Supporting Information

for

Attraction by repulsion: compounds with like charges undergo self-assembly in water that improves in high salt and persists in real biological fluids

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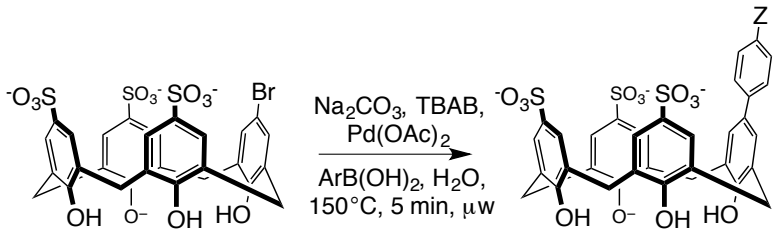
Experimental Section

General

Proton nuclear magnetic resonance spectra (^{1}H NMR) were recorded at 500 MHz at 23 °C unless otherwise stated. Proton chemical shifts are expressed in parts per million (ppm, δ scale) downfield from tetramethylsilane, and are referenced to residual proton in the NMR solvent (DOH δ 4.79, CD_2HOD = 3.35). Data are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sext = sextet, m = multiplet and/or multiple resonances, br = broad), coupling constant in Hertz, and integration. Carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 125 MHz at 23 °C. Carbon chemical shifts are reported in parts per million downfield from tetramethylsilane and are referenced to residual carbon resonances of the solvent or to the deuterium lock reference in the case of D_2O. Infrared (IR) spectra were obtained using a Perkin Elmer 1000 FT-IR spectrometer. Data are represented as follows: frequency of absorption (cm^{-1}), intensity of absorption (s = strong, m = medium, w = weak, br = broad). High-resolution electrospray ionization mass spectrometry (HR-ESI-MS) was obtained from the UVic-Genome BC Proteomics Centre on a LTQ Velos Orbitrap or in-house on a Micromass Q-TOF II. Samples were prepared in 1:1 solution of CH_3OH:H_2O. Melting points were collected on a Gallenkamp Melting Point apparatus. Boronic acids were obtained from

Matrix Scientific. All other reagents and solvents for synthesis were purchased from Sigma-Aldrich and used as obtained.

Synthesis

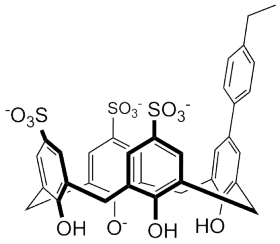


A

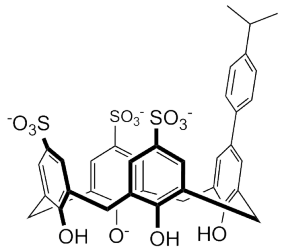
1: Z = H, 46%
2: Z = Me, 49%
3: Z = Et, 41%
4: Z = iPr, 40%
5: Z = tBu, 53%
6: Z = $CH_2NH_3^+$, 48%

The syntheses of compounds **A**, **1**, **2**, and **6** have been previously published.[1, 2] New hosts were made using **A** as starting material, following the generalized synthetic procedure below. **A** (0.1011 g, 0.136 mmol), 4-methylphenylboronic acid (0.0204 g, 1.1 equiv., 0.150 mmol, $Pd(OAc)_2$ (0.0061 g, 20 mol%) and sodium carbonate (0.0548 g, 3.8 equiv., 0.517 mmol) were dissolved in 5 mL of deionized water inside a microwave vial and irradiated to a temperature of 150 °C for 5 minutes with cooling air and stirring on (Biotage Initiator Microwave Reactor). HPLC purification was performed on a 250 mm x 22 mm preparative C18 Alltech Apollo 10 μm column, using a Shimadzu Prominence HPLC system with UV detection at 280 nm. A gradient running from 90% H_2O (with 0.1% TFA)/10% CH_3CN (with 0.1% TFA) to 90% CH_3CN (with 0.1% TFA)/10% H_2O (with 0.1% TFA) over 30 minutes was used. Lyophilization of collected fractions afforded a white powder in 49% yield (0.0489 g).

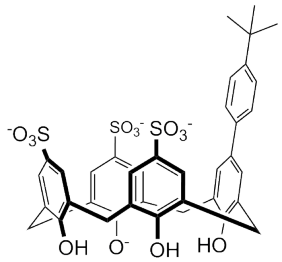
Characterization data for new compounds



5-(4-ethylphenyl)-25, 26, 27, 28-tetrahydroxy-11-17-23-trisulfonatocalix[4]arene **(3)**
Mp: 240 °C (dec). IR (KBr pellet): 3383br, 3221br, 2957sh, 2935sh, 1474s, 1457s, 1264w, 1205s, 1152s, 1113s, 1040s, 886w, 816w, 783m, 668m, 657m, 626m, 542m. ^{1}H NMR (500 MHz, D_2O): d 7.75 (d, J = 2.2 Hz, 2H), 7.70 (d, J = 2.2 Hz, 2H), 7.62 (s, 2H), 7.29 (s, 2H), 6.86 (d, J = 8.0 Hz, 2H), 6.24 (d, J = 7.6 Hz, 2H), 4.07 (s, br, 8H), -0.30 (s, 2H) –1.56 (s, 3H). ^{13}C NMR (125 MHz, D_2O): d 151.7, 151.0, 147.0, 143.1, 136.7, 136.4, 135.1, 128.9, 128.6, 128.3, 128.1, 127.6, 127.1, 126.8, 126.8, 126.6, 125.3, 30.8, 30.6, 26.1, 11.1 HR-ESI-MS: m/z observed: 767.09475 ($[M-H]^-$, $C_{36}H_{31}O_{13}S_3^-$; calcd 767.09320).

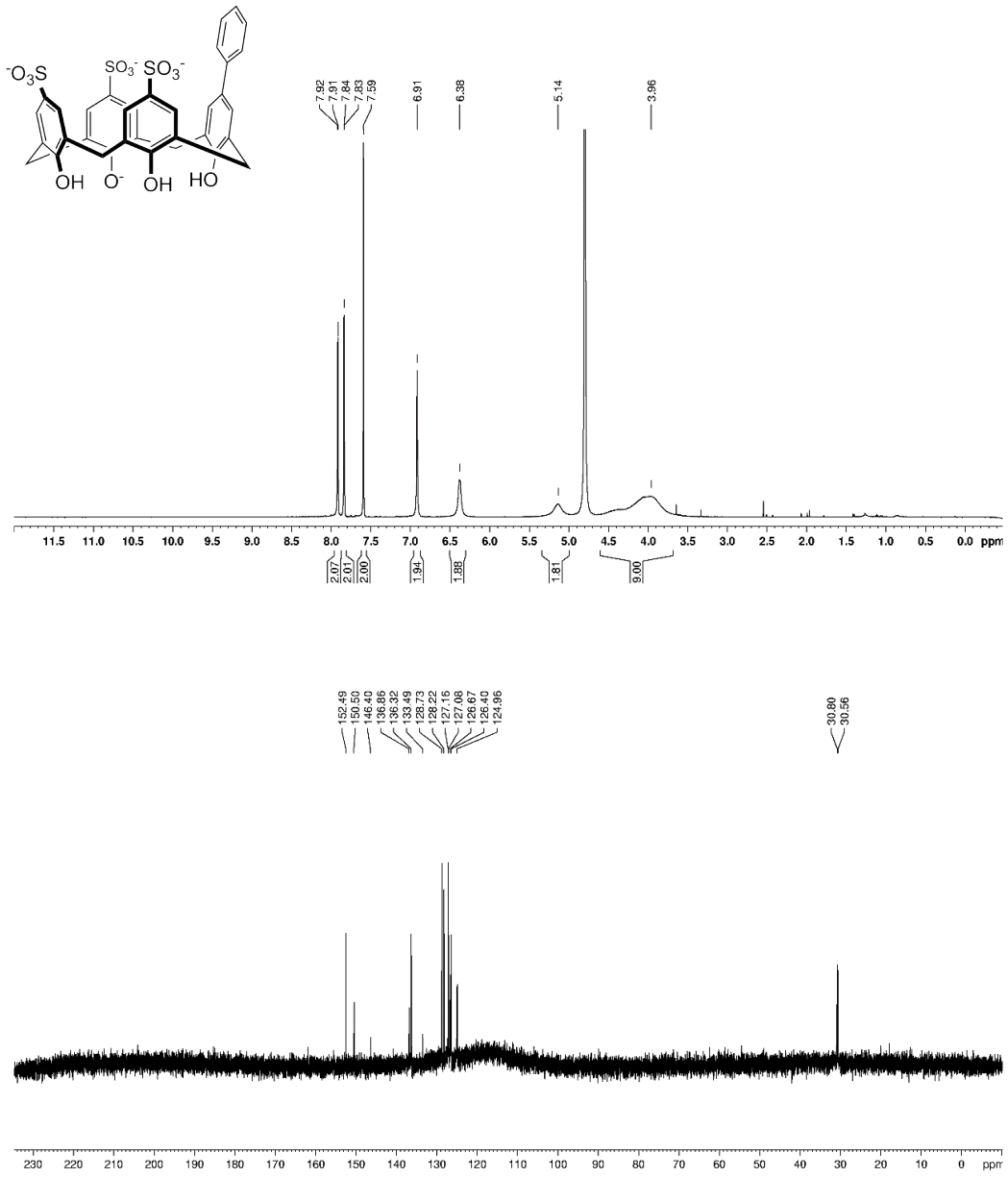


5-(4-*iso*propylphenyl)-25, 26, 27, 28-tetrahydroxy-11-17-23-trisulfonatocalix[4]arene **(4)**
Mp: 240 °C (dec). IR (KBr pellet): 3411br, 3215br, 2957sh, 2918sh, 1476s, 1448s, 1381w, 1264s, 1241s, 1155s, 1113s, 1040s, 881w, 830w, 783m, 735w, 663m, 654m, 623m, 551m. ^{1}H NMR (500 MHz, D_2O): d 7.73 (s, 2H), 7.70 (s, 2H), 7.65 (s, 2H), 7.28 (s, 2H), 6.89 (d, J = 7.6 Hz, 2H), 6.28 (d, J = 7.3 Hz, 2H), 4.08 (d, br, 8H), 0.99 (s, 1H) –1.10 (s, 6H). ^{13}C NMR (125 MHz, D_2O): d 151.5, 151.1, 147.4, 147.1, 136.8, 136.7, 135.3, 135.3, 129.0, 128.5, 128.2, 128.0, 127.2, 126.9, 126.9, 126.6, 126.3, 125.5, 31.2, 30.8, 20.3 HR-ESI-MS: m/z observed: 781.10965 ($[M-H]^-$, $C_{37}H_{34}O_{13}S_3^-$; calcd 781.10885).

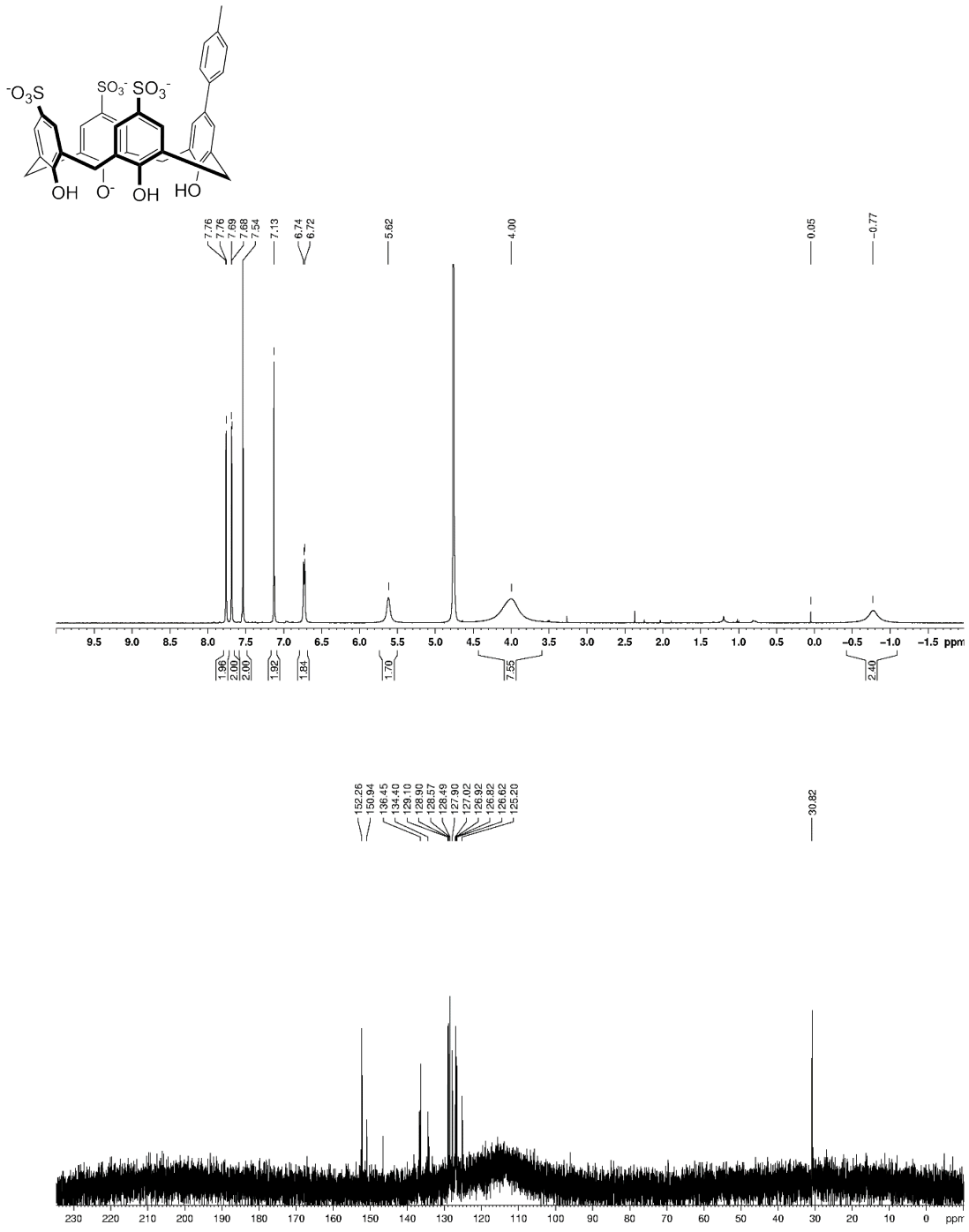


5-(4-*t*-butylphenyl)-25, 26, 27, 28-tetrahydroxy-11-17-23-trisulfonatocalix[4]arene (**5**)
Mp: 240 °C (dec). IR (KBr pellet): 3410br, 3208br, 2949s, 1475s, 1453s, 1266w, 1216s, 1155s, 1111s, 1040s, 885w, 827w, 784m, 665m, 626m, 543w. ^{1}H NMR (500 MHz, D_2O): d 7.77 (d, J = 1.6 Hz, 2H), 7.72 (d, J = 1.6 Hz, 2H), 7.66 (s, 2H), 7.25 (s, 2H), 6.90 (d, J = 7.8 Hz, 2H), 6.40 (d, J = 7.3Hz, 2H), 4.09 (d, br, 8H), –0.62 (s, 9H) ^{13}C NMR (125 MHz, D_2O): d 151.8, 150.9, 149.5, 146.8, 137.0, 136.5, 135.3, 135.2, 128.8, 128.2, 128.0, 128.0, 127.0, 127.0, 126.8, 125.3, 125.3, 32.0, 31.0, 28.7 HR-ESI-MS: m/z observed: 795.12575 ($[M-H]^-$, $C_{38}H_{35}O_{13}S_3^-$; calcd 795.12450).

