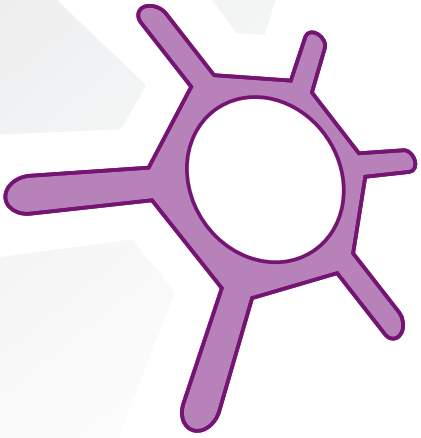


ICCS

International Conference
on Chemical Structures

9th International Conference on Chemical Structures

June 5-9, 2011 ◆ Noordwijkerhout ◆ The Netherlands

Exhibitor's Newsletter

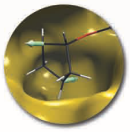
www.int-conf-chem-structures.org

MOE

MOLECULAR OPERATING ENVIRONMENT

MOE is a fully integrated drug discovery software package. MOE runs on Windows, Linux, Unix, and Mac OS X. MOE contain a toolbox for adapting existing and creating new applications. With MOE, molecular modelers, medicinal chemists and occasional users can benefit from sharing the same software system.

MOE 2010.10 HIGHLIGHTS



Streamlined Interactive Modeling Interface

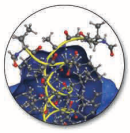
- Toggle ligands, proteins and surfaces on/off.
- Analyze and optimize multiple ligand:receptor complexes.
- Create surfaces, calculate properties and display substitution points.

Integration of NAMD Engine in MOE

- Export parameters and scripts automatically.
- Import NAMD trajectories into MOE database.
- Run simulations on a cluster with restart capability.

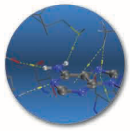
Structure-Based Medicinal Chemistry Transformations

- Transform molecules in 3D using reaction style rules.
- Refine structures in an active site and apply 3D filters.
- Integrated with scaffold replacement, fragment linking, growing and BREED.



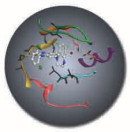
Enhanced Graphics

- Faster real-time GPU ray-tracing.
- 3D Stereo with anaglyph glasses.
- Clip molecular surfaces only.



Non-bonded Interaction Visualization

- Display H-bonds, CH...X, proton-π and VdW interactions.
- Show strengths or energies and set thresholds.
- Control visualization for ligand, receptor and solvent combinations.



Kinase Database and Explorer

- Search database of 3D aligned kinase structures.
- Add in-house structures with automated protocol.
- Browse kinases by core, pocket or canonical structural views.

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3D QSAR using Molecular Fields and Field Points

cresset
smarter chemistry | smarter decisions

Cresset produces software tools that enable chemists and biologists to gain better understanding of the biological activity of their molecules. Our products enable specific tasks, such as the generation of binding hypotheses from a series of active molecules in the absence of protein crystal structure data (e.g. GPCR or ion channel targets).

We are developing a new 3D QSAR product to enable the analysis of models of compound activities. These models are generated by aligning a set of known actives and creating sets of 3D descriptors for them (based on Cresset's unique molecular Field Points). The activity data are then analysed using the 3D Field descriptors (typically using PLS tools).

The Cresset 3D QSAR approach offers major benefits:

- The molecular alignments are not structurally biased – the alignment uses the Field Points for each molecule in a series against a single active conformer, or against a template created from a series of known actives.
- Fewer, more accurate descriptors - the descriptors are not grid-based, allowing the chemical features of the compound series to drive the sampling. This gives fewer but more accurate descriptor vectors for each molecule.
- The process is very rapid, allowing interactive feedback

Example Project : Analysis of Antagonists of a GPCR Target

Target – Human tachykinin receptor 3, (neurokinin receptor 3 or NK3), with pharmaceutical potential for treatment of a series of CNS disorders including schizophrenia.

Compounds – a series of 81 analogues derived by traditional medicinal chemistry from an initial starting hit "scaffold 1", by our collaboration partner Euroscreen. Testing against human NK3 assay show activity values (pIC50) ranging from 8.7 to 4.6 (equivalent to low nM to low mM activity).

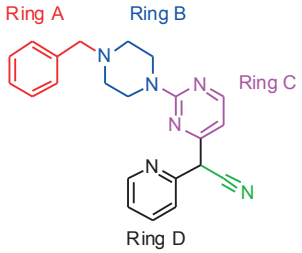

Figure 1. The key areas of the "scaffold 1" compounds for possible analogue exploration

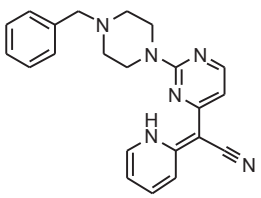

Figure 2. The actual enantiomer seen in proton NMR

Method: Generate a template for NK3 activity based on a FieldTemplater analysis of two of the most active "scaffold 1" compounds plus three other known NK3 actives. This yields a hypothesis for the active bound conformations of these molecules, which can then be used to generate an alignment for all 81 "scaffold 1" analogues.

