New Journal of Chemistry

Supporting Information

Cucurbit[8]uril Forms Tight Inclusion Complexes with Cationic Triamantanes

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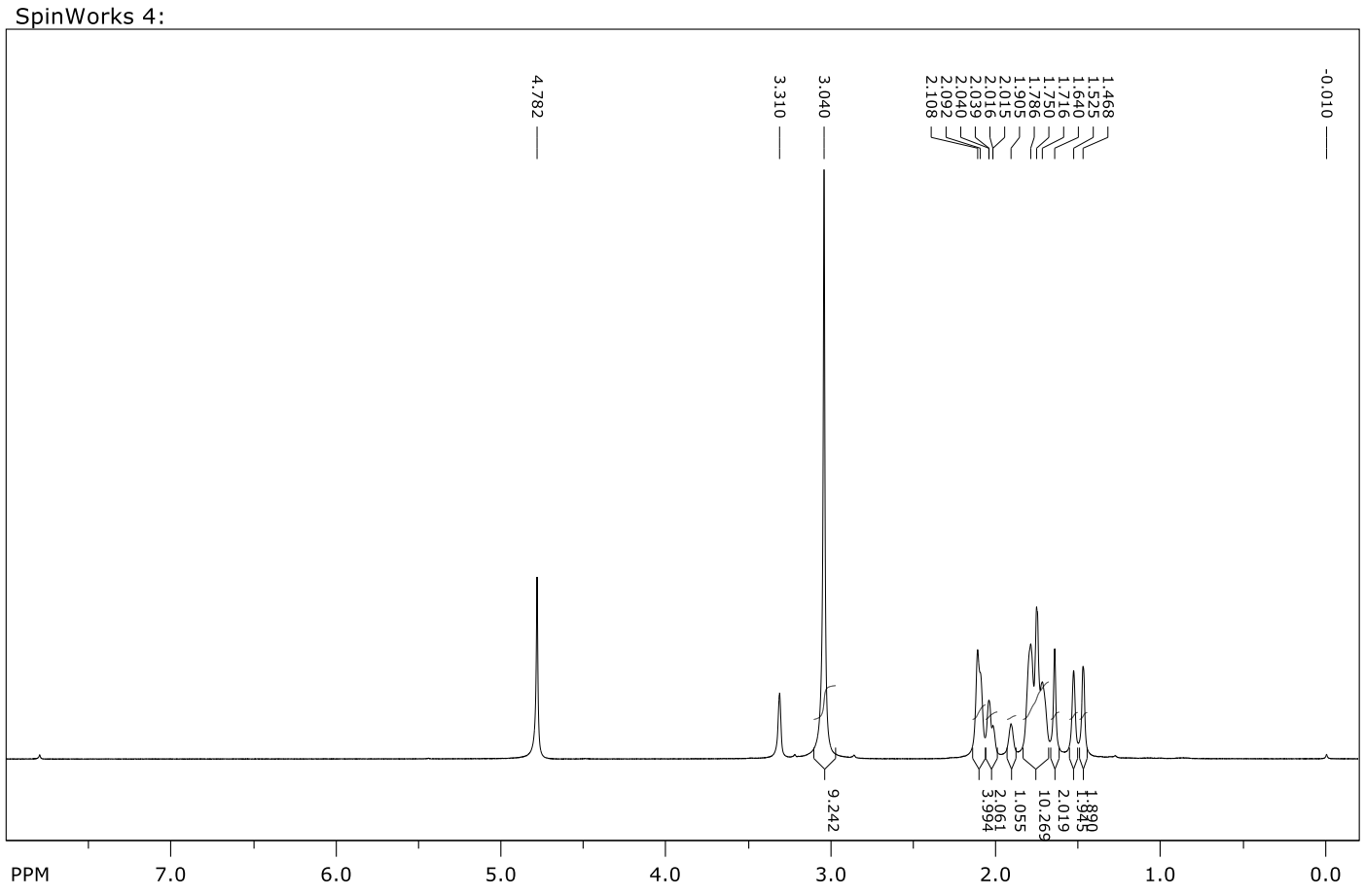

Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$ + few drops of CD_3OD) recorded for *N*,*N*,*N*-trimethyltriamantane-9-aminium iodide (**G1**•I^-).

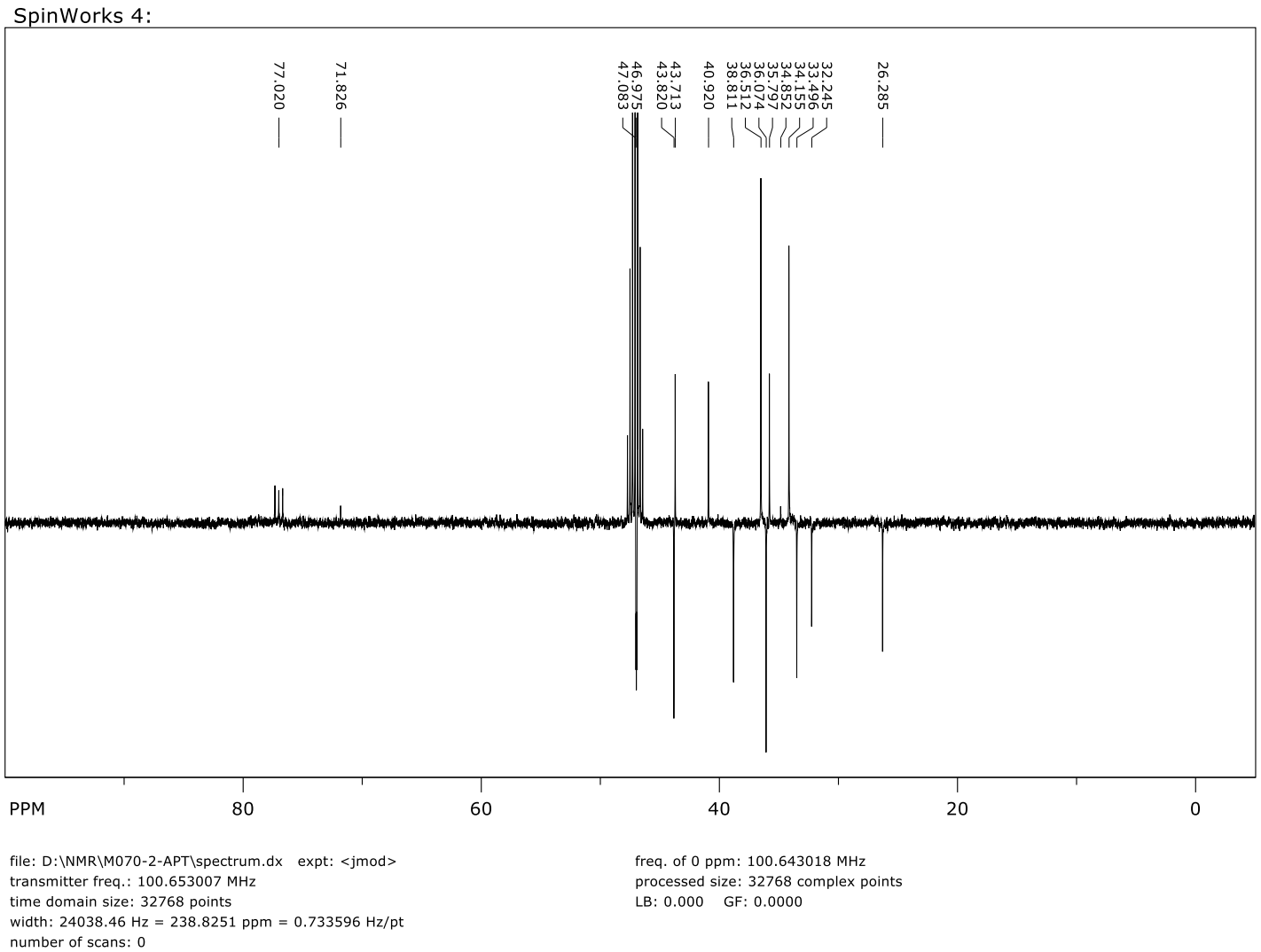

Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$ + few drops of CD_3OD) of *N*,*N*,*N*-trimethyltriamantane-9-aminium iodide (**G1**•I^-).

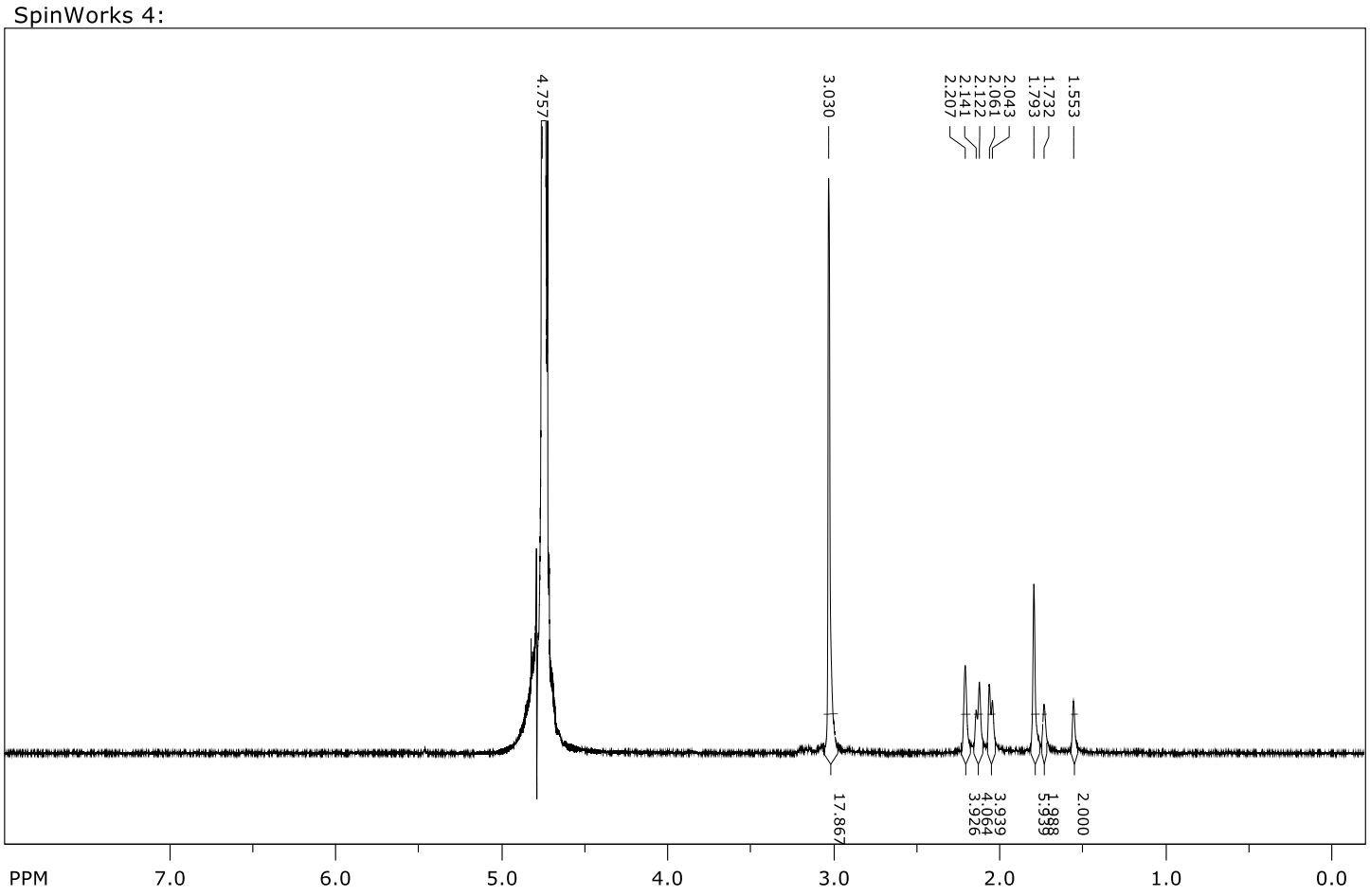

Figure S3. ^{1}H NMR (600 MHz, D_2O) recorded for *N*,*N*,*N*,*N*',*N*',*N*'-hexamethyltriamantane-9,15-diaminium diiodide (**G3**•2I^{-}).

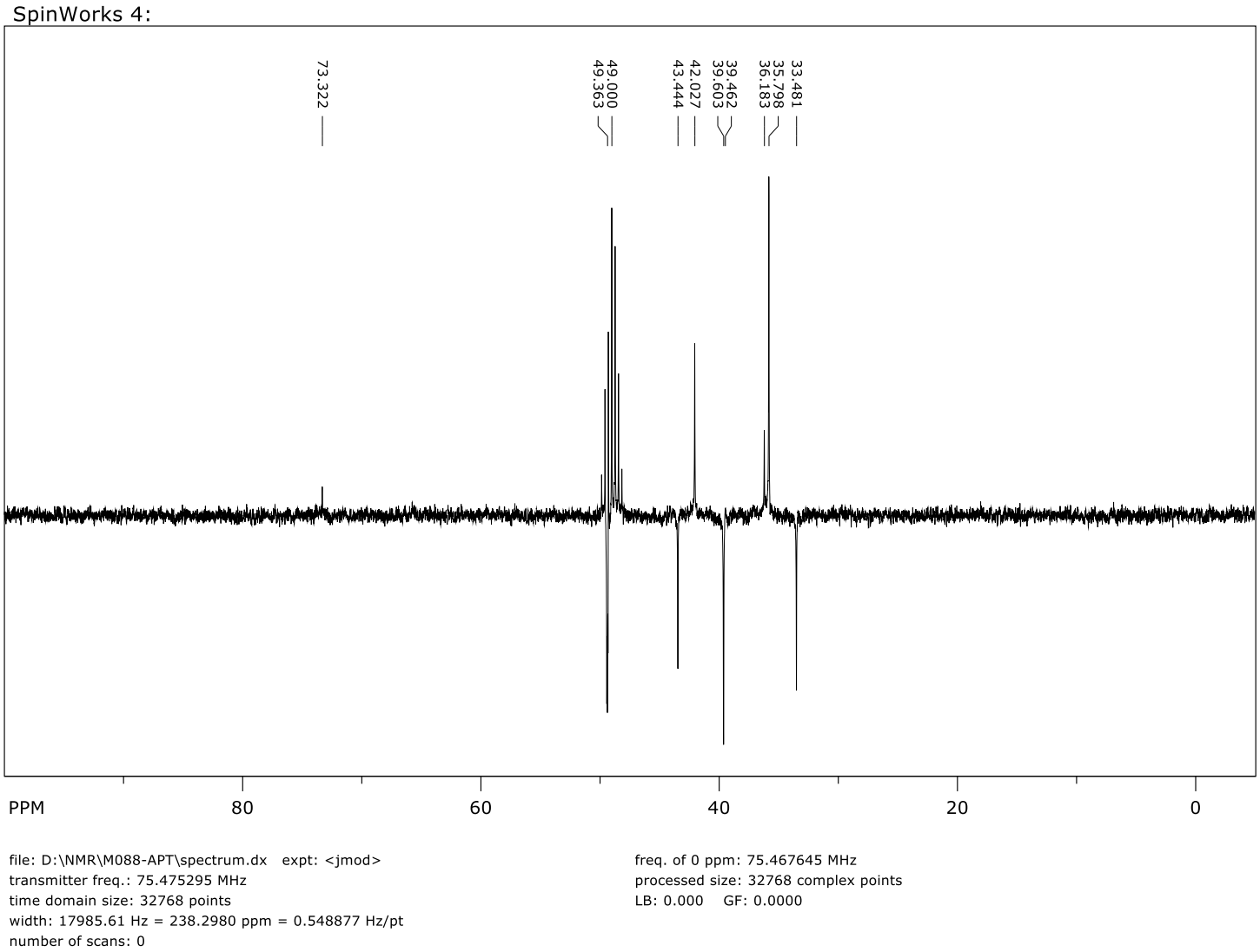

Figure S4. ^{13}C NMR (75 MHz, CD_3OD) recorded for *N*,*N*,*N*,*N*',*N*',*N*'-hexamethyltriamantane-9,15-diaminium diiodide (**G3**•2I$^-$).

^{1}H NMR binding studies for CB[7] and CB[8] toward triamantanes G1 – G4

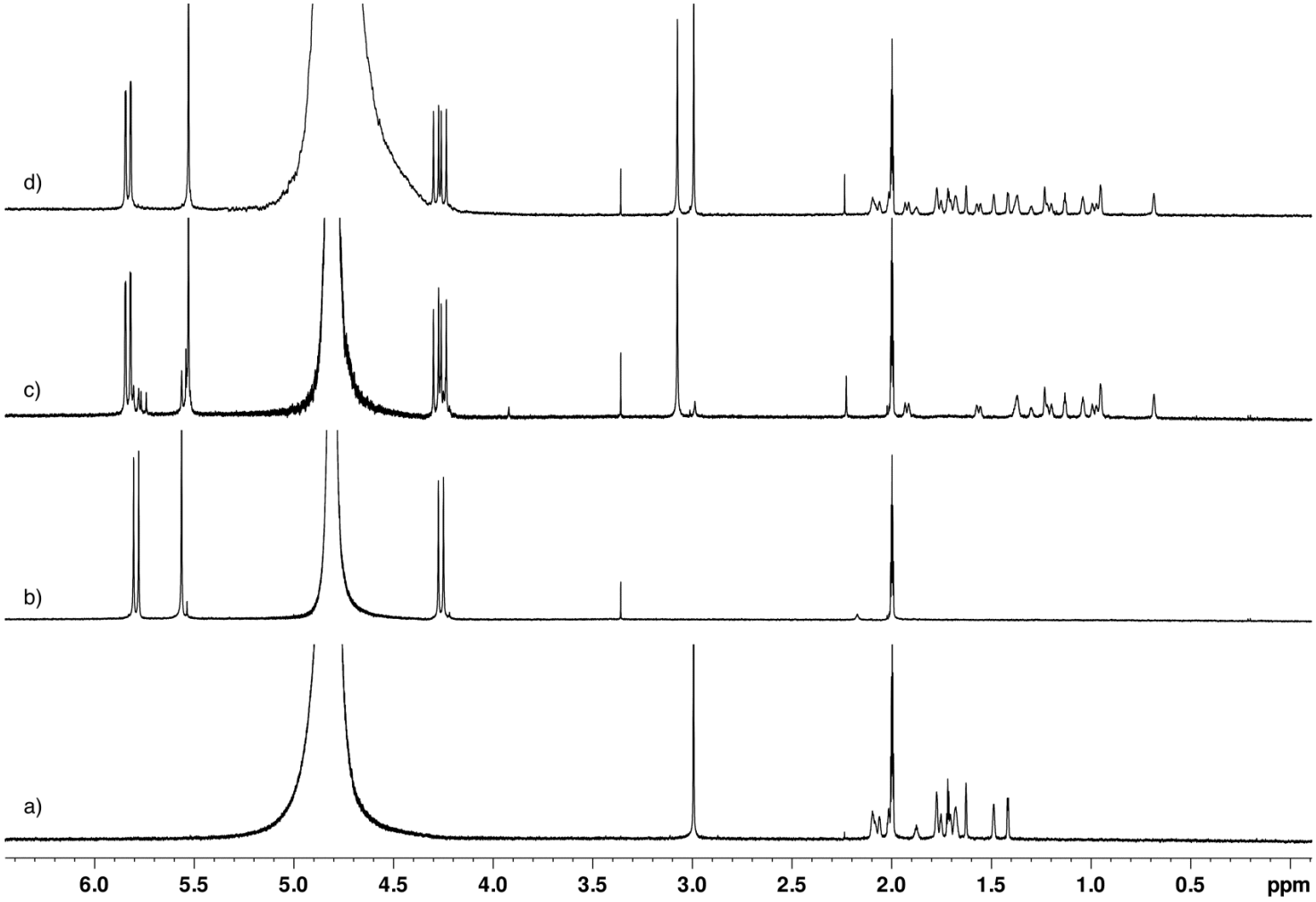

Figure S5. ^{1}H NMR spectra recorded (600 MHz, RT, 50 mM NaO_2CCD_3, pD 4.74) for: a) **G1** (0.5 mM), b) CB[7] (0.2 mM), c) an equimolar mixture of **G1** and CB[7] (0.2 mM), and d) a mixture of **G1** (0.4 mM) and CB[7] (0.2 mM).

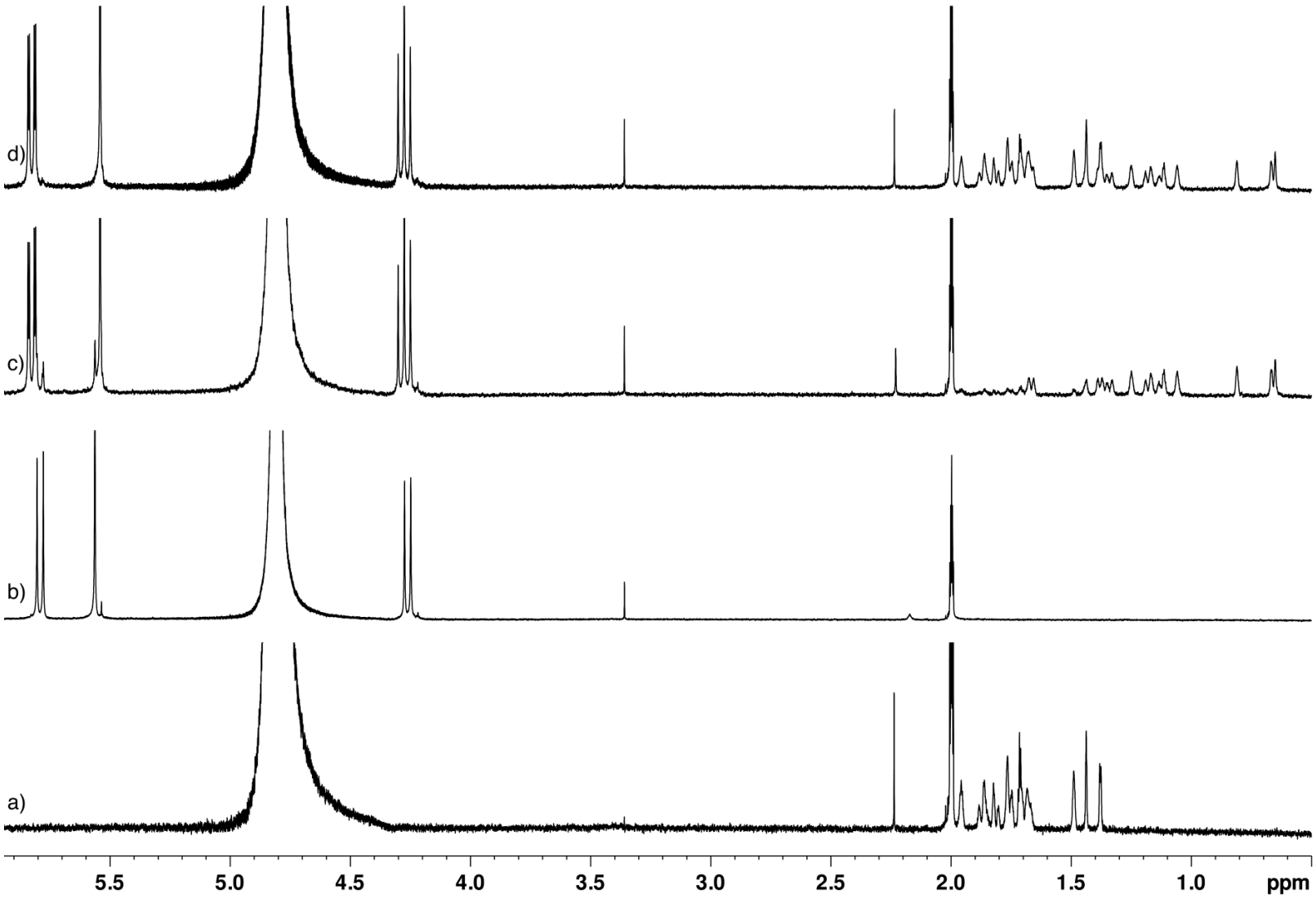

Figure S6. ^{1}H NMR spectra recorded (600 MHz, RT, 50 mM NaO_2CCD_3, pD 4.74) for: a) **G2** (0.5 mM), b) CB[7] (0.2 mM), c) an equimolar mixture **G2** and CB[7] (0.2 mM), and d) a mixture of **G2** (0.4 mM) and CB[7] (0.2 mM).

