Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Information

A Supramolecular Switch Based on Three Binding States of a Pyrene Derivate: A Reversible Three-State Switch with Only Two Stimuli

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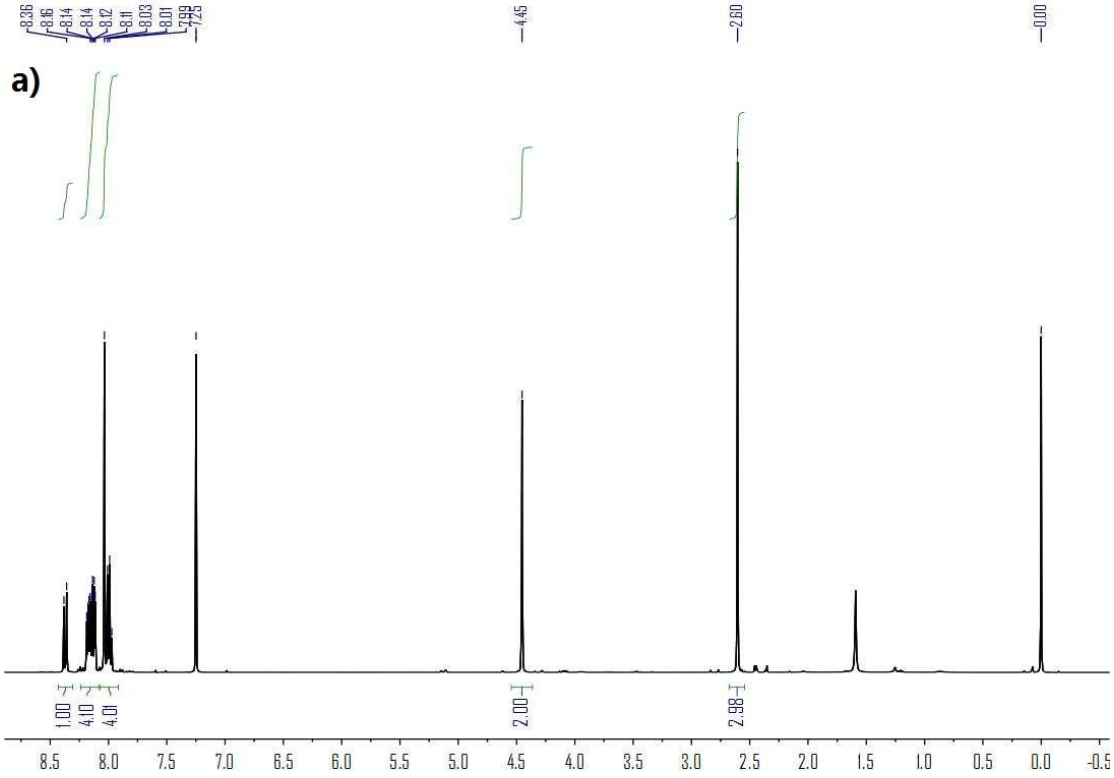


