Host-[2]Rotaxane: the Advantage of Converging Functional Groups for Guest Recognition

Inese Smukste, Brian E. House, and David B. Smithrud*

<u>Content</u>	<u>Page</u>
Table S1. NMR properties of the calix[4]arenes in CDCl ₃ at 25 °C, which show that they are held in a cone conformation	S2
Fig. S1 A typical binding plot, which shows the change in fluorescence of pyrene caused by the addition of Rotaxane 1.	S2
Table S2. Concentration ranges used in the fluorescence assays.	S3

Table S1. NMR properties of the calix[4]arenes in CDCl₃ at 25 °C, which show that they are held in a cone conformation

Calix[4]arene	Ar-CH _a H _b -Ar (ppm)	Ar-CH _a H _b -Ar (ppm)	$\Delta\sigma$ (ppm)	Ar-CH ₂ -Ar (ppm)
5	4.34-4.21(m)	3.46 (d)	0.9	30.09
6	4.43 (d)	3.59 (d)	0.84	30.55
7	4.55 (d)	3.52 (d)	1.03	31.64
8	4.57-4.45 (m)	3.51-3.41 (m)	~1.04	31.65 and 31.45
3	4.50 (d)	3.45 (d)	1.05	31.65
11	4.53-4.44 (m)	3.53-3.38	~1.03	31.43 and 31.27

Figure S1 A typical binding plot, which shows the change in fluorescence of pyrene caused by the addition of Rotaxane **1**.

Table S2. Concentration ranges used in the fluorescence assays.

General range of the concentrations of the assay solutions used to derive K_A 's are: [2]rotaxane **1** (5×10^{-6} M to 5×10^{-5} M) and *N*-Ac-Trp (1×10^{-5} M), [2]rotaxane **1** (4×10^{-6} M to 4×10^{-5} M) and indole (1×10^{-5} M) in DMSO and DMSO/buffer (80/20 (v/v)), [2]rotaxane **1** (4×10^{-6} M to 4×10^{-5} M) and indole (1×10^{-5} M) in DMSO and DMSO/buffer solutions (80/20 (v/v)), [2]rotaxane **1** (8×10^{-6} M to 1×10^{-4} M) and indole (5×10^{-5} M) in DMSO/buffer solutions (50/50 and 25/75 (v/v)), [2]rotaxane **1** (3×10^{-6} M to 3×10^{-5} M) and (L)- or (D)-Trp (5×10^{-6} M), [2]rotaxane **1** (1×10^{-8} M to 1.4×10^{-6} M) and fluorescein (5×10^{-8} M), [2]rotaxane **1** (4×10^{-8} M to 5×10^{-6} M) and pyrene (1×10^{-7} M), [2]rotaxane **1** (3×10^{-7} M to 7×10^{-6} M) and 1,5-DNS (1.6×10^{-6} M), calix[4]arenes **2** or **3** (4×10^{-6} M to 1×10^{-4} M) and *N*-Ac-Trp or indole (5×10^{-5} M), calix[4]arenes **2** or **3** (2×10^{-6} M to 1×10^{-4} M) and fluorescein (1×10^{-6} M), calix[4]arenes **2** (2×10^{-6} M to 9×10^{-5} M) and pyrene (5×10^{-6} M), calix[4]arenes **3** (8×10^{-7} M to 1×10^{-5} M) and pyrene (1×10^{-6} M), calix[4]arenes **2** or **3** (2×10^{-6} M to 1×10^{-4} M) and 1,5-DNS (5×10^{-6} M).