Electronic Supplementary Information for Dalton Transactions

<Supporting Information>

A Truncated Octahedral Nanocage for Fluorescent Detection of Nucleoside

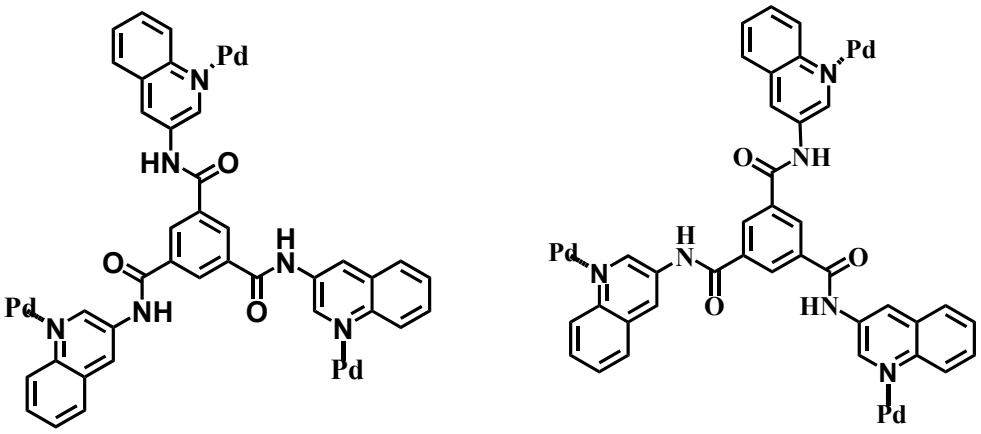
Yang Liu, Xiao Wu, Cheng He,* Rong Zhang and Chunying Duan*

State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116012, China. E-mail: cyduan@dlut.edu.cn

Contents

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.



syn-type ***anti-type***

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.

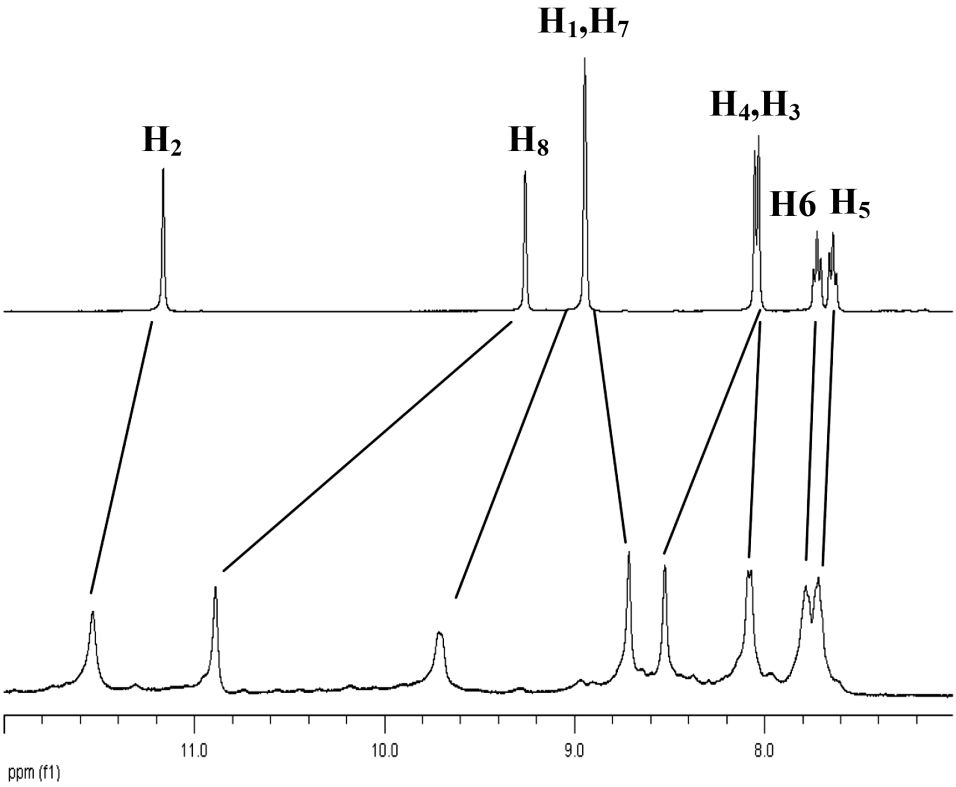
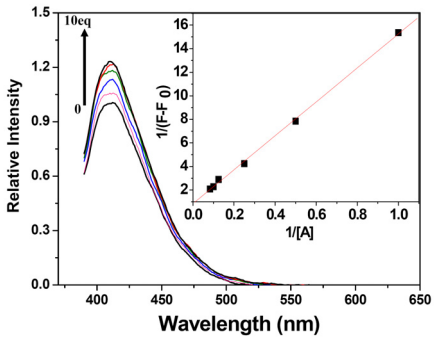
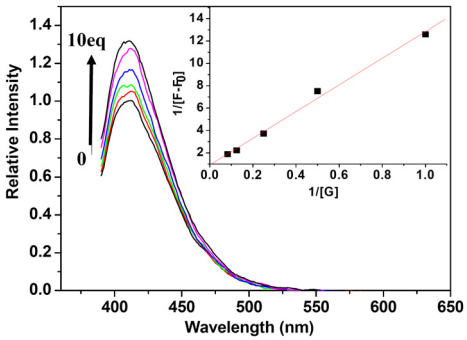


