Chemical Structure Association Trust

ISSUE 1

NEWSLETTER

SPRING 2002

From the Chairman of the CSA Trust

With this first Chemical Structure Association Trust Newsletter, I cordially invite all former members of the Chemical Structure Association to become sponsors of the Trust by donating the minimum sum of £25 for individuals (no minimum for students) and £100 for corporations. All donors will be listed on the Trust's sponsorship list

Be assured that your donation will be put to good use in continuing the educational activities of the CSA by the expanded CSA Trust and you will continue to receive the Newsletter on a regular basis.

After many discussions during 2001 and thorough investigation of the issues, the incorporation of the activities of CSA into the Trust was approved unanimously at the Annual General Meetings of both organisations. Concomitantly, all members of the CSA Executive Committee were elected Trustees (see report on Page 2).

The expanded body of Trustees will be well suited to organise and manage these activities, such as continued publication of the Newsletter, participation in and sponsorship of conferences, and training programmes. Through these activities the Trust will enhance its position to promote its aims and objectives and better serve the chemical information community.

These activities (combined with the newly established Michael Lynch Award of the Chemical Structure Association Trust, to be awarded triennially) will also lead to a greater international awareness of the Trust. In addition to the award, the Trust will continue to provide bursaries to worthy candidates for furthering their research through attending conferences, collaborating with other research groups or acquiring tools needed in their research.

During the transition period in 2002, a committee consisting of members of both organisations will study and solve all outstanding issues and make its final recommendations at the 6th International Conference on Chemical Structures in Noordwijkerhout in June. Full incorporation is expected to be completed in the latter half of 2002.

Please help us to achieve the stated goals of the Trust by becoming a sponsor. I am looking forward to meeting many of you during the next year at conferences and the Annual General Meeting in December.

Guenter Grethe
Chairman, CSA Trust

Sponsorship Secretary John Holliday will maintain the register of donors. Please send donations to him: Dr John Holliday, Department Of Information Studies, University of Sheffield, Sheffield, S10 2TN, UK. Tel: +44-(0)114-222-2685; e-mail: J.D.Holliday@sheffield.ac.uk

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Inside...

From your 'new' old CSA Chairman

The bad news is that you're stuck with me again as your Chairman but fortunately the good news is for just a short period of time! I'm very pleased to tell you that the reason for this is that at the respective AGMs of the CSA and the CSA Trust (CSAT), it was unanimously agreed to incorporate the activities of the CSA within the framework of the CSAT. Some might say about time too! It's probably lost in the mists of time but it was always intended that the CSA activities would be incorporated into the CSAT when it was set up. However, it turned out to be a little too complicated to accomplish in 1988 (it took over 3 years just to set up the Trust!)

The draft proposals spelt out on Page 2 of the Autumn 2001 CSA Newsletter have been accepted and the main point I should like to emphasise is that all the activities of the CSA will continue without interruption. All your current CSA Executive Committee members, and our President, are now Trustees. The only major differences you'll notice as CSA members is that you will no longer pay a 'subscription' to the CSA in 2002 but instead be asked to make a donation to the CSAT. The minimum amount is £25 for full members ($35 in the US) and there is no minimum amount for students but, of course, any higher level of donation will be gratefully received! Then you become a donor to the CSAT.

The Newsletter is now the CSAT Newsletter. It is envisaged in the future that the vast majority of donors will want to access the Newsletter via the Web site.

It is now be possible to receive Corporate donations. This means that organisations making corporate donations can, for example, download multiple copies of the Newsletter.

A small sub-committee has been set up from both the CSA Executive committee and the CSAT Trustees to oversee the smooth transition of the CSA activities into the CSAT over the next few months. The immediate objective is to report on the progress of this transition at the Noordwijkerhout meeting in June. The CSA would then be formally wound up at an AGM in December 2002.

Peter Nichols

Round-up of 2001 CSA and CSA Trust AGMs

Incorporation of CSA activities within the CSA Trust

The AGMs of both the CSA and the CSA Trust were held on Monday 3rd December 2001. One of the major items on the two Agendas was the proposal that, in future, all the CSA educational activities should be carried out by the Trust.

The Trust AGM was held first, but CSA members were invited to attend the item on the amalgamation. The Trustees unanimously approved that the activities, objects and funds of the CSA should be incorporated within the framework of the Trust. Those members of the CSA Executive Committee who were not already Trustees were then elected to the Board of Trustees.

