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Electronic Supplementary Information

Solution- and Gas-Phase Study of Binding of Ammonium and Bisammonium Hydrocarbons with Oxacalix[4]arene Carboxylate

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NMR titration

Stepwise association constants were evaluated using (Bindfit) online tools at supramolecular.org.[1,2] The 1:2 NMR binding model with "full flavor" was used in Bindfit, which does not assume any specific relation: (i) between chemical shifts of HG and HG_2; (ii) between stepwise association constants (K_{11}, K_{12}). Cooperativity was expressed as $\alpha = 4K_{12}/K_{11}$.[2]

Table S1. Titration data points and binding constants of 1:2 complexes of host **1** with guests **2-13** (entry 1-12) and molecule **22** with guests **2**, **11** and **12** (entry 13, 14 and 15 and marked with an asterisks) in methanol-d_4 at 298 K.

Entry	Guest	K_a (M^{-1})	Data points fitted
1	**2**	K_{11} 167.1 ± 1.7 K_{12} 15.9 ± 0.1	64
2	**3**	K_{11} 97.1 ± 0.9 K_{12} 5.67 ± 0.05	76
3	**4**	K_{11} 105 ± 1 K_{12} 7.2 ± 0.1	76
4	**6**	K_{11} 103 ± 2 K_{12} 5.6 ± 0.1	57
5	**7**	K_{11} 46 ± 2 K_{12} 3.3 ± 0.1	72
6	**8**	Proton transfer to host	
7	**9**	Proton transfer to host	
8	**10**	Proton transfer to host	
9	**11**	K_{11} 124 ± 1 K_{12} 8.73 ± 0.08	76

10	**12**	K_{11} 818 ± 30 K_{12} 104 ± 5	72
11	**13**	K_{11} 536 ± 8 K_{12} 31.4 ± 0.5	76
12	**14**	K_{11} 113 ± 2 K_{12} 3.13 ± 0.08	76
13	**2***	K_{11} 250 ± 20 K_{12} 17 ± 1	68
14	**11***	K_{11} 500 ± 100 K_{12} 6.0 ± 0.4	76
15	**12***	K_{11} 2000 ± 200 K_{12} 100 ± 7	68

^{1}H NMR titration data of host **1** and guest **2** complex in methanol-d_4

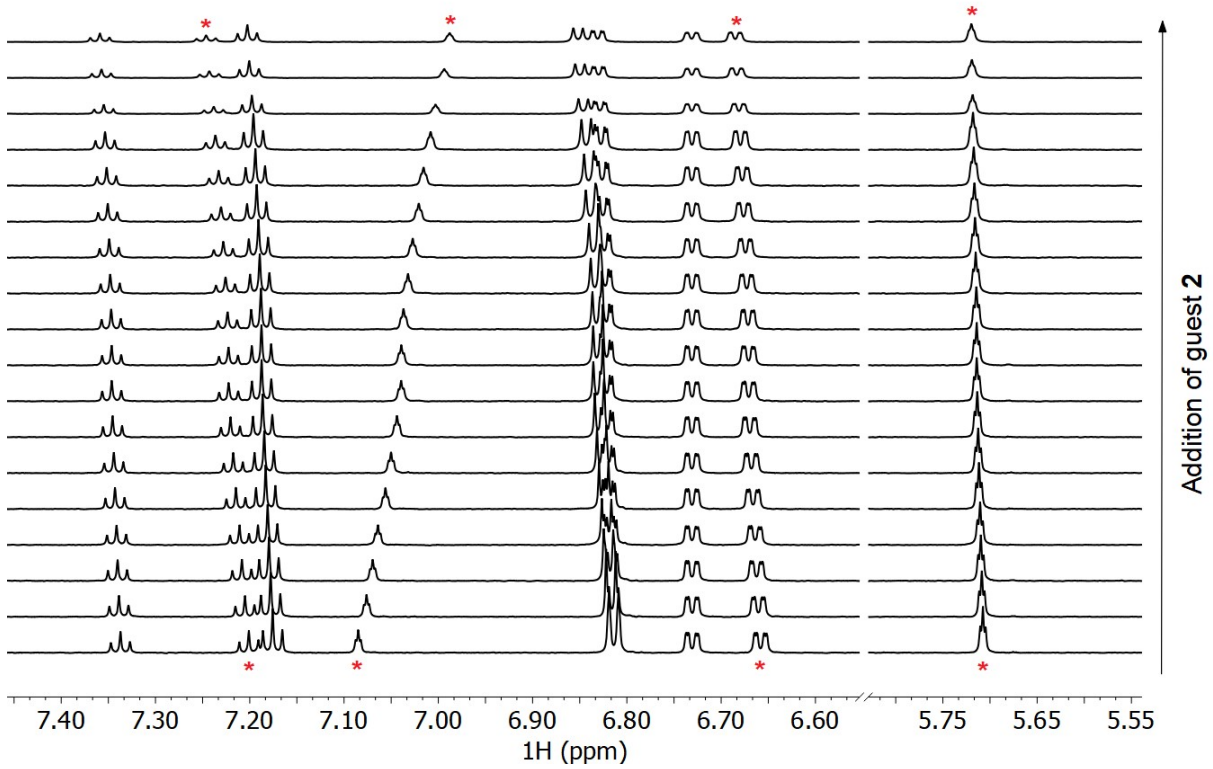

Figure S1. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.7 mM) titration with **2** at 298 K. On the figure are shown the 18 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **2** concentration (M) in samples 0, 0.0013, 0.0026, 0.0040, 0.0065, 0.0090, 0.0120, 0.0145, 0.0147, 0.0165, 0.0203, 0.0255, 0.0338, 0.0417, 0.0581, 0.0740, 0.1120, 0.1437. The results of the K_a determination based on 16 titration points and 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 binding model results

^{1}H NMR titration data of host **1** and guest **3** complex in methanol-d_4

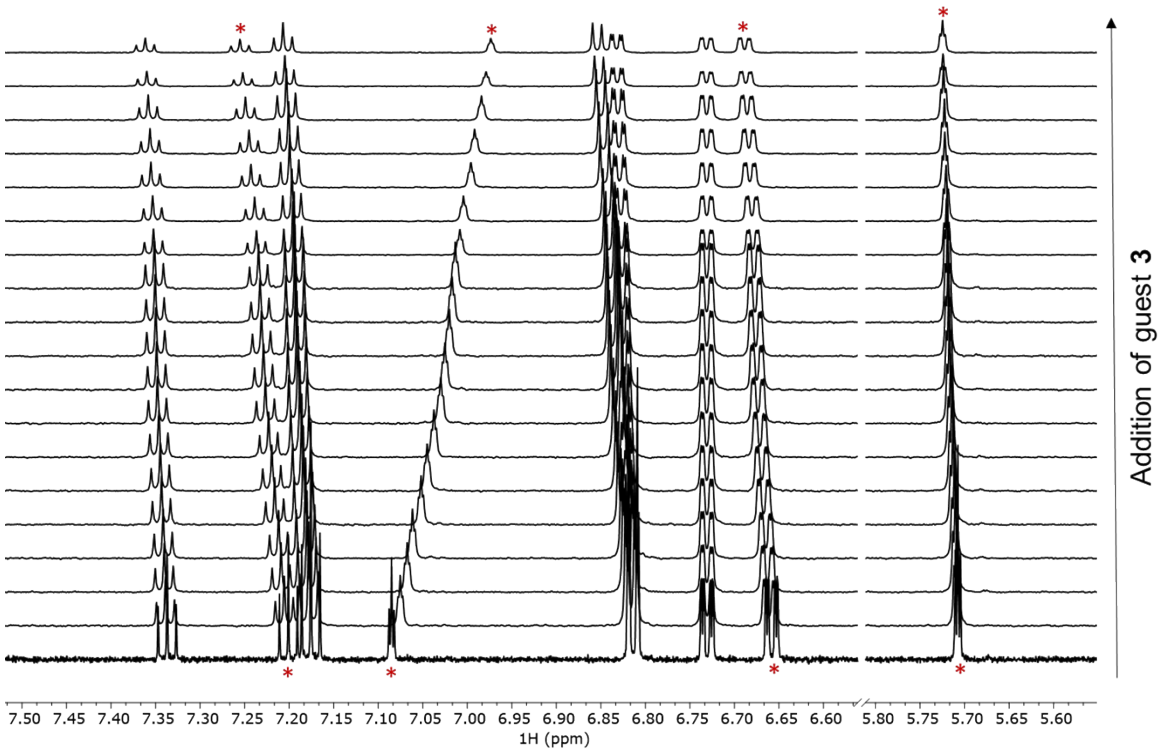

Figure S2. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.7 mM) titration with **3** at 298 K. On the figure are shown the 19 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **3** concentration (M) in samples 0, 0.0017, 0.0034, 0.0052, 0.0087, 0.0119, 0.0172, 0.0232, 0.0281, 0.0349, 0.0397, 0.0455, 0.0570, 0.0663, 0.0962, 0.1158, 0.1594, 0.1966, 0.2555. The results of the K_a determination based on 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

^{1}H NMR titration data of host **1** and guest **4** complex in methanol-d_4

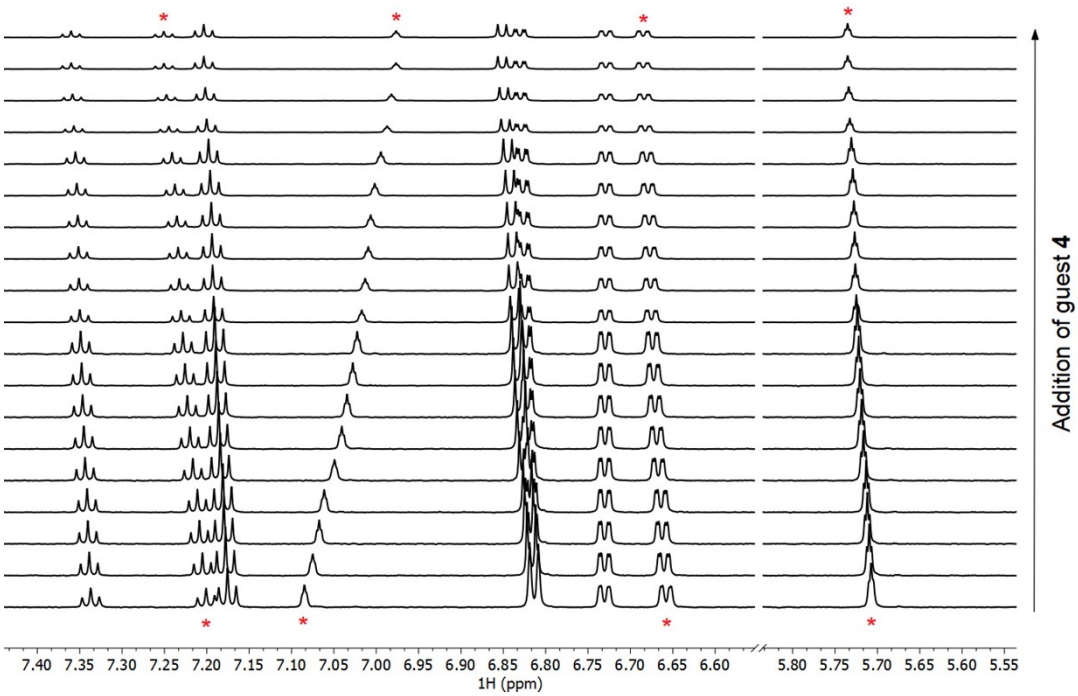

Figure S3. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.7 mM) titration with **4** at 298 K. On the figure are shown the 19 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **4** concentration (M) in samples 0, 0.0018, 0.0036, 0.0054, 0.0103, 0.0150, 0.0200, 0.0262, 0.0326, 0.0413, 0.0496, 0.0551, 0.0626, 0.0760, 0.1014, 0.1407, 0.1758, 0.2256, 0.2284. The results of the K_a determination based on 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

^{1}H NMR titration data of host **1** and guest **6** complex in methanol-d_4

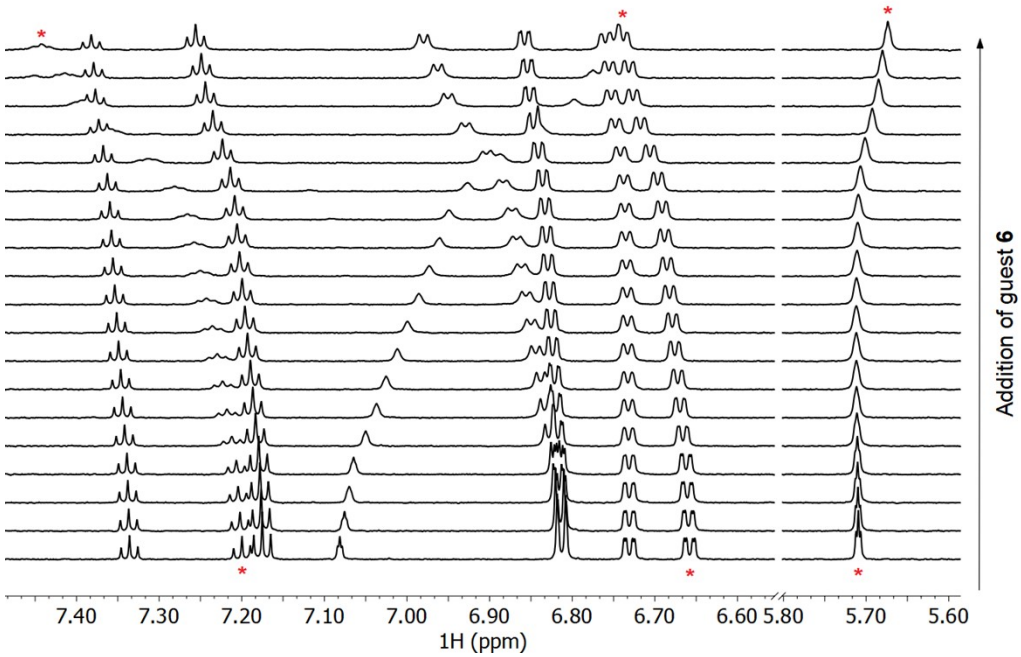

Figure S4. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.2 mM) titration with **6** at 298 K. On the figure are shown the 19 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **6** concentration (M) in samples 0, 0.0003, 0.0006, 0.0010, 0.0019, 0.0029, 0.0038, 0.0049, 0.0064, 0.0078, 0.0093, 0.0106, 0.0125, 0.0152, 0.0203, 0.0279, 0.0360, 0.0395, 0.0475. The results of the Ka determination based on 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

