

High pKa variability of cysteine residues in structural databases and the effect of H-bond contributions

[Yapısal veritabanlarındaki sistein kalıntılarında pKa değerinin yüksek oranda değişkenlik göstermesi ve H-bağı katkılarının etkisi]

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Table. Comparison of different propka implementations (all residues), results with three replicas (random 1,000 points sampling)

	ppka3 [pKa] [#]	ppka3 SD	ppka1 [pKa]	ppka1 SD	ΔpKa (ppka3 – ppka1)	p-value (t-test, n=1000**)
CYS	10.957	1.287	9.198	2.008	1.759	7.68E-189
CYS	10.854	1.235	9.091	1.957	1.763	1.55E-190
CYS	11.101	1.438	9.148	1.978	1.953	3.02E-187
ASP	3.404	0.658	3.236	0.707	0.168	1.39E-19
ASP	3.440	0.677	3.234	0.764	0.206	1.03E-21
ASP	3.481	0.639	3.287	0.738	0.193	3.38E-21
GLU	4.422	0.753	4.146	0.781	0.276	1.372E-12
GLU	4.413	0.655	4.136	0.706	0.277	1.215E-11
GLU	4.422	0.667	4.133	0.745	0.289	5.73E-09
TYR	11.164	1.051	10.624	1.290	0.540	4.284E-08
TYR	11.166	1.107	11.000	1.304	0.165	6.417E-05
TYR	11.277	1.235	10.774	1.160	0.502	5.28E-07
HIS	5.802	1.080	5.953	1.832	-0.151	0.4878652
HIS	6.024	1.067	5.999	1.450	0.025	0.4477804
HIS	5.849	0.989	6.066	1.751	-0.218	0.8380233
ARG	12.524	0.530	12.006	0.589	0.518	1.199E-54
ARG	12.482	0.725	12.054	0.528	0.428	1.592E-53
ARG	12.558	0.634	12.063	0.518	0.495	2.48E-58
LYS	10.552	0.448	10.418	0.204	0.134	1.291E-11
LYS	10.523	0.439	10.314	0.234	0.209	3.323E-09
LYS	10.559	0.450	10.307	0.216	0.252	2.99E-12

[#]legend: [pKa]=average pKa for each type, SD=Standard deviation; ΔpKa (ppka3 – ppka1) = ppka3 [pKa] - ppka1 [pKa]; t-test described in Methods. ** Each line reports statistics (t-test derived p-values, last column, as in Table 1, main text) obtained by randomly selecting 1,000 points (out of the full dataset of 750 proteins, 40605 residues); random selections were repeated three times for each residue (hence, three rows per residue are reported in this table), reflecting three independent replicas of the calculations reported in Table 1 (to which Table S3 should be compared for validation purposes; see main text).