ICCS

International Conference
on Chemical Structures

10th International Conference on Chemical Structures
10th German Conference on Chemoinformatics

June 1–5 2014 // Noordwijkerhout // The Netherlands

Exhibitor Newsletter

GCC

German Conference
on Chemoinformatics

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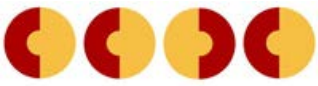

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We would like to thank CCL.NET and Jan Labanowski for adding the conference to the CCL conferences webpage. We are also grateful to the Center of Bioinformatics of the University of Hamburg for hosting the conference webpage.

Exhibition

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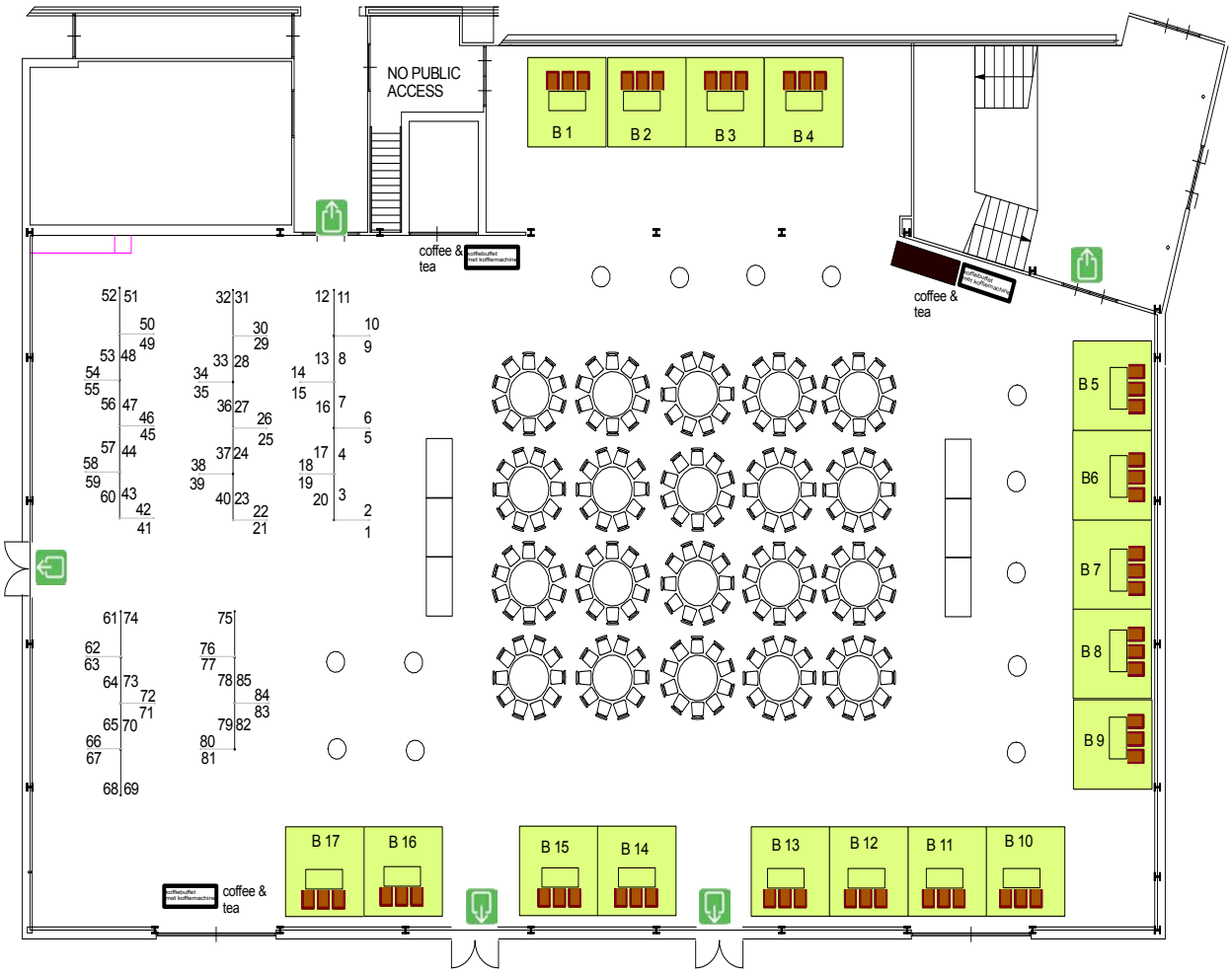
Exhibition Layout



Exhibitors

Exhibitor	Booth	Exhibitor	Booth
Simulations Plus, Inc.	B 1	NextMove Software	B 10
Certara	B 2	Chemical Abstracts Service	B 11
Chemical Computing Group	B 3	Schrödinger	B 12
OpenEye Scientific Software	B 4	Dotmatics	B 13
Cambridge Crystallographic Data Centre	B 5	KNIME	B 14
Cresset	B 6	Xemistry	B 15
c.a.r.u.s. HMS GmbH	B 7	MEDIT	B 16
PerkinElmer	B 8	GVK BIO	B 17
ChemAxon	B 9		

Exhibition Hours

- Monday June 2, 2014 14:30 – 19:30
- Tuesday June 3, 2014 14:30 – 19:30

c.a.r.u.s. HMS GmbH is a software company with over 60 employees located in northern Germany near Hamburg. C.a.r.u.s has been successfully developing IT solutions in the fields of healthcare, life sciences and customized software for over 20 years.

Within the healthcare sector, we provide and continually develop our hospital information system myMedis. The system is based on meeting the demands of small outpatient-hospitals as well as large clinics such as the university-hospital of Hamburg-Eppendorf. Our medical information system is composed of individual modules which can be used in combination or as stand-alone solutions. Via integrated interfaces these modules are designed to communicate with every single IT-system within healthcare.

For life science c.a.r.u.s. offers a data-management platform called ViSoR that combines a customizable set of modules and functionalities for drug discovery approaches. This browser-based IT platform is a digital workplace for interdisciplinary teams to manage and compare results from *in vitro* as well as *in silico* screens. It facilitates the integration of historic data-sets, brings together remote teams and enables a secured data-transfer to customers.
Additionally we offer a data-management-software for an automated quality control of primer sets such as PCR-Kits for infectious diseases.

