

Supplementary Material:

Conceptual DFT Descriptors of Amino Acids with Potential Corrosion Inhibition Properties Calculated with the Latest Minnesota Density Functionals

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\*Correspondence: Dr. Daniel Glossman-Mitnik daniel.glossman@cimav.edu.mx **Table S1A.** HOMO and LUMO orbital energies (eV), ionization potential I and electron affinity A (eV), global electronegativity  $\chi$ , chemical hardness  $\eta$ , global electrophilicity  $\omega$ , electrodonating power  $\omega^-$ , electroaccepting power  $\omega^+$  and net electrophilicity  $\Delta \omega^{\pm}$  of natural amino acids bearing a ionizable side-chain at different pHs calculated with the M11L density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of the KID procedure and the lower part shows the results derived from the calculated vertical  $\Delta$ SCF energies.

	НОМО	LUMO	$\chi_K$	$\eta_K$	$\omega_K$	$\omega_K^-$	$\omega_K^+$	$\Delta \omega_K^{\pm}$
Arg1	-6.959	-1.421	4.190	5.538	1.585	5.611	1.421	7.032
Arg2	-6.489	-0.403	3.446	6.086	0.976	4.055	0.609	4.664
Arg3	-6.003	-0.339	3.171	5.664	0.887	3.714	0.544	4.258
Arg4	-5.850	0.065	2.893	5.915	0.707	3.231	0.338	3.569
Asp1	-7.712	-1.390	4.551	6.322	1.638	5.946	1.395	7.342
Asp2	-6.403	-1.119	3.761	5.284	1.339	4.889	1.127	6.016
Asp3	-6.084	-0.401	3.243	5.683	0.925	3.827	0.584	4.411
Asp4	-5.612	0.115	2.748	5.727	0.659	3.051	0.303	3.354
Glu1	-7.397	-1.395	4.396	6.003	1.610	5.793	1.397	7.190
Glu2	-6.146	-1.362	3.754	4.785	1.473	5.121	1.367	6.489
Glu3	-6.039	-0.256	3.148	5.784	0.856	3.648	0.501	4.149
Glu4	-5.885	0.228	2.828	6.113	0.654	3.105	0.276	3.381
His1	-6.977	-1.523	4.250	5.454	1.656	5.778	1.528	7.305
His2	-6.426	-1.413	3.920	5.013	1.532	5.338	1.418	6.756
His3	-5.685	-0.444	3.065	5.241	0.896	3.652	0.587	4.239
His4	-5.354	-0.143	2.748	5.211	0.725	3.149	0.401	3.550
Lys1	-7.726	-1.369	4.547	6.357	1.626	5.924	1.376	7.300
Lys2	-6.472	-0.627	3.550	5.845	1.078	4.296	0.746	5.043
Lys3	-5.991	-0.594	3.293	5.397	1.004	3.993	0.700	4.693
Lys4	-5.952	0.117	2.918	6.069	0.701	3.241	0.323	3.564
	Ι	А	$\chi$	$\eta$	ω	$\omega^{-}$	$\omega^+$	$\Delta \omega^{\pm}$
Arg1	I 7.449	A	χ 4.319	$\eta$	$\omega$	$\omega^{-}$	$\omega^+$	$\Delta \omega^{\pm}$
Arg1 Arg2	I 7.449 6.831	A 1.189 0.374	$\chi$ 4.319 3.602	$\eta$ 6.260 6.458	$\omega$ 1.490 1.005	$\omega^{-}$ 5.531 4.214	$\omega^+$ 1.212 0.612	$\Delta \omega^{\pm}$ 6.742 4.826
Arg1 Arg2 Arg3	I 7.449 6.831 6.365	A 1.189 0.374 0.319	$\chi$ 4.319 3.602 3.342	$\eta$ 6.260 6.458 6.046	$\omega$ 1.490 1.005 0.924	$\omega^{-}$ 5.531 4.214 3.896	$\omega^+$ 1.212 0.612 0.554	$\Delta \omega^{\pm}$ 6.742 4.826 4.450
Arg1 Arg2 Arg3 Arg4	I 7.449 6.831 6.365 6.093	A 1.189 0.374 0.319 -0.023	$\chi$ 4.319 3.602 3.342 3.035	$\eta$ 6.260 6.458 6.046 6.115	$\omega$ 1.490 1.005 0.924 0.753	$\omega^{-}$ 5.531 4.214 3.896 3.406	$\omega^+$ 1.212 0.612 0.554 0.371	$\Delta \omega^{\pm}$ 6.742 4.826 4.450 3.777
Arg1 Arg2 Arg3 Arg4 Asp1	I 7.449 6.831 6.365 6.093 8.106	A 1.189 0.374 0.319 -0.023 1.189	$\chi$ 4.319 3.602 3.342 3.035 4.648	$\eta$ 6.260 6.458 6.046 6.115 6.917	$\omega$ 1.490 1.005 0.924 0.753 1.561	$\omega^{-}$ 5.531 4.214 3.896 3.406 5.879	$\omega^+$ 1.212 0.612 0.554 0.371 1.231	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2	$I \\ 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\$	A 1.189 0.374 0.319 -0.023 1.189 0.975	$\chi$ 4.319 3.602 3.342 3.035 4.648 3.844	$\eta$ 6.260 6.458 6.046 6.115 6.917 5.738	$\omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\$	$\omega^-$ 5.531 4.214 3.896 3.406 5.879 4.856	$\omega^+$ 1.212 0.612 0.554 0.371 1.231 1.012	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3	$I \\ 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\$	A 1.189 0.374 0.319 -0.023 1.189 0.975 0.394	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \end{array}$	$\eta$ 6.260 6.458 6.046 6.115 6.917 5.738 6.083	$\begin{matrix} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \end{matrix}$	$\omega^-$ 5.531 4.214 3.896 3.406 5.879 4.856 4.039	$\omega^+$ 1.212 0.612 0.554 0.371 1.231 1.012 0.603	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4	$I \\ 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\$	A 1.189 0.374 0.319 -0.023 1.189 0.975 0.394 -0.037	$\chi$ 4.319 3.602 3.342 3.035 4.648 3.844 3.436 2.945	$\eta$ 6.260 6.458 6.046 6.115 6.917 5.738 6.083 5.965	$\begin{matrix} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \end{matrix}$	$\omega^-$ 5.531 4.214 3.896 3.406 5.879 4.856 4.039 3.300	$\omega^+$ 1.212 0.612 0.554 0.371 1.231 1.012 0.603 0.354	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1	$I \\ 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\$	$\begin{array}{c} A\\ 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \end{array}$	$\eta$ 6.260 6.458 6.046 6.115 6.917 5.738 6.083 5.965 6.618	$\begin{matrix} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \end{matrix}$	$\omega^-$ 5.531 4.214 3.896 3.406 5.879 4.856 4.039 3.300 5.667	$\omega^+$ 1.212 0.612 0.554 0.371 1.231 1.012 0.603 0.354 1.198	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2	$I \\ \hline 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\ 6.461 \\ \hline$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131 \end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \end{array}$	$\begin{matrix} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \end{matrix}$	$\omega^-$ 5.531 4.214 3.896 3.406 5.879 4.856 4.039 3.300 5.667 4.934	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3	$I \\ \hline 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\ 6.461 \\ 6.342 \\ \hline$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131\\ 0.268\end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \\ 3.305 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \\ 6.073 \end{array}$	$\begin{matrix} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \\ 0.899 \end{matrix}$	$\begin{array}{c} \omega^- \\ 5.531 \\ 4.214 \\ 3.896 \\ 3.406 \\ 5.879 \\ 4.856 \\ 4.039 \\ 3.300 \\ 5.667 \\ 4.934 \\ 3.831 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \\ 0.526 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \\ 4.356 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4	$I \\ \hline 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\ 6.461 \\ 6.342 \\ 6.125 \\ \hline$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131\\ 0.268\\ -0.142 \end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \\ 3.305 \\ 2.992 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \\ 6.073 \\ 6.267 \end{array}$	$\begin{array}{c} \omega \\ \hline 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \\ 0.899 \\ 0.714 \end{array}$	$\begin{array}{c} \omega^- \\ 5.531 \\ 4.214 \\ 3.896 \\ 3.406 \\ 5.879 \\ 4.856 \\ 4.039 \\ 3.300 \\ 5.667 \\ 4.934 \\ 3.831 \\ 3.316 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \\ 0.526 \\ 0.324 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \\ 4.356 \\ 3.640 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1	$\begin{matrix} & I \\ & 7.449 \\ & 6.831 \\ & 6.365 \\ & 6.093 \\ & 8.106 \\ & 6.713 \\ & 6.477 \\ & 5.927 \\ & 7.779 \\ & 6.461 \\ & 6.342 \\ & 6.125 \\ & 7.304 \end{matrix}$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131\\ 0.268\\ -0.142\\ 1.282 \end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \\ 3.305 \\ 2.992 \\ 4.293 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \\ 6.073 \\ 6.267 \\ 6.021 \end{array}$	$\begin{array}{c} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \\ 0.899 \\ 0.714 \\ 