

Chemical Information and Computer Applications Group

Spring 2008 Newsletter

<http://www.rsc.org/CICAG>



Spring Meeting, 2008 - Open Access Publishing in the Chemical Sciences

The spring meeting of the Group will revisit the area of open-access publishing. It is over three years since our last meeting on this subject, and there have been many developments since then, particularly regarding chemistry.

This meeting will provide an update of these developments in this important area, presented by a panel of distinguished speakers, including:-

Simon Coles, Southampton University
Peter Murray-Rust, Cambridge University
Diana Leitch, Manchester University
Bryan Vickery, Chemistry Central
Christoph Steinbeck, EBI
David Hoole, Nature Publishing Group

together with other relevant organisations.

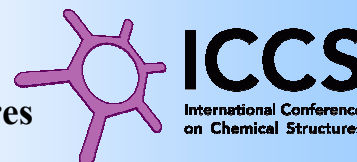
[See the section starting on page 3 about the 'Open Access Dilemma']

This will be a one-day meeting, held at the RSC, Burlington House, Piccadilly, London on Thursday, May 22nd. Further details, including the full programme and application forms, will be circulated shortly in the Group newsletter, but mark the date in your diaries now.

Funding to help students attend this meeting may be available. If you wish to pursue this possibility please contact Doug Veal – dougveal@waitrose.com

Doug Veal
Secretary, CICAG

8th International Conference on Chemical Structures



NH Leeuwenhorst Conference Hotel, Noordwijkerhout, The Netherlands.
1 - 5 June 2008

The meeting is jointly sponsored and organised by a number of societies- including RSC/CICAG

The 8th International Conference on Chemical Structures is seeking presentations of novel research and emerging technologies for the following plenary sessions:

- ✚ Cheminformatics
- ✚ Structure-Activity and Structure-Property Prediction
- ✚ Structure-Based Drug Design and Virtual Screening
- ✚ Analysis of Large Data Sets
- ✚ Informatics for Bridging Between Chemistry and Biology
- ✚ Virtual Chemistry

Submission of papers on both applications and case studies as well as on method development and algorithmic work is encouraged. The final program will be a balance of these two aspects.

Posters can be submitted for any of the above and related areas, but contributions in any aspect of the computer handling of chemical structure information is also welcome, such as:

- ✚ representation and manipulation of organic and inorganic compounds, biomacromolecules and polymers
- ✚ new algorithms for searching and managing chemical structures and reactions
- ✚ 3D databases and pharmacophore modeling
- ✚ (automatic) structure elucidation
- ✚ combinatorial chemistry, diversity analysis
- ✚ web technology and its effect on chemical information
- ✚ electronic publishing
- ✚ searching/dealing with patent spaces
- ✚ MM or QM/MM simulations
- ✚ practical free energy calculations
- ✚ material sciences

The conference will feature a new product review session for commercial presentations.

The deadline for the submission of abstracts is 15 February 2008.

Visit the conference website at www.int-conf-chem-structures.org for more information, including details on procedures for online abstract submission and conference registration. The deadline to take advantage of the early registration discount is **25th March 2008.**

Funding to help students attend this meeting may be available. If you wish to pursue this possibility please contact Doug Veal – dougveal@waitrose.com

Items from the literature

Brief abstracts from the reviews are shown please follow the links to the full article and acknowledgements.

Chemistry's Open Access Dilemma

Chemistry World, 2007, December

It was no surprise when, on 13 November, President Bush vetoed a bill that aimed to make all National Institutes of Health (NIH)-funded research publications freely available on the web. After all, the 'open access' policy was just a tiny part of a \$150 billion multi-agency proposition which Bush had lambasted as 'a spending spree'.

But the saga has highlighted a widening rift in the chemical community over open access publishing - and the contentious provision could yet be revived.

The bill, would have forced over 200,000 researchers worldwide, including many chemists, to post all peer reviewed findings on PubMed Central (PMC) within 12 months of publication in a traditional journal. The agency's current policy of simply asking grantees to deposit their articles on PMC has resulted in only 4 per cent actually doing so.

