ICCS

International Conference on Chemical Structures

11th International Conference on Chemical Structures

May 27 – 31, 2018 ♦ Noordwijkerhout ♦ The Netherlands

Exhibition Newsletter

www.int-conf-chem-structures.org

Preface

Dear Colleagues and Friends,

Welcome to the 11th International Conference on Chemical Structures (ICCS). The organizers decided to deviate from the triennial ICCS schedule by one year, the event, as a result, being organized in 2018. The conference builds on a long and successful history, which started with a NATO Advanced Study Workshop in 1973 and with the previous edition being jointly organized with the German Conference on Cheminformatics. The ICCS meeting is among the most important events in this area of science and gives an accurate picture of the state-of-the-art in the computer handling and manipulation of chemical structures.

We have received 145 abstract submissions from over 24 different countries from 4 continents. All submissions were subject to a review process carried out by a Scientific Advisory Board of 20 international reviewers from academia and industry. This allowed us to compile an outstanding scientific program of 34 plenary and 78 poster presentations.

Additionally, the conference hosts an exhibition with booths from 17 vendors who will present their latest applications, content and software. This exhibition newsletter is intended to inform you in detail about the conference workshops, the exhibition and our exhibitors and to help you to plan your attendance. At this point, we would also like to thank the many sponsors for their financial support, which helped us to provide bursaries to a considerable number of PhD-student attendants.

We hope that you enjoy the conference!

Markus Wagener (ICCS Chair), Frank Oellien (ICCS Co-Chair), Chris de Graaf, Lars Ridder, Egon Willighagen, and Gerard van Westen

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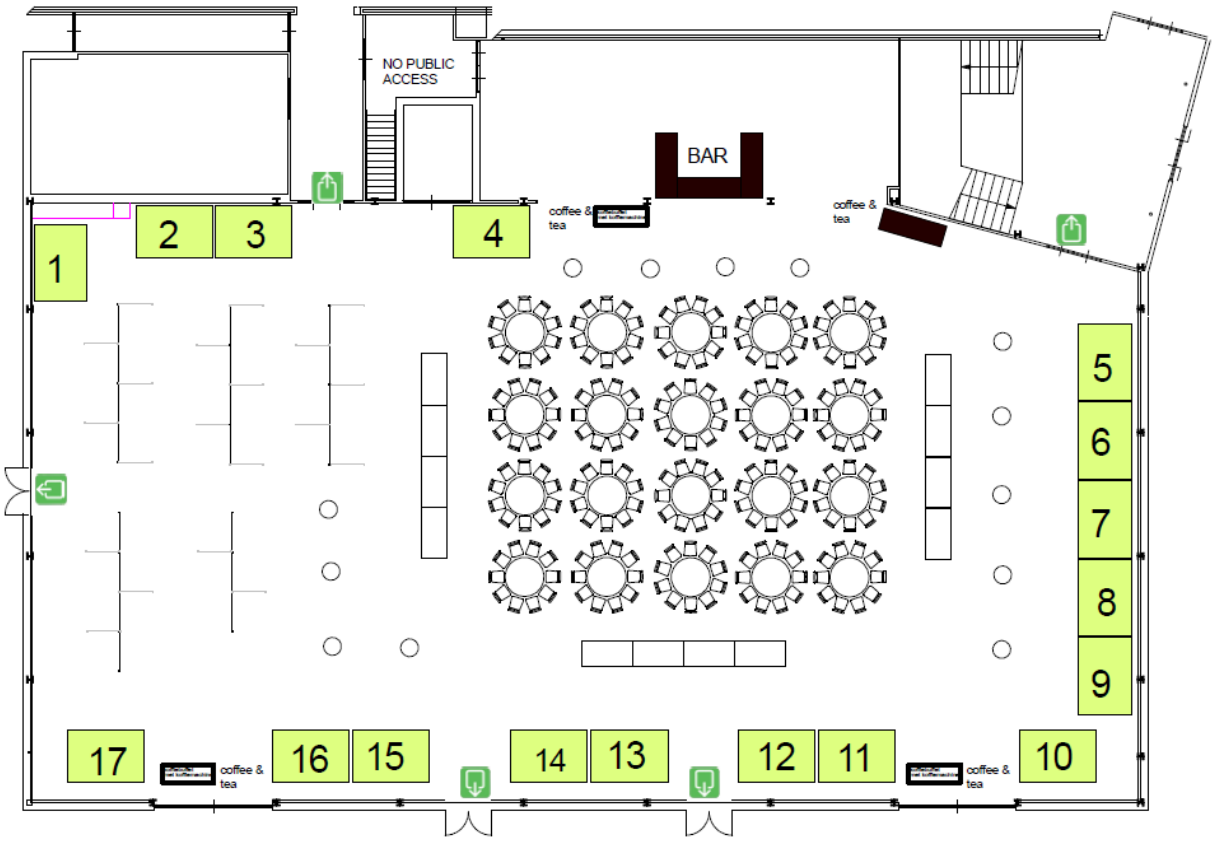
We would like to thank CCL.NET and Jan Labanowski for adding the conference to the CCL Conferences webpage. We would also like to thank the Center of Bioinformatics of the University of Hamburg for hosting the conference webpage.

Exhibition

Exhibition Layout



Exhibitor	Booth	Exhibitor	Booth
Acellera	B1	Cresset	B10
Discngine	B2	CCDC	B11
SilcsBio	B3	inte:ligand	B12
Schrödinger	B4	NextMove Software	B13
Collaborative Drug Design	B5	Dotmatics	B14
Chemical Abstract Service	B6	Xemistry	B15
Certara	B7	Chemical Computing Group	B16
Knime	B8	OpenEye	B17
Culgi	B9		

Exhibition Hours

- Monday, May 28th 2018, 14:30 – 19:30
- Tuesday, May 29th 2018, 14:30 – 19:30

- Exhibition Setup: May 27th 2018 (afternoon)
- Exhibition Dismantle: May 30th 2018 (morning)

Exhibitors

Chemical Computing Group

OpenEye

Xemistry

Dotmatics

NextMove Software

Collaborative Drug Design

KNIME

Inte:ligand

Schrödinger

Cresset

Chemical Abstract Service

Certara

CCDC

SilcsBio

Discngine

Acellera

Culgi

Workshops

Chemical Computing Group Workshop: *Application of Matched Molecular Pairs to Interactive SAR Exploration*

Sunday May 27th 2018, 15:00-17:00, NH Conference Hotel Noordwijkerhout, Room: Boston 13

Managing and analyzing structure activity/property relationship data in medicinal chemistry projects is becoming ever more challenging, with larger data sets and parallel development of different structural series. Tools and methods for the efficient visualization, analysis and profiling of structures therefore remain of deep interest.

