Construction of Supramolecular Polymers with Different Topologies by Orthogonal Self-Assembly of Cryptand–Paraquat Recognition and Metal Coordination

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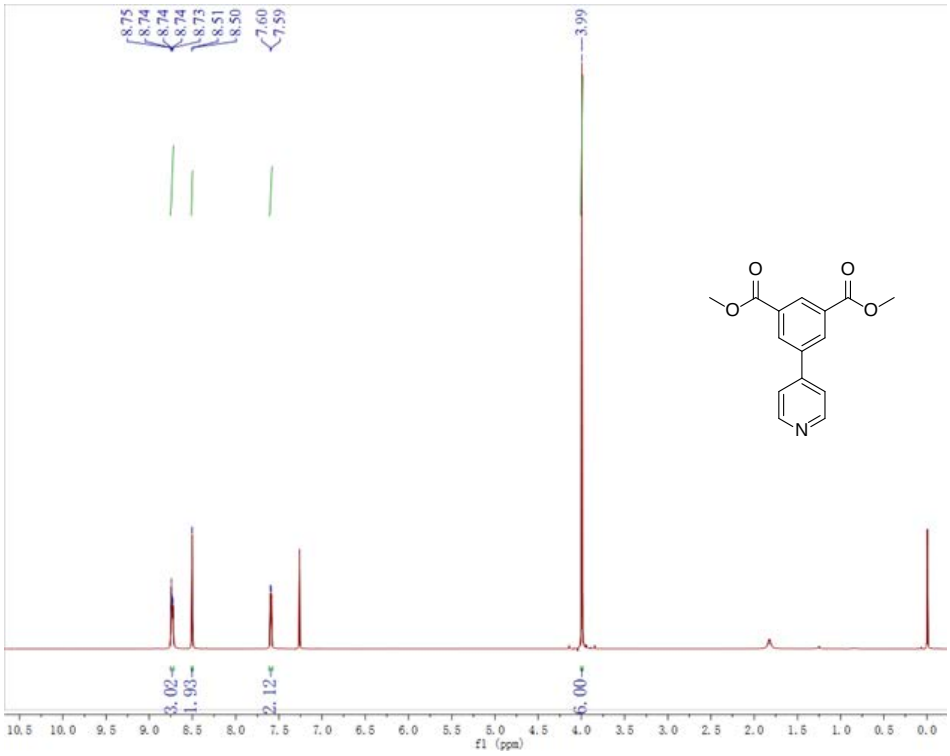

Figure S1. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298 K) of **1**.

