

Correction: Folding Very Short Peptides Using Molecular Dynamics

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In *PLoS Computational Biology*, volume 2, issue 4:

The abbreviation GB/SA had an incorrect definition in the Abstract, Introduction, and Abbreviations list. The correct definition of GB/SA is generalized-Born/surface area.

Table 4 has several rows that did not appear in bold font in the published article, and Table 5 had four rows with incorrect spacing in the published article. Both tables appear correctly below.

This correction note may be found online at DOI: 10.1371/journal.pcbi.0020060.

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Table 4. Ground Mesostrings of β -Sheet Proteins

Name	Sequence	RMSD in Å	Mesosting		P1 in Percent	ΔF in kcal/mol	TS in kcal/mol	Native Structure	
			Native	Ground					
Chymotrypsin inhibitor	seq1	1-NLKTEWPE	5.2	bbbabbba	Bbaaabb-	65	0.89	0.90	Loop
	seq2	4-TEWPELVG	4.2	abbaaab1	b-baaaaab	85	1.6	0.57	3₁₀ helix
	seq3	7-PELVGKSV	2.9	aaablbbba	baabbaab	15	0.24	1.65	
	seq4	10-VGKSVVEEA	4.1	b1bbbaaa	abaaaaabb	34	0.51	1.39	
	seq5	13-SVEEAKKV	0.5	baaaaaaaa	-aaaaaaaa	63	0.82	0.92	Helix
	seq6	16-EAKKVILQ	4.3	aaaaaaaa	baaaaaaa	24	0.14	1.32	
	seq7	19-KVILQDKP	3.9	aaaaaaba	babaaabb	34	0.45	1.16	
	seq8	22-LQDKPEAQ	2.7	aaabaabb	Bbabaaa-	45	0.81	1.39	Helix-cap
	seq9	25-KPEAQIIV	4.9	baabbbbbb	bbaaabbb	41	0.71	1.17	
	seq10	28-AQIIVLPV	5.7	bbbbbbbbb	b-aaabbb	64	0.68	0.91	Strand
	seq11	31-IVLPVGTI	3.1	bbbbblbb	bbbaaaab	20	0.14	1.54	
	seq12	34-PVGTIVTM	4.2	bb1bbbbb	bbbaaaaa	12	0.06	1.87	
	seq13	37-TIVTMEYR	4.0	bbbabbbb	aaaaabba	30	0.44	1.23	
	seq14	40-TMEYRDDR	3.7	babbaaab	bb-aaaaa	64	0.87	1.02	Loop-turn
	seq15	43-YRIDRVRL	3.2	bbaabbbb	bbbaaaaa	48	0.17	0.75	
	seq16	46-DRVRLFVD	6.4	abbbbbbb	abbaabbb	40	0.64	1.18	
	seq17	49-RLFVDKLD	4.2	bbbbbaa1	babaaabb	37	0.07	0.83	
seq18	52-VDKLDNIA	4.1	hbba1bba	ba-aaabb	64	1.06	1.09	Hairpin-turn	
seq19	55-LDNIAEVP	3.3	albbabbb	babaaabb	22	0.15	1.36		
seq20	58-IAEVPRVG	3.7	babbbbbb	baabba-b	66	0.97	0.99	Bulge	
α Spectrin	seq1	1-KELVLALY	4.3	bbbbbbbab	-aaaaaaaa	64	0.90	1.01	Strand
	seq2	4-VLALYDYQ	3.7	bbbabbbb	aaaaaaaa	34	0.31	1.29	
	seq3	7-LYDYQEKS	4.0	abbbbbbab	baaaaaaa	55	0.78	0.88	Loop
	seq4	10-YQEKSRE	3.6	bbbabaab	baaabbaa	44	0.53	0.90	
	seq5	13-KSPREVTM	3.8	abaabbbb	Bbbbaaa-	58	1.01	1.06	Loop
	seq6	16-REVTMKKG	4.5	abbbbbb1	abaaaaa-	48	0.86	1.18	Diverging-turn
	seq7	19-TMKKGDIL	2.7	bbbblbbb	babbbbbb	23	0.18	1.45	
	seq8	22-KGDILTLL	4.4	b1bbbbba	b-baaaaa	78	1.73	0.97	Strand
	seq9	25-ILTLLNST	3.9	bbbabaaa	b-aaaaaa	75	1.42	0.93	Strand
	seq10	28-LLNSTNKD	4.0	babaabaa	Bbbbaaa-	53	1.06	1.25	Hairpin-turn
	seq11	31-STNKDWWK	3.2	aabaabbb	bbbaaabb	36	0.22	1.15	
	seq12	34-KDWWKVEV	5.8	aabbbbbb	b-baabbb	43	0.70	1.32	
	seq13	37-WKVEVNDR	3.8	bbbbblab	bbbaaaaa	46	0.60	1.01	Hairpin-turn
	seq14	40-EVNDRQGF	3.7	bb1abbbb	baaaaaab	25	0.07	1.33	
	seq15	43-DRQGFVPA	5.6	abbbbbbba	abbbabbb	12	0.07	1.62	
	seq16	46-GFVPAAYV	3.2	bbbbaaab	bbbaaabb	36	0.78	1.42	
	seq17	49-PAAYVKKLD	3.3	baaabbbbbb	abaaaaaa	41	0.14	0.93	

RMSD is the most likely value of RMSD extracted from the free-energy profile of RMSD. The ground mesosting is sometimes nearly identical to less-populated mesostrings. If the most populated mesostrings differ by only one mesostate, we group them into a consensus mesosting, which contains one indefinite mesostate signified by [-].

