Chemical Structure Association Trust

NEWSLETTER

Spring 2005 Issue 9

Awards for Trustees

Congratulations to three of our Trustees who have been honoured for their work. Johnny Gasteiger is the recipient of the 2005 Mike Lynch CSA Trust Award (see page 2); Peter Nichols received the Ernie Hyde Award (pictured right) and Peter Willett received the 2005 ACS Award for Computers in Chemical and Pharmaceutical Research (page 5).

Following the sad death of former Trustee, Jacques-Émile Dubois, the CSA Trust is establishing a new Award in his name.

A delighted Peter Nichols receives the Ernie Hyde Award from Guenter Grethe (page 2)

Report from the Chair

This being the first Newsletter of 2005, I will briefly summarise some of the Trust's activities during the past year. After the flurry of work connected with merging the activities of CSA into the CSA Trust, 2004 went by calmly with all subcommittees carrying out their tasks. In 2004, Trustees met at the National ACS Meeting in Anaheim and at the AGM in November in London. Recently, nine Trustees met at the 2005 Spring ACS meeting in San Diego. Main topics during this meeting included a discussion about the format of the newly established award honoring Jacques-Émile Dubois (obituary on page 3) and the future involvement of the Trust in the organisation of the prestigious International Conference on Chemical Structures in Noordwijkerhout, The Netherlands (page 6).

During the year, the Trust was involved in co-organising several joint meetings with other organisations. Guenter Grethe organised a highly successful CINF/CSA Trust symposium entitled 'The Future of Scientific Publishing'. A summary of the symposium provided by Wendy Warr can be found in this Newsletter on page 4. The Trust also continued to support financially and collaborate with MGMS on the triennial Sheffield meeting on Chemoinformatics, and co-organised with RSC-CIG a one day course on Chemical Information for Non-Chemists. As in previous years, the CSA Trust co-sponsored the ExemplarChem meeting with a prize of £250, which was awarded to Philip Holmes from Plymouth University.

The 2005 International Conference on Chemical Structures will take place during the first week of June in Noordwijkerhout, the Netherlands. As in previous years, the Trust is a co-organiser of the conference and is providing several student bursaries. Based on the number of abstracts submitted (more than 150) and the high number of registrants, it promises to be another successful conference. The highlight will certainly be the award address by Johnny Gasteiger, the 2005 recipient of the CSA Trust Mike Lynch Award (see below).

The $1,000 CSA Trust Grant for 2005 was awarded to students at the Department of Information Studies at the University of Sheffield for attending the Noordwijkerhout conference. Peter Nichols is the recipient of the 2004 Ernie Hyde Award for his many contributions, in particular for his involvement in the educational activities of the Trust (see below).

After many years of service, Sue Jackson and Rob Brown resigned from the Board of Trustees. Dr Phil McHale (Elsevier MDL), a long-standing member of CSA, was unanimously elected to the Board for a three-year term.

The Trust thanks Clive Weeks for his outstanding work over many years as Secretary for the Trust; we'll miss him. David Walsh will take his place in 2005.

Guenter Grethe

2005 Mike Lynch Award for Johnny Gasteiger

Professor Dr Johann Gasteiger will be honoured with the 2005 CSA Trust Mike Lynch Award. The CSA Trust acknowledges Professor Gasteiger's outstanding accomplishments in the field of computational chemistry and structure elucidation. The award will be presented at the 7th International Conference on Chemical Structures in Noordwijkerhout, the Netherlands, in June 2005.

Professor Dr Gasteiger was born in 1941 in southern Germany, and studied chemistry at the universities of Munich and Zurich. In 1971, he achieved his PhD. After a postdoc stay at University of California, Berkeley in 1971/72, he returned to Munich, where he became Professor in 1988. At the University of Erlangen–Nürnberg he founded the 'Computer-Chemie-Centrum' in 1994.

Professor Gasteiger is a member of the ACS, CSA Trust, MGMS, the German Chemical Society and of several editorial boards.

The Mike Lynch Award will be given on a tri-annual basis, consisting of $5,000 and an appropriate memento.

New Trustee Phil McHale

Phil McHale is VP of Corporate Communications & Scientific Affairs at MDL Information Systems, Inc., based in their San Leandro, CA headquarters. He has a PhD in organic chemistry from the University of Oxford, England, and has over 30 years experience in the informatics industry. He has worked for the Chemical Society (London), Wellcome, Pergamon and Derwent Information. Since joining MDL in 1988, he has held a variety of positions in product planning and marketing, and assumed his current position in 2002.

Peter Nichols awarded 2004 Ernie Hyde Award

The 2004 Ernie Hyde Award for exceptional contributions to the CSA Trust was unanimously awarded to Peter Nichols at the AGM. Peter was instrumental in the CSA/CSATrust merger and subsequently headed the subcommittee on Meetings and Training. He worked tirelessly to fulfil an important objective of the Trust, the development of professionals in Chemical Information and related sciences. He has been one of the most active Trustees with particular involvement in co-organising one-day training courses with the RSC–CIG, and he has represented the Trust at the ExemplarChem competition. His persuasive touch and good-humoured approach to solving problems made him many friends and helped him getting others involved in Trust activities. His award is well deserved.