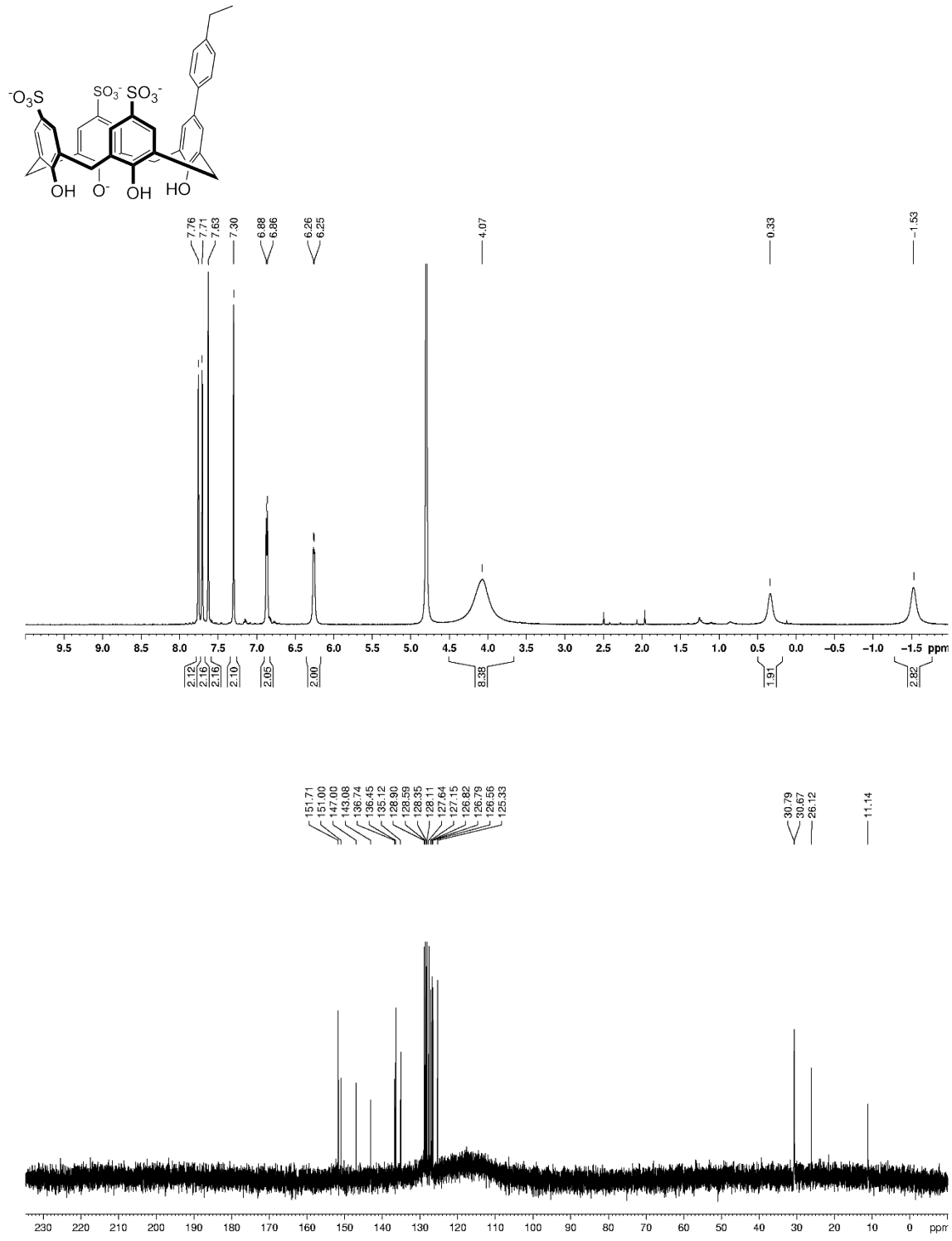
^{1}H and ^{13}C NMR spectra for all compounds