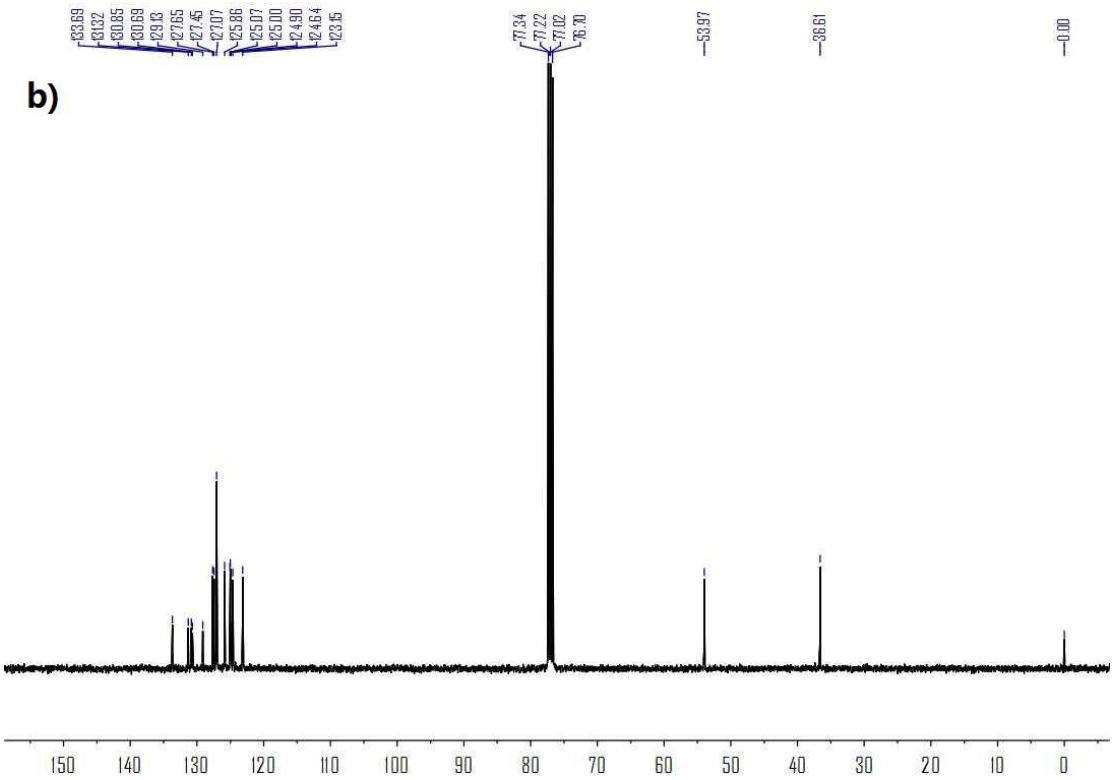


Figure S-1. a) ^{1}H NMR spectrum of N-methyl-pyrenemethylamine (MPA) and b) ^{13}C NMR spectrum of MPA in $CDCl_3$.

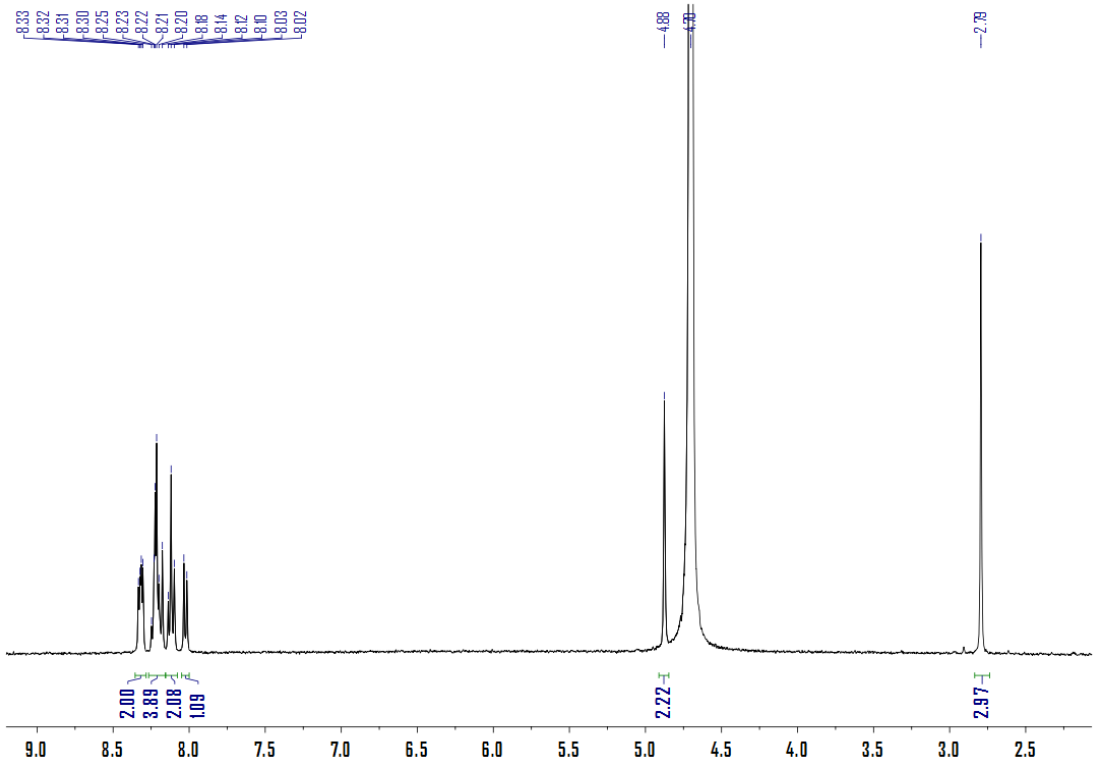


Figure S-2. ^{1}H NMR spectrum of 1 mM N-methyl-pyrenemethylammonium (MPA^{+}) in D_2O.

