

Web interface with advanced query properties for the Binding Interface (BIF) database

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The amount of structural and energetic data on biomacromolecules and their complexes is constantly growing. The data is of great value for applications such as molecular modeling, drug discovery, or chemogenomics.^[1] Currently, the data is distributed over many different databases. To integrate the information, the Binding Interface (BIF) database has been developed in our group as a MySQL-based relational database system.^[2] At the heart of the BIF is the structural information from the PDB. This information is augmented with additional relations based on a hierarchical molecule model and a mol2 atom type classification. Ligands, potential binding pockets, and binding interfaces are identified and integrated. Energetic information from the PDBbind database and the BindingDB, DrugScore potential fields, and information from the catalytic site atlas (CSA), the SCOP and the CATH database are added.

To fully exploit the large amounts of available data in the BIF database, an efficient data handling capability is crucial. To this aim, a web interface is currently under development that provides a powerful, yet intuitive tool for accessing the data. The interface can be queried by PDB code, or by any structural or energetic property of the molecules. The search results can be saved as pdb- or mol2-file, or as tabular report in a text file. In addition, statistical analyses will be possible. To visualize the results, the retrieved data can directly be piped to Pymol, where the hierarchical molecule model will be kept.

We expect the BIF – in conjunction with its new interface – to be a valuable tool for drug discovery and structural bioinformatics. It will be possible to generate datasets for testing or developing new docking tools and scoring functions, and to extract various types of knowledge from the data. In addition, the BIF is believed to be an interesting tool for chemogenomics applications, such as analyzing the similarity between different binding pockets. The BIF and its interface are designed and implemented in such a way that the database can easily be expanded.

[1] J. C. Hermann, R. Marti-Arbona, A. A. Fedorov, E. Fedorov, S.C. Almo, B. K. Shoichet, F. M. Raushel, *Nature* **2007**, *448*, 775-779.

[2] T. Jimenez, S. Derksen, E. Schmidt, S. Radestock, C. Wendel, H. Gohlke, *Unpublished results*.