^{1}H NMR titration data of host **1** and guest **7** complex in methanol-d_4

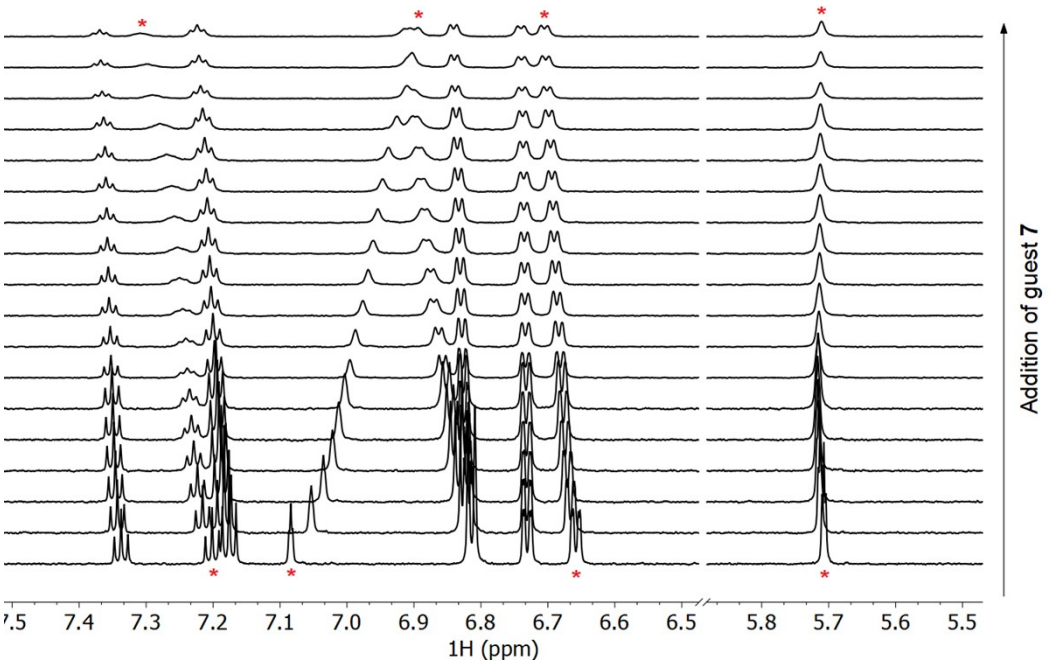

Figure S5. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.7 mM) titration with **7** at 298 K. On the figure are shown the 18 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **7** concentration (M) in samples 0, 0.0057, 0.0112, 0.0167, 0.0221, 0.0274, 0.0302, 0.0379, 0.0455, 0.0527, 0.0608, 0.0665, 0.0732, 0.0839, 0.1121, 0.1469, 0.1782, 0.2096. The results of the K_a determination based on 1:1 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

^{1}H NMR titration data of host **1** and guest **8** complex in methanol-d_4

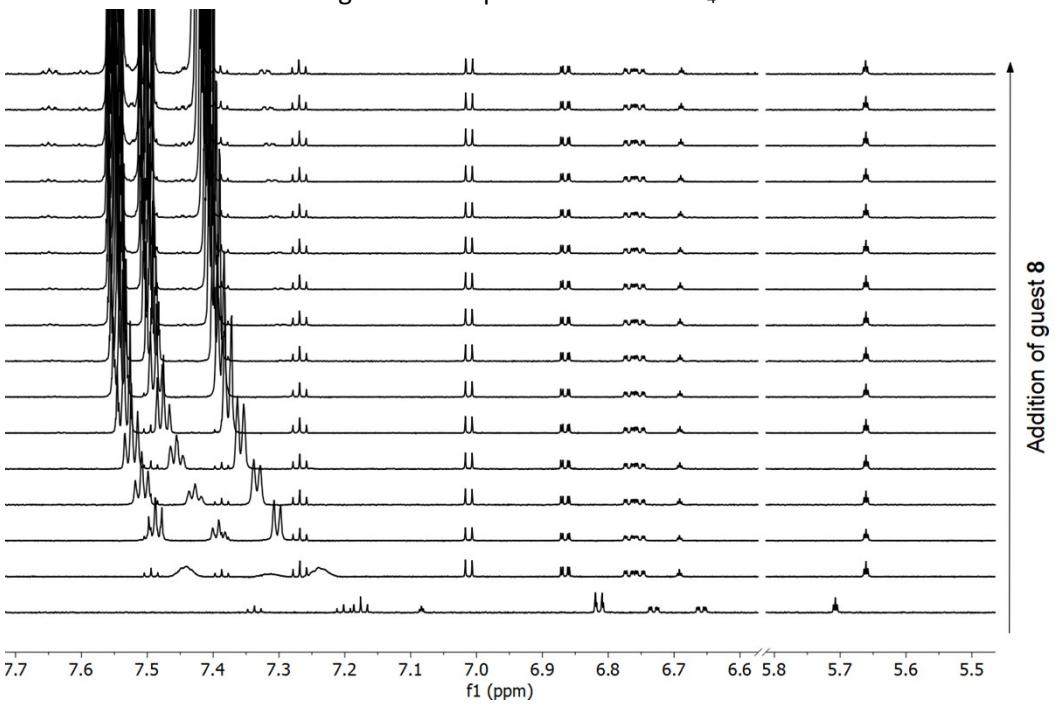

Figure S6. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (1.0 mM) titration with **8** at 298 K. Guest **8** concentration (M) in samples 0, 0.001, 0.002, 0.003, 0.005, 0.007, 0.01, 0.0148, 0.0196, 0.0243, 0.0289, 0.0335, 0.0380, 0.0467, 0.0552, 0.0715, 0.0868, 0.1215, 0.1402.

^{1}H NMR titration data of host **1** and guest **9** complex in methanol-d_4

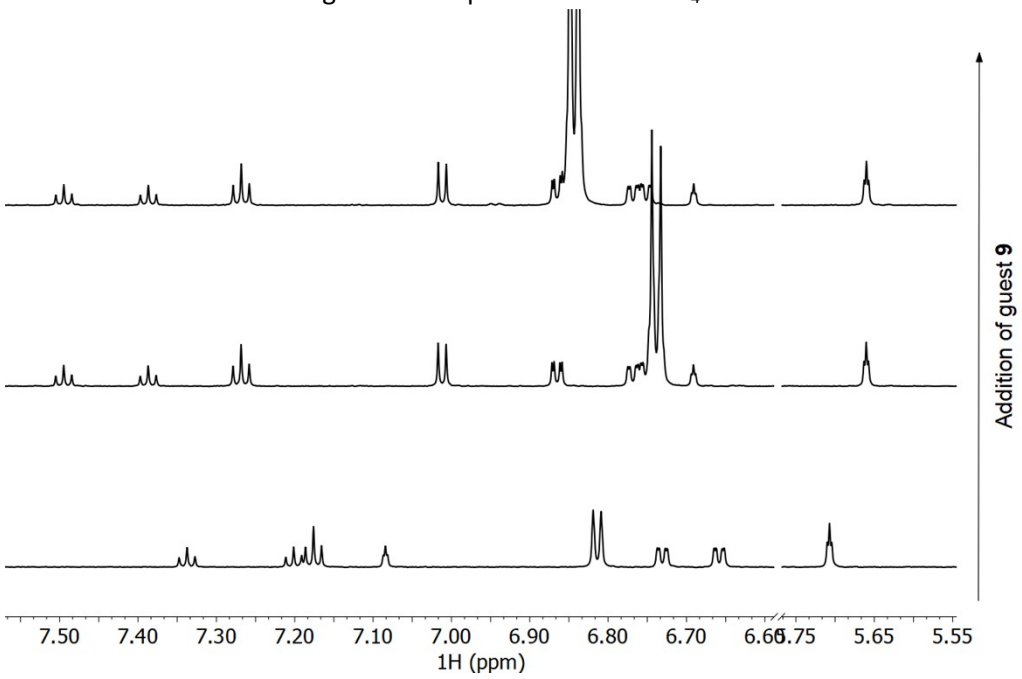

Figure S7. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.7 mM) titration with **9** at 298 K. Guest **9** added to samples in 0, 1 and 2 equivalents.

^{1}H NMR titration data of host **1** and guest **10** complex in methanol-d_4

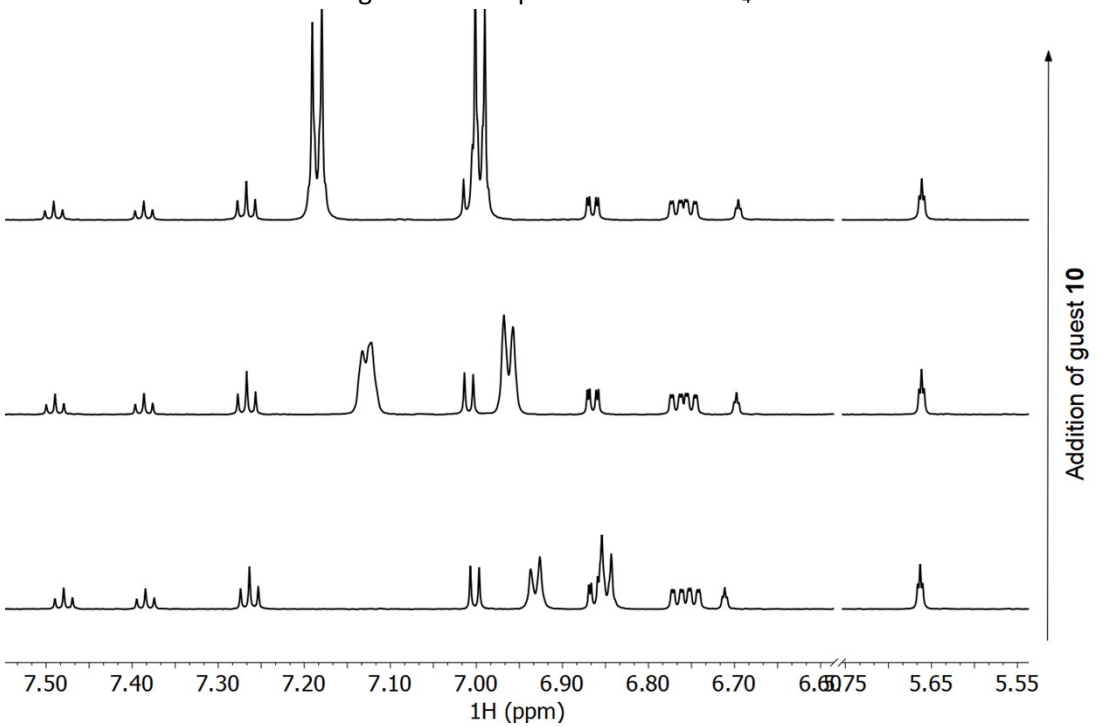

Figure S8. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.7 mM) titration with **10** at 298 K. Guest **10** added to samples in 1.5, 3.1 and 4.5 equivalents.