In addition c.a.r.u.s. uses its proprietary Java Enterprise Frameworks to develop individual software-solutions for customers. This expertise enables us to meet the demands by customized software solutions of the highest quality in a short period of time.
C.a.r.u.s delivers IT-solutions as an efficient tool for our customers with the best possible support. So far every single customer-project of c.a.r.u.s. was finished successfully, which makes us a preferred partner for software projects in medical and life science sectors.

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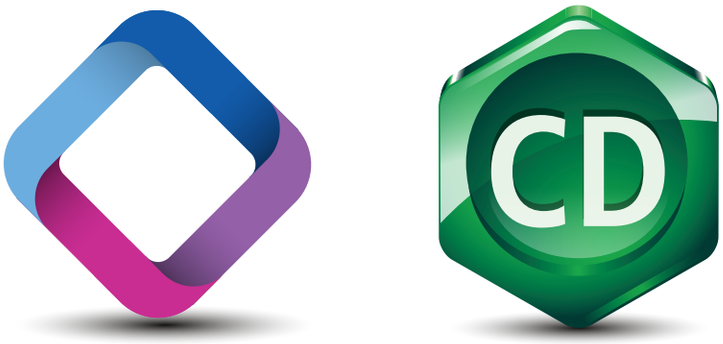

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The world's most comprehensive source of chemistry information—SciFinder®—is now searchable directly from ChemDraw®. You can search substances and reactions from the comfort of your favorite drawing tool. That means more information—and inspiration—for your research in less time. Sounds like a simple choice to us.

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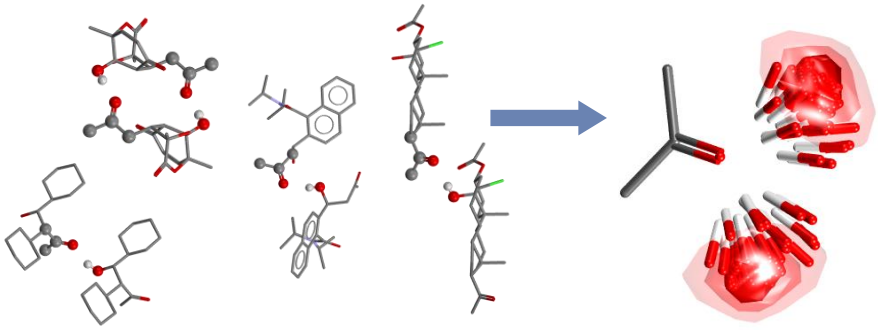
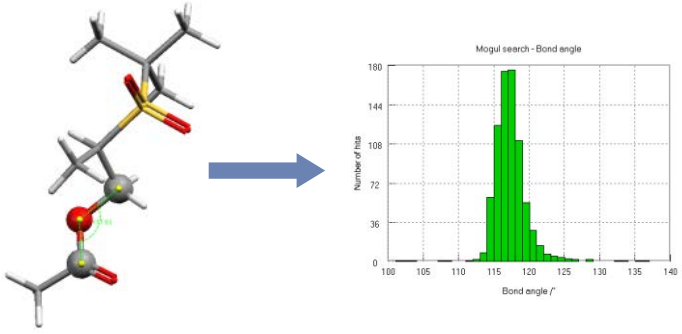
PerkinElmer®
For the Better

at ICCS/GCC, Noordwijkerhout

The Cambridge Structural Database (CSD) is the world's leading repository of organic and metal-organic crystal structure information. It currently contains more than 700,000 entries.





Meet our staff at booth B5 and see the latest developments in the CSD, its associated software, and the other tools for crystallography, drug discovery and drug development provided by the CCDC.

Come along to our workshop (Thurs 5th June, 14:00-16:00) to learn more about our pre-computed libraries of intramolecular geometry and intermolecular interactions and how they can be used to inform decisions in different aspects of the drug discovery process.

MOE

MOLECULAR OPERATING ENVIRONMENT

Structure-Based Design

> Active Site Detection & Visualization
> Protein: Ligand Interaction Diagrams
> Contact Statistics, Electrostatic, & Interaction Maps
> Scaffold Replacement, Fragment Linking/Growing
> Ligand-Receptor Docking
> Multi-Fragment Search
> BREED: 3D Ligand Generator
> Medicinal Chemistry Transformation

Pharmacophore Discovery

> Ligand & Structure-Based Query Editor
> Partial Matches, SMARTS Patterns, Constraints, & Shape
> Custom Features & Boolean Expressions
> Automatic Query Generation
> High-Throughput Conformation Generation
> Pharmacophore Search (.mdb, .oeb)
> Linker & Lead-like Conformational Databases
> Ligand & Structure-Based Scaffold Replacement

Protein & Antibody Modeling

> Protonate3D: Protonation State Prediction
> Protein Structure, Family, & Fab Databases
> Remote Homology & Fold Identification
> Multiple Sequence/Structure Alignment & Analysis
> Homology Modeling & Macromolecular Simulation
> Knowledge-based Antibody Modeling
> Mutation & Rotamer Exploration
> Protein Geometry Quality Assessment

Molecular Modeling & Simulations

> MMFF, Amber, & CHARMM Forcefields
> Explicit or Implicit Solvent Models
> Molecular Mechanics & Dynamics
> Conformation Generation, Analysis, & Clustering
> Molecular Surfaces & Electron Density Display
> Non-linear Poisson-Boltzmann Electrostatics
> Quantum & Semi-Empirical Calculations