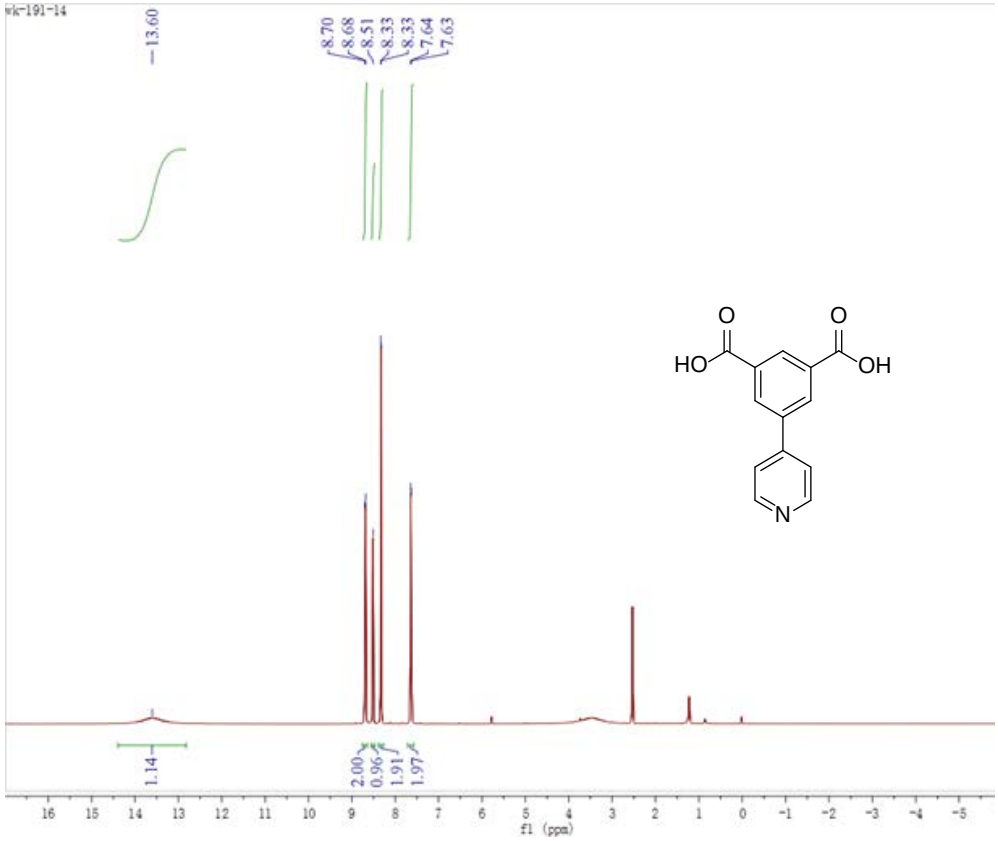

Figure S2. ^{1}H NMR spectrum (500 MHz, DMSO-d_6, 298 K) of **2**.

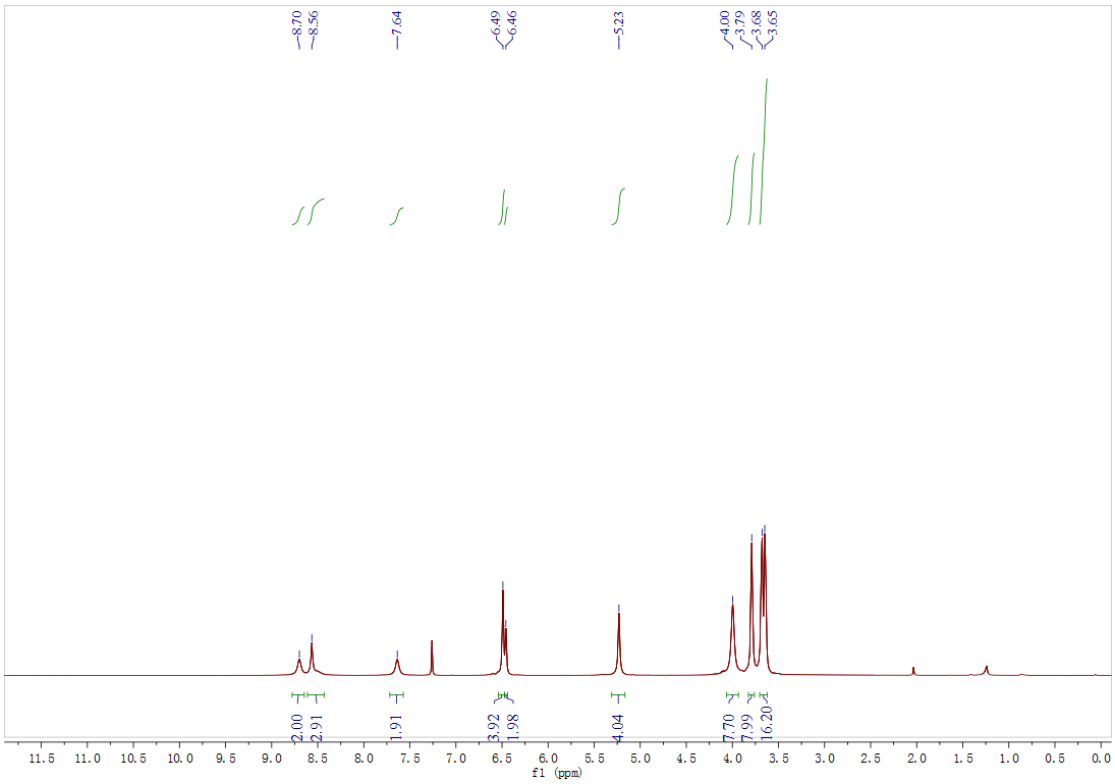

Figure S3. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298 K) of **4**.

