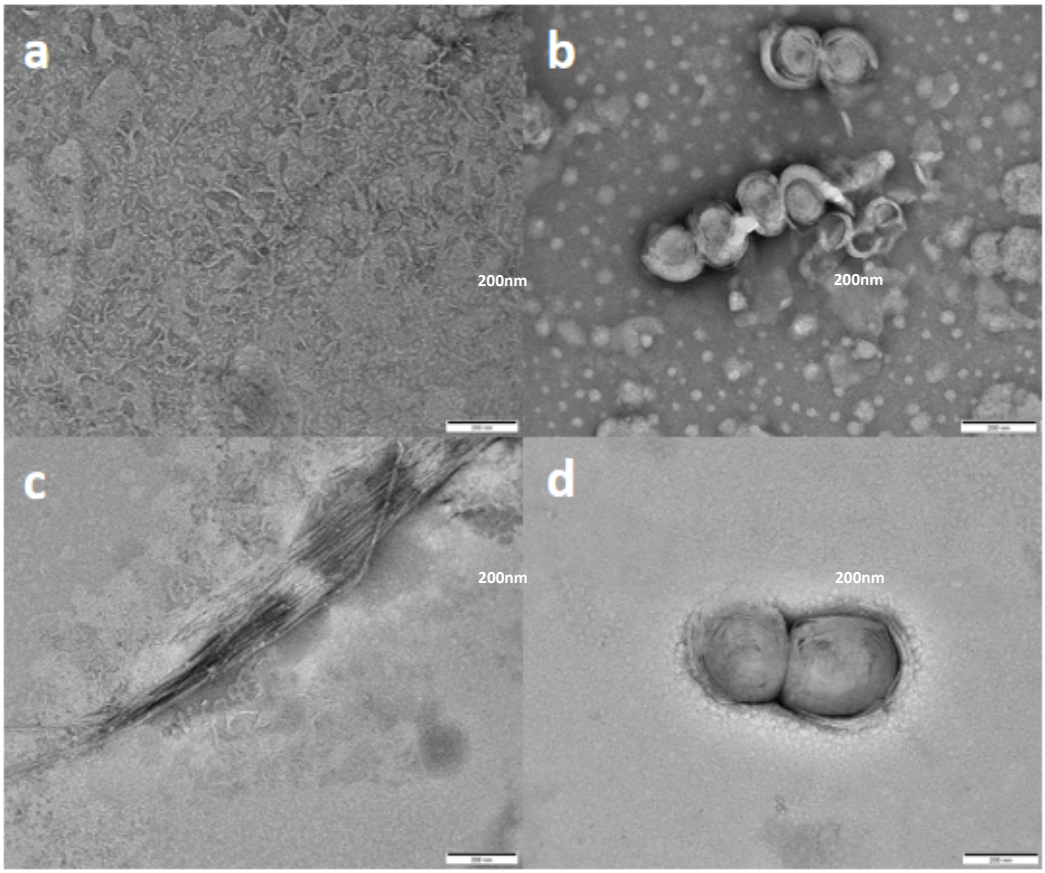



**Figure S11.** TEM image of molecule **1-4**, (a) molecule 1, (b) molecule 2, (c) molecule 3, and (d) molecule 4. [c]=25 μM