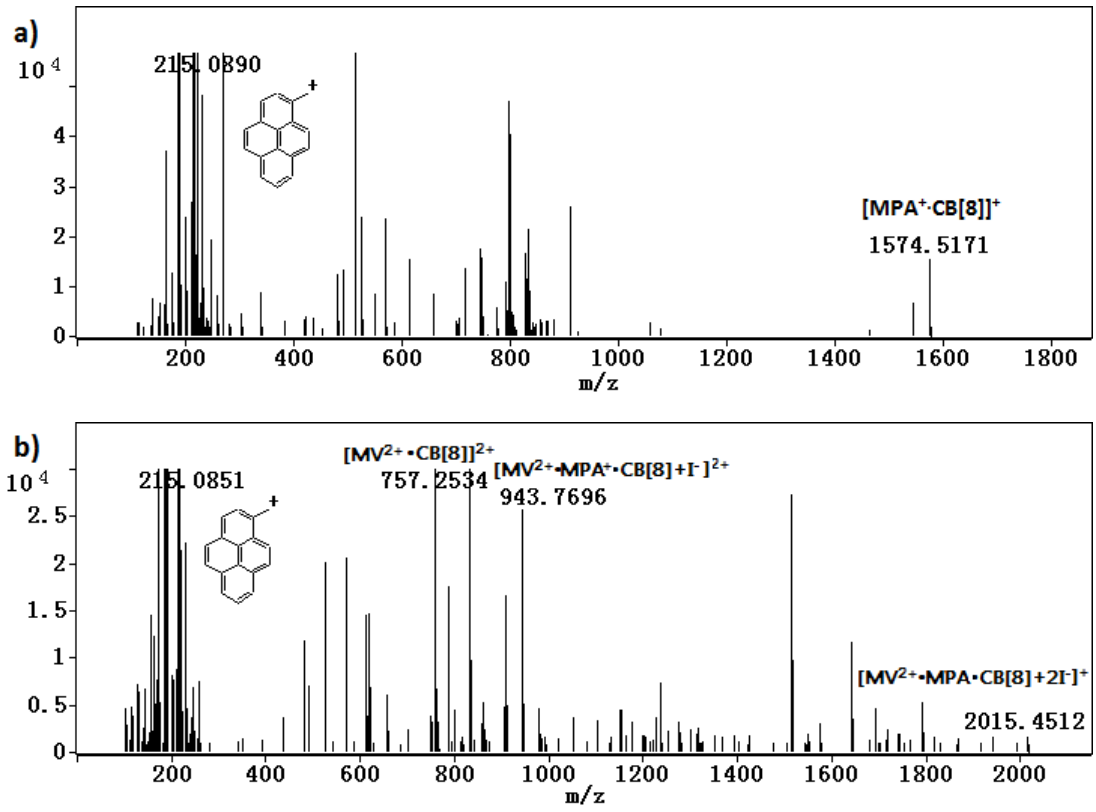
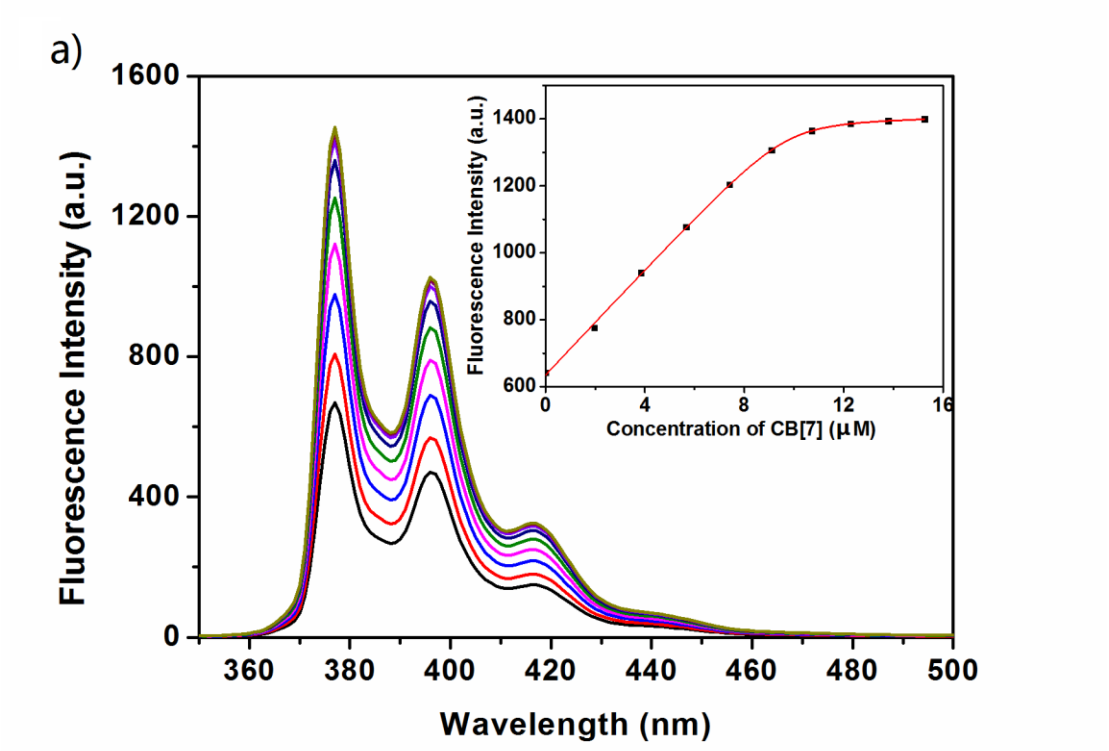
