Thermodynamics and Structural Aspects of Propofol Inclusion in Native and Substituted β-Cyclodextrins in Water

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SUPPORTING INFORMATION

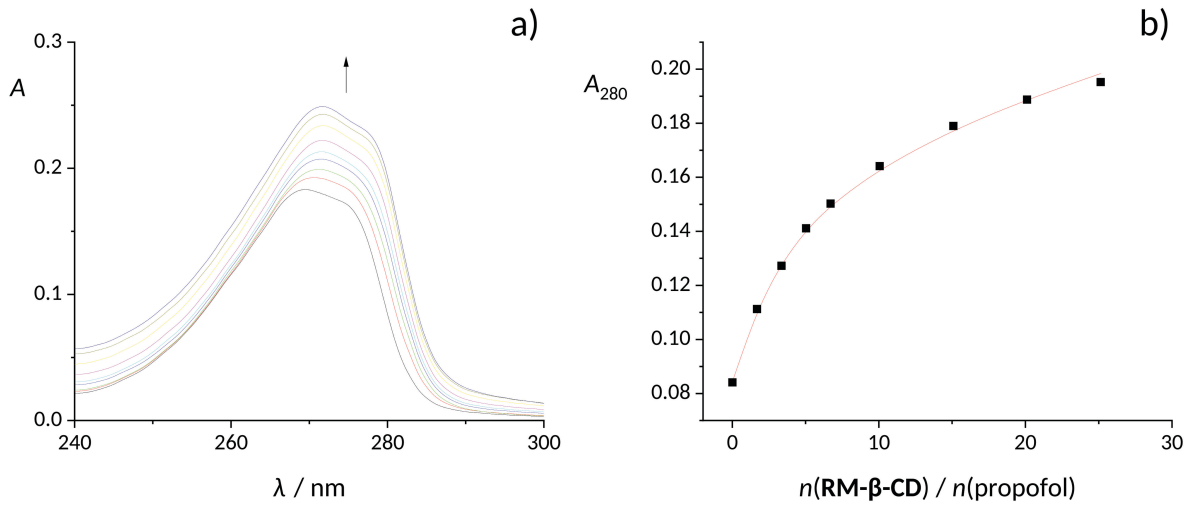

Figure S1. UV spectrophotometric titration of propofol (c_0 = 1.37 × 10^{-4} mol dm^{-3}) with **RM-β-CD** (c = 1.02 × 10^{-2} mol dm^{-3}) in H_2O at 298 K; l = 1 cm. a) Spectra corrected for dilution. b) Dependence of the absorbance at 280 nm on the receptor-to-guest mole ratio. ■ experimental; – calculated.

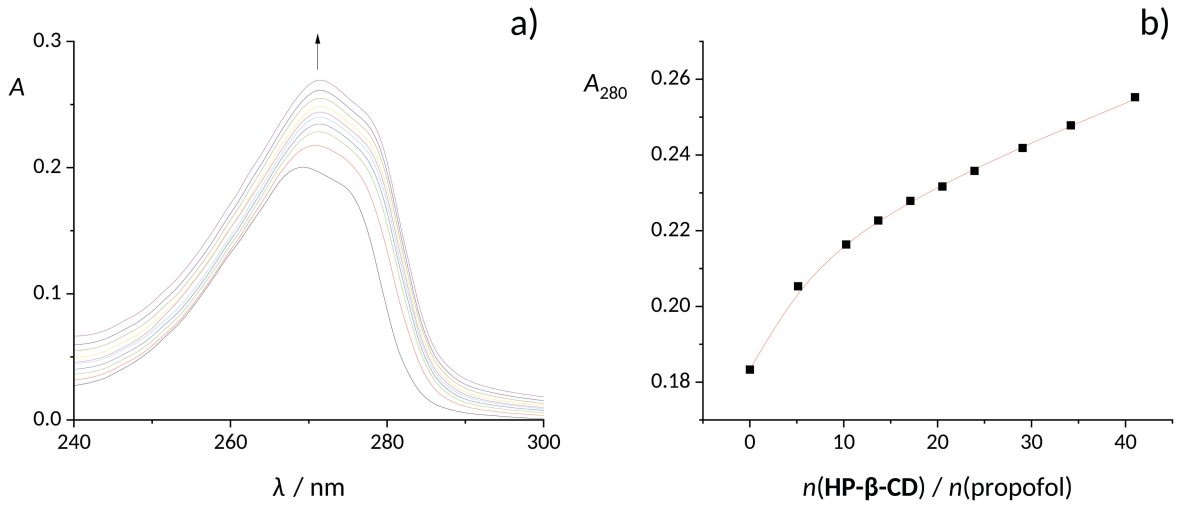

Figure S2. UV spectrophotometric titration of propofol (c_0 = 1.37 × 10^{-4} mol dm^{-3}) with **HP-β-CD** (c = 1.10 × 10^{-2} mol dm^{-3}) in H_2O at 298 K; l = 1 cm. a) Spectra corrected for dilution. b) Dependence of the absorbance at 280 nm on the receptor-to-guest mole ratio. ■ experimental; – calculated.

