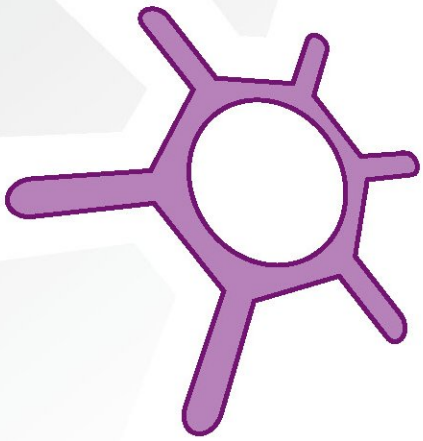


ICCS

International Conference on Chemical Structures

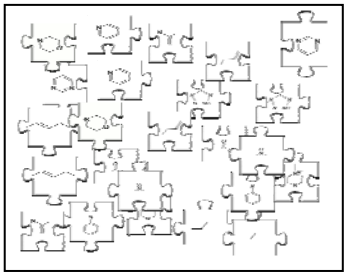
8th International Conference on Chemical Structures

June 1-5, 2008 ◆ Noordwijkerhout ◆ The Netherlands

Exhibitor's Newsletter

www.int-conf-chem-structures.org

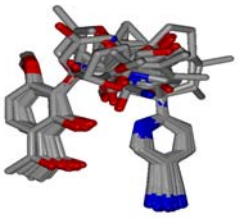
Visit us at Booth B9



BioSolveIT is a dynamic and established innovative leader in the virtual screening software market. The company supplies software and services to industry and academia, and has many established partnerships with pharmaceutical companies and world renowned academic groups. In recent years BioSolveIT have significantly improved and enlarged their software portfolio. Access to BioSolveIT software has immensely improved with tool specific GUI's and interfaces to popular software platforms such as MOE® and Pipeline Pilot®. In addition, the company now also specialises in providing one of the most complete, diverse and highly efficient software offerings available for *de novo* drug design.

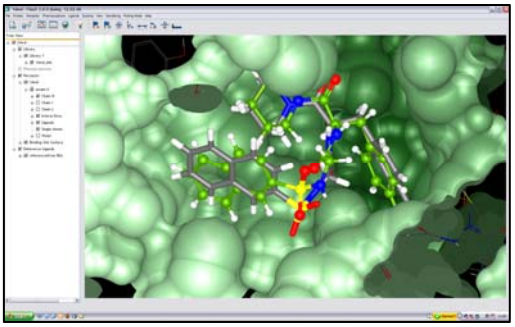
The company's core software offerings cover the following areas of virtual screening:

De Novo & Fragment Based Drug Design

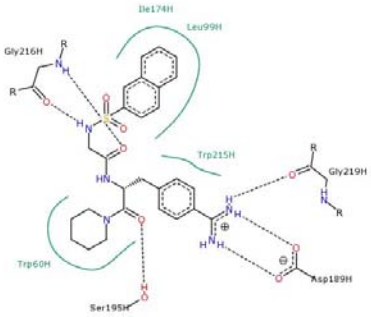


CoLibri: generate, manipulate and maintain your fragment spaces
FlexNovo: sensible fragment & docking based novel compound generation
FTrees-FS: invest 5mins to search 10^{18} virtual synthesizable products
ReCore: instant scaffold replacement & fragment linking with 2 clicks

Structure-based design



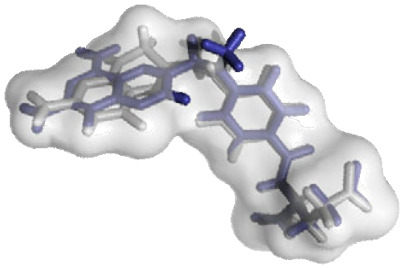
FlexX 3.0:
The best enriching docking engine has just gone graphical:
* docking speeds of less than 1 second per compound
* protein flexibility * pharmacophores, * combinatorics **...**



PoseView – visualize protein-ligand complexes at an atomistic level

DDB – An integrated, Oracle based platform for docking analysis

Ligand-based screening

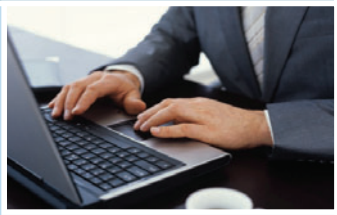


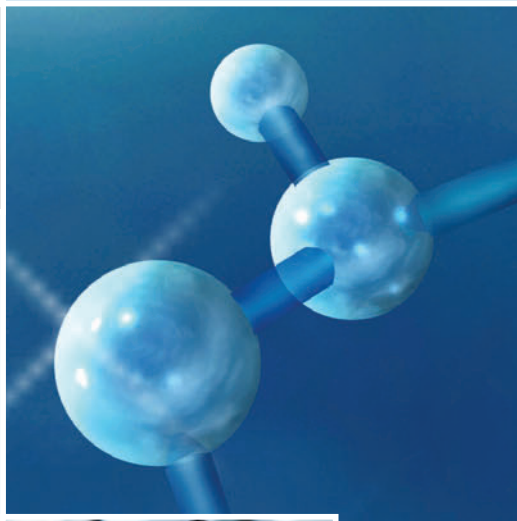
FTrees: orthogonal scaffold hopper to diversify your hits
FlexS – 3D molecular alignment for 3D QSAR, compound mimic design and virtual screening

BioSolveIT GmbH
An der Ziegelei 75
53757 Sankt Augustin

Phone: +49 2241 25 25 0
Fax: +49 2241 25 25 525

Email: contact@biosolveit.de
Web: www.biosolveit.de





CAS: the Leading Source of Chemical Information

CAS, a division of the American Chemical Society, is the global leader in chemical information, providing the most comprehensive databases of disclosed research in chemistry and related sciences.