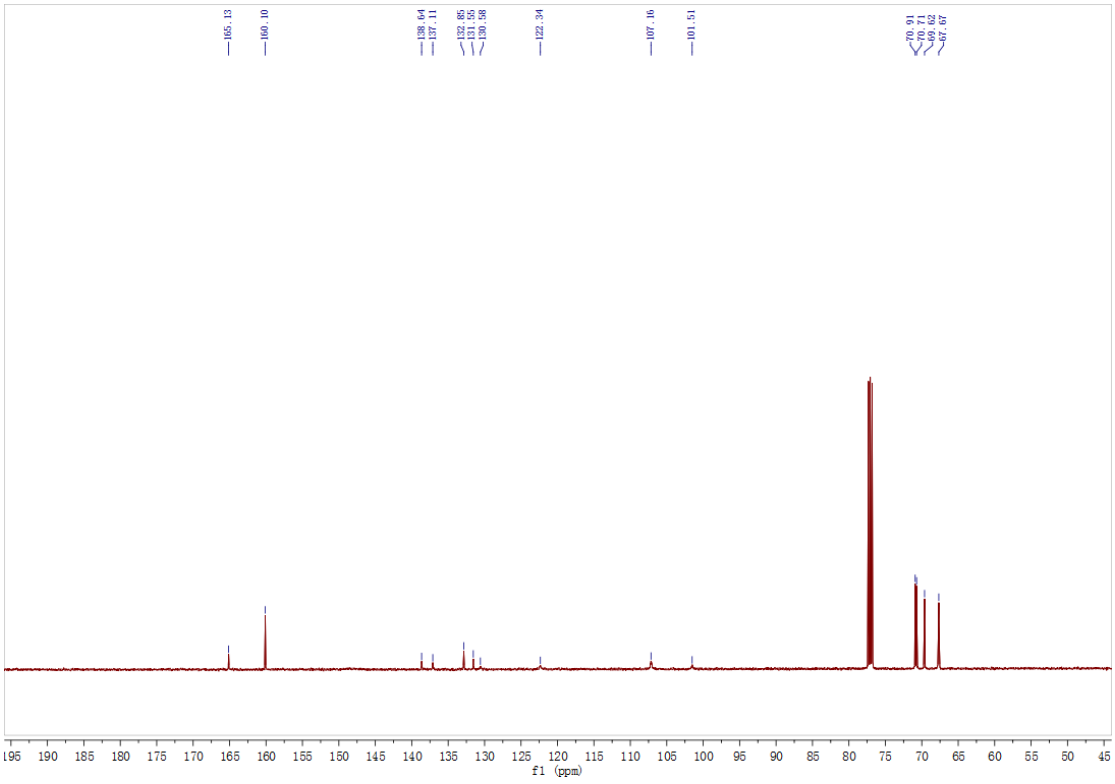

Figure S4. ^{13}C NMR spectrum (126 MHz, $CDCl_3$, 298 K) of **4**.