The CSA AGM followed, and a similar motion was unanimously approved by the 14 CSA members present and by 6 proxy votes. A Select Committee will oversee the incorporation and will submit a final report to the Trust in June 2002. Members of this committee are: Peter Rusch (Chairman), Janet Ash (former CSA Chairman), Geoff Downs (Trust Treasurer), Guenter Grethe (Trust Chairman), Bonnie Lawlor (Trustee), Peter Nichols (CSA Chairman), Suzanne Pears (CSA Treasurer), Clive Weeks (Trust Secretary).

The Trust becomes responsible for Newsletter production, conference organisation and training programmes.

There has always been an overlap between the aims and objectives of the CSA and the Trust, but now that all the activities will be carried out by the CSA Trust, we shall be in a better position to make a positive contribution to chemical information worldwide.

CSA Trust Mike Lynch Award

Guidelines for the future CSA Trust Awards and Grants were discussed and approved, and the Trust Award will in future be named the 'CSA Trust Mike Lynch Award', in honour of the outstanding contribution that Mike has made to the field of chemical information.

Ernie Hyde Awards

At the CSA AGM, two people were presented with an Ernie Hyde Award for their contributions to the CSA. Rob Brown received an award for his work on setting up and maintaining the CSA website for the past 5 years, and Rosemary Downs was rewarded for all her work on examining the legal implications of the incorporation of the CSA within the Trust.

CSA Committee

New officers were elected to the CSA Committee, with Peter Nichols as Chairman and Helen Schofield as Vice-Chairman. All other Committee members were re-elected. The Committee will ensure a smooth transition of CSA activities to the Trust before the CSA is formally wound up later this year.

Personalia

Steve Maginn of the Cambridge Crystallographic Data Centre is going to run Chemical Computing Group's UK office, performing both technical and commercial contacts, being the first contact for both in the UK, Netherlands and Scandanavia. The office will be in Cambridge.

Pierre Buffet of Questel.Orbit has been awarded the Online Information Lifetime Achievement Award.

Roger Sayle has left Metaphorics (Daylight) and is working for OpenEye.

Bill Fitch is now working for Roche in California.

Sheila Ash has moved to Accelrys' Cambridge (UK) office.

Allan Marchington has been appointed senior vice president of productivity at Millennium Pharmaceuticals in Cambridge, MA.

Matthew Clark (previously at EMAX) is now Director of Scientific Computation at LOCUS Discovery.

CINF/CSA Symposium

223rd American Chemical Society National Meeting
Orlando, Florida
Sunday April 7 2002

Chemical Descriptors I

Cosponsored with Chemical Structure Association (CSA)

B. A. Vickery, Organiser

9:00 **Introductory Remarks**

9:10 **1. An efficient representation for chemical descriptors**
J. M. Blaney, J. K. Lanctot

9:40 **2. A hierarchy of structure representation**
J. Gasteiger, T. Kleinöder, J. Sadowski, M. Wagener, M. C. Hemmer

10:10 **3. Use of molecular descriptors based on medicinal chemistry building blocks**
P. E. Blower Jr., K. Cross, M. Fligner, J. Verducci

10:40 **4. Molecular descriptors as a tool for data mining the Registry file**
J. M. Wilson, R. J. Schenck

11:10 **5. Multiresolution analysis of topological representations of structural and physico-chemical properties of pharmacological molecules**
J. Binamé, L. Leherte, D. P. Vercauteren

Chemical Descriptors II

B. A. Vickery, Organiser

1:30 **Introductory Remarks**

1:40 **6. Combinatorial descriptors for virtual screening**
V. S. Lobanov, D. K. Agrafiotis, H. Xu

2:10 **7. Prediction of drug solubility: cohesive interactions modeled by Monte Carlo simulations**
A. Filikov

2:40 **8. Collection of chemically intuitive molecular descriptors proven as highly effective and fast predictors of ADME properties**
R. Fraczkiewicz, B. Steere, M. B. Bolger

3:10 **9. An efficient bitmap container package for very high-dimensional fingerprints**
P. Fox, L. Naerum, H. Thogersen, R. Clark, T. Heritage

3:40 **10. Controlling degeneracy with the extended valence sequence Signature molecular descriptor**
J. Faulon, C. J. Churchwell, D. P. Visco

ExemplarChem 2001

A massed audience of young chemists, chemistry lecturers, sponsors and organisers gathered at the Scientific Societies Lecture theatre in London on 24th October 2001 to attend the annual ExemplarChem Prize winners meeting. You may remember from last year's report by Janet Ash (who was unable to attend this meeting, hence a far less impressive report by yours truly) that ExemplarChem is an Internet exhibition of exemplary chemistry student project work initiated by Henry Rzepa of Imperial College.

