

## Organic pollutants in water-soluble cavitands and capsules: contortions of molecules in nanospace

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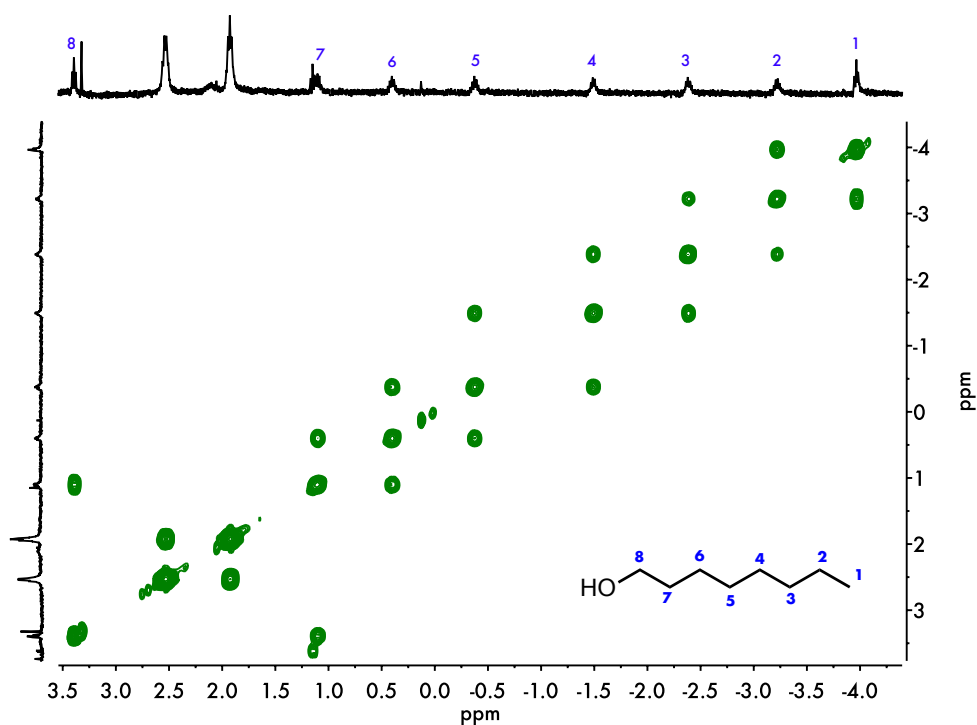
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Electronic Supplementary Information

**Table S1.**  $\Delta\delta$  data of  $C_8H_{17}OH$ - $C_{10}H_{21}OH$  in cavitand **1**<sup>a</sup>

$\Delta\delta$	$C_8H_{17}OH$	$C_9H_{19}OH$	$C_{10}H_{21}OH$
1/(Me)	-4.76	-4.75	-4.73
2	-4.47	-4.48	-4.44
3	-3.63	-3.65	-3.64
4	-2.73	-2.78	-2.8
5	-1.62	-1.7	-1.74
6	-0.85	-0.93	-0.98
7	-0.39	-0.4	-0.45
8	-0.16	-0.17	-0.19
9		-0.05	-0.04
10			0.1

<sup>a</sup>  $\Delta\delta = \delta_{\text{bound guest}} - \delta_{\text{free guest}}$



**Figure S1.** Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of *n*-C<sub>8</sub>H<sub>17</sub>OH in cavitand **1**.

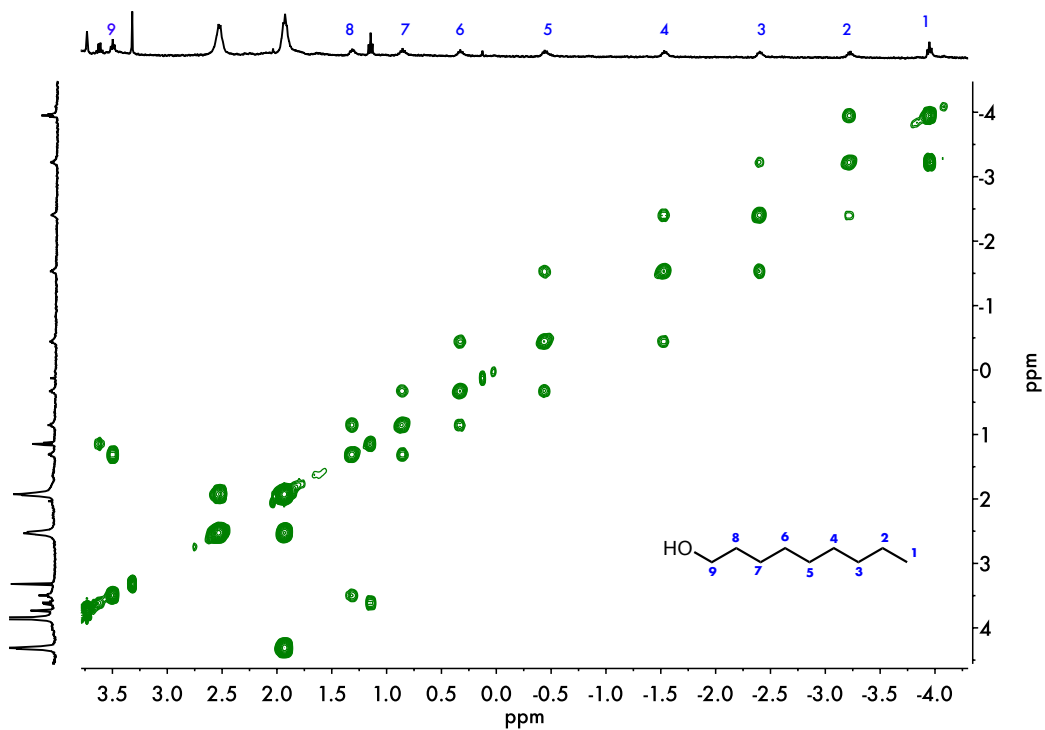


Figure S2. Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of *n*-C<sub>9</sub>H<sub>19</sub>OH in cavitan 1.

