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ADDITIONS AND CORRECTIONS

Energetic Determinants of Oligomeric State Specificity in Coiled Coils[*J. Am. Chem. Soc.* **2006**, *128*, 15499−15510]. Jorge Ramos and Themis Lazaridis*

Pages 15503, 15505, 15506, and 15507 respectively: Tables 2, 3, 4, and 5 contain an error (column V is identical to column I). The corrected tables are provided below. The text is not affected by this error. We thank David Minde for pointing out the error.

Table 2. Average Free Energy ($W - T\Delta S^{conf}$) per Residue for the GCN4-p1 Sequence during Four 0.6 ns (300 Frames) Nosé−Hoover MD Simulations[a]

residue	I	II	III	IV	V
Ace	−4.04	−3.31	−4.58	−4.60	−4.58
Arg^{2g}	4.04	3.39	6.29	6.93	5.34
Met^{3a}	−1.97	−1.62	−1.18	−0.75	−1.94
Lys^{4b}	0.86	1.26	1.05	0.88	0.88
Gln^{5c}	−8.50	−8.61	−8.49	−8.28	−8.27
Leu^{6d}	−4.21	−6.92	−5.90	−5.49	−6.00
Glu^{7e}	−3.49	−4.53	−4.12	−3.66	−4.67
Asp^{8f}	−10.47	−10.84	−10.64	−10.33	−10.82
Lys^{9g}	−1.17	−0.99	−0.66	−0.56	−0.34
Val^{10a}	−2.53	−4.63	−4.82	−4.30	−4.47
Glu^{11b}	−4.15	−4.79	−4.45	−3.97	−4.43
Glu^{12c}	−4.45	−4.86	−4.44	−4.06	−4.40
Leu^{13d}	−4.68	−7.70	−6.08	−6.78	−7.18
Leu^{14e}	−5.78	−5.81	−5.86	−6.45	−5.40
Ser^{15f}	−8.21	−7.96	−7.81	−8.41	−7.98
Lys^{16g}	0.14	0.71	1.52	1.04	1.51
Asn^{17a}	−11.57	−11.19	−12.22	−10.81	−10.68
Tyr^{18b}	−1.42	−1.57	−1.18	−0.51	−0.83
His19c	−3.32	−3.28	−3.41	−3.70	−4.14
Leu^{20d}	−4.52	−6.60	−6.31	−6.49	−5.92
Glu^{21e}	−4.19	−4.63	−4.36	−4.60	−3.68
Asn^{22f}	−11.63	−11.35	−11.49	−11.14	−11.12
Glu^{23g}	−3.97	−3.74	−4.16	−4.04	−3.99
Val^{24a}	−2.61	−3.68	−4.46	−3.87	−4.40
Ala^{25b} [b]	−5.51	−6.39	−6.21	−5.93	−6.14
Arg^{26c}	1.24	1.87	1.96	1.76	2.14
Leu^{27d}	−4.03	−6.81	−6.45	−6.35	−6.70
Lys^{28e}	1.30	0.59	1.10	1.33	1.33
Lys^{29f}	1.75	1.61	1.85	1.65	2.71
Leu^{30g}	−1.78	−1.70	−1.70	−2.40	−2.86
Val^{31a}	2.20	2.17	1.08	1.32	0.31
Cbx	−1.41	−1.39	−1.44	−1.62	−1.97
$\sum[W - T\Delta S^{conf}]$	−108.08	−123.32	−117.58	−114.15	−118.69

[a] All entries are in units of kcal/(mol·helix). Lowest energy values among the oligomers are underlined. The monomer energies have been included for completeness, but only the multimers are compared. The values reported here do not include the constant $\sum_i \Delta G_i^{ref_{solv}}$ contribution. The error bar on these values is around 0.1 kcal/mol. Ace is the acetyl blocking group, and Cbx, the methyl amide blocking group. [b] The stabilization observed for Ala^{25b} is an artifact, resulting from the rebuilding of part of helix A of the trimer (see Methods). This rebuilding results in a suboptimal hydrogen bond between Ala^{25b} and Lys.^{29f}