Through the auspices of a group of generous sponsors, namely CAS, CSA, Inpharmatica, ISI, GlaxoSmith-Kline, MGMS and Pfizer, the Royal Society of Chemistry were able to organise a very interesting programme of speakers, serving to warm up the audience with some thought-provoking papers prior to the main event of the Prize Giving, whilst feeding us all with an excellent lunch and providing a wine reception to round off a most enjoyable and rewarding day.

The speakers and their topics were:

- Henry Rzepa (Imperial College): 'The world is getting more global'
- David Alker (Pfizer): 'Getting a job: partnership or big brother'
- Barry Dunne (CAS): 'A walk through the world of scientific information'
- Ben Johnson (Graphic Science): "Working with audiences"

Following the invited papers there was a short discussion led by Dr Sean McWhinnie of the RSC on the future of ExemplarChem and plans for 2002 and then on to the Awards ceremony itself.

Your Chairman, representing the CSA, was delighted to present an Award to Nicola Whitehead and Dan Morgan of Loughborough University for their project on 'Preparation of Ceramic Electrolyte Microtubes by means of Electrodeposition} and, ever willing to appear before the camera, his picture and that of the prize winners is shown below for your delectation.

Full details including a complete list of the 2001 winners, Guide Lines and Timetable for 2002 can be found at: www.chemsoc.org/exemplarchem/

In light of the fact that one of the CSA's raison d'être as stated in our publicity flyer is 'Chemistry on the Internet', this is a very worthwhile activity to support, also, it does give the CSA good exposure to chemistry students.

Peter Nichols

Peter Nichols with the Exemplarchem 2001 prize winners and co-ordinator from Loughborough University

Applications Invited for CSA Trust Grants for 2003

The Chemical Structure Association (CSA) Trust is an internationally recognised organisation established to promote the critical importance of chemical information to advances in chemical research. In support of its charter, the Trust has created a unique Grant Program, and is currently inviting the submission of grant applications for 2003.

Purpose of the Grants:

The Grant Program has been created to 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 compounds.

Grants will be awarded up to a maximum of one thousand US dollars ($1,000) each. Grants are awarded for specific purposes, and within one year each grantee is required to submit a brief written report detailing how the grant funds were allocated.

Who is eligible?

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, are invited to submit applications. While the primary focus of the Grant Program is the career development of young researchers, additional bursaries may be made available at the discretion of the Trust. All requests must follow the application procedures noted below and will be weighed against the same criteria.

What activities are eligible?

Grants may be awarded to acquire the tools necessary to support research activities, or 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, or to acquire unique research techniques in support of one's research.

Application requirements:

Applications 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, etc.). The relevance of the above-stated 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.

Three copies of the complete application document must be supplied for distribution to the Grants Committee.

Deadline for applications:

Applications must be received no later than October 18, 2002. Successful applicants will be notified by December 18, 2002.

Address for submission of applications:

Three copies of the application documentation should be forwarded to:

Bonnie Lawlor
CSA Trust Grant Committee Chair
276 Upper Gulph Road
Radnor
PA 19087
USA

E-mail submissions, if complete, may be forwarded to the Grant Committee at chescot@aol.com.

What shape is my molecule?

Is the representation of molecular structures on a computer little more than fine art with a practical use? David Bradley considers.

Long gone are the days of chemists sitting at a desk to draw their molecules with a pencil and chemical template, with its bond lines, hexagons, and cyclohexane chairs and boats. And it's the rare student who works with plastic ball and stick models. These days there are sophisticated software packages around that can render a chemical sketch in three dimensions on screen in seconds, or import a fully formatted structure from a database, such as CambridgeSoft's ChemFinder, or a website like Ron Rinehart's Molecular Heaven, which links to numerous resources for finding all kinds of molecular structures (http://www.mpcfaculty.net/ron_rinehart/molechev.htm). Like many other programs, the ArgusLab Molecular Modeling Program (now at version 3.0 beta) (http://www.planaria-software.com) features extensive support for rendering molecular surfaces. It can build three-dimensional interactive molecules, and crucially optimise structures for the entire periodic table so that it provides a conformation as close to the likely 'real' shape of a molecule in the real world.

Computational techniques built into this package and others such as those from ACD's ACD/HNMR (http://www.acdlabs.com/products/spec_lab/predict_nmr/hnmr/) allow aspects of chemistry such as nuclear magnetic resonance spectra to be predicted from the geometry-optimised structure.