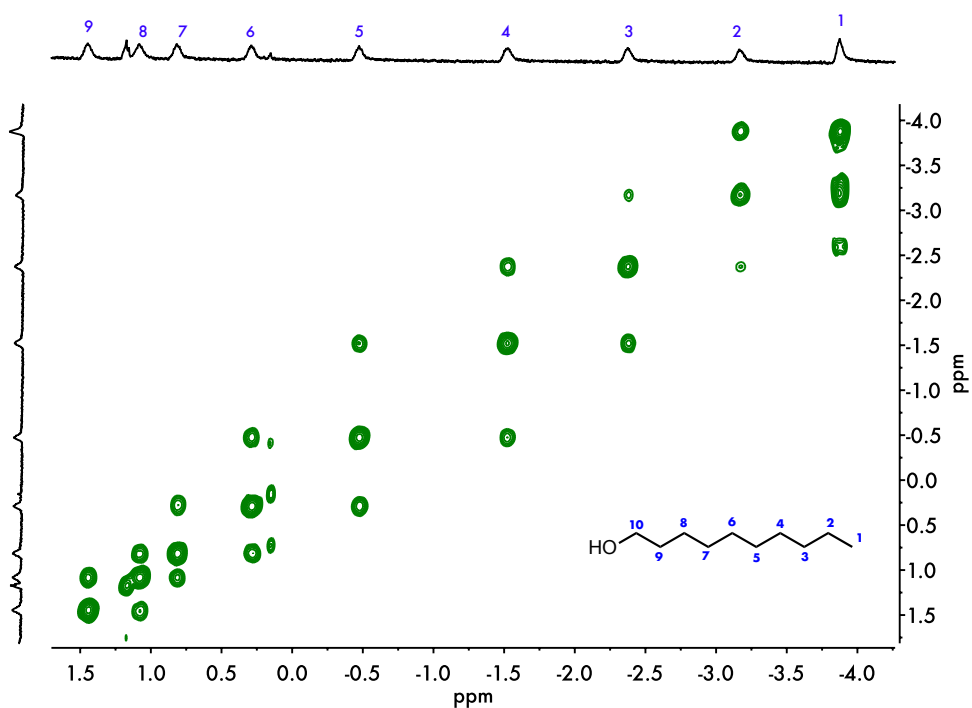
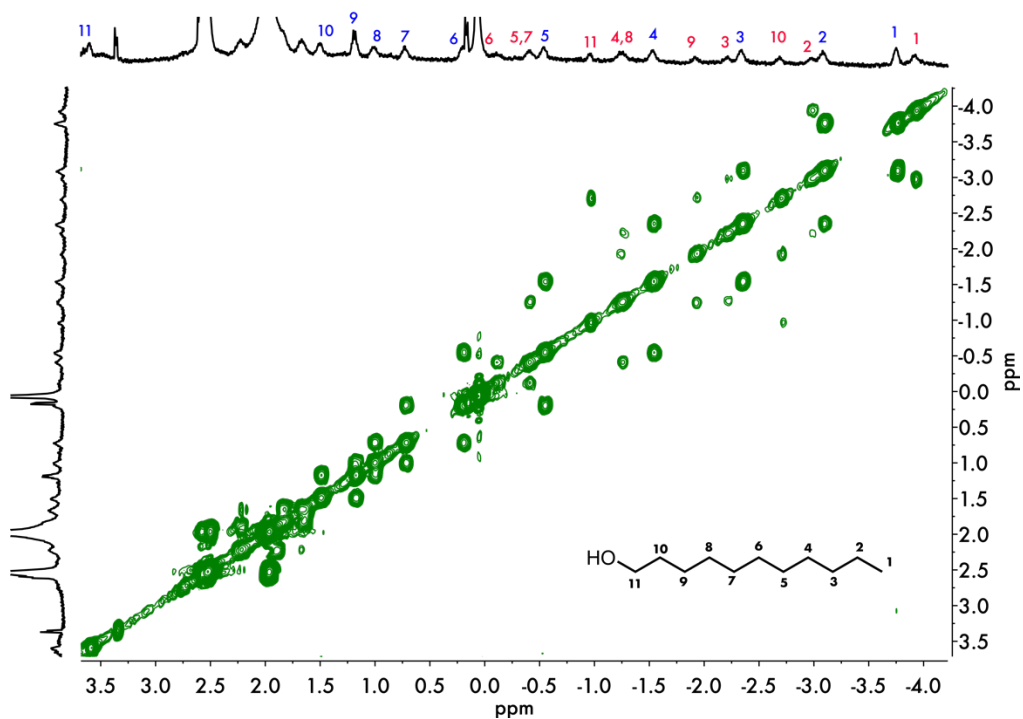
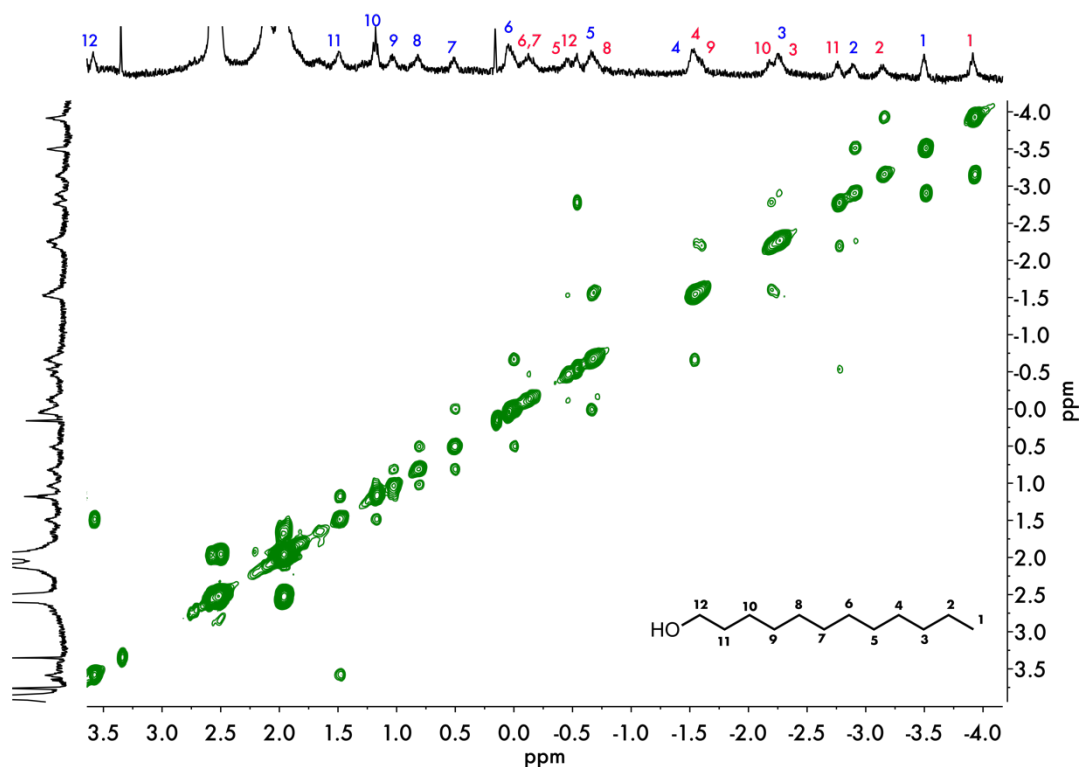


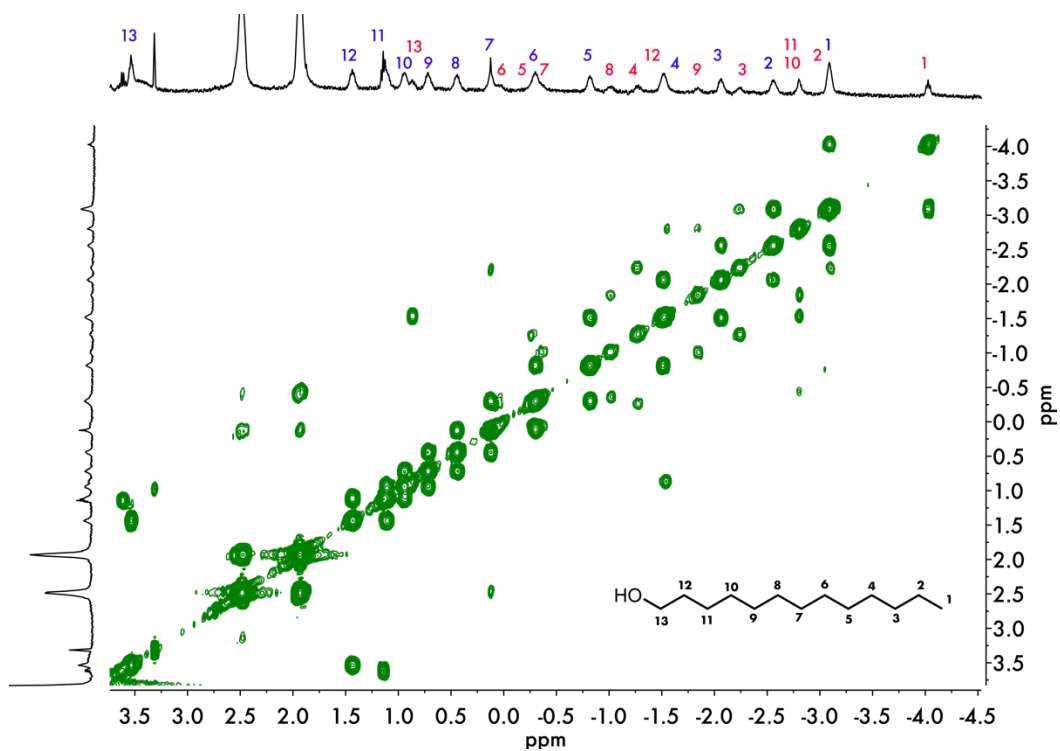
Figure S3. Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of *n*-C<sub>10</sub>H<sub>21</sub>OH in cavitan 1.



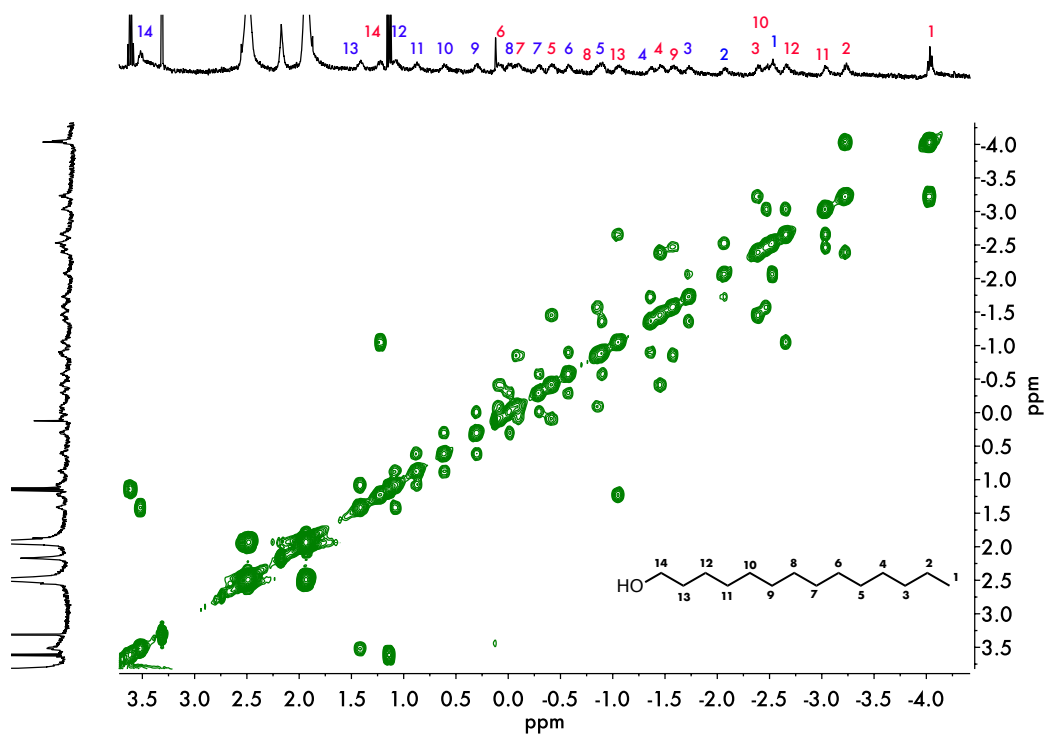
**Figure S4.** Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of *n*-C<sub>11</sub>H<sub>23</sub>OH in both cavitant **1** (the guest with blue labeled numbers) and capsule **1.1** (the guest with red labeled numbers).



