

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

Autumn 2003 Newsletter

Future meetings:

One-day Training Course on Chemical Information

30th October 2003 Burlington House, London Organised jointly by CSA Trust and RSC-CIG

This one day training course will contain a series of presentations which will provide an impartial and critical overview of Chemical Information products. It will be given by specialists from academic information departments, vendor representatives and the pharmaceutical industry.

The theme of the presentations will cover structure searching in relation to chemical reactions, chemical properties and chemicals reported in patents

A booking form is included at the end of the newsletter.

Provisional programme:

- 9:30 Registration/coffee
- 10:00 Beilstein/Crossfire, Helen Schofield
- 11:15 Coffee/tea
- 11:30 CASReact, Barry Dunne
- 12:30 Cheminformatics at Sheffield, Val Gillet
- 1:15 Lunch
- 2:15 Markush searching on STN
- 3:30 Tea
- 3:35 User Perspective, Suzanne Pears, AZ

See CSA at <http://www.chem-structure.org>

The Third Joint Sheffield Conference on Chemoinformatics - 21-23 April 2004

will be held at the Octagon Centre and Tapton Hall of Residence, The University of Sheffield, UK.

The meeting is sponsored by the Chemical Structure Association Trust and the Molecular Graphics and Modelling Society.

The call for papers will be announced later in the summer and further details will be placed on

<http://cisrg.shef.ac.uk/shef2004/>

Reports on Past Meetings:

The Future of Chemical Information in the UK

The Chemical Information Group held a well-attended meeting on this subject on Tuesday, May 27th 2003, at Burlington House. The meeting had been organised at the suggestion of, and in close liaison with, the RSC Librarian, Nigel Lees.

Nigel himself opened the proceedings by sketching out the background to the topic. He reviewed the RSC's role in chemical information as the pre-eminent learned society in chemistry in the UK. He noted changes in the chemistry sector, in particular the decline in higher education in chemistry. As a result the RSC faced a number of key questions regarding its future information activities. These included the extent to which it made its archives electronic, the use of remote access by members, and the extent of collaboration with other bodies active in the area.

The second speaker was Julia Stocken, Head of Science, Technology and Innovation at the British Library. She also reviewed current changes, especially in scientific publishing, driven by, inter alia, technology, research behaviour, financial pressures, and the growth of open archiving. Publishers had responded by making electronic copies of their journals available through 'big deals,' but Julia did not believe this was sustainable. Better exploitation of electronic resources had to come, but Julia still believed there was a role for large repositories.

The third speaker, Joanne Yeomans, Faculty team Librarian at Leeds University, took a look into the future. She began by looking back at some projections on the future of scientific information made back in 1968. She foresaw a world of essentially electronic information, probably web-based. From the users' viewpoint, access needed to be available on all platforms and browsers, and there needed to be better integration of resources and easy searching and navigation via links. There would be increasing use of pre-prints and

content management software. This implied new roles for librarians, who will need skills in IT, project management, and teaching, as well as specialised subject knowledge.

Finally, Gillian Sinclair, Resource Guide Adviser for the Physical Sciences, spoke about the Resource Guide Initiative being undertaken under the auspices of JISC. The objective is to produce a series of resource guides to aid users to locate information resources in seven areas. Chemistry is covered by the Physical Sciences area. Each area has an expert Advisory Committee. The Resource Guides are basically aimed at the Higher education sector. Printed guides are available, as are free training materials. The information is also available on-line at: www.jisc.ac.uk/resoureguides/.

The meeting concluded with a discussion session, in which all the speakers took part. The main point to emerge from this was the need for better training, especially at undergraduate level, in use of information resources.

The Powerpoint slides used in the presentations are available on the Group website at: <http://cds3.dl.ac.uk/cds/CIG/cig.html>.

Doug Veal - CIG Secretary

The discussion forum from this meeting has been available since the end of May - but only two people have posted anything!

It's available from our Web site or you can go straight there using this link

<http://www.guestforum.com/forum.mx?Account=cigmembers>

Would you prefer to receive this newsletter as a web link or e-mail? For those who do not live in the UK especially this would cut postage costs! Please let us know by contacting any of us via <http://cds3.dl.ac.uk/cds/CIG/cig.html>

Software Updates

VEGA1.5.0

(<http://www.ddl.unimi.it/>), a program to convert, manage and visualize 3D structures for several platforms (Win32, Linux, Irix, AmigaOs).

Marvin Applets and Marvin Beans 3.1.3 have been released. The packages contain software development tools and applications for chemistry. Marvin Applets and JavaBeans support drawing/displaying chemical structures and handling molecule objects.

Information for the newsletter could be sent to me -

Dot Parker e-mail: gvpdjp@talk21.com (01371 870 435) and I would be very pleased to receive it!

NEWS

All of **Bentham Science's journals** published in the year 2000, 2001 and 6 months of 2002 are now available free on-line in full text PDF form in collaboration with Ingenta (offer is only available in the year 2003).

<http://www.bentham.org/>

Failed Reactions Database

The Failed Reactions Database is a compilation of reactions with unexpected results (unexpected product, further reactions or simply no reaction).

see: http://www.accelrys.com/chem_db/failedreact.html

Retrospective digitization of RSC journals

The RSC has just announced a program for digitizing its old journal issues. The backfile will contain all articles published by the Royal Society of Chemistry (and its forerunner societies) from 1841 to 1996. It is estimated the backfile will contain 200,000 articles in 1,200,000 pages. More details at:

<http://www.rsc.org/is/journals/retrodigitisation.htm>

Web of Science/MIMAS

(for UK academic community only)

A new version of the Web of Science (version 5) has been introduced at MIMAS: a preview is now available at: <http://wos.mimas.ac.uk/news/wokpreview.html>. The full implementation, under the new Web of Knowledge Platform, is due to be introduced at the end of June.

