



The Royal Society of Chemistry

**Chemical  
Information  
Group**

## NEWSLETTER

October 2002

### Register online and receive free RSC news by e-mail

The RSC is now offering all RSC Interest Groups a free monthly e-mail service. This will provide us with a quick and convenient way of sending communications to CIG members who have registered their e-mail addresses with the RSC. We therefore urge you to register your e-mail address, if you have one, via the RSC website at: [www.rsc.org/CFReg/](http://www.rsc.org/CFReg/)

### RSC Interest Groups

With the broadening of the RSC membership, new forums in the areas of Chemical Biology and Materials Chemistry have been established. Another new forum, for the Environment/Energy, is under consideration. In the interests of promoting greater involvement in the current Divisions and new Forums, from 2003 **members will be able to join any number of Divisions and Forums free of charge.**

### Next Meeting

#### Information at the Chemistry/Biology Interface

**20th November 2002 at Burlington House, London.**

As the boundaries between Chemistry and Biology become increasingly indistinct, this meeting will look at new initiatives being developed to stimulate information exchange between these two subject areas. Speakers include:-

Simon Edwards, Life Sciences Manager for the Royal Society of Chemistry.

Stephen Baker, Centre for Chemical Biology, Leicester University.

Kim Henrick, Head of Structural Databases at the EBI, Hinxton.

Leslie Thompson Programme Manager for the Life Sciences Interface Programme (EPSRC).

Denise Harrison (Sheffield Science Librarian)

Simon Alcock (Derwent)

and Barry Dunne (CAS)

### Review of Past Meetings

#### 6th International Conference on Chemical Structures

#### June 2002

Another successful conference was held at Noorwijkerhout, The Netherlands with 157 participants from 17 different countries attending the 6th meeting in this well established series that began in 1973 and is held every three years. The Conference brings together an international group interested in handling chemical structures

and related topics and fosters cooperation among organizations and researchers involved in the merging fields of cheminformatics and bioinformatics. A number of organisations sponsor this event, including the CIG. The conference this year consisted of 22 presentations and 13 product reviews (though on one or two occasions it was difficult to tell the difference) along with 40 posters. Attendees and speakers were split fairly evenly between academics, industrials and software people. Although some people had attended before, there were a large number of first time attendees.

This year saw more presentations concerned with consolidation as opposed to innovation, with some talks being more non-scientific, such as the approach to tools.

The opening address was given by Peter Willett, University of Sheffield, who received the first CSA Trust Mike Lynch Award.

Other talks came under the 5 main sessions: 'New Algorithms for Searching and Managing Chemical Structures', 'Combinatorial Chemistry & Molecular Diversity', 'Structure-Activity & Structure-Property Relationships', 'Molecular Modelling & Managing 3D Databases' and 'Synthesis'. Sponsored receptions after the talks provided an excellent way of meeting people, as did the excursion on Wednesday afternoon and evening.

## **Chemical Information: Maximizing the Opportunities and minimizing the challenges.**

### **April 2002**

This UKOLUK meeting was held in conjunction with CIG at the University of Leeds. Themes for the meeting ranged from delivering an information service in academia and industry, evaluating databases to aid purchase decisions [see F. Cooke and H. Schofield. A framework for the evaluation of chemical structure databases. *Journal of Chemical Information and Computer Sciences*, 41(5), 1131-1140, 2001], to the new PsiGate Internet gateway [see also <http://www.freepint.com/issues/040402.htm#feature>], the RSC Library and Information Centre and the Chemoinformatics course at Sheffield.

## **Future Meeting**

### **THE FUTURE OF CHEMICAL INFORMATION IN THE UK**

What is the future of access to chemical information in the UK? This is not a particular easy question to answer, not least because chemistry is becoming more of an interdisciplinary subject these days. It seems to be under threat from many sources (see UK chemistry under pressure, *Chemical & Engineering News* April 15 2002, p31-36). The RSC, as Europe's leading Chemical Society, is obviously concerned about these issues; no more so than its Library & Information Centre (LIC), one of the world's finest information resources in chemistry. In an ongoing review of its role and services the LIC is asking a number of questions, in particular: what sort of chemistry information provision should the LIC make for future researchers? What services should the LIC supply? How can we make use of our collection of chemistry materials (in print and electronic media)? As a result, discussions have had to take in how chemical information, as a whole, is being collected, delivered, accessed and archived and has not just focussed solely on the library. It was thought useful to widen these discussions to the RSC's Chemical Information Group. The following might be of interest to you.

