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

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

- Systems Toxicology
- Knowledge Management in R&D

Further details on www.innovationwell.net

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For further information, abstracts, and speaker bios, see www.echeminfo.com
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)

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

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

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

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

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

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

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

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

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)

Thank you to our sponsors:
SimBioSys Inc.
Schering-Plough

Don’t miss this evening’s Poster Session
**Wednesday 17**

### 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)

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

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

**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)

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

### Structure-based Drug Design
**Chair: Jose Duca (Schering-Plough)**

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

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

**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)

**Realistic Virtual Screening Assessment in Kinases**
- Natasja Brooijmans (Wyeth)

### Systems Toxicology

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

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

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

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

**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 Stabile Isotope Labeled Metabolites, Laszlo G. Boros (SIDMAP)**

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

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**Thank you to our sponsors:**

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

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

- Bayesian Modeling of Numerical Data for ADME Property Prediction
  Athony Klon (Pharmacopeia Drug Discovery)

- Predicting Phospholipidosis Inducing Potential
  Dennis Pelletier (Pfizer)

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

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

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**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

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**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–Chemoinformatics in Support of Predictive Toxicology
  Ann Richard (EPA)

- 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)

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

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**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

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www.echeminfo.com
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.

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

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**Program** | **Morning** | **Afternoon**
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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

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**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

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**Registration Fees**

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<th></th>
<th><strong>Regular</strong></th>
<th><strong>Academic</strong></th>
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<tr>
<td>Full Pass (Meeting &amp; Workshops)</td>
<td>$1400</td>
<td>$700</td>
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<td>Day Pass (any single day)</td>
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<td>Screening &amp; Docking only</td>
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<td>Predictive Tox/ADME only</td>
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Payments can be made by bank transfer, cheque or credit card: Amex, MasterCard, Visa

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