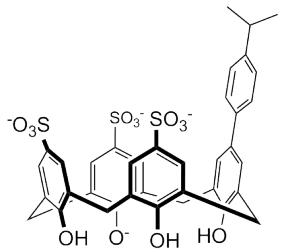
Compound **(phenyl)** (25.4 mM) in D_2O

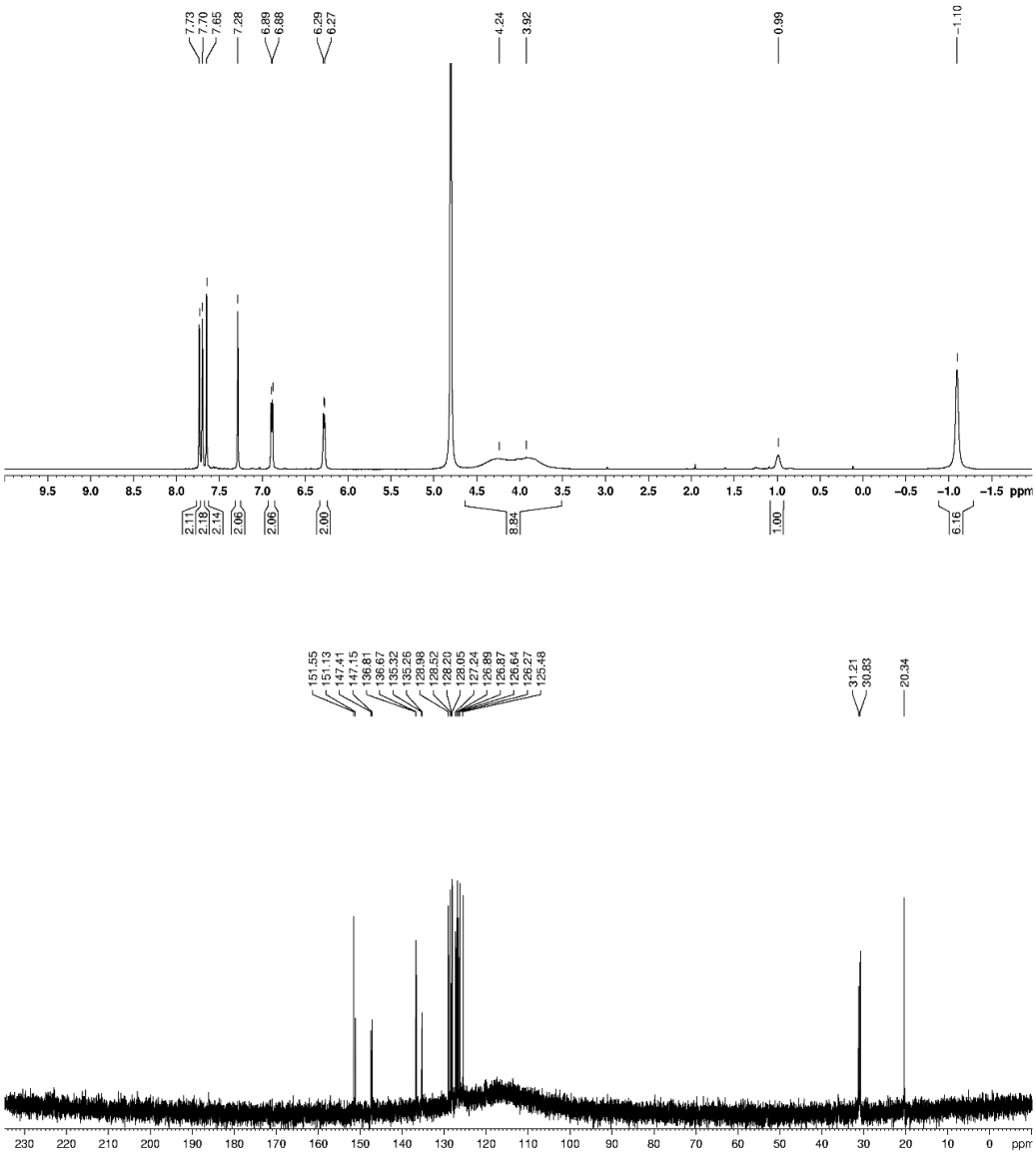


Compound **(tolyl)** (20.3 mM) in D_2O

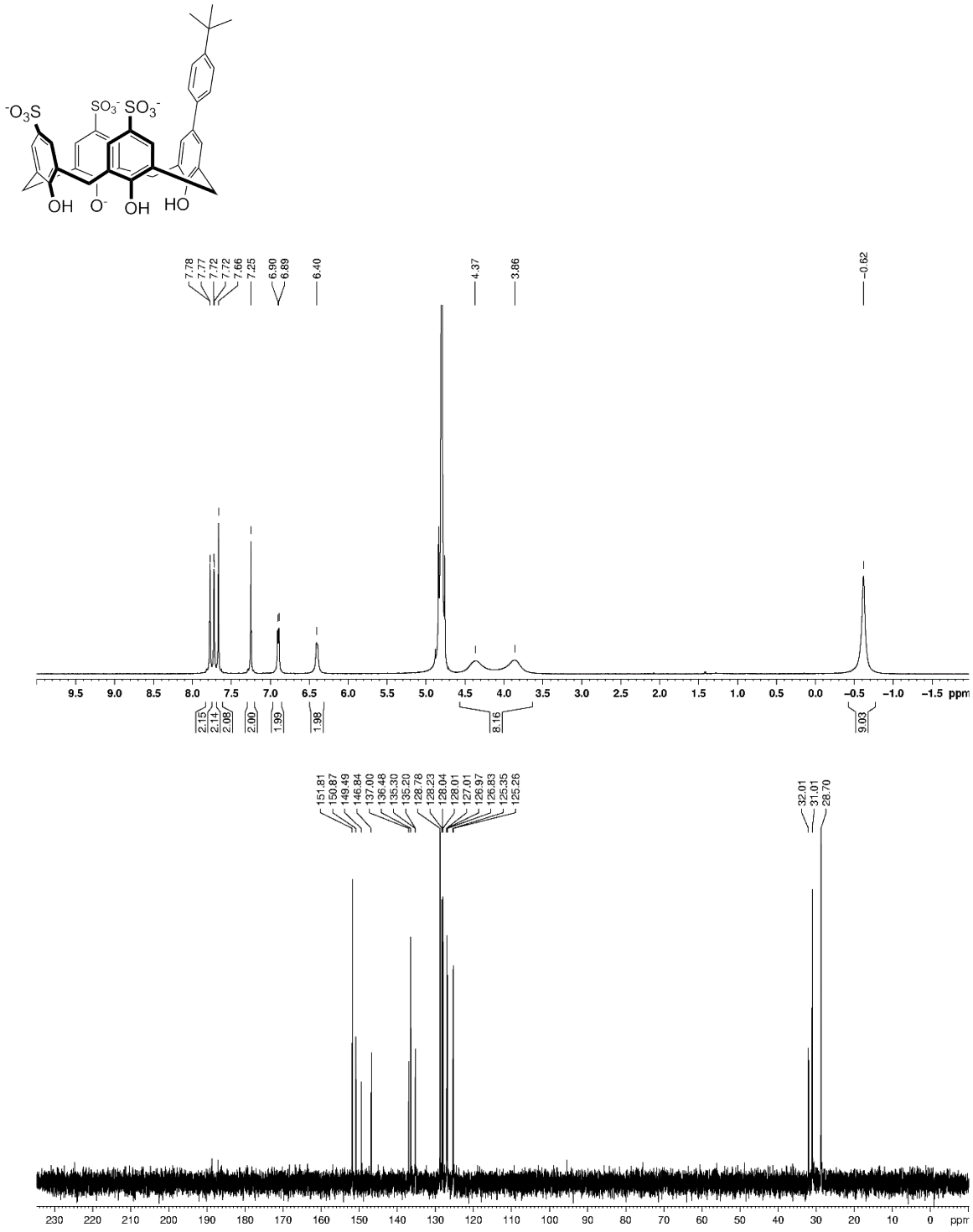


Compound **(ethyl)** (26.0 mM) in D_2O

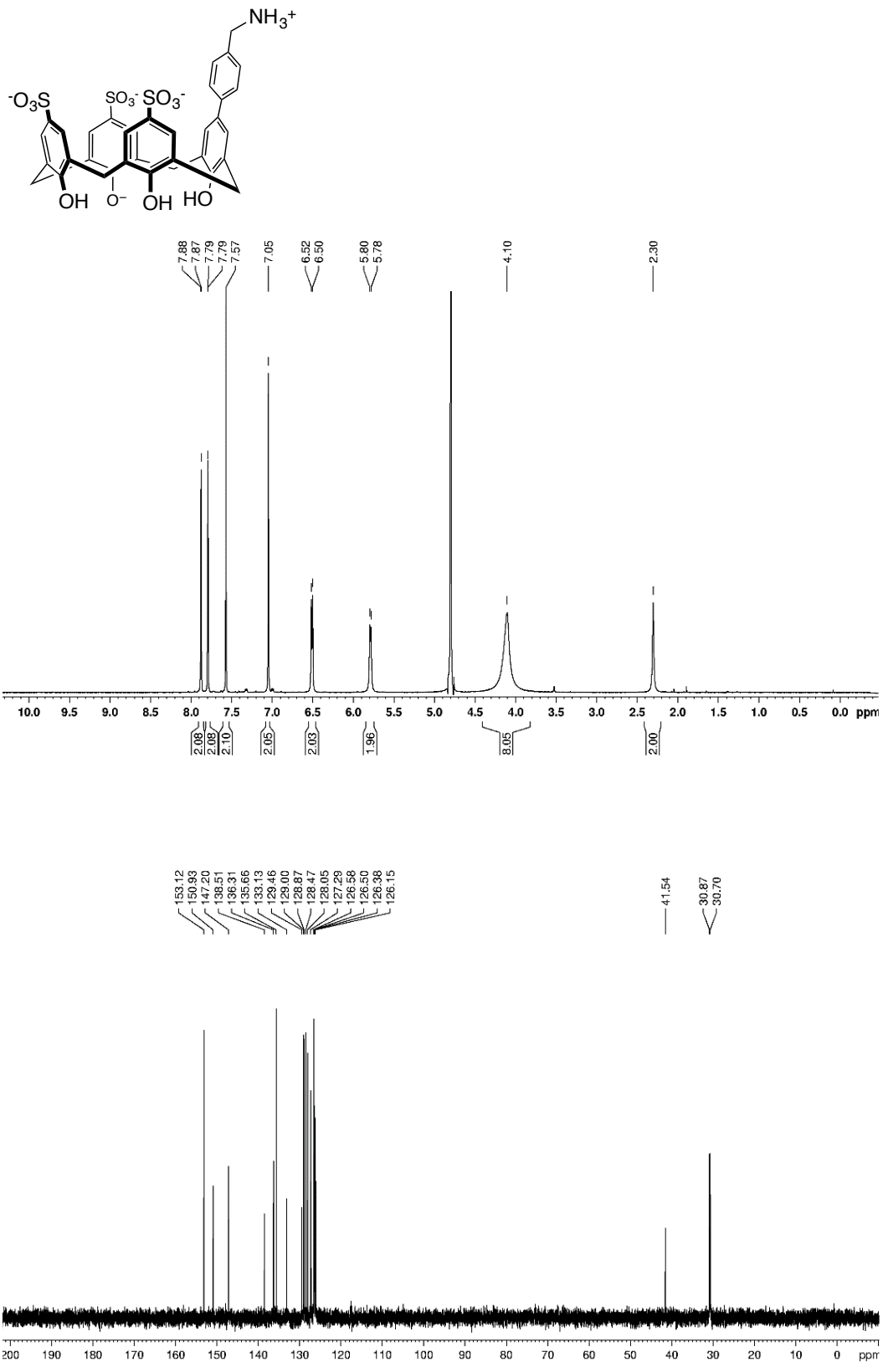




Compound **(isopropyl)** (24.8 mM) in D_2O



Compound **(tbutyl)** (24.0 mM) in D_2O



Compound (**aminomethyl**) (20.4 mM) in D_2O

Supplementary NMR spectra for characterization of assemblies

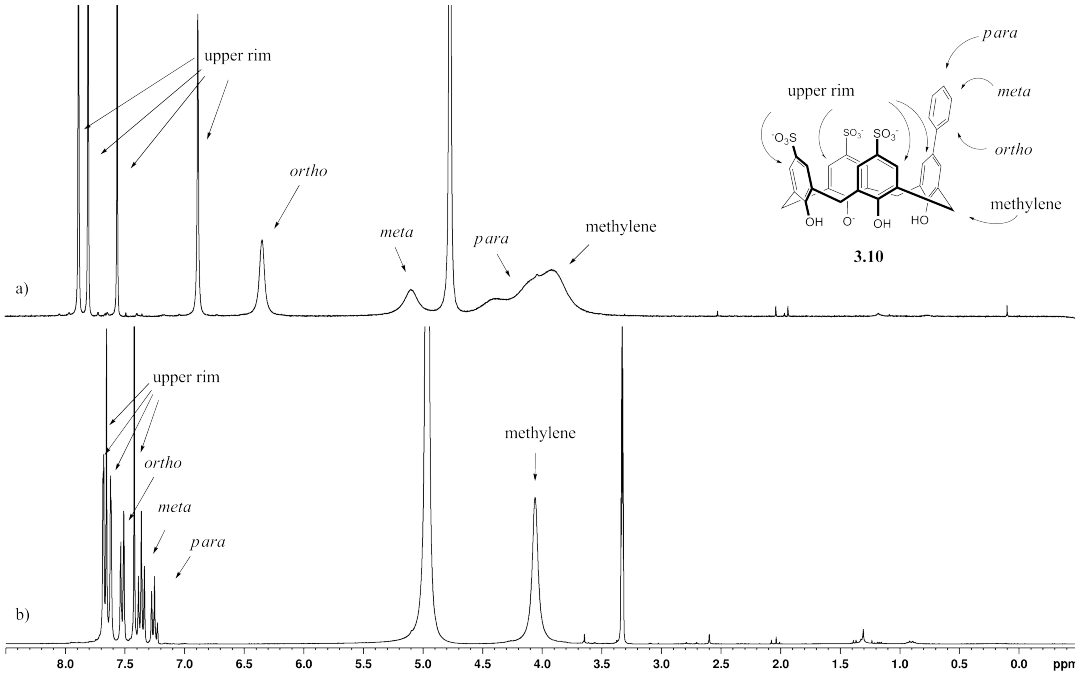


Figure S1. ^{1}H NMR spectra of calixarene 1 in D_2O and CD_3OD shows the solvent dependence on self-association. a) ^{1}H NMR spectra of calixarene **1** in D_2O (25.4 mM) shows upfield shifting of several resonances. b) ^{1}H NMR spectra of the same calixarene **1** in CD_3OD (21.3 mM). The upfield shifting observed in D_2O, is completely absent from the CD_3OD spectra.

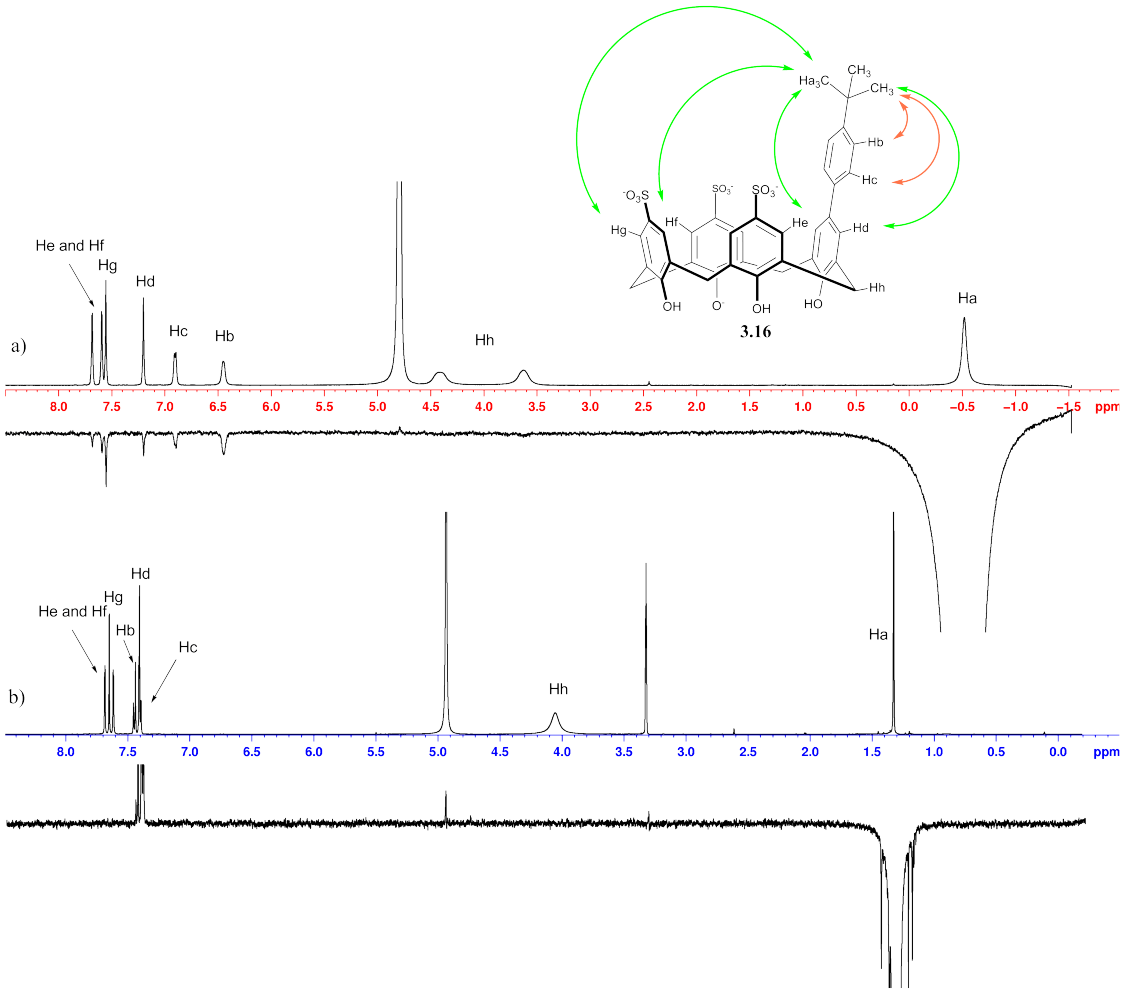


Figure S2. NOE spectra of host 5 **give evidence for assembly in D_2O and not in CD_3OD.** a) 1D ^{1}H NMR and corresponding NOE spectrum of a solution of host **5** in D_2O shows clear NOE correlations between all aromatic protons and the *t*-butyl functionality of the tip of the pendant arm. Orange arrows represent correlations that might be the result of intramolecular NOE, whereas green arrow correlations can only be explained by intermolecular self-association with the *t*-butyl group in contact with the pocket and upper rim of another monomer. b) 1D ^{1}H NMR and corresponding NOE spectrum of host **5** in CD_3OD shows intramolecular NOE contacts to Ha and Hc but not the upper rim protons He, Hf and Hg. No correlations were observed to the methylene protons in either spectrum. X-axes are coloured to highlight that they are scaled differently.

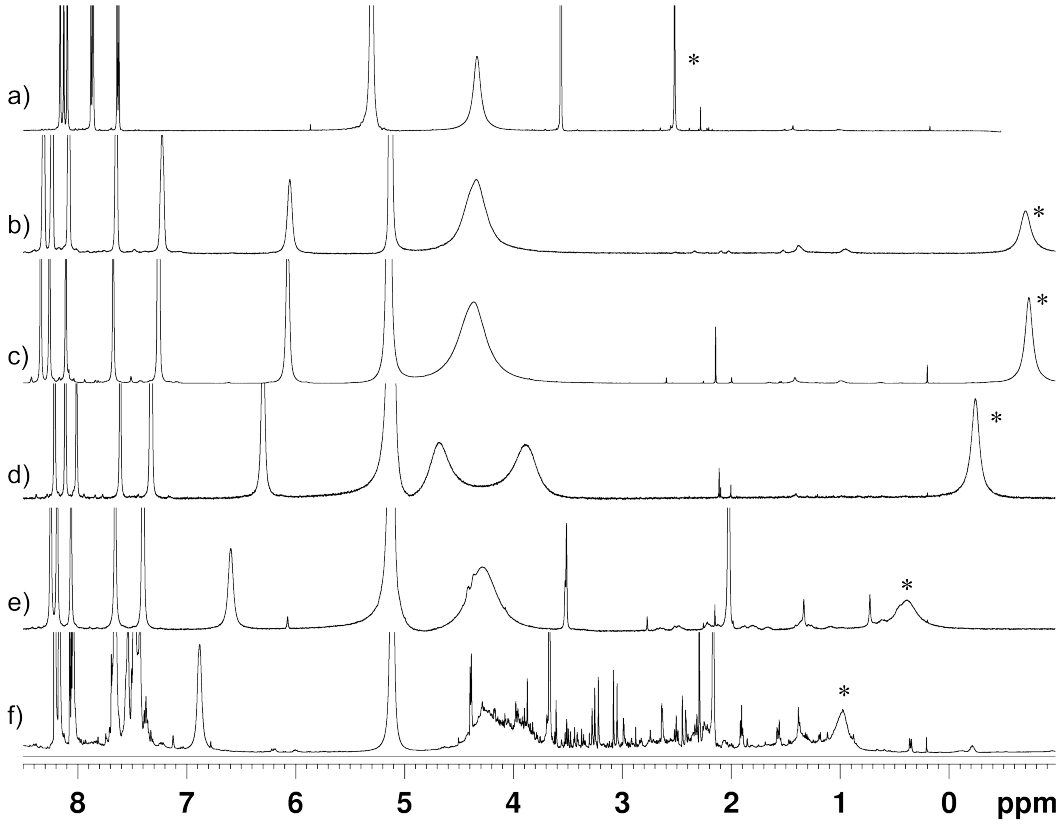
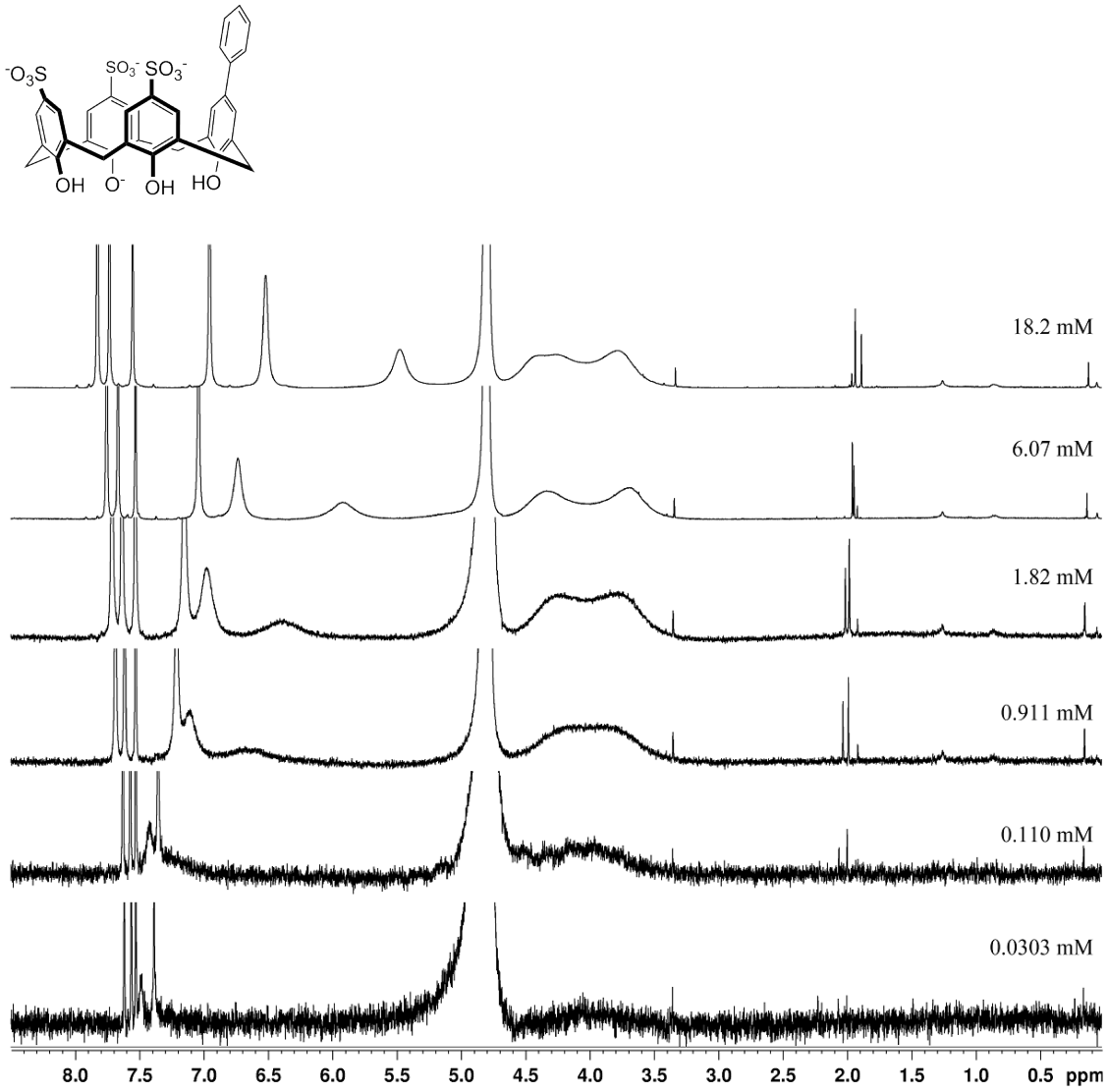


Figure S3. NMR shows that compound 2 assembles in competitive media. NMR spectra of **(2)** in: a) MeOD (22.1 mM) b) D_2O (20.3 mM), c) 100 mM Na_2HPO_4 pD 7.0 (18.4 mM), d) mock serum (100 mM Na_2HPO_4 pD 7.4, 138 mM NaCl, 2.7 mM KCl, 0.5 mM $MgCl_2$, (20.0 mM), e) mock urine (136 mM NaCl, 22.0 mM KCl, 15.1 mM K_2SO_4, 223 mM urea, 13.2 mM creatinine, 0.13 mM corticosterone) (20.0 mM), f) real urine with 10% D_2O (20.0 mM). The key methyl resonance whose shift is diagnostic of assembly is indicated with an asterisk.