Table 3. Average Free Energy ($W - T\Delta S^{conf}$) per Residue for the H38-p1 Sequence during Four 0.6 ns (300 Frames) Nosé−Hoover MD Simulations[a]

residue	I	II	III	IV	V
Ace	−4.67	−3.46	−4.91	−4.80	−4.65
Arg^{2g}	3.79	2.10	3.71	3.79	3.72
Ile^{3a}	−0.20	−0.98	−1.32	−0.07	−0.79
Lys^{4b}	0.58	1.35	0.80	1.03	0.90
Gln^{5c}	−8.16	−8.20	−8.43	−7.78	−8.41
Gln^{6d}	−9.33	−10.37	−10.86	−10.84	−10.45
Glu^{7e}	−4.03	−3.95	−4.10	−3.79	−4.43
Asp^{8f}	−10.62	−10.87	−10.63	−10.44	−10.87
Lys^{9g}	−2.35	−1.22	−2.45	−2.45	−1.69
Leu^{10a}	−4.30	−4.22	−6.24	−6.28	−6.21
Glu^{11b}	−4.81	−4.92	−4.74	−4.21	−4.90
Glu^{12c}	−4.95	−5.47	−5.13	−4.83	−4.98
Thr^{13d}	−4.85	−5.16	−5.35	−5.65	−5.32
Leu^{14e}	−5.24	−5.24	−5.53	−5.05	−4.00
Ser^{15f}	−8.11	−7.75	−7.78	−8.13	−8.09
Lys^{16g}	0.03	0.64	1.18	1.23	1.22
Ile^{17a}	−3.11	−3.12	−4.66	−4.02	−3.71
Tyr^{18b}	−1.30	−1.19	−1.21	−0.23	−0.71
His^{19c}	−3.51	−3.67	−3.45	−3.68	−4.05
Leu^{20d}	−4.76	−7.36	−6.93	−7.08	−6.53
Glu^{21e}	−3.56	−3.26	−3.49	−4.18	−2.97
Asn^{22f}	−11.28	−11.43	−11.40	−11.15	−10.87
Glu^{23g}	−4.10	−3.79	−4.29	−5.01	−4.09
Ile^{24a}	−1.89	−1.57	−3.77	−3.22	−3.46
Ala^{25b}	−5.61	−6.16	−6.13	−6.01	−6.09
Arg^{26c}	1.22	1.95	1.17	1.22	1.40
Val^{27d}	−2.71	−3.45	−4.74	−4.64	−4.27
Lys^{28e}	1.36	0.73	1.07	1.31	1.59
Lys^{29f}	1.96	1.94	1.88	1.84	2.00
Leu^{30g}	−1.92	−1.94	−2.05	−3.15	−3.09
Leu^{31a}	1.21	1.94	−0.03	−1.24	−1.41
Cbx	−1.39	−1.26	−1.56	−1.66	−1.91
$\sum[W - T\Delta S^{conf}]$	−106.62	−109.35	−121.36	−119.17	−117.13

[a] All entries are in units of kcal/(mol·helix). Lowest energy values among the oligomers are underlined. The monomer energies have been included for completeness, but only the multimers are compared. The values reported here do not include the constant $\sum_i \Delta G_i^{ref_{solv}}$ contribution. The error bar on these values is around 0.1 kcal/mol. Ace is the acetyl blocking group, and Cbx, the methyl amide blocking group.

Table 4. Average Free Energy ($W - T\Delta S^{conf}$) per Residue for the Gcn4-LI Sequence during Four 0.6 ns (300 Frames) Nosé−Hoover MD Simulations[a]

residue	I	II	III	IV	V
Ace	−4.78	−3.39	−4.45	−4.56	−4.30
Arg^{2g}	5.27	4.10	5.85	6.49	6.11
Met^{3a}	−2.12	−1.23	−0.54	−1.22	−1.65
Lys^{4b}	0.02	1.55	0.78	0.50	0.89
Gln^{5c}	−9.21	−8.75	−8.43	−8.31	−8.46
Ile^{6d}	−1.68	−3.20	−3.91	−3.92	−3.66
Glu^{7e}	−4.07	−4.10	−4.06	−3.72	−4.20
Asp^{8f}	−10.19	−10.72	−10.52	−10.14	−10.38
Lys^{9g}	−1.40	−1.41	−0.50	−0.86	−0.24
Leu^{10a}	−4.17	−4.87	−5.71	−7.18	−7.33
Glu^{11b}	−4.73	−4.70	−5.01	−4.55	−4.96
Glu^{12c}	−4.32	−4.76	−4.53	−4.18	−4.45
Ile^{13d}	−2.21	−3.04	−4.39	−4.97	−4.41
Leu^{14e}	−5.72	−6.05	−6.14	−6.53	−5.50
Ser^{15f}	−8.06	−7.93	−7.73	−7.95	−7.93
Lys^{16g}	−0.14	−0.32	1.38	0.66	0.43
Leu^{17a}	−5.56	−6.49	−7.09	−7.71	−7.56
Tyr^{18b}	−1.36	−1.44	−1.33	−0.60	−1.01
His^{19c}	−3.53	−3.47	−3.35	−3.78	−4.47
Ile^{20d}	−2.40	−2.52	−4.23	−4.95	−4.62
Glu^{21e}	−3.38	−3.78	−3.56	−4.21	−3.41
Asn^{22f}	−11.30	−11.56	−11.51	−11.08	−10.87
Glu^{23g}	−3.82	−3.85	−3.90	−4.67	−3.87
Leu^{24a}	−4.15	−4.63	−5.74	−7.31	−7.73
Ala^{25b}	−5.71	−6.29	−6.31	−6.23	−6.39
Arg^{26c}	0.89	1.41	1.63	1.23	1.74
Ile^{27d}	−1.61	−2.54	−4.22	−4.21	−4.22
Lys^{28e}	1.60	0.86	0.65	1.01	1.13
Lys^{29f}	1.80	2.06	1.33	1.82	1.86
Leu^{30g}	−2.09	−2.06	−1.96	−3.09	−3.17
Leu^{31a}	0.77	2.04	−0.14	−1.60	−1.56
Cbx	−1.35	−1.20	−1.58	−1.68	−1.94
$\sum[W - T\Delta S^{conf}]$	−98.70	−102.28	−109.22	−117.52	−116.15