The workshop will start with a presentation about the use of interactive MMP analysis and R-group profiling to enhance typical medicinal chemistry workflows by interrogating the SAR data, thereby guiding a medicinal chemistry campaign in its development.

The presentation will be followed by working through some real examples of the use of the new MOEsaic application, and some complementary capabilities in the MOE (Molecular Operating Environment) software system;

R-Group Profiles and Analysis / MOEsaic / MMP Analysis / Template-Forced Docking / Scaffold Replacement / MedChem Transformations

Trial copies of MOE can be provided; see www.chemcomp.com/Product-Free_Trial.htm

OpenEye Workshop: *Orion - CADD on the Cloud*

Sunday May 27th 2018, 15:00-17:00, NH Conference Hotel Noordwijkerhout, Room: Boston 15

The cloud will increasingly become the destination for a wide variety of tasks, in computational chemistry and elsewhere. In this workshop we will introduce Orion, OpenEye's new cloud-native CADD platform. By seamlessly integrating almost limitless computing capacity with well validated workflows and powerful analysis tools Orion substantially increases the scale of problems that can be addressed and makes finding solutions to those problems easy for anyone.

In this workshop we will use Orion to address a frequent problem in medicinal chemistry – using protein structural knowledge to find new lead compounds from a large number of molecules and understanding how these active compounds interact with the protein binding site. To solve this problem effectively we will use a variety of approaches; docking at various levels of accuracy, re-scoring and pose refinement using higher levels of theory. This workflow will proceed from a pool of millions of molecules to produce a few 10's of high probability candidates for experimental validation.

The ability to set up and monitor a large-scale calculation on the cloud, analyse its results, share that analysis and make decisions based on it, all through the same interface, a standard web browser, is extremely powerful. We will illustrate all these capabilities in the course of the workshop.

Schrödinger Workshop: ***Maximizing the impact of Computational Modelling on Drug Design***

Thursday May 31th 2018, 14:00-16:00, NH Conference Hotel Noordwijkerhout, Room: Boston 13

LiveDesign is a novel platform delivering cheminformatics and expert computational models side by side in a highly collaborative and intuitive web-based tool. By presenting experimental data alongside predictive data and models, a broad range of scientists can drive new ideas by asking the key questions and easily exploring chemical space.

In this workshop we will introduce LiveDesign in the context of real-world medicinal chemistry workflows. This will range from rapid querying of the existing SAR, through to graphical exploration of experimental and predictive data to aid profiling and prioritization of new ideas. Embedded 3D docking and pharmacophore model visualization is a key component of the LiveDesign platform and we will show how to make the most of this information. We will also show how the administration interface allows modelers to publish validated Glide1 docking models, for use in a selectivity study of COX1 and COX22. Finally we will show how new ideas can easily be pushed and pulled into Maestro for deeper analysis with more complex computational methods, for a truly cyclic workflow.

1. Friesner, R. A.; Murphy, R. B.; Repasky, M. P.; Frye, L. L.; Greenwood, J. R.; Halgren,T. A.; Sanschagrin, P. C.; Mainz, D. T., "Extra Precision Glide: Docking and Scoring Incorporating a Model of Hydrophobic Enclosure for Protein-Ligand Complexes" J. Med. Chem., 2006, 49, 6177–6196

2. Plount-Price, M. L.; Jorgensen W. L., “Analysis of Binding Affinities for Celecoxib Analogues with COX-1 and COX-2 from Combined Docking and Monte Carlo Simulations and Insight into the COX-2/COX-1 Selectivity” J. Am. Chem. Soc., 2000, 122 (39), pp 9455–9466

Joint Xemistry & KNIME Workshop: ***Chemistry Data Workflows – Leveraging Explorative Native KNIME Technology and Xemistry Custom Nodes***

Thursday May 31th 2018, 14:00-16:00, NH Conference Hotel Noordwijkerhout, Room: Boston 15

The KNIME software has quickly become a prime player in the chemistry data processing arena. Additional chemistry capabilities are continuously added – as built-in support features, packaged standard nodes, and third-party vendor offerings.

Xemistry and KNIME will present a joint workshop highlighting new chemistry-related developments in and around the KNIME software.

In the first part, Daria Goldmann of KNIME will explain and demonstrate new core chemistry features and interactive analysis and exploration capabilities which support the implementation of reproducible KNIME workflows for chemistry data.

In the second part, Wolf Ihlenfeldt of Xemistry introduces the CACTVS KNIME node builder environment – for those occasions where you need a custom chemistry data processing node which is not available as a turnkey solution, and you really do not want to dig into the intricacies of native KNIME Java development.

Towards computerized drug discovery

COMPANY

- SME Founded in 2006
- Social Headquarters in London, UK
- Research & Development in Barcelona, ESP

OUR MISSION

Accelerate the transition to a rational, computerized drug discovery via simulations and machine learning.

OUR VISION

We work with our customers by becoming a key technology partner, boosting their discovery workflow with the most innovative solutions.

OUR VALUES

Science, research, innovation and development.

CONTACT US

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carrer Aiguader nr 88
08003 Barcelona - Spain
tel. +34 93 018 69 14
@ info@acellera.com

CONTEXT

Every year about 50 drugs are launched on the market to cure close to 30.000 diseases. There is a need to increase the discovery of new molecules of interest.

Recent technological advances allow to harness the capacity of computerized methods and run in silico experiments to discover new drugs.

SOLUTION

Accelerating the discovery of new drugs by developing and democratizing the use of innovative computerized methods.

