Electronic Supplementary Material (ESI) for Chemical Communications

Supplementary Information for:

Different Superstructures formed by Janus-type Nucleosides

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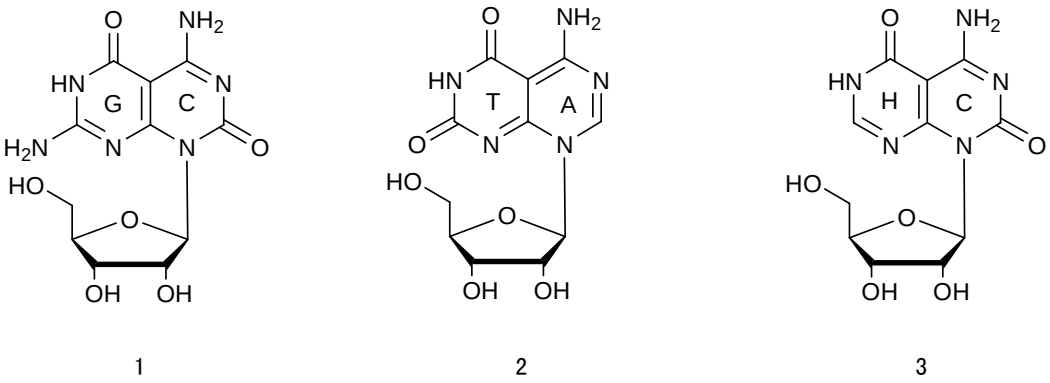
Abbreviations

DMF (N,N–dimethylformamide); H_2O (deionized NanoPure water); MeOH (methanol); h (hour); Tapping mode atomic force microscopy (TM-AFM); SEM (scanning electron microscopy); TEM (transmission electron microscopy); ESI–MS (electrospray ionization mass spectrometry); CD (circular dichroism)

General

The samples were prepared by dissolving (compound **1**-**3**, 1 mg/mL) in DMF. The solutions were heated to ~100°C and allowed to cool to room temperature for ~48 h, then investigated by SEM, AFM and TEM.



1 2 3

Figure S1. The structures of compound **1**-**3.**

SEM Imaging

SEM was performed using a high resolution INSPECT F50. All SEM images were obtained without staining. Samples were prepared by dissolving (compound **1**-**3**, 1 mg/mL) in DMF. The solutions were heated to ~100°C and allowed to cool to room temperature for ~48 h.

