Protein Structure Comparison Using Computational Geometry Methods

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Methods of computational geometry provide a robust and effective approach to studying topology and architecture of molecular systems, including proteins. In this approach a protein is represented by a set of points in three-dimensional space, where each point designate an amino acid residue. The Delaunay tessellation of this set of points generates an aggregate of space-filling irregular tetrahedra, or Delaunay simplices. The vertices of each simplex define objectively four nearest neighbor residues and a collection of all simplices describes the topology of a protein. This description can be used to compare protein structures, based on the analysis of the specific patterns of spatial proximity of residues forming Delaunay simplices and their positions in the primary sequence. Applications of this method for pairwise protein structure comparison and clustering of proteins into structurally similar groups is discussed.