Binding interactions between the host cucurbit[7]uril and dendrimer guests containing a single ferrocenyl residue

David Sobransingh and Angel E. Kaifer*

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

ELECTRONIC SUPPLEMENTARY INFORMATION

Determination of equilibrium association constants. The association constants were determined by NMR using competitive binding between the ferrocene containing guest and 2,7-dimethyldiazapyrenium as a reference guest. The association constant between CB7 and 2,7-dimethyldiazapyrenium, was determined by UV spectroscopy at pH 2 and pH 7. Stock solutions containing dimethyl-diazapyrenium (1 equiv) and CB7 (0.7 equivalents) were prepared in pD 7 and pD 2 buffers (0.1 M Na₃PO₄) also containing 0.1 M NaCl. The ferrocene containing guest was added (1-2 equiv) and from NMR spectral integration, the concentrations of bound and free 2,7-dimethyldiazapyrenium were determined. The amount of 2,7-dimethyldiazapyrenium displaced from its CB7 complex was used to calculate the value for the association constant of the ferrocene-containing guest.



Fig. ESI-1. Cyclic voltammograms of 1.0 mM **FG1** (solid line) and **FG1** in the presence of 1.5 equiv of **CB7**(dotted line) at a scan rate of 100 mV s⁻¹ in pH 7 (0.1 M phosphate) buffer, 0.1 M NaCl.



Fig. ESI-2. Cyclic voltammograms of 1.0 mM **FG1** (solid line) and **FG1** in the presence of 1.0 equivalents of **CB7** (dotted line) at a scan rate of 100 mV s⁻¹ in pH 2 (0.1 M phosphate) buffer, 0.1 M NaCl.



Fig. ESI-3. MALDI-TOF spectra of **FG1** in the presence of 1.5 equivalents of **CB7** in pH 2 (0.1 M phosphate) buffer, 0.1 M NaCl (HCCA matrix). The peak corresponding to the complex appears at a m/z value of 1,621.



Fig. ESI-4. MALDI-TOF spectra of **FG3** in the presence of 1.5 equivalents of **CB7** in pH 2 (0.1 M phosphate) buffer, 0.1 M NaCl (HCCA matrix). The peak corresponding to the complex appears at a m/z value of 4,372.