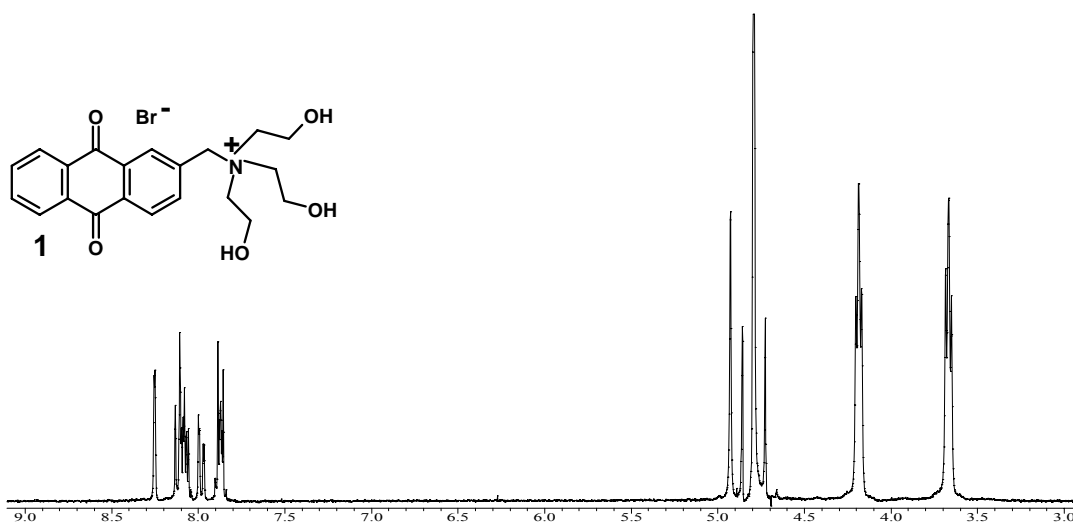


## Inclusion of anthraquinone derivatives by the cucurbit[7]uril host

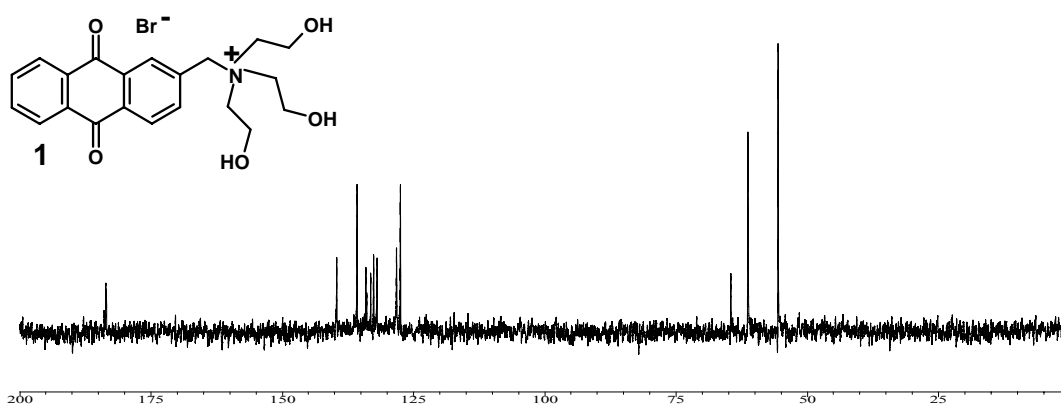
Vladimir Sindelar, Samantha E. Parker and Angel E. Kaifer\*

*Center for Supramolecular Science and Department of Chemistry, University of Miami,  
Coral Gables, FL 33124-0431*

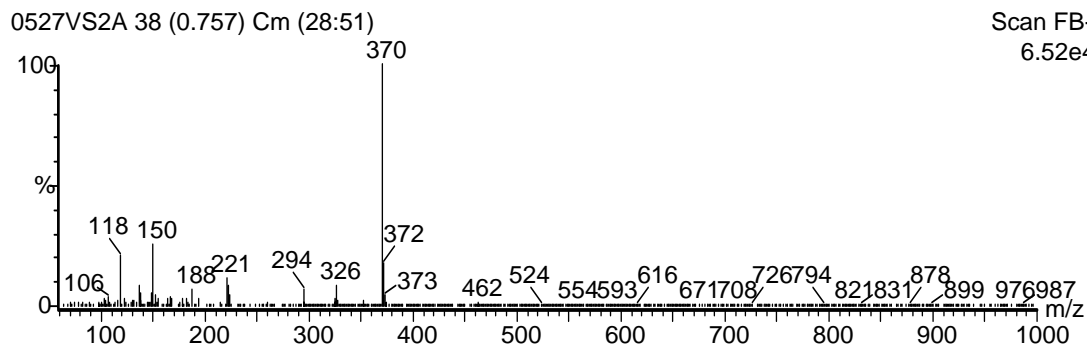
### Electronic Supplementary Information



