Supporting Information

Study of Cavity Size and Nature of Bridging Units on Recognition of Nucleotides by Cyclophanes

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Figure S1. Relative changes in the absorbance of the different cyclophanes **CP–1**, **CP–2**, **CP–3** and **CP–4** with the addition of various nucleosides and nucleotides in phosphate buffer (10 mM, pH 7.4).



Figure S2. Changes in the emission spectrum of **CP-1** (11 μ M) with the addition of (A) 5'-GTP and (B) 5'-ATP in 10 mM phosphate buffer (pH 7.4). [5'-GTP or 5'-ATP], (a) 0 and (g) 500 μ M (λ_{ex} = 355 nm).



Figure S3. ¹H NMR spectra of the **CP-1** in D_2O in the (a) absence and (b) presence of 5'-ATP (0.35 mM).



Figure S4. Changes in the absorption spectrum of HPTS (7 μ M) with gradual addition of **CP–1** in phosphate buffer (pH 7.4). Inset shows the Benesi–Hildebrand fit for fluorescence quenching of HPTS by **CP–1**. [**CP–1**], (a) 0, (b) 1.25, (c) 2.51, (d) 3.78, (e) 5.05 and (f) 6.25 μ M.



Figure S5. Changes in the emission spectrum of HPTS (3.3 μ M) with gradual addition of **CP-4** in phosphate buffer (pH 7.4). [**CP-4**], (a) 0, (b) 3.14, (c) 6.23, (d) 9.27, (e) 12.26, (f) 15.2, (g) 18.1, (h) 20.94 and (i) 23.75 μ M (λ_{ex} = 364 nm).



Figure S6. Fluorescence decay profile of HPTS (3.0 μ M) alone and in the presence of the cyclophane **CP–2**. [**CP–2**] (a) 0, (b) 3.5 and (c) 4.3 μ M.



Figure S7. Effect of temperature on the emission spectrum of the complex [**CP**– **3**·HPTS] in phosphate buffer (10 mM, pH 7.4). (a) 298 to (g) 358 K (λ_{ex} = 364 nm).



Figure S8. Relative fluorescence quenching of HPTS by **CP-4** at different salt concentrations.



Figure S9. Changes in the emission spectrum of HPTS (6.6 μ M) with gradual addition of **OC-4** in phosphate buffer (pH 7.4). [**OC-4**], (a) 0, (b) 1.25, (c) 2.51, (d) 3.78, (e) 5.05 and (f) 6.25 μ M. (λ_{ex} = 364 nm).



Figure S10. Fluorescence indicator displacement from the complexes (A) [**CP-2**·HPTS] and (B) [**CP-3**·HPTS] by 5'–GTP in phosphate buffer (pH 7.4). [5'–GTP], (a) 0 and (i) 1.6 mM (λ_{ex} = 364 nm).



Figure S11. Fluorescence indicator displacement from the complex [**CP-4**·HPTS] by 5'-GTP in phosphate buffer (pH 7.4). [5'-GTP], (a) 0 and (i) 0.56 mM ($\lambda_{ex} = 364$ nm).



Figure S12. ¹H NMR spectrum of **CP–1** in DMSO-*d*₆.



Figure S13. ¹H NMR spectrum of **CP–2** in DMSO-*d*₆.



Figure S14. ¹H NMR spectra of **CP–3** in DMSO- d_6 .



Figure S15. ¹H NMR spectra of **CP–4** in DMSO- d_6 +D₂O.



Figure S16. ¹H NMR spectra of **OC–4** in D_2O .