Cheminformatics & (HTS) QSAR

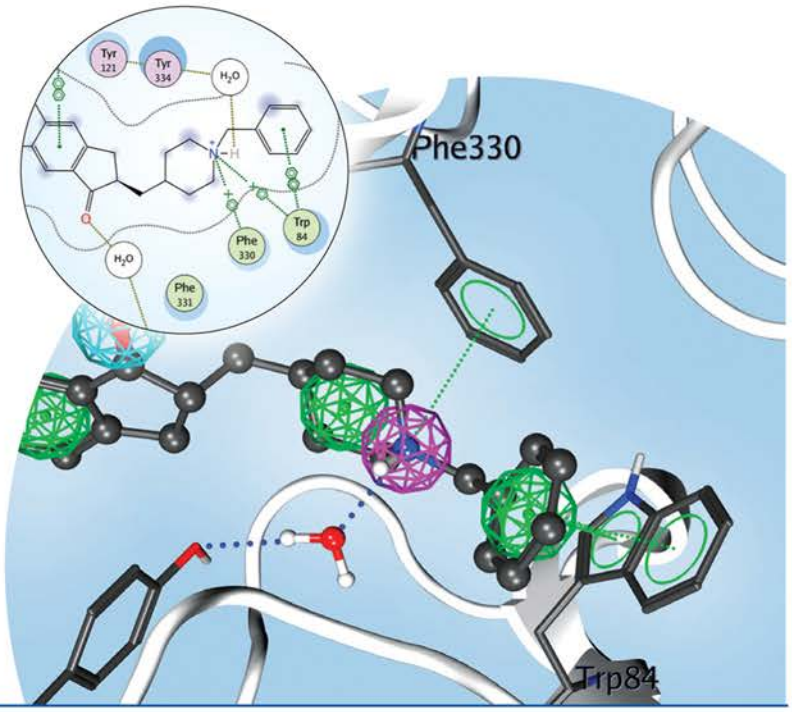
> SD Command Tools for Pipeline Workflows
> Washing, Filtering, Tautomer & Titration Enumeration
> 600+ Molecule Descriptors
> PLS, PCR, Binary QSAR, & Recursive Partitioning
> Similarity, Diversity, & Fingerprints
> 3D Conformer Generation from SMILES or 2D
> Combinatorial Library Design
> Automatic Publication-Quality 2D Depiction

Medicinal Chemistry Applications

> MOE/web: Web Browser Applications
> Protein: Ligand Interaction Diagrams
> Contact Statistics, Electrostatic, & Interaction Maps
> LigX: Ligand Optimization in Pocket
> Ligand & Structure-Based Scaffold Replacement
> Multiple Molecule Flexible Alignment
> Conformation Generation, Analysis, & Clustering
> Synthetic Feasibility Descriptor

Methods Development & Deployment

> Scientific Vector Language (SVL)
> Background (batch) & Cluster Computing
> Platform Independent (Windows, Mac OS X, Linux, Unix)
> URL (HTTP/FTP) & TCP-IP Sockets
> Relational Database Connectivity (JDBC)
> MOE/web: Web Browser Application Framework
> Soap Server & KNIME nodes



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Life Science Molecular Modeling and Simulation

Multi-Criteria Drug Design ***Lead Identification*** ***Lead Optimization*** ***Off-Target Modeling***

Muse

Identify and Optimize Lead Compounds

Muse® is a molecular design workflow that accelerates the identification and optimization of lead candidates. Using Muse, CADD Scientists and Medicinal Chemists can identify novel structures, scaffolds, or side-chains that meet specific design objectives; explore lead- and scaffold-hopping; invent new R-groups around a fixed scaffold and generate ideas that meet multiple design criteria. With Muse, scientists can:

- Design new candidates that mimic the shape and pharmacophore features of your lead structures
- Elaborate fragments in the context of a protein binding site for fragment based drug design
- Generate ideas based on multiple design criteria you choose
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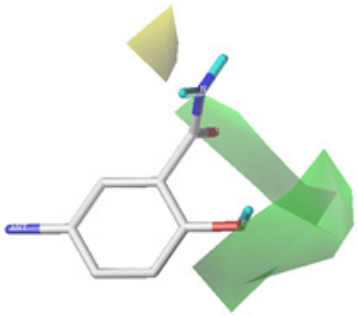
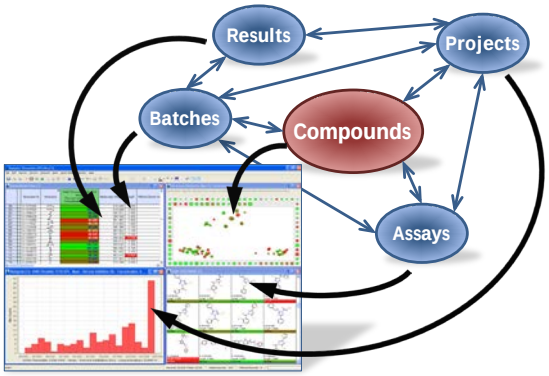


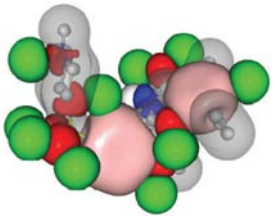
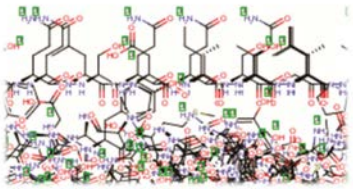
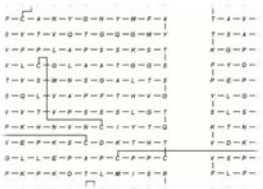
SYBYL®-X has everything you need for drug design and other molecular discovery projects, from HTS through Lead Optimization. Easily move from building a homology model for a target of interest to identifying potential lead candidates and multi-criteria drug design, to lead optimization projects, or to building a homology model for a target of interest. If you need **library design, scaffold hopping, structure based design, ligand based design, cheminformatics,** or tools to build a **protein model**, SYBYL-X has it…and more.

D360

Access, Analyze and Share Your Scientific Data

D360 provides life science researchers with 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 from early discovery through pre-clinical and clinical drug development, 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, scientists report that as many as fifty (50) mouse clicks are reduced to just one, and that assembly of a project SAR dataset can be reduced from hours to minutes, allowing researchers to spend more time at the bench.



Recent articles & posters

ChemAxon

Articles

Screen3D: A Novel Fully Flexible High-Throughput Shape-Similarity Search Method – Adrián Kalászi et al.

J. Chem. Inf. Model., 2014, 54 (4), pp 1036-1049

3D shape- or volume-based virtual screening is a broadly used approach in drug discovery. In recent years a large number of publications have appeared in which these tools were compared not only to competitive methods but to docking studies as well. Studies often showed that the effectiveness of docking could be highly variable due to a large number of possible confounding factors, while ligand-based, shape-based approaches were more consistent. Here, we describe a novel, fully flexible shape-based virtual screening algorithm that does not require previous 3D conformation or conformer generation…

New Approaches to Virtual Screening – Ivan Solt et al.