1.530 \end{array}$	$\begin{array}{c} \omega^- \\ 5.531 \\ 4.214 \\ 3.896 \\ 3.406 \\ 5.879 \\ 4.856 \\ 4.039 \\ 3.300 \\ 5.667 \\ 4.934 \\ 3.831 \\ 3.316 \\ 5.584 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \\ 0.526 \\ 0.324 \\ 1.291 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \\ 4.356 \\ 3.640 \\ 6.874 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2	$I \\ \hline 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\ 6.461 \\ 6.342 \\ 6.125 \\ 7.304 \\ 6.722 \\ \hline end{tabular}$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131\\ 0.268\\ -0.142\\ 1.282\\ 0.985 \end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \\ 3.305 \\ 2.992 \\ 4.293 \\ 3.853 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \\ 6.073 \\ 6.267 \\ 6.021 \\ 5.736 \end{array}$	$\begin{array}{c} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \\ 0.899 \\ 0.714 \\ 1.530 \\ 1.294 \end{array}$	$\begin{array}{c} \omega^- \\ 5.531 \\ 4.214 \\ 3.896 \\ 3.406 \\ 5.879 \\ 4.856 \\ 4.039 \\ 3.300 \\ 5.667 \\ 4.934 \\ 3.831 \\ 3.316 \\ 5.584 \\ 4.874 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \\ 0.526 \\ 0.324 \\ 1.291 \\ 1.020 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \\ 4.356 \\ 3.640 \\ 6.874 \\ 5.894 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3	$I \\ \hline 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\ 6.461 \\ 6.342 \\ 6.125 \\ 7.304 \\ 6.722 \\ 5.962 \\ \hline \end{cases}$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131\\ 0.268\\ -0.142\\ 1.282\\ 0.985\\ 0.395\\ \end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \\ 3.305 \\ 2.992 \\ 4.293 \\ 3.853 \\ 3.179 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \\ 6.073 \\ 6.267 \\ 6.021 \\ 5.736 \\ 5.566 \end{array}$	$\begin{array}{c} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \\ 0.899 \\ 0.714 \\ 1.530 \\ 1.294 \\ 0.908 \end{array}$	$\begin{array}{c} \omega^- \\ 5.531 \\ 4.214 \\ 3.896 \\ 3.406 \\ 5.879 \\ 4.856 \\ 4.039 \\ 3.300 \\ 5.667 \\ 4.934 \\ 3.831 \\ 3.316 \\ 5.584 \\ 4.874 \\ 3.752 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \\ 0.526 \\ 0.324 \\ 1.291 \\ 1.020 \\ 0.574 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \\ 4.356 \\ 3.640 \\ 6.874 \\ 5.894 \\ 4.326 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4	$I \\ \hline 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\ 6.461 \\ 6.342 \\ 6.125 \\ 7.304 \\ 6.722 \\ 5.962 \\ 5.616 \\ \hline \end{cases}$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131\\ 0.268\\ -0.142\\ 1.282\\ 0.985\\ 0.395\\ 0.395\\ 0.199\\ \end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \\ 3.305 \\ 2.992 \\ 4.293 \\ 3.853 \\ 3.179 \\ 2.907 \end{array}$	$\begin{array}{c} \eta \\ 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \\ 6.073 \\ 6.267 \\ 6.021 \\ 5.736 \\ 5.566 \\ 5.416 \end{array}$	$\begin{array}{c} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \\ 0.899 \\ 0.714 \\ 1.530 \\ 1.294 \\ 0.908 \\ 0.780 \end{array}$	$\begin{array}{c} \omega^- \\ 5.531 \\ 4.214 \\ 3.896 \\ 3.406 \\ 5.879 \\ 4.856 \\ 4.039 \\ 3.300 \\ 5.667 \\ 4.934 \\ 3.831 \\ 3.316 \\ 5.584 \\ 4.874 \\ 3.752 \\ 3.353 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \\ 0.526 \\ 0.324 \\ 1.291 \\ 1.020 \\ 0.574 \\ 0.446 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \\ 4.356 \\ 3.640 \\ 6.874 \\ 5.894 \\ 4.326 \\ 3.799 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4 Lys1	$\begin{matrix} I \\ \hline 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\ 6.461 \\ 6.342 \\ 6.125 \\ 7.304 \\ 6.722 \\ 5.962 \\ 5.616 \\ 8.165 \end{matrix}$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131\\ 0.268\\ -0.142\\ 1.282\\ 0.985\\ 0.395\\ 0.395\\ 0.199\\ 1.149 \end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \\ 3.305 \\ 2.992 \\ 4.293 \\ 3.853 \\ 3.179 \\ 2.907 \\ 4.657 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \\ 6.073 \\ 6.267 \\ 6.021 \\ 5.736 \\ 5.566 \\ 5.416 \\ 7.015 \end{array}$	$\begin{array}{c} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \\ 0.899 \\ 0.714 \\ 1.530 \\ 1.294 \\ 0.908 \\ 0.780 \\ 1.546 \end{array}$	$\begin{array}{c} \omega^- \\ 5.531 \\ 4.214 \\ 3.896 \\ 3.406 \\ 5.879 \\ 4.856 \\ 4.039 \\ 3.300 \\ 5.667 \\ 4.934 \\ 3.831 \\ 3.316 \\ 5.584 \\ 4.874 \\ 3.752 \\ 3.353 \\ 5.858 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \\ 0.526 \\ 0.324 \\ 1.291 \\ 1.020 \\ 0.574 \\ 0.446 \\ 1.201 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \\ 4.356 \\ 3.640 \\ 6.874 \\ 5.894 \\ 4.326 \\ 3.799 \\ 7.060 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4 Lys1 Lys2	$\begin{matrix} I \\ \hline 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\ 6.461 \\ 6.342 \\ 6.125 \\ 7.304 \\ 6.722 \\ 5.962 \\ 5.616 \\ 8.165 \\ 6.812 \end{matrix}$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131\\ 0.268\\ -0.142\\ 1.282\\ 0.985\\ 0.395\\ 0.395\\ 0.199\\ 1.149\\ 0.522 \end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \\ 3.305 \\ 2.992 \\ 4.293 \\ 3.853 \\ 3.179 \\ 2.907 \\ 4.657 \\ 3.667 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \\ 6.073 \\ 6.267 \\ 6.021 \\ 5.736 \\ 5.566 \\ 5.416 \\ 7.015 \\ 6.290 \end{array}$	$\begin{array}{c} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \\ 0.899 \\ 0.714 \\ 1.530 \\ 1.294 \\ 0.908 \\ 0.780 \\ 1.546 \\ 1.069 \end{array}$	$\begin{array}{c} \omega^- \\ 5.531 \\ 4.214 \\ 3.896 \\ 3.406 \\ 5.879 \\ 4.856 \\ 4.039 \\ 3.300 \\ 5.667 \\ 4.934 \\ 3.831 \\ 3.316 \\ 5.584 \\ 4.874 \\ 3.752 \\ 3.353 \\ 5.858 \\ 4.365 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \\ 0.526 \\ 0.324 \\ 1.291 \\ 1.020 \\ 0.574 \\ 0.446 \\ 1.201 \\ 0.698 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \\ 4.356 \\ 3.640 \\ 6.874 \\ 5.894 \\ 4.326 \\ 3.799 \\ 7.060 \\ 5.063 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu2 Glu3 Glu3 His1 His2 His3 His4 Lys1 Lys2 Lys3	$\begin{matrix} I \\ \hline 7.449 \\ 6.831 \\ 6.365 \\ 6.093 \\ 8.106 \\ 6.713 \\ 6.477 \\ 5.927 \\ 7.779 \\ 6.461 \\ 6.342 \\ 6.125 \\ 7.304 \\ 6.722 \\ 5.962 \\ 5.616 \\ 8.165 \\ 6.812 \\ 6.351 \end{matrix}$	$\begin{array}{c} A\\ \hline 1.189\\ 0.374\\ 0.319\\ -0.023\\ 1.189\\ 0.975\\ 0.394\\ -0.037\\ 1.161\\ 1.131\\ 0.268\\ -0.142\\ 1.282\\ 0.985\\ 0.395\\ 0.395\\ 0.199\\ 1.149\\ 0.522\\ 0.494 \end{array}$	$\begin{array}{c} \chi \\ 4.319 \\ 3.602 \\ 3.342 \\ 3.035 \\ 4.648 \\ 3.844 \\ 3.436 \\ 2.945 \\ 4.470 \\ 3.796 \\ 3.305 \\ 2.992 \\ 4.293 \\ 3.853 \\ 3.179 \\ 2.907 \\ 4.657 \\ 3.667 \\ 3.422 \end{array}$	$\begin{array}{c} \eta \\ 6.260 \\ 6.458 \\ 6.046 \\ 6.115 \\ 6.917 \\ 5.738 \\ 6.083 \\ 5.965 \\ 6.618 \\ 5.330 \\ 6.073 \\ 6.267 \\ 6.021 \\ 5.736 \\ 5.566 \\ 5.416 \\ 7.015 \\ 6.290 \\ 5.856 \end{array}$	$\begin{array}{c} \omega \\ 1.490 \\ 1.005 \\ 0.924 \\ 0.753 \\ 1.561 \\ 1.288 \\ 0.970 \\ 0.727 \\ 1.509 \\ 1.352 \\ 0.899 \\ 0.714 \\ 1.530 \\ 1.294 \\ 0.908 \\ 0.780 \\ 1.546 \\ 1.069 \\ 1.000 \end{array}$	$\begin{array}{c} \omega^- \\ 5.531 \\ 4.214 \\ 3.896 \\ 3.406 \\ 5.879 \\ 4.856 \\ 4.039 \\ 3.300 \\ 5.667 \\ 4.934 \\ 3.831 \\ 3.316 \\ 5.584 \\ 4.874 \\ 3.752 \\ 3.353 \\ 5.858 \\ 4.365 \\ 4.077 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.212 \\ 0.612 \\ 0.554 \\ 0.371 \\ 1.231 \\ 1.012 \\ 0.603 \\ 0.354 \\ 1.198 \\ 1.138 \\ 0.526 \\ 0.324 \\ 1.291 \\ 1.020 \\ 0.574 \\ 0.446 \\ 1.201 \\ 0.698 \\ 0.655 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.742 \\ 4.826 \\ 4.450 \\ 3.777 \\ 7.110 \\ 5.867 \\ 4.642 \\ 3.654 \\ 6.865 \\ 6.072 \\ 4.356 \\ 3.640 \\ 6.874 \\ 5.894 \\ 4.326 \\ 3.799 \\ 7.060 \\ 5.063 \\ 4.732 \end{array}$

