Chemical Database Service

NEWSLETTER

Issue 24. Winter 2006

EPSRC to close down CDS

EPSRC announced on the 11th October 2006 that the Chemical Database Service (CDS) is to close on 31 March 2007.

The full announcement is on the EPSRC site:
http://www.epsrc.ac.uk/ResearchFunding/Programmes/Chemistry/NCS.htm

See Page 2 for more details.

A summary of the main articles

What the Changes Mean to You; Why has this happened? and What can you do about it (page 2)

Comments by just some of our users. (page 3)

Details of the packages that will be lost in the organic synthesis and spectroscopy area which you may have to subscribe to and the support service (pages 4-5)

Proposals by CDS at to what happens next can be found on page 6

Results of the ACD Labs I-Lab trial.(page 7)

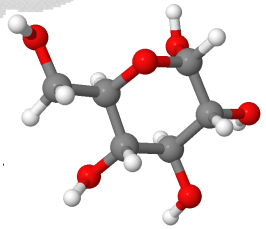
Improvements to the crystallography web front end - CrystalWeb (page 8)

Two articles from our list of Research Highlights from 2005/2006 (pages 9 and 10)

For a list of all the packages currently available see page 11.

A list of contact details and information can be found on page 12.

Inside this issue:



CCLRC Daresbury Laboratory

CDS ON-LINE

See http://cds.dl.ac.uk/cds/newsletters.html for this and previous editions of our newsletter

What the Changes Mean to You

If you use the

- Cambridge Structural Database
- Inorganic Chemistry Structural Database
- DETHERM, the thermo physical properties database

The EPSRC will continue to provide access until at least 2010. A procurement process is underway to provide such a service by an alternative, yet to be specified mechanism. CDS will continue to run these as best we can until the tender exercise has been completed.

After 1st April 2007 there will be no funding to any other component of the CDS.

(see Page 4 for more details of other components)

Note that if the new provider is **not** CDS, then it is very unlikely that **CrystalWeb** and our various utilities (Bedlam, CRAD) will continue to be available.

Also note that there is no provision for continued access to the metals and intermetallics crystal structure database (**CrystMet**) nor the Crystal Data Identification File (**CDIF**).

Why has this happened?

The EPSRC response to e-mails included the following statements:-

"The Chemistry Programme has a finite budget, which has to cover the full range of both responsive and targeted activities; the funding for these services comes directly from the responsive mode budget. The Chemistry Programme does not have the budget to support all chemistry research in the UK nor is it in our Programme objectives to do so. Our objectives include maintaining the health of the chemistry discipline through the support of high quality research.

Each of the services has to demonstrate that they are supporting high quality research comparable to that funded through responsive mode. The review panel concluded that the CDS no longer met key criteria of a Chemistry National Service, including demonstration of high demand and high quality research supported across the whole suite of databases. "

The Service believes that the Review process itself and the subsequent conclusions are seriously flawed for a number of compelling reasons.

(A document has been sent to EPSRC pointing out these flaws - this may be made publicly available later).

A leading expert in the field had this to say about the report "The Review Report is really dire, and certainly not something that EPSRC should be proud of: some of it is simply ludicrous .., some of it impractical .., and some simply weird."

Around 2,000 users per year will be effected by this decision, over half of these use the databases that are to be stopped.

What can you do about it

1. Write to EPSRC (carmine.ruggiero@epsrc.ac.uk) and express your views (please copy us in).

2. Get your colleagues to express their views as well to the EPSRC.

3. Join the CDS-UK discussion list and join the debate (http://www.jiscmail.ac.uk/lists/CDS-UK.html)

4. Make other arrangements to access required databases -

(see page 6)

Below are just some of the comments our users had to make about the decision:

"In my experience, as a synthetic organic chemist, SciFinder is vastly inferior compared to Crossfire for reaction searches, certainly on 'simpler' structures, and Crossfire, in turn, is not as good as ISIS-Base. . . . the hitset in ISIS/Base is of higher quality and more relevant (the other databases often yield results which are not relevant)."

"I am distressed to learn that the CDS service will close. It is vital for my work, and it will seem like going back to the stone age if I can no longer access the various crystallographic databases."

"I think the proposed shutdown of the CDS services is an appalling state of affairs which will be very damaging to us all. . . . routine access to these facilities has proven not only valuable but essential for the progress of our work. To close down the CDS services would be a crying shame and extremely detrimental to the chemistry community. In the long-term it doesn't seem like this would be a cost effective solution either."

"I am appalled that this excellent and uniquely useful service is being chopped by EPSRC without (it would seem) any consultation with the synthetic chemistry community" who use it."