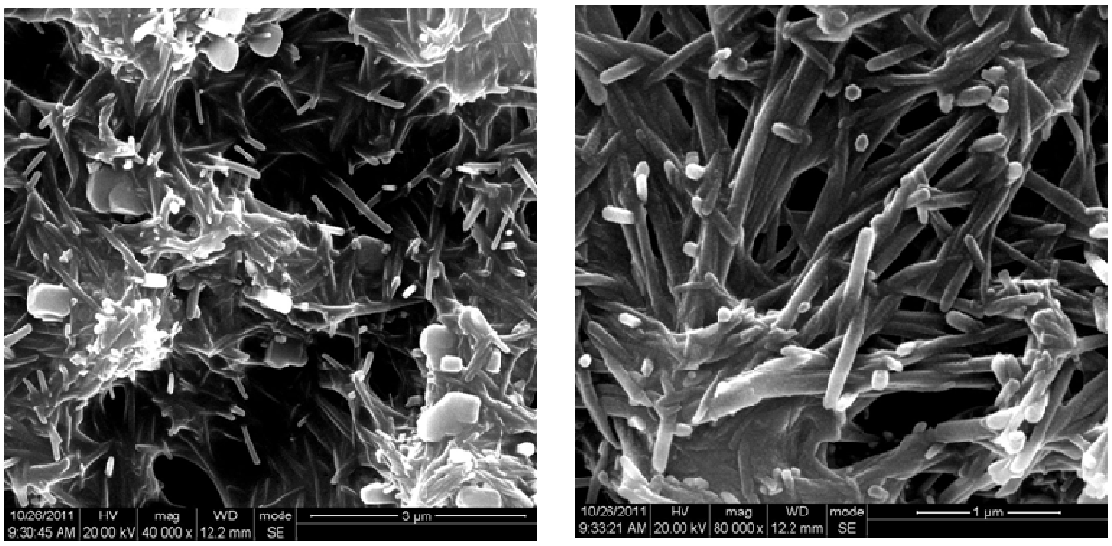


Figure S2. SEM images of compound **1** (1 mg/mL in DMF) recorded on INSPECT F50

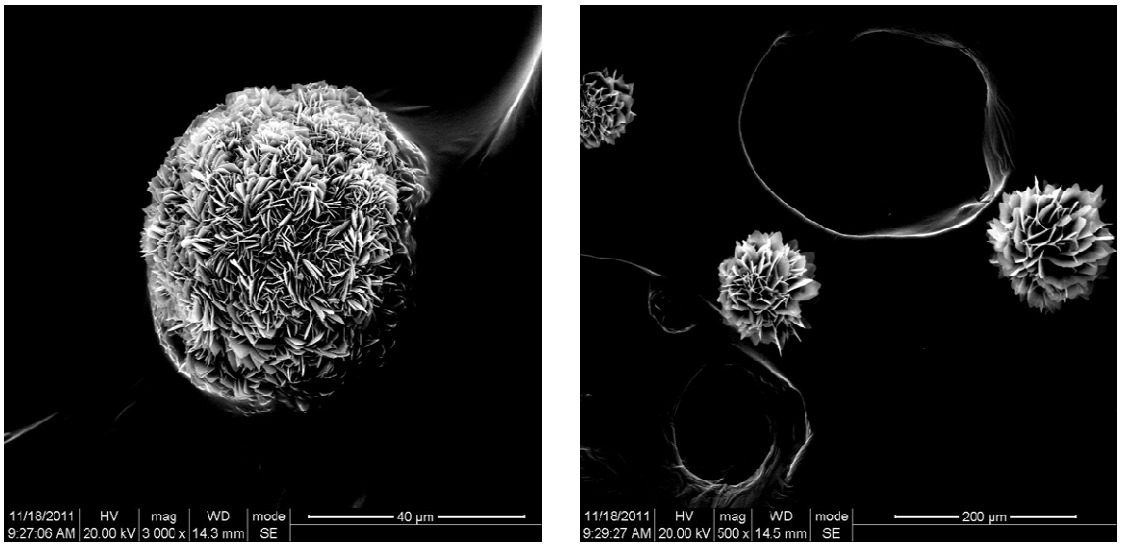


Figure S3. SEM images of compound **2** (1 mg/mL in DMF) recorded on INSPECT F50

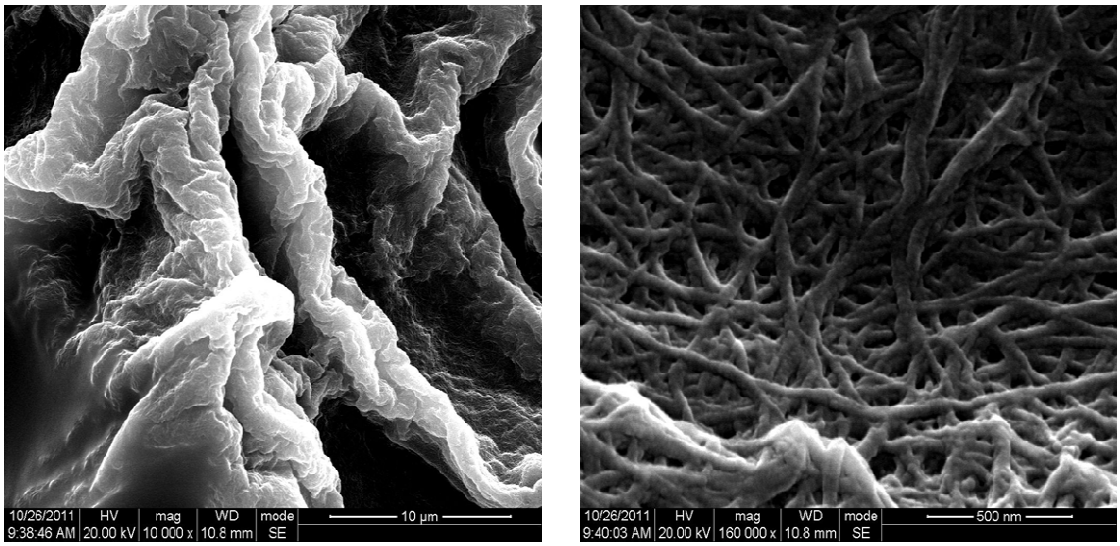


Figure S4. SEM images of compound **3** (1 mg/mL in DMF) recorded on INSPECT F50

AFM Imaging

AFM measurements were performed in tapping mode (TM–AFM) at amplitude setpoint of 1 V using SPI4000 (Seiko Instruments, Chiba, Japan). Soft silicon cantilevers were chosen (SI-DF2000, K-A102001604, Japan) with spring constant of 5 N/m. Clean mica substrates (1×1 cm^2) were prepared and 5 µL of the RNT samples (1 mg/mL in DMF) were deposited onto a freshly cleaved mica surface. The mica surface with the adsorbed samples was then dried in air and imaged immediately.

