Binding of alkyl halides in water-soluble cavitands with urea rims

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Supporting Information

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Instrumentation. ^{1}H NMR spectra were obtained at 600 MHz on a Bruker DRX-600 spectrometer equipped with a 5 mm DCH cryoprobe. Spectra were recorded at 298 K unless otherwise stated. Chemical shifts are expressed in parts per million (δ scale) with respect to tetramethylsilane and are referenced to the proton signal of residual, non-deuterated solvent [D_2O: δ 4.79 for ^{1}H NMR;] for ^{1}H NMR.

Materials. All reagents and solvents were purchased from commercial suppliers.

A general statement. The orientations of the tumbling guests were calculated from the percent of the maximum Δδ that the observed CH_3 signals represent. For example, the CH_3 of the 1-chlorohexane appears at Δδ = -3.9 ppm (binding with cavitand **2**) which represents 80 % of the maximum Δδ of -4.8 ppm (CH_3 is down and at the bottom of cavitand **2**) with 20% of Δδ of -0.4 ppm (CH_3 is up and near the rim).

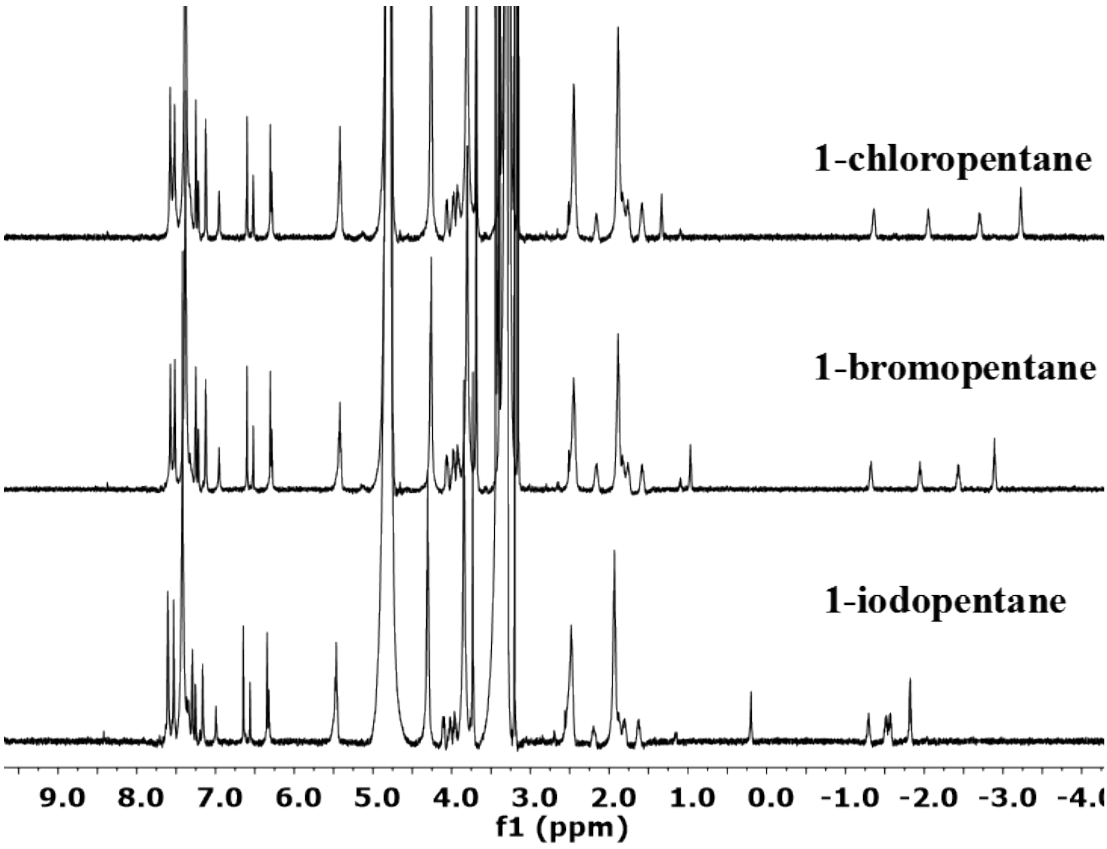

Figure S1. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **2** (1.0 mM) + 1-chloropentane (0.5 mM), cavitand **2** (1.0 mM) + 1-bromopentane (0.5 mM), cavitand **2** (1.0 mM) + 1-iodopentane (0.5 mM).