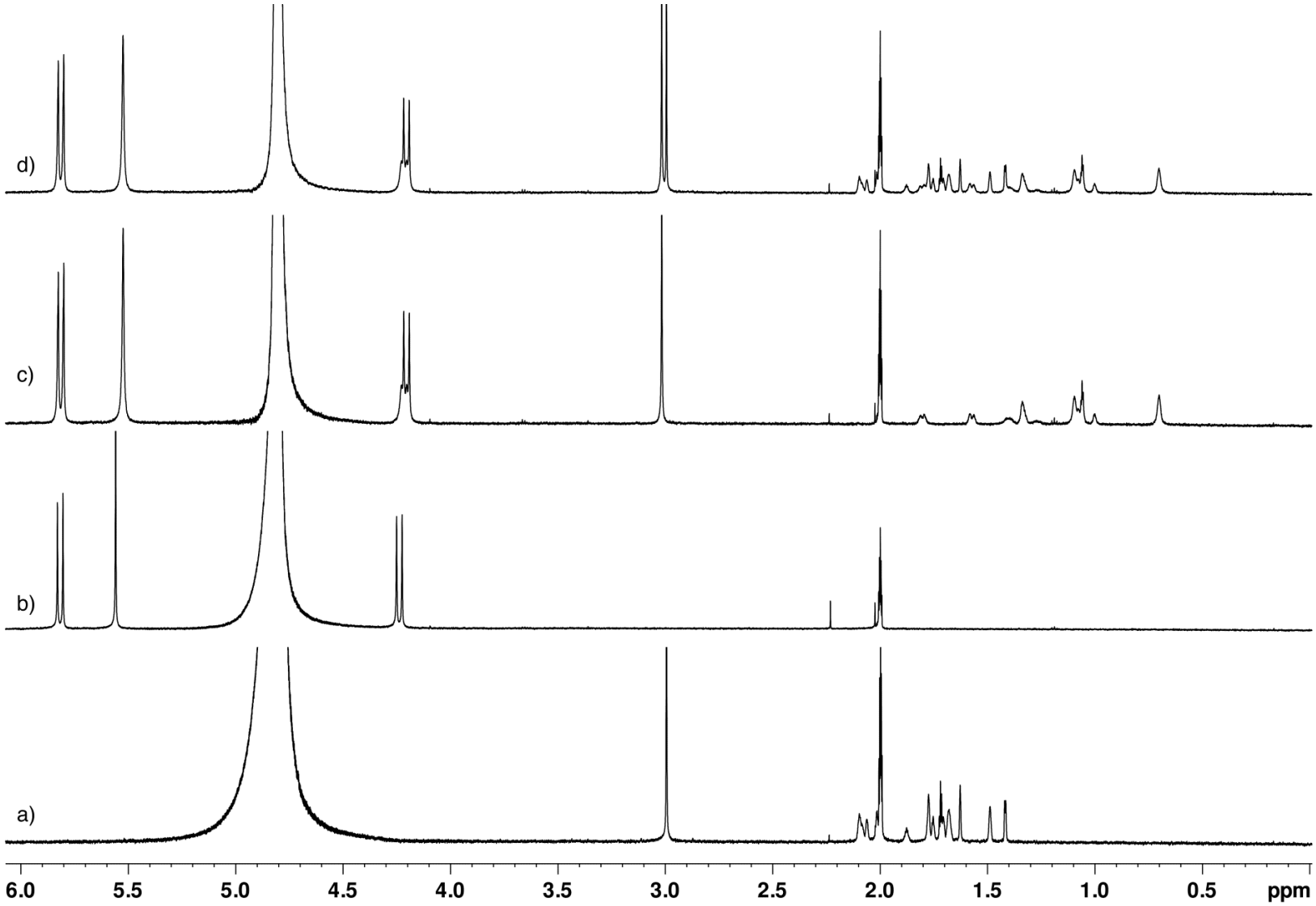

Figure S7. ^{1}H NMR spectra recorded (600 MHz, RT, 50 mM NaO_2CCD_3, pD 4.74) for: a) **G1** (0.5 mM), b) CB[8] (0.2 mM), c) an equimolar mixture of **G1** and CB[8] (0.2 mM), and d) a mixture of **G1** (0.4 mM) and CB[8] (0.2 mM).

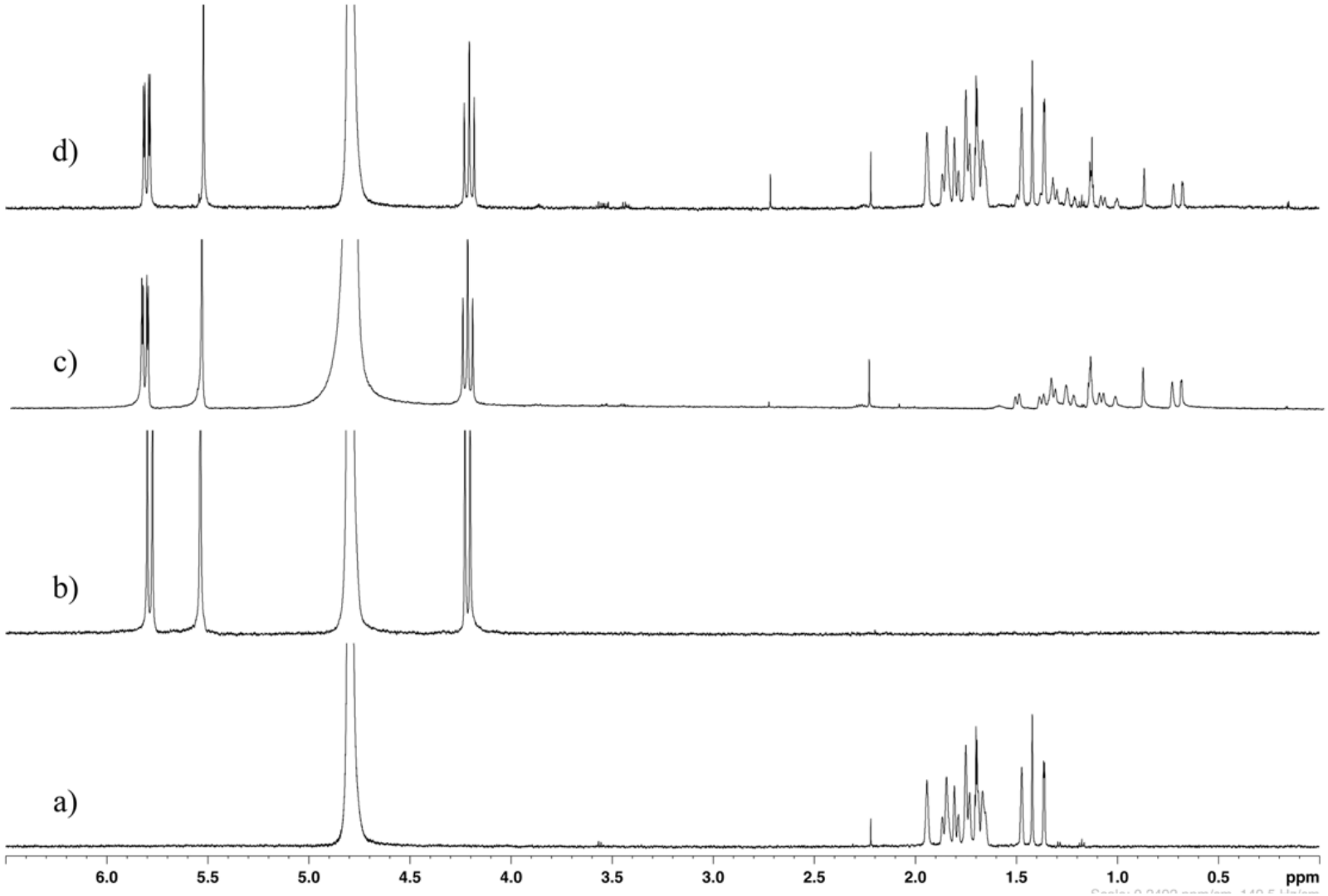

Figure S8. ^{1}H NMR spectra recorded (600 MHz, RT, D_2O) for: a) **G2** (0.5 mM), b) CB[8] (0.2 mM), c) an equimolar mixture of **G2** and CB[8] (0.2 mM), and d) a mixture of **G2** (0.4 mM) and CB[8] (0.2 mM). The CB[8]•**G2** complex precipitates from solution but can be made temporarily soluble by heating to obtain the NMR spectra given above.

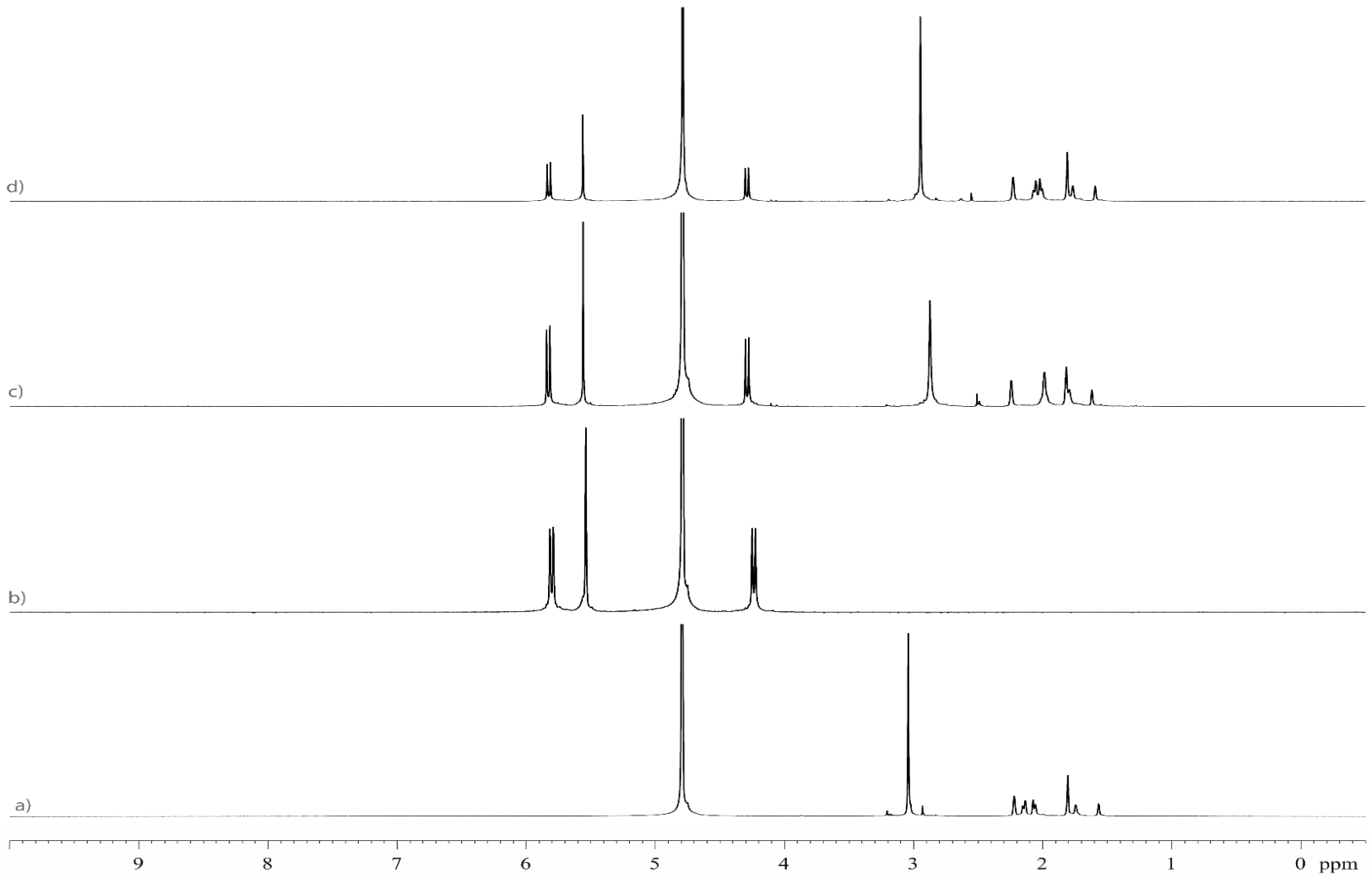

Figure S9. ^{1}H NMR spectra recorded for (600 MHz, RT, D_2O) for: a) **G3** (1.0 mM), b) CB[7] (1.0 mM), c) an equimolar mixture of **G3** and CB[7] (1.0 mM), and d) a mixture of **G3** (2.0 mM) and CB[7] (1.0 mM).

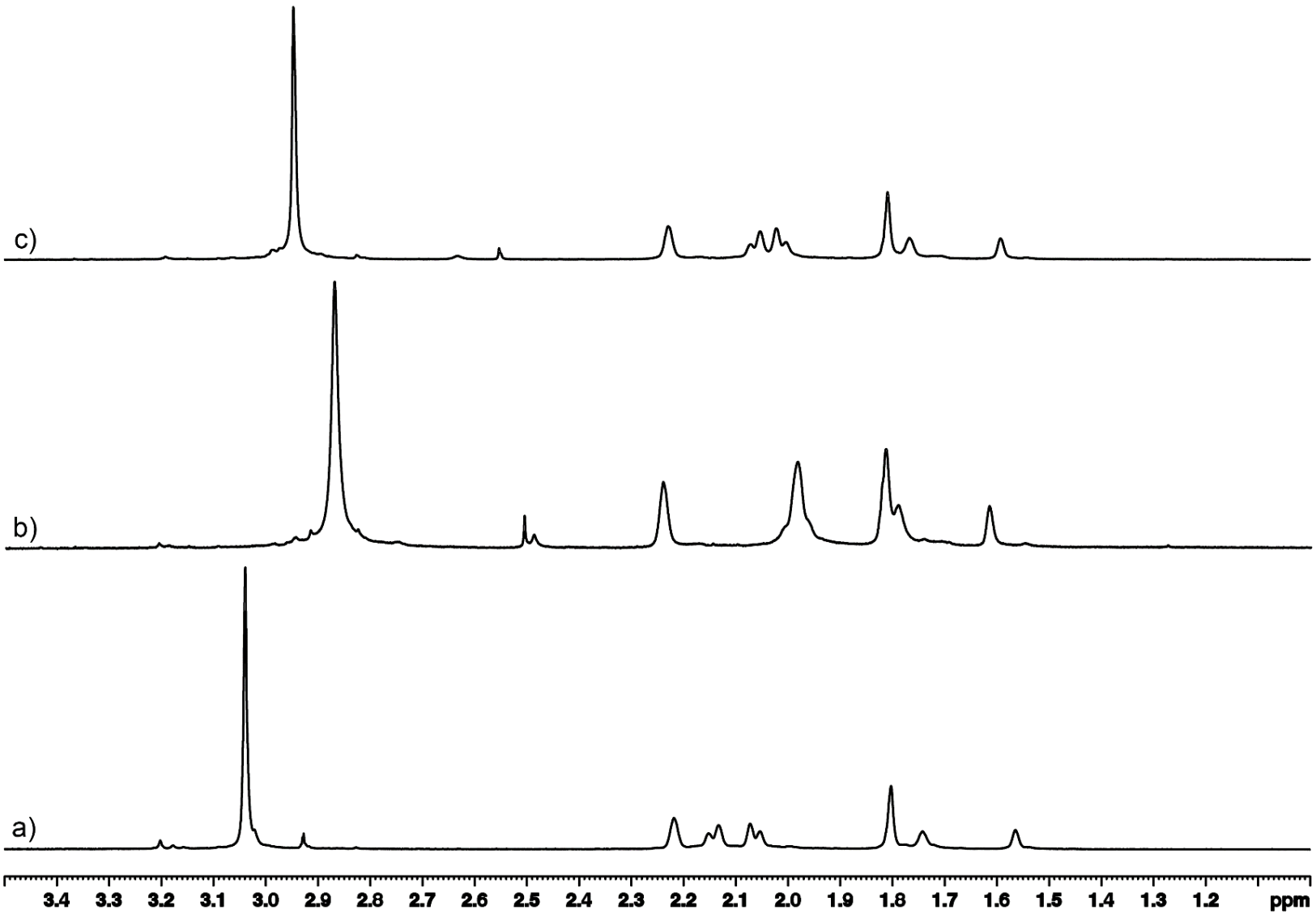

Figure S10. The expanded guest region for ^{1}H NMR spectra recorded for (600 MHz, RT, D_2O) for: a) **G3** (1.0 mM), b) an equimolar mixture of **G3** and CB[7] (1.0 mM), and c) a mixture of **G3** (2.0 mM) and CB[7] (1.0 mM).

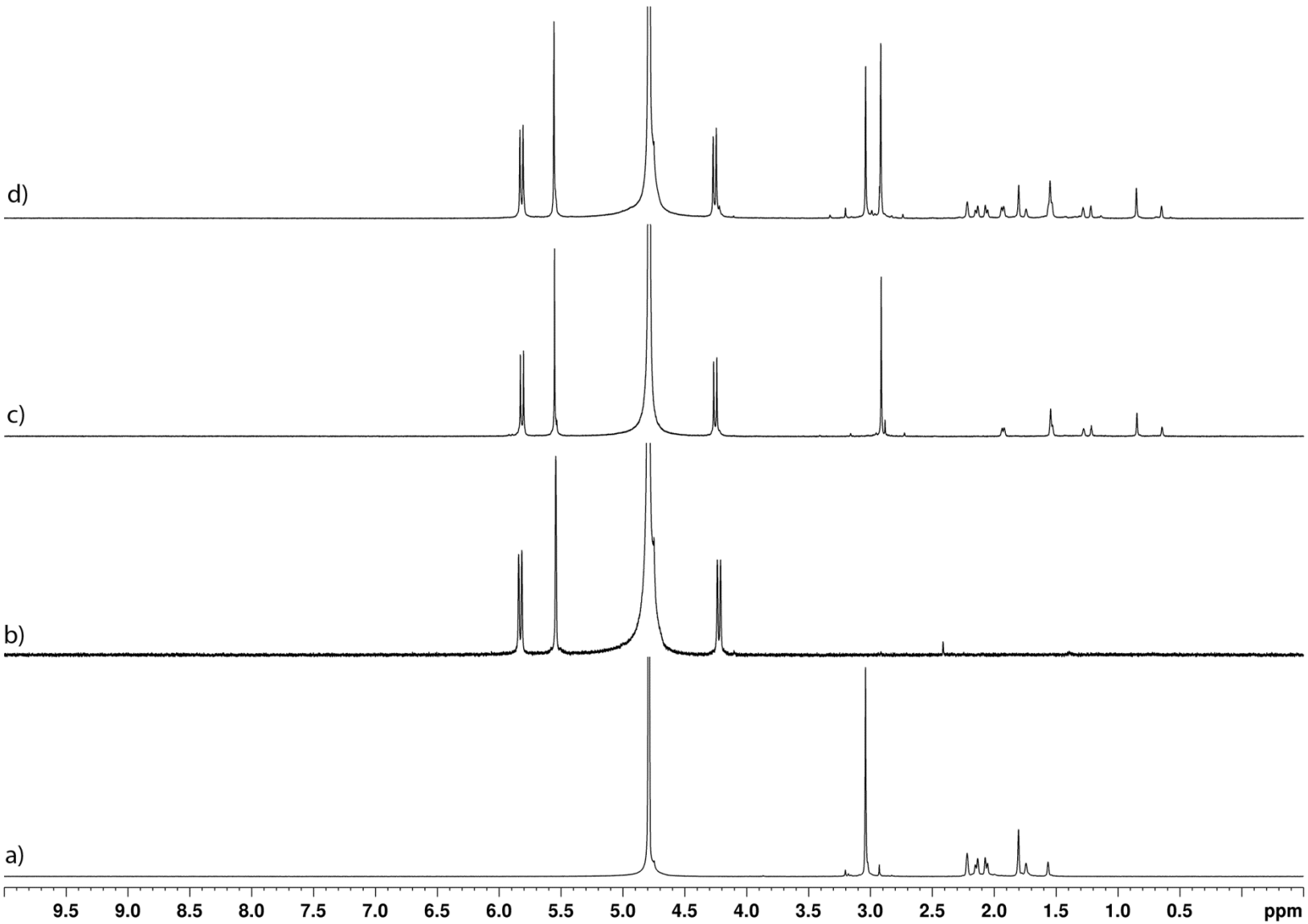

Figure S11. ^{1}H NMR spectra recorded for (600 MHz, RT, D_2O) for: a) **G3** (1.0 mM), b) CB[8] (0.5 mM), c) an equimolar mixture of **G3** and CB[8] (0.5 mM), and d) a mixture of **G3** (1.0 mM) and CB[8] (0.5 mM).

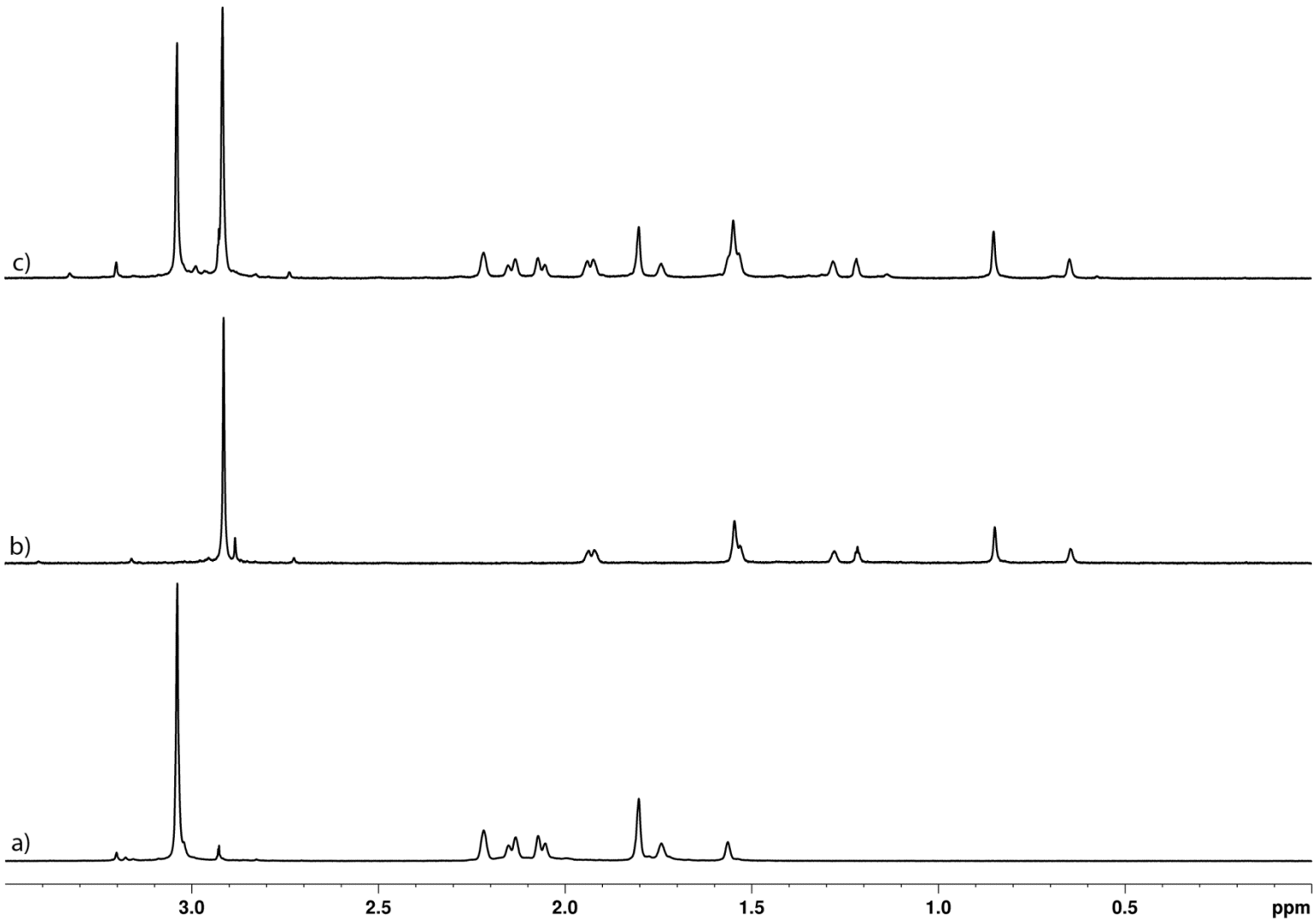

Figure S12. The expanded guest region for ^{1}H NMR spectra recorded for (600 MHz, RT, D_2O) for: a) **G3** (1.0 mM), b) an equimolar mixture of **G3** and CB[8] (0.5 mM), and c) a mixture of **G3** (1.0 mM) and CB[8] (0.5 mM).