Guenter Grethe

Obituary: Jaques-Émile Dubois 1920–2005

We are very sad to report the death of former Trustee Jacques-Émile Dubois, who died at his home in Paris on 2 April 2005, at the age of 84.

Born on 13 April 1920 in Lille, Jacques-Émile Dubois was only 20 years old when the Second World War started. He was evacuated to Grenoble, where he played an important role in the French resistance.

From 1948 to 1950 he was a scientific assistant to the Cultural Counsellor at the French Embassy in London and was a research worker in Professor Ingold's laboratory at University College London. In 1949, he became Professor and created the Chemistry Institute of Sarrebrück University. On his return to France, at the end of 1957, he became the first Chair of Organic Physical Chemistry which was created at the Faculty of Sciences of Paris. He was then founder and director of the Organic Physical Chemistry Laboratory which in 1977 became part of the Institute of Topology and Dynamic Systems.

Jacques-Émile Dubois was one of the pioneers of chemical information systems, particularly in using mathematical methods for encoding organic substances. In 1965, he was the inventor of the DARC (Description, Acquisition, Restitution, and Conception) system, which allowed exploration of structure-property correlations. The system was also used for similarity searching in chemical structure databanks, for helping to develop new drugs in the pharmaceutical industry and for prediction of properties. He extended the system to deal with Markush Structures found in patents (INPI-Questel Markush-DARC).

Jacques-Émile Dubois also played an important role in the creation of the University Paris 7. In parallel to his scientific activities, he held many important positions including: Directeur Adjoint de l'Enseignement Supérieur (1963–65), Directeur des Recherches et Moyens d'Essai (DRME) at the National Defence Ministry (1965–1977), President of the French Physical Chemistry Society (1974–1976), co-Director of the Biology Section of the Curie Institute (1977–1980), Member of the Administrative Council and Directorate of the Centre National de la Recherche Scientifique (CNRS) (1965–1977) and of the Office de la Recherche Scientifique et Technique d'Outre-Mer (Orstom) (1963–1975), Member of the Conseil Scientifique du Commissariat à l'Énergie Atomique (CEA) (1971–1977), Vice-president of the Centre National de l'Information Chimique (1973–1990), Scientific Director of Compagnie Générale d'Électricité (CGE) (1979–1983), President of the Interdivisional Committee of IUPAC, (1969–1977), Vice-president of CODATA (1981–1988), President of CODATA-ICSU (1994–1998).

He received many scientific honours including: Grand prix de l'invention technique de la ville de Paris for the development of the DARC system (1975), Grand prix d'animation graphique at the Festival of Angers (1986), Doctor honoris causa, Regensburg University and the Herman Skolnik Award of the American Chemical Society (1992).

Jacques-Émile Dubois was Commander of the Légion d'Honneur and of the Ordre National du Mérite; received the Resistance medal; was Commandeur des Palmes Académiques; and received various international honours.

Obituary: Clayton F. Callis

We regret to announce the death of Clayton F. Callis, president of the American Chemical Society in 1989. Dr Callis died on March 9, 2005, at the age of 81.

He came out of retirement to serve as interim director of Chemical Abstracts Service in 1991, at a time when CAS was undergoing more than a little turmoil. Bob Massie, current president of CAS, paid tribute to Dr Callis in the Open Meeting of the Committee on Chemical Abstracts Service on March 14, at the National ACS Meeting in San Diego. He emphasised, in particular, the genuine personal interest Dr Callis had shown in the staff in Columbus. He went out of his way to meet every single person who served under him.

An obituary appeared in *Chemical and Engineering News* on March 21.

People and Places

Edlyn Simmons, section manager for patent information in the Intellectual Property and Business Information Services Department at Proctor & Gamble in the US, is to be awarded the International Patent Information (IPI) Award for 2005. Ms Simmons co-founded the Patent Information Users Group (PIUG) which has grown to be a major force in patent information. She chaired PIUG from 1990–1992 and has been a director-at-large since 2000. She has also played a major role as advisor or Board Member to various other associations and vendor organisations. She co-authored, with Stu Kaback, the chapter on patent information in the *Kirk-Othmer Encyclopedia of Chemical Technology*.

Arie Jongejan, previously CEO of Elsevier's Science & Technology Division, has been appointed the new CEO of Swets Information Services.

Wendy Cornell, (who runs the programme committee for ACS COMP division) has moved from Novartis to Merck & Co.

Jason Theodosiou is back at MDL.

The Future of Scientific Publishing

Two symposia at the ACS Meeting held in San Diego in March were of particular interest to our readers. One was the symposium honouring Peter Willett as the winner of the ACS Award for Computers in Chemical and Pharmaceutical Research (see page 5). The other, co-sponsored by the CSA Trust and the ACS Division of Chemical Information (CINF), is the subject of the current article.

The opening talk was a devilishly amusing presentation by Steve Heller (slides on hellers.com). There was less factual content in this presentation on Open Access (OA) than in Bill Town's talk in Peter Willett's symposium, but Steve held the audience in thrall. In his examples of OA journal policies he took a stab at ACS Publications' recent announcement of more 'open' policies and gave the first public revelation of the *Beilstein Journal of Organic Chemistry*.

