



*Chemical Structure Association*

# **NEWSLETTER**

Issue 58

Autumn  
2001

## **Personalia**

Rudy Potenzzone, formerly senior vice president for marketing and development at MDL, is now president and CEO of LION Bioscience's US operations.

Daniel Keesman is now global vice president, sales and marketing for LION bioscience. He was formerly vice president for MDL Europe and managing director of MDL Frankfurt.

Mark Canales, formerly vice president of product development at MDL, has been appointed senior vice president, cheminformatics development for LION's US operations.

Herschel Weintraub has left Genentech and is consulting as SciCom Scientific Computing.

Dr Stuart Kaback is the recipient of the 'International Patent Information (IPI) Award' for 2001.

Jin Li, formerly of Protherics Molecular Design, is now director, chemical computing, at AstraZeneca in Mölndal.

Anthony Baxter, formerly chief scientific officer of Oxford Asymmetry International, is now CEO of Argenta Discovery.

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*Please note: John Holliday (+44-(0)114-222-2685) maintains a current membership list with full addresses and telephone numbers of all CSA members. If you change your address or telephone number, please let him know. If you need the telephone number of a CSA member then John can help you.*

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## **THE FUTURE!**

We will be asking you to vote, at the AGM in December, on the proposal to incorporate the existing CSA activities within the framework of the CSA Trust. A substantial part of this Newsletter is devoted to giving you some information about the Trust and an outline of the draft proposals for combining the two organisations. If you have any comments or questions about the proposals, please e-mail me on ash@euronet.nl. Don't forget to make a note of the date of the AGM and Dinner (see below).

**Janet Ash**  
*CSA Chairman*

## **AGM and Annual Dinner**

The CSA and the CSA Trust AGMs will be held at the Linnean Society, Burlington House, Piccadilly, in the afternoon of Monday 3rd December, followed by the Annual Dinner at 7.00 pm for 7.30 pm at the Cadogan Hotel, Sloane Street, London. Full details and an Agenda will be circulated nearer the time.

## **Inside...**

### **Personalia**

### **The CSA and the CSA Trust**

### **CSA Trust Awards and Grants**

### **Training**

### **Course Report**

### **Nîmes program**

### **Web-linking**

### **CSA/MGMS Meeting**

### **Events 2001-2002**

### **Product News**

### **MSc in Chemo- informatics**

### **CSA/CINF Symposium**

### **Contact Details**

### **Next Copy Date**

## ***The CSA and the CSA Trust***

At the CSA AGM in December 2000, the Executive Committee was given the task of investigating the possibility of incorporating the activities of the CSA within the framework of the CSA Trust.

The Trust was set up in 1989 as a UK Registered Charity, which provided the best way to use the surplus funds generated from the CSA conferences for grants and awards to enable students and other worthy candidates to further their research. The Trust has its own constitution (Deed of Covenant), which unambiguously defines it as a Charity. Further details of the Trust, including a list of the current Trustees, are given on page 3 of this Newsletter. The CSA activities are mainly 'educational' and would fall within the objectives and aims of the CSA Trust.

When the Trust was set up it was envisaged that, at some time in the future, all the activities of the CSA would be carried out by the Trust. Following legal advice, we have drafted some proposals as to how this could now be achieved. The draft proposals are given below, and if you have any comments on these, please e-mail Janet Ash at ash@euronet.nl.

Your comments and any concerns that you may have can then be addressed before the final proposals are put to the membership at the CSA AGM, to be held in London on December 4th 2001.

If you would like to see a copy of the Trust Deed, please contact the Secretary of the Trust, Clive Weeks, at drcliveweeks@netscapeonline.co.uk

## ***Draft proposals for the incorporation of the activities of the CSA within the framework of the CSA Trust***

### ***Membership***

Current members of the CSA would cease to pay their subscriptions in 2002, and make an equivalent 'donation' to the Trust, in the same way that anyone can make donations to the Trust.

### ***Newsletter, Conference Organisation and Training***

These activities would be undertaken and controlled by Trustees, assisted by volunteers (who would be selected, but not necessarily exclusively, from those making donations to the Trust).

### ***Executive Committee***

Any current CSA Executive Committee members and the President, who are not already Trustees, would be appointed Trustees at the CSA Trust AGM in December 2001, subject to their approval. This would be possible within the maximum allowed 30 Trustees. One third of the Trustees have to retire every year, but are eligible for re-appointment.

### ***Benefits to Donors and Corporate Donations***

Newsletters and preferential rates at conferences, etc. would be made available to all those who donated a minimum of £25 (the current CSA subscription). Companies that donated (say) £100 would receive up to 4 copies of the Newsletter. The CSA Trust would maintain a list of donors. Current CSA Emeritus members could continue to receive CSA Newsletters if they wish, regardless of whether or not they make a donation to the Trust.

### ***Website***

A single website will be created, giving details of all existing Trust activities as well as all the activities currently undertaken by the CSA. The CSA website is being revamped and could be expanded to include all the Trust activities.

### ***Awards and Prizes***

The Ernie Hyde Award, and Prizes (such as ExemplarChem) could be discussed with Trustees, just as

would be the case for any other CSA Trust Award or Prize.