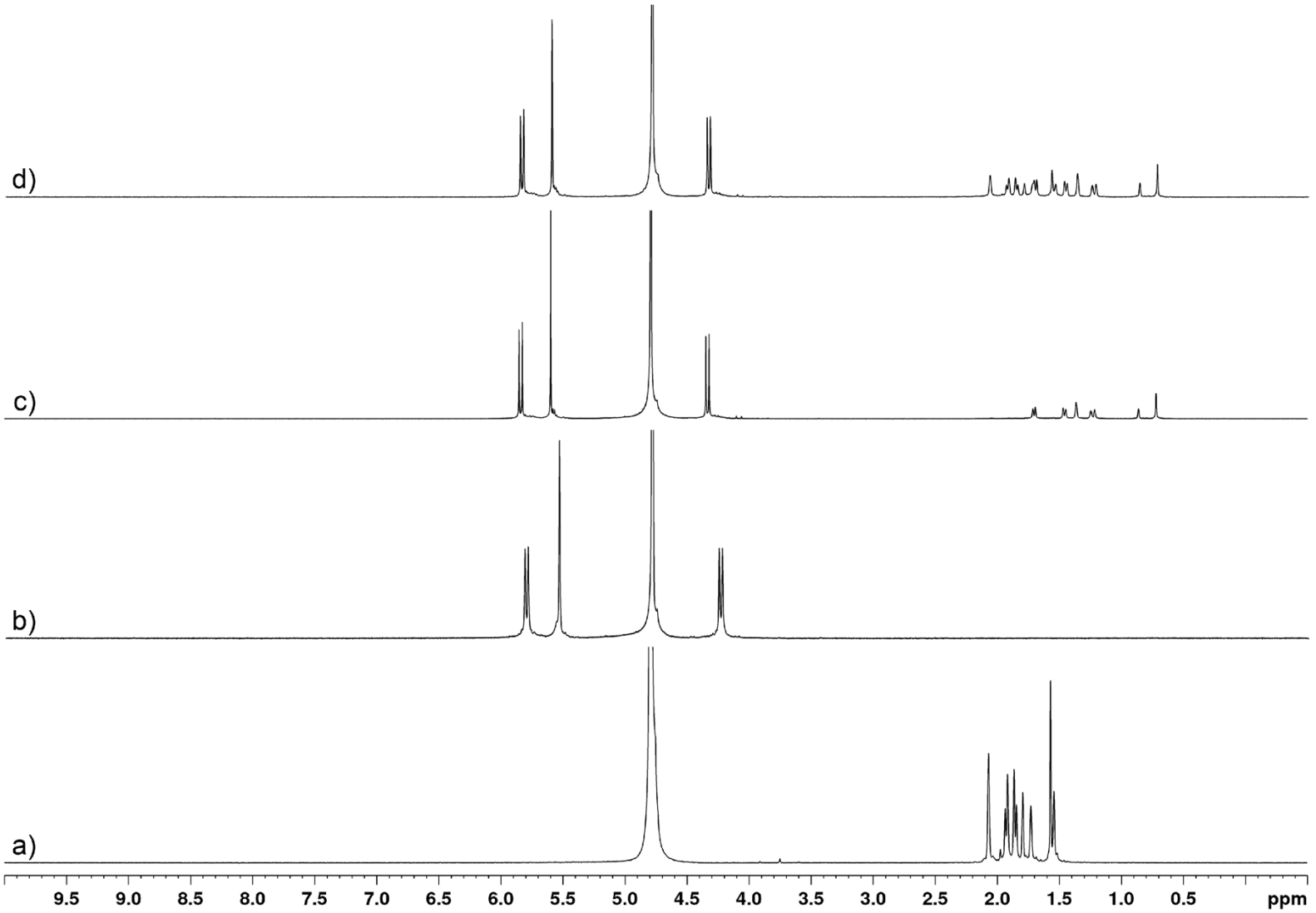

Figure S13. ^{1}H NMR spectra recorded for (600 MHz, RT, D_2O) for: a) **G4** (1.0 mM), b) CB[7] (1.0 mM), c) an equimolar mixture of **G4** and CB[7] (1.0 mM), and d) a mixture of **G4** (2.0 mM) and CB[7] (1.0 mM).

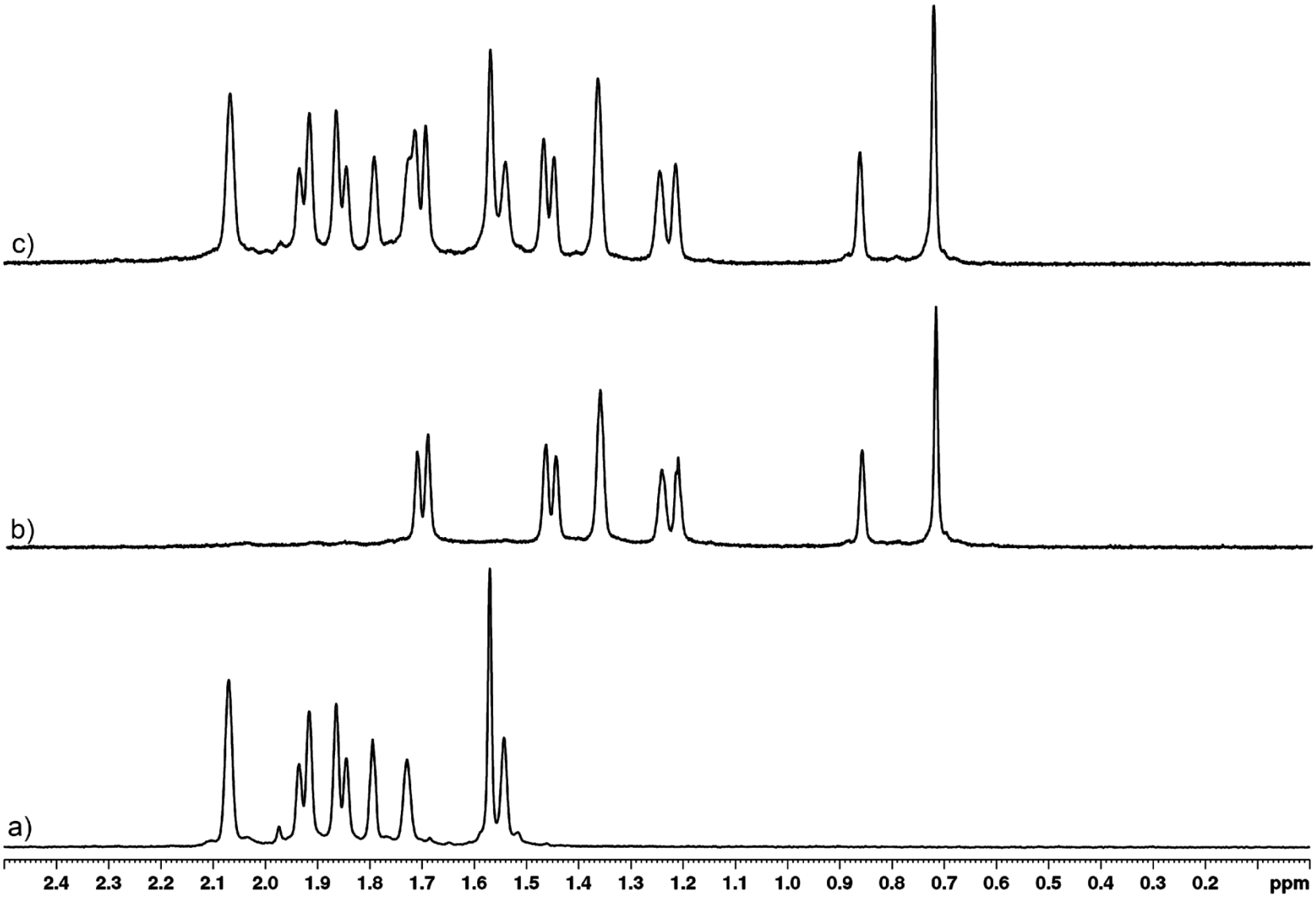

Figure S14. The expanded guest region for ^{1}H NMR spectra recorded for (600 MHz, RT, D_2O) for: a) **G4** (1.0 mM), b) an equimolar mixture of **G4** and CB[7] (1.0 mM), and c) a mixture of **G4** (2.0 mM) and CB[7] (1.0 mM).

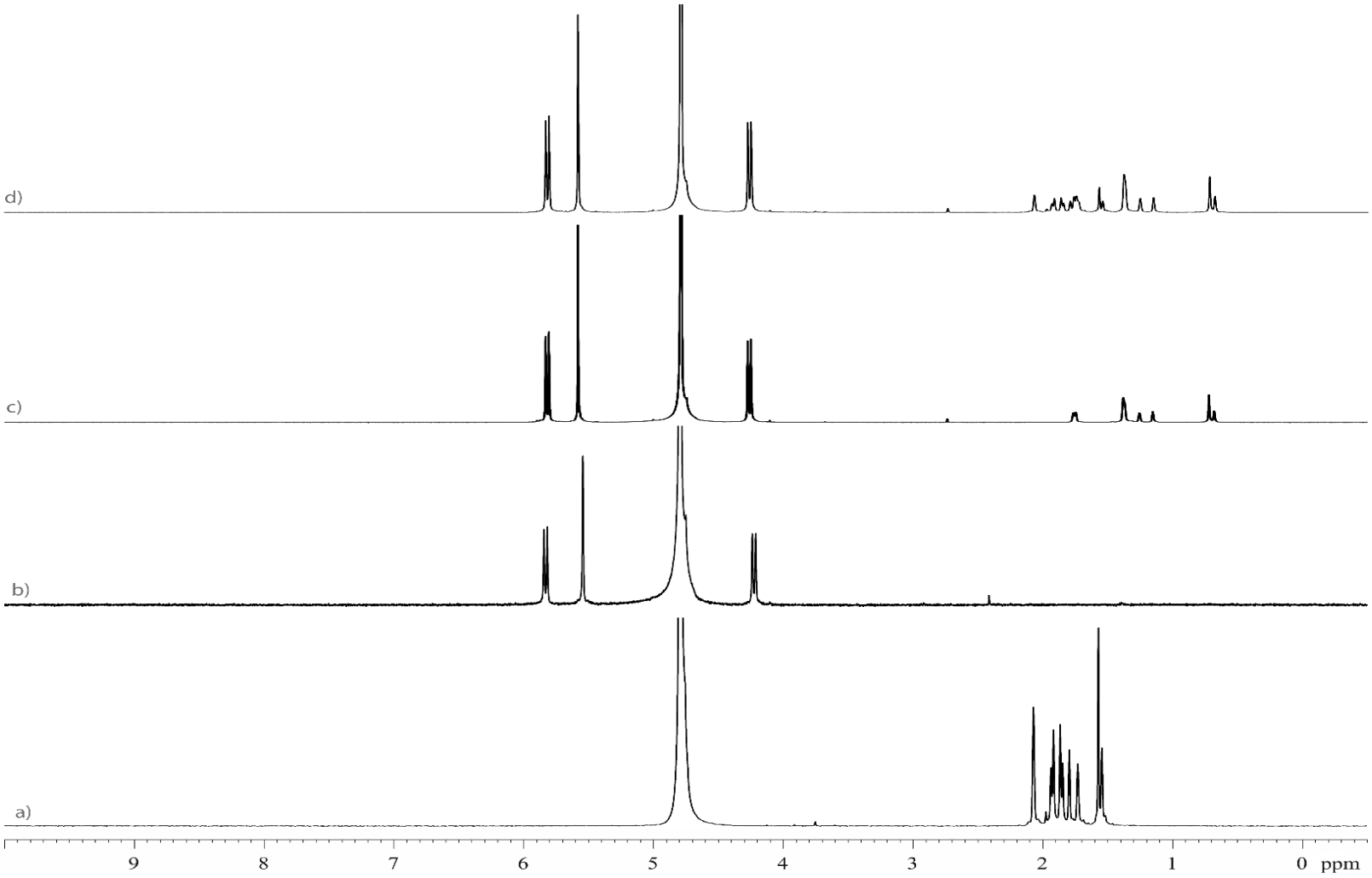

Figure S15. ^{1}H NMR spectra recorded for (600 MHz, RT, D_2O) for: a) **G4** (1.0 mM), b) CB[8] (0.5 mM), c) an equimolar mixture of **G4** and CB[8] (1.0 mM), and d) a mixture of **G4** (2.0 mM) and CB[8] (1.0 mM).

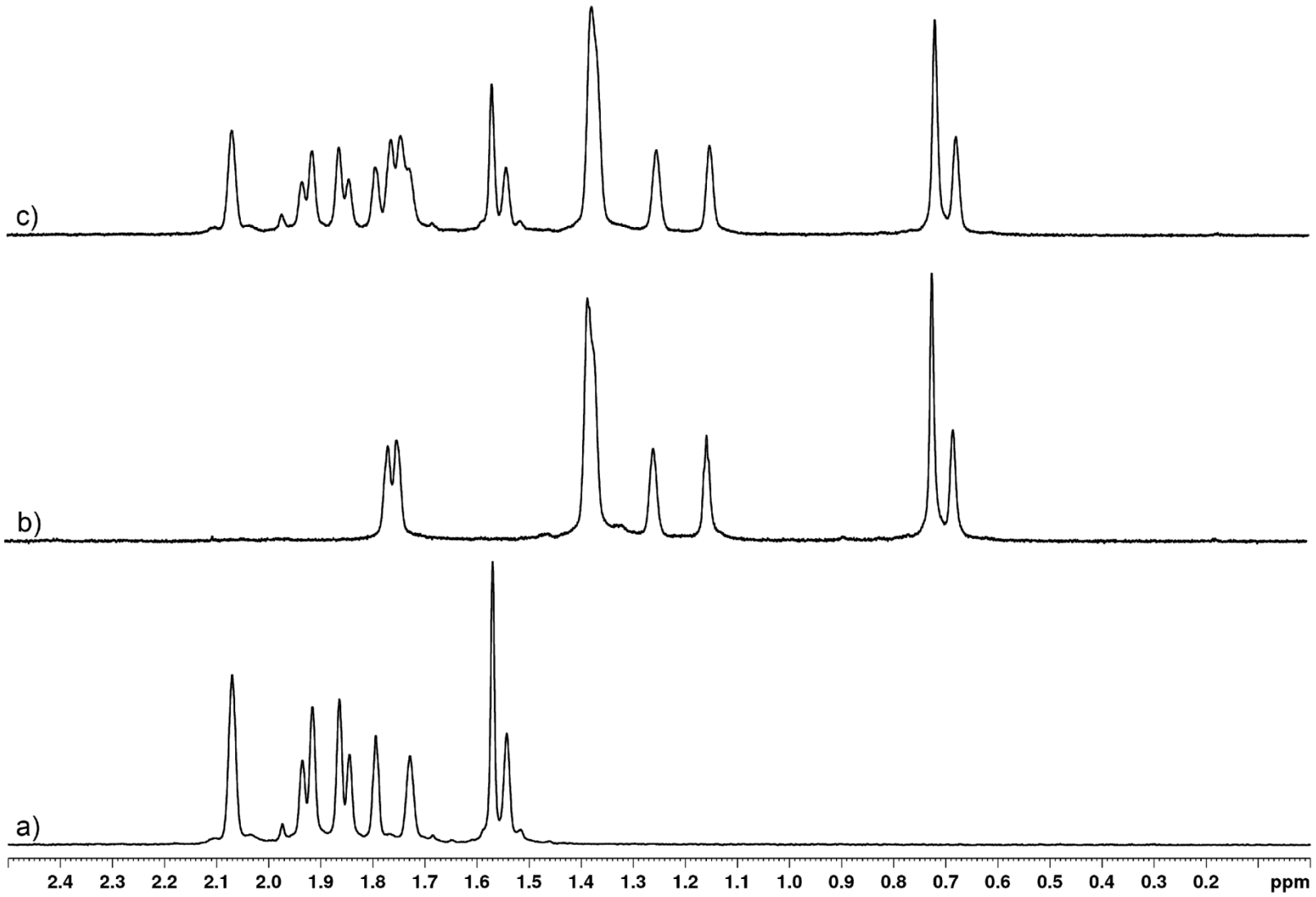

Figure S16. The expanded guest region for ^{1}H NMR spectra recorded for (600 MHz, RT, D_2O) for: a) **G4** (1.0 mM), b) an equimolar mixture of **G4** and CB[8] (1.0 mM), and c) a mixture of **G4** (2.0 mM) and CB[8] (1.0 mM).

Determination of K_a of Cucurbit[7]uril towards G1, G2 and G4 using Isothermal Titration Calorimetry (ITC).

The binding data was fitted using the single set of sites binding model in MicroCal PEAQ-ITC analysis software.

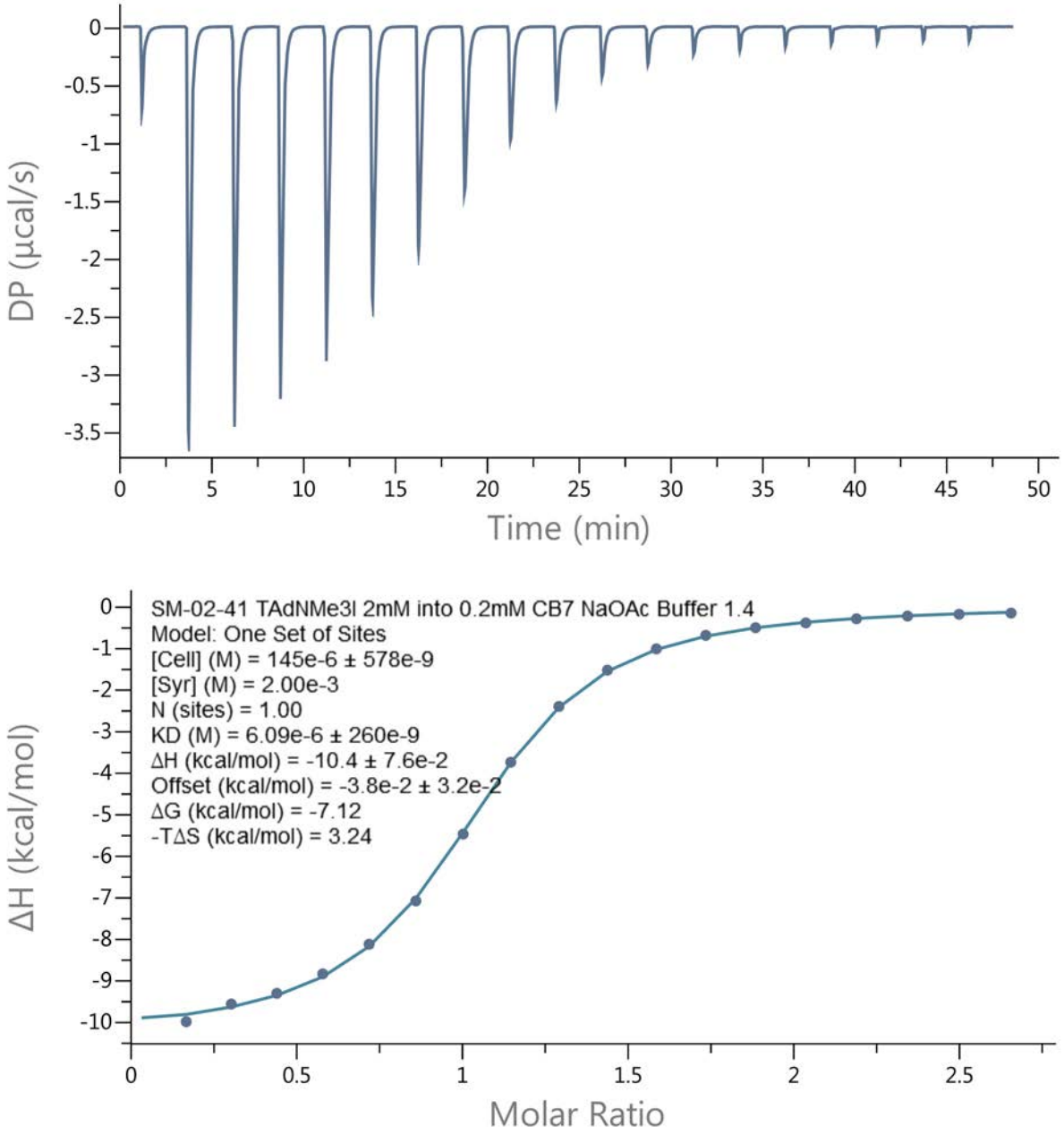

Figure S17. a) Plot of change in DP vs time from the titration of CB[7] (0.145 mM) with **G1** (0 – 0.362 mM) in 50 mM NaOAc buffered H_2O, pH = 4.74. b) Plot of the ΔH as a function of molar ratio of CB[7]:**G1**. The solid line represents the best non-linear fit of the data to a 1:1 binding model (K_a = (1.6 ± 0.1) × 10^5 M^{-1}; ΔH = (–10.4 ± 0.076) kcal mol^{-1}).

