

Supporting information

Controllable Supramolecular Polymerization through Self-

Sorting of Aliphatic and Aromatic Motifs

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1. Characterization of molecular weight of supramolecular polymers by AUC

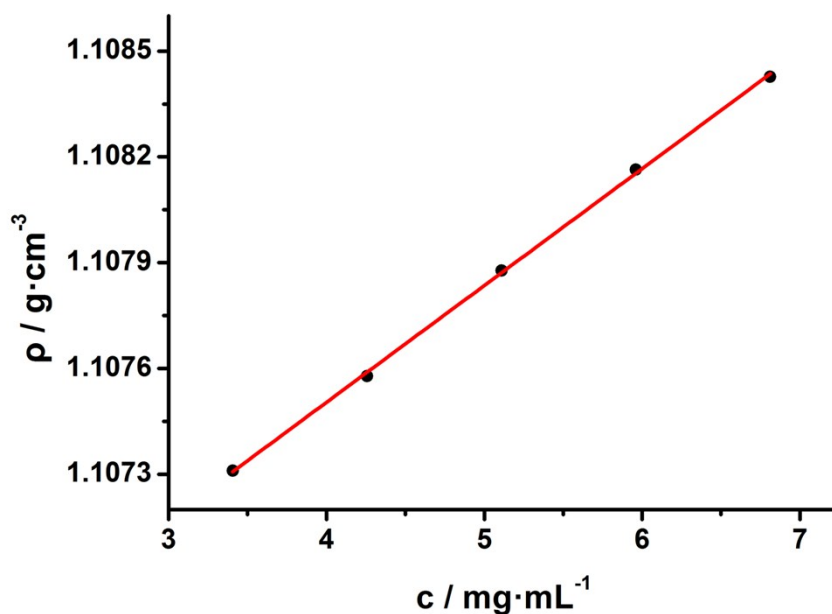


Fig. S1 Fitting curve of the concentration-dependent density data of supramolecular polymers.

As shown in Fig. S1, the partial specific volume was calculated to be $0.605 \text{ mg}^{-1}\text{mL}$, and the equation was $y = 1.10618 x + 0.00033118$ studied by an Anton Paar DMA 5000 densimeter.

2. Characterization of the difference of absorbance after adding CB[7] to Np-C₆-Np-CB[8] by UV-vis spectra.

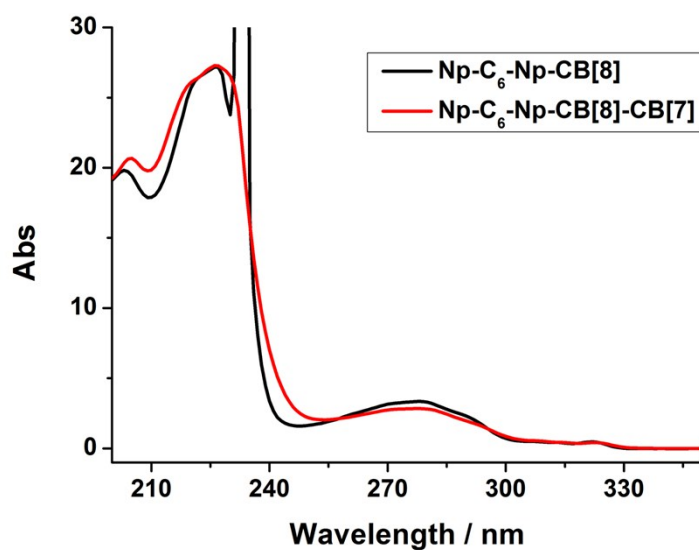


Fig. S2 Absorbance of Np-C₆-Np-CB[8] and Np-C₆-Np-CB[8]-CB[7].