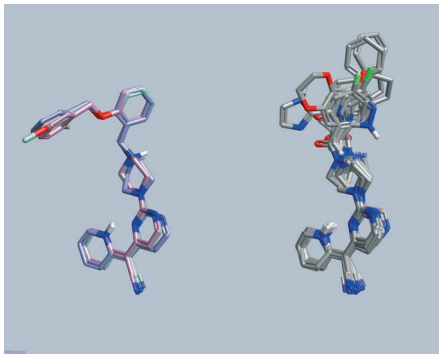

Figure 3. Template (left) and selection of aligned molecules (right)

Once we have generated the alignment for all 81 compounds we then generate a series of 3D descriptors for these molecules.

The descriptors are based on sampling the molecular Field values for each molecule at a series of points in space. The specific points used for sampling the field values are determined by analysis of the molecular Field Points associated with the whole series of molecules. These descriptor vectors, along with the activity data from the NK3 assay are then used in a statistical PLS procedure, which then yields a model of activity versus the descriptors.

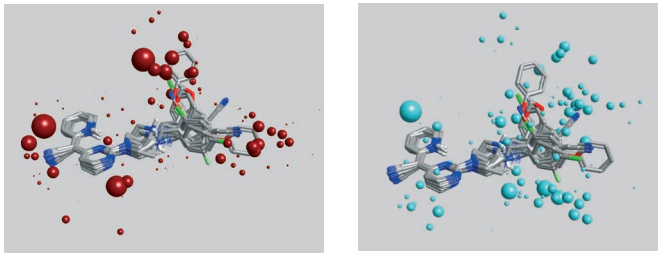

Figure 4. Areas where more positive electrostatic field is good (left), and in contrast where more negative electrostatic field is good (right).

Armed with this model we are now able to analyse the factors which lead some compounds to be more active than others.

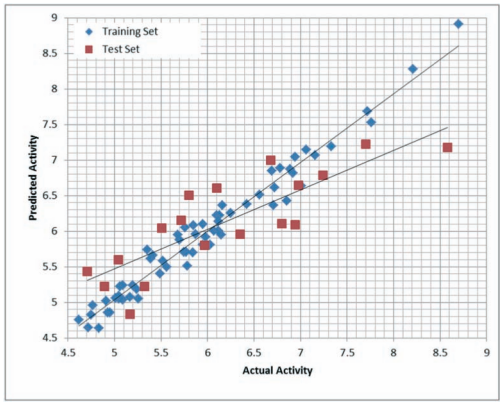

Figure 5. Model performance showing both Training set and an independent Test set of compounds

For more information please visit www.cresset-group.com

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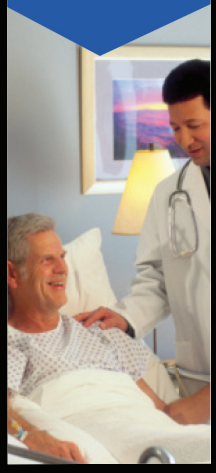

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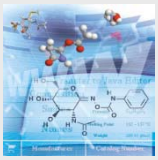
CORINA *et al.*

Molecular Networks at the 9th ICCS

Molecular Networks – maker of **CORINA** – offers innovative chemoinformatics software products, consulting, development and research services to increase the quality and productivity of discoveries in chemical, pharmaceutical and biotechnology R&D. Molecular Networks' areas of activities range from synthesis design of chemical compounds to the prediction of their chemical, physical and biological properties, their chemical reactivity and metabolic or environmental fate.

New Collaboration



Molecular Networks has recently entered into a Research Collaboration Agreement with the U.S. FDA Center for Food Safety and Applied Nutrition (CFSAN) to jointly develop the Office of Food Safety's food additives knowledge base CERES using Molecular Networks' chemoinformatics platform **MOSES**. The Chemical Evaluation and Risk Estimation System (CERES) is a centralized, chemical structure oriented knowledge base, which will establish a sustainable data/information management and storage system to provide decision support for both pre-market and post-market safety assessments for food ingredients and food-contact substances. Included in CERES is the development of structural alerts, computational toxicology and metabolism prediction models and structural categories for a threshold of toxicological concern approach to food ingredients.

New Service

Inspired by the collaboration with U.S. FDA CFSAN, Molecular Networks makes the core set of molecular descriptors of **ADRIANA.*Code*** publicly available to the scientific community. This core set, called **MOSES.Descriptors**, includes the most versatile and widely applicable descriptors in the areas of drug design, ADME and toxicity prediction, for modeling chemical reactivity and to support the use of computational tools in risk assessment of chemicals.

