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

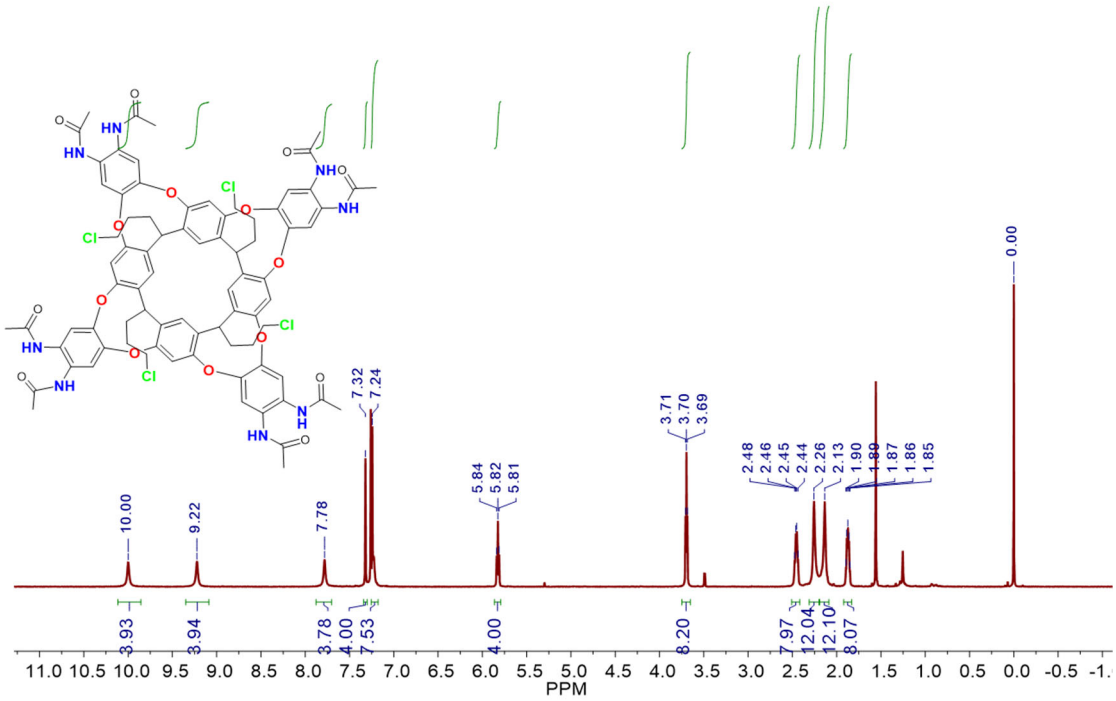

Fig. S1 ^{1}H NMR spectrum of cavitand **3** in chloroform-*d* at rt

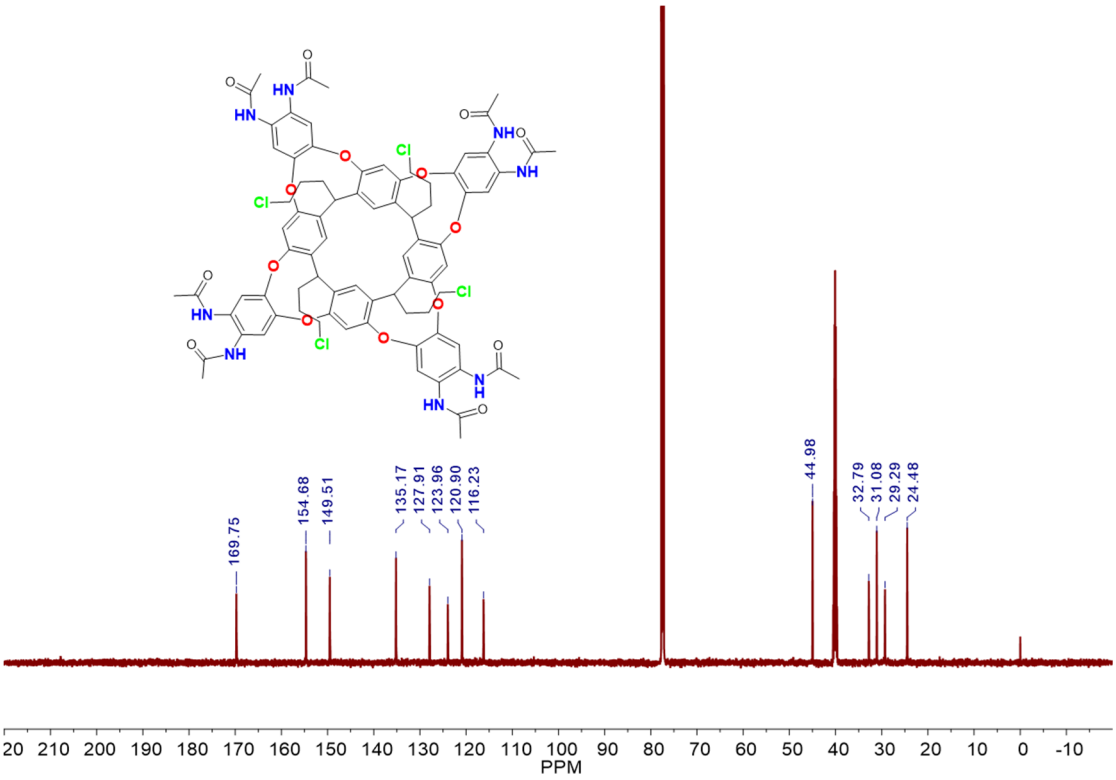

Fig. S2 ^{13}C NMR spectrum of cavitand **3** in chloroform-*d*/DMSO-d_6 (vol/vol = 9 :1) at rt

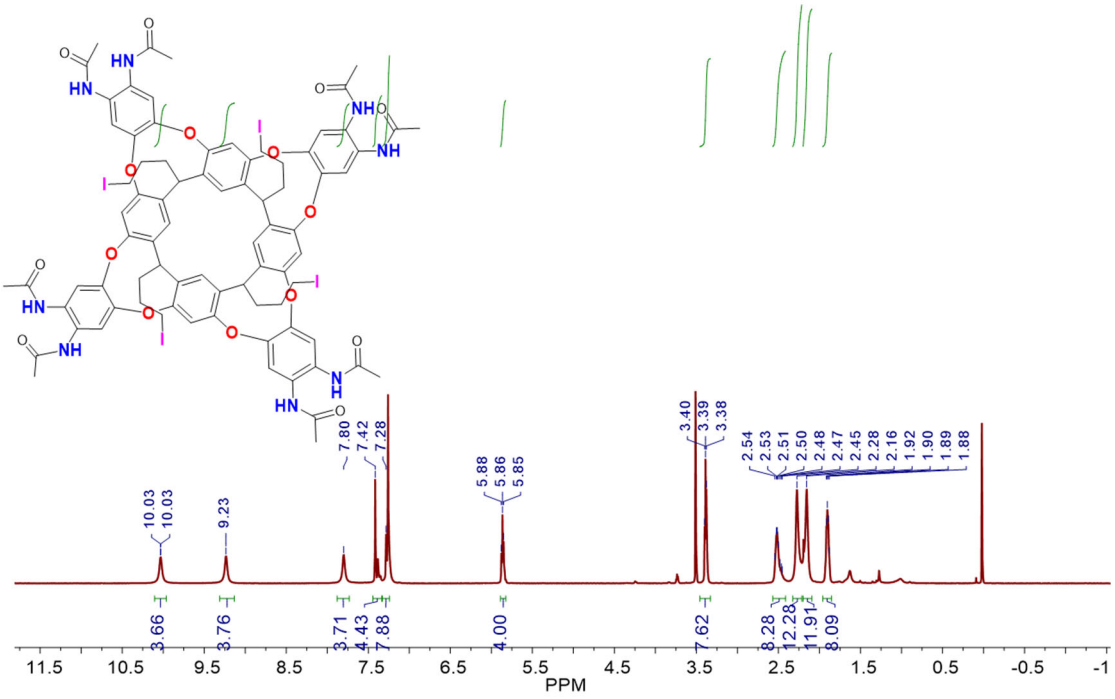

Fig. S3 ^{1}H NMR spectrum of cavitand **2** in chloroform-*d* at rt

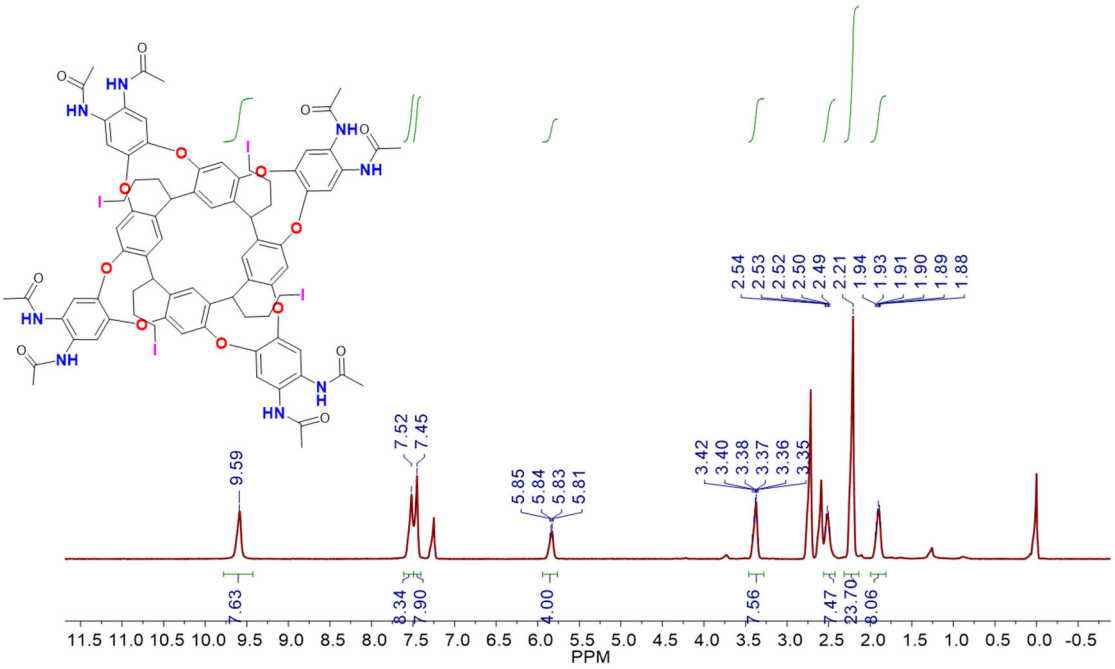

Fig. S4 ^{1}H NMR spectrum of cavitand **2** in chloroform-*d*/DMSO-d_6 (vol/vol = 9 :1) at rt