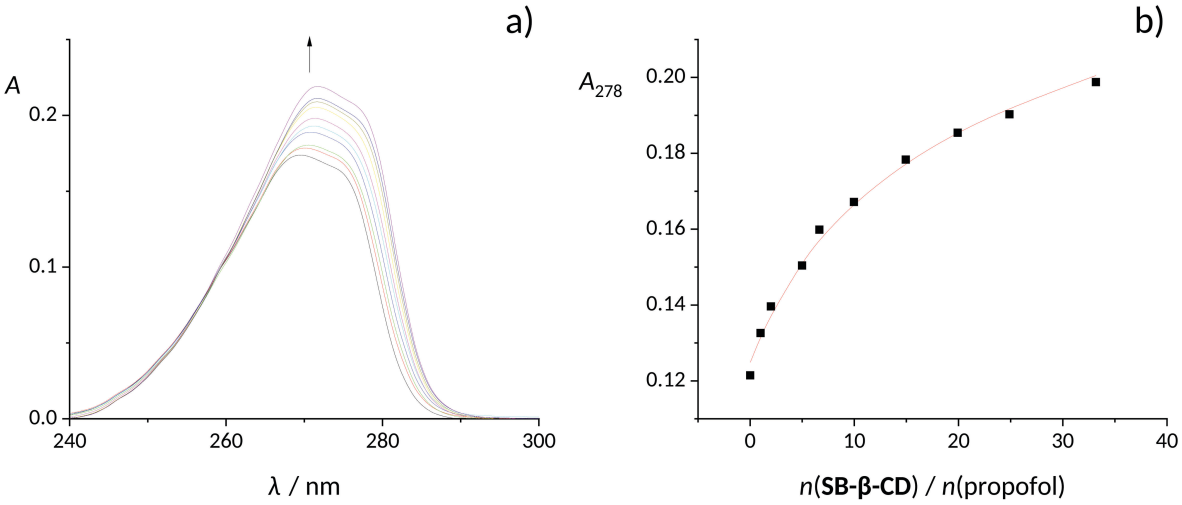

Figure S3. UV spectrophotometric titration of propofol (c_0 = 1.37 × 10^{-4} mol dm^{-3}) with **SB-β-CD** (c = 1.11 × 10^{-2} mol dm^{-3}) in H_2O at 298 K; l = 1 cm. a) Spectra corrected for dilution. b) Dependence of the absorbance at 280 nm on the receptor-to-guest mole ratio. ■ experimental; – calculated.

