

CORRECTION

Protein Science 11:2714-2726 (2002)

Distance-scaled, finite ideal-gas reference state improves structure-derived potentials of mean force for structure selection and stability prediction

Hongyi Zhou and Yaoqi Zhou

A bug was discovered in our original program that generated the DFIRE potential of mean force. As a result, some results were changed. The number of atomic pairs for 1011 proteins is 57 millions at the distance shell of 14Å-15Å. The radius of each reference sphere is $1.225R_g$. The value of α is now 1.61. The constant prefactor (η) is now 0.0157. We also set the potential for zero occurrence to 2η kcal/mole, same as that in RAPDF and atomic KBP for comparison. The change of these values does not change the accuracy of the DFIRE potential, nor the conclusion of the paper. For multiple decoy sets, the number of correctly identified proteins continues to be 27 out of 32 decoy sets. The average Z-score of the 32 sets increases further from 4.27 to 4.52. The accuracy of loop prediction among 11 loop decoys is unchanged. The average correlation coefficient between the scores and the rmsd values for the *4state-reduced* set is reduced (improved) slightly from 0.63 to 0.61 whereas the average correlation coefficient for the loop decoys is unchanged. The correlation coefficient between theoretically predicted and experimentally measured change in stability due to mutation is unchanged where rmsd is reduced slightly from 1.52 kcal/mole to 1.49 kcal/mole. Full detailed corrections on figures and tables can be found in supplement (also in <http://theory.med.buffalo.edu>).

SUPPLEMENT FOR THE CORRECTION

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Distance-scaled, finite ideal-gas reference state improves structure-derived potentials of mean force for structure selection and stability prediction

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Table 1: Number of correctly identified decoys from single decoy sets by different potentials.

	RAPDF	Atomic KBP	DFIRE-A	DFIRE-A _{1.50} *	DFIRE-A _{1.70}	DFIRE-B
misfold	25/25	25/25	25/25	25/25	25/25	23/25
asilomar	33/33	33/33	33/33	33/33	32/33	32/33
pdberr & sgpa	5/5	5/5	5/5	5/5	5/5	5/5
ifu	31/44	33/44	33/44**	33/44	32/44**	18/44

*: DFIRE-A_{1.45} is now replaced by DFIRE-A_{1.50} to reflect the increase of α from 1.57 to 1.61. **: Bold numbers are different from old result.

Table 2: Native rank and Z-score of different potentials using multiple decoy sets.