The internet is threatening the way in which the scientific publishing industry has done business for many decades. The scholarly community needs organisations to accept, review, disseminate and archive manuscripts but the costs of the current system are too high and it is proving difficult to institute change. Peer review is about to collapse under the weight of too many poor manuscripts, all of which are too easily submitted via the internet. The solution, independent of any new or old economic model of publishing, is to charge for submission of manuscripts, and charge a second fee for acceptance under the OA model.

While librarians and publishers have to some extent adapted to the new technologies over the past decade, for researchers it has been 'business as usual': they publish wherever they want and fail to use new electronic facilities to enhance their manuscripts. Researchers need to stop publishing partial results on a regular basis. Journals need to charge authors for frivolous submissions. The real villains are the researchers. Of the 34,000 signatories to the Public Library of Science letter, about 34 have actually published in an OA journal. Steve predicts that university provosts will soon mandate researchers to put up their publications on either institutional or public websites.

If OA prevails, the only losers will be the publishers. Why do publishers think evolution does not apply to them? Nowhere in the Constitution is there a guaranteed right for a company to remain in business. Open Access will provide global, universal free access to information; resolve the serials crisis; accelerate scientific progress and research; enhance research productivity; and improve quality.

René Deplanque of FIZ Chemie Berlin described how the everyday work of the scientist has changed. The use of databases today is commonplace but with the advance of the internet, evolving Grid technology and OA initiatives, new ways of handling and distribution of data will change the functions and applications of

Room with a view: delegates at the March ACS meeting enjoyed the splendours of Spring in San Diego

information systems. Yesterday, users were satisfied if they found what they were looking for; nowadays the direct application of information within the scientific process is what matters. Networking of computers to calculate huge amounts of experimental data, networking of experiments, and easy access to full text publications are changing the landscape. In a related talk, Robert Schlögl of the Max Planck Gesellschaft (MPG) addressed the need to link and exchange information content over national, institutional and disciplinary borders. MPG's vision is to integrate the internet into scientific work flows, networking strategic partners and institutions in building institutional repositories and a digital archive.

Also in evidence were the dynamic duo of the chemical semantic web, Peter Murray-Rust and Henry Rzepa. In an interesting and impassioned presentation, Peter told us how the World Wide Molecular Matrix stands up for the rights of molecules in the face of publishers whose interest seems to be to destroy the supplementary data submitted with a learned paper. He exemplified his case with demonstrations of OSCAR for understanding the data in free text, and InChI, the IUPAC international chemical identifier. He also attacked ACS for applying its copyright terms to supplementary data that are not actually the property of ACS. He recommends the use of a Creative Commons licence: an example is his presentation now mounted on the Cambridge website.

Henry bemoaned the fact that, although he can carry hours of music on his iPod and transfer it to a PC, he cannot do the equivalent with his scientific publications. In his presentation (available on his website) he talked about crystallising information and 'intertwingling' (a superior form of 'intermingling'). The challenge is to create a culture that values chemical metadata and open data. It is the 'datument' rather than the document that matters. Henry produces datuments using the Adobe eXtensible Metadata platform (XMP), an RDF vocabulary that can be embedded in SVG, CML, PDF or JPEG documents. Molecular structures are represented as unique InChI identifiers and embedded in electronic articles as part of the XMP.

OA is inevitable: it is not a case of 'if' but of 'when', asserted Ann Wolpert of MIT in a masterly exposition of the economic and social factors. Scientists work in multi-disciplinary teams, based in more than one institution and they collaborate over time and space. Conflicts can occur when they have different access rights to information. It is not acceptable for publishers to retain control of a discipline through the literature. Tuition fees cannot rise at the rate of inflation, there is less research money, and the payout from endowments is falling. MIT has had to add three staff positions to negotiate licences with vendors and address restrictive clauses such as 'walk-in' exclusions. This money could be spent on better things. If organised properly, OA respects the roles of societies, the critical value of peer review, and the changing nature of research and education, but recognises the inability of higher education to support the appetite of each discipline.

Since the final speaker, Derk Haank of Springer, as on previous occasions, failed to grace us with his presence, Pieter Bolman of the STM Association was the sole defender of the publishers' viewpoint. There are two models for OA: the author-pays, value model, and the self–archiving model that presupposes that the continuation of the current system. STM does not recognise the superiority of any particular model. Both profit and non-profit publishers are experimenting with OA. Any business model must be financially sustainable and generate income by adding value for all the customers (authors, readers and libraries). It should generate enough profit to encourage innovation, and attract investment and the best people. In principle, it seems logical that customers should pay in proportion to the value delivered but, in practice, the situation is not so straightforward. Pieter gave lengthy, reasoned arguments around sustainability and value. All the models used in current OA experiments have drawbacks, possibly fatal ones, but STM wishes them well: experiments are to be encouraged. Remember that governments can get it wrong. The market must decide which model is best within social responsibility constraints.

Guenter Grethe is to be commended on organising a very interesting symposium. I had wondered if I would regret missing some of the Lipinski-Oprea symposium on safe exchange of chemical structures in order to hear oft-repeated arguments about OA. I was proved wrong: this symposium was a credit to the Trust and, from my selfish point of view, will be good for sales of the 25th report in my ACS meeting series!

Dr Wendy Warr,
Wendy Warr & Associates
http://www.warr.com

ACS Award for Peter Willett

The ACS Award for Computers in Chemical and Pharmaceutical Research recognises outstanding individual achievement for the use of computers in education, product development, or research in the chemical and biological sciences. In 2005, the award was presented to Peter Willett, Professor of Information Studies at the University of Sheffield, UK (pictured right).

