

Supplementary Materials

Recognition of Hydrophilic Cyclic Compounds by a Water-soluble Cavitand

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Content

¹ H NMR, ¹³ C NMR spectra of the cavitands.....	1
Mass (HR) spectra of cavitands.....	5
¹ H NMR spectra of the host-guest complex formed between cavitand 1 with different guests.....	8

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

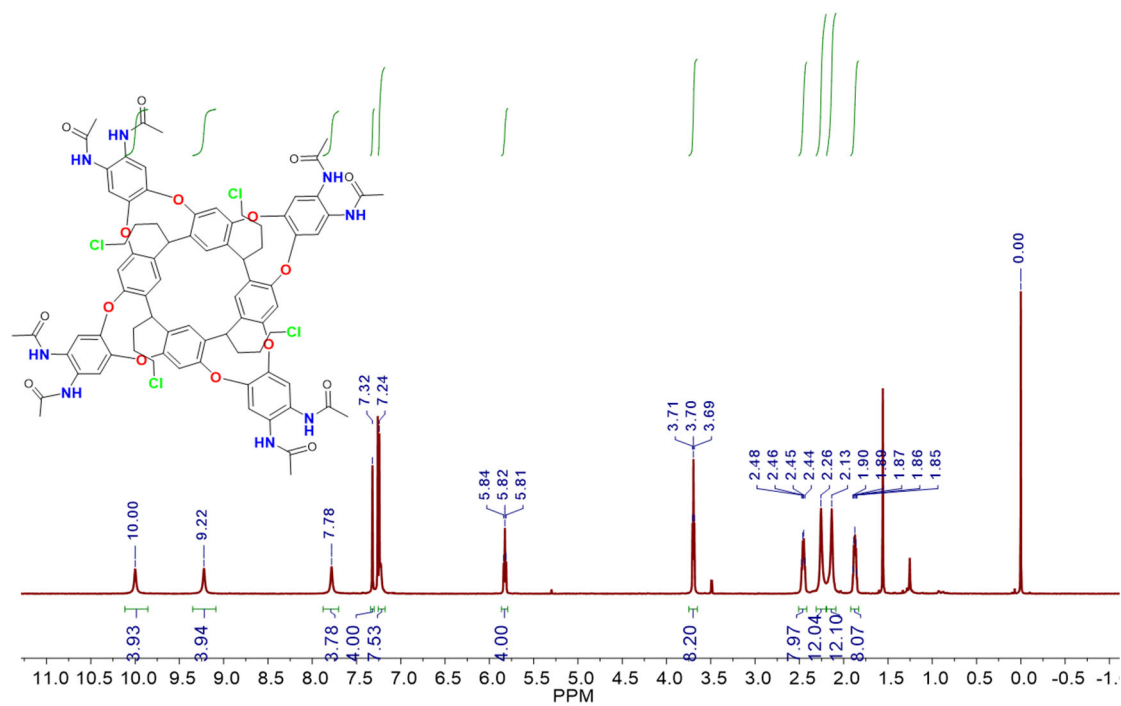


Fig. S1 ^1H NMR spectrum of cavitand 3 in chloroform- d at rt

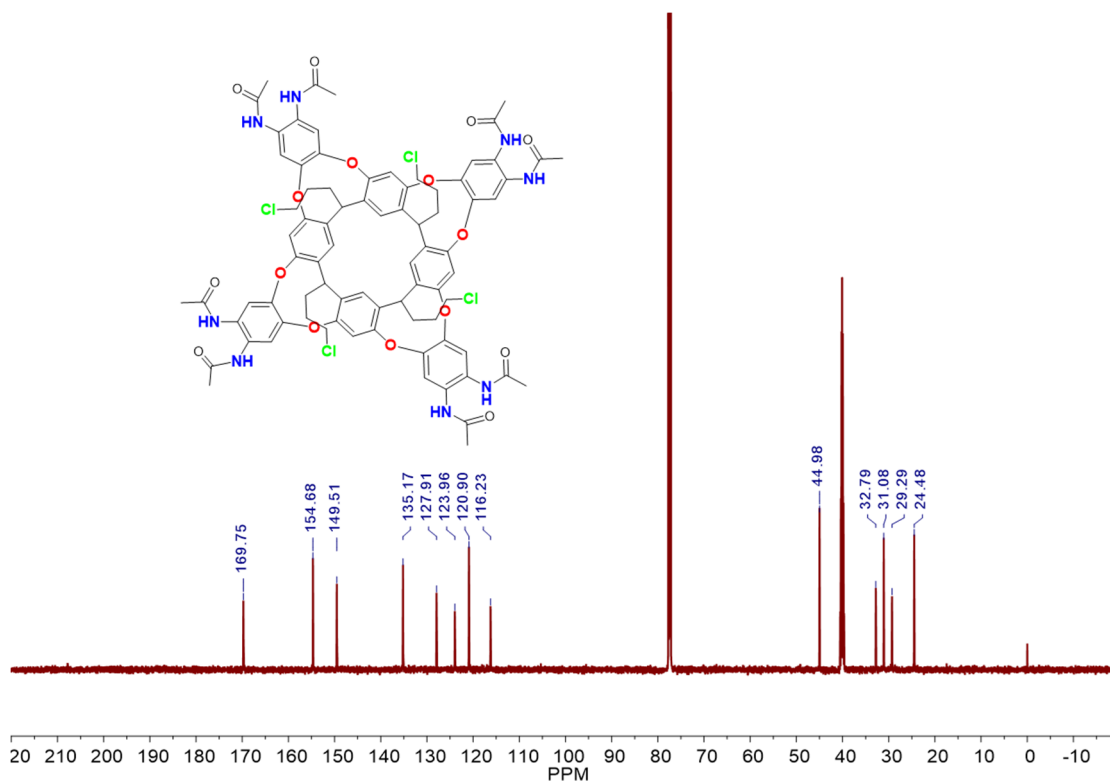


Fig. S2 ^{13}C NMR spectrum of cavitand 3 in chloroform- d /DMSO- d_6 (vol/vol = 9:1) at rt

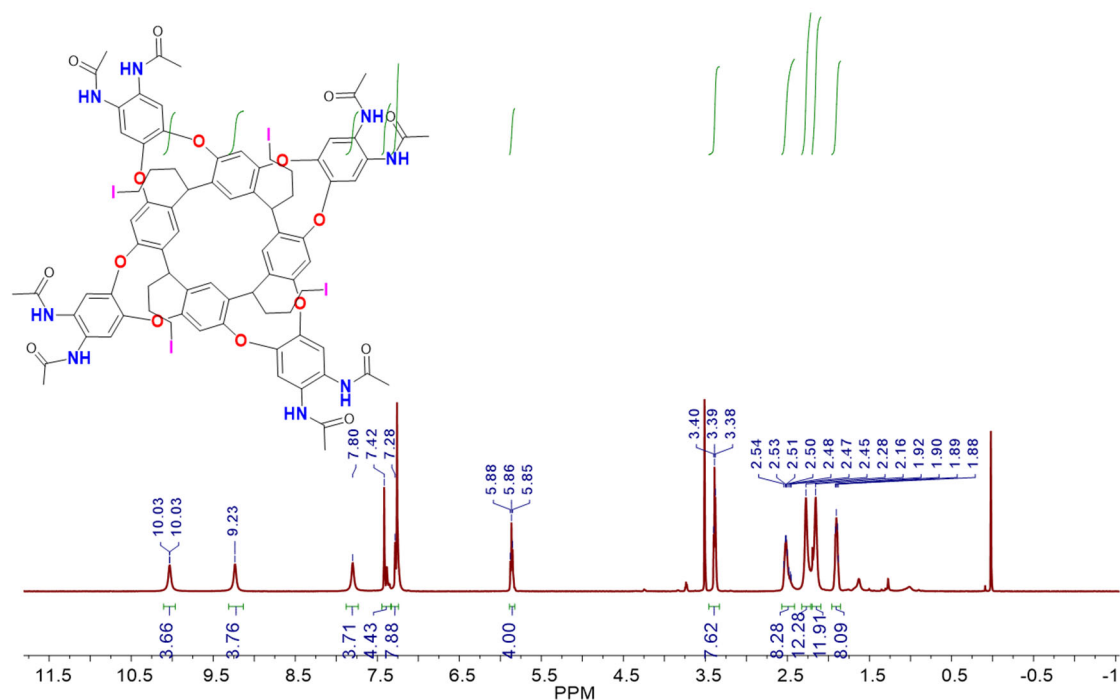


Fig. S3 ^1H NMR spectrum of cavitand 2 in chloroform- d at rt

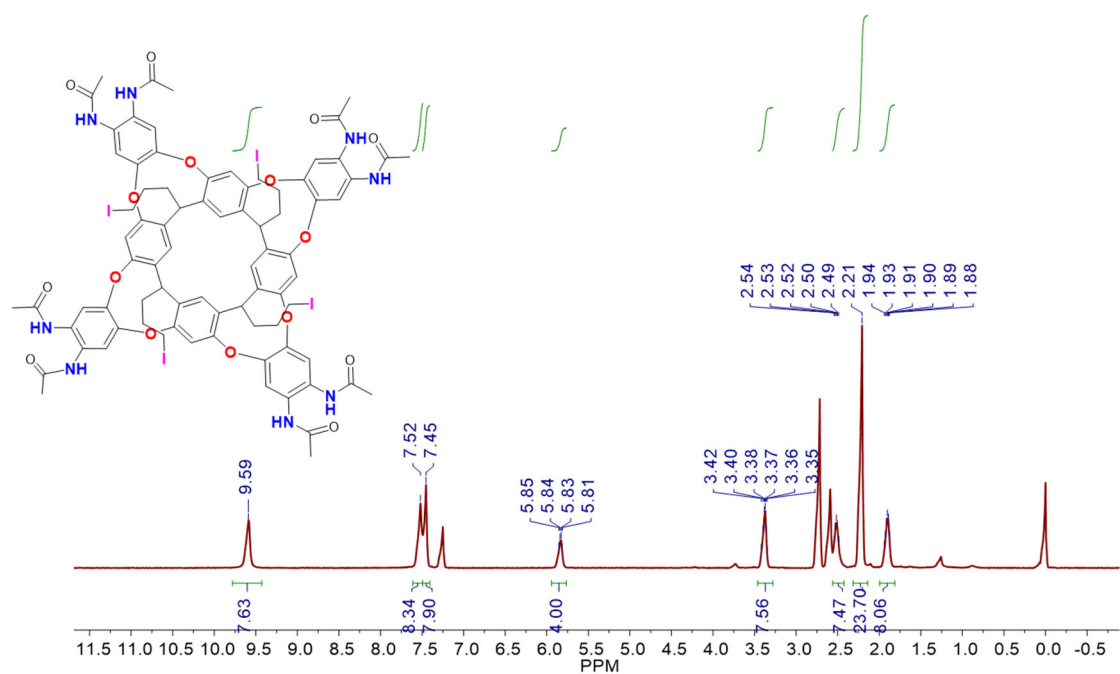


Fig. S4 ^1H NMR spectrum of cavitand 2 in chloroform- d /DMSO- d_6 (vol/vol = 9:1) at rt

