Supporting Information

for

Chalcogen Bonding and Hydrophobic Effects Force Molecules into Small Spaces

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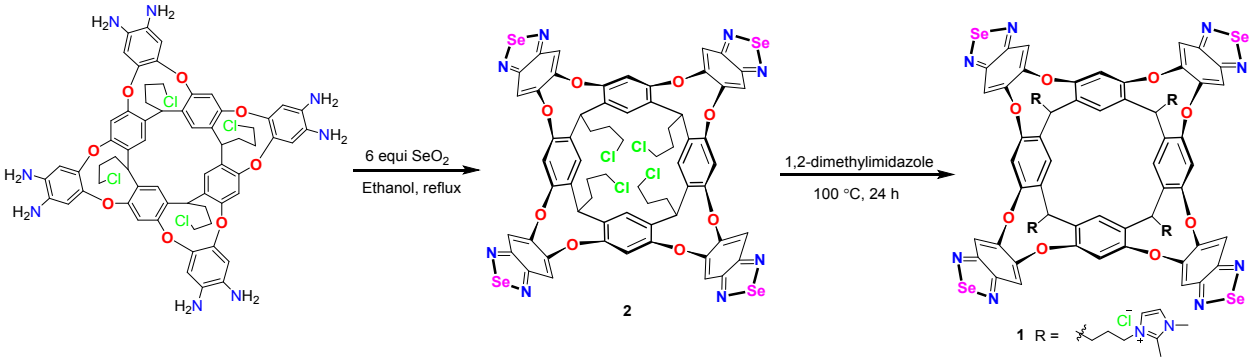
Contents

Experimental

General experimental

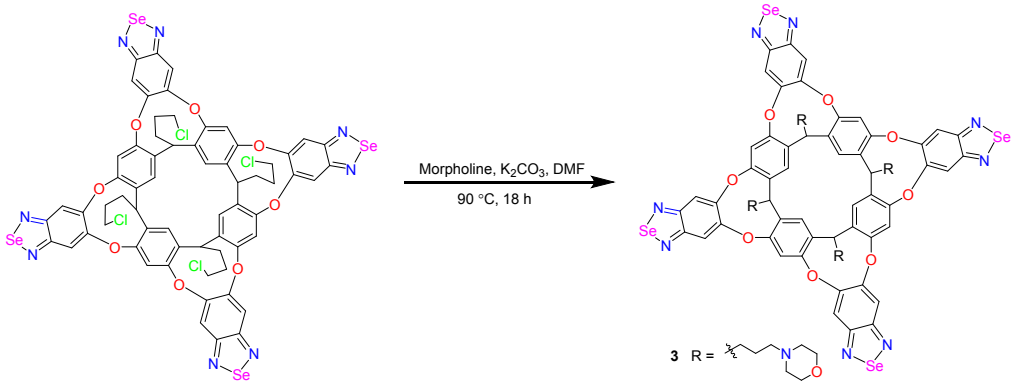
All analytical grade solvents and reagents purchased from commercial sources were used without further purification. SeO_2 was purchased from Energy Chemical Company Ltd., Shanghai China. D_2O, DMSO-d_6, $CDCl_3$ and CD_3OD were used as NMR analysis solvents. ^{1}H and ^{13}C NMR analyses were performed using Bruker AVANCE III HD 600 MHz spectrophotometer. Positive ions high-resolution mass analyses were performed on Bruker micrOTOF II machine.



Procedure for the synthesis of cavitand 2

A solution of 60 mg (0.54 mmol) of SeO_2 in 5 mL of water was added dropwise to a stirred solution of 121 mg (0.1 mmol) of octa-amino cavitand[1, 2] in 25 mL of ethanol at rt. The light orange mixture obtained was heated in an oil bath and maintained at reflux for 5 h. The mixture was

cooled to rt and a pale solid precipitated. It was filtered washed successively with water and ethanol and dried under high vacuum. The product **2** (140 mg) was obtained in 93% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.56 (s, 8H), 8.19 (s, 4H), 7.84 (s, 4H), 5.70 (t, J = 8.1 Hz, 4H), 3.81 (t, J = 6.5 Hz, 8H), 2.61 (d, J = 7.9 Hz, 8H), 1.84 (p, J = 6.7 Hz, 8H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 157.5, 155.0, 154.7, 135.6, 124.8, 116.9, 116.2, 45.4, 33.4, 31.4, 29.0.



Procedure for the synthesis of cavitand 3

A solution of 300 mg (0.2 mmol) of **2** in 20 mL of DMF was treated with 8 equivalents (1.6 mmol) of K_2CO_3 and 5 equivalents (1 mmol) of morpholine. The mixture was stirred and heated at 90 °C for 20 h. The mixture was cooled to rt and 80 mL of water was added. The solid precipitate obtained was filtered and washed successively with water and ethanol. The solid was further suspended in 30 mL ethanol, sonicated for 1 h, then filtered and washed with ethanol. After drying under high vacuum 250 mg of a pale colored compound was obtained in 73% yield. HR-MS (ESI): Calcd. for chemical formula $C_{80}H_{77}N_{12}O_{12}Se_4$: $[M+H]^{1+}$ = 1715.2482, found: 1715.2479, $C_{80}H_{78}N_{12}O_{12}Se_4$: $[M+2H]^{2+}$ = 572.4209, found: 572.4221, ^{1}H NMR (600 MHz, chloroform-*d*) δ 7.85 (s, 8H), 7.51 (s, 4H), 7.43 (s, 4H), 5.86 (t, J = 8.1 Hz, 4H), 3.78 (q, J = 4.7 Hz, 16H), 2.62 – 2.53 (m, 24H), 2.40 (q, J = 7.3 Hz, 8H), 1.69 – 1.62 (m, 8H). ^{13}C NMR (150 MHz, chloroform-*d*) δ 156.9, 155.3, 154.6, 135.6, 123.5, 116.0, 115.1, 66.9, 58.9, 53.9, 33.5, 29.9, 24.8.

Procedure for the synthesis of water-soluble cavitand 1

A solution of 100 mg **2** in 10 mL of 1,2-dimethylimdazole and heated and stirred at 100 °C for 24 h. The mixture was cooled to rt and 50 mL of acetonitrile was added. The precipitated solid was filtered and washed thoroughly with acetonitrile. The pale solid recovered was suspended in 30 mL of acetonitrile and heated with stirring at 80 °C for 3 h. The solid precipitate from the cooled mixture was filtered and washed with acetonitrile and dried under high vacuum to give 113 mg **1** (90% yield) was recovered. (The ^{1}H NMR spectrum of the product showed acetonitrile solvent signals) HR-MS (ESI): Calcd. for chemical formula $C_{84}H_{76}N_{16}O_8Se_4Cl_3$: $[M\text{-}Cl]^{1+}$ = 1859.1779, found: 1859.1782, $C_{84}H_{76}N_{16}O_8Se_4Cl_2$: $[M\text{-}2Cl]^{2+}$ = 912.1046, found: 912.1062, $C_{84}H_{76}N_{16}O_8Se_4Cl$: $[M\text{-}3Cl]^{3+}$ = 596.4134, found: 596.4145, ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.50 (s, 8H), 8.27 (s, 4H), 8.12 (s, 4H), 8.08 (s, 4H), 7.79 (s, 4H), 5.55 (t, J = 7.9 Hz, 4H), 4.37 (s, br, 8H), 3.85 (s, 12H), 2.84 (s, br, 8H), 2.76 (s, 12H), 1.77 (s, br, 8H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 156.8, 154.4, 154.1, 144.4, 135.2, 125.8, 122.2, 121.1, 116.0, 115.5, 47.8, 34.7, 33.6, 28.2, 27.8, 9.5.

^{1}H NMR, ^{13}C NMR spectra of cavitands

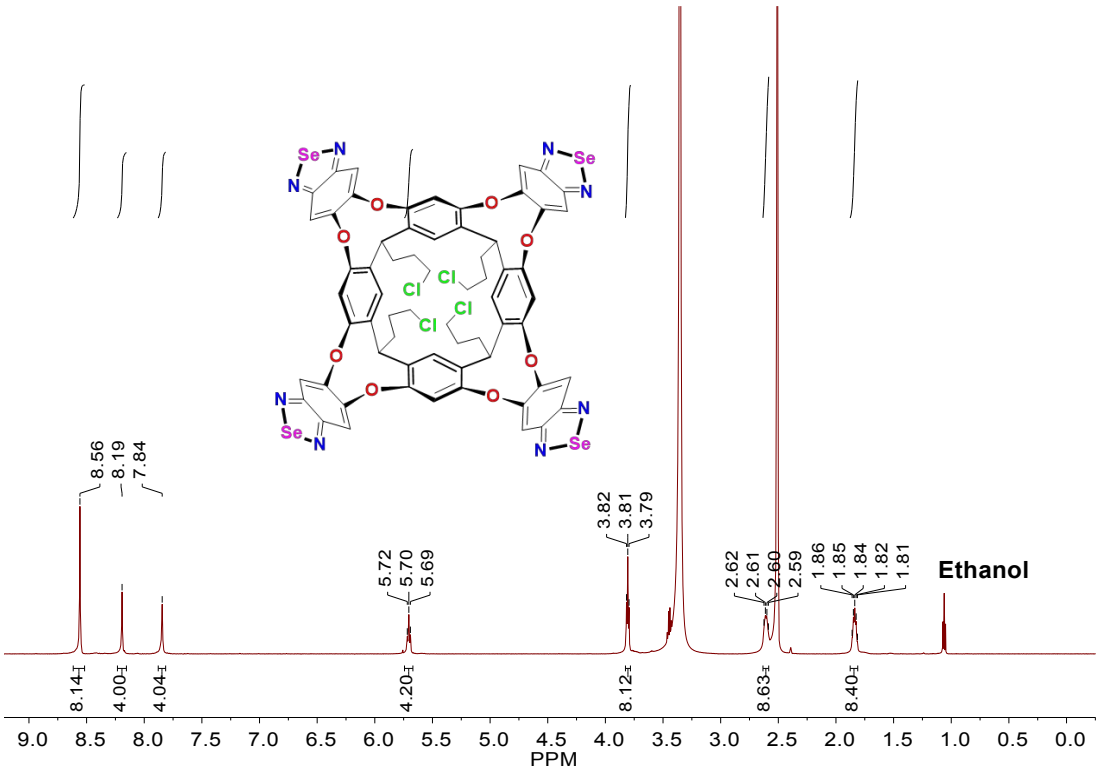


Fig. S1 ^{1}H NMR spectrum of **2** in DMSO-d_6, analyzed at rt

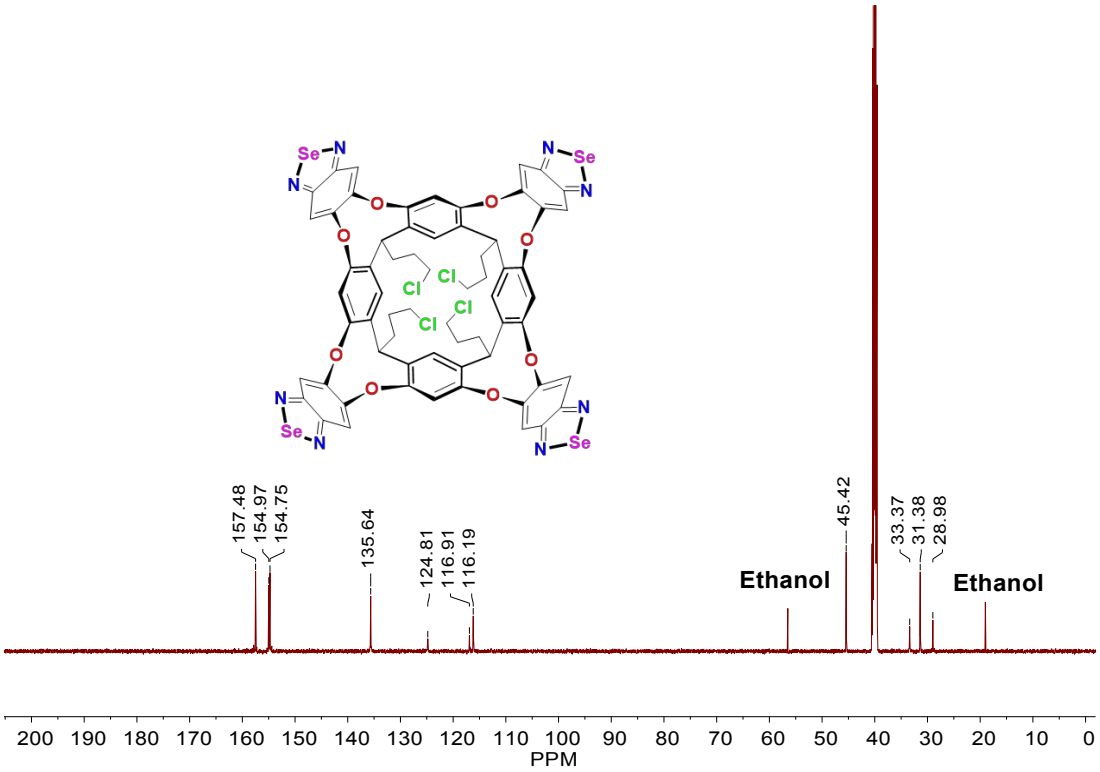


Fig. S2 ^{13}C NMR spectrum of **2** in DMSO-d_6, analyzed at rt

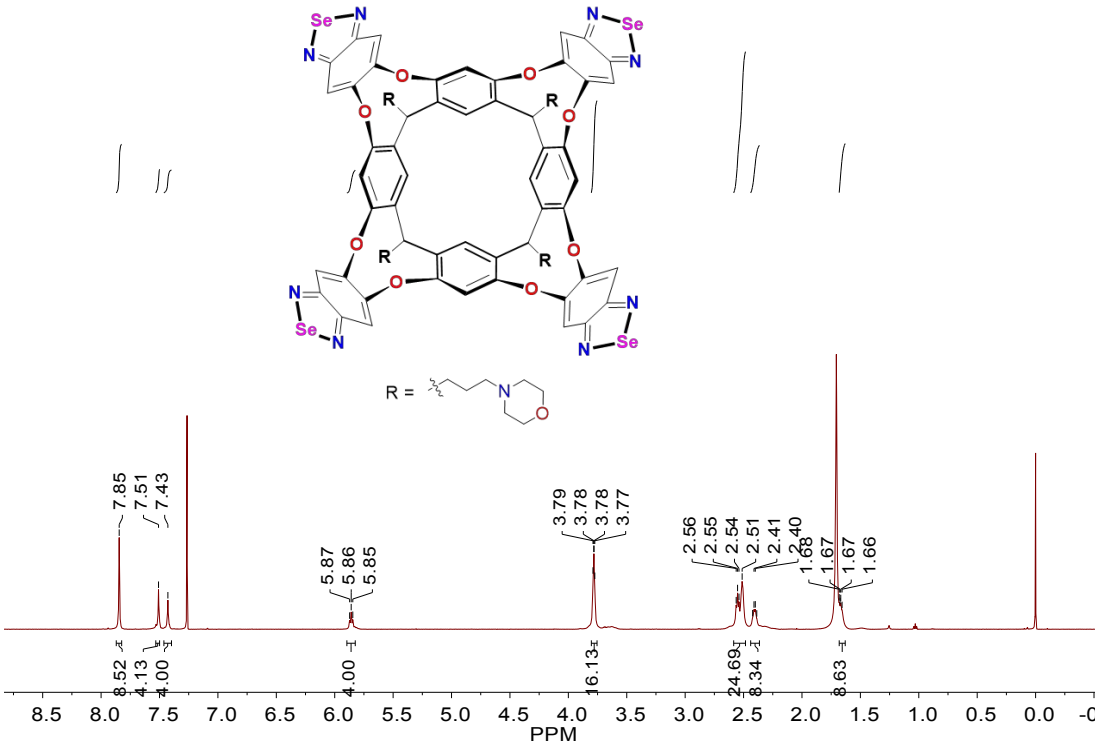


Fig. S3 ^{1}H NMR spectrum of **3** in $CDCl_3$, analyzed at rt

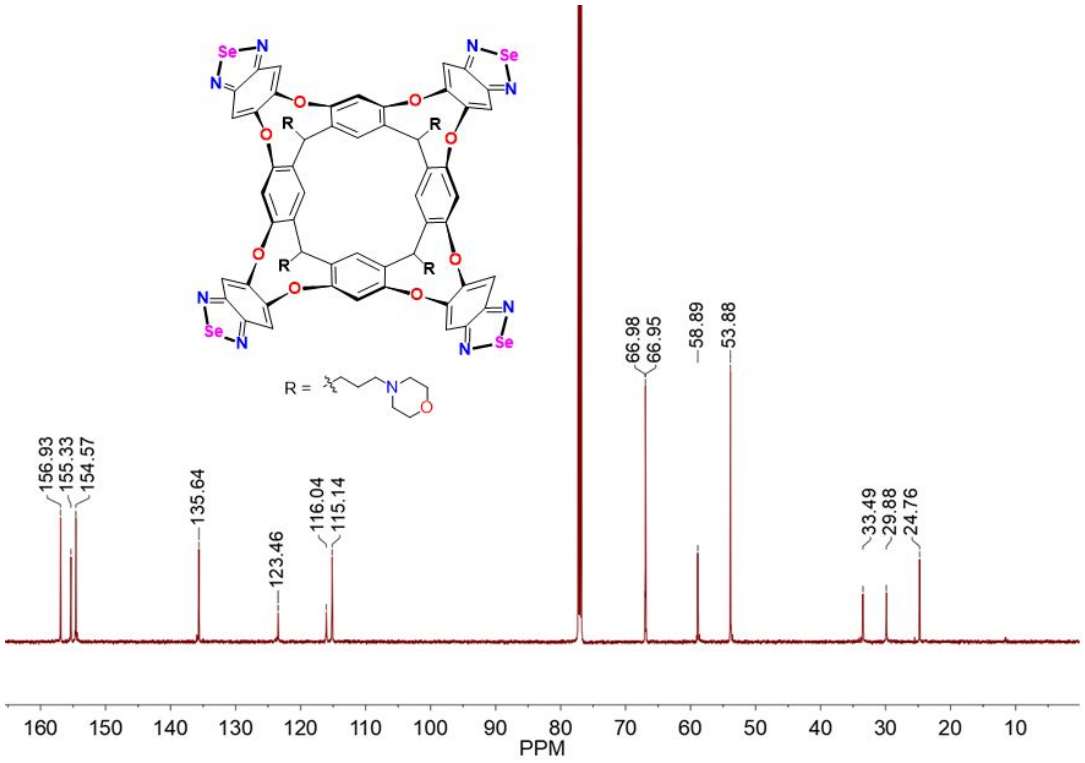


Fig. S4 ^{13}C NMR spectrum of **3** in $CDCl_3$, analyzed at rt

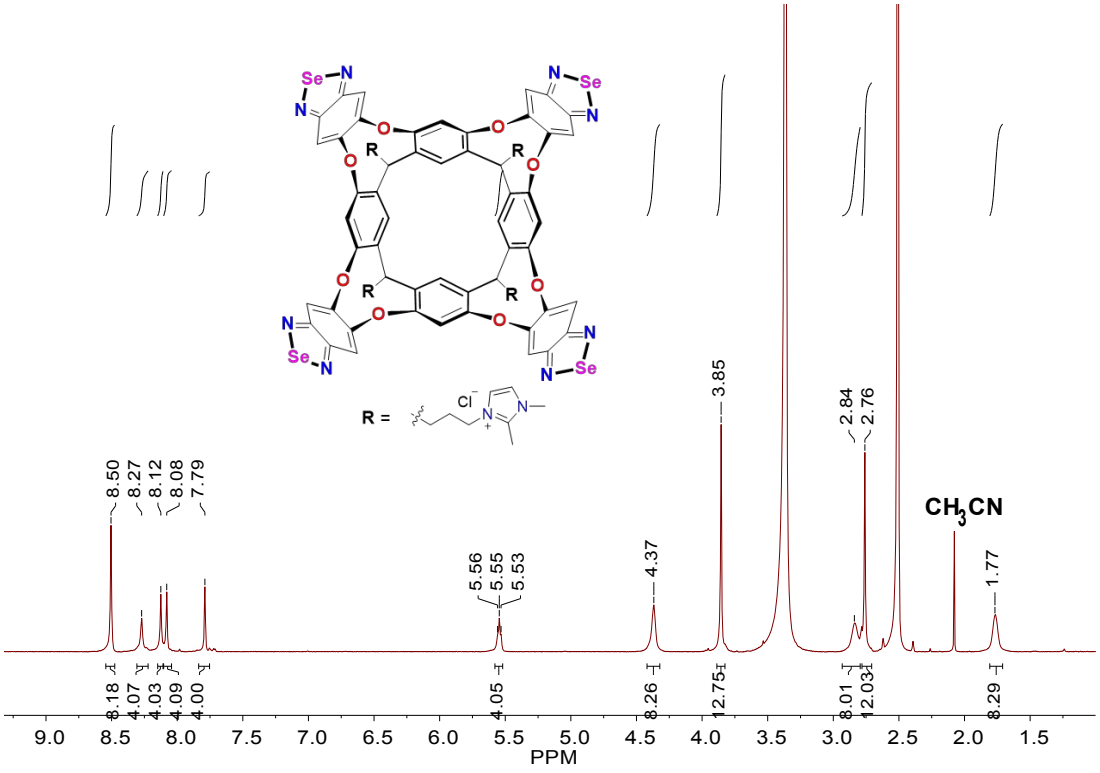


Fig. S5 ^{1}H NMR spectrum of **1** in DMSO-d_6, analyzed at rt

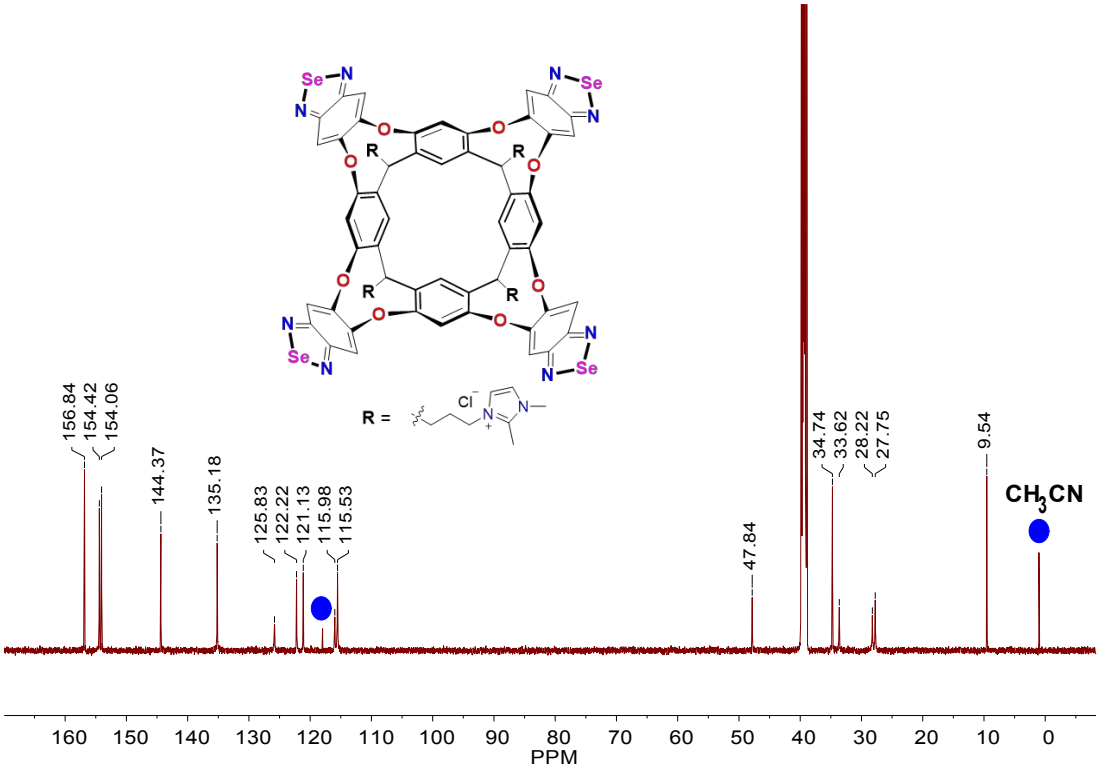


Fig. S6 ^{13}C NMR spectrum of **1** in DMSO-d_6, analyzed at rt

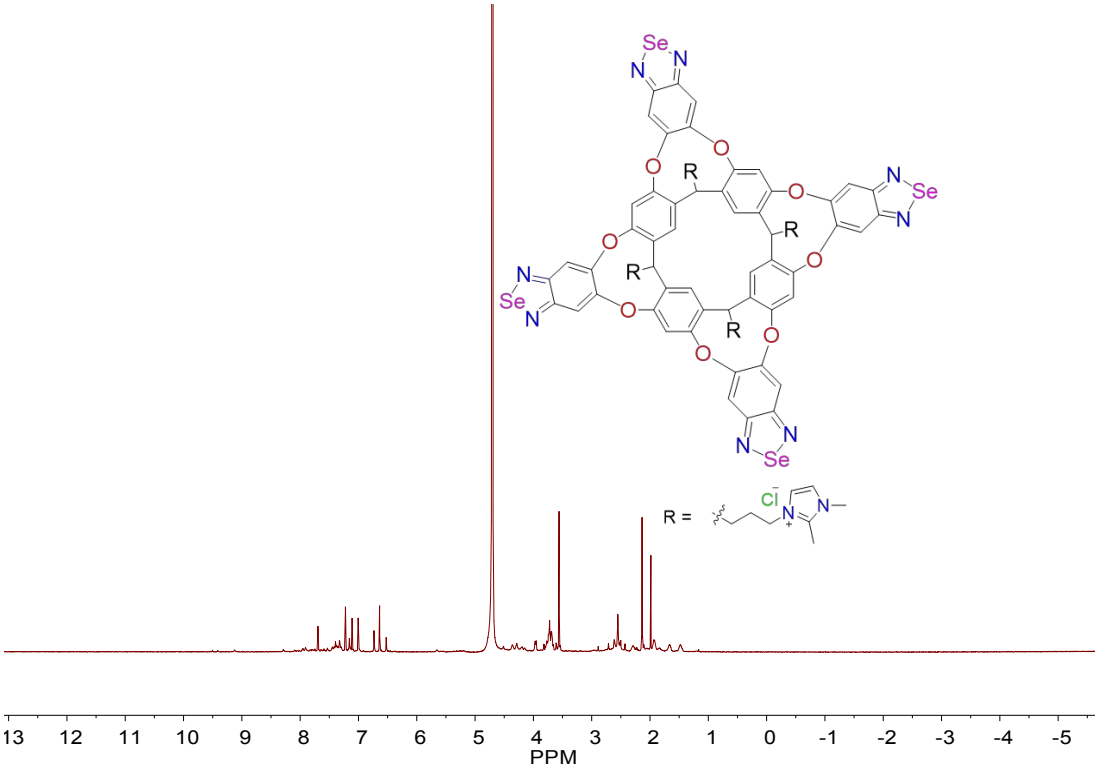


Fig. S7 ^{1}H NMR spectrum of **1** in D_2O, analyzed at rt

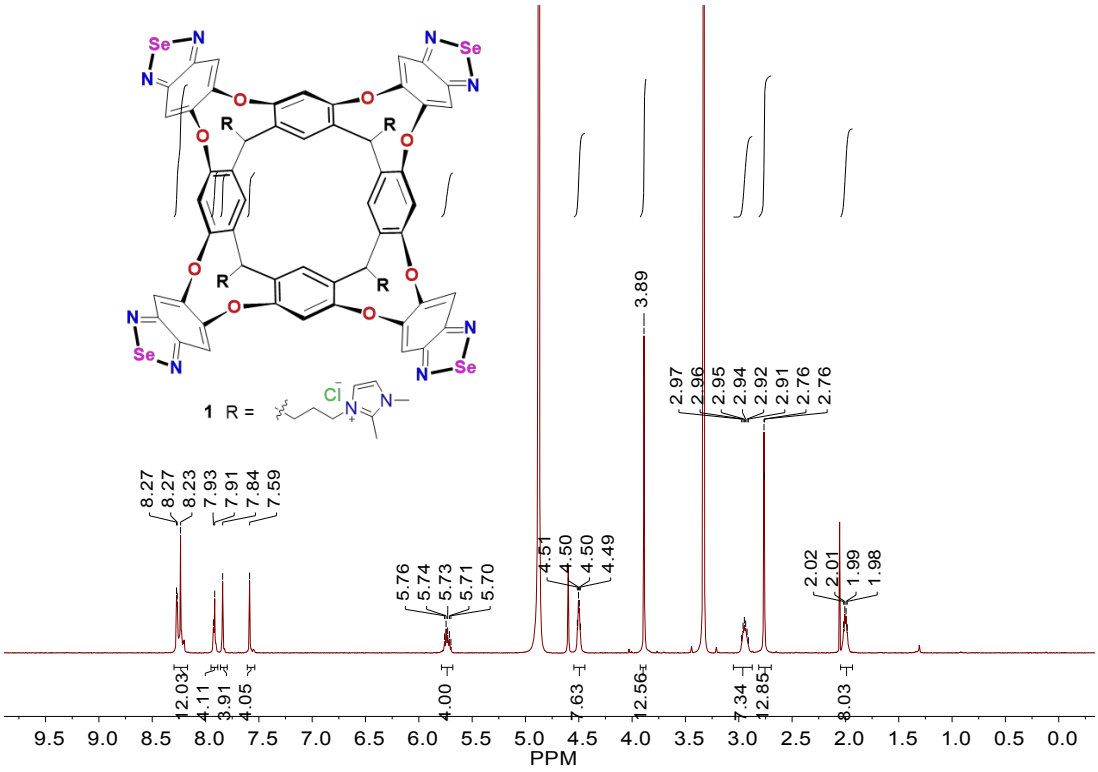


Fig. S8 ^{1}H NMR spectrum of **1** in methanol-d_4, analyzed at rt

Mass (HR) spectra of cavitands

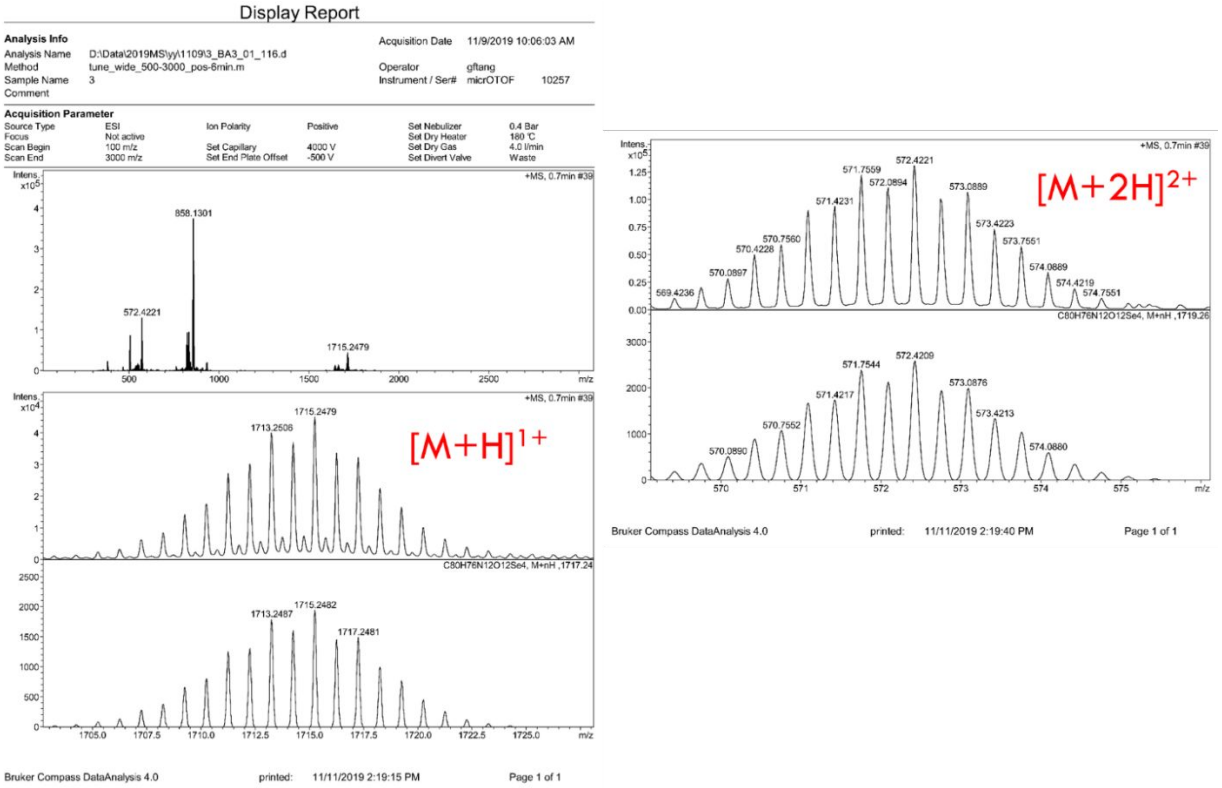


Fig. S9 Mass spectrum of **3**, cationic species formed by the addition on nH cations

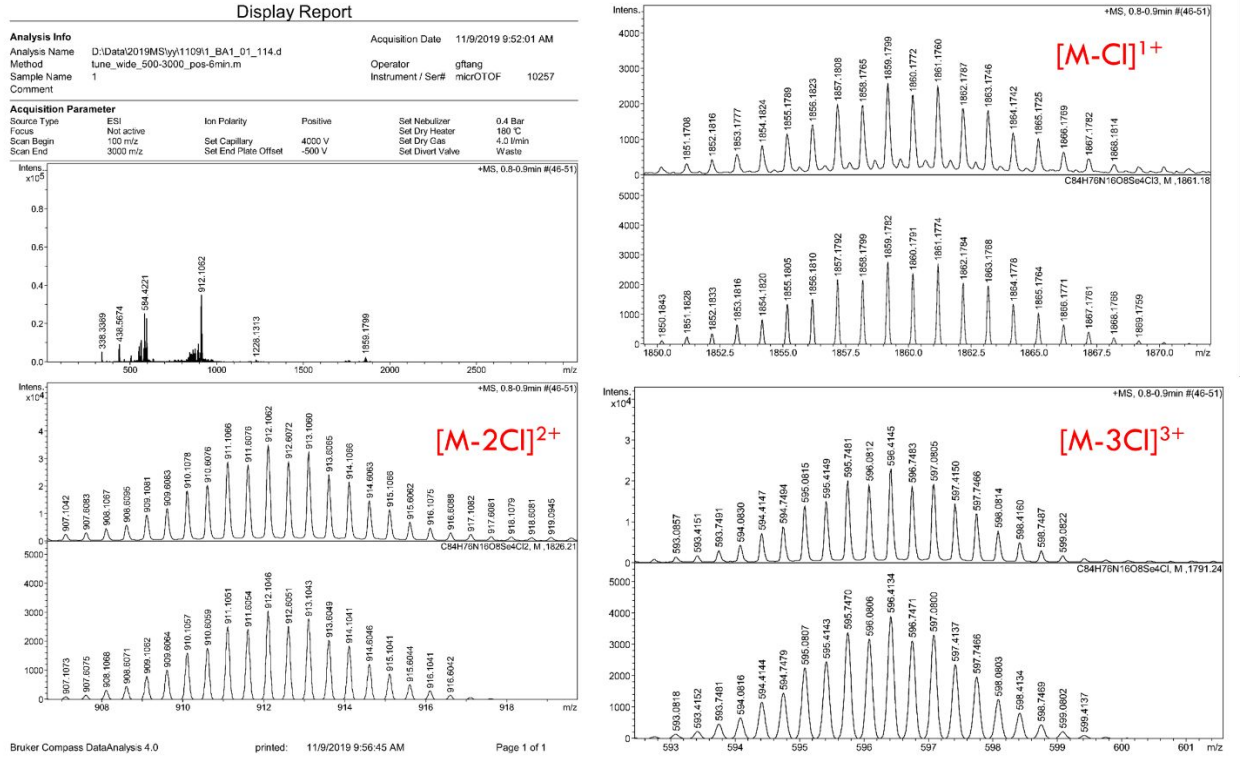


Fig. S10 Mass spectrum of **1**, cationic species formed by the loss of nCl anions

^{1}H NMR spectra of 1 in water in the presence of *n*-alkane as guest

General procedure for the binding analyses

1 mM, 0.5 mL of **1** in D_2O was taken in the NMR tube and excess pure *n*-alkane (~0.5 µL or ~0.5 mg) was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^{1}H NMR spectroscopy at rt.