The award was established in 1984 by Digital Equipment Corporation, and sponsored by them from 1984 to 1995. IBM North America, Scientific and Technical Systems and Solutions sponsored the award from 1996 to 1998. Since 2001, the award has been sponsored by Accelrys.

This award is given annually, and consists of a cash prize and a certificate. The monetary award is $5,000, plus a $1,000 travel allowance to attend the meeting at which the award is presented.

7th International Conference on Chemical Structures

June 5 – June 9, 2005

NH Leeuwenhorst Conference Hotel, Noordwijkerhout, The Netherlands

Technical Program

SUNDAY JUNE 5

Welcome and Introduction, Bob Snyder, ICCS Program Chair

CSA Trust Mike Lynch Award Address:

My Love Affair with Molecules – and Reactions

Johnny Gasteiger, Universität Erlangen–Nürnberg

MONDAY JUNE 6

Cheminformatics

- *Similarity-Based Virtual Screening Using Data Fusion*
  Peter Willett, University of Sheffield
- *Quest for the Rings – A Cheminformatics Analysis to Identify Novel Bioactive Heterocyclic Systems*
  Peter Ertl, Novartis Institutes for Biomedical Research
- *Classification of Reactions by Type or Name*
  Guenter Grethe
- *Molecular Similarity Searching Using the Conductor-Like Screening Model (COSMOsim)*
  Andreas Bender, Unilever Centre for Molecular Science Informatics
- *Aligning Ligand Ensembles in Multiplet Space*
  Robert D. Clark, Tripos, Inc
- *Structure-Based 3D Pharmacophores: An Alternative to Docking?*
  Gerhard Wolber, Inte:Ligand Softwareentwicklungs- und Consultig GmbH
- *The Molecule Evoluator: An Interactive Evolutionary Algorithm for Designing Drug-Like Molecules*
  AD IJzerman, Leiden Center for Drug Research
- *Open Access/Open Source and the IUPAC International Chemical Identifier*
  Stephen Heller, NIST
- *ErG: A Two-Dimensional Pharmacophore Approach to Scaffold Hopping*
  Nikolaus Stiefl, Lilly Forschung GmbH
- *Improving Conformer Generation: A Sisyphean Task?*
  Matthew Stahl, OpenEye Scientific Software

TUESDAY JUNE 7

Structure-Based Design and Virtual Screening

- *FlexNovo: Structure-Based Searching in Chemistry Spaces*
  Jörg Degen, Zentrum für Bioinformatik
- *Recent Advances in De Novo Ligand Design and Optimisation*
  Krisztina Boda, University of Leeds
- *Combining the Power of Combinatorial Chemistry With the Efficiency of Pharmacophore-Based Docking*
  Holger Claussen, BioSolveIT GmbH
- *Using Molecular Fields to Derive Bound Conformations*
  Andy Vinter, Cresset BioMolecular Design Ltd
- *Generation and Selection of Potential ER Ligands Using the De Novo Structure-Based Design Tool, SkelGen*
  Henriette Willems, De Novo Pharmaceuticals
- *Knowledge-Based Design of Target-focused Libraries*
  Donovan Chin, Biogen Idec
- *Towards an Expert System for Binding Site Definitions*
  Maria Kontoyianni, P&G Pharmaceuticals, Inc
- *Successful Virtual Screening for Tat-TAR RNA Interaction Inhibitors With a Fuzzy Pharmacophore Model*
  Steffen Renner, University of Frankfurt
- *An Effective Virtual Screening Protocol for Beta-Secretase (BACE1)*
  Tímea Polgár, Richter Gedeon Ltd
- *PPAR-alpha Agonists Designed Using A Knowledge-Based De Novo Technology*
  Suresh Singh, Vitae Pharmaceuticals

WEDNESDAY JUNE 8

Structure-Activity and Structure-Property Prediction

- *Modelling Cytochrome P450 Inhibition Using Large Datasets of in vitro Assays for CYP 2D6 and CYP 3A4*
  Boryeu Mao, Cerep Inc
- *SPORCalc – Fingerprint Based Probabilistic Scoring of Metabolic Sites*
  Catrin Hasselgren Arnby, AstraZeneca
- *Relationships Between Molecular Complexity, Biologic Activity and Structural Diversity*
  Ansgar Schuffenhauer, Novartis Pharma AG
- *In silico Prediction of Buffer Solubility Based on Quantum-Mechanical, HQSAR- and Topology-Based Descriptors*
  Andreas Göller, Bayer Healthcare
- *MC4PC: A Computational Tool for the Rational Evaluation of the Hazard Potential of New Pharmaceuticals and other Organic Chemicals*
  Gilles Klopman, Case Western Reserve University
- *Characterising Bitterness: Identification of the Key Structural Features*
  Sarah Rodgers, Unilever Research
- *Comparing Vector Versus Structural Coding for Predicting ADMETox Data Sets*
  Jörg Kurt Wegner, Universität Tübingen