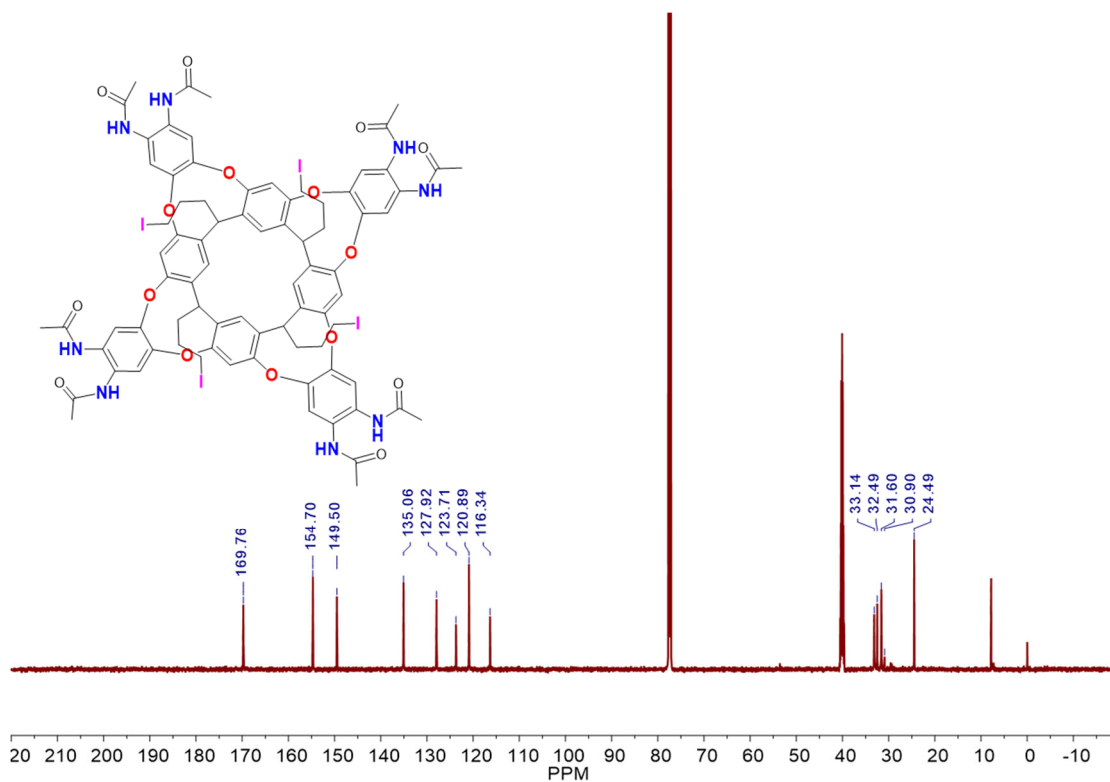


Fig. S5 ¹³C NMR spectrum of cavitand 2 in chloroform-*d*/DMSO-*d*₆ (vol/vol = 9:1) at rt

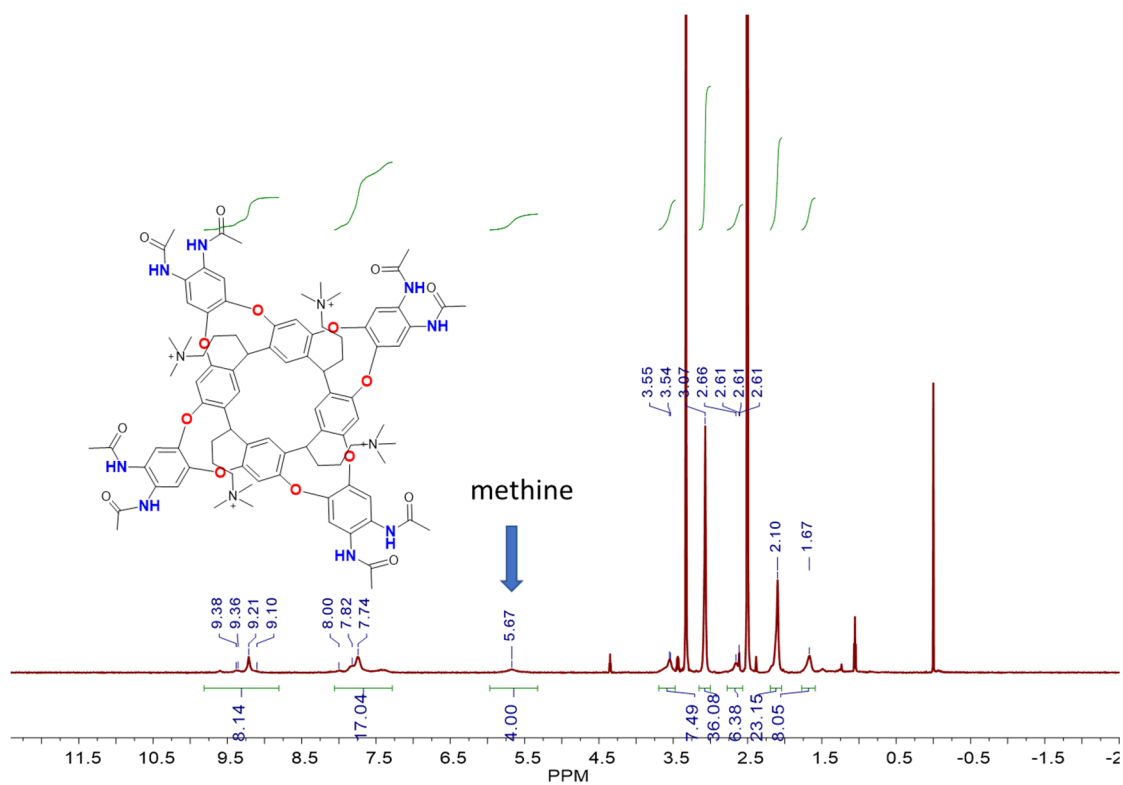


Fig. S6 ¹H NMR spectrum of cavitand 1 in DMSO-*d*₆ at rt, the cavitand display vase form exclusively

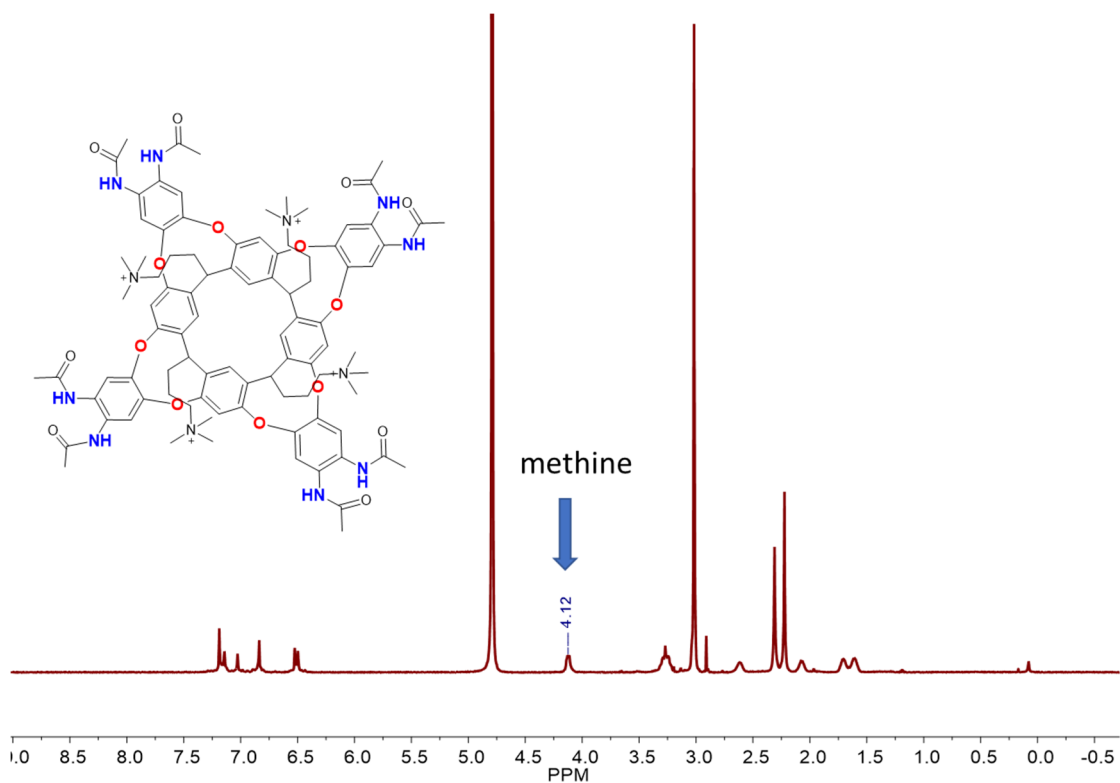


Fig. S7 ^1H NMR spectrum of cavitand **1** in D_2O at rt, the cavitand display kite form exclusively

