Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Functional Self-Assembled Nanovesicles Based on β-Cyclodextrin, Liposomes and Adamantyl Guanidines as Potential Nonviral Gene Delivery Vectors

Adela Štimac,[a] Matea Tokić,[b] Ajasja Ljubetič,[c] Tomislav Vuletić,[d] Marina Šekutor,[e] Josip Požar [b] Katarina Leko,[b] Marko Hanževački,[f] Leo Frkanec,[e] and Ruža Frkanec*[a]*

[a] University of Zagreb, Centre for Research and Knowledge Transfer in Biotechnology, Rockefellerova 10, 10 000 Zagreb, Croatia

[b] University of Zagreb, Faculty of Science, Horvatovac 102a, 10 000 Zagreb, Croatia

[c] National Institute of Chemistry, Hajdrihova ulica 19, 1000 Ljubljana, Slovenia

[d] Institute of Physics, Bijenička cesta 46, 10 000 Zagreb, Croatia

[e] Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10 000 Zagreb, Croatia.

[f] Department of Physical Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10 000 Zagreb, Croatia.

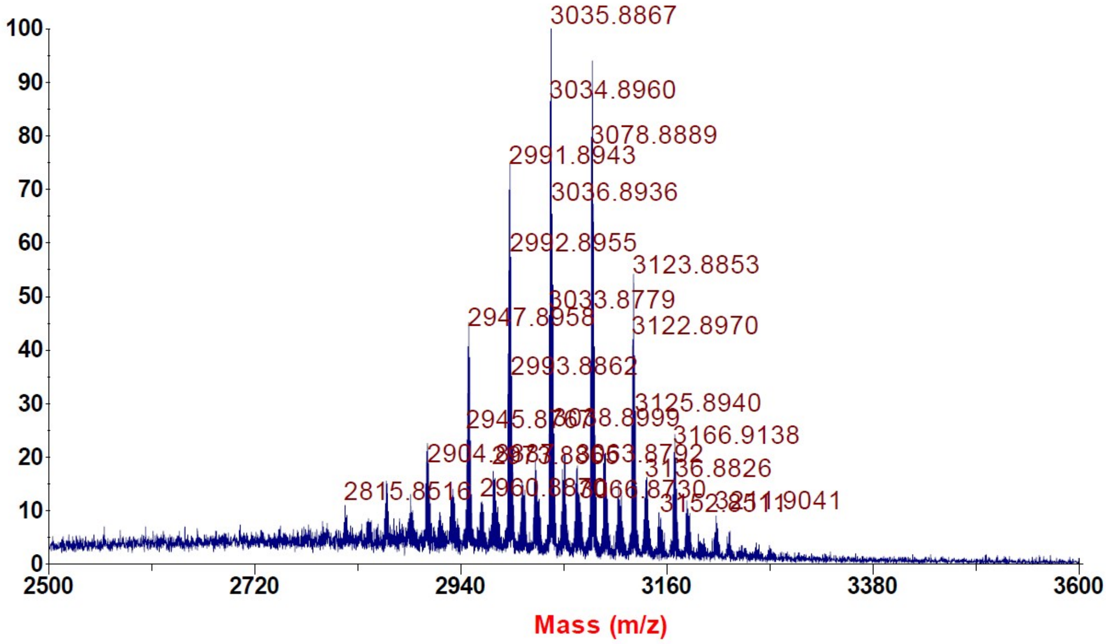


Figure S1. HRMS spectrum of amphiphilic derivative of β-cyclodextrin, heptakis[6-deoxy-6-dodecylthio-2-O-oligo(ethylene glycol)]-β-cyclodextrin (EO-CD-SR), Maldi TOF mass spectra acquired on Applied Biosystems Voyager DE STR instrument (Foster City, CA).

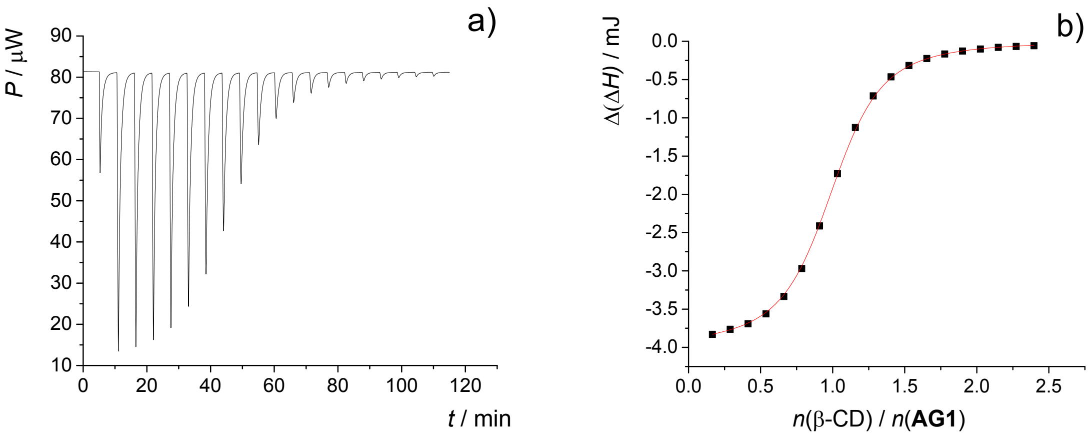


Figure S2. a) Microcalorimetric titration of **AG1** (c = 8.76 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 1.03 × 10^{-2} mol dm^{-3}) in water at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

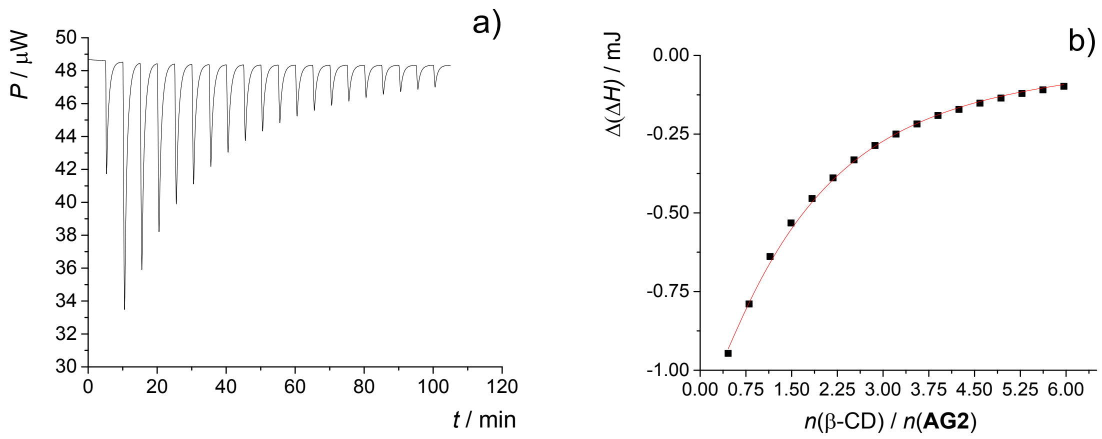


Figure S3. a) Microcalorimetric titration of **AG2** (c = 2.34 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 7.60 × 10^{-3} mol dm^{-3}) in water at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

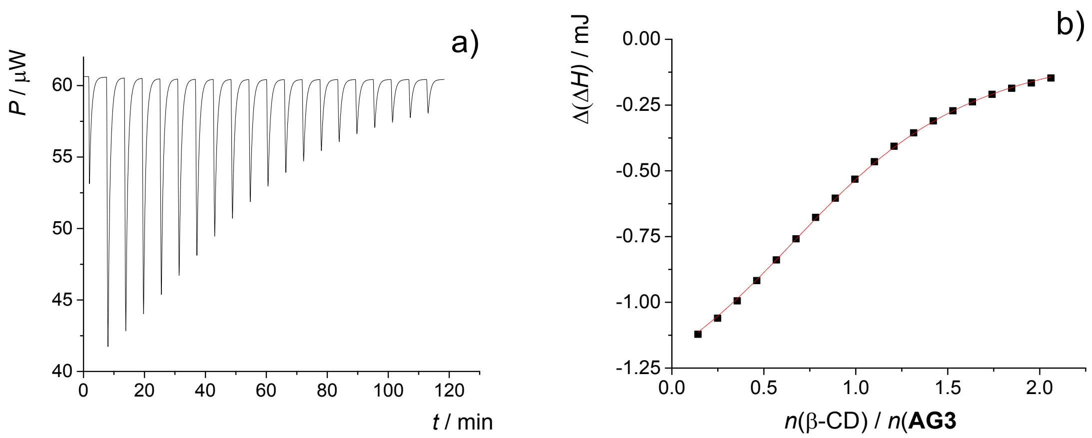


Figure S4 a) Microcalorimetric titration of **AG3** (c = 4.55 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 4.59 × 10^{-3} mol dm^{-3}) in water at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

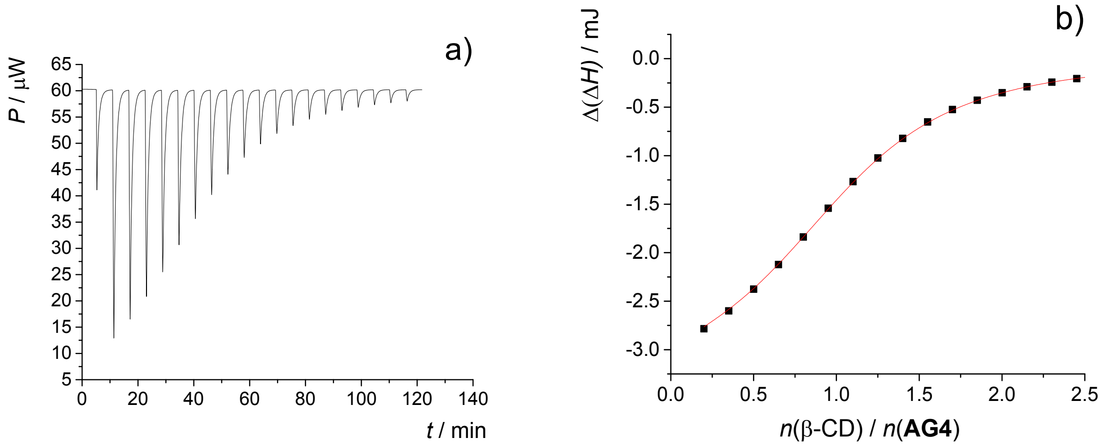


Figure S5. a) Microcalorimetric titration of **AG4** (c = 7.28 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 1.03 × 10^{-2} mol dm^{-3}) in water at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

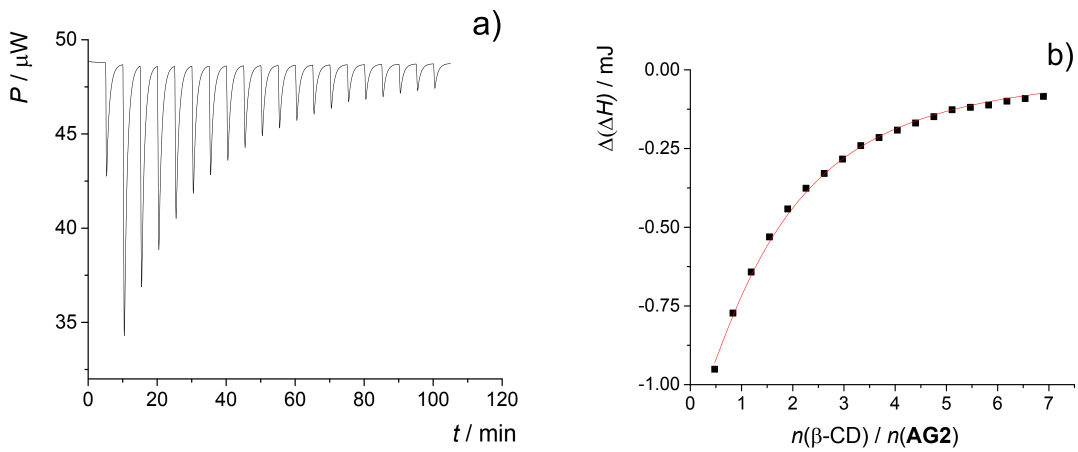


Figure S6. a) Microcalorimetric titration of **AG2** (c = 2.35 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 7.96 × 10^{-3} mol dm^{-3}) in HEPES buffer at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

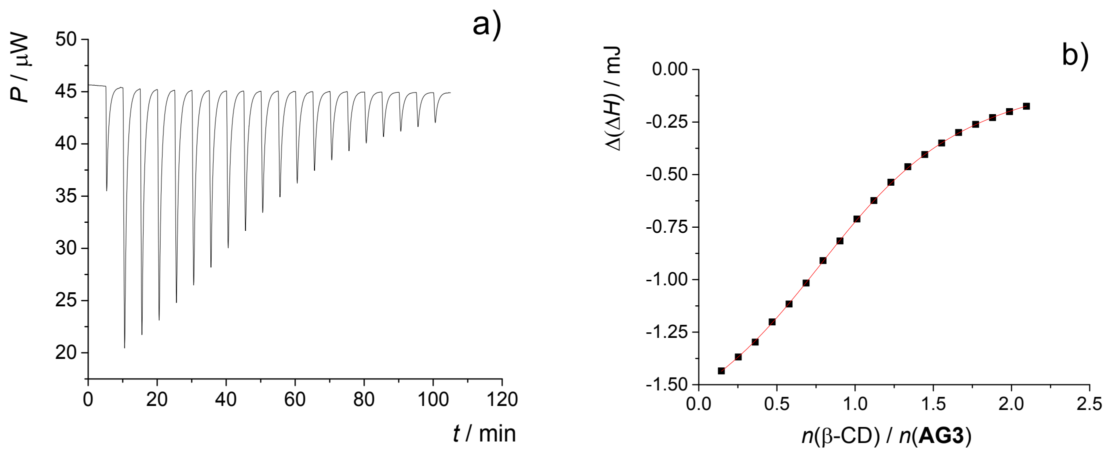


Figure S7. a) Microcalorimetric titration of **AG3** (c = 5.80 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 5.98 × 10^{-3} mol dm^{-3}) in HEPES buffer at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

