Supporting Information

Synthesis and Inclusion Properties of a β-Cyclodextrin Heptaphosphoramidate

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I. NMR Spectra

NMR Spectra of compound **6**

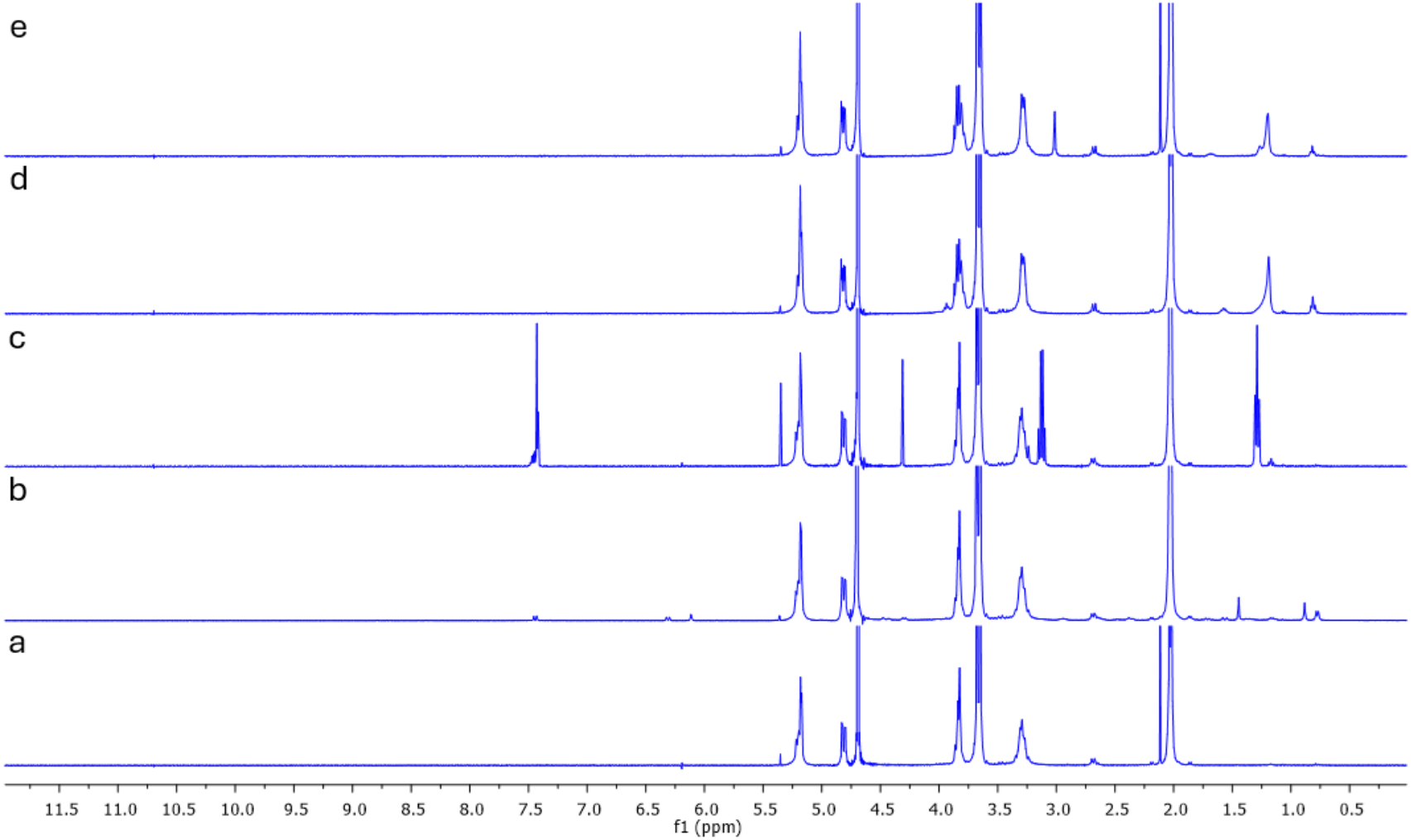
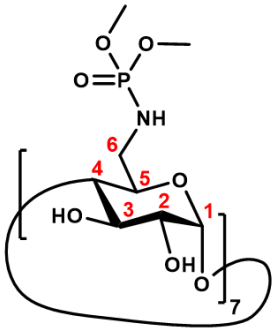


Figure S1: ^{1}H NMR Spectra of compound **6** (spectrum **a**) and inclusion studies with Dex-P (**7**, spectrum **b**), *N*-benzyltriethylammonium chloride (spectrum **c**), sodium dodecyl sulfate (spectrum **d**) and *N*-hexadecyltrimethylammonium bromide (spectrum **e**) in D_2O.

NMR Spectra of compound **4**



4

Figure S2: ^{1}H NMR Spectrum of compound **4** in D_2O.

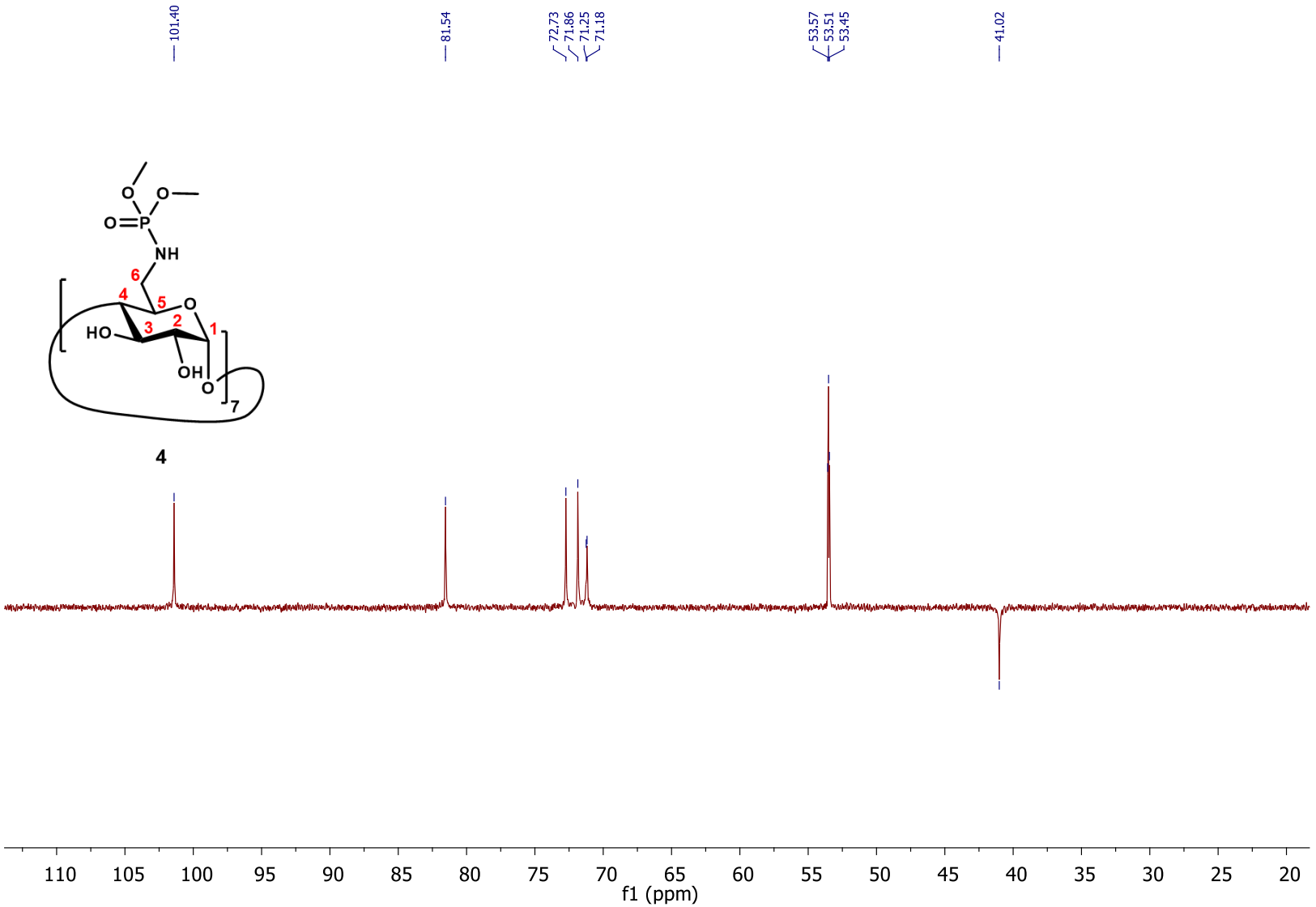


Figure S3: ^{13}C NMR Spectrum of compound **4** in D_2O.