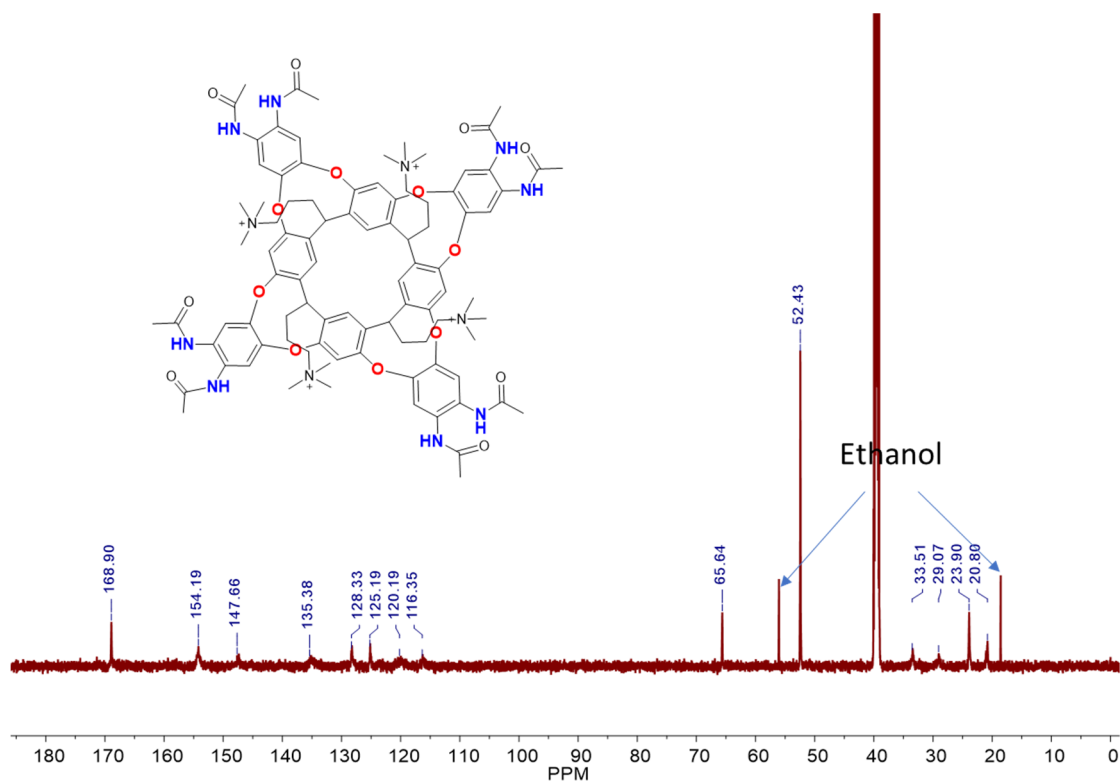


Fig. S8 ^{13}C NMR spectrum of cavitand **1** in $\text{DMSO}-d_6$ at rt

Mass (HR) spectra of cavitands

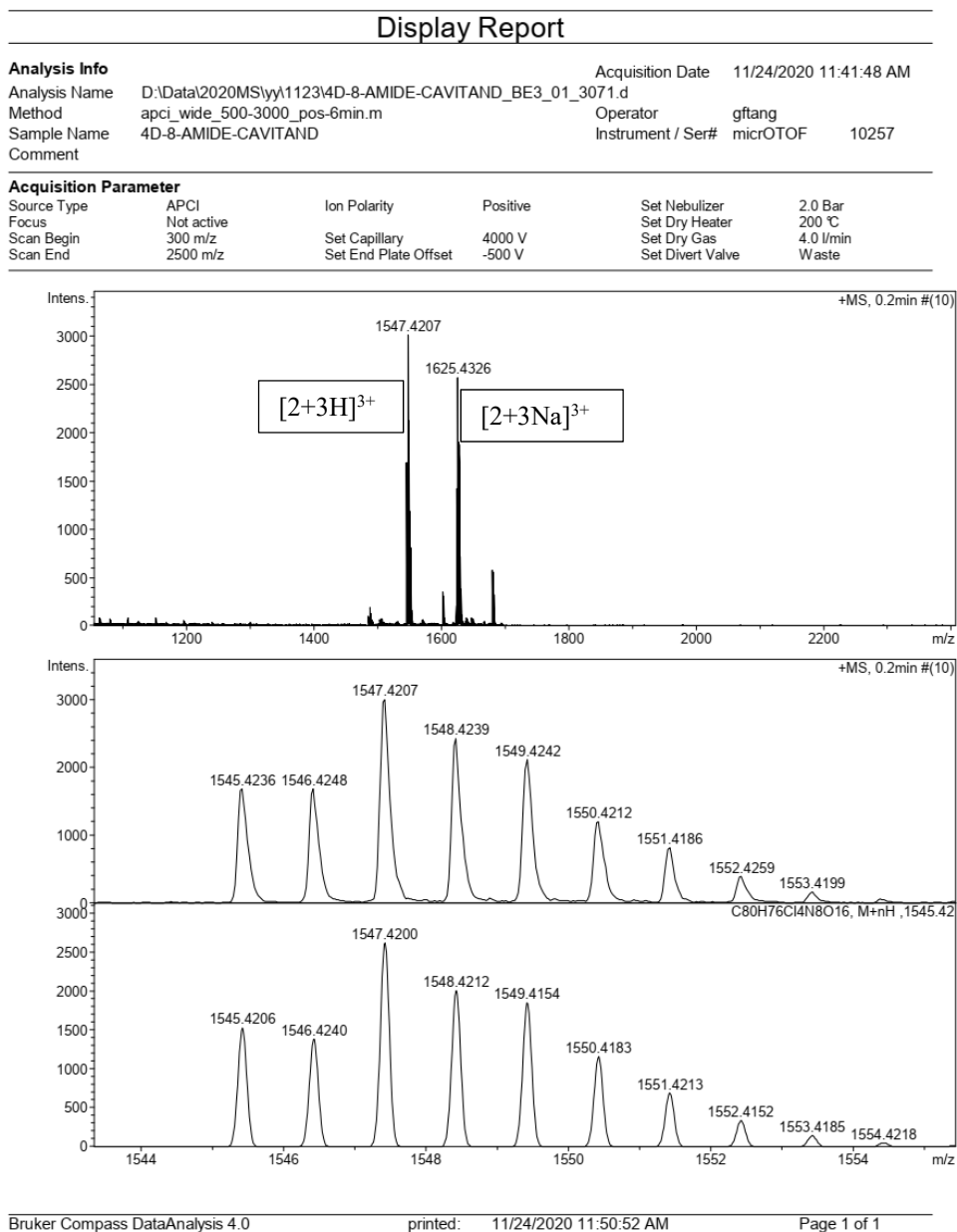


Fig. S9 Mass spectrum of cavitand 2

Display Report

Analysis Info

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Method tune_wide_500-3000_pos-6min.m
Sample Name 151
Comment

Acquisition Date 8/5/2020 9:37:35 AM

Operator gftang
Instrument / Ser# micrOTOF 10257

Acquisition Parameter

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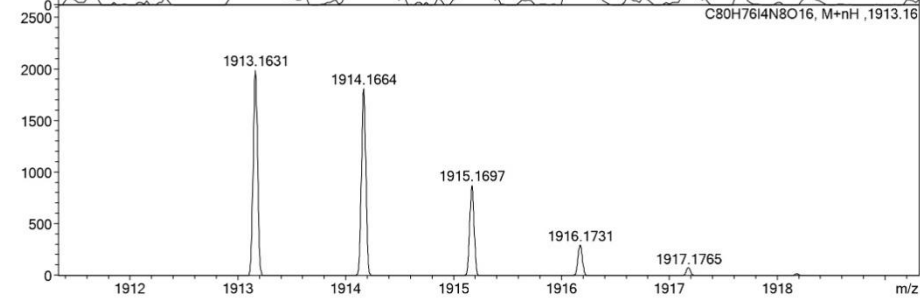
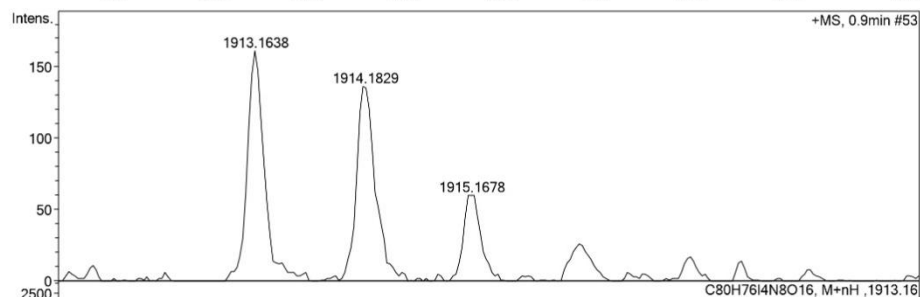
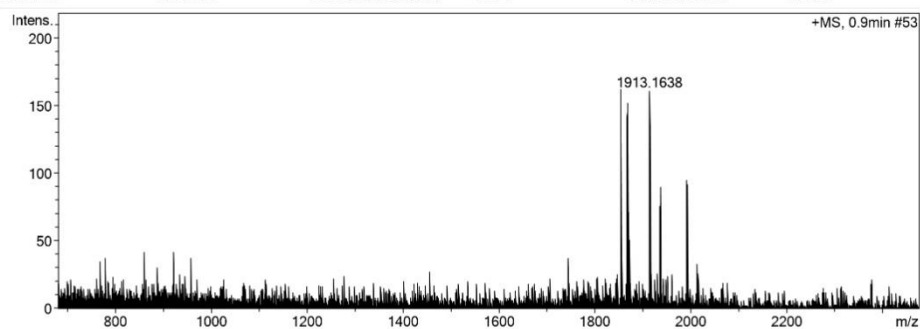


Fig. S10 Mass spectrum of cavitand 3

Display Report

Analysis Info

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Method tune_wide_500-3000_pos-6min.m
Sample Name 156
Comment

