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Supporting Information

Probing Reversible Chemistry in Coenzyme B₁₂-Dependent Ethanolamine Ammonia Lyase with Kinetic Isotope Effects

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Table S1. Tabulated proton inventory data from Figure 2.

n	$k_{\text{obs } 1} \text{ (s}^{-1}\text{)}$	$k_{\text{obs } 2} \text{ (s}^{-1}\text{)}$	$\text{KIE}_{\text{obs } 1}$
0	191.9 ± 5.2	5.73 ± 1.14	1.00 ± 0.04
0.25	144.4 ± 6.5	4.71 ± 1.08	1.33 ± 0.07
0.5	109.0 ± 3.4	5.31 ± 0.80	1.76 ± 0.07
0.75	77.0 ± 4.5	6.11 ± 1.14	2.49 ± 0.16
0.99	48.2 ± 4.3	6.11 ± 3.84	3.98 ± 0.37

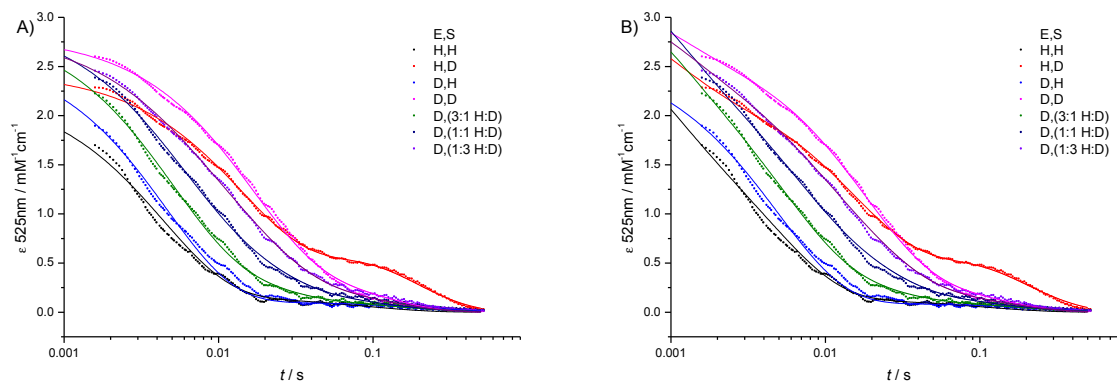


Figure S1. Comparison of the global fitting of the resampled data from Figures 1 and 2 to a 2-step (A) and 3-step (B; redrawn from Figure 3) mechanism. The fits are almost indistinguishable, and fitted parameters are given in Table S2.

Table S2. Fitted parameters determined by global fitting of the data in Figure 3.^a

Parameter	2-step mechanism		3-step mechanism	
	Objective value 1.45		Objective value 1.18	
	value	standard error	value	standard error
k_1	-	-	562.219	61.176
k_{-1}	-	-	582.262	82.748
k_{12}	208.821	1.448	497.245	67.708
k'_2	19.594	0.925	44.987	4.664
k_{-2}	16.871	1.677	24.265	2.601
k'_{-2}	11.203	0.284	11.011	0.331
k_3	12.183	0.414	10.276	0.350
KIE ₂	3.896	0.041	4.629	0.196
KIE ₋₂	2.247	0.262	3.712	0.370
KIE' ₋₂	39.447	6.139	37.452	5.202
enzyme concentration uncertainty (fraction of initial concentration)				
H,H	0.700	0.068	0.700	0.093
H,D	0.786	0.001	1.087	0.108
D,H	1.300	0.133	1.300	0.186
D,D	1.040	0.035	1.300	0.132
D,(3:1 H:D)	0.851	0.021	1.066	0.120
D,(1:1 H:D)	0.843	0.002	1.139	0.120
D,(1:3 H:D)	0.925	0.011	1.241	0.126
time uncertainty (ms)				
H,H	0.593	0.474	0.354	0.296
H,D	1.600	0.139	-0.459	0.296
D,H	-1.610	0.485	-1.894	0.384
D,D	-0.995	0.631	-0.947	0.343
D,(3:1 H:D)	1.083	0.148	-0.172	0.254
D,(1:1 H:D)	1.600	0.054	-0.155	0.248
D,(1:3 H:D)	0.780	0.151	-0.753	0.277

^a Selected parameters for the 3-step model are also presented in Table 3.