CAS resources include the following databases and services:

- The world's most authoritative collection of disclosed chemical substance information, including the CAS Registry℠, incorporating records for more than 35 million organic and inorganic substances and more than 59 million sequences—CAS databases also contain records for more than 14 million reactions; the CAS Registry is the authoritative source of CAS Registry Number® identifiers, the recognized standard for identifying chemical substances;

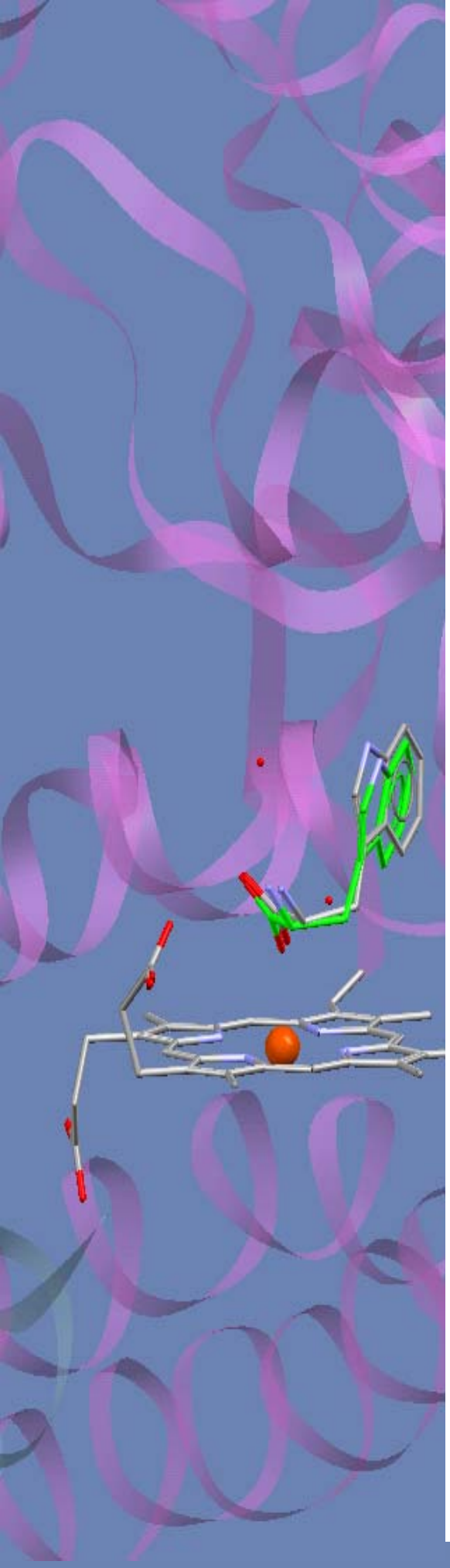
- CAS' comprehensive database of scientific literature: the only database of its kind that integrates information for both chemistry-related journal articles and patents;
- Search tools, including SciFinder®, for easy-to-use access to the wealth of scientific information in CAS databases, and STN®, the premier collection of scientific databases;
- For visualization and analysis, there's STN® AnaVist™, a breakthrough in patent and competitive intelligence analysis, and SubScape™ for visualizing and managing substance answer sets retrieved in SciFinder.

CAS makes information accessible to virtually any scientific researcher worldwide in industry, governmental research institutions, and academia.

For more information, visit **www.cas.org** or e-mail **help@cas.org**.

CAS®

A division of the American Chemical Society



www.ccdc.cam.ac.uk

The GOLD Suite

Intuitive Protein-Ligand Docking Package

The GOLD Suite provides all the functionality required to set up individual dockings or virtual screening runs, to post-process docking results and to visualise and manipulate structures in 3D, both pre- and post-docking. Raw PDB files can be set up for use within GOLD; no third party software is needed to prepare the binding site.

The GOLD Suite consists of:

- **Hermes** for comprehensive structure visualisation, structure editing, and for definition and calculation of descriptors post-docking.
- **GOLD** for protein-ligand docking.
- **GoldMine** for post-processing docking solutions.

Benefits of using the GOLD Suite:

- Easy to use interface with instructive wizard
- Features for protein preparation and pre-docking setup
- A choice of scoring functions
- Comprehensive post-processing tools
- Options for validating output ligand geometries and protein-ligand interactions
- Options for tailoring dockings

For further information, or to arrange a free evaluation, please contact Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK
www.ccdc.cam.ac.uk • Tel: +44 1223 336408 • Fax: +44 1223 336033 • Email: admin@ccdc.cam.ac.uk
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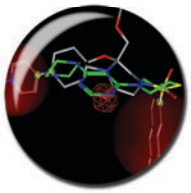
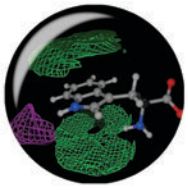
MOE

CHEMICAL COMPUTING GROUP
Scalable Software, Scalable Science.