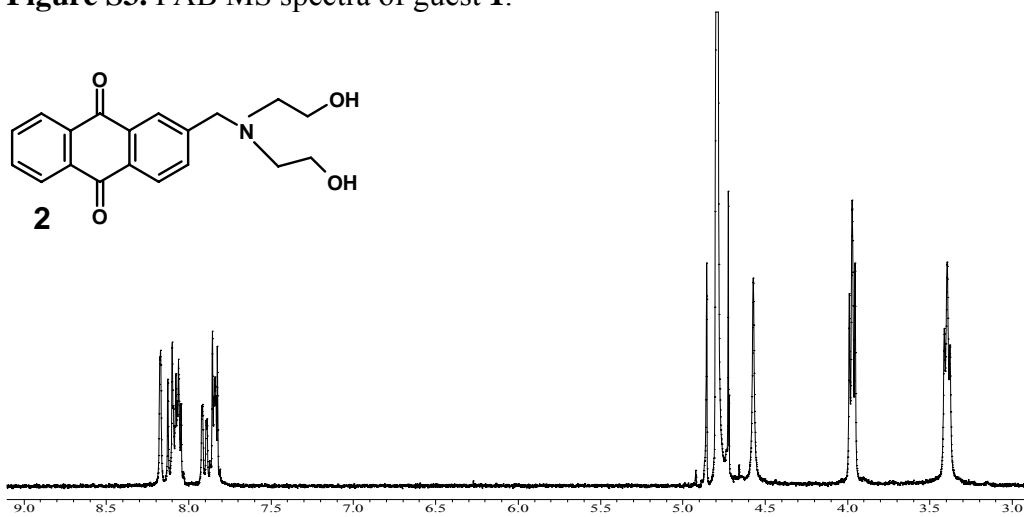
**Figure S1.**  $^1\text{H}$  NMR spectra (DCl/D<sub>2</sub>O, pH = 2.0) of guest **1**.



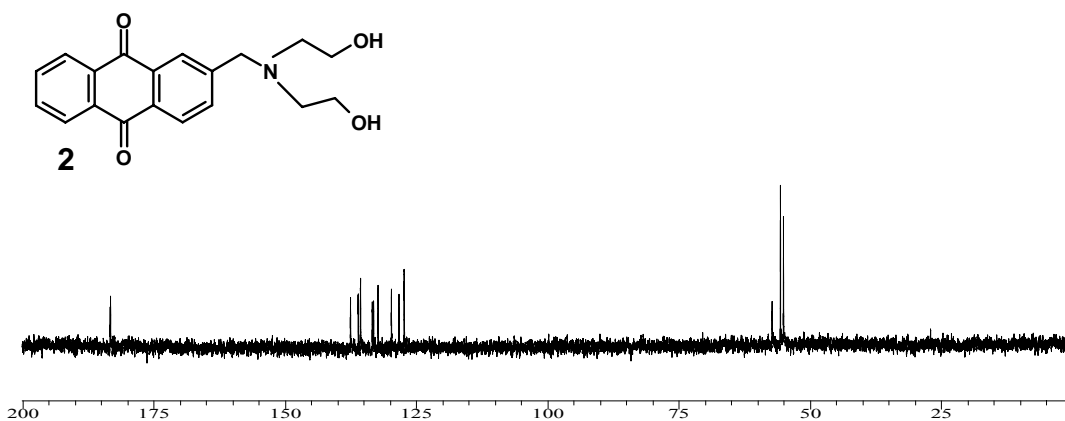
**Figure S2.**  $^{13}\text{C}$  NMR spectra (DCl/D<sub>2</sub>O, pH = 2.0) of guest **1**.



