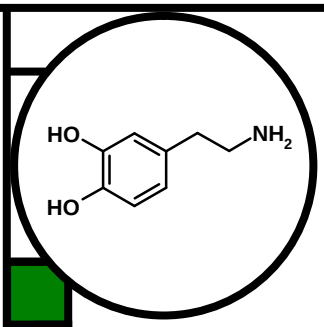
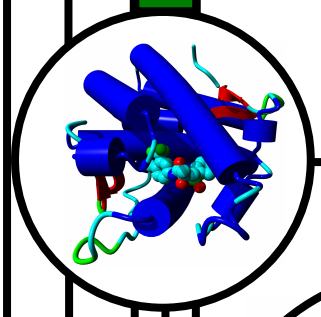
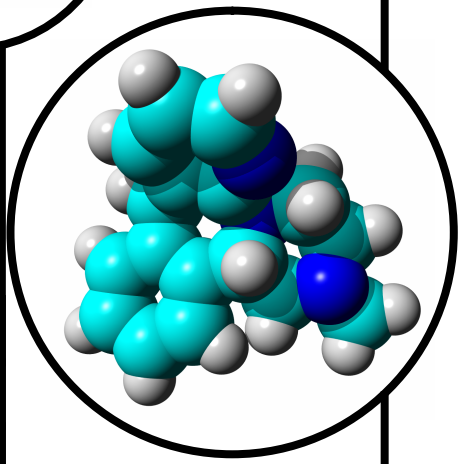


SEVENTH INTERNATIONAL
CONFERENCE ON

CHEMICAL STRUCTURES



Exhibitor Newsletter



June 5 - 9, 2005
Noordwijkerhout, The Netherlands

www.int-conf-chem-structures.org

Preface

Welcome to the Seventh International Conference on Chemical Structures!

This *Exhibition Newsletter* gives you a preview of the companies that will be exhibiting at the Seventh International Conference on Chemical Structures next week, the exhibition schedule, and information on the latest products showcased by these companies at the conference.

The technical program for the Seventh International Conference on Chemical Structures can be found on the conference web site at www.int-conf-chem-structures.org with the titles linked to the abstracts.

See you Sunday June 5th in Noordwijkerhout.

Cheers,
Bob Snyder, Program Chair
Markus Wagener, Vice Chair

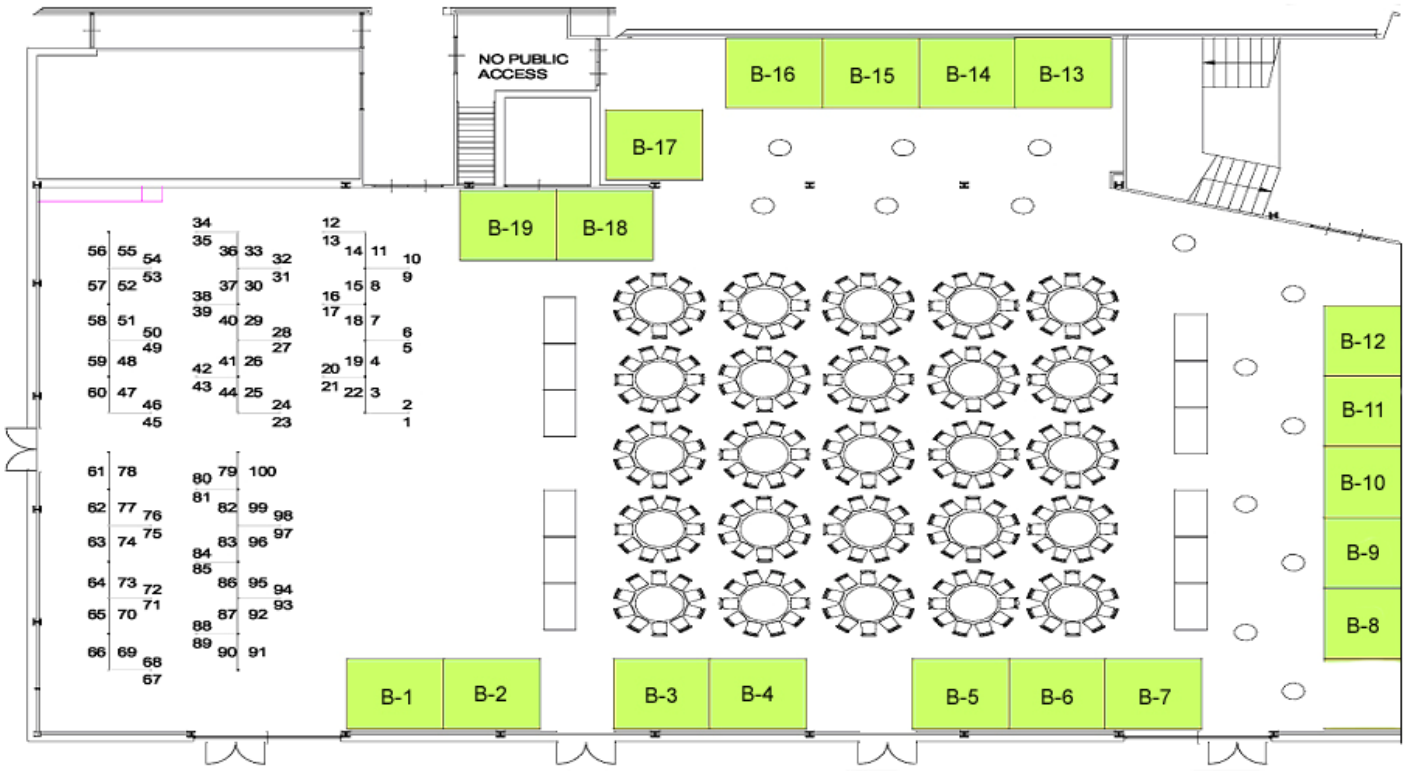
List of Exhibitors

Booth	Exhibitor	URL
B-1	Tripos	www.tripos.com
B-2	ChemAxon	www.chemaxon.com
B-3	Chemical Computing Group	www.chemcomp.com
B-4	Akos Consulting & Solutions	www.akosgmbh.de
B-5	CambridgeSoft	www.cambridgesoft.com
B-6	CAS	www.cas.org
B-7	FIZ CHEMIE Berlin	www.fiz-chemie.de
B-8	Elsevier MDL	www.mdl.com
B-9	Advanced Chemistry Development	www.acdlabs.com
B-10	Molecular Networks GmbH	www.mol-net.com
B-11	Barnard Chemical Information	www.bci.gb.com
B-12	Cambridge Crystallographic Data Centre	www.ccdc.cam.ac.uk
B-13	SciTegic	www.scitegic.com
B-14	Accelrys Ltd.	www.accelrys.com
B-15	Inte:Ligand	www.inteligand.com
B-16	COSMOlogic GmbH & Co. KG	www.cosmologic.de
B-17	OpenEye Scientific Software	www.eyesopen.com
B-18	Bio-Rad Laboratories, Informatics Division	www.bio-rad.com
B-19	Bioreason	www.bioreason.com

