

Supplementary Information

Unravelling Binding Effects in Cyclodextrin Inclusion Complexes with Diamondoid Ammonium Salt Guests

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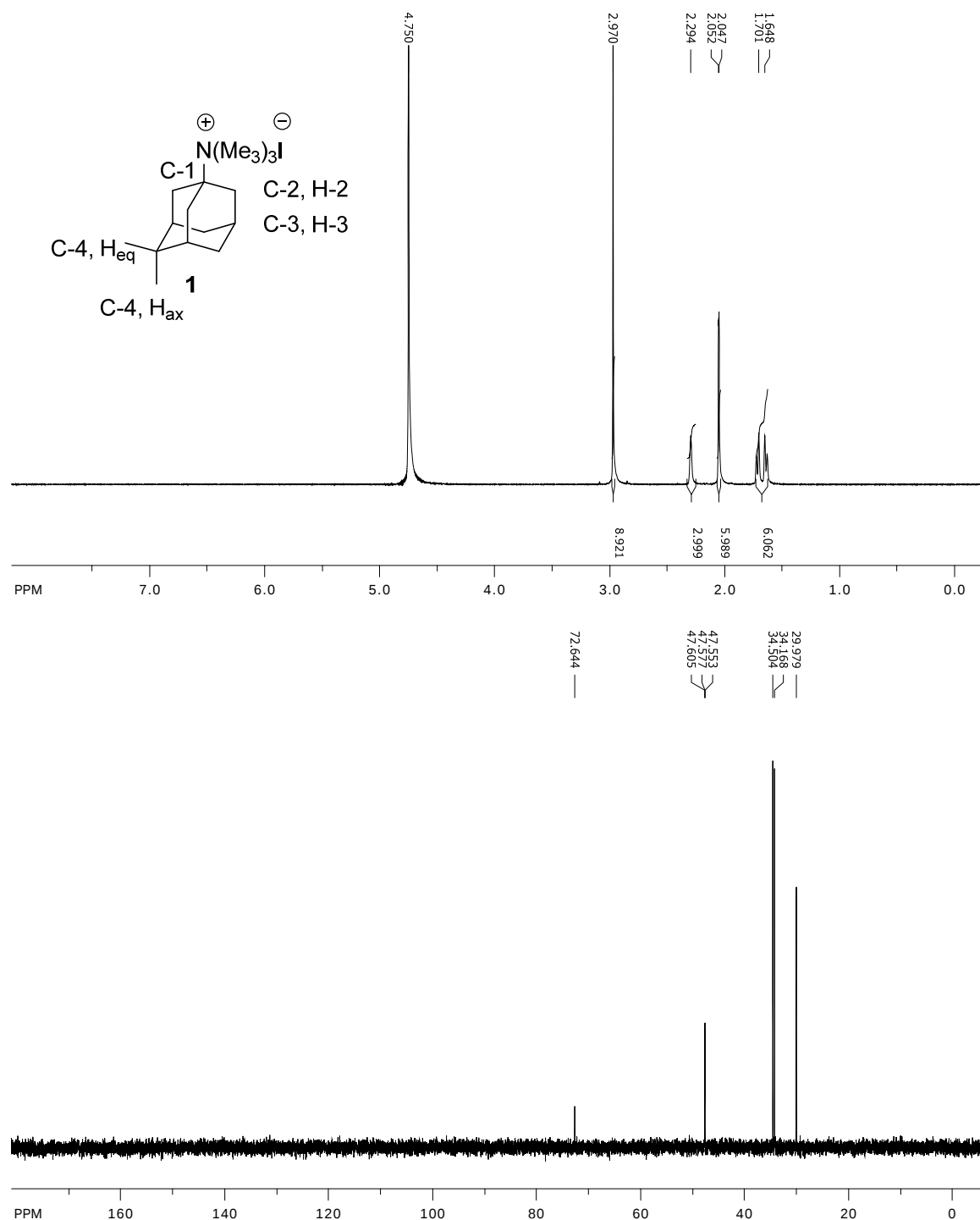
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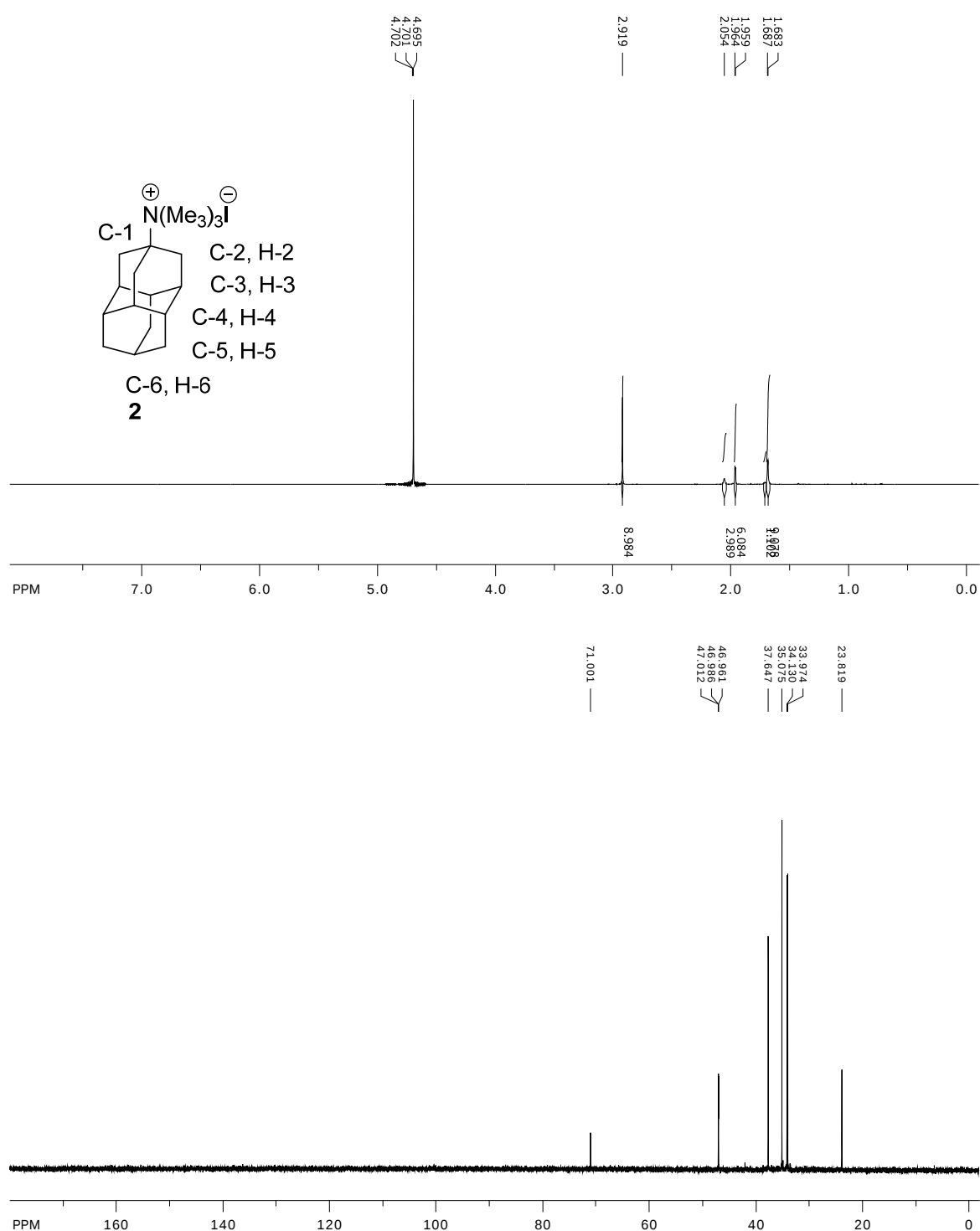
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Figure S1. ^1H (D_2O , 600 Hz) and ^{13}C NMR spectra (D_2O , 150 Hz) of *N,N,N*-trimethyladamantane-1-aminium iodide (**1**).