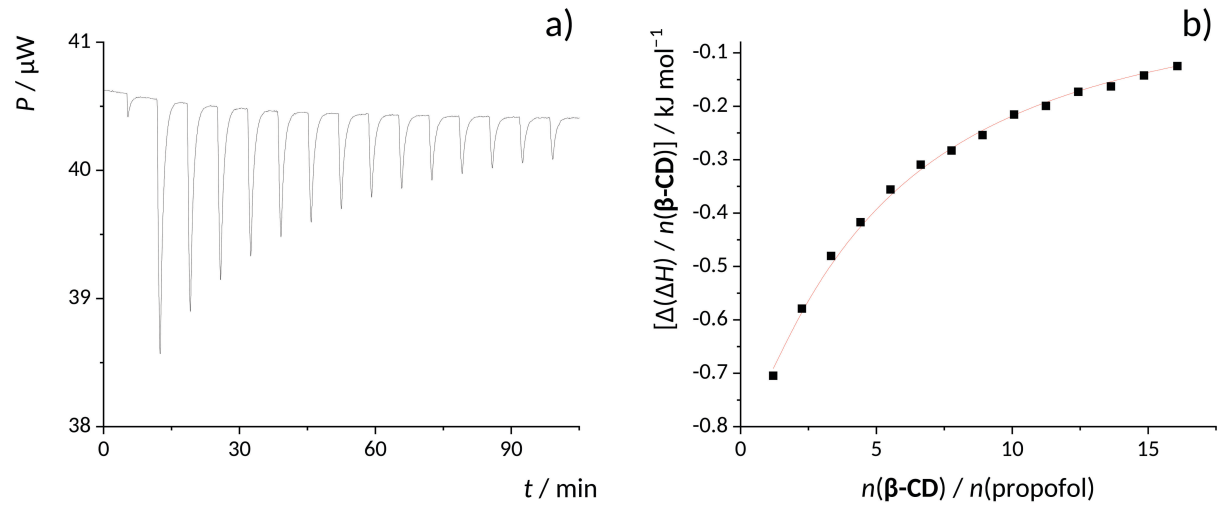

Figure S4. Microcalorimetric (ITC) titration of propofol ($c_0 = 1.37 \times 10^{-4}$ mol dm^{-3}) with **β-CD** ($c = 1.01 \times 10^{-2}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) Dependence of the normalized successive enthalpy change on the receptor-to-guest mole ratio. ■ experimental; – calculated.

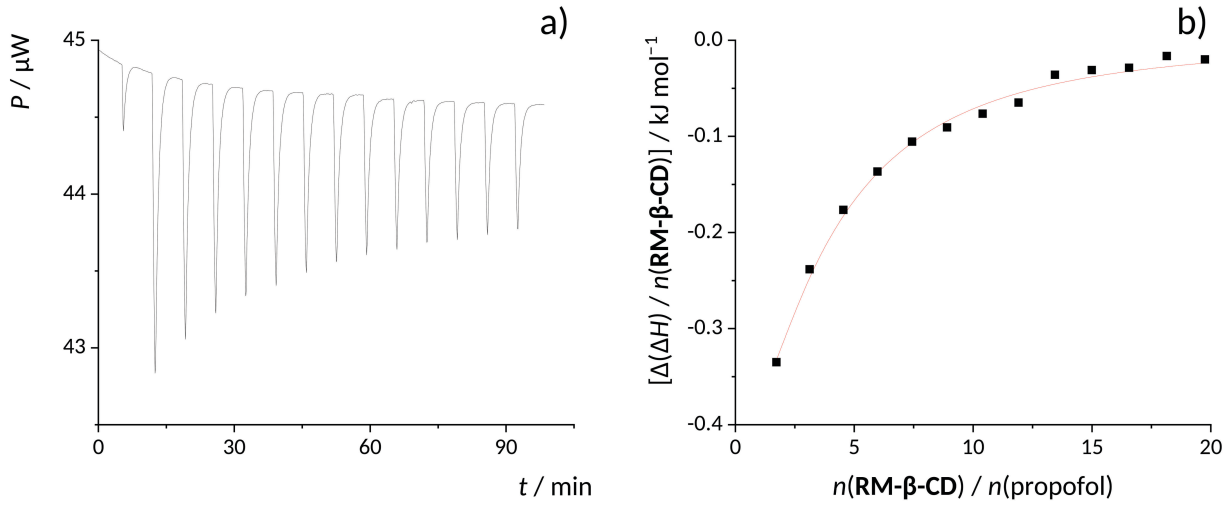

Figure S5. Microcalorimetric (ITC) titration of propofol ($c_0 = 1.37 \times 10^{-4}$ mol dm^{-3}) with **RM-β-CD** ($c = 1.02 \times 10^{-2}$ mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) Dependence of the normalized successive enthalpy change on the receptor-to-guest mole ratio. ■ experimental; – calculated.