### ***Finance***

All accounts and financial transactions would need to go through the CSA Trust Treasurer. The increased turnover of the CSA Trust from increased activities would mean having to submit far more detailed accounts to the Charity Commission. There will be a small additional accountancy cost involved but this should be offset by the fact that only one set of accounts will need to be audited.

### ***Meetings of Trustees***

Regular meetings of Trustees will take place to monitor activities, initiate new actions, report on progress, etc. However, a quorum of Trustees is only two people. This means that a meeting can take place if all Trustees have been informed, given opportunities to attend, able to send apologies and/or contribute in written form at meetings. Electronic meetings will be held where possible.

## *The Chemical Structure Association Trust*

The Chemical Structure Association Trust is an internationally recognised registered Charity established to promote the critical importance of chemical information to advances in chemical research. In particular, the Trust aims to create a greater awareness of the essential role that is played in scientific research by the systems and methodologies used for the storage, processing and retrieval of information related to chemical structures, reactions and properties.

Research in this area has been strikingly successful and the results are rapidly reflected in practice. For example, both similarity searching and 3D structure searching are now well established even though much of the research was done only in the 1980s. There is still a pressing need for research in chemical information. Combinatorial chemistry and molecular diversity, for example, are new and exciting fields. However, universities have substantial problems in funding research while industry has difficulty in recruiting suitably trained personnel. The Chemical Structure Association Trust makes funds available to support research in the field of chemical information worldwide.

The Chemical Structure Association Trust is managed by an internationally recognised Board of Trustees listed below:

- Dr Guenter Grethe (Chairman), MDL Information Systems Inc, USA
- Dr Clive Weeks (Secretary), Consultant, UK
- Dr G. M. Downs (Treasurer), Barnard Chemical Information, UK
- Janet E. Ash, Consultant, UK
- M. P. Buffet, Questel. Orbit, France
- Dr J. Buckingham, CRC Press (UK)
- Mr Harry Collier, Infonortics Ltd, UK
- Dr R. Deplanque, Fachinformationszentrum Chemie GmbH, Germany
- Professor Dr J. Gasteiger, Universität Erlangen-Nürnberg, Germany
- Professor A. P. Johnson, University of Leeds, UK
- Ms Bonnie Lawlor, Chescot Publishing Inc., USA
- Dr Diana M. Leitch, University of Manchester, UK
- Professor M. Lynch, University of Sheffield, UK
- Dr R. Massie, Chemical Abstracts Service, USA
- Peter W. L. Nichols, Hampden Data Services, UK
- Dr P. F. Rusch, Consultant, USA
- Dr W. G. Town, ChemWeb Inc, UK
- Dr S. E. Ward, TFPL Ltd, UK
- Dr W. A. Warr, Wendy Warr & Associates, UK
- Dr D. Winkler, CSIRO Molecular Science, Australia
- Ms J. L. Witiak, Rohm and Haas Co., USA

Corporate donors to the Trust include:

- American Chemical Society
- BASIC Group
- Chemical Abstracts Service
- Chemical Notation Association
- Chemical Structure Association
- Derwent
- Elsevier
- GlaxoWellcome
- Hoffmann-La Roche
- Pfizer
- Unilever
- Wendy Warr & Associates
- ZENECA Specialties

Some of the people who have benefited from Awards and Grants in the past include:

- Marina Molchanova, Zelinsky Institute, Moscow (graph-theoretical and combinatorial algorithms for structure generation)
- Weifan Zheng, University of North Carolina (QSAR and combinatorial chemistry)
- Aniko Simon, University of Leeds (chemical literature data extraction)
- Eugene Babaev, Moscow State University (computer-assisted synthesis)
- Gareth Jones, University of Sheffield (paper on genetic algorithm at ACS National Meeting)
- Vladimir Kvasnicka, Slovak Technical University (neural networks for prediction of physiochemical properties)
- Rainer Herges, University of Erlangen-Nürnberg (reaction databases and quantum chemistry)
- Dimitry Lushnikov and Vladimir Shcherbukhin, Zelinski Institute, Moscow (reaction mechanisms and heterocyclic ring transformations)

Some of the recipients of bursaries are:

- Dr. Horst Boegel, Institute of Physical Chemistry, University of Halle, Merseburg, Germany
- Dr. Serge Tratch, Chemical Department of the Moscow State University, Moscow, Russia
- Jan Baber, School of Chemistry, University of Leeds, UK
- Kevin Jernigan, Department of Chemistry, Moscow State University, Moscow, Russia
- Mr. M. Karthikeyan, Division of Organic Synthesis, National Chemical Laboratory, Pune, India
- Michael Wright, Imperial College, London, UK
- Dr Zaneta Nikolovska-Coleska, University of Skopje, Macedonia.

## CHEMICAL STRUCTURE ASSOCIATION TRUST AWARD & GRANTS

### Draft guidelines

The CSA Trust is currently preparing new Guidelines for its Awards and Grants programmes. The outline of these is given below, and the final details will be available after they have been formally approved at the CSA AGM in December. These programmes are financed by investments managed by the CSA Trust and through funds donated by industrial, academic, and government organisations that recognise the value of and benefit from research, development, and education in the fields supported by the CSA Trust.

