Supplementary Material (ESI) for Chemical Communications

Supporting Information

A synthetic receptor for phosphocholine esters

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Instruments, Materials and General Methods

NMR spectra were recorded with a Bruker DRX 600 MHz. ESI mass spectra were recorded with an Agilent ESI-TOF spectrometer. The ITC experiments were carried out on a VP-ITC MicroCalorimeter, MicroCal, LLC (Northhampton, MA) and the UV-Vis titration with a Varian Cary 50-Bio spectrophotometer. The error limit of the binding constant are in the order of ± 15%. Non linear least square calculation of the binding data were carried out with Microcal Origin 5.0 (MicroCal Software, Inc.) for the ITC measurements and with SigmaPlot 8.0 (SPSS, Inc.) for the other experiments.
Deuterated chloroform (Cambridge Isotope Laboratories, Inc.) and chloroform extra dry (Acros) were used for the NMR spectra and the other experiment respectively without further purification. The *DOPC* was available from commercial sources (Avanti Polar Lipids, Inc. 20mg/mL chloroform solution) and was used without any further purification. For the NMR experiments the commercial solution of *DOPC* was evaporated under vacuum and the residue dissolved in $CDCl_3$. Compounds **1**-Zn,[1] **2**-Zn[1] and **3**[2] were synthesized as described previously.

Isothermal Titration Calometry (ITC) Studies

A typical titration experiment is described.. The titration cell was filled with a solution of the host in chloroform (0.13mM). The reference cell was filled with chloroform. The syringe was loaded with 250µl of a 5mM guest solution in chloroform. Experimental setting: 1) Injection volume: 2µl for 1st, then 7µl; 2) Total number of injections: 33; 3) Cell T = 300K; 4) Injection interval: 180 sec; 5) Stirring speed: 490 sec; 6) Feedback: High; 7) ITC equilibration: Fast, Auto. All experiments were duplicated. See Figure 1 as example.

[1] S. Richeter and J. Rebek, Jr., *J. Am. Chem. Soc.,* 2004, **126**, 16280-16281.
[2] B. Purse, A. Gissot and J. Rebek, Jr., *J. Am. Chem. Soc.*, 2005, **127**, 11222-11223.