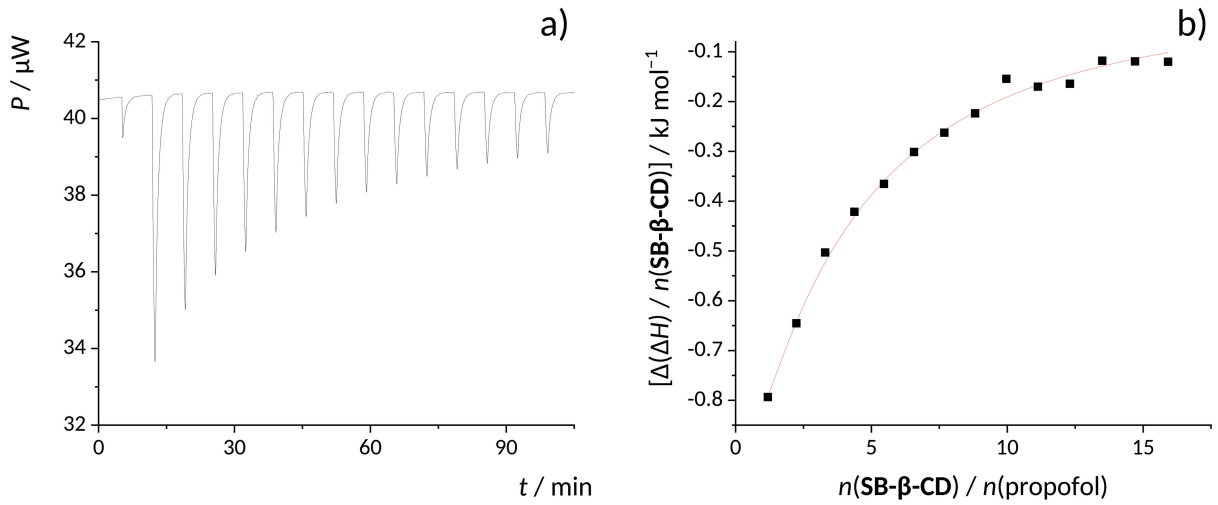

Figure S6. Microcalorimetric (ITC) titration of propofol (c_0 = 1.37 × 10^{-4} mol dm^{-3}) with **SB-β-CD** (c = 1.11 × 10^{-2} mol dm^{-3}) in H_2O at 298 K. a) Thermogram. b) Dependence of the normalized successive enthalpy change on the receptor-to-guest mole ratio. ■ experimental; – calculated.

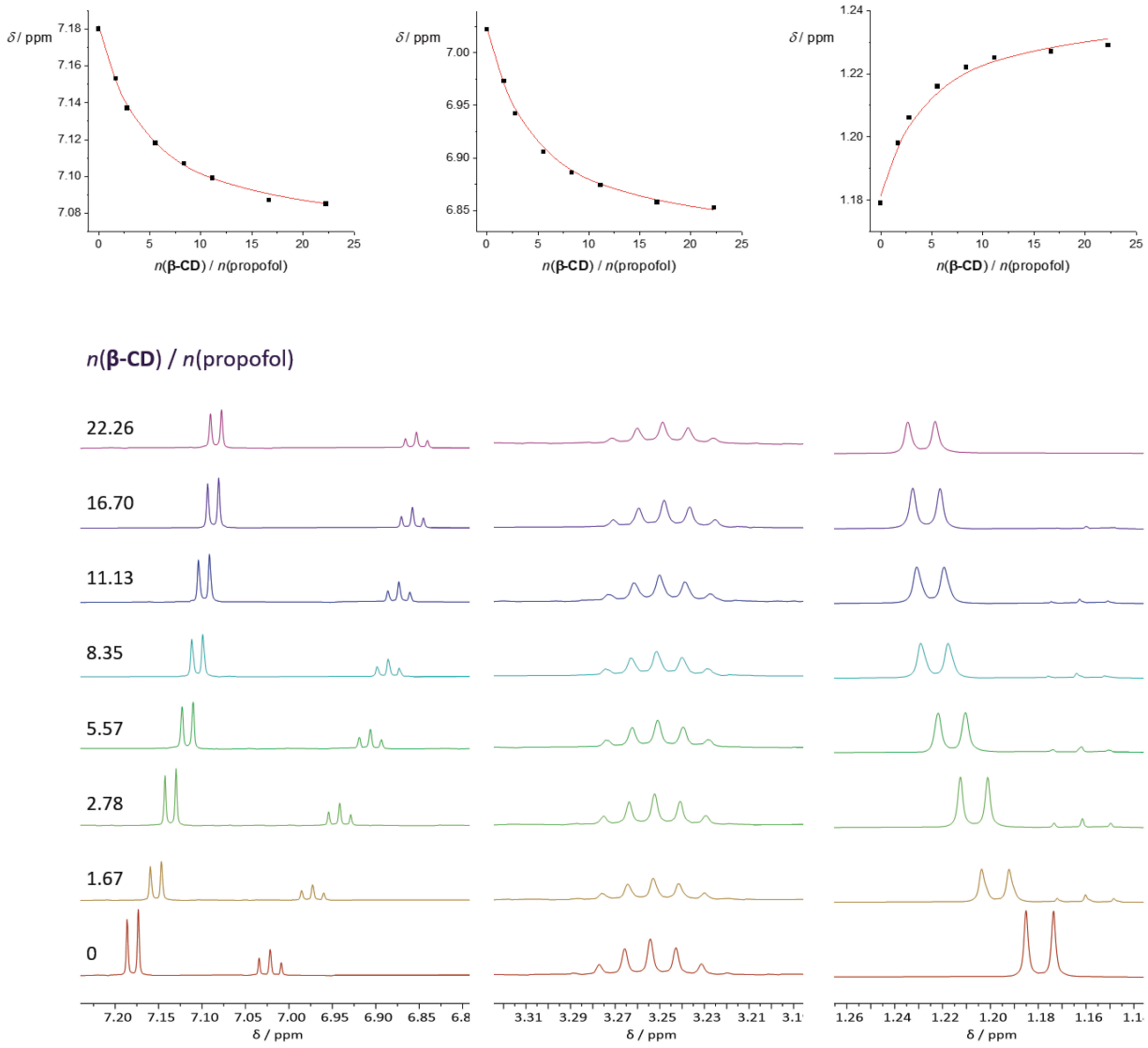

Figure S7. ^{1}H NMR titration of propofol ($c_0 = 4.0 \times 10^{-4}$ mol dm^{-3}) with **β-CD** ($c = 2.0 \times 10^{-2}$ mol dm^{-3}) in D_2O.