3. ITC studies of self-sorting system.

(1) Host-guest interaction between Np and cucurbiturils

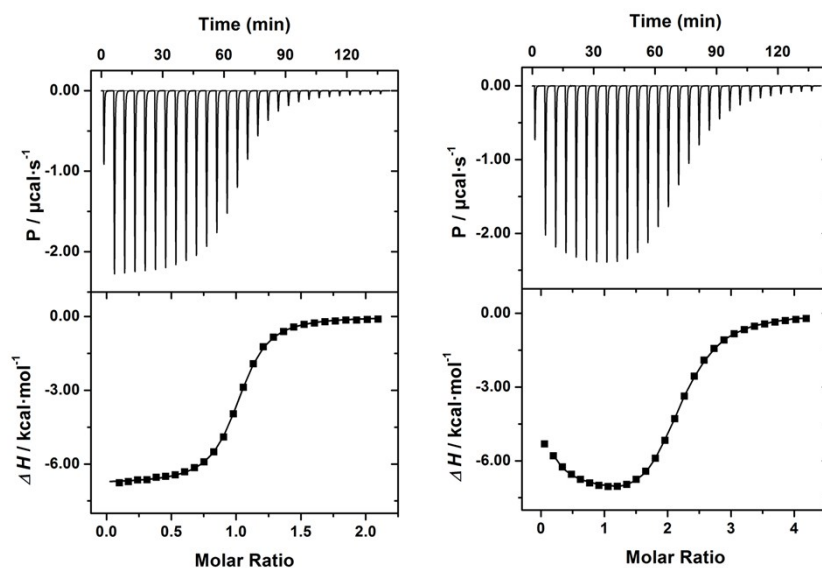


Fig. S3 Fitting the ITC data for titration experiments of a) NpTA (1.0 mM) into CB[7] (0.1 mM) with a one-sites binding model and b) NpTA (1.0 mM) into CB[8] (0.05 mM) with a sequential binding model.

As shown in Fig. S3, the binding constant of Np and CB[7] was $7.80 \times 10^5 \text{ M}^{-1}$, and the two step binding constant of Np and CB[8] was $K_{a1} = 5.53 \times 10^5 \text{ M}^{-1}$ and $K_{a2} = 2.90 \times 10^5 \text{ M}^{-1}$.

(2) Host-guest interaction between C_4 and CB[7]

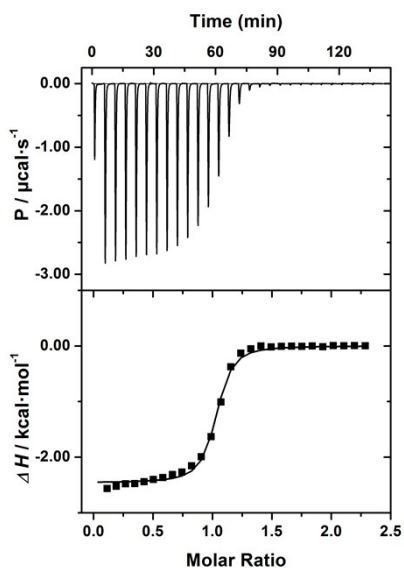


Fig. S4 Fitting the ITC data for titration experiments of a) C_4DA (1.0 mM) into CB[7] (0.1 mM) with a one-sites binding model.

As shown in Fig. S4, the binding constant of C_4 and CB[7] was $7.71 \times 10^5 \text{ M}^{-1}$, and the binding of C_4 and CB[8] could not be detected.

(3) Host-guest interaction between C_6 and cucurbiturils

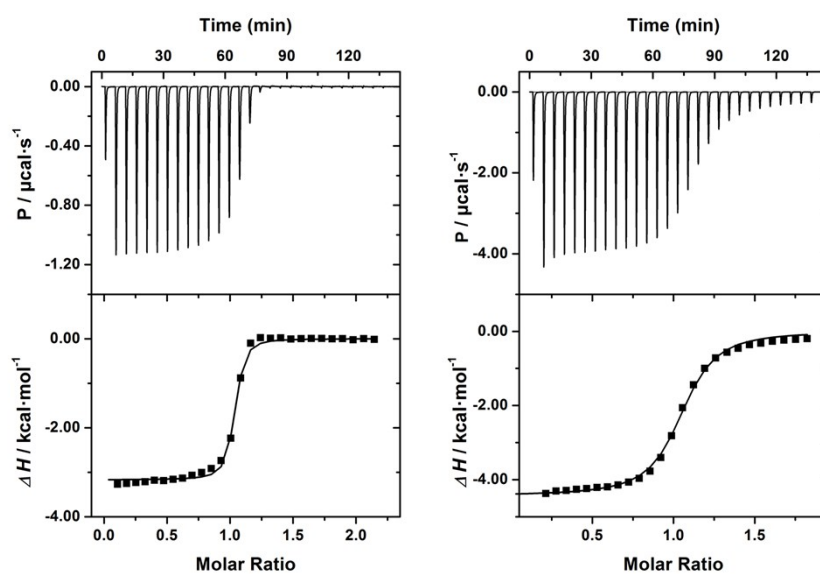


Fig. S5 Fitting the ITC data for titration experiments of a) C₆DA (1.0 mM) into CB[8] (0.1 mM) with a one-sites binding model and b) CB[7] (3.0 mM) into C₆DA-CB[8] (0.3 mM) with a competitive binding model.