ACTIVITIES

- Drug Discovery software development partner
- Software & hardware development and sales
- Drug discovery services
- EU project partner (CompBioMed)

PRODUCTS

- ACEMD, code for running MD on Nvidia GPU
- HTMD, suite compatible with Amber, Charmm, Gromos for MD preparation, production and analysis
- AceFlow, automated workflow for MD
- AceCloud, application to run MD in the Cloud, available on AWS marketplace
- PlayMolecule, platform of ML based applications
- Metrocubo, 4GPU workstation designed for MD
- Metrocubo-cluster, customized cluster for MD and ML

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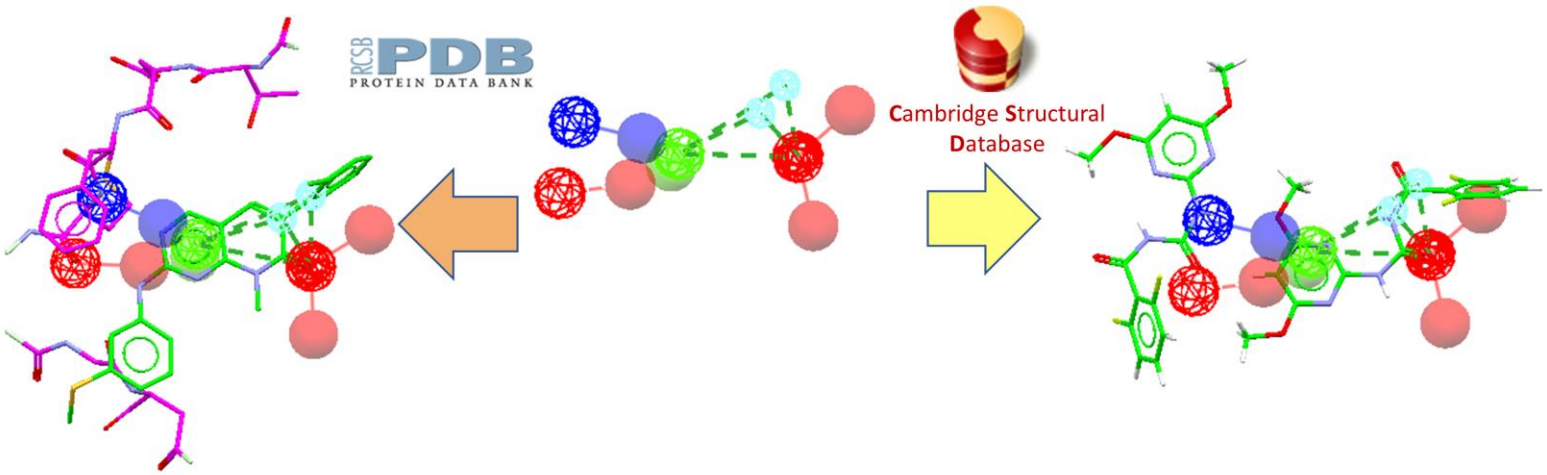
The Cambridge Crystallographic Data Centre

ICCS
International Conference on Chemical Structures

Noordwijkerhout

The CCDC curates the world's leading database for organic and metal-organic crystal structures (the CSD). In addition, we develop software solutions to derive insight from the data contained in the CSD as well as provide world class, data-driven cheminformatic applications for drug discovery and development.

CSD-CrossMiner



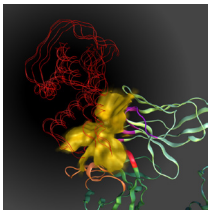
Our most recent application, CSD-CrossMiner, allows users to mine both the CSD and the PDB using pharmacophore- or substructure-based searching interactively to find repeated patterns of interactions or possible suggestions for potential scaffold hops.

Come chat with Dr. Jason Cole at booth B9 who can tell you about what we do and what we can provide for your organisation.

NEW IN MOE 2018.01

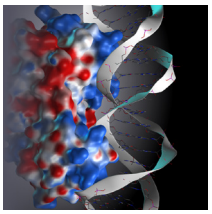
MOE 2018.01

NEW IN VERSION 2018.01



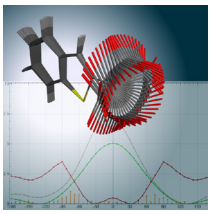
Epitope Mapping and Analysis

- Identify epitopes automatically during protein-protein docking
- Analyze and cluster Protein-Protein Interaction Fingerprints
- Visualize annotated epitope sequences and browse through associated protein poses



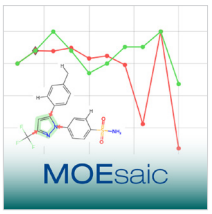
RNA/DNA Builder

- Build, edit, align and superpose DNA and RNA polynucleotide sequences
- Mutate and explore nucleotide conformations
- Introduce non-natural nucleobases for synthetic polynucleotide design



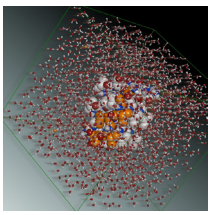
Torsion Scanning and Analysis

- Calculate bond torsions and plot energy curves using MM and QM
- Generate ligand conformers and identify optimal conformations and torsion angles
- Browse and compare QM torsion energy plots against Mogul statistics



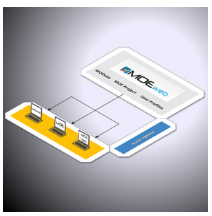
MOEsaic – SAR and MMP Analysis

- Calculate and plot R-group contributions to molecular properties
- Search and filter matched molecular pair lists to find activity cliffs
- Improved plot capabilities



Unified Molecular Dynamics Interface to AMBER

- Launch AMBER for MD simulations using a streamlined interface
- Generate and convert parameters automatically through MOE
- Run MD on parallel clusters or GPU and analyze trajectories in MOE



MOE/web Enhancements

- Update client machines with new or customized SVL applications
- Build and deploy custom project and user profiles across client computers
- Run remote Scaffold Replacement searches against large fragment databases

To learn more about MOE, please visit: chemcomp.com

About MOE

MOE is a leading drug discovery software platform that integrates visualization, modeling and simulations, as well as methodology development, in one package. MOE scientific applications are used by biologists, medicinal chemists and computational chemists in pharmaceutical, biotechnology and academic research. MOE runs on Windows, Linux, Unix, and MAC OS X.

