

Supporting Information for:

**Nitroxide biradicals as thread unit in paramagnetic Cucurbituril-based
rotaxanes**

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2D-ROESY of [3]Rotaxane 3b	S2
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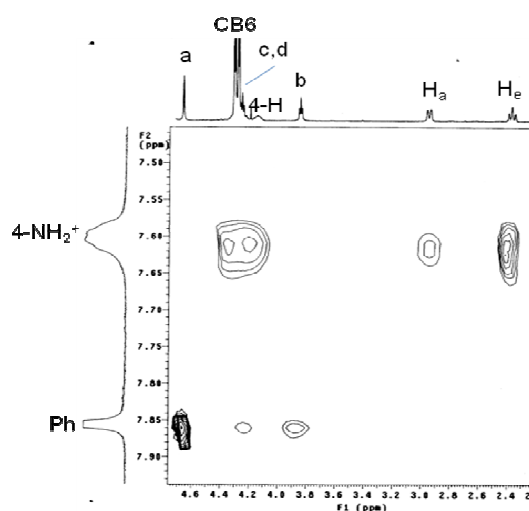


FIGURE S1. Partial 2D ROESY (600 MHz, D₂O, 298 K) spectrum of **3b** (1mM). The signals were assigned by using the labels reported in the molecular structure. In the spectrum ammonium protons (4-NH₂⁺) show connections with 4-H, H_a and H_e protons of the piperidine heterocycle and with **d** signals.

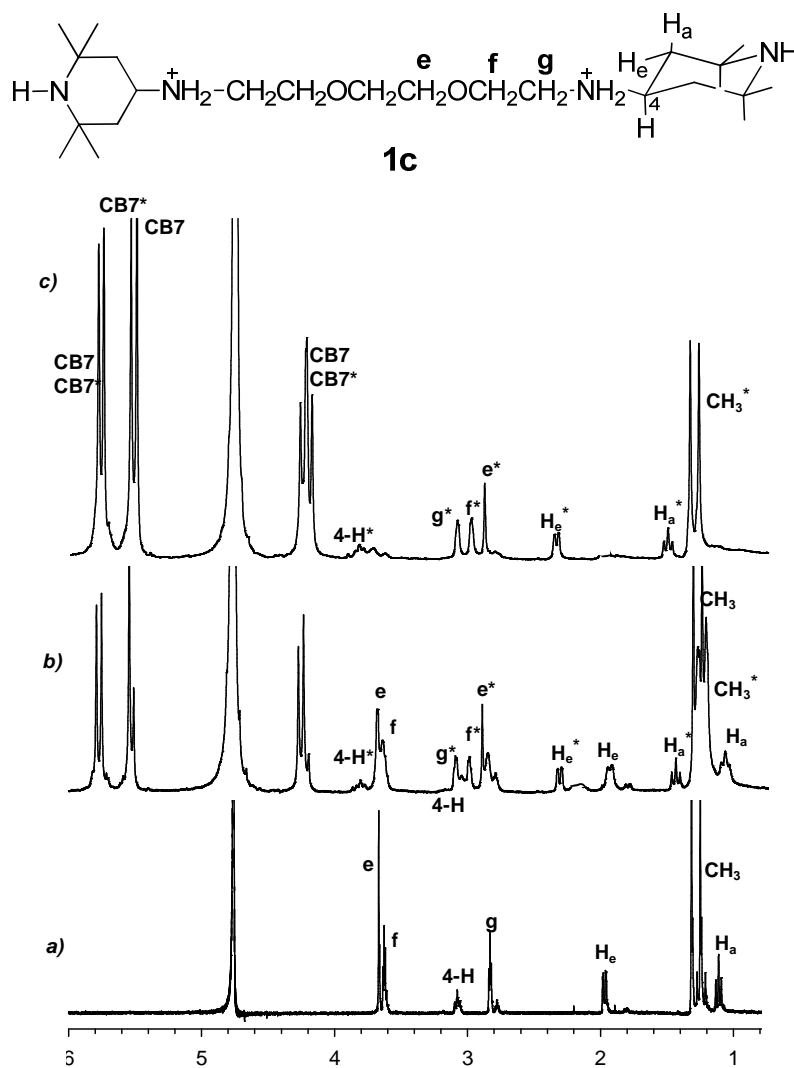


FIGURE S2. Spectra of **1c** (3.4 mM, 400 MHz, D₂O, 298 K) a) in absence of CB7, b) in the presence of CB7 1.9 mM, c) in the presence of CB7 9.8 mM. The signals were assigned by using the labels reported in the molecular structure. The starred labels indicate the chemical shifts of the complex **1c@CB7**.