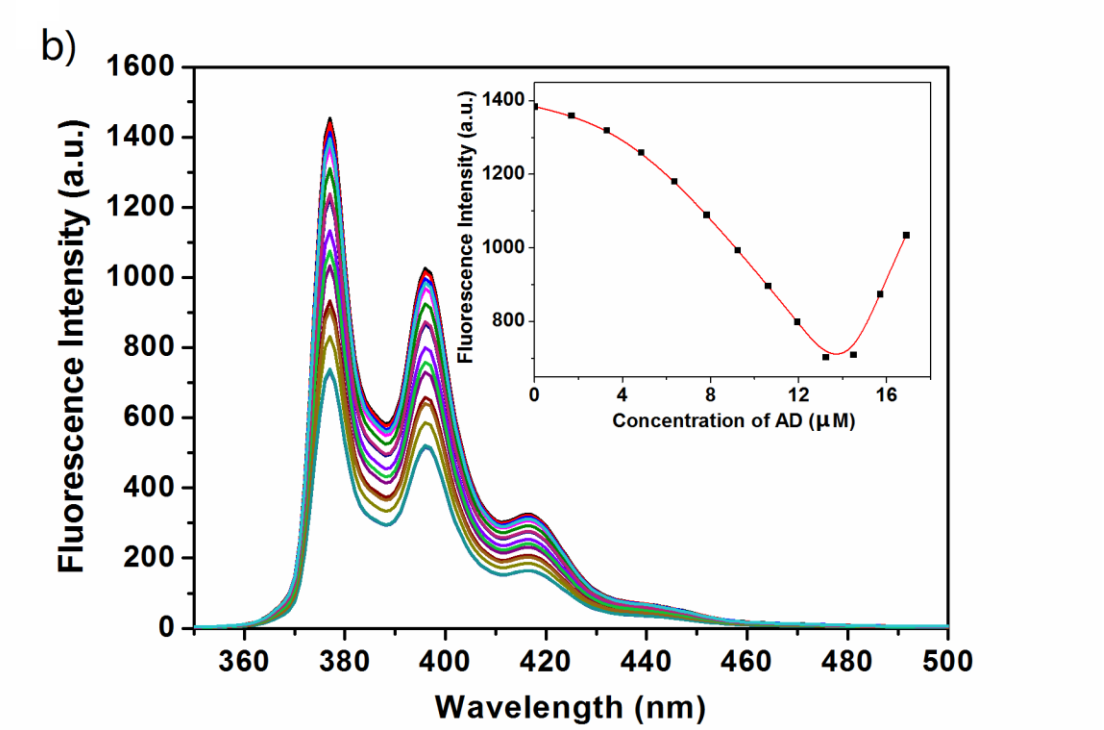
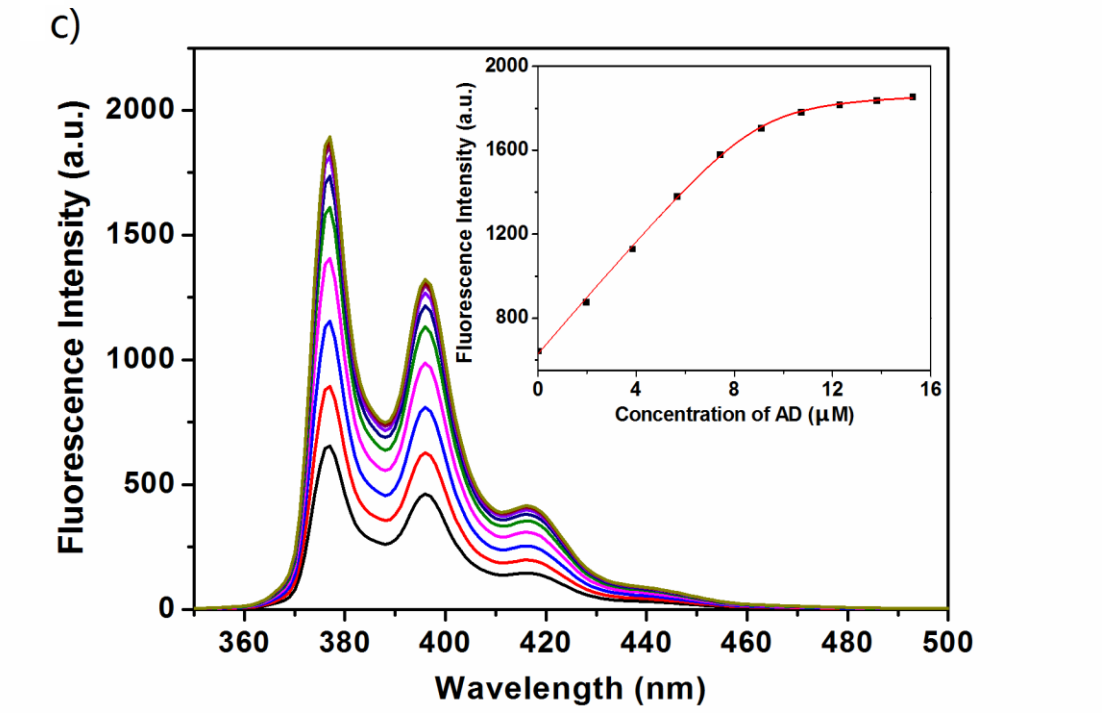


