SUPPORTING INFORMATION:

Electronic Properties of Amino Acids and Nucleobases: Similarity Classes and Pairing Principles from Chemical Reactivity Indices

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1. Amino Acids: Chemical Reactivity Indices for Individual Classes

Table 1: Mean, maximum and minimum values of the electronegativity χ, the chemical hardness η and the electronphilicity ω for the individual amino acid classes he$^+$, me^0, me$^+$ and se$^-$. The values for the amino acids MET and TRP which are not part of any class are also shown.

Property	he$^+$	me^0	me$^+$	se$^-$	MET	TRP
$\langle\chi\rangle$	2.85	3.17	2.59	3.48	2.83	3.30
$\chi_{\min}$	2.68	3.08	2.54	3.47	–	–
$\chi_{\max}$	2.98	3.30	2.65	3.49	–	–
$\langle\eta\rangle$	5.34	4.85	4.79	4.16	4.47	3.70
$\eta_{\min}$	5.17	4.58	4.73	4.02	–	–
$\eta_{\max}$	5.47	4.99	4.84	4.30	–	–
$\langle\omega\rangle$	0.75	1.04	0.70	1.45	0.89	1.47
$\omega_{\min}$	0.69	0.96	0.67	1.41	–	–
$\omega_{\max}$	0.85	1.18	0.74	1.50	–	–

2. Nucleobases: Chemical Reactivity Indices for Individual Classes

Table 2: Mean, maximum and minimum values of the electronegativity χ, the chemical hardness η and the electronphilicity ω for the individual nucleobase classes Nse^+, Nse^0 and Nse^-.

Property	Nse^+	Nse^0	Nse^-
$\langle \chi \rangle$	2.36	3.33	3.95
χ_{min}	–	–	3.80
χ_{max}	–	–	4.15
$\langle \eta \rangle$	3.09	3.39	3.90
η_{min}	–	–	3.79
η_{max}	–	–	3.98
$\langle \omega \rangle$	0.90	1.63	2.00
ω_{min}	–	–	1.84
ω_{max}	–	–	2.14

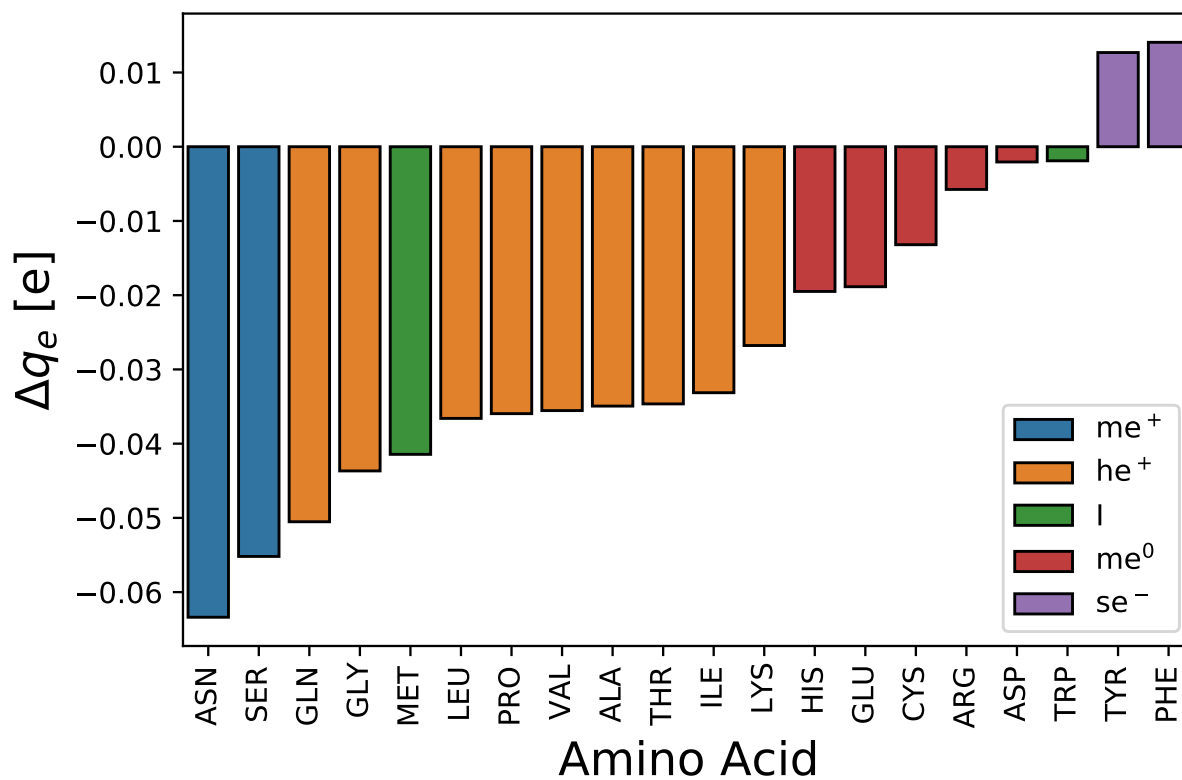# 3. Transferred Charge between Amino Acids and Water Molecules