Exhibition Schedule

Monday	10:35	-	11:10	Morning Break in Atrium
	13:00	-	14:00	Lunch in Atrium
	15:50	-	16:30	Afternoon Break in Atrium
	16:30	-	18:30	Poster Session in Atrium
	18:30	-	19:30	Reception in Atrium
	19:30	-	21:30	Buffet Dinner in Atrium
Tuesday	10:35	-	11:10	Morning Break in Atrium
	13:00	-	14:00	Lunch in Atrium
	15:50	-	16:30	Afternoon Break in Atrium
	16:30	-	18:30	Poster Session in Atrium
	18:30	-	19:30	Reception in Atrium
	19:30	-	21:30	Buffet Dinner in Atrium

Exhibition Layout



1. Tripos
2. ChemAxon
3. Chemical Computing Group
4. Akos Consulting & Solutions
5. CambridgeSoft
6. CAS
7. FIZ CHEMIE Berlin
8. Elsevier MDL
9. Advanced Chemistry Development
10. Molecular Networks GmbH
11. Barnard Chemical Information
12. Cambridge Crystallographic Data Centre
13. SciTegic
14. Accelrys Ltd.
15. Inte:Ligand
16. COSMOlogic GmbH & Co. KG
17. OpenEye Scientific Software
18. Bio-Rad Laboratories, Informatics Division
19. Bioreason

ChemAxon

ChemAxon is a leader in providing Java based chemical software development platforms for the biotechnology and pharmaceutical industries.

By focusing upon active interaction with users and core portability, ChemAxon creates leading edge cross platform solutions to power modern cheminformatics and chemical communication.

Presentations at 7th ICCS

Making Real Molecules in Virtual Space P-9

High throughput virtual library enumeration using reaction rules to obtain chemically meaningful and synthetically feasible structures. The software uses our native Chemical Terms language to filter library output to refine structures generated.

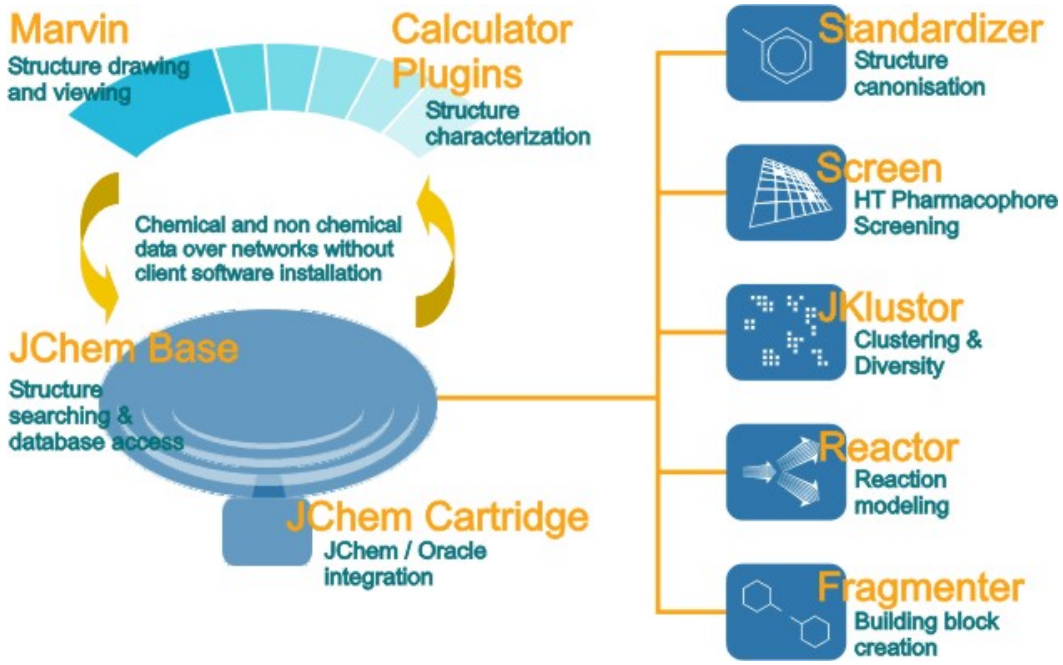
Advanced Structural Search Using ChemAxon Tools P-26

Substructure, exact, superstructure, MCS (maximum common substructure) and similarity searching is demonstrated via JChem Base and other tools (also available directly from Oracle environment via JChem Cartridge). Performance and relevance will be shown.

ChemAxon: Platform for Cheminformatics PR-6

Brief overview of ChemAxon's cheminformatics platform and introduction to recently launched toolkits. We introduce here our OpenGL based 3D structure visualization component, MarvinSpace, and invite comments and input during it's pre-product development.

Current product lineup



Current Calculator Plugin lineup

pKa ¤ logP, logD ¤ polar surface area (PSA) ¤ charge distribution ¤ polarizability ¤ topology analysis ¤ H-bond acceptor/donor ¤ major microspecies ¤ Huckel analysis ¤ refractivity