	$J_I$	$J_A$	$\mathbf{J}_{HL}$	$J_{\chi}$	$J_{\eta}$	$J_{\omega}$	$J_{D1}$	$J_{\omega^-}$	$\mathbf{J}_{\omega^+}$	${\rm J}_{\Delta\omega^{\pm}}$	$J_{D2}$
Arg1	0.49	0.23	0.54	0.13	0.72	0.09	0.74	0.08	0.21	0.29	0.37
Arg2	0.34	0.03	0.34	0.16	0.37	0.03	0.40	0.16	0.00	0.16	0.23
Arg3	0.36	0.02	0.36	0.17	0.38	0.04	0.42	0.18	0.01	0.19	0.26
Arg4	0.24	0.04	0.25	0.14	0.20	0.05	0.25	0.18	0.03	0.21	0.27
Asp1	0.39	0.20	0.44	0.10	0.60	0.08	0.61	0.07	0.16	0.23	0.29
Asp2	0.31	0.14	0.34	0.08	0.45	0.05	0.46	0.03	0.12	0.15	0.19
Asp3	0.39	0.01	0.39	0.19	0.40	0.05	0.45	0.21	0.02	0.23	0.31
Asp4	0.32	0.08	0.33	0.20	0.24	0.07	0.32	0.25	0.05	0.30	0.39
Glu1	0.38	0.23	0.45	0.07	0.62	0.10	0.63	0.13	0.20	0.32	0.40
Glu2	0.31	0.23	0.39	0.04	0.55	0.12	0.56	0.19	0.23	0.42	0.51
Glu3	0.30	0.01	0.30	0.16	0.29	0.04	0.33	0.18	0.02	0.21	0.28
Glu4	0.24	0.09	0.26	0.16	0.15	0.06	0.23	0.21	0.05	0.26	0.34
His1	0.33	0.24	0.41	0.04	0.57	0.13	0.58	0.19	0.24	0.43	0.53
His2	0.30	0.43	0.52	0.07	0.72	0.24	0.76	0.46	0.40	0.86	1.06
His3	0.28	0.05	0.28	0.11	0.32	0.01	0.34	0.10	0.01	0.09	0.13
His4	0.26	0.06	0.27	0.16	0.21	0.06	0.27	0.20	0.04	0.25	0.32
Lys1	0.44	0.22	0.49	0.11	0.66	0.08	0.67	0.07	0.18	0.24	0.30
Lys2	0.34	0.11	0.36	0.12	0.45	0.01	0.46	0.07	0.05	0.02	0.09
Lys3	0.36	0.10	0.37	0.13	0.46	0.00	0.48	0.08	0.05	0.04	0.10
Lys4	0.28	0.03	0.28	0.16	0.25	0.05	0.30	0.19	0.03	0.22	0.29
Average	0.33	0.13	0.37	0.13	0.43	0.07	0.46	0.16	0.11	0.26	0.33

**Table S1B.** Descriptors  $J_I$ ,  $J_A$ ,  $J_{HL}$ ,  $J_{\chi}$ ,  $J_{\eta}$ ,  $J_{\omega}$ ,  $J_{D1}$ ,  $J_{\omega^-}$ ,  $J_{\omega^+}$ ,  $J_{\Delta\omega^{\pm}}$  and  $J_{D2}$  for the natural amino acids bearing a ionizable side-chain at different pHs calculated from the results of Table S1A

**Table S2A.** HOMO and LUMO orbital energies (eV), ionization potential I and electron affinity A (eV), global electronegativity  $\chi$ , chemical hardness  $\eta$ , global electrophilicity  $\omega$ , electrodonating power  $\omega^-$ , electroaccepting power  $\omega^+$  and net electrophilicity  $\Delta \omega^{\pm}$  of natural amino acids bearing a ionizable side-chain at different pHs calculated with the MN12L density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of the KID procedure and the lower part shows the results derived from the calculated vertical  $\Delta$ SCF energies.