^{1}H NMR titration data of host **1** and guest **11** complex in methanol-d_4

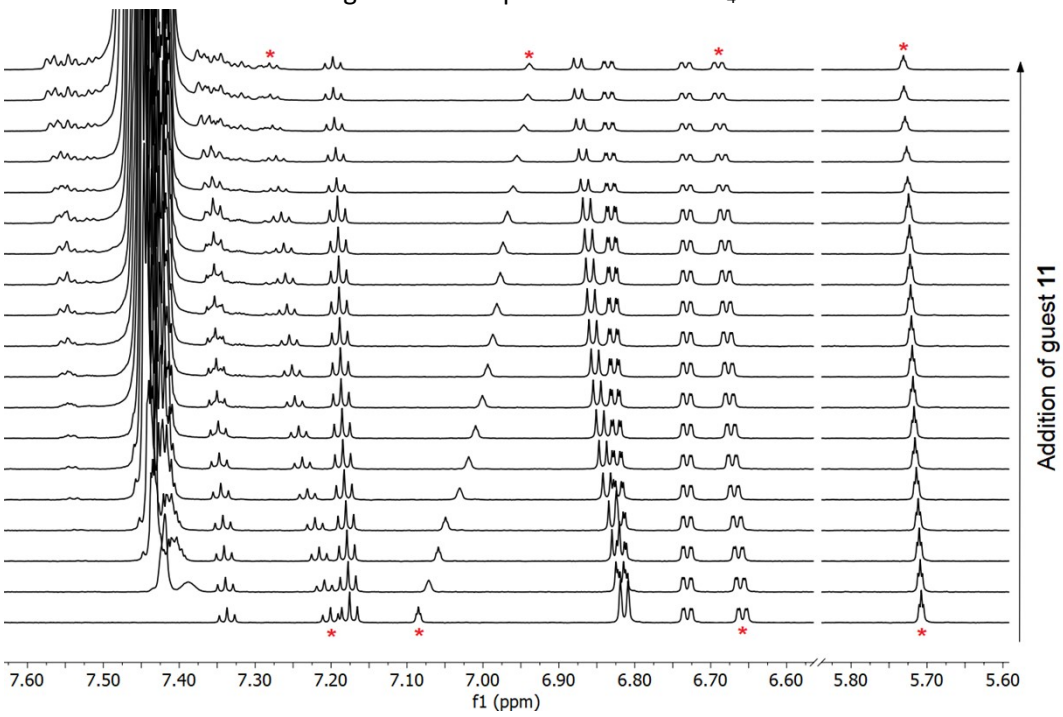

Figure S9. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.6 mM) titration with **11** at 298 K. On the figure are shown the 19 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **11** concentration (M) in samples 0, 0.0013, 0.0029, 0.0044, 0.0084, 0.0124, 0.0166, 0.0211, 0.0262, 0.0336, 0.0387, 0.0455, 0.0511, 0.0633, 0.0805, 0.1006, 0.1417, 0.1773, 0.1968. The results of the K_a determination based on 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

^{1}H NMR titration data of host **1** and guest **12** complex in methanol-d_4

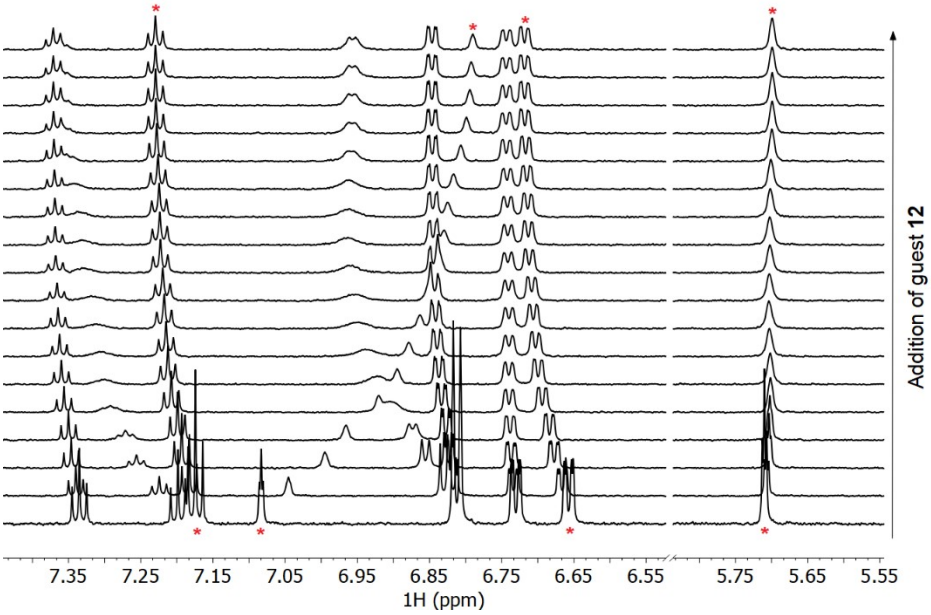

Figure S10. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.2 mM) titration with **12** at 298 K. On the figure are shown the 18 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **12** concentration (M) in samples 0, 0.0003, 0.0009, 0.0013, 0.0026, 0.0038, 0.0053, 0.0068, 0.0084, 0.0124, 0.0143, 0.0166, 0.0204, 0.0286, 0.0386, 0.0478, 0.0546, 0.0590. The results of the K_a determination based on 13 titration points and 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

^{1}H NMR titration data of host **1** and guest **13** complex in methanol-d_4

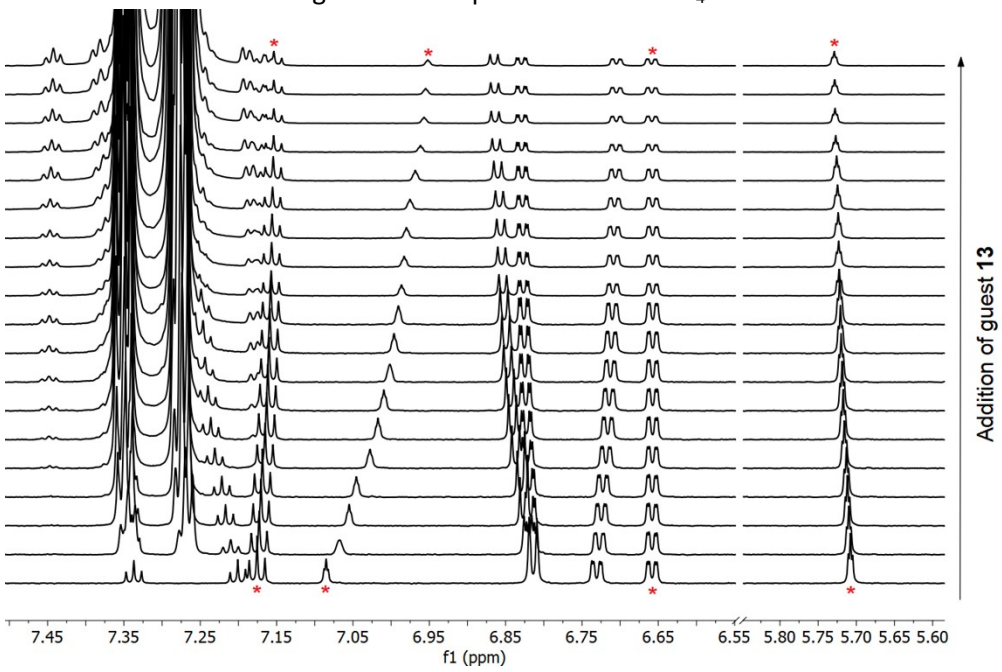

Figure S11. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.2 mM) titration with **13** at 298 K. On the figure are shown the 19 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **13** concentration (M) in samples 0, 0.0005, 0.0009, 0.0014, 0.0028, 0.0041, 0.0054, 0.0073, 0.0089, 0.0113, 0.0131, 0.0150, 0.0172, 0.0214, 0.0290, 0.0398, 0.0498, 0.0555, 0.0639. The results of the K_a determination based on 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

^{1}H NMR titration data of host **1** and guest **14** complex in methanol-d_4

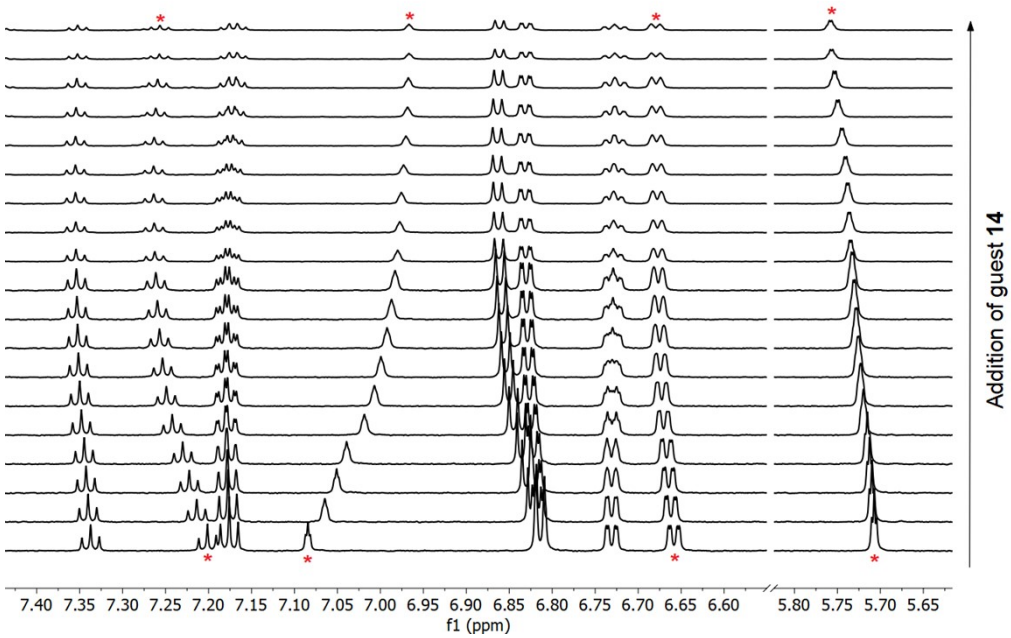

Figure S12. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.7 mM) titration with **14** at 298 K. On the figure are shown the 19 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **14** concentration (M) in samples 0, 0.0017, 0.0033, 0.0054, 0.0112, 0.0166, 0.0215, 0.0290, 0.0355, 0.0442, 0.0524, 0.0602, 0.0681, 0.0839, 0.1110, 0.1558, 0.1943, 0.2312, 0.2442. Bindfit 1:2 model results

^{1}H NMR titration data of host **1** added nitrobenzene **15** in methanol-d_4

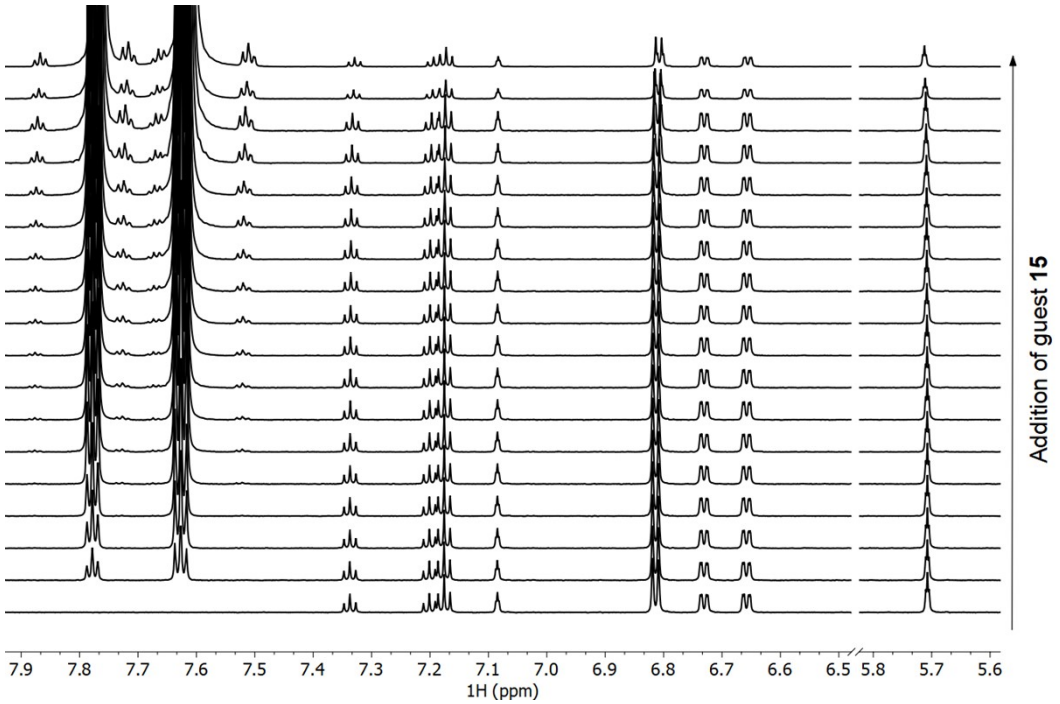

Figure S13. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.7 mM) titration with nitrobenzene at 298 K. On the figure are shown the 18 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **15** concentration (M) in samples 0, 0.0017, 0.0031, 0.005, 0.01, 0.0157, 0.0209, 0.0265, 0.0344, 0.0429, 0.0505, 0.0594, 0.0683, 0.0838, 0.1172, 0.1424, 0.1993, 0.2623. No complex formation was observed. See ion mobility section for further information.

^{1}H NMR titration data of host **1** and guest **16** complex in methanol-d_4

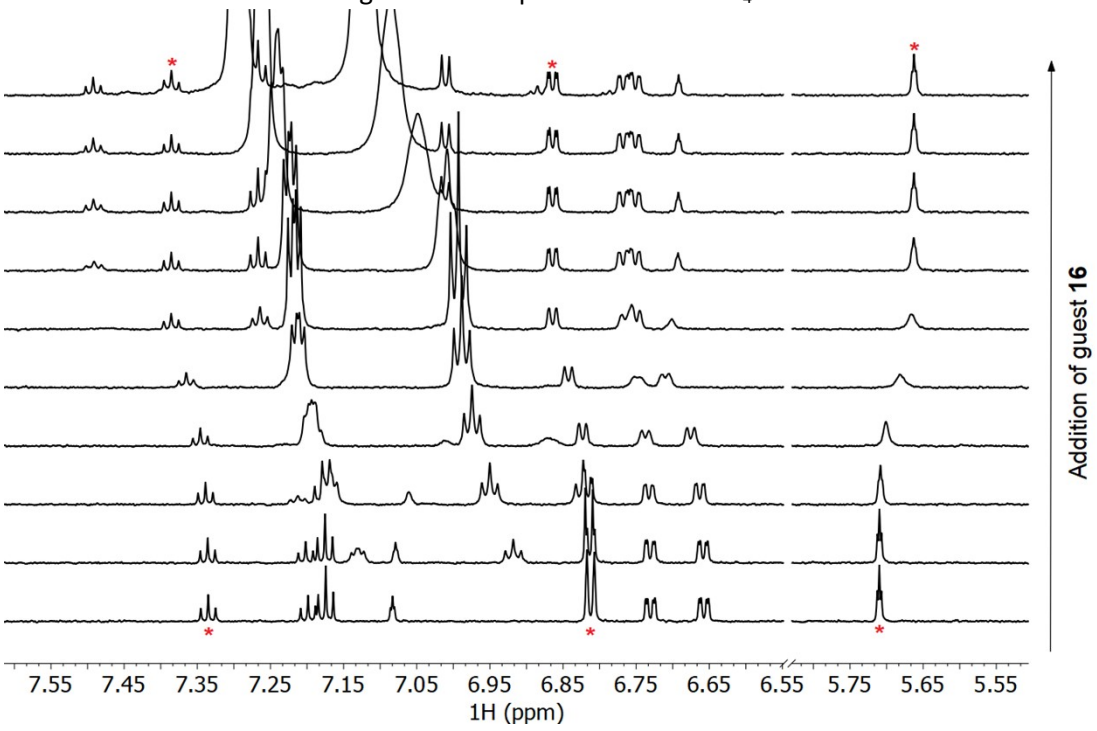

Figure S14. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.2 mM) titration with **16** at 298 K. On the figure are shown the 10 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **16** added to samples from 0.2 to 9.7 equivalents.

