Relative orientation of the electric dipole moments of proteins in protein complexes.

ABSTRACT

In most biological processes there is a need for cooperation of proteins, which act in tandem. Protein complexes can be formed by a variety of non -covalent interactions, including hydrogen bonds, Van-der Waals and electrostatic interactions. In order to understand the interaction of proteins experimental techniques of high efficiency have been developed for the detection of interacting proteins. Scientists trying to surpass the inability of the experimental techniques to define the relative orientation of interacting proteins develop computational methods capable to provide automatically the three-dimensional structure of protein complexes, such as protein docking.

Our goal was to study the relative orientation of the electric dipole moments of proteins in protein complexes. This is a parameter that could be used in protein docking to identify the probable protein orientations. The result of this study is to obtain probability distributions of the angle between the electric dipole moments of proteins in the complexes. These probability distributions can be then used to improve the results obtained from protein docking.