Supporting Information for:

The effects of hexafluoroisopropanol on guest binding by water-soluble capsule and cavitand hosts

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Table of Contents

Experimental Procedures

General. Cavitand **1** was prepared as previously described.[1] All guests were obtained from TCI-America, Sigma-Aldrich, or Acros and used as received. ^{1}H and spectra were recorded using either a Bruker AV 600 or Bruker DRX 600 (^{1}H: 600.0 MHz) spectrometer at 298 K. Chemical shifts (δ) are reported in ppm shifted from tetramethylsilane (TMS, δ_H 0.00) and referenced to the solvent peak. The relative chemical shift of the solvent to free TMS was determined experimentally at various percentages of HFIP in D_2O (Fig. S1), and the chemical shift of the solvent peak at the relevant amount of HFIP was referenced for titration experiments. All NMR spectra were processed using MestReNova NMR processing software.

NMR Complexation Studies. Solutions of **1** were prepared to a final concentration ranging from 0.0008-0.0029 M. In each case, 400 μL of this solution was transferred to an NMR tube. Insoluble guests were added in excess, in neat 2 μL portions for liquids and as a spatula tip full for solids. In all cases the NMR tubes containing the host/guest mixtures were sonicated for ≥ 2 h to promote host-guest complex formation.

Discussions

HFIP Induced Conformational Transition. The ^{1}H NMR spectra of dilute solutions of **1** in D_2O (0.8 mM) show two distinct sets of signals. These are characteristic of an equilibrium between the D_{2d} symmetric "kite" and C_{4v} symmetric "vase" conformations (Fig. S2),[1,2] and are present in an approximately 2.8:1 ratio, respectively. The former conformation exists in a dimeric velcrand complex (Fig. S2, top). Dilution with HFIP results in a small shift to the vase conformation (~2.1:1 kite/vase) at 5% HFIP v/v, and at 15-50% HFIP v/v the cavitand exists completely in the vase conformation. This well-established conformational transition[3,4] is indicated primarily by the absence of peaks in the NMR between 6.0-7.0 ppm. Although the size, shape and propensity of HFIP to solubilize hydrophobic compounds[5] make it ideal to stabilize the "vase" conformation by its inclusion within the cavity of **1** it is not readily observed by ^{19}F NMR (at least in slow exchange on the NMR timescale).

Complexes of 1 with *n*-alkanes in 15% HFIP v/v in D_2O. The determination of binding motifs of *n*-alkanes with **1** (cavitand *versus* capsule) in 15% HFIP v/v are, in part, based on comparisons to the

complexes analyzed in 100% D_2O (Fig. S16)[2] and the relative integrations between the resorcinarene core meso-protons of **1** in the "vase" conformation and the bound guests. The integrations for the complexation of C_8 (Fig. S3) are reasonable for residing in a monomeric cavitand. For complexes with C_9-C_{14}, the integration values (Figs. S4-S9) agree quite well for binding to the dimeric capsule **1.1**. Presumably, the increasing insolubility and/or binding cavity volume needs of the larger guests C_{15}-C_{18} prevent complete uptake of the guests by **1**, and the relative integration values between host and guest are not reliable. However, comparison of these spectra (Figs. S10-S13) to the 100% D_2O system suggest capsular binding of "curled" guests in 15% HFIP v/v as well.

Computational Details

General. Density functional theory (DFT) calculations[6] have been carried out employing the M062X functional[7] and the 6-31G(d,p) basis set.[8] All calculations have been carried out with the aid of Gaussian 09.[9]

Geometry Optimizations. Optimized geometries have been determined for the encapsulated complexes, whereby different initial guesses have been employed in different optimizations in order to obtain the lowest minimum. The coordinates of all the atoms in the capsule and the guest were included in the optimization. The two main initial guesses involved (a) the substituent (-CN, -OH, -COOH) pointing directly towards the end of the capsule or (b) the substituent not pointing towards the end of the capsule. In the case of 1,12-dodecanediol, the lowest minimum (Fig. S24a) results from the optimization with initial guess (a) while initial guess (b) leads to a minimum higher than (a) by 2.0 kcal mol^{-1} (Fig. S24b). In the case of the 1,12-dicyanododecane, initial guess (a) and subsequent optimizations leads to a minimum structure (Fig. S24c) bound 14 kcal mol^{-1} higher than the lowest minimum (Fig. S24d) by 26 kcal mol^{-1}. Initial guess (a) for the 1,14-tetradecanedicarboxylic acid system, leads to a minimum energy structure for the encapsulated complex unbound with respect to the free guest+capsule, while the optimum structure (Fig. S24e) is bound by 58 kcal mol^{-1}. The coordinates for structures in Fig. S24 are included below.

Calculation of NMR Shifts. The method GIAO[10] provided by Gaussian 09 was employed. The results were calibrated relative to TMS at B3LYP/6-311+ G(2d,p) GIAO also provided by Gaussian 09. The values in the figures are the average of the calculated shifts over the hydrogen atoms which would be equivalent in the free guest, for comparison with the way the experimental results are presented.

1D NMR Spectra

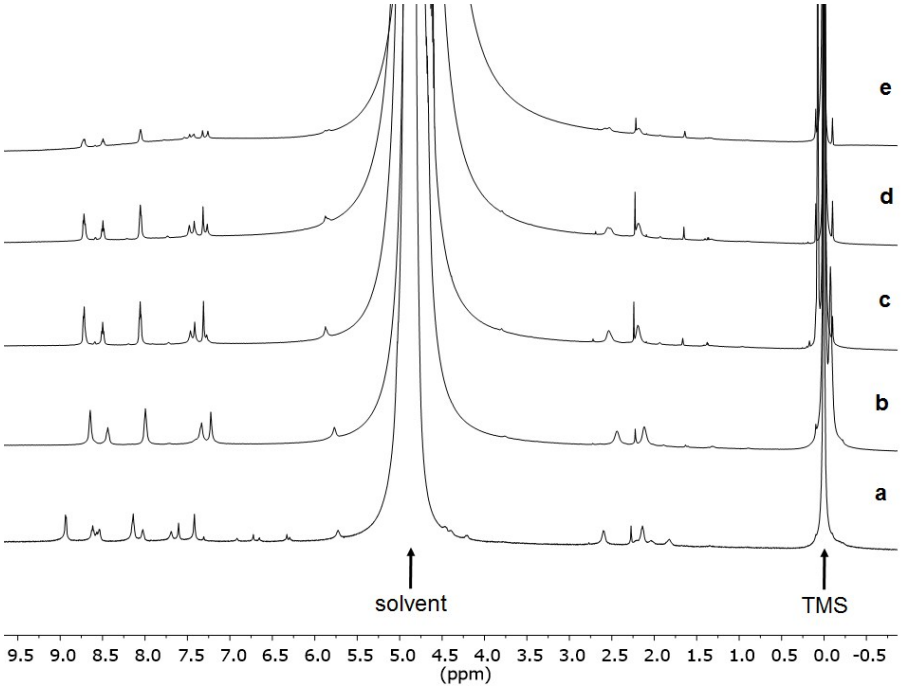


Fig. S1 ^{1}H NMR spectra of **1** and chemical shift of solvent relative to TMS (0.00 ppm) at (a) 5% (4.906 ppm), (b) 15% (4.799 ppm), (c) 25% (4.745 ppm), (d) 35% (4.673 ppm) and 50% (4.603 ppm) HFIP in D_2O.

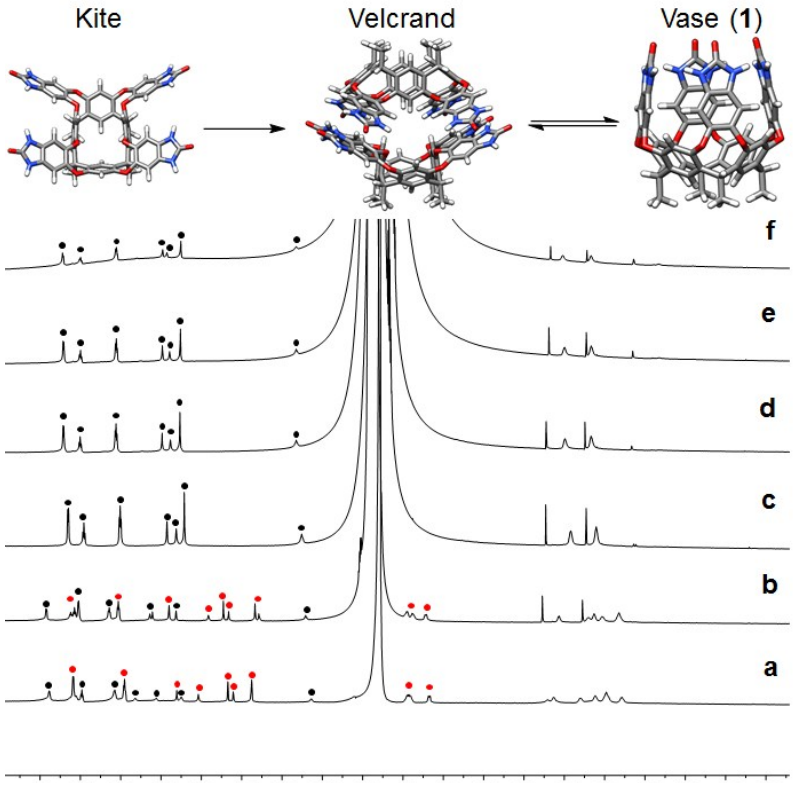


Fig. S2 Representation (top) of the various conformational states of 1 and ^{1}H NMR spectra (bottom) of 1 in D_2O at 298 K with (a) 0%, (b) 5%, (c) 15%, (d) 25%, (e) 35%, and 50% HFIP. The principal resonances for the "kite" and "vase" conformations are indicated by (•) and (•), respectively.

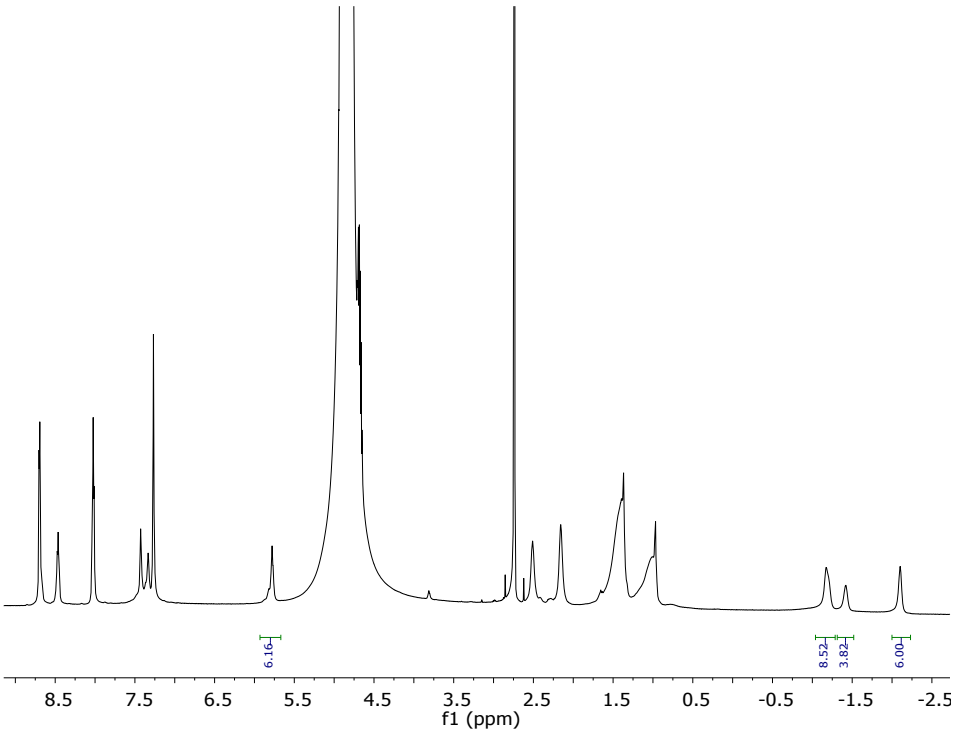


Fig. S3 ^{1}H NMR spectrum of the **1**•C_8 complex in 15% HFIP v/v in D_2O.

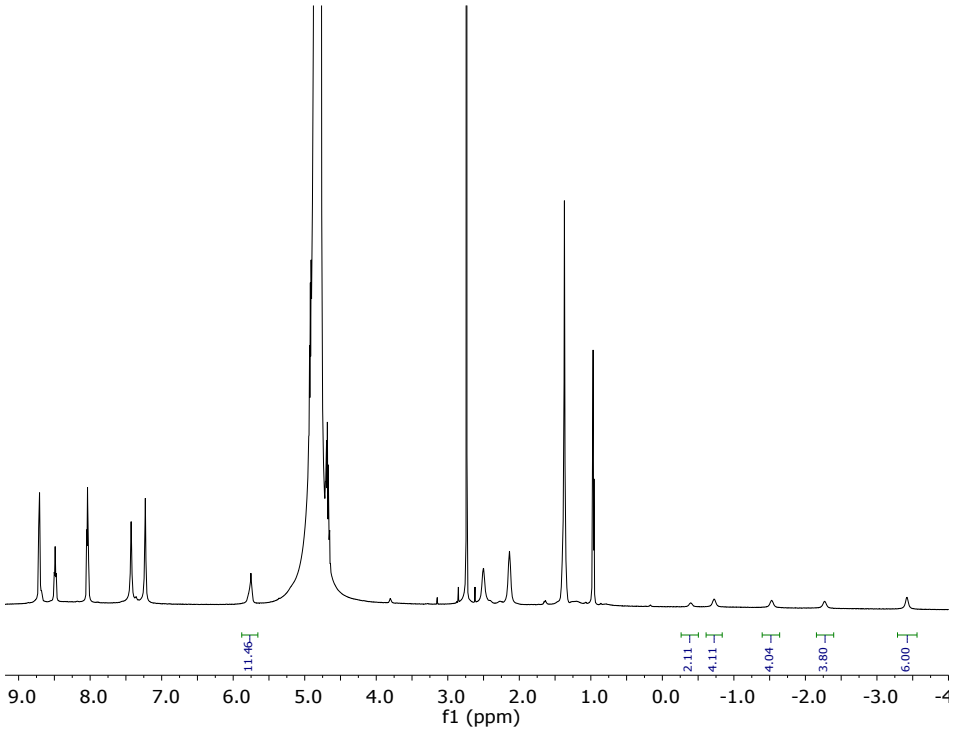


Fig. S4 ^{1}H NMR spectrum of the **1.1**•C_9 complex in 15% HFIP v/v in D_2O.

