Binding of aromatic mono- and di-N-oxides in water by resorcinarene sulfonates

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SUPPORTING INFORMATION

CONTENTS

I. NMR Spectroscopy

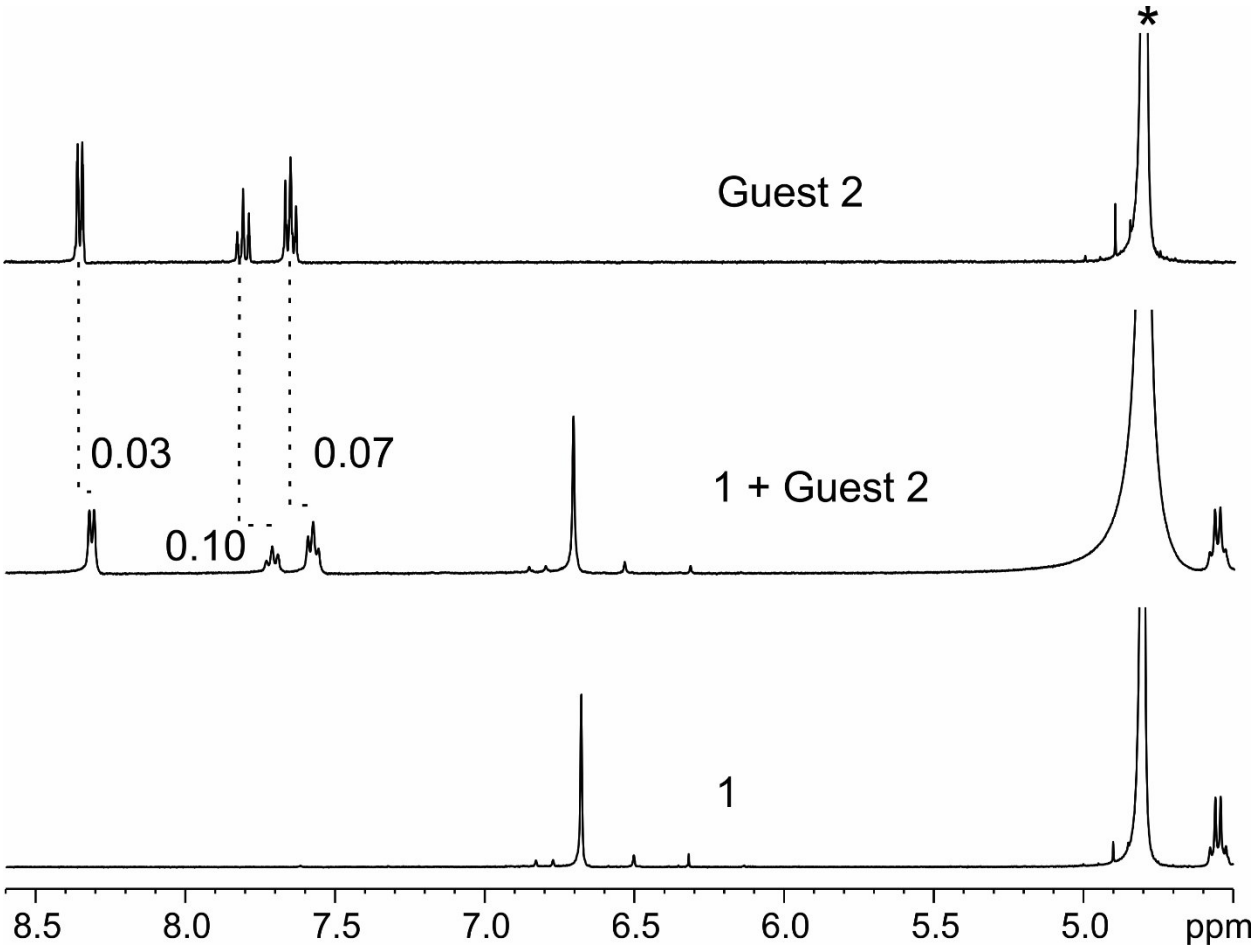


Figure S1: ^{1}H NMR spectra (D_2O, 298 K) of **1**, equimolar mixtures of **2**@**1** and **2**. The dash lines give an indication of the signal changes in ppm. Asterisks is the residual NMR solvent.

