Supporting Information for

The flight of a cytidine deaminase complex with an imperfect transition state analogue inhibitor: mass spectrometric evidence for the presence of a trapped water molecule

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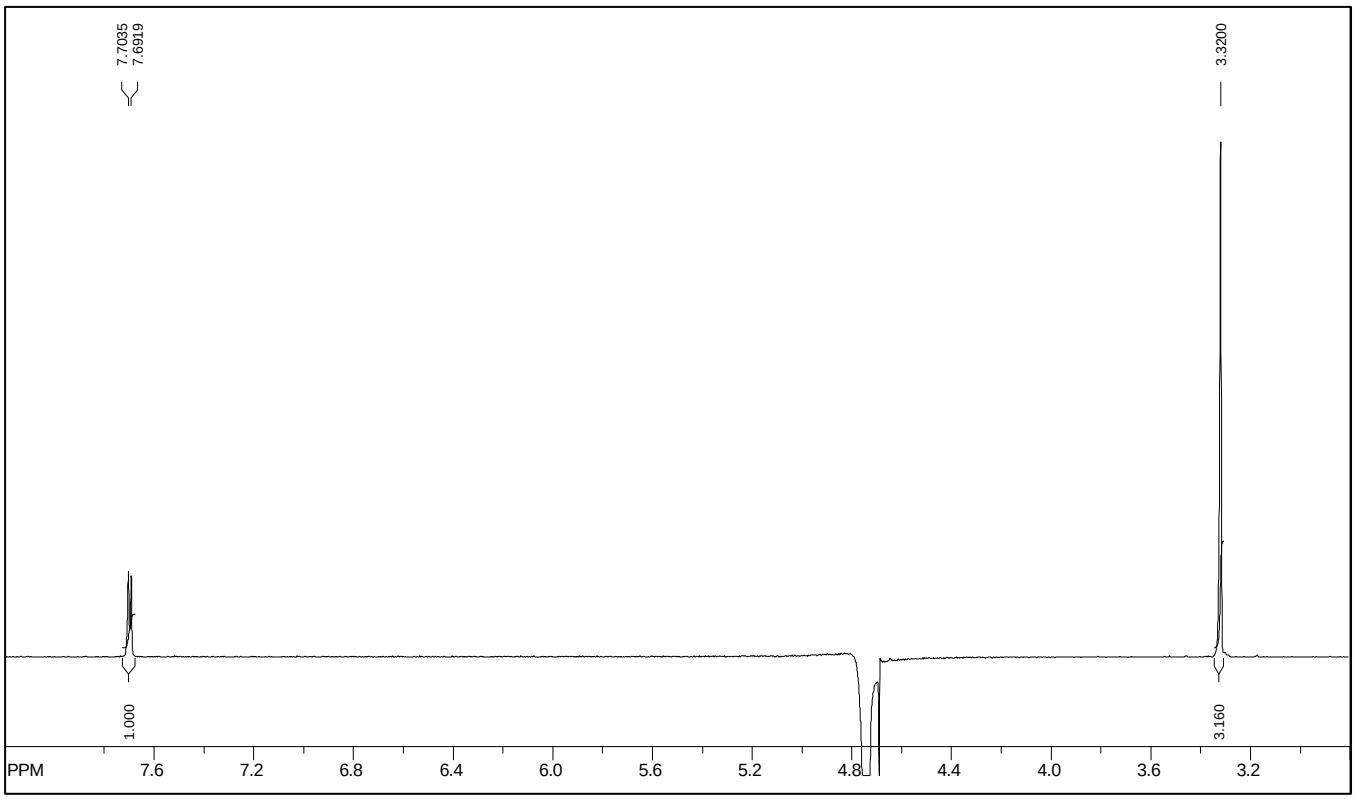