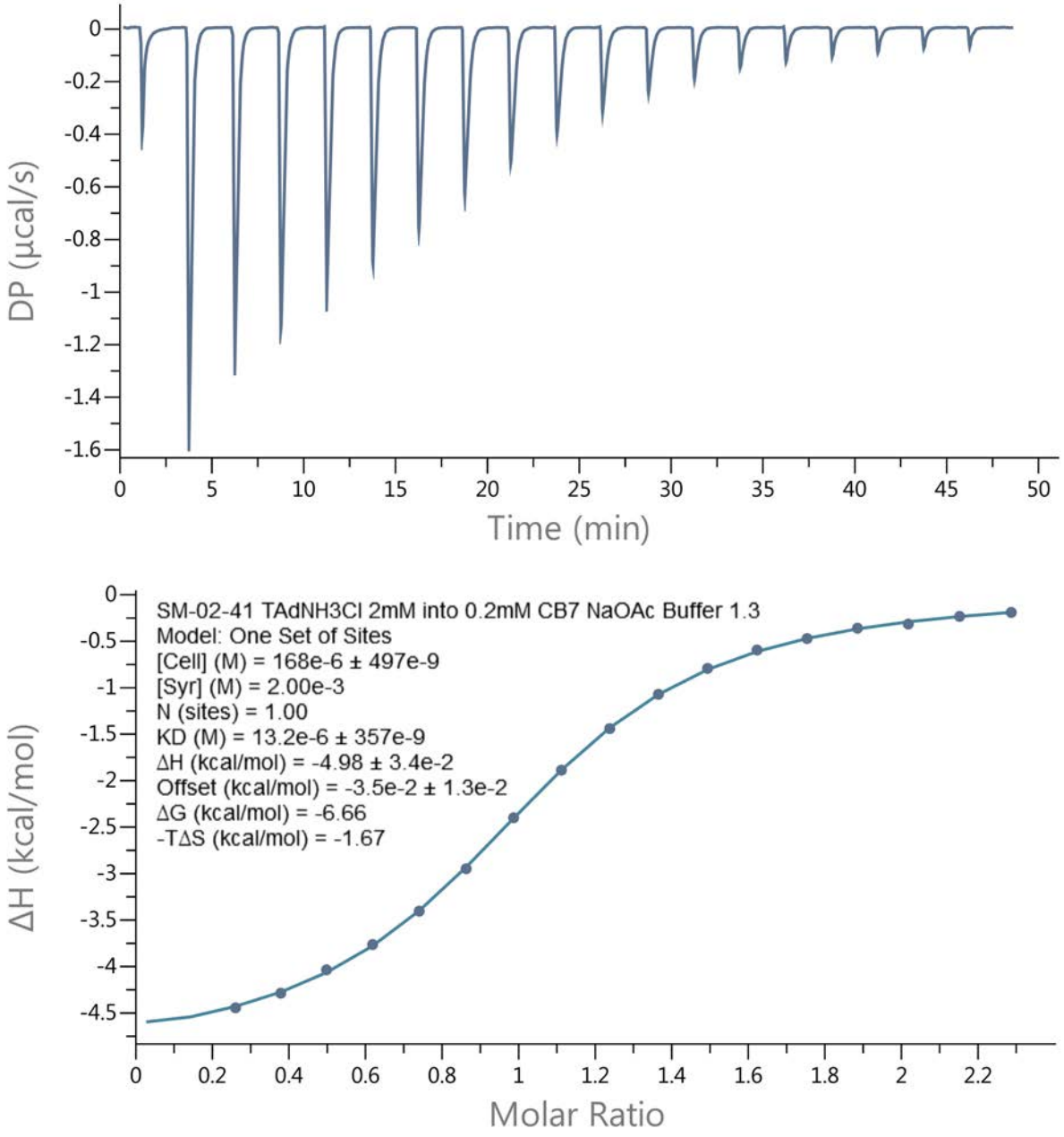

Figure S18. a) Plot of change in DP vs time from the titration of CB[7] (0.168 mM) and with **G2** (0 – 0.375 mM) in 50 mM NaOAc buffered H_2O, pH = 4.74. b) Plot of the ΔH as a function of molar ratio of CB[7]•**G2**. The solid line represents the best non-linear fit of the data to a 1:1 binding model (K_a = (7.5 ± 0.2) × 10^4 M^{-1}; ΔH = (–4.98 ± 0.034) kcal mol^{-1}).

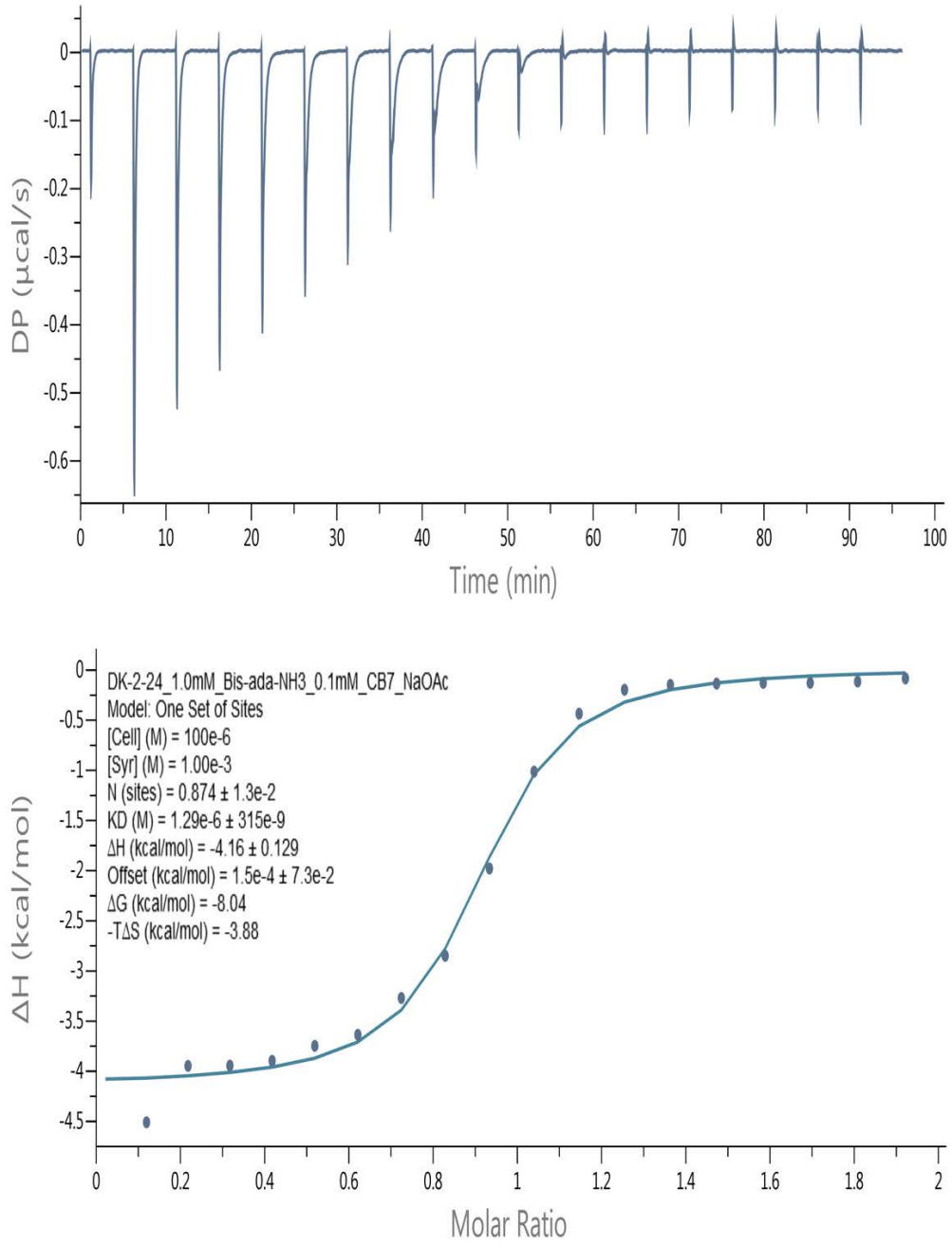

Figure S19. Isothermal Titration Calorimetry (ITC) curve obtained through direct binding titration studies. A solution of CB[7] (0.100 mM) in the cell was titrated with **G4** (1.00 mM) in the syringe at 298.0 K in 50 mM sodium acetate buffered water at pH 4.74. K_a = (7.75 ± 1.89) × 10^5 M^{-1}. Average of 3 measurements: K_a = (6.73 ± 1.41) × 10^5 M^{-1}; ΔH = (–3.79 ± 0.10) kcal mol^{-1}; $-T\Delta S$ = (–4.16 ± 0.15 kcal mol^{-1}); ΔG = (–7.96 ± 0.11) kcal mol^{-1}.

Determination of K_a of CB[7] and CB[8] towards 1, 7, and 8 using ^{1}H NMR Competition

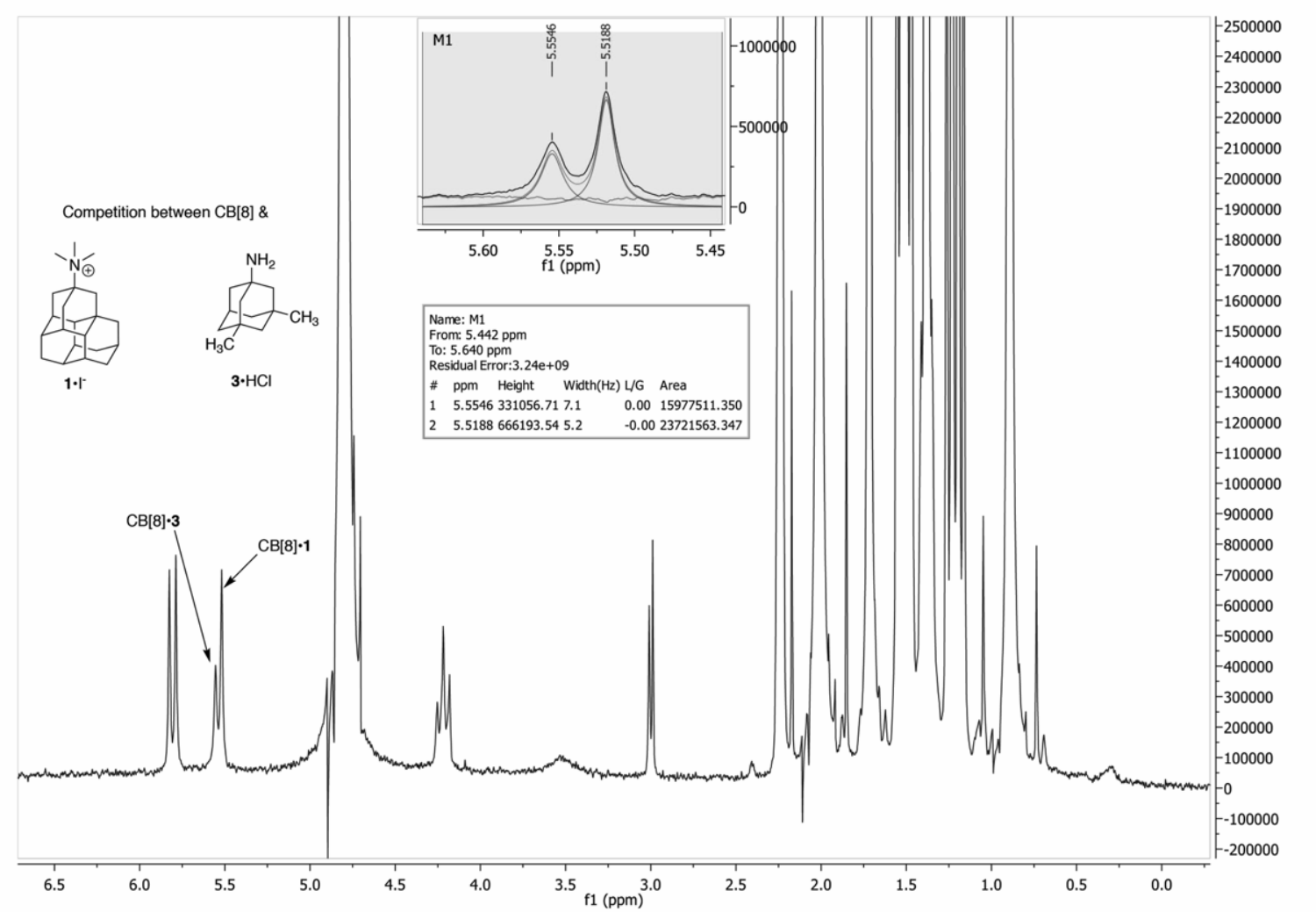

Figure S20. ^{1}H NMR spectra recorded (600 MHz, RT, 50 mM NaOAc Buffered D_2O, pH = 4.74) for a competitive mixture of CB[8] (0.100 mM), **C1** (16.5 mM), and **G1** (0.11 mM) at equilibrium. K_{rel} = 493.8 (Equilibrium was studied starting from both directions and gave the same K_{rel} value).

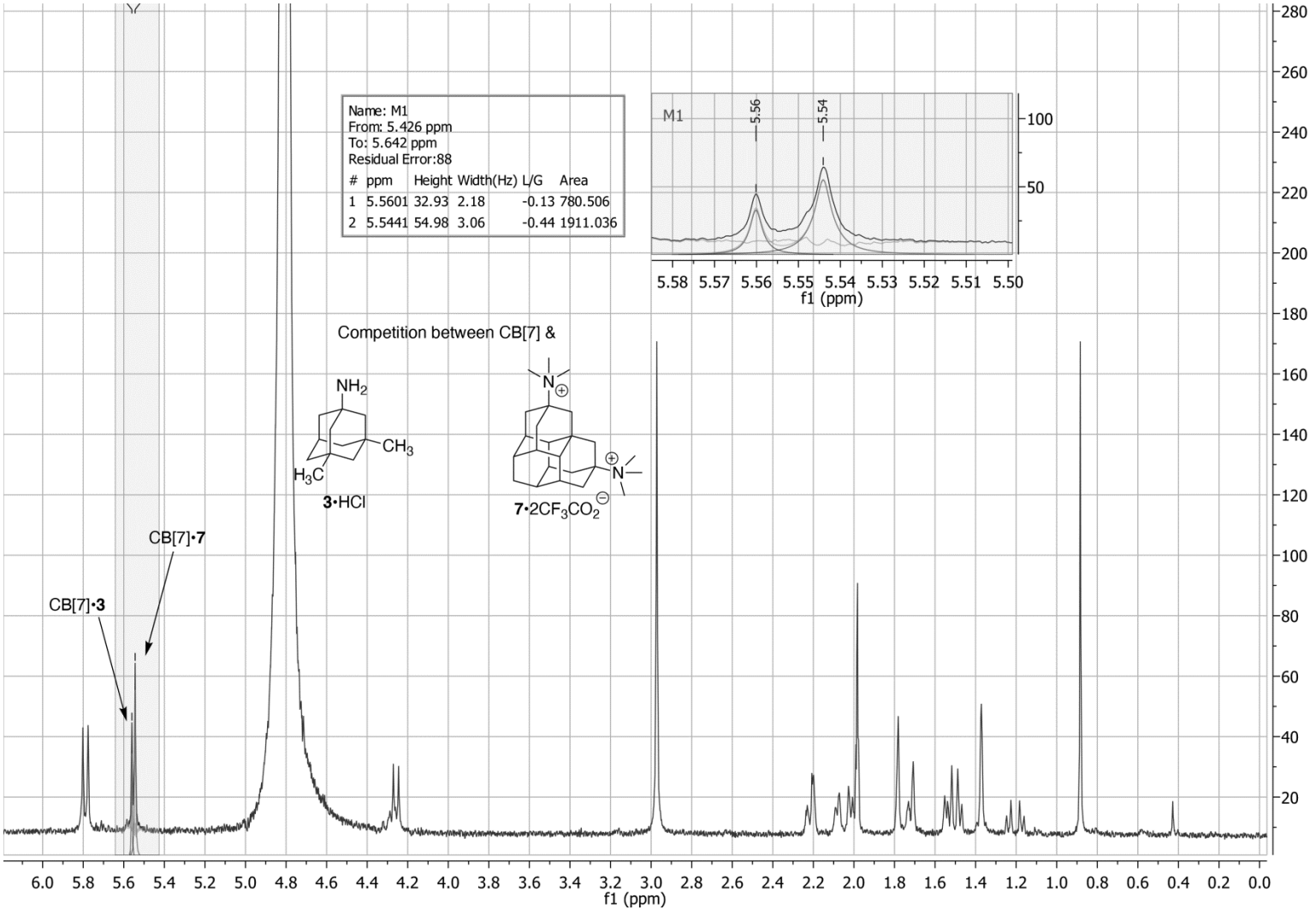

Figure S21. ^{1}H NMR spectra recorded (600 MHz, RT, 50 mM NaOAc Buffered D_2O, pH = 4.74) for a competitive mixture of CB[7] (0.100 mM), **C1** (0.22 mM), and **G3** (0.11 mM) at equilibrium. K_{rel} = 11.99 (Equilibrium was studied starting from both directions and gave the same K_{rel} value).

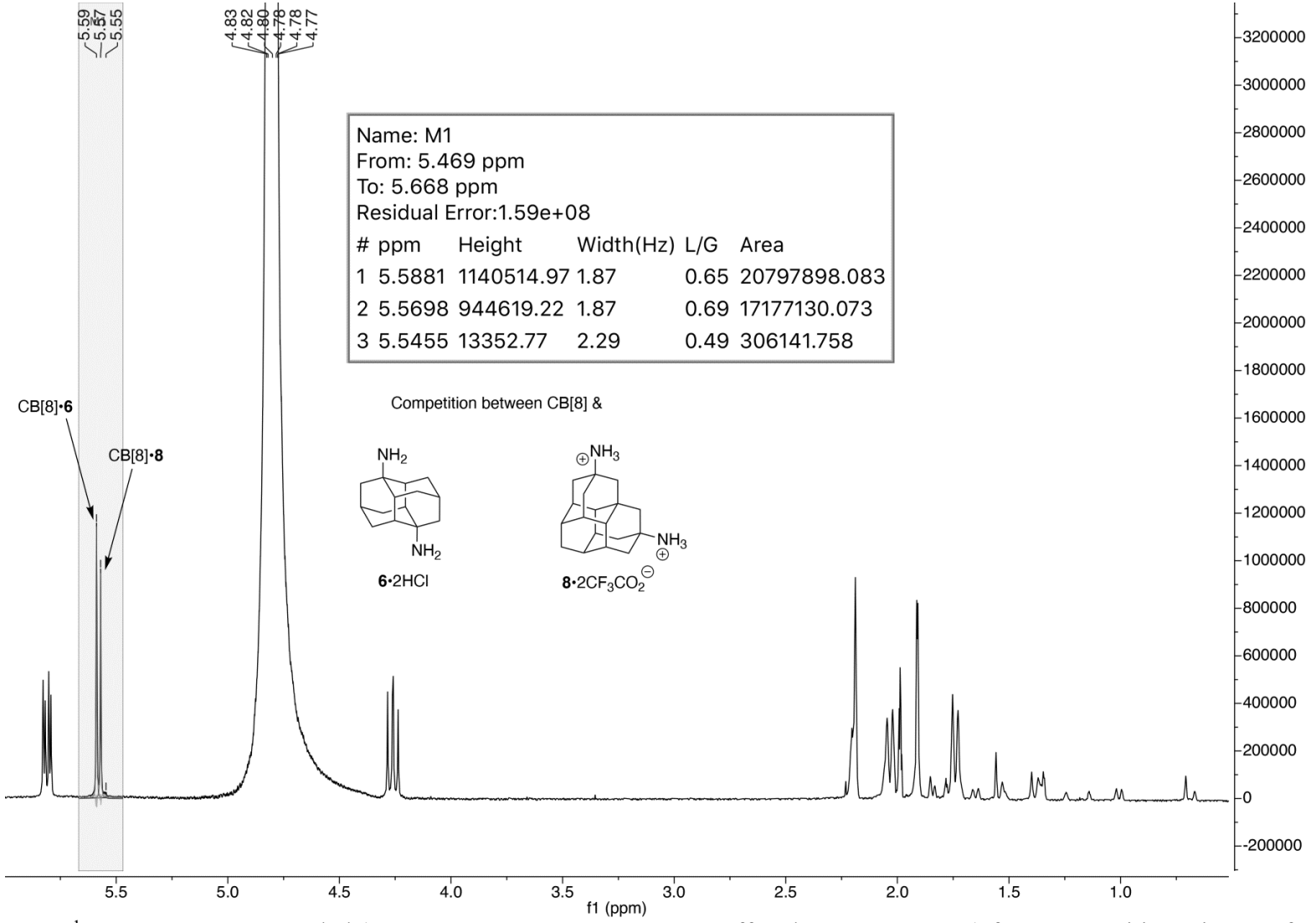

Figure S22. ^{1}H NMR spectra recorded (600 MHz, RT, 50 mM NaOAc Buffered D_2O, pH = 4.74) for a competitive mixture of CB[8] (0.100 mM), **C2** (0.33 mM), and **G4** (0.11 mM) at equilibrium. K_{rel} = 3.46 (Equilibrium was studied starting from both directions and gave the same K_{rel} value).

Affinimeter Output Files from the Competitive Titration of CB[8] + C3 with G3 or G4.

Experiment 1: Measuring the binding affinity of **C3** and CB[8]

Figure S23. Cartoon representation of the stepwise 1:2 binding model used in Affinimeter for both titrations of **C3** (A) and CB[8] (M) outlined in Figures S24-S29.

Results

- Global χ^2: *2.76e+00*
  - χ^2 for curve [1]: *4.15e+00*

Table 1: Correction parameters† *† fitted parameters in blue*

ΔH_{dil} [cal·mol^{-1}]	Q_{db} [cal]	r_M	r_A	r_B
(1.1029 ± 0.0081)e+03	0.000e+00	1.000e+00	(9.8192 ± 0.0309)e-01	1.000e+00

Table 2: Reaction parameters† *† fitted parameters in blue*

Reaction	K [M^{-n}]	ΔH [cal·mol^{-1}]
[1] Free species ⟺ M_1A_1	(2.6699 ± 0.3224)e+07	(-9.2300 ± 0.0419)e+03
[2] M_1A_1 + A_1 ⟺ M_1A_2	(7.4697 ± 1.7486)e+06	(-8.2808 ± 0.0638)e+03

Figure S24. Results from the titration of **C3** (A) titrated into CB[8] (B) as a part of the global fit for experiment 1. ΔH_{dil} = heat of dilution; r_A = % of active **C3** concentration for titration 1. Cell: CB[8] (0.02 mM); Syringe: **C3** (0.350 mM); Number of Injections: 18.

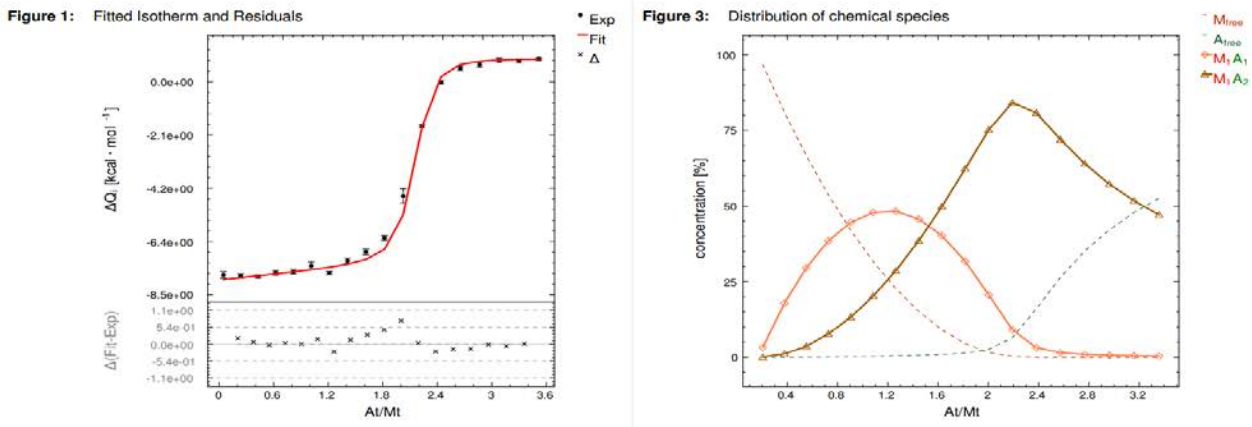

Figure S25. Left) Integrated signal from titration 1 and best fit line from global fit (top) and the residuals of the fit (bottom). Right) Percent concentration of each species present in the cell over time with respect to the total CB[8] concentration (M_{free}) or total **C3** concentration (A_{free}, M_1A_1, M_1A_2).