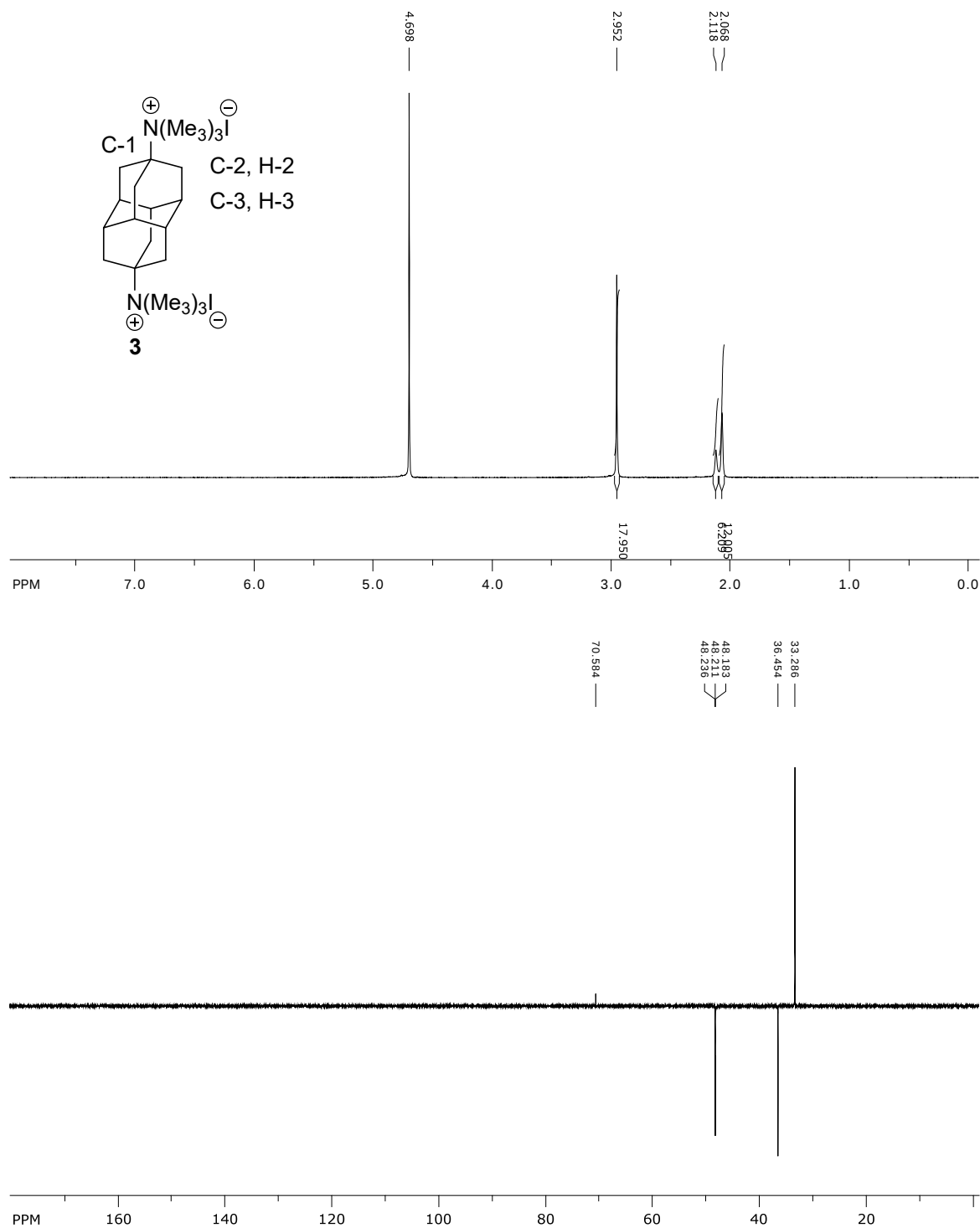
1: ^1H (D_2O , 600 MHz, 25 °C) δ 3.02 (9H, s, CH_3), 2.35 (3H, s, H-3), 2.10 (6H, d, $J = 2.03$ Hz, H-2), 1.71 (3H, d, $J = 12.3$ Hz, H_{eq}), 1.64 (3H, d, $J = 12.3$ Hz, H_{ax}) ppm. ^{13}C (D_2O , 150 MHz, 25 °C) δ 72.5 (C-1), 47.54 (CH_3), 47.51 (CH_3), 47.49 (CH_3), 34.4 (C-4), 34.1 (C-2), 29.9 (C-3) ppm. HRMS (MALDI): calcd. for $[\text{C}_{13}\text{H}_{24}\text{IN}]^+$ 194.1909; found 194.1916.

Figure S2. ^1H (D_2O , 600 Hz) and ^{13}C NMR (D_2O , 150 Hz) spectra of *N,N,N*-trimethyldiamantane-4-aminium iodide (**2**).



2: ^1H (D_2O , 600 MHz, 25 $^\circ\text{C}$) δ 3.02 (9H, s, CH_3), 2.16 (3H, s, H-3), 2.07 (6H, d, $J = 2.98$ Hz, H-2), 1.76 (s, 1H, H-6), 1.75-1.72 (9H, m, H-4, H-5) ppm. ^{13}C (D_2O , 150 MHz, 25 $^\circ\text{C}$) δ 71.9 (C-1), 47.92 (CH_3), 47.90 (CH_3), 47.87 (CH_3), 38.6 (C-3), 36.0 (C-4 or C-5), 35.0 (C-2), 34.9 (C-4 or C-5), 24.7 (C-6) ppm. HRMS (MALDI): calcd. for $[\text{C}_{17}\text{H}_{28}\text{N}]^+$ 246.2216; found 246.2228.

Figure S3. ^1H (D_2O , 600 Hz) and ^{13}C NMR (D_2O , 150 Hz) spectra of *N,N,N,N',N',N'*-hexamethyldiamantane-4,9-diaminium diiodide (**3**).



3: ^1H (D_2O , 600 MHz, 25 °C) δ 2.95 (18H, s, CH_3), 2.11 (6H, s, H-2), 2.06 (12H, s, H-3) ppm. ^{13}C (D_2O , 150 MHz, 25 °C) δ 70.6 (C-1), 48.23 (CH_3), 48.21 (CH_3), 48.18 (CH_3), 36.4 (C-3), 33.3 (C-2) ppm. HRMS (MALDI): calcd. for $[\text{C}_{20}\text{H}_{36}\text{N}_2\text{I}]^+$ 431.1918; found 431.1928.

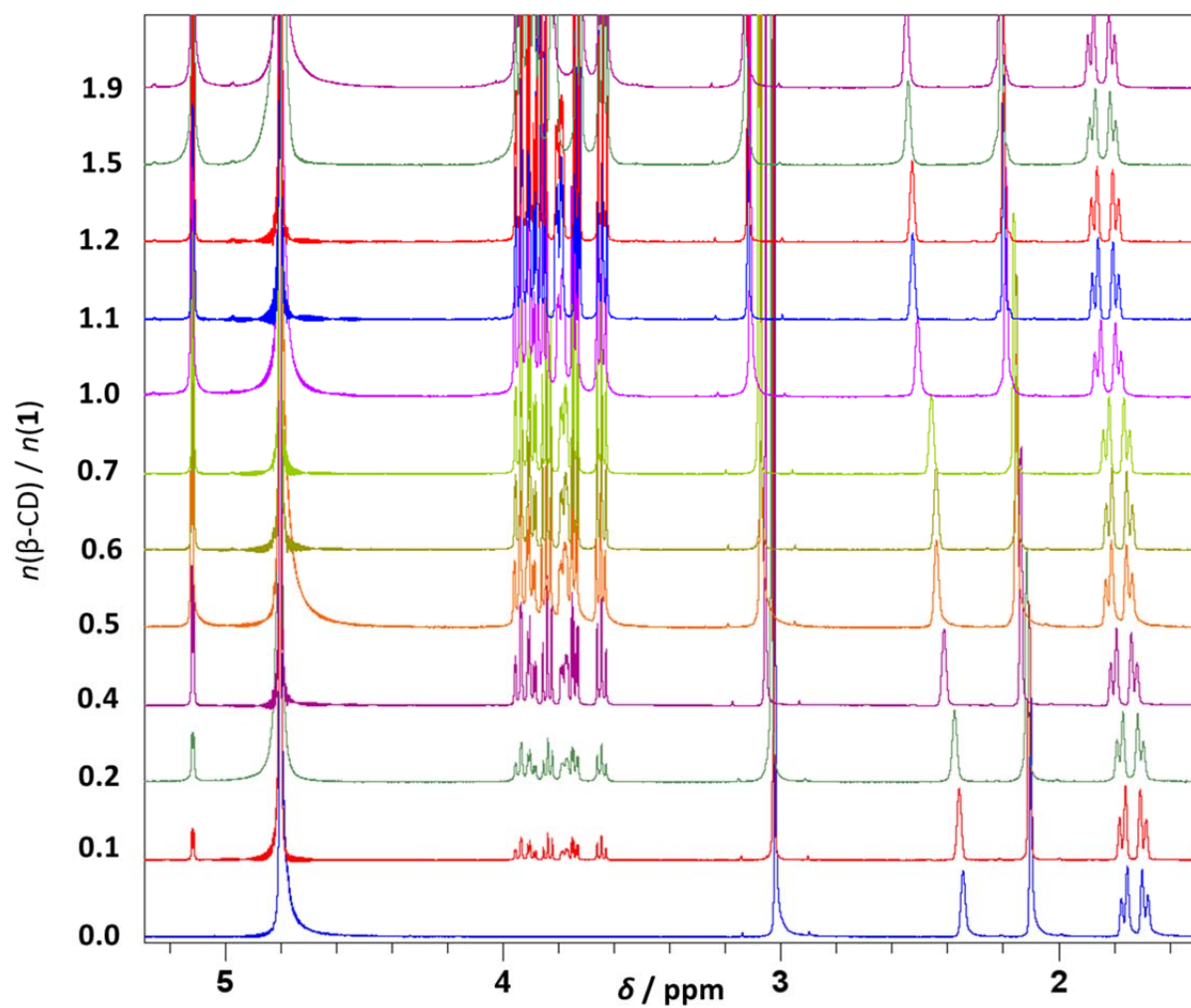


Figure S4. ^1H NMR (600 MHz, 25 $^\circ\text{C}$) spectra obtained by titration of **1** with added equivalents of $\beta\text{-CD}$ in D_2O (to the top).