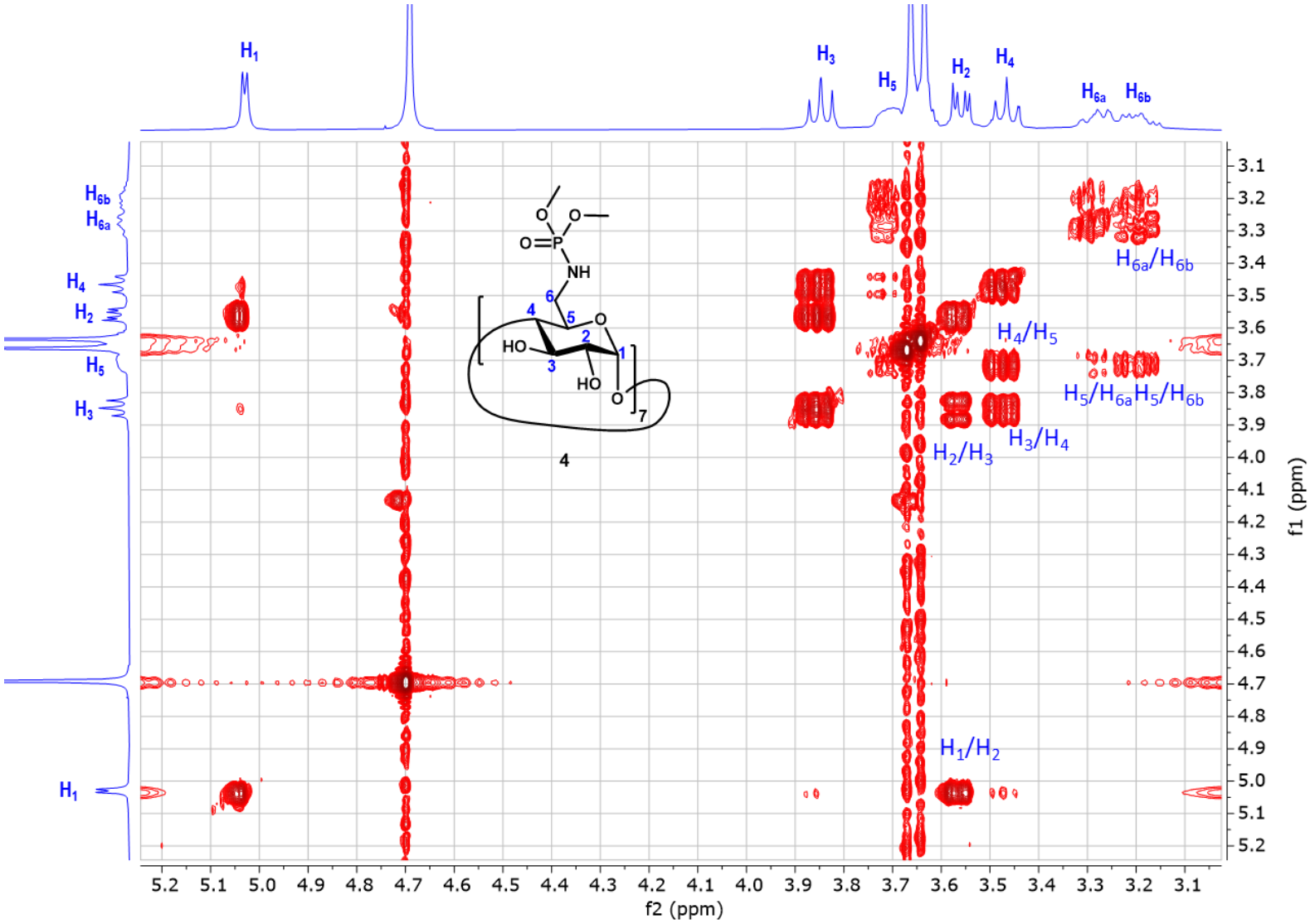


Figure S4: ^{1}H-^{1}H COSY NMR Spectrum of compound **4** in D_2O.

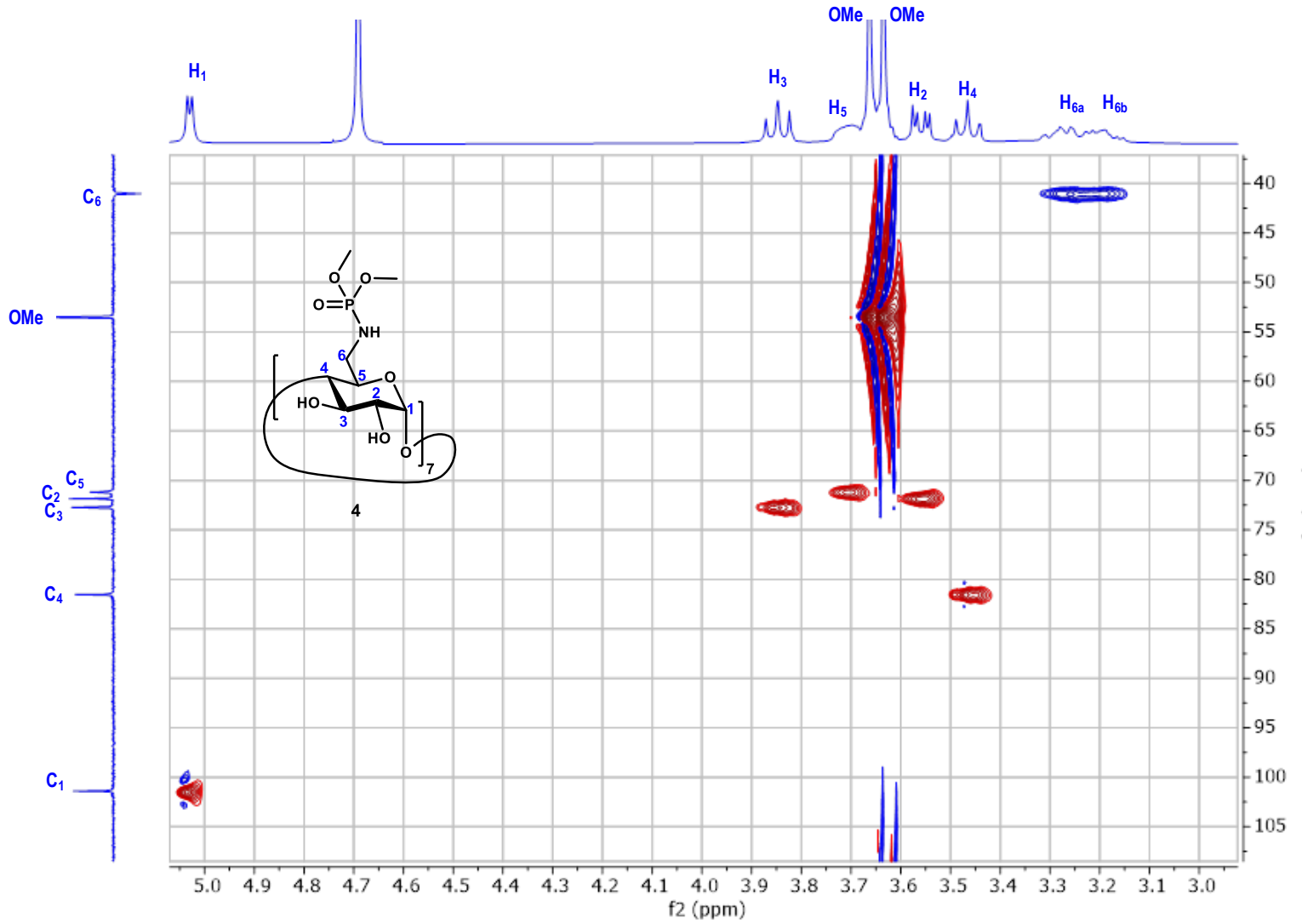


Figure S5: ^{1}H-^{13}C HSQC NMR Spectrum of compound **4** in D_2O.

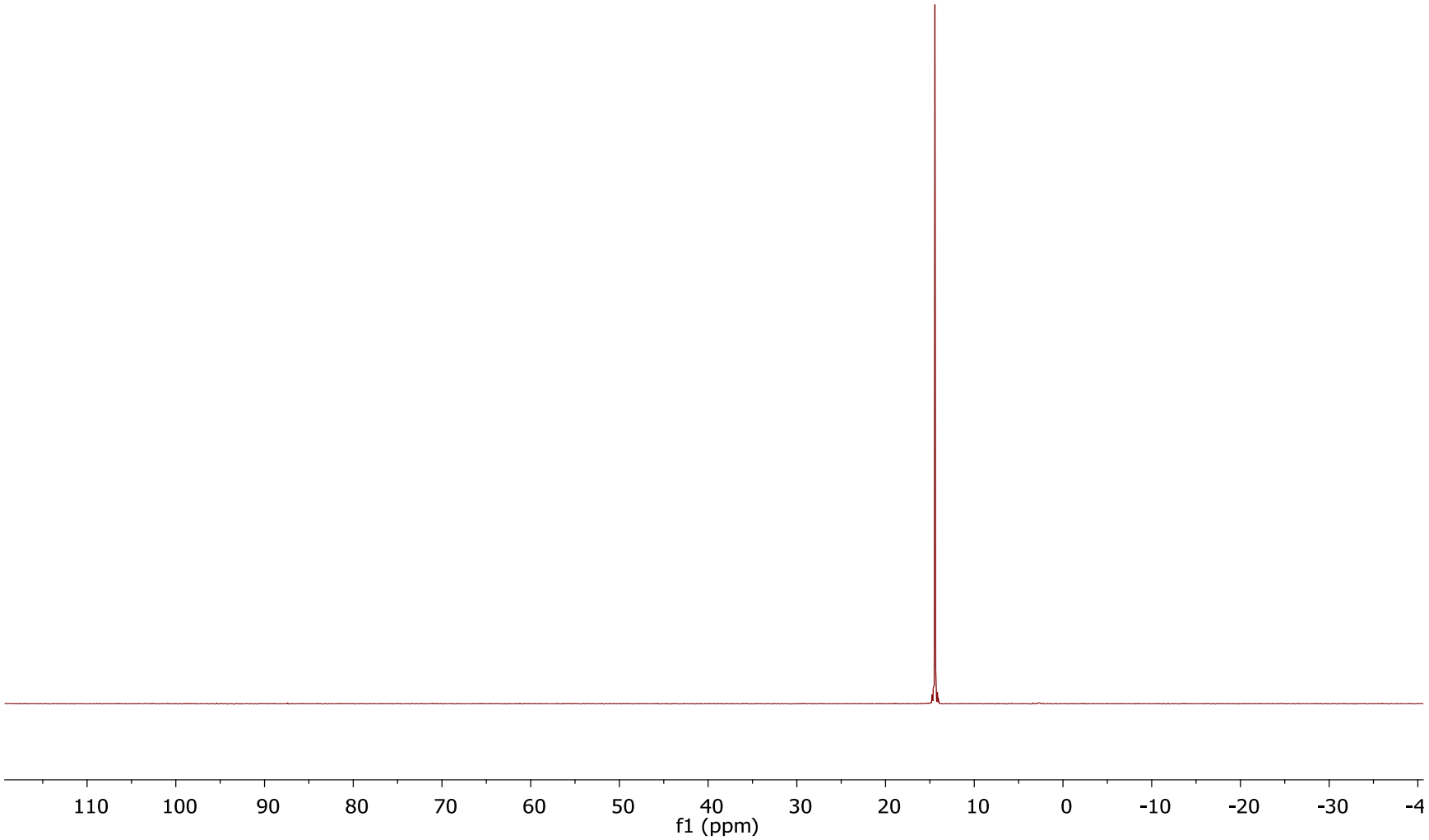


Figure S6: ^{31}P-NMR Spectrum of compound **4** in D_2O.