Drug Discovery & Development (dddmag.com), 2013

Virtual screening (VS) aims to reduce the enormous virtual space of chemical compounds (a practical virtual library might comprise ~1015 molecules) to a more manageable number for further synthesis and screening against biological targets, which could lead to potential drug candidates...

Chemical Weapons – Aurora Costache et al.

European Biopharmaceutical Review, Spring 2014

One of the most important business management challenges for chemistry departments in the global life sciences industry is dealing with controlled substance compliance…

Posters

Chemical Patent Curation and Management – new tools and capabilities – Arpad Figyelmesi et al.

Here we present Chemaxon's new Patent Curation Tool that is designed to offer unique solutions for patent miners…

Plexus – A Flexible Library Design Platform to Conduct Innovative Chemistry – Krisztian Niesz et al.

We describe Plexus, ChemAxon's new discovery platform providing easy to use cheminformatics tools for the bench researchers. Plexus allows chemists to easily get on the most common virtual library design processes, including compound enumeration, property based filtering, pharmacophore similarity searching and clustering as simple and straightforward as possible…

Compliance Checker: A simple compliance tool that helps you stay on the safe side – Krisztian Niesz et al.

Have you ever been in a situation when you or your peers worked with a controlled substance without even knowing about it?...

HELM: an open standard for handling large Biologics – Roland Knispel at al.

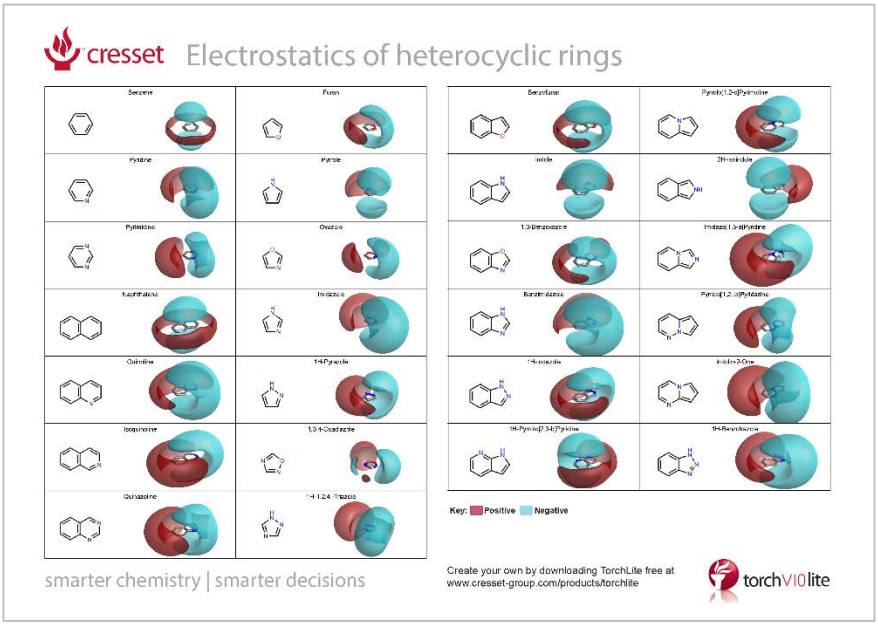
…leveraging the HELM standard for transforming and consolidating structure management of large bio-molecules with novel tools, currently in the making.

cresset

Oral presentation: Monday, June 2 | 14:00 – 14:30
Multi-dimensional activity cliff analysis

Poster presentation: Bioisosteres in accessible chemistry space

Visit booth B6 for a limited edition complimentary copy of the poster ‘Electrostatics of heterocyclic rings’.



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Integrate, query and browse multiple data sets at once with *Browser*

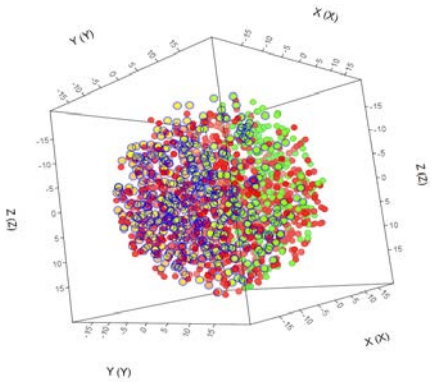
- Images as well as chemical, biological, analytical, and many other types of data can be unified and presented to users in a single view
- Schedule searches and automatic trigger email notifications

Track the progression of samples through their complete lifecycle with *Cascade*

- Configure tests to suit your organisation's business practices
- Flexible templates enable the close mapping of your workflow and business practices even if they change regularly
- Supports all types of test requests including chemistry, biology, formulations, purifications etc.
- Supports a battery of analyses to enable a single click submission of tests around one or more samples

Analyse and visualise scientific data with *Vortex*

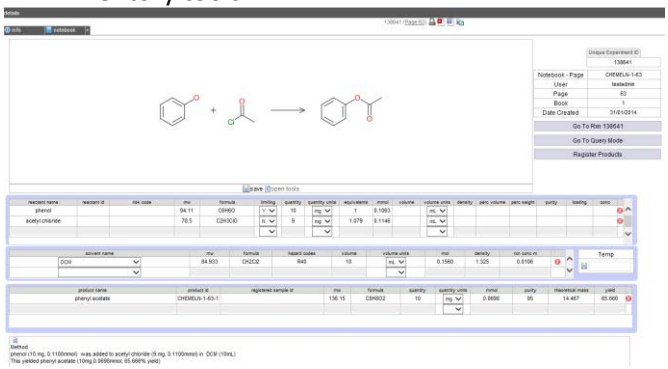
- Designed to dynamically import, combine, mine and analyse large datasets including chemical structures, biological assays, text and numeric data
- Includes a set of scientific property calculators and functionalities designed to assist scientists from diverse disciplines