## 2.6 AFM images of molecule 1-4

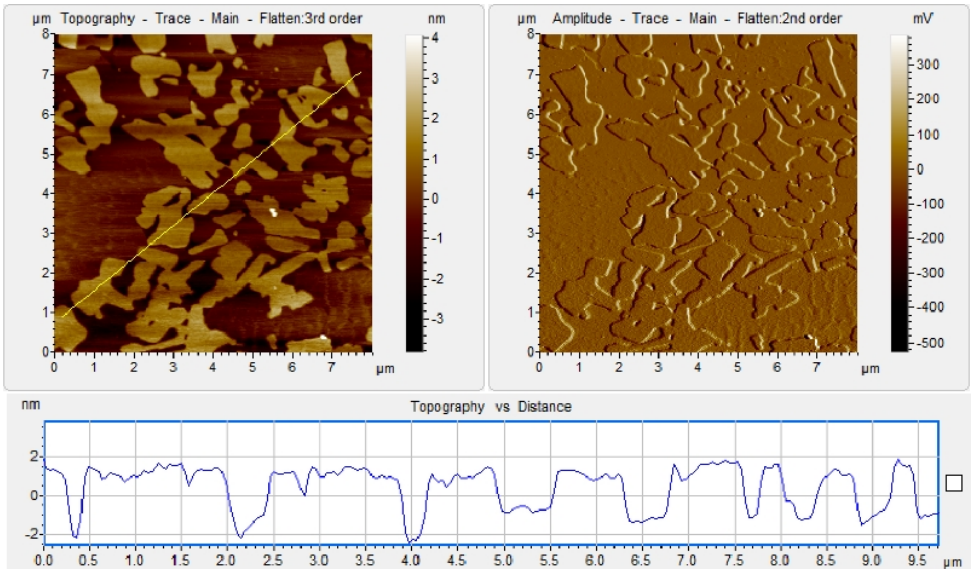



**Figure S12.** AFM image of molecule **1**, [c]=100 µM.

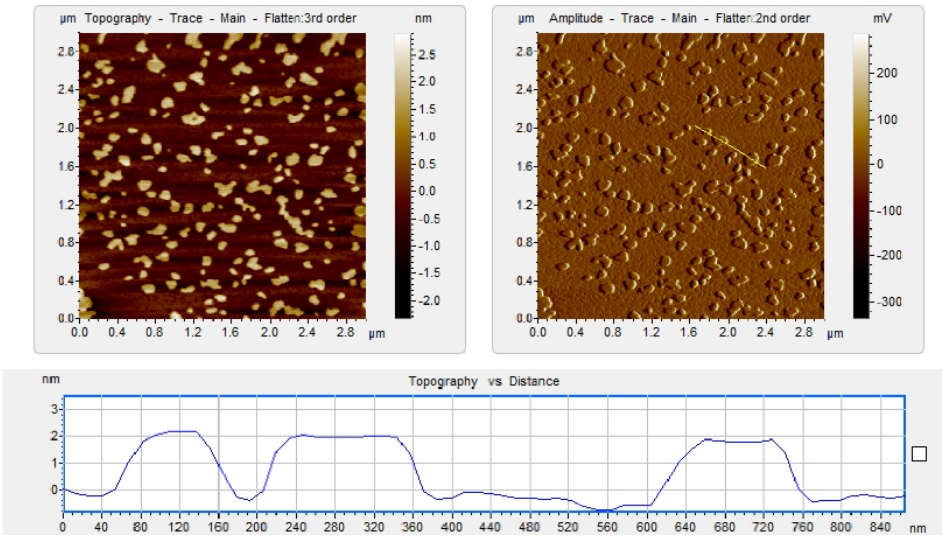



**Figure S13.** AFM image of molecule **2**, [c]=100 µM.