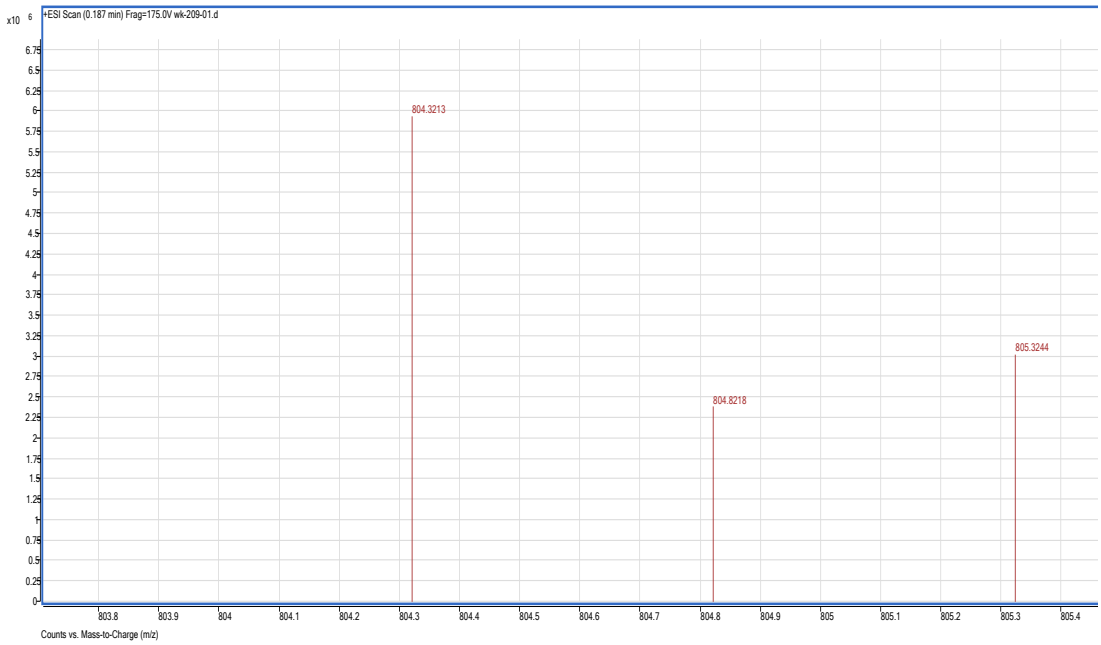

Figure S5. ESI-MS spectrum of **4** (*m/z* = 804.3213 $[M + H]^+$).

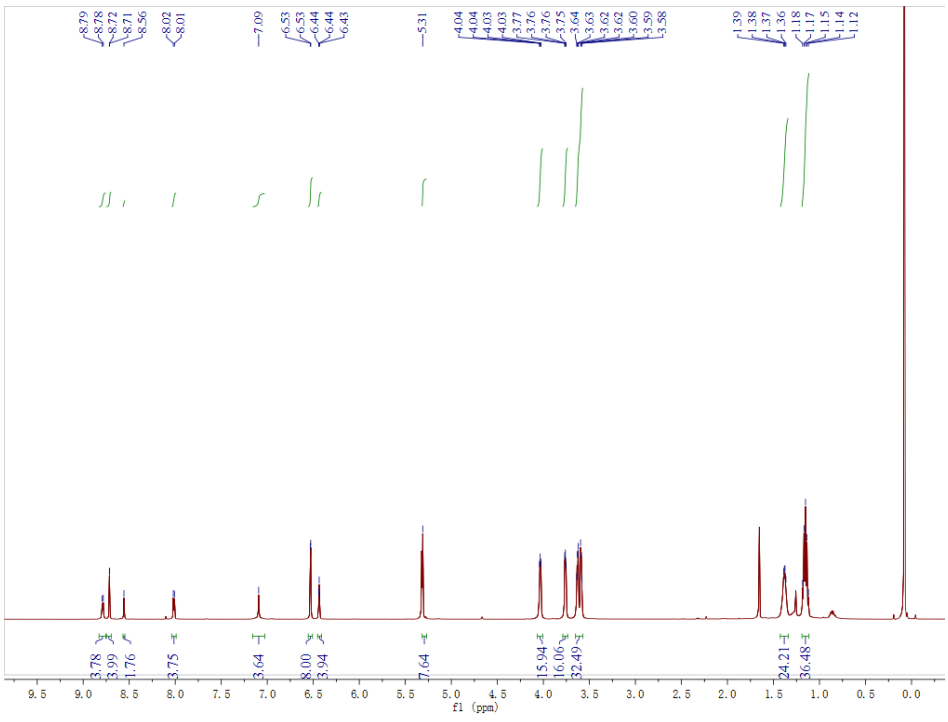

Figure S6. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2, 298 K) of **8**.

