GCC 2015

11th German Conference on Chemoinformatics

Exhibition Newsletter

TOPICS

- Workshops
- Exhibition
- Floor Plans
- Sponsors
- Software News

www.gdch.de/gcc2015

Welcome

Welcome to the *11. German Conference on Chemoinformatics (GCC2015)*

Dear GCC2015 participant,

In 2015 we have again managed to attract the leading software companies and publishers as exhibitors at the Germen Conference on Chemoinformatics. You will be able to get information about their newest technologies in Molecular Modelling, Data Mining, Data Analysis Information Management and much more. In order to plan your visit we provide you information about the pre-conference workshops and the conference exhibition in this **Exhibition Newsletter**.

The newsletter contains a floor plan, a summarized exhibition schedule, detailed information about the content and location of the **two pre-conference workshops.** 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/gcc2015. A link to the corresponding abstracts can also be found on the web site.

See you on Sunday, November 8 in Fulda, Germany.

Sincerely

Guido Kirsten

GCC Organizing team

Exhibitors

AKos GmbH	AKos	http://www.akosgmbh.de
Biovariance GmbH	biovariance	http://www.biovariance.com
CCDC	CCDC	http://www.ccdc.cam.ac.uk
CCG	CHEMICAL COMPUTING GROUP	http://www.chemcomp.com
Discngine S.A.S.	discngine	http://www.discngine.com
dotmatics	dotmatics knowledge solutions	http://www.dotmatics.com
IDBS Ltd.	idbs	https://www.idbs.com
KNIME.com AG	Open for Innovation KNIME	http://www.knime.com
OpenEye	OpenEye SCIENTIFIC	http://www.eyesopen.com
Xemistry	Xemistry chemoinformatics	http://www.xemistry.com

Sponsors

Main Sponsor

Further Sponsors

Non-Exhibiting Sponsors

JOURNAL OF
CHEMICAL INFORMATION
AND MODELING

Exhibition & Workshop Schedule

Sunday, 8th

12:00 – 13:30 Pre-Conference Workshops

This year OpenEye and KNIME will offer free pre-conference workshops.

• ***Getting your Chemistry right with KNIME*** **Salon Bonifatius**

KNIME

• ***OpenEye toolkits and iPython notebooks*** **Saal Köln**

OpenEye

16:00 – 16:30 Coffee & Exhibition Foyer

Monday, 9th

10:30 – 11:00 Coffee & Exhibition Foyer

16:00 – 20:00 Coffee & Exhibition & Poster Sessions Foyer

Tuesday, 10th

10:30 – 11.00 Coffee & Exhibition Foyer

Pre-Conference Workshops

OpenEye toolkits and iPython notebooks: A do-it-yourself workshop around chemoinformatic problems

With the advance of computing power in recent years more and more data can be generated quickly. Efficient data processing and decision making is more important than ever. OpenEye toolkits are designed to be robust and efficient and in combination with iPython Notebooks they become almost interactive to use.

During the course we will first give a general introduction on how to work with the OENotebook package. This is our in-house extension to the IPython Notebooks. After that, we will explain and modify a 2D/3D virtual screening analysis workflow on the fly.

Participants who bring their own laptop will be able to work in their browser on Online-Notebooks the same way as if they had a full installation of iPython Notebook and all toolkits on their local machine. In case participants want to keep a copy of their work - there will be a possibility to download the notebook at the end of the course.