### Awards

An Award will be given on a tri-annual basis beginning in 2002, consisting of five thousand US dollars (\$5,000) and an appropriate memento. The purpose of the Award is to recognise and encourage outstanding accomplishments in education, research and development activities that are related to the systems and methods used to store, process and retrieve information about chemical structures, reactions and properties. The Award will be presented at a prestigious, relevant conference to be identified prior to each presentation. The recipient of the Award will be asked to give a presentation at the conference.

The Trust Award will be granted to an individual for outstanding achievement in a specific scientific area supported by the Trust. Any individual, except a member of the Trust Awards Committee, may submit one nomination or one seconding letter for the Award in any given year.

Nomination of an individual must be accompanied by the following documentation:

- 1) A letter that evaluates the nominee's accomplishments and the specific relevant work that is to be recognised
- 2) A biographical sketch, including a statement of academic qualifications, as well as contact information
- 3) At least two seconding letters that support the nomination and provide additional factual information with regard to the scientific achievements of the nominee
- 4) If appropriate, a list of the nominee's publications and/or patents may also be submitted.

The CSA Trust Awards Committee, consisting of five members of the Board of Trustees, will examine the

applications and decide on the recipient of the Award. If no-one meets the Award criteria, no Award will be given. The Awards Committee will also provide guidance to the recipient of the award regarding the nature of the presentation that he/she will be requested to be given at the conference.

### Grants

In addition to the Award programme, there will also be Trust Career Development Grants, which will provide funding for the career development of young researchers who have demonstrated excellence in their education, research or development activities that are related to the systems and methods used to store, process and retrieve information about chemical structures, reactions and properties.

Each year the Trust will allocate funds to be given in grants. The value of each grant may vary, but no grant will exceed one thousand US dollars (\$1,000). Grants will be awarded for specific purposes, and within one year each recipient of a grant will be required to submit a brief written report detailing how the grant funds were allocated.

Trust grants will be awarded each year to the applicant(s), age 35 or younger, who have demonstrated excellence in their chemical information related research and who are developing careers that have the potential to have a positive impact on the utility of chemical information relevant to chemical structures, reactions, and compounds. While the primary focus of the Grant programme is the career development of young researchers, additional bursaries may be made available at the discretion of the Trust. Requests for age-neutral bursaries will follow the same procedure as that for the grant applications and such requests will be evaluated against the same criteria. The awarding of age-neutral bursaries in any given year will be determined by the availability of funds.

Anyone working in the field of chemical information who is 35 years of age or younger may apply for a Trust Career Development Grant that will assist in furthering their research, development or education activities where such activities relate to the specific scientific areas supported by the Trust. Grants may be awarded for travel to collaborate with research groups, to attend a conference relevant to one's area of research, to gain

access to special computational facilities, to acquire unique research techniques in support of one's research, or to acquire the tools necessary to support their research.

Applications for grants must include the following documentation:

- 1) A letter that details the work upon which the grant application is to be evaluated as well as details on research recently completed by the applicant
- 2) The amount of grant funds being requested and the details regarding the purpose for which the grant will be used (e.g. cost of equipment, travel expenses if the request is for financial support of meeting attendance, and so on). The relevance of the purpose to the Trust's objectives and the clarity of this statement are essential in the evaluation of the application)
- 3) A brief biographical sketch, including a statement of academic qualifications
- 4) Two reference letters in support of the application. Additional materials may be supplied at the discretion of the applicant only if relevant to the application and if such materials provide information not already included in items 1-4.

The number of grants to be offered in any given year will be determined by the Board of Trustees and will be determined by the availability of funds. Grants will not be given in any year in which the applications do not meet the selection criteria.

The CSA Trust Grant Committee will consist of three members of the Board of Trustees, who are not serving on the Awards Committee. It will be up to the Grant Committee to establish a schedule to ensure that all applications for grants to be awarded in a given year are received by mid-October of the preceding year. The Committee will review the applications and present their decision regarding the distribution of grant funds for Board approval at the Annual Meeting of the Board of Trustees in December.

All applicants will be informed of the results of the Board's decision after the Annual Meeting of the Board of Trustees once it is determined that the necessary funds can be secured either from existing funds or from fundraising.

The names of all grant winners as well as the names of those awarded any age-neutral bursaries for any given year will be published in the Trust's publication(s) and at any conference(s) deemed relevant by the committee.

## CSA Trust Grants 2001

The CSA Trust has announced details of grants made to two PhD students as part of the Awards and Grants programme for 2001.

George V. Gkoutos, from Imperial College, London, UK, receives £500, to attend the International Chemical Information Conference in Nîmes in October 2001. George is working on new resource discovery tools in chemo/bioinformatics, as the web is generally regarded as a low quality chemo/bioinformatics resource discovery tool.

The new tools and methods developed include:

- a demonstration of the use of metadata in chemistry;
- automated ways of converting chemical related sites and information to XHTML and XML (JChemTidy);
- automated generation of Dublin Core and chemical metadata (JChemMeta);
- automated digital signing of databases to establish a level of trust for the XHTML/XML conversions and transformations (JChemSign);
- new resources for creation and conversion of XML content;
- automated digital signing of XHTML/XML chemical documents on the Web (JChemValidate);
- advanced indexing and searching methods (JChemdig);
- resource discovery via molecular XML repositories (Peer to Peer Systems).