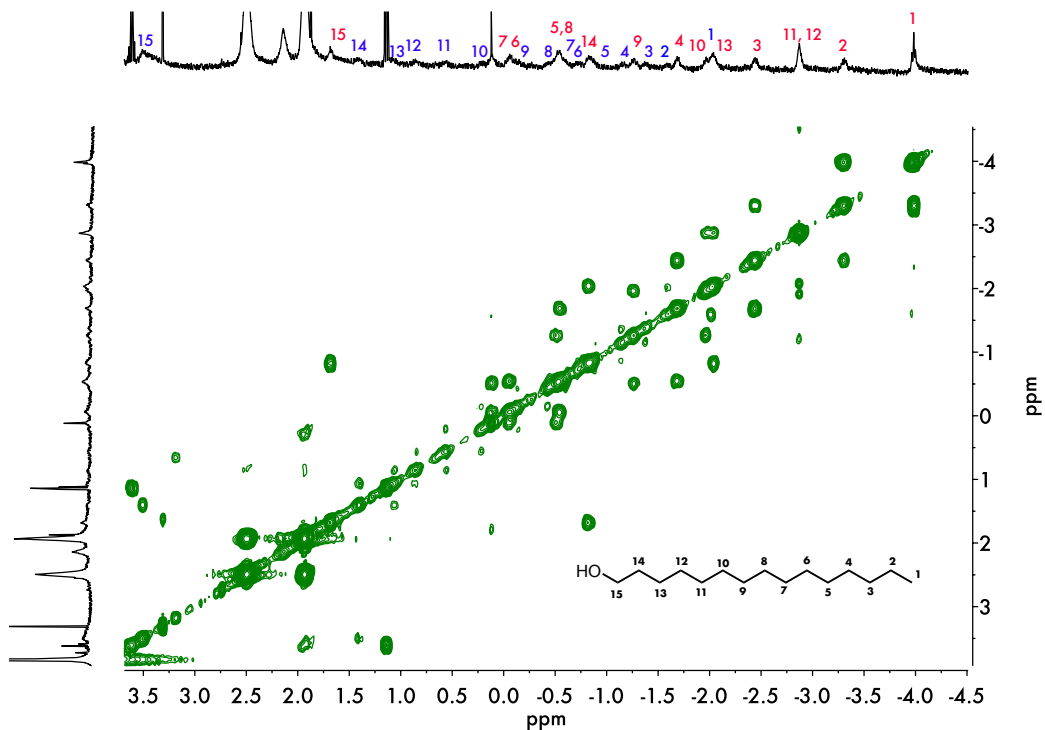
**Figure S5.** Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of *n*-C<sub>12</sub>H<sub>25</sub>OH in both cavitant **1** (the guest with blue labeled numbers) and capsule **1.1** (the guest with red labeled numbers).



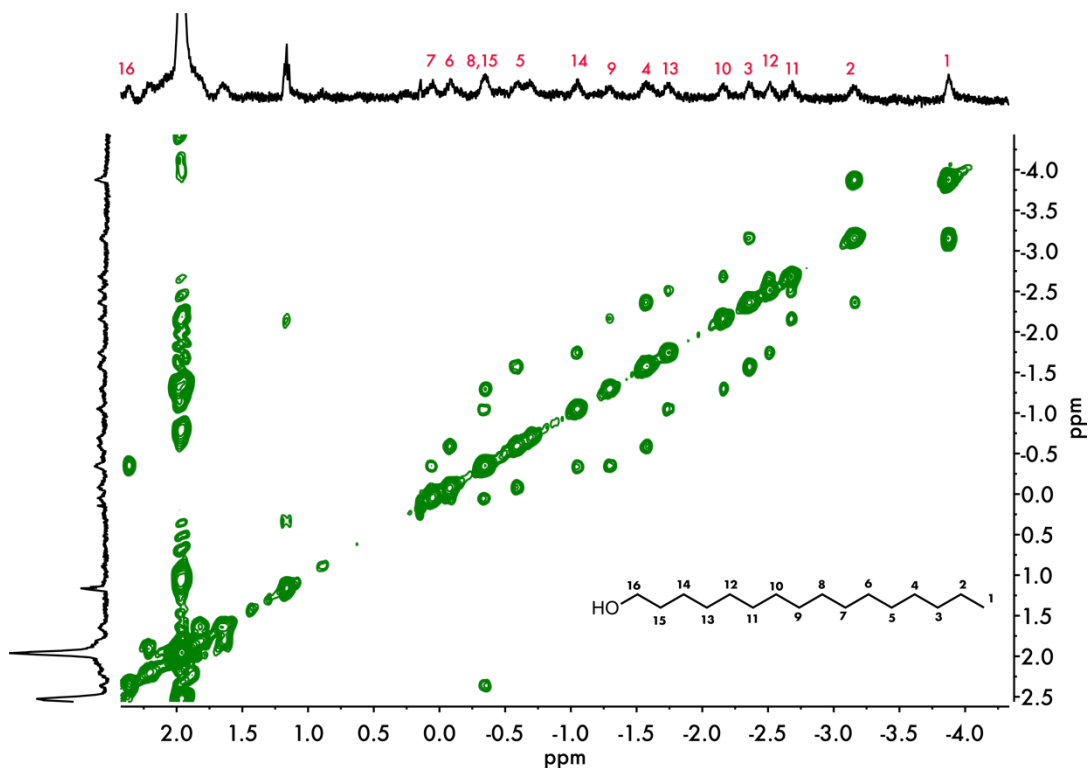
**Figure S6.** Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of *n*-C<sub>13</sub>H<sub>27</sub>OH in both cavitaand **1** (the guest with blue labeled numbers) and capsule **1.1** (the guest with red labeled numbers).



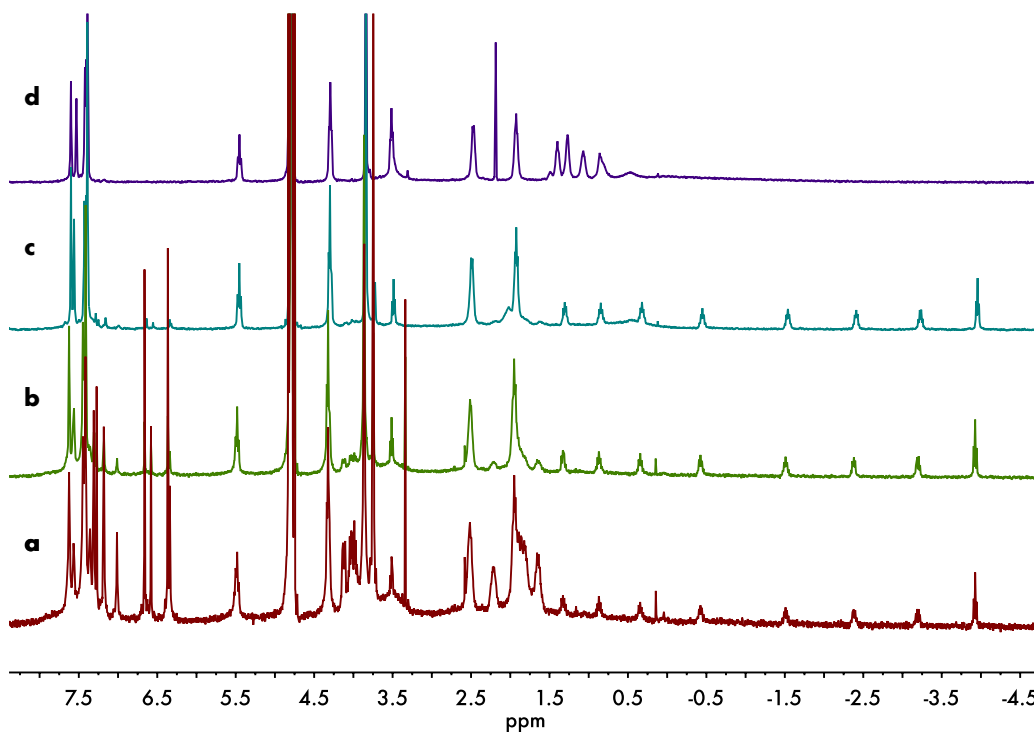
**Figure S7.** Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of *n*-C<sub>14</sub>H<sub>29</sub>OH in both cavitaand **1** (the guest with blue labeled numbers) and capsule **1.1** (the guest with red labeled numbers).