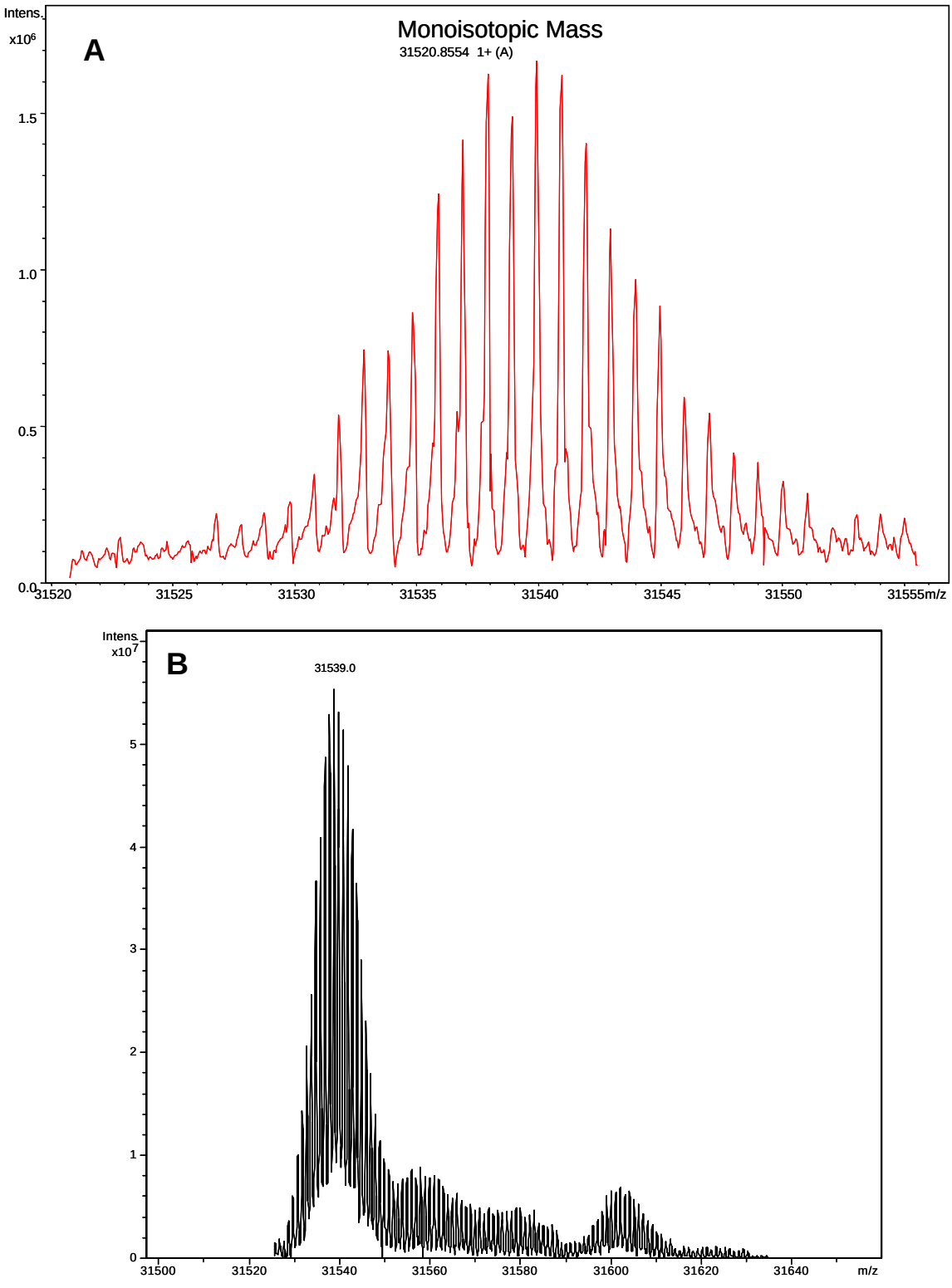
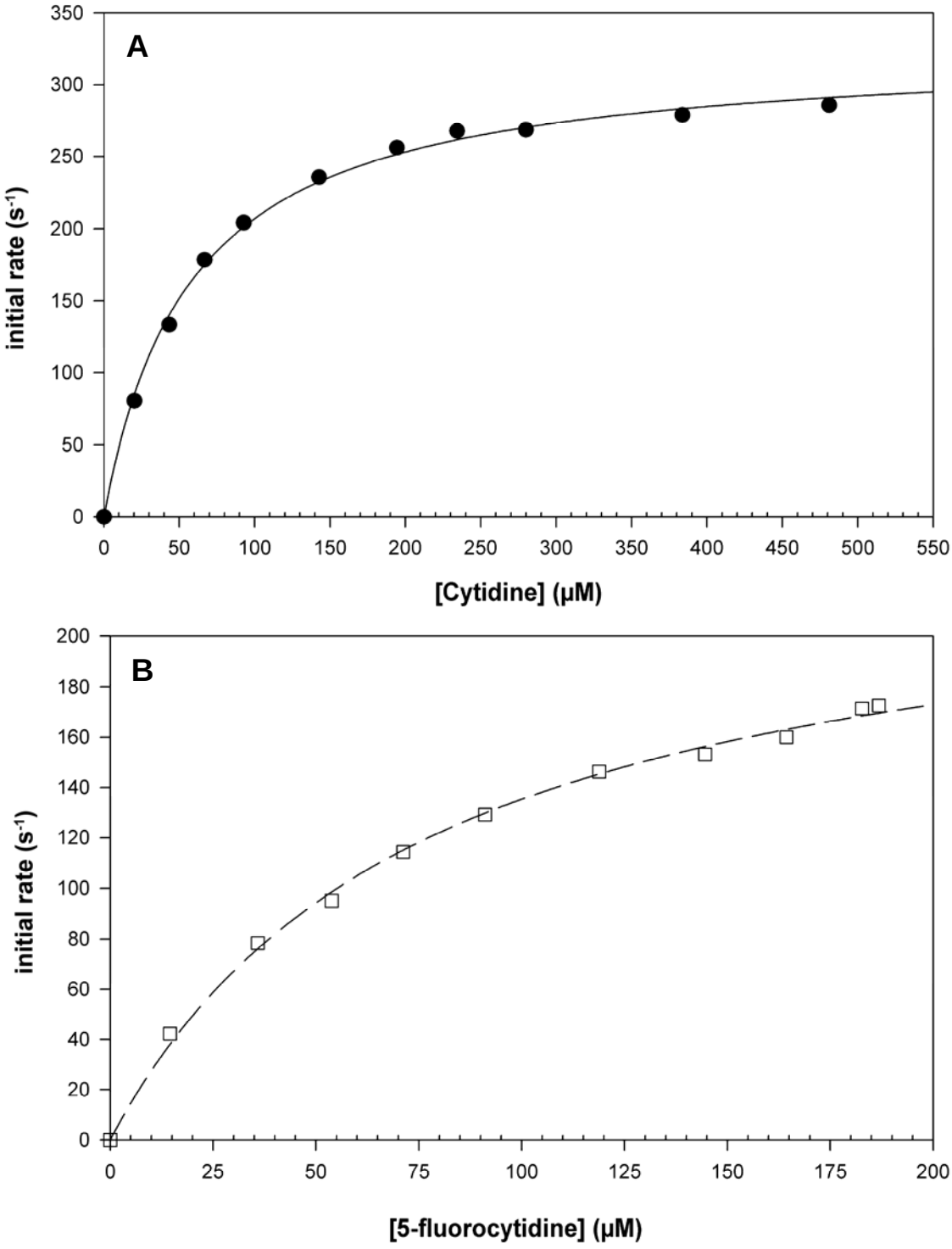
Additional ^{1}H NMR and MS spectra, along with Michaelis-Menten plots, uncatalyzed kinetic time course data, van't Hoff plots and ITC results are