A) <i>4state_reduced</i>	RAPDF	Atomic KBP	DFIRE-A	DFIRE-A _{1.50}	DFIRE-A _{1.70}	DFIRE-B
1ctf	1/3.26	1/3.53	1/3.85	1/3.44	1/4.01	1/3.02
1r69	1/3.49	1/3.76	1/4.23	1/3.91	1/4.18	1/2.96
1sn3	1/3.26	1/3.50	1/3.81	1/3.98	1/3.38	1/3.41
2cro	1/2.93	1/2.91	1/3.29	1/3.06	1/3.28	2/2.75
3icb	1/2.22	1/2.41	4/2.25	1/2.16	5/2.27	27/1.64
4pti	1/3.12	1/3.47	1/3.64	1/3.67	1/3.35	1/3.13
4rxn	1/2.79	1/3.12	1/3.39	1/2.98	1/3.47	17/1.90
\bar{Z}	3.01	3.24	3.49	3.31	3.42	2.69
B) <i>fisa</i>	RAPDF	Atomic KBP	DFIRE-A	DFIRE-A _{1.50}	DFIRE-A _{1.70}	DFIRE-B
1fc2	497/-2.74	413/-1.05	169/0.56	340/-0.32	53/1.07	1/3.26
1hdd-C	17/2.00	25/1.78	1/4.78	1/4.47	1/4.69	1/7.23
2cro	14/1.93	24/1.64	1/6.67	1/6.32	1/6.45	1/8.35
4icb	1/3.89	6/2.46	1/7.18	1/6.96	1/7.18	1/9.01
\bar{Z}	1.27	1.21	4.80	4.36	4.85	6.96
C) <i>fisa_casp3</i>	RAPDF	Atomic KBP	DFIRE-A	DFIRE-A _{1.50}	DFIRE-A _{1.70}	DFIRE-B
1bg8-A	1/4.39	2/2.84	1/5.32	1/5.67	1/4.87	1/3.76
1bl0	1/3.19	215/0.76	1/4.28	1/4.22	1/3.97	3/2.22
1jwe	1/4.69	4/2.64	1/6.59	1/6.06	1/5.69	1/4.93
\bar{Z}	4.09	2.08	5.40	5.32	4.84	3.64
D) <i>lmds</i>	RAPDF	Atomic KBP	DFIRE-A	DFIRE-A _{1.50}	DFIRE-A _{1.70}	DFIRE-B
1b0n-B	359/-0.45	74/1.03	424/-1.06	399/-0.78	427/-1.19	256/0.03
1bba	501/-11.11	500/-3.51	501/-15.48	501/-17.78	501/-12.62	501/-20.18
1fc2	501/-7.75	501/-8.86	501/-5.54	501/-6.35	501/-4.54	441/-1.26
1ctf	1/2.84	1/3.45	1/3.61	1/3.66	1/3.52	1/2.74
1dtk	116/-0.08	31/1.16	1/2.86	23/1.32	1/3.57	5/2.59
1igd	1/4.21	1/4.16	1/5.23	1/5.73	1/4.62	1/4.63
1shf-A	1/5.15	2/2.83	1/6.78	1/6.49	1/6.52	1/5.46
2cro	416/-0.96	175/0.40	1/5.09	10/2.16	1/6.29	1/4.75
2ovo	4/2.76	1/2.86	1/3.29	1/3.46	1/3.07	26/1.52
4pti	157/0.20	13/1.75	1/4.23	1/2.97	1/4.72	1/3.60
\bar{Z}	-0.52	0.53	0.90	0.09	1.40	0.39
E) <i>lattice_ssfit</i>	RAPDF	Atomic KBP	DFIRE-A	DFIRE-A _{1.50}	DFIRE-A _{1.70}	DFIRE-B
1beo	1/9.79	1/9.47	1/12.31	1/12.80	1/8.73	1/8.31
1ctf	1/6.99	1/7.20	1/10.17	1/7.94	1/9.43	1/6.92
1dkt-A	1/6.78	1/6.78	1/7.93	1/7.73	1/5.73	1/5.43
1fca	1/5.57	1/3.36	1/7.31	1/6.84	1/6.02	1/5.34
1nkl	1/8.33	1/8.16	1/10.33	1/8.53	1/8.45	1/6.29
1pgb	1/8.42	1/6.86	1/12.76	1/10.74	1/10.56	1/10.26
1trl-A	1/4.84	1/5.58	1/6.61	1/5.43	1/5.87	1/3.85
4icb	1/6.68	1/5.65	1/8.31	1/6.81	1/8.07	1/4.42
\bar{Z}	7.18	6.61	9.47	8.35	7.86	6.35
Summary	RAPDF	Atomic KBP	DFIRE-A	DFIRE-A _{1.50}	DFIRE-A _{1.70}	DFIRE-B
# Correct/Total	22/32	18/32	27/32	26/32	27/32	23/32
\bar{Z}	2.83	2.87	4.52	3.88	4.21	3.51

Table 3: The rmsd (\AA) of the lowest-energy conformation from the *loops* decoy set.