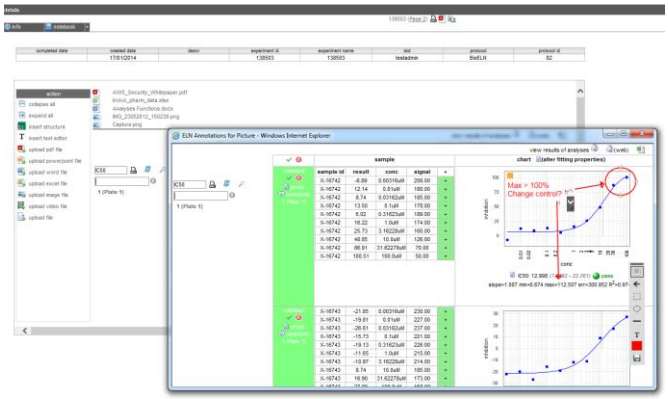
Interactive 3D Scatterplot in Vortex

Flexible and fully searchable Electronic Laboratory Notebook: *Studies Notebook*

- Multi-discipline, highly customisable ELN
- Configured to fulfil the informatics requirements of different laboratories within an organisation
- Integrated with chemical registration and sample inventory tools



Example of Studies Notebook for Chemistry



Example of Studies Notebook for Biology

Register chemicals or biologicals and track assets with *Register* and *BioRegister*

- Adaptable, fully integrated biologicals and chemistry registration systems
- Meets requirements of scientists and regulatory officials in education, government and industry.

Add chemical intelligence to Excel, Word, Outlook and PowerPoint with *Dotmatics for Office (D4O)*

- Speed up report writing with preformatted paragraphs or tables of chemistry data

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Biggest Repository of Compound Bio-activity Data

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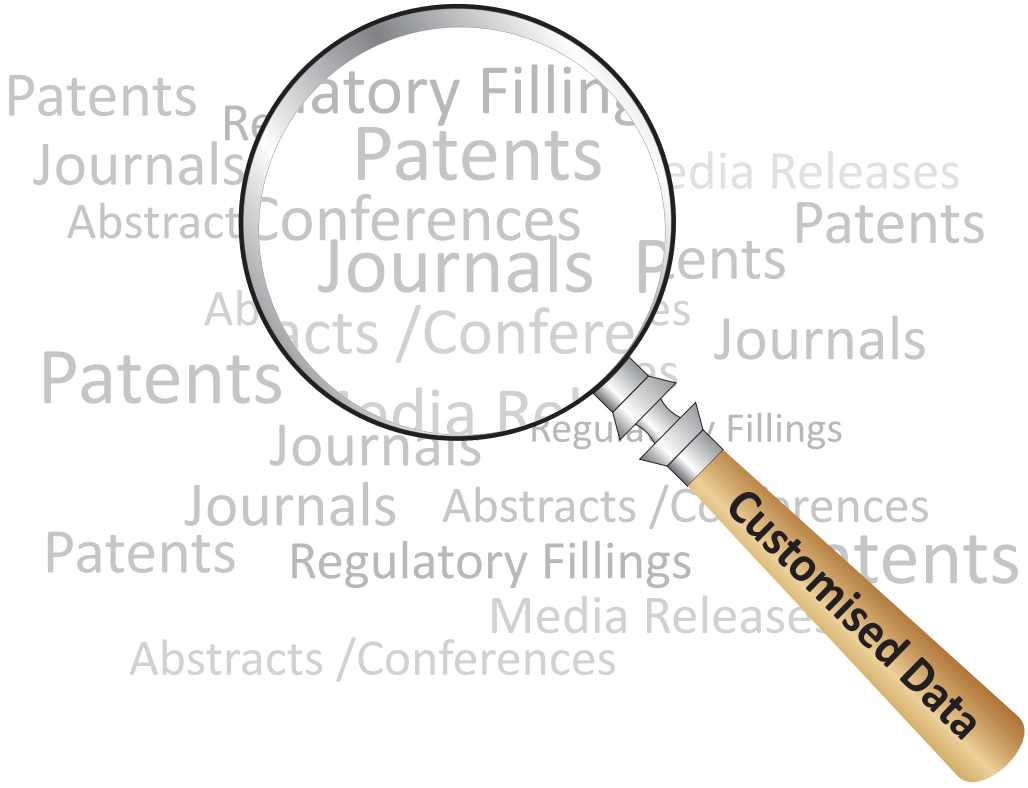

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• Phone: + 49 (0) 69 800 865 0 • Email: aniket@evolvus.com

www.evolvus.com

GVK Biosciences (GVK BIO) is Asia's leading Contract Research Organization from India, which offers comprehensive services from Informatics, chemistry synthesis to clinical trial. Currently, we provide holistic services to nearly 200 companies, offering specialized services to our clients from various verticals from Chemistry, Biology to Informatics and Predictive Analytics to cater requirements of clients in different domains with flexible business models customized to suit client needs.

The **Informatics division** of GVK BIO is one of the oldest and largest informatics service providers in India. We have over 500 scientists working to provide the Informatics services and proprietary Bio/Chemical databases to our customers. GVK BIO's Informatics group has more than 12 years of experience in data mining, curation and analysis aspects from data published in literature references, patents, company websites, and regulatory documents as well confidential documents from client's side. Our scientists have expertise in multiple areas such as Chemistry, Pharmacology, Biology, Biomarker and Clinical data. Significant number of scientist are working on client specific project where objective and scope of data mining, curation and overall outcome of project has been defined by client with stringent quality control processes.

GVK BIO databases:

- **GOSTAR**: Small Molecule Structure Activity Relationship Database- over 6 Mn compounds with 20 Mn SAR points curated from Journal articles, patents, company websites etc.
- **GOBIOM**: Biomarker database with over 35,000 biomarkers from exploratory, preclinical and clinical areas
- **Clinical trial outcome databases**: Indication specific summary level meta data captured from clinical trials, currently we have hands on experience to develop over 82 indication specific databases