Miss Pornpan Pungpo, from Thailand, receives £1,500 to attend the 14th European Symposium on QSAR at Bournemouth, UK in September 2002. Miss Pungpo has been a staff member of the chemistry department, Faculty of Science, Ubonratchathani University since 1994 and has worked in the area of QSAR for 5 years.

Miss Pungpo is now studying for a PhD in computer aided molecular design in the Chemistry Department, Kasetsart University, working on molecular modelling and inhibitor-enzyme interaction study of HIV-1 RT inhibitor, based on quantum chemical calculations. Details of the work have been published in the *Journal of Computer-Aided Molecular Design*, the *Journal of Molecular Graphics and Modelling* and the *Journal of Chemical Information and Computer Sciences*.

A formal announcement about the Trust grants will be made at the International Chemical Information Conference in Nîmes in October.

## CSA Training Initiatives

The CSA Executive met in May at Roche, Welwyn Garden City to consider the role that the CSA could play in developing training in chemical information.

The CSA has previously been active in providing independent professional training courses but these ceased some time ago and the meeting considered whether it was time for the CSA to step back into the training arena, and to define some feasible objectives. Representatives from academic and industrial perspectives identified issues in chemical information training which needed to be explored. The academic approach to chemical information was limited by access to resources and the availability of competent instructors across many UK academic institutions, both issues being addressed by MIMAS.

In industry, resource issues were not seen as such an issue, but there was some concern that end users of information tools were not using the available resources effectively.

Both sectors had identified the need of some objective, independent and basic training. This was a critical analysis of what products (databases, software etc.) are available and when they are the most useful.

## A Practical Introduction to Chemoinformatics Course Report

For some years now, the Molecular Graphics and Modelling Society (MGMS) have organised an annual short course in chemical and biological computing. The rapid developments in bioinformatics and in chemoinformatics over the past few years have meant that there is now far too much material for a single short course. The MGMS hence took the decision to run two courses, one on bioinformatics (for details, see <http://www.york.ac.uk/depts/chem/extern/extcourses/bioinf01.htm>) and one on chemoinformatics, and approached the Department of Information Studies at the University of Sheffield to organise the latter. This course 'A Practical Introduction to Chemoinformatics' was presented for the first time, jointly sponsored by the MGMS and the CSA, in Sheffield on June 12th–June 15th, 2001.

The course was advertised at the 2nd Sheffield Chemoinformatics conference (see page 9) and attracted a total of 14 delegates, who received an intensive two and a half days of lectures and practical sessions from a 5-strong lecturing team: Dr Andrew Leach from GlaxoSmithKline; Dr Robin Taylor from the

Another topic which could prove interesting would be an investigation into the processes operating 'behind the click', to give some understanding of the mechanisms of structure searching, markush search systems and the like.

Traditional classroom type presentations with speakers/presenters and also electronic distance learning techniques via the Web were both thought to be useful in presenting chemical information techniques, to different audiences.

In order to develop the themes identified at this meeting, we need to find out if other members are willing to participate in training initiatives and to establish their area(s) of expertise. A suggestion arising from this is the compilation of a database of members' expertise.

Many thanks to Helen Schofield, Peter Nichols, John Holliday for attending and Sue Jackson for hosting this meeting. Comments and suggestions regarding CSA training initiatives are warmly welcomed.

*David Walsh*  
*david.walsh@dial.pipex.com*  
*6 North Street, Deal,*  
*Kent CT14 6NA*

Cambridge Crystallographic Data Centre; and Dr Val Gillet (the organiser of the course), Dr. John Holliday and Prof. Peter Willett from the University of Sheffield.

The sessions were intended to provide a wide-ranging overview of chemoinformatics techniques for relatively new workers in the field, and covered the following topics:

- 2D Databases and database searching;
- Diversity and compound selection methods;
- 3D:3D data sources and database searching;
- Combinatorial library design.

Out-of-session activities included sampling hostelrys, both local and in the Peak District, and a stomach-expanding conference dinner in Sheffield's restaurant of the year. Attendees' responses to the course (full details of which are at [http://cisrg.shef.ac.uk/ci\\_course/](http://cisrg.shef.ac.uk/ci_course/)) were highly favourable and it is hoped that the course will be offered on an annual basis in the future.

## **International Chemical Information Conference, Nîmes, France, 21-24 October 2001**

### **SUNDAY 21**

Welcome cocktail and buffet dinner sponsored by Chemical Abstracts Service

### **MONDAY 22**

Opening Keynote address

Arnoud de Kemp, Springer-Verlag, Heidelberg, Germany

An Information Community Overview with Reference to the Potential Impact of Peer-to-Peer Networking on Scientific and Technical Information

#### ***Session One: The Old and the New: Coexistence?***

Jonathan Goodman, University of Cambridge, UK

Evaluating Chemical Information Sources on the World Wide Web

Dr Alfred Steinhardt, Hoffmann-La Roche, Basel, Switzerland

New Information Management Technologies to Improve the Drug Development Process

Pierre Buffet, Questel-Orbit, Paris, France

Virtual Databases: Integrating Web and Internal Data Searching

*New Product Information Presentations from ISI, CAS, Accelrys and Questel-Orbit*

Chemical Structure Association  
Presentation of the 2001 Awards

#### ***Session Two: And Now the User...***

Deborah Kahn

DK Associates, London, UK

Information at the Desktop: What have we learned?

