GCC 2012

8th German Conference on Chemoinformatics

Exhibition Newsletter

TOPICS

- List of Exhibitors
- Pre-Conference Workshops
- Free Software Session
- Room Plans
- Exhibitor One-Pagers

Welcome

Welcome to the *8. German Conference on Chemoinformatics (GCC2012)*

Dear GCC2012 participant,

this ***Exhibition Newsletter*** will inform you about the conference exhibition, the free software session and the pre-conference workshops.

In addition, the newsletter contains a floor plan, a summarized exhibition schedule, detail information about the content and location of the **two pre-conference workshops** and the Free Software Session. Furthermore, it includes one-pagers of our exhibitors including latest product news.

The technical program for the conference can be found on the conference web site as PDF or online version at http://www.gdch.de/gcc2012. A link to the corresponding abstracts can also be found on the web site.
The GCC2012 can also be followed via Twitter using the tag #goslarcheminf

See you on Sunday, November 11 in Goslar, Germany.

Sincerely

Frank Oellien
GDCh CIC Chairman

List of Exhibitors

Exhibitor	URL
AKos	www.akosgmbh.de
CERTARA	www.certara.com
ChemAxon	www.chemaxon.com
Chemical Computing Group	www.chemcomp.com
Dotmatics	www.dotmatics.com
OpenEye	www.eyesopen.com
Xemistry	www.xemistry.com

List of Sponsors

Conference Main Sponsor

Chemical Computing Group

FIZ Chemie Berlin Award Sponsor

FIZ CHEMIE Berlin

Poster Session Sponsor

Journal of Cheminformatics

Conference Dinner Sponsor

Journal of Chemical Information and Modelling

Exhibition & Marketplace Schedule

Sunday, 11th

14:00 – 15:30 Free Software Session **Großer Saal**

- **Get your Chemistry right with KNIME**
  Meinl, T., Konstanz/D
- **RDKit**
  Landrum, G., Basel/CH

15:00 Build-up of the Exhibition **Barbarasaal**

16:00 – 18:00 Pre-Conference Workshops (Chemoinformatics Marketplace)

This year Chemical Computing Group, and ChemAxon will offer free pre-conference workshops during the market place event on Sunday afternoon.

- ***New Developments of the MOE 2012 Release*** **Großer Saal**
  Chemical Computing Group

- **Using ChemAxon's Discovery Toolkit within Workflow Tools: KNIME and Pipeline Pilot** **Großer Saal**
  ChemAxon

Monday, 12th

10:30 – 11:00 Coffee & Exhibition **Barbarasaal**

16:30 – 19:00 Exhibition (including exhibition rallye) **Barbarasaal**

Tuesday, 13th

10:05 – 11.00 Coffee & Exhibition **Barbarasaal**

15.30 – 16.00 Coffee & Exhibition **Barbarasaal**

Workshop Details

In parallel to the Free-Software-Session **two free pre-conference workshops** will be organized on Sunday afternoon right before the official conference opening. The pre-conference workshops and the Free-Software-Session will be held in the room **"Großer Saal"** in the conference venue "Der Achtermann".

Chemical Computing Group, Free Workshop:
New Developments of MOE 2012 Release

16:00-17:00

The workshop will describe the new developments in the 2012 release of the Molecular Operating Environment, MOE. These include:

- A new reaction-based Combinatorial Library enumeration application
- A new capability for locating and visualising predicted water locations in binding sites, based on 3D-RISM calculations
- Prediction of protein properties (sequence and atom-based)
- An application for protein design, based on targeted mutations, including exploration of alanine / cysteine scanning, etc.
- A protein "patch analyser", allowing visualisation of surface properties and their relation to sequence and secondary structure

Please contact Steve Maginn (smaginn@chemcomp.com) for details.

