Protein-ligand interactions from the perspective of binding specificity

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Abstract

A large number of in-vitro experiments on the inhibition of kinases and proteases are reported in literature, and compiled by ProLINT database. Using this powerful wealth of knowledge, we have carried our an analysis of ligand specificity of these two classes of proteins. Each of the proteases and kinases included in the database has been assigned a consensus ligand fragment signature, based on the available information about its interaction with different ligands. A set of 43 fragments efficiently represent every ligand. We have then organized the consensus fragment signatures for every protein in form of a cluster-tree diagram. This tree is also constructed from other sequence, structure and physical considerations. Cluster-cluster comparison between these analyzes provide a valuable information about ligand specific interactions and similarities between proteins.