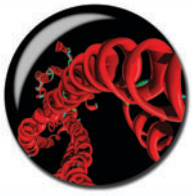
PHARMACOPHORE DISCOVERY

- Scaffold Replacement
- Pharmacophore Elucidation
- Pharmacophore Search
- High Throughput Conformational Analysis
- Pharmacophore Query Editor
- Pharmacophore Consensus



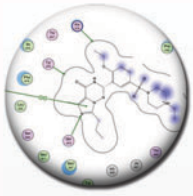
STRUCTURE-BASED DESIGN

- Active Site Detection
- Ligand: Protein Interaction Diagrams
- Molecular Surfaces and Maps
- Protonate3D
- Ligand-Receptor Docking
- Multi-Fragment Search
- LigX: Ligand Explorer



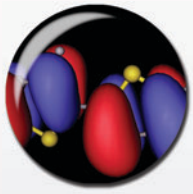
PROTEIN MODELING AND BIOINFORMATICS

- Protein Structure and Family Databases
- Fold Identification
- Structural Family Analysis
- Mutation and Rotamer Exploration
- Multiple Alignment
- Homology Modeling
- Structural Quality Assessment



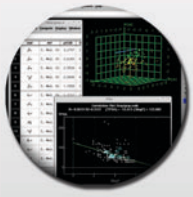
MEDICINAL CHEMISTRY APPLICATIONS

- MOE/web
- LigX : Ligand Explorer
- Ligand:Protein Interaction Diagrams
- Molecular Surfaces and Maps
- Scaffold Replacement
- Molecular Descriptors
- Flexible Alignment of Small Molecules



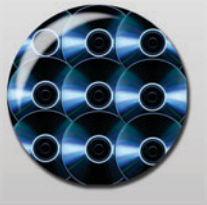
MOLECULAR MODELING AND SIMULATIONS

- Builders & Data Import/Export
- Molecular Mechanics & Dynamics
- Implicit Solvent Electrostatics
- Conformational Analysis
- Flexible Alignment of Small Molecules
- Diffraction Simulation
- Quantum Calculations



CHEMINFORMATICS AND QSAR

- SD Pipeline Command Line Tools
- Tautomer and Titration Enumeration
- Molecular Descriptors
- Similarity, Diversity & Fingerprints
- High Throughput Conformational Search
- QSAR/QSPR Predictive Modeling
- Consensus Modeling



HIGH THROUGHPUT DISCOVERY

- VSA Descriptors
- HTS-Binary QSAR
- Focused Combinatorial Library Design
- Diverse Combinatorial Library Design
- Combinatorial Library Enumeration
- RECAP Analysis and Synthesis

METHODS DEVELOPMENT AND DEPLOYMENT

- Scientific Vector Language (SVL)
- Background Computing
- Cluster Computing
- Platform Independent (Windows, MacOSX, Linux, Unix)
- Java Subsystem
- MOE/web

Contact us for a free evaluation of the new MOE release.

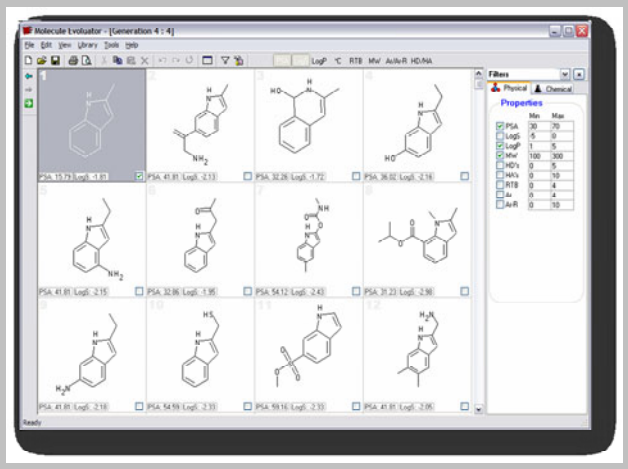
info@chemcomp.com | www.chemcomp.com | 514.393.1055

www.cidrux.com

Drug Discovery through Evolutionary Optimization

Drug design is still a daunting task, requiring innovation as early up as possible in the drug discovery process to reduce cost as much as possible. While the search space of drug like molecules, 10^{20} to 10^{60} structures in total, can never be inspected exhaustively, modern evolutionary search methods combined with the expertise of the medicinal chemist open up a creative path to success. CIDRUX' software products, the **Molecule Evoluator™** and the **Molecule Commander™**, provide an easy-to-use, powerful approach for creating and optimizing innovative structures.