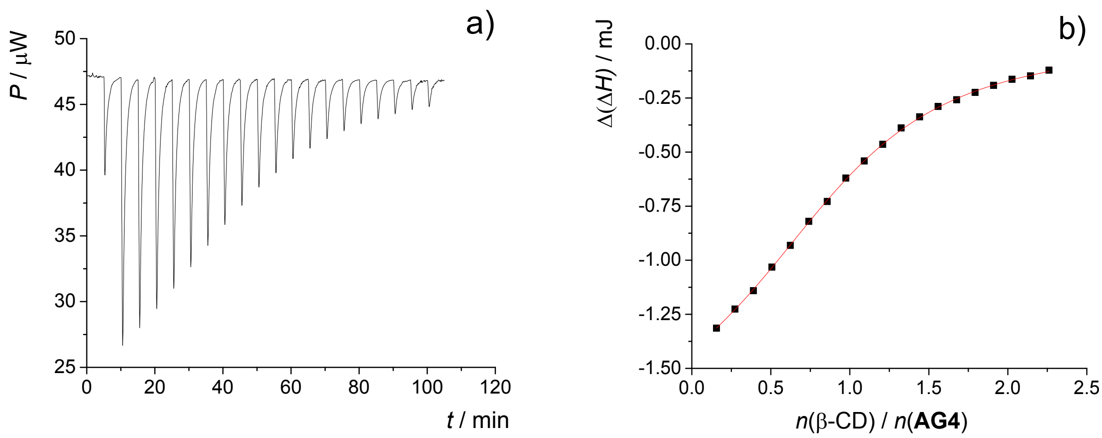


Figure S8. a) Microcalorimetric titration of **AG4** (c = 5.38 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 5.98 × 10^{-3} mol dm^{-3}) in HEPES buffer at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

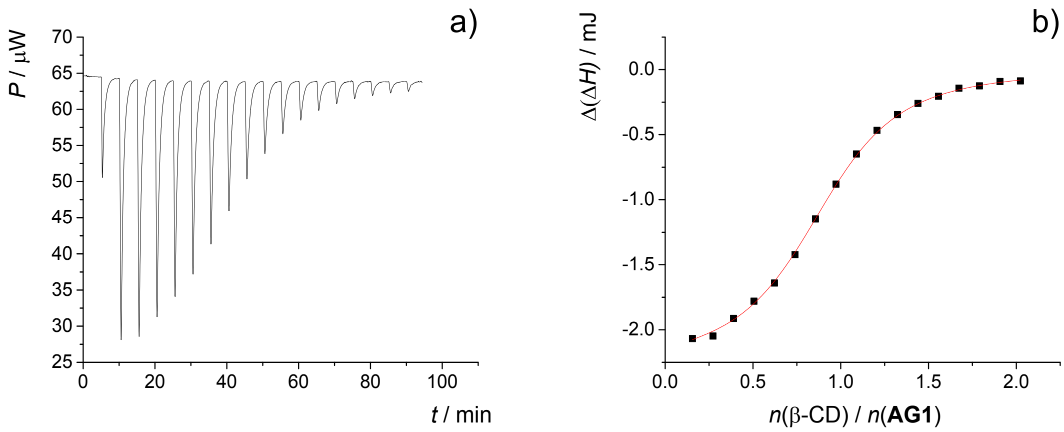


Figure S9. a) Microcalorimetric titration of **AG1**(c = 5.56 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 6.14 × 10^{-3} mol dm^{-3}) in HCl (c = 5 × 10^{-3} mol dm^{-3}) at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

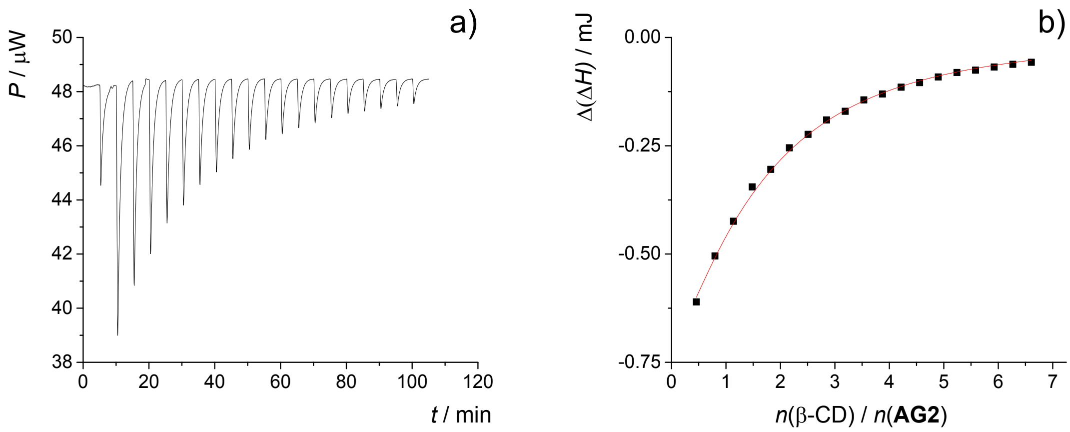


Figure S10. a) Microcalorimetric titration of **AG2** (c = 1.89 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 6.14 × 10^{-3} mol dm^{-3}) in HCl (c = 5 × 10^{-3} mol dm^{-3}) at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

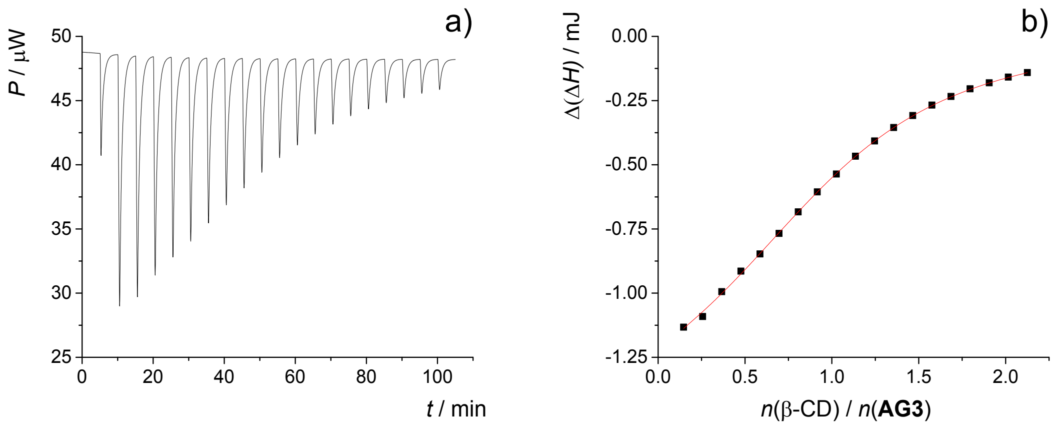


Figure S11. a) Microcalorimetric titration of **AG3** (c = 4.49 × 10^{-4} mol dm^{-3}, V = 1.42 mL) with **β-CD** (c = 4.67 × 10^{-3} mol dm^{-3}) in HCl (c = 5 × 10^{-3} mol dm^{-3}) at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

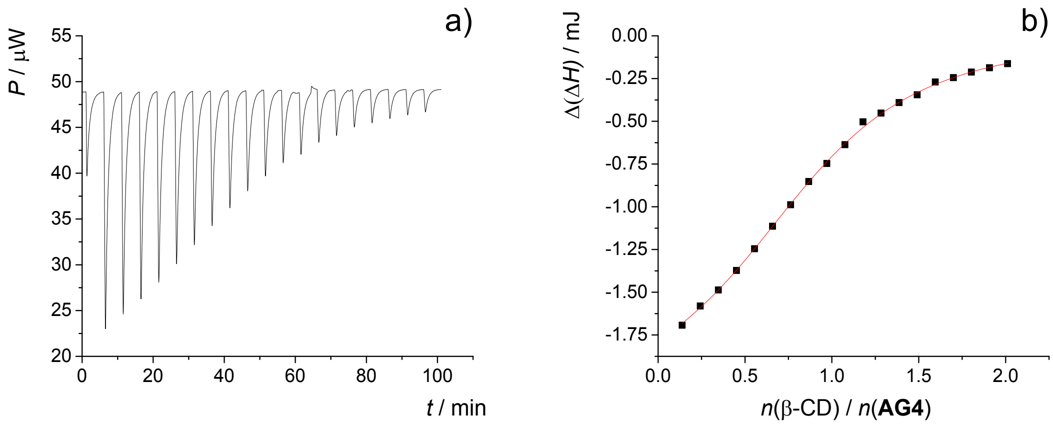


Figure S12. a) Microcalorimetric titration of **AG4** (c = 6.60 × 10^{-4} mol dm^{-3}, V = 1.42mL) with **β-CD** (c = 6.58 × 10^{-3} mol dm^{-3}) in HCl (c = 5 × 10^{-3} mol dm^{-3}) at 25 °C; **b)** Dependence of successive enthalpy change on host to guest molar ratio. ■ experimental; — calculated.

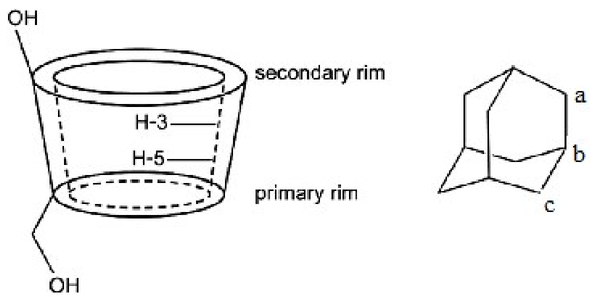


Figure S13. Schematic structure of β-CD and adamantane**.**

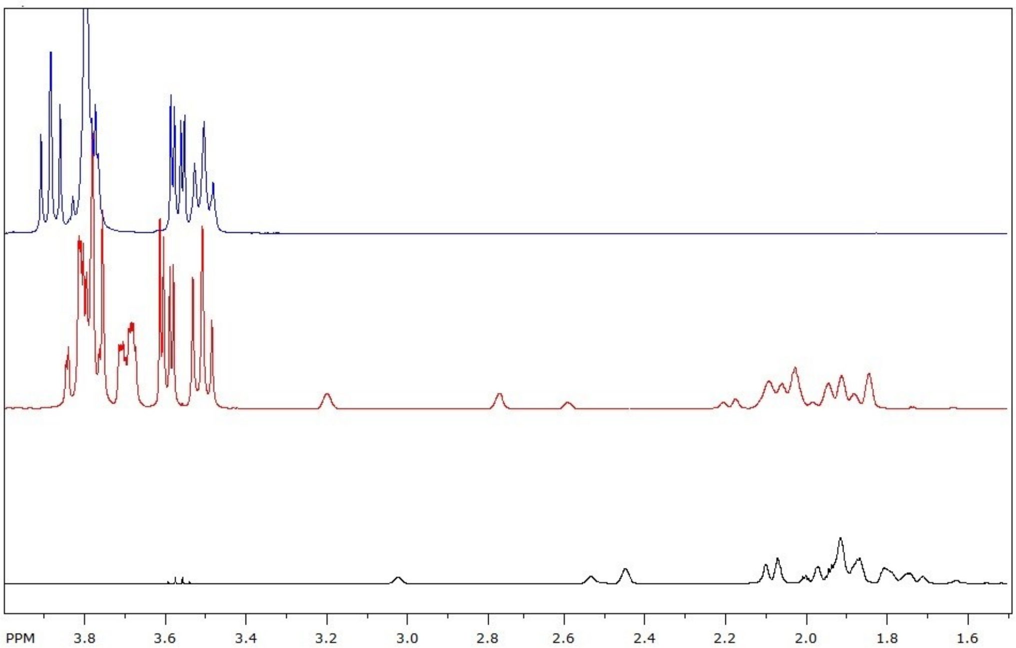


Figure S14. Overlapped ^{1}H NMR spectra of **AG1** upon β-CD addition (β-CD blue line, complex [**AG1**/β-**CD**] red line and **AG1** black line) at 25 °C in D_2O.

