

Supporting Information

Recognition of Hydrophilic Molecules in Deep Cavitand Hosts with Water-mediated Hydrogen Bonds

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Table of Contents	Error! Bookmark not defined.
1. Materials and Methods	2
2. Water solubility of guest molecules	2
3. Experimental procedures and characterization data	3
3.1 Scheme of the synthesis of water soluble Cavitand 1a	3
3.2 Synthesis and characterization of water soluble Cavitand 1a	3
3.3 Scheme of the synthesis of water soluble cavitand 1b	5
3.4 Synthesis and characterization of water soluble Cavitand 1b	6
4. ¹H NMR, ¹³C NMR spectrum and HR-MS spectrum of cavitands	7
5. ¹H NMR of the complexes and relative $\Delta\delta$ calculation for guests	14
5.1 Relevant guests used in cavitand 1a and 1b	14
5.2 ¹ H NMR for the complexation of cavitand 1a with guests.	16
5.3 ¹ H NMR for the complexation of cavitand 1b with guests.	31
5.4 Host-guest complexed of cavitand 1a and cycloalkane	47
6. Isothermal titration calorimetry (ITC) experiments of cavitand 1b	49
7. Computational details	53
8. Models with different numbers of water molecules	53

8.1. Binding of THF.....	55
8.2. Binding of cyclopentanone.	56
8.3. Binding of cyclopentanol.	59
8.4. Binding of 1,4-dioxane.	Error! Bookmark not defined.
8.5. Binding of 1,3-dioxane.	59
9. Non-covalent interaction plots	60
10. Cartesian coordinates	61
11. References.....	117

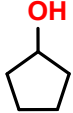
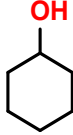
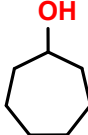
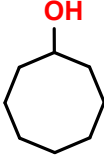
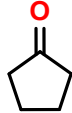
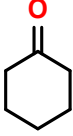
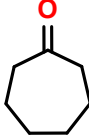
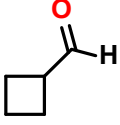
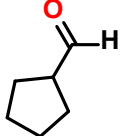
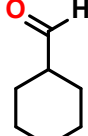
1. Materials and Methods

All commercially available compounds, purchased from TCI, Alfa, Energy chemical or Meryer were used without further purification. ^1H NMR, ^{13}C NMR spectra were recorded using Bruker AVANCE III HD 600 MHz spectrometer with cryoprobe at the temperatures indicated. NMR solvents were purchased from Cambridge Isotope Laboratories, Inc. Chemical shifts were reported in ppm using the residue solvent peaks: D_2O $\delta = 4.79$ ppm (^1H NMR); $\text{DMSO-}d_6$ $\delta = 2.50$ ppm (^1H NMR). Data were presented as follows: 1) Chemical shift, 2) multiplicity (s = single, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiple and/or multiple resonances, br = broadened signal, app = apparent splitting pattern), 3) coupling constant (J, in Hz), 4) integration. Positive ion high-resolution mass spectrometry analyses were performed on Bruker micrOTOF II machine.

2. Water solubility of guest molecules

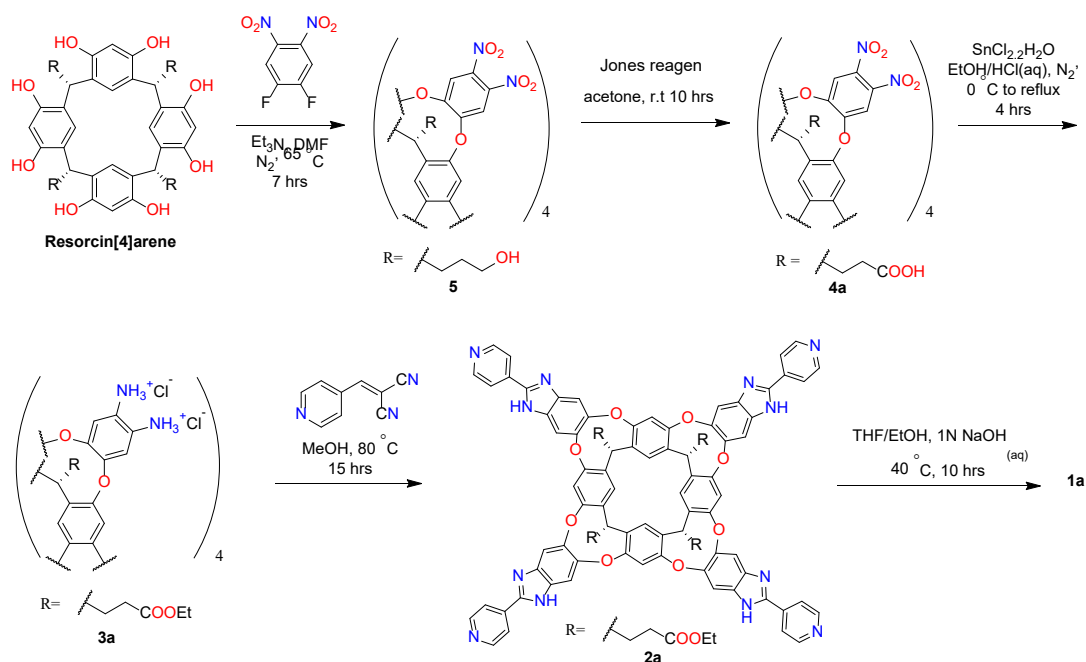
Table S1: structure and water solubility of the relevant guests in this article.

Compounds					
Water solubility	Miscible	80.2g/L	Miscible	Miscible	Unknown

Compounds					
Water solubility	Slightly soluble	40g/L	Immiscible	6.57g/L	9.2g/L
Compounds					
Water solubility	150g/L	Insoluble	Soluble	Soluble	Slightly soluble

3. Experimental procedures and characterization data

3.1 Scheme of the synthesis of water soluble Cavitand **1a**.



Scheme 1. Synthesis of water soluble cavitand **1a**.

3.2 Synthesis and characterization of water soluble cavitand **1a**

3.2.1 Synthesis of cavitand **5**

Synthesis of resorcin[4]arene and cavitand **5** followed the previously reported procedures.¹ The characterization data are in accordance with the previous report.

3.2.2 Synthesis of malononitrile ylide

2-(pyridin-4-ylmethylene)malononitrile was prepared based on the previously reported

procedure.² The characterization data are in accordance with the previous report.

3.2.3 Synthesis of cavitand **4a**

To a solution of cavitand **5** (500 mg, 0.36 mmol, 1 eq.) in acetone (80 mL) cooled to 0 °C, a small portion of Jones reagent (0.85 mL, 10 eq.) was added slowly with continuous stirring.³ The reaction mixture was warmed to room temperature and stirred for 10 hrs, then quenched by adding 2-propanol (20 mL) and filtered. The filtrate was concentrated under reduced pressure and the solid was washed thoroughly with acetone (3 × 50 mL) and MeOH (3 × 50 mL). Cavitand **4a** (450 mg, 83%) was obtained as a green solid. ¹H NMR (600 MHz, DMSO-*d*₆, δ ppm) 12.27 (s, 4H), 8.85 (s, 8H), 8.29 (s, 4H), 7.90 (s, 4H), 5.60 (s, 4H), 2.66 (s, 8H), 2.24 (s, 8H). ¹³C NMR (151 MHz, DMSO-*d*₆, δ ppm) 174.36, 155.55, 154.52, 140.25, 136.14, 126.45, 122.55, 116.93, 33.49, 32.45, 27.21. HRMS (ESI): Calcd for chemical formula C₆₄H₄₀N₈O₃₂: 1432.1749, found: 1431.1679 [M-H]⁻.

3.2.4 Synthesis of cavitand **3a**

Cavitand **4a** (500 mg, 0.26 mmol, 1 eq.) was suspended in precooled EtOH (0 °C, 40 mL). To the suspension, tin (II) chloride dihydrate (7.2 g, 32 mmol, 120 eq.) and 10 mL of 37% (wt/wt) HCl(aq) was added slowly. The reaction flask was degassed, then immersed in an oil bath at 110 °C and stirred vigorously for 4 hrs.¹ After cooling to room temperature, the precipitate was filtered. The solid obtained was washed with 3 N HCl (3 × 20 mL, 0 °C), acetonitrile (5 × 10 mL, 0 °C) and diethyl ether (5 × 20 mL). Cavitand **3a** (290 mg, 64%) was obtained as a white solid. ¹H NMR (600 MHz, DMSO-*d*₆, δ ppm) 7.81 (s, 4H), 7.63 (s, 8H), 7.22 (s, 4H), 5.59 (t, *J* = 9.5 Hz, 4H), 4.06 (d, *J* = 7.1 Hz, 8H), 2.26 (t, *J* = 7.6 Hz, 8H), 1.19 (t, *J* = 7.1 Hz, 12H).

3.2.5 Synthesis of cavitand **2a**

Cavitand **3a** (500 mg, 1 eq.) was dissolved in MeOH (80 mL) and 15 mL ammonium hydroxide (25% - 28%) was added. The octa amine cavitand **3a** precipitated as a white solid and was collected by filtration. The octa amine cavitand **3a** was dissolved in MeOH (100 mL) and freshly prepared 2-(pyridin-4-ylmethylene)malononitrile (714 mg, 12 eq.) was added slowly at RT (at this time, the reaction solution is heterogeneous). The reaction mixture was heated at 80 °C with vigorous stirring for 15 hrs. After cooling, the solid was filtered and washed with water (2 × 30 mL), MeOH (2 × 30 mL) and DCM (2 × 30 mL) to give cavitand **2a** (412 mg, 65%) as a yellow solid.

¹H NMR of cavitand **2a** (600 MHz, 10% D₂O/ DMSO-*d*₆, δ ppm) 8.58 (d, 8H), 8.07 (s, 8H), 7.85 (m, 12H), 7.72(s, 4H), 5.61 (t, 4H), 4.05 (t, 8H), 2.62 (t, 8H), 2.29 (t, 8H), 1.18 (t, 12H). ¹³C NMR (151 MHz, DMSO-*d*₆ /10% D₂O, δ ppm) 173.29, 155.96, 150.10, 149.74,

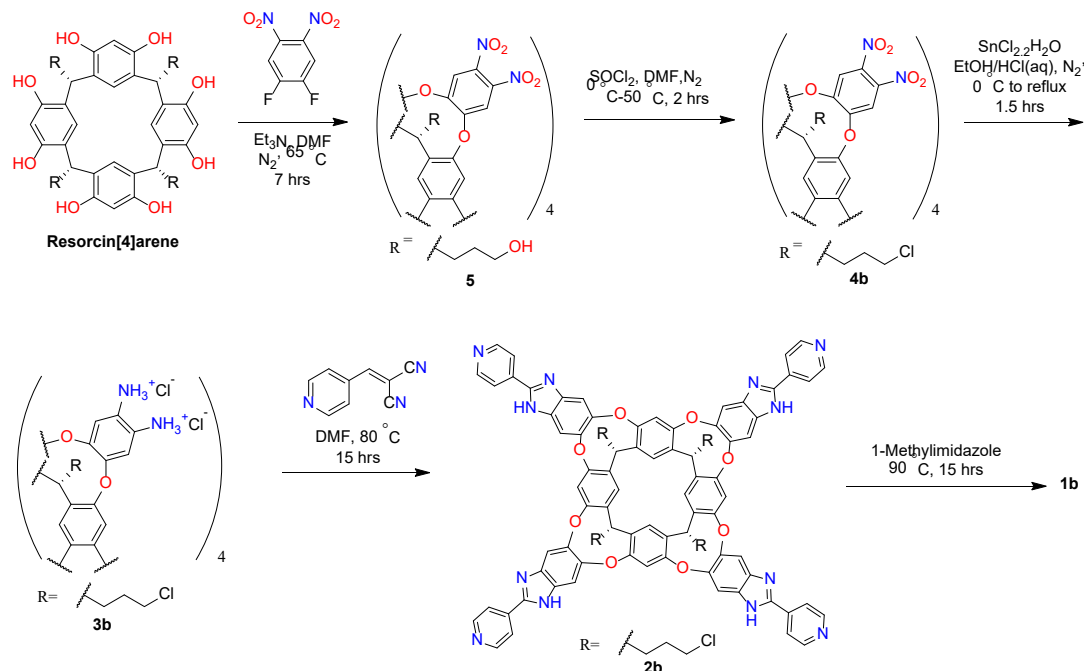
136.84, 135.29, 135.17, 125.00, 124.36, 117.32, 60.63, 50.54, 33.36, 32.72, 27.49, 18.56, 14.46. HRMS (ESI): Calcd for chemical formula $C_9H_7N_{12}O_{16}$: 1652.5502, found: 1653.56 $[M+H]^+$.

3.2.6 Synthesis of cavitand **1a**

Cavitand **2a** (400 mg, 0.24 mmol, 1 eq.) was added to a 50 mL round-bottom flask containing ethanol (15 mL) and tetrahydrofuran (15 mL), then aqueous sodium hydroxide (1N, 1.2 mL, 5 eq.) was added at 0 °C. The reaction mixture was warmed to 40 °C and stirred for 10 hrs.⁴ The solid was filtered and washed with ethanol (3×20 mL). The solid was suspended in 50 mL of acetone then vigorously stirred and refluxed for 1 h. The suspension was cooled to room temperature, filtered and washed with excess acetone (100 mL), then dried under high vacuum. Cavitand **1a** (310 mg, 78%) was obtained as a yellow solid.

1H NMR of cavitand **1a** (600 MHz, 10% D_2O / $DMSO-d_6$, δ ppm) 8.78 (d, 8H), 7.87 - 7.72 (m, 20H), 7.63 (s, 4H), 5.67 (t, 4H), 2.64 (t, 8H), 2.25 (t, 8H). ^{13}C NMR (151 MHz, D_2O /10% $DMSO-d_6$, δ ppm) 183.43, 166.41, 157.19, 150.65, 149.80, 141.32, 137.05, 125.77, 122.40, 118.52, 111.75, 37.43, 35.04, 29.85. HRMS (ESI): Calcd for chemical formula $C_{88}H_{56}N_{12}O_{16}H_4$: 1540.4250, found: 1538.41 $[M-2H]^{2-}$.

3.3 Scheme of the synthesis of water soluble cavitand **1b**



Scheme 2. Synthesis of water soluble cavitand **1b**.

3.4 Synthesis and characterization of water soluble Cavitand **1b**

3.3.1 Synthesis of cavitand **4b** and cavitand **3b**

Cavitands **4b** and **3b** were synthesized following the previously reported procedure.¹ The characterization data are in accordance with the previous report.

3.3.2 Synthesis of cavitand **2b**

Cavitand **3b** (500mg, 1 eq.) was dissolved in MeOH (80 mL) and then 15 mL ammonium hydroxide (25% - 28%) was added. The octa amine cavitand **2b** precipitated as a white solid. The solid was dissolved in DMF (150 mL) and 2-(pyridin-4-ylmethylene)malononitrile (768 mg, 12 eq.) was added to the flask; then the mixture was stirred at 80 °C for 15 hrs. After completion of the reaction, the solvent was removed under vacuum, and MeOH (100 mL) was added to give a solid. The resulting precipitate was filtered and washed with H₂O (2 × 30 mL), MeOH (2 × 30 mL) and DCM (2 × 30 mL). Cavitand **2b** (370 mg, 57%) was obtained as a yellow solid.

¹H NMR of cavitand **2b** (600 MHz, DMSO-*d*₆, δ ppm) 12.94 (br, 4H), 8.68 (s, 4H), 8.04 (s, 8H), 7.69 (s, 4H), 7.42 (s, 4H), 5.59 (t, 4H), 3.74 (s, 8H), 1.76 (s, 8H). ¹³C NMR (151 MHz, DMSO-*d*₆, δ ppm) 155.89, 150.57, 149.98, 136.54, 135.38, 124.95, 120.30, 117.39, 45.44, 33.13, 31.36, 29.26. HRMS (ESI): Calcd for chemical formula C₈₈H₆₄Cl₄N₁₂O₈:1556.3724, found: 1557.38 [M+H]⁺.

3.3.3 Synthesis of cavitand **1b**

Compound **2b** (250 mg) and 1-methylimidazole (25 mL) was taken in 50 mL round bottom flask, then sonicated for 10 min for complete dissolution. The mixture was heated at 90 °C with continuously stirring under nitrogen atmosphere for 15 hrs. After cooling to room temperature, 250 mL of acetone was added with vigorous stirring resulting in the precipitation of a white solid. The solid was centrifuged (4000 rpm, 10 min) and washed thoroughly with excess acetone. The recovered solid was re-suspended in 50 mL of acetone, vigorously stirred and heated at reflux for 2 hrs. It was cooled to room temperature and centrifuged (4000 rpm, 10 min) to get a white solid. This product was washed with excess acetone (50 mL) and dried under high vacuum. Cavitand **1b** (255 mg, 84%) was obtained as a white solid.

¹H NMR of cavitand **1b** (600 MHz, D₂O 10 %/ DMSO-*d*₆, δ ppm) 9.11 (d, 4H), 8.53 (d, 8H), 8.04 (s, 8H), 7.92 (s, 6H), 7.79 (t, 14H), 7.58 (t, 4H), 5.48 (t, 4H), 4.31 (t, 8H), 3.81 (s, 12H), 2.63 (t, 8H), 1.72 (s, 8H). ¹³C NMR (151 MHz, MeOD-*d*₄, δ ppm) 156.31, 150.28, 149.52, 137.15, 136.62, 134.97, 125.40, 123.77, 122.54, 120.51, 116.87, 35.25, 33.40, 28.96, 28.22. HRMS (ESI): Calcd for chemical formula C₁₀₄H₈₈N₂₀O₈Cl₄:1884.5848, found: 1814.65 [M-2Cl]²⁻.

4. ^1H NMR, ^{13}C NMR and HR-MS spectra of cavitands

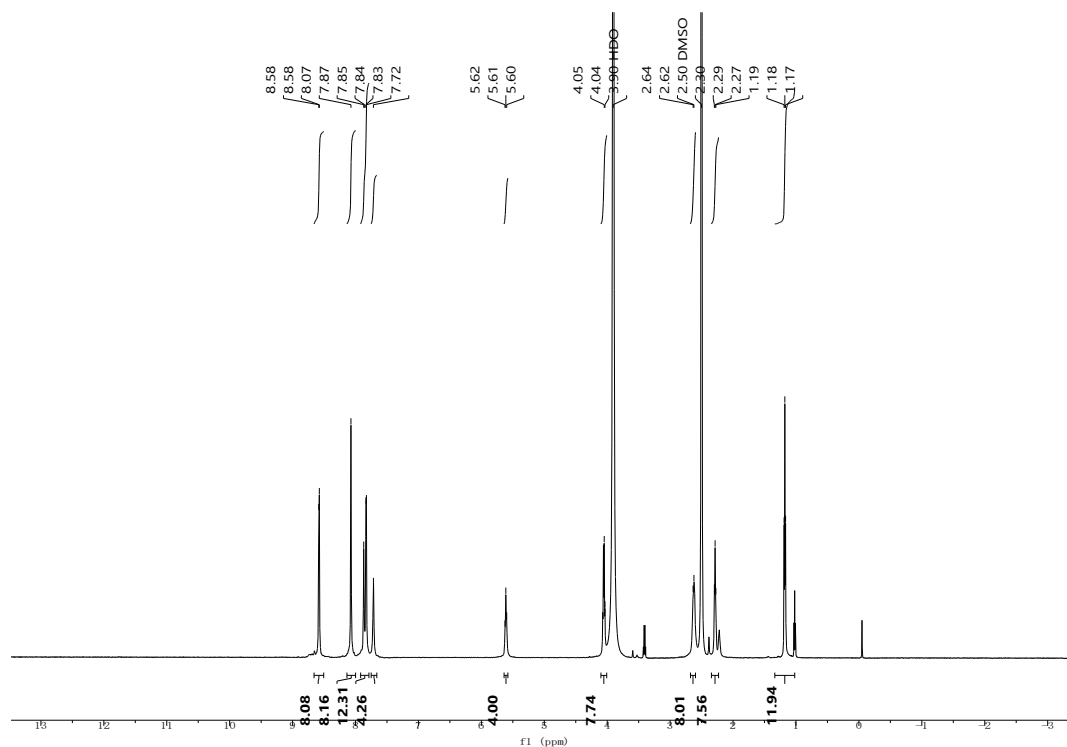


Figure S1. ^1H NMR spectrum (600 MHz, 298 K) of cavitand **2a** in 10% $\text{D}_2\text{O}/\text{DMSO}-d_6$.

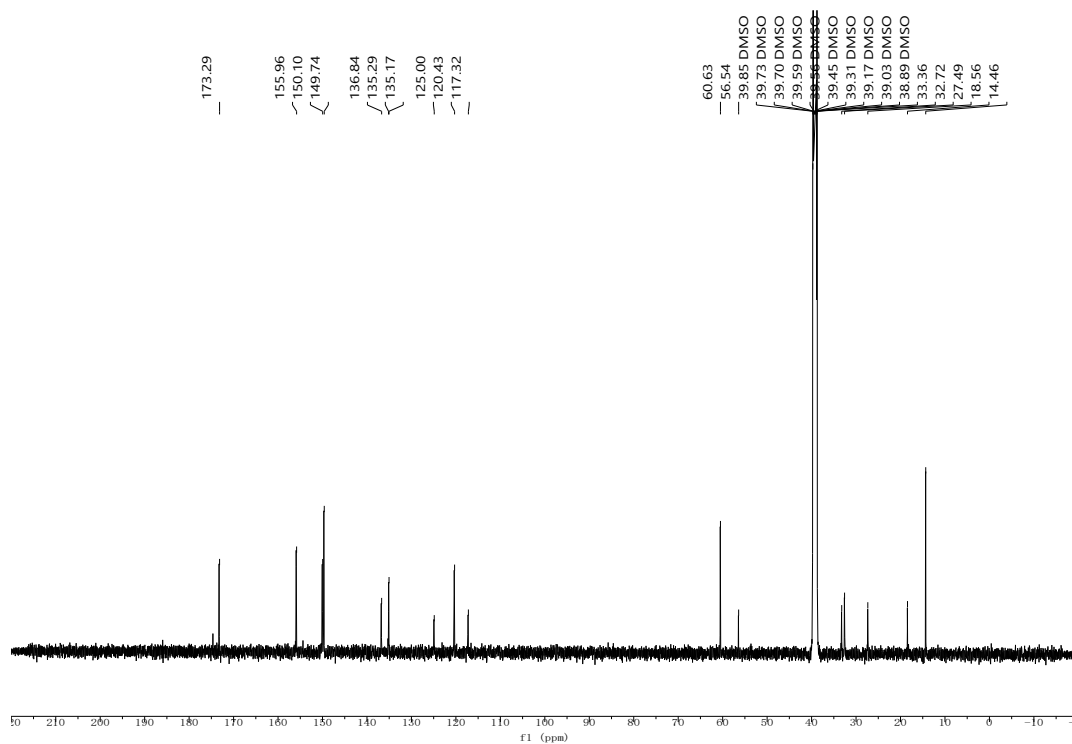


Figure S2. ^{13}C NMR spectrum of cavitand **2a** in 10% $\text{D}_2\text{O}/\text{DMSO}-d_6$.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
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Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

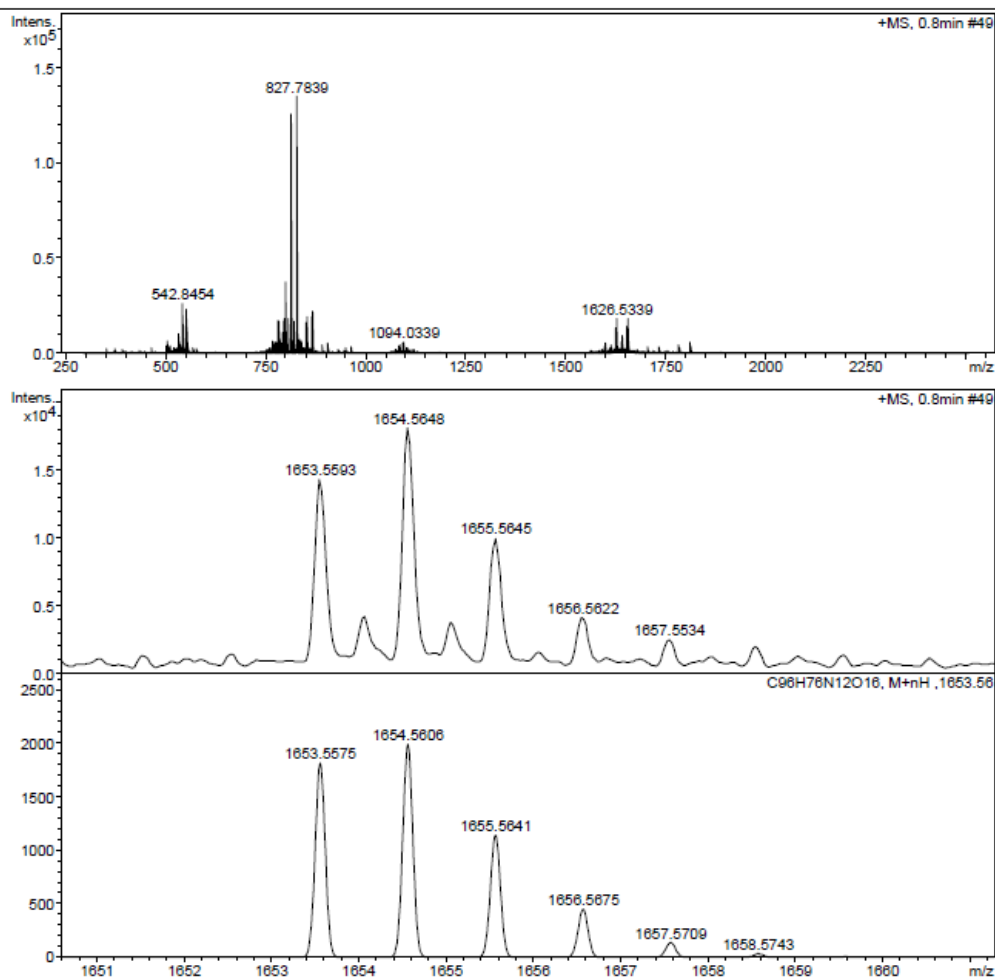


Figure S3. HR-MS spectrum of cavitand **2a**.

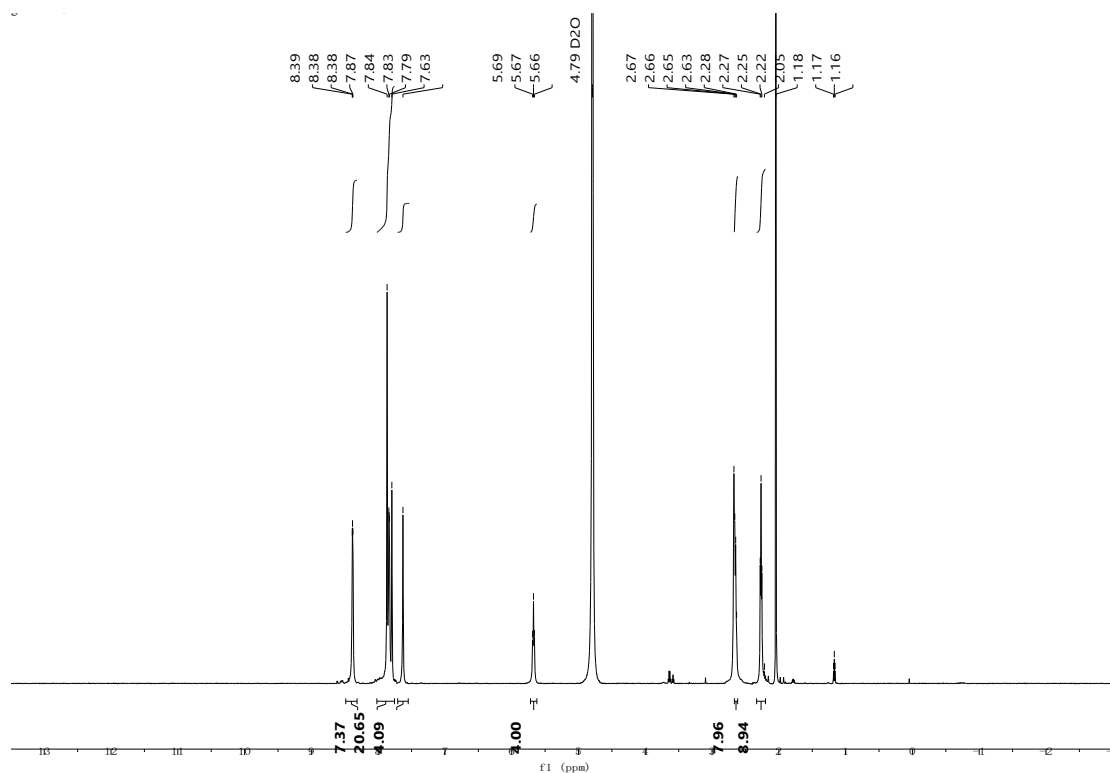


Figure S4. ¹H spectrum (600 MHz, 298 K) of cavitand **1a** in 10% DMSO-*d*₆/D₂O.

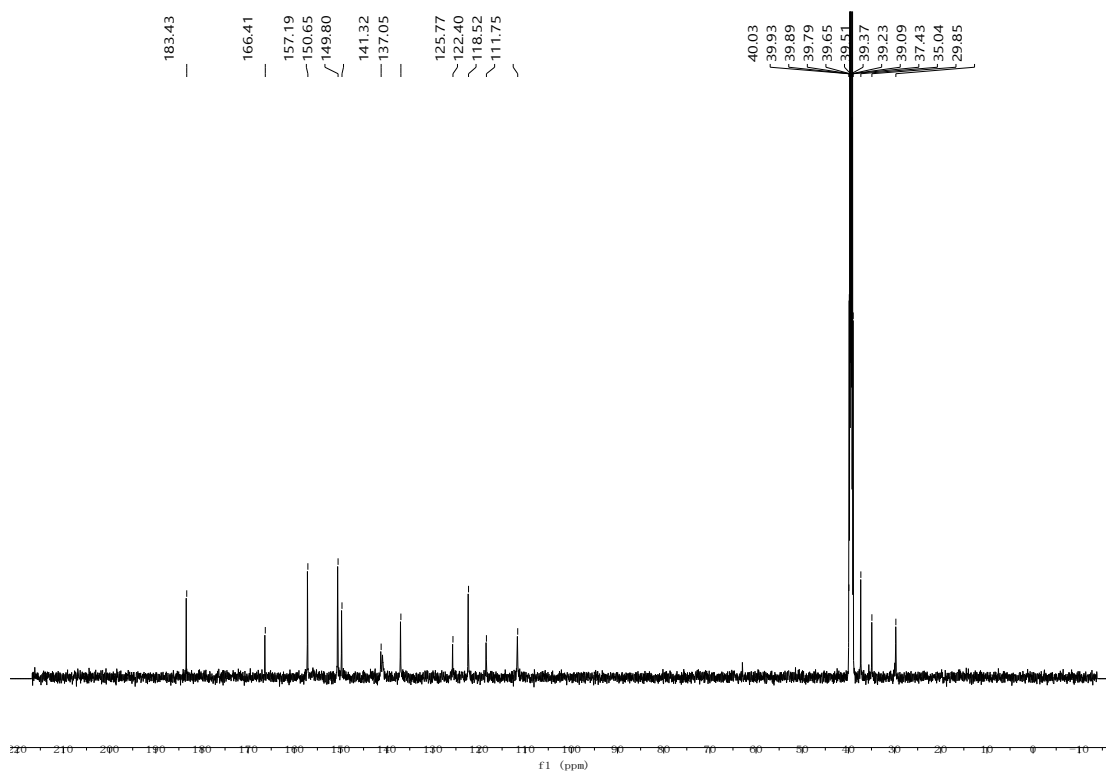


Figure S5. ¹³C NMR spectrum of cavitand **1a** in 10% DMSO-*d*₆/D₂O.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.0 Bar
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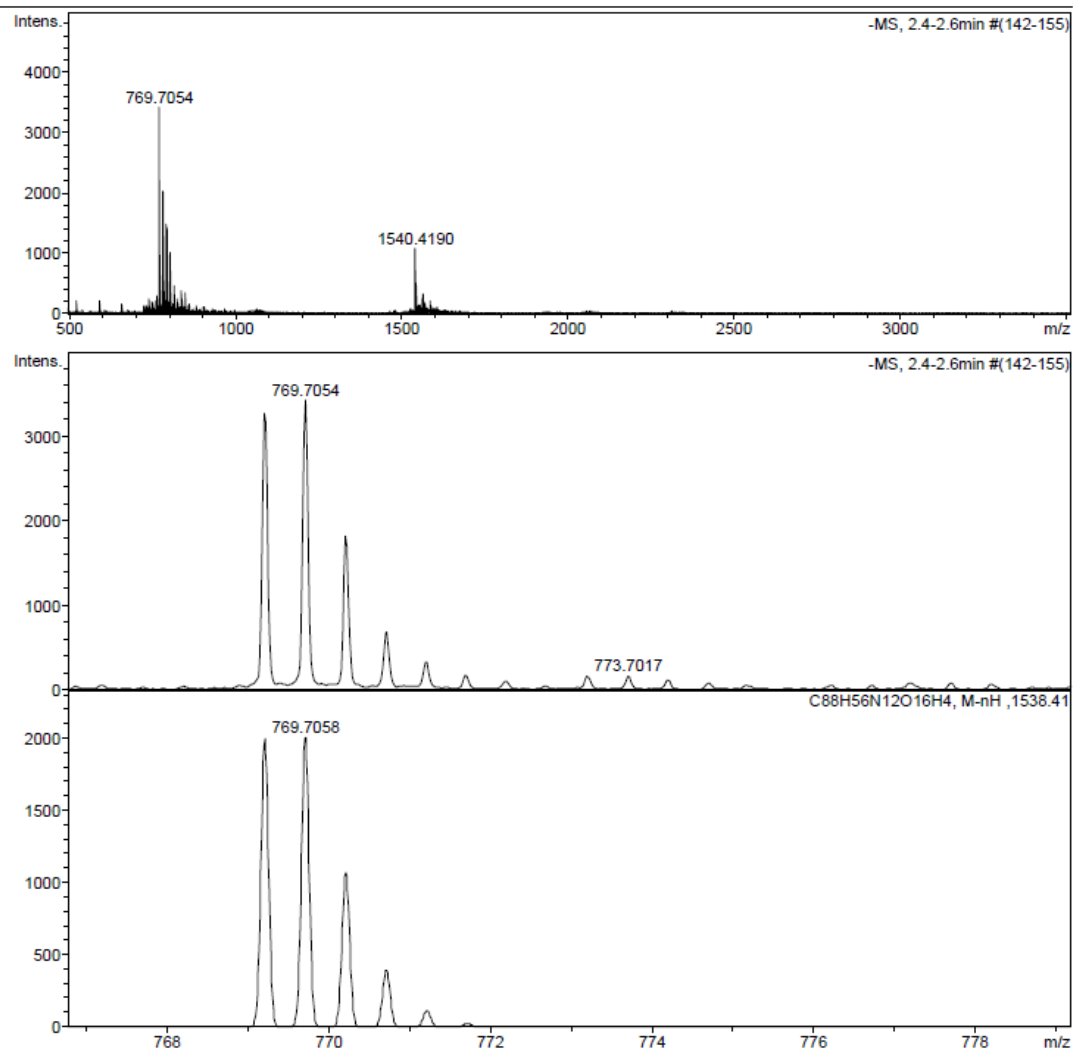


Figure S6. HR-MS spectrum of cavitand **1a**.

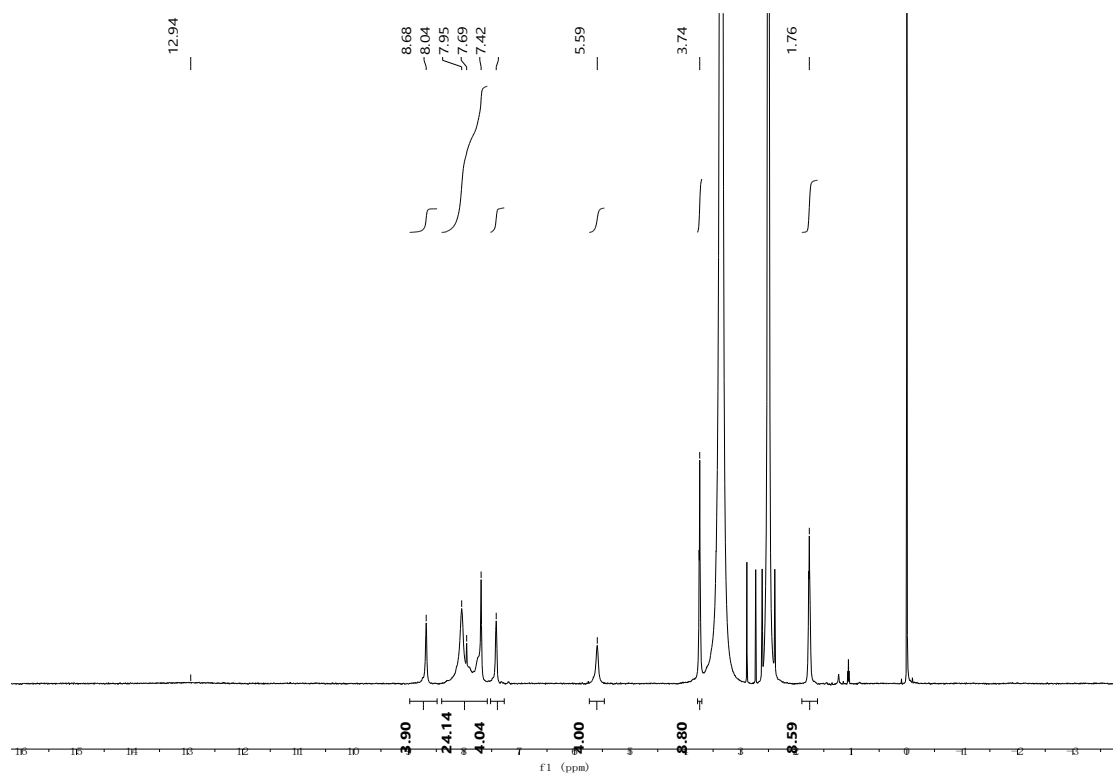


Figure S7. ¹H spectrum (600 MHz, 298 K) of cavitand **2b** in DMSO-*d*₆.

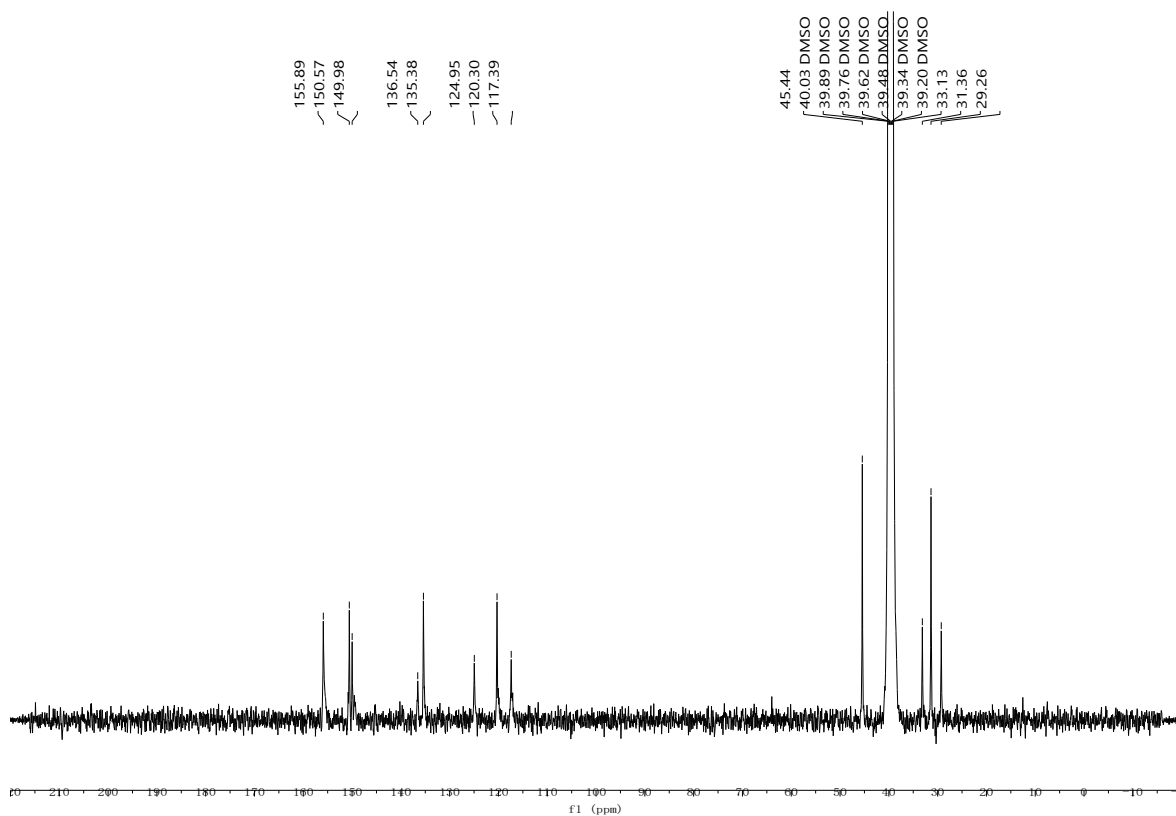


Figure S8. ¹³C NMR spectrum of cavitand **2b** in 10% D₂O/ DMSO-*d*₆.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
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Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

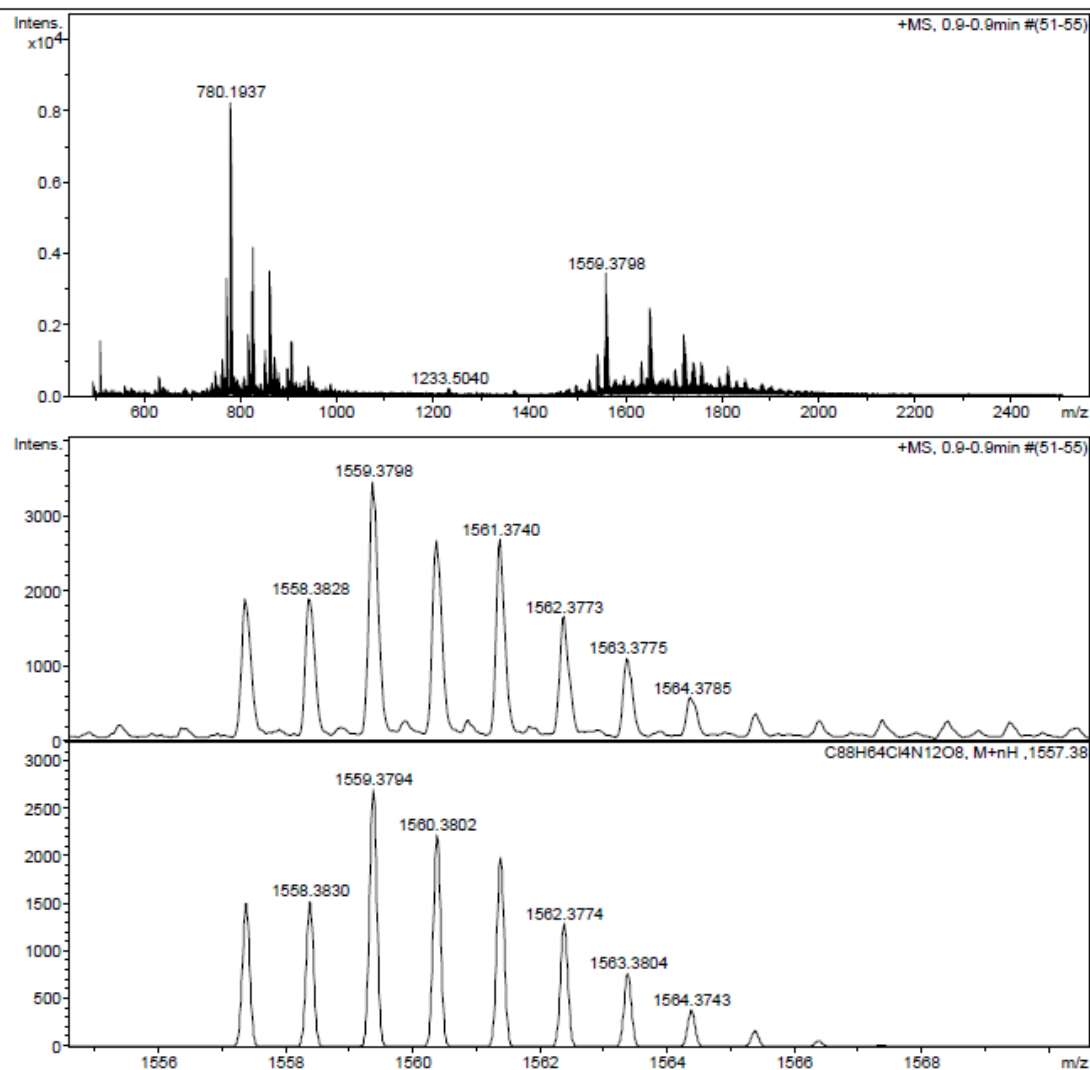


Figure S9. HR-MS spectrum of cavitand **2b**.

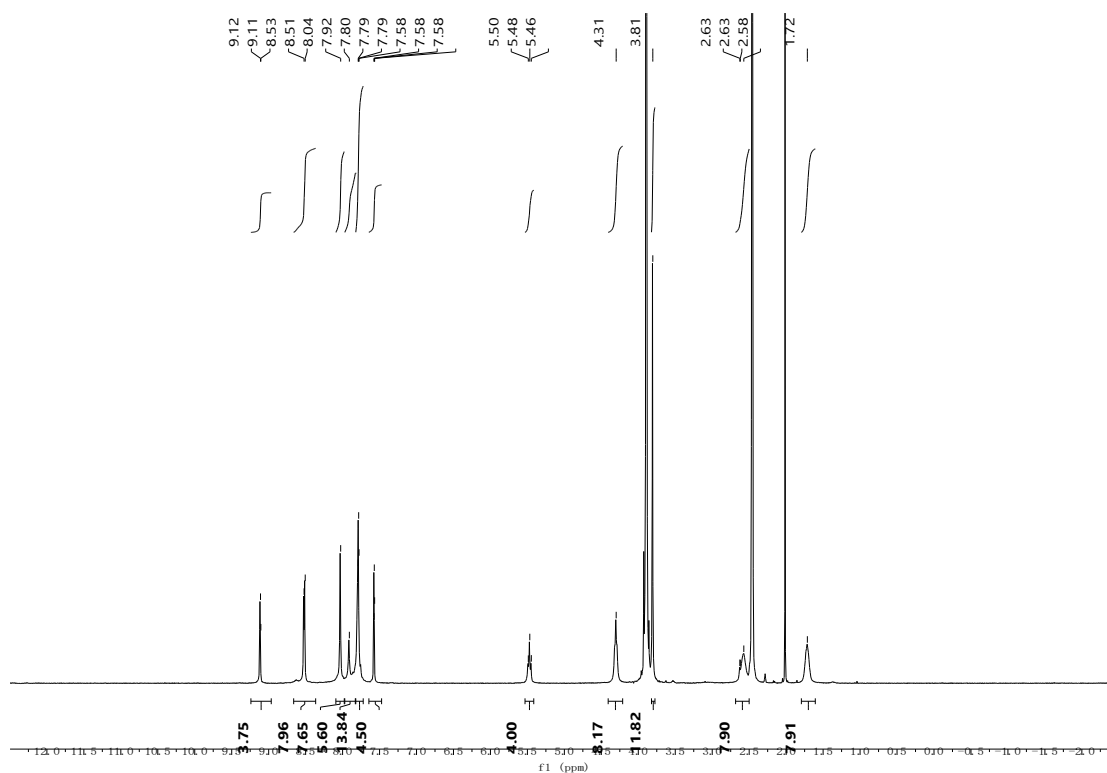


Figure S10. ¹H NMR spectrum (600 MHz, 298 K) of cavitand **1b** in 10% D₂O/ DMSO-*d*₆.

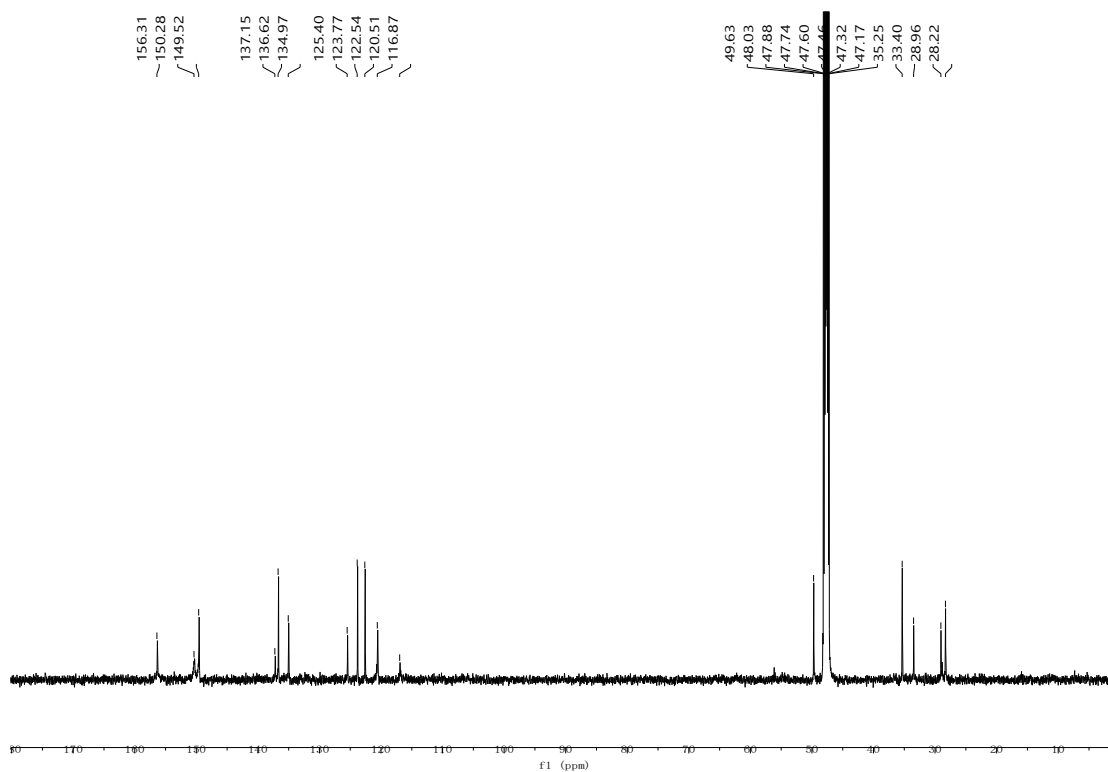


Figure S11. ¹³C NMR spectrum of cavitand **1b** in MeOD-*d*₄

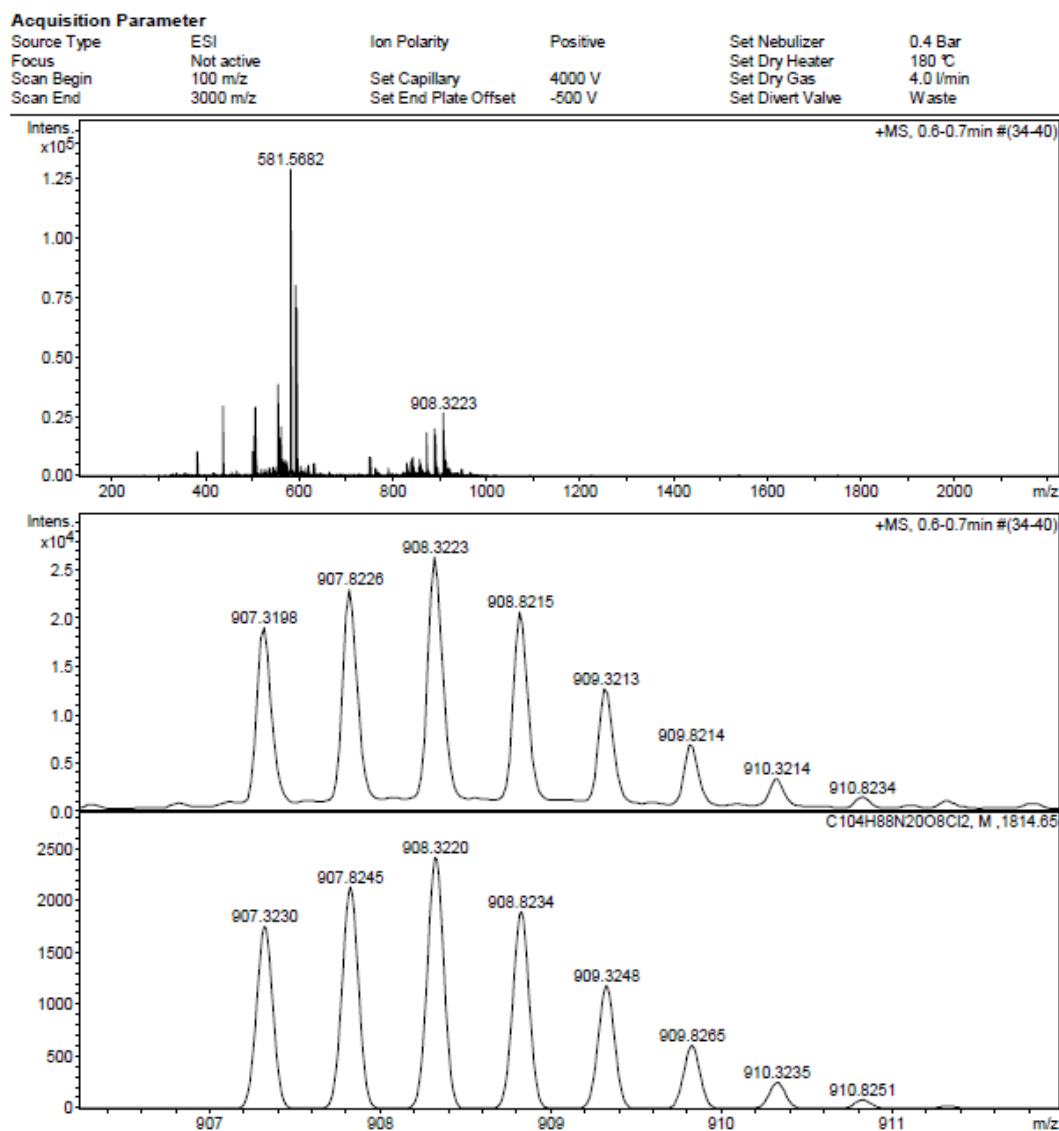


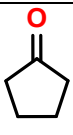
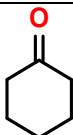
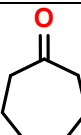
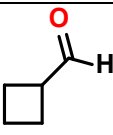
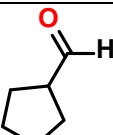
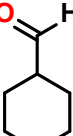
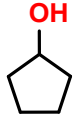
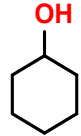
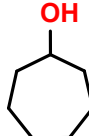
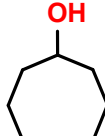
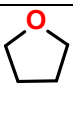
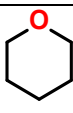
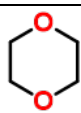
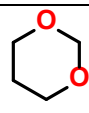
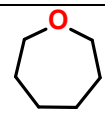
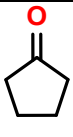
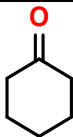
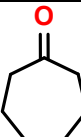
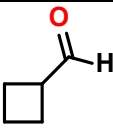
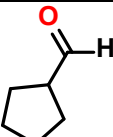
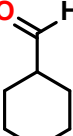
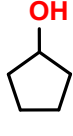
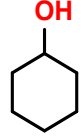
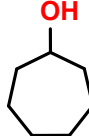
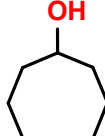
Figure S12. HR-MS spectrum of cavitand **1b**.