Acquisition Date 8/5/2020 9:23:29 AM

Operator gftang
Instrument / Ser# micrOTOF 10257

Acquisition Parameter

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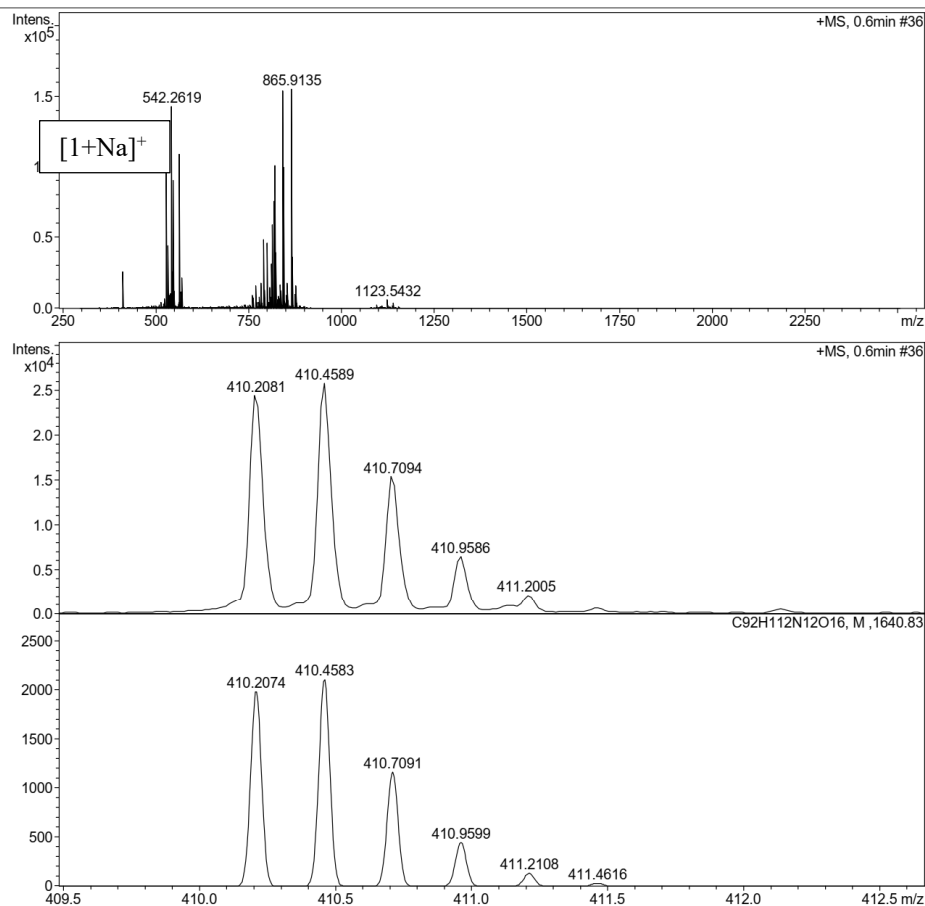


Fig. S11 Mass spectrum of cavitand 1

^1H NMR spectra of the host-guest complex formed between cavitand **1** with different guests

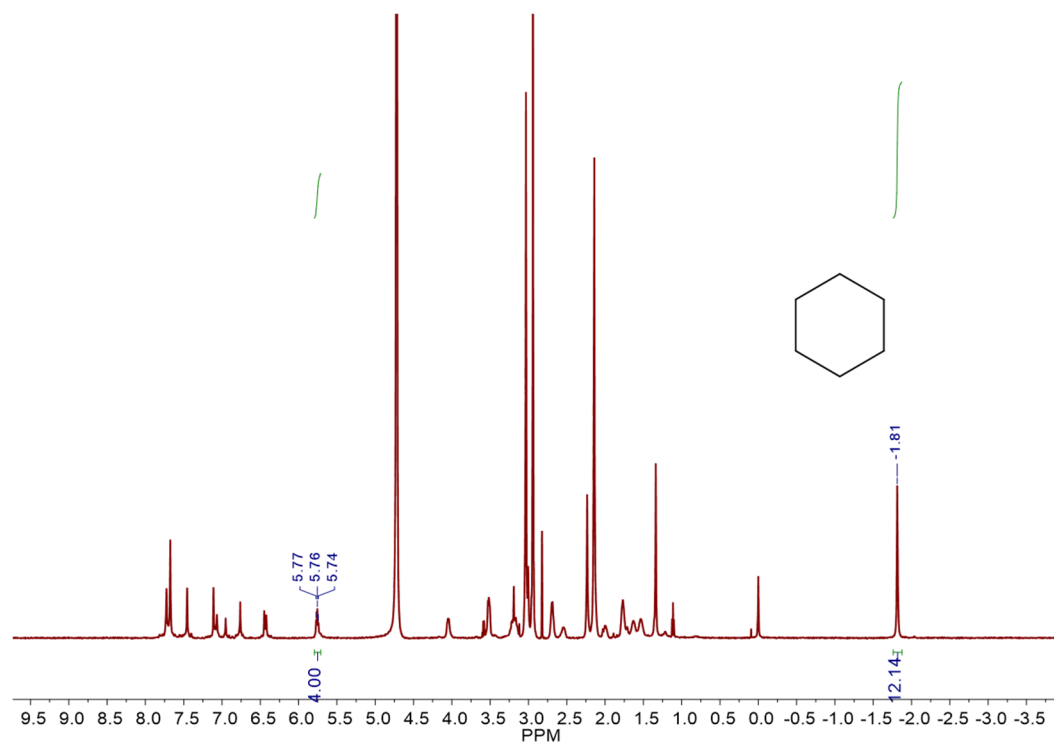


Fig. S12 ^1H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexane in D_2O

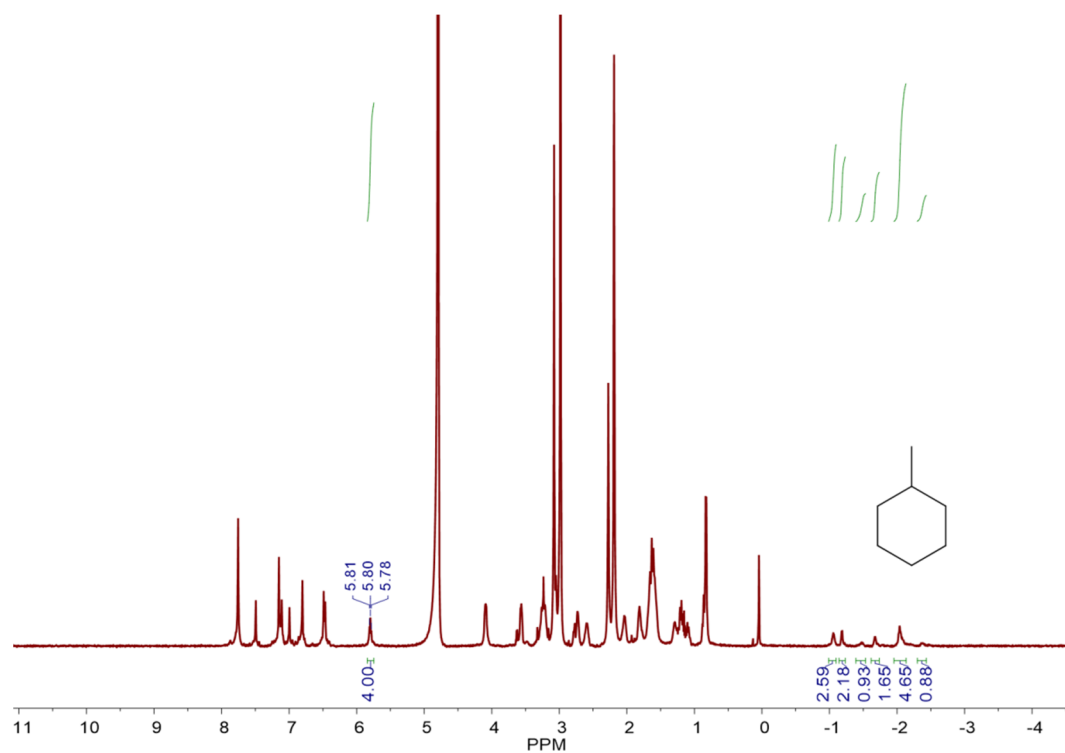


Fig. S13 ^1H NMR spectrum of the complex formed between cavitand **1** and excess of methylcyclohexane

