

Supporting Information for:

Folded alkyl chains in water-soluble capsules and cavitands

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Experimental Procedures

General. All guests were obtained from TCI-America, Sigma-Aldrich, or Acros and used as received. ^1H and spectra were recorded using either a Bruker AV 600 or Bruker DRX 600 (^1H : 600.0 MHz) spectrometer at 298 K. Chemical shifts (δ) are reported in ppm shifted from tetramethylsilane (δ_{H} 0.00) and referenced to residual non-deuterated solvent HDO (D_2O : δ_{H} 4.79 ppm).¹ All NMR spectra were processed using MestReNova NMR processing software.

NMR Titrations. Solutions of **1a** were prepared to a final concentration ranging from 0.0080-0.0010 M. In each case, 400 μL of this solution was transferred to an NMR tube. Water insoluble guests including *n*-alkanes and 11-aminoundecanoic acid were added in excess, in neat 2 μL portions for liquids and as a spatula tip full for solids. The diol-based guests were dissolved in D_2O with concentrations ranging from 0.013-0.042 M, and were added to achieve a 1:1 host/guest molar ratio in the NMR tube. In all cases the NMR tubes containing the host/guest mixtures were sonicated for ≥ 3 h.

Alkane Competition Experiments

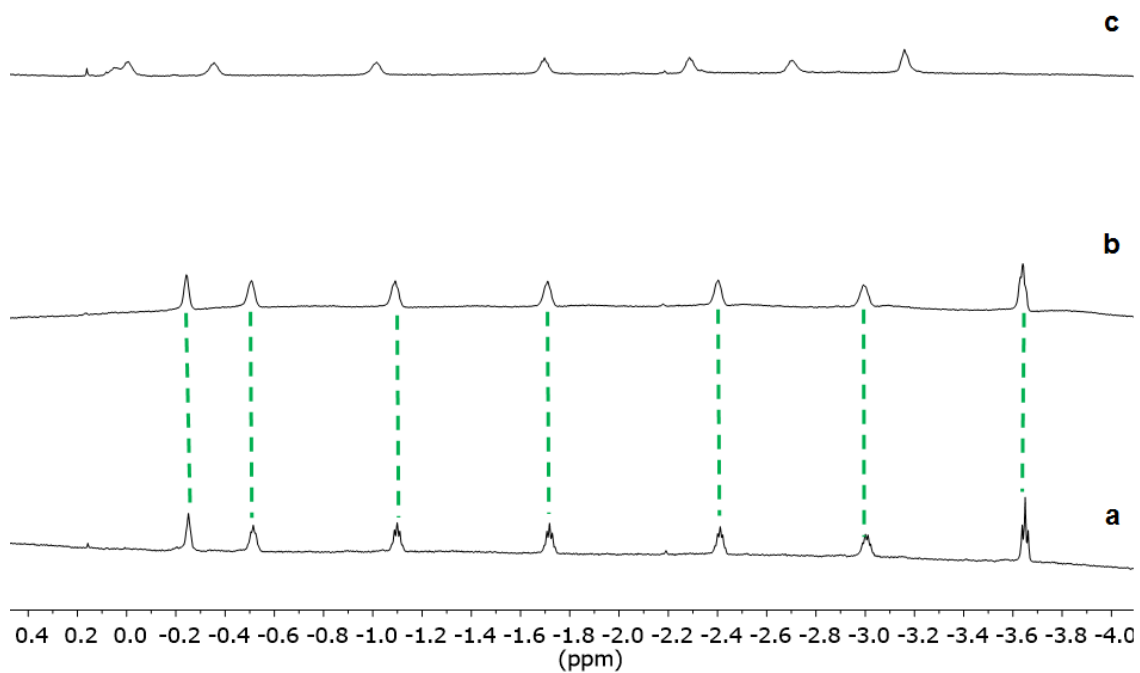


Fig. S1 Partial ^1H NMR (D₂O, 600 MHz) spectra of the upfield shifted resonances of **1.1** in the presence of a) *n*-tetradecane and *n*-pentadecane, b) *n*-tetradecane only and c) *n*-pentadecane only showing encapsulated guest(s).