MAIN APPLICATION AREAS

- Structure-Based Design
- Fragment-Based Design
- Pharmacophore Discovery
- Medicinal Chemistry Applications
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- Protein and Antibody Modeling
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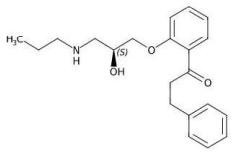
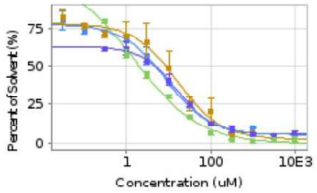
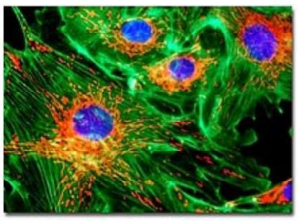
	Chemical Properties	Cell-based ELISA	Pharmacological Activity				Cytometry IC50
Molecule	Molecular weight (g/mol)	Dose-response Plot	pIC50	LE	LipE	clogP	Microscopy Image
CDD-1413022 	341.451	 Flag outliers & Override	6.48	0.37	2.84	3.64	

Activity & Registration
Store and organize your data

Store, Search, Analyze, & Report

CDD Vault is a modern web application for your chemical registration, assay data management and SAR analysis. It lets you organize drug discovery data and collaborate across project teams. It is simple to use and extremely secure.

Visualization
Plot datasets and mine them

Interact, Calculate, Compare & Publish

CDD Vault is a dynamic analysis tool for drug discovery data. It lets you plot and analyze large data sets to find interesting patterns, activity hotspots and outliers. With publication quality graphics, it is easy to illustrate and share results across project teams.

Inventory
Keep track of compounds

Debit, Track & Locate

CDD Vault is an Integrated inventory system for your compounds and reagents. Stay informed of the current status of your inventory whether in-house or shared externally.

ELN
Document all your research

Capture, Search, Protect & Work Together

CDD Vault is the ultimate electronic lab notebook, integrated directly with the chemical and biological assay data repositories and our full analysis and visualization environment. Designed for project teams, you can archive and search all of your experiments with ease and collaborate securely.

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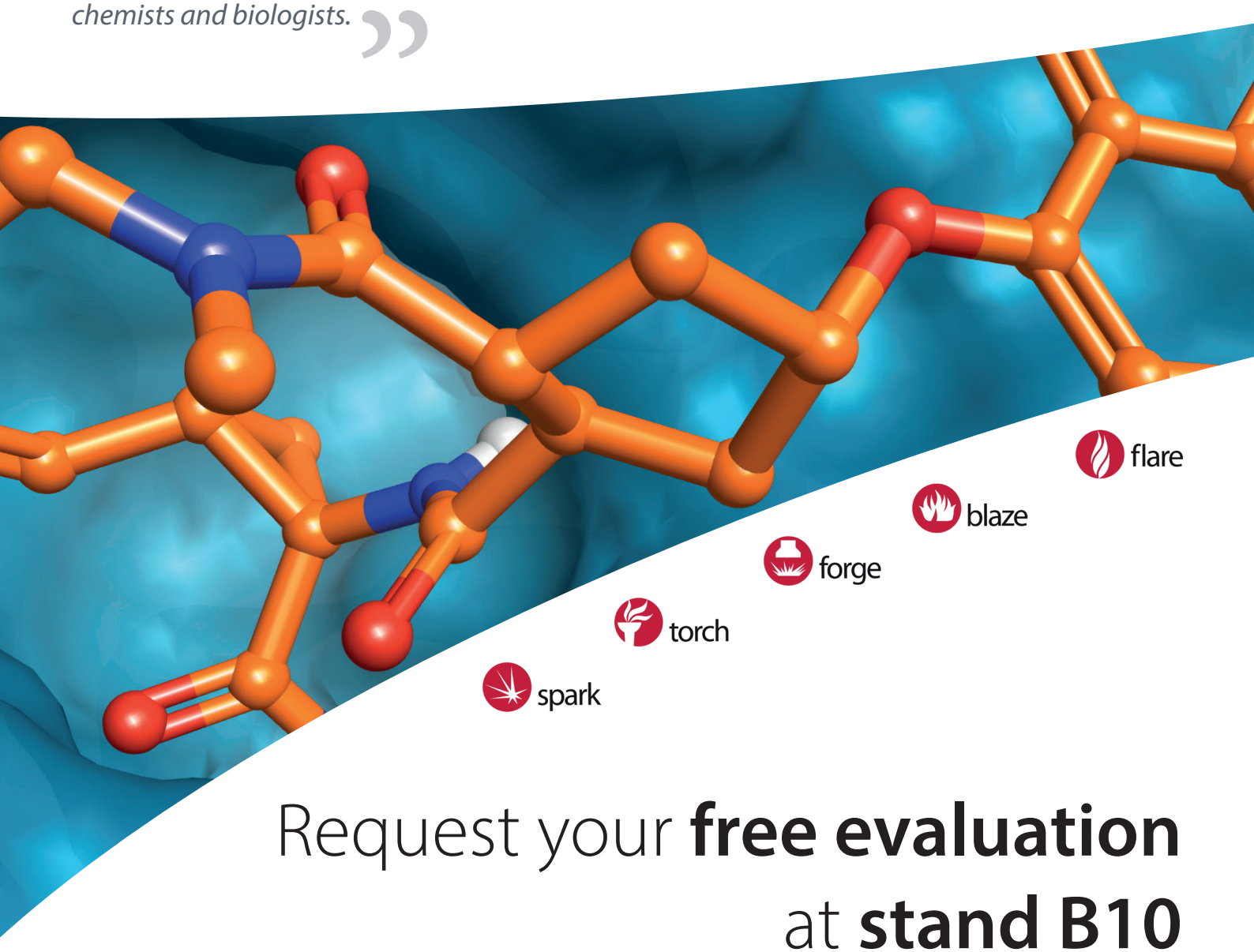

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CULGI covers all aspects of multiscale modeling in chemistry, from quantum chemistry to molecular and coarse-grained modeling, chemical informatics and thermodynamics, and machine learning.

https://www.culgi.com

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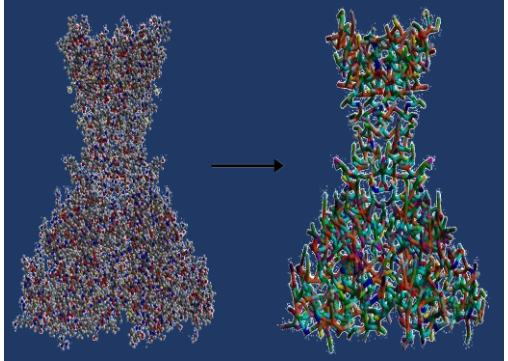

Atomistic (left) and coarse-grained (right) representation of the hERG voltage-gated potassium channel. The coarse-grained representation of hERG is obtained using the mapper function in the Culgi software.

