echeminfo

Community of Practice for
Drug Discovery & Development

Latest Advances in Drug Discovery & Planning Methods

Advanced Training Workshop

Oxford University, June 25-29, 2007

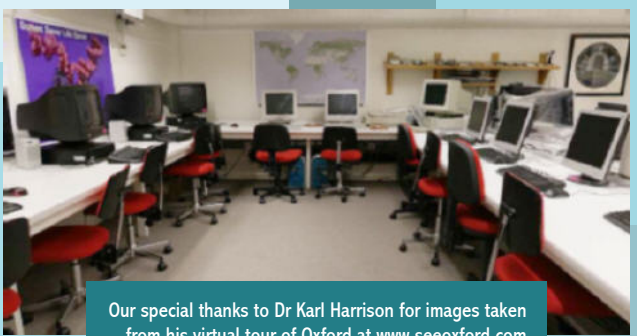
Interactive pragmatic workshops with leading experts and industry practitioners...

- Protein Target & Ligand Modelling
- Virtual Screening & Docking
- Structure-based Drug Design
- Pharmacophore Models
- Focused Library Design
- ADME, QSAR & Predictive Toxicology
- Lead Optimisation
- Pharmacokinetics & Dynamics
- Data Mining, Analysis & Visualisation

A hands-on focus to drug discovery problems using leading-edge software. Discuss practical examples, methods and emerging techniques.

- Class facilitation, discussions and support led by Community Manager Dr. Barry Hardy, Dr. Karl Harrison (Oxford University) and an international faculty team of expert drug discovery application practitioners
- Use leading drug discovery software packages from CCG, Chemaxon, Fujitsu, OpenEye, Schrodinger, SimBioSys, Simulations Plus and Tripos
- Further exercises and trial software licences provided for continuing work beyond class
- One year's membership of eCheminfo included 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.



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

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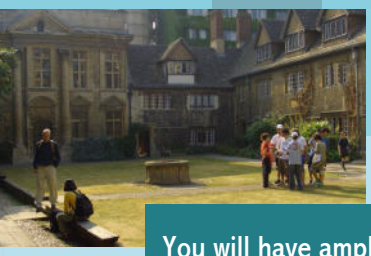
Advanced Protein Modeling
Ulrike Uhrig (Tripos)

- Build 3D Protein Models from Sequences
- Include Structural Information in Sequence Alignment
- Search Databases for Homologous Protein Families
- Choose Protein Template Structures Effectively
- Evaluate Strength of Model
- Determine Binding Site using Molecular Surfaces

"I must say I took home a lot of new ideas – things I would like to try out as soon as possible to improve the support of the work of our medicinal chemists." UW, 2006



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.

Pharmacophore Derivation, Elucidation and Searching
Steve Maginn (Chemical Computing Group)

- Pharmacophore Query Derivation & Elucidation
- Database Searching for new Leads
- Ligand-based Searching without Crystallographic Knowledge
- Target-based Searching without Activity Knowledge
- Using Crystal Structure Knowledge of Target/Ligand Complexes
- Using Capabilities of Molecular Operating Environment

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, Bioisostere Identification
- 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.

"A very useful workshop which is a very good starting point for development and use of new approaches to common tasks. Format and method of carrying out this training is optimal" AC, 2006

Ligand Filtering, Virtual Screening & Docking
Darryl Reid (SimBioSys)

- Create Pseudo-Pharmacophores for Rapid Screening
- Fragment-based Docking & Virtual Screening
- Binding Pose Prediction of Ligands
- Analyse Ligand-Receptor Interactions
- Design Workflow from Database to Lead
- Analyse Interaction Results

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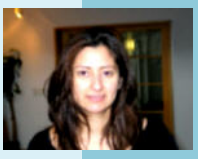
Focused Library Design
Jas Gata-Aura and Gerd Rather (Schrodinger)

- Design Optimised Ligands – Benzothiophene Core in Raloxifene
- Design Subtype-selective Ligands for Estrogen Receptors
- Screening a 20M+ Library to select Focused Libraries
- Analyse Enrichment Factors in Focused Library Design
- Graphically Building & Executing Workflows
- Data Analysis Pipelines for Processing of Library Designs



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

"That was a great opportunity. I had a global overview of topics and met very interesting people. With pleasure I'd participate in future events." GG, 2006

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

Analysing SAR Data using Advanced Structure Searching & Predictions
Tim Dudgeon (ChemAxon)

- Rapidly Analyse Large Chemical & Biological Databases
- Use Advanced Structure Searching Techniques
- Prediction of Chemical Properties
- Database Storing & Searching of Chemical Information
- Application of Chemical Terms for Molecular Calculations
- Prediction of Partitioning, Solubility & Bioavailability

Prediction of Pharmacological Properties & QSAR Analysis
Wojciech Plonka (Fujitsu Group)

- Study Molecular Structure-Biological Activity Relationships
- Generate Molecular Descriptors
- Develop Quantitative Structure-Activity Relationships (QSAR)
- Detect Descriptors Relevant for Modeled Properties
- Predict Toxicity, Carcinogenicity & Human Intestinal Absorption
- Apply Semiempirical Quantum Chemistry Calculations

"Plenty of diversity in topics. Excellent facilities. I did not realise how many tools were out there. The course structure was good. Social events especially punting facilitated discussion. Good contacts made. Put a lot in context. Hands-on approach a big bonus over lectures." MM, 2006

ADMET, Gastrointestinal Simulation & Pharmacokinetics
Michael Bolger (Simulations Plus & USC School of Pharmacy)

- ADMET, Property Estimation, log P, log D, pKa, Solubility
- Permeability, Diffusivity, Dissolution Rate
- Distribution, Carcinogenicity, Mutagenicity
- Maximal Therapeutic Dose, hERG K+ Channel Inhibition
- Physiologically-based Gastrointestinal Simulation, Bioavailability
- Clearance, Pharmacokinetics & Dynamics, PBPK, Virtual Clinical Trials

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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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Bursary Award Sponsored by CCG

CHEMICAL COMPUTING GROUP
Scalable Software. Scalable Science.

A bursary award sponsored by Chemical Computing Group (CCG) will be used to support the attendance of one academic participant who is working in an area of drug discovery research.

To apply for the bursary, please send an email to eCheminfo at douglasconnect.com by February 28, 2007. Your appilcation must include descriptions of your research and training needs (ca. 500 words each), and your CV. The recipient of the award will be selected based on an evaluation of the quality and innovation of the described research and the potential positive impact of the training on their research progress and will be notified by 15 March.

I felt the workshop was extremely beneficial and interesting in the sense it covered a diverse range of topics within the drug design field. It was extremely useful for determining what I would like to do in the future. The accommodation at St Edmunds was excellent and the location was perfect. Thank you for an excellent week."
AM, 2006

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 (25-29 June, 2007). Registration Fee: Regular £1350 / Academic £675
- ❑ 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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