Free evaluation download available at our website

Free provision for teaching and academic research

Free for free web sites

Chemical Computing Group's
Molecular Operating Environment (MOE)™

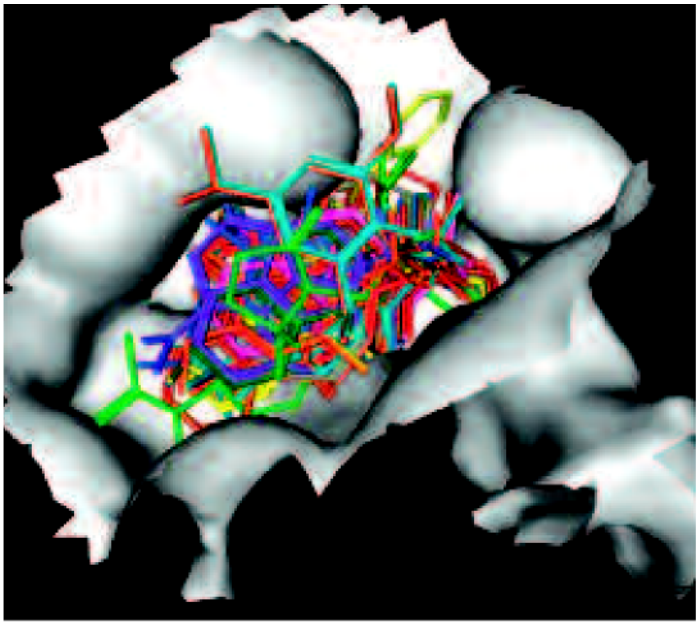
Chemical Computing Group, Inc. (CCG) is a developer and worldwide supplier of scientific software for Life Sciences. CCG's flagship software platform, MOE™ (Molecular Operating Environment), combines visualization, simulation and methodology development into a single integrated package. MOE 's collection of built-in applications, which include tools for protein modeling, molecular modeling, structure-based drug design, high throughput discovery, cheminformatics and bioinformatics, appeal to a wide audience of users ranging from computational experts to occasional users. MOE applications are built on the Scientific Vector Language (SVL), a high-level programming system designed specifically for life science application development. SVL allows users to customize MOE applications and to develop their own novel tools. Users are free to run MOE on a variety of hardware platforms and operating systems, including Windows, Linux, Mac OS X, IBM AIX, HP-UX, Sun Solaris, and Silicon Graphics Irix.

Protein Modeling and Bioinformatics

MOE's CASP-validated protein structure and bioinformatics applications are intuitive, easy-to-use and communicate seamlessly with other MOE applications. MOE's complete sequence-to-structure prediction suite integrates homologue identification, multiple sequence-structure alignment, conserved core analysis and structural refinement tools into a straightforward workflow that allows users to make more effective use of their 2D and 3D protein information. MOE also includes a structural family database that allows dependable functional inferences to be made between distantly related proteins.

Molecular Modeling and Simulations

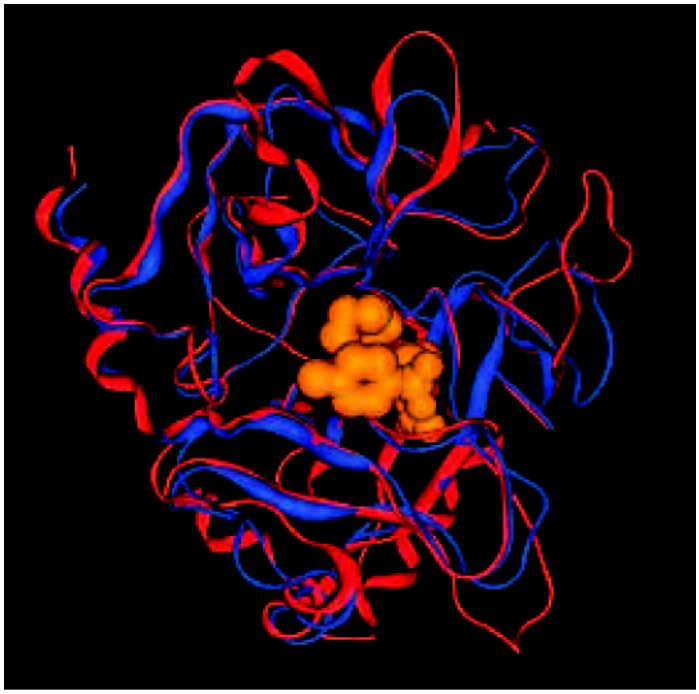
MOE's internal representation of organic chemical structures, and flexible architecture, provide a solid foundation for molecular modeling and computational chemistry. Intuitive molecular editors, file format handling, choice of



validated force fields, semi-empirical calculations, and superior modeling applications make for a fully scalable and customizable software package. Applications include molecular mechanics, diffraction simulation, molecular builders and data import/ex port, flexible molecular alignment and (high throughput) conformational search.

Structure-based Drug Design

MOE provides a collection of utilities for visualizing and understanding details of receptor active sites and receptor-ligand interactions. MOE applications for active site



detection, ligand-receptor docking, 3D pharmacophore searching, multi-fragment searching and probabilistic contact potentials can all be used to recommend improvements to known ligands or to screen ligand databases for candidate binders.

High Throughput Discovery and Cheminformatics

MOE cheminformatics tools include descriptor and fingerprint calculators, QSAR model building applications (including the patented Binary QSAR methodology), similarity searching methods, compound clustering algorithms, subset selection tools and a variety of data plotting options. Cheminformatics data can be conveniently stored in the proprietary MOE molecular database format, which allows for easy visualization and manipulation of numeric, character and 3D molecular data. Additional applications include an array of HTS-QSAR data analysis and focused combinatorial library design tools.

Unique Software Architecture

The majority of MOE's applications are written in the Scientific Vector Language (SVL), a built-in, chemistry aware programming language created by CCG. SVL application source code is provided in the distribution of MOE, allowing users to rapidly customize and modify existing applications, automate workflows, and create new approaches. The underlying architecture is inherently portable, allowing users to run MOE and SVL on a wide range of hardware (personal computers, workstations and heterogeneous clusters) and OS platforms.

CCG is based in Montreal, Canada, with offices in Germany and the UK. For further information, or for a free evaluation of MOE, please consult the CCG website at www.chemcomp.com for details on how to contact CCG.

CHEMICAL COMPUTING GROUP
Scalable Software. Scalable Science.

PASS: Prediction of Activity Spectra for Substances

The majority of known biologically active substances possess many kinds of biological activity, comprising of pharmacological effects, biochemical mechanisms of action, carcinogenicity, mutagenicity, etc. We often call this the biological profile. It is very difficult to screen every compound in all available biological assays; and as a consequence about 30% of projects fail because serious adverse or toxic effects are discovered too late.

PASS predicts the biological activity spectra on the basis of the 2D structural formula. This provides the opportunity to select compounds with desirable effects and without unwanted side effects in the early stage of drug discovery. PASS version 1.932.1 (January 2005) predicts 1000 kinds of biological activity with an average accuracy of 85% (leave one out cross-validation). Based on the calculated values of probability to be active and inactive (Pa and Pi respectively), one may define a flexible criteria for selecting the most promising leads with desirable level of novelty. Calculation of biological activity spectra for 100,000 compounds on a PC takes about 20 min. PASS can be effectively used to analyze large databases.