Figure S-3. Accurate mass Q-TOF spectra of a) MPA^+ with CB[8] (1:1 in mole) , and b) MPA^+ with MV^{2+} and CB[8] (1:1:1 in mole)

(MPA^+ is not stable under mass spectroscopy condition and most of it decomposed into methyl pyrene cation. Thus the signals of target complexes are weak and background signals are strong.)







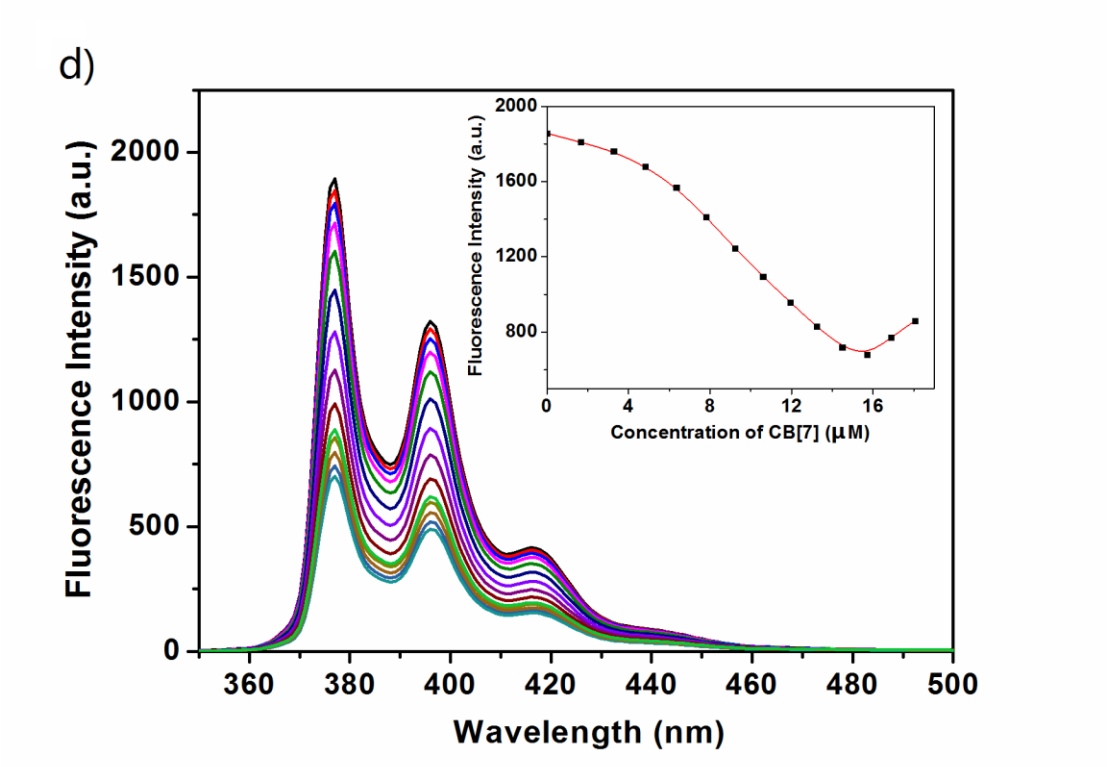


Figure S-4. Emission spectra of a) the titration of $MPA^{+}\cdot MV^{2+}\cdot$CB[8] (10μM) with CB[7], b) the titration of $MPA^{+}\cdot