Scientific Web Tool for the Analysis and Visualization of the Packing of Biological Macromolecules

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This Project entails the development of a web tool for the analysis of biological macromolecules, most notably proteins and RNA molecules, and the subsequent visualization of the results. The underlying algorithm uses a Delaunay Triangulation to find and calculate the position and size of cavities. The packing density of atoms is further calculated with a modified Voronoi method. Cavities are biologically significant since they can contain small molecules such as water, which interact with the larger molecule in a variety of ways and are essential for their structure, dynamics and thereby also function. The packing density of a certain region in a molecule is often tied directly to its dynamics and the general density of a structure can be an indicator of the quality of the model. The web tool offers users the possibility of calculation own structures, but also provides a database of pre-calculated structures, coming from the RCSB Protein Data Bank, which is updated weekly with new structures.

Awards Won:

Fourth Award of $500