THURSDAY JUNE 9

Analysis of Large Data Sets

- *Hit Selection From HTS Assays: Enhancing Hit Quality And Diversity*
  Iain McFadyen, Wyeth Research
- *Use of Multiple-Category Bayesian Modeling to Predict Side Effects*
  Robert Brown, SciTegic, Inc
- *Scaffold-Hopping Using Clique Detection Applied to Reduced Graphs*
  Eleanor Gardiner, University of Sheffield
- *A First Look into ABCD*
  Dmitrii Rassokhin, Johnson & Johnson Pharmaceutical R&D

Bridging the Cheminformatics–Bioinformatics Gap

- *Integration of Chemical and Biological Data: The NCBI PubChem Project*
  Wolf Ihlenfeldt, National Institutes of Health
- *StARLITe – a Chemogenonics Knowledge Base*
  Edith Chan, Inpharmatica
- *A Searchable Database for Comparing Protein-Ligand Binding Sites for the Discovery of Structure-Function Relationships*
  Richard Jackson, University of Leeds

- Conference Closing Remarks
  Markus Wagener, ICCS Vice Chair

Open Access Publishing: an Overview

Open Access (OA) is one of the most heated topics in the field of scholarly communications. It has been the subject of numerous studies, government reviews and conference sessions in recent years. This article is based on a talk I gave in a conference session on Open Access which I co-organised at the ACS meeting in Philadelphia in 2004. The CSA Trust co-sponsored (with CINF) a session on OA at the ACS meeting in San Diego (see Page 4).

Open Access is a method for disseminating the result of scientific research: a method that makes no charge to readers or their institutions for online access and permits printing, copying, onward distribution and creation of derivative works, subject only to community-defined standards of attribution and integrity. A number of developments have driven the Open Access movement. Academics and librarians are complaining about the current 'toll-access' system. Governments around the world are considering whether publicly funded research should lead to free-of-charge access. The Wellcome Foundation has led an initiative in OA. Recently, the UK House of Commons Select Committee issued a report on access to scientific publications and NIH has issued a policy statement on the publication of research funded by NIH.

There are many potential advantages to Open Access. Some believe that it signals a return to a core value of scholarship: free exchange of information. The number of accesses to OA e-journals is claimed to be higher than for toll-access e-journals and there is some evidence that OA articles get more citations than those in toll-access journals. There is a moral and ethical argument in that everyone around the world can get access. The impact argument is that more eyeballs mean greater spread of ideas. Open Access also cuts down costs for libraries.

There are, however, some disadvantages. Scholars as authors have concerns about peer review, cost, prestige, archiving, and information overload. There are copyright issues. Not everyone has access to the web, especially in developing countries. Also, Open Access merely shifts the costs from libraries to the funding agencies or employers.

Some fundamental issues need addressing: who owns the intellectual property generated by universities and the publicly funded research they undertake? Should access to that knowledge be free or restricted? How should it be provided and who should pay for it? Where do you draw the line between what is owned by the public body that does the research and what is owned by the individual scientist? Is there a difference between electronic content and print?

The first route to Open Access (the so-called green route), Open Access self-archiving, involves the posting of articles to either authors' personal or institutional websites, or a subject-based archive on the web. The posted article may be archived before peer review, after peer review, or as the published PDF file. Qualifying websites are interoperable and use special protocols to enable seamless recognition by search engines. Many commercial publishers have recently clarified their support for this approach as long as the final PDF is used and their electronic journal websites are cited.

The second route to Open Access (the so-called gold route), Open Access publishing, involves creation of new journals that require authors to pay a manuscript processing fee. The fees charged by Open Access journals (currently $500 to $1,500) are recovered by authors from institutions or grant funds. As regards shifting the costs, it is a zero sum game: someone has to pay for the system one way or another. In the author pays model for OA journals, costs per article to break even have been estimated to range from $500 to $2000; to make a profit, the publisher needs even more. The Springer Open Choice option, for example, costs $3000. There is no reason why OA cannot be profit-making.

There is also the question of submission fees *versus* publication fees. If the fee is for submission and the article gets rejected, the authors have wasted their money. If the fee is for publication, it is paid only if the article is accepted, but then successful authors are subsidising poor authors. There is no easy answer but most journals go for a publication (acceptance) fee; a few go for a mixture of the two.

Who actually pays the fees for publishing in OA journals? If a funding agency pays, the cost is incorporated into the bid but there will then be fewer funding awards overall. If the employer, e.g., a university, pays, what else gets cut to pay for it? If the library pays, it is no better off than it was before. It is rare for the authors themselves to pay. Fees are often waived if the author pleads poverty but then richer authors are subsidising them. Some subject areas, such as humanities, are not funded much by funding agencies so they may not get OA journals, though there is no reason why institutional repositories should not be set up in the humanities.

Early entrants in the Open Access arena were PubMed Central, BioMed Central, the Open Society Institute, the Budapest Open Access Initiative, Public Library of Science, and there have been some responses from commercial publishers (notably Springer and Blackwells).

In Open Access publishing, all papers are peer reviewed in the 'traditional' way and are permanently archived in secure repositories such as those of PubMed Central, the Institut de l'Information Scientifique et Technique (INIST) in France, and the Koninklijke Bibliotheek in the Netherlands. Papers are searchable and retrievable: they are included in PubMed, Scirus, Google, CrossRef, and the Health InterNetwork Access to Research Initiative (HINARI). Some OA journals are indexed in MEDLINE, BIOSIS and CAS, and increasing numbers are tracked by ISI for citations.

