



SPRING 2009

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NEXT MEETING

SCIENTIFIC TEXT AND DATA MINING 20TH MAY 2009, BURLINGTON HOUSE, LONDON

This meeting explores the tools and methods for mining chemical information such as text, structures and data.

DRAFT PROGRAMME

10.30 to 11.00	<i>Registration & Tea/Coffee</i>
11.00 to 11.40	"Annotating Chemical Names" - Peter Corbett, Unilever Centre for Molecular Informatics, Cambridge
11.40 to 12.20	TBA - Sophia Ananiadou, NaCTeM, Manchester
12.20 to 13.00	"Text Mining with Pipeline Pilot: a Bibliography Platform Example" - Stéphane Vellay, Accelrys
13.00 to 13.50	LUNCH
13.50 to 14.30	"From high throughput to high frustration: data mining in drug discovery" - Darren Green, GSK
14.30 to 15.10	TBA - Jeanette Eldridge, AstraZeneca
15.10 to 15.40	"Mining scientific information: pitfalls and possibilities" - Neil Stutchbury, RSC
15.40 to 16.10	"Mining and meaning: applying standards to chemical content" - Richard Kidd, RSC

This will be followed by an AGM with wine and cheese.

There is a booking form available at the end of this Newsletter and for download at the CICAG home page

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

PAST MEETINGS

RSC LAW GROUP EVENT: SEARCHING AND SORTING - 25TH NOVEMBER 2008 BURLINGTON HOUSE, LONDON

Speakers included:

Marian Challis, an examiner at the UK-IPO

Steve Royle, a professional searcher from Perquisitum Limited

Jannette Mole, an IP scientist at AstraZeneca R&D Charnwood

Nazma Masud, a chemical information specialist from the RSC (interactive session on RSC virtual library resource)

This session started with an overview of the patent process and the role of patent examiners and the sources they used when examining a patent.

Steve Royle discussed aspects of outsourcing patent searching and offered guidelines of how to select the most appropriate organization for your needs and how to implement the work.

He suggested that you could expect to spend time and money establishing the outsourcing relationship and that quality expectations and service parameters should be clearly defined. One approach would be to provide the prospective firm with a variety of projects of the type they would be expected to complete and evaluate their deliverables against your quality standards.

Jannette Mole presented a novel approach to organizing the mountains of information we have gathered around us with mind maps, a pictorial map of linking ideas on a topic, which could be used as an index to your electronic repository of saved searches and other important documents.

The session finished with an interactive demonstration of the resources available to members of the Royal Society of Chemistry through RSC Virtual Library.

236TH ACS NATIONAL MEETING AND EXPOSITION - PHILADELPHIA, PA, AUGUST 17-21, 2008

Chemical Information and Computation 2008, Number Two

The contents list is on the Web at <http://www.warr.com/morepubs.html>.

A 12-page extract is available free at <http://www.warr.com/phillyacs08.pdf>.

The report includes:

1. News from more than 70 companies (including some not exhibiting)
2. Condensed press releases for the last six months of 2008
3. Accurate transcripts of presentations, complete with color figures and literature references, with the following themes:
 - Herman Skolnik Award Symposium, Awardee Gerry Maggiora.
 - Data mining and text mining approaches to drug discovery.
 - ADME informatics, converting raw data to useful knowledge for drug discovery predictive properties.
 - A retrosynthesis search engine.
 - Working with IUPAC names.
 - Open meetings of the ACS committees on ACS Publications and CAS.

Contact me by email for further details.

Wendy

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FROM THE LITERATURE

NEW TOOL: AUTHORMAPPER.COM

<http://www.authormapper.com/>

"AuthorMapper.com is a free interactive tool that visualizes scientific research areas and trends in an easy and refined way. It will assist the scientific research community by plotting authors, subjects and institutions on a world map as well as identifying scientific trends through timeline graphs, statistics and regions. Start mapping your scientific community today!"

NEWS FROM THE CHEMICAL DATABASE SERVICE, DARESBURY

CDS were successful in renewing the license for the ACD/Labs set of spectroscopy and physical chemistry databases and they will now be available for (at least) another 2 years.

Institutional logins via Shibboleth are now available for two databases - "Available Chemicals" and "Screening Compounds". It is hoped to extend this to all the databases by the end of April 2009.

Eligible users (any UK 'academic') are also able to register very quickly using the express online registration route where a CDS ID and password should be e-mailed back within 10 minutes as long as you use an .ac.uk e-mail address.

The SPRESI database, the world's third largest molecule database is now available for at least the next year to all registered users via a web interface.

More details can be found on the home page <http://cds.dl.ac.uk>

MOLECULAR NETWORKS

Molecular Networks announced the first commercial release of its new reaction database-driven synthesis planning tool THERESA.

THERESA is a new web-based, easy-to-use program system that supports chemists in planning their organic synthesis strategy by providing a novel method to search in reaction databases.

For further information about THERESA, please refer to the THERESA product page on the web site of Molecular Networks (www.molecular-networks.com/software/theresa/) or contact them at info@molecular-networks.com.

COUNTER 3

RSC Publishing can now provide customers with COUNTER 3 compliant journal usage statistics, thanks to a new service delivered by MPS Technologies.

The publishing arm of the UK's Royal Society of Chemistry, RSC Publishing is the first chemistry publisher to announce the availability of COUNTER 3 statistics for its journal customers. Full details are available on the website: http://www.rsc.org/Publishing/librarians/News/COUNTER_3.asp

The RSC Publishing journal portfolio is about to see further expansion with the announcement that two new peer-reviewed titles, **Nanoscale** and **Analytical Methods**, will be launching in autumn 2009.

Nanoscale will publish experimental and theoretical work across the breadth of nanoscience and nanotechnology.

Analytical Methods will highlight new and improved methods for the practical application of analytical science.

Visit www.rsc.org/methods and www.rsc.org/nanoscale to find out more.

REAXYS LAUNCHED, JANUARY 1, 2009

Reaxys is Elsevier's new interface to the Beilstein and Gmelin databases and also includes the Patent Chemistry Database.

For more information go to <http://info.reaxys.com>



* Please delete as appropriate

I/We* would like to attend "Scientific Text and Data Mining" on Wednesday 20th May 2009, at the Royal Society of Chemistry, Burlington House, London.

Name

Organisation

Address

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..... Postcode

Telephone Fax

E-mail

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

Cost of the meeting: Member of the CICAG/USTLG (£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. 00589218)

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.....

Please return the booking form by 8th May 2008 to:

Chris Evans
RSC-CIGAG Treasurer
22 Coburn Gardens
Cheltenham
GL51 0GE
tel. +44 (0)1242 510778
e-mail: chrisevans72@btinternet.com

Further details will be sent 1-2 weeks before the event

Please notify us of any cancellations to assist with catering