ELECTRONIC SUPPLEMENTARY INFORMATION

A new cucurbit[8]uril-based fluorescent receptor for indole derivatives

Yonghua Ling, Wei Wang and Angel E. Kaifer*

Center for Supramolecular Chemistry and Department of Chemistry, University of Miami, Coral Gables, FL 33124-0431

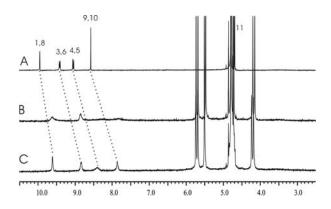


Figure SI-1. 1 H NMR spectrum (0.1MNaCl/D₂O, 300MHz) of 1.0 mM DPT $^{2+}$ in the presence of 0 equiv (A), 0.5 equiv (B) and 1.0 equiv CB8.

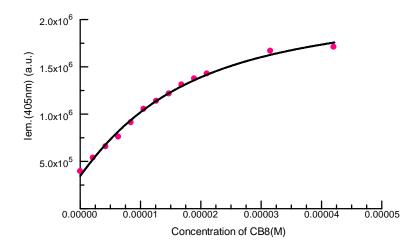


Figure SI-2. Fluorescence intensity at 405nm from a solution of 10 μ M DPT²⁺ as a function of the added CB8 concentration. The data is best fitted to 1:1 binding model to obtain the equilibrium constant $K = 7.8 \times 10^4 \,\mathrm{M}^{-1}$.

Ling, Wang and Kaifer Page SI1

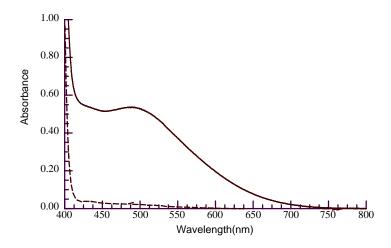


Figure SI-3. Electronic absorption spectra obtained in H_2O for a mixture of 0.52 mM DPT²⁺ and 1.05 mM serotonin (dashed line), and 0.52mM CB8 ,0.54mM DPT²⁺ and 1.05mM serotonin mixture (solid line)

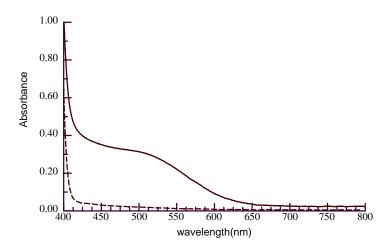


Figure SI-4. Electronic absorption spectra obtained in H_2O for a mixture of 0.5 mM DPT²⁺ and 1.73 mM tryptophan (dashed line), and 0.5 mM CB8 ,0.5 mM DPT²⁺ and 1.73mM tryptophan (solid line)

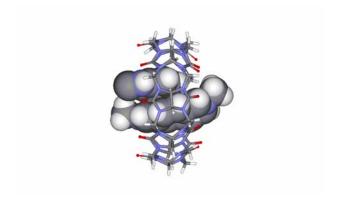


Figure SI-5. Energy- minimized structure of the I • DPT²⁺@CB8 ternary complex (PM3)

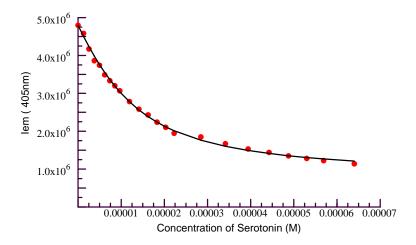


Figure SI-6. Fluorescence intensity at 405nm from a solution of 10 μ M DPT²⁺ and 10 μ M CB8 as a function of the added serontonin concentration. The data is best fitted to 1:1 binding model to obtain the equilibrium constant $K=1.45\times10^5\,\mathrm{M}^{-1}$.

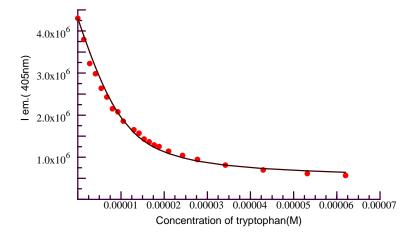


Figure SI-7. Fluorescence intensity at 405nm from a solution of 10 μ M DPT²⁺ and 10 μ M CB8 as a function of the added tryptophan concentration. The data is best fitted to 1:1 binding model to obtain the equilibrium constant $K=4.16\times10^5\,\mathrm{M}^{-1}$.