The KNIME Analytics Platform -- Bringing Science to your Data

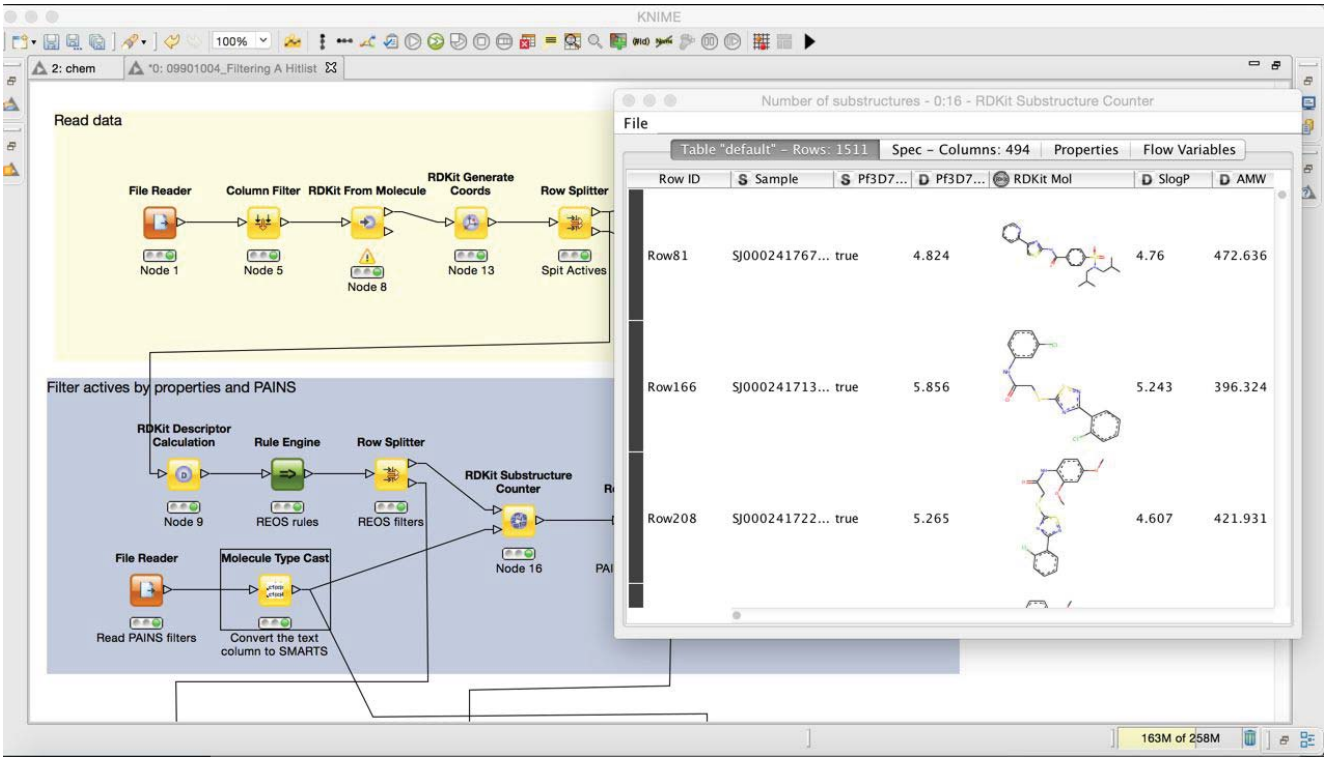
Jon Fuller[1,*], Thorsten Meinl[1]

[1] KNIME.com AG, Technoparkstr. 1, 8005 Zurich, Switzerland
[*] jon.fuller@knime.com

KNIME [1] is the leading open platform for data-driven innovation helping organizations to stay ahead of change. It is a tool for data analysis, manipulation, visualization and reporting, based on the graphical programming paradigm. A diverse array of life science extensions in KNIME add cheminformatics, molecular modeling, bioinformatics, image processing and visualization capabilities to KNIME Analytics Platform [2].

In this workshop you'll learn how to access typical chemistry formats like mol2, sdf and pdb. Then you'll learn how to generate molecular properties, and molecular fingerprints. We will cover the basics of building a classifier for compounds that are active or inactive against malaria. Finally we'll show a few examples of how to deploy KNIME workflows in a research and development environment.

