

## Supporting Information

### **Fabrication of *nor-seco-cucurbit*[10]uril based supramolecular polymers via self-sorting**

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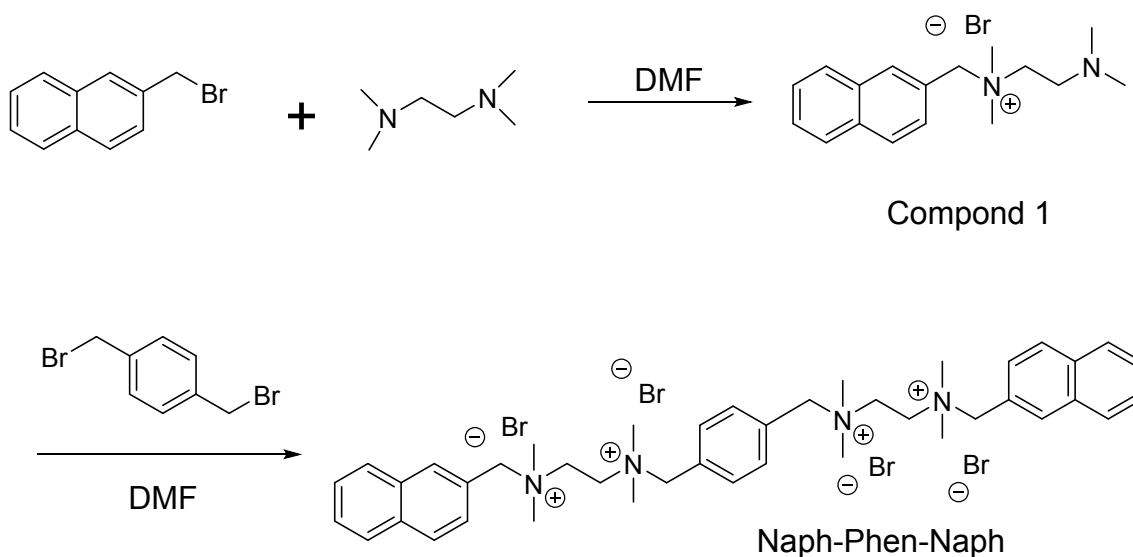
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## 1. Materials and instruments

All the chemical materials we used were from commercial suppliers without further purification. JOEL JNM-ECA 600 spectrometer (600 MHz) and JOEL JNM-ECA 400 spectrometer (400 MHz) were used to get the  $^1\text{H}$  NMR spectra and DOSY. Isothermal titration calorimetry (ITC) experiments were carried out with a Microcal VP-ITC apparatus in PBS buffer solution at 298.15 K. ESI-MS was carried out on a LTQ LC/MS apparatus. *Nor-seco-cucurbit[10]uril*<sup>1</sup> and *cucurbit[7]uril*<sup>2</sup> were prepared according to the reported literatures.

## 2. Synthesis of molecules

### 2.1 Synthesis of Np-PhDi-Np



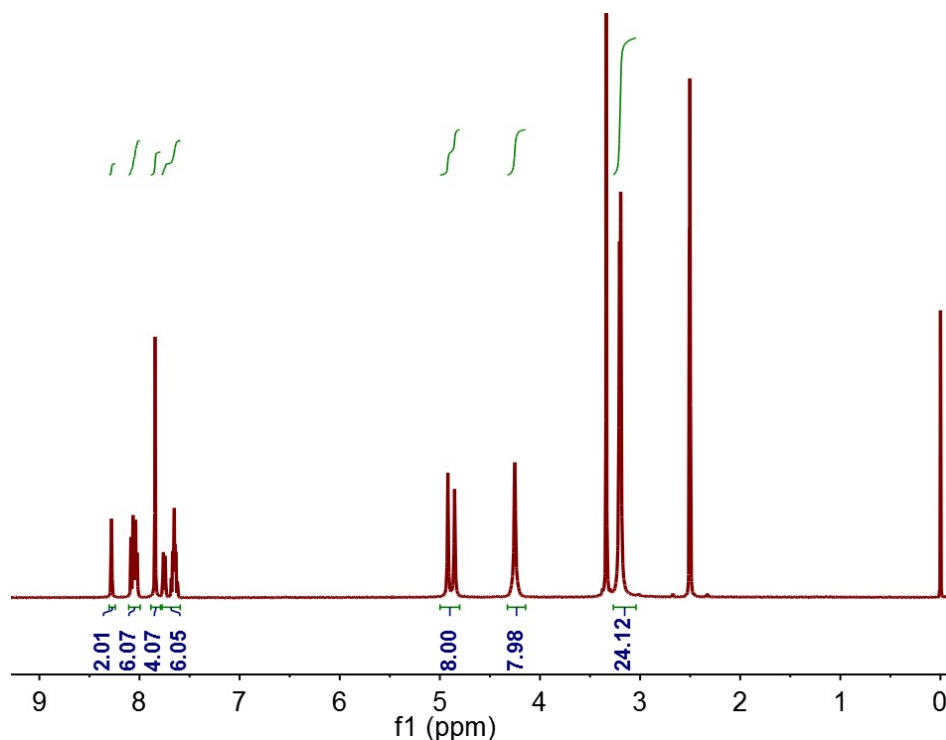
Scheme S1. Synthesis of Naph-Phen-Naph.