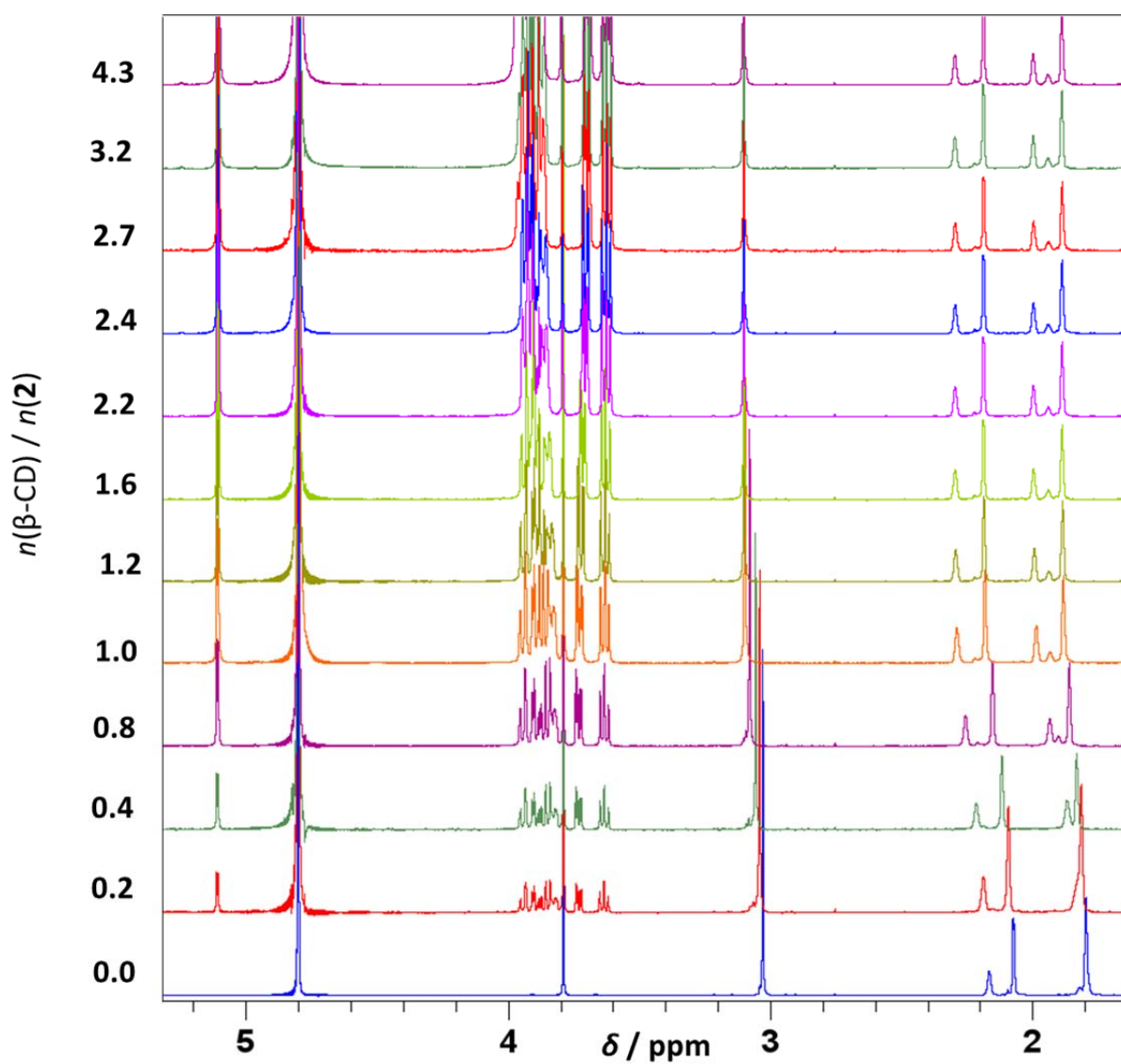


Figure S5. ¹H NMR (600 MHz, 25 °C) spectra obtained by titration of **2** with added equivalents of β-CD in D₂O (to the top).

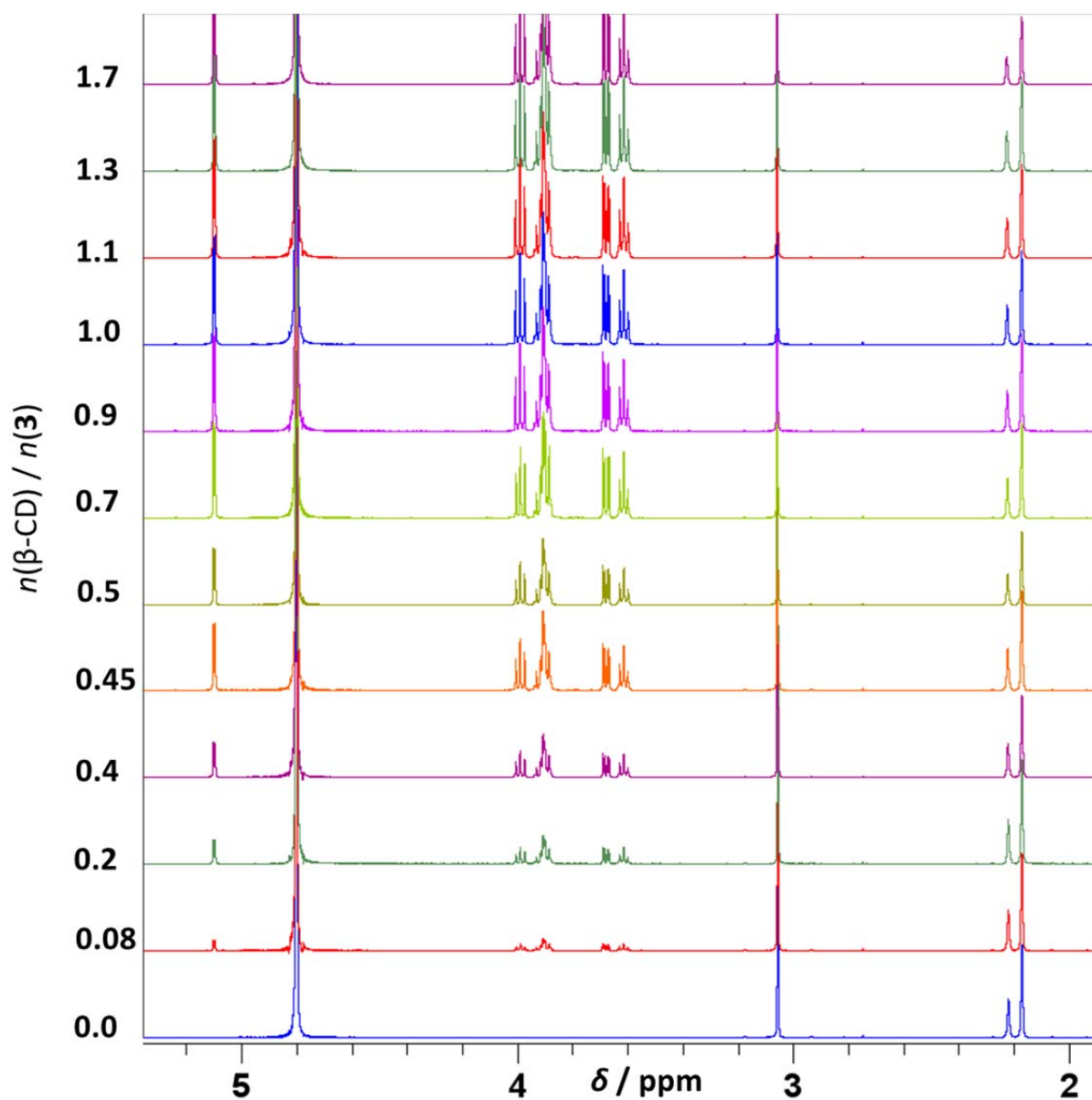


Figure S6. ¹H NMR (600 MHz, 25 °C) spectra obtained by titration of **3** with added equivalents of β-CD in D₂O (to the top).