"I am profoundly upset that this service is being withdrawn. . . I can only assume that this is a further sign of the demise of Chemistry as a subject, which makes me rather depressed."

"I am very surprised at this move as the CDS is for myself, my group and most people in my department an absolutely pivotal service. The ACD in particular is used on a daily basis. The EPSRC support for CDS should be continued, as it serves to support invaluable services to UK science. Without the support of this service we are going to slip behind the US, Japan and leading European research countries, who will no doubt be laughing at the unmatched ability of the UK to undermine its own scientific base."

It is with considerable alarm that I read about the closure of the CDS at Daresbury and the implication that continued provision of vital database access is unlikely to be guaranteed under the present arrangements. My group makes extensive use of the Cambridge Structural Database and ICSD and we would be severely hampered if access to these databases were curtailed for any length of time. In addition, I have the highest regard for the service provided by the CSD and remain puzzled as to the EPSRC's decision to close it at all. Certainly, the announcement I saw on the EPSRC website left me none the wiser. I would strongly urge the EPSRC to reexamine very carefully the CDS and the important service it has provided the UK academic community for many years.

SERVICES and DATA THAT WILL CLOSE IN APRIL 2007

The databases in these areas which EPSRC will no longer be funding cover:-

1. The Data

Synthetic Methodology

A variety of chemical databases are available that cover 60 years of published literature. They provid established and current awareness in synthetic organic chemistry and now contain around 1.5 Million searchable reactions. Unlike the molecule databases such as Beilstein, the entries in these databases are carefully selected because of the transformation and contain not only single-stage reactions but also overall reactions. The databases available are:-

- REFLIB (Reference Library) - consisting of :-
  - THEILHEIMER (Synthetic Methods)
  - CLF (Current Literature File)
  - CHIRAS (Asymmetric Synthesis)
  - METALYSIS (Transition metal-mediated transformation)
  - ORAC/CORE (Established Literature)
  - CHC (Comprehensive Heterocyclic Chemistry)
- DJSM (Derwent Journal of Synthetic Methods)
- CHEMINFORM (CIRX - current awareness)
- ORGSYN (Organic Synthesis)
- SPG (Protecting Groups) [Not available from MDL via DiscoveryGate]
- SPS (Solid Phase Synthesis) [MDL have a similar, smaller database]
- BIOCATALYSIS (Enzymes etc. as catalysts) [Not available from MDL via DiscoveryGate]

Additional Databases

- CHIRBASE (Chiral Separations by chromatography). A unique tool for preparative or analytical resolution of drugs, agrochemicals, etc. [Not available via DiscoveryGate]

Access to the data is via:-

- Client/Host software - ISIS/Base
- Web Browser using ChimePro Plugin

Chemical Sourcing and Logistics

The databases contain information such as supplier, catalogue number, amount of compound, purity and price for entries that range from bulk, readily available, off-the-shelf compounds to rare compound in small quantities that you may have to wait for a few months for delivery. A number of databases also contain extra information like Number of H Donors, Number of H Acceptors, Number of Rotational Bonds and Calculated LogP. The databases available are:-

- MDL's Available Chemicals Directory (ACD) – over 1/2Million compounds from 706 Suppliers. Direct links to around 15,000 Material Safety Data Sheets is also available.
- Screening Compounds Database (SCD) - a collection by CDS of 25 Suppliers and amounts to over 4.8 Million compounds.
- Molecular Diversity Preservation International (MDPI) - over 9,000 compounds (10mg-100g) deposited by research workers. [Not available via DiscoveryGate]

Access to the data is via:-

- Client/Host software - ISIS/Base
- Web Browser using ChimePro Plugin (including structure searching of ACD and SCD from Macs using Java applet)

3-D Molecular Databases

These databases contain calculated 3-D coordinate information (using the CORINA package) along with other data. The databases available are:-

- MDL's Available Chemicals Directory (ACD) - supports 3-D search and display.
- National Cancer Institute Collection (NCI) structures and data from the main NCI Collection plus the Plated Compounds, Cancer Screened and AIDS Screened Collections.

Access to the data is via:-

- Client/Host software - ISIS/Base
- Web Browser using ChimePro Plugin (Java applet for Macs)

Spectroscopy

Spectroscopy databases can aid the chemist in spectral interpretation and structure elucidation. Searches can be conducted by inputting then matching a query spectrum (or fragment), a (sub-) structure or bibliographic information such as name, formula or CAS number. The ability to predict an NMR spectra for any trial structure using statistical information taken from the spectra stored in a database can be very useful in identifying a molecule.

- SpecInfo - a multi-technique spectroscopic database system, covering NMR, MS and IR spectroscopy.