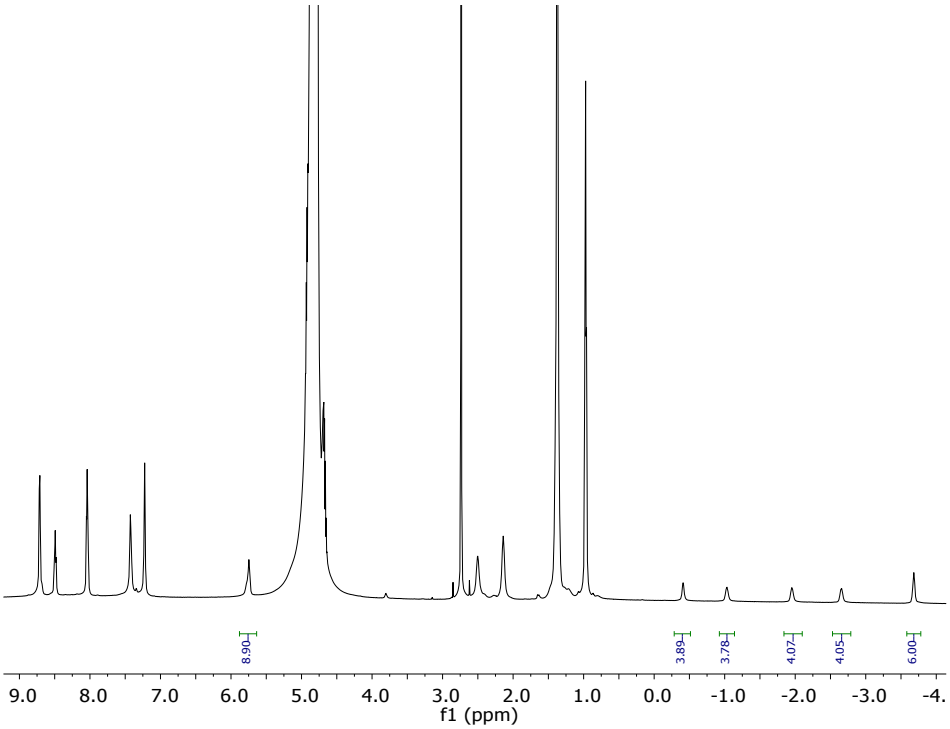


Fig. S5 ^{1}H NMR spectrum of the **1.1**•C_{10} complex in 15% HFIP v/v in D_2O.

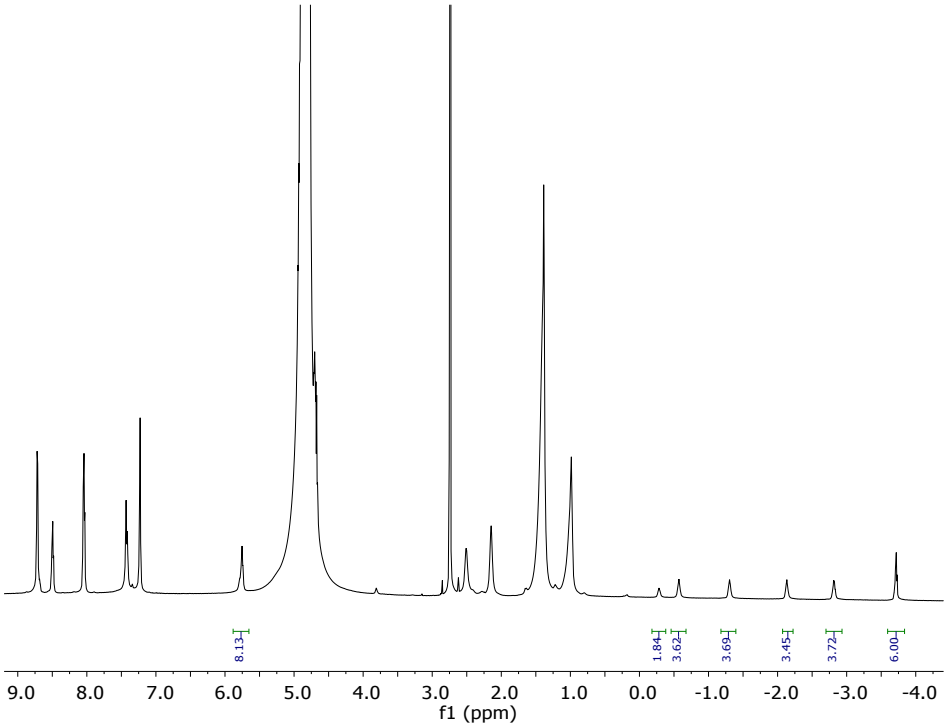


Fig. S6 ^{1}H NMR spectrum of the **1.1**•C_{11} complex in 15% HFIP v/v in D_2O.

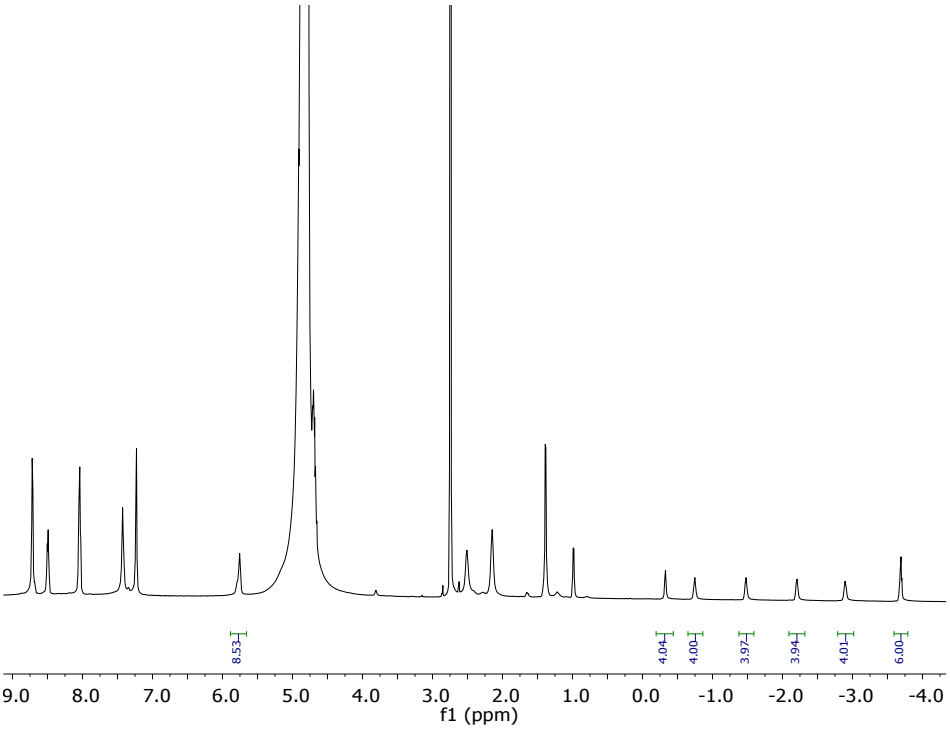


Fig. S7 ^{1}H NMR spectrum of the **1.1**•C_{12} complex in 15% HFIP v/v in D_2O.

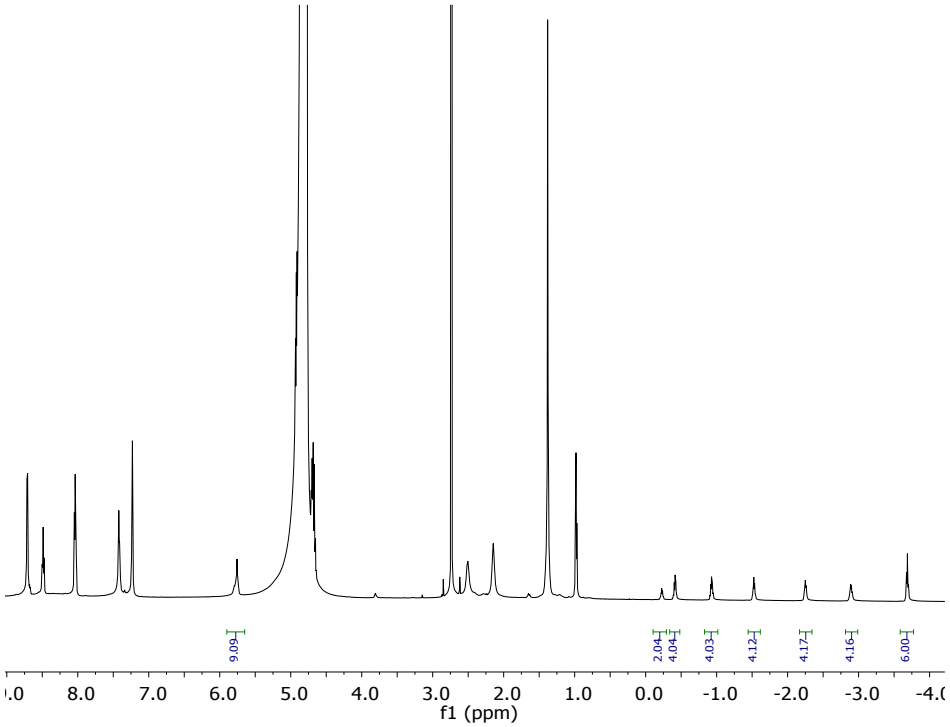


Fig. S8 ^{1}H NMR spectrum of the **1.1**•C_{13} complex in 15% HFIP v/v in D_2O.

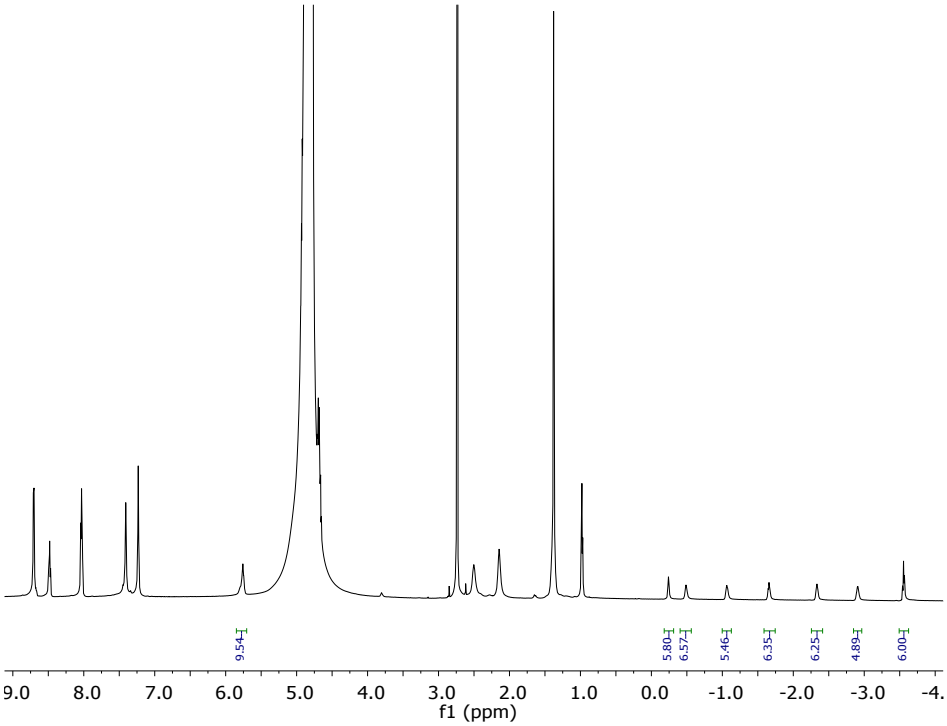


Fig. S9 ^{1}H NMR spectrum of the **1.1**•C_{14} complex in 15% HFIP v/v in D_2O.

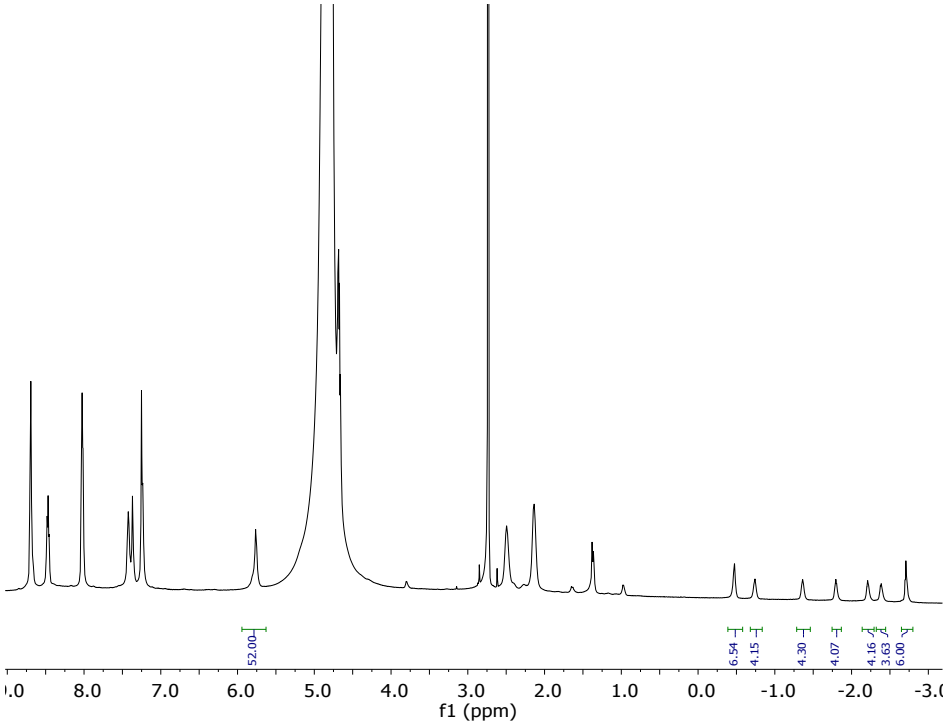


Fig. S10 ^{1}H NMR spectrum of the **1.1**•C_{15} complex in 15% HFIP v/v in D_2O.

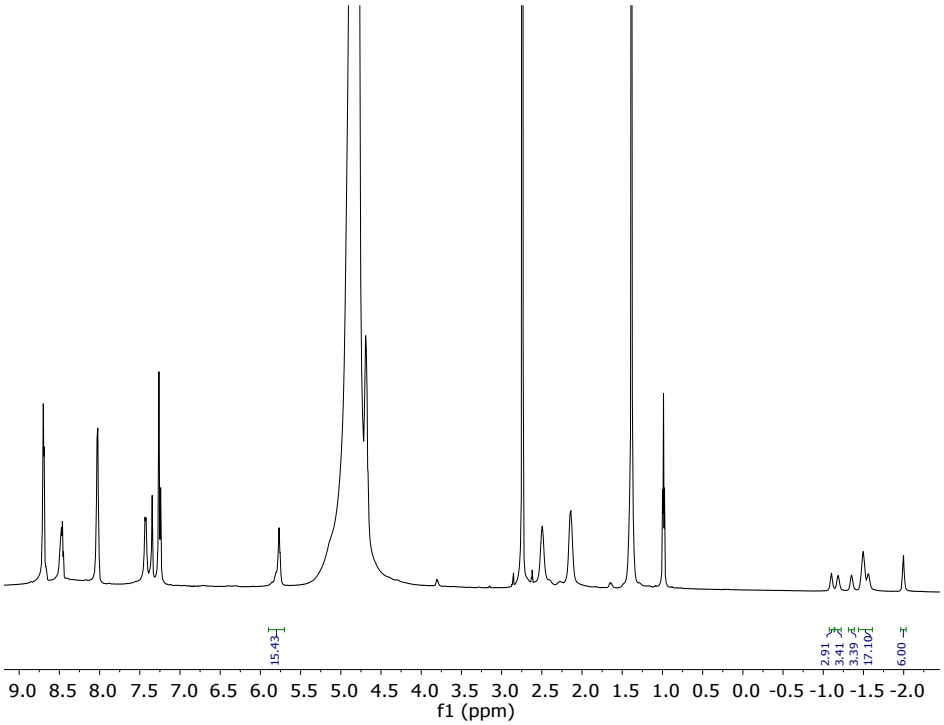


Fig. S11 ^{1}H NMR spectrum of the **1.1**•C_{16} complex in 15% HFIP v/v in D_2O.