ChemAxon, Free Workshop:
Using ChemAxon's Discovery Toolkit within Workflow Tools: KNIME and Pipeline Pilot

17:00-18:00

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

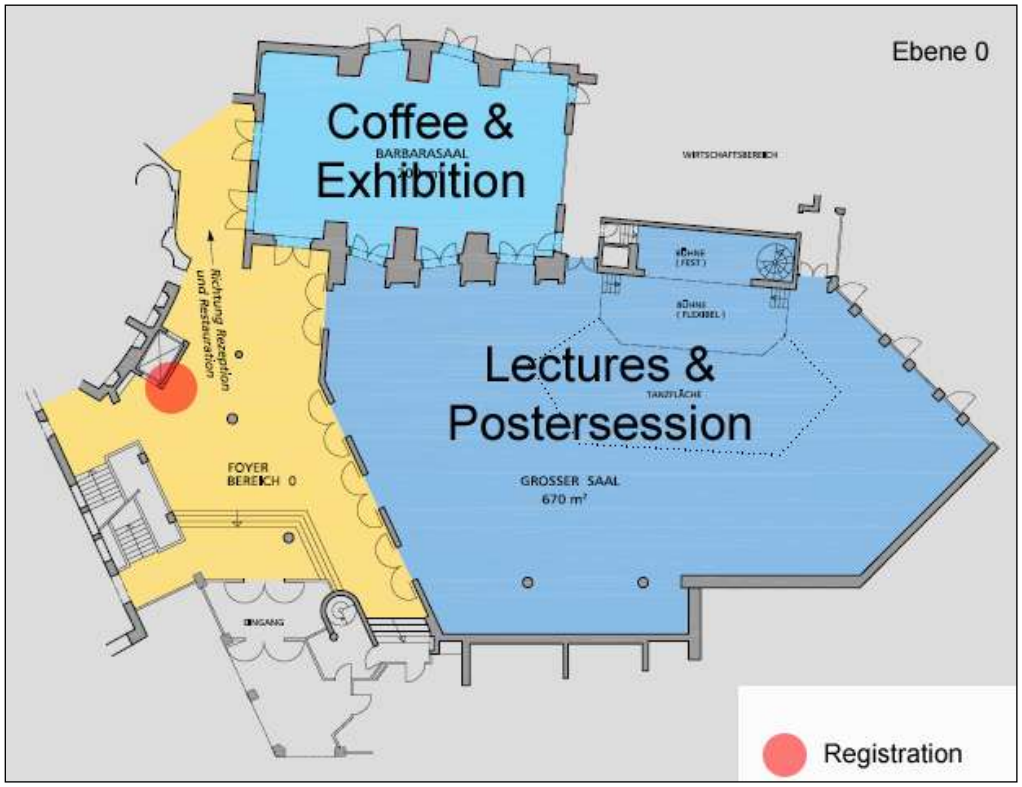
ChemAxon has an extensive API for working with chemical structures. The majority of functionality can be accessed through nodes and components for the KNIME and Pipeline Pilot workflow platforms, enabling end-users to quickly build and re-use workflows to generate analyses and reports.