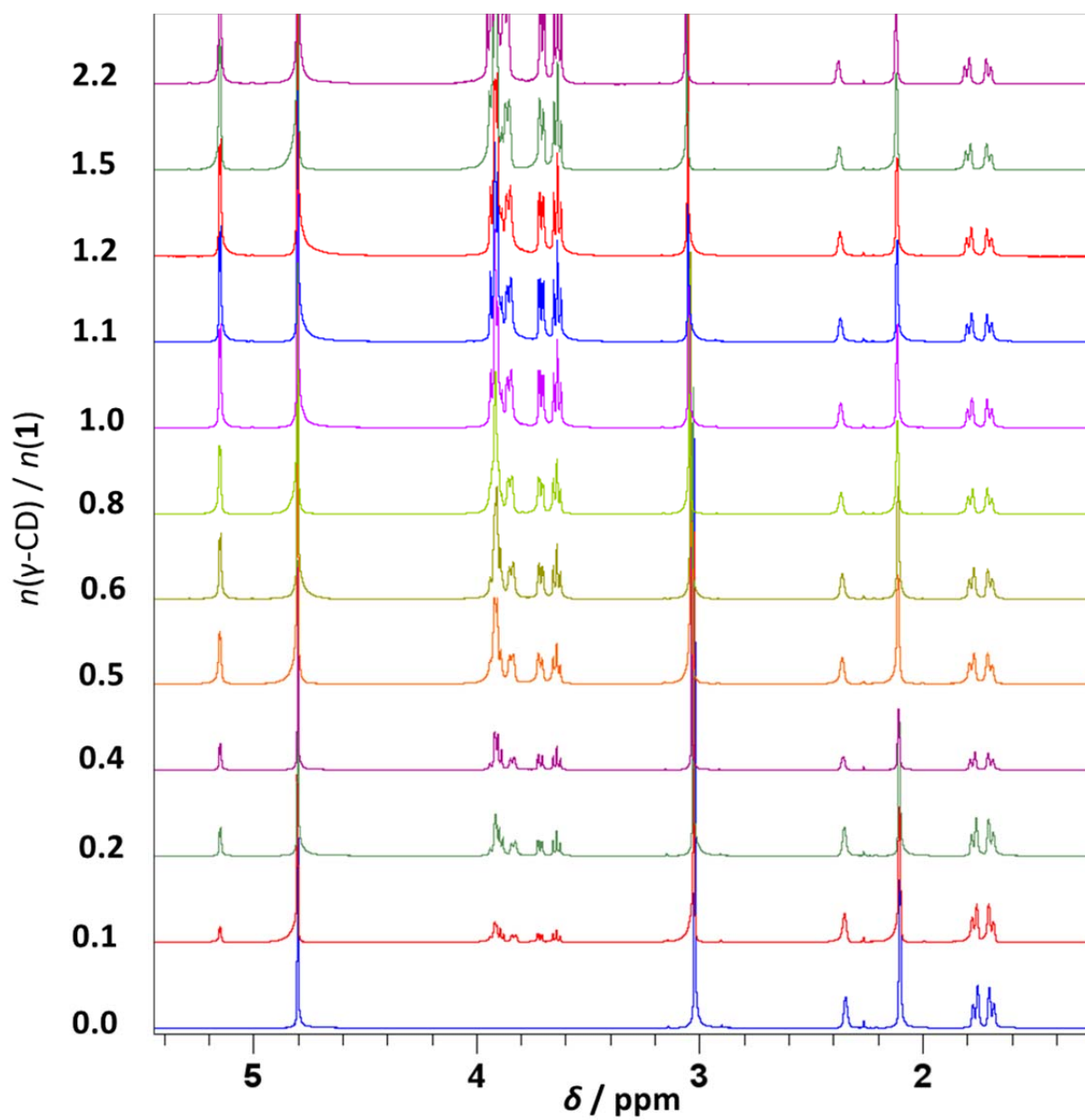


Figure S7. ^1H NMR (600 MHz, 25 $^\circ\text{C}$) spectra obtained by titration of **1** with added equivalents of γ -CD in D_2O (to the top).

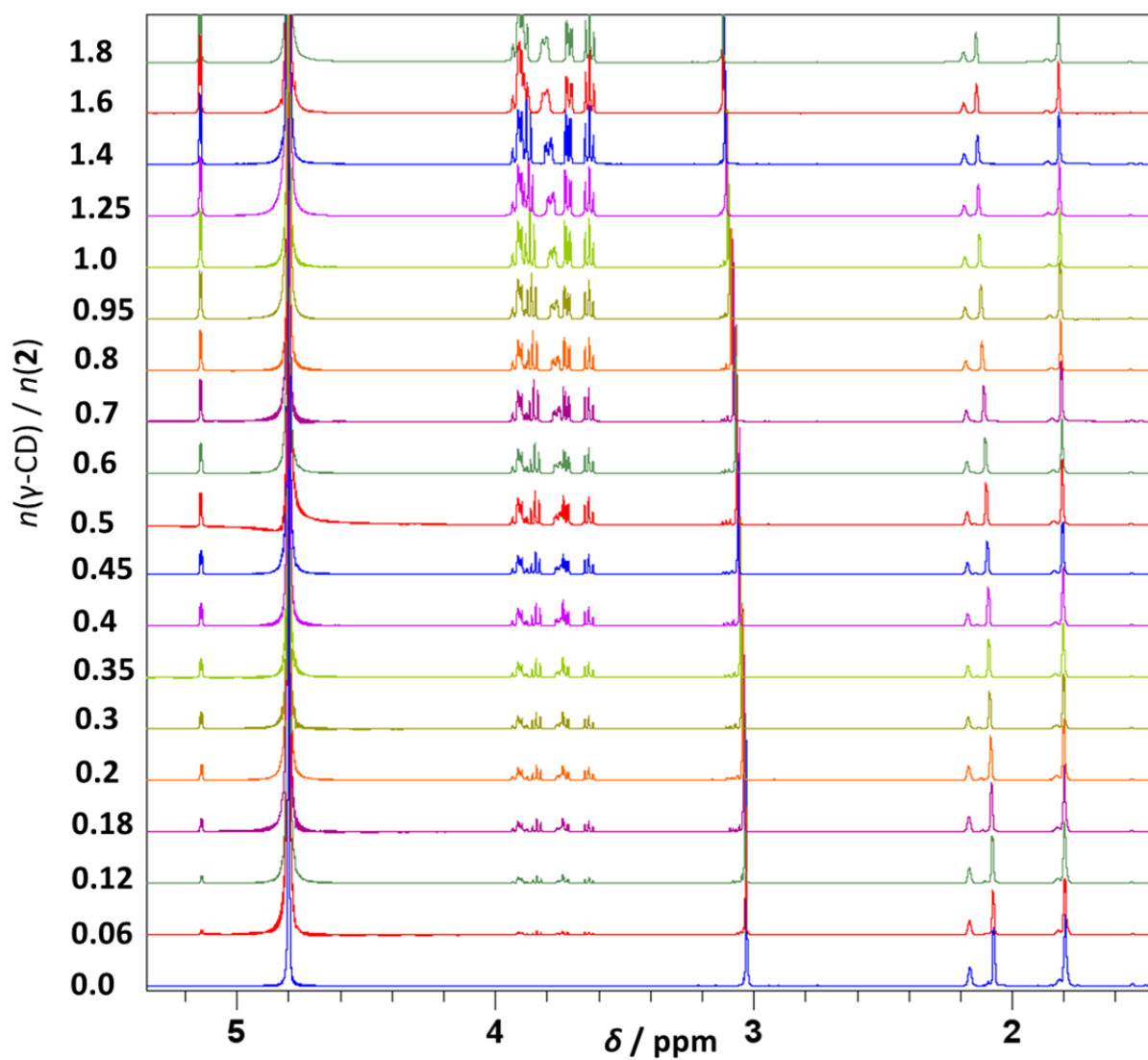


Figure S8. ¹H NMR (600 MHz, 25 °C) spectra obtained by titration of **2** with added equivalents of γ-CD in D₂O (to the top).