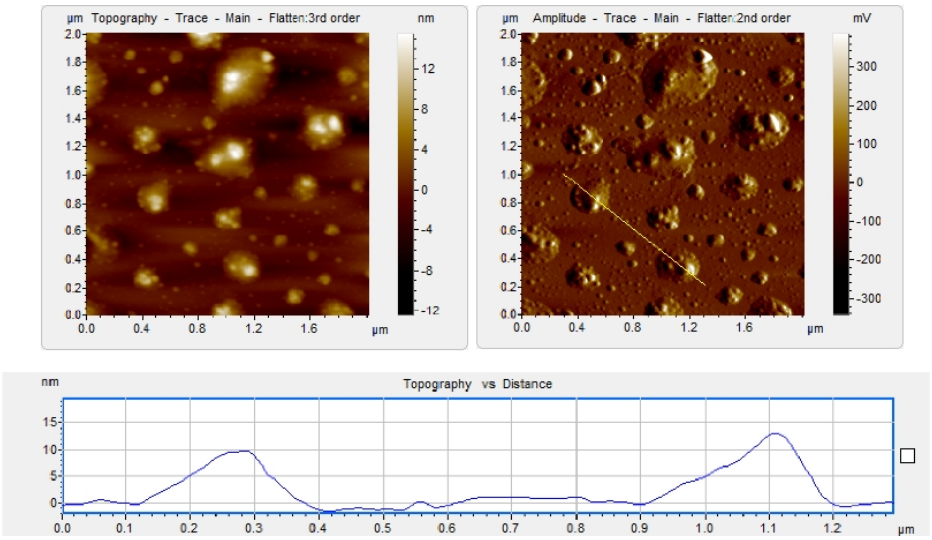



**Figure S14.** AFM image of molecule **3**, [c]=100 µM.

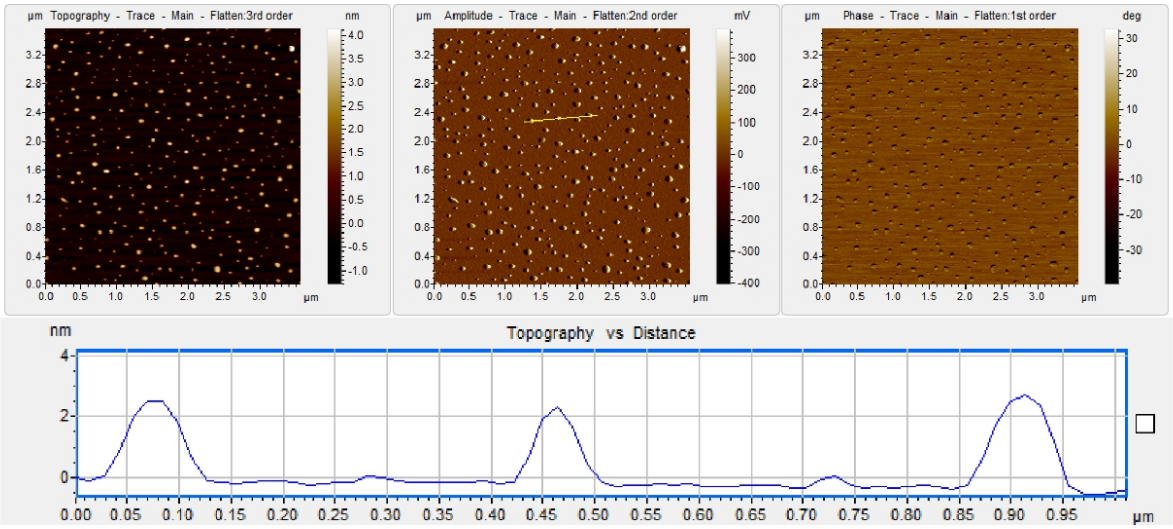



**Figure S15.** AFM image of molecule **3** with small aggregates, [c]=100 µM.