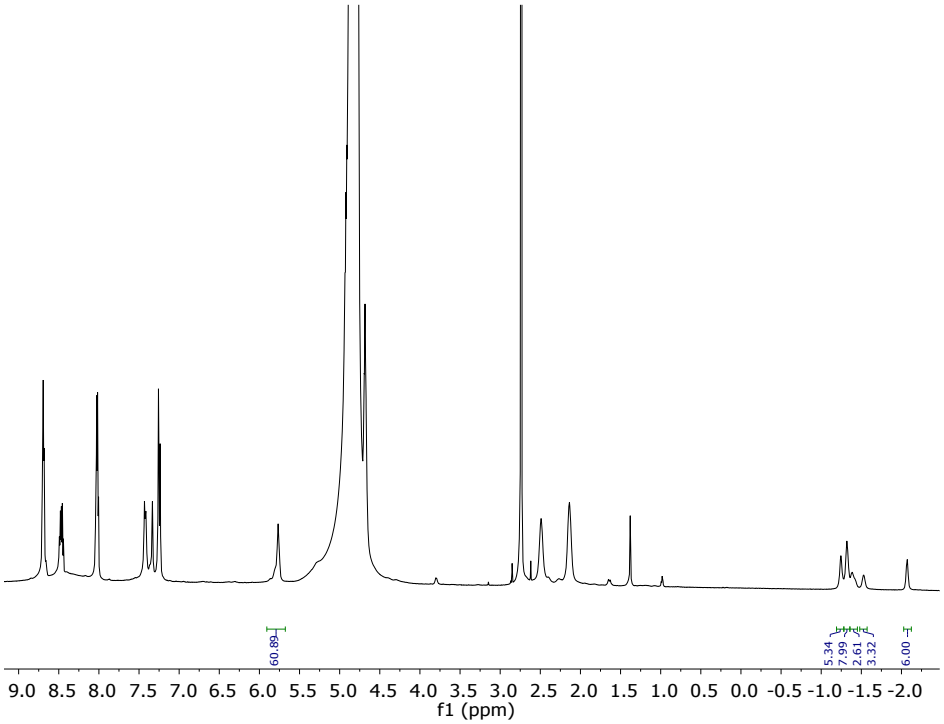


Fig. S12 ^{1}H NMR spectrum of the **1.1**•C_{17} complex in 15% HFIP v/v in D_2O.

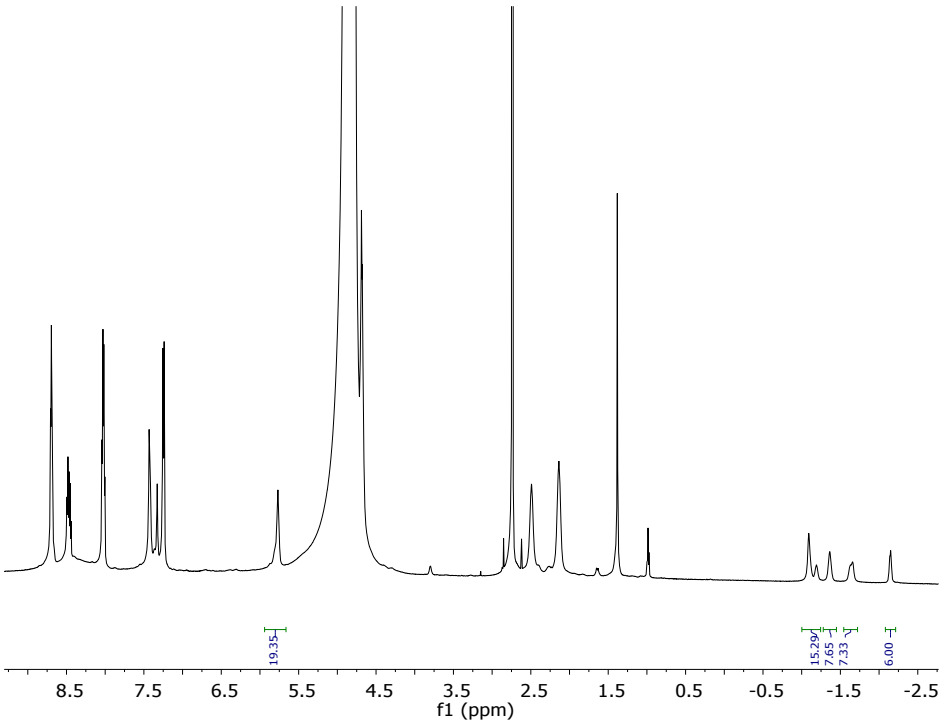


Fig. S13 ^{1}H NMR spectrum of the **1.1**•C_{18} complex in 15% v/v HFIP v/v in D_2O.

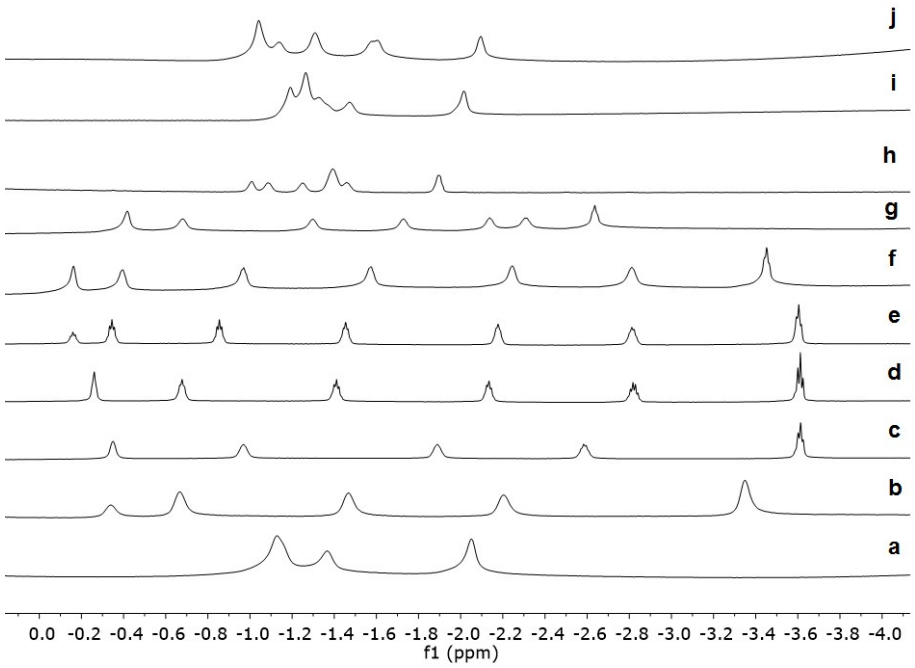


Fig. S14 Partial ^{1}H NMR spectra showing the upfield region of complexes of **1** and **1.1** with *n*-alkanes (a) C_8, (b) C_9, (c) C_{10}, (d) C_{12}, (e) C_{13}, (f) C_{14}, (g) C_{15}, (h) C_{16}, (i) C_{17} and (j) C_{18} in 50% v/v HFIP in D_2O.

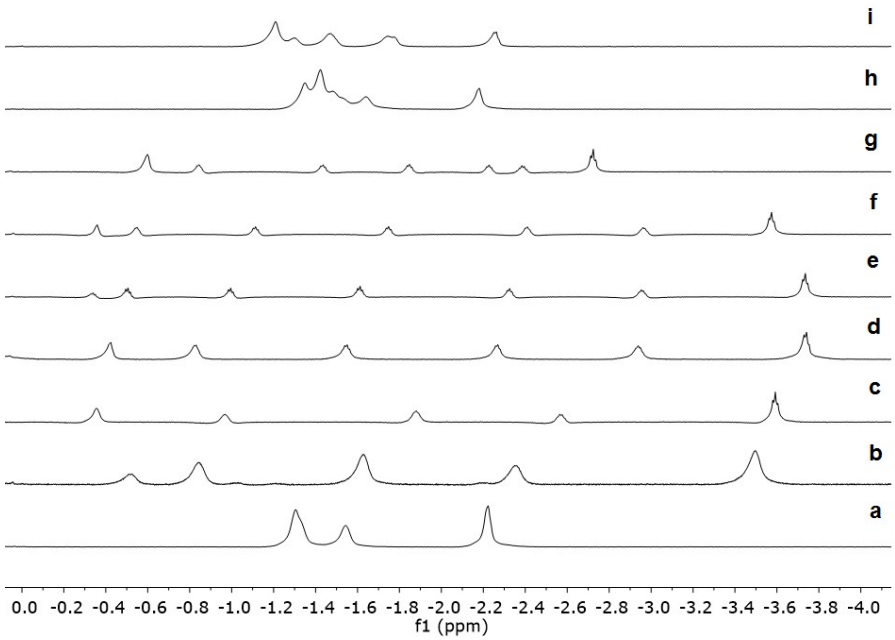


Fig. S15 Partial ^{1}H NMR spectra showing the upfield region of complexes of **1** and **1.1** with *n*-alkanes (a) C_8, (b) C_9, (c) C_{10}, (d) C_{12}, (e) C_{13}, (f) C_{14}, (g) C_{15}, (h) C_{17} and (i) C_{18} in 85% v/v HFIP in D_2O.

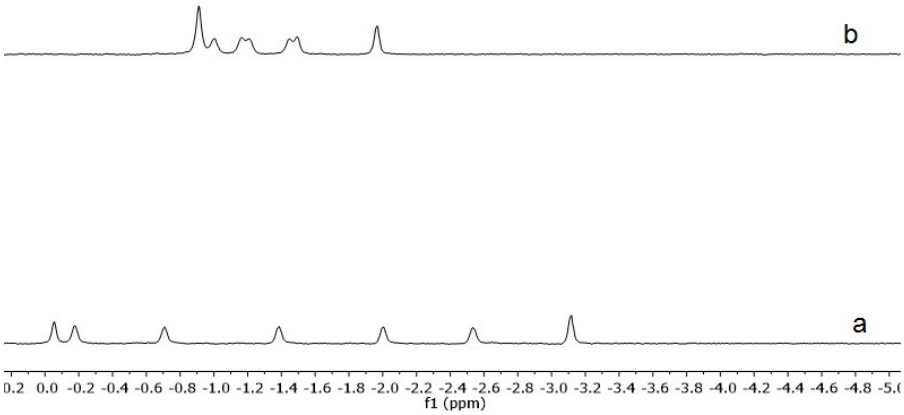


Fig. S16 Partial ^{1}H NMR spectra showing the upfield region of complexes of **1** and **1.1** with *n*-alkanes (a) C_{14}, (b) C_{18} in 100% HFIP

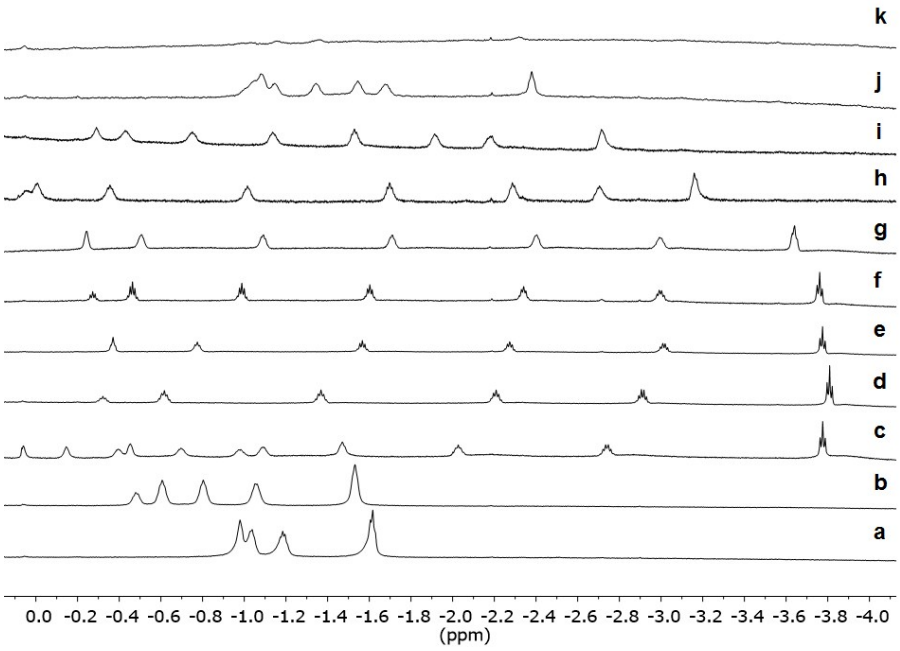


Fig. S17 Previously reported partial ^{1}H NMR spectra showing the upfield region of complexes of **1** and **1.1** with *n*-alkanes (a) C_8, (b) C_9, (c) C_{10}, (d) C_{11}, (e) C_{12}, (f) C_{13}, (g) C_{14}, (h) C_{15}, (i) C_{16}, (j) C_{17} and (k) C_{18} in 100% D_2O.

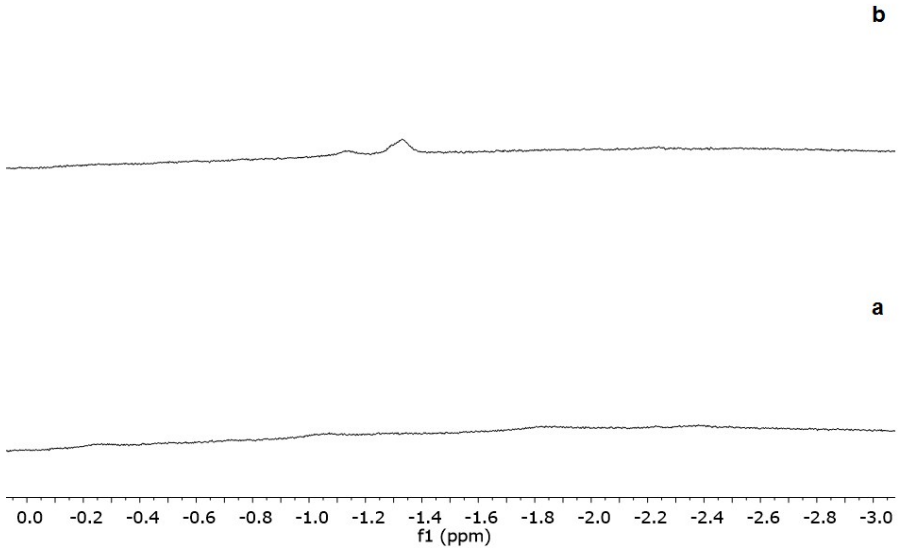


Fig. S18 Partial ^{1}H NMR spectra showing the upfield region of complexes of **1.1** with (a) 1,14-tetradecanediol and (b) 1,16-hexadecanediol in 15% HFIP v/v in D_2O.