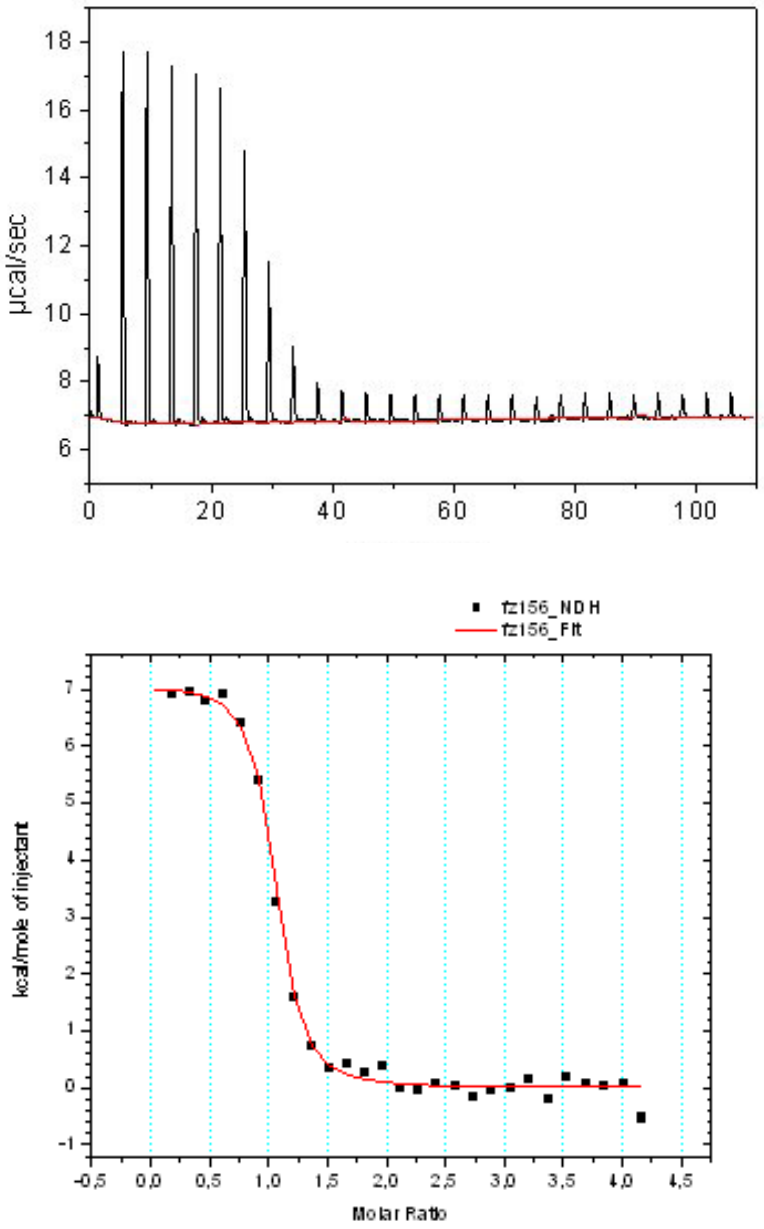

Figure 1 ITC profile and corresponding fitting for the titration of **1**-Zn with *DOPC*

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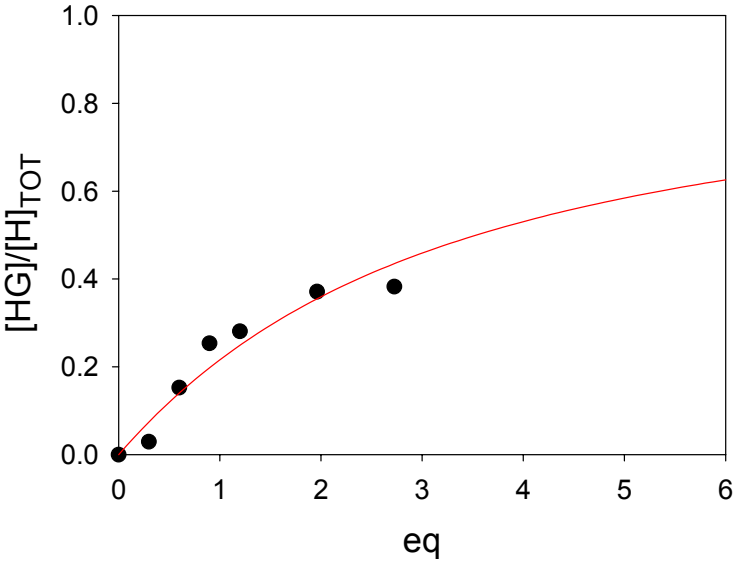
^{1}H-NMR Titrations

Titration of **3** with *DOPC*

600µl of a 2 mM solution of **3** was titrated with a 70 mM solution of *DOPC* in $CDCl_3$. T = 300K. The concentrations of free and bound guest were monitored by integration of the peaks of the methine protons of the free and the bound host at δ=3.3 ppm and δ=-0.32 ppm, respectively.