Figure 1: Transferred charge Δq_e between the amino acids and water molecules.
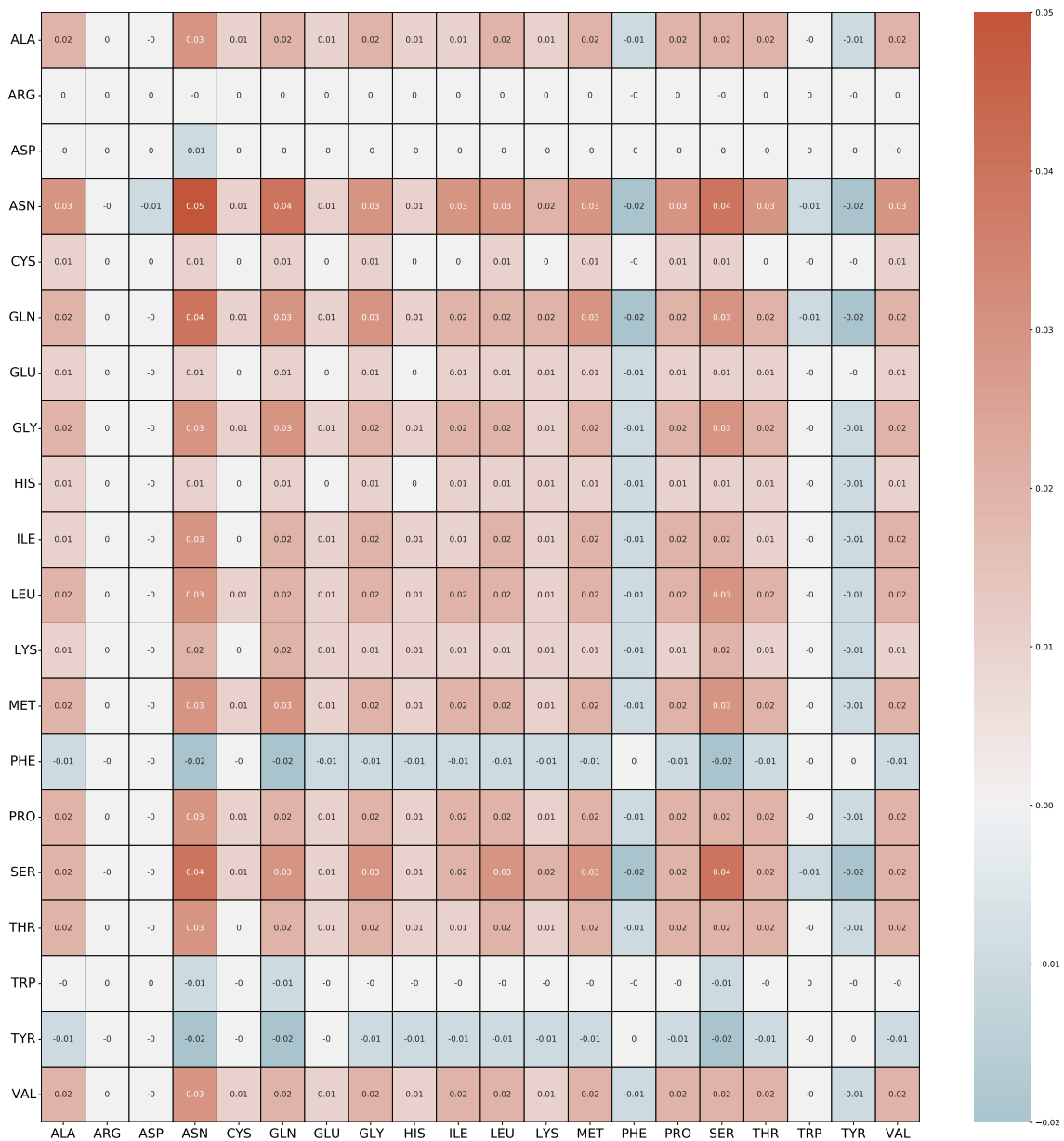
4. Interaction Energies for Amino Acids

