

Supplementary materials

Self-Assembled Nanotubes Based on Chiral H₈-BINOL Modified with 1,2,3-Triazole to Recognize Bi³⁺ Efficiently by ICT Mechanism

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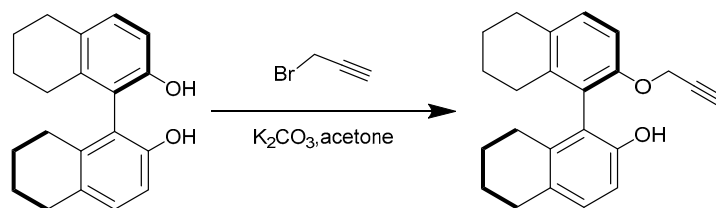
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1.Synthesis of R-P



R-H₈-BINOL (2.0 g, 6.79 mmol), potassium carbonate (1.88 g, 13.6 mmol) and acetone (15.0 mL) as solvent were added to a 100 mL three-necked flask at room temperature. 3-Bromopropargyl (0.94 mL, 10.87 mmol) was slowly added to the three-necked flask and stirred at room temperature for 5-7 min, heated to 60°C and refluxed for 12 h. The solution was then analyzed by TLC. The reaction was quenched when TLC detection (EA:PE=1:4) showed complete reaction of the raw material. The system was cooled to room temperature, the reaction liquid was filtered through a recirculating pump and the filtrate was washed three times with acetone. About 200-300 mesh of silica was added to the filtrate and the solvent was dried on a rotary evaporator to give a yellow-brown powder. Column chromatography using petroleum ether and ethyl acetate as eluents (V(PE):V(EA) = 15:1) yielded 1.56 g of yellow-brown solid in 69.3% yield. ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.73 (s, 1H), 7.13 (d, J = 8.4 Hz, 1H), 7.02 (d, J = 8.4 Hz, 1H), 6.95 (d, J = 8.2 Hz, 1H), 6.77 (d, J = 8.2 Hz, 1H), 4.73 (d, J = 2.5 Hz, 2H), 3.57 (s, 1H), 2.88 – 2.73 (m, 4H), 2.73 – 2.64 (m, 4H), 2.45 – 2.26 (m, 2H), 2.09 (dd, J = 30.4, 17.0 Hz, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 152.02, 151.58, 135.90, 135.24, 129.30, 127.99, 127.74, 126.55, 126.15, 122.86, 112.50, 110.30, 79.69, 77.18, 55.08, 28.51, 26.48, 26.35, 22.55, 22.45.

2. ^1H NMR, ^{13}C NMR of 1-azido-2,3,4,6-tetra-O-acetyl- β -D-glucose (DMSO- D_6)

