

Electronic Supplementary Information (ESI)

Separation of phenylenediamine isomers by using decamethylcurbit[5]uril

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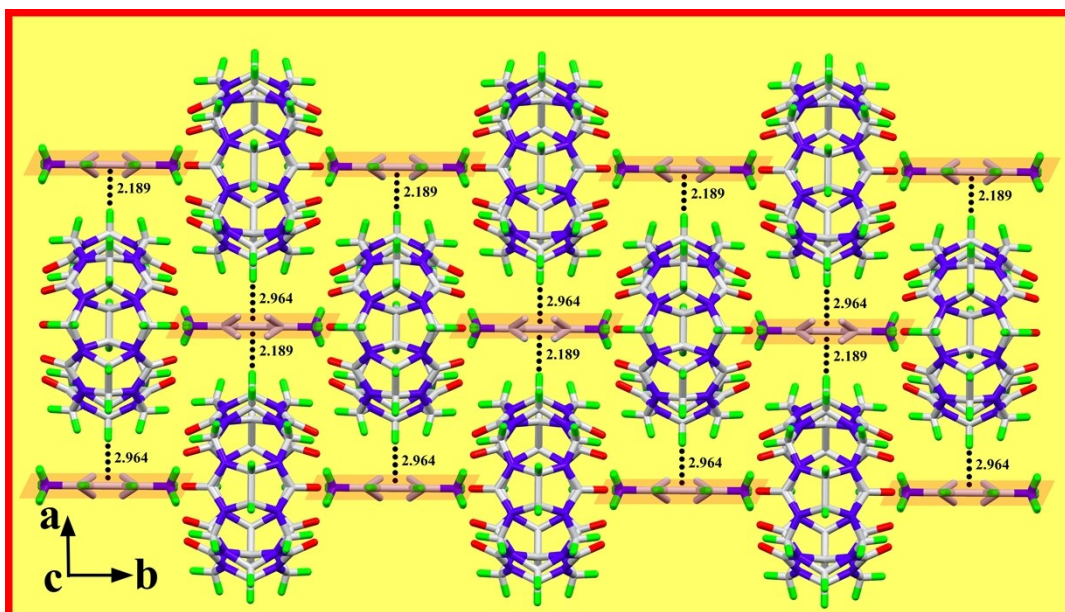


Figure S1 Crystal structure of Q[5]-*p*-PDA-based supramolecular chains.

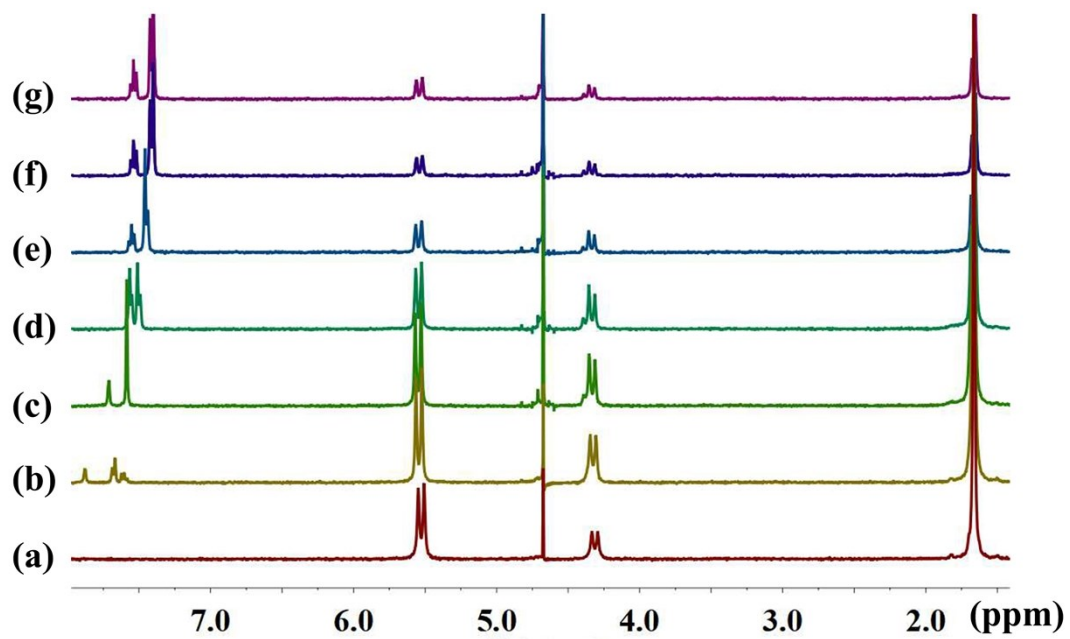


Figure S2. Titration ^1H NMR spectra of $\text{Me}_{10}\text{Q}[5]$ ($1\ \mu\text{M}$) upon addition with molar equivalents of *m*-PDA: (a) 0; (b) 0.5; (c) 1.5; (d) 2.5; (e) 5; (f) 5.5; (g) 6.