	НОМО	LUMO	$\chi_K$	$\eta_K$	$\omega_K$	$\omega_K^-$	$\omega_K^+$	$\Delta \omega_K^{\pm}$
Arg1	-6.875	-1.072	3.974	5.803	1.361	5.071	1.097	6.168
Arg2	-6.384	0.193	3.096	6.578	0.728	3.416	0.320	3.736
Arg3	-5.923	0.285	2.819	6.208	0.640	3.078	0.259	3.336
Arg4	-5.658	0.741	2.458	6.398	0.472	2.574	0.115	2.689
Asp1	-7.651	-1.115	4.383	6.537	1.469	5.539	1.156	6.695
Asp2	-6.262	-0.791	3.527	5.471	1.137	4.379	0.852	5.231
Asp3	-5.959	0.116	2.921	6.074	0.703	3.245	0.324	3.569
Asp4	-5.517	0.693	2.412	6.211	0.468	2.531	0.119	2.650
Glu1	-7.311	-1.083	4.197	6.228	1.414	5.316	1.119	6.435
Glu2	-6.005	-0.984	3.495	5.021	1.216	4.493	0.999	5.492
Glu3	-5.908	0.269	2.820	6.177	0.644	3.083	0.263	3.347
Glu4	-5.757	0.899	2.429	6.655	0.443	2.517	0.088	2.605
His1	-6.835	-1.188	4.011	5.647	1.425	5.208	1.197	6.405
His2	-6.197	-0.945	3.571	5.252	1.214	4.541	0.970	5.511
His3	-5.522	0.077	2.722	5.599	0.662	3.035	0.312	3.347
His4	-5.173	0.398	2.387	5.571	0.511	2.565	0.178	2.742
Lys1	-7.655	-1.064	4.359	6.591	1.442	5.475	1.115	6.590
Lys2	-6.374	-0.083	3.228	6.291	0.828	3.664	0.436	4.100
Lys3	-5.929	-0.050	2.989	5.879	0.760	3.382	0.393	3.774
Lys4	-5.889	0.742	2.573	6.631	0.499	2.700	0.126	2.826
	Ι	А	χ	η	ω	$\omega^{-}$	$\omega^+$	$\Delta \omega^{\pm}$
			70	,				
Arg1	7 971	0 705	2 000	6 546	1.221	4.850	0.852	5.702
0	1.211	0.725	5.990	0.040		<b>1.000</b>	0.004	
Arg2	6.598	-0.138	3.998 3.230	6.736	0.774	3.585	0.355	3.940
Arg2 Arg3	$6.598 \\ 6.129$	0.725 -0.138 -0.307	$3.998 \\ 3.230 \\ 2.911$		$0.774 \\ 0.658$	$3.585 \\ 3.174$	$0.355 \\ 0.263$	$3.940 \\ 3.437$
Arg2 Arg3 Arg4	$\begin{array}{c} 7.271 \\ 6.598 \\ 6.129 \\ 5.891 \end{array}$	0.725 -0.138 -0.307 -0.475	3.998 3.230 2.911 2.708	$\begin{array}{c} 0.540 \\ 6.736 \\ 6.436 \\ 6.366 \end{array}$	$0.774 \\ 0.658 \\ 0.576$	$3.585 \\ 3.174 \\ 2.903$	$\begin{array}{c} 0.352 \\ 0.355 \\ 0.263 \\ 0.196 \end{array}$	$3.940 \\ 3.437 \\ 3.099$
Arg2 Arg3 Arg4 Asp1	$\begin{array}{c} 7.271 \\ 6.598 \\ 6.129 \\ 5.891 \\ 7.938 \end{array}$	$\begin{array}{c} 0.725 \\ -0.138 \\ -0.307 \\ -0.475 \\ 0.754 \end{array}$	3.998 3.230 2.911 2.708 4.346	$\begin{array}{c} 0.340 \\ 6.736 \\ 6.436 \\ 6.366 \\ 7.184 \end{array}$	$\begin{array}{c} 0.774 \\ 0.658 \\ 0.576 \\ 1.314 \end{array}$	3.585 3.174 2.903 5.251	$\begin{array}{c} 0.352 \\ 0.355 \\ 0.263 \\ 0.196 \\ 0.905 \end{array}$	$3.940 \\ 3.437 \\ 3.099 \\ 6.156$
Arg2 Arg3 Arg4 Asp1 Asp2	$\begin{array}{c} 7.271 \\ 6.598 \\ 6.129 \\ 5.891 \\ 7.938 \\ 6.466 \end{array}$	$\begin{array}{c} 0.725 \\ -0.138 \\ -0.307 \\ -0.475 \\ 0.754 \\ 0.454 \end{array}$	$\begin{array}{c} 3.998 \\ 3.230 \\ 2.911 \\ 2.708 \\ 4.346 \\ 3.460 \end{array}$	$\begin{array}{c} 0.340 \\ 6.736 \\ 6.436 \\ 6.366 \\ 7.184 \\ 6.012 \end{array}$	$\begin{array}{c} 0.774 \\ 0.658 \\ 0.576 \\ 1.314 \\ 0.996 \end{array}$	$\begin{array}{c} 3.585\\ 3.174\\ 2.903\\ 5.251\\ 4.097\end{array}$	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\end{array}$	$\begin{array}{c} 3.940 \\ 3.437 \\ 3.099 \\ 6.156 \\ 4.735 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3	$\begin{array}{c} 7.271 \\ 6.598 \\ 6.129 \\ 5.891 \\ 7.938 \\ 6.466 \\ 6.245 \end{array}$	$\begin{array}{c} 0.725 \\ -0.138 \\ -0.307 \\ -0.475 \\ 0.754 \\ 0.454 \\ -0.068 \end{array}$	$\begin{array}{c} 3.998 \\ 3.230 \\ 2.911 \\ 2.708 \\ 4.346 \\ 3.460 \\ 3.089 \end{array}$	$\begin{array}{c} 0.340 \\ 6.736 \\ 6.436 \\ 6.366 \\ 7.184 \\ 6.012 \\ 6.312 \end{array}$	$\begin{array}{c} 0.774 \\ 0.658 \\ 0.576 \\ 1.314 \\ 0.996 \\ 0.756 \end{array}$	$\begin{array}{c} 3.585\\ 3.174\\ 2.903\\ 5.251\\ 4.097\\ 3.450\end{array}$	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\end{array}$	$\begin{array}{c} 3.940 \\ 3.437 \\ 3.099 \\ 6.156 \\ 4.735 \\ 3.812 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4	$\begin{array}{c} 7.271 \\ 6.598 \\ 6.129 \\ 5.891 \\ 7.938 \\ 6.466 \\ 6.245 \\ 5.763 \end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\end{array}$	$\begin{array}{c} 3.998 \\ 3.230 \\ 2.911 \\ 2.708 \\ 4.346 \\ 3.460 \\ 3.089 \\ 2.653 \end{array}$	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\end{array}$	$\begin{array}{c} 3.585\\ 3.174\\ 2.903\\ 5.251\\ 4.097\\ 3.450\\ 2.848 \end{array}$	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194 \end{array}$	$\begin{array}{c} 3.940 \\ 3.437 \\ 3.099 \\ 6.156 \\ 4.735 \\ 3.812 \\ 3.042 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1	$\begin{array}{c} 7.271 \\ 6.598 \\ 6.129 \\ 5.891 \\ 7.938 \\ 6.466 \\ 6.245 \\ 5.763 \\ 7.587 \end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\end{array}$	$\begin{array}{c} 3.998\\ 3.230\\ 2.911\\ 2.708\\ 4.346\\ 3.460\\ 3.089\\ 2.653\\ 4.180\end{array}$	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814 \end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282 \end{array}$	$\begin{array}{c} 3.585\\ 3.174\\ 2.903\\ 5.251\\ 4.097\\ 3.450\\ 2.848\\ 5.080 \end{array}$	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ \end{array}$	$\begin{array}{c} 3.940 \\ 3.437 \\ 3.099 \\ 6.156 \\ 4.735 \\ 3.812 \\ 3.042 \\ 5.980 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2	$\begin{array}{c} 7.271 \\ 6.598 \\ 6.129 \\ 5.891 \\ 7.938 \\ 6.466 \\ 6.245 \\ 5.763 \\ 7.587 \\ 6.209 \end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\end{array}$	3.998 3.230 2.911 2.708 4.346 3.460 3.089 2.653 4.180 3.423	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ \end{array}$	$\begin{array}{c} 3.585\\ 3.174\\ 2.903\\ 5.251\\ 4.097\\ 3.450\\ 2.848\\ 5.080\\ 4.162\\ \end{array}$	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ \end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3	$\begin{array}{c} 7.271 \\ 6.598 \\ 6.129 \\ 5.891 \\ 7.938 \\ 6.466 \\ 6.245 \\ 5.763 \\ 7.587 \\ 6.209 \\ 6.104 \end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\\ -0.204 \end{array}$	3.998 3.230 2.911 2.708 4.346 3.460 3.089 2.653 4.180 3.423 2.950	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\\ 6.308\end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ 0.690\\ \end{array}$	$\begin{array}{c} 3.585\\ 3.174\\ 2.903\\ 5.251\\ 4.097\\ 3.450\\ 2.848\\ 5.080\\ 4.162\\ 3.248\\ \end{array}$	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ 0.299\end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901\\ 3.547 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4	$\begin{array}{c} 7.271 \\ 6.598 \\ 6.129 \\ 5.891 \\ 7.938 \\ 6.466 \\ 6.245 \\ 5.763 \\ 7.587 \\ 6.209 \\ 6.104 \\ 5.912 \end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\\ -0.204\\ -0.550\end{array}$	3.998 3.230 2.911 2.708 4.346 3.460 3.089 2.653 4.180 3.423 2.950 2.681	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\\ 6.308\\ 6.461 \end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ 0.690\\ 0.556\end{array}$	3.585 3.174 2.903 5.251 4.097 3.450 2.848 5.080 4.162 3.248 2.857	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ 0.299\\ 0.176\end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901\\ 3.547\\ 3.032 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1	$\begin{array}{c} 7.271\\ 6.598\\ 6.129\\ 5.891\\ 7.938\\ 6.466\\ 6.245\\ 5.763\\ 7.587\\ 6.209\\ 6.104\\ 5.912\\ 7.220\end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\\ -0.204\\ -0.550\\ 0.949\end{array}$	3.998 3.230 2.911 2.708 4.346 3.460 3.089 2.653 4.180 3.423 2.950 2.681 4.084	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\\ 6.308\\ 6.461\\ 6.271 \end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ 0.690\\ 0.556\\ 1.330\\ \end{array}$	3.585 3.174 2.903 5.251 4.097 3.450 2.848 5.080 4.162 3.248 2.857 5.095	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ 0.299\\ 0.176\\ 1.010\\ \end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901\\ 3.547\\ 3.032\\ 6.105 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2	$\begin{array}{c} 7.271\\ 6.598\\ 6.129\\ 5.891\\ 7.938\\ 6.466\\ 6.245\\ 5.763\\ 7.587\\ 6.209\\ 6.104\\ 5.912\\ 7.220\\ 6.422 \end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\\ -0.204\\ -0.550\\ 0.949\\ 0.619\end{array}$	3.998 3.230 2.911 2.708 4.346 3.460 3.089 2.653 4.180 3.423 2.950 2.681 4.084 3.520	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\\ 6.308\\ 6.461\\ 6.271\\ 5.803 \end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ 0.690\\ 0.556\\ 1.330\\ 1.068\end{array}$	3.585 3.174 2.903 5.251 4.097 3.450 2.848 5.080 4.162 3.248 2.857 5.095 4.258	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ 0.299\\ 0.176\\ 1.010\\ 0.738\end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901\\ 3.547\\ 3.032\\ 6.105\\ 4.997 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3	$\begin{array}{c} 7.271\\ 6.598\\ 6.129\\ 5.891\\ 7.938\\ 6.466\\ 6.245\\ 5.763\\ 7.587\\ 6.209\\ 6.104\\ 5.912\\ 7.220\\ 6.422\\ 5.825\end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\\ -0.204\\ -0.550\\ 0.949\\ 0.619\\ -0.152\end{array}$	3.998 3.230 2.911 2.708 4.346 3.089 2.653 4.180 3.423 2.950 2.681 4.084 3.520 2.837	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\\ 6.308\\ 6.461\\ 6.271\\ 5.803\\ 5.976\end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ 0.690\\ 0.556\\ 1.330\\ 1.068\\ 0.673\\ \end{array}$	3.585 3.174 2.903 5.251 4.097 3.450 2.848 5.080 4.162 3.248 2.857 5.095 4.258 3.138	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ 0.299\\ 0.176\\ 1.010\\ 0.738\\ 0.302 \end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901\\ 3.547\\ 3.032\\ 6.105\\ 4.997\\ 3.440 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4	$\begin{array}{c} 7.271\\ 6.598\\ 6.129\\ 5.891\\ 7.938\\ 6.466\\ 6.245\\ 5.763\\ 7.587\\ 6.209\\ 6.104\\ 5.912\\ 7.220\\ 6.422\\ 5.825\\ 5.437\end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\\ -0.204\\ -0.550\\ 0.949\\ 0.619\\ -0.152\\ -0.240\\ \end{array}$	3.998 3.230 2.911 2.708 4.346 3.089 2.653 4.180 3.423 2.950 2.681 4.084 3.520 2.837 2.599	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\\ 6.308\\ 6.461\\ 6.271\\ 5.803\\ 5.976\\ 5.677\end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ 0.690\\ 0.556\\ 1.330\\ 1.068\\ 0.673\\ 0.595 \end{array}$	3.585 3.174 2.903 5.251 4.097 3.450 2.848 5.080 4.162 3.248 2.857 5.095 4.258 3.138 2.844	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ 0.299\\ 0.176\\ 1.010\\ 0.738\\ 0.302\\ 0.245 \end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901\\ 3.547\\ 3.032\\ 6.105\\ 4.997\\ 3.440\\ 3.089 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4 Lys1	$\begin{array}{c} 7.271\\ 6.598\\ 6.129\\ 5.891\\ 7.938\\ 6.466\\ 6.245\\ 5.763\\ 7.587\\ 6.209\\ 6.104\\ 5.912\\ 7.220\\ 6.422\\ 5.825\\ 5.437\\ 7.973\end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\\ -0.204\\ -0.550\\ 0.949\\ 0.619\\ -0.152\\ -0.240\\ 0.714 \end{array}$	3.998 3.230 2.911 2.708 4.346 3.089 2.653 4.180 3.423 2.950 2.681 4.084 3.520 2.837 2.599 4.344	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\\ 6.308\\ 6.461\\ 6.271\\ 5.803\\ 5.976\\ 5.677\\ 7.259\end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ 0.690\\ 0.556\\ 1.330\\ 1.068\\ 0.673\\ 0.595\\ 1.300\\ \end{array}$	3.585 3.174 2.903 5.251 4.097 3.450 2.848 5.080 4.162 3.248 2.857 5.095 4.258 3.138 2.844 5.225	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ 0.299\\ 0.176\\ 1.010\\ 0.738\\ 0.302\\ 0.245\\ 0.881\\ \end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901\\ 3.547\\ 3.032\\ 6.105\\ 4.997\\ 3.440\\ 3.089\\ 6.106\end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4 Lys1 Lys2	$\begin{array}{c} 7.271\\ 6.598\\ 6.129\\ 5.891\\ 7.938\\ 6.466\\ 6.245\\ 5.763\\ 7.587\\ 6.209\\ 6.104\\ 5.912\\ 7.220\\ 6.422\\ 5.825\\ 5.437\\ 7.973\\ 6.581\end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\\ -0.204\\ -0.550\\ 0.949\\ 0.619\\ -0.152\\ -0.240\\ 0.714\\ -0.014\end{array}$	3.998 3.230 2.911 2.708 4.346 3.089 2.653 4.180 3.423 2.950 2.681 4.084 3.520 2.837 2.599 4.344 3.284	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\\ 6.308\\ 6.461\\ 6.271\\ 5.803\\ 5.976\\ 5.677\\ 7.259\\ 6.595\\ \end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ 0.690\\ 0.556\\ 1.330\\ 1.068\\ 0.673\\ 0.595\\ 1.300\\ 0.818 \end{array}$	3.585 3.174 2.903 5.251 4.097 3.450 2.848 5.080 4.162 3.248 2.857 5.095 4.258 3.138 2.844 5.225 3.689	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ 0.299\\ 0.176\\ 1.010\\ 0.738\\ 0.302\\ 0.245\\ 0.881\\ 0.405 \end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901\\ 3.547\\ 3.032\\ 6.105\\ 4.997\\ 3.440\\ 3.089\\ 6.106\\ 4.094 \end{array}$
Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4 Lys1 Lys2 Lys3	$\begin{array}{c} 7.271\\ 6.598\\ 6.129\\ 5.891\\ 7.938\\ 6.466\\ 6.245\\ 5.763\\ 7.587\\ 6.209\\ 6.104\\ 5.912\\ 7.220\\ 6.422\\ 5.825\\ 5.437\\ 7.973\\ 6.581\\ 6.262\end{array}$	$\begin{array}{c} 0.725\\ -0.138\\ -0.307\\ -0.475\\ 0.754\\ 0.454\\ -0.068\\ -0.456\\ 0.773\\ 0.636\\ -0.204\\ -0.550\\ 0.949\\ 0.619\\ -0.152\\ -0.240\\ 0.714\\ -0.014\\ -0.040\\ \end{array}$	3.998 3.230 2.911 2.708 4.346 3.089 2.653 4.180 3.423 2.950 2.681 4.084 3.520 2.837 2.599 4.344 3.284 3.111	$\begin{array}{c} 6.340\\ 6.736\\ 6.436\\ 6.366\\ 7.184\\ 6.012\\ 6.312\\ 6.219\\ 6.814\\ 5.572\\ 6.308\\ 6.461\\ 6.271\\ 5.803\\ 5.976\\ 5.677\\ 7.259\\ 6.595\\ 6.302\\ \end{array}$	$\begin{array}{c} 0.774\\ 0.658\\ 0.576\\ 1.314\\ 0.996\\ 0.756\\ 0.566\\ 1.282\\ 1.051\\ 0.690\\ 0.556\\ 1.330\\ 1.068\\ 0.673\\ 0.595\\ 1.300\\ 0.818\\ 0.768 \end{array}$	3.585 3.174 2.903 5.251 4.097 3.450 2.848 5.080 4.162 3.248 2.857 5.095 4.258 3.138 2.844 5.225 3.689 3.486	$\begin{array}{c} 0.355\\ 0.263\\ 0.196\\ 0.905\\ 0.637\\ 0.361\\ 0.194\\ 0.900\\ 0.739\\ 0.299\\ 0.176\\ 1.010\\ 0.738\\ 0.302\\ 0.245\\ 0.881\\ 0.405\\ 0.374 \end{array}$	$\begin{array}{c} 3.940\\ 3.437\\ 3.099\\ 6.156\\ 4.735\\ 3.812\\ 3.042\\ 5.980\\ 4.901\\ 3.547\\ 3.032\\ 6.105\\ 4.997\\ 3.440\\ 3.089\\ 6.106\\ 4.094\\ 3.860\\ \end{array}$

