

## Electronic Supplementary Information

# Inclusion Complex of Cucurbit[7]uril with Benzimidazolyl Benzyl Viologen Showing Fluorescence and Photochromic Properties

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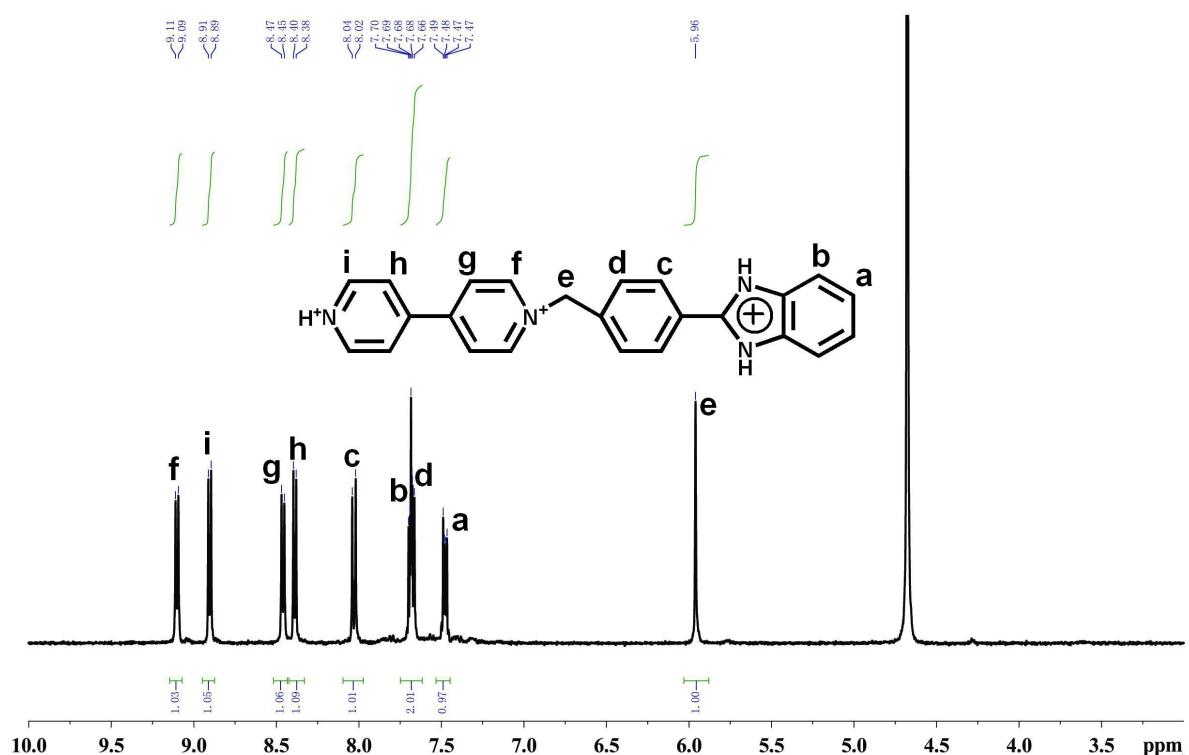
