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

![Graph showing concentration-dependent density data](image)

**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 mg⁻¹mL⁻¹, and the equation was \( y = 1.10618 x + 0.00033118 \) studied by an Anton Paar DMA 5000 densimeter.

![UV-vis spectra](image1)

**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

![ITC data](image2)

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

(2) Host-guest interaction between C$_4$ and CB[7]

![Fitting the ITC data for titration experiments of a) C$_4$DA (1.0 mM) into CB[7] (0.1 mM) with a one-sites binding model.](image)

As shown in Fig. S4, the binding constant of C$_4$ and CB[7] was $7.71 \times 10^5$ 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 $1.19 \times 10^9$ M⁻¹, and the binding constant of C₆ and CB[8] was $7.10 \times 10^6$ 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 $2.16 \times 10^9$ M⁻¹, and the binding constant of C₈ and CB[8] was $7.79 \times 10^6$ M⁻¹.
(5) Host-guest interaction between C\textsubscript{10} and cucurbiturils

Fig. S7 Fitting the ITC data for titration experiments of a) C\textsubscript{10}DA (1.0 mM) into CB[8] (0.1 mM) with a one-sites binding model and b) CB[7] (3.0 mM) into C\textsubscript{10}DA-CB[8] (0.3 mM) with a competitive binding model.

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