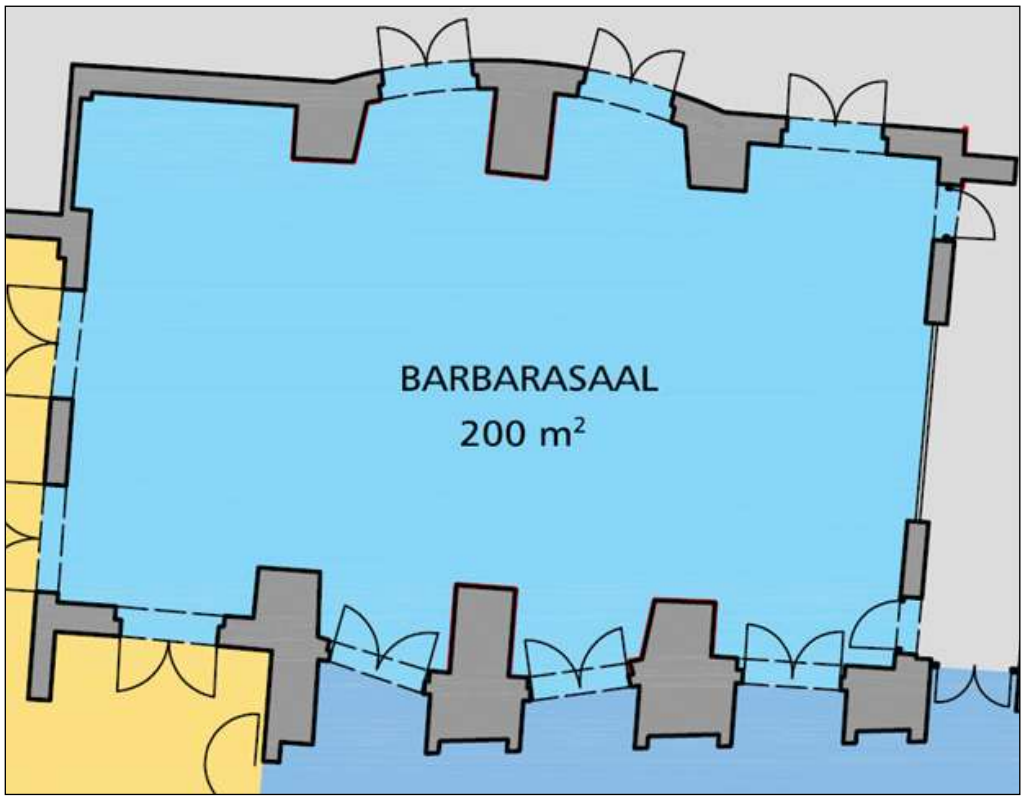
Based around ChemAxon's Discovery Toolkit we will give an introduction to the technology available in workflow tools, including virtual enumeration, property prediction and screening and provide workflows corresponding to some common discovery processes. The workshop will primarily use the KNIME platform and will highlight practical user aspects through real life examples, mainly focusing on virtual library design and analysis, as well as document processing for chemical research.

Please contact Alex Allardyce (aallardyce@chemaxon.com) for details.

Floor Plans / Room Plans

The exhibition will take place in the **Barbarasaal** (basement, Ebene 0) of the hotel.