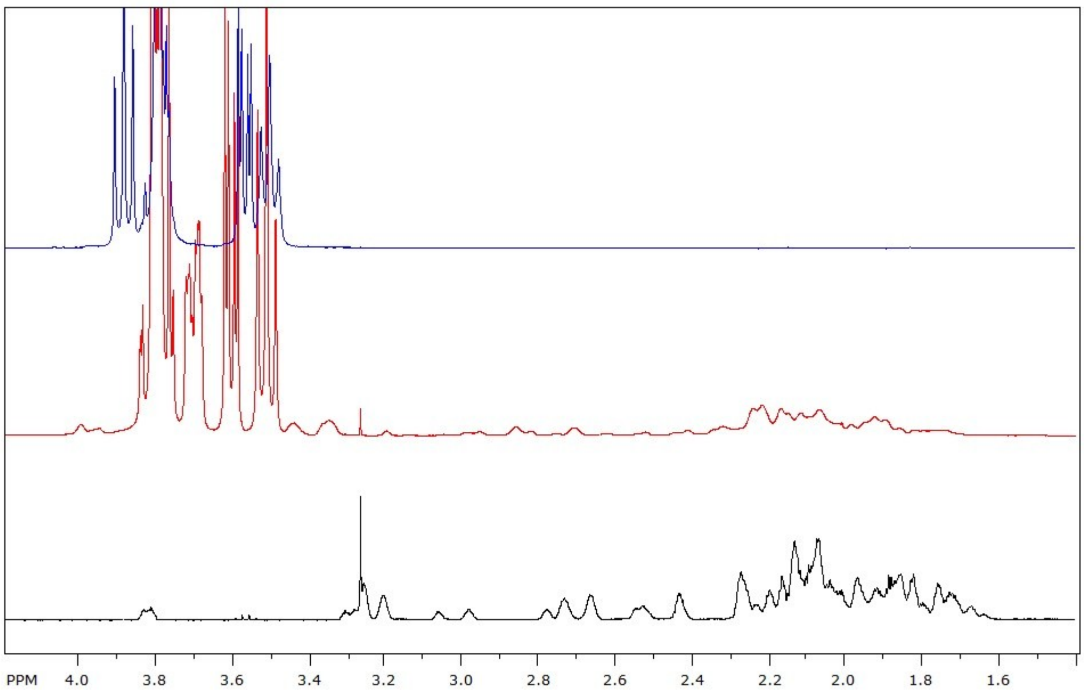


Figure S15 Overlapped ^{1}H NMR spectra of **AG2** upon β-CD addition (β-CD blue line, complex [**AG2**/β-**CD**] red line and **AG2** black line) at 25 °C in D_2O.

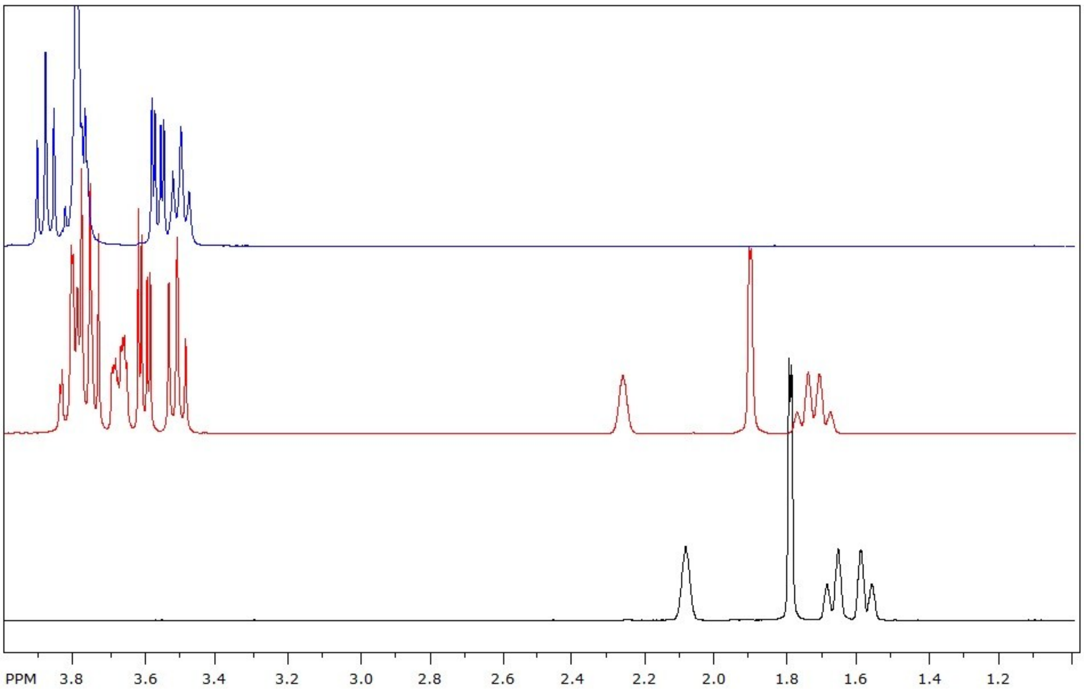


Figure S16. Overlapped ^{1}H NMR spectra of **AG3** upon β-CD addition (β-CD blue line, complex [**AG3**/β-**CD**] red line and **AG3** black line) at 25 °C in D_2O.

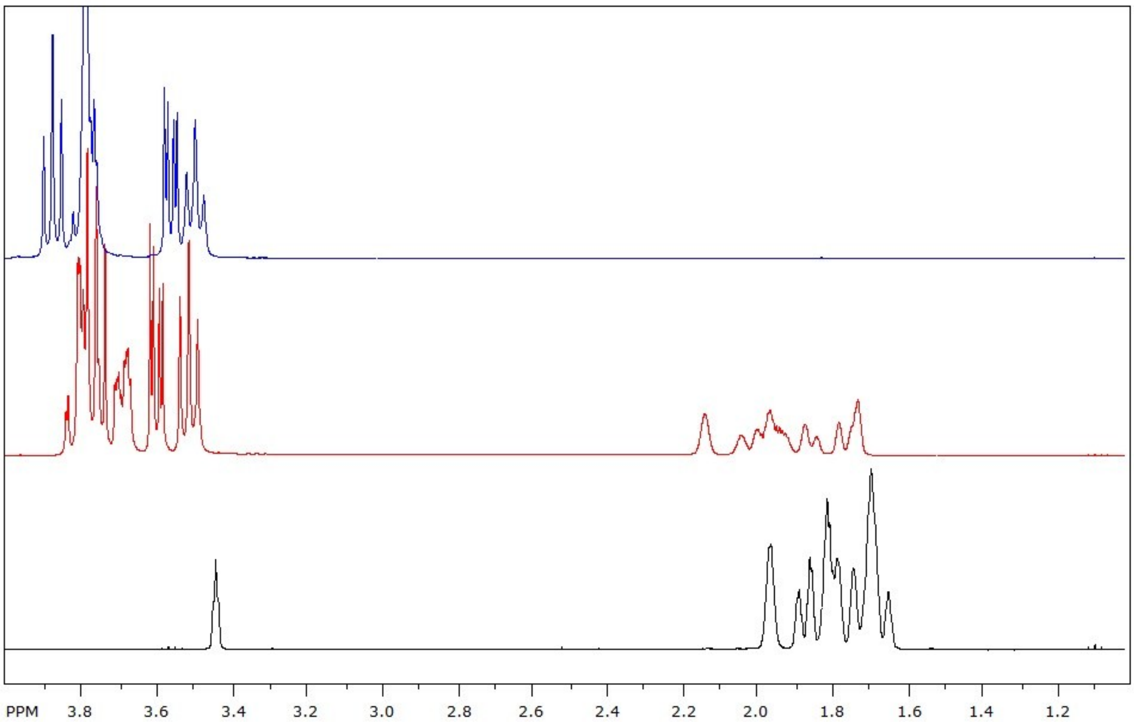
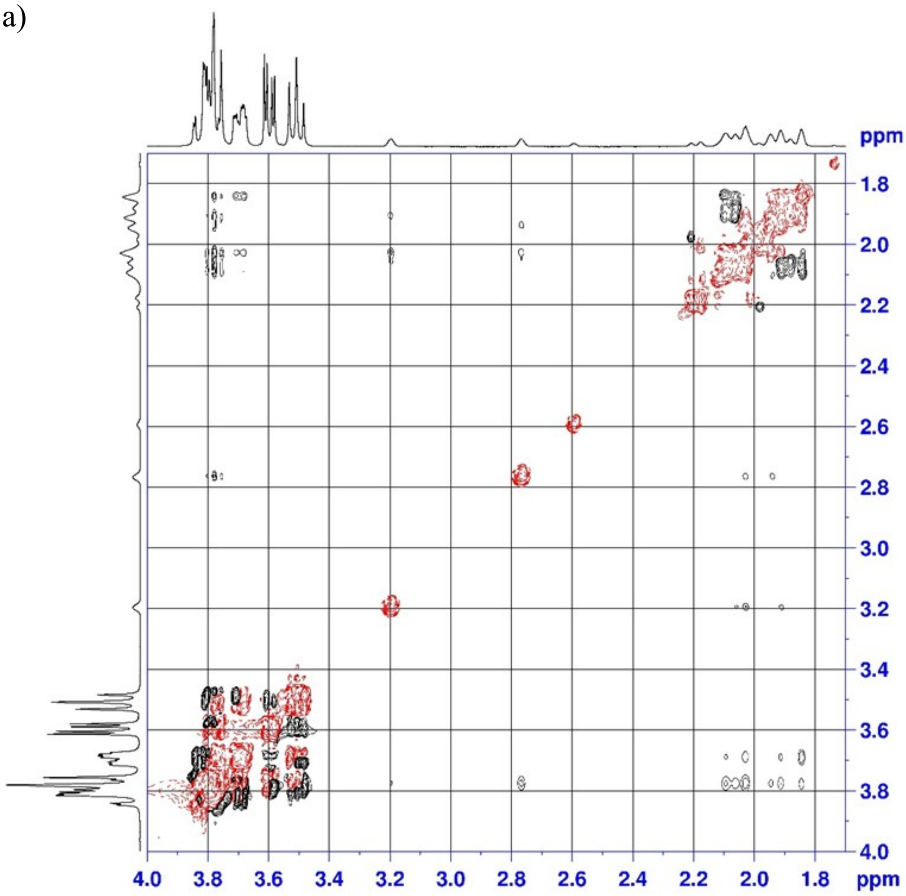


Figure S17. Overlapped ^{1}H NMR spectra of **AG4** upon β-CD addition (β-CD blue line, complex [**AG4**/β-**CD**] red line and **AG4** black line) at 25 °C in D_2O.

a)



b)

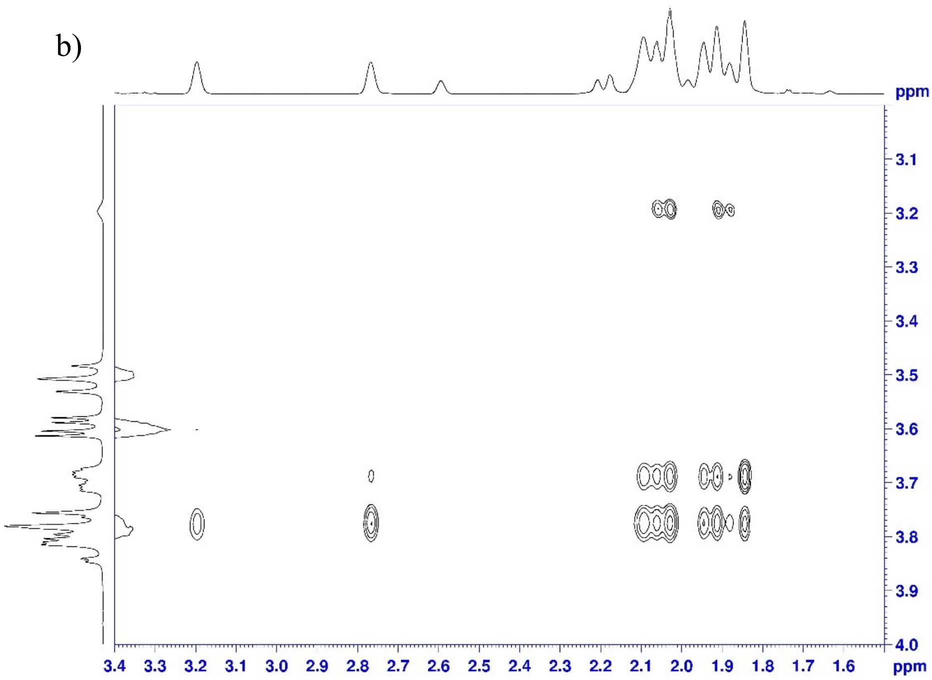
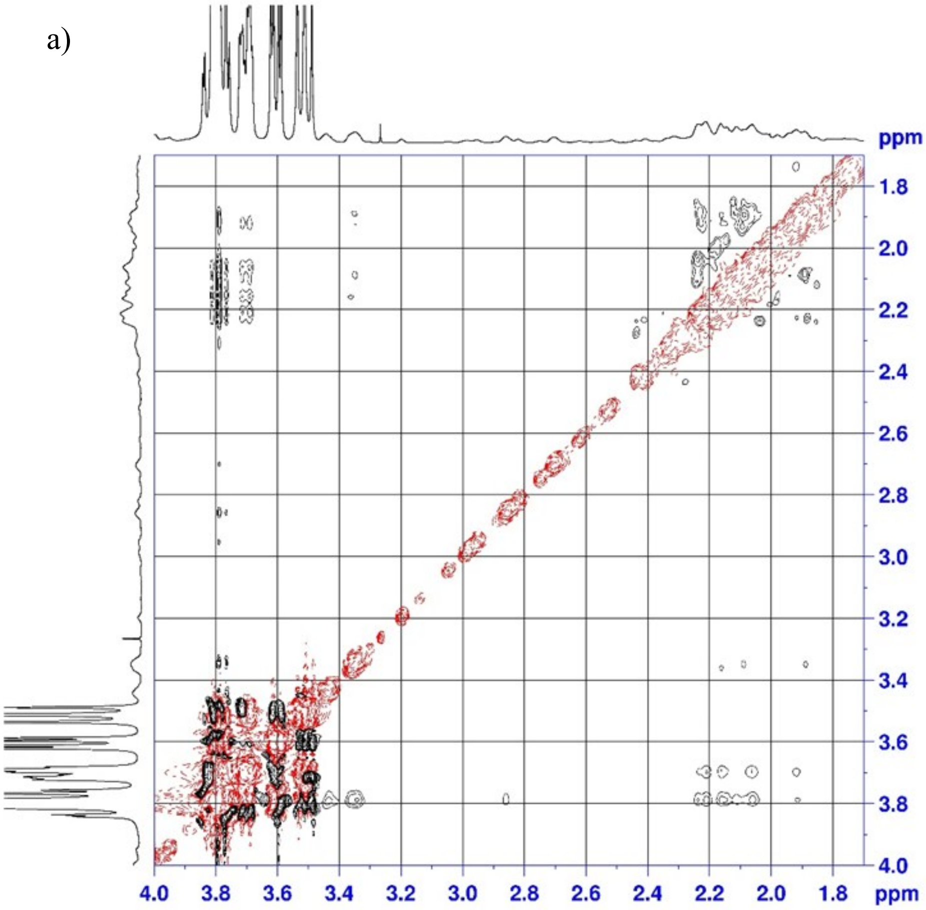