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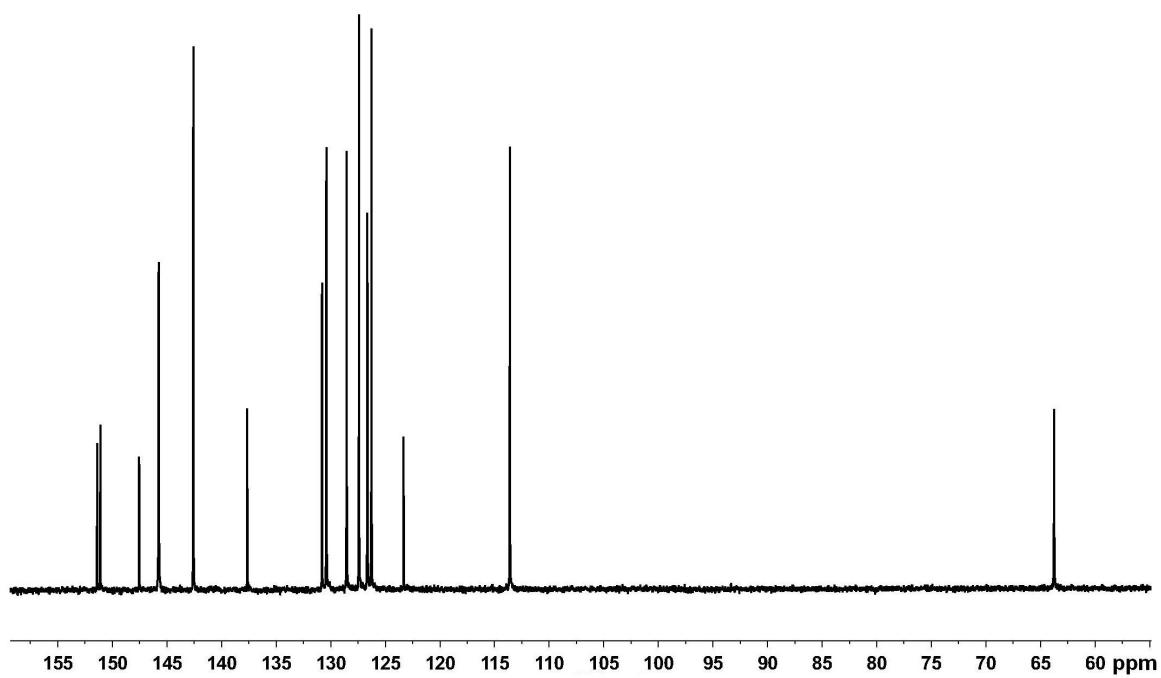
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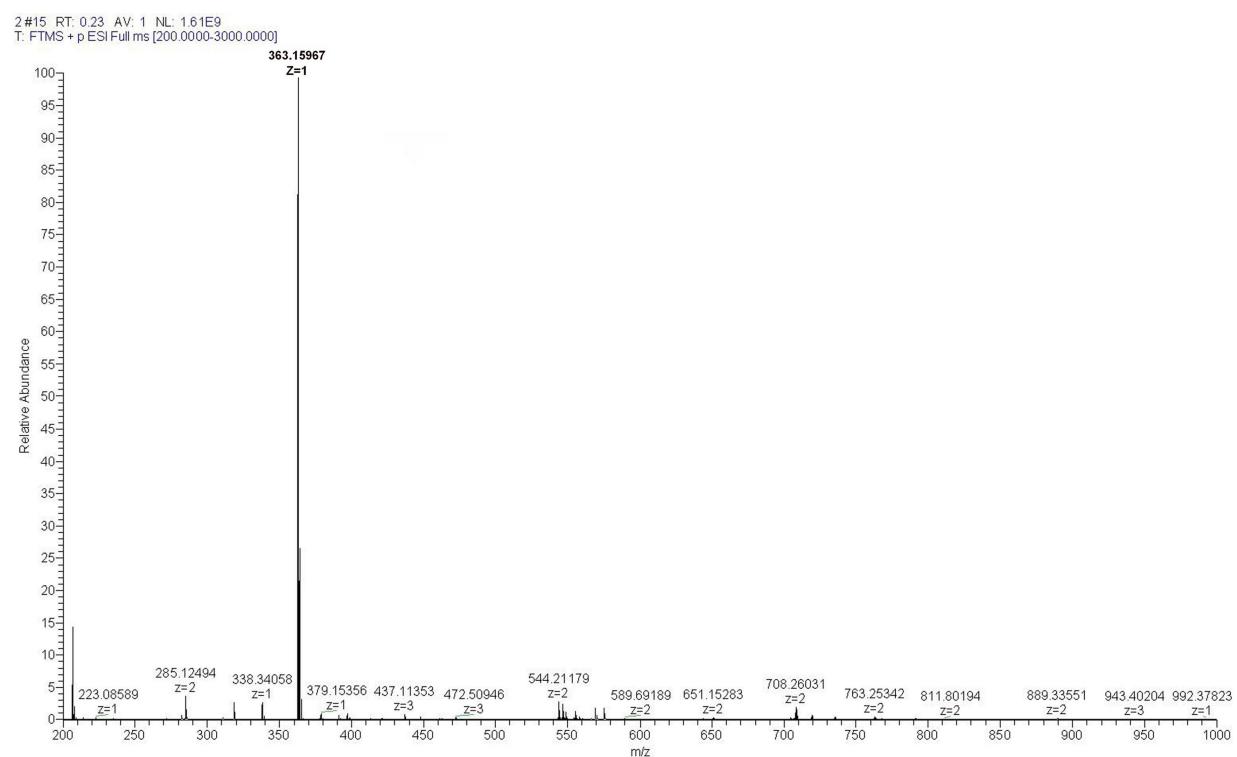
**Fig. S1.**  $^1\text{H}$  NMR of guest molecule **1**·Cl<sub>3</sub> in D<sub>2</sub>O.