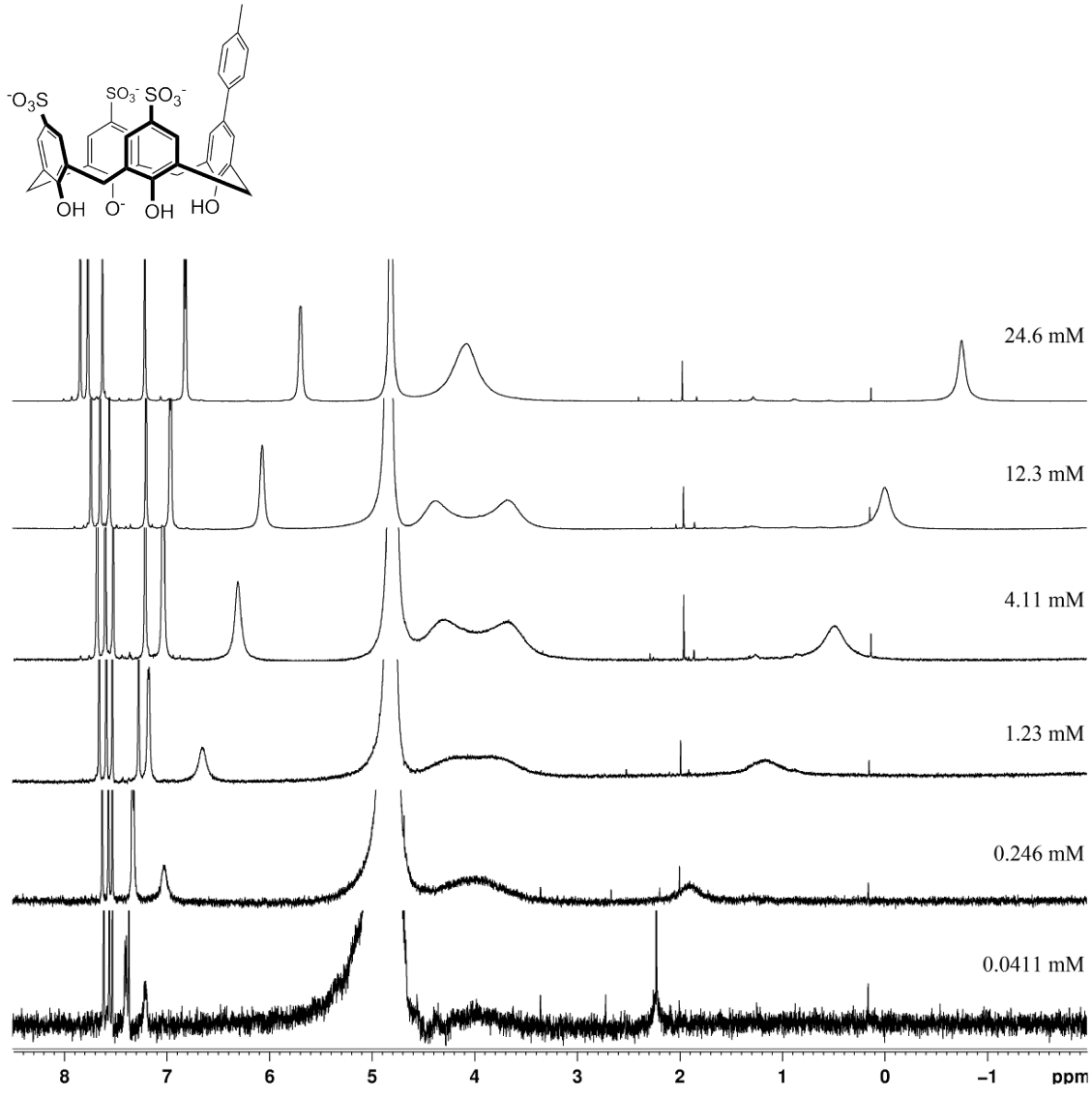
^{1}H NMR Dilution Titrations – Method

All dilution titrations were recorded using a 500 MHz AC Bruker NMR using a BBI probe at 23 °C with the aid of a cassette autosampler. Calixarene samples in buffered D_2O were prepared in 1.5 mL microfuge tubes using an autopipette. Titrations were performed in either unbuffered D_2O, phosphate buffer [100 mM Na_2HPO_4 D_2O (pD 7.0)[3]], or PBS [100 mM Na_2HPO_4 buffered D_2O (pD 7.0) containing 138 mM, NaCl, 2.7 mM KCl, and 0.5 mM $MgCl_2$]. All buffers were prepared from EMD Millipore D_2O, 99.9%.

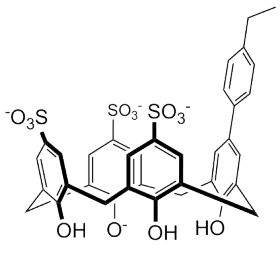
Dilution titrations in phosphate buffer

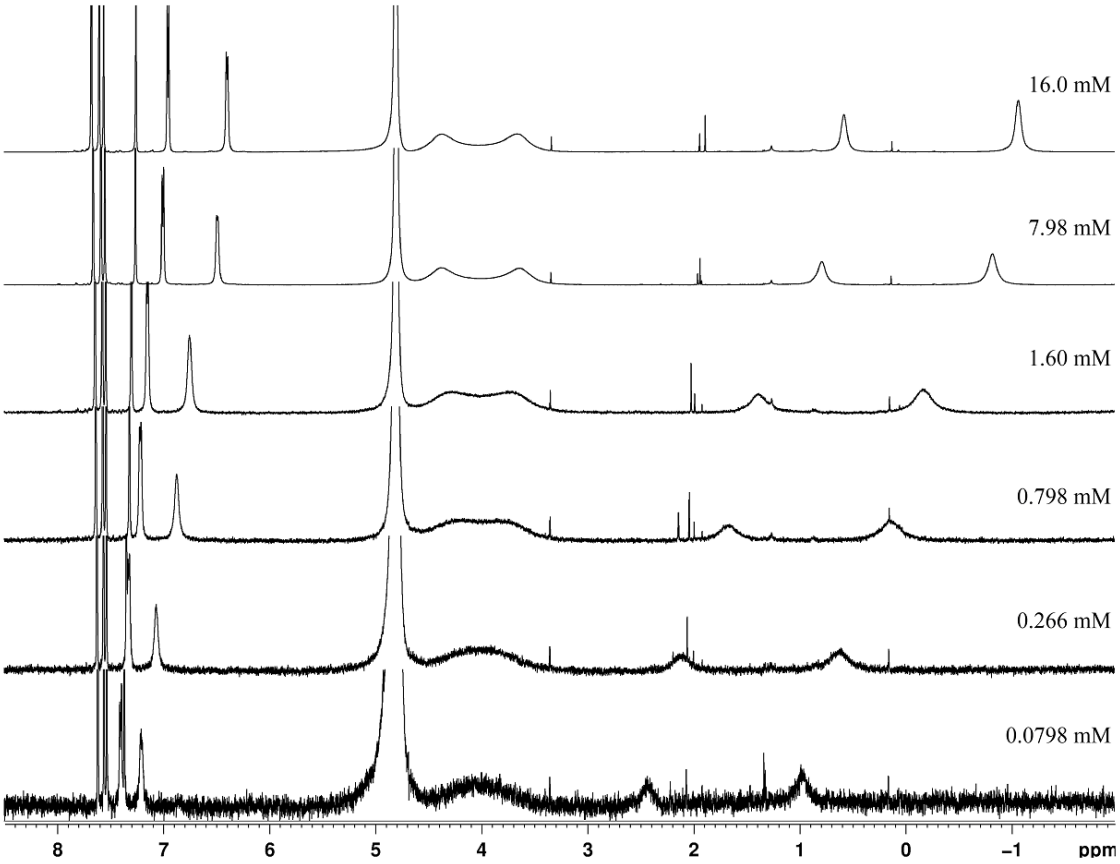


Dilution titration (**phenyl**) in phosphate buffer

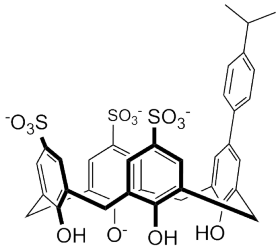


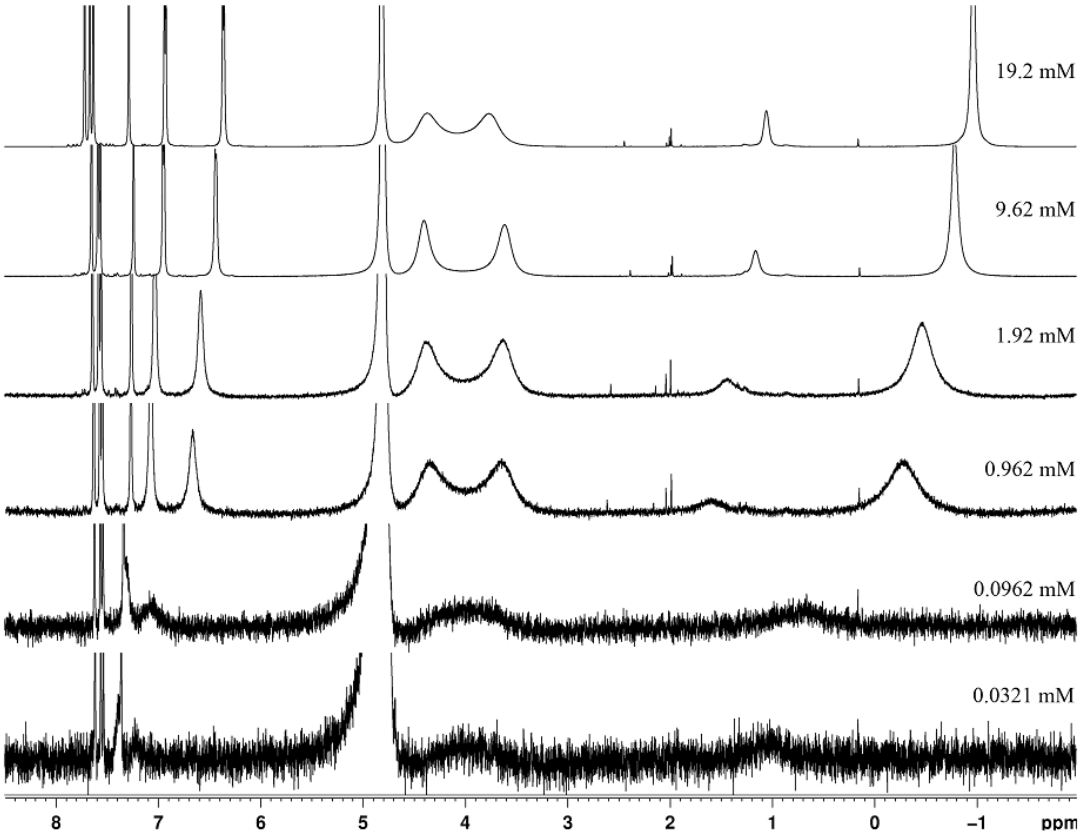
Dilution titration of **(tolyl)** in phosphate buffer



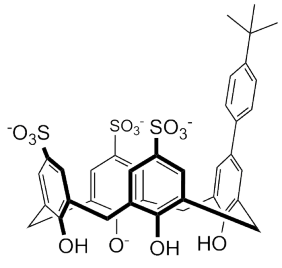


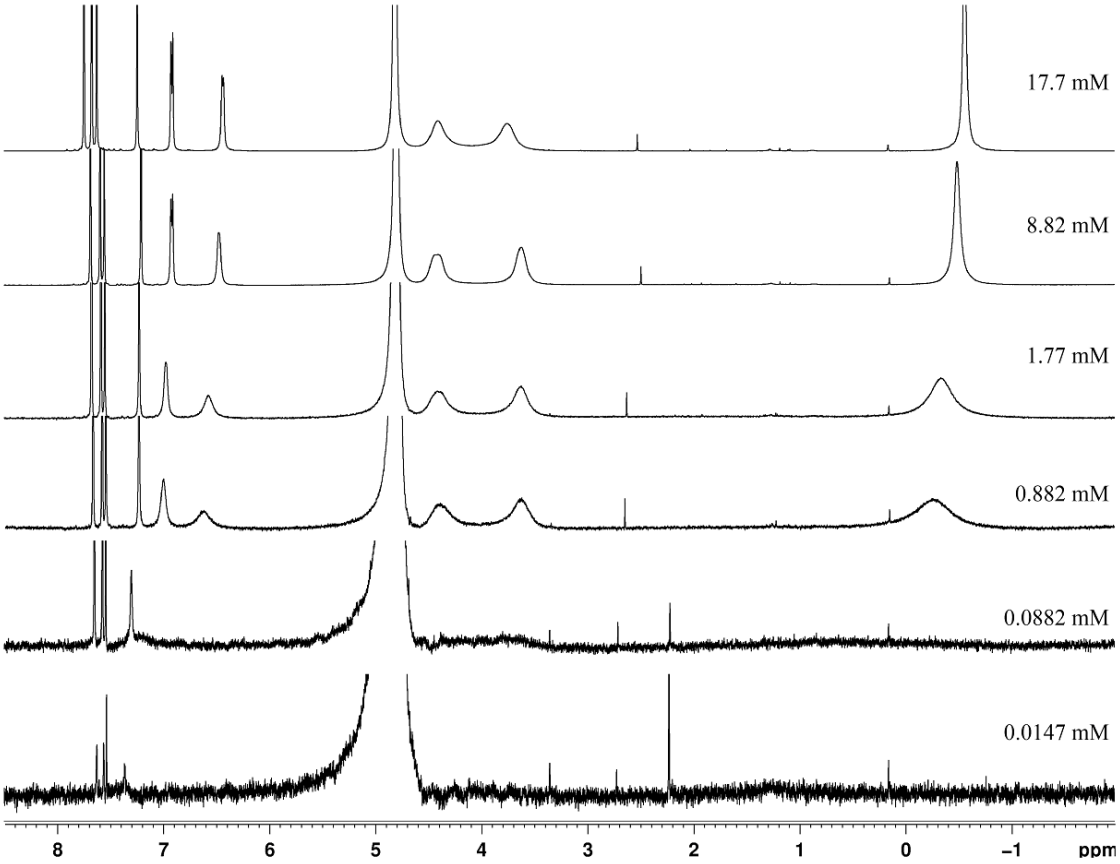
Dilution titration of **(ethyl)** in phosphate buffer