	$J_I$	$J_A$	$\mathbf{J}_{HL}$	$J_{\chi}$	$J_{\eta}$	$J_{\omega}$	$J_{D1}$	$J_{\omega^-}$	$\mathbf{J}_{\omega^+}$	$J_{\Delta\omega^{\pm}}$	$J_{D2}$
Arg1	0.40	0.35	0.53	0.02	0.74	0.14	0.76	0.22	0.25	0.47	0.57
Arg2	0.21	0.06	0.22	0.13	0.16	0.05	0.21	0.17	0.03	0.20	0.27
Arg3	0.21	0.02	0.21	0.09	0.23	0.02	0.25	0.10	0.00	0.10	0.14
Arg4	0.23	0.27	0.35	0.25	0.03	0.10	0.27	0.33	0.08	0.41	0.53
Asp1	0.29	0.36	0.46	0.04	0.65	0.15	0.67	0.29	0.25	0.54	0.66
Asp2	0.20	0.34	0.39	0.07	0.54	0.14	0.56	0.28	0.21	0.50	0.61
Asp3	0.29	0.05	0.29	0.17	0.24	0.05	0.30	0.20	0.04	0.24	0.32
Asp4	0.25	0.24	0.34	0.24	0.01	0.10	0.26	0.32	0.08	0.39	0.51
Glu1	0.28	0.31	0.41	0.02	0.59	0.13	0.60	0.24	0.22	0.45	0.56
Glu2	0.20	0.35	0.40	0.07	0.55	0.16	0.58	0.33	0.26	0.59	0.73
Glu3	0.20	0.06	0.21	0.13	0.13	0.05	0.19	0.17	0.04	0.20	0.26
Glu4	0.15	0.35	0.38	0.25	0.19	0.11	0.34	0.34	0.09	0.43	0.55
His1	0.39	0.24	0.45	0.07	0.62	0.09	0.64	0.11	0.19	0.30	0.37
His2	0.23	0.33	0.40	0.05	0.55	0.15	0.57	0.28	0.23	0.51	0.63
His3	0.30	0.07	0.31	0.11	0.38	0.01	0.39	0.10	0.01	0.09	0.14
His4	0.26	0.16	0.31	0.21	0.11	0.08	0.25	0.28	0.07	0.35	0.45
Lys1	0.32	0.35	0.47	0.02	0.67	0.14	0.68	0.25	0.23	0.48	0.59
Lys2	0.21	0.10	0.23	0.06	0.30	0.01	0.31	0.03	0.03	0.01	0.04
Lys3	0.33	0.09	0.35	0.12	0.42	0.01	0.44	0.10	0.02	0.09	0.14
Lys4	0.18	0.24	0.31	0.21	0.06	0.09	0.24	0.29	0.07	0.36	0.47
Average	0.26	0.22	0.35	0.12	0.36	0.09	0.43	0.22	0.12	0.34	0.43

**Table S2B.** Descriptors  $J_I$ ,  $J_A$ ,  $J_{HL}$ ,  $J_{\chi}$ ,  $J_{\eta}$ ,  $J_{\omega}$ ,  $J_{D1}$ ,  $J_{\omega^-}$ ,  $J_{\omega^+}$ ,  $J_{\Delta\omega^{\pm}}$  and  $J_{D2}$  for the natural amino acids bearing a ionizable side-chain at different pHs calculated from the results of Table S2A

**Table S3A.** HOMO and LUMO orbital energies (eV), ionization potential I and electron affinity A (eV), global electronegativity  $\chi$ , chemical hardness  $\eta$ , global electrophilicity  $\omega$ , electrodonating power  $\omega^-$ , electroaccepting power  $\omega^+$  and net electrophilicity  $\Delta \omega^{\pm}$  of natural amino acids bearing a ionizable side-chain at different pHs calculated with the MN12SX density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of the KID procedure and the lower part shows the results derived from the calculated vertical  $\Delta$ SCF energies.