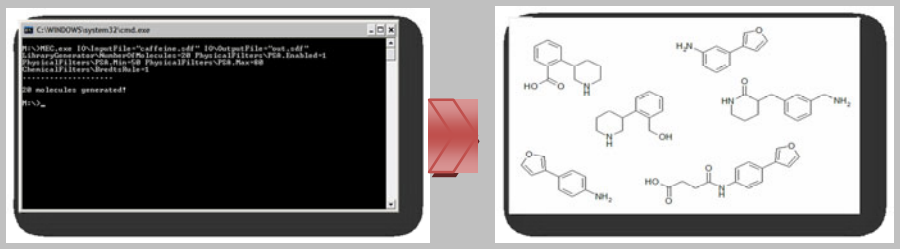
The Molecule Evoluator™



- ✓ Combines automatic and interactive creation of structures in an unprecedented way for finding novel chemical structures.
- ✓ Automatic calculation of physicochemical properties such as polar surface area, logP, logS, molecular weight, and others.
- ✓ Optional automatic filtering of molecules to generate only molecules with physicochemical properties within a predefined range.
- ✓ Chemical feasibility such as Bredt's rule, and the absence or presence of certain chemical groups can be controlled by the user.
- ✓ Interface for external structure scoring functions provided.
- ✓ Import and export of molecule structures and libraries in .mol and .sd file format.
- ✓ Easy to use, Windows™ user interface (Windows™ 2000 and higher).

Applications: New structure generation, lead optimization of proprietary molecules, structural differentiation away from competitor's molecules.

The Molecule Commander™



- ✓ Command-line based user interface, facilitating seamless integration into drug discovery workflows.
- ✓ Fully automatic library creation of new chemical entities.
- ✓ All chemical and physicochemical properties and filtering features of the Molecule Evoluator™ available.

Applications: Automatic generation of libraries of any size and desired physicochemical properties, „front load" generator for any drug discovery workflow.

About CIDRUX Pharminformatics:

CIDRUX Pharminformatics was established in 2002. The company focuses on supporting the lead finding and lead optimization process in the early stages of drug design. CIDRUX' software products, the Molecule Evoluator™ and the Molecule Commander™, offer a breakthrough in the interactive design of new molecules by means of state-of-the-art technology from evolutionary optimization and computational intelligence. The founders of CIDRUX, Prof. Dr. Ad IJzerman and Prof. Dr. Thomas Bäck, are world-renowned experts in medicinal chemistry and evolutionary computation, respectively. Our clients include Allergan (San Diego, CA), BayerSchering (Berlin, Germany), NIH (Bethesda, MD), and Vertex Pharmaceuticals (San Diego, CA) among others.

Visit www.cidrux.com for information on how to order our software products. If you do, download our Polar Surface Area Software – for you, for free.

Contact:

Cidrux Pharminformatics
Park Oosterspaarn 6
2036MB Haarlem
The Netherlands

info@cidrux.com
www.cidrux.com

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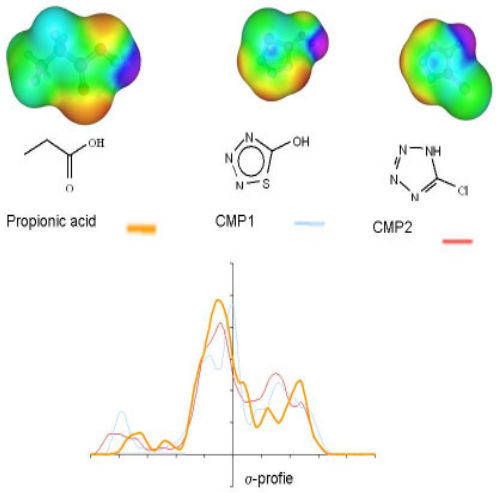
COSMOlogic GmbH & Co. KG
Your Competent Partner for
Computational Chemistry and Fluid Thermodynamics

Carsten Wittekindt and Andreas Klamt
COSMOlogic GmbH & Co. KG, Leverkusen, Germany
info@cosmologic.de www.cosmologic.de

Life Science Applications of COSMO-RS

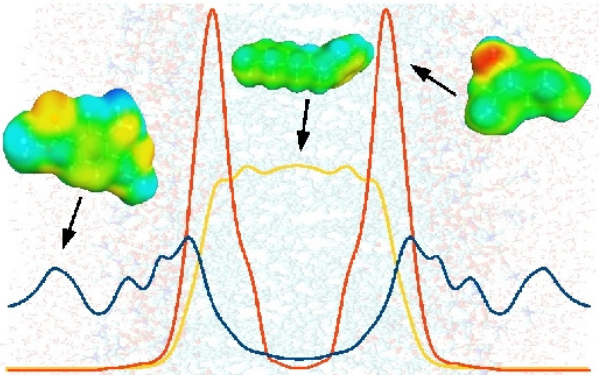
The **COSMO-RS** method gives access to a wide range of properties that are of interest for the life sciences industry. Models for the prediction of relevant ADME properties are available within our **COSMO*frag*** suite, which is of special interest for high throughput projects.

- Intestinal Absorption Coefficient
- Blood-Brain Partitioning Coefficient
- Human Serum Albumin Binding
- Octanol-Water Partition Coefficient
- Water solubility
- Abraham models



Our COSMO-RS theory has shown that the σ-profiles provide crucial information for most physicochemical behaviour. Suitable σ-profiles are a necessary (though not sufficient) precondition for good receptor binding. We therefore developed ***COSMOsim*** for bio-isoster search. Since the similarity search is based on surface polarity, not on chemical similarity, scaffold hopping is automatically included. Using **COSMO*frag*** we calculated the σ-profiles for 8,850,000 compounds retrieved from the PubChem database. It takes less than 30 min on 1 CPU to screen the database for similarity.