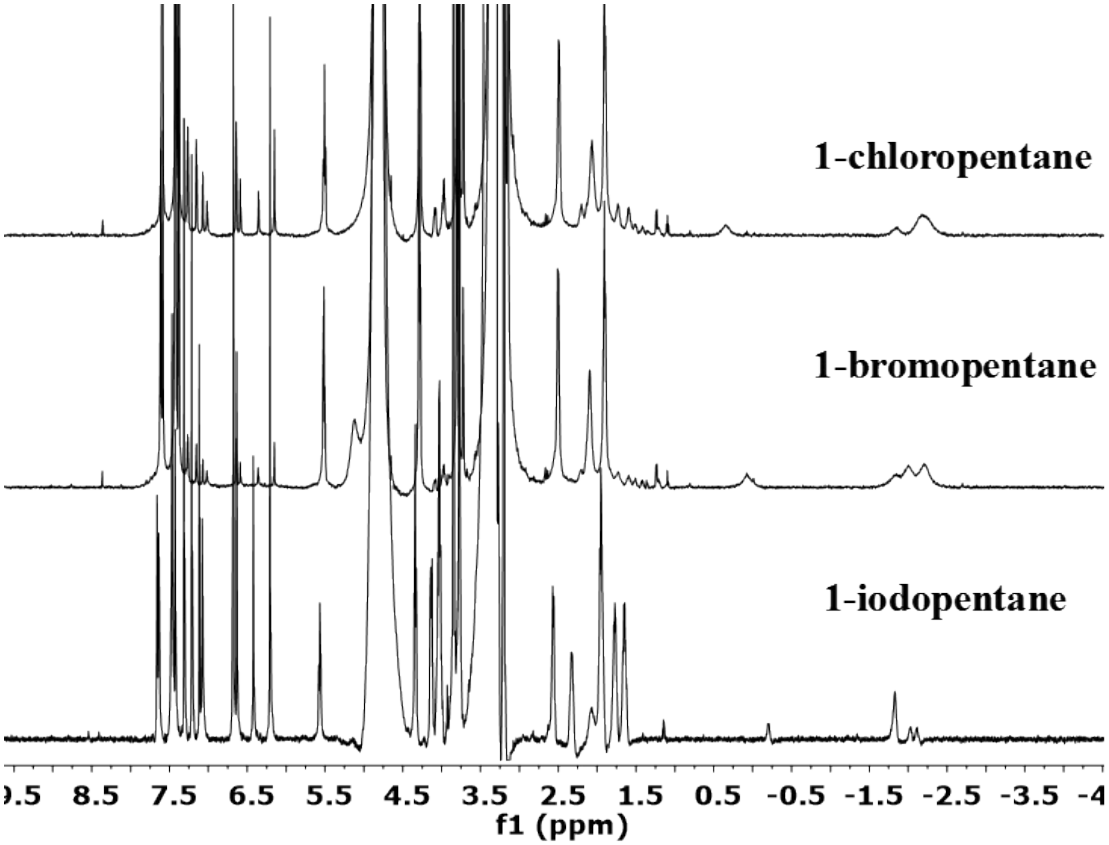

Figure S2. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **3** (1.0 mM) + 1-chloropentane (0.5 mM) , cavitand **3** (1.0 mM) + 1-bromopentane (0.5 mM), cavitand **3** (1.0 mM) + 1-iodopentane (0.5 mM).