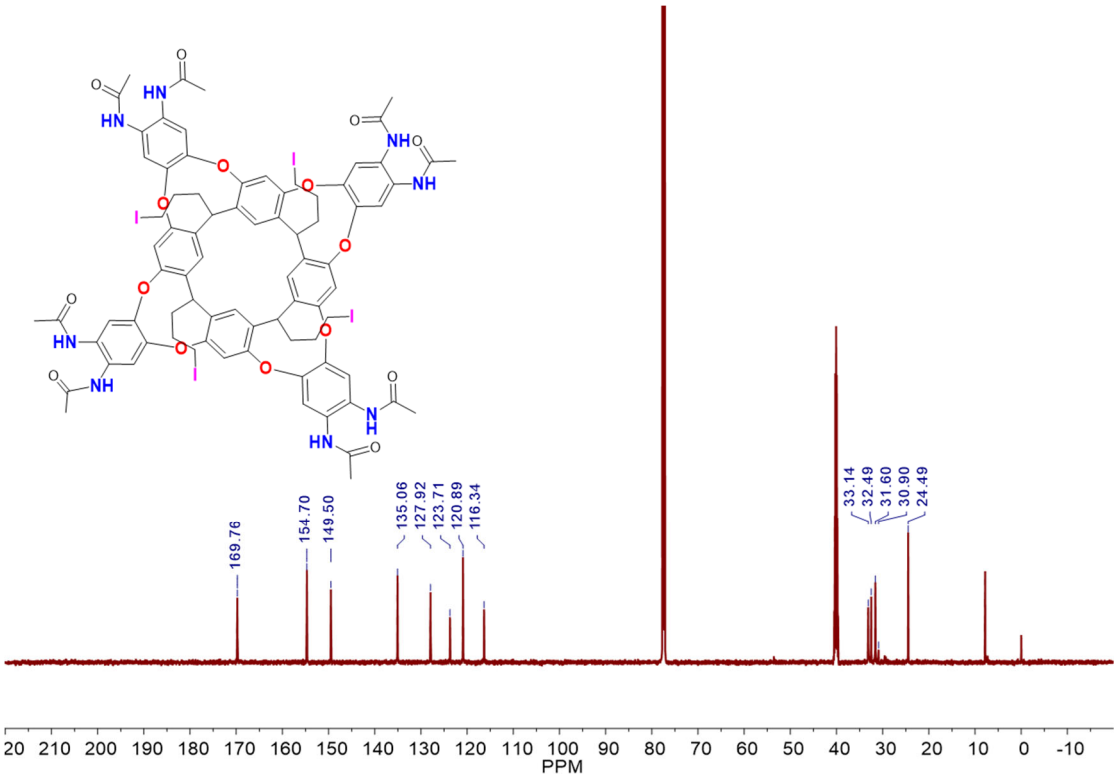

Fig. S5 ^{13}C NMR spectrum of cavitand **2** in chloroform-*d*/DMSO-d_6 (vol/vol = 9 :1) at rt

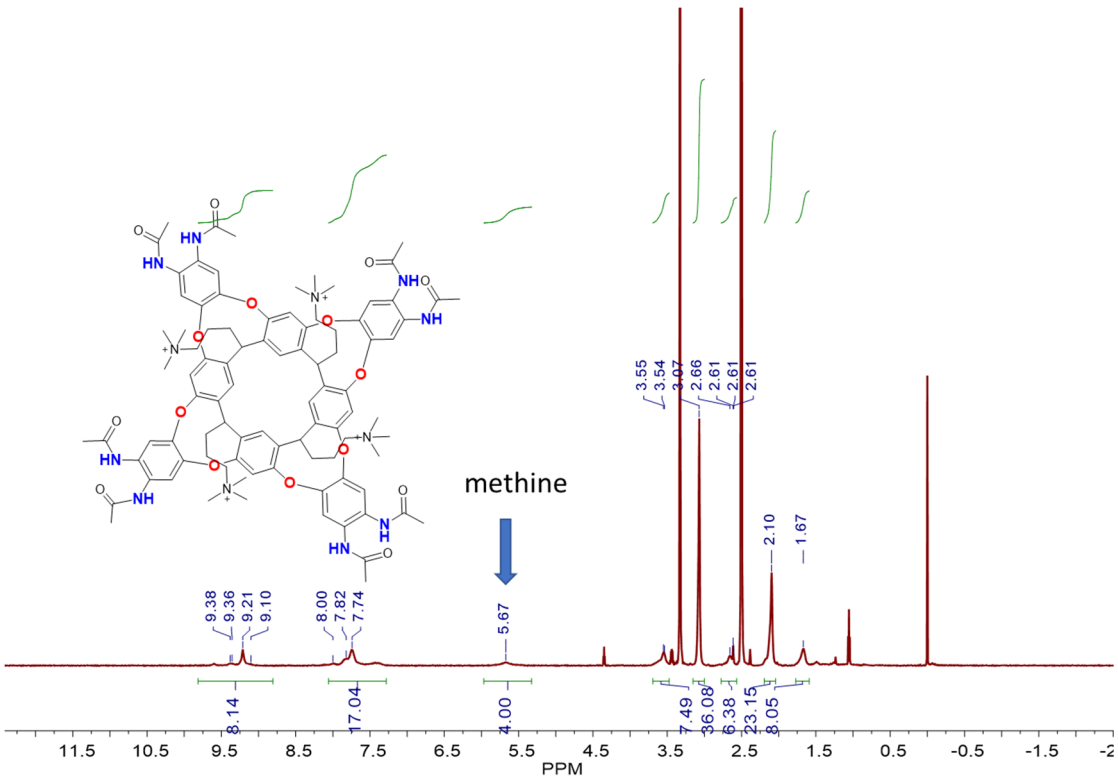

Fig. S6 ^{1}H NMR spectrum of cavitand **1** in DMSO-d_6 at rt, the cavitand display vase form exclusively

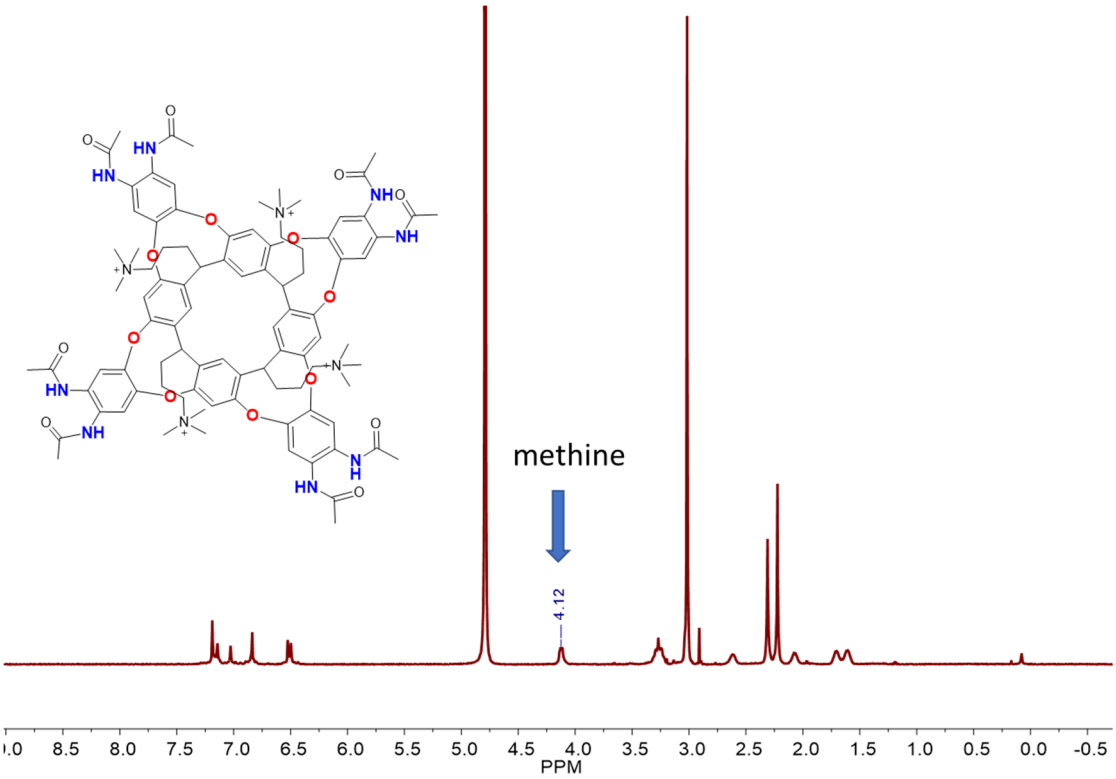

Fig. S7 ^{1}H NMR spectrum of cavitand **1** in D_2O at rt, the cavitand display kite form exclusively