COSMO*mic* calculates the overall partition coefficient of chemicals in micelles and biomembranes as well as the internal distribution of the chemicals within such membranes. In the space of a minute it thus gives access to the description of processes like permeability, toxic effects of protonophores and washout rates of drugs which determine their half-life.



Graphical user interfaces are available for most of our software. In addition, COSMO*logic* is partner of SciTegic's Pipeline Pilot; components for standard applications are available.

We would be happy to welcome you at our booth (B12) and discuss how we can assist you in your special research.

COSMO*therm*, COSMO*frag*, COSMO*sim*, and COSMO*mic*

Fast drug design based on fundamental science. It's more than just QSAR!

CRESSET BIOMOLECULAR DISCOVERY

Cresset BioMolecular Discovery has developed unique technology to understand ligand-protein binding. We went back to basics and created the XED forcefield which redefines the electron distribution around a ligand, allowing us to generate accurate electronic, steric and hydrophobic molecular fields. These fields define what the protein 'feels' as a ligand approaches and what interactions the ligand can make with the protein.

Field technology can be applied throughout the drug discovery process, including:

- Hit-finding (via virtual screening)
- Finding the bioactive conformation of ligands (in the absence of target x-ray data)
- Qualitative field SAR
- Supporting H2L and LO through lead hopping and bioisoteric replacements

Cresset works with small biotechs and global pharma companies to find novel hits for their targets through screening only a few hundred compounds. We are the top global virtual screening provider, having undertaken >40 projects with an 80% success rate and hit rates commonly in the range 5-30%. A large diversity of chemotypes is found because we work with fields rather than chemical structure.

You can work with us on a consultancy basis or lease our software.

digital chemistry

See our posters P-21 and P-22, and join us at stand B3 for a Torus:Server demonstration, and to claim your free software

Torus:Server

Version 1.2.6 now available

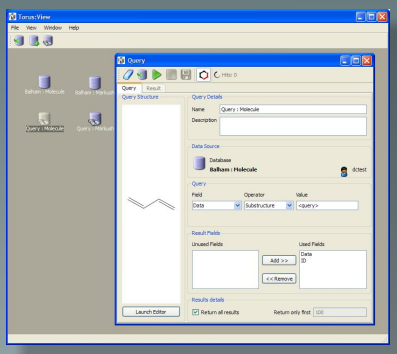
Oracle data cartridge (9i and 10g) for the storage and retrieval of both Markush and single-molecule structures

- Supports multiple, industry standard formats
- Molecule and/or Markush capable, **without** enumeration
- Transparent handling of chemistry types. Single columns may contain mixed Molecule / Markush structures, all in a completely open schema
- Functions for exact and substructure searching, property calculation, Markush overlap and enumeration

New in 1.2.6

- Improved indexing allows much larger and complex Markush structures to be handled more efficiently
- Improved property binning allowing vast Markush libraries to be evaluated in seconds

Torus:View



Torus:View Windows client for Torus:Server database

- Allows Daylight SMILES and ISIS/Draw query submission
- Tabular result set display of both Molecule and Markush hits
- Import of complex SD files into a Torus:Server database

BCI Toolkits

Version 7.14 now available

Comprehensive SDK covering a range of Cheminformatics functions

- Components available for Clustering, Diversity, Fingerprinting, Dictionary Generation and Molecule/Markush analysis. All components are fully integrated and allow seamless data transfer
- Clustering module allows vast datasets to be clustered in a number of hierarchical and non-hierarchical forms, both for binary and floating-point dataprints
- Markush/Molecule module allows property calculation, enumeration and searching from within vast Markush libraries - **without** enumeration
- Language support for C/C++, Java, PERL, PYTHON and Visual Basic
- Supports Windows, Linux and Solaris platforms

New in 7.14

- RGroup decomposition allowing Markush creation from sets of Molecules
- SMILES canonicalisation

Theilheimer

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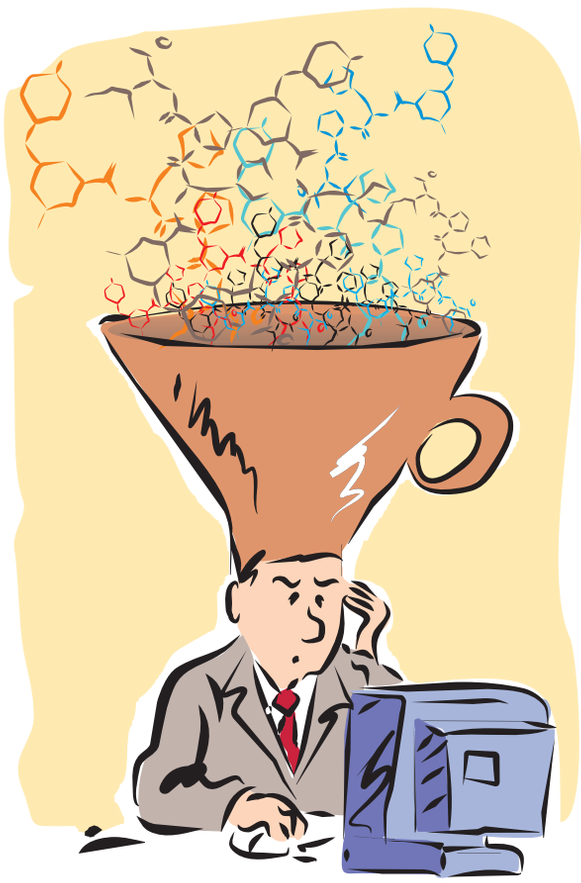
There are a plethora of tools available for data analysis, but very few reliable data sources.