PDB ID	Residue range	rmsd range	RAPDF	Atomic KBP	DFIRE-A	DFIRE-A _{1.50}	DFIRE-A _{1.70}	DFIRE-B
3dfr	20 – 23	0.75 – 4.58	0.88	0.88	0.75	0.75	0.75	4.17
3dfr	27 – 30	0.81 – 3.47	0.87	1.69	1.10	1.69	1.10	1.26
3dfr	64 – 67	0.89 – 4.19	2.32	2.61	1.24	2.41	1.24	1.82
3dfr	120 – 124	0.57 – 2.91	0.75	1.28	1.18	0.62	1.18	1.25
3dfr	136 – 139	1.39 – 2.15	1.57	1.71	1.54	1.54	1.67	1.66
2sga	35 – 39	1.20 – 3.17	1.32	1.22	1.33	1.33	1.33	1.23
2sga	97 – 101	0.60 – 3.34	0.79	3.34	0.63	0.63	0.61	1.08
2sga	116 – 119	0.47 – 4.91	0.99	1.09	1.05	0.99	1.05	4.28
2sga	132 – 136	0.97 – 2.58	1.29	1.56	1.62	1.62	1.62	1.53
2fbj	265 – 269	0.96 – 3.90	3.90	3.67	1.03	2.07	1.10	2.15
2hfl	264 – 268	1.11 – 2.81	1.46	1.50	1.50	1.44	1.50	1.58

Table 4: The correlation coefficients between the scores and the rmsd values for the *4state_reduced* set.

PDB ID	RAPDF	Atomic KBP	DFIRE-A
1ctf	0.73	0.67	0.70
1r69	0.72	0.70	0.64
1sn3	0.47	0.49	0.30
2cro	0.76	0.73	0.75
3icb	0.86	0.83	0.82
4pti	0.52	0.53	0.44
4rxn	0.61	0.59	0.65
ave.	0.67	0.65	0.61

Table 5: The correlation coefficients between scores and rmsd values for the *loops* decoy set.

PDB ID	Residue range	rmsd range	RAPDF	Atomic KBP	DFIRE-A
3dfr	20 – 23	0.75 – 4.58	0.83	0.60	0.92
3dfr	27 – 30	0.81 – 3.47	0.60	0.56	0.72
3dfr	64 – 67	0.89 – 4.19	0.48	0.20	0.77
3dfr	120 – 124	0.57 – 2.91	0.93	0.84	0.92
3dfr	136 – 139	1.39 – 2.15	0.61	0.14	0.64
2sga	35 – 39	1.20 – 3.17	0.61	0.72	0.78
2sga	97 – 101	0.60 – 3.34	0.83	0.44	0.93
2sga	116 – 119	0.47 – 4.91	0.82	0.82	0.75
2sga	132 – 136	0.97 – 2.58	0.30	0.08	0.29
2fbj	265 – 269	0.96 – 3.90	-0.84	-0.10	0.82
2hfl	264 – 268	1.11 – 2.81	0.45	0.23	0.63
ave.			0.51	0.41	0.74

