

Supporting Information

for

A Zinc-Salophen/Bile-Acid Conjugate Receptor Solubilized by CTABr Micelles Binds Phosphate in Water

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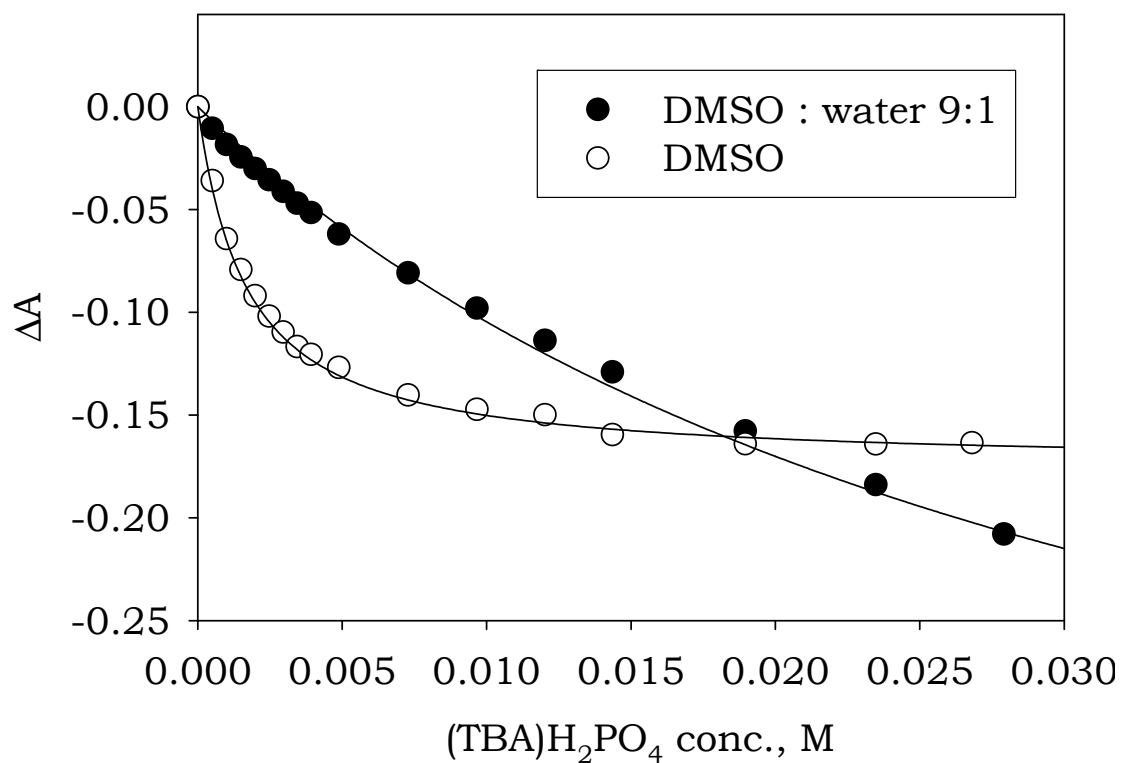


Figure S1. Plots of the absorption variations of **1** upon addition of $(TBA)H_2PO_4$ in DMSO (\circ) and in a 10%water/DMSO mixture (\bullet), recorded at 300 K. Lines represent the best fit curves (1:1 binding isotherm equation).