0.54 g 2-(Bromomethyl)naphthalene and 10 mL N, N, N', N'-Tetramethylethylenediamine were mixed in a flask with 10 mL DMF. The mixture was heated at 80 °C in a nitrogen environment overnight (around 12 h). After the reaction was completed, the light yellow solution was added dropwise into 150 mL of diethyl ether and the precipitate was filtered. The filter residue was washed by diethyl ether for three times. The white solid was compound 1, with a yield of 88%.

0.12 g 4,4'-Bis(bromomethyl)biphenyl and 1.1 g compound 1 were mixed with 20 mL DMF in a flask and then heated up to 90 °C for 10 h in a nitrogen environment. After the reaction was completed, the white solid precipitate was filtered directly and washed by acetonitrile and diethyl ether for three times. The yield was 95%.

$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ): 8.24 (s, 2H), 8.10-7.95 (m, 6H), 7.81 (s, 4H), 7.75-7.55 (m, 6H), 4.88 (s, 4H), 4.81 (s, 4H), 4.21 (s, 8H), 3.15 (m, 24H).

ESI-MS: m/z 168.16 [M-4Br-2Naph]<sup>2+</sup>



## 2.2 Synthesis of Naph



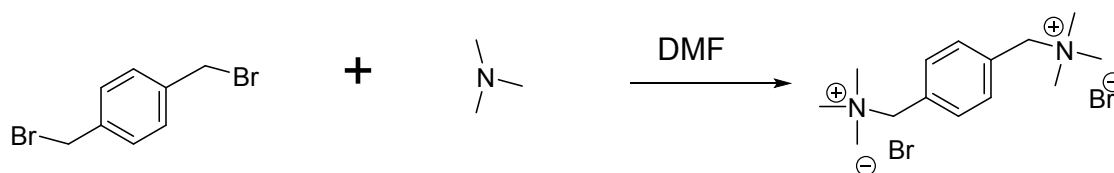
Scheme S2. Synthesis of Naph.

2-(bromomethyl) naphthalene (200 mg) and trimethyl amine (2.0 mL) were heated in 15 mL acetonitrile at 70 °C for 5 h. After the reaction was completed, the mixture was added dropwise into 150 mL diethyl ether. The precipitate was filtrated then dried in vacuum to give a white solid, yielding 90%.

<sup>1</sup>H NMR (400 MHz, D<sub>2</sub>O): 8.00-8.25 (m, 4H), 7.60-7.75 (m, 3H), 4.68 (s, 2H), 3.17 (s, 9H).

ESI-MS: m/z 200.14 [M-Br]<sup>+</sup>

### 2.3 Synthesis of Phen



Scheme S3. Synthesis of Phen.

Phen 1,4-bis(bromomethyl) benzene (300 mg) and trimethyl amine (3.0 mL) were heated in 15 mL acetonitrile at 70 °C for 5 h. After the reaction was completed, the mixture was added dropwise into 150 mL diethyl ether. The precipitate was filtrated and dried in vacuum to give a white solid, yielding 92%.

$^1\text{H}$  NMR (400 MHz,  $\text{D}_2\text{O}$ ): 7.73 (s, 4H), 4.60 (s, 4H), 3.16 (s, 18H).

ESI-MS:  $m/z$  111.11  $[\text{M}-2\text{Br}]^{2+}$

### 3. $^1\text{H}$ NMR spectra of Naph-Phen-Naph and supramolecular polymer

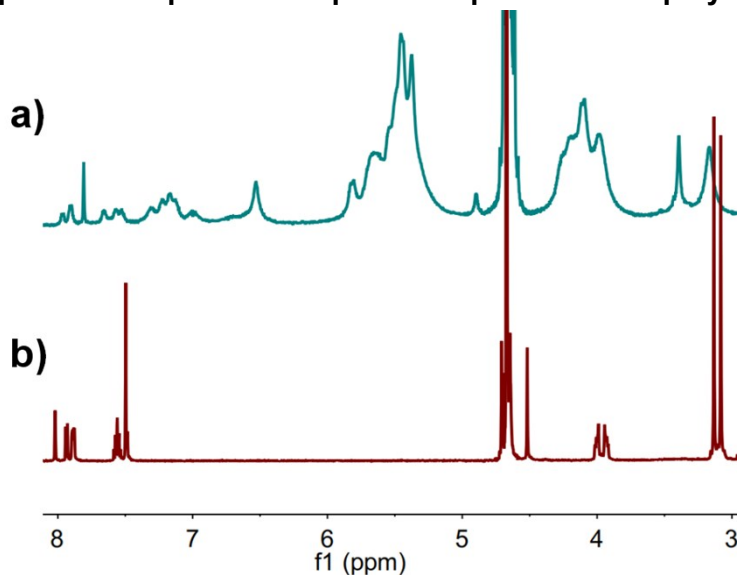


Figure S1  $^1\text{H}$  NMR spectra of a) supramolecular polymer and b) Naph-Phen-Naph.

From  $^1\text{H}$  NMR spectra we found that when *ns*-CB[10], Naph-Phen-Naph and CB[7] were mixed together in water with the ratio of 1:1:1, the peaks of Naph and Phen moieties all shifted up-field and broadened, which suggested the formation of supramolecular polymer.

## Reference

1. W.-H. Huang, S. Liu, P. Y. Zavalij and L. Isaacs, J. Am. Chem. Soc. 2006, 128, 14744-14745
2. A. Day, A. P. Arnold, R. J. Blanch, and B. Snushall, J. Org. Chem. 2001, 66, 8094-8100