

Structural Classification and Analysis of Homo Oligomer Interfaces of Proteins

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We tried to classify and analyze all the protein-protein interfaces to further understand the protein-protein interactions, paying attention to the interface of homo oligomer (homo-interface) and the molecular surface of proteins with physicochemical properties on the surfaces.

First, 374 homo-interfaces assumed to be biological interactions were selected for the analyses from 867 SCOP-fold representatives. Then they are classified into *dimer-type*, *cyclic-oligomer-type* and *twisted-type* interfaces according to the rotational symmetry of the interfaces, and the dimer-type interfaces are further classified into *parallel*, *perpendicular* and *circular* classes according to the direction of spreads of interfaces against the crystallographic two-fold axis. In addition, we have analyzed the correlation between the classification and physicochemical properties such as hydrophobic interactions, electrostatic interactions and the shape complementarities of the molecular surface at the interaction sites.

As the results, we have found some strong tendencies between the classification and the physicochemical properties. For examples, (1) for the twisted-type interface, hydrophobic interactions and shape complementarities are preferably used, and (2) the parallel dimer-type interfaces tend to use hydrophobic interactions, but the perpendicular dimer-type interfaces are usually used electrostatic interactions.

Keywords: structure-function relationships, protein-protein interactions, interface surface