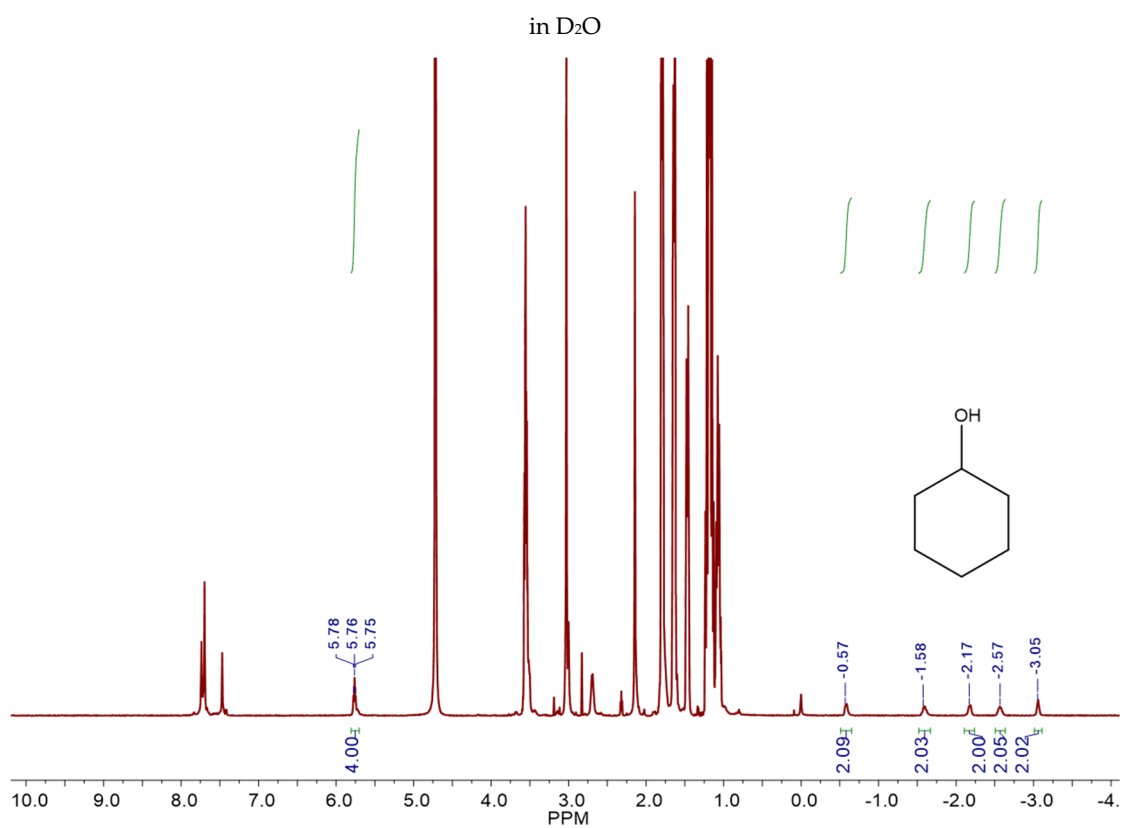


Fig. S14 ¹H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexanol in

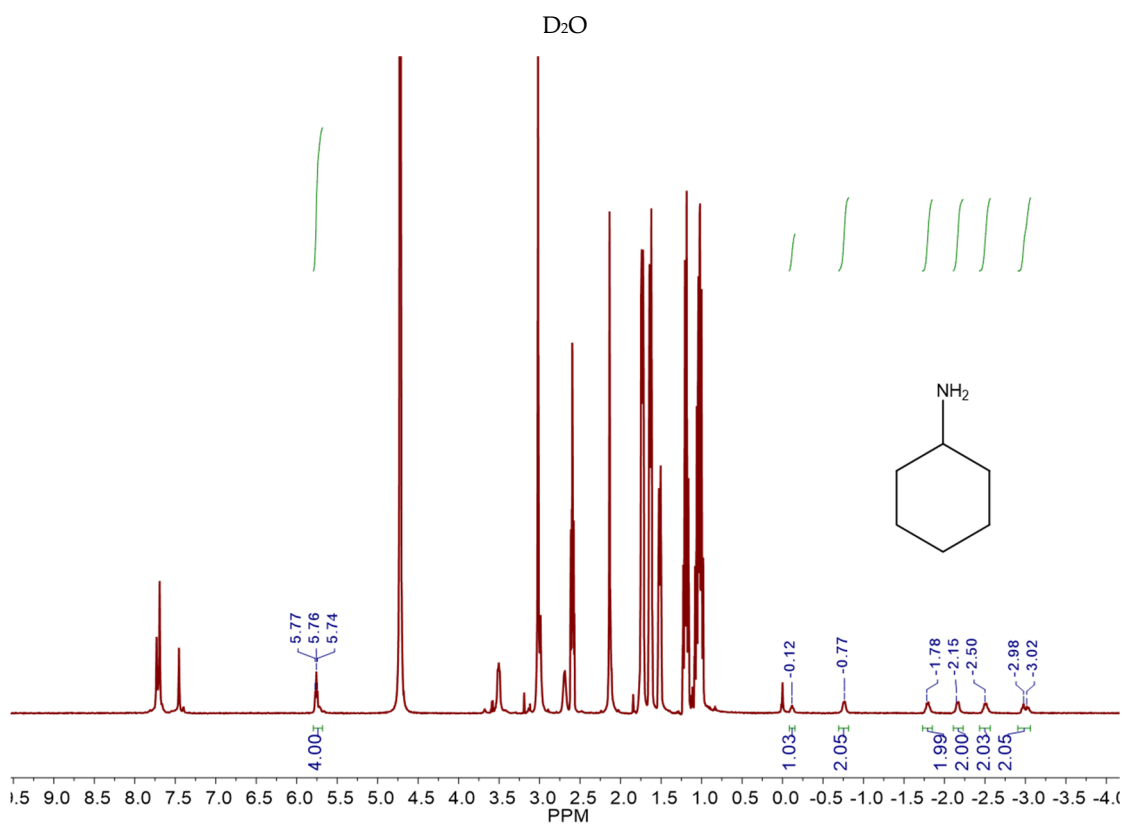


Fig. S15 ¹H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexylamine in

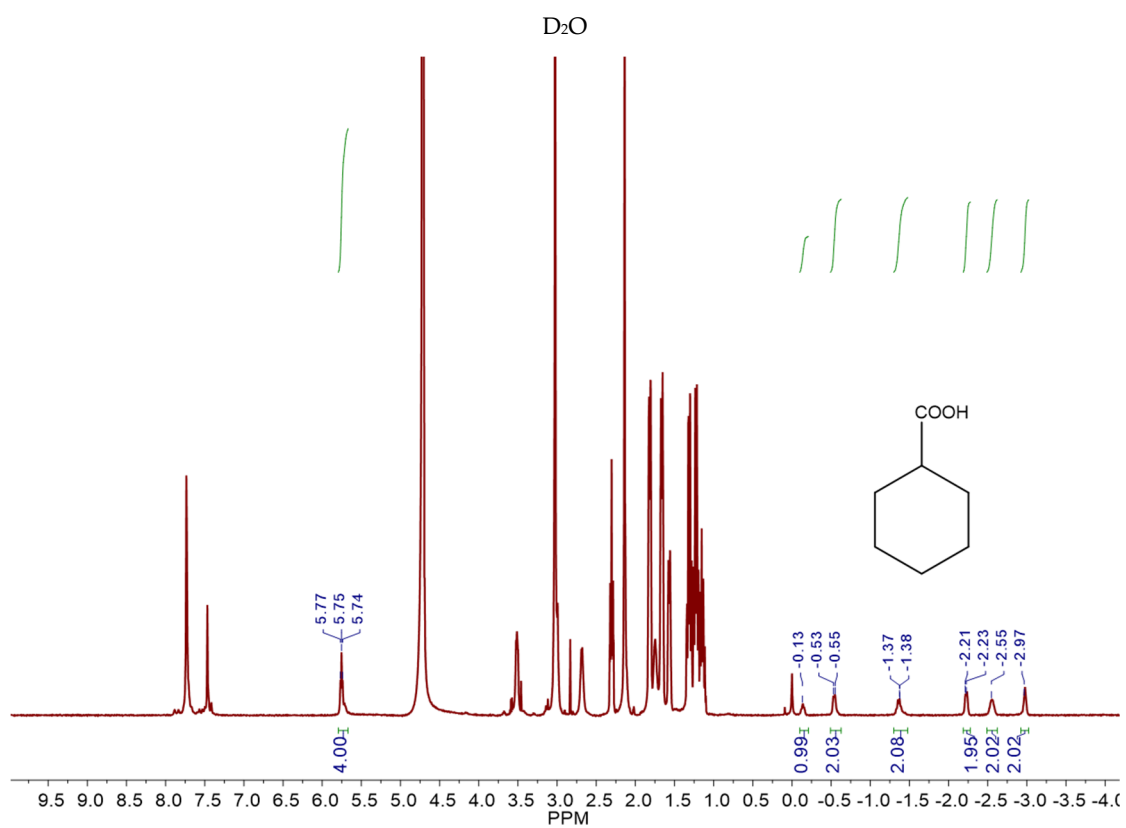


Fig. S16 ¹H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexanecarboxylic acid in D₂O

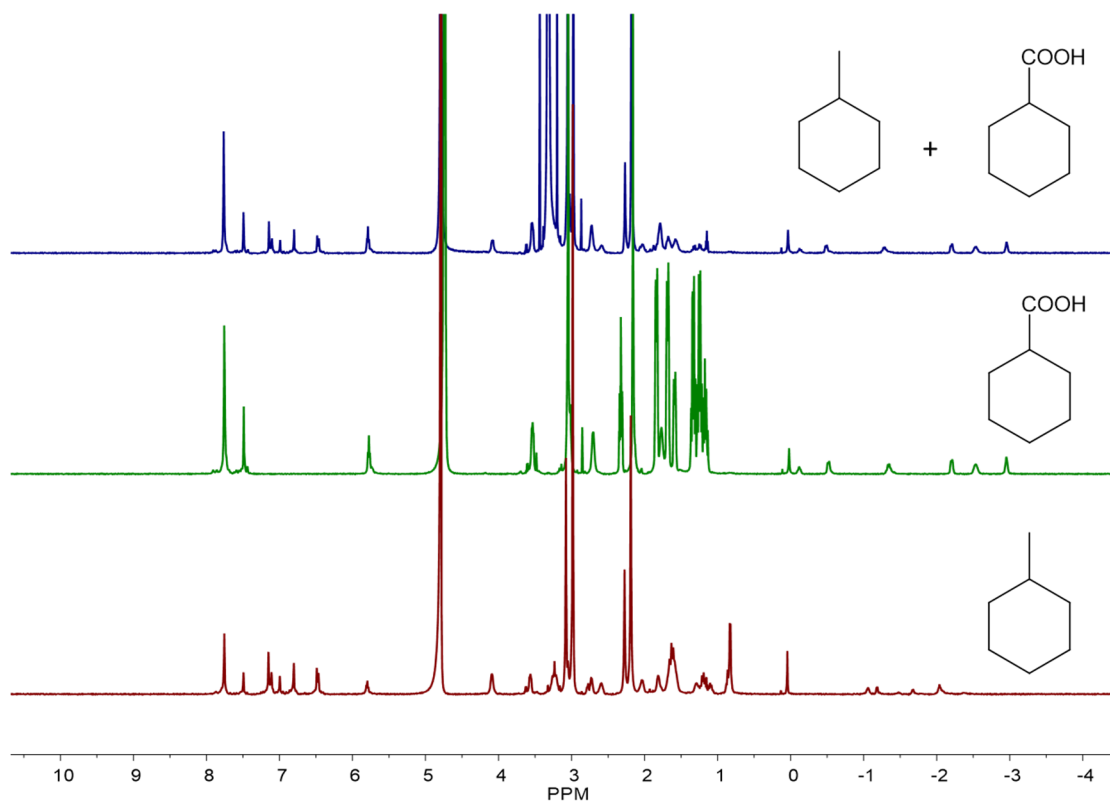


Fig. S17 ^1H NMR spectra of the complexes formed between cavitand **1**, 1mmol + from bottom to top, excess of methylcyclohexane, cyclohexanecarboxylic acid, and equimolar methylcyclohexane + cyclohexanecarboxylic acid (1:1) mixture.

