

NEWSLETTER Spring 2012

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Chemical Information & Computer Applications Group: <http://www.rsc.org/CICAG>

Linked in  <http://www.linkedin.com/groups?gid=1989945>

Twitter: https://twitter.com/RSC_CICAG/

Chemical Information & Computer Applications Group

Contributed by Keith White, RSC CICAG Chairman

CICAG aims to keep its members abreast of the latest activities, services, and developments in all aspects of chemical information, from generation through to archiving, and in the computer applications used in this rapidly changing area through meetings, newsletters and professional networking.

CICAG Committee Members

Welcome to **Dr Stephanie North**, our newest committee member. Stephanie is Director of Allyl Consulting Limited and is currently working as a consultant, providing representation for InfoChem GmbH in the UK. She began her career as a medicinal chemist at Glaxo then moved into Information Services where she was responsible for the chemical information team. Stephanie pioneered the introduction of end-user searching and led the evaluation, deployment and training for chemical applications. She then progressed to leading groups of information analysts delivering a range of services across R&D. Following the GlaxoSmithKline merger, Stephanie transferred into Research Data Management and had global responsibility for the information exchange critical for external collaborations. Stephanie left GSK to start her consulting business specialising in chemical information and collaboration knowledge management for the Pharma, Biotech and Informatics community. Stephanie holds a PhD in chemistry and is a Fellow of the Royal Society of Chemistry.

A full list of the current RSC CICAG Committee Officers and Members, with their affiliations and contact details, can be found on the CICAG website:

<http://www.rsc.org/Membership/Networking/InterestGroups/CICAG/committee.asp>

If you are interested in joining the committee, please contact the RSC CICAG Chairman (Dr Keith White; email: keith.white@matthey.com). Enquiries are particularly welcome from younger members of the profession.

N.B. It is now an RSC requirement that all new group committee members are also members of the RSC.

RSC now has an e-Membership category, which costs just £20 and provides electronic access to Chemistry World and access to Specialist Interest Groups and other RSC networks via MyRSC. See: <http://www.rsc.org/Membership/e-Membership/>

As well as the **LinkedIn** Group: <http://www.linkedin.com/groups?gid=1989945>
CICAG is now on **Twitter**: https://twitter.com/RSC_CICAG/

RSC CICAG Autumn 2011 Meeting Report

The Future Information Needs of Pharmaceutical and Medicinal Chemistry
Monday 28th November 2011

Meeting Summary

Contributed by Stuart Newbold, Head of Information, Astex Pharmaceuticals

Following on from the 2010 Meeting, when conference speakers looked back to a 'Celebration of the History of Chemical Information', this year's RSC CICAG conference instead was an attempt to look forward to 'The Future Information Needs of Pharmaceutical and Medicinal Chemistry'. This year's attendees were fortunate in not having to brave the snowy weather of 2010. They were also provided with a very

agreeable venue in the shape of the Linnean Society, located diagonally opposite the RSC across the courtyard.

The programme commenced with **Dr Wendy Warr**, who set the scene by reviewing the progress of the pharmaceutical industry since the 1970s, the state of the industry and challenges facing it today including declining productivity, bearing down on costs by mergers and acquisitions, and changes in the way R&D is undertaken including by collaborations with biotechs and universities. Wendy was followed by **Dr Frank Cooke** of GlaxoSmithKline (GSK), who provided an industrial perspective with a case study on how GSK use information today, with a particular emphasis on how the company continues to embrace technology to both deliver information to scientists and also measure its use and effectiveness across the organisation.

Frank was followed by **Dr Anne Hersey** from European Bioinformatics Institute (EBI), who described how the ChEMBL open access database has been developed to provide users with structure-activity data for druglike, bioactive compounds. Collaborative ventures and integration of database information were themes which were repeated during the day, and ChEMBL proved to be the first example of a new, curated, database with links to other resources where information about common chemical structures (or targets) exists, and which has input from other partners including non-profit, university and big Pharma. The morning concluded with **Prof Jeremy Frey** from the University of Southampton, who provided a fascinating insight into a more integrated, high-tech future by use of semantic web technology. Jeremy espoused the capture of all data in research experiments and the use of metadata in particular. Jeremy provided a number of examples of enabling technology including the use of virtual research environments.

In the afternoon, and following the lead from Anne Hersey, **Richard Kidd**, Head of Informatics at the RSC, gave a presentation on the RSC's collaborative public-private project, Open PHACTS, which itself is derived from the Innovative Medicines Initiative between the European Community and the European Federation of Pharmaceutical Industries and Associations and whose members include a range of pharmaceutical companies. Themes included integration of information via elimination of 'data silos' as well as the construction of new ontologies. Attendees then had a chance to listen to a publisher's perspective, in this case from **Paul Peters** of Chemical Abstracts Services. Initially Paul's focus was on the challenges facing the Pharma industry and what CAS does today as a provider of timely, high value-added information. But Paul also looked ahead, highlighting some emerging trends and illustrated a shift to the provision of information solutions with the development of a completely new STN which will be appearing in the market this year. The day's most entertaining presentation was saved until last. This was from **Dr Bill Town**, President of Kilmorie Consulting, with his 'Reflections on the Past and Future'. Bill firstly took a look back over some personal milestones and the role that technology had played in his achievements. The talk included many fascinating examples of how the publishing and pharmaceutical industries had changed in the last 30 years, highlighted some amusing past predictions of the future, before concluding with his own view of what the future may hold for the Pharma and information industries.