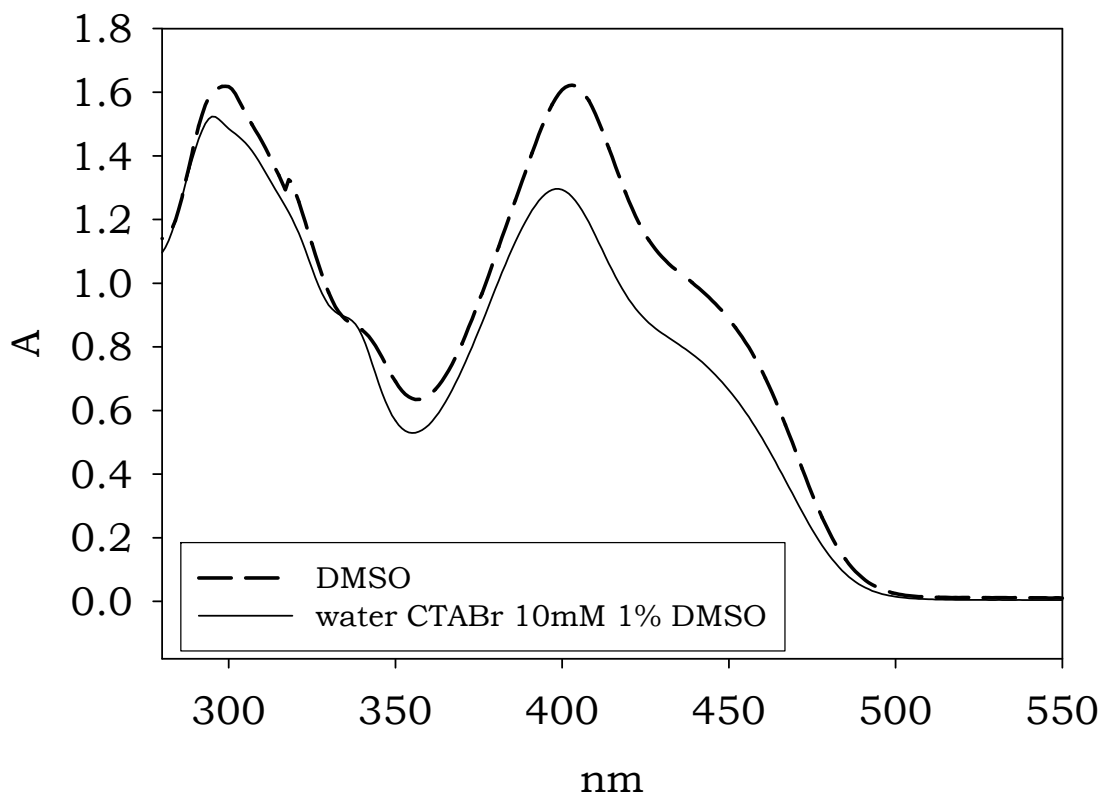


Figure S2. Absorption spectra of a 0.1mM solution of **1** in DMSO (- -) and in water (-) (CTABr, 10mM – 1%DMSO).

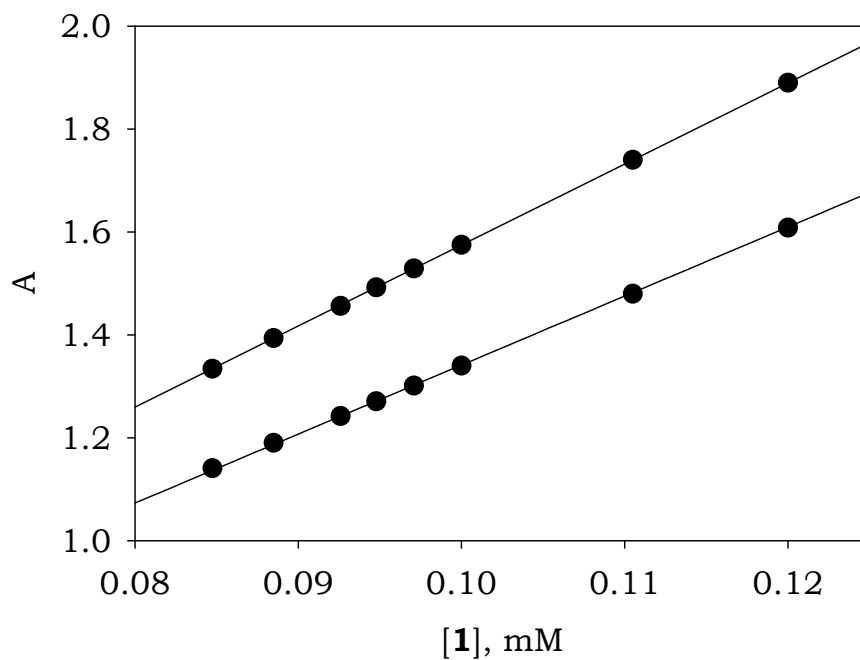


Figure S3. Plot of Absorption vs. [**1**] at 295 and 400 nm, and linear fit of the data (-)