5. ^1H NMR of the complexes and relative $\Delta\delta$ calculation for guests

5.1 Relevant guests used in cavitand **1a** and **1b**

Table S2: Summary of guest molecules for cavitand **1a** and **1b** in this work

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cavitand 1a					
					
cavitand 1b					
					
					

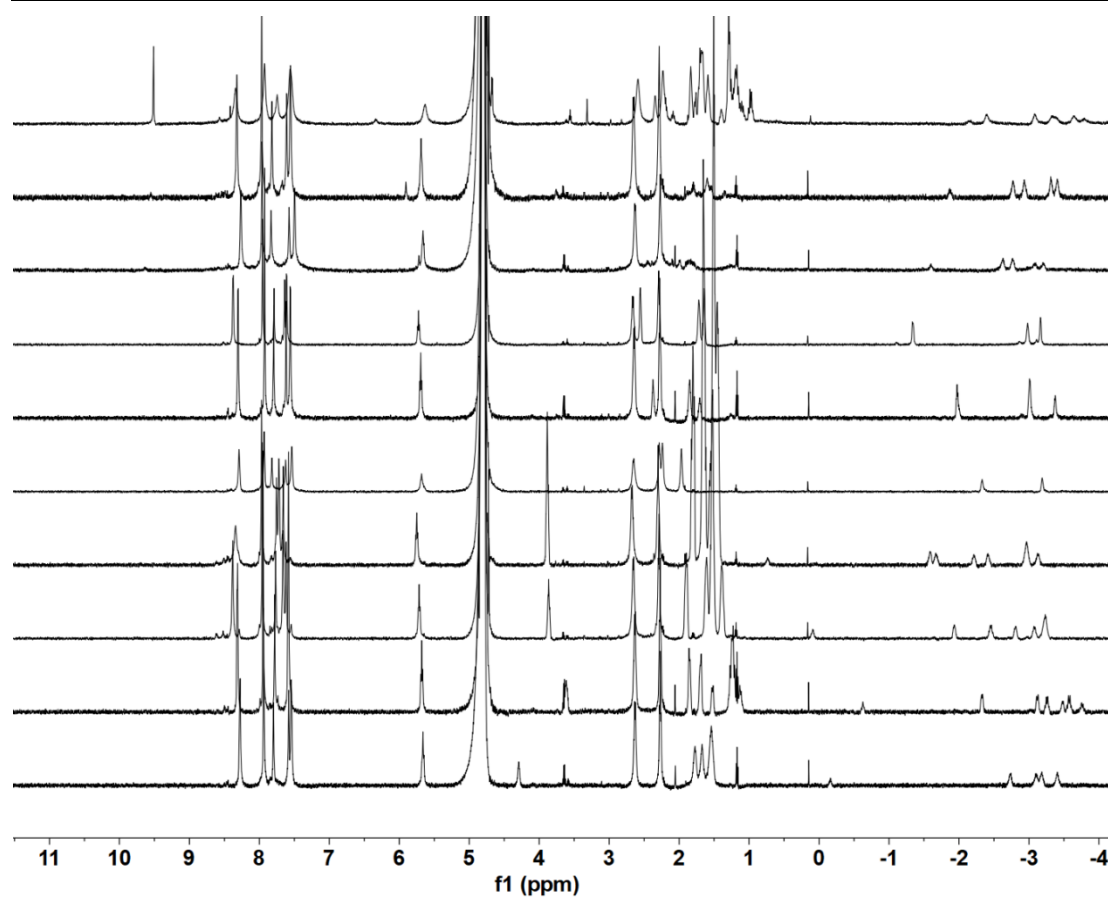


Figure S13: ¹H NMR spectra (600 MHz, 298 K) of the host **1a** and guest complexes, from top to bottom: cyclohexanecarbaldehyde, cyclopentanecarbaldehyde, cyclobutanecarbaldehyde, cycloheptanone, cyclohexanone, cyclopentanone, cyclooctanol, cycloheptanol, cyclohexanol, and cyclopentanol.

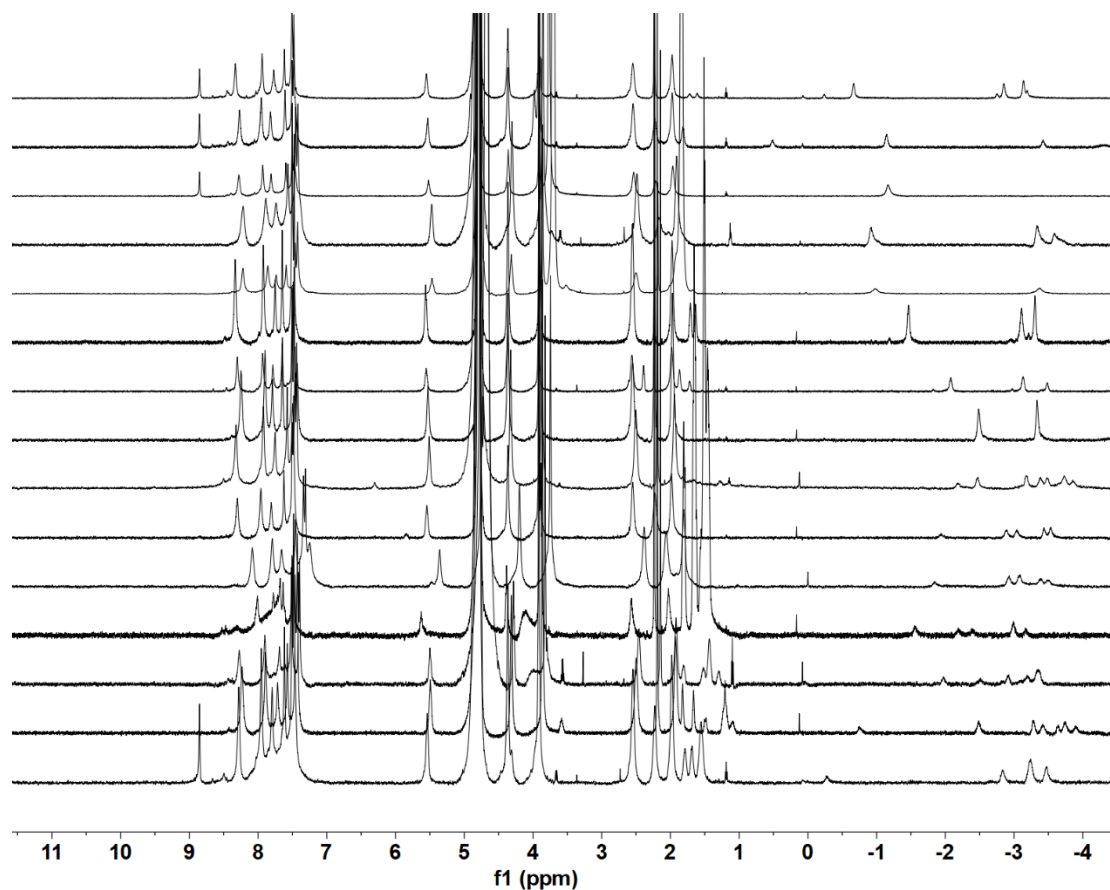
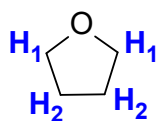


Figure S14: ^1H NMR spectra (600 MHz, 298 K) of the host **1b** and guest complexes, from top to bottom: oxepane, 1,3-dioxane, 1,4-dioxane, THP, THF, cycloheptanone, cyclohexanone, cyclopentanone, cyclohexanecarbaldehyde, cyclopentanecarbaldehyde, cyclobutanecarbaldehyde, cyclooctanol, cycloheptanol, cyclohexanol, and cyclopentanol.

5.2 ^1H NMR for the complexation of cavitand **1a** with guests.

5.2.1 Guest:



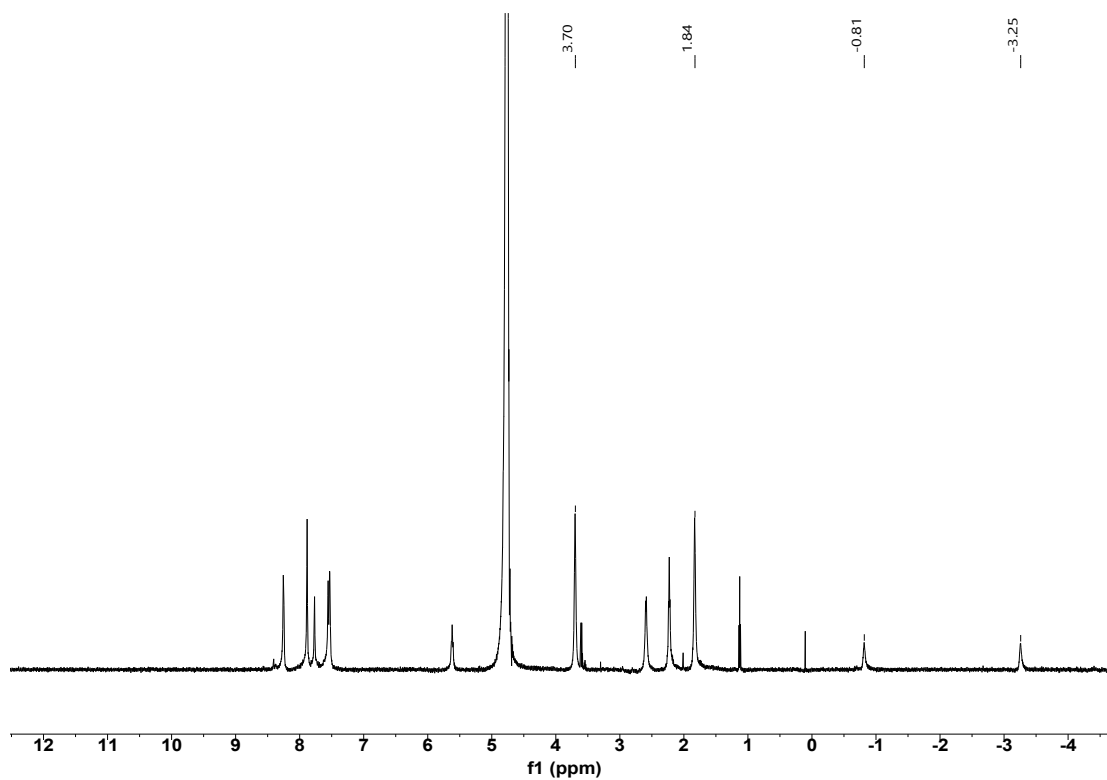
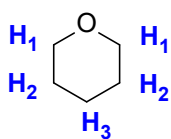


Figure S15. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL)

Table S3: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.70	-0.81	-4.51
H ₂	1.84	-3.25	-5.09

5.2.2 Guest:



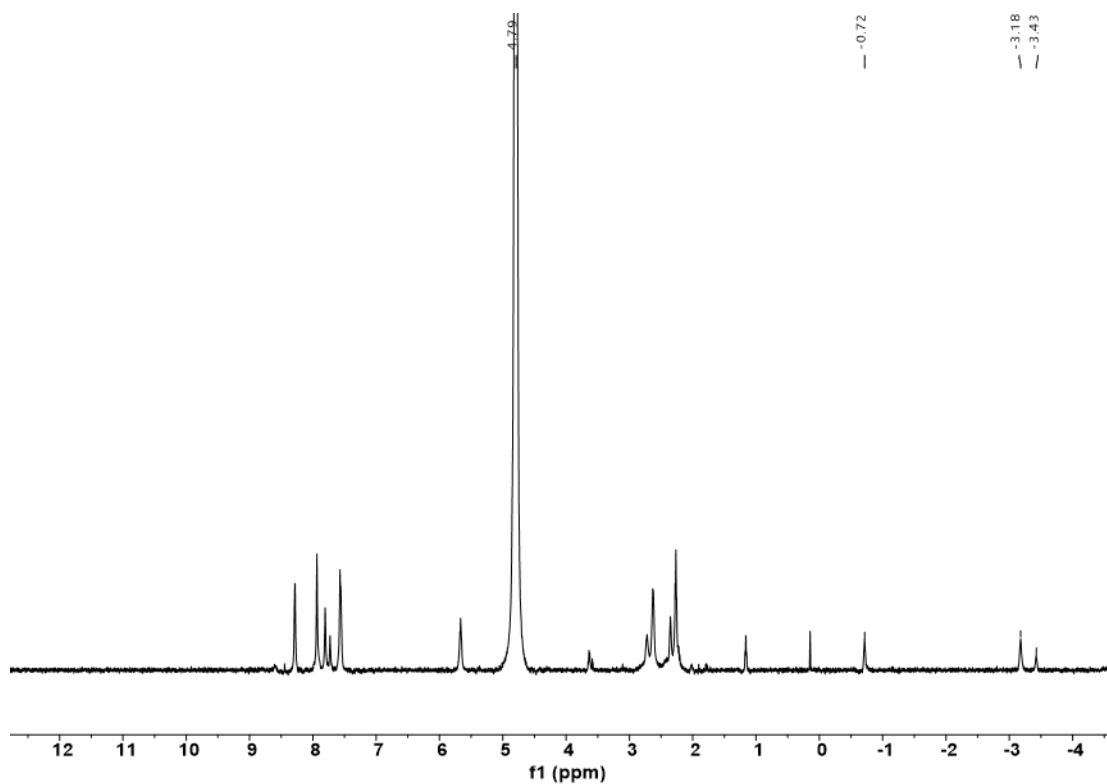
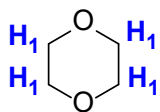


Figure S16. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S4: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.60	-0.72	-4.32
H ₂	1.60	-3.18	-4.78
H ₃	1.60	-3.43	-5.03

5.2.3 Guest:



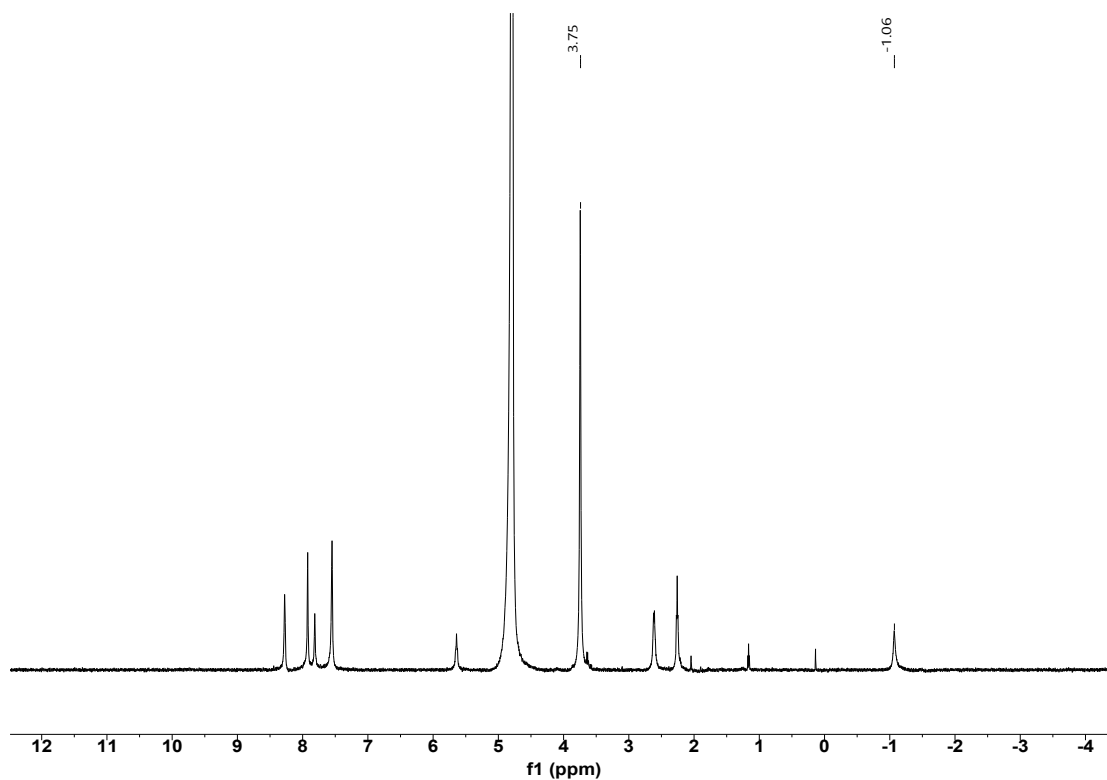
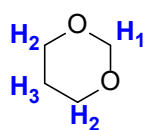


Figure S17. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S5: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.75	-1.06	-4.81

5.2.4 Guest:



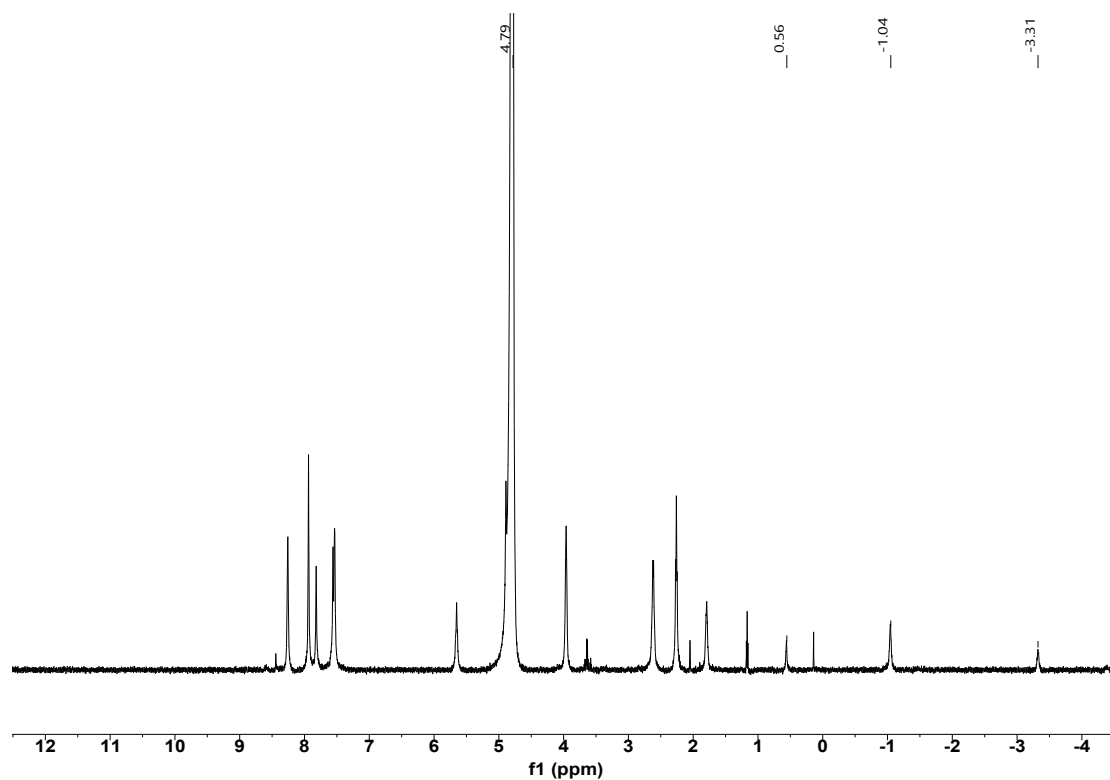
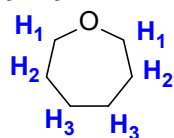


Figure S18. ^1H NMR spectrum (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S6: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	4.89	0.56	-4.33
H ₂	3.97	-1.04	-5.01
H ₃	1.80	-3.31	-5.11

5.2.5 Guest:



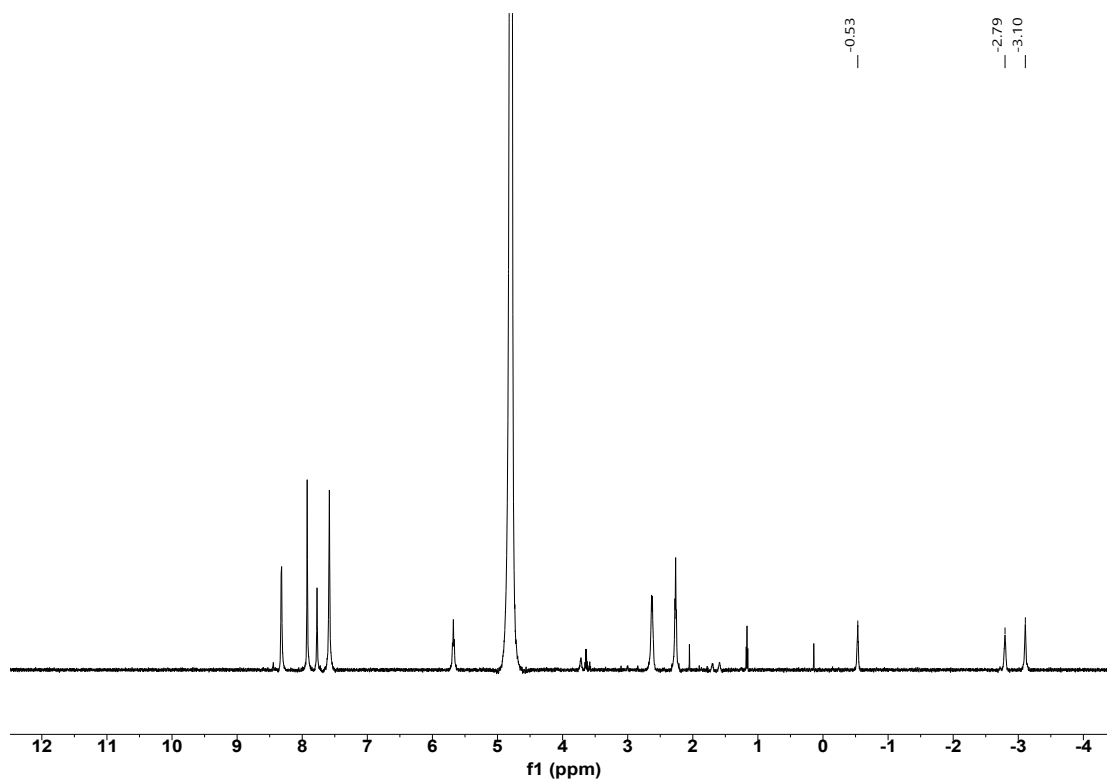
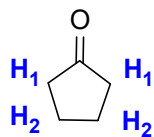


Figure S19. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S7: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.35	-0.53	-3.88
H ₂	1.44	-2.79	-4.23
H ₃	1.60	-3.10	-4.70

5.2.6 Guest:



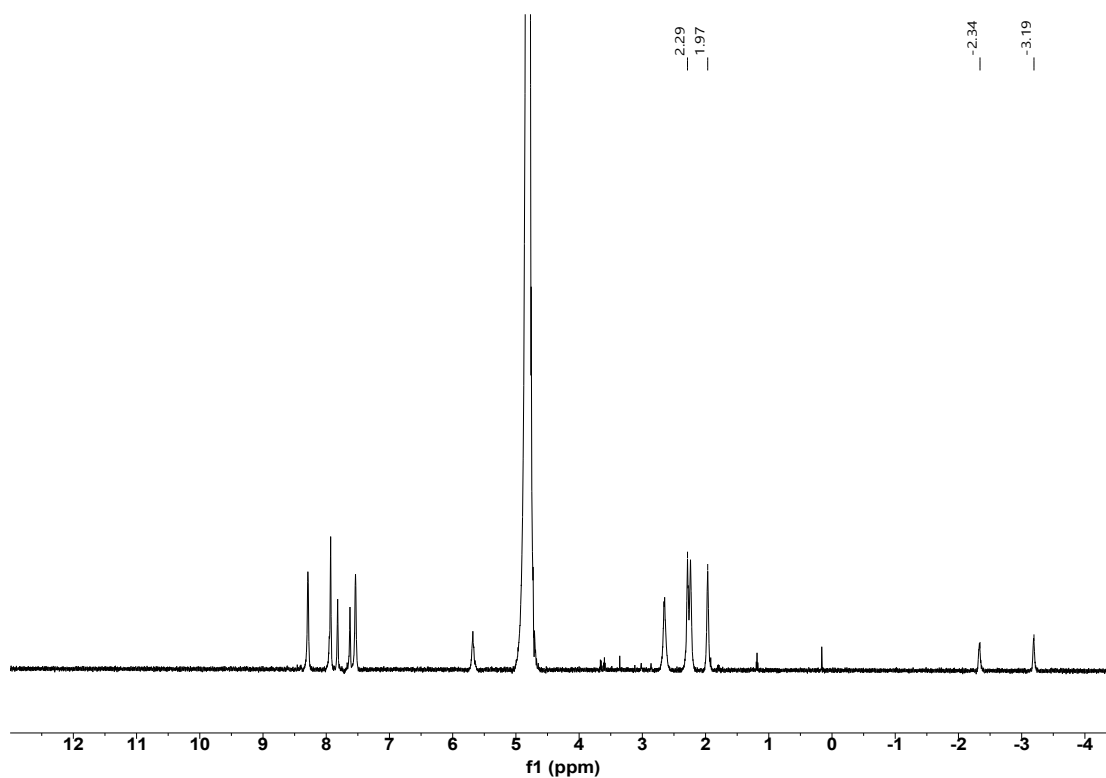
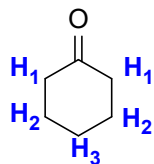


Figure S20. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S8: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	2.29	-2.34	-4.63
H ₂	1.97	-3.19	-5.16

5.2.7 Guest:



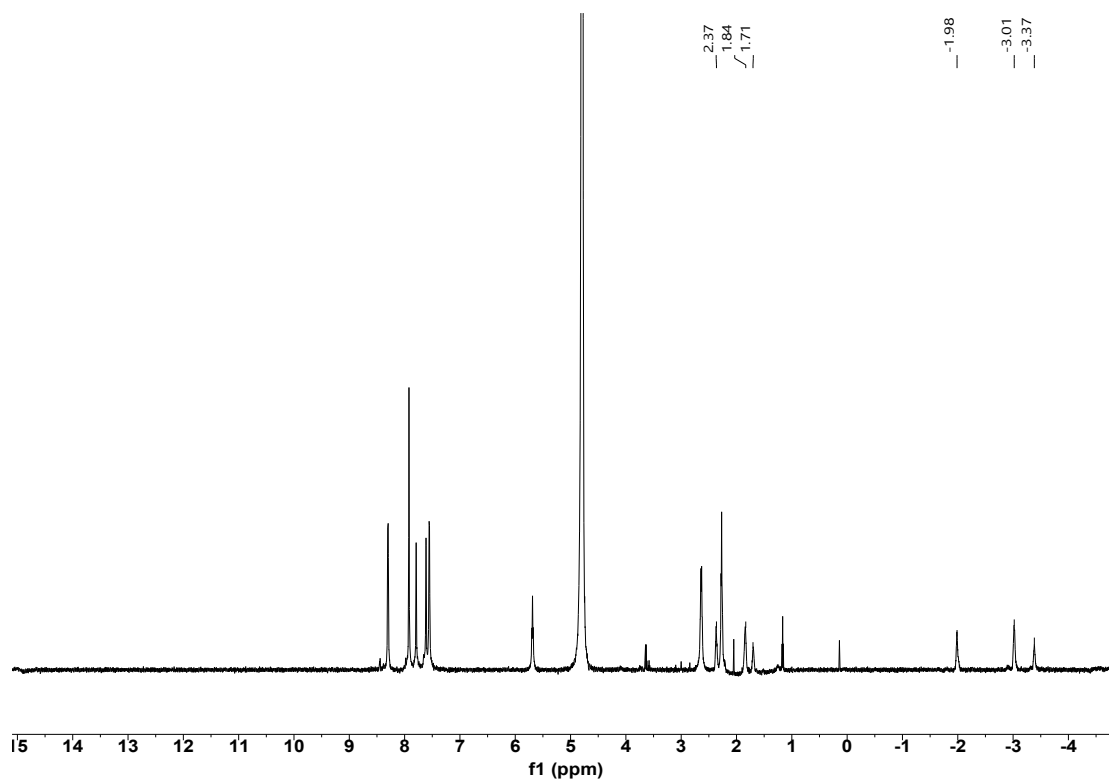
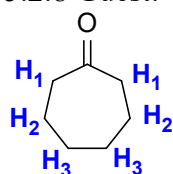


Figure S21. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S9: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	2.37	-1.98	-4.35
H ₂	1.84	-3.01	-4.85
H ₃	1.70	-3.37	-5.07

5.2.8 Guest:



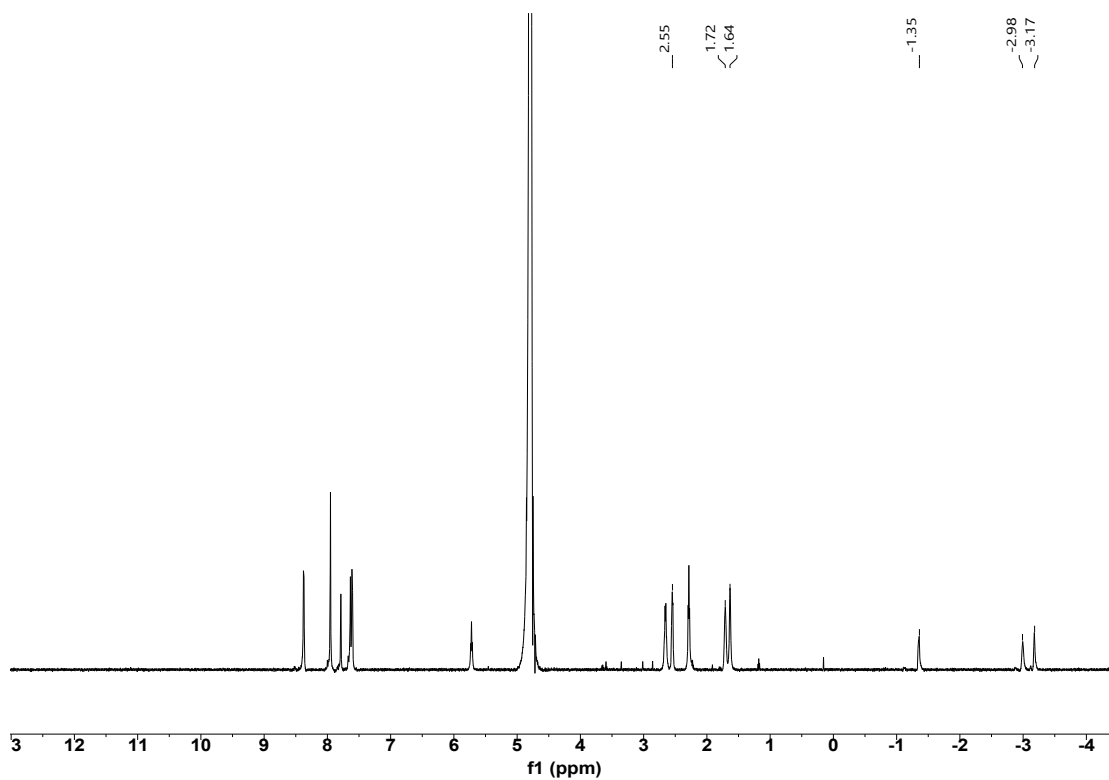
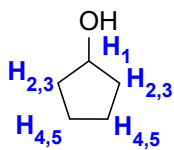


Figure S22. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S10: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	2.25	-1.35	-3.60
H ₂	1.72	-2.98	-4.70
H ₃	1.64	-3.17	-4.81

5.2.9 Guest:



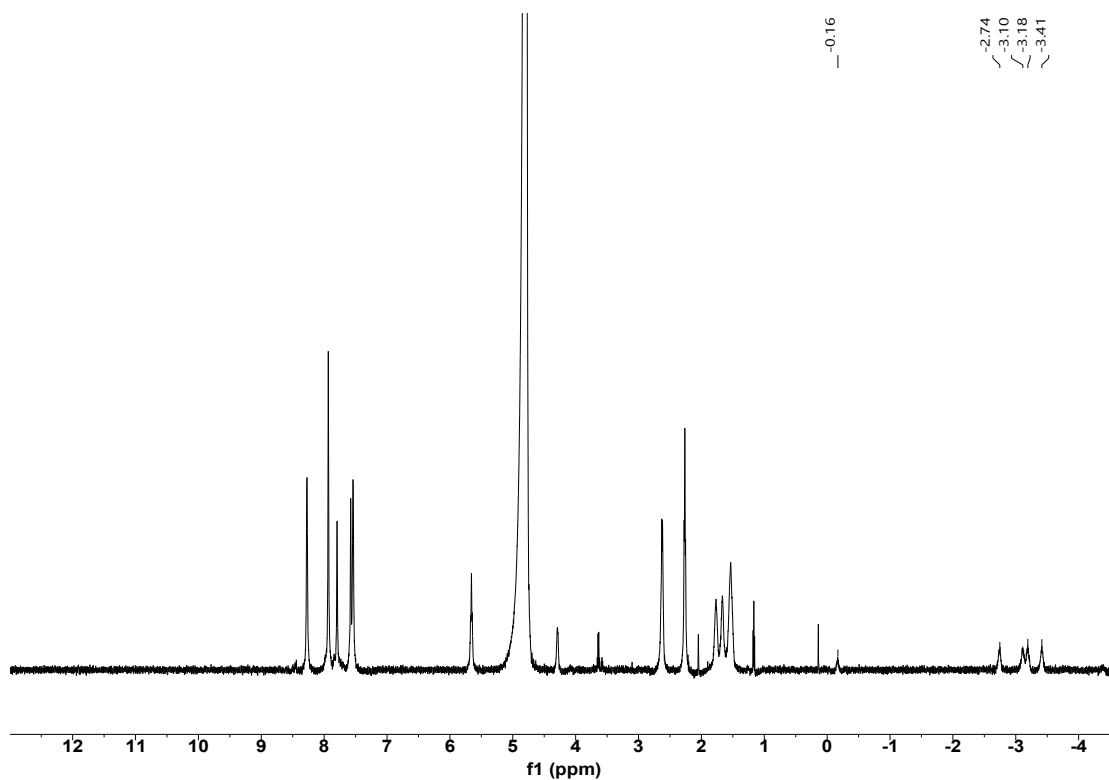
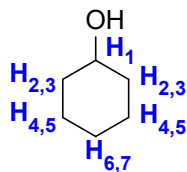


Figure S23. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S11: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	4.30	-0.16	-4.46
H ₂	1.78	-2.74	-4.52
H ₃	1.54	-3.10	-4.64
H ₄	1.67	-3.18	-4.85
H ₅	1.71	-3.41	-5.12

5.2.10 Guest:



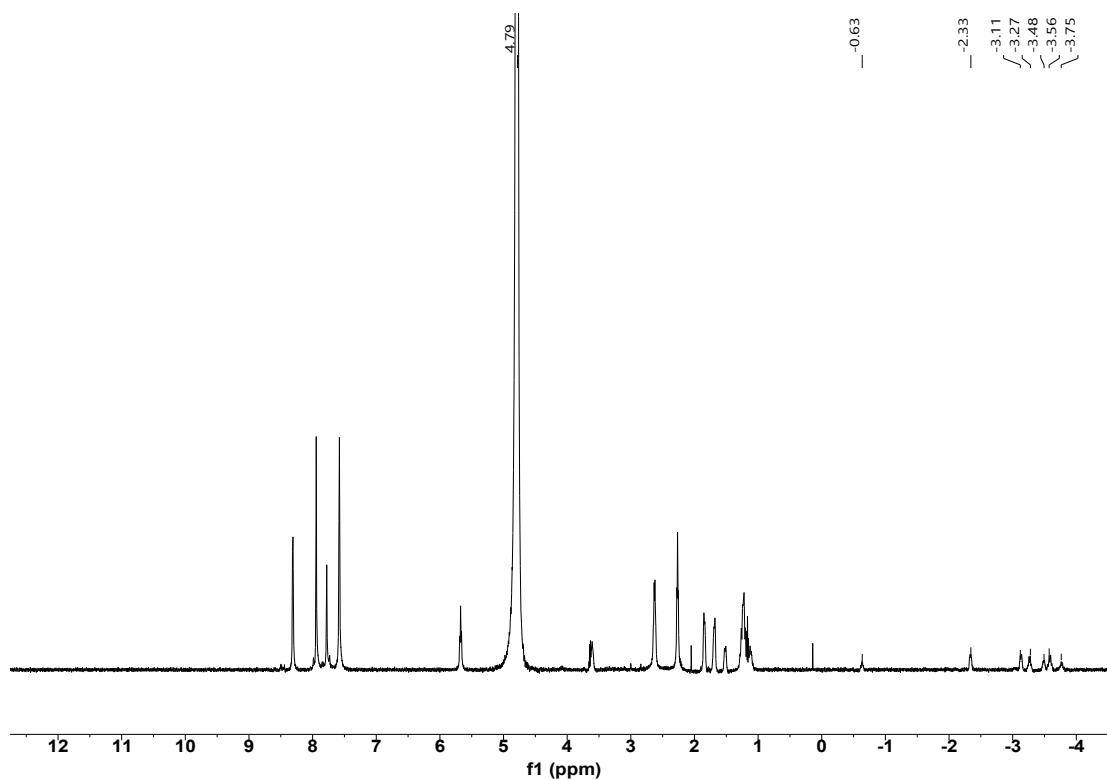
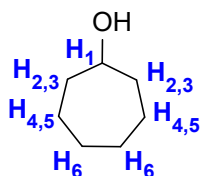


Figure S24. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S12: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.62	-0.63	-4.25
H ₂	1.85	-2.33	-4.18
H ₃	1.68	-3.11	-4.79
H ₄	1.53	-3.27	-4.79
H ₅	1.51	-3.48	-4.99
H ₆	1.46	-3.56	-5.16
H ₇	1.44	-3.75	-5.19

5.2.11 Guest:



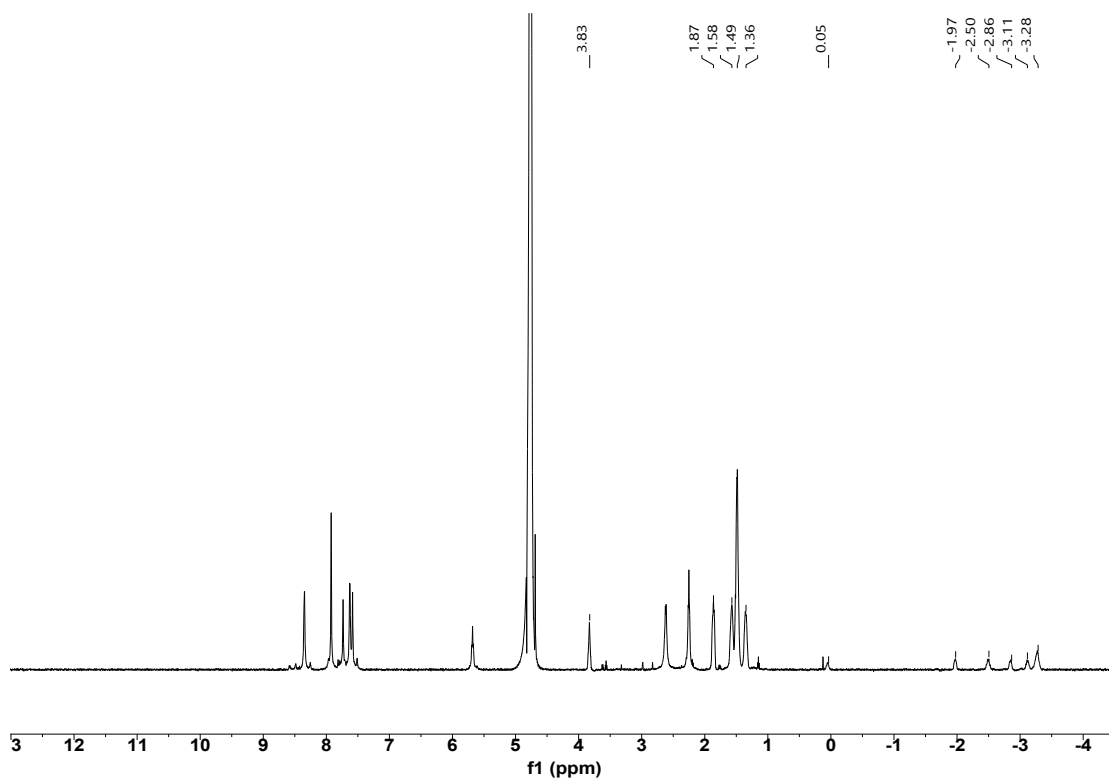
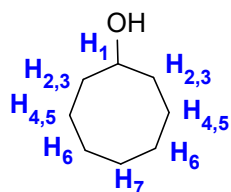


Figure S25. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S13: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.83	-0.05	-3.88
H ₂	1.87	-1.97	-3.84
H ₃	1.52	-2.50	-4.02
H ₄	1.58	-2.86	-4.44
H ₅	1.49	-3.11	-4.60
H ₆	1.36	-3.28	-4.64

5.2.12 Guest:



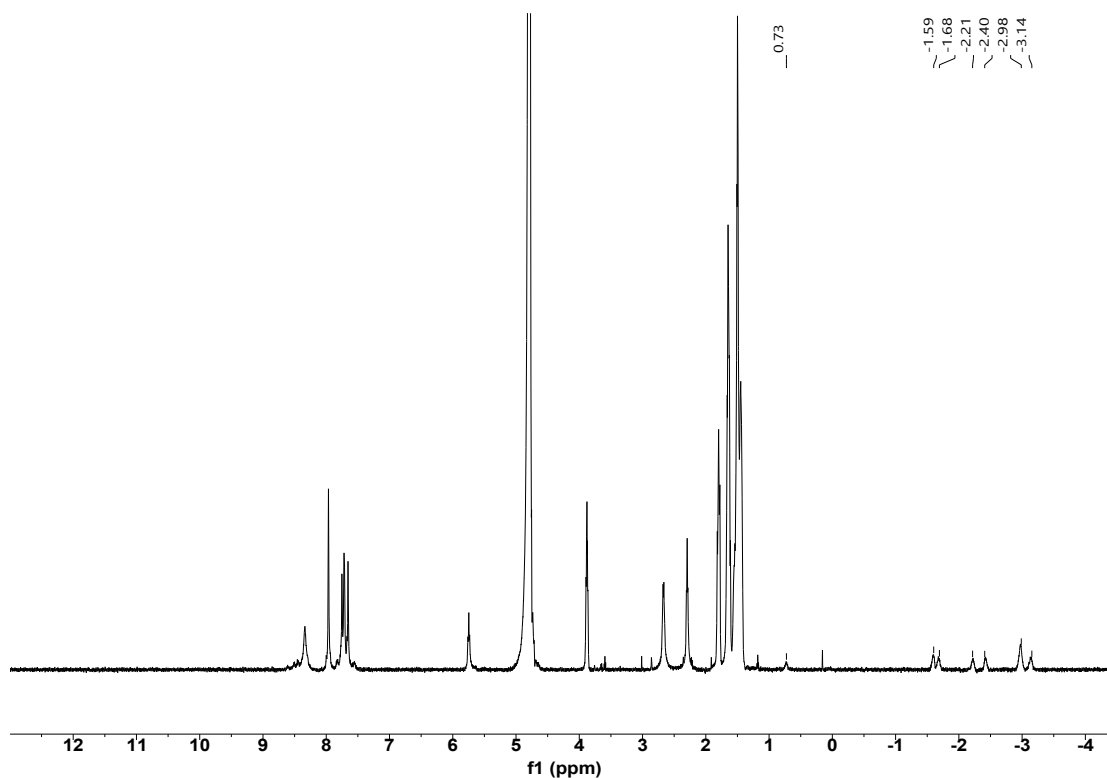
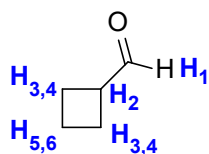


Figure S26. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S14: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.88	0.73	-3.15
H ₂	1.80	-1.59	-3.39
H ₃	1.65	-1.68	-3.33
H ₄	1.62	-2.21	-3.83
H ₅	1.56	-2.40	-3.96
H ₆	1.51	-2.98	-4.49
H ₇	1.45	-3.14	-4.59

5.2.13 Guest:



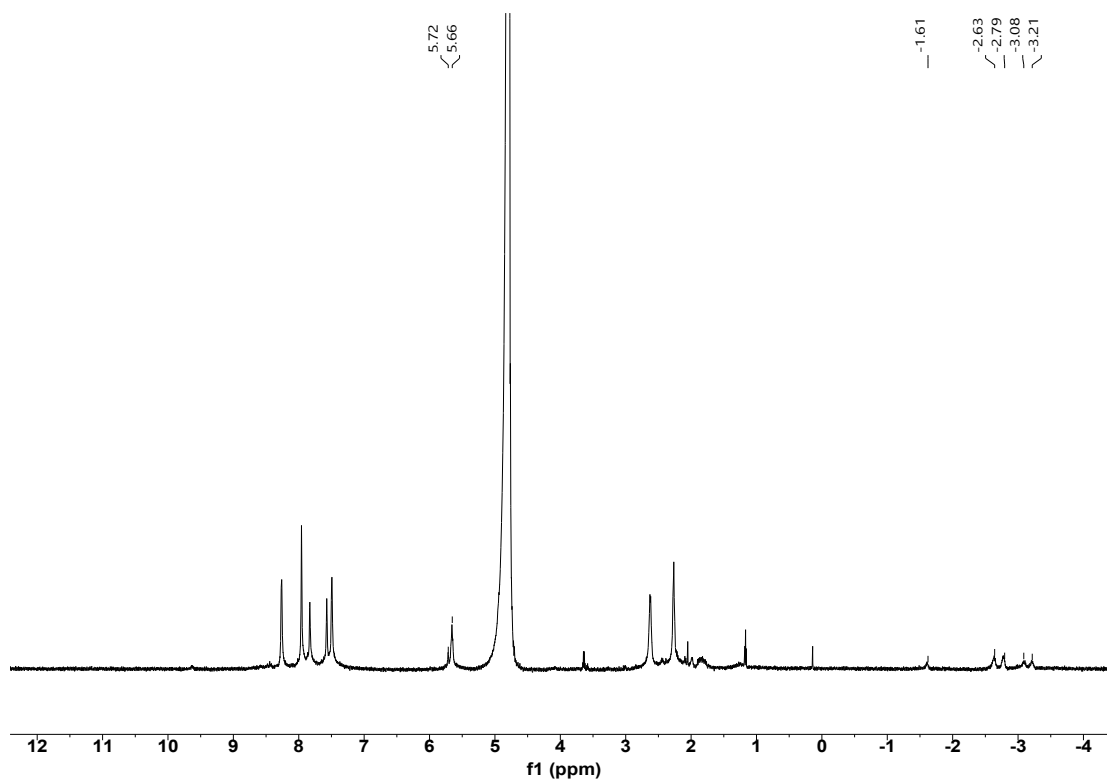
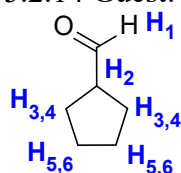


Figure S27. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S15: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	9.63	5.72	-3.91
H ₂	3.01	-1.61	-4.62
H ₃	1.98	-2.63	-4.61
H ₄	1.85	-2.79	-4.64
H ₅	1.70	-3.08	-4.78
H ₆	1.60	-3.21	-4.81

5.2.14 Guest:



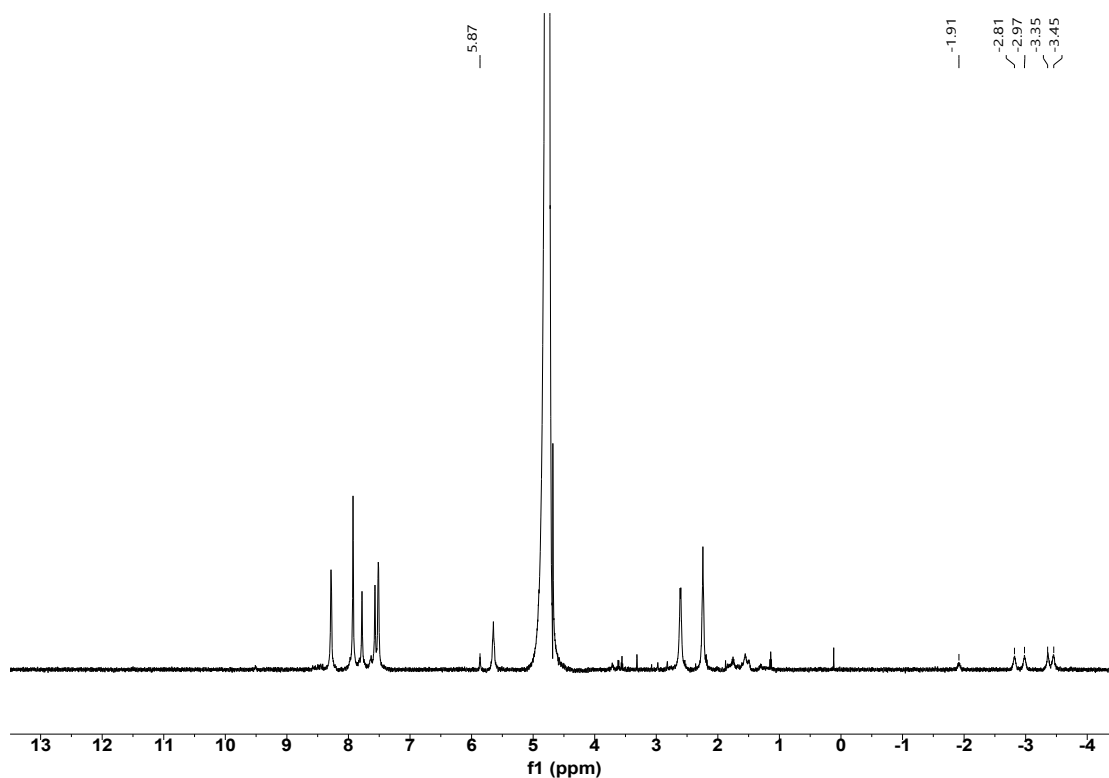
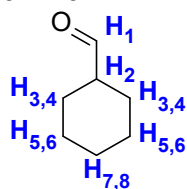


Figure S28. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S16: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	9.52	5.87	-3.65
H ₂	2.37	-1.91	-4.28
H ₃	1.60	-2.81	-4.41
H ₄	1.85	-2.97	-4.82
H ₅	1.63	-3.35	-4.98
H ₆	1.73	-3.45	-5.18

5.2.15 Guest:



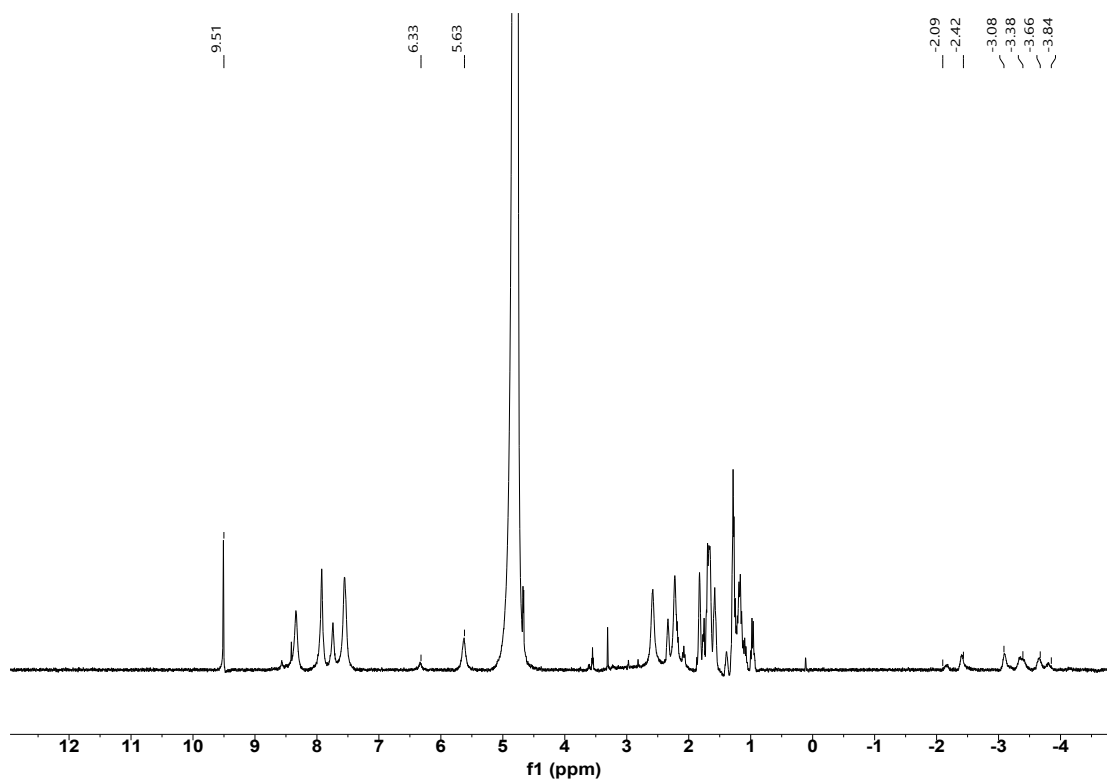


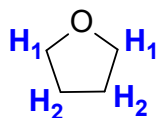
Figure S29. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1a** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S17: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	9.51	6.33	-3.18
H ₂	2.30	-2.09	-4.39
H ₃	1.77	-2.42	-4.19
H ₄	1.75	-3.08	-4.83
H ₅	1.57	-3.38	-4.95
H ₆	1.53	-3.40	-4.93
H ₇	1.52	-3.66	-5.18
H ₈	1.44	-3.84	-5.28

5.3 ^1H NMR for the complexation of cavitand **1b** with guests.