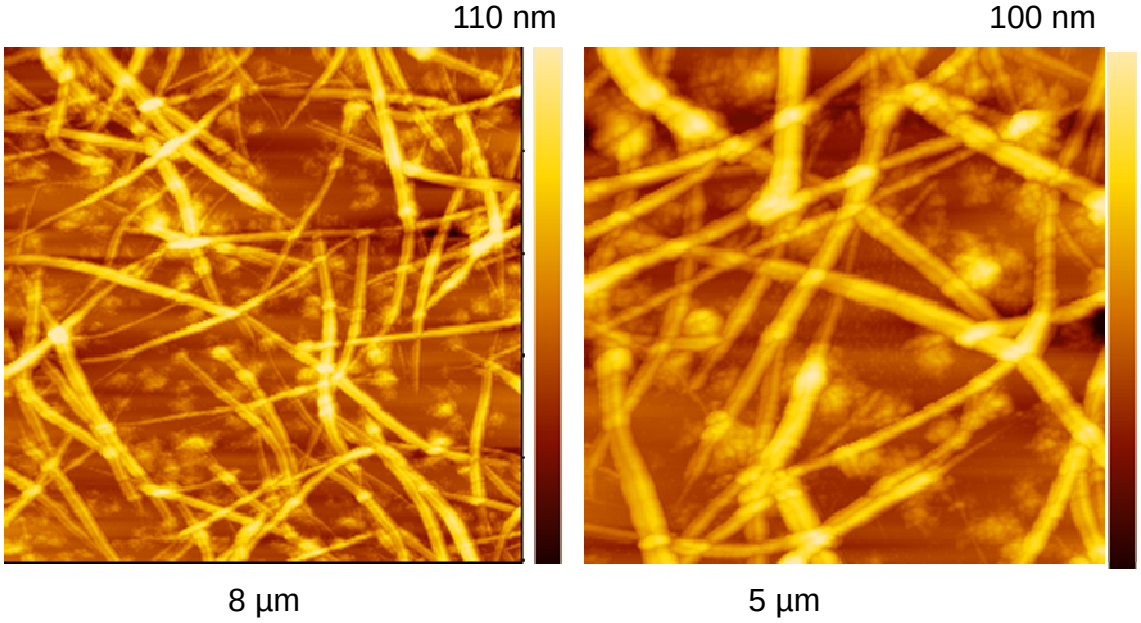


Figure S5. TM–AFM height and amplitude images of compound **1** (1 mg/mL in DMF).

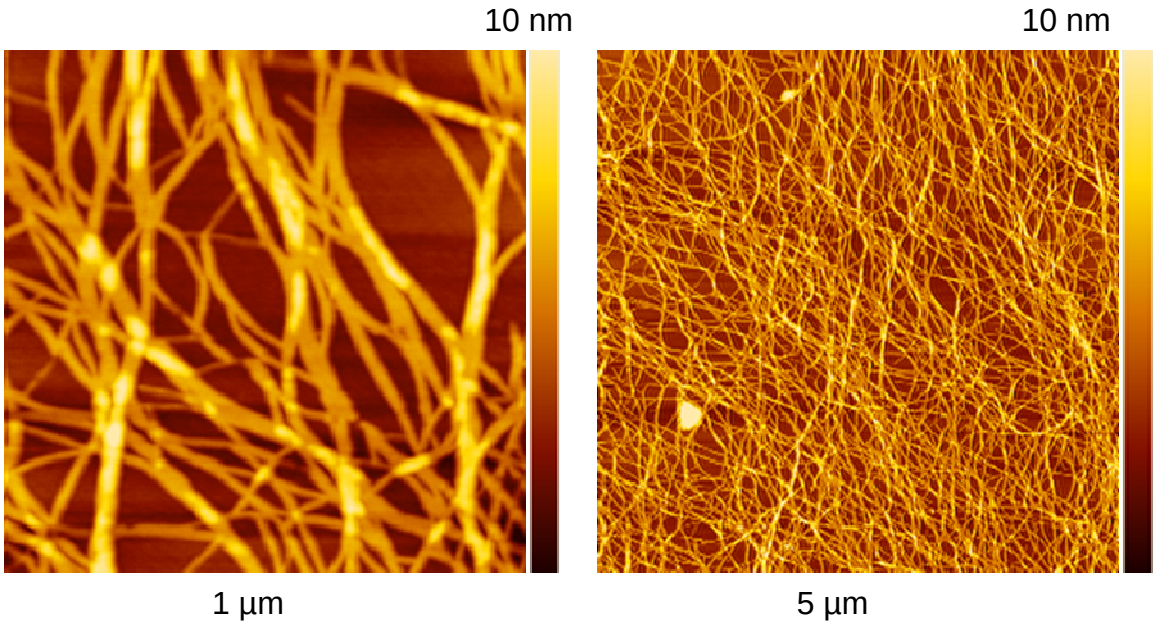


Figure S6. TM–AFM height and amplitude images of compound **3** (1 mg/mL in DMF).

TEM Imaging

TEM images were recorded on a Tecnai G^2 F_{20} microscope operated at 200KV, 5 µL of each solution were placed on micro ultra-thin carbon coated TEM grid for 1 min before excess material was blotted with filter paper. All the samples were air-dried for 2 h at room temperature. The grids were staining with phosphotungstic acid and dried at room temperature before imaging.