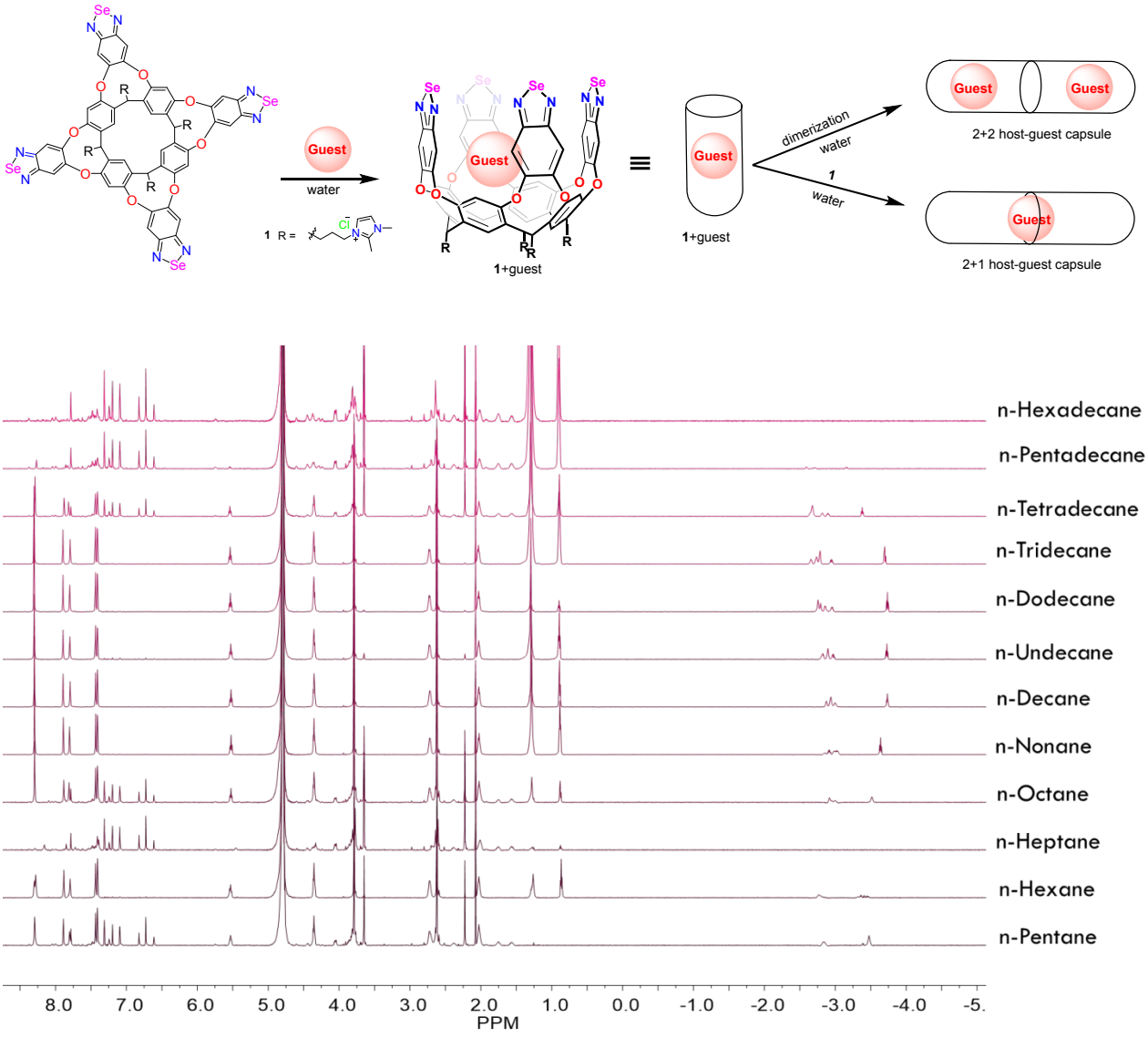


Fig. S11 ^{1}H NMR spectra of the complexes formed between **1**, 1 mM + from bottom to top, *n*-pentane, *n*-hexane, *n*-heptane, *n*-octane, *n*-nonane, *n*-decane, *n*-undecane, *n*-dodecane, *n*-tridecane, *n*-tetradecane, *n*-pentadecane and *n*-hexadecane in D_2O, each mixture was sonicated for 1 h at rt and analyzed at rt

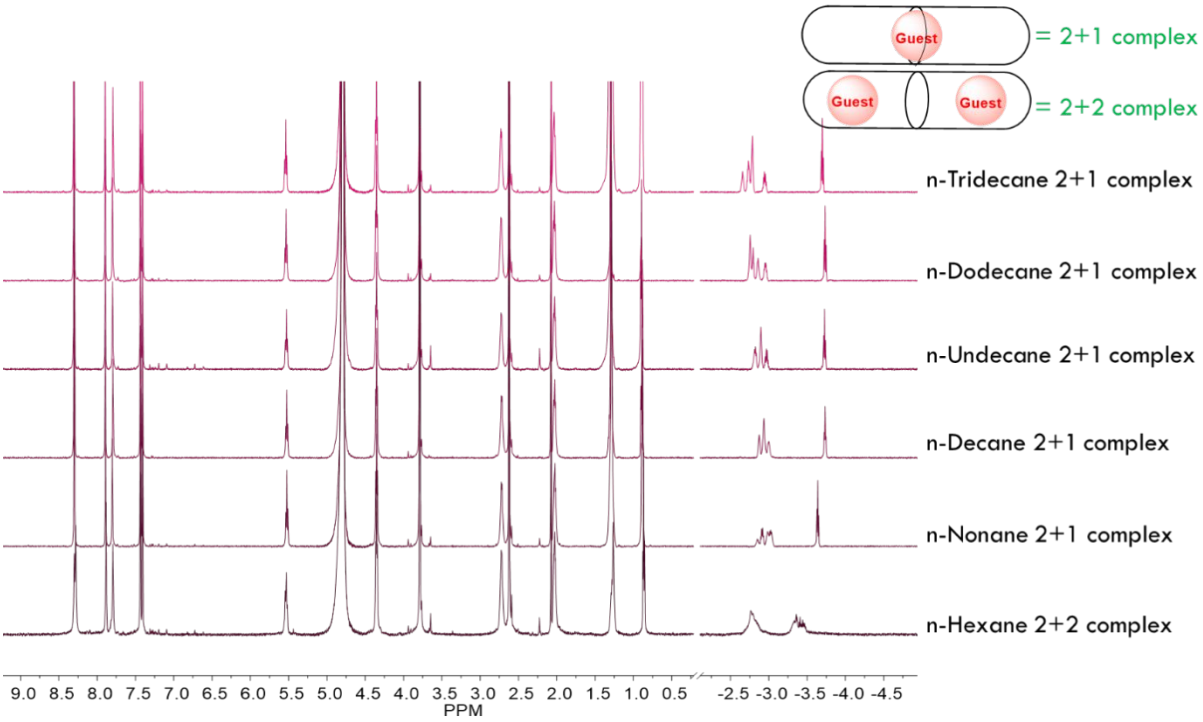


Fig. S12 ^{1}H NMR spectra of the capsular complexes formed between **1** and particular guest; 2 + 2 complex in which two host molecules make a capsule by encapsulation of two molecules of the guest (n-hexane); 2 + 1 complex in which the host capsule encapsulate one molecule of particular guest (*n*-heptane, *n*-octane, *n*-nonane, *n*-decane, *n*-undecane, *n*-dodecane, *n*-tridecane); The NMR spectra were taken in D_2O at rt

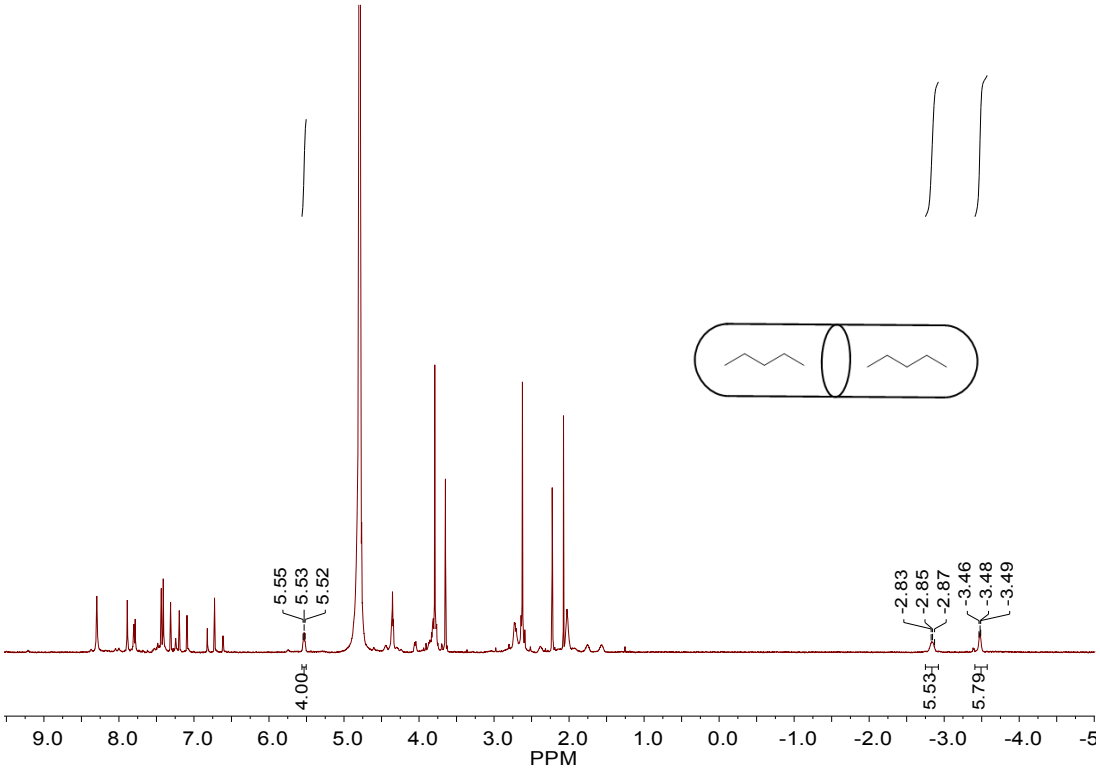


Fig. S13 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-pentane in D_2O, analyzed at rt

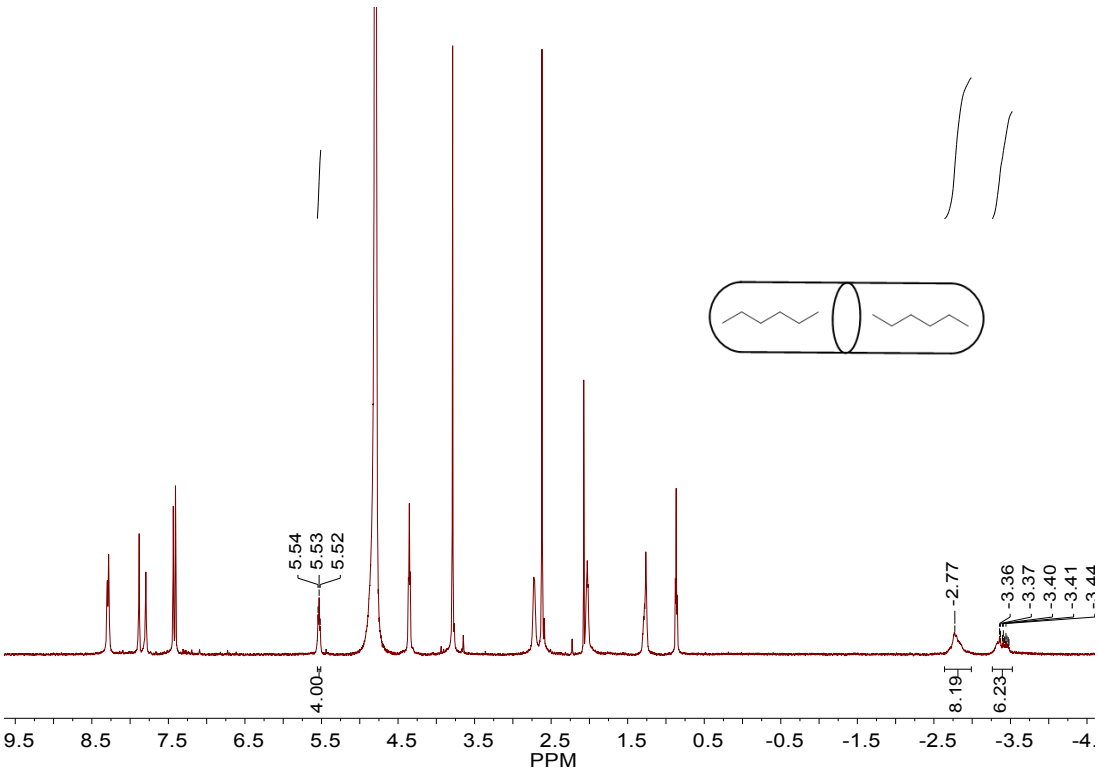


Fig. S14 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-hexane in D_2O, analyzed at rt

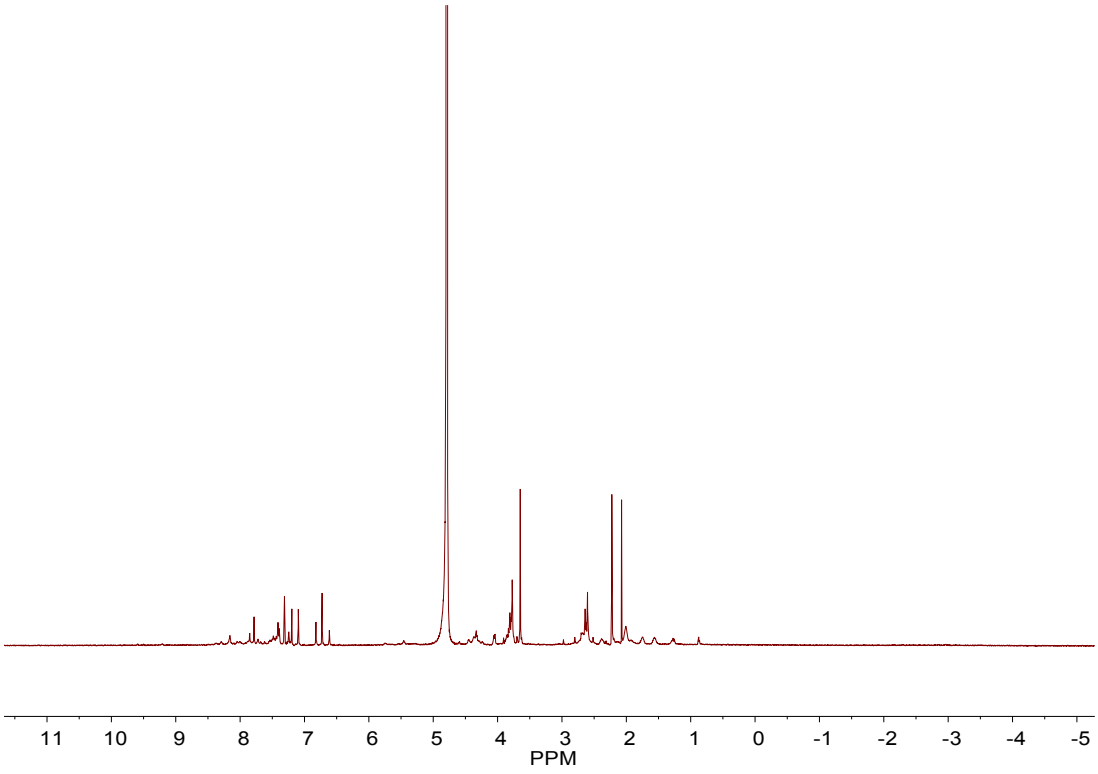


Fig. S15 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-heptane in D_2O, analyzed at rt

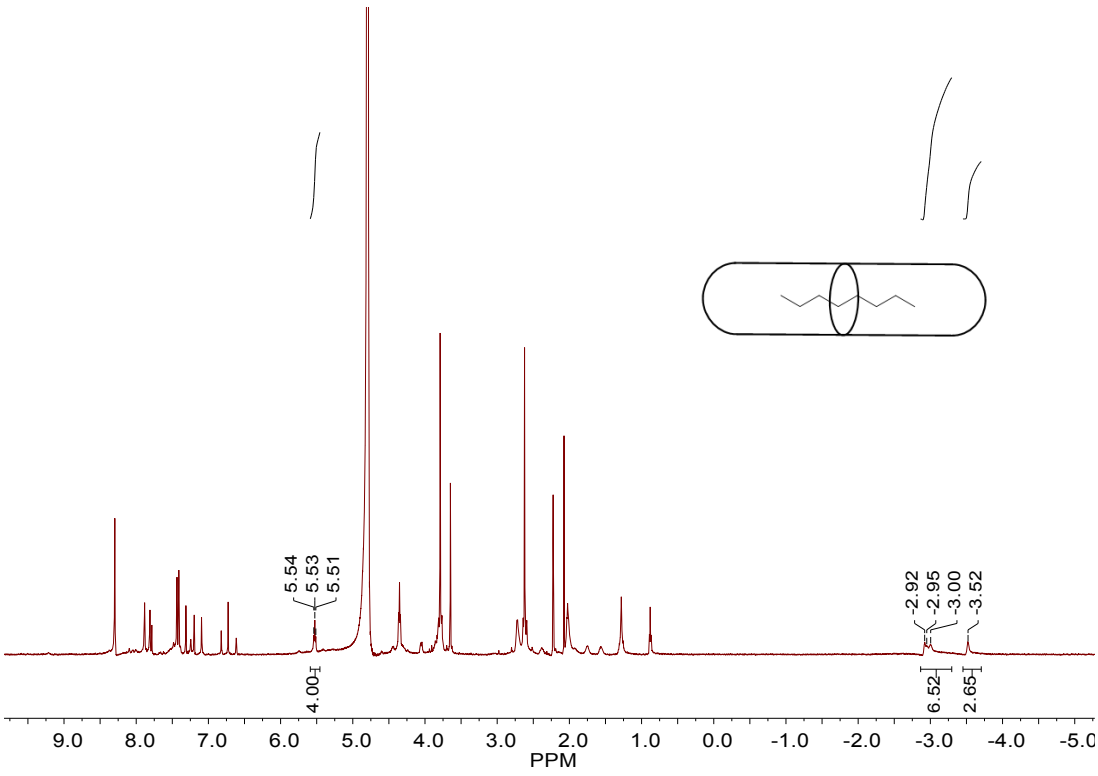


Fig. S16 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-octane in D_2O, analyzed at rt

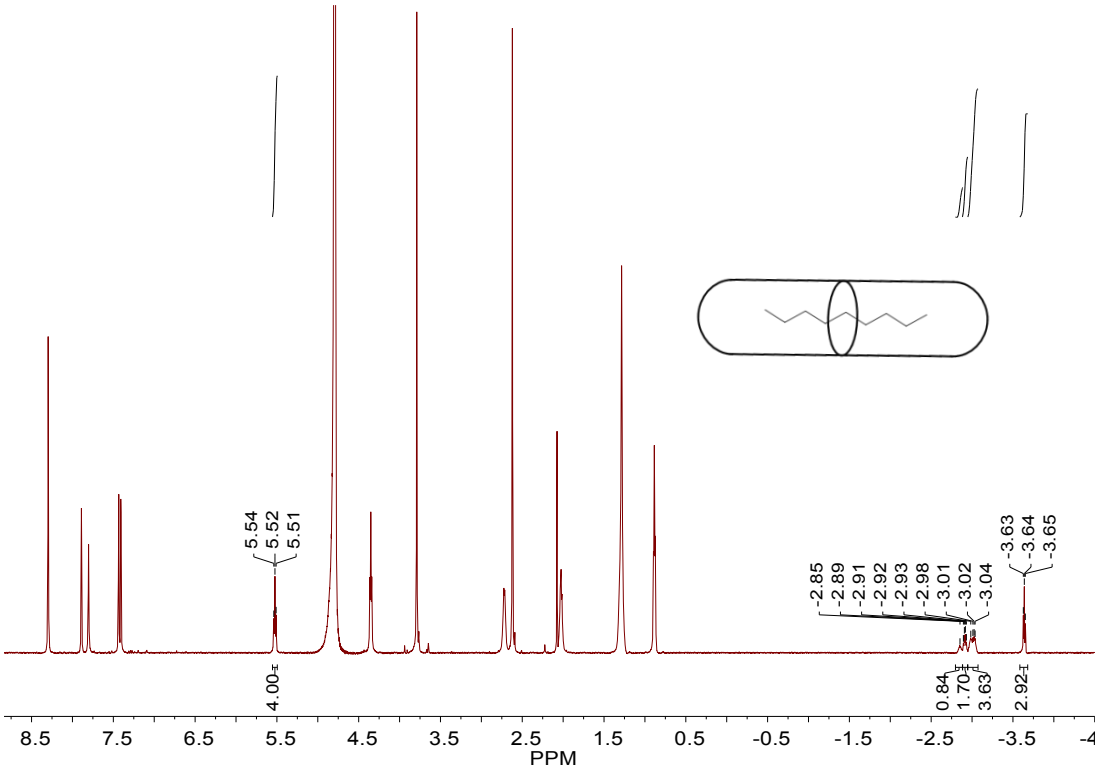


Fig. S17 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-nonane in D_2O, analyzed at rt

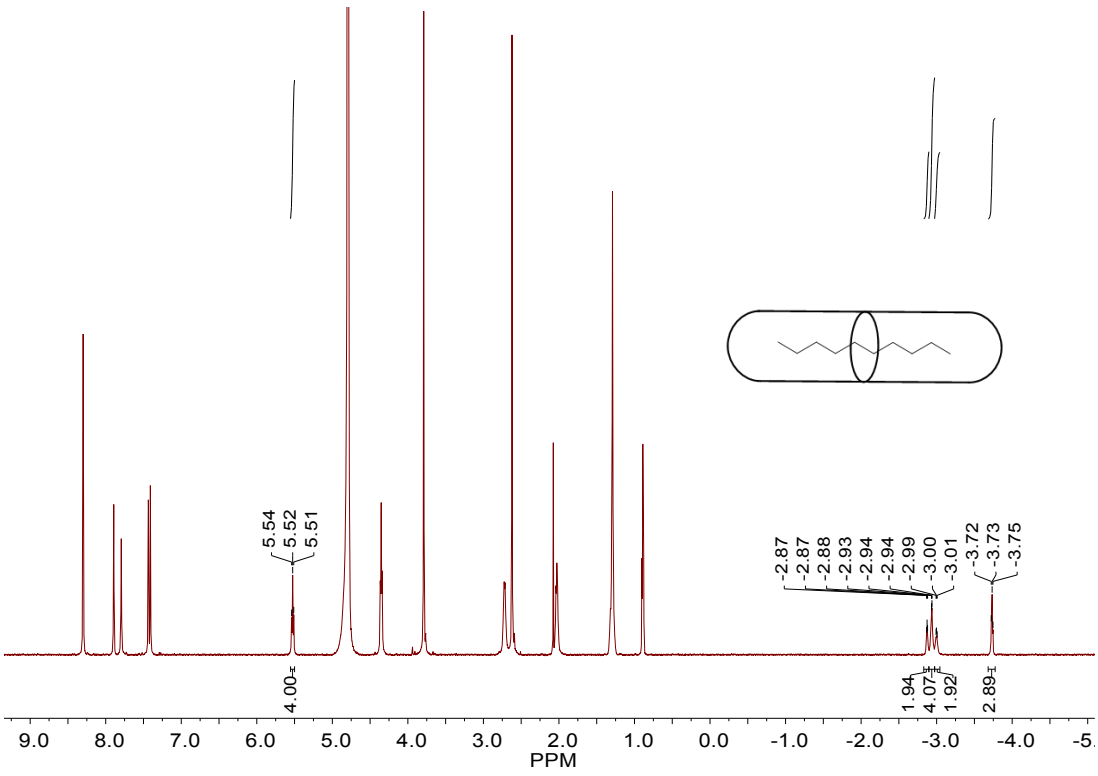


Fig. S18 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-decane in D_2O, analyzed at rt

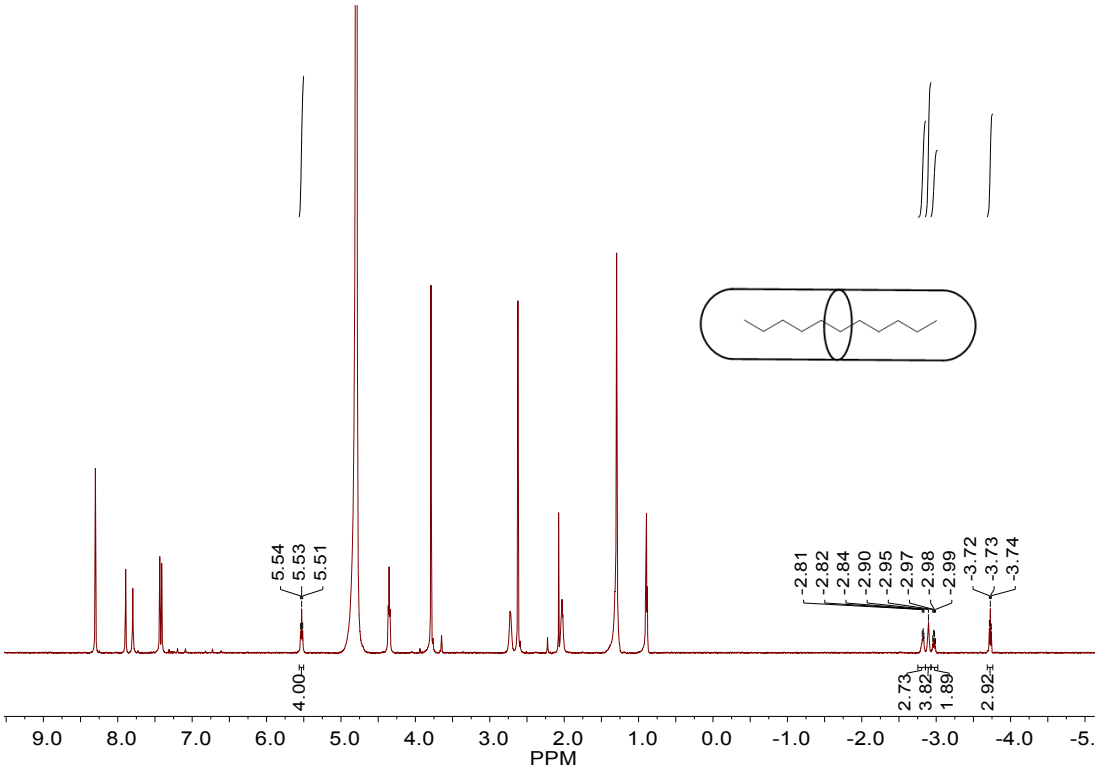


Fig. S19 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-undecane in D_2O, analyzed at rt

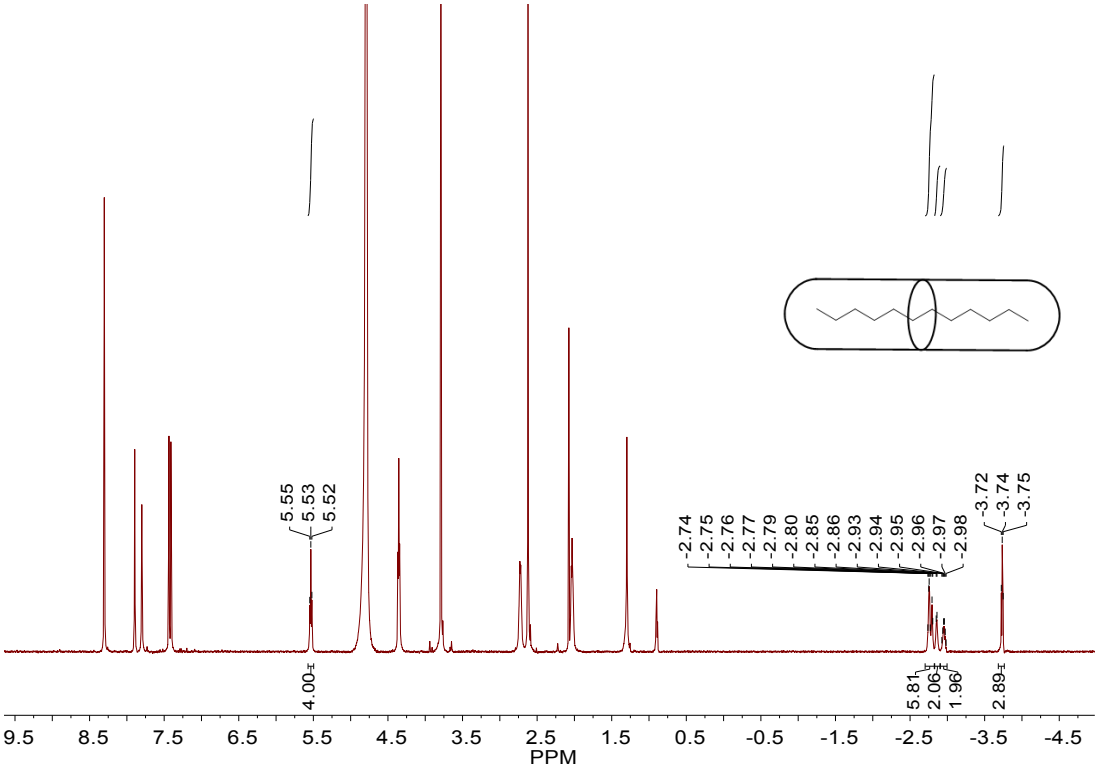


Fig. S20 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-dodecane in D_2O, analyzed at rt

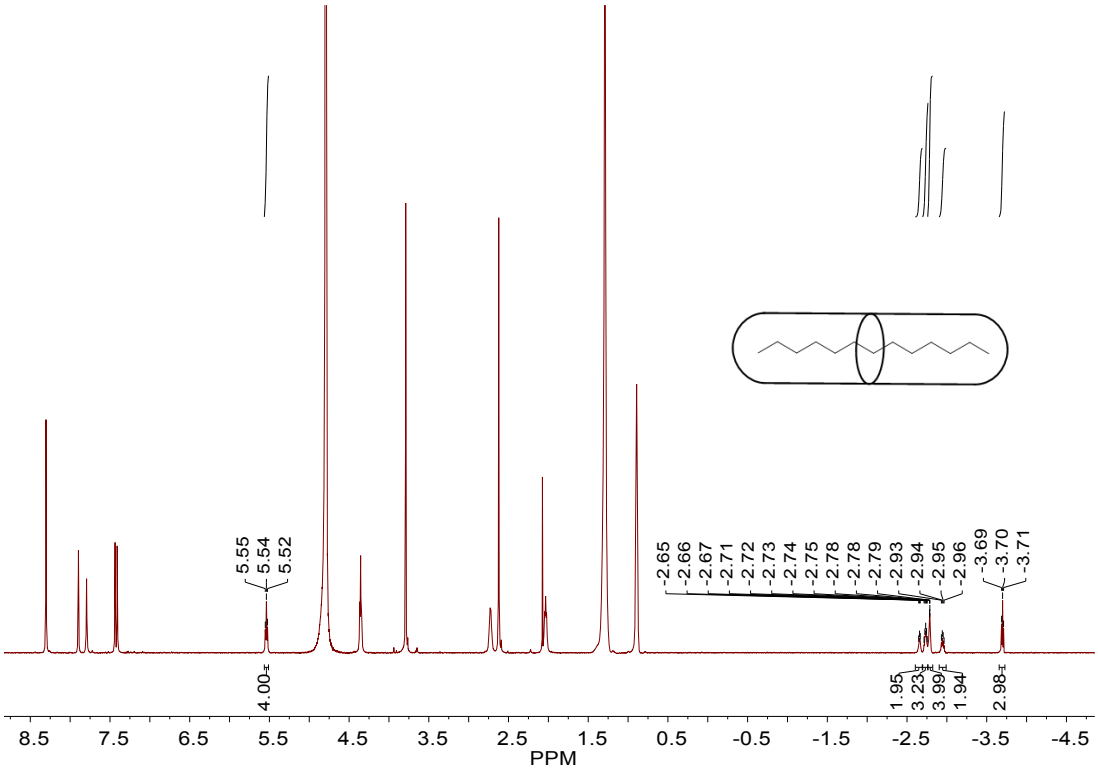


Fig. S21 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-tridecane in D_2O, analyzed at rt

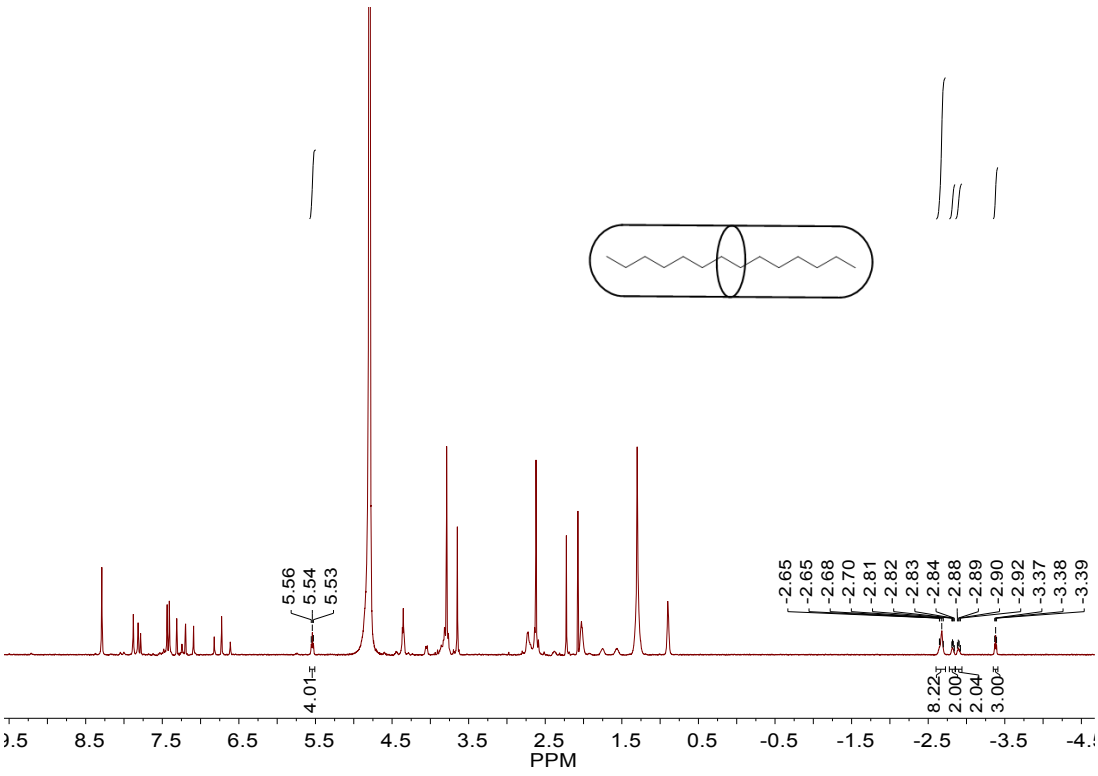


Fig. S22 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-tetradecane in D_2O, analyzed at rt