Figure S18. a) 2D ROESY spectrum of the **AG1@ β-CD** (molar ratio 1:1) in D_2O at 25 °C, and b) the partial contour plot of the same ROESY spectrum (Ad and β-CD region).

a)



b)

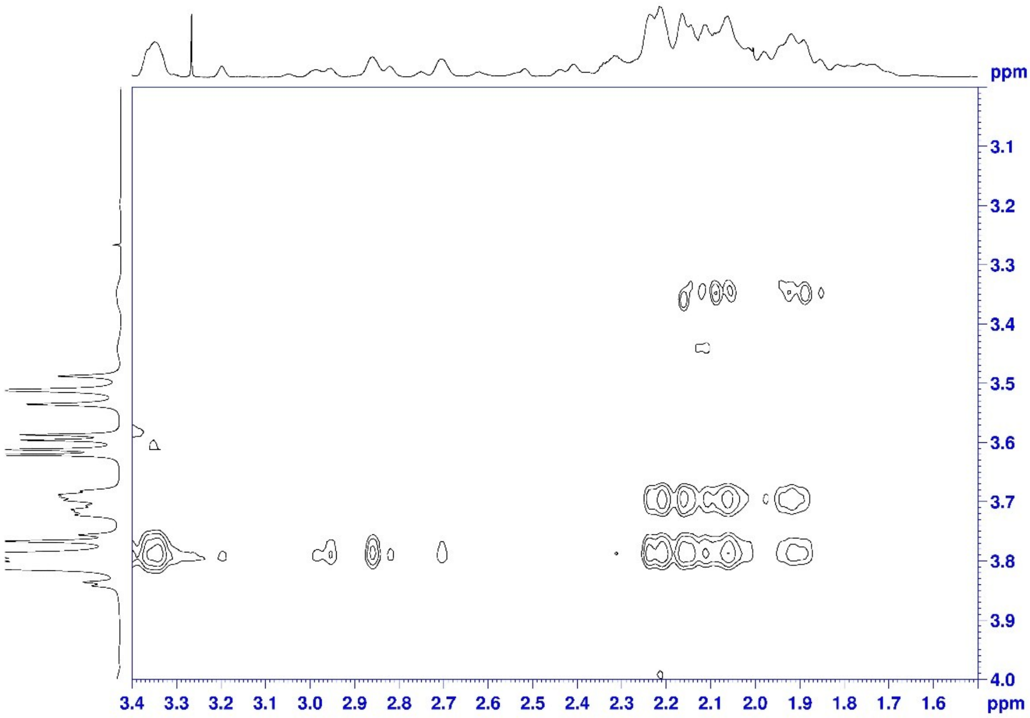
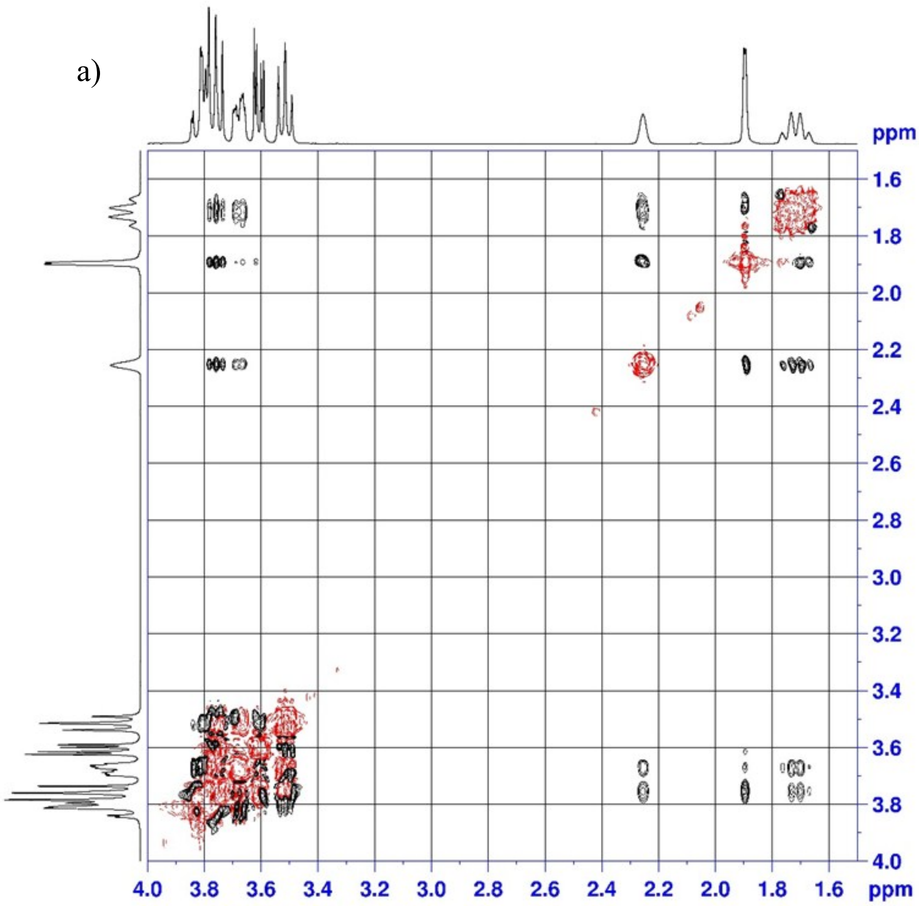


Figure S19. a) 2D ROESY spectrum of the **AG2 @β-CD** (molar ratio 1:1) in D_2O at 25 °C, and b) the partial contour plot of the same ROESY spectrum (Ad and β-CD region).

a)



b)

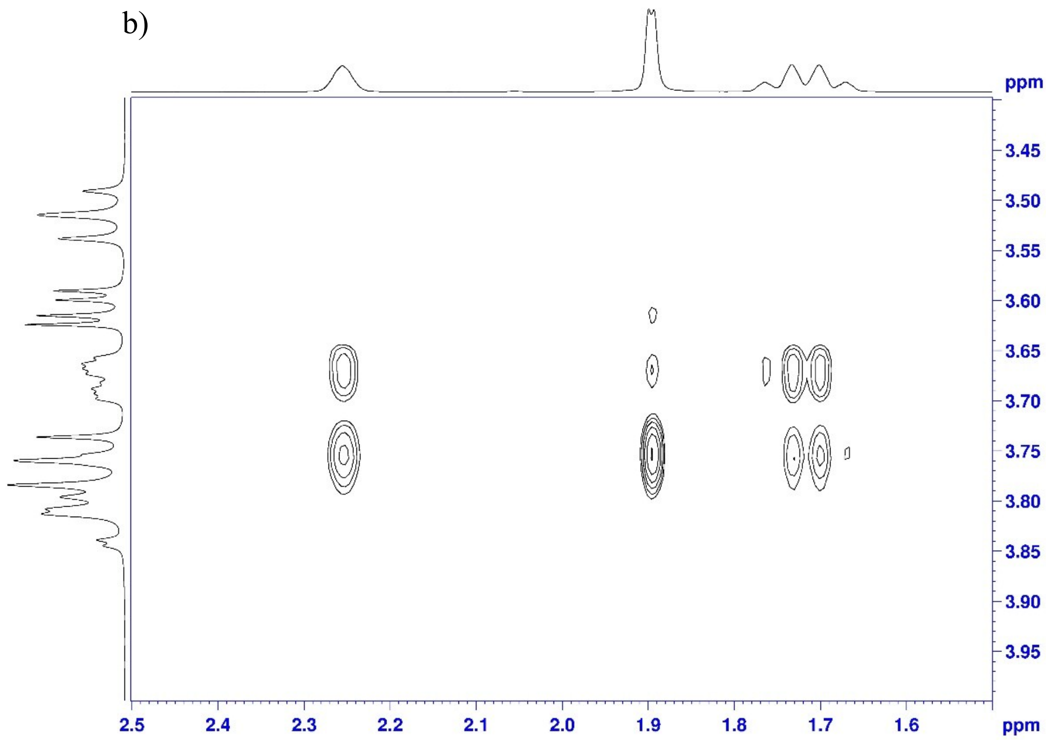
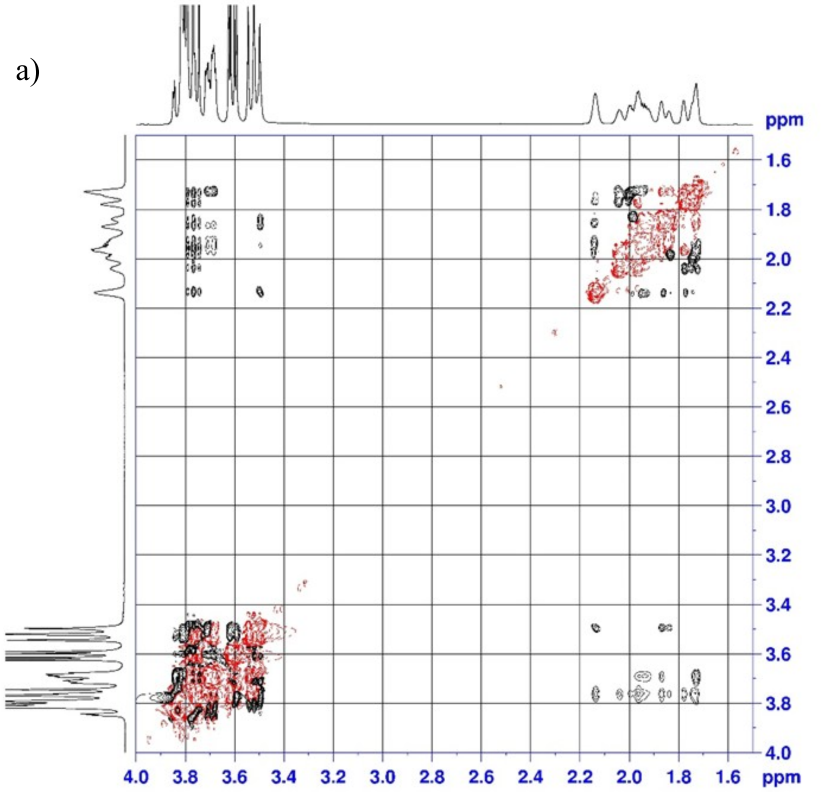


Figure S20. a) 2D ROESY spectrum of the **AG3@β-CD** (molar ratio 1:1) in D_2O at 25 °C and b) the partial contour plot of the same ROESY spectrum (Ad and β-CD region).

a)



b)

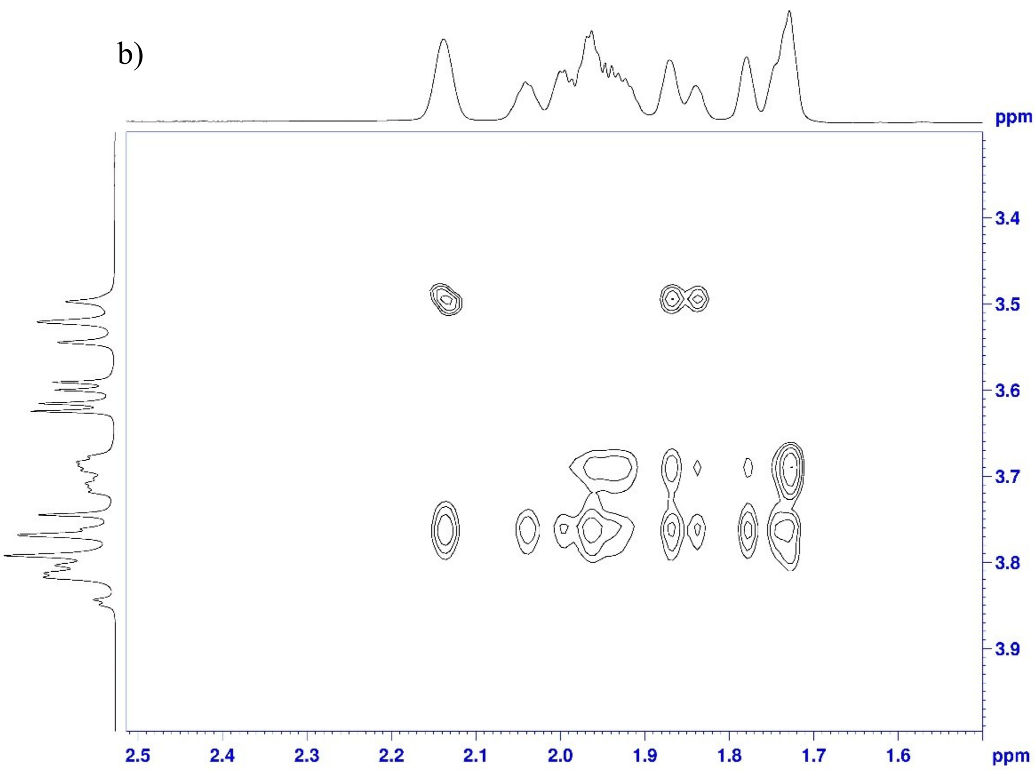


Figure S21. a) 2D ROESY spectrum of the **AG4@β-CD** (molar ratio 1:1) in D_2O at 25 °C and b) the partial contour plot of the same ROESY spectrum (Ad and β-CD region).