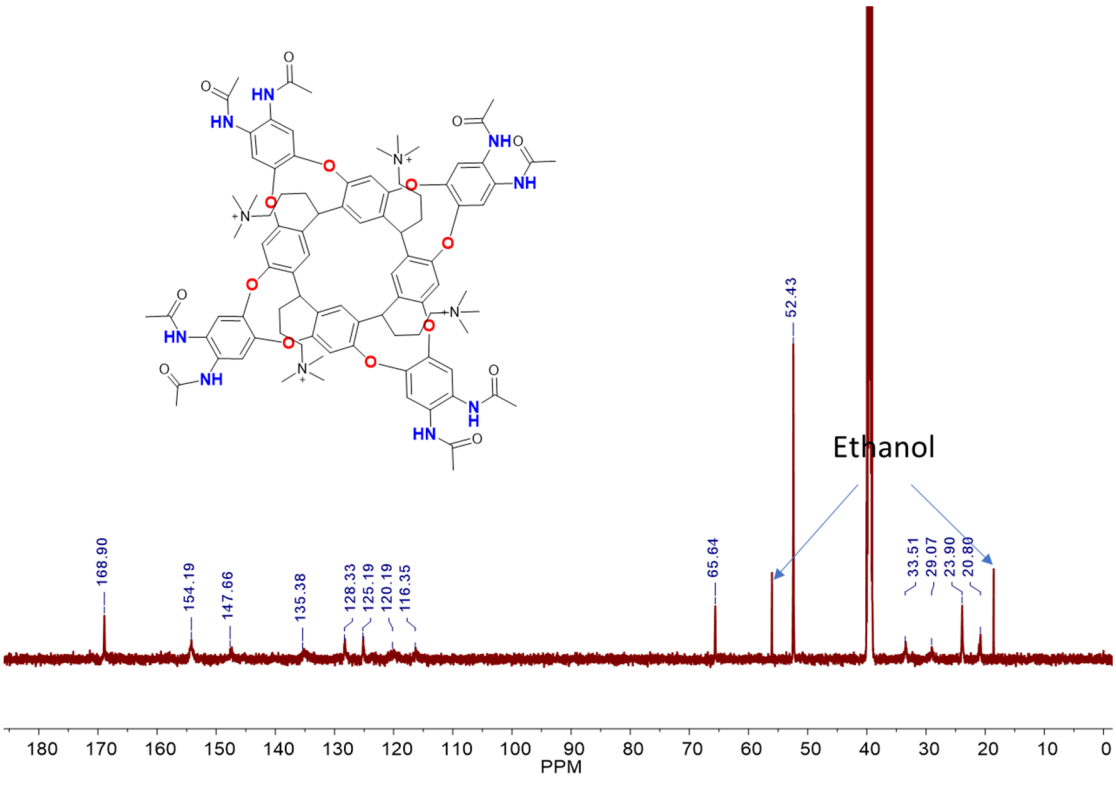

Fig. S8 ^{13}C NMR spectrum of cavitand **1** in DMSO-d_6 at rt

Mass (HR) spectra of cavitands

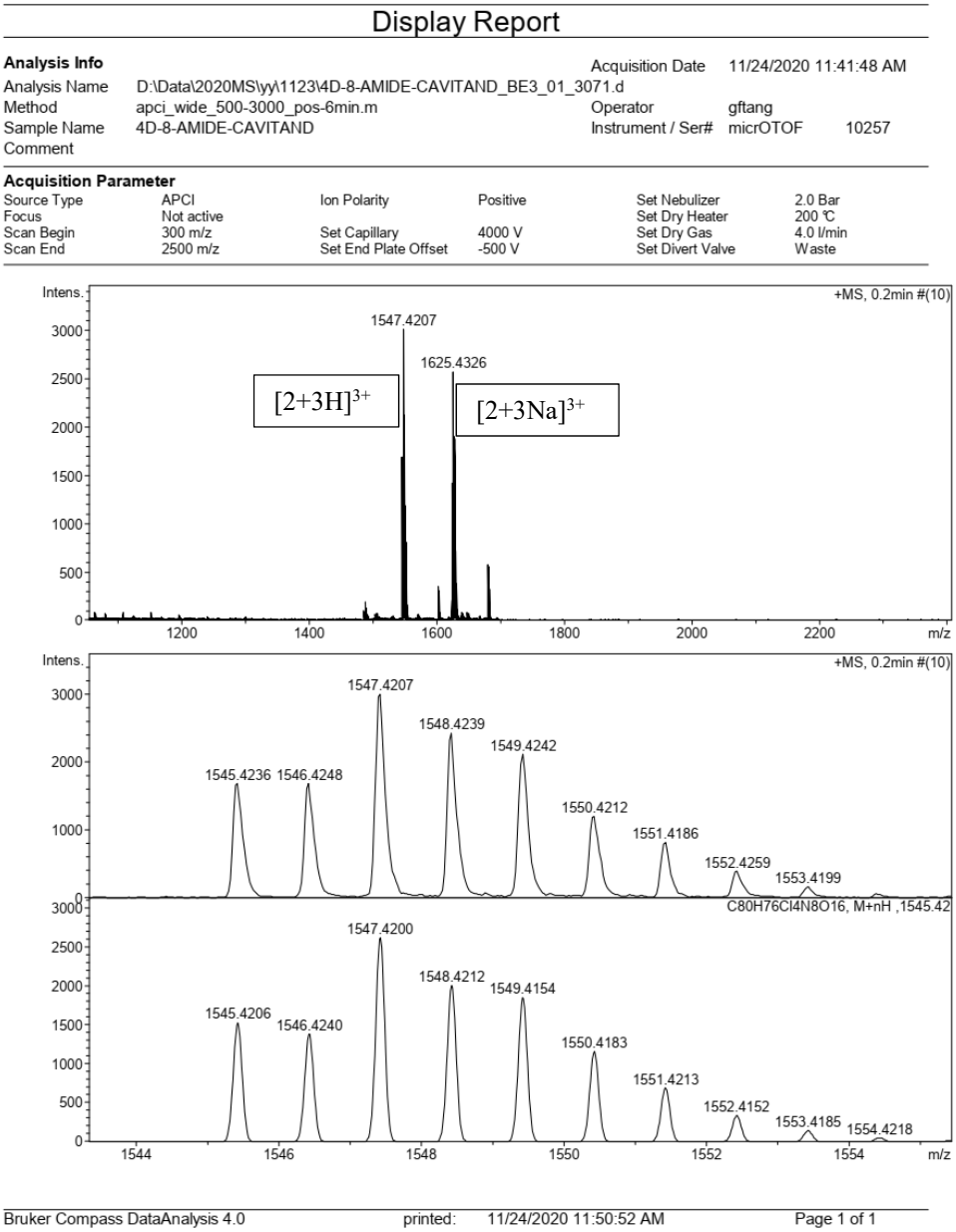

Fig. S9 Mass spectrum of cavitand **2**

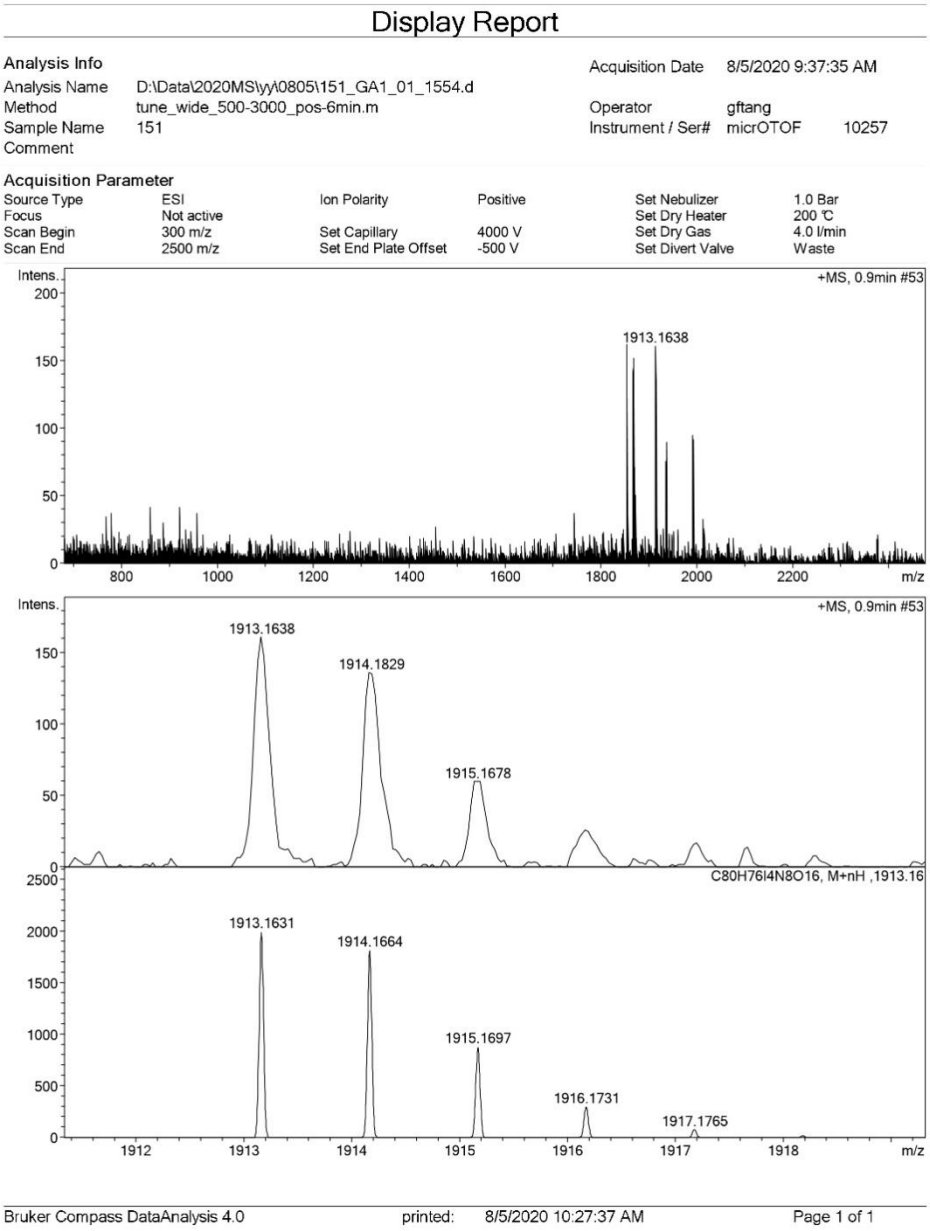

Fig. S10 Mass spectrum of cavitand **3**

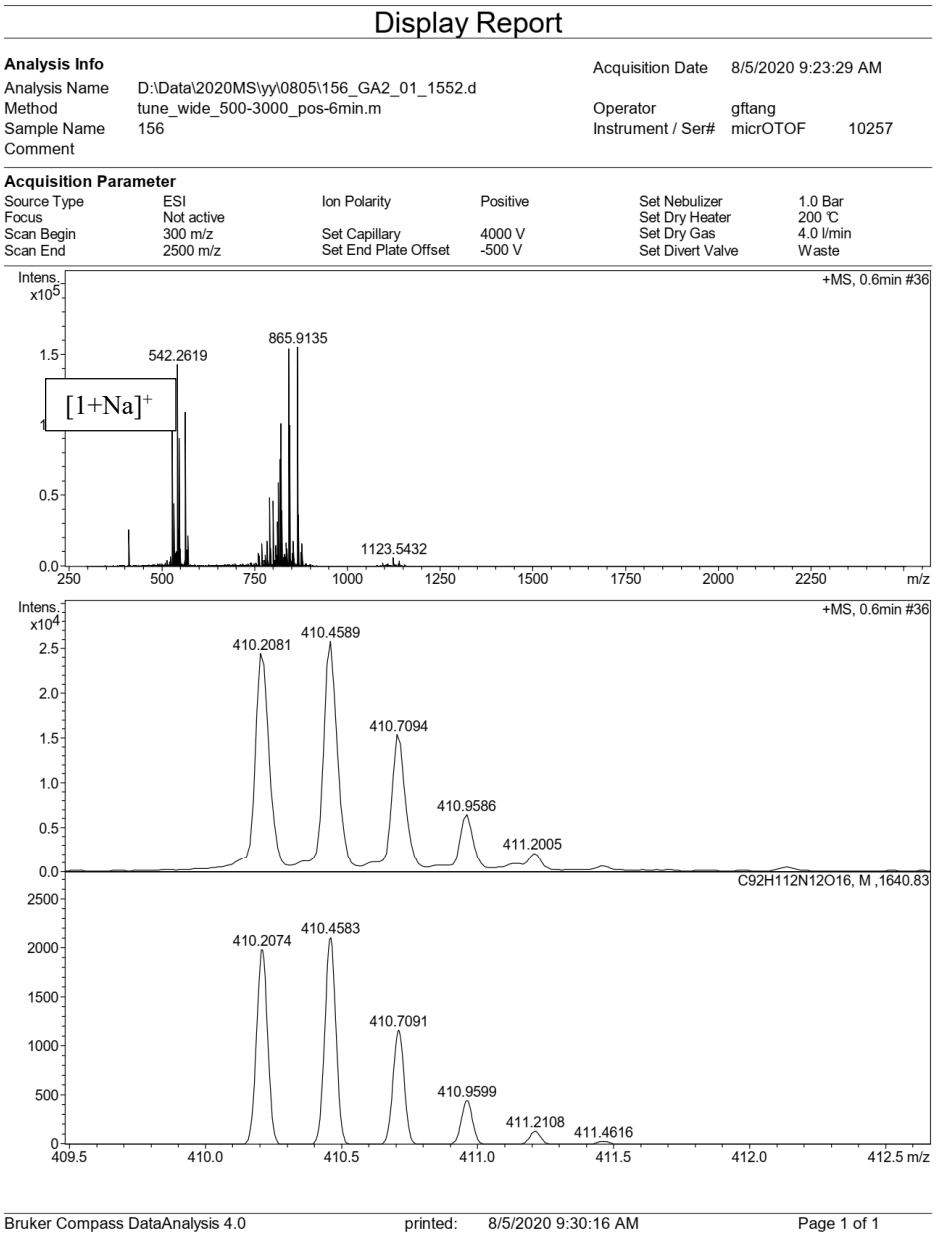