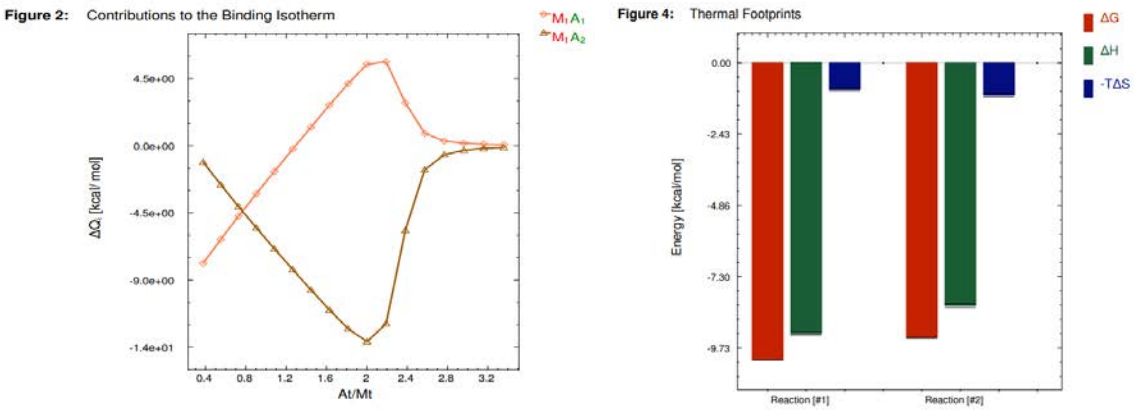

Figure S26. Left) Total contribution of each complexation reaction to the overall integrated signal over time for titration 2. Right) Graphical representation of ΔG, ΔH, and -TΔS for each complexation reaction.

Results

- Global χ^2: *2.76e+00*
  - χ^2 for curve [2]: *2.29e+00*

Table 3: Correction parameters† *† fitted parameters in blue*

ΔH_{dil} [cal·mol^{-1}]	Q_{db} [cal]	r_M	r_A	r_B
(-2.9819 ± 0.0212)e+03	0.000e+00	1.000e+00	(1.0325 ± 0.0023)e+00	1.000e+00

Figure S27. Results from the titration of **C3** (A) titrated into CB[8] (B) as a part of the global fit for experiment 1. ΔH_{dil} = heat of dilution; r_A = % of active **C3** concentration for titration 1. Cell: CB[8] (0.005 mM); Syringe: **C3** (0.040 mM); Number of Injections: 54.

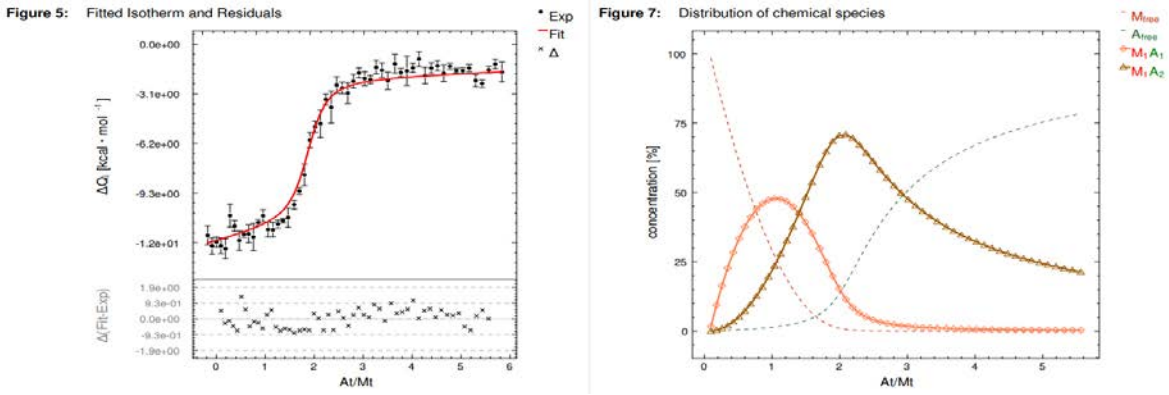

Figure S28. Left) Integrated signal from titration 2 and best fit line from global fit (top) and the residuals of the fit (bottom). Right) Percent concentration of each species present in the cell over time with respect to the total CB[8] concentration (M_{free}) or total **C3** concentration (A_{free}, M_1A_1, M_1A_2).

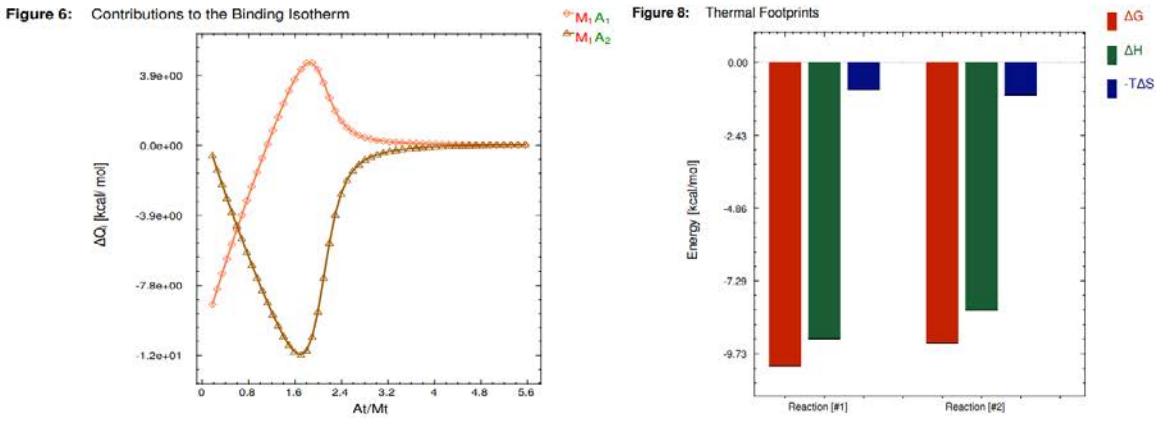

Figure S29. Left) Total contribution of each complexation reaction to the overall integrated signal over time for titration 2. Right) Graphical representation of ΔG, ΔH, and -TΔS for each complexation reaction.

Experiment 2: Measuring the binding affinity of **G3** and CB[8] by using **C3** as a competitor.

Figure S30. Cartoon representation of the stepwise 1:2 binding model used in Affinimeter for both titrations of **C3** (A) and CB[8] (M) outlined in Figures S31-S36.

Results

- Global χ^2: ***2.81e+00***
  - χ^2 for curve [1]: ***4.09e+00***

Table 1: Correction parameters† *† fitted parameters in blue*

ΔH_{dil} [cal·mol^{-1}]	Q_{db} [cal]	r_M	r_A	r_B
(1.1023 ± 0.0061)e+03	0.000e+00	1.000e+00	(9.8076 ± 0.0224)e-01	1.000e+00

Figure S31. Results from the titration of **C3** (A) titrated into CB[8] (M) as a part of the global fit for experiment 2. ΔH_{dil} = heat of dilution; r_A = % of active **C3** concentration for titration 1. Cell: CB[8] (0.02 mM); Syringe: **C3** (0.350 mM); Number of Injections: 18.

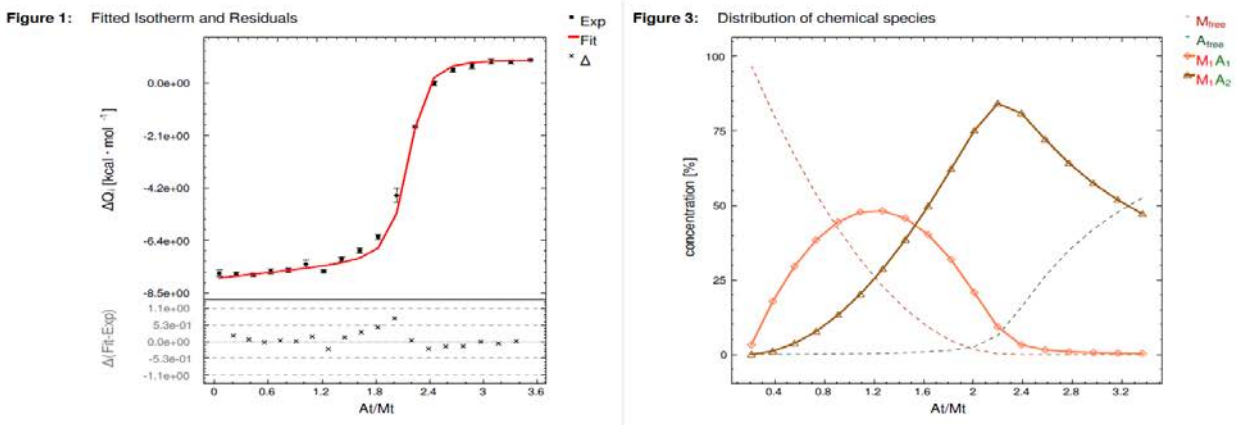

Figure S32. Left) Integrated signal from titration 1 and best fit line from global fit (top) and the residuals of the fit (bottom). Right) Percent concentration of each species present in the cell over time with respect to the total CB[8] concentration (M_{free}) or total **C3** concentration (A_{free}, M_1A_1, M_1A_2).

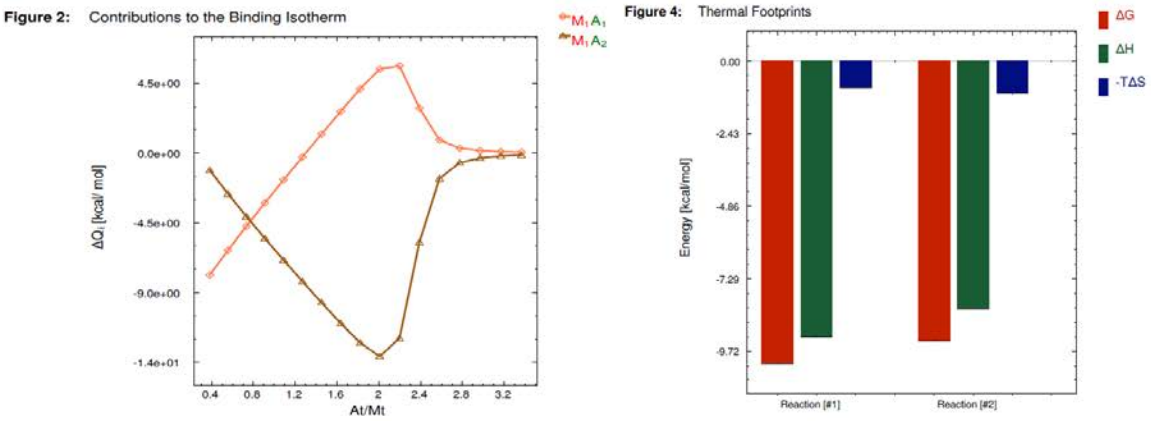

Figure S33. Left) Total contribution of each complexation reaction to the overall integrated signal over time for titration 1. Right) Graphical representation of ΔG, ΔH, and -TΔS for each complexation reaction.

Results

- Global χ^2: **2.81e+00**
  - χ^2 for curve [2]: **2.27e+00**

Table 3: Correction parameters† *† fitted parameters in blue*

ΔH_{dil} [cal·mol^{-1}]	Q_{db} [cal]	r_M	r_A	r_B
(-2.9759 ± 0.0157)e+03	0.000e+00	1.000e+00	(1.0323 ± 0.0017)e+00	1.000e+00

Figure S34. Results from the titration of **C3** (A) titrated into CB[8] (B) as a part of the global fit for experiment 2. ΔH_{dil} = heat of dilution; r_A = % of active **C3** concentration for titration 2. Cell: CB[8] (0.005 mM); Syringe: **C3** (0.040 mM); Number of Injections: 54.

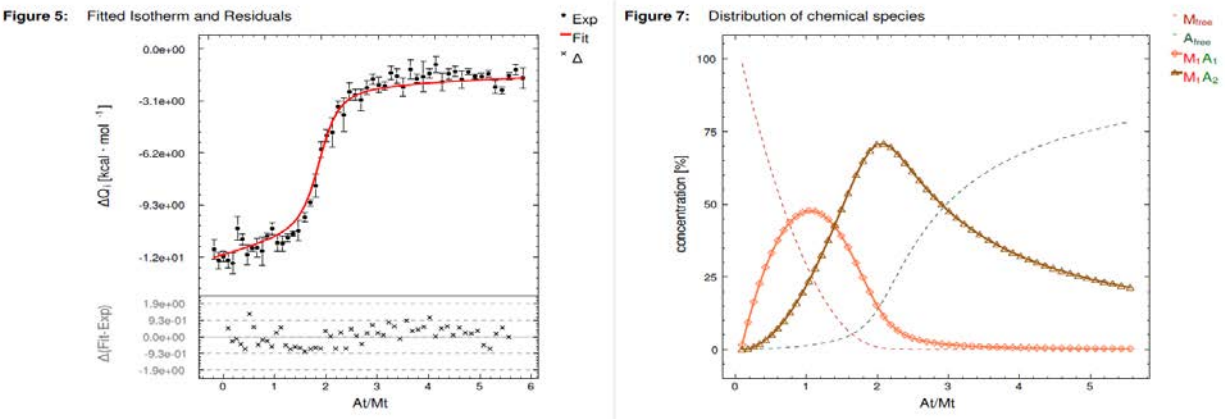

Figure S35. Left) Integrated signal from titration 2 and best fit line from global fit (top) and the residuals of the fit (bottom). Right) Percent concentration of each species present in the cell over time with respect to the total CB[8] concentration (M_{free}) or total **C3** concentration (A_{free}, M_1A_1, M_1A_2).

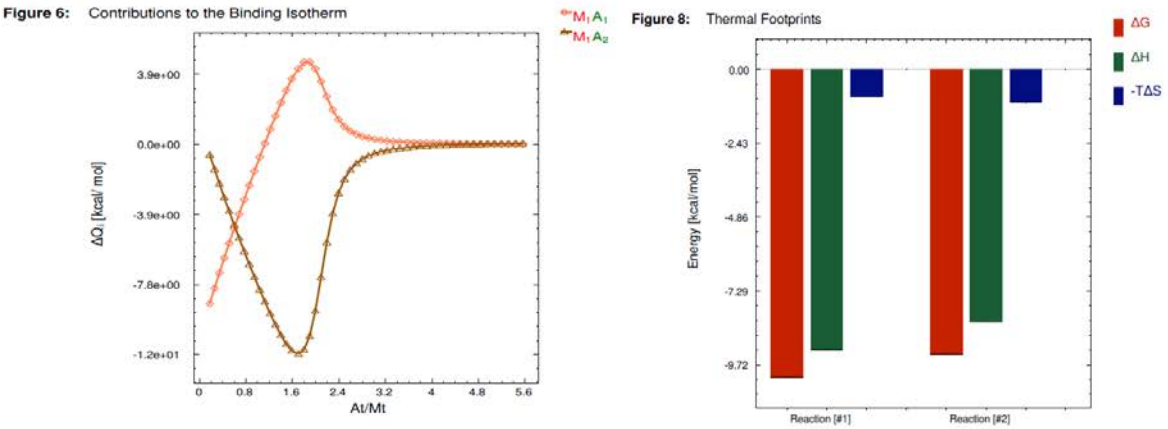

Figure S36. Left) Total contribution of each complexation reaction to the overall integrated signal over time for titration 2. Right) Graphical representation of ΔG, ΔH, and -TΔS for each complexation reaction.

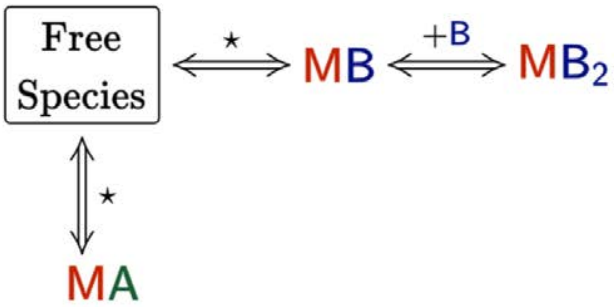

Figure S37. Cartoon representation of the stepwise competition binding model used in Affinimeter for the titration of **G3** (A) into a mixture of CB[8] (M) and **C3** (B) outlined in Figures S41-S43.

Results

- Global χ^2: *2.81e+00*
  - χ^2 for curve [3]: *2.93e+00*

Table 5: Correction parameters† *† fitted parameters in blue*

ΔH_{dil} [cal·mol^{-1}]	Q_{db} [cal]	r_M	r_A	r_B
(-8.3660 ± 0.1136)e+02	*0.000e+00*	*1.000e+00*	(8.5858 ± 0.0145)e-01	(1.4040 ± 0.0115)e+00

Table 6: Reaction parameters† *† fitted parameters in blue*

Reaction	K [M^{-n}]	ΔH [cal·mol^{-1}]
[1] Free species ⟹ M_1B_1	(2.6496 ± 0.2385)e+07	(-9.2416 ± 0.0310)e+03
[2] M_1B_1 + B_1 ⟹ M_1B_2	(7.4659 ± 1.2976)e+06	(-8.2917 ± 0.0472)e+03
[3] Free species ⟹ M_1A_1	(1.1486 ± 0.1689)e+13	(-1.0076 ± 0.0045)e+04

Figure S38. Results from the titration of **G3** (A) into a mixture of CB[8] (M) and **C3** (B) as a part of the global fit for experiment 2. ΔH_{dil} = heat of dilution; r_A = % of active **C3** concentration for titration 3. Cell: CB[8] (0.030 mM), **C3** (0.175 mM); Syringe: **G3** (0.100 mM); Number of Injections: 54.

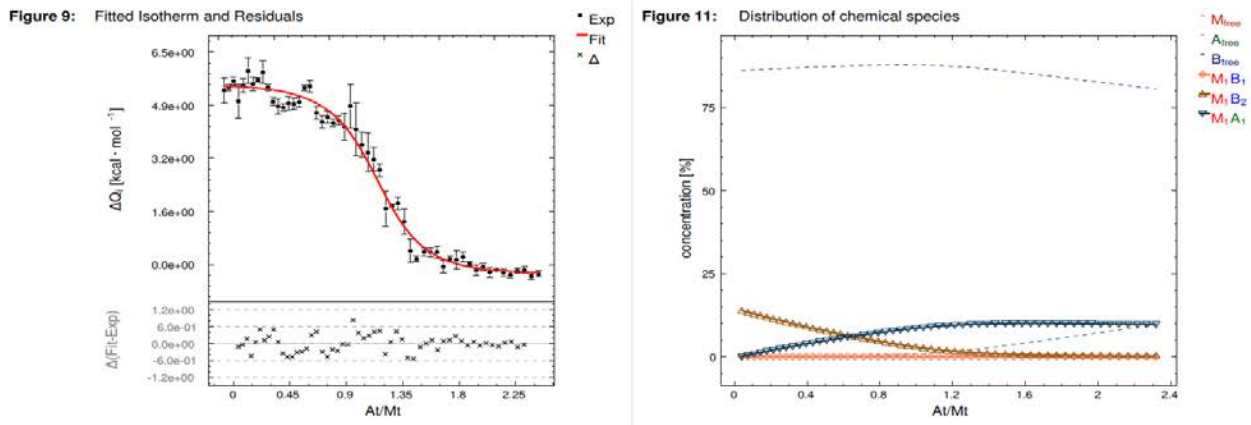

Figure S39. Left) Integrated signal from titration 3 and best fit line from global fit (top) and the residuals of the fit (bottom). Right) Percent concentration of each species present in the cell over time with respect to the total CB[8] concentration (M_{free}), total **C3** concentration (B_{free}, M_1B_1, M_1B_2), or total **G3** concentration (A_{free}, M_1A_1).

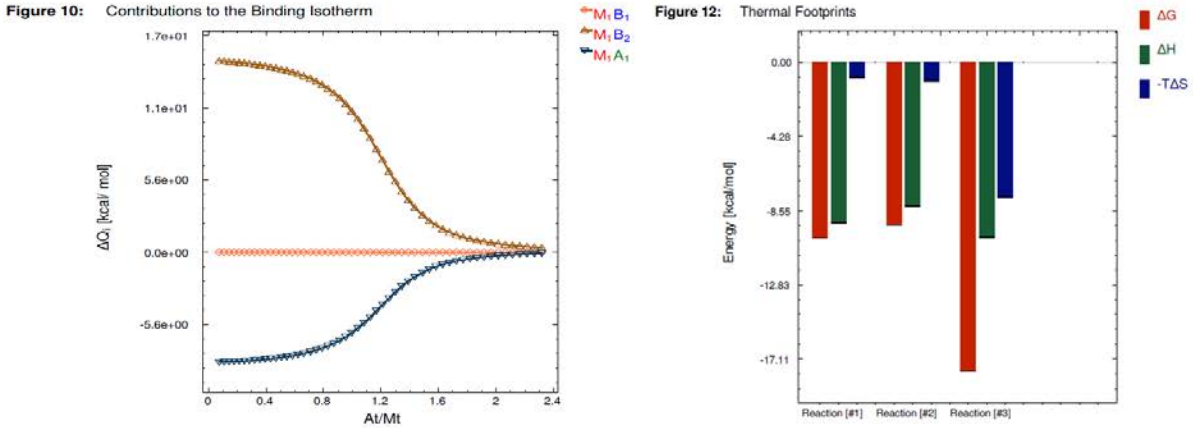

Figure S40. Left) Total contribution of each complexation reaction to the overall integrated signal over time for titration 3. Right) Graphical representation of ΔG, ΔH, and -TΔS for each complexation reaction.

Experiment 3: Measuring the binding affinity of **G4** and CB[8] by using **C3** as a competitor

Figure S41. Cartoon representation of the stepwise 1:2 binding model used in Affinimeter for both titrations of **C3** (A) and CB[8] (M) outlined in Figures S42-S47.

Results

- Global χ^2: *3.98e+00*
  - χ^2 for curve [3]: *1.22e+01*

Table 5: Correction parameters† *† fitted parameters in blue*

ΔH_{dil} [cal·mol^{-1}]	Q_{db} [cal]	r_M	r_A	r_B
(1.4547 ± 0.0191)e+03	0.000e+00	1.000e+00	(9.7919 ± 0.0324)e-01	1.000e+00

Figure S42. Results from the titration of **C3** (A) titrated into CB[8] (B) as a part of the global fit for experiment 3. ΔH_{dil} = heat of dilution; r_A = % of active **C3** concentration for titration 1. Cell: CB[8] (0.02 mM); Syringe: **C3** (0.350 mM); Number of Injections: 18.

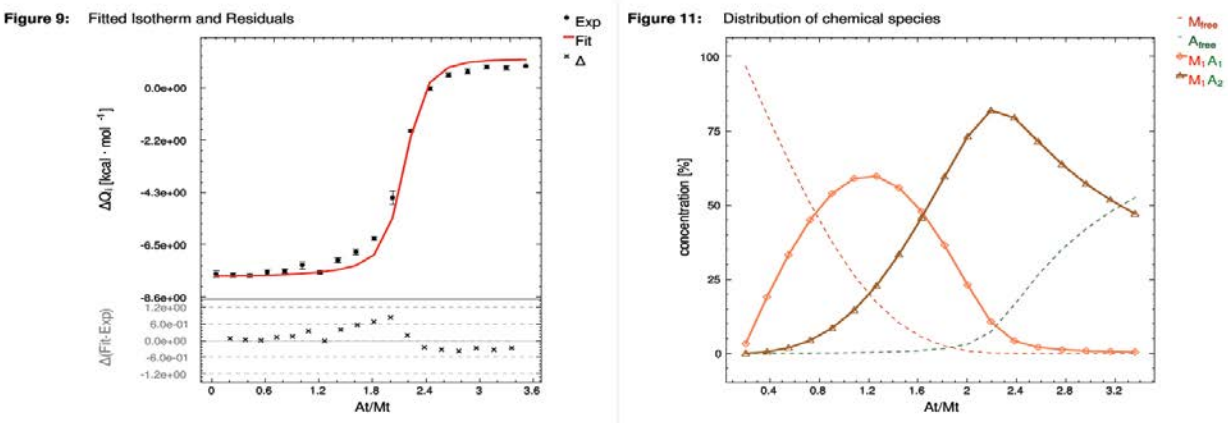

Figure S43. Left) Integrated signal from titration 1 and best fit line from global fit (top) and the residuals of the fit (bottom). Right) Percent concentration of each species present in the cell over time with respect to the total CB[8] concentration (M_{free}) or total **C3** concentration (A_{free}, M_1A_1, M_1A_2).