PharmaExpert helps to analyze the prediction taking into account a huge knowledgebase of activity-activity relationships. It provides the means for interactive selecting the most advantageous compounds. Structures are visualized using the Chime plug-in. Compounds can be profiled based on user-defined criteria. Selected compounds can be exported in SD-file format.

PASS CL is the command line version for inclusion in other in-house applications, or into programs like SciTegic's Pipeline Pilot.

The programs are working on PCs under Windows using MOL and SDF input formats; TXT, SDF and CSV output formats.

Contact: Dr. Alexander Kos
AKos Consulting & Solutions GmbH
Postfach 141
CH-4010 Basel
alexander.kos@akosgmbh.de,
www.akosgmbh.com

FIZ CHEMIE BERLIN
Fachinformationszentrum Chemie GmbH

Welcome at stand B-7
FIZ CHEMIE Berlin

ICCS 2005

FIZ CHEMIE Berlin (The Chemistry Information Centre) is a German information agency providing high quality information services concerning chemistry, chemical engineering and related fields to academia, industry and the general public.

General Activities

- Online and Inhouse Databases
- Multimedia Based Teachware
- eScience and Web Technology
- Printed Information Services
- Search Engines
- Data Inquiry by Order
- Workshops and Help Desk
- Internet Hosting
- Marketing Representative for the Chemical Abstracts Service for the German Speaking Countries

Main Products

• ChemInform	Reaction databases and reports in printed and electronic form covering synthetic organic and metal-organic chemistry
• Infotherm	Database with thermophysical properties of mixtures and pure substances
• Chemgaroo	Web based, interactive multimedia platform for education and advanced training in chemistry
• eScience	Web based infrastructures for scientific institutions, work-flow and project management, publication and archiving systems
• Search Engines	ChemGuide, MedPharmGuide and PublishersGuide: Expert searches in evaluated websites of chemistry, medicine, pharmacology and scientific publishers

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Elsevier MDL

Patents are an important and under-used source of information in chemistry and life sciences research. While many text-based systems already exist for accessing patent information, structure-based searching offers a more powerful and flexible way for scientists to mine this vast pool of important information.

To provide this capability, Elsevier MDL offers the new structure-searchable **MDL® Patent Chemistry Database**, a factual database indexing reactions, substances and their properties from organic chemistry and life science patent publications (World and European since 1978, U.S. since 1976). For researchers, the new database offers compelling benefits, including:

- **More effective synthesis planning**
  Reactions have the complete reaction text from the patent and spectral data (peaks) from the reaction products. Reactions are classified with InfoChem ClassCodes to allow seamless linking to other DiscoveryGate® reaction databases.
- **Better bioactivity profiling and lead discovery**
  Bio- and medicinal chemists can export chemical structures and their numerical bioactivity data* (e.g. EC50, IC50, LD100) to SAR tables.
- **Easy relevance checking**
  Markush structures and reactions* are displayed together with the claims text in an easy-to-view format, enabling researchers to check the relevance of located patents quickly and easily. For quick reference to original patent documents, the Patent Chemistry Database includes the location (page number)* of reactions or substance properties in the patent document.
- **Access to complementary information**
  The Patent Chemistry Database can be used as a complementary database in prior-art-searches as it indexes more than 800,000 prophetic compounds since 1976 that are rarely covered elsewhere.

The Patent Chemistry Database is available on the **DiscoveryGate** content platform, which is now faster, simpler and easier to use, displaying hits as soon as they are retrieved and requiring fewer clicks and windows to achieve results. See www.discoverygate.com.

ELSEVIER

MDL

* For patent applications published from December 2003 onwards

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info@mol-net.com

Molecular Networks GmbH

Inspiring Chemical Discovery

Molecular Networks is a chemoinformatics company that provides tools, consulting and development services to the chemical, pharmaceutical and biotechnology industry. The company's core expertise is the handling and processing of chemical structures and files for chemical information, the modeling of biological and physicochemical properties and the handling and modeling of chemical reactions.

Molecular Networks' product portfolio includes a suite of software tools that are used by over one hundred customers and partners worldwide and cover the following areas of application (tools that are available as SciTegic's Pipeline Pilot components are marked with "PP"):

Handling and processing of chemical structures

- Controlling structural state & integrity **CHECK** (PP)
- Generating 2D coordinates **2DCOOR** (PP)
- Enumerating stereoisomers & tautomers **STERGEN** & **TAUTOMER**
- Generating 3D models and conformations **CORINA** (PP) & **ROTATE**
- Warehousing structures, conformations and data **C@ROL**
- Warehousing structures and data of biochemical pathways **BioPath**

Calculating and analyzing properties and descriptors

- Computing physicochemical, 2D, 3D, and surface-based molecular descriptors **ADRIANA.*Code*** (PP)
- Analyzing and modeling data **SONNIA**

Handling and processing of chemical reactions

- Designing synthesis **WODCA**
- Warehousing reactions **C@ROL**
- Warehousing reactions and data of biochemical pathways **BioPath**

Handling and processing of files for chemical information

- Converting and manipulating files **CONVERT** (PP), **TABLE** & **SPLIT/JOIN&MERGE**
- Drawing and printing **IMAGE** & **PAGE**

Free evaluation copies can be downloaded from Molecular Networks' web server at http://www.mol-net.com/php/profile.php.

Currently, Molecular Networks is directing its expertise and proprietary technology to expand its business activities in the areas of the prediction of chemical reactivity and synthetic accessibility of compounds. A new product range covering these areas will be available from 2005.

For further information, please come to meet Molecular Networks' representatives at the exhibition of the 7th ICCS at **Booth #10**, contact info@mol-net.com or visit the home page at http://www.mol-net.com.

Barnard Chemical Information Ltd

Chemical Informatics Software and Consultancy Services

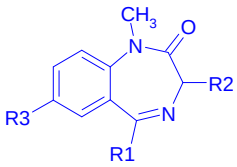
http://www.bci.gb.com

20 Years
1985-2005

Combinatorial Libraries

BCI's Markush technology for combinatorial library handling allows order-of-magnitude speed improvements over enumeration-based approaches. Virtual libraries of millions or even billions of compounds can be handled efficiently with features for

- ultra-fast enumeration
- fingerprint generation
- Lipinski and other properties
- topological indices
- full structure and substructure searching
- library overlap identification



R_1 = phenyl / cyclohexyl / ...
R_2 = H / methyl / ...
R_3 = H / Cl / NO_2 / ...

