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Supporting Information

Fabrication of chiral networks for tri-substituted anthraquinone derivative using molecular self-assembly

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1. Synthesize:

TTA molecule was synthesized from the commercially available 1,2,4-trihydroxyanthraquinone with $BrC_{13}H_{27}$ in DMF (dry, 150 ℃, 50 mL) along with Cs_2CO_3 added. The reaction finished twenty hours later and proved to be quite successful with a yield of 99%. The desired products were obtained by repeated recrystallization for the sake of high degree purity. TTA is a kind of crystal. The solvent was purchased from Tokyo Chemical Industry without further purification.

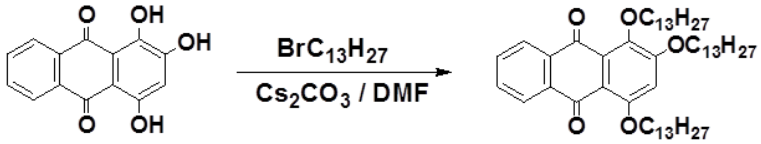

Fig. S1 Synthesis of TTA.

2. Characterization data：

TTA：^{1}H NMR (400 MHz $CDCl_3$) δ 8.21 (m, 2H), 7.70 (m, 2H), 6.79 (s, 1H), 4.09 (m, 6H), 1.92 (m, 66H), 1.58 (m, 9H)

MS: 825 [$C_{53}H_{86}NaO_5$] (Fig. S2)

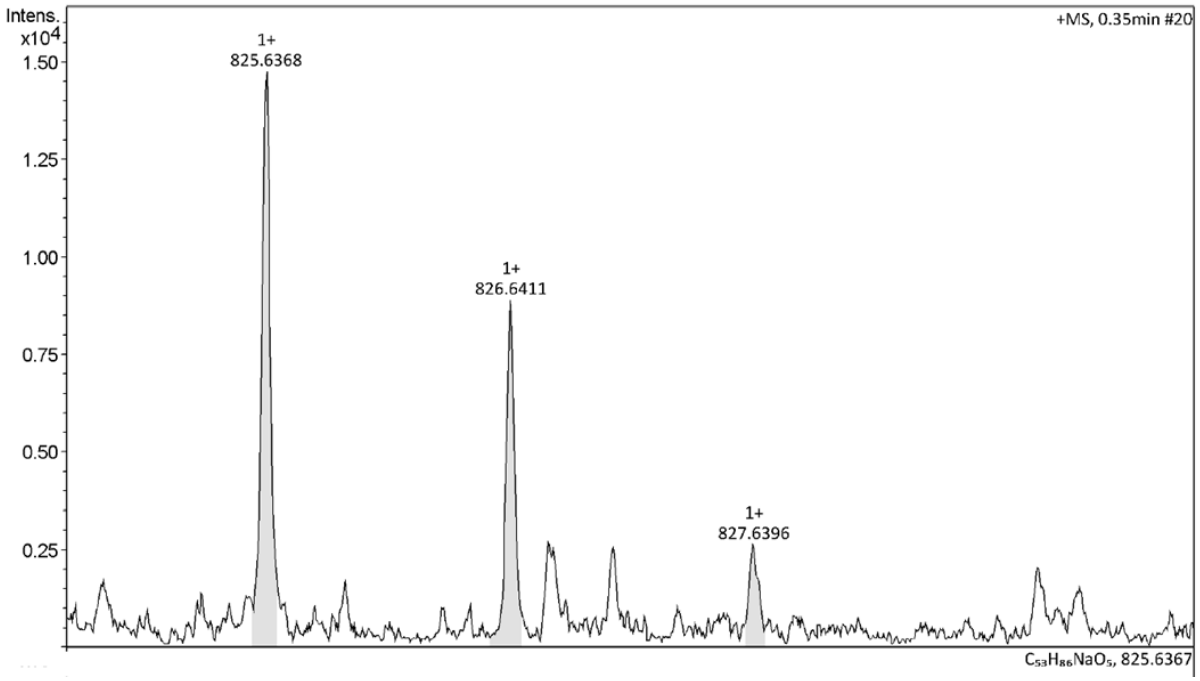

Fig. S2 MS image for TTA.

