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Analysing Protein-Protein Interface using JPIV

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Short Abstract: In this work we present Java Protein Interface Viewer (JPIV). It is a web-based software designed to visualize and analyze protein-protein interfaces. It uses Delaunay triangulation in order to define the interface, and the STING_DB physical-chemical parameters to the analysis process.

Long Abstract:

The interest in protein-protein interactions network is increasing at a faster pace because of their central role in a large number of processes inside and outside the cells, and their key role in controlling most of the cellular regulation pathways. These protein-protein interactions occur mainly in the interface regions of the complex surface. Thus, the knowledge of structures and properties of these interface areas, forces involved and physical-chemical parameters capable of defining these interfaces is of special importance for protein-protein binding sites identification or prediction (Neuvirth et al., 2004; Mintz et al., 2005). Moreover, it is important to bear in mind that this is a special kind of molecular recognition apparatus and the comprehension of this machinery can shed some light over the complex regulatory and metabolic pathways that occur in living organisms, and also help to design drugs for blocking or modifying these interactions. Identification of these interaction patches and their respective properties is a major step to understand the complexes formation (Jiang et al., 2002). One first step in this direction is to make the term interface mathematically precise. More than one characterization is possible. For example, it is common to define the interface taking into account the Solvent Accessible Surface – SAS, or taking other concept from computational geometry. The former is used in Java Protein Dossier – JPD (Neshich et al., 2004) for labeling the Interface Forming Residues (IFR), and the latter is used for defining the average surface between two chains in a protein (Ray et al., 2005). In Ray et al. the authors use Delanauy triangulation and the marching tetrahedra algorithm to render the surface. In this work, the marching tetrahedra algorithm is extended in a twofold way. First, two surfaces are defined, being one for each chain, instead of defining an average surface. This difference is crucial, since only the average of any parameter can be defined over the average surface, resulting in information being lost. Second, the STING_DB was used to introduce a large number of protein sequence and structure parameters. According to

Neshich et. al. (2005) there is more than 300 physical-chemical parameters available in STING_DB. These parameters are used to define both surfaces, i. e., a huge number of physical-chemical parameters can be used to visualize and analyze the interface using JPIV (Java Protein Interface Viewer), which is a new STING suite module. This is performed using a friendly user graphical interface, which enormously facilitate the analysis.

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