

# digital briefs

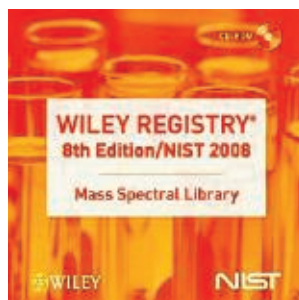
NEW SOFTWARE AND WEBSITES FOR THE CHEMICAL ENTERPRISE

## DATABASE

**PSILO** is a database system that provides a central repository for protein-drug-complex and macromolecule structural data and computational models. Crystallographers and computational modelers can use PSILO's Web-based interface to search and download structures from public sources, such as the Protein Data Bank (PDB), or to store proprietary structures. The software safeguards such proprietary data and allows collaborative edits to and annotation of in-house structures by multiple users. PSILO integrates into Web browser search bars and enables users

management programs installed. **Chemical Computing Group**, [www.chemcomp.com](http://www.chemcomp.com)

The **Wiley Registry 8th Edition/NIST 2008 Mass Spectral Library**, a combination of two trusted collections in mass spectrometry, was recently released by John Wiley & Sons. The updated database



now features an electron ionization mass spec library with more than 560,000 spectra, a

structure library with more than 348,000 searchable structures, and more than 2 million chemical names and synonyms. The complete NIST software suite—including MS Search, MS Interpreter v2.0, and AMDIS—comes with every Wiley registry/NIST 2008 library license. Users can search the collection for small-molecule organics, pharmaceuticals, illegal drugs, poi-

sons, steroids, chemical warfare agents, and environmental pollutants. The database software is compatible with instruments manufactured by most mass spec instrumentation companies, including Agilent, Bruker, JEOL, Leco, PerkinElmer, ThermoFisher Scientific, Varian, and Waters. **John Wiley & Sons**, [www.wiley.com/go/databases](http://www.wiley.com/go/databases)

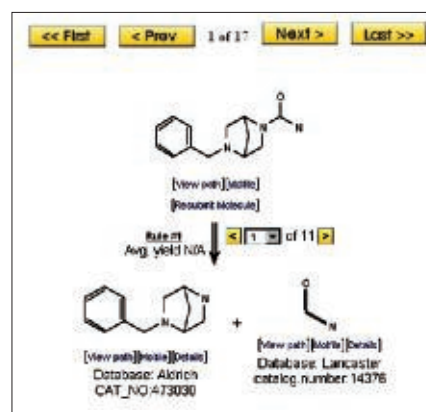
## SOFTWARE

**ActivityBase v7.2** is a drug discovery data management system that can be used by scientists to capture, analyze, and store experimental data from high-throughput screening, secondary screening, or compound profiling and complex in vitro assays. The software can be used

in conjunction with plate-based and non-plate-based assays, including RNAi assays, ELISA, TaqMan assays, and MS/HPLC. Users can process data collected from a few plates to hundreds of plates, which can generate hundreds of thousands of data points. ActivityBase allows vi-

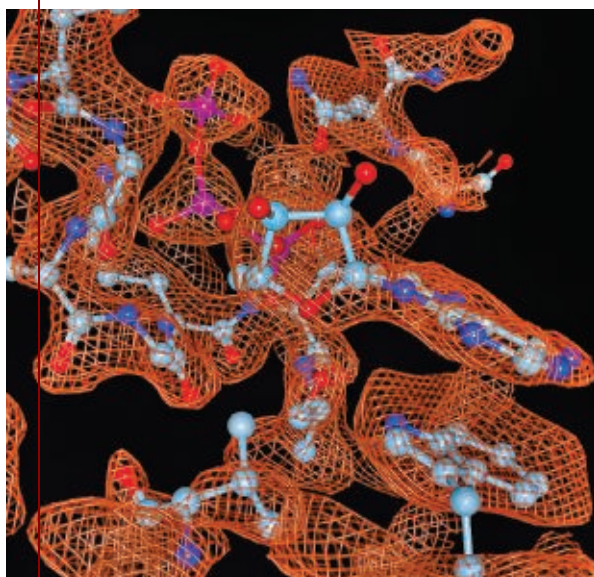
ualization of data in two and three dimensions, enabling identification of trends in results and potential experimental errors. Chemists using the software can register, search for, and display chemical information with associated biological data. Advanced structure searching includes substructure, superstructure, exact match, and similarity, and an advanced stereochemistry representation system is also available. The ActivityBase suite is integrated with Microsoft Excel and now includes the Excel Designer, a user-friendly front-end tool for building and editing data analysis templates quickly. **IDBS**, [www.idbs.com/ActivityBase](http://www.idbs.com/ActivityBase)

**ARChem** (Automated Retrosynthetic Chemistry) Route Designer is a new software tool that aids synthetic chemists in planning organic synthesis. The software employs reaction databases such as CrossFire and Accelrys' Methods of Organic Synthesis (MOS), starting material catalogs such as those from Aldrich and Lancaster, and optional user input to aid in viable synthetic route design. With chemical perception algorithms, ARChem identifies reaction cores and generalizes reaction rules to make a retrosynthetic "solution tree" for a user's target molecule. The tree can be navigated, and every step along the chosen route is illustrated with examples from the literature. ARChem's exhaustive analysis is controlled by algorithms and rules that prevent combinatorial explosion. In addition, users can adjust the search depth and scope by targeting



and protecting bonds. ARChem has a Web-based user interface and can be integrated with electronic notebooks in the lab. **SimBioSys**, [www.simbiosys.ca](http://www.simbiosys.ca)

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to track favorite searches and hit lists. In addition, the system is capable of graphically comparing structure files, displaying electron densities for structures (shown), and illustrating active-site protein-ligand interactions. PSILO can be customized to work with nonstandard PDB files but requires users to already have either Oracle or MySQL database