Major scholarly societies joined the Association of American Publishers (AAP) in lobbying against the proposal, including the American Chemical Society (ACS), the American Association for Clinical Chemistry, the Biochemical Society, and the RSC

If it is ever signed into law, the new NIH policy could filter down to other US federal agencies and affect disciplines beyond the biomedical sciences.

For the moment, that looks unlikely. Bush vetoed the bill because, in his words, legislators were 'acting like a teenager with a new credit card', and not specifically because of the open access provision.

<http://www.rsc.org/chemistryworld/Issues/2007/December/ChemistrysOpenAccessDilemma.asp>

However, the White House has also recently warned that any open access policy should consider 'the possible impact that grant conditions could have on scientific research publishing, scientific peer review and on the United States' longstanding leadership in upholding strong standards of protection for intellectual property'.

Meanwhile, in the UK, progress on the issue has ground to a halt. Nearly four years ago, the House of Commons Science and Technology Committee launched an inquiry into the scientific publishing industry. The committee's July 2004 recommendations, which included a proposal to make all publicly funded scientific research in the UK freely available online, were ultimately rejected by the government.

But the call for open access publishing has been growing louder over the last decade.

PubMed Central now contains over one million items, such as articles and editorials, and is said to be growing by at least 7 per cent annually (although similar growth is seen across conventional journals, too).

And physicists have arXiv - which houses preprint articles dating back to 1991 and has more recently been expanded to include disciplines like mathematics and computer science. The database contains over 440,000 e-prints with around 4000 added every month.

Chemistry, however, has yet to embrace either open access or pre-print archives (see 'Surfing Web2O', p46) . While there are more than 60 small open access chemistry journals (see figure), no major chemistry publications are fully open access.

According to Bryan Vickery, editorial director of Chemistry Central - an offshoot of open access publisher BioMed Central - the most important resources for chemists, like Chemical Abstracts and the Beilstein Database, are still locked behind hefty subscription fees.

'Many of the problems we are helping to solve are biology-related,' he said. 'We need to be maximising the visibility of our outstanding research, not hiding it behind subscription barriers.'

The fields that have more readily welcomed open access are those with a pressing need for widespread collaboration. For example, high energy physics traditionally has a very strong preprint culture, partly because researchers must cooperate to efficiently use the incredibly expensive technology they need.

Many chemists, on the other hand, are not eager to share their data before publication because their experiments could be repeated quickly and easily in another lab. In addition, unlike particle physics, significant areas of chemistry lend themselves to patentability and commercial exploitation.

.... the steps taken by the RSC and ACS to enter this new world of publishing have received a stilted response from chemists. For roughly a year, the RSC has had an Open Science service that allows authors to pay to make their article freely accessible to all. The basic fee for a primary research article is £1600 with a 15 per cent discount for RSC members, owner societies of RSC journals, and authors from subscribing organisations..

So far, just four authors have participated and only 40 articles are available through AuthorChoice, the ACS's one-year-old foray into open access, which has an upfront fee of \$3000 for non-ACS members with discounted rates for members and subscribing institutions.

Rebecca Trager, US correspondent for Research Day USA

Helping RSS help researchers Research Information, December/January 2007

Scholarly journal publishing is a major business. It is worth more than \$5 billion per year and around 2,000 STM publishers are estimated to publish between 20,000 and 25,000 peer reviewed scholarly journals worldwide(1).

New articles reveal the results of recent research, often for the first time, so it is important that researchers know about them as soon as possible. This is particularly true now that many research funding bodies require submission of research output to institutional or subject repositories within a few months of publication in scholarly journals.

If researchers do not hear about new papers when they are first published then they could choose to go straight to the repository and bypass the publisher altogether – a situation that could cause concerns for the publisher's accountants.

Traditionally, keeping up with the literature meant physically browsing journals in a library or scanning clippings, abstracting services or Tables of Contents (TOCs) online or by email.

Roddy MacLeod is senior subject librarian at Heriot-Watt University, UK.

UK scholarly journals: baseline report. RIN, RCUK and DTI, 2006. www.rin.ac.uk/data-scholarly-journals

http://www.researchinformation.info/features/feature.php?feature_id=152

eTBLAST

Chemical & Engineering News: Science & Technology, February 4, 2008, Volume 86, Number 05, pp. 26-28

This review compares [eTBLAST](#) a new unique search engine for searching biomedical literature, with **Pubmed**

[eTBLAST](#) sorts results by relevance, while PubMed sorts by **date**.