Table S1. [1]H-NMR Chemical shifts (δ, ppm) for CH protons of β-CD alone, **AG3** alone and their shifts after complexation (*CIS* = $\delta_{\mathbf{complex}}$ **-** δ_{guest}) in D_2O at 25 °C.

	CH protons	**H-3**	**H-6**	**H-5**	**H-2**	**H-4**
βCD	δ alone	3.89	3.80	3.77	3.57	3.50
	CIS	0.13	0.04	0.10	-0.04	-0.01
	CH protons	**Hβ**	**Hα**	**Hγ**		
AG3	δ alone	2.08	1.78	1.62		
	CIS	-0.18	-0.11	-0.11		

Table S2. Electronic energies, zero-point vibrational energies, enthalpies and Gibbs energies of **AG1@β-CD** and **AG4@β-CD** in hartree.[a]

Compound	*E*	*ZPVE*	*H*	*G*
AG1@ β-CD[b]	-4923.300453	1.521130	-4921.689895	-4921.901851
AG4@ β-CD[b]	-4924.497185	1.542902	-4922.862830	-4923.082668
AG1@ β-CD[c]	-4926.784872	–	–	–
AG4@ β-CD[c]	-4927.999731	–	–	–

[a] Optimized geometries obtained by CPCM(water)/B3LYP/6-31G and CPCM(water)/B3LYP-D3(BJ)/311+G(d,p) levels of theory were comparable and the coordinates differed only slightly. [b] Computed at the CPCM(water)/B3LYP/6-31G level of theory. [c] Computed at the CPCM(water)/B3LYP-D3(BJ)/311+G(d,p) level of theory.

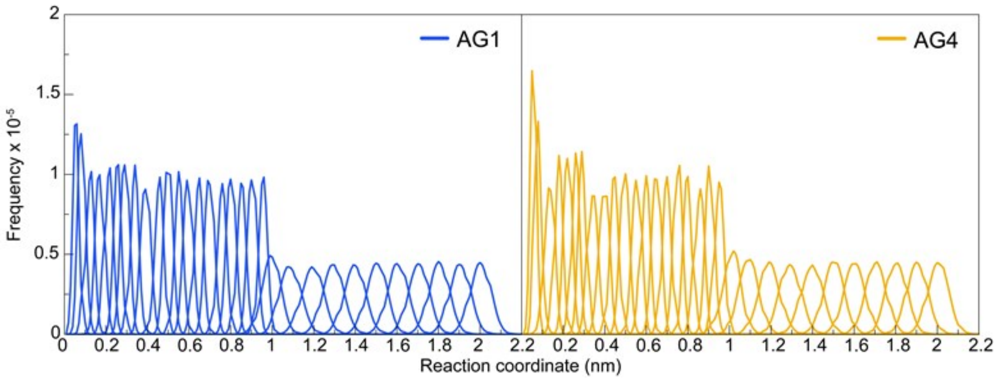


Figure S22. Histograms used to produce the free energy profiles using the WHAM method for AG1 and AG4 binding to the β-CD in water at 300 K.

Table S3. Geometries in Cartesian coordinates in Å computed at the CPCM(water)/B3LYP/6-31G level of theory.

AG1@β-CD			
6	0.186439000	-1.222880000	-0.391992000
1	0.880757000	-2.024129000	-0.115765000
1	-0.767081000	-1.434391000	0.109117000
6	-0.013101000	-1.216936000	-1.935918000
1	-0.437564000	-2.165944000	-2.275359000
6	1.348263000	-0.946575000	-2.638901000
1	1.215451000	-0.958830000	-3.728552000
1	2.056753000	-1.746151000	-2.391124000
6	1.902572000	0.420423000	-2.179709000
1	2.868155000	0.609324000	-2.667300000
6	0.901073000	1.525859000	-2.580592000
1	1.285408000	2.513247000	-2.301493000
1	0.756732000	1.533615000	-3.668690000
6	2.085401000	0.417412000	-0.642025000
1	2.814003000	-0.347580000	-0.352397000
1	2.481523000	1.383728000	-0.312166000
6	0.736145000	0.146711000	0.059357000
1	0.879638000	0.145793000	1.147589000
6	-0.267408000	1.254874000	-0.322196000

1	-1.230093000	1.084364000	0.175689000
1	0.096637000	2.232260000	0.011348000
6	-0.464424000	1.279191000	-1.870354000
1	-1.161874000	2.077786000	-2.134762000
6	-0.967149000	-0.090130000	-2.277683000
7	-2.085678000	-0.416780000	-2.839381000
7	-3.010485000	0.582900000	-3.189732000
1	-2.918161000	1.577925000	-2.932493000
6	-4.163121000	0.150101000	-3.740869000
7	-4.984647000	1.087628000	-4.289305000
1	-5.882971000	0.817275000	-4.664644000
1	-4.590656000	1.948094000	-4.646324000
7	-4.493999000	-1.138723000	-3.713224000
1	-3.963796000	-1.819023000	-3.153747000
1	-5.297952000	-1.473622000	-4.223505000
6	-5.334066000	-2.947865000	1.474088000
1	-5.655784000	-3.948630000	1.768173000
8	-4.007430000	-2.973554000	0.896652000
6	-6.315802000	-2.292042000	0.510571000
1	-7.315741000	-2.323181000	0.956662000
8	-6.326677000	-3.051564000	-0.737240000
1	-6.923569000	-2.583462000	-1.360510000
6	-5.926960000	-0.850161000	0.214363000
1	-4.979454000	-0.853991000	-0.337092000
8	-6.990481000	-0.320033000	-0.608966000
1	-6.641142000	0.480626000	-1.091167000
6	-5.714692000	-0.027763000	1.491454000
1	-6.686014000	0.233381000	1.929719000
6	-4.828767000	-0.767839000	2.504258000
1	-3.801419000	-0.796269000	2.130928000

8	-5.300549000	-2.165251000	2.677799000
6	-4.862851000	-0.181822000	3.906492000
1	-5.892882000	-0.201381000	4.287391000
1	-4.511445000	0.850473000	3.886820000
8	-3.969019000	-0.908716000	4.791416000
1	-4.215187000	-1.856777000	4.753200000
6	-1.153211000	-5.690311000	-0.605210000
1	-0.775411000	-6.643614000	-0.981105000
8	-0.054566000	-4.794266000	-0.315120000
6	-2.087966000	-5.025413000	-1.634483000
1	-2.824148000	-5.783083000	-1.930892000
8	-1.363955000	-4.618324000	-2.817674000
1	-0.384163000	-4.752109000	-2.718497000
6	-2.861603000	-3.839661000	-1.030887000
1	-2.165463000	-3.014374000	-0.857035000
8	-3.881473000	-3.395026000	-1.973468000
1	-4.761094000	-3.281257000	-1.516212000
6	-3.499390000	-4.220442000	0.314432000
1	-4.326850000	-4.921594000	0.149256000
6	-2.469812000	-4.833308000	1.265541000
1	-1.678443000	-4.105766000	1.470264000
8	-1.871416000	-6.011483000	0.600151000
6	-3.026998000	-5.371232000	2.574831000
1	-3.836045000	-6.086126000	2.376007000
1	-3.410296000	-4.554696000	3.188474000
8	-1.967489000	-6.002159000	3.348337000
1	-1.583956000	-6.716132000	2.796410000
6	4.169449000	-4.673668000	-0.133744000
1	5.194253000	-5.038742000	-0.046985000
8	4.113579000	-3.243777000	0.005665000

6	3.527760000	-5.077005000	-1.469423000
1	3.631601000	-6.159109000	-1.589345000
8	4.178913000	-4.396357000	-2.590558000
1	4.649817000	-5.033302000	-3.163065000
6	2.050977000	-4.690635000	-1.475853000
1	1.975344000	-3.603184000	-1.393848000
8	1.394831000	-5.131667000	-2.698296000
1	1.878744000	-4.778121000	-3.473651000
6	1.307511000	-5.328988000	-0.304674000
1	1.279719000	-6.418283000	-0.430588000
6	1.995461000	-4.959651000	1.017702000
1	1.919554000	-3.881574000	1.187828000
8	3.433480000	-5.321953000	0.926048000
6	1.510421000	-5.716284000	2.245544000
1	1.587290000	-6.797243000	2.067206000
1	0.475254000	-5.467596000	2.479396000
8	2.297225000	-5.328540000	3.406988000
1	3.237833000	-5.513536000	3.201581000
6	6.493197000	0.194502000	0.601124000
1	7.357640000	0.794385000	0.892533000
8	5.343992000	1.025690000	0.365274000
6	6.778442000	-0.657442000	-0.637744000
1	7.695586000	-1.228940000	-0.453347000
8	6.983201000	0.208001000	-1.790184000
1	6.988269000	-0.359334000	-2.590787000
6	5.632814000	-1.621071000	-0.918155000
1	4.733350000	-1.039222000	-1.151420000
8	6.036763000	-2.399666000	-2.066869000
1	5.309000000	-3.023529000	-2.328787000
6	5.341565000	-2.492313000	0.301816000

1	6.166545000	-3.189128000	0.484081000
6	5.105007000	-1.636226000	1.555070000
1	4.178839000	-1.063804000	1.446997000
8	6.243575000	-0.691813000	1.715841000
6	5.085370000	-2.429017000	2.854098000
1	4.290122000	-3.175727000	2.830419000
1	4.902632000	-1.742784000	3.689495000
8	6.329185000	-3.159793000	3.047510000
1	7.066109000	-2.513314000	3.038208000
6	3.916167000	4.992197000	0.184471000
1	3.938983000	6.079737000	0.278081000
8	2.579750000	4.514663000	0.002877000
6	4.803627000	4.516793000	-0.960996000
1	5.770038000	5.026878000	-0.874996000
8	4.151175000	4.912469000	-2.202888000
1	4.682491000	4.581836000	-2.956244000
6	5.048127000	3.010886000	-0.941899000
1	4.115295000	2.506079000	-1.222149000
8	6.071841000	2.768299000	-1.928230000
1	6.327609000	1.804449000	-1.943058000
6	5.442575000	2.488212000	0.448584000
1	6.468894000	2.785047000	0.694468000
6	4.454597000	2.982391000	1.513566000
1	3.452669000	2.618761000	1.270265000
8	4.439882000	4.477553000	1.439013000
6	4.769916000	2.610104000	2.957126000
1	5.523265000	3.305911000	3.351768000
1	5.181987000	1.599022000	2.983964000
8	3.582371000	2.571608000	3.790965000
1	3.054338000	3.405770000	3.707059000

6	-1.464427000	5.701045000	0.103874000
1	-2.297671000	6.402324000	0.169311000
8	-1.945078000	4.342172000	0.215802000
6	-0.695290000	5.860753000	-1.210314000
1	-0.505374000	6.926973000	-1.376436000
8	-1.546333000	5.353476000	-2.283842000
1	-1.071034000	5.438045000	-3.135520000
6	0.628680000	5.112169000	-1.177209000
1	0.414777000	4.038721000	-1.146924000
8	1.345471000	5.445756000	-2.386634000
1	2.286799000	5.129331000	-2.338595000
6	1.448239000	5.448772000	0.070033000
1	1.817484000	6.480470000	0.014781000
6	0.631618000	5.239240000	1.354217000
1	0.381085000	4.179785000	1.468193000
8	-0.614825000	6.030164000	1.219060000
6	1.252210000	5.772253000	2.653834000
1	0.496061000	5.715799000	3.437975000
1	1.539462000	6.822643000	2.524013000
8	2.383570000	4.989583000	3.122190000
1	3.184645000	5.090111000	2.549668000
6	-5.662393000	2.404715000	0.797795000
1	-6.742087000	2.293275000	0.910668000
8	-4.969633000	1.192649000	1.155844000
6	-5.272943000	2.812262000	-0.631553000
1	-5.783078000	3.752144000	-0.872502000
8	-5.727022000	1.778975000	-1.535273000
1	-5.540338000	1.984912000	-2.476374000
6	-3.755435000	3.011400000	-0.701185000
1	-3.263636000	2.090403000	-0.376070000

8	-3.366769000	3.275327000	-2.082644000
1	-2.692109000	4.012229000	-2.143402000
6	-3.394100000	4.146212000	0.257899000
1	-3.891956000	5.071038000	-0.053377000
6	-3.830656000	3.803372000	1.693333000
1	-3.257700000	2.944792000	2.057725000
8	-5.275790000	3.465575000	1.695713000
6	-3.704281000	4.969885000	2.662001000
1	-2.660823000	5.275724000	2.747456000
1	-4.069097000	4.657400000	3.647212000
8	-4.429996000	6.139859000	2.185575000
1	-5.374299000	5.898209000	2.082302000