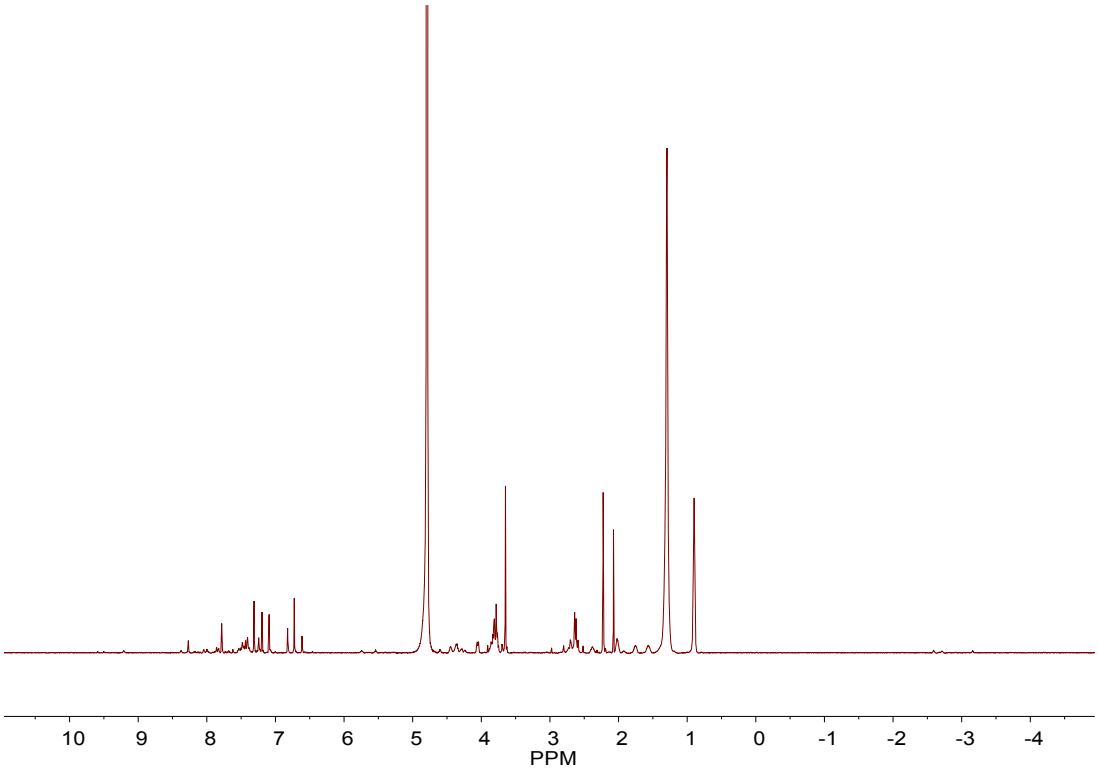


Fig. S23 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-pentadecane in D_2O, analyzed at rt

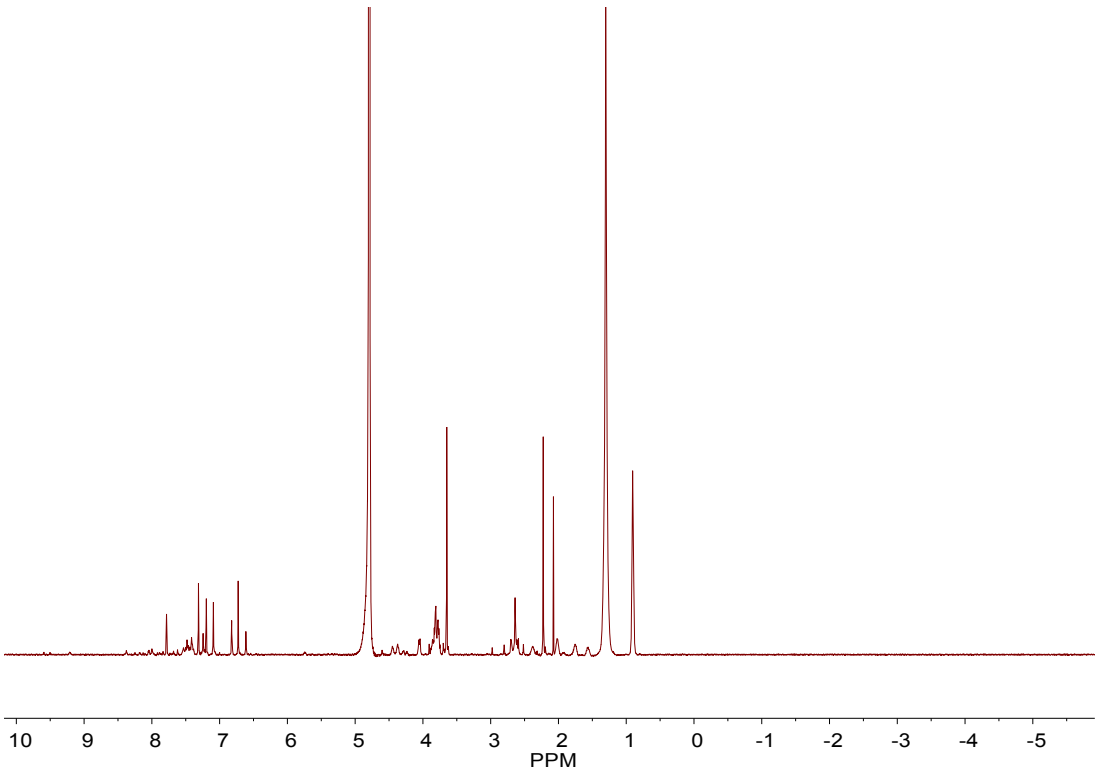


Fig. S24 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + *n*-hexadecane in D_2O, analyzed at rt

^{1}H NMR spectra of 1 in water in the presence of cycloalkane

General procedure for the binding analyses

1 mM, 0.5 mL of **1** in D_2O was taken in NMR tube and excess pure cycloalkane (0.5 µL or ~0.5 mg) was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^{1}H NMR spectroscopy at rt.

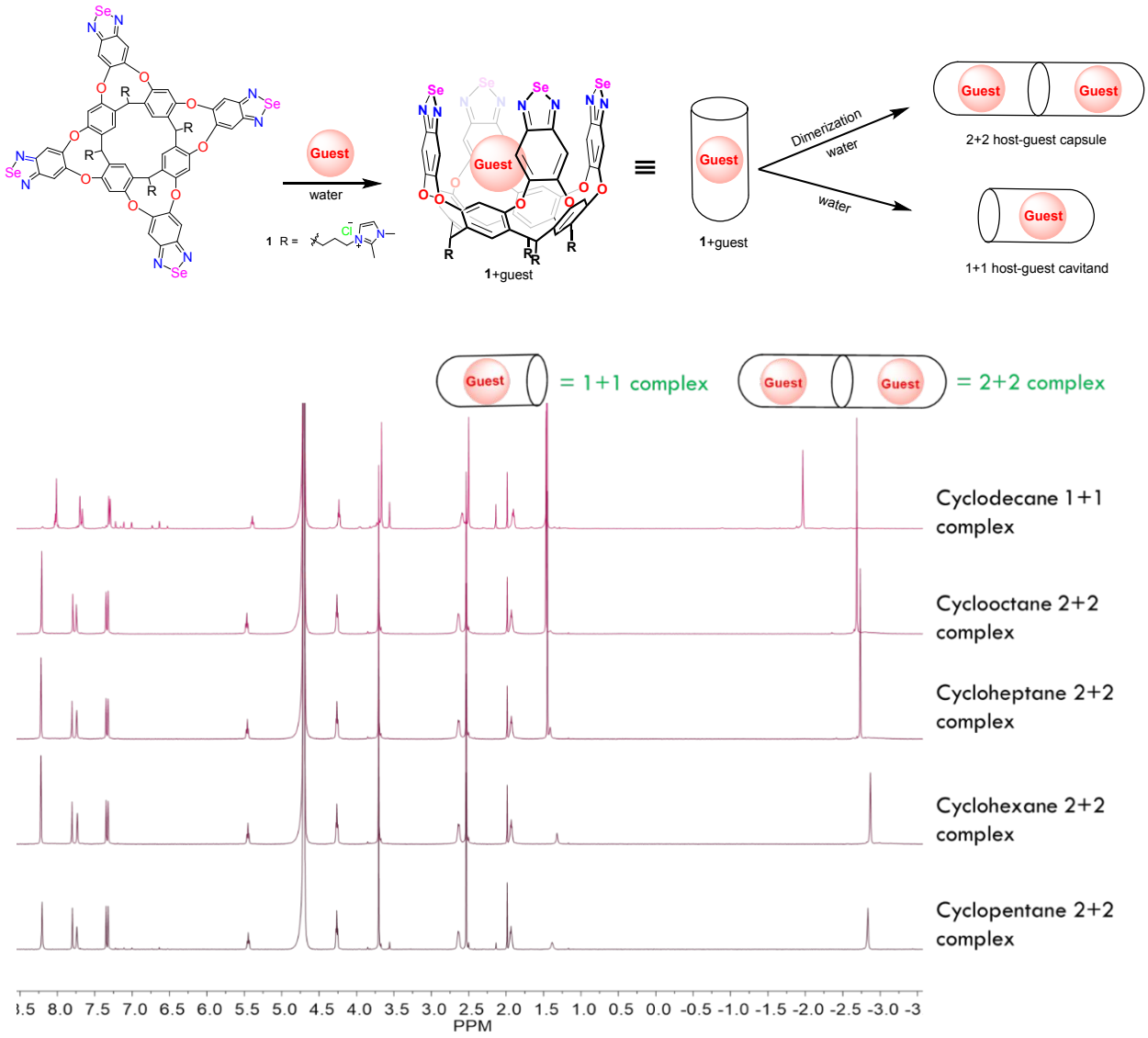


Fig. S25 ^{1}H NMR spectrum 1H NMR spectra of the complexes formed between **1**, 1 mM + from bottom to top, cyclopentane, cyclohexane, cycloheptane, cyclooctane, cyclodecane in D_2O, each mixture was sonicated for 1 h at rt and analyzed at rt

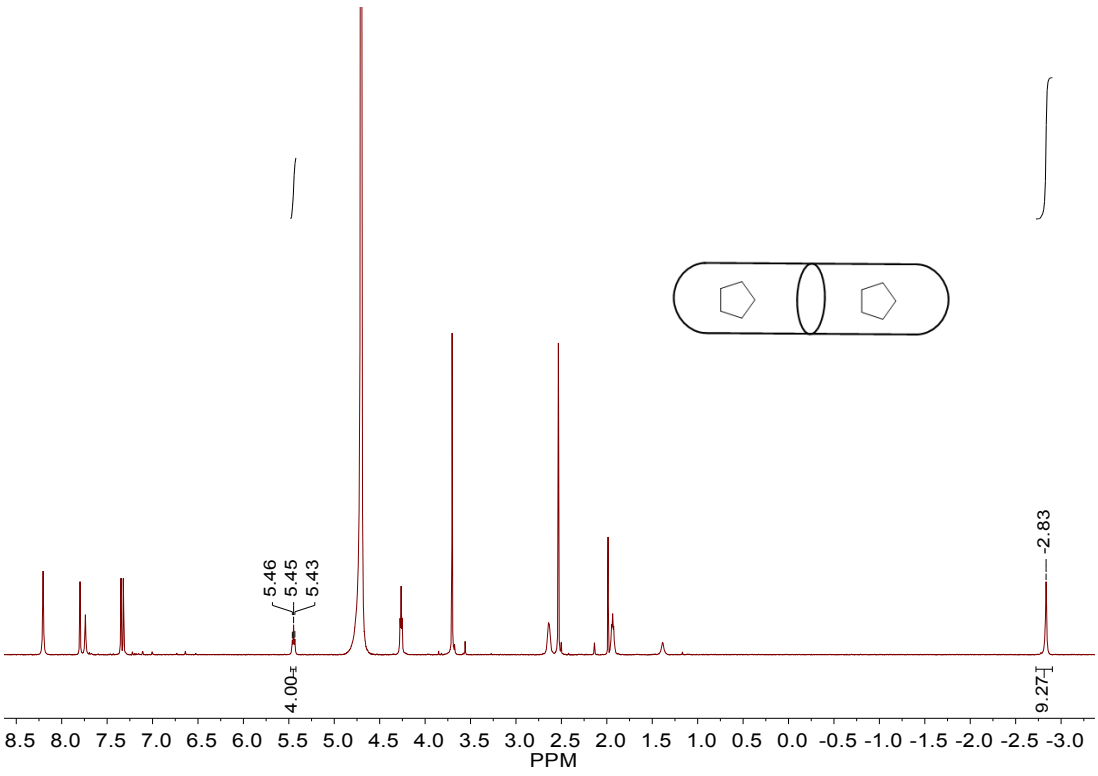


Fig. S26 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + cyclopentane in D_2O, analyzed at rt

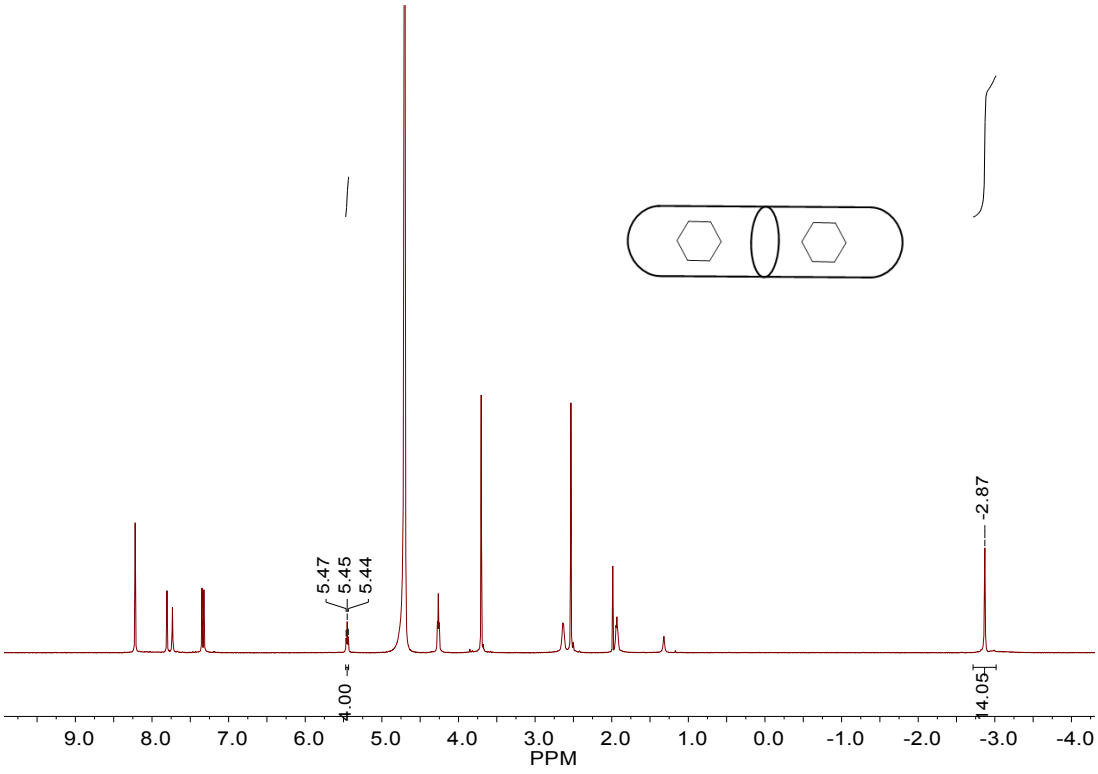


Fig. S27 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + cyclohexane in D_2O, analyzed at rt

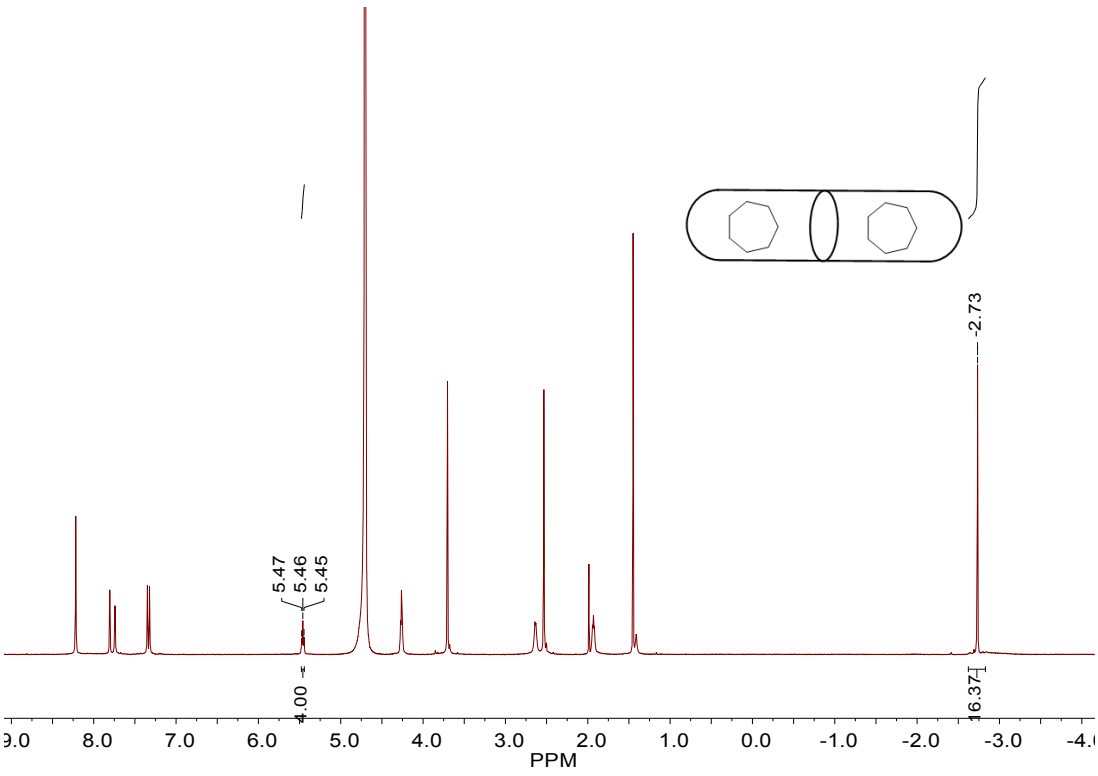


Fig. S28 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + cycloheptane in D_2O, analyzed at rt

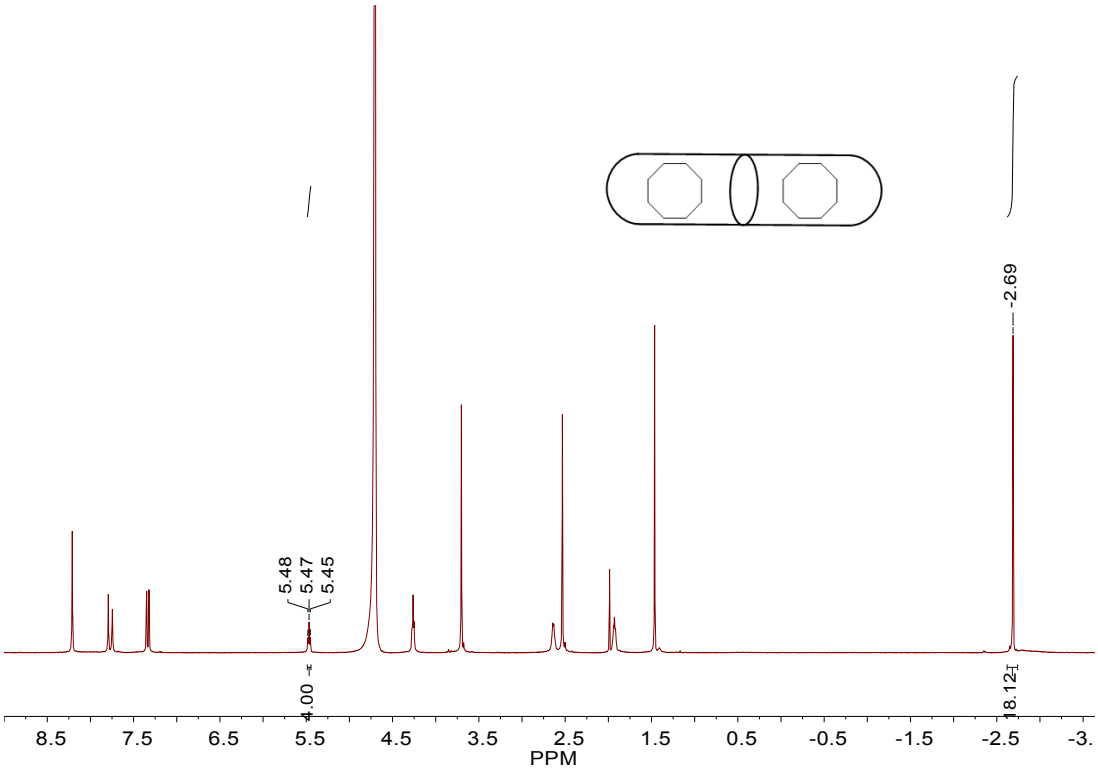


Fig. S29 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + cyclooctane in D_2O, analyzed at rt

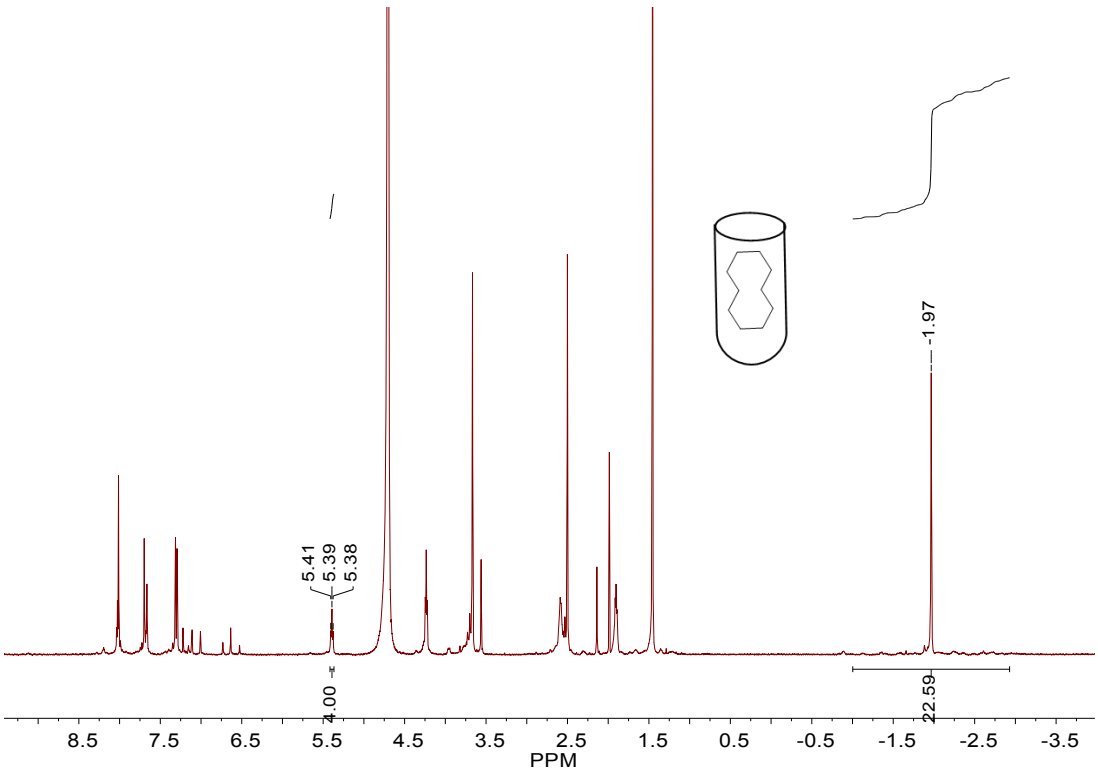


Fig. S30 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + cyclodecane in D_2O, analyzed at rt

^{1}H NMR spectra of 1 in water showing assembly with different branched chain or cyclic carboxylic acid

General procedure for the binding analyses

1 mM, 0.5 mL of **1** in D_2O was taken in NMR tube and excess pure branched chain or cyclic carboxylic acid (~0.5 µL or ~0.5 mg) was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^{1}H NMR spectroscopy at rt.

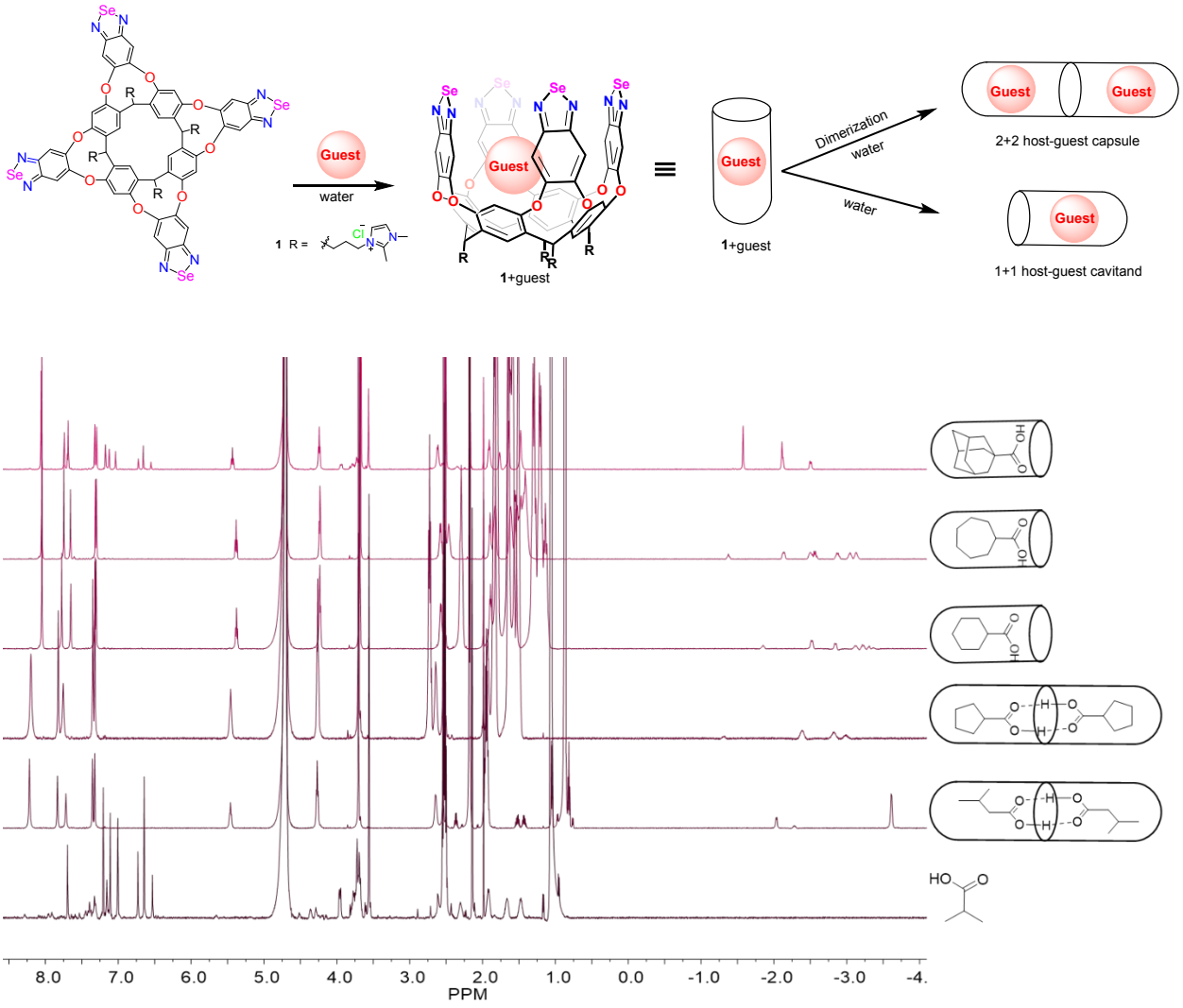


Fig. S31 ^{1}H NMR spectra of the complexes formed between **1**, 1 mM + from bottom to top, 2-methylpropanoic acid, 3-methylbutanoic acid, cyclopentane carboxylic acid, cyclohexane carboxylic acid, cycloheptane carboxylic acid and adamantane carboxylic acid in D_2O, each mixture was sonicated for 1 h at rt and analyzed at rt; 3-methylbutanoic acid and cyclopentane carboxylic acid formed 2 + 2 capsule stabilized by inter molecular acid-acid hydrogen bonding, while the other acid formed 1 + 1 cavitand complex

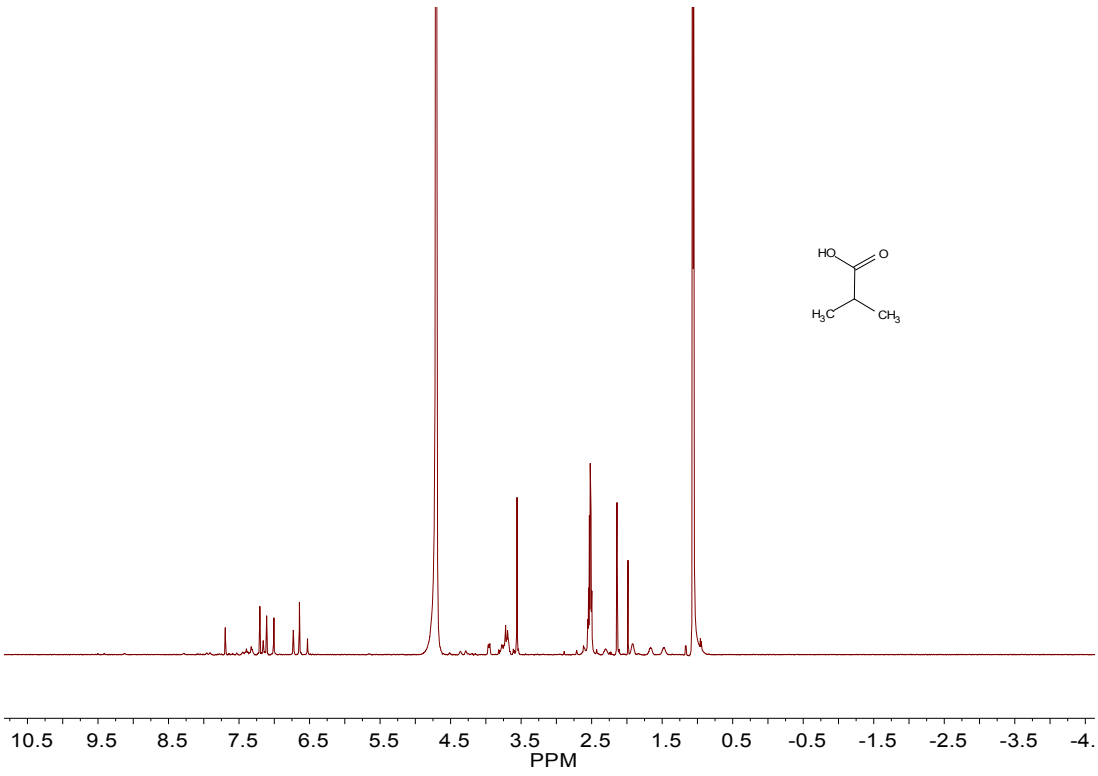


Fig. S32 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + 2-methylpropanoic acid in D_2O, analyzed at rt

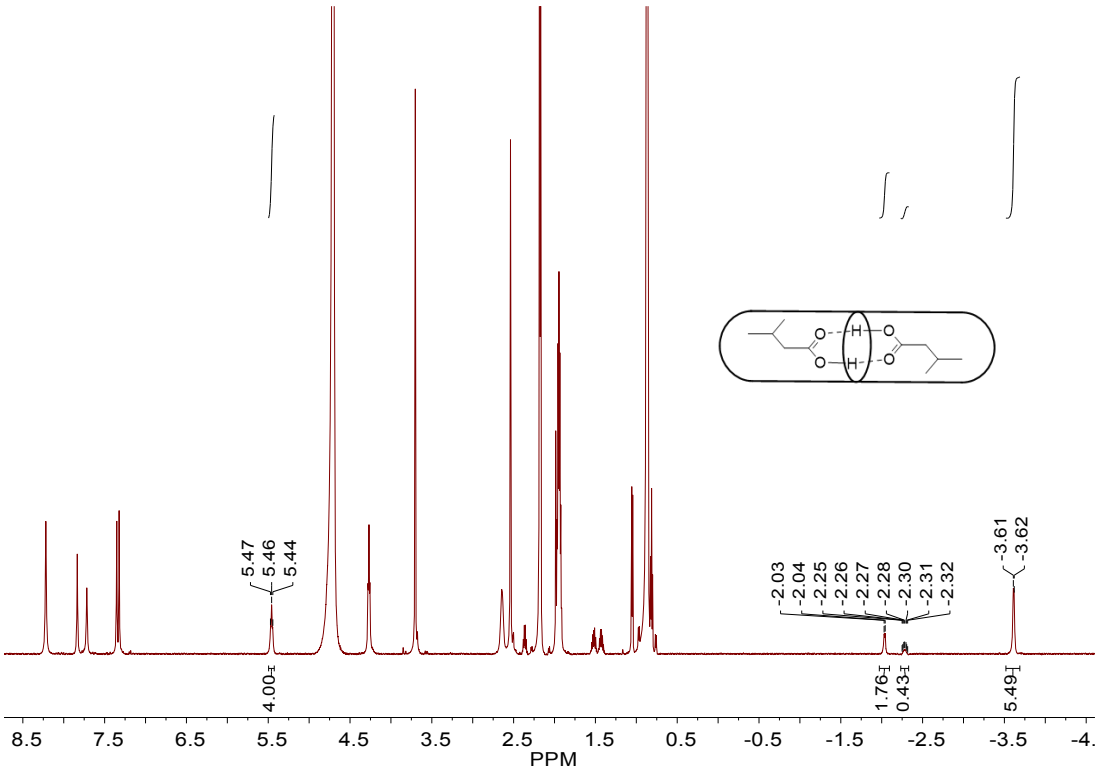


Fig. S33 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + 3-methylbutanoic acid in D_2O, analyzed at rt