Quality content which can be customized is difficult to come by.

Our Offerings

- **Target specific ligand databases with PK/PD and bioassay data**
- **Annotation of Chemical structures**
- **Indexing of chemical and assay data, from public and patent sources**
- **Structured and unstructured data mining (automated and manual)**
- **ADMET and Reaction databases**

We provide customised solutions and cost effective scalable resources, in the areas of Patent Chemistry Data Abstraction, Indexing of Markush Structures, and Annotation of Clinical, Pharmacological, Biochemical, Chemical and Pharmacogenomic Data.

Using extensive chemical ontologies and semantic data mining, coupled with our strong manual quality assurance methodologies, we are able to construct target and ligand specific knowledge databases from a variety of sources such as journals, patents and public databases.

Our unique delivery model combines elements of both onshore and offshore resourcing to ensure the highest levels of quality at a significantly lower cost than local alternatives.

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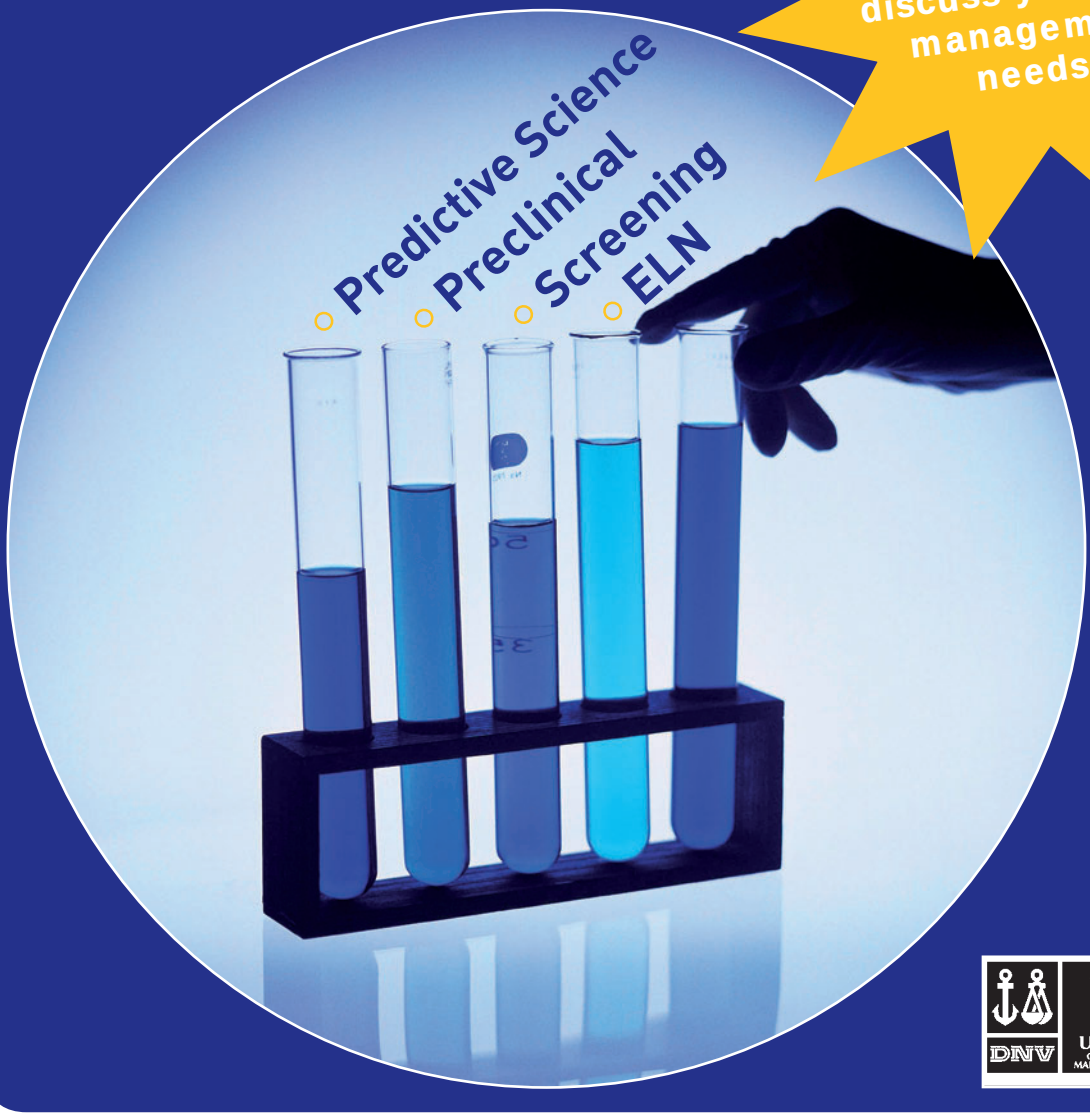
idbs

IDBS: multiple solution provider

IDBS provides quality data management software with services to match

One integrated framework for all your research data

Come to our booth # B7 to discuss your data management needs!



idbsSolutions

www.idbs.com

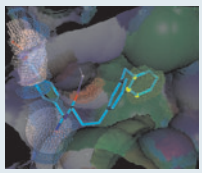
Keymodule Ltd.