- **MOSES.Descriptors** and its application in toxicity prediction are presented on **poster P-50**

New Developments

CSRML (Chemical Subgraph Representation Markup Language) is a new, flexible XML-based specification to define chemical substructures that overcomes some of the limitations of the existing standards. In addition to a reference implementation, a graphical editor, Chemical Subgraph Editor (**CSE**), has been developed and is freely available to conveniently define, edit and annotate CSRML-based queries and documents.

- **CSRML**, **CSE** and its applications in Chemoinformatics are presented on **poster P-18**

Evergreens

- **CORINA** for generating high-quality three-dimensional molecular models
- **ROTATE** for exploring the conformation space and generating conformational ensembles
- **MN.Tools** for representing, processing and manipulating chemical structure & reaction information

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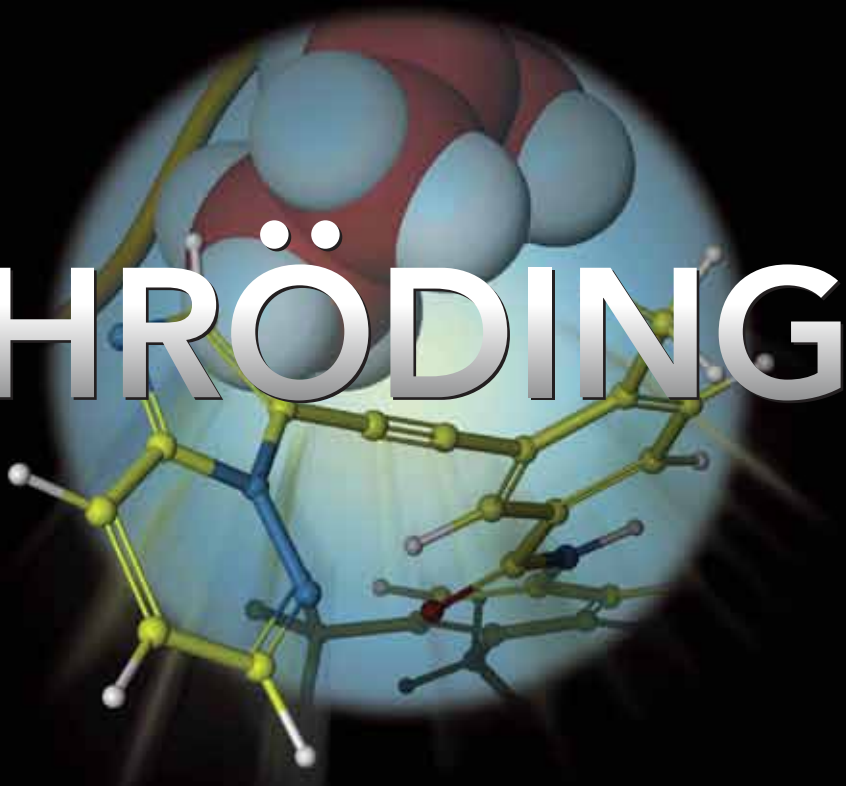

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Lead Optimization: cheminformatics using Canvas, 2D/3D QSAR using Phase, QikProp, and Strike, combinatorial chemistry using CombiGlide, fragment-based design using Glide, ligand-based design using Phase, structure-based design using CombiGlide, Glide XP, Induced-Fit Docking, Prime, absolute and relative binding affinity predictions using Desmond FEP, Prime MM-GB/SA, and MCPRO+

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Small Molecule Modeling & Simulations: conformation generation and clustering using ConfGen and MacroModel, Property Generation and filtering using LigPrep and QikProp, 1D/2D to 3D structure generation using Epik and LigPrep, molecular mechanics using MacroModel, molecular dynamics using Desmond, quantum mechanics using Jaguar

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Expect Actives: BioSolveIT's New Tools!

- HYDE Affinity Assessment: *Predict and Understand Binding!*
- ReCore Fragment-Based Design: *Grow, Link, Merge on-the-fly!*

Affinity Assessment with HYDE

Small molecule affinity estimation with HYDE is the state-of-the-art, award-winning approach to see IF and WHY something binds - or why it doesn't bind.

Patented by Bayer and Hamburg University, this approach integrated into BioSolveIT's LeadIT suite will suppress false positives drastically - resulting in unrivaled hit rates.

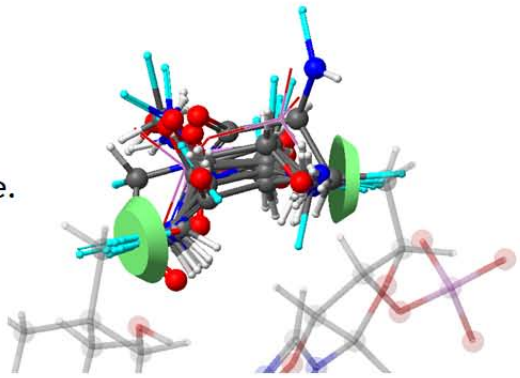
Come see the new affinity predictor HYDE at our booth.