included herein. This material is available free of charge via the Internet at http://pubs.acs.org.



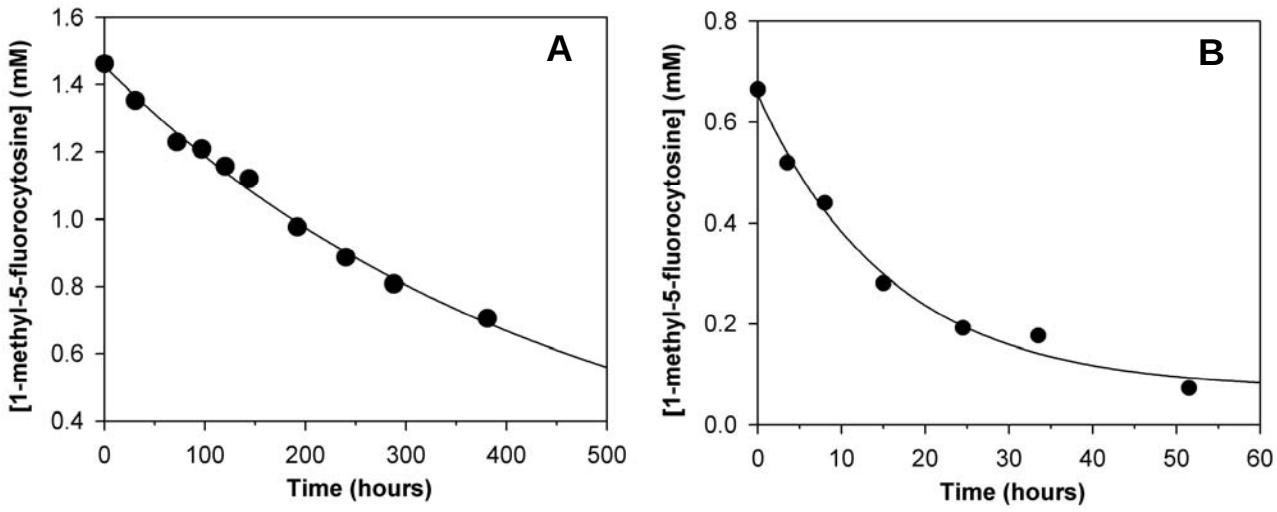
Supporting Information Figure S1. ^{1}H NMR spectrum (500 MHz) of recrystallized 1-*N*-methyl-5-fluorocytosine in D_2O.