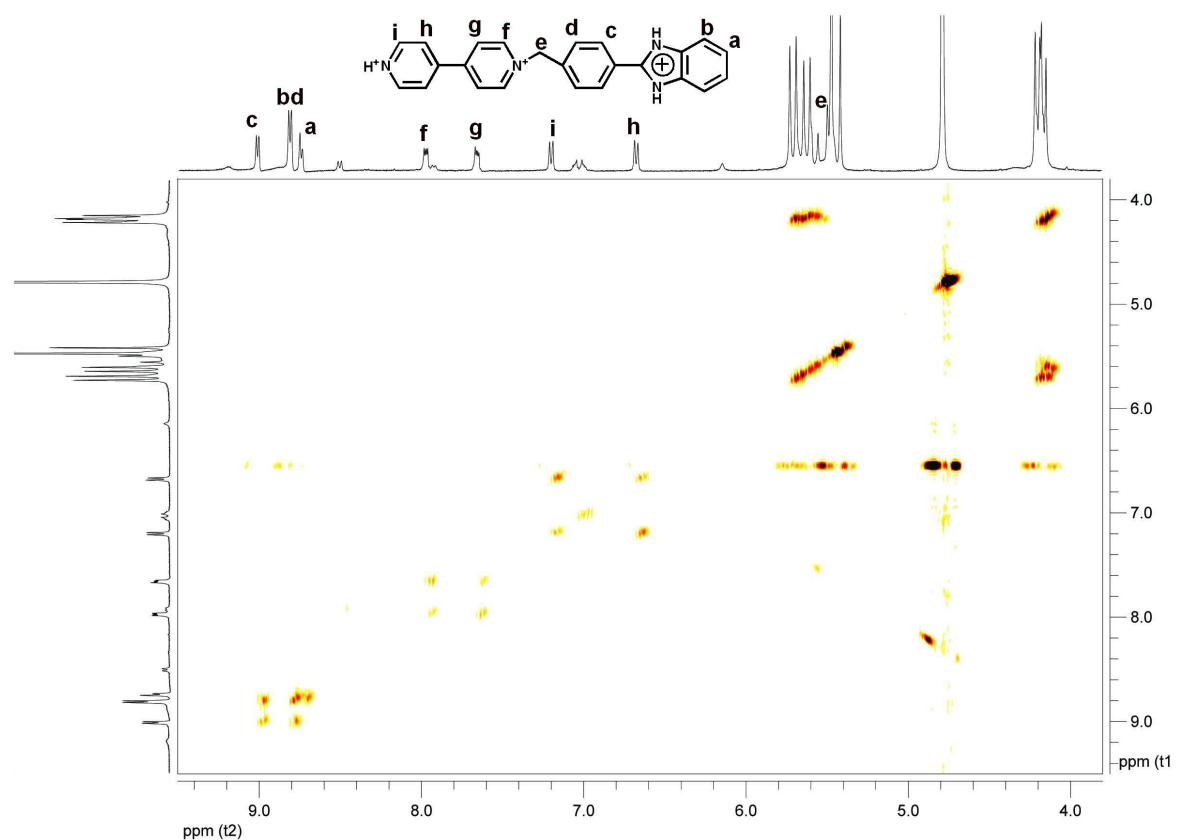
**Fig. S2.**  $^{13}\text{C}$  NMR of guest molecule **1**· $\text{Cl}_3$  in  $\text{D}_2\text{O}$ .