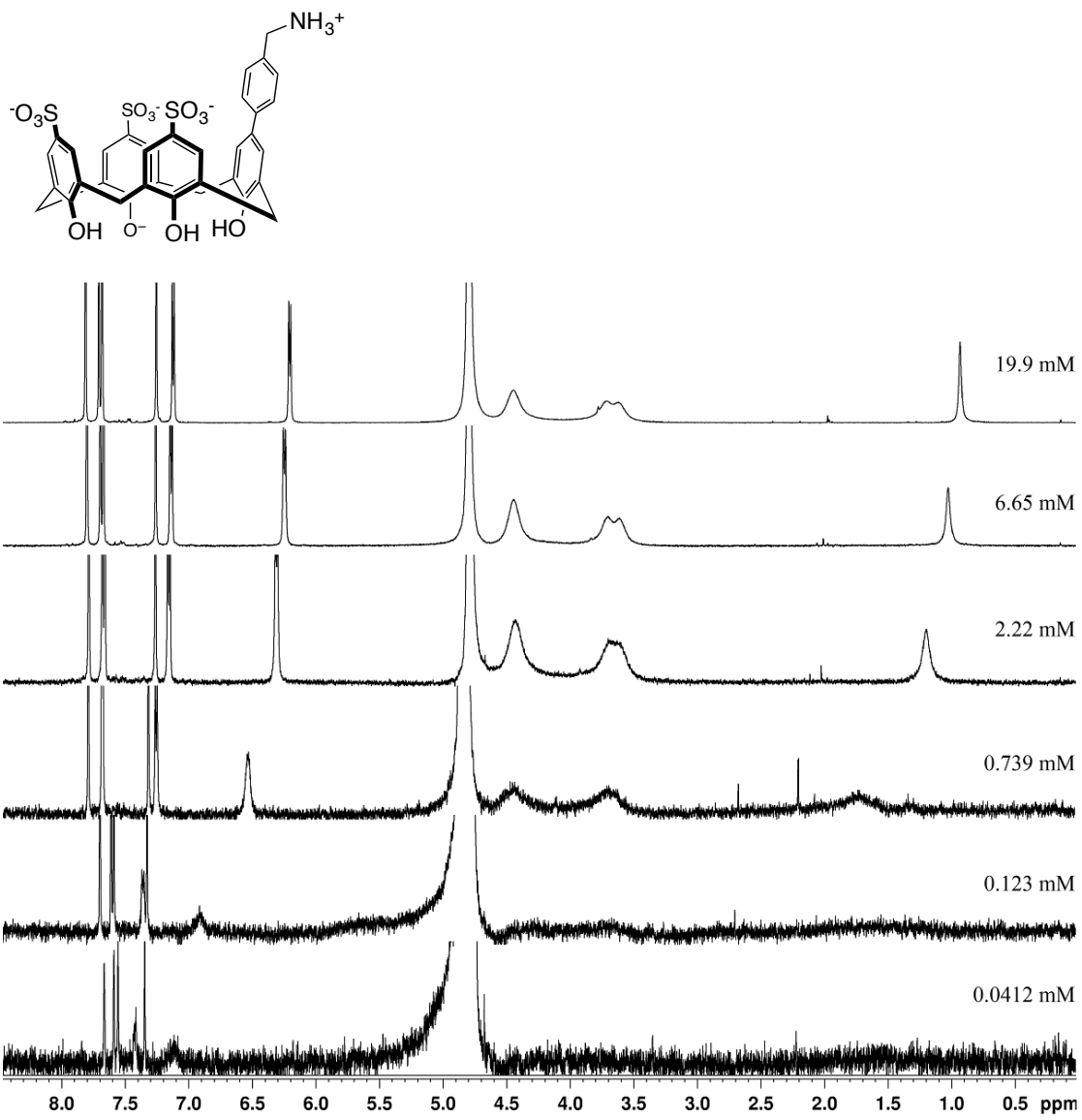


Dilution titration of **(isopropyl)** in phosphate buffer



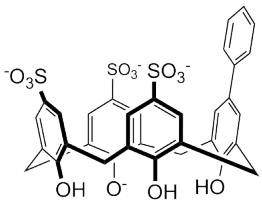


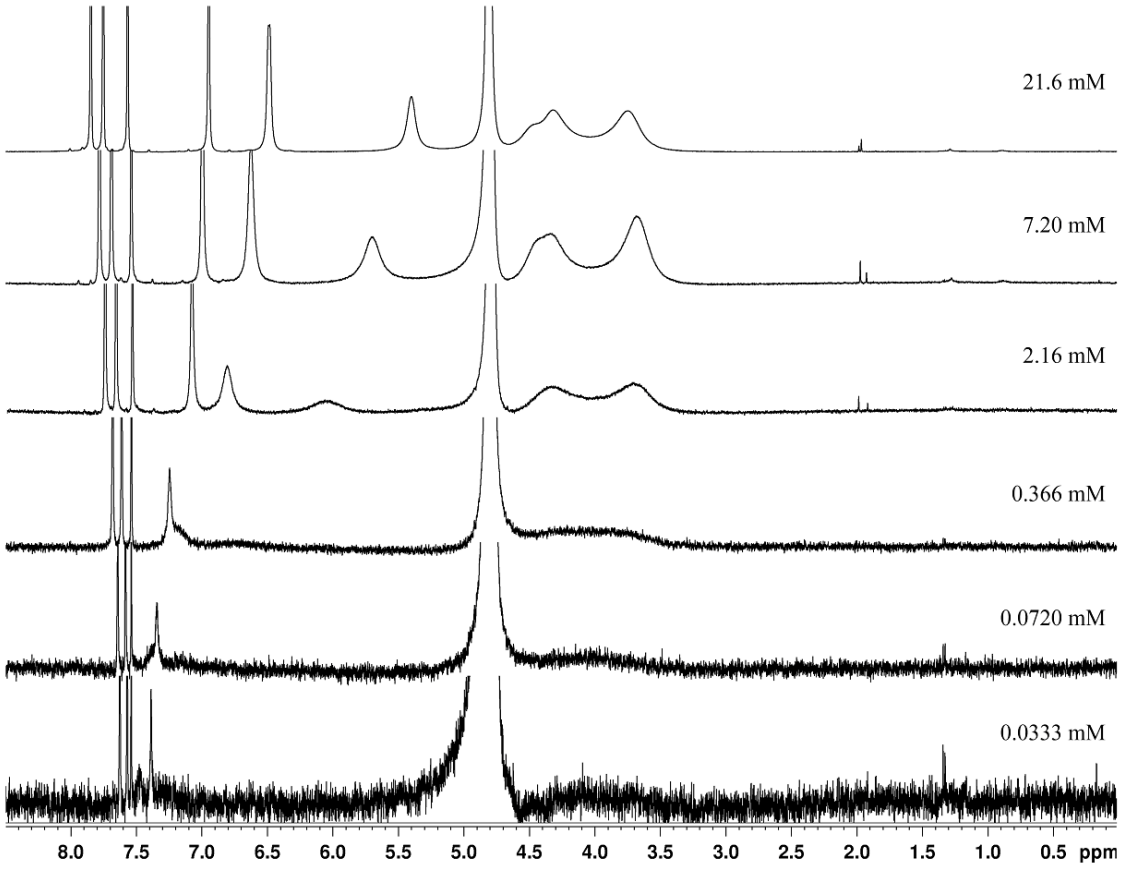
Dilution titration of **(tbutyl)** in phosphate buffer



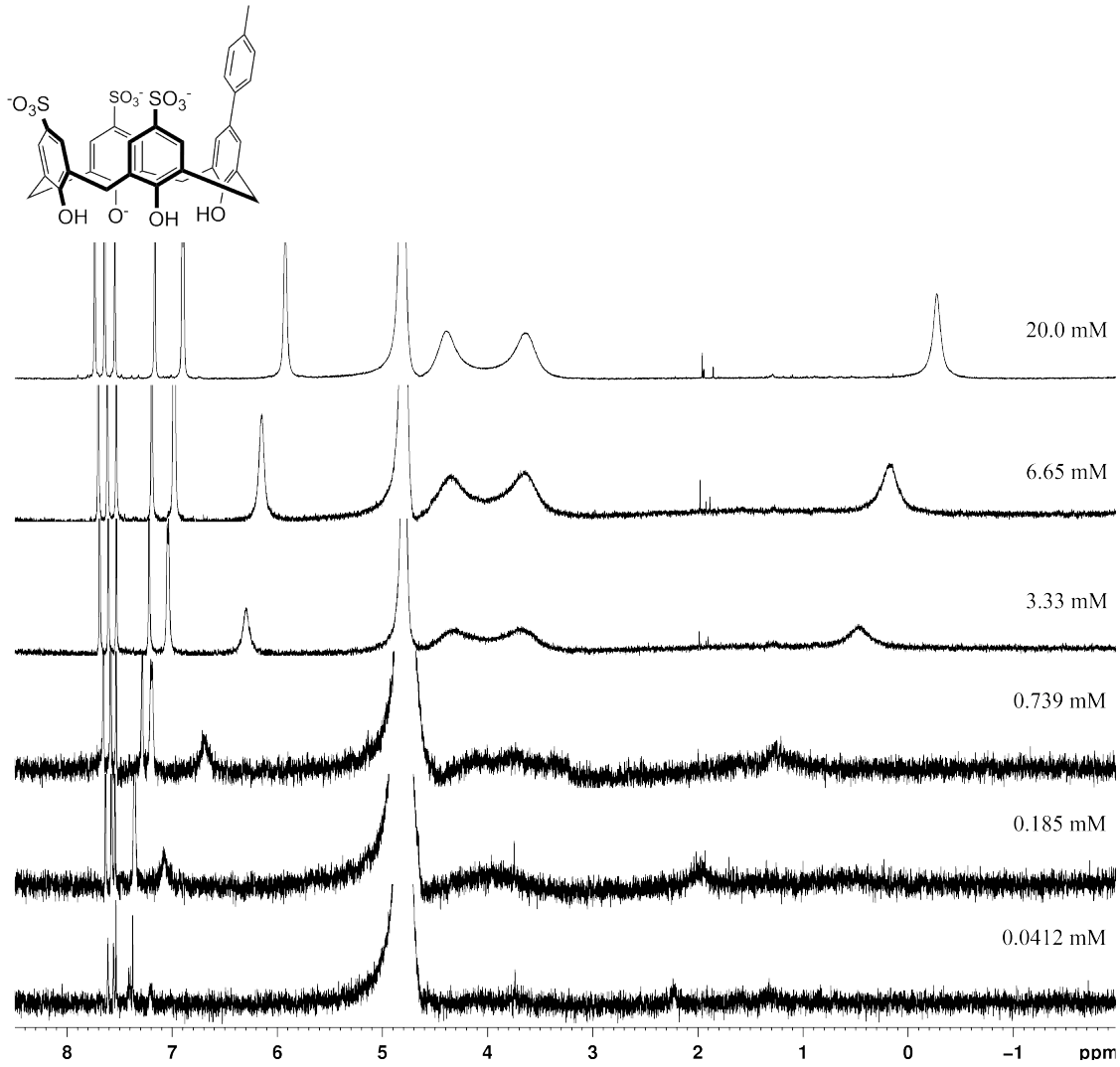
Dilution titration of (**aminomethyl**) in phosphate buffer

