

Latest Advances in Drug Discovery & Development

InterAction Meeting • October 2007

Bryn Mawr College, Philadelphia, PA

Join industry experts to find out
what's new in these fields...

- ▶ **Virtual Screening & Docking**
- ▶ **Structural Biology**
- ▶ **Fragment-based Drug Discovery**
- ▶ **Structure-based Drug Design**
- ▶ **Predictive ADME/Toxicology**



...with a format designed to maximize
InterAction...

- ▶ **Seminars and panel discussions**
- ▶ **Associated workshops to explore and discuss topics further**
- ▶ **Poster session and networking events in the evenings**



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...and also attend InnovationWell's
related sessions...

- ▶ **Systems Toxicology**
- ▶ **Knowledge Management in R&D**

Further details on www.innovationwell.net

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Research Laboratories

Pre-meeting Forum & Workshop on Virtual Screening (full day)

Join the experts to discuss and advance best practices and build trust in comparison studies...

- Practices for target preparation
- Practices for ligand preparation
- Rules and execution of comparison studies
- Practices for scoring
- Practices for docking (including placement, energy & entropy calculation, constraints)
- Wiki-supported documentation and discussions pre- and post-workshop

Facilitated by: Christopher Austin (NIH), Jerome Hert (UCSF), Gerard Kleywegt (Univ. Uppsala), Xavier Barril (Univ. Barcelona), Barry Hardy (Douglas Connect), Paul Hawkins (OpenEye Scientific Software), Darryl Reid (SimBioSys), Kay Perry (Univ. Pennsylvania), Woody Sherman (Schrodinger)

Virtual Screening & Docking Chair: Christopher Austin (National Institutes of Health)

Pharmacological Networks of Proteins Derived from the Similarity between their Ligand-Sets
Jerome Hert (UCSF)

De Novo and Fast-follower Design of Novel Therapeutic Compounds
Wilfried Langenaeker (Silicos)

How Important is Binding Entropy of Relative Motions in Protein-Ligand Docking & Virtual Screening?
Anatoly Ruvinsky (University of Kansas)

Selectivity, Diversity and Pose Quality in Virtual Screening: the case for post-docking analysis
John W. Liebeschuetz (CCDC)

Generation and Analysis of Large Quantitative High Throughput Screening Datasets
Christopher Austin (NIH)

Combining Methods for VHTS: Ligand-based LASSO & Structure-based eHITS
Zsolt Zsoldos (SimBioSys)

A Computational Protocol to Fragment-based Drug Design
François Delfaud (Medit)

Best Practice: Avoiding Bias in Virtual Screening
Gunther Stahl (Tripos)

Dealing with Active Site Plasticity using GOLD
Robin Taylor (CCDC)

Further Adventures in Shape Space
Paul Hawkins (OpenEye Scientific Software)

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SimBioSys Inc.

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Structural Biology Chair: Max Cummings (Johnson & Johnson PR&D)

A Small Change with Large Consequences: a tale of two conformations
Charles Lesburg (Schering-Plough)

Protein Crystallography: not as simple as ABC then?
Gerard Kleywegt (University of Uppsala)

Fundamental Differences between High- and Low-Affinity Complexes of Enzymes and Neo-Enzymes
Heather Carlson (University of Michigan)

Drug target Modeling: ligands tell us more than we think
Ajay Jain (UCSF)

Structure-based Prediction of Small-Molecule Druggability
Alan Cheng (Amgen)

Assignment of Protonation States & Geometries to Macromolecular Structures Using Unary Quadratic Optimization
Paul Labute (Chemical Computing Group)

Don't miss this evening's
Poster Session

Fragment-based Drug Discovery

Chair: Maria Kontoyianni (Crystax Pharmaceuticals)

KEYNOTE: Fragment-based Discovery of Selective, orally Bioavailable Tyrosine Kinase Inhibitors for Targeted Treatment of Human Cancers
Stephen Burley (SGX Pharmaceuticals)

NMR in Target Profiling and Compound File Enhancement
Chaohong Sun (Abbott)

Using Fragments to Couple Ligand- and Structure-based Approaches
Woody Sherman (Schrodinger)

Fragment-based Discovery by SPR Imaging of Chemical Microarrays
Renate Sekul (Graffinity)

Fragment Evolution Strategies: Mastering Hyperspace Jumps
Xavier Barril (University of Barcelona)

Design of Beta-Secretase (BACE-1) Inhibitors: optimizing leads through in silico property-based fragment-scanning
Georgia McGaughey (Merck)

Thank you to our sponsors:



Our special thanks go to Collene Wells for some of the images of Bryn Mawr Campus used in this brochure

Structure-based Drug Design

Chair: Jose Duca (Schering-Plough)

Cross-Docking vs. Scoring: is overfitting the third wheel?
Jose Duca (Schering-Plough)

Taking Advantage of Current Computational Capacities: applications of high-resolution techniques in computer-assisted drug design
Daniel Cheney (Bristol-Myers Squibb)