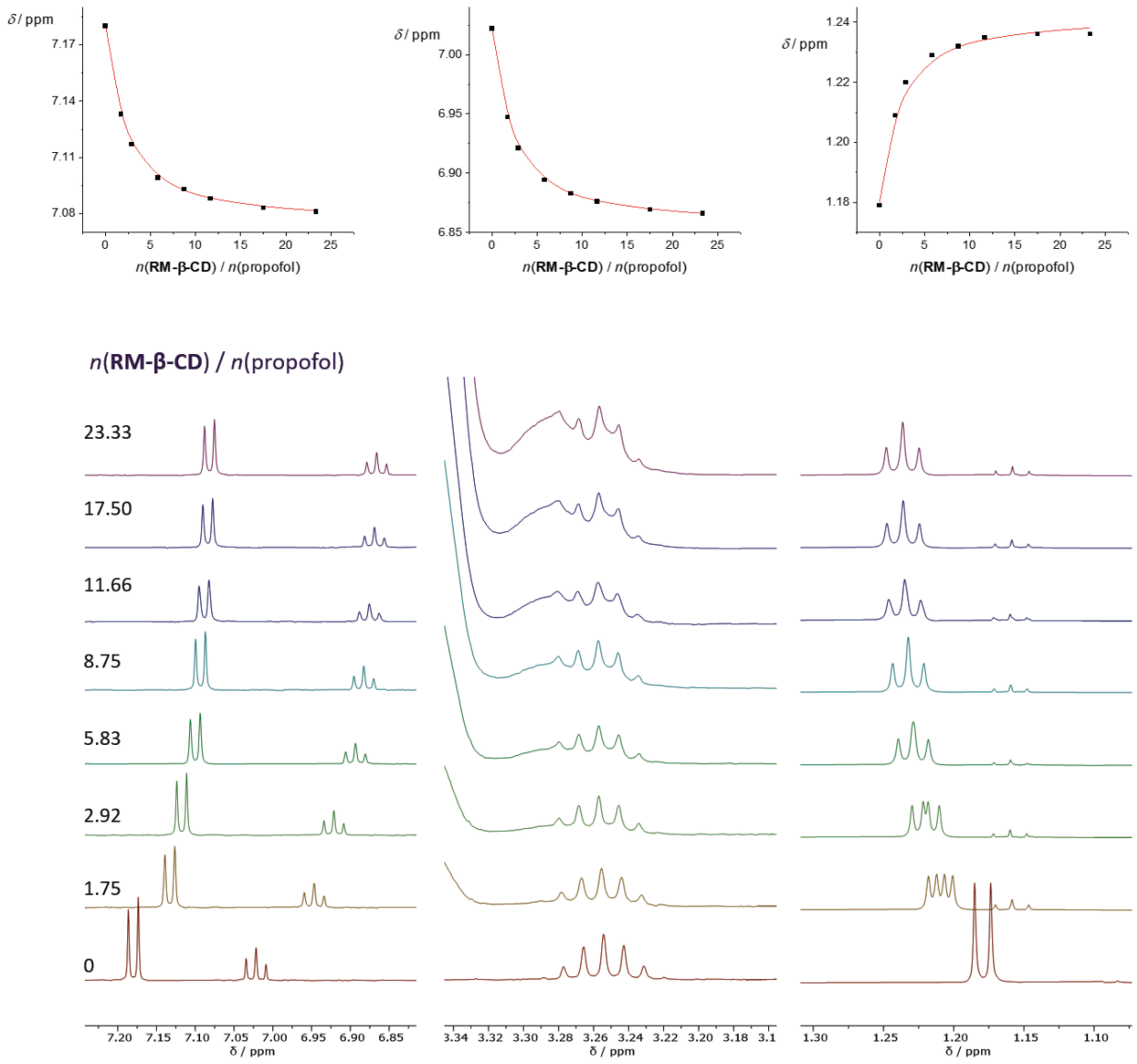

Figure S8. ^{1}H NMR titration of propofol (c_0 = 4.0 × 10^{-4} mol dm^{-3}) with **RM-β-CD** (c = 2.0 × 10^{-2} mol dm^{-3}) in D_2O.