Access to the data is via:-

- Web Browser - SpecSurf.

A full description of all of the databases can be found on the CDS web site at http://cds.dl.ac.uk/cds

2. Support

Staff at CDS, Daresbury LaboratoryCDS provide a full range of user support.

We provide a help desk to answer all queries and extensive on-line help through our web pages, which include user guides, FAQ database, tutorials and exercises as well as Flash movies that show what the different packages can do. Site visits (Road Shows) and training courses are available on request with no cost to the user.

CDS provide web front ends for a number of molecule databases including ACD, SCD, NCI and ChiBase (not availble from the Supplier) and have recently enabled Mac users to access these databases using a Java applet for drawing and viewing the molecules.

Linking to full text biblographic data from the MDL and Accelrys databases has been enabled (also availble in ICSD, CSD (ConQuest)and CrystalWeb) and we have also added data to other databases to LitLink enable them - such as ChirBase.

CDS negotiate, on behalf of the academic community, site wide deals on all the databases which not only save a lot of money (cf. individual licenses and hardware) but also save on time and effort on keeping the data and machines up-to-date.

CDS has run a number of trials of databases in the past and has just finished the ACD Labs trial of their I-Lab spectroscopy databases - which was run on our own machine. The CDS team were able to identify and find solutions to a few small problems to our users with this trial. We originally introduced Beilstein to the community by this mechanism - running it for a year free of charge. We had planned on running a trial of the SPRESI database (5.0 million molecules 3.7 million reactions) via a web interface for PC and Mac users which could link to SpecSurf and I-Lab.

If CDS do not win the tender bid then other support services will be effected. CrystalWeb is produced by CDS as a web front end to all the crystallography databases. We are continually adding to it and improving it (see page 7). The file format converter, Bedlam, has been produced by CDS and handles crystallographic data better than Babel, which is also made available. DL Visualise [displays and edits crystal structures] can obtain crystal data directly from the CDS databases.

ACCESS TO THESE DATABASES AND SUPPORT FUNCTIONS WILL CEASE IN APRIL

What Happens Next

We believe that the initial goal should be to get EPSRC to extend the closure date for another 9-12 months. This will :-

1. Allow sufficient time for users to apply for funding to cover any alternative arrangements.

2. Allow CDS to provide all databases until alternatives arrangements are made (this would also help with license agreements)

3. Allow a more wide ranging review of current and future needs for cheminformatics to take place without prejudicing the outcome.

EPSRC has stated that '***Under Full Economic Costing, Research Councils will fund the element of database provision which relates to individual research grants. From 31 March 2007, a number of the databases currently supported by CDS will have to be accessed via a charging arrangement either directly from the vendor or though an intermediary such as CDS or an equivalent; the relevant component of such costs can be included on any Research Council proposal.*** '

Therefore, a proposal for a CDS subscription service is included below.

Possible Subscription Service

The CDS would like to continue offering databases in the areas of Synthetic Methodology, Available Chemicals, Screening Compounds, 3-D Molecular Databases and Spectroscopy as shown on the previous pages. If enough users are interested in the ACD Labs databases following the trial then it may be possible for CDS to run a (separate) subscription service

CDS would continue to offer our full range of user support.

Final pricing can not been fixed it this time as it depends on the number of Institutes that take up the offer. The offer may be for an annual subscription or would be for a three year period.

However, if a reasonable number of Institutes subscribe to this service then the cost, for the components that are to be lost, is likely to be in the region of £3,500 per year. [DiscoveryGate would cost, on average, 9,350 Euros (£6,300) per year]

CDS would like to hear from the community about interest in a subscription service.

You can e-mail us at:- cdsbb@dl.ac.uk

ACD Labs I-Lab Trial

The trial ran over the summer months from July to October. During that time over 200 users from over 50 Institutes used the database, with over 3,500 accesses and making over 2,600 calculations.

The number of accesses via the ChemSketch software was twice as high as the number of accesses via the web, but more users used the web interface. This may be due to the fact that it was easy to have a quick look at the available data by using the web rather than download and install a piece of software. However, users found the ChemSketch method much easier to use and view the results once the effort had been made and so accessed the data more.

For the NMR data, prediction of 1H NMR spectra proved to be the most popular, scoring the highest calculation rate (786 calculations). This was followed by prediction of 13C NMR spectra (441) then 31P NMR spectra (143 calculations).
Searching the databases also followed this trend of 1H NMR followed by 13C NMR then 31P NMR.

The ability to generate a Name also proved popular. Producing a name according to IUPAC rules recorded the third highest in the list of all calculations (over 300). 59 Calculations were conducted to generate a structure from a chemical name.