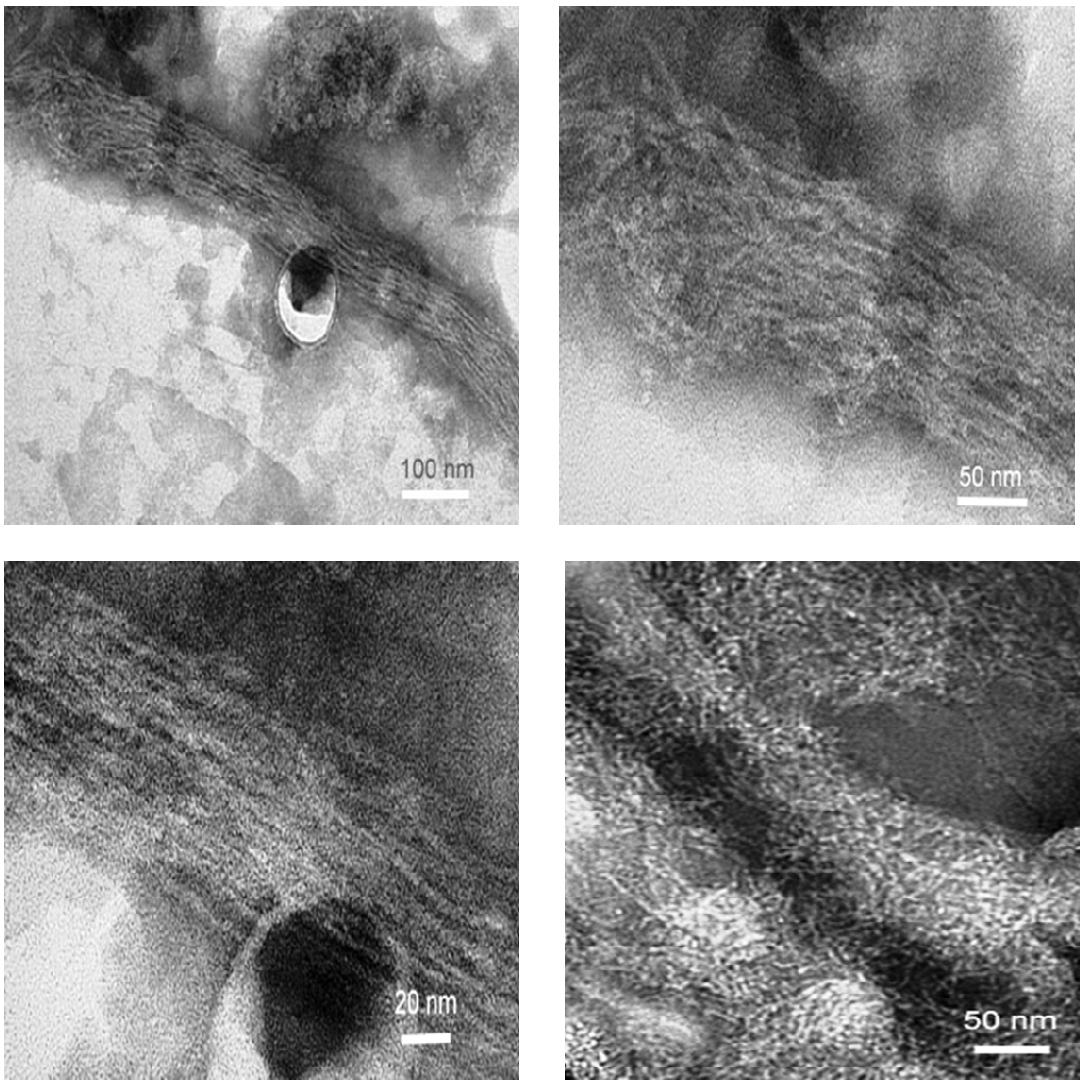


Figure S7. TEM images of compound **1**

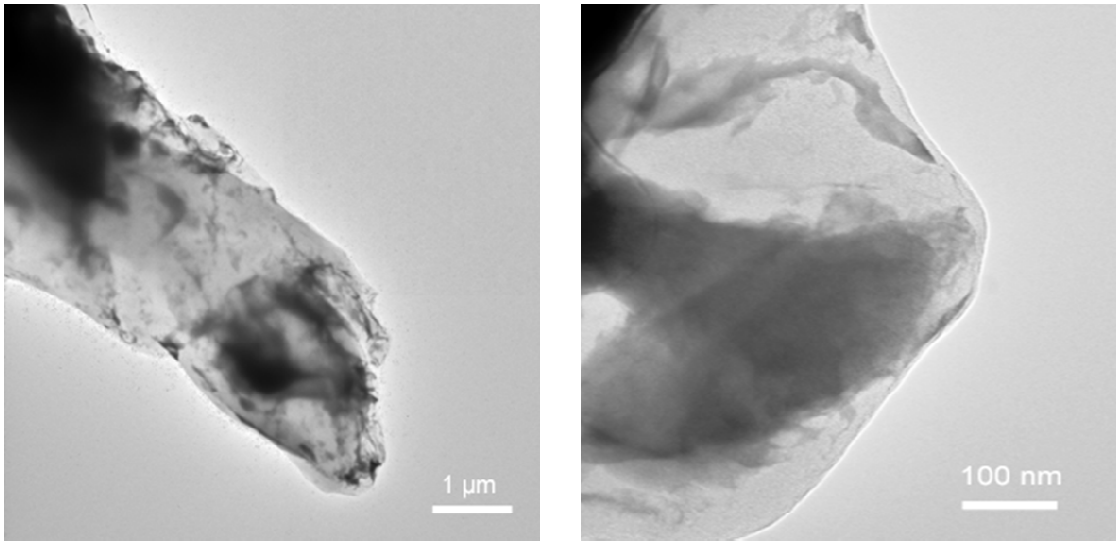


Figure S8. TEM images of compound **2**

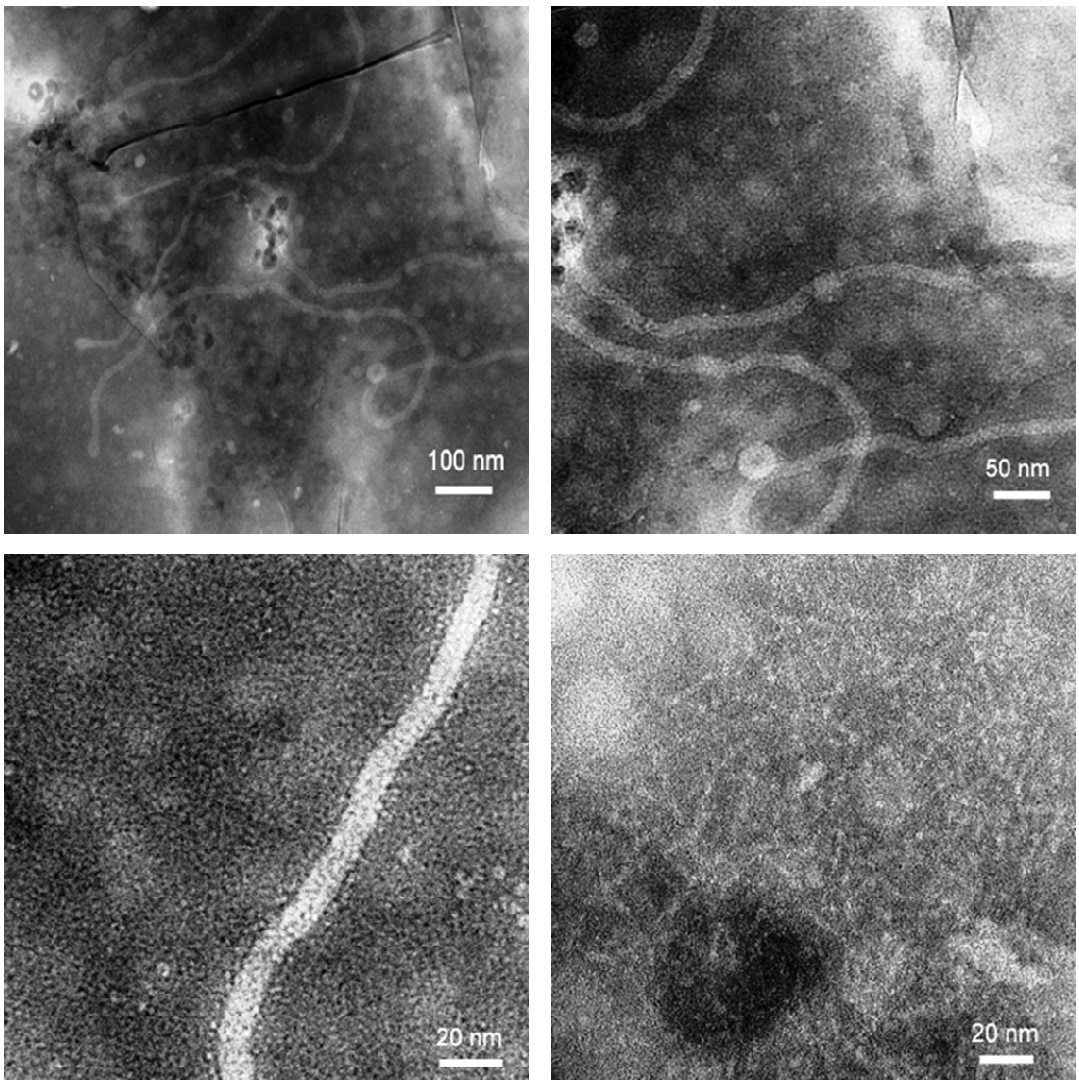


Figure S9. TEM images of compound **3**

ESI-MS

MS data was got on ESI-Q-TOF (micrOTOF-Q) in the solution of **1** and **3** (0.1 mM in MeOH/H_2O=1:1). The peaks correspond to the noncovalent intermediate species of the self-assembled supermacrocycle (1-mer to 6-mer)