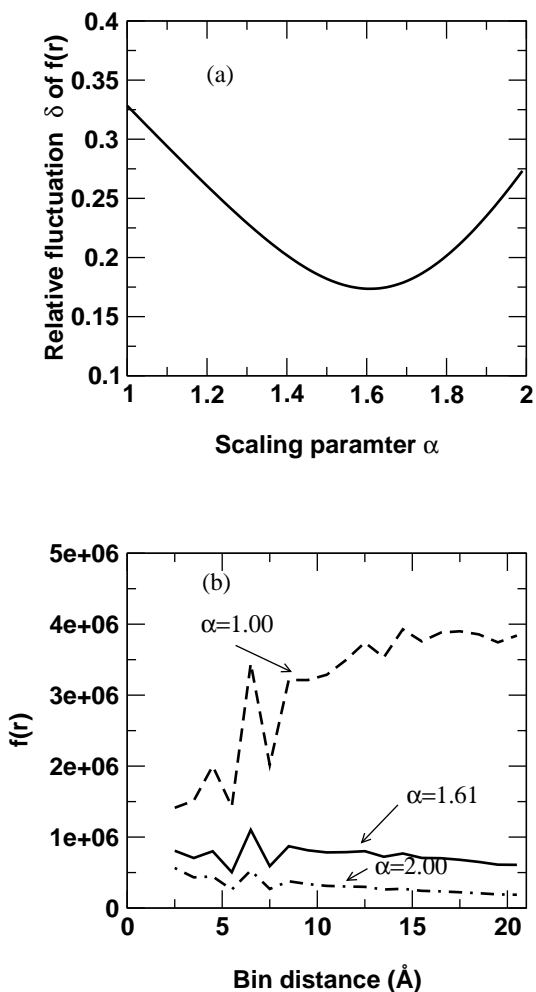


Figure 1: Scaling behavior of uniformly distributed heavy atoms in 1011 spheres. Number of pairs was counted in every 1\AA shell and r is the middle point of the shell. a) Relative fluctuation δ and b) Reduced distance-dependent function $f(r) = N(r)/r^\alpha$

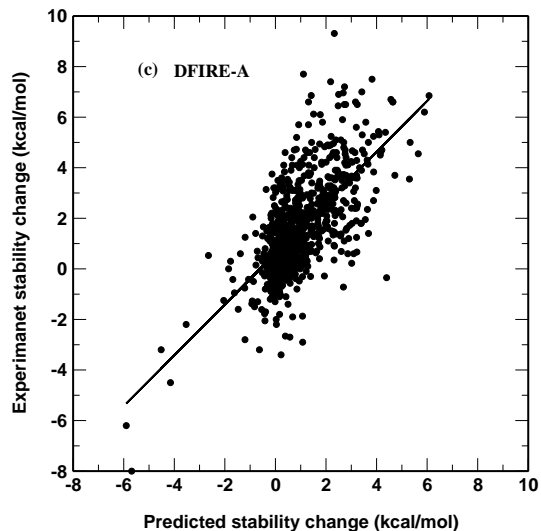


Figure 2: The experimentally measured changes in stability versus theoretically predicted ones in a database of 895 large-to-small mutations. (c) DFIRE-A. Lines represent the results from linear regression fit. The correlation coefficients are 0.52, 0.55, and 0.67 for RAPDF, atomic KBP and DFIRE-A, respectively.