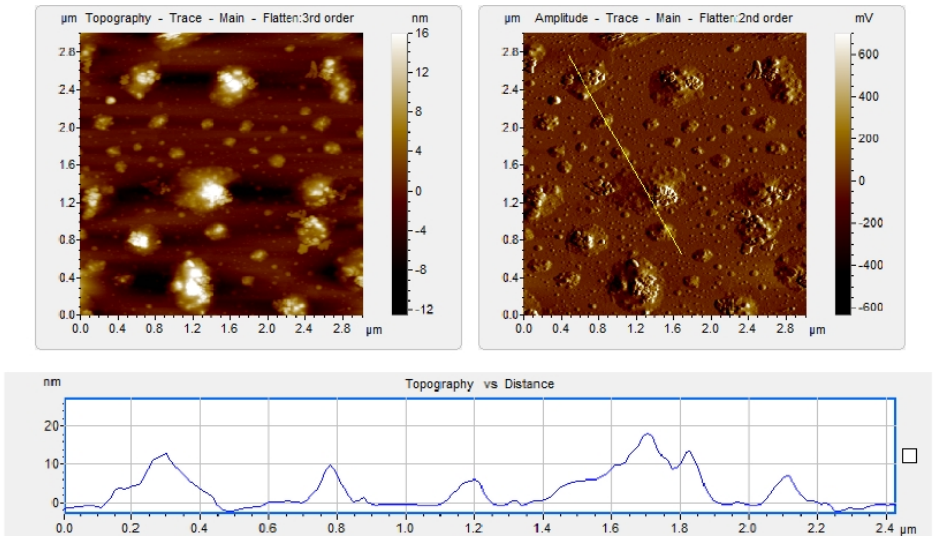



**Figure S16.** AFM image of molecule **4**, [c]=100 µM.

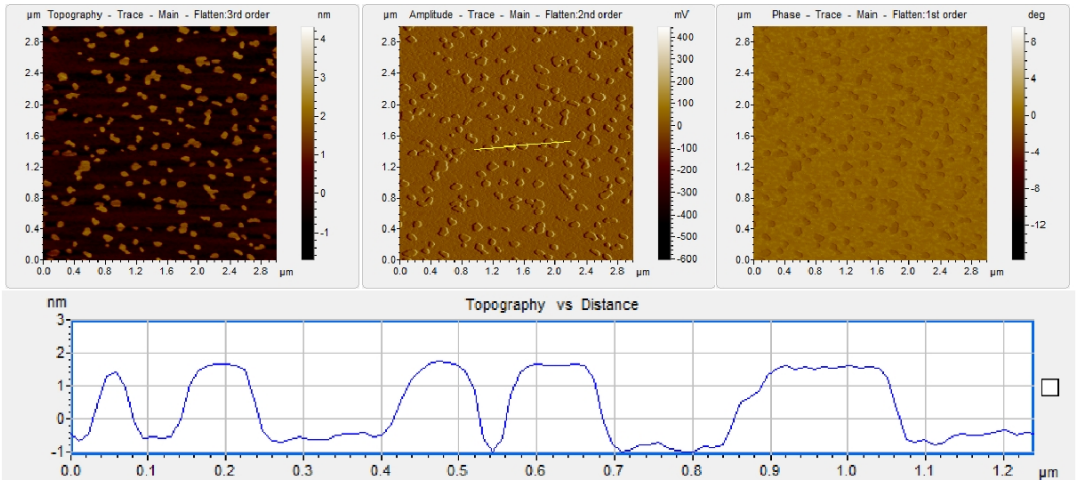



**Figure S17.** AFM image of molecule **4** with small aggregates, [c]=100 µM.

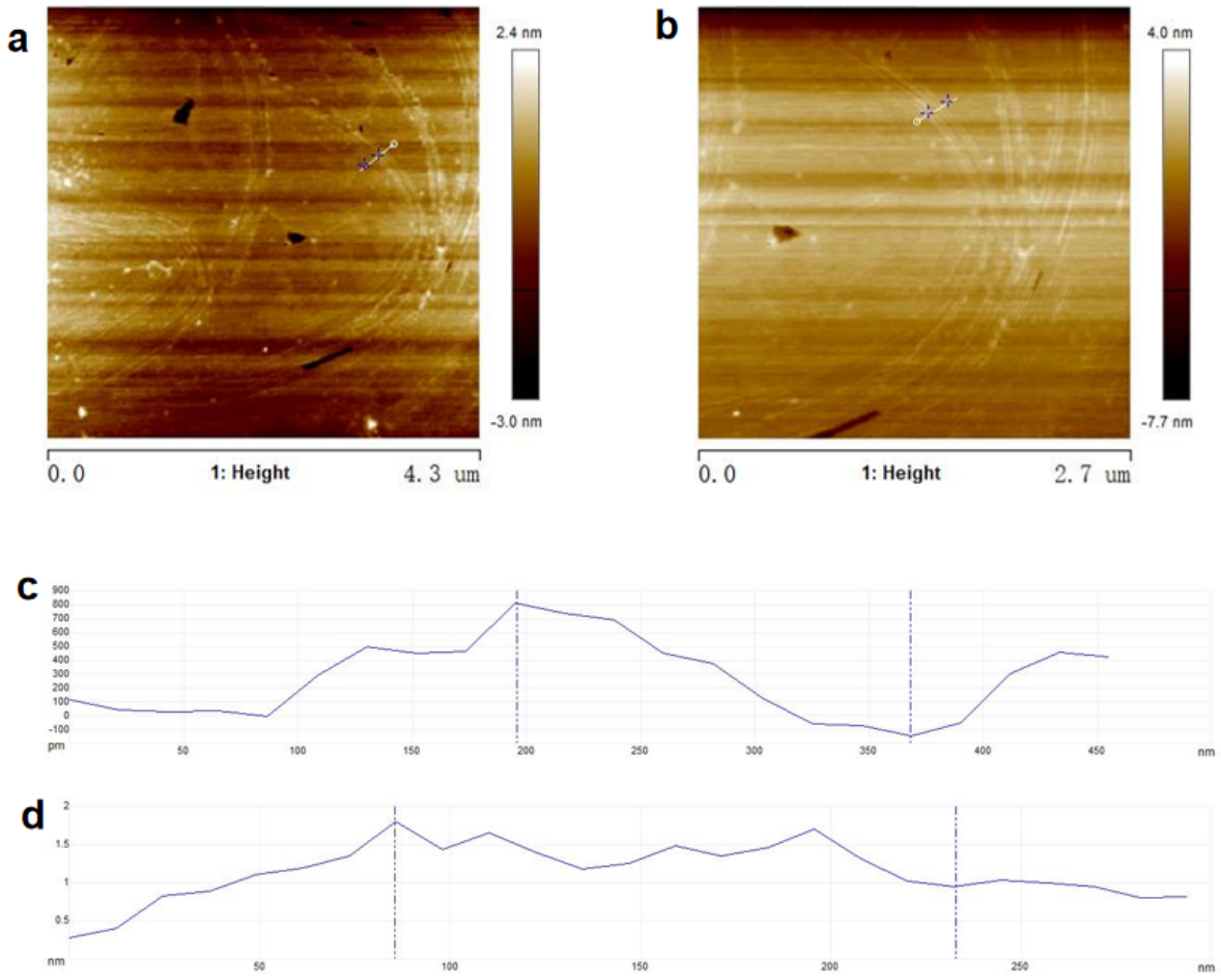