AG4@β-CD			
6	-1.872119000	-0.734572000	-3.291527000
1	-2.734125000	-1.322771000	-2.951956000
1	-1.955365000	-0.647959000	-4.383476000
6	-0.559271000	-1.470997000	-2.918984000
1	-0.548208000	-2.466010000	-3.382693000
6	-0.455869000	-1.597832000	-1.376400000
1	0.457950000	-2.129238000	-1.073396000
1	-1.296353000	-2.197585000	-1.006656000
6	-0.469106000	-0.193589000	-0.729524000
1	-0.397107000	-0.292989000	0.361239000
6	0.738132000	0.615760000	-1.258397000
1	0.749074000	1.613499000	-0.800672000
1	1.679322000	0.124274000	-0.977689000
6	-1.786312000	0.527059000	-1.101833000
1	-2.639959000	-0.050764000	-0.721413000
1	-1.827044000	1.515406000	-0.625675000

6	-1.886934000	0.671538000	-2.641407000
1	-2.819401000	1.188041000	-2.905790000
6	-0.678852000	1.485940000	-3.167240000
1	-0.751914000	1.607289000	-4.257017000
1	-0.672314000	2.494034000	-2.731983000
6	0.640146000	0.760819000	-2.795919000
1	1.493920000	1.345358000	-3.161771000
6	0.627326000	-0.642376000	-3.476954000
1	0.474762000	-0.519552000	-4.558454000
7	1.890700000	-1.391083000	-3.285790000
1	1.892155000	-2.158153000	-2.626993000
6	3.060682000	-1.093928000	-3.877842000
7	3.177946000	-0.123646000	-4.792682000
1	4.105909000	0.020149000	-5.173071000
1	2.399675000	0.421811000	-5.119941000
7	4.172552000	-1.784660000	-3.531437000
1	4.130548000	-2.537804000	-2.828317000
7	5.395137000	-1.352426000	-4.078524000
1	5.894706000	-2.083337000	-4.570016000
1	5.945083000	-0.810903000	-3.416385000
6	-6.509314000	-0.575617000	0.242719000
1	-7.360866000	-1.245868000	0.375953000
8	-5.290652000	-1.312784000	0.045696000
6	-6.704442000	0.367107000	-0.952764000
1	-7.668873000	0.873640000	-0.850807000
8	-6.664578000	-0.368401000	-2.214828000
1	-7.564260000	-0.569558000	-2.539743000
6	-5.583805000	1.399330000	-1.006641000
1	-4.634980000	0.886608000	-1.189372000
8	-5.828452000	2.361879000	-2.070602000

1	-5.917834000	1.887232000	-2.922335000
6	-5.497608000	2.168017000	0.306419000
1	-6.398156000	2.774792000	0.449532000
6	-5.338494000	1.205671000	1.494478000
1	-4.377353000	0.687034000	1.425378000
8	-6.435617000	0.204863000	1.455402000
6	-5.475060000	1.878853000	2.851286000
1	-4.694490000	2.630435000	2.973792000
1	-5.369377000	1.122612000	3.637886000
8	-6.743486000	2.582463000	2.974026000
1	-7.468905000	1.934596000	2.852519000
6	-3.664251000	-5.169052000	0.049513000
1	-3.590343000	-6.256552000	0.113370000
8	-2.350871000	-4.561642000	0.079632000
6	-4.326004000	-4.721024000	-1.260920000
1	-5.290067000	-5.230340000	-1.352796000
8	-3.537203000	-5.146196000	-2.393309000
1	-2.569938000	-5.104494000	-2.188457000
6	-4.579681000	-3.207391000	-1.237022000
1	-3.613776000	-2.687125000	-1.260224000
8	-5.369962000	-2.858638000	-2.393809000
1	-5.669901000	-1.914923000	-2.330876000
6	-5.305624000	-2.782860000	0.050572000
1	-6.342663000	-3.139974000	0.016226000
6	-4.600311000	-3.295766000	1.307133000
1	-3.604484000	-2.852793000	1.389488000
8	-4.445075000	-4.763345000	1.187914000
6	-5.368179000	-3.089293000	2.602851000
1	-6.366820000	-3.534610000	2.539313000
1	-5.460781000	-2.027111000	2.829611000

8	-4.635752000	-3.692911000	3.722994000
1	-4.733753000	-4.666018000	3.668180000
6	1.683444000	-5.485269000	0.996012000
1	2.495114000	-6.111864000	1.365830000
8	2.152003000	-4.134069000	0.782011000
6	1.102428000	-6.022452000	-0.318610000
1	0.929882000	-7.098891000	-0.194021000
8	2.100051000	-5.817830000	-1.360644000
1	1.756007000	-6.137691000	-2.219230000
6	-0.208896000	-5.322865000	-0.673178000
1	0.000656000	-4.286283000	-0.935216000
8	-0.791293000	-5.880064000	-1.892291000
1	-1.009963000	-6.830797000	-1.783231000
6	-1.194279000	-5.340157000	0.501985000
1	-1.503080000	-6.367913000	0.736629000
6	-0.535876000	-4.716287000	1.743865000
1	-0.236742000	-3.684421000	1.538418000
8	0.680364000	-5.519381000	2.025037000
6	-1.370835000	-4.727750000	3.025173000
1	-0.698087000	-4.977804000	3.854444000
1	-2.153344000	-5.494098000	2.977177000
8	-1.941832000	-3.408854000	3.227201000
1	-2.889943000	-3.472496000	3.516883000
6	5.776714000	-2.003846000	1.291829000
1	6.824101000	-1.834045000	1.546577000
8	5.093404000	-0.756941000	1.043034000
6	5.614667000	-2.896250000	0.056228000
1	6.106403000	-3.855627000	0.246294000
8	6.276967000	-2.251852000	-1.064321000
1	6.523673000	-2.902247000	-1.748203000

6	4.120961000	-3.110560000	-0.202620000
1	3.625736000	-2.136719000	-0.266554000
8	3.946840000	-3.801164000	-1.467919000
1	3.227879000	-4.496001000	-1.422964000
6	3.575229000	-3.877960000	1.000745000
1	4.098698000	-4.832375000	1.108006000
6	3.767044000	-3.052793000	2.287390000
1	3.168809000	-2.137259000	2.225796000
8	5.195617000	-2.672224000	2.426235000
6	3.386940000	-3.809294000	3.545515000
1	2.295378000	-3.884695000	3.593948000
1	3.745996000	-3.251502000	4.417945000
8	3.988223000	-5.137349000	3.488304000
1	3.694118000	-5.670032000	4.252805000
6	5.390415000	3.378844000	0.556523000
1	5.790298000	4.394727000	0.557103000
8	3.957142000	3.391198000	0.397664000
6	6.011681000	2.529303000	-0.549735000
1	7.101744000	2.591809000	-0.457140000
8	5.609980000	3.079821000	-1.838966000
1	5.959413000	2.499835000	-2.546958000
6	5.588600000	1.069244000	-0.448891000
1	4.515215000	0.995304000	-0.664877000
8	6.358833000	0.363766000	-1.456374000
1	6.327152000	-0.621798000	-1.296534000
6	5.827717000	0.511167000	0.957542000
1	6.894599000	0.342502000	1.129278000
6	5.264049000	1.433593000	2.048966000
1	4.170902000	1.437781000	1.985555000
8	5.748684000	2.817216000	1.833723000

6	5.673706000	1.024308000	3.450116000
1	5.151120000	0.095661000	3.707549000
1	5.371086000	1.808276000	4.154088000
8	7.117611000	0.827129000	3.475002000
1	7.394059000	0.495151000	4.351423000
6	0.653307000	6.001313000	-0.043505000
1	0.147218000	6.964169000	-0.130840000
8	-0.297159000	4.943272000	0.152907000
6	1.514943000	5.713789000	-1.275365000
1	2.136670000	6.598081000	-1.460607000
8	0.639839000	5.494396000	-2.416259000
1	1.177508000	5.193797000	-3.177219000
6	2.432982000	4.512192000	-1.073912000
1	1.820318000	3.606906000	-0.971842000
8	3.254657000	4.436554000	-2.258347000
1	4.035528000	3.833282000	-2.118601000
6	3.258189000	4.663620000	0.206558000
1	3.986190000	5.476076000	0.090325000
6	2.339031000	4.928324000	1.401887000
1	1.667972000	4.075303000	1.545066000
8	1.522416000	6.130707000	1.105421000
6	3.038809000	5.257593000	2.709578000
1	3.688605000	6.132417000	2.575493000
1	3.644405000	4.413113000	3.040509000
8	2.054191000	5.502029000	3.753955000
1	1.474788000	6.231564000	3.448424000
6	-4.456955000	4.447135000	0.516612000
1	-5.491146000	4.690058000	0.768092000
8	-4.326088000	3.033941000	0.217076000
6	-3.977020000	5.236116000	-0.712235000

1	-4.141046000	6.301019000	-0.517245000
8	-4.782495000	4.917569000	-1.861880000
1	-4.965997000	3.943182000	-1.930503000
6	-2.472653000	5.020174000	-0.929285000
1	-2.295206000	3.973953000	-1.211482000
8	-2.024285000	5.915885000	-1.968760000
1	-1.090698000	5.696023000	-2.230274000
6	-1.702594000	5.311698000	0.369335000
1	-1.767297000	6.386944000	0.579988000
6	-2.229751000	4.521056000	1.566344000
1	-2.074615000	3.448304000	1.416070000
8	-3.685285000	4.777858000	1.684895000
6	-1.664092000	4.953597000	2.912054000
1	-1.817704000	6.033362000	3.043441000
1	-0.596595000	4.739981000	2.973061000
8	-2.293642000	4.210529000	3.993423000
1	-3.256336000	4.388538000	3.954794000

Table S4. Geometries in Cartesian coordinates in Å computed at the CPCM(water)/B3LYP-D3(BJ)/311+G(d,p) level of theory.

AG1@β-CD			
6	0.245179000	-1.163166000	-0.196912000
1	0.975313000	-1.926415000	0.085041000
1	-0.672098000	-1.365575000	0.364330000
6	-0.026937000	-1.257810000	-1.714731000
1	-0.450754000	-2.228236000	-1.974693000
6	1.295387000	-1.017669000	-2.485815000
1	1.123416000	-1.116870000	-3.561779000
1	2.026858000	-1.777805000	-2.201029000

6	1.839446000	0.378216000	-2.152894000
1	2.777597000	0.543144000	-2.691371000
6	0.813725000	1.435445000	-2.577994000
1	1.198000000	2.437301000	-2.377902000
1	0.617756000	1.374543000	-3.652632000
6	2.082666000	0.495261000	-0.640306000
1	2.858747000	-0.203729000	-0.328153000
1	2.443755000	1.499512000	-0.411949000
6	0.783006000	0.236369000	0.136493000
1	0.975461000	0.310347000	1.210773000
6	-0.257141000	1.288329000	-0.268737000
1	-1.196040000	1.122869000	0.267887000
1	0.084705000	2.291426000	-0.008883000
6	-0.505210000	1.219443000	-1.795755000
1	-1.218252000	1.991517000	-2.077721000
6	-0.996915000	-0.171368000	-2.111020000
7	-2.089729000	-0.517349000	-2.681816000
7	-2.936941000	0.486565000	-3.119431000
1	-2.734959000	1.480993000	-3.003340000
6	-4.096168000	0.134083000	-3.683044000
7	-4.820682000	1.115035000	-4.280494000
1	-5.663479000	0.843366000	-4.766973000
1	-4.305542000	1.862496000	-4.726759000
7	-4.535342000	-1.109464000	-3.614019000
1	-4.091390000	-1.803686000	-3.004378000
1	-5.376164000	-1.374323000	-4.103437000
6	-5.177125000	-2.560726000	1.669856000
1	-5.505652000	-3.524279000	2.062441000
8	-3.955009000	-2.690036000	0.966199000
6	-6.245984000	-1.949716000	0.767775000

1	-7.176681000	-1.883299000	1.340513000
8	-6.437902000	-2.811539000	-0.359195000
1	-7.053774000	-2.360710000	-0.953515000
6	-5.821073000	-0.565309000	0.309207000
1	-4.938616000	-0.669926000	-0.329782000
8	-6.904949000	-0.031643000	-0.440718000
1	-6.546363000	0.685865000	-0.996209000
6	-5.421838000	0.323577000	1.491424000
1	-6.319467000	0.658654000	2.023122000
6	-4.474284000	-0.414044000	2.444445000
1	-3.504686000	-0.527589000	1.952010000
8	-4.983789000	-1.720968000	2.778033000
6	-4.288784000	0.308667000	3.765005000
1	-5.252459000	0.365118000	4.286019000
1	-3.934759000	1.321382000	3.575782000
8	-3.309144000	-0.329348000	4.581080000
1	-3.584196000	-1.247427000	4.694323000
6	-1.461576000	-5.665080000	-0.476248000
1	-1.140275000	-6.661614000	-0.783366000
8	-0.359271000	-4.781196000	-0.430681000
6	-2.475645000	-5.095433000	-1.477309000
1	-3.290199000	-5.819818000	-1.567743000
8	-1.902300000	-4.954653000	-2.766645000
1	-0.943119000	-4.806023000	-2.686105000
6	-3.066813000	-3.782450000	-0.953463000
1	-2.283850000	-3.019393000	-0.927935000
8	-4.099952000	-3.333146000	-1.833793000
1	-4.910756000	-3.158280000	-1.316373000
6	-3.592391000	-3.978431000	0.467988000
1	-4.469676000	-4.634191000	0.437752000