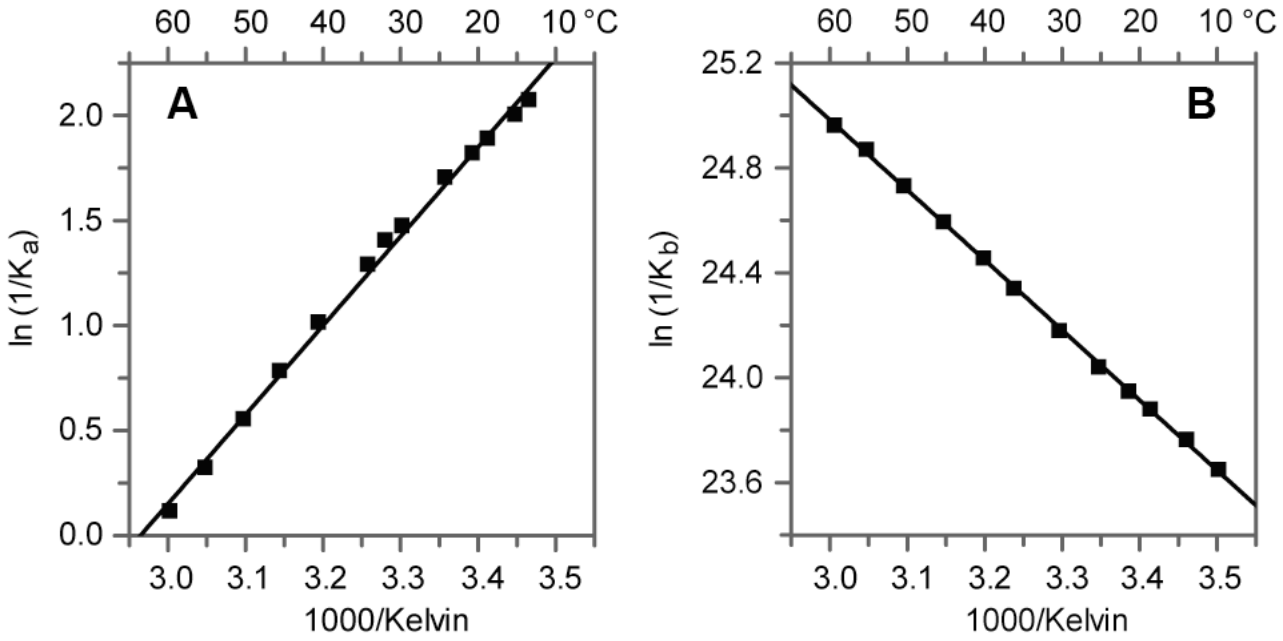
Supporting Information Figure S2. Mass spectrum of the CDA monomer. A) Monoisotopic mass, acquired under denaturing conditions. B) Most abundant isotopic mass, acquired under non-denaturing conditions.