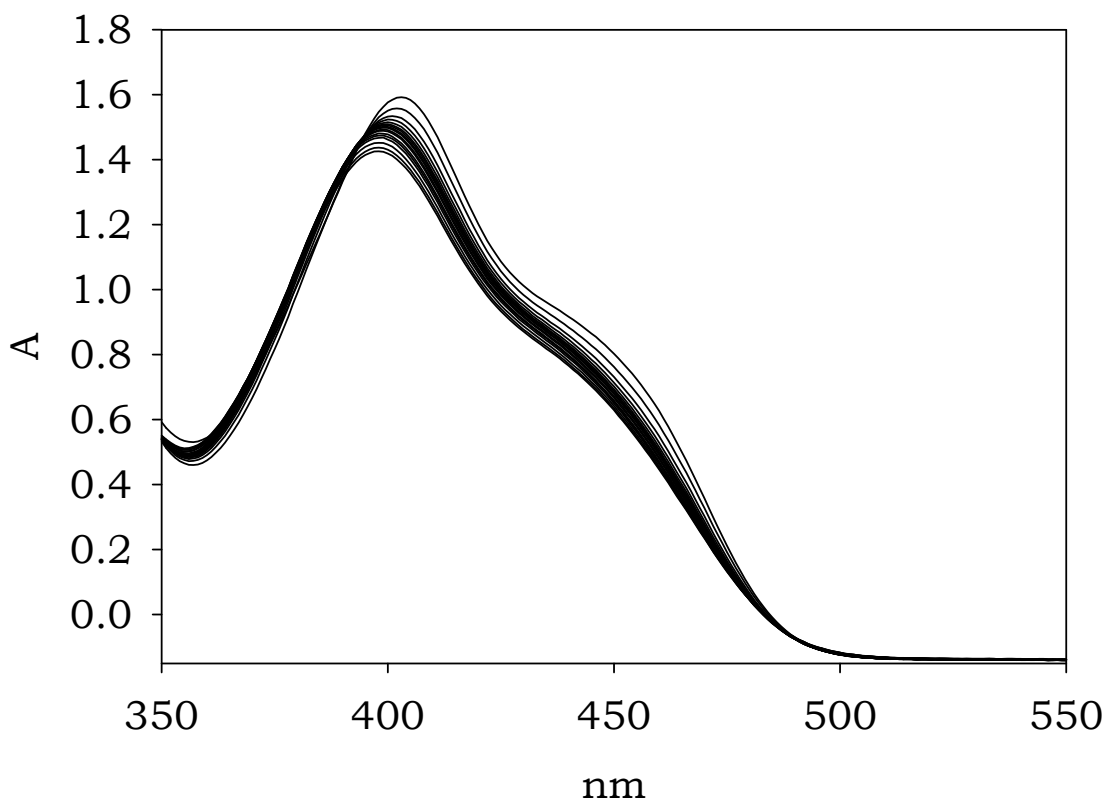


Figure S4. UV-vis variation of a 0.1 mM solution of **1** in DMSO upon addition of (TBA)H₂PO₄ at 300 K.