In an article of this length, it has not been possible to cover much of the detail or many of the recent developments relating to Open Access. Instead, I have tried to give a brief overview of the field to a reader who is new to the topic.

Bill Town,
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Publicly available chemical services in China

Major chemistry related electronic services such as ScienceDirect and ISI Web of Knowledge have been made accessible in major academic institutions in China in the past three to five years. A few research institutions now have access to chemical databases such as CA on CD and Beilstein/Gmelin Crossfire. SciFinder Scholar became available recently in Nanjing University. There are hardly any public services specifically dedicated to chemistry, but the following scientific services resulting from several government supported projects has made the searching of Chinese chemical journal articles much easier.

The National Science and Technology Library (NSTL) is a government-supported virtual alliance of seven scientific libraries in China, started since June 2000. NSTL integrates scientific and technical information resources in general as well as by discipline, such as agriculture, medicine and the chemical industry, and provides united services based on the member libraries. China's Information Center for Chemical Industry, formerly part the Ministry of Chemical Industry, is one of the member libraries focusing services on the chemical industry. The website of NSTL is the most attractive scientific service publicly available in China. NSTL now provides the following free services:

(1) Free abstracts searching covering Chinese journal articles, conference proceedings, degree theses and standards. The service has good coverage of Chinese journal articles after 1989, but is incomplete in conference proceedings, degree theses and standards.

(2) Online consulting on information searching: NSTL launched the service in August 2004. An experienced librarian from member libraries of NSTL is online and answers questions interactively when posted. The whole process is logged and an e-mail recording the consulting details is sent to the user for future reference. Offline consulting is also freely available by online posting; the answer e-mail will be sent to the user within three days.

(3) NSTL serves as a nationwide access gateway to the full text of journals. The current service includes the full text of ten journals in material science (1999–2002) from Maney Publishing and four journals from the Royal Society, UK.

Both ScienceChina (http://sdb.csdl.ac.cn/) and China's National United Catalog of Journals (http://union.csdl.ac.cn/Reader/query.jsp) are two free services made available as projects of the Chinese Science Digital Library (CSDL). Science China is a citation database of China's scientific journals since 1980, launched in May 2004. This citation analysis tool has fully linked features in cited references, citations, authors, keywords, categories and fund information. The United Catalog integrates the online catalogs of 400 academic libraries in China. This service helps find full text sources for over 7000 journal titles. The service is also the searching gateway of a new Inter-Library Loan service among the research libraries of the Chinese Academy of Sciences.

Xiaoxia Li
Chinese Academy of Sciences

Meetings in 2005 in China

The 40th IUPAC Congress will be held in August 14 – 19, Beijing, China. A session dedicated to chemical information, entitled 'Information Technology in Chemistry and Computational Chemistry' will be chaired by Professor Kaixian Chen, former Director of Shanghai Institute of Materia Medica, Chinese Academy of Sciences. The co-Chairman is Professor J. Andrew McCammon, UCSD, US. The session will focus on computer aided molecular design and computations in theoretical chemistry. The proposed program is at http://www.ccs.ac.cn/IUPAC2005/iupac2005-2c.htm.

The 3rd International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2005) will be held from 29 October to 1 November, 2005 in Shanghai under the joint auspices of the Shanghai Institute of Organic Chemistry (SIOC), the Chinese Academy of Sciences (CAS) and the University Paris7-Denis Diderot (ITODYS-CNRS UMR 7086). Information about the symposium is available at http://www.sioc.ac.cn/CMTPI2005/.

Pacifichem 2005

Pacifichem is an international conference of the Pacific Basin Societies which is held every five years in Honolulu, Hawaii. The 2005 conference will take place from December 15 to 20. A symposium on 'Drug Discovery in a Systems Biology World: Integration of Biology and Chemistry Information' is part of the Biological Chemistry section of the conference.

Advances in the 'omics' sciences (genomics, proteomics, metabolomics, toxicogenomics) have recently enabled the development of better-focused and more rational approaches towards target identification, validation and prioritisation. Such advances have also produced very large and complex datasets, which are growing at an exponential rate, reflecting the complexity of life and biological pathways. The integration of biology and chemistry has led to a new set of informatics challenges and knowledge management. The purpose of the symposium is to offer an occasion to present and discuss the latest developments in the area of systems biology and new ideas for linking biological and chemical information, combinatorial chemistry, interpreting biological networks, and clustering algorithms for data analysis and visualisation.

The symposium consists of three half-day sessions plus a poster session. The major topics included are:

- Genomics
- Proteomics
- Small Molecule Lead Identification and Optimisation
- Metabolomics
- Toxicogenomics.

An overriding theme of all sections is the integration of biological and chemical information as the drug discovery process moves from target identification to small molecule synthesis to safety and efficacy assessment to clinical studies.

Details can be found at:
http://www.pacifichem.org

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Kilmorie Consulting

Kilmorie Consulting (www.kilmorie.com) helps organizations to make the best use of their information resources, develop new information services or products, and bring them to market. A group of independent consultants, each with extensive experience in diverse areas of electronic publishing, we cover all aspects of information dissemination, from creating a strategy to implementation, including market research, product development, training, and website creation. For each project, the exact needs will be assessed and an appropriate team assembled from a wide group of experienced independent consultants.

Kilmorie Consulting was founded by Bill 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 Chemical Abstracts Service) 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.