The final part of proceedings was a question and discussion session, chaired by **Dr Diana Leitch** in which a common theme for those of us in the West was of a somewhat challenging and possibly insecure future. Only time will tell whether we were being too pessimistic! Our thanks go to all the speakers who were excellent.

The comprehensive summary of 'The Future Information Needs of Pharmaceutical and Medicinal Chemistry' meeting by Dr Wendy Warr, plus copies of several of the presentations, can be downloaded at:

<http://www.rsc.org/Membership/Networking/InterestGroups/CICAG/meetings.asp>

Further thoughts on points raised in discussion at the end of the meeting

Contributed by Alan Tonge

I would like to add my own observations about some of the points raised by members of the audience in Questions & Discussion section at the end of the meeting.

While Wendy Warr is correct in suggesting that the mood of the meeting was pessimistic and that we must be able to adapt in order to survive and move forward in the rapidly changing (and currently contracting) world of chemical information in the pharmaceutical industry, I think that there were a number of additional points made by attendees in the Discussion that deserve consideration:

- i) If medicinal chemists are now being required to manage their own information resources, rather than rely upon information specialists, this surely requires that they will have less time to devote to laboratory chemistry.
- ii) While the pharmaceutical industry is busy further re-structuring itself by 'outsourcing' services to *e.g.* China and India, where are the next generation of UK chemists who can currently manage these services going to come from? The consequence is that we will lose the ability to maintain a viable UK industry.
- iii) Chemistry has been removed from centre-stage in the lead discovery process for drug development.

For me it is this last point which we need to disseminate - much of the creative input of chemists has been lost and arguably needs to be replaced. As a discipline, part of the process of survival must be to stand up for ourselves.

Speakers' Abstracts

"Adapt and Survive: the Way Forward in Research IS", Dr Wendy Warr, Wendy Warr & Associates

Chemists involved in drug discovery are heavy users of information, both internal and external. I will give an introduction to the changing economics and environment of the pharmaceutical industry, and the workflows of "hit-to-lead" and "lead optimization". There are information resources and tools that can be used in decision making at every stage and I will discuss a selection of these in context.

"Case Study: Use of Information in the Pharmaceutical Industry Today", Dr Frank Cooke, Published Information Manager, GlaxoSmithKline

In this presentation I will look at the use of published information within GlaxoSmithKline (GSK). Over the last decade we have seen dramatic changes in the way users access and use published information. Significant changes along the way have been the downsizing and eventual elimination of the traditional library, provision of greater access to electronic resources, the integration / de-integration of information sources, the changing model of expectations set on our users and the way we gather, archive and utilize usage data to drive our licensing, marketing and training efforts.

"How the ChEMBL Database is Meeting the Chemical and Biological Information Needs of Scientists of the Future", Dr Anne Hersey, Group Coordinator, ChEMBL Group, EBI (European Bioinformatics Institute)

The landscape of pharmaceutical development is changing with the reduction in the size of many large pharmaceutical companies and an increase in early stage work being done in academic groups and small companies. There is an interest in open data and pre-competitive initiatives to help facilitate this. ChEMBL is an open bioactivity database containing manually extracted and curated structure-activity relationship (SAR) data from the medicinal chemistry literature. It is a resource used by drug discovery scientists in

large pharmaceutical companies as well as small companies and academic organisations. The database and its content will be described as well as the work done to integrate it with other resources such as PubChem. The challenges in doing this will be discussed as well as ideas on future integration.

“Semantic Web Technology in the Chemistry Laboratory”, Prof Jeremy Frey, School of Chemistry, University of Southampton

While the World Wide Web has altered the way we present and access research and information in Chemistry, it could be argued that it has not fundamentally changed the way we undertake the research in the laboratory, unlike some aspects of the ‘online society’. In my talk I will describe the work we have undertaken to apply and develop some of the techniques of the semantic web and ideas of social networks to facilitate experimental chemistry, with for example electronic laboratory notebooks and related ideas.

“Pharmacological Information Discovery with the Public-Private Project Open PHACTS”, Mr Richard Kidd, Head of Informatics, Royal Society of Chemistry

Open PHACTS is a European project funded by the Innovative Medicines Initiative, and is an industry / academia public-private partnership with 8 EFPIA partners and 14 academic / not-for-profit / SME partners. It aims to reduce the barriers to drug discovery by applying semantic technologies to available data resources, creating an Open Pharmacological Space. Currently, pharmaceutical companies expend significant and duplicated efforts aligning and integrating internal information with public data sources, and to address this problem Open PHACTS will deliver a single view across available data resources, and will be freely available to users.