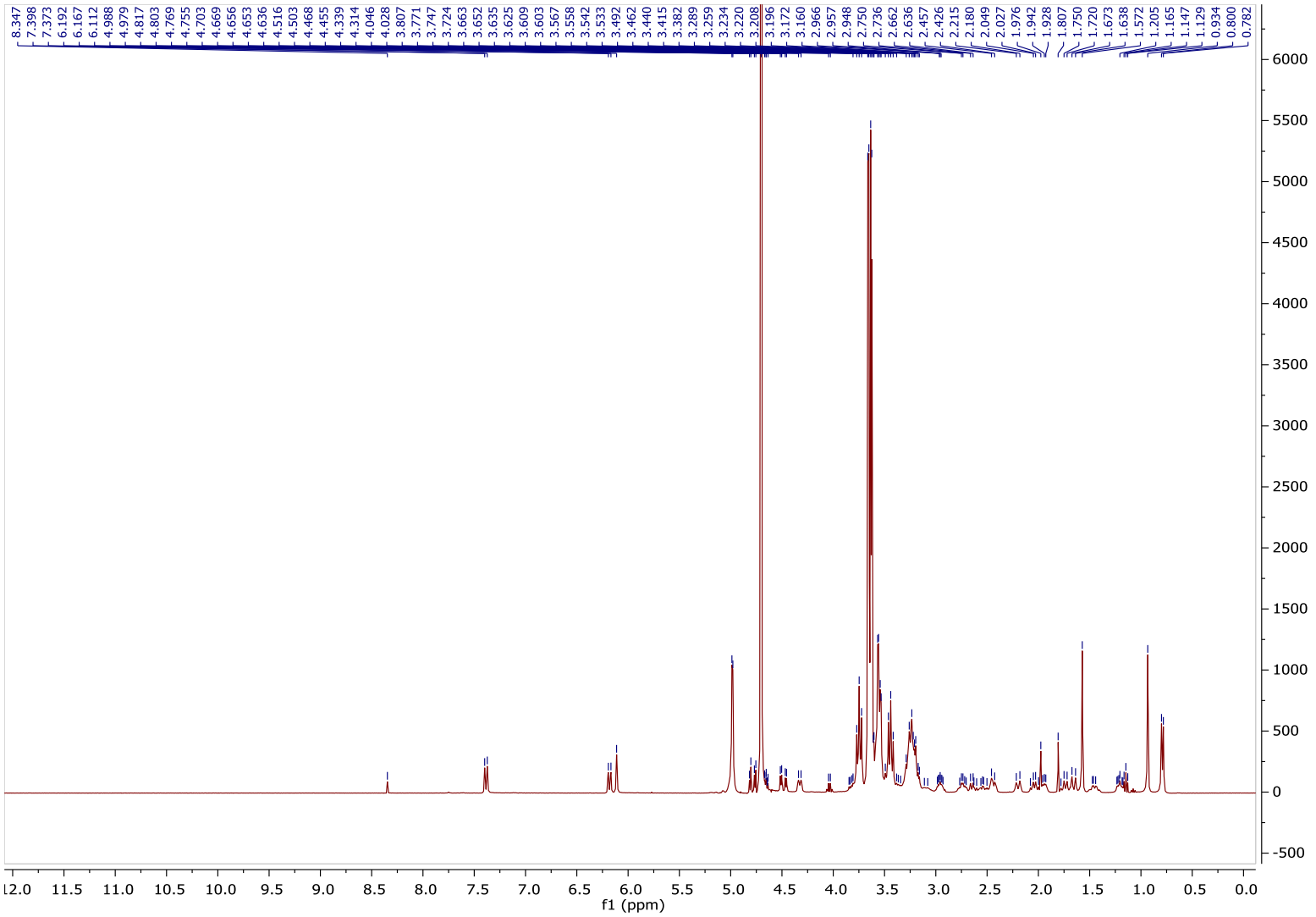


Figure S7: ^{1}H NMR Spectrum of compound **4** + Dexamethasone Sodium Phosphate (Dex-P, **7**) in D_2O.

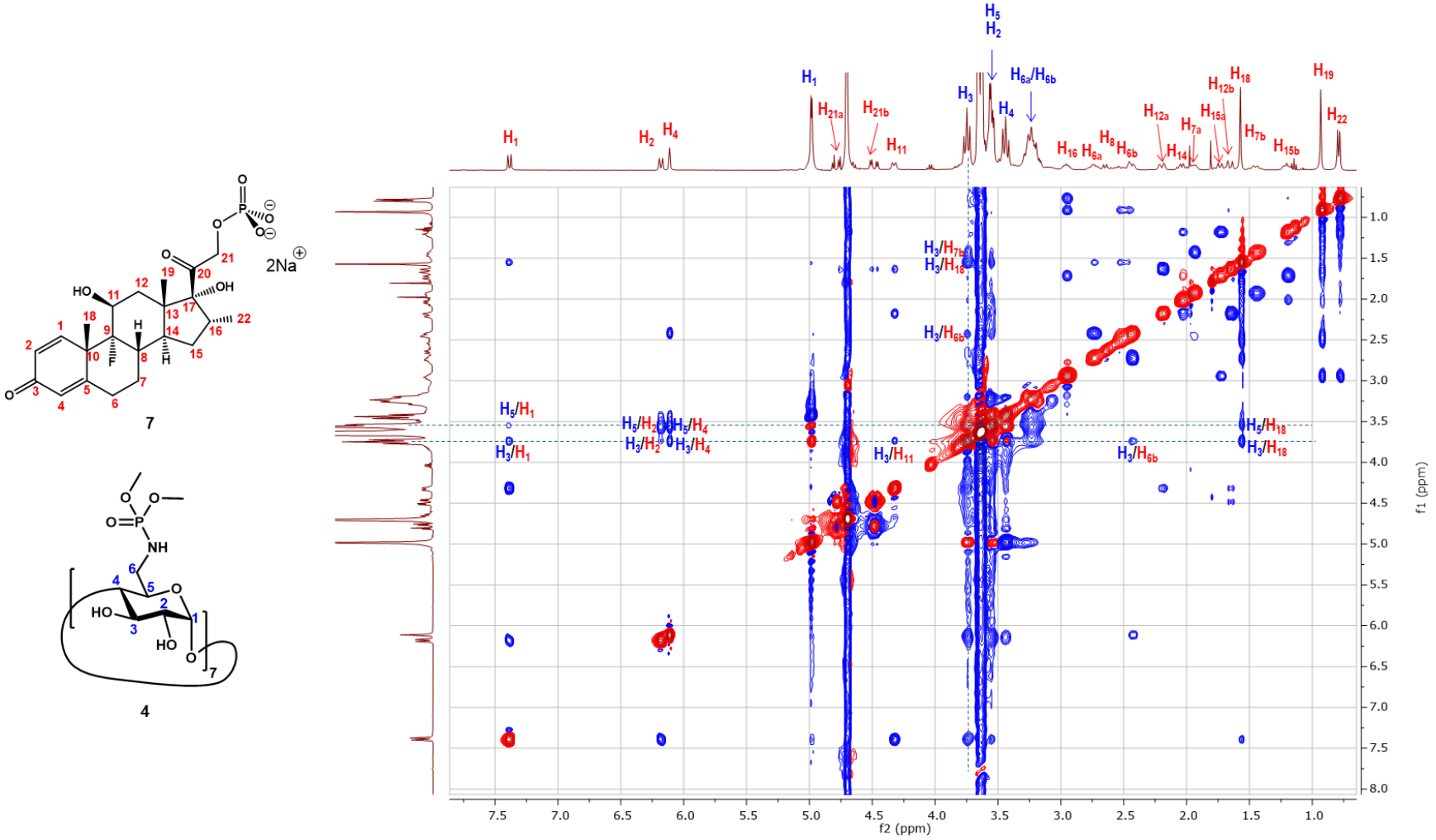


Figure S8: ^{1}H–^{1}H ROESY Spectrum of compound **4** + Dexamethasone Sodium Phosphate (DEX-P, **7**) in D_2O.

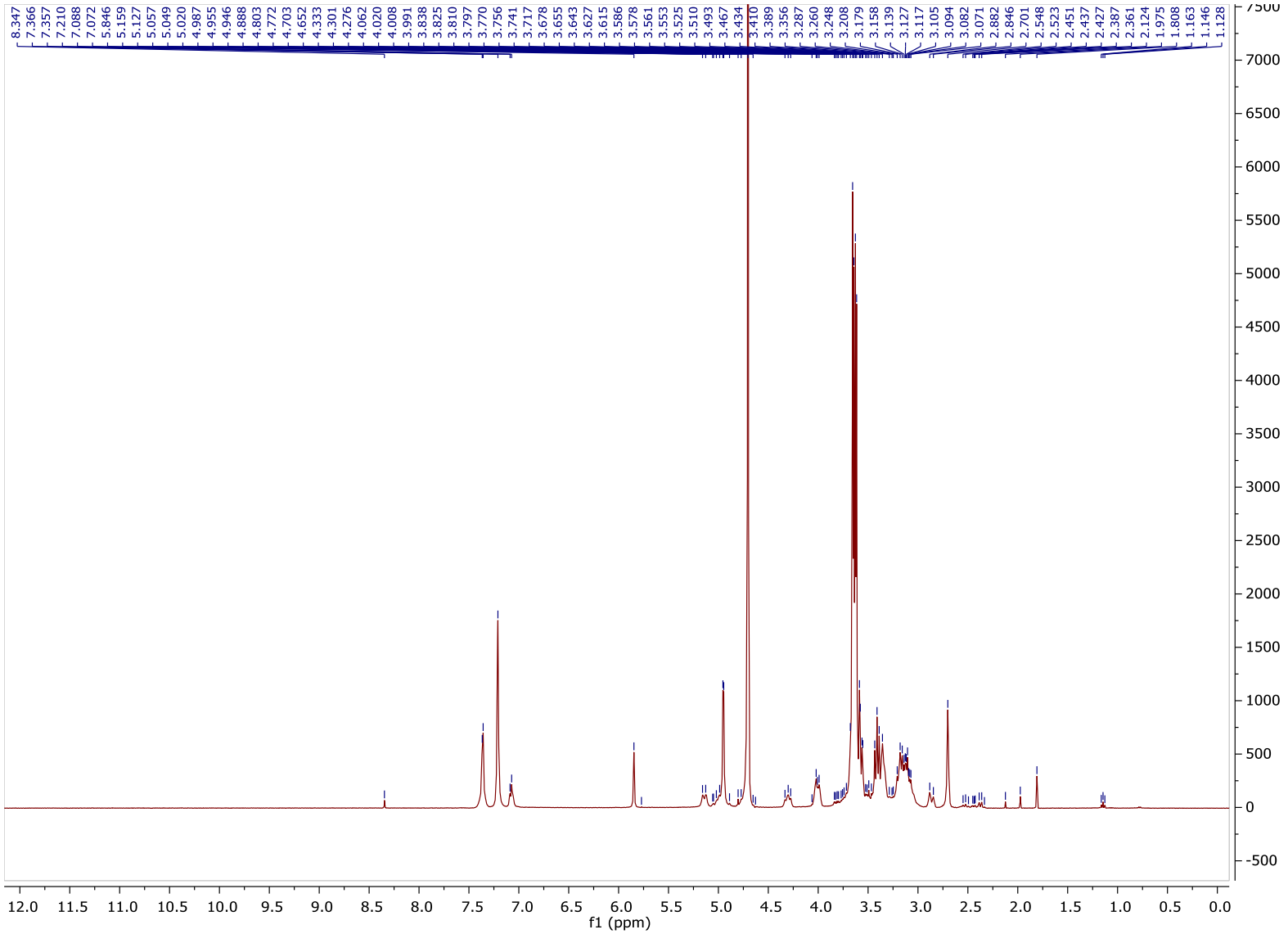


Figure S9: ^{1}H NMR Spectrum of compound **4** + Nefopam HCl (**9**) in D_2O.

