Chemical Database Service

NEWSLETTER

Issue 13   January 2001

The **Chemscape** system is now running on the CDS server. This provides access via the web to the organic databases normally accessed through **ISIS**. The major reaction databases are available via **ReactionWeb** and the Available Chemicals Directory (ACD) is also accessible. The articles on pages 2, 3 and 5 give more details.

There have been significant **hardware upgrades** to the main server since the last Newsletter. Typical searches now run **twice as fast** as they did 6 months ago. See the article on page 9 for more details of the upgrades.

IsoStar performance has been improved with the introduction of a client/server system for PCs. More information and details of how to obtain the client software are given on page 10.

MDL's **LitLink** is now available from CDS. The LitLink system provides automatic linking from citations retrieved from a database to original journal articles stored on literature websites. This single click reference service works with ReactionWeb as well as with the ISIS Reaction Browser on a PC. It also operates with Beilstein Commander on references retrieved from the Beilstein database. A fuller description is provided in the article on page 7.

All **CDS support** calls should now be sent directly to us (email: cdsbb@dl.ac.uk, phone: 01925 603162) and not to the Computer Helpdesk/User Interface Group.

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Chemscape Server

Chemscape is the web based equivalent of ISIS. It allows access, via a web browser, to the organic databases otherwise available through the ISIS client/server system. A Chemscape server is currently running on CDS together with four applications, giving access to a number of databases. These are:

- ACD - Available Chemicals Directory
- ReactionWeb - main organic reaction databases
- MDPI - Molecular Diversity Preservation International database
- Chirbase - Chirbase Chiral Separation by Chromatography database

The ACD and ReactionWeb applications are described later in this newsletter. The MDPI and Chirbase applications access the ISIS databases of the same name.

Browser requirements to use Chemscape

In order to use the Chemscape system, you need the Chime Pro plugin installed in your browser (note that this is not the same as the freely available Chime plugin). This plugin is available, to registered CDS users only, from the download section of the CDS website. Hardware and software requirements are listed on the site, but in summary Chime Pro works with Internet Explorer and Netscape on a PC or with Netscape on a Mac. No other platforms are supported.

For the preparation of structural queries, the Chemscape system uses ISIS/Draw, though other drawing packages can be used. ISIS/Draw can be downloaded from the CDS website (as part of the ISIS/Client package), for those who do not already have it on their machines. It is also freely available for academic use from MDL's website at http://www.mdli.com.

Accessing the databases

The databases can be accessed by following the links for access to data on the CDS website, or directly using the following URLs:

http://cds.dl.ac.uk/acd	ACD
http://cds.dl.ac.uk/rxnweb	ReactionWeb
http://cds.dl.ac.uk/mdpi	MDPI
http://cds.dl.ac.uk/chirbase	Chirbase

ReactionWeb

ReactionWeb is the web based equivalent of the ISIS Reaction Browser. It contains most of the functionality of the Browser and runs under the Chemscape System (see the article above on Chemscape for web browser requirements).

ReactionWeb provides access to nearly 1,000,000 reactions from the same databases which are available in the Reaction Browser, except for Solid Phase Synthesis and BioCatalysis. These last two databases should be available shortly.

ReactionWeb can be accessed from the link on the CDS website or directly using the URL

http://cds.dl.ac.uk/rxnweb

You will be prompted for a username and password and should use your usual CDS id and password.

ReactionWeb 'transformation' query form.

Using ReactionWeb

Using ReactionWeb is very similar to using the Reaction Browser. Queries are composed on one of several query forms (the picture above shows a query in the 'transformations' query form) selected on login. Text search fields are selected using pop-up lists and many fields have associated vocabulary lists. Structural queries are prepared in ISIS/Draw, which is started by double clicking in the appropriate structure box.

Like the Reaction Browser, the results page has a number of different 'forms' which display data about the hits (see picture below). In addition, you can specify the number of hits displayed per page or you can view the complete set of data available for an individual hit. A clustering option is also available. This allows you to group the hits into clusters based on a field you have selected, with all the hits in a given cluster having the same value for that field.