Chemistry is a subject that has embraced electronic media whole heartedly, but is there still a role for print? The print versus electronic issue is not only about delivery of content but also about archiving chemistry as a subject. Is a library of a learned society (i.e. the RSC) to be considered an official archive library or is this just the preserve of the British Library and other copyright depository libraries? Would it matter much if the LIC decided to go totally electronic and not collect print or even get rid of a large part of its printed collection? Just whose responsibility is it to collect for posterity? Archiving chemistry is of great concern to us all. Publishers are enticing libraries to go fully electronic with some pricing deals, yet publishers still produce print. Will libraries decide to go fully electronic or will we have dual media for many years to come?

The LIC has been collecting for just over 160 years and has many long runs of journals from volume 1; does this constitute a viable archive? Could there or should there be greater collaboration on maintaining and developing a “national collection on chemistry”? Or is chemistry becoming part of a much larger diffuse interdisciplinary physical science? Is there really a future for individual subject collections such as in chemistry, geology, medicine or mechanical engineering, for example?

Should we actively “Map” chemistry resources in the UK, to find gaps, duplication, and needs of the collection? Medicine has been successfully “Mapped” and has a much higher profile as a result.

How do smaller companies, universities and colleges get access to the information they require now and how will they be supplied in the future? Does a specialist information centre such as the LIC have a role in providing resources for this sector? How do we make sure that all those who wish to gain access to information, at a reasonable price, will be able to?

The RSC’s LIC are grappling with all these questions and more and are keen to 'place' the Library in a position as a centre of excellence. However, how do they do this given many of the issues above? The RSC’s CIG and LIC would like your views and feed back on the above. A one-day informal chemistry brain-storm to discuss this and other related issues will be arranged for spring next year. We hope you will attend, share your views, come up with new ideas and have some fun! In the meantime, you can send any views directly to Nigel Lees Manager, Library and Archival Services, Royal Society of Chemistry.

## Minutes of the 2002 AGM held at Burlington House on 23rd May 2002

Apologies: One apology was received.

Previous minutes: Minutes for the 2001 AGM were not available. There were no matters arising.

Membership: Membership has remained approximately constant throughout the year.

Finances: The 2002 Treasurer’s report indicated that we are financially sound and the accounts were adopted. They have been circulated to those present and to the RSC. We do not need an auditor unless requested by the RSC.

Chair – Don Parkin stands

Treasurer – Chris Evans stands

Election of Officers: Secretary – Dot Parker resigned and Doug Veal took over.

Peter Rhodes resigned as Newsletter Editor and as a member of the Committee. Dot Parker offered to help with the Newsletter. A note of thanks will be sent to Peter.

Members – Jan Davies (STN); Barry Dunne (CAS)

Requirement for new members for the committee: After discussion it was agreed that we need new fresh faces from both industry and academia. Existing committee to identify and approach people who may be suitable.

Future Meetings:

- It was agreed that better publicity was required for any future Meetings for members.
- It was suggested that we should find suitable speakers in the field of Chemical Information – then build in the meeting topic around them.
- Next meeting - Thursday 31st October (subsequently changed to November 20th - see details elsewhere in this newsletter).
- It was agreed to leave subscriptions/cost of meetings as they are, but try and provide better value. This will be reviewed in 2003

Membership status: The conditions allowing membership have changed within the RSC and this was discussed. It was felt that the RSC guidelines were flexible enough and this would not cause the Group any problem.

- Remit of the group: The RSC advised us that it would be a good opportunity to revise the objectives of subject groups with the changes in Membership conditions. It was decided that the CIG would not make any changes.
- AOB: RSC wishes to set up a Chemistry librarians forum. Nigel Lees to be contacted to discuss how the CIG might help. The Secretary will invite him to the next Committee meeting.
- Autumn 2002  
20th November, "Information at the Biology/Chemistry interface."  
4th International Chemical Information Conference, Manchester, autumn 2003. The Group assisted UMIST, along with the CSA, in the organisation and underwriting of the 3rd
- Future meetings: Conference, and had provisionally agreed to do the same for the 4th. Chairman and Secretary to liaise with UMIST and CSA.
- Other topics suggested were:-  
Forensics  
Chemistry libraries