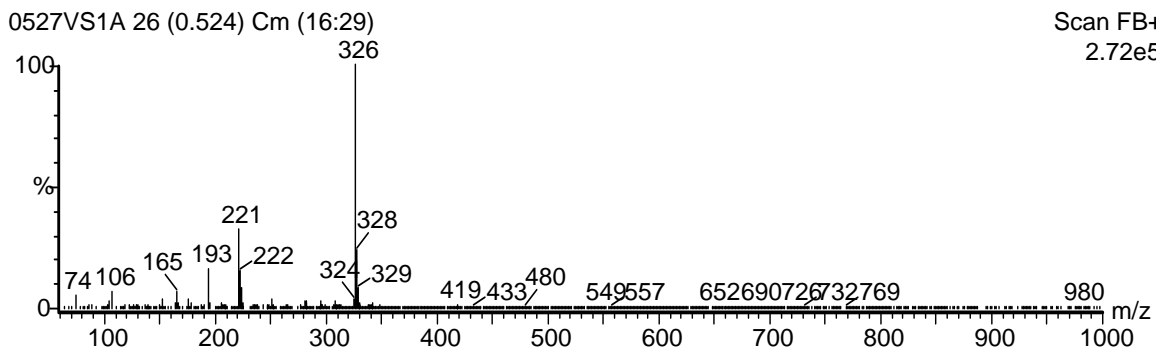
**Figure S3.** FAB MS spectra of guest 1.



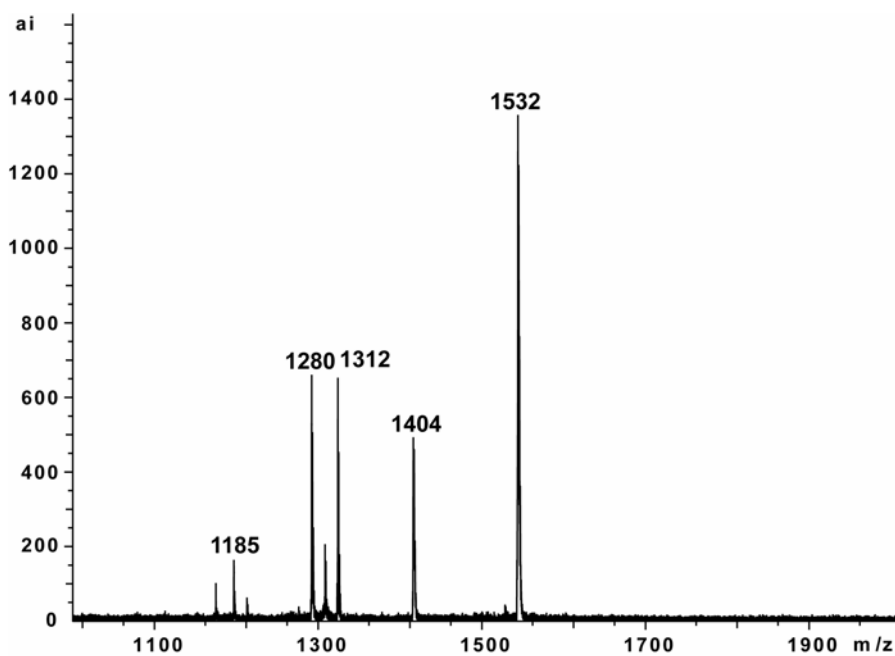
**Figure S4.**  $^1\text{H}$  NMR spectra (DCI/ $\text{D}_2\text{O}$ , pH = 2.0) of guest 2.