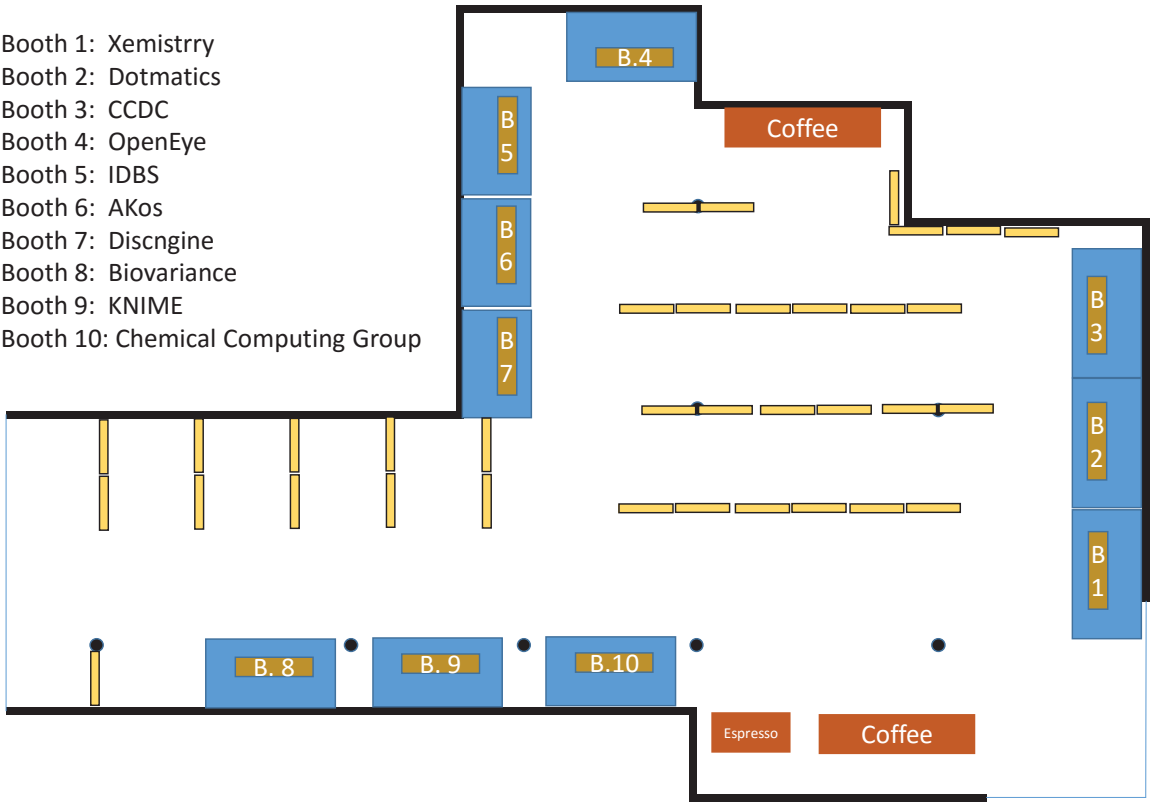
In combination with the KNIME Server & WebPortal [3], KNIME Analytics Platform also provides the nimble yet robust application architecture that is called for in Life Science Discovery Informatics [4] where High Content Screening and Next Generation Sequencing present a tough combination of high data volume, high data velocity and high data variety. 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.