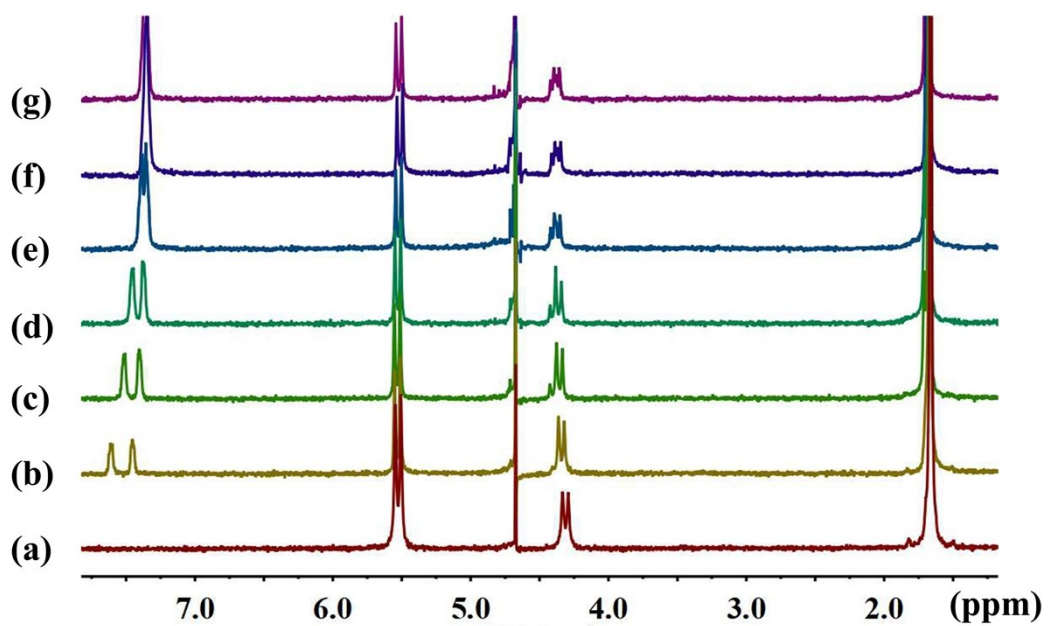


Figure S3. Titration ^1H NMR spectra of $\text{Me}_{10}\text{Q}[5]$ ($1\ \mu\text{M}$) upon addition with molar equivalents of *o*-PDA: (a) 0; (b) 1; (c) 2.5; (d) 4.5; (e) 5.5; (f) 6; (g) 7.