Fig. S11 Mass spectrum of cavitand **1**

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

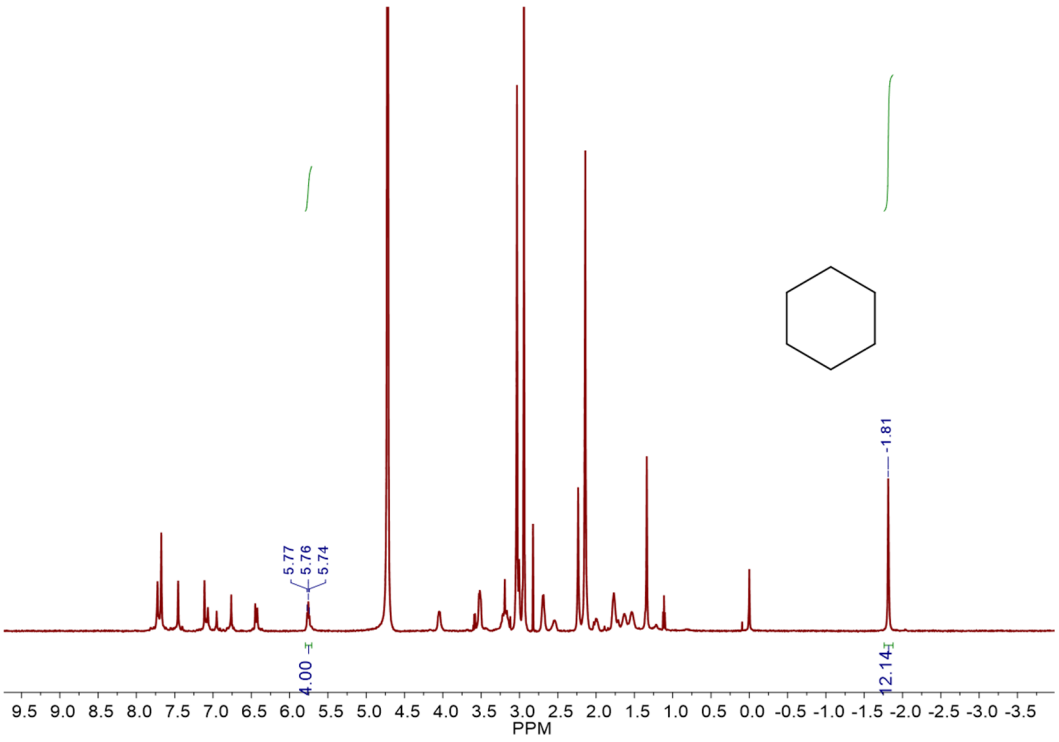

Fig. S12 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexane in D_2O

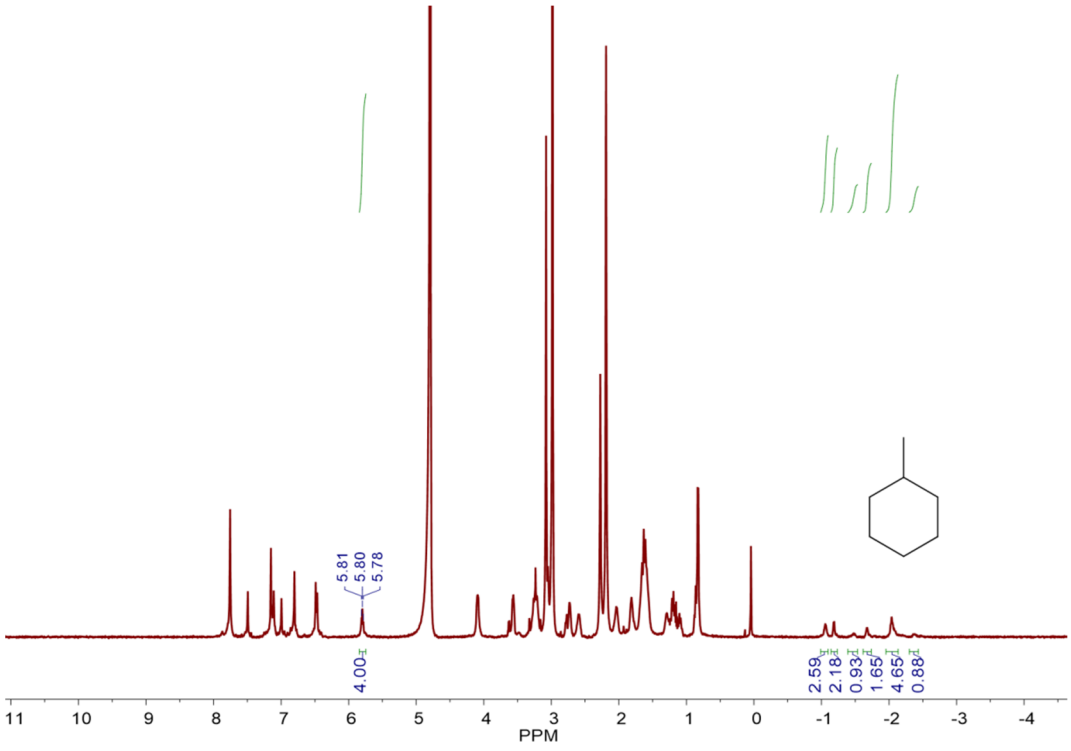

Fig. S13 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of methylcyclohexane

