

Supporting Material for

Inclusion complex formation of sanguinarine alkaloid with cucurbit[7]uril:

Inhibition of nucleophilic attack and photooxidation

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¹H-NMR spectra

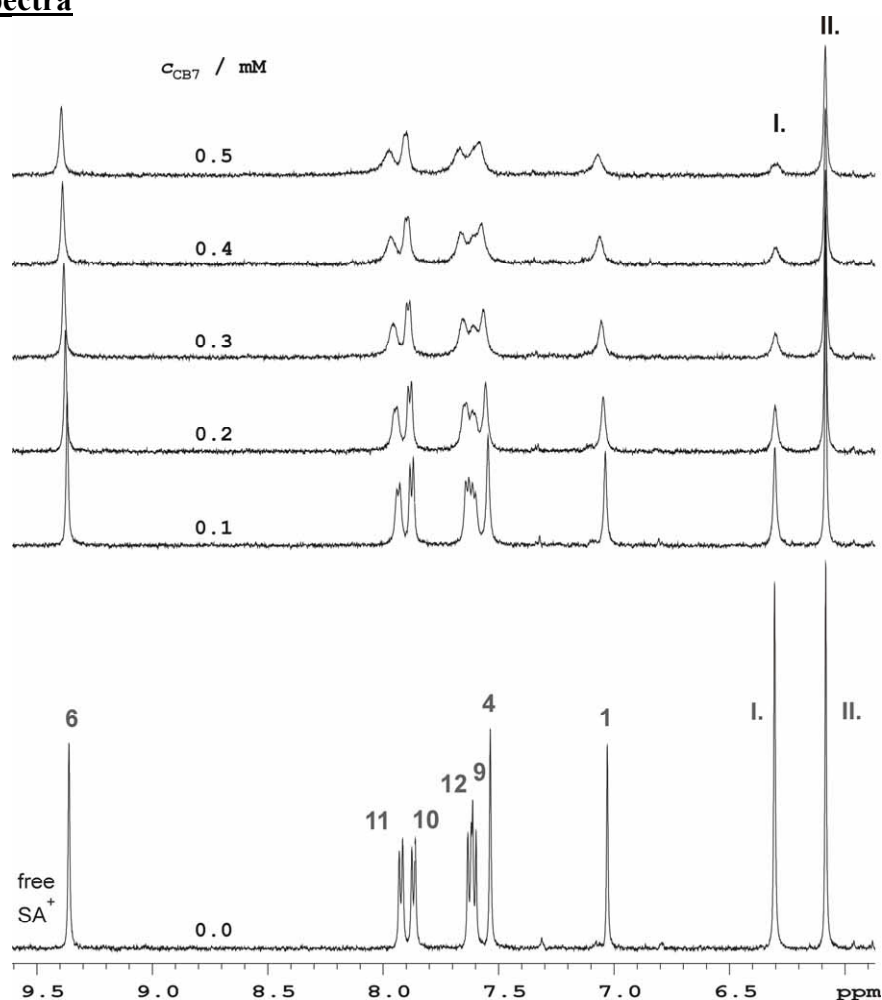


Figure S1: ¹H-NMR (600 MHz) titration of 4mM SA⁺ with CB7 in D₂O at 283 K. The broadening and population change effects seen on the resonances are related to the multisite exchange shown in Scheme 2.

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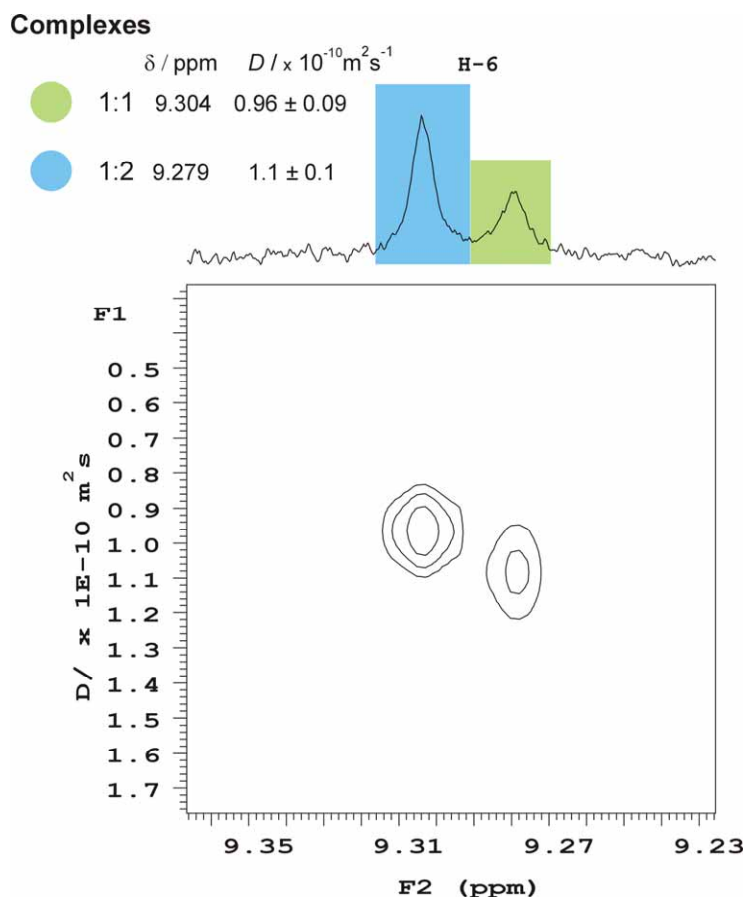


Figure S2: Cross-peaks for the H-6 protons in the ^1H -DOSY-NMR spectrum (600 MHz) of 0.3 mM SA^+ in the presence of 1 mM CB7 in D_2O at 283 K

Supporting information for ^1H -DOSY^[1-3]:

The ^1H -DOSY experiments were carried out in a 5-mm tube at 283 K. A Performa IV XYZ gradient amplifier was used with a 60 Gauss.cm^{-1} maximum Z-gradient capability. The gradient strength was calibrated by using 5% (w/w) sucrose in D_2O at 298 K ($D = 5.22 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$). The bipolar pulse-pair stimulated-echo (Dbppste) pulse sequence was used for acquiring diffusion data with 50 ms diffusion delay, 8 squared increments for gradient levels and 256 transients. The Varian DOSY package was used for measuring and processing.

References for the DOSY technique

- [1] K. F. Morris, C. S. Johnson Jr., *J. Am. Chem. Soc.* 1992, **114**, 3139–3141.
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- [3] D. Wu, A. Chen, C. S. Johnson Jr., *J. Magn. Reson., Ser. A* 1995, **115**, 260–264.