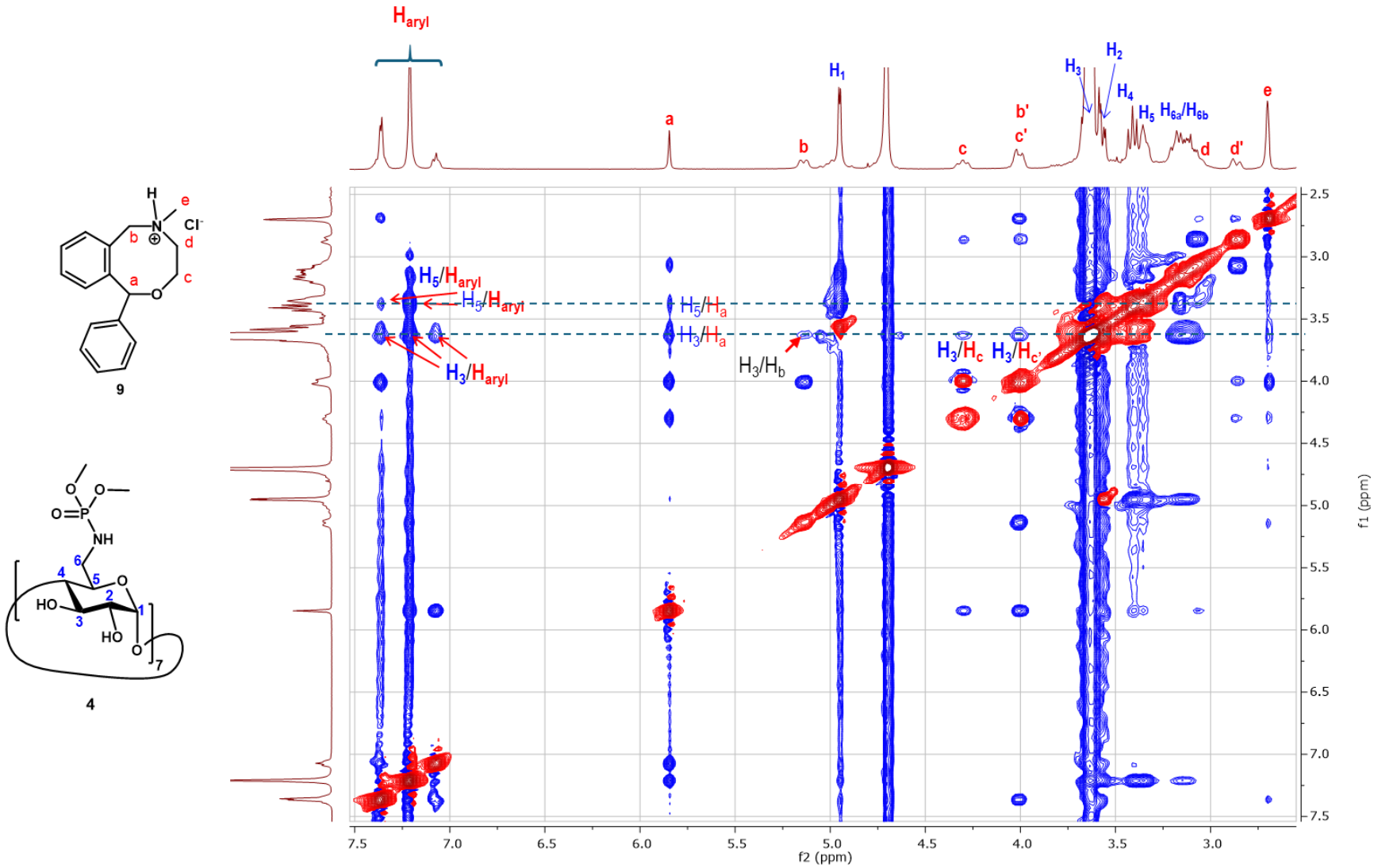


Figure S10: ^{1}H–^{1}H ROESY Spectrum of compound **4** + Nefopam HCl (**9**) in D_2O.

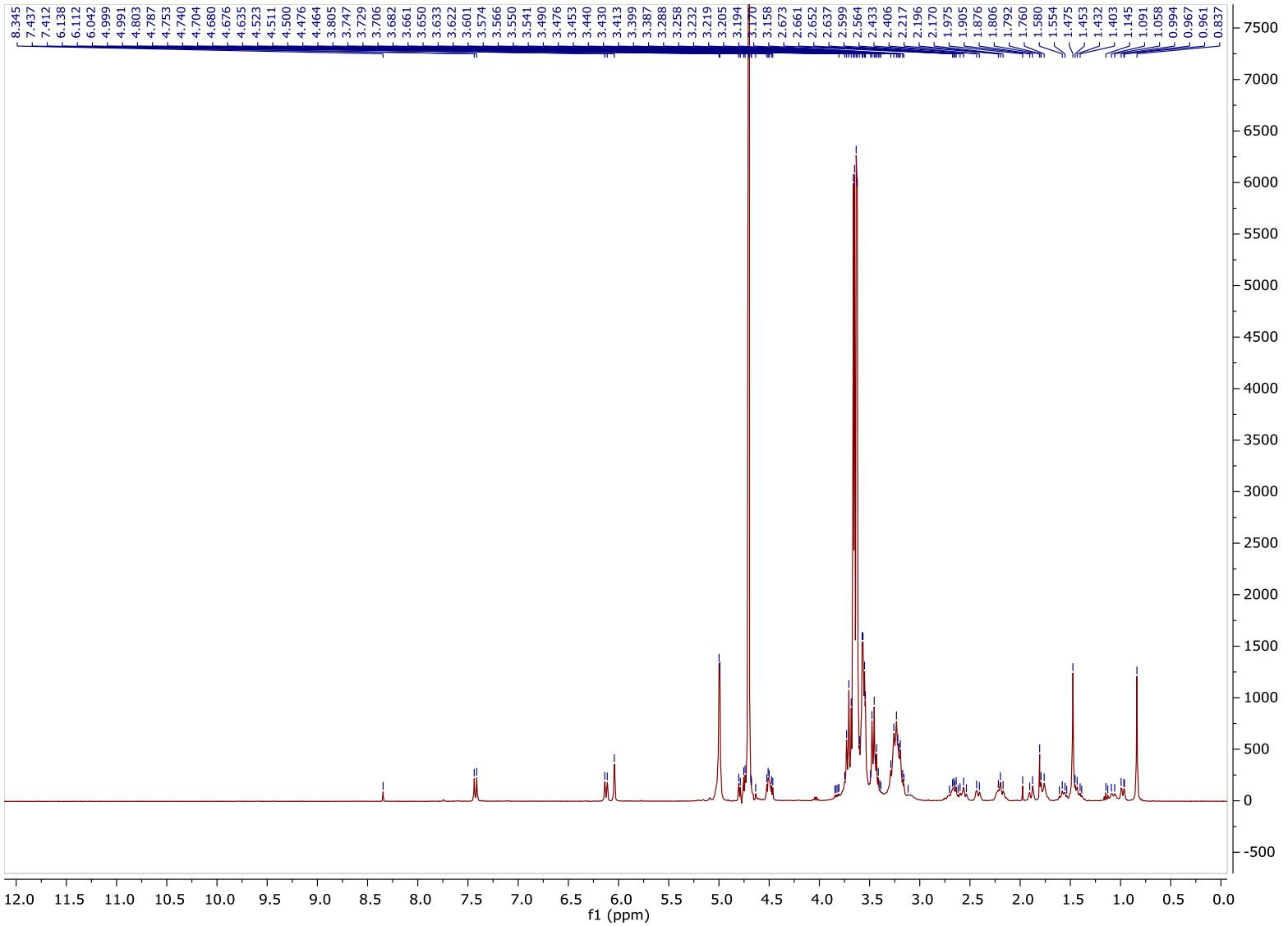


Figure S11: ^{1}H NMR Spectrum of compound **4** + Prednisolone Disodium Phosphate (Prd-P, **8**) in D_2O.