6	-2.524650000	-4.598701000	1.374862000
1	-1.691250000	-3.896764000	1.476501000
8	-2.045222000	-5.825150000	0.797828000
6	-3.057808000	-4.958103000	2.752755000
1	-3.907554000	-5.643750000	2.650713000
1	-3.394124000	-4.053061000	3.258389000
8	-2.048689000	-5.532459000	3.578731000
1	-1.777045000	-6.361709000	3.167673000
6	3.798597000	-4.737384000	-0.335615000
1	4.817106000	-5.124206000	-0.290340000
8	3.785006000	-3.338822000	-0.176213000
6	3.141098000	-5.087691000	-1.676705000
1	3.220744000	-6.166799000	-1.823235000
8	3.796677000	-4.400351000	-2.752434000
1	4.159254000	-5.048013000	-3.366540000
6	1.674313000	-4.680811000	-1.647676000
1	1.618332000	-3.597572000	-1.526015000
8	0.990865000	-5.061429000	-2.840714000
1	1.404899000	-4.601037000	-3.581820000
6	0.960207000	-5.324604000	-0.468438000
1	0.915597000	-6.409614000	-0.611623000
6	1.712212000	-4.998008000	0.828104000
1	1.655465000	-3.920685000	1.010899000
8	3.095108000	-5.383025000	0.705855000
6	1.186467000	-5.742506000	2.040478000
1	1.246062000	-6.822910000	1.860437000
1	0.147313000	-5.474020000	2.212988000
8	1.905003000	-5.385291000	3.218886000
1	2.834132000	-5.593842000	3.062287000
6	6.298029000	-0.153222000	0.689782000

1	7.163663000	0.392381000	1.068664000
8	5.266543000	0.731083000	0.325277000
6	6.672957000	-1.001576000	-0.527255000
1	7.503487000	-1.654755000	-0.238012000
8	7.092520000	-0.138137000	-1.584291000
1	7.138442000	-0.673180000	-2.388255000
6	5.489304000	-1.853369000	-0.952541000
1	4.676781000	-1.191888000	-1.272588000
8	5.918559000	-2.656204000	-2.044310000
1	5.155503000	-3.173235000	-2.362987000
6	4.998152000	-2.690722000	0.223388000
1	5.751559000	-3.438949000	0.483838000
6	4.720053000	-1.807324000	1.445983000
1	3.867755000	-1.154243000	1.237591000
8	5.880958000	-1.000736000	1.740289000
6	4.425546000	-2.596360000	2.709103000
1	3.543540000	-3.215498000	2.551934000
1	4.214877000	-1.892146000	3.520992000
8	5.489091000	-3.477388000	3.065265000
1	6.279317000	-2.940369000	3.199952000
6	4.055541000	4.702374000	0.376428000
1	4.114168000	5.775912000	0.562038000
8	2.753365000	4.326281000	0.011788000
6	5.044583000	4.301859000	-0.716773000
1	6.017613000	4.728318000	-0.450336000
8	4.583981000	4.870351000	-1.942968000
1	5.173849000	4.569428000	-2.645953000
6	5.185348000	2.792130000	-0.826768000
1	4.249653000	2.387093000	-1.228485000
8	6.251456000	2.540654000	-1.729488000

1	6.423498000	1.579673000	-1.756744000
6	5.414833000	2.136035000	0.536974000
1	6.421655000	2.365218000	0.901478000
6	4.359881000	2.619486000	1.537094000
1	3.373034000	2.327613000	1.175020000
8	4.419983000	4.071972000	1.596065000
6	4.522645000	2.085571000	2.950744000
1	5.262198000	2.696828000	3.482177000
1	4.893148000	1.061884000	2.902685000
8	3.289320000	2.024182000	3.665964000
1	2.840260000	2.883727000	3.625113000
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1	-1.952734000	6.479883000	-0.086310000
8	-1.667620000	4.437487000	-0.039596000
6	-0.312193000	5.890668000	-1.374245000
1	-0.034845000	6.944185000	-1.482899000
8	-1.135786000	5.490490000	-2.473263000
1	-0.604158000	5.533906000	-3.278067000
6	0.945986000	5.047259000	-1.282925000
1	0.645363000	3.995228000	-1.277337000
8	1.742155000	5.321354000	-2.426336000
1	2.642755000	4.979510000	-2.277542000
6	1.707294000	5.307012000	0.014439000
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6	0.777650000	5.166268000	1.229707000
1	0.441313000	4.128471000	1.315122000
8	-0.356755000	6.033329000	1.031889000
6	1.354754000	5.617592000	2.576672000
1	0.517903000	5.708763000	3.269427000
1	1.814138000	6.606749000	2.470745000

8	2.270623000	4.698550000	3.161993000
1	3.104746000	4.696675000	2.660261000
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1	-6.416593000	2.559305000	0.870833000
8	-4.677877000	1.444954000	1.011016000
6	-5.029551000	3.030341000	-0.742452000
1	-5.526792000	3.980070000	-0.964489000
8	-5.546002000	2.008477000	-1.583126000
1	-5.377584000	2.207613000	-2.515027000
6	-3.520285000	3.195485000	-0.884444000
1	-3.039076000	2.261546000	-0.581544000
8	-3.195286000	3.459120000	-2.251492000
1	-2.446001000	4.085567000	-2.294230000
6	-3.083991000	4.302473000	0.066775000
1	-3.566157000	5.240783000	-0.222309000
6	-3.485991000	3.947447000	1.507524000
1	-2.926289000	3.060672000	1.821911000
8	-4.900792000	3.677349000	1.570939000
6	-3.230783000	5.065472000	2.502724000
1	-2.167350000	5.297912000	2.525731000
1	-3.537675000	4.722643000	3.496484000
8	-3.905605000	6.272953000	2.150776000
1	-4.850143000	6.079195000	2.113585000

AG4@β-CD			
6	-1.684814000	-0.533237000	-1.649576000
1	-2.397130000	-1.289811000	-1.309930000
1	-2.028900000	-0.177744000	-2.626723000
6	-0.292526000	-1.172633000	-1.781256000
1	-0.329915000	-1.994553000	-2.503330000

6	0.159216000	-1.693451000	-0.404637000
1	1.138344000	-2.179275000	-0.458696000
1	-0.544016000	-2.459942000	-0.071797000
6	0.216263000	-0.533343000	0.602963000
1	0.537885000	-0.912869000	1.577377000
6	1.221971000	0.516676000	0.100546000
1	1.277576000	1.351283000	0.805896000
1	2.226387000	0.091262000	0.034877000
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1	-1.895558000	-0.628526000	1.101645000
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6	-1.628213000	0.633603000	-0.649239000
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6	-0.621991000	1.682217000	-1.152510000
1	-0.942343000	2.077208000	-2.122914000
1	-0.586628000	2.528707000	-0.462941000
6	0.776792000	1.049677000	-1.270628000
1	1.487750000	1.806687000	-1.614524000
6	0.688359000	-0.102832000	-2.297689000
1	0.304358000	0.285998000	-3.246874000
7	1.986982000	-0.745247000	-2.570700000
1	2.069546000	-1.721933000	-2.329251000
6	2.924774000	-0.269905000	-3.395586000
7	2.845819000	0.944343000	-3.929438000
1	3.641216000	1.260541000	-4.467436000
1	2.086920000	1.571014000	-3.725507000
7	3.973049000	-1.054310000	-3.705726000
1	4.175691000	-1.878141000	-3.127678000
7	5.033383000	-0.480303000	-4.432507000
1	5.220931000	-1.061850000	-5.243103000

1	5.854449000	-0.475796000	-3.831837000
6	-5.834428000	-2.307298000	-0.289419000
1	-6.442730000	-3.210438000	-0.223146000
8	-4.469066000	-2.633440000	-0.400395000
6	-6.233588000	-1.476878000	-1.515923000
1	-7.312042000	-1.307566000	-1.476391000
8	-5.889610000	-2.163644000	-2.725517000
1	-6.690220000	-2.517853000	-3.127639000
6	-5.516460000	-0.134288000	-1.503982000
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8	-5.990127000	0.715945000	-2.549589000
1	-5.766193000	0.306068000	-3.394193000
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6	-5.378525000	-0.335821000	0.994830000
1	-4.300918000	-0.526572000	0.966703000
8	-6.094579000	-1.581491000	0.893436000
6	-5.733566000	0.246476000	2.350742000
1	-5.199552000	1.185021000	2.485254000
1	-5.413844000	-0.453561000	3.129832000
8	-7.123390000	0.541921000	2.472305000
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1	-1.700178000	-6.937010000	0.412778000
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1	-4.778602000	-4.325245000	2.527615000
1	-4.210544000	-2.661565000	2.328152000
8	-3.019275000	-3.813254000	3.515058000
1	-3.001727000	-4.739612000	3.781442000
6	3.206195000	-4.859261000	0.898373000
1	4.177005000	-5.149745000	1.299401000
8	3.238467000	-3.506636000	0.478135000
6	2.829967000	-5.738106000	-0.299075000
1	2.918790000	-6.783856000	0.017661000
8	3.760134000	-5.474880000	-1.348752000
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1	1.345428000	-4.425388000	-1.104898000
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1	1.038437000	-7.190165000	-1.591847000
6	0.440180000	-5.582950000	0.444809000
1	0.363745000	-6.632660000	0.752563000
6	0.919112000	-4.723824000	1.626250000
1	0.859680000	-3.673707000	1.336255000
8	2.289006000	-5.048377000	1.944230000
6	0.096202000	-4.926128000	2.897980000

1	0.656130000	-5.593588000	3.558692000
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8	-0.151545000	-3.696793000	3.580524000
1	-1.104200000	-3.515939000	3.518034000
6	5.887729000	-0.319112000	0.722143000
1	6.818610000	0.209263000	0.932350000
8	4.859672000	0.587458000	0.392801000
6	6.054522000	-1.279449000	-0.467872000
1	6.869569000	-1.974669000	-0.254985000
8	6.354701000	-0.545445000	-1.663160000
1	7.313078000	-0.471183000	-1.743567000
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1	3.951689000	-1.345998000	-0.833780000
8	4.872876000	-2.940660000	-1.765370000
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6	4.465889000	-2.798551000	0.650458000
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6	4.361478000	-1.803389000	1.814023000
1	3.520176000	-1.127171000	1.630820000
8	5.577370000	-1.036356000	1.895318000
6	4.132286000	-2.471714000	3.152061000
1	3.131896000	-2.912213000	3.148405000
1	4.181414000	-1.709093000	3.936239000
8	5.124810000	-3.480850000	3.357228000
1	4.900749000	-3.966109000	4.157868000
6	3.947449000	4.621750000	0.361610000
1	4.085009000	5.698100000	0.473745000
8	2.589161000	4.315140000	0.146275000
6	4.760044000	4.097095000	-0.822369000
1	5.800439000	4.407254000	-0.676820000

8	4.250390000	4.683264000	-2.021583000
1	4.665561000	4.231767000	-2.767878000
6	4.699565000	2.581368000	-0.876377000
1	3.667207000	2.274995000	-1.080183000
8	5.548265000	2.163990000	-1.936792000
1	5.681409000	1.201298000	-1.867214000
6	5.115741000	1.991096000	0.465530000
1	6.179920000	2.171042000	0.635684000
6	4.301615000	2.610731000	1.607102000
1	3.250747000	2.333941000	1.481039000
8	4.419052000	4.046426000	1.560384000
6	4.740432000	2.142998000	2.977194000
1	4.502768000	1.079654000	3.066777000
1	4.176476000	2.696397000	3.735430000
8	6.145768000	2.357808000	3.129048000
1	6.422579000	1.964271000	3.962842000
6	-1.180738000	6.045405000	0.280588000
1	-1.934134000	6.815765000	0.451256000
8	-1.788811000	4.804160000	0.024196000
6	-0.292290000	6.417929000	-0.908413000
1	0.109504000	7.419682000	-0.719734000
8	-1.096127000	6.440197000	-2.086977000
1	-0.503048000	6.496051000	-2.847323000
6	0.864903000	5.441369000	-1.037217000
1	0.468444000	4.446392000	-1.269234000
8	1.689321000	5.899683000	-2.099994000
1	2.497328000	5.353386000	-2.133268000
6	1.624498000	5.358164000	0.283120000
1	2.128000000	6.313199000	0.469747000
6	0.670881000	5.045168000	1.439102000

1	0.252348000	4.042998000	1.302114000
8	-0.400599000	6.008513000	1.459229000
6	1.342810000	5.134438000	2.797479000
1	1.741461000	6.146306000	2.939057000
1	2.171526000	4.429864000	2.839644000
8	0.449509000	4.791950000	3.854755000
1	-0.267664000	5.436886000	3.846748000
6	-5.499631000	2.969756000	0.261648000
1	-6.554420000	2.841108000	0.507178000
8	-4.941158000	1.745846000	-0.181099000
6	-5.329035000	3.993627000	-0.868745000
1	-5.830919000	4.916876000	-0.567265000
8	-5.982446000	3.549215000	-2.044461000
1	-5.762487000	2.613610000	-2.206347000
6	-3.846282000	4.300759000	-1.078362000
1	-3.345821000	3.403044000	-1.462616000
8	-3.728064000	5.365532000	-2.009994000
1	-2.786595000	5.603218000	-2.092132000
6	-3.194811000	4.672597000	0.256311000
1	-3.605192000	5.630262000	0.595246000
6	-3.453033000	3.607238000	1.322216000
1	-2.982193000	2.665581000	1.027327000
8	-4.873404000	3.403335000	1.447842000
6	-2.957450000	4.009283000	2.699033000
1	-3.426573000	4.955159000	2.996304000
1	-1.879900000	4.152135000	2.666407000
8	-3.206799000	2.995444000	3.670704000
1	-4.162615000	2.884412000	3.732858000

Table S5. Size and polydispersity index (PdI) of tested vesicles. The results are expressed as an average value ± standard deviation of ten measurements.

