Prediction of the inhibitor specificity to protein kinases based on the amino acid sequences

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The original algorithm was applied for the prediction of protein kinase inhibitors, which allows detection the amino acid positions determining the specificity of a protein to a ligand. The developed method can be applied for the study of other protein families.

Keywords: protein kinases; prediction of the inhibitors; amino acid sequences; specificity patterns; diverged protein families.

The protein kinases present the enzyme family involved into the many normal and pathological processes. The search of selective kinase inhibitors is one of promising direction in the drug design. This task is rather complex due to the significant intersection of ligand specificity among proteins of the given family.

Different methods are used for prediction of the inhibitor specificity to protein kinases, including 3D modelling, phylogenetic analysis and study of the combinatorial protein-ligand space. We applied the original algorithm for obtaining the scores of specificity of the amino acid positions regarding to the certain ligands. Our approach based on the estimation of local similarity in examined amino acid sequence with the sequences from the training set classified in accordance with the protein inhibitor interactions.

Validation with 3D structures of protein kinase complexes with their inhibitors was performed, it confirms the accuracy of our method. In further work our approach will be applied to some other protein families.