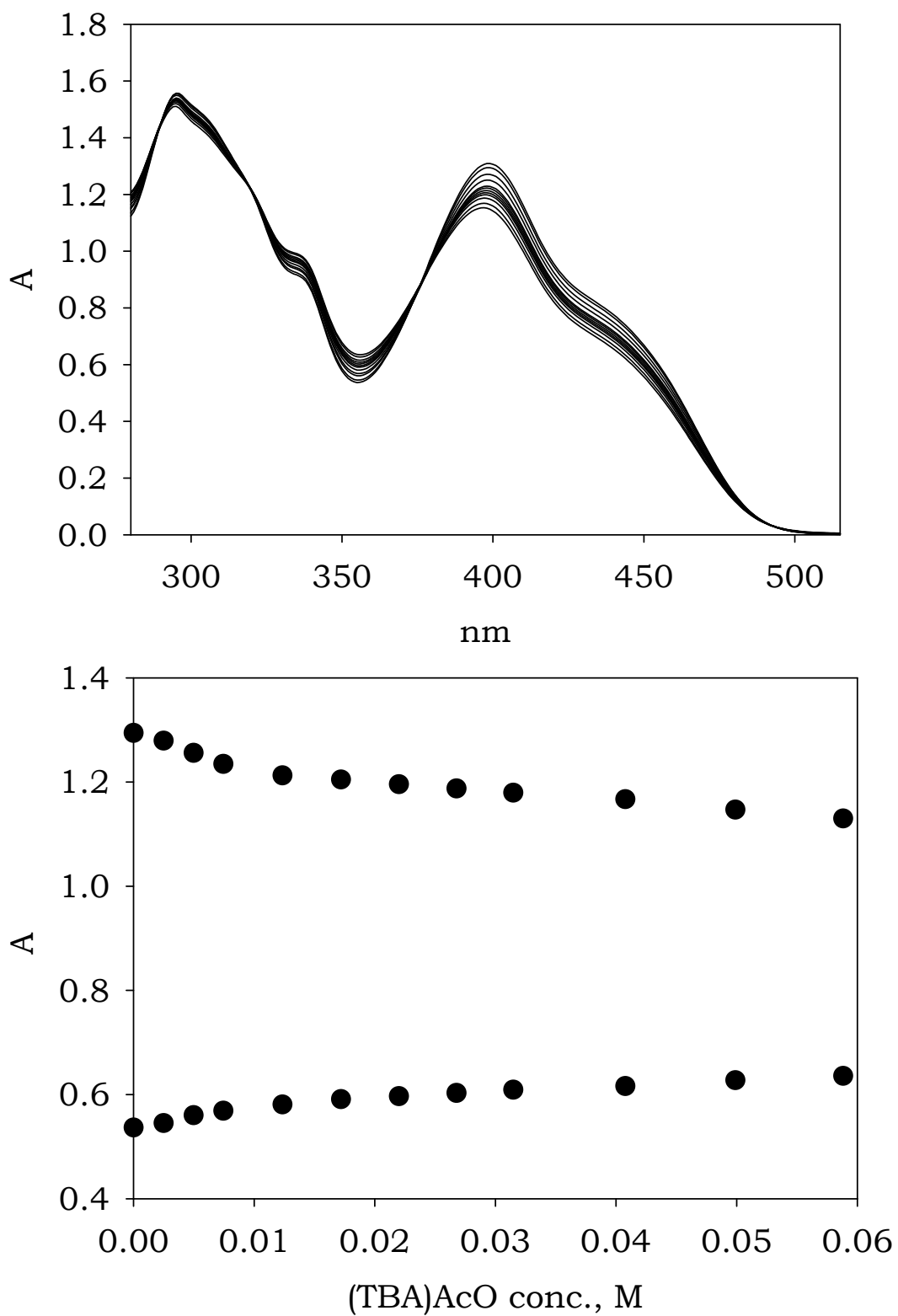


Figure S5. top) UV-vis variation of a 0.1 mM solution of **1** in water (CTABr 10 mM, 1% DMSO) upon addition of (TBA)AcO at 300 K; bottom) Plot of the Abs v. AcO conc. at 355 and 400 nm.