Frank Cooke and \* Helen Schofield  
GlaxoSmithKline, Pennsylvania, USA  
and \* UMIST, Manchester, UK

Mining for Education Nuggets: Assessment of End-Users' Search Techniques to Assist with Training and Purchase Decisions

*New Product Information Presentations from Springer Verlag and STN International*

#### ***Session Three: Challenges to the Scientific and Technical Information Community***

Arie Jongejan (Elsevier, Amsterdam, The Netherlands)

Robert Massie (Chemical Abstracts Service, Ohio, USA)

Jacques Michel (European Patent Office, The Hague, The Netherlands)

Michael Tansey (Thomson Scientific, Philadelphia, USA)

Conference Cocktail sponsored by MDL/ScienceDirect/ChemWeb

### **TUESDAY 23**

Day Two Keynote address

Stephen E Arnold  
AIT, Kentucky, USA

Content Management: A Matter of Discontent

#### ***Session Four: Data Exploration & Integration***

Jean Marie Devès and Isabelle Morelon, Institut Français du Pétrole, Rueil-Malmaison, France

Text Mining: Ali Baba's Cave?

Thérèse Vachon, Novartis, Basel, Switzerland

Interactive Exploration of Patent Data for Competitive Intelligence: Applications in Ulix (Novartis Knowledge Miner)

Anthony Trippe, Aurigin Consulting, California, USA

A Comparison of Ideologies: Intellectually Assigned Co-Coding Clustering vs Themescape Automatic Thematic mapping

*New Product Information Presentations from Micropatent, Chemical News & Intelligence, Invention-Machine, FIZ Karlsruhe and Thomson Financial*

#### ***Session Five: Indexing, Analysis & Categorisation***

Valery Tsourikov, Invention-Machine, New York, USA

Semantic Processing with Causal Reasoning: Applications in Patent Intelligence and Text Mining

Marc Krier and Francesco Zaccà, European Patent Office, The Hague, The Netherlands

Automatic Categorisation of Patent Data

#### ***Session Six: Information Acquisition & Management***

Matthew Toussant, Chemical Abstracts Service, Ohio, USA

The Changing Landscape of Chemical Patent Information and Its Impact On Chemical Research: from Gene Sequences and Biotech Property to Application Publication Changes

Susan Jackson, Roche Products, Welwyn, UK

Document Linking

Ralph Schroeder, Delphion, Illinois, USA

Intellectual Asset Management Capabilities

*New Product Information Presentations from Bio-Rad Laboratories, John Wiley & Sons, SPECS and BioSPECS, and CambridgeSoft*

### **WEDNESDAY 24**

#### ***Session Seven: A Virtual World***

Guy Hibbert, Sift Groups, Bristol, UK  
The Role of Virtual Communities in Professional Scientific and Technical Domains: an Applications Service Provider Viewpoint

Peter Hoefer, Bayer, Leverkusen, Germany

The Bayer Virtual Library

#### ***Session Eight: Data Search & Management***

Rudolph Potenzzone, LION Bioscience Inc, California, USA

Integrating Disparate Databases to Support the Drug Discovery Process

Erno Pretsch, P. Portmann, M.E. Munk and E. Zass, ETH, Zürich, Switzerland

A New Versatile Structure Search System

Paul Fretwell, Accelrys, Leeds, UK  
Commercial Reaction Databases in Oracle

End of 2001 programme at about 13.00

## ***The revolution in web linking for chemists***

***Jenny Drey***

Chemists are benefiting increasingly from advances in technology which allow them to add value to chemical information on the Internet. First and most obvious is the immediacy with which chemists all around the world can access the latest research, without having to wait for postal systems to delay its arrival on their desks. Journal issues can be archived electronically, and searched through easily. Large data sets can be transmitted, which could not otherwise have been printed and distributed unless at great cost. Chemists have benefited from this in particular, since paper journals were only able to present a rather one-dimensional approach to chemical information, the very nature of which is three-dimensional. Chemists communicate in structures, which are difficult to represent in two dimensions, and processes, which are impossible to represent on the printed page.

Elsevier Science recently announced its plans to upgrade radically its online offerings for chemists. Their Dymond Linking (Dynamic Metadata on Demand) initiative allows readers of chemistry journals to pinpoint a chemical object in an online article and click on it to initiate a search for that structure or reaction in third party databases or applications. In just two clicks, they can directly access further information about their chosen object. Dymond Linking was developed by Elsevier Science in conjunction with ChemWeb.com and MDL Information Systems, and was announced at the Pacificchem meeting in Honolulu. This radical new linking mechanism brings the database and the journal much closer together – journals are taking on a completely new dimension, and becoming more integrated with information stored in databases. A user can hop out of the journal, into the database, and then hop back into another journal article which also features the compound of interest. It is now possible to go from an online article to a list of search results for a compound of interest in just two clicks. The demonstration version showed how a link from bold numbers in the full text (structure identifiers) can be activated to become 'clickable'. When clicked, an intermediate window

opens up to show the search options, along with a Chime representation of the compound. The user can then choose to search Beilstein CrossFire, The Combined Chemical Dictionary, or generate a IUPAC name for the compound using AutoNom.