Has anyone got any other ideas or volunteers for speakers

## News

### Dialog Expands Scientific & Technical Content Collection

**CARY, N.C., USA (October 4, 2002)** — Dialog, will be adding or enhancing more than 10 scientific and technical files of content, expanding its collection used by scientific and technical information professionals. New files to be added or enhanced include: market research from Adis International; evidence-based journals from BMJ Publishing; Catfile Plus; Controlled Trials Register; HealthScout; National Patent Databases from Germany, France and the United Kingdom (provided in native language with integrated English language machine translations); Regulatory Affairs Journal from PJB Publications; and an expanded version of ToxFile. Additionally, The Cochrane Database of Systematic Reviews currently available on Dialog DataStar will be made available to Dialog users in 2003, providing access to one of the most important sources in evidence-based medicine. The agreement with Cochrane signalled Dialog's commitment to evidence-based medicine, one of the fastest growing areas of medical interest. The journal from BMJ Publishing and the Controlled Trials Register will round off this collection.

Also, the IMS R&D focus file will be enhanced with images, and American Medical Association journals will be launched on Dialog DataStar by the end of 2002.

In the last year, Dialog has completed a number of initiatives to improve its scientific and technical information, including providing DialogWeb Guided Search customers with the capability to order displayable abstracts of journal articles, patents and other documents published by Chemical Abstracts Service (CAS®). Announced earlier this year and scheduled for availability later this month, the CAS linking will allow users to request and then purchase multiple corresponding full abstracts when searching CA Search® files (file numbers 308-314, 399). These files include more than 16 million bibliographic references and indexing in chemistry and related science (from 1967 onward) produced by CAS.

For information on the addition or enhancement of more than 30 content sources, the launching of three new services designed to support information professionals and researchers in scientific and technical fields: (E-Journal Linking Dialogs re-entry to the document delivery market in August 2002, and major and long-awaited enhancements to the Dialog AlertsSM service ) please see [www.Dialog.com](http://www.Dialog.com)

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### Organic & Biomolecular Chemistry Journal

In January 2003 J. Chem. Soc. Perkin Trans. 1 and 2 are merging to form a new journal Organic & Biomolecular Chemistry ([www.rsc.org/is/journals/current/obc/obcpub.htm](http://www.rsc.org/is/journals/current/obc/obcpub.htm)). Organic & Biomolecular

Chemistry will bring molecular design, synthesis, structure, function and reactivity together in one journal and will publish fundamental work on synthetic, physical and biomolecular organic chemistry as well as all organic aspects of: chemical biology, medicinal chemistry, natural product chemistry, supramolecular chemistry, macromolecular chemistry, theoretical chemistry and catalysis. Organic & Biomolecular Chemistry will replace Perkin 1 and 2 in RSC Packages A and B and the 2003 subscription price will be less than the 2002 combined price of Perkin 1 and 2.

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## Organic Chemistry Newsletter

A free monthly newsletter for organic chemists has recently been launched. Covered topics include:

- New websites useful for organic chemists
- New software, instruments, books etc. useful in organic chemistry labs
- Special offers and/or promotions for organic chemists

Issue 1.1 is now available at <http://www.organicworldwide.net/newsletter.html>

## On-Line Resources

### TOXNET and Haz-Map

The Toxicology and Environmental Health Information Program of the National Library of Medicine's Division of Specialized Information Services (<http://tox.nlm.nih.gov>) recently launched several new and improved resources.

1. New look for **TOXNET** search interface. (<http://toxnet.nlm.nih.gov>)

TOXNET is a cluster of databases on toxicology, environmental health and hazardous chemicals.

2. New database, **Haz-Map** (<http://hazmap.nlm.nih.gov>).

Haz-Map, an occupational health and toxicology database, links jobs and hazardous job-related tasks to exposure to chemicals and occupational diseases and their symptoms.

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### Chemistry Portal to Nature

**Nature** now has a portal for Chemistry, that allows you to search for articles in Nature group publications (Nature, the newly launched Nature Materials, Nature Biotechnology, etc.) in the field of Chemistry: . Of course you, or your institution, must have a subscription in order to get access to the full-text articles.