Quite a number of physical property predictions were also undertaken such as pKa (152), WSol (111) and LogP (102).

The trial also served to highlight slight problems with this package. Some users experienced difficulties logging on to I-Lab via ChemSketch because their local server blocked the connection. The cause for this was investigated and we found that going through a proxy server remedied this problem. It was also noted that the window, produced after conducting a prediction or search using the web interface, lacked one or two buttons at the top. The window could not be resized so these buttons could not be displayed. These points have been passed on to ACD Labs.

ACD Labs I-Lab Trial

As the EPSRC no longer think that there is a high enough demand for spectroscopy databases which supports high quality research, they are unlikely to fund this. Therefore, in order to continue using the ACD Labs databases, at some point you will need to subscribe to a service.
If enough users are interested then it may be possible for CDS to run such a subscription service.

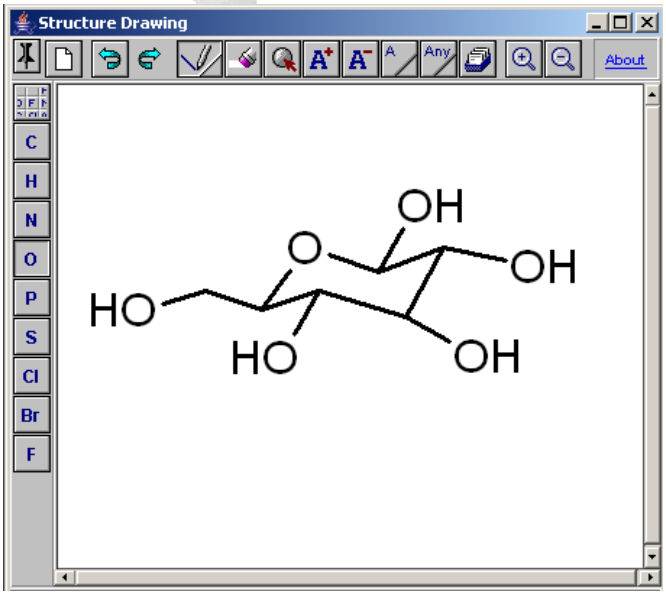
CDS are now seeking feedback from the community as regards the value of the system. Please take a moment to answer the questions on the questionnaire at:-
http://cds.dl.ac.uk/cds/ACDtrial.html

Otherwise you should be able to subscribe directly with ACD Labs. The contact information for the UK account manager is:-

Paul Hubberstey
Account Manager
Advanced Chemistry Development, UK and Ireland
Tel: +44 (0) 1344 668030
Fax: +44 (0) 1344 668230
Email: paul.hubberstey@acdlabs.com
http://www.acdlabs.com/

What's New?

Mac users are now able to access the Available Chemicals Directory (**ACD**), the Screening Compounds Database (**SCD**) and the National Cancer Institute (**NCI**) database over the web by using a Java applet to draw structures.