This developers believe that this technology represents a revolution in web-linking. Up until now, all web links have been based on underlying text strings, but these links are based on chemical structures and therefore allow one application to pass this structure information on to many other applications. Initially, Dymond Linking will offer access to the three applications in the demonstration version, but will also be offering property and spectra predictions for the linked structure in a future release, and any database or application provider who allows structure searching could, in theory, be linked to from the online article. By linking into third-party databases, the user has access to a substantial backfile of in-

formation for that structure – and the user is not restricted to Elsevier journal titles alone. It is expected that many users may click out of an Elsevier journal into an extensive database such as CrossFire and then into a journal from the ACS, for example. The Elsevier and the ACS articles are linked not by text, but by the fact that the same structure is quoted in both articles. The initiative offers links that are indirect, and not always obvious, between articles that may not be linked when using text search strings. Dymond's advantage will be that it uses the language of the chemist: structures. Dymond Linking is currently offered free of charge from Tetrahedron Letters, exclusively on ChemWeb.com. During the course of the year, extra functionalities and linking possibilities will be made, with links also being offered from other journals. Dymond Linking will also be available to customers of Elsevier's ScienceDirect package from mid-2001.

This revolutionary new tool for chemists has potentially far-reaching implications. If it were to become universal, would there actually be a need for a chemical indexing service?

The future of chemical information delivery is exciting, with many major developments taking place that will greatly improve the way chemists carry out their research. Not only will chemists be able to access more information more quickly, they will be able to access and exchange a whole new quality of information over the Web which has never before been possible.

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***In just two clicks  
you can go from  
an online article  
to search results***

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**2nd Joint CSA/MGMS  
Sheffield Conference on Chemoinformatics  
April 9th–11th 2001**

About 170 delegates from 17 countries gathered in Stephenson Hall, at the University of Sheffield, for the second joint Chemical Structure Association/ Molecular Graphics and Modelling Society conference.

The conference was organised mainly by members of the Department of Information Studies at the University of Sheffield and thanks go to Peter Willett, Val Gillet and John Holliday for all the work that went into making the second International Conference on Chemoinformatics at least as successful as the first (held in 1998).

The programme consisted of a series of oral presentations, posters sessions, and a commercial software and hardware exhibition. The oral presentations were divided into sessions on Library Design, QSAR, Molecular Interactions, Virtual Screening and High-Throughput Screening. Abstracts are available on the website at <http://cisrg.shef.ac.uk/shef2001/abstracts.htm>.

As before, the Cutlers Hall in Sheffield provided a splendid opportunity for the delegates to meet together socially.

Both the CSA Trust and MGMS provided bursaries for students to attend the conference. The CSA Trust sponsored Kamaldeep Chohan from the University of Leicester, and Szabolcs Csepregi, from the University of Leeds. Brief conference reports by these students are given below.

Abstracts of the posters exhibited at the conference, including those of Kam Chohan and Szabolcs Csepregi, can be found at <http://cisrg.shef.ac.uk/shef2001/posters.htm>.

**Report by Kam Chohan  
Department of Chemistry,  
University of Leicester**

The conference provided an excellent opportunity to find out about many aspects of drug discovery, and how different companies and institutions implement them. The reassuring part is that, although they are using different leads, they use similar methodologies to underpin their work. I found the talks extremely useful, interesting and diverse, helping to extend my general knowledge of the area.

I particularly enjoyed Mike Hann's presentation on 'Making lead discovery less complex'. He explained the need to use simple approaches first as a crude filter, followed by more sophisticated approaches on a smaller data set, as a practical approach to drug discovery. Dimitris Agrafiotis presented an approach 'towards the unthinkable'. He predicted molecular properties of products from simple chemical building blocks. I was incredibly impressed with his ability to obtain a  $q^2=0.98$  overnight – while most of us were fast asleep! I found all the presentations relating to specific protein-ligand docking programs (for example, DOCK and FLEXX) extremely useful, as these are packages I have utilised in my work. Overall, it was fantastic to have so many interesting presentations throughout.

There were a large number of posters to see, and this provided another excellent opportunity to have more open discussions. There were so many good quality posters that it was very difficult to pick favourites. Attending the poster session

gave me plenty of opportunity to interact with other PhD students. I am very grateful to the CSA for giving me the opportunity to come to Sheffield for an excellent conference and many thanks to the organisers for a warm welcome and an enjoyable couple of days.

**Report from Szabolcs  
Csepregi, ICAMS, School  
of Chemistry  
University of Leeds**

I think it was an excellent conference. A large subject was covered and I have learned much about areas that I am not closely in touch with: in particular, library design, QSAR, High-Throughput Screening and dis-similarity. For myself, as an author of a docking method, the most interesting sessions were about molecular interactions and virtual screening.

The talks I liked the best were by Michael Hann, Robin Taylor, Peter Johnson, Jonathan Goodman, Matthias Rarey, Andrew Good, Bohdan Waszkowycz, Geoff Downs and Joseph Durant. The poster session was also very interesting. I found the discussions, questions and suggestions regarding my poster from conference delegates very valuable and helpful.

The organisation of the conference was professional. Everything went smoothly and was on time. At the beginning there seemed to be some problem with the microphones, but the talks were always intelligible. The environment was also very nice. Both Stephenson Hall and the Cutlers Hall were great buildings and the cooks gave us a real treat.