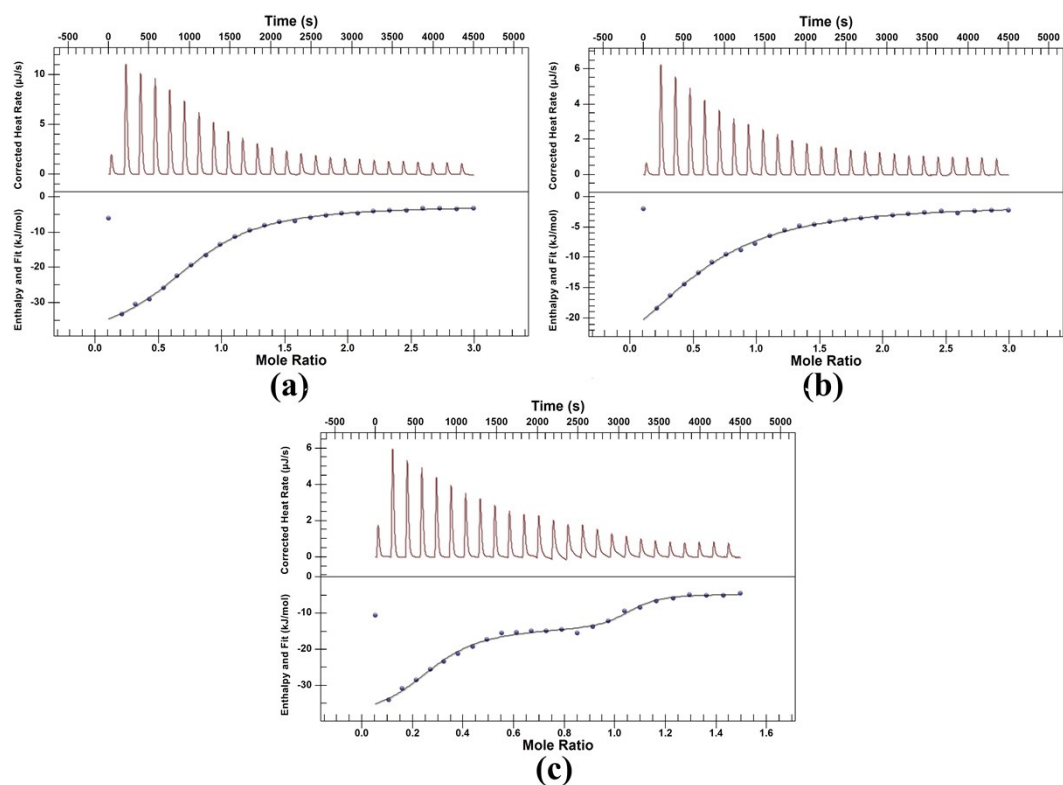


Figure S4. Isothermal titration calorimetry profiles obtained for $\text{Me}_{10}\text{Q}[5]$ in the presence of (a) *o*-PDA, (b) *m*-PDA and (a) *p*-PDA, respectively in an aqueous HCl solution (0.05M) at 298.15 K.

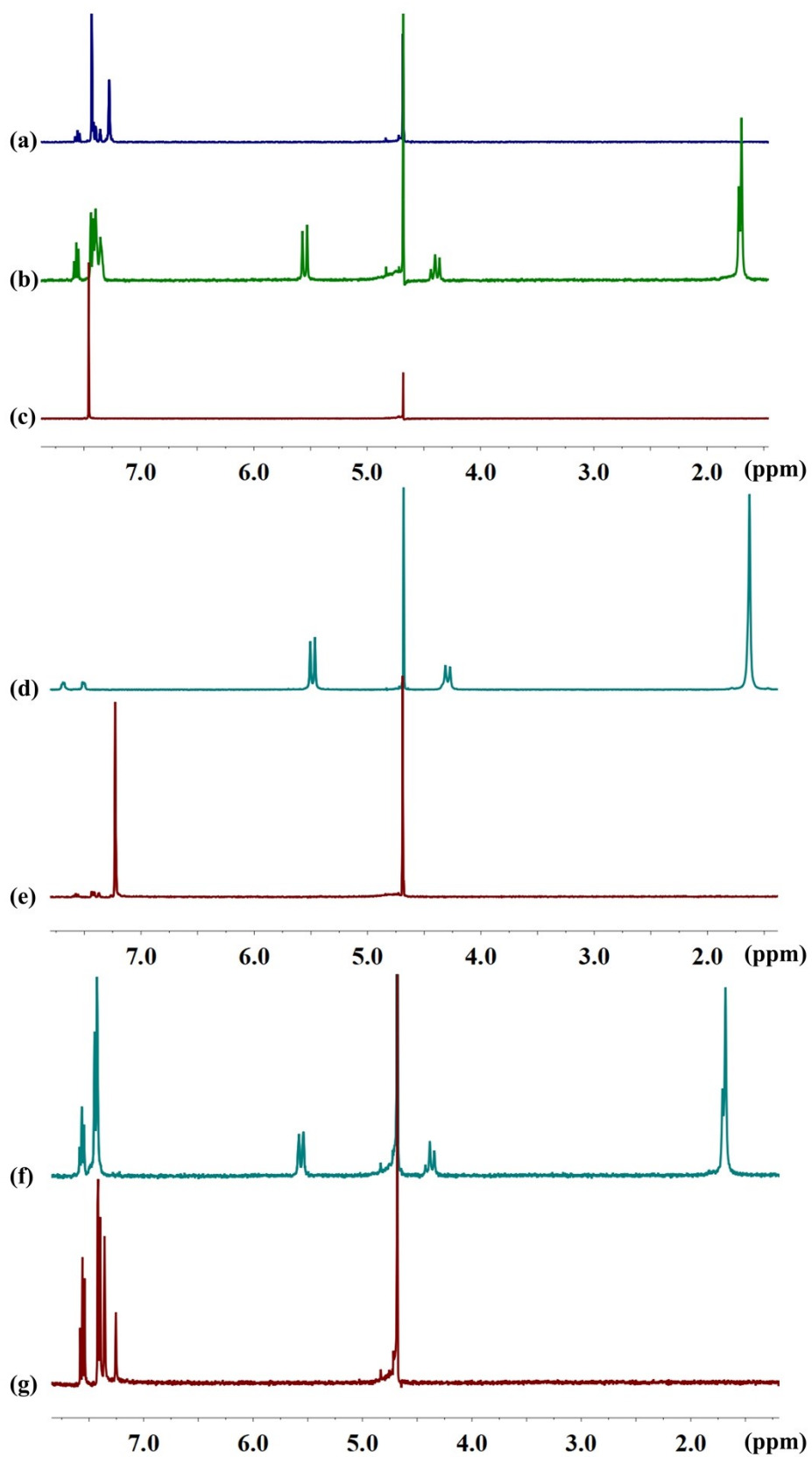


Figure S5. ¹H NMR spectra of sample of (a) Figure 5a; (b) Figure 5b; (c) Figure 5c (d) Figure 5d; (e) Figure 5e (f) Figure 5f and (g) Figure 5g.