“Meeting the Challenges of Pharmaceutical and Medicinal Chemistry, a Publisher Perspective”, Mr Paul Peters, Director, EMEA Sales, CAS


The information user faces many challenges in locating quality information. The patent searcher for example needs to be confident they have identified all prior art. The laboratory scientist may be looking for a quicker, cleaner method to synthesize their compound. The PhD student will need to be sure they are working on a novel area of science. Likewise, the scientist preparing a paper for publication is interested in any previous work in the area. With the explosive growth in the quantity of data, the increasingly complex patents prepared by attorneys and the large volume of non-English literature, the job of the information user is not getting easier. So how are publisher organizations meeting these challenges? Significant technology advancements at CAS allow for fast and precise structure, reaction, sequence and Markush searching. Close collaboration with patent offices worldwide means we are in step with the changing trends in patenting. Novel analysis and visualization technologies provide new insights into existing data. The trend is similar with other publisher organizations who are, for example, working in pre-competitive environments to provide data, tools and technologies to assist pharma partners in fully utilizing the volumes of information today. In this talk, the focus will mainly be CAS with a short mention of the new STN platform which will be available in 2012.

“Some Reflections on the Past and Future”, Dr Bill Town, President, Kilmorie Consulting

Since over fifty years have passed since I started my first chemistry degree course, I'm reaching an age where my own personal reflections are approaching historical dimensions. In this brief talk, I will consider changes in information and communication technology over this period, their impact on the delivery of chemical information and, in parallel, changes which have occurred in the pharmaceutical and publishing industries. Predicting the future has always been difficult but I'll also attempt to gaze into my crystal ball to see if the fog clears.


Details of Speakers

Dr Wendy Warr, MA, DPhil (Oxon), CChem, FRSC, FCLIP



Dr Warr has Master's and Doctor's degrees in Chemistry from the University of Oxford, England. She is a Chartered Chemist, a Fellow of the Royal Society of Chemistry and a Fellow of the Chartered Institute of Library and Information Professionals. She has over 40 years' experience in information systems and research computing including nearly 20 years in the pharmaceutical industry. She is active in the Chemical Information Division of the American Chemical Society (ACS) and serves on several international scientific committees, including the scientific advisory board of the German Chemical Society's Conference on Cheminformatics. She has been an Editor of the ACS Journal of Chemical Information and Modeling (formerly Journal of Chemical Information and Computer Sciences) since 1989. She is also a columnist for the Journal of Computer-Aided Molecular Design. She is General Secretary of the International Council for Scientific and Technical Information (ICSTI) where she represents the International Union of Pure and Applied Chemistry (IUPAC). Wendy Warr & Associates offer consultancy services in the fields of cheminformatics, computational chemistry and electronic publishing. Clients include pharmaceutical companies, pharmaceutical industry partners, software companies, publishers, and scientific database producers.

Dr Frank Cooke



Dr Cooke received his BSc in Chemistry from Imperial College, London and also his PhD from the same institution although most of his research was done while at the Ohio State University. He worked for Eastman Kodak in Kingsport, Tennessee for 18 years where he did research in a number of areas including custom synthesis for drug intermediates, textile and photographic dyes and enteric coatings for drug delivery systems. Beyond the research environment he held positions in chemical development and large scale production before returning to the research labs. At this point he had a career change and moved into chemical information and led a group of information specialists while developing IT solutions to provide more timely access to company chemical data. In 1996, Frank joined SmithKline Beecham to manage a small group of information scientists who supported a number of desktop tools. Although he went through a merger and numerous upsizings and downsizings of his group he continues to manage a group supporting desktop information products. However, the current support model offers very different challenges and benefits compared to earlier times. He has developed systems to comprehensively track usage of both internal and external information sources and these have been employed very successfully in right-sizing contracts and targeted marketing efforts. Frank enjoys running, cycling, swimming and golf although years of competitive abuse have slowed his current pace!

Dr Anne Hersey

Dr Hersey obtained a degree in Chemistry and PhD from the University of Kent. She then worked for many years at GlaxoSmithKline and its former companies. Firstly she worked on physicochemical property measurement and then led a team developing models for the prediction of ADMET properties for use by drug discovery teams. Currently she is the Group Coordinator of the ChEMBL Group at EMBL-EBI near Cambridge.

Professor Jeremy Frey



Professor Frey is Professor of Physical Chemistry at the University of Southampton, and is currently involved with the UK e-Science programme, as Principal Investigator (PI) of the CombeChem project (<http://www.combechem.org/>) looking at the ways in which e-Science and Grid infrastructure can be developed to provide support for and carry out chemical research, for example in Electronic Laboratory Notebooks (ELNs) with the Smart Tea Project, generating and applying a “Semantic Chemical Grid” and applying Web 2.0 & Social Network ideas with Chemical Blogs and related technologies. Fundamental to the ideas of “Publication @ Source” for scientific data is his work on the interaction of e-print repositories with chemistry in the work on the e-Bank & e-Crystals projects (<http://ecrystals.chem.soton.ac.uk/>).