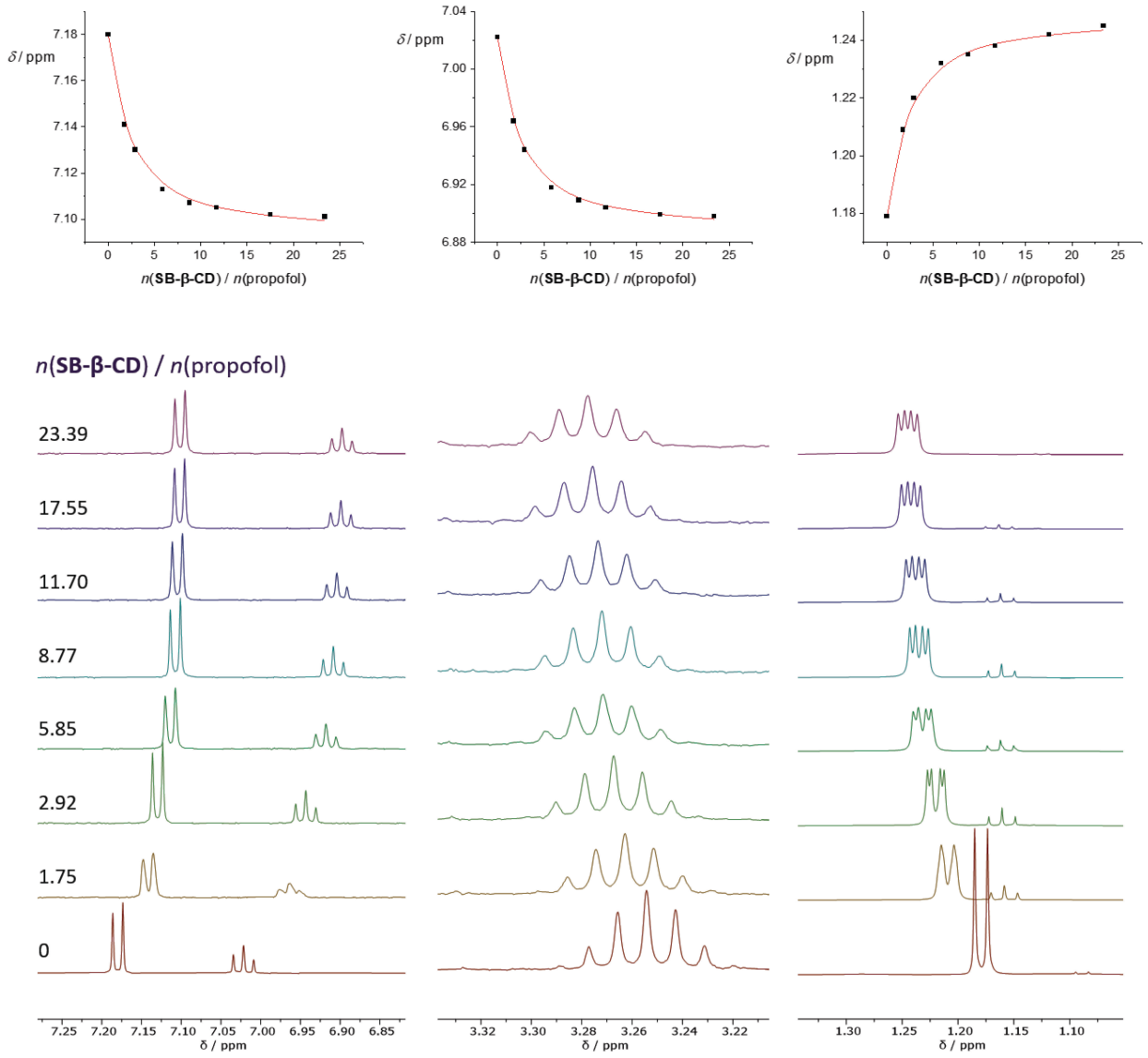

Figure S9. ^{1}H NMR titration of propofol ($c_0 = 4.0 \times 10^{-4}$ mol dm^{-3}) with **SB-β-CD** ($c = 2.0 \times 10^{-2}$ mol dm^{-3}) in D_2O.