MV^{2+}\cdot$CB[8] (10μM) and CB[7] (15μM) with AD, c) the titration of $MPA^{+}\cdot MV^{2+}\cdot$CB[8] (10μM) with AD and d) the titration of $MPA^{+}\cdot MV^{2+}\cdot$CB[8] (10μM) and AD (15μM) with CB[7], inserts show the fluorescence intensity at 376nm versus the concentration of titrator.

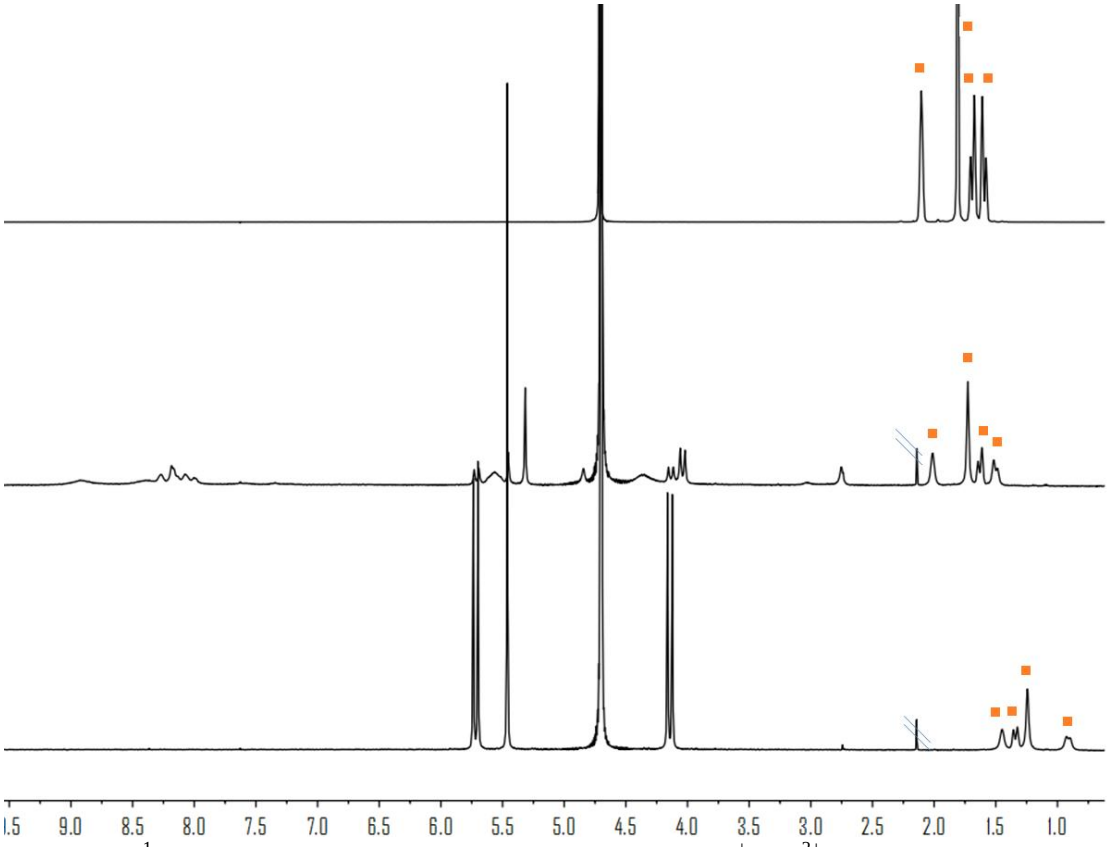


Figure S-5. ^{1}H NMR spectra of 1mM AD (upper), 1 mM MPA^{+}·MV^{2+}·CB[8] with 1.5 mM AD (middle) and 1 mM AD·CB[8] (bottom). Peaks of AD are highlighted with orange squares.