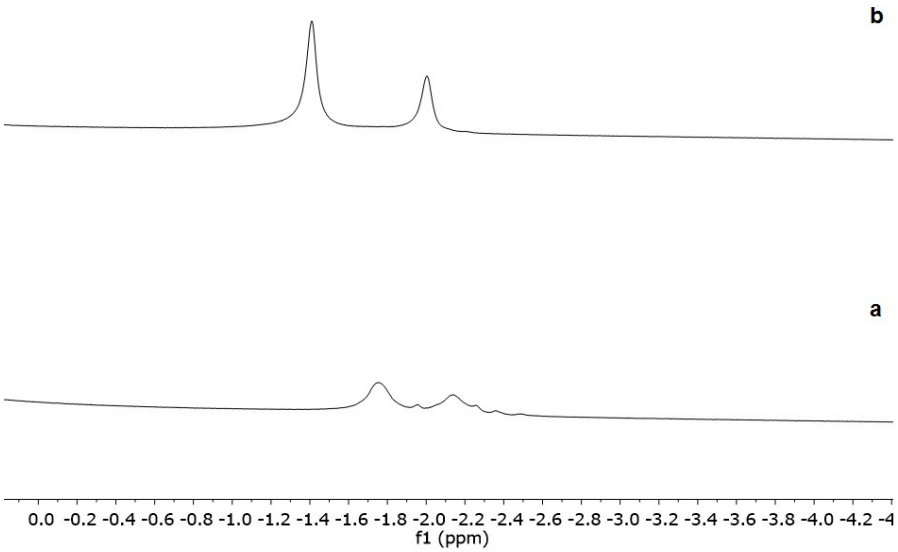


Fig. S19 Partial ^{1}H NMR spectra showing the upfield region of complexes of **1.1** with (a) *n*-hexane and (b) *n*-heptane in 15% HFIP v/v in D_2O.

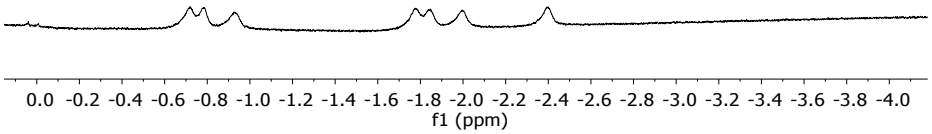
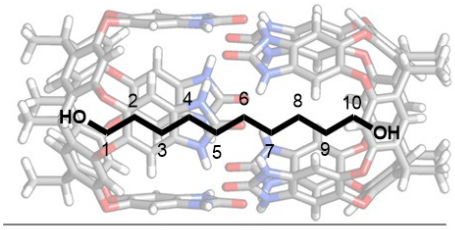


Fig. S20 Partial (unreferenced) ^{1}H NMR spectra of **1.1** with 1,14-tetradecanedicarboxylic acid in 83% HFIP/D_2O indicating formation of inclusion complex in the presence of high amounts of HFIP.

Chemical Shift and 2D COSY NMR Data for Bolaamphiphiles



Peaks	Free δ (ppm)	Bound δ (ppm)	Δδ (ppm)
1,10	3.565	-1.026	-4.591
2,9	1.516	-2.436	-3.952
3,8	1.257	-1.753	-3.01
4,7	1.257	-0.96	-2.217
5,6	1.257	-0.397	-1.654

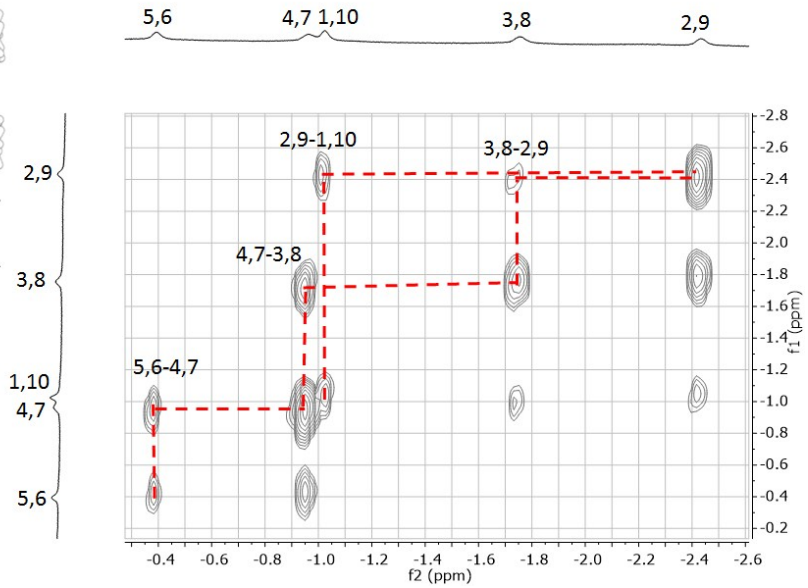
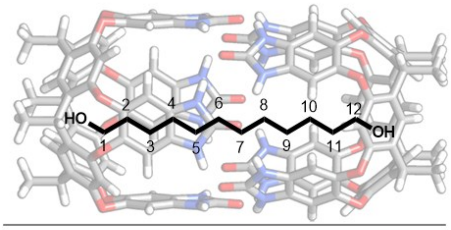


Fig. S21 Change in chemical shift (ppm) of free versus bound guest and assigned COSY NMR data for 1,10-decanediol in 15% HFIP/D_2O.



Peaks	Free δ (ppm)	Bound δ (ppm)	Δδ (ppm)
1,12	3.56	-0.94	-4.5
2,11	1.512	-2.606	-4.118
3,10	1.241	-1.947	-3.188
4,9	1.241	-1.302	-2.543
5,8	1.241	-0.651	-1.892
6,7	1.241	-0.301	-1.542

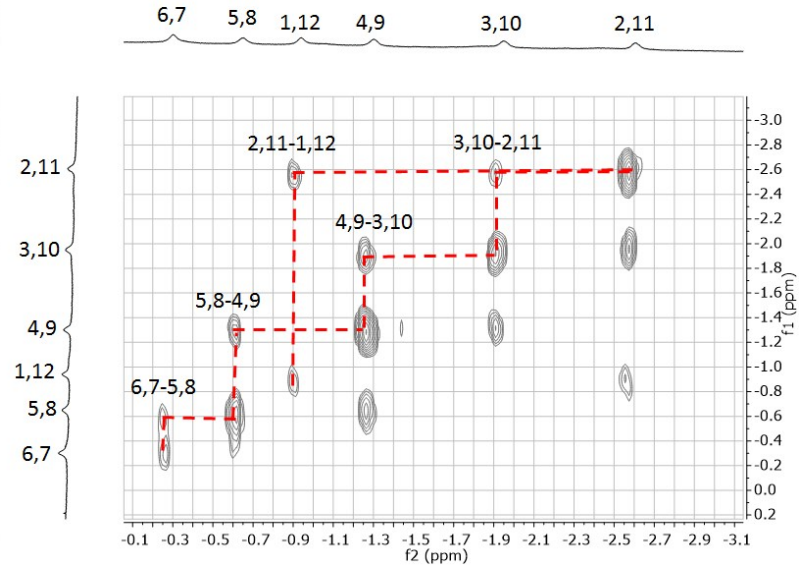
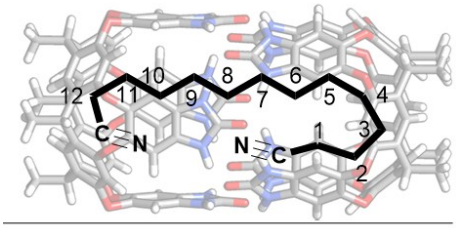


Fig. S22 Change in chemical shift (ppm) of free versus bound guest and assigned COSY NMR data for 1,12-dodecanediol in 15% HFIP/D_2O.



Peaks	Free δ (ppm)	Bound δ (ppm)	Δδ (ppm)
1,12	2.309	-2.052	-4.361
2,11	1.618	-2.665	-4.283
3,10	1.397	-1.998	-3.395
4,9	1.292	-1.29	-2.582
5,8	1.292	-0.597	-1.889
6,7	1.292	-0.022	-1.314

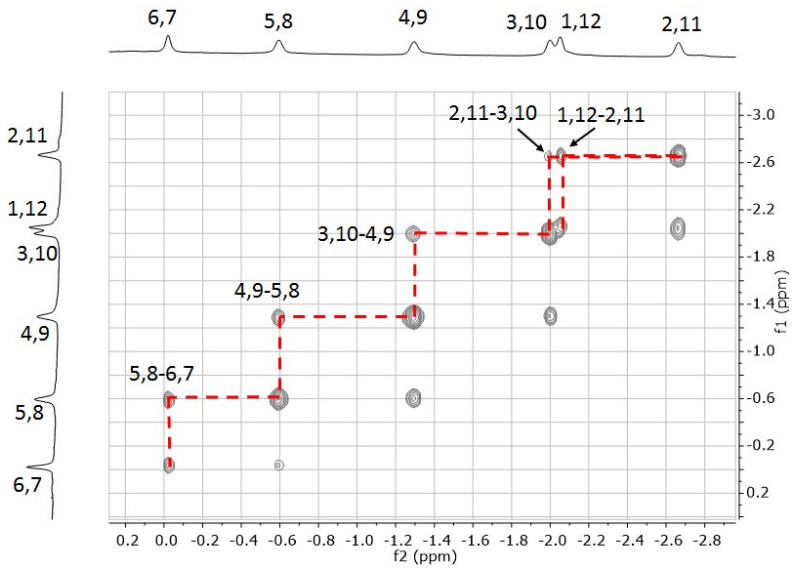
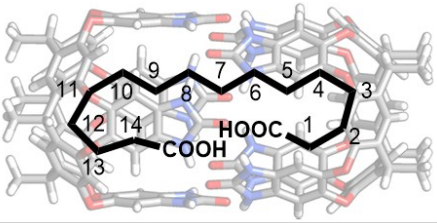


Fig. S23 Change in chemical shift (ppm) of free versus bound guest and assigned COSY NMR data for tetradecanedioic dinitrile in 15% HFIP/D_2O.



Peaks	Free δ (ppm)	Bound δ (ppm)	Δδ (ppm)
1,14	2.287	-0.802	-3.089
2,13	1.561	-1.802	-3.363
3,12	1.241	-2.413	-3.654
4,11	1.241	-1.972	-3.213
5,10	1.241	-1.802	-3.043
6,9	1.241	-0.858	-2.099
7,8	1.241	-0.619	-1.86

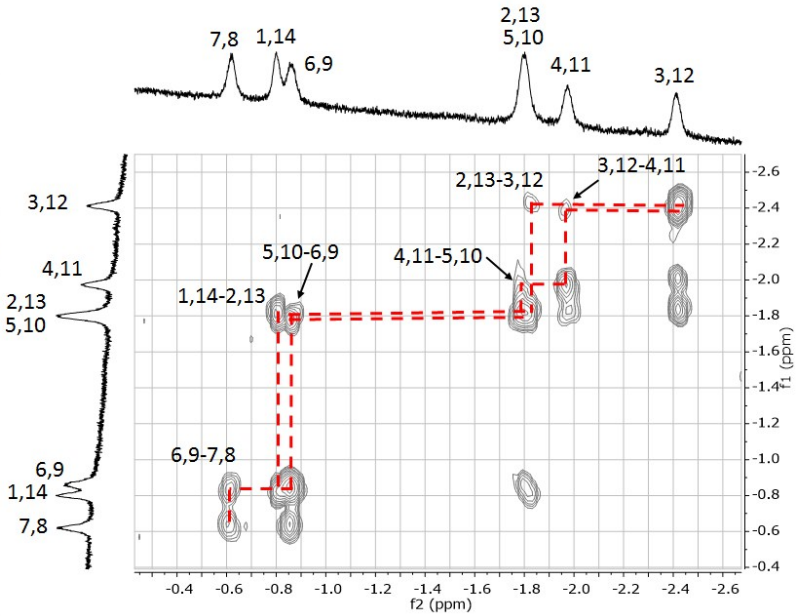


Fig. S24 Change in chemical shift (ppm) of free versus bound guest and assigned COSY NMR data for hexadecanedioic acid in 15% HFIP/D_2O.

DFT Structures of Capsular Complexes

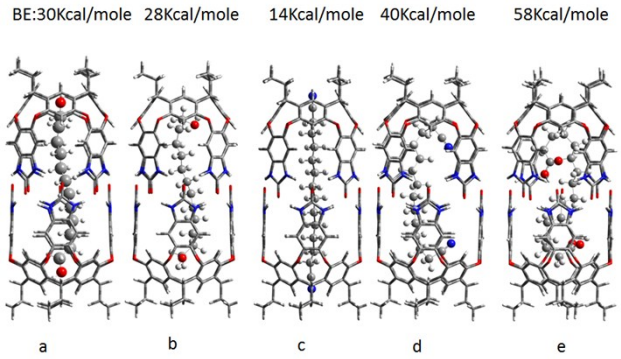


Fig. S25 The optimum structures obtained by the calculations: (a), (b) optimum structures resulting from initial guesses (a) and (b) for the 1,12-dodecanediol complex, (c) and (d) are the corresponding structures for the 1,12-dicyanododecane complex and (e) the lowest energy minimum structure determined for the encapsulated 1,14-tetradecanedicarboxylic acid.