[eTBLAST](#) **saves time and effort** of creating a complicated query.

[eTBLAST](#) lets you **iterate** your search over **several** good papers to narrow your focus.

This can provide the **full MEDLINE abstract** in the results, and a link to the PubMed page and send your results to your **email**.

This **free** service is provided by the University of Texas Southwestern Medical Center. No registration necessary!

A paper detailing the operation of eTBLAST by James Lewis, Stephan Ossowski, Justin Hicks, Mounir Errami, Harold R. Garner, called *Text similarity: an alternative way to search MEDLINE*, *Bioinformatics* Sep 15, 2006; 22: 2298-2304 has been published at <http://bioinformatics.oxfordjournals.org/reports/mfr1.dtl>

Scientists cloning more papers than ever Telegraph, 23/01/2008, A new computer program reveals the questionable practice is on the rise, reports Roger Highfield

One scientific paper in every 100 has been cloned by researchers to improve their publication record in the endless quest to win more funding, according to a computerised trawl through millions of articles.

[eTBLAST](#)

The study, which reveals that the duplicates have risen in incidence by almost four fold in the past three decades, comes from researchers who have used the new computer-based text-searching tool to compare multiple documents in a database for similarities, providing a more efficient method to carry out literature searches, as well as offering scientific journal editors a new tool to thwart questionable publication practices.

Nature Launches Two New Websites:

Nature Precedings at: <http://precedings.nature.com>

Contains pre-publication research, unpublished manuscripts, presentations, posters, white papers, technical papers, supplementary findings, and other scientific documents.

Submissions are screened by their professional curation team for relevance and quality, but are not subjected to peer review. They welcome high-quality contributions from biology, medicine (except clinical trials), chemistry and the earth sciences."

Scintilla at: <http://scintilla.nature.com>

"Scintilla collects data from hundreds of news outlets, scientific blogs, journals and databases and then makes it easy to organise, share and discover the information that you're interested in."

It serves as an aggregator for news about science, and lets users recommend stories to each other and join social networks of scientists with similar interests.

ACS Nanotation

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

In October 2007, ACS Publications launched ACS Nanotation, a new website created to bring together the worldwide nano community. This free online resource enables nanoscientists to save time by reading reviews that identify the most significant, new research.

2collab

Elsevier Announces Launch of 2collab, New Research 2.0 Platform Elsevier, 27 November 2007

2collab is a social research application that provides a new way of processing scholarly information from any source. It provides a platform for researchers to connect with others in their fields, making it possible to explore, share and collaborate, increasing the chances to discover new research opportunities and mine the collective wisdom of the its member community. See

http://www.elsevier.com/wps/find/authored_newsitem.cws_home/companynews05_00800

ScienceDirect

4,000 eBooks Now Available on ScienceDirect - Elsevier, 10 September 2007

Elsevier now have more than 4,000 eBooks available on ScienceDirect. eBooks comprises high-quality selected titles published from 1995 to the present. Including scientific and technical books spanning 18 subject areas, as well as books from publishers including Pergamon and Academic Press.

ScienceDirect plans to add approximately 700 newly published titles each year. To review the list of titles available, or to inquire about signing up for eBooks on ScienceDirect, please visit

www.info.sciencedirect.com/books.

Scitopia

....Moves Into Next Phase With Full Launch Information Today, Inc., October 22, 2007

Back in April, a new sci-tech search portal was announced called Scitopia (www.scitopia.org). At the time, this joint project of 13 sci-tech scholarly society publishers promised to launch the federated searching service at the SLA annual meeting in early June. They met that deadline with a product still in beta. Now they have released the final version. (For the time being!) See <http://newsbreaks.infotoday.com/nbReader.asp?ArticleId=39927>

Scitopia now contains

- Some 3 million documents, mostly peer-reviewed journals and some conference proceedings.
- 50 million patents from the U.S. Patent and Trademark Office, the Japan Patent Office, and the European Patent Office.
- Government reports through a connection to the U.S. Department of Energy's Information Bridge (www.osti.gov/bridge).

