

## <Supporting Information>

### A Truncated Octahedral Nanocage for Fluorescent Detection of Nucleoside

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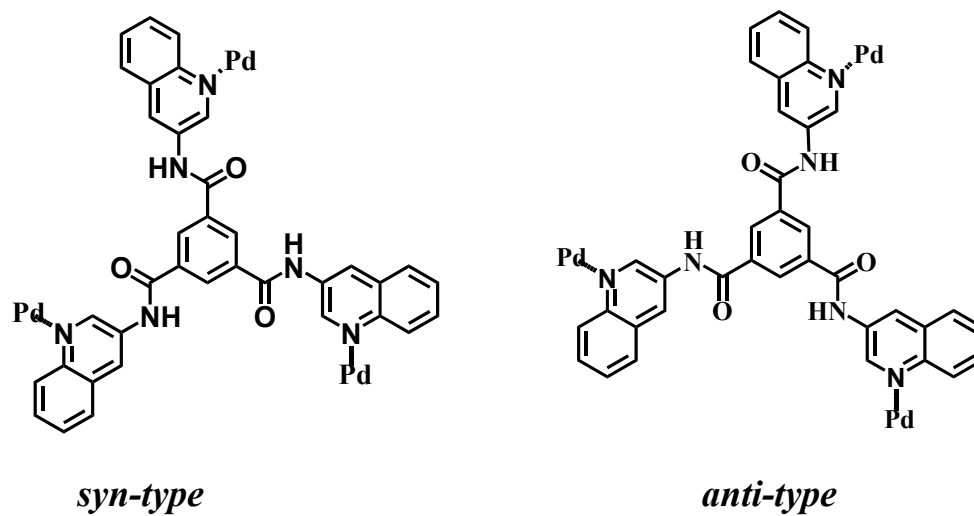
**Figure S1.** <sup>1</sup>H-NMR spectra of QA and compound **DL1**, Pd<sub>6</sub>(QA)<sub>8</sub>(NO<sub>3</sub>)<sub>12</sub>.

**Figure S2** Fluorescent responses of compound **DL1**, Pd<sub>6</sub>(QA)<sub>8</sub>(NO<sub>3</sub>)<sub>12</sub> upon the addition of Adenosine, Guanosine, Cytidine and Uridine, and the Association Constant Calculation.

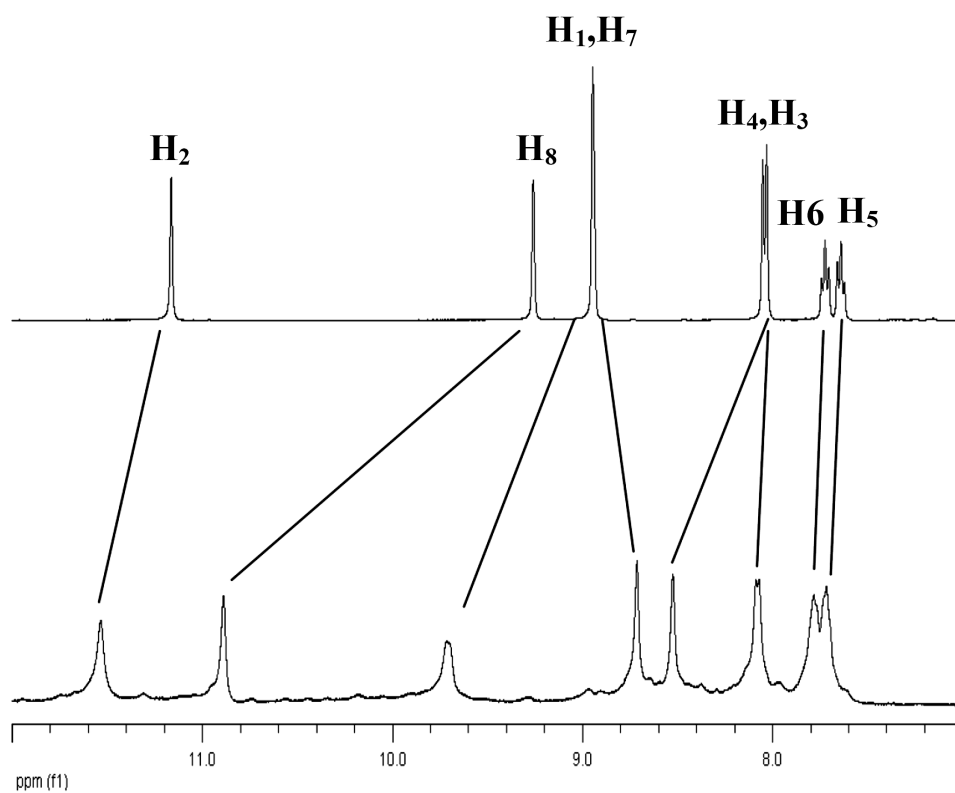
**Figure S3** ESI-TOF spectra of compound **DL1**, Pd<sub>6</sub>(QA)<sub>8</sub>(NO<sub>3</sub>)<sub>12</sub> in the presence of uridine and the simulation of the peaks.