Fragment-Based Design with ReCore

ReCore replaces or finds fitting fragments for a query within seconds.

Typical query scenarios could be:

- We have two binding fragments in two subsites.
  How can we link or merge the two ?
- We have a fragment binding and another, empty subsite.
  How can we grow into this site?
- We have a molecule, but we don't like a part of it.
  How can we replace this part?



ReCore combines your inhouse expertise to solve these problems: It has been specifically designed to support team building between medicinal and computational chemists.

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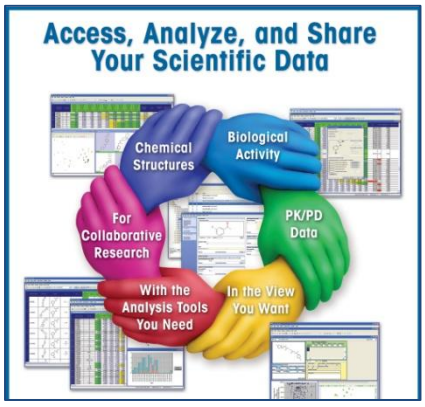

Discovery 360° (D360) is the first comprehensive product solution that provides life science researchers a single point of access to retrieve, analyze, and share scientific data. Eliminating time-consuming, error prone, non-productive hours that scientists spend merging and manipulating data from multiple, disparate sources, D360 provides quick and easy access to data and enables scientists to deal with data across projects, as well as within a given project. Using D360, assembly of a project SAR dataset can be reduced from hours to minutes, allowing researchers to spend more time at the bench. ***Learn more:*** ***www.tripos.com/discovery360***

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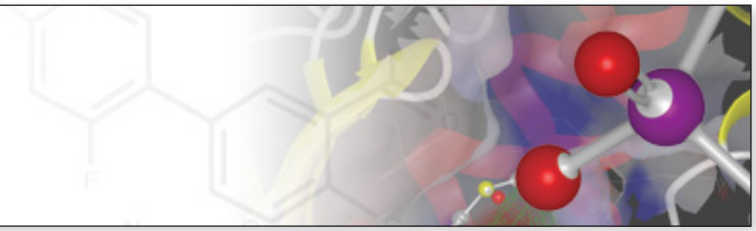


Come see our talk from Geoff Skillman, M.D., Ph.D. • **Wednesday, June 8 at 12:30 – 13:00**

"An Analysis of Fragment-Spaces and Their Impact on Fragment Replacement"

in the "Analysis of Large Chemistry Spaces" Session

OpenEye Scientific Software develops large-scale applications and toolkits for drug design and molecular modeling. The software is designed for scientific rigor, speed, scalability and platform independence. Its primary aim is virtual screening and lead-hopping. Areas of expertise include cheminformatics, conformer generation, docking, shape comparison, electrostatics, crystallography and visualization. Our latest application and toolkit releases include the following:

BROOD *Fragment replacement and molecular design*

BROOD assists in the exploration of chemical and property space around hit or lead molecules. BROOD fragment searching applications include core-replacement, side-chain enumeration, SAR expansion, property-directed optimization, filling holes in SAR, and patent breaking.

- Lead optimization and SAR expansion using fragment replacement
- 3D shape, chemistry and electrostatic fragment similarity
- Multidimensional analysis of very large property spaces
- Multiple criteria for selecting hits
  - Probability of activity
  - Synthetic accessibility
  - Fit to binding site
- Graphical interface for query customization in the active site, constraint generation, property analysis, and results visualization
- Custom interface for efficient analysis of results, includes hitlist cluster-viewer, protein-ligand interaction perception, 2D and 3D visualization, property visualization, probability of activity and favorites management
- Non-obvious bioisosteric replacement

SZMAP *Water…where it matters, when it matters*

SZMAP is a hybrid method that combines a single explicit probe water with a continuum water model to analyze the effects of moleular surfaces on solvent thermodynamics. In binding sites, a better understanding of these effects will improve lead-optimization and other aspects of drug design.

- Produces 3D grids mapping various thermodynamic quantities across holo, apo and ligand structures
- Performs very rapid calculations at specified sets of coordinates such as atom centers of bound ligands
- Includes a facility for integrating grids to quantify SZMAP results
- Prediction of changes in water activity on ligand binding
- Output of key waters and orientational preferences
- Variable resolution
- Results can be visualized in 3D using VIDA
- 2D Grapheme diagrams present SZMAP results in a format that is natural for a chemist
- Includes tools to convert output grids to different formats and perform various mathematical operations on grids

FastROCS *Real-time shape similarity for virtual screening, lead hopping and shape clustering*

FastROCS is an extremely fast shape comparison application, based on the idea that molecules have similar shape if their volumes overlay well and any volume mismatch is a measure of dissimilarity.

