A Tool for Aligning Cavities of Macromolecules

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Dealing with the difficult problem of the structural alignment of proteins, we built a tool that aligns two protein cavities. The approach consists in projecting geometrical and physico-chemical properties from two cavities onto two discretized spheres located inside the cavities, and then in finding the best correspondence between the descriptors describing the two spheres. This best correspondence gives the alignment of the two cavities. The tool is able to successfully align cavities of G-protein-coupled receptors (built by homology modelling), that can share very low sequence identity (below 5%) on the residues of the cavities.