ReactionWeb is LitLink enabled (see article later in this newsletter about LitLink). Clicking on any retrieved reference will transfer you to our LitLink Server and display a list of links to sites from where the article can be retrieved.

Unlike the Reaction Browser, however, ReactionWeb has no list saving functionality. Neither hitlists or queries can be saved for later use.

ReactionWeb results display using 'summary' form
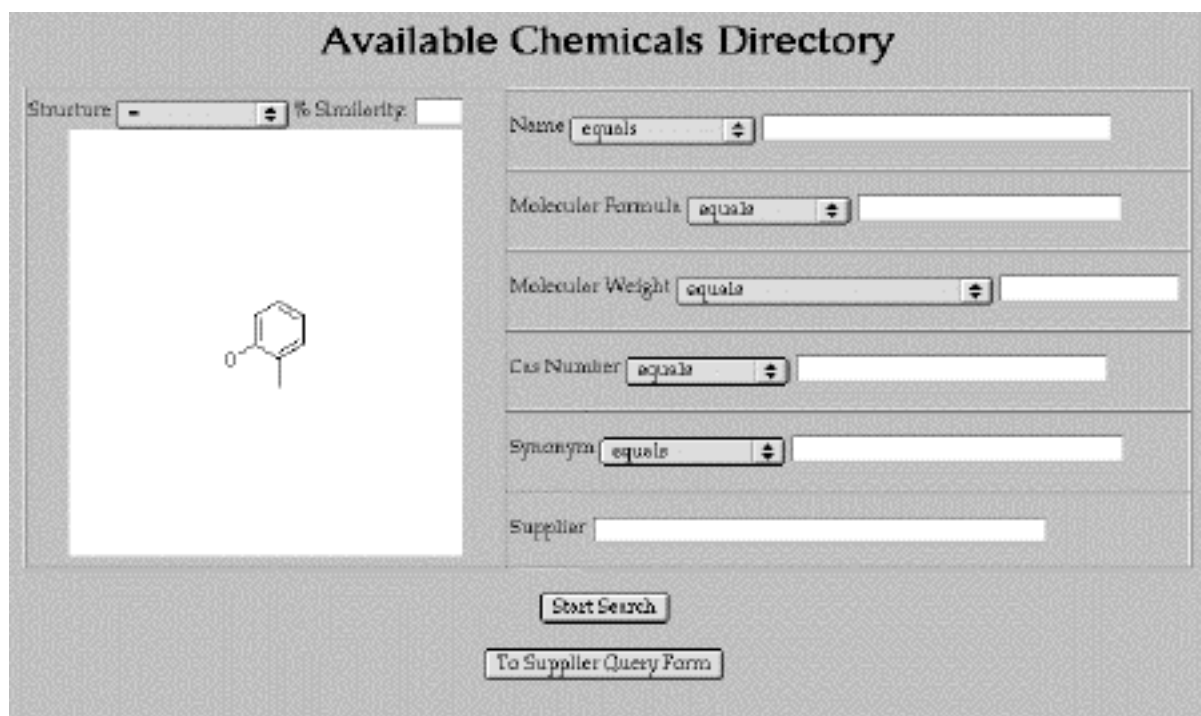
Available Chemicals Directory via the web

A search system for the Available Chemicals Directory (ACD) is now available via the web. It contains most of the functionality of the ISIS ACD Finder and runs under the Chemscape System (see the article above on Chemscape for web browser requirements).

It can be accessed from the link on the CDS website or directly using the URL

http://cds.dl.ac.uk/acd

You will be prompted for a username and password and should use your usual CDS id and password.

A search form similar to the ISIS form is displayed. In addition there is a separate supplier query form for finding supplier details.
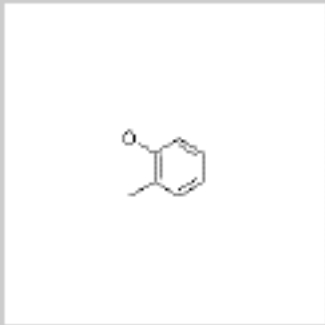

ACD search form

Results can be printed directly from the browser window or details can be cut and pasted to another application. In common with the other Chemscape applications there is no mechanism for the saving of hitlists on the server.