5.3.1 Guest:



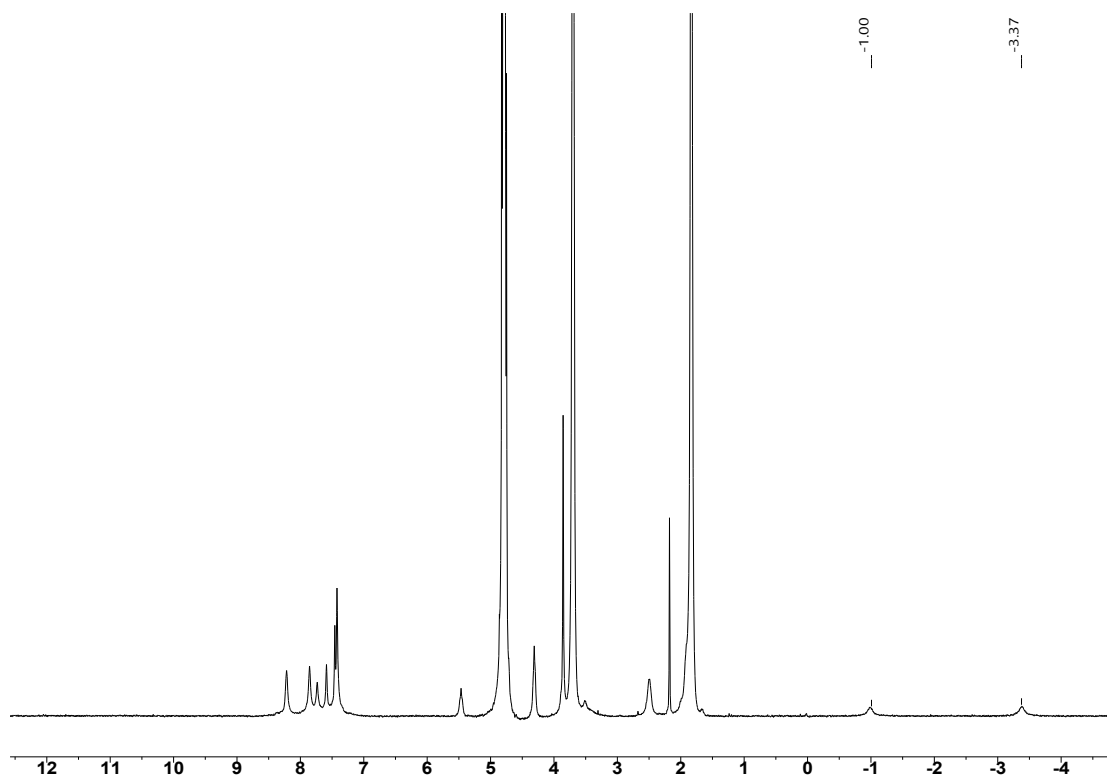
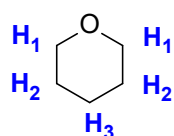


Figure S30. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S18: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H_1	3.70	-1.00	-4.70
H_2	1.84	-3.37	-5.11

5.3.2 Guest:



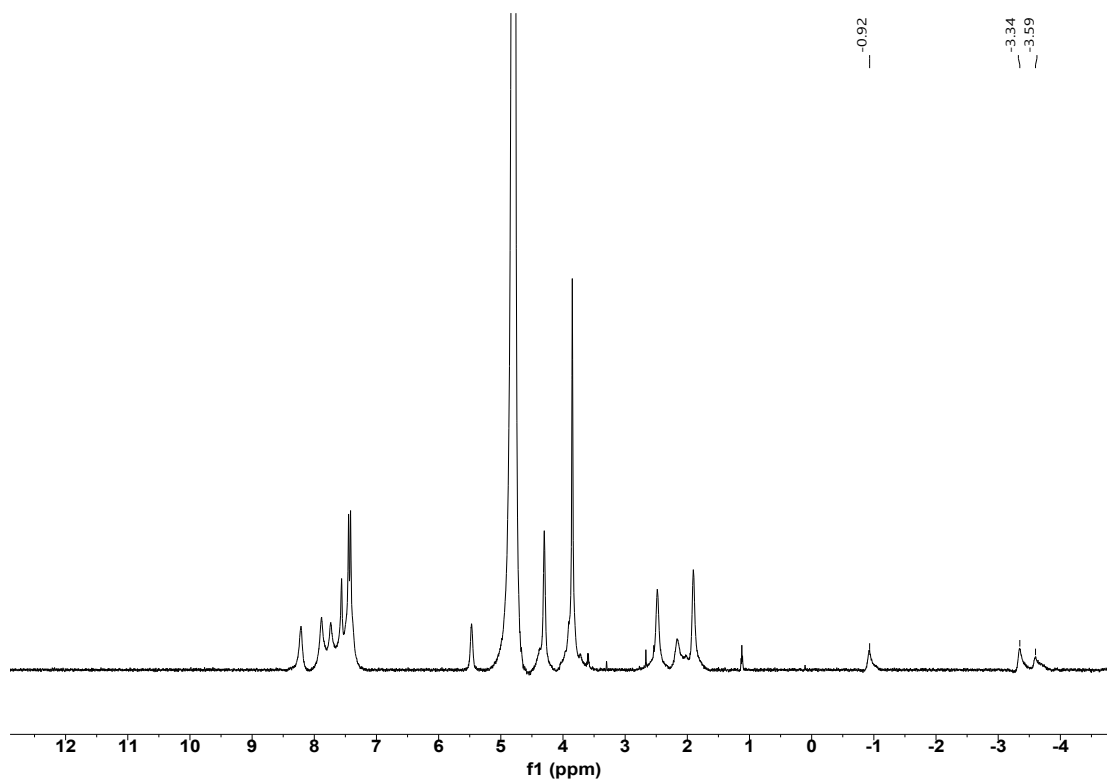
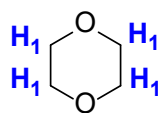


Figure S31. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S19: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.60	-0.92	-4.52
H ₂	1.60	-3.34	-4.94
H ₃	1.60	-3.59	-5.19

5.3.3 Guest:



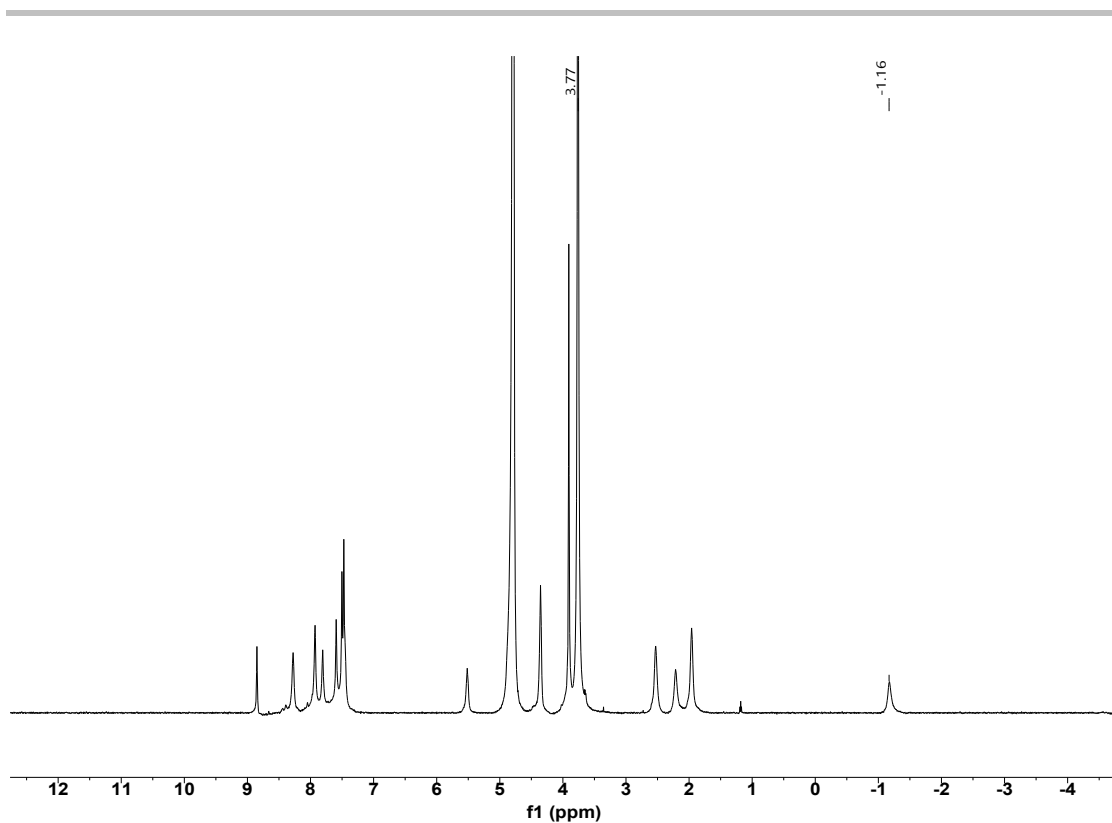
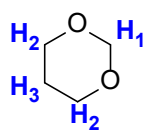


Figure S32. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S20: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H_1	3.77	-1.16	-4.93

5.3.4 Guest:



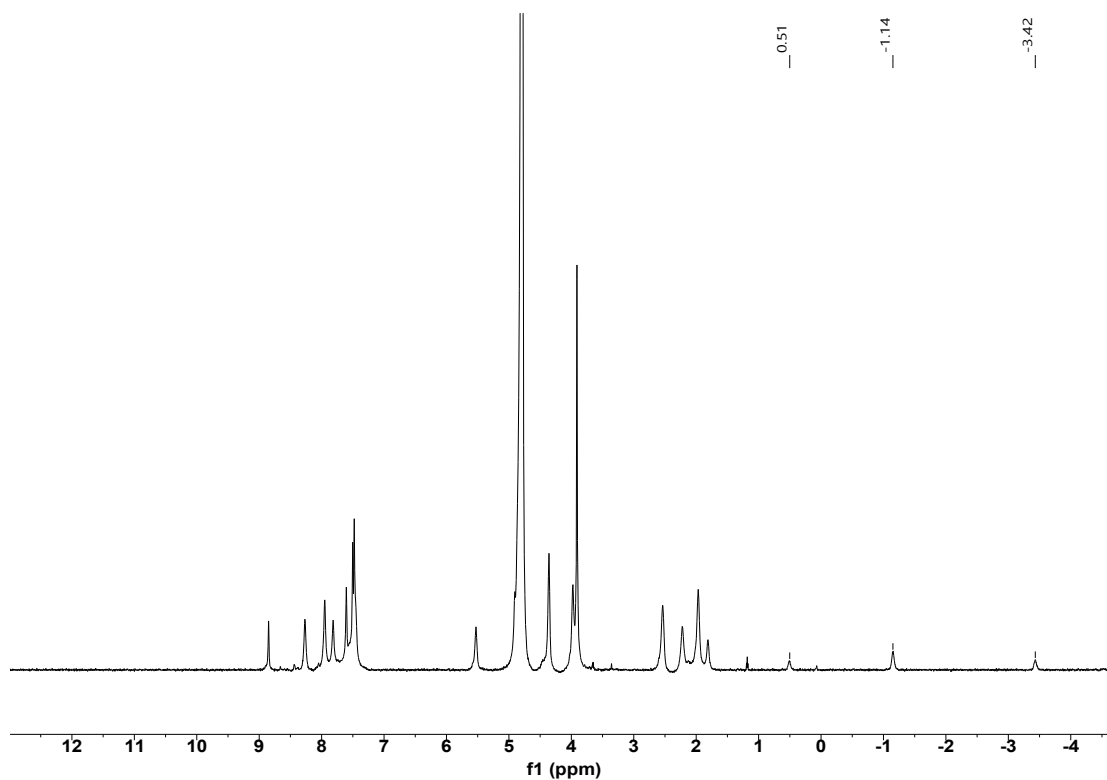
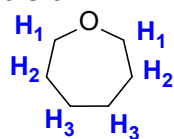


Figure S33. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S21: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	4.89	0.51	-4.38
H ₂	3.97	-1.14	-5.11
H ₃	1.80	-3.42	-5.22

5.3.5 Guest:



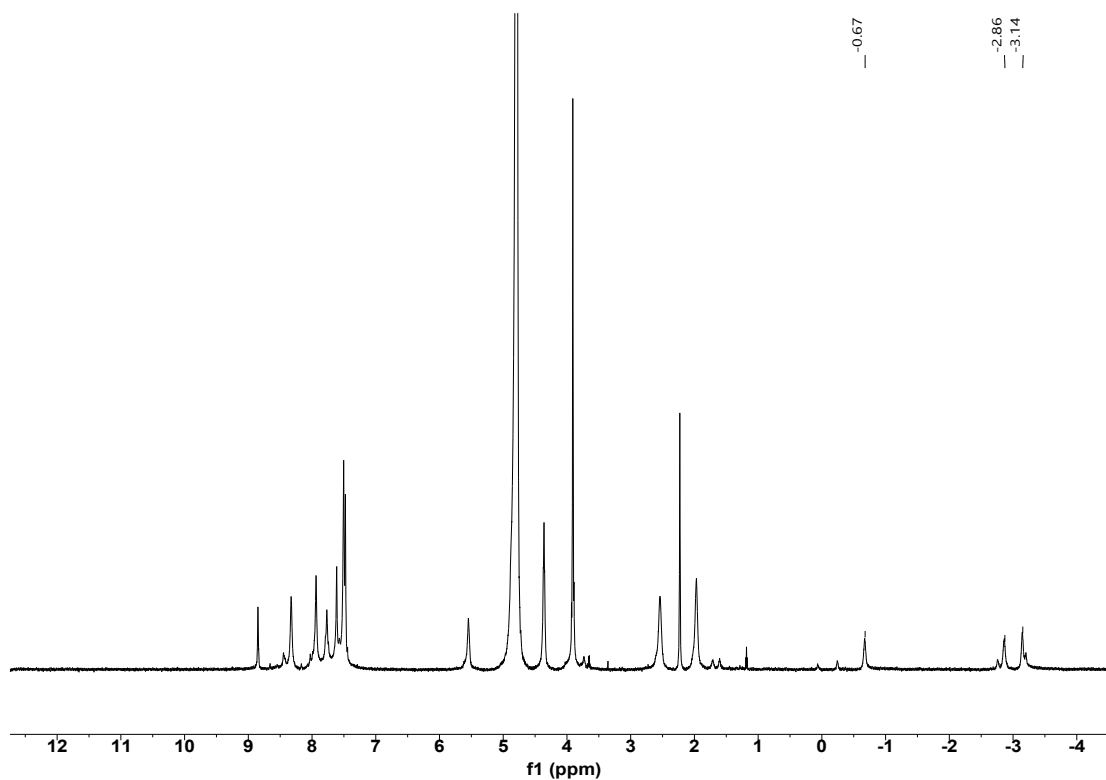
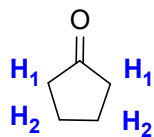


Figure S34. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S22: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.35	-0.67	-4.02
H ₂	1.44	-2.86	-4.30
H ₃	1.60	-3.14	-4.74

5.3.6 Guest:



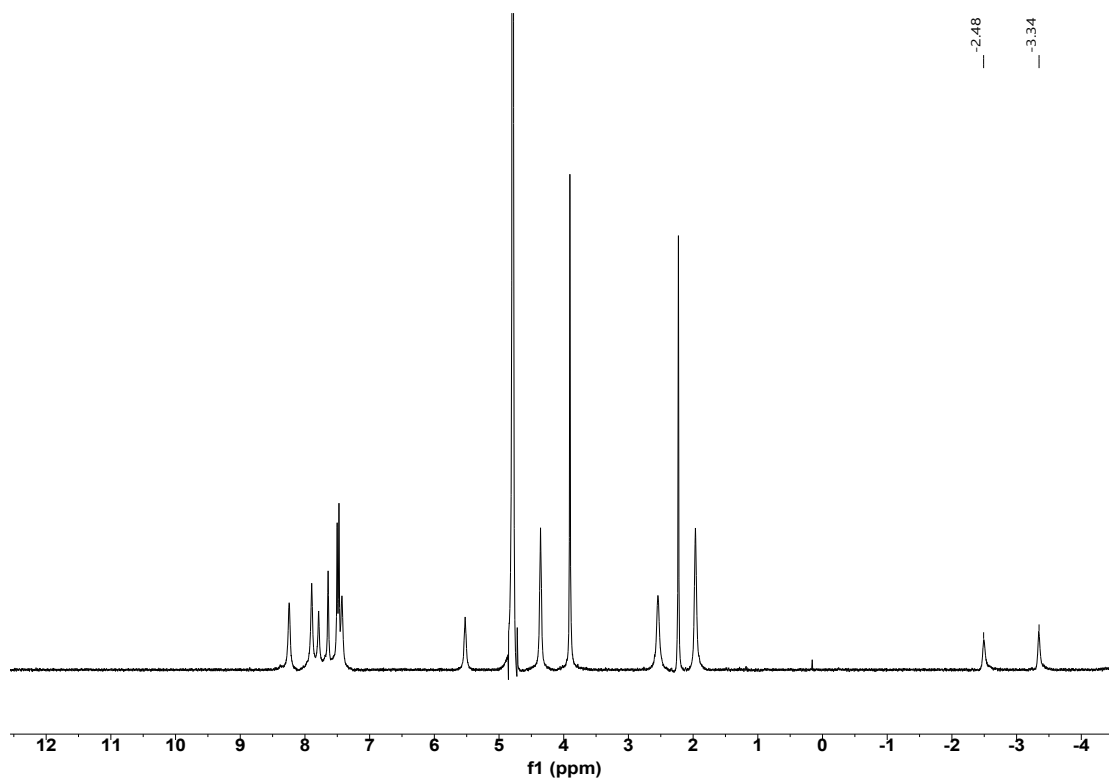
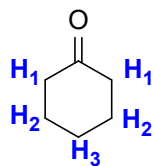


Figure S35. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S23: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	2.29	-2.48	-4.77
H ₂	1.97	-3.34	-5.31

5.3.7 Guest:



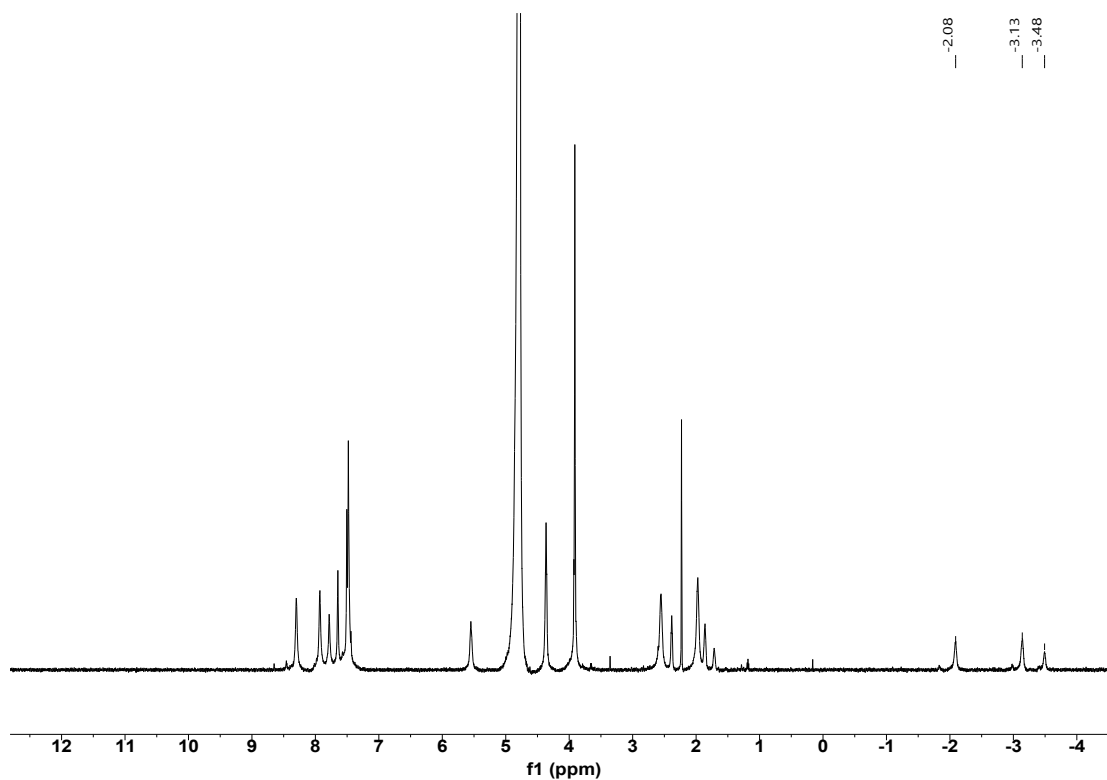
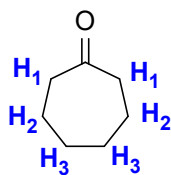


Figure S36. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S24: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	2.37	-2.08	-4.45
H ₂	1.84	-3.13	-4.97
H ₃	1.70	-3.48	-5.18

5.3.8 Guest:



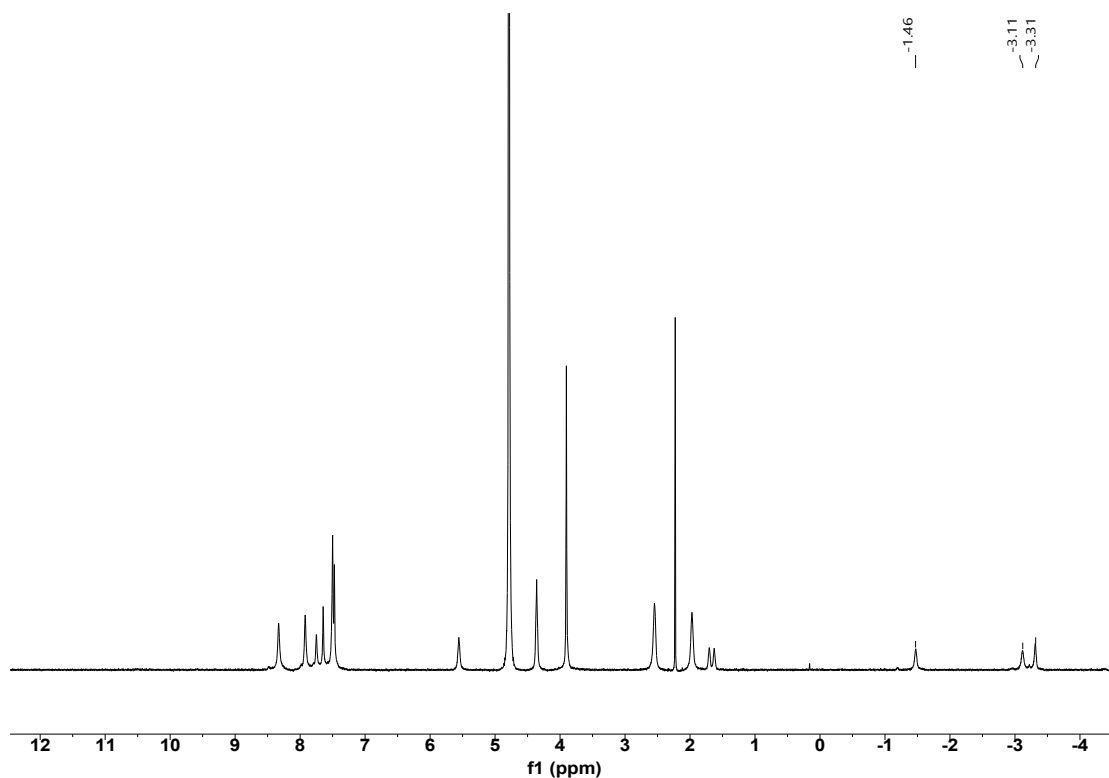
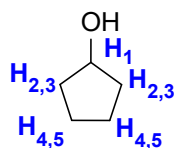


Figure S37. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S25: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	2.25	-1.46	-3.71
H ₂	1.72	-3.11	-4.83
H ₃	1.64	-3.31	-4.95

5.3.9 Guest:



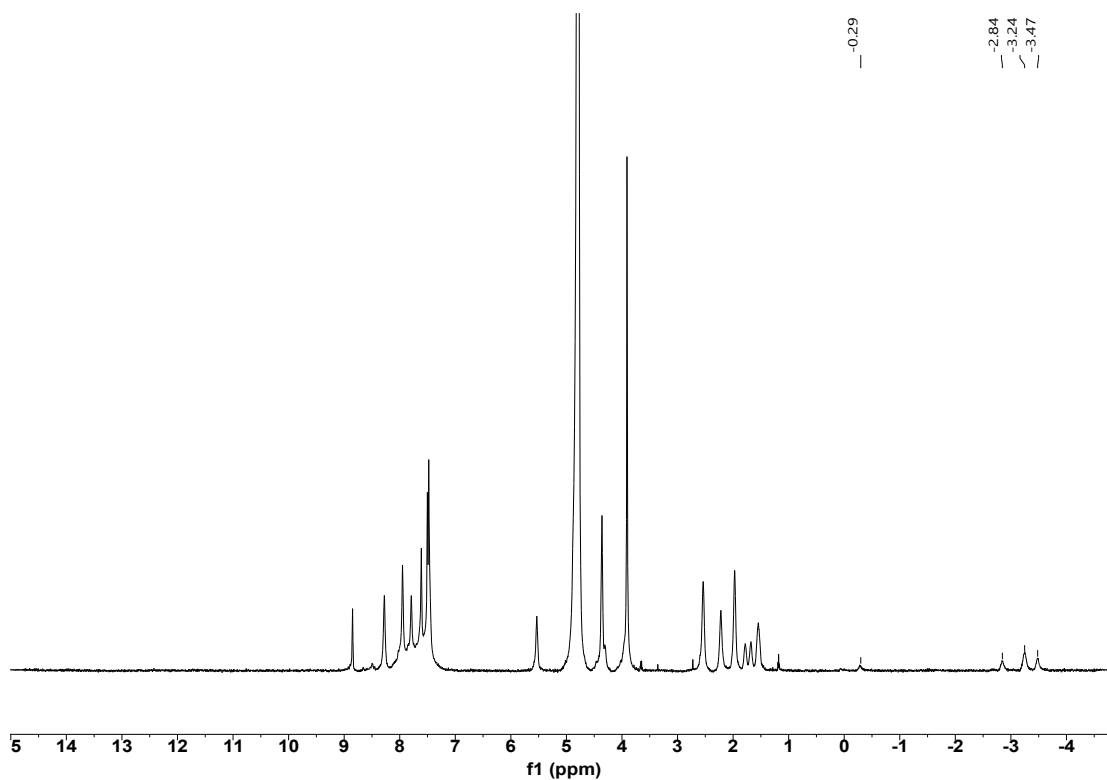
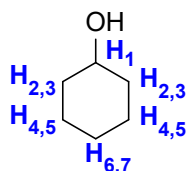


Figure S38. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S26: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H_1	4.30	-0.29	-4.59
$\text{H}_{2,3}$	1.78	-2.84	-4.62
H_4	1.67	-3.24	-4.91
H_5	1.71	-3.47	-5.18

5.3.10 Guest:



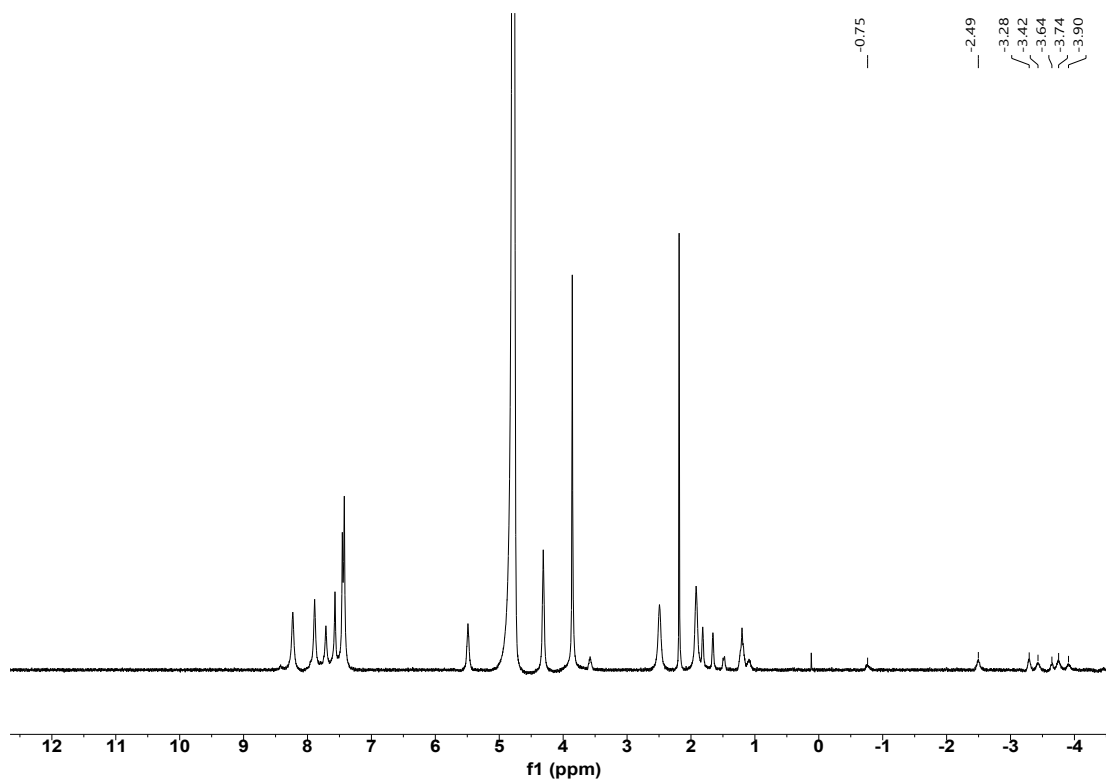
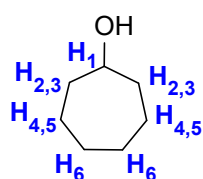


Figure S39. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S27: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.58	-0.75	-4.33
H ₂	1.85	-2.49	-4.07
H ₃	1.68	-3.28	-4.96
H ₄	1.53	-3.42	-4.95
H ₅	1.51	-3.64	-4.99
H ₆	1.46	-3.74	-5.20
H ₇	1.44	-3.90	-5.34

5.3.11 Guest:



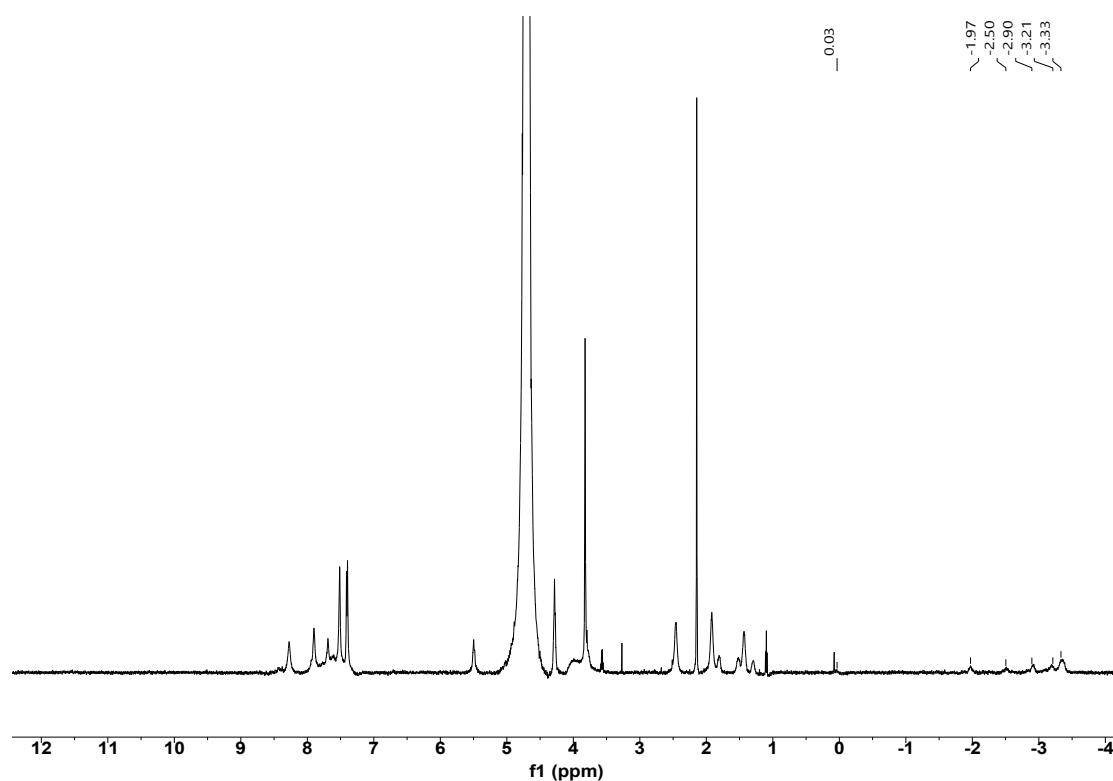
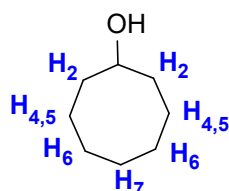


Figure S40. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S28: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	3.83	-0.03	-3.85
H ₂	1.87	-1.97	-3.84
H ₃	1.52	-2.50	-4.02
H ₄	1.58	-2.90	-4.48
H ₅	1.49	-3.21	-4.70
H ₆	1.36	-3.33	-4.69

5.3.12 Guest:



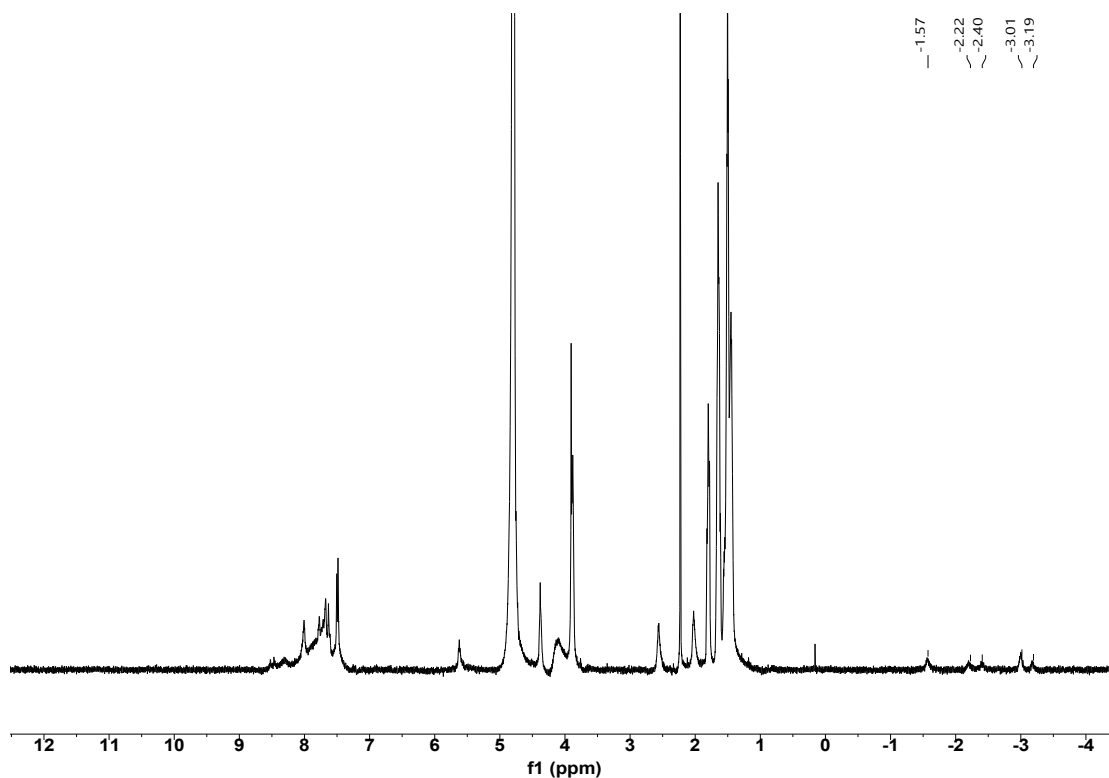
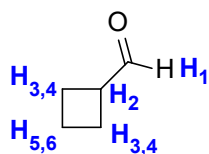


Figure S41. ^1H NMR spectra (600 MHz, 298 K) of the complex between host **1b** (1 mM) and guest (1: 1) mixture in D_2O

Table S29: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₂	1.80	-1.57	-3.37
H ₄	1.62	-2.22	-3.84
H ₅	1.56	-2.40	-3.96
H ₆	1.51	-3.01	-4.52
H ₇	1.45	-3.19	-4.64

5.3.13 Guest:



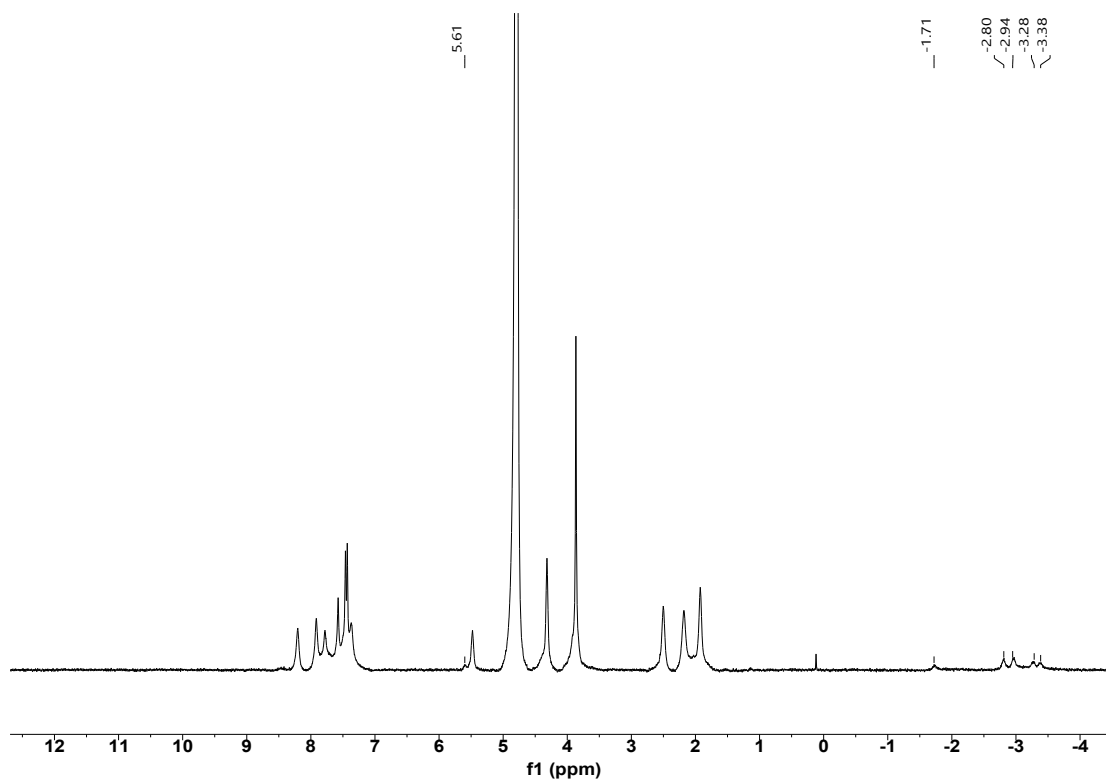
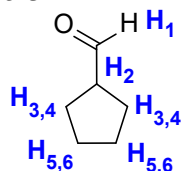


Figure S42. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S30: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	9.63	5.61	-4.02
H ₂	3.01	-1.71	-4.72
H ₃	1.98	-2.80	-4.72
H ₄	1.85	-2.94	-4.79
H ₅	1.70	-3.28	-4.98
H ₆	1.60	-3.38	-4.98

5.3.14 Guest:



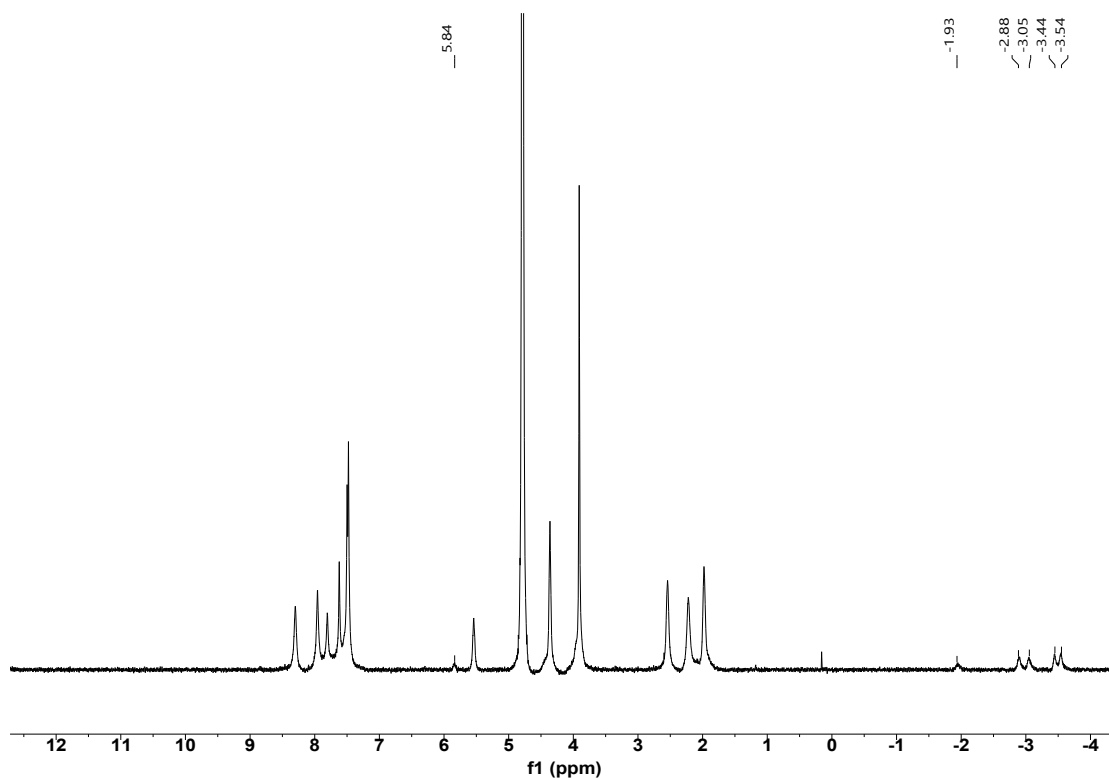
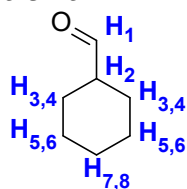


Figure S43. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S31: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	9.52	5.84	-3.68
H ₂	2.37	-1.93	-4.30
H ₃	1.60	-2.88	-4.48
H ₄	1.85	-3.05	-4.90
H ₅	1.63	-3.44	-5.07
H ₆	1.73	-3.54	-5.27

5.3.15 Guest:



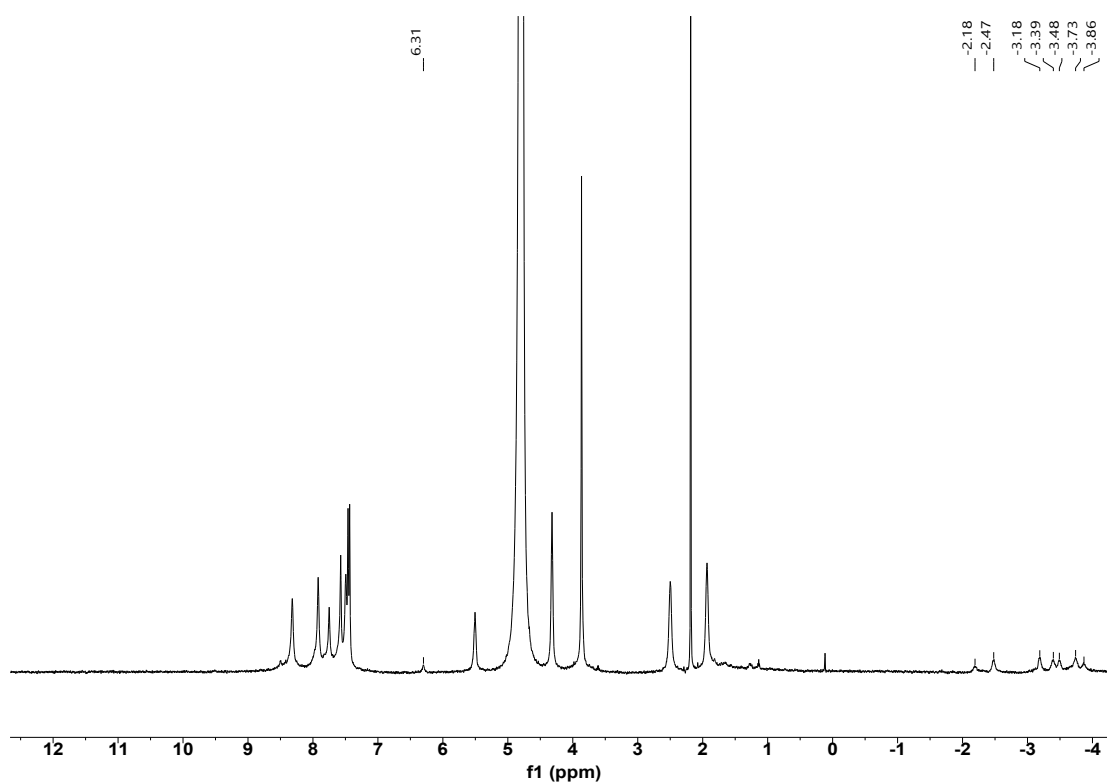


Figure S44. ^1H NMR spectra (600 MHz, D_2O , 298 K) of the complex between host **1b** (1 mM, 500 μL) and guest (100 mM, 5 μL).

Table S32: $\Delta\delta$ calculation of guest molecules.

Hydrogen	δ in D_2O (ppm)	δ in Cavitand (ppm)	$-\Delta\delta$ (ppm)
H ₁	9.51	6.31	-3.20
H ₂	2.30	-2.18	-4.48
H ₃	1.77	-2.47	-4.24
H ₄	1.75	-3.18	-4.93
H ₅	1.57	-3.39	-4.96
H ₆	1.53	-3.48	-5.01
H ₇	1.52	-3.73	-5.25
H ₈	1.44	-3.86	-5.30

5.4 Host-guest complexes of cavitand **1a** and cycloalkanes

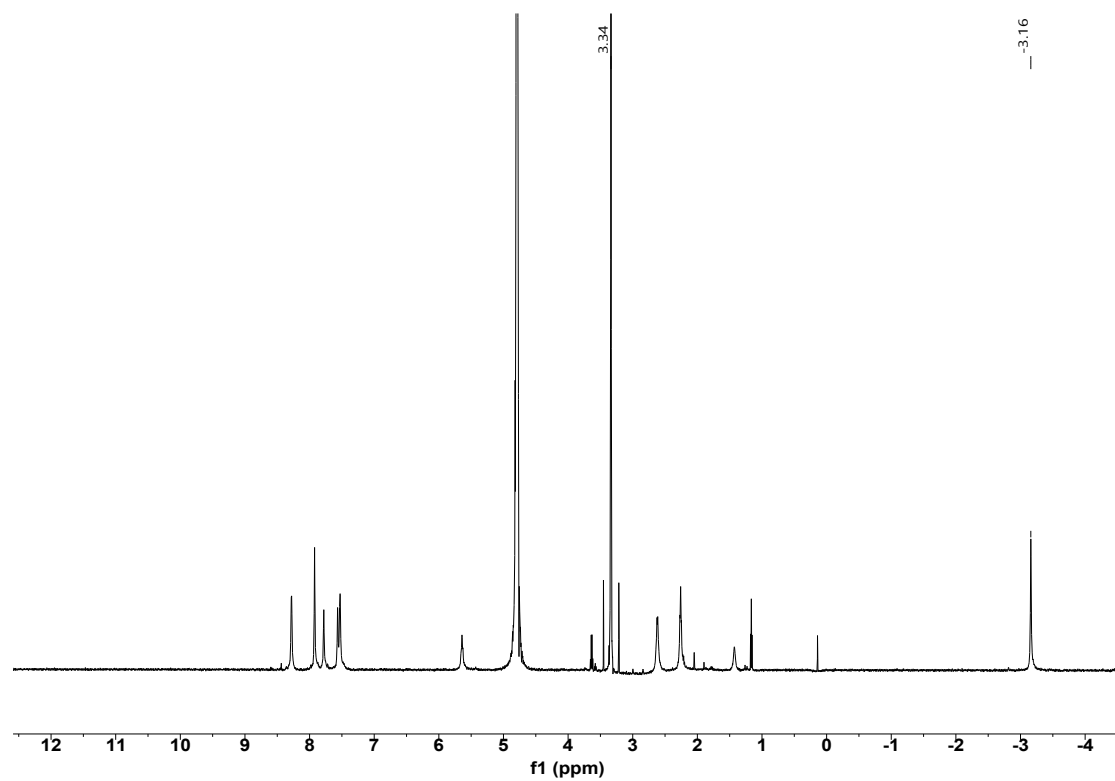


Figure S45. ^1H NMR spectra (600 MHz, 298 K, D_2O) of the complex between host **1a** and cyclopentane.

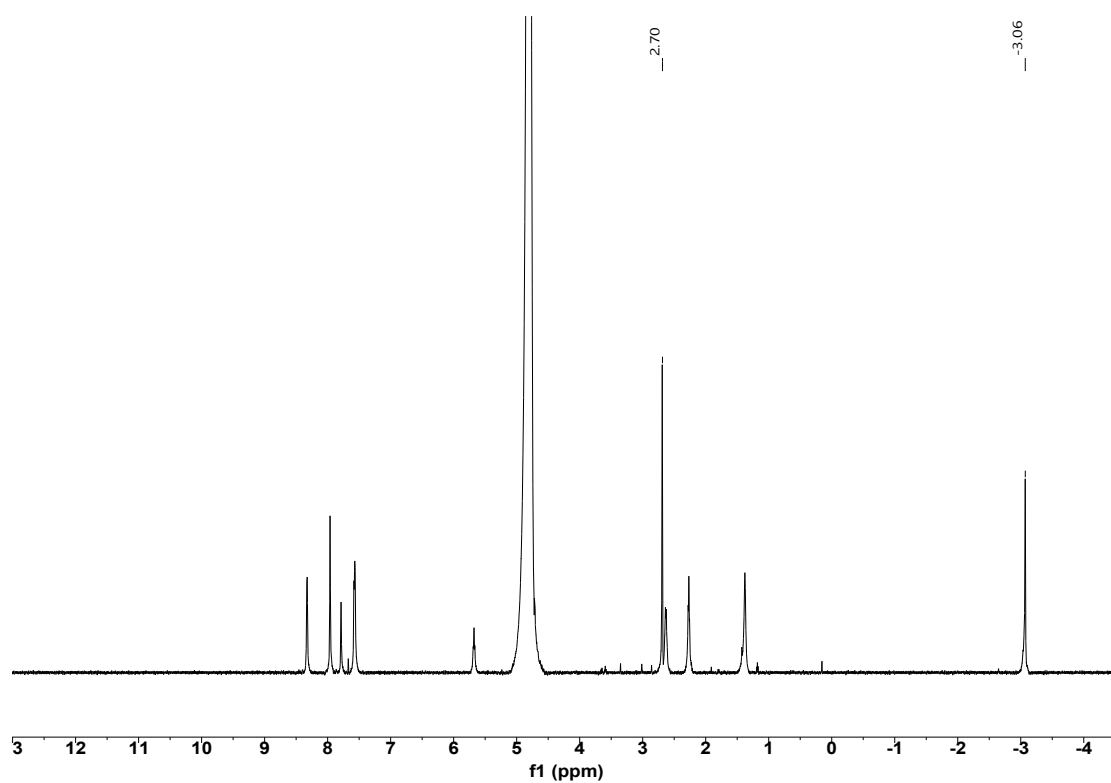


Figure S46. ^1H NMR spectra (600 MHz, 298 K, D_2O) of the complex between host **1a** and cyclohexane.

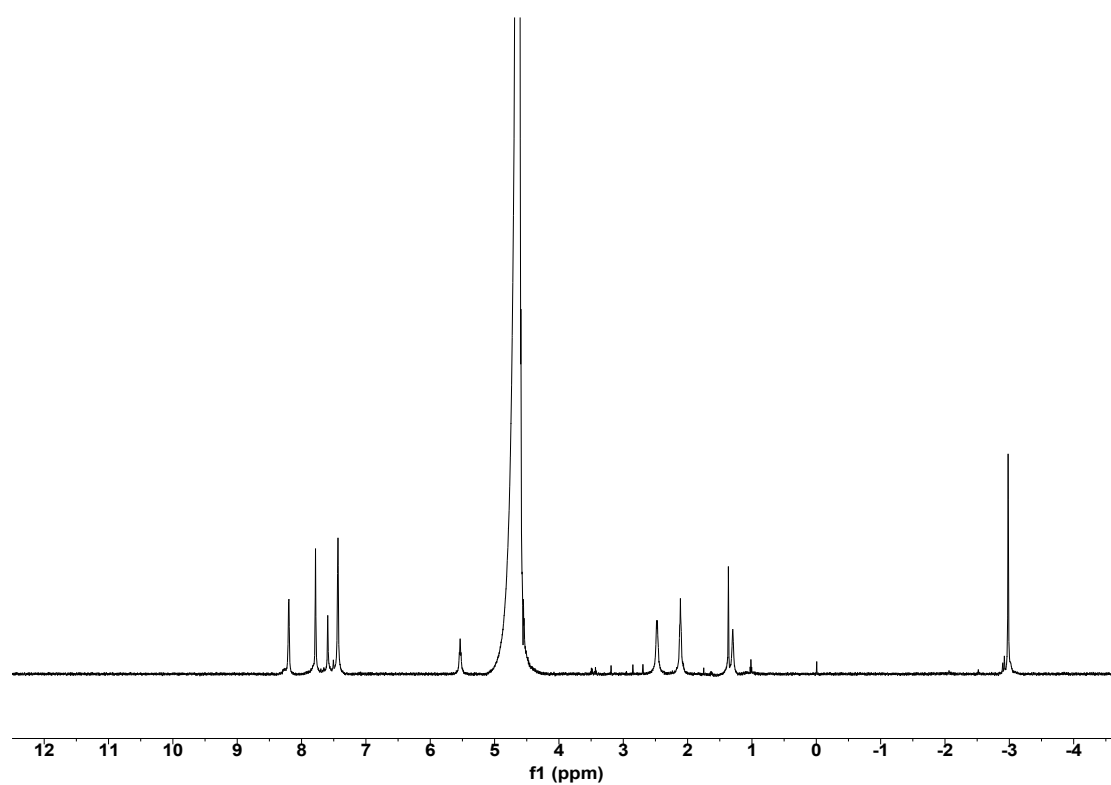


Figure S47. ^1H NMR spectra (600 MHz, 298 K, D_2O) of the complex between host **1a** and cycloheptane.

6. Isothermal titration calorimetry (ITC) experiments of cavitand **1b**

The binding constant was calculated by isothermal titration calorimetry (ITC), using cavitand **1b** as host and different guests (THF, 1,4-dioxane and cyclohexanone). ITC data were obtained on a VP-ITC MicroCalo-rimeter, MicroCal, LLC (North hampton, MA). Titrations were performed at 25°C with a host concentration of approximately 1 mM in the cell (1.45 mL), and a guest concentration of approximately 10 mM in the syringe. All solutions were prepared with distilled water. Injection volumes varied from 5 to 10 μ L, with a 360 s spacing between injections. After the reference titration was subtracted, the revised data were fitted to atheoretical titration curve using the One Set of Sites model of the Origin7.0 software provided by MicroCal, LLC.

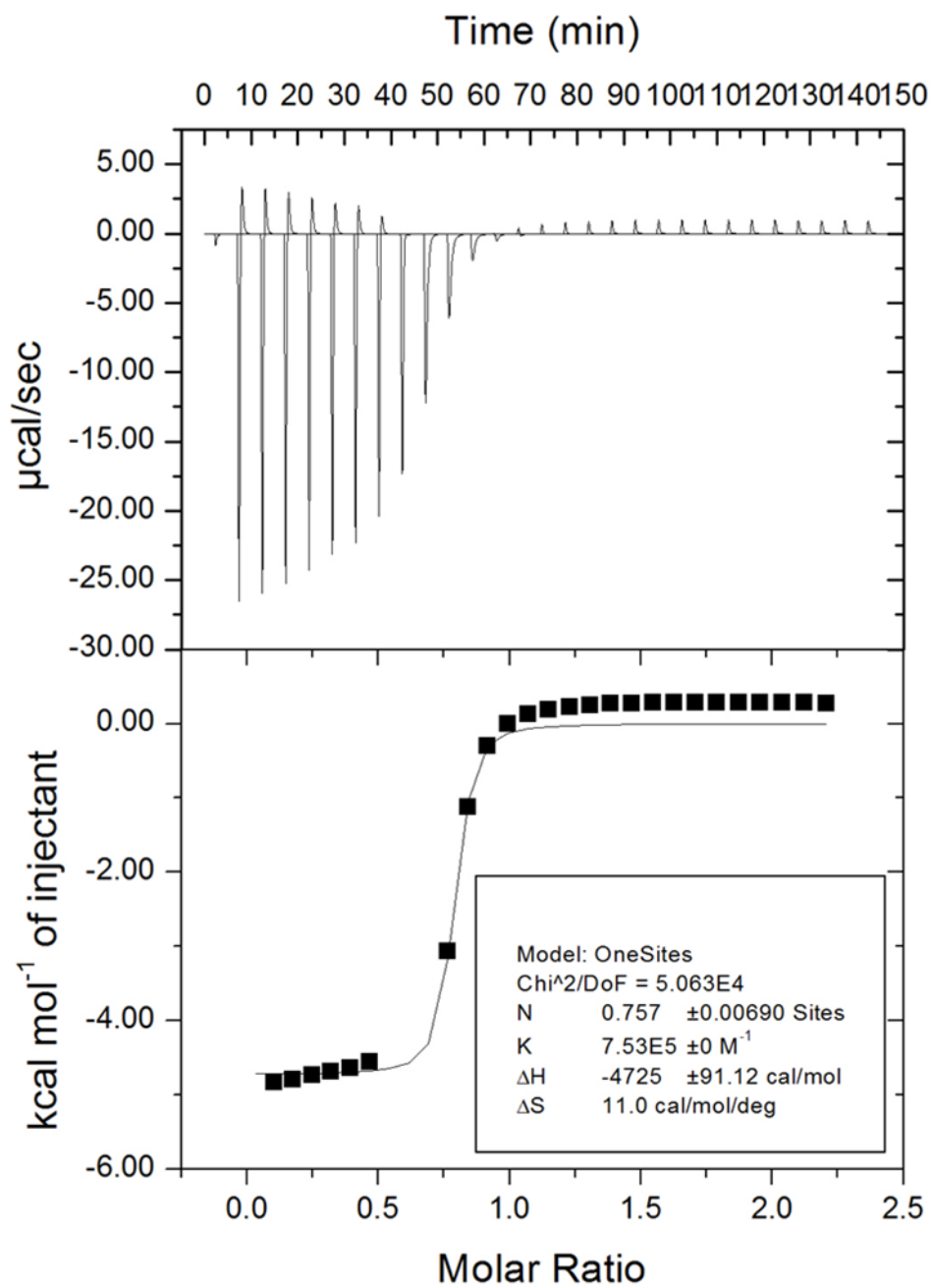


Figure S48. ITC experiments (298K) of cavitand **1b** and cyclohexanone, $K = 7.53 \times 10^5 \text{ M}^{-1}$.

