

Electronic Supplementary Information

Metal Ion-induced Supramolecular pK_a Tuning and Fluorescence Regeneration of *p*-Sulfonatocalixarene Encapsulated Neutral Red Dye

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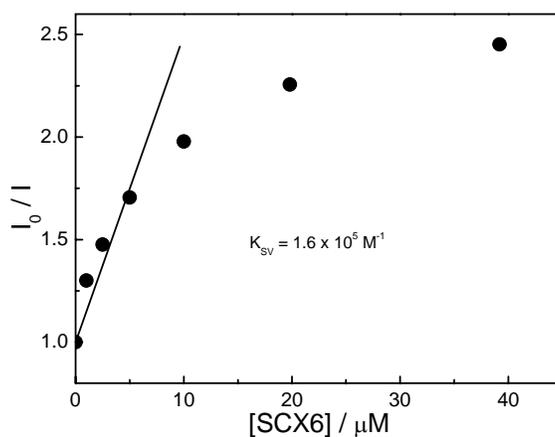


Figure S1. Stern-Volmer plots obtained from the fluorescence intensity quenching of NRH⁺ by SCX6 at pH 5. The emission was monitored at 635 nm.

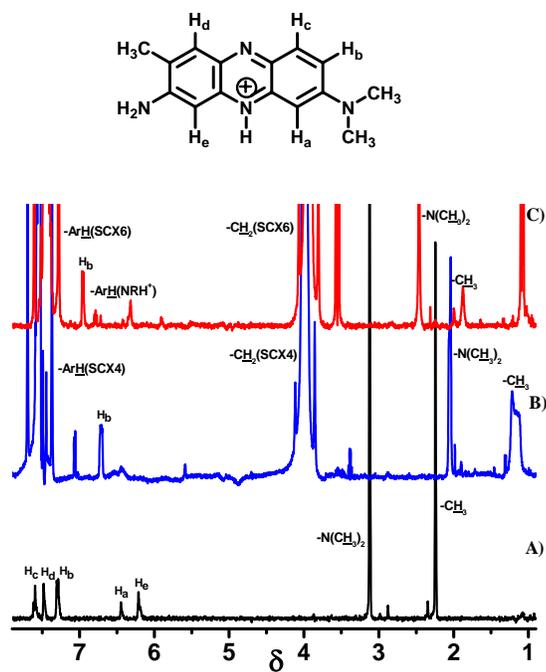


Figure S2. ¹H NMR spectra of NRH⁺ in the absence (A) and in the presence of SCX4 (B) and SCX6 (C) in D₂O.

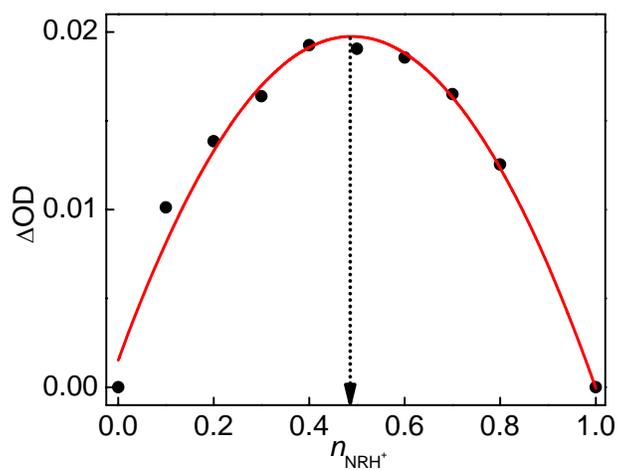
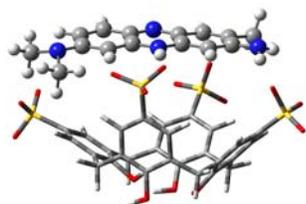


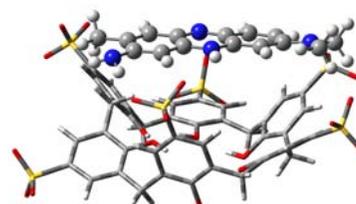
Figure S3. Job plot evaluated by the absorbance changes at 535 nm for the SCX4:NRH⁺ complex. n_{NRH^+} represents the mole fraction of NRH⁺.

(A)



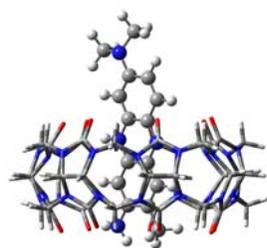
($\Delta H_f = -223$ kcal/mol)

(B)



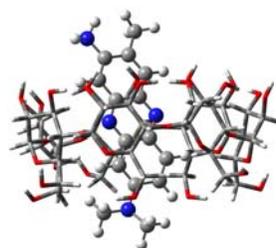
($\Delta H_f = -260$ kcal/mol)

(C)



($\Delta H_f = -35.6$ kcal/mol)

(D)



($\Delta H_f = -7.5$ kcal/mol)

Figure S4. Energy-optimized structures of SCX4:NRH⁺ (A); SCX6:NRH⁺ (B); CB7:NRH⁺ (C) and β -CD:NR (D) complexes.