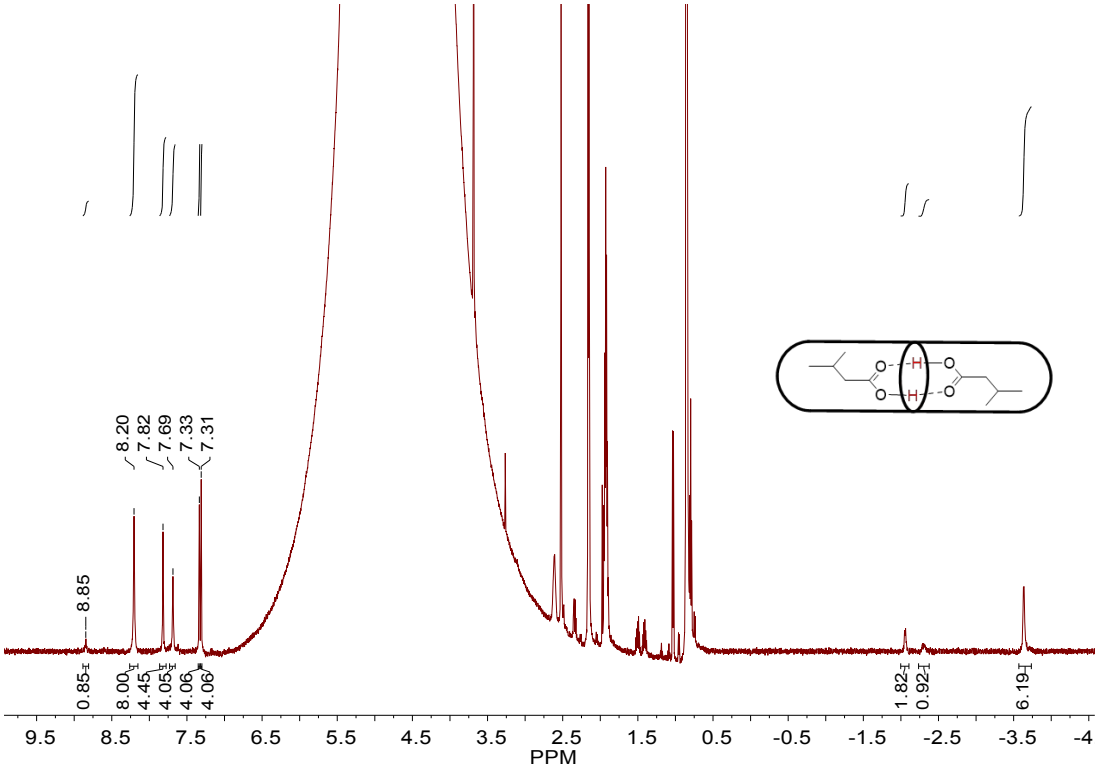


Fig. S34 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + 3-methylbutanoic acid in 10% D_2O in H_2O, analyzed at rt

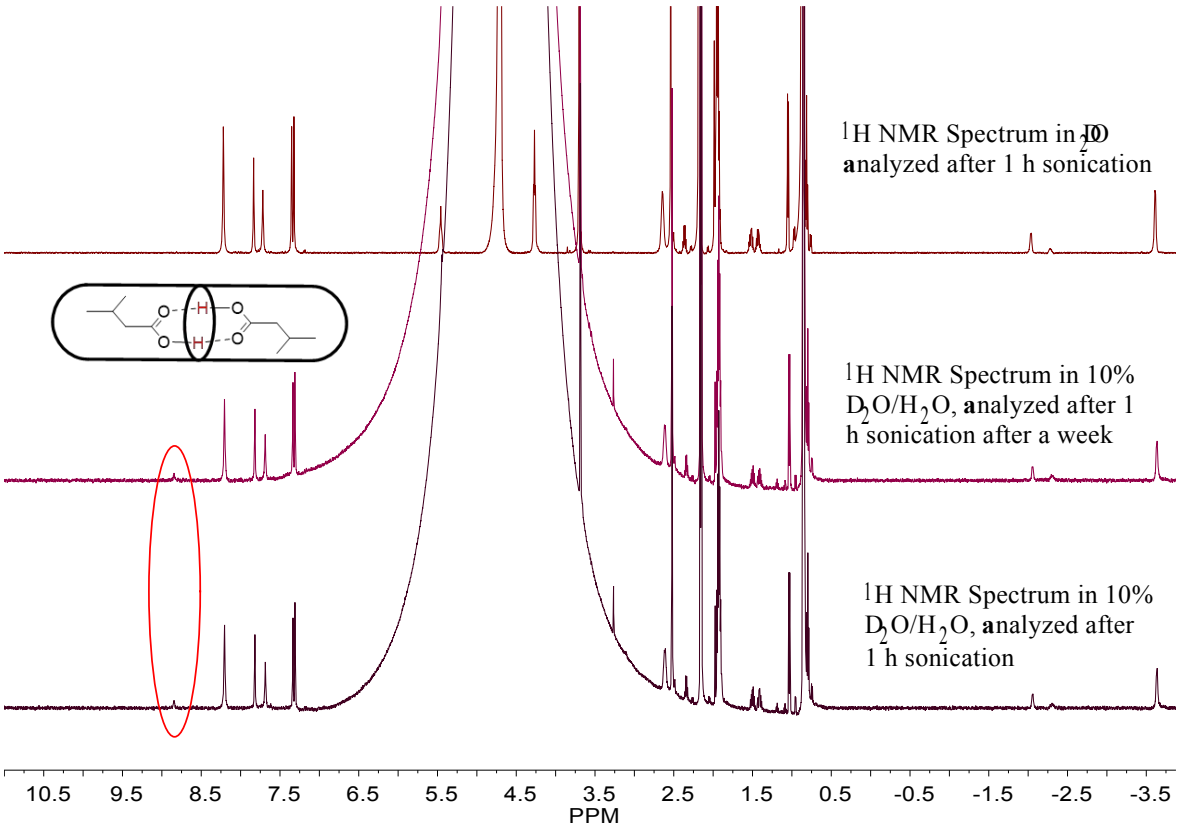


Fig. S35 ^{1}H NMR spectrum of the complex formed between 1, 1 mM + 3-methylbutanoic acid in 10% D_2O in H_2O, analyzed at rt

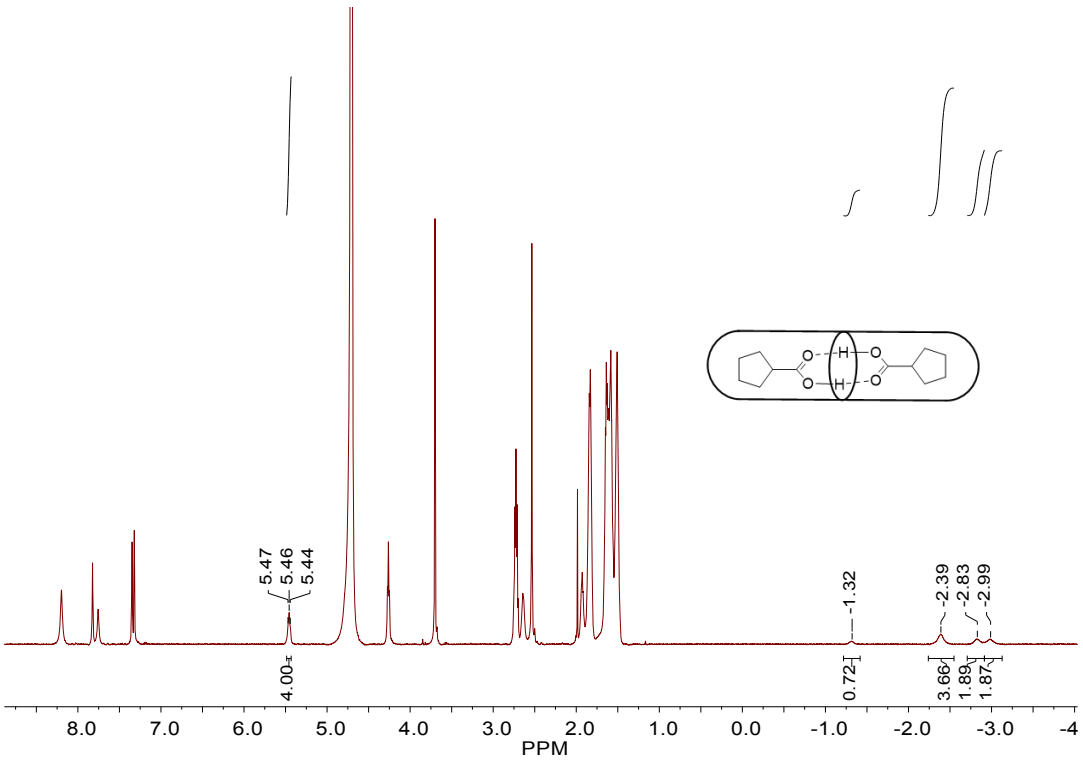


Fig. S36 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + cyclopentane carboxylic acid in D_2O, analyzed at rt

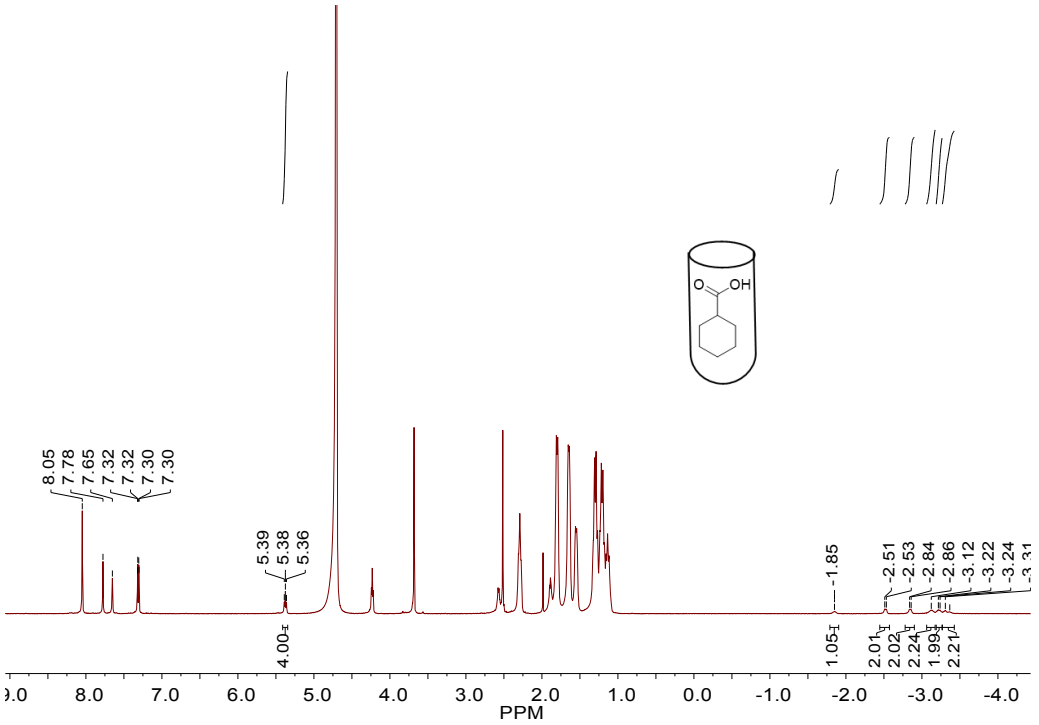


Fig. S37 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + cyclohexane carboxylic acid in D_2O, analyzed at rt

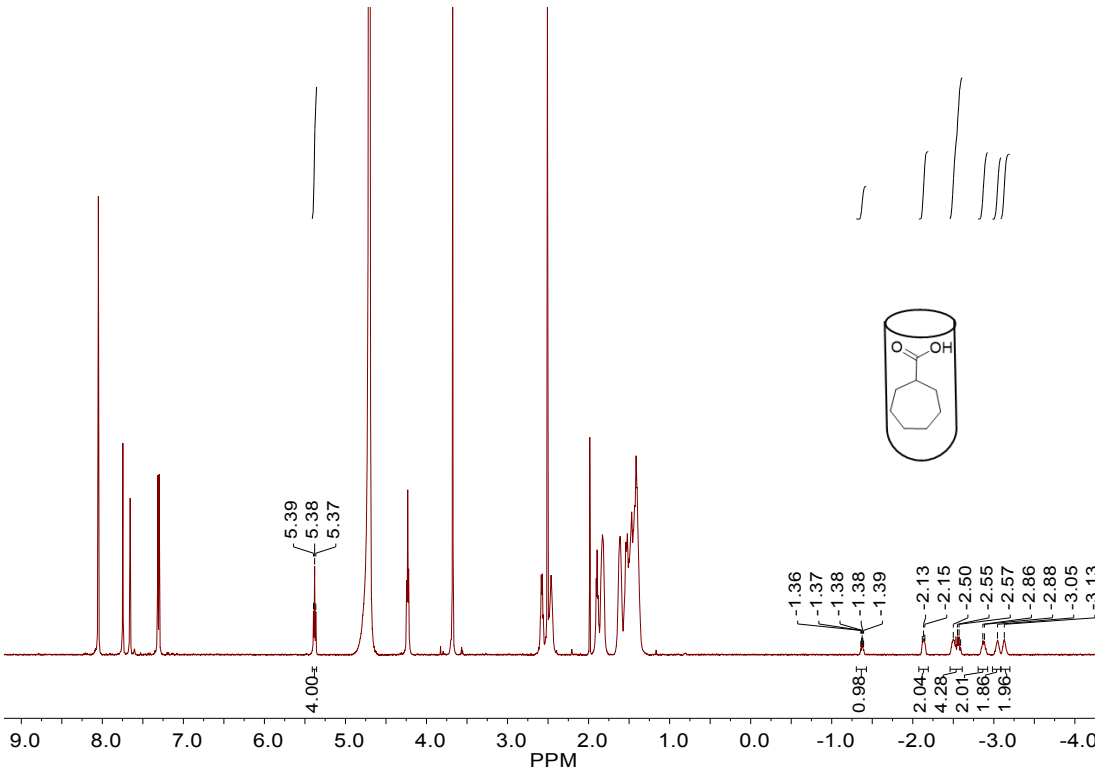


Fig. S38 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + cycloheptane carboxylic acid in D_2O, analyzed at rt

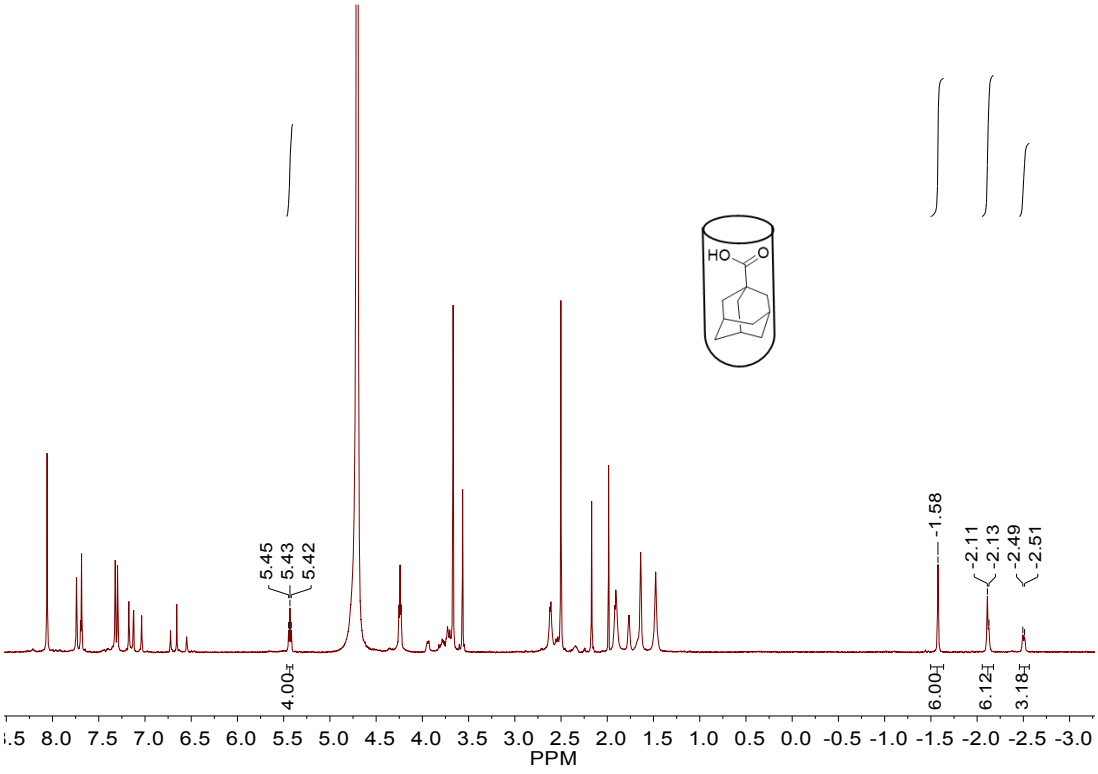


Fig. S39 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + adamantane carboxylic acid in D_2O, analyzed at rt

^{1}H NMR spectra of 1 in water in the presence of different carboxylic acid amide

General procedure for the binding analyses

1 mM, 0.5 mL of **1** in D_2O was taken in NMR tube and 0.5 equivalent of acid amide (as stock solution in acetonitrile-d_3) was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^{1}H NMR spectroscopy at rt.

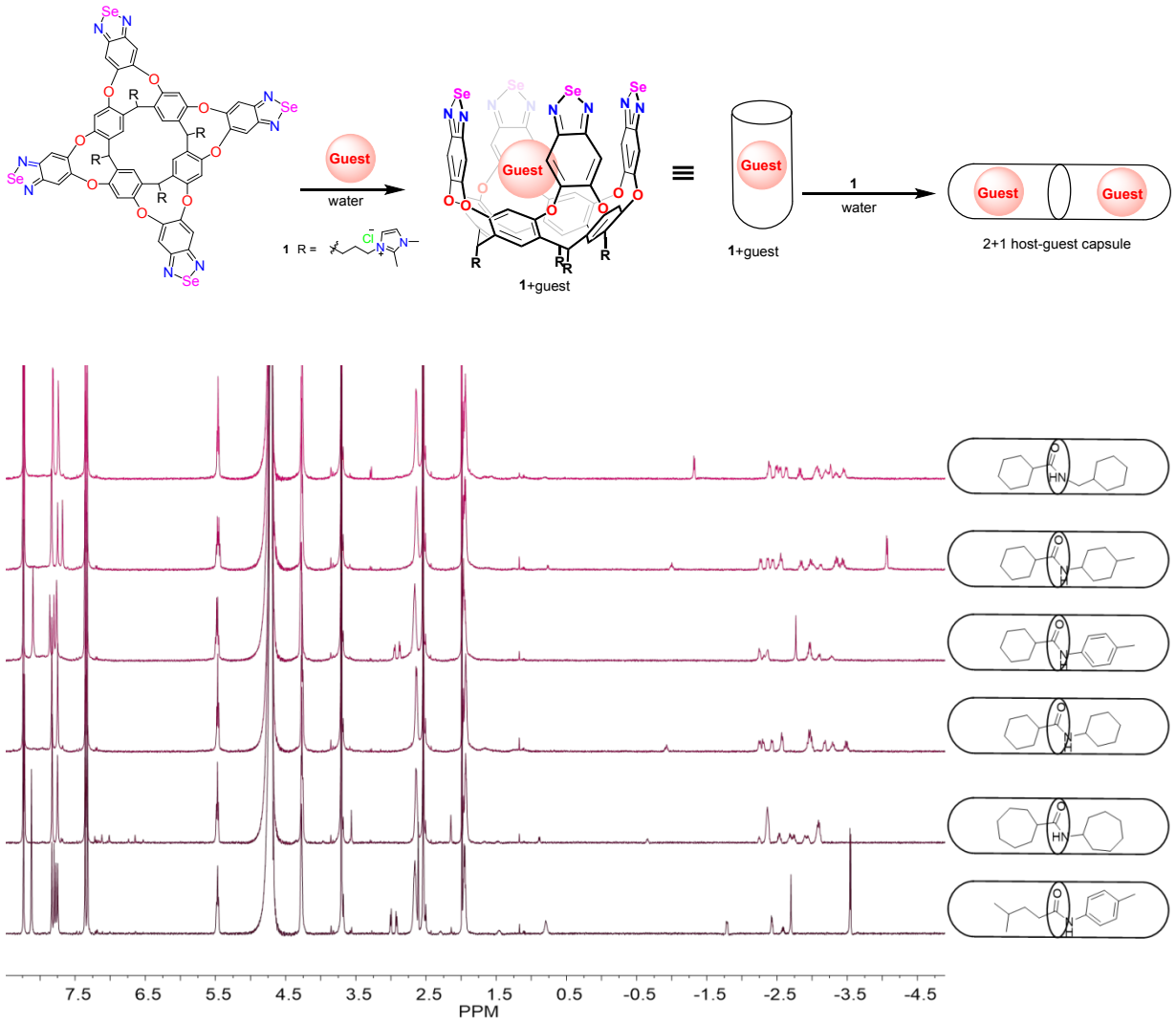


Fig. S40 ^{1}H NMR spectra of the complexes formed between **1**, 1 mM + 0.5 equivalent of, from bottom to top, 4-methyl-N-(p-tolyl)pentanamide, N-cycloheptylcycloheptanecarboxamide, N-cyclohexylcyclohexanecarboxamide, N-(p-tolyl)cyclohexanecarboxamide, N-(4-methylcyclohexyl)cyclohexanecarboxamide, N-(cyclohexylmethyl)cyclohexanecarboxamide in D_2O, stock solution of amide in CD_3CN (50 mM), 5 µL was added to 0.5 mL 1 mM solution of **1**, each mixture was sonicated for 1 h at rt and analyzed at rt; every amide formed a stable capsule

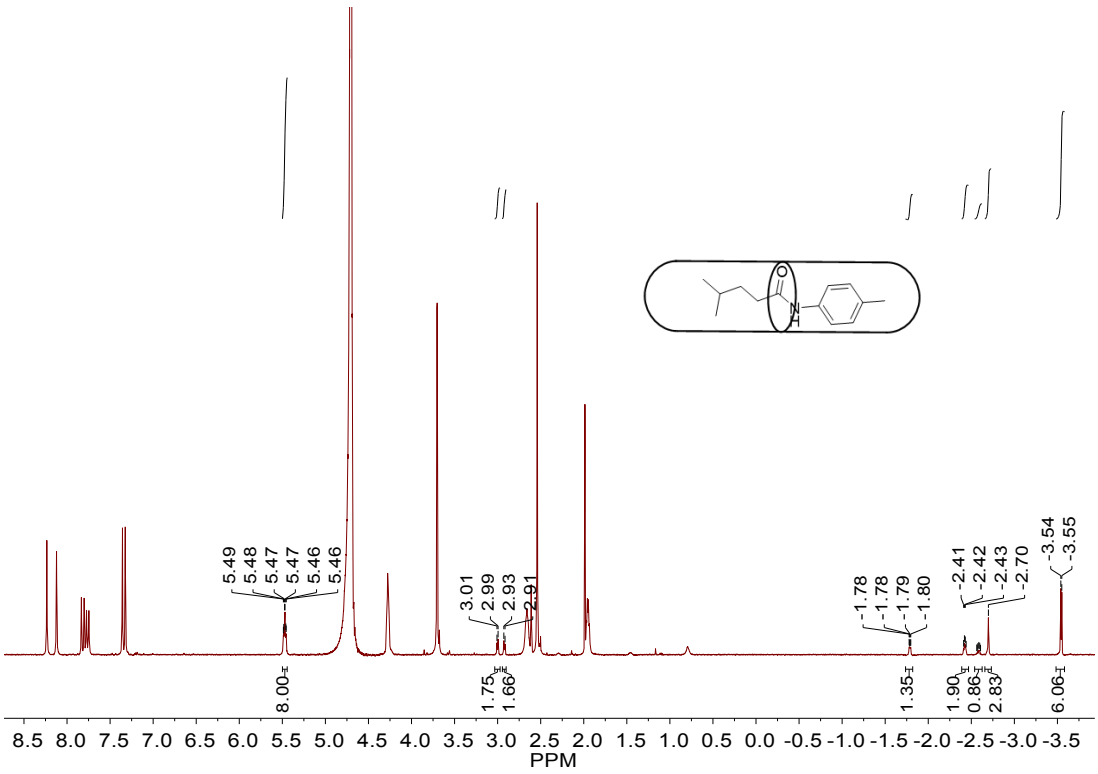


Fig. S41 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + 0.5 equivalent of 4-methyl-N-(p-tolyl)pentanamide in D_2O, analyzed at rt

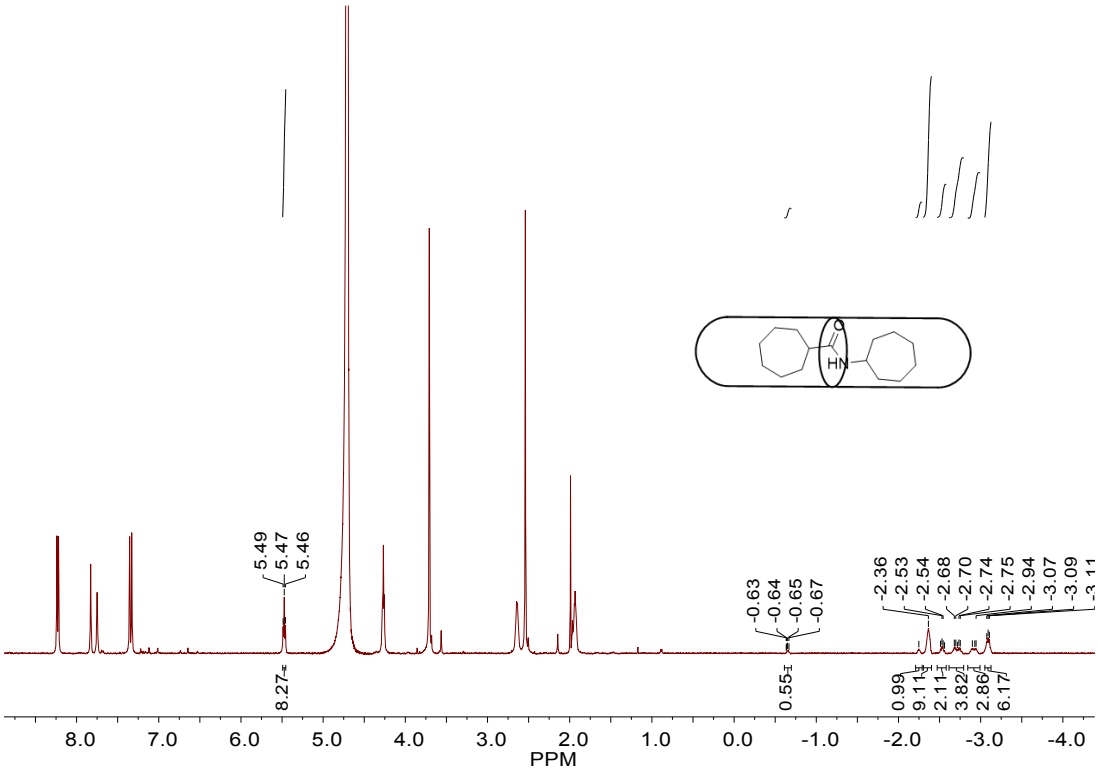


Fig. S42 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + 0.5 equivalent of N-cycloheptylcycloheptanecarboxamide in D_2O, analyzed at rt

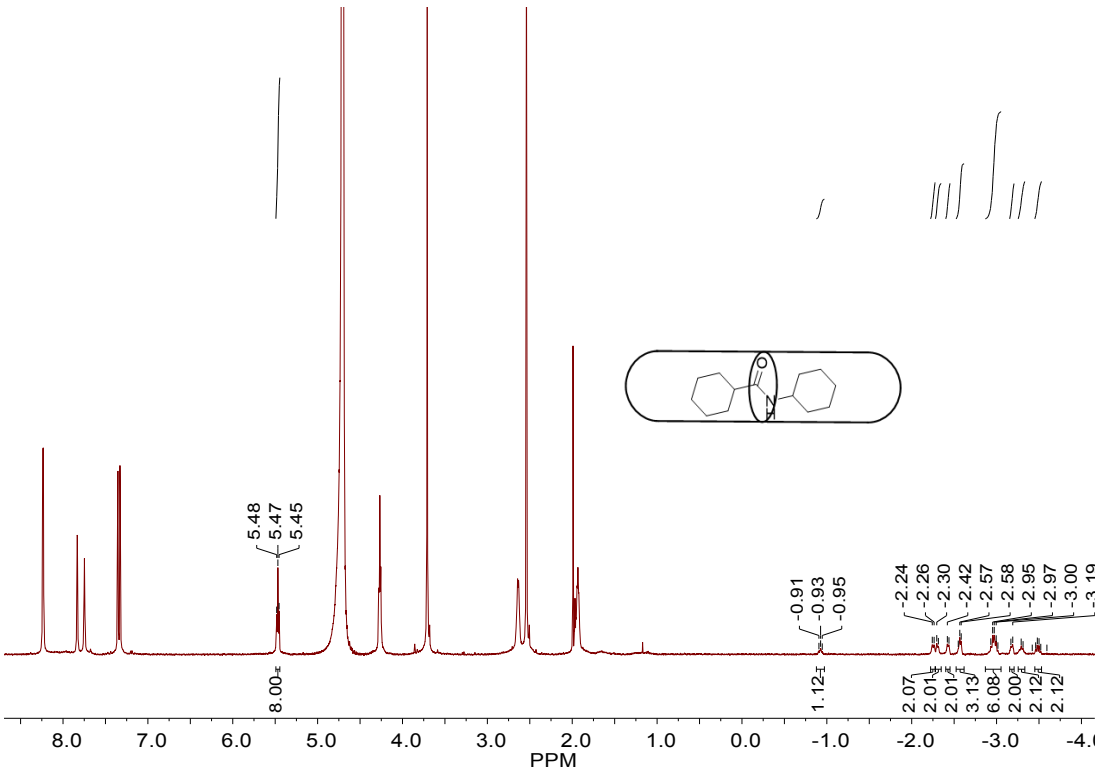


Fig. S43 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + 0.5 equivalent of N-cyclohexylcyclohexanecarboxamide in D_2O, analyzed at rt

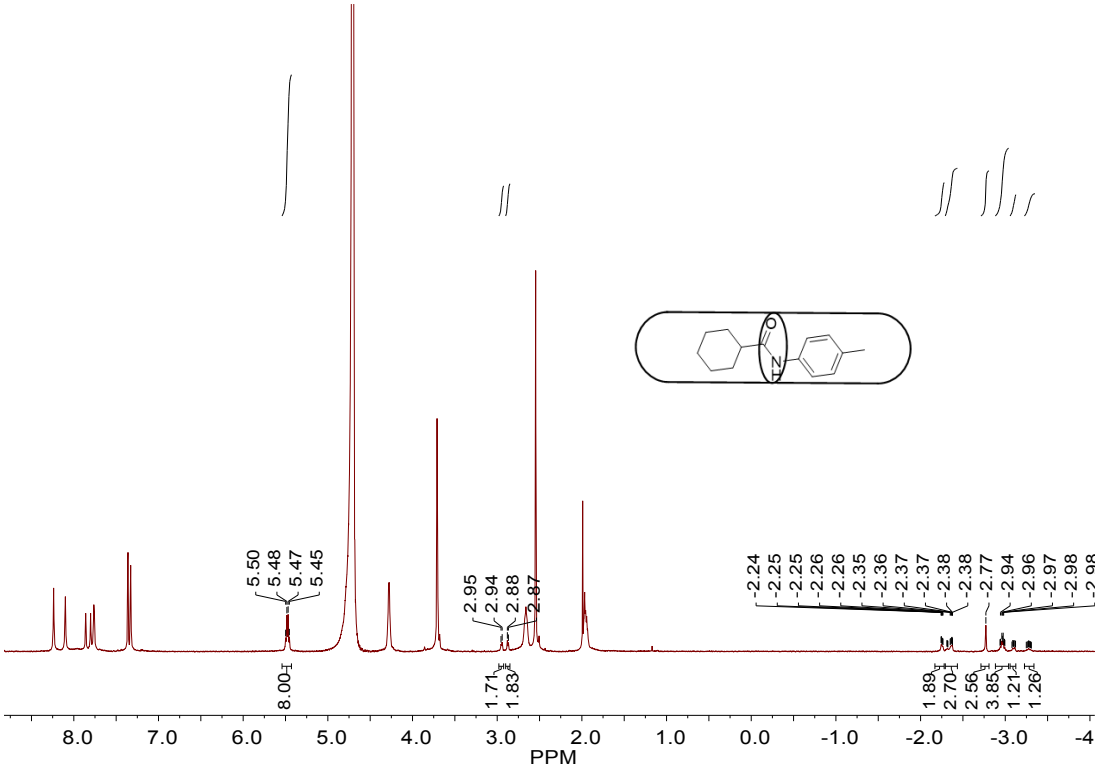


Fig. S44 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + 0.5 equivalent of N-(p-tolyl)cyclohexanecarboxamide in D_2O, analyzed at rt

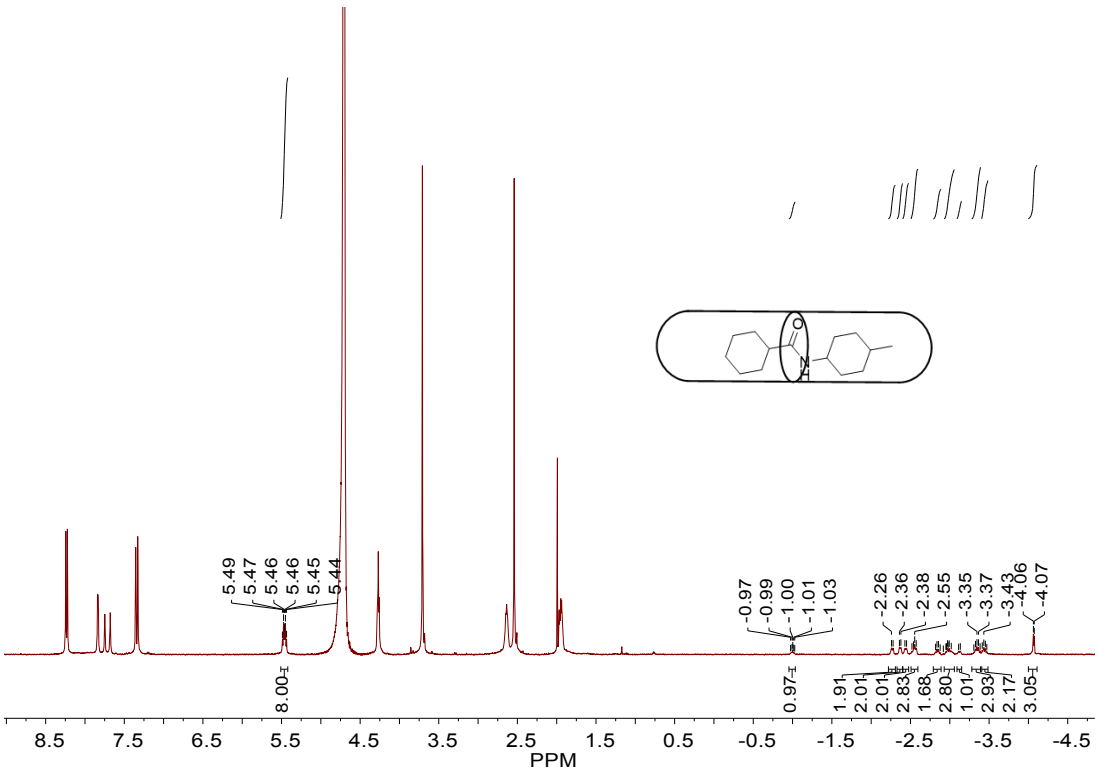


Fig. S45 [1]H NMR spectrum of the complex formed between **1**, 1 mM + 0.5 equivalent of N-(4-methylcyclohexyl)cyclohexanecarboxamide in D_2O, analyzed at rt

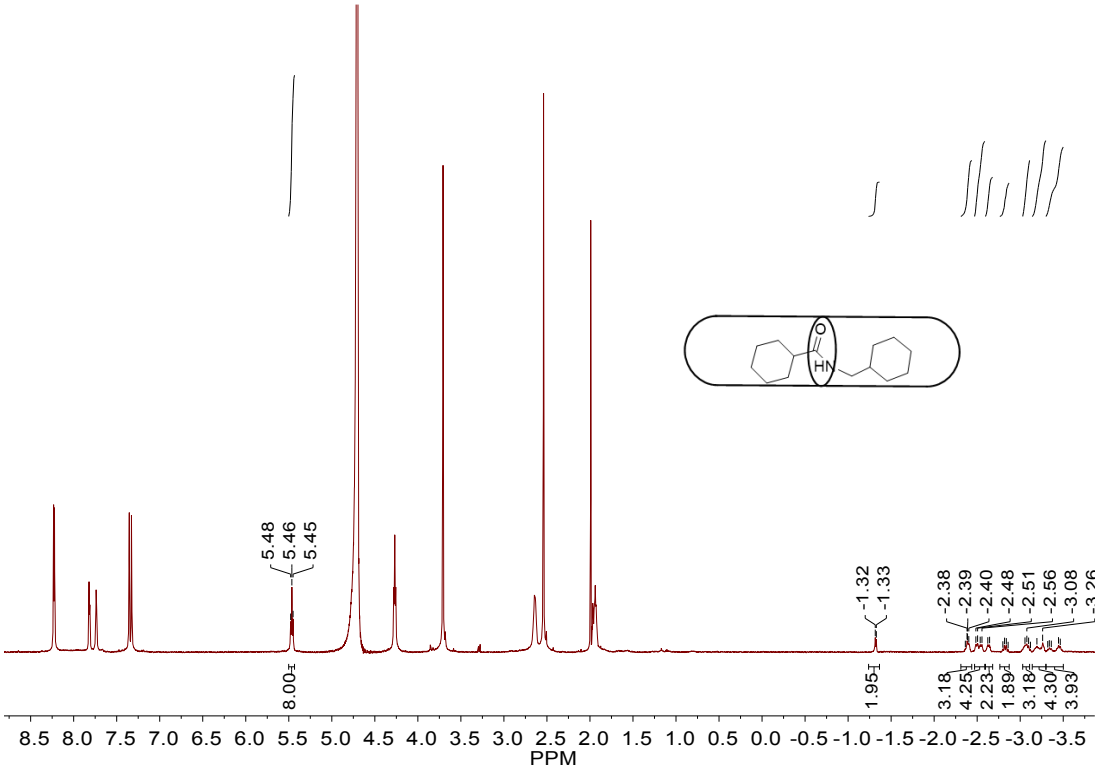


Fig. S46 [1]H NMR spectrum of the complex formed between **1**, 1 mM + 0.5 equivalent of N-(cyclohexylmethyl)cyclohexanecarboxamide in D_2O, analyzed

Capsular assembly confirmation by ^{1}H DOSY NMR spectroscopy

We prepared a solution containing an equimolar mixture of **1** and cyclohexane carboxylic acid. The ^{1}H NMR spectrum of the mixture evidenced that the cyclohexane carboxylic acid formed the 1+1 cavitand complex with the expected orientation of the guest included in **1**. As mentioned above, the size of cyclohexane carboxylic acid appears to be too large for the assembly of 2+2 capsular complex and possibly too small to template a 2+1 host-guest capsular counterpart (ESI Figure S47). We also dissolved in water one equivalent of the cyclohexane carboxylic acid anhydride with two equivalents of **1**. The cyclohexane carboxylic acid anhydride induced the assembly of **1** in a 1+2 encapsulation complex that was stable over two weeks; no changes were observed in any of the guest's chemical shifts, demonstrating that the capsule protected the anhydride from being hydrolyzed by water (ESI Figure S48-S49). As shown in Scheme, we mixed both solution to obtain a complex mixture that was analyzed using ^{1}H DOSY NMR spectroscopy (ESI Figure S50-S52). The two assemblies were identified in the DOSY spectrum of the mixture owing to the different diffusion constants assigned to the protons of **1** in the two assemblies and the slow chemical exchange regime that was operative between them in both the chemical shift and diffusion timescales. The 2+1 cyclohexane carboxylic acid anhydride capsule's methine and benzoselenadiazole protons' chemical shifts are downfield shifted compared to those of the 1+1 cavitand complex formed by the cyclohexane carboxylic acid.