**Figure S18.** AFM images (a, b) and thickness (c, d) of molecule **3**, [c]=25 μM.

## 2.7 Molecular size calculation

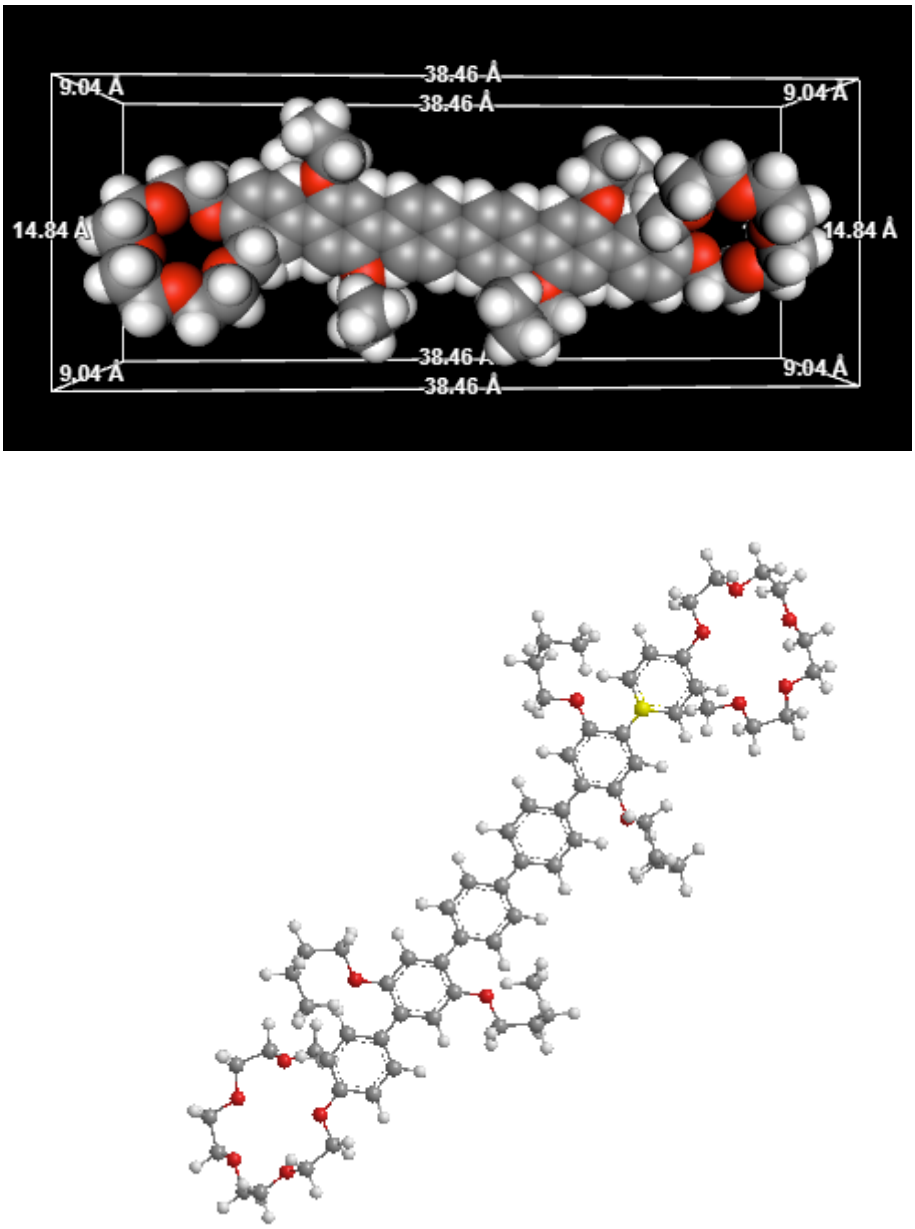
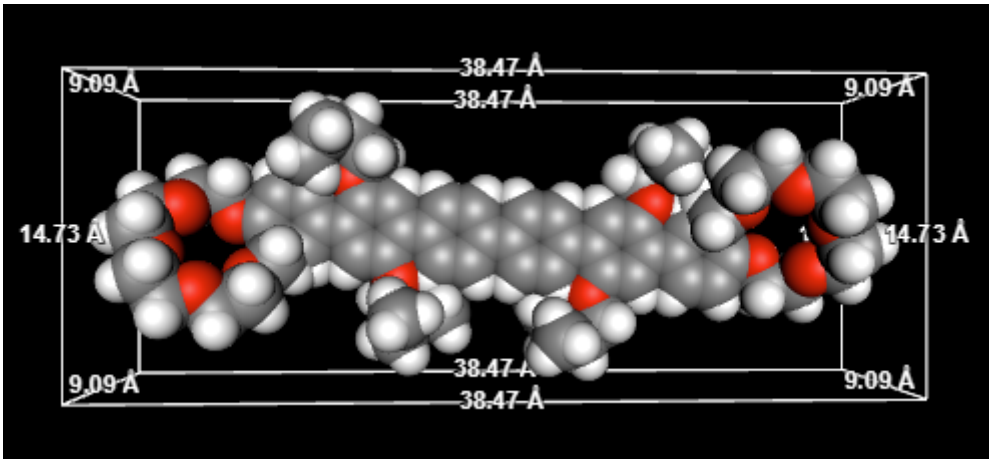