Dilution titrations in PBS

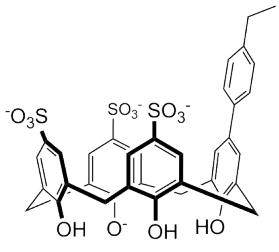


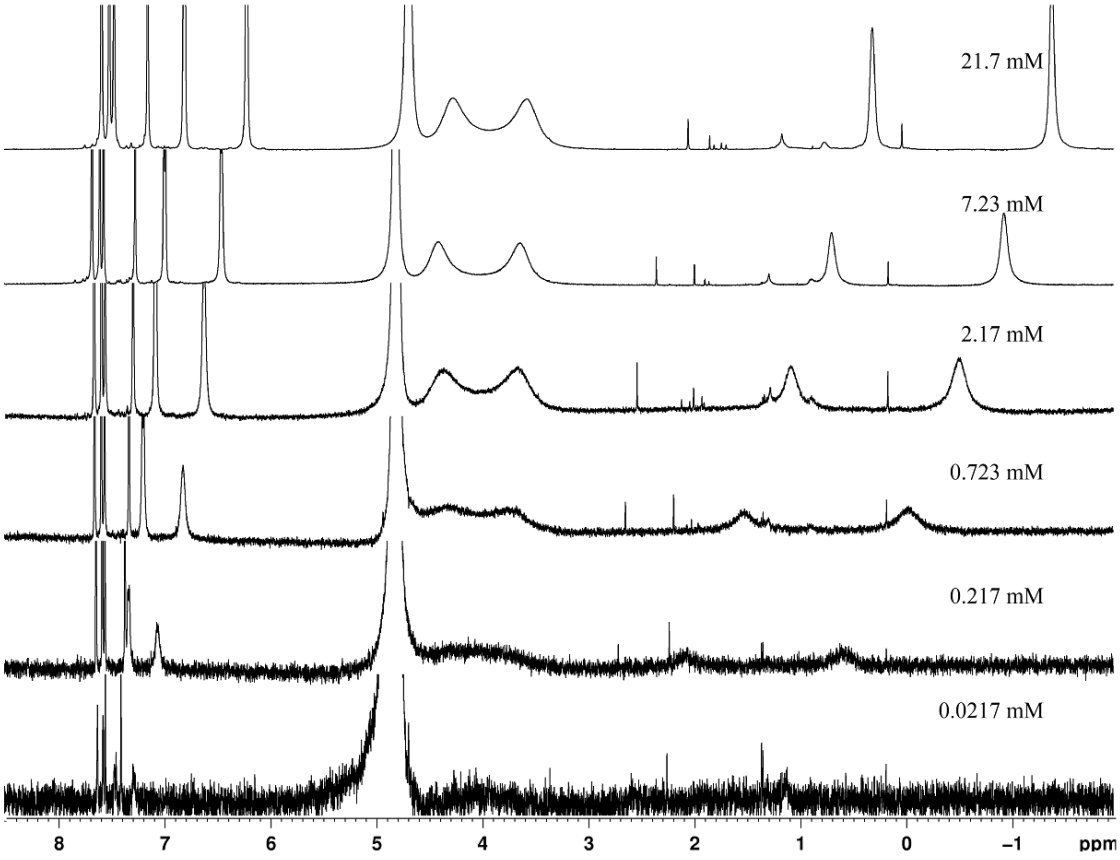


Dilution titration of **(phenyl)** in PBS

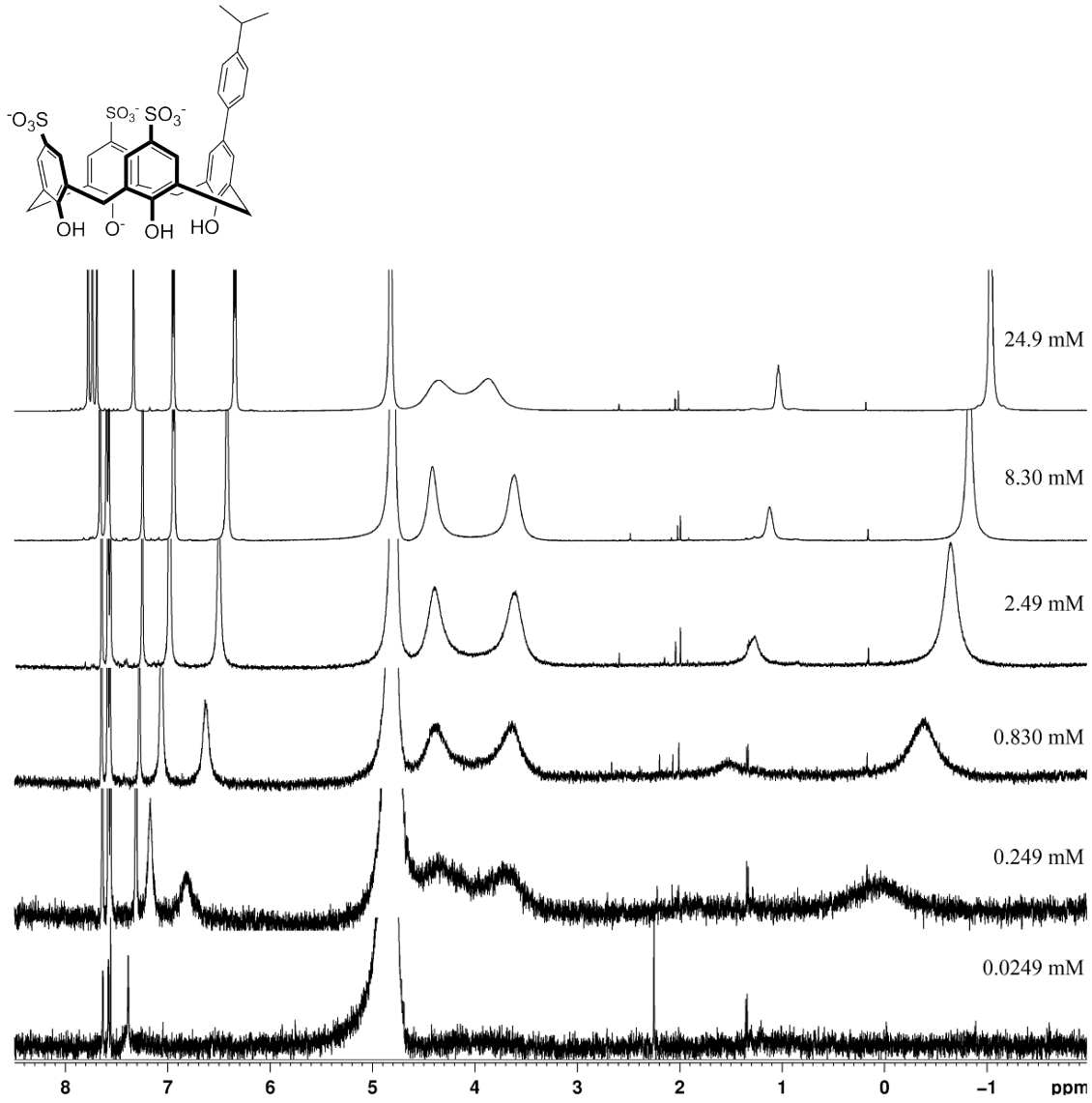


Dilution titration of **(tolyl)** in PBS

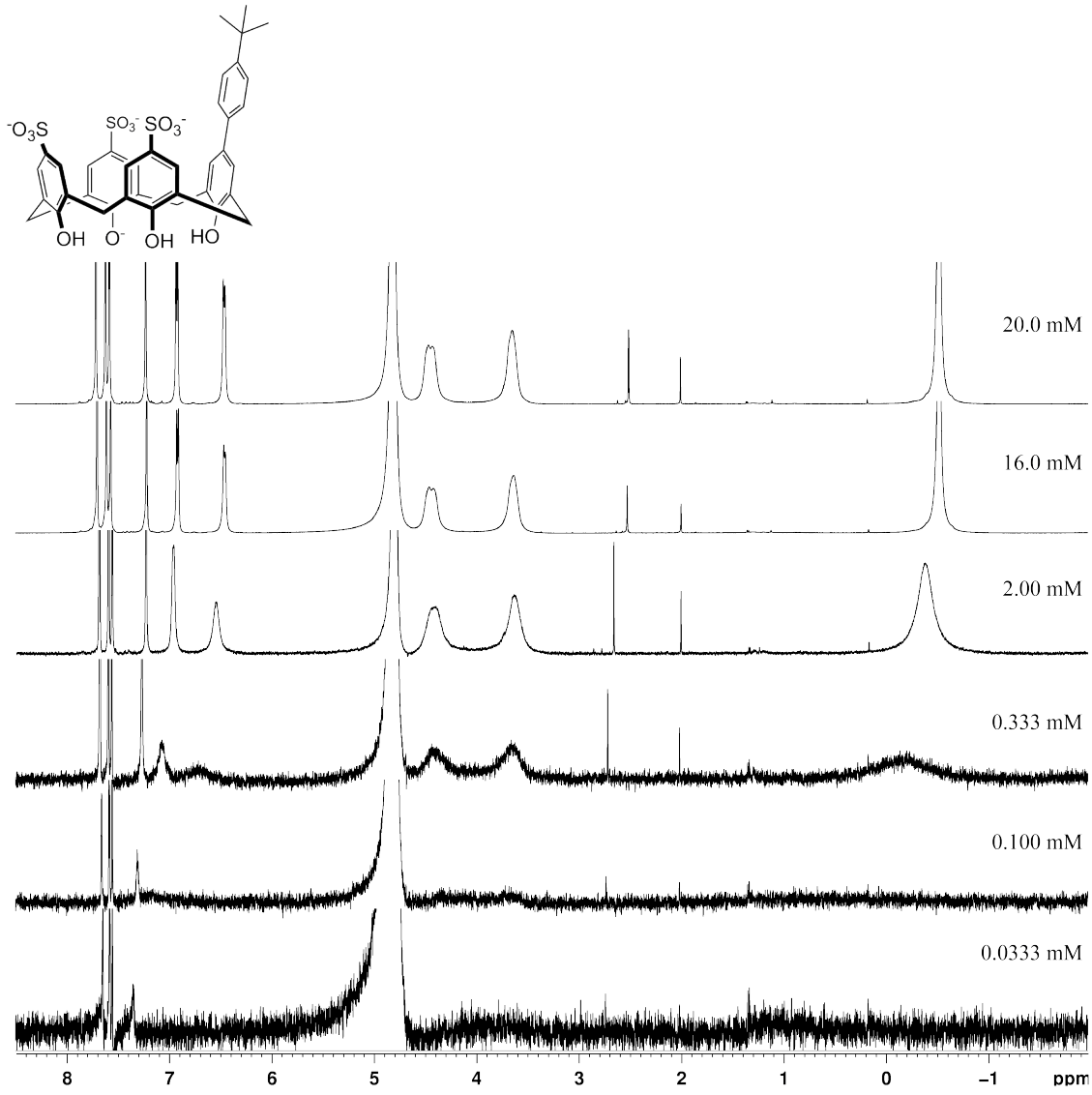




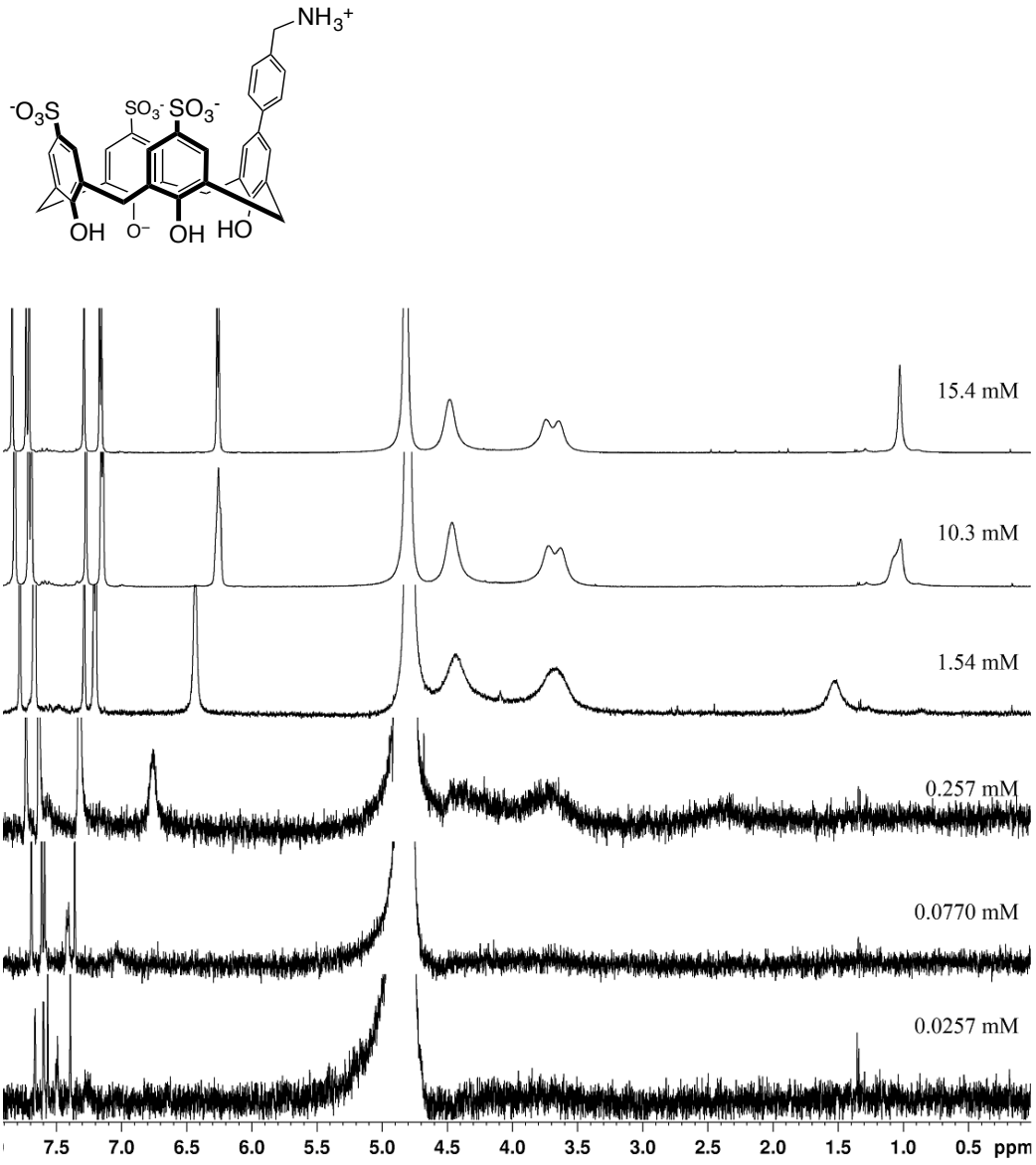
Dilution titration of **(ethyl)** in PBS



Dilution titration **(isopropyl)** in PBS



Dilution titration of **(tbutyl)** in PBS



Dilution titration of **(aminomethyl)** in PBS

X-ray crystallography

Diffraction intensities were collected at 200(2) K on a Bruker Apex2 CCD diffractometer with a micro-focus Incoatec *IμS* tube with CuKα radiation, λ = 1.54178 Å. Space groups were determined based on systematic absences. Absorption corrections were applied by SADABS.[5] Structures were solved by direct methods and Fourier techniques and refined on F2 using full matrix least-squares procedures. All non-H atoms were refined with anisotropic thermal parameters. H atoms were refined in calculated positions in a rigid group model. Although a strong micro-focus Incoatec *IμS* Cu source was used for data collection diffraction from crystals at high angles are very weak and data were collected up to $2\theta_{max}$ = 100 degrees. The structures three calix units are joint via a Na atom located on a 3-fold axis. Two additional Na atoms are in general positions and bonded to solvent water molecules. Relatively big empty space between the mentioned structural units in the crystal structure are filled by disordered solvent water molecules and additional Na atoms needed to provide the charge balance. We could not find solution for this disordered part of the structure and it was treated by SQUEEZE.[6] Corrections of the X-ray data by SQUEEZE 160 electron is close to 127 electron for 12 solvent molecules and 0.666Na atom in the symmetrically independent part. All calculations were performed by the Bruker SHELXTL (v. 6.10) package.[7]

Table S1. Crystal data and structure refinement for cu_hofr7_0m_a (Compound 5).

Identification code	cu_hofr7_0m_a	
Empirical formula	C38 H70 Na3 O32 S3	
Formula weight	1204.09	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Trigonal	
Space group	P-31c	
Unit cell dimensions	a = 27.0902(13) Å	a= 90°.
	b = 27.0902(13) Å	b= 90°.
	c = 30.1891(16) Å	g = 120°.
Volume	19186.9(17) $Å^3$	
Z	12	
Density (calculated)	1.251 Mg/m^3	
Absorption coefficient	1.971 mm^{-1}	
F(000)	7620	
Crystal size	0.14 x 0.12 x 0.09 mm^3	
Theta range for data collection	1.88 to 50.43°.	
Index ranges	-10<=h<=27, -26<=k<=10, -27<=l<=30	
Reflections collected	35587	
Independent reflections	6710 [R(int) = 0.0331]	
Completeness to theta = 50.43°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8425 and 0.7699	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6710 / 0 / 571	
Goodness-of-fit on F^2	1.110	
Final R indices [I>2sigma(I)]	R1 = 0.0794, wR2 = 0.2433	
R indices (all data)	R1 = 0.0989, wR2 = 0.2670	
Largest diff. peak and hole	0.443 and -0.374 $e.Å^{-3}$	

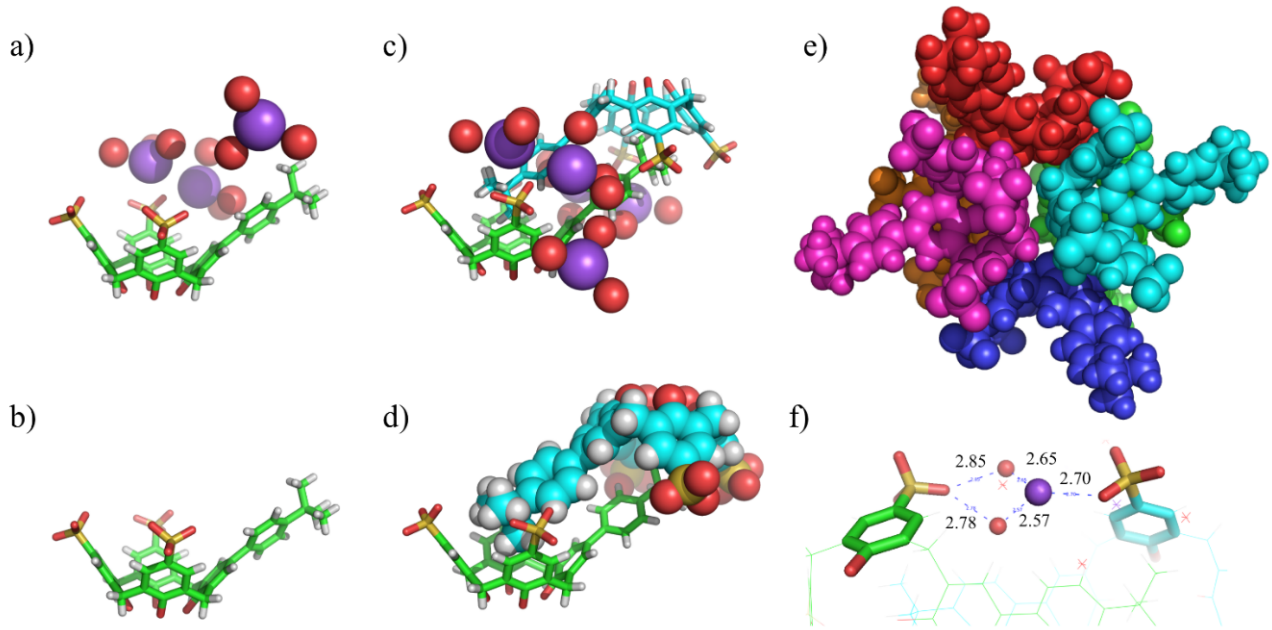


Figure S4. X-ray diffraction crystal structure of compound 5. a) The monomer asymmetric unit with associated Na^+ (purple) and H_2O (red). b) the same monomer structure with Na^+ and H_2O hidden. c) the dimeric interaction adjacent monomers in the crystal, with Na^+ (purple) and H_2O (red). d) the dimeric interaction adjacent monomers in the crystal, space filling model with Na^+ and H_2O hidden. e) the rosette structure of six symmetry-related monomers, with each of the 6 calixarene units colour coded differently. f) hydrogen bonding network between the two sulfonates that approach each other the closest in the solid state dimer, bridged through Na^+ (purple) and H_2O (red)

ITC Titrations – Method

Isothermal titration calorimetry (ITC) dilution titrations of hosts **1-6** were performed on a MicroCal VP-ITC. Buffer solutions were prepared exactly as described for NMR experiments, except using Milli-Q deionized H_2O and with vacuum degassing prior to use. Titrations were performed at 303 K in buffered H_2O by titrating a concentrated sample of calixarene into the sample cell containing a matched solution of blank buffer. The resulting isotherms were fitted to a curve using the manufacturer's supplied fitting equation in Origin using an added correction factor (Qd) as a fittable vertical offset parameter to account for the heat of dimer dilution, which is assumed to be a constant for any given dimer under these experimental conditions. This offset adjustment is described in the literature.[4]

Gas-phase calculations

At the request of a referee the charge density of relevant anions, and repulsive forces experienced by monomers of **5** were calculated. The volume of each anion was determined from the crystallographically determined structure (for **5**) or from the energy-minimized structure (for Cl^-, HPO_4^-, TsO^-) in Spartan '12 (HF 6-31G+*).

Table S2. Charge density of **5** compared to other relevant anions.