[a] All entries are in units of kcal/(mol·helix). Lowest energy values among the oligomers are underlined. The monomer energies have been included for completeness, but only the multimers are compared. The values reported here do not include the constant $\sum_i \Delta G_i^{ref_{solv}}$ contribution. The error bar on these values is around 0.1 kcal/mol. Ace is the acetyl blocking group, and Cbx, the methyl amide blocking group.

Table 5. Average Free Energy ($W - T\Delta S^{conf}$) per Residue for the Comp Sequence during Four 0.6 ns (300 Frames) Nosé−Hoover MD Simulations[a]

residue	I	II	III	IV	V
Ace	−3.16	−3.33	−3.75	−3.68	−3.71
Leu^{2g}	−3.27	−2.92	−2.71	−2.42	−2.74
Ala^{3a}	0.09	−0.41	−0.48	0.14	−0.93
Pro^{4b}	5.56	5.48	5.25	4.84	4.98
Gln^{5c}	−8.04	−8.38	−8.46	−8.46	−8.65
Met^{6d}	−4.51	−3.87	−4.33	−4.09	−4.57
Leu^{7e}	−5.05	−4.76	−5.23	−5.07	−5.23
Arg^{8f}	1.46	1.55	1.44	2.21	1.84
Glu^{9g}	−5.91	−6.04	−6.36	−6.28	−5.65
Leu^{10a}	−4.57	−4.92	−6.29	−6.71	−6.76
Gln^{11b}	−8.65	−8.44	−8.60	−8.49	−8.94
Glu^{12c}	−5.20	−5.42	−5.52	−4.94	−5.43
Thr^{13d}	−4.57	−4.39	−6.06	−5.23	−5.34
Asn^{14e}	−10.59	−10.99	−11.43	−10.56	−11.26
Ala^{15f}	−6.72	−6.81	−6.68	−6.64	−6.18
Ala^{16g}	−6.56	−7.12	−7.20	−7.42	−7.92
Leu^{17a}	−4.15	−4.78	−5.09	−5.55	−5.64
Gln^{18b}	−8.99	−9.20	−9.16	−8.50	−8.95
Asp^{19c}	−10.33	−10.17	−10.63	−10.45	−9.65
Val^{20d}	−3.07	−4.01	−4.35	−5.27	−4.92
Arg^{21e}	2.48	2.36	3.30	2.54	1.73
Glu^{22f}	−4.44	−4.24	−4.44	−4.20	−4.31
Leu^{23g}	−4.95	−5.27	−5.20	−6.27	−7.06
Leu^{24a}	−4.40	−5.37	−6.46	−6.86	−6.88
Arg^{25b}	2.95	2.23	2.44	3.62	3.00
Gln^{26c}	−9.63	−8.74	−9.50	−10.01	−9.25
Gln^{27d}	−8.00	−7.63	−9.67	−9.31	−10.24
Val^{28e}	−1.49	−2.27	−2.09	−2.98	−4.01
Lys^{29f}	1.85	1.90	1.89	1.31	2.40
Glu^{30g}	−1.38	−1.78	−1.60	−1.77	−0.95
Ile^{31a}	3.57	3.53	2.45	2.16	1.69
Cbx	−1.48	−1.29	−1.48	−1.58	−2.03
$\sum[W - T\Delta S^{conf}]$	−121.15	−125.51	−135.98	−135.94	−141.56

[a] All entries are in units of kcal/(mol·helix). Lowest energy values among the oligomers are underlined. The monomer energies have been included for completeness, but only the multimers are compared. The values reported here do not include the constant $\sum_i \Delta G_i^{ref_{solv}}$ contribution. The error bar on these values is around 0.1 kcal/mol. Ace is the acetyl blocking group, and Cbx, the methyl amide blocking group.

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