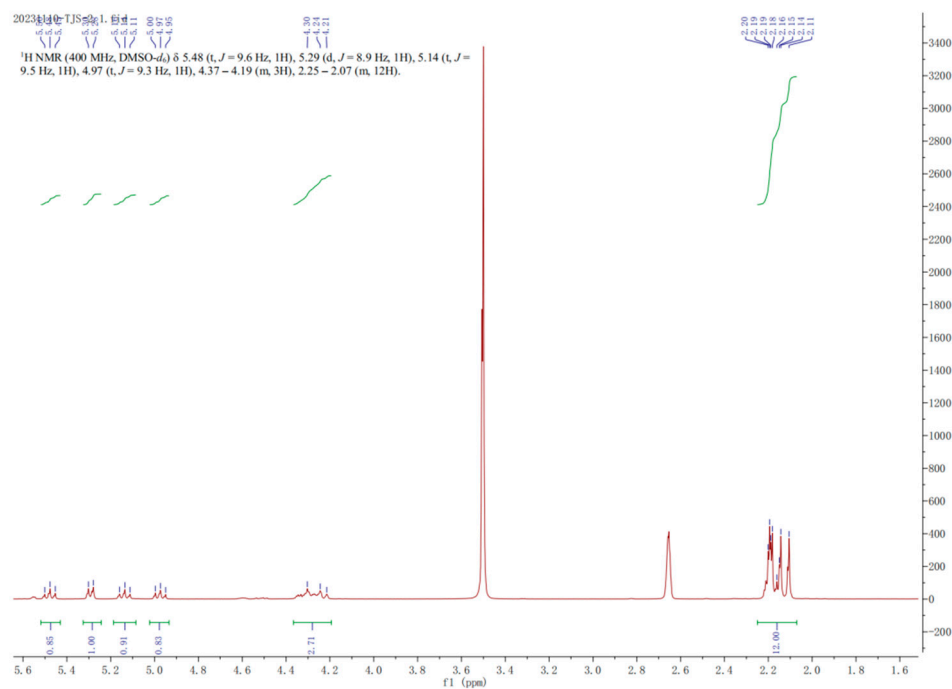


Figure S1. ^1H NMR of 1-azido-2,3,4,6-tetra-O-acetyl- β -D-glucose (DMSO- d_6)

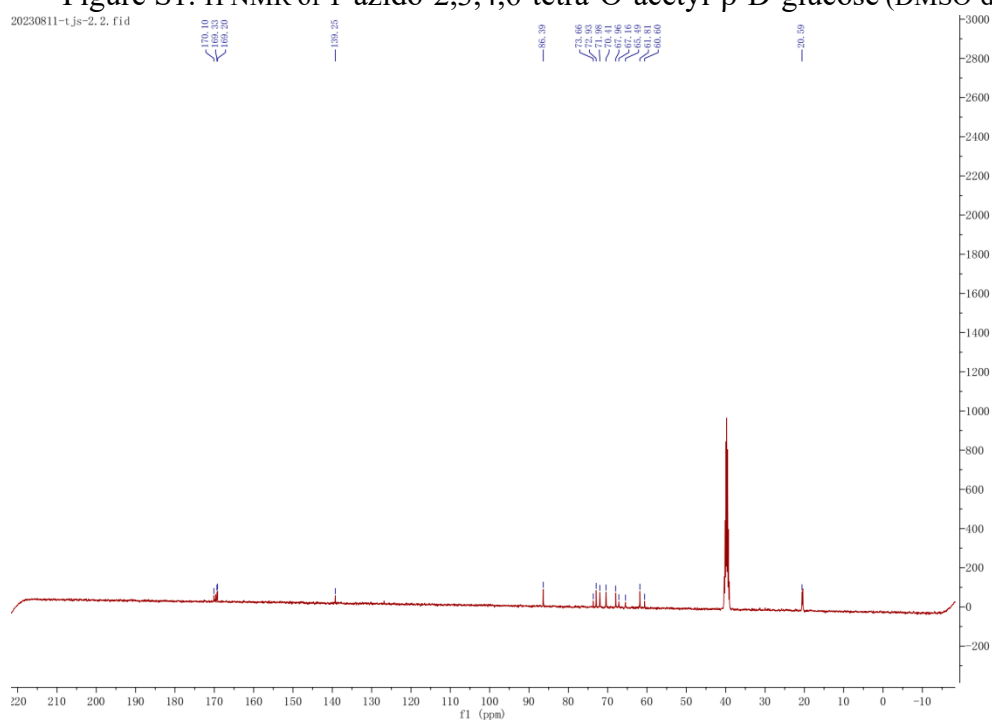


Figure S2 ^{13}C NMR of 1-azido-2,3,4,6-tetra-O-acetyl- β -D-glucose (DMSO- d_6)

3. ^1H NMR, ^{13}C NMR of *R*-**P** (DMSO- D_6)