	НОМО	LUMO	$\chi_K$	$\eta_K$	$\omega_K$	$\omega_K^-$	$\omega_K^+$	$\Delta \omega_K^{\pm}$
Arg1	-7.554	-1.079	4.316	6.475	1.439	5.440	1.124	6.564
Arg2	-7.289	-0.429	3.859	6.860	1.086	4.529	0.670	5.200
Arg3	-6.778	-0.383	3.581	6.395	1.002	4.195	0.614	4.809
Arg4	-6.347	0.119	3.114	6.466	0.750	3.461	0.347	3.807
Asp1	-8.591	-1.108	4.849	7.483	1.571	6.035	1.186	7.220
Asp2	-7.257	-0.924	4.090	6.333	1.321	5.083	0.992	6.075
Asp3	-6.981	-0.422	3.702	6.559	1.045	4.350	0.648	4.998
Asp4	-6.346	0.296	3.025	6.642	0.689	3.305	0.280	3.586
Glu1	-8.267	-1.060	4.664	7.207	1.509	5.800	1.136	6.937
Glu2	-7.012	-1.002	4.007	6.009	1.336	5.051	1.044	6.095
Glu3	-6.885	-0.357	3.621	6.528	1.004	4.227	0.606	4.833
Glu4	-6.651	0.302	3.175	6.954	0.725	3.471	0.297	3.768
His1	-7.419	-1.159	4.289	6.260	1.469	5.474	1.185	6.659
His2	-7.052	-0.814	3.933	6.238	1.240	4.836	0.903	5.738
His3	-6.119	-0.476	3.298	5.643	0.963	3.928	0.631	4.559
His4	-5.801	-0.043	2.922	5.759	0.741	3.304	0.382	3.685
Lys1	-8.588	-1.072	4.830	7.516	1.552	5.988	1.159	7.147
Lys2	-7.273	-0.698	3.986	6.575	1.208	4.820	0.834	5.654
Lys3	-6.765	-0.666	3.715	6.099	1.132	4.502	0.787	5.289
Lys4	-6.719	0.158	3.280	6.877	0.782	3.635	0.354	3.989
	Ι	А	$\chi$	$\eta$	ω	$\omega^{-}$	$\omega^+$	$\Delta \omega^{\pm}$
Arg1	I 7.491	A	$\chi$ 4.260	$\eta$ 6.462	$\omega$	$\omega^{-}$	$\omega^+$	$\Delta \omega^{\pm}$
Arg1 Arg2	I 7.491 6.885	A 1.029 -0.307	$\chi$ 4.260 3.289	$\eta$ 6.462 7.193	$\omega$ 1.404 0.752	$\omega^{-}$ 5.342 3.598	$\omega^+$ 1.082 0.309	$\frac{\Delta\omega^{\pm}}{6.425}$
Arg1 Arg2 Arg3	I 7.491 6.885 6.680	A 1.029 -0.307 -0.363	$\chi$ 4.260 3.289 3.158	$\eta$ 6.462 7.193 7.043	$\omega$ 1.404 0.752 0.708	$\omega^{-}$ 5.342 3.598 3.436	$\omega^+$ 1.082 0.309 0.277	$\Delta \omega^{\pm}$ 6.425 3.907 3.713
Arg1 Arg2 Arg3 Arg4	I 7.491 6.885 6.680 6.209	A 1.029 -0.307 -0.363 -0.637	$\chi$ 4.260 3.289 3.158 2.786	$\eta$ 6.462 7.193 7.043 6.847	$\omega$ 1.404 0.752 0.708 0.567	$\omega^{-}$ 5.342 3.598 3.436 2.955	$\omega^+$ 1.082 0.309 0.277 0.169	$\Delta \omega^{\pm}$ 6.425 3.907 3.713 3.124
Arg1 Arg2 Arg3 Arg4 Asp1	I 7.491 6.885 6.680 6.209 8.402	A -0.307 -0.363 -0.637 0.997	$\chi$ 4.260 3.289 3.158 2.786 4.699	$\eta$ 6.462 7.193 7.043 6.847 7.405	$\omega$ 1.404 0.752 0.708 0.567 1.491	$\omega^{-}$ 5.342 3.598 3.436 2.955 5.795	$\omega^+$ 1.082 0.309 0.277 0.169 1.095	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2	I 7.491 6.885 6.680 6.209 8.402 6.756	A 1.029 -0.307 -0.363 -0.637 0.997 0.756	$\chi$ 4.260 3.289 3.158 2.786 4.699 3.756	$\eta \\ 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\$	$\begin{matrix} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \end{matrix}$	$\omega^-$ 5.342 3.598 3.436 2.955 5.795 4.605	$\omega^+$ 1.082 0.309 0.277 0.169 1.095 0.848	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3	I 7.491 6.885 6.680 6.209 8.402 6.756 6.489	A 1.029 -0.307 -0.363 -0.637 0.997 0.756 -0.137	$\begin{array}{c} \chi \\ 4.260 \\ 3.289 \\ 3.158 \\ 2.786 \\ 4.699 \\ 3.756 \\ 3.176 \end{array}$	$\eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ \hline$	$\begin{matrix} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \end{matrix}$	$\omega^-$ 5.342 3.598 3.436 2.955 5.795 4.605 3.524	$\omega^+$ 1.082 0.309 0.277 0.169 1.095 0.848 0.348	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ \hline$	A 1.029 -0.307 -0.363 -0.637 0.997 0.756 -0.137 -0.573	$\chi$ 4.260 3.289 3.158 2.786 4.699 3.756 3.176 2.839	$\eta$ 6.462 7.193 7.043 6.847 7.405 6.000 6.626 6.823	$\begin{matrix} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \end{matrix}$	$\omega^-$ 5.342 3.598 3.436 2.955 5.795 4.605 3.524 3.027	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.188 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ \hline$	$\begin{array}{c} A\\ \hline 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\end{array}$	$\chi$ 4.260 3.289 3.158 2.786 4.699 3.756 3.176 2.839 4.476	$\eta$ 6.462 7.193 7.043 6.847 7.405 6.000 6.626 6.823 6.899	$\begin{matrix} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \end{matrix}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \end{array}$	$\omega^+$ 1.082 0.309 0.277 0.169 1.095 0.848 0.348 0.188 1.097	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ \hline$	$\begin{array}{c} A\\ \hline 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944 \end{array}$	$\chi$ 4.260 3.289 3.158 2.786 4.699 3.756 3.176 2.839 4.476 3.726	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \end{array}$	$\begin{matrix} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \end{matrix}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.348 \\ 1.097 \\ 0.980 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ 6.413 \\ \hline ext{absolute}$	$\begin{array}{c} A\\ \hline 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944\\ -0.371 \end{array}$	$\chi$ 4.260 3.289 3.158 2.786 4.699 3.756 3.176 2.839 4.476 3.726 3.021	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \\ 6.785 \end{array}$	$\begin{matrix} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \\ 0.673 \end{matrix}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \\ 3.280 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.348 \\ 1.097 \\ 0.980 \\ 0.259 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \\ 3.538 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ 6.413 \\ 6.485 \\ \hline ext{abs}$	$\begin{array}{c} A\\ \hline 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944\\ -0.371\\ -0.796\end{array}$	$\chi$ 4.260 3.289 3.158 2.786 4.699 3.756 3.176 2.839 4.476 3.726 3.021 2.845	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \\ 6.785 \\ 7.281 \end{array}$	$\begin{matrix} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \\ 0.673 \\ 0.556 \end{matrix}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \\ 3.280 \\ 2.989 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.348 \\ 1.097 \\ 0.980 \\ 0.259 \\ 0.144 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \\ 3.538 \\ 3.133 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ 6.413 \\ 6.485 \\ 7.449 \\ \hline$	$\begin{array}{c} A\\ \hline 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944\\ -0.371\\ -0.796\\ 1.122 \end{array}$	$\chi$ 4.260 3.289 3.158 2.786 4.699 3.756 3.176 2.839 4.476 3.726 3.021 2.845 4.286	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \\ 6.785 \\ 7.281 \\ 6.326 \end{array}$	$\begin{matrix} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \\ 0.673 \\ 0.556 \\ 1.452 \end{matrix}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \\ 3.280 \\ 2.989 \\ 5.441 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.348 \\ 1.097 \\ 0.980 \\ 0.259 \\ 0.144 \\ 1.156 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \\ 3.538 \\ 3.133 \\ 6.597 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ 6.413 \\ 6.485 \\ 7.449 \\ 6.910 \\ \hline $	$\begin{array}{c} A\\ \hline 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944\\ -0.371\\ -0.796\\ 1.122\\ 0.879 \end{array}$	$\begin{array}{c} \chi \\ 4.260 \\ 3.289 \\ 3.158 \\ 2.786 \\ 4.699 \\ 3.756 \\ 3.176 \\ 2.839 \\ 4.476 \\ 3.726 \\ 3.021 \\ 2.845 \\ 4.286 \\ 3.895 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \\ 6.785 \\ 7.281 \\ 6.326 \\ 6.031 \end{array}$	$\begin{array}{c} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \\ 0.673 \\ 0.556 \\ 1.452 \\ 1.258 \end{array}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \\ 3.280 \\ 2.989 \\ 5.441 \\ 4.840 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.348 \\ 0.188 \\ 1.097 \\ 0.980 \\ 0.259 \\ 0.144 \\ 1.156 \\ 0.945 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \\ 3.538 \\ 3.133 \\ 6.597 \\ 5.784 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ 6.413 \\ 6.485 \\ 7.449 \\ 6.910 \\ 6.096 \\ \hline $	$\begin{array}{c} A\\ \hline 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944\\ -0.371\\ -0.796\\ 1.122\\ 0.879\\ -0.270\\ \end{array}$	$\begin{array}{c} \chi \\ 4.260 \\ 3.289 \\ 3.158 \\ 2.786 \\ 4.699 \\ 3.756 \\ 3.176 \\ 2.839 \\ 4.476 \\ 3.726 \\ 3.021 \\ 2.845 \\ 4.286 \\ 3.895 \\ 2.913 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \\ 6.785 \\ 7.281 \\ 6.326 \\ 6.031 \\ 6.366 \end{array}$	$\begin{array}{c} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \\ 0.673 \\ 0.556 \\ 1.452 \\ 1.258 \\ 0.667 \end{array}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \\ 3.280 \\ 2.989 \\ 5.441 \\ 4.840 \\ 3.188 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.188 \\ 1.097 \\ 0.980 \\ 0.259 \\ 0.144 \\ 1.156 \\ 0.945 \\ 0.275 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \\ 3.538 \\ 3.133 \\ 6.597 \\ 5.784 \\ 3.462 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ 6.413 \\ 6.485 \\ 7.449 \\ 6.910 \\ 6.096 \\ 5.766 \\ \hline \end{cases}$	$\begin{array}{c} A\\ \hline 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944\\ -0.371\\ -0.796\\ 1.122\\ 0.879\\ -0.270\\ -0.328 \end{array}$	$\begin{array}{c} \chi \\ 4.260 \\ 3.289 \\ 3.158 \\ 2.786 \\ 4.699 \\ 3.756 \\ 3.176 \\ 2.839 \\ 4.476 \\ 3.726 \\ 3.021 \\ 2.845 \\ 4.286 \\ 3.895 \\ 2.913 \\ 2.719 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \\ 6.785 \\ 7.281 \\ 6.326 \\ 6.031 \\ 6.366 \\ 6.093 \end{array}$	$\begin{array}{c} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \\ 0.673 \\ 0.556 \\ 1.452 \\ 1.258 \\ 0.667 \\ 0.607 \end{array}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \\ 3.280 \\ 2.989 \\ 5.441 \\ 4.840 \\ 3.188 \\ 2.954 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.188 \\ 1.097 \\ 0.980 \\ 0.259 \\ 0.144 \\ 1.156 \\ 0.945 \\ 0.275 \\ 0.235 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \\ 3.538 \\ 3.133 \\ 6.597 \\ 5.784 \\ 3.462 \\ 3.188 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4 Lys1	$I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ 6.413 \\ 6.485 \\ 7.449 \\ 6.910 \\ 6.096 \\ 5.766 \\ 8.275 \\ \hline \end{cases}$	$\begin{array}{c} A\\ 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944\\ -0.371\\ -0.796\\ 1.122\\ 0.879\\ -0.270\\ -0.328\\ 1.014 \end{array}$	$\begin{array}{c} \chi \\ 4.260 \\ 3.289 \\ 3.158 \\ 2.786 \\ 4.699 \\ 3.756 \\ 3.176 \\ 2.839 \\ 4.476 \\ 3.726 \\ 3.021 \\ 2.845 \\ 4.286 \\ 3.895 \\ 2.913 \\ 2.719 \\ 4.644 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \\ 6.785 \\ 7.281 \\ 6.326 \\ 6.031 \\ 6.366 \\ 6.093 \\ 7.261 \end{array}$	$\begin{array}{c} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \\ 0.673 \\ 0.556 \\ 1.452 \\ 1.258 \\ 0.667 \\ 0.607 \\ 1.485 \end{array}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \\ 3.280 \\ 2.989 \\ 5.441 \\ 4.840 \\ 3.188 \\ 2.954 \\ 5.746 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.188 \\ 1.097 \\ 0.980 \\ 0.259 \\ 0.144 \\ 1.156 \\ 0.945 \\ 0.275 \\ 0.235 \\ 1.102 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \\ 3.538 \\ 3.133 \\ 6.597 \\ 5.784 \\ 3.462 \\ 3.188 \\ 6.849 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4 Lys1 Lys2	$\begin{matrix} I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ 6.413 \\ 6.485 \\ 7.449 \\ 6.910 \\ 6.096 \\ 5.766 \\ 8.275 \\ 6.869 \end{matrix}$	$\begin{array}{c} A\\ 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944\\ -0.371\\ -0.796\\ 1.122\\ 0.879\\ -0.270\\ -0.328\\ 1.014\\ -0.227\end{array}$	$\begin{array}{c} \chi \\ 4.260 \\ 3.289 \\ 3.158 \\ 2.786 \\ 4.699 \\ 3.756 \\ 3.176 \\ 2.839 \\ 4.476 \\ 3.726 \\ 3.021 \\ 2.845 \\ 4.286 \\ 3.895 \\ 2.913 \\ 2.719 \\ 4.644 \\ 3.321 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \\ 6.785 \\ 7.281 \\ 6.326 \\ 6.031 \\ 6.366 \\ 6.093 \\ 7.261 \\ 7.096 \end{array}$	$\begin{array}{c} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \\ 0.673 \\ 0.556 \\ 1.452 \\ 1.258 \\ 0.667 \\ 0.607 \\ 1.485 \\ 0.777 \end{array}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \\ 3.280 \\ 2.989 \\ 5.441 \\ 4.840 \\ 3.188 \\ 2.954 \\ 5.746 \\ 3.658 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.348 \\ 1.097 \\ 0.980 \\ 0.259 \\ 0.144 \\ 1.156 \\ 0.945 \\ 0.275 \\ 0.235 \\ 1.102 \\ 0.337 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \\ 3.538 \\ 3.133 \\ 6.597 \\ 5.784 \\ 3.462 \\ 3.188 \\ 6.849 \\ 3.996 \end{array}$
Arg1 Arg2 Arg3 Arg4 Asp1 Asp2 Asp3 Asp4 Glu1 Glu2 Glu3 Glu4 His1 His2 His3 His4 Lys1 Lys2 Lys3	$\begin{matrix} I \\ \hline 7.491 \\ 6.885 \\ 6.680 \\ 6.209 \\ 8.402 \\ 6.756 \\ 6.489 \\ 6.251 \\ 7.925 \\ 6.508 \\ 6.413 \\ 6.485 \\ 7.449 \\ 6.910 \\ 6.096 \\ 5.766 \\ 8.275 \\ 6.869 \\ 6.435 \end{matrix}$	$\begin{array}{c} A\\ 1.029\\ -0.307\\ -0.363\\ -0.637\\ 0.997\\ 0.756\\ -0.137\\ -0.573\\ 1.026\\ 0.944\\ -0.371\\ -0.796\\ 1.122\\ 0.879\\ -0.270\\ -0.328\\ 1.014\\ -0.227\\ -0.256\end{array}$	$\begin{array}{c} \chi \\ 4.260 \\ 3.289 \\ 3.158 \\ 2.786 \\ 4.699 \\ 3.756 \\ 3.176 \\ 2.839 \\ 4.476 \\ 3.021 \\ 2.845 \\ 4.286 \\ 3.895 \\ 2.913 \\ 2.719 \\ 4.644 \\ 3.321 \\ 3.089 \end{array}$	$\begin{array}{c} \eta \\ \hline 6.462 \\ 7.193 \\ 7.043 \\ 6.847 \\ 7.405 \\ 6.000 \\ 6.626 \\ 6.823 \\ 6.899 \\ 5.564 \\ 6.785 \\ 7.281 \\ 6.326 \\ 6.031 \\ 6.366 \\ 6.093 \\ 7.261 \\ 7.096 \\ 6.691 \end{array}$	$\begin{array}{c} \omega \\ 1.404 \\ 0.752 \\ 0.708 \\ 0.567 \\ 1.491 \\ 1.176 \\ 0.761 \\ 0.591 \\ 1.452 \\ 1.248 \\ 0.673 \\ 0.556 \\ 1.452 \\ 1.258 \\ 0.667 \\ 0.607 \\ 1.485 \\ 0.777 \\ 0.713 \end{array}$	$\begin{array}{c} \omega^- \\ 5.342 \\ 3.598 \\ 3.436 \\ 2.955 \\ 5.795 \\ 4.605 \\ 3.524 \\ 3.027 \\ 5.573 \\ 4.706 \\ 3.280 \\ 2.989 \\ 5.441 \\ 4.840 \\ 3.188 \\ 2.954 \\ 5.746 \\ 3.658 \\ 3.389 \end{array}$	$\begin{array}{c} \omega^+ \\ 1.082 \\ 0.309 \\ 0.277 \\ 0.169 \\ 1.095 \\ 0.848 \\ 0.348 \\ 0.348 \\ 1.097 \\ 0.980 \\ 0.259 \\ 0.144 \\ 1.156 \\ 0.945 \\ 0.275 \\ 0.235 \\ 1.102 \\ 0.337 \\ 0.300 \end{array}$	$\begin{array}{c} \Delta \omega^{\pm} \\ \hline 6.425 \\ 3.907 \\ 3.713 \\ 3.124 \\ 6.890 \\ 5.453 \\ 3.873 \\ 3.215 \\ 6.670 \\ 5.686 \\ 3.538 \\ 3.133 \\ 6.597 \\ 5.784 \\ 3.462 \\ 3.188 \\ 6.849 \\ 3.996 \\ 3.689 \end{array}$

