Supporting Information

Inclusion of 4-pyrrolidinopyridine derivatives in a symmetrical α,α',δ,δ'-tetramethyl-cucurbit[6]uril and a Ba^{2+}-driven pseudorotaxane with characteristic UV absorption changes

Bo Yang, Xin Xiao,* Yun-Qian Zhang, Qian-Jiang Zhu, Sai-Feng Xue, Zhu Tao,* and Gang Wei*
Fig. S1 Interaction of g2 and TMeQ[6]: $^1$H NMR spectra (400 MHz, D$_2$O) of (A) g2 (ca. 2 mM) in the absence TMeQ[6], (B) in the presence of 1.19 equiv of TMeQ[6], and (C) neat TMeQ[6].
Fig. S2 Interaction of g2 and TMeQ[6]: (A) absorption spectra of g2 (20 μM) in aqueous solution at different TMeQ[6] concentrations, (B) concentrations and the corresponding $A$ vs $N_{\text{TMeQ}[6]}/N_{g2}$ curve and (C) concentrations and the corresponding $\Delta A$ vs $N_{g2}/(N_{\text{TMeQ}[6]}+N_{g2})$ curve (inset).
Fig. S3 Isothermal titration calorimetry profiles of TMeQ[6] with g2 in aqueous solution at 298.15 K. A) Nano ITC data for 30 sequential injections (each of 6 mL) of g2 solution (1.0 mM) into TMeQ[6] solution (0.1 mM). B) Apparent reaction heat obtained from integration of the calorimetric traces.
Fig. S4 UV pH titrations of $g^0$ (□) (282nm) and TMeQ[6]$\cdot g^0$ complexes (●) (282nm)
Fig. S5 The MALDI-TOF mass spectrum for TMeQ[6]·g0.
Fig. S6 The MALDI-TOF mass spectrum for TMeQ[6]·g1.
Fig. S7 The MALDI-TOF mass spectrum for TMeQ[6]·g2.
Table S1 Microcalorimetric titration data for TMeQ[6] with g2 in aqueous solution at 298.15 K.

<table>
<thead>
<tr>
<th>Complex</th>
<th>$n$</th>
<th>$K_a \text{ (M}^{-1}\text{)}$</th>
<th>$\Delta H \text{ (kJ mol}^{-1}\text{)}$</th>
<th>$T \Delta S \text{ (kJ mol}^{-1}\text{)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>g2-TMeQ[6]</td>
<td>0.94±0.02</td>
<td>(1.08±0.32) ×10^6</td>
<td>−36.60±0.87</td>
<td>−2.16</td>
</tr>
</tbody>
</table>