in D_2O

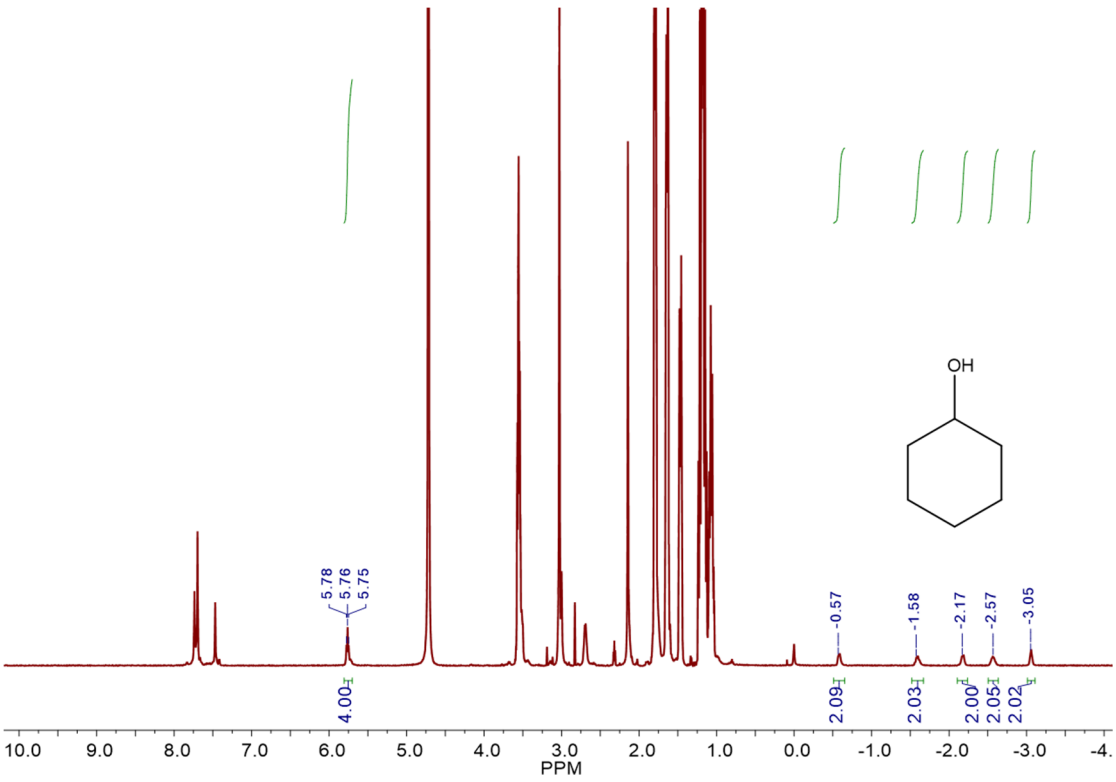

Fig. S14 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexanol in D_2O

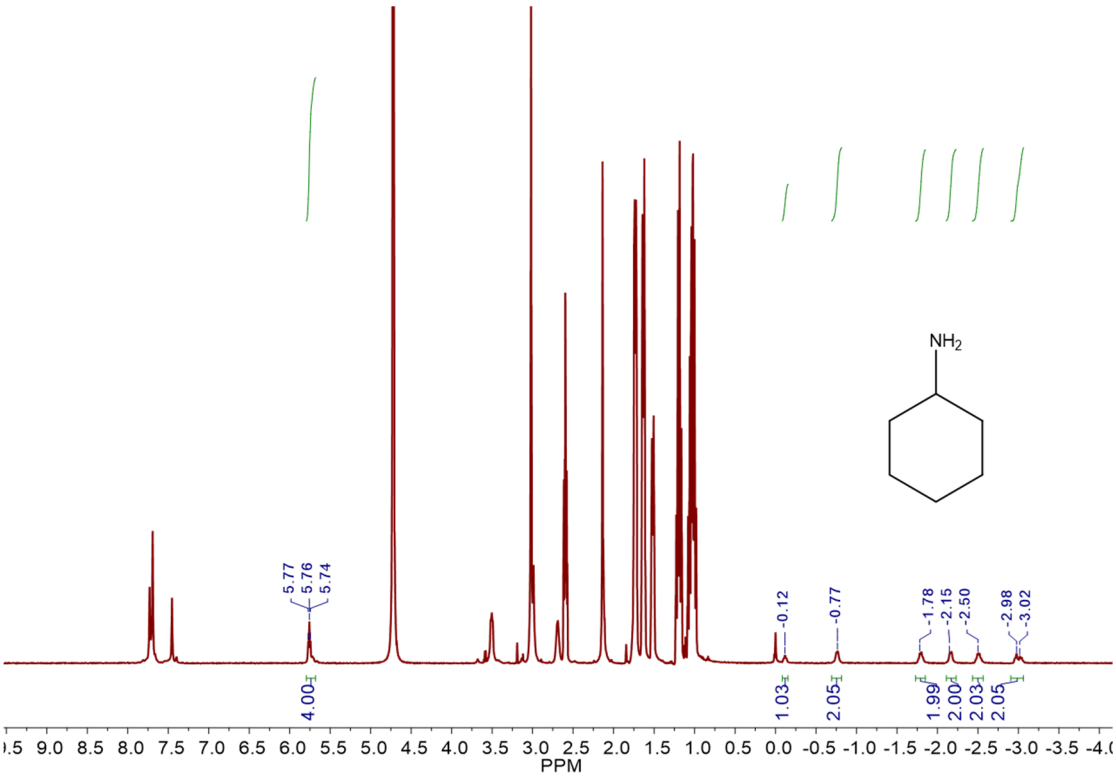

Fig. S15 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexylamine in

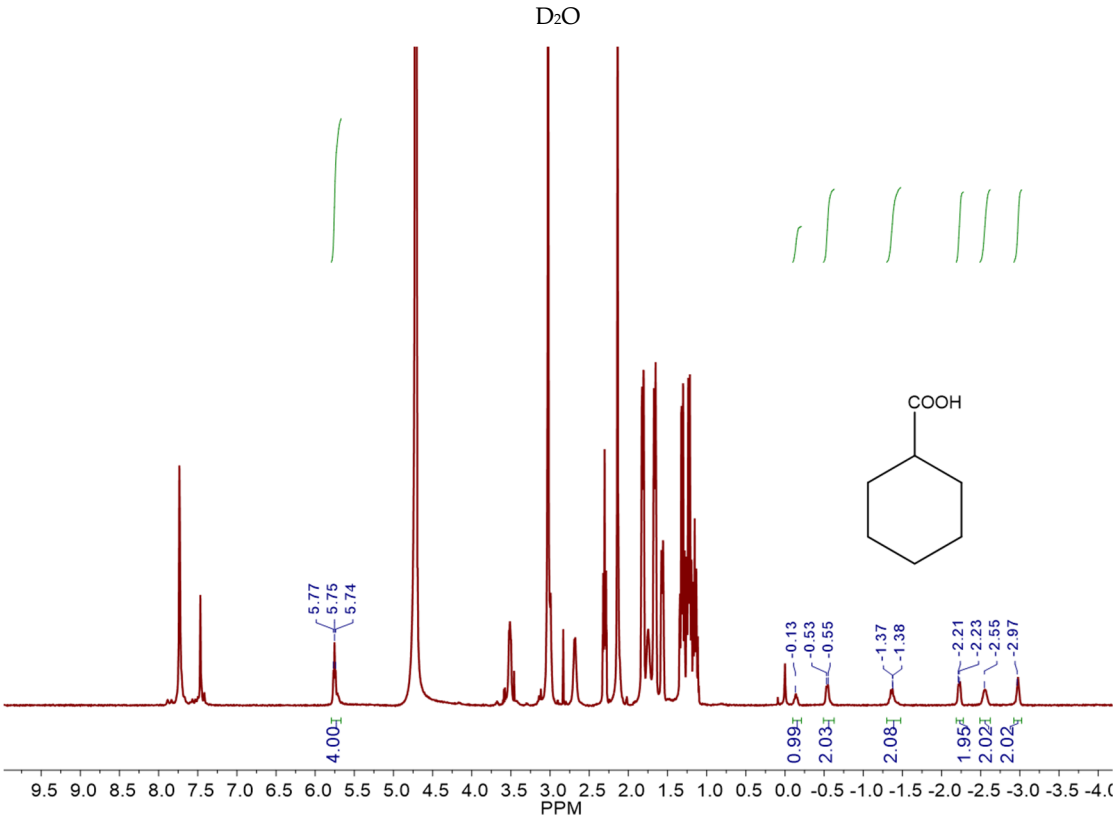

Fig. S16 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexanecarboxylic acid in D_2O

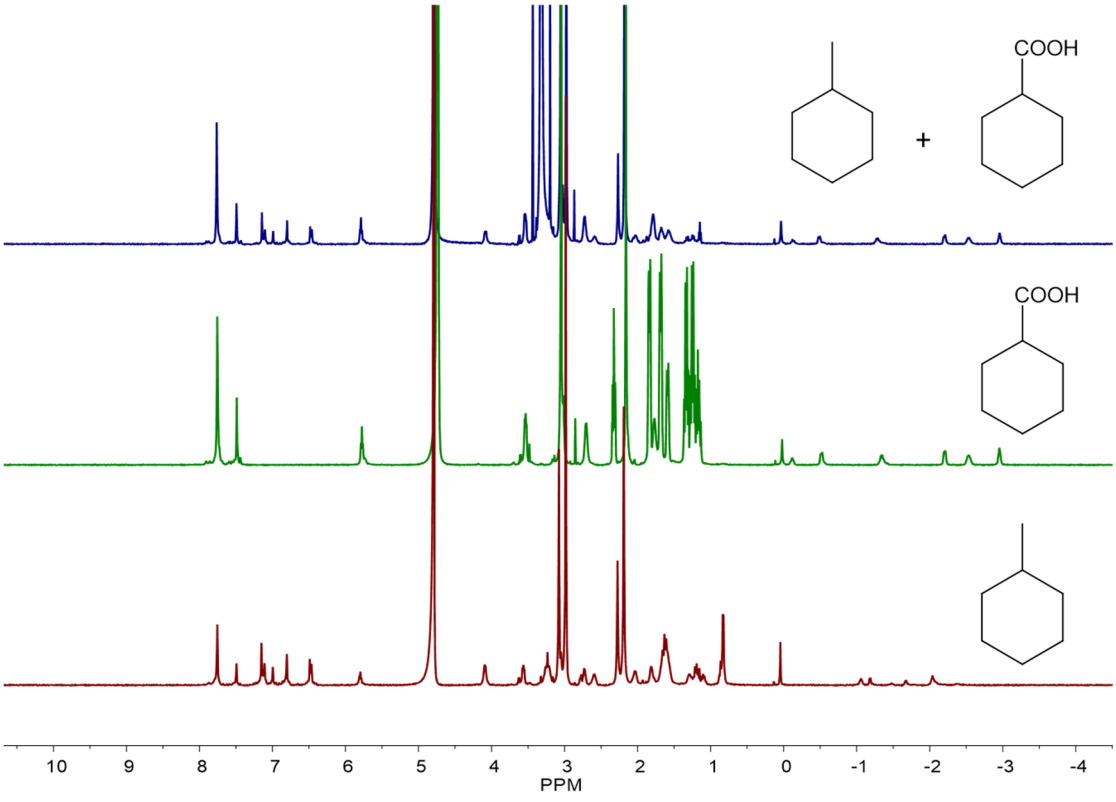

Fig. S17 ^{1}H NMR spectra of the complexes formed between cavitand **1**, 1mmol + from bottom to top, excess of methylcyclohexane, cyclohexanecarboxylic acid, and equimolar methylcyclohexane + cyclohexanecarboxylic acid (1:1) mixture.