**Figure S19.** Structure and simulated size of molecule **1**.



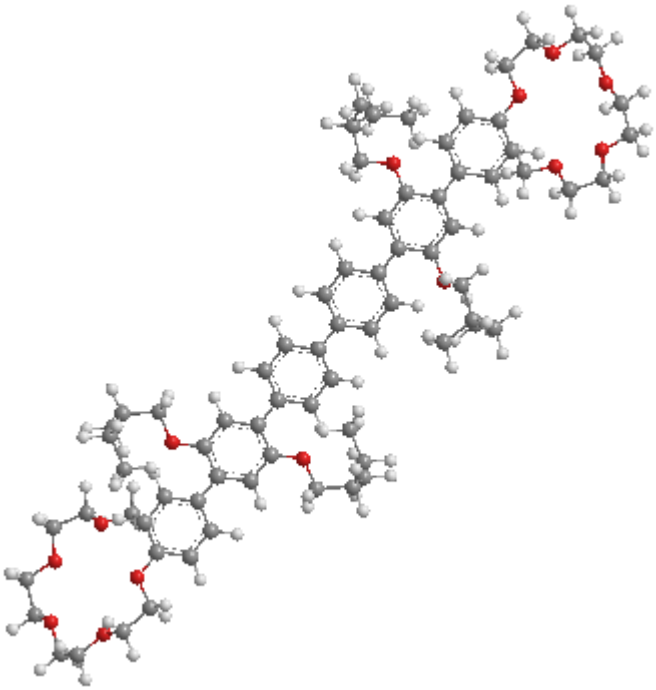



**Figure S20.** Structure and simulated size of molecule **2**.

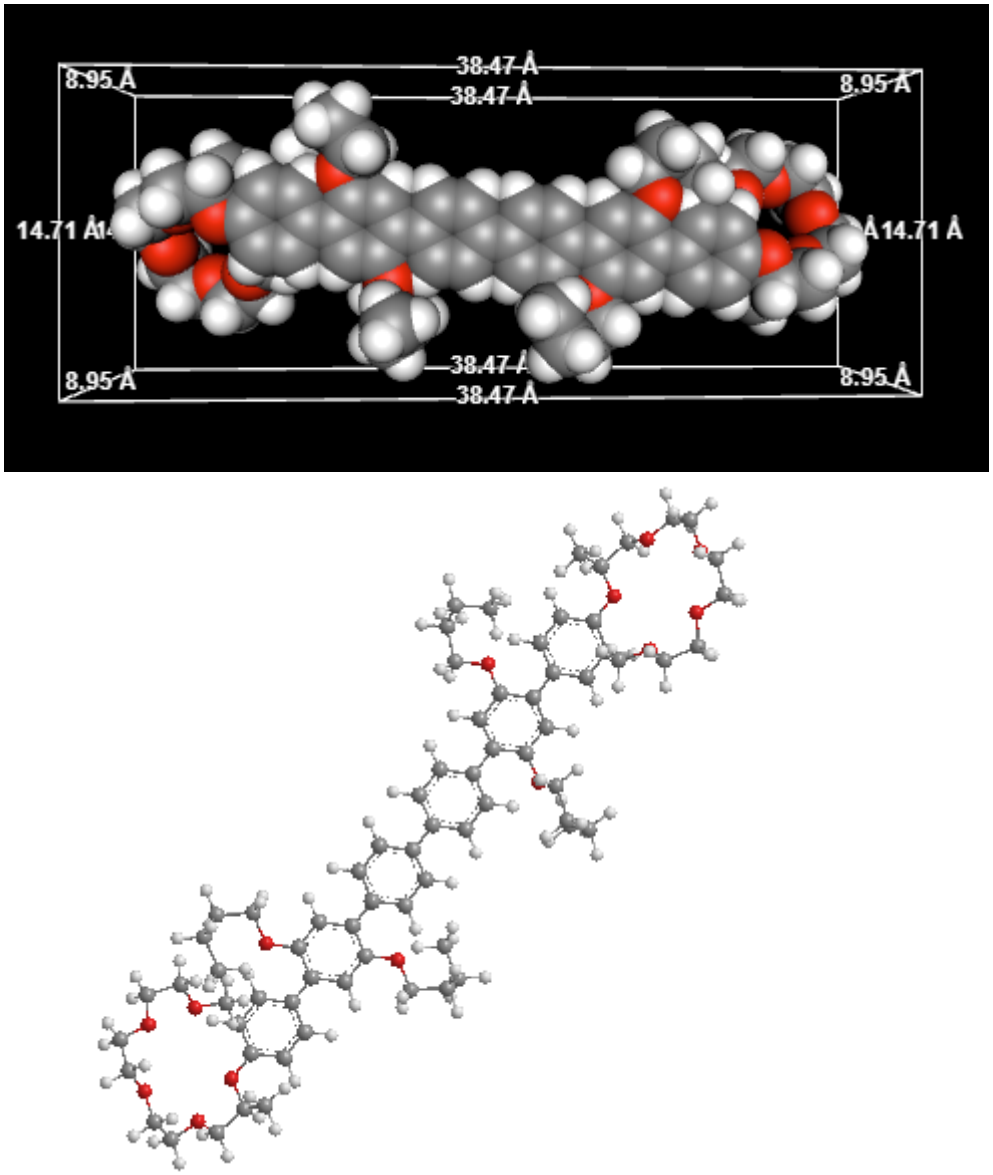



**Figure S21.** Structure and simulated size of molecule **3**.

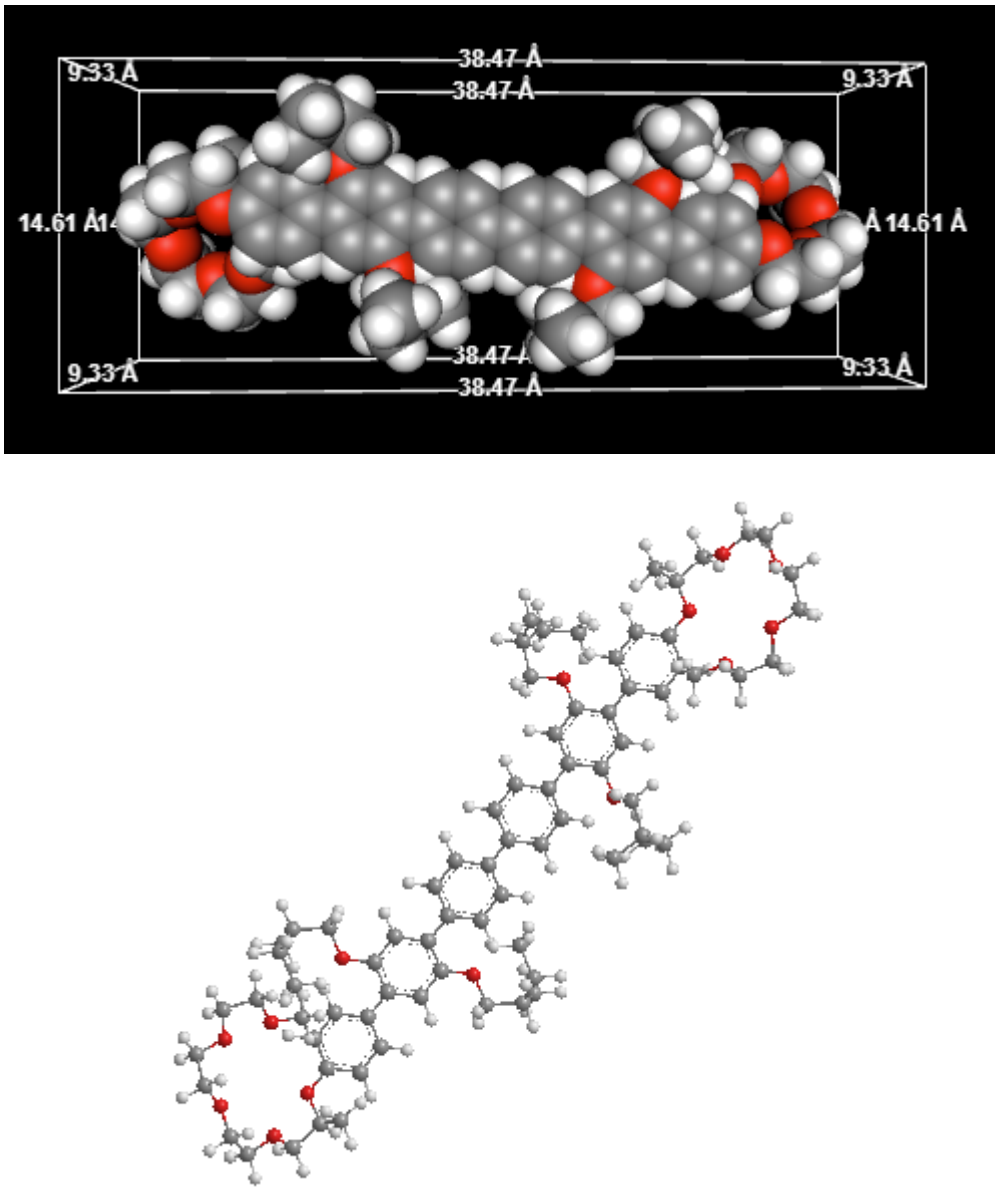



**Figure S22.** Structure and simulated size of molecule **4**.