The early chemistry drawing packages used the 2D structure, that most fundamental of structural representations, akin to a freehand sketch. From this beginning, the familiar structure drawing packages have all evolved tremendously over the years; good examples of this evolution are ChemDraw (http://www.cambridgesoft.com/products/family.cfm?FID=2), MDL Information Systems' ISIS/Draw (http://www.mdli.com/cgi/dynamic/product.html?uid=$uid&key=$key&id=43), and ChemWindow now at version 6 (http://www.softshell.com/cw/cw.html). Now, the latest version of a package such as ChemDraw Ultra 6.0 will recognise the stereochemistry inherent in a molecule, check the valencies of every atom, clean up the bond lengths and angles and even produce a systematic name from one's structure using IUPAC chemical nomenclature rules.

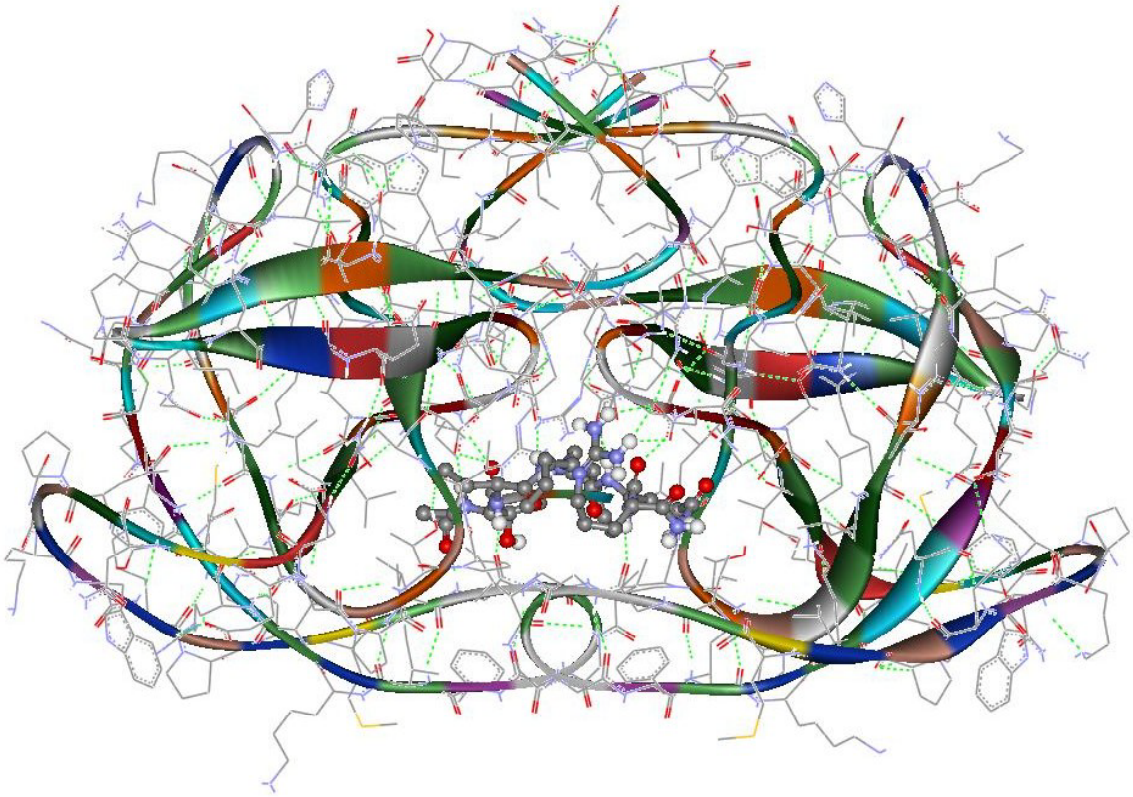
The 2D structures and their ball-and-stick relatives hinge on the rules of covalent bonds described by G.N. Lewis. A single line represents a bond between the atoms at each of its end. While chemists can 'see' very clearly what a 2D diagram represents, such a diagram encapsulates only one aspect of a chemical, the purported interconnectivity of its atoms at the covalent level. But, molecules are three-dimensional.

Rendering a 2D structure as a 3D molecule is the forte of a whole range of programs including the parent suites of ChemDraw, ChemWindow itself and the web-browser based Chime program from MDL. Molecules-3D from Molecular Arts Corporation (http://www.molecules.com/m3d25web.shtml) also provides fine structures. Accelrys' Materials Studio provides great control of the display of molecular structure.