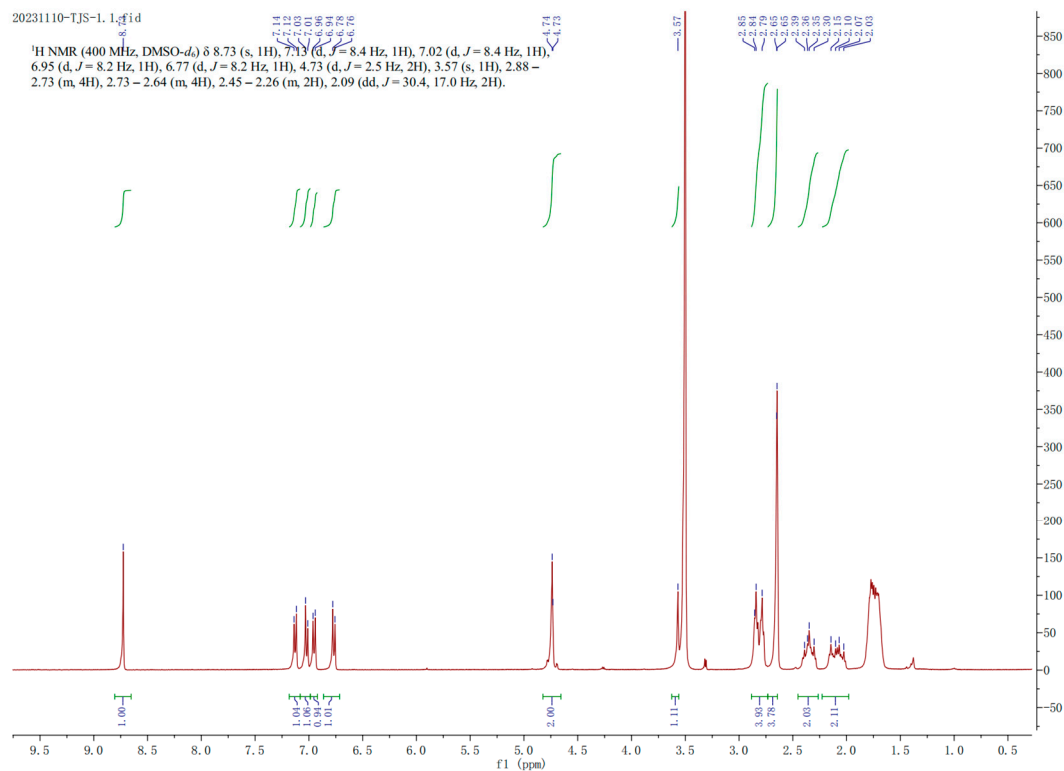


Figure S3 ^1H NMR of *R*-**P** (DMSO- d_6)

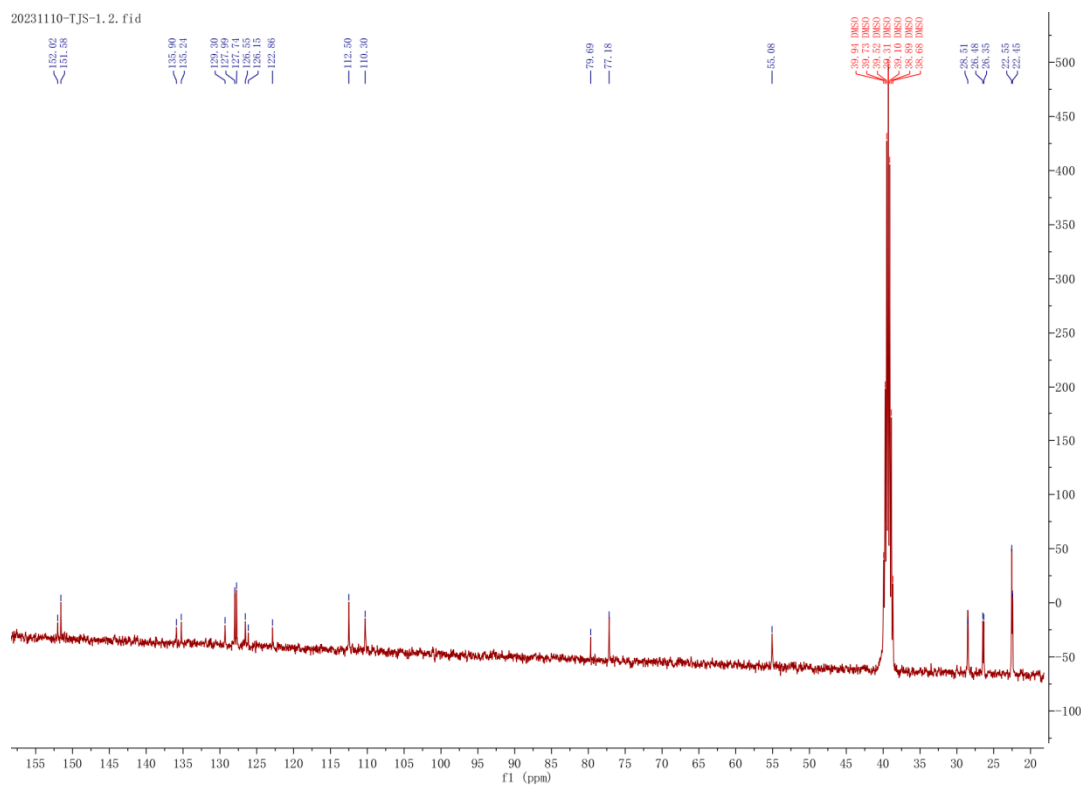


Figure S4 ^{13}C NMR of *R*-**P** (DMSO- d_6)