## 2.8 CD spectra of molecule 4

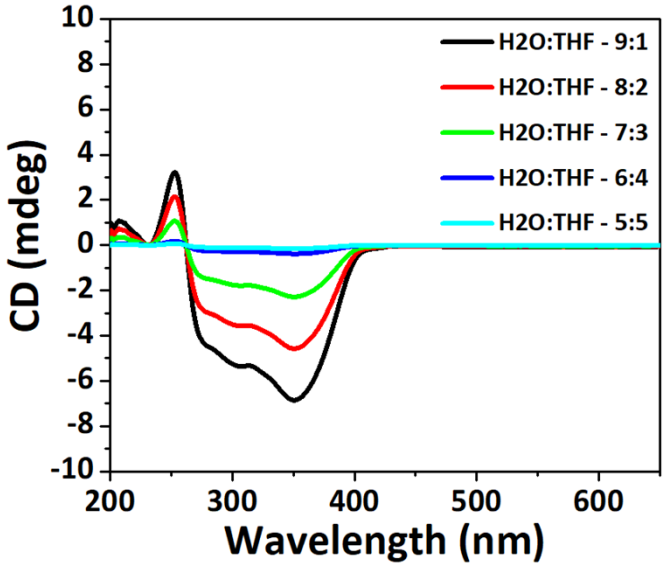



**Figure S23.** CD spectra of molecule **4** in $H_2O$/THF mixed solvent with various volume ratios under the concentration of 25 μM. The absorption anisotropy factor, $g_{abs}$, was calculated to be $6.83*10^{-6}$, $1.23*10^{-5}$, $5.62*10^{-5}$, $1.22*10^{-4}$, $2.18*10^{-4}$, for water content of 50%, 60%, 70%, 80%, 90%, respectively.