Thomson Scientific Launches New Citation Impact Forum

Thomson Scientific announced the launch of Citation Impact Forum (www.scientific.thomson.com/citationimpactforum), an online forum promoting scholarly discussion about all facets of citation-based research evaluation.

The company hopes that by promoting an understanding and discussion of scholarly metrics, those in the industry will be encouraged to use metrics more effectively.

It will feature interviews with and commentary from industry leaders, bibliometricians, researchers, and publishers—about scholarly evaluation. Thomson Scientific said it will also use the forum to address, or to clarify, inaccuracies and common misinterpretations circulating among the scientific community printed in journals, blogs, and other forums.

Microsoft Ventures In to Open Access Chemistry

29 January 2008

Computational chemists have secured funding from computing giant Microsoft to showcase how chemistry can benefit from open access data sharing on the internet.

The two-year eChemistry pilot project represents 'a major test case' for proposed new protocols for sharing scholarly information over the web, said Lee Dirks, director of scholarly communications at Microsoft Research. Microsoft's support is also a boost for the small band of chemists keen to promote open access internet publishing.

..... Most chemical information on the web is published in closed journals and databases which guarantee high quality but also require a subscription to view. Pre-print servers, collaborative documents, open databases, video sites, online lab notebooks and blogs provide other ways of communicating research. Combining the lot offers the enticing prospect of a vast, free-to-access repository. This could transform the sharing of scientific research if the disparate data sources were machine-readable, so that a search engine could automatically gather data about a particular molecule from a crystal structure, a movie, an online lab book, and an archived article, for example.

<http://www.rsc.org/chemistryworld/News/2008/January/29010803.asp>

RSC A Chemical Conversion:

How many of you actually read any of the publications that we are regularly sent out? I admit that I do not always read either Grapevine or RSC News or any of the other publications.

There is an item in RSC News for February 2008 entitled "A Chemical Conversion" which discusses the changes being made at Burlington house. These changes will involve the closure of the library and the necessity to use many of the resources online or by phone.

I was pleased to see that "All original features in the library will be carefully restored. New features will include glass partitions across the alcoves...and a bridge to connect the two upper levels to improve access.

Adjacent to the main reading room there will be an area for light refreshment and informal meetings...

Online resources - during the closure of the library the Virtual library www.rsc.org/virtuallibrary and the Chemical enquiry Helpdesk www.rsc.org/library/cehd will continue to be available to all members. The Virtual Library offers access to millions of full text articles and chapters from key chemistry journals and ebooks. In preparation for the closure the Virtual Library will be expanded to include remote-access to Elsevier journals and over 300 more ebooks. In addition free prepaid article tokens will continue to be offered to members.

The enquiry helpdesk service has access to other premium resources and Information Officers will be able to find the information you previously would have visited the library for.

Any additions to the Virtual library will be notified in RSC News or via GrapeVine, the RSC's e-alerting service

A Note from your committee

We hope you all like this version of the newsletter - all comments and articles to include in the next edition should be sent to:

Dr. Don Parkin

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Email: d.parkin@dl.ac.uk

BOOKING FORM

RSC | Advancing the
Chemical Sciences



CICAG
Chemical Information and
Computer Applications Group

* Please delete as appropriate

I/We* would like to attend “**Open Access in the Chemical Sciences**” on **Thursday 22nd May 2008**, at the Royal Society of Chemistry, Burlington House, London W1J 0BA

Name Mr/Miss/Mrs/Ms/Dr/Professor*

Organisation

Address

.....

.....

..... Postcode

Telephone Fax

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

Cost of the meeting: Member of the CICAG (£30) Non-member (£40)

Payment by cheque (enclosed) - payable to RSC-CIG

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

Please send invoice to above address

Please send invoice to address below

Name Mr/Miss/Mrs/Ms/Dr/Professor*

Organisation

Address

.....

.....

..... Postcode

Please return the booking form by 12th May to

Chris Evans,
22 Coburn Gardens,
Cheltenham
GL51 0GE

Email: chrisevans72@btinternet.com

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

Please notify us of any cancellations to assist with catering.