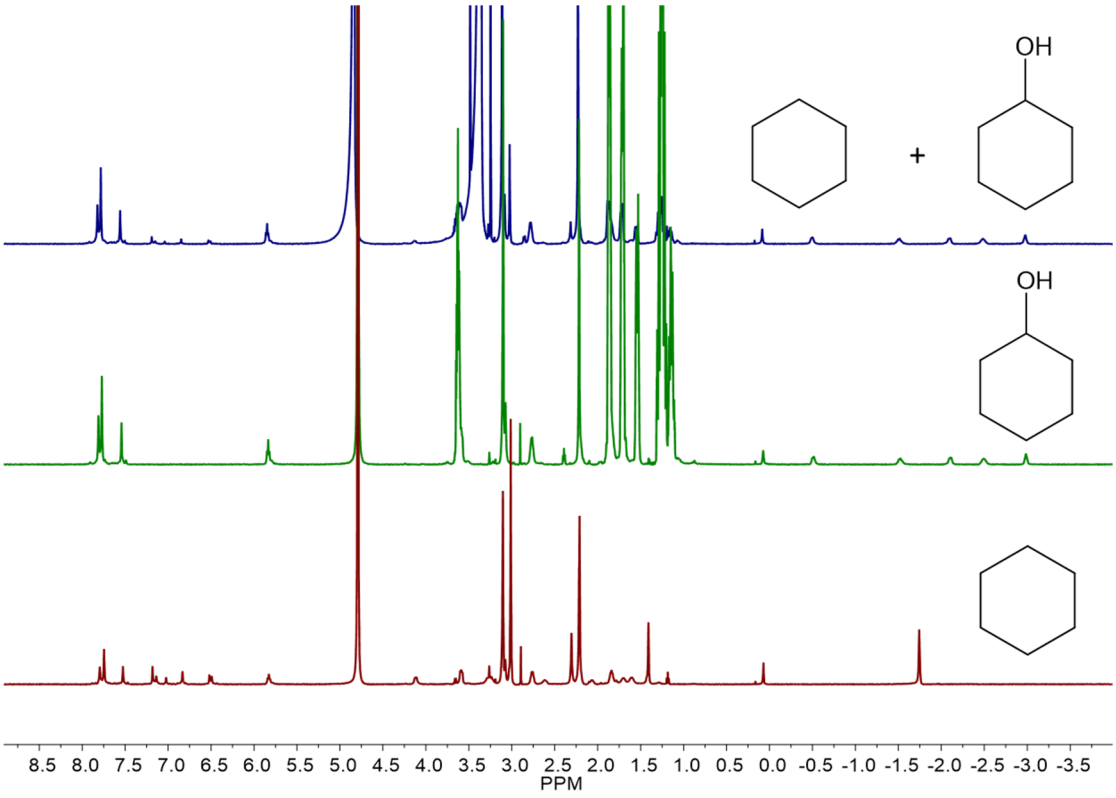

Fig. S18 ^{1}H NMR spectra of the complexes formed between cavitand **1**, 1mmol + from bottom to top, excess of cyclohexane, cyclohexanol, and equimolar cyclohexane + cyclohexanol (1:1) mixture.

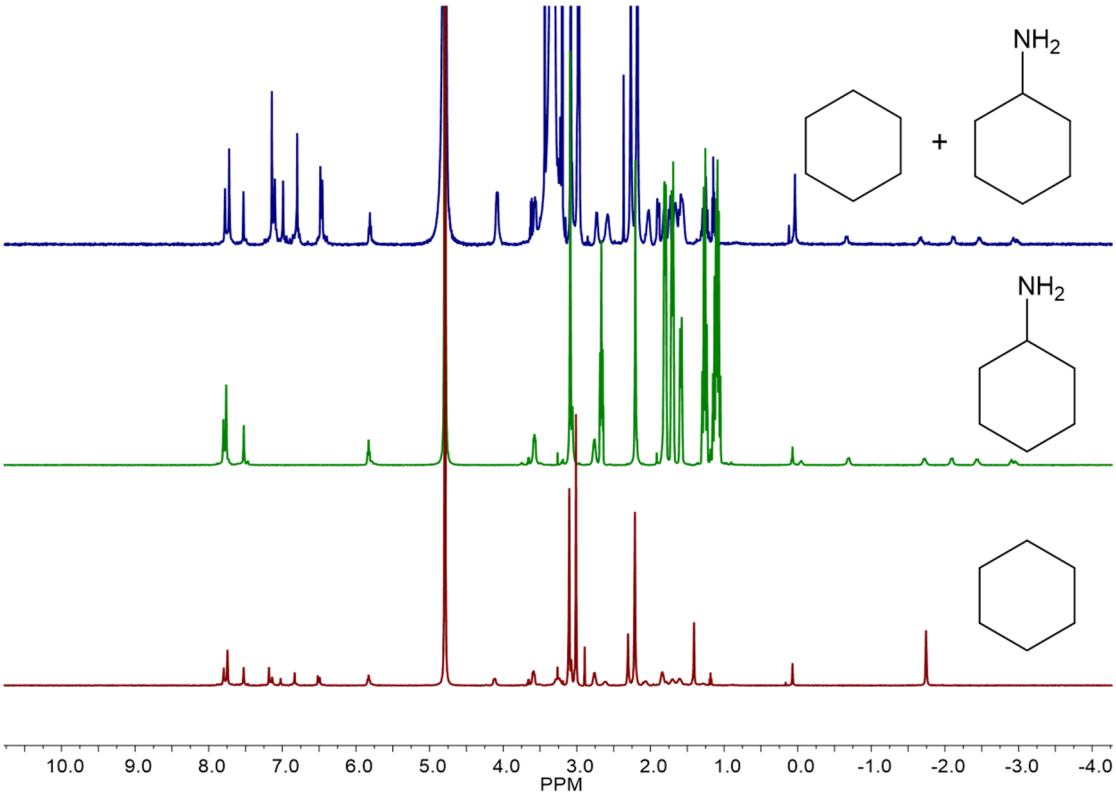

Fig. S19 ^{1}H NMR spectra of the complexes formed between cavitand **1**, 1mmol + from bottom to top, excess of cyclohexane, cyclohexylamine, and equimolar cyclohexane + cyclohexylamine (1:1) mixture

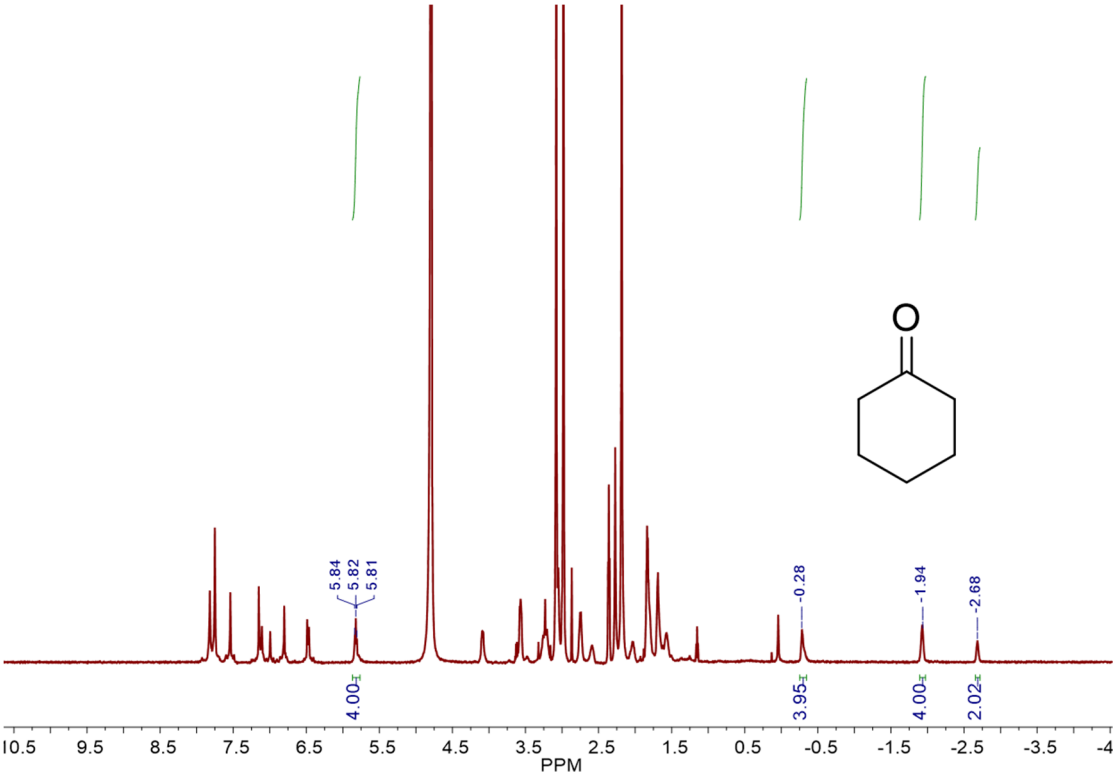

Fig. S20 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of cyclohexanone in D_2O