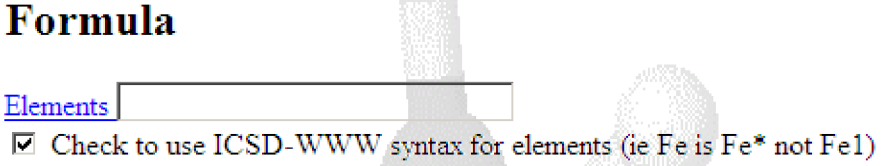


Improvements to CrystalWeb

Formula Searching

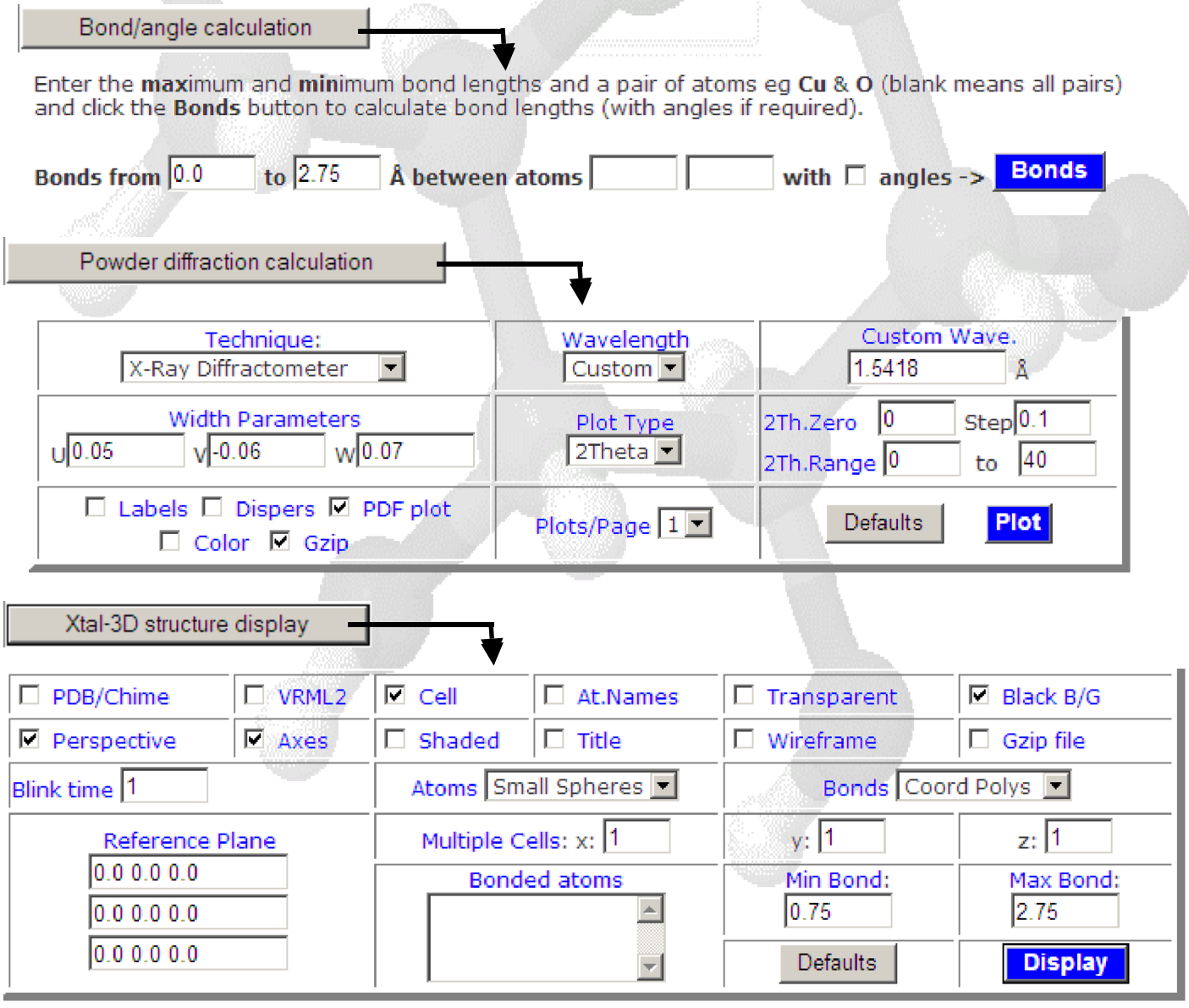
A new wild card option for element type has been added for formula searching. This is of particular value when searching for inorganic substances. For instance the following search formula: *1 Cu O2 in conjunction with element count 3 will retrieve Ba(CuO2), SrCuO2, CuAlO2, etc.

CrystalWeb formula searching now has the ICSD-WWW tick box option selected by default. Thus the formula search "Cu O" with element count 2 will retrieve: CuO, Cu2O, Cu4O3, etc rather than simply CuO.



Greater integration with ICSD-WWW

Buttons are now provided for calculations and display that take you directly to ICSD-WWW where the calculation or display is performed.



Note: Since April 2006, CosmoPlayer (VRML viewer) no longer works in MSIE, but still works well in FireFox.

Rational Design of Molecularly Imprinted Polymers - Kal Karim

Cranfield Biotechnology Centre, Cranfield University at Silsoe

Introduction

Our present research is the development of a general method for the rational design of Molecularly Imprinted Polymers (MIPs). Using molecular modelling & computer simulation it is possible to predict & tailor the polymer properties for specific applications. Areas of applicability include drug discovery, detection of toxins/environmental pollutants, both natural & industrial, sensors & assays, separation & in drug development. MIPs have been previously synthesised with high selectivity sensitivity for target compounds such as triazine herbicides, pesticides, algal and fungal toxins, explosives, peptides and a variety of drugs. Their synthesis is via straightforward and inexpensive procedures.

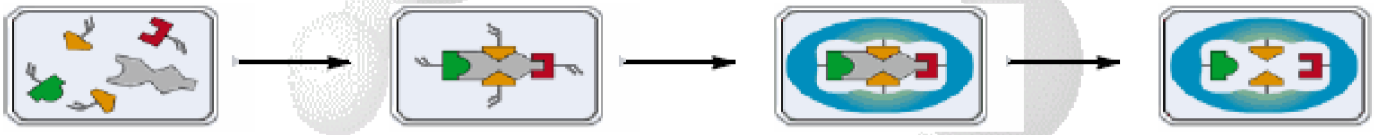
Current Work

Our research has allowed the predictive design of polmer specificity & affinity, new synthetic ligands, further development in the chemistry of conjugated polymers (PANI & polythiophenes) & the ability to incorporate them into transducers such as QCM, SPR, optical & electrochemical detection methods.