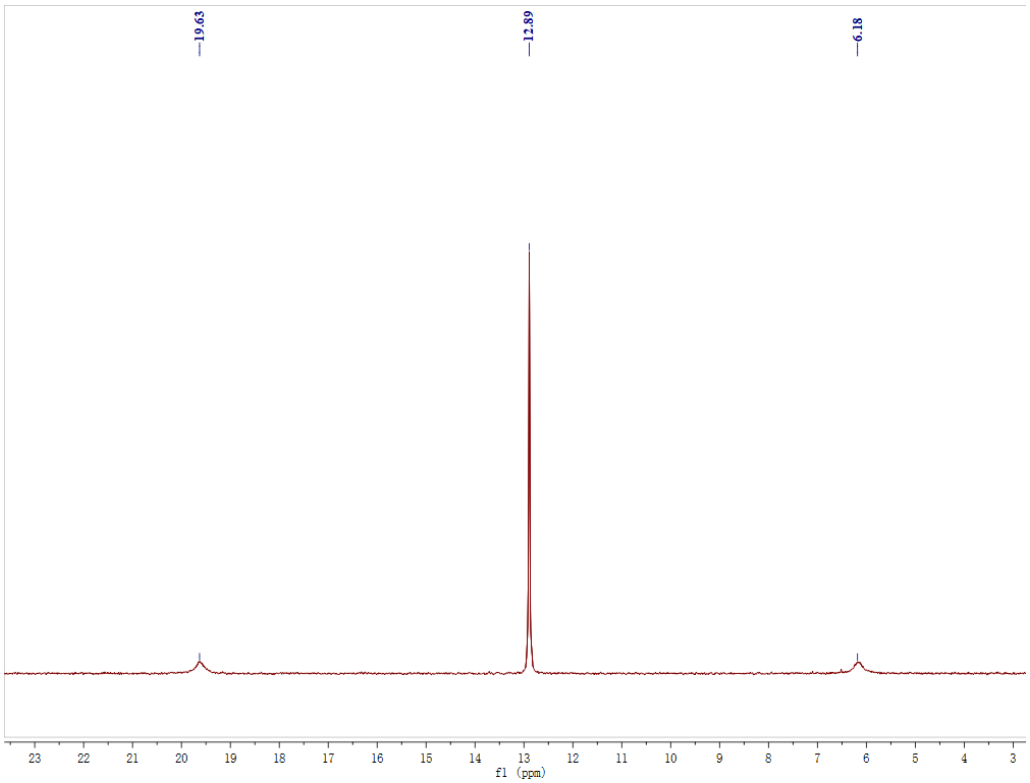

Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum (202 MHz, CD_2Cl_2, 298 K) of **8**.

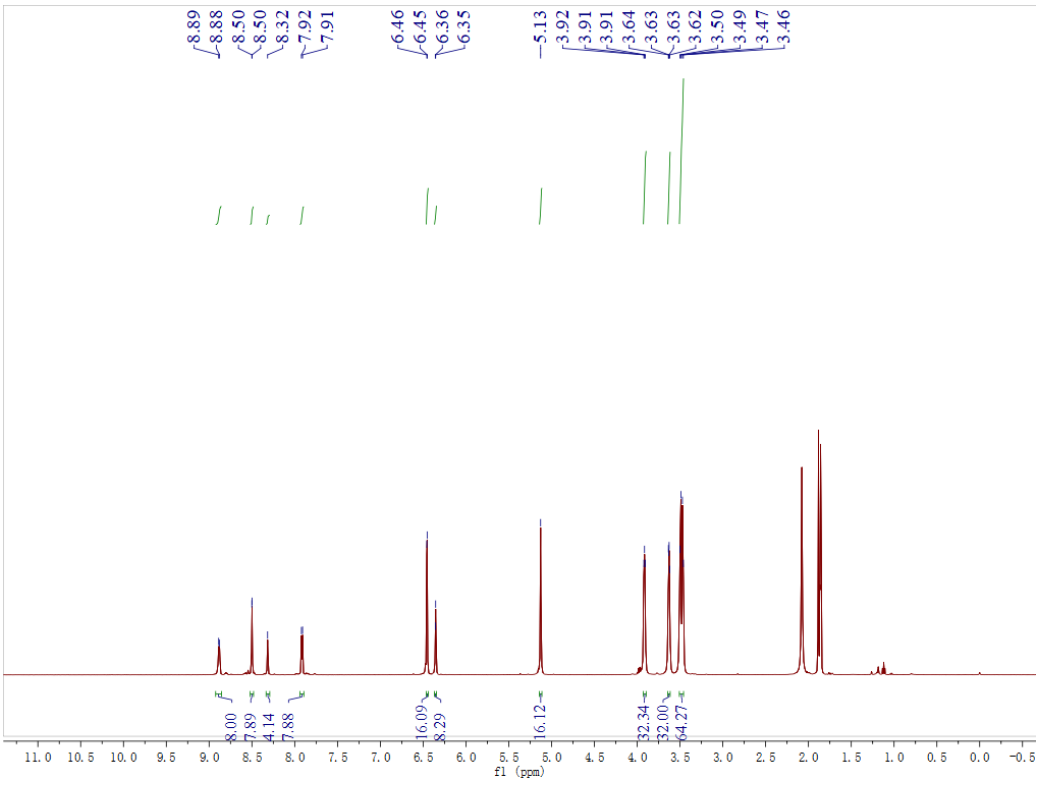

Figure S8. ^{1}H NMR spectrum (500 MHz, CD_3CN, 298 K) of **9**.