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
- Build structures using imported fragments - recore as standard feature
- Excellent synergy with fragment based hit discovery
- Predicts binding affinity and synthetic feasibility (via complexity analysis)
- 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-LeadOpt

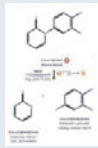
- Optimize hit compounds within the target's active site
- Synthetic constraints ensure only synthetically accessible structures are generated
- Two modes of optimization - core extension and monomer replacement

Chemical Document Processing

CLiDE Pro

- Convert images of chemical structures into computer readable formats (e.g. MDL MOL and RG files)
- Recognize generic structures
- Load PDF documents and raster image files, TIFF and BMP
- Tools to modify extracted molecules and text
- User interface or batch mode execution

Computer-Aided Synthesis Planning



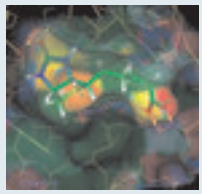
ARChem: Route Designer

- Fully automated retrosynthetic analysis of target organic molecules
- Reaction rules automatically extracted from reaction databases (including very large databases, e.g. Beilstein)
- Integrated with reaction databases for literature references and reporting
- Contains over 100,000 starting materials, with catalog references

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
- Very straightforward to setup and run

eHiTS Score

- Statistically derived empirical scoring function
- Uses temperature factors of PDB files for more accurate statistics collection
- Reliably predicts binding affinity

CheVi

- Molecular visualization suite - Interface to eHiTS docking
- Specifically designed to show how ligands interact with receptor active sites

QSAR Similarity Tools

eHiTS LASSO

- QSAR descriptor based on surface properties of ligands
- Trained on small number of active ligands
- Conformation independent
- Ideally suited for scaffold hopping hit discovery

Visit Keymodule Ltd. at Booth 15

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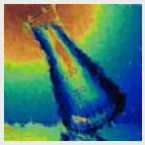
CORINA *et al.*

Molecular Networks at the 8th ICCS, June 2008 - Booth B2

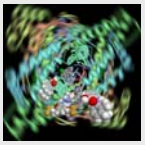
Molecular Networks – maker of **CORINA** – offers innovative chemoinformatics software products, consulting, development and research services to increase the quality and productivity of discoveries in chemical, pharmaceutical and biotechnology R&D. Its areas of activities range from the design and synthesis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

New Products



SYLVIA rapidly evaluates the ease of synthesis of organic compounds

- Prioritizes thousands of structures, *e.g.*, generated by *de novo* design experiments, according to their synthetic complexity



isoCYP predicts the isoform specificity of human cytochrome P450 substrates

- Includes the isoform specificities for CYP450 3A4, 2D6 and 2C9 substrates
- Designed for drug-like molecules

New Versions

Molecular descriptor package **ADRIANA.*Code*** Version 2.2 available now!

- Parametrized for charged molecules
- New global molecular descriptors
- New shape- and size-related descriptors

Biochemical pathway database **BioPath** and **BioPath.*Explore*** Version 2.0 availabe now!

- Over 2.000 biochemical structures and 2.800 biochemical reactions
- Evaluation copy for download available

New Developments

THERESA is a web-based, easy-to-use tool for the stepwise retrosynthetic analysis of a given target compound. It uses a knowledge base of different reaction types automatically derived from reaction databases and simultaneously scans catalogs of available chemicals for the proposed precursors.

- The method will be presented in paper D-2 on Wednesday morning, June 4, 2008 at the 8th ICCS

Evergreens

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

Molecular Networks
Inspiring Chemical Discovery

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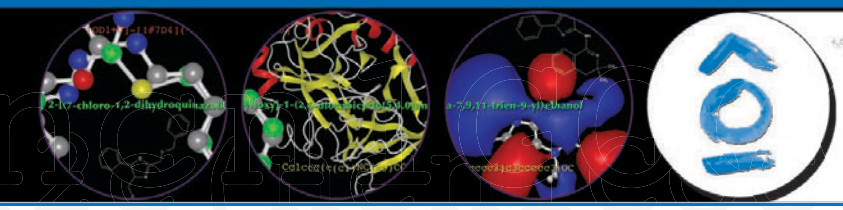
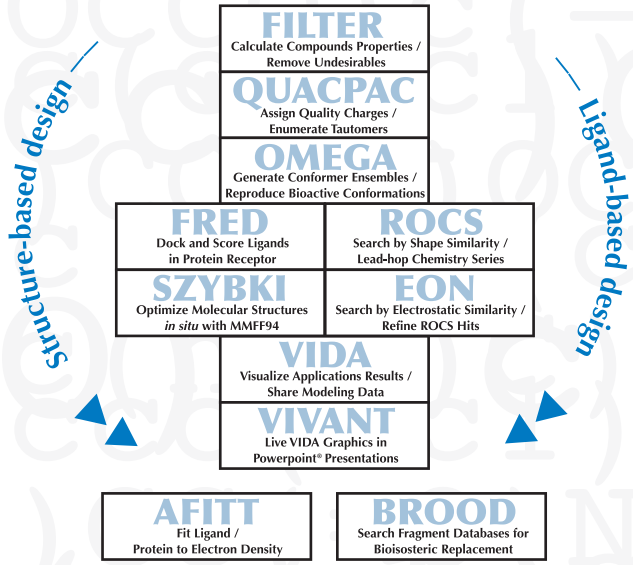
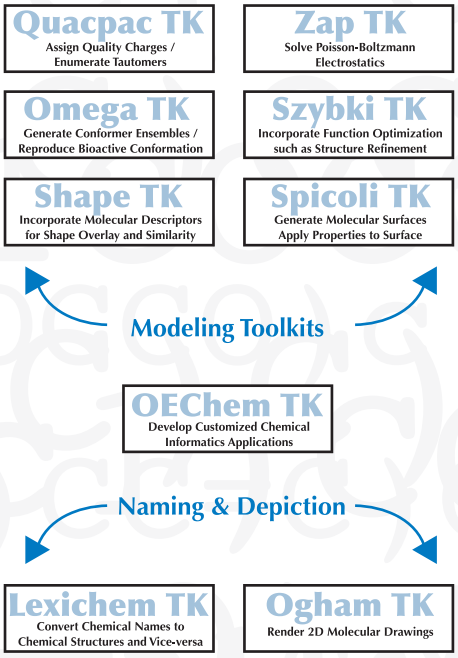