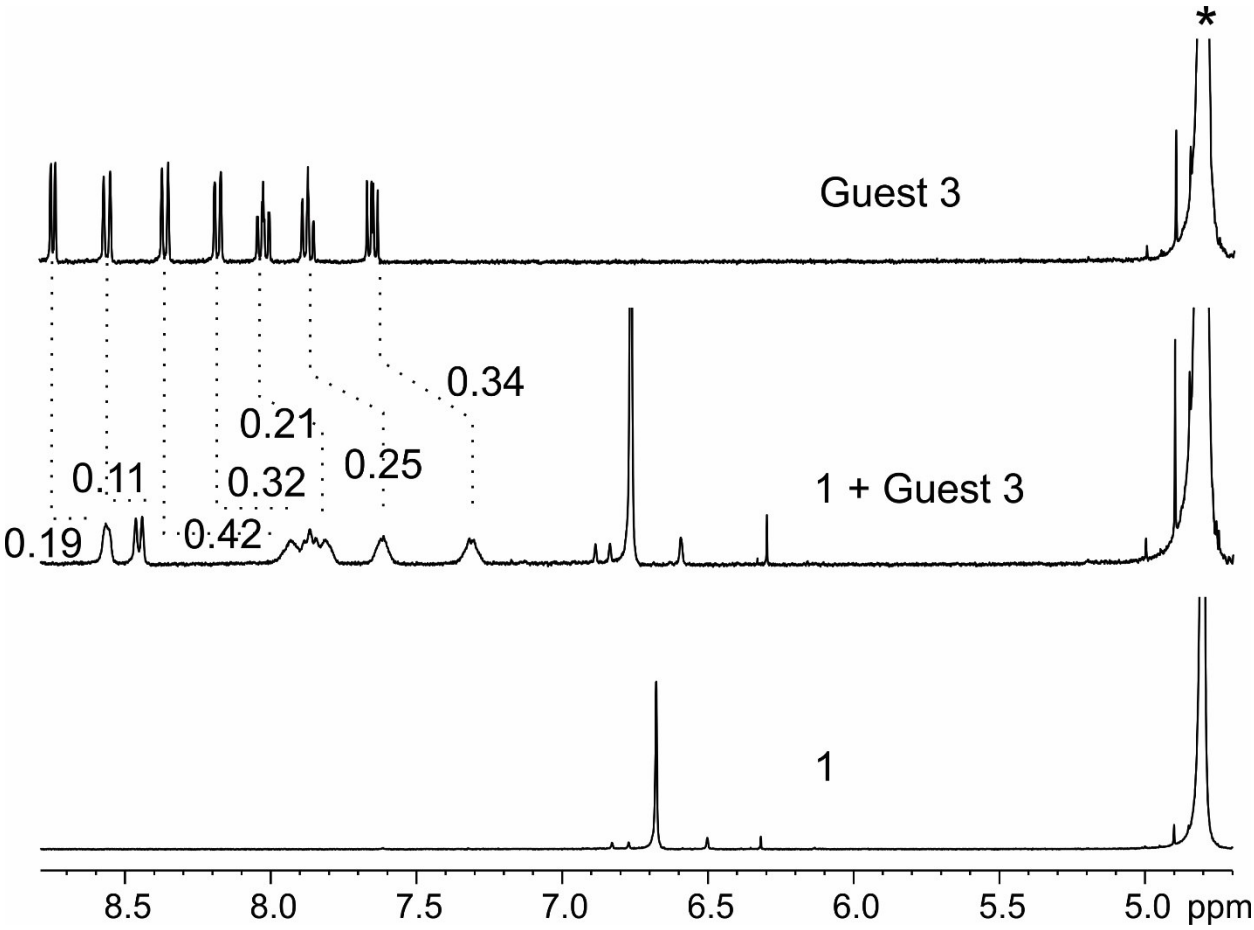


Figure S2: ^{1}H NMR spectra (D_2O, 298 K) of **1**, equimolar mixtures of **3**@**1** and **3**. The dash lines give an indication of the signal changes in ppm. Asterisks is the residual NMR solvent.