## EVENTS 2001–2002

### September

**13–14 September:** EuroMUG'01 Daylight European User Meeting, University Arms Hotel, Cambridge, UK. Contact: Dr John Bradshaw, Sheraton House, Castle Park, Cambridge CB3 0AX, UK. Tel: +44-(0)1223-390-099; fax: +44-(0)1223-390-040; email: johnb@daylight.com; website: <http://www.daylight.com/europe/emug01/>

**18–22 September:** 7th International Symposium on Solid Phase Synthesis and Combinatorial Chemical Libraries, University of Southampton, UK. Contact: Professor Roger Epton, P.O. Box 13, Kingswinford, West Midlands, DY6 0HR, UK. Tel: +44-(0)1384-279324; fax: +44-(0)1384-294463; email: r.epton@mayflower.demon.co.uk; website: <http://www.biocom.co.uk/sps2001.htm#PI>

**30 September–October 3:** EUSIDIC Annual Conference. Information Value Chain, Status and Future Developments, Kongreßhaus, Baden-Baden, Germany. Contact: Ms. Dagmar Marek, EUSIDIC Secretariat, c/o FIZ Karlsruhe, 76344 Eggenstein Leopoldshafen, Germany. Tel: +49-(0)7247-808-403; fax: +49-(0)7247-808-114; e-mail: eusidic@fiz-karlsruhe.de; website: <http://www.eusidic.org>

### October

**10–11 October:** Online Information for the City, London, UK. Contact: Learned Information Europe Ltd, Woodside, Hinksey Hill, Oxford OX1 5BE, UK. Tel: +44-(0)1865-388000; fax: +44-(0)1865-736354; website: <http://www.online-information-city.co.uk/>

**21–24 October:** The 2001 International Chemical Information Conference and Exhibition, Novotel Atria Hotel, Nîmes, France. Contact: Harry Collier, Infonortics Ltd., 15 Market Place, Tetbury, Gloucestershire, GL8 8DD, UK. Tel: +44-(0)1666-505-772; fax: +44-(0)1666-505-774; e-mail: contact@infonortics.com; website: <http://www.infonortics.com/chemical/index.html>. Program on page 7

### November

**4–7 November:** Combinatorial Chemistry: Applying the Technology, Dolder Grand Hotel, Zurich, Switzerland. Contact: Kate Herrick-Stare, ACS ProSpectives, 1155 16th Street, NW, Washington DC, 20036 US. Tel:

+1-800-227-5558/ +1-(202)-872-6286; fax: +1-(202)-872-6013; e-mail: [acsprospectives@acs.org](mailto:acsprospectives@acs.org); website: <http://www.acs.org/acsperspectives>

**5–7 November:** 18th European MDL Software Users' Group Meeting, Prague, Czech Republic. Contact: Ariane Ludwig, MDL Information Systems AG, Gewerbestrasse 12, CH-4123 Allschwil 2, Switzerland. Tel: +41-61-486-88-88; fax: +41-61-486-88-89; e-mail: [ArianeL@mdli.com](mailto:ArianeL@mdli.com); website: <http://www.mdli.com/>

**15–16 November:** CombiCat 2001: Combinatorial Catalysis and Catalyst Optimization, Park Hyatt Hotel Philadelphia, Pennsylvania, US. Contact: The Catalyst Group Resources, PO Box 640, Spring House, PA 19477, US. Tel: +1-(215)-628-4447; fax: +1-(215)-628-2267; e-mail: [cnf@catalystgrp.com](mailto:cnf@catalystgrp.com); website: <http://www.catalystgrp.com/conferences.html>

### December

**3 December:** CSA and the CSA Trust AGMs, the Linnean Society, Burlington House, Piccadilly

**3 December:** CSA Annual Dinner, 7.00 pm for 7.30 pm at the Cadogan Hotel, Sloane Street, London.

**4 December:** SCI Bioactive Sciences and Fine Chemicals Groups Conference. ADME: Perspectives in High Throughput and in Silico Approaches, London, UK. Contact: Conference Secretariat, Society of Chemical Industry, 14/15 Belgrave Square, London SW1X 8PS, UK. Tel: +44-(0)20-7598-1564; fax: +44-(0)20-7235-7743; e-mail: [alex.jennings@soci.org](mailto:alex.jennings@soci.org); website: <http://www.soci.org/>

**4–6 December:** Online Information 2001, Grand Hall, Olympia, London, UK. Contact: Rebekah Hart, Learned Information Europe Ltd, Woodside, Hinksey Hill, Oxford OX1 5BE, UK. Tel: +44-(0)1865-388000; fax: +44-(0)1865-736354; e-mail: [rebekah\\_hart@learned.co.uk](mailto:rebekah_hart@learned.co.uk); website: <http://www.online-information.co.uk>

## 2002

### April

**7–12 April:** 223rd American Chemical Society National Meeting, Orlando, US. Contact: ACS Meetings Department, 1155 Sixteenth Street, N.W., Washington DC, 20036 US. Tel: +1-(202)-872-4396; fax: +1-(202)-872-6128; email: [natlmtgs@acs.org](mailto:natlmtgs@acs.org)

## Chemweb

*Tetrahedron Letters* is available free via the Organic Chemistry Forum at <http://organic.chemweb.com>, from ChemWeb.com, until 1 October 2001. This includes back issues to Volume 39. The journal is published weekly and covers developments in techniques, structures, methods and conclusions in experimental and theoretical chemistry. Membership of ChemWeb.com is required to access ChemWeb.com or the Organic Chemistry Forum. Membership is also free.