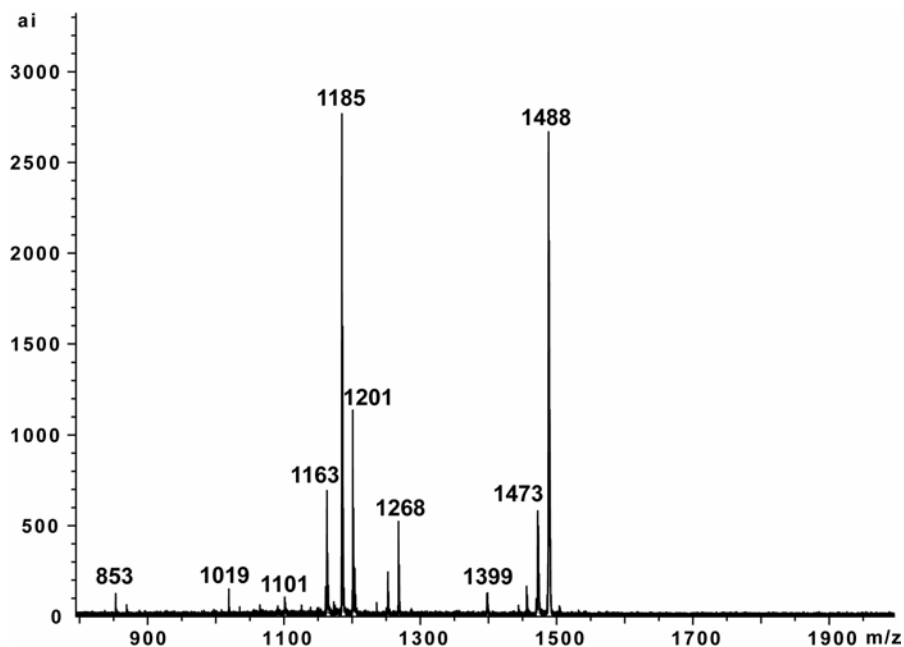
**Figure S5.**  $^{13}\text{C}$  NMR spectra (DCI/ $\text{D}_2\text{O}$ , pH = 2.0) of guest 2.



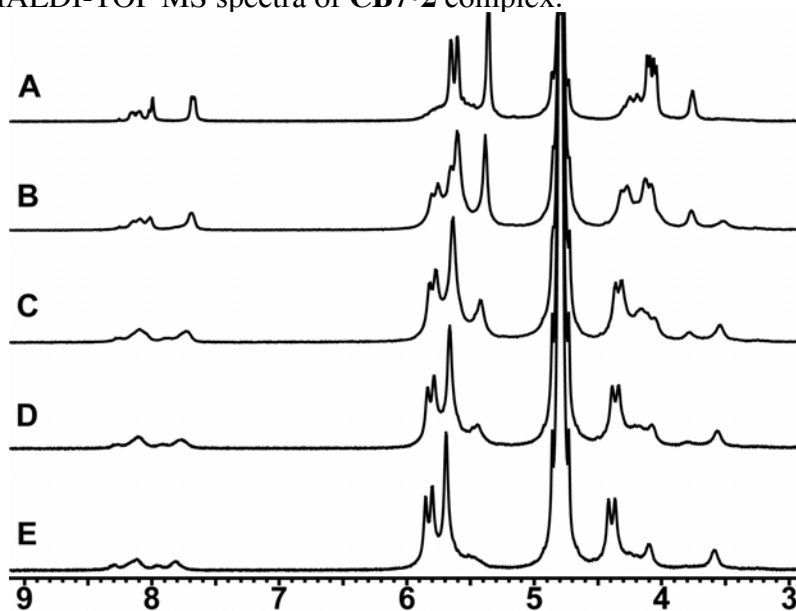
**Figure S6.** FAB MS spectra of guest **2**.



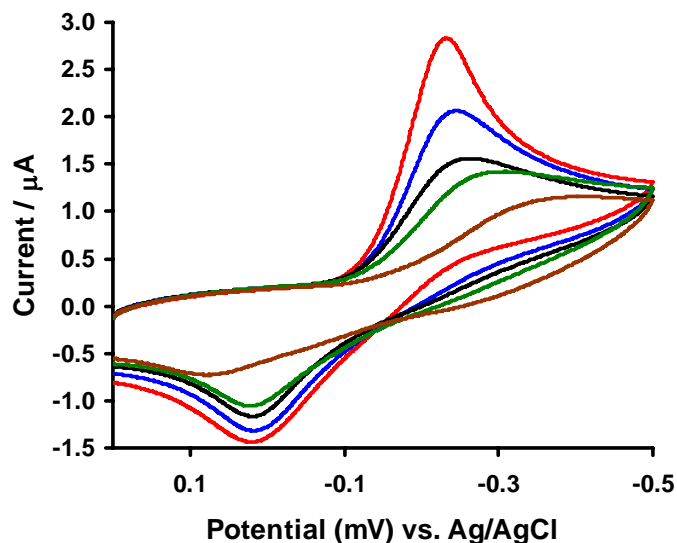
**Figure S7.** MALDI-TOF MS spectra of **CB7•1** complex.