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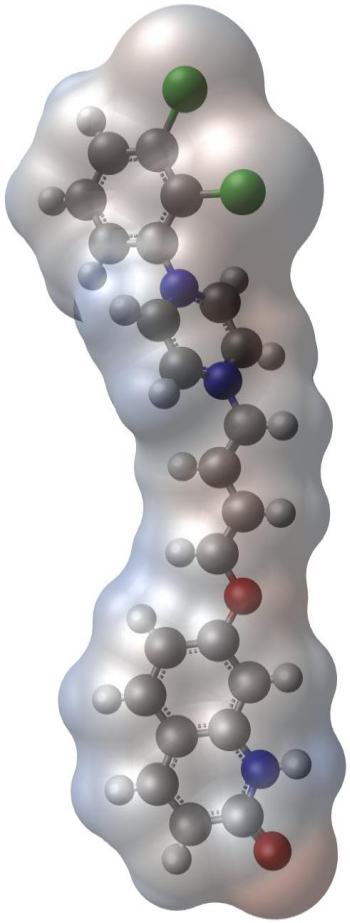
MOLECULAR MODEL: The screening charge density surface around the aripiprazole drug molecule. Aripiprazole is the recommended drug for the treatment of schizophrenia.



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Ideal tool for the broader aspects of digitalization of chemical R&D, in particular, IP protection

- ✓ Unique CULGI Graphical Programming Environment
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- ✓ Fast solution for a wide variety of problems
- ✓ CULGI scripting language or python
- ✓ Workflow as a simple end-user graphical user interface
- ✓ Operates from intra-clouds

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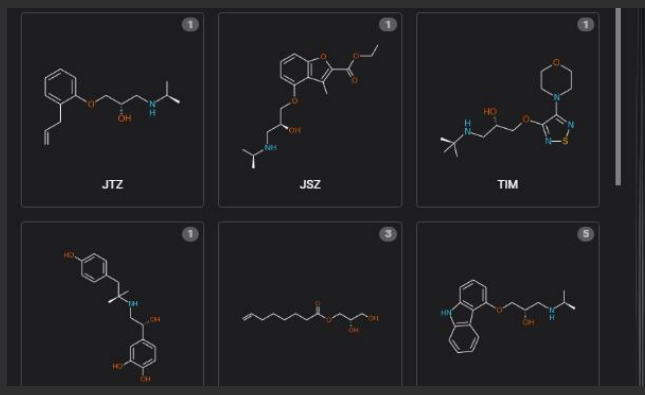

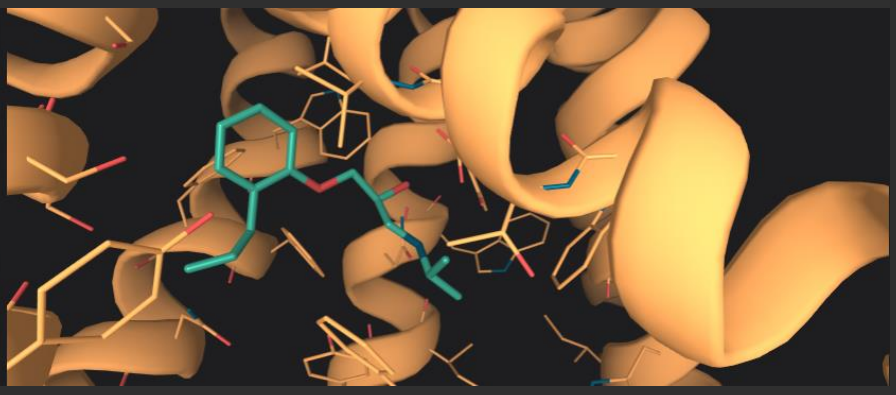

Increase your productivity

Save time comparing similar pockets and ligands. Create and test hypotheses on the fly. Visualize hot spots or mutation in 3D with one click. Share ideas with colleagues quickly and easily.

Benefit from collective intelligence

Extract and apply knowledge that has been generated over time by different project teams and research programs. Maximize the value of your data by keeping it alive and searchable.

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Inte:Ligand is the scientific leader in developing modern scientific software solutions known for intuitive and inspiring graphical user interfaces. We offer unique algorithms, software platforms, and research services for molecule discovery, trusted by scientists worldwide in the pharmaceutical, cosmetic, agrochemical, and nutrition industries.

Our innovative solutions include:

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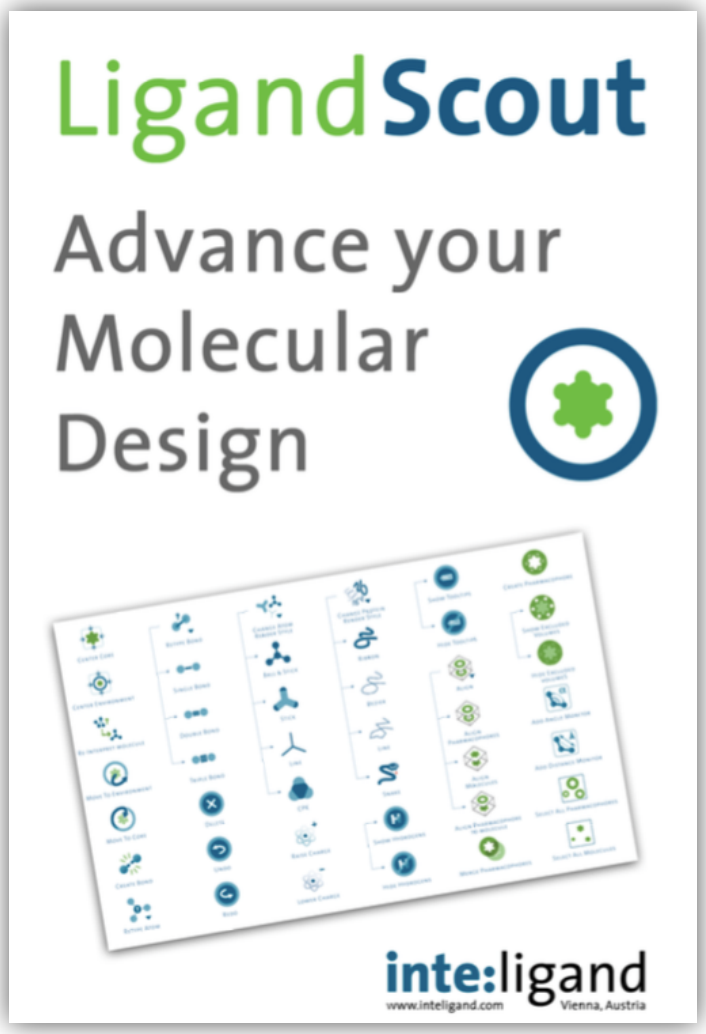
- Tackling PPIs.
- Fragment-based design.
- Hit triaging.
- Compound library creation & management.
- Activity-profiling.
- Tox prediction.
- Chemistry decision support .
- A full range of chemoinformatics tools.



