

# Chemical Information and Computer Applications Group

## Summer 2008 Newsletter

RSC | Advancing the  
Chemical Sciences



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

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

One-day meeting, Thursday, May 22<sup>nd</sup>, RSC, Burlington House, Piccadilly, London

See <http://www.rsc.org/ConferencesAndEvents/conference/alldetails.cfm?evid=101553>

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. The cost is a very modest £30 for Group members and £40 for non-members. This includes coffee, lunch and tea.

The programme and application form for the meeting are given below.

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

The Final programme for the one-day meeting at Burlington House on May 22<sup>nd</sup>, 2008 can be seen on the next page. A booking form is available at the end of this Newsletter.

### Notice of Annual General Meeting

The 2008 AGM of the Chemical Information and Computer Applications Group of the Royal Society of Chemistry will be held on **Tuesday, June 10<sup>th</sup>** starting at **4.00pm at Burlington House, Piccadilly, London**. The agenda for the AGM is given below. In conjunction with the AGM, Mark Peplow, Editor of Chemistry World, will give a talk on the RSC publications for members – past, present and future.

#### Programme

- |           |   |
|-----------|---|
| 3.30-4.00 | Registration and tea/coffee   |
| 4.00-4.45 | Lecture – ‘RSC member publications: from <i>Chemistry in Britain</i> to <i>Chemistry World</i> ,’ Mark Peplow, Editor, <i>Chemistry World</i><br>(allowing time for questions afterwards) |
| 4.45-5.15 | CICAG AGM   |
| 5.15-6.15 | Wine and cheese reception   |

Please note that attendance at this meeting is completely free of charge. However, if you are planning to attend, please contact the Group Secretary, to allow us to establish numbers for catering purposes .

Doug Veal, CICAG Secretary ([dougveal@waitrose.com](mailto:dougveal@waitrose.com))

**Final programme for the one-day meeting at Burlington House on May 22nd, 2008.**

<b>Time</b>	<b>Topic and Speaker</b>
0930	Registration and coffee
1000	<i>Welcome and Introduction to the meeting</i> Barry Dunne, CICAG Chairman
1010	<i>Open Data – why it must become universal</i> Peter Murray-Rust, University of Cambridge
1045	Coffee
1100	<i>Open Access – the publishers' perspective</i> Ian Russell, Association of Learned and Professional Society Publishers
1135	<i>Open Access and the Wellcome Trust</i> Robert Kiley, The Wellcome Trust
1210	<i>Some new chemistry in European Bioinformatics</i> Christoph Steinbeck, European Bioinformatics Institute
1315	Lunch
1415	<i>Designing data repositories to support preservation &amp; publication for the chemistry community</i> Simon Coles, University of Southampton
1445	<i>Title to be announced</i> Diana Leitch, University of Manchester
1520	<i>Growth of support for Open Access, and its spread from biomedicine</i> Bryan Vickery, ChemistryCentral
1555	Tea
1610	<i>How will NPG provide better access and impact with chemistry content?</i> David Hoole, Nature Publishing Group
1645	General Discussion                      All
1700	Close of Meeting



## **Nominations invited for the Tony Kent Strix Award**

The UKeiG Tony Kent Strix Award is given *annually* to an individual or a team based in any country of the world in recognition of an outstanding contribution to the field of information retrieval

*Dr Tony Kent, a past Fellow of the Institute of Information Scientists and Director of Information at the RSC, died in 1997. He made a major contribution to the development of information retrieval and information services both in the UK and internationally, particularly in the field of chemistry. The name Strix was chosen both to reflect Tony's interest in ornithology, and the name of one of the last and most successful information retrieval packages which he created.*

Nominations will be judged by a panel of experts, and the statuette of an owl will be presented to the winner during the annual Online Information Meeting in London, December 2-4<sup>th</sup> 2008. The Panel will assess the nominations on the basis of one or more of the following criteria:

- Development of, or significant improvement in, mechanisms for the retrieval of information, either generally or in a specialised field;
- Development of, or significant improvement in, accessibility to an information service;
- A sustained contribution over a period of years to the field of information retrieval; for example, by running an information service or by contributing at national or international level to organisations active in the field;
- A major and/or sustained contribution to the theoretical or experimental understanding of the information retrieval process;
- A major contribution to fostering the education, training and/or general awareness of the importance and the technicalities of information retrieval.

Key characteristics that the judges will look for in nominations are innovation and initiative, and in particular the originality and practicality of approach that Tony Kent exemplified.

Past winners have been:

2007	Mats Lindqvist
2006	Stella Dextre Clarke
2005	Jack Mills
2004	Professor Cornelis Joost (Keith) van Rijsbergen
2003	Dr Herbert van Sompel
2002	Malcolm Jones
2001	Professor Peter Willett
2000	Dr Martin Porter
1999	Dr Donna Harman
1998	Professor Stephen Robertson

Nominations should take the form of a short description (no more than 3 sides of A4) of the work in question, together with full contact details of both the nominee and the nominator. Do not forget to include any documentation, references or URLs which may support the nomination.

Nominations should be send to

Alan Gilchrist,  
32 Friar Road,  
Brighton BN1 6NH  
UK.  
Tel: 01273 705226  
E-mail: [cura@fastnet.co.uk](mailto:cura@fastnet.co.uk)

The closing date is Friday September 19th 2008.  
(Electronic format is preferable, but not obligatory)

The Strix Award is endorsed by the International Society for Knowledge Organization (UK Chapter)

Further details can be found on the UKeiG website at:  
<http://www.ukeig.org.uk/awards/tonykentstrix.html>

*Notes:*

UKeiG is an established professional group for all information professionals, users and developers of electronic information resources. The Group encourages communication and the exchange of best practice and knowledge across all sectors; and offers an e-journal, a mailing list, an annual programme of training courses; and an array of awards and bursaries. UKeiG is a Special Interest Group of CILIP: the Chartered Institute of Library and Information Professionals. 7 Ridgmount Street, London, WC1E 7AE. Registered Charity No. 313014.