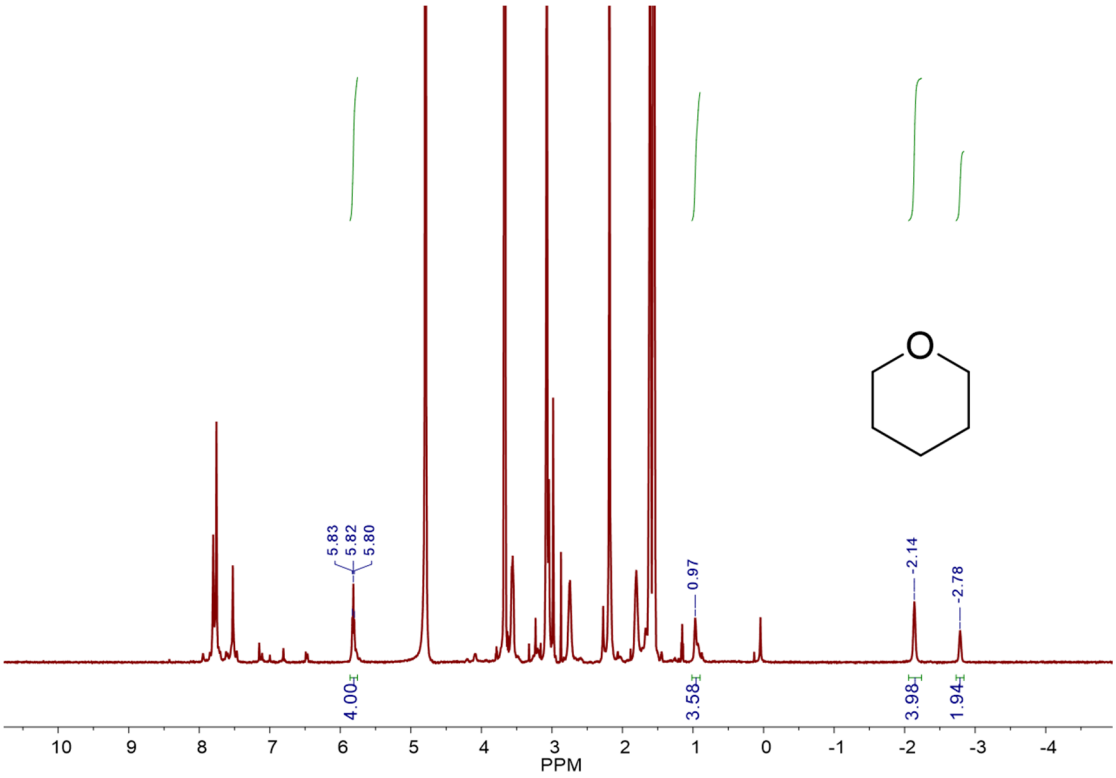

Fig. S21 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of tetrahydropyran in D_2O

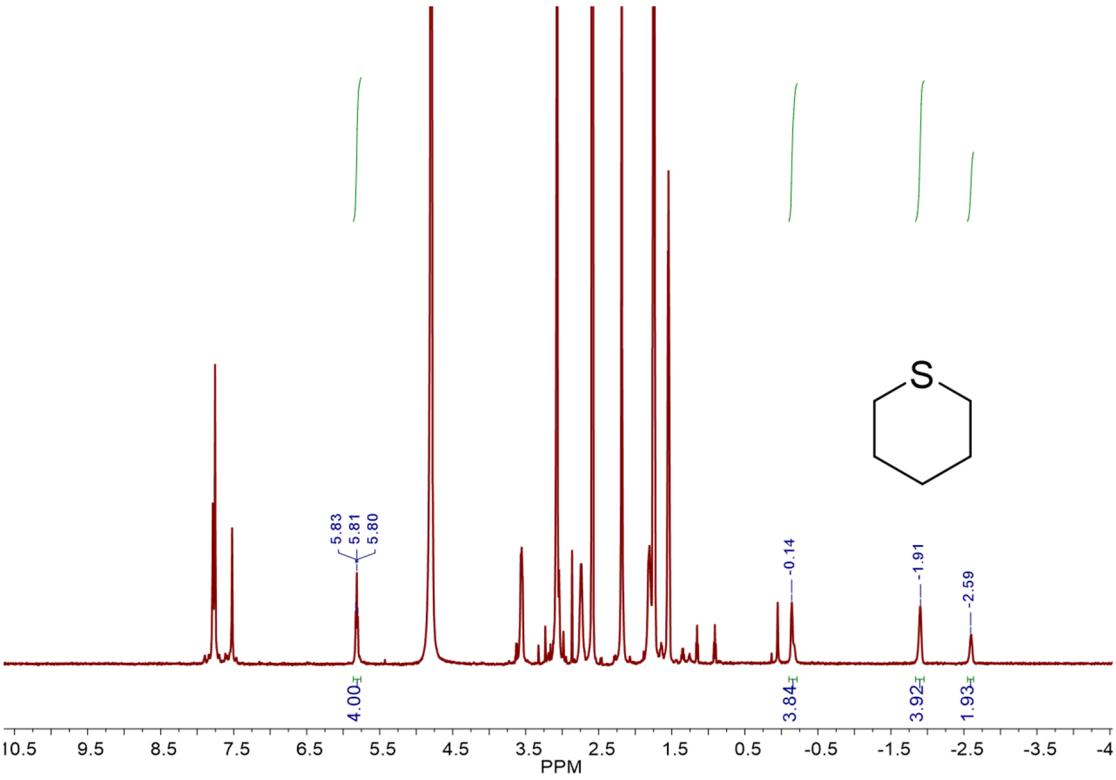

Fig. S22 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of thiane in D_2O

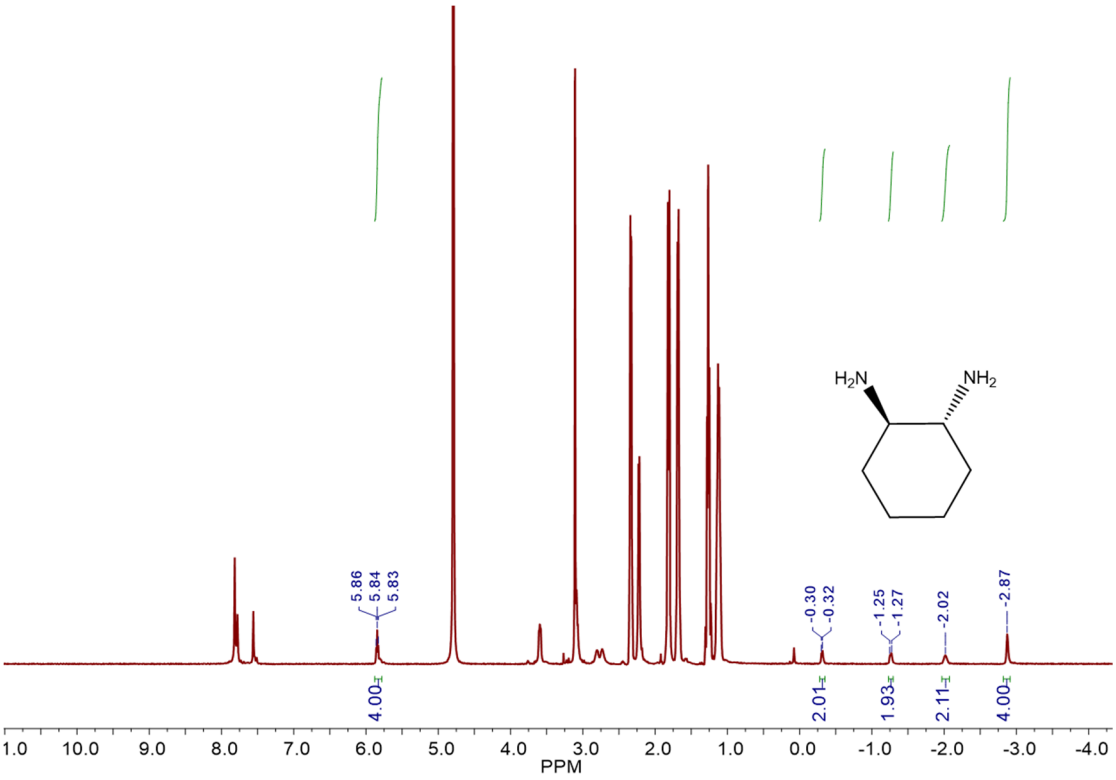

Fig. S23 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of trans-1,2-diaminocyclohexane in D_2O