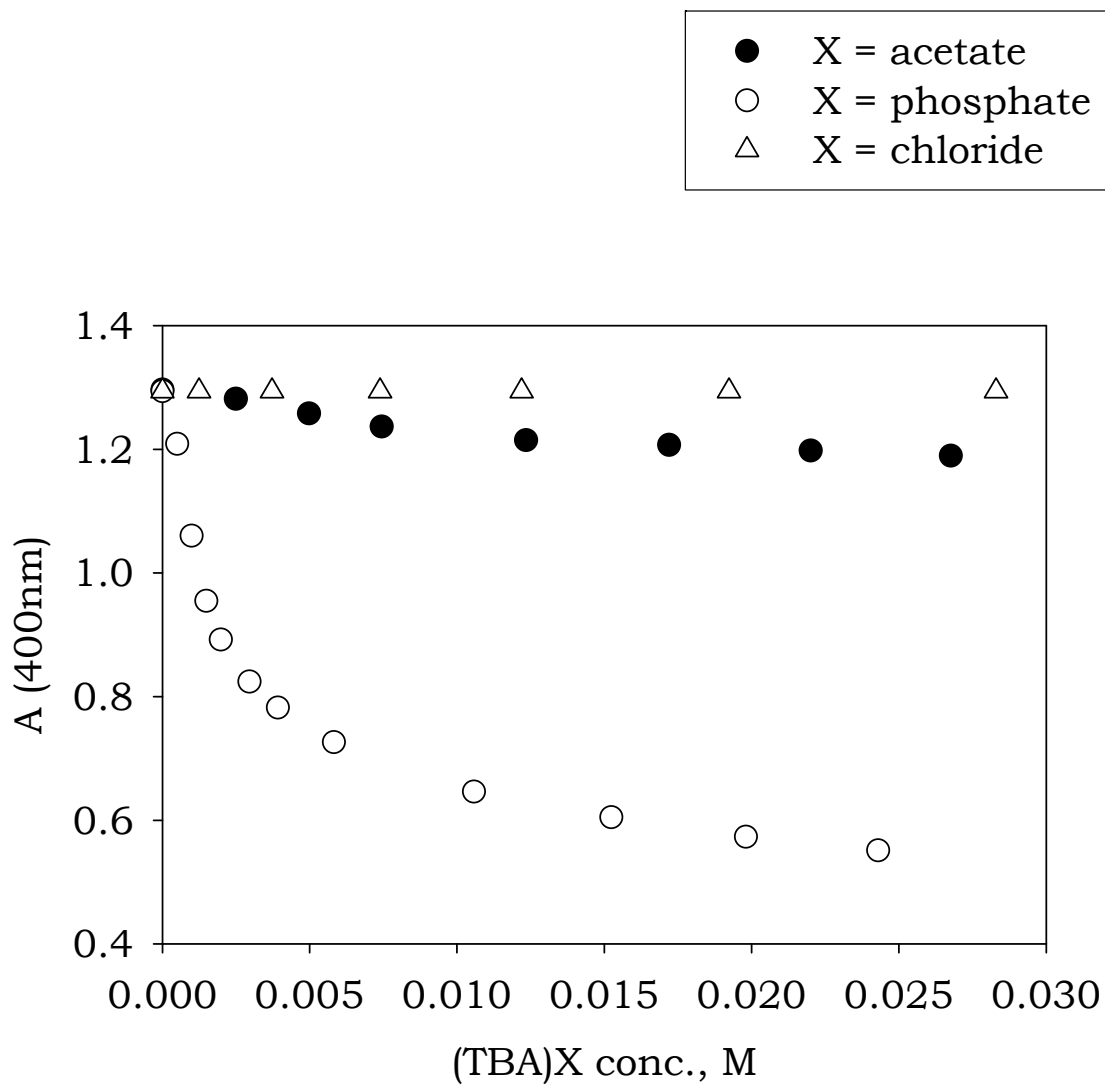


Figure S6. Absorption variation observed upon addition of (TBA)X (X= chloride (Δ), acetate (\bullet) and phosphate (\circ)) to a 0.1 mM solution of **1** in water (CTABr 10mM, 1%DMSO).