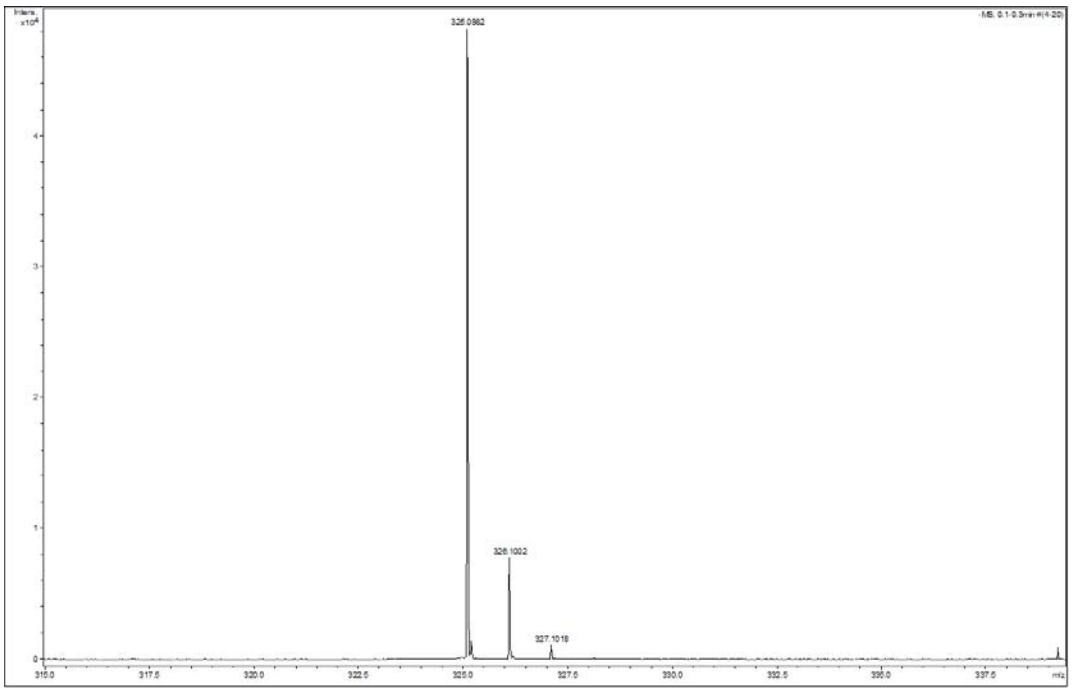


Figure S10. Compound **1** in MeOH/H_2O (1:1) was investigated by negative ESI-MS mode , the 1-mer peaks at 325.09

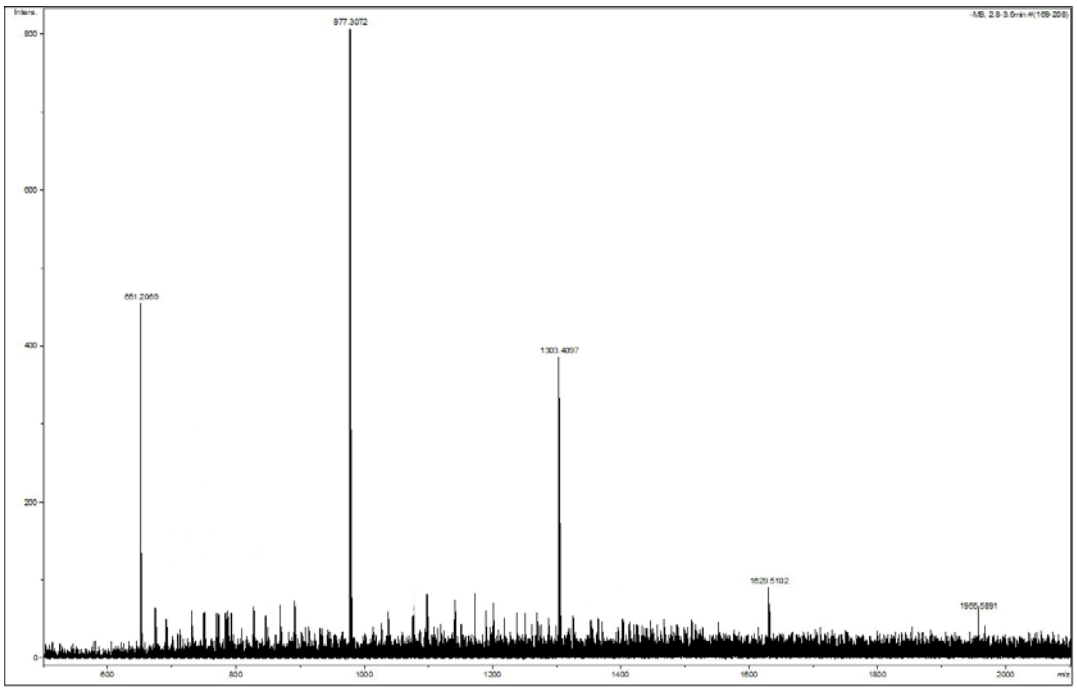


Figure S11. Compound **1** in MeOH/H_2O (1:1) was investigated by negative ESI-MS mode, the 2-mer to 6-mer peaks at 651.21 to 1955.59.