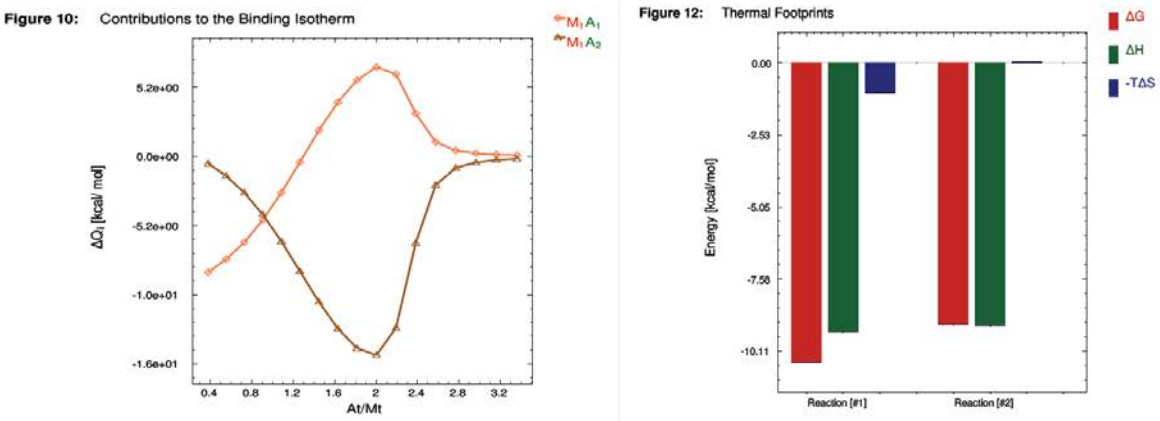

Figure S44. Left) Total contribution of each complexation reaction to the overall integrated signal over time for titration 1. Right) Graphical representation of ΔG, ΔH, and -TΔS for each complexation reaction.

Results

- Global χ^2: *3.98e+00*

Table 3: Correction parameters† *† fitted parameters in blue*

ΔH_{dil} [cal·mol^{-1}]	Q_{db} [cal]	r_M	r_A	r_B
(-2.7148 ± 0.0169)e+03	0.000e+00	1.000e+00	(1.0176 ± 0.0017)e+00	1.000e+00

Figure S45. Results from the titration of **C3** (A) titrated into CB[8] (B) as a part of the global fit for experiment 3. ΔH_{dil} = heat of dilution; r_A = % of active **C3** concentration for titration 2. Cell: CB[8] (0.005 mM); Syringe: **C3** (0.040 mM); Number of Injections: 54.

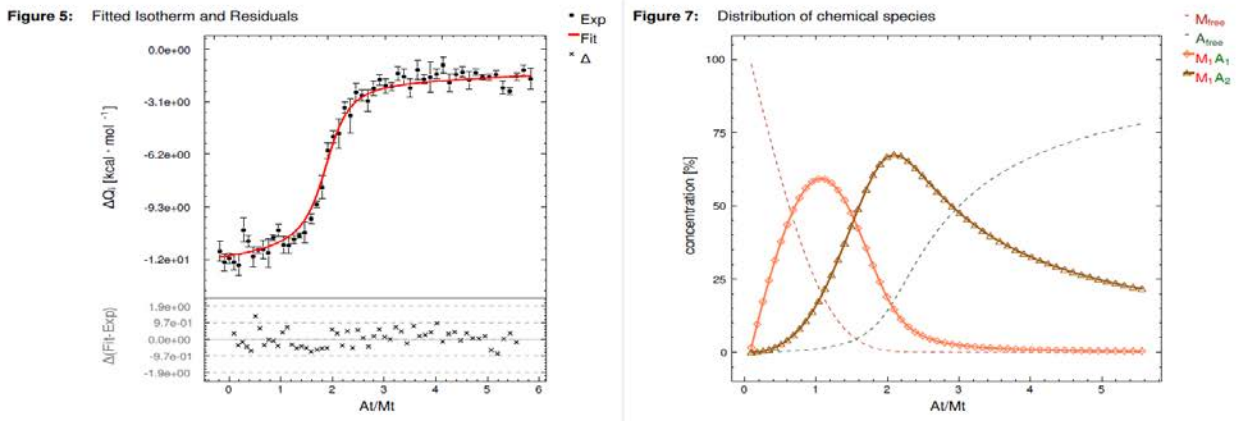

Figure S46. Left) Integrated signal from titration 2 and best fit line from global fit (top) and the residuals of the fit (bottom). Right) Percent concentration of each species present in the cell over time with respect to the total CB[8] concentration (M_{free}) or total **C3** concentration (A_{free}, M_1A_1, M_1A_2).

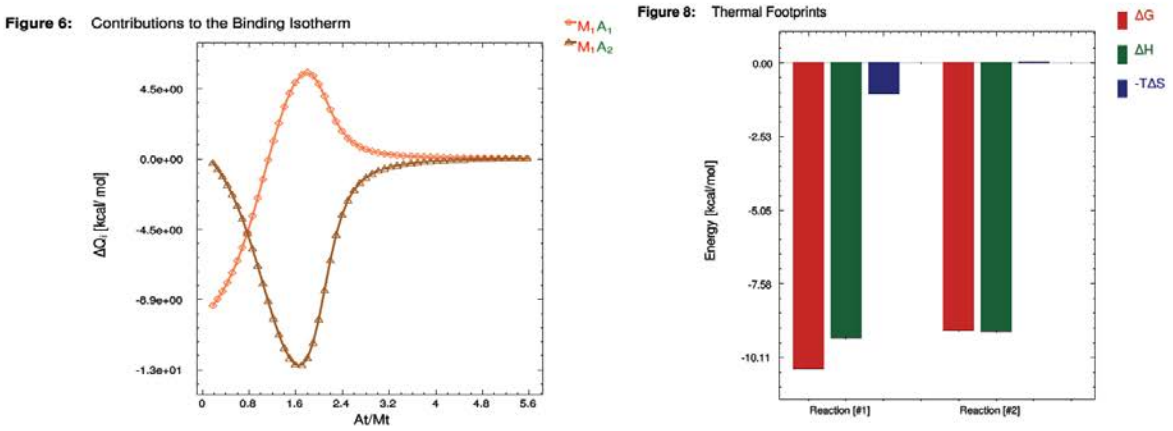

Figure S47. Left) Total contribution of each complexation reaction to the overall integrated signal over time for titration 2. Right) Graphical representation of ΔG, ΔH, and -TΔS for each complexation reaction.

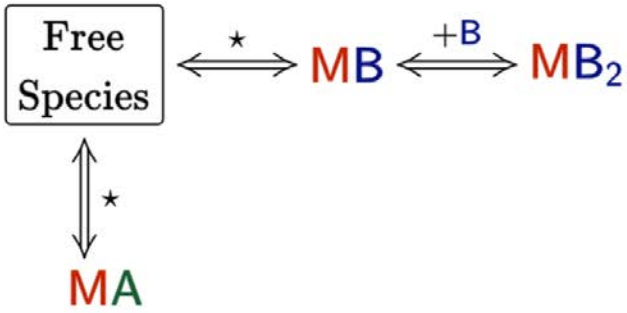

Figure S48. Cartoon representation of the stepwise competition binding model used in Affinimeter for the titration of **G4** (A) into a mixture of CB[8] (M) and **C3** (B) outlined in Figures S52-S57.

Results

- Global χ^2: *3.98e+00*
  - χ^2 for curve [1]: *4.38e+00*

Table 1: Correction parameters† *† fitted parameters in blue*

ΔH_{dil} [cal·mol^{-1}]	Q_{db} [cal]	r_M	r_A	r_B
(-1.4297 ± 0.0316)e+03	0.000e+00	1.000e+00	(9.2598 ± 0.0330)e-01	(1.0598 ± 0.0060)e+00

Table 2: Reaction parameters† *† fitted parameters in blue*

Reaction	K [M^{-n}]	ΔH [cal·mol^{-1}]
[1] Free species ⟹ M_1B_1	(4.9349 ± 0.3942)e+07	(-9.4436 ± 0.0416)e+03
[2] M_1B_1 + B_1 ⟹ M_1B_2	(5.4213 ± 0.6600)e+06	(-9.2195 ± 0.0661)e+03
[3] Free species ⟹ M_1A_1	(1.1418 ± 0.2161)e+14	(-1.1501 ± 0.0050)e+04

Figure S49. Results from the titration of **G4** (A) into a mixture of CB[8] (M) and **C3** (B) as a part of the global fit for experiment 3. ΔH_{dil} = heat of dilution; r_A = % of active **C3** concentration for titration 3. Cell: CB[8] (0.020 mM), **C3** (0.015 mM); Syringe: **G4** (0.070 mM); Number of Injections: 54.

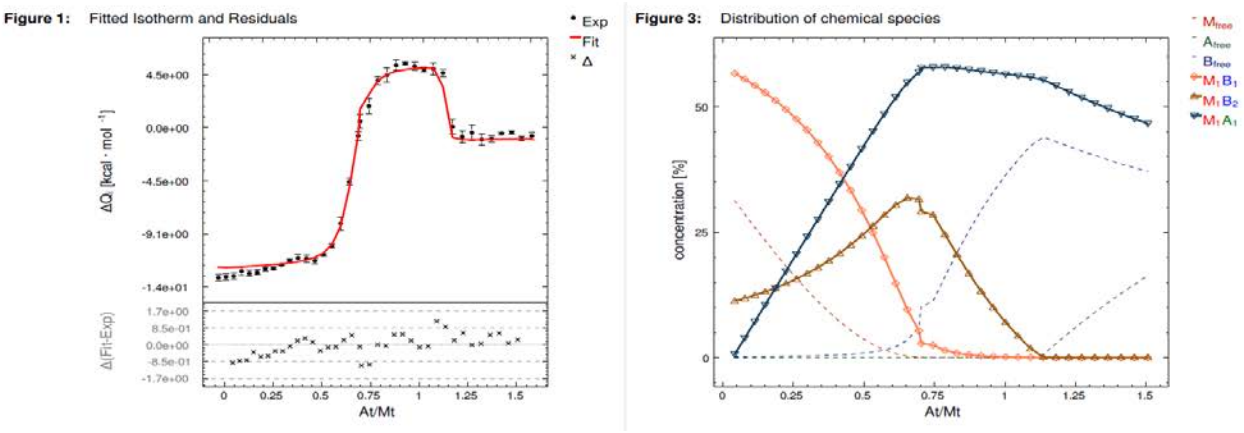

Figure S50. Left) Integrated signal from titration 3 and best fit line from global fit (top) and the residuals of the fit (bottom). Right) Percent concentration of each species present in the cell over time with respect to the total CB[8] concentration (M_{free}), total **C3** concentration (B_{free}, M_1B_1, M_1B_2), or total **G4** concentration (A_{free}, M_1A_1).

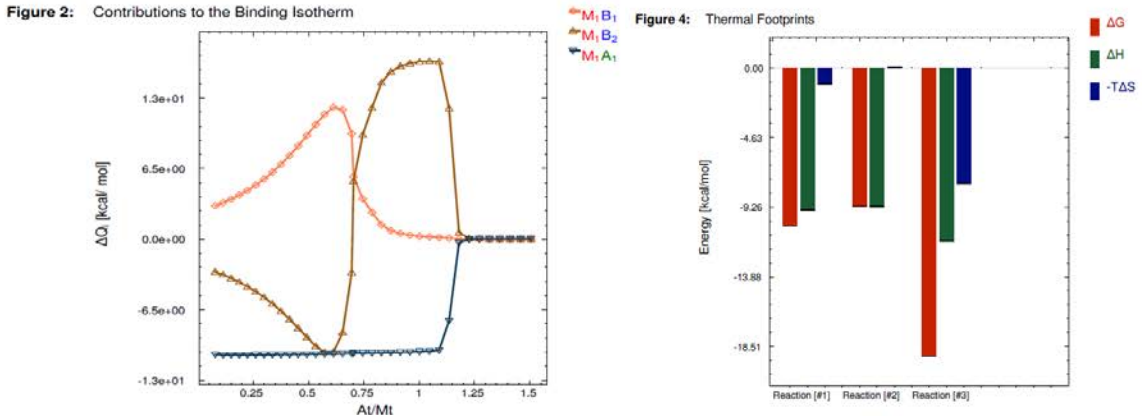

Figure S51. Left) Total contribution of each complexation reaction to the overall integrated signal over time for titration 3. Right) Graphical representation of ΔG, ΔH, and -TΔS for each complexation reaction.

Results

- Global χ^2: *3.98e+00*
  - χ^2 for curve [4]: *2.68e+00*

Table 7: Correction parameters† *† fitted parameters in blue*

ΔH_{dil} [cal·mol^{-1}]	Q_{db} [cal]	r_M	r_A	r_B
(-4.8798 ± 0.0191)e+02	0.000e+00	1.000e+00	(7.9695 ± 0.0300)e-01	(8.8648 ± 0.0244)e-01

Figure S52. Results from the titration of **G4** (A) into a mixture of CB[8] (M) and **C3** (B) as a part of the global fit for experiment 3. ΔH_{dil} = heat of dilution; r_A = % of active **C3** concentration for titration 4. Cell: CB[8] (0.020 mM), **C3** (0.040 mM); Syringe: **G4** (0.150 mM); Number of Injections: 54.

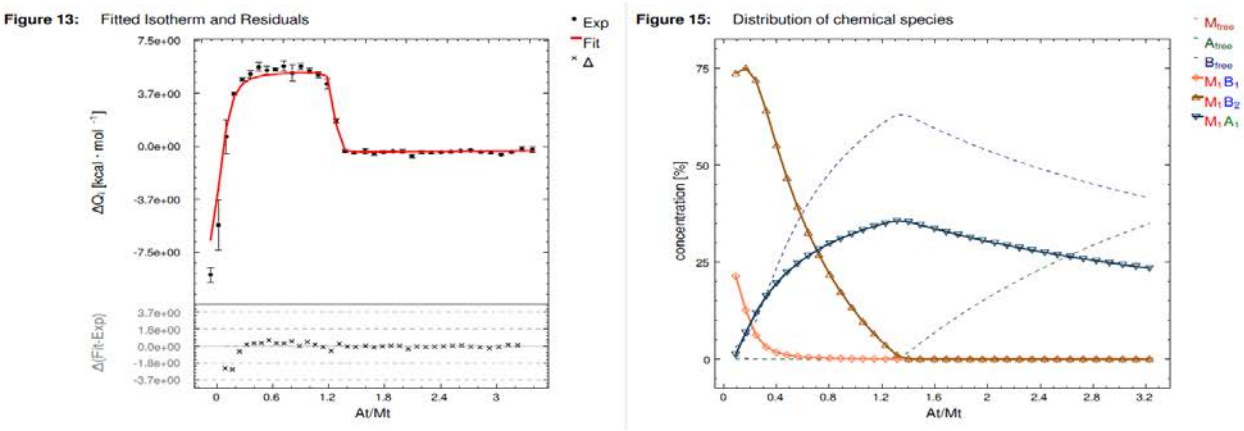

Figure S53. Left) Integrated signal from titration 4 and best fit line from global fit (top) and the residuals of the fit (bottom). Right) Percent concentration of each species present in the cell over time with respect to the total CB[8] concentration (M_{free}), total **C3** concentration (B_{free}, M_1B_1, M_1B_2), or total **G4** concentration (A_{free}, M_1A_1).

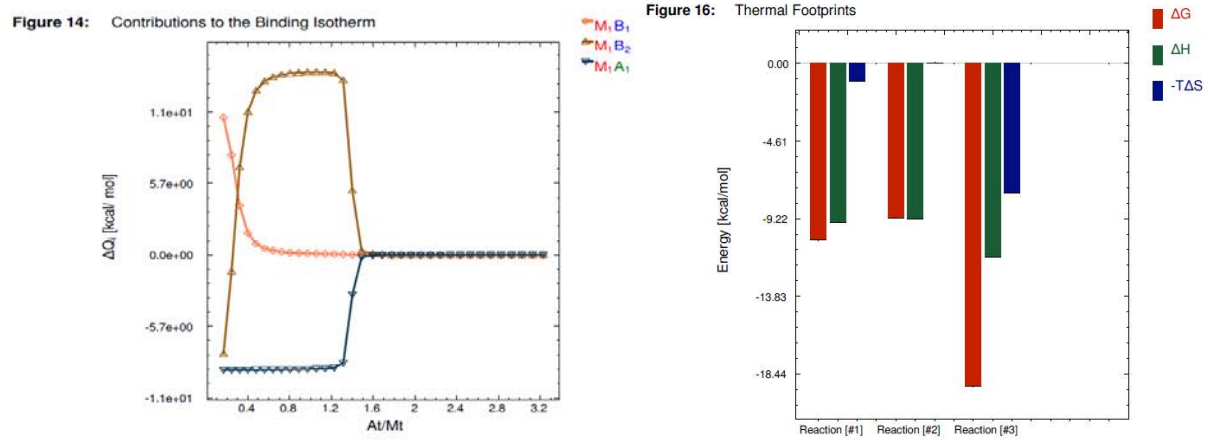

Figure S54. Left) Total contribution of each complexation reaction to the overall integrated signal over time for titration 4. Right) Graphical representation of ΔG, ΔH, and -TΔS for each complexation reaction.

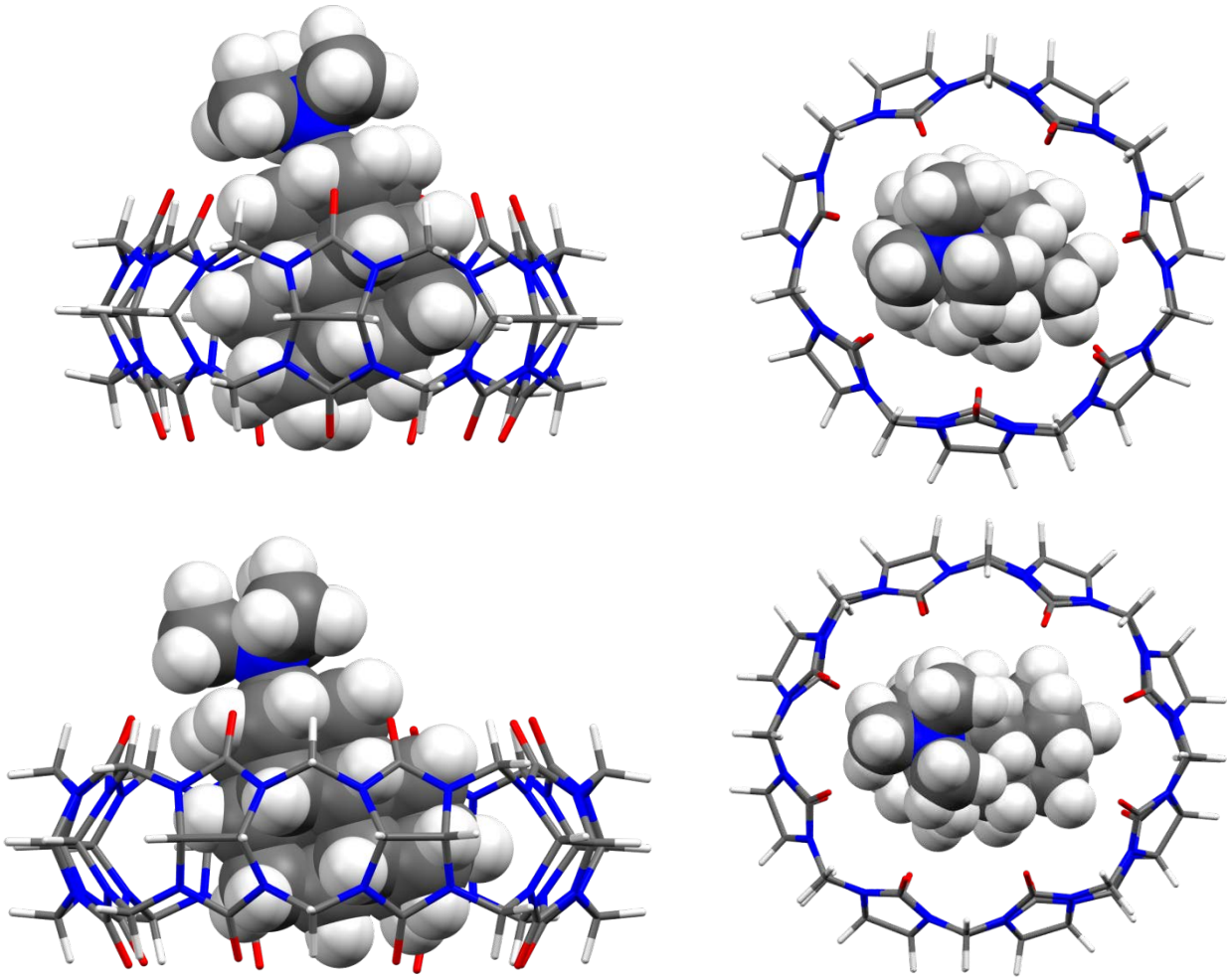

Figure S55. Representations of the minimized geometries of CB[7]•**G1** (top) and CB[8]•**G1** (bottom). Color coding: C, gray; H, white; O, red; N, blue.

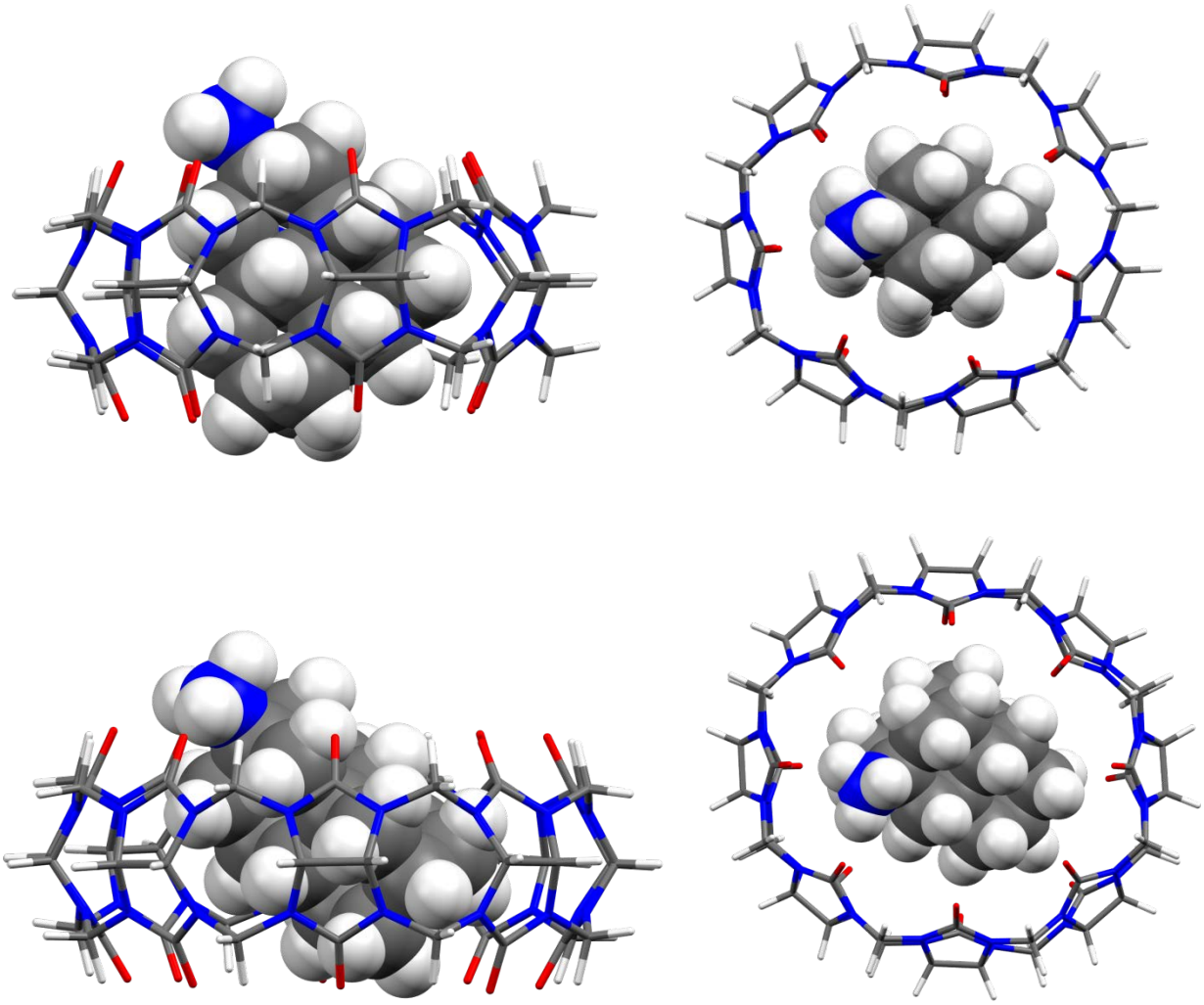

Figure S56. Representations of the minimized geometries of CB[7]•**G2** (top) and CB[8]•**G2** (bottom). Color coding: C, gray; H, white; O, red; N, blue.