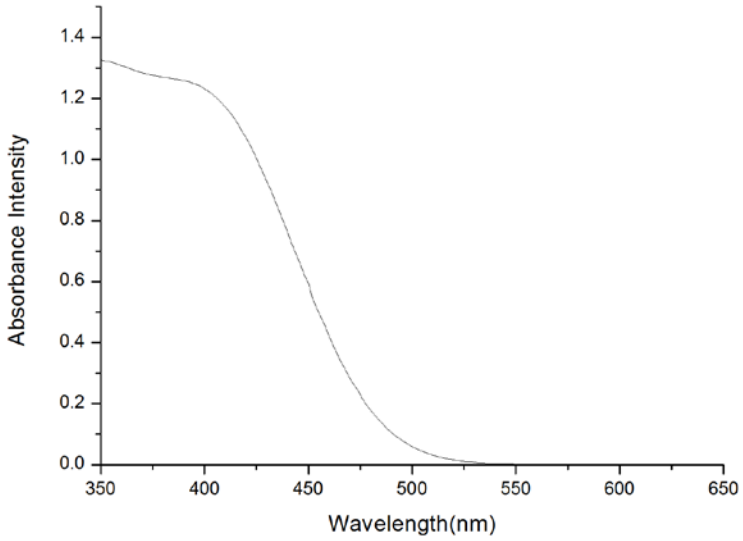

Figure S9. UV-vis absorption spectrum of 2.00 mM **4** and **6** in acetone.

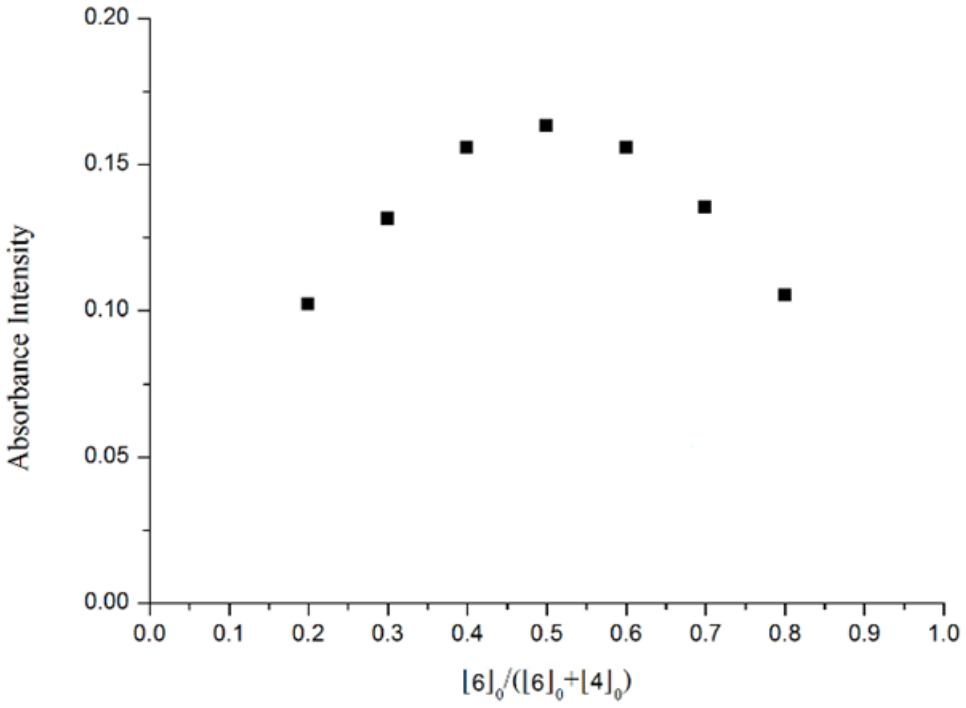

Figure S10. Job plot showing the 1:1 stoichiometry of the complex of **4** and **6** in acetone. $[\mathbf{4}]_0 + [\mathbf{6}]_0 = 2.00$ mM, $\lambda = 400$ nm; $[\mathbf{4}]_0$ and $[\mathbf{6}]_0$ are the initial concentrations of **4** and **6**.