## Organic Syntheses Goes Electronic

Organic Syntheses has released a website, [www.orgsyn.org](http://www.orgsyn.org). This site is available free of charge to all chemists and contains all of the nine Collective as well as Annual Volumes and Indices. Each preparation published in OS is peer-reviewed for correctness and reproducibility, making it unique in the organic chemical literature, and contains detailed information on starting materials, equipment, reaction and purification procedures, and safety precautions. In recent volumes, editors have attempted to standardise the style of experimental procedures and the presentation of spectroscopic data. Increasing emphasis on the toxicology of organic compounds has led to the inclusion of additional hazard warnings. The website is the result of a collaboration between the Board of Directors of OS, CambridgeSoft Corporation and DataTrace Publishing Company. All the information in the OS Collective Volumes, Annual Volumes and Indices has been digitised, mapped and converted to XML documents by DataTrace. CambridgeSoft has developed the website incorporating the databases linking text and chemical structures using their ChemOffice Webserver software. Reaction diagrams are stored in a Chem-Finder database to facilitate structure-based searching.

The OS website is fully searchable using a variety of techniques. With the free ChemDraw plugin for Netscape Navigator or Microsoft Internet Explorer, chemists can draw structural queries directly on the web page, and combine structural or reaction transformation queries with full-text and bibliographic search terms.

## iMRW

Integrated Major Reference Works (iMRW) permits linking between MDL's synthetic methodology databases and specific reference works on synthetic methods thanks to a partnership between MDL and InfoChem. The following major reference works are available in the initial iMRW product offering:

Comprehensive Asymmetric Catalysis (CAC) from Springer-Verlag

- reviews catalytic methods for asymmetric organic synthesis
- contains 6,000 evaluated reactions

Comprehensive Organic Functional Group Transformations (COFGT) from Elsevier

- highlights the preparation and transformations of functional groups
- covers all known functional groups and the methods of their construction, introduction, and interconversion.

Encyclopedia of Reagents for Organic Synthesis (EROS) from John Wiley & Sons, Ltd.

- electronic version of an eight-volume reference of reagents
- will contain approximately 48,000 reactions and 3,500 reagents used by organic chemists
- regular updates will add about 200 new reagents annually.
- intended to help synthetic chemists find the most suitable reagents for particular reactions.

Website: <http://www.mdli.com>.

# PRODUCT NEWS

## Introducing new software company Accelrys

Molecular Simulations Inc. (MSI), Synopsys Scientific Systems, Oxford Molecular, and the Genetics Computer Group (GCG) have been combined and now exists as Accelrys, a subsidiary of Pharmacoepia. This new company develops and commercialises molecular modelling and simulation software for the life sciences and materials research, cheminformatics and decision

support systems, and bioinformatics tools for gene sequence analysis. The business also provides consulting services to its customers in drug discovery and chemical development. Accelrys has bases in San Diego CA, Princeton NJ, and Madison WI, in the US and Cambridge and Leeds, in the UK. The company's website is at [www.accelrys.com](http://www.accelrys.com).

**Contact Details****Chair****Janet Ash****Tel: +44-(0)1580-852270****e-mail: ash@euronet.nl****Vice Chair****Peter Nichols****Tel: +44-(0)20-8441-7495****e-mail: hds peter@aol.com****Treasurer****Suzanne Pears****Tel: +44-(0)1509-644384****e-mail: suzanne.pears@astrazeneca.com****Secretary****David Walsh****e-mail: david.walsh@****dial.pipex.com****Membership Secretary****John Holliday****Tel: +44-(0)114-222-2685****e-mail: J.D.Holliday@sheffield.ac.uk****Newsletter Editor****Frances Daniel****Tel: +44-(0)1949-844837****e-mail: francesdaniel@bottesford65.fsnet.co.uk****Next Copy Date****February 15 2002**

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**MSc in Chemoinformatics  
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An exciting programme in chemoinformatics has been developed in collaboration with a consortium of leading agrochemical, pharmaceutical and chemical software companies. The programme aims to develop the skills required for the many posts now available in chemoinformatics.

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**Further information and an application form are available from:**

**The Graduate Admissions Secretary,  
Department of Information Studies,  
University of Sheffield,  
Western Bank, Sheffield S10 2TN.**

**Tel: 0114 2222630****Fax: 0114 2780300****Email: dis@sheffield.ac.uk****Website:****<http://www.shef.ac.uk/~is/courses/pgrad/mscci/mscci.html>****CSA/CINF joint meeting, San Diego**

At the National American Chemical Society (ACS) Meeting held in San Diego, California, in April 2001, the CSA sponsored a day and a half symposium on 'Electronic Chemistry Publishing'. The speakers were from all segments of the endeavour and demonstrated the international character of this work. The papers were of good quality and the attendance was excellent in spite of the threat of blackouts due to the problems in the California electrical distribution system. Many of the presentations can be viewed at the CINF (ACS Division of Chemical Information) website (<http://www.acs-cinf.org>).