

Poster B-63

2D Maps of Protein Surface



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Short Abstract: In this work, we present 2DIM (Two Dimensional Interface Maps). It is a graphical interface that permits to visualize the protein-protein interfaces in 2D maps.

Long Abstract:

In this work, we present 2DIM (Two Dimensional Interface Maps). It is a graphical interface that permits to visualize the protein-protein interfaces in 2D maps. It is known that more than 50% of the Protein Data Bank (PDB) files describe macromolecular structures with two or more chains. It is desirable to get a better understanding of how the protein complexes are gathered together. Although the surface complementarity is a key factor in complexes formation, the physical-chemical properties also play an important role. JPIV (Java Protein Interface Viewer), which is a new STING module, is designed to render the proteins interfaces in 3D, and over them, all the STING DB physical-chemical properties can be painted what greatly facilitated their analyses. Now, 2DIM and JPIV are completely integrated, and it is possible to visualize the 3D JPIV interfaces in 2D maps through 2DIM. The 3D protein interface surfaces were modeled as Graphs and using the Shape Preserving algorithm, they were mapped onto the plane. This mapping introduces some inevitable deformation, nevertheless the local shape is preserved which is essential in the process of matching the corresponding regions in both surfaces. This matching task is almost impossible to 3D due to the surface complexity in the space.