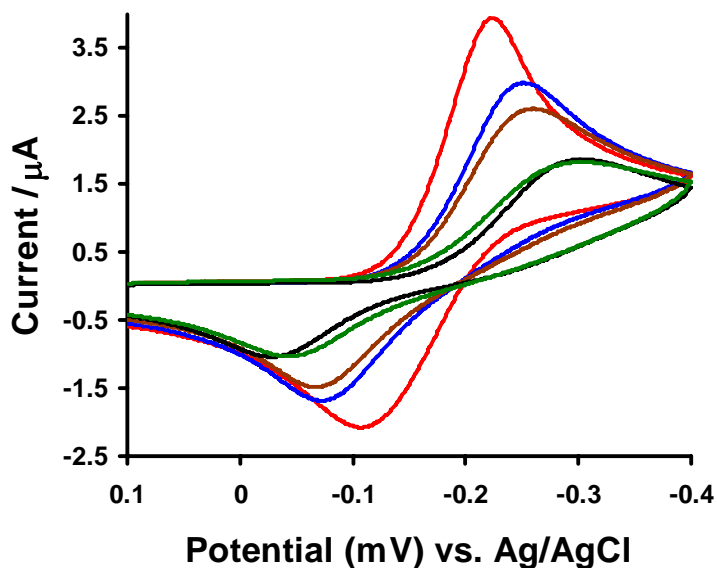
**Figure S8.** MALDI-TOF MS spectra of **CB7•2** complex.



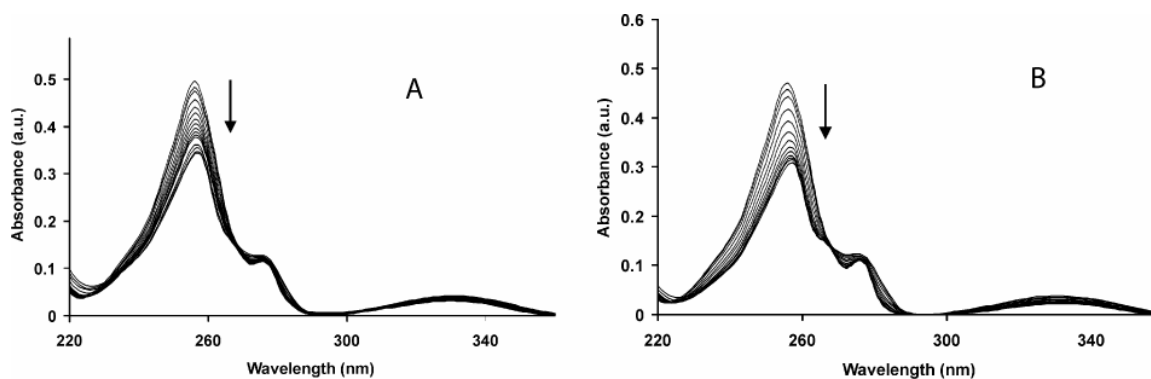
**Figure S9.** <sup>1</sup>H NMR spectra (DCl/D<sub>2</sub>O, pH = 2.0) of guest **2** in the presence of 1.5 equiv of CB7 and 0 equiv (**A**), 62.7 equiv (0.3 M) (**B**), 104.5 equiv (0.5 M) (**C**) 146.4 equiv (0.7 M) (**D**) and 230.0 equiv (1.1 M) (**E**) of NaCl.



**Figure S10.** Cyclic voltammetric response on glassy carbon ( $0.071 \text{ cm}^2$ ) of guest **1** in 0.1 M HCl solution in the absence (red) and in the presence of 0.5 equiv (blue), 1.0 equiv (black), 1.5 equiv (green) and 2.0 equiv (brown) **CB7**. Scan rate: 0.1 V/sec.



**Figure S11.** Cyclic voltammetric response on glassy carbon ( $0.071 \text{ cm}^2$ ) of guest **2** in 0.1 M pH 2 phosphate buffer (also containing 0.1 M NaCl) solution in the absence (red) and in the presence of 0.5 equiv (blue), 1.0 equiv (brown), 1.5 equiv (green) and 2.0 equiv (black) **CB7**. Scan rate: 0.1 V/sec.



**Figure S12.** Electronic absorption spectra (25 °C, 0.01 M HCl) of (A) 10  $\mu$ M guest **1** and (B) 10  $\mu$ M guest **2** in the presence of increasing concentrations (0-80  $\mu$ M) of CB7.