ACD search results display

CDS support

Due to an internal reorganisation here at Daresbury, the Computer Help Desk/User Interface Group (UIG) no longer provide front line user support for CDS. All CDS queries should be sent directly to us at the following addresses:

Email: cdsbb@dl.ac.uk
Telephone: 01925 603162

These email and telephone numbers have not changed.

LitLink

The LitLink system provides automatic linking from citations in the organic reaction databases to original journal articles stored on literature websites such as Elsevier (ScienceDirect), ScienceServer, SwetsNet, American Chemical Society, or Royal Society of Chemistry.

Major chemistry journals available through LitLink include J. Chem. Soc., Chemical Communications; Perkin Trans.; Tetrahedron; Tetrahedron Letters; J. Am. Chem. Soc. and J. Org. Chem.

LitLink is a web based system which takes the citation data from a LitLink enabled application, parses it and using data from its knowledge base prepares an appropriate set of hyperlinks to websites which have the article available. Where no sites are available, LitLink produces an email link, which prepares a draft email containing the citation which can be sent to a document delivery service. Note that LitLink does not automatically allow access to any of the sites that it produces links for. These will only work if the user or their University has an appropriate licence to use the site.

Current LitLink enabled applications are the ISIS Reaction Browser and Beilstein Commander on the PC and the web application ReactionWeb (see the article earlier in this newsletter). It is unlikely that there will be a LitLink enabled version of the ISIS Reaction Browser for the Mac. In order to use LitLink from a PC, either for ISIS or Beilstein, you need to install the LitLink client software. This is available, along with installation and configuration instructions, from the download area of the CDS website.

Using LitLink

Using LitLink with the ISIS Reaction Browser is simple, once the client software has been installed and configured. Whenever you browse a retrieved hitlist you will see the LitLink button on the left of the page. Simply select the reference of interest and click on this button (currently LitLink only works with the MDL supplied databases - the button will be greyed out and will not work in other cases). Once selected your browser will start and after prompting for your CDS id and password will present a screen like the picture below.

Beilstein Commander works similarly. Each retrieved citation has an automatically generated link labeled LitLink with the citation number, which will take you straight to the LitLink page.

The LitLink page gives a list of links to sites where the document or abstract is available. Clicking on a link should take you straight to the document. The choice of which link to use will depend upon which sites your University has licence agreements to use. CDS does not provide free access to these literature sites.

LitLink and ReactionWeb

The ReactionWeb system is automatically configured for LitLink. Whenever you display a hitlist, the references are already hyperlinked to the LitLink server. Clicking on one takes you straight to the LitLink page, similar to the one shown below.

Typical LitLink output page, giving a list of links to sources for the requested reference.

CDS can customise the knowledge base that comes with LitLink. Thus we can add new sites which are appropriate for the UK academic community. We can also add information on other journals not currently in the knowledge base, which could be important if we wish to LitLink enable other applications we support.

In order to keep the knowledge base as correct as possible, it would be helpful if you could let us know of any links which do not work correctly. In addition we would like to know of any additional literature sites which are not displayed by LitLink but ought to be present. Please send any comments/information to cdsbb@dl.ac.uk.
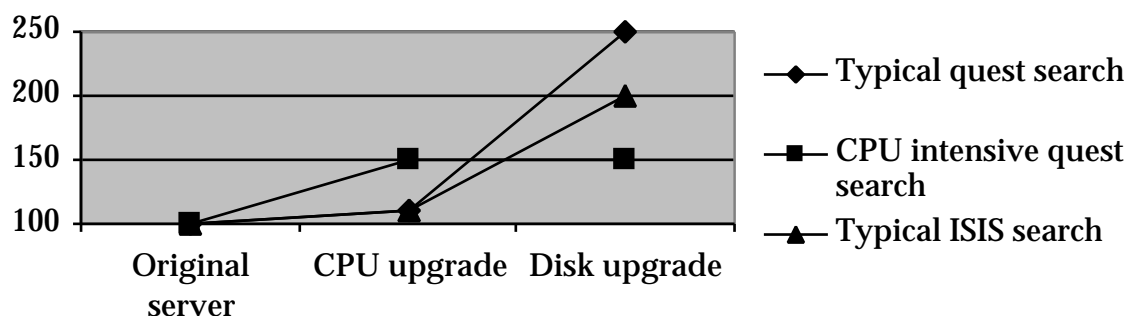
Server upgrades

The main CDS server was upgraded on June 28th last year. The new configuration has two R12k 270 MHz processors, giving a 50% increase in cpu power, and 512 MB of main memory (a two fold increase). The total downtime was less than 90 minutes for the entire upgrade.