Toolkits

The full range of BCI's technology is now available as software toolkit components, which can be incorporated into users' own programs. Toolkit components are available for applications including

- fingerprint generation
- substructure search
- clustering
- diversity analysis
- Markush-based processing of combinatorial libraries
- query format conversion

An extensive range of operating systems is supported, and a number of language interfaces are available including C/C++, Visual Basic, Java and Perl.

Fingerprints

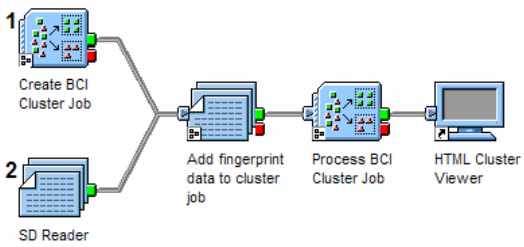
BCI's fragment-dictionary-based fingerprints have been found to perform well for both clustering and diversity analysis in several published studies.

Clustering

During its 20-year existence, BCI has been at the forefront of the development of clustering methods for large chemical datasets. As well as producing highly-efficient implementations of standard clustering methods such as Ward's and K-means, BCI has also identified and implemented novel algorithms such as "Divisive K-means", which allow datasets of millions of compounds to be clustered in reasonable time on modest hardware.

SOAP Servers

BCI's technology is now also available as SOAP services, which be called from any client supporting the SOAP protocol, such as SciTegic's Pipeline Pilot. Initially two servers are being offered, for fingerprint generation and for clustering, with a Markush server under development. A range of hardware and operating system platforms is supported, including processor farms for clustering of very large datasets.



Visit us at Exhibition Stand B-11

The Cambridge Crystallographic Data Centre: 40 Years of Service to the Scientific Community

www.ccdc.cam.ac.uk 40 1965 - 2005

Cambridge Structural Database

The CCDC originated from a small group set up in 1959 by J. D. Bernal and Olga Kennard, initially at Birkbeck College, London and from 1962 at the Chemistry Department in Cambridge, collecting data on organic and metal-organic crystal structures and using these to investigate intermolecular arrangements and forces. In 1965, the CCDC was formally established with a grant from the U.K. Office of Scientific and Technical Information. Data acquisition accelerated from then on, particularly after the introduction of the Crystallographic Information File (CIF) in the early nineties. Forty years on, the Cambridge Structural Database (CSD) contains 335,276 structures. Figure 1 shows the growth rate of the CSD for the period 1970 to 2004. At the current rate of growth, the 500,000th structure will be added to the CSD in 2009.

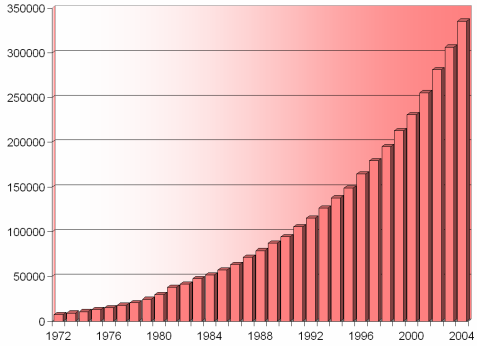


Fig.: Growth of the CSD 1970-1994.

CSD Applications

The first papers that made use of the CSD for fundamental research began to appear in the late 1970s. This type of research became more popular in the 1980s and has driven improvements made to the search and analysis tools (the CSD System). The CCDC maintains a web-accessible database of more than 1,200 published applications of the CSD System, as well as its other products, available from http://www.ccdc.cam.ac.uk/free_services/webcite/.

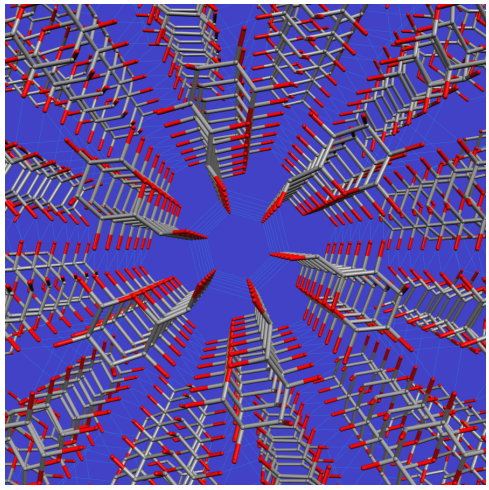


Fig. 2: Perspective view of β-D-allose (CSD refcode COKBIN).

CSD System

The CSD System comprises software for searching, visualising and analysing the valuable structural information contained in the CSD. Two structural *knowledge bases* are also supplied which allow instant access to inter- and intra-molecular geometric data derived from the CSD.

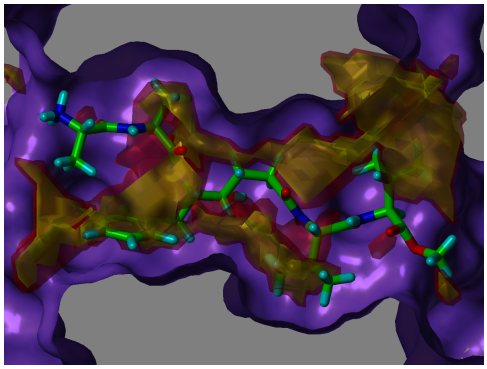


Fig. 3: SuperStar contour map of an HIV protease binding site (1AAQ) using aromatic CH probe. The ligand is a hydroxyethylene isostere of a substrate peptide.