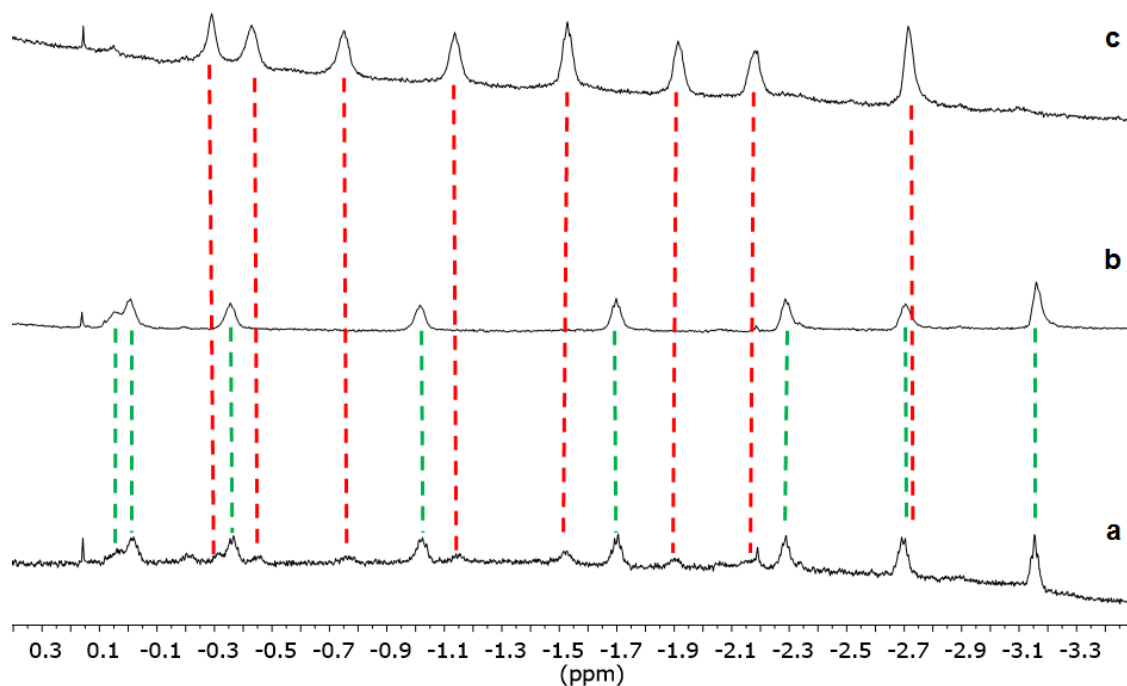


Fig. S2 Partial ^1H NMR spectra (D₂O, 600 MHz) of the upfield shifted resonances of **1.1** in the presence of a) *n*-pentadecane and *n*-hexadecane, b) *n*-pentadecane only and c) *n*-hexadecane only showing encapsulated guest(s).