4. ^1H NMR, ^{13}C NMR of *R*- β -D-1

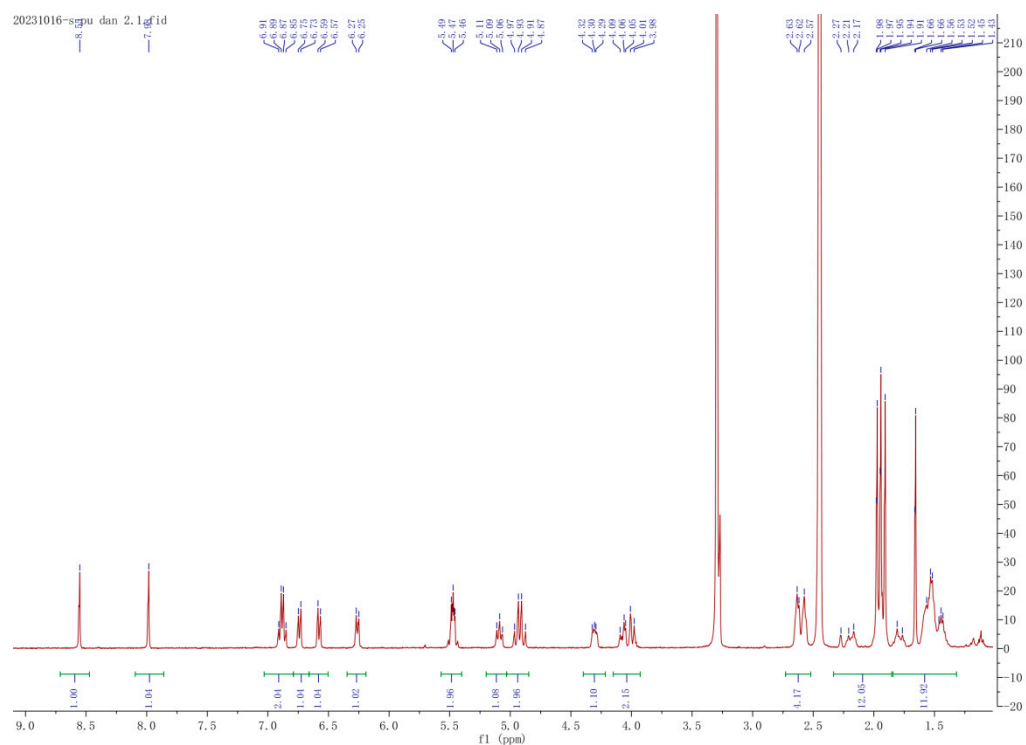


Figure S5 ^1H NMR of *R*- β -D-1 (DMSO- d_6)