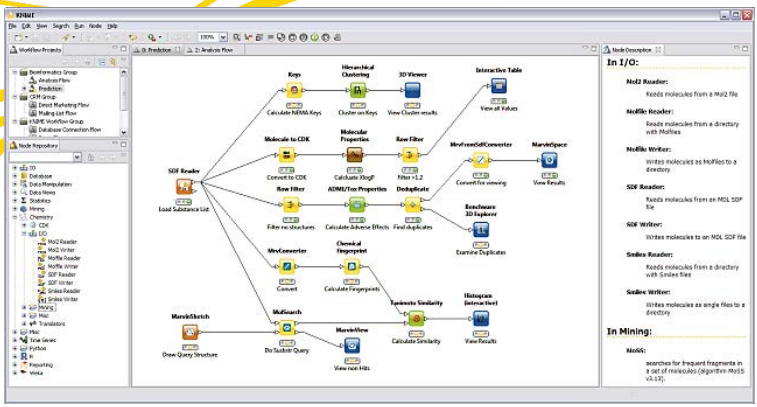
Custom Data Service Portfolio:

- Technical and Scientific Abstracting & Indexing
- Database Creation
- Scientific data Excerption
- Indexing of scientific literature
- Clinical data extraction
- Chemical compound and reaction information
- Taxonomy, Ontology
- ADME Toxicology
- Content Conversion into required format
- Legacy and Archived data conversion into electronic format
- Indexing of scientific literature

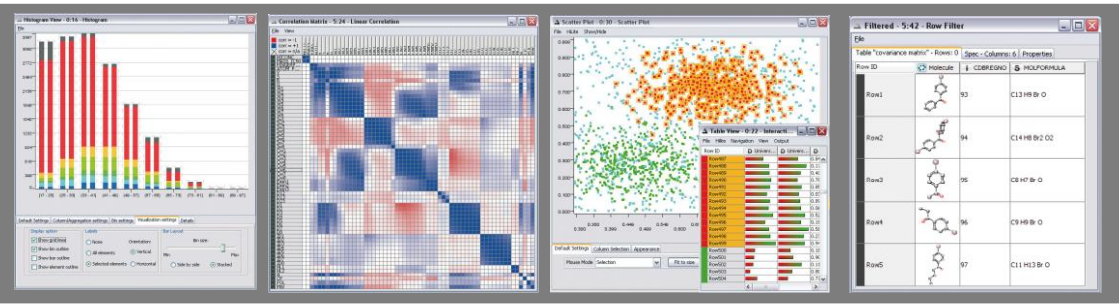
Why GVK BIO?

- Quality and transparent communication
- Multilingual expertise
- Flexibility and scalability
- Complete confidentiality
- Quick turnaround time
- On time delivery

Joining Data, Tools and Science



- Life Science extensions for chemo- and bioinformatics
- High Content Analytics (HCS)
- Molecular structure and cell assay image support



About KNIME: KNIME is the leading open platform for data-driven innovation helping organizations to stay ahead of change. Innovative organizations use our open-source, enterprise-grade analytics platform to discover the potential hidden in their data, mine for fresh insights, or predict new futures.

Quick to deploy, easy to scale and intuitive to use, KNIME is used in over 60 countries on data of every kind: from numbers to images, molecules to humans, signals to complex networks, from kilo- to petabytes, or simple reports to complex analyses.

Visit our booth at ICSS/GCC!

KNIME.com AG
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8005 Zurich, Switzerland
info@KNIME.com

Learn more at http://www.knime.com

MEDIT SA software to crossmine 3D 2D 1D data

2 rue du belvedere, 91120 Palaiseau France - info@medit.fr - www.medit.fr

FC-Bioisostere = NEW software for bioisosteric replacement (rules from PDB local pocket similarities)

***FC-Bioisostere* software co-developed with *Felix Concordia SARL* opens access to 3D bioisosteric replacement onto your molecule of interest to find chemical groups having similar 3D biological interactions. While maintaining target potencies, it helps Chemists to optimize additional properties in pharmacokinetics and metabolic response, and/or to escape from existing patents by selecting alternative equivalent chemical groups.**

***FC-Bioisostere* is a 2 step application:**

First, users can automatically build a database of 3D bioisosteres from:

a. an input set of pre-aligned ligands (3D SD files) where pairs of 3D overlapping fragments are detected and stored ; or

b. by driving *MED-SuMo MEDIT SA* software to extract from the *PDB* files (*Protein Data Bank*, ~90000 protein) and/or your in-house biostructural data all local protein-ligand similar superpositions (defined by charges, Hbond, hydrophobic, aromatic, ... interactions); or

c. alternatively we provide pre-computed databases of bioisostere pairs built upon the whole *PDB* prepared by our experts.

Second, the chemist input molecule of interest is deconvoluted and/or splitted in fragments (6 methods are available). Once fragments to be replaced are selected, all fitting replacement pairs of fragment are retrieved from the database. Different methods to merge/fuse those fragments into the input molecule are provided to generate full 3D bioisosteres. 1D/2D/3D chemical and protein scoring filters help to sort/focus on the best bioisostere candidates.

FC-Bioisostere* is a new component of the *C2P* consortium *(Chemo-Proteomic Platform) to cross-mine altogether biostructural, structure-activities and chemical libraries data. *C2P* includes :

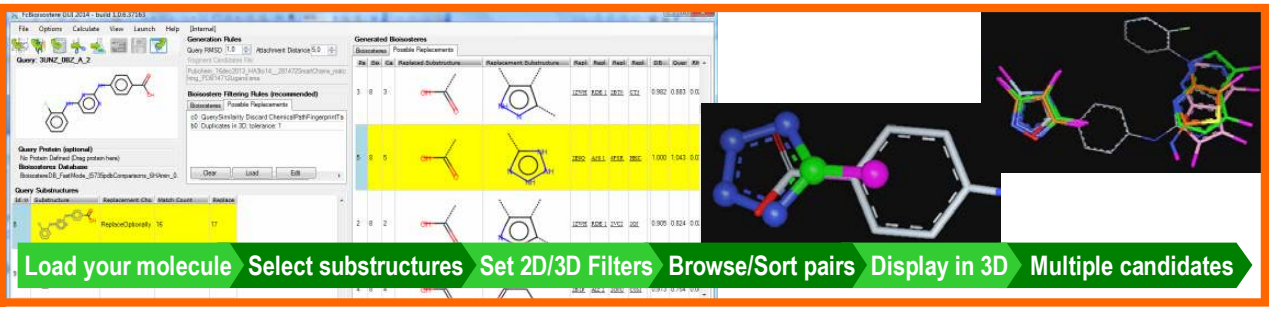
1. *MED-SuMo* to detect/superpose 3D protein surface interactions,
2. *MEDP-Fragmentor* to deconvolute protein-ligand structure in pocket-fragment interactions,
3. *MEDP-SiteClassifier* to navigate in all intra-familly/inter-family binding site similarities across the whole PDB,
4. *MED-Ligand* to explore 1D/2D/3D ligand/fragment similarities,
5. *MEDL-Hybridise* to combine in 3D fragments,
6. *MEDL-filter* to filter/score according to 1D/2D/3D (protein)-ligand properties.