Recent projects undertaken by Kilmorie Consulting include: conference reports on the ICSTI International Seminar on Open Access (Paris, 2003) and the International Patent Information Conference and Exposition (Lisbon, 2004); surveys of information habits of bench chemists, of strategic directions in the scientific information industry and of the take-up of XML production technology by publishers; advising a scientific society during a potential change of journals publisher; a number of confidential business development projects for venture capitalists, publishers and information providers; and a report on STM book publishing. Bill Town was also co-organiser of a recent seminar on Open Access publishing at the Fall ACS meeting in Philadelphia.

Kilmorie Consulting is now an operating division of Kilmorie Clarke Ltd (www.kilmorieclarke.com) whose activities also include corporate video production and conference production.

CSA Trust Grant Report: Development of the MCM on the world wide web

Atmospheric research at the University of Leeds, UK, encompasses a wide variety of topics relevant to atmospheric processes. A collaborative project has been funded by the Department for Environment, Food and Rural Affairs (DEFRA), to develop and apply predictive models to the formation of tropospheric ozone on a range of different geographical scales. An essential part of the project is the Master Chemical Mechanism (MCM), as this mechanism underpins much of the current ozone modelling undertaken for DEFRA.

The Master Chemical Mechanism is a near-explicit chemical mechanism describing the degradation of 135 volatile organic compounds in the troposphere. First developed to investigate ozone production in the troposphere, the mechanism also aims to provide a research tool for investigating areas where detailed chemistry is required, eg the generation of intermediates.

The CSA Trust Grant provided tools for the development and updating of the MCM on the web, from my new research base at the University of Western Australia, Perth (UWA). The $1000 was used to fund the purchase of a Pentium PC box, and Linux operating system to initially set up a mirror MCM website at UWA. The Linux box is also vital for some of the in-house software tools needed for generating updates of the binary web-based MCM reaction database and reconstruction of the website when updates are made. ChemOffice Ltd 2000 software was also purchased to continue with the chemical representation of the reaction codes.

The primary MCMv3 website was updated in November 2003, to MCMv3.1. The new Perth-based web server was installed and tested, then used to host a backup site of the entire MCMv3 website, while further developments were undertaken, and launched in March 2004 (see http://www.chem.leeds.ac.uk/Atmospheric/MCM/mcmproj.html).

The establishment of the hardware and software at UWA has enabled continued work on MCM developments. This has included various aspects of MCM scheme writing and updating, new project and modelling initiatives, and continued links with the Leeds UK group, and contributing to the first MCM Developer and User Group workshop in December 2004.

The CSA Trust Grant 2004 has provided valuable assistance in establishing an ongoing research base at UWA.

Sam Saunders
School of Earth and Geographical Science
Faculty of Natural & Agricultural Sciences
The University of Western Australia

EVENTS 2005

May		
19–20	ChemAxons Inaugural User Group Meeting, Budapest, Hungary	http://www.chemaxon.hu/forum/ftopic272.html
21–26	2005 PIUG Annual Conference – The Future of Patent Information – Tools and Techniques for Adding Value Hyatt Regency Crystal City, Arlington, VA, US	Tel: (703) 418-1234 http://www.crystalcity.hyatt.com
June		
5–9	7th International Conference on Chemical Structures, the Congress Center, Noordwijkerhout, the Netherlands	http://www.int-conf-chem-structures.org/
July		
3–7	CONNECT2005, 12th Royal Australian Chemical Institute National Convention, Sydney, Australia	http://www.pco.com.au/connect2005/
August		
14–19	40th IUPAC Congress, Beijing, China.	http://www.ccs.ac.cn/IUPAC2005/iupac2005-2c.htm
24–26	11th Asian Chemical Congress, Seoul	http://www.11acc.org/
28 August – September 1	230th American Society Meeting, Washington DC	http://www.chemistry.org/portal/a/c/s/1/acsdisplay.html?DOC=meetings%5cwashington2005%5chome.html
September		
11–14	Biomolecular Simulations: from Prediction to Practice MGMS International Meeting 2005 Trinity College Dublin, Ireland	E-mail: mgms2005@tchpc.tcd.ie http://www.tchpc.tcd.ie/mgms/
October		
16–19	The 2005 International Chemical Information Conference and Exhibition,Nîmes, France	E-mail: contact@infonortics.com http://www.infonortics.com/chemical/index.htm
21–26	International Computational Methods in Sciences and Engineering 2005 (ICCMSE 2005), Hotel Poseidon Resort, Loutraki, Korinthos, Greece	E-mail: secretary@ieccs.net
29 October – November 1	3rd International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2005), Shanghai, China	http://www.sioc.ac.cn/CMTPI2005/
November		
14–16	AccelrysWorld 2005, Tower Thistle Hotel, London, UK	http://www.accelrys.com/accelrysworld/
29 November – December 1	Online Information, Olympia, London, UK	http://www.online-information.co.uk
December		
15– 20	Pacifichem 2005 (International Chemical Congress of Pacific Basin Societies) Honolulu, Hawaii, US	E-mail: Pacifichem@comcast.net http://www.pacifichem.org

Product News

CAS Mobile

Chemical Abstracts Service (CAS) demonstrated the delivery of chemical information, including structures, via live interaction using BlackBerry and other handheld devices at the recent CAS European conference in Vienna. More than 20 handheld devices were used simultaneously by conference participants to retrieve hundreds of literature references as well as molecular structure and related data for specific substances in real time.