OpenEye: Booth 6

www.eyesopen.com



Molecular Modeling & Cheminformatics



Applications

OpenEye's portfolio of molecular modeling applications is presented as a workflow involving ligand- and structure-based design strategies. **FILTER** and **QUACPAC** prepare the input data by removal of undesirables and consistent molecular representation. Next, **OMEGA** generates high quality 3D conformer ensembles. **ROCS** corresponds to the ligand-based approach where libraries are searched by 3D shape (and chemistry) matching. **EON** may then be used to refine the search by electrostatic similarity. **FRED** is OpenEye's docking and scoring application. Hit structures may then be optimized with **SZYBKI**. **VIDA** is a powerful graphical interface for visualization and effective communication of results, which **VIVANT** can then export live into PowerPoint® presentations or web pages. **AFITT** is a standalone application for ligand fitting to crystalographic density, and **BROOD**, searches fragment databases for bioisosteric replacement.

Toolkits

OpenEye has an extensive portfolio of cheminformatics and molecular modeling toolkits. Toolkits are programming libraries for creating customized applications with object-oriented accessibility to a given set of capabilities. Central to the portfolio is the **OEChem TK**, OpenEye's programming library for chemistry and cheminformatics, on top of which a number of other toolkits have been built. Among the six modeling toolkits, four (**Quacpac TK**, **Omega TK**, **Shape TK** and **Szybki TK**) have been made partially available as applications, while two are only available as toolkits (**Zap TK** and **Spicoli TK**). In addition, **Lexichem TK** and **Ogham TK** are two specific toolkits for naming and depiction. All the toolkits are written in C++ and have a stable, documented API. Functionality is also accessible via Python and Java wrappers.

Visit us at Booth 6 to find out more!

OpenEye Scientific Software

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business@eyesopen.com

Transition State Technology Co. Ltd.

(Will be established at June, 2009)

TS TECHNOLOGY

Launched from YAMAGUCHI UNIVERSITY

Supported by Japan Science and Technology Agency

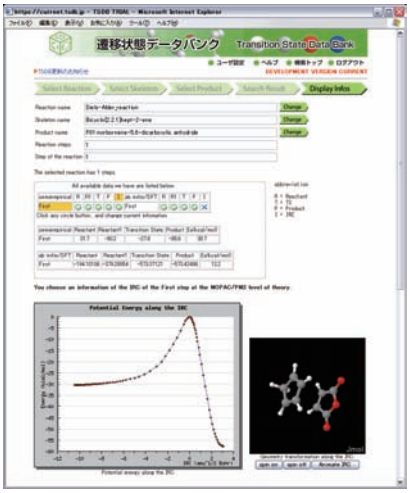
TS Technology

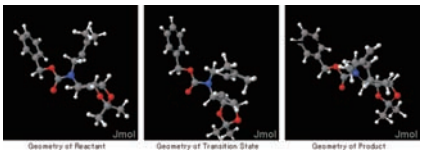
is a Japanese Computational Chemical Venture Company launched at June 2009 from Yamaguchi University. We are now developing the *in silico* screening for synthesis route developments based on quantum chemical calculations. We would like to contribute to reducing costs and periods for synthesis route developments using our *in silico* technology combined with the TSDB and offer sustainable methods for organic synthesis and delivering safety drugs.

Our services and products

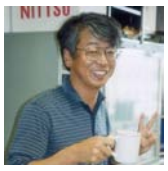
are listed.

- Teoretical calculations
- Reaction analysis and optimization
- Consultant services for synthesis route development
- The TSDB, which supports your calculations and analysis of organic reactions, and is now accessible at **https://trial.tsdb.jp/**





Screenshots of the web-based TSDB



Come to our exhibition booth!

- Introducing our company, services and products
- Demonstration of The TSDB and our softwares
- Setting up your free TSDB account
- A nice souvenir on a fast-come-fast-served basis

TS TECHNOLOGY

Transition State Technology Company Limited

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