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### Chemical Registry System

The US Environmental Protection Agencies (EPA) Chemical Registry System provides identification information on more than 70,000 chemicals. "The system provides a common basis for identifying chemicals listed in EPA regulations and data systems, and chemicals of interest from other sources, such as publications." Searches can be done by name, chemical abstracts service (CAS) number, or keyword/identifier. Results include ID information, listings of chemicals in regulations, and listings of agency programs, as well as sometimes providing molecular formula, molecular weight, and alternative identification information. The system can be found at :- <http://www.epa.gov/crs/>

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Elsevier Science's **Scirus** is a comprehensive science-specific search engine available on the Internet. It currently covers over 105 million science-related pages, consisting of 90 million science-related Web pages, including 43 million .edu sites, 5.8 million .org sites and 5.7 million .ac.uk sites

In addition to Web pages, Scirus indexes 17 million records from a number of journal sources including 12.8 million MEDLINE citations and 1.6 million ScienceDirect full-text articles.

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## Molecular Property Calculation

There is an interactive web service for the calculation of molecular properties relevant to drug design and QSAR. Properties calculated include logP, molecular polar surface area, and Rule of 5 parameters. Soon also a drug likeness index will be available.

Property calculation is available at the Molinspiration Cheminformatics web site :-

<http://www.molinspiration.com/cgi-bin/properties>

Molinspiration is offering this as a free service to internet chemistry community.

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## The Chemical Information Sources Discussion List, CHMINF-L

CIG continues to be a sponsor of The Chemical Information Sources Discussion List, CHMINF-L, a discussion list for all those involved in any way with chemical information. The list is organised by Gary Wiggins, Head of the Indiana University Chemistry Library. The list serves as a forum for discussion of, and an information source for, chemistry reference questions and the sources used to find information needed by chemists.

Members of the CIG are entitled to use it. You need to register, but it is free.

To subscribe, send mail to [LISTSERV@LISTSERV.INDIANA.EDU](mailto:LISTSERV@LISTSERV.INDIANA.EDU) with the command: SUBSCRIBE CHMINF-L.

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### *CIG Web Site*

CIG has a web site which gives up-to-date information on CIG, including forthcoming meetings. The web site, which is organised by Don Parkin, can be accessed on:

<http://cds.dl.ac.uk/cds/CIG/cig.html>

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## News from CDS, Daresbury.

A web interface to the crystallography databases - **CrystalWeb** - is available for users. The interface allows bibliographic (author, journal etc), cell data, reduced cell and basic formula searching of the databases. Retrieved structures can be displayed and manipulated using the Chime or ChimePro plugin and the references are automatically LitLink enabled, giving single click access to electronic sources of the articles.

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## News from CAS & STN

Jan Davies, STN Agency (UK) / Dr Barry Dunne, SII/CAS

### STN Express® with Discover!™ - V6.01 for Windows®

STN Express V6.01 for Windows is now available. New features include enhancements to the post-processing tools, as well as additional predefined reports and tables. Transcripts from STN® on the WebSM are supported for post-processing, along with the ability to transfer answer keys from SciFinder® into an STN session. This new version also includes a full interface to BLAST® sequence similarity searching, previously only available via STN on the Web. The free upgrade can be downloaded from <http://www.cas.org/Support/express60/win/patches/patches.html>

### SciFinder / SciFinder® Scholar™

New 2002 releases of both tools are now available, with enhanced features including powerful stereochemistry analysis and easy navigation along synthetic pathways.

### CAS File Enhancements

CA/CAPLUS content continues to grow with data now available online from 1907. In total there are now more than 21 million records, including nearly 4 million patent records. Searchable data includes bibliographic information and the abstract text.

Subject and substance indexing from the 7th Collective Index period (1962-66) corresponding to the print index letters A-N has been added to CA/CAPLUS. This work will be ongoing until all of the 'old' subject and substance indexing has been added.

A new Section Thesaurus is now available online. This feature guides searchers through the relationships and historical changes in the 80 sections of Chemical Abstracts™.

Over 1 million experimental property values for over 830,000 compounds have been added to the REGISTRYSM and ZREGISTRY files. The 5 properties with experimental values are melting point, boiling point, refractive index, optical rotatory power and density, as well as associated conditions, if available. Further information on these and the existing calculated property values is available by entering HELP PROPERTIES in the REGISTRY file. CASREACT® has been enriched with 99,000 reactions from approximately 54,000 documents published between 1907-1985. The new reactions are from the Rxn: Core Reactions database from the French organisation, INPI (Institut National de la Propriete Industrielle). The database is rich in preparations of steroids, heterocyclic compounds, and carbohydrates. Together with last year's additions from the VINITI/ZIC reaction collection covering journals from 1974-1991 and patents from 1982-1991, this brings the total number of reactions to more than 6.3 million reactions from over 398,000 document records.