Quantum conformational transition in biological macromolecule

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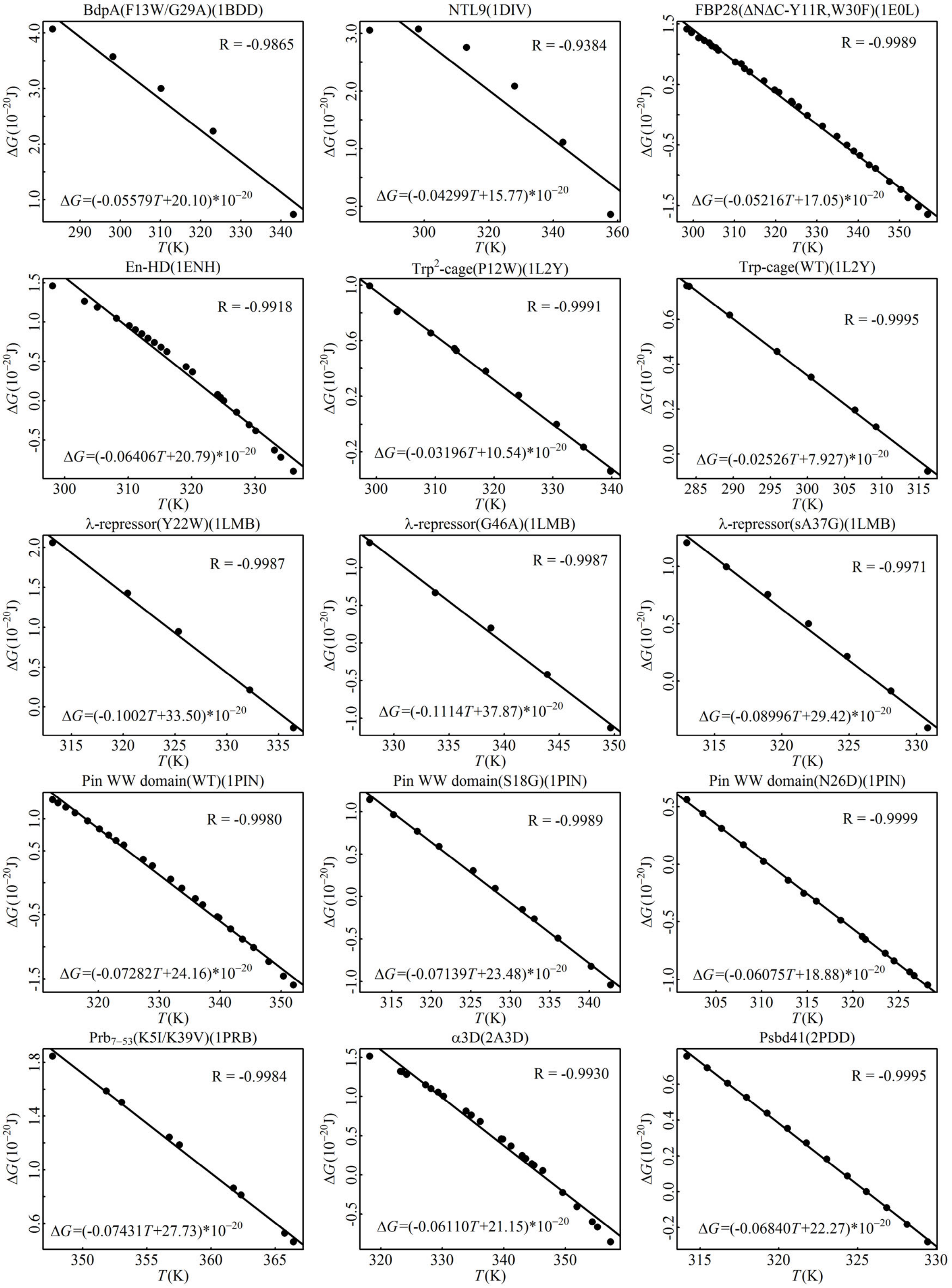

Figure S1. Linear relation between protein free energy ΔG and temperature. Experimental free energies ΔG changing with temperature are plotted for 15 proteins. The regression analysis shows a good linear relation existing between ΔG and T for each protein. ΔG in unit J, T in unit Kelvin. The experimental data of the temperature dependence of ΔG were given in ref 12 to ref 23 of the text.

