echeminfo

Community of Practice for Applications of Cheminformatics & Chemical Modeling to Drug Discovery

Latest Advances in Drug Discovery & Planning Methods

Advanced Training Workshop

Oxford University, July 3-7, 2006

Interactive pragmatic workshops with leading experts and industry practitioners...

- Virtual Screening & Docking
- Structure-based Drug Design
- Reaction Planning & Library Design
- Latest advances in ADME & Predictive Toxicology
- Data Analysis & Visualisation
- Integration of Cheminformatics & Bioinformatics Tools & Data

Study problems in detail using leading-edge software. Discuss practical examples, methods and emerging techniques.

AND take home....

- A free copy of Quantum CAChe for Windows
- A full suite of OpenEye software for Windows and Linux with 30 day licence
- A one-year license of Schrodinger's Maestro valued at £300
- Two advanced textbooks by Lennart Eriksson on Multi- and Megavariate Data Analysis
- A CD with demonstration versions of Umetrics software
- One year's membership to eCheminfo (value £175) and access to the online library of eCheminfo meeting proceedings (2003-present)

The workshops will take place at the Chemistry Information Technology Center, part of the new, state-of-the-art Chemistry Research Laboratory at Oxford University.

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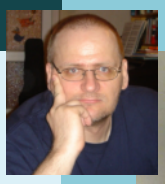
In silico Library Enumeration of Synthetically Feasible Libraries Gyorgy Pirok (ChemAxon) and Daniel Butler (Inhibox)



- Optimum conditions for 'synthetically accessible' libraries
- Create virtual libraries with provided software
- Designing properties for drug discovery and development
- Extend chemical space coverage with diversity
- Discuss real world workflows, limitations and liberations
- Discuss experiences and results from Inhibox case-study

Reaction Modelling and Prediction of Reaction Thermodynamics & Kinetics, David Gallagher (CAChe, BioSciences Group, Fujitsu)

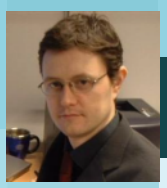
- Qualitative and quantitative aspects of reaction modelling
- Visualization of reaction paths, sterics, molecular orbitals
- Estimation of free energies of reactions, regioselectivity
- Examine effects of reaction conditions and catalysts
- Analysis of transition state energies and insights on yields
- Prediction of relative reaction rates of competing reactions

You will have ample opportunity to discuss your perspectives and criticisms of the methods studied and you'll take-away key nuggets of understanding from these intensive sessions.

Applications of Filtering and Similarity in Virtual Screening Paul Hawkins (OpenEye Scientific Software)

- Database filtering, conformer generation and sorting
- Virtual screening using shape-based similarity
- Examine targets without structural information, e.g., GPCRs
- Investigate electrostatic similarity for ranking possible hits
- Filtering hits for ADMET
- Examine datasets from recent screening publications

A fully equipped IT classroom and a variety of software packages will be at your disposal to work through the problems posed by the instructors.



Compound Database Preparation & Scoring Functions for Virtual Screening, David Lloyd (Hitachi Professor, Trinity College Dublin)

- Case study on Estrogen Receptor Scoring Functions
- Enrichment, False Positive and real-score distribution analysis
- Scaffold and substituent retrieval
- Fingerprint analysis for processing conformers
- Enumeration of protonated, tautomeric, stereochemical states
- Docking of "multimeric" compound representations

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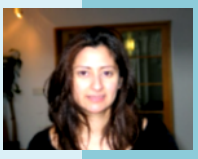
Advances in Virtual Screening and Structure-based Drug Design
Jas Gata-Aura and Gerd Rather (Schrodinger)

- Accurate treatment of ligand and receptor flexibility in docking
- Use of polarizable charges derived from quantum mechanics
- Docking to conformational ensembles to reduce false negatives
- Improving enrichment factors in database screens
- Automating large set screenings with hierarchical approach
- Incorporation of ADME properties into lead optimization



You may also bring your own laptop to test software on your own test problems.

Data Analysis & Visualisation in Discovery Chemistry & Biology
Lennart Eriksson (Umetrics)

- Principal Components, PLS, & Orthogonal-PLS Analysis
- Large data sets with many variables, indicators, features
- Clustering and relationships in heterogeneous data sets
- Non-independence of both observations and variables
- Selection bias in cases with different amounts of data recorded
- Drift in data measured at different times

Return to your lab with new ideas, best practices and software experiences to maximise productivity in your own drug discovery research activities.

Predictive Toxicology, Scott McDonald (Lhasa Limited) and Mark Cronin (Liverpool John Moores University)

- Predicting toxicology for screens in lead generation
- Use of QSAR by regulatory agencies, especially US FDA
- Examine chemical structure processing and compound alerts
- Predicted metabolites and toxicity prediction
- Work flow exercises in lead generation and lead optimisation
- New advances in toxicology, lessons learnt from REACH

Discovery Data Mining using Data Pipelining
Rob Brown (Scitegic)

- Data pipelining and rapid construction of analysis workflows
- Organization and mining of discovery data
- Organizing screening hits into chemical families
- Building SAR tables of chemical series
- Developing statistically-based screens from experimental data
- Gain experience in building workflows to perform analysis

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Join this international community of leading scientists...

Founded in 2003, eCheminfo is an ongoing Community of Practice (CoP) committed to the core value of outreach with diverse groups in the commercial, government and academic sectors for the sharing of best practices and the development of strategies, resources and methodologies that address specific issues in improved drug discovery and productivity.

The CoP involves a diversity of subject matter expertise comprised of experienced professionals from the life science and pharmaceutical industry, vendors, research institutes, universities and government.

A blended approach is used for community interaction. Presentations (with audio) are made available through the collaborative website, periodic teleconferences are held on specific topics, and face-to-face InterAction Meetings are also held in the US and Europe. For those unable to participate directly, all materials can be accessed from the site at any time or from any location.

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Chemical Computing Group www.chemcomp.com

CHEMICAL COMPUTING GROUP
Scalable Software. Scalable Science.

Chemical Computing Group are the producers and suppliers of MOE (Molecular Operating Environment), a state of the art software system for drug discovery and protein modeling. MOE contains a full range of applications, from bioinformatics and protein structure modeling, through structure-based drug design, to cheminformatics, QSAR modeling and library design.

Based in its own programming language, SVL (Scientific Vector Language), MOE can be deployed on a full range of computing platforms; SVL also allows CCG's support to be the most responsive in the industry, as customizations and upgrades can be provided to MOE users on a very short timescale.

Our special thanks go to Karl Harrison for images taken from his virtual tour of Oxford at www.seeoxford.com

Register now for eCheminfo's Advanced Training Workshop on

Drug Discovery Design & Planning Methods

5 ways to register...

- ✓ **Online** at echeminfo.com (Ticket Office is only visible after login)
- ✓ **Email** echeminfo at douglasconnect.com
- ✓ **Phone** Nicki Douglas on +41 61 851 04 61
- ✓ **Fax** +44 870 112 38 44 (eFax)
- ✓ **Post** Douglas Connect, Baermeggenweg 14 4314 Zeiningen, Switzerland

Please select

- ❑ I wish to register for the eCheminfo Training Week taking place at Oxford University (3-7 July, 2006). Registration Fee £1350.
- ❑ Please contact me over local accommodation options for staying in one of the nearby colleges during the training week (subject to availability).

All registration payments must be received in advance of the Training Week.

Payments can be made by bank transfer, cheque or credit card: Amex, MasterCard, Visa

Name

Company/institute

Tel:

Email:

Billing Address

City Postcode

Country

Signed Date

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