We have expanded our monomer database library which we use to screen and select possible monomer candidates for polymer preparation by searching for commercially available functional monomers which are polymerisable but have the necessary substituents to form a complex with a given target. The expansion of the library for virtual screening is a direct result of searching monomers using the MDL Available Chemicals Directory, to which we have ready access via the EPSRC Chemical Database Service (CDS). 3D structures can then be generated using Molecular Mechanics and Molecular Dynamics simulations.

Cranfield Health has a newly acquired multinuclear NMR spectrometer able to investigate samples in both solid and solution phase. This is part of the Science Research Investment Fund (SRIF) and will ensure that novel monomers can be synthesised for many applications. Access to the wide range of reaction databases also available via the CDS allows us to design compounds via viable, cost effective synthetic routes. The main targets are novel multifunctional monomers, which will act as superior monomer candidates for polymer preparation to those currently available, and crosslinkers, which can further enhance the stability of the monomer-template complex. In some cases it may be possible to make polymers with specificity and affinity from these novel multidentate monomers where the template is not required.

A schematic representation of the Molecular Imprinting Polymerisation process



a. Selection b. Self-Assembly c. Polymerisation d. Extraction

Addition Role of the CDS

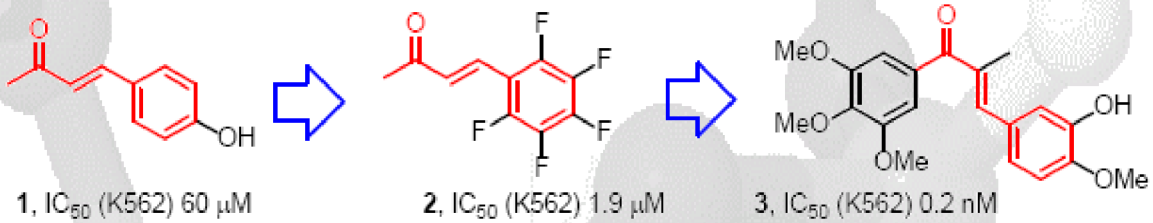
In addition the CDS has supported our Bioinformatics masters course since its inception 4 years ago, specifically in helping run the “Molecular Modelling and Chemoinformatics” module with great success (giving lectures and running practical sessions).

The synthesis of indanones related to combretastatin A-4 *via* microwave- assisted Nazarov cyclization of chalcones

*Nicholas Lawrence, **Alan McGown, **Sylvie Ducki
* H Lee Moffitt Cancer Center, Tampa, Florida and **Centre for Molecular Drug Design, University of Salford.

Our research groups have a long-standing interest in anti-cancer agents, especially those derived from natural products. In 1996, as part of a plant-screening program, we identified Scutellaria barbata D. Don (Labiatae) as a potential source of anticancer agents. The dried whole plant, readily available from herb wholesalers, is used in traditional Chinese medicine as an anti-inflammatory and antitumour agent. It is a component of Shan Ci Gu soup, a herbal prescription for stomach cancer.

Bioassay guided fractionation of the herb extract, using the MTT assay to determine cytotoxicity, revealed the presence of many cytotoxic components. One such fraction had an IC50 (K562) of 10 µg/mL. The fraction was predominantly the simple enone 1 (IC50 60 µM) [1]. Preparation of a library of butenones revealed that those possessing electronwithdrawing groups were the most active [2] The pentafluorophenylbutenone 2 was over 30 times more active than the natural product 1.

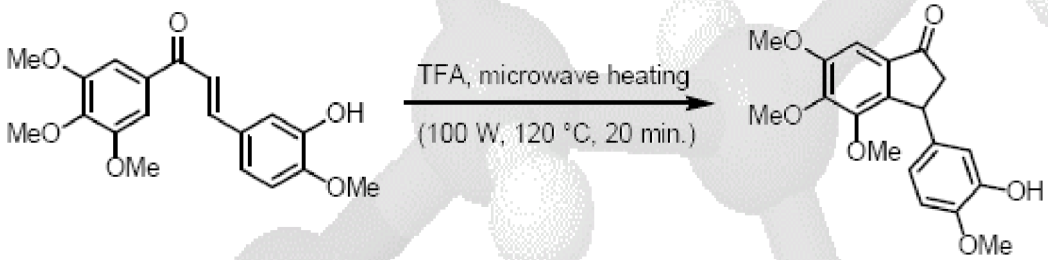


1, IC_{50} (K562) 60 µM **2**, IC_{50} (K562) 1.9 µM **3**, IC_{50} (K562) 0.2 nM