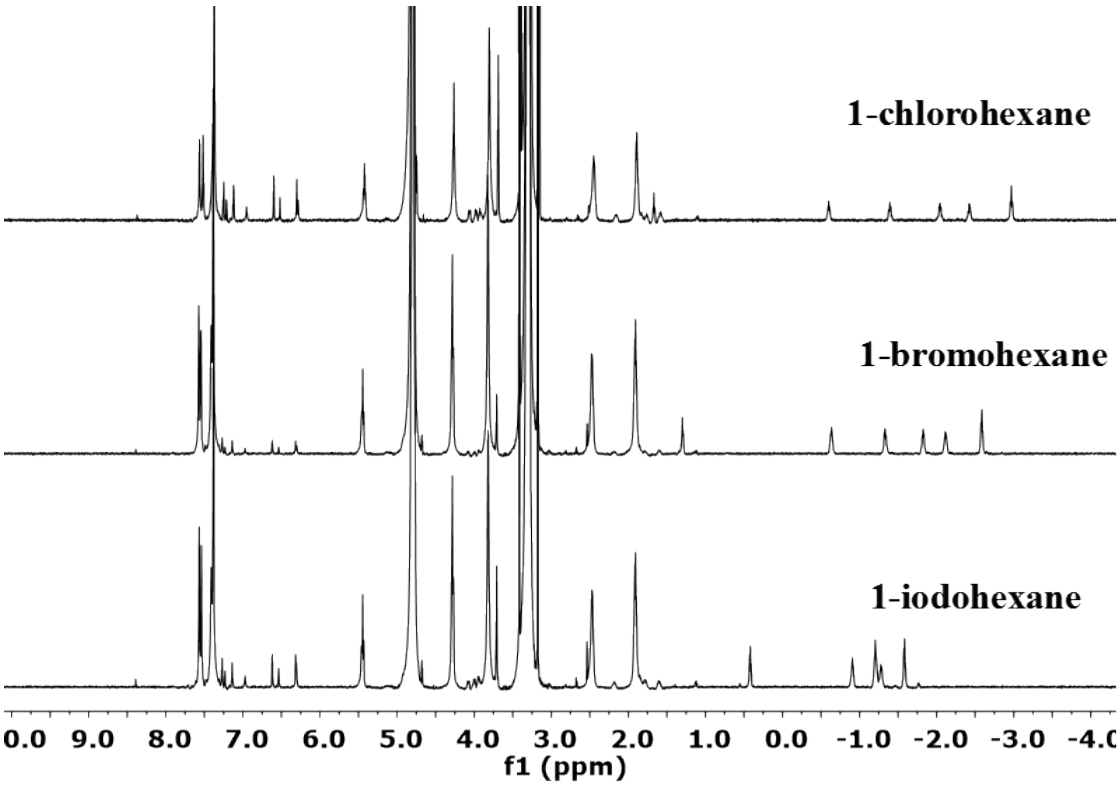

Figure S3. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **2** (1.0 mM) + 1-chlorohexane (0.5 mM), cavitand **2** (1.0 mM) + 1-bromohexane (0.5 mM), cavitand **2** (1.0 mM) + 1-iodohexane (0.5 mM).