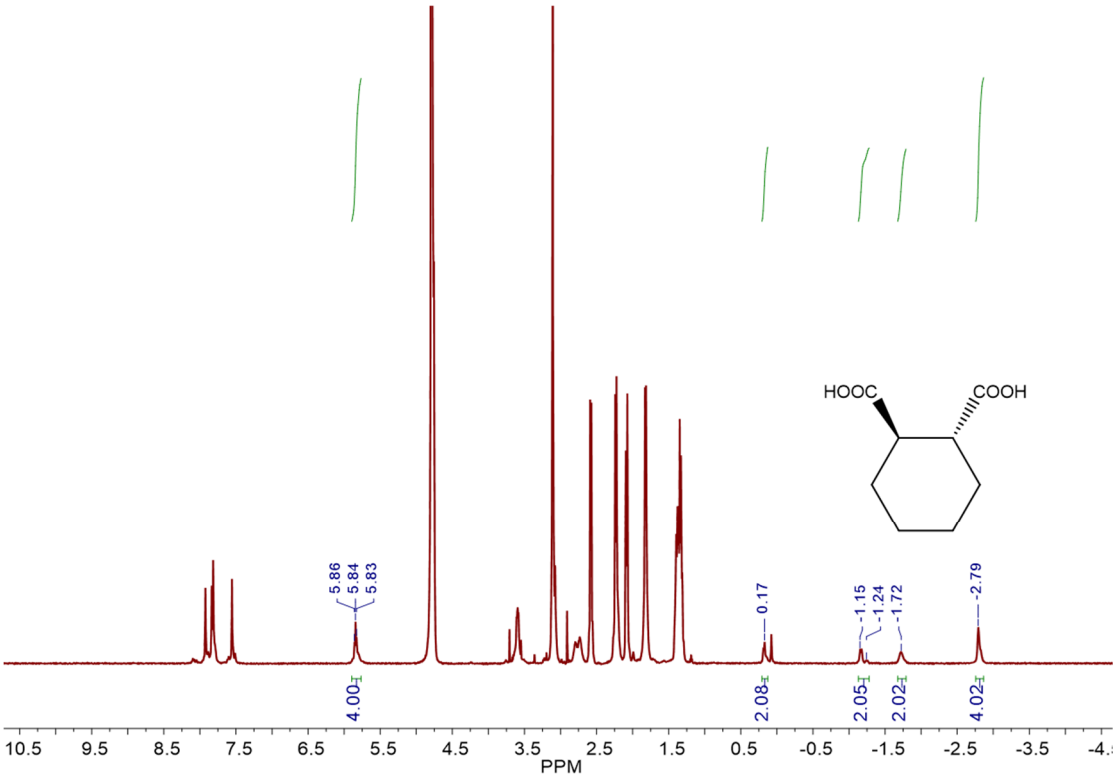

Fig. S24 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of trans-1,2-Cyclohexanedicarboxylic acid in D_2O

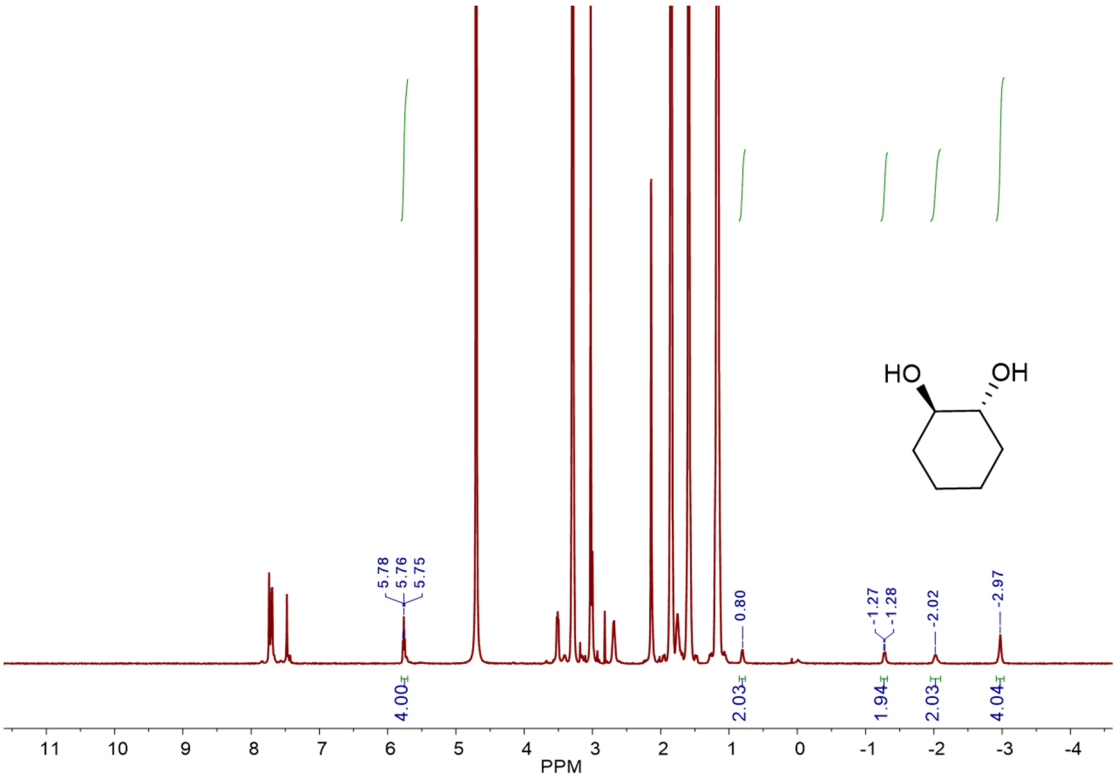

Fig. S25 ^{1}H NMR spectrum of the complex formed between cavitand **1** and excess of trans-1,2-Cyclohexanediol in D_2O

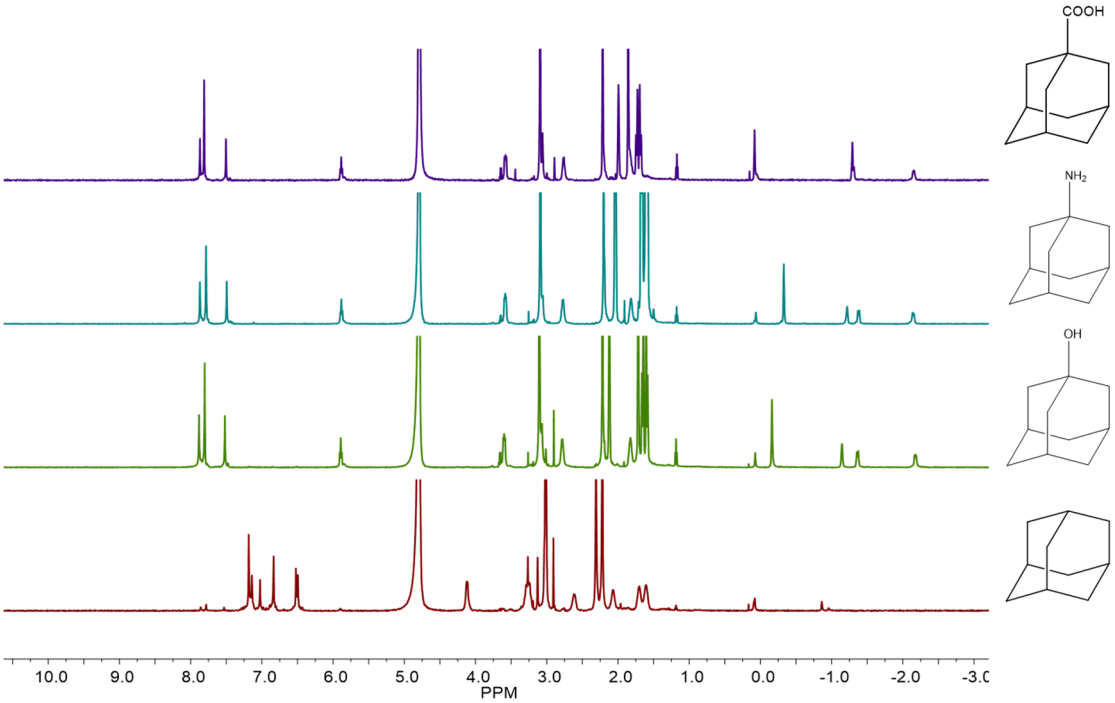

Fig. S26 ^{1}H NMR spectra of the complexes formed between cavitand **1**, 1mmol + from bottom to top, excess of admantane, 1-adamantanol, amantadine, 1-adamantanecarboxylic acid

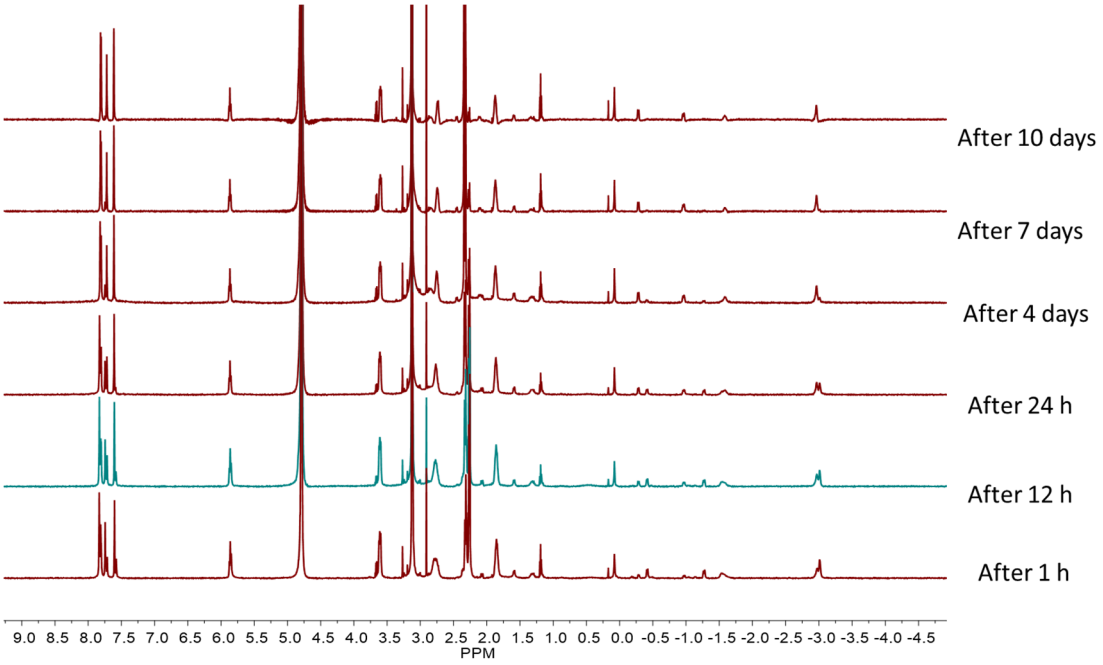

Fig. S27 Comparative ^{1}H NMR spectra of the host-guest complex formed between equimolar oxaliplatin and cavitand **1** in D_2O, after stand for from bottom to top 1h, 12 h, 24 h, 4 days ,7 days and 10 days