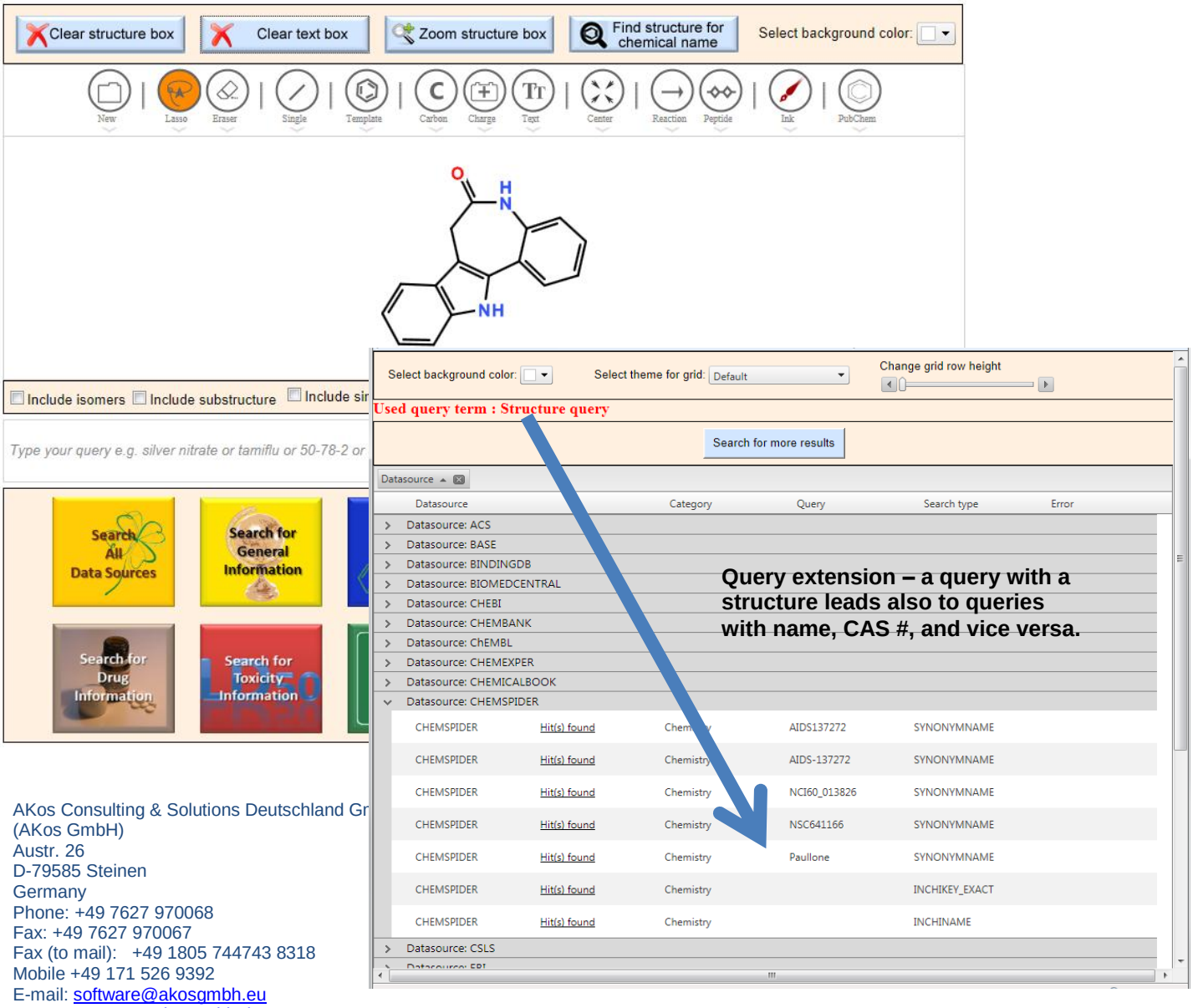




RunsEverywhere Global Search should replace Google as search engine for chemists and biologist searching for scientific information.

- **More comprehensive**
  - Google covers a lot, but by far not everything. For instance Google cannot search in a database
- **Much less link results**
  - Would you open a link to Google with 1 million hits, or to PubChem with one hit?
- **Sort and group the results**
- **Choose the sources**
  - Google searches over everything, here you can choose your databases/sources
- **Query extension**.

Try it out: http://cwmglobalsearch.com/gsaspdev/default.aspx



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Multi-Criteria Drug Design • Lead Identification • Lead Optimization • Predictive Safety • Off-Target Prediction

Muse®

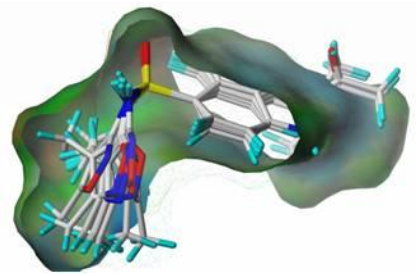
Identify and Optimize Lead Compounds

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.

- 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
- Integrate your own properties or CADD models (e.g. docking, ADME prediction, etc.)
- Intuitive and easy to use for medicinal chemists, casual modelers and expert computational chemists

SYBYL®-X

Molecular Data Explorer, QSAR Project Manager, and more!