The display of a molecule as a 3D structure is amenable to all kinds of representations. These range from the basic 3D version of the simple stick diagram and the ball-and-stick to the space-filling model, also known as a CPK model after its inventors, Corey, Pauling and Kulton. In the space-filling model, atoms are rendered as spheres with their scaled 'real' radius, their Van der Waals radius, the distance out from the nucleus into which the electrons extend, showing how atoms sit together in a molecule with no leggy bonds. The physical bulk of some chemical groups becomes immediately apparent with the space-filling model, as atoms jostle for position in a molecule.

There is much more to a molecule than simply its atoms and bonds. There are the interactions between different parts of the molecule, how they behave in solvents, when other molecules are present, or when they crystallise. One feature that a program like ArgusLab can be used to create while you are browsing molecules embedded in web pages is to show the electrostatic outline, or surface, of a molecule. This rendering provides a view of how a molecule 'feels' to solvent or other molecules. In one sense it smoothes out the troughs between atoms, but in a more scientific manner it represents the electrostatic potential of the molecule as a whole, with its highs and lows smoothed out between atoms, as there are no gaps in this field.

Although this is all well and good for simple small molecules, when it comes to rendering in 3D the structure of a macromolecule, for example, a nucleic acid or



Visualisation packages produce beautiful pictures, such as this stunning structure of a protein

a protein, then ball and stick representations just look like so many entangled bead necklaces, while space-filling models engulf the interesting parts of the structure in a seemingly amorphous mass.

Proteins have their own library of motifs, which are incorporated into visualisation packages. A ribbon-like curl, a spaghetti string, and a flash of blue tape then represent regions of secondary structure, the alpha-helices, the long, plain stretches of amino acids, the beta-pleated sheets.

Some of the packages allow one to vary the parameters used to generate the protein model. For instance, they can be rendered as a flat ribbon, a shadowed 3D ribbon, or as a pure schematic where helices might be represented by chunky red cylinders and the beta-sheets as stark, pointing arrows.

Crystal structures too give little away of their internal symmetries when rendered as space-filling models. The polyhedral representation of co ordination possible with Materials Studio, the aptly named Diamond (http://www.crystalimpact.com) and other packages, is much more adept at providing chemists with a clear view of their material. It allows one to gloss over the details of atom shape and view the overall crystal stacking and packing of a compound.

So, what exists in reality? Visualisation tools produce beautiful pictures – impressions of the molecule, even cubist representations. Do they answer the question, 'What does a molecule look like?' Probably not. A molecular structure is a word in the language of chemistry. Much as you cannot sit on the word 'chair' so molecular drawings, no matter how sophisticated, are not the word themselves. What is certain is that chemists could do without molecular visualisations just as well as the rest of us can do without words.

David Bradley is a freelance science writer based in Cambridge; he can be contacted through his website at http://www.sciencebase.com

Current Challenges facing Information and Knowledge Management in the International Pharmaceutical Industry

43rd AGM of the Pharma Documentation Ring (P-D-R)

The Pharma Documentation Ring (P-D-R) held its 43rd Annual General Meeting (AGM) in Kent, UK during October 2001. The P-D-R is an association whose members represent the scientific information departments of the leading research and development-based pharmaceutical corporations. The 24 companies represented account for approximately 60% of the total global turnover of ethical drugs.

This year's meeting, hosted by Pfizer, was attended by delegates from over 30 different sites in Europe and North America. Given the tragic events of September 11th in the US, it is a reflection of the importance of this meeting to P-D-R representatives and their companies that so many members made a special effort to attend the meeting. Bristol Myers Squibb participated in a P-D-R meeting for the first time. Mr Anton Theodorou of PharmaTransfer hosted an informal reception for delegates prior to the official opening of the meeting.

In his opening address, Sandy Mullen (Bayer AG), the President of the P-D-R, discussed the omnipresent information explosion and the increasing use of the internet, the total amount of information available doubling every three to five years – the internet itself is expanding by 100% every three months. Nearly 60% of the US adult population now accesses the internet for an average of 10 hours each month. Although, much of the scientific information available on the Internet is of limited usefulness and questionable quality, the challenge to information/knowledge management professionals is to identify the useful sources via text mining and other techniques and thereby assist their users to find the solutions to the tasks at hand.

Just as the Internet is growing rapidly, so is the quantity of information held in corporate intranets. It is a major challenge to classify and organise this information more effectively to facilitate later retrieval, as well as to provide advice and training on what is relevant and where to find it. Improving information literacy within their organisation is becoming an important knowledge management activity in several P-D-R companies.