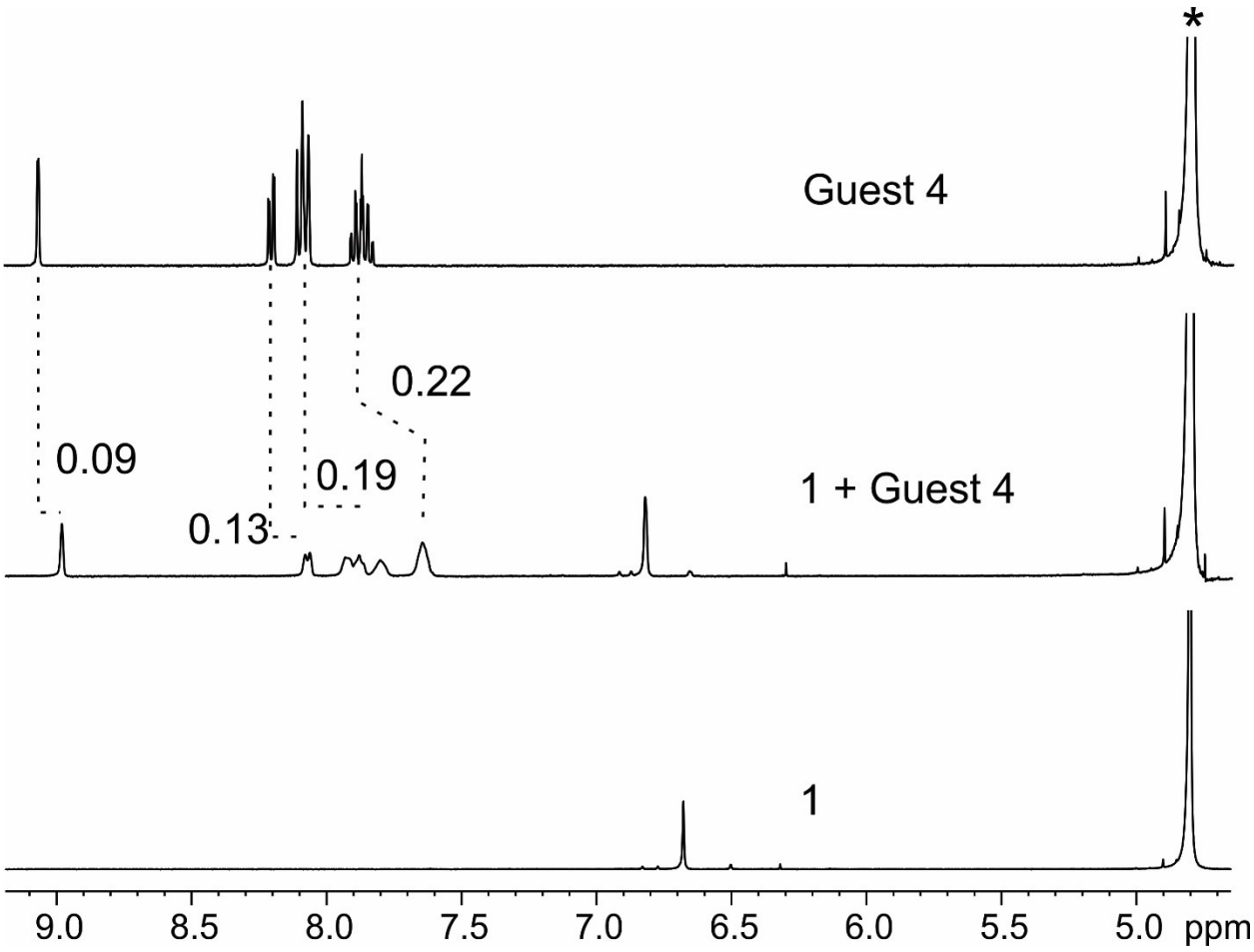


Figure S3: ^{1}H NMR spectra (D_2O, 298 K) of **1**, equimolar mixtures of **4**@**1** and **4**. The dash lines give an indication of the signal changes in ppm. Asterisks is the residual NMR solvent.