## **Experimental Section.**

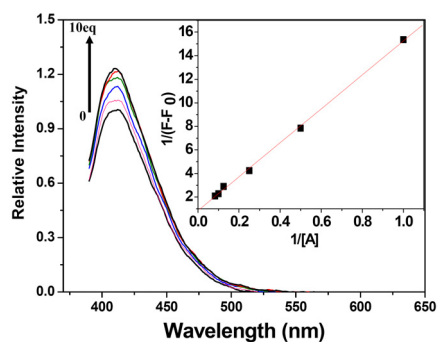
All chemicals were of reagent grade quality obtained from commercial sources and the solvents used were purification by standard procedure. The elemental analyses of C, H and N were performed on a Vario EL III elemental analyzer.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were measured on a 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.



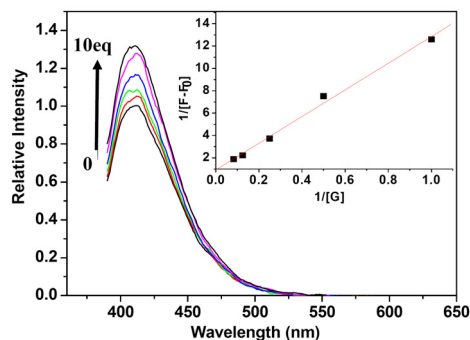
**Scheme S1.** Two possible ligand conformations in the complex **DL1**. When the quinoline nitrogen and amide oxygen of the ligand are on the same side, the conformation of the ligand was defined as *syn-type* and when in the opposite side, as *anti-type*.



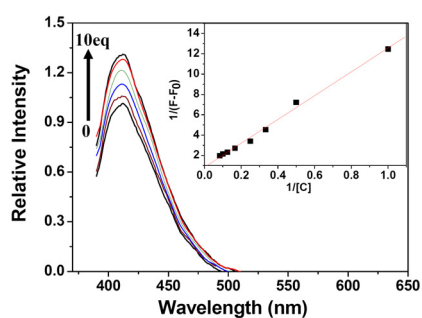
**Figure S1.** <sup>1</sup>H-NMR spectra of **QA** (top) and complex **DL1** (bottom) in d<sup>6</sup>-DMSO, showing the broadened and overall chemical shifted resonance signals.



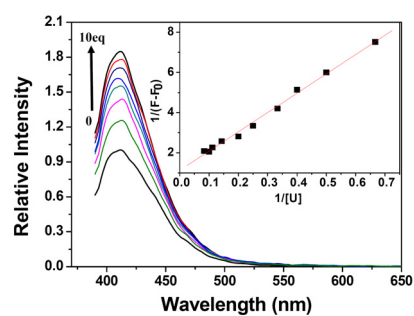
**A** ( $\log K=3.54\pm 0.01$ )



**G** ( $\log K= 3.62 \pm 0.02$ )



**C** ( $\log k=3.63\pm 0.02$ )

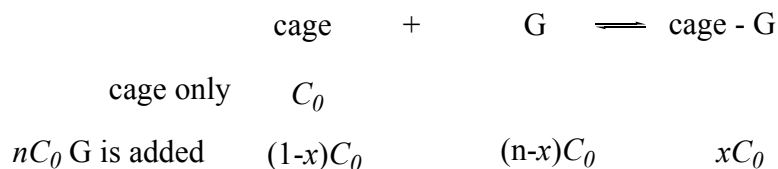


**U** ( $\log k = 3.72 \pm 0.01$ )

**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  $x C_0$  to be the concentration of complexed species cage-nG, when the concentration of the added guest anion is  $n C_0$  with the original concentration of the cage being fixed at  $C_0$ :



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

When the value of  $x \ll n$ :

$$K = \frac{x}{n(1-x)C_0} \quad 2$$

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 ( $n C_0$ ) of G, the fluorescent intensity becomes:

$$F = F_1 x + F_0 (1-x) \quad 3$$

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:

$$\frac{F-F_0}{F_1-F_0} = x \quad 4$$

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

$$\frac{1}{K C_0 (F_1 - F_0)} \cdot \frac{1}{n} = \frac{1}{F - F_0} \quad 5$$

$K$  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  $d_6$ -DMSO solution in the presence of equivalent molar ratio of uridine, showing the measured and simulated isotopic patterns of each peak, respectively.