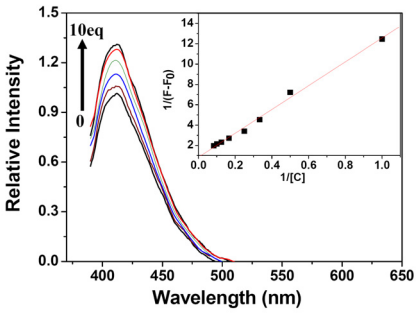
Figure S1. ^{1}H-NMR spectra of **QA** (top) and complex **DL1** (bottom) in d^{6}-DMSO, showing the broadened and overall chemical shifted resonance signals.



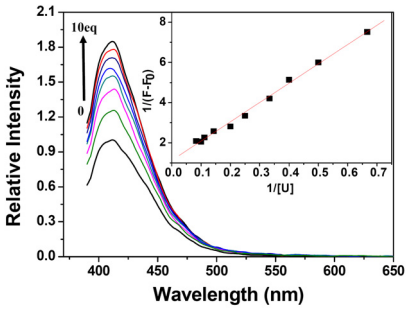
A (logK=3.54±0.01)



G (logK= 3.62 ± 0.02)



C (logk=3.63±0.02)



U (logk = 3.72 ± 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 xC_0 to the concentration of complexes species cage-nG, when the concentration of the added guest anion is a nC_0 with the original concentration of the cage being fixed at C_0:

	cage	+	G	⟶	cage - G
cage only	C_0				
nC_0 G is added	$(1-x)C_0$		$(n-x)C_0$		xC_0

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

When the value of x << n:

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

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 (nC_0) of G, the fluorescent intensity becomes:

$$\mathbf{F = F_1\, x + F_0\,(1-x)} \qquad 3$$

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:

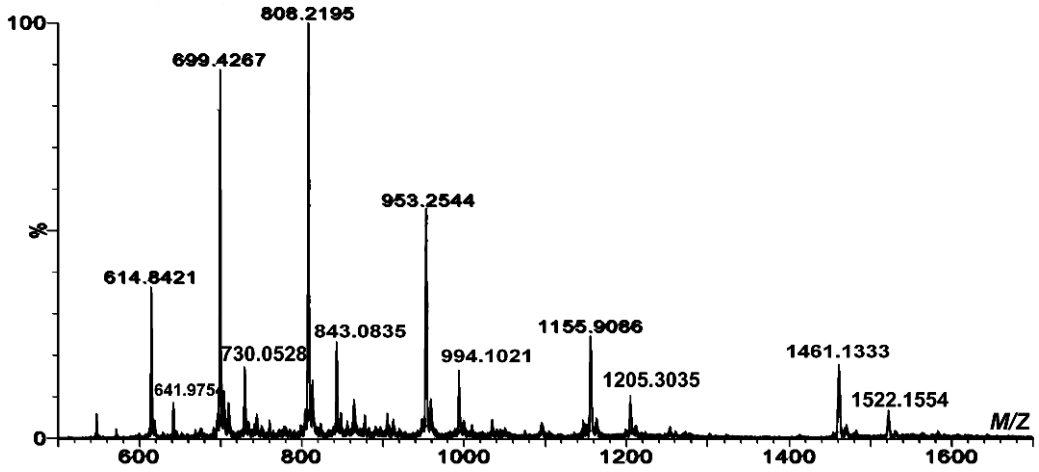
$$\frac{F-F_0}{F_1-F_0} = x \qquad 4$$

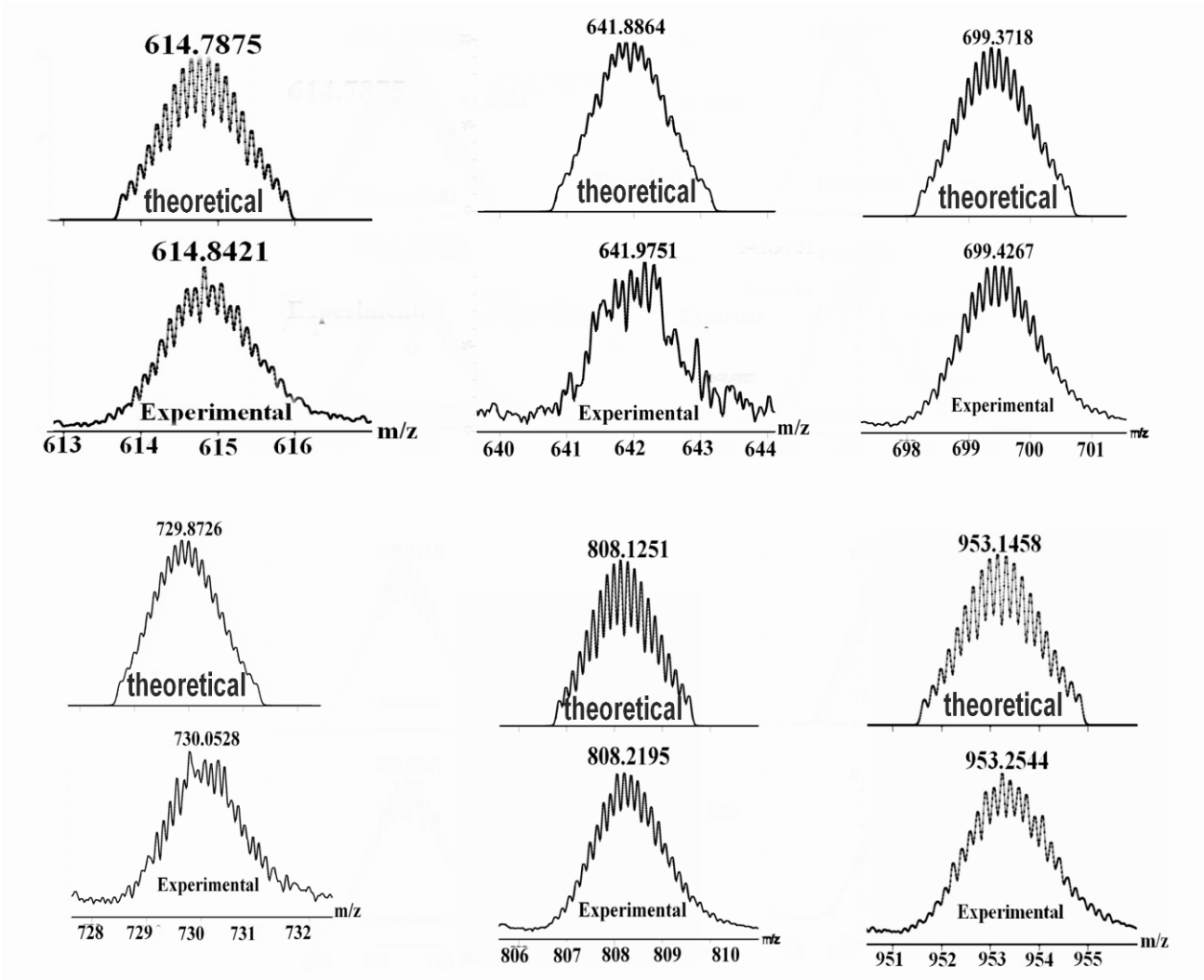
From eqs (2) and (4), we can obtain the equation:

