

**Electronic Supplementary Information (ESI)**

**Mixed behavior of *p*-phenylenediaminium guest binding with  
inverted cucurbit[6]uril host**

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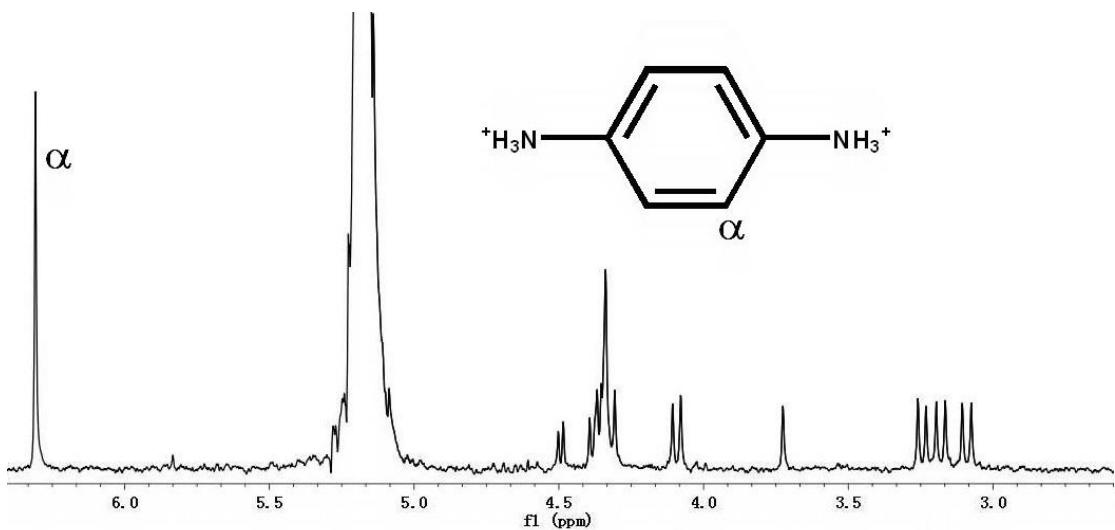
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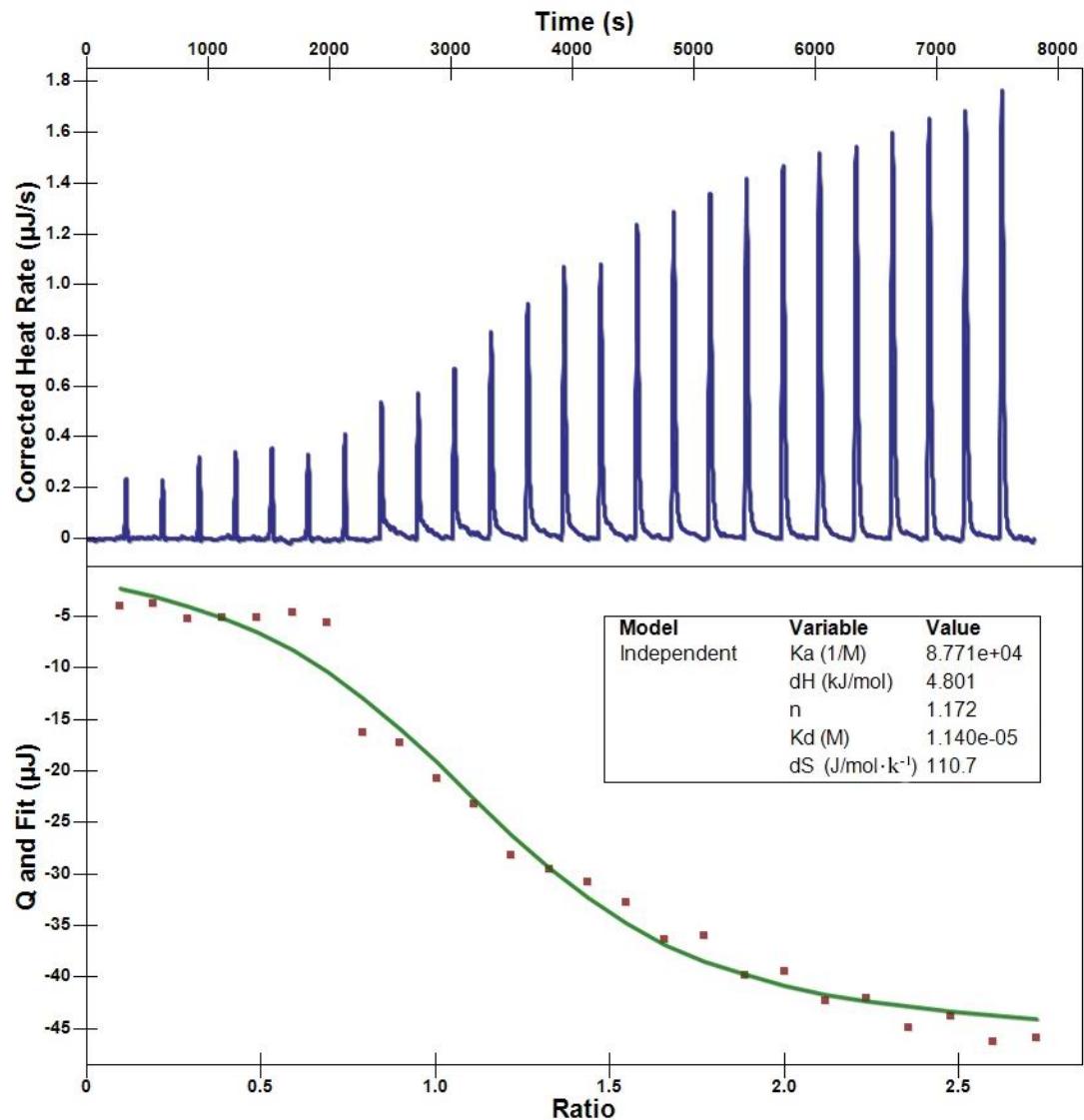
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**Figure S1.**  $^1\text{H}$  NMR spectra (400 MHz) of *p*-phenylenediaminium in the presence of 0.44 equiv of *i*Q[6] in 4.0 M DCl at 278.15 K.



**Figure S2** ITC profile of *i*Q[6] with *p*-phenylenediaminium at 298.15 K.