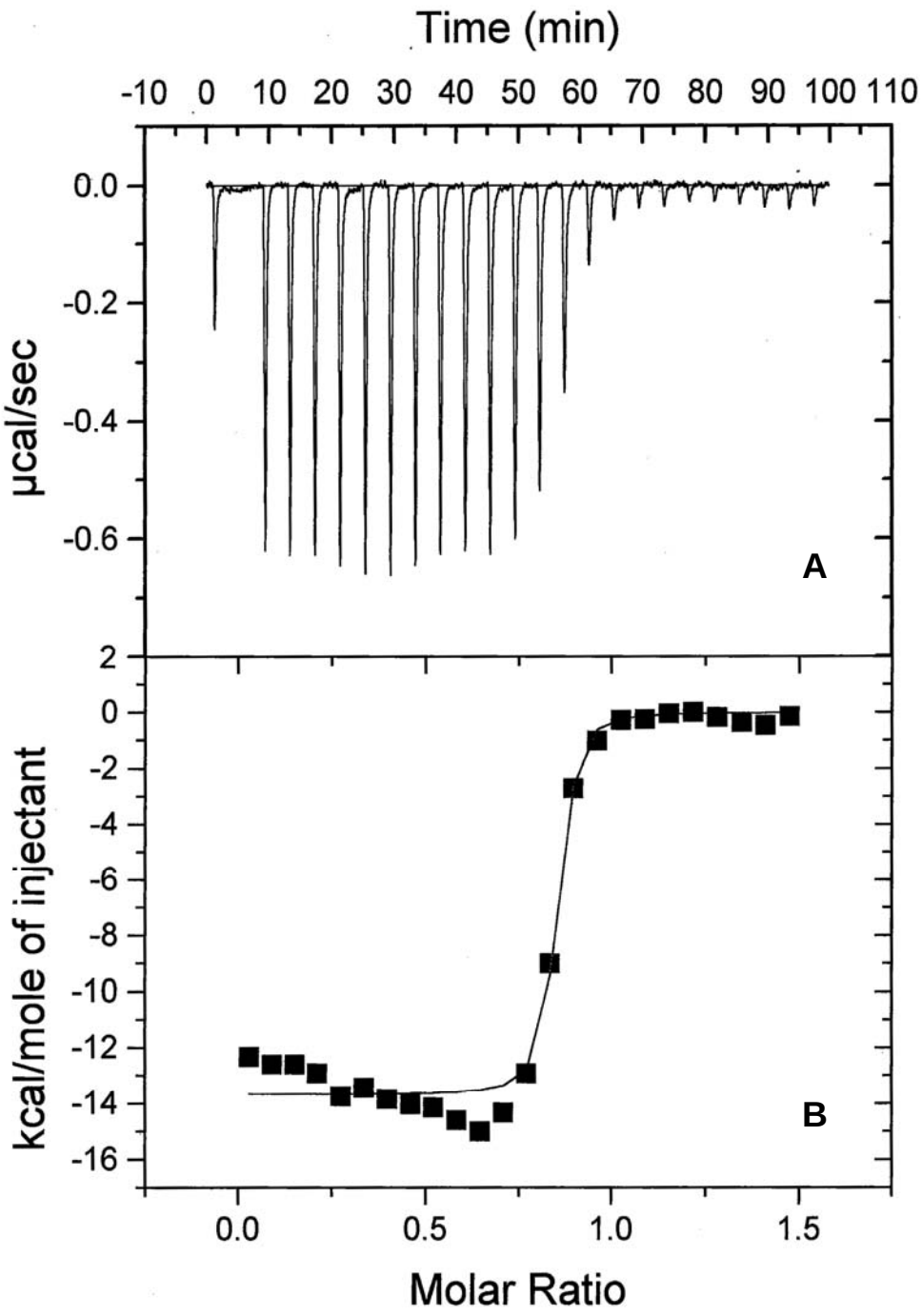
Supporting Information Figure S3. A plot of initial rates for CDA catalyzed deamination versus substrate concentration. (A) Deamination of substrate cytidine fit to the Michaelis-Menten equation (solid line) satisfactorily ($R^2 = 0.99$). B) Deamination of 5-fluorocytidine fit to the Michaelis-Menten equation (dashed line) satisfactorily ($R^2 = 0.99$).



Supporting Information Figure S4. A plot of 1-*N*-methyl-5-fluorocytosine concentration versus time at high temperature under neutral conditions. A) Data collected at 98 °C followed first order exponential decay satisfactorily (R^2 = 0.99). B) Data collected at 140 °C followed first order exponential decay satisfactorily (R^2 = 0.99).



Supporting Information Figure S5. van't Hoff plots of the equilibrium constants for (A) proton dissociation from 5-fluoro-1-methyl-2-oxopyrimindine and (B) addition of hydroxide ion to the 5-fluoro-1,3-dimethyl-2-oxopyrimindinium cation, both obtained from the temperature dependence of their respective pK_a values.



Supporting Information Figure S6. Isothermal calorimetric titration of cytidine deaminase with FZeb at 25 °C in phosphate buffer (0.10 M, pH 7). (A) Heat effects associated with each injection after baseline correction. (B) Integrated heats (■) fitted to a one-site binding model (solid line, best fit curve).