Mr Richard Kidd



Richard Kidd has worked at the Royal Society of Chemistry for many years on the underlying data and production processes behind its publications. Richard's team developed the Project Prospect semantic enhancement of its journals, and is currently integrating publications and tools with the RSC's public access ChemSpider database.

Mr Paul Peters



Paul Peters got a BSc in Chemical Engineering from the HTS in Amsterdam. He worked as an information professional for the Dutch Labour Inspectorate before working for 8 years as the STN representative for the Netherlands at Cobidoc BV. In 1995 Paul joined the newly founded sales and support organization Science Information International which is a wholly owned subsidiary of the American Chemical Society tasked with the sales and support of CAS products in Europe, the Middle East and Africa. Paul leads a team of more than 20 staff and agents around Europe and the Middle East who work with patent experts and scientists in companies, academia, patent offices and other research organizations providing access to STN and SciFinder to solve a variety of chemistry and related questions.

Dr Bill Town



Dr Town is a senior manager with an exceptional record of innovation in patent and scientific information web publishing and software development. Kilmorie Consulting was founded by Dr Town who has over 30 years experience in the software, publishing and electronic information industries. In 1983, he founded Hampden Data Services (now a wholly owned subsidiary of the American Chemical Society) which was instrumental in developing many software products including STN Express. Before establishing Kilmorie Consulting in 2002, he worked as Managing Director of ChemWeb, Inc. and before that in many roles at Derwent Information Ltd. Kilmorie Consulting is now an operating division of Kilmorie Clarke Ltd whose activities also include corporate video production and conference production.

RSC CICAG Meeting May 2012

Our next meeting will be held on Tuesday 15th May 2012 in the Science Room, RSC, Burlington House, London.

Provisional title:

CICAG Networking and Personal Development Meeting: Members and Students

This meeting is still at the planning stage but will be an opportunity for networking and personal development. We are hoping to arrange for a keynote speaker to talk about aspects of personal development. The meeting will also enable students to showcase their research. Put the date in your diaries; further details will be available soon on the CICAG website: <http://www.rsc.org/CICAG/>

Bursaries:

A limited number of student bursaries are available. These will cover UK travel costs and the meeting fee, to enable selected students to attend the meeting at no cost whatsoever. Please contact Dr Keith White, Chairman of RSC CICAG, email: keith.white@matthey.com

RSC CICAG AGM 2012

The 2012 CICAG AGM will take place immediately after the above meeting, on Tuesday 15th May 2012 at 4.30 pm in the Science Room, RSC, Burlington House.

Further details of the Group can be found on its website at:

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

USTLG Autumn meeting on Data Management

Report by Hannah Morgan, University of Nottingham Medical Library

The autumn 2011 meeting of the University Science and Technology Librarians' Group (USTLG) was held in Clare College, Cambridge, conveniently located next to the imposing University Library on 28th November 2011. The day's focus on data management started with a talk by Laura Molloy about the Data Management Skills Support Initiative. This project evolved from the realisation that essential data management skills were not currently widely embedded in postgraduate training. Laura explained how they have worked with institutions to create usable and open access training materials for information literacy and their plan to engage with professional bodies to create career profiles stressing the importance of data management in a variety of jobs.

Continuing the theme of data management in research, Yvonne Nobis from Cambridge University, presented her current work trying to help academics in different disciplines share data, focussing on the use of computer codes. Yvonne highlighted that many postgraduate students write their own computer codes to aid their research but do not publish it, and this large amount of data created is likely to be beneficial to someone else, either working in the same field or in a completely different discipline. As was the case for the historian who was able to use code, created by geneticists to look at gene trees, for his study of the history of manuscripts. However this and all of the other cases of collaboration that Yvonne came across had arisen from serendipity, usually during conversation at a college lunch, and therefore Yvonne is continuing to investigate if, and how, librarians can facilitate data sharing across academic disciplines.

In a slight break from data management we were then introduced to the new USTLG website, www.ustlg.org, incorporating a new logo and a blog to enable more members to contribute to its content. During lunch there was the opportunity to see some of the rare science manuscripts held by the Cambridge University Library. These included some of Isaac Newton's notebooks and Ernest Rutherford's lab diaries, which we were warned were still slightly radioactive. Also on display were a few draft pages of Charles Darwin's 'On the Origin of Species', interestingly only kept by Darwin because his children had used the other side to draw upon.

After lunch, Rachel Berrington from the Institute of Electrical and Electronics Engineers (IEEE) gave an overview of the current updates and the future plans of IEEE. These included several new journals starting in 2012 and the facility to now search the IEEE Xplore database on mobile devices. The final talk was given by Anna Collins on 'Supporting Research Data Management', featuring the Incremental Project, a collaboration between the Universities of Cambridge and Glasgow about how best to deliver data management training to postgraduate students. This was a good end to the day providing many practical hints and tips both on delivering data management training and data management itself.

