Electronic Supplementary information

Bifunctional receptor triad for efficient recognition of mono and dicarboxylic acids

Karol Kacprzak[a] , Jacek Gawroński*[a]

Experimental

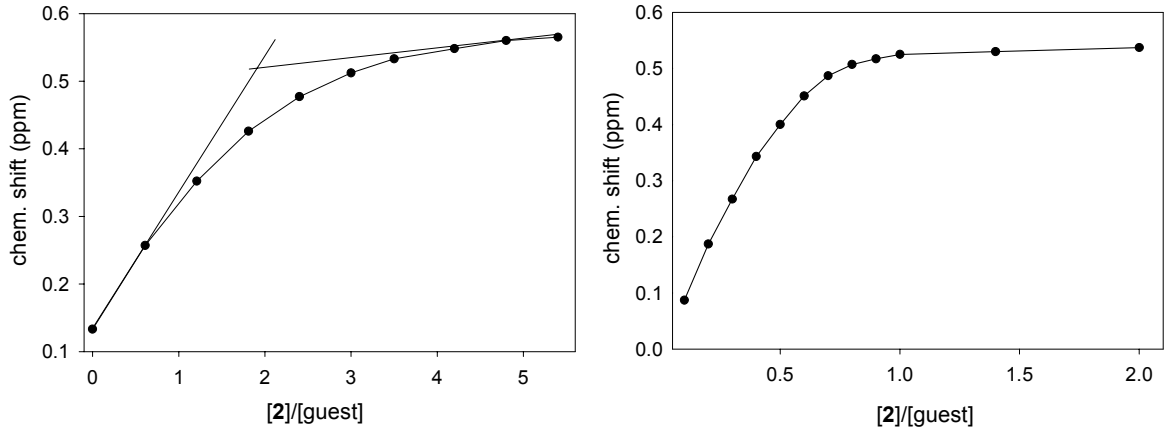
^{1}H NMR spectra were recorded on a Varian 300 MHz spectrometer. Rotational barriers for **1** and **2** were calculated (± 10% accuracy) from the ^{1}H NMR spectra registered at various temperatures (in DMSO) according to the procedure given by Eliel (E.L. Eliel, *Stereochemistry of Organic Compounds*, Wiley 1992, 643).
Spectrometric ^{1}H NMR titration for the determination of stoichiometry of the complexes was carried out as follows. To the triad **2** (1 mmol) in 0.6 ml of solvent ($CDCl_3$-CD_3OD, 2:1) the solid guest was gradually added, and the spectrum was registered after each addition.
ESI MS spectra were recorded with the Waters-Micromass ZQ HPLC-MS system.

Table 1. Recognition of acids by triad **1**[a]

Guest (mol eq.)	Signal of the imide protons	Conformer distribution (%) *anti*:*syn*
none	8.22 (s) – *anti*, 8.0 (s) - *anti* 8.12 (s) – *syn*	50:50
Trifluoroacetic acid[b] (2)	8.16 (s), 7.99 (s)	100:0
Benzoic acid (3)	8.18 (s), 7.61 (s) 7.82 (s)	~80:20
(*R*,*R*)-Tartaric acid (1)	8.13 (s)	0:100
(*S*,*S*)-Tartaric acid (1)	8.16 (s)	0:100

(s) – singlet
[a] measurements in $CDCl_3$:CD_3OD (2:1), c_{triad} = 0.011 mol/dm^{-3}, [b] in $CDCl_3$

Spectrometric titration of triad **2** by benzoic acid (left) and succinic acid (right).



ESMS spectrum of the complex of guest **2** with (*R*,*R*)-tartaric acid