

**EXPLORING RELATEDNESS OF PROTEINS BASED ON ELECTROSTATIC PROPERTIES -  
APPLICATION TO ESTIMATION OF ENZYME KINETIC PARAMETERS**

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Protein molecular interaction fields like electrostatic potentials are key determinants of protein function. PIPSA (Protein Interaction Property Similarity Analysis) is a procedure to compare and analyze protein molecular interaction fields. For the calculation of protein similarity, first the protein electrostatic potential is calculated from the protein structure. From all-pairwise comparisons of the electrostatic potentials, similarity indices are calculated. These indices can then be used for clustering and visualization of proteins as epograms (tree-like diagrams showing electrostatic potential differences) or heat maps. This procedure is automated and can be used via the webPIPSA webserver ([pipsa.eml.org](http://pipsa.eml.org)). PIPSA may assist in protein functional assignment, classification of proteins, the comparison of binding properties and the estimation of enzyme kinetic parameters. Depending on the rate limiting step of the enzyme reaction, the enzyme kinetic parameters can be correlated with differences in molecular interaction fields within a set of enzymes sharing the same structural fold. This allows the estimation of unknown kinetic parameters for proteins where the structure is known or can be modeled using comparative modeling approaches.