<Supporting Information>

A Truncated Octahedral Nanocage for Fluorescent Detection of Nucleoside

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Experimental Section.

All chemicals were of reagent grade quality obtained from commercial sources and the solvents used were purification by standard procedure. The elemental analyses of C, H and N were performed on a Vario EL III elemental analyzer. $^1$H NMR and $^{13}$C NMR spectra were measured on a Varian INOVA 400M spectrometer. API mass spectra were recorded on HP1100LC/MSD spectrometer. ESI mass spectra were carried out on a HPLC-Q-Tof MS spectrometer using methanol as mobile phase. The solution fluorescent spectra were measured on JASCO FP-6500 in DMF solution. Both excitation and emission slit widths were 3 nm.
Scheme S1. Two possible ligand conformations in the complex **DL1**. When the quinoline nitrogen and amide oxygen of the ligand are on the same side, the conformation of the ligand was defined as syn-type and when in the opposite side, as anti-type.
Figure S1. $^1$H-NMR spectra of QA (top) and complex DL1 (bottom) in d$^6$-DMSO, showing the broadened and overall chemical shifted resonance signals.
Figure S2 Fluorescent response of complex DL1 upon the addition of Adenosine (A), Guanosine (G), Cytidine (C) and Uridine (U), excited at 370 nm. Insert: linear fitting of the intensity recorded on 410 nm, $R^2 = 0.999$ (A), 0.996 (G), 0.997 (C) and 0.997 (U), respectively.
**Association Constant Calculation:**

Generally, for the formation of 1:1 complexed species formed by the cage compound and the guest anion (G), if we assume $xC_0$ to the concentration of complexes species cage-nG, when the concentration of the added guest anion is $nC_0$ with the original concentration of the cage being fixed at $C_0$:

$$\text{cage} + G \rightleftharpoons \text{cage - G}$$

$cage$ only $C_0$

$nC_0$ G is added $(1-x)C_0$ $(n-x)C_0$ $xC_0$

$$K = \frac{[\text{cage-G}]}{[\text{cage}][G]} = \frac{xC_0}{(n-x)C_0(1-x)C_0} = \frac{x}{(n-x)(1-x)C_0}$$

When the value of $x \ll n$:

$$K = \frac{x}{n(1-x)C_0}$$

The measurements are performed under the conditions where the intensity value of the free cage compound in such a concentration is $F_0$, after addition of a given amount ($nC_0$) of G, the fluorescent intensity becomes:

$$F = F_1x + F_0(1-x)$$

where $F_1$ is the intensity of the saturated value in the presence of excess guest anions.

It is easy to derive the usual equation:

$$\frac{F-F_0}{F_1-F_0} = x$$

From eqs (2) and (4), we can obtain the equation:

$$\frac{1}{KC_0(F_1-F_0)} \cdot \frac{1}{n} = \frac{1}{F-F_0}$$

$K$ can be obtained by a linear analysis of $1/n$ ($X$) versus $1/(F-F_0)$ ($Y$).
Figure S3 ESI-TOF spectra of compound DL1 in d₆-DMSO solution in the presence of equivalent molar ratio of uridine, showing the measured and simulated isotopic patterns of each peak, respectively.