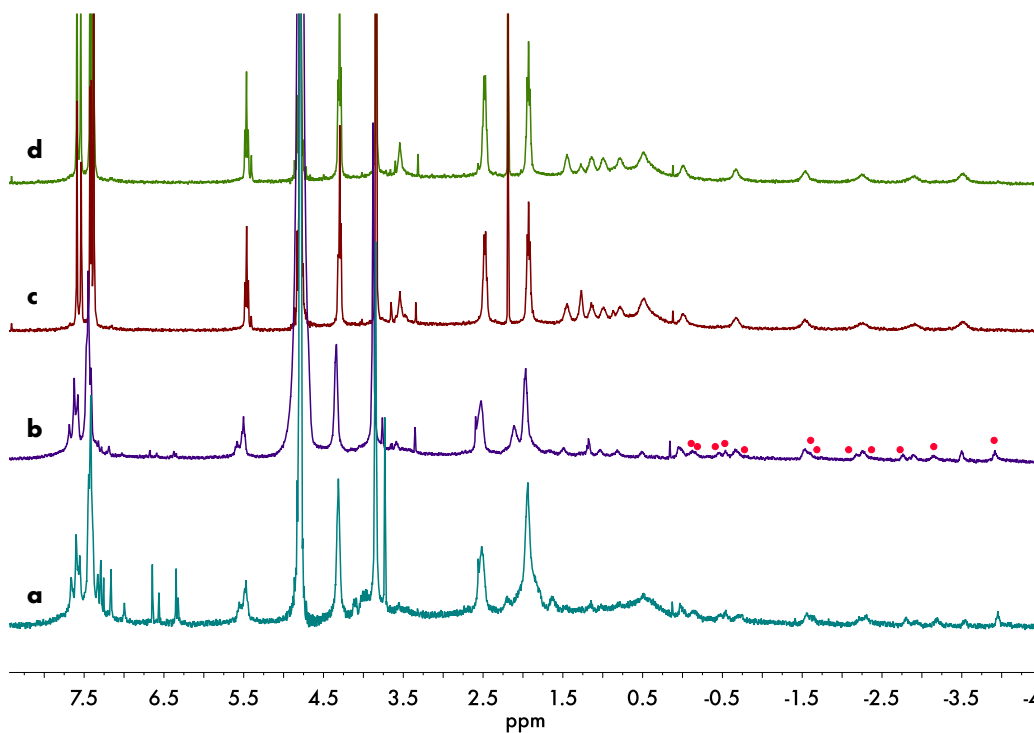
**Figure S8.** Partial COSY NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ , 298K) of  $n\text{-C}_{15}\text{H}_{31}\text{OH}$  in both cavitanol **1** (the guest with blue labeled numbers) and capsule **1.1** (the guest with red labeled numbers).



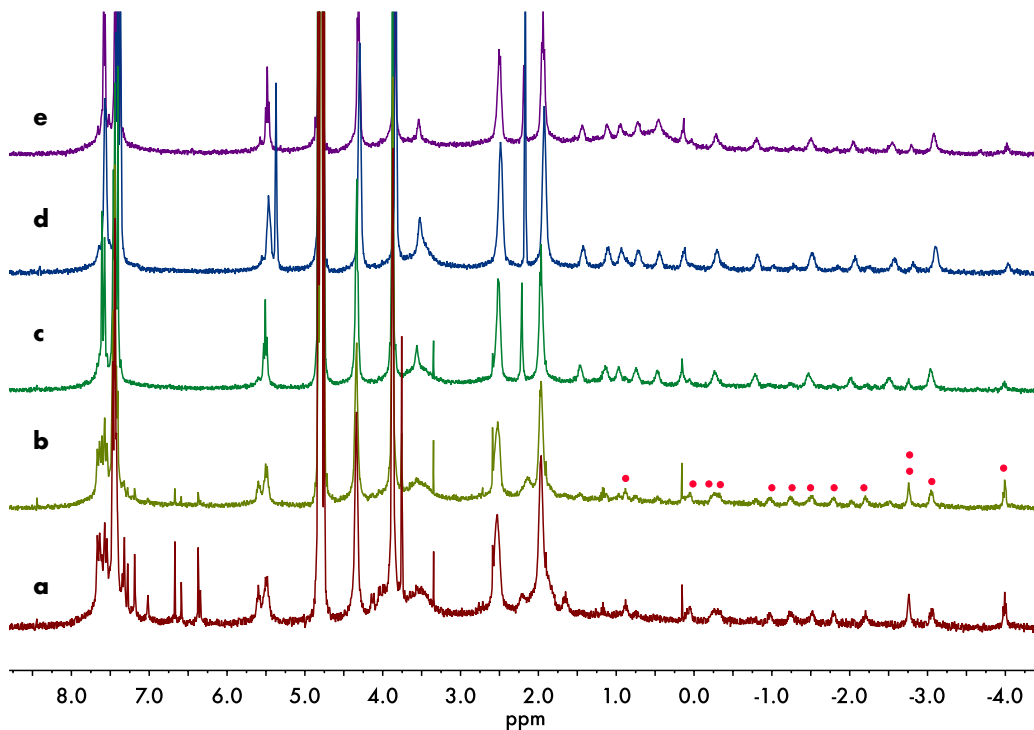
**Figure S9.** Partial COSY NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ , 298K) of  $n\text{-C}_{16}\text{H}_{33}\text{OH}$  in capsule **1.1**.



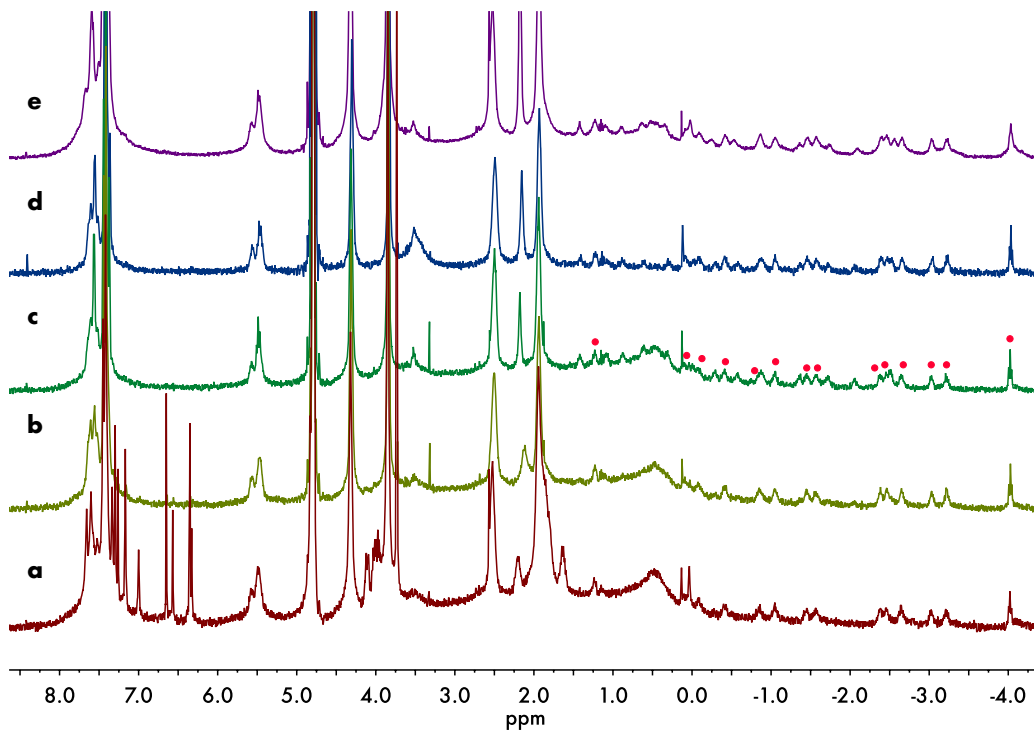
**Figure S10.** Stacked partial  $^1\text{H}$  NMR spectra (400 MHz,  $\text{D}_2\text{O}$ , 298K) of different equivalents of  $n\text{-C}_9\text{H}_{19}\text{OH}$  in cavitaud **1**. a) 0.2 equivalent; b) 0.5 equivalent; c) 1.0 equivalent and d) 4.0 equivalent.