Ideas, Approaches & Progress in Structure-based Drug Design
Julian Tirado-Rives (Yale)

Ligand/Protein Binding in Structure-based Drug Design: examples of the role of water and caveats in its treatment
Terry Stouch (JCAMD)

Realistic Virtual Screening Assessment in Kinases
Natasja Brooijmans (Wyeth)

Don't miss this evening's Poster Session with refreshments & barbecue

Systems Toxicology

Biomarker Discovery, Validation & Implementation in Translational Medicine
Salvatore Alesci (Wyeth Research)

Metabonomics of Acute Renal Failure in Children during Cardiopulmonary Bypass Surgery
Richard Beger (FDA)

Multivariate Approach to the Informative Set of Genes
Darius M. Dziuda (Central Connecticut State University)

Structured Knowledge Transfer & Integration of Pre-Clinical Biomarker Data for Decision-Making in Drug Development
Fred Cohen (Fast Track Systems)

Determination of New Biomarkers for Liver Toxicity in the Form of Stable Isotope Labeled Metabolites, Laszlo G. Boros (SIDMAP)

Thank you to our sponsors:



Predictive ADME/Toxicology
Chair: Tony Hopfinger (University of New Mexico College of Pharmacy)

Comparison of TEFs and REPs Predicted by Quantitative Spectrometric Data-Activity Relationships and REPs Determined by a Luciferase Gene Expression Assay for 1,3,7,8-TCDD and 1,2,3,4,7-PeCDD

Richard Beger (FDA)

Predictive ADMET at the NCI
 Joseph Tomaszewski (NCI)

Predicting Phospholipidosis Inducing Potential
 Dennis Pelletier (Pfizer)

Towards Cognizant Data Models for SAR and Modeling of ADME/Tox Properties
 Eric Jamois (Strand Life Sciences)

Bayesian Modeling of Numerical Data for ADME Property Prediction
 Anthoy Klou (Pharmacopeia Drug Discovery)

Drugs, Drug-Likeness, Metabolism, Antimicrobials
 Artem Cherkasov (University of British Columbia)

Predictive ADME/Toxicology Forum & workshop activity

- Latest advances in QSAR and ADME/Tox methodologies and resources
- Impact of government and regulatory policy and legislation in the US & Europe
- Potential barriers for replacing animal testing by alternative approaches
- Actions for data integration and knowledge-sharing between initiatives
- The role of semantic web approaches in uniting structured data from multiple resources
- The role of natural language processing for processing unstructured information
- Extraction of data from the scientific literature
- Application of advanced search and agent technologies



Predictive ADME/Toxicology
Chair: Tony Hopfinger (University of New Mexico College of Pharmacy)

QSAR Screening for Carcinogenic Potential Using Multiple Models and Software Platforms
 Joseph Contrera (FDA)

Toxico-Cheminformatics in Support of Predictive Toxicology
 Ann Richard (EPA)

Application of Global and Local in Silico Models to Predict Pharmacokinetic Properties
 Judith Madden (Liverpool John Moores University)

Bio- and Chemoinformatics Applications in Discovery of Multitargeted Drugs
 Vladimir Poroikov (Russian Academy of Sciences)

In-silico Prediction of Chemical Toxicity: Lazy-Structure-Activity-Relationships (LASAR) and the OpenTox Framework
 Christoph Helma (Univ. of Freiburg and in-silico toxicology)

ADME/Tox Modeling from Informatics to Structure-based Paradigms
 Tony Hopfinger (Univ. New Mexico)

Predictive ADME/Toxicology Forum & Workshop

- Methods and procedures for secure testing of commercial data that could be acceptable to industry
- Impact of knowledge management approaches
- Frameworks for computational model testing and validation
- Collaboration & community support structures and environments

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.



Program	Morning	Afternoon
Virtual Screening & Docking	15, 16	15, 16
Structural Biology		16
Fragment-based Drug Discovery	17	
Structure-based Drug Design		17
Predictive Toxicology/ADME	17, 18, 19	17, 18, 19

Register now for eCheminfo's InterAction Meeting on Latest Advances in Drug Discovery & Development

5 ways to register...

✓	Online	echeminfo.com (Ticket Office is only visible after login)
✓	eMail	echeminfo@douglasconnect.com
✓	Phone	+41 61 851 04 61
✓	eFax	+44 870 112 38 44
✓	Post	Douglas Connect, Baermeggenweg 14, 4314 Zeiningen, Switzerland

Registration Fees	Regular	Academic
<input type="checkbox"/> Full Pass (Meeting & Workshops)	\$1400	\$700
<input type="checkbox"/> Day Pass (any single day)	\$500	
<input type="checkbox"/> Screening & Docking only	\$1000	
<input type="checkbox"/> Predictive Tox/ADME only	\$1000	
Payments can be made by bank transfer, cheque or credit card: Amex, MasterCard, Visa		

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