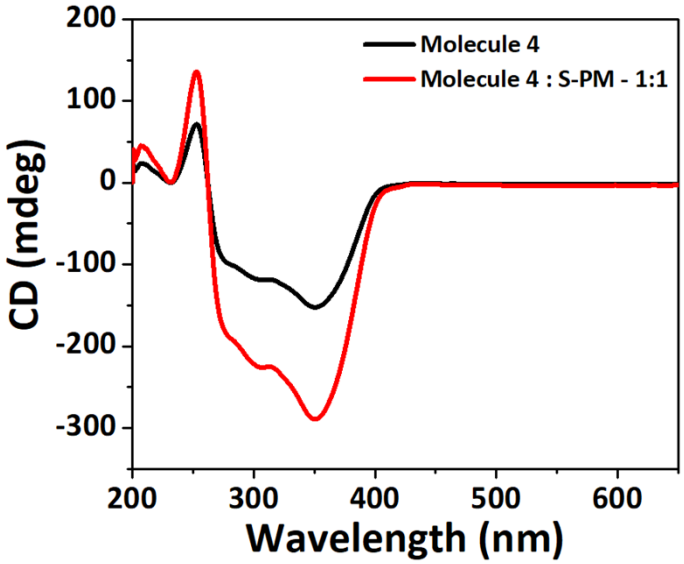



**Figure S24.** CD spectra of molecule **4** in the presence of *S*-PM-Ts.

## 2.9 Enantioselective synthesis results of molecule 1-4

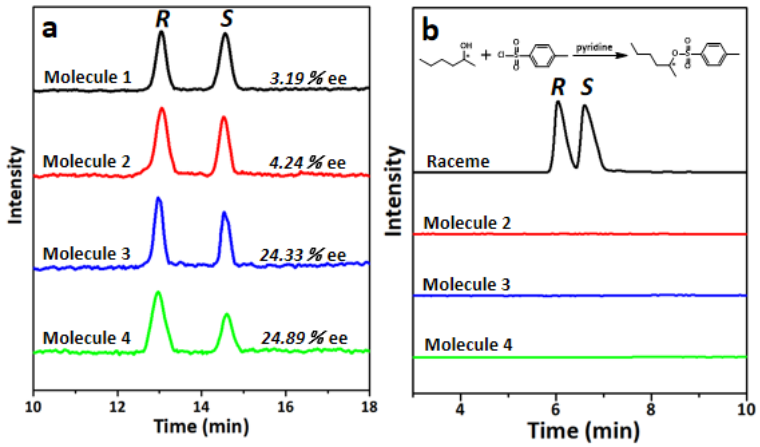



**Figure S25.** Chiral HPLC chromatograms results of nucleophilic substitution reaction from a) racemic 1-methoxypropan-2-ol (PM) and TsCl in the presence of molecule **1**-**4**, b) from racemic 2-hexanol and TsCl in the presence of molecule **2**-**4**.

## 2.10 Emission spectra of aggregates and absorption spectra of dye

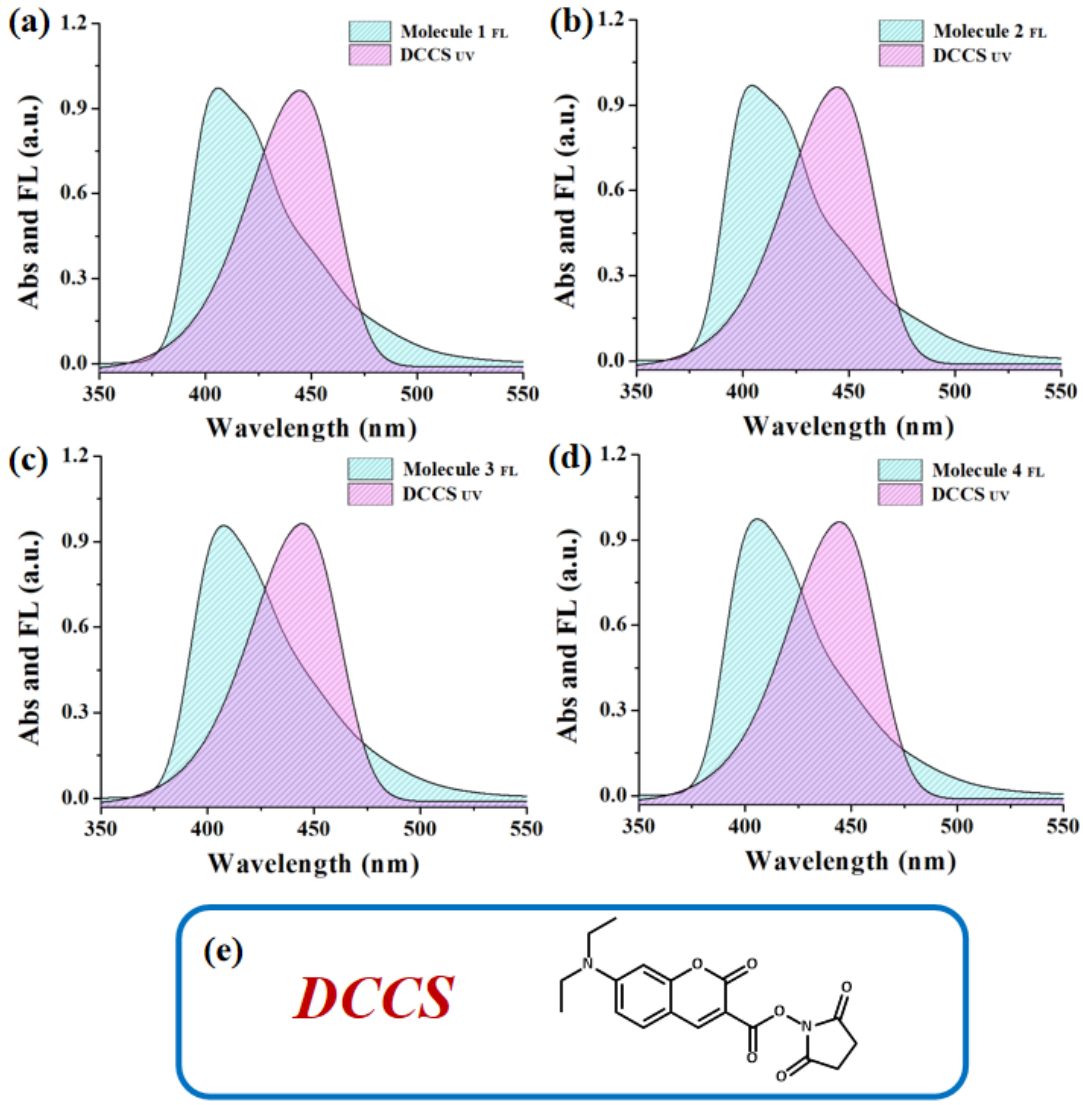



**Figure S26.** (a, b, c, d) Normalized emission spectra (filled with cyan) of the molecules **1-4** and absorption spectra (filled with pink) of DCCS respectively. (e) Molecular structure of DCCS.