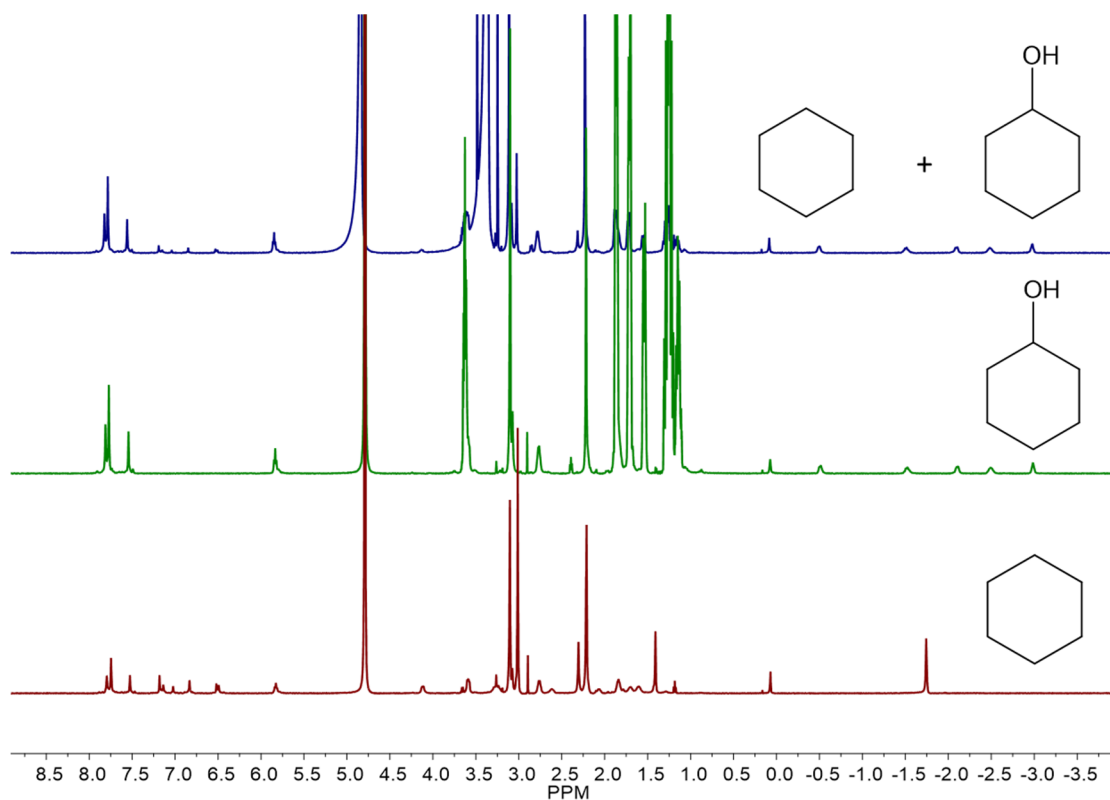


Fig. S18 ^1H NMR spectra of the complexes formed between cavitand **1**, 1mmol + from bottom to top, excess of cyclohexane, cyclohexanol, and equimolar cyclohexane + cyclohexanol (1:1) mixture.

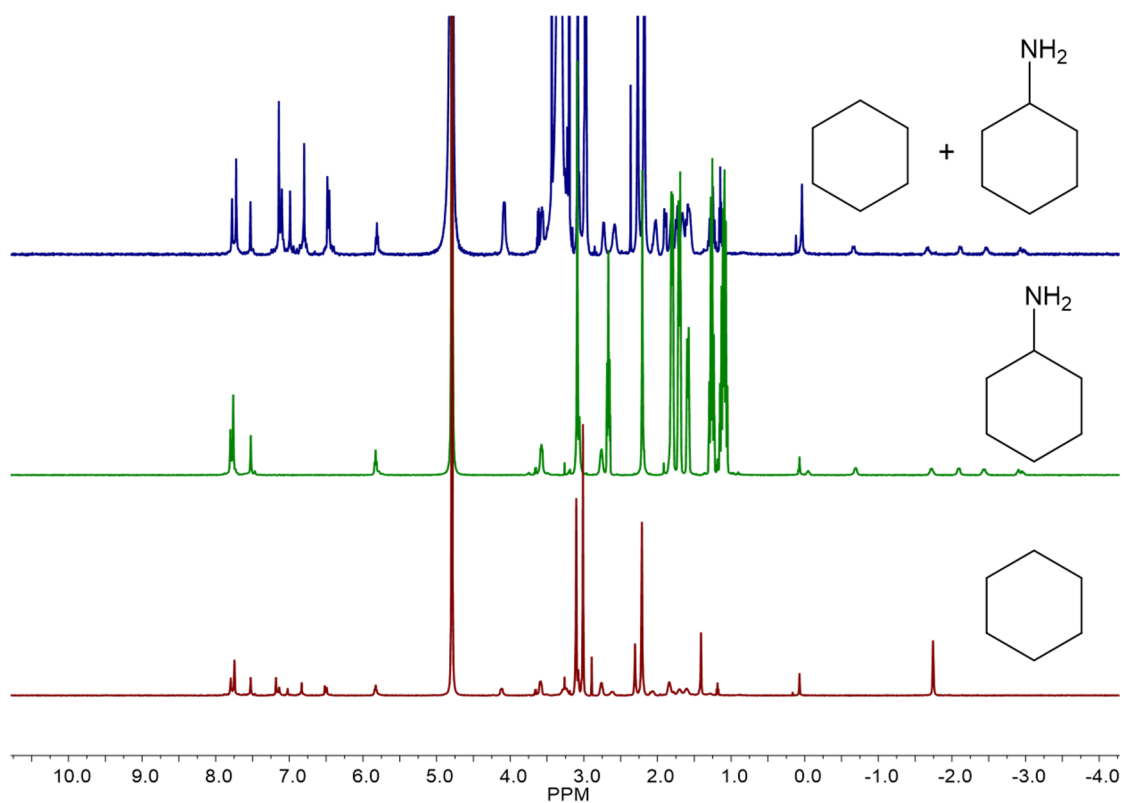


Fig. S19 ^1H NMR spectra of the complexes formed between cavitand **1**, 1mmol + from bottom to top, excess of cyclohexane, cyclohexylamine, and equimolar cyclohexane + cyclohexylamine (1:1) mixture