P₁ is the probability of the ground mesosting.

ΔF is the free-energy difference between the ground mesosting and the next mesosting.

TS is the entropy of the mesostrings.

Native Structure is the description of the structure of the peptide in the native structure.

Bolded rows highlight structured peptides: P₁ > 45%, and ΔF > 0.6 kcal/mol.

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Table 5. Comparison of the Structural Bias with the Native Structure

Name	Lines	Structure per Residue
Protein G	1	MTYKLI L N G K T L K G E T T T E A V D A A T A E K V F K Q Y A N D N G V D G E W T Y D D A T K T F T V T F E
	2	-SSSSSSS-----SSSSSSS--HHHHHHHHHHHHH-----SSSSSTT--SSSSS-
	3	bbbbbbbababbbbbbbbabaaaaaaaaaaaaaaaaalbbabbbbaalbbbbbba
	4	-----aa-----aaaaaa-aaaaaaaaaaaa-----aaaaa-----
	5	_____HHHHHHHHHHHH S_TTT_S
Protein L	1	KANLIFANGSTQTAEFKGTFEKATSEAYAYADTLKKNNGEYTVVDVADKGYTLNFKFAG
	2	-SSS-----SSS-----HHHHHHHHHHHH-----SS--S----S---SS--
	3	bbbbbaalbbbbbbbbbbaaaaaaaaaaaaaabalalbbbbblllabbbbbba
	4	-----aaaa-----aaa-----aaa-----aaaaar-----aaaa-----
	5	_____HHHHHHHHHH HH_GGG
Protein A	1	QQNAFYELHLPNLNEEQRNGFIQSLKDDPSQSANLLAEAKKLND
	2	-HHHHHHHH-----HHHHHHHHHHHH--TT-HHHHHHHHHHHHH--
	3	aaaaaaaaabaabbaaaaaaaaaaaaaabaaaaaaaaaaaaaaaa
	4	-----aaa-----aaaaaa-aaaaaa-aaaaaa-
	5	_____HHHHHHHH HH_GGG
Myoglobin	1	MVLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHPETLEKDFRKHLEAEEMKASEDLKAGVTVLT
	2	---HHHHHHHHHHHHHH--HHHHHHHHHHHH--HHH33-TT-TT---HHHHHH--HHHHHHHHHHHH
	3	bbbbaaaaaaaaaaaaaabaaaaaaaaaaaaabaaaaabaaaaabaaaaabaaaaaaaaaaaa
	4	-----aaaaaa-----aaaaaa-aaaaaa-----r-----aaaa-----
	5	_____HHHH_GGG
	1	ALGAILKKKGHEAELEKPLAQSHATKHKIPIKYLEFISEAIIHVLHSRHPGNFGADAQGAMNKALELFRKD
	2	HHHHHHHH-----HHHHHHHHHHHH-----HHHHHHHHHHHHHHHH--TT---HHHHHHHHHHHHHH
	3	aaaaaaaaalbaaaaaaaaaaaaaalbbbaaaaaaaaaaaaaabaaabbaaaaaaaaaaaaa
	4	-----aaaa-----aaaaar-----r-----aaaa
	5	_____HHHH HHHHHHHHHH
	1	IAAKYKELGYQG
	2	HHHHHHHH-----
	3	aaaaaaaaalala
	4	aaaa-----
	5	
Chymotrypsin inhibitor 2	1	NLKTEWPELVGKSVVEAKKVI L Q D K P E A Q I I V L P V G T I V T M E Y R I D R V R L F V D K L D N I A E V P R V G
	2	---S-333TT---HHHHHHHHHH--TT-SSSSS-----TTSSSSS--TT--S---S--
	3	bbbabbaaablbbaaaaaaaaaabaabbbbbbbbbbabbabbbaabbbbbbbaalbbabbbbbb
	4	--aaa-aaaa-----aaaaaa-----aaa-aaa-----aaaa-----aaa-r-----
	5	
α Spectrin	1	KELVLALYDYQEKSPREVTMKGDI L T L L N S T N K D W K V E V N D R Q G F V P A A Y V K K L D
	2	--SSSS--S-----TT---S-TT-SSSSS-----SSS-TT-SSSSS333SSSS-
	3	bbbbbbabbbbababbbbbbllbbbbbabaabaabbbbbbllabbbbbbbaabbbbbb
	4	-aaaaaaaaaaaa-aaaaa-aaaaaaaa-----aaaa-----
	5	_____EETT_E

Line 1 is the amino-acid sequence.
 Line 2 is the secondary structure in the native structure (3, 310 helix; H, α-helical; S, sheet; T, H-bonded-turn).
 Line 3 is the mesostring of the native structure.
 Line 4 is the ground mesostring predicted from the peptides (aaa, helical-turn; rr, reverse-turn).
 Line 5 is the I-sites predictions (__, other; E, extended but not H-bonded; G, other helical-turn; H, α-helical; S, sheet; T, turn).
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