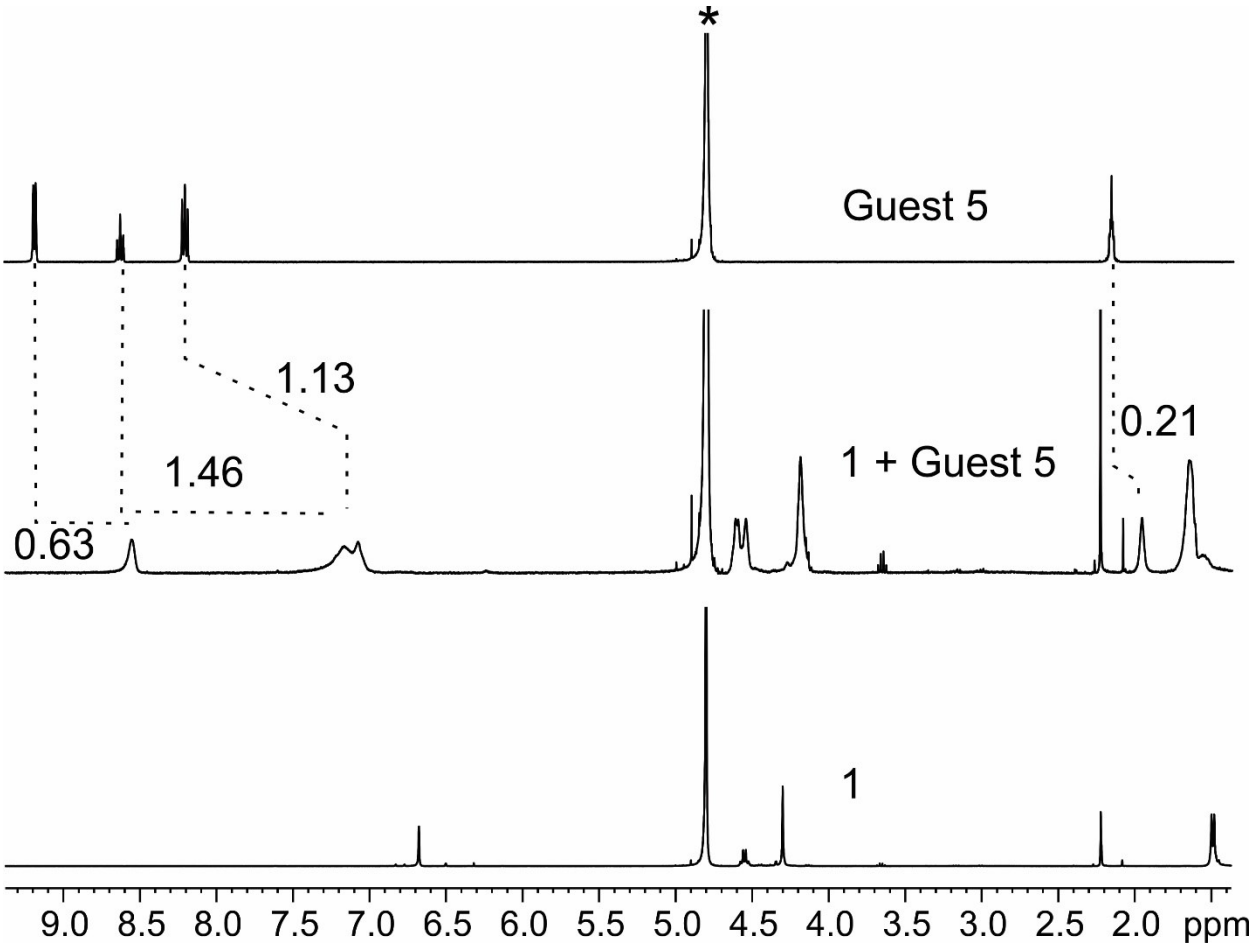


Figure S4: ^{1}H NMR spectra (D_2O, 298 K) of **1**, equimolar mixtures of **5@1** and **5**. The dash lines give an indication of the signal changes in ppm. Asterisks is the residual NMR solvent.