Vesicles	Size / nm	PdI
PC	165 ± 9	0.4 ± 0.1
PC : EO-CD-SR	102 ± 2	0.2 ± 0.1
EO-CD-SR	143 ± 5	0.5 ± 0.1

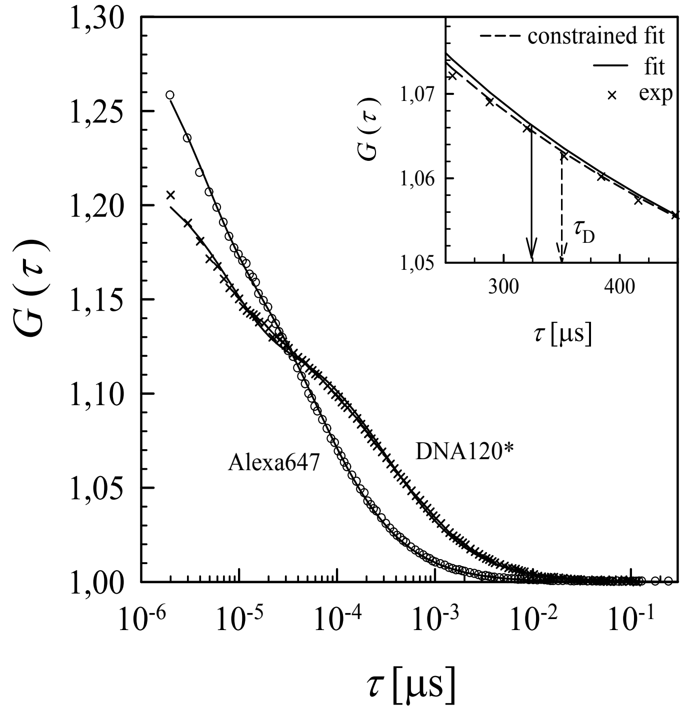

Figure S23. Experimental autocorrelation functions G(τ) recorded for 20 nM (molecules) DNA120* in HEPES buffer aqueous envorinment. For comparison, the data is shown for 20 nM Alexa647 fluorophore in pure water, without any DNA. We also performed the calibration measurement of diffusion time τ_{ref} =~50 μs for the free Alexa647 fluorophore, whose diffusion coefficient is known,[39] D_{ref} = 3.3 × 10^{-10} m²/s. The diffusion time for DNA120* is ~350 μs, corresponding to diffusion coefficient ~ 4 × 10^{-11} m²/s. This coefficient correspond well to a theoretical value for a rodlike 120 basepair DNA molecule of a length L=bN (*N*=120, *b* = 0.34 nm) and diameter *d* = 2.6 nm.

The inset emphasizes different fits to autocorrelation data. Constrained fit is executed by constraining the values that describe the triplet contribution to *G(t)* (triplet time τ_T, triplet fraction *T*) in order to improve the fit to data points in the region more relevant to the properties (i.e. characteristic diffusion time τ_D) of the system under study. The difference in τ_D

between the fits is, however, not significant for this study. The experimental values of *G(τ)* are shown with symbols and the respective fits with solid and dashed lines.

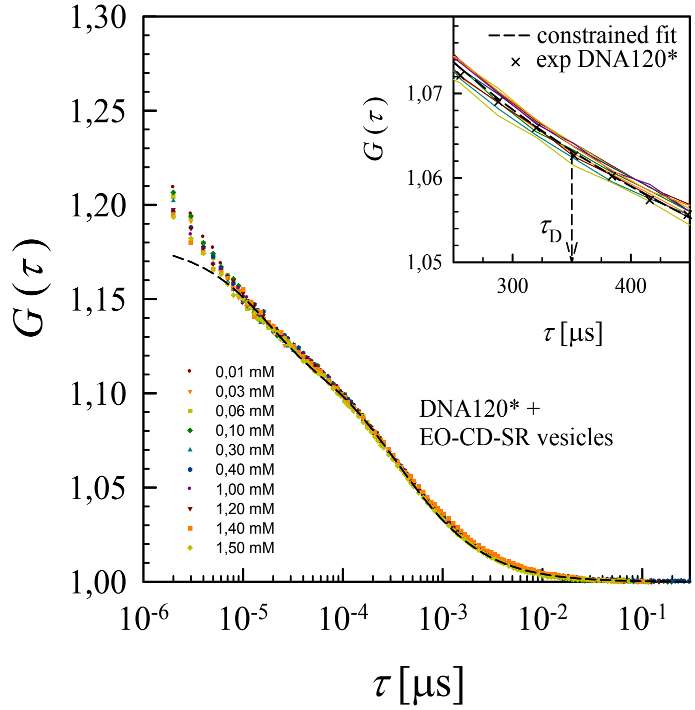

Figure S24. Experimental autocorrelation functions *G(τ)* recorded for 20 nM DNA120* in aqueous buffer environments with an increasing content of unmodified EO-CD-SR vesicles. Vesicle content is defined by the molecular concentration of constituents of the vesicle membrane. The experimental values of *G(τ)* are shown with symbols and may be compared to the fit to *G(τ)* for the Cy5 labeled DNA120* in an environment without vesicles. The inset zooms the correlation time range 250−450 µs. Here the experimental values of *G(τ)* for DNA120* in varying vesicle concentrations environment are given by colored lines. The arrow in the inset denotes the diffusion time τ_D for DNA120* in an aqueous environment without vesicles. The diffusion times for different vesicle concentration samples vary around τ_D in an uncorrelated manner, which indicates that τ_D is not influenced by the presence of unmodified vesicles.

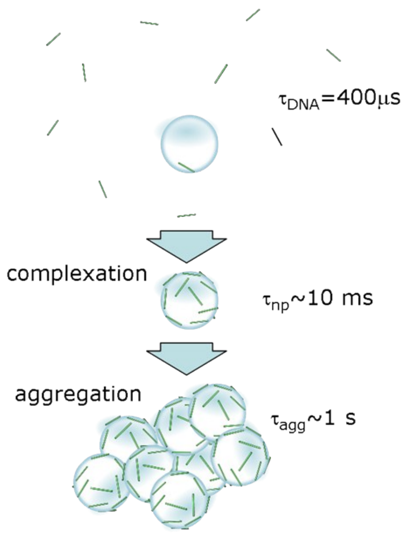

Figure S25. A schematic representation of the processes in the nanoparticle solution. AG modified nanoparticles (spheres) and DNA120* (rods) are shown to scale. DNA is 40 nm long and presented as rodlike since the 120bp fragment is shorter than DNA persistence length. DNA120* diffusion time is ~400 µs. At concentrations of amphiphiles (0.1 – 1.5 mM) that we tested, corresponding nanovesicles concentrations (1-10 nM) are comparable to DNA120* concentration (10-20 nM). Nanovesicles concentration is such that we find one nanovesicles every 0.6-1.2 µm, while DNA concentration gives average DNA distance of 0.4-0.5 µm. Above certain threshold concentrations of nanovesicles these would remove all free DNA from solution and complex it. FCS would then detect the diffusion time (~10 ms) of the DNA-vesicle complex, i.e. of the vesicle, which is quite larger entity. Change in the surface charge of nanovesicles due to complexation would, in some cases, lead to aggregation that was observed as extremely high characteristic diffusion times (~1 s).

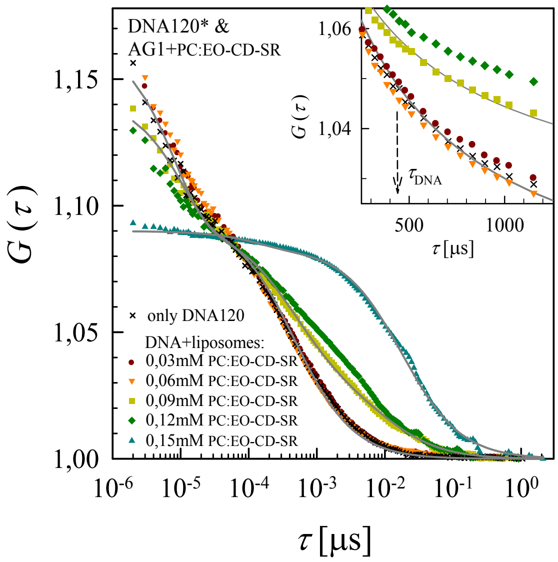

Figure S26. Experimental autocorrelation functions G(τ) recorded for 20 nM (molecules) DNA120* titrated with a stock solution of PC : EO-CD-SR liposomes modified with **AG1**. Stock concentration of amphiphiles was 1.5 mM and the corresponding final concentrations are shown. The liposome concentrations are taken to be proportional to nominal amphiphile concentration. The solid grey lines are fits to experimental data. The inset focuses on the range of correlation times that correspond to DNA120* characteristic diffusion time (~400 μs). When DNA 120* binds to nanovesicles its diffusion time is enhanced. The mixture of the bound and unbound DNA120* species shows in FCS as the autocorrelation function that deviates from the one for only DNA120* - at 0,09 mM amphiphile this deviation is quite apparent indicating that significant fraction of DNA120* is bound and we take 0,09 mM as threshold concentration.

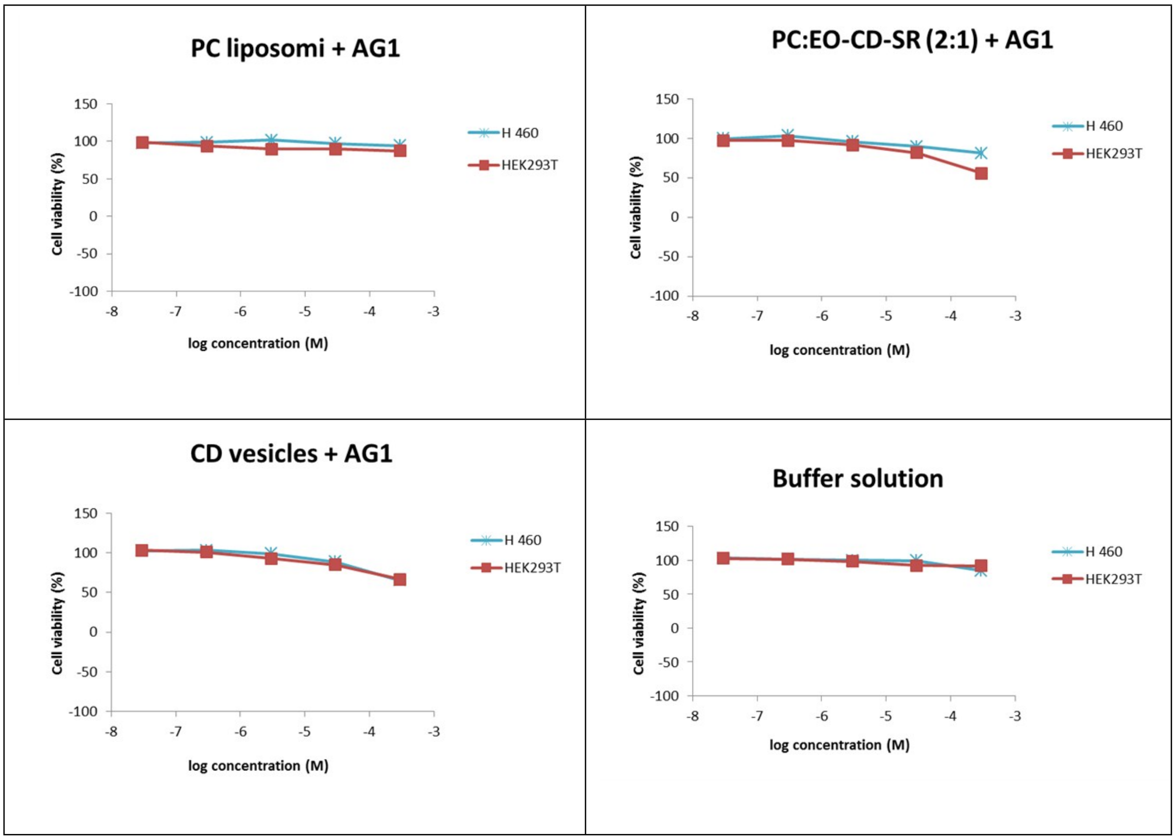

Figure S27. Dose-response profiles for cell viability in the presence of tested nanovesicles and buffer solution, tested *in vitro* on HEK293T and H 460 cell lines for 72 hrs incubation.

Cell toxicity study

The experiments were carried out on two human cell lines: HEK293T (embryonic kidney) and H 460 (lung carcinoma). Briefly, cells were grown in DMEM medium with the addition of 10% fetal bovine serum (FBS), 2 mM L-glutamine, 100 U/mL penicillin and 100 µg/mL streptomycin, and cultured as monolayers at 37 °C in a humidified atmosphere with 5% CO_2. Cells were seeded at 1.6×10^4 cells/ml in a standard 96-well microtiter plates and left to attach for 24 h. Next day, test compounds were added in five serial 10-fold dilutions. After 72 hours of incubation, the cell viability was evaluated by the MTT assay, a colorimetric assay system that measures the reduction of a tetrazolium component (MTT) into an insoluble formazan product by the mitochondria of viable cells. The absorbance was determined spectrophotometrically at 570 nm on a microplate reader (Multiscan, Thermo Labsystems, Waltham, MA, USA) and was directly proportional to the cell viability. The cell viability of the treated cells was expressed as a percentage compared to the untreated control cells. Each result represents an average value from at least two separate experiments performed in quadruplicate.