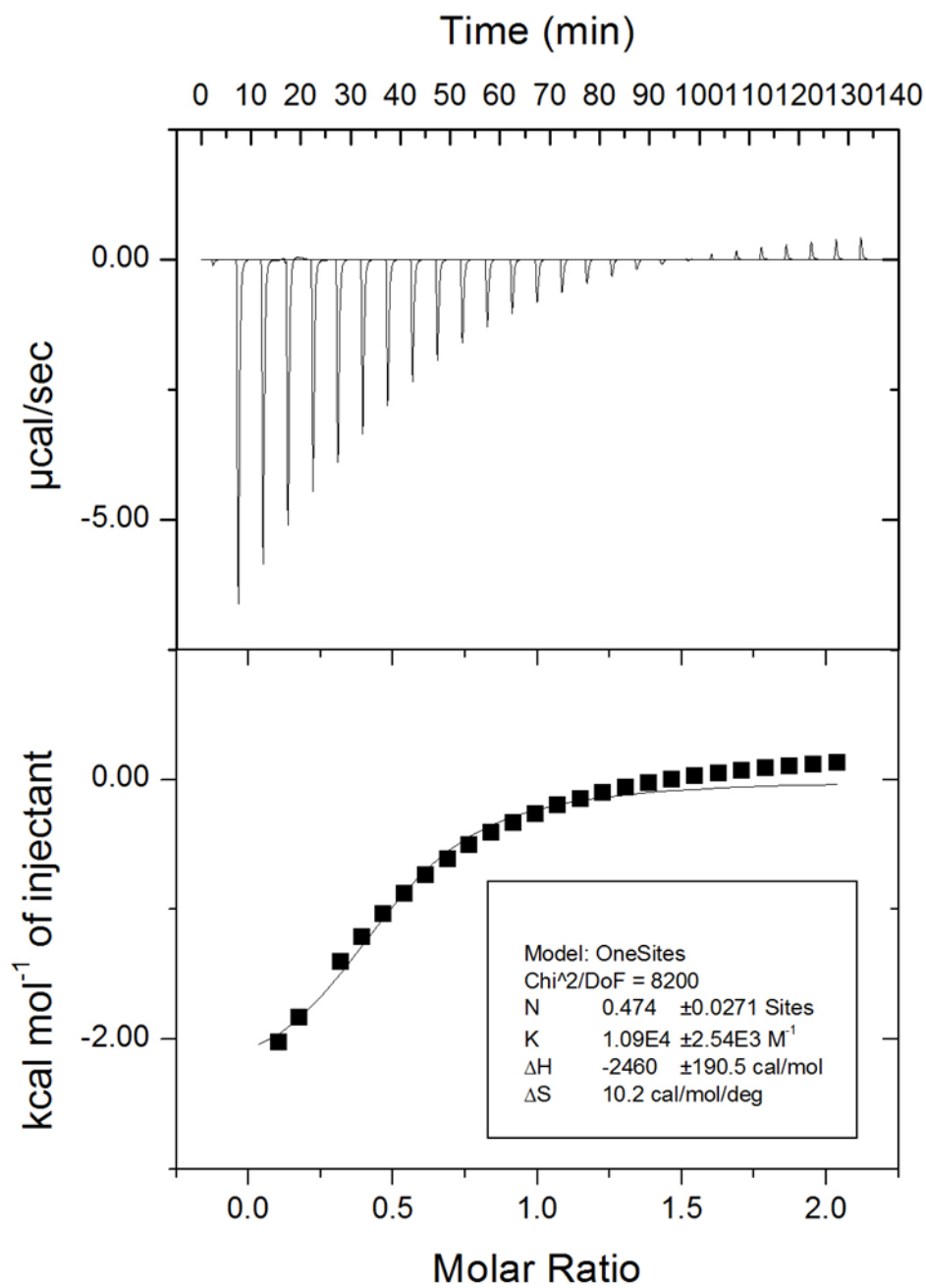


Figure S49. ITC experiments (298K) of cavitand **1b** and 1,4-dioxane, $K = 1.09 \times 10^4 \text{ M}^{-1}$.

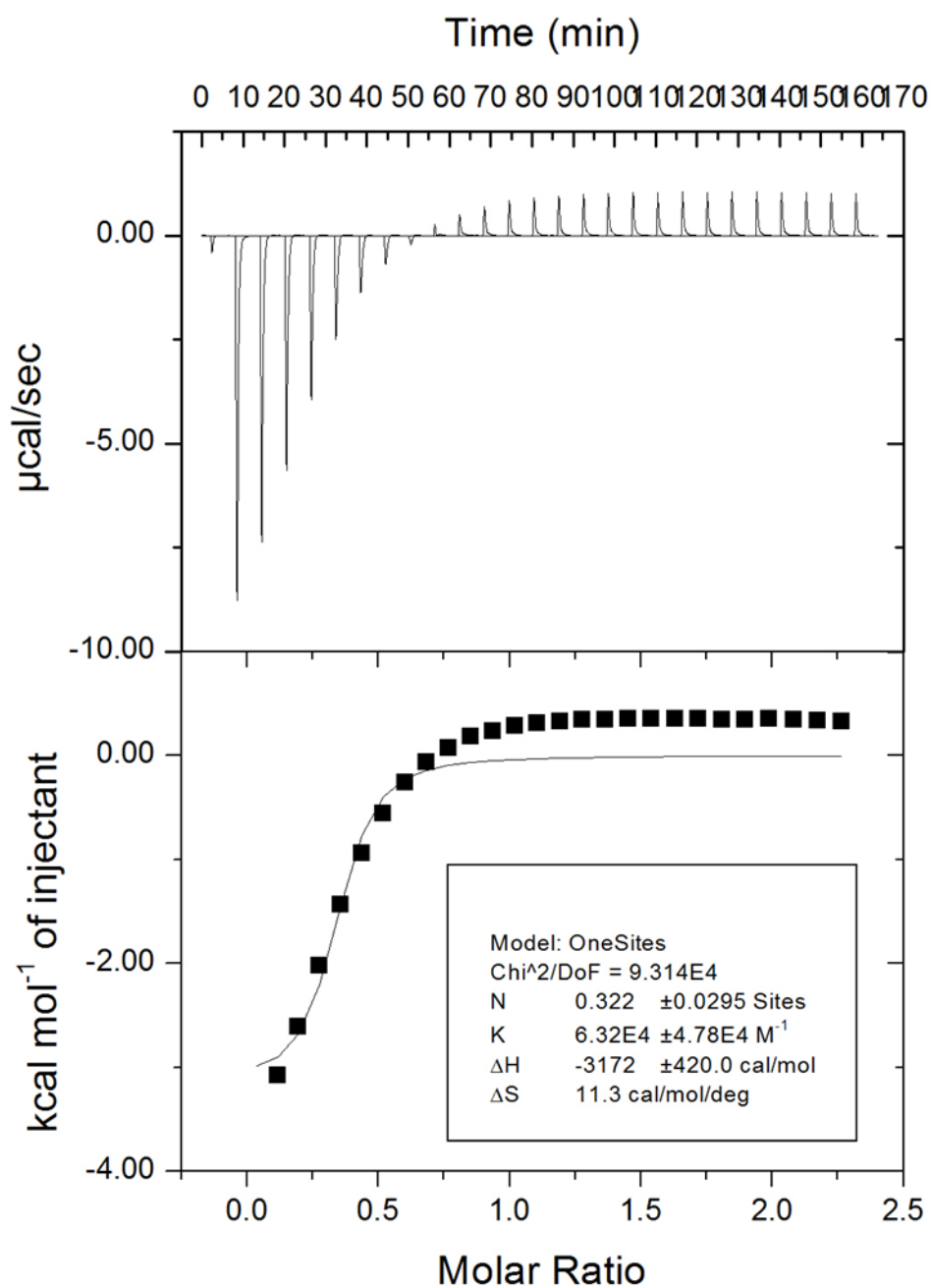


Figure S50. ITC experiments (298K) of cavitand **1b** and THF, $K = 6.32 \times 10^4 \text{ M}^{-1}$.

7. Computational details

All calculations were carried out using the B3LYP-D3(BJ) hybrid functional⁵ as implemented in the Gaussian 16 software package, revision C.01.⁶ The calculations included corrections for dispersion energy using Grimme's D3 dispersion method, coupled with the Becke-Johnson damping function.⁷

Geometry optimizations were performed using the 6-31G(d,p) basis set. The energies of these structures were then corrected for solvation using the SMD model⁸ employing the same basis set. The electronic energies were further refined by calculating single-point energies using the 6-311+G(2d,2p) basis set.

Frequencies were calculated at the same level of theory as the geometry optimizations to ensure that every structure is a minimum without imaginary frequencies and to provide Gibbs free energy corrections. The quasi-rigid-rotor-harmonic-oscillator approach (qRRHO) was then applied to correct the entropic contribution from low-frequency vibrational modes (i.e. smaller than 100 cm⁻¹).⁹

In all calculations, the feet of the cavitand were replaced by methyl groups, as has been done in previous studies.¹⁰

A number of conformations were examined for each host-guest complex in order to obtain the lowest-energy structure, with special attention being given to hydrogen bonding patterns between the guest and solvent molecules, as well as guest orientation inside the cavitand.

8. Models with different numbers of water molecules

We considered initially host-guest models with different numbers of water molecules (0, 4, 8, or 12) with THF as a representative guest. Geometries with a direct hydrogen bond between THF and the benzimidazole NH donor could not be located in any of the models. As shown in Figure S1, it was found that a total of twelve water molecules, four bridging at the seam and eight inside the cavitant, make a good geometric fit.

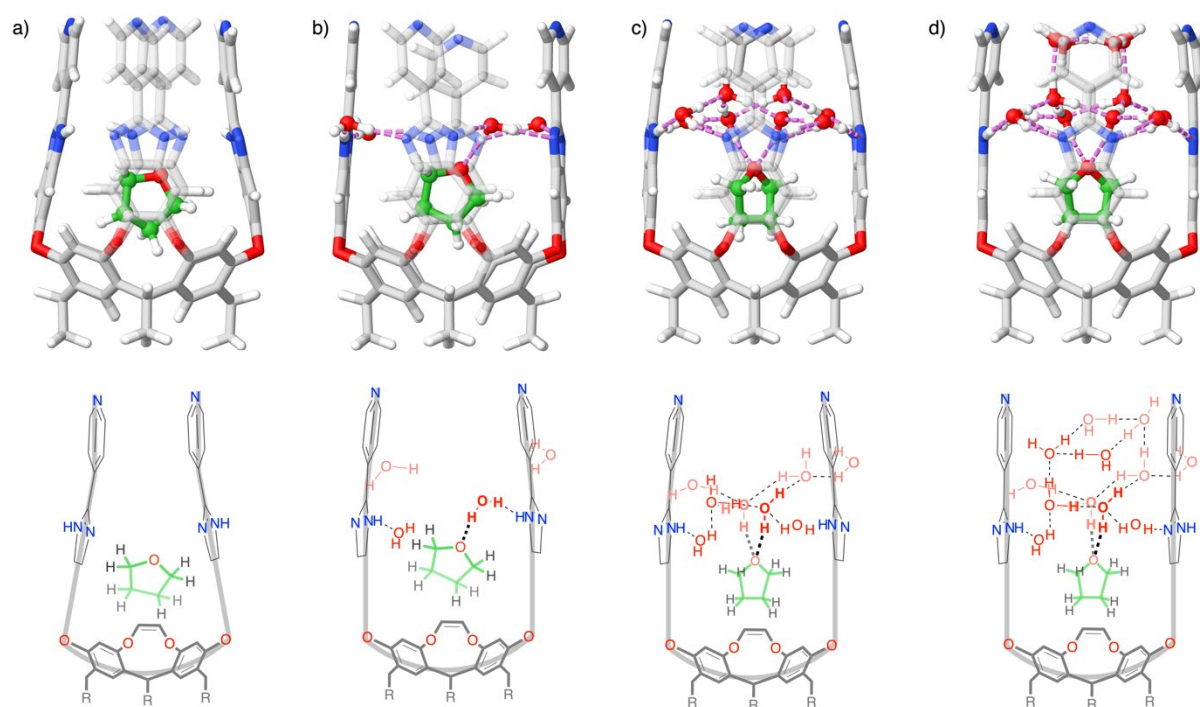


Figure S51. Models of THF binding in the cavitant considering a) zero, b) four, c) eight, and d) twelve water molecules.

8.1. Binding of THF

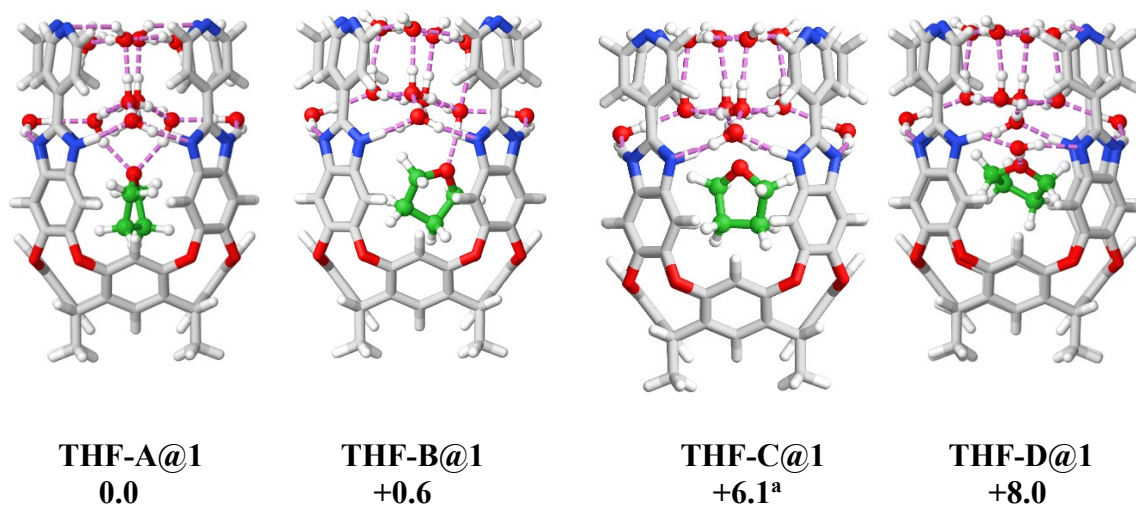


Figure S52. Different binding modes of THF in cavitant **1**. Relative energies are indicated in kcal/mol.

^a A small imaginary frequency ($6i\text{ cm}^{-1}$) was found in the vibrational analysis of this structure. It could not be eliminated despite many attempts to re-optimize the geometry. This imaginary frequency was treated as real in the qRRHO calculations of the thermal corrections to Gibbs free energy.

8.2. Binding of cyclopentanone

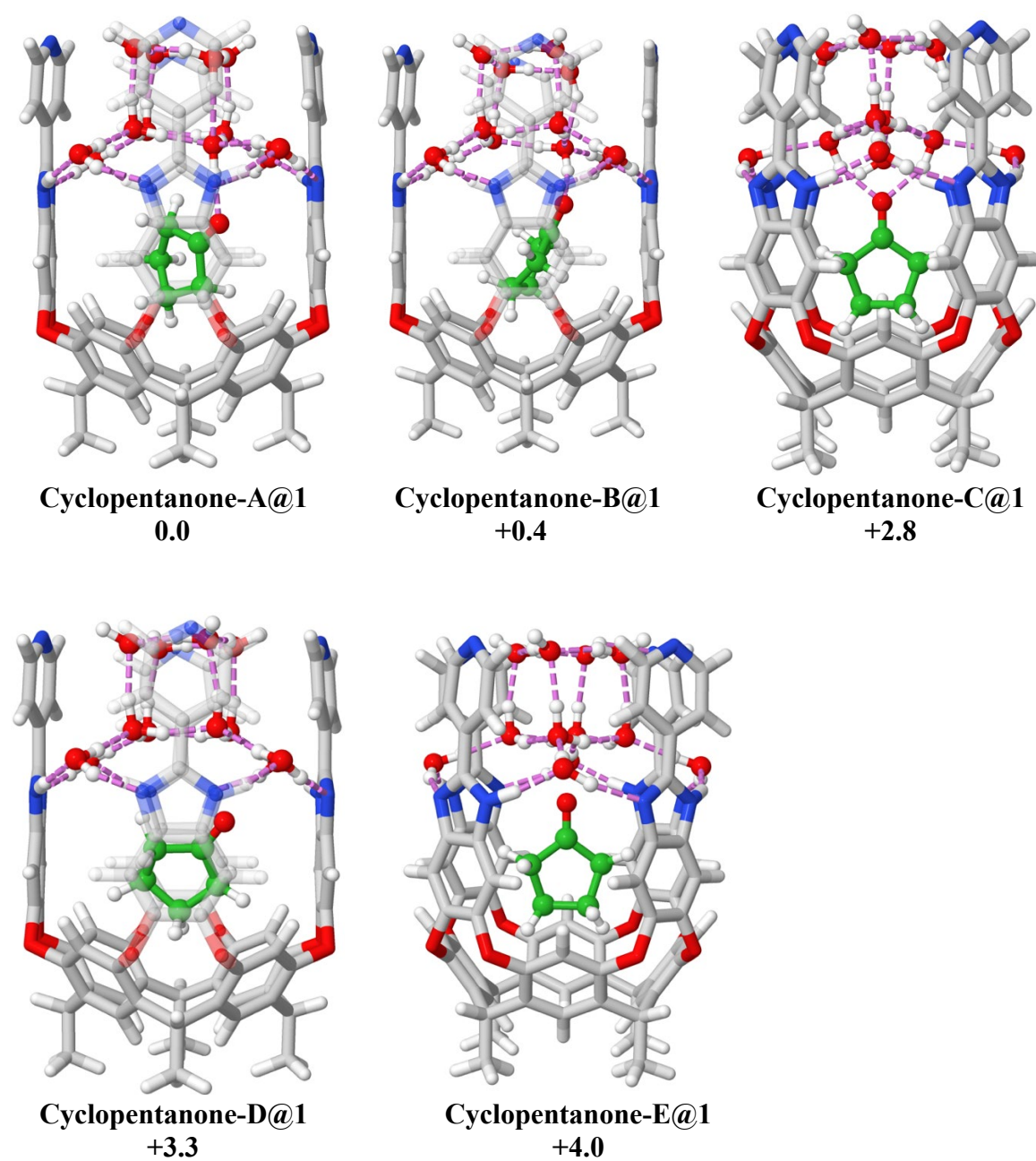


Figure S53. Different binding modes of cyclopentanone in cavitand **1**. Relative free energies are indicated in kcal/mol.

8.3. Binding of cyclopentanol

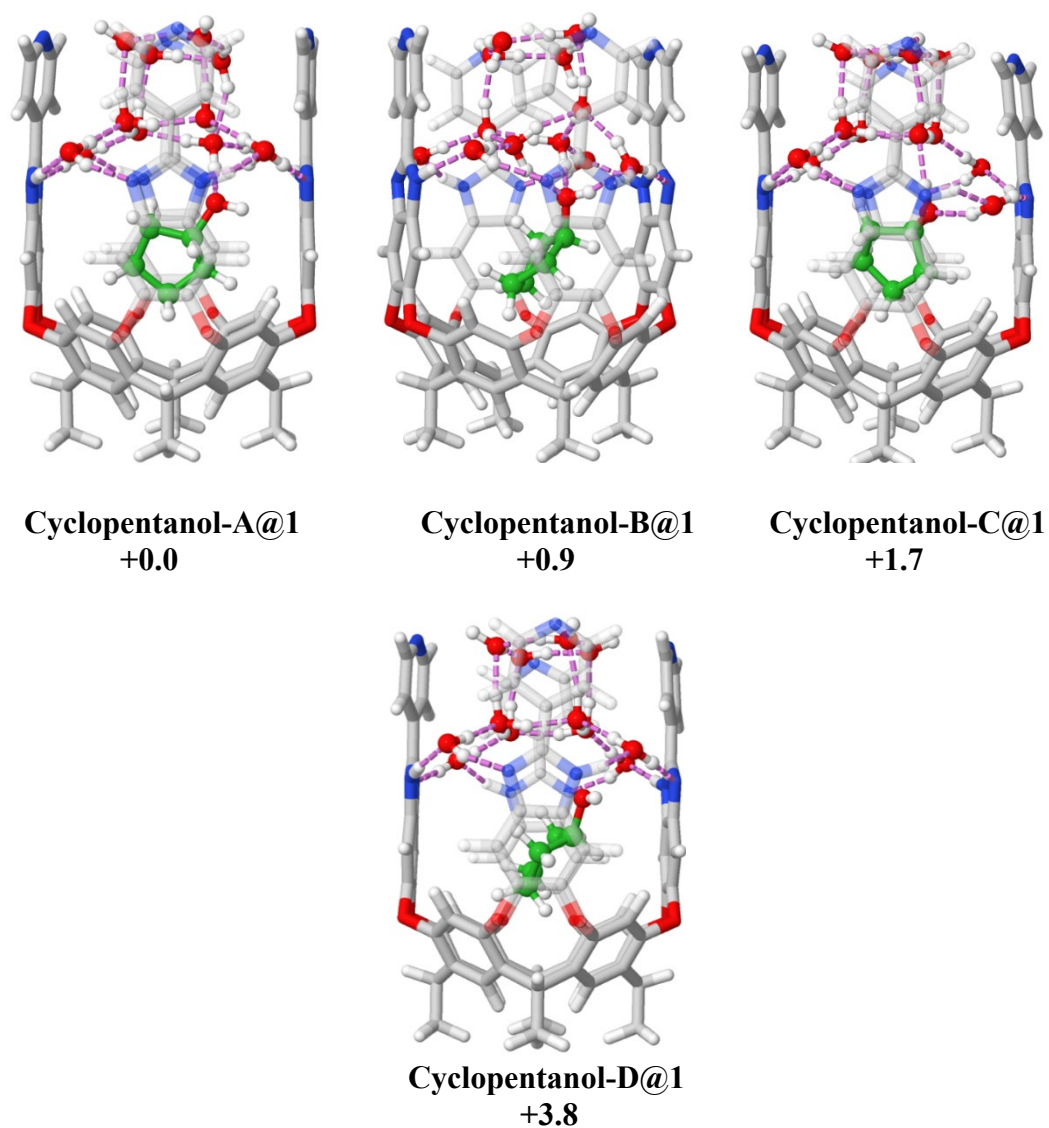


Figure S54. Different binding modes of cyclopentanol in cavitand **1**. Relative free energies are indicated in kcal/mol.

8.4. Binding of 1,4-dioxane

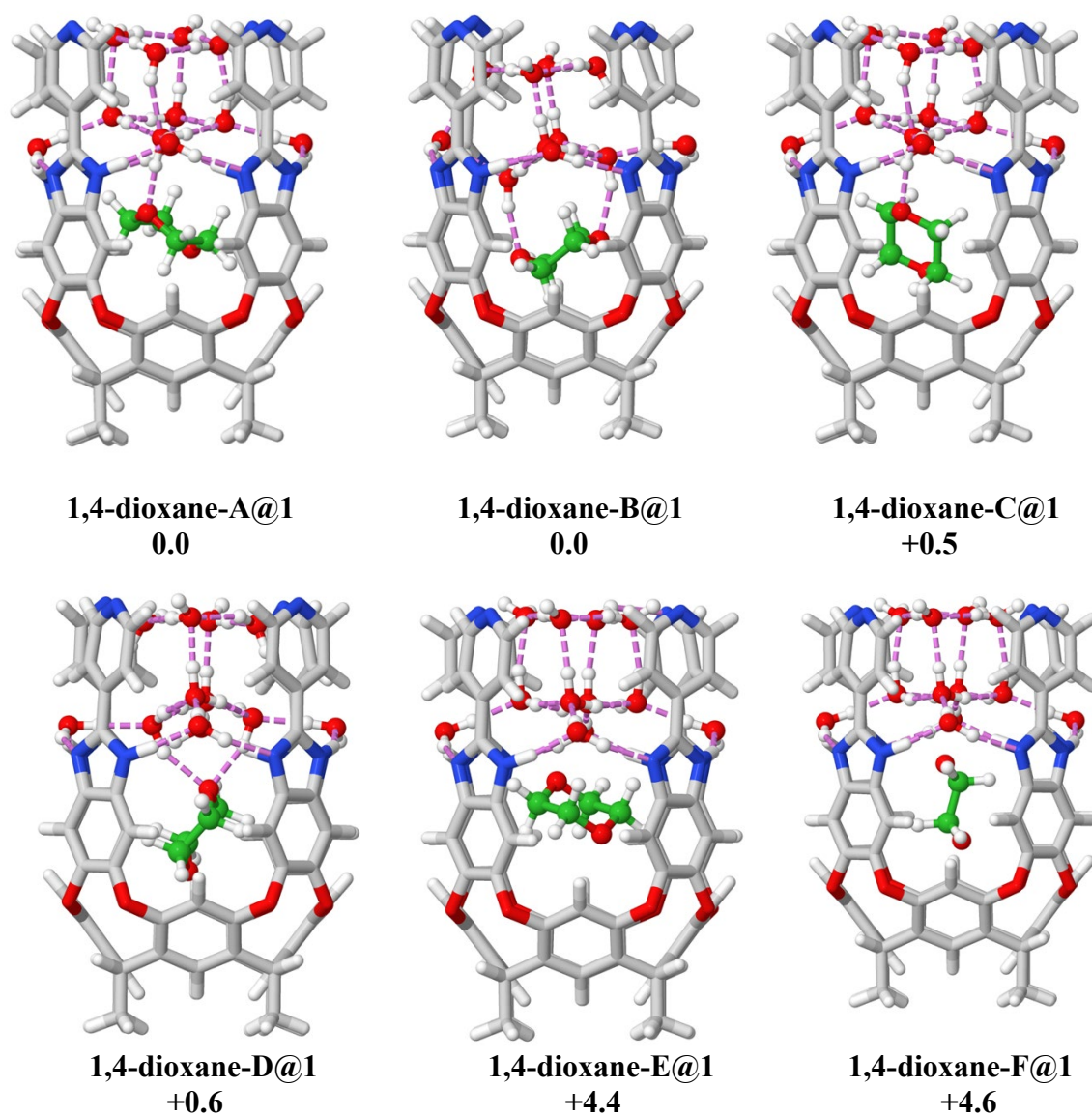


Figure S55. Different binding modes of 1,4-dioxane in cavitand **1**. Relative free energies are indicated in kcal/mol.

8.5. Binding of 1,3-dioxane

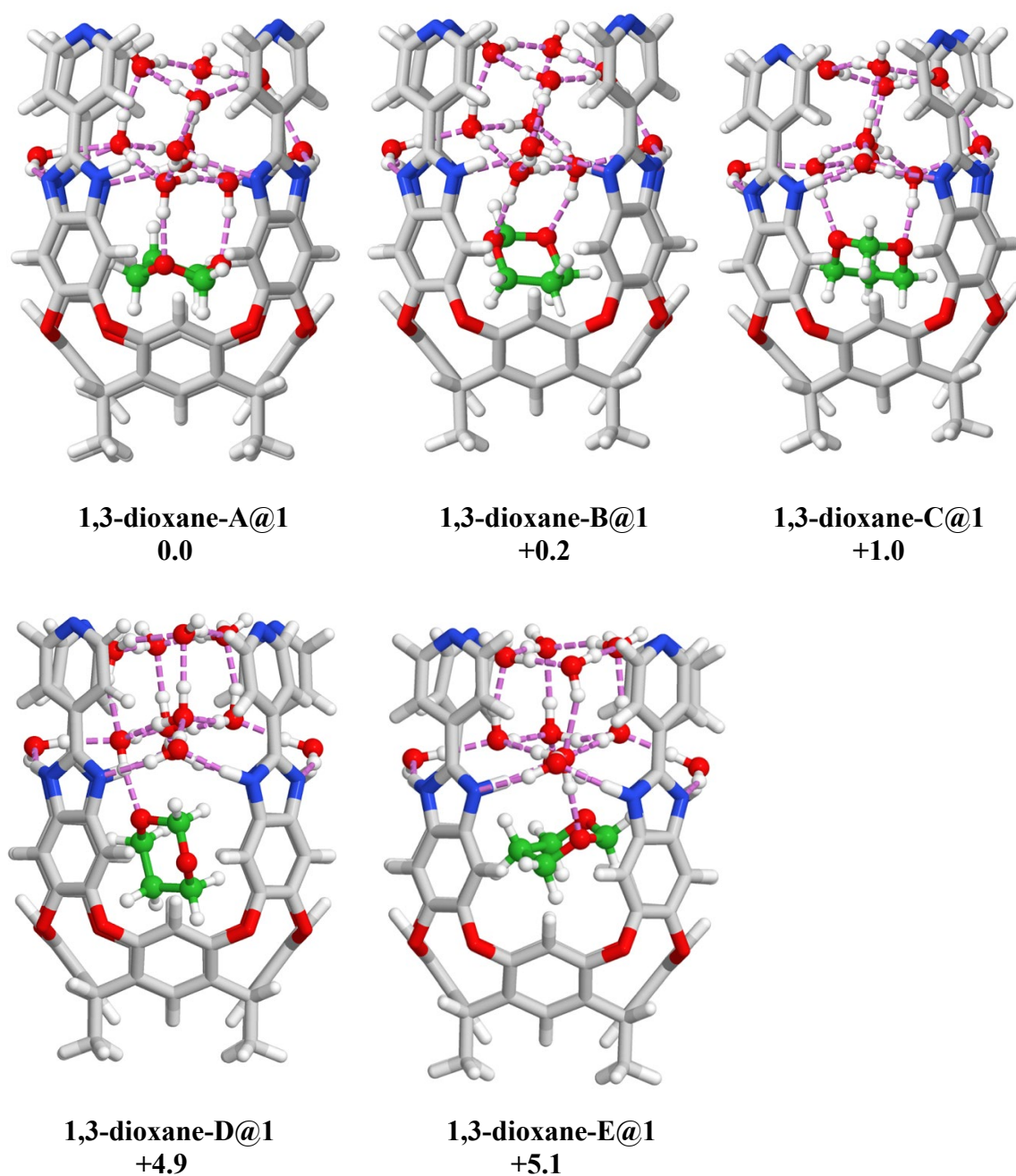


Figure S56. Different binding modes of 1,3-dioxane in cavitand **1**. Relative free energies are indicated in kcal/mol.

9. Non-covalent interaction plots

The non-covalent interaction (NCI) index enables the identification and classification of non-covalent interactions through a topological analysis of the electron density.[7] The calculations were carried out with NCIPLOT 4.0.1, using promolecular approximation, and cutoff values of 0.5 au for density and 1.0 au for reduced density gradient. The color scale in the figures below is $-0.04 < \rho < 0.04$ au, where green regions represent weak van der Waals interactions and blue regions represent attractive non-covalent interactions.

In the model without water molecules (Figure S57a), the THF and the cavitand interact through weak dispersion interactions. When water is included in the model (Figure S57b), the oxygen of THF establishes additional favorable hydrogen bonds with a water molecule (blue arrows). The water molecules interact with the cavitand either via hydrogen bonds with the benzimidazoles panels at the seam (Figure S57c, blue arrow), or via van der Waals interactions with the upper parts of the panel (Figure S57c, green arrow).

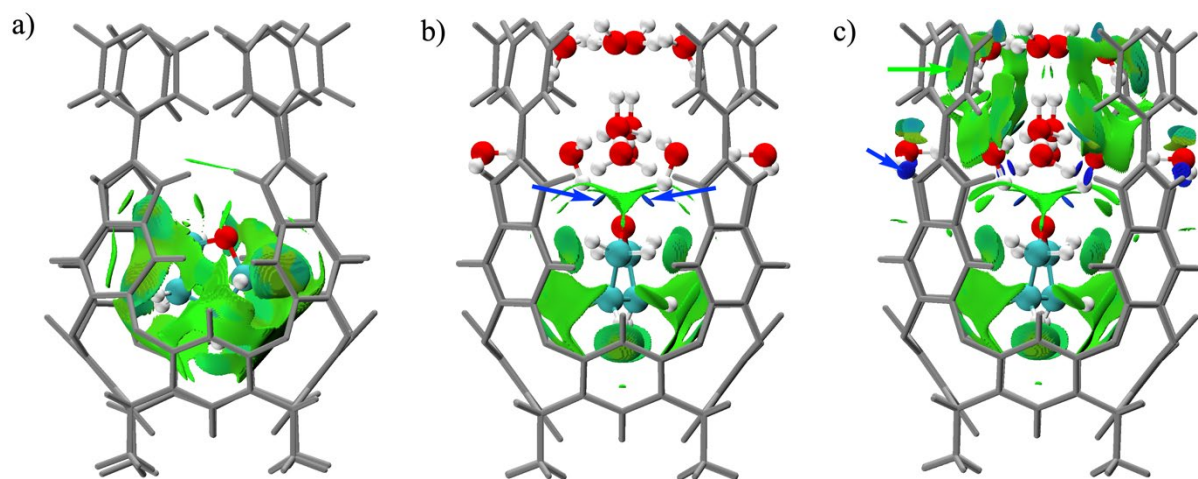


Figure S57. NCI plots for the intermolecular interactions in the host-guest complexes with THF. a) In the absence of water molecules, b) and c) with water molecules present. For clarity, b) shows the intramolecular interactions involving only the guest, while in c) all interactions are presented.