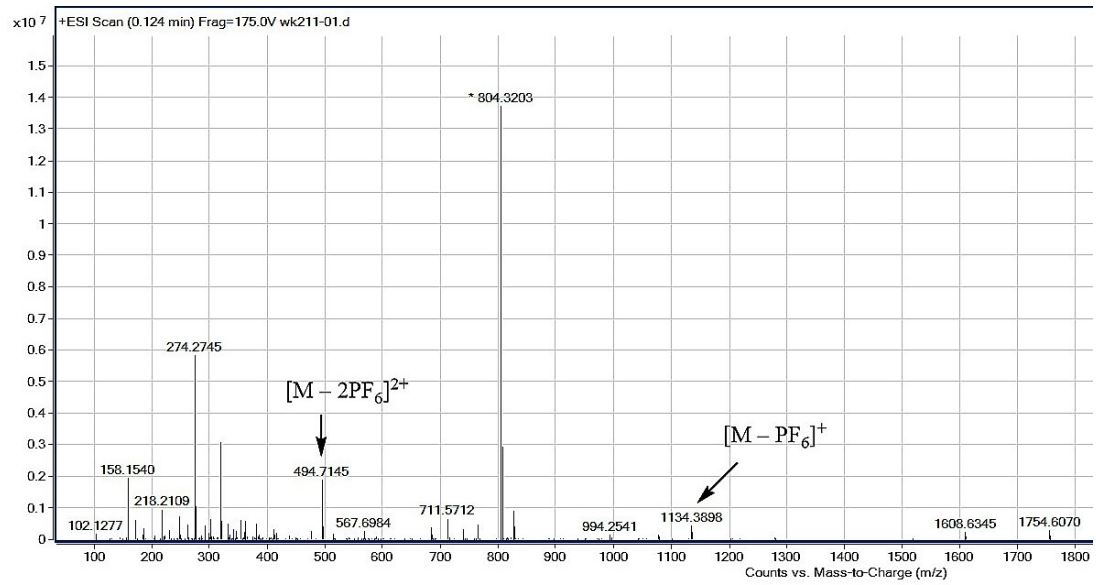

Figure S11. The positive electrospray ionization mass spectrum of an equimolar mixture of **4** and **6** in CH_3CN. Mass fragment at *m*/*z* 494.7145 for [**4**⊃**6** – $2PF_6$]$^{2+}$ and 1134.3898 for [**4**⊃**6** – PF_6]$^{+}$ confirmed the 1:1 complexation stoichiometry.