Applications Software

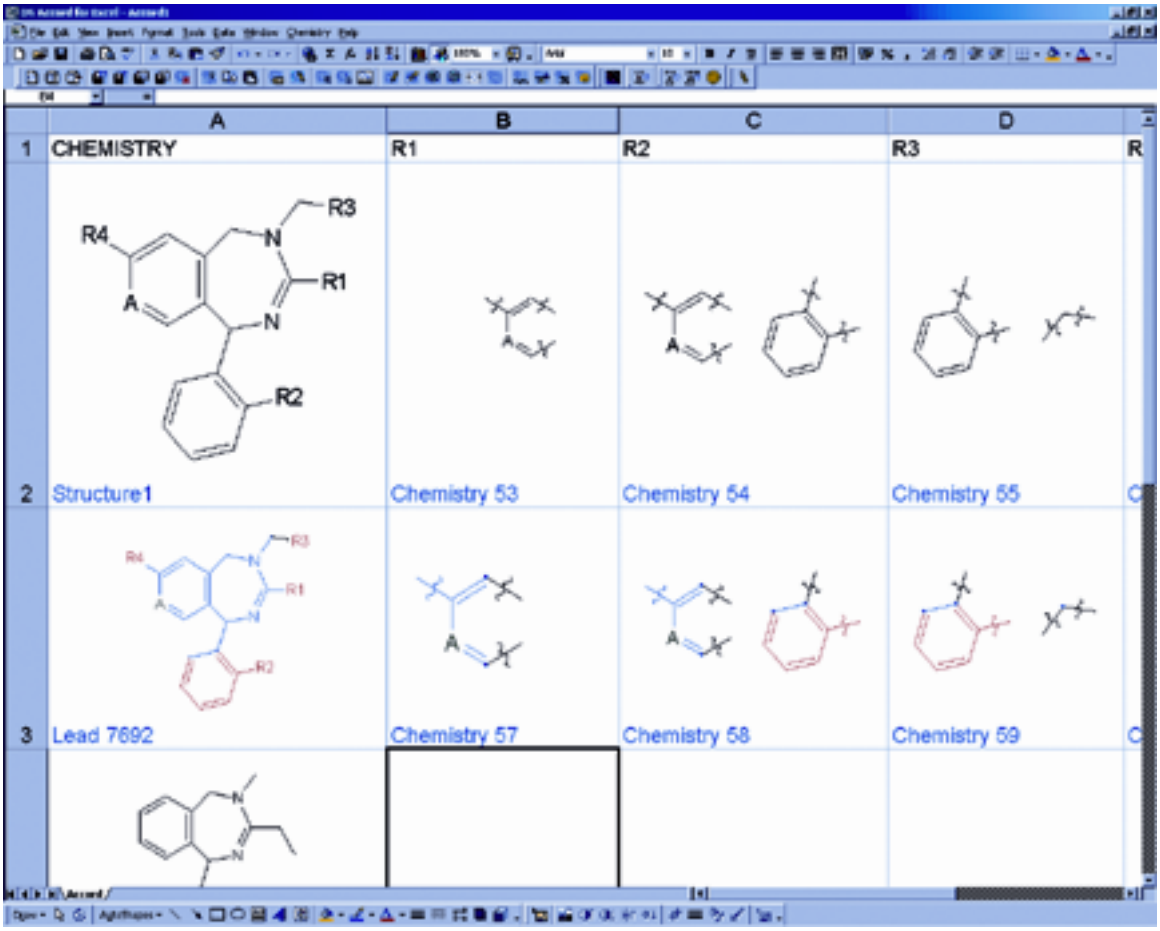
Recent years have seen the CCDC diversify into developing and distributing software applications for rational drug design (*SuperStar*, *GOLD* and *Relibase+*), and for structure solution from powder diffraction data (*DASH*). All of these products make use of crystal structure data from the CSD or PDB in some way, and all except *SuperStar* are being developed through collaborations with industry and academia.

We look forward to the next 40 years.

Chemically Intelligent Informatics Solutions from Accelrys

Accelrys (www.accelrys.com) develops and delivers innovative scientific software applications and services that help to solve critical R&D challenges. These applications include modeling, simulation, and informatics solutions that help transform the discovery and development of innovative pharmaceuticals, chemicals, and materials.

Accelrys, through its Accord product range, provides flexible, industry-leading informatics solutions that scale from the individual researcher to the enterprise, enabling the storage, mining, and analysis of chemical and biological data and information. The Accord software suite ranges from individual function-specific software components, to programming toolkits, desktop applications and enterprise-wide solutions, providing both off-the-shelf applications and tools to allow custom development.



Drop by the Accelrys booth (#B14) for a hands-on demonstration of Accelrys cheminformatics solutions and talk to our scientists about, amongst other topics, stereochemistry capabilities and Markush handling.

For a sneak peak before the event, visit www.accelrys.com/technologies/informatics/cheminformatics/

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Your partner for in-silico drug discovery.

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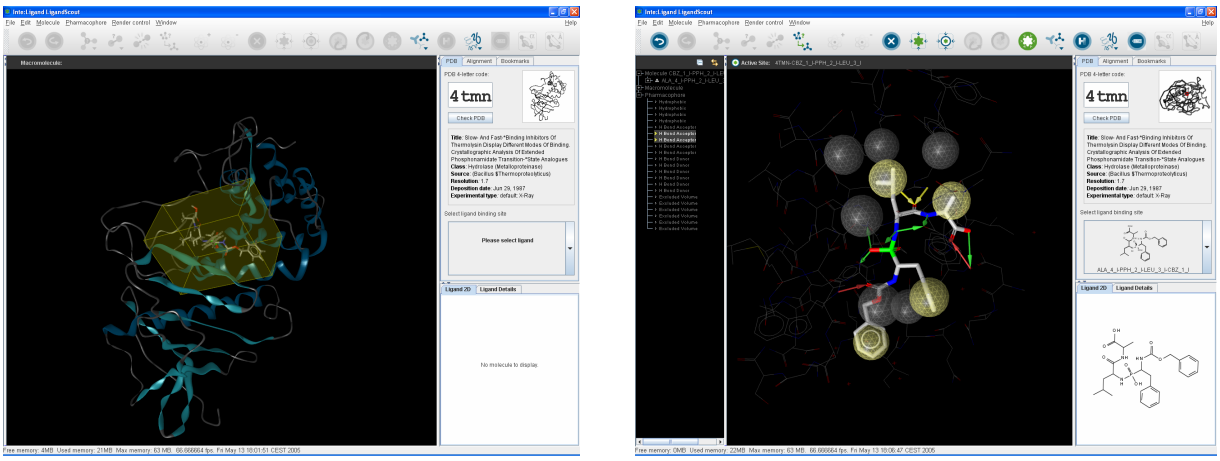
www.inteligand.com
office@inteligand.com

Inte:Ligand has specialized in the development of algorithms and software that support scientists in in-silico bio-activity prediction. Besides contract research services, we offer direct access to our software allowing high quality 3D pharmacophore modeling and virtual library generation.