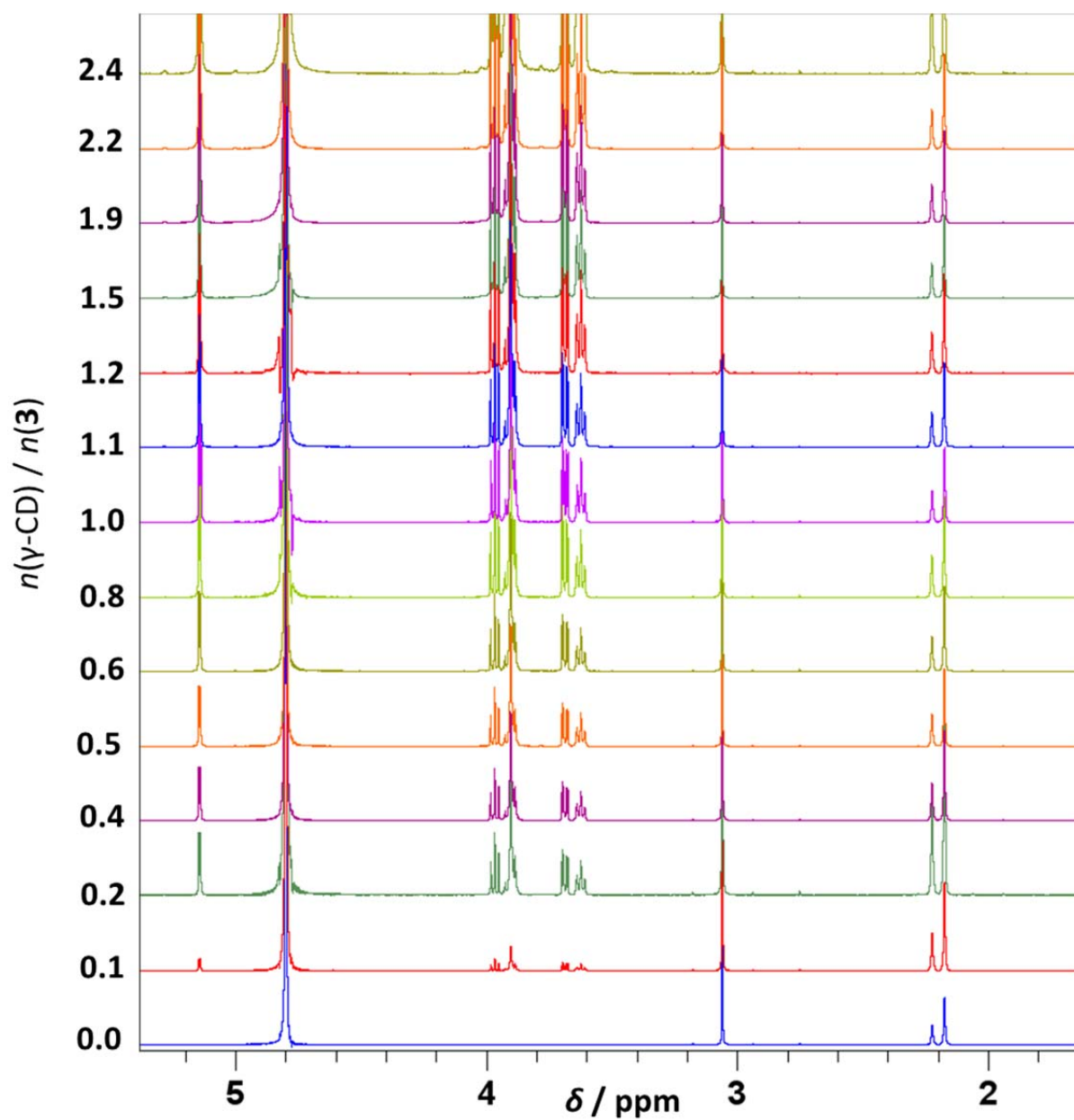


Figure S9. ^1H NMR (600 MHz, 25 °C) spectra obtained by titration of **3** with added equivalents of $\gamma\text{-CD}$ in D_2O (to the top).

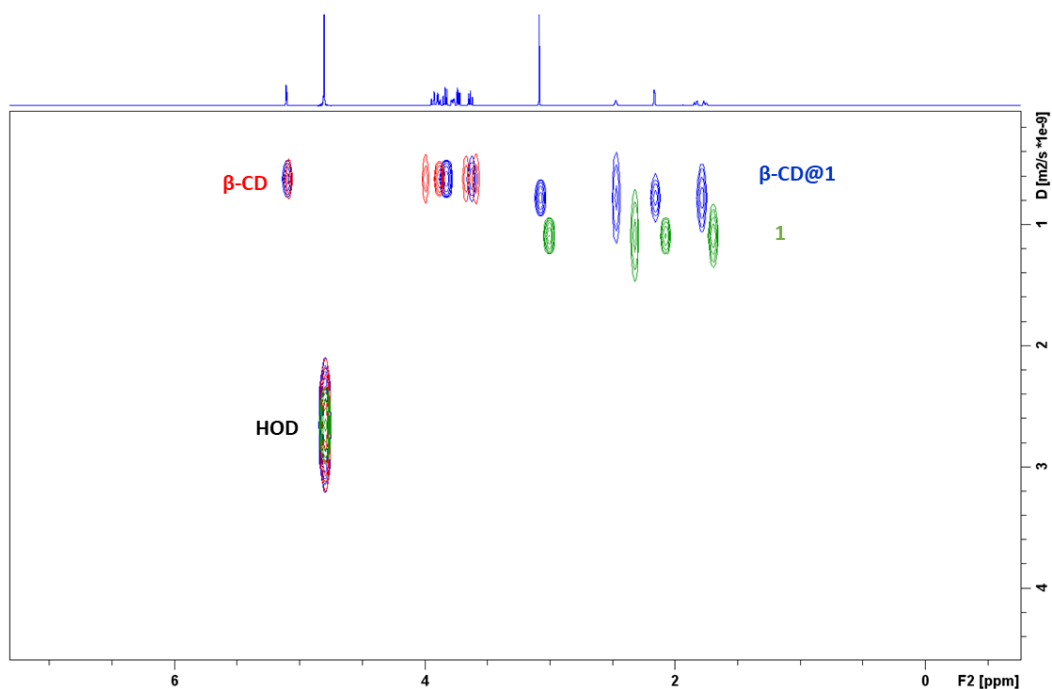


Figure S10. $\beta\text{-CD}$, **1** and **1@ $\beta\text{-CD}$** ^1H NMR DOSY (600 MHz, D_2O , 25 $^\circ\text{C}$). The one-dimensional ^1H NMR spectrum of **1@ $\beta\text{-CD}$** is shown at the top.

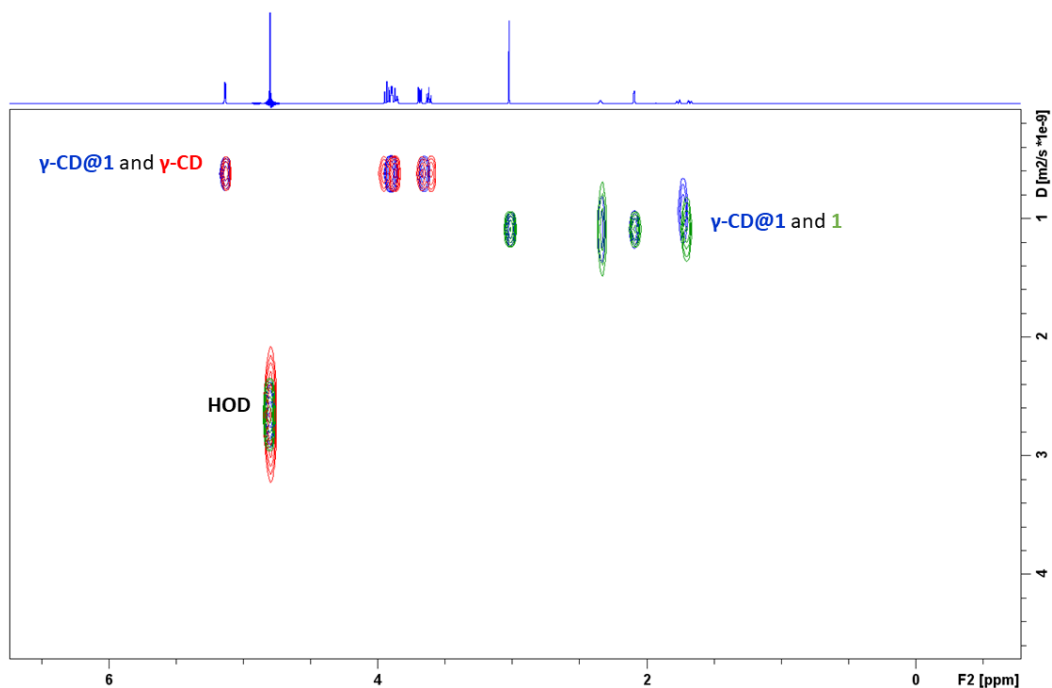


Figure S11. $\gamma\text{-CD}$, **1** and **1@ $\gamma\text{-CD}$** ^1H NMR DOSY (600 MHz, D_2O , 25 $^\circ\text{C}$). The one-dimensional ^1H NMR spectrum of **1@ $\gamma\text{-CD}$** is shown at the top.