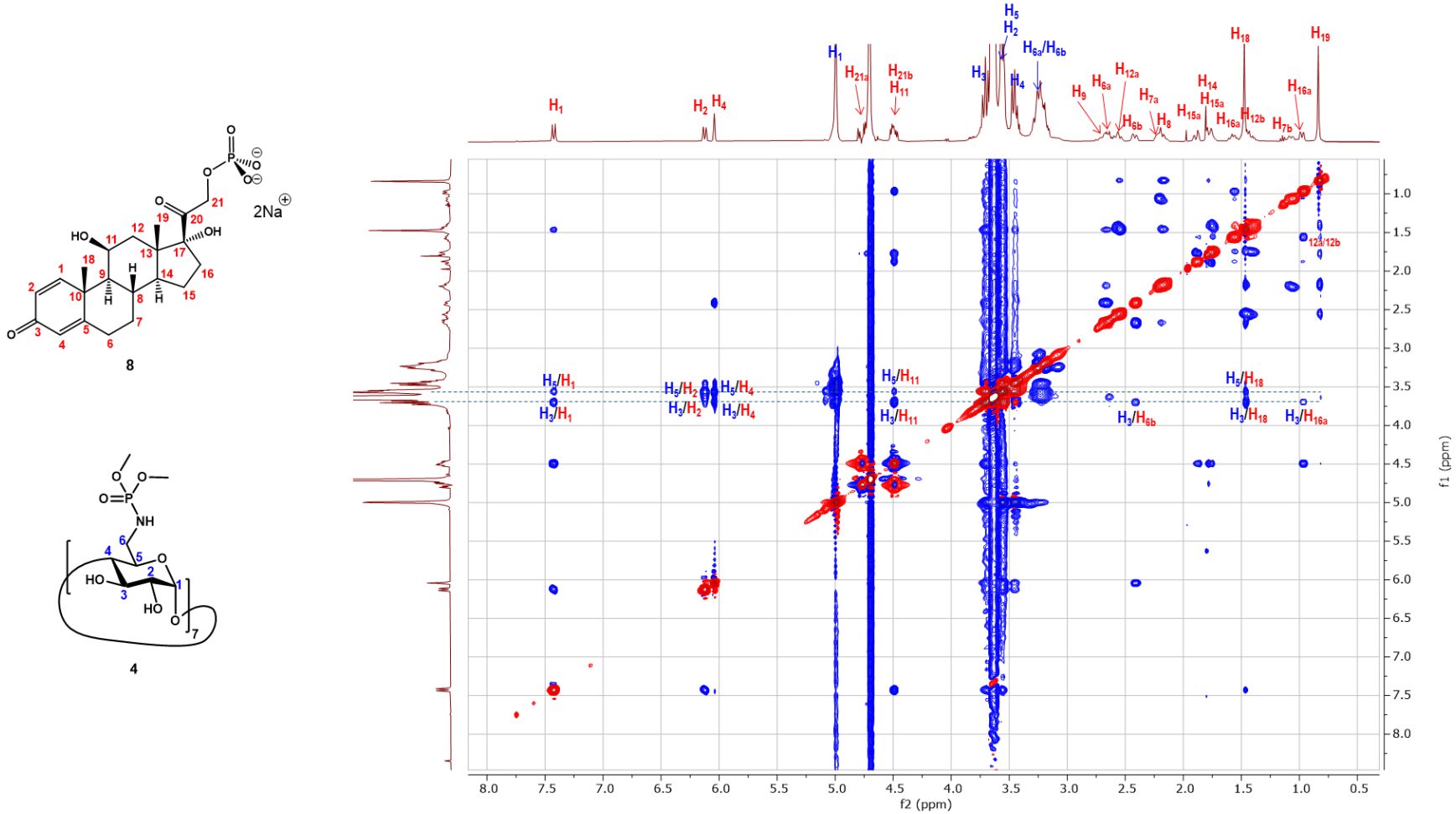


Figure S12: ^{1}H–^{1}H ROESY Spectrum of compound **4** + Prednisolone Disodium Phosphate (**8**) in D_2O.

II. Isothermal Titration Calorimetry (ITC)

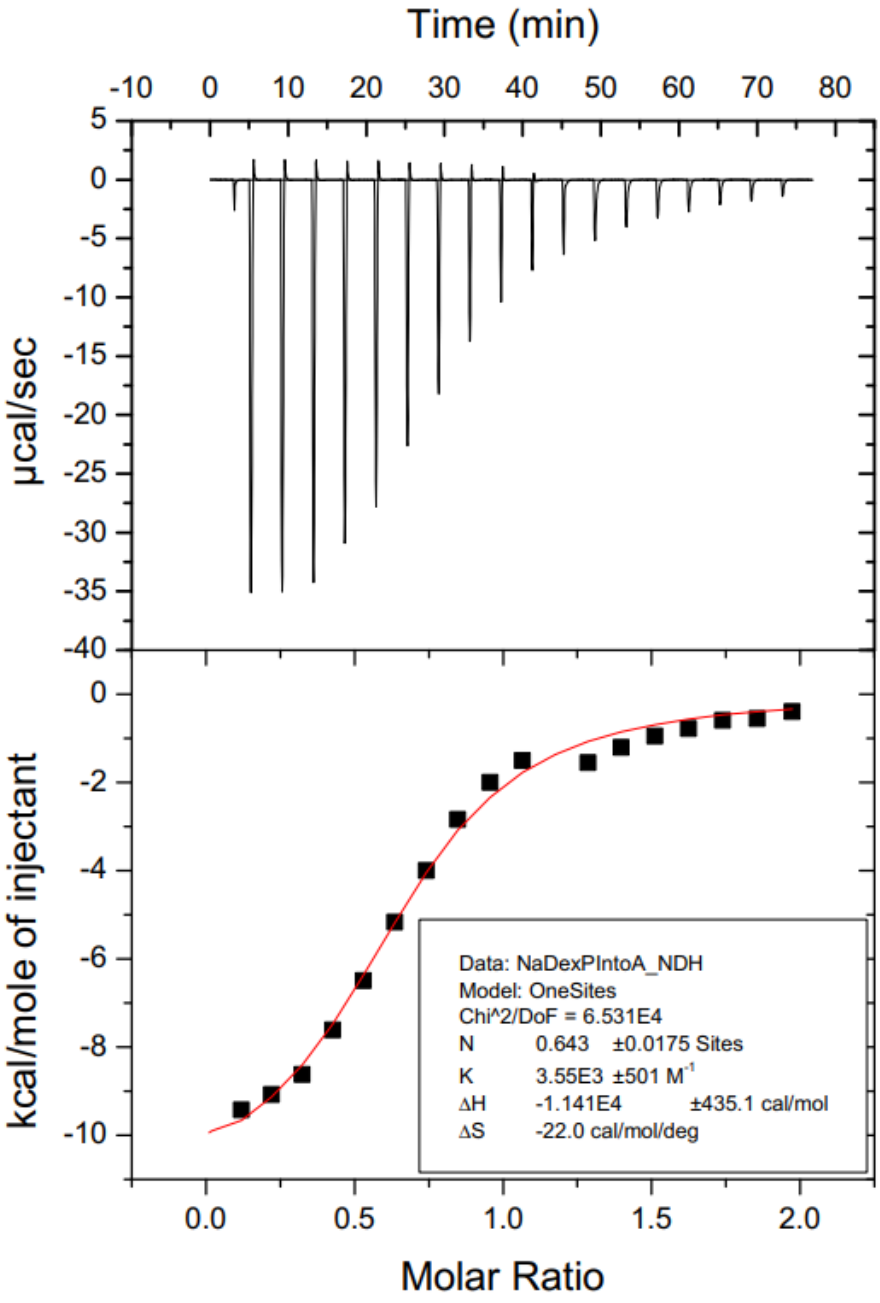


Figure S13: ITC Titration of Dex-P (**7**) into compound **4**.

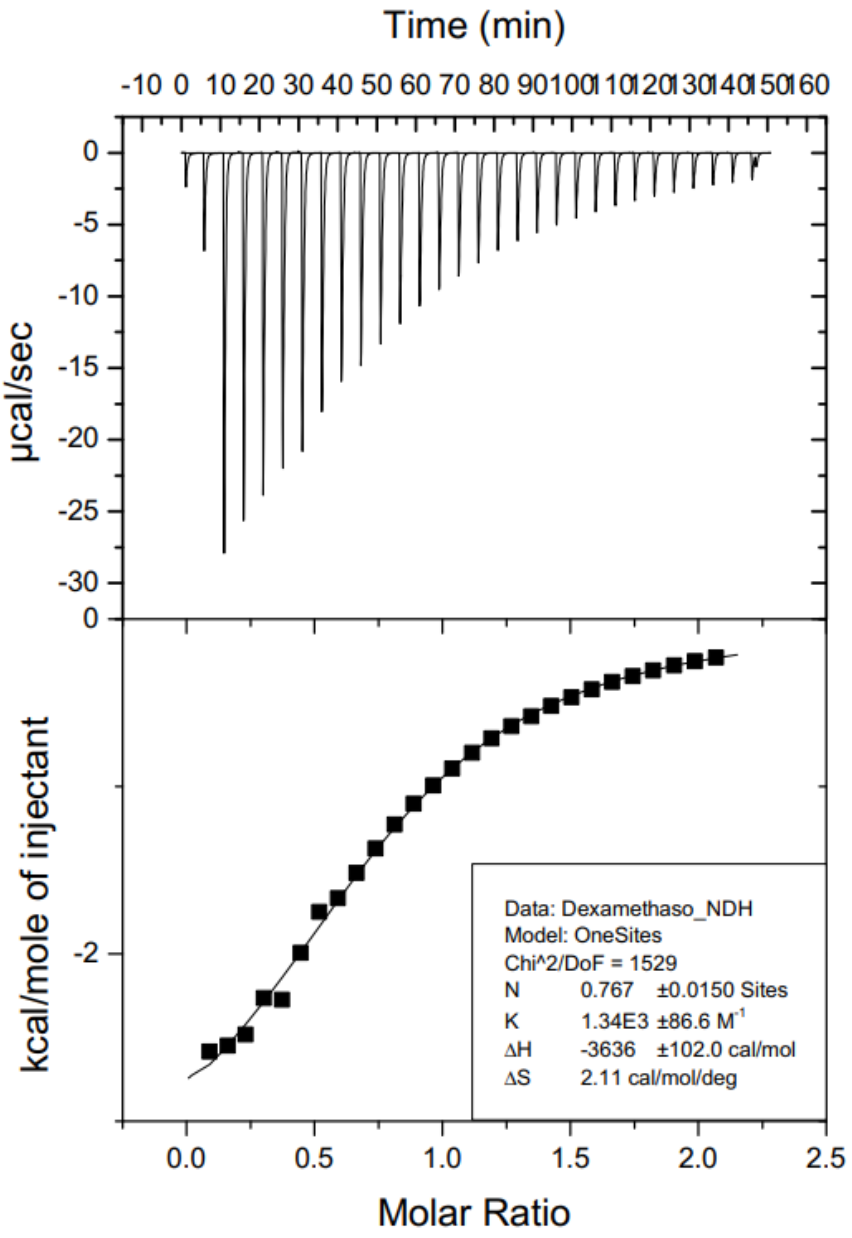


Figure S14: ITC Titration of Dex-P (**7**) into HPBCD (**1**).