***FC-Bioisostere* & *MED-SuMo* are unique technology for Chemist to better take advantage of 3D biostructral data**. Please come to our booth to test FC-bioisostere and/or to discover case studies.

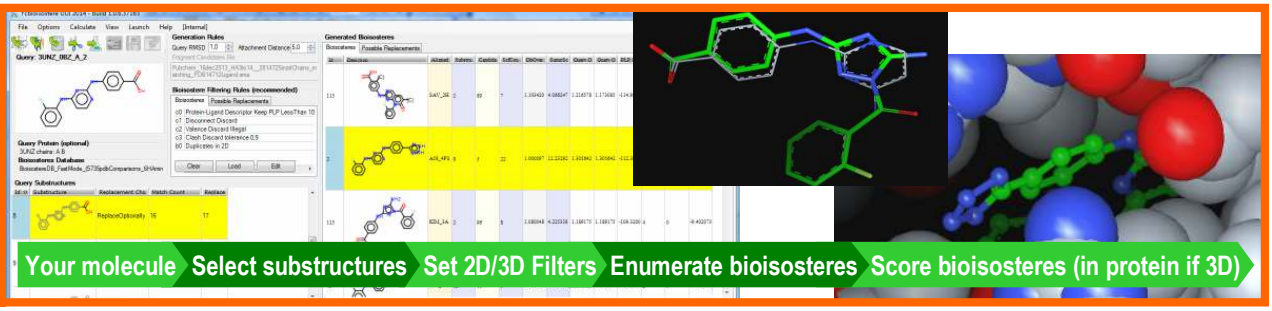
Ref: Moriaud F, Adcock SA, Vorotyntsev A, Doppelt-Azeroual O, Richard SB and Delfaud F, ACS Symposium series1076, Chapter book 5, p71-88 (2011)

(1) Build or buy bioisostere database

(2a) Explore possible replacements



(2b) Score bioisostere candidates



Replace substructures in your molecule of interest by equivalent functions to optimize the pharmacokinetic profile

(PDB based material, experimental structures are worth)

NextMove Software

Innovative solutions for difficult problems

- ELNs & Reactions
- Patents/Text Mining
- Biologics
- Similarity & Search

NextMove Software develops and markets scientific software solutions for the pharmaceutical and life sciences industries.

CaffeineFix

CaffeineFix is used to rapidly match chemical names or terms against a dictionary or grammar (e.g. a grammar for IUPAC names). As well as use in text mining, it can be used to provide autocomplete functionality and spell-correction.

HazELNut

HazELNut is a suite of tools used to extract, normalize and analyse reactions from Electronic Lab Notebooks (ELNs). This can be used to export to a data warehouse or search system, identify duplicates, find similar reactions and so on.

LeadMine

LeadMine is used to mine text for chemical names and terms. It incorporates NextMove's CaffeineFix technology to find terms that match appropriate dictionaries or grammars. It has enhanced functionality to handle the patent literature.

Matsy

Matsy is a set of tools for creating and analysing Matched Molecular Series (the general form of Matched Molecular Pairs). In Particular, it can be used to suggest what compound to make next in a medicinal chemistry campaign.

MPSearch

MPSearch rapidly searches a chemical database to find Matched Pairs related to a query molecule. This type of search is used to explore previous medicinal chemistry strategies.

NameRXN

NameRXN is used to classify and name reactions. It is particularly useful in the context of ELN analysis but also as a plugin to chemical drawing software. NameRXN builds upon NextMove Software's Patsy technology.

Patsy

Patsy is used to speed up SMARTS pattern matching by creating optimized SMARTS patterns or source code. Speed gains are particularly large when multiple SMARTS patterns are matched against a single structure.

SmallWorld

SmallWorld is an index of chemical space based on more than 4 billion molecular substructures. It can be used to measure similarity based on Graph-Edit Distance (GED), find the MCS of a set of molecules, analyse HTS results, and much more.

Sugar & Splice

Sugar & Splice can be used to perceive and depict biopolymer structure. This makes It easy to interconvert between small molecule representations (e.g. SMILES, MOL) and biopolymer representations (HELM, FASTA, IUPAC line notation).

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Cambridge Science Park,
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England CB4 0EY

www.nextmovesoftware.com

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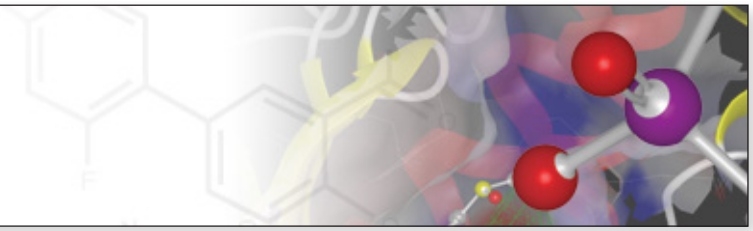

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"Combining methods to increase efficiency in virtual screening: a quantitative approach"

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.