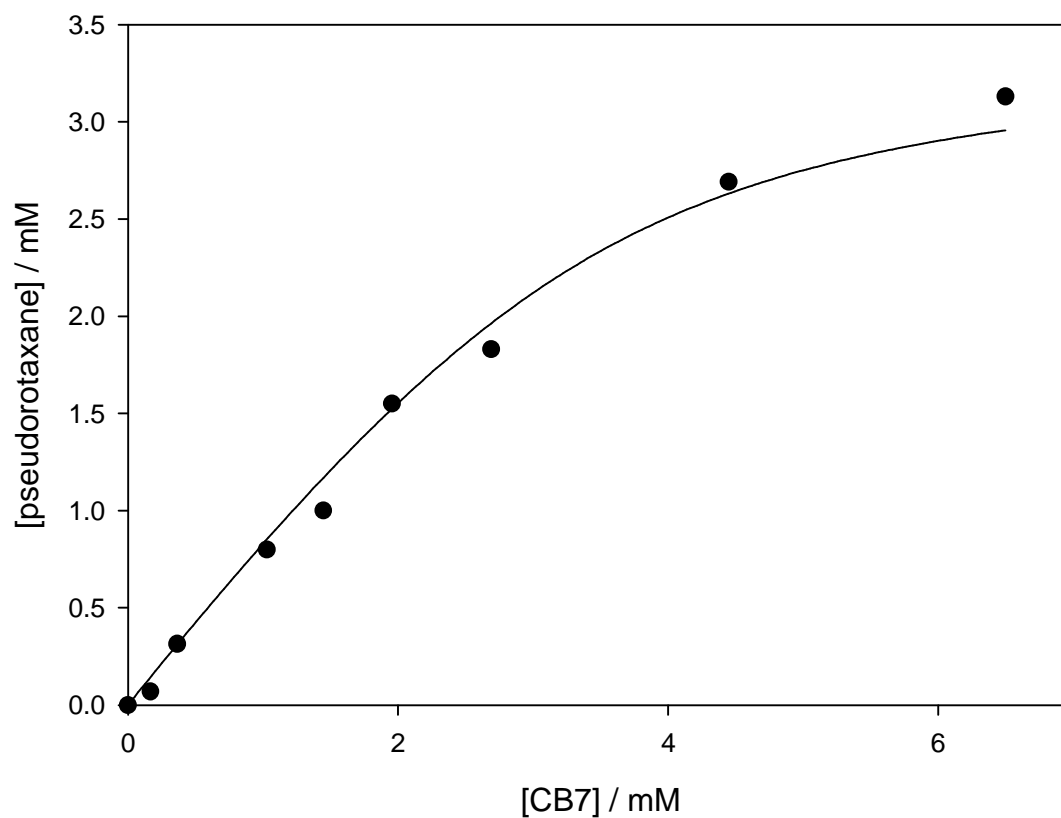


FIGURE S3. **1c@CB7** pseudorotaxane concentration as function of **CB7** concentration at room T in water as determined by H-NMR (starting **1c** concentration is 3.4 mM).

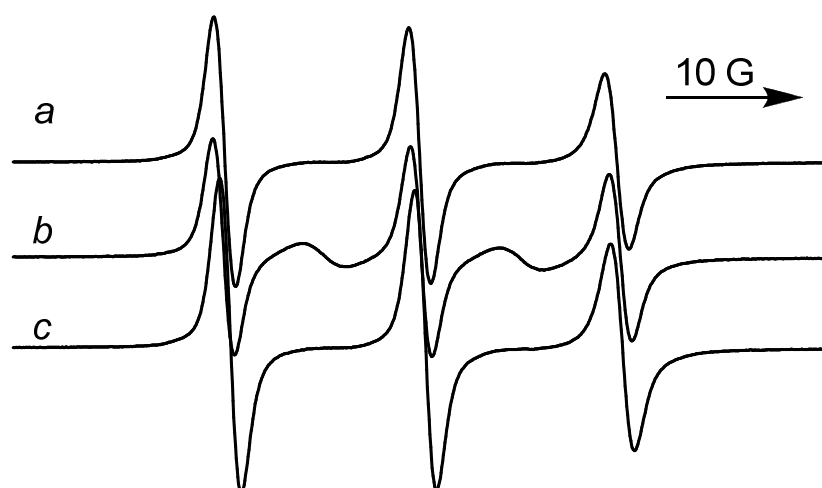


FIGURE S4. (a) EPR Spectrum of **1a** in the presence of CB7 in water. (b) EPR spectrum of sample *a* after addition of NaOH 0.01 M. (c) EPR spectrum of sample *b* after addition of HCl 0.01 M