K = 180 ± 15%

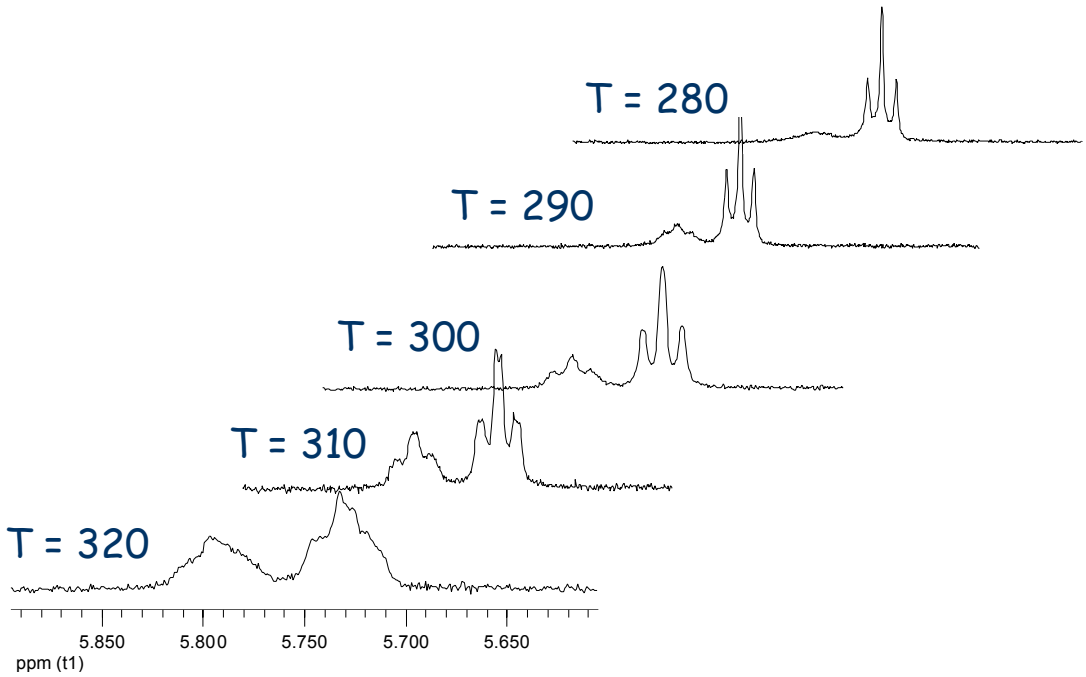
The value of K was obtained by the fitting of the experimental data with the equation:

$$\frac{[HG]}{H_{TOT}} = \frac{KH_{TOT} + KG_{TOT} + 1 - \sqrt{(KH_{TOT} + KG_{TOT} + 1)^2 - 4K^2 H_{TOT} G_{TOT}}}{2KH_{TOT}}$$

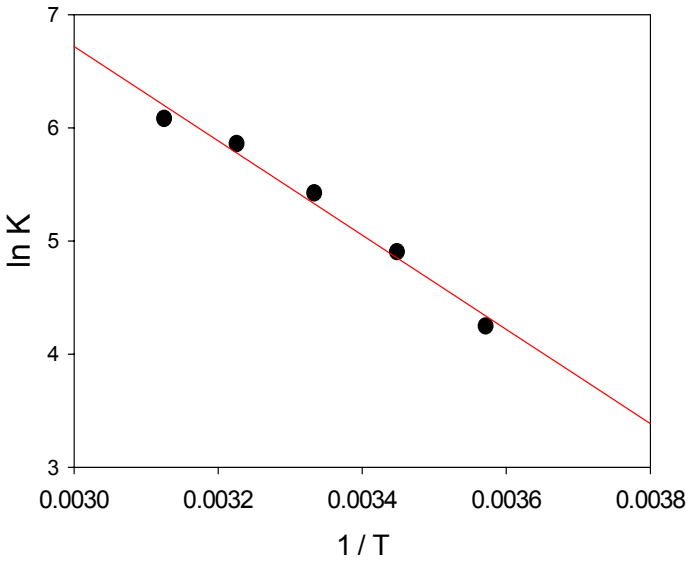
where [HG] is the equilibrium concentration of the Host-Guest complex and H_{TOT} and G_{TOT} the total concentrations of the Host and the Guest respectively.
The binding constant between **3** and *DOPC* was measured also at different temperature (280-320 K). The experimental data were fitted by equation eq1a obtaining the value for the ΔH° and the ΔS° of the binding reaction.

(a) $\Delta G^\circ = -RT\ln K = \Delta H^\circ - T\Delta S^\circ$ (b) $\ln K = -\frac{\Delta H^\circ}{R}\frac{1}{T} + \frac{\Delta S^\circ}{R}$ eq 1

a)



b)



$\Delta H° = 8300$ cal/mol
$\Delta S° = 38$ e.u.

Figure 2 a) Signals of the methine protons of the bound and unbound host at different temperatures. b) Fitting of the experimental data of the binding constants at different temperatures according to eq1b.