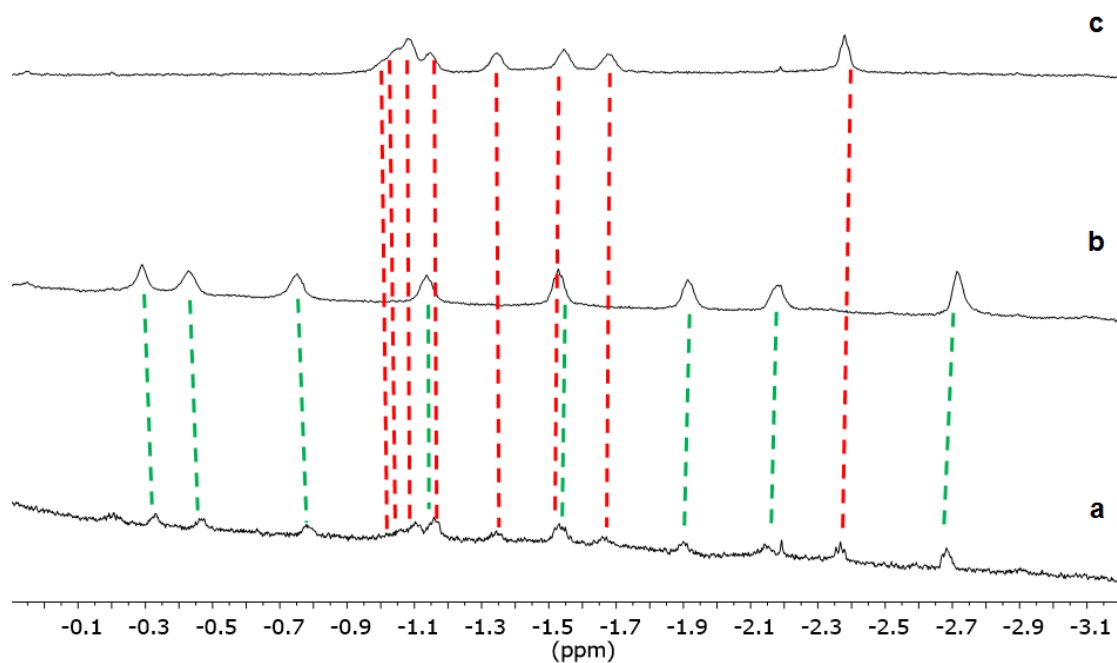


Fig. S3 Partial ^1H NMR (D_2O , 600 MHz) spectra of the upfield shifted resonances of **1.1** in the presence of a) *n*-hexadecane and *n*-heptadecane, b) *n*-hexadecane only and c) *n*-heptadecane only showing encapsulated guest(s).

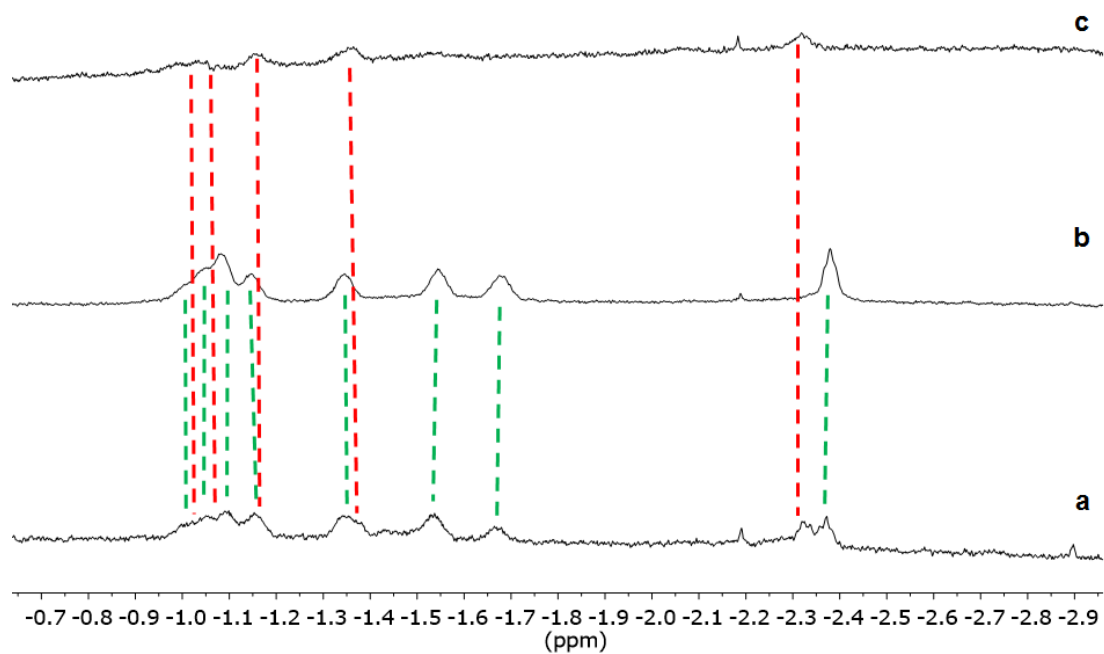


Fig. S4 Partial ^1H NMR (D_2O , 600 MHz) spectra of the upfield shifted resonances of **1.1** in the presence of a) *n*-heptadecane and *n*-octadecane, b) *n*-heptadecane only and c) *n*-octadecane only showing encapsulated guest(s).