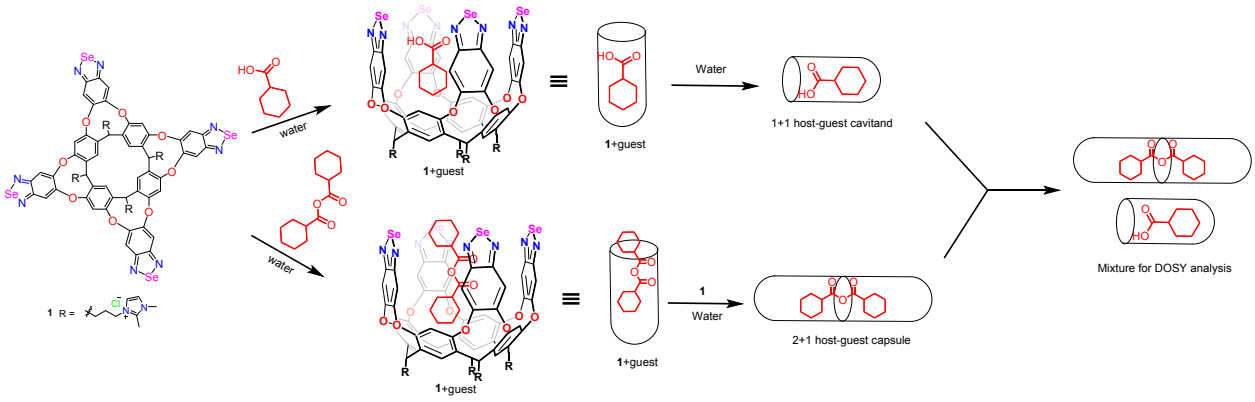
^{1}H DOSY NMR confirmation of the capsule formed by 1 in the presence of guest

General procedure for preparation of the samples for binding analyses

- 1 mM, 0.5 mL of cavitand solution in D_2O was taken in NMR tube and 1 equivalent of cyclohexane carboxylic acid was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^{1}H NMR spectroscopy at rt Fig. ESI. S47.

- Similarly, 1 mM, 0.5 mL of cavitand solution in D_2O was taken in NMR tube and 0.5 equivalent of cyclohexane carboxylic acid anhydride was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^{1}H NMR spectroscopy at rt Fig. ESI. S48.

- Both of the above samples were mixed and analyzed by ^{1}H NMR (Fig. ESI S52) and DOSY spectroscopy at rt.



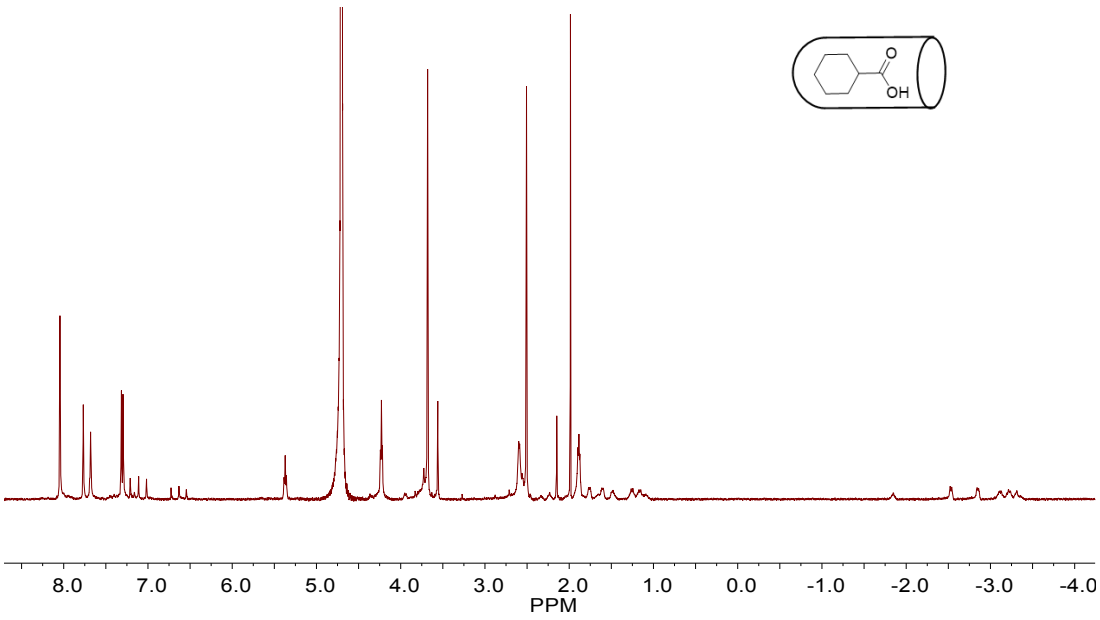


Fig. S47 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 1 equivalent of cyclohexane carboxylic acid, analyzed at rt

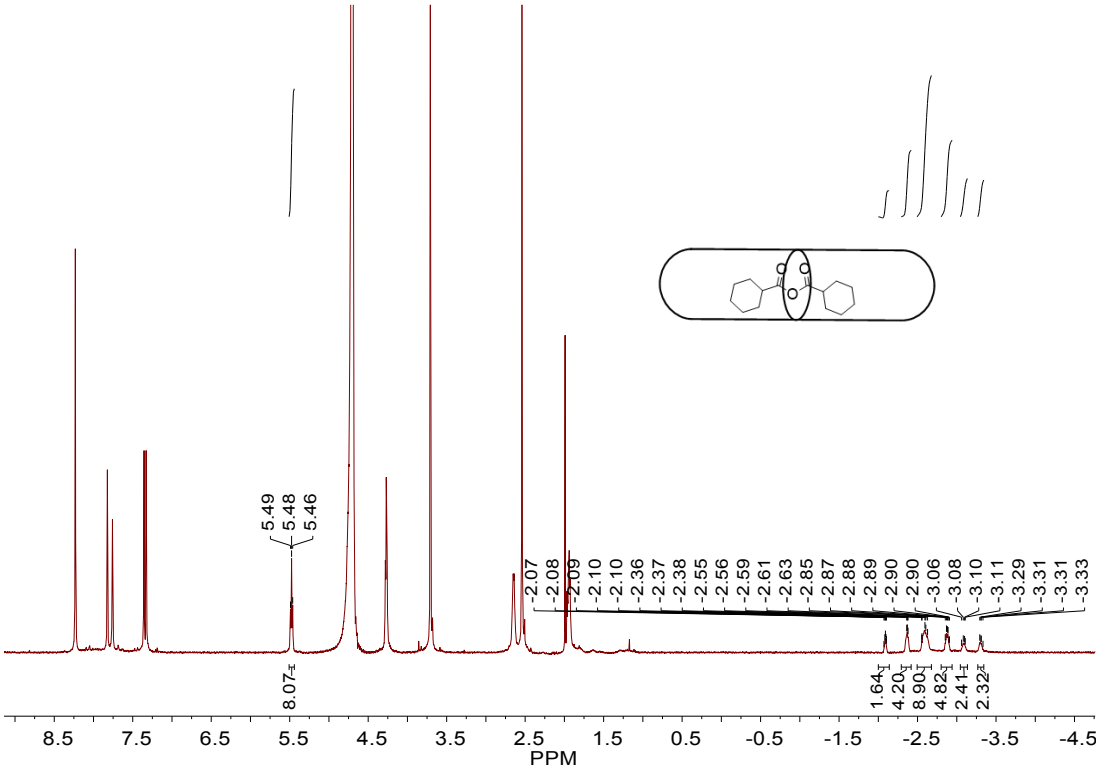


Fig. S48 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 0.5 equivalent of cyclohexane carboxylic acid anhydride (added as 5 µL, 100 mM stock solution in CD_3CN), analyzed at rt

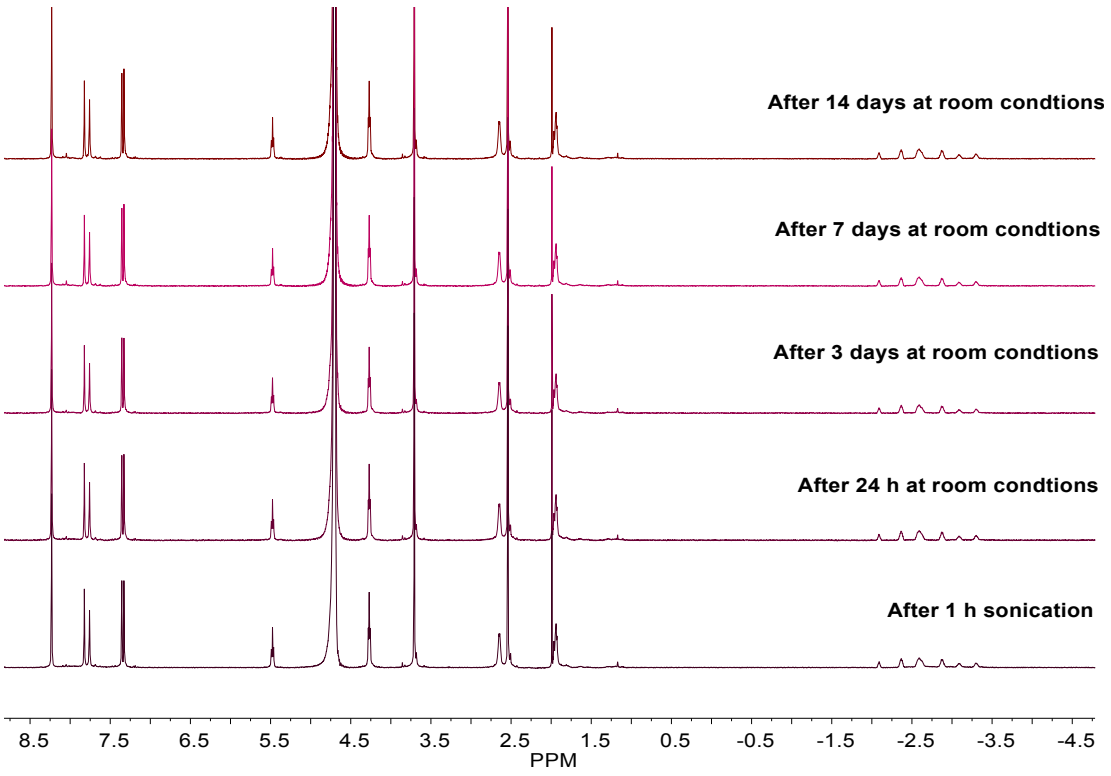


Fig. S49 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 0.5 equivalent of cyclohexane carboxylic acid anhydride (added as 5 µL, 100 mM stock solution in CD_3CN), analyzed over mentioned time points at rt

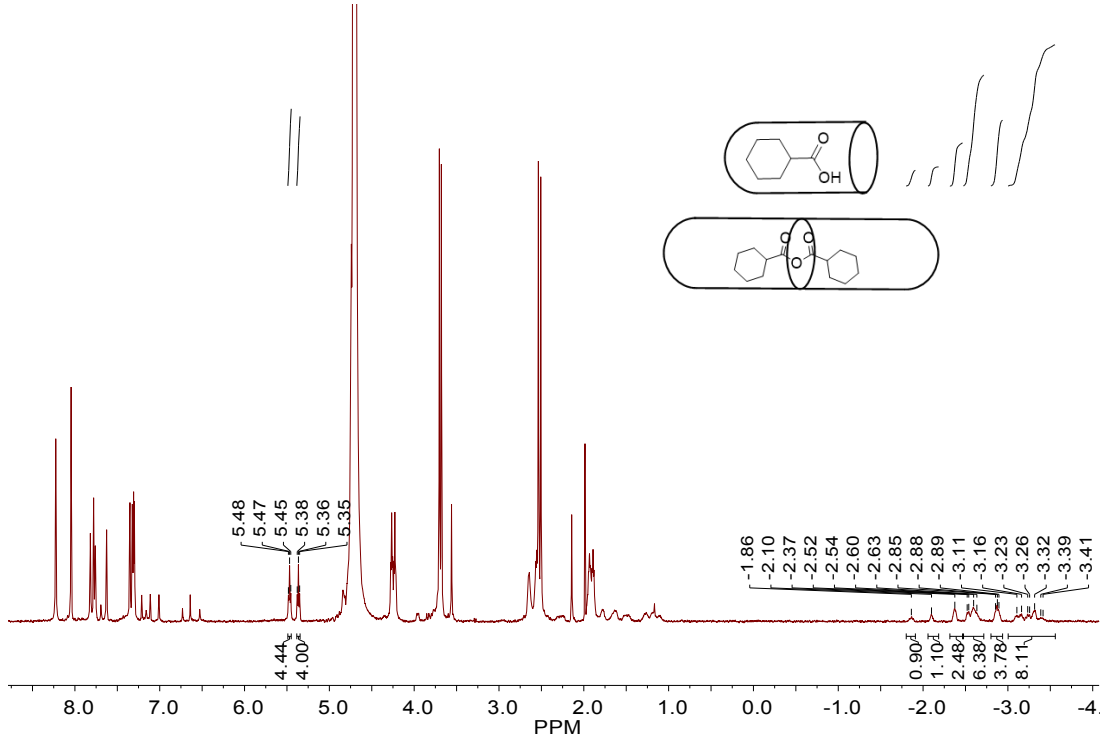


Fig. S50 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 0.5 equivalent of cyclohexane carboxylic acid and 1, 1 mM in D_2O + 0.5 equivalent of cyclohexane carboxylic acid anhydride (added as 5 µL, 100 mM stock solution in CD_3CN), mixed and analyzed by ^{1}H NMR spectroscopy (mixture of sample displayed in Fig. S47 and Fig. S48)

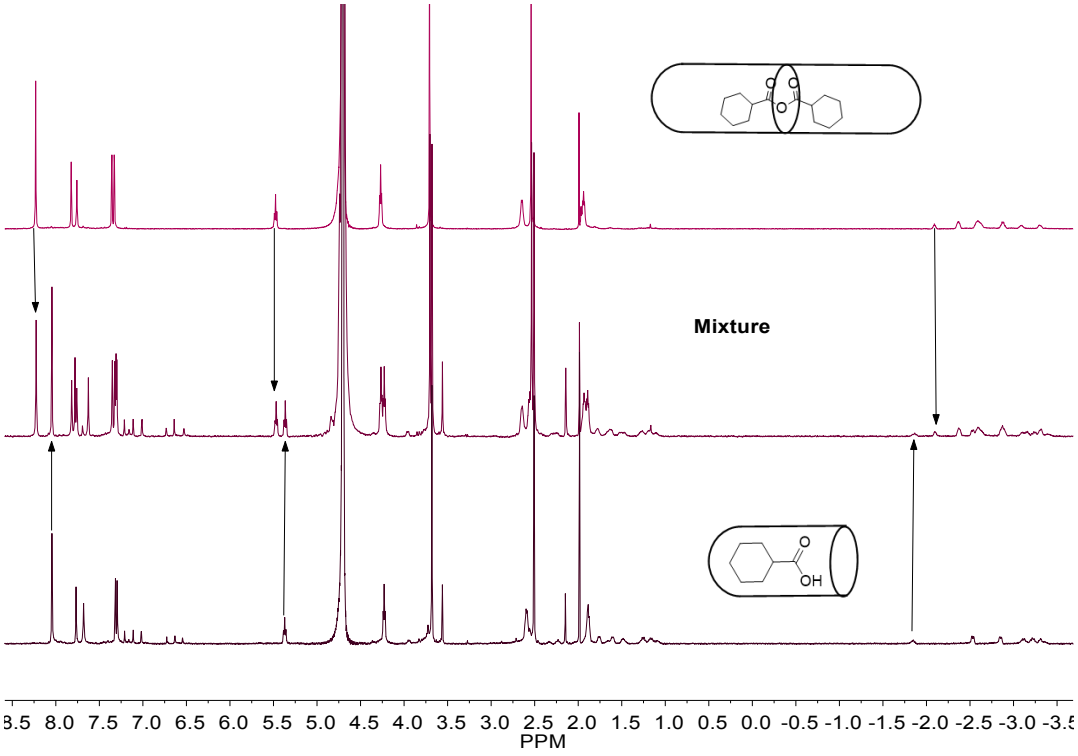


Fig. S51 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 1 equivalent of cyclohexane carboxylic acid (bottom), **1**, 1 mM in D_2O + 0.5 equivalent of cyclohexane carboxylic acid anhydride (added as 5 µL, 100 mM stock solution in CD_3CN) (top), mixture of both these samples (middle)

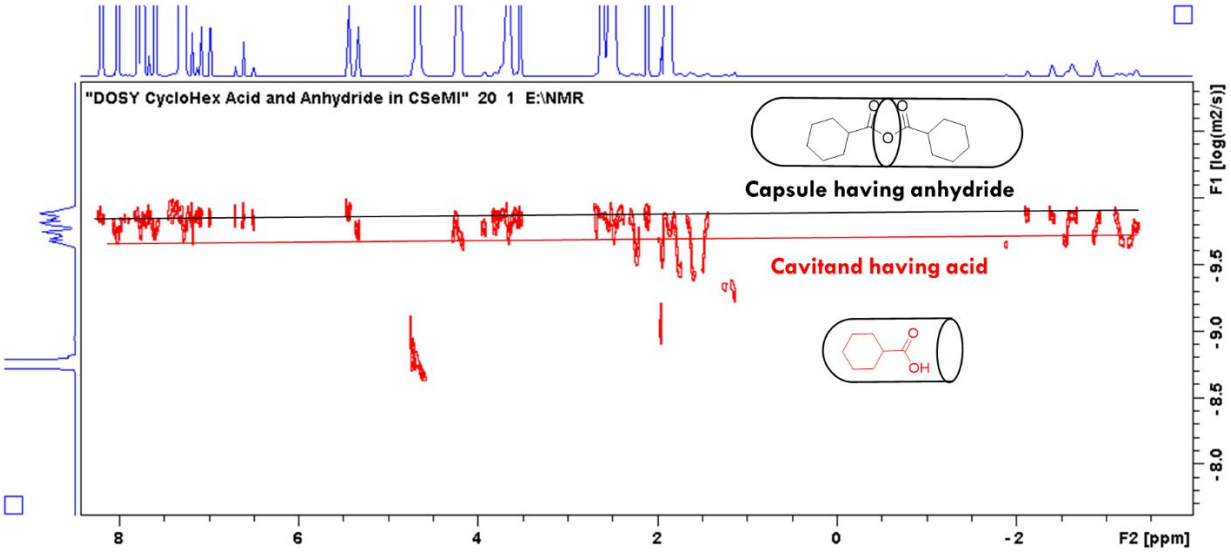


Fig. S52 ^{1}H DOSY NMR spectrum of the cavitand and capsule mixture formed by **1** in the presence of cyclohexane carboxylic acid and cyclohexane carboxylic acid anhydride respectively; 1 mM of **1** was added with 1 equivalent of cyclohexane carboxylic acid or cyclohexane carboxylic acid anhydride separately and then both these samples were mixed and analyzed by DOSY NMR spectroscopy.

Binding selectivity for saturated cyclic hydrocarbons over their unsaturated ones

When benzene was added as a guest to a D_2O solution of **1**, the broadened signal around 7.2 ppm indicated the relatively fast exchange of benzene in and out of the cavitand, rather than the formation of a dimeric capsule (ESI Figure S53). This was also deduced from the methine proton's chemical shift of the 1+1 cavitand complex of **1** with benzene, observed upfield as compared to that of 2+2 capsule of **1** formed with cyclohexane (ESI Figure S53 and S56). Additional competitive binding experiments using 1:1 host-guest ratios showed the same binding preference for cyclohexane (ESI Figure S58-S60).

Addition of toluene to **1** in D_2O formed a 1+1 cavitand complex that was easily recognized from its methine proton chemical shift and integration of the bound toluene methyl's protons (ESI Figure S62). Toluene was bound in a way that its methyl group was deep in the cavity with a ^1H signal of the $-CH_3$ protons resonating at -2.27 ppm with $\Delta\delta$ = - 4.47 ppm (ESI Figure S62). The addition of a 1:1 mixture of toluene and methyl cyclohexane to **1** gave only a dimeric capsule with two molecules of methyl cyclohexane in the inner space (ESI Figure S64). Furthermore, methyl cyclohexane replaced toluene from its complex with **1** to generate a 2+2 capsular assembly (ESI Figure. S63). Selectivity in equivalent quantities of host and guests showed the same binding preference for methyl cyclohexane (ESI Figure S66-S68).

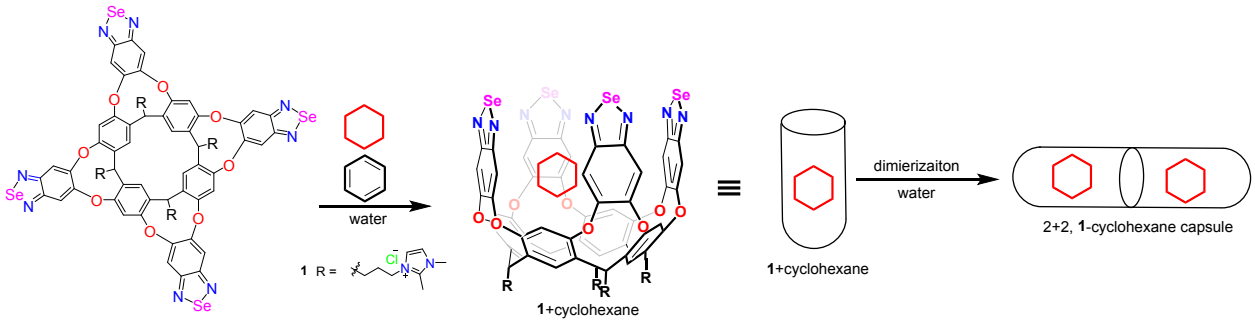
Binding selectivity of 1 for benzene and cyclohexane

General procedure for the binding analyses using excess guest

1 mM, 0.5 mL of cavitand solution in D_2O was taken in NMR tube and excess of the guest was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^1H NMR spectroscopy at rt.

General procedure for the binding analyses using 1:1 host and guest ratio

1 mM, 0.5 mL of **1** in D_2O was taken in NMR tube and 0.5 equivalent of the guest (as stock solution in acetonitrile-d_3) was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^1H NMR spectroscopy at rt.



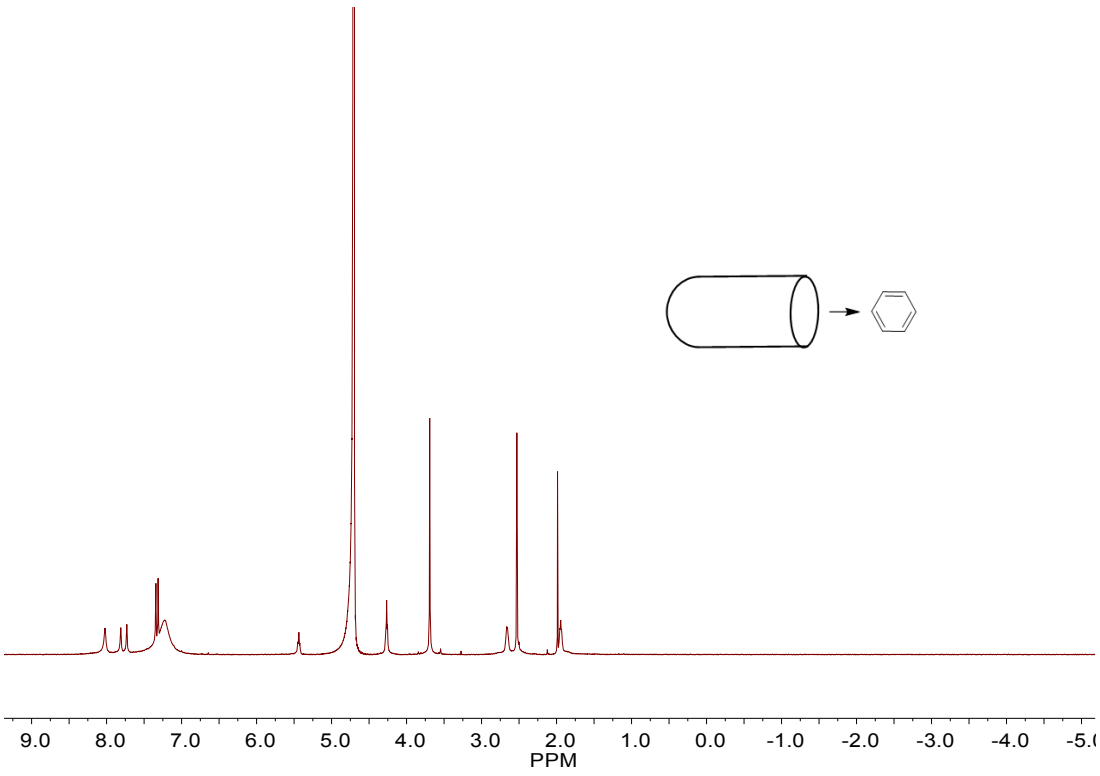


Fig. S53 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + excess benzene, in D_2O, analyzed at rt

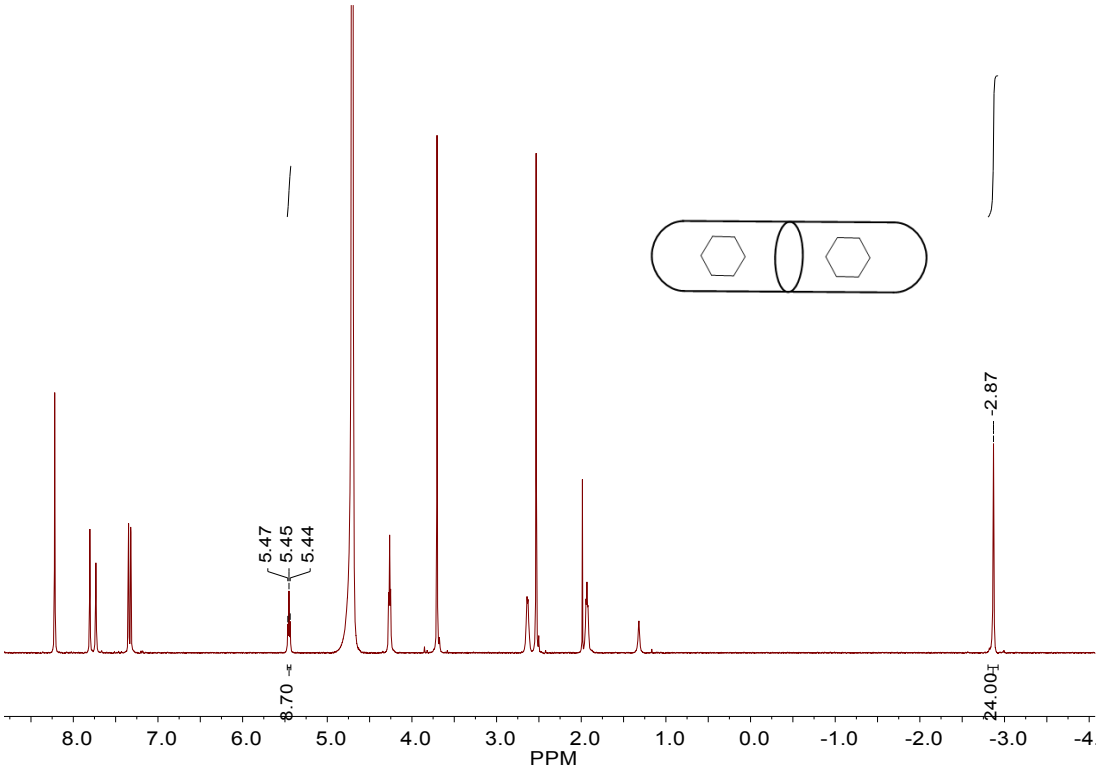


Fig. S54 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + excess cyclohexane, in D_2O, analyzed at rt

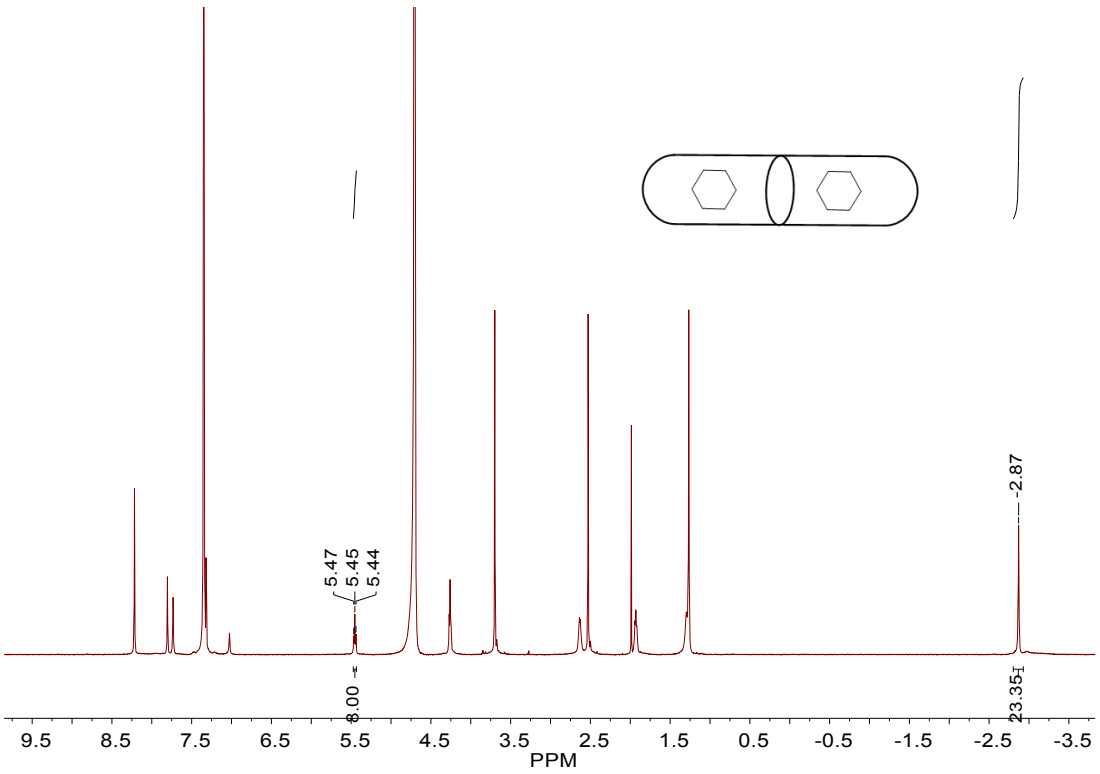


Fig. S55 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + excess cyclohexane and benzene (1:1) mixture, in D_2O, analyzed at rt

