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Optimization of the binding properties of a synthetic anion receptor using rational and combinatorial strategies

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Structure of compounds **2** and **3**:

Concentration-dependent NMR spectra: 2 in CDCl₃ (a) 2 mM, (b) 0.2 mM, (c) 0.02 mM (Bruker DRX 500 / 500 MHz)

Concentration-dependent NMR spectra: 3 in CDCl₃ (a) 2 mM, (b) 0.2 mM, (c) 0.02 mM (Bruker DRX 500 / 500 MHz)

¹H-NMR spectra: **2** (1 mM) in CDCl₃ (a), **2** (1 mM) + 1 equiv of *n*-butyltrimethylammonium iodide in CDCl₃ (b).

NOESY NMR spectrum: 2 (1 mM) in d_6 -DMSO (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).

NOESY NMR spectrum: 3 (1 mM) in d_6 -DMSO (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).

NOESY NMR spectrum: **2** (1 mM) in CDCl₃ (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).

NOESY NMR spectrum: **3** (1 mM) in CDCl₃ (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).

NOESY NMR spectrum: **2** (1 mM) after the addition of 3 equiv. of *n*-butyltrimethylammonium tosylate in CDCl₃ (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).

FT-IR spectrum: 2 in 1% [d₆]DMSO/CDCl₃ (c = 2mM)

FT-IR spectrum: 3 in CDCl₃ (c = 2mM)

Job-Plot: **2** + *n*-butyltrimethylammonium iodide in *d*₆-DMSO ($\Delta\delta$ = variation of the shift of the ProH(α) (squares) and the APAH(3) signal (circles) of **2**).

NMR Titration: Experimental (circles, squares) and calculated (line) saturation curves for the complex formation between **2** and *n*-butyltrimethylammonium iodide in *d*₆-DMSO ($\Delta\delta$ = variation of the shift of the ProH(α) (squares) and the APAH(3) signal (circles) of **2**)