Supplementary Material for Organic & Biomolecular Chemistry

Supplementary data

Table 1S

Pseudo-first-order rate constants for the reaction of SNAP with Captopril. The effect of captopril concentration on the first stage.

[SNAP] = 3 mM, [EDTA] = 50 μM, λ = 590 nm, temp = 25 ^{o}C, pH = 7.30

[Captopril]/mM	$k_{obs}/10^{-2}$ **s^{-1}**
40	6.43
50	7.65
60	9.35
70	10.7

Table 2S

Pseudo-first-order rate constants for the reaction of SNAP with Captopril. The effect of captopril concentration on the second stage.

[SNAP] = 0.4 mM, [EDTA] = 50 μM, λ = 332 nm, temp = 25 °C, pH = 7.38

[Captopril]/mM	k_{obs}/ 10^{-4} s^{-1}
6	1.81
10	3.53
15	5.17
20	6.77
25	8.15
30	9.63
40	13.5

Table 3S

Pseudo-first-order rate constants for the reaction of SNAP with Captopril. The effect of pH variation on the first stage.

[SNAP] = 3 mM, [captopril] = 40 mM, [EDTA] = 50 μM, I = 0.5 M (NaCl), θ = 20.0, 25.0, 30.0, 37.0 ^{o}C; λ = 590 nm.

	k_{obs} / s^{-1}							
	Expt.	**Calc.**	**Expt.**	**Calc.**	**Expt.**	**Calc.**	**Expt.**	**Calc.**
pH	*20.0 ^{o}C*		*25.0^{o}C*		*30.0 ^{o}C*		*37.0 ^{o}C*	
6.33	0.013	0.004	0.037	0.005	-	-	0.041	0.011
6.81	0.024	0.010	0.041	0.015	0.062	0.022	0.086	0.033
7.30	0.044	0.032	0.062	0.047	0.10	0.068	0.15	0.10
7.63	0.078	0.070	0.11	0.10	0.21	0.15	0.29	0.21
8.23	0.32	0.27	0.42	0.39	0.67	0.57	1.02	0.84
8.62	0.68	0.64	1.01	0.93	1.54	1.34	2.34	2.00
9.17	1.83	1.95	2.89	2.84	4.18	4.10	6.26	6.05
9.41	3.03	2.97	4.28	4.33	6.14	6.25	8.99	9.22

NB: rate constants are the averages of two determinations with errors ≤ 5 %

Expt. **stands for Experimental data and *Calc*. stands for calculated data obtained from Sigma Plot non-linear regression.**

Table 4S

Pseudo-first-order rate constants for the reaction of SNAP with Captopril. The effect of pH variation on the second stage.

[SNAP] = 0.4 mM, [captopril] = 15 mM, [EDTA] = 50 μM, I = 0.5 M (NaCl), θ = 20.0, 25.0, 30.0, 37.0 ^{o}C; λ = 332 nm.

	k_{obs} / 10^{-4} s^{-1}			
pH	*20.0 ^{o}C*	*25.0^{o}C*	*30.0 ^{o}C*	*37.0 ^{o}C*
6.28	1.10	1.45	2.90	4.41
6.57	1.64	2.69	3.65	5.04
6.82	2.17	3.31	4.64	6.48
7.09	2.65	3.73	5.51	6.83
7.31	3.43	4.79	6.45	8.92
7.51	3.60	5.54	7.70	11.1
7.75	4.66	6.24	7.52	11.7
8.37	4.78	7.79	10.6	11.5
8.65	5.85	8.28	9.35	13.7
8.80	4.71	7.50	10.3	14.3
9.19	5.67	6.60	9.53	13.1
9.40	5.89	6.71	8.55	13.6