Organizing 3D Project Data for Structure-Based Drug Design

Markus Kossner

Chemical Computing Group
Kaiser-Wilhelm-Ring 11, 50672 Köln, Germany

It is often desirable to organize disparate crystallographic project data into a common homogeneous format, ready to use for modelling. We present a web-based application that permits users to specify numerous options controlling superposition and alignment of structures in a family or project, ligand specification, and whether electron densities or other grids are to be included. The final result is a project database containing superposed structures all in the same frame of reference. From here, structures can be dynamical regrouped, for example by scaffold class, for easy management, and can be easily browsed and used as a starting point for further research. The system is able to handle multi-subunit complexes, including structures which may be missing subunits, by using a novel algorithm to determine which subunits of each complex correspond to each other.

Specific applications of the output database files include family-based homology modeling, which benefit from a highly enriched source for templates and loop conformations; and family-specific searching and further filtering of structures.