^{1}H NMR titration data of host **1** and guest **17** complex in methanol-d_4

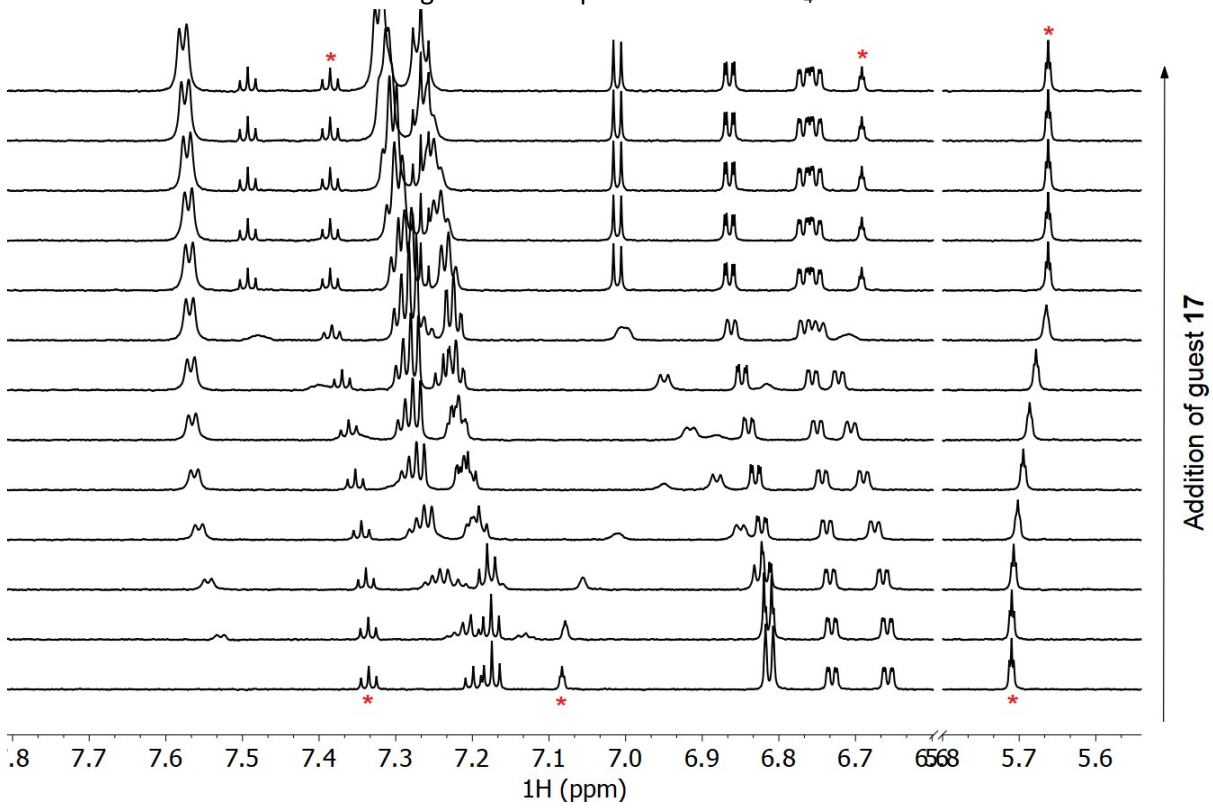

Figure S15. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.2 mM) titration with **17** at 298 K. On the figure are shown the 13 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **17** added to samples from 0.2 to 2.6 equivalents.

^{1}H NMR titration data of host **1** and guest **18** complex in methanol-d_4

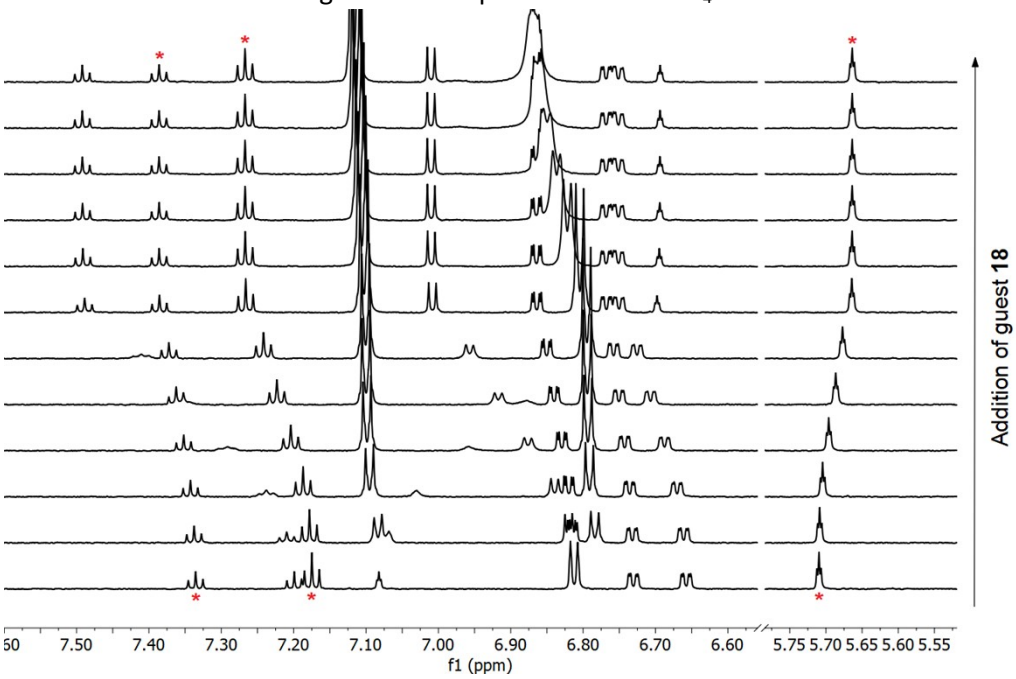

Figure S16. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.2 mM) titration with **18** at 298 K. On the figure are shown the 12 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **18** added to samples from 0.4 to 2.3 equivalents.

^{1}H NMR titration data of host **1** and guest **19** complex in methanol-d_4

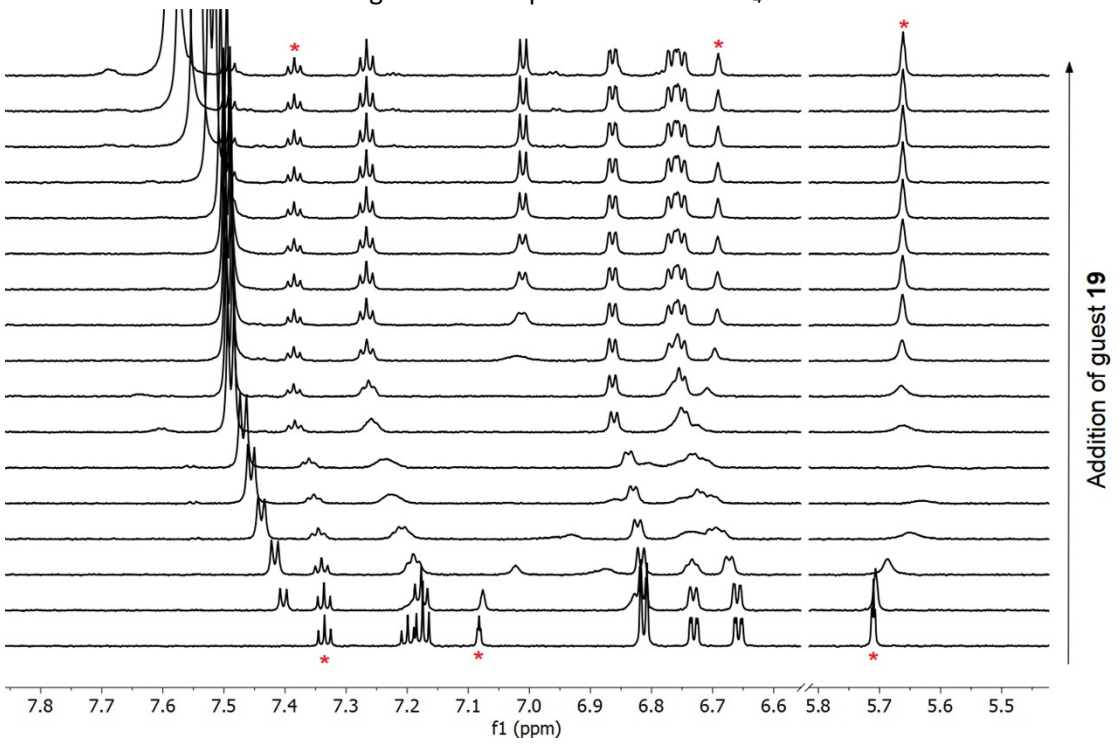

Figure S17. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.2 mM) titration with **19** at 298 K. On the figure are shown the 17 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **19** added to samples from 0.3 to 10.3 equivalents.

^{1}H NMR titration data of host **1** and guest **20** complex in methanol-d_4

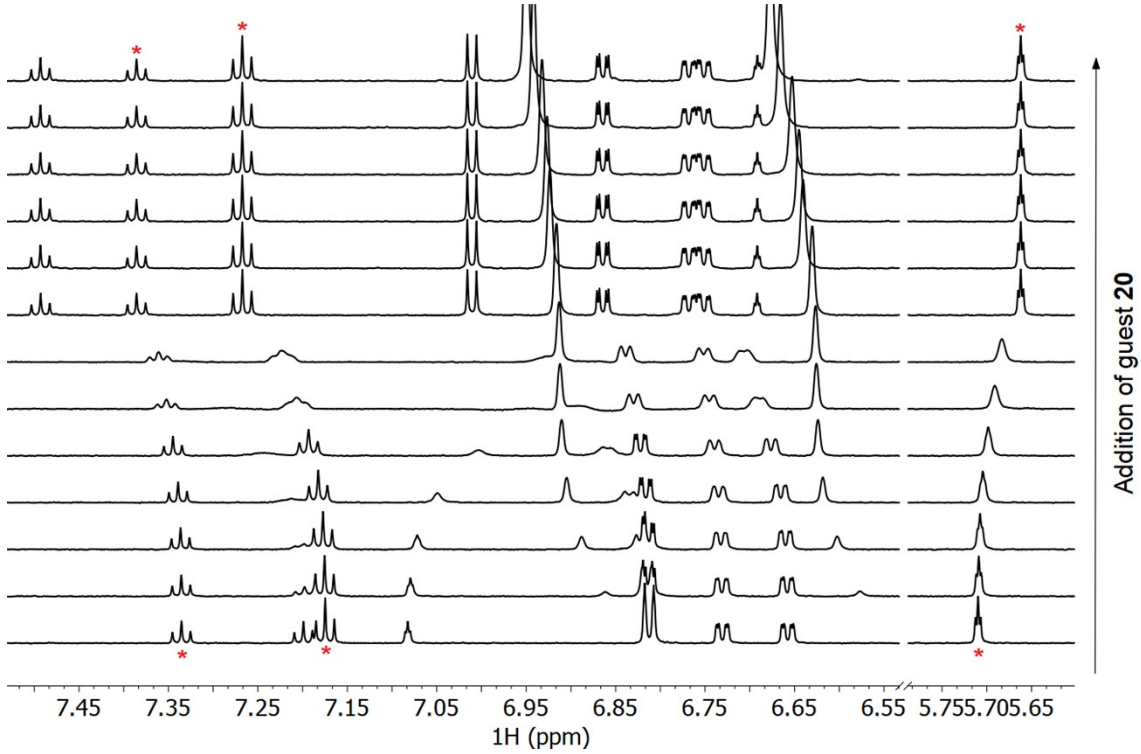

Figure S18. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.2 mM) titration with **20** at 298 K. On the figure are shown the 13 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **20** added to samples from 0.2 to 5.8 equivalents.