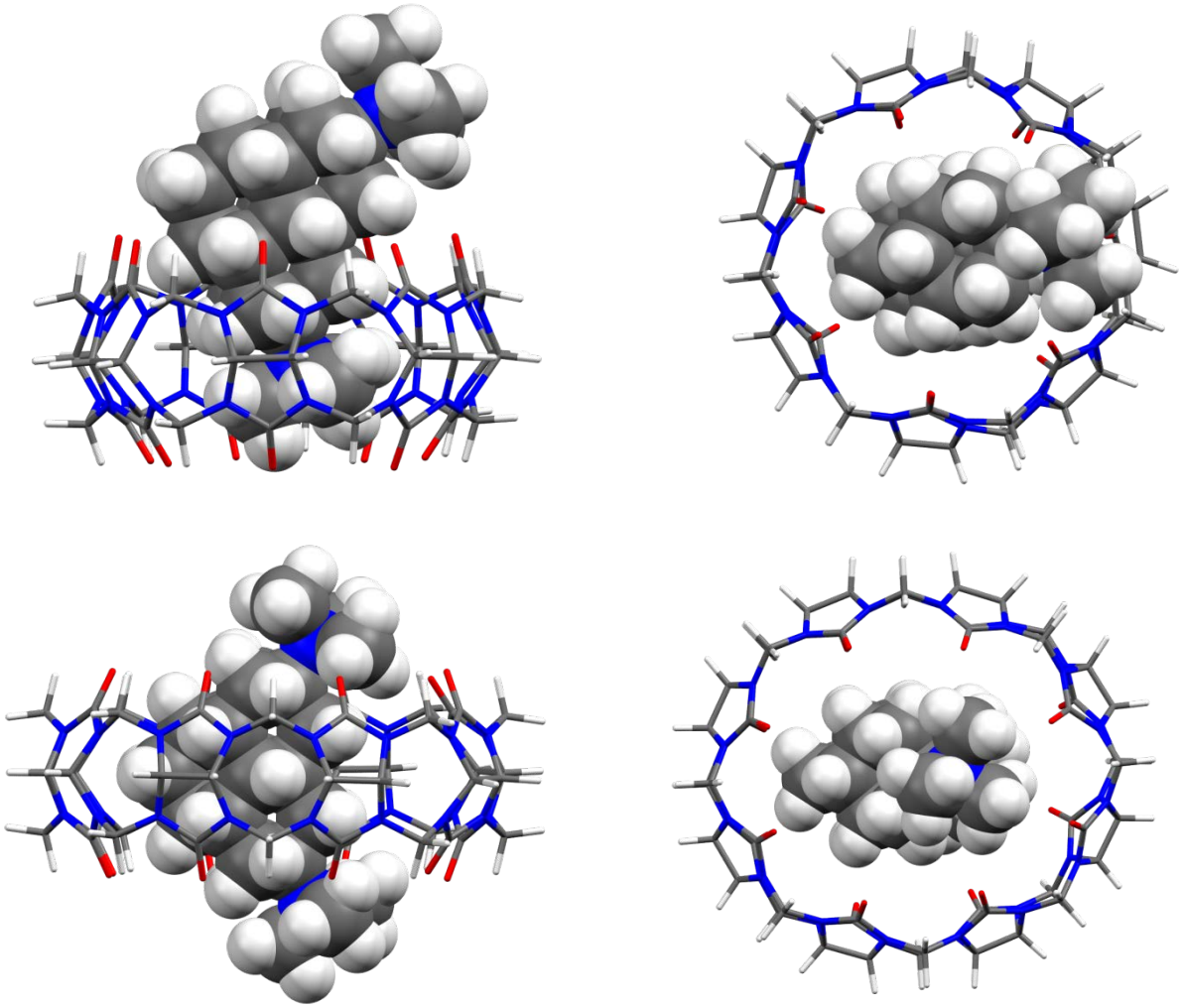

Figure S57. Representations of the minimized geometries of CB[7]•**G3** (top) and CB[8]•**G3** (bottom). Color coding: C, gray; H, white; O, red; N, blue.

Table S1. Electronic energies, zero-point vibrational energies, enthalpies and Gibbs energies of guests **G1**–**G4**, CB[7] and CB[8], and the corresponding complexes in Hartree computed using the GFN2-xTB method. The interaction energies (difference between the energy of the complex and the energy of the guest and the host molecules) for the complexes in kcal mol^{-1} are given in parentheses.

compound	*E*	*ZPVE*	*H*	*G*
G1	-64.055694	0.495235	-63.544051	-63.599693
G2	-54.570637	0.410876	-54.146303	-54.196330
G3	-77.160562	0.607646	-76.531822	-76.595677
G4	-58.192044	0.438754	-57.738041	-57.790919
CB[7]	-251.174100	0.923189	-250.186362	-250.339766
CB[8]	-287.050977	1.055132	-285.921884	-286.093340
CB[7]•G1	-315.272746 **(-27.0)**	1.424573	-313.767545 **(-23.3)**	-313.947474 **(-5.0)**
CB[7]•G2	-305.783942 **(-24.6)**	1.339440	-304.367502 **(-21.9)**	-304.540738 **(-2.9)**
CB[7]•G3 unstable	-328.322615 **(7.6)**	1.539372	-326.698337 **(12.5)**	-326.884910 **(31.7)**
CB[7]•G3 exclusion	-328.361297 **(-16.7)**	1.535884	-326.738713 **(-12.9)**	-326.931129 **(2.7)**
CB[7]•G4	-309.422823 **(-35.6)**	1.369077	-307.975832 **(-32.3)**	-308.149194 **(-11.6)**
CB[8]•G1	-351.159698 **(-33.3)**	1.554003	-349.514316 **(-30.4)**	-349.717460 **(-15.3)**
CB[8]•G2	-341.674384 **(-33.1)**	1.469324	-340.117704 **(-31.1)**	-340.312876 **(-14.6)**
CB[8]•G3	-364.265517 **(-33.9)**	1.668273	-362.501204 **(-29.8)**	-362.711852 **(-14.3)**
CB[8]•G4	-345.307439 **(-40.4)**	1.497598	-343.720905 **(-38.3)**	-343.919089 **(-21.9)**

Table S2. Geometries of guests **G1**–**G4**, CB[7] and CB[8], and the corresponding complexes in Cartesian coordinates in Å obtained using the GFN2-xTB method and from CREST sampling.

G1			
6	-1.977600000	1.142300000	-1.092500000
6	-2.723300000	-0.191200000	-1.083800000
6	-2.329800000	-0.945200000	0.185500000
6	-2.345300000	1.970300000	0.143000000
6	-0.451700000	0.935200000	1.381700000
6	-2.699500000	-0.131100000	1.429700000
6	-1.959800000	1.213700000	1.421500000
6	-2.356600000	-1.009200000	-2.318900000
6	-0.090100000	0.056100000	-2.359900000
6	-0.852200000	-1.270500000	-2.331200000
6	-0.444400000	-2.043100000	-1.074900000
6	1.060900000	-2.303100000	-1.079100000
6	1.805300000	-0.969100000	-1.106000000
6	1.416000000	-0.199200000	-2.367000000
6	-0.473600000	0.874900000	-1.126100000
6	1.431500000	-0.150200000	0.128600000
6	-0.827600000	-1.222500000	0.157900000
6	-0.077200000	0.111500000	0.140000000
7	-2.327200000	2.043800000	2.676200000
1	2.885400000	-1.153500000	-1.109400000
1	-2.260900000	1.707700000	-1.986800000
1	-3.803800000	-0.009700000	-1.085200000
1	-2.869400000	-1.897900000	0.220500000
1	-1.813900000	2.917700000	0.070500000
1	-3.417000000	2.157700000	0.102800000
1	-0.133000000	0.365100000	2.253200000
1	0.119000000	1.861600000	1.336300000
1	-3.778700000	0.011400000	1.417600000
1	-2.427200000	-0.725100000	2.300500000
1	-2.897100000	-1.958800000	-2.311900000
1	-2.645700000	-0.469200000	-3.223800000
1	-0.366900000	0.611100000	-3.264300000
1	-0.592000000	-1.858100000	-3.219200000
1	-0.976700000	-3.001600000	-1.052700000
1	1.332400000	-2.898300000	-1.954200000
1	1.344400000	-2.872400000	-0.190700000
1	1.955800000	0.749900000	-2.408000000
1	1.690900000	-0.774900000	-3.254000000
1	0.065800000	1.828700000	-1.159000000
1	1.724500000	-0.695400000	1.028700000
1	1.976300000	0.796600000	0.115400000
1	-0.544300000	-1.786600000	1.054200000
6	-1.627500000	3.345100000	2.699800000
6	-3.775400000	2.331100000	2.740000000
6	-1.971300000	1.339900000	3.925700000
1	-0.903500000	1.155100000	3.976500000
1	-2.508100000	0.400900000	4.008900000
1	-2.246900000	1.962600000	4.773500000
1	-4.094300000	2.911900000	1.881100000
1	-3.981800000	2.911900000	3.635900000
1	-4.351300000	1.413400000	2.793300000
1	-1.895600000	3.946000000	1.837500000
1	-0.551900000	3.206900000	2.727500000
1	-1.921300000	3.888700000	3.594600000

G2			
6	-1.977000000	1.150300000	-1.094800000
6	-2.723300000	-0.186100000	-1.075900000
6	-2.331700000	-0.950600000	0.191200000
6	-2.341900000	1.975700000	0.141800000
6	-0.440300000	0.934300000	1.384200000
6	-2.698000000	-0.134900000	1.433700000
6	-1.943700000	1.191000000	1.388800000
6	-2.359600000	-1.004200000	-2.312100000
6	-0.091500000	0.059000000	-2.356400000
6	-0.855200000	-1.266800000	-2.326100000
6	-0.446100000	-2.041000000	-1.070900000
6	1.058500000	-2.305400000	-1.081900000
6	1.807400000	-0.973900000	-1.112800000
6	1.414000000	-0.200400000	-2.370500000
6	-0.470600000	0.878500000	-1.121100000
6	1.441500000	-0.155100000	0.123600000
6	-0.825000000	-1.220500000	0.163700000
6	-0.065500000	0.111600000	0.143600000
7	-2.296500000	1.995000000	2.604800000
1	2.886800000	-1.162100000	-1.122300000
1	-2.255700000	1.705200000	-1.996400000
1	-3.803500000	-0.004100000	-1.076500000
1	-2.865500000	-1.906000000	0.214200000
1	-1.812700000	2.928300000	0.100300000
1	-3.414900000	2.169400000	0.133600000
1	-0.140900000	0.378600000	2.273800000
1	0.112000000	1.874600000	1.358300000
1	-3.775400000	0.033500000	1.441000000
1	-2.425400000	-0.703700000	2.323400000
1	-2.900400000	-1.953700000	-2.305300000
1	-2.648900000	-0.464400000	-3.217100000
1	-0.369800000	0.614400000	-3.260300000
1	-0.597000000	-1.854500000	-3.214900000
1	-0.980100000	-2.998700000	-1.048500000
1	1.323800000	-2.902400000	-1.957800000
1	1.344600000	-2.875000000	-0.194500000
1	1.956500000	0.747200000	-2.411900000
1	1.683100000	-0.774700000	-3.260300000

1	0.070300000	1.831200000	-1.156200000
1	1.736300000	-0.701300000	1.022400000
1	1.988300000	0.790400000	0.109100000
1	-0.540500000	-1.786400000	1.058300000
1	-1.800700000	2.894400000	2.596000000
1	-3.306500000	2.179400000	2.630700000
1	-2.035600000	1.487000000	3.458500000

G3

6	-1.971000000	1.134200000	-1.103000000
6	-2.718300000	-0.198400000	-1.092900000
6	-2.322600000	-0.953300000	0.175100000
6	-2.331000000	1.961400000	0.135700000
6	-0.429400000	0.922000000	1.365400000
6	-2.683500000	-0.138300000	1.421600000
6	-1.938100000	1.203600000	1.411600000
6	-2.352800000	-1.016300000	-2.328900000
6	-0.083000000	0.042600000	-2.367000000
6	-0.849200000	-1.279100000	-2.344600000
6	-0.434900000	-2.045100000	-1.089200000
6	1.074000000	-2.311900000	-1.095700000
6	1.846600000	-0.985600000	-1.122400000
6	1.428200000	-0.211500000	-2.380300000
6	-0.467800000	0.866300000	-1.139800000
6	1.445200000	-0.163500000	0.110700000
6	-0.821300000	-1.232400000	0.144900000
6	-0.069000000	0.097800000	0.119600000
7	-2.292400000	2.033500000	2.669400000
7	3.372800000	-1.244100000	-1.123500000
1	-2.259300000	1.702100000	-1.993700000
1	-3.798200000	-0.016700000	-1.093200000
1	-2.866500000	-1.902900000	0.213500000
1	-1.805400000	2.911900000	0.061000000
1	-3.402900000	2.148100000	0.102600000
1	-0.116400000	0.353700000	2.239500000
1	0.134800000	1.851900000	1.320400000
1	-3.761900000	0.009700000	1.413600000
1	-2.416200000	-0.733900000	2.292900000
1	-2.896200000	-1.964100000	-2.322100000
1	-2.645900000	-0.476500000	-3.232400000
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1	-0.956200000	-3.007800000	-1.066200000
1	1.294800000	-2.914100000	-1.975200000
1	1.310000000	-2.890500000	-0.204200000
1	1.924100000	0.756200000	-2.433600000
1	1.656300000	-0.774500000	-3.283700000
1	0.063900000	1.823300000	-1.172100000
1	1.693600000	-0.696600000	1.026700000
1	1.947100000	0.802500000	0.109800000
1	-0.545500000	-1.795400000	1.042900000
6	-1.584200000	3.331000000	2.691900000
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6	3.793200000	-2.038000000	-2.296900000
6	4.145800000	0.015600000	-1.154200000
6	3.807800000	-1.986100000	0.078900000
1	-0.864300000	1.147000000	3.968000000
1	-2.468400000	0.386400000	3.999800000
1	-2.210000000	1.944400000	4.767100000
1	-4.059800000	2.915900000	1.887400000
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1	-4.320900000	1.414900000	2.794300000
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1	-0.510000000	3.187000000	2.733800000
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1	3.922200000	0.588300000	-2.047900000
1	5.207200000	-0.220500000	-1.166100000
1	3.946800000	0.615400000	-0.272700000
1	3.319200000	-2.952800000	0.138300000
1	3.608800000	-1.416500000	0.980200000
1	4.880100000	-2.157400000	0.020700000
1	3.562900000	-1.519100000	-3.221600000
1	3.317400000	-3.013100000	-2.298800000
1	4.869200000	-2.190100000	-2.257000000

G4

6	-1.926400000	1.165400000	-1.057900000
6	-2.672000000	-0.171600000	-1.040200000
6	-2.282100000	-0.936100000	0.227500000
6	-2.291700000	1.990300000	0.179200000
6	-0.390700000	0.949900000	1.424700000
6	-2.648900000	-0.120300000	1.470100000
6	-1.894500000	1.206100000	1.427200000
6	-2.304800000	-0.989900000	-2.275800000
6	-0.039000000	0.075400000	-2.316900000
6	-0.800700000	-1.252200000	-2.288300000
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6	1.848000000	-0.953900000	-1.068800000
6	1.470100000	-0.182100000	-2.330400000
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6	1.491900000	-0.136700000	0.169100000
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1	3.606000000	-1.725000000	-0.231600000

CB7

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8	2.611500000	-3.143900000	2.996400000
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8	2.566900000	3.196000000	2.933300000
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8	-3.701800000	-1.813500000	-2.948300000
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8	4.143500000	0.002000000	-2.960900000
8	2.597800000	3.164500000	-2.995800000
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1	6.067300000	-2.898100000	-1.634600000
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1	4.850500000	2.309500000	-2.849300000
1	6.070500000	2.922900000	-1.660400000
6	2.941200000	3.622200000	-1.926600000
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1	1.483200000	6.474600000	-1.723800000
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1	5.243000000	-4.517200000	0.026200000
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6	4.238900000	4.058600000	-0.027300000
1	5.218500000	4.555600000	-0.024200000
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1	3.243000000	6.079200000	-0.044200000

CB8

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8	16.955400000	8.656100000	7.773200000
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1	17.168500000	6.861000000	3.970900000
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1	15.189900000	6.795300000	2.539100000
1	14.526600000	8.393400000	2.008700000
6	15.590100000	6.682400000	6.202700000
1	15.707100000	6.655100000	7.292100000
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6	13.559300000	6.574200000	4.686200000
1	13.945800000	5.627000000	4.286200000
7	14.189200000	6.871700000	5.946900000
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8	12.306900000	9.089300000	2.585700000
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8	13.549400000	7.354100000	8.105100000
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6	12.047100000	6.587600000	5.029200000
1	11.515800000	5.640200000	4.865400000
7	12.028300000	6.929500000	6.430200000
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8	8.992300000	10.388000000	3.625900000
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7	7.305800000	14.299400000	6.927200000	6	17.523100000	15.995800000	8.583700000
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6	10.891700000	18.941400000	6.795300000	7	18.686300000	12.074000000	3.969900000
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1	12.465400000	20.174400000	8.662300000	1	19.448300000	10.524400000	2.828700000
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6	13.901900000	17.634900000	9.760600000				

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8	4.056349559	1.421897645	3.306556674
8	1.182351047	3.727415172	3.356192751
8	-2.614977724	3.444470444	3.507211960
8	-4.441845938	0.261984076	3.435924564
8	-2.986843132	-3.096274477	3.499727455
8	0.747113125	-4.224988232	-2.739684835
8	3.927847578	-2.035310639	-2.763270114
8	4.159355763	1.643712233	-2.749282962
8	1.286973017	4.177351829	-2.741517073
8	-2.337422846	3.231924870	-2.546398012
8	-4.418376736	0.210170335	-2.699194404
8	-2.791570169	-2.942108426	-2.545961660
7	-0.229654286	-4.953882497	1.586646132
7	1.969213329	-4.628834141	1.578161857
7	3.995968916	-3.318187402	1.516366815
7	5.267207729	-1.501912125	1.513097117
7	5.418505577	0.904215364	1.522973068
7	4.381573677	2.862505529	1.541853204
7	2.504825273	4.378483850	1.586796262
7	0.357625499	4.952891740	1.588085630
7	-2.047042137	4.674071857	1.642368078
7	-3.928716312	3.498454288	1.616886623
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7	-5.285848927	-0.805207028	1.579030988
7	-4.323878961	-3.023963015	1.627245892
7	-2.592668314	-4.413271802	1.648827615
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7	1.977627291	-4.712182103	-0.853856078
7	4.027341528	-3.393709331	-0.908990406
7	5.212287353	-1.505807650	-0.928684822
7	5.362624533	0.936852462	-0.918411341
7	4.428170018	2.960362731	-0.884030439
7	2.548562805	4.510759462	-0.841580537
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1	-3.525220748	-5.810335487	0.405021098
6	1.069720303	1.209018595	-1.555582151
6	1.916413134	-0.037943528	-1.339379171
6	1.046357511	-1.259380235	-1.593119132
6	0.550639703	1.242654380	-2.992784737
6	-1.474064014	0.027805493	-2.235778028
6	0.510855218	-1.244991607	-3.022942972
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6	1.308569157	-0.066698928	1.076853149
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6	1.747071009	-0.467153157	2.085985361
6	0.505932545	-1.340525537	2.233766413
6	-0.676622884	-0.459794164	2.620508196
6	-1.222876257	-0.123009945	0.190868995
6	0.209405760	-2.034850438	0.906799098
6	1.212154714	-0.126434905	-0.347363713
6	-0.032375981	-1.004671513	-0.192656912
7	-0.799031162	-1.386448824	-3.897798562
1	0.673266936	-2.099709510	3.007255247
1	-2.309937690	1.536768133	-0.652092990
1	-0.397323375	2.527144329	-1.833555796
1	1.847713459	1.542181668	-1.550431139
1	-2.665978099	-0.392210571	-2.177119454
1	-1.933396750	0.984325578	-3.004468861
1	0.493484764	-2.343706520	-1.786799068
1	-1.237848845	-2.294747807	-1.407629328
1	0.506636670	0.993585556	-3.534612481
1	1.521253266	-0.376175183	-3.092645556
1	0.942954039	3.103482482	0.163150306
1	-0.783764741	3.083373611	0.550815150
1	-1.765501420	1.204910374	1.805687530
1	0.531773064	1.948534069	2.306444867
1	2.396092864	1.194708156	0.891378005
1	1.958041220	0.052099997	3.025433741
1	2.620637092	-1.082690929	1.865502040
1	-1.562801655	-1.071628350	2.785262899
1	-0.471480218	0.056306767	3.562976100
1	-2.115087385	-0.751675976	0.313020432
1	1.057353728	-2.672435228	0.646658646
1	-0.673079896	-2.668282089	1.027779254
1	2.070165959	-0.757325801	-0.615991685
1	-1.488014877	-2.141556577	-3.763762518
1	-1.121515463	-0.748839086	-4.631090333
1	0.088797429	-1.830436111	-4.190230607

CB[7]•G3 unstable complex

8	-0.842990169	4.211123394	2.879903492
8	-3.507138596	1.743424153	2.776210821
8	-3.539224678	-1.916159158	2.854481237
8	-0.578497544	-4.669760117	2.773561327
8	3.025732731	-4.021331810	2.726308857
8	4.641370141	-0.342974439	2.760360510
8	2.703563202	3.103129074	2.686555925
8	-1.203365530	4.465903428	-3.360106845
8	-4.522958087	2.227596204	-3.353590767
8	-3.709587607	-1.639270178	-3.253460546
8	-0.637704668	-3.984872463	-3.209222567
8	2.585199626	-3.453937697	-3.282445057
8	4.028099450	-0.247194030	-3.370111729
8	2.731360559	3.380786639	-3.510373579
7	0.031846523	5.130875560	0.970270166
7	-2.153544856	4.725473060	1.067810970
7	-4.002973912	3.190786071	1.066832485
7	-4.896542022	1.146485562	1.057048945
7	-4.800948646	-1.258620694	1.057238785
7	-3.714118391	-3.207786179	0.950558536
7	-1.920982906	-4.859721999	0.914408537
7	0.163779595	-5.686007646	0.840769529
7	2.609360030	-5.247527950	0.817709203
7	4.268473848	-3.729481793	0.809755970
7	5.140270916	-1.430842948	0.780889908
7	5.096847120	0.807432783	0.824988829
7	4.011354154	2.976642162	0.804739569
7	2.344098028	4.465464401	0.878180845
7	-0.083652882	5.125435288	-1.456347732
7	-2.294752321	4.759380645	-1.358298148
7	-4.243859147	3.315928579	-1.339767260
7	-5.137967798	1.270927121	-1.352204525
7	-4.901598483	-1.142763893	-1.353306810
7	-3.823603082	-3.096709588	-1.470479774
7	-1.987416460	-4.677371100	-1.487061272
7	0.102119697	-5.438408371	-1.582772903
7	2.462980450	-5.022382204	-1.605652257
7	4.146463235	-3.574996851	-1.603898798
7	5.078656050	-1.362536739	-1.649340508
7	4.960752810	0.862224223	-1.586531259
7	3.992631345	3.072603385	-1.618404691
7	2.256282411	4.478681757	-1.538104246
6	-0.974658326	4.633012481	1.759853899
6	-3.419291635	4.368226503	1.652231688