Our standard response measurement showed a 10% increase in the speed of a typical search due to this upgrade, though more cpu intensive searches e.g. using complex geometric constraints in quest, should show a larger increase. The machine copes better now when under heavy load.

A significant number of database searches are limited by how fast the program can retrieve data from the disks. In December we moved the organic reaction (ISIS) databases to a new, faster access disk. This has cut search times in half when using ISIS. In mid-January the crystallographic data was similarly moved to a faster access disk. A typical quest search is now some 2.5 times faster. Very cpu intensive searches are much less affected, though they experience more benefit from the cpu upgrade. The spectroscopy data has just been moved and we see about a 20% increase in the speed of SpecInfo searches.

The old machine has been reconfigured and is now in use running the LitLink server (see article on page 7). In the longer run it will be used for other services, probably ISIS, thus reducing the load on the main server.
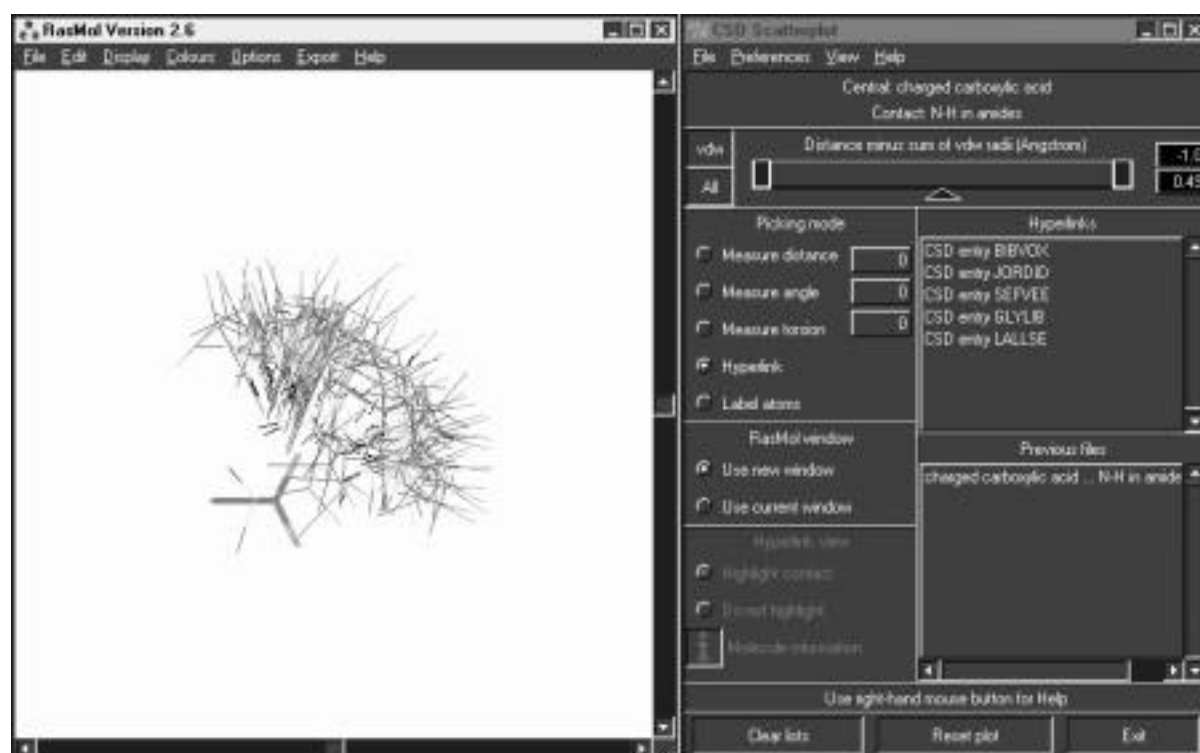
Relative search speed increases due to server upgrades