3. Experimental Section

3.1 X-ray diffraction

The powder X-ray diffraction (XRD) pattern is recorded using a Bruker D8-ADVANCE diffractometer with Cu Kα rddiation. A step-scan mode was adopted with a sampling time of 0.1 s and a scanning step of 0.02 °. The XRD peaks of all samples can be indexed using the Dicvol program.

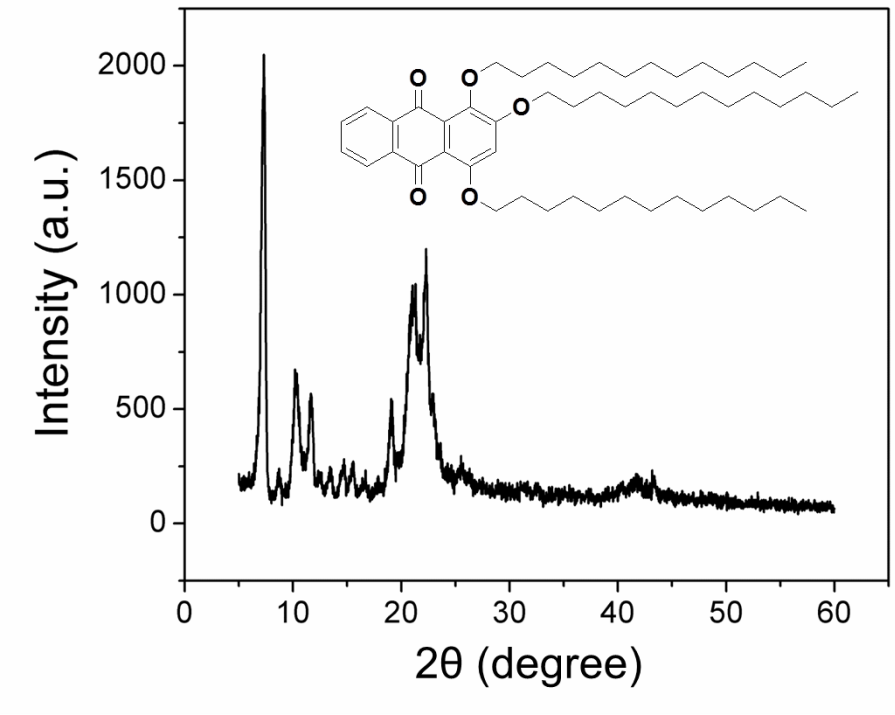

Fig. S3 X-ray diffraction patterns of TTA.

3.2 STM and molecular modeling

All of the solvents were purchased from TCI and used without further purification. The samples were prepared by depositing a droplet (about 1 μL) of solution onto a freshly cleaved atomically flat surface of HOPG (quality ZYB, Bruker, USA). STM experiments were performed on a Nanoscope IIIa Multimode SPM (Bruker, USA) under ambient condition (temperature: 15−20 ℃, humidity: 45−60%). The tips were mechanically cut from Pt/In wires (80/20). Different tips and samples were used to check the reproducibility of the results. All images were recorded with constant current mode and shown without further processing. Material studio 4.0 was used to build molecular models of the assembled structures. The models were constructed based on the inter-molecular distances and angles, and analysis of the STM results. Also, they were tested to be right according to the ideal overlap with the high-resolution STM images.

4. STM images and molecular models

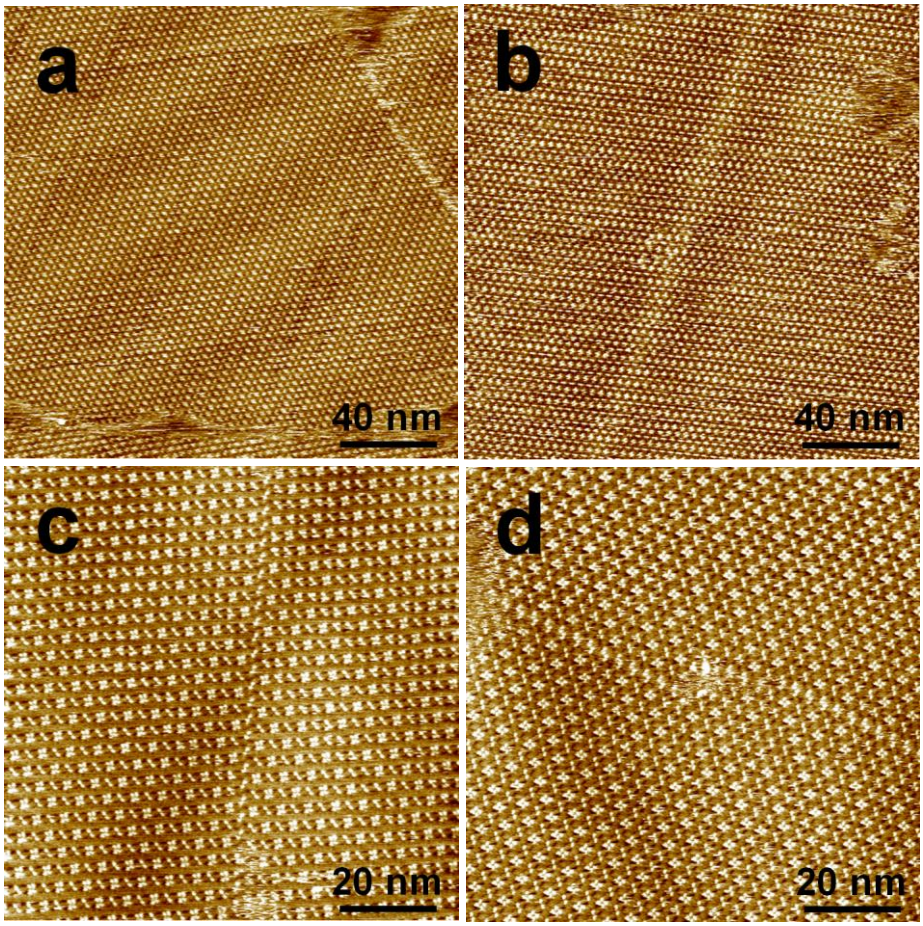

Fig.S4 Large-scale STM images of TTA molecules at the 1-octanoic acid/HOPG interface. (a) and (c) are for the CCW configuration, (b) and (d) are for the CW configuration. Imaging condition: I_t = 500 to 600 pA, V_{bias} = 600 to 880 mV.

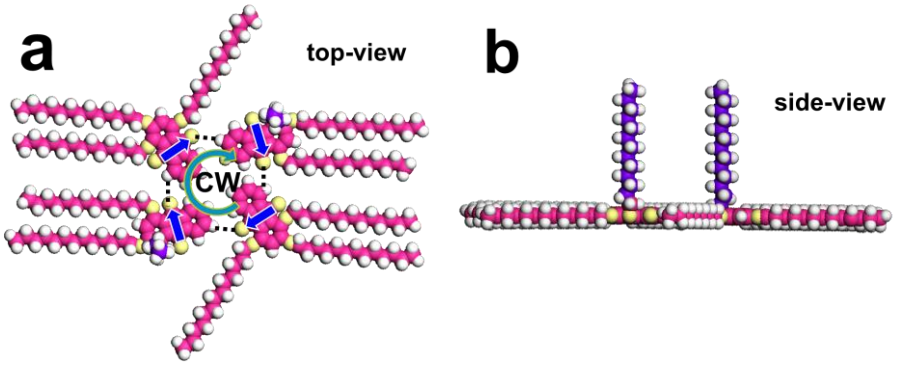

Fig. S5 Molecular models of the Flower-like tetramer from (a) top-view and (b) side view. The black dotted lines represent the hydrogen bonds and a set of blue arrows indicate the CW handedness.