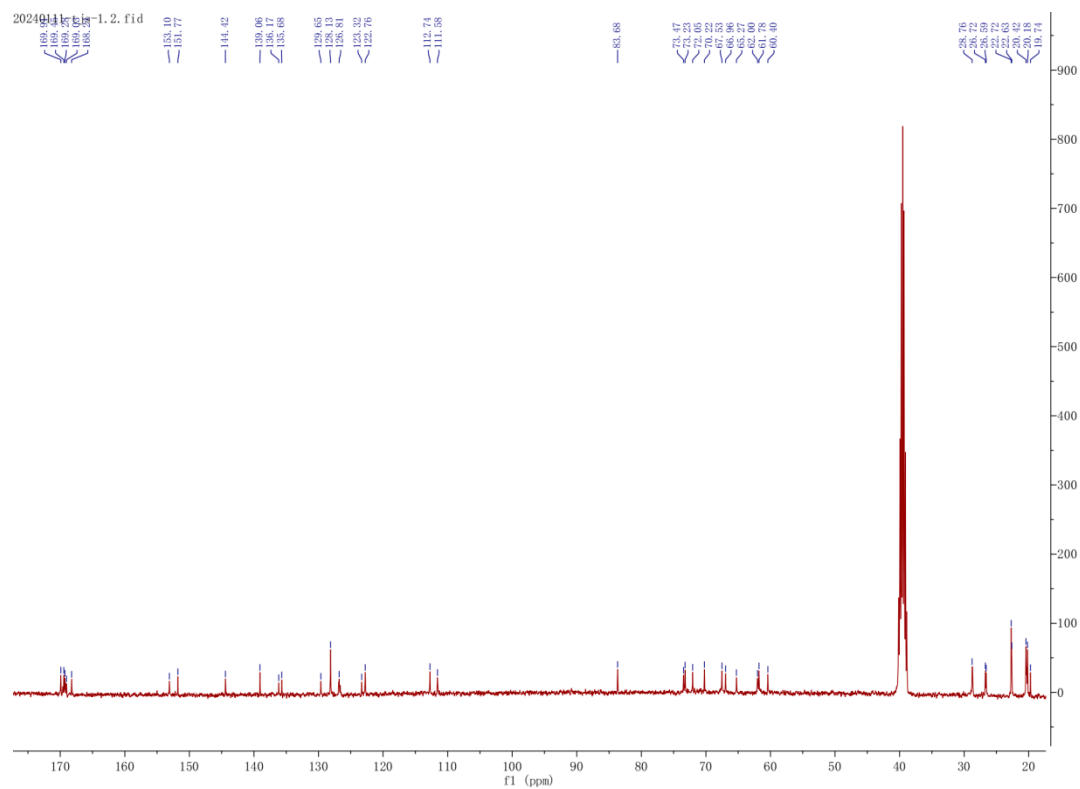


Figure S6 ^{13}C NMR of *R*- β -D-1 (DMSO- d_6)

5. MS plot of *R*- β -D-1

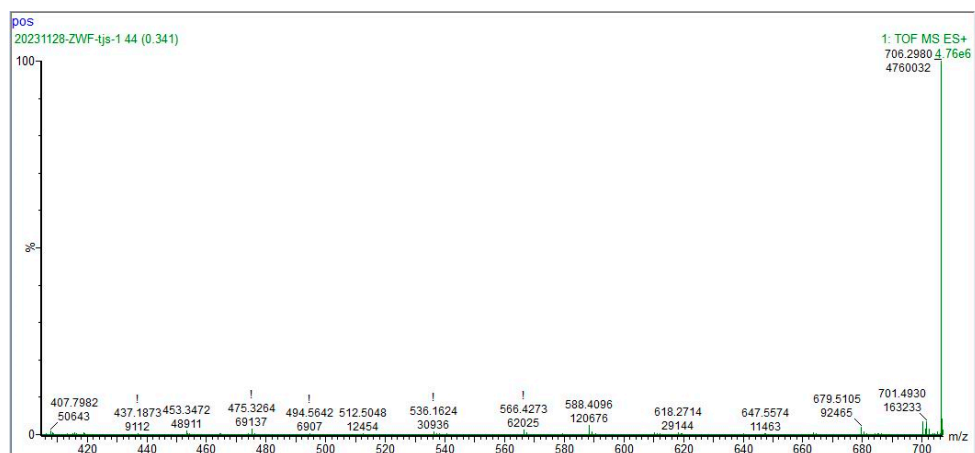


Figure S7 mass spectrometry of *R*- β -D-1

6. Histogram of *R*- β -D-1 with Bi^{3+} in the presence of different anions

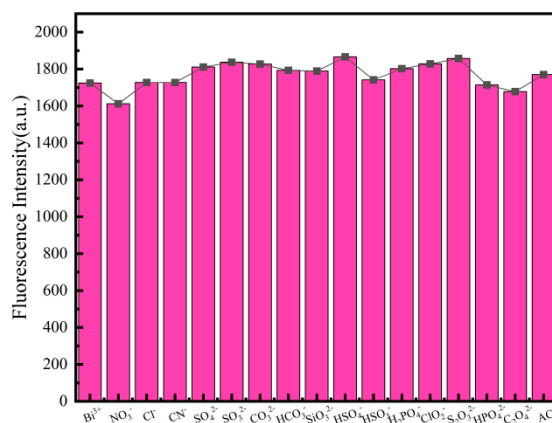


Figure S8 Fluorescence histogram of *R*- β -D-1 versus Bi^{3+} in the presence of different anions

7. Preparation of fluorescence test samples

7 mg of probe *R*- β -D-1 in a 10 mL volumetric flask, add chromatographic methanol to dissolve and quantify to 10 mL, at this time, the concentration of the test masterbatch is 0.001 M. Next, the masterbatch will be diluted to 2.0×10^{-5} M, and taken at any time when needed.