- Processes 2 million conformations per sec on a Quad Fermi box
- Returns overlays based on the quality of the 3D shape and color match against the query
- Overlays are intuitive and visually informative
- Available as a web service
- Jobs can be launched and the subsequent results viewed directly from within VIDA
- Reports rigorous shape and color tanimoto measurement

OEDocking *Docking with the lights on*

OEDocking is a robust suite of well validated molecular docking tools each specifically designed to address its own unique application to the docking problem.

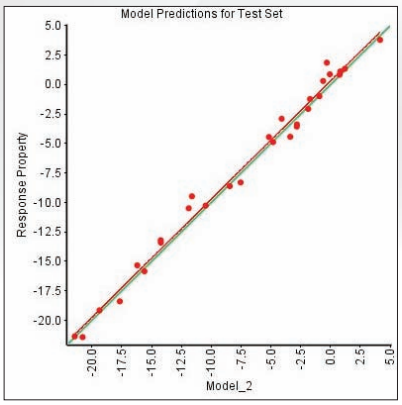
- **FRED** - *Fast exhaustive docking for virtual screening.*
  - Among the best (and fastest) docking programs available for structure-based virtual screening
  - Shown to produce the lowest variability in separate exhaustive studies of virtual screening methods.
- **HYBRID** - *Ligand guided docking for virtual screening.*
  - Takes advantage of reference ligand to guide the initial docking process
  - Significantly improved enrichment in cases where a reference ligand is available
  - Docking is hard enough, why throw out useful information?
- **POSIT** - *Cross docking and pose prediction.*
  - Directed pose prediction guided by one or more reference ligands in existing or related protein structures
  - Predictions accompanied by meaningful statistics assessing the quality and reliability of the prediction
- **OEDocking TK** - *Programming library for docking (C++, Python, .NET)*
  - All the functionality of FRED and HYBRID in toolkit form
  - Common and well supported framework for the development of new docking and scoring applications
  - Create custom docking network services

To learn more about our other Applications and Toolkits, please stop by our booth, or visit us at: www.eyesopen.com

Accelrys: focusing on science

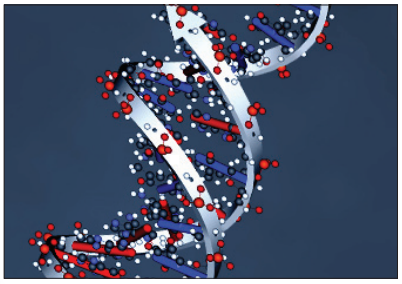
The new Accelrys Enterprise R&D Architecture draws on Accelrys' deep domain expertise in chemistry, biology and materials science; it combines the product portfolios of Accelrys and Symyx; and it leverages the Pipeline Pilot™ platform. The architecture offers customers a broad solution set of configurable applications for handling the diversity of science, experimental processes and information requirements encountered across the R&D value

Accelrys QSAR Workbench: Rapidly develop, validate and deploy QSAR models
Developed in a collaboration between the Accelrys Professional Services team and pharmaceutical company GlaxoSmithKline, the Accelrys QSAR Workbench is a commercially available, web-based solution that automates and accelerates the development, validation and deployment of predictive Quantitative Structure-Activity Relationship (QSAR) models.

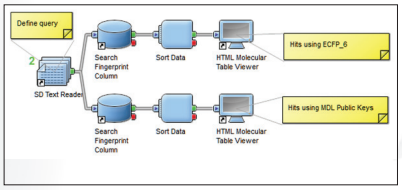


Built on the Pipeline Pilot platform, the QSAR Workbench utilizes native QSAR methods and easily integrates with other statistical tools—helping experts and non-experts alike save time, reduce costs, collaborate more effectively and speed research by leveraging robust, predictive models. The QSAR Workbench reduces modeling time from days to hours and enables chemists to make faster, better decisions.

Building Novel Applications with Pipeline Pilot to drive Next Generation Sequencing
The Next Generation Sequencing (NGS) Collection for Pipeline Pilot enables scientists and informaticians to build and perform complex analyses of DNA sequence information in dramatically streamlined fashion. Key benefits of the NGS Collection include simpler DNA sequencing workflows such as quality assessment and filtering, visualizing gene content or density, identifying and comparing SNPs and other variants and comparing RNA expression across experiments or individuals.



Access Accelrys Direct 7.0 using Pipeline Pilot 8.0: Collection Update 3
Pipeline Pilot's Component Collections are the "scientific building blocks" of the scientific informatics platform and are grouped by category of science or function. Collection Update 3 (CU3) extends the Cheminformatics Collection to integrate with the Accelrys Direct 7.0 data cartridge (previously Symyx Direct). The new components cover all aspects of creating, maintaining and searching structure and reaction databases in Accelrys Direct and include a comprehensive set of examples.