10. Cartesian coordinates

THF-A@1:

```
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C -4.9384260000 -0.6258330000 -3.1469810000
C -4.9481220000 -2.7155770000 -1.7634780000
H -5.2083190000 -2.5929570000 -3.8494050000
C -5.4781170000 0.5069280000 -2.5323230000
C -3.8111160000 -0.4390730000 -3.9549510000
C -5.4844450000 -2.5516080000 -0.4821870000
C -3.8398310000 -3.5629420000 -1.8927180000
C -4.9600370000 1.7938550000 -2.7079880000
H -6.3500130000 0.3847270000 -1.9003660000
C -3.2720280000 0.8252000000 -4.1635890000
O -3.2824420000 -1.5313330000 -4.6342550000
C -4.9795320000 -3.2000010000 0.6480180000
H -6.3385560000 -1.8953500000 -0.3617240000
C -3.3140680000 -4.2308860000 -0.7919350000
O -3.3053240000 -3.8120210000 -3.1540390000
C -5.5769110000 3.0134060000 -2.0363150000
C -3.8350710000 1.9286770000 -3.5317440000
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C -4.9593310000 -1.7944380000 2.7084780000
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O -3.3717860000 -4.7372550000 1.5591280000
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C -7.1115790000 2.9849960000 -2.0287610000
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C -0.9094220000 -3.1656610000 3.8128480000
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H	-0.9003840000	-2.5919140000	4.7309650000	C	3.7828060000	3.9812010000	-2.4846940000
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C	-0.8951580000	-3.8584270000	-3.0670600000	C	5.8006260000	4.8280160000	-1.4861050000
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C	-0.8811430000	-1.4188190000	-4.5671680000	C	5.9619200000	3.0767950000	-2.9445430000
H	-0.8828860000	-0.5241300000	-5.1752640000	H	4.1507750000	2.3287210000	-3.8370190000
C	-0.9105890000	3.1660870000	-3.8130210000	H	6.3087880000	5.5217640000	-0.8198230000
H	-0.9016160000	2.5924590000	-4.7312140000	H	6.5961690000	2.3395350000	-3.4280980000
C	-0.9735500000	4.7810900000	-1.4496290000	C	3.8431070000	-2.6427700000	-3.7256130000
H	-1.0053880000	5.4319750000	-0.5859550000	C	4.5625900000	-1.6622980000	-4.4275920000
N	1.6041270000	3.3414940000	-3.5321600000	C	4.5792070000	-3.6084690000	-3.0230420000
N	1.5339930000	4.6205130000	-1.6838610000	C	5.9557240000	-1.6989110000	-4.3927000000
N	1.6204930000	3.6143900000	3.1737430000	H	4.0637280000	-0.8715360000	-4.9749600000
N	1.6214360000	1.7045820000	4.3513250000	C	5.9688480000	-3.5441990000	-3.0568770000
N	1.6052600000	-3.3408920000	3.5316480000	H	4.0821160000	-4.3756380000	-2.4444680000
N	1.5350030000	-4.6203390000	1.6836510000	H	6.5277860000	-0.9421570000	-4.9237210000
N	1.6208480000	-3.6148120000	-3.1741760000	H	6.5545750000	-4.2829140000	-2.5135480000
N	1.6215580000	-1.7044040000	-4.3507290000	C	3.7838660000	-3.9806370000	2.4842280000
H	1.8453280000	-4.8756090000	0.7240410000	C	4.4222170000	-4.9014560000	1.6391870000
H	1.9443710000	-0.7623200000	-4.6263890000	C	4.5899410000	-3.0641860000	3.1738080000
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H	1.9445800000	0.7624910000	4.6267110000	H	3.8623420000	-5.6390010000	1.0797130000
O	2.5542890000	-4.6722740000	-0.7980170000	C	5.9628790000	-3.0761550000	2.9444570000
H	2.0941030000	-4.5472080000	-1.6611800000	H	4.1514570000	-2.3280800000	3.8365030000
H	2.8526900000	-3.7564720000	-0.5992480000	H	6.3101550000	-5.5209230000	0.8195740000
O	2.5376650000	0.8439430000	-4.3280620000	H	6.5970650000	-2.3389090000	3.4281310000
H	2.1359250000	1.7422790000	-4.3629340000	N	6.5769680000	-3.9226420000	2.1020960000
H	2.5553150000	0.6660580000	-3.3607240000	N	6.6662380000	-2.6167980000	-3.7264710000
O	2.5537720000	4.6719590000	0.7976310000	N	6.5758280000	3.9233450000	-2.1021220000
H	2.8516690000	3.7560130000	0.5988220000	N	6.6660220000	2.6175480000	3.7272160000
H	2.0933880000	4.5473500000	1.6607390000	C	2.3226030000	-3.9630090000	2.5981370000
O	2.5376130000	-0.8431710000	4.3266340000	C	2.3771390000	2.6702000000	3.7300400000
H	2.1363200000	-1.7417420000	4.3618830000	C	2.3215290000	3.9633990000	-2.5985890000
H	2.5538060000	-0.6651770000	3.3592530000	C	2.3773970000	-2.6703100000	-3.7300780000
C	3.8428340000	2.6427880000	3.7255980000	C	-0.5780640000	-1.1935530000	-0.0757710000
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C	4.5788770000	3.6080340000	3.0224060000	C	-0.5738670000	1.1921600000	0.0693520000
C	5.9555700000	1.6999660000	4.3940070000	C	-1.9841690000	0.7191450000	-0.2710580000
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H 2.9090410000 -0.9476770000 1.0848540000
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THF-B@1:

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C -5.4999860000 0.5608820000 -2.5106990000
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C -3.8376840000 -3.4803770000 -1.9747180000
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H -6.3588630000 0.4117990000 -1.8667960000
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O -3.3227100000 -1.3946720000 -4.7128750000

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H -6.3668220000 -1.8930720000 -0.4082440000
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C -5.5883810000 -3.0612480000 1.9642850000
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O -3.3661120000 3.3005000000 -3.7077470000
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O	-3.3943280000	1.4219930000	4.7521680000	N	1.6147350000	-3.4015620000	-3.2512840000
C	0.2686180000	-3.5596230000	3.1342400000	N	1.5850440000	-1.5088450000	-4.4569210000
C	-2.1641280000	3.1477450000	3.6155620000	H	1.8589520000	-4.7500470000	0.6289600000
C	-2.1742040000	1.9363060000	4.3571030000	H	1.9006960000	-0.5576560000	-4.7090580000
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C	-7.1546270000	1.9223740000	3.0578950000	O	2.5654730000	-4.4519580000	-0.8779750000
H	-7.5358320000	1.4495060000	3.9670100000	H	2.1135090000	-4.2811920000	-1.7402590000
H	-7.5691290000	1.3763150000	2.2059280000	H	2.9003120000	-3.5629500000	-0.6253220000
C	-7.1438920000	3.0090180000	-1.9227490000	O	2.5628750000	1.0267450000	-4.3902090000
H	-7.5382630000	3.9119050000	-1.4487750000	H	2.1122050000	1.9011230000	-4.3241720000
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C	-7.0914570000	-1.9475720000	-3.0335110000	O	2.4879830000	4.5466350000	1.0017670000
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H	-7.5205320000	-1.4040080000	-2.1872000000	H	2.0417100000	4.4421170000	1.8738220000
C	-7.1233610000	-3.0547290000	1.9494610000	O	2.5792620000	-0.9045320000	4.5198040000
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H	-7.5439210000	-2.2065370000	1.4022000000	H	2.8906210000	-0.6554810000	3.6200800000
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H	-7.4646110000	-2.9742190000	-2.9876160000	C	4.4050690000	1.5681810000	4.8314220000
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C	-0.9943550000	1.3182220000	4.7462420000	H	3.8610930000	0.9215380000	5.5071250000
H	-1.0107560000	0.4185570000	5.3466870000	C	5.9093140000	3.0825580000	3.1466120000
C	-0.9720340000	3.7739890000	3.2739150000	H	4.0806290000	4.0094170000	2.4944360000
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C	-0.9309150000	-3.1920240000	3.7599080000	H	6.5338240000	3.6656330000	2.4738330000
H	-0.9349550000	-2.6463270000	4.6948820000	C	3.7440200000	4.0564790000	-2.3870900000
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H	-0.9449780000	2.7675940000	-4.6810610000	H	6.5724820000	2.6214260000	-3.5866080000
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H 6. 0296820000 -0. 7125360000 -1. 6227310000
O 6. 2612260000 -1. 7913960000 -0. 0747580000
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THF-C@1:

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C -5.0351680000 2.9141710000 -1.4763830000
H -5.3118680000 4.6823810000 -0.3653960000
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C -3.9335340000 3.7339990000 1.5841460000
C -5.5697130000 1.7158880000 -1.9602690000
C -3.9128280000 3.4304640000 -2.1372550000
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H -6.4476470000 1.5147450000 1.2705370000
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H -6.4351930000 1.2989320000 -1.4585130000
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O -3.3771860000 4.6543350000 -1.7422750000
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C -3.9396510000 2.1832820000 3.4222040000
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C -2.1861770000 4.7386290000 0.3415050000
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O	-3.4169730000	0.9781600000	-4.8290750000	C	-7.1877400000	-0.2490370000	-3.5852590000
C	-5.6178170000	-1.6457060000	1.9869050000	H	-7.5590320000	0.5922220000	-4.1767940000
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H	3.1733270000	1.1335990000	-1.1397400000	C	-3.8632410000	-3.9523820000	-0.9607600000
H	4.2807020000	2.0722350000	0.5647270000	H	-2.4527700000	-4.2728820000	-2.5499420000
O	6.2422820000	-0.1484520000	1.8838430000	C	-2.0618620000	-1.8066700000	-4.3320120000
H	6.3054330000	0.7432640000	1.4543160000	H	-5.3583660000	4.5028850000	-1.1466980000
H	6.6903290000	-0.0451130000	2.7376620000	C	-5.0705390000	3.1727100000	0.4635020000
O	6.1275530000	1.9999630000	0.3664980000	O	-3.4147800000	4.3101220000	-2.4992100000
H	6.4833170000	2.8987340000	0.2533390000	C	-5.0141630000	-2.6766350000	1.9023890000
H	6.2992960000	1.5579760000	-0.5034150000	H	-5.2827130000	-4.6000400000	1.0817840000
O	3.6554760000	-1.8140280000	-0.6641130000	O	-3.3605230000	-4.9853910000	-0.1733210000
H	4.6279160000	-1.9314880000	-0.6034370000	C	-5.5762520000	2.1719060000	1.2973210000
H	3.4423190000	-1.1352100000	0.9535790000	C	-3.9693510000	3.8981520000	0.9296180000
O	3.4697490000	0.5469690000	-1.8673640000	C	-2.2079220000	4.4398010000	-1.8325800000
H	4.4288870000	0.7003010000	-1.9678840000	C	0.2901960000	-0.3966180000	-4.6228770000
H	3.5321380000	-0.9620550000	-1.1750950000	C	-5.5494310000	-1.4134720000	2.1747660000
O	6.3236930000	0.4920650000	-1.7987800000	C	-3.8950870000	-3.0749330000	2.6445460000
H	6.8059610000	0.4475800000	-2.6397030000	C	-2.1441020000	-4.7808670000	0.4466920000
H	6.4667310000	-0.3889420000	-1.3731600000	C	0.3260860000	-1.7694480000	-4.2848080000
O	6.4306790000	-1.6836770000	-0.2767140000	C	-5.0441590000	1.8822920000	2.5576970000
H	6.4785100000	-1.2373390000	0.6054040000	H	-6.4286840000	1.5970610000	0.9544800000
H	6.9369490000	-2.5055180000	-0.1750260000	C	-3.4158580000	3.6475750000	2.1799100000

1,4-dioxane-A@1:

C	-5.5454080000	-0.9034500000	-3.5310230000	H	-6.4141530000	-1.0882190000	1.6079990000
C	-4.9671060000	0.4698580000	-3.2118700000	C	-3.3559180000	-2.2528010000	3.6262910000
C	-4.9560180000	-1.9660840000	-2.6118530000	O	-3.3624720000	-4.3527080000	2.4689010000
H	-5.2041580000	-1.1496550000	-4.5371460000	C	-2.1388360000	-4.4567460000	1.8302270000
C	-5.5196810000	1.3107950000	-2.2426020000	C	-5.6372390000	0.8064830000	3.4590920000
C	-3.8487230000	0.9449620000	-3.9069460000	C	-3.9390350000	2.6346390000	2.9766230000
C	-5.5113540000	-2.2727380000	-1.3655010000	H	-2.6057980000	4.2568680000	2.5529870000
C	-3.8222510000	-2.6879160000	-3.0050970000	C	0.1856360000	4.4892180000	-1.7860860000
C	-5.0245900000	2.5877050000	-1.9608900000	C	-3.9120870000	-1.0013410000	3.8595410000
H	-6.3829840000	0.9606580000	-1.6889400000	H	-2.5307800000	-2.6039510000	4.2281970000
C	-3.3300060000	2.2116000000	-3.6612290000	C	0.2258740000	-4.7908910000	0.4521710000
O	-3.3015500000	0.1677700000	-4.9235490000	H	-5.3223650000	1.0544350000	4.4733600000
C	-4.9966390000	-3.2605840000	-0.5211250000	O	-3.4083070000	2.4386270000	4.2479980000
H	-6.3877720000	-1.7232200000	-1.0419600000	C	0.1248950000	4.7887780000	-0.4036750000
C	-3.2868920000	-3.6847930000	-2.1969590000	O	-3.4054650000	-0.2019370000	4.8788290000

C	0.2570640000	-4.4759970000	1.8319070000	N	1.6054060000	-0.0021380000	-4.7106250000
C	-2.1834240000	1.7942950000	4.3371930000	H	1.8567750000	-4.7331300000	-0.9235960000
C	-2.1880370000	0.4110850000	4.6570700000	H	1.9148450000	0.9812070000	-4.6585480000
C	0.2061060000	1.7924950000	4.3448080000	H	1.7327230000	4.7759150000	1.0018970000
C	0.1783200000	0.4099710000	4.6443960000	H	1.8189010000	-0.9567320000	4.6567520000
C	-7.1723940000	0.7933660000	3.4393160000	O	2.5619770000	-3.9266910000	-2.2360020000
H	-7.5490920000	0.0520040000	4.1491700000	H	2.1284900000	-3.4778620000	-3.0035310000
H	-7.5868690000	0.5471180000	2.4577510000	H	2.9386730000	-3.1789400000	-1.7220620000
C	-7.1944690000	3.4356630000	-0.9225960000	O	2.5383780000	2.3985240000	-3.8361400000
H	-7.5981210000	4.1387430000	-0.1890100000	H	2.0807780000	3.2040200000	-3.4997330000
H	-7.5960810000	2.4469450000	-0.6843110000	H	2.6897010000	1.8811980000	-3.0171180000
C	-7.0806530000	-0.9122090000	-3.5455400000	O	2.4333150000	3.9913160000	2.3512760000
H	-7.4527940000	-0.1767040000	-4.2638240000	H	2.6778000000	3.1917590000	1.8341630000
H	-7.5203780000	-0.6728890000	-2.5733410000	H	1.9996400000	3.5939850000	3.1440440000
C	-7.1410400000	-3.5808540000	0.8208720000	O	2.5543030000	-2.3415910000	3.9433150000
H	-7.5118130000	-4.2933890000	0.0789880000	H	2.1016750000	-3.1201890000	3.5426680000
H	-7.5634760000	-2.6025420000	0.5755260000	H	2.8639790000	-1.8276540000	3.1643030000
H	-7.5267820000	-3.8677380000	1.8028360000	C	3.7235670000	1.0692820000	4.5062140000
H	-7.4467610000	-1.9003430000	-3.8369500000	C	4.3889890000	-0.0579420000	5.0137180000
H	-7.5677890000	3.7120550000	-1.9123660000	C	4.5118090000	2.1100340000	3.9917540000
H	-7.5601920000	1.7756920000	3.7223960000	C	5.7751300000	-0.1142370000	4.9330810000
C	-1.0079220000	-0.2962700000	4.8234780000	H	3.8459880000	-0.8973140000	5.4280860000
H	-1.0199270000	-1.3391530000	5.1100680000	C	5.8919580000	1.9447310000	3.9524390000
C	-0.9957130000	2.4995180000	4.1995610000	H	4.0555390000	3.0076110000	3.5930380000
H	-1.0046800000	3.5650790000	4.0074880000	H	6.3033340000	-0.9893550000	5.3054110000
C	-0.9477080000	-4.3267610000	2.5365950000	H	6.5166870000	2.7244450000	3.5228120000
H	-0.9591040000	-4.1233970000	3.6000510000	C	3.6853820000	4.6424300000	-0.9707960000
C	-0.9615710000	-4.9647220000	-0.2550050000	C	4.3156750000	5.1644690000	0.1699740000
H	-0.9735830000	-5.2554050000	-1.2969800000	C	4.5030460000	4.1231020000	-1.9849180000
C	-0.8663060000	-2.4898280000	-4.1510200000	C	5.7009480000	5.0991670000	0.2602650000
H	-0.8623590000	-3.5513210000	-3.9389760000	H	3.7474550000	5.5805920000	0.9912110000
C	-0.9024170000	0.2906620000	-4.8347400000	C	5.8799330000	4.0998240000	-1.7876450000
H	-0.9254880000	1.3280460000	-5.1415800000	H	4.0755580000	3.7028750000	-2.8865140000
C	-1.0018050000	4.3305290000	-2.5156910000	H	6.2044310000	5.4836880000	1.1445770000
H	-0.9890150000	4.1365840000	-3.5809030000	H	6.5245070000	3.6533940000	-2.5397500000
C	-1.0785220000	4.9484130000	0.2787880000	C	3.8443600000	-1.0552530000	-4.4216740000
H	-1.1149610000	5.2294930000	1.3226550000	C	4.5424940000	0.0777450000	-4.8662680000
N	1.5120960000	4.3963300000	-2.1766920000	C	4.6022580000	-2.1627710000	-4.0092680000
N	1.4296740000	4.8921290000	0.0152650000	C	5.9356090000	0.0489410000	-4.8725130000
N	1.5214260000	2.2160100000	4.2615720000	H	4.0263380000	0.9768070000	-5.1800280000
N	1.4929010000	0.0230290000	4.7484130000	C	5.9899460000	-2.0776600000	-4.0575790000
N	1.5764970000	-4.3519580000	2.2430010000	H	4.1223080000	-3.0640860000	-3.6511340000
N	1.5389880000	-4.8776090000	0.0558670000	H	6.4903170000	0.9229320000	-5.2050860000
N	1.6415920000	-2.1758460000	-4.1569620000	H	6.5924840000	-2.9258680000	-3.7388730000

C	3.7718260000	-4.5502960000	1.0529860000
C	4.4154720000	-5.0685340000	-0.0817500000
C	4.5767190000	-3.9639580000	2.0407020000
C	5.7902670000	-4.9115910000	-0.2085450000
H	3.8610210000	-5.5492370000	-0.8764190000
C	5.9432270000	-3.8494140000	1.8060480000
H	4.1432440000	-3.5664350000	2.9495420000
H	6.2984340000	-5.2890310000	-1.0932130000
H	6.5763830000	-3.3561610000	2.5395380000
N	6.5590450000	-4.2864470000	0.6956840000
N	6.6695000000	-1.0006310000	-4.4802410000
N	6.4896770000	4.5581870000	-0.6815390000
N	6.5352620000	0.8499060000	4.3911070000
C	2.3101600000	-4.5874020000	1.1565010000
C	2.2612430000	1.1335820000	4.4945770000
C	2.2238910000	4.6309360000	-1.0756290000
C	2.3799010000	-1.0967240000	-4.4069120000
O	3.5198730000	-0.7881090000	1.8305970000
H	3.2145680000	0.9159950000	1.3443840000
H	4.4916330000	-0.7163020000	1.9773510000
O	3.2308010000	1.7736210000	0.8533520000
H	2.8820860000	1.1892170000	-0.7279570000
H	4.1936380000	1.9830110000	0.7744710000
O	6.2555530000	-0.3895940000	1.7367860000
H	6.2372250000	0.5334080000	1.3657080000
H	6.7748410000	-0.3186690000	2.5535960000
O	5.9048330000	1.8749500000	0.4601130000
H	6.4456440000	2.6772930000	0.3854310000
H	5.8514840000	1.4980700000	-0.4736840000
O	3.5770270000	-1.8005680000	-0.7108930000
H	4.5634290000	-1.8569950000	-0.7544520000
H	3.4457760000	-1.2706950000	0.9704630000
O	2.7589350000	0.6992240000	-1.5838780000
H	1.8087650000	0.4148580000	-1.5726460000
H	3.3423360000	-0.9442550000	-1.1370150000
O	5.7016650000	0.7681060000	-1.8659940000
H	4.7774170000	0.6612520000	-2.1421080000
H	6.0681290000	-0.1333160000	-1.7713660000
O	6.3044440000	-1.6467810000	-0.6474750000
H	6.4425180000	-1.2792020000	0.2581180000
H	6.7632440000	-2.5011970000	-0.6303280000
C	-0.8086650000	1.2270630000	0.4219830000
C	-0.7909000000	0.8886670000	-1.0627310000
C	-0.0316450000	-1.2983800000	-0.5354220000

C	-0.0675860000	-0.9365550000	0.9449530000
H	-1.7718950000	0.5163380000	-1.3846860000
H	-0.5245680000	1.7554030000	-1.6698100000
H	0.1515030000	1.6856930000	0.7115230000
H	-1.6118240000	1.9323750000	0.6466310000
H	-0.9852090000	-1.7474780000	-0.8414700000
H	0.7782380000	-1.9940740000	-0.7661340000
H	-0.3386070000	-1.8081180000	1.5439230000
H	0.9244130000	-0.5829450000	1.2680540000
O	0.1998270000	-0.1208930000	-1.3305750000
O	-1.0514970000	0.0596950000	1.1989100000

1,4-dioxane-B@1:

C	-5.4938880000	-0.6283520000	-3.5675660000
C	-4.9141030000	0.7188220000	-3.1553570000
C	-4.9150910000	-1.7574080000	-2.7240190000
H	-5.1499770000	-0.8062010000	-4.5870520000
C	-5.4678280000	1.4958630000	-2.1353540000
C	-3.7953030000	1.2377490000	-3.8174450000
C	-5.4773610000	-2.1458370000	-1.5045700000
C	-3.7933140000	-2.4683200000	-3.1692040000
C	-4.9747710000	2.7532440000	-1.7740390000
H	-6.3305800000	1.1104020000	-1.6049690000
C	-3.2767940000	2.4866370000	-3.4912780000
O	-3.2489170000	0.5245680000	-4.8796860000
C	-4.9834410000	-3.2043930000	-0.7372690000
H	-6.3434180000	-1.6058200000	-1.1399810000
C	-3.2827560000	-3.5380610000	-2.4413720000
O	-3.2344780000	-2.1606230000	-4.4059670000
C	-5.6129940000	3.5746450000	-0.6625390000
C	-3.8562030000	3.2309680000	-2.4690960000
H	-2.4508280000	2.8962000000	-4.0547420000
C	-2.0314960000	-0.0948330000	-4.6619060000
C	-5.6041790000	-3.6163800000	0.5904130000
C	-3.8644420000	-3.8854040000	-1.2270030000
H	-2.4577560000	-4.1120510000	-2.8370040000
C	-2.0203930000	-1.4922350000	-4.4122820000
H	-5.3053140000	4.6074900000	-0.8277410000
C	-5.0308530000	3.1616540000	0.6825710000
O	-3.3643160000	4.5080640000	-2.1985300000
C	-5.0117750000	-2.7806790000	1.7162740000
H	-5.2897150000	-4.6445360000	0.7714680000

O	-3.3763840000	-4.9782400000	-0.5124900000	C	-7.1387490000	-3.5959320000	0.5663300000
C	-5.5445470000	2.1058780000	1.4399370000	H	-7.5097780000	-4.2563380000	-0.2222040000
C	-3.9249590000	3.8434740000	1.2005720000	H	-7.5521550000	-2.6005540000	0.3818130000
C	-2.1579930000	4.5918740000	-1.5220410000	H	-7.5332360000	-3.9425150000	1.5253090000
C	0.3373740000	-0.0717780000	-4.5985600000	H	-7.3980580000	-1.5946250000	-3.9473820000
C	-5.5375130000	-1.5336730000	2.0676830000	H	-7.5139250000	3.8836330000	-1.6597520000
C	-3.9015720000	-3.2387050000	2.4362170000	H	-7.5402180000	1.5497310000	3.8208240000
C	-2.1631130000	-4.8212200000	0.1299260000	C	-1.0075120000	-0.6209630000	4.8280060000
C	0.3676040000	-1.4635450000	-4.3496630000	H	-1.0252660000	-1.6821770000	5.0368590000
C	-5.0182660000	1.7250320000	2.6780930000	C	-0.9823820000	2.2109890000	4.4021580000
H	-6.3989800000	1.5621350000	1.0541800000	H	-0.9873180000	3.2870260000	4.2816190000
C	-3.3766870000	3.5015810000	2.4314470000	C	-0.9706410000	-4.4858890000	2.2446730000
O	-3.4254580000	4.9368610000	0.4955360000	H	-0.9847180000	-4.3448300000	3.3179880000
C	-2.1961070000	4.7934620000	-0.1156600000	C	-0.9774330000	-4.9550390000	-0.5784160000
C	-5.0187530000	-0.7490440000	3.0995090000	H	-0.9867140000	-5.1799010000	-1.6366160000
H	-6.3960030000	-1.1636910000	1.5193160000	C	-0.8271420000	-2.1876830000	-4.2669620000
C	-3.3610340000	-2.4886700000	3.4740250000	H	-0.8265410000	-3.2607900000	-4.1245840000
O	-3.3838290000	-4.5088160000	2.1756950000	C	-0.8524060000	0.6310640000	-4.7679080000
C	-2.1611210000	-4.5812850000	1.5306320000	H	-0.8719630000	1.6862030000	-5.0068410000
C	-5.6200360000	0.5924070000	3.5000120000	C	-0.9515270000	4.5440430000	-2.2120470000
C	-3.9115610000	2.4403020000	3.1538290000	H	-0.9396340000	4.4374180000	-3.2896580000
H	-2.5636210000	4.0772810000	2.8486520000	C	-1.0292110000	4.9195990000	0.6246670000
C	0.2363410000	4.6406810000	-1.4717950000	H	-1.0651000000	5.1098900000	1.6887990000
C	-3.9082250000	-1.2500150000	3.7861600000	N	1.5634610000	4.5686200000	-1.8655510000
H	-2.5451490000	-2.8871330000	4.0590370000	N	1.4776270000	4.8780480000	0.3604590000
C	0.2085470000	-4.8145400000	0.1388280000	N	1.5340400000	1.9157240000	4.4550690000
H	-5.3093250000	0.7685520000	4.5303950000	N	1.4957470000	-0.3060450000	4.7924210000
O	-3.3945840000	2.1556230000	4.4146380000	N	1.5538630000	-4.4877070000	1.9584840000
C	0.1739260000	4.8199080000	-0.0689350000	N	1.5233610000	-4.8772910000	-0.2576090000
O	-3.4052860000	-0.5263460000	4.8632320000	N	1.6816050000	-1.8826410000	-4.2518860000
C	0.2357790000	-4.5826840000	1.5353490000	N	1.6541650000	0.3221710000	-4.6627420000
C	-2.1736440000	1.5017660000	4.4759940000	H	1.8472740000	-4.6679930000	-1.2234810000
C	-2.1853280000	0.0989830000	4.6979190000	H	1.9674030000	1.2996560000	-4.5572520000
C	0.2167790000	1.4926330000	4.5091830000	H	1.7751640000	4.6852090000	1.3361480000
C	0.1827860000	0.0926020000	4.7123320000	H	1.8177750000	-1.2775340000	4.6261260000
C	-7.1551620000	0.5874470000	3.4726170000	O	2.5756050000	-3.7771380000	-2.4672100000
H	-7.5382150000	-0.1991800000	4.1282830000	H	2.1541900000	-3.2688470000	-3.2037440000
H	-7.5661980000	0.4108980000	2.4747140000	H	2.9581440000	-3.0719330000	-1.8997940000
C	-7.1471350000	3.5349760000	-0.6905690000	O	2.5931310000	2.6783570000	-3.6635780000
H	-7.5520420000	4.1851730000	0.0896230000	H	2.1337590000	3.4558940000	-3.2695340000
H	-7.5539290000	2.5333960000	-0.5262090000	H	2.7644370000	2.1100810000	-2.8836910000
C	-7.0293910000	-0.6300520000	-3.5882320000	O	2.4580880000	3.7976880000	2.6363150000
H	-7.3958990000	0.1540110000	-4.2563030000	H	2.6849500000	3.0316990000	2.0630890000
H	-7.4717250000	-0.4554400000	-2.6035260000	H	2.0214420000	3.3586030000	3.4041800000

O	2.5447680000	-2.6050750000	3.8009400000	C	2.2682700000	0.8163080000	4.6131210000
H	2.0842390000	-3.3509980000	3.3507230000	C	2.2734600000	4.7039170000	-0.7463160000
H	2.8423590000	-2.0365440000	3.0554730000	C	2.4245960000	-0.7933390000	-4.4338220000
C	3.7303850000	0.7437580000	4.6135380000	O	3.5003350000	-0.9216200000	1.7846550000
C	4.3916970000	-0.4174050000	5.0436570000	H	3.2039660000	0.8038690000	1.3999380000
C	4.5213760000	1.8115200000	4.1627250000	H	4.4701410000	-0.8628200000	1.9478370000
C	5.7773330000	-0.4746850000	4.9544090000	O	3.2320530000	1.6938240000	0.9694940000
H	3.8457680000	-1.2792520000	5.4045800000	H	2.9314470000	1.2254680000	-0.6615020000
C	5.9005680000	1.6430180000	4.1083640000	H	4.1968520000	1.9022670000	0.9204290000
H	4.0676670000	2.7338620000	3.8216370000	O	6.2433670000	-0.5317040000	1.7429810000
H	6.3027140000	-1.3745460000	5.2668780000	H	6.2311080000	0.4138870000	1.4332870000
H	6.5276450000	2.4456840000	3.7271680000	H	6.7604530000	-0.5167540000	2.5641620000
C	3.7344500000	4.6957760000	-0.6336440000	O	5.9141560000	1.8134030000	0.6158580000
C	4.3605030000	5.1205070000	0.5491280000	H	6.4593500000	2.6160560000	0.6058180000
C	4.5557650000	4.2526820000	-1.6803600000	H	5.8810510000	1.4997240000	-0.3423660000
C	5.7445770000	5.0382580000	0.6428300000	O	3.6190650000	-1.7617620000	-0.8181150000
H	3.7898020000	5.4745080000	1.3972850000	H	4.6056060000	-1.8213350000	-0.8534250000
C	5.9309310000	4.2012150000	-1.4758000000	H	3.4408820000	-1.3489150000	0.8945590000
H	4.1321490000	3.9111890000	-2.6162660000	O	2.8356610000	0.8031510000	-1.5564520000
H	6.2444800000	5.3488620000	1.5577360000	H	1.8824960000	0.5293630000	-1.6019320000
H	6.5776450000	3.8099820000	-2.2562770000	H	3.3960680000	-0.8812710000	-1.1964610000
C	3.8889520000	-0.7589770000	-4.4506580000	O	5.7646290000	0.8689050000	-1.7838500000
C	4.5924770000	0.3955990000	-4.8256250000	H	4.8430130000	0.7823120000	-2.0766380000
C	4.6406980000	-1.8943770000	-4.1092870000	H	6.1285740000	-0.0375230000	-1.7443230000
C	5.9853690000	0.3589340000	-4.8375930000	O	6.3454790000	-1.6257760000	-0.7186430000
H	4.0807700000	1.3154030000	-5.0818150000	H	6.4634950000	-1.3173930000	0.2116290000
C	6.0287960000	-1.8147190000	-4.1563890000	H	6.7946380000	-2.4854570000	-0.7432110000
H	4.1556620000	-2.8129740000	-3.8059200000	C	-1.2142130000	-1.3620790000	0.0057800000
H	6.5447570000	1.2485100000	-5.1166960000	C	0.2212810000	-1.0529700000	-0.3922670000
H	6.6270450000	-2.6843650000	-3.8921950000	C	-0.4258100000	1.2115600000	-0.7663700000
C	3.7532020000	-4.6213240000	0.7674190000	C	-1.8459130000	0.8510870000	-0.3582270000
C	4.3996580000	-5.0733460000	-0.3936480000	H	0.8152970000	-0.8130980000	0.5020350000
C	4.5562510000	-4.1005900000	1.7926060000	H	0.6833390000	-1.8925170000	-0.9172270000
C	5.7754740000	-4.9141390000	-0.5055670000	H	-1.7766570000	-1.6982840000	-0.8772550000
H	3.8466320000	-5.5024020000	-1.2182140000	H	-1.2372330000	-2.1490040000	0.7606470000
C	5.9242670000	-3.9785480000	1.5712460000	H	0.1314710000	1.5912360000	0.1025630000
H	4.1204670000	-3.7570130000	2.7220790000	H	-0.4194630000	1.9646580000	-1.5547980000
H	6.2857160000	-5.2380580000	-1.4099740000	H	-2.3286580000	1.7020000000	0.1275660000
H	6.5562840000	-3.5340020000	2.3361360000	H	-2.4295560000	0.5737770000	-1.2487070000
N	6.5428070000	-4.3486320000	0.4382420000	O	0.2564140000	0.0611880000	-1.3055560000
N	6.7110540000	-0.7175680000	-4.5136790000	O	-1.8340020000	-0.2177440000	0.5801550000
N	6.5360850000	4.5664440000	-0.3331620000				
N	6.5400670000	0.5194790000	4.4739830000				
C	2.2906180000	-4.6574900000	0.8623300000				

1,4-dioxane-C@1:

				C	-5.0187530000	-0.7490440000	3.0995090000
C	-5.4938880000	-0.6283520000	-3.5675660000	H	-6.3960030000	-1.1636910000	1.5193160000
C	-4.9141030000	0.7188220000	-3.1553570000	C	-3.3610340000	-2.4886700000	3.4740250000
C	-4.9150910000	-1.7574080000	-2.7240190000	O	-3.3838290000	-4.5088160000	2.1756950000
H	-5.1499770000	-0.8062010000	-4.5870520000	C	-2.1611210000	-4.5812850000	1.5306320000
C	-5.4678280000	1.4958630000	-2.1353540000	C	-5.6200360000	0.5924070000	3.5000120000
C	-3.7953030000	1.2377490000	-3.8174450000	C	-3.9115610000	2.4403020000	3.1538290000
C	-5.4773610000	-2.1458370000	-1.5045700000	H	-2.5636210000	4.0772810000	2.8486520000
C	-3.7933140000	-2.4683200000	-3.1692040000	C	0.2363410000	4.6406810000	-1.4717950000
C	-4.9747710000	2.7532440000	-1.7740390000	C	-3.9082250000	-1.2500150000	3.7861600000
H	-6.3305800000	1.1104020000	-1.6049690000	H	-2.5451490000	-2.8871330000	4.0590370000
C	-3.2767940000	2.4866370000	-3.4912780000	C	0.2085470000	-4.8145400000	0.1388280000
O	-3.2489170000	0.5245680000	-4.8796860000	H	-5.3093250000	0.7685520000	4.5303950000
C	-4.9834410000	-3.2043930000	-0.7372690000	O	-3.3945840000	2.1556230000	4.4146380000
H	-6.3434180000	-1.6058200000	-1.1399810000	C	0.1739260000	4.8199080000	-0.0689350000
C	-3.2827560000	-3.5380610000	-2.4413720000	O	-3.4052860000	-0.5263460000	4.8632320000
O	-3.2344780000	-2.1606230000	-4.4059670000	C	0.2357790000	-4.5826840000	1.5353490000
C	-5.6129940000	3.5746450000	-0.6625390000	C	-2.1736440000	1.5017660000	4.4759940000
C	-3.8562030000	3.2309680000	-2.4690960000	C	-2.1853280000	0.0989830000	4.6979190000
H	-2.4508280000	2.8962000000	-4.0547420000	C	0.2167790000	1.4926330000	4.5091830000
C	-2.0314960000	-0.0948330000	-4.6619060000	C	0.1827860000	0.0926020000	4.7123320000
C	-5.6041790000	-3.6163800000	0.5904130000	C	-7.1551620000	0.5874470000	3.4726170000
C	-3.8644420000	-3.8854040000	-1.2270030000	H	-7.5382150000	-0.1991800000	4.1282830000
H	-2.4577560000	-4.1120510000	-2.8370040000	H	-7.5661980000	0.4108980000	2.4747140000
C	-2.0203930000	-1.4922350000	-4.4122820000	C	-7.1471350000	3.5349760000	-0.6905690000
H	-5.3053140000	4.6074900000	-0.8277410000	H	-7.5520420000	4.1851730000	0.0896230000
C	-5.0308530000	3.1616540000	0.6825710000	H	-7.5539290000	2.5333960000	-0.5262090000
O	-3.3643160000	4.5080640000	-2.1985300000	C	-7.0293910000	-0.6300520000	-3.5882320000
C	-5.0117750000	-2.7806790000	1.7162740000	H	-7.3958990000	0.1540110000	-4.2563030000
H	-5.2897150000	-4.6445360000	0.7714680000	H	-7.4717250000	-0.4554400000	-2.6035260000
O	-3.3763840000	-4.9782400000	-0.5124900000	C	-7.1387490000	-3.5959320000	0.5663300000
C	-5.5445470000	2.1058780000	1.4399370000	H	-7.5097780000	-4.2563380000	-0.2222040000
C	-3.9249590000	3.8434740000	1.2005720000	H	-7.5521550000	-2.6005540000	0.3818130000
C	-2.1579930000	4.5918740000	-1.5220410000	H	-7.5332360000	-3.9425150000	1.5253090000
C	0.3373740000	-0.0717780000	-4.5985600000	H	-7.3980580000	-1.5946250000	-3.9473820000
C	-5.5375130000	-1.5336730000	2.0676830000	H	-7.5139250000	3.8836330000	-1.6597520000
C	-3.9015720000	-3.2387050000	2.4362170000	H	-7.5402180000	1.5497310000	3.8208240000
C	-2.1631130000	-4.8212200000	0.1299260000	C	-1.0075120000	-0.6209630000	4.8280060000
C	0.3676040000	-1.4635450000	-4.3496630000	H	-1.0252660000	-1.6821770000	5.0368590000
C	-5.0182660000	1.7250320000	2.6780930000	C	-0.9823820000	2.2109890000	4.4021580000
H	-6.3989800000	1.5621350000	1.0541800000	H	-0.9873180000	3.2870260000	4.2816190000
C	-3.3766870000	3.5015810000	2.4314470000	C	-0.9706410000	-4.4858890000	2.2446730000
O	-3.4254580000	4.9368610000	0.4955360000	H	-0.9847180000	-4.3448300000	3.3179880000
C	-2.1961070000	4.7934620000	-0.1156600000	C	-0.9774330000	-4.9550390000	-0.5784160000

H	-0.9867140000	-5.1799010000	-1.6366160000	C	4.5557650000	4.2526820000	-1.6803600000
C	-0.8271420000	-2.1876830000	-4.2669620000	C	5.7445770000	5.0382580000	0.6428300000
H	-0.8265410000	-3.2607900000	-4.1245840000	H	3.7898020000	5.4745080000	1.3972850000
C	-0.8524060000	0.6310640000	-4.7679080000	C	5.9309310000	4.2012150000	-1.4758000000
H	-0.8719630000	1.6862030000	-5.0068410000	H	4.1321490000	3.9111890000	-2.6162660000
C	-0.9515270000	4.5440430000	-2.2120470000	H	6.2444800000	5.3488620000	1.5577360000
H	-0.9396340000	4.4374180000	-3.2896580000	H	6.5776450000	3.8099820000	-2.2562770000
C	-1.0292110000	4.9195990000	0.6246670000	C	3.8889520000	-0.7589770000	-4.4506580000
H	-1.0651000000	5.1098900000	1.6887990000	C	4.5924770000	0.3955990000	-4.8256250000
N	1.5634610000	4.5686200000	-1.8655510000	C	4.6406980000	-1.8943770000	-4.1092870000
N	1.4776270000	4.8780480000	0.3604590000	C	5.9853690000	0.3589340000	-4.8375930000
N	1.5340400000	1.9157240000	4.4550690000	H	4.0807700000	1.3154030000	-5.0818150000
N	1.4957470000	-0.3060450000	4.7924210000	C	6.0287960000	-1.8147190000	-4.1563890000
N	1.5538630000	-4.4877070000	1.9584840000	H	4.1556620000	-2.8129740000	-3.8059200000
N	1.5233610000	-4.8772910000	-0.2576090000	H	6.5447570000	1.2485100000	-5.1166960000
N	1.6816050000	-1.8826410000	-4.2518860000	H	6.6270450000	-2.6843650000	-3.8921950000
N	1.6541650000	0.3221710000	-4.6627420000	C	3.7532020000	-4.6213240000	0.7674190000
H	1.8472740000	-4.6679930000	-1.2234810000	C	4.3996580000	-5.0733460000	-0.3936480000
H	1.9674030000	1.2996560000	-4.5572520000	C	4.5562510000	-4.1005900000	1.7926060000
H	1.7751640000	4.6852090000	1.3361480000	C	5.7754740000	-4.9141390000	-0.5055670000
H	1.8177750000	-1.2775340000	4.6261260000	H	3.8466320000	-5.5024020000	-1.2182140000
O	2.5756050000	-3.7771380000	-2.4672100000	C	5.9242670000	-3.9785480000	1.5712460000
H	2.1541900000	-3.2688470000	-3.2037440000	H	4.1204670000	-3.7570130000	2.7220790000
H	2.9581440000	-3.0719330000	-1.8997940000	H	6.2857160000	-5.2380580000	-1.4099740000
O	2.5931310000	2.6783570000	-3.6635780000	H	6.5562840000	-3.5340020000	2.3361360000
H	2.1337590000	3.4558940000	-3.2695340000	N	6.5428070000	-4.3486320000	0.4382420000
H	2.7644370000	2.1100810000	-2.8836910000	N	6.7110540000	-0.7175680000	-4.5136790000
O	2.4580880000	3.7976880000	2.6363150000	N	6.5360850000	4.5664440000	-0.3331620000
H	2.6849500000	3.0316990000	2.0630890000	N	6.5400670000	0.5194790000	4.4739830000
H	2.0214420000	3.3586030000	3.4041800000	C	2.2906180000	-4.6574900000	0.8623300000
O	2.5447680000	-2.6050750000	3.8009400000	C	2.2682700000	0.8163080000	4.6131210000
H	2.0842390000	-3.3509980000	3.3507230000	C	2.2734600000	4.7039170000	-0.7463160000
H	2.8423590000	-2.0365440000	3.0554730000	C	2.4245960000	-0.7933390000	-4.4338220000
C	3.7303850000	0.7437580000	4.6135380000	O	3.5003350000	-0.9216200000	1.7846550000
C	4.3916970000	-0.4174050000	5.0436570000	H	3.2039660000	0.8038690000	1.3999380000
C	4.5213760000	1.8115200000	4.1627250000	H	4.4701410000	-0.8628200000	1.9478370000
C	5.7773330000	-0.4746850000	4.9544090000	O	3.2320530000	1.6938240000	0.9694940000
H	3.8457680000	-1.2792520000	5.4045800000	H	2.9314470000	1.2254680000	-0.6615020000
C	5.9005680000	1.6430180000	4.1083640000	H	4.1968520000	1.9022670000	0.9204290000
H	4.0676670000	2.7338620000	3.8216370000	O	6.2433670000	-0.5317040000	1.7429810000
H	6.3027140000	-1.3745460000	5.2668780000	H	6.2311080000	0.4138870000	1.4332870000
H	6.5276450000	2.4456840000	3.7271680000	H	6.7604530000	-0.5167540000	2.5641620000
C	3.7344500000	4.6957760000	-0.6336440000	O	5.9141560000	1.8134030000	0.6158580000
C	4.3605030000	5.1205070000	0.5491280000	H	6.4593500000	2.6160560000	0.6058180000

H	5.8810510000	1.4997240000	-0.3423660000	C	-3.2827560000	-3.5380610000	-2.4413720000
O	3.6190650000	-1.7617620000	-0.8181150000	O	-3.2344780000	-2.1606230000	-4.4059670000
H	4.6056060000	-1.8213350000	-0.8534250000	C	-5.6129940000	3.5746450000	-0.6625390000
H	3.4408820000	-1.3489150000	0.8945590000	C	-3.8562030000	3.2309680000	-2.4690960000
O	2.8356610000	0.8031510000	-1.5564520000	H	-2.4508280000	2.8962000000	-4.0547420000
H	1.8824960000	0.5293630000	-1.6019320000	C	-2.0314960000	-0.0948330000	-4.6619060000
H	3.3960680000	-0.8812710000	-1.1964610000	C	-5.6041790000	-3.6163800000	0.5904130000
O	5.7646290000	0.8689050000	-1.7838500000	C	-3.8644420000	-3.8854040000	-1.2270030000
H	4.8430130000	0.7823120000	-2.0766380000	H	-2.4577560000	-4.1120510000	-2.8370040000
H	6.1285740000	-0.0375230000	-1.7443230000	C	-2.0203930000	-1.4922350000	-4.4122820000
O	6.3454790000	-1.6257760000	-0.7186430000	H	-5.3053140000	4.6074900000	-0.8277410000
H	6.4634950000	-1.3173930000	0.2116290000	C	-5.0308530000	3.1616540000	0.6825710000
H	6.7946380000	-2.4854570000	-0.7432110000	O	-3.3643160000	4.5080640000	-2.1985300000
C	-1.2142130000	-1.3620790000	0.0057800000	C	-5.0117750000	-2.7806790000	1.7162740000
C	0.2212810000	-1.0529700000	-0.3922670000	H	-5.2897150000	-4.6445360000	0.7714680000
C	-0.4258100000	1.2115600000	-0.7663700000	O	-3.3763840000	-4.9782400000	-0.5124900000
C	-1.8459130000	0.8510870000	-0.3582270000	C	-5.5445470000	2.1058780000	1.4399370000
H	0.8152970000	-0.8130980000	0.5020350000	C	-3.9249590000	3.8434740000	1.2005720000
H	0.6833390000	-1.8925170000	-0.9172270000	C	-2.1579930000	4.5918740000	-1.5220410000
H	-1.7766570000	-1.6982840000	-0.8772550000	C	0.3373740000	-0.0717780000	-4.5985600000
H	-1.2372330000	-2.1490040000	0.7606470000	C	-5.5375130000	-1.5336730000	2.0676830000
H	0.1314710000	1.5912360000	0.1025630000	C	-3.9015720000	-3.2387050000	2.4362170000
H	-0.4194630000	1.9646580000	-1.5547980000	C	-2.1631130000	-4.8212200000	0.1299260000
H	-2.3286580000	1.7020000000	0.1275660000	C	0.3676040000	-1.4635450000	-4.3496630000
H	-2.4295560000	0.5737770000	-1.2487070000	C	-5.0182660000	1.7250320000	2.6780930000
O	0.2564140000	0.0611880000	-1.3055560000	H	-6.3989800000	1.5621350000	1.0541800000
O	-1.8340020000	-0.2177440000	0.5801550000	C	-3.3766870000	3.5015810000	2.4314470000

1,4-dioxane-D@1:

C	-5.4938880000	-0.6283520000	-3.5675660000	H	-6.3960030000	-1.1636910000	1.5193160000
C	-4.9141030000	0.7188220000	-3.1553570000	C	-3.3610340000	-2.4886700000	3.4740250000
C	-4.9150910000	-1.7574080000	-2.7240190000	O	-3.3838290000	-4.5088160000	2.1756950000
H	-5.1499770000	-0.8062010000	-4.5870520000	C	-2.1611210000	-4.5812850000	1.5306320000
C	-5.4678280000	1.4958630000	-2.1353540000	C	-5.6200360000	0.5924070000	3.5000120000
C	-3.7953030000	1.2377490000	-3.8174450000	C	-3.9115610000	2.4403020000	3.1538290000
C	-5.4773610000	-2.1458370000	-1.5045700000	H	-2.5636210000	4.0772810000	2.8486520000
C	-3.7933140000	-2.4683200000	-3.1692040000	C	0.2363410000	4.6406810000	-1.4717950000
C	-4.9747710000	2.7532440000	-1.7740390000	C	-3.9082250000	-1.2500150000	3.7861600000
H	-6.3305800000	1.1104020000	-1.6049690000	H	-2.5451490000	-2.8871330000	4.0590370000
C	-3.2767940000	2.4866370000	-3.4912780000	C	0.2085470000	-4.8145400000	0.1388280000
O	-3.2489170000	0.5245680000	-4.8796860000	H	-5.3093250000	0.7685520000	4.5303950000
C	-4.9834410000	-3.2043930000	-0.7372690000	O	-3.3945840000	2.1556230000	4.4146380000
H	-6.3434180000	-1.6058200000	-1.1399810000	C	0.1739260000	4.8199080000	-0.0689350000

O	-3.4052860000	-0.5263460000	4.8632320000	N	1.6816050000	-1.8826410000	-4.2518860000
C	0.2357790000	-4.5826840000	1.5353490000	N	1.6541650000	0.3221710000	-4.6627420000
C	-2.1736440000	1.5017660000	4.4759940000	H	1.8472740000	-4.6679930000	-1.2234810000
C	-2.1853280000	0.0989830000	4.6979190000	H	1.9674030000	1.2996560000	-4.5572520000
C	0.2167790000	1.4926330000	4.5091830000	H	1.7751640000	4.6852090000	1.3361480000
C	0.1827860000	0.0926020000	4.7123320000	H	1.8177750000	-1.2775340000	4.6261260000
C	-7.1551620000	0.5874470000	3.4726170000	O	2.5756050000	-3.7771380000	-2.4672100000
H	-7.5382150000	-0.1991800000	4.1282830000	H	2.1541900000	-3.2688470000	-3.2037440000
H	-7.5661980000	0.4108980000	2.4747140000	H	2.9581440000	-3.0719330000	-1.8997940000
C	-7.1471350000	3.5349760000	-0.6905690000	O	2.5931310000	2.6783570000	-3.6635780000
H	-7.5520420000	4.1851730000	0.0896230000	H	2.1337590000	3.4558940000	-3.2695340000
H	-7.5539290000	2.5333960000	-0.5262090000	H	2.7644370000	2.1100810000	-2.8836910000
C	-7.0293910000	-0.6300520000	-3.5882320000	O	2.4580880000	3.7976880000	2.6363150000
H	-7.3958990000	0.1540110000	-4.2563030000	H	2.6849500000	3.0316990000	2.0630890000
H	-7.4717250000	-0.4554400000	-2.6035260000	H	2.0214420000	3.3586030000	3.4041800000
C	-7.1387490000	-3.5959320000	0.5663300000	O	2.5447680000	-2.6050750000	3.8009400000
H	-7.5097780000	-4.2563380000	-0.2222040000	H	2.0842390000	-3.3509980000	3.3507230000
H	-7.5521550000	-2.6005540000	0.3818130000	H	2.8423590000	-2.0365440000	3.0554730000
H	-7.5332360000	-3.9425150000	1.5253090000	C	3.7303850000	0.7437580000	4.6135380000
H	-7.3980580000	-1.5946250000	-3.9473820000	C	4.3916970000	-0.4174050000	5.0436570000
H	-7.5139250000	3.8836330000	-1.6597520000	C	4.5213760000	1.8115200000	4.1627250000
H	-7.5402180000	1.5497310000	3.8208240000	C	5.7773330000	-0.4746850000	4.9544090000
C	-1.0075120000	-0.6209630000	4.8280060000	H	3.8457680000	-1.2792520000	5.4045800000
H	-1.0252660000	-1.6821770000	5.0368590000	C	5.9005680000	1.6430180000	4.1083640000
C	-0.9823820000	2.2109890000	4.4021580000	H	4.0676670000	2.7338620000	3.8216370000
H	-0.9873180000	3.2870260000	4.2816190000	H	6.3027140000	-1.3745460000	5.2668780000
C	-0.9706410000	-4.4858890000	2.2446730000	H	6.5276450000	2.4456840000	3.7271680000
H	-0.9847180000	-4.3448300000	3.3179880000	C	3.7344500000	4.6957760000	-0.6336440000
C	-0.9774330000	-4.9550390000	-0.5784160000	C	4.3605030000	5.1205070000	0.5491280000
H	-0.9867140000	-5.1799010000	-1.6366160000	C	4.5557650000	4.2526820000	-1.6803600000
C	-0.8271420000	-2.1876830000	-4.2669620000	C	5.7445770000	5.0382580000	0.6428300000
H	-0.8265410000	-3.2607900000	-4.1245840000	H	3.7898020000	5.4745080000	1.3972850000
C	-0.8524060000	0.6310640000	-4.7679080000	C	5.9309310000	4.2012150000	-1.4758000000
H	-0.8719630000	1.6862030000	-5.0068410000	H	4.1321490000	3.9111890000	-2.6162660000
C	-0.9515270000	4.5440430000	-2.2120470000	H	6.2444800000	5.3488620000	1.5577360000
H	-0.9396340000	4.4374180000	-3.2896580000	H	6.5776450000	3.8099820000	-2.2562770000
C	-1.0292110000	4.9195990000	0.6246670000	C	3.8889520000	-0.7589770000	-4.4506580000
H	-1.0651000000	5.1098900000	1.6887990000	C	4.5924770000	0.3955990000	-4.8256250000
N	1.5634610000	4.5686200000	-1.8655510000	C	4.6406980000	-1.8943770000	-4.1092870000
N	1.4776270000	4.8780480000	0.3604590000	C	5.9853690000	0.3589340000	-4.8375930000
N	1.5340400000	1.9157240000	4.4550690000	H	4.0807700000	1.3154030000	-5.0818150000
N	1.4957470000	-0.3060450000	4.7924210000	C	6.0287960000	-1.8147190000	-4.1563890000
N	1.5538630000	-4.4877070000	1.9584840000	H	4.1556620000	-2.8129740000	-3.8059200000
N	1.5233610000	-4.8772910000	-0.2576090000	H	6.5447570000	1.2485100000	-5.1166960000

H	6.6270450000	-2.6843650000	-3.8921950000	C	-0.4258100000	1.2115600000	-0.7663700000
C	3.7532020000	-4.6213240000	0.7674190000	C	-1.8459130000	0.8510870000	-0.3582270000
C	4.3996580000	-5.0733460000	-0.3936480000	H	0.8152970000	-0.8130980000	0.5020350000
C	4.5562510000	-4.1005900000	1.7926060000	H	0.6833390000	-1.8925170000	-0.9172270000
C	5.7754740000	-4.9141390000	-0.5055670000	H	-1.7766570000	-1.6982840000	-0.8772550000
H	3.8466320000	-5.5024020000	-1.2182140000	H	-1.2372330000	-2.1490040000	0.7606470000
C	5.9242670000	-3.9785480000	1.5712460000	H	0.1314710000	1.5912360000	0.1025630000
H	4.1204670000	-3.7570130000	2.7220790000	H	-0.4194630000	1.9646580000	-1.5547980000
H	6.2857160000	-5.2380580000	-1.4099740000	H	-2.3286580000	1.7020000000	0.1275660000
H	6.5562840000	-3.5340020000	2.3361360000	H	-2.4295560000	0.5737770000	-1.2487070000
N	6.5428070000	-4.3486320000	0.4382420000	O	0.2564140000	0.0611880000	-1.3055560000
N	6.7110540000	-0.7175680000	-4.5136790000	O	-1.8340020000	-0.2177440000	0.5801550000
N	6.5360850000	4.5664440000	-0.3331620000				
N	6.5400670000	0.5194790000	4.4739830000				
C	2.2906180000	-4.6574900000	0.8623300000	1,4-dioxane-E@1:			
C	2.2682700000	0.8163080000	4.6131210000	C	-5.5454080000	-0.9034500000	-3.5310230000
C	2.2734600000	4.7039170000	-0.7463160000	C	-4.9671060000	0.4698580000	-3.2118700000
C	2.4245960000	-0.7933390000	-4.4338220000	C	-4.9560180000	-1.9660840000	-2.6118530000
O	3.5003350000	-0.9216200000	1.7846550000	H	-5.2041580000	-1.1496550000	-4.5371460000
H	3.2039660000	0.8038690000	1.3999380000	C	-5.5196810000	1.3107950000	-2.2426020000
H	4.4701410000	-0.8628200000	1.9478370000	C	-3.8487230000	0.9449620000	-3.9069460000
O	3.2320530000	1.6938240000	0.9694940000	C	-5.5113540000	-2.2727380000	-1.3655010000
H	2.9314470000	1.2254680000	-0.6615020000	C	-3.8222510000	-2.6879160000	-3.0050970000
H	4.1968520000	1.9022670000	0.9204290000	C	-5.0245900000	2.5877050000	-1.9608900000
O	6.2433670000	-0.5317040000	1.7429810000	H	-6.3829840000	0.9606580000	-1.6889400000
H	6.2311080000	0.4138870000	1.4332870000	C	-3.3300060000	2.2116000000	-3.6612290000
H	6.7604530000	-0.5167540000	2.5641620000	O	-3.3015500000	0.1677700000	-4.9235490000
O	5.9141560000	1.8134030000	0.6158580000	C	-4.9966390000	-3.2605840000	-0.5211250000
H	6.4593500000	2.6160560000	0.6058180000	H	-6.3877720000	-1.7232200000	-1.0419600000
H	5.8810510000	1.4997240000	-0.3423660000	C	-3.2868920000	-3.6847930000	-2.1969590000
O	3.6190650000	-1.7617620000	-0.8181150000	O	-3.2756150000	-2.4711730000	-4.2664520000
H	4.6056060000	-1.8213350000	-0.8534250000	C	-5.6603630000	3.4831760000	-0.9059650000
H	3.4408820000	-1.3489150000	0.8945590000	C	-3.9067820000	3.0186150000	-2.6868370000
O	2.8356610000	0.8031510000	-1.5564520000	H	-2.5053670000	2.5843330000	-4.2513790000
H	1.8824960000	0.5293630000	-1.6019320000	C	-2.0792250000	-0.4292000000	-4.6737840000
H	3.3960680000	-0.8812710000	-1.1964610000	C	-5.6063160000	-3.5881940000	0.8357150000
O	5.7646290000	0.8689050000	-1.7838500000	C	-3.8632410000	-3.9523820000	-0.9607600000
H	4.8430130000	0.7823120000	-2.0766380000	H	-2.4527700000	-4.2728820000	-2.5499420000
H	6.1285740000	-0.0375230000	-1.7443230000	C	-2.0618620000	-1.8066700000	-4.3320120000
O	6.3454790000	-1.6257760000	-0.7186430000	H	-5.3583660000	4.5028850000	-1.1466980000
H	6.4634950000	-1.3173930000	0.2116290000	C	-5.0705390000	3.1727100000	0.4635020000
H	6.7946380000	-2.4854570000	-0.7432110000	O	-3.4147800000	4.3101220000	-2.4992100000
C	-1.2142130000	-1.3620790000	0.0057800000	C	-5.0141630000	-2.6766350000	1.9023890000
C	0.2212810000	-1.0529700000	-0.3922670000	H	-5.2827130000	-4.6000400000	1.0817840000

O	-3.3605230000	-4.9853910000	-0.1733210000	C	-7.1410400000	-3.5808540000	0.8208720000
C	-5.5762520000	2.1719060000	1.2973210000	H	-7.5118130000	-4.2933890000	0.0789880000