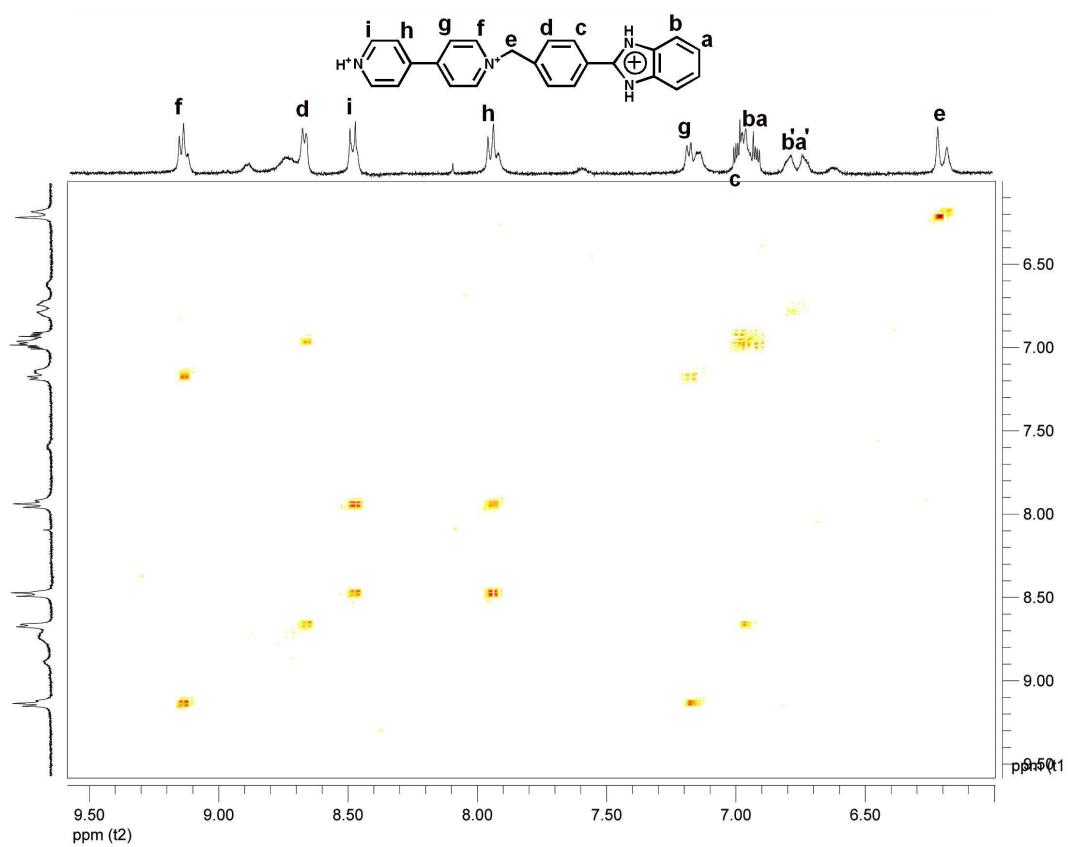
**Fig. S3.** HRMS of guest molecule (**1-2H**)<sup>+</sup>.



