



reference management systems, Word or Excel files or PDF – a great improvement from the rather clumsy output created by CrossFire Commander. Alternatively to the built-in Marvin Sketch structure editor one can use the CrossFire editor or Symyx Draw.

Reaxys is 100 per cent web based (using Java), and the developers have learned from previous experience, for example with CrossFire Web. The power-user would prefer to install an application with much reduced loading times; one can only hope that speed bottlenecks are solved in the future.

The synthesis planning feature is reminiscent of the reaction planner in Symyx Isentris. Reaxys's display of chemical reactions is almost perfect in readability and gives a better overview of reaction sequences compared to SciFinder. Clearly with Reaxys, the importance of the specialised CrossFire suite of databases as a necessary addition to the comprehensive Chemical Abstracts databases is strengthened.

Query options include reactions, substances and properties, text, authors and more. Intuitively one can create even complicated reaction pathways called synthesis

**Reaxys simplifies chemical database searching**

**'Reaxys creates a renaissance for the use of data from the formerly known Beilstein and related databases'**

plans by asking for syntheses of intermediates. This will not only help research chemists find syntheses of known compounds or precedence of analogous reactions; it also helps students to get an excellent overview of any areas they might be interested in. Markush queries will find prophetic substances from patents.

In summary Reaxys clearly creates a renaissance for the use of data from the formerly known Beilstein and related databases. With these high quality, deeply indexed data in the background, Reaxys might replace the concept of Beilstein. As it also includes very important patent information drilled down to reaction procedure texts, the scientific community will also become increasingly aware of the importance of patents, too.

For more information see [www.info.reaxys.com](http://www.info.reaxys.com)

**iLabber**

**Contur Software AB**

*Reviewed by Evert Homan, Beactica AB, Sweden*

In September 2008, Beactica implemented iLabber, an electronic

laboratory notebook (ELN) system available as an online service from Contur Software. iLabber is based on the company's server-based enterprise ELN solution ConturELN.

Being a small specialist drug discovery company, Beactica opted for a software as a service model, as it was much cheaper to implement with no up-front costs.

This means that we have benefited from a full-scale ELN system without having to invest in any hardware, licenses or maintenance. As it is also fully scalable, more users can be easily added as the need grows.

Getting started with iLabber was straightforward, as users only need to download the desktop client. The system is very intuitive and even users without previous experience with electronic lab notebooks were using iLabber directly.

Our scientists have easy access to their own experiments, both ongoing and finished ones, in iLabber's 'My Lab Notebook'. Colleagues' notebooks and project notebooks are readily accessible in the notebook library.

The search tool in iLabber is powerful, comprising a flexible free

text search function that searches through all textual content in the experiments. Searching can also be done by chemical structure, project, date intervals and more. Chemical search capabilities are powered by ChemAxon's JChem Cartridge.

The Related Experiment section allows for creating cross-references between experiments, which is very helpful. By using the Share Experiment function colleagues can be invited to different workgroups and share experiments. Experiments can also be cloned and converted to user-sharable templates, which saves documentation time.

A much appreciated function with the iLabber software is the digital countersigning option. Securing intellectual property in a reliable, tractable system is vital for Beactica's business. As all experiment records are stored as PDF files, it doesn't require the need to print and store submitted experiments on paper. All data is securely and confidentially backed up by Contur.

For further information visit [www.ilabber.com](http://www.ilabber.com)

## WebCSD

**Cambridge Crystallographic Data Centre**  
Reviewed by Susan Boyd, *CompChem Solutions, UK*

The Cambridge Structural Database (CSD) has been around for many years, and is now firmly established as an invaluable resource for crystallographers, medicinal chemists and molecular modellers, comprising around 500 000 small molecule crystal structures. Recently the Cambridge Crystallographic Data Centre (CCDC) has developed a web portal to query the database, making access easier than ever before. No software installation is needed, and users see updates to the database as soon as they have been processed. With such a setup, the system is ideally placed for running e-practicals in the classroom, as well as enabling easier rollout for commercial organisations.

But it is not just a new look and feel; new functionality has also been added to the WebCSD interface. The fingerprint-based similarity search

**'CCDC has developed a web portal to query their database'**

may be of particular interest for exploring the crystal structures of compounds similar to a query, and the use of hyperlinked referencing on top of an SQL-based relational database system should impress most users with the Google-like search speeds it can achieve for full-text searching. Results are presented with the aid of an integrated molecular visualiser, showing both 2D and 3D molecular representations together with keyword hyperlinks to other CSD entries. Results can be exported in several formats.

At present users can only access WebCSD via the internet, but later this year an intranet version of the system is planned, to support users who would like to query proprietary data with the portal.

A demo version of WebCSD which accesses the 'teaching database' subset of the CSD can be found at [http://webcsd.ccdc.cam.ac.uk/teaching\\_database\\_demo.php](http://webcsd.ccdc.cam.ac.uk/teaching_database_demo.php) and can be used for teaching purposes as well as for familiarisation with the WebCSD structure browsing system.

The screenshot displays the WebCSD web portal interface. At the top, there is a navigation bar with tabs for Home, Substructure Search, Similarity Search, Text/Numeric Search, Reduced Cell Search, Browse CSD, News, and Help. The main content area shows search results for entry KEJBUW, identified as 3-Chloro-2-phenylbenzo-γ-pyrone. A 3D ball-and-stick model of the molecule is shown on the left, and a 2D chemical structure diagram is on the right. The diagram includes the molecular formula C<sub>15</sub>H<sub>11</sub>ClO<sub>2</sub>, space group P 2<sub>1</sub>/n, unit cell parameters a 9.317(3), b 14.991(2), c 8.848(4), angles α 90, β 94.45(3), γ 90, R-Factor 5.4%, and temperature (K) Room Temp. (283-303). The interface also includes a search filter sidebar, a 'Show Symmetry' section with radio buttons for None, Unit Cell, and Packing, and a 'Launch External Viewer' button. At the bottom, it states: 'Added to CSD: 7th September 1990; Last modified: 13th July 2002; Published in WebCSD: 18th March 2009 23:44:33'.