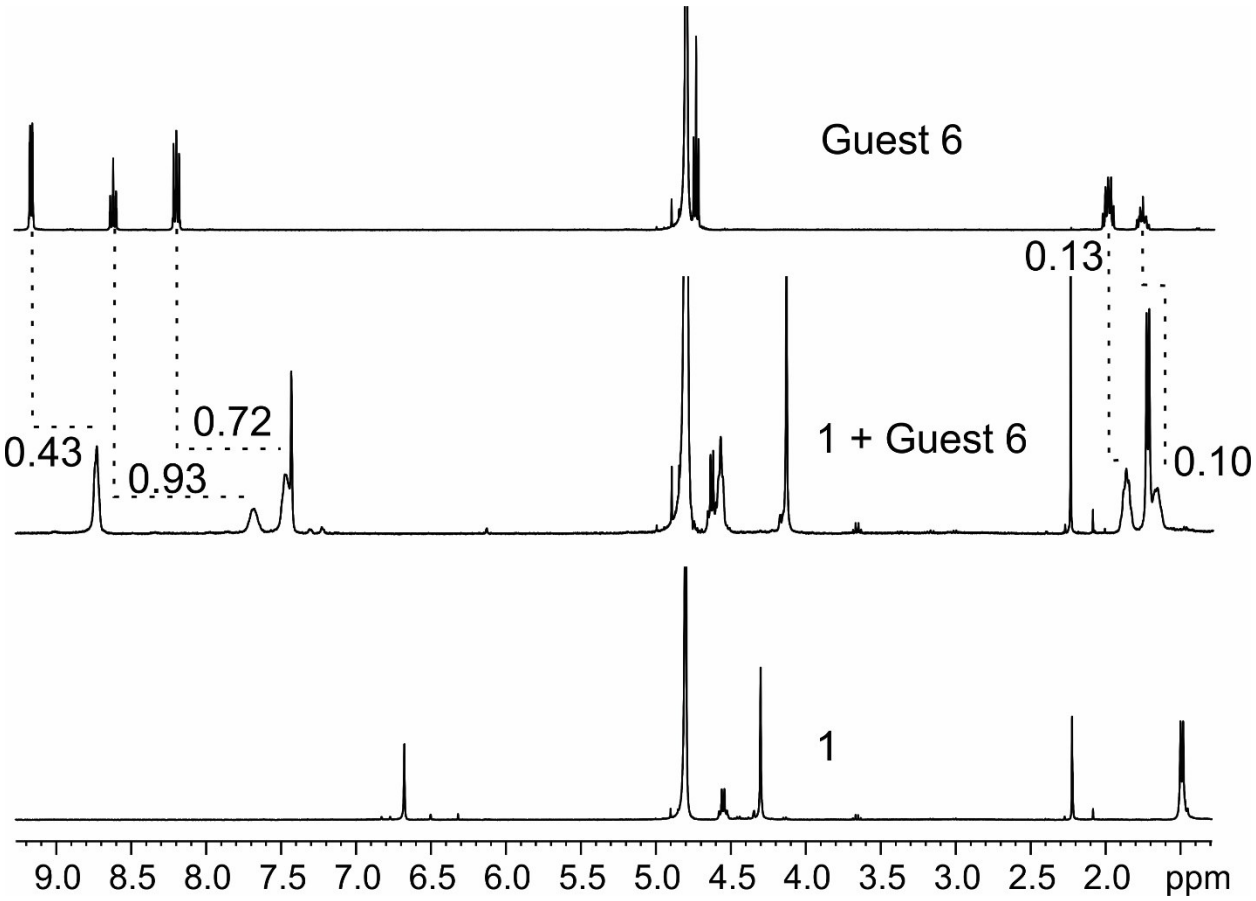


Figure S5: ^{1}H NMR spectra (D_2O, 298 K) of **1**, equimolar mixtures of **6@1** and **6**. The dash lines give an indication of the signal changes in ppm. Asterisks is the residual NMR solvent.