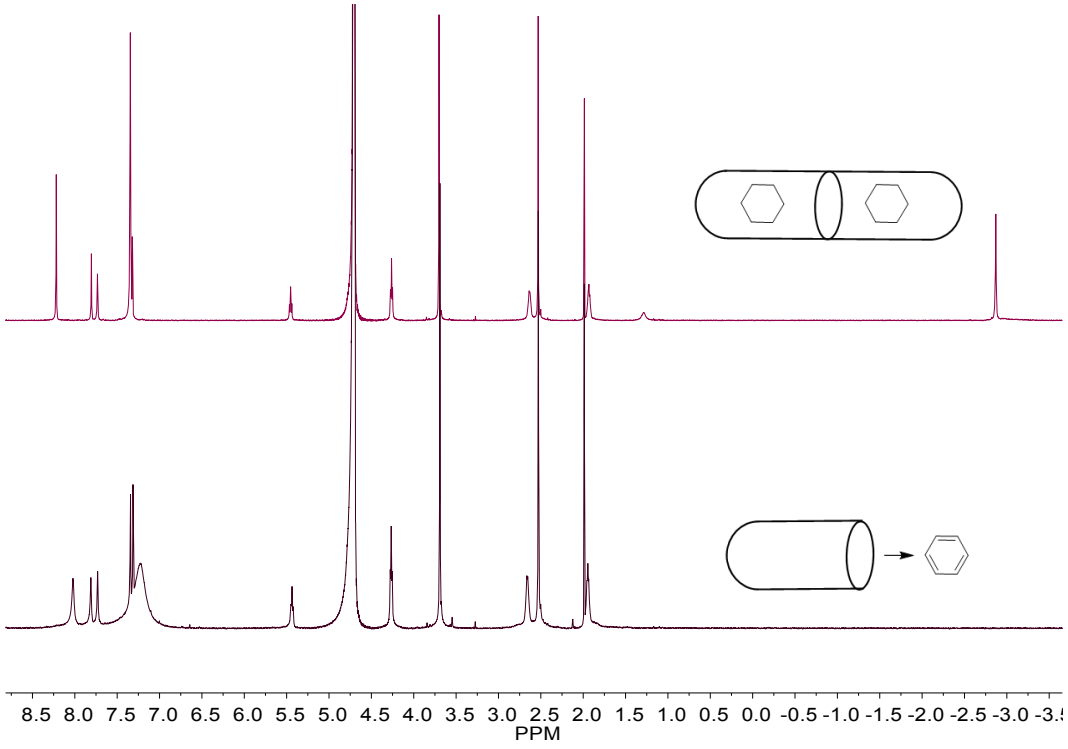


Fig. S56 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + excess benzene sonicated for 1 h and analyzed by ^{1}H NMR spectroscopy (bottom), Then excess cyclohexane was added sonicated for 1 h and analyzed by ^{1}H NMR spectroscopy (top), in D_2O, analyzed at rt

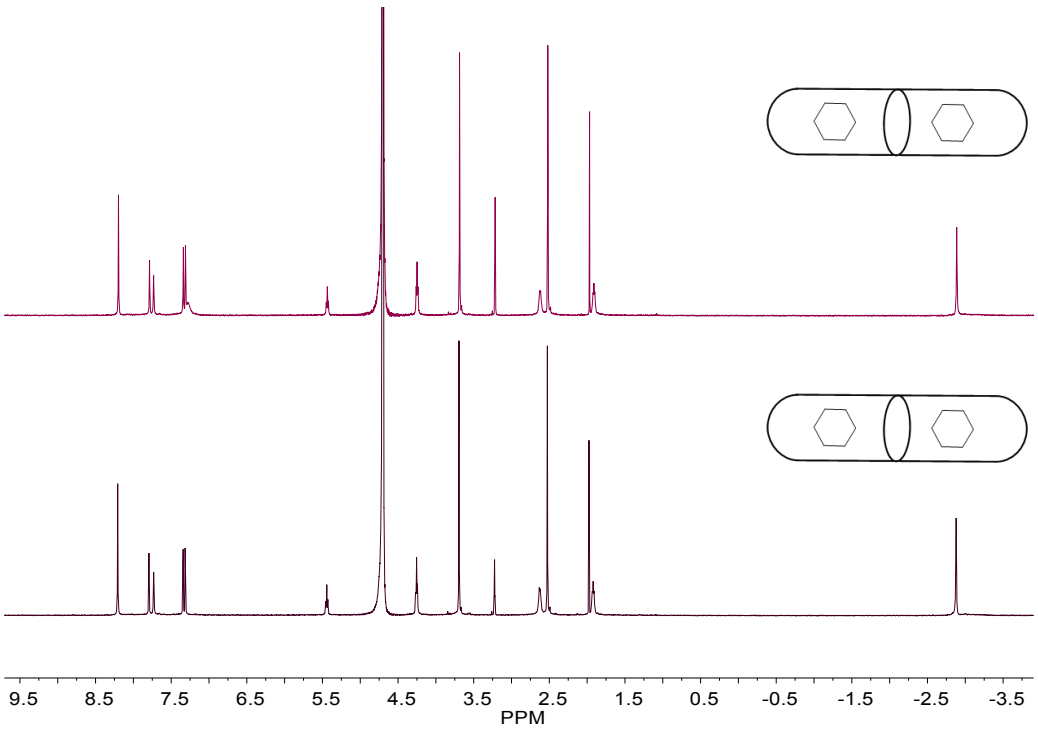


Fig. S57 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM + excess cyclohexane sonicated for 1 h and analyzed by ^{1}H NMR spectroscopy (bottom), Then excess benzene was added sonicated for 1 h and analyzed by ^{1}H NMR spectroscopy (top), in D_2O, analyzed at rt

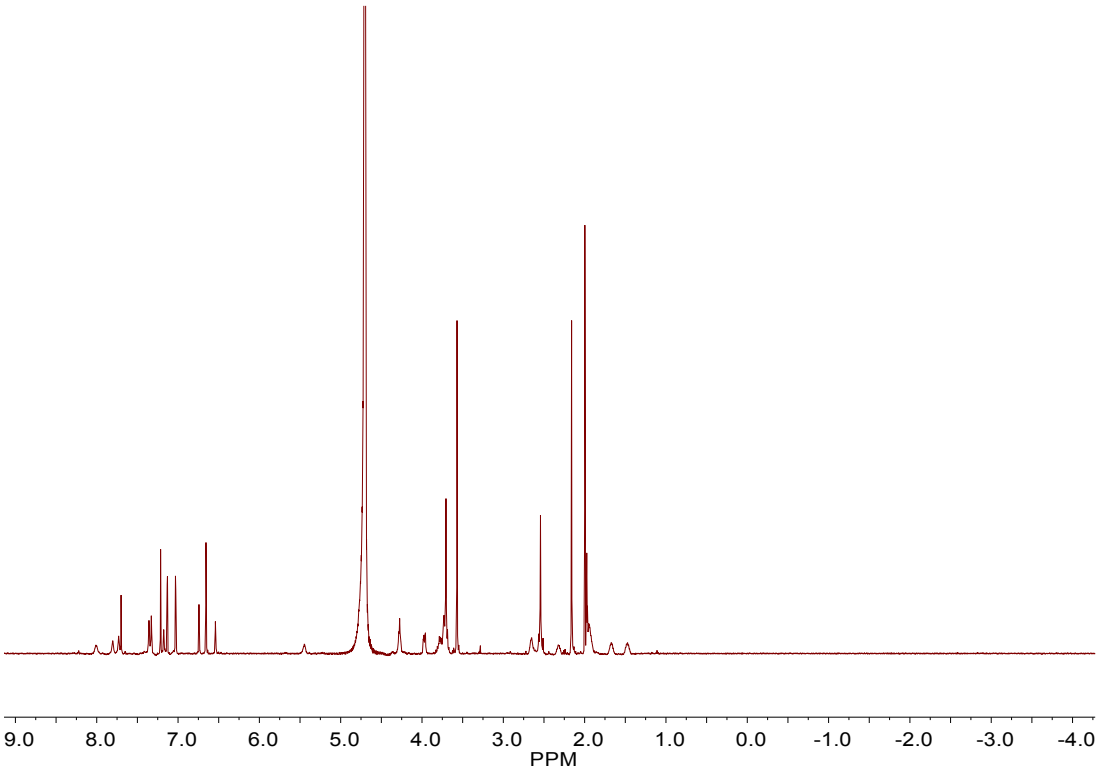


Fig. S58 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 1 equivalent benzene (added as 5 µL, 100 mM stock solution in CD_3CN), analyzed at rt

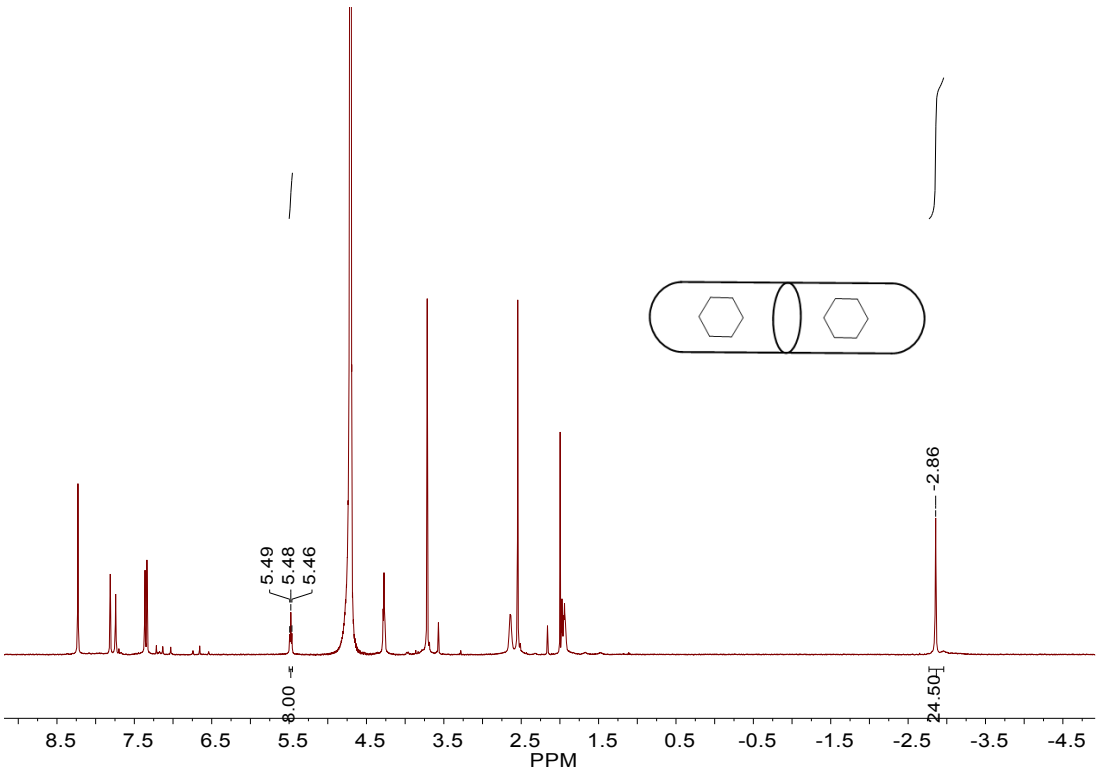


Fig. S59 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 1 equivalent cyclohexane (added as 5 µL, 100 mM stock solution in CD_3CN), analyzed at rt

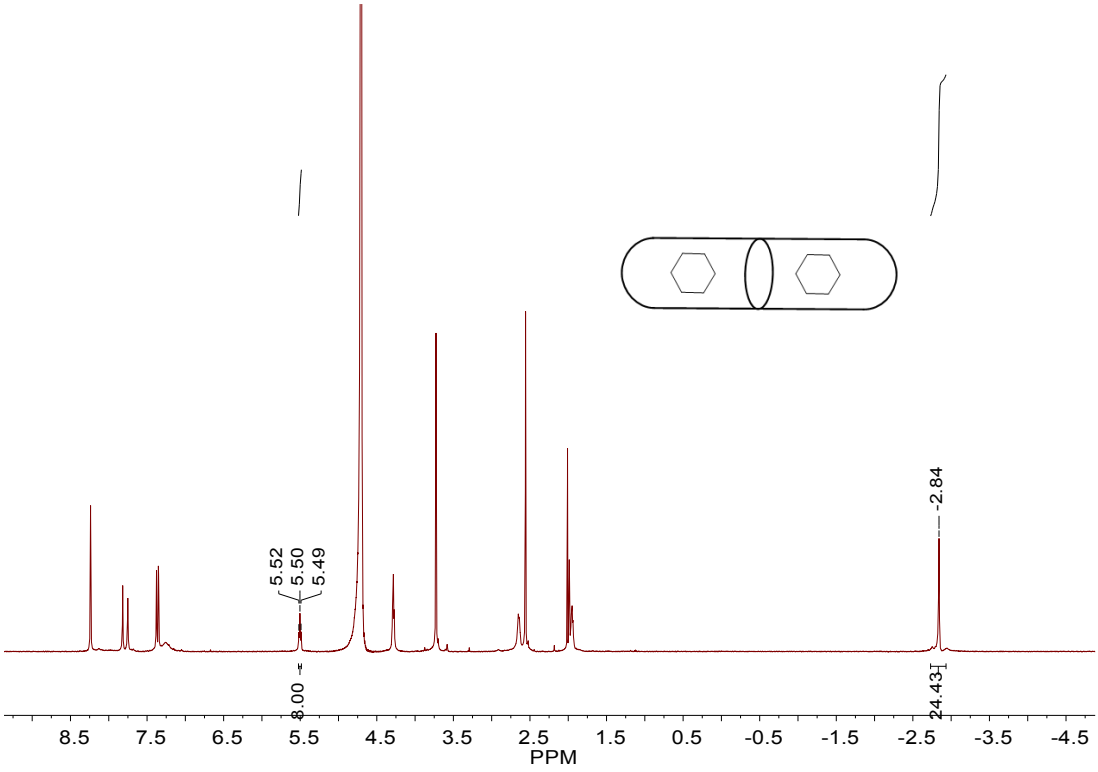


Fig. S60 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 1 equivalent each benzene and cyclohexane (each one added as 5 µL, 100 mM stock solution in CD_3CN), analyzed at rt

Binding selectivity for toluene and methyl cyclohexane

General procedure for the binding analyses using excess guest

1 mM, 0.5 mL of cavitand solution in D_2O was taken in NMR tube and excess of the guest was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^1H NMR spectroscopy at rt.

General procedure for the binding analyses using 1:1 host and guest ratio

1 mM, 0.5 mL of **1** in D_2O was taken in NMR tube and 0.5 equivalent of the guest (as stock solution in methanol-d_4) was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^1H NMR spectroscopy at rt.

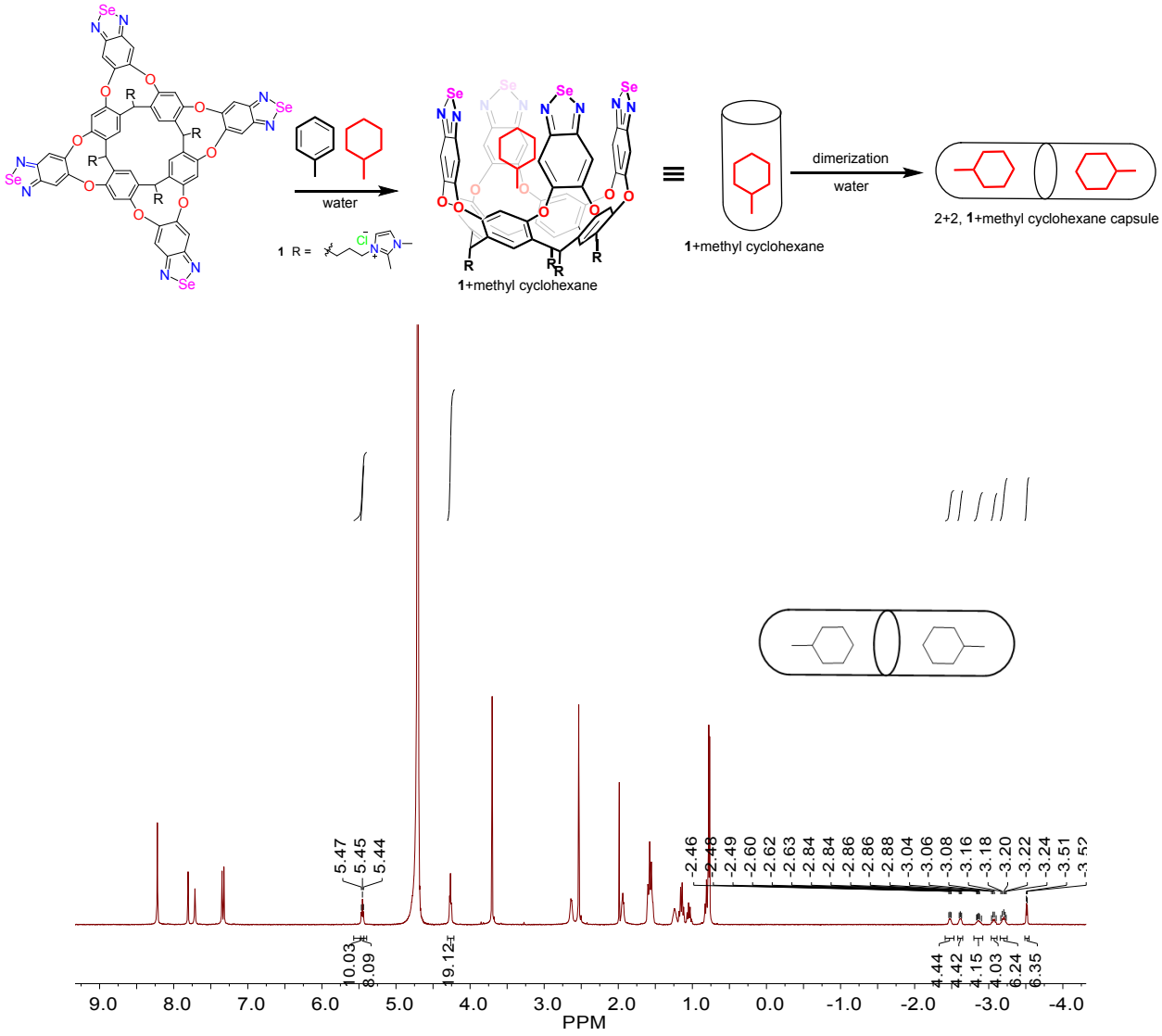


Fig. S61 ^1H NMR spectrum of the complex formed between **1**, 1 mM , in D_2O + excess methyl cyclohexane, analyzed at rt

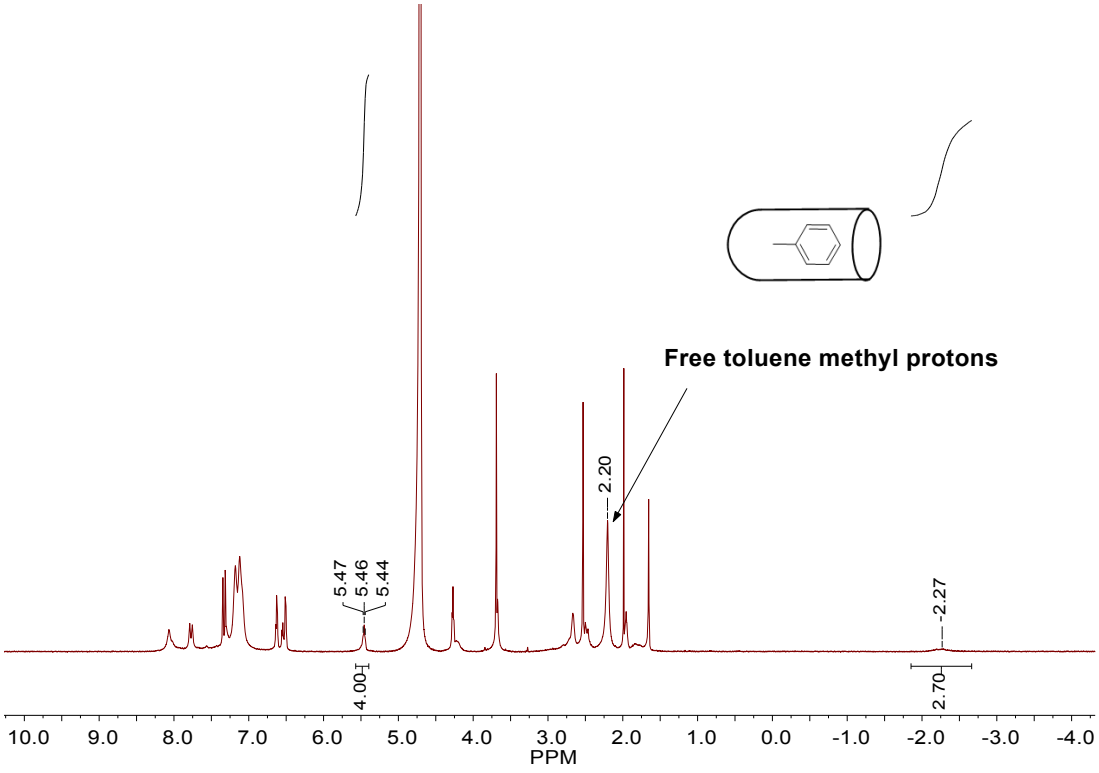


Fig. S62 [1]H NMR spectrum of the complex formed between **1**, 1 mM, in D_2O + excess toluene, analyzed at rt

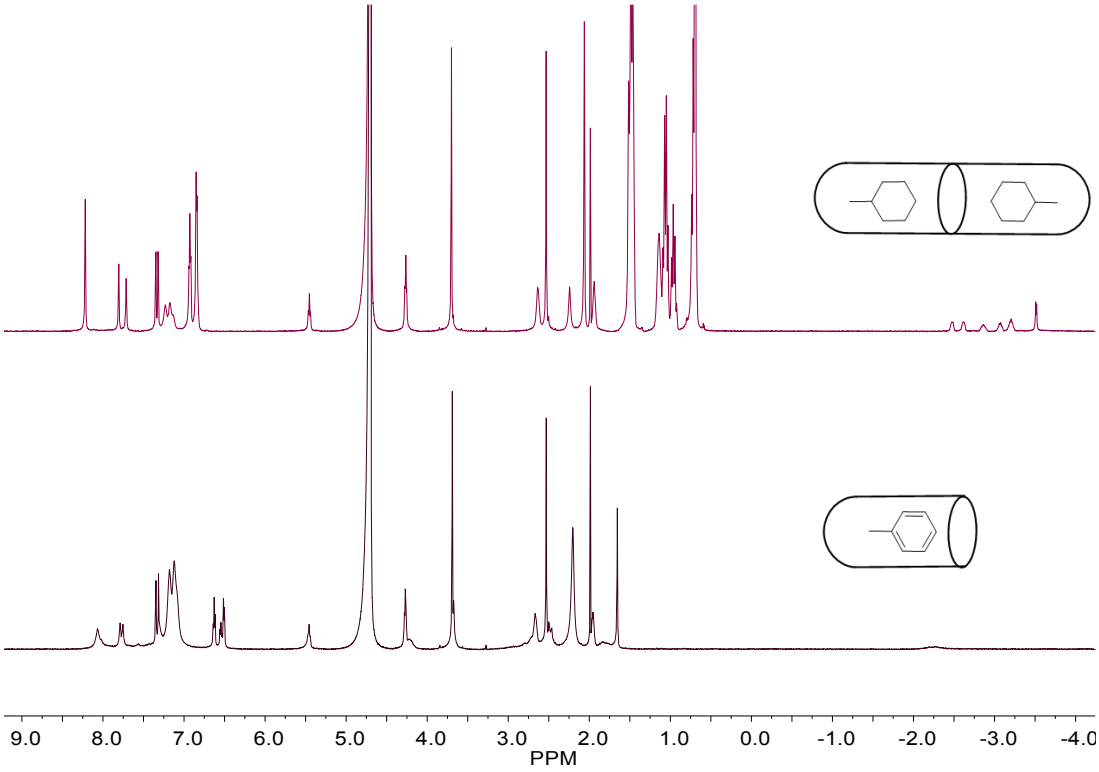


Fig. S63 [1]H NMR spectrum of the complex formed between **1**, 1 mM + excess toluene sonicated for 1 h and analyzed by [1]H NMR spectroscopy (bottom), Then excess methyl cyclohexane was added sonicated for 1 h and analyzed by [1]H NMR spectroscopy (top), in D_2O, analyzed at rt, toluene was completely replaced by methyl cyclohexane to covert unstable cavitand to stable capsule while encapsulating two molecules of methyl cyclohexane

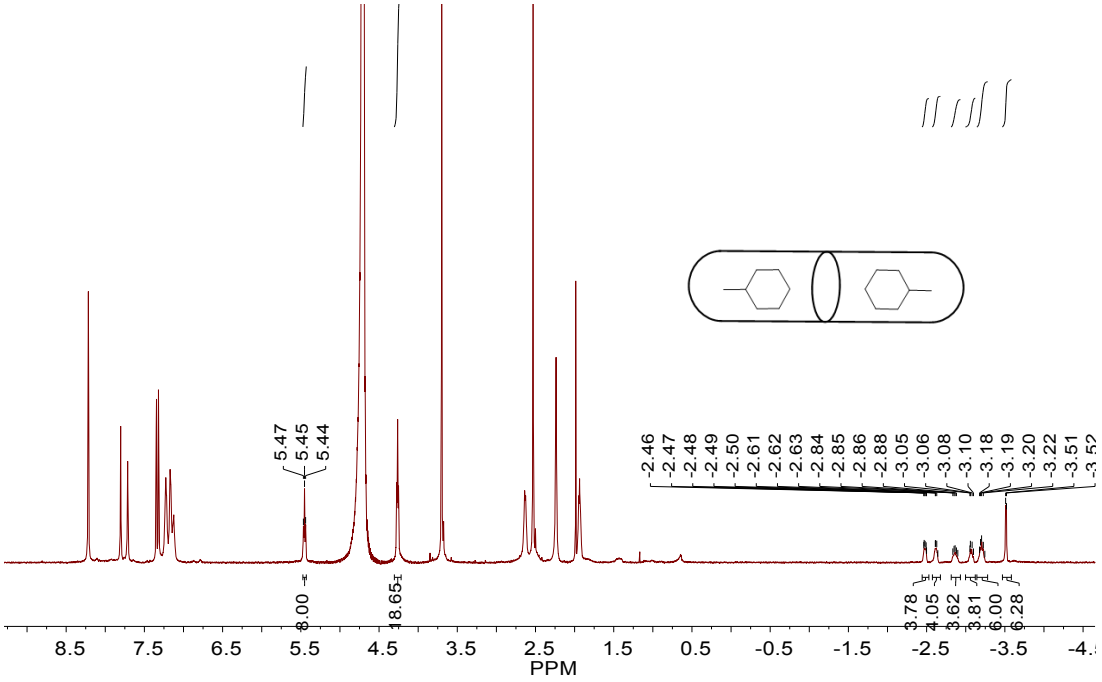


Fig. S64 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM, in D_2O + excess methyl cyclohexane and toluene (1:1) mixture, analyzed at rt

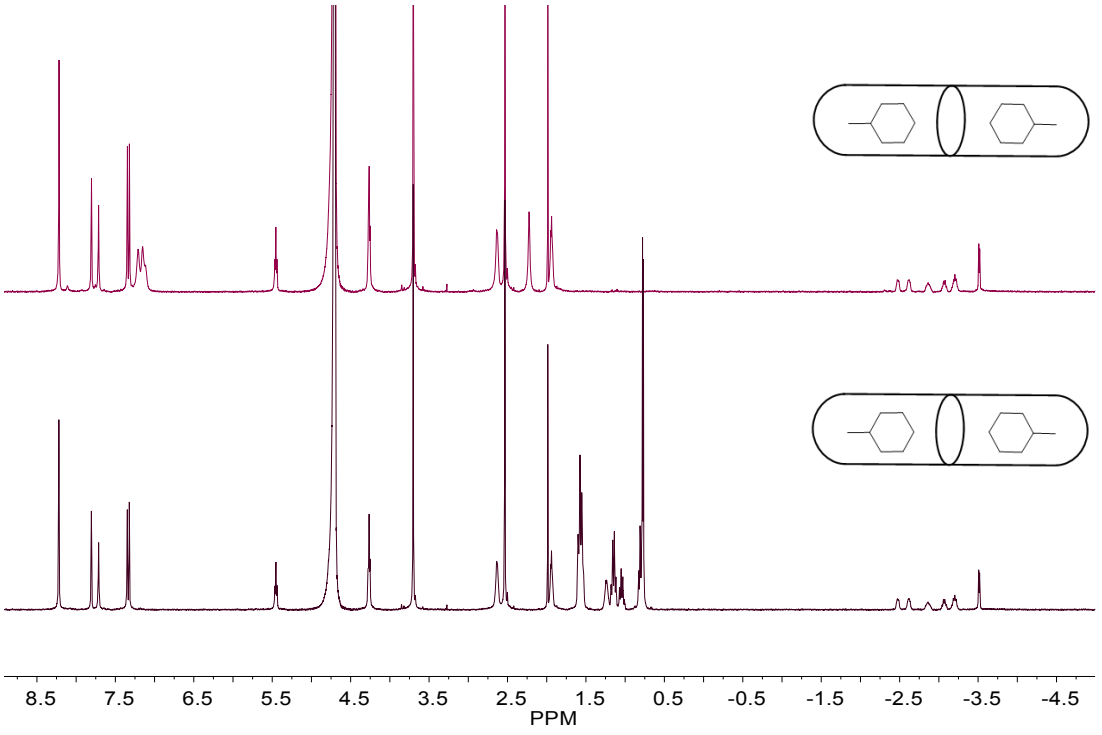


Fig. S65 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + excess cyclohexane sonicated for 1 h and analyzed by ^{1}H NMR spectroscopy (bottom), Then excess toluene was added sonicated for 1 h and analyzed by ^{1}H NMR spectroscopy (top), methyl cyclohexane was not replaced by toluene as a stable capsule encapsulating two molecules of methyl cyclohexane will not covert to unstable cavitand bearing toluene in the cavity.

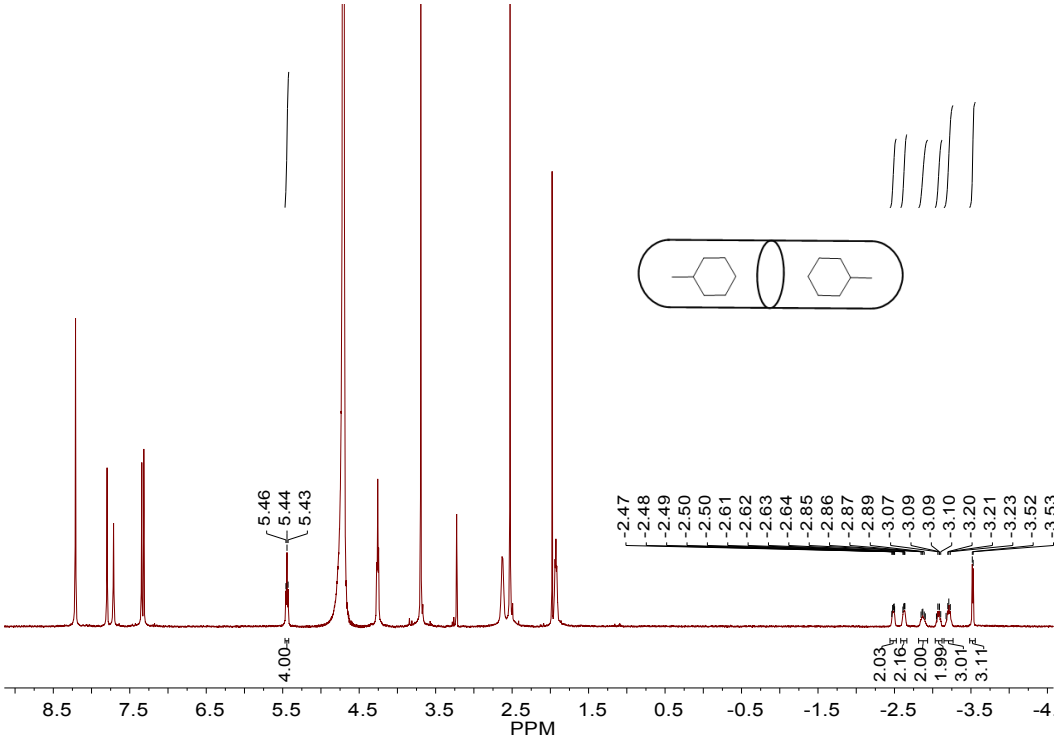


Fig. S66 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 1 equivalent methyl cyclohexane (added as 5 µL, 100 mM stock solution in methanol-d_4), analyzed at rt

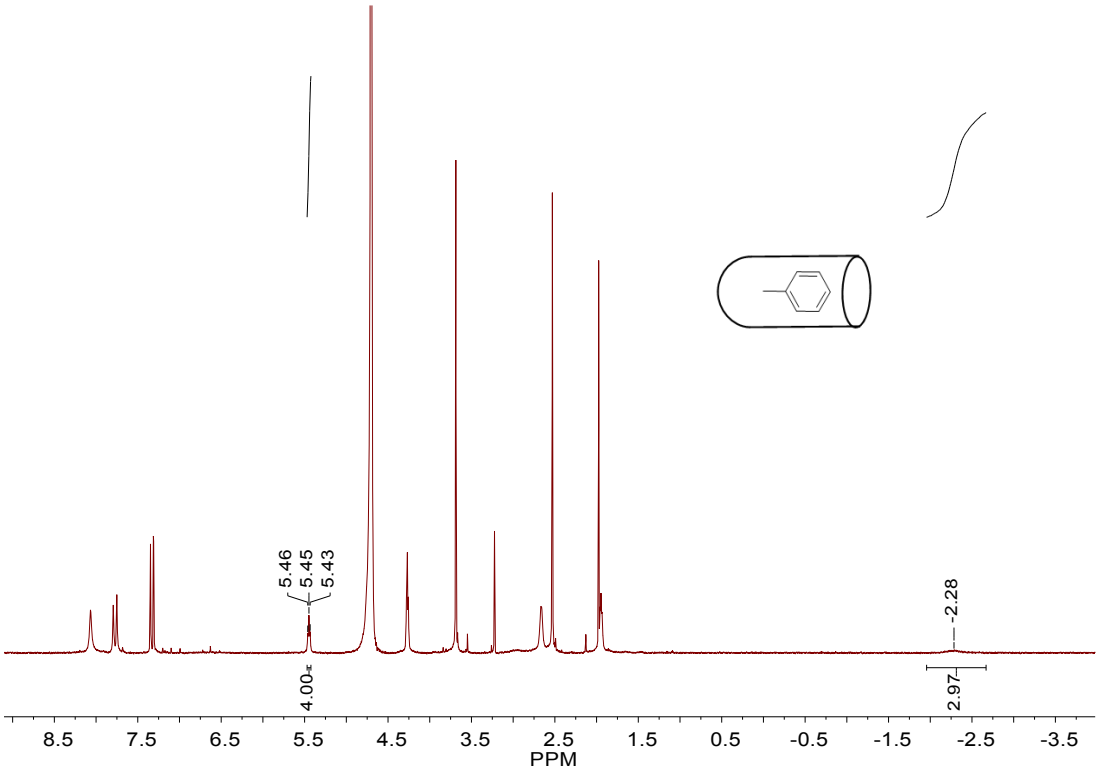


Fig. S67 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 1 equivalent toluene (added as 5 µL, 100 mM stock solution in methanol-d_4), analyzed at rt

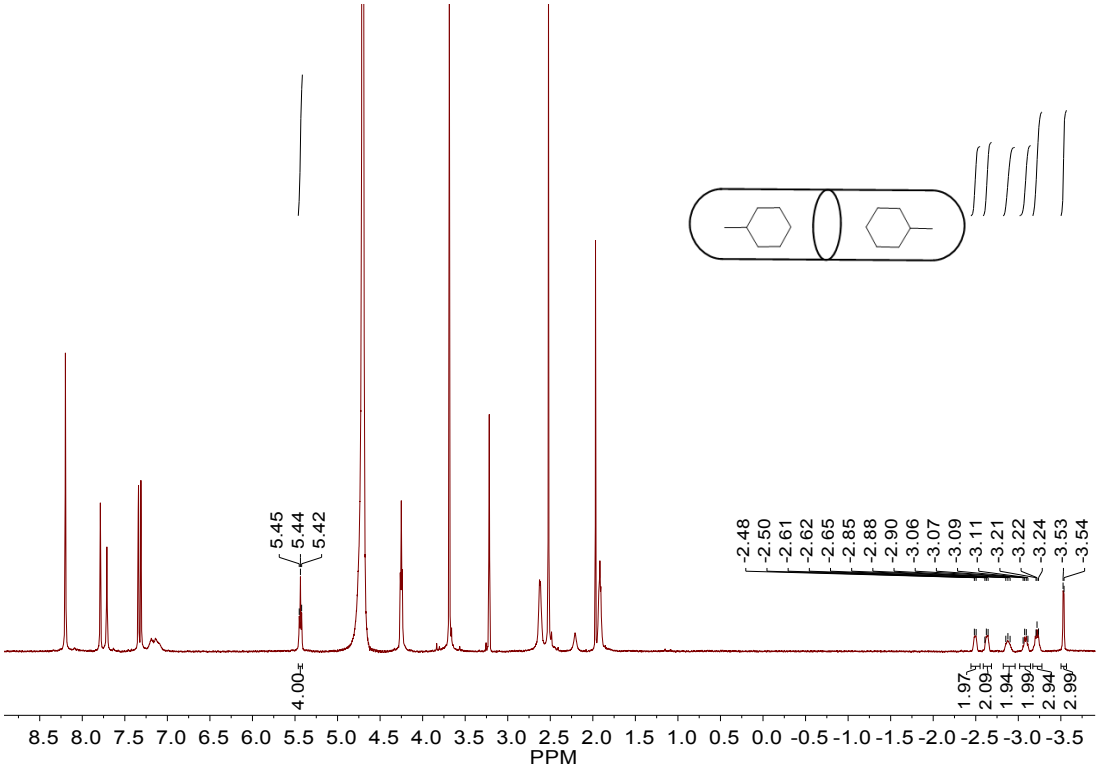


Fig. S68 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 1 equivalent of toluene and 1 equivalent of methyl cyclohexane (each one added as 5 µL, 100 mM stock solution in methanol-d_4), analyzed at rt

^{1}H NMR spectra of 1 in water in the presence of miscellaneous guests

General procedure for the binding analyses

A 1 mM solution of **1** in 0.5 mL D_2O was placed in an NMR tube and 0.5 equivalent of guest (4,4'-dimethylbiphenyl, as stock solution in DMSO-d_6) or excess (dibromooctane, or halooctane) was added, and the tube was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^{1}H NMR spectroscopy at rt.

