

Supplementary Information

Thymidylate Synthase Catalyzed H-transfers: Two Chapters in One Tale

Zhen Wang and Amnon Kohen*

Department of Chemistry, University of Iowa, Iowa City, IA 52242

*Author to whom correspondences should be addressed. E-mail: amnon-kohen@uiowa.edu Phone #: 319-

335-0234

Data Tables:

Table S1: Observed V/K KIEs presented in Figure 2B in the main text.

Temperature °C	Observed H/T KIE	Observed D/T KIE
5	2.08±0.01	1.46±0.01
15	2.22±0.02	1.440±0.007
25	2.236±0.006	1.38±0.01
35	2.102±0.007	1.31±0.01

This table presents the observed H/T and D/T KIEs on the proton transfer catalyzed by TSase, obtained from the competitive KIE experiments. The experimental details have been described in the main text.

Table S2: Intrinsic KIEs presented in Figure 2B in the main text.

Temperature °C	Intrinsic KIE (H/T)	Intrinsic KIE (H/D)	Intrinsic KIE (D/T)
5	16.3±1.3	6.9±0.4	2.30±0.06
15	10.2±0.7	5.0±0.2	2.00±0.04
25	6.2±0.7	3.5±0.3	1.72±0.06
35	3.8±0.4	2.5±0.2	1.49±0.05

This table presents the intrinsic KIEs (H/T, H/D, and D/T) on the proton transfer catalyzed by TSase. These values are calculated from the observed KIE data (Table S1) using Northrop's method as described in the main text. The errors are calculated at 95% confidence level.