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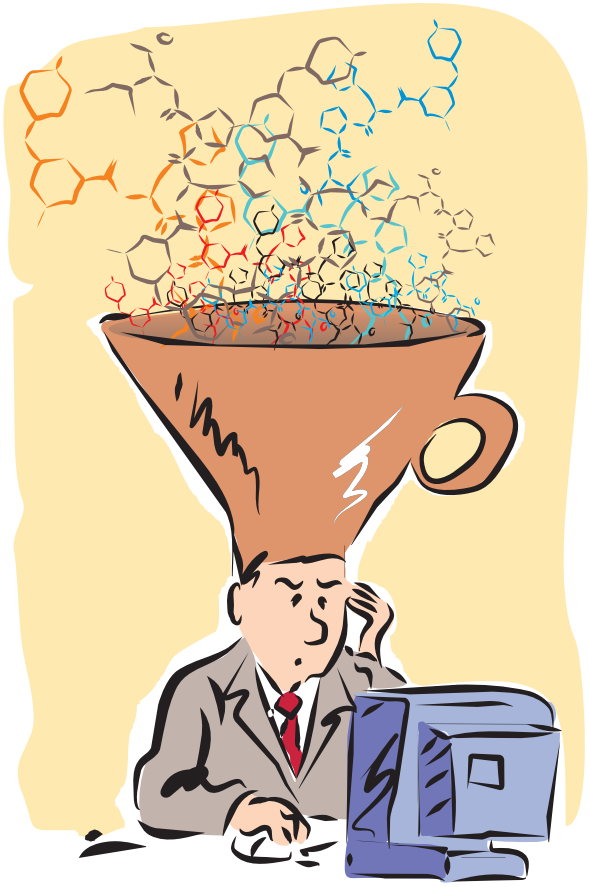

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Keymodule Ltd.

SimBioSys, Inc.

Focused on Research

Our focus is on the provision of leading edge drug design software tools for scientific research in the biotechnology and pharmaceutical industries. Our range of software applications include tools for structure-based de novo design of novel ligands and scaffolds, virtual high throughput screening (both protein- and ligand based), estimation of synthetic feasibility and synthetic route design, and automated mining of the chemical literature.

De Novo Ligand Design

SPROUT
- Sophisticated de novo design tool
- Design new hit molecules from scratch within the active site of your target
- Excellent synergy with fragment based hit discovery
- Predicts binding affinity and synthetic feasibility
- Recore as standard feature
- Proven record of success

SynSPROUT
- Generate synthetically accessible ligands by virtual chemistry within protein cavity
- Use a library of readily available starting materials (monomers)
- Editable reaction knowledge base

SPROUT-HitOpt
- Optimize hit compounds within the target's active site
- Synthetic constraints ensure only realistic structures are generated
- Two modes of optimization - core extension and monomer replacement

Chemical Document Processing

CLiDE Standard
- Extract molecules from documents one by one

CLiDE Professional
- Extract large amounts of molecules from documents by a simple mouse click

CLiDE Batch
- Extract molecules from documents in batch processing mode

Computer Aided Synthesis Planning

ARChem: Route Designer
- Full retrosynthetic analysis of target molecules back to readily available starting materials
- Reaction rules automatically extracted from reaction databases covering the full breadth of chemical literature
- Integrated with reaction databases for literature references and reporting
- Expandable starting materials collection, including the major chemical vendors

CAESA
- Rapidly estimate synthetic feasibility of target molecules
- Great addition to any de novo design pipeline

Flexible Ligand Docking and Scoring

eHiTS
- Fragment based flexible ligand docking
- Highly accurate docking
- The only truly exhaustive docking method
- Automated protonation state handling

eHiTS Score
- Statistically derived empirical scoring function
- Protein-family based score tuning for improved performance
- Tuning utility available for users to customize scoring function for the system of interest
- Reliably predicts activity in virtual screening scenarios

CheVi
- Molecular visualization suite - Interface to eHiTS docking
- Specifically designed to highlight the main ligand-receptor interactions and their eHiTS scores

QSAR Similarity Tools

eHiTS LASSO
- High speed ligand-based screening tool
- QSAR descriptor based on surface properties of ligands
- Trainable on small number of active ligands
- Conformation independent
- Ideally suited for scaffold hopping hit discovery

Contact us for more information about our software solutions and to arrange a free evaluation version of our products: info@keymodule.co.uk

CambridgeSoft from PerkinElmer For the Better

Visit the CambridgeSoft booth at the Ninth International Conference on Chemical Structures, chat with CambridgeSoft staff and get demos of our suite of industry-leading chemistry tools and applications.

ChemDraw – continues to set the standard for chemical structure representation, database input, query formulation and presentation quality graphics. And now with added biological content.

Chem3D – Chem3D brings workstation-quality molecular graphics and rigorous computational methods to your desktop. Integration with molecular analysis makes Chem3D the ideal software for chemists and biochemists. Features include state-of-the-art protein visualization, open GL graphics and stereo glasses, molecular mechanics and semi-empirical calculations with interfaces to MOPAC, Jaguar GAMESS and Gaussian

Chemical Nomenclature – our name-to-structure and structure-to-name algorithms continue to extend the range of names and structural types which can be handled correctly. We detect and flag ambiguous names and deal tolerantly and intelligently with reasonable but not-IUPAC-correct names.