The first to develop technology to automatically detect 3D-interactions between large and small molecules in a click of a button, we continue advancing the field by being the first to develop interactive tools to interface our 3D-pharmacophore technology with docking and molecular dynamics simulations.

Find out more about research services, software packages, algorithms and chemoinformatics tools to advance your discovery projects by visiting our booth at the ICCS 2018, Nordwijkerhout Expo.

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KNIME

Bringing Science to your Data

KNIME in the Life Sciences

KNIME Analytics Platform is a tool for data analysis, manipulation, visualization, and reporting, based on the graphical programming paradigm.

A diverse array of life science extensions adds cheminformatics, molecular modeling, bioinformatics, image processing and visualization capabilities.

Combined with KNIME Server and WebPortal, KNIME allows you to securely share your workflows and easily make them available as web applications or REST-based web services that can be used by your colleagues.

With KNIME, you have the power and simplicity to rapidly prototype ideas, share complex analyses with colleagues, articulate complex processes easily, and load and integrate data from diverse data sources.

In Brief

- Nodes for data I/O, preprocessing, cleansing, etc.
- Extensive support for machine learning, including deep learning
- Integration with R and Python
- Wide range of interactive views, i.e. scatter plots & parallel coordinates
- Tools from leading cheminformatics vendors
- Community contributed extensions for working with chemistry, biology, and image data.

Powerful Analytics

Powerful: A large library of native nodes, community contributions, and tool integrations makes KNIME Analytics Platform the perfect toolbox for any data scientist.

Reliable and Trusted: Hardened in the field since 2008 with bi-annual software releases and thousands of dedicated users.

Scalable: Toggle easily between single computer, streaming, and big data execution. Integrate new capabilities on top of, alongside, or within your existing infrastructure.

Room to Grow: Extend the capabilities of KNIME Analytics Platform with KNIME Server for collaboration, automation, and deployment functionalities.

Data and Tool Blending

Data Blending: Simple text files, databases, documents, images, networks, even data based on Apache Hadoop, can all be combined within the same visual workflow.

Integrating R and Python: Include R and Python code in your KNIME workflows, reusing expertise, which is graphically documented and shared among data scientists.

Tool Blending: KNIME Big Data Extensions integrate Apache Hadoop, Spark, and MLlib. Additional integrations include deep learning frameworks and other machine learning libraries (H2O, Weka, and more). Blend state of the art tools with the ease of use of KNIME workflows.

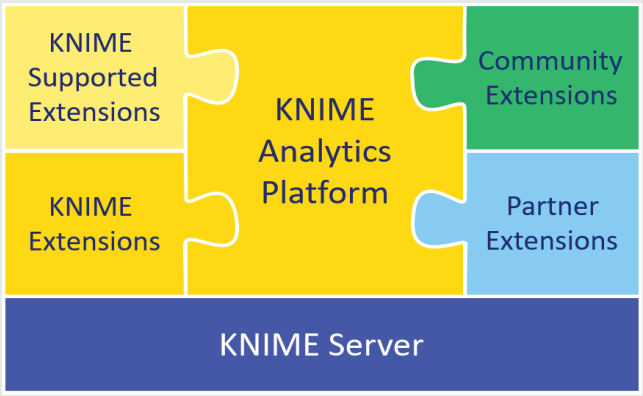
Visual Documentation: Easy to learn graphical interface means that coding is optional and work is documented visually.

Open for Innovation

Portable and Durable: Backwards compatibility ensures that existing workflows continue to function with new versions, future proofing your work. Industry leading PMML support allows effortless model portability and deployment.

Open Platform: Be inspired by hundreds of example workflows available on the public example server and fully functional, real world use cases.

Unrestricted Open Source: We release our latest, complete code base under the GPLv3 license, with support for major operating systems. The only restriction is your creativity.



About KNIME

At KNIME®, we build software for fast, easy and intuitive access to advanced data science, helping organizations drive innovation.

For over a decade, a thriving community of data scientists in over 60 countries has been working with our platform on every kind of data: from numbers to images, molecules to humans, signals to complex networks, and simple statistics to big data analytics.

Our headquarters are based in Zurich, with additional offices in Konstanz, Berlin, and Austin. We're open for innovation®, so visit us at KNIME.com.

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NextMove Software develops scientific software solutions for the pharmaceutical and life sciences industries. Our current best selling products include:

ARTHOR	Arthor provides fast state-of-the-art substructure and chemical similarity search capabilities for ultra-large databases of hundreds of millions of compounds, using SMARTS optimization, Just-In-Time compilation and/or GPUs.
CASANDRA	Casandra is an in-house web service for providing real time chemical safety warnings of experimental hazards and incompatibilities directly to the (Perkin-Elmer) Electronic Laboratory Notebook (ELN) client as planned by the chemist.
HAZELNUT	HazELNut is a suite of tools used to extract, normalize and analyze reactions from Electronic Lab Notebooks (ELNs). This can be used to export to a data warehouse or search system, identify duplicates, name/classify reactions and so on.
LEADMINE	LeadMine is used to mine text for chemicals and other entities, using CaffeineFix technology to (spell-correct) match terms from dictionaries, ontologies and grammars. PatFetch simplifies analysis of patents as a web service GUI.
MATSY	Matsy is a suite of tools for creating and analysing Matched Molecular Series (the general form of Matched Molecular Pairs). In particular, it can be used to propose compounds to make/test next in a medicinal chemistry campaign.
PISTACHIO	Pistachio is a reaction dataset browser providing loading, querying, and analytics of chemical reactions. With over 7 million chemical reactions extracted from US & EPO patents, it demonstrates an AI interface to faceted (structure) search.
SMALLWORLD	SmallWorld is an index of chemical space based on more than 69 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 structures. This makes it easy to interconvert between small molecule representations (e.g. SMILES, MOL) and biopolymer representations (HELM, FASTA, PLN, IUPAC line notation).