1	-3.228495597	4.148499431	2.709298290	6	2.968910677	3.612781073	-2.357892951
1	-4.119841546	5.207608551	1.554573059	6	1.219987338	5.347600418	-2.053297474
6	-4.069789007	1.994530485	1.744401033	1	1.511533772	6.396458301	-1.898699595
6	-5.361908778	-0.082228820	1.655190172	1	1.127530136	5.138733213	-3.125743587
1	-5.032200455	-0.074686509	2.701370483	6	-0.481580305	5.754912436	-0.220535851
1	-6.457867188	-0.118194933	1.593662082	1	-0.211632860	6.824383676	-0.233532782
6	-3.957645017	-2.107187212	1.746073867	6	-2.010846901	5.485203393	-0.145402673
6	-3.153460052	-4.419818932	1.516695207	1	-2.628948044	6.397430938	-0.094440812
1	-2.929670851	-4.201782888	2.568196329	6	-4.897261898	3.220758947	-0.056980922
1	-3.901308090	-5.224681023	1.444444760	1	-5.632471303	4.034396707	0.060299477
6	-0.751736989	-5.026584174	1.643546073	6	-5.519434156	1.794242984	-0.064841135
6	1.496651493	-6.034380642	1.310711667	1	-6.616544090	1.777705093	0.045927284
1	1.476728889	-5.876485232	2.395695348	6	-5.302184034	-1.839675368	-0.154980947
1	1.680294739	-7.089245789	1.073283762	1	-6.400659298	-1.929027630	-0.114751976
6	3.263740340	-4.298004572	1.586143118	6	-4.547248719	-3.194532964	-0.231653640
6	5.220613992	-2.777055543	1.331434172	1	-5.203291588	-4.080793501	-0.241578754
1	6.237848331	-3.163819826	1.174244452	6	-1.881686080	-5.553272256	-0.346963389
1	5.007481761	-2.683258684	2.403339988	1	-2.658041498	-6.334583708	-0.386166757
6	4.922065839	-0.331222695	1.593359418	6	-0.423390213	-6.093709848	-0.416902630
6	5.039988699	2.131288044	1.379667576	1	-0.346753748	-7.187088871	-0.528762375
1	6.013452184	2.628690240	1.257309904	6	3.242689292	-5.430521862	-0.466789964
1	4.801417094	2.015034280	2.443742097	1	3.561246050	-6.479175574	-0.582717872
6	2.989096488	3.467989055	1.576862151	6	4.414596903	-4.403523333	-0.458090224
6	1.365507477	5.330964804	1.479213826	1	5.415637112	-4.857290461	-0.538397718
1	1.337198387	5.098217501	2.550206757	6	5.793144434	-1.034214747	-0.451309389
1	1.662046232	6.377243317	1.324307446	1	6.811847370	-1.455507220	-0.488073168
6	-1.194214339	4.754779689	-2.195870151	6	5.742110845	0.518164937	-0.427127360
6	-3.643633276	4.529808210	-1.844691929	1	6.730831724	1.005919086	-0.472051781
1	-3.584597656	4.423987181	-2.934547482	6	4.198970549	3.774701950	-0.383619672
1	-4.270741034	5.392162061	-1.581285622	1	5.197282688	4.243430356	-0.370337963
6	-4.625003656	2.264748973	-2.159946396	6	3.017098061	4.784512660	-0.348108989
6	-5.606653861	0.006360179	-1.874354137	1	3.325467142	5.843528348	-0.352863329
1	-5.432586202	0.036527872	-2.956799348	6	1.590494021	-0.674596460	-0.852418573
1	-6.679526660	-0.105343574	-1.664883508	6	0.726648089	-1.924860327	-0.807165074
6	-4.096769282	-1.935223998	-2.154125754	6	-0.739944873	-1.550096805	-0.674562686
6	-3.218561955	-4.248879705	-2.093494005	6	1.242072524	0.124086642	-2.090993193
1	-2.977725576	-3.954787661	-3.122301944	6	-0.490961553	1.333085961	-0.790506681
1	-3.938271420	-5.081065767	-2.086530880	6	-1.134887383	-0.782378192	-1.914200396
6	-0.806784758	-4.620034741	-2.206464292	6	-0.249244365	0.450950317	-2.062603684
6	1.371024625	-5.755193756	-2.176928375	6	1.150556805	-2.735560301	0.386871426
1	1.308927052	-5.451373446	-3.229524924	6	1.741558565	-0.699228975	1.634768366
1	1.557149679	-6.831810343	-2.086372697	6	0.894049705	-1.961570427	1.666712284
6	3.004236456	-3.951029909	-2.275595207	6	-0.566295851	-1.555973141	1.789282799
6	5.077955419	-2.679058859	-2.225959061	6	-0.764079924	-0.788287164	3.086538778
1	6.090600940	-3.100503095	-2.172970512	6	0.097903208	0.471627298	3.080741608
1	4.753698730	-2.561493746	-3.267594071	6	1.570752235	0.099237472	2.918217795
6	4.611570113	-0.258047058	-2.323414828	6	1.367944138	0.138317028	0.416206051
6	4.961244586	2.167684589	-2.189988405	6	-0.301848232	1.334176875	1.845632375
1	4.679077672	2.038172852	-3.242191309	6	-0.957833117	-0.720127525	0.579999513
1	5.964380879	2.610526551	-2.110799249	6	-0.102130987	0.545509515	0.512402999

7	-0.606751413	1.065651252	-3.438316835	8	-0.794200000	4.186500000	2.303800000
7	-0.089112003	1.176880126	4.457850200	8	-3.397000000	1.482600000	2.111000000
1	2.641523646	-0.970089904	-0.907474806	8	-3.638600000	-2.415500000	1.965300000
1	0.869833290	-2.493006322	-1.729349327	8	-0.773100000	-5.020700000	1.589300000
1	-1.343920473	-2.457867661	-0.605322383	8	3.175000000	-4.107400000	1.439600000
1	1.835134274	1.038505500	-2.101553197	8	4.585900000	-0.497700000	1.641000000
1	1.523527268	-0.472303081	-2.956918069	8	2.626800000	2.905100000	1.855600000
1	-1.543227010	1.614847474	-0.706778119	8	-0.962800000	3.801600000	-3.761300000
1	0.105316662	2.248290063	-0.837153567	8	-4.001400000	1.822300000	-3.897400000
1	-1.038831083	-1.463939778	-2.754964251	8	-3.885800000	-1.688800000	-4.088900000
1	-2.171863966	-0.466814882	-1.823374020	8	-1.068300000	-3.728100000	-4.407200000
1	0.616278566	-3.671451028	0.396130208	8	2.375600000	-2.874600000	-4.500900000
1	2.212851389	-2.917720313	0.291762621	8	4.066500000	0.175800000	-4.402900000
1	2.781931551	-0.999396153	1.550285135	8	2.617300000	3.350500000	-4.150800000
1	1.175342654	-2.577314127	2.524632685	7	0.045700000	5.098800000	0.372900000
1	-1.193474584	-2.445491852	1.829390115	7	-2.107200000	4.560400000	0.455400000
1	-0.482078323	-1.469587501	3.885329668	7	-3.922600000	2.966000000	0.440000000
1	-1.819711796	-0.544636915	3.188287693	7	-4.788400000	0.912100000	0.365900000
1	2.191321808	0.990046305	2.857187377	7	-4.835000000	-1.507600000	0.226300000
1	1.939129341	-0.520557515	3.733288853	7	-3.957500000	-3.541800000	-0.020000000
1	1.995321613	1.038970558	0.388172268	7	-2.084800000	-5.060700000	-0.294900000
1	-1.346395511	1.627957379	1.930548251	7	0.091900000	-5.511900000	-0.492200000
1	0.316562382	2.230609035	1.815755606	7	2.461300000	-4.965500000	-0.579600000
1	-2.015700035	-0.436878732	0.658565934	7	4.219500000	-3.592600000	-0.539000000
6	0.333041259	2.133603727	-3.799548219	7	5.236600000	-1.395300000	-0.378800000
6	-0.557754518	0.078566616	-4.546448188	7	5.126000000	0.820400000	-0.161700000
6	-1.970937540	1.597164863	-3.436281146	7	4.020900000	2.973000000	0.019800000
6	0.111879149	0.229504934	5.577843810	7	2.367300000	4.460000000	0.189400000
6	0.857222307	2.285841709	4.661449200	7	-0.039800000	5.026500000	-2.045000000
6	-1.436233607	1.742256101	4.631287741	7	-2.203900000	4.528400000	-1.962600000
1	-2.096771718	2.296555411	-2.620453668	7	-4.114900000	3.071000000	-1.968500000
1	-2.689166182	0.787070875	-3.359508546	7	-5.139100000	1.109700000	-2.026500000
1	-2.171957160	2.128714485	-4.363310813	7	-5.085600000	-1.283300000	-2.167300000
1	0.352182982	-0.514026898	-4.522628019	7	-4.124700000	-3.262500000	-2.426200000
1	-0.581970898	0.630555879	-5.483946738	7	-2.238000000	-4.713700000	-2.688500000
1	-1.419412401	-0.583991238	-4.527064386	7	-0.075000000	-5.141300000	-2.886400000
1	1.286596190	1.725436334	-4.120530368	7	2.251600000	-4.584600000	-2.965700000
1	0.487479015	2.790190859	-2.953926217	7	4.012700000	-3.242200000	-2.926300000
1	-0.073560543	2.733604377	-4.609756162	7	5.086700000	-1.105400000	-2.785500000
1	1.881878649	1.933058255	4.701305860	7	5.098100000	1.098000000	-2.564100000
1	0.623888926	2.786734890	5.598774133	7	4.096900000	3.269900000	-2.387700000
1	0.757644567	3.009823329	3.861538751	7	2.311400000	4.566800000	-2.222100000
1	-2.204739828	1.007345793	4.422436153	6	-0.933200000	4.555400000	1.161800000
1	-1.566585400	2.592837743	3.971773713	6	-3.356900000	4.149500000	1.041700000
1	-1.551976007	2.083530317	5.657868608	1	-3.143800000	3.911000000	2.089500000
1	1.029716496	-0.338716050	5.461028846	1	-4.085100000	4.965000000	0.969900000
1	-0.729493960	-0.451983946	5.664627793	6	-3.966800000	1.752700000	1.078700000
1	0.183330588	0.796605386	6.504363322	6	-5.281700000	-0.325700000	0.923400000
				1	-4.887200000	-0.402500000	1.943300000
CB[7]•G3 exclusion complex				1	-6.378600000	-0.302700000	0.934400000

6	-4.080100000	-2.478600000	0.841900000	6	-1.995300000	5.313100000	-0.771800000
6	-3.345700000	-4.793400000	0.358400000	1	-2.678900000	6.173200000	-0.757200000
1	-3.134300000	-4.738200000	1.432600000	6	-4.801900000	3.012900000	-0.698900000
1	-4.044100000	-5.611800000	0.145300000	1	-5.505500000	3.852100000	-0.608100000
6	-0.901700000	-5.164700000	0.396100000	6	-5.456600000	1.607600000	-0.714000000
6	1.434300000	-5.847400000	-0.069600000	1	-6.544200000	1.596900000	-0.558300000
1	1.454600000	-5.759000000	1.022800000	6	-5.462900000	-2.000100000	-0.977200000
1	1.660800000	-6.877000000	-0.375800000	1	-6.556700000	-2.004700000	-0.866000000
6	3.261700000	-4.199000000	0.237500000	6	-4.818500000	-3.397300000	-1.171000000
6	5.275800000	-2.781500000	0.021700000	1	-5.528800000	-4.235000000	-1.219900000
1	6.246800000	-3.207800000	-0.258500000	6	-1.980400000	-5.636100000	-1.614900000
1	5.143300000	-2.807900000	1.109600000	1	-2.639800000	-6.512100000	-1.701700000
6	4.928800000	-0.374700000	0.488300000	6	-0.465900000	-5.941300000	-1.756400000
6	5.043300000	2.086400000	0.525300000	1	-0.220700000	-6.998000000	-1.937900000
1	6.014900000	2.593800000	0.470900000	6	3.048400000	-5.117700000	-1.892900000
1	4.787400000	1.854800000	1.565800000	1	3.282000000	-6.175400000	-2.082800000
6	2.965300000	3.385200000	0.797900000	6	4.277100000	-4.171300000	-1.860300000
6	1.390500000	5.296200000	0.844800000	1	5.247300000	-4.664200000	-2.019000000
1	1.388000000	5.025800000	1.906300000	6	5.857400000	-0.900900000	-1.585300000
1	1.679300000	6.344400000	0.712500000	1	6.859600000	-1.337500000	-1.701400000
6	-1.058000000	4.386000000	-2.704100000	6	5.827700000	0.640000000	-1.411300000
6	-3.510300000	4.260600000	-2.503200000	1	6.815300000	1.121300000	-1.370300000
1	-3.392000000	4.090200000	-3.579400000	6	4.249200000	3.874500000	-1.091400000
1	-4.160900000	5.123000000	-2.316800000	1	5.240200000	4.340700000	-1.005400000
6	-4.366800000	1.976500000	-2.752600000	6	3.050400000	4.853700000	-1.013800000
6	-5.721000000	-0.068300000	-2.602000000	1	3.320100000	5.918000000	-0.974300000
1	-5.569200000	0.002200000	-3.685200000	6	1.674700000	-1.243300000	1.398200000
1	-6.788500000	-0.109000000	-2.357700000	6	0.697800000	-2.372200000	1.686300000
6	-4.305900000	-2.035000000	-3.007500000	6	-0.716100000	-1.840100000	1.514600000
6	-3.554400000	-4.365200000	-3.145100000	6	1.490300000	-0.701800000	-0.025200000
1	-3.457100000	-4.045100000	-4.189200000	6	-0.183000000	0.929100000	0.829300000
1	-4.211000000	-5.238700000	-3.061100000	6	-0.914800000	-1.329000000	0.082900000
6	-1.118400000	-4.435800000	-3.426400000	6	0.059600000	-0.180300000	-0.199800000
6	1.169400000	-5.297900000	-3.581600000	6	0.896800000	-2.894500000	3.105700000
1	1.030600000	-4.867500000	-4.580400000	6	1.641700000	-0.629200000	3.841200000
1	1.423400000	-6.362900000	-3.643900000	6	0.661700000	-1.769800000	4.104100000
6	2.824100000	-3.489600000	-3.559400000	6	-0.757900000	-1.227100000	3.954300000
6	5.001100000	-2.358100000	-3.478500000	6	-0.995900000	-0.093400000	4.956100000
1	5.977700000	-2.855200000	-3.465300000	6	-0.015000000	1.053300000	4.683900000
1	4.690200000	-2.128700000	-4.504600000	6	1.418300000	0.526000000	4.821800000
6	4.669300000	0.067000000	-3.358300000	6	1.454500000	-0.126800000	2.411200000
6	5.098100000	2.461500000	-3.020300000	6	-0.216700000	1.535000000	3.246800000
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1	6.087000000	2.901600000	-2.849400000	6	0.034600000	0.401200000	2.254800000
6	2.963400000	3.679100000	-3.037500000	7	-0.151900000	0.366800000	-1.638900000
6	1.203700000	5.353100000	-2.691900000	7	-0.261500000	2.223600000	5.657500000
1	1.417500000	6.418700000	-2.547200000	1	2.690700000	-1.625800000	1.506200000
1	1.090600000	5.121700000	-3.757300000	1	0.867500000	-3.190300000	0.982300000
6	-0.488000000	5.674500000	-0.836900000	1	-1.422200000	-2.649600000	1.706000000
1	-0.268900000	6.750500000	-0.877800000	1	2.218400000	0.096900000	-0.168700000

1	1.708600000	-1.502100000	-0.736200000
1	-1.208700000	1.288700000	0.784700000
1	0.497500000	1.767000000	0.678800000
1	-0.742800000	-2.164400000	-0.597600000
1	-1.950600000	-1.002600000	-0.021600000
1	0.200000000	-3.714800000	3.284300000
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1	-0.375200000	2.610100000	7.718700000

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8	-2.987267201	-3.555197693	-2.497912526
8	-4.560301184	-0.210761607	-2.314064081
8	-2.785481631	3.223595697	-2.501540691
8	0.357746327	4.342059218	-3.170092271
8	2.956040658	1.997673988	-3.614744505
8	4.134639586	-1.817801607	2.407823483
8	1.356114828	-4.219609723	2.857265211
8	-2.010510230	-3.512826300	3.437456477
8	-3.629558769	-0.192617744	3.810529294
8	-1.839282275	3.326469794	3.368843917
8	1.473691246	4.382571001	2.767045100
8	3.890832458	2.042980005	2.258261578
7	4.502020797	-1.137743415	-2.023539125
7	3.747877038	-3.228450013	-1.870695599
7	1.970969723	-4.834839667	-1.511108980
7	-0.126859529	-5.483966019	-1.155788962
7	-2.469968205	-4.981145292	-0.764910568
7	-4.109565340	-3.506006426	-0.490553301
7	-5.045456526	-1.283474737	-0.333235948
7	-4.938321900	0.937259535	-0.359307918
7	-3.968961030	3.139492371	-0.524662953
7	-2.431182086	4.720207679	-0.800152729
7	-0.187992746	5.468558729	-1.246410070
7	1.938913585	4.957798161	-1.619685009
7	3.728894598	3.368424413	-1.949072729
7	4.510902351	1.288936871	-2.067309679
7	4.904678005	-1.095010878	0.366585136
7	4.112170505	-3.165314362	0.538736841
7	2.366226353	-4.802193390	0.874382467
7	0.277902876	-5.464952105	1.247620827
7	-2.062438748	-4.948717540	1.637905875
7	-3.716331589	-3.483482565	1.895391465
7	-4.692708417	-1.274332225	2.078696345
7	-4.542392543	0.947917774	2.032293524
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7	-2.027252869	4.738865358	1.574262405
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7	2.389505840	5.020683746	0.761681125
7	4.135250487	3.399016144	0.424830715
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1	2.768847638	-4.288171117	-3.315916010
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1	-1.632177844	-5.562647036	-2.533566676
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1	-5.098427048	-2.502793949	-1.973214075
1	-6.129194200	-3.040530423	-0.590625013
6	-4.803365665	-0.191314572	-1.129025319
6	-5.011135263	2.245830425	-0.954589979

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6	-3.033344127	3.642036615	-1.392764765	6	-4.119341050	-4.252642351	0.742970734
6	-1.587772333	5.633539532	-1.529856305	1	-5.110029219	-4.698719164	0.910197971
1	-1.889072959	6.660735210	-1.302041994	6	-5.537700377	-0.907729358	0.970349666
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6	0.668275995	4.859519136	-2.119340761	6	-5.452565748	0.641437832	0.953684171
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1	2.751916490	4.414065061	-3.419663748	1	-5.060964395	4.266082262	0.866124026
6	3.657577345	2.192982670	-2.641991006	6	-2.964101695	4.997611678	0.508164999
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6	-2.527395928	-3.923955843	2.423446064	6	-1.487582884	-0.539803874	-1.120482661
6	-4.604197776	-2.606421259	2.617935160	6	1.000490366	-0.268729596	-2.605717465
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6	4.689393392	-3.135095859	-0.783647131	1	0.789210902	-0.937440563	-3.441786334
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8	1.367738864	4.369784326	3.308744474
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6	6.651668978	-1.304638365	0.573947593
1	7.744794983	-1.202628314	0.604451914
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1	-3.523922776	-6.548545299	0.065414452	6	-2.459689394	4.416666234	-1.601015545
7	-2.854570242	-4.897685245	-1.033646510	8	-2.161280299	3.775371105	-2.583315944
6	-4.301365861	-4.721133683	1.923512512	7	-1.765905254	5.475119976	1.465394835
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1	-4.151471291	-4.490431266	2.984391261	1	-2.236479308	7.001278526	0.114366554
6	-4.084880713	-4.541416224	-1.682201151	7	-1.635141985	5.289962772	-0.936073245
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1	-4.733566133	-5.426517939	-1.720057576	1	-0.663773323	7.144636537	2.001680065
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6	-5.661735506	-3.620235745	0.085801667	6	-0.459720325	5.834070666	-1.559973131
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7	-4.804458465	-3.462866030	-1.063204877	1	-0.399099048	5.392248332	-2.561118538
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8	-4.782390010	-2.179505138	3.160590373	6	1.805001118	-0.479701838	-0.088893783
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7	-6.048467520	-1.629476894	-1.093871666	6	1.372715936	-0.603983741	1.370190043
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1	2.014812963	5.531421882	-2.908942885	6	1.478347360	-0.961982467	2.195128316
7	3.427830528	4.861131102	1.046636456	6	0.763240030	-0.522172032	-0.173102901
6	4.034964667	5.101016088	-0.239445366	6	1.681356064	1.336674398	1.235228314
1	4.430323106	6.123708588	-0.293572615	6	-0.743726606	1.295378342	0.622600942
7	3.151647276	4.838835928	-1.350140659	6	0.676561710	0.977470905	0.138460286
6	3.957978375	3.779683665	1.687278839	7	0.298739270	2.239143774	-3.434161126
8	3.638535963	3.372461069	2.784613807	7	2.390742347	0.894596257	3.532396166
6	3.531872881	3.738025996	-2.069840567	1	-0.172640283	-1.932730501	-1.519590569
8	2.973650216	3.314048984	-3.060165034	1	-2.373484700	-0.808224647	-1.569999653
7	4.941994747	3.254079509	0.896112229	1	-2.757534533	1.186077017	-0.141736485
6	5.093552375	3.971617890	-0.345858020	1	1.078642767	-0.312955000	-2.900195987
1	6.130459043	4.308623794	-0.473742889	1	-0.643276711	-0.334746829	-3.318035615
7	4.659812103	3.219336759	-1.499348816	1	0.935834292	2.846477666	-0.906783684
6	5.912714406	2.327540989	1.408525244	1	1.989130026	1.532719902	-1.473473202
1	6.920562215	2.724094713	1.236404486	1	-2.171192879	1.514617112	-2.517143656
1	5.718481362	2.222752091	2.481495338	1	-1.518049028	2.824944113	-1.532348125
6	5.488319639	2.262624839	-2.180868225	1	-2.967062950	-1.138067357	0.826823653
1	6.507952761	2.659942348	-2.262740621	1	-1.899631318	-2.421464380	0.253229998
1	5.052580746	2.111651580	-3.174999085	1	0.541620780	-2.392997746	0.888455661
7	5.825862654	1.013596230	0.830175583	1	-1.186744434	-1.587497747	2.463772524

1	-2.041205525	0.732672956	2.257497194
1	-0.263710309	0.304608036	3.888379234
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1	2.486879645	-1.220320441	1.868529972
1	1.260299346	-1.557562129	3.082694526
1	1.773538095	-0.765121693	-0.525621213
1	1.595886946	2.399893832	1.464318842
1	2.694349860	1.125002672	0.888422651
1	-0.820668817	2.363469939	0.859184962
1	-0.159655320	1.852655471	-4.263598440
1	-0.019318562	3.223150748	-3.315748003
1	1.318453200	2.284574049	-3.590055918
1	2.546018070	1.915912427	3.555649379
1	3.309774402	0.464286180	3.308460563
1	2.097495559	0.571106293	4.457671221