Inte:Ligand's software: ilib diverse and preview of LigandScout

At the 7th International Conference on Chemical Structures Inte:Ligand is presenting its virtual combinatorial library generation software "ilib diverse" and giving a preview on its new pharmacophore modeling tool "LigandScout." ilib diverse is a software package for flexibly drafting and creating new libraries of drug-like organic molecules suitable for rational lead structure discovery. LigandScout allows the structure-based creation and editing of 3D pharmacophores describing the interaction of small organic ligands with macromolecular structures.



LigandScout screen shots

Visit us at **booth number #15**: Preview LigandScout, use ilib diverse, discuss with us and get your personal LigandScout mouse pad!

Products

- COSMOtherm: Software for Life Science and Fluid Phase Thermodynamics.
- COSMObase: Database of 3500 DFT/COSMO-files for common solvents and compounds.
- COSMOfrag: Software for rapid screening and HTS applications with COSMOtherm, including various options for structure and conformational analysis and tautomer generation.
- COSMOsim: Software for similarity search based on σ-profiles.
- TURBOMOLE: Fast Quantum Chemical Program (Prof. R. Ahlrichs, Univ. of Karlsruhe, redistribution and support by COSMOlogic).

Services

- Consulting in Computational Chemistry and Fluid Phase Thermodynamics.
- Contract calculations in the context of COSMOtherm.
- Contract reseach, development, and programming in Computational Chemistry related areas.
- General programming of interfaces and tools for Chemistry and Chemical Engeneering.

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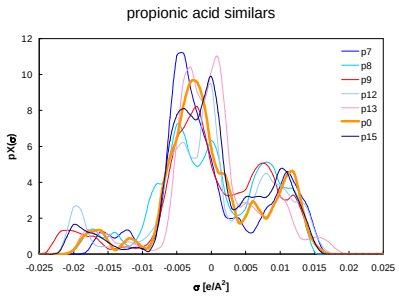
Web www.cosmologic.de

COSMOlogic GmbH & Co. KG

Your Competent Partner for Computational Chemistry and Fluid Thermodynamics

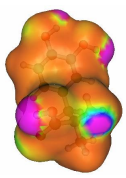
COSMOsim – Bio-isoster search based on σ-profiles

COSMOsim is a novel approach for the quantification of drug similarity which makes use of the surface polarities σ as defined in the quantum chemistry based COSMO-RS method. The histograms of the surface polarities, the σ-profiles, have been proven to be the key for the calculation of all kinds of partition and adsorption coefficients, and thus of relevant ADME parameters as solubility, logBB and many others. They also carry a large part of the information required for the estimation of desolvation and binding processes responsible for the inhibition of enzyme receptors by drug molecules. Consequently, a large degree of similarity with respect to the σ-profiles appears to be a necessary condition for drugs of similar physiological action. Driven by this insight, we have developed a σ-profile based drug similarity measure SMS for the detection of new bioisosteric drug candidates. In several examples and in a number of real drug design projects COSMOsim already has demonstrated its statistical and pharmaceutical plausibility, its practicability for real drug research projects, and its unique independence from the chemical structure which enables scaffold hopping in a natural way.

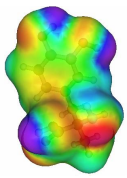


COSMOtherm – A novel access to solubility, partitioning, and molecular interactions for drug design and development

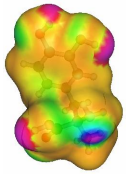
COSMOtherm is our approved program for the quantitative calculation of fluid phase thermodynamics based on quantum chemical COSMO calculations. Besides many features primarily developed for chemical engineering mixture thermodynamics, COSMOtherm allows for predictive calculations of many properties relevant for life-science research, as solubility in any solvent, partition coefficients between any solvents, and pKA. It has predefined models for blood-brain partitioning, intestinal absorption, albumin binding, and allows for the definition of other models. COSMOtherm now includes a graphical user interface and is subject to constant improvement and extension.



Methyldopamin colored by Intestinal Absorption



Methyldopamin colored by σ



Methyldopamin colored by Blood-Brain Partition Coefficient

OpenEye Scientific Software

1998

OMEGA

Omega remains the single most important product at OpenEye. Without a good sampling of conformers likely to be bioactive, all the techniques for assessing and quantifying shape and electrostatics are severely limited. By exhaustive sampling and comprehensive rotor enumeration, OMEGA provides the backbone to high-throughput molecular modeling at OpenEye.

1999

2000

FILTER

Filter began as an exercise, only to take on a life of its own as a useful tool for library preparation. Rewritten with OEChem, it can rapidly screen out compounds with undesirable physical or chemical properties.

ROCS

ROCS was the first search program to define molecular similarity purely on the basis of shape. Enormously fast, able to compare a thousand conformers per second, ROCS is the most useful program OpenEye sells.

VIDA

VIDA is OpenEye's primary visualization package. Designed from the ground-up as a program to inspect thousands of structures, either from docking or shape-analysis, VIDA was cross-platform and totally unique. Redesigned in 2004 to use OEChem, VIDA II will be released Summer '05.

2001

OEChem

In some ways, OpenEye's first professional software product. The result of six man-years of intense effort (half the company for two years), OEChem is arguably the best cheminformatics tool available. With wide support for file format interpretation and conversion, SMILES and SMARTS processing, 3D bond perception, protein and nucleic acid support, compressed file handling and comprehensive chemical expertise, OEChem became the code-base for all subsequent OE programs. OEChem, its Python and up-coming Java wrappers, are perfect for small-scale and industrial-scale programming.

ZAP

ZAP was OpenEye's first product. Combining ideas from Barry Honig on Poisson-Boltzmann electrostatics, Mike Holst on multigrid methods for solving elliptical PDEs, and from Andrew Grant on Gaussian representations of volume, ZAP was the first commercial PB solver of known accuracy. It also introduced solvent forces that could be included in dynamics or minimization.

FRED

Developed initially as a validation tool, FRED has become the only truly exhaustive docking tool for lead discovery. Capable of searching all possible alignments within an active-site of a given conformer in milliseconds, FRED has won a reputation as the most effective large-scale docking program.

EON

The sound of the other shoe dropping is EON. OpenEye has maintained a consistent philosophy that shape and electrostatics are the key molecular properties. While ROCS enables rapid analysis of shape similarity, EON compares external electrostatic fields using the alignment from ROCS and the potentials generated by ZAP.