NextMove Software Limited,
Innovation Centre (Unit 23),
Cambridge Science Park,
Milton Road, Cambridge,
England CB4 0EY

www.nextmovesoftware.com

Attend our Pre-Conference Workshop on Sunday, May 27th 2018 from 15:00-17:00

"Orion - CADD on the Cloud"

- Orion is OpenEye's reimagining of all the elements of CADD conducted entirely within a cloud service, in our case Amazon Web Services (AWS), delivered as either a hosted system or an in-house VPC solution
- As a 'cloud native' platform Orion completely automates and manages access to large scale AWS processing and storage
- In-cloud facilities include molecular design, 3D visualization, data analysis, results/method sharing and project organization
- All of OpenEye science is included, enabling users to construct innovative workflows with Floe, our pipelining tool
- As an open platform Orion allows for straightforward integration of third-party code (customer, academic, vendor)
- Interaction with Orion is via a simple webpage, deliverable on any internet-enabled device

Interact with Orion via web browser on any internet-enabled device.

OpenEye has built a solid reputation as a scientific leader in the field of molecular design based on two decades of delivering useful applications and programming toolkits. Our scientific approach has focussed on the power of molecular 3D structure to inform and guide, in particular via the concept of shape similarity. We have changed industry perception of what is possible with the speed, robustness and scalability of our tools and have recently built these into a ground-up, cloud-native platform, Orion. Combining unlimited computation and storage with powerful tools for data sharing, visualization and analysis in an open development platform, Orion offers unprecedented capabilities for drug discovery and optimization.

OpenEye SCIENTIFIC

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

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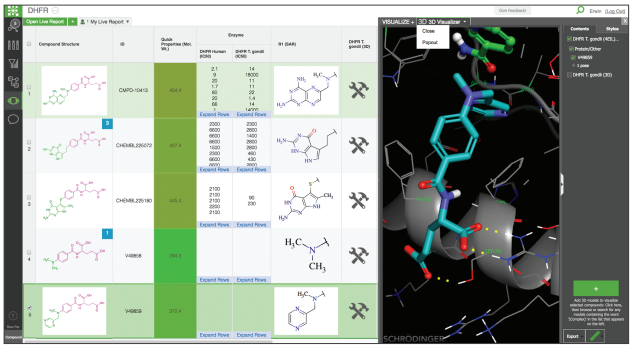
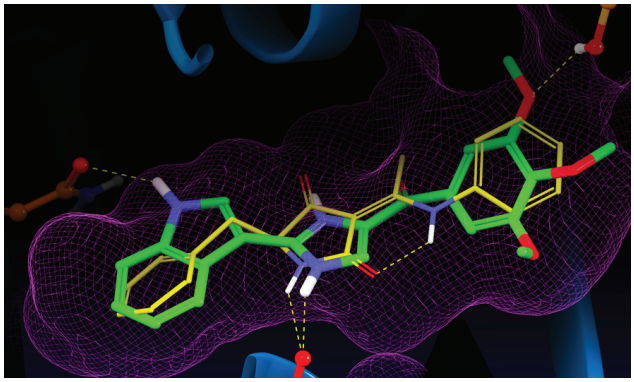


Real-time Collaboration with LiveDesign

LiveDesign is a highly-collaborative web-based platform for workflow management and computational modeling alongside experimental data analysis and powerful cheminformatics.

Learn more at https://www.schrodinger.com/livedesign



Try the Small-Molecule Drug Discovery Suite

A comprehensive suite to accelerate lead discovery and lead optimization. This suite features a wide range of virtual screening options, including the industry-leading Glide, advanced computations to estimate binding affinity, analysis to assist in structure prediction, and much more!

Request a trial evalution at https://www.schrodinger.com/request-trial-license

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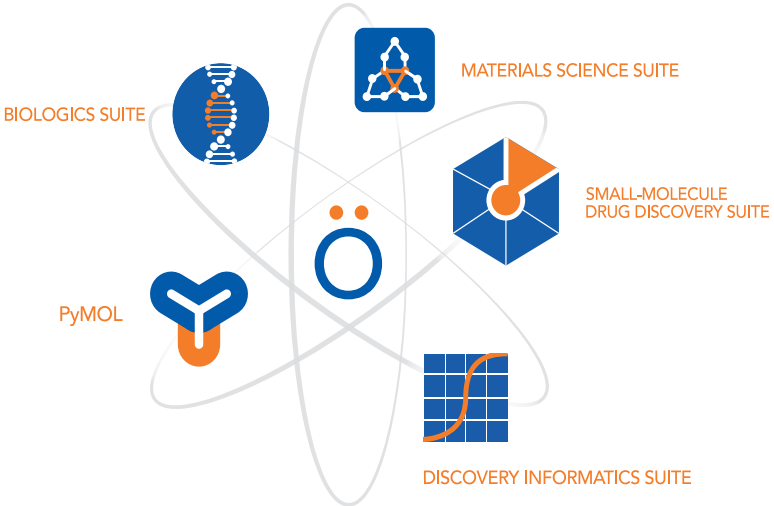
A scientific leader in computational chemistry, providing software solutions and services for life sciences and materials research

Schrödinger aims to provide integrated software solutions and services that truly meet its customers' needs. We want to empower researchers around the world to achieve their goals of improving human health and quality of life through advanced computational techniques that transform the way chemists design compounds and materials.

By building and deploying breakthrough collaborations and partnerships, we help scientists accelerate their research and development activities, reduce costs, and make novel discoveries that might otherwise not be possible.