**Figure S11.** Stacked partial  $^1\text{H}$  NMR spectra (400 MHz,  $\text{D}_2\text{O}$ , 298K) of host-guest complex between different equivalents of  $n\text{-C}_{12}\text{H}_{25}\text{OH}$  and cavitaud **1**. a) 0.2 equivalent; b) 0.5 equivalent; c) 1.0 equivalent and d) 4.0 equivalent. The NMR signals labeled with red circle are from the guest inside the capsule **1.1**.

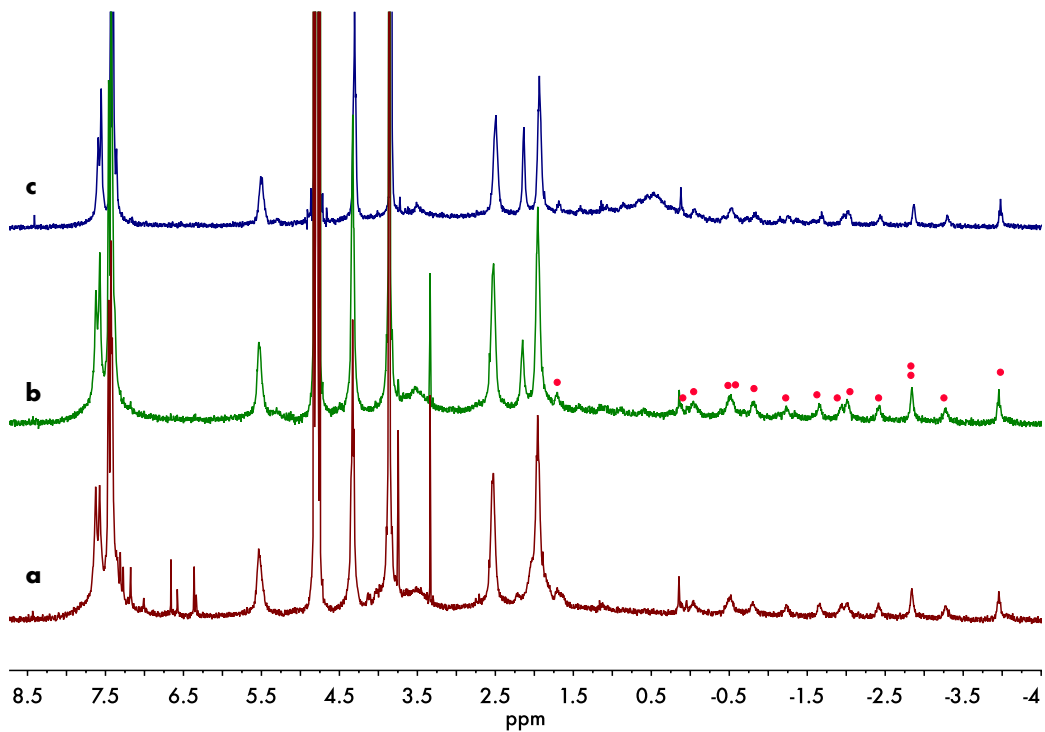


**Figure S12.** Stacked partial <sup>1</sup>H NMR spectra (400 MHz, D<sub>2</sub>O, 298K) of host-guest complex between different equivalents of *n*-C<sub>13</sub>H<sub>27</sub>OH and cavitanol **1.1**. a) 0.3 equivalent; b) 0.4 equivalent; c) 1.0 equivalent; d) 3.0 equivalent and e) 10.0 equivalent. The NMR signals labeled with red circle are from the guest inside the capsule **1.1**.

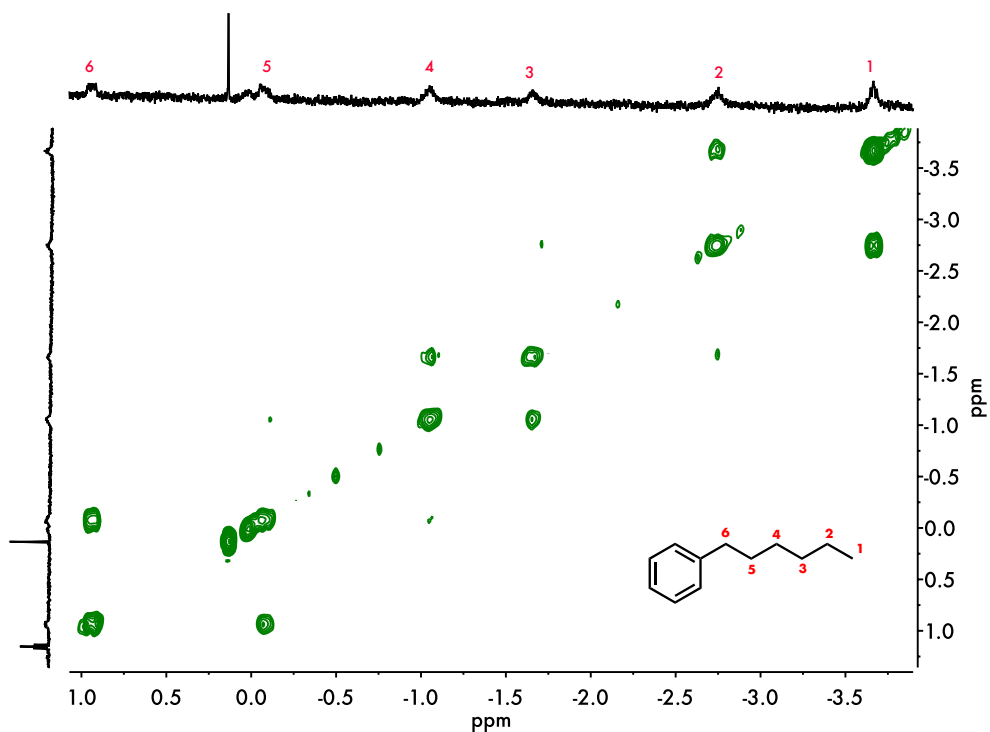


**Figure S13.** Stacked partial <sup>1</sup>H NMR spectra (400 MHz, D<sub>2</sub>O, 298K) of host-guest complex between different equivalents of *n*-C<sub>14</sub>H<sub>29</sub>OH and cavitanol **1.1**. a) 0.5 equivalent; b) 1.0 equivalent; c) 2.0 equivalent; d) 4.0 equivalent and e) 10.0 equivalent. The NMR signals labeled with red circle are from the guest inside the capsule **1.1**.

