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Exploring protein function prediction and ligand-protein associations via computational chemogenomics

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Abstract

Chemogenomics matches target space with ligand space, and vice versa. The underlying assumption of this field are: i) Molecules with enough similarity to ligands for which a target profile is known have a high probability of sharing the same target; ii) Targets sharing similar ligands should have similar binding sites. Protein function is typically associated with the recognition of endogenous ligands. Given the number of available, not yet annotated proteins, it follows that functional prediction will continue to be instrumental in drug discovery programs. To date, putative function for targets with no known ligands has been determined from liganded homologous proteins using sequence and structure comparisons. Problems have long plagued both approaches, thus leading to more focused and concerted efforts employing active site comparisons. We will present our approach toward computational chemogenomics by answering two questions that is, what the putative function of 'a' protein is and what the binding protein partner of 'a' ligand is.Descriptors representing distinct properties of binding pockets of a wide spectrum of proteins (434 complexes or 17 protein families) have been calculated and analyzed statistically in order to predict protein function. Our best model using discriminant function analysis had correct classification rates of 90%. Similarly, descriptors representing features of the ligands bound to these proteins were employed in order to predict the proteins to which they are bound with satisfactory classification rates. Implications and challenges of our approach will also be discussed.

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