^{1}H NMR titration data of host **1** and guest **21** complex in methanol-d_4

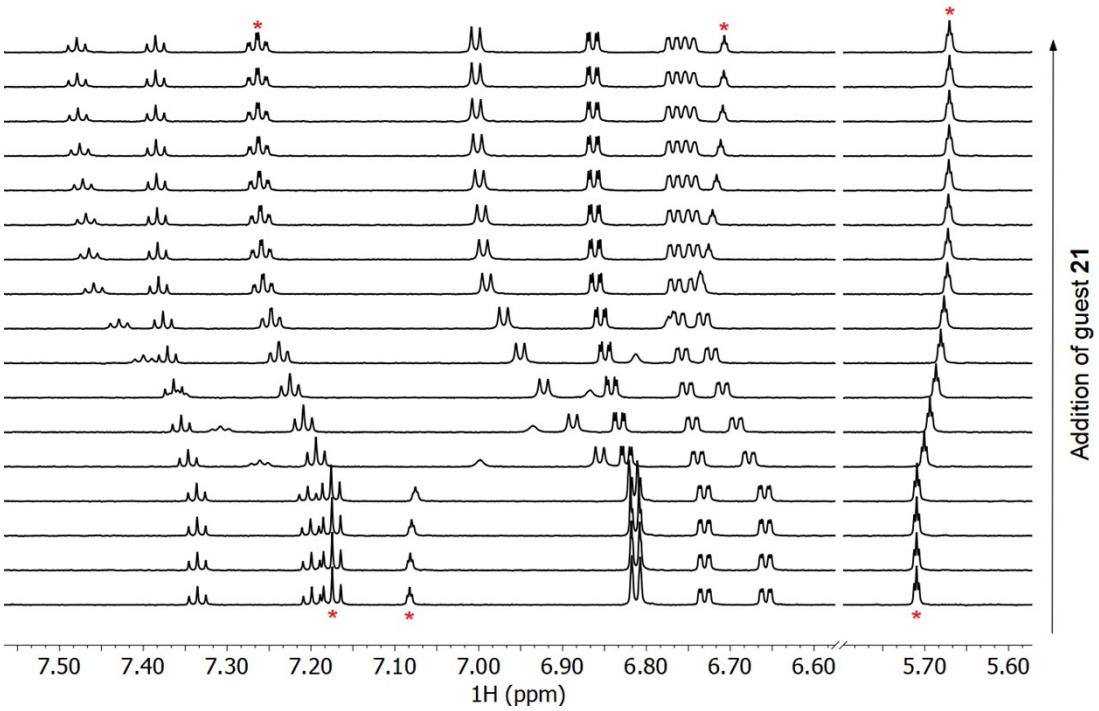

Figure S19. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of **1** (0.2 mM) titration with **21** at 298 K. On the figure are shown the 17 titration points representing all the macrocycles´ peaks with followed protons marked with asterisk (*). Guest **21** added to samples from 0.2 to 7.6 equivalents.

^{1}H NMR titration data of 2,6-dimethoxybenzoic acid and guest **2** complex in methanol-d_4

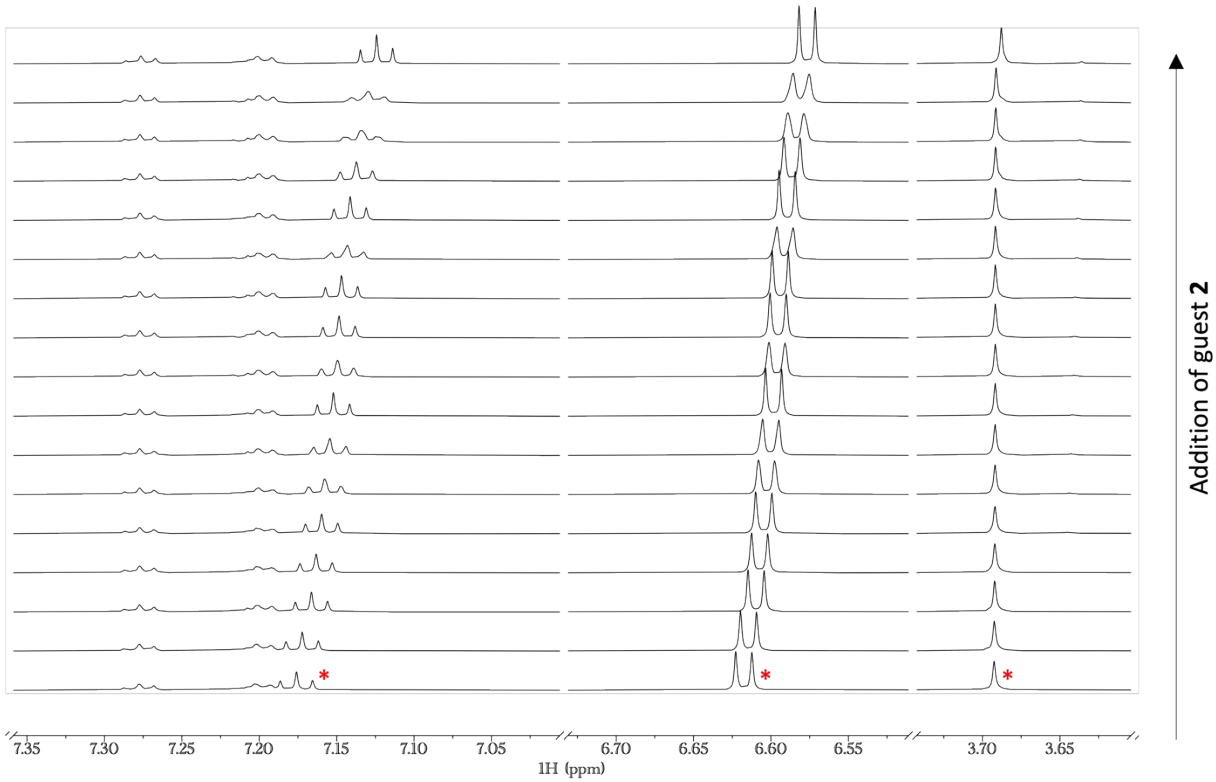

Figure S20. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of 2,6-dimethoxybenzoic acid (0.7 mM) titration with **2** at 298 K. On the figure are shown the 17 titration points representing all the 2,6-dimethoxybenzoic acid peaks with followed protons marked with asterisk (*). Guest **2** concentration (M) in samples 0, 0.0013, 0.0026, 0.0040, 0.0065, 0.0091, 0.0122, 0.0147, 0.0165, 0.0204, 0.0257, 0.0342, 0.0423, 0.0592, 0.0752, 0.1140, 0.1464. The results of the K_a determination based on 15 titration points and 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

^{1}H NMR titration data of host 2,6-dimethoxybenzoic acid and guest **11** **c**omplex in methanol-d_4

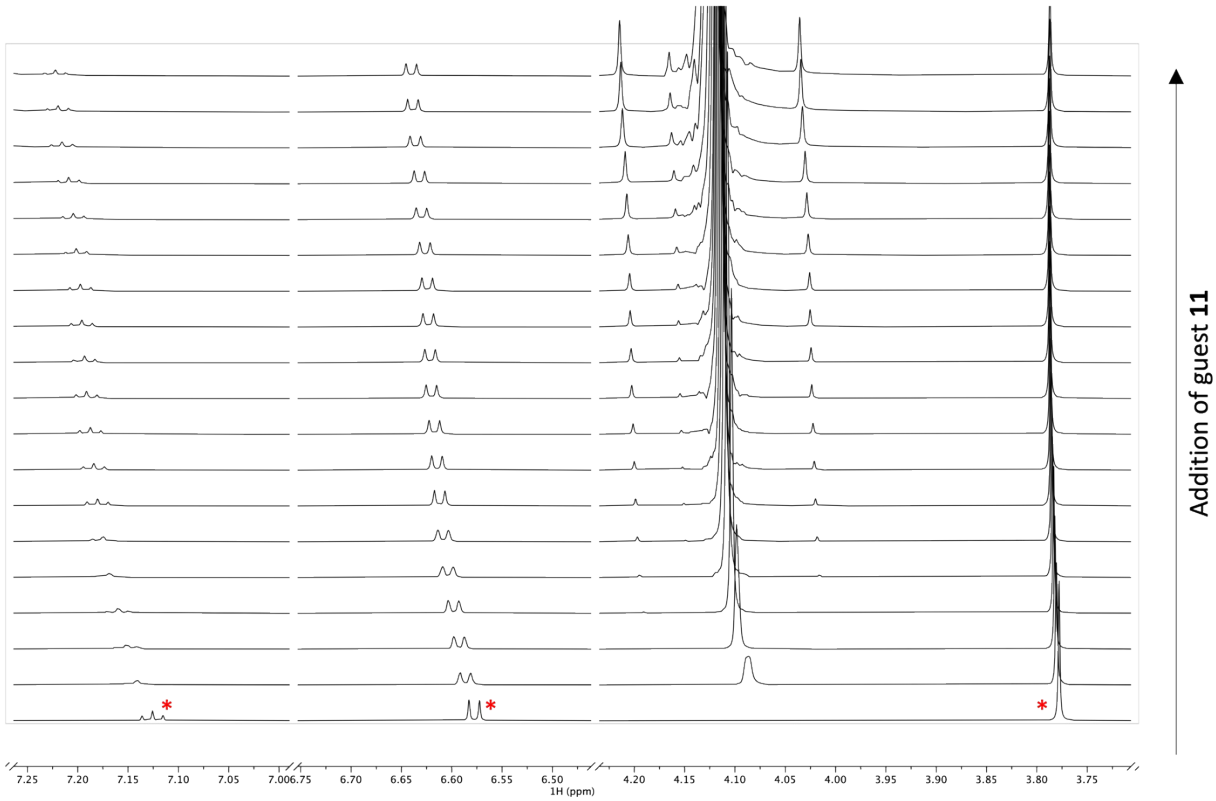

Figure S21. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of 2,6-dimethoxybenzoic acid (0.7 mM) titration with **11** at 298 K. On the figure are shown the 19 titration points representing all the 2,6-dimethoxybenzoic acid peaks with followed protons marked with asterisk (*). Guest **11** concentration (M) in samples 0, 0.0013, 0.0026, 0.0040, 0.0065, 0.0091, 0.0122, 0.0147, 0.0165, 0.0204, 0.0257, 0.0342, 0.0423, 0.0592, 0.0752, 0.1140, 0.1464. The results of the K_a determination based on 14 titration points 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

^{1}H NMR titration data of host 2,6-dimethoxybenzoic acid and guest **12** complex in methanol-d_4

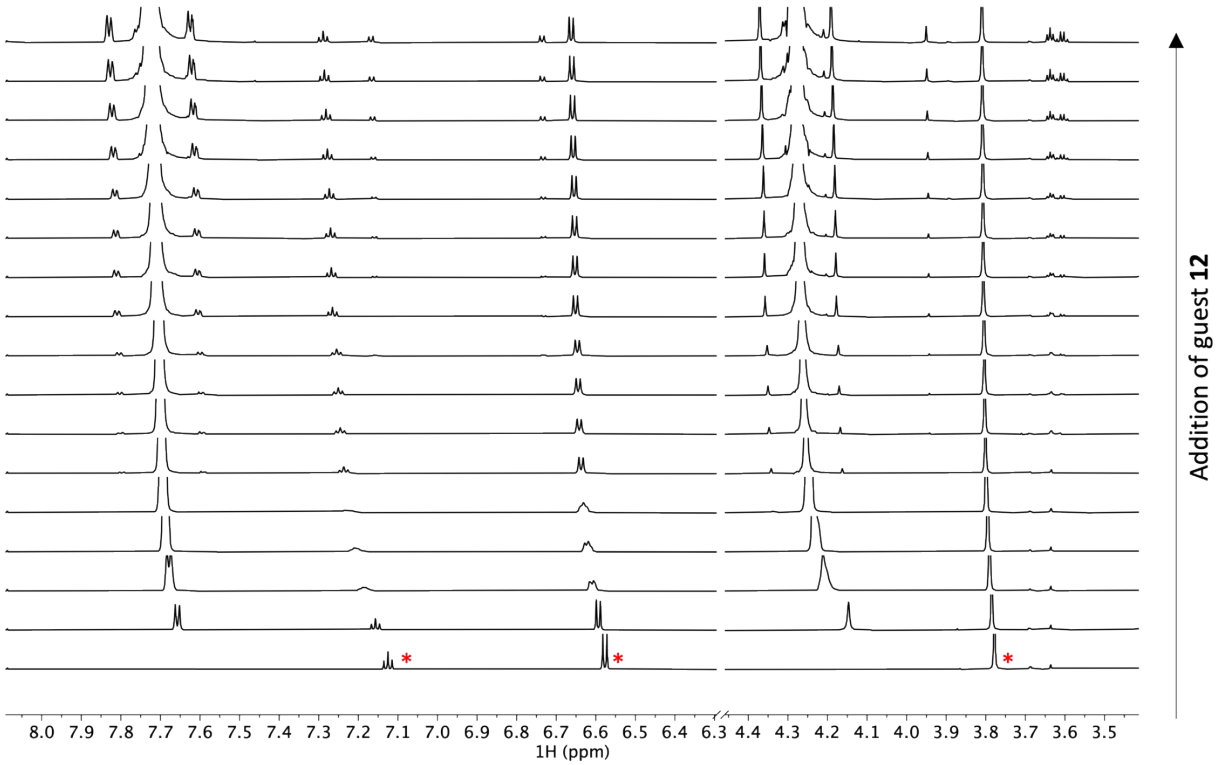

Figure S22. ^{1}H NMR (methanol-d_4, 800.13 MHz) spectra of 2,6-dimethoxybenzoic acid (0.7 mM) titration with 12 at 298 K. On the figure are shown the 17 titration points representing all the 2,6-dimethoxybenzoic acid peaks with followed protons marked with asterisk (*). Guest **12** concentration (M) in samples 0, 0.0013, 0.0026, 0.0040, 0.0065, 0.0091, 0.0122, 0.0147, 0.0165, 0.0204, 0.0257, 0.0342, 0.0423, 0.0592, 0.0752, 0.1140, 0.1464. The results of the K_a determination based on 14 titration points 1:2 binding model of Bindfit are accessible at the following link: Bindfit 1:2 model results

ESI-MS

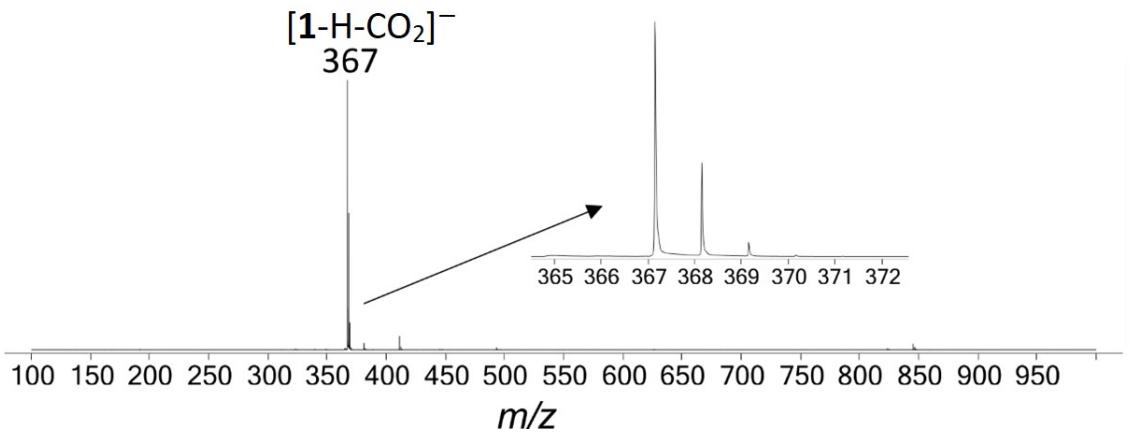

Figure S23. (−)ESI-MS spectrum of host **1** in acetonitrile. Inset shows zoomed view for isotopic distribution.

