

CORRIGENDUM

Corrigendum to: “Solvation Effects and Driving Forces for Protein Thermodynamic and Kinetic Cooperativity: How Adequate is Native-Centric Topological Modeling?”

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Hüseyin Kaya and Hue Sun Chan*

Because of a typographical error in the kinetic simulation program, Figure 9 in the original paper was inaccurate. Figure 9, its legend and supporting Table 3 should be replaced by the following. We thank Dr Zhirong Liu of our group for his assistance in preparing the corrected Figure and Table.

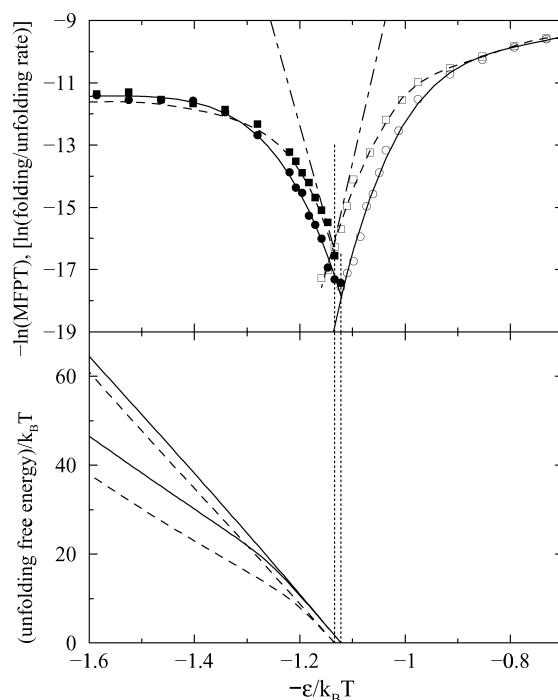


Figure 9. Same as Figure 8 but for the with-solvation models at $T = 0.82$. Simulation details not identical to that in Figure 8 are as follows. Upper panel: MFPTs are from the $0.5 \leq \epsilon \leq 1.30$ entries in Table 3. Otherwise the kinetic definitions of folding and unfolding are the same as that in Figure 8. Significant chevron rollovers are observed here as well. Lower panel: Stability curves are given by the natural logarithm of the Boltzmann weight of the folded state minus that of the denatured chain population with ≤ 30 native contacts (upper curves) or that with ≤ 80 (lower curves). The folded state is defined here by conformations with exactly $Q = 1$ (cf. Figure 4C). The stability curves are obtained by histogram techniques from simulations at $\epsilon = 0.93$ (NCS1) and 0.92 (NCS2).

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Table 3. Same as Table 1, but for the with-solvation models ($T = 0.82$, Figure 9)

ϵ	Unfolding				ϵ	Folding			
	NCS1		NCS2			NCS1		NCS2	
	MFPT/ 10^5	N_t	MFPT/ 10^5	N_t		MFPT/ 10^5	N_t	MFPT/ 10^5	N_t
0.40	0.0559	100	0.0552	100	1.50	0.9366	97	2.4917	100
0.50	0.0930	100	0.0874	100	1.40	0.7541	97	1.0181	100
0.60	0.1428	100	0.1465	100	1.30	0.8596	97	0.8972	100
0.65	0.1840	100	0.1913	100	1.25	0.8049	97	1.0368	100
0.70	0.2583	100	0.2855	100	1.20	1.0222	97	1.0351	100
0.75	0.3779	100	0.4583	100	1.15	1.1630	98	1.0671	100
0.80	0.5884	100	1.0106	100	1.10	1.4094	97	1.5428	100
0.825	1.0430	100	–	–	1.05	2.2543	98	3.2245	100
0.83	–	–	2.7883	100	1.00	5.5415	97	10.628	100
0.85	1.9525	100	5.2280	100	0.99	7.4727	93	17.457	100
0.86	–	–	10.725	100	0.98	10.829	97	20.435	100
0.87	–	–	21.265	100	0.97	14.755	49	42.888	100
0.875	5.6643	100	–	–	0.96	23.857	50	57.242	50
0.88	–	–	31.558	50	0.95	35.767	96	89.698	19
0.89	–	–	84.652	50	0.94	53.492	48	227.72	28
0.90	13.436	100	184.72	71	0.93	155.01	25	332.80	18
0.91	31.860	100	272.36	27	0.92	–	–	371.22	8
0.92	66.267	92	427.37	18					
0.93	116.97	50	–	–					
0.94	243.74	28	–	–					
0.95	320.08	25	–	–					