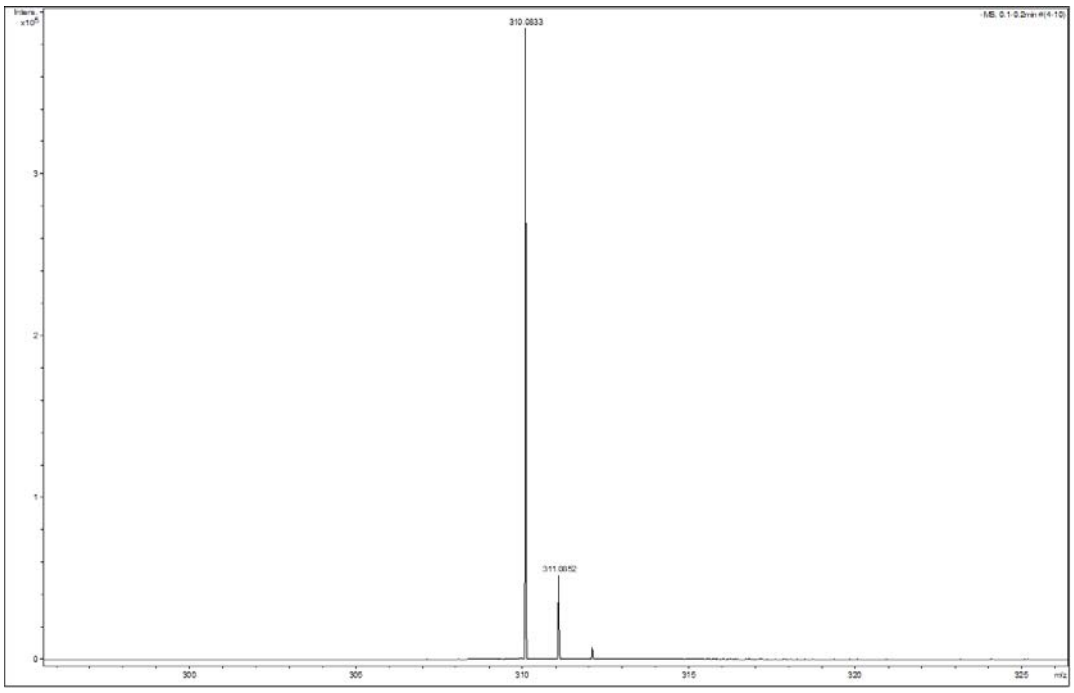


Figure S12. Compound **3** in MeOH/H_2O (1:1) was investigated by negative ESI-MS mode, the 1-mer peaks at 310.08

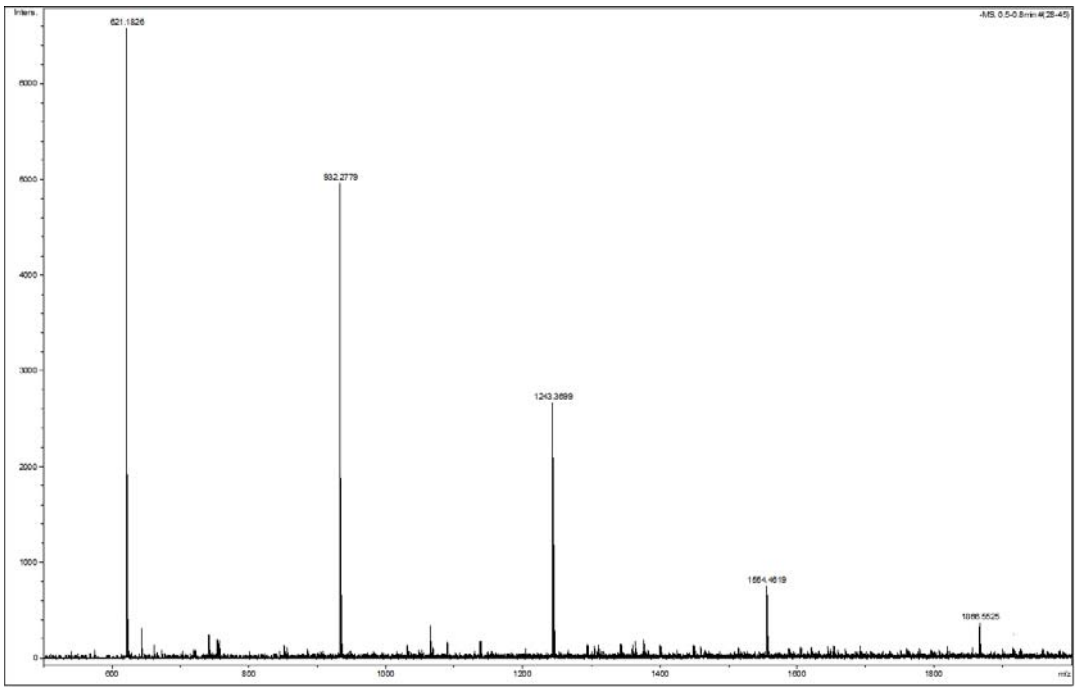


Figure S13. Compound **3** in MeOH/H_2O (1:1) was investigated by negative ESI-MS mode, the 2-mer to 6-mer peaks at 621.18 to 1866.55.

CD

CD spectra were recorded on circular dichroism spectrometer (Aviv Biomedical, Inc.). The samples were prepared by dissolving (compound **1** and **3**, 0.5 mg/mL) in H_2O. The solutions were heated to ~90°C and allowed to cool to room temperature for ~48 h, then investigated by CD.