## **It's All About Access**

Collections of digital resources expand, enhancing current and ensuring future access to scientific data .

Sophie L. Rovner

**MORE AND MORE** scientific journal articles, books, and data are flowing into online archives and databases, potentially broadening access to the material for both scientists and the public. This trend raises issues such as who should have access to what material, what should be saved for the long haul, and how best to preserve the information.

See the full article at <http://pubs.acs.org/cen/science/86/8605sci1.html>

## News From the Chemical Database Service, Daresbury

The EPSRC has awarded the CDS group at Daresbury a contract for chemical database provision to the UK community beyond 1st April 2008. This replaces the previous long lasting grant funding arrangements, which terminated on the 31st March.

The new service covers the following components:

- The Cambridge Structural Database
- The Inorganic Crystal Structure Database
- The CrystMet database system
- The NIST Crystal Data Identification File
- DETHERM, thermophysical properties database
- The SpecInfo spectroscopic system
- The ACD/Labs I-Lab spectroscopic and physical properties prediction system

The New Contract arrangements came into operation on 1st April 2008. The contract is for 3 years with a possibility of an extension to 4 or possibly 5 years. I-Lab provision, however, will be reviewed after the first year.

More information can be found at: <http://cds.dl.ac.uk/cds/contract.html>

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### CALL FOR PAPERS

4th German Conference on Chemoinformatics

Hotel 'Der Achtermann', Goslar, Germany ; 9 - 11 November 2008

The CIC division of the German Chemical Society announces the 4th German Conference on Chemoinformatics (<http://www.gdch.de/gcc2008>)

They are inviting the submission of abstracts for talks and posters in the following plenary sessions:

- \* Chemoinformatics and Drug Development
- \* Chemical Information
- \* Molecular Modelling
- \* Computational Material Science and Nanotechnology and other highlights in the field of Computational Chemistry.

The submission of papers on both applications and case studies as well as on method development and algorithmic work is encouraged.

Visit the conference website at [www.gdch.de/gcc2008](http://www.gdch.de/gcc2008) for more information, including a link to the online abstract submission interface, a more detailed, downloadable PDF version of the 1st circular as well as additional information.

The deadline for the submission of abstracts is 29 July 2008.

Invited Speakers are:

Jürgen Bajorath, University of Bonn, D. Michael Berthold, University of Konstanz , D. Marcus Elstner, University of Braunschweig, D. Robert Glen, Cambridge University, UK Kurt Varmuza, Technical University of Vienna, A. Brian Vickery, Chemistry Central, London, UK

Because of the strong increase of the number of attendees during the last two conferences, a limit for the number of conference participants is imposed this year (200 max).

<http://www.gdch.de/vas/tagungen/tg/circular1.pdf>



## CAS agrees to cooperate with Wikipedia

In a positive turnaround Chemical Abstracts Service (CAS) has announced that it will support the '[CAS Number Validation project](#)' started at Wikipedia Chemistry to assist in producing a curated dataset.



New ScienceDirect features meet researchers' needs

- New to ScienceDirect are features that make the platform more user friendly and deliver better, clearer result.
- Preview tabs that provide quick access to the important article assessment components: the abstract, figures/tables and references.
- We have made it possible to view reference information within the body of a paper when the cursor moves over a [reference marker](#).
- A new [article toolbox](#) brings together all of the article-related functionality.
- Researchers are interested to know how other experts rate articles they read

For more information, contact your local sales manager or visit the [ScienceDirect Info site](#)



University of Southampton announces institutional Open Access mandate.

The University became the first (or second - Stirling University announced its own [mandate](#) on 9 April) in the UK to announce that it would henceforth require all academic staff to make all their published research available online.



## Web Version of SciFinder

SciFinder provides scientists with web access to the most comprehensive scientific information available. [View a demo of the web version of SciFinder](#).

For information about enabling access to the web version of SciFinder at your organization, contact [CAS Customer Care](#)

SciFinder is a research discovery tool that allows you to explore the CAS databases that contain literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!

You can explore one single source for scientific information in journals and patent literature from around the world.

## RSC Prospect Journal

RSC Publishing announced the release of more new features for RSC Prospect. The new features added to the enhanced HTML articles include:

- Structure and sub-structure searching
- Links to patent information (via SureChem)
- New chemical ontology terms (via ChEBI, the Chemical Entities of Biological Interest ontology)
- Links to compounds in PubChem

These new features, added to the existing biomedical ontology terms (from Gene, Sequence and Cell Ontologies) linked to definitions and related papers, hyperlinked compound information in the text and links to the IUPAC Gold Book, are another step in the transformation of scientific publishing.

You can read the news item at:

[http://www.rsc.org/Publishing/Journals/ProjectProspect/News/structure\\_search.asp](http://www.rsc.org/Publishing/Journals/ProjectProspect/News/structure_search.asp)

# BOOKING FORM



**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 22<sup>nd</sup> May 2008, at the Royal Society of Chemistry, Burlington House, London W1J 0BA

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

Organisation .....

Address .....

.....

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..... 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 .....

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..... Postcode .....

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Please return the booking form to

Chris Evans,

22 Coburn Gardens,

Cheltenham

GL51 0GE

Email: [chrisevans72@btinternet.com](mailto: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.