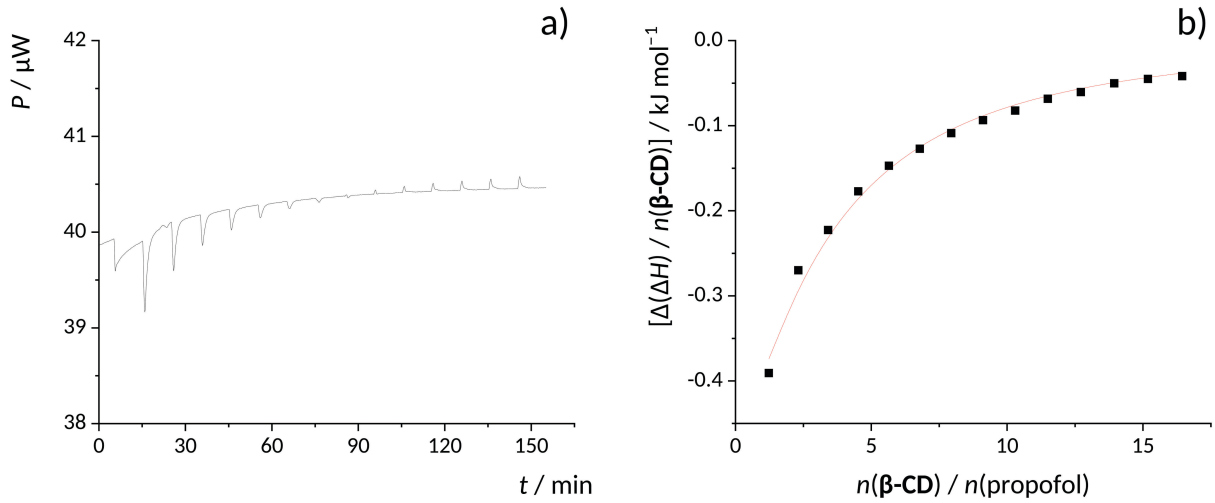

Figure S10. Microcalorimetric (ITC) titration of propofol (c_0 = 1.37 × 10^{-4} mol dm^{-3}) with **β-CD** (c = 1.01 × 10^{-2} mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) Dependence of the normalized successive enthalpy change on the receptor-to-guest mole ratio. ■ experimental; – calculated.

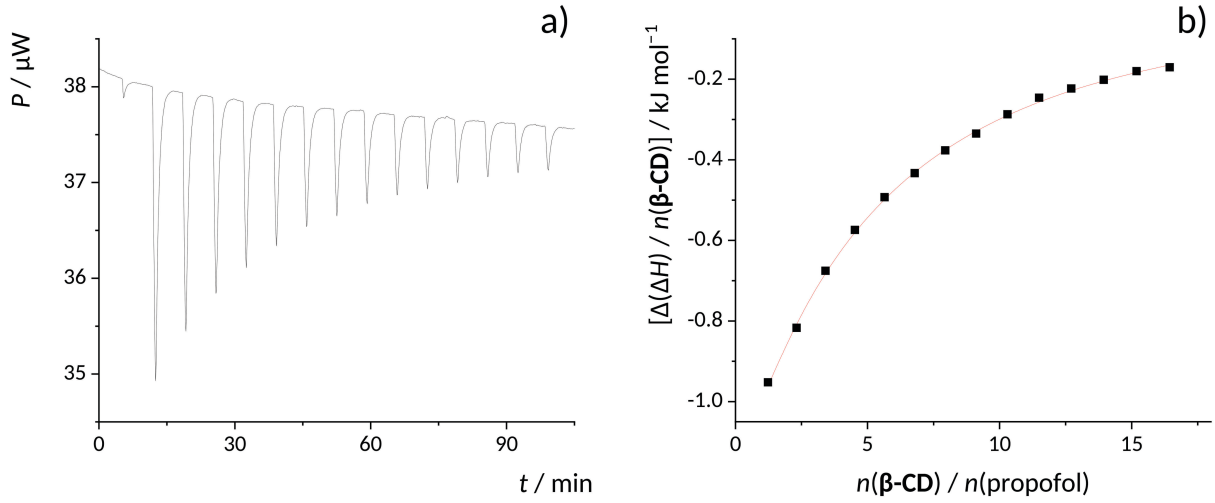

Figure S11. Microcalorimetric (ITC) titration of propofol (c_0 = 1.37 × 10^{-4} mol dm^{-3}) with **β-CD** (c = 1.01 × 10^{-2} mol dm^{-3}) in H_2O at 310 K. a) Thermogram. b) Dependence of the normalized successive enthalpy change on the receptor-to-guest mole ratio. ■ experimental; – calculated.