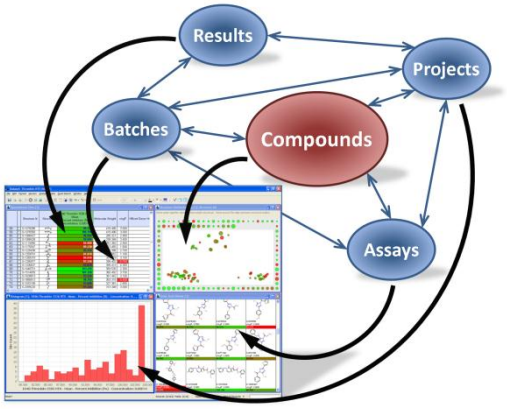


SYBYL-X has everything you need for drug design and other molecular discovery projects, from HTS follow-up through late Lead Optimization. Easily move from building a homology model for a target of interest to identifying potential lead candidates and multi-criteria drug design, to lead optimization 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.

PredictFX™

Identify and Address Drug Safety Issues

PredictFX is a modeling and simulation suite that provides improved opportunities to identify, monitor, and address safety issues earlier in the drug discovery process by predicting the off-target pharmacology, and its potentially associated side-effect profile, from the 2D structure of molecules. Developed by Chemotargets, a spin-off company from Jordi Mestres' lab, leaders in predictive safety, PredictFX enables scientists engaged at any stage of drug discovery and development to identify safety risks in order to guide optimization more effectively, and better manage attrition.



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.

About ChemAxon

ChemAxon makes desktop applications and software toolkits for structure visualization and management, structure based property predictions, virtual synthesis, screening and clustering. Our products work on all major operating systems and can be implemented into larger systems and web environments.

ChemAxon's software is used by leading commercial and academic research groups worldwide. We support academic teaching and research via our free academic package.

ChemAxon's Discovery Toolit

ChemAxon's Discovery Toolkit is a software suite which provides API, command line and (for some capabilities) integration within ChemAxon's desktop applications - Marvin, Instant JChem and JChem for Excel. By making the functionality available from various access points we ensure the relevance for a wide range of users.

Marvin & Calculator Plugins

Marvin is a collection of tools for drawing, displaying and characterizing chemical structures, reactions and queries. Calculator Plugins are modules of Marvin and JChem cheminformatics platforms. They include a wide range of structure-based prediction tools to explore the physico-chemical properties of chemical compounds (e.g. elemental analysis, pKa, logP, polarizability, conformers, etc.).

Fragmenter

Fragmenter is ChemAxon's solution for creating molecular fragment libraries based on various cleavage rules.

- Customizable fragmentation rules
- RECAP fragmentation & R-Group decomposition modules
- Fragmentation information is stored with fragments
- Generate fragment statistics

Reactor

Reactor allows the user to perform various multi-step virtual syntheses, using generic reaction equations and ChemAxon's Chemical Terms scripting language.

- Pre-built generic reaction library
- Fast enumeration
- No limitations in reaction type (inter/intra-molecular) reactants and product numbers
- No need to preselect reagents

Screen

The Screen suite provides tools for pharmacophore analysis and ligand-based high throughput virtual screening.

- Flexible Pharmacophore building (fragment & calculation-based solutions)
- Configurable Molecule Descriptor Generation (optimization through training)
- Suitable for ligand based approaches
- Available (batch, API, workflow nodes, etc.)

JKlustor

JKlustor is ChemAxon's solution to explorative data mining in combinatorial chemistry and drug design processes, where a large number of chemical compounds need to be analyzed.

- Wide range of clustering methods
- Flexible search options; Interactive display
- Efficient
- Available (batch, API, Web Services,workflow nodes, desktop applications,MCS viewer Applet)

You can try and evaluate all of our software for free.