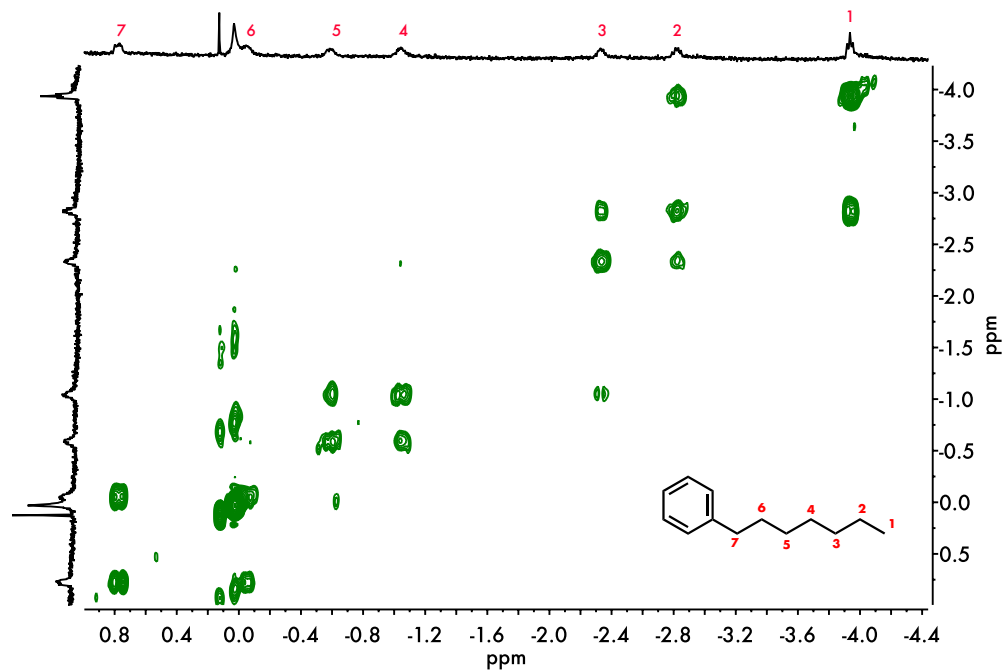




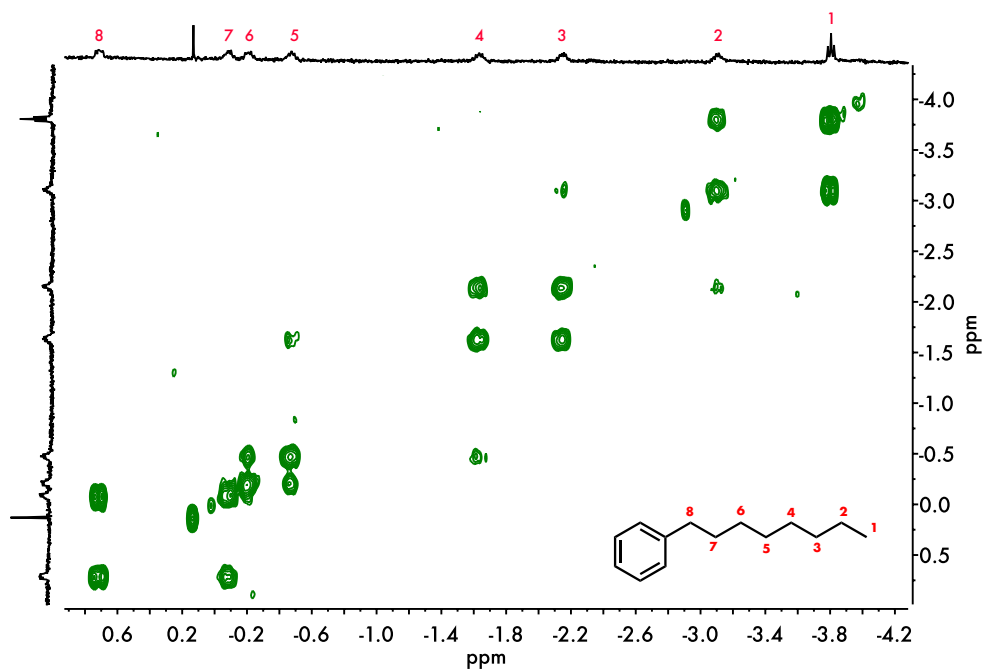
**Figure S14.** Stacked partial  $^1\text{H}$  NMR spectra (400 MHz,  $\text{D}_2\text{O}$ , 298K) of host-guest complex between different equivalents of  $n\text{-C}_{15}\text{H}_{31}\text{OH}$  and cavitaud **1**. a) 0.5 equivalent; b) 1.0 equivalent and c) 4.0 equivalent. The NMR signals labeled with red circle are from the guest inside the capsule **1.1**.



**Figure S15.** Partial COSY NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ , 298K) of  $\text{C}_6\text{H}_{13}\text{Ph}$  in capsule **1.1**.



**Figure S16.** Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of C<sub>7</sub>H<sub>15</sub>Ph in capsule 1.1.



**Figure S17.** Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of C<sub>8</sub>H<sub>17</sub>Ph in capsule 1.1.

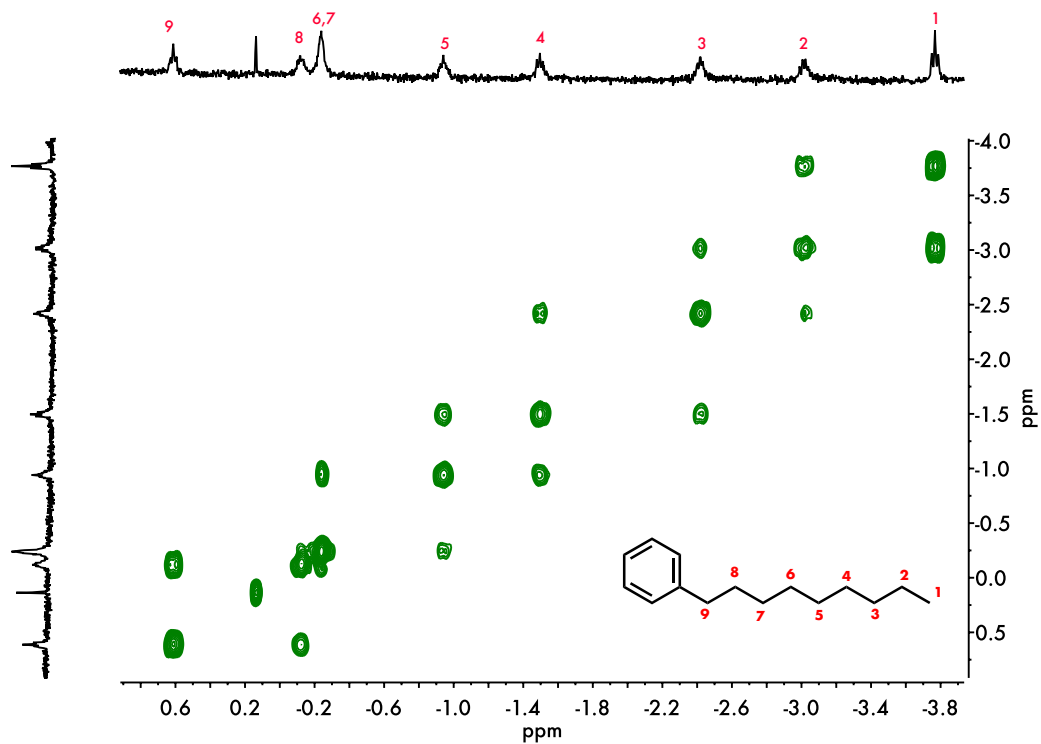


Figure S18. Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of C<sub>9</sub>H<sub>19</sub>Ph in capsule 1.1.

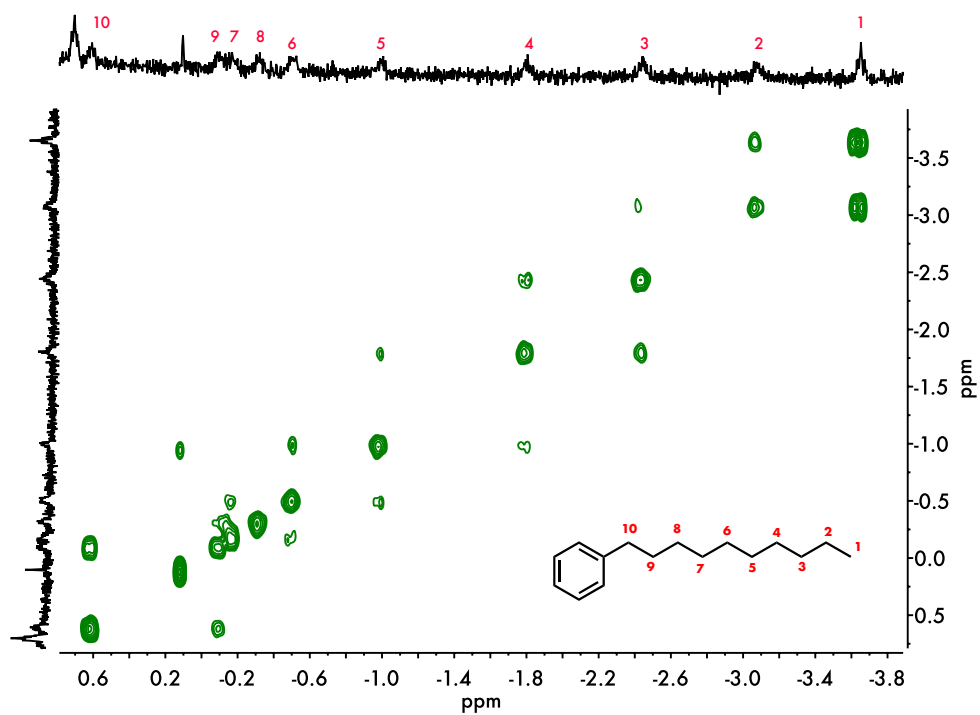


Figure S19. Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of C<sub>10</sub>H<sub>21</sub>Ph in capsule 1.1.