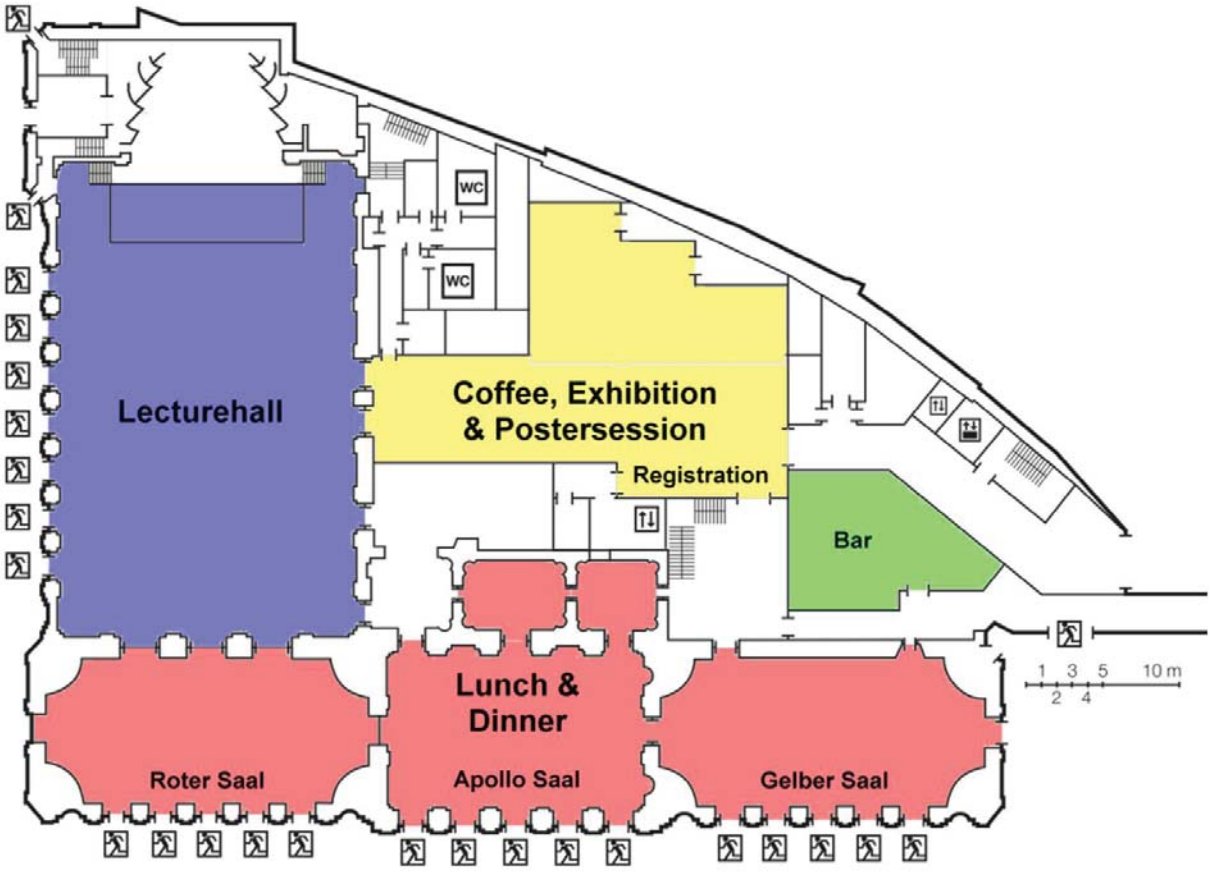


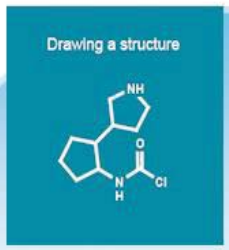
[1] http://www.knime.org/
[2] https://tech.knime.org/community
[3] http://www.knime.com/knimeserver
[4] https://www.knime.org/blog/knime-and-rest-a-dream-team-for-life-sciences-discovery-informatics

Floorplan Poster Session and Exhibition

Booth 1: Xemistrry
Booth 2: Dotmatics
Booth 3: CCDC
Booth 4: OpenEye
Booth 5: IDBS
Booth 6: AKos
Booth 7: Discngine
Booth 8: Biovariance
Booth 9: KNIME
Booth 10: Chemical Computing Group



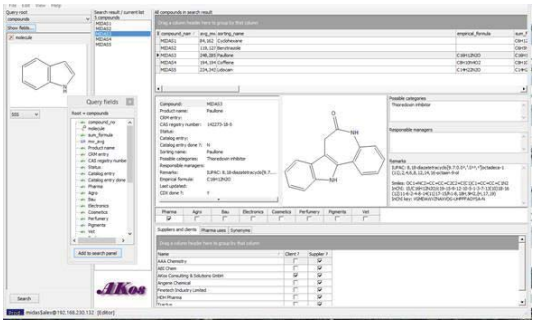




AKos
Consulting & Solutions GmbH

iScienceSearch
search the Internet by structure

AKosSamples
order samples



Services: We offer with ChemRPS (Chemical Registration and Publishing System) a complete chemical information system. We offer services to adjust the system to your needs. We have a lot of experience cleaning your data before we register them into the system:

Structure checker: This application checks the correct valence, weeds out wrong structures

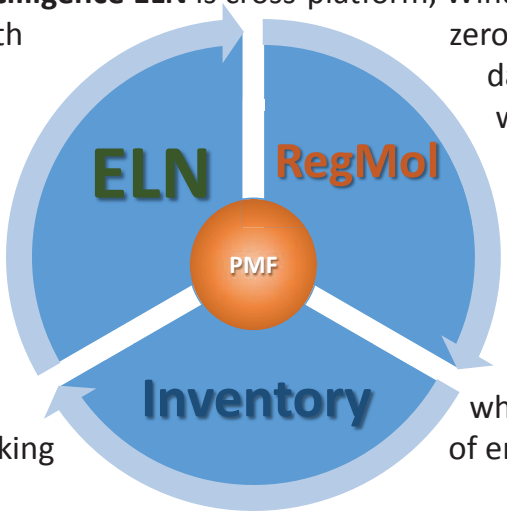
Standardize structures, for instance converts 5 valence nitrogen in 3 valence nitrogen (e.g. uncharged nitro groups gets converted in charged nitro groups)

Name checker: This application is able to correct errors in names, i.e. if words are spelled wrong like immidazole instead of imidazole. Such a correction cannot be 100%, but it finds many errors.

CAS number checker: This application checks if the CAS Registry Number is a valid CAS number. It finds incorrect assigned CAS numbers. Often the CAS number given is in reality for a salt and not for the parent. We only have access to CAS numbers that are in the public domain, but these are already quite a lot.

Data enrichment: This application can add synonyms, CAS Registry Numbers, IUAPAC names PASS parameters (predicted biological activities), …and more to a compound record.