C	-3.9693510000	3.8981520000	0.9296180000	H	-7.5634760000	-2.6025420000	0.5755260000
C	-2.2079220000	4.4398010000	-1.8325800000	H	-7.5267820000	-3.8677380000	1.8028360000
C	0.2901960000	-0.3966180000	-4.6228770000	H	-7.4467610000	-1.9003430000	-3.8369500000
C	-5.5494310000	-1.4134720000	2.1747660000	H	-7.5677890000	3.7120550000	-1.9123660000
C	-3.8950870000	-3.0749330000	2.6445460000	H	-7.5601920000	1.7756920000	3.7223960000
C	-2.1441020000	-4.7808670000	0.4466920000	C	-1.0079220000	-0.2962700000	4.8234780000
C	0.3260860000	-1.7694480000	-4.2848080000	H	-1.0199270000	-1.3391530000	5.1100680000
C	-5.0441590000	1.8822920000	2.5576970000	C	-0.9957130000	2.4995180000	4.1995610000
H	-6.4286840000	1.5970610000	0.9544800000	H	-1.0046800000	3.5650790000	4.0074880000
C	-3.4158580000	3.6475750000	2.1799100000	C	-0.9477080000	-4.3267610000	2.5365950000
O	-3.4755850000	4.9429590000	0.1502850000	H	-0.9591040000	-4.1233970000	3.6000510000
C	-2.2453470000	4.7576090000	-0.4481330000	C	-0.9615710000	-4.9647220000	-0.2550050000
C	-5.0313150000	-0.5566920000	3.1484440000	H	-0.9735830000	-5.2554050000	-1.2969800000
H	-6.4141530000	-1.0882190000	1.6079990000	C	-0.8663060000	-2.4898280000	-4.1510200000
C	-3.3559180000	-2.2528010000	3.6262910000	H	-0.8623590000	-3.5513210000	-3.9389760000
O	-3.3624720000	-4.3527080000	2.4689010000	C	-0.9024170000	0.2906620000	-4.8347400000
C	-2.1388360000	-4.4567460000	1.8302270000	H	-0.9254880000	1.3280460000	-5.1415800000
C	-5.6372390000	0.8064830000	3.4590920000	C	-1.0018050000	4.3305290000	-2.5156910000
C	-3.9390350000	2.6346390000	2.9766230000	H	-0.9890150000	4.1365840000	-3.5809030000
H	-2.6057980000	4.2568680000	2.5529870000	C	-1.0785220000	4.9484130000	0.2787880000
C	0.1856360000	4.4892180000	-1.7860860000	H	-1.1149610000	5.2294930000	1.3226550000
C	-3.9120870000	-1.0013410000	3.8595410000	N	1.5120960000	4.3963300000	-2.1766920000
H	-2.5307800000	-2.6039510000	4.2281970000	N	1.4296740000	4.8921290000	0.0152650000
C	0.2258740000	-4.7908910000	0.4521710000	N	1.5214260000	2.2160100000	4.2615720000
H	-5.3223650000	1.0544350000	4.4733600000	N	1.4929010000	0.0230290000	4.7484130000
O	-3.4083070000	2.4386270000	4.2479980000	N	1.5764970000	-4.3519580000	2.2430010000
C	0.1248950000	4.7887780000	-0.4036750000	N	1.5389880000	-4.8776090000	0.0558670000
O	-3.4054650000	-0.2019370000	4.8788290000	N	1.6415920000	-2.1758460000	-4.1569620000
C	0.2570640000	-4.4759970000	1.8319070000	N	1.6054060000	-0.0021380000	-4.7106250000
C	-2.1834240000	1.7942950000	4.3371930000	H	1.8567750000	-4.7331300000	-0.9235960000
C	-2.1880370000	0.4110850000	4.6570700000	H	1.9148450000	0.9812070000	-4.6585480000
C	0.2061060000	1.7924950000	4.3448080000	H	1.7327230000	4.7759150000	1.0018970000
C	0.1783200000	0.4099710000	4.6443960000	H	1.8189010000	-0.9567320000	4.6567520000
C	-7.1723940000	0.7933660000	3.4393160000	O	2.5619770000	-3.9266910000	-2.2360020000
H	-7.5490920000	0.0520040000	4.1491700000	H	2.1284900000	-3.4778620000	-3.0035310000
H	-7.5868690000	0.5471180000	2.4577510000	H	2.9386730000	-3.1789400000	-1.7220620000
C	-7.1944690000	3.4356630000	-0.9225960000	O	2.5383780000	2.3985240000	-3.8361400000
H	-7.5981210000	4.1387430000	-0.1890100000	H	2.0807780000	3.2040200000	-3.4997330000
H	-7.5960810000	2.4469450000	-0.6843110000	H	2.6897010000	1.8811980000	-3.0171180000
C	-7.0806530000	-0.9122090000	-3.5455400000	O	2.4333150000	3.9913160000	2.3512760000
H	-7.4527940000	-0.1767040000	-4.2638240000	H	2.6778000000	3.1917590000	1.8341630000
H	-7.5203780000	-0.6728890000	-2.5733410000	H	1.9996400000	3.5939850000	3.1440440000

O	2.5543030000	-2.3415910000	3.9433150000	C	2.2612430000	1.1335820000	4.4945770000
H	2.1016750000	-3.1201890000	3.5426680000	C	2.2238910000	4.6309360000	-1.0756290000
H	2.8639790000	-1.8276540000	3.1643030000	C	2.3799010000	-1.0967240000	-4.4069120000
C	3.7235670000	1.0692820000	4.5062140000	O	3.5198730000	-0.7881090000	1.8305970000
C	4.3889890000	-0.0579420000	5.0137180000	H	3.2145680000	0.9159950000	1.3443840000
C	4.5118090000	2.1100340000	3.9917540000	H	4.4916330000	-0.7163020000	1.9773510000
C	5.7751300000	-0.1142370000	4.9330810000	O	3.2308010000	1.7736210000	0.8533520000
H	3.8459880000	-0.8973140000	5.4280860000	H	2.8820860000	1.1892170000	-0.7279570000
C	5.8919580000	1.9447310000	3.9524390000	H	4.1936380000	1.9830110000	0.7744710000
H	4.0555390000	3.0076110000	3.5930380000	O	6.2555530000	-0.3895940000	1.7367860000
H	6.3033340000	-0.9893550000	5.3054110000	H	6.2372250000	0.5334080000	1.3657080000
H	6.5166870000	2.7244450000	3.5228120000	H	6.7748410000	-0.3186690000	2.5535960000
C	3.6853820000	4.6424300000	-0.9707960000	O	5.9048330000	1.8749500000	0.4601130000
C	4.3156750000	5.1644690000	0.1699740000	H	6.4456440000	2.6772930000	0.3854310000
C	4.5030460000	4.1231020000	-1.9849180000	H	5.8514840000	1.4980700000	-0.4736840000
C	5.7009480000	5.0991670000	0.2602650000	O	3.5770270000	-1.8005680000	-0.7108930000
H	3.7474550000	5.5805920000	0.9912110000	H	4.5634290000	-1.8569950000	-0.7544520000
C	5.8799330000	4.0998240000	-1.7876450000	H	3.4457760000	-1.2706950000	0.9704630000
H	4.0755580000	3.7028750000	-2.8865140000	O	2.7589350000	0.6992240000	-1.5838780000
H	6.2044310000	5.4836880000	1.1445770000	H	1.8087650000	0.4148580000	-1.5726460000
H	6.5245070000	3.6533940000	-2.5397500000	H	3.3423360000	-0.9442550000	-1.1370150000
C	3.8443600000	-1.0552530000	-4.4216740000	O	5.7016650000	0.7681060000	-1.8659940000
C	4.5424940000	0.0777450000	-4.8662680000	H	4.7774170000	0.6612520000	-2.1421080000
C	4.6022580000	-2.1627710000	-4.0092680000	H	6.0681290000	-0.1333160000	-1.7713660000
C	5.9356090000	0.0489410000	-4.8725130000	O	6.3044440000	-1.6467810000	-0.6474750000
H	4.0263380000	0.9768070000	-5.1800280000	H	6.4425180000	-1.2792020000	0.2581180000
C	5.9899460000	-2.0776600000	-4.0575790000	H	6.7632440000	-2.5011970000	-0.6303280000
H	4.1223080000	-3.0640860000	-3.6511340000	C	-0.8086650000	1.2270630000	0.4219830000
H	6.4903170000	0.9229320000	-5.2050860000	C	-0.7909000000	0.8886670000	-1.0627310000
H	6.5924840000	-2.9258680000	-3.7388730000	C	-0.0316450000	-1.2983800000	-0.5354220000
C	3.7718260000	-4.5502960000	1.0529860000	C	-0.0675860000	-0.9365550000	0.9449530000
C	4.4154720000	-5.0685340000	-0.0817500000	H	-1.7718950000	0.5163380000	-1.3846860000
C	4.5767190000	-3.9639580000	2.0407020000	H	-0.5245680000	1.7554030000	-1.6698100000
C	5.7902670000	-4.9115910000	-0.2085450000	H	0.1515030000	1.6856930000	0.7115230000
H	3.8610210000	-5.5492370000	-0.8764190000	H	-1.6118240000	1.9323750000	0.6466310000
C	5.9432270000	-3.8494140000	1.8060480000	H	-0.9852090000	-1.7474780000	-0.8414700000
H	4.1432440000	-3.5664350000	2.9495420000	H	0.7782380000	-1.9940740000	-0.7661340000
H	6.2984340000	-5.2890310000	-1.0932130000	H	-0.3386070000	-1.8081180000	1.5439230000
H	6.5763830000	-3.3561610000	2.5395380000	H	0.9244130000	-0.5829450000	1.2680540000
N	6.5590450000	-4.2864470000	0.6956840000	O	0.1998270000	-0.1208930000	-1.3305750000
N	6.6669500000	-1.0006310000	-4.4802410000	O	-1.0514970000	0.0596950000	1.1989100000
N	6.4896770000	4.5581870000	-0.6815390000				
N	6.5352620000	0.8499060000	4.3911070000				
C	2.3101600000	-4.5874020000	1.1565010000				

1,4-dioxane-F@1:

C	-5.5454080000	-0.9034500000	-3.5310230000	H	-6.4141530000	-1.0882190000	1.6079990000
C	-4.9671060000	0.4698580000	-3.2118700000	C	-3.3559180000	-2.2528010000	3.6262910000
C	-4.9560180000	-1.9660840000	-2.6118530000	O	-3.3624720000	-4.3527080000	2.4689010000
H	-5.2041580000	-1.1496550000	-4.5371460000	C	-2.1388360000	-4.4567460000	1.8302270000
C	-5.5196810000	1.3107950000	-2.2426020000	C	-5.6372390000	0.8064830000	3.4590920000
C	-3.8487230000	0.9449620000	-3.9069460000	C	-3.9390350000	2.6346390000	2.9766230000
C	-5.5113540000	-2.2727380000	-1.3655010000	H	-2.6057980000	4.2568680000	2.5529870000
C	-3.8222510000	-2.6879160000	-3.0050970000	C	0.1856360000	4.4892180000	-1.7860860000
C	-5.0245900000	2.5877050000	-1.9608900000	C	-3.9120870000	-1.0013410000	3.8595410000
H	-6.3829840000	0.9606580000	-1.6889400000	H	-2.5307800000	-2.6039510000	4.2281970000
C	-3.3300060000	2.2116000000	-3.6612290000	C	0.2258740000	-4.7908910000	0.4521710000
O	-3.3015500000	0.1677700000	-4.9235490000	H	-5.3223650000	1.0544350000	4.4733600000
C	-4.9966390000	-3.2605840000	-0.5211250000	O	-3.4083070000	2.4386270000	4.2479980000
H	-6.3877720000	-1.7232200000	-1.0419600000	C	0.1248950000	4.7887780000	-0.4036750000
C	-3.2868920000	-3.6847930000	-2.1969590000	O	-3.4054650000	-0.2019370000	4.8788290000
O	-3.2756150000	-2.4711730000	-4.2664520000	C	0.2570640000	-4.4759970000	1.8319070000
C	-5.6603630000	3.4831760000	-0.9059650000	C	-2.1834240000	1.7942950000	4.3371930000
C	-3.9067820000	3.0186150000	-2.6868370000	C	-2.1880370000	0.4110850000	4.6570700000
H	-2.5053670000	2.5843330000	-4.2513790000	C	0.2061060000	1.7924950000	4.3448080000
C	-2.0792250000	-0.4292000000	-4.6737840000	C	0.1783200000	0.4099710000	4.6443960000
C	-5.6063160000	-3.5881940000	0.8357150000	C	-7.1723940000	0.7933660000	3.4393160000
C	-3.8632410000	-3.9523820000	-0.9607600000	H	-7.5490920000	0.0520040000	4.1491700000
H	-2.4527700000	-4.2728820000	-2.5499420000	H	-7.5868690000	0.5471180000	2.4577510000
C	-2.0618620000	-1.8066700000	-4.3320120000	C	-7.1944690000	3.4356630000	-0.9225960000
H	-5.3583660000	4.5028850000	-1.1466980000	H	-7.5981210000	4.1387430000	-0.1890100000
C	-5.0705390000	3.1727100000	0.4635020000	H	-7.5960810000	2.4469450000	-0.6843110000
O	-3.4147800000	4.3101220000	-2.4992100000	C	-7.0806530000	-0.9122090000	-3.5455400000
C	-5.0141630000	-2.6766350000	1.9023890000	H	-7.4527940000	-0.1767040000	-4.2638240000
H	-5.2827130000	-4.6000400000	1.0817840000	H	-7.5203780000	-0.6728890000	-2.5733410000
O	-3.3605230000	-4.9853910000	-0.1733210000	C	-7.1410400000	-3.5808540000	0.8208720000
C	-5.5762520000	2.1719060000	1.2973210000	H	-7.5118130000	-4.2933890000	0.0789880000
C	-3.9693510000	3.8981520000	0.9296180000	H	-7.5634760000	-2.6025420000	0.5755260000
C	-2.2079220000	4.4398010000	-1.8325800000	H	-7.5267820000	-3.8677380000	1.8028360000
C	0.2901960000	-0.3966180000	-4.6228770000	H	-7.4467610000	-1.9003430000	-3.8369500000
C	-5.5494310000	-1.4134720000	2.1747660000	H	-7.5677890000	3.7120550000	-1.9123660000
C	-3.8950870000	-3.0749330000	2.6445460000	H	-7.5601920000	1.7756920000	3.7223960000
C	-2.1441020000	-4.7808670000	0.4466920000	C	-1.0079220000	-0.2962700000	4.8234780000
C	0.3260860000	-1.7694480000	-4.2848080000	H	-1.0199270000	-1.3391530000	5.1100680000
C	-5.0441590000	1.8822920000	2.5576970000	C	-0.9957130000	2.4995180000	4.1995610000
H	-6.4286840000	1.5970610000	0.9544800000	H	-1.0046800000	3.5650790000	4.0074880000
C	-3.4158580000	3.6475750000	2.1799100000	C	-0.9477080000	-4.3267610000	2.5365950000
O	-3.4755850000	4.9429590000	0.1502850000	H	-0.9591040000	-4.1233970000	3.6000510000
C	-2.2453470000	4.7576090000	-0.4481330000	C	-0.9615710000	-4.9647220000	-0.2550050000
C	-5.0313150000	-0.5566920000	3.1484440000	H	-0.9735830000	-5.2554050000	-1.2969800000

C	-0.8663060000	-2.4898280000	-4.1510200000	C	5.7009480000	5.0991670000	0.2602650000
H	-0.8623590000	-3.5513210000	-3.9389760000	H	3.7474550000	5.5805920000	0.9912110000
C	-0.9024170000	0.2906620000	-4.8347400000	C	5.8799330000	4.0998240000	-1.7876450000
H	-0.9254880000	1.3280460000	-5.1415800000	H	4.0755580000	3.7028750000	-2.8865140000
C	-1.0018050000	4.3305290000	-2.5156910000	H	6.2044310000	5.4836880000	1.1445770000
H	-0.9890150000	4.1365840000	-3.5809030000	H	6.5245070000	3.6533940000	-2.5397500000
C	-1.0785220000	4.9484130000	0.2787880000	C	3.8443600000	-1.0552530000	-4.4216740000
H	-1.1149610000	5.2294930000	1.3226550000	C	4.5424940000	0.0777450000	-4.8662680000
N	1.5120960000	4.3963300000	-2.1766920000	C	4.6022580000	-2.1627710000	-4.0092680000
N	1.4296740000	4.8921290000	0.0152650000	C	5.9356090000	0.0489410000	-4.8725130000
N	1.5214260000	2.2160100000	4.2615720000	H	4.0263380000	0.9768070000	-5.1800280000
N	1.4929010000	0.0230290000	4.7484130000	C	5.9899460000	-2.0776600000	-4.0575790000
N	1.5764970000	-4.3519580000	2.2430010000	H	4.1223080000	-3.0640860000	-3.6511340000
N	1.5389880000	-4.8776090000	0.0558670000	H	6.4903170000	0.9229320000	-5.2050860000
N	1.6415920000	-2.1758460000	-4.1569620000	H	6.5924840000	-2.9258680000	-3.7388730000
N	1.6054060000	-0.0021380000	-4.7106250000	C	3.7718260000	-4.5502960000	1.0529860000
H	1.8567750000	-4.7331300000	-0.9235960000	C	4.4154720000	-5.0685340000	-0.0817500000
H	1.9148450000	0.9812070000	-4.6585480000	C	4.5767190000	-3.9639580000	2.0407020000
H	1.7327230000	4.7759150000	1.0018970000	C	5.7902670000	-4.9115910000	-0.2085450000
H	1.8189010000	-0.9567320000	4.6567520000	H	3.8610210000	-5.5492370000	-0.8764190000
O	2.5619770000	-3.9266910000	-2.2360020000	C	5.9432270000	-3.8494140000	1.8060480000
H	2.1284900000	-3.4778620000	-3.0035310000	H	4.1432440000	-3.5664350000	2.9495420000
H	2.9386730000	-3.1789400000	-1.7220620000	H	6.2984340000	-5.2890310000	-1.0932130000
O	2.5383780000	2.3985240000	-3.8361400000	H	6.5763830000	-3.3561610000	2.5395380000
H	2.0807780000	3.2040200000	-3.4997330000	N	6.5590450000	-4.2864470000	0.6956840000
H	2.6897010000	1.8811980000	-3.0171180000	N	6.6669500000	-1.0006310000	-4.4802410000
O	2.4333150000	3.9913160000	2.3512760000	N	6.4896770000	4.5581870000	-0.6815390000
H	2.6778000000	3.1917590000	1.8341630000	N	6.5352620000	0.8499060000	4.3911070000
H	1.9996400000	3.5939850000	3.1440440000	C	2.3101600000	-4.5874020000	1.1565010000
O	2.5543030000	-2.3415910000	3.9433150000	C	2.2612430000	1.1335820000	4.4945770000
H	2.1016750000	-3.1201890000	3.5426680000	C	2.2238910000	4.6309360000	-1.0756290000
H	2.8639790000	-1.8276540000	3.1643030000	C	2.3799010000	-1.0967240000	-4.4069120000
C	3.7235670000	1.0692820000	4.5062140000	O	3.5198730000	-0.7881090000	1.8305970000
C	4.3889890000	-0.0579420000	5.0137180000	H	3.2145680000	0.9159950000	1.3443840000
C	4.5118090000	2.1100340000	3.9917540000	H	4.4916330000	-0.7163020000	1.9773510000
C	5.7751300000	-0.1142370000	4.9330810000	O	3.2308010000	1.7736210000	0.8533520000
H	3.8459880000	-0.8973140000	5.4280860000	H	2.8820860000	1.1892170000	-0.7279570000
C	5.8919580000	1.9447310000	3.9524390000	H	4.1936380000	1.9830110000	0.7744710000
H	4.0555390000	3.0076110000	3.5930380000	O	6.2555530000	-0.3895940000	1.7367860000
H	6.3033340000	-0.9893550000	5.3054110000	H	6.2372250000	0.5334080000	1.3657080000
H	6.5166870000	2.7244450000	3.5228120000	H	6.7748410000	-0.3186690000	2.5535960000
C	3.6853820000	4.6424300000	-0.9707960000	O	5.9048330000	1.8749500000	0.4601130000
C	4.3156750000	5.1644690000	0.1699740000	H	6.4456440000	2.6772930000	0.3854310000
C	4.5030460000	4.1231020000	-1.9849180000	H	5.8514840000	1.4980700000	-0.4736840000

O	3.5770270000	-1.8005680000	-0.7108930000	O	3.0659840000	5.0693450000	-0.5779140000
H	4.5634290000	-1.8569950000	-0.7544520000	C	5.3334740000	-1.2199420000	-3.4959350000
H	3.4457760000	-1.2706950000	0.9704630000	C	3.5291900000	0.4679570000	-4.0571180000
O	2.7589350000	0.6992240000	-1.5838780000	H	2.0745070000	1.9631820000	-4.5557830000
H	1.8087650000	0.4148580000	-1.5726460000	C	1.7620650000	4.1527000000	-2.3858400000
H	3.3423360000	-0.9442550000	-1.1370150000	C	5.4512890000	1.4865780000	3.1929050000
O	5.7016650000	0.7681060000	-1.8659940000	C	3.6548790000	3.1258260000	2.4885820000
H	4.7774170000	0.6612520000	-2.1421080000	H	2.2397100000	4.6244220000	1.8843980000
H	6.0681290000	-0.1333160000	-1.7713660000	C	1.8208620000	4.7790180000	-1.1126670000
O	6.3044440000	-1.6467810000	-0.6474750000	H	4.9964150000	-1.6096740000	-4.4567400000
H	6.4425180000	-1.2792020000	0.2581180000	C	4.7964790000	-2.1733810000	-2.4360660000
H	6.7632440000	-2.5011970000	-0.6303280000	O	3.0248650000	-0.4548240000	-4.9667400000
C	-0.8086650000	1.2270630000	0.4219830000	C	4.8987140000	0.0701870000	3.1177470000
C	-0.7909000000	0.8886670000	-1.0627310000	H	5.1504970000	1.8795560000	4.1643290000
C	-0.0316450000	-1.2983800000	-0.5354220000	O	3.1832580000	3.0610400000	3.7945110000
C	-0.0675860000	-0.9365550000	0.9449530000	C	5.3486370000	-2.2472460000	-1.1545680000
H	-1.7718950000	0.5163380000	-1.3846860000	C	3.7158330000	-3.0177310000	-2.7190160000
H	-0.5245680000	1.7554030000	-1.6698100000	C	1.8428020000	-1.1053800000	-4.6567520000
H	0.1515030000	1.6856930000	0.7115230000	C	-0.6104620000	4.1416350000	-2.2575450000
H	-1.6118240000	1.9323750000	0.6466310000	C	5.4111110000	-0.8751150000	2.2236870000
H	-0.9852090000	-1.7474780000	-0.8414700000	C	3.8540890000	-0.3354220000	3.9579220000
H	0.7782380000	-1.9940740000	-0.7661340000	C	2.0107420000	2.3778480000	4.0570060000
H	-0.3386070000	-1.8081180000	1.5439230000	C	-0.5674760000	4.8107330000	-1.0100930000
H	0.9244130000	-0.5829450000	1.2680540000	C	4.8931860000	-3.1317240000	-0.1732780000
O	0.1998270000	-0.1208930000	-1.3305750000	H	6.1831400000	-1.5983670000	-0.9155510000
O	-1.0514970000	0.0596950000	1.1989100000	C	3.2328000000	-3.9140640000	-1.7677450000
1,3-dioxane-A@1:				O	3.1767830000	-3.0120590000	-4.0042550000
C	5.2730380000	3.5017950000	-1.5067590000	C	1.9280940000	-2.4383960000	-4.1733570000
C	4.6645540000	2.4182910000	-2.3887300000	C	4.9404890000	-2.1877150000	2.1454610000
C	4.7210620000	3.3826440000	-0.0928740000	H	6.2236840000	-0.5784050000	1.5706780000
H	4.9145070000	4.4540840000	-1.8982650000	C	3.3602330000	-1.6377850000	3.9113360000
C	5.2276010000	1.1452120000	-2.5161280000	O	3.3557690000	0.5569560000	4.9056920000
C	3.4941890000	2.6780190000	-3.1125620000	C	2.0996610000	1.0981580000	4.6685530000
C	5.2844940000	2.5182550000	0.8514890000	C	5.5437160000	-3.2178540000	1.2000310000
C	3.6045930000	4.1302630000	0.3018690000	C	3.8127020000	-3.9614100000	-0.5016040000
C	4.6929330000	0.1535990000	-3.3443550000	H	2.4332180000	-4.5958350000	-2.0210810000
H	6.1332450000	0.9238080000	-1.9636900000	C	-0.5478880000	-1.2212540000	-4.6083480000
C	2.9367090000	1.7211080000	-3.9521630000	C	3.8851340000	-2.5451720000	2.9941860000
O	2.9483110000	3.9570050000	-3.0663000000	H	2.5877950000	-1.9461500000	4.6017270000
C	4.7909960000	2.3802710000	2.1508100000	C	-0.3577020000	2.2634180000	4.1772720000
H	6.1562130000	1.9412680000	0.5655090000	H	5.2768170000	-4.1948710000	1.6031480000
C	3.0747560000	4.0081760000	1.5833760000	O	3.3843060000	-4.9136090000	0.4214810000
				C	-0.4397250000	-2.5519460000	-4.1363640000
				O	3.4306840000	-3.8610440000	2.9720790000

C	-0.2847630000	1.0021020000	4.8153850000	N	-1.9513170000	4.0008450000	-2.5526910000
C	2.1801140000	-4.6824430000	1.0718530000	H	-2.0867890000	3.2389990000	3.4073360000
C	2.2067530000	-4.1182920000	2.3767940000	H	-2.3193580000	3.3211260000	-3.2298630000
C	-0.2120620000	-4.7695310000	1.1479850000	H	-1.9653750000	-3.7786600000	-3.3429050000
C	-0.1670800000	-4.1889670000	2.4380610000	H	-1.7664320000	-3.3793060000	3.5828320000
C	7.0764060000	-3.1425390000	1.1402240000	O	-2.6546910000	3.7346500000	1.7594790000
H	7.4964250000	-3.2710820000	2.1413890000	H	-2.3428160000	4.4194900000	1.1272540000
H	7.4451860000	-2.1901350000	0.7494340000	H	-2.2204460000	2.8972840000	1.4541710000
C	6.8675100000	-1.1684800000	-3.5262600000	O	-2.8075140000	1.5843970000	-3.6313410000
H	7.2720250000	-2.1694540000	-3.6984310000	H	-2.5207570000	0.9104870000	-4.2875890000
H	7.3036190000	-0.7945240000	-2.5957430000	H	-2.3886610000	1.2367160000	-2.7993890000
C	6.8069050000	3.5253860000	-1.5541220000	O	-2.3609990000	-4.3761560000	-1.7937900000
H	7.1481590000	3.6596570000	-2.5840820000	H	-2.5002280000	-3.4776360000	-1.4150880000
H	7.2631160000	2.6070400000	-1.1741940000	H	-1.9710850000	-4.8514050000	-1.0236340000
C	6.9849960000	1.5293380000	3.1287180000	O	-2.3403660000	-2.0235000000	4.3714940000
H	7.3361300000	2.5583550000	3.2431790000	H	-1.9164130000	-1.2781480000	4.8520140000
H	7.3864490000	1.1480890000	2.1856680000	H	-2.5674120000	-1.6061050000	3.5066680000
H	7.4099240000	0.9246140000	3.9343130000	C	-3.7149410000	-4.2277470000	1.7440880000
H	7.1868240000	4.3540300000	-0.9506090000	C	-4.4066580000	-3.7453110000	2.8654570000
H	7.2044380000	-0.5130610000	-4.3338480000	C	-4.4565540000	-4.4362710000	0.5719780000
H	7.4650520000	-3.9350180000	0.4951110000	C	-5.7613570000	-3.4484680000	2.7430510000
C	1.0314050000	-3.8801060000	3.0789570000	H	-3.9061960000	-3.5519190000	3.8055340000
H	1.0592890000	-3.4720410000	4.0807350000	C	-5.8088230000	-4.1083500000	0.5657650000
C	0.9806370000	-5.0404590000	0.4656420000	H	-3.9808160000	-4.7944060000	-0.3305970000
H	0.9784820000	-5.4984800000	-0.5155300000	H	-6.3030400000	-3.0507620000	3.5985930000
C	0.9607550000	0.4180310000	5.0784630000	H	-6.3905200000	-4.2459050000	-0.3438590000
H	1.0415960000	-0.5354330000	5.5855710000	C	-4.0152300000	-2.0573450000	-4.1898040000
C	0.7815680000	2.9783690000	3.8130840000	C	-4.6305220000	-3.2158250000	-3.6896670000
H	0.7270930000	3.9608810000	3.3632660000	C	-4.8445660000	-0.9911770000	-4.5593820000
C	0.6646090000	5.1343950000	-0.4299150000	C	-6.0158020000	-3.2338560000	-3.5611260000
H	0.7228750000	5.6633680000	0.5131460000	H	-4.0547130000	-4.0720730000	-3.3613330000
C	0.5440110000	3.8228410000	-2.9714350000	C	-6.2184570000	-1.1085490000	-4.3711910000
H	0.5066580000	3.3681100000	-3.9522840000	H	-4.4227770000	-0.0783380000	-4.9577390000
C	0.6158940000	-0.4950270000	-4.8912320000	H	-6.5109080000	-4.1223500000	-3.1740550000
H	0.5698070000	0.5079070000	-5.2956160000	H	-6.8711470000	-0.2745050000	-4.6140420000
C	0.7841050000	-3.1851230000	-3.9275140000	C	-4.1153350000	4.6253570000	-1.4682910000
H	0.8527740000	-4.2128750000	-3.5954350000	C	-4.9148530000	4.1154470000	-2.4960880000
N	-1.8872650000	-0.8760420000	-4.7071740000	C	-4.7608200000	5.2140070000	-0.3703330000
N	-1.7289210000	-2.9968400000	-3.9770140000	C	-6.3006770000	4.1858560000	-2.3645000000
N	-1.5307370000	-4.9178270000	0.7596280000	H	-4.4850560000	3.6417540000	-3.3700380000
N	-1.4766720000	-4.0136240000	2.8126580000	C	-6.1498440000	5.2368630000	-0.3460110000
N	-1.5610330000	0.5247790000	5.0394430000	H	-4.1848830000	5.6362970000	0.4424710000
N	-1.7032080000	2.5309850000	4.0461930000	H	-6.9360500000	3.7685370000	-3.1412770000
N	-1.8558600000	5.0543310000	-0.5701160000	H	-6.6703200000	5.6851740000	0.4976700000

C	-3.8362720000	1.2865100000	4.4265920000	H	2.5035220000	-0.9973470000	-1.1448780000
C	-4.6318480000	2.2056590000	3.7259600000	H	0.9471840000	-1.5256410000	-1.8148320000
C	-4.4705320000	0.1582580000	4.9665520000	H	-0.1286770000	-1.3428460000	0.4070100000
C	-5.9837230000	1.9237850000	3.5495490000	H	1.3361230000	-2.3085700000	0.6009420000
H	-4.2107650000	3.0964510000	3.2764580000	H	2.6635010000	1.2752300000	-0.3795420000
C	-5.8288540000	-0.0222020000	4.7315370000	H	1.2171090000	2.3271330000	-0.5928680000
H	-3.9051670000	-0.5896730000	5.5036510000	O	1.0274210000	0.4467630000	-1.3163050000
H	-6.6070860000	2.6061580000	2.9762240000	C	1.4980760000	-0.2958780000	1.3591900000
H	-6.3327580000	-0.9028240000	5.1236640000	H	1.0918120000	-0.4370900000	2.3598330000
N	-6.5889850000	0.8229290000	4.0181810000	H	2.5923310000	-0.3383990000	1.4160330000
N	-6.9254580000	4.7315750000	-1.3164350000	O	1.1147990000	1.0373470000	0.9572510000
N	-6.8145640000	-2.2017170000	-3.8727470000				
N	-6.4697000000	-3.6065280000	1.6177400000				
C	-2.3837710000	1.4422360000	4.5376880000	1,3-dioxane-B@1:			
C	-2.2594980000	-4.4243290000	1.7611010000	C	5.3404870000	3.4362810000	-1.4728690000
C	-2.5594000000	-1.9519670000	-4.3013160000	C	4.7371760000	2.3628460000	-2.3731080000
C	-2.6553790000	4.5567270000	-1.5092310000	C	4.7844080000	3.3335000000	-0.0578330000
O	-2.8374570000	-0.9959820000	1.8583430000	H	4.9925120000	4.3918160000	-1.8666330000
H	-2.7671430000	-1.6992030000	0.1872950000	C	5.2972640000	1.0905140000	-2.5104290000
H	-3.8043870000	-0.7938590000	1.8410460000	C	3.5830920000	2.6350280000	-3.1195710000
O	-2.8336670000	-1.8133630000	-0.7920870000	C	5.3447740000	2.4885480000	0.9056290000
H	-2.0781100000	-0.3630680000	-1.3055510000	C	3.6746570000	4.0969820000	0.3256130000
H	-3.8004080000	-1.6876530000	-0.9764300000	C	4.7816870000	0.1118090000	-3.3673550000
O	-5.4237430000	-0.3418870000	1.4294810000	H	6.1837630000	0.8527450000	-1.9342130000
H	-5.6498260000	-0.7772210000	0.5695320000	C	3.0538660000	1.6980730000	-4.0004280000
H	-6.1845340000	-0.3913060000	2.0239260000	O	3.0237760000	3.9034150000	-3.0508770000
O	-5.4422220000	-1.1947050000	-1.0788480000	C	4.8555000000	2.3827830000	2.2107500000
H	-6.0960320000	-1.7367980000	-1.5395910000	H	6.2099440000	1.8964890000	0.6306600000
H	-5.3835000000	-0.3143580000	-1.5881260000	C	3.1503730000	4.0097640000	1.6121680000
O	-1.6001550000	1.3483780000	1.1295770000	O	3.1379870000	5.0173870000	-0.5694890000
H	-1.8190540000	1.1880770000	0.1774320000	C	5.4172550000	-1.2668890000	-3.4853140000
H	-2.3898430000	-0.1259340000	1.7255940000	C	3.6437960000	0.4424790000	-4.1153110000
O	-1.7060770000	0.5485550000	-1.4421620000	H	2.2076620000	1.9552050000	-4.6214220000
H	-0.7301850000	0.4682750000	-1.5296500000	C	1.8355660000	4.0802240000	-2.3648680000
H	-0.6190340000	1.2917490000	1.1682740000	C	5.5067130000	1.4875130000	3.2575510000
O	-5.2089540000	1.1076370000	-2.1800960000	C	3.7264260000	3.1453660000	2.5376530000
H	-4.4490050000	1.2138320000	-2.7872470000	H	2.3217230000	4.6408160000	1.9000220000
H	-4.9569690000	1.6071080000	-1.3670050000	C	1.8919980000	4.7164380000	-1.0981230000
O	-4.3692960000	1.9096780000	0.2379440000	H	5.0865200000	-1.6764170000	-4.4400650000
H	-4.8022920000	1.2749850000	0.8420960000	C	4.8623900000	-2.1908000000	-2.4078010000
H	-4.1150880000	2.6899110000	0.7549610000	O	3.1366060000	-0.4635890000	-5.0437560000
C	0.9647460000	-1.3124270000	0.3588570000	C	4.9387110000	0.0780430000	3.1689020000
C	1.4142230000	-0.9176240000	-1.0423500000	H	5.2024290000	1.8804520000	4.2279050000
C	1.5661430000	1.3283930000	-0.3500790000	O	3.2380050000	3.1057160000	3.8410730000

C	5.4068420000	-2.2687710000	-1.1231590000	H	7.3982640000	2.5466390000	3.3197590000
C	3.7555020000	-3.0013040000	-2.6863610000	H	7.4440150000	1.1388040000	2.2589500000
C	1.9333660000	-1.0823410000	-4.7288230000	H	7.4572180000	0.9107910000	4.0071420000
C	-0.5358820000	4.1032950000	-2.2540470000	H	7.2575150000	4.2730800000	-0.9029490000
C	5.4483030000	-0.8749630000	2.2816830000	H	7.2995500000	-0.5873910000	-4.3206790000
C	3.8614710000	-0.3035150000	3.9777610000	H	7.4644540000	-3.9711480000	0.5789950000
C	2.0538690000	2.4304460000	4.0846940000	C	0.9649260000	-3.8132940000	3.0577850000
C	-0.4933590000	4.7882890000	-1.0159890000	H	0.9788780000	-3.3964290000	4.0561130000
C	4.9163290000	-3.1290990000	-0.1354090000	C	0.9494830000	-4.9929280000	0.4496990000
H	6.2596540000	-1.6437430000	-0.8848480000	H	0.9605140000	-5.4655540000	-0.5244250000
C	3.2454190000	-3.8795090000	-1.7348920000	C	0.9775320000	0.4605890000	5.0604850000
O	3.2200780000	-2.9736800000	-3.9692530000	H	1.0459200000	-0.4983280000	5.5581730000
C	1.9843730000	-2.3753140000	-4.1424370000	C	0.8287210000	3.0328200000	3.8151750000
C	4.9427780000	-2.1737650000	2.1815040000	H	0.7834800000	4.0225140000	3.3798280000
H	6.2857100000	-0.5972790000	1.6521470000	C	0.7376220000	5.0947680000	-0.4264530000
C	3.3241760000	-1.5855760000	3.9009800000	H	0.7969040000	5.6398560000	0.5073740000
O	3.3746680000	0.5951650000	4.9253280000	C	0.6185340000	3.7546590000	-2.9542360000
C	2.1246780000	1.1438640000	4.6839530000	H	0.5804030000	3.2968230000	-3.9339190000
C	5.5449710000	-3.2175020000	1.2488370000	C	0.7207960000	-0.4681560000	-5.0257900000
C	3.8174970000	-3.9333290000	-0.4668920000	H	0.7010290000	0.4952760000	-5.5200410000
H	2.4322740000	-4.5443550000	-1.9866700000	C	0.8243740000	-3.0590420000	-3.8135600000
C	-0.4621020000	-1.1408200000	-4.6825890000	H	0.8636740000	-4.0557740000	-3.3956060000
C	3.8522050000	-2.5034230000	2.9973110000	N	-1.7945210000	-0.7868000000	-4.8309070000
H	2.5221110000	-1.8770830000	4.5634090000	N	-1.6791600000	-2.8170360000	-3.8710780000
C	-0.3195910000	2.3117030000	4.1451270000	N	-1.5655540000	-4.9014880000	0.7241310000
H	5.2556380000	-4.1881970000	1.6524530000	N	-1.5403510000	-3.9822290000	2.7720230000
O	3.3570680000	-4.8715210000	0.4531970000	N	-1.5410090000	0.5720800000	4.9836880000
C	-0.3830660000	-2.4163760000	-4.0725130000	N	-1.6632200000	2.5842090000	3.9965250000
O	3.3692050000	-3.8076640000	2.9726060000	N	-1.7817490000	5.0667800000	-0.5961500000
C	-0.2606700000	1.0465620000	4.7768820000	N	-1.8756450000	3.9894920000	-2.5654440000
C	2.1388680000	-4.6264550000	1.0691860000	H	-2.0375220000	3.2683210000	3.3260380000
C	2.1479910000	-4.0517500000	2.3690960000	H	-2.2436520000	3.2944050000	-3.2290560000
C	-0.2519380000	-4.7302020000	1.1211180000	H	-1.9483250000	-3.5695540000	-3.2055450000
C	-0.2244900000	-4.1410980000	2.4081190000	H	-1.8433950000	-3.3481530000	3.5374120000
C	7.0791330000	-3.1677710000	1.2124840000	O	-2.5796610000	3.6435610000	1.6474240000
H	7.4818450000	-3.2957320000	2.2207870000	H	-2.2857020000	4.3414650000	1.0175750000
H	7.4696900000	-2.2245500000	0.8204730000	H	-2.1390040000	2.8116460000	1.3461250000
C	6.9515840000	-1.2229360000	-3.5019950000	O	-2.6671790000	1.5838300000	-3.6196590000
H	7.3528120000	-2.2293950000	-3.6478630000	H	-2.3989060000	0.9581250000	-4.3298690000
H	7.3805110000	-0.8302520000	-2.5758570000	H	-2.2928250000	1.1381440000	-2.8177490000
C	6.8752950000	3.4480330000	-1.5098620000	O	-2.5081180000	-4.3283250000	-1.8149510000
H	7.2248760000	3.5801630000	-2.5372420000	H	-2.8285780000	-3.4926670000	-1.4025940000
H	7.3210590000	2.5255670000	-1.1273700000	H	-2.0380200000	-4.7549690000	-1.0614320000
C	7.0405110000	1.5204080000	3.2009640000	O	-2.4079710000	-1.9795310000	4.3298960000

H	-1.9453890000	-1.2351290000	4.7747350000	C	-2.4890760000	-1.8059800000	-4.3235480000
H	-2.7012610000	-1.5722100000	3.4808000000	C	-2.5804150000	4.5761310000	-1.5409480000
C	-3.7731090000	-4.2928060000	1.7050890000	O	-3.1414910000	-1.0145710000	1.8515160000
C	-4.4780740000	-3.7269200000	2.7782350000	H	-3.2334780000	-1.7663650000	0.2175770000
C	-4.5141470000	-4.6591090000	0.5721540000	H	-4.1031760000	-0.7862260000	1.8728770000
C	-5.8442950000	-3.4974130000	2.6386720000	O	-3.3321110000	-1.9077800000	-0.7550440000
H	-3.9830760000	-3.4225840000	3.6915810000	H	-2.5022360000	-0.5552750000	-1.3171120000
C	-5.8785800000	-4.3866070000	0.5439820000	H	-4.2983730000	-1.7688280000	-0.9317060000
H	-4.0304540000	-5.0936880000	-0.2914700000	O	-5.6738300000	-0.2335670000	1.4502110000
H	-6.3958190000	-3.0319760000	3.4529570000	H	-5.9812310000	-0.6379330000	0.6016800000
H	-6.4599770000	-4.6431540000	-0.3393950000	H	-6.4160540000	-0.1634700000	2.0671480000
C	-3.9488020000	-1.8877360000	-4.2329320000	O	-5.8572780000	-1.0858550000	-1.0576820000
C	-4.5873090000	-3.0438930000	-3.7566840000	H	-6.5459930000	-1.4994610000	-1.5963000000
C	-4.7604440000	-0.8055110000	-4.5969510000	H	-5.5919390000	-0.2320830000	-1.5385460000
C	-5.9709080000	-3.0362430000	-3.6200830000	O	-1.7192840000	1.1761510000	1.0314610000
H	-4.0299690000	-3.9218430000	-3.4558960000	H	-1.8515610000	0.9643210000	0.0705580000
C	-6.1356020000	-0.9002230000	-4.4078410000	H	-2.6801690000	-0.1627760000	1.6607400000
H	-4.3247320000	0.1058070000	-4.9825760000	O	-1.8781800000	0.2086440000	-1.4601260000
H	-6.4798390000	-3.9182670000	-3.2368780000	H	-0.9853940000	-0.2064290000	-1.4430770000
H	-6.7732670000	-0.0519560000	-4.6416590000	H	-0.8288450000	0.8121820000	1.2358670000
C	-4.0385260000	4.6758390000	-1.5162120000	O	-5.0952880000	1.1407590000	-2.0798880000
C	-4.8412730000	4.1342380000	-2.5252170000	H	-4.3342080000	1.2240610000	-2.6820520000
C	-4.6774860000	5.3257970000	-0.4507820000	H	-4.8914310000	1.6704110000	-1.2694910000
C	-6.2254340000	4.2393320000	-2.4063510000	O	-4.7890340000	2.2041670000	0.3548120000
H	-4.4152890000	3.6136620000	-3.3740800000	H	-5.0361860000	1.4445640000	0.9148710000
C	-6.0655490000	5.3791450000	-0.4377410000	H	-4.1260070000	2.7334290000	0.8299460000
H	-4.0953220000	5.7733080000	0.3446540000	C	1.9800240000	0.8313600000	-0.3300540000
H	-6.8651910000	3.8015160000	-3.1684360000	C	1.8583440000	0.3839750000	1.1201180000
H	-6.5818470000	5.8754430000	0.3811870000	C	0.4413980000	-1.3775450000	0.4617480000
C	-3.8109040000	1.3698400000	4.3930290000	H	2.6591530000	-0.3170140000	1.3836290000
C	-4.5990800000	2.3075770000	3.7105030000	H	1.8811920000	1.2198690000	1.8143030000
C	-4.4604070000	0.2562760000	4.9465880000	H	1.2535860000	1.6242260000	-0.5400510000
C	-5.9597550000	2.0563680000	3.5560410000	H	2.9776040000	1.2370690000	-0.5140300000
H	-4.1678700000	3.1881000000	3.2520730000	H	1.2419860000	-2.1011060000	0.6578150000
C	-5.8258710000	0.1056730000	4.7356850000	H	-0.5372640000	-1.8154150000	0.6529780000
H	-3.9024900000	-0.5037060000	5.4745930000	O	0.5871030000	-0.2711690000	1.3294150000
H	-6.5727200000	2.7474900000	2.9833360000	C	1.7290400000	-0.3636570000	-1.2407680000
H	-6.3415940000	-0.7652740000	5.1340210000	H	1.6416200000	-0.0768630000	-2.2857750000
N	-6.5793210000	0.9676100000	4.0342570000	H	2.5321930000	-1.1034540000	-1.1442320000
N	-6.8446690000	4.8481560000	-1.3903940000	O	0.4773400000	-0.9998200000	-0.9004110000
N	-6.7506820000	-1.9845760000	-3.9120610000				
N	-6.5518560000	-3.8008440000	1.5433880000				
C	-2.3539020000	1.4979420000	4.4827490000				
C	-2.3102860000	-4.4232820000	1.7226390000				
				1,3-dioxane-C@1:			
				C	-5.2994460000	-1.4045620000	-3.5161860000

C	-4.6623080000	-0.0234350000	-3.4490990000	C	-3.5156730000	-1.3570890000	3.9561820000
C	-4.7902970000	-2.2790940000	-2.3786780000	O	-3.5515100000	-3.6390240000	3.1943150000
H	-4.9396050000	-1.8628050000	-4.4377620000	C	-2.3026000000	-3.9122210000	2.6499630000
C	-5.2020960000	1.0136490000	-2.6851940000	C	-5.6202600000	1.6950750000	3.0155160000
C	-3.4949590000	0.2527940000	-4.1713410000	C	-3.8185270000	3.3204570000	2.2800920000
C	-5.3830300000	-2.2774460000	-1.1121040000	H	-2.3615010000	4.7459690000	1.6066460000
C	-3.6988880000	-3.1329840000	-2.5797220000	C	0.6508280000	3.9788330000	-2.6066690000
C	-4.6479960000	2.2961430000	-2.6330350000	C	-4.0141510000	-0.0585960000	3.8992530000
H	-6.1019840000	0.8184410000	-2.1137420000	H	-2.7543040000	-1.6172440000	4.6776310000
C	-2.9268650000	1.5212690000	-4.1646340000	C	0.1241200000	-4.5469600000	1.5040850000
O	-2.9486650000	-0.7380320000	-4.9772470000	H	-5.3514000000	2.1376010000	3.9749280000
C	-4.9475460000	-3.0921660000	-0.0638610000	O	-3.3982480000	3.3807760000	3.6053730000
H	-6.2328360000	-1.6266530000	-0.9415940000	C	0.5498210000	4.5549410000	-1.3172830000
C	-3.2359600000	-3.9601800000	-1.5592660000	O	-3.5382100000	0.9072520000	4.7826640000
O	-3.1319290000	-3.2202880000	-3.8490250000	C	0.0850390000	-3.9914720000	2.8041640000
C	-5.2716060000	3.4072180000	-1.8001220000	C	-2.2131220000	2.7366630000	3.9299410000
C	-3.4895700000	2.5272520000	-3.3859820000	C	-2.2902690000	1.4499100000	4.5267020000
H	-2.0661760000	1.7350640000	-4.7818990000	C	0.1748770000	2.6763660000	4.0783920000
C	-1.7801020000	-1.3516120000	-4.5616290000	C	0.0796300000	1.3856460000	4.6523630000
C	-5.6302930000	-3.1165290000	1.2971510000	C	-7.1513030000	1.7208890000	2.9033440000
C	-3.8466500000	-3.9223950000	-0.3077650000	H	-7.5960110000	1.1520300000	3.7242240000
H	-2.4279330000	-4.6521300000	-1.7501180000	H	-7.5212630000	1.2909760000	1.9683830000
C	-1.8750180000	-2.6614730000	-4.0213150000	C	-6.8041610000	3.4328450000	-1.8889880000
H	-4.9004980000	4.3449010000	-2.2146950000	H	-7.1971670000	4.2829190000	-1.3249100000
C	-4.7632960000	3.3450060000	-0.3653710000	H	-7.2729190000	2.5292640000	-1.4894660000
O	-2.9295390000	3.8006110000	-3.4216960000	C	-6.8321240000	-1.3520200000	-3.5895630000
C	-5.0565880000	-2.0359900000	2.2028800000	H	-7.1458550000	-0.7592900000	-4.4530030000
H	-5.3645090000	-4.0700070000	1.7540360000	H	-7.2898980000	-0.9068930000	-2.7018240000
O	-3.4276080000	-4.7865570000	0.6981310000	C	-7.1614540000	-3.0592120000	1.1960710000
C	-5.3720240000	2.5668500000	0.6226240000	H	-7.5274860000	-3.8893260000	0.5859290000
C	-3.6461480000	4.0997270000	0.0099600000	H	-7.5280730000	-2.1331700000	0.7445200000
C	-1.7419770000	3.9887160000	-2.7295780000	H	-7.6054030000	-3.1368960000	2.1921150000
C	0.5876880000	-1.4671250000	-4.4162310000	H	-7.2361490000	-2.3623590000	-3.6953380000
C	-5.5392280000	-0.7242140000	2.1855270000	H	-7.1174580000	3.5318680000	-2.9317130000
C	-4.0210550000	-2.3320930000	3.0996270000	H	-7.5134200000	2.7510970000	2.9572190000
C	-2.2428810000	-4.4917980000	1.3545130000	C	-1.1427790000	0.7675490000	4.9115090000
C	0.5047120000	-2.7969010000	-3.9403710000	H	-1.2088270000	-0.1989890000	5.3935890000
C	-4.9318260000	2.5364050000	1.9498580000	C	-0.9915050000	3.3684590000	3.7292230000
H	-6.2365490000	1.9717750000	0.3521850000	H	-0.9510720000	4.3665480000	3.3117180000
C	-3.1854010000	4.1076860000	1.3224380000	C	-1.1488890000	-3.6856580000	3.3918860000
O	-3.0545210000	4.9267230000	-0.9391510000	H	-1.2128760000	-3.2832570000	4.3952240000
C	-1.8151520000	4.5660730000	-1.4333570000	C	-1.0274160000	-4.8322130000	0.7745790000
C	-5.0527040000	0.2815040000	3.0237000000	H	-0.9902320000	-5.3015240000	-0.1997530000
H	-6.3415130000	-0.4796980000	1.4990600000	C	-0.7393120000	-3.4037970000	-3.7387070000

H	-0.8185390000	-4.4257100000	-3.3894660000	H	4.1796720000	5.2066130000	0.2308380000
C	-0.5489990000	-0.7372180000	-4.7627740000	C	6.3239700000	4.1435280000	-2.7293920000
H	-0.4907860000	0.2520760000	-5.1971410000	H	4.5085730000	3.6494940000	-3.7812320000
C	-0.5193830000	3.6999050000	-3.3277360000	H	6.6441830000	5.3954420000	0.2563310000
H	-0.4817420000	3.3088210000	-4.3367680000	H	6.9740740000	3.8262440000	-3.5406100000
C	-0.6668240000	4.8600590000	-0.7136660000	C	4.0625900000	-2.3944770000	-3.9140200000
H	-0.7220070000	5.3419520000	0.2532920000	C	4.9140790000	-1.3493450000	-4.2941740000
N	1.9895420000	3.8352770000	-2.9403940000	C	4.6508730000	-3.5534990000	-3.3845190000
N	1.8395410000	4.7728920000	-0.9037820000	C	6.2849800000	-1.4906750000	-4.0869400000
N	1.5080130000	3.0133170000	3.9258350000	H	4.5290140000	-0.4253830000	-4.7078630000
N	1.3736870000	0.9678800000	4.8463130000	C	6.0314020000	-3.5936480000	-3.2352540000
N	1.3773700000	-3.7990840000	3.2566020000	H	4.0392010000	-4.3817420000	-3.0553730000
N	1.4559970000	-4.6847280000	1.1979380000	H	6.9541300000	-0.6716550000	-4.3364880000
N	1.7736460000	-3.2932520000	-3.7274440000	H	6.5052120000	-4.4809360000	-2.8201360000
N	1.9390730000	-1.1850730000	-4.4780680000	C	3.6343460000	-4.0543860000	2.2214590000
H	1.7975160000	-4.8077930000	0.2280440000	C	4.3807270000	-4.4683080000	1.1066940000
H	2.3362710000	-0.2385700000	-4.5215440000	C	4.3340460000	-3.4414880000	3.2700460000
H	2.0858790000	4.9267460000	0.0865530000	C	5.7472610000	-4.2074110000	1.0775480000
H	1.6400820000	-0.0319020000	4.9563150000	H	3.9170760000	-4.9474780000	0.2537470000
O	2.3615790000	-4.3975890000	-1.2992840000	C	5.7033850000	-3.2344810000	3.1331920000
H	2.0369850000	-4.2869590000	-2.2199500000	H	3.8170360000	-3.0823050000	4.1487520000
H	2.6610810000	-3.4879640000	-1.0561350000	H	6.3313980000	-4.5069350000	0.2092580000
O	3.0016130000	1.2828180000	-3.6762280000	H	6.2535290000	-2.7419340000	3.9324550000
H	2.6862900000	2.2133100000	-3.7264880000	N	6.4191580000	-3.5925360000	2.0592330000
H	2.5604390000	0.9525040000	-2.8475080000	N	6.8537450000	-2.5821970000	-3.5579300000
O	2.4127250000	4.3086240000	1.6629490000	N	6.9320590000	4.6179060000	-1.6364640000
H	2.3783600000	3.3730460000	1.3553200000	N	6.4195100000	1.3357800000	3.9812690000
H	2.0358530000	4.2159140000	2.5658930000	C	2.1728070000	-4.1902950000	2.2603190000
O	2.2181310000	-1.5351910000	4.5297930000	C	2.1944100000	1.9581590000	4.3613260000
H	1.7858280000	-2.4064090000	4.3638800000	C	2.6665950000	4.3141300000	-1.8969640000
H	2.4203150000	-1.2548920000	3.6079310000	C	2.6070070000	-2.3056440000	-4.0352080000
C	3.6492020000	1.7849290000	4.2888350000	O	2.2616600000	-0.7423250000	1.8654430000
C	4.2846000000	0.6988180000	4.9080380000	H	2.4412820000	0.9310150000	1.3142440000
C	4.4500450000	2.6662930000	3.5473910000	H	1.3475320000	-0.9666560000	1.5892680000
C	5.6507470000	0.5205460000	4.7156640000	O	2.5303820000	1.7125730000	0.7138310000
H	3.7319040000	-0.0278180000	5.4884480000	H	2.0695510000	0.9156390000	-0.6925930000
C	5.8095440000	2.3962210000	3.4305850000	H	3.5078680000	1.8003270000	0.5511230000
H	4.0126570000	3.5118890000	3.0324770000	O	5.7091650000	-0.3784260000	1.5025020000
H	6.1517380000	-0.3314610000	5.1700210000	H	5.5798080000	0.5479370000	1.1989590000
H	6.4442930000	3.0588310000	2.8455040000	H	6.3977320000	-0.3341820000	2.1785710000
C	4.1224690000	4.4178490000	-1.8009980000	O	5.1278780000	1.9119000000	0.1989260000
C	4.7494240000	4.9172810000	-0.6450680000	H	5.4847950000	2.8049600000	0.2891270000
C	4.9414770000	4.0356580000	-2.8677400000	H	5.2604660000	1.6448670000	-0.7715340000
C	6.1394690000	5.0003700000	-0.6234210000	O	3.1447230000	-1.9193130000	-0.4701170000

H	2.7473670000	-1.1536110000	-0.9495060000	C	-5.5678530000	3.5043890000	-1.0915160000
H	2.8129550000	-1.2319280000	1.2111700000	C	-3.8167330000	2.9268250000	-2.8431650000
O	1.9319600000	0.3060360000	-1.4683850000	H	-2.4220060000	2.3943250000	-4.3819120000
H	0.9714610000	0.0850680000	-1.4943770000	C	-2.0277800000	-0.6338070000	-4.6281710000
H	4.1149850000	-1.8681720000	-0.6456730000	C	-5.6359420000	-3.4561970000	1.0299790000
O	5.4281020000	1.0111710000	-2.1881500000	C	-3.8893000000	-3.9529800000	-0.7346280000
H	4.6350940000	1.0951620000	-2.7570400000	H	-2.4555800000	-4.3555000000	-2.2806610000
H	5.5171480000	0.0701250000	-1.9237000000	C	-2.0229980000	-1.9843780000	-4.1922830000
O	5.7533710000	-1.3989050000	-0.8793130000	H	-5.2476090000	4.5061070000	-1.3795770000
H	5.9435480000	-1.1237060000	0.0634870000	C	-4.9940790000	3.2538020000	0.2964830000
H	6.4586490000	-1.9787100000	-1.1931940000	O	-3.3010240000	4.2162530000	-2.7181930000
C	-1.3710590000	-0.3948590000	1.3372830000	C	-5.0407600000	-2.4902150000	2.0466820000
H	-2.3016380000	-0.9754610000	1.3606680000	H	-5.3258260000	-4.4549680000	1.3387910000
H	-1.1100520000	-0.1198740000	2.3583860000	O	-3.4089020000	-4.9541140000	0.1066000000
C	-1.5105570000	0.8176770000	0.4223690000	C	-5.5272560000	2.3126220000	1.1808460000
H	-2.3780710000	1.4148220000	0.7175280000	C	-3.8799460000	3.9804810000	0.7298520000
H	-0.6216020000	1.4526760000	0.5088260000	C	-2.0939370000	4.3549020000	-2.0525710000
O	-0.3088660000	-1.2498550000	0.8635760000	C	0.3406520000	-0.6105480000	-4.5671250000
O	-0.6052040000	-0.5761300000	-1.3608910000	C	-5.5648990000	-1.2093800000	2.2508570000
C	-0.5495690000	-1.6689780000	-0.4611830000	C	-3.9270390000	-2.8595220000	2.8128140000
H	-1.4977570000	-2.2186090000	-0.5081540000	C	-2.1876040000	-4.7294040000	0.7143000000
H	0.2825960000	-2.3037630000	-0.7645360000	C	0.3636190000	-1.9586340000	-4.1408900000
C	-1.6714890000	0.3388570000	-1.0174750000	C	-5.0140560000	2.0891700000	2.4628050000
H	-1.6105960000	1.1536480000	-1.7374080000	H	-6.3884130000	1.7361920000	0.8634840000
H	-2.6299970000	-0.1784530000	-1.1577220000	C	-3.3431380000	3.7928430000	1.9980520000

1,3-dioxane-D@1:

C	-5.5017820000	-1.0153150000	-3.4741550000	H	-6.4243290000	-0.9057330000	1.6644440000
C	-4.9088960000	0.3670350000	-3.2334360000	C	-3.3886340000	-1.9944380000	3.7585460000
C	-4.9327520000	-2.0302770000	-2.4906740000	O	-3.4038910000	-4.1426360000	2.6970310000
H	-5.1574510000	-1.3249170000	-4.4615390000	C	-2.1783870000	-4.2875690000	2.0632800000
C	-5.4494340000	1.2640670000	-2.3089570000	C	-5.6348880000	1.0762340000	3.4163470000
C	-3.7874140000	0.7926190000	-3.9553180000	C	-3.8994750000	2.8448430000	2.8500020000
C	-5.5042590000	-2.2638700000	-1.2361360000	H	-2.5232660000	4.4063750000	2.3413660000
C	-3.8044030000	-2.7862780000	-2.8335540000	C	0.3000320000	4.3838010000	-1.9992950000
C	-4.9395950000	2.5482720000	-2.0960870000	C	-3.9345120000	-0.7277010000	3.9261840000
H	-6.3148740000	0.9528360000	-1.7356020000	H	-2.5734420000	-2.3247300000	4.3850340000
C	-3.2534580000	2.0642280000	-3.7762960000	C	0.1792500000	-4.7479970000	0.7176280000
O	-3.2452810000	-0.0449270000	-4.9239840000	H	-5.3268120000	1.3742960000	4.4191200000
C	-5.0124150000	-3.2176910000	-0.3391380000	O	-3.3916490000	2.7198500000	4.1408320000
H	-6.3754500000	-1.6861270000	-0.9494300000	C	0.2367300000	4.7455170000	-0.6319300000
C	-3.2968370000	-3.7522910000	-1.9747280000	O	-3.4274920000	0.1160070000	4.9099810000
O	-3.2415880000	-2.6359040000	-4.0972560000	C	0.2130560000	-4.3011760000	2.0599720000

C	-2.1758520000	2.0701220000	4.2864570000	H	1.8140950000	-4.8089290000	-0.6502580000
C	-2.2002340000	0.7038290000	4.6736160000	H	1.9817180000	0.7463610000	-4.6933040000
C	0.2155560000	2.0440070000	4.3222580000	H	1.8359410000	4.8044110000	0.7784180000
C	0.1694940000	0.6772800000	4.6883950000	H	1.7954680000	-0.7081990000	4.7564500000
C	-7.1695920000	1.0836610000	3.3798700000	O	2.5489100000	-4.0438580000	-1.9966650000
H	-7.5645580000	0.3872520000	4.1244150000	H	2.1405220000	-3.6268340000	-2.7955310000
H	-7.5775070000	0.7908650000	2.4084690000	H	2.9268050000	-3.2766460000	-1.5141770000
C	-7.1024480000	3.4799430000	-1.1187890000	O	2.6531620000	2.2095470000	-3.9712210000