Table S1. Parameters in the statistical analysis of the denaturant concentration dependence of protein folding /unfolding rates.

Protein	$\ln W^0$	$\ln W_u^0$	m_f(M^{-1})	m_u(M^{-1})	m'(M^{-2})	$\Delta G^{(0)}$(kJ/mol)	N	ζ (kJ/mol)	$\varpi\delta\theta$ (×10^{11})
GW1	3.66	−4.03	−2.94	4.11	−0.4865	19.04	344	186.79	3.3252
U1A	4.80	−14.98	−0.064	4.61	−0.2826	48.98	415	71.56	2.0083

Columns 2 – 6 are parameters obtained from experimental fitting of relaxation rate constant (see Eq 17 to 19 in text), $\Delta G^{(0)} = RT\ln\frac{W^{(0)}}{W_u^{(0)}}$, N- torsion number of the protein sequence, ζ and $\varpi\delta\theta$ are calculated from theory in text .

Table S2. Data of 38 multi-state protein folding.

PDB	$\ln k_f$	$\ln W$	$\Delta G/k_BT$	N	f	Ref
1A6N	1.1	3.74	4.9	597	81	33
1AON	−1.5	−0.86	4.2	590	1	34
1AU7	9.7	8.08	4.9	253	81	35
1AUE	6.0	7.24	11.4	390	81	36
1BD8	2.9	2.90	5.2	572	25	37
1BFE	3.0	2.50	6.4	349	1	38
1BTB	3.4	2.37	6.1	353	1	39
1CBI	−3.2	0.55	6.6	531	1	40
1EAL	1.3	0.79	6.2	492	1	41
1ENH	10.5	7.86	2.9	237	81	42
1GM1	0.8	1.62	3.1	341	1	43
1GXT	4.4	3.19	11.2	347	1	44
1HCD	4.0	2.60	13.0	444	1	45
1HNG	1.8	2.71	9.4	380	1	46
1IFC	3.4	1.03	8.0	524	1	40
1IGS	−4.6	−1.26	9.0	908	1	47
1JOO	2.3	1.13	10.7	602	1	48
1OPA	1.4	1.58	10.6	536	1	40
1PHP_C	−3.9	−1.50	6.9	816	1	49
1PHP_N	2.3	−0.70	6.5	677	1	50
1QOP	−2.5	0.58	6.4	980	25	51
1RA9	−3.2	−1.61	2.9	613	1	52
1RNB	2.6	2.68	11.7	415	1	53
1SCE	4.2	2.62	10.3	403	1	54
1ST7	8.5	5.45	2.1	352	81	55
1TIU	3.6	3.22	11.2	344	1	56
1TTF	5.5	3.21	13.9	332	1	57
1UZC	7.6	7.68	6.2	292	81	58
1V9E	−4.2	1.47	19.8	992	1	59
2A5E	3.5	2.46	3.3	540	25	60
2CRO	3.7	7.67	4.2	265	81	61
2LZM	4.1	5.40	18.1	646	25	62
2MYO	4.7	4.91	7.9	451	25	63
2RN2	0.1	1.44	12.1	604	1	62
2VIL	5.0	1.67	9.1	484	1	64
3CHY	1.0	0.55	5.4	490	1	65
3F6R	3.6	1.07	8.4	533	1	66
3H08	1.9	2.33	15.9	544	1	67

First column – PDB code of the protein, 2nd column – experimental logarithm rate, 3rd column – theoretical logarithm rate, 4th column – free energy , N – torsion number and f – structure-related shape parameter of the protein whose value can be found in Ref. 3 of the text. The experimental folding rate and free energy can be found in references in the text whose number is listed in the last column.