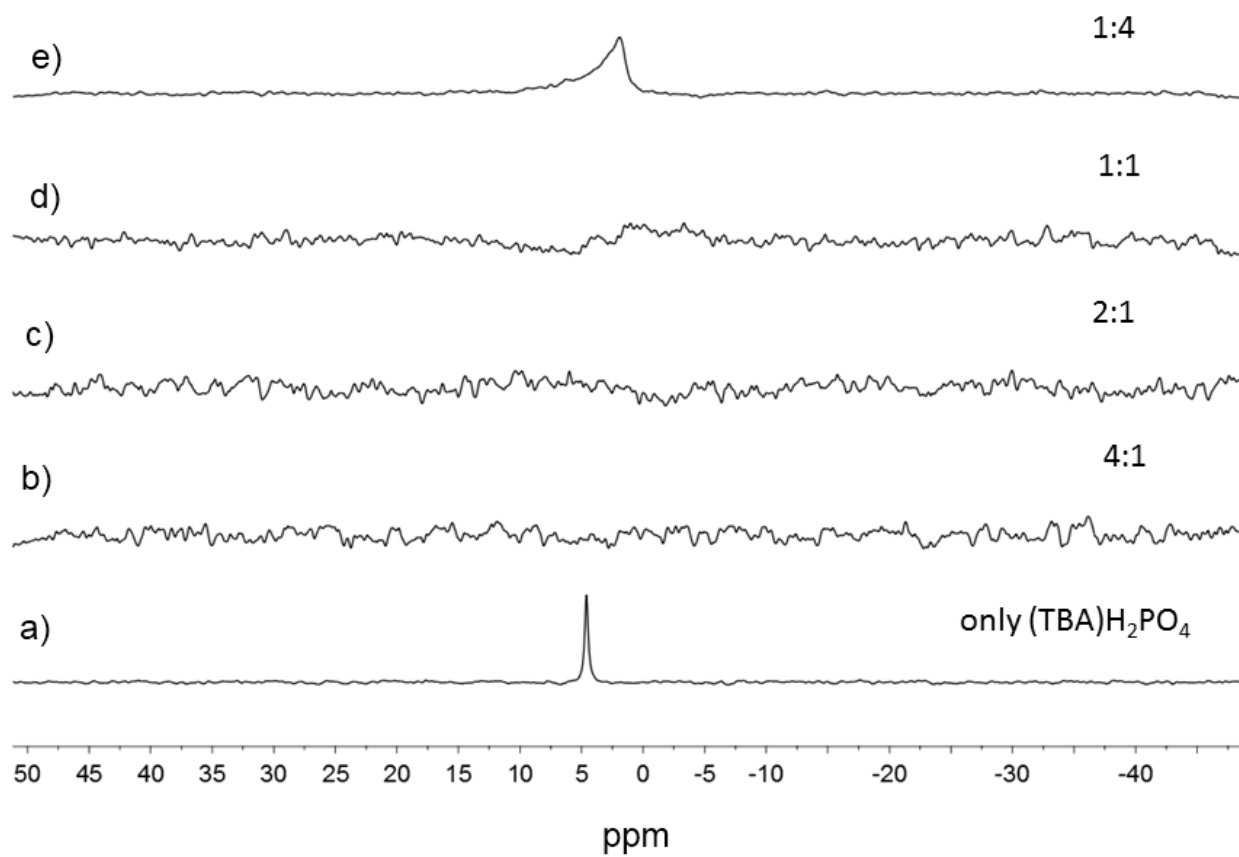


Figure S7. ³¹P-NMR in DMSO; a) (TBA)H₂PO₄ 5mM, b) **1** : (TBA)H₂PO₄ 4:1 (20mM : 5mM); c) **1** : (TBA)H₂PO₄ 2:1 (20mM : 10mM); d) **1** : (TBA)H₂PO₄ 1:1 (20mM : 20mM) and e) **1** : (TBA)H₂PO₄ 1:4 (20mM : 80mM).

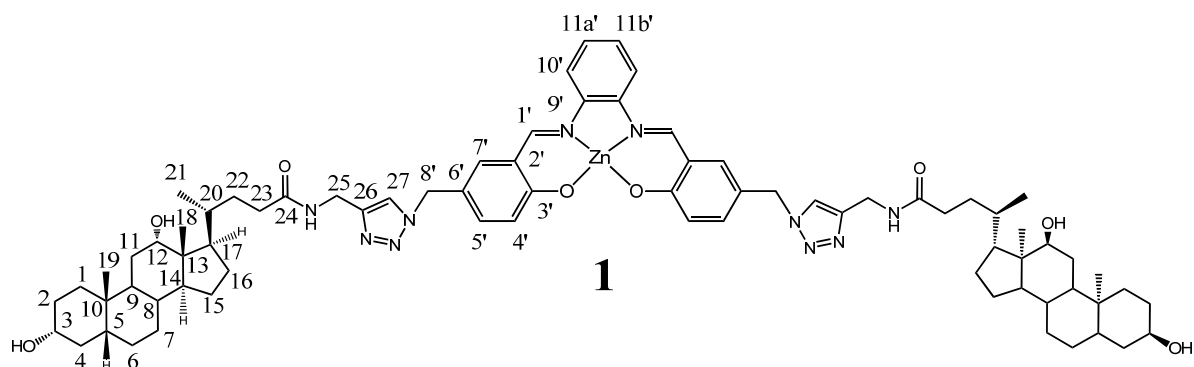


Figure S8. Numbering of **1**, including numbering of **4**; the assignment of individual ^1H and ^{13}C signals was carried out by comparing them with NMR data of parental compounds published in the literature,¹ by heteronuclear 2D experiments PFG ^1H , ^{13}C HMQC, and supported by data predicted by software ACD/ChemSketch C+H NMR Predictors and DB (Product version 10.04). ^1H chemical shifts were referenced to the trace signal of CHCl_3 (7.26 ppm from int. TMS) or DMSO (2.5 ppm) and ^{13}C chemical shifts to the center peak of the solvent signal (77.00 ppm from int. TMS for CDCl_3 , and 39.52 ppm for DMSO-*d*6).

¹ S. Ikonen, H. Macíčková-Cahová, R. Pohl, M. Šanda, and M. Hocek, *Org. Biomol. Chem.*, 2010, **8**, 1194-1201; A. Valkonen, M. Lahtinen, Virtanen E., S. Kaikkonen and E. Kolehmainen, *Biosens. Bioelectron.* 2004, **20**, 1233-1241.