	$J_I$	$J_A$	$\mathbf{J}_{HL}$	$J_{\chi}$	$J_{\eta}$	$J_{\omega}$	$J_{D1}$	$J_{\omega^-}$	$\mathbf{J}_{\omega^+}$	$J_{\Delta\omega^{\pm}}$	$J_{D2}$
Arg1	0.06	0.05	0.08	0.06	0.01	0.03	0.07	0.10	0.04	0.14	0.17
Arg2	0.40	0.74	0.84	0.57	0.33	0.33	0.74	0.93	0.36	1.29	1.63
Arg3	0.10	0.75	0.75	0.42	0.65	0.29	0.83	0.76	0.34	1.10	1.37
Arg4	0.14	0.52	0.54	0.33	0.38	0.18	0.53	0.51	0.18	0.68	0.87
Asp1	0.19	0.11	0.22	0.15	0.08	0.08	0.19	0.24	0.09	0.33	0.42
Asp2	0.50	0.17	0.53	0.33	0.33	0.15	0.49	0.48	0.14	0.62	0.80
Asp3	0.49	0.56	0.75	0.53	0.07	0.28	0.60	0.83	0.30	1.13	1.43
Asp4	0.10	0.28	0.29	0.19	0.18	0.10	0.28	0.28	0.09	0.37	0.47
Glu1	0.34	0.03	0.34	0.19	0.31	0.06	0.37	0.23	0.04	0.27	0.35
Glu2	0.50	0.06	0.51	0.28	0.45	0.09	0.53	0.35	0.06	0.41	0.54
Glu3	0.47	0.73	0.87	0.60	0.26	0.33	0.73	0.95	0.35	1.29	1.64
Glu4	0.17	0.49	0.52	0.33	0.33	0.17	0.49	0.48	0.15	0.63	0.81
His1	0.03	0.04	0.05	0.00	0.07	0.02	0.07	0.03	0.03	0.06	0.08
His2	0.14	0.07	0.16	0.04	0.21	0.02	0.21	0.00	0.04	0.05	0.06
His3	0.02	0.75	0.75	0.38	0.72	0.30	0.87	0.74	0.36	1.10	1.37
His4	0.04	0.37	0.37	0.20	0.33	0.13	0.41	0.35	0.15	0.50	0.63
Lys1	0.31	0.06	0.32	0.19	0.25	0.07	0.32	0.24	0.06	0.30	0.39
Lys2	0.40	0.92	1.01	0.66	0.52	0.43	0.95	1.16	0.50	1.66	2.08
Lys3	0.33	0.92	0.98	0.63	0.59	0.42	0.96	1.11	0.49	1.60	2.01
Lys4	0.09	0.57	0.57	0.33	0.47	0.19	0.61	0.51	0.19	0.70	0.89
Average	0.24	0.41	0.52	0.32	0.33	0.18	0.51	0.51	0.20	0.71	0.90

**Table S3B.** Descriptors  $J_I$ ,  $J_A$ ,  $J_{HL}$ ,  $J_{\chi}$ ,  $J_{\eta}$ ,  $J_{\omega}$ ,  $J_{D1}$ ,  $J_{\omega^-}$ ,  $J_{\omega^+}$ ,  $J_{\Delta\omega^{\pm}}$  and  $J_{D2}$  for the natural amino acids bearing a ionizable side-chain at different pHs calculated from the results of Table S3A

**Table S4A.** HOMO and LUMO orbital energies (eV), ionization potential I and electron affinity A (eV), global electronegativity  $\chi$ , chemical hardness  $\eta$ , global electrophilicity  $\omega$ , electrodonating power  $\omega^-$ , electroaccepting power  $\omega^+$  and net electrophilicity  $\Delta \omega^{\pm}$  of natural amino acids bearing a ionizable side-chain at different pHs calculated with the N12SX density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of the KID procedure and the lower part shows the results derived from the calculated vertical  $\Delta$ SCF energies.