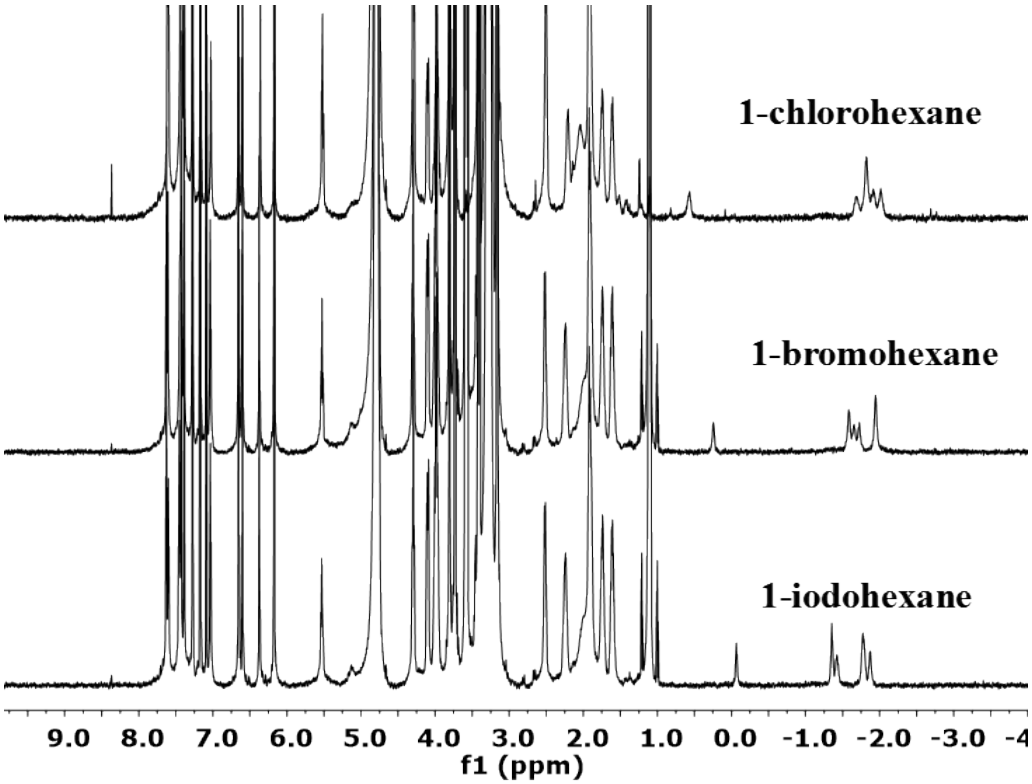

Figure S4. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **3** (1.0 mM) + 1-chlorohexane (0.5 mM), cavitand **3** (1.0 mM) + 1-bromohexane (0.5 mM), cavitand **3** (1.0 mM) + 1-iodohexane (0.5 mM).