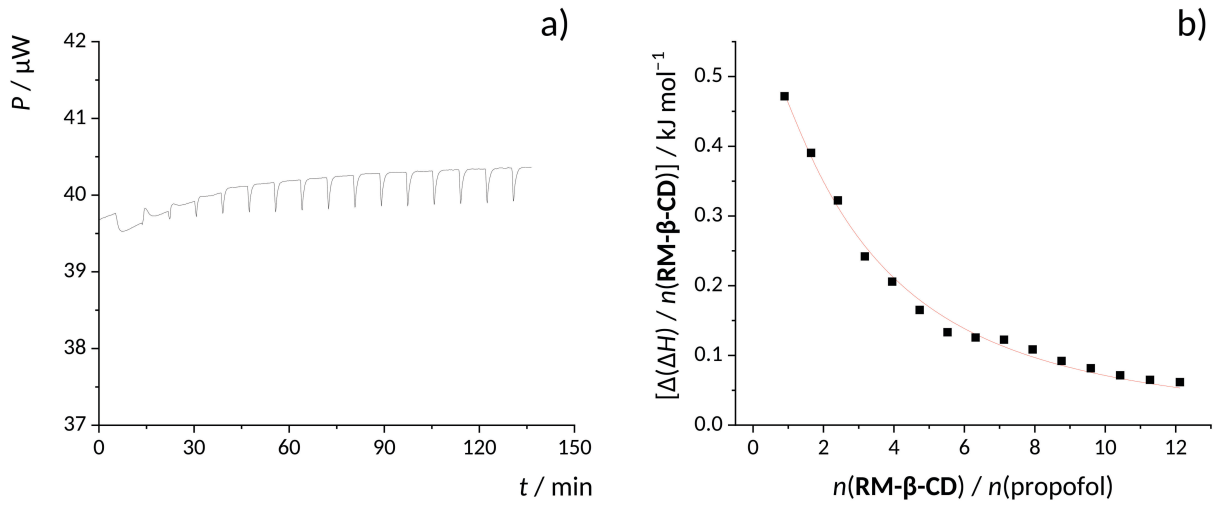

Figure S12. Microcalorimetric (ITC) titration of propofol (c_0 = 1.37 × 10^{-4} mol dm^{-3}) with **RM-β-CD** (c = 1.02 × 10^{-2} mol dm^{-3}) in H_2O at 278 K. a) Thermogram. b) Dependence of the normalized successive enthalpy change on the receptor-to-guest mole ratio. ■ experimental; – calculated.

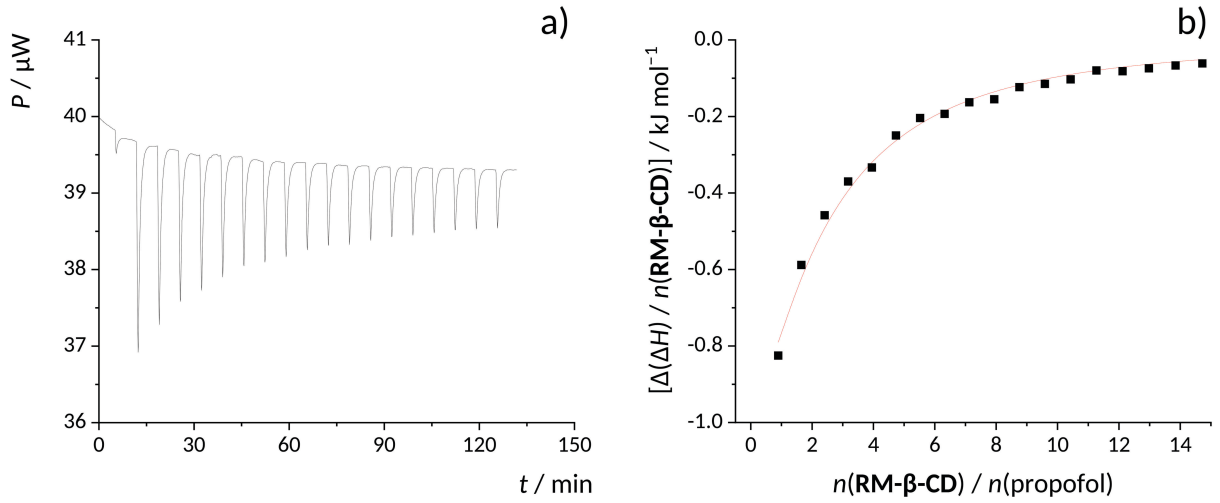

Figure S13. Microcalorimetric (ITC) titration of propofol (c_0 = 1.37 × 10^{-4} mol dm^{-3}) with **RM-β-CD** (c = 1.02 × 10^{-2} mol dm^{-3}) in H_2O at 310 K. a) Thermogram. b) Dependence of the normalized successive enthalpy change on the receptor-to-guest mole ratio. ■ experimental; – calculated.