The activity appears to be associated with ability to act as an alkylating agent. Further structural modification and library design [3] led to discovery of alpha-methylchalcone 3, which operates biologically by a different mechanism [4]. This chalcone shows potent cytotoxicity, and inhibits cell growth, over a period of several days, by binding strongly to tubulin, a protein essential for cell division [5]. Perhaps more exciting is its ability to cause selective damage to tumor vasculature in a matter of minutes. This effect is also thought to be related to its tubulin binding property. In this way tumors are starved of oxygen and nutrients and their constituent cells die. Compounds such as these that target tumor vasculature clearly have significant clinical promise for the treatment of cancer.

As part of a recent study to determine the features of the chalcone that lead to good biological activity we have developed a fast and efficient microwave-assisted synthesis of indanones [6]. Microwave irradiation provides a useful alternative to traditional heating techniques to promote the trifluoroacetic acid (TFA) catalyzed Nazarov cyclization of chalcones.

The use of the microwave reactor is ideal for handling potentially hazardous reagents such as TFA. The reactions can be performed quickly, conveniently and safely: both the temperature and the pressure of the reaction vial are monitored continuously. The exposure to pressurized reaction vessels containing TFA is thereby significantly reduced.



Throughout the study we have made frequent use of the CDS. Specinfo was useful for assigning structures of the natural products derived from the herbs. Structural and activity analysis of products was also helped by access to the Cambridge Crystallographic database. We made regular use of the CDS reaction databases with particular emphasis on the various 'specialist' systems including SPS. (solid phase synthesis) and Chirbase (chiral separation by chromatography). The Available Chemical Directory is very useful for quickly sourcing starting materials and building blocks for library design. In summary our research has been greatly aided by our access to the Service.

1. Ducki, S.; Hadfield, J. A.; Lawrence, N. J.; Liu, C. Y.; McGown, A. T.; Zhang, X. G., Isolation of E-1-(4'-hydroxyphenyl)-but-1-en-3-one from Scutellaria barbata. Planta Medica 1996, 62, 185-186.
2. Ducki, S.; Hadfield, J. A.; Hepworth, L. A.; Lawrence, N. J.; Liu, C. Y.; McGown, A. T., Synthesis and cell growth inhibitory properties of substituted (E)-1-phenylbut-1-en-3-ones. Bioorg. Med.Chem. Lett. 1997, 7, 3091-3094.
3. Lawrence, N. J.; Rennison, D.; McGown, A. T.; Ducki, S.; Gul, L. A.; Hadfield, J. A.; Khan, N., Linked Parallel Synthesis and MTT Bioassay Screening of Substituted Chalcones. J. Combi.Chem. 2001, 3, 421-426.
4. Ducki, S.; Forrest, R.; Hadfield, J. A.; Kendall, A.; Lawrence, N. J.; McGown, A. T.; Rennison, D., Potent antimitotic and cell growth inhibitory properties of substituted chalcones. Bioorg. Med. Chem. Lett. 1998, 8, 1051-1056.
5. Lawrence, N. J.; McGown, A. T.; Ducki, S.; Hadfield, J. A., The interaction of chalcones with tubulin. Anti-Cancer Drug Design 2000, 15, 135-141.
6. Lawrence, N. J.; Armitage, E. S. M.; Greedy, B.; Cook, D.; Ducki, S.; McGown, A. T., The synthesis of indanones related to combretastatin A-4 via microwave-assisted Nazarov cyclization of chalcones. Tetrahedron Lett. 2006, 47, 1637-1640.

Databases available from the Chemical Database Service (CDS)

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

STRUCTURES

The Structures databases contain a comprehensive collection of organic, organo-metallic and inorganic compounds, metals, alloys and protein **crystal structure data**.

CSD - **C**ambridge **S**tructural **D**atabase.
Crystal structure data for over **390,000 organic and organo-metallic compounds**. New releases of this database are received and mounted bimonthly.

*ConQuest is the graphical front end which has 3D search capabilities.

*VISTA performs numerical, statistical and graphical analyses.

*Mercury provides comprehensive facilities for visualising crystal structures in three dimensions.

***IsoStar** A knowledge base of non-bonded interactions derived from the CSD, the Protein Data Bank (PDB) and molecular orbital calculations. Uses a simple web interface.

* **Mogul** A knowledge base of molecular geometries using data derived from the CSD.