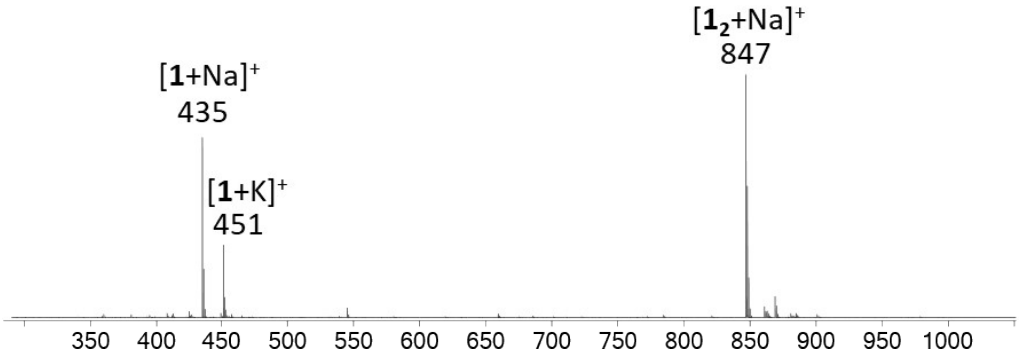

Figure S24. (+)ESI-MS spectrum of host **1** in acetonitrile.

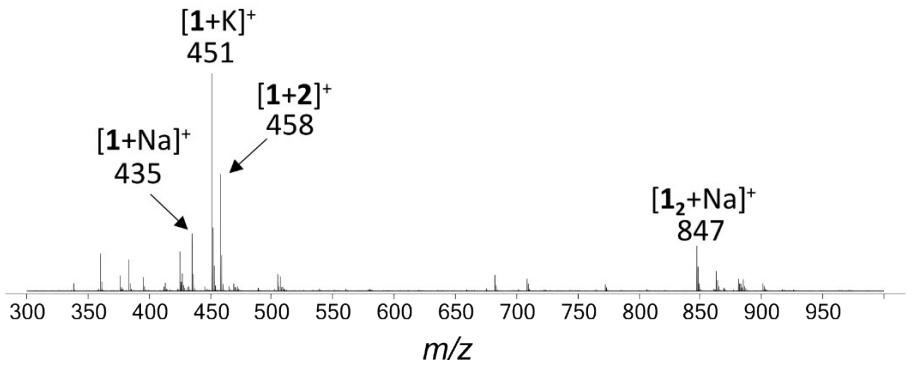

Figure S25. (+)ESI-MS spectrum 1:1 mixture of host **1** with guest **2**.

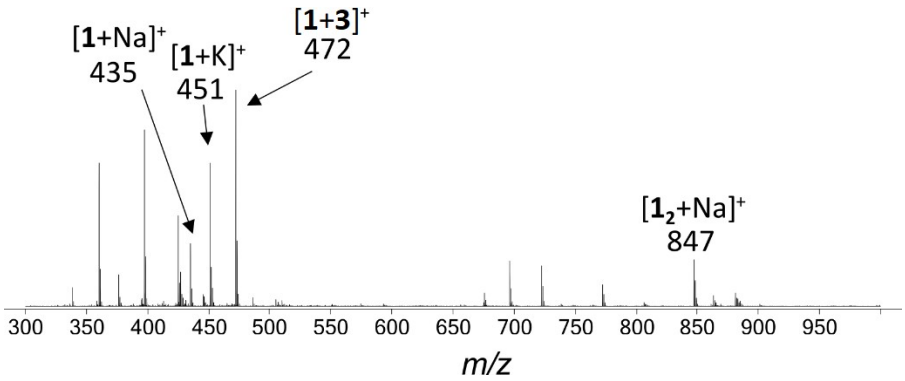

Figure S26. (+)ESI-MS spectrum 1:1 mixture of host **1** with guest **3**.

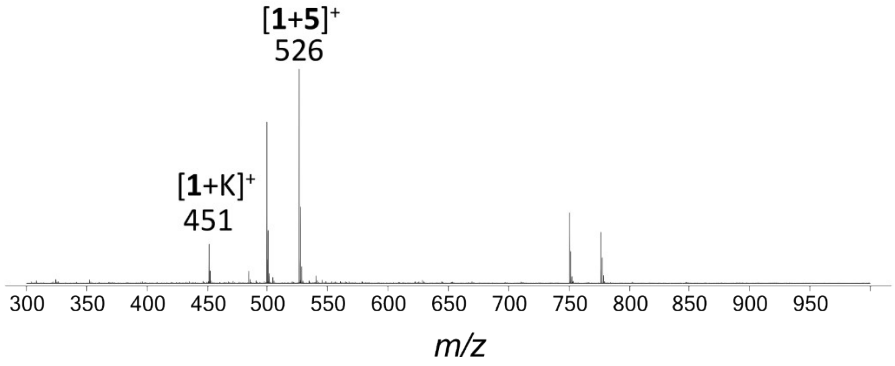

Figure S27. (+)ESI-MS spectrum 1:1 mixture of host **1** with guest **5**.

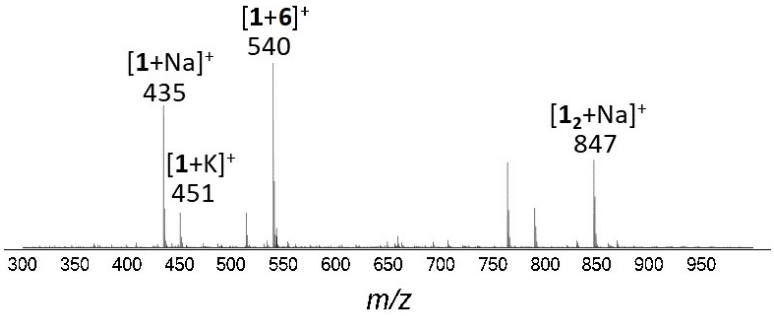

Figure S28. (+)ESI-MS spectrum 1:1 mixture of host **1** with guest **6**.

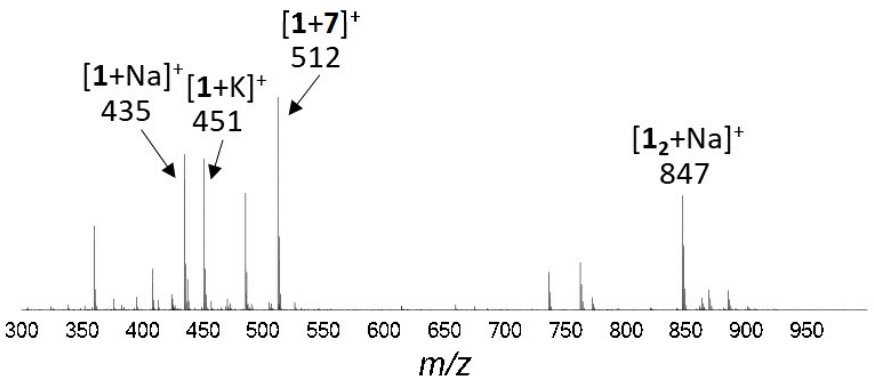

Figure S29. (+)ESI-MS spectrum 1:1 mixture of host **1** with guest **7**.

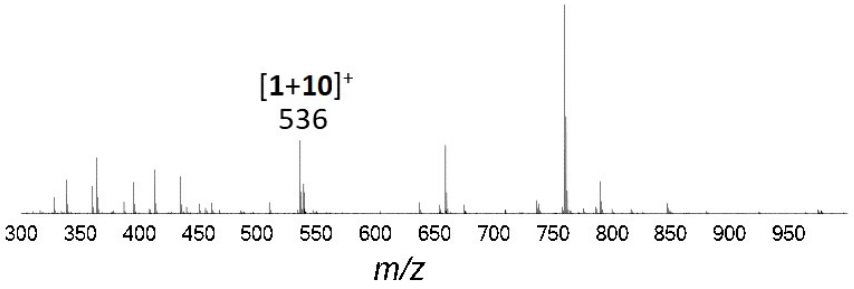

Figure S30. (+)ESI-MS spectrum 1:1 mixture of host **1** with guest **10**.

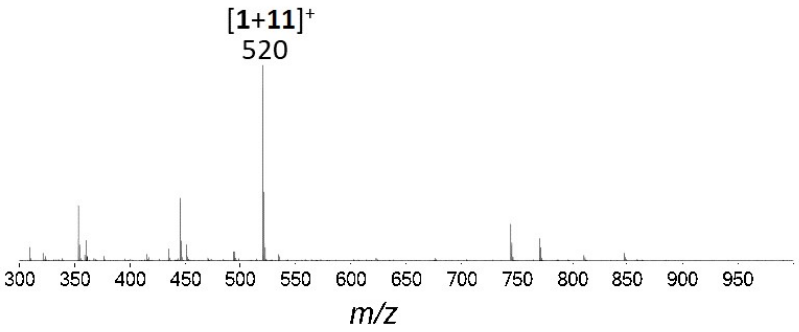

Figure S31. (+)ESI-MS spectrum 1:1 mixture of host **1** with guest **11**.

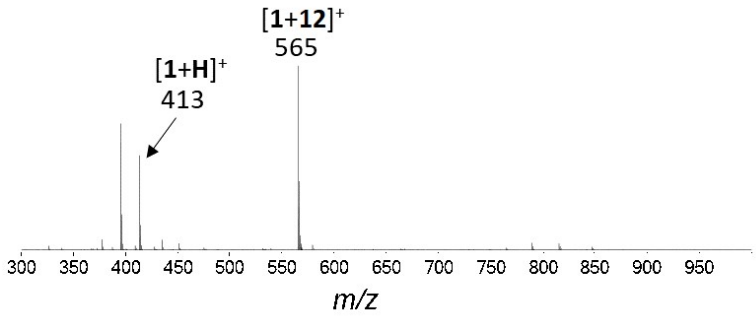

Figure S32. (+)ESI-MS spectrum 1:1 mixture of host **1** with guest **12**.

Ion mobility mass spectrometry

Figure 4 shows that all the ions of the complexes have drift times slightly longer than the free host, evidencing that the ammonium guests are located outside the oxacalixarene cavity with only the ammonium unit connected to the macrocycle's binding site. In the [**1**+Na]$^+$ drift spectrum the second ion with longer drift time belongs to [$\mathbf{1_2}$+Na]$^+$ complex that appears due to the post-drift tube fragmentation. This is evidenced by the $\mathbf{1_2}$ dimers drift time that is 35.08 ms, whereas in the [**1**+Na]$^+$ drift spectrum the second ions drift time is 34.89 ms. In [**1**+**12**]$^+$ drift spectrum the second less abundant ion population with longer drift time likely belongs to [$\mathbf{1_2}$+**12**]$^+$ ion, where two macrocycles are interacting with the guest with one interaction taking place due to hydrogen bonding and the other with the nitro group.

