Supporting information

Host-guest interaction of cucurbit[8]uril with N-(3-Aminopropyl)cyclohexylamine: cyclohexylalkane encapsulation triggered ternary complex

Yu Xia¹, Chuan-Zeng Wang¹, Mengkui Tian¹, Zhu Tao¹, Xin-Long Ni^{1*}, Timothy J. Prior² and Carl Redshaw^{2*}

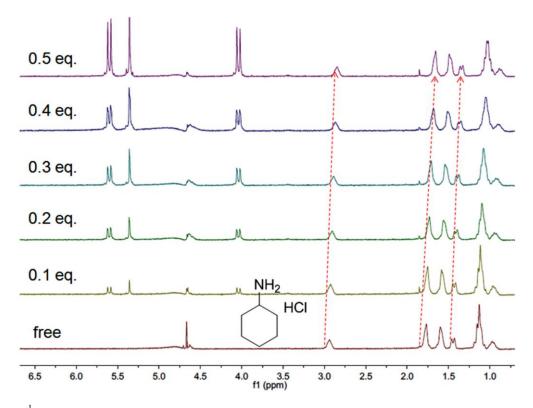


Figure S1. H NMR titration spectra of the \mathbf{CyA} guest in D_2O (1.0 mmol, pD = 2.45) with increasing concentrations of the Q[8] host at room temperature.

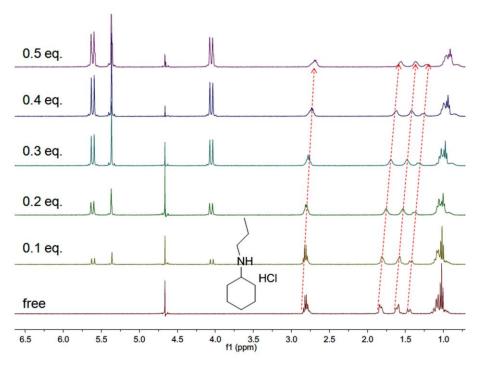


Figure S2. ^{1}H NMR titration spectra of the **NECyA** guest in $D_{2}O$ (1.0 mmol, pD = 2.45) with increasing concentrations of Q[8] host at room temperature.

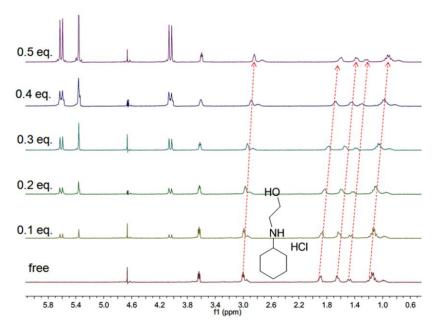


Figure S3. ^{1}H NMR titration spectra of the **NCyEA** guest in $D_{2}O$ (1.0 mmol, pD = 2.45) with increasing concentrations of the Q[8] host at room temperature.

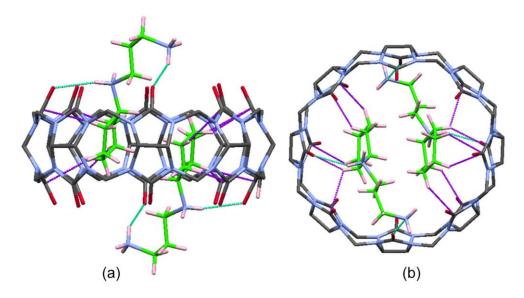


Figure S4. X-ray strucure of Q[8]•N3ACyA: (a) side view; (b) top view; hydrogen bond (green), $C-H\cdots\pi$ interaction (magenta). Hydrogen atoms, solvate water molecules, and $[CdCl_4]^{2^*}$ dianions are omitted for clarity.