2002

2003

SMACK

The Daylight SMARTS language is one of the most popular and most approachable means for describing chemical patterns. However, easy of construction does not mean efficiency of search. SMACK is a self-contained application that applies a canonical set of rules to improve throughput. SMACK. You know you want it.

WABE

The product of a unique collaboration within OpenEye, WABE is our first lead optimization tool. WABE takes a known structure and applies a set of local substitutions that retain the shape of the molecule, while varying the electrostatics. From a protein structure and bound ligand, it can automatically recalculate the electrostatic component of binding faster than the structures can be produced. In reviews of literature series, WABE was able to accurately reproduce trends found in medicinal chemistry.

QuacPac

A major concern at OpenEye is the bad application of electrostatics. Key to many physical interactions, such as protein-ligand binding, it requires considerable expertise and knowledge. QuacPac is a collection of programs that attempt to bridge the gap that often exists in the correct application of ZAP. The main application is molcharge, a simple program that will apply a variety of charging schemes, from force-field charging, e.g. MMFF, electronegativity schemes such as VC2003, up to semi-empirical methods such as AM1 and the highly accurate AM1-BCC. QuacPac also includes programs to enumerate tautomer and pKa states, protein pKas, molecular dipoles and simple electrostatic descriptors.

2004

Lexichem

Lexichem contains three core-technologies: the facility to depict a description of molecular connectivity (so-called 2D information), a complex set of rules to translate IUPAC names into SMILES, and the algorithms to reverse the process, i.e. take SMILES strings and produce accurate chemical names. Available in library form, Lexichem provides a mechanism of broadening the appeal and usability of OpenEye tools, as well as spurring us in new directions.

SZYBKI

It means 'fast' in Polish and is pronounced "Ship-key". Szybki is an efficient implementation of the Merck Molecular Force Field (MMFF) and can be applied to ligands, ligands in the context of a protein and to proteins. In the latter case, Szybki can 'regularize', i.e. optimize hydrogen positions, and check for correct HIS, ASN and GLN alignments. Applied to ligands, it allows the application of both MMFF and solvation forces from PB. Finally, ligand-protein interactions can be optimized with MMFF, PB and surface area terms.

AFITT

As OpenEye advanced into lead optimization, it was clear that crystallographic refinement utilizing the chemical and physics-based expertise at OpenEye would be of value. The AFITT project, a partnership with five major pharma, is set to deliver its first offering this summer. It will include real-time and real-space fitting using MMFF and electron-density shape, as well as OEChem information handling and OMEGA conformation generation.

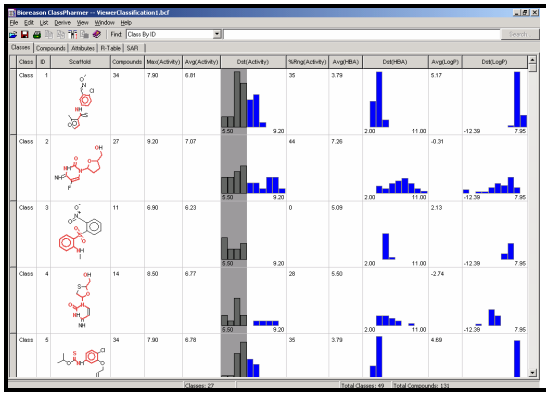
SAESAR

When there is little or no structural information on ligands of known, or suspected, activity, the OpenEye conjecture that shape and electrostatics are the key variables suggests that SAR ought incorporate both. SAESAR (Shape And Electrostatics SAR) is a tool that combines that ansatz with the statistical and clustering expertise of Mesa Analytics. Due later in 2005.

2005

ClassPharmer™ Suite

Intuitive Software for Screening Data Analysis, Hit-to-lead Development, Lead Optimization and Predictive Toxicology



ClassPharmer™ for *Intuitive Classifications*

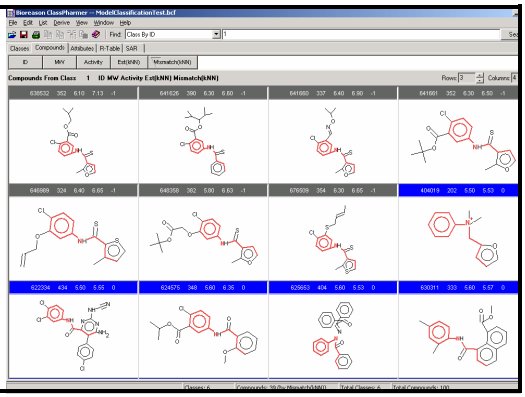
Benefit from Bioreason's **proprietary classification** algorithms on up to **100,000** molecules within a **very intuitive, easy-to-use graphical interface**.

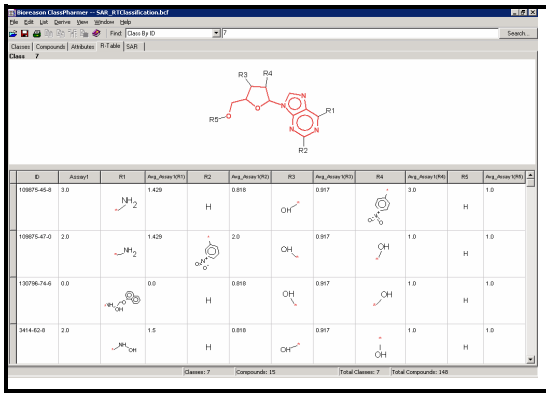
- **Learn novel scaffolds** and identify those that are well-known;
- **Rationalize library design** by considering **scaffold diversity**;
- **Identify mechanisms of action** from the classification.

ClassPharmer™ for Lead Identification

Benefit from advanced modeling and list generation capabilities facilitating **Lead Identification**.

- **Improve HTS triage** with **diverse** and **active-enriched** lists;
- **Detect false +/- more accurately** via **local** predictive models;
- **Find similar, predicted active compounds** from other libraries.





ClassPharmer™ for Lead Optimization

Benefit from Bioreason's **proprietary Rtable generation and SAR extraction** algorithms for efficient **Lead Optimization**.

- **Understand R-group information** via scaffolds with **R-tables**;
- **Extract SAR/SPR rules automatically** for all R-groups;
- **Examine** particular **toxicophores** from SPR exploration;
- **Test virtual compounds** derived from learned hypotheses.

Visit booth 19 at the 7th ICCS in Noordwijkerhout, June 5-9, 2005

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