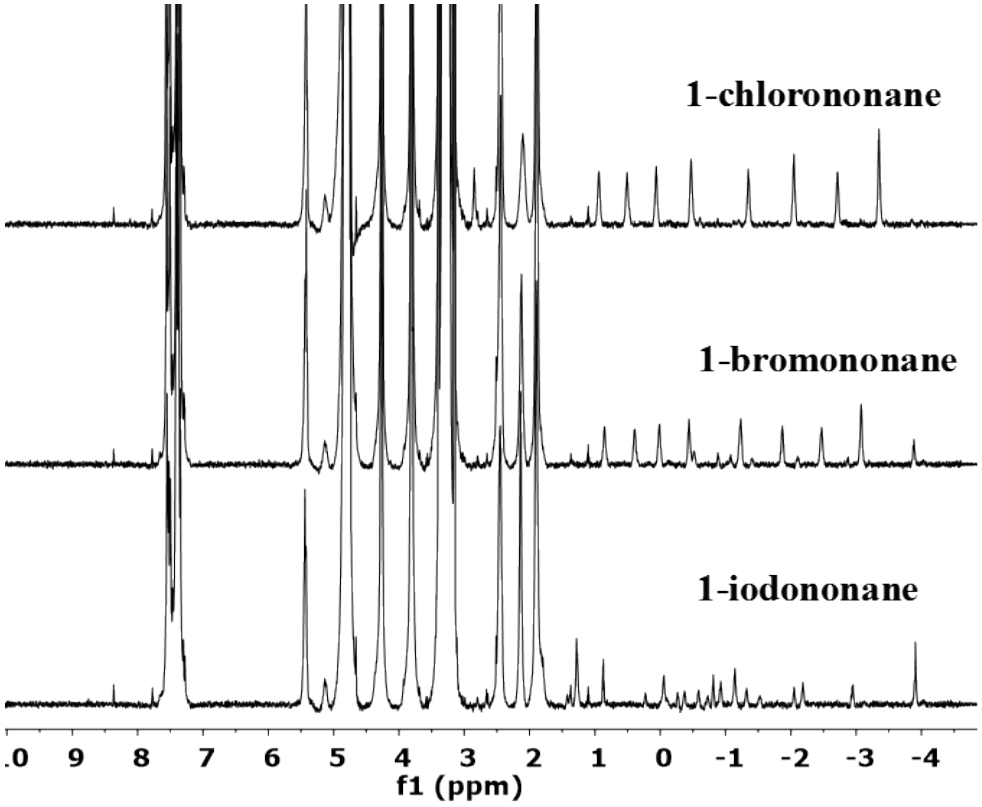

Figure S5. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **2** (1.0 mM) + 1-chlorononane (0.5 mM) (2:1), cavitand **2** (1.0 mM) + 1-bromononane (0.5 mM) (2:1), cavitand **2** (1.0 mM) + 1-iodononane (0.5 mM) (2:1).

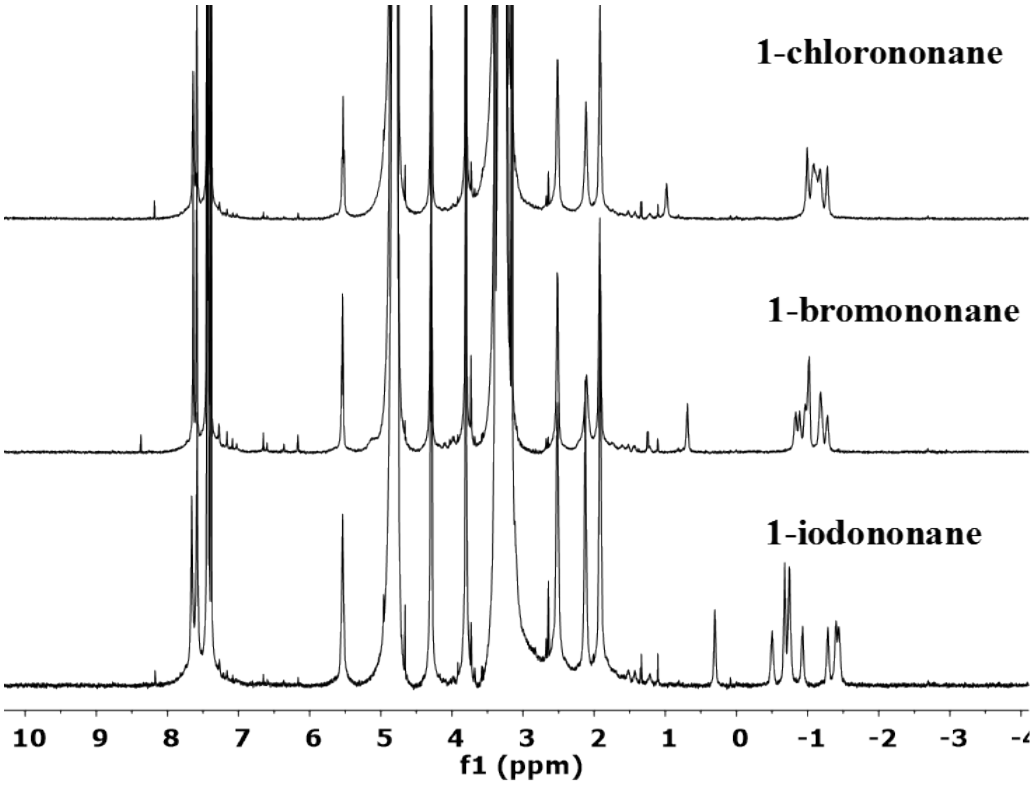

Figure S6. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **3** (1.0 mM) + 1-chlorononane (0.5 mM), cavitand **3** (1.0 mM) + 1-bromononane (0.5 mM), cavitand **3** (1.0 mM) + 1-iodononane (0.5 mM).