	НОМО	LUMO	$\chi_K$	$\eta_K$	$\omega_K$	$\omega_K^-$	$\omega_K^+$	$\Delta \omega_K^{\pm}$
Arg1	-7.405	-1.028	4.216	6.377	1.394	5.295	1.078	6.373
Arg2	-6.985	0.315	3.335	7.300	0.762	3.647	0.312	3.960
Arg3	-6.177	0.341	2.918	6.517	0.653	3.173	0.255	3.428
Arg4	-6.064	0.866	2.599	6.930	0.487	2.707	0.108	2.815
Asp1	-8.287	-1.017	4.652	7.270	1.489	5.758	1.105	6.863
Asp2	-6.865	-0.740	3.803	6.126	1.180	4.645	0.842	5.486
Asp3	-6.582	0.502	3.040	7.085	0.652	3.267	0.227	3.495
Asp4	-6.018	0.957	2.531	6.975	0.459	2.619	0.089	2.708
Glu1	-7.986	-1.070	4.528	6.916	1.482	5.660	1.133	6.793
Glu2	-6.605	-0.993	3.799	5.612	1.286	4.822	1.023	5.845
Glu3	-6.502	0.642	2.930	7.144	0.601	3.114	0.183	3.297
Glu4	-6.253	1.087	2.583	7.340	0.455	2.660	0.076	2.736
His1	-7.356	-1.131	4.244	6.226	1.446	5.403	1.160	6.563
His2	-6.825	-0.891	3.858	5.934	1.254	4.809	0.950	5.759
His3	-5.950	0.264	2.843	6.213	0.650	3.110	0.268	3.378
His4	-5.653	0.520	2.566	6.173	0.533	2.736	0.170	2.905
Lvs1	-8.320	-1.003	4.662	7.317	1.485	5.758	1.097	6.855
Lvs2	-6.988	0.479	3.255	7.467	0.709	3.513	0.258	3.771
Lvs3	-6.382	0.521	2.931	6.904	0.622	3.141	0.210	3.351
Lvs4	-6.333	1.058	2.638	7.392	0.471	2.722	0.084	2.806
	Ι	А	$\chi$	$\eta$	ω	$\omega^{-}$	$\omega^+$	$\Delta \omega^{\pm}$
Arg1	7.399	1.085	4.242	6.313	1.425	5.366	1.124	6.489
Arg2	6.832	-0.282	3.275	7.114	0.754	3.590	0.315	3.905
Arg3	6.169	-0.307	2.931	6.476	0.663	3.197	0.266	3.463
Arg4	5.969	-0.663	2.653	6.633	0.531	2.802	0.149	2.951
Asp1	8.216	1.070	4.643	7.147	1.508	5.785	1.142	6.927
Asp2	6.672	0.806	3.739	5.866	1.192	4.620	0.880	5.500
Asp3	6.399	-0.214	3.092	6.613	0.723	3.405	0.313	3.719
Asp4	6.007	-0.729	2.639	6.737	0.517	2.774	0.135	2.910
Glu1	7.872	1.123	4.497	6.749	1.498	5.667	1.170	6.873
Glu2	6.517	1.047	3.782	5.470	1.307	4.847	1.065	5.913
Glu3	6.412	-0.506	2.953	6.917	0.630	3.169	0.216	3.386
Glu4	6.173	-0.806	2.684	6.979	0.516	2.810	0.126	2.936
His1	7.365	1.185	4.275	6.180	1.478	5.480	1.206	6.686
His2	6 75 4	0.000	3 861	5,785	1.289	4.869	1 008	5.877
His3	0.734	0.969	0.001	0.100	1.200	1.000	1.000	0.011
$\mathbf{U}_{a}$	$\begin{array}{c} 0.754 \\ 5.904 \end{array}$	-0.179	2.862	6.083	0.673	3.158	0.296	3.454
11184	$     \begin{array}{r}       0.754 \\       5.904 \\       5.599 \\     \end{array}   $	-0.179 -0.414	$2.862 \\ 2.592$	$6.083 \\ 6.014$	$0.673 \\ 0.559$	$3.158 \\ 2.790$	$0.296 \\ 0.197$	$3.454 \\ 2.987$
Lys1		-0.179 -0.414 1.061	$\begin{array}{c} 3.801 \\ 2.862 \\ 2.592 \\ 4.644 \end{array}$	$6.083 \\ 6.014 \\ 7.167$	$0.673 \\ 0.559 \\ 1.505$	$3.158 \\ 2.790 \\ 5.780$	$\begin{array}{c} 1.000\\ 0.296\\ 0.197\\ 1.135\end{array}$	$3.454 \\ 2.987 \\ 6.915$
Lys1 Lys2	$\begin{array}{c} 6.754 \\ 5.904 \\ 5.599 \\ 8.228 \\ 6.824 \end{array}$	$\begin{array}{c} 0.969\\ -0.179\\ -0.414\\ 1.061\\ -0.192\end{array}$	$\begin{array}{c} 3.801 \\ 2.862 \\ 2.592 \\ 4.644 \\ 3.316 \end{array}$	6.083 6.014 7.167 7.016	$\begin{array}{c} 0.673 \\ 0.559 \\ 1.505 \\ 0.784 \end{array}$	$3.158 \\ 2.790 \\ 5.780 \\ 3.664$	$\begin{array}{c} 0.296 \\ 0.197 \\ 1.135 \\ 0.348 \end{array}$	3.454 2.987 6.915 4.011
Lys1 Lys2 Lys3	$\begin{array}{c} 6.754 \\ 5.904 \\ 5.599 \\ 8.228 \\ 6.824 \\ 6.402 \end{array}$	$\begin{array}{c} 0.969\\ -0.179\\ -0.414\\ 1.061\\ -0.192\\ -0.221 \end{array}$	$\begin{array}{c} 3.301 \\ 2.862 \\ 2.592 \\ 4.644 \\ 3.316 \\ 3.091 \end{array}$	$\begin{array}{c} 6.083 \\ 6.014 \\ 7.167 \\ 7.016 \\ 6.623 \end{array}$	$\begin{array}{c} 0.673 \\ 0.559 \\ 1.505 \\ 0.784 \\ 0.721 \end{array}$	$\begin{array}{c} 3.158 \\ 2.790 \\ 5.780 \\ 3.664 \\ 3.401 \end{array}$	$\begin{array}{c} 0.296 \\ 0.197 \\ 1.135 \\ 0.348 \\ 0.311 \end{array}$	$\begin{array}{c} 3.454 \\ 2.987 \\ 6.915 \\ 4.011 \\ 3.712 \end{array}$

	$J_I$	$J_A$	$\mathbf{J}_{HL}$	$J_{\chi}$	$J_{\eta}$	$J_{\omega}$	$J_{D1}$	$J_{\omega^-}$	$\mathbf{J}_{\omega^+}$	$J_{\Delta\omega^{\pm}}$	$J_{D2}$
Arg1	0.01	0.06	0.06	0.03	0.06	0.03	0.08	0.07	0.05	0.12	0.14
Arg2	0.15	0.03	0.16	0.06	0.19	0.01	0.19	0.06	0.00	0.05	0.08
Arg3	0.01	0.03	0.03	0.01	0.04	0.01	0.04	0.02	0.01	0.04	0.04
Arg4	0.09	0.20	0.22	0.05	0.30	0.04	0.30	0.10	0.04	0.14	0.17
Asp1	0.07	0.05	0.09	0.01	0.12	0.02	0.12	0.03	0.04	0.06	0.08
Asp2	0.19	0.07	0.20	0.06	0.26	0.01	0.27	0.02	0.04	0.01	0.05
Asp3	0.18	0.29	0.34	0.05	0.47	0.07	0.48	0.14	0.09	0.22	0.28
Asp4	0.01	0.23	0.23	0.11	0.24	0.06	0.27	0.15	0.05	0.20	0.26
Glu1	0.11	0.05	0.13	0.03	0.17	0.02	0.17	0.01	0.04	0.04	0.06
Glu2	0.09	0.05	0.10	0.02	0.14	0.02	0.14	0.03	0.04	0.07	0.08
Glu3	0.09	0.14	0.16	0.02	0.23	0.03	0.23	0.06	0.03	0.09	0.11
Glu4	0.08	0.28	0.29	0.10	0.36	0.06	0.38	0.15	0.05	0.20	0.26
His1	0.01	0.05	0.05	0.03	0.05	0.03	0.06	0.08	0.05	0.12	0.15
His2	0.07	0.08	0.11	0.00	0.15	0.03	0.15	0.06	0.06	0.12	0.15
His3	0.05	0.08	0.10	0.02	0.13	0.02	0.13	0.05	0.03	0.08	0.09
His4	0.05	0.11	0.12	0.03	0.16	0.03	0.16	0.05	0.03	0.08	0.10
Lys1	0.09	0.06	0.11	0.02	0.15	0.02	0.15	0.02	0.04	0.06	0.08
Lys2	0.16	0.29	0.33	0.06	0.45	0.07	0.46	0.15	0.09	0.24	0.30
Lys3	0.02	0.30	0.30	0.16	0.28	0.10	0.34	0.26	0.10	0.36	0.46
Lys4	0.05	0.27	0.27	0.11	0.32	0.06	0.34	0.16	0.05	0.21	0.27
Average	0.08	0.14	0.17	0.05	0.21	0.04	0.22	0.08	0.05	0.13	0.16

**Table S4B.** Descriptors  $J_I$ ,  $J_A$ ,  $J_{HL}$ ,  $J_{\chi}$ ,  $J_{\eta}$ ,  $J_{\omega}$ ,  $J_{D1}$ ,  $J_{\omega^-}$ ,  $J_{\omega^+}$ ,  $J_{\Delta\omega^{\pm}}$  and  $J_{D2}$  for the natural amino acids bearing a ionizable side-chain at different pHs calculated from the results of Table S4A