This year's meeting format had been restructured to enable delegates to participate in smaller groups on topics that had been identified as of strategic interest. Four topics were discussed in two parallel streams

- Future Information Department Roles
- Impact of New Emerging Information Technologies
- Global Information Management
- Measuring what we are doing in the Information/ Knowledge Management Areas

These more practical sessions proved particularly useful as there was a healthy and open discussion among delegates on the issues faced, the different approaches that had been tried, and an indication as to what had worked well and what had not. During these sessions, it emerged that a very broad set of new information-/ knowledge management-related roles were being established within individual P-D-R companies to deliver higher added value services to end users. There was overwhelming support for these strategic sessions to be held again in 2002 and the P-D-R Board agreed to identify further topics for discussion.

In the company reports sessions, the content of which is an excellent basis for informal benchmarking, it was apparent that several P-D-R companies continue to undergo major internal restructuring, as a result of further merger and acquisition activity in this very active industry sector. The larger companies are putting considerable efforts into establishing global licences with scientific and technical publishers and database providers,and an ever increasing number of electronic journals are being licensed and made available to R&D and other staff at all sites, particularly via the exploitation of linkage technology i.e. database records to e-articles.

Two external speakers gave presentations during the meeting. Clare Markillie (Editorial Development Manager, Pharmaprojects) described the changes that had taken place in Pharmaprojects to deliver improvements to the accuracy and timeliness of the information in this important drug pipeline file. Clare also went on to describe new web based solutions which will be made available to customers early in 2002. Rachel MacAdam (European Account Manager, Micropatent Inc.) outlined the enhancements that had been made to the patent coverage and full text search and display features of Micropatent. Rachel also reported that they were also

forming a number of alliances with other key information providers, to enable linking between the content from different sources.

P-D-R representatives had completed a questionnaire on electronic newsfeeds prior to the AGM. The analysis of the results showed that a large number of both fee-based and gratis services are being used within P-D-R companies. Each newsfeed service was assessed for content, usability and cost. In the streaming newsfeed section, Bloomberg and News Edge Insight were the preferred sources. In the Pharmaceutical News section, Scrip and Prous Daily Essentials were viewed as delivering the most comprehensive content, though Marketletter and Prous Daily Essentials were seen as the most cost effective sources. Marketletter had the most consistent overall rating in terms of coverage, cost and user-friendliness. An analysis of the information from these sources revealed that an increasing percentage of the content was freely available, though without some of the added value comment.

An important recent development discussed during the meeting was the adoption of the Directive on the harmonisation of certain aspects of copyright and related rights in the information society by the European Council of Ministers. The Directive entered into effect in June 2001, and member states have until December 22, 2002, to incorporate the Directive into National Law. The implementation of the Directive is likely to have cost implications for the Library Groups within P-D-R companies.

The 44th P-D-R AGM will be held on 8th – 11th October 2002, in Newmarket, Sussex, England and will be hosted by Glaxo SmithKline.

In summary, this was a highly successful meeting and a survey conducted amongst attendees indicated there had been, once again, a very high level of relevant and good quality presentations by P-D-R members and invited speakers.

This meeting is regarded by many participants as the major annual event of its type for the pharmaceutical industry.

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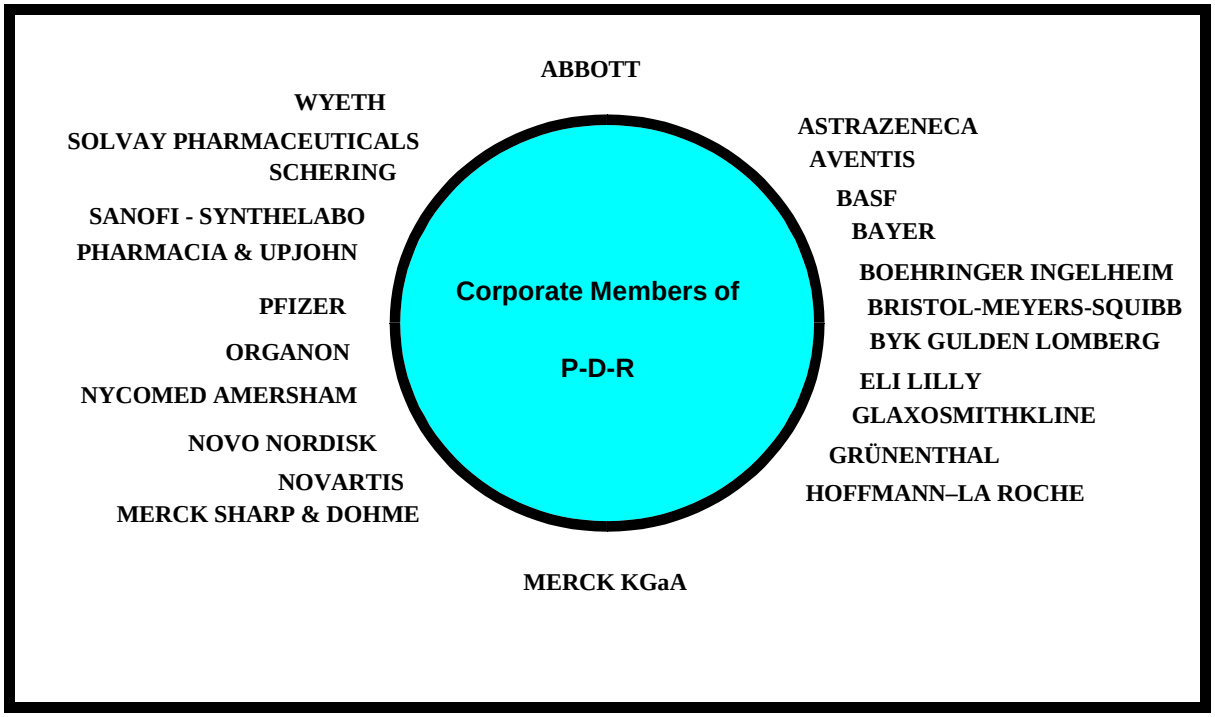