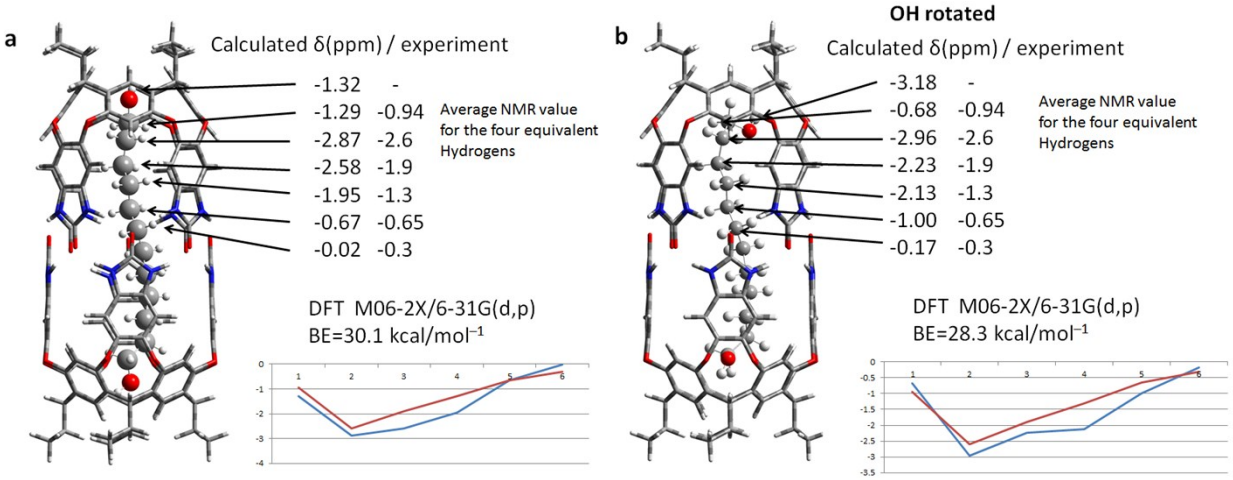


Fig. S26 DFT (M06-2X/6-31G(d,p) structures, calculated versus experimental chemical shifts (δ, ppm), and binding energies of encapsulated 1,12-dodecanediol by **1.1** (a) with the terminal hydroxyls directed toward the aromatic capsule "floors", and (b) with the hydroxyls rotated away from the aromatic "floors". In the charts, horizontal axis gives the carbon-atom numbering as in the main article, vertical axis gives the NMR δ(ppm)

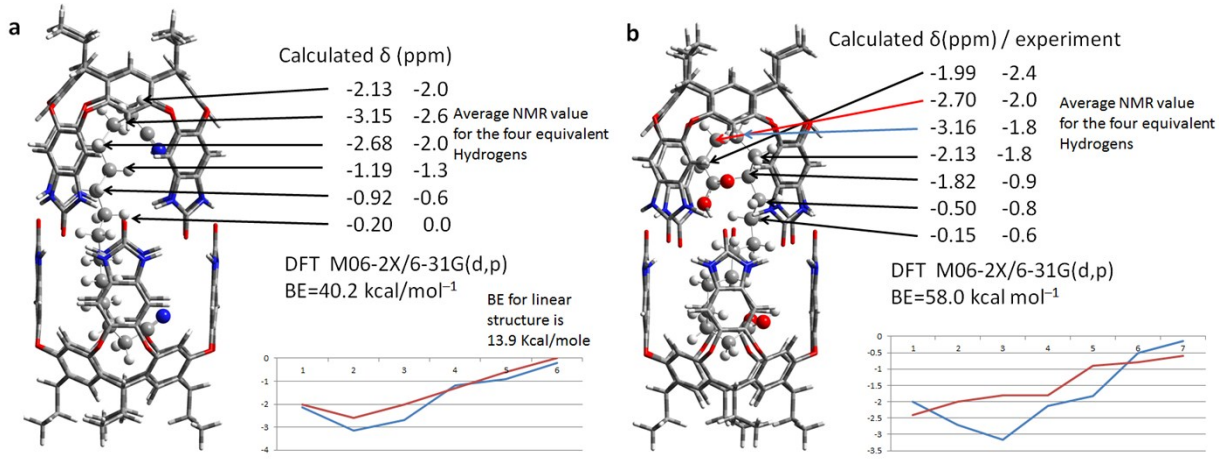


Fig. S27 DFT (M06-2X/6-31G(d,p) structures, calculated versus experimental chemical shifts (δ, ppm), and binding energies of encapsulated (a) 1,12-dicyanododecane and (b) 1,14-tetradecanedicarboxylic acid by **1.1**. In the charts, horizontal axis gives the carbon-atom numbering as in the main article, vertical axis gives the NMR δ(ppm)

Calculated Structure Coordinates

Coordinates in Angstrom units for the lowest minimum energy geometry of 1,12-dodecanediol (structure a)

C	-8.88886100	-0.13534700	-3.59849100
C	-8.32442900	1.14388000	-2.98197300
C	-8.28075600	-1.37991000	-2.96007600
H	-8.56039600	-0.13701100	-4.64230500
C	-8.89137600	1.77599500	-1.87013600
C	-7.18516400	1.73689500	-3.52937800
C	-8.81618700	-1.96601000	-1.81257400
C	-7.14460500	-1.98508600	-3.50422100
C	-8.36967300	2.93089100	-1.27824000
H	-9.78138800	1.33036100	-1.43427300
C	-6.65472100	2.90420000	-2.99897600
O	-6.62003500	1.20520500	-4.67960500
C	-8.26677500	-3.08221500	-1.17930200
H	-9.68767900	-1.50169100	-1.36222800
C	-6.58870900	-3.11953300	-2.93189000
O	-6.58966700	-1.49124300	-4.67957800
C	-8.99629200	3.59268800	-0.04466300
C	-7.23022500	3.47982600	-1.87681100
H	-5.82513200	3.39355900	-3.48962300
C	-5.40175400	0.57311000	-4.55246200
C	-8.86172400	-3.66495700	0.10016600
C	-7.13304500	-3.64609700	-1.76883300
H	-5.75238700	-3.61339300	-3.40789500
C	-5.38567300	-0.83108900	-4.55958300

H	-8.68412000	4.64119000	-0.07519500
C	-8.42073200	3.01878200	1.24958800
O	-6.70325000	4.67281200	-1.40110600
C	-8.28802800	-2.98746000	1.34102100
H	-8.52861100	-4.70644100	0.14330700
O	-6.57106200	-4.79883700	-1.23362200
C	-8.98368000	1.92492500	1.92060800
C	-7.26321000	3.56793100	1.81252800
C	-5.48775000	4.59928000	-0.75563900
C	-3.02649400	0.59904600	-4.43834100
C	-8.86555100	-1.86365600	1.94170100
C	-7.13740800	-3.50173700	1.94234500
C	-5.35786700	-4.66154800	-0.59419600
C	-3.00832700	-0.80365000	-4.44617100
C	-8.40135300	1.30537000	3.03564900
H	-9.92419400	1.52471900	1.54374000
C	-6.69766900	3.03195800	2.95933900
O	-6.71833500	4.72070300	1.27461600
C	-5.49351500	4.61841800	0.64675000
C	-8.33548300	-1.22276900	3.06664900
H	-9.77045000	-1.46028400	1.49535400
C	-6.60921400	-2.93179900	3.09057100
O	-6.57047400	-4.66889100	1.45527400
C	-5.35632800	-4.58196600	0.80825100
C	-8.96092500	0.03403500	3.67916200
C	-7.23692300	1.89463100	3.54093700
H	-5.84952900	3.51908500	3.41958000
C	-3.10936400	4.58259800	-0.74405900
C	-7.18872100	-1.79413400	3.62985100

H	-5.77500600	-3.40321500	3.59095700
C	-2.97746500	-4.63956800	-0.59593900
H	-8.63280500	0.05738100	4.72284100
O	-6.66206600	1.40431500	4.70080700
C	-3.11569800	4.60081500	0.65917200
O	-6.65377200	-1.26856500	4.79762900
C	-2.97656500	-4.55295300	0.80433600
C	-5.44022700	0.76879400	4.60048000
C	-5.43808700	-0.63183200	4.66852700
C	-3.06313700	0.76367300	4.50826500
C	-3.06299400	-0.63862500	4.57336300
C	-4.30376100	4.64023400	1.37342900
C	-4.29047800	4.60120500	-1.47052300
C	-4.21658200	1.30576400	-4.50995800
C	-4.18296700	-1.53653700	-4.52577300
C	-4.24640300	1.48767700	4.54119000
C	-4.24555300	-1.35345200	4.67739800
C	-4.16345400	-4.70694100	-1.31243200
C	-4.16148000	-4.53919100	1.52569600
H	-4.31748100	4.72584900	2.45272900
H	-4.29607300	4.65220000	-2.55213300
H	-4.25010800	2.57030300	4.55504300
H	-4.23517200	2.38680900	-4.56297200
H	-4.25507500	-2.42980800	4.79342000
H	-4.18015400	-2.61787400	-4.58103300
H	-4.17715500	-4.83109900	-2.38815500
H	-4.16982600	-4.53949500	2.60851500
C	-0.96815100	4.62954200	-0.03294900
C	-0.87648900	-0.07167600	-4.35082000

C	-0.83338500	-4.64319000	0.10801500
C	-0.91951000	0.05994300	4.50179900
N	-1.73273000	-1.04094200	4.58159600
N	-1.73228700	1.16348400	4.48330100
N	-1.64587800	-4.57317100	1.20810700
N	-1.64640100	-4.71321900	-0.99428600
N	-1.67141200	-1.18715100	-4.40043100
N	-1.70247600	1.01810200	-4.39807800
N	-1.77738400	4.61875600	-1.14004200
N	-1.78730100	4.64779900	1.06655900
H	-1.34281000	1.94335500	-4.15144500
H	-1.40991800	4.39229300	1.98210400
H	-1.35461200	-1.96013800	4.34552100
H	-1.26513300	-4.47229600	-1.91095700
C	-10.39788400	-3.68050200	0.09458500
C	-10.96850500	-4.52104400	-1.04430900
H	-10.80134800	-2.66321100	0.03247300
H	-10.73136300	-4.07936300	1.05916000
H	-12.05872400	-4.57056600	-0.98728700
H	-10.69716300	-4.10188000	-2.01728200
H	-10.58008600	-5.54324000	-1.00202000
C	-10.49592400	-0.01494900	3.68155500
C	-11.11913500	1.13752000	4.46503000
H	-10.79579000	-0.97252400	4.12049100
H	-10.89177000	-0.01884800	2.65893600
H	-12.20676900	1.04023000	4.50483900
H	-10.74297600	1.15316300	5.49236400
H	-10.88240300	2.10357600	4.01011500
C	-10.53175200	3.56923000	-0.07224700

C	-11.10334700	4.34326300	-1.25678000
H	-10.89265800	4.00132700	0.86791200
H	-10.90782000	2.53968400	-0.09655700
H	-12.19573700	4.34174800	-1.23691800
H	-10.76483900	5.38359400	-1.23778800
H	-10.77977200	3.90627700	-2.20567600
C	-10.42457400	-0.17337200	-3.60563000
C	-11.03284300	0.95453800	-4.43421400
H	-10.82316600	-0.13469800	-2.58538400
H	-10.73182100	-1.14380500	-4.01115900
H	-12.12253500	0.87802700	-4.46373900
H	-10.77220200	1.93339700	-4.02117200
H	-10.66255200	0.92032500	-5.46333200
O	0.32069400	0.05543500	4.47984800
H	-1.35951100	2.07205400	4.19185100
H	-1.26412500	-4.25607300	2.10313600
H	-1.39045300	4.34143700	-2.04429300
H	-1.29072600	-2.09741700	-4.13126900
O	0.36462000	-0.05014400	-4.30053400
O	0.40849700	-4.66310400	0.10758300
O	0.27172400	4.65083100	-0.02879700
C	8.92502800	2.68254800	-2.53483600
C	8.36604400	1.33003600	-2.98214200
C	8.30771800	3.12412000	-1.20662100
H	8.58772800	3.40787100	-3.28123800
C	8.94923400	0.10364400	-2.63331100
C	7.20801900	1.27358800	-3.76617500
C	8.84711700	2.77481700	0.03516500
C	7.15551300	3.91926400	-1.18947600

C	8.40164700	-1.14223100	-2.96227800
H	9.87714600	0.11761000	-2.06302400
C	6.66994000	0.06001000	-4.16556000
O	6.63631200	2.44250000	-4.23853100
C	8.27800800	3.13419400	1.26096800
H	9.75132400	2.16988500	0.05574200
C	6.58807600	4.33666500	0.00327800
O	6.61351500	4.38236200	-2.38067600
C	8.99435700	-2.46995100	-2.48977200
C	7.23974800	-1.13053300	-3.74171600
H	5.82205100	0.04313500	-4.83568600
C	5.41400800	2.81424300	-3.71446800
C	8.85410100	2.70119200	2.60587200
C	7.13132200	3.92853800	1.21272300
H	5.74299700	5.01087700	-0.00774400
C	5.40351400	3.83753500	-2.75566900
H	8.67843200	-3.21886400	-3.22234800
C	8.39236100	-2.90849700	-1.15398900
O	6.68811900	-2.32391100	-4.17227700
C	8.27704200	1.36282200	3.05685100
H	8.50796900	3.44111700	3.33360200
O	6.56843600	4.40258800	2.38844400
C	8.90485000	-2.49262900	0.07849500
C	7.28385200	-3.76194200	-1.11884500
C	5.48630900	-2.71453800	-3.61397200
C	3.03658100	2.74140800	-3.66147200
C	8.84846000	0.13952400	2.70352200
C	7.13811300	1.31700300	3.86432100
C	5.35646900	3.85898000	2.76146300

C	3.02634400	3.77085600	-2.70746800
C	8.36591000	-2.87305400	1.31199800
H	9.76026400	-1.82309900	0.08334900
C	6.73165500	-4.17775500	0.08244500
O	6.74366800	-4.25758200	-2.29893300
C	5.51551500	-3.73857300	-2.65618300
C	8.33407500	-1.09741900	3.09574300
H	9.71870000	0.14795100	2.05459600
C	6.61817800	0.11109400	4.31197400
O	6.55918100	2.49862200	4.30976900
C	5.35371700	2.86095700	3.74856300
C	8.94832700	-2.41739400	2.64726500
C	7.25480200	-3.71876900	1.28273900
H	5.91770200	-4.88982500	0.08442500
C	3.10839700	-2.69956300	-3.52191600
C	7.20090400	-1.08247800	3.91326600
H	5.78419700	0.10542700	5.00046900
C	2.97960000	3.80043800	2.68913200
H	8.63819800	-3.16615000	3.38236400
O	6.70681400	-4.18596800	2.46914200
C	3.13595800	-3.73312100	-2.57215600
O	6.67895000	-2.27788800	4.39574000
C	2.97602300	2.79492200	3.66716700
C	5.48844400	-3.66344800	2.85334400
C	5.47530400	-2.68527900	3.86042900
C	3.10652400	-3.63956300	2.79968800
C	3.09512600	-2.66614700	3.81051300
C	4.33597500	-4.27759000	-2.14060000
C	4.27639400	-2.19226100	-4.07117800

C	4.22505900	2.26568000	-4.19526400
C	4.20450600	4.34548000	-2.25640400
C	4.29829500	-4.16396100	2.32181000
C	4.27255900	-2.18998900	4.36483900
C	4.16510200	4.35670300	2.23481000
C	4.15635700	2.32568000	4.22293300
H	4.37138200	-5.11537500	-1.45521200
H	4.25662800	-1.45171700	-4.86079900
H	4.31791400	-4.95395100	1.58107900
H	4.23948600	1.52271500	-4.98301900
H	4.27471000	-1.47774100	5.18047000
H	4.20746800	5.18042600	-1.56695700
H	4.17918000	5.17520700	1.52587600
H	4.16082600	1.59826700	5.02507100
C	0.97804400	-3.26492900	-3.04122200
C	0.88781900	3.21999300	-3.16802600
C	0.83481800	3.28726700	3.15994800
C	0.95669500	-3.13034800	3.25922800
N	1.76101600	-2.38322500	4.08030800
N	1.77834600	-3.91718600	2.49649300
N	1.64381100	2.51065400	3.94604500
N	1.64941000	4.09227700	2.40857800
N	1.69255700	4.05484900	-2.43739600
N	1.70853600	2.43736500	-3.93855300
N	1.77170700	-2.44232100	-3.79732800
N	1.81324900	-4.07029400	-2.30865700
H	1.34210200	1.57604100	-4.35029200
H	1.44626900	-4.56858900	-1.49565300
H	1.38008400	-1.55106100	4.53303400