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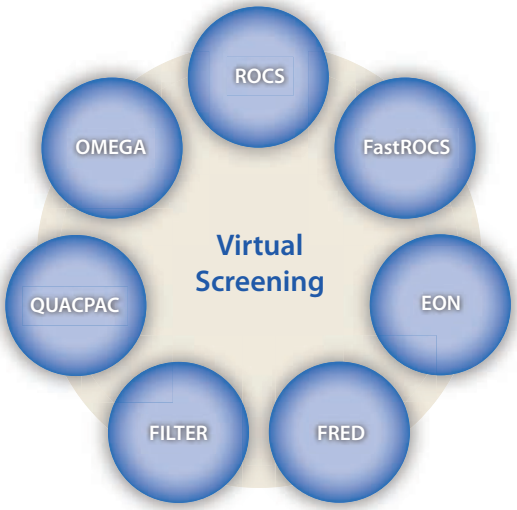
About OpenEye, Our Philosophy and Product Line

OpenEye Scientific Software has been developing large scale applications and toolkits for drug design and molecular modeling since 1997. Our software is designed to accurately quantify the shape and electrostatics of molecules, which we strongly believe are the main drivers in molecular interactions. OpenEye's software product line focuses primarily on virtual screening and lead hopping, and as such includes tools for conformer generation, docking, shape comparison, electrostatics, crystallography, visualization and cheminformatics. OpenEye also makes most of its technology available as toolkits - programming libraries suitable for custom development.



Virtual Screening

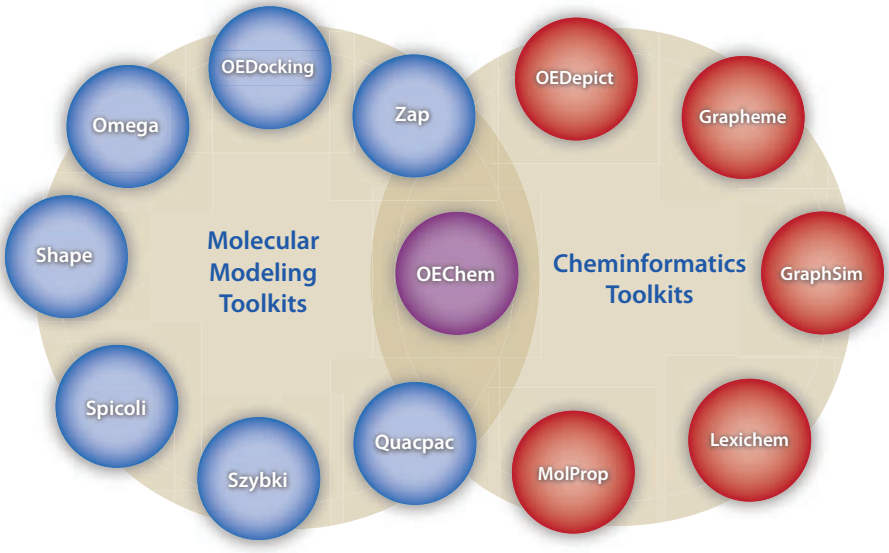
OpenEye's Virtual Screening applications include the following: FILTER, QUACPAC, OMEGA, ROCS, FastROCS, EON and FRED.

Input compounds are prepared by removal of undesirables (FILTER) and application of a variety of charge models (QUACPAC). OMEGA generates high quality 3D conformer ensembles. For ligand-based virtual screening, ROCS and FastROCS search compound libraries for 3D shape (and chemistry) similar molecules. EON is frequently used in conjunction with ROCS hitlists to identify lead-hops with electrostatic similarity to a query. For structure-based virtual screening, FRED is an exhaustive, rigid docking and scoring application.

Lead Optimization

OpenEye has developed novel, award-winning products for lead optimization. Our applications include: BROOD, FRED, SZYBKI, SZMAP, and POSIT.

Replacement of fragments with BROOD allows for lead-hopping and SAR exploration. Docking with FRED is useful for lead optimization, in addition to being an effective virtual screening tool. SZYBKI optimizes structures, optionally within a protein binding site. SZMAP explores the environment water encounters in a binding site to guide molecular design. POSIT utilizes information from known ligands to make very accurate, low strain pose positions.