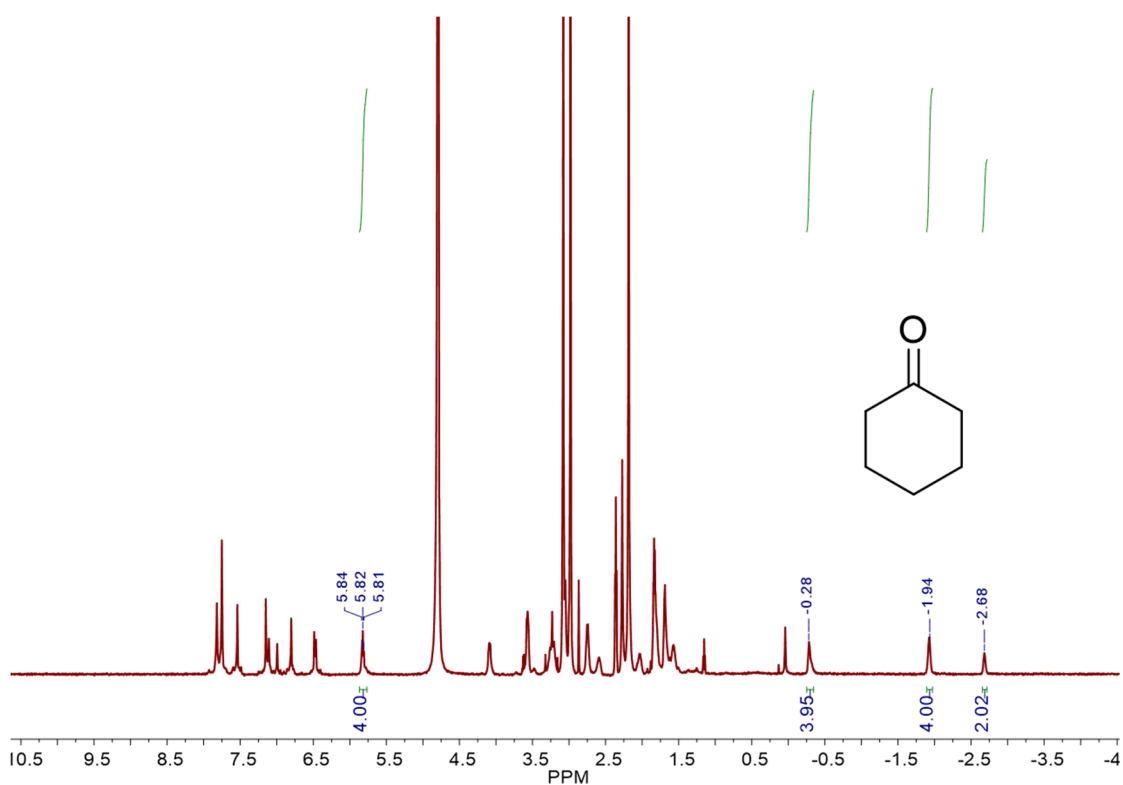


Fig. S20 ^1H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexanone in D_2O

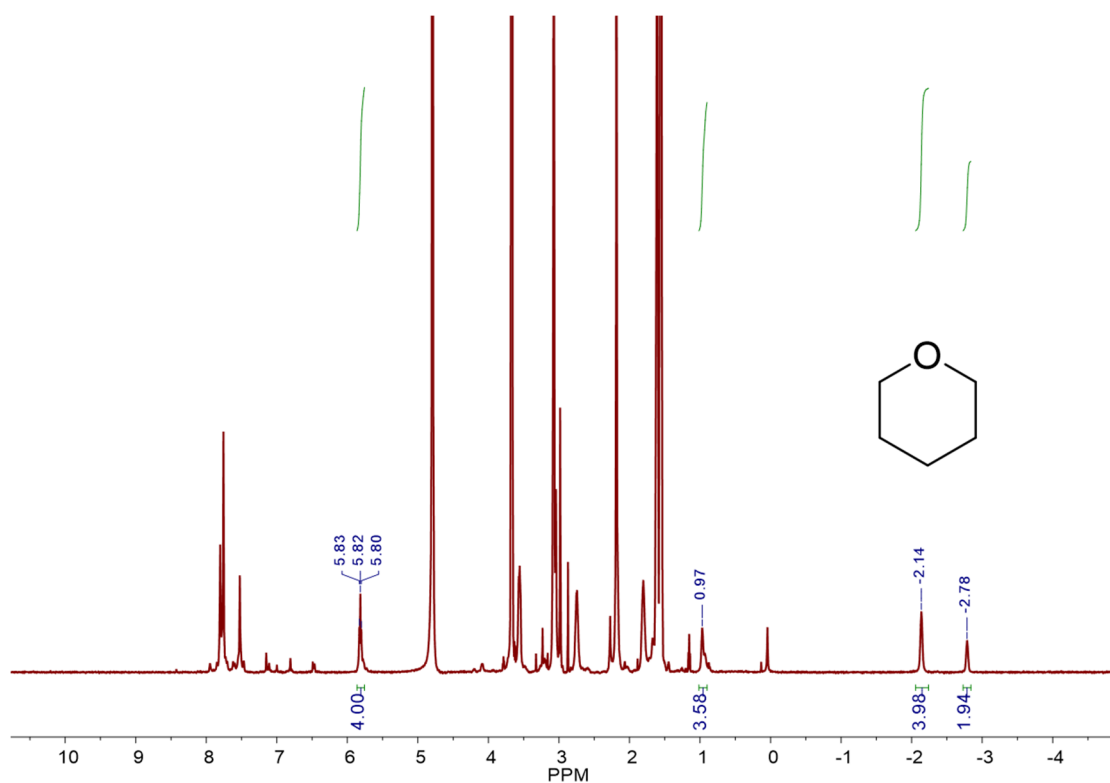


Fig. S21 ^1H NMR spectrum of the complex formed between cavitand 1 and excess of tetrahydropyran in D_2O

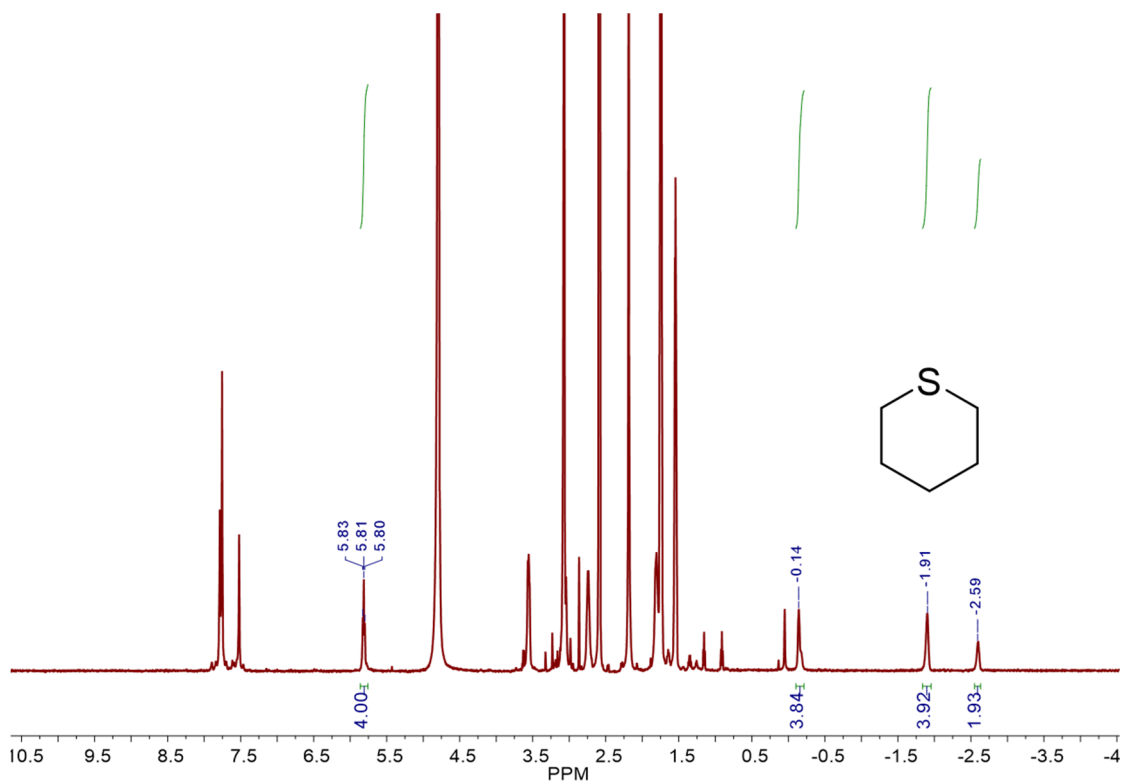


Fig. S22 ^1H NMR spectrum of the complex formed between cavitand 1 and excess of thiane in D_2O

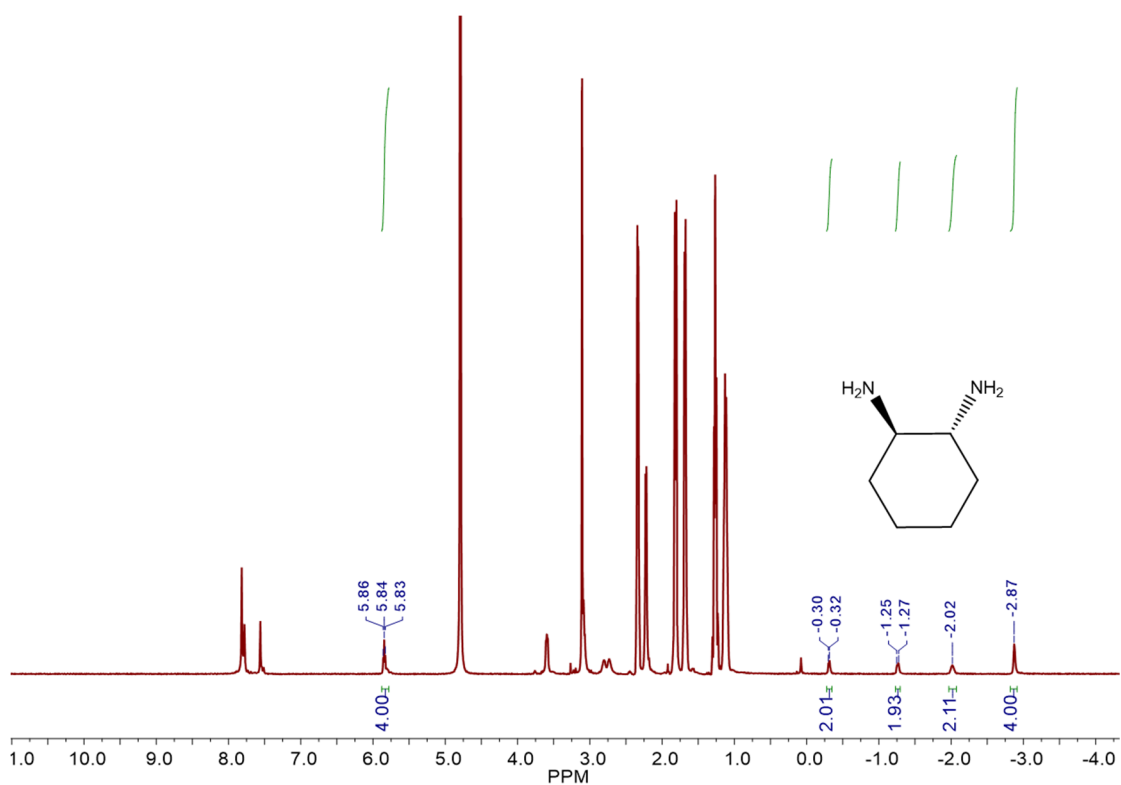


Fig. S23 ^1H NMR spectrum of the complex formed between cavitand **1** and excess of trans-1,2-diaminocyclohexane in D_2O