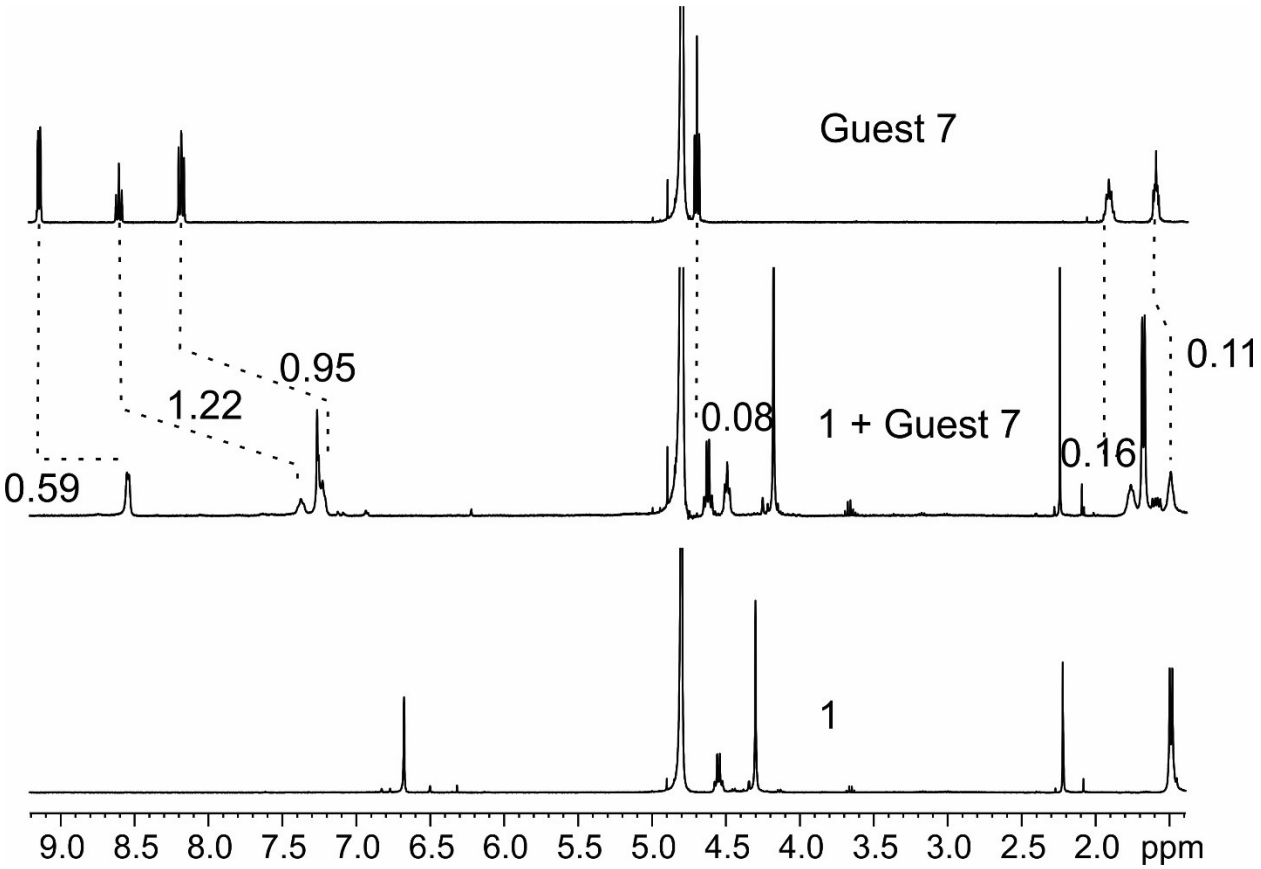


Figure S6: ^{1}H NMR spectra (D_2O, 298 K) of **1**, equimolar mixtures of **7**@**1** and **7**. The dash lines give an indication of the signal changes in ppm. Asterisks is the residual NMR solvent.

II. Isothermal Titration Calorimetry

Table S1: Thermodynamic binding parameters of formed complexes between the receptors and the guests in H_2O by ITC.

Complexes	K_1 **(× 10^4) M^{-1}**	ΔH_1 **kcal/mol**	$T\Delta S_1$ **kcal/mol**	ΔG_1 **kcal/mol**	K_2 **(× 10^3) M^{-1}**	ΔH_2 **kcal/mol**	$T\Delta S_2$ **kcal/mol**	ΔG_2 **kcal/mol**
2@1	-	-	-	-				
3@1	0.66±0.07	-28.4±1.92	-23.15	-5.25				
4@1	0.19±0.05	-0.57±0.07	3.87	-4.44				
5@1	1.32±0.12	-6.99±0.02	-1.29	-5.70	3.36±0.84	4.57±0.31	8.75	-4.18
6@1	2.65±0.81	-10.96±0.55	-4.59	-6.37	2.64±0.17	-16.87±0.84	-11.37	-5.50
7@1	3.15±0.36	-3.94±0.05	2.20	-6.14	1.37±0.34	-1.52±0.25	2.75	-4.27

Table S2: Complexation derived interaction parameter (α) that describes cooperativity in binding constants for thermodynamics in deionized H_2O.

