echeminfo

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

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

Thank you to our sponsors:

Johnson & Johnson PHARMACEUTICAL RESEARCH & DEVELOPMENT

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

- Critical Paths in Drug Development
- Mechanisms, Metabolism & 'omics
- Systems Biology, Biomarkers & Endpoints
- Knowledge Management in R&D

Further details on www.innovationwell.net

Thank you to our sponsors:

MERCK Research Laboratories

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

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Monday 15

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), Darryl Reid (SimBioSys), Paul Hawkins (OpenEye Scientific Software), Kay Perry (Univ. Pennsylvania)

Tuesday 16

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)

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

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

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:

Schering-Plough

Virtual Screening Hands-on Workshop Activity in IT Classroom

User-Friendly Ligand Filtering and Virtual Screening / Docking, Results and Visualization
Workshop Instructor: Darryl Reid (SimBioSys)

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

Thank you to our sponsors:

SimBioSys Inc.

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Wednesday 17

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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)

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

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

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

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)

Virtual Screening Workshop Activity

Thank you to our sponsors:

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

Dealing with Active Site Plasticity Using GOLD
Workshop Instructor: Robin Taylor (CCDC)

Thank you to our sponsors:

Tripos

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)

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

Realistic Virtual Screening Assessment in Kinases
Natasja Brooijmans (Wyeth)

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 (Lexicon Pharmaceuticals)

KEYNOTE
Julian Tirado-Rives (Yale)

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

Forum & Workshop on Predictive ADME/Toxicology

- 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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Thursday 18

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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
Anthohy Klon (Pharmacopeia Drug Discovery)

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

Predictive ADME/Toxicology
Forum & workshop activity

- To maximize interaction, discussion, issue resolution and action plans for cooperation
- To address specific challenges to progress in the field, and areas where collaboration can support integration and alignment of programs and resources and reduction of duplication
- Innovation Café format wherein the group defines a scenario in which optimum confidence in predictive toxicology methods is reached and then prioritizes steps for achieving that goal.
- The resulting roadmap should support action plans where cooperation between initiatives can accelerate the contribution of predictive toxicology methods to enhanced confidence in safety of new healthcare products and progress the goal of reduction and replacement of animal testing through computational methods

Friday 19

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)

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)

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

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)

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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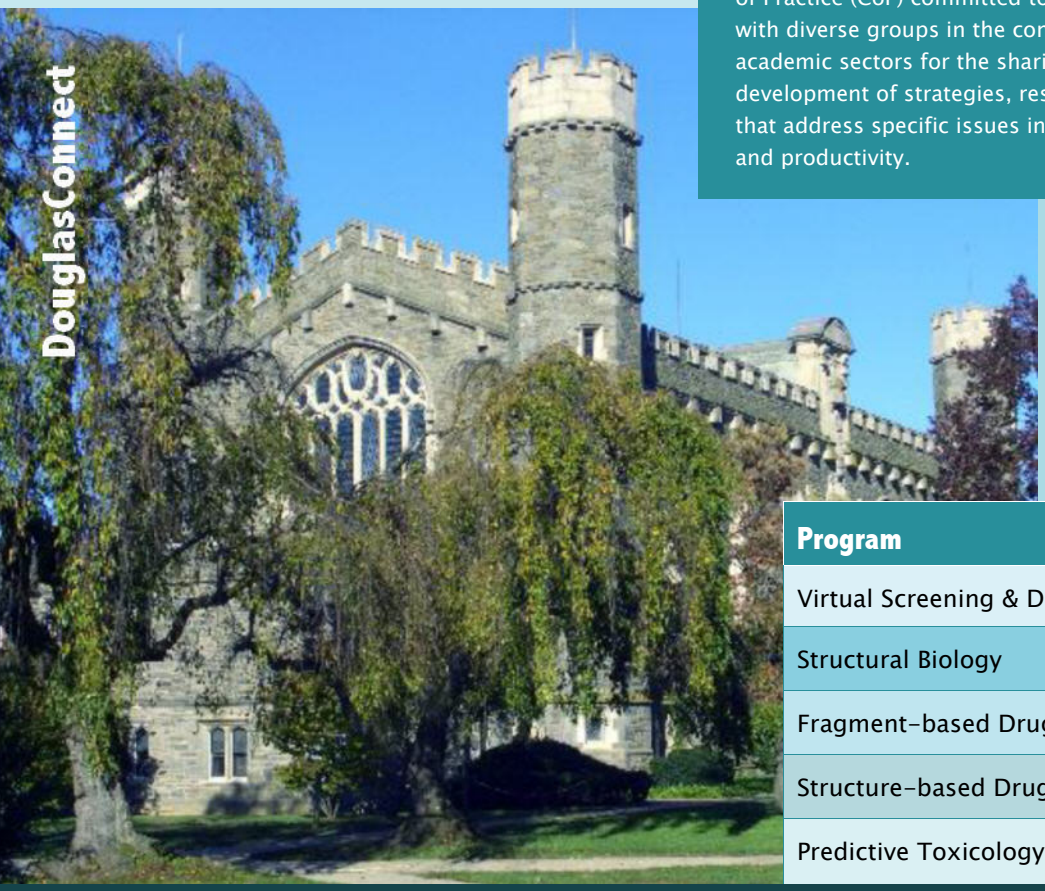

Founded in 2003, eCheminfo is an ongoing Community of Practice (CoP) committed to the core value of outreach with diverse groups in the commercial, government and academic sectors for the sharing of best practices and the development of strategies, resources and methodologies that address specific issues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

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Program	Morning	Afternoon
Virtual Screening & Docking	15, 16 , 17	15, 16
Structural Biology		16
Fragment-based Drug Discovery	17	
Structure-based Drug Design		17
Predictive Toxicology/ADME	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
□ Full Pass (Meeting & Workshops)	$1400	$700
□ Day Pass (any single day)	$500	
□ Screening & Docking only	$1000	
□ Predictive Tox/ADME only	$1000	
Payments can be made by bank transfer, cheque or credit card: Amex, MasterCard, Visa		

Name

Company/institute

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