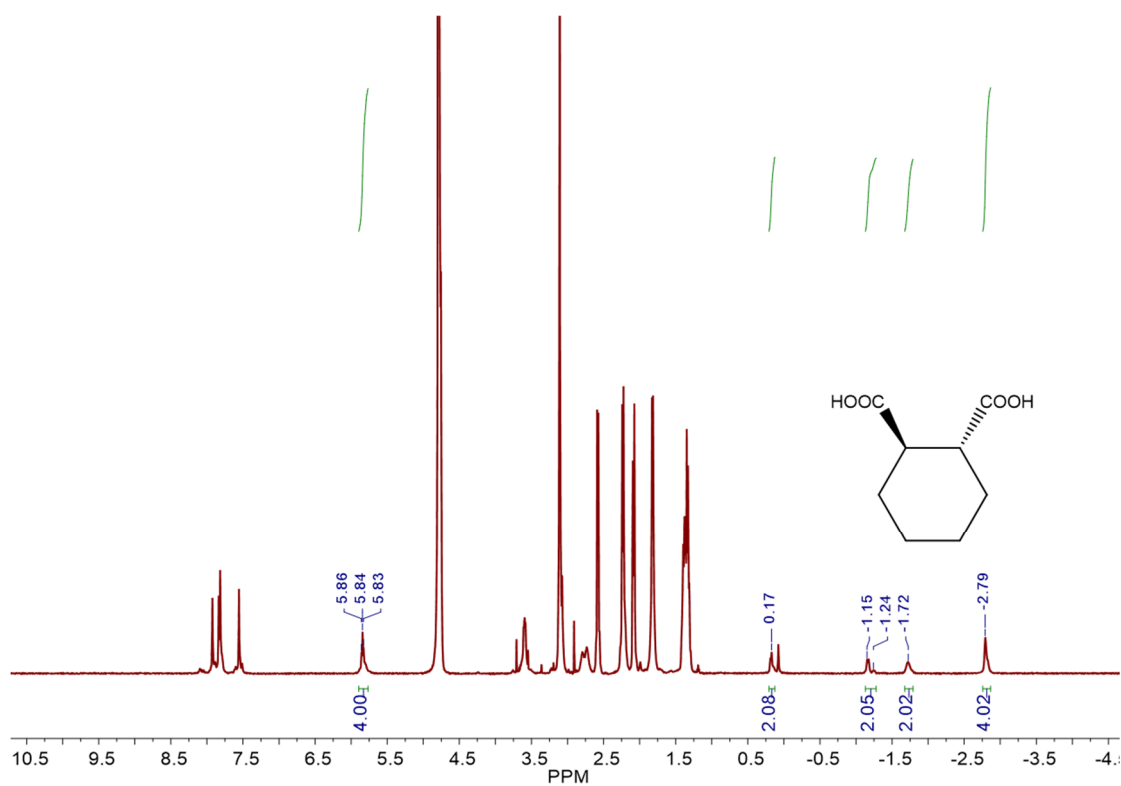


Fig. S24 ^1H NMR spectrum of the complex formed between cavitand **1** and excess of trans-1,2-Cyclohexanedicarboxylic acid in D_2O

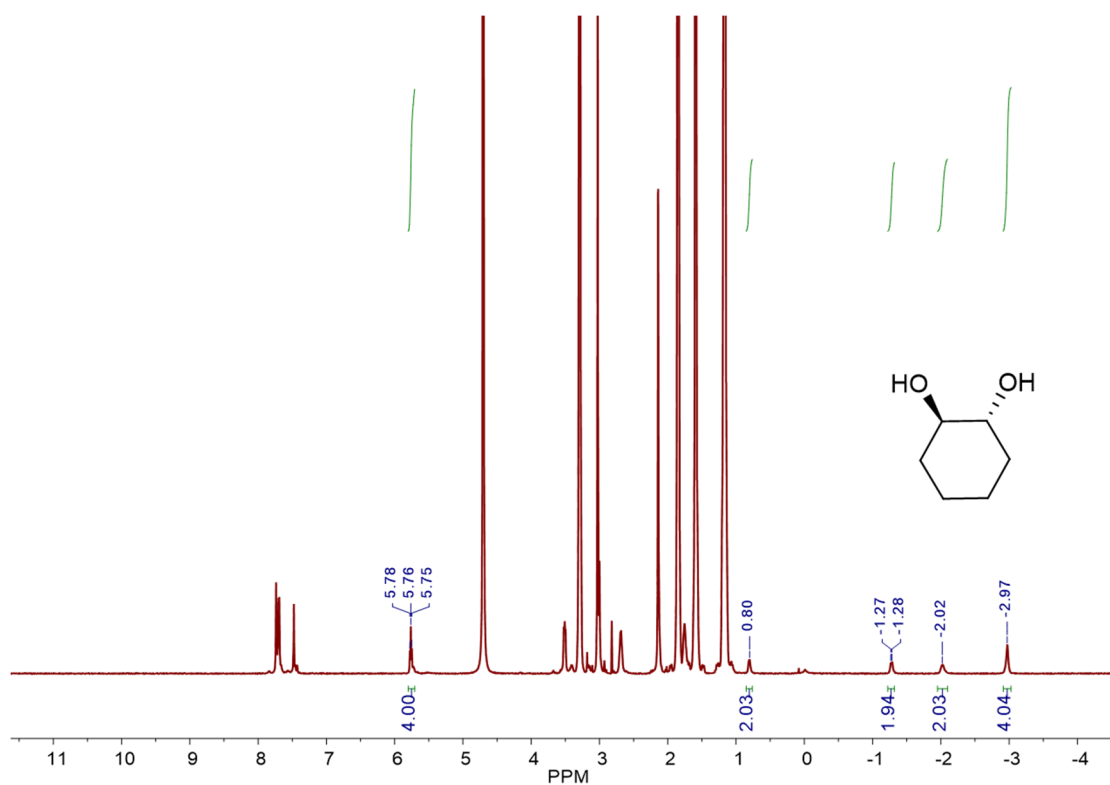


Fig. S25 ^1H NMR spectrum of the complex formed between cavitand **1** and excess of trans-1,2-Cyclohexanediol in D_2O

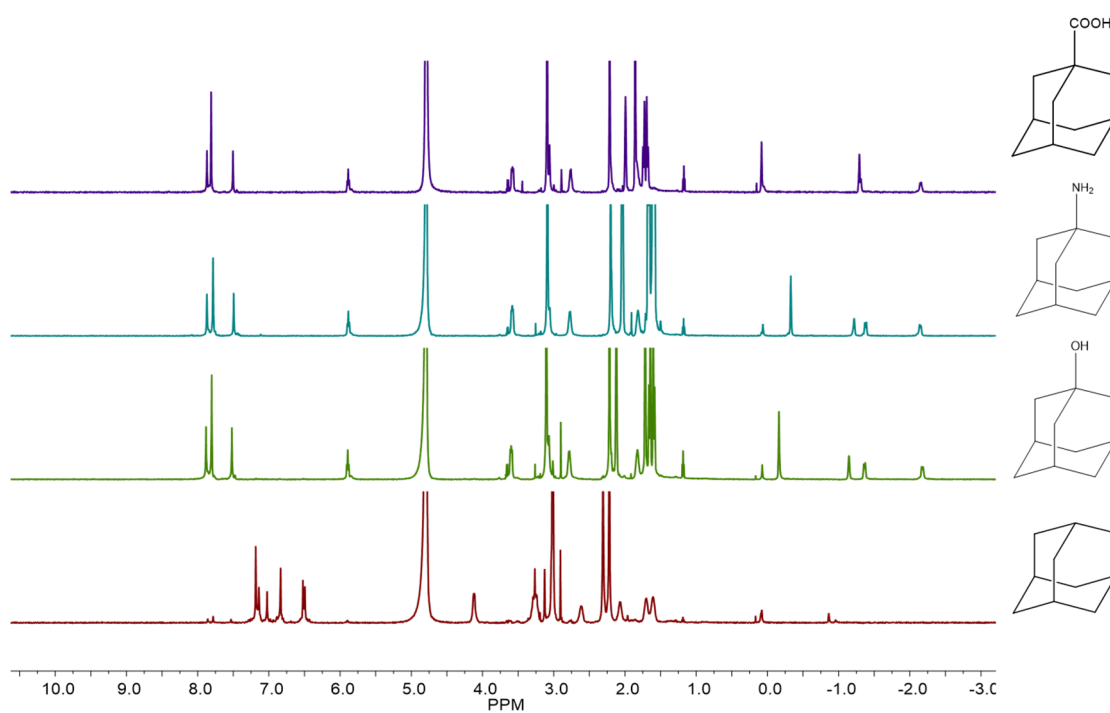


Fig. S26 ^1H NMR spectra of the complexes formed between cavitand **1**, 1mmol + from bottom to top, excess of adamantane, 1-adamantanol, amantadine, 1-adamantanecarboxylic acid

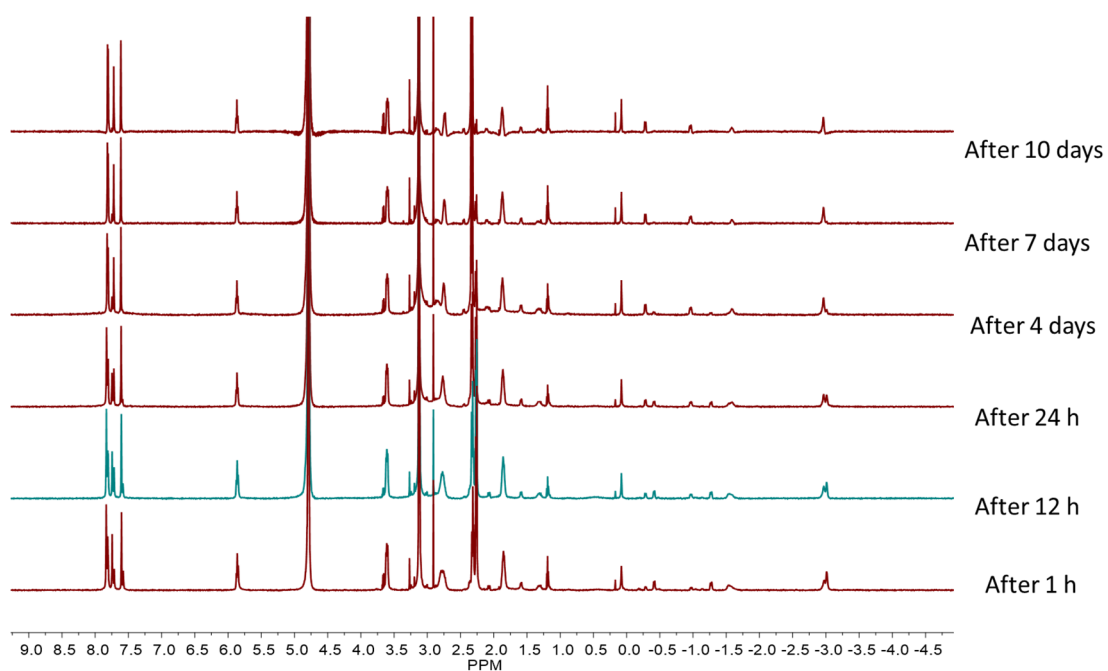


Fig. S27 Comparative ^1H NMR spectra of the host-guest complex formed between equimolar oxaliplatin and cavitand **1** in D_2O , after stand for from bottom to top 1h, 12 h, 24 h, 4 days, 7 days and 10 days