Cartridge – the CambridgeSoft Cartridge stores molecules and reactions and provides the structure repository for CambridgeSoft's Enterprise suite. The CambridgeSoft Cartridge supports CDX, CDXML, Molfile, RXN, and SMILES formats making it flexible enough to be included with both new and legacy data, without the need for conversion.

E-Notebook – CambridgeSoft's electronic lab notebook is the most widely deployed ELN in industry, and through its flexible configuration it can be tailored to your specific workflows and UI requirements, whether you are a synthetic or medicinal chemist, an assay biologist or a DMPK researcher. You can get immediate personal productivity gains while building a sharable corporate archive of essential intellectual property.

KNIME - CambridgeSoft licenses, supports, and services the KNIME workflow platform in enterprise R&D environments, and works collaboratively with KINIME.com to tighten the integration of KNIME with CambridgeSoft products and deliver CambridgeSoft capabilities as KNIME nodes.

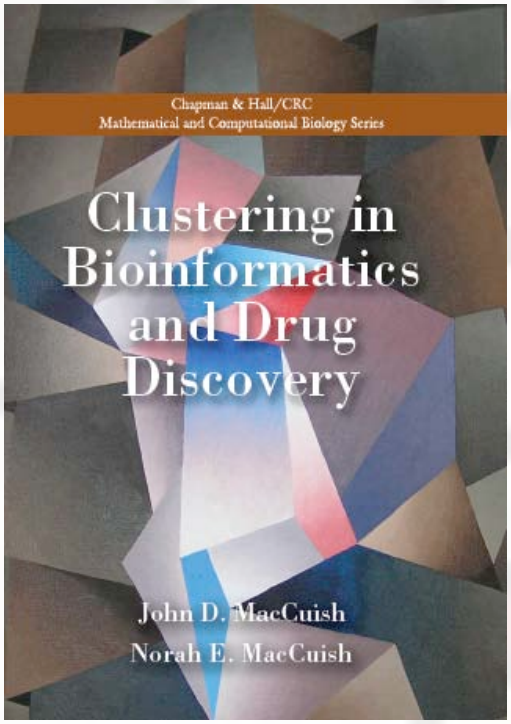
Chemical Structure Workflows – through a combination of our nomenclature tools, ChemScript chemical scripting language and KNIME, it is possible to automate, streamline and share many different chemical structure workflows including file reading, merging and comparison, property calculations, filtering and reporting and display.

ChemBioViz – the new search interface for the ChemBioOffice Suite, ChemBioViz uses the organizational power of DataViews to provide flexible views of underlying data, with configurable search screens. ChemBioViz provides form-, table- and card-views of search results for easy display and navigation, and includes plotting and filtering to speed exploration of data sets. ChemBioViz for Excel provides search and display from within Excel, and a new integration with Spotfire gives access to leading analysis and visualization tools.

MESA ANALYTICS & COMPUTING
Custom Data Mining Solutions

Mesa Analytics & Computing, Inc. provides R&D consulting services and software for clients outsourcing their complex problems in data mining and knowledge discovery, including areas such as cheminformatics, drug discovery, and compound acquisition. Mesa employs specialists in statistics, mathematics, computer science, software engineering, medicinal and computational chemistry to help companies design and develop custom solutions to their data mining problems. Mesa serves clients in the US, Europe, and Asia.

Recent Publication



"Clustering in Bioinformatics and Drug Discovery", Chapman & Hall, Mathematics and Computational Biology Series, 2010, by John and Norah MacCuish

Mesa Established 1999

by John and Norah MacCuish

SERVICES

We offer consulting and software expertise in data analysis and visualization including:

- Compound Acquisition
- Computational Chemistry
- Dynamic Web Applications
- Control Systems
- Simulation

We employ state-of-the-art tools and techniques, including:

- Statistical Modeling
- Cluster Analysis
- Anomaly Detection
- Chemical Diversity Analysis

SOFTWARE

GroupBase

Parallel and sequential clustering with similarity searching tools, from small (~1000s) to massive scale (many millions) with both 2D and 3D descriptors, or others

FingerprinterBase

2D key-based (320 and 768) molecular fingerprints

WebflowDD

Drug Design dynamic web application

New! ShapeBase

quasi-Monte Carlo integration based methods for molecular shape fingerprints, volume, alignment, and pharmacophore methods. Works with GroupBase

New! ChemTattoo3D

Open Source shape and phamacophore analysis

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A Better Way to Turn Data into Decisions

ACD/Labs provides chemical and analytical knowledge management that captures and utilizes the relationship between chemical structure and disparate forms of data. Our product portfolio includes a complete array of tools for the prediction of molecular physical and ADMET properties from structure; unparalleled accuracy in chemical nomenclature; and the unique capability to bring together disparate forms of analytical and chemical information.