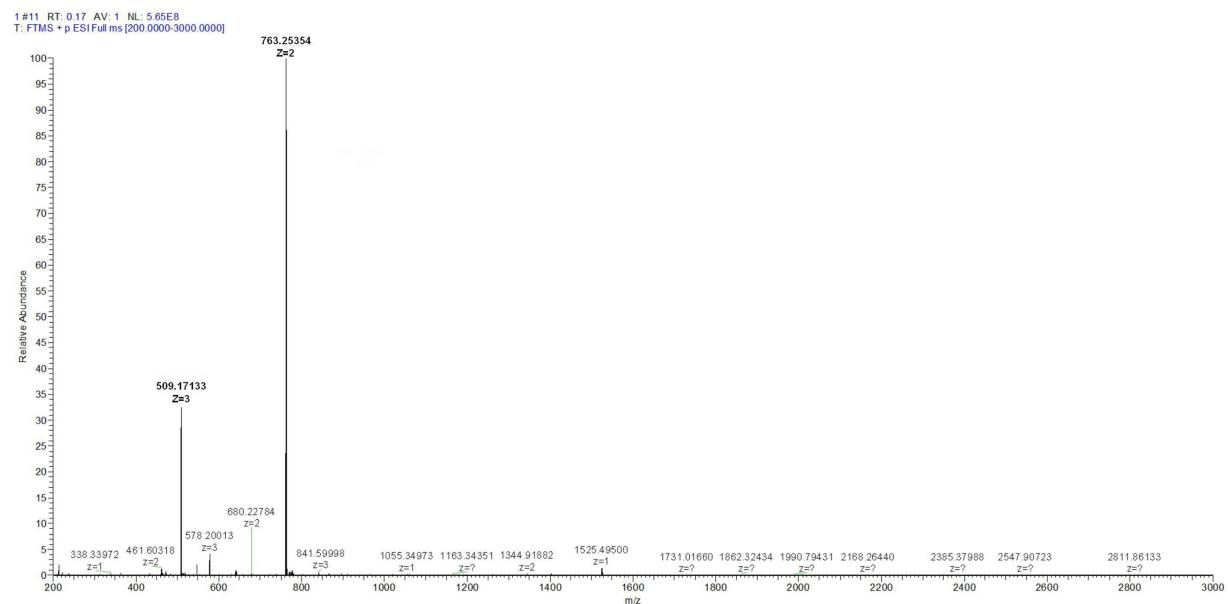
**Fig. S4.** 2D gCOSY spectrum of the inclusion complex  $\mathbf{1}^{3+}@\text{Q}[7]$  in  $\text{D}_2\text{O}$ .



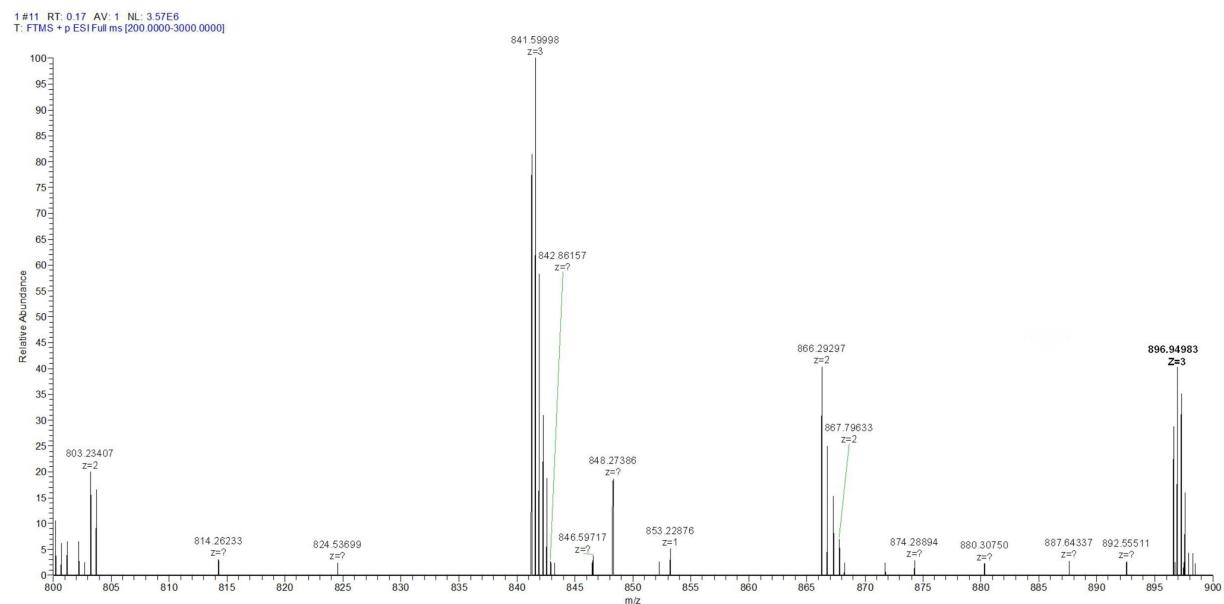
**Fig. S5.** 2D gCOSY spectrum of the inclusion complex **1**<sup>3+</sup>@Q[7]<sub>2</sub> in D<sub>2</sub>O.



