echeminfo

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

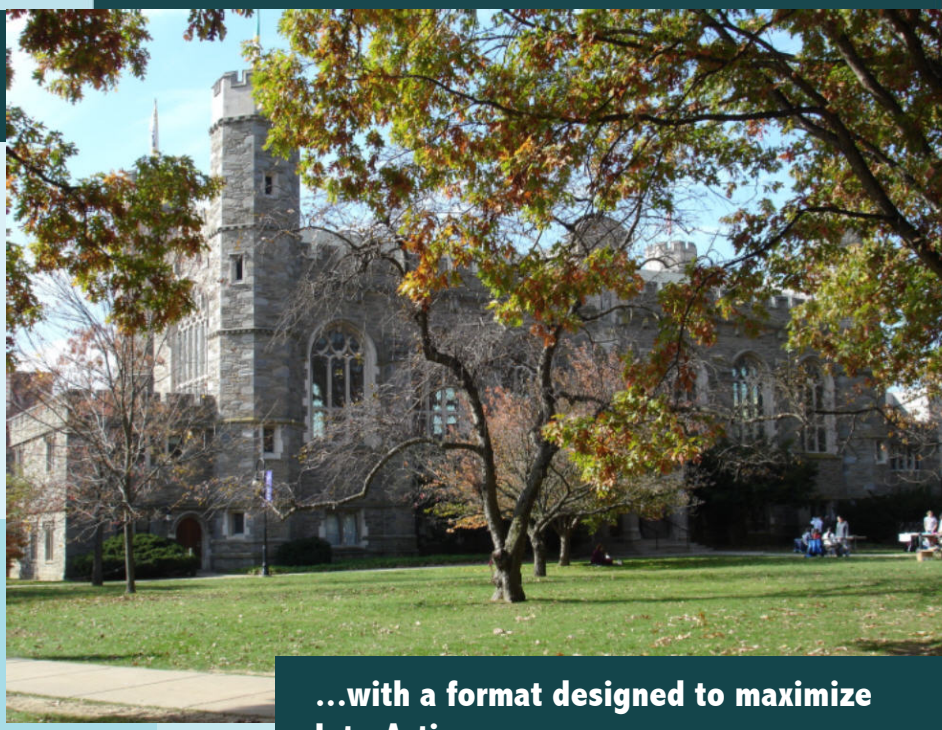
Latest Advances in Drug Discovery & Development

InterAction Meeting 2006, October 16-19

Bryn Mawr College, Philadelphia, PA

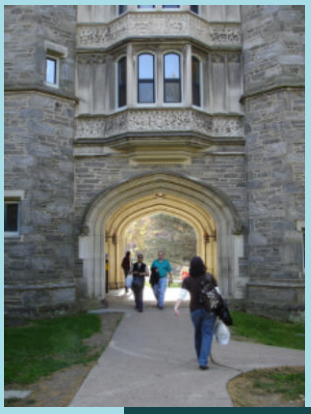
Join industry experts to find out what's new in these fields...

- Structure-based Drug Design
- Screening & Docking
- Discovery Tools & Modeling
- Medicinal Chemistry
- Predictive Toxicology



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

- Seminars and panel discussions in the mornings
- Associated workshops in the afternoons to explore the topics in greater depth
- Poster session and networking events in the evenings



Thank you to our sponsors:

Johnson & Johnson PHARMACEUTICAL RESEARCH & DEVELOPMENT

...and also attend related drug development sessions...