As shown in Fig. S5, the binding constant of C₆ and CB[7] was $1.19 \times 10^9 \text{ M}^{-1}$, and the binding constant of C₆ and CB[8] was $7.10 \times 10^6 \text{ M}^{-1}$.

(4) Host-guest interaction between C₈ and cucurbiturils

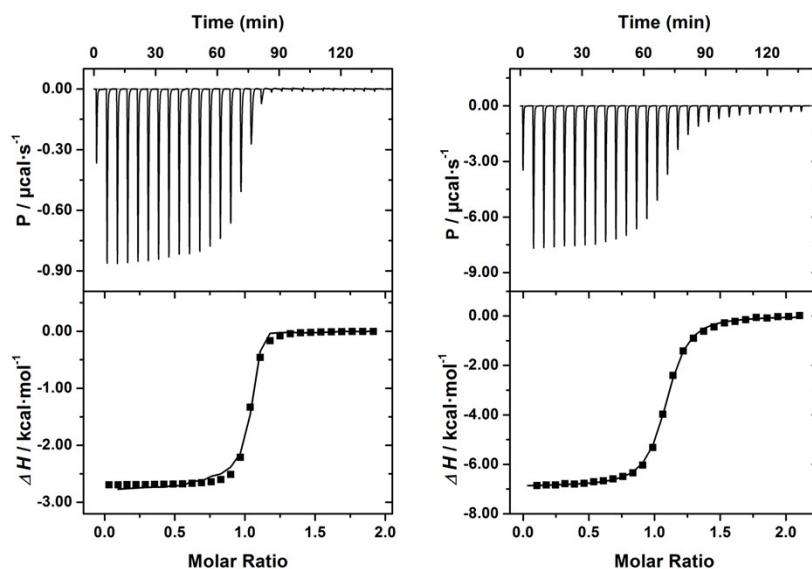


Fig. S6 Fitting the ITC data for titration experiments of a) C₈DA (1.0 mM) into CB[8] (0.1 mM) with a one-sites binding model and b) CB[7] (3.0 mM) into C₈DA-CB[8] (0.3 mM) with a competitive binding model.

As shown in Fig. S6, the binding constant of C₈ and CB[7] was $2.16 \times 10^9 \text{ M}^{-1}$, and the binding constant of C₈ and CB[8] was $7.79 \times 10^6 \text{ M}^{-1}$.

(5) Host-guest interaction between C₁₀ and cucurbiturils

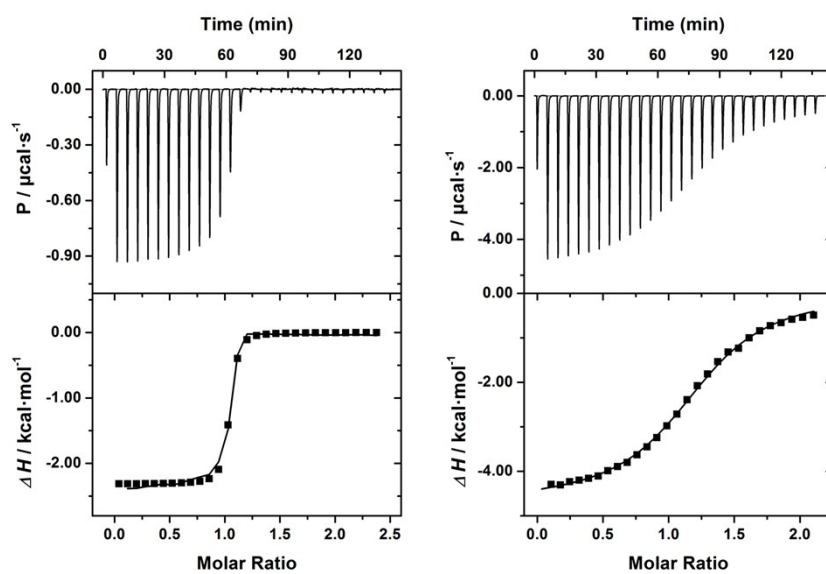


Fig. S7 Fitting the ITC data for titration experiments of a) C₁₀DA (1.0 mM) into CB[8] (0.1 mM) with a one-sites binding model and b) CB[7] (3.0 mM) into C₁₀DA-CB[8] (0.3 mM) with a competitive binding model.

As shown in Fig. S7, the binding constant of C₁₀ and CB[7] was $2.27 \times 10^8 \text{ M}^{-1}$, and the binding constant of C₁₀ and CB[8] was $9.34 \times 10^6 \text{ M}^{-1}$.