H	1.27506100	4.56618800	1.58384600
C	10.39016600	2.72014200	2.63487100
C	10.96309700	4.10953000	2.36722400
H	10.80684000	2.00752800	1.91326700
H	10.70795600	2.36668400	3.62175600
H	12.05247400	4.10836000	2.45357800
H	10.70234800	4.45875900	1.36403500
H	10.56749000	4.83509700	3.08444400
C	10.48462700	-2.38770400	2.64917000
C	11.09761200	-3.75884000	2.37627000
H	10.80876100	-2.01982800	3.62880300
H	10.86494900	-1.66645700	1.91639800
H	12.18777100	-3.72133700	2.44338300
H	10.73852100	-4.49429200	3.10262600
H	10.83098900	-4.11938400	1.37863600
C	10.53054800	-2.46983000	-2.46736300
C	11.13626800	-2.23241200	-3.84829000
H	10.85646300	-3.43991200	-2.07667600
H	10.91386200	-1.72137800	-1.76360800
H	12.22713300	-2.28429300	-3.81287200
H	10.78408900	-2.98630500	-4.55884100
H	10.85605400	-1.25079800	-4.24145600
C	10.46029000	2.72519500	-2.51351900
C	11.07083300	2.48251000	-3.89117000
H	10.86582600	1.99788200	-1.79986300
H	10.75948000	3.70979900	-2.13793700
H	12.15977100	2.56549200	-3.85779700
H	10.81772500	1.48689300	-4.26706100
H	10.69686700	3.21449400	-4.61324600

O	-0.28470900	-3.11577100	3.23555700
H	1.40769900	-4.40590700	1.67650500
H	1.27094700	1.66742200	4.39044700
H	1.37195600	-1.60467700	-4.22935100
H	1.30937600	4.54300300	-1.62486500
O	-0.35223900	3.19735100	-3.15577300
O	-0.40707700	3.28616400	3.15118700
O	-0.26155900	-3.29888200	-3.04767700
C	-6.69109400	0.31071600	0.29465800
H	-6.56580900	1.40164400	0.19238100
H	-6.47026000	0.05074500	1.34401100
C	-5.69774800	-0.38459400	-0.60270200
C	-4.31473000	0.16563000	-0.30116300
H	-5.96712300	-0.21933700	-1.65303800
H	-5.73975700	-1.46761900	-0.42032500
C	-3.17511600	-0.73047200	-0.74790200
H	-4.20920300	1.16543000	-0.74783900
H	-4.22380100	0.31195000	0.78693100
C	-1.85646600	-0.22141500	-0.19792100
H	-3.35324800	-1.75149900	-0.37854000
H	-3.14241800	-0.79847700	-1.84368700
H	-1.66161100	0.79381300	-0.57403000
H	-1.95286300	-0.12582200	0.89407400
C	-0.66376300	-1.10782900	-0.50225300
C	0.52772500	-0.70065600	0.34550100
H	-0.40625900	-1.05038800	-1.56990000
H	-0.92009500	-2.15789300	-0.30841300
C	1.82704900	-1.35946400	-0.07279900
H	0.31724000	-0.91469100	1.40398500

H	0.65108600	0.39041600	0.27637100
C	3.01357400	-0.79025800	0.68557700
H	1.97955200	-1.18501900	-1.15024000
H	1.76143000	-2.44914300	0.05753600
C	4.33404800	-1.16318200	0.04477000
H	2.93207100	0.30630800	0.69799400
H	2.98950600	-1.10570600	1.73741700
C	5.54274800	-0.47917400	0.67870700
H	4.28018400	-0.88420900	-1.02083100
H	4.47405300	-2.25351200	0.05503100
C	6.53933300	-0.17358200	-0.41484600
H	5.25903100	0.44568900	1.19950800
H	6.01787000	-1.12805200	1.42264300
H	6.61821100	-1.05877200	-1.06296300
H	6.16450300	0.65619600	-1.04035900
O	-7.99519600	-0.08333700	-0.05153500
H	-8.58541800	0.33073500	0.58569600
O	7.78529500	0.14509300	0.15295000
H	8.34310000	0.46468200	-0.56251200

Coordinates in Angstrom units for the second lowest minimum energy geometry of 1,12-dodecanediol (structure b)

C	8.86234900	-2.76784500	2.37904600
C	8.30486000	-1.43899100	2.87396800
C	8.24370700	-3.13761900	1.03633700
H	8.52485400	-3.52732400	3.08892800
C	8.86497500	-0.20591100	2.54125600
C	7.17493400	-1.43411200	3.69721900

C	8.75500200	-2.64026100	-0.16590500
C	7.13567000	-3.97531500	0.96298200
C	8.35769700	1.02189600	2.99889000
H	9.74263200	-0.19078200	1.90120400
C	6.65667300	-0.23977500	4.18977900
O	6.61582200	-2.63219900	4.10073700
C	8.21412000	-2.95674400	-1.41444800
H	9.61528600	-1.97912200	-0.12950900
C	6.57982000	-4.33153600	-0.25803200
O	6.58683100	-4.51152500	2.12357700
C	8.98647500	2.36260200	2.62739200
C	7.23686300	0.96537700	3.83017400
H	5.83156300	-0.25880500	4.88446000
C	5.39887700	-2.98800600	3.54001600
C	8.81958300	-2.42362800	-2.70874600
C	7.11067000	-3.80355700	-1.43726600
H	5.75542700	-5.02343500	-0.30211600
C	5.38787600	-3.96233600	2.53838300
H	8.67556900	3.06511000	3.40668400
C	8.41115700	2.90694100	1.32258500
O	6.72214400	2.13225200	4.37794200
C	8.26462800	-1.04774000	-3.05890500
H	8.47691800	-3.09766300	-3.49875600
O	6.55034000	-4.19415800	-2.64359800
C	8.95926100	2.61023000	0.06731100
C	7.28644400	3.73128500	1.34691700
C	5.51415700	2.56552700	3.87131400
C	3.01983000	-2.87811400	3.46847900
C	8.86330600	0.14864600	-2.64921000

C	7.13327200	-0.95335400	-3.86835800
C	5.34168600	-3.60863500	-2.97932800
C	3.00993600	-3.86140200	2.47584700
C	8.42443900	3.09499500	-1.14071800
H	9.83151300	1.96874400	0.02337200
C	6.74054700	4.24476200	0.17194100
O	6.74231900	4.12442000	2.55724900
C	5.51766000	3.58643100	2.92184600
C	8.37909800	1.41103400	-3.01283800
H	9.74417900	0.09535900	-2.01393600
C	6.64289600	0.27964700	-4.27992700
O	6.55504500	-2.10399300	-4.37417900
C	5.34360700	-2.52338400	-3.85326400
C	9.00593300	2.70948500	-2.50497800
C	7.29717200	3.90613600	-1.05162700
H	5.90848200	4.92669400	0.22159800
C	3.13496300	2.56058600	3.85418900
C	7.24803500	1.44377600	-3.83284600
H	5.81250600	0.32391100	-4.96598400
C	2.96092000	-3.58443700	-2.94832900
H	8.68771300	3.49467300	-3.19755800
O	6.72866100	4.43778500	-2.20449000
C	3.13716800	3.58453500	2.90095600
O	6.72062300	2.66297000	-4.24121100
C	2.95873300	-2.49098600	-3.82032700
C	5.51102500	3.91617600	-2.61130000
C	5.50831800	3.01349200	-3.67161200
C	3.12947000	3.83282700	-2.53242500
C	3.12758900	2.92850100	-3.60074400

C	4.33055700	4.13137800	2.43293600
C	4.30953600	2.04695800	4.37189600
C	4.21702400	-2.44133000	4.03510800
C	4.17838100	-4.43025500	2.00293100
C	4.31623700	4.36007200	-2.03350700
C	4.31008000	2.51963100	-4.20529800
C	4.14311400	-4.17178000	-2.52050400
C	4.15282300	-1.94982100	-4.30256700
H	4.34228800	4.96661200	1.75178800
H	4.32045700	1.30340000	5.15585300
H	4.32313700	5.10533400	-1.25274200
H	4.23247500	-1.72732000	4.84364300
H	4.31767700	1.87640700	-5.06922900
H	4.18151600	-5.21489300	1.25984600
H	4.15544300	-5.05005700	-1.89520600
H	4.16122700	-1.14642600	-5.02046000
C	0.99763100	3.10835700	3.39617100
C	0.87521700	-3.26071300	2.91325800
C	0.83610000	-3.05294100	-3.41854500
C	0.95849600	3.34401300	-3.03050800
N	1.80307500	2.65285200	-3.89711300
N	1.80626000	4.08440900	-2.21470500
N	1.63383200	-2.19914500	-4.10257200
N	1.62335600	-3.92303500	-2.73317200
N	1.66839400	-4.08747100	2.15216600
N	1.70548800	-2.54335900	3.72896300
N	1.79617500	2.29718200	4.15757600
N	1.81047900	3.91290600	2.65298500
H	1.34284400	-1.71777500	4.22429100

H	1.43297800	4.40252400	1.83544100
H	1.41450600	1.86040300	-4.41006600
H	1.24318900	-4.43154500	-1.93075000
C	10.35585900	-2.46217000	-2.71323100
C	10.90561600	-3.87739300	-2.54665100
H	10.77035000	-1.81712900	-1.92979800
H	10.69578300	-2.03754400	-3.66383400
H	11.99553200	-3.88499400	-2.61858200
H	10.62585000	-4.29742400	-1.57664400
H	10.51033000	-4.53966200	-3.32304400
C	10.53957300	2.67169000	-2.51985000
C	11.16168300	4.02221400	-2.17820700
H	10.85321500	2.35467000	-3.52025500
H	10.92074800	1.90856200	-1.83011900
H	12.25113100	3.98206800	-2.25442700
H	10.80248400	4.79726800	-2.86187200
H	10.90451100	4.33093600	-1.16058900
C	10.52250100	2.32741000	2.63211500
C	11.09166100	1.99358900	4.00741900
H	10.88041900	3.31089600	2.30683200
H	10.90250200	1.60993300	1.89478400
H	12.18434900	2.01469400	3.99721600
H	10.74606700	2.71524100	4.75467800
H	10.77487000	0.99954100	4.33675500
C	10.39806000	-2.81191700	2.35497400
C	11.00487300	-2.64005400	3.74481900
H	10.80447100	-2.04918900	1.68098600
H	10.69669700	-3.77699700	1.93135500
H	12.09460600	-2.71548600	3.70980200

H	10.74534200	-1.66666400	4.17094800
H	10.63352800	-3.41070000	4.42674700
O	-0.23785600	3.32307200	-3.01634100
H	1.42563200	4.48236000	-1.34931000
H	1.25581800	-1.31961000	-4.48073500
H	1.41200400	1.45192000	4.57207200
H	1.28977100	-4.50944500	1.30786200
O	-0.36179200	-3.20424100	2.88218200
O	-0.43461600	-3.05750500	-3.43344600
O	-0.25228400	3.12454900	3.41062200
C	-8.92038600	-0.03189300	3.64264500
C	-8.37946400	-1.28957200	2.96673200
C	-8.28065400	1.23088300	3.06631500
H	-8.58504200	-0.08983500	4.68434600
C	-8.99884700	-1.88074800	1.84414100
C	-7.23680000	-1.89980400	3.45677300
C	-8.80581600	1.89107200	1.95355800
C	-7.14958200	1.79700700	3.66269700
C	-8.46387400	-3.01401000	1.19021600
H	-9.89613800	-1.42923800	1.45136900
C	-6.71196500	-3.05164500	2.86060300
O	-6.64764500	-1.43246300	4.62019000
C	-8.25162400	3.05917600	1.41803400
H	-9.68785500	1.47486100	1.47425700
C	-6.58091700	2.96067100	3.17184600
O	-6.61394200	1.24002000	4.81576200
C	-9.06497500	-3.54070900	-0.12057300
C	-7.31095400	-3.55462200	1.72065400
H	-5.86419200	-3.54217000	3.30329400

C	-5.41758800	-0.80534600	4.53781200
C	-8.83133300	3.77064500	0.20290000
C	-7.11408500	3.57184700	2.04138100
H	-5.74768600	3.41724100	3.68666900
C	-5.40736900	0.59279000	4.66526700
H	-8.74668200	-4.58785900	-0.18899200
C	-8.44139400	-2.83782400	-1.33916300
O	-6.73582700	-4.68723000	1.13544400
C	-8.25405200	3.19726800	-1.08466100
H	-8.47597100	4.80478700	0.25906500
O	-6.55209700	4.75343300	1.59044700
C	-8.95330900	-1.63633000	-1.85074300
C	-7.32497900	-3.35889000	-1.95970300
C	-5.53122100	-4.52653400	0.48741900
C	-3.03854800	-0.81726900	4.45327000
C	-8.82405200	2.08299500	-1.71660700
C	-7.13709100	3.76431100	-1.68110500
C	-5.33947600	4.65420300	0.93689700
C	-3.03130000	0.58192300	4.58688000
C	-8.37832300	-0.97307400	-2.95290600
H	-9.83017900	-1.19851100	-1.38900800
C	-6.73561900	-2.74994700	-3.05964800
O	-6.77652700	-4.57171100	-1.53140300
C	-5.55246100	-4.48919100	-0.90897900
C	-8.31743000	1.54024400	-2.90425800
H	-9.68467700	1.61250700	-1.25878700
C	-6.63473800	3.28575400	-2.88585700
O	-6.54383600	4.88904400	-1.11454900
C	-5.34222200	4.70780900	-0.47080400

C	-8.95472700	0.31146700	-3.54427100
C	-7.26106900	-1.54939400	-3.53109300
H	-5.91801100	-3.22340200	-3.57395600
C	-3.15399500	-4.44323800	0.44499000
C	-7.21658000	2.16289000	-3.47157200
H	-5.81464200	3.78947500	-3.37119800
C	-2.96329500	4.54115400	0.93877300
H	-8.63868500	0.32214500	-4.59428900
O	-6.71469100	-0.99174700	-4.68434400
C	-3.16844700	-4.41865800	-0.95465200
O	-6.68915500	1.70360000	-4.67623000
C	-2.96368300	4.57884900	-0.46693700
C	-5.49550600	-0.36464900	-4.59179000
C	-5.48066600	1.04488000	-4.60188200
C	-3.11375000	-0.38240200	-4.55301400
C	-3.10232700	1.02190600	-4.56088300
C	-4.36981600	-4.46068100	-1.65549900
C	-4.31890600	-4.52055300	1.19120700
C	-4.23660700	-1.52875300	4.44998500
C	-4.20426200	1.30148700	4.71215700
C	-4.30503100	-1.09135500	-4.58705300
C	-4.27840500	1.74728700	-4.60102300
C	-4.14978300	4.59154900	1.65229600
C	-4.14025900	4.68115900	-1.18476800
H	-4.39880300	-4.51086500	-2.73420700
H	-4.30562700	-4.61733700	2.26553200
H	-4.32249500	-2.17368500	-4.62759000
H	-4.24571700	-2.61155300	4.41488400
H	-4.28166500	2.83309700	-4.65623800