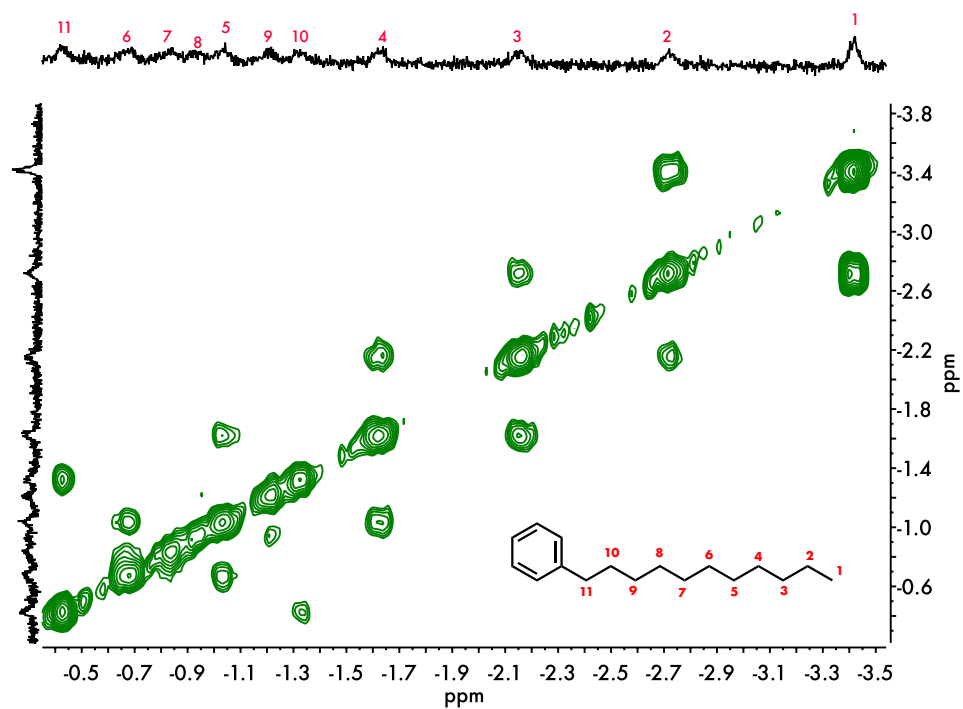


Figure S20. Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of C<sub>11</sub>H<sub>23</sub>Ph in capsule 1.1.

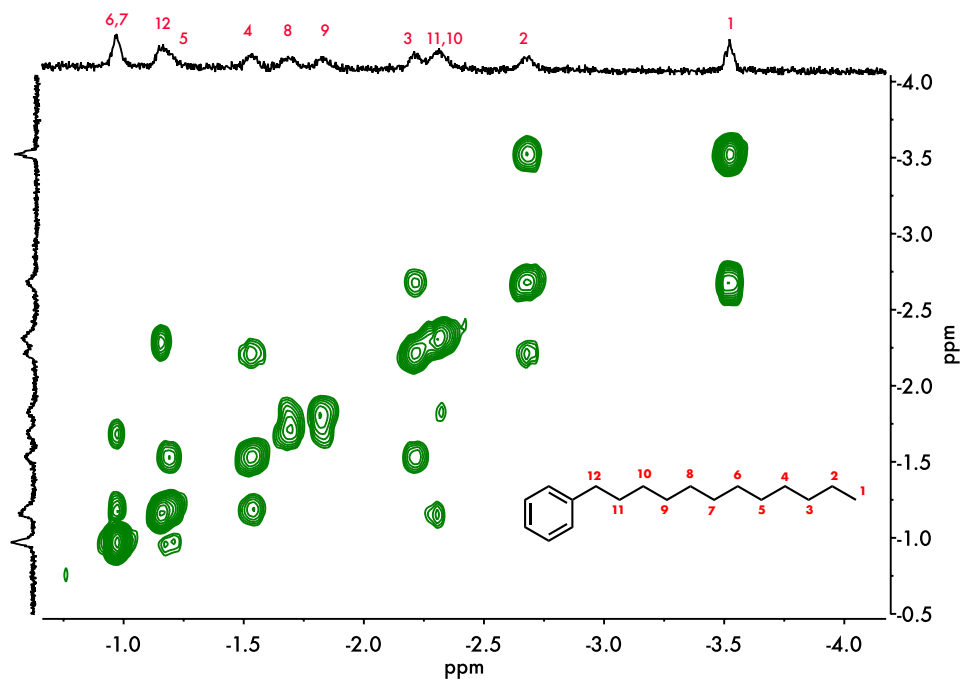


Figure S21. Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of C<sub>12</sub>H<sub>25</sub>Ph in capsule 1.1.

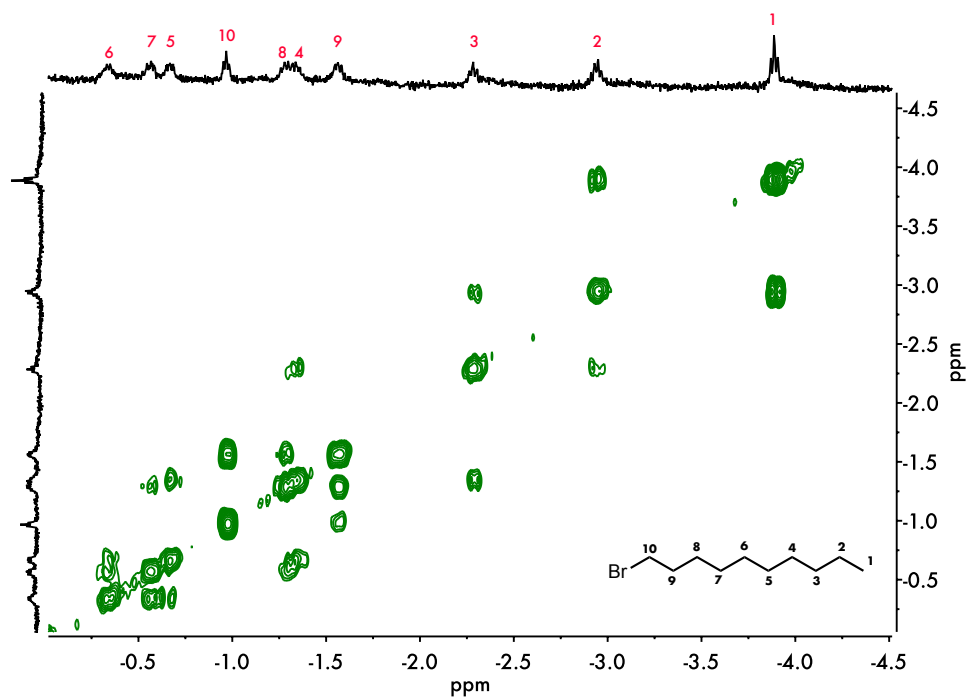


Figure S22. Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of C<sub>10</sub>H<sub>21</sub>Br in capsule 1.1.

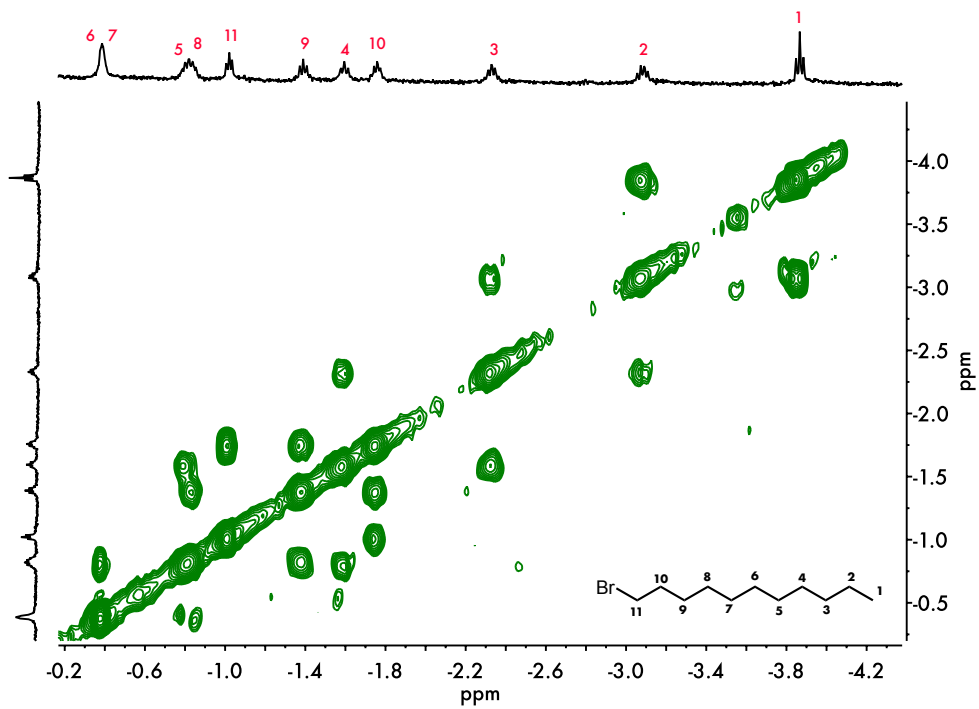
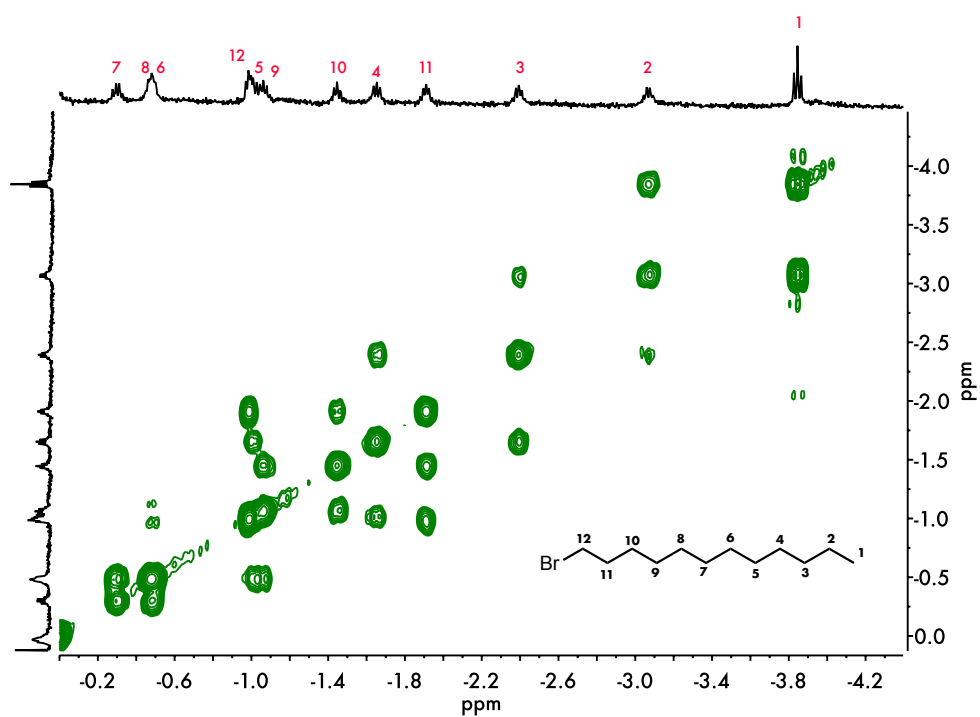