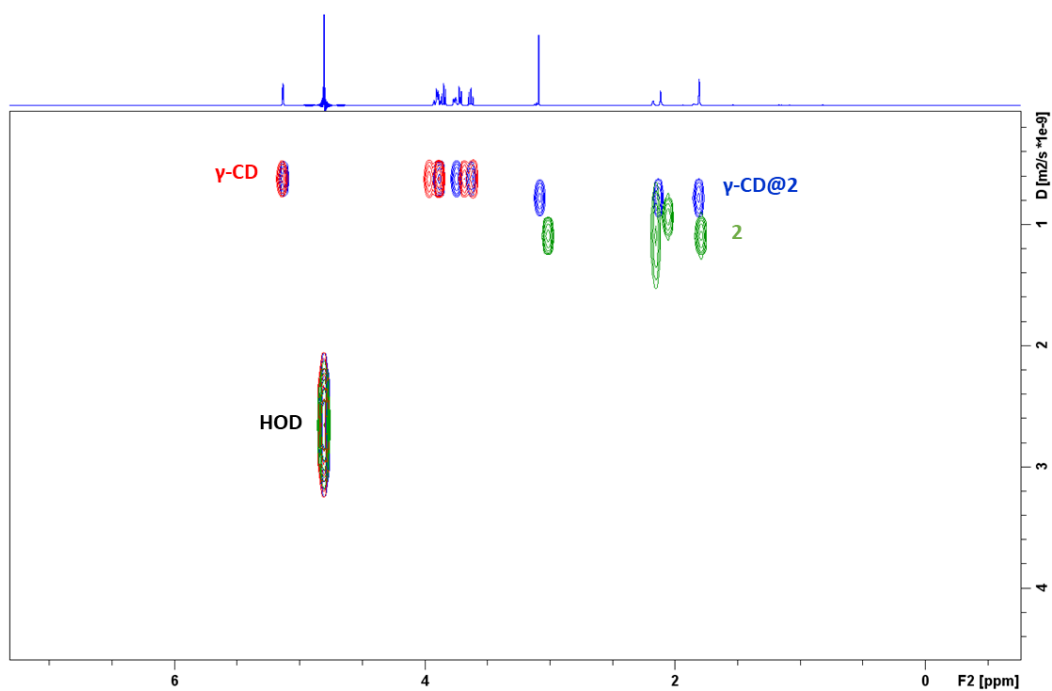


Figure S12. γ -CD, **2** and **2**@ γ -CD 1H NMR DOSY (600 MHz, D_2O , 25 $^{\circ}C$). The one-dimensional 1H NMR spectrum of **2**@ γ -CD is shown at the top.

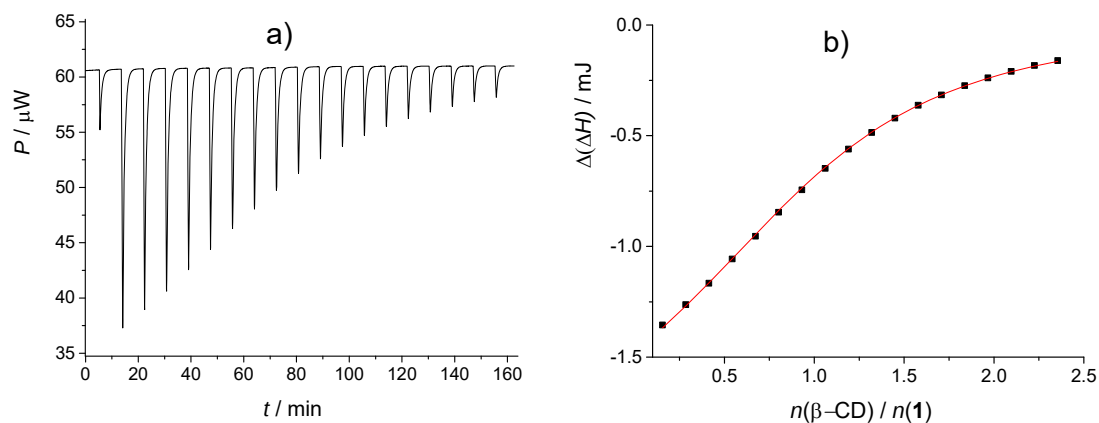


Figure S13. Microcalorimetric titration of **1** ($c = 4.3 \times 10^{-4} \text{ mol dm}^{-3}$, $V = 1.4265 \text{ mL}$) with β -CD ($c = 5.30 \times 10^{-3} \text{ mol dm}^{-3}$) in water at $25.0 \text{ }^\circ\text{C}$; b) Dependence of successive enthalpy change on β -CD to **1** molar ratio; $\blacksquare$ measured, $-$ calculated.

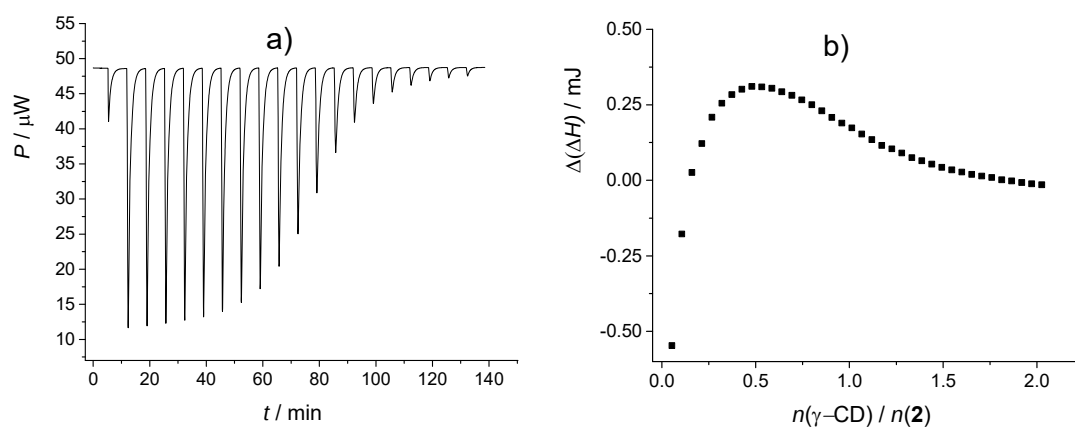


Figure S14. Microcalorimetric titration of **2** ($c = 4.95 \times 10^{-3} \text{ mol dm}^{-3}$, $V = 1.425 \text{ mL}$) with γ -CD ($c = 4.70 \times 10^{-2} \text{ mol dm}^{-3}$) in water at $25.0 \text{ }^\circ\text{C}$; b) Dependence of successive enthalpy change on γ -CD to **2** molar ratio.

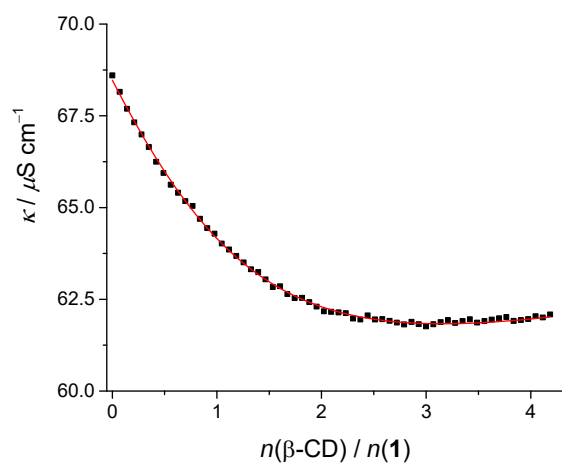


Figure S15. Conductometric titration of **1** ($c = 6.87 \times 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 15 \text{ ml}$) with β -CD ($c_0 = 5.243 \times 10^{-3} \text{ mol dm}^{-3}$); $\blacksquare$ measured, $-$ calculated.

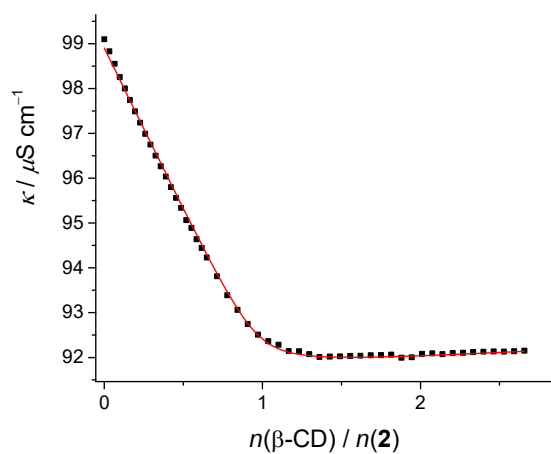
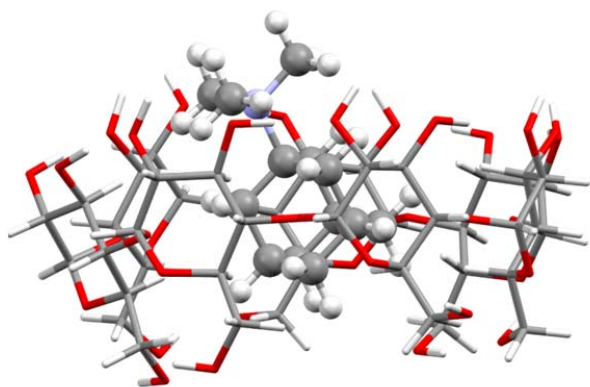
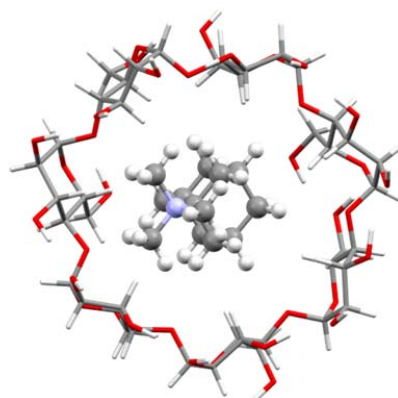