Complex	$\alpha = (4K_2/K_1)$
2@1	-
3@1	-
4@1	-
5@1	1.02
6@1	0.40
7@1	0.17

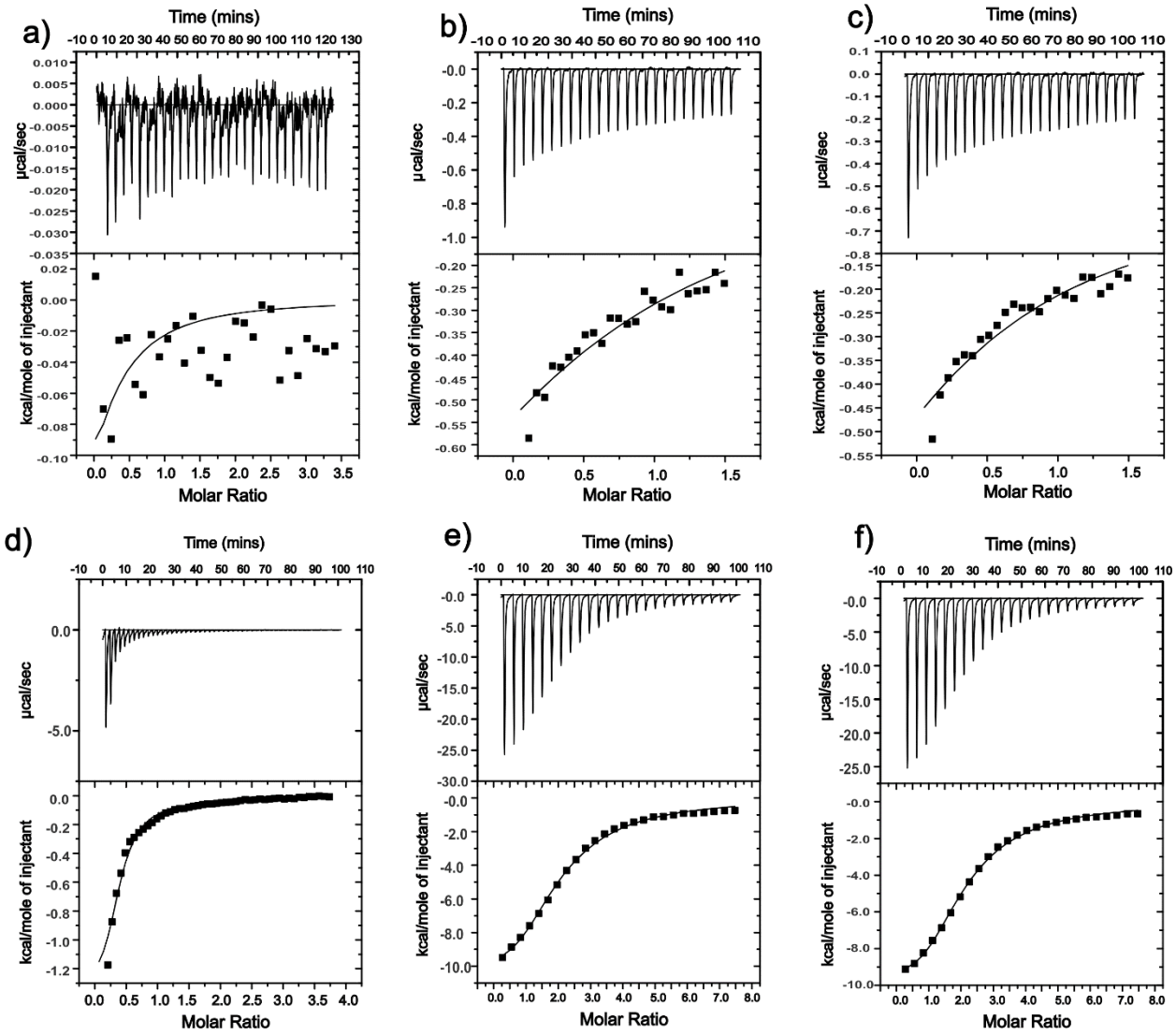


Figure S7: ITC traces of the titration of receptor 1 with n-oxides (**2-7**) in 10mM Tris buffer, pH 7.4 at 298 K. (a) **2@1**, (b) **3@1**, (c) **4@1** were fitted to a one set of site binding model**.** (d) **5@1** (e) **6@1** (f) **7@1** were fitted to sequential two set of sites binding model.