Journal Citation Reports

(provide citation data, journal ranking and impact factors for nearly 5,000 leading science journals) - Data for the year 2002 is now available: <http://wos.mimas.ac.uk/jcrweb/>

psci-comlit

A database of journal, newspaper and book references on science communication, public engagement with science and the wider issues of science in society; from the Wellcome Library at: <http://www.psci-com.org.uk/psicomlit/>

CAS Databases have been enriched with Additional Indexing, More Citations, and Additional Patent Coverage

- CAS databases have been enriched with new content including subject and chemical substance indexing for the 7th Collective Index period (7CI, 1962-1966), the 6th Collective Index (6CI, 1957-1961) and the 5th Collective Index (5CI, 1947-1956). Indexing for the 4th Collective Index (4CI, 1937-1946) has begun.
- The CA Section Thesaurus is now available in the CASM and CAplusSM files on STN[®], this facilitates comprehensive retrieval by section codes over the period 1907-present.
- The CAS databases now include more than 80 million citations, including citations from 1998 to the present. CAS coverage now includes 44 active patent issuing authorities, with the addition most recently of national patent offices for Estonia, New Zealand, Monaco, Bulgaria, Slovenia and Hong Kong plus the African Regional Industrial Property Organization (ARIPO). Current information on the database can be obtained by entering the command NEWS FILE in CA/CAplus on STN.
- REGISTRYSM has been enhanced with over 9,300 additional synonyms for pharmaceuticals from the compendium, *Drugs: Synonyms and Properties*, published by Ashgate.
- Over 174 million new predicted values have been added to more than 11.5 million REGISTRY substances for the following properties:

Bioconcentration factor, Boiling point, Enthalpy of vaporization, Flash point, Organic carbon absorption coefficient, Vapour pressure.

These values were calculated using CAS connection tables and software developed by Advanced Chemistry Development, Inc. (ACD), Toronto, Canada.

CAS Science SpotlightSM Honors Presented

The most-requested article and journals of 2002 have been identified by CAS Science Spotlight, the first real time, real usage rating system for scientific publications. Those honoured are Yukio Takahashi and Tomoya Ogawa, authors of the most-requested article, Total Synthesis of Cyclomaltohexaose, 1987, published in *Carbohydrate Research*, represented by Derek Horton, editor in 1987; Elsevier, publisher of *Carbohydrate Research*, represented by Jim Milne. For most-requested journals, those honoured are ACS Publications, whose journals published the greatest number of most-requested articles, represented by Robert

Bovenschulte; *Journal of the American Chemical Society*, the publication with the greatest number of most-requested articles, represented by Peter J. Stang, editor. All honourees received Science Spotlight sculptures at the March 24 ceremony. More information on Science Spotlight is available at <http://www.cas.org/spotlight/index.html>
Dr Barry Dunne, SII/CAS, bdunne@cas.org

JISC funds BioMed Central membership for all UK universities.

More than 80,000 biology and medical researchers working at UK universities can now share their research findings freely with fellow researchers, funding bodies, students, journalists, and the general public worldwide. Making the results of science and medical research openly available will aid the global advancement of science and healthcare. Publishing in freely accessible online journals will also make the UK higher education system more cost-effective, by reducing the amount of money spent on journal subscriptions.

The landmark deal announced by **The Joint Information Systems Committee (JISC)**, a joint committee of the UK further and higher education funding bodies, and open access publisher BioMed Central places the UK at the forefront of the drive to make scientific research freely available on the Internet. The 15 month BioMed Central membership agreement commences on the 1 July. From this date article-processing charges will be waived - for all UK higher education staff - when publishing in any of BioMed Central's 90+ peer-reviewed journals in which all research content is freely accessible.

Free registration is required; there is a sophisticated advanced search facility, and search results can be exported directly into Endnote.

Journal titles include:

- BMC Biochemistry
- BMC Structural Biology
- Proteome Science
- BMC Biotechnology
- Journal of Nanobiotechnology
- BMC Chemical Biology

For a full list see:

<http://www.biomedcentral.com/browse/bysubject/>

BOOKING FORM

**‘The One-day Training Course on Chemical Information’ on
30th October 2003 at Burlington House, London**

I/We* would like to attend

Name:	Mr/Miss/Mrs/Ms/Dr/Professor
Organisation:	
Address:	
	Postcode:
Phone:	
E-mail:	
Fax:	

Please tick boxes below. We regret we CANNOT ACCEPT CREDIT CARD bookings.

Cost of the meeting: Member of the CIG (£15.00)

Non-Member of the CIG (£25.00)

Payment by cheque enclosed:

Payment by bank transfer

(Lloyds TSB, Sort code: 30-92-76 Account: RSC Chemical Information Group Trust Account No. 0589218)

Invoice to address as above **Invoice to contact as shown here:**

Please return the booking form by 17th October 2003 to The Treasurer

Chris Evans

Information Officer

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Details will be sent upon receipt of this form 1-2 weeks before the event.