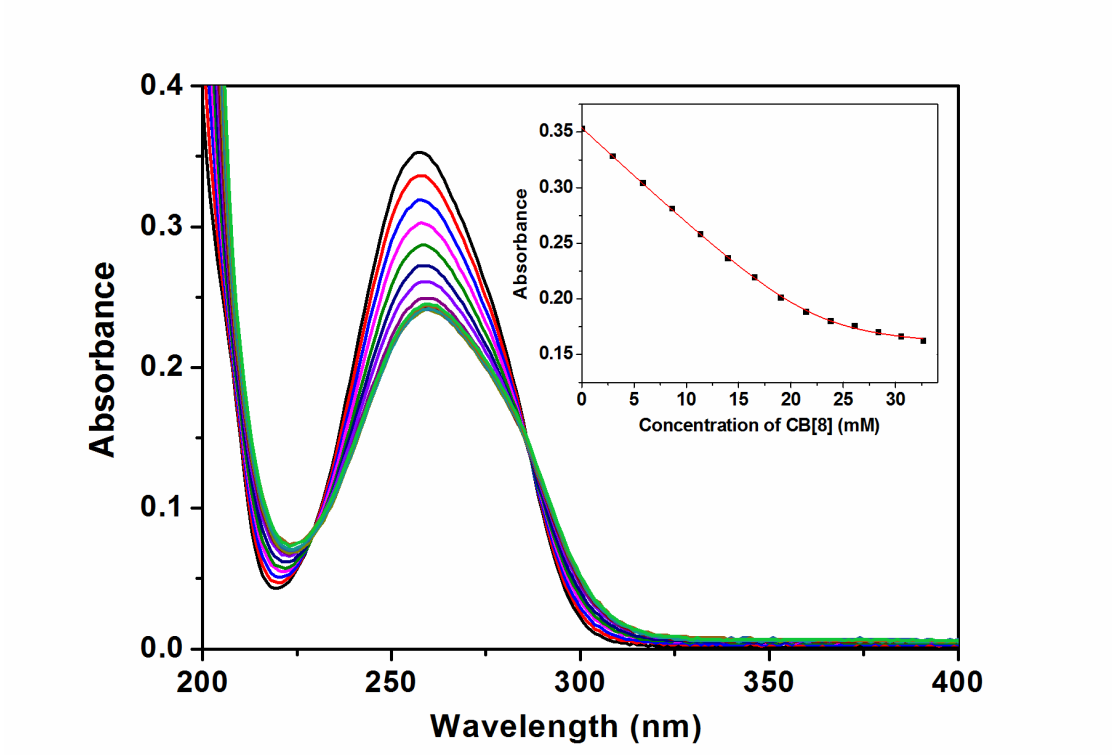


Figure S-6. UV-vis spectra of the titration of MV^{2+} (16 μM) with CB[8] (insert shows the absorbance at 258 nm with different amount of CB[8], corrected for the absorbance of CB[8])

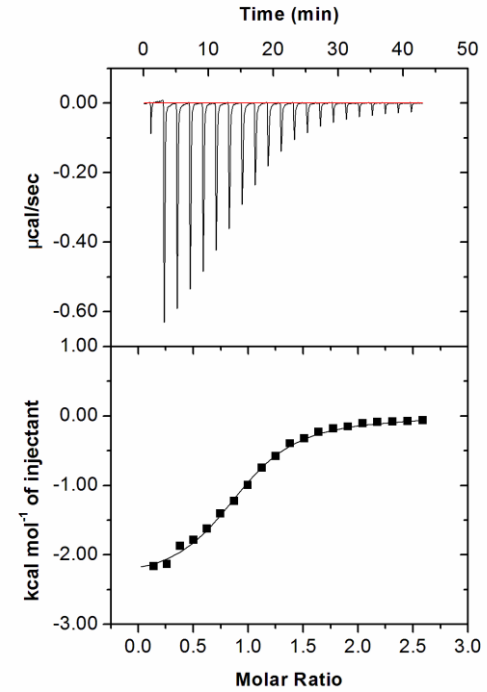


Figure S-7. ITC data for the binding of AD to CB[8] (compete with 6.4 mM MV^{2+})