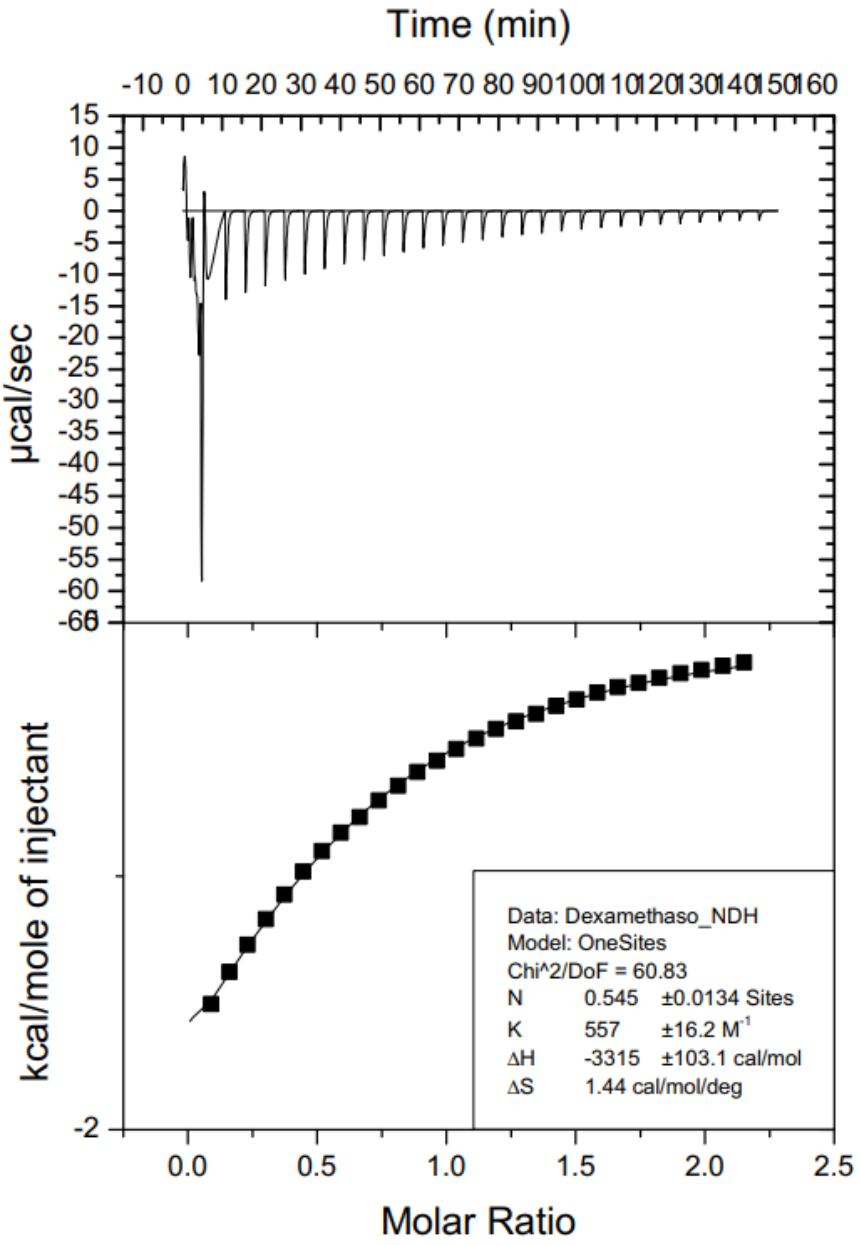


Figure S15: ITC Titration of Dex-P (**7**) into RMBCD (**2**).

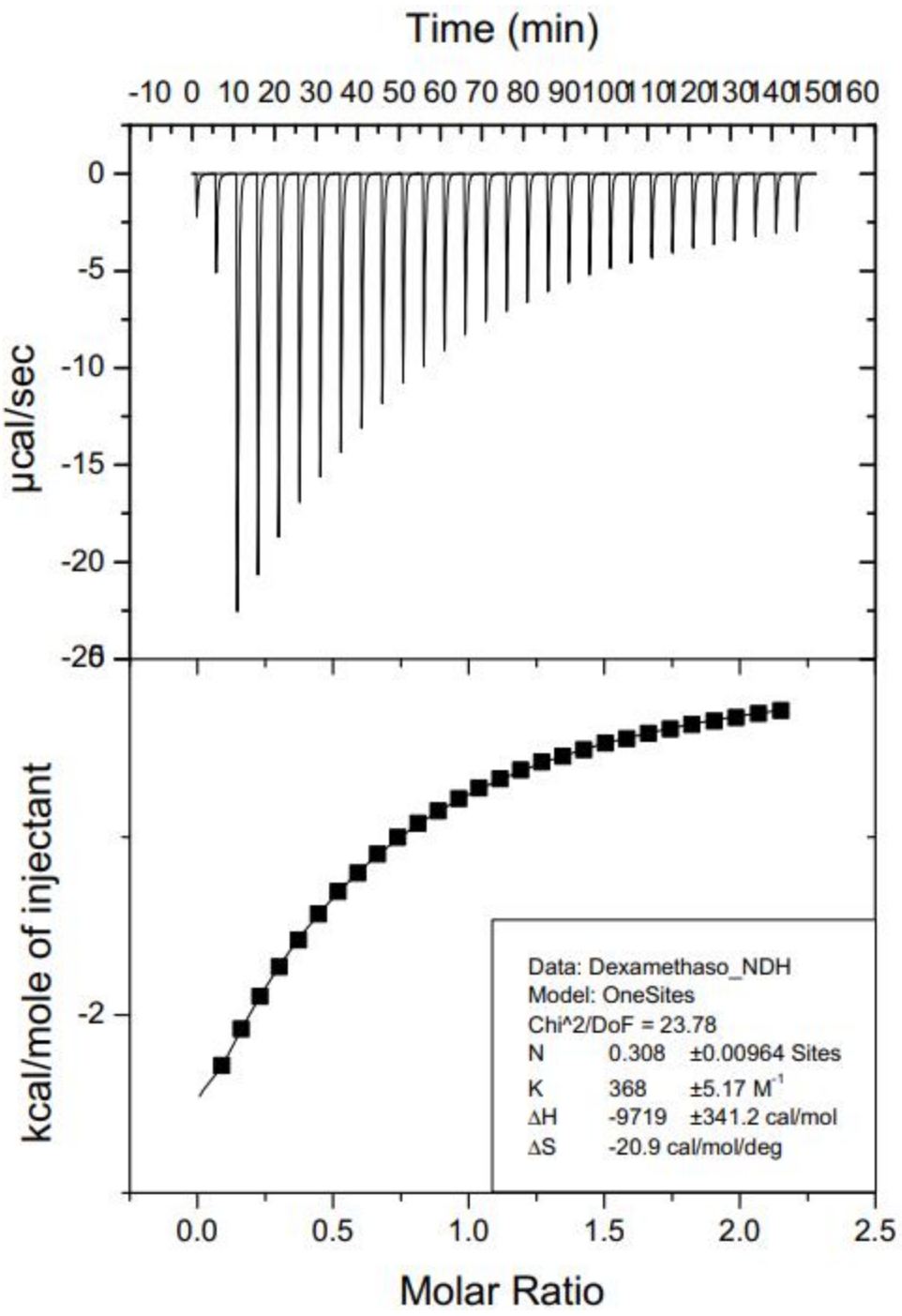


Figure S16: ITC Titration of Dex-P (**7**) into SBEBCD (**3**).

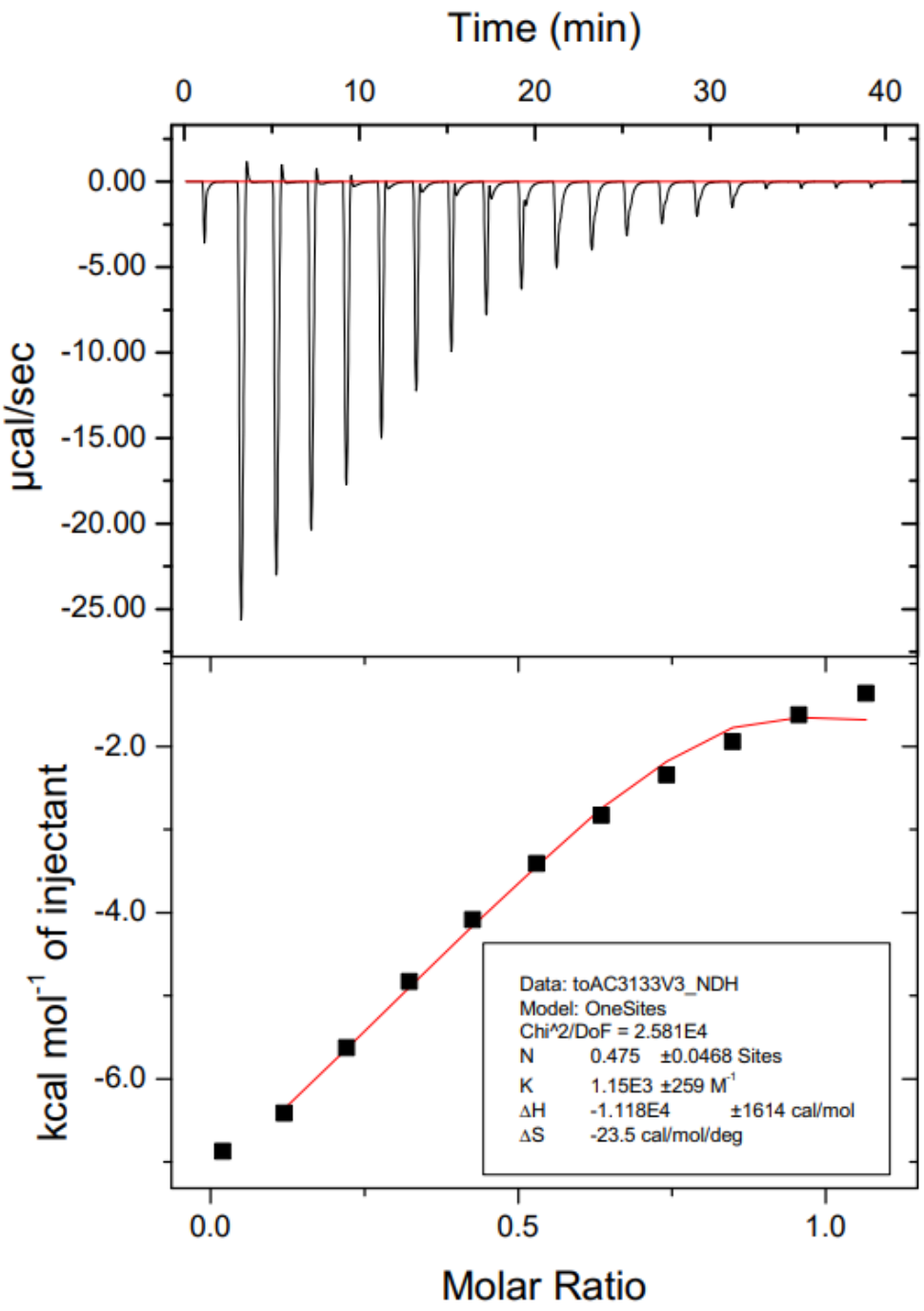


Figure S17: ITC Titration of Prd-P (**8**) into compound **4**.