2-D NMR of 1a with 11-Aminoundecanoic Acid

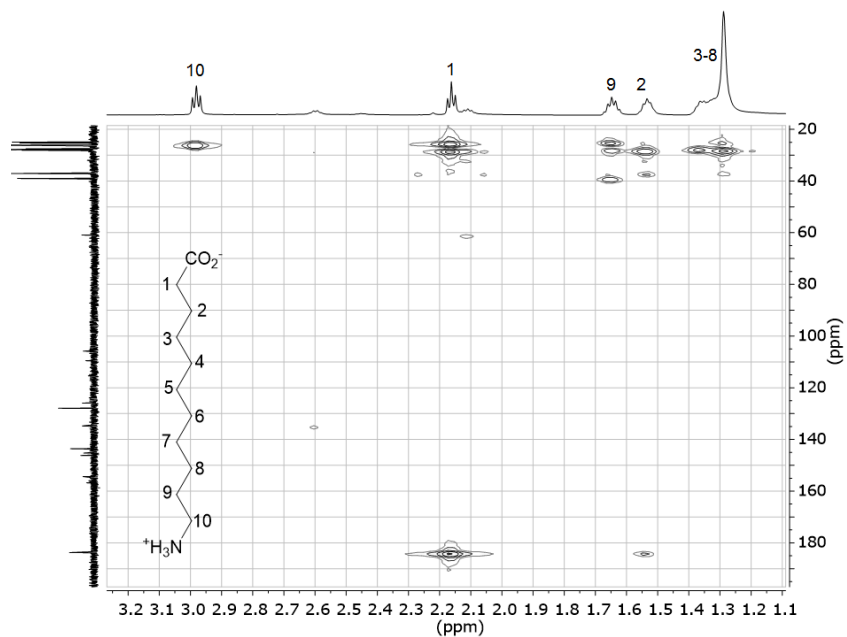


Fig. S5 Partial ^1H - ^{13}C HMBC spectra (D_2O) of **1a** with 11-aminoundecanoic acid highlighting that the methylene alpha to the ammonium in the “free” guest is the furthest downfield. This resonance is anticipated to be the furthest downfield for the “bound” species as well, and this assumption was made for the assignment of the “bound” signals in subsequent 2-D NMR analysis.

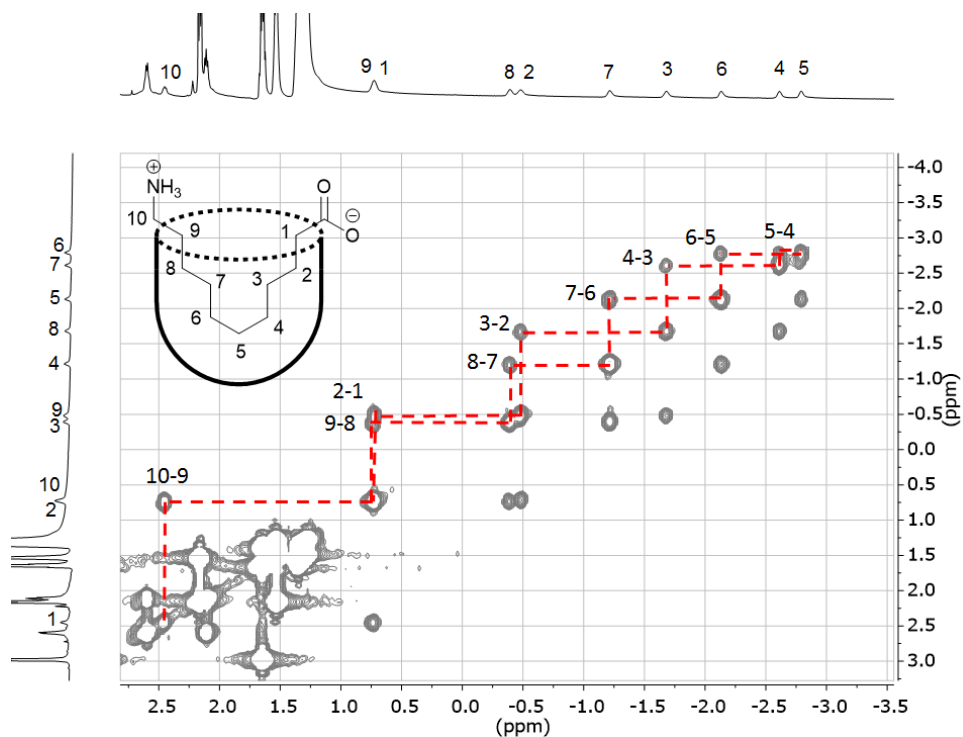


Fig. S6 Partial ^1H - ^1H COSY NMR spectra (D_2O) of **1a** with 11-aminoundecanoic acid.

Cartesian coordinates of calculated structures

The Capsule with encapsulated C17 was minimized at the Hartree-Fock methods (*ab initio*) and 6-31G* basis set with Gaussian 09 software.² The propyl pyridinium “feet” were replaced with hydrogens to reduce computation time.

O	1.29741400	7.14230800	0.22514900
H	1.70483500	7.90456200	0.61485800
H	0.89138300	6.65405900	0.94709900
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H	1.71872900	-7.86249000	-0.61271900
H	0.91406000	-6.60004300	-0.91863600
O	-1.22758100	-6.97277500	1.35324900
H	-0.95335900	-6.34490000	2.02000000
H	-0.43339400	-7.42423600	1.09015900

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