Schrödinger Product Suites



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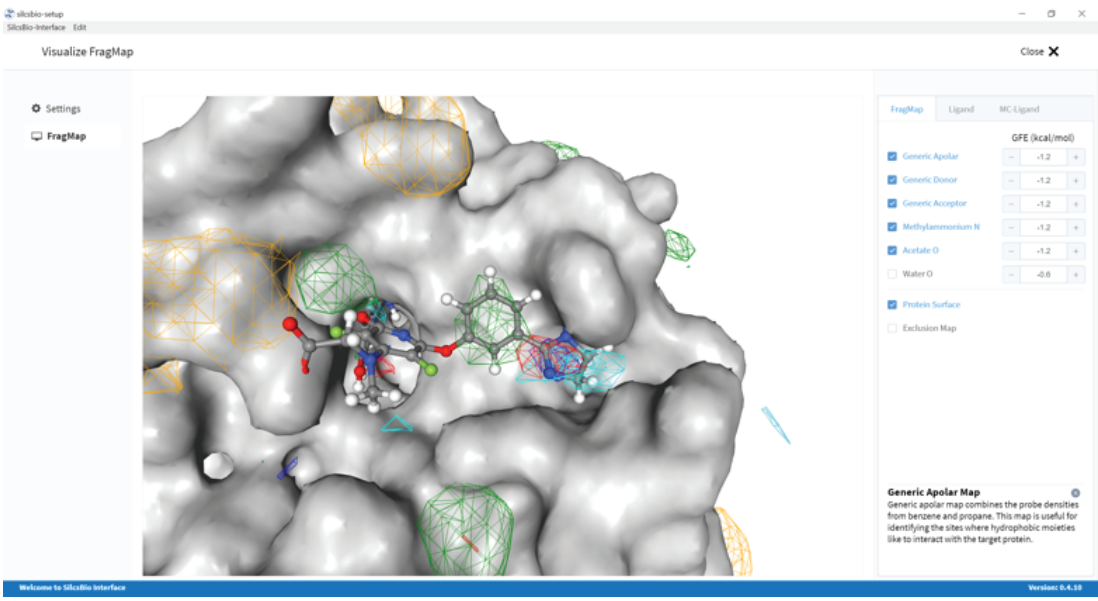
SILCSBIO

SilcsBio offers proprietary computer-aided drug design software and related services. Our main products include SILCS. Single-Step FEP. and the CGenFF program. Visit our booth at ICCS to test drive the new GUI. explore FragMaps. and learn more about the CGenFF Parameter Optimizer!

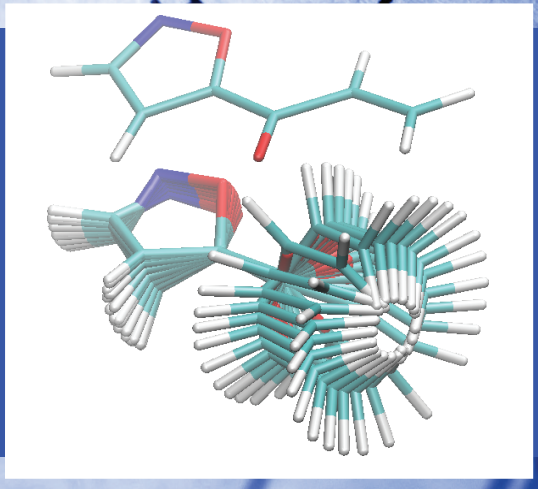
Graphical User Interface

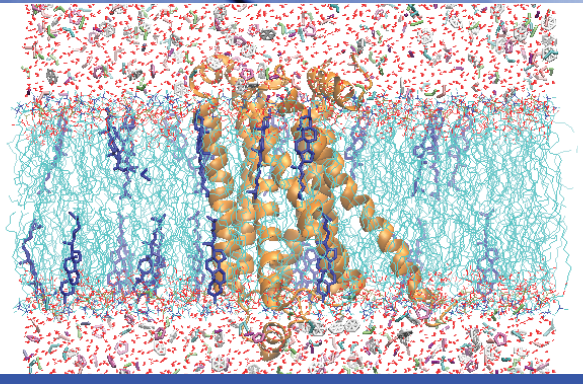
-Easy set up for SILCS and SSFEP projects
-Simple job submission to remote host
-Convenient job progress tracking
-All-in-one results visualization: SILCS FragMaps. SILCS-MC. and SSFEP



CGenFF Parameter Optimizer

Conveniently optimize dihedral angles receiving high penalty scores with QM dihedral scans in Psi4.





SILCS with Transmembrane Receptors

A new command-line tool automates SILCS simulation setup for GPCRs and other transmembrane proteins.

SilcsBio. LLC 8 Market Place. Suite 300. Baltimore MD 21202 www.silcsbio.com

The Xemistry Tools Universe

We develop multi-platform tools allowing you to effectively bridge the gaps between applications, or to rapidly implement your own chemistry data processing ideas without dealing with all the low-level details.

At the core: The CACTVS Toolkit – the universal foundation for chemical information processing

KNIME Node Compiler – script your own networked KNIME nodes without Java programming

Python Scripting Interface – standalone interpreter, or loadable module for any Python3-enabled software

Database Cartridges – add chemistry query functions and in-database scripting to Mysql, PostgreSQL, SQLite, …

Tcl Scripting Interface – stand-alone truly multithreading interpreter, or loadable module for any Tcl-enabled software

Web scripting – develop interactive chemistry Web tools with (F)CGI backends and ExtJS JavaScript framework integration

Custom Libraries – planning on developing new commercial software? We provide libraries for cheminformatics core functions

Script Wrapper – transform your scripts into independent stand-alone ready-to-run applications

Xemistry chemoinformatics

Please visit us at our booth.

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- Division of Chemical Information (CINF)
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- Royal Netherlands Chemical Society (KNCV)
- Computers in Chemistry Division (CIC)
  German Chemical Society (GDCh)
- The Chemical Structure Association Trust
  (CSA Trust)
- Chemical Information and Computer Applications Group (CICAG)
  Royal Society of Chemistry (RSC)
- Division of Chemical Information and Computer Science
  Chemical Society of Japan (CSJ)
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- European Association of Chemical and Molecular Sciences (EuCheMS)