Figure 2: Heatmap of interaction energies $\Delta\Delta E_s$ for all pairs of amino acids.
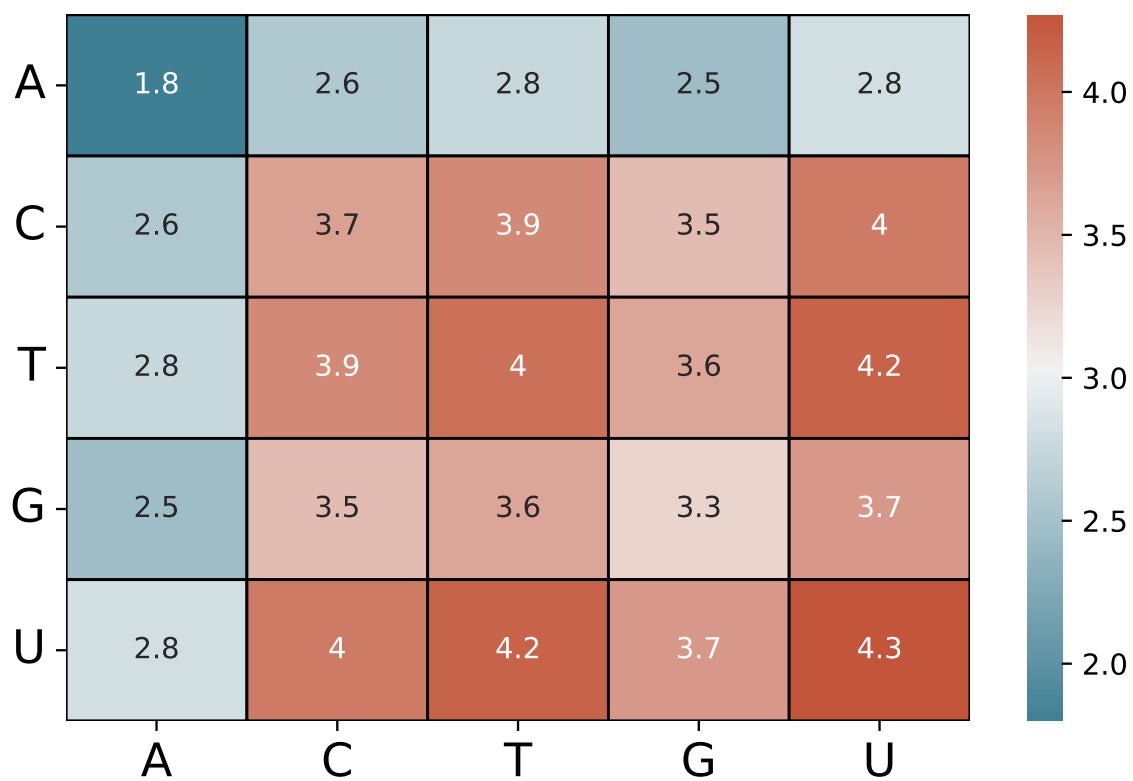
5. Electrophilicity Values for Nucleobase Pairs

Figure 3: Heatmap of product electrophilicities ω_{XY} for all pairs of nucleobases X and Y.