



interactions between functionalities on the protein and those on the ligand. It is even possible to search the database for similar active site cavities to a given query (done on the basis of homology) and superimpose the retrieved complexes in the supplied 3D structural viewer.

Relibase+ extends the functionality of Relibase by supporting input of proprietary protein structures to a locally installed version of the PDB, by allowing users to store and manipulate (via Boolean algebra) retrieved hitlists and by supporting cavity similarity searching on the basis of shape and detected binding features (CavBase). WaterBase allows crystallographers and modellers to explore water clusters in crystal structures, and will warn users if it detects the likelihood of a wrongly-assigned water molecule, for example. If used alongside the Cambridge Structural Database (CSD), Relibase+ can assess whether ligand geometry is optimal by checking the occurrence of each given bond length, distance or torsion angle in the CSD, and graphing the data for ease of interpretation.

Check out the web site to explore Relibase – but unless you're an academic user you need to do that in the next couple of months, as, from January 2008, Relibase will only be available free of charge to academic users.

**Relibase supports cavity similarity searching on the basis of shape and binding features**

For more information, or to arrange an evaluation of Relibase+, contact the CCDC ([admin@ccdc.cam.ac.uk](mailto:admin@ccdc.cam.ac.uk)).

## Instant-JChem

**ChemAxon**

*Reviewed by Tobias Kind, University of California at Davis, US*

Instant-JChem is an out-of-the-box desktop application for storing and searching chemical structures and their properties from ChemAxon. It is a multi-platform (LINUX, Windows, Mac OS X) and multiprocessor friendly program. The Personal Edition is free for everyone and the Enterprise version is free for academic teaching and research. Instant-JChem is very intuitive and aimed at beginners and experts in the field of cheminformatics and bioinformatics. It can import and export the most common file formats like SDF, SMILES and RDF reaction files.

The integrated molecule editor can be used to curate 2D and 3D molecular structures within the database. The 'Standardizer' module allows a pre-treatment of structures during import such as aromatisation and canonicalisation for proper database search and steps like salt and fragment removal which are important for handling diverse structural datasets.



The project window contains the different projects and user databases in a compact folder style setting. The compound view includes a grid view showing multiple structures at a time or a form editable, single record report view for compound warehousing or drug data handling.

The query window is used for substructure, similarity and fragment search. It includes a powerful chemical terms filter which can be used to filter compounds according to their bioavailability, or Lipinski Rule of Five, or other single or combined structure based arguments.

Chemical terms can be computed for every structure in the database and includes functions like IUPAC-Name, logP, pKa, logD and hundreds of other properties, as well as molecular topology descriptors and more complex calculations like number of tautomers and stereoisomers.

Local database search is fast and hundreds of thousands of structures can be handled on a commodity laptop or personal computer. The overlap function allows a quick overlap calculation of two different databases and is a highlight among many other functions.

IJC Personal is free for all and the free academic package permits all IJC functionality (as well as all of other ChemAxon products). Given that IJC is a most powerful device for working with chemistry and other data, and that most of the functionality is included in the free Personal version, this should be very good news for anyone interested in working with chemical data.

For more information contact [sales@chemaxon.com](mailto:sales@chemaxon.com)

## ConturRDC

**Contur**

*Reviewed by Bo Skoog, Biovitrum, Sweden*

We are in the process of switching to ConturRDC to take control of the raw data from our instruments. Previously we saved the raw data manually every month and also manually entered the file names into our electronic lab notebooks (ELN). ConturRDC automates this process