Commonly used ion configuration (BaCl_2 , MnCl_2 , CuCl , CaCl_2 , KCl , CoCl_3 , CrCl_3 , ZnCl_2 , AlCl_3 , MgCl_2 , PbCl_2 , AgCl , CdCl_2 , GdCl_3 , LiCl , NaCl , NH_4Cl , NiCl_2 , BiCl_3 configured into a concentration of 0.1 M)(Methanol solution, need to be ready to use, room temperature 25°C, take 2mL test solution added to 3.5mL high transparent quartz fluorescence cuvette, add 2 μL of ions to be tested, fluorescence test).

Commonly used anionic formulations (KNO_3 , NaCl , NaCN , Na_2SO_4 , Na_2SO_3 , Na_2CO_3 , NaHCO_3 , Na_2SiO_3 , NaHSO_4 , NaHSO_3 , NaH_2PO_4 , NaClO_2 , $\text{Na}_2\text{S}_2\text{O}_3$, NaHPO_4 , $\text{Na}_2\text{C}_2\text{O}_4$, and CH_3COONa configured into a concentration of 0.1 M) (water solution, the solution should be ready to use, room temperature 25°C , take 2mL of the test solution and add it into a 3.5mL high transparent quartz fluorescence cuvette, add 2 μL Bi^{3+} ions, then add 2 μL of the anionic to be tested for the fluorescence test).

8. Method of calculating charge density difference (CDD)

Ab initio calculations were performed with the periodic density functional theory (DFT) code Vienna ab initio simulation package (VASP) [1,2]. The exchange and correlation energy was calculated within the generalized gradient approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE) functional [3,4]. To include van der Waals forces, we added the D3 correction as implemented by Grimme et al [5,6]. The electron-core interaction was described with the projector augmented wave (PAW) method [7]. The electronic wave functions were expanded using a plane wave basis set with an energy cutoff of 400 eV. Gamma type k-point meshes of $1 \times 1 \times 1$ were used for electronic structure analysis [8-12].

9. SEM plots of the sensor *R*- β -D-1 with Bi^{3+} in methanol

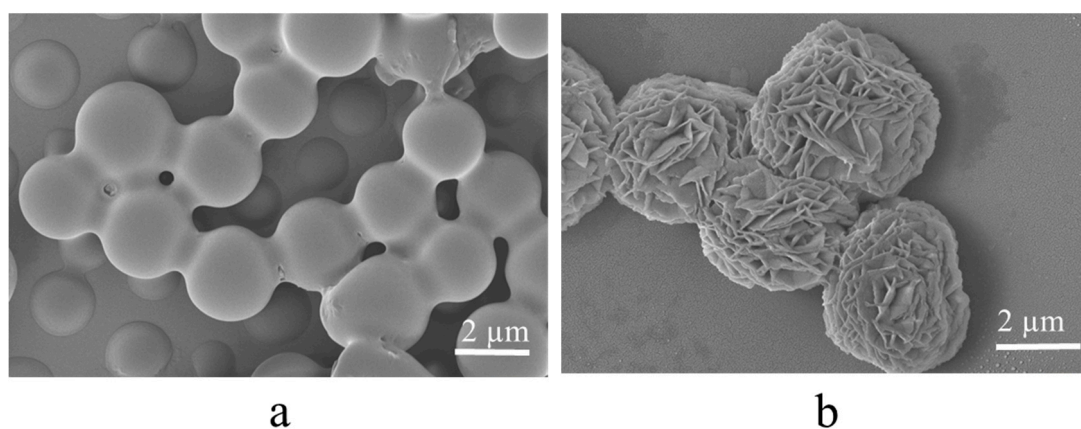


Figure S9 a SEM image of *R*- β -D-1 in methanol solvent, b is the SEM morphology change of *R*- β -D-1 with the addition of Bi^{3+} .

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