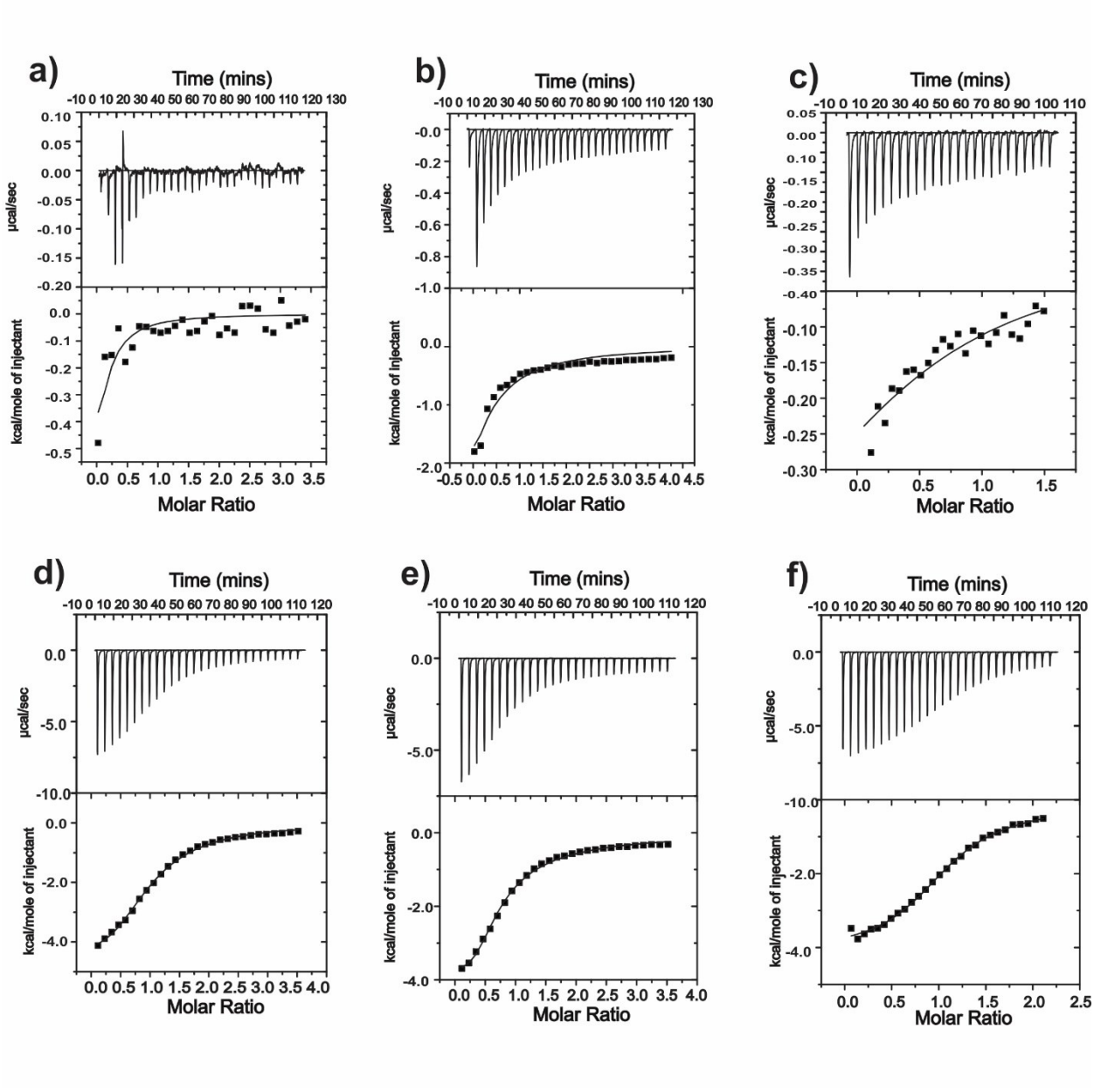
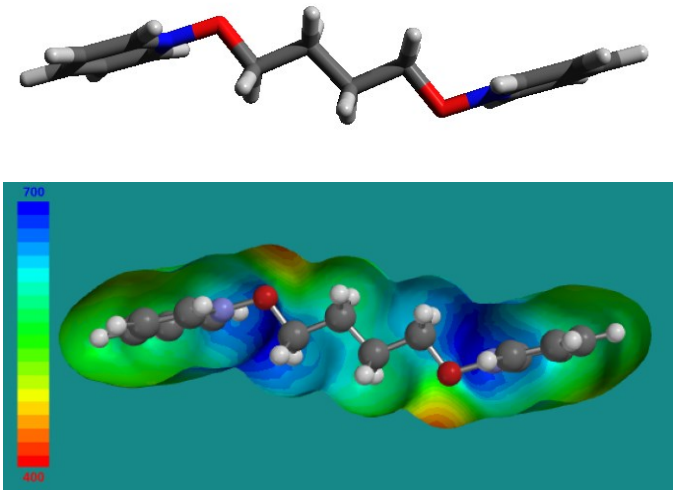
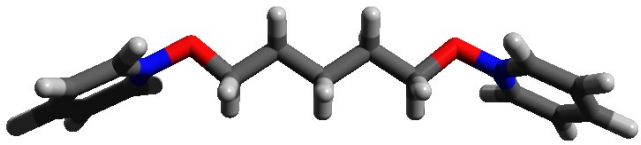
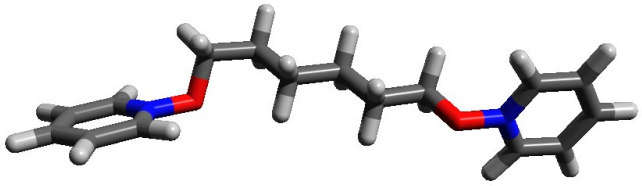


Figure S8: ITC traces of the titration of receptor 1 with n-oxides (**2-7**) in water at 298 K. (a) **2@1**, (b) **3@1**, (c) **4@1** were fitted to a one set of site binding model**.** (d) **5@1** (e) **6@1** (f) **7@1** were fitted to sequential two set of sites binding model.

III. Computation Calculations

Table S2. Equilibrium structures and properties of guest molecules from B3LYP-D3 calculation with 6-31G** basis set within the implicit PCM water solvent; the electrostatic potential scale shown is in kJ/mole.

	Symmetry: C_{2h} μ=0.0 D N---N=8.43 Å
	Symmetry: C_{2v} μ=4.38 D N---N=9.71 Å
	Symmetry C_1 μ=0.50 D N---N=10.10 Å