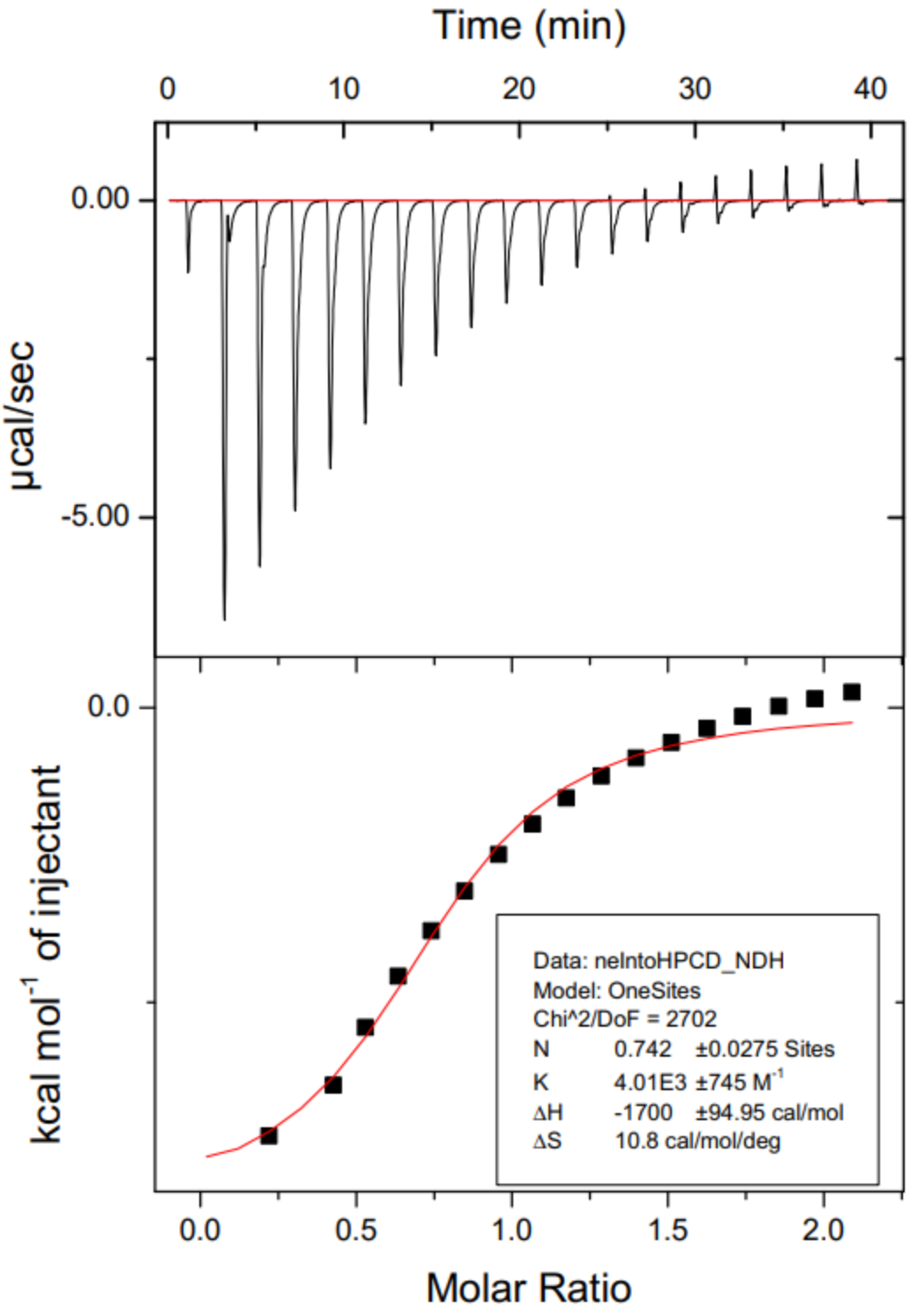


Figure S18: ITC Titration of Prd-P (**8**) into HPBCD (**1**).

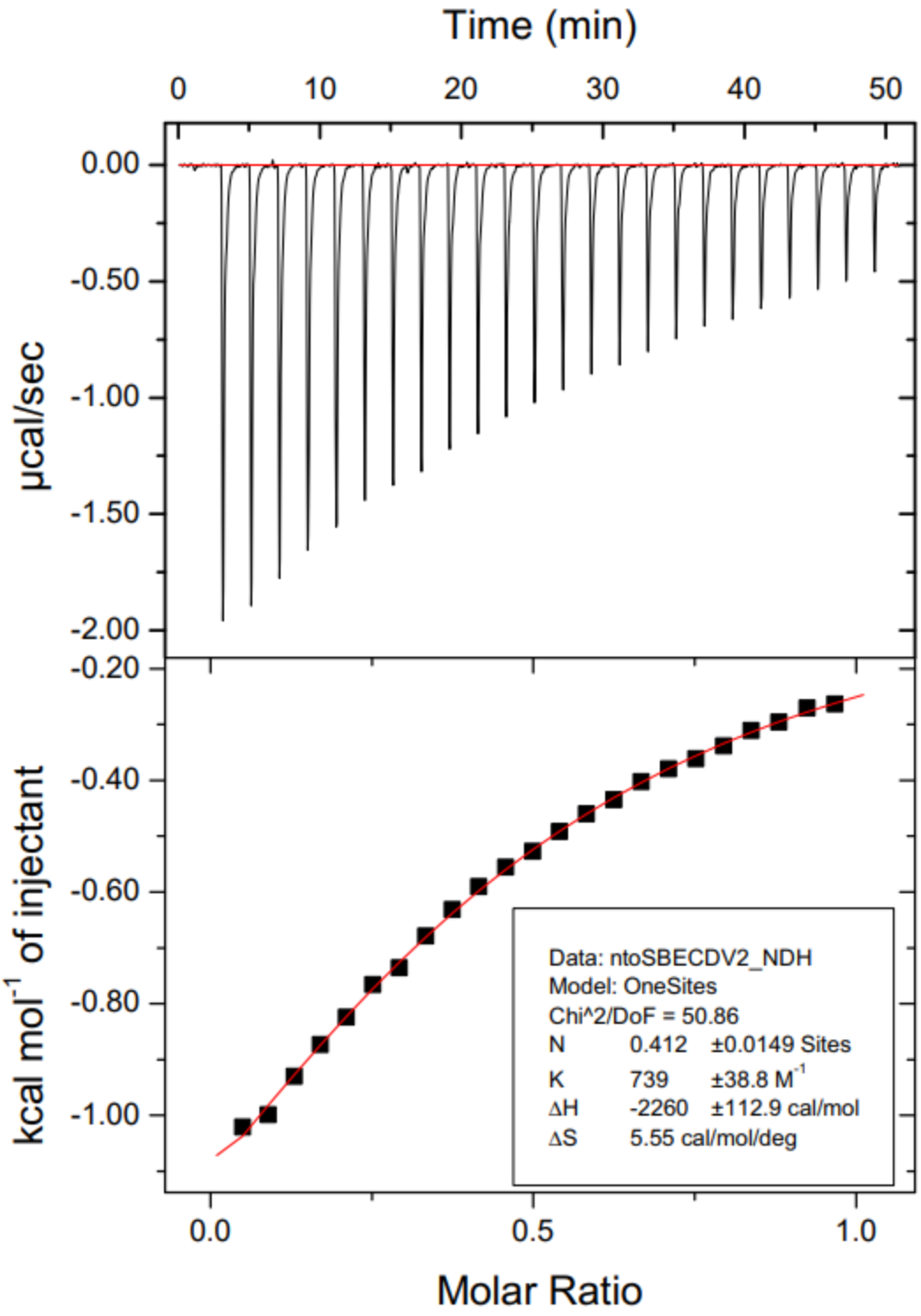


Figure S19: ITC Titration of Prd-P (**8**) into SBEBCD (**3**).

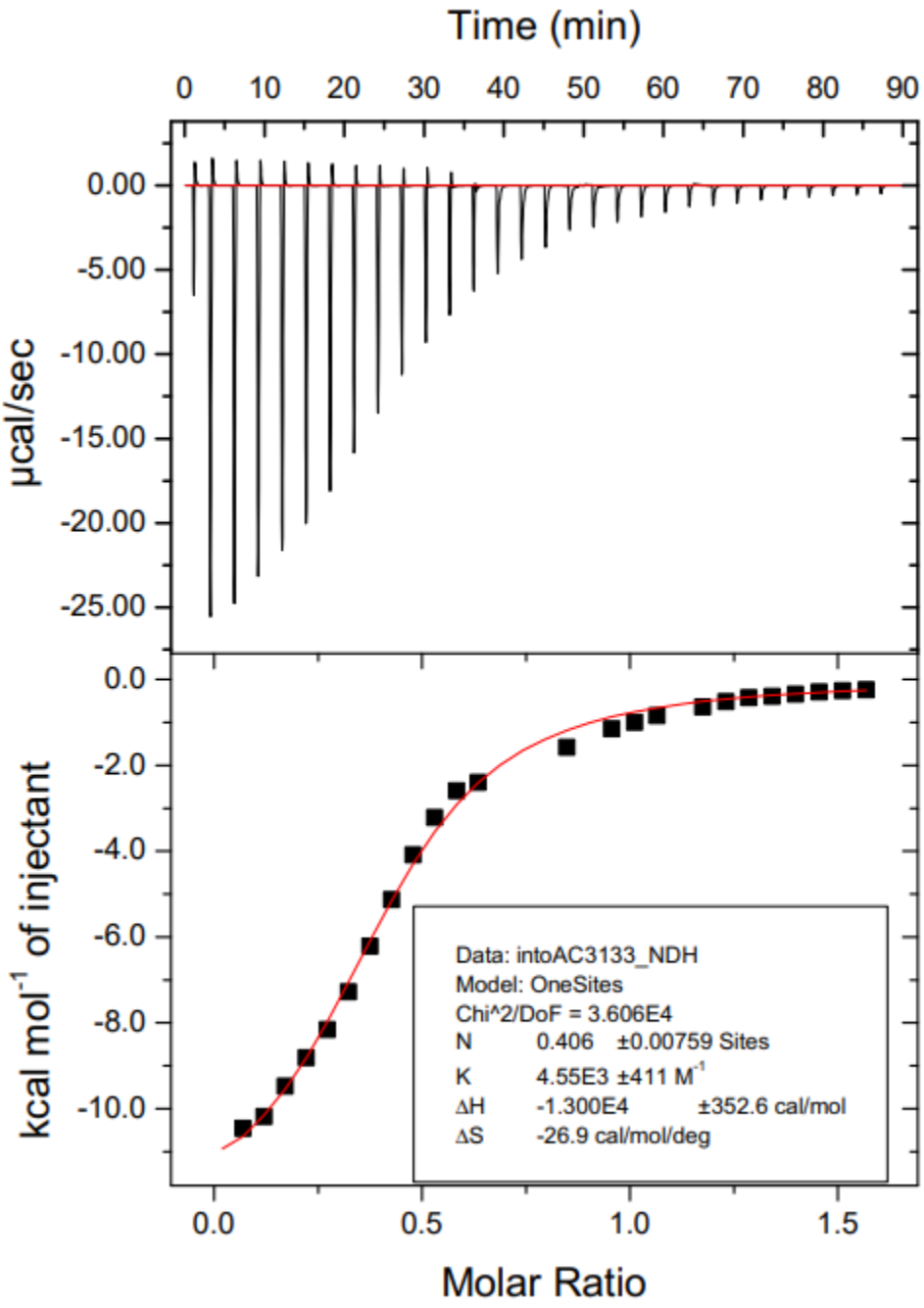


Figure S20: ITC Titration of Nefopam HCl (**9**) into compound **4** .