H	-7.5010600000	4.2230350000	-0.4228090000	H	2.1942070000	3.0275290000	-3.6693670000
H	-7.5215120000	2.5096860000	-0.8384120000	H	2.8067740000	1.7350020000	-3.1274860000
C	-7.0370230000	-1.0046490000	-3.4989070000	O	2.5027900000	4.0952560000	2.1940700000
H	-7.3949530000	-0.3091090000	-4.2628300000	H	2.7302630000	3.2641020000	1.7194870000
H	-7.4792890000	-0.7011290000	-2.5459090000	H	2.0509520000	3.7567870000	3.0019640000
C	-7.1703060000	-3.4306150000	1.0035140000	O	2.5230730000	-2.1096750000	4.0907440000
H	-7.5443710000	-4.1826250000	0.3035810000	H	2.0635440000	-2.8979680000	3.7137120000
H	-7.5783890000	-2.4642400000	0.6945230000	H	2.8363560000	-1.6301270000	3.2911220000
H	-7.5673380000	-3.6521150000	1.9978970000	C	3.7228790000	1.2815980000	4.5199420000
H	-7.4146960000	-2.0037080000	-3.7324780000	C	4.3720260000	0.1729350000	5.0852710000
H	-7.4630640000	3.7149990000	-2.1237540000	C	4.5245950000	2.2799520000	3.9463050000
H	-7.5454180000	2.0852670000	3.6054450000	C	5.7567150000	0.0888110000	5.0007230000
C	-1.0276940000	-0.0069520000	4.8870730000	H	3.8176450000	-0.6336330000	5.5466580000
H	-1.0540640000	-1.0348360000	5.2229590000	C	5.9016680000	2.0898690000	3.9097870000
C	-0.9775250000	2.7549610000	4.1298700000	H	4.0815420000	3.1614340000	3.4997790000
H	-0.9728920000	3.8092040000	3.8829280000	H	6.2724960000	-0.7739700000	5.4164760000
C	-0.9880180000	-4.0873990000	2.7513710000	H	6.5366610000	2.8344360000	3.4353260000
H	-0.9943000000	-3.7946400000	3.7936210000	C	3.7976220000	4.5588600000	-1.1778210000
C	-1.0089820000	-4.9880640000	0.0331850000	C	4.4242540000	5.1258970000	-0.0566490000
H	-1.0254280000	-5.3638620000	-0.9811010000	C	4.6179470000	3.9920760000	-2.1638630000
C	-0.8335380000	-2.6601670000	-3.9596520000	C	5.8087500000	5.0590230000	0.0435210000
H	-0.8366610000	-3.7026090000	-3.6689840000	H	3.8540340000	5.5794430000	0.7432740000
C	-0.8467160000	0.0681630000	-4.8292420000	C	5.9936390000	3.9696280000	-1.9573330000
H	-0.8625450000	1.0824390000	-5.2056870000	H	4.1930290000	3.5370820000	-3.0497460000
C	-0.8866390000	4.2005150000	-2.7250330000	H	6.3095490000	5.4802150000	0.9125780000
H	-0.8722220000	3.9567420000	-3.7799410000	H	6.6400240000	3.4875890000	-2.6855170000
C	-0.9668790000	4.9415720000	0.0398820000	C	3.8899760000	-1.2916300000	-4.3220450000
H	-1.0036090000	5.2704670000	1.0696900000	C	4.6033670000	-0.1980660000	-4.8359450000
N	1.6273860000	4.2679210000	-2.3807170000	C	4.6333650000	-2.3798450000	-3.8376320000
N	1.5399570000	4.8626570000	-0.2142220000	C	5.9960400000	-0.2443960000	-4.8359670000
N	1.5364550000	2.4467770000	4.2202290000	H	4.0993870000	0.6852540000	-5.2084940000
N	1.4788970000	0.2794250000	4.8159570000	C	6.0220900000	-2.3155680000	-3.8881620000
N	1.5325700000	-4.1561720000	2.4623820000	H	4.1421800000	-3.2512650000	-3.4248260000
N	1.4936760000	-4.8812140000	0.3336570000	H	6.5623040000	0.5998600000	-5.2217040000
N	1.6760610000	-2.3681020000	-3.9889370000	H	6.6131060000	-3.1494600000	-3.5148280000
N	1.6603450000	-0.2339760000	-4.6782840000	C	3.7281980000	-4.4863380000	1.3090410000

C	4.375000000	-5.085855000	0.216841000	H	0.711659000	-2.063492000	-1.036085000
C	4.533687000	-3.850854000	2.265907000	H	-0.095491000	1.217000000	0.324998000
C	5.753175000	-4.957506000	0.094377000	H	-0.423888000	1.824802000	-1.316198000
H	3.821069000	-5.608139000	-0.551336000	H	-2.551450000	1.289534000	0.036845000
C	5.903906000	-3.773801000	2.039941000	H	-2.429270000	0.423501000	-1.503987000
H	4.098252000	-3.391408000	3.144071000	O	0.249563000	-0.096771000	-1.252613000
H	6.263420000	-5.397167000	-0.759849000	O	-1.191908000	-1.759455000	-0.454520000
H	6.538015000	-3.246251000	2.748336000	C	-2.044062000	-0.814983000	0.211006000
N	6.523701000	-4.288929000	0.965565000	H	-3.046066000	-1.243435000	0.193930000
N	6.713499000	-1.276062000	-4.376255000	H	-1.727663000	-0.714017000	1.261546000
N	6.599829000	4.473578000	-0.869310000				
N	6.528923000	1.009605000	4.403813000				
C	2.266104000	-4.497286000	1.404791000	1,3-dioxane-E@1:			
C	2.260665000	1.367215000	4.508209000	C	5.521447000	-3.217689000	1.868891000
C	2.336756000	4.549170000	-1.289102000	C	4.944236000	-2.029251000	2.626622000
C	2.425064000	-1.314806000	-4.306668000	C	4.938061000	-3.282650000	0.463665000
O	3.503768000	-0.686297000	1.894873000	H	5.169133000	-4.110312000	2.386857000
H	3.232231000	0.976340000	1.312642000	C	5.501257000	-0.749784000	2.557162000
H	4.475766000	-0.627221000	2.044121000	C	3.811964000	-2.192100000	3.432827000
O	3.270187000	1.814264000	0.787498000	C	5.501547000	-2.587568000	-0.611188000
H	2.952587000	1.172118000	-0.782101000	C	3.799470000	-4.056338000	0.204682000
H	4.237276000	2.002451000	0.712260000	C	4.996313000	0.346146000	3.263825000
O	6.251270000	-0.342941000	1.809173000	H	6.375031000	-0.601546000	1.933307000
H	6.253870000	0.559347000	1.390065000	C	3.284089000	-1.130043000	4.157296000
H	6.763769000	-0.239110000	2.626767000	O	3.261415000	-3.461635000	3.576703000
O	5.952343000	1.856710000	0.411686000	C	4.994417000	-2.648724000	-1.911977000
H	6.506387000	2.645818000	0.303817000	H	6.380254000	-1.979996000	-0.427848000
H	5.908083000	1.432704000	-0.502553000	C	3.271731000	-4.149547000	-1.078334000
O	3.583367000	-1.831919000	-0.591362000	O	3.242074000	-4.822844000	1.224194000
H	4.568819000	-1.910855000	-0.616710000	C	5.638304000	1.725311000	3.181368000
H	3.427432000	-1.216026000	1.062991000	C	3.866152000	0.128861000	4.062311000
O	2.839516000	0.644976000	-1.617435000	H	2.448154000	-1.287909000	4.822937000
H	1.885255000	0.382546000	-1.614053000	C	2.039588000	-3.698458000	2.973763000
H	3.376932000	-0.997183000	-1.069534000	C	5.621511000	-1.897171000	-3.079705000
O	5.776797000	0.636720000	-1.859567000	C	3.859662000	-3.440131000	-2.119708000
H	4.854840000	0.530885000	-2.143682000	H	2.433767000	-4.803929000	-1.268115000
H	6.124774000	-0.264810000	-1.710726000	C	2.025577000	-4.413966000	1.747686000
O	6.314041000	-1.721296000	-0.507811000	H	5.323275000	2.262425000	4.0766220

C	3.9724970000	3.3440710000	2.1762330000	H	7.5775270000	-1.4319710000	-2.1695990000
C	2.1598630000	1.7271700000	4.4490550000	H	7.5567010000	-1.4157820000	-3.9328170000
C	-0.3298540000	-3.6452660000	2.9611340000	H	7.4189120000	-4.1433560000	1.3736000000
C	5.6034900000	0.5828460000	-2.4569700000	H	7.5268330000	1.1524130000	4.0799750000
C	3.9440260000	-0.2144870000	-3.9831450000	H	7.6624490000	3.8762130000	-1.2184930000
C	2.1563230000	-2.9679080000	-3.6915980000	C	1.1362040000	3.3780840000	-3.6072460000
C	-0.3638820000	-4.3682480000	1.7461570000	H	1.1566950000	2.8660280000	-4.5599290000
C	5.1156690000	3.1464640000	-0.3766580000	C	1.1052660000	4.8428200000	-1.1463630000
H	6.4685550000	1.7742120000	0.5491060000	H	1.1088720000	5.4306400000	-0.2371290000
C	3.4513760000	4.0879840000	1.1239440000	C	0.9863700000	-1.1168410000	-4.7878220000
O	3.4475430000	3.4976370000	3.4558420000	H	1.0086280000	-0.2049490000	-5.3712180000
C	2.2105660000	2.9381270000	3.7087270000	C	0.9647880000	-3.5862190000	-3.3389960000
C	5.1154680000	1.8898070000	-2.5368050000	H	0.9640000000	-4.5448270000	-2.8375000000
H	6.4586850000	0.3900970000	-1.8196800000	C	0.8308240000	-4.7699590000	1.1352300000
C	3.4341000000	1.0748840000	-4.0927430000	H	0.8295840000	-5.3593900000	0.2270050000
O	3.4009830000	-1.2234790000	-4.7736240000	C	0.8620280000	-3.3141440000	3.6007770000
C	2.1684690000	-1.7399420000	-4.4032640000	H	0.8834380000	-2.8056110000	4.5555430000
C	5.7336630000	3.0494140000	-1.7657120000	C	0.9478800000	1.1599410000	4.8258100000
C	4.0110660000	3.9762810000	-0.1441660000	H	0.9243400000	0.2631700000	5.4319930000
H	2.6429490000	4.7835750000	1.2947660000	C	1.0517900000	3.5911300000	3.3146230000
C	-0.2319850000	1.7969770000	4.4151750000	H	1.0962570000	4.5355730000	2.7892440000
C	4.0093450000	2.1097430000	-3.3643290000	N	-1.5617540000	1.4688040000	4.6225110000
H	2.6205800000	1.2731370000	-4.7750570000	N	-1.4567770000	3.3821950000	3.4476050000
C	-0.2124720000	-2.9332030000	-3.6927560000	N	-1.4121560000	4.7079780000	-1.4214500000
H	5.4423260000	3.9579380000	-2.2937850000	N	-1.3680140000	3.5651680000	-3.3581750000
O	3.5192990000	4.7785240000	-1.1717290000	N	-1.5349400000	-1.3208130000	-4.6219840000
C	-0.1571100000	2.9956320000	3.6653430000	N	-1.5302450000	-3.2613560000	-3.4886810000
O	3.5353810000	3.4101750000	-3.5203030000	N	-1.6798760000	-4.5534950000	1.3595970000
C	-0.2242610000	-1.7152330000	-4.4132810000	N	-1.6455500000	-3.4206350000	3.2964500000
C	2.2988770000	4.4321050000	-1.7282060000	H	-1.8603590000	-3.8829220000	-2.7262070000
C	2.3132880000	3.7118850000	-2.9528770000	H	-1.9554930000	-2.6943470000	3.9615020000
C	-0.0930140000	4.4843560000	-1.7804590000	H	-1.7457690000	4.0281990000	2.6892410000
C	-0.0558660000	3.7576670000	-2.9945140000	H	-1.6873620000	2.7875850000	-3.9709870000
C	7.2675440000	2.9987630000	-1.7376290000	O	-2.5886600000	-4.3412200000	-1.2511040000
H	7.6601610000	2.9914730000	-2.7580020000	H	-2.1737560000	-4.6123280000	-0.3971890000
H	7.6587750000	2.1129370000	-1.2296760000	H	-2.9691040000	-3.4550890000	-1.0514400000
C	7.1724800000	1.6725400000	3.1860070000	O	-2.6010840000	-1.1169950000	4.4137600000
H	7.5819980000	2.6863160000	3.1871910000	H	-2.1391280000	-0.3165230000	4.7542540000
H	7.5867980000	1.1524650000	2.3178640000	H	-2.7345510000	-0.8857900000	3.4698260000
C	7.0561980000	-3.2462830000	1.8826010000	O	-2.3878650000	4.4970790000	1.1754460000
H	7.4211660000	-3.2586760000	2.9131630000	H	-2.6217770000	3.5684760000	0.9496430000
H	7.5062610000	-2.3822880000	1.3857970000	H	-1.9294760000	4.8043950000	0.3587310000
C	7.1560660000	-1.9231420000	-3.0510780000	O	-2.3935590000	1.2942710000	-4.3545500000
H	7.5124410000	-2.9567670000	-3.0517410000	H	-1.9867240000	0.4414170000	-4.6435760000

H	-2.7118650000	1.0931850000	-3.4448980000	C	-2.4189990000	-3.9672820000	2.2996070000
C	-3.6054350000	4.0625850000	-2.4285120000	O	-3.3797730000	0.7830730000	-1.8103330000
C	-4.2584600000	3.6292970000	-3.5929210000	H	-3.1223140000	1.5901430000	-0.2766800000
C	-4.4028010000	4.3869760000	-1.3207860000	H	-4.3584350000	0.8716210000	-1.8726220000
C	-5.6402290000	3.4827480000	-3.5749670000	O	-3.1517570000	1.8672460000	0.6751470000
H	-3.7084120000	3.3660590000	-4.4863790000	H	-2.8376940000	0.3168510000	1.3843470000
C	-5.7774340000	4.1974020000	-1.4103980000	H	-4.1161850000	1.9609250000	0.8678530000
H	-3.9580500000	4.7338280000	-0.3965610000	O	-6.1356750000	0.9835160000	-1.5137400000
H	-6.1579520000	3.1260380000	-4.4626300000	H	-6.1308680000	1.3655540000	-0.5955200000
H	-6.4078870000	4.4055710000	-0.5491290000	H	-6.6324960000	1.6251640000	-2.0465090000
C	-3.7222360000	2.5310510000	3.9624700000	O	-5.8304970000	1.6641130000	1.0026930000
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C	-4.5510400000	1.4552820000	4.3113810000	H	-5.7951280000	0.7339460000	1.3918790000
C	-5.7257560000	3.7570130000	3.4444980000	O	-3.5704870000	-1.7849150000	-0.7644410000
H	-3.7614470000	4.5858880000	3.2471930000	H	-4.5561990000	-1.8153080000	-0.7786770000
C	-5.9278370000	1.5996390000	4.1722770000	H	-3.2285340000	-0.1650810000	-1.5835910000
H	-4.1320810000	0.5125140000	4.6403520000	O	-2.7295250000	-0.6361140000	1.6420680000
H	-6.2205030000	4.6644150000	3.1047300000	H	-1.7743210000	-0.8306880000	1.4730210000
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C	-3.8837460000	-3.9304190000	2.3271650000	O	-5.6881750000	-0.7722810000	1.8486720000
C	-4.5853100000	-3.4399520000	3.4389310000	H	-4.7706210000	-1.0637420000	1.9690760000
C	-4.6389020000	-4.4034170000	1.2422610000	H	-6.0614150000	-1.3208230000	1.1297250000
C	-5.9784520000	-3.4406130000	3.4083210000	O	-6.3068250000	-1.5750710000	-0.7201170000
H	-4.0719820000	-3.0393250000	4.3043330000	H	-6.4035220000	-0.6743160000	-1.1130140000
C	-6.0267710000	-4.3545890000	1.3224850000	H	-6.7739700000	-2.1579010000	-1.3367220000
H	-4.1581380000	-4.7897070000	0.3534170000	C	0.3702840000	1.0916920000	-0.0016530000
H	-6.5351460000	-3.0530970000	4.2580390000	C	0.7822470000	-0.0002950000	0.9890550000
H	-6.6266860000	-4.7142610000	0.4889330000	C	-0.2023350000	-1.6157340000	-0.4193190000
C	-3.7471420000	-2.2851930000	-3.9690540000	H	1.7930820000	-0.3728040000	0.7709860000
C	-4.4168010000	-3.4544740000	-3.5764910000	H	0.7606260000	0.3464590000	2.0234910000
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C	-5.7974200000	-3.4216510000	-3.4227110000	H	1.1398300000	1.8704100000	-0.0426310000
H	-3.8792460000	-4.3669930000	-3.3555080000	H	0.8060190000	-1.9367080000	-0.7258900000
C	-5.9046080000	-1.2305210000	-4.0508250000	H	-0.8870200000	-2.4608150000	-0.4139560000
H	-4.0719140000	-0.2296750000	-4.5743440000	O	-0.1330320000	-1.1165050000	0.9141170000
H	-6.3270290000	-4.3168430000	-3.1033840000	C	0.1605070000	0.4774080000	-1.3890920000
H	-6.5228160000	-0.3529980000	-4.2243990000	H	-0.3197600000	1.1716780000	-2.0779610000
N	-6.5486360000	-2.3287510000	-3.6246590000	H	1.1200390000	0.1640610000	-1.8277710000
N	-6.7069610000	-3.8862750000	2.3783750000	O	-0.7126710000	-0.6591890000	-1.3028250000
N	-6.5268260000	2.7188810000	3.7322470000	Cyclopentanone-A@1:			
N	-6.4064800000	3.7320610000	-2.5022100000	C	5.5278660000	-2.9996160000	-2.1182710000
C	-2.2844260000	-2.2552910000	-4.0420940000	C	4.9330590000	-3.2185390000	-0.7337340000
C	-2.1430150000	4.1320430000	-2.3738950000	C	4.9462960000	-1.7442780000	-2.7551160000
C	-2.2624010000	2.4288970000	4.0218710000				

H	5.1903910000	-3.8359690000	-2.7312980000	C	2.1530060000	3.3109310000	-3.3988710000
C	5.4596360000	-2.6111580000	0.4089350000	C	5.6449110000	2.9063920000	2.0844220000
C	3.8186480000	-4.0486490000	-0.5622710000	C	3.9006420000	1.7986170000	3.5596540000
C	5.5017810000	-0.4752020000	-2.5612530000	H	2.5180390000	0.8153580000	4.8689260000
C	3.8171500000	-1.8351770000	-3.5790870000	C	-0.3089600000	-3.2587400000	3.4040560000
C	4.9409700000	-2.8089350000	1.6915290000	C	3.9445160000	3.9813490000	0.5440530000
H	6.3192000000	-1.9607610000	0.2962840000	H	2.5757880000	4.9162230000	-0.8217850000
C	3.2793150000	-4.2780480000	0.6987270000	C	-0.2126700000	2.1446960000	-4.2001330000
O	3.2822320000	-4.7049440000	-1.6660880000	H	5.3395940000	3.7563060000	2.6956660000
C	4.9948210000	0.6808270000	-3.1622130000	O	3.4002780000	3.0638470000	3.8563350000
H	6.3740630000	-0.3859700000	-1.9240980000	C	-0.2467450000	-2.0881700000	4.1969560000
C	3.2921600000	-0.7097310000	-4.2035750000	O	3.4456350000	4.6562010000	1.6547970000
O	3.2697360000	-3.0837740000	-3.8547140000	C	-0.2416170000	3.3085560000	-3.3945800000
C	5.5595080000	-2.1504420000	2.9176500000	C	2.1872380000	3.4236570000	3.2919660000
C	3.8238930000	-3.6467430000	1.8109680000	C	2.2154820000	4.2531850000	2.1395240000
H	2.4498920000	-4.9590980000	0.8199180000	C	-0.2044120000	3.4776480000	3.2793720000
C	2.0614190000	-4.2423640000	-2.1297510000	C	-0.1552800000	4.2908410000	2.1214300000
C	5.6115050000	2.0598180000	-2.9602710000	C	7.1793310000	2.8649930000	2.0769020000
C	3.8698720000	0.5349950000	-3.9810350000	H	7.5767330000	3.7955310000	1.6627390000
H	2.4638870000	-0.8127580000	-4.8885890000	H	7.5838020000	2.0419780000	1.4812510000
C	2.0518120000	-3.3960810000	-3.2696650000	C	7.0945110000	-2.1680230000	2.8933420000
H	5.2355170000	-2.7398400000	3.7759830000	H	7.4884020000	-1.7417480000	3.8199420000
C	4.9864160000	-0.7537350000	3.1200560000	H	7.5173330000	-1.5956460000	2.0630190000
O	3.2919490000	-3.9190420000	3.0683250000	C	7.0630780000	-3.0132940000	-2.1151870000
C	5.0240820000	2.7306310000	-1.7248940000	H	7.4280840000	-3.9590070000	-1.7056640000
H	5.2964780000	2.6622920000	-3.8129520000	H	7.4982150000	-2.2075890000	-1.5173950000
O	3.3728980000	1.6535580000	-4.6440210000	C	7.1463220000	2.0307890000	-2.9524820000
C	5.5278790000	0.3867000000	2.5203540000	H	7.5167570000	1.5998020000	-3.8864830000
C	3.8719570000	-0.5749410000	3.9469540000	H	7.5602660000	1.4386220000	-2.1316300000
C	2.0828150000	-3.3186070000	3.3889640000	H	7.5406490000	3.0459860000	-2.8565420000
C	-0.3091100000	-4.1886680000	-2.0792400000	H	7.4410540000	-2.9063940000	-3.1355340000
C	5.5589350000	2.5290840000	-0.4487010000	H	7.4561340000	-3.1956190000	2.8011240000
C	3.9152340000	3.5810760000	-1.8285550000	H	7.5563390000	2.7484510000	3.0964920000
C	2.1567030000	2.1484530000	-4.2141100000	C	1.0447730000	4.7085840000	1.5494470000
C	-0.3374660000	-3.3537560000	-3.2204970000	H	1.0763060000	5.3733020000	0.6964340000
C	5.0195790000	1.6739210000	2.7258000000	C	0.9863770000	3.0493520000	3.8823820000
H	6.3924810000	0.2706810000	1.8771560000	H	0.9779520000	2.4582810000	4.7894130000
C	3.3381550000	0.6877240000	4.1780210000	C	0.9629410000	3.9108750000	-3.0016150000
O	3.3508210000	-1.6788550000	4.6136420000	H	0.9738860000	4.8254900000	-2.4222090000
C	2.1205760000	-2.1478700000	4.1923640000	C	0.9735410000	1.5585750000	-4.6343580000
C	5.0505550000	3.1386750000	0.7015990000	H	0.9834550000	0.7026650000	-5.2957320000
H	6.4133870000	1.8701810000	-0.3475050000	C	0.8593050000	-2.9604950000	-3.8324410000
C	3.3908670000	4.2165580000	-0.7086620000	H	0.8592470000	-2.3570920000	-4.7311790000
O	3.3786120000	3.8744480000	-3.0798620000	C	0.8810650000	-4.6563260000	-1.5272630000

H	0.8983880000	-5.3268530000	-0.6787440000	H	-4.2117270000	-4.0650220000	2.3584870000
C	0.8764870000	-3.8895360000	3.0023660000	H	-6.3165100000	-0.8790330000	5.4187020000
H	0.8598520000	-4.8031460000	2.4222780000	H	-6.6600420000	-3.7240480000	2.4500060000
C	0.9556520000	-1.5233730000	4.6132700000	C	-3.8611210000	-3.7302190000	-2.6242900000
H	0.9911810000	-0.6607280000	5.2649160000	C	-4.5694350000	-4.5859130000	-1.7672080000
N	-1.6355210000	-3.5876320000	3.1788960000	C	-4.6099750000	-2.9087440000	-3.4816700000
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N	-1.5257860000	3.2432320000	3.6206320000	H	-4.0617380000	-5.2387080000	-1.0680330000
N	-1.4651810000	4.5448820000	1.7874730000	C	-5.9983450000	-2.9821780000	-3.4333800000
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N	-1.5260150000	1.8202370000	-4.4391950000	H	-6.5240480000	-5.2202760000	-1.1354650000
N	-1.6506450000	-3.0732990000	-3.5523750000	H	-6.5930680000	-2.3525460000	-4.0923670000
N	-1.6272530000	-4.4047540000	-1.7454520000	C	-3.7590960000	2.6620490000	-3.8019030000
H	-1.8503370000	0.8660100000	-4.6975280000	C	-4.4065910000	1.8132780000	-4.7130860000
H	-1.9493320000	-4.7201130000	-0.8159310000	C	-4.5630100000	3.3921170000	-2.9143630000
H	-1.8458620000	-0.7848160000	4.7331050000	C	-5.7899860000	1.6915290000	-4.6548740000
H	-1.7821940000	4.7995250000	0.8319760000	H	-3.8519220000	1.2253690000	-5.4319620000
O	-2.5797570000	-0.6462910000	-4.4976100000	C	-5.9384750000	3.1828710000	-2.9341010000
H	-2.1346240000	-1.5205220000	-4.3767330000	H	-4.1239940000	4.0775130000	-2.2004970000
H	-2.8918210000	-0.4388680000	-3.5881600000	H	-6.3034860000	1.0270370000	-5.3466410000
O	-2.6922540000	-4.5542320000	0.7827340000	H	-6.5739610000	3.7102620000	-2.2266640000
H	-2.2020720000	-4.4677590000	1.6353640000	N	-6.5630140000	2.3370490000	-3.7687390000
H	-2.9304500000	-3.6239100000	0.6020580000	N	-6.6850860000	-3.7925530000	-2.6161800000
O	-2.5142840000	0.7980480000	4.5524940000	N	-6.6143360000	-2.2815730000	3.9297380000
H	-2.7733110000	0.6091300000	3.6221580000	N	-6.5131390000	3.8524740000	2.2906660000
H	-2.0499370000	1.6630630000	4.4716120000	C	-2.2957030000	2.7425070000	-3.7726750000
O	-2.5301470000	4.5718160000	-0.6983130000	C	-2.2485210000	3.8811860000	2.7027900000
H	-2.0803260000	4.4611190000	-1.5697760000	C	-2.3467490000	-2.6539480000	3.8081390000
H	-2.8349200000	3.6606120000	-0.4878460000	C	-2.3951380000	-3.7071980000	-2.6489430000
C	-3.7110210000	3.9115520000	2.6181820000	C	-0.0985890000	0.4166970000	-0.2907420000
C	-4.3624440000	4.7988370000	1.7474790000	C	1.9470030000	-0.8858010000	0.2133350000
C	-4.5107640000	3.0390420000	3.3716280000	C	2.3252890000	0.5049010000	-0.3197690000
C	-5.7448520000	4.7265290000	1.6229830000	C	1.0800220000	1.3656960000	-0.0184550000
H	-3.8111130000	5.5039040000	1.1399940000	H	-0.3594190000	0.4065540000	-1.3593620000
C	-5.8856290000	3.0467830000	3.1633700000	H	-1.0154500000	0.6377020000	0.2611720000
H	-4.0677020000	2.3398630000	4.0695470000	H	2.1514720000	-0.9660200000	1.2904460000
H	-6.2612070000	5.3918240000	0.9344990000	H	2.4452230000	-1.7303320000	-0.2649820000
H	-6.5174320000	2.3488120000	3.7076280000	H	3.2337220000	0.9019130000	0.1350140000
C	-3.8076900000	-2.5677990000	3.8745790000	H	2.4931380000	0.4546860000	-1.4009720000
C	-4.4321440000	-1.6747480000	4.7604530000	H	1.0805740000	1.6624880000	1.0360190000
C	-4.6328560000	-3.3519740000	3.0557270000	H	1.0397690000	2.2762420000	-0.6174690000
C	-5.8181570000	-1.5766650000	4.7489490000	O	-3.4981480000	2.0207970000	-0.0530860000
H	-3.8604750000	-1.0374850000	5.4222490000	H	-3.3134360000	0.9349780000	1.3457250000
C	-6.0099810000	-3.1631830000	3.1158410000	H	-4.4753280000	2.1242440000	0.0223690000

O	-3.3556170000	0.1729390000	1.9747060000	H	-2.4801730000	2.2932680000	-4.4084460000
H	-3.0277670000	-1.1433710000	0.8812530000	C	-2.0273410000	-0.7533390000	-4.5889620000
H	-4.3227570000	0.0335700000	2.1205710000	C	-5.5732740000	-3.5307360000	1.0769100000
O	-6.2468970000	1.8040880000	0.2024360000	C	-3.8253040000	-4.0308100000	-0.6858630000
H	-6.2872150000	1.1153080000	0.9192490000	H	-2.4197250000	-4.4678330000	-2.2513630000
H	-6.7522130000	2.5562310000	0.5503930000	C	-2.0087390000	-2.1115470000	-4.1783830000
O	-6.0311700000	-0.2311050000	1.8458920000	H	-5.3562590000	4.4137570000	-1.4600880000
H	-6.5898110000	-0.5905770000	2.5529020000	C	-5.0748140000	3.1965230000	0.2381230000
H	-5.9584330000	-0.9686550000	1.1593610000	O	-3.4074430000	4.1326870000	-2.7886110000
O	-3.4706490000	0.0134110000	-1.9207420000	C	-5.0005910000	-2.5410220000	2.0817140000
H	-4.4540080000	-0.0060950000	-2.0101840000	H	-5.2453490000	-4.5195800000	1.3988990000
H	-3.3826680000	1.3977490000	-0.8129410000	O	-3.3212900000	-5.0055900000	0.1705300000
O	-2.8981110000	-1.7618800000	0.1163470000	C	-5.5805470000	2.2500460000	1.1334240000
H	-1.9121410000	-1.8822400000	0.0634730000	C	-3.9777100000	3.9551290000	0.6608860000
H	-3.2518000000	-0.7026050000	-1.2778870000	C	-2.1996940000	4.2991410000	-2.1284630000
O	-5.7676840000	-2.0040870000	-0.0134780000	C	0.3435930000	-0.7136720000	-4.5231770000
H	-4.8265500000	-2.1990120000	-0.1590290000	C	-5.5495070000	-1.2675730000	2.2656930000
H	-6.0827410000	-1.5631880000	-0.8271210000	C	-3.8808900000	-2.8790770000	2.8532520000
O	-6.2150990000	0.0384160000	-1.8319380000	C	-2.1069400000	-4.7393300000	0.7781470000
H	-6.3801670000	0.7610530000	-1.1805300000	C	0.3813550000	-2.0710170000	-4.1236030000
H	-6.6733450000	0.3273350000	-2.6345770000	C	-5.0569780000	2.0489760000	2.4149900000
C	0.4427930000	-0.9659010000	0.0476120000	H	-6.4278680000	1.6491910000	0.8240170000
O	-0.2265520000	-1.9854850000	0.1711210000	C	-3.4339070000	3.7928170000	1.9302390000
Cyclopentanone-B@1:				O	-3.4729590000	4.9365460000	-0.1874530000
C	-5.4974330000	-1.1537290000	-3.4572160000	C	-2.2398060000	4.7008870000	-0.7670490000
C	-4.9353180000	0.2441830000	-3.2320940000	C	-5.0433820000	-0.3413840000	3.1815570000
C	-4.9030520000	-2.1480520000	-2.4675950000	H	-6.4134480000	-0.9888520000	1.6736780000
H	-5.1499180000	-1.4645110000	-4.4431430000	C	-3.3597460000	-1.9897910000	3.7856230000
C	-5.5041920000	1.1518600000	-2.3347970000	O	-3.3366570000	-4.1568100000	2.7568140000
C	-3.8118800000	0.6728680000	-3.9495260000	C	-2.1093910000	-4.2931690000	2.1260800000
C	-5.4564890000	-2.3634920000	-1.2017400000	C	-5.6564030000	1.0384230000	3.3862310000
C	-3.7764640000	-2.9058860000	-2.8130400000	C	-3.9593670000	2.8350690000	2.7908470000
C	-5.0174490000	2.4488580000	-2.1434800000	H	-2.6271430000	4.4283830000	2.2645600000
H	-6.3703390000	0.8380460000	-1.7639310000	C	0.1936710000	4.3393300000	-2.0802350000
C	-3.3076480000	1.9596450000	-3.7994620000	C	-3.9285190000	-0.7300490000	3.9319730000
O	-3.2486140000	-0.1788060000	-4.8931100000	H	-2.5372730000	-2.2937400000	4.4160090000
C	-4.9511680000	-3.2984300000	-0.2936560000	C	0.2645940000	-4.7101580000	0.7833190000
H	-6.3271020000	-1.7850160000	-0.9149940000	H	-5.3529720000	1.3606350000	4.3829700000
C	-3.2513870000	-3.8530150000	-1.9400060000	O	-3.4411360000	2.7308540000	4.0791780000
O	-3.2224500000	-2.7765310000	-4.0823230000	C	0.1302740000	4.7225400000	-0.7187680000
C	-5.6581800000	3.4120440000	-1.1528660000	O	-3.4349470000	0.1399570000	4.8987260000
C	-3.8973780000	2.8325820000	-2.8919000000	C	0.2857690000	-4.2762270000	2.1315190000
				C	-2.2154090000	2.1003880000	4.2288520000
				C	-2.2177860000	0.7427410000	4.6457570000

C	0.1768110000	2.1100670000	4.2606390000	H	1.7385710000	4.8092880000	0.6843770000
C	0.1523970000	0.7504630000	4.6543980000	H	1.8028650000	-0.6077700000	4.7409570000
C	-7.1912430000	1.0182050000	3.3516240000	O	2.6743470000	-4.0681880000	-1.9265910000
H	-7.5734340000	0.3291980000	4.1096230000	H	2.2012730000	-3.6705570000	-2.6968710000
H	-7.5946690000	0.7001920000	2.3862350000	H	3.0328270000	-3.2834530000	-1.4553910000
C	-7.1922150000	3.3605100000	-1.1719200000	O	2.5948180000	2.1608620000	-4.0283540000
H	-7.6003710000	4.1097650000	-0.4882530000	H	2.1094510000	2.9634100000	-3.7271980000
H	-7.5927360000	2.3887420000	-0.8701990000	H	2.8219350000	1.7190440000	-3.1815840000
C	-7.0326290000	-1.1803890000	-3.4755160000	O	2.4414140000	4.1297960000	2.0899870000
H	-7.4099890000	-0.4984240000	-4.2422340000	H	2.7007420000	3.2986430000	1.6313750000
H	-7.4783010000	-0.8818640000	-2.5225720000	H	1.9935450000	3.7939670000	2.9018570000
C	-7.1079000000	-3.5356220000	1.0435010000	O	2.5637150000	-2.0004550000	4.1029360000
H	-7.4643830000	-4.3037750000	0.3520030000	H	2.1169630000	-2.8050410000	3.7476130000
H	-7.5334410000	-2.5813910000	0.7207930000	H	2.8868970000	-1.5417960000	3.2940540000
H	-7.5042410000	-3.7522710000	2.0391640000	C	3.6960980000	1.4081840000	4.4824610000
H	-7.3870410000	-2.1895920000	-3.7016890000	C	4.3591530000	0.3236140000	5.0773890000
H	-7.5620540000	3.5697800000	-2.1792620000	C	4.4853710000	2.4066950000	3.8924290000
H	-7.5843930000	2.0171230000	3.5586140000	C	5.7455310000	0.2606660000	5.0048050000
C	-1.0342290000	0.0538750000	4.8707910000	H	3.8146940000	-0.4811400000	5.5532980000
H	-1.0449670000	-0.9665380000	5.2294620000	C	5.8656640000	2.2388710000	3.8700290000
C	-1.0270030000	2.7987520000	4.0546190000	H	4.0315500000	3.2705910000	3.4231240000
H	-1.0382050000	3.8475190000	3.7855610000	H	6.2723000000	-0.5839650000	5.4433560000
C	-0.9218590000	-4.0797500000	2.8175320000	H	6.4917150000	2.9826590000	3.3828110000
H	-0.9368580000	-3.7867560000	3.8597500000	C	3.6920780000	4.5687380000	-1.2719900000
C	-0.9198990000	-4.9676730000	0.0965640000	C	4.3105730000	5.1677320000	-0.1629190000
H	-0.9267310000	-5.3470870000	-0.9166280000	C	4.5215940000	3.9950170000	-2.2461600000
C	-0.8124960000	-2.7830590000	-3.9576850000	C	5.6952920000	5.1187070000	-0.0584520000
H	-0.8092790000	-3.8326940000	-3.6926830000	H	3.7339700000	5.6321680000	0.6257950000
C	-0.8498470000	-0.0388250000	-4.7724580000	C	5.8968650000	3.9898860000	-2.0352850000
H	-0.8710640000	0.9812930000	-5.1326850000	H	4.1052660000	3.5229140000	-3.1268700000
C	-0.9929510000	4.1398640000	-2.8001770000	H	6.1890520000	5.5641170000	0.8025380000
H	-0.9789660000	3.8833070000	-3.8520710000	H	6.5497940000	3.4983000000	-2.7510060000
C	-1.0739460000	4.9264670000	-0.0490930000	C	3.8984110000	-1.3618520000	-4.3073540000
H	-1.1103520000	5.2739310000	0.9746550000	C	4.5918130000	-0.2567560000	-4.8239140000
N	1.5207200000	4.2291690000	-2.4645010000	C	4.6597830000	-2.4360940000	-3.8216790000
N	1.4341750000	4.8578910000	-0.3070200000	C	5.9847580000	-0.2784490000	-4.8244460000
N	1.4914690000	2.5312760000	4.1519860000	H	4.0726590000	0.6170850000	-5.1984930000
N	1.4679160000	0.3750700000	4.7889780000	C	6.0474900000	-2.3468040000	-3.8715550000
N	1.6011190000	-4.1219530000	2.5427110000	H	4.1832150000	-3.3113130000	-3.3999770000
N	1.5808630000	-4.8256070000	0.4046200000	H	6.5362460000	0.5749470000	-5.2112770000
N	1.6964900000	-2.4725340000	-3.9848980000	H	6.6531330000	-3.1679980000	-3.4937210000
N	1.6578830000	-0.3238870000	-4.6329660000	C	3.8057520000	-4.4302620000	1.3991190000
H	1.9131720000	-4.7436510000	-0.5806040000	C	4.4607970000	-5.0429040000	0.3198350000
H	1.9682610000	0.6617040000	-4.6584780000	C	4.6012430000	-3.7725430000	2.3485630000

C	5.8375300000	-4.9006770000	0.1974150000	O	5.8972170000	0.6578430000	-1.8675500000
H	3.9132440000	-5.5811510000	-0.4417630000	H	4.9632840000	0.5199340000	-2.1047120000
C	5.9710000000	-3.6828430000	2.1236870000	H	6.2789480000	-0.2281790000	-1.7160570000
H	4.1587010000	-3.3013180000	3.2167080000	O	6.5151090000	-1.6727370000	-0.4535270000
H	6.3542750000	-5.3467140000	-0.6493710000	H	6.6051210000	-1.2286440000	0.4223990000
H	6.5973670000	-3.1344490000	2.8229580000	H	6.9455760000	-2.5336050000	-0.3268200000
N	6.5976750000	-4.2075420000	1.0581840000	C	-0.1762040000	-0.4694020000	-0.7368610000
N	6.7202410000	-1.2966200000	-4.3622490000	O	0.9042470000	-0.8662240000	-1.1588150000
N	6.4946990000	4.5216520000	-0.9560000000				
N	6.5067000000	1.1807440000	4.3931260000				
C	2.3421400000	-4.4478490000	1.4851670000				
C	2.2324760000	1.4693040000	4.4615920000				
C	2.2306880000	4.5360970000	-1.3801520000				
C	2.4332390000	-1.4060390000	-4.2869170000				
C	-1.1764240000	-1.3178150000	0.0196460000				
C	-0.7186910000	0.9426000000	-0.8797050000				
C	-2.1760840000	0.8473120000	-0.3997630000				
C	-2.1627940000	-0.3064920000	0.6245890000				
H	-1.6770780000	-1.9517120000	-0.7250610000				
H	-0.6805090000	-1.9865650000	0.7257770000				
H	-0.1214840000	1.5902480000	-0.2214180000				
H	-0.5850950000	1.3162230000	-1.8982310000				
H	-2.5452070000	1.7805550000	0.0235180000				
H	-2.8239790000	0.5854520000	-1.2411810000				
H	-1.7890940000	0.0497240000	1.5915280000				
H	-3.1537960000	-0.7292120000	0.7933420000				
O	3.5829920000	-0.6398010000	1.8848970000				
H	3.2689220000	1.0048810000	1.2641960000				
H	4.5515460000	-0.5588160000	2.0431420000				
O	3.2965170000	1.8412260000	0.7355830000				
H	3.0608030000	1.1861550000	-0.8566280000				
H	4.2614350000	2.0427850000	0.6675770000				
O	6.3304270000	-0.2360550000	1.8322210000				
H	6.3120070000	0.6553090000	1.3906920000				
H	6.8205820000	-0.0918330000	2.6574940000				
O	5.9881190000	1.9238770000	0.3813850000				
H	6.5133670000	2.7302240000	0.2561800000				
H	5.9806510000	1.4709640000	-0.5218040000				
O	3.7890280000	-1.8607150000	-0.5574780000				
H	4.7759900000	-1.9118610000	-0.5774840000				
H	3.5292070000	-1.1919740000	1.0653100000				
O	3.0278720000	0.6634100000	-1.7000470000				
H	2.1567630000	0.1933260000	-1.6691380000				
H	3.5653030000	-1.0533340000	-1.0614550000				

C	-0.2532370000	-1.7494150000	4.2869590000	H	7.5099330000	-2.8841900000	3.0993700000
C	5.5509330000	-0.6450630000	-2.5584970000	H	7.5414140000	3.0826940000	2.8626960000
C	3.8960440000	-2.1198480000	-3.4558290000	H	7.5099490000	2.8834900000	-3.0998660000
C	2.1552590000	-4.3480830000	-1.8028030000	C	0.9330660000	1.1374660000	-4.6927590000
C	-0.2700370000	-2.9796340000	3.5864300000	H	0.9404950000	0.2278110000	-5.2786250000
C	5.0055470000	2.5886470000	-1.9343130000	C	0.9344740000	3.6185340000	-3.2643310000
H	6.4079340000	1.8589070000	-0.4928600000	H	0.9449580000	4.5800780000	-2.7671320000
C	3.3398900000	4.1135510000	-1.0358900000	C	0.9446700000	-3.3458860000	-3.6825140000
O	3.3801420000	4.7274220000	1.2860860000	H	0.9488240000	-2.8712580000	-4.6558740000
C	2.1560720000	4.3483300000	1.8026720000	C	0.9774490000	-4.7045240000	-1.1614030000
C	5.0151950000	0.4503470000	-3.2407350000	H	0.9941840000	-5.2681880000	-0.2383580000
H	6.4181230000	-0.4844250000	-1.9288640000	C	0.9343210000	-3.6183830000	3.2644060000
C	3.3431100000	-1.0557570000	-4.1593330000	H	0.9446410000	-4.5798790000	2.7671120000
O	3.3641420000	-3.3930420000	-3.6396950000	C	0.9333490000	-1.1375330000	4.6932160000
C	2.1401160000	-3.6636950000	-3.0461420000	H	0.9409560000	-0.2279370000	5.2791720000
C	5.6031820000	1.8513870000	-3.1277490000	C	0.9453940000	3.3458300000	3.6821510000
C	3.8832010000	3.4094710000	-2.1040570000	H	0.9494920000	2.8709550000	4.6553890000
H	2.5165250000	4.7916660000	-1.2026490000	C	0.9782930000	4.7051760000	1.1614360000
C	-0.2543190000	3.6827470000	3.0369810000	H	0.9951090000	5.2690620000	0.2385260000
C	3.8844130000	0.2177340000	-4.0328110000	N	-1.5765610000	3.4905360000	3.4093350000
H	2.5096310000	-1.2283120000	-4.8243550000	N	-1.5233670000	4.5627390000	1.4333680000
C	-0.2149590000	-4.3481960000	-1.7875830000	N	-1.5793990000	3.3572650000	-3.3519890000
H	5.2728950000	2.3930700000	-4.0148750000	N	-1.5755880000	1.4109600000	-4.4699760000
O	3.3465490000	3.5931690000	-3.3752600000	N	-1.5773200000	-3.4902690000	-3.4096180000
C	-0.2141560000	4.3488760000	1.7875500000	N	-1.5241720000	-4.5618080000	-1.4332990000
O	3.3386890000	1.2664410000	-4.7661900000	N	-1.5795130000	-3.3568470000	3.3523580000
C	-0.2550790000	-3.6824750000	-3.0372310000	N	-1.5753700000	-1.4107430000	4.4707140000
C	2.1212570000	2.9975640000	-3.6326620000	H	-1.8532000000	-4.7236640000	-0.4560870000
C	2.1210650000	1.7719590000	-4.3477560000	H	-1.9053460000	-0.4575110000	4.7044050000
C	-0.2699920000	2.9798690000	-3.5861280000	H	-1.8524410000	4.7247460000	0.4561990000
C	-0.2534040000	1.7495280000	-4.2864390000	H	-1.9056810000	0.4578160000	-4.7038410000
C	7.1382510000	1.8556270000	-3.1229860000	O	-2.5924590000	-4.4777860000	1.0226980000
H	7.5173200000	1.3682200000	-4.0252120000	H	-2.1071310000	-4.2670670000	1.8563100000
H	7.5658530000	1.3326870000	-2.2629940000	H	-3.0196610000	-3.6218220000	0.7944390000
C	7.1549260000	3.0834720000	1.8400250000	O	-2.5808280000	1.1056170000	4.4050900000
H	7.5328740000	3.9709240000	1.3254750000	H	-2.1325080000	1.9802190000	4.3145520000
H	7.5693350000	2.2085880000	1.3313880000	H	-2.8239970000	0.8945460000	3.4773470000
C	7.1383420000	-1.8562890000	3.1225110000	O	-2.5918500000	4.4788740000	-1.0225550000
H	7.5175380000	-1.3689100000	4.0246970000	H	-3.0187080000	3.6227690000	-0.7942010000
H	7.5659230000	-1.3334010000	2.2624750000	H	-2.1066460000	4.2682230000	-1.8562610000
C	7.1543710000	-3.0841970000	-1.8405440000	O	-2.5816160000	-1.1052860000	-4.4052820000
H	7.5322490000	-3.9716800000	-1.3259950000	H	-2.1332760000	-1.9798920000	-4.3149370000
H	7.5689570000	-2.2093490000	-1.3319920000	H	-2.8251000000	-0.8946120000	-3.4775400000
H	7.5407490000	-3.0835200000	-2.8632560000	C	-3.8016210000	2.3876830000	-3.9024160000

C	-4.5271870000	1.3766160000	-4.5522480000	C	1.0577580000	0.3994830000	1.1701050000
C	-4.5334750000	3.4081050000	-3.2771640000	C	2.4663220000	-0.0600060000	0.7676890000
C	-5.9195400000	1.4298270000	-4.5312740000	C	2.4659340000	0.0606370000	-0.7678820000
H	-4.0348420000	0.5494610000	-5.0487550000	H	1.0110220000	-1.4991700000	-1.2338020000
C	-5.9236640000	3.3572510000	-3.3175680000	H	0.6769150000	-0.0102180000	-2.1163370000
H	-4.0347200000	4.2101140000	-2.7504780000	H	1.0083880000	1.4967630000	1.2348940000
H	-6.4957580000	0.6474710000	-5.0187050000	H	0.6776240000	0.0066540000	2.1166440000
H	-6.5046290000	4.1364330000	-2.8287560000	H	3.2525720000	0.5296760000	1.2326760000
C	-3.7661790000	4.0631610000	2.3258320000	H	2.6139790000	-1.1042380000	1.0601440000
C	-4.3846970000	4.9267200000	1.4081290000	H	2.6114140000	1.1051490000	-1.0604550000
C	-4.5952540000	3.2283830000	3.0880200000	H	3.2531750000	-0.5275330000	-1.2331040000
C	-5.7632030000	4.8616120000	1.2462630000	O	-3.1269670000	-0.3673950000	-1.7463850000
H	-3.8091950000	5.6093250000	0.7974100000	H	-3.5987100000	1.2967600000	-0.9561820000
C	-5.9648620000	3.2350940000	2.8376190000	H	-2.2220700000	-0.2130430000	-1.4012610000
H	-4.1801030000	2.5546330000	3.8264170000	O	-3.7635770000	2.0159280000	-0.3107220000
H	-6.2536630000	5.5074190000	0.5213590000	H	-3.4423920000	1.0723620000	1.1228090000
H	-6.6144040000	2.5468300000	3.3705160000	H	-4.7509730000	2.1236490000	-0.2939080000
C	-3.8015640000	-2.3870480000	3.9030330000	O	-6.2111530000	-0.1830990000	-1.8933530000
C	-4.5269990000	-1.3758260000	4.5527730000	H	-6.4877490000	0.6840750000	-1.5298470000
C	-4.5335530000	-3.4074210000	3.2778600000	H	-5.3033700000	-0.0546720000	-2.2044670000
C	-5.9193610000	-1.4288590000	4.5318010000	O	-6.4240310000	1.8803470000	-0.1256500000
H	-4.0345490000	-0.5486690000	5.0491690000	H	-6.9095720000	2.6522310000	0.2064110000
C	-5.9237380000	-3.3563760000	3.3182340000	H	-6.3828440000	1.2579150000	0.6545200000
H	-4.0348930000	-4.2095250000	2.7512260000	O	-3.7657170000	-2.0156030000	0.3111750000
H	-6.4954820000	-0.6463980000	5.0191840000	H	-4.7530580000	-2.1237090000	0.2940820000
H	-6.5048090000	-4.1355050000	2.8294670000	H	-3.4436250000	-1.0727290000	-1.1222690000
C	-3.7669630000	-4.0626000000	-2.3259390000	O	-3.1264890000	0.3664690000	1.7466350000
C	-4.3854020000	-4.9260370000	-1.4080630000	H	-2.2220190000	0.2106340000	1.4009820000
C	-4.5961230000	-3.2281130000	-3.0883510000	H	-3.6013090000	-1.2960480000	0.9563500000
C	-5.7639280000	-4.8611360000	-1.2463220000	O	-6.2112260000	0.1831400000	1.8933470000
H	-3.8098250000	-5.6084110000	-0.7971550000	H	-5.3037470000	0.0540440000	2.2050570000
C	-5.9657450000	-3.2349670000	-2.8380120000	H	-6.4885130000	-0.6838910000	1.5300570000
H	-4.1810370000	-2.5544420000	-3.8268540000	O	-6.4261350000	-1.8801920000	0.1255560000
H	-6.2543370000	-5.5068790000	-0.5213270000	H	-6.3842740000	-1.2578070000	-0.6546210000
H	-6.6153560000	-2.5469050000	-3.3710860000	H	-6.9116550000	-2.6519550000	-0.2068160000
N	-6.5571430000	-4.0145090000	-1.9185240000	C	0.1893170000	-0.0017160000	0.0002550000
N	-6.6258220000	-2.3935100000	3.9293870000	O	-1.0407910000	-0.0024570000	0.0003200000
N	-6.5563250000	4.0147170000	1.9182350000				
N	-6.6258760000	2.3945270000	-3.9287960000				
C	-2.3036000000	-4.0194510000	-2.4255270000				
C	-2.3342630000	2.3978520000	-3.8849420000				
C	-2.3028180000	4.0200950000	2.4254350000				
C	-2.3342070000	-2.3974310000	3.8855390000				
C	1.0581390000	-0.4017540000	-1.1697030000				
				Cyclopentanone-D@1:			
				C	5.6164690000	-0.0355960000	-3.5591740000
				C	5.0295090000	-1.2817500000	-2.9075230000
				C	5.0127680000	1.2269170000	-2.9576640000
				H	5.2953070000	-0.0583750000	-4.6011320000

C	5.5623230000	-1.8575700000	-1.7520200000	C	5.5969210000	0.0764660000	3.6318780000
C	3.9152400000	-1.9077810000	-3.4771100000	C	3.8865060000	-1.8018390000	3.5949940000
C	5.5440350000	1.8306870000	-1.8134750000	H	2.5367170000	-3.4648170000	3.5686900000
C	3.8990200000	1.8386900000	-3.5482370000	C	-0.1904550000	-4.7371730000	-0.6128960000
C	5.0491960000	-3.0208450000	-1.1689040000	C	3.8838520000	1.9403270000	3.5430210000
H	6.4214560000	-1.3861490000	-1.2891370000	H	2.5162550000	3.5949420000	3.4777440000
C	3.3841220000	-3.0731260000	-2.9370110000	C	-0.1834100000	4.6812850000	-0.7709370000
O	3.3906950000	-1.3916330000	-4.6567800000	H	5.2678270000	0.0926060000	4.6715230000
C	5.0294930000	3.0048410000	-1.2580210000	O	3.3413730000	-1.2861960000	4.7684790000
H	6.4041780000	1.3708130000	-1.3410140000	C	-0.1531960000	-4.6750880000	0.8011310000
C	3.3611530000	3.0096290000	-3.0252070000	O	3.3567190000	1.4295790000	4.7255240000
O	3.3718200000	1.3263370000	-4.7309090000	C	-0.2284920000	4.7355940000	0.6431640000
C	5.6577160000	-3.6232000000	0.0900030000	C	2.1227460000	-0.6337530000	4.6759460000
C	3.9383160000	-3.6152620000	-1.7822020000	C	2.1369740000	0.7861960000	4.6465230000
H	2.5634100000	-3.5765420000	-3.4261940000	C	-0.2693630000	-0.6158140000	4.6536710000
C	2.1691530000	-0.7489840000	-4.5847450000	C	-0.2318820000	0.7988160000	4.6123630000
C	5.6268610000	3.6608100000	-0.0204800000	C	7.1322630000	0.0802990000	3.6304170000
C	3.9151830000	3.5746360000	-1.8826240000	H	7.5048560000	0.9748880000	4.1367080000
H	2.5407920000	3.4948660000	-3.5331060000	H	7.5601710000	0.0710170000	2.6241490000
C	2.1530770000	0.6699900000	-4.6465980000	C	7.1923680000	-3.5937730000	0.0898810000
H	5.3460640000	-4.6678820000	0.1120830000	H	7.5761750000	-4.0890810000	0.9859230000
C	5.0502290000	-2.9682060000	1.3233960000	H	7.6024610000	-2.5801570000	0.0745890000
O	3.4256490000	-4.8113560000	-1.2836290000	C	7.1518090000	-0.0263330000	-3.5460430000
C	5.0174470000	3.0527290000	1.2349300000	H	7.5356030000	-0.9199350000	-4.0456390000
H	5.3092250000	4.7037030000	-0.0419660000	H	7.5720790000	-0.0091650000	-2.5366380000
O	3.4091930000	4.7749440000	-1.3882720000	C	7.1617350000	3.6410950000	-0.0144950000
C	5.5562920000	-1.7929240000	1.8846410000	H	7.5458030000	4.1403980000	-0.9081750000
C	3.9309350000	-3.5419660000	1.9355500000	H	7.5780540000	2.6300740000	0.0005000000
C	2.2029360000	-4.7511400000	-0.6281650000	H	7.5401660000	4.1651530000	0.8673250000
C	-0.1985450000	-0.7625750000	-4.5528790000	H	7.5262930000	0.8556090000	-4.0727050000
C	5.5376440000	1.8962480000	1.8245710000	H	7.5775600000	-4.1169840000	-0.7895030000
C	3.8976020000	3.6376920000	1.8396140000	H	7.5101800000	-0.8007970000	4.1560060000
C	2.1859200000	4.7247900000	-0.7480070000	C	0.9598630000	1.5198780000	4.6217030000
C	-0.2390980000	0.6500820000	-4.6367650000	H	0.9787720000	2.6011720000	4.6462290000
C	5.0076760000	-1.1886270000	3.0205930000	C	0.9284220000	-1.3434160000	4.6967310000
H	6.4219160000	-1.3320470000	1.4232030000	H	0.9298600000	-2.4236080000	4.7696100000
C	3.3608620000	-2.9768000000	3.0699760000	C	0.9661770000	4.7943020000	1.3749600000
O	3.4376990000	-4.7441420000	1.4377690000	H	0.9631970000	4.8697000000	2.4549580000
C	2.2162040000	-4.7046240000	0.7908240000	C	1.0115680000	4.6946170000	-1.4860100000
C	5.0043970000	1.3198460000	2.9799720000	H	1.0349380000	4.7055610000	-2.5673210000
H	6.4026590000	1.4300300000	1.3674990000	C	0.9583090000	1.3781100000	-4.6954110000
C	3.3428720000	3.0964930000	2.9934060000	H	0.9607550000	2.4563470000	-4.7947990000
O	3.3806140000	4.8301770000	1.3342000000	C	0.9931780000	-1.4815880000	-4.5402190000
C	2.1645920000	4.7646700000	0.6722590000	H	1.0096010000	-2.5626760000	-4.5261790000

C	1.0083200000	-4.7928440000	-1.3371410000	H	-6.2326340000	-4.9856930000	2.4036430000
H	1.0102580000	-4.8701930000	-2.4169040000	H	-6.5304030000	-4.1095760000	-1.6165830000
C	1.0379350000	-4.6793930000	1.5225740000	C	-3.7450940000	-0.1357240000	-4.6078170000
H	1.0558740000	-4.6901230000	2.6041100000	C	-4.3834040000	-1.3670030000	-4.8236580000
N	-1.5082660000	-4.7489550000	-1.0371450000	C	-4.5590110000	0.9871980000	-4.3944400000
N	-1.4647620000	-4.6625320000	1.2107650000	C	-5.7694170000	-1.4283010000	-4.7567810000
N	-1.5881640000	-1.0387220000	4.6659640000	H	-3.8183740000	-2.2728960000	-4.9977950000
N	-1.5434700000	1.2089010000	4.6175410000	C	-5.9367660000	0.8107120000	-4.3374090000
N	-1.5505700000	4.7324720000	1.0594980000	H	-4.1245610000	1.9658860000	-4.2332530000
N	-1.4926590000	4.6627840000	-1.1884820000	H	-6.2768060000	-2.3795960000	-4.9014570000
N	-1.5590180000	1.0681400000	-4.6586610000	H	-6.5825080000	1.6617880000	-4.1326250000
N	-1.5058550000	-1.1773510000	-4.5474020000	C	-3.7356990000	4.6826490000	-0.1484230000
H	-1.8084600000	4.2866670000	-2.1049670000	C	-4.3738470000	4.8957230000	-1.3805520000
H	-1.8239540000	-2.0911500000	-4.1595810000	C	-4.5504190000	4.4672170000	0.9736920000
H	-1.7927960000	-4.2920700000	2.1222050000	C	-5.7601060000	4.8259290000	-1.4428360000
H	-1.8661210000	2.1315620000	4.2681670000	H	-3.8102270000	5.0726790000	-2.2866300000
O	-2.5548480000	3.2064780000	-3.1968320000	C	-5.9280220000	4.4085410000	0.7961500000
H	-2.0938280000	2.6125840000	-3.8383130000	H	-4.1181360000	4.3084070000	1.9536140000
H	-2.8562500000	2.5869350000	-2.4949170000	H	-6.2668970000	4.9696800000	-2.3945540000
O	-2.5659240000	-3.2007730000	-3.1339490000	H	-6.5738950000	4.2045450000	1.6472630000
H	-2.0467590000	-3.8064530000	-2.5547870000	N	-6.5459680000	4.5612040000	-0.3875060000
H	-2.8472360000	-2.4833840000	-2.5218900000	N	-6.5551250000	-0.3726500000	-4.4915540000
O	-2.5911560000	-3.2243030000	3.2309130000	N	-6.5065730000	-4.5173030000	0.4087660000
H	-2.9070180000	-2.6226500000	2.5191970000	N	-6.5926800000	0.3640580000	4.5676350000
H	-2.1250070000	-2.6155790000	3.8507470000	C	-2.2737180000	4.6814380000	-0.0576910000
O	-2.6033870000	3.2599010000	3.2036080000	C	-2.3181020000	0.0739190000	4.6348920000
H	-2.1170710000	3.8865090000	2.6170170000	C	-2.2379050000	-4.6918720000	0.0734020000
H	-2.9035000000	2.5538730000	2.5875010000	C	-2.2838330000	-0.0485520000	-4.5941790000
C	-3.7798150000	0.1524490000	4.6531430000	C	0.2983560000	0.8032780000	-0.8444450000
C	-4.4269090000	1.3757410000	4.8877940000	C	1.4814490000	-1.2218050000	-0.0397360000
C	-4.5845830000	-0.9750860000	4.4292840000	C	2.3649280000	0.0195540000	0.1534660000
C	-5.8146340000	1.4240910000	4.8368220000	C	1.3570730000	1.1887990000	0.2001440000
H	-3.8695590000	2.2849060000	5.0708450000	H	0.6361160000	1.0818210000	-1.8527520000
C	-5.9646550000	-0.8107400000	4.3890850000	H	-0.6954960000	1.2381700000	-0.7070590000
H	-4.1422960000	-1.9477110000	4.2519450000	H	1.1326930000	-1.6176860000	0.9235800000
H	-6.3298480000	2.3679560000	5.0016790000	H	1.9530320000	-2.0498100000	-0.5696100000
H	-6.6043650000	-1.6649750000	4.1793100000	H	2.9928150000	-0.0338940000	1.0453870000
C	-3.6999260000	-4.6889100000	0.1600560000	H	3.0317040000	0.1408650000	-0.7081070000