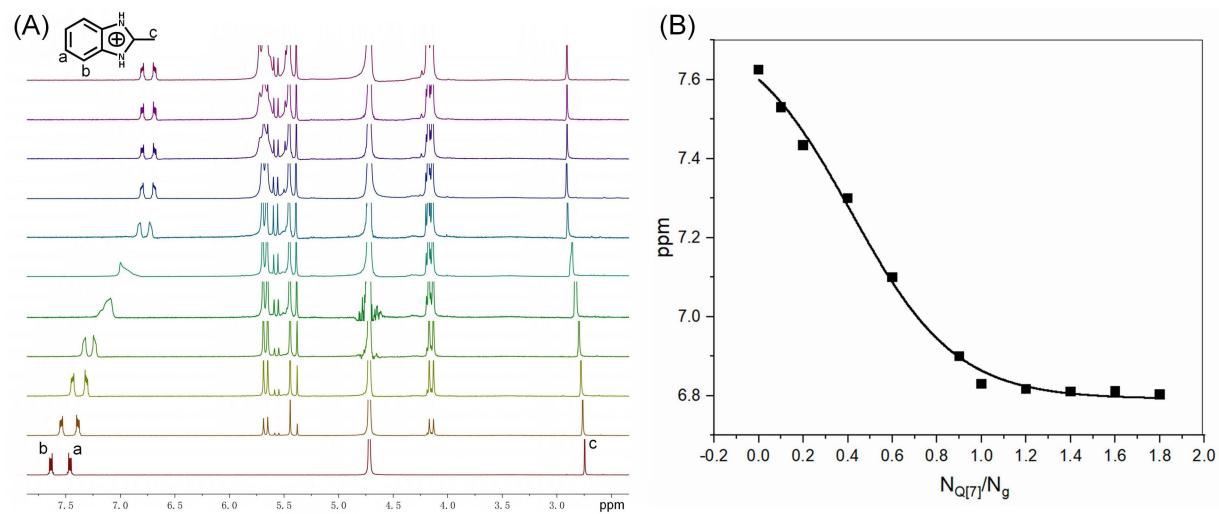
**Fig. S6.** The ESI-MS for the inclusion complex  $\mathbf{1}^{3+}@\text{Q}[7]$ .



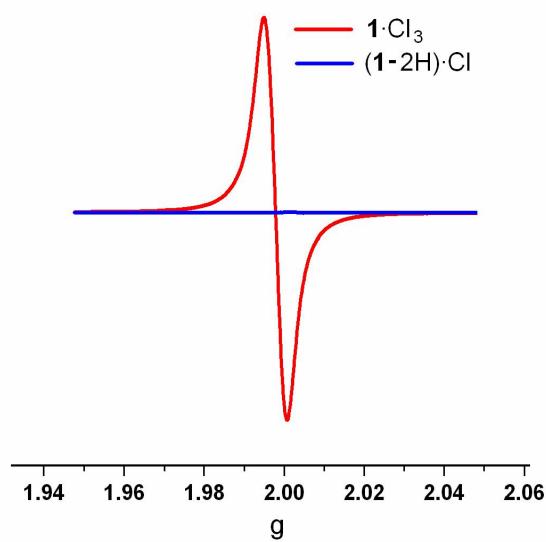
**Fig. S7.** The ESI-MS for the inclusion complex  $\mathbf{1}^{3+}@\text{Q[7]}_2$ .



**Fig. S8.** (A)  $^1\text{H}$  NMR spectra (400 MHz,  $\text{D}_2\text{O}$ ) of 2-methylbenzimidazolium chloride in different equiv. of Q[7] at 20 °C. (B)  $^1\text{H}$  NMR titration curve of 2-methylbenzimidazolium chloride by addition of Q[7] in  $\text{D}_2\text{O}$ .



**Fig. S9.** ESR spectra of the compounds **1**·Cl<sub>3</sub> and (**1**-2H)·Cl.



**Fig. S10.** ESR spectra of the compounds 2-methylbenzimidazolium chloride and methyl viologen.