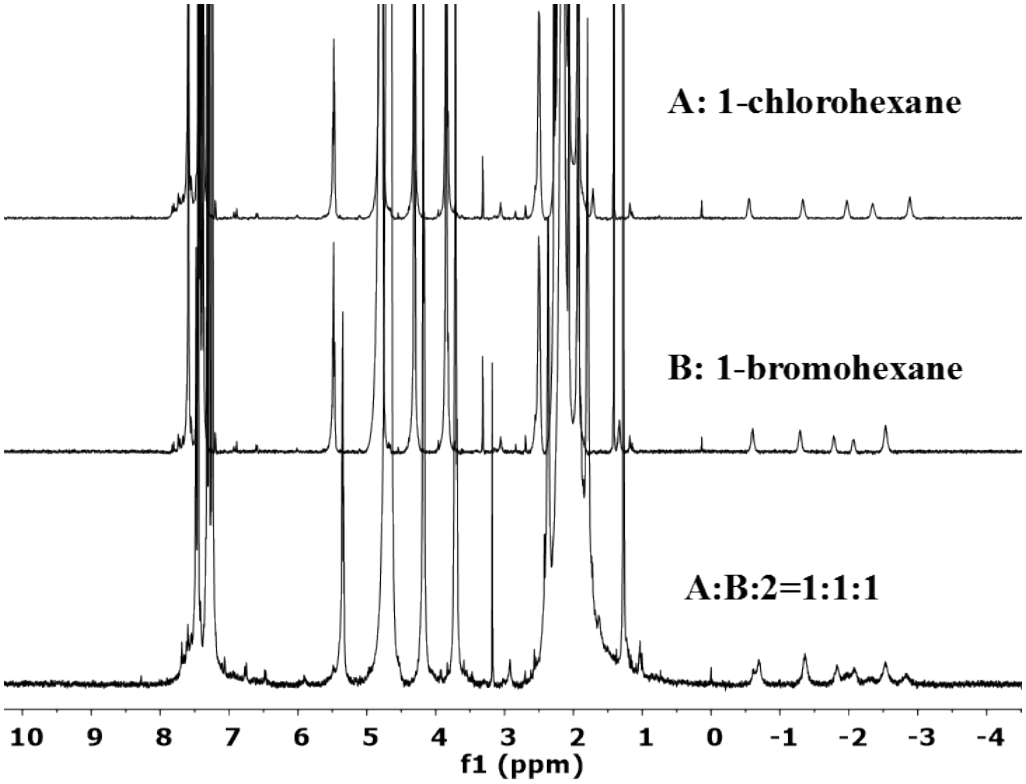

Figure S7. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **2** (1.0 mM) + 1-chlorohexane (1.0 mM) (1:1), cavitand **2** (1.0 mM) + 1-bromohexane (1.0 mM) (1:1), cavitand **2** (1.0 mM) + 1-chlorohexane (1.0 mM) + 1-bromohexane (1.0 mM) (1:1:1).