EVENTS 2002

April

3–5 April: Biomolecular Interactions: Molecular Graphics and Modelling Society Annual International Conference, with the British Biophysical Society Wills Hall, University of Bristol, Bristol, UK. Contact Dr. Adrian Mulholland, School of Chemistry, University of Bristol, UK. E-mail: Adrian.Mulholland@bris.ac.uk; website: http://www.chm.bris.ac.uk/enzyme/mgms/outline.html

7–12 April: 223rd American Chemical Society National Meeting, Orlando, Florida, US. Note that this meeting includes the CINF symposium (see page 3). Contact ACS Meetings Department, 1155 Sixteenth Street, N.W., Washington DC, 20036 US. Tel: +1-(202)-872-4396; fax: +1-(202)- 872-6128; e-mail: natlmtgs@acs.org; website: http://chemistry.org/portal/Chemistry?PID=\orlando2002\index.html

May

13–16 May: Beilstein Workshop Molecular Informatics: Confronting Complexity, Hotel Schloss Korb, Bozen, Italy. Website: www.beilstein-institut.de

13–17 May: 2002 MDL User Conference, Sheraton Inner Harbor Hotel, 300 S. Charleston, Baltimore, MD 21201. For more information, please contact: Valerie Lukecart, MDL Information Systems, Inc., 14600 Catalina Street, San Leandro, CA 94577. E-mail: valeriel@mdli.com

June

2–6 June: 6th International Conference on Chemical Structures, Golden Tulip Conference Hotel, Noordwijkerhout, Netherlands. Contact Dr. Guenter Grethe, MDL Information Systems, Inc., 14600 Catalina Street, San Leandro, CA 94577, US. Tel: +1-(510)-357-2222, ext. 1430; fax: +1-(510)-614-3616; e-mail: guenter@mdli.com; website: http://www.chemwebcom/docs/6iccs/6iccs.html. See also page 12

25–28 June: A Practical Introduction to Chemoinformatics, University of Sheffield. See opposite page

30 June–5 July: 9th biennial Gordon Conference on Computational Chemistry, Colby-Sawyer College, New London, New Hampshire, USA. Contact Dr. Bernard Brooks (brb@nih.gov) or Dr. William Swope (swope@almaden.ibm.com). Very preliminary information is available at http://www.grc.uri.edu/programs/2002/compchem.htm

July

31 July–2 August: Exploring Modern Computational Chemistry, Nottingham University/RSC Theoretical Chemistry Group (Faraday Division), University of Nottingham, School of Chemistry, Nottingham, UK. Contact Dr Jonathan Hirst, University of Nottingham, School of Chemistry, University Park, Nottingham, NG7 2RD, UK. Tel: +44-(0)115-951-3478; fax: +44-(0)115-951-3562; e-mail: jonathan.hirst@nottingham.ac.uk; website: http://www.nottingham.ac.uk/chemistry/emc2

August

4-9 August: Drug Discovery Technology 2002, IBC's Annual World Congress, Hynes Convention Center, Boston, MA, USA. Website: http://www.drugdisc.com/

18–22 August: 224th ACS National Meeting, Boston, MA, USA. See April for contact details