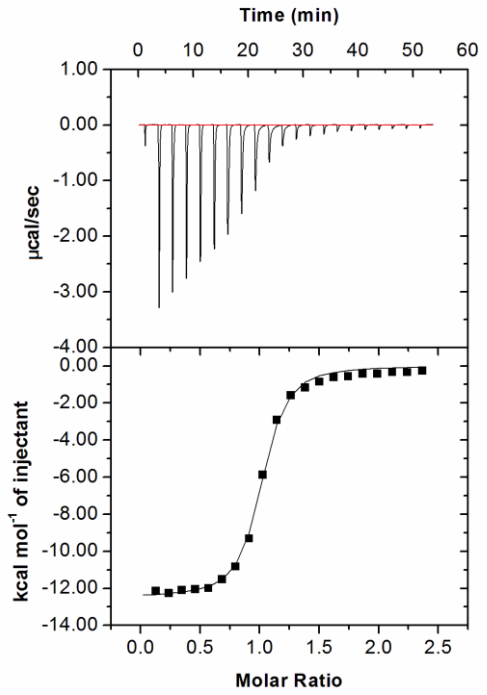


Figure S-8. ITC data for the binding of L-Phenylalanine to CB[7]

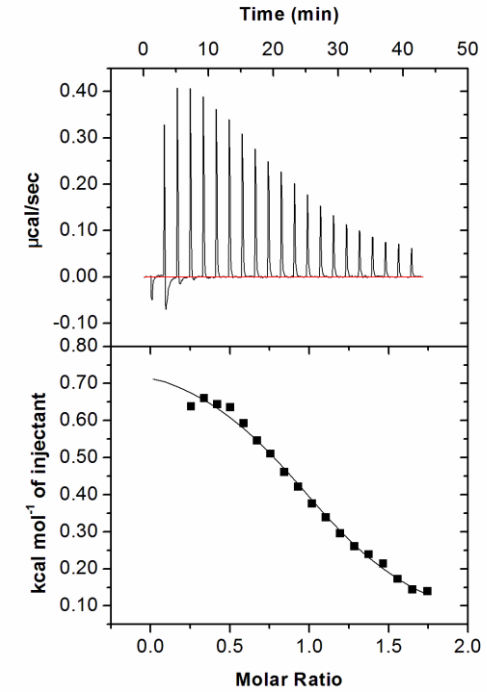


Figure S-9. ITC data for the binding of MV^{2+} to CB[7] (compete with 10.0 mM L-Phenylalanine)

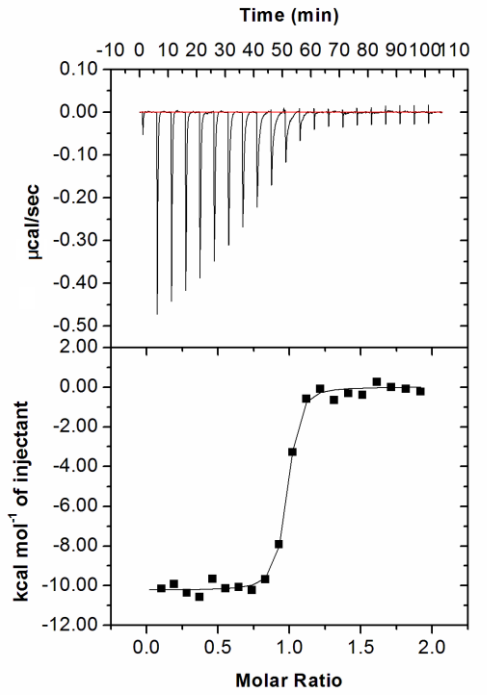


Figure S-10. ITC data for the binding of AD to CB[7] (compete with 8.0 mM MV^{2+})

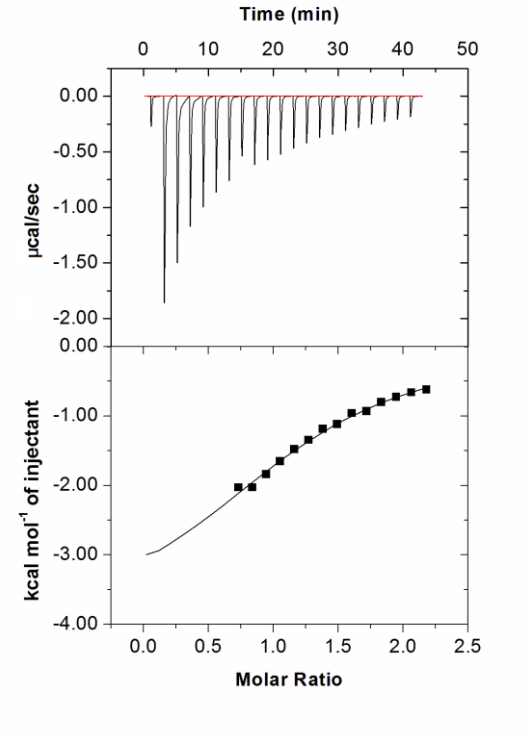


Figure S-11. ITC data for the binding of MPA^+ to CB[7]