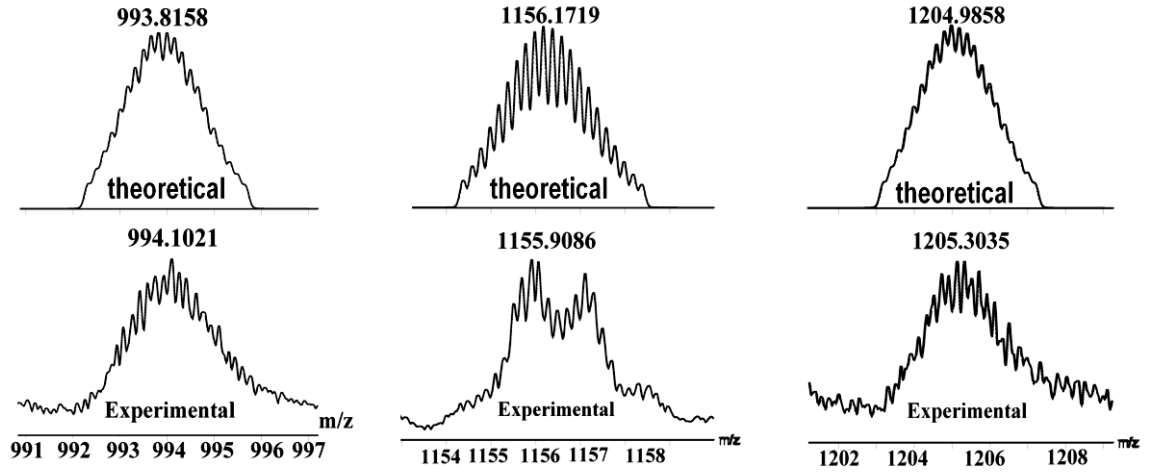
$$\frac{\mathbf{1}}{\mathbf{KC_0(F_1-F_0)}} \cdot \frac{1}{n} = \frac{\mathbf{1}}{\mathbf{F-F_0}} \qquad 5$$

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.



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theoretical
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m/z
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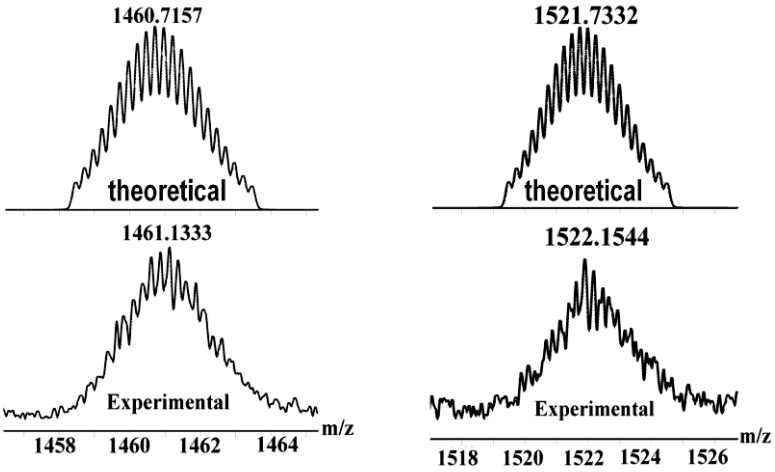
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Experimental
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