September

1–6 September: 4th European Computational Chemistry Conference (EUCO-CC4), Università di Perugia, La Cittadella, Assisi, Italy. Contact: Antonio Laganà, Dipartimento di Chimica, Via Elce di sotto 8, 06123 Perugia, Italy. Tel: +39-0755855515; fax: +39-0755-855606; e-mail: lag@unipg.it; website: http://www.chm.unipg.it/chimgen/mb/cong/EUCO-CC4/index.html

22–26 September: High Information Content Screening – 8th Annual Conference and Exhibition, Netherlands Congress Centre, The Hague, Netherlands. Contact: Society for Biomolecular Screening, 36 Tamarack Avenue, #348 Danbury, CT 06811, US. Tel: +1 203-743-1336; fax: +1-203-748-7557; e-mail: email@sbsonline.org; website: http://www.sbsonline.org

October

20–23 October: ICIC 2002 (International Chemical Information Conference), Nîmes, France. Website: http://www.infonortics.com/chemical/index.html

December

3–5 December: Online Information 2002, Olympia, 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.co.uk.

A Practical Introduction to Chemoinformatics

25–28 June 2002

University of Sheffield

Sheffield, UK

This intensive short course is intended to provide an introduction to the major aspects of chemoinformatics, with particular emphasis on applications in modern drug discovery. The course will comprise a mixture of hands-on workshops, lectures, and informal discussions. A key focus will be on the underlying rationale/theory, rather than teaching which buttons to press in a particular piece of software.

Two key learning objectives are:

What is the most appropriate method (or methods) to use for a particular problem?
Why does a particular method give a particular result?

Topics covered

- 2D databases and database searching (substructure search, virtual screening, property searching, similarity searching)
- Diversity and compound selection (clustering, DBCS, cell-based approaches)
- Moving into 3D: experimental data sources (small-molecule crystallographic data: CSD, intermolecular interactions: IsoStar, SuperStar, Relibase)
- Computational methods for 3D (introduction to molecular mechanics and conformational analysis)
- 3D databases (database searching, pharmacophore generation)
- Combinatorial libraries (molecular descriptors, diversity vs focused library design, lead- and drug-like concepts, enumeration and monomer selection)
- Analysis of high-throughput screening data (data mining, data visualisation)

Course Venue

The course will be organised and run within the Department of Information Studies at the University of Sheffield, which is recognised as one of the world's leading centres in chemoinformatics, and will take place in the Department's new chemoinformatics research laboratory. A variety of commercial software packages will be used for the hands-on elements of the course.

En-suite accommodation will be provided in Halifax Hall of Residence.

Course Tutors

The course tutors are Professor. Peter Willett and Dr Val Gillet from the University of Sheffield, Dr Andrew Leach from GlaxoSmithKline and Dr Robin Taylor from the Cambridge Crystallographic Data Centre. They have many years of practical experience in the field, in both academic and industrial environments. There will be ample opportunity for participants to discuss their own chemoinformatics problems with the tutors.

Course Fee

The registration fee of £600 covers all tuition, the necessary computing facilities and handouts, accommodation, meals and refreshments and the special course dinner on Thursday 27 June.

Registration

For more details please contact:

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Noordwijkerhout 2002

6th International Conference on Chemical Structures

The 6th International Conference on Chemical Structures will take place at the Golden Tulip Conference Hotel, Leewenhorst, Noorwijkerhout, The Netherlands from 2–6 June 2002. This conference, which continues the well-established conference series, brings together an international group interested in handling chemical structures and related topics. Participants discuss research and development in the processing, storage, retrieval and use of chemical structures. The conference fosters co-operation among organisations and researchers involved in the merging fields of chemoinformatics and bioinformatics.

The conference will open with a keynote address on Sunday afternoon, June 2, and will continue until lunchtime on Thursday, June 6. The main technical program will be divided into separate plenary sessions, taking place each morning. A new-product review session for commercial presentations and an extended poster session will be part of the scientific program. An exhibition featuring both commercially available software and also software from research projects and Special Interest Group (SIG) sessions will form an integral part of the conference.

Registration for the entire conference, including full board and four nights lodging, excursion and conference dinner, and conference proceedings is Euro 975 (currently about US$ 880) for single room accommodation. Student (Euro 150) discounts are available and a limited number of bursaries will be offered. Attendees requiring help for partial reimbursement of conference expenses should apply to the Guenter Grethe (guenter@mdli.com) giving the following information:

1. the amount and the reason for the request
2. a brief biography giving details of experience and current research work
3. a letter of support from a supervisor or colleague to justify your request

The registration form and full details of the conference, as they become available, will be posted on the web site at http://www.chemweb.com/docs/6iccs/structure.html