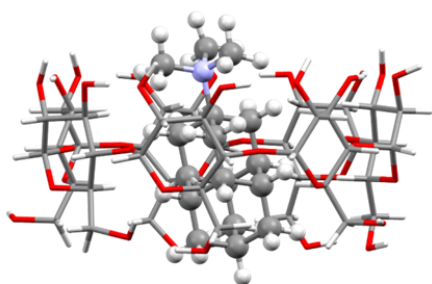
Figure S16. Conductometric titration of **2** ($c = 5.5 \times 10^{-4} \text{ mol dm}^{-3}$, $V_0 = 15 \text{ ml}$) with β -CD ($c = 5.31 \times 10^{-3} \text{ mol dm}^{-3}$); $\blacksquare$ measured, $-$ calculated.



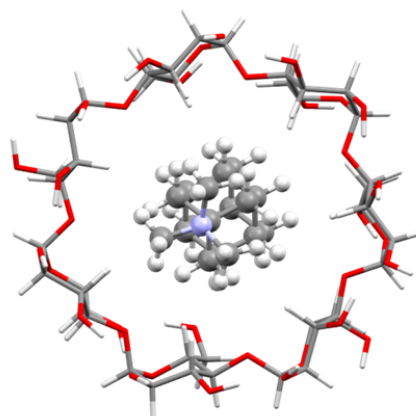
1@β-CD – side view



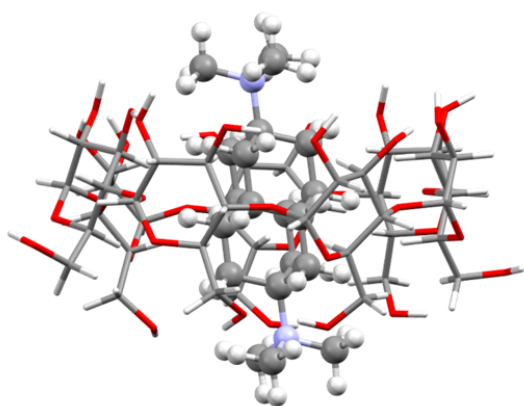
1@β-CD – top view



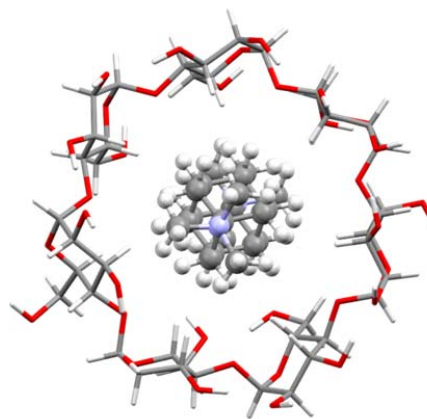
2@β-CD – side view



2@β-CD – top view

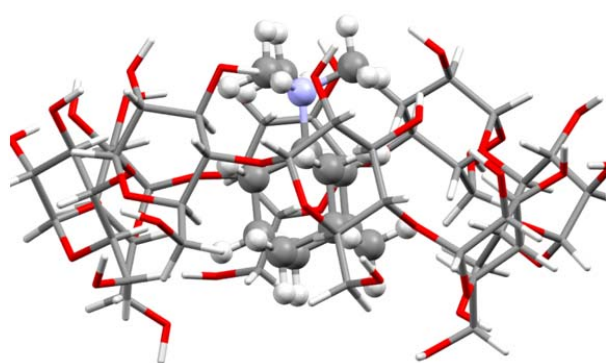


3@β-CD – side view

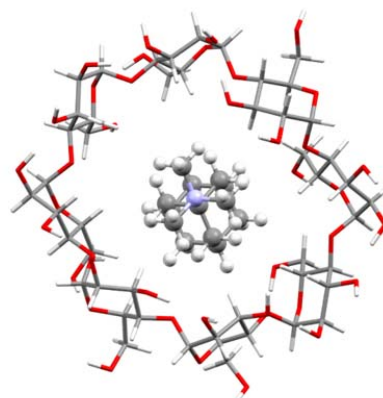


3@β-CD – top view

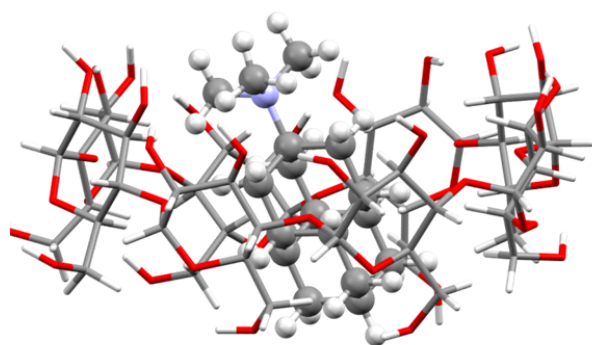
Figure S17. Optimized structures of complexes of compounds 1–3 with β-cyclodextrin computed at the B3LYP-D3/6-31G level of theory.



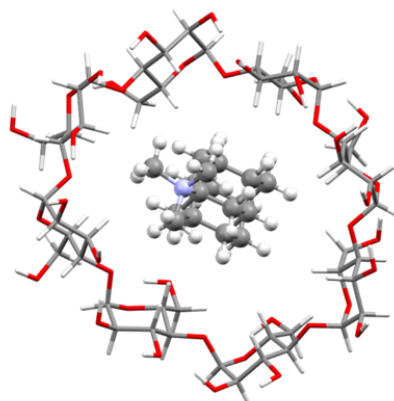
1@ γ -CD – side view



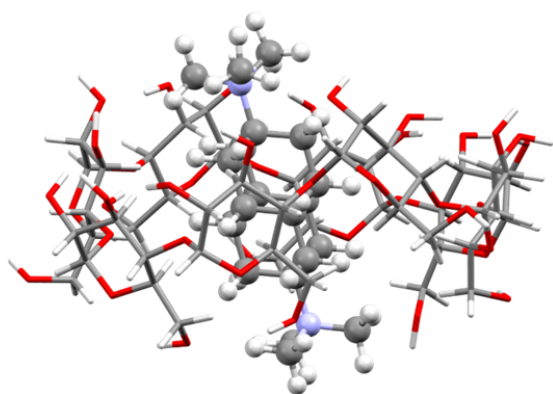
1@ γ -CD – top view



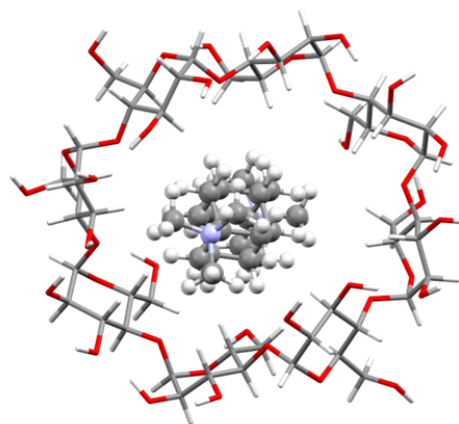
2@ γ -CD – side view



2@ γ -CD – top view



3@ γ -CD – side view



3@ γ -CD – top view

Figure S18. Optimized structures of complexes of compounds **1–3** with γ -cyclodextrin computed at the B3LYP-D3/6-31G level of theory.

Table S1. Electronic energies, zero-point vibrational energies, enthalpies and Gibbs energies of complexes of compounds **1–3** with β - and γ -cyclodextrins in Hartree computed at the CPCM(water)/B3LYP-D3(BJ)/6-31G level of theory.

compound	<i>E</i>	<i>ZPVE</i>	<i>H</i>	<i>G</i>
1@β-CD	-4838.7444 98	1.580824	-4837.074870	-4837.284255
2@β-CD	-4993.586752	1.653114	-4991.843376	-4992.058568
3@β-CD	-5167.302495	1.771530	-5165.434516	-5165.657670
1@γ-CD	-5449.327574	1.751186	-5447.477191	-5447.710756
2@γ-CD	-5604.171129	1.826748	-5602.241959	-5602.480916
3@γ-CD	-5777.886259	1.945463	-5775.833169	-5776.080482

Table S2. Geometries of complexes of compounds **1–3** with β - and γ -cyclodextrins in Cartesian coordinates in Å computed at the CPCM(water)/B3LYP-D3(BJ)/6-31G level of theory.