Table S2. (+)ESI-MS detected ions of [**1** + guest]$^+$ 1:1 complexes in acetonitrile with their corresponding CCS values.

ion	m/z$_{exp}$	*m/z*$_{theor}$	Δ*m/z* (mDa)	Experimental $^{DT}CCS_{N2}$ (Å^2)	Theoretical $^{TMLJ}CCS_{N2}$ (Å^2)[a]	Δ*CCS (%)*
[**1**+Na]$^+$	435.0837	435.0839	0.20	196.9	178.3[c]	9.4
[**1**+**2**]$^+$	458.1604	458.1598	0.60	202.1	192.1	4.9
[**1**+**3**]$^+$	472.1757	472.1755	0.20	205.0	199.4	2.7
[**1**+**5**]$^+$	526.2228	526.2224	0.40	218.1	-	-
[**1**+**6**]$^+$	540.2367	540.2381	-1.40	221.5	-	-
[**1**+**7**]$^+$	512.2073	512.2068	0.50	214.5	-	-
[**1**+**10**]$^+$	536.1687	536.1704	1.70	212.7	-	-
[**1**+**11**]$^+$	520.1762	520.1755	0.70	211.8	216.2	2.1
[**1**+**12**]$^+$	565.1590	565.1605	-1.50	216.9	211.5	2.5

[a] Theoretical $^{TMLJ}CCS_{N2}$ values calculated based on DFT calculated structures optimized at B97D/6-311+G(2d,p) level of theory. [b] Free host [**1**+Na]$^+$ ion *m/z* value and experimental $^{DT}CCS_{N2}$ value. [c] For reference is given theoretical $^{TMLJ}CCS_{N2}$ calculation of **1**, based on the coordinates obtained from the SCXRD analysis of the macrocycle.
Ions of cyclohexane containing guests (**5** and **6**) exhibited highest CCS values (218.1 Å and 221.5 Å) indicating a slightly different binding geometry from aromatic ammonium guests.

DFT calculations

The procedure for generating initial structures for sampling gas-phase PES of each single-charged host-guest pair of oxacalix[4]arene **1** with monoammonium guest species **2**, **3**, **11**, and **12** is based on multi-stage approach. The optimized geometry of the macrocycle was taken from the previous report.[3] Six structures of its complex, with randomly chosen positions of the sodium cation binding sites characterized by representative spatial locations either within or in close proximity to macrocycle cavity were generated and the full geometry optimizations were carried out in the gas phase for each structure at B3LYP/6-311+G(2d,p) level of theory. This sampling resulted in a preferential position of the Na^+ ion being located at the extension of O=C bond axis of carboxylic acid group towards the cavity with Boltzmann probability of 99%. Based on that finding, the starting structures of ammonium guest complexes were constructed with nitrogen atom always positioned at the same atomic coordinates as was established for Na^+ ion while for each complex, 5 to 10 alternative structures were considered with distinct variations in the terminal ring or chain orientation. Again, B3LYP/6-311+G(2d,p) method was chosen for geometry optimizations. The few representative low-energy structures of each complex were re-optimized using B97D[4]/6-311+G(2d,p)[5,6] level of theory with empirical dispersion corrections. Subsequently, the absence of imaginary eigenvalues was confirmed by vibrational normal mode analysis for each optimized structure using the same theoretical method. The reliability of theoretical procedure for obtaining these true minima structures of the complexes was confirmed by close match between experimental and theoretical CCS values.

The similar conformational sampling procedure starting from the variety of initial configurations was used for elucidating the lowest-energy structures of the charge-neutral ion pairs formed in methanol as a result of complexation of monoammonium guest species **8**, **11**, and **12** with carboxylate form of oxacalix[4]arene **1**, with one notable exception – all geometry optimizations and vibrational normal mode calculations were carried out at PCM/B97D/6-311+G(2d,p) level where the solvent effects were treated in the framework of polarized continuum approximation.

The DFT calculations were performed with the Gaussian 09[7] quantum chemistry suite.

Molecular Cartesian coordinates of the **[1+8]**$^{+}$ host-guest complex in MeOH (Å)

O	3.75591300	1.03934500	-0.04109600
O	1.38299000	-3.07474600	-1.01071600
O	2.45203800	-0.01724000	-2.75094300
O	0.53459400	-0.22617100	-1.56279900
O	-0.59072700	2.75014300	1.36035200
O	-2.42602200	-1.71905500	1.71697600
C	3.44494800	-0.28583200	0.22742400
C	2.51489100	-0.99279400	-0.55795100
C	2.26314000	-2.33143900	-0.22493200
C	1.83761700	-0.35538700	-1.74948600
C	2.71696600	1.96657800	-0.08690800
C	2.92772500	-2.96721900	0.82391100
H	2.70539300	-4.00895900	1.03981800
C	4.11539800	-0.90313800	1.28454600
H	4.81863200	-0.32033200	1.87383600
C	1.57075100	1.81870400	0.70268800
H	1.45437900	0.95734000	1.35199200
C	0.03639500	-3.07258300	-0.67564900
C	2.89286600	3.06688500	-0.92817200
H	3.79185400	3.14618900	-1.53339900
C	-0.89276500	1.60905300	2.10457900
C	-1.84914200	-2.38159000	0.64432100
C	-0.46966700	-2.36614400	0.41867200
H	0.18405800	-1.78507900	1.05911400
C	0.57027000	2.79227000	0.61541900
C	-1.40271700	0.47743100	1.46529800
H	-1.50338300	0.44657800	0.38525500
C	3.86309000	-2.24761200	1.57229600
H	4.38631600	-2.73081500	2.39418300
C	-0.80424300	-3.81367300	-1.51452900
H	-0.38363400	-4.35073800	-2.36093800
C	-1.80367000	-0.60169100	2.26272100
C	0.71555000	3.90308500	-0.22774600
H	-0.07839600	4.64357300	-0.27878700
C	-0.76305800	1.67889200	3.49352100
H	-0.35875300	2.57869900	3.95012500
C	1.88165000	4.03232800	-0.98476900
H	1.99874700	4.89110200	-1.64280000
C	-2.17584100	-3.83209100	-1.24659800
H	-2.83837600	-4.40258500	-1.89455800
C	-2.71403400	-3.11590700	-0.17337100
H	-3.78175400	-3.11086600	0.02825500
C	-1.16908500	0.58531600	4.26526700
H	-1.07634500	0.62402300	5.34848700
C	-1.68867700	-0.56072000	3.65556100
H	-2.01066200	-1.41723500	4.24260600
N	-1.13910900	0.91711300	-3.28028900
H	-1.38434400	0.24967800	-4.00777100
H	-0.81629000	1.77972100	-3.71110300
H	0.05255200	0.22154300	-2.35418400
C	-2.19448100	1.12568300	-2.34242800
C	-3.00693500	0.04744100	-1.95828700
C	-2.35505200	2.37300700	-1.72193300
C	-3.98819900	0.22868100	-0.98065100
H	-2.85684100	-0.93112000	-2.41088500
C	-3.33494000	2.54288300	-0.74029600
H	-1.70413200	3.19992400	-2.00012000

C	-4.15991600	1.47546300	-0.36730200
H	-4.60687400	-0.61594300	-0.68554400
H	-3.44460000	3.51284900	-0.25942500
H	-4.91710400	1.60917500	0.40237100

Molecular Cartesian coordinates of the **[1+11]**$^{+}$ host-guest complex in MeOH (Å)

O	2.73970800	2.44155900	-0.40326100
O	2.85263400	-2.34732400	-0.37517400
O	4.24625500	0.07018600	-2.42895200
O	2.02048200	0.00959200	-2.70495700
O	-1.79528400	2.35936100	1.43289100
O	-1.68896800	-2.44714000	1.44274300
C	3.02644600	1.24807800	0.27177000
C	2.99230700	0.05151900	-0.45746200
C	3.08347800	-1.13378200	0.28588200
C	3.08248400	0.04314700	-1.99384500
C	1.42441400	2.87949300	-0.33229400
C	3.35829300	-1.13823700	1.65329900
H	3.42738500	-2.08707700	2.17943500
C	3.29953300	1.28128600	1.63941000
H	3.32248100	2.23835000	2.15454400
C	0.48082200	2.31756000	0.54503500
H	0.75481000	1.51004400	1.21288600
C	1.55187600	-2.82993600	-0.31886900
C	1.07280700	3.93562100	-1.17991900
H	1.81225900	4.35007000	-1.85996200
C	-1.53100200	1.16169900	2.10241200
C	-0.69702200	-2.87981300	0.57607100
C	0.58925300	-2.31884300	0.56845100
H	0.83688600	-1.51852900	1.25532000
C	-0.82156900	2.83929300	0.57127500
C	-1.76774100	-0.04463300	1.44237500
H	-2.17580800	-0.05588500	0.43762000
C	3.49714900	0.07964600	2.32635500
H	3.71346400	0.09101000	3.39184200
C	1.23668000	-3.87806800	-1.19039600
H	1.99032900	-4.25242200	-1.87804800
C	-1.47836200	-1.23645300	2.10806100
C	-1.19348200	3.89457400	-0.26938300
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C	-1.05243600	1.19313200	3.41284100
H	-0.87252400	2.14873300	3.89842000
C	-0.23497700	4.42954800	-1.13546800
H	-0.51579700	5.24582900	-1.79785600
C	-0.05482600	-4.41421600	-1.16160600
H	-0.30792400	-5.22360500	-1.84334100
C	-1.03297400	-3.92756700	-0.28891200
H	-2.03737200	-4.34177900	-0.27247400
C	-0.80139500	-0.01739100	4.06980100
H	-0.42757800	-0.00680200	5.09105500
C	-0.99975600	-1.24090300	3.41872700
H	-0.77867200	-2.18544200	3.90892300
N	-0.28722400	-0.02440100	-1.63903300
H	0.75672800	-0.01031500	-2.08287900
H	-0.38108400	0.80001900	-1.03580200
H	-0.36109400	-0.85119800	-1.03697800

C	-1.36218300	-0.03523700	-2.69359100
H	-1.19386900	-0.92718600	-3.30374500
H	-1.20733000	0.85670900	-3.30737600
C	-2.72225200	-0.04399700	-2.04386000
C	-3.33611700	1.16404100	-1.68067900
C	-3.32556200	-1.25987000	-1.68920300
C	-4.53360700	1.15689400	-0.95914100
H	-2.86357600	2.10839200	-1.94571700
C	-4.52315100	-1.26813800	-0.96761700
H	-2.84453500	-2.19793200	-1.96137900
C	-5.12594800	-0.05944800	-0.59776800
H	-4.99852800	2.09797100	-0.67232300
H	-4.98027700	-2.21510300	-0.68771200
H	-6.05399400	-0.06541800	-0.02939400

Molecular Cartesian coordinates of the **[1+12]**$^{+}$ host-guest complex in MeOH (Å)

O	3.19981900	2.45778200	-0.27559000
O	3.38887200	-2.32376200	-0.21374300
O	4.89288300	0.11326900	-2.17387100
O	2.72255800	0.00016100	-2.64381600
O	-1.42008500	2.33368000	1.33436700
O	-1.25043300	-2.47691500	1.33382100
C	3.46492400	1.27865900	0.42474900
C	3.49387800	0.07463100	-0.29284700
C	3.56194500	-1.10957700	0.45564600
C	3.72455300	0.06319500	-1.80355800
C	1.87497200	2.88514900	-0.26686800
C	3.75693700	-1.09998200	1.83621200
H	3.81138600	-2.04441400	2.37134200
C	3.65736200	1.31950800	1.80571300
H	3.63349300	2.27840000	2.31681300
C	0.89907300	2.32129500	0.57067200
H	1.14466800	1.52142400	1.25839000
C	2.08522500	-2.81377900	-0.24249000
C	1.55476600	3.92747400	-1.14270800
H	2.32194000	4.34276400	-1.79074600
C	-1.19269700	1.13421400	2.01377800
C	-0.20935000	-2.88505800	0.51468400
C	1.07633400	-2.33329000	0.60714300
H	1.27834800	-1.55041700	1.32802900
C	-0.40985600	2.82175600	0.52157700
C	-1.32594000	-0.07161800	1.32464100
H	-1.59928400	-0.08174800	0.27670100
C	3.83567800	0.12399700	2.50753600
H	3.98952000	0.14401400	3.58358900
C	1.82356800	-3.83044500	-1.16643100
H	2.61583100	-4.17985100	-1.82304900
C	-1.10834300	-1.26489700	2.01455700
C	-0.75245500	3.86552700	-0.34539800
H	-1.77386200	4.23554100	-0.36919000
C	-0.87246800	1.16316900	3.37171900
H	-0.77088100	2.11771500	3.88145700
C	0.24073700	4.40604000	-1.16766000
H	-0.01678900	5.21270000	-1.85092100
C	0.53219300	-4.36363100	-1.23278500
H	0.31871700	-5.14791400	-1.95605800

C	-0.49513900	-3.90106600	-0.40457900
H	-1.50022400	-4.30991000	-0.46327900
C	-0.68230500	-0.04840900	4.04715900
H	-0.43301900	-0.03932700	5.10576400
C	-0.78841400	-1.27092500	3.37272600
H	-0.62113100	-2.21576500	3.88321400
N	0.35321000	-0.06206300	-1.71784600
H	1.73021800	-0.02847900	-2.19228000
H	0.22034400	0.72503000	-1.07922000
H	0.22427400	-0.91160800	-1.16505000
C	-0.66156800	-0.00680000	-2.80912500
H	-0.49697400	-0.87174000	-3.45984800
H	-0.48314800	0.90737400	-3.38451500
C	-2.05619100	-0.01905700	-2.22798800
C	-2.67755000	1.18619800	-1.86367900
C	-2.67712100	-1.23839500	-1.91029100
C	-3.88335700	1.18286600	-1.16667600
H	-2.19669900	2.13265200	-2.09966600
C	-3.88373900	-1.26206400	-1.21532300
H	-2.19760400	-2.17536300	-2.18457100
C	-4.46785800	-0.04617200	-0.84337400
H	-4.35925300	2.10964300	-0.86469000
H	-4.36109600	-2.19969700	-0.95137000
N	-5.73355700	-0.06113500	-0.07836900
O	-6.24319900	-1.15599300	0.18472500
O	-6.22080000	1.02181200	0.26438900

Molecular Cartesian coordinates of the **[1+2]**$^{+}$ host-guest complex (Å)

