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Enhanced Applications of Molecular Libraries

There are many methods to analyze molecular libraries (e.g. peptide libraries, nucleic acid libraries, libraries of polymeric or multipart structures) in terms of their functional properties. Often, these methods relate the covalent structure of the molecules in libraries to their function based on consensus sequence analysis. However, many biological interactions cannot be explained using such simple models. Methods are needed that consider higher order interactions between multiple components of each library molecule, both adjacent to and distributed within the structure.

Prof. Neal Woodbury at the Biodesign Institute of Arizona State University has developed a suite of novel methods, systems and algorithmic processes, for molecular library and array analyses. In one method, the information from one or more molecular libraries is used to relate the primary structure of molecules (e.g. amino acid sequence of a peptide) in a library to their function and to predict the function of molecules not present in the library from their primary structure. Another method uses competitive binding to aid in detecting common functional characteristics among a plurality of molecules on an array to determine complex patterns of interactions. Other methods utilize novel algorithms to analyze molecular array or library data using normalization strategies.

One example application involves using binding data from a target (protein, antibody, nucleic acid, sugar polymer, etc.) binding to a peptide array to generate a closed form equation that predicts what sequences (e.g. in the entire human proteome) that the target would bind to and how that binding would map onto a specific protein.

Another example application involves creating a closed form equation for the immune response to a disease from IgG binding using a series of blood samples from patients and controls. This equation can in turn predict what antigens in the relevant proteome give rise to the immune response, and exactly where on those antigens the interactions take place, providing potential leads for vaccine components or drug targets.

Potential Applications

- Antibody/protein characterization & epitope mapping onto proteomes

- Drug discovery
- Diagnostics, prognoses or treatment specification
- Design of new molecular libraries
- Vaccines – antigen discovery
- Ligand discovery and prediction of protein-protein interactions
- Catalyst development
- Development of coatings with specific properties
- Creation of functional surfaces

Benefits and Advantages

- Provides a closed form equation relating primary structure (sequence) to function that can be applied to any sequence or to proteomes
- Applicable to any molecular library system (peptides, nucleic acids, proteins, sugars & sugar polymers, any of the listed molecules but with non-natural components)
- Can predict the function of molecules in the library and not in the library
- Takes into consideration higher order interactions
- Known biological constraints can be applied to the system to get better predictions
- Enables more defined and better designed array sequences

For more information about the inventor(s) and their research, please see Dr. Woodbury's departmental webpage