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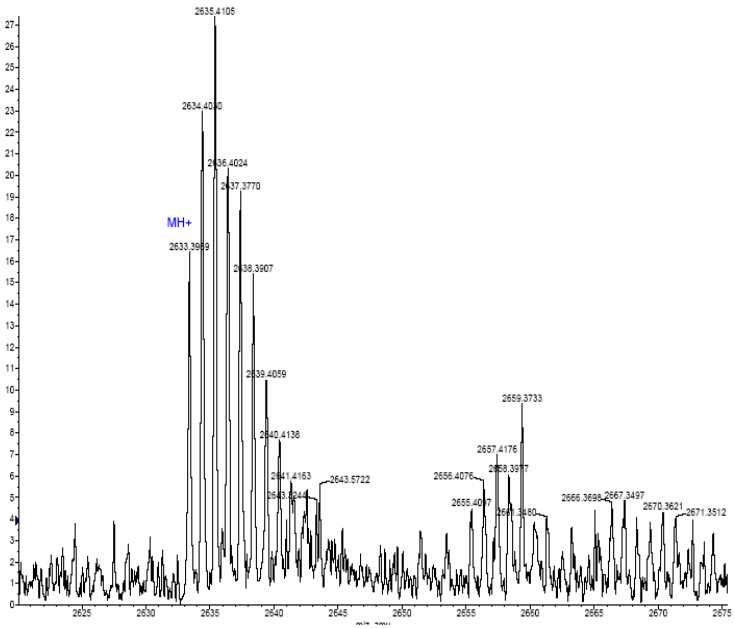
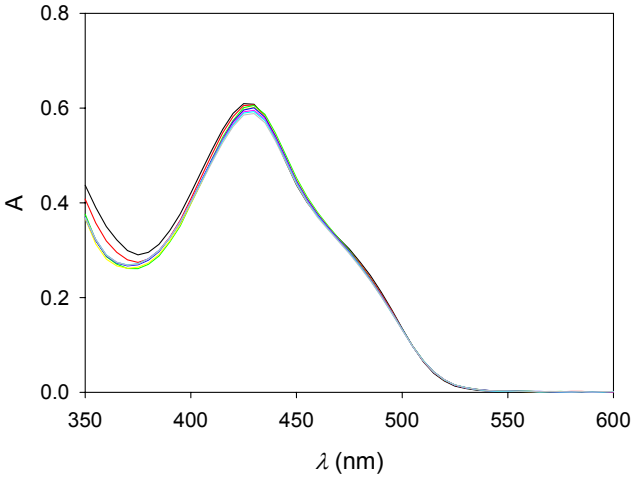
ESI-TOF spectrum of a solution of 1-Zn and *DOPC*

[**1**-Zn·*DOPC*+H^+] 2633.3969 (calculated 2633.3964)

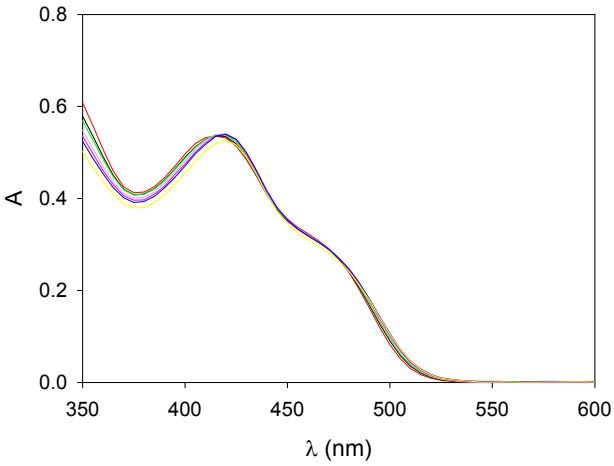


UV-VIS Experiments

UV-VIS Spectra for the titration of **1**-Zn (a) and **2**-Zn (b) with 0-2 equivalents of *DOPC*.
In these experiments the initial concentration of the complex is $4.0 \cdot 10^{-5}$, T=300K, $CHCl_3$
The Absorbance variation is too slight to measure an accurate value of the binding constant.



(a)



(b)