- Critical Paths in Drug Development
- Metabolomics
- Biomarkers
- Decision Support in R&D

Further details on http://innovationwell.net

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

Monday 16

Structure-based Drug Design
Chair: Frank Hollinger (Locus Pharmaceuticals)

Structure-Based Design of Estrogen Receptor-beta Selective Compounds
Mike Malamas (Wyeth)

Using *ab initio* Calculations as Routine Tools to Help Design CDK2 Inhibitors
Jose Duca (Schering-Plough)

Small Molecule Inhibitors of Protein-Protein Interactions
Max Cummings
(Johnson & Johnson PR&D)

Structure-based Drug Design Targeting Infectious Disease
Erin Duffy (Rib-X)

High Strain Energies of Bound Ligands
Paul Labute (Chemical Computing Group)

Structural Interactions of CCR5 with HIV-1 Entry Inhibitors
Debananda Das
(National Cancer Institute)

Harnessing the Power of Structure-based Drug Design using a Fragment Based Approach
Frank Hollinger (Locus Pharmaceuticals)

Session sponsored by:
Chemical Computing Group

Associated afternoon workshops...

- Lance Westerhoff (QuantumBio), Quantum Biochemistry Workflows
- Zenon Konteatis and Jennifer L. Ludington (Locus Pharmaceuticals) Fragment- and Structure-Based Drug Design
- Osman F. Güner (Turquoise Consulting) Advanced Techniques in Pharmacophore Perception and Successful Applications in Drug Design
- Hege Beard and Shashi Rao (Schrodinger) Advances in Virtual Screening and Structure-based Drug Design
- Alex Clark (Chemical Computing Group), Hypothesis Generation from Docking Results Using Activity Measurements, Interaction Fingerprints, Clustering and 2D Visualization Methods

Tuesday 17

Screening & Docking
Chair: Stan Young (National Institute of Statistical Sciences)

Analysis of HTS Data Using Recursive Partitioning, Stan Young (National Institute of Statistical Sciences)

A new Self-organizing Algorithm for Molecular Alignment and Pharmacophore Development
Deepak Bandyopadhyay (Johnson & Johnson PR&D)

Development of Angiogenesis Inhibitors - from Screening to the Clinic
William Douglas Figg (National Cancer Institute)

Investigating Bias in Docking Screens with Target, Ligand and Decoy Benchmarking Sets
John Irwin (UCSF)

Virtual Ligand Screening with eHiTS
Darryl Reid (SimBioSys)

A Critical Assessment of Docking Programs and Scoring Functions
Neysa Nevins (GlaxoSmithKline Pharmaceuticals)

Associated afternoon workshops...

- Paul Hawkins (OpenEye) Applications of Filtering and Similarity in Virtual Screening
- Darryl Reid (SimBioSys), Docking and Screening
- Roundtable Discussion on Virtual Screening & Docking Study
  This session will discuss current virtual screening and docking methods and software, results of existing validation and comparison studies, and procedures for community of practice studies to be undertaken.

Session sponsored by:

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Join us on Tuesday evening for an open event on Knowledge Management in R&D including demonstrations of Electronic Laboratory Notebooks, open seminars & panel discussion, followed by a Knowledge Café and reception.

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Wednesday 18

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Bench Scientists' & Modelers' Discussions on Discovery Tools & Modeling

In this session a panel of experimental and computational chemists will discuss their experiences in using computational modeling methods in drug discovery. They will discuss where the methods and software are having success, and where current methods are not yet meeting their needs, are failing or have challenges or complications. Short presentations on drug discovery experiences will be used to seed discussion of cheminformatics-driven medicinal chemistry and lead optimization and conversations on where new developments could aid improvement in practice and tools.

Panel: Chris Cooper (BMS), James Arnold (AstraZeneca), Phil Edwards (AstraZeneca), Pete Connolly (Johnson & Johnson PRD), Victor Lobanov (Johnson & Johnson PRD), Jim Wikel (Coalesix)

Associated afternoon workshops...

- Michael B. Bolger (Simulations Plus and USC School of Pharmacy) *in silico* Technology in Drug Discovery and Development
- Sanji Bhal and Karim Kassam (ACD/Labs), Using Physicochemical Property Predictions to Overcome ADME Concerns at Lead Optimization
- Gilles Klopman (Multicase), Machine Intelligence in the Design of New Biologically Active Chemicals
- Bob Clark (Tripos), Challenges of ADME/Tox Prediction

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

Thursday 19

Predