

Electronic Supporting Information:

Experimental section:

Otherwise noted, materials were obtained from commercial suppliers and were used without further purification. ^1H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra were recorded by using a Varian Gemini 200 or a Bruker DRX- 500 spectrometer respectively. CDCl_3 was used as solvent and TMS as internal standard, otherwise specified. Matrix-assisted laser desorption ionization time of-flight (MALDI-TOF) mass spectra were recorded by using an Applied Biosystems Voyager-DE STR, using a-Cyano-4-hydroxycinnamic acid as the matrix, observing reflector-positive ions. Malvern Autosizer 4700 and ALV/SP-125 laser light scattering (LLS) spectrometers were used. DLS measurements were performed at a fixed scattering angle (q) of 90. TEM observations were performed by using a Philips CM 120 electron microscope. For all TEM observations, the solutions of aggregates were dropped onto the carbon-coated copper grids. SEM was conducted by using a Tescan 5136 MM scanning electron microscope. The AFM images were acquired in tapping mode by using a Nanoscope IV from Digital Instruments equipped with a silicon cantilever with 125 Pmand E-type vertical engage piezoelectric scanner. For SEM and AFM observations, the samples were prepared by drying the solution on freshly cleaved mica at RT. X-ray diffraction (XRD) spectra were registered with a Philips diffractometer composed of a $\text{CuK}\alpha$ ($\lambda = 1.54 \text{ \AA}$) source, a quartz monochromator, and a goniometric plate.

The derivatives of calix[6]arene (**1**, **2**, **3**) were synthesized as the literatures reported.¹ Synthesis of **TAC**: Compound **3** (200 mg) was added to a stirring 20 ml solution of 1, 3-diaminopropane under N_2 . After 12 h stirring, the solution was poured into 300 ml water and stirred for 1 h. The residue was re-crystallized by ethanol and gave 37% (77 mg) yield for product.

^1H NMR(CDCl_3 , 298 K): δ 1.14 (18 H, s), 1.23 (22 H, m), 1.40 (18 H, s), 1.44 (4 H, br), 2.49 (2 H, t), 2.53-3.20 (6 H, m), 3.22-3.69 (24 H, m), 3.90-4.48 (14 H, m), 4.66 (2 H, d, $J=14.4$), 6.81 (2 H, s), 6.99 (2 H, br), 7.07 (2 H, s), 7.10 (4 H, s), 7.19 (2 H, s), 7.30 (2 H, s);

MALDI-TOF: calculated for $[\text{M}+\text{Na}^+]$ $m/z = 1451.9$; found, $m/z = 1452.2$.

^{13}C NMR(CDCl_3 , 298 K): δ 169.7, 153.5, 153.1, 152.1, 146.4, 145.9, 145.7, 134.2, 133.1, 132.9, 132.7, 132.2, 131.5, 128.4, 127.3, 126.2, 125.4, 124.8, 73.1, 72.3, 72.1, 71.4, 69.4, 69.0, 39.3, 38.5, 34.4, 34.3, 31.8, 31.6, 31.5, 30.4, 30.2, 29.9, 26.9, 26.6.

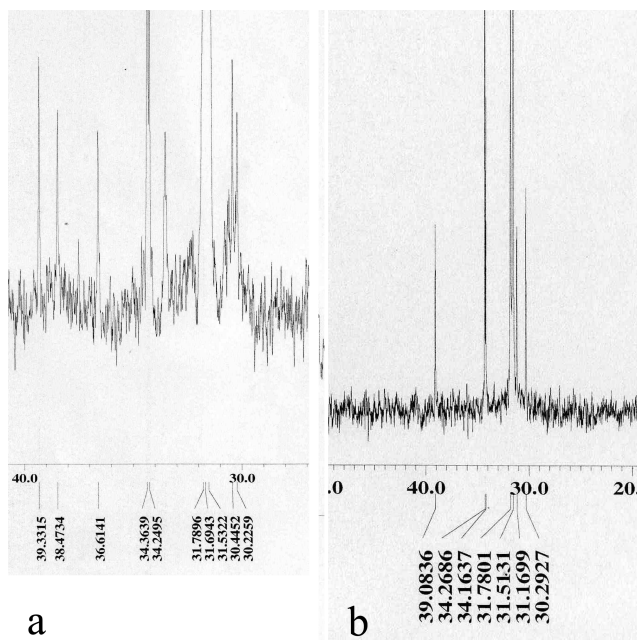
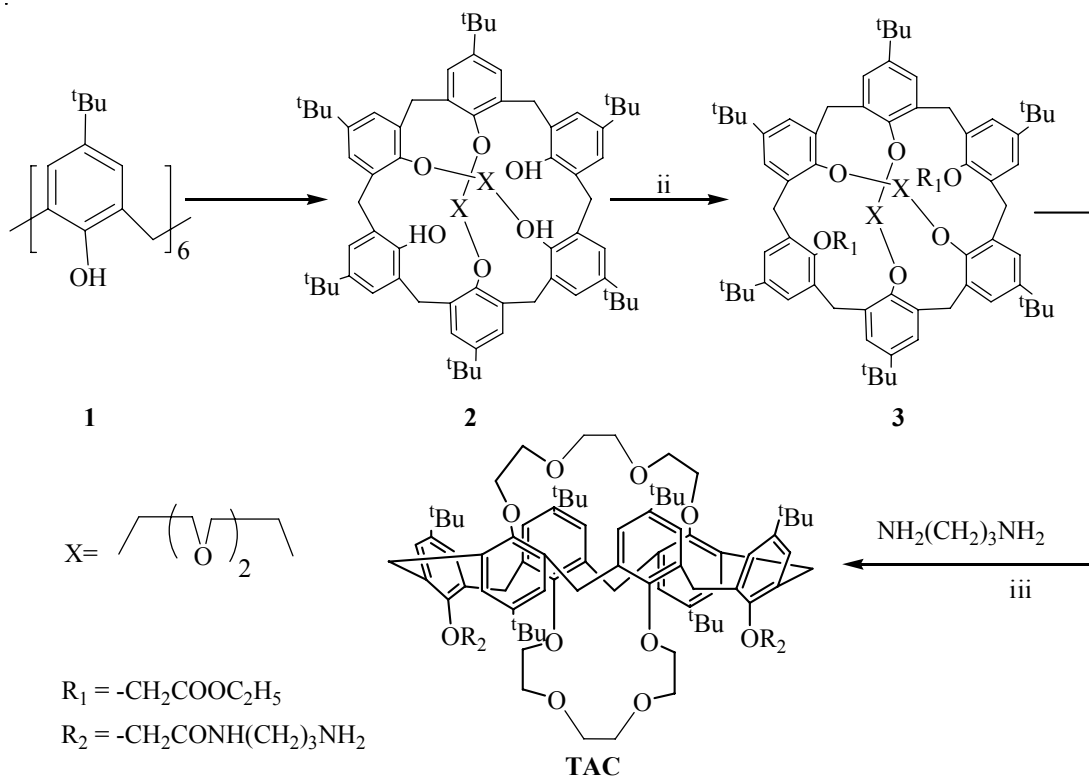


Figure. S1. Sections of the ^{13}C NMR spectra of **TAC** (a) and its precursory compound **3** (b)

The peaks of the bridging methylenes of **TAC** (39 ppm and 31 ppm) are almost the same as those in the precursor compound showing no change in the conformation after aminolysis reaction.²

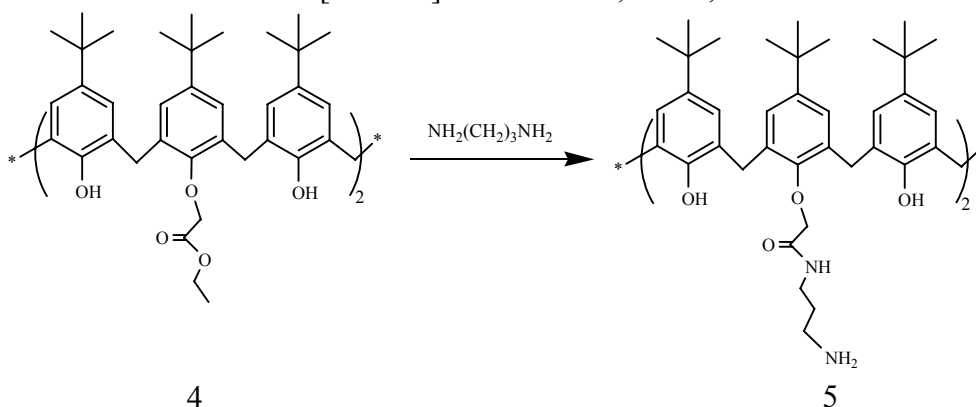


Scheme 1. Reagents and reaction: (i) K_2CO_3 /xylene, triethylene glycol ditosylates, reflux, 12 h, 52%; (ii) K_2CO_3 /MeCN, ethyl bromoacetate, reflux, 12 h, 65%. (iii)

1,3-Propanediamine, r.t..

Synthesis of compound **5**: Compound **4** was added to a stirring 20 ml solution of 1, 3-diaminopropane under N₂. After 12 h stirring, the solution was poured into 300 ml water and stirred for 1 h. The residue was purified by preparative TLC and gave 89% yield for product. It should be noted that the compound **5** is flexible and the product was the conformational mixture.³

MALDI-TOF: calculated for [M+Na⁺] m/z = 1224.7; found, m/z = 1225.0



Scheme 2. Reagents and reaction: 1,3-Propanediamine, r.t..

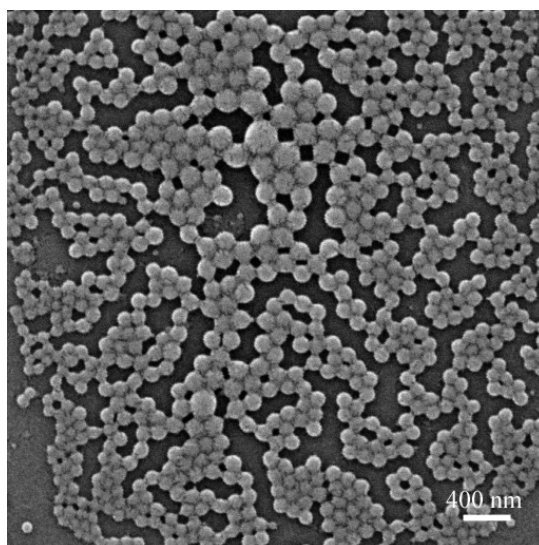


Figure. S2. SEM image of the aggregates (TAC) in solution (the volume ratio of water:ethanol = 1:3)

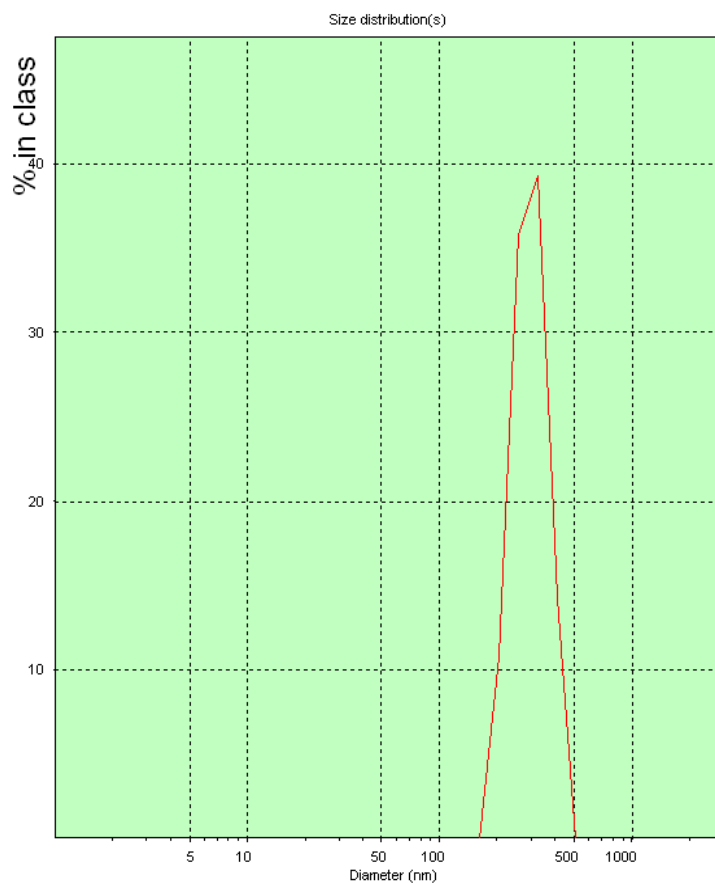


Figure. S3. DLS results obtained from ethanol-water mixture of **TAC** at 25 °C (the volume ratio of water:ethanol = 1:3); polydispersity is 0.192 and the diameter of the aggregates is approximate 289 nm.

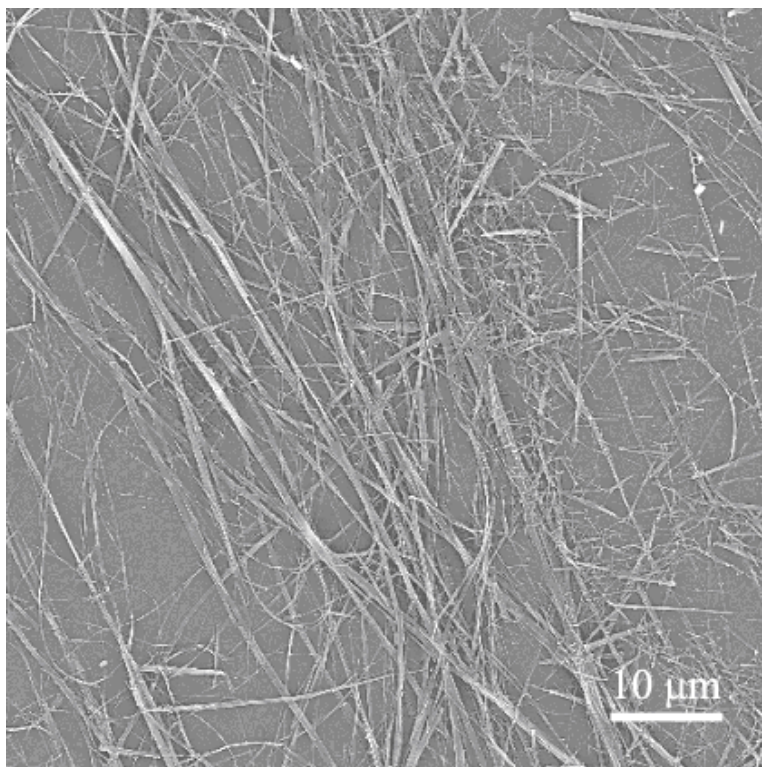


Figure. S4. SEM image of the stack of the aggregates (the volume ratio of water : ethanol = 1:1)

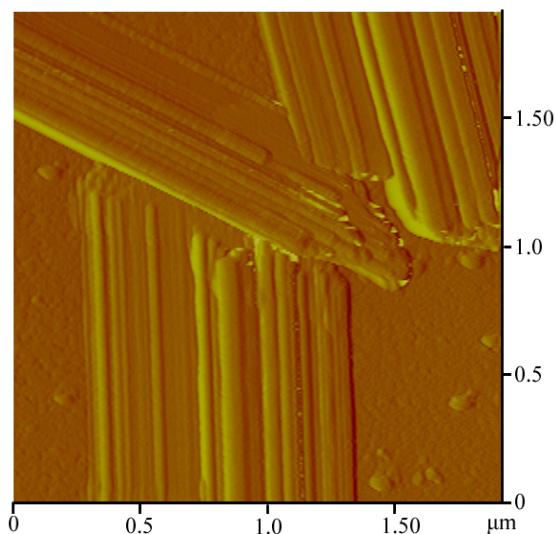


Figure. S5. AFM image of the stack of the aggregates (the volume ratio of water : ethanol = 1:1)

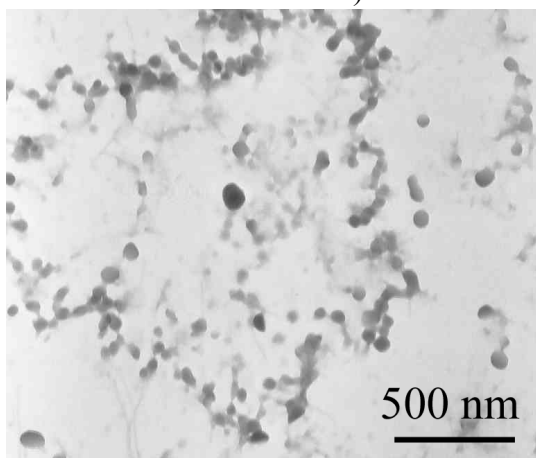


Figure. S6. TEM image the aggregates (compound **5**) in solution (the volume ratio of water:ethanol = 1:3)

References:

1. Guan, B.; Gong, S. L.; Wu, X. J.; Chen, Y. Y. *Tetrahedron Lett.* **2005**, *46*, 6041-6044.
2. Jaime, C.; Demendoza, J.; Prados, P.; Nieto, P. M.; Sanchez, C. *J. Org. Chem.* **1991**, *56*, 3372-3376.
3. Nam, K. C.; Park, K. S. *Bull. Korean Chem. Soc.* **1995**, *16*, 153-157