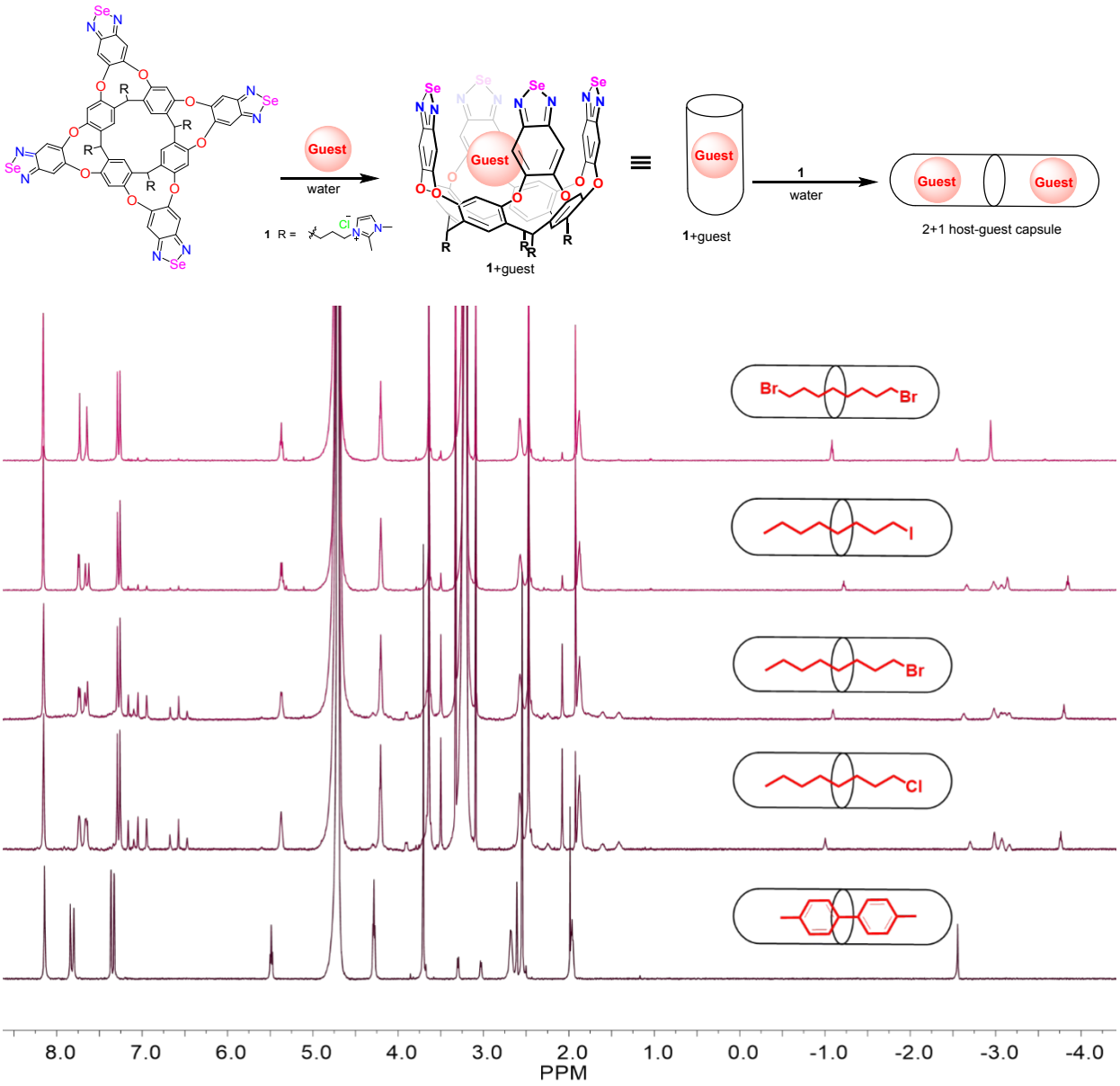


Fig. S69 ^{1}H NMR spectra comparative plot of the complexes formed between **1**, 1 mM in D_2O + from bottom to top, 0.5 equivalent of 4,4'-dimethylbiphenyl (added as 2.5 µL, 100 mM stock solution in DMSO-d_6) or excess of 1-chlorooctane, 1-bromooctane, 1-iodooctane or 1,8-dibromooctane, analyzed at rt

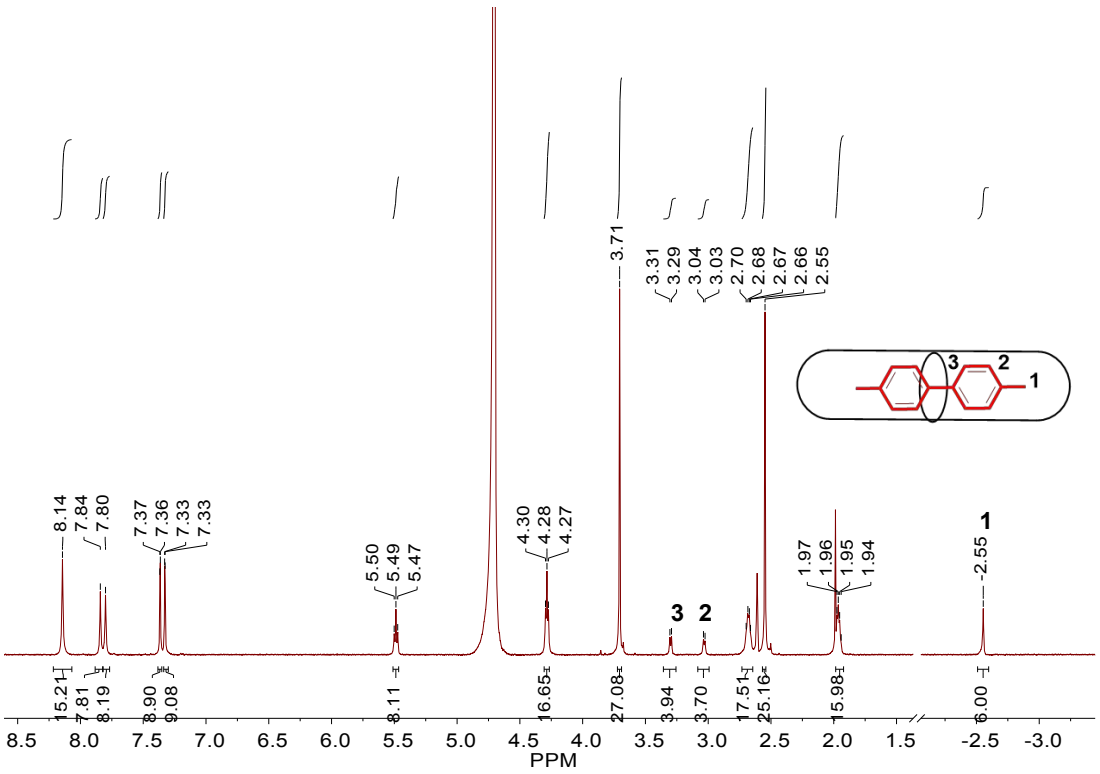


Fig. S70 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + 0.5 equivalent of 4,4'-dimethylbiphenyl (added as 2.5 µL, 100 mM stock solution in DMSO-d_6), analyzed at rt

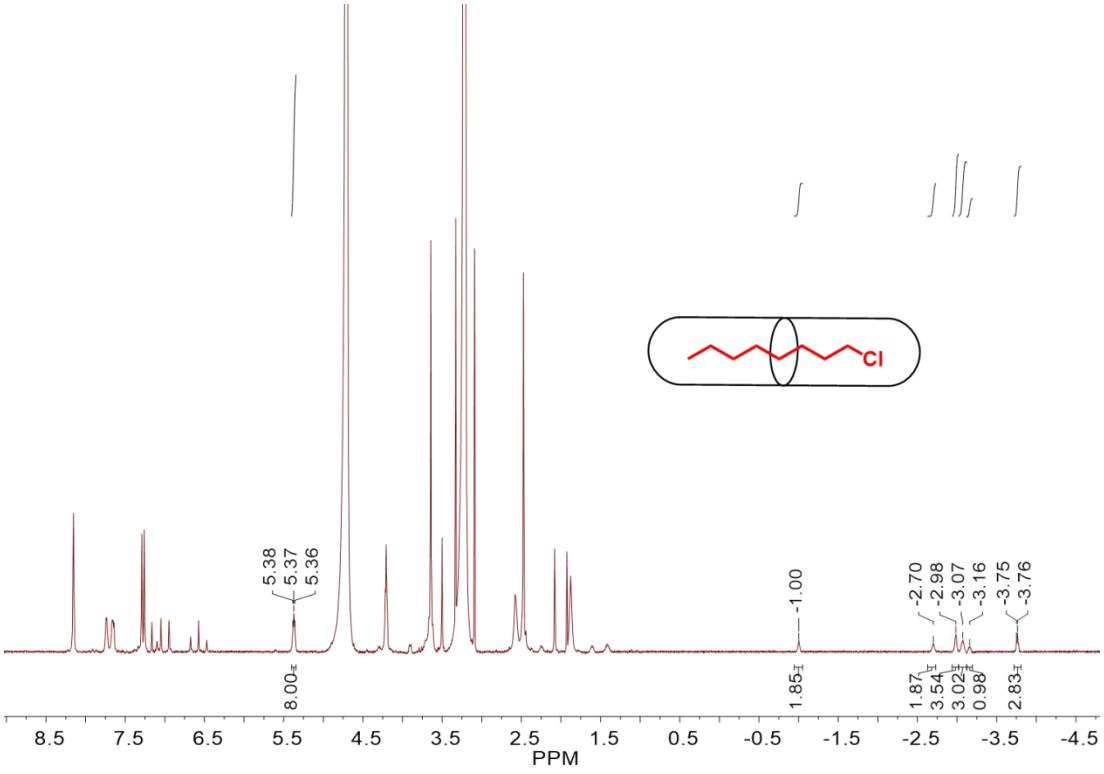


Fig. S71 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + excess 1-chlorooctane, analyzed at rt

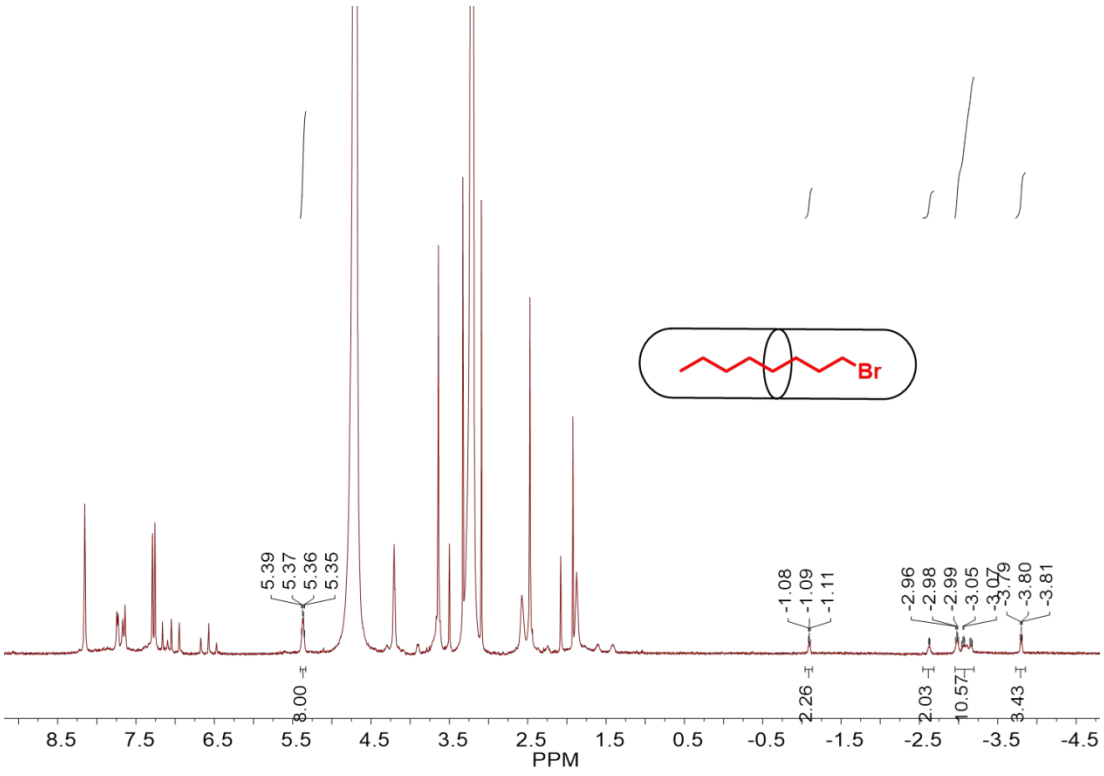


Fig. S72 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + excess 1-bromooctane, analyzed at rt

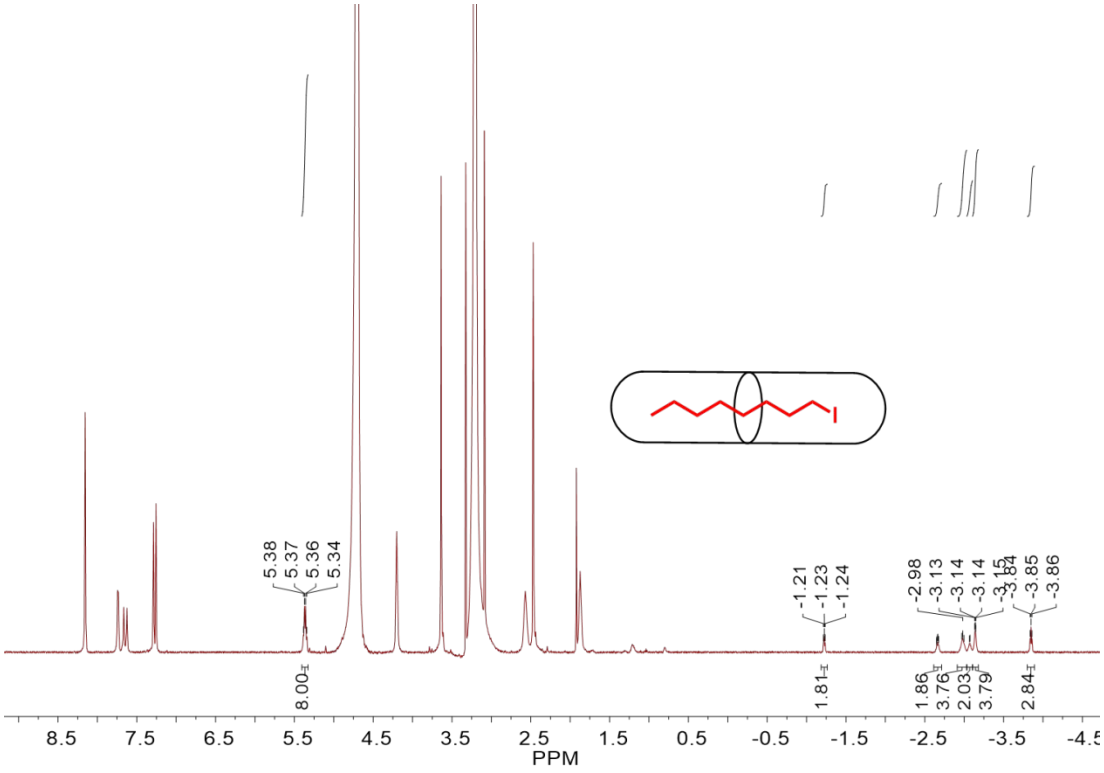


Fig. S73 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + excess 1-iodooctane, analyzed at rt

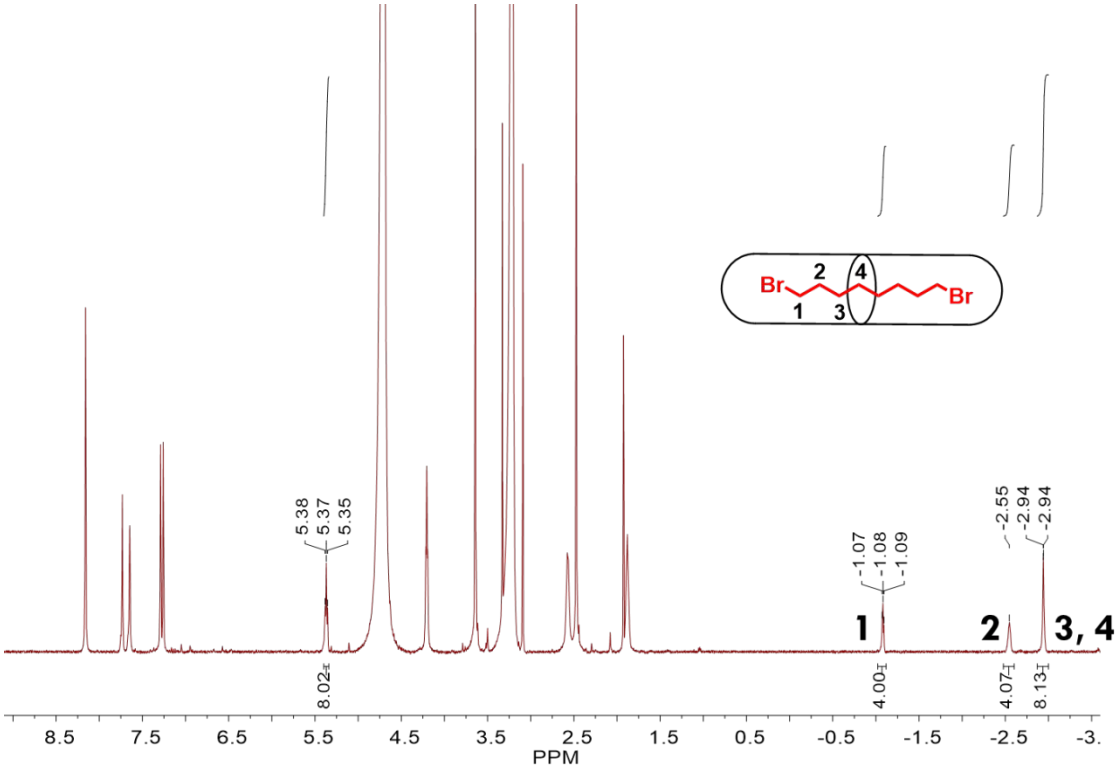


Fig. S74 ^{1}H NMR spectrum of the complex formed between **1**, 1 mM in D_2O + excess 1,8-dibromooctane, analyzed at rt

Crystallographic details for single crystal analysis of 3

Table S1: Crystal structure parameters of **3**

CCDC Number[1]	1967953
Empirical formula	$C_{166}H_{164}N_{24}O_{24}Se_8$
Formula weight	3510.88
Crystal system	Triclinic
Temperature (K)	173(2)
Wavelength (Å)	1.34139
Space group	P-1
Unit cell dimensions	
a (Å)	23.5179(18)
b (Å)	41.767(4)
c (Å)	43.084(4)
α (°)	84.628(5)
β (°)	89.020(5)
γ (°)	79.679(5)
Volume ($Å^3$)	41453(6)
Z	8
Density (calculated) (Mg/m^3)	1.125
Absorption coefficient (mm^{-1})	1.405
F(000)	14336
Crystal size (mm^3)	0.100 x 0.100 x 0.100
Theta range for data collection (°)	1.661 to 51.741
Index ranges	-27<=h<=27, -48<=k<=48, -50<=l<=50
Reflections collected	569355
Independent reflections	136738 [R(int) = 0.1571]
Completeness to theta = 51.741°	98.2
Refinement method	Full-matrix-block least-squares on F2
Data / restraints / parameters	136738/10392/7948
Goodness-of-fit on F^2	1.002
Final R indices [I>2sigma(I)]	R1 = 0.1521, wR2 = 0.3570
R indices (all data)	R1 = 0.2449, wR2 = 0.4054
Largest diff. peak and hole($e.Å^{-3}$)	2.095 and -0.831

[1] Crystallographic data for **3**, CCDC: can be obtained from Cambridge Crystallographic Data Center 12 Union Road, Cambridge CB2 1EZ, UK; Tel: +44-1223336408; fax: +44-1223336003; e-mail: deposit@ccdc.cam.ac.uk.

Theoretical Calculations

DFT geometry optimization calculations were carried out at the M06-2X[3]/LANL2DZ[4] level of theory. Dipole moments, dipole electric field isotropic and anisotropic polarizabilities, and NMR spectra were calculated at the PBE0[4]/6-31G(d,p)[5]//M06-2X/LANL2DZ level of theory.[6] NMR shielding tensors have been computed with the Gauge-Independent Atomic Orbital (GIAO) method.[7] All calculations were carried out via the Gaussian16 program.[8]

Table S2: Dipole moments μ (Debye), isotropic polarizability (au) and anisotropic polarizabilities (au) at PBE0/6-31G(d,p)//M06-2X/LANL2DZ.

	Figure **4A**/Scheme 3(first)		Figure **4B**/Scheme 3(second)		Figure **4C**/Scheme 3(third)	
	capsule	capusle+C_9H_{20}	capsule	capusle+C_9H_{20}	capsule	capusle+C_9H_{20}
μ	0.045	0.332	0.973	0.565	0.015	1.617
isotropic polarizability	1518	1579	1858	1931	1273	1329
anisotropic polarizability	920	960	1303	1350	540	599

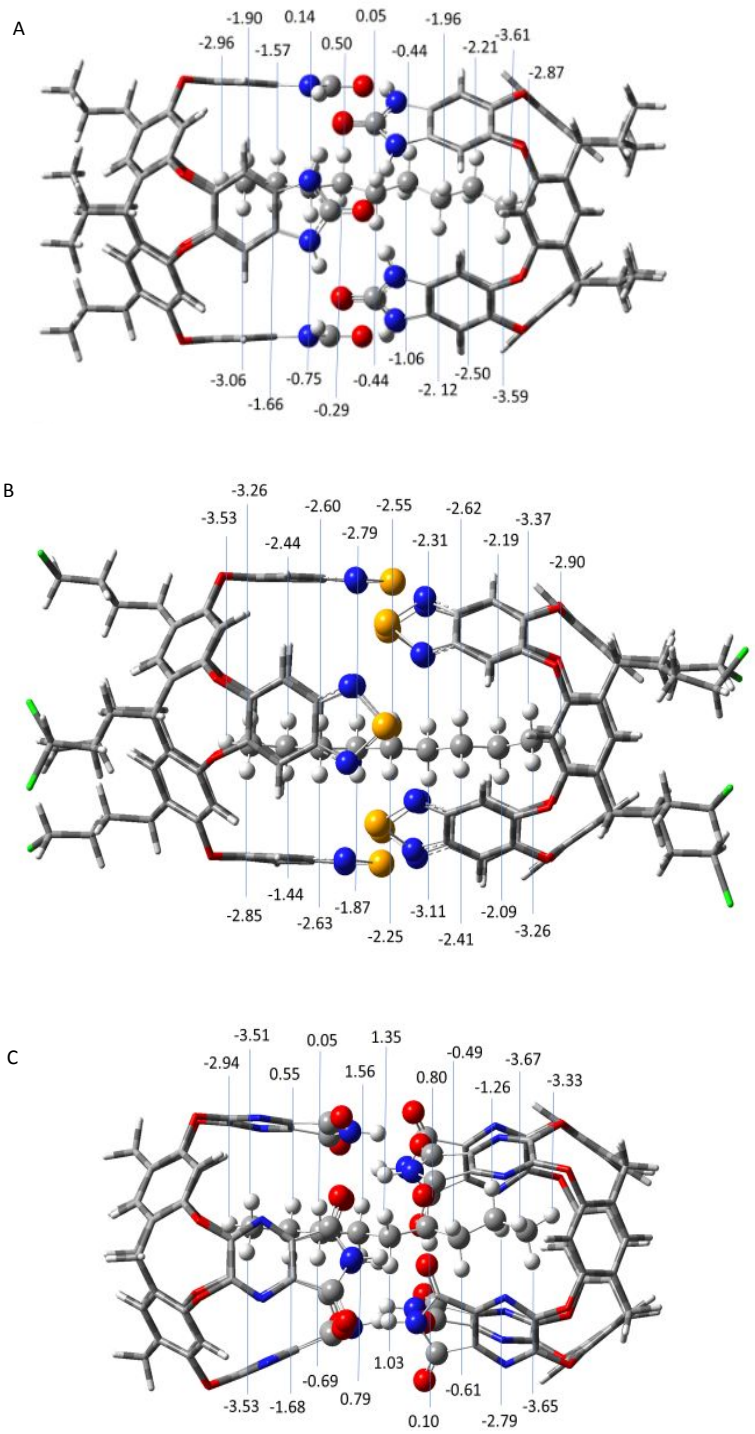


Fig. S75 **Calculated structures and ^{1}H NMR shifts for the 2+1 C_9H_{20} capsule (4B) and the corresponding capsules for the –(NH)2CO (4A) and –$(CO)_2$NH (4C) panels corresponding to Scheme 3.**

Table S3 (XYZ geometries)

Table S3-1 Capsule+C_9H_{20} (Figure 4A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.923121	-2.852497	-2.233364
2	6	0	8.343986	-3.095335	-0.841854
3	6	0	8.317468	-1.596798	-2.853261
4	1	0	8.606994	-3.695780	-2.855714
5	6	0	8.864498	-2.476999	0.307401
6	6	0	7.263873	-3.973349	-0.664392
7	6	0	8.842640	-0.310795	-2.640891
8	6	0	7.198302	-1.703531	-3.694719
9	6	0	8.356294	-2.705572	1.596873
10	6	0	6.743547	-4.244246	0.599767
11	8	0	6.714871	-4.651016	-1.782129
12	6	0	8.296032	0.843878	-3.227539
13	6	0	6.642142	-0.587873	-4.315989
14	8	0	6.662855	-2.982993	-3.980210
15	6	0	8.956502	-2.053051	2.838590
16	6	0	7.275909	-3.595547	1.711523
17	1	0	5.957882	-4.979560	0.721599
18	6	0	5.471242	-4.185656	-2.248410
19	6	0	8.885958	2.237422	-3.019208
20	6	0	7.177424	0.673034	-4.057089
21	1	0	5.834635	-0.703244	-5.027739
22	6	0	5.445776	-3.326477	-3.365501
23	1	0	8.644095	-2.660373	3.694246
24	6	0	8.372641	-0.659225	3.059101
25	8	0	6.738858	-3.894455	2.989335
26	6	0	8.319063	2.889312	-1.760481
27	1	0	8.551575	2.846343	-3.865329
28	8	0	6.610998	1.797829	-4.704908
29	6	0	8.905534	0.498607	2.467687
30	6	0	7.267497	-0.494581	3.908531
31	6	0	5.502097	-3.294564	3.293351
32	6	0	3.086177	-4.128408	-2.146248
33	6	0	8.862458	2.668560	-0.483043
34	6	0	7.227331	3.767703	-1.849156
35	6	0	5.395295	2.285786	-4.192862
36	6	0	3.062139	-3.270635	-3.269335
37	6	0	8.380870	1.782875	2.694328
38	6	0	6.738090	0.763534	4.186888
39	8	0	6.715826	-1.624767	4.557009
40	6	0	5.492750	-2.118408	4.069650
41	6	0	8.359163	3.279037	0.678878
42	6	0	6.716594	4.414879	-0.725894
43	8	0	6.654277	4.053584	-3.114066
44	6	0	5.415854	3.444694	-3.391469
45	6	0	8.966882	3.041886	2.058926
46	6	0	7.280938	1.883392	3.560178
47	1	0	5.946139	0.874042	4.916523
48	6	0	3.117689	-3.248753	3.185627
49	6	0	7.265654	4.146463	0.526273
50	1	0	5.925105	5.146486	-0.829684
51	6	0	3.016217	2.205726	-4.017800
52	1	0	8.657276	3.882741	2.687863
53	8	0	6.744263	3.159054	3.861123
54	6	0	3.110552	-2.058309	3.947730
55	8	0	6.733944	4.817193	1.656630
56	6	0	3.034708	3.374991	-3.223778
57	6	0	5.510243	3.491279	3.273843
58	6	0	5.504005	4.345687	2.153061

59	6	0	3.124442	3.413813	3.230467
60	6	0	3.116153	4.279010	2.112507
61	6	0	4.290395	-1.491558	4.419965
62	6	0	4.309699	-3.892245	2.864990
63	6	0	4.286397	-4.617230	-1.637332
64	6	0	4.234666	-2.874935	-3.905358
65	6	0	4.315081	3.029082	3.839787
66	6	0	4.301630	4.770430	1.571419
67	6	0	4.188687	1.659989	-4.531262
68	6	0	4.229743	4.019014	-2.915116
69	1	0	4.291586	-0.619346	5.061235
70	1	0	4.333914	-4.829584	2.323007
71	1	0	4.332373	2.420984	4.735367
72	1	0	4.321168	-5.319165	-0.813364
73	1	0	4.312665	5.475499	0.749603
74	1	0	4.226298	-2.263631	-4.798934
75	1	0	4.182288	0.801703	-5.191038
76	1	0	4.258788	4.943272	-2.351794
77	6	0	0.960805	-2.639118	3.531352
78	6	0	0.920567	-3.673957	-2.645181
79	6	0	0.873745	2.752838	-3.520777
80	6	0	0.964213	3.817790	2.668736
81	7	0	1.769157	4.504094	1.785579
82	7	0	1.784455	3.139262	3.543349
83	7	0	1.697702	3.681666	-2.924906
84	7	0	1.671095	1.838555	-4.171575
85	7	0	1.714421	-2.999128	-3.545654
86	7	0	1.749528	-4.350406	-1.778366
87	7	0	1.776364	-3.578076	2.939021
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92	1	0	1.304459	0.915137	-4.453864
93	1	0	9.772085	0.399333	1.818734
94	1	0	9.706952	-1.799612	0.194387
95	1	0	9.719079	-0.205123	-2.007147
96	1	0	9.712604	1.998461	-0.389942
97	6	0	10.510562	3.029269	2.023804
98	6	0	11.117114	2.968770	3.434010
99	1	0	10.843397	3.941316	1.513481
100	1	0	10.888002	2.188513	1.427637
101	1	0	12.210278	3.009194	3.394644
102	1	0	10.766572	3.811225	4.040713
103	1	0	10.829774	2.045246	3.949053
104	6	0	10.430563	2.235059	-3.028689
105	6	0	10.998627	1.735932	-4.366184
106	1	0	10.831920	1.622758	-2.210847
107	1	0	10.769391	3.260866	-2.839065
108	1	0	12.091285	1.801146	-4.377462
109	1	0	10.718599	0.693083	-4.551354
110	1	0	10.613171	2.337699	-5.196914
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112	6	0	11.068665	-4.155059	-1.763132
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114	1	0	10.798250	-2.605476	-3.259574
115	1	0	12.161131	-4.139024	-1.830107
116	1	0	10.794921	-4.364841	-0.723211
117	1	0	10.701853	-4.984025	-2.378787
118	6	0	10.500750	-2.052977	2.805921
119	6	0	11.104389	-1.572233	4.134341
120	1	0	10.880710	-1.430517	1.985543
121	1	0	10.833608	-3.076624	2.593935
122	1	0	12.197655	-1.621478	4.110897

123	1	0	10.815587	-0.537147	4.348519
124	1	0	10.752998	-2.194801	4.964754
125	1	0	1.336223	-2.206252	-4.087080
126	1	0	1.407569	-4.204190	2.208557
127	1	0	1.342389	4.297360	-2.178353
128	1	0	1.423535	2.343076	4.089912
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130	8	0	-0.402561	2.752487	-3.493233
131	8	0	-0.315807	-2.651397	3.544608
132	8	0	-0.355946	-3.683535	-2.631699
133	6	0	-8.841079	-3.574394	0.644530
134	6	0	-8.262718	-3.129170	-0.696975
135	6	0	-8.231945	-2.761097	1.782249
136	1	0	-8.523747	-4.611708	0.793048
137	6	0	-8.791621	-2.058296	-1.437563
138	6	0	-7.164369	-3.806831	-1.247474
139	6	0	-8.745437	-1.515613	2.182867
140	6	0	-7.118036	-3.250878	2.482780
141	6	0	-8.267169	-1.652351	-2.677201
142	6	0	-6.635174	-3.458070	-2.487369
143	8	0	-6.608403	-4.915339	-0.565122
144	6	0	-8.191583	-0.761782	3.231549
145	6	0	-6.552466	-2.545212	3.541998
146	8	0	-6.578681	-4.518589	2.152930
147	6	0	-8.858058	-0.500051	-3.484248
148	6	0	-7.170416	-2.373266	-3.176325
149	1	0	-5.841980	-4.047788	-2.928955
150	6	0	-5.368155	-4.716850	0.067401
151	6	0	-8.772517	0.573425	3.690152
152	6	0	-7.074559	-1.300900	3.887574
153	1	0	-5.744474	-2.978236	4.117835
154	6	0	-5.352509	-4.523093	1.463001
155	1	0	-8.537662	-0.647110	-4.520909
156	6	0	-8.271583	0.836971	-3.035094
157	8	0	-6.617221	-2.039209	-4.437314
158	6	0	-8.204026	1.728721	2.871726
159	1	0	-8.432501	0.722493	4.720163
160	8	0	-6.495962	-0.602219	4.974082
161	6	0	-8.806292	1.588530	-1.974677
162	6	0	-7.165632	1.378654	-3.708577
163	6	0	-5.382188	-1.364470	-4.410955
164	6	0	-2.982864	-4.627893	0.025585
165	6	0	-8.753461	2.128354	1.641397
166	6	0	-7.107179	2.461761	3.351811
167	6	0	-5.277238	0.056746	4.731636
168	6	0	-2.966840	-4.441607	1.426903
169	6	0	-8.283237	2.831416	-1.578720
170	6	0	-6.636968	2.621821	-3.368822
171	8	0	-6.604465	0.683879	-4.806366
172	6	0	-5.377473	0.033084	-4.584307
173	6	0	-8.253770	3.210619	0.896522
174	6	0	-6.597639	3.555990	2.656502
175	8	0	-6.527567	2.127135	4.600892
176	6	0	-5.292348	1.454213	4.553004
177	6	0	-8.868447	3.647811	-0.429695
178	6	0	-7.182231	3.323502	-2.296681
179	1	0	-5.842514	3.057324	-3.961199
180	6	0	-3.000989	-1.356285	-4.247304
181	6	0	-7.156049	3.904940	1.429116
182	1	0	-5.802968	4.153359	3.085380
183	6	0	-2.900021	0.054236	4.520404
184	1	0	-8.559728	4.685315	-0.593453
185	8	0	-6.648397	4.595045	-1.975268
186	6	0	-2.998301	0.048046	-4.410071