Student Bursaries

In order to encourage young chemists to consider careers in chemical information and computer applications, the CICAG committee is prepared to consider applications from students for bursaries to attend any relevant chemical information or computer applications conference or meeting.

Initial enquiries should be made to the CICAG Chairman, Dr Keith White, email: keith.white@matthey.com

Tony Kent Strix Award 2011

Contributed by Doug Veal

As announced in the last newsletter, the 2011 Tony Kent Strix award was presented to Prof. Alan Smeaton, School of Computing, Dublin City University, for his sustained contributions to the field of natural language processing techniques for textual information retrieval and to the indexing and retrieval of image, audio and video data.

The award was presented on Monday 24th October at the Enterprise Search Europe event at the Hilton London Olympia. The award is administered by the CILIP UK e-Information Group and sponsored by the CICAG and Aslib.

The picture shows the award being presented with, from the left, Martin White, conference organiser and Chair of UKeIG, Graham Coult representing Aslib, Prof. Smeaton and Doug Veal, Chair of the Strix Award Panel and representing CICAG.

Further details of the Tony Kent Strix Award, including a list of past winners, can be found at: <http://www.ukeig.org.uk/awards/tony-kent-strix>



Other Awards

CSA Trust Jacques-Émile Dubois Grants

The Chemical Structure Association (CSA) Trust is an internationally recognized organization established to promote the critical importance of chemical information to advances in chemical research. In support of its charter, the Trust has created a unique Grant Program, renamed in honor of Professor Jacques-Émile Dubois who made significant contributions to the field of cheminformatics. The Trust is currently inviting the submission of grant applications for 2012.

The deadline for applications is March 14, 2012. For full details see:

http://www.csa-trust.org/?page_id=9



2012 CINF Scholarship for Scientific Excellence Sponsored by FIZ Chemie Berlin

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society funded by FIZ Chemie Berlin is designed to reward graduate and postdoctoral students in chemical information and related sciences for scientific excellence and to foster their involvement in CINF.

Closing date: 31st March 2012. For further details see:

<http://www.acscinf.org/about/news/20120125.php>



Reaxys PhD Prize: Call for Submissions

The Reaxys PhD Prize recognizes research and publication excellence in organic, inorganic, and organometallic chemistry. The Prize is open to all students studying for a PhD (or having completed a PhD after January 1, 2011) in chemistry.

Submissions are reviewed and judged for originality, importance, applicability, rigor or approach and publication quality, by an external board of internationally renowned chemists. Submissions close on February 15, 2012. For further details see:

<http://prize.reaxys.com>



RSC Publishing News

Contributed by Louise Peck, Library Marketing Specialist, RSC

RSC Mobile app now available on iOS and Android

RSC Mobile provides readers with access to search more than 30 RSC journals from our RSC Publishing Platform. If your institution/organisation pays for RSC journals, then you can access exactly the same content on this app using your institutions/organisations wireless network.

See: <http://blogs.rsc.org/technical/2012/01/11/rsc-mobile-android/>

Chemistry World Mobile app now available

We have just launched the iPad and Android apps for Chemistry World and these are now available completely free of charge on the App Store and Android Market, respectively, until 1 April.

See: <http://prospect.rsc.org/blogs/cw/2012/01/12/chemistry-world-app/>

Shibboleth Compliance

Japanese RSC Publishing is pleased to announce Shibboleth compliance with the Japanese Federation GakuNin, for more information

See: <http://blogs.rsc.org/technical/2011/12/22/shibbolethjapan/>

FREE Access Content Updates

RSC Publishing would like to announce updates to our free access content model for RSC scientific journal articles and eBooks, for more information please

See: <http://blogs.rsc.org/rscpublishing/2011/12/19/freeaccessupdates/>

RSC Publishing announces new partnership for South Africa and Botswana

RSC Publishing, the award-winning publishing division of the Royal Society of Chemistry announces new partnership in South Africa and Botswana

See: <http://blogs.rsc.org/rscpublishing/2011/12/16/newpartnershipsandbotswana/>

RSC Publishing attended Online Information, London

We're really pleased that our recycled cardboard stand stood the test of time and survived the exhibition, proving to be a great asset and receiving lots of positive comments and photographs. See:

<http://blogs.rsc.org/rscpublishing/2011/12/23/online-information-show-2011-winners/>