Software from Scilligence: AKos GmbH is a reseller of **Chrawler** that can search structures & reactions in unstructured data (Word, PPT, Excel, OneNote, Chemical files, pdf, image files, etc.). **Chem4SharePoint** enables chemistry intelligence and biologics informatics in Microsoft SharePoint. **Scilligence ELN** is cross-platform, Windows, MAC, iPAD, Android, Linux and Chromebook with zero installation. **RegMOL** is a cloud based or in-house database for molecules and biologics R&D informatics, which can be extended to the **Inventory application.** **TouchMol for Office** puts structures with connec- tion table (searchable) into Excel, Word, OneNote and PowerPoint. **SAR** **Analyzer** is a grid with embedded structures and graphics. **Scilligence PMF** (Project and Material Management) let's you organize the daily workflow by showing on a timeline what to do, enables project based sharing of files, tracking of email, tasks and issues.



AKos GmbH is a **distributor of more than 25 million** of building blocks, and screening samples. A big part of the business is custom synthesis done in labs around the world.

biovariance

Komplexe Datenanalysen und Softwareentwicklung im Pharma- und Gesundheitsbereich

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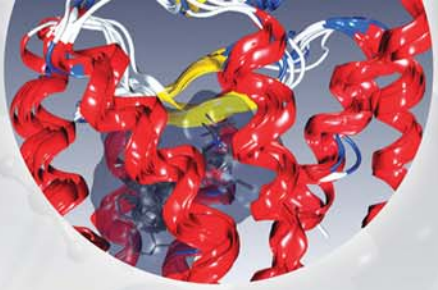
Berufseinstieg nach der Ausbildung und Praktika sind bei uns jederzeit möglich



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

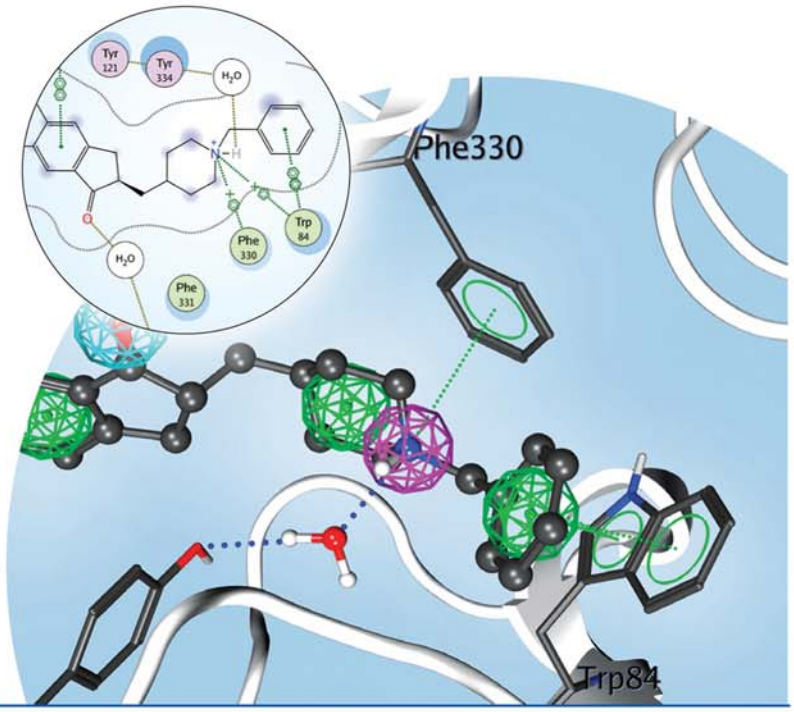
> SD Command Tools for Pipeline Workflows
> Washing, Filtering, Tautomer & Titration Enumeration
> 600+ Molecule Descriptors
> PLS, PCR, Binary QSAR, & Recursive Partitioning
> Similarity, Diversity, & Fingerprints
> 3D Conformer Generation from SMILES or 2D
> Combinatorial Library Design
> Automatic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

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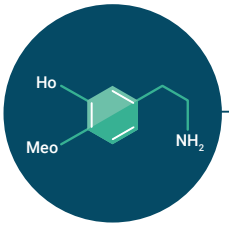
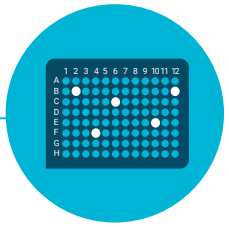
Decision Making

Sample Tracking

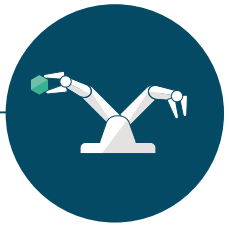


Cheminformatics



Screening

Scientific Computing



Robotics

Sometimes things make more sense

when you look at them differently

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knowledge solutions

Wisdom within arms reach. Imagine that. Innovation is about insight. It's a code cracked, complexity unravelled. Data turned into intelligence.