Anion	Charge	Volume (nm^3)	Charge density (nm^{-3})
Calixarene monomer **5**	–4	0.677	–5.91
p-toluenesulfonate	–1	0.153	–6.54
$H_2PO_4^-$	–1	0.068	–14.60
Cl^-	–1	0.023	–43.48

The Coulombic interaction potential energies for adjacent monomers of **5** were calculated using atomic partial charges (HF 6-31G+*) and the atomic coordinates from the X-ray structure of **5** with waters and counterions removed. The sum of all intermolecular Coulombic interaction energies between all atoms in monomer A and all atoms in monomer B was calculated as:

$$U = \frac{1}{4\pi\varepsilon_0\varepsilon}\sum q_A q_B / r$$

In gas phase: U = +362 kcal/mol

In water: U = +4.5 kcal/mol (using ε = 80.1 for H_2O at 20°C)

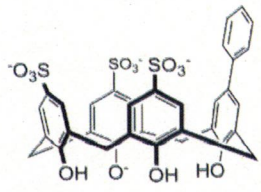
References

1. Daze, K. D.; Ma, M. C. F.; Pineux, F.; Hof, F., Synthesis of New Trisulfonated Calix[4]arenes Functionalized at the Upper Rim, and Their Complexation with the Trimethyllysine Epigenetic Mark. *Org. Lett.* **2012,** *14*, 1512-1515.
2. Tabet, S.; Douglas, S. F.; Daze, K. D.; Garnett, G. A. E.; Allen, K. J. H.; Abrioux, E. M. M.; Quon, T. T. H.; Wulff, J. E.; Hof, F., Synthetic trimethyllysine receptors that bind histone 3, trimethyllysine 27 (H3K27me3) and disrupt its interaction with the epigenetic reader protein CBX7. *Bioorg. Med. Chem.* **2013,** *21* (22), 7004-7010.
3. Glasoe, P. K.; Long, F. A., Use of a glass electrode to measure acidities in deuterium oxide. *J. Phys. Chem.* **1960,** *64* (1), 188-190.
4. Velazquez-Campoy, A.; Leavitt, S.; Freire, E., Characterization of Protein-Protein Interactions by Isothermal Titration Calorimetry. In *Protein-Protein Interactions*, Fu, H., Ed. Humana Press: 2004; Vol. 261, pp 35-54.
5. Sheldrick, G. M. *SADABS v. 2.01, Bruker/Siemens area detector absorption correction program*, Bruker/AXS: Madison, WI, USA, 1998.
6. Van der Sluis, P. V.; Spek, A. L., BYPASS: an effective method for the refinement of crystal structures containing disordered solvent regions. *Acta Crystallographica Section A: Foundations of Crystallography* **1990,** *46* (3), 194-201.
7. *SHELXTL-6.10 "Program for Structure Solution, Refinement and Presentation"*, BRUKER AXS Inc.: 5465 East Chery Parkway, Madison WI, 53711-5373 USA.

Host - 1x phenyl 3x HSO3 c4a
100mM Phosphate buffer, pH 7.4

PHOS

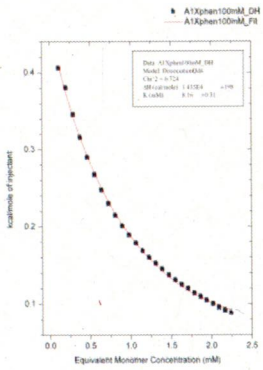
Compound 1



Oct 8b
Data: A1Xphen100mM_DH
Model: DissociationQd4
Chi^2 = 6.724

DH (cal/mc	1.44E+04	198
K (mM)	8.16	0.31

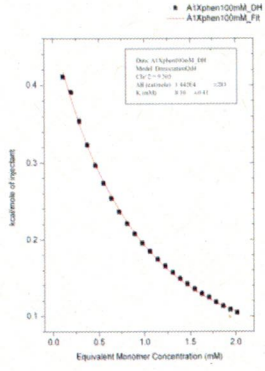
-119.1665 <--Qd



Oct 9a
no L trim, 3 points R
Data: A1Xphen100mM_DH
Model: DissociationQd4
Chi^2 = 9.305

DH (cal/mc	1.44E+04	283
K (mM)	8.10	0.41

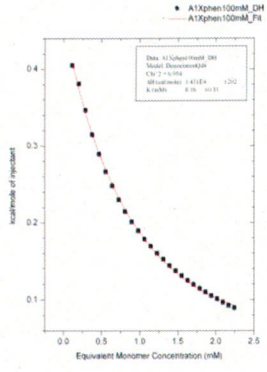
-114.6333 <--Qd



Oct9b
no trim
Data: A1Xphen100mM_DH
Model: DissociationQd4
Chi^2 = 6.954

DH (cal/mc	1.43E+04	202
K (mM)	8.16	0.31

-118.285 <--Qd



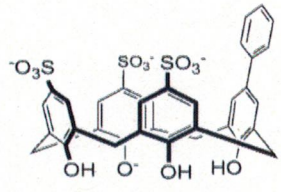
100mM phosphate deltG= -RT ln(keq) 303.15K

	Average		SD	%RSD		
Kd	8.14	mM	0.028284	0.347473		avg
Keq (M-1)	122.8501	/M			qd (kcal	-117.3616
						avg
ΔH	-14.36	kcal/mol	0.045461	0.316578	Kd uncert	0.343333
ΔG	-2.894745	kcal/mol			ΔH uncert	227.6667
(-)TΔS	11.46525	kcal/mol				
ΔS	-0.037839	cal/K				

Host - 1x phenyl 3x HSO3 c4a
100mM PBS, pH 7.4

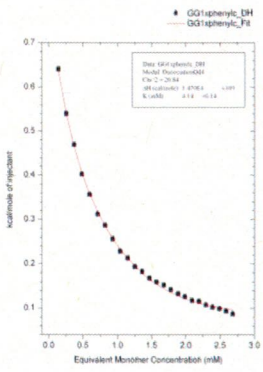
PBS

Compound 1



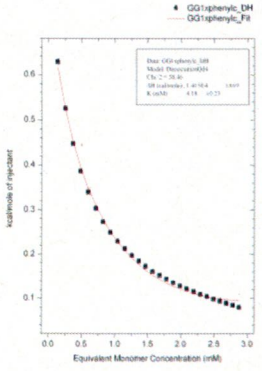
Sept17a
Data: GG1xphenylc_DH
Model: DissociationQd4
Chi^2 = 20.84

DH (cal/mc	1.47E+04	109
K (mM)	4.14	0.14
-169.4674		



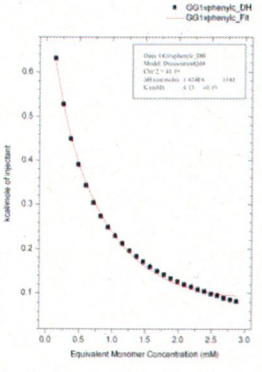
Sept17b
Data: GG1xphenylc_DH
Model: DissociationQd4
Chi^2 = 58.46

DH (cal/mc	1.42E+04	169
K (mM)	4.18	0.23
-159.3087		



Sept18a
Data: GG1xphenylc_DH
Model: DissociationQd4
Chi^2 = 41.19

DH (cal/mc	1.42E+04	141
K (mM)	4.13	0.19
-161.3823		



100mM PBS deltG= -RT ln(keq) 303.15K

	Average		SD	%RSD
Kd	4.15	mM	0.02	0.520541
Keq (M-1)	240.96	/M		
ΔH	-14.36	kcal/mol	0.24	1.677034
ΔG	-3.30	kcal/mol		
(-)TΔS	11.06	kcal/mol		
ΔS	-0.037	cal/K		

	avg
qd (kcal	-163.39

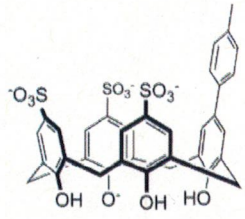
	avg
Kd uncert	0.186667
ΔH uncert	139.6667

Host - 1x tolyl 3x HSO3 c4a

100mM Phosphate buffer, pH 7.4

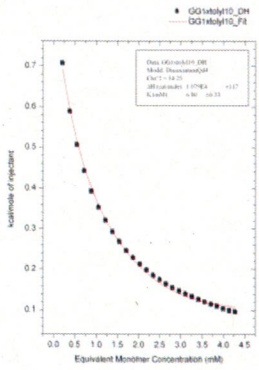
PHOS

Compound 2



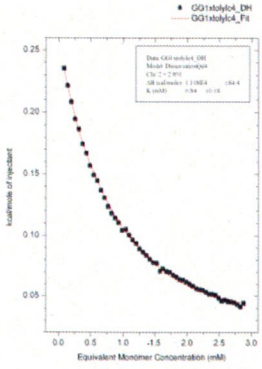
June24a
Data: GG1xtolyl10_DH
Model: DissociationQd4
Chi^2 = 54.25

DH (cal/mc	1.08E+04	117
K (mM)	6.8	0.33
-182.1398		



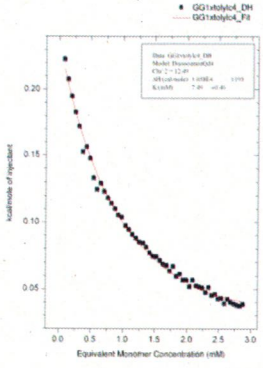
June18A
Data: GG1xtolylc4_DH
Model: DissociationQd4
Chi^2 = 2.891

DH (cal/mc	1.11E+04	84.4
K (mM)	6.84	0.18
-58.69822		



June18B
Data: GG1xtolylc4_DH
Model: DissociationQd4
Chi^2 = 12.49

DH (cal/mc	1.06E+04	195
K (mM)	7.49	0.46
-58.53054		



100mM phosphate deltG= -RT ln(keq) 303.15K

	Average		SD	%RSD
Kd	7.04	mM	0.32	4.490245
Keq (M-1)	141.98	/M		
ΔH	-10.82	kcal/mol	0.20	1.895161
ΔG	-2.98	kcal/mol		
(-)TΔS	7.83	kcal/mol		
ΔS	-0.026	cal/K		

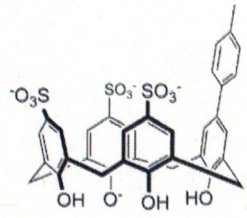
	avg
qd (kcal	-99.79

	avg
Kd uncert	0.323333
ΔH uncert	132.1333

Host - 1x tolyl 3x HSO3 c4a
100mM PBS buffer, pH 7.4

PBS

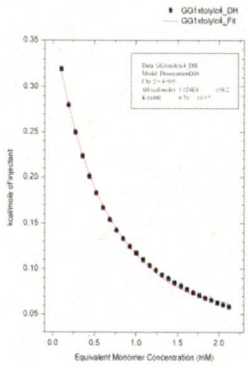
Compound 2



Sept5b
Data: GG1xtolylc4_DH
Model: DissociationQd4
Chi^2 = 4.995

DH (cal/mc	1.02E+04	98.2
K (mM)	4.7	0.17

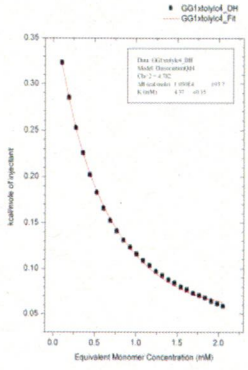
-77.56357



Spept 6A
Data: GG1xtolylc4_DH
Model: DissociationQd4
Chi^2 = 4.782

DH (cal/mc	1.03E+04	93.7
K (mM)	4.37	0.15

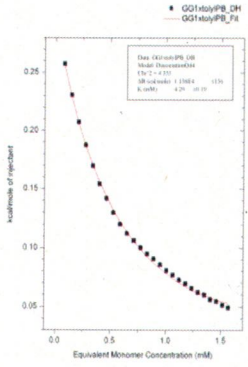
-77.79667



Nov28a
Data: GG1xtolylPB_DH
Model: DissociationQd4
Chi^2 = 4.355

DH (cal/mc	1.14E+04	156
K (mM)	4.29	0.19

-68.30582



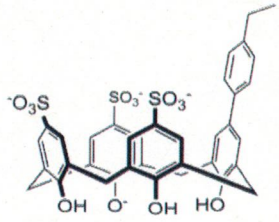
100mM PBS deltG= -RT ln(keq) 303.15K

	Average		SD	%RSD	
Kd	4.45	mM	0.18	3.98468	
Keq (M-1)	224.55	/M			
					avg
					qd (kcal -74.56
					avg
ΔH	-10.64	kcal/mol	0.52	4.923233	**Kd uncert** 0.17
ΔG	-3.26	kcal/mol			**ΔH uncert** 115.9667
(-)TΔS	7.38	kcal/mol			
ΔS	-0.024	cal/K			

Host - 1x ethyphenyl 3x HSO3 c4a
100mM Phosphate buffer, pH 7.4

PHOS

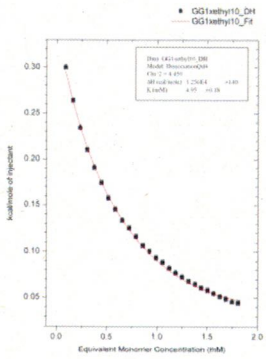
Compound 3



Dec-26
Data: GG1xethyl10_DH
Model: DissociationQd4
Chi^2 = 4.459

DH (cal/mc	1.26E+04	140
K (mM)	4.95	0.18

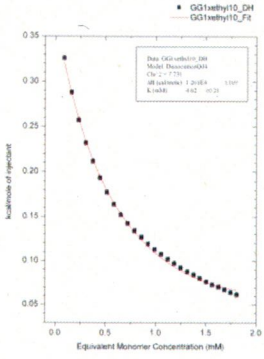
-100.613



Dec27a
Data: GG1xethyl10_DH
Model: DissociationQd4
Chi^2 = 7.731

DH (cal/mc	1.26E+04	169
K (mM)	4.62	0.21

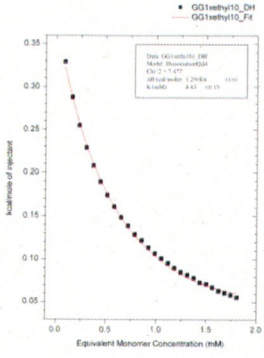
-81.24548



Dec27b
Data: GG1xethyl10_DH
Model: DissociationQd4
Chi^2 = 7.477

DH (cal/mc	1.29E+04	160
K (mM)	4.45	0.19

-90.77656



100mM phosphate deltG= -RT ln(keq) 303.15K

	Average		SD	%RSD
Kd	4.67	mM	0.21	4.441768
Keq (M-1)	213.98	/M		
ΔH	-12.69	kcal/mol	0.15	1.181157
ΔG	-3.23	kcal/mol		
(-)TΔS	9.46	kcal/mol		
ΔS	-0.031	cal/K		

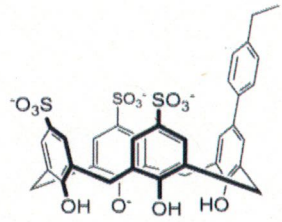
	avg
qd (kcal	-90.88

	avg
Kd uncert	0.193333
ΔH uncert	156.3333

Host - 1x ethyphenyl 3x HSO3 c4a
100mM PBS, pH 7.4

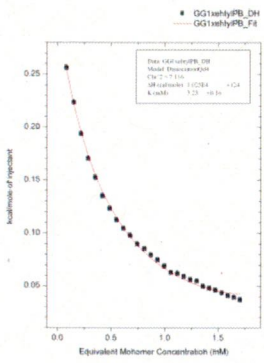
PBS

Compound 3



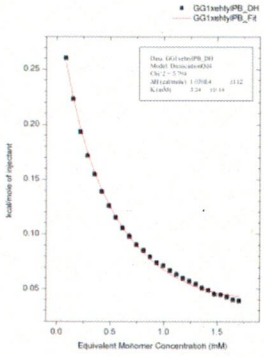
Nov 26a
Data: GG1xehtylPB_DH
Model: DissociationQd4
Chi^2 = 7.116

DH (cal/mc	1.03E+04	124
K (mM)	3.23	0.16
-69.63248		



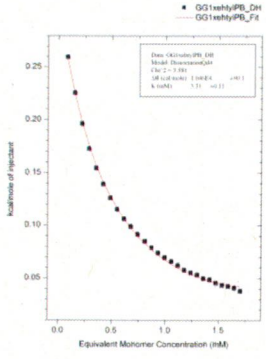
Nov 27a
Data: GG1xehtylPB_DH
Model: DissociationQd4
Chi^2 = 5.794