187	8	0	-6.631111	5.028334	0.742793
188	6	0	-2.914038	1.457285	4.349150
189	6	0	-5.410612	4.622488	-1.308136
190	6	0	-5.401329	4.850327	0.082467
191	6	0	-3.024174	4.553217	-1.314579
192	6	0	-3.013567	4.787348	0.079645
193	6	0	-4.179318	0.757951	-4.603647
194	6	0	-4.188327	-2.082958	-4.263680
195	6	0	-4.178543	-4.787520	-0.669647
196	6	0	-4.146209	-4.404404	2.165911
197	6	0	-4.216946	4.490524	-2.029612
198	6	0	-4.197764	4.958359	0.792347
199	6	0	-4.074518	-0.661184	4.733697
200	6	0	-4.104932	2.177290	4.379808
201	1	0	-4.184190	1.823538	-4.794899
202	1	0	-4.204339	-3.163536	-4.195773
203	1	0	-4.237352	4.375709	-3.106054
204	1	0	-4.202931	-4.996267	-1.731784
205	1	0	-4.206436	5.194396	1.849137
206	1	0	-4.147601	-4.321723	3.245583
207	1	0	-4.071669	-1.726828	4.924437
208	1	0	-4.128479	3.257078	4.303119
209	6	0	-0.846457	-0.649204	-4.274913
210	6	0	-0.819852	-4.536882	0.700503
211	6	0	-0.755858	0.761758	4.323468
212	6	0	-0.862339	4.658242	-0.633658
213	7	0	-1.666212	4.840007	0.470950
214	7	0	-1.684386	4.470192	-1.723318
215	7	0	-1.576780	1.862205	4.217501
216	7	0	-1.556145	-0.346408	4.485869
217	7	0	-1.619162	-4.380851	1.812545
218	7	0	-1.644707	-4.673476	-0.393074
219	7	0	-1.659057	-1.754986	-4.156488
220	7	0	-1.656779	0.455205	-4.407520
221	1	0	-1.278054	-4.530833	-1.347070
222	1	0	-1.290765	1.410410	-4.262040
223	1	0	-1.283065	4.717901	1.419523
224	1	0	-1.190682	-1.300655	4.331489
225	1	0	-9.671497	1.197020	-1.445338
226	1	0	-9.647774	-1.522735	-1.035365
227	1	0	-9.614827	-1.120860	1.663825
228	1	0	-9.605637	1.579296	1.250496
229	6	0	-10.411655	3.617822	-0.399288
230	6	0	-11.023325	4.219482	-1.673653
231	1	0	-10.742591	4.186764	0.478107
232	1	0	-10.786818	2.595514	-0.261774
233	1	0	-12.116327	4.235423	-1.616346
234	1	0	-10.674716	5.247935	-1.820025
235	1	0	-10.738131	3.641792	-2.560027
236	6	0	-10.317036	0.574171	3.703891
237	6	0	-10.885992	-0.478912	4.667196
238	1	0	-10.722879	0.405333	2.698048
239	1	0	-10.650265	1.574621	4.005792
240	1	0	-11.978352	-0.422353	4.710178
241	1	0	-10.610395	-1.492070	4.354528
242	1	0	-10.497147	-0.324533	5.679994
243	6	0	-10.384612	-3.548255	0.665549
244	6	0	-10.990943	-4.501934	-0.375319
245	1	0	-10.766993	-2.533520	0.495461
246	1	0	-10.713114	-3.835689	1.672091
247	1	0	-12.083443	-4.514390	-0.307871
248	1	0	-10.716673	-4.202637	-1.392911
249	1	0	-10.628565	-5.524126	-0.218741
250	6	0	-10.402184	-0.507194	-3.466409

251	6	0	-10.993410	0.533346	-4.429682
252	1	0	-10.788422	-0.328727	-2.454552
253	1	0	-10.738306	-1.512096	-3.750635
254	1	0	-12.086940	0.485339	-4.438622
255	1	0	-10.700397	1.549399	-4.142551
256	1	0	-10.636296	0.359653	-5.450926
257	1	0	-1.238377	-3.953822	2.669827
258	1	0	-1.290063	-2.643181	-3.784471
259	1	0	-1.221265	2.752905	3.837693
260	1	0	-1.320235	4.031393	-2.581991
261	8	0	0.413034	4.676834	-0.648823
262	8	0	0.521047	0.772326	4.300027
263	8	0	0.430670	-0.651818	-4.294233
264	8	0	0.456164	-4.563143	0.689278
265	6	0	4.264102	-1.398656	0.226793
266	6	0	3.024799	-0.836593	-0.488949
267	1	0	5.191573	-1.150945	-0.305173
268	1	0	4.342709	-1.002540	1.249768
269	1	0	4.203006	-2.492898	0.299534
270	6	0	1.712073	-1.178838	0.236810
271	1	0	3.111898	0.254970	-0.585099
272	1	0	2.980703	-1.233062	-1.514753
273	1	0	1.668344	-2.263671	0.427303
274	1	0	1.700438	-0.684597	1.223634
275	6	0	0.464697	-0.763644	-0.562678
276	6	0	-0.843933	-0.923886	0.227142
277	1	0	0.406378	-1.362234	-1.485729
278	1	0	0.565063	0.284405	-0.887224
279	6	0	-2.097213	-0.747099	-0.647850
280	1	0	-0.866375	-1.915210	0.707245
281	1	0	-0.862158	-0.190821	1.049418
282	1	0	-1.988727	0.164945	-1.259620
283	1	0	-2.165179	-1.591719	-1.353972
284	6	0	-3.393176	-0.650560	0.173144
285	6	0	-4.653235	-0.461968	-0.688406
286	1	0	-3.310954	0.192994	0.876803
287	1	0	-3.509701	-1.557875	0.789550
288	6	0	-5.912888	-0.257628	0.169988
289	1	0	-4.512992	0.402303	-1.356823
290	1	0	-4.785419	-1.342214	-1.337497
291	1	0	-6.810803	-0.124258	-0.447575
292	1	0	-6.080381	-1.126464	0.823211
293	1	0	-5.810890	0.628835	0.813044

Table S3-2 Capsule+C_9H_{20} (Figure 4B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.364964	3.223322	-1.771107
2	6	0	7.777011	2.016796	-2.499395
3	6	0	7.772334	3.331393	-0.368536
4	1	0	8.039276	4.111929	-2.320682
5	6	0	8.324397	0.726375	-2.401875
6	6	0	6.644407	2.176353	-3.310926
7	6	0	8.304456	2.642653	0.732669
8	6	0	6.656349	4.151889	-0.134071
9	6	0	7.788002	-0.380454	-3.079022
10	6	0	6.084499	1.107431	-4.009756
11	8	0	6.118222	3.476186	-3.494177
12	6	0	7.783511	2.758541	2.032337
13	6	0	6.112557	4.302258	1.139669

14	8	0	6.129790	4.916992	-1.202801
15	6	0	8.383909	-1.783660	-2.992515
16	6	0	6.647401	-0.158749	-3.867830
17	1	0	5.255258	1.268740	-4.686488
18	6	0	4.867619	3.791738	-2.951355
19	6	0	8.388797	2.013278	3.220868
20	6	0	6.671926	3.597333	2.205601
21	1	0	5.294558	4.991879	1.308877
22	6	0	4.873498	4.577920	-1.720080
23	1	0	8.075137	-2.317228	-3.896932
24	6	0	7.784683	-2.539215	-1.809917
25	8	0	6.115045	-1.244162	-4.600804
26	6	0	7.806767	0.603999	3.300079
27	1	0	8.063917	2.541843	4.122401
28	8	0	6.152695	3.803541	3.507796
29	6	0	8.300056	-2.415731	-0.510877
30	6	0	6.694667	-3.403728	-1.986956
31	6	0	4.873286	-1.775556	-4.237420
32	6	0	2.457351	3.866199	-2.992194
33	6	0	8.364375	-0.498860	2.630042
34	6	0	6.656789	0.375847	4.071793
35	6	0	4.893581	3.266535	3.809141
36	6	0	2.461534	4.667581	-1.756395
37	6	0	7.792856	-3.126531	0.588660
38	6	0	6.157022	-4.127996	-0.924958
39	8	0	6.166974	-3.604426	-3.286369
40	6	0	4.901061	-3.064666	-3.552425
41	6	0	7.810668	-1.788167	2.701792
42	6	0	6.086288	-0.890308	4.186405
43	8	0	6.132041	1.447068	4.831156
44	6	0	4.882291	1.983201	4.506372
45	6	0	8.405622	-2.996417	1.982079
46	6	0	6.701580	-3.977320	0.349345
47	1	0	5.351404	-4.832188	-1.094090
48	6	0	2.463287	-1.818359	-4.217655
49	6	0	6.655083	-1.949416	3.482068
50	1	0	5.247876	-1.057320	4.850044
51	6	0	2.481216	3.334116	3.874662
52	1	0	8.102124	-3.884463	2.546407
53	8	0	6.181100	-4.767919	1.403379
54	6	0	2.488621	-3.128439	-3.545886
55	8	0	6.126622	-3.250829	3.631102
56	6	0	2.471612	2.032416	4.565006
57	6	0	4.913312	-4.424193	1.894284
58	6	0	4.884718	-3.570664	3.078017
59	6	0	2.501999	-4.526060	1.892569
60	6	0	2.476264	-3.644604	3.071775
61	6	0	3.757254	-3.737496	-3.235908
62	6	0	3.698490	-1.171082	-4.574824
63	6	0	3.705837	3.458117	-3.582393
64	6	0	3.718207	5.023928	-1.147538
65	6	0	3.771117	-4.909446	1.327111
66	6	0	3.710110	-3.195874	3.660703
67	6	0	3.741577	3.939381	3.523791
68	6	0	3.717375	1.389638	4.894295
69	1	0	3.781859	-4.720040	-2.781330
70	1	0	3.667686	-0.243908	-5.132667
71	1	0	3.799176	-5.590324	0.485396
72	1	0	3.699324	2.930016	-4.527485
73	1	0	3.679256	-2.616462	4.574569
74	1	0	3.725691	5.657369	-0.269435
75	1	0	3.754399	4.918514	3.061557
76	1	0	3.704719	0.470488	5.466046
77	7	0	1.267054	-3.338075	3.528543

78	7	0	1.309810	-4.904563	1.437095
79	7	0	1.268549	1.527950	4.821307
80	7	0	1.283105	3.842796	3.598117
81	7	0	1.261783	4.989655	-1.280417
82	7	0	1.256221	3.564569	-3.474548
83	7	0	1.254922	-1.321212	-4.454064
84	7	0	1.297077	-3.651942	-3.270325
85	1	0	9.141130	-1.745821	-0.351682
86	1	0	9.206420	0.585560	-1.783141
87	1	0	9.166225	1.998603	0.577752
88	1	0	9.265202	-0.352270	2.041155
89	6	0	9.947002	-2.961771	1.936397
90	6	0	10.530522	-4.277689	1.395855
91	1	0	10.328840	-2.780012	2.947017
92	1	0	10.311852	-2.129358	1.318068
93	1	0	10.405551	-5.071925	2.140743
94	1	0	9.978435	-4.591977	0.497398
95	6	0	9.931205	2.015157	3.204741
96	6	0	10.502371	3.444088	3.244843
97	1	0	10.325268	1.496179	2.320154
98	1	0	10.279144	1.446435	4.077301
99	1	0	10.214080	3.992852	2.340888
100	1	0	10.084970	3.990859	4.098689
101	6	0	9.907886	3.222850	-1.752480
102	6	0	10.498565	3.251436	-3.173753
103	1	0	10.303145	2.348953	-1.215995
104	1	0	10.238953	4.106625	-1.190599
105	1	0	10.219971	2.342209	-3.718677
106	1	0	10.086236	4.099391	-3.733232
107	6	0	9.927547	-1.763191	-2.956492
108	6	0	10.522744	-3.180908	-2.883819
109	1	0	10.299741	-1.182327	-2.101263
110	1	0	10.280759	-1.247144	-3.859363
111	1	0	10.236161	-3.656079	-1.938276
112	1	0	10.118201	-3.805874	-3.688723
113	6	0	12.042188	-3.136306	-2.980407
114	1	0	12.395479	-2.889395	-3.981213
115	1	0	12.485495	-2.458897	-2.248384
116	6	0	11.994411	-4.167488	0.995961
117	1	0	12.420198	-5.116711	0.676432
118	1	0	12.157370	-3.410319	0.226017
119	6	0	12.016668	3.365014	-3.122178
120	1	0	12.349399	4.318483	-2.712044
121	1	0	12.475187	2.539659	-2.575729
122	6	0	12.021294	3.411018	3.353558
123	1	0	12.361887	2.996020	4.302136
124	1	0	12.484438	2.878258	2.521986
125	17	0	12.710191	5.142777	3.284277
126	17	0	12.727234	3.280233	-4.844192
127	17	0	12.754469	-4.819469	-2.595451
128	17	0	13.034433	-3.618563	2.454132
129	34	0	-0.051290	2.693689	4.211918
130	34	0	-0.067262	4.309385	-2.397284
131	34	0	-0.035785	-4.181191	2.505245
132	34	0	-0.052248	-2.510840	-3.867549
133	6	0	-8.375652	-3.562617	-0.724549
134	6	0	-7.780487	-2.645729	-1.790693
135	6	0	-7.772732	-3.221516	0.635087
136	1	0	-8.054716	-4.580376	-0.967467
137	6	0	-8.316355	-1.381366	-2.088941
138	6	0	-6.646749	-3.050460	-2.510154
139	6	0	-8.301385	-2.226623	1.473788
140	6	0	-6.637226	-3.911695	1.090920
141	6	0	-7.768650	-0.533562	-3.064224

142	6	0	-6.072020	-2.242479	-3.490662
143	8	0	-6.137930	-4.354372	-2.307376
144	6	0	-7.750095	-1.913089	2.727836
145	6	0	-6.067040	-3.642543	2.332713
146	8	0	-6.129309	-4.980995	0.316340
147	6	0	-8.348592	0.836890	-3.403933
148	6	0	-6.626910	-0.990295	-3.742660
149	1	0	-5.240347	-2.605507	-4.080855
150	6	0	-4.881350	-4.513801	-1.713050
151	6	0	-8.336628	-0.839833	3.643492
152	6	0	-6.619602	-2.640768	3.129821
153	1	0	-5.235315	-4.234671	2.693424
154	6	0	-4.876578	-4.855258	-0.294403
155	1	0	-8.033537	1.071837	-4.425502
156	6	0	-7.740864	1.906833	-2.500182
157	8	0	-6.088974	-0.185427	-4.772083
158	6	0	-7.758169	0.531484	3.299629
159	1	0	-8.000759	-1.076937	4.657917
160	8	0	-6.077631	-2.412770	4.418060
161	6	0	-8.265839	2.194431	-1.230795
162	6	0	-6.642741	2.667972	-2.926624
163	6	0	-4.841381	0.418795	-4.587337
164	6	0	-2.475312	-4.671453	-1.767660
165	6	0	-8.313311	1.371608	2.319799
166	6	0	-6.631012	1.007970	3.987129
167	6	0	-4.825841	-1.792101	4.503025
168	6	0	-2.470993	-5.027998	-0.339473
169	6	0	-7.760668	3.210668	-0.405945
170	6	0	-6.100164	3.679856	-2.134871
171	8	0	-6.116681	2.460678	-4.225722
172	6	0	-4.857008	1.853886	-4.319258
173	6	0	-7.787025	2.638692	2.017976
174	6	0	-6.088677	2.266801	3.733243
175	8	0	-6.082325	0.219528	5.026594
176	6	0	-4.828951	-0.366847	4.820865
177	6	0	-8.384360	3.544260	0.947065
178	6	0	-6.654434	3.932351	-0.881598
179	1	0	-5.291094	4.294242	-2.510317
180	6	0	-2.430937	0.441037	-4.581476
181	6	0	-6.658885	3.059197	2.739684
182	1	0	-5.266173	2.641257	4.329282
183	6	0	-2.415810	-1.782250	4.448119
184	1	0	-8.086406	4.569051	1.191553
185	8	0	-6.150838	5.006938	-0.110558
186	6	0	-2.445931	1.891795	-4.328553
187	8	0	-6.153345	4.362294	2.517138
188	6	0	-2.419739	-0.342143	4.758708
189	6	0	-4.897888	4.872049	0.500179
190	6	0	-4.898725	4.524544	1.919420
191	6	0	-2.489388	5.027577	0.530947
192	6	0	-2.489553	4.685902	1.963961
193	6	0	-3.706805	2.578625	-4.215849
194	6	0	-3.673457	-0.270643	-4.730448
195	6	0	-3.727547	-4.436289	-2.437816
196	6	0	-3.717840	-5.123839	0.374588
197	6	0	-3.741314	5.133197	-0.174391
198	6	0	-3.741583	4.453325	2.639258
199	6	0	-3.665411	-2.491800	4.350793
200	6	0	-3.671281	0.337725	4.968127
201	1	0	-3.719653	3.652062	-4.074924
202	1	0	-3.653960	-1.322070	-4.986958
203	1	0	-3.744986	5.447494	-1.210553
204	1	0	-3.733554	-4.244655	-3.503457
205	1	0	-3.743702	4.261378	3.704856

206	1	0	-3.716619	-5.439769	1.410279
207	1	0	-3.659715	-3.559909	4.174458
208	1	0	-3.667325	1.380926	5.256791
209	7	0	-1.288987	4.603204	2.531559
210	7	0	-1.289216	5.204903	-0.014974
211	7	0	-1.225664	0.236953	4.776939
212	7	0	-1.218359	-2.320659	4.248039
213	7	0	-1.268021	-5.233515	0.194772
214	7	0	-1.275967	-4.590221	-2.342835
215	7	0	-1.226158	-0.113126	-4.652026
216	7	0	-1.252341	2.462125	-4.202444
217	1	0	-9.118491	1.617349	-0.882379
218	1	0	-9.196143	-1.052364	-1.542673
219	1	0	-9.179748	-1.678409	1.142747
220	1	0	-9.191507	1.032462	1.777574
221	6	0	-9.925270	3.491012	0.911557
222	6	0	-10.509066	4.564965	-0.020975
223	1	0	-10.308977	3.641212	1.926601
224	1	0	-10.287333	2.503783	0.591102
225	1	0	-10.366683	5.556849	0.423297
226	1	0	-9.969171	4.563589	-0.979883
227	6	0	-9.879555	-0.836030	3.649183
228	6	0	-10.453277	-2.177616	4.139714
229	1	0	-10.284931	-0.612705	2.652667
230	1	0	-10.212996	-0.022783	4.307346
231	1	0	-10.174781	-2.984521	3.452241
232	1	0	-10.028856	-2.429502	5.118772
233	6	0	-9.917619	-3.547752	-0.704998
234	6	0	-10.509285	-4.027705	-2.042631
235	1	0	-10.308044	-2.546170	-0.476821
236	1	0	-10.252095	-4.203708	0.110023
237	1	0	-10.224329	-3.344113	-2.850623
238	1	0	-10.102581	-5.013275	-2.297933
239	6	0	-9.892248	0.843632	-3.369583
240	6	0	-10.473274	2.222585	-3.730298
241	1	0	-10.271203	0.551129	-2.380552
242	1	0	-10.249705	0.082675	-4.076207
243	1	0	-10.180921	2.958515	-2.972194
244	1	0	-10.063726	2.571020	-4.685804
245	6	0	-11.993154	2.164595	-3.811218
246	1	0	-12.349990	1.633010	-4.693005
247	1	0	-12.441257	1.740553	-2.910856
248	6	0	-11.980358	4.348652	-0.343203
249	1	0	-12.404000	5.147441	-0.948877
250	1	0	-12.162548	3.384082	-0.821691
251	6	0	-12.027947	-4.110396	-1.960875
252	1	0	-12.365729	-4.869607	-1.255467
253	1	0	-12.483512	-3.147710	-1.724806
254	6	0	-11.970903	-2.105049	4.246909
255	1	0	-12.300527	-1.400282	5.010269
256	1	0	-12.443582	-1.873140	3.291593
257	17	0	-12.659904	-3.761049	4.757983
258	17	0	-12.734735	-4.606644	-3.613601
259	17	0	-12.691287	3.891744	-3.947490
260	17	0	-12.998929	4.318854	1.228850
261	34	0	0.109217	-1.029449	4.483105
262	34	0	0.043383	-5.001141	-1.100530
263	34	0	0.034373	4.978460	1.276059
264	34	0	0.090445	1.188251	-4.430605
265	6	0	4.882311	-0.731901	-0.468070
266	6	0	3.588970	-1.459761	-0.069018
267	1	0	5.774848	-1.265581	-0.118398
268	1	0	4.952788	-0.631662	-1.560982
269	1	0	4.910017	0.279642	-0.041562

270	6	0	2.325170	-0.697122	-0.499475
271	1	0	3.575150	-2.468789	-0.512701
272	1	0	3.567270	-1.600792	1.023909
273	1	0	2.362921	0.324122	-0.090743
274	1	0	2.314528	-0.592088	-1.597460
275	6	0	1.030526	-1.384507	-0.039181
276	6	0	-0.233672	-0.588210	-0.399636
277	1	0	1.067992	-1.533520	1.053578
278	1	0	0.977073	-2.387863	-0.490174
279	6	0	-1.539564	-1.306217	-0.020165
280	1	0	-0.199793	0.388977	0.106068
281	1	0	-0.236591	-0.379334	-1.482117
282	1	0	-1.612213	-2.255025	-0.579389
283	1	0	-1.512712	-1.575365	1.048812
284	6	0	-2.785504	-0.447519	-0.298373
285	6	0	-4.105227	-1.127833	0.103195
286	1	0	-2.821337	-0.191847	-1.369903
287	1	0	-2.693087	0.504501	0.246854
288	6	0	-5.324780	-0.210432	-0.093362
289	1	0	-4.237485	-2.044353	-0.493468
290	1	0	-4.046073	-1.447204	1.155644
291	1	0	-6.259848	-0.714711	0.183645
292	1	0	-5.238847	0.697233	0.520585
293	1	0	-5.412211	0.103133	-1.144277

Table S3-3 Capsule+C_9H_{20} (Figure 4C)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-8.276667	-0.783999	-3.236973
2	6	0	-8.863943	0.578369	-3.587085
3	6	0	-9.054976	1.348825	2.080713
4	6	0	-8.504901	2.579122	1.683883
5	6	0	-9.138583	3.457216	0.612880
6	6	0	-8.526779	3.197766	-0.756363
7	6	0	-8.956809	2.102255	-1.529234
8	6	0	-8.364619	1.752168	-2.752732
9	6	0	-8.841559	-1.601193	-2.245727
10	6	0	-8.965664	-3.673633	-0.788083
11	6	0	-8.392999	-3.287937	0.570798
12	6	0	-8.955547	-2.299450	1.391466
13	6	0	-8.409854	-1.953419	2.643937
14	6	0	-8.446528	0.538967	3.056018
15	6	0	-9.009160	-0.817512	3.463938
16	6	0	-7.311607	2.568635	-3.194412
17	6	0	-7.500670	3.993243	-1.290352
18	6	0	-6.887212	3.699455	-2.508298
19	6	0	-7.271169	-3.356873	-2.699743
20	6	0	-7.173912	-1.310464	-3.928191
21	6	0	-6.676175	-2.588971	-3.701817
22	6	0	-7.313744	2.984018	2.307733
23	6	0	-7.269742	1.023756	3.646290
24	6	0	-6.682942	2.240386	3.301195
25	6	0	-7.290831	-2.682788	3.077518
26	6	0	-7.244833	-3.933347	1.053217
27	6	0	-6.692286	-3.675954	2.300982
28	1	0	-5.775942	2.588456	3.782881
29	1	0	-9.984867	1.015322	1.624575
30	1	0	-9.003756	4.508261	0.878422
31	1	0	-10.211664	3.245440	0.568394
32	1	0	-9.777602	1.494573	-1.152753

33	1	0	-6.084957	4.321110	-2.891497
34	1	0	-5.838938	-2.973462	-4.274695
35	1	0	-9.702038	-1.230066	-1.692295
36	1	0	-9.846980	-1.776078	1.051092
37	1	0	-5.823323	-4.217041	2.659440
38	1	0	-10.094003	-0.810223	3.317091
39	1	0	-8.804878	-0.989057	4.523304
40	1	0	-10.044797	-3.489506	-0.779942
41	1	0	-8.800148	-4.740393	-0.956311
42	1	0	-8.657080	0.786383	-4.640032
43	1	0	-9.950368	0.516489	-3.463360
44	8	0	-6.518651	-0.480593	-4.887492
45	8	0	-6.614885	2.190063	-4.381498
46	8	0	-6.675398	-4.915927	0.210568
47	8	0	-6.741395	-4.664479	-2.474998
48	8	0	-6.737918	-2.432051	4.365749
49	8	0	-6.705252	0.236725	4.677747
50	8	0	-7.033479	5.138703	-0.583246
51	8	0	-6.816583	4.253172	1.939126
52	6	0	-5.435584	1.526987	-4.125891
53	6	0	-5.383509	0.127191	-4.398517
54	7	0	-4.302466	-0.612062	-4.124124
55	7	0	-4.412246	2.183733	-3.565180
56	6	0	-3.277386	0.066238	-3.588418
57	6	0	-3.331649	1.432063	-3.308833
58	6	0	-1.932437	-0.446689	-3.168673
59	6	0	-2.023966	1.830540	-2.685979
60	7	0	-1.232772	0.676707	-2.729879
61	8	0	-1.524972	-1.611169	-3.160820
62	1	0	-0.220485	0.709874	-2.522979
63	8	0	-1.690106	2.910948	-2.191853
64	6	0	-5.503641	-4.658037	-1.848350
65	6	0	-5.489870	-4.645662	-0.421193
66	6	0	-8.345757	-2.880399	-1.929763
67	7	0	-4.380472	-4.402401	0.279057
68	7	0	-4.382944	-4.598828	-2.571325
69	6	0	-5.499567	-0.380665	4.451857
70	6	0	-5.505119	-1.802605	4.355960
71	6	0	-5.757483	4.985048	-0.059684
72	6	0	-5.646870	4.402435	1.240145
73	7	0	-4.384265	-2.517686	4.220781
74	7	0	-4.383118	0.339937	4.339382
75	7	0	-4.691490	5.335821	-0.779726
76	7	0	-4.471092	4.076992	1.779126
77	6	0	-3.253355	-4.447228	-1.850925
78	6	0	-3.402960	4.409142	1.028426
79	6	0	-3.267627	-4.281993	-0.464418
80	6	0	-3.266952	-0.389036	4.175485
81	6	0	-3.255689	-1.784387	4.147155
82	6	0	-3.504871	5.063024	-0.198749
83	6	0	-2.113374	5.372461	-0.692373
84	6	0	-1.947084	4.215478	1.351175
85	6	0	-1.818977	-4.389944	-2.314363
86	6	0	-1.868654	-4.000407	-0.001389
87	6	0	-1.866621	0.112696	3.983553
88	6	0	-1.819476	-2.233509	4.005835
89	7	0	-1.260322	4.840087	0.306066
90	7	0	-1.082937	-1.033394	3.894264
91	7	0	-1.081482	-4.114810	-1.136243
92	8	0	-1.466011	3.635370	2.323297
93	8	0	-1.764750	5.957499	-1.710049
94	8	0	-1.509502	1.286749	3.883064
95	8	0	-1.348806	-3.366402	4.009735
96	8	0	-1.341048	-4.559236	-3.429190

97	8	0	-1.487890	-3.705849	1.138360
98	1	0	-0.051496	-4.047000	-1.122165
99	1	0	-0.059284	-1.042224	3.800811
100	1	0	-0.246903	4.988763	0.320604
101	1	0	10.147114	-2.599974	1.999848
102	6	0	9.072218	-2.786179	2.092080
103	6	0	8.409849	-1.547743	2.684609
104	6	0	8.515860	-3.137752	0.719736
105	1	0	8.925376	-3.630079	2.770224
106	6	0	8.915019	-0.251066	2.502615
107	6	0	7.240339	-1.671333	3.450003
108	6	0	9.013445	-2.497976	-0.432695
109	6	0	7.484677	-4.072561	0.537045
110	6	0	8.294803	0.884828	3.057250
111	1	0	9.823583	-0.117155	1.918925
112	6	0	6.608873	-0.592687	4.061008
113	8	0	6.736530	-2.980279	3.626788
114	6	0	8.479956	-2.710653	-1.713032
115	1	0	9.844088	-1.803387	-0.320638
116	6	0	6.918040	-4.322255	-0.712752
117	8	0	6.964424	-4.801547	1.649440
118	6	0	8.841846	2.282570	2.811118
119	6	0	7.157635	0.672445	3.852624
120	1	0	5.726693	-0.727819	4.677397
121	6	0	5.587476	-3.340465	2.968426
122	6	0	9.042925	-2.026294	-2.956182
123	6	0	7.403606	-3.608248	-1.801086
124	1	0	6.107422	-5.034469	-0.825436
125	6	0	5.689443	-4.398963	2.018389
126	1	0	9.928837	2.217792	2.696918
127	1	0	8.625753	2.910025	3.679272
128	6	0	8.268660	2.949941	1.566321
129	8	0	6.566447	1.785372	4.513776
130	7	0	4.432925	-2.728183	3.231703
131	6	0	8.417599	-0.665593	-3.225363
132	1	0	8.880961	-2.674878	-3.820651
133	1	0	10.121750	-1.898139	-2.820315
134	8	0	6.795870	-3.790605	-3.070461
135	7	0	4.616671	-4.950014	1.444783
136	6	0	8.825744	2.762372	0.293312
137	6	0	7.156434	3.803472	1.646551
138	6	0	5.343872	2.199878	4.023924
139	6	0	3.368906	-3.251764	2.599839
140	6	0	8.941038	0.509189	-2.649794
141	6	0	7.286928	-0.525321	-4.043585
142	6	0	5.594515	-3.153492	-3.274998
143	6	0	3.442468	-4.376089	1.777166
144	6	0	8.317701	3.385365	-0.863356
145	1	0	9.681631	2.098019	0.189274
146	6	0	6.660775	4.504880	0.554188
147	8	0	6.527173	3.956344	2.905645
148	6	0	5.338485	3.285982	3.100390
149	7	0	4.224226	1.577883	4.403908
150	6	0	1.942599	-2.793756	2.664424
151	6	0	8.327253	1.761347	-2.806940
152	1	0	9.856515	0.440485	-2.065816
153	6	0	6.621997	0.689063	-4.212232
154	8	0	6.782408	-1.666361	-4.735012
155	6	0	5.569029	-2.107370	-4.243159
156	7	0	4.508499	-3.503390	-2.580589
157	6	0	2.035937	-4.748962	1.372573
158	6	0	8.900250	3.049325	-2.226927
159	6	0	7.254287	4.283789	-0.689586
160	1	0	5.827592	5.191297	0.664083

161	7	0	4.232118	3.668480	2.456151
162	6	0	3.103495	2.027695	3.810474
163	7	0	1.224984	-3.736000	1.945310
164	8	0	1.512001	-1.774602	3.216409
165	6	0	7.137605	1.794818	-3.551148
166	1	0	5.733621	0.761424	-4.829566
167	7	0	4.440138	-1.497942	-4.615205
168	6	0	3.388859	-2.847938	-2.929374
169	8	0	1.630817	-5.710940	0.733091
170	1	0	8.701816	3.871275	-2.919225
171	1	0	9.984751	2.936108	-2.129635
172	8	0	6.703024	4.988816	-1.810269
173	6	0	3.116018	3.013671	2.823793
174	6	0	1.672325	1.617993	4.048346
175	1	0	0.198951	-3.726957	1.845370
176	8	0	6.497144	3.048095	-3.670062
177	6	0	3.340684	-1.905070	-3.957975
178	6	0	2.013982	-2.988801	-2.353010
179	6	0	5.441399	4.505012	-2.124294
180	6	0	1.706084	3.211914	2.331065
181	7	0	0.921358	2.421900	3.162887
182	8	0	1.238558	0.776084	4.828420
183	6	0	5.373161	3.334374	-2.943179
184	6	0	1.912473	-1.458513	-4.126334
185	7	0	1.204885	-2.174697	-3.130229
186	8	0	1.661552	-3.668225	-1.379149
187	7	0	4.358036	5.051275	-1.575350
188	8	0	1.344791	3.894524	1.365888
189	1	0	-0.105932	2.426021	3.156726
190	7	0	4.271810	2.584786	-3.018062
191	8	0	1.418154	-0.673257	-4.925826
192	1	0	0.178718	-2.127434	-3.060218
193	6	0	3.221029	4.351920	-1.759937
194	6	0	3.202145	3.103129	-2.382938
195	6	0	1.825015	4.683841	-1.313703
196	6	0	1.823297	2.526762	-2.232637
197	7	0	1.067227	3.535529	-1.657292
198	8	0	1.385132	5.697665	-0.788627
199	8	0	1.429142	1.383646	-2.515490
200	1	0	0.047451	3.474562	-1.560586
201	6	0	-4.792259	0.033882	0.806708
202	6	0	-3.446669	0.779216	0.776675
203	1	0	-5.627595	0.705304	1.042131
204	1	0	-5.002786	-0.445470	-0.159662
205	1	0	-4.774598	-0.765455	1.564114
206	6	0	-2.267214	-0.173101	0.510297
207	1	0	-3.470959	1.559151	-0.004454
208	1	0	-3.286647	1.309643	1.728455
209	1	0	-2.286030	-0.992055	1.249131
210	1	0	-2.398739	-0.663198	-0.471511
211	6	0	-0.894965	0.514615	0.572890
212	6	0	0.269409	-0.431645	0.241734
213	1	0	-0.749142	0.920963	1.583627
214	1	0	-0.872263	1.388174	-0.102238
215	6	0	1.633428	0.163213	0.625730
216	1	0	0.129171	-1.380895	0.784683
217	1	0	0.264323	-0.690212	-0.831776
218	1	0	1.701875	1.201408	0.260200
219	1	0	1.692620	0.202814	1.723513
220	6	0	2.815753	-0.656429	0.092112
221	6	0	4.155770	-0.293412	0.752863
222	1	0	2.890161	-0.516316	-1.000112
223	1	0	2.616560	-1.730063	0.252663
224	6	0	5.313113	-1.129062	0.182060

225	1	0	4.360993	0.779464	0.607713
226	1	0	4.075515	-0.456656	1.839689
227	1	0	6.254845	-0.959490	0.721177
228	1	0	5.071915	-2.202592	0.232714
229	1	0	5.487151	-0.887265	-0.877122

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