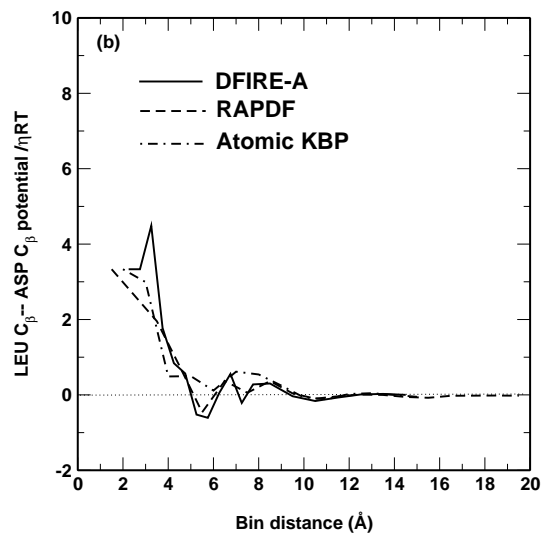
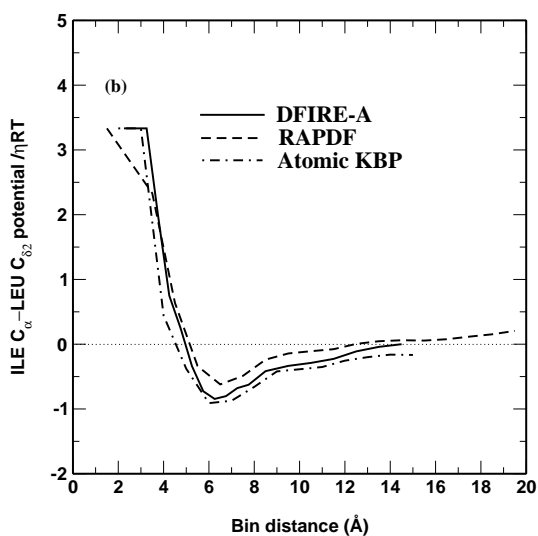
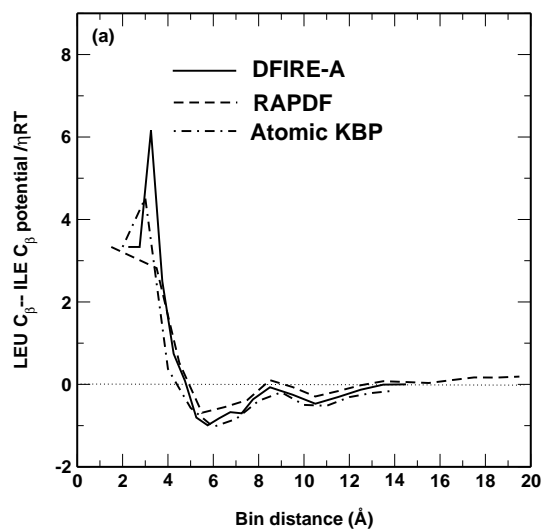
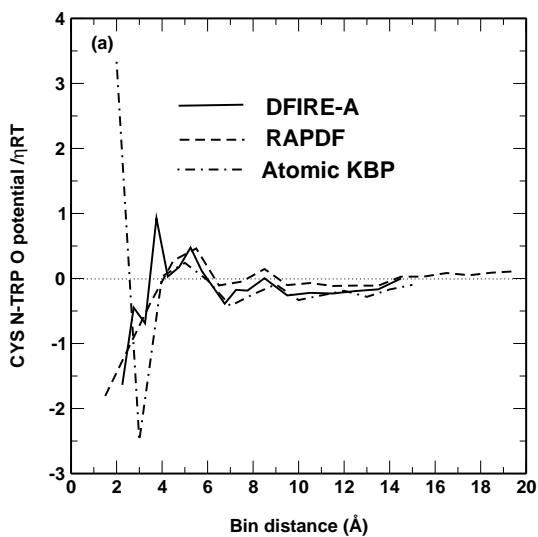


Figure 3: The distance dependence of three knowledge-based potentials a) between atom N of residue Cys and atom O of residue Trp and b) between atom C_α of residue Ile and atom $C_{\delta 2}$ of residue Leu.

Figure 4: The distance dependence of three knowledge-based potentials a) between C_β atoms of Leu and Ile residues and b) between C_β atoms of Leu and Asp residues.

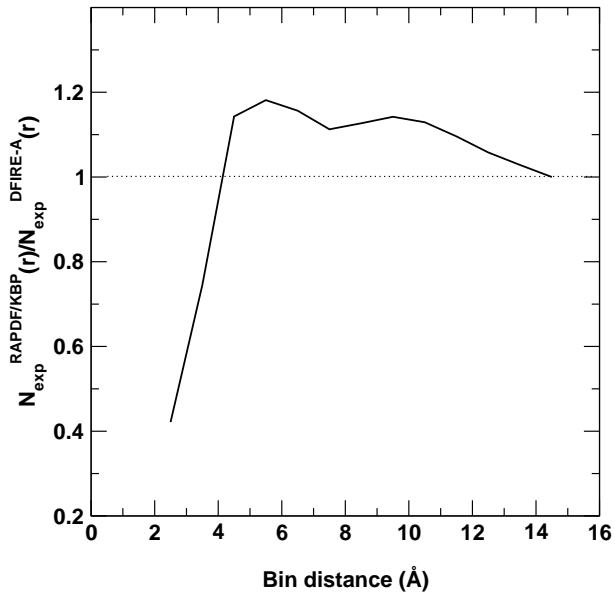


Figure 5: The distance dependence of $N_{\text{exp}}^{\text{RAPDF/KBP}}(r)/N_{\text{exp}}^{\text{DFIRE-A}}(r)$.