Structure Based Property Prediction

- Predict an array of physicochemical properties including pK_a, log*D*, aqueous solubility, and solubility in DMSO
- Predict ADME properties such as P-gp specificity, oral bioavailability, passive absorption, and P450 substrates and inhibitors
- Predict toxicity endpoints including CYP inhibition, hERG inhibition, and genotoxicity
- Explore structure optimization to achieve desired physicochemical, ADME, and toxicity characteristics

Learn More

ACD/Percepta

Built on 16 years of expertise, the new generation of ACD/Labs' physicochemical and ADME/Tox software currently in development–ACD/Percepta–will combine our industry-standard tools into one platform. The single interface will provide entire organizations with consistent information, while making available different levels of detail appropriate to individual tasks, such as screening and profiling, advanced study of individual properties, and structure-based design.

ACD/Spectrus

Analytical and Chemical Knowledge Management

For more than a decade, ACD/Labs has excelled in bringing together disparate forms of analytical and chemical information. Building upon our unique ability to handle live analytical data and molecular structures in a chemically relevant manner, ACD/Labs is developing ACD/Spectrus, the next generation of software, to include:

- All-in-one processing, confirmation, and reporting software designed to assist in the interpretation of analytical, chromatographic, and chemical project data
- Powerful databasing for improved storage and retrieval of live spectral and chromatographic data, analytical and chemical information, reactions, and schemas
- The ability to easily customize and integrate with LIMS, ELNs, registry, and other software packages, making ACD/Spectrus an integral part of corporate knowledge management infrastructure on the laboratory or organizational level

Learn More

Visit us in the Exhibit Hall

ACD/Labs

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dotmatics

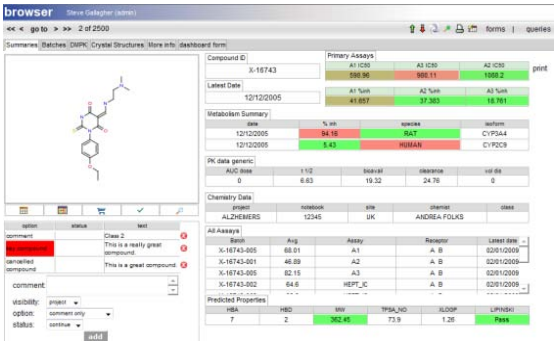
knowledge solutions

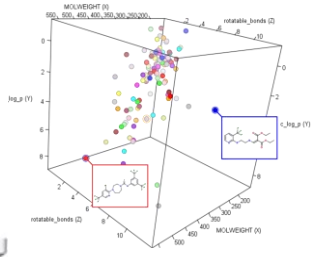
Dotmatics Informatics Suite: Information into Knowledge

Browser

Query and visualization tool for biological and chemical datasets. Key features include:

- Connect to any database or data architecture
- Search & query any data in the database including structures, text and numbers
- Built in spreadsheet, pivot table and report style data views. Simple exports to Word, Excel, Powerpoint, .csv, .sdf etc
- Simple form design





Vortex

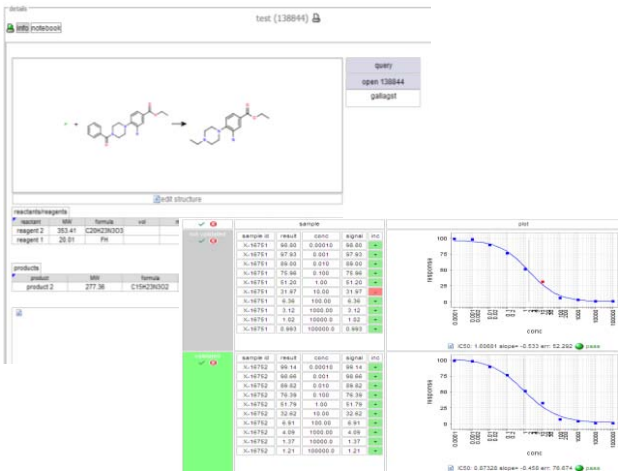
World-class visualization and analytics platform for scientific data. Key features include:

- Creating and manipulating plots
- Drill-downs and filters based on structures, text and numbers
- Chemical property calculation
- Simple extension with python scripts

Studies and Studies Notebook

The new standard in screening data management and Electronic Laboratory notebook. Key features include:

- Creating plate-based assays & ad-hoc experiments
- Managing, integrating & reporting from biological data
- ELN for Both chemistry and Biology scientists



Register

Web-based tool for single and batch compound registration. Key features include:

- Register chemical structure or macromolecule sequence data
- InChI codes handle duplicates and tautomers
- Upload and store QC data and lab book information

Gateway

A centralised solution for sharing information with colleagues and external collaborators.

dotmatics

knowledge solutions

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