O	3.17400000	-1.75000000	0.78200000
O	-1.63500000	-1.91900000	1.50800000
O	1.33000000	-3.28900000	-0.71800000
H	1.16700000	-3.47900000	-1.66000000
O	-0.34200000	-1.84500000	-1.10300000
O	2.13300000	2.28300000	-1.75600000
O	-2.15700000	2.79300000	0.37600000
C	2.05600000	-1.65700000	1.57500000
C	0.74900000	-1.86800000	1.06400000
C	-0.33100000	-1.70200000	1.95200000
C	0.51100000	-2.29500000	-0.34300000
C	3.25200000	-0.95500000	-0.36200000
C	-0.13800000	-1.39500000	3.29600000
H	-1.00500000	-1.29800000	3.94500000
C	2.25600000	-1.34300000	2.91900000
H	3.27300000	-1.18200000	3.26800000
C	2.59700000	0.28100000	-0.43100000
H	2.01100000	0.64100000	0.40700000
C	-2.37700000	-0.81500000	1.15100000
C	4.04600000	-1.42500000	-1.40600000
H	4.54700000	-2.38500000	-1.31300000
C	1.36500000	2.77900000	-0.70900000
C	-2.62400000	1.51700000	0.56300000
C	-1.80800000	0.45400000	0.98000000
H	-0.75300000	0.61600000	1.16300000
C	2.74200000	1.05000000	-1.59200000
C	0.00100000	2.48900000	-0.68100000
H	-0.43600000	1.86200000	-1.45300000

C	1.16200000	-1.23000000	3.77900000
H	1.32200000	-0.99200000	4.82800000
C	-3.74400000	-1.03600000	0.92800000
H	-4.16200000	-2.02400000	1.09600000
C	-0.77600000	3.02000000	0.35100000
C	3.52800000	0.60100000	-2.66000000
H	3.63000000	1.22100000	-3.54700000
C	1.95300000	3.58800000	0.26600000
H	3.01800000	3.79800000	0.21500000
C	4.17800000	-0.63000000	-2.55000000
H	4.79900000	-0.97800000	-3.37300000
C	-4.54000000	0.04100000	0.52400000
H	-5.60500000	-0.11200000	0.36600000
C	-3.99400000	1.31600000	0.31800000
H	-4.61100000	2.15700000	0.01400000
C	1.15000000	4.11700000	1.28100000
H	1.59500000	4.75700000	2.04000000
C	-0.21900000	3.83200000	1.33700000
H	-0.85300000	4.23600000	2.12200000
N	-2.53400000	-0.52700000	-2.05700000
H	-1.69400000	-0.87900000	-1.54100000
H	-2.22300000	0.04800000	-2.84400000
H	-3.08300000	0.07100000	-1.41900000
C	-3.37600000	-1.68800000	-2.54200000
C	-4.62400000	-1.18400000	-3.25500000
H	-3.61500000	-2.26400000	-1.64500000
H	-2.73200000	-2.28800000	-3.19200000
H	-5.22300000	-2.03900000	-3.58700000
H	-5.24000000	-0.57400000	-2.58300000
H	-4.36600000	-0.58800000	-4.14100000

Molecular Cartesian coordinates of the **[1+3]**$^{+}$ host-guest complex (Å)

O	3.19600000	-1.96600000	0.88700000
O	-1.42500000	-1.15200000	2.17600000
O	0.94900000	-3.46400000	0.02700000
H	0.62300000	-3.82500000	-0.81800000
O	-0.53800000	-1.87300000	-0.50900000
O	2.34700000	1.50800000	-2.42800000
O	-1.46200000	3.20300000	-0.01200000
C	2.23400000	-1.51000000	1.75600000
C	0.84800000	-1.60500000	1.46400000
C	-0.05200000	-1.06500000	2.40200000
C	0.34500000	-2.28500000	0.23800000
C	3.20800000	-1.47400000	-0.41800000
C	0.38100000	-0.50400000	3.60000000
H	-0.35600000	-0.12000000	4.30000000
C	2.67500000	-0.94400000	2.95100000
H	3.74500000	-0.88300000	3.13200000
C	2.72700000	-0.19300000	-0.71300000
H	2.32800000	0.44100000	0.07200000
C	-2.05500000	-0.04500000	1.65000000
C	3.76400000	-2.29500000	-1.39800000
H	4.13600000	-3.27900000	-1.13000000
C	1.82000000	2.35000000	-1.45500000
C	-2.06500000	2.10100000	0.53900000
C	-1.35000000	1.03600000	1.10500000

H	-0.26600000	1.04900000	1.11400000
C	2.79800000	0.25900000	-2.03600000
C	0.44900000	2.30800000	-1.20200000
H	-0.18100000	1.60600000	-1.74000000
C	1.75000000	-0.45800000	3.87700000
H	2.09800000	-0.02400000	4.81100000
C	-3.45700000	-0.07100000	1.65400000
H	-3.97700000	-0.91000000	2.10900000
C	-0.08300000	3.18100000	-0.25000000
C	3.34500000	-0.54500000	-3.04400000
H	3.39500000	-0.16700000	-4.06200000
C	2.65400000	3.24700000	-0.78400000
H	3.71800000	3.25700000	-1.00500000
C	3.82900000	-1.81100000	-2.71000000
H	4.26400000	-2.43600000	-3.48700000
C	-4.14900000	1.00600000	1.09300000
H	-5.23700000	1.00700000	1.10600000
C	-3.47200000	2.08800000	0.51600000
H	-4.00600000	2.93200000	0.08800000
C	2.09400000	4.11900000	0.15500000
H	2.73200000	4.82900000	0.67800000
C	0.72300000	4.08900000	0.43500000
H	0.27600000	4.76100000	1.16300000
N	-2.67200000	-0.47000000	-1.48600000
H	-1.81000000	-0.82800000	-1.01200000
H	-2.42700000	-0.16100000	-2.43000000
H	-3.02000000	0.34700000	-0.96000000
C	-3.73200000	-1.54800000	-1.53500000
C	-5.01700000	-1.02000000	-2.16300000
H	-3.88300000	-1.85700000	-0.49700000
H	-3.30800000	-2.38500000	-2.09800000
H	-5.36200000	-0.14600000	-1.59100000
H	-4.81100000	-0.67700000	-3.18900000
C	-6.10500000	-2.10500000	-2.18000000
H	-6.33900000	-2.44000000	-1.16100000
H	-7.02500000	-1.71800000	-2.63200000
H	-5.78100000	-2.97800000	-2.76200000

Molecular Cartesian coordinates of the **[1+11]**$^{+}$ host-guest complex (Å)

O	3.98200000	0.93100000	-1.64900000
O	-0.06600000	-1.65300000	-2.43200000
O	1.61700000	1.88500000	-2.89600000
H	1.06200000	2.68500000	-2.84000000
O	0.00200000	1.12200000	-1.53800000
O	2.07700000	1.57900000	2.79300000
O	-0.84600000	-2.22500000	2.34500000
C	3.31100000	-0.24800000	-1.87100000
C	1.90400000	-0.29200000	-2.05400000
C	1.31000000	-1.55600000	-2.22800000
C	1.07600000	0.94500000	-2.10700000
C	3.58900000	1.73300000	-0.57800000
C	2.06600000	-2.72400000	-2.27600000
H	1.56000000	-3.67300000	-2.43200000
C	4.07300000	-1.41500000	-1.91100000
H	5.14600000	-1.33900000	-1.75800000
C	3.00600000	1.17900000	0.56700000

H	2.84300000	0.10900000	0.63900000
C	-0.85100000	-1.96300000	-1.34200000
C	3.84700000	3.09900000	-0.68400000
H	4.31000000	3.49300000	-1.58400000
C	1.85600000	0.21300000	2.92900000
C	-1.23700000	-2.22000000	1.03000000
C	-0.36200000	-1.93800000	-0.02900000
H	0.67700000	-1.70200000	0.16900000
C	2.66300000	2.03200000	1.62300000
C	0.62800000	-0.31100000	2.52300000
H	-0.12100000	0.34100000	2.08500000
C	3.45200000	-2.64700000	-2.13000000
H	4.05100000	-3.55400000	-2.16800000
C	-2.19000000	-2.27600000	-1.61300000
H	-2.53500000	-2.31000000	-2.64300000
C	0.39400000	-1.67700000	2.69200000
C	2.90300000	3.40900000	1.54300000
H	2.63500000	4.04800000	2.38000000
C	2.83600000	-0.59900000	3.50200000
H	3.78200000	-0.16100000	3.80900000
C	3.50100000	3.92500000	0.39200000
H	3.70100000	4.99300000	0.32900000
C	-3.04000000	-2.56700000	-0.54200000
H	-4.07700000	-2.83000000	-0.73800000
C	-2.58700000	-2.52600000	0.78300000
H	-3.24400000	-2.75600000	1.61700000
C	2.57200000	-1.96200000	3.67200000
H	3.32500000	-2.60300000	4.12500000
C	1.35200000	-2.51400000	3.26200000
H	1.13600000	-3.57100000	3.38800000
N	-2.32500000	0.67000000	-0.16500000
H	-1.36500000	0.63800000	-0.57700000
H	-2.31900000	1.26500000	0.66700000
H	-2.59800000	-0.28200000	0.12800000
C	-3.32500000	1.21200000	-1.18200000
H	-3.28800000	0.51400000	-2.02200000
H	-2.93300000	2.18400000	-1.49800000
C	-4.69200000	1.31000000	-0.56700000
C	-5.04500000	2.44200000	0.18300000
C	-5.60400000	0.25200000	-0.69700000
C	-6.29400000	2.51200000	0.80500000
H	-4.35000000	3.27900000	0.26500000
C	-6.85500000	0.32400000	-0.07900000
H	-5.33600000	-0.62000000	-1.29200000
C	-7.19800000	1.45200000	0.67600000
H	-6.56700000	3.39600000	1.37800000
H	-7.56400000	-0.49400000	-0.19000000
H	-8.17400000	1.50900000	1.15400000

Molecular Cartesian coordinates of the **[1+12]**$^{+}$ host-guest complex (Å)

O	-1.75475600	-3.67627500	-0.23395800
O	-3.75231000	0.74370800	-0.59135100
O	-2.13525200	-2.27186100	-2.62247200
H	-1.63910400	-2.07030200	-3.43670600
O	-1.46346800	-0.18670100	-2.14530300
O	2.31096300	-1.35861800	1.13995900
O	-0.06159800	2.79042300	1.84599400

C	-2.58738300	-2.67646100	0.20830300
C	-2.72010400	-1.45134700	-0.49617100
C	-3.56261600	-0.47143200	0.06377600
C	-2.03868600	-1.21648200	-1.80036800
C	-0.38924800	-3.41340100	-0.32228500
C	-4.28194000	-0.70070000	1.23378800
H	-4.93345900	0.08225500	1.61219200
C	-3.29891400	-2.90991100	1.38387600
H	-3.15828200	-3.85871800	1.89435700
C	0.22065400	-2.43293800	0.47029600
H	-0.36143900	-1.83752700	1.16570500
C	-3.02018300	1.82340900	-0.14534400
C	0.34630600	-4.21843900	-1.19231200
H	-0.16106500	-4.97434900	-1.78506400
C	1.62515000	-0.48505700	1.97641400
C	-1.16717900	2.82053300	1.04027100
C	-1.90539400	1.68034700	0.69117800
H	-1.60926500	0.70442000	1.05711500
C	1.60829000	-2.27478700	0.38162500
C	1.02174000	0.65416300	1.43827600
H	1.02827700	0.82520300	0.36714000
C	-4.15669900	-1.92890100	1.88560400
H	-4.71677400	-2.11593000	2.79884400
C	-3.42461500	3.08115900	-0.61668900
H	-4.31464700	3.16206400	-1.23541300
C	0.44406500	1.57129300	2.31862300
C	2.37581200	-3.07529200	-0.47445900
H	3.45425200	-2.94450400	-0.50034800
C	1.64133600	-0.72201500	3.35133300
H	2.13033400	-1.61441200	3.73266700
C	1.73294500	-4.04084300	-1.25150100
H	2.32373800	-4.67248300	-1.91163500
C	-2.68023500	4.20551900	-0.24483900
H	-2.99385600	5.19064800	-0.58464500
C	-1.54009500	4.09070200	0.55998600
H	-0.96712100	4.96318600	0.86264500
C	1.04651200	0.20986800	4.20716100
H	1.06100100	0.04118400	5.28135700
C	0.44210400	1.36388700	3.69716500
H	-0.00850500	2.10607000	4.35075500
N	-0.82388400	2.48467300	-2.27244300
H	-1.60996300	2.90389800	-2.77639900
H	-1.06004800	1.47868200	-2.09863400
H	-0.77938200	2.95812100	-1.35651400
C	0.48816500	2.63258300	-3.02462500
H	0.64730400	3.70555800	-3.17129600
H	0.34504100	2.14994600	-3.99567500
C	1.60813700	1.99733500	-2.24353600
C	1.94107300	0.65388000	-2.47081700
C	2.30752900	2.73633600	-1.27708800
C	2.97484600	0.05338400	-1.75546000
H	1.39550400	0.07681800	-3.21444800
C	3.32465000	2.13755000	-0.53257100
H	2.06138000	3.78289900	-1.10345100
C	3.64452300	0.80456800	-0.79076800
H	3.25039300	-0.98129700	-1.92337900
H	3.86538700	2.68341600	0.23405600
N	4.72877500	0.15125300	0.00464300

O	5.08936700	0.71968900	1.03155500
O	5.17865300	-0.90878600	-0.42463600

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