With E-WorkBook 10, organizations can improve their ability to extract insights from data more simply than ever.

E-WorkBook 10
Let's achieve

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Save the Date!

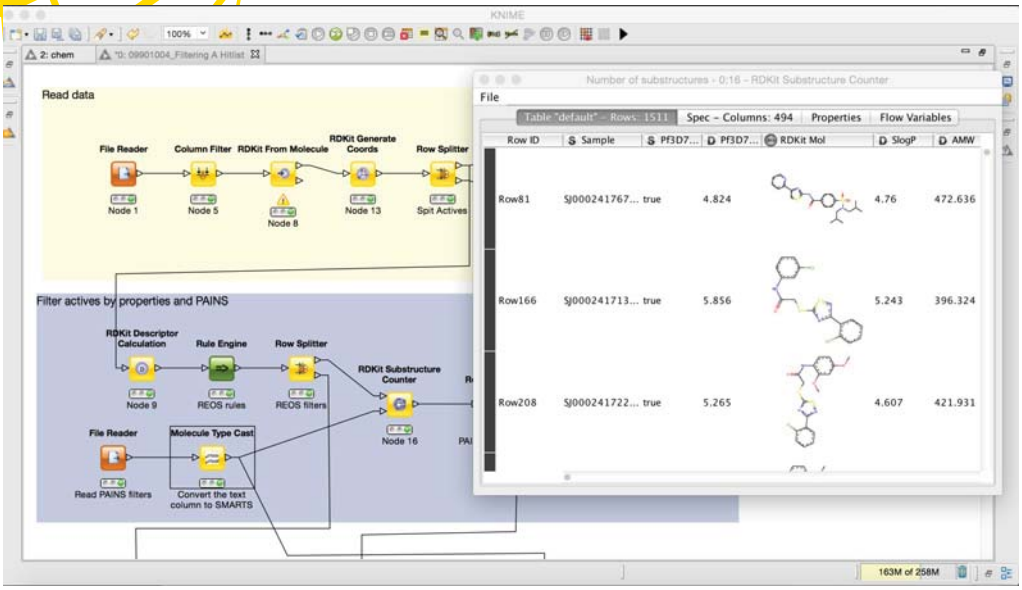
KNIME Spring Summit

Feb 24-26, 2016

DBB Forum Berlin

Open for Innovation
KNIME

KNIME Analytics Platform – Bringing Science to Your Data



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

Quick to deploy, easy to scale, and intuitive, 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.

KNIME in the Life Sciences

It is a tool for data analysis, manipulation, visualization and reporting, based on the graphical programming paradigm. A diverse array of life science extensions in KNIME add cheminformatics, molecular modeling, bioinformatics, image processing and visualization capabilities to KNIME Analytics Platform. In combination with the KNIME Server & WebPortal, KNIME Analytics Platform also provides the nimble yet robust application architecture that is called for in Life Science Discovery Informatics where High Content Screening and Next Generation Sequencing present a tough combination of high data volume, high data velocity and high data variety. 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.
- Wide range of interactive views, i.e. scatter plots & parallel coordinates
- Chemical structure representation
- Tools from leading cheminformatics vendors
- Community contributed chemistry plugs, molecular structures, cell assay images

KNIME TeamSpace

All of the KNIME Analytics Platform functionality, plus:

- Sharing workflows...
- ...metanodes, subnodes...
- ...and data within your team

KNIME Server Lite

All KNIME TeamSpace functionality, plus

- Remote and...
- ...scheduled execution
- User rights management

KNIME Server

All KNIME Server Lite functionality, plus

- SOAP and RESTful web service API
- Web access & execution of workflows
- Enhanced support

Open for Innovation
KNIME

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OpenEye SCIENTIFIC

Please register for our workshop / Sunday, November 8 at 12:00 – 13:30

"OpenEye toolkits and iPython notebooks: A do-it-yourself workshop around chemoinformatic problems"

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

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

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- Fully open access peer-reviewed journal with high visibility through global exposure
- Fast publication ensures the readers keep abreast of the most recent research results

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