Supramolecular Self-Assemblies of β-Cyclodextrins with Aromatic Tethers: Factors Governing the Helical Columnar versus Linear Channel Superstructures

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Figure S1  The molecular structure of Mono[6-O-(4-bromobenzene)]-β-CD (1)
Figure S2  The molecular structure of Mono[6-O-(4-nitro-phenyl)]-β-CD (2)
Figure S3  The molecular structure of Mono[6-O-(4-formyl-phenyl)]-β-CD (3)
Figure S4  The molecular structure of Mono(6-phenylseleno-6-deoxy)-β-CD (4)
Figure S5  The molecular structure of Mono[6-O-(4-hydroxybenzoyl)]-β-CD (5)
Figure S6  The dimeric structure of the compound 5.
Figure S7  Plot from $^1$H NMR data of 2 as a function of total concentration to determine the aggregation equilibrium constant. The closed circles are the experimental data points, and the line is the theoretical curve based on the calculated values as equation $\delta_{\text{obsd}} = \delta_\text{m} + f_d (\delta_\text{m} - \delta_\text{n}) = \delta_\text{m} + (\delta_\text{m} - \delta_\text{n}) \left( \frac{1 + 8 \text{K}_a \text{C}}{(1 + 8 \text{K}_a \text{C})^{1/2}} - \frac{1}{1 + 8 \text{K}_a \text{C}} \right)$.
Figure S8  ITC titration data of $\beta$-CD (13.0 mM) with mono[6–O-(4–nitrobenzene)]-$\beta$-CD (0.62 mM) (2) in H$_2$O at 25 °C.