ChemSpider News

Contributed by Richard Kidd, Informatics Manager, RSC



<http://www.chemspider.com>

Learn Chemistry Wiki (<http://www.rsc.org/learn-chemistry/wiki/>) was launched at the beginning of 2012 as part of the overall **Learn Chemistry** (<http://www.rsc.org/learn-chemistry/>) site. The Learn Chemistry Wiki contains over 2000 "substance" pages which correspond to simple compounds that would commonly be encountered during the last years of school and first years of University. The Learn Chemistry Wiki also goes a step further and not only contains compound information in isolation but also contains

laboratory experiments (with parallel sections which contain an overview, teachers' notes and students' handouts) for each, quizzes, and tutorials which are linked to the compound information to put them into context. The wiki is based on the MediaWiki platform (which allows multiple users to contribute collaboratively since the website is intended to be a community website), but extends it to incorporate functionality similar to that of ChemSpider, invoked via custom-made extensions. For example, it is possible to draw structures using GGA's Ketcher in order to find structures, or to draw answers to quiz questions (for example to specify the product of a particular reaction). It is also possible to include an interactive spectrum retrieved from ChemSpider in any wiki page, using the ChemDoodle spectrum viewing widget in browsers which support canvases or JSpecView applet in those that don't.

<http://www.chemspider.com/blog/learn-chemistry-wiki-is-launched.html>

ChemSpider plugin for IDBS ELN

In collaboration with IDBS and Cambridge's Chemistry department, we have made a plug-in which could both dynamically retrieve information from ChemSpider into their ELN, and publish to it the other way. The Chemistry department at Cambridge have been very helpful in granting access to their ELN to write the plug-in, and will be its first users, but the results will be freely available for any existing IDBS E-WorkBook suite user.

<http://www.chemspider.com/blog/chemspider-plugin-for-idbs-eln.html>

CAS News

Contributed by Dr Anne Jones, CAS Applications Specialist UK & Ireland



A division of the American Chemical Society

New SciFinder Features Help Scientists Quickly Find Substances Most Relevant to Their Research

Key enhancements in the recent SciFinder update (December 2011) include relevance ranking of structure search answer sets, additional mass spec and NMR data for ~75,000 substances, new streamlined display formats for references and substances, and the introduction of bioactivity and target indicators to substance detail displays and substance Analyze options. With bioactivity and target indicators, you can now use SciFinder to easily assess the biological relevance of substances (e.g., for new drug applications).

New STN[®] Revolutionizes Patent Searching for Professionals

Redesigned STN retains what customers value most while phasing in advanced search and analysis capabilities beginning in 2012.

The STN partners, Chemical Abstracts Service (CAS) in the U.S. and FIZ Karlsruhe in Germany, are pleased to announce that a completely new STN will be phased into the market beginning in 2012.

The new platform will bring improved efficiency and usability at the expert level. Powerful new elements will include:

- Project-oriented workflow,
- Combined text and structure queries,
- Simultaneous query and results interaction,
- Real-time analysis of results, and
- Virtually no system limits.

"While New STN will offer a wide range of advancements, it will retain the unique values of STN that are trusted by patent search professionals today, including the STN command

line, search precision and high-quality content," said Sabine Brunger-Weilandt, President and CEO of FIZ Karlsruhe.

"Our focus on patent professionals also encompasses the STN commitment to a secure and confidential research environment, as well as training and support by our scientists, which will be hallmarks of the new system," said Robert J. Massie, President of CAS.

Teams of information technology professionals at FIZ Karlsruhe and CAS have designed and developed the new system with active guidance and insights from a global customer advisory council. "It is exciting to be part of the development process of the new STN platform," stated Dr. Mark Harper, patent information analyst at Sanofi and member of the STN Advisory Council. "The new system will greatly improve efficiency when searching STN, resulting from improved workflow support for patent experts."

An alpha release to the STN Advisory Council was completed in late 2011, and a release to global STN fixed fee customers will follow this year. The initial customer release will comprise the core databases of CAS and Thomson Reuters, a number of full-text patent files, and a suite of critical features and functions. Subsequent releases will be enhanced with additional databases and functionality.

The current STN system, including STN Express and STN on the Web, will continue to be available and fully supported throughout the development of the new platform.

<http://www.cas.org/newsevents/releases/newstn102411.html>

CAS Expands Global Patent Coverage - Intellectual Property Corporation of Malaysia Becomes 62nd Authority on CASM/CAplusSM

In mid-November, CAS enhanced its extensive patent authority coverage in CA/CAplus by adding the Intellectual Property Corporation of Malaysia. Malaysia (country code MY) is the 62nd authority covered by CAS.

Malaysian patent documents expand CAS' already substantial coverage of the world's major patent authorities. CAS actively continues to expand coverage, particularly from smaller patent authorities which would otherwise be largely inaccessible to many patent searchers.

You can quickly access multiple sources with broad coverage of 62 patent authorities covered by CAS. Coverage of Malaysian kind code A is retroactive to January 15, 2010. This includes granted patents and utility models. Malaysian A patents are eligible to be covered as basics or added to existing patent families. Approximately 1,000 patents are expected per year (approximately 200 basic patents) from Malaysia.

CA/CAplus Now Includes Examiner Citations for Japanese Patents

CAS is pleased to expand our coverage in the CA/CAplus databases to include Japanese patent examiner citations. Intellectually translated examiner citations include links to other CAplus records for quick access to the exact information you need such as inventor names and patent assignees.