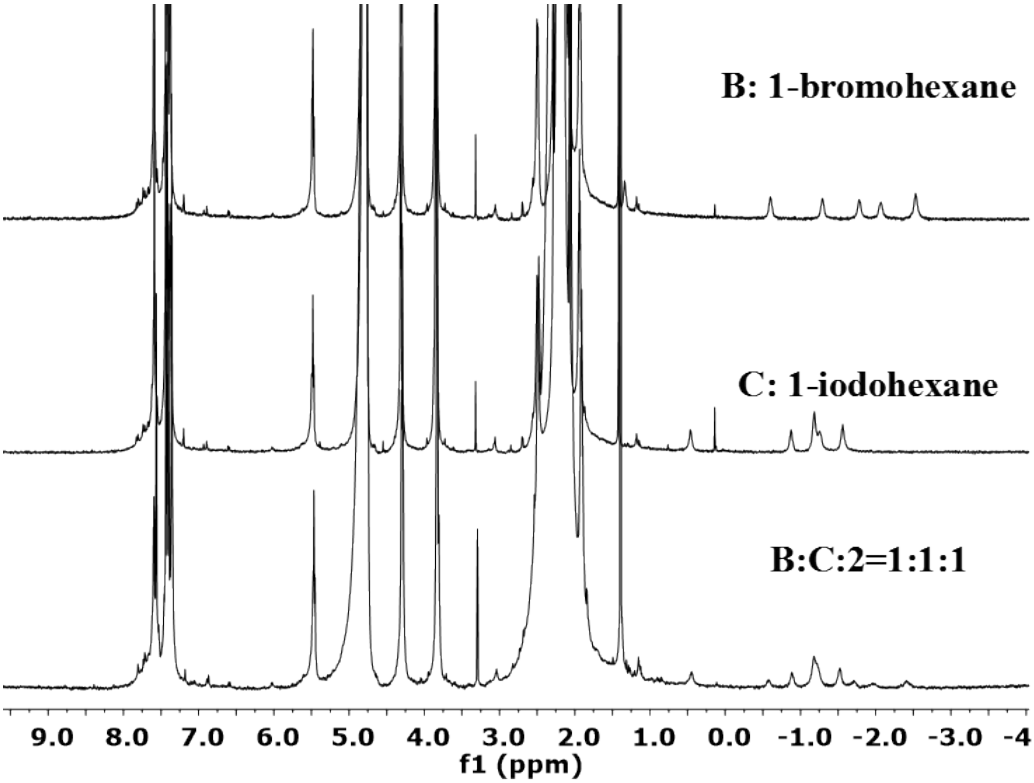

Figure S8. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **2** (1.0 mM) + 1-bromohexane (1.0 mM) (1:1), cavitand **2** (1.0 mM) + 1-iodohexane (1.0 mM) (1:1), cavitand **2** (1.0 mM) + 1-bromohexane (1.0 mM) + 1-iodohexane (1.0 mM) (1:1:1).

