

Prediction-based Fingerprints of Protein Interactions

Aleksey Porollo (joint work with Jarek Meller)

The recognition of protein interaction sites is an important intermediate step towards identification of functionally relevant residues and understanding protein function, facilitating experimental efforts in that regard. Toward that goal we propose a novel representation that integrates enhanced relative solvent accessibility (RSA) predictions with high resolution structural data. In particular, we demonstrate that the difference between the predicted and actual (i.e. observed in an unbound structure) RSA of an amino acid residue can be used to significantly improve the discrimination between interacting and non-interacting sites, compared to evolutionary conservation, physico-chemical characteristics, structure-derived and other features considered before. Based on these observations, we develop a new method for the prediction of protein-protein interaction sites, using machine learning approaches to combine the most informative features into the final predictor.