H	-4.20888000	2.37251300	4.87350600
H	-4.16055100	4.61913900	2.73780900
H	-4.14901400	4.77373800	-2.26439500
C	-1.01152000	-4.46085800	-0.29243000
C	-0.89770600	-0.13802400	4.48956900
C	-0.82652100	4.52736600	0.24107100
C	-0.96073900	0.29790300	-4.50752900
N	-1.76327400	1.40757300	-4.54785400
N	-1.78761500	-0.79927900	-4.54092400
N	-1.62813000	4.57952500	-0.86706600
N	-1.63374500	4.52477300	1.33717400
N	-1.69244200	0.97037800	4.62379100
N	-1.71712400	-1.22359300	4.41711100
N	-1.81193400	-4.47781000	0.83233900
N	-1.85142800	-4.44514900	-1.36978200
H	-1.34685500	-2.11565700	4.06118700
H	-1.47649800	-4.17249800	-2.29455900
H	-1.37627500	2.30553800	-4.25397800
H	-1.25988400	4.24167700	2.25066200
C	-10.36584300	3.81542700	0.20290200
C	-10.92499200	4.56644300	1.40706200
H	-10.78932600	2.80451200	0.17297200
H	-10.68434500	4.30267100	-0.72572200
H	-12.01371900	4.63960700	1.35351100
H	-10.66391000	4.06340300	2.34283800
H	-10.51912900	5.58212300	1.45165600
C	-10.48714000	0.36088900	-3.53156500
C	-11.11406700	-0.76170400	-4.35498900
H	-10.79372100	1.33402300	-3.93105300

H	-10.87437000	0.32097400	-2.50658200
H	-12.20214600	-0.66927200	-4.37975400
H	-10.74773100	-0.73357100	-5.38554900
H	-10.86503000	-1.74276100	-3.93980800
C	-10.59469900	-3.51249900	-0.14383600
C	-11.21507700	-4.35219200	0.97074700
H	-10.92058600	-3.88382900	-1.12136200
H	-10.96863400	-2.48359400	-0.07558000
H	-12.30488300	-4.35633100	0.89762700
H	-10.86628300	-5.38712000	0.91311200
H	-10.94232800	-3.96450600	1.95630700
C	-10.45314000	0.04545700	3.66185600
C	-11.08523400	-1.10522700	4.44038800
H	-10.85938900	0.06585100	2.64313700
H	-10.73329000	1.00242700	4.11500000
H	-12.17254200	-1.00239000	4.47907300
H	-10.85255700	-2.07067700	3.98242300
H	-10.71030500	-1.12643000	5.46809500
O	0.27833500	0.28494300	-4.47979700
H	-1.42278400	-1.72886100	-4.33053400
H	-1.25228300	4.33579700	-1.78353500
H	-1.41507600	-4.23989500	1.73405000
H	-1.30875000	1.89528600	4.43894200
O	0.35348000	-0.14051600	4.47019200
O	0.42650900	4.51840100	0.24257700
O	0.22258100	-4.49462200	-0.30288100
C	6.64974700	0.26433500	0.09168800
H	6.64583300	0.94198100	0.96797300
C	5.72195200	-0.87822500	0.34158800

C	4.32315500	-0.31846900	0.63710400
H	6.07245000	-1.50656900	1.15255200
H	5.69179100	-1.49166200	-0.57228000
C	3.18875700	-1.19376900	0.13161800
H	4.21827400	-0.12980600	1.70998000
H	4.24236100	0.64535200	0.13373700
C	1.89188200	-0.39981600	0.12996000
H	3.41147000	-1.50932000	-0.89143200
H	3.08751100	-2.10224300	0.72391700
H	1.67173900	-0.03329900	1.14073000
H	2.04119300	0.48981000	-0.49174400
C	0.69562800	-1.17080100	-0.39639900
C	-0.42673900	-0.20426300	-0.73147100
H	0.35530600	-1.90713800	0.34035300
H	0.97976800	-1.74245100	-1.28931300
C	-1.77053300	-0.86856700	-0.95158200
H	-0.15094700	0.39343700	-1.60960200
H	-0.52957400	0.50834300	0.10097200
C	-2.86766800	0.16981000	-1.08831800
H	-1.99504600	-1.51412600	-0.08742600
H	-1.73638400	-1.52970800	-1.82881300
C	-4.24305800	-0.43372500	-0.89522800
H	-2.72137700	0.94100100	-0.32022500
H	-2.79078400	0.69141100	-2.05356400
C	-5.36586300	0.60779200	-0.89398000
H	-4.24149400	-0.96267900	0.06568200
H	-4.44310300	-1.20529100	-1.64680500
C	-6.36732700	0.25378700	0.16855700
H	-4.97642900	1.61448900	-0.73107300

H	-5.86935300	0.60866500	-1.87028300
H	-5.97824100	0.51662200	1.17441000
H	-7.31274900	0.80610000	0.02691000
H	7.69411000	-0.07627800	-0.05484200
O	6.15379800	0.90989500	-1.04923500
H	6.83334700	1.58526600	-1.31542100
O	-6.59057400	-1.13506200	0.08041200
H	-7.44035600	-1.31534300	0.43444500

Coordinates in Angstrom units for the lowest minimum energy geometry of 1,12-dicyanododecane (structure d)

C	-8.82332900	-2.08566600	2.78223900
C	-8.27660000	-2.69994400	1.49588000
C	-8.20475100	-0.72229000	3.05820400
H	-8.48867900	-2.74007900	3.59266500
C	-8.84433600	-2.43231100	0.24732500
C	-7.20510800	-3.60071400	1.52207900
C	-8.75537000	0.48186000	2.61010000
C	-7.02364300	-0.64311000	3.80220900
C	-8.41801700	-3.02830800	-0.94264000
H	-9.66603200	-1.72132300	0.19889900
C	-6.76531100	-4.22614200	0.36344800
O	-6.62108800	-3.95977200	2.72820200
C	-8.18021700	1.72849200	2.87559400
H	-9.68064200	0.44974400	2.04013900
C	-6.42782700	0.57624000	4.09231800
O	-6.50619200	-1.80304600	4.35352000
C	-9.02834700	-2.65652800	-2.28768200

C	-7.35396700	-3.93218700	-0.85869900
H	-5.96960000	-4.95782700	0.42174500
C	-5.37967400	-3.41997200	3.00967000
C	-8.77505200	3.04069400	2.38606000
C	-6.99576600	1.75096100	3.61884600
H	-5.56011200	0.61521100	4.73512900
C	-5.32468400	-2.29134400	3.84229000
H	-8.75616400	-3.45573100	-2.98271000
C	-8.38198100	-1.38138300	-2.81416600
O	-6.88405600	-4.56863200	-2.00267600
C	-8.20240700	3.36635600	1.01691500
H	-8.41456900	3.81769600	3.06533000
O	-6.46759200	2.97170500	3.99697500
C	-8.85662300	-0.10462800	-2.50015200
C	-7.25522400	-1.46251700	-3.63799700
C	-5.64262400	-4.13887000	-2.43787000
C	-2.99943200	-3.48685700	2.94671700
C	-8.73919100	2.81717300	-0.15025100
C	-7.08753500	4.20148100	0.88560000
C	-5.27005700	3.37955200	3.43940500
C	-2.95272700	-2.34921800	3.76724700
C	-8.26929400	1.07222500	-2.97667900
H	-9.73750600	-0.02221300	-1.86841500
C	-6.66480500	-0.32067100	-4.15968200
O	-6.76711900	-2.71110400	-3.99232100
C	-5.58432900	-3.13843100	-3.42157900
C	-8.22503000	3.06661700	-1.42395700
H	-9.59184500	2.14865600	-0.05985000
C	-6.56806100	4.49490200	-0.36692400

O	-6.54098900	4.81446300	2.00516300
C	-5.30536000	4.35191400	2.42962300
C	-8.83161300	2.46142300	-2.68314900
C	-7.14708700	0.93199500	-3.80011400
H	-5.85373400	-0.40124500	-4.87123500
C	-3.25915600	-4.22105200	-2.36197200
C	-7.12159800	3.92124200	-1.50315700
H	-5.73726200	5.18195700	-0.45501800
C	-2.89991800	3.35264800	3.32974400
H	-8.50499600	3.09721200	-3.51126800
O	-6.56356600	2.05910900	-4.34949400
C	-3.20484000	-3.20224800	-3.32650300
O	-6.60168400	4.25125900	-2.74730900
C	-2.92757400	4.34260900	2.33796300
C	-5.36759000	2.50150200	-3.81576500
C	-5.38416800	3.66898900	-3.03868800
C	-2.99527000	2.45240200	-3.66902200
C	-3.01120200	3.64449400	-2.92825100
C	-4.35562000	-2.66860600	-3.88560000
C	-4.47905600	-4.71918800	-1.92582300
C	-4.21245700	-4.04128900	2.56214000
C	-4.10580600	-1.74718500	4.23895800
C	-4.16428500	1.87779900	-4.14253900
C	-4.20334200	4.27062500	-2.60847100
C	-4.06100400	2.88776400	3.92278600
C	-4.12889600	4.87736100	1.89597500
H	-4.30939900	-1.93090800	-4.67689900
H	-4.54929800	-5.52983400	-1.21010400
H	-4.15055200	1.00023100	-4.77684900

H	-4.26674300	-4.94456300	1.96639100
H	-4.23369300	5.20690000	-2.06574900
H	-4.06987500	-0.91548000	4.93063100
H	-4.03967200	2.17350100	4.73625300
H	-4.17287200	5.66182700	1.14981900
C	-1.08711600	-3.75490500	-2.78606800
C	-0.83666000	-3.01940900	3.39911600
C	-0.77221800	3.77838400	2.71780100
C	-0.86228100	3.05082100	-3.25319700
N	-1.68712400	3.99427100	-2.70198100
N	-1.66203900	2.11650500	-3.86310000
N	-1.60038800	4.60237300	1.99948300
N	-1.56442200	3.04282500	3.56116200
N	-1.61617300	-2.08899000	4.03257500
N	-1.68030300	-3.88273000	2.74540700
N	-1.93939200	-4.55545700	-2.06303900
N	-1.86348200	-2.95010800	-3.57931000
H	-1.31883100	-4.48171200	1.99981500
H	-1.46510400	-2.08869700	-3.96768400
H	-1.30862500	4.63704900	-2.00272300
H	-1.21074900	2.17967300	3.97620200
C	-10.30944400	3.07409600	2.42327200
C	-10.85903900	2.89403400	3.83601100
H	-10.74004500	2.31198000	1.76300000
H	-10.62968200	4.03909100	2.01597800
H	-11.94793600	2.98508100	3.84849300
H	-10.59481900	1.91261600	4.24001600
H	-10.44840400	3.65175800	4.51010000
C	-10.36877800	2.49780700	-2.65914300

C	-10.99146300	2.10074900	-3.99468300
H	-10.66821800	3.51809300	-2.39630700
H	-10.76634700	1.85570200	-1.86431000
H	-12.07961400	2.19693600	-3.96138000
H	-10.62035400	2.74240800	-4.79966300
H	-10.75100000	1.06610000	-4.25554500
C	-10.56219900	-2.57744600	-2.25497900
C	-11.20496600	-3.91395700	-1.89659500
H	-10.90107600	-2.24875100	-3.24395700
H	-10.90293100	-1.81058400	-1.54958900
H	-12.29505100	-3.84391900	-1.92148400
H	-10.89877900	-4.69305700	-2.60126200
H	-10.90876100	-4.23678000	-0.89409600
C	-10.35959500	-2.06084700	2.82131000
C	-10.96679300	-3.45990800	2.76683800
H	-10.76598600	-1.45444400	2.00317000
H	-10.66040500	-1.55754000	3.74711700
H	-12.05605200	-3.41780300	2.84240100
H	-10.71132200	-3.96618600	1.83140600
H	-10.59382000	-4.07569500	3.59088600
O	0.37746500	3.06361500	-3.23069500
H	-1.30683200	1.18570800	-4.10282200
H	-1.24760800	5.04185000	1.14825500
H	-1.57983600	-5.02021500	-1.23102200
H	-1.21937200	-1.18394800	4.30570700
O	0.40224400	-3.08659000	3.44442000
O	0.46557600	3.72697700	2.64354400
O	0.15073600	-3.77417100	-2.74912500
C	8.88283800	-3.64480000	0.24839500

C	8.29559200	-2.90487500	1.44042700
C	8.25449500	-3.12216500	-1.03206200
H	8.57080000	-4.68789200	0.34592200
C	8.78791000	-1.66637700	1.85681600
C	7.21225200	-3.43506200	2.14830500
C	8.74026500	-2.00461000	-1.71549600
C	7.13358300	-3.76620000	-1.56386700
C	8.26793500	-0.94932200	2.93698500
H	9.62680300	-1.23733300	1.31375300
C	6.69905400	-2.77868600	3.25927500
O	6.66179500	-4.64887400	1.76062500
C	8.15330300	-1.50700100	-2.88353600
H	9.61473400	-1.49401600	-1.31912700
C	6.53814900	-3.31593700	-2.73086300
O	6.66053800	-4.92277500	-0.95879900
C	8.87417000	0.37887700	3.38455300
C	7.19685600	-1.53277400	3.62382500
H	5.90273200	-3.23136200	3.83587100
C	5.45064200	-4.62659300	1.08923800
C	8.68431300	-0.29082400	-3.63005100
C	7.03246400	-2.18554900	-3.36821600
H	5.71143700	-3.86125900	-3.16426100
C	5.45063600	-4.81547100	-0.30334100
H	8.56444100	0.51546900	4.42482100
C	8.30449800	1.56702800	2.61809100
O	6.63453100	-0.88513300	4.71399300
C	8.12030500	1.02656000	-3.10474400
H	8.31317300	-0.38484100	-4.65455000
O	6.42343300	-1.76180700	-4.53861900

C	8.87940100	2.08309400	1.45256600
C	7.18175000	2.23269000	3.11711200
C	5.42974800	-0.24948100	4.46705200
C	3.06451000	-4.63833800	1.07124100
C	8.72859400	1.74407900	-2.07384200
C	7.00848000	1.62047100	-3.71209800
C	5.21423900	-1.11449600	-4.36101800
C	3.06828200	-4.85851800	-0.31523600
C	8.37904500	3.20589300	0.78680000
H	9.76300900	1.59493300	1.04772400
C	6.67391700	3.36777300	2.49952300
O	6.63220700	1.81026900	4.31818500
C	5.43098200	1.13700200	4.25300600
C	8.30812700	3.01352500	-1.66926500
H	9.57895600	1.29748600	-1.56411800
C	6.58674600	2.89667200	-3.36581600
O	6.35816100	0.95223000	-4.73853800
C	5.19073800	0.28769700	-4.41533100
C	8.97619100	3.73243000	-0.50935900
C	7.25637200	3.83640300	1.33010800
H	5.86158100	3.91406100	2.95772300
C	3.05764500	-0.27563000	4.26480000
C	7.21587900	3.57923700	-2.33261300
H	5.76250600	3.35533000	-3.89694900
C	2.85817000	-1.15564600	-4.04355200
H	8.68979300	4.78448000	-0.58244000
O	6.80060500	5.00501200	0.74497300
C	3.06219800	1.11156300	4.04951100
O	6.77594500	4.85081400	-1.98509100