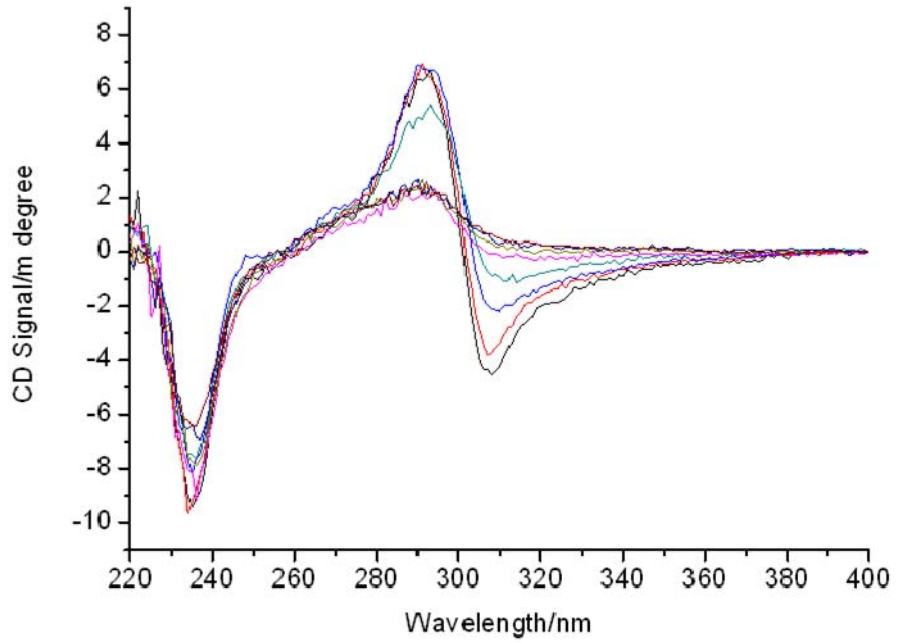


Figure S14. Temperature-dependent CD spectra of unbuffered aqueous solution for compound **1** (0.5 mg/mL in H_2O), The arrow indicates the trend of temperature increasing: 10℃, 20℃, 30℃, 40℃, 50℃, 60℃, 70℃, 80℃; Wavelength start: 400 nm, wavelength end: 220 nm.

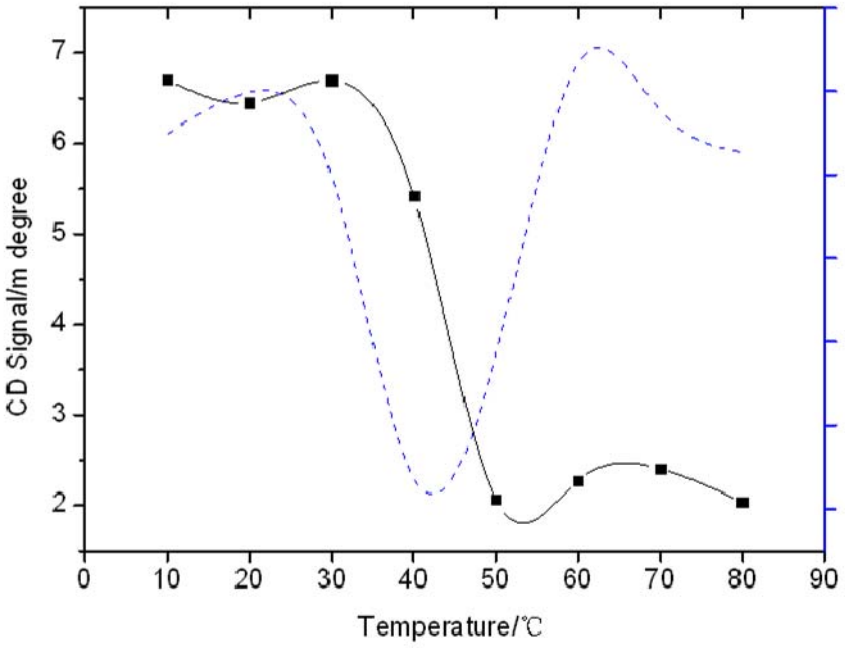


Figure S15. Temperature dependence of compound **1** at 293 nm. Tm: 42.5 ℃.

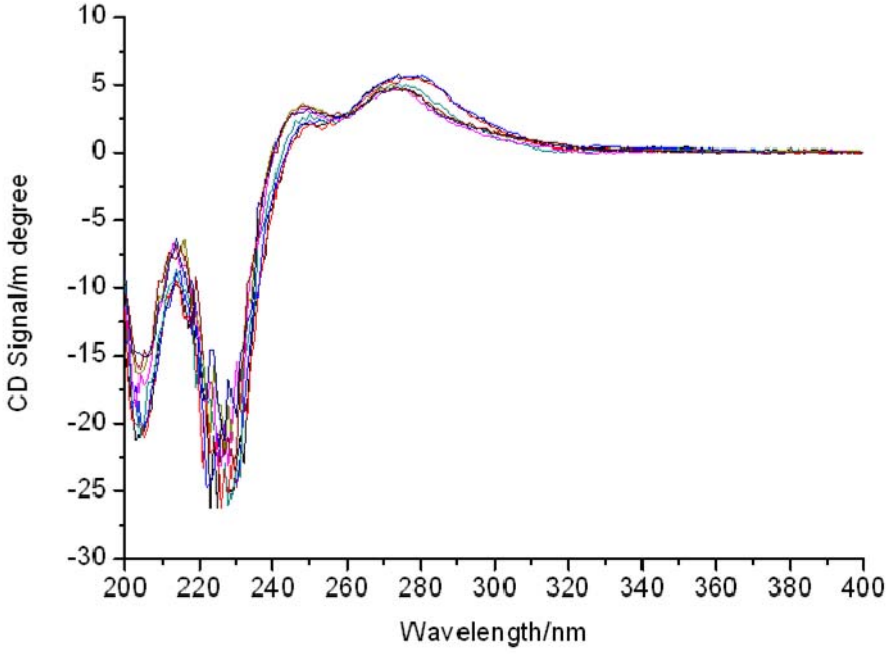


Figure S16. Temperature-dependent CD spectra of unbuffered aqueous solution for compound **3** (0.5 mg/mL in H_2O), The arrow indicates the trend of temperature increasing: 10℃, 20℃, 30℃, 40℃, 50℃, 60℃, 70℃, 80℃; Wavelength start: 400 nm, wavelength end: 200 nm.