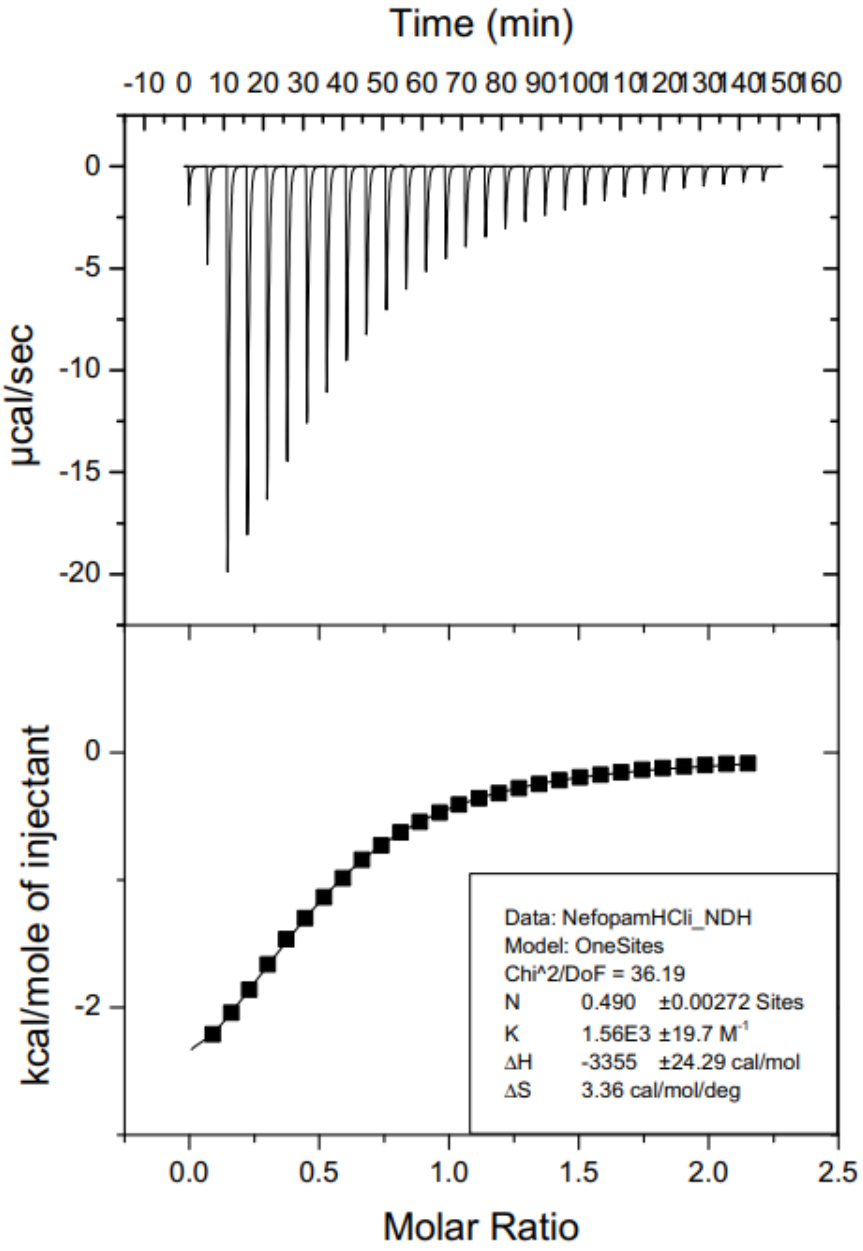


Figure S21: ITC Titration of Nefopam HCl (9) into HPBCD (1).

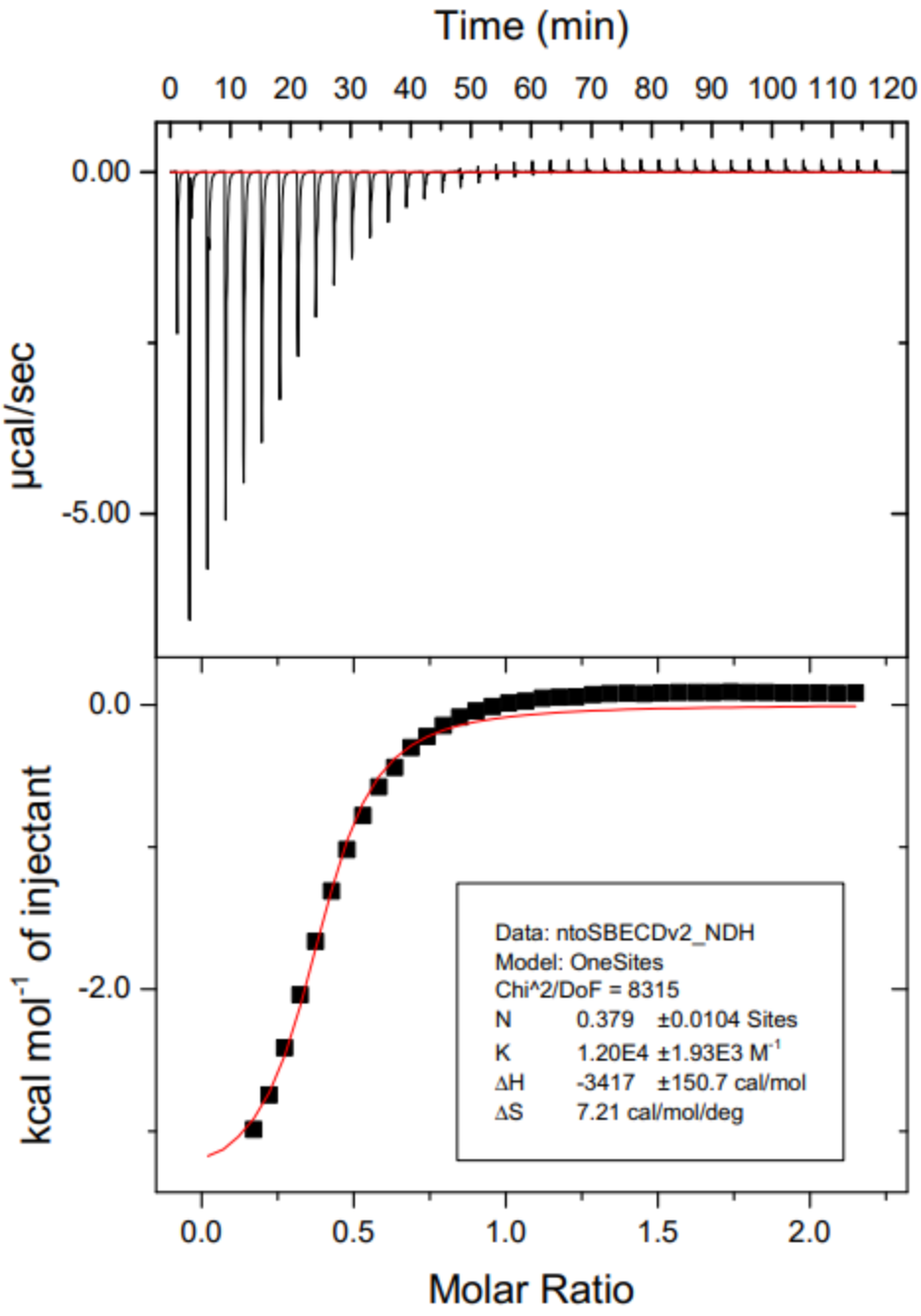


Figure S22: ITC Titration of Nefopam HCl (**9**) into SBEBCD (**3**).

HRMS Spectra

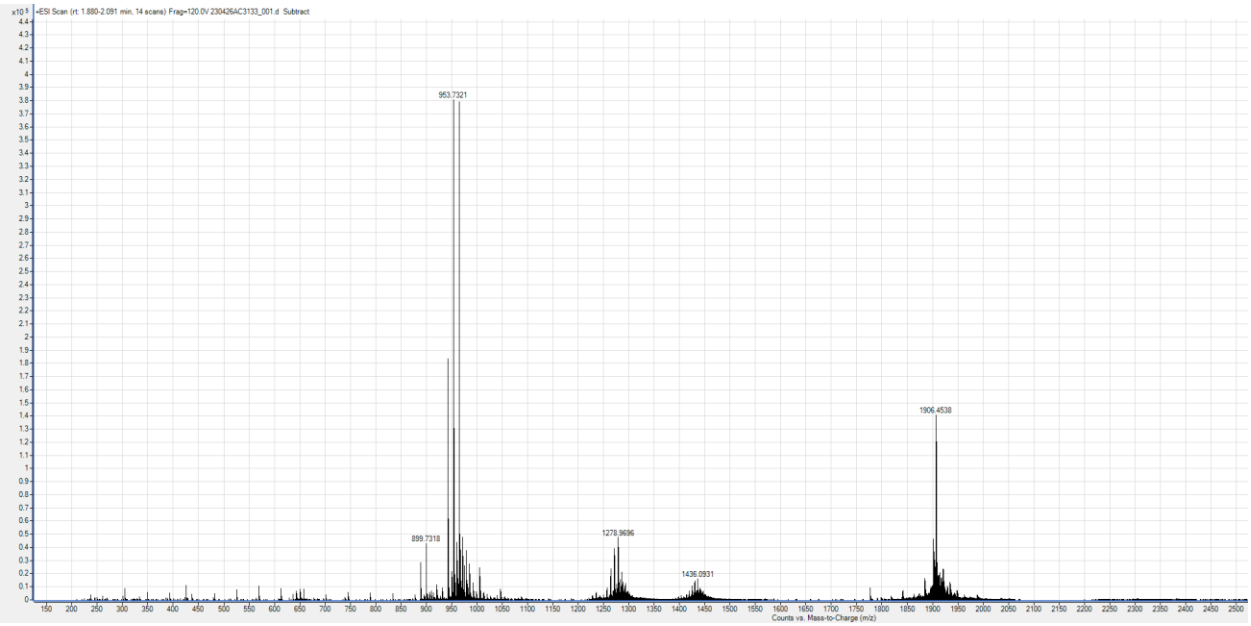


Figure S23: HRMS Spectra of Compound **4**