Database coverage includes Japanese B1 and B2 patents processed as basics and published September 21, 2011 or later. Patent examiner citations are available for about 95 percent of the Japanese B1 and B2 patents processed so far.

The numerous countries and authorities available with examiner citations in CA/CAplus include:

CA DE EP FR GB WO US

CAS Learning Solutions

CAS Learning Solutions resource centre provides access to a full portfolio of SciFinder[®] and STN training options. Choose from a variety of tutorials and "how-to" guides to sign-

up for instructor-led training events and weekly practice sessions. Defined curricula will help both new and experienced searchers take their search skills to the next level. Click on the hyperlink and explore! <http://cas.org/support/learning/>

CAS Training in the UK 2012

In addition to the e-learning resource CAS Learning Solutions, we still offer training sessions for both STN and SciFinder in the UK.

In partnership with FIZ Karlsruhe, we will be coordinating a series of STN public training events this year based in London and Manchester.

We will cover include a number of search topics including chemical structure, markush structures (Marpat), sequences, patents as well as a series of general STN skills workshops to cover all abilities from beginners to advanced searchers.

We are also able to conduct 'in-house' training sessions or WebEx sessions on all aspects of CAS based STN or SciFinder searching. Also, if you wish to know more about any of the CAS products or would like further information or help with STN or SciFinder then please contact annejones@cas.org

CAS/InfoChem Collaboration in ChemInformatics

CAS/InfoChem Press release - Columbus, Ohio (December 12, 2011)

World leader in chemistry content partners with leading chemistry software provider to create new technologies to enhance the discovery of chemical patents and more

Chemical Abstracts Service (CAS), a division of the American Chemical Society and the world's authority for chemical information, today announced a long term collaboration with InfoChem, GmbH (InfoChem), a leader in chemical structure and reaction technology as well as datamining in chemical science documents, headquartered in Munich, Germany.

Under the new collaboration, research teams at CAS and InfoChem will work together to explore the technology frontiers in the field of cheminformatics. For example, the joint team is now researching and developing technology to identify chemical information in text and to semantically enrich chemical information documents. The partners will also continue to focus on chemical substance information and the ways to extract, derive, store, communicate and interpret that information.

"We are delighted to expand our relationship with InfoChem to undertake research in advanced technologies in the chemical information space," said Robert J. Massie, President of CAS. Since 1997 CAS and InfoChem have successfully worked together in the area of chemical information content. "Chemistry, in addition to being the central science, is a global enterprise. CAS has strong relationships with scientific and commercial organizations around the world, and we are delighted to enhance our collaboration with InfoChem in their area of expertise."

With the project "ChemProspector" InfoChem was one of the participants in the prestigious "THESEUS" research program, an initiative of the German Ministry of Economics and Technology. The subject of this project was: "Advanced mining and searching of chemical content in patent documents". "We are excited to collaborate with the leader in chemical information, CAS," said Peter Loew, PhD, Managing Director of InfoChem. "This project will enable InfoChem to enhance our successful research and development from the THESEUS initiative and create significant value for chemists and the chemical enterprise."

<http://www.infochem.de/news/releasedisplay.shtml?release1101.shtml>

InfoChem News

Contributed by Stephanie North, InfoChem GmbH



New Version of Chemisches Zentralblatt Structure Database released in January 2012: <http://beta.infochem.de/products/databases/czb.shtml>

InfoChem is pleased to announce the successful release of Chemisches Zentralblatt Structural Database Version 1.1.



CHEMISCHES
ZENTRALBLATT
Structural Database

Chemisches Zentralblatt is one of the most important abstracts journals covering the period 1830-1969. The content is relevant to all types of chemistry search, in particular to novelty and prior-art searching. InfoChem provides a structure searchable web-based service offering the benefits of language independent access to around 1 million unique chemical names and 500,000 unique chemical structures. New Features include:

New design for hit lists

This is the major improvement in version 1.1. Molecule results show a list of the hits with detailed information and direct links to the pages of Chemisches Zentralblatt, where the name of the molecule is highlighted. Document results are listed showing a strip with all molecules described in the document page. A click on the molecules gives detailed information.

Direct link to pdf documents

The direct link to the pdf documents has been improved as login is no longer necessary.

Easy surfing in original document

Users interested in scrolling the original work are now able to do this easily by clicking on the buttons "previous page" or "next page" of the pdf document.

Online Guide

An online help guide is now available in this version.

Improved search fields

The user is now able to recognize at a glance which kind of search options are offered in the two categories: "molecule-specific and document-specific".

Please contact Stephanie North (sn@infochem.de) if you would like more information or a demonstration.

Chemical Database Service News

Contributed by Don Parkin, CDS

New CDS Powder Diffraction Peak searching utility 'PeakQuest' now available

PeakQuest is a combination of the CMPR/LOGIC Software by Brian Toby (ANL) and powder diffraction data from CDS (> 133,000 patterns).