C	2.83881500	0.24727100	-4.07277400
C	5.58088400	4.98001600	0.09372800
C	5.56831300	4.92564900	-1.30803400
C	3.20523400	5.04114300	0.11908200
C	3.18847800	4.99143900	-1.28124100
C	4.24118800	1.83596800	4.05485000
C	4.23580100	-0.97108000	4.48756600
C	4.24754000	-4.54108800	1.79174000
C	4.25968300	-4.96418200	-1.01575900
C	4.39790100	5.07145000	0.82220700
C	4.36684700	4.97153100	-2.01288300
C	4.04451200	-1.85501800	-4.19164000
C	3.99476500	0.98666300	-4.26473100
H	4.24613100	2.91122500	3.93607100
H	4.24156800	-2.03283500	4.70096300
H	4.42305300	5.17307500	1.89996300
H	4.24900600	-4.43518300	2.87003000
H	4.37156000	4.97561500	-3.09630000
H	4.28577400	-5.18023400	-2.07697600
H	4.07123500	-2.93682500	-4.22429600
H	3.97444100	2.06742400	-4.32743400
C	0.91989200	0.41657300	4.05274200
C	0.91842900	-4.80152200	0.37988800
C	0.71340000	-0.47516300	-3.92084500
C	1.04820700	5.04679500	-0.54689900
N	1.84772800	5.02683200	-1.66627000
N	1.88064700	5.10671300	0.54035400
N	1.50912300	0.63258800	-3.98909500
N	1.53569700	-1.57015900	-3.94413400

N	1.73959100	-4.98372800	-0.70652600
N	1.73397900	-4.62200400	1.47033400
N	1.72753300	-0.67416400	4.25935000
N	1.73840500	1.50570600	3.92392600
H	1.35362300	-4.24617300	2.34394900
H	1.37722100	2.40633600	3.59023100
H	1.46394100	4.64600700	-2.52783100
H	1.17578400	-2.49608400	-3.70324300
C	10.22027000	-0.26703800	-3.70432000
C	10.79354300	-1.49666800	-4.40321900
H	10.66148900	-0.17647000	-2.70354800
H	10.51167400	0.64127500	-4.24286400
H	11.87884800	-1.41695700	-4.50531800
H	10.57180300	-2.41038300	-3.84390700
H	10.36588600	-1.60754700	-5.40447500
C	10.50876200	3.66766400	-0.56357000
C	11.16510900	4.50874000	0.52793100
H	10.81949300	4.02581300	-1.55118300
H	10.86655400	2.63379200	-0.49422300
H	12.25346600	4.50358200	0.42706900
H	10.82478100	5.54696000	0.47300500
H	10.91487700	4.12953900	1.52338400
C	10.41241100	0.36260800	3.36781200
C	11.00139300	-0.67734100	4.31671600
H	10.75619300	1.36407800	3.65031700
H	10.79494500	0.18951600	2.35476700
H	12.09337500	-0.63664100	4.31119200
H	10.66120400	-0.50265100	5.34205700
H	10.69832500	-1.68953600	4.03300600

C	10.41855500	-3.62862500	0.22016400
C	11.02410700	-4.31921500	1.43923300
H	10.80284600	-2.60436300	0.15063500
H	10.73996000	-4.13495600	-0.69692100
H	12.11469200	-4.34353700	1.37723600
H	10.74838900	-3.80211500	2.36302600
H	10.66591700	-5.35046700	1.51661200
O	-0.19049200	5.04444000	-0.52107600
H	1.51279500	4.86152100	1.46034900
H	1.15070200	1.58294400	-3.81651300
H	1.35996200	-1.62492400	4.17357700
H	1.34564500	-4.85467200	-1.63738800
O	-0.32030600	-4.82025800	0.37732300
O	-0.53065800	-0.48869900	-3.88771200
O	-0.32086800	0.42355100	4.02277100
C	-6.28303500	0.29531200	0.19192000
H	-6.66157500	-0.16561900	1.11114400
H	-7.11498200	0.82378800	-0.27962400
C	-5.71187600	-0.78335500	-0.73395900
C	-4.52699800	-1.52376400	-0.11602500
H	-5.41991700	-0.32746400	-1.68856600
H	-6.52752200	-1.47164700	-0.94467500
C	-3.18303700	-0.97111100	-0.56211200
H	-4.59653500	-1.47881500	0.98541000
H	-4.57043500	-2.58833100	-0.37262600
C	-2.02844800	-1.60141100	0.19099000
H	-3.06034100	-1.13721000	-1.64300400
H	-3.14745800	0.11404000	-0.41567000
H	-2.09459400	-1.30946500	1.25086400

H	-2.10322700	-2.69992700	0.16936000
C	-0.68444400	-1.17640600	-0.37018700
C	0.45318400	-1.40526200	0.60758700
H	-0.71551500	-0.11306100	-0.64535300
H	-0.47879100	-1.71939500	-1.30303100
C	1.79243900	-1.33391400	-0.09785200
H	0.33555400	-2.38087000	1.08968100
H	0.39795800	-0.65968900	1.41521800
C	2.99005500	-1.18027300	0.82131500
H	1.78830600	-0.47781700	-0.79023800
H	1.91270800	-2.22758900	-0.73145600
C	4.26591000	-1.18307600	-0.00440300
H	2.90836000	-0.22349700	1.35901500
H	3.00524100	-1.96680100	1.58978200
C	5.50911900	-0.70878800	0.74424800
H	4.08671300	-0.51770100	-0.86082800
H	4.44022200	-2.18013800	-0.43296100
C	6.42441700	0.07434300	-0.20380400
H	5.23134200	-0.05271000	1.58079200
H	6.05347200	-1.55559700	1.15809100
H	7.37252000	0.36754200	0.25885300
H	6.64879600	-0.51941500	-1.09460700
C	5.67209300	1.27023900	-0.59051700
N	4.92777700	2.14514100	-0.73317000
C	-5.25279500	1.25887200	0.57591000
N	-4.35783200	1.94508500	0.84979400

Coordinates in Angstrom units for the lowest minimum energy geometry of 1,14-tetradecanedicarboxylic acid (structure e)

C	8.81849400	-3.08004300	-1.87652900
C	8.25824100	-3.16524100	-0.46467300
C	8.15332400	-1.93741800	-2.62115800
H	8.52190100	-4.00060600	-2.38598700
C	8.75559700	-2.38540200	0.57954100
C	7.21367200	-4.04319400	-0.16480600
C	8.63770900	-0.62811200	-2.56751500
C	7.01796500	-2.17623900	-3.39789800
C	8.28227400	-2.46719400	1.89182100
H	9.55848200	-1.68392400	0.36301500
C	6.73370600	-4.17084500	1.12827500
O	6.69095500	-4.85005100	-1.17023400
C	8.02732400	0.43415600	-3.23418300
H	9.54288800	-0.43237900	-1.99871000
C	6.38709000	-1.14631400	-4.08150800
O	6.56353000	-3.48283400	-3.54897300
C	8.87991700	-1.62122100	3.00870000
C	7.24920900	-3.37402000	2.14155800
H	5.95351400	-4.88628400	1.35180400
C	5.45618900	-4.49909300	-1.67388600
C	8.59286900	1.84656800	-3.24794100
C	6.86535400	0.15022800	-3.95646200
H	5.54701800	-1.35344800	-4.73165200
C	5.39291500	-3.82006200	-2.90384600
H	8.56982800	-2.09261500	3.94567500
C	8.28311600	-0.22198300	3.01946200

O	6.73543800	-3.51635000	3.42530200
C	8.05980900	2.67939900	-2.09377100
H	8.21646300	2.31494200	-4.16152200
O	6.24308400	1.18167400	-4.64116700
C	8.84336400	0.86303300	2.34184100
C	7.12130300	0.01709900	3.76034700
C	5.48764500	-2.93900200	3.58944900
C	3.07204200	-4.55041300	-1.57657500
C	8.62873400	2.61926600	-0.81976300
C	6.99816400	3.56942700	-2.27816600
C	5.10538600	1.72990000	-4.08785900
C	3.01151300	-3.87736900	-2.80779300
C	8.30021500	2.15055400	2.38810100
H	9.74938900	0.70365700	1.76280600
C	6.58481300	1.29275200	3.87474900
O	6.57848300	-1.02069700	4.49131200
C	5.41343000	-1.61576400	4.04867800
C	8.21383200	3.41618400	0.24875900
H	9.43741600	1.91305900	-0.65033000
C	6.55964200	4.38212400	-1.24021100
O	6.39227500	3.68501400	-3.52745800
C	5.16463500	3.05179500	-3.61135600
C	8.87848600	3.32666100	1.61508900
C	7.15929800	2.34221200	3.17121400
H	5.75950100	1.47160600	4.55031700
C	3.11833000	-3.02880500	3.43753600
C	7.15243800	4.29548500	0.01328500
H	5.76462700	5.09679600	-1.41187600
C	2.78019900	1.67711600	-3.60861900

H	8.59157000	4.22945700	2.16103000
O	6.65627300	3.62705700	3.30734600
C	3.05283000	-1.68504500	3.82923600
O	6.70060100	5.13057400	1.03137700
C	2.81840900	3.02535600	-3.22193400
C	5.45495500	3.95074500	2.71179900
C	5.47944800	4.77591100	1.57525900
C	3.07653900	3.98448800	2.67127800
C	3.09875200	4.85152800	1.56835000
C	4.18798000	-0.96873100	4.17006900
C	4.33762800	-3.67656900	3.31817100
C	4.29196000	-4.88255300	-1.00509000
C	4.16412300	-3.52850600	-3.49664400
C	4.24478400	3.55212700	3.27769400
C	4.29960900	5.26819300	1.01420800
C	3.90574500	1.02287900	-4.08055100
C	4.01178700	3.73058700	-3.21968700
H	4.12318600	0.04164800	4.55300600
H	4.41513800	-4.71819600	3.03066200
H	4.22704600	2.94620300	4.17458600
H	4.35597200	-5.43264300	-0.07485000
H	4.34421500	5.95438000	0.17674700
H	4.12685200	-3.05539300	-4.47023700
H	3.86331100	-0.00412300	-4.41941000
H	4.07202500	4.76600300	-2.90661200
C	0.94203000	-2.43175400	3.57814600
C	0.90053000	-4.29718800	-2.13262800
C	0.71874000	2.26438100	-2.95327400
C	0.94113100	4.44778000	2.10955800

N	1.77308200	5.14311700	1.26720900
N	1.74280500	3.77013000	2.99746300
N	1.51951400	3.36936000	-2.86432100
N	1.47419800	1.24433800	-3.44112700
N	1.66696700	-3.75608200	-3.13932200
N	1.75952400	-4.81197400	-1.19854900
N	1.80243100	-3.46465500	3.30059800
N	1.70907900	-1.34640400	3.90496600
H	1.41070800	-5.09434100	-0.27789700
H	1.33273200	-0.39290800	3.92990500
H	1.38558800	5.49625100	0.39573200
H	1.11437700	0.27735400	-3.49633100
C	10.12886200	1.87882900	-3.32263200
C	10.66978000	1.19833300	-4.57723900
H	10.57606000	1.41940300	-2.43331800
H	10.43691300	2.92989300	-3.30437500
H	11.75601100	1.30018200	-4.63957700
H	10.42788600	0.13176900	-4.58610800
H	10.23611100	1.64563300	-5.47692400
C	10.41204100	3.31349300	1.52438100
C	11.07850400	3.37647900	2.89609800
H	10.71441200	4.17600300	0.92068200
H	10.76849500	2.42937200	0.98269000
H	12.16590900	3.42711700	2.80083400
H	10.74584700	4.26135200	3.44712700
H	10.83122600	2.49784000	3.49868000
C	10.41634300	-1.61453100	2.98709500
C	11.00111500	-3.00859000	3.19596800
H	10.76134800	-0.93901600	3.77835400

H	10.79559600	-1.19908600	2.04604800
H	12.09318100	-2.97871700	3.21474000
H	10.65646200	-3.43418600	4.14324200
H	10.69339100	-3.68781000	2.39546800
C	10.35288900	-3.01236400	-1.91386000
C	11.00141500	-4.25831200	-1.31757600
H	10.72283800	-2.12433200	-1.38824800
H	10.65676800	-2.89313000	-2.96018200
H	12.09024100	-4.21039500	-1.39599800
H	10.74199100	-4.36834600	-0.26058100
H	10.66296900	-5.15873600	-1.83911100
O	-0.29554800	4.46252100	2.09091800
H	1.38249700	2.94040100	3.47596100
H	1.18648100	4.18145200	-2.33973000
H	1.46351800	-4.28125500	2.79333200
H	1.26660000	-2.99261800	-3.68335900
O	-0.33700200	-4.32836700	-2.10162300
O	-0.49366700	2.20638400	-2.65486200
O	-0.29897200	-2.48469500	3.57402600
C	-8.79219600	-3.55546200	1.04786700
C	-8.21998500	-3.29192500	-0.33515500
C	-8.13921400	-2.61284900	2.04234300
H	-8.48632400	-4.56776800	1.32550500
C	-8.73342800	-2.30003100	-1.16921200
C	-7.13027100	-4.02847900	-0.80888400
C	-8.62152200	-1.32496100	2.28484300
C	-7.00647900	-3.02396000	2.74907600
C	-8.22414400	-2.02260300	-2.43889300
H	-9.56957000	-1.70608200	-0.80851500

C	-6.63214900	-3.82098900	-2.08687300
O	-6.59218300	-5.03898600	-0.02446100
C	-8.02799300	-0.44934300	3.19544200
H	-9.51251500	-0.99699800	1.75518800
C	-6.38646200	-2.18189600	3.65970200
O	-6.55354900	-4.32814100	2.60689000
C	-8.81480700	-0.92628700	-3.31269800
C	-7.15707100	-2.80899100	-2.88136500
H	-5.82982400	-4.44326300	-2.46193900
C	-5.36990300	-4.83281300	0.58619600
C	-8.60916700	0.91545900	3.53819700
C	-6.88216800	-0.89959100	3.85369800
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C	-5.35233500	-4.50770700	1.95329100
H	-8.48230000	-1.13797200	-4.33289400
C	-8.25063800	0.44564600	-2.96549800
O	-6.61713200	-2.60176900	-4.14557700
C	-8.11788700	2.01077500	2.60454700
H	-8.21912000	1.16673100	4.52855400
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C	-8.84528900	1.31345300	-2.04662100
C	-7.12672700	0.91424400	-3.65369800
C	-5.39678200	-1.94891300	-4.11775300
C	-2.99160100	-4.99971900	0.61085700
C	-8.75296400	2.30065400	1.39640800
C	-7.02529100	2.81053500	2.95601000
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C	-8.38208400	2.61206700	-1.81554200

H	-9.72499000	0.97374200	-1.50572200
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O	-1.94300000	1.98842700	-0.13289000
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