The demonstration illustrated the ability to retrieve and analyse information from CAS' principal databases, CAplus and CAS Registry. The Registry database contains records for more than 25 million organic and inorganic substances, including small molecules, and more than 56 million sequences.

CAS will be making this new mobile route to scientific databases, called CAS Mobile, available through its STN and SciFinder services in the near future.

Sequence Analysis Collection

SciTegic has announced the release of the Sequence Analysis Collection for the data pipelining software, Pipeline Pilot. With the Sequence Analysis Collection, it is now possible to analyse, annotate, and compare biological sequences in an environment where modular tools can be linked together to create practical bioinformatics routines. SciTegic's pipelining platform has been well validated in other informatics disciplines, and has been deployed in cheminformatics for five years. While over 50 bioinformatics tools have been incorporated into the collection, Scitegic believe that the strength of the system is how easily customers can integrate additional in-house algorithms and third party software tools.

Combined Chemical Dictionary

The Chapman & Hall/CRC Combined Chemical Dictionary, available via CHEMnetBASE, has just added 5,900 new compounds. The CCD now contains 188,000 natural products, 46,000 drugs, 276,000 organic compounds and 103,000 inorganic/organometallic compounds. Literature coverage is current to mid-2004. Searching the database (including browsing and viewing hit lists) is completely free of charge. If wanting to view or print the full product entries, however, a current subscription is needed, or access to the appropriate older print volumes. The website is at http://www.chemnetbase.com/scripts/ccdweb.exe

LITHIUM 2.1

Tripos, Inc. has released LITHIUM 2.1, the latest version of its 3-D molecular data desktop tool. Specifically designed to foster communications between front-line life sciences researchers and expert computational chemists, LITHIUM allows researchers to view, evaluate and share insights on molecular data among their colleagues. Enhancements to the software include new scientific, graphic and operational features, hyperlink captions, and an integrated web browser that lets users apply chemical knowledge to corresponding 3-D molecular structures. The release contains two components:

- LITHIUM Base, the enterprise platform that allows users to automate repetitive tasks through automatically generated procedures that can be played back later on the same or other relevant models and shared with others
- LITHIUM Developer, the platform for LITHIUM-based applications that supports custom interfaces and applications based on organisations' specific needs

More information can be found at http://www.tripos.com/

SPRESI^{web} 2.1

InfoChem has a new version of its web-based structure and reaction research platform SPRESI^{web}. The system offers internet access to 4.5 million compounds and 3.6 million reactions from 565,000 references, including 156,000 patents. Over 28 million facts such as chemical and physical properties, reaction conditions and keywords abstracted from the primary literature are searchable. SPRESI^{web} 2.1 features an innovative prototype of name reactions search in addition to common search types such as 'substructure search', 'isomer search', 'parent search' and 'flex match'.

The new SPRESIweb version offers:

- export of hit sets in SD, RD and BibTeX format for import in own database
- name reactions search
- direct links from reference to publishers site via DOI
- sorting of hit lists by certain criteria
- possibility to include hit lists in new query
- compact hit list view for reactions and references
- customisable link to company-/campus internal LitLink server

More information can be found at http://www.spresi.com.

SPROUT v6.0

The ability to design drugs that bind strongly within a receptor site has long been a goal of medicinal/computational chemists. SPROUT v6.0 brings chemists closer to that goal. SPROUT v6.0 is a mature de novo ligand design package featuring:

- Exhaustive and systematic coverage of the search space
- Excellent visualisation capabilities
- Generic skeletons that represent all interesting chemical space
- Improved loan pair directionality
- Complexity analysis for ranking and pruning structures
- Specific library for peptide generation

SPROUT v6.0 is highly tuned for Linux and Silicon Graphics IRIX operating systems. To receive a free evaluation version of SPROUT v6.0, please email SimBioSys at info@simbiosys.ca or visit the website at http://www.simbiosys.ca.

Nominations Required for 2006 Herman Skolnik Award

The ACS Division of Chemical Information established this Award to recognise outstanding contributions to and achievements in the theory and practice of chemical information science. The Award is named in honour of the first recipient, Herman Skolnik.

Through this Award, the ACS Division of Chemical Information is committed to encouraging the continuing preparation, dissemination and advancement of chemical information science and related disciplines through individual and team efforts. Examples of such advancement include, but are not limited to, the following:

- Design of new and unique computerised information systems
- Preparation and dissemination of chemical information
- Editorial innovations
- Design of new indexing, classification, and notation systems
- Chemical nomenclature
- Structure-activity relationships
- Numerical data correlation and evaluation
- Advancement of knowledge in the field

The Award consists of a $3000 honorarium and a plaque. The recipient is expected to give an address at the time of the Award presentation. In recent years, the Award Symposium has been organised by the recipient.

Nominations for the Award should describe the nominee's contributions to the field of chemical information and should include supportive materials such as a biographical sketch and a list of publications and presentations. Three seconding letters are also required. Nominations and supporting material should be sent by e-mail to Bill Town, CINF Awards Chair (bill.town@kilmorie.com). Paper submissions are no longer acceptable. The deadline for nominations is June 1, 2005.

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