CMPR is a multipurpose program and can be used for displaying diffraction data, manual- & auto-indexing and peak fitting. The LOGIC program can be used to locate entries in the powder diffraction database that match specified conditions, i.e. contain certain elements and not others, have peaks in certain locations, but do not have peaks in certain other locations.

PeakQuest: <http://cds.dl.ac.uk/cds/peakquest/peakquest.html>

CPMR: <http://cds.dl.ac.uk/cds/peakquest/cmpr.html>

LOGIC: <http://cds.dl.ac.uk/cds/peakquest/logicdoc.html>

Forthcoming Meetings/Conferences

Advances and Progress in Drug Design

20th - 21st February 2012, London

<http://www.smi-online.co.uk/2012drugdesign.asp>

Academic Drug Discovery: Programmes and Collaborations

1st March 2012, SCI HQ, London

<http://www.soci.org/General-Pages/Display-Event?EventCode=FCHEM347>

ICSTI Winter Workshop: Delivering Data in Science

5th March 2012, Paris

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

International Patent Information Conference & Exposition, IPI-ConfEx 2012

11th - 14th March 2012, Barcelona, Spain

<http://www.ipi-confex.com/>

2nd RSC Symposium on Chemical Biology for Drug Discovery

20th - 21st March 2012, AstraZeneca, Alderley Park, Macclesfield

<http://www.maggichurchosevents.co.uk/bmcs>

UKSG 35th Annual Conference and Exhibition

26th - 28th March 2012, Glasgow

<http://www.uksg.org/event/conference12>

International Information Conference on Search, Data Mining & Visualization (II-SDV)

16th - 17th April 2012, Nice, France

<http://www.ii-sdv.com>

23rd Symposium on Medicinal Chemistry in Eastern England

26th April 2012, Eisai European Knowledge Centre, Hatfield, Hertfordshire

<http://www.maggichurchosevents.co.uk/bmcs>

A Practical Introduction to Chemoinformatics

12th - 15th June 2012, University of Sheffield

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

New Horizons in Toxicity Prediction - 3rd International Lhasa Symposium

5th - 6th September 2012, Cambridge

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

ALPSP International Conference

11th - 13th September 2012, The Belfry, Sutton Coldfield

<http://www.alpsp.org/Ebusiness/TrainingAndEvents/ALPSPInternationalConference.aspx>

4th RSC/SCI Symposium on GPCRs in Medicinal Chemistry

17th-19th September 2012, Lilly UK, Erl Wood, Windlesham, Surrey

<http://www.maggichurchosevents.co.uk/bmcs>

Other News Items

The 2011 UKeig Jason Farradane Award has been awarded to the United Kingdom Council of Research Repositories (UKCoRR), a professional membership-driven organisation managed for and by those staff working throughout the UK as Open Access repository administrators and managers.

<http://www.ukeig.org.uk/awards/jason-farradane>

Academia grows its role in drug discovery

Chemistry World, 08 December 2011

<http://www.rsc.org/chemistryworld/News/2011/December/08121104.asp>

British Library sparks Amazon row

BBC News Entertainment & Arts, 17 October 2011

<http://www.bbc.co.uk/news/entertainment-arts-15332307>

CAS and InfoChem Enter into Long Term Collaboration in ChemInformatics

World leader in chemistry content partners with leading chemistry software provider to create new technologies to enhance the discovery of chemical patents and more
CAS News Releases, December 12, 2011

<http://www.cas.org/newsevents/releases/infochem121211.html>

New STN® Revolutionizes Patent Searching for Professionals

Redesigned STN retains what customers value most while phasing in advanced search and analysis capabilities beginning in 2012

PRNewswire, Oct. 24, 2011

<http://www.prnewswire.com/news-releases/new-stn-revolutionizes-patent-searching-for-professionals-132466373.html>

PubChem Gets More Data

Research: IBM contributes information on more than 2.4 million compounds to NIH chemical database

Chemical & Engineering News, December 13, 2011

<http://cen.acs.org/articles/89/web/2011/12/PubChem-Data.html>

RSC and IDBS Automate Online Publishing of Chemistry Research

Alliance with University of Cambridge Creates 'Instant Messaging' of Chemistry Data via ChemSpider, Fostering Collaboration and Streamlining Research

IDBS - Data-Management News | Press Releases, December 6, 2011

<http://www.idbs.com/Data-Management-News/press-release/royal-society-of-chemistry-and-idbs-automate-online-publishing-of-chemistry-research/>

Berlin's Chemistry Information Centre FIZ CHEMIE GmbH Up For Sale

<http://www.fiz-chemie.de/en/home/news-schedule/newsdetail/article/pressemitteilung-fiz-chemie.html>

<http://newsbreaks.infotoday.com/Digest/Chemistry-Information-Centre-Berlin-FIZ-CHEMIE-Up-For-Sale-80424.asp>

Please send items for future CICAG Newsletters to the newsletter editor:

Lindsay Battle, email: lindsay.battle@chem.ox.ac.uk