Figure S23. Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of C<sub>11</sub>H<sub>23</sub>Br in capsule 1.1.

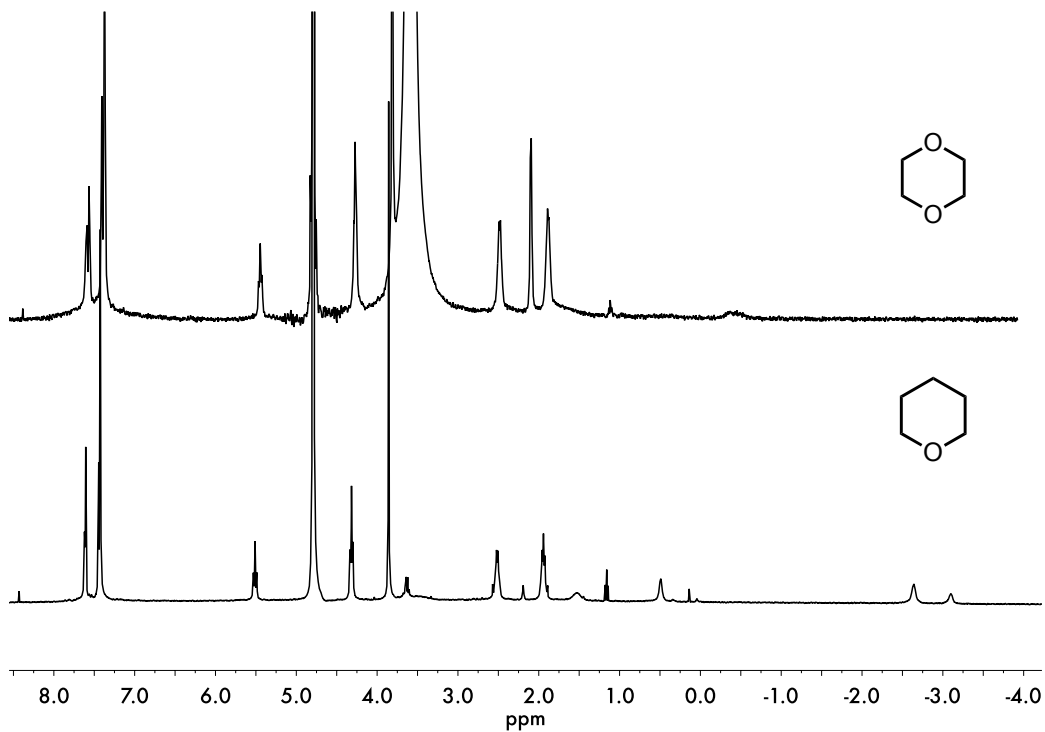


**Figure S24.** Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of C<sub>12</sub>H<sub>25</sub>Br in capsule **1.1**.

**Table S2.**  $\Delta\delta$  data of C<sub>10</sub>H<sub>21</sub>Br-C<sub>12</sub>H<sub>25</sub>Br in capsule **1.1**<sup>a</sup>

$\Delta\delta$	C <sub>10</sub> H <sub>21</sub> Br	C <sub>11</sub> H <sub>23</sub> Br	C <sub>12</sub> H <sub>25</sub> Br
1/(Me)	-4.78	-4.74	-4.73
2	-4.25	-4.36	-4.37
3	-3.58	-3.62	-3.70
4	-2.64	-2.89	-2.95
5	-1.97	-2.10	-2.32
6	-1.64	-1.69	-1.79
7	-1.87	-1.69	-1.61
8	-2.73	-2.13	-1.79
9	-3.40	-2.82	-2.37
10	-4.31	-3.58	-2.88
11		-4.35	-3.74
12			-4.33

<sup>a</sup>  $\Delta\delta = \delta_{\text{bound guest}} - \delta_{\text{free guest}}$

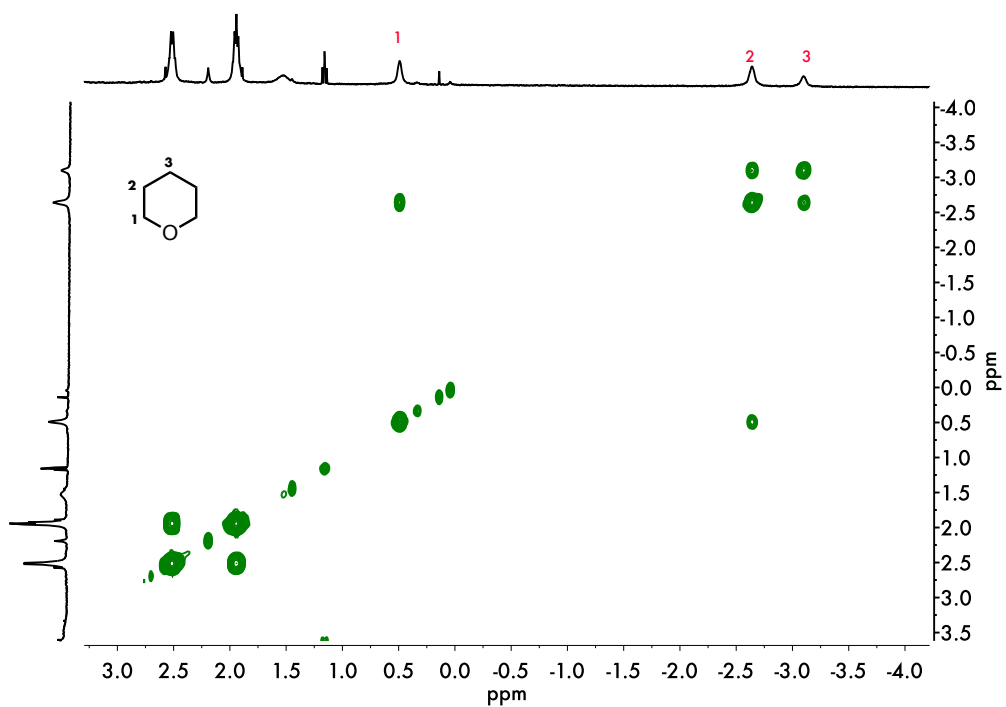


**Figure S25.** Stacked <sup>1</sup>H NMR spectra (400 MHz, D<sub>2</sub>O, 298K) of 1,4-dioxane (top) and tetrahydropyran (bottom) in cavitaand **1**.

**Table S3.**  $\Delta\delta$  data of tetrahydropyran and 1,4-dioxane in cavitaand **1**<sup>a</sup>

$\Delta\delta$	Tetrahydropyran	1,4-Dioxane
1	-3.19	
2	-4.25	-4.01
3	-4.68	

<sup>a</sup>  $\Delta\delta = \delta_{\text{bound guest}} - \delta_{\text{free guest}}$



**Figure S26.** Partial COSY NMR spectrum (400 MHz, D<sub>2</sub>O, 298K) of tetrahydropyran in cavitanol **1**.