Supporting information available

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- brombenzene)]- 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 $\delta_{obsd} = \delta_m + f_d(\delta_d - \delta_m) = \delta_m + (\delta_d - \delta_m) \frac{(1 + 8KaC_t)^{1/2} - 1}{(1 + 8KaC_t)^{1/2} + 1}$



Figure S8 ITC titration data of β -CD (13.0 mM) with mono[6–O-(4–nitrobenzene)]- β -CD (0.62 mM) (2) in H₂O at 25 °C.