ICSD - **I**norganic **C**rystal **S**tructure **D**ata File.
Over **93,000 inorganic structures** - the companion file to the Cambridge organic file (though in a different format). ***WWW interface available.***

CRYSTMET (**MDF - M**etals **D**ata **F**ile)
Crystal structure data for over **74,000 metals, alloys and intermetallics.**.

CDIF - **C**rystal **D**ata **I**dentification **F**ile.
Crystal class and unit cell data for **237,671 crystal structures**.

CrystalWeb - a simple **web interface to all of the crystallographic databases** that allows bibliographic and cell data searching along with structure display.

Calculated 3D structures are also available from the NCI and ACD databases (see Organic Synthesis column)

PHYSICAL CHEMISTRY

DETHERM

One of the world's largest thermophysical property databases of pure compounds and compound mixtures Contains over **5 Million data sets** for around **122,000 systems** (around **25,000 pure substances** and **97,000 mixtures**) covering around **500 property fields**.

UTILITY PROGRAMS

A variety of utility programs are available, including links to electronic literature, chemical file format conversion and molecule viewers.

LitLink - Links citations to electronic literature.

Crad - A **c**rystal **rad**ial distribution calculation program.

BABEL and **BEDLAM** file format converters.

ORGANIC SYNTHESIS

ISIS - Chemical reaction information management system allowing search, retrieval and display of molecules, reactions and their associated data. ISIS is a client/server system requiring ISIS/Draw and ISIS/Base on your desktop machine, but now ***available via your Web browser*** (using ChimePro).

Currently ISIS can access **around 1.4 Million searchable reactions** from the following databases:-

REFLIB (Reference Library) - consisting of :-
THEILHEIMER (Synthetic Methods)
CLF (Current Literature File)
CHIRAS (Asymmetric Synthesis)
METALYSIS (Metal-mediated transformation)
ORAC CORE (Established Literature)
CHC (Comprehensive Heterocyclic Chemistry)
REACCS-JSM (Journal of Synthetic Methods)
CHEMINFORM (CIRX - current awareness)
ORGSYN (Organic Synthesis)
SPG (Protecting Groups)
SPS (Solid Phase Synthesis)
BIOCATALYSIS (Enzymes etc. as catalysts)
CHIRBASE (Chiral Separations by chromatography)
NCI (National Cancer Institute Database).

Access via ISIS/Base or Web

AVAILABLE COMPOUNDS

ACD (**A**vailable **C**hemicals **D**irectory) - a database of readily available chemicals. It contains over **500,000 unique compounds** from over **700 different suppliers**.

3D search and display now available.

SCD (Screening Compounds Database) - **over 4.8 Million compounds** for use in screening compound libraries and diversity synthesis.

Access via ISIS/Base or Web

SPECTROSCOPY

The Spectroscopy databases are designed to aid the chemist in structure elucidation and spectral interpretation problems.

SPECINFO - SpecInfo is a multi-technique spectroscopic database system which covers NMR, IR and mass spectra. A variety of features are available within the program to help with spectrum prediction and searching. It contains spectral data sets with their associated structure connection tables. The database currently contains:-

^{13}C NMR	^{15}N NMR	^{17}O NMR	^{31}P NMR	^{19}F NMR	^{1}H NMR	IR SPECTRA	MASS SPECTRA
102,369	992	856	16,561	25,442	117,379	20,898	138,727

This includes:-
Natural Products ^{13}C NMR Spectral Collection.
Fluka ^{1}H-NMR Spectral Collection.
Aldrich ^{1}H-NMR Spectral Collection.
HNMR Spectral Collection 2 & 3.

SpecInfo is accessed using **SpecSurf**, a **Web graphical user interface** that makes drawing structures, creating peaklists and viewing hit lists easy.

The Chemical Database Service (CDS) provides on-line access to a variety of quality databases in the field of Chemistry, plus support, training and advice.

The service is available **free of charge at point of access** 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.

Remit:
To provide Chemical Database Service and support to UK academic community as well as helping to maintain/ improve the service according to the service level agreement with the EPSRC

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

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

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

Documentation:
Most documentation is available online and some can be downloaded from the CDS web site.

CDS Helpdesk:
cdsbb@dl.ac.uk or
01925-603-162

CDS (main service machine):
Internet name: cds.dl.ac.uk
Internet number: 193.62.124.35

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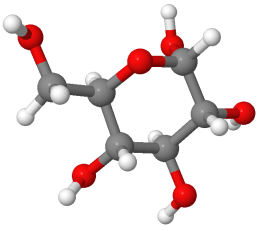

CDS
ON-LINE