Toolkits

OpenEye toolkits are programming libraries for creating customized applications which utilize OpenEye technology. Central to the portfolio is OEChem TK, OpenEye's programming library for chemistry and cheminformatics, on top of which a number of other toolkits have been built. Among the seven modeling toolkits, five
All the toolkits are written in C++ and have a stable, documented API. Functionality is also accessible via Python, Java and .NET wrappers.

www.eyesopen.com

OpenEye Scientific Software

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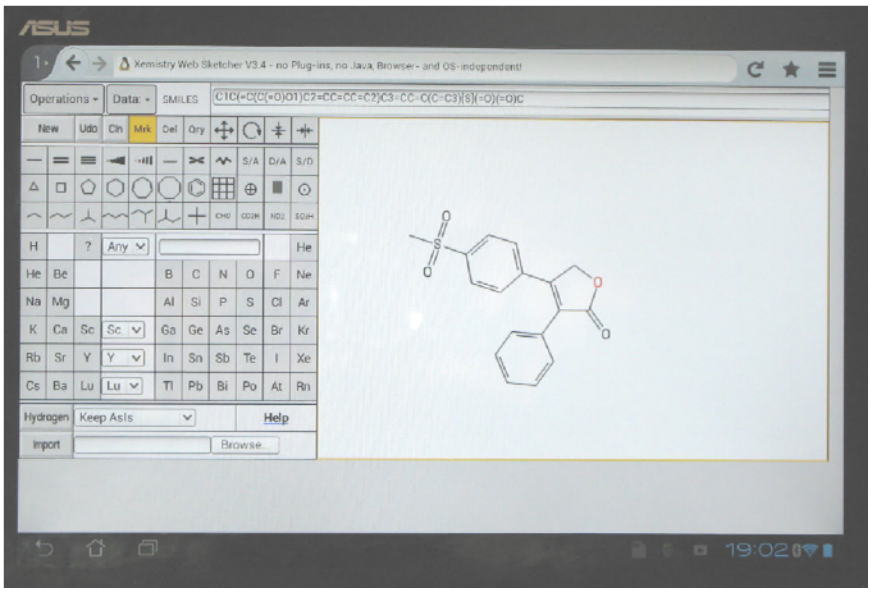
Technology Highlight:
Next Generation Structure Handling in a Web Context

Working with chemical structures and reactions in a Web context has become a standard chemoinformatics technique. However, new technologies and the demise of established approaches constantly require the re-evaluation of the suitability of tools and techniques used for both public and in-house Web portals:

- Java Applets have become a security nightmare, and generally fell out of fashion – Java is no longer installed by default or even available on many computers.
- The advent of new hardware, such as iOS- or Android-based Tablets makes it impossible to use platform-dependent PC plug-ins, even if that was a feasible option for controlled company environments until recently.
- This new hardware also poses interesting challenges in user interfaces – drawing a structure on a touchscreen, without keyboard and mouse, and with a 100x180 effective resolution and a small screen where a fingertip is larger than a standard bond length requires rethinking of interface paradigms.
- On the other hand, ever more potent JavaScript capabilities, JavaScript toolkits, document models and finally widely supported Web standards such as SVG as well as overlooked capabilities of portable formats such as PDF allow the implementation of advanced rendering modules, interactivity and intelligence in standard-conforming Web environments that are transparently accessible from PCs, Tablets and even Smartphones regardless of their brand.
- Moving applications to a Web environment poses unique integration issues –convenient drag&drop and clipboard data transfer with mainstream software such as MS Word or ChemDraw is a challenge – but can be done, as we show in our exhibition.

Please visit our booth and ask for a demonstration and discussion of our tools and components.



Picture: Xemistry Web Structure Sketcher on an Asus Transformer Android Tablet