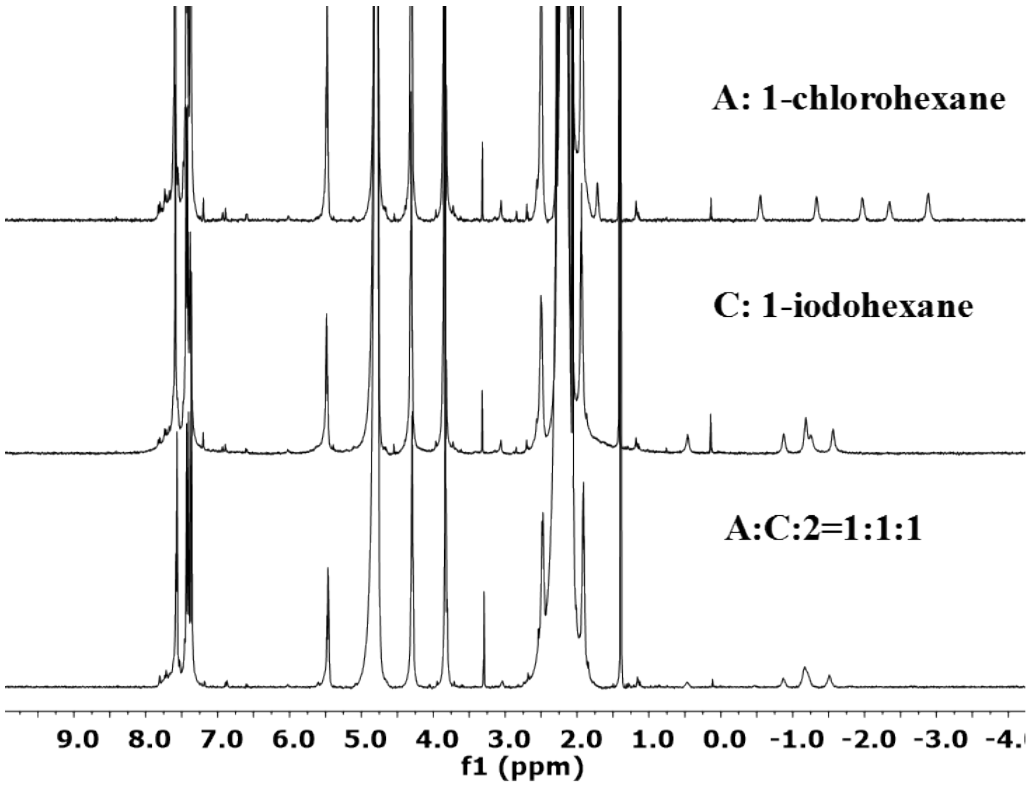

Figure S9. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **2** (1.0 mM) + 1-chlorohexane (1.0 mM) (1:1), cavitand **2** (1.0 mM) + 1-iodohexane (1.0 mM) (1:1), cavitand **2** (1.0 mM) + 1-chlorohexane (1.0 mM) + 1-iodohexane (1.0 mM) (1:1:1).

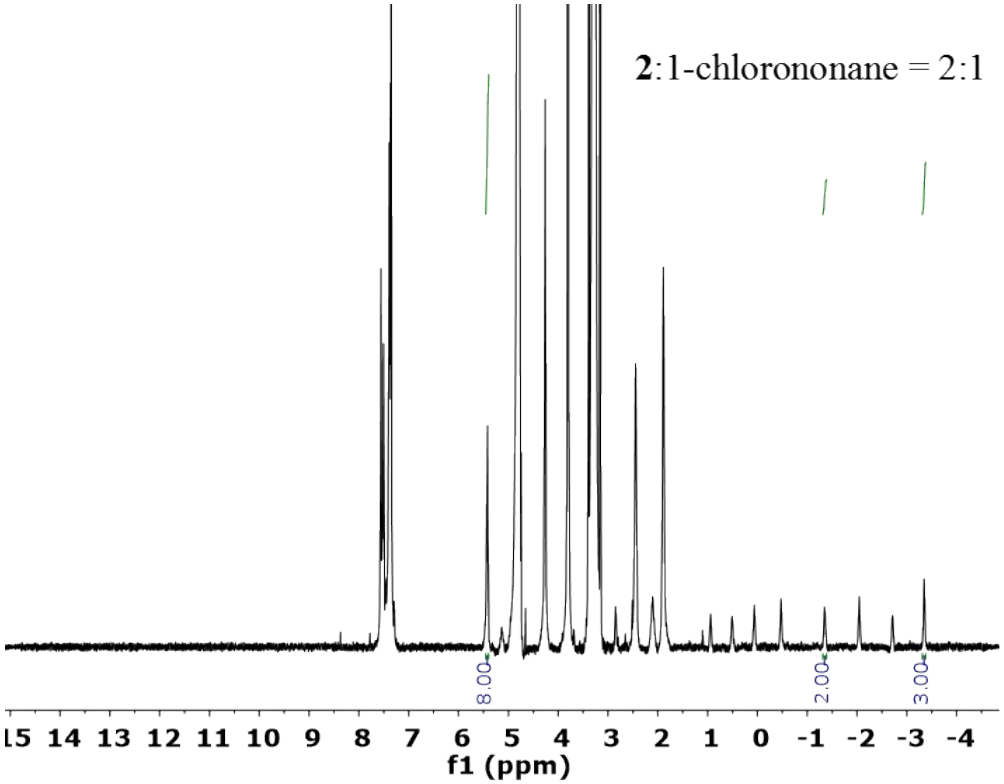

Figure S10. ^{1}H NMR spectra (600MHz, D_2O, 298K) of cavitand **2** (1.0 mM) + 1-chlorononane (0.5 mM) (2:1).