IsoStar client

The IsoStar database contains information about the geometries, energies and frequencies of occurrence of thousands of different types of non-bonded contacts. The data is derived from the Cambridge Structural Database (CSD), the Brookhaven Protein Data Bank (PDB) and molecular orbital calculations. Normally, IsoStar is accessed from CDS via X-Windows. However, in this case, manipulation of the rasmol display can be very slow, especially when the network is congested. A solution to this problem is to use the new IsoStar client software, which is available for the PC.

The IsoStar client software accesses the data on the CDS server, but does the manipulation and display on your local machine. This lowers the network traffic considerably, resulting in a much faster response.

The IsoStar client software is only available for Windows. It can be downloaded, together with installation instructions, from the download area of the CDS website.

**IsoStar running on a PC showing the rasmol display
and the scatterplot control box**

Summary of databases available from the Chemical Database Service

A brief description of all the databases currently available from the CDS at Daresbury.

ISIS A chemical reaction information management system allowing search, retrieval and display of molecules, reactions and their associated data. Currently contains 1,011,000 searchable reactions. Specialist databases available include Protecting Groups, Solid Phase Synthesis, BioCatalysis and Chiral Separations.

In addition there is the Available Chemicals Directory (ACD) which contains supplier information on 315,000 different compounds from over 630 different suppliers.

SPEC SpecInfo is a multi-technique spectroscopic database package intended to cover NMR, IR and mass spectra. The package is designed to aid the chemist in spectral interpretation and structure elucidation problems. The database currently contains 99,059 ^{13}C NMR; 999 ^{15}N NMR; 856 ^{17}O NMR; 2,183 ^{31}P NMR; 1,825 ^{19}F NMR; 5,000 ^{1}H NMR; 20,898 infrared spectra and 128,000 mass spectra.

CSD The Cambridge Structural Database. Crystal structure data for over 224,000 organic and organometallic compounds. Currently available under Cambridge's Quest and ConQuest retrieval software and our in-house software (CSSR).

IsoStar A database of non-bonded interactions taken from the CSD, PDB and theoretical calculations.

ICSD Inorganic Crystal Structure Data File. Over 57,000 inorganic structures - the companion file to the Cambridge organic file. ICSD is now accessible via the CDS website.

MDF Metals Data File. Crystal structure data for nearly 61,000 metals, alloys and intermetallics.

CDIF Crystal Data Identification File. Crystal class and unit cell data for over 237,000 crystal structures.

ELYS Electrolyte Solutions Database. Thermodynamic and transport property data such as density, viscosity and diffusion coefficients. Currently contains about 10,000 entries.

Information

General queries:

Chemical Database Service (CDS)
Room C18, Daresbury Laboratory
Daresbury, Warrington
WA4 4AD
(01925) 603162
Email cdsbb@dl.ac.uk

For ISIS specific problems:

Dr. D. Parkin
Email D.Parkin@dl.ac.uk
(01925) 603162

For SpecInfo specific problems:

Dr. D.A. Fletcher
Email D.A.Fletcher@dl.ac.uk
(01925) 603162

For crystallography specific problems:

Dr. R. F. McMeeking
Email R.F.McMeeking@dl.ac.uk
(01925) 603162

World Wide Web Site

Information about CDS, including
online help and documentation is
available over the World Wide Web at
the CDS website, URL:

    http://cds.dl.ac.uk/cds

Web based interfaces to selected
databases are also available from this
site.

Registration of new accounts:

You can now register online for a CDS
account from the CDS website.

Documentation:

Most documentation is available online
and some can be downloaded from the
CDS web site. Printed manuals can still
be ordered from us at the above
address.

Access:

The service is available free of charge to
UK academic research groups for non-
commercial work. Each individual user
will be issued with a unique ID. It is not
our policy to allow shared IDs.

cds (main service machine):

Internet number: 193.62.124.35
Internet name: cds.dl.ac.uk

Comments:

All comments, questions and
suggestions about this newsletter
should be sent to:

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