DH (cal/mc	1.03E+04	112
K (mM)	3.24	0.14
-69.0608		



Nov27b
Data: GG1xehtylPB_DH
Model: DissociationQd4
Chi^2 = 3.581

DH (cal/mc	1.05E+04	90.1
K (mM)	3.31	0.11
-72.12943		



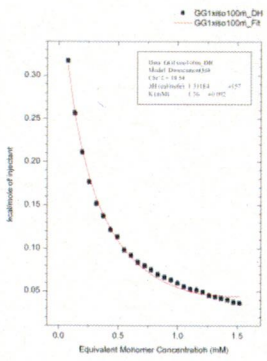
100mM PBS deltG= -RT ln(keq) 303.15K

	Average		SD	%RSD
Kd	3.26	mM	0.04	1.091726
Keq (M-1)	306.75	/M		
ΔH	-10.34	kcal/mol	0.09	0.866497
ΔG	-3.45	kcal/mol		
(-)TΔS	6.89	kcal/mol		
ΔS	-0.023	cal/K		

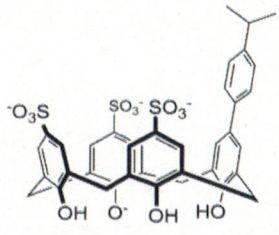
	avg
qd (kcal	-70.27

	avg
Kd uncert	0.136667
ΔH uncert	108.7

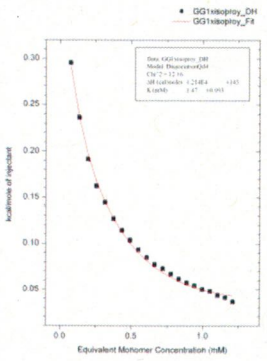
Host - 1x isopropylphenyl 3x HSO3 c4a
100mM Phosphate buffer, pH 7.4



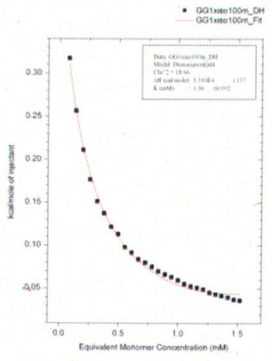
PHOS
Compound 4



Nov17a		
Data: GG1xiso100m_DH		
Model: DissociationQd4		
Chi^2 = 18.54		
DH (cal/mc	1.31E+04	157
K (mM)	1.56	0.092
-77.27094		



Nov18b		
Data: GG1xisoproy_DH		
Model: DissociationQd4		
Chi^2 = 12.16		
DH (cal/mc	1.21E+04	145
K (mM)	1.47	0.093
-70.47738		



Nov-20		
Data: GG1xiso100m_DH		
Model: DissociationQd4		
Chi^2 = 18.66		
DH (cal/mc	1.31E+04	157
K (mM)	1.56	0.092
-77.17424		

100mM phosphate deltG= -RT ln(keq) 303.15K

	Average		SD	%RSD
Kd	1.53	mM	0.04	2.772968
Keq (M-1)	653.59	/M		
ΔH	-12.78	kcal/mol	0.45	3.558725
ΔG	-3.90	kcal/mol		
(-)TΔS	8.88	kcal/mol		
ΔS	-0.029	cal/K		

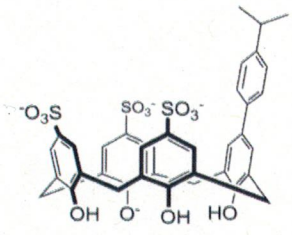
	avg
qd (kcal	-74.97

	avg
Kd uncert	0.092333
ΔH uncert	153

Host - 1x isopropylphenyl 3x HSO3 c4a
100mM PBS, pH 7.4

PBS

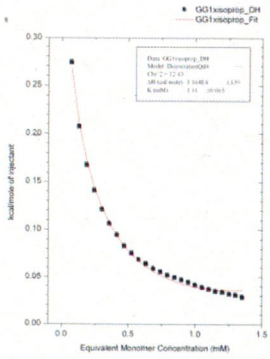
Compound 4



Nov 22a
Data: GG1xisoprop_DH
Model: DissociationQd4
Chi^2 = 12.43

DH (cal/mc	1.16E+04	139
K (mM)	1.11	0.065

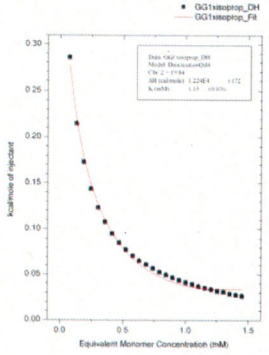
-64.13776



Nov 22b
Data: GG1xisoprop_DH
Model: DissociationQd4
Chi^2 = 19.84

DH (cal/mc	1.22E+04	172
K (mM)	1.15	0.076

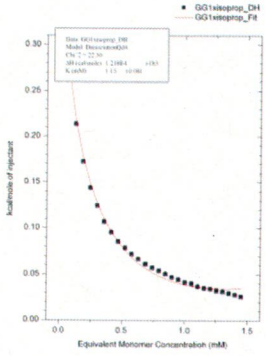
-71.48807



Nov 23a
Data: GG1xisoprop_DH
Model: DissociationQd4
Chi^2 = 22.30

DH (cal/mc	1.22E+04	183
K (mM)	1.15	0.081

-70.31031



100mM PBS deltG= -RT ln(keq) 303.15K

	Average		SD	%RSD
Kd	1.14	mM	0.02	1.658902
Keq (M-1)	879.77	/M		
ΔH	-12.02	kcal/mol	0.27	2.244715
ΔG	-4.08	kcal/mol		
(-)TΔS	7.94	kcal/mol		
ΔS	-0.026	cal/K		

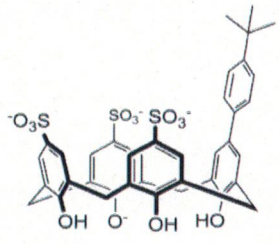
	avg
qd (kcal	-68.65

	avg
Kd uncert	0.074
ΔH uncert	164.6667

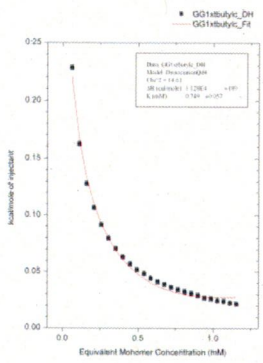
Host - 1x t-butylphenyl 3x HSO3 c4a
100mM Phosphate buffer, pH 7.4

PHOS

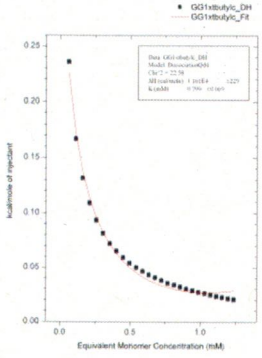
Compound 5



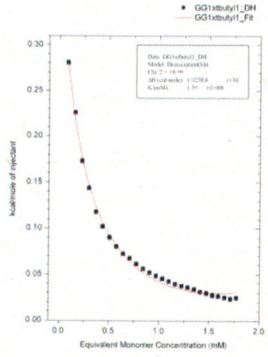
Jul-17		
Data: GG1xtbutylc_DH		
Model: DissociationQd4		
Chi^2 = 14.61		
DH (cal/mc	1.13E+04	189
K (mM)	0.749	0.057
-52.91181		



Jul-18		
Data: GG1xtbutylc_DH		
Model: DissociationQd4		
Chi^2 = 22.58		
DH (cal/mc	1.16E+04	229
K (mM)	0.80	0.069
-56.35282		



June28a		
Data: GG1xtbutyl1_DH		
Model: DissociationQd4		
Chi^2 = 18.99		
DH (cal/mc	1.02E+04	138
K (mM)	1.39	0.088
-77.83342		



100mM phosphate deltG= -RT ln(keq) 303.15K

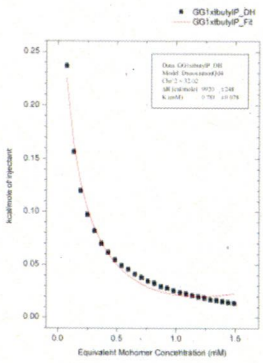
	Average		SD	%RSD
Kd	0.98	mM	0.29	29.72448
Keq (M-1)	1021.10	/M		
ΔH	-11.04	kcal/mol	0.59	5.329598
ΔG	-4.17	kcal/mol		
(-)TΔS	6.87	kcal/mol		
ΔS	-0.023	cal/K		

	avg
qd (kcal	-62.37

	avg
Kd uncert	0.071333
ΔH uncert	185.3333

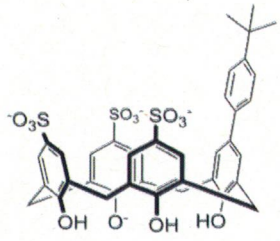
Host - 1x t-butylphenyl 3x HSO3 c4a

100mM PBS, pH 7.4

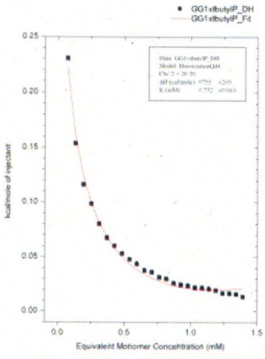


PBS

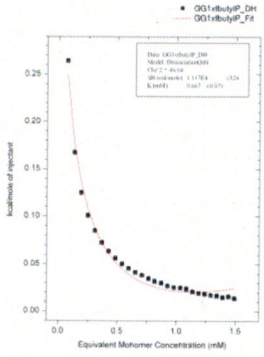
Compound 5



Nov-29		
Data: GG1xtbutylP_DH		
Model: DissociationQd4		
Chi^2 = 32.02		
DH (cal/mc	9.92E+03	248
K (mM)	0.781	0.078
-63.67423		



Dec2a		
2points R trim		
Data: GG1xtbutylP_DH		
Model: DissociationQd4		
Chi^2 = 20.20		
DH (cal/mc	9.755.00	203
K (mM)	0.732	0.063
-61.19541		



Dec2b		
Data: GG1xtbutylP_DH		
Model: DissociationQd4		
Chi^2 = 46.64		
DH (cal/mc	1.12E+04	324
K (mM)	0.667	0.071
-71.47569		

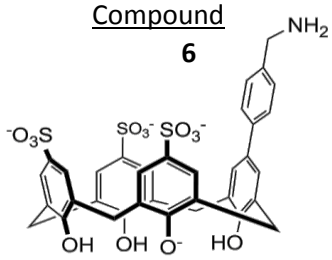
100mM PBS deltG= -RT ln(keq) 303.15K

	Average		SD	%RSD		avg
Kd	0.726667	mM	0.046693	6.425622		
Keq (M-1)	1376.147	/M			**qd (kcal**	-65.44844
						avg
ΔH	-10.28167	kcal/mol	0.625	6.078781	**Kd uncert**	0.070667
ΔG	-4.348493	kcal/mol			**ΔH uncert**	258.3333
(-)TΔS	5.933174	kcal/mol				
ΔS	-0.019581	cal/K				

Host - 1x 4-aminomethylphenyl 3x HSO3 c4a
100mM Phosphate buffer, pH 7.4

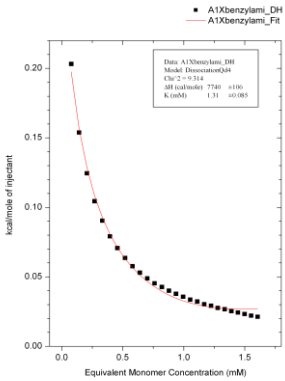
PHOS

Compound **6**



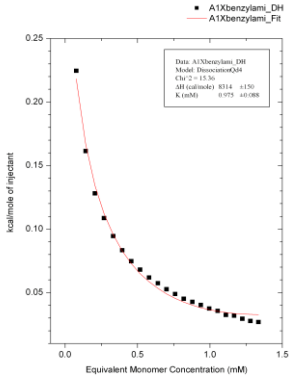
Sept 24a
Data: A1Xbenzylami_DH
Model: DissociationQd4
Chi^2 = 9.314

DH (cal/mc	7.74E+03	106
K (mM)	1.31	0.085
-47.344		



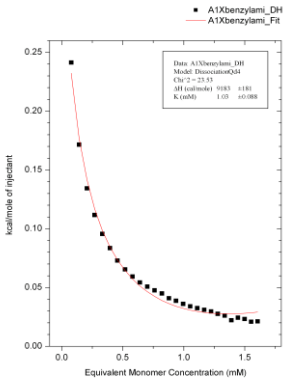
Sept 25b
Data: A1Xbenzylami_DH
Model: DissociationQd4

Chi^2 = 15.36		150
DH (cal/mc	8.31E+03	0.088
K (mM)	0.98	
-44.0984		



Sept 26b
Data: A1Xbenzylami_DH
Model: DissociationQd4
Chi^2 = 23.53

DH (cal/mc	9.18E+03	181
K (mM)	1.03	0.088
-57.897		



100mM phosphate deltG= -RT ln(keq) 303.15K

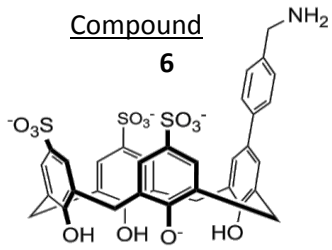
	Average		SD	%RSD	
Kd	1.11	mM	0.15	13.27472	
Keq (M-1)	904.98	/M			
					avg
					qd (kcal -49.78
ΔH	-8.41	kcal/mol	0.59	7.051451	
ΔG	-4.10	kcal/mol			**avg**
(-)TΔS	4.32	kcal/mol			**Kd uncert** 0.0865
ΔS	-0.014	cal/K			**ΔH uncert** 95.696

Host - 1x 4-aminomethylphenyl 3x HSO3 c4a

100mM PBS, pH 7.4

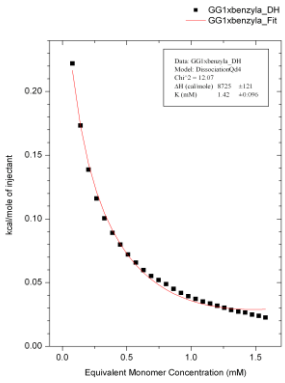
PBS

Compound **6**



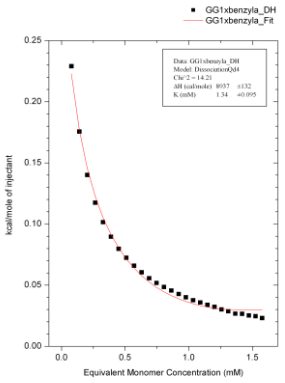
OCt22b
Data: GG1xbenzyla_DH
Model: DissociationQd4
Chi^2 = 12.07

DH (cal/mc	8.73E+03	121
K (mM)	1.42	0.096
-54.0414		



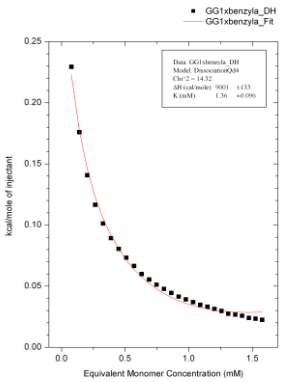
Oct23a
Data: GG1xbenzyla_DH
Model: DissociationQd4
Chi^2 = 14.21

DH (cal/mc	8.94E+03	132
K (mM)	1.34	0.095
-54.9043		



OCt23b
Data: GG1xbenzyla_DH
Model: DissociationQd4
Chi^2 = 14.32

DH (cal/mc	9.00E+03	133
K (mM)	1.36	0.096
-56.6081		



100mM PBS deltG= -RT ln(keq) 303.15K

	Average		**SD**	**%RSD**
Kd	1.37	mM	0.03	2.475252
Keq (M-1)	728.16	/M		
ΔH	-8.89	kcal/mol	0.12	1.327153
ΔG	-3.97	kcal/mol		
(-)TΔS	4.92	kcal/mol		
ΔS	-0.016	cal/K		

	avg
qd (kcal	-55.18

	avg
Kd uncert	0.095667
ΔH uncert	128.6667