- Maps various thermodynamic properties across holo, apo and ligand structures
- Identifies key water sites and their orientational preferences
- Predicts changes in water activity on ligand binding
- Performs very rapid calculations at specified sets of coordinates such as atom centers of bound ligands
- GAMEPLAN allows for rapid calculation and analysis of SZMAP result to suggest ligand modification hypotheses
- Results can be visualized in 3D using VIDA
- 2D Grapheme representations present SZMAP results in a format that is natural for a chemist
- Improved speed and full parallelization through MPI
- 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.*
  - A fast, and among the best, docking program 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(s) to guide the initial docking process
  - Significantly improved enrichment
  - Docking is hard enough, why throw out useful information?
- **POSIT** - *Pose prediction for lead optimization.*
  - The maximum leveraging of all structural information to produce best in class pose prediction performance
  - Predictions are uniquely assessed by probability of success - a reliable metric that is target independent
- **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

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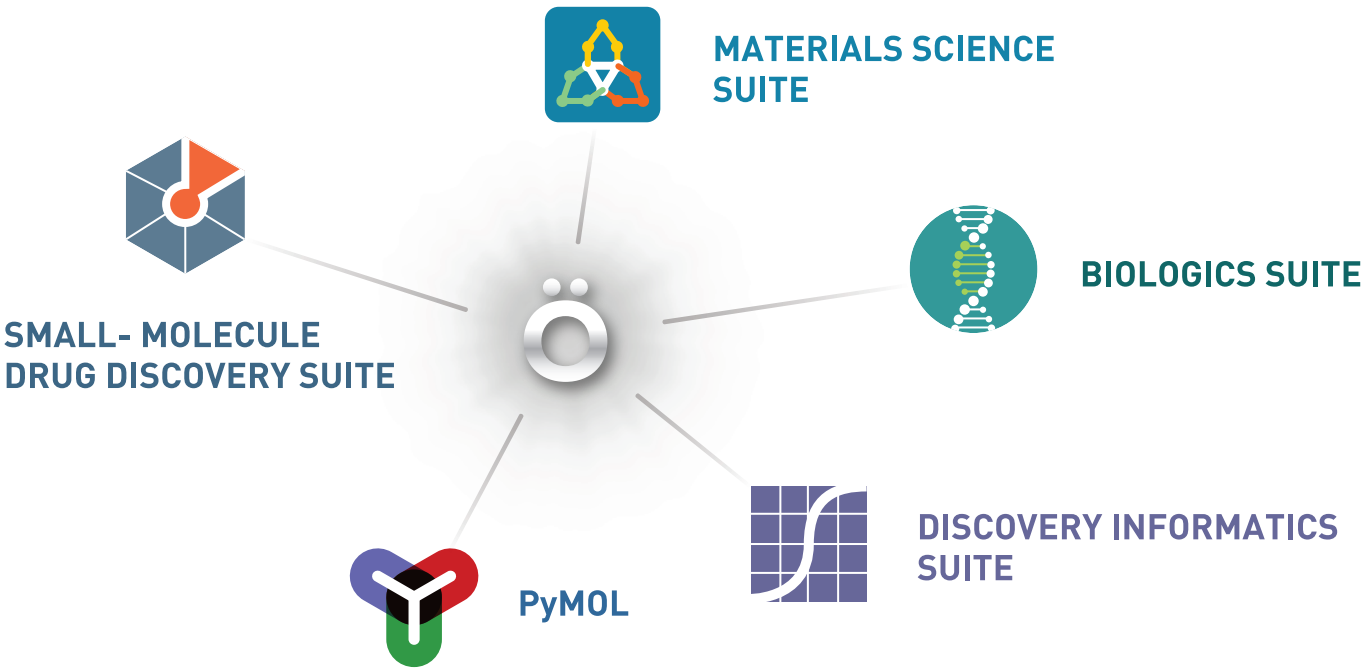

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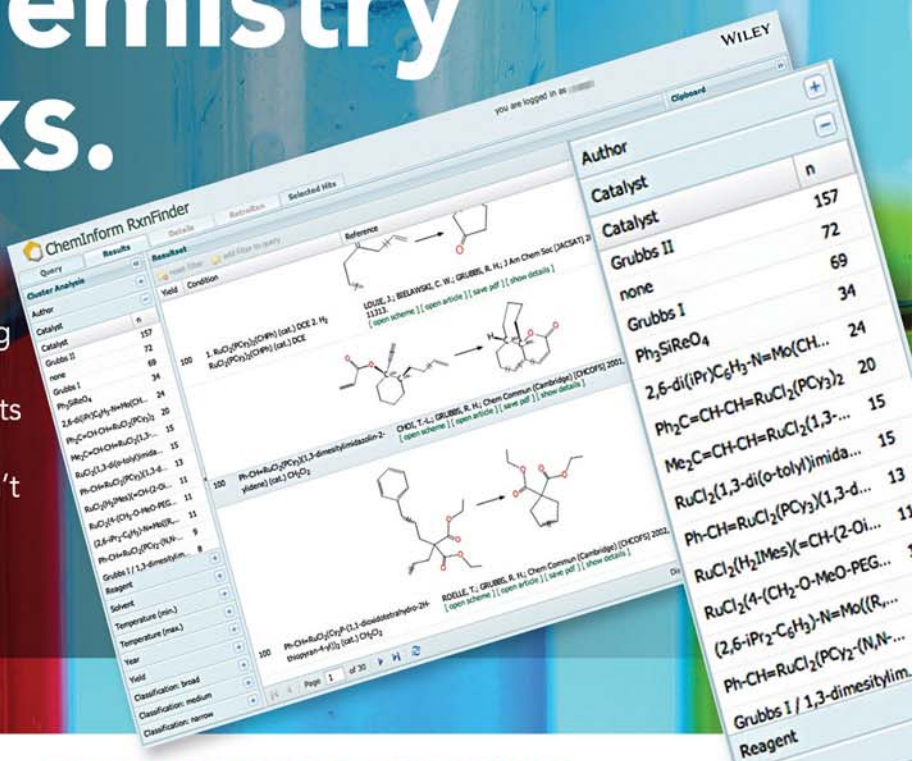

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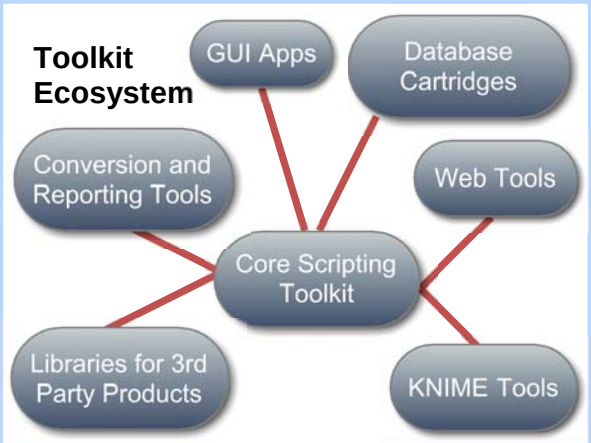

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