1@β-CD			
6	0.868616000	0.957126000	1.069286000
1	1.905620000	1.287897000	0.927827000
1	0.536348000	1.310656000	2.052896000
6	0.793012000	-0.582435000	0.995938000
1	1.440090000	-1.016979000	1.765200000
6	1.288836000	-1.058881000	-0.399591000
1	1.266257000	-2.152047000	-0.427195000
1	2.329047000	-0.744436000	-0.521578000
6	0.384614000	-0.449822000	-1.497159000
7	0.883482000	-0.927497000	-2.952917000
6	-1.070348000	-0.919174000	-1.269724000
1	-1.741264000	-0.514944000	-2.033151000
1	-1.138287000	-2.010527000	-1.298525000
6	0.449143000	1.092271000	-1.419479000
1	1.471590000	1.451653000	-1.571479000
1	-0.189577000	1.550456000	-2.179541000
6	-0.035309000	1.558220000	-0.024699000
1	0.012671000	2.651377000	-0.002236000
6	-1.488832000	1.098412000	0.198891000
1	-1.830023000	1.434740000	1.184644000
1	-2.151554000	1.551894000	-0.547608000
6	-1.556503000	-0.437859000	0.122155000
1	-2.592999000	-0.763762000	0.248307000
6	-0.661153000	-1.048796000	1.217145000
1	-1.008741000	-0.729876000	2.207314000

6	1.786027000	-5.794847000	0.144717000
1	2.629644000	-6.477329000	0.245854000
8	2.211204000	-4.431276000	0.266639000
6	1.069090000	-5.966230000	-1.190661000
1	0.820128000	-7.025233000	-1.318111000
8	1.968140000	-5.546288000	-2.253743000
1	1.492170000	-5.585367000	-3.108147000
6	-0.206996000	-5.138854000	-1.229546000
1	0.059444000	-4.082464000	-1.124877000
8	-0.817585000	-5.377489000	-2.509601000
1	-1.774097000	-5.089066000	-2.519826000
6	-1.109901000	-5.475362000	-0.048842000
1	-1.498675000	-6.496478000	-0.134030000
6	-0.340086000	-5.288786000	1.255993000
1	-0.027575000	-4.244606000	1.346783000
8	0.873331000	-6.137596000	1.210071000
6	-1.066599000	-5.712656000	2.515686000
1	-1.346296000	-6.771774000	2.448436000
1	-1.968059000	-5.114226000	2.651265000
8	-0.219376000	-5.470304000	3.674024000
1	0.619263000	-5.958535000	3.533705000
6	5.658104000	-2.196260000	0.927459000
1	6.643594000	-1.892638000	1.282893000
8	4.916806000	-1.052592000	0.426232000
6	5.764428000	-3.243997000	-0.190409000
1	6.350359000	-4.088047000	0.183447000
8	6.508087000	-2.703506000	-1.298425000
1	6.023719000	-1.946451000	-1.723257000
6	4.368240000	-3.743557000	-0.570668000
1	3.817533000	-2.916724000	-1.038061000
8	4.489721000	-4.855140000	-1.478596000
1	3.602048000	-5.066342000	-1.872665000
6	3.592654000	-4.175594000	0.679783000
1	4.034998000	-5.096207000	1.077905000
6	3.557587000	-3.096688000	1.750797000
1	3.040670000	-2.215860000	1.370298000
8	4.952004000	-2.709383000	2.064399000
6	2.954527000	-3.511059000	3.077230000
1	3.547213000	-4.325747000	3.514085000
1	1.926340000	-3.849261000	2.950111000
8	2.900920000	-2.365367000	3.972717000
1	3.802409000	-1.983429000	4.023241000
6	5.240709000	2.973765000	-0.590643000
1	5.649482000	3.959013000	-0.813373000
8	3.822914000	3.034356000	-0.375294000
6	5.505140000	1.974308000	-1.714184000
1	6.576195000	1.965501000	-1.931393000

8	4.752182000	2.347227000	-2.916178000
1	5.354172000	2.604840000	-3.642006000
6	5.043469000	0.586283000	-1.291439000
1	3.955611000	0.609960000	-1.187041000
8	5.412763000	-0.412153000	-2.281737000
1	5.230734000	-0.091758000	-3.187397000
6	5.633863000	0.156446000	0.050975000
1	6.704346000	-0.047887000	-0.053876000
6	5.366250000	1.239358000	1.096720000
1	4.284056000	1.340590000	1.213960000
8	5.914531000	2.513457000	0.592555000
6	5.993986000	1.068127000	2.464348000
1	7.088242000	1.094714000	2.375893000
1	5.694841000	0.111756000	2.898890000
8	5.510338000	2.101769000	3.360551000
1	5.501543000	2.985736000	2.915071000
6	0.958025000	6.073378000	0.110897000
1	0.568088000	7.067846000	0.329481000
8	-0.098962000	5.109262000	0.015024000
6	1.744399000	6.034095000	-1.199980000
1	2.517690000	6.809573000	-1.168662000
8	0.831536000	6.307195000	-2.298652000
1	1.289257000	6.105200000	-3.140778000
6	2.401745000	4.675159000	-1.373525000
1	1.622002000	3.911345000	-1.474654000
8	3.203036000	4.732762000	-2.574225000
1	3.605146000	3.843355000	-2.749612000
6	3.248573000	4.353599000	-0.147238000
1	4.054015000	5.084475000	-0.033960000
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1	1.556519000	3.669149000	1.017739000
8	1.829126000	5.738331000	1.217127000
6	3.119064000	4.053680000	2.408869000
1	3.241912000	2.975867000	2.505105000
1	2.516006000	4.410721000	3.250205000
8	4.475536000	4.582951000	2.475396000
1	4.474069000	5.537433000	2.683288000
6	-4.254283000	4.652461000	0.432865000
1	-5.275329000	4.918636000	0.710178000
8	-4.138665000	3.267130000	0.115916000
6	-3.752360000	5.478324000	-0.746410000
1	-3.953032000	6.535258000	-0.539311000
8	-4.503118000	5.058756000	-1.920747000
1	-4.125710000	5.506693000	-2.705806000
6	-2.258099000	5.299232000	-0.976432000
1	-2.074477000	4.270702000	-1.315939000
8	-1.885076000	6.246416000	-1.994683000

1	-0.906452000	6.194204000	-2.178133000
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1	-1.505241000	6.544188000	0.643069000
6	-2.004308000	4.562131000	1.397685000
1	-1.977321000	3.541741000	1.014878000
8	-3.438360000	4.931471000	1.605474000
6	-1.302602000	4.591950000	2.747469000
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8	-1.282893000	3.280886000	3.376264000
1	-2.209078000	2.929526000	3.454104000
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8	-5.021066000	-1.076314000	-0.007755000
6	-6.487001000	0.583000000	-0.958150000
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8	-6.495828000	-0.206933000	-2.181053000
1	-6.556496000	0.405173000	-2.943446000
6	-5.414626000	1.655001000	-1.029863000
1	-4.452047000	1.179489000	-1.257764000
8	-5.796606000	2.564672000	-2.082623000
1	-5.219946000	3.375245000	-2.075521000
6	-5.281411000	2.376420000	0.307360000
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6	-5.035835000	1.395363000	1.458953000
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8	-6.141085000	0.410640000	1.437798000
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8	-2.209191000	-4.514458000	-0.100814000
6	-4.252623000	-4.470272000	-1.378386000
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8	-5.162053000	-2.587319000	-2.497510000
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6	-5.067838000	-2.534974000	-0.038892000
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6	-4.350931000	-3.092611000	1.190883000
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8	-6.453760000	-3.424431000	2.406089000
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6	1.308998000	0.828143000	-0.538978000
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6	0.336372000	-1.498329000	-0.512739000
1	-0.392871000	-2.188081000	-0.946396000
1	1.330227000	-1.948526000	-0.617311000
6	0.016581000	-1.333407000	0.987828000
1	0.069129000	-2.313907000	1.470927000
6	1.044836000	-0.392368000	1.663771000
6	0.737126000	-0.256183000	3.165753000
1	2.047185000	-0.813952000	1.518771000
6	0.970596000	0.985124000	0.960643000
1	1.705858000	1.665214000	1.407757000
6	-0.447618000	1.573008000	1.161025000
6	-0.762390000	1.712341000	2.664830000

6	-0.745724000	6.154400000	-0.029205000
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8	3.498159000	-3.824961000	-0.100086000
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1	0.806484000	-1.241512000	3.642148000
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6	-0.848150000	0.739113000	-3.154436000
6	-0.136590000	-1.600278000	-3.026133000
6	1.517620000	0.202516000	-2.787902000
1	1.635665000	0.085572000	-3.865053000
1	1.686592000	1.245858000	-2.526124000
1	2.223009000	-0.447335000	-2.276508000
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6	-1.318884000	5.970787000	0.616781000
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1	-2.681874000	-5.083309000	-3.567643000
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