C	-4.3408590000	-4.9254320000	1.3865120000	H	0.9026860000	1.2495650000	1.1967550000
C	-4.5118700000	-4.4332970000	-0.9556000000	H	1.8244450000	2.1516720000	-0.0028380000
C	-5.7248440000	-4.8280560000	1.4546260000	O	-3.5601040000	1.1929830000	1.5651920000
H	-3.7793340000	-5.1400560000	2.2856660000	H	-3.4555640000	-0.6100280000	1.4510560000
C	-5.8875390000	-4.3506640000	-0.7729450000	H	-4.5308240000	1.2021460000	1.7118610000
H	-4.0758570000	-4.2557580000	-1.9310240000	O	-3.5869640000	-1.5574410000	1.2094150000

H	-3.4483690000	-1.4226920000	-0.6020730000
H	-4.5596470000	-1.6894480000	1.2140510000
O	-6.3436650000	0.8599100000	1.6899020000
H	-6.4661440000	-0.1119000000	1.5440760000
H	-6.7912690000	1.0431140000	2.5316470000
O	-6.3796620000	-1.6668930000	0.8892100000
H	-6.7878040000	-2.5339930000	1.0540940000
H	-6.5111100000	-1.5076730000	-0.0787350000
O	-3.5294650000	1.5300740000	-1.1656180000
H	-4.4965370000	1.6997650000	-1.1846960000
H	-3.4423630000	1.4143930000	0.6083180000
O	-3.6340000000	-1.1628670000	-1.5347980000
H	-4.6085710000	-1.2050770000	-1.6354780000
H	-3.4372630000	0.5737070000	-1.4152940000
O	-6.4270910000	-0.8447690000	-1.6302630000
H	-6.8482360000	-0.9996950000	-2.4922340000
H	-6.4954040000	0.1312030000	-1.4851070000
O	-6.3150520000	1.6895710000	-0.8351390000
H	-6.4298090000	1.5313870000	0.1349420000
H	-6.7603440000	2.5363200000	-1.0039160000
C	0.2535790000	-0.7246220000	-0.8016990000
O	-0.6125270000	-1.4261820000	-1.2895410000

Cyclopentanone-E@1:

C	-5.6352860000	2.9848410000	2.0591610000
C	-5.0353450000	1.7456370000	2.7129950000
C	-5.0373340000	3.1962630000	0.6746350000
H	-5.3141010000	3.8338450000	2.6635940000
C	-5.5579620000	0.4612820000	2.5361530000
C	-3.9130620000	1.8708710000	3.5387010000
C	-5.5659720000	2.5722010000	-0.4603630000
C	-3.9186400000	4.0206510000	0.4930630000
C	-5.0259220000	-0.6745800000	3.1562460000
H	-6.4253720000	0.3406050000	1.8975560000
C	-3.3602800000	0.7694720000	4.1798650000
O	-3.3986480000	3.1403310000	3.7828600000
C	-5.0406630000	2.7418680000	-1.7433530000
H	-6.4269460000	1.9256310000	-0.3372490000
C	-3.3767600000	4.2237410000	-0.7708140000
O	-3.3827130000	4.7173810000	1.5739530000
C	-5.6304320000	-2.0610650000	2.9706220000
C	-3.9049190000	-0.4930690000	3.9767560000
H	-2.5359560000	0.8939120000	4.8661610000

C	-2.1769620000	3.4480380000	3.2163080000
C	-5.6306720000	2.0598630000	-2.9712580000
C	-3.9230430000	3.5739780000	-1.8706930000
H	-2.5497600000	4.9069730000	-0.8958820000
C	-2.1616320000	4.2836510000	2.0683170000
H	-5.3088400000	-2.6499400000	3.8303940000
C	-5.0400600000	-2.7428640000	1.7427840000
O	-3.3754620000	-1.5739930000	4.6770770000
C	-5.0257320000	0.6735580000	-3.1567750000
H	-5.3091280000	2.6488200000	-3.8309930000
O	-3.3989740000	3.8089970000	-3.1382040000
C	-5.5652440000	-2.5733910000	0.4597090000
C	-3.9221210000	-3.5745030000	1.8702700000
C	-2.1567620000	-2.0741980000	4.2452770000
C	0.1928400000	3.4184770000	3.2149090000
C	-5.5575610000	-0.4625030000	-2.5368300000
C	-3.9045240000	0.4924120000	-3.9770660000
C	-2.1753500000	3.2372400000	-3.4317630000
C	0.2322040000	4.2643770000	2.0799580000
C	-5.0361810000	-3.1972140000	-0.6752180000
H	-6.4264310000	-1.9271270000	0.3364770000
C	-3.3753230000	-4.2239070000	0.7704340000
O	-3.3982840000	-3.8095200000	3.1378850000
C	-2.1748390000	-3.2375290000	3.4316770000
C	-5.0344420000	-1.7466610000	-2.7135350000
H	-6.4252110000	-0.3421200000	-1.8985050000
C	-3.3593510000	-0.7699320000	-4.1799470000
O	-3.3753990000	1.5734760000	-4.6774110000
C	-2.1568810000	2.0740350000	-4.2455390000
C	-5.6340620000	-2.9860780000	-2.0598210000
C	-3.9171610000	-4.0211100000	-0.4934940000
H	-2.5480670000	-4.9068110000	0.8955950000
C	0.2357300000	-2.0814010000	4.2171560000
C	-3.9118970000	-1.8714960000	-3.5389010000
H	-2.5348010000	-0.8940940000	-4.8660190000
C	0.1948510000	3.2342420000	-3.3955450000
H	-5.3124690000	-3.8349730000	-2.6641930000
O	-3.3810140000	-4.7178960000	-1.5742250000
C	0.1953650000	-3.2340580000	3.3957380000
O	-3.3970120000	-3.1407590000	-3.7829090000
C	0.2356010000	2.0817660000	-4.2172080000
C	-2.1599430000	-4.2840040000	-2.0684410000
C	-2.1752940000	-3.4481420000	-3.2162230000
C	0.2338670000	-4.2643290000	-2.0797480000

C	0.1944900000	-3.4180200000	-3.2144090000	H	1.8275860000	-2.3590360000	-4.1044770000
C	-7.1690890000	-2.9732840000	-2.0540870000	O	2.5763810000	4.4682250000	-0.8611080000
H	-7.5463020000	-2.8820920000	-3.0762500000	H	2.1035590000	4.6645180000	-0.0179640000
H	-7.5890940000	-2.1463220000	-1.4748500000	H	2.8828400000	3.5381490000	-0.7446370000
C	-7.1655330000	-2.0473050000	2.9636880000	O	2.5811570000	0.8702470000	4.4449600000
H	-7.5487640000	-3.0687850000	2.8919490000	H	2.1056280000	0.0269420000	4.6327020000
H	-7.5856310000	-1.4802410000	2.1283420000	H	2.8967440000	0.7531850000	3.5176560000
C	-7.1703130000	2.9714730000	2.0532190000	O	2.5776660000	-4.4685990000	0.8618200000
H	-7.5476260000	2.8801050000	3.0753300000	H	2.8839240000	-3.5384870000	0.7451110000
H	-7.5899250000	2.1443690000	1.4739000000	H	2.1050640000	-4.6652540000	0.0186900000
C	-7.1657680000	2.0457000000	-2.9645280000	O	2.5826540000	-0.8696770000	-4.4450910000
H	-7.5492830000	3.0670790000	-2.8928640000	H	2.1064120000	-0.0267060000	-4.6323240000
H	-7.5858370000	1.4785450000	-2.1292290000	H	2.8985730000	-0.7528550000	-3.5178220000
H	-7.5409240000	1.5963920000	-3.8879860000	C	3.7436920000	-3.7938440000	-2.7064740000
H	-7.5521780000	3.9010240000	1.6224970000	C	4.3813710000	-3.2989190000	-3.8545860000
H	-7.5409350000	-1.5981160000	3.8871040000	C	4.5575740000	-4.2224220000	-1.6471830000
H	-7.5506630000	-3.9029650000	-1.6233860000	C	5.7672160000	-3.2015050000	-3.8668180000
C	-0.9984470000	-3.0120660000	-3.8079070000	H	3.8173270000	-2.9556230000	-4.7113940000
H	-1.0175900000	-2.4129100000	-4.7082110000	C	5.9349610000	-4.0708900000	-1.7618810000
C	-0.9641570000	-4.7150180000	-1.5061130000	H	4.1245300000	-4.6242560000	-0.7397110000
H	-0.9654290000	-5.3906560000	-0.6600360000	H	6.2738830000	-2.8022930000	-4.7427930000
C	-0.9608130000	1.5001820000	-4.6592200000	H	6.5804600000	-4.3602070000	-0.9356590000
H	-0.9600810000	0.6431400000	-5.3207200000	C	3.7449910000	-2.7199700000	3.7724340000
C	-0.9991270000	3.8367970000	-3.0044610000	C	4.3874340000	-3.8682750000	3.2843800000
H	-1.0198000000	4.7496180000	-2.4243500000	C	4.5545820000	-1.6583930000	4.2036240000
C	-0.9658320000	4.7146790000	1.5060240000	C	5.7739390000	-3.8784900000	3.1957570000
H	-0.9670780000	5.3900640000	0.6597480000	H	3.8269280000	-4.7266060000	2.9390830000
C	-1.0001110000	3.0124360000	3.8083120000	C	5.9330100000	-1.7714550000	4.0616920000
H	-1.0192830000	2.4134920000	4.7087590000	H	4.1176520000	-0.7507880000	4.6008950000
C	-0.9608570000	-1.4999870000	4.6589400000	H	6.2845550000	-4.7545380000	2.8017070000
H	-0.9603570000	-0.6428050000	5.3202600000	H	6.5754340000	-0.9437200000	4.3535290000
C	-0.9984380000	-3.8369460000	3.0046540000	C	3.7420690000	3.7943390000	2.7070740000
H	-1.0188710000	-4.7498630000	2.4246860000	C	4.3796960000	3.2994520000	3.8552340000
N	1.5554650000	-1.7368290000	4.4588360000	C	4.5560240000	4.2229200000	1.6478330000
N	1.5062220000	-3.5777450000	3.1675070000	C	5.7655380000	3.2020260000	3.8675420000
N	1.5543710000	-4.5085810000	-1.7380460000	H	3.8156360000	2.9561580000	4.7120260000
N	1.5045970000	-3.1789790000	-3.5514860000	C	5.9334020000	4.0713610000	1.7625960000
N	1.5554450000	1.7375350000	-4.4587930000	H	4.1230550000	4.6247370000	0.7403210000
N	1.5055990000	3.5782140000	-3.1670970000	H	6.2721510000	2.8027960000	4.7435390000
N	1.5527190000	4.5085900000	1.7382330000	H	6.5789490000	4.3606690000	0.9364100000
N	1.5029490000	3.1796970000	3.5521900000	C	3.7446270000	2.7211750000	-3.7720510000
H	1.8285800000	4.1401080000	-2.3537630000	C	4.3866890000	3.8695410000	-3.2836370000
H	1.8259830000	2.3598350000	4.1052650000	C	4.5545690000	1.6599860000	-4.2035470000
H	1.8294420000	-4.1399540000	2.3545400000	C	5.7731860000	3.8801720000	-3.1949590000

H	3.8258830000	4.7275940000	-2.9381380000
C	5.9329530000	1.7734460000	-4.0615350000
H	4.1179410000	0.7523640000	-4.6011140000
H	6.2835160000	4.7562600000	-2.8006270000
H	6.5756570000	0.9460080000	-4.3536030000
N	6.5552320000	2.8483480000	-3.5482760000
N	6.5509530000	3.5520820000	2.8372420000
N	6.5556460000	-2.8463160000	3.5487950000
N	6.5525760000	-3.5516060000	-2.8364870000
C	2.2824810000	2.6448940000	-3.8103690000
C	2.2814500000	-3.8395120000	-2.6307740000
C	2.2828170000	-2.6441190000	3.8106680000
C	2.2798240000	3.8399520000	2.6312880000
C	-0.8221250000	1.2390440000	0.0572710000
C	-0.8272280000	-1.2392710000	-0.0576370000
C	-2.2331910000	-0.7189610000	0.2750920000
C	-2.2309180000	0.7243450000	-0.2720410000
H	-0.7776190000	1.6175930000	1.0877250000
H	-0.4410720000	2.0311670000	-0.5921180000
H	-0.7866400000	-1.6180810000	-1.0881490000
H	-0.4478380000	-2.0328530000	0.5909390000
H	-3.0294660000	-1.3282730000	-0.1526990000
H	-2.3781340000	-0.7024360000	1.3612490000
H	-2.3786490000	0.7084380000	-1.3578210000
H	-3.0235480000	1.3369690000	0.1576600000
O	3.5599440000	-0.6288560000	-1.8589180000
H	3.3477770000	-1.5113170000	-0.2599650000
H	4.5345740000	-0.7031360000	-1.9322420000
O	3.5447060000	-1.8704400000	0.6374340000
H	3.3868730000	-0.2807770000	1.5148050000
H	4.5206080000	-1.9443820000	0.6875600000
O	6.3596410000	-0.8845060000	-1.6534190000
H	6.4645290000	-1.3117180000	-0.7666740000
H	6.7932710000	-1.4917640000	-2.2744770000
O	6.3497760000	-1.6541910000	0.8830170000
H	6.7839910000	-2.2769980000	1.4880060000
H	6.4577570000	-0.7686590000	1.3115100000
O	3.5436630000	1.8700640000	-0.6375230000
H	4.5195240000	1.9444510000	-0.6876340000
H	3.3874560000	0.2802060000	-1.5156660000
O	3.5585980000	0.6283170000	1.8584660000
H	4.5331630000	0.7032030000	1.9319160000
H	3.3469550000	1.5106690000	0.2598250000
O	6.3586630000	0.8855010000	1.6536490000

H	6.7918160000	1.4932650000	2.2745580000
H	6.4627680000	1.3128960000	0.7669070000
O	6.3493040000	1.6552690000	-0.8827900000
H	6.4577650000	0.7698660000	-1.3114110000
H	6.7830490000	2.2784560000	-1.4877270000
C	0.0662690000	-0.0018910000	-0.0012190000
O	1.2827330000	-0.0042850000	-0.0025250000

Cyclopentanol-A@1:

C	5.5169200000	-3.6292830000	0.8164510000
C	4.9469930000	-2.7084420000	1.8862870000
C	4.9077320000	-3.2902470000	-0.5363880000
H	5.1769740000	-4.6354600000	1.0632320000
C	5.4951070000	-1.4542930000	2.1675070000
C	3.8280260000	-3.1011130000	2.6282470000
C	5.4425010000	-2.2984530000	-1.3646890000
C	3.7717470000	-3.9688530000	-0.9940200000
C	4.9933840000	-0.6029910000	3.1562000000
H	6.3591070000	-1.1305960000	1.5990100000
C	3.3039480000	-2.2885010000	3.6259790000
O	3.2868800000	-4.3691410000	2.4145640000
C	4.9094010000	-1.9774820000	-2.6155150000
H	6.3202310000	-1.7615730000	-1.0243540000
C	3.2153870000	-3.6815100000	-2.2355480000
O	3.2420580000	-5.0129070000	-0.2353630000
C	5.6315650000	0.7459870000	3.4653150000
C	3.8752490000	-1.0452310000	3.8751670000
H	2.4791130000	-2.6318680000	4.2329970000
C	2.0620790000	-4.4428090000	1.7815820000
C	5.5183040000	-0.9185420000	-3.5254800000
C	3.7750620000	-2.6852240000	-3.0276750000
H	2.3781200000	-4.2591640000	-2.5988370000
C	2.0350710000	-4.7870590000	0.4031420000
H	5.3266560000	0.9996140000	4.4811550000
C	5.0601060000	1.8357910000	2.5661470000
O	3.3785080000	-0.2718980000	4.9204780000
C	4.9588450000	0.4612380000	-3.2029590000
H	5.1793620000	-1.1544570000	-4.5347800000
O	3.2545830000	-2.4386720000	-4.2943820000
C	5.5868350000	2.1328160000	1.3069100000
C	3.9652630000	2.5946670000	2.9948320000
C	2.1743370000	0.3808070000	4.7096150000
C	-0.3107590000	-4.3755650000	1.8023580000

C	5.5288190000	1.2852960000	-2.2278960000	H	7.5299780000	-0.0579120000	4.1397590000
C	3.8507120000	0.9620230000	-3.8991460000	H	7.6283590000	4.0848460000	-0.1349520000
C	2.0467810000	-1.7704570000	-4.3597670000	C	1.0867810000	4.2907470000	-2.4948420000
C	-0.3574130000	-4.7320100000	0.4327260000	H	1.0952660000	4.0634790000	-3.5523660000
C	5.0845860000	3.1474990000	0.4860800000	C	1.0863290000	5.0152830000	0.2734860000
H	6.4329530000	1.5557810000	0.9524830000	H	1.1013850000	5.3239660000	1.3112140000
C	3.4407830000	3.6170910000	2.2114710000	C	0.8702940000	0.3205540000	-4.8476140000
O	3.4543060000	2.3704230000	4.2698100000	H	0.8878430000	1.3626390000	-5.1407170000
C	2.2196420000	1.7566740000	4.3609420000	C	0.8578510000	-2.4655510000	-4.1879010000
C	5.0572740000	2.5685640000	-1.9393150000	H	0.8614630000	-3.5296630000	-3.9921310000
H	6.3842090000	0.9141590000	-1.6755010000	C	0.8331640000	-4.9539600000	-0.2745900000
C	3.3651490000	2.2414270000	-3.6528280000	H	0.8235430000	-5.2649670000	-1.3116000000
O	3.2818340000	0.2105300000	-4.9239380000	C	0.8889120000	-4.2463970000	2.4991590000
C	2.0549130000	-0.3879470000	-4.6840820000	H	0.9196050000	-4.0170100000	3.5559260000
C	5.6896900000	3.4563720000	-0.8763330000	C	0.9661690000	-0.2758350000	4.9082900000
C	3.9886780000	3.8798410000	0.9606070000	H	0.9470800000	-1.3119750000	5.2216130000
H	2.6356240000	4.2322060000	2.5858100000	C	1.0578240000	2.4952870000	4.1914230000
C	-0.2159230000	0.4520970000	4.7172850000	H	1.0990870000	3.5528640000	3.9678330000
C	3.9533610000	3.0254230000	-2.6665310000	N	-1.5432420000	0.0727290000	4.8283310000
H	2.5514890000	2.6296150000	-4.2476720000	N	-1.4500510000	2.2503310000	4.2792940000
C	-0.3228300000	-1.7398340000	-4.3250840000	N	-1.4345810000	4.9456230000	0.0057950000
H	5.3975070000	4.4789270000	-1.1167620000	N	-1.4154400000	4.3694840000	-2.1686930000
O	3.4987170000	4.9513900000	0.2149610000	N	-1.6512650000	0.0691280000	-4.7483330000
C	-0.1480140000	1.8199980000	4.3602890000	N	-1.6399080000	-2.1206990000	-4.2412940000
O	3.4874330000	4.3176410000	-2.4393390000	N	-1.6803200000	-4.7853950000	0.0167880000
C	-0.3381080000	-0.3632440000	-4.6545520000	N	-1.6228510000	-4.2405800000	2.1953250000
C	2.2733390000	4.7886580000	-0.4130600000	H	-1.9695350000	-2.9403740000	-3.6953600000
C	2.2723940000	4.4444680000	-1.7909970000	H	-1.9236970000	-3.7078860000	3.0321990000
C	-0.1201540000	4.8329550000	-0.4176760000	H	-1.7468300000	3.0856730000	3.7404630000
C	-0.0985080000	4.4629860000	-1.7839690000	H	-1.7521450000	3.8020780000	-2.9717120000
C	7.2234980000	3.3962520000	-0.8814890000	O	-2.6880700000	-3.8115400000	-2.4246180000
H	7.6058880000	3.6840920000	-1.8645480000	H	-2.2317040000	-4.2961460000	-1.6996590000
H	7.6151210000	2.4004170000	-0.6562710000	H	-3.0488610000	-3.0067170000	-1.9870950000
C	7.1659470000	0.6981410000	3.4388750000	O	-2.5583200000	-2.3367180000	3.8794880000
H	7.5756540000	1.6691820000	3.7297320000	H	-2.1004160000	-1.6529220000	4.4236820000
H	7.5706340000	0.4537700000	2.4527960000	H	-2.7297880000	-1.8523020000	3.0428070000
C	7.0517030000	-3.6480500000	0.7966480000	O	-2.4032840000	3.9568170000	2.4243000000
H	7.4346390000	-3.9509310000	1.7748970000	H	-2.6303210000	3.1314800000	1.9390490000
H	7.4900240000	-2.6746400000	0.5600950000	H	-1.9440970000	4.4923300000	1.7357370000
C	7.0533750000	-0.9523300000	-3.5310090000	O	-2.5425770000	2.5231350000	-3.7956600000
H	7.4048080000	-1.9428750000	-3.8322430000	H	-2.1232000000	1.7859720000	-4.2998210000
H	7.4909830000	-0.7324250000	-2.5532940000	H	-2.8722260000	2.0750130000	-2.9839680000
H	7.4420890000	-0.2146150000	-4.2380740000	C	-3.6413010000	4.6096300000	-1.1170100000
H	7.4083860000	-4.3597920000	0.0472350000	C	-4.3065640000	4.5535320000	-2.3518580000

C	-4.4292590000	4.5938650000	0.0437530000	C	2.3531480000	0.1657990000	0.2716230000
C	-5.6893730000	4.4172420000	-2.3668260000	C	1.4479010000	1.2311120000	-0.4219040000
H	-3.7645290000	4.5694720000	-3.2877260000	H	-0.4892480000	0.9034250000	-1.4579320000
C	-5.8060990000	4.4501110000	-0.0865650000	H	-0.5715250000	0.8174640000	0.3063860000
H	-3.9760100000	4.6434790000	1.0257500000	H	0.9673720000	-0.9970720000	1.5036860000
H	-6.2156640000	4.3468950000	-3.3161330000	H	1.9767120000	-2.0042640000	0.4610970000
H	-6.4288520000	4.3940520000	0.8031580000	H	2.7885020000	0.5341270000	1.2025370000
C	-3.7098670000	1.2743920000	4.5305540000	H	3.1894270000	-0.1046310000	-0.3797690000
C	-4.3336370000	2.5311730000	4.4801090000	H	1.3981630000	2.1608470000	0.1466120000
C	-4.5333590000	0.1395610000	4.5493350000	H	1.8492420000	1.4820940000	-1.4055690000
C	-5.7205690000	2.5892380000	4.4136680000	O	-3.5534090000	1.2742250000	-1.5181450000
H	-3.7597440000	3.4483420000	4.4587320000	H	-3.1987150000	1.6067200000	0.1930350000
C	-5.9113750000	0.3119860000	4.4679050000	H	-4.5249110000	1.4398580000	-1.5191110000
H	-4.1091630000	-0.8561910000	4.5817530000	O	-3.2065510000	1.5875800000	1.1825520000
H	-6.2202660000	3.5542500000	4.3620230000	H	-2.9145420000	-0.1142900000	1.4066180000
H	-6.5618070000	-0.5573750000	4.4292830000	H	-4.1669130000	1.6273070000	1.4086120000
C	-3.8726820000	-4.4380620000	1.1439050000	O	-6.2890500000	1.4294800000	-1.1293930000
C	-4.5574280000	-4.2814780000	2.3583040000	H	-6.2530260000	1.5138140000	-0.1385030000
C	-4.6423590000	-4.5730970000	-0.0218030000	H	-6.7685750000	2.2199360000	-1.4276340000
C	-5.9504400000	-4.2608650000	2.3457840000	O	-5.8980820000	1.3147010000	1.4614290000
H	-4.0316410000	-4.1490570000	3.2955090000	H	-6.4351860000	1.6234310000	2.2077140000
C	-6.0292360000	-4.5371860000	0.0859890000	H	-5.8724830000	0.3096650000	1.5495460000
H	-4.1763040000	-4.6889570000	-0.9910130000	O	-3.7434620000	-1.4705330000	-1.3087690000
H	-6.4947890000	-4.1283020000	3.2774390000	H	-4.7307290000	-1.5002390000	-1.3168360000
H	-6.6407030000	-4.6356180000	-0.8085100000	H	-3.4843960000	0.2914660000	-1.5879100000
C	-3.8614170000	-1.0579500000	-4.4443330000	O	-2.8730370000	-1.1058510000	1.3724950000
C	-4.5253010000	-2.2937700000	-4.4107610000	H	-2.0127040000	-1.3172150000	0.9300930000
C	-4.6483400000	0.1016100000	-4.3937880000	H	-3.4874770000	-1.4382810000	-0.3644940000
C	-5.9064650000	-2.3125770000	-4.2599880000	O	-5.7620670000	-1.2655320000	1.5466960000
H	-3.9829560000	-3.2288610000	-4.4571580000	H	-4.8271630000	-1.5331140000	1.5262980000
C	-6.0233960000	-0.0329490000	-4.2302570000	H	-6.1639220000	-1.5897880000	0.7176130000
H	-4.1947350000	1.0838430000	-4.4356190000	O	-6.4681670000	-1.2619950000	-1.1524650000
H	-6.4325250000	-3.2636270000	-4.2124480000	H	-6.5619440000	-0.2833840000	-1.2390490000
H	-6.6454380000	0.8544970000	-4.1429050000	H	-6.9316470000	-1.6143770000	-1.9276640000
N	-6.6619410000	-1.2106310000	-4.1391710000	C	0.3550490000	-0.9143190000	-0.5528160000
N	-6.6933260000	-4.3868320000	1.2400890000	H	0.7510630000	-1.2194890000	-1.5310780000
N	-6.5167450000	1.5086810000	4.3846780000	O	-0.8419180000	-1.6697130000	-0.2946990000
N	-6.4465350000	4.3372370000	-1.2620540000	H	-0.6386700000	-2.6122910000	-0.3768020000
C	-2.3981990000	-1.0007890000	-4.4846950000	Cyclopentanol-B@1:			
C	-2.1774340000	4.6494270000	-1.0587560000				
C	-2.2497390000	1.1659580000	4.5472880000	C	-5.5861840000	1.5968920000	3.2273460000
C	-2.4072920000	-4.4804890000	1.0918310000	C	-4.9919930000	0.1942560000	3.2197510000
C	0.0541520000	0.5827940000	-0.5643610000	C	-4.9970610000	2.4459910000	2.1075810000
C	1.4425770000	-1.0541800000	0.5164530000				

H	-5.2608470000	2.0588450000	4.1600760000	C	-2.1703230000	3.9560360000	-2.7344820000
C	-5.5242880000	-0.8450520000	2.4528910000	C	-5.5441040000	-1.5957180000	-3.2280790000
C	-3.8727810000	-0.1010490000	4.0065180000	C	-3.8304250000	-3.2457630000	-2.3369570000
C	-5.5320060000	2.4550870000	0.8153890000	H	-2.4780870000	-4.7110440000	-1.5476260000
C	-3.8929480000	3.2723370000	2.3515730000	C	0.2173470000	-4.0368420000	2.8198200000
C	-5.0074000000	-2.1445130000	2.4584850000	C	-3.8416810000	0.1152410000	-3.9921670000
H	-6.3864890000	-0.6368510000	1.8302530000	H	-2.4927890000	1.6318850000	-4.6951990000
C	-3.3385830000	-1.3837480000	4.0514690000	C	0.1704610000	4.5836260000	-1.4251600000
O	-3.3411220000	0.8927510000	4.8212760000	H	-5.2097980000	-2.0530590000	-4.1598250000
C	-5.0289140000	3.2531850000	-0.2157660000	O	-3.2981900000	-3.3319490000	-3.6230090000
H	-6.3849520000	1.8196750000	0.6064570000	C	0.1808460000	-4.6348930000	1.5389370000
C	-3.3717940000	4.0891880000	1.3540080000	O	-3.3058760000	-0.8765420000	-4.8093750000
O	-3.3608570000	3.3474840000	3.6368390000	C	0.2234850000	3.9699680000	-2.6996860000
C	-5.6120580000	-3.2554060000	1.6110210000	C	-2.0820480000	-2.7146870000	-3.8609890000
C	-3.8955010000	-2.3921600000	3.2733320000	C	-2.0894330000	-1.4231520000	-4.4547230000
H	-2.5165950000	-1.6076320000	4.7157030000	C	0.3083860000	-2.7160610000	-3.8922470000
C	-2.1297720000	1.4454600000	4.4474860000	C	0.2836920000	-1.4167170000	-4.4518940000
C	-5.6249160000	3.2607550000	-1.6178120000	C	-7.0794750000	-1.6057930000	-3.2310730000
C	-3.9263840000	4.0625820000	0.0791880000	H	-7.4552990000	-1.0429300000	-4.0897080000
H	-2.5577800000	4.7616260000	1.5812870000	H	-7.5135420000	-1.1604190000	-2.3317010000
C	-2.1362590000	2.7336230000	3.8501300000	C	-7.1465400000	-3.2282350000	1.5866450000
H	-5.3050990000	-4.1949600000	2.0712020000	H	-7.5268960000	-4.0782330000	1.0137130000
C	-4.9952730000	-3.2375890000	0.2183440000	H	-7.5533130000	-2.3196550000	1.1342410000
O	-3.3968800000	-3.6897290000	3.3848250000	C	-7.1216920000	1.5906760000	3.2224790000
C	-5.0044130000	2.1514960000	-2.4564860000	H	-7.4971440000	1.0217470000	4.0773590000
H	-5.3165120000	4.2005460000	-2.0766930000	H	-7.5459400000	1.1440480000	2.3189120000
O	-3.4273680000	4.9061450000	-0.9108370000	C	-7.1595320000	3.2245000000	-1.6147160000
C	-5.4957710000	-2.4470670000	-0.8187410000	H	-7.5523730000	4.0746090000	-1.0504980000
C	-3.8782630000	-4.0318350000	-0.0625670000	H	-7.5666100000	2.3155430000	-1.1630990000
C	-2.1762250000	-3.9658000000	2.7927460000	H	-7.5386430000	3.2808630000	-2.6387070000
C	0.2416020000	1.4365600000	4.3816370000	H	-7.5004230000	2.6139600000	3.2912510000
C	-5.5104340000	0.8481370000	-2.4516190000	H	-7.5385060000	-3.2914510000	2.6053010000
C	-3.8864580000	2.4055510000	-3.2613320000	H	-7.4475930000	-2.6330010000	-3.2994340000
C	-2.1998660000	4.5781960000	-1.4586180000	C	-0.9068700000	-0.7610090000	-4.7601290000
C	0.2540230000	2.7319480000	3.8123850000	H	-0.9234680000	0.2074120000	-5.2418300000
C	-4.9493440000	-2.4355960000	-2.1056270000	C	-0.8905500000	-3.3794850000	-3.6004500000
H	-6.3592230000	-1.8228710000	-0.6207850000	H	-0.8971700000	-4.3833290000	-3.1948010000
C	-3.3038380000	-4.0490710000	-1.3299140000	C	-0.9689920000	3.6686890000	-3.3723630000
O	-3.4010230000	-4.8837110000	0.9309660000	H	-0.9633730000	3.2376290000	-4.3655520000
C	-2.1856990000	-4.5788170000	1.5115150000	C	-1.0277630000	4.9123610000	-0.7958750000
C	-4.9630880000	-0.1879660000	-3.2124280000	H	-1.0554440000	5.4257630000	0.1559400000
H	-6.3759260000	0.6341850000	-1.8354910000	C	-0.9522460000	3.3935160000	3.5495550000
C	-3.3170810000	1.4011700000	-4.0364250000	H	-0.9677030000	4.3960960000	3.1413720000
O	-3.3835120000	3.6999900000	-3.3559440000	C	-0.9407840000	0.7833820000	4.7249130000

H	-0.9445990000	-0.1828290000	5.2113560000	H	4.1384580000	-2.8420840000	3.6040690000
C	-0.9849170000	-3.7152470000	3.4661280000	H	6.1840930000	-5.4758030000	0.0175300000
H	-0.9969490000	-3.2879580000	4.4609600000	H	6.5575120000	-2.7141090000	3.0560600000
C	-1.0048770000	-4.9333740000	0.8761440000	C	3.7851800000	2.1112800000	4.0485910000
H	-1.0196960000	-5.4346140000	-0.0824910000	C	4.5127340000	1.0452680000	4.6042410000
N	1.5415580000	-3.8483030000	3.2007750000	C	4.5151350000	3.1852550000	3.5192100000
N	1.4941380000	-4.8290480000	1.1747720000	C	5.9047030000	1.1139000000	4.6097930000
N	1.6224100000	-3.1076800000	-3.7073620000	H	4.0192060000	0.1736490000	5.0174020000
N	1.6033320000	-1.0510260000	-4.6072460000	C	5.9053580000	3.1419410000	3.5733130000
N	1.5487180000	3.7755340000	-3.0602610000	H	4.0135560000	4.0235220000	3.0546360000
N	1.4769200000	4.7707360000	-1.0444610000	H	6.4836580000	0.2975410000	5.0349100000
N	1.5618580000	3.1344610000	3.6184250000	H	6.4850250000	3.9662930000	3.1629540000
N	1.5638230000	1.0833790000	4.5267900000	C	3.7265470000	4.2756040000	-1.9254940000
H	1.7905190000	4.8682280000	-0.0562270000	C	4.3453740000	5.0762840000	-0.9526090000
H	1.8913620000	0.1142670000	4.6721520000	C	4.5549420000	3.4865530000	-2.7360660000
H	1.7913570000	-4.7550710000	0.1929390000	C	5.7239680000	5.0006930000	-0.7960000000
H	1.9209340000	-0.0697400000	-4.7208050000	H	3.7704110000	5.7189290000	-0.2999410000
O	2.5234680000	4.4493930000	1.4015500000	C	5.9248840000	3.4806870000	-2.4891800000
H	2.0506390000	4.2036580000	2.2330370000	H	4.1379840000	2.8594050000	-3.5138820000
H	2.8473230000	3.5764120000	1.0870150000	H	6.2149740000	5.5996030000	-0.0319890000
O	2.5264890000	-1.4372270000	4.2140900000	H	6.5747360000	2.8299170000	-3.0665870000
H	2.0881040000	-2.3151630000	4.1438570000	N	6.5182150000	4.2018860000	-1.5238820000
H	2.6361450000	-1.1715290000	3.2729580000	N	6.6094000000	2.1372810000	4.1096090000
O	2.1352360000	-3.5959890000	-1.1039320000	N	6.4868060000	-4.0735090000	1.5043430000
H	2.9868880000	-3.1247240000	-0.9334720000	N	6.6451430000	-2.0735950000	-3.9448620000
H	2.0059840000	-3.6241180000	-2.0870650000	C	2.2652400000	4.2553510000	-2.0444580000
O	2.5458760000	1.4466490000	-4.2202970000	C	2.3663550000	-2.0859510000	-4.1292160000
H	2.1027090000	2.3139130000	-4.0556200000	C	2.2688010000	-4.3063710000	2.1875300000
H	2.7529060000	1.1287060000	-3.3138460000	C	2.3190550000	2.1241910000	4.0417000000
C	3.8288760000	-2.0669620000	-4.0844370000	C	-1.2185650000	-1.1744250000	0.4970330000
C	4.5821510000	-0.9992860000	-4.5942970000	C	-0.5522290000	0.6424910000	-1.0262250000
C	4.5272420000	-3.1403770000	-3.5119130000	C	-1.9700870000	0.9105720000	-0.5090810000
C	5.9715530000	-1.0582300000	-4.5012410000	C	-2.0127920000	0.1158990000	0.8070320000
H	4.1088930000	-0.1272750000	-5.0300760000	H	-1.8943450000	-2.0010070000	0.2669760000
C	5.9162030000	-3.0888060000	-3.4631350000	H	-0.5948290000	-1.4979310000	1.3357030000
H	3.9931740000	-3.9941450000	-3.1150090000	H	0.1731870000	1.2172040000	-0.4342930000
H	6.5731410000	-0.2369660000	-4.8816520000	H	-0.4012740000	0.8991350000	-2.0781520000
H	6.4738340000	-3.9063610000	-3.0113630000	H	-2.1808780000	1.9718220000	-0.3742120000
C	3.7256130000	-4.2781010000	2.0355820000	H	-2.7079390000	0.5142420000	-1.2158190000
C	4.3368390000	-5.0457800000	1.0311830000	H	-1.5147150000	0.6896900000	1.5964550000
C	4.5526150000	-3.4558790000	2.8134840000	H	-3.0290990000	-0.0878900000	1.1488750000
C	5.7006660000	-4.9056120000	0.8076230000	O	3.0844170000	0.3468990000	-1.7066960000
H	3.7622720000	-5.7349580000	0.4246410000	H	3.9222930000	-1.1172570000	-0.9886050000
C	5.9082950000	-3.3879200000	2.5041520000	H	2.2513230000	-0.1217500000	-1.4579580000

O	4.1028960000	-1.8971200000	-0.4204380000	C	-3.9315100000	2.8284190000	2.8677250000
H	3.4429190000	-1.1341480000	1.0351180000	H	-2.5830300000	4.4148860000	2.3624080000
H	5.0922710000	-2.0012050000	-0.3988150000	C	-2.2064070000	4.7378220000	-0.6617670000
O	6.1869980000	0.4041540000	-1.8186110000	C	-5.5767240000	-1.0351670000	-3.4624430000
H	6.5698910000	-0.4659340000	-1.5889990000	C	-3.8695920000	0.7716430000	-3.9202960000
H	5.2997910000	0.2320450000	-2.1672660000	H	-2.5049830000	2.3745640000	-4.3502950000
O	6.7383260000	-1.7896410000	-0.2426100000	C	-2.1748850000	4.3366540000	-2.0239920000
H	7.1429630000	-2.6220710000	0.0548600000	H	-5.3294300000	1.3377030000	4.4414840000
H	6.6609030000	-1.2464430000	0.5891060000	C	-5.0503370000	-0.3419680000	3.2016600000
O	3.4238610000	1.9282860000	0.4777530000	O	-3.4033660000	2.6903240000	4.1500020000
H	4.4100140000	2.0293780000	0.4989760000	C	-4.9787580000	-2.0554270000	-2.5030550000
H	3.1877160000	1.0383970000	-1.0003850000	H	-5.2445700000	-1.3244540000	-4.4600070000
O	2.8237090000	-0.5867130000	1.5785270000	O	-3.3417460000	-0.0753900000	-4.8894360000
H	1.9917390000	-0.6966180000	1.0673780000	C	-5.5679670000	-1.2368270000	2.2620870000
H	3.2247630000	1.1678020000	1.0679420000	C	-3.9406400000	-0.7639180000	3.9414460000
O	6.3768650000	-0.2861730000	1.9141010000	C	-2.1876230000	2.0363920000	4.2712080000
H	5.5224060000	-0.3011220000	2.3642240000	C	0.1632060000	4.7241590000	-0.6159050000
H	6.4657160000	0.6337710000	1.5783040000	C	-5.5209150000	-2.2784950000	-1.2336400000
O	6.1194330000	1.8935740000	0.3565350000	C	-3.8620820000	-2.8187900000	-2.8687060000
H	6.1727810000	1.3476160000	-0.4787420000	C	-2.1229060000	-0.6693180000	-4.6277320000
H	6.5991710000	2.7088530000	0.1419000000	C	0.2173420000	4.3380100000	-1.9765660000
C	-0.3408930000	-0.8493210000	-0.7417570000	C	-5.0399840000	-2.5139480000	2.0495180000
H	-0.6667950000	-1.4430770000	-1.6008460000	H	-6.4254330000	-0.9296550000	1.6747160000
O	1.0677130000	-1.1125090000	-0.5371710000	C	-3.3924530000	-2.0294180000	3.7675450000
H	1.2625580000	-2.0683790000	-0.6938330000	O	-3.4284370000	0.0798330000	4.9232880000

Cyclopentanol-C@1:

C	-5.6397010000	3.4854440000	-1.0556930000	H	-6.3814850000	-1.6929310000	-0.9319580000
C	-5.0507870000	3.2420290000	0.3276180000	C	-3.3342290000	-3.7750520000	-2.0075950000
C	-5.0220120000	2.5260590000	-2.0637730000	O	-3.3239610000	-2.6958680000	-4.1487980000
H	-5.3235250000	4.4861520000	-1.3517160000	C	-2.1066320000	-2.0428860000	-4.2665520000
C	-5.5654380000	2.2883030000	1.2095940000	C	-5.6338650000	-3.4748370000	1.0288080000
C	-3.9453670000	3.9829250000	0.7580940000	C	-3.9286540000	-2.8880340000	2.8154350000
C	-5.5377630000	1.2440220000	-2.2806080000	H	-2.5741750000	-2.3600410000	4.3899730000
C	-3.8980010000	2.9037260000	-2.8097820000	C	0.2048520000	2.0081310000	4.2725590000
C	-5.0397290000	2.0617300000	2.4852320000	C	-3.9037350000	-3.9662790000	-0.7539050000
H	-6.4199990000	1.7014580000	0.8932770000	H	-2.5087500000	-4.3909950000	-2.3335640000
C	-3.3995280000	3.7951260000	2.0221930000	C	0.2448980000	-0.6448690000	-4.5946700000
O	-3.4350110000	4.9763760000	-0.0747470000	H	-5.3207260000	-4.4747120000	1.3307600000
C	-4.9946290000	0.3487140000	-3.2049230000	O	-3.4077080000	-4.1753650000	2.6929410000
H	-6.4069480000	0.9355640000	-1.7113450000	C	0.1625270000	0.6447020000	4.6504430000
C	-3.3334940000	2.0412950000	-3.7431490000	O	-3.4137440000	-4.9661010000	0.0844890000
O	-3.3861550000	4.1936240000	-2.6835270000	C	0.2864230000	-2.0208050000	-4.2655260000
C	-5.6441040000	1.0402500000	3.4405860000	C	-2.1872210000	-4.3192930000	2.0539730000

C	-2.1971010000	-4.7324280000	0.6944470000	H	1.7833720000	4.7657820000	0.7795260000
C	0.2060130000	-4.3295150000	2.0455770000	H	1.7937900000	-0.7353560000	4.7130820000
C	0.1721790000	-4.7307980000	0.6887340000	H	1.8007740000	-4.7493090000	-0.6831440000
C	-7.1686950000	-3.4546200000	1.0068760000	O	2.5884460000	2.1331820000	-3.9427610000
H	-7.5427550000	-4.2029380000	0.3028750000	H	2.1030270000	2.9044680000	-3.5661060000
H	-7.5809670000	-2.4873630000	0.7066670000	H	2.9104240000	1.6444430000	-3.1496250000
C	-7.1793660000	1.0390600000	3.4175040000	O	2.5431440000	4.0490470000	2.1532030000
H	-7.5645130000	0.3389030000	4.1638300000	H	2.0700300000	3.6681160000	2.9310870000
H	-7.5933260000	0.7460880000	2.4487000000	H	2.8288030000	3.2503230000	1.6549570000
C	-7.1745220000	3.4599610000	-1.0646480000	O	2.5412630000	-2.1198600000	4.0283380000
H	-7.5650970000	4.2071230000	-0.3684380000	H	2.8323570000	-1.6369390000	3.2213580000
H	-7.5893450000	2.4913670000	-0.7722310000	H	2.0666900000	-2.9052230000	3.6667040000
C	-7.1120340000	-1.0446700000	-3.4630130000	O	2.4732090000	-3.9350790000	-2.0271770000
H	-7.4900410000	-0.3430840000	-4.2116100000	H	2.1113400000	-3.5587560000	-2.8679660000
H	-7.5434060000	-0.7597020000	-2.4994500000	H	2.9080620000	-3.1779120000	-1.5709000000
H	-7.4810760000	-2.0450420000	-3.7048970000	C	3.7184320000	-4.5043260000	1.2935130000
H	-7.5480290000	3.6882390000	-2.0666090000	C	4.3629880000	-5.0738500000	0.1841690000
H	-7.5588600000	2.0382090000	3.6479520000	C	4.5253080000	-3.9259610000	2.2848530000
H	-7.5611250000	-3.6844900000	2.0011740000	C	5.7453350000	-4.9816530000	0.0864250000
C	-1.0168420000	-4.9583280000	0.0006960000	H	3.8047030000	-5.5454240000	-0.6135110000
H	-1.0338690000	-5.3134190000	-1.0210950000	C	5.8999020000	-3.8821690000	2.0828210000
C	-0.9944030000	-4.1374070000	2.7434890000	H	4.0871790000	-3.4791230000	3.1685940000
H	-1.0005090000	-3.8637850000	3.7908930000	H	6.2564340000	-5.3970050000	-0.7792600000
C	-0.9104110000	-2.7337820000	-4.1075460000	H	6.5389010000	-3.4009200000	2.8196780000
H	-0.9140110000	-3.7932500000	-3.8830260000	C	3.7127730000	1.2619710000	4.5069420000
C	-0.9463660000	0.0444550000	-4.7997460000	C	4.3546900000	0.1604050000	5.0942190000
H	-0.9642000000	1.0798570000	-5.1115420000	C	4.5232500000	2.2707320000	3.9636050000
C	-0.9723470000	4.1574310000	-2.6960210000	C	5.7422800000	0.0948350000	5.0648860000
H	-0.9617890000	3.8972180000	-3.7468470000	H	3.7932250000	-0.6528570000	5.5344180000
C	-1.0372450000	4.9490100000	0.0538830000	C	5.9026340000	2.0985000000	3.9804550000
H	-1.0693300000	5.2933110000	1.0788860000	H	4.0856640000	3.1485440000	3.5042490000
C	-0.9904910000	2.7178780000	4.0901210000	H	6.2530120000	-0.7607020000	5.5015860000
H	-0.9887590000	3.7702900000	3.8361020000	H	6.5464940000	2.8520230000	3.5323510000
C	-1.0317210000	-0.0374230000	4.8681570000	C	3.7190620000	4.5352460000	-1.1905930000
H	-1.0543790000	-1.0630490000	5.2109180000	C	4.3530800000	5.1235900000	-0.0849450000
N	1.5252340000	2.4120340000	4.1644870000	C	4.5376370000	3.9758410000	-2.1839310000
N	1.4726580000	0.2498160000	4.7791060000	C	5.7388520000	5.0744270000	0.0029620000
N	1.5250510000	-4.1963570000	2.4507350000	H	3.7861440000	5.5790700000	0.7157020000
N	1.4853400000	-4.8505870000	0.2989640000	C	5.9142180000	3.9734130000	-1.9899980000
N	1.6076140000	-2.4235590000	-4.1597330000	H	4.1081040000	3.5179040000	-3.0661930000
N	1.5528980000	-0.2422240000	-4.6968960000	H	6.2422630000	5.5107610000	0.8630160000
N	1.5410140000	4.2084960000	-2.3647910000	H	6.5627890000	3.5099800000	-2.7300460000
N	1.4706750000	4.8409420000	-0.2071090000	C	3.7918280000	-1.2483330000	-4.4270530000
H	1.8672020000	0.7447170000	-4.6044170000	C	4.4324460000	-0.1359590000	-4.9945530000

C	4.6034310000	-2.2511160000	-3.8755180000	H	3.4427610000	1.1762430000	-0.9742130000
C	5.8178730000	-0.0544140000	-4.9373940000	O	6.2847060000	1.8887250000	0.3964910000
H	3.8692530000	0.6732790000	-5.4401290000	H	6.7154230000	2.7570610000	0.3368330000
C	5.9807060000	-2.0607880000	-3.8581770000	H	6.4422180000	1.4692590000	-0.4860840000
H	4.1680900000	-3.1400480000	-3.4371300000	O	6.4280230000	0.3872700000	-1.7856950000
H	6.3271160000	0.8088030000	-5.3605700000	H	6.5508070000	-0.4980030000	-1.3611120000
H	6.6239730000	-2.8074540000	-3.3981060000	H	6.8602010000	0.3079180000	-2.6512290000
N	6.6004470000	-0.9784740000	-4.3584070000	C	-0.3777920000	-0.6766410000	-0.9678010000
N	6.5283250000	4.4896920000	-0.9115380000	H	-1.0242130000	-0.9939720000	-1.7997220000
N	6.5257430000	1.0265590000	4.4994440000	O	0.9481980000	-1.1586230000	-1.1752090000
N	6.5212400000	-4.3743040000	0.9974450000	H	0.9098560000	-2.1173900000	-1.2911990000
C	2.3312150000	-1.3337230000	-4.4080990000	Cyclopentanol-D@1:			
C	2.2571040000	-4.5009330000	1.3818430000	C	-5.5028890000	-3.0562760000	-2.3061280000
C	2.2513740000	1.3369240000	4.4633600000	C	-4.9689760000	-1.7370320000	-2.8481950000
C	2.2580450000	4.5074430000	-1.2837790000	C	-4.8845960000	-3.3500990000	-0.9463020000
C	-0.3697270000	0.8537370000	-0.8862940000	H	-5.1426270000	-3.8332880000	-2.9811510000
C	-1.0298580000	-1.1038650000	0.3530870000	C	-5.5572150000	-0.5022600000	-2.5588560000
C	-2.1937960000	-0.1121210000	0.4928720000	C	-3.8387530000	-1.7312640000	-3.6719390000
C	-1.6452110000	1.2238020000	-0.0846540000	C	-5.4304060000	-2.8428360000	0.2370980000
H	0.5365070000	1.1548720000	-0.3470180000	C	-3.7324820000	-4.1389760000	-0.8375120000
H	-0.3292310000	1.3217100000	-1.8731570000	C	-5.0764720000	0.7094720000	-3.0650880000
H	-1.3489740000	-2.1484280000	0.3564260000	H	-6.4335310000	-0.4841610000	-1.9213870000
H	-0.2981120000	-0.9697610000	1.1605190000	C	-3.3388840000	-0.5505720000	-4.2064430000
H	-3.0477700000	-0.4571860000	-0.1011740000	O	-3.2607520000	-2.9472090000	-4.0264210000
H	-2.5458860000	-0.0141810000	1.5221340000	C	-4.8915610000	-3.0991620000	1.4997680000
H	-2.3923380000	1.7088100000	-0.7160560000	H	-6.3193580000	-2.2264050000	0.1709080000
H	-1.4089660000	1.9299050000	0.7153740000	C	-3.1711410000	-4.4204990000	0.4022160000
O	3.6537790000	-1.8390830000	-0.6547280000	O	-3.1779900000	-4.7248930000	-1.9753040000
H	3.4039230000	-1.1927910000	0.9858240000	C	-5.7384740000	2.0467350000	-2.7604850000
H	4.6322210000	-1.9086880000	-0.6507470000	C	-3.9449070000	0.6586440000	-3.8885290000
O	3.5039180000	-0.6821830000	1.8281040000	H	-2.5107370000	-0.5726980000	-4.8986940000
H	3.3633260000	0.9919130000	1.2012670000	C	-2.0281660000	-3.2501800000	-3.4831670000
H	4.4717490000	-0.6483910000	1.9869830000	C	-5.5072160000	-2.5611390000	2.7845270000
O	6.4380590000	-1.7952830000	-0.2868990000	C	-3.7391550000	-3.8896500000	1.5532910000
H	6.4948830000	-1.3632510000	0.6016500000	H	-2.3148210000	-5.0752700000	0.4674030000
H	6.8525350000	-2.6667480000	-0.1670570000	C	-1.9778010000	-4.1992870000	-2.4269860000
O	6.2896350000	-0.2972180000	1.9007650000	H	-5.4519970000	2.7195560000	-3.5693450000
H	6.7323030000	-0.2089170000	2.7605440000	C	-5.1651620000	2.6474340000	-1.4833220000
H	6.3856340000	0.5920120000	1.4759650000	O	-3.4793480000	1.8281670000	-4.4786620000
O	3.6209360000	0.6858230000	-1.8110250000	C	-4.9750370000	-1.1679910000	3.0933880000
H	4.5955840000	0.6852050000	-1.9141630000	H	-5.1505650000	-3.2075350000	3.5872440000
H	3.4351230000	-1.0186350000	-1.1588100000	O	-3.2004980000	-4.2095380000	2.7970210000
O	3.4881540000	1.8369520000	0.7035920000	C	-5.6649120000	2.3250590000	-0.2200970000
H	4.4585230000	1.9835520000	0.6892850000				

C	-4.1073190000	3.5623420000	-1.5393210000	H	-7.4952530000	-2.0127340000	1.9993010000
C	-2.2917590000	2.3681750000	-4.0147740000	H	-7.4338470000	-2.2802980000	3.7411860000
C	0.3375250000	-3.1156640000	-3.4594470000	H	-7.3662890000	-4.1058600000	-1.9472120000
C	-5.5719390000	-0.0125300000	2.5783780000	H	-7.6376530000	1.5794790000	-3.6987790000
C	-3.8613250000	-0.9995460000	3.9263010000	H	-7.7346750000	3.3858690000	1.9294150000
C	-2.0032090000	-3.6097460000	3.1334730000	C	-1.1856470000	2.6546560000	4.1120360000
C	0.4118750000	-4.0780910000	-2.4234110000	H	-1.1796020000	1.9569670000	4.9381510000
C	-5.1786580000	2.8859000000	0.9636130000	C	-1.2374530000	4.5942780000	2.0049500000
H	-6.4805270000	1.6144300000	-0.1550930000	H	-1.2551470000	5.3206540000	1.2030800000
C	-3.5908080000	4.1408610000	-0.3830460000	C	-0.8553260000	-1.9237940000	4.4885770000
O	-3.6287460000	3.9606380000	-2.7877440000	H	-0.8858520000	-1.1207260000	5.2140870000
C	-2.3780490000	3.5027910000	-3.1599940000	C	-0.8069000000	-4.1257720000	2.6580760000
C	-5.1225070000	1.2766740000	2.8741850000	H	-0.7948910000	-4.9904140000	2.0082350000
H	-6.4309540000	-0.1231230000	1.9268530000	C	-0.7661550000	-4.6361410000	-1.9064650000
C	-3.3958290000	0.2679790000	4.2559810000	H	-0.7402520000	-5.3967140000	-1.1363150000
O	-3.2634640000	-2.1093820000	4.5203100000	C	-0.8705060000	-2.7009110000	-4.0149230000
C	-2.0294990000	-2.5128050000	4.0361320000	H	-0.9132260000	-2.0118880000	-4.8474400000
C	-5.7786530000	2.5332610000	2.3183210000	C	-1.0664550000	1.8677930000	-4.4359950000
C	-4.1162850000	3.7936740000	0.8587250000	H	-1.0162900000	1.0190160000	-5.1054540000
H	-2.8012710000	4.8763810000	-0.4478940000	C	-1.2417570000	4.1804210000	-2.7499940000
C	0.0948080000	2.5087010000	-3.9804260000	H	-1.2992350000	5.0520620000	-2.1124370000
C	-4.0146390000	1.3905580000	3.7197670000	N	1.4343600000	2.2107730000	-4.1658600000
H	-2.5815900000	0.3721690000	4.9574630000	N	1.2642890000	4.0697820000	-2.9181350000
C	0.3635370000	-3.5109990000	3.0962700000	N	1.2797760000	4.4706840000	2.2064950000
H	-5.5075580000	3.3452140000	2.9935760000	N	1.3159870000	2.9195110000	3.8356090000
O	-3.6432660000	4.4345250000	2.0051790000	N	1.6694280000	-2.0602520000	4.2846240000
C	-0.0204790000	3.6634640000	-3.1732360000	N	1.6859910000	-3.7952690000	2.8532370000
O	-3.5846490000	2.6624410000	4.0854950000	N	1.7413890000	-4.3192860000	-2.1159240000
C	0.3621530000	-2.4246200000	4.0043520000	N	1.6381870000	-2.7998160000	-3.7726040000
C	-2.4093990000	4.0408050000	2.5006410000	H	2.0314320000	-4.3063310000	2.0191940000
C	-2.3819600000	3.0973640000	3.5639020000	H	1.9302370000	-1.9200430000	-4.2399940000
C	-0.0233360000	4.1439410000	2.5412310000	H	1.4699480000	4.6746800000	-2.1119210000
C	-0.0120800000	3.1668880000	3.5650040000	H	1.6916310000	2.0604240000	4.2824960000
C	-7.3110310000	2.4444110000	2.2894230000	O	2.8118750000	-4.5748190000	0.4915500000
H	-7.6936740000	2.2520160000	3.2955480000	H	2.3230310000	-4.6753750000	-0.3584580000
H	-7.6827490000	1.6475110000	1.6393620000	H	3.1425810000	-3.6496450000	0.4565030000
C	-7.2715220000	1.9659770000	-2.7436630000	O	2.6314130000	-0.3428520000	-4.4439020000
H	-7.6966620000	2.9605330000	-2.5839490000	H	2.0969970000	0.4866070000	-4.4723170000
H	-7.6583870000	1.3142430000	-1.9553600000	H	3.0049300000	-0.3576310000	-3.5355720000
C	-7.0363700000	-3.1231320000	-2.2948630000	O	0.9579540000	4.9744690000	-0.4508780000
H	-7.4258070000	-2.9613840000	-3.3037100000	H	0.6908590000	4.0316740000	-0.3743500000
H	-7.4937430000	-2.3739450000	-1.6427570000	H	1.2877680000	5.1495530000	0.4545610000
C	-7.0411420000	-2.6272390000	2.7815490000	O	2.5930320000	0.5948390000	4.4932350000
H	-7.3708010000	-3.6574250000	2.6216100000	H	2.1574890000	-0.2806550000	4.6178520000

H	2.9407770000	0.5372180000	3.5763300000	C	2.4413640000	-3.5406120000	-2.9386090000
C	3.5003060000	3.6611700000	2.9245340000	C	-1.3356030000	1.2830430000	0.2242210000
C	4.2539850000	3.2058730000	4.0143510000	C	0.1640580000	-0.1582630000	-0.9890980000
C	4.1862860000	4.0514450000	1.7652720000	C	-0.9169790000	-1.0784700000	-0.3998820000
C	5.6362580000	3.1399500000	3.8880530000	C	-2.0094970000	-0.1122610000	0.1419110000
H	3.7755450000	2.8842060000	4.9306400000	H	-1.5188640000	1.7916910000	1.1714170000
C	5.5706030000	3.9363250000	1.7425790000	H	-1.7004790000	1.9381150000	-0.5725750000
H	3.6320890000	4.3874210000	0.8969550000	H	-0.1334200000	0.2029150000	-1.9812750000
H	6.2411040000	2.7817010000	4.7181560000	H	1.1434520000	-0.6379630000	-1.0870890000
H	6.1243440000	4.1990660000	0.8444070000	H	-1.3091640000	-1.7871970000	-1.1310360000
C	3.5494810000	3.2581280000	-3.3628880000	H	-0.4966520000	-1.6707410000	0.4217920000
C	4.1271950000	4.2998850000	-2.6175490000	H	-2.8742340000	-0.0817620000	-0.5276000000
C	4.4170370000	2.3289340000	-3.9574760000	H	-2.3812260000	-0.4437630000	1.1159210000
C	5.5081450000	4.3474160000	-2.4804950000	O	3.7034650000	0.3962160000	1.9221770000
H	3.5196940000	5.0561730000	-2.1348480000	H	3.5263600000	1.3142530000	0.4797540000
C	5.7839160000	2.4662270000	-3.7501820000	H	4.6710980000	0.5406470000	2.0252620000
H	4.0280990000	1.4984800000	-4.5341370000	O	3.5155410000	1.6775670000	-0.4429020000
H	5.9699510000	5.1409740000	-1.8968460000	H	3.5968930000	0.2850040000	-1.4168490000
H	6.4714500000	1.7397260000	-4.1773950000	H	4.4275530000	1.9880610000	-0.6098780000
C	3.8999610000	-3.4819520000	-3.0394790000	O	6.4423060000	0.8219510000	1.7093490000
C	4.5161450000	-2.8442110000	-4.1277070000	H	6.4810850000	1.2719290000	0.8256380000
C	4.7335960000	-4.0510030000	-2.0647590000	H	6.8217020000	1.4773520000	2.3185970000
C	5.9020140000	-2.7553730000	-4.1598300000	O	6.3212880000	1.7204770000	-0.7732890000
H	3.9353190000	-2.3874980000	-4.9184980000	H	6.7362500000	2.4220060000	-1.3062880000
C	6.1090210000	-3.8932800000	-2.1896090000	H	6.5003740000	0.8808080000	-1.2624940000
H	4.3165990000	-4.5670060000	-1.2089070000	O	3.8156000000	-1.9563970000	0.5006660000
H	6.3932420000	-2.2473860000	-4.9867920000	H	4.7882230000	-2.0285060000	0.6166830000
H	6.7705010000	-4.2914890000	-1.4234380000	H	3.6221330000	-0.5117050000	1.5390390000
C	3.8920430000	-2.9408970000	3.5719730000	O	3.7438630000	-0.5837880000	-1.8739790000
C	4.5695130000	-4.0390880000	3.0190780000	H	4.7162910000	-0.6581610000	-1.9834070000
C	4.6692460000	-1.8993180000	4.1012910000	H	3.6926930000	-1.5731540000	-0.4029680000
C	5.9576500000	-4.0192010000	2.9697410000	O	6.5446850000	-0.7711280000	-1.6866690000
H	4.0348870000	-4.8806840000	2.5985050000	H	6.9737890000	-1.3300750000	-2.3563480000
C	6.0529130000	-1.9766240000	3.9878340000	H	6.6870050000	-1.2404990000	-0.8288540000
H	4.2029340000	-1.0321390000	4.5522870000	O	6.5903880000	-1.6764570000	0.8226870000
H	6.4955920000	-4.8556060000	2.5288320000	H	6.6629410000	-0.8109060000	1.2957130000
H	6.6714940000	-1.1609570000	4.3551720000	H	7.0267590000	-2.3153710000	1.4100450000
N	6.7093910000	-3.0008270000	3.4163210000	C	0.1574780000	1.0403000000	-0.0284790000
N	6.7071610000	-3.2409600000	-3.2014420000	H	0.6552880000	0.7550200000	0.9129790000
N	6.3438650000	3.4424580000	-3.0144520000	O	0.7735320000	2.2193110000	-0.5497710000
N	6.3025300000	3.4771060000	2.7730910000	H	1.7376150000	2.0810810000	-0.6021440000
C	2.4292430000	-2.8957120000	3.5793920000				
C	2.0428910000	3.7057090000	2.9734020000				
C	2.1005820000	3.1506210000	-3.4962900000				

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