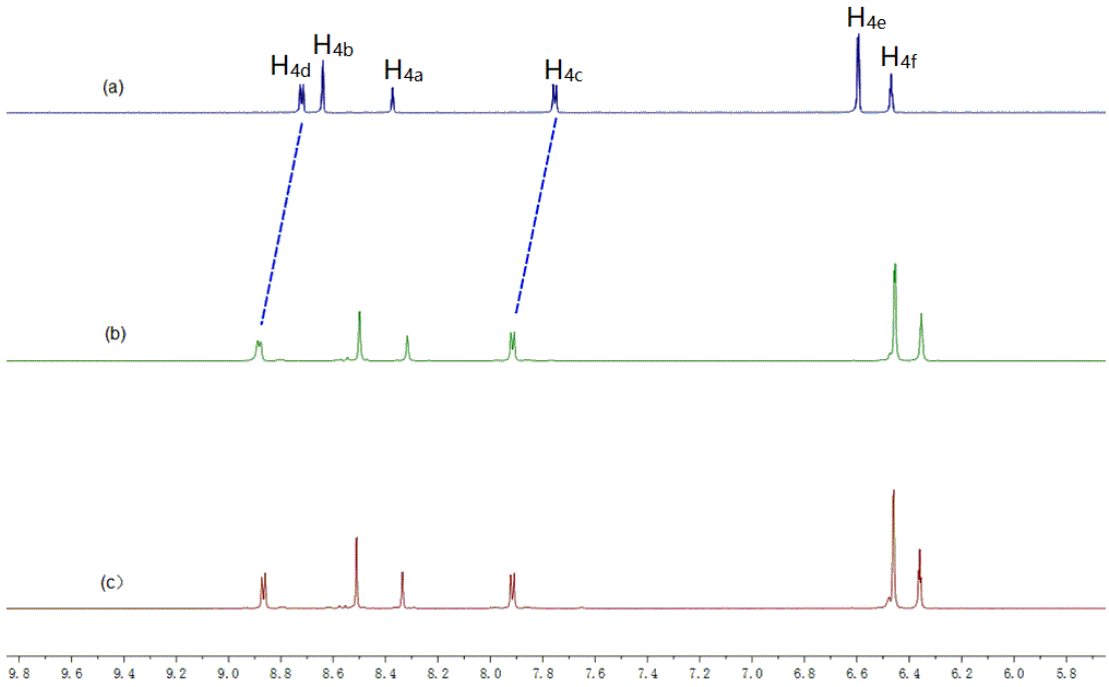

Figure S12. ^{1}H NMR spectra (500 MHz, CD_3CN, 298 K) of (a) cryptand **4**; (b) tetra-cryptand **9** and (c) tetra-cryptand **9** after 7 days.

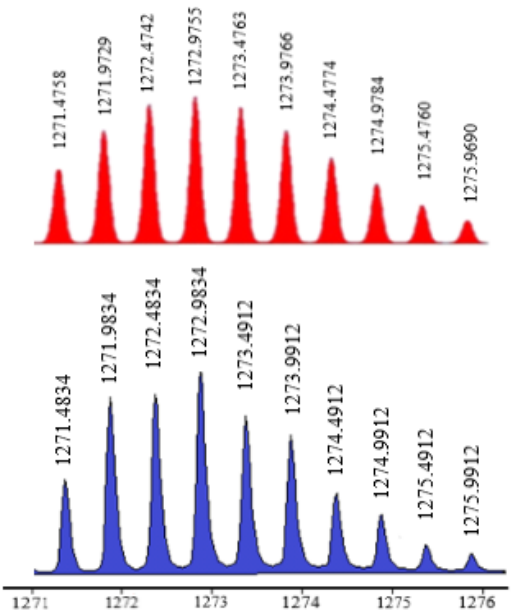

Figure S13. Experimental (red) and calculated (blue) ESI-TOF-MS spectra of **8** $[M– 2OTf]^{2+}$.

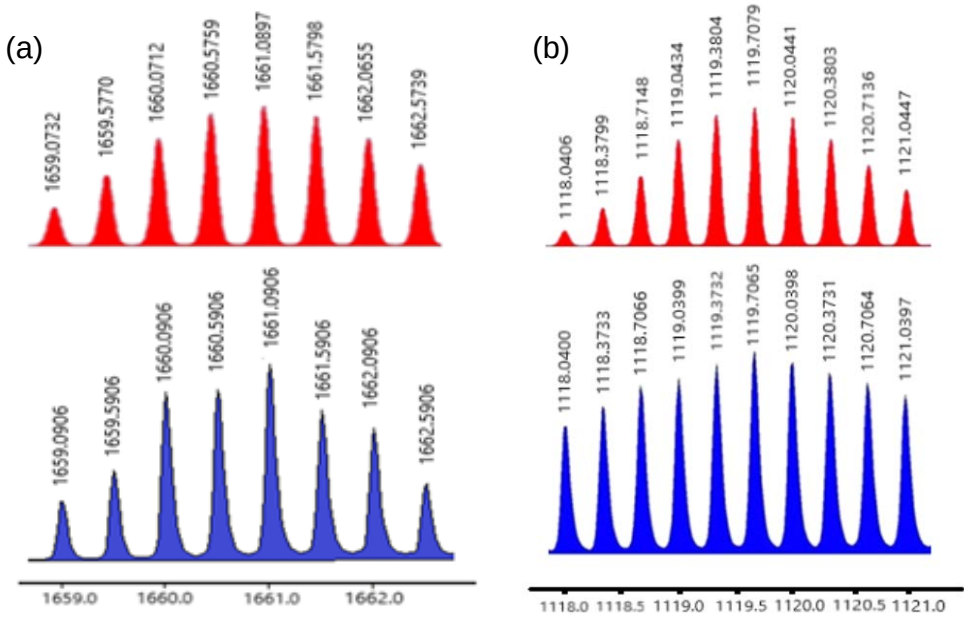

Figure S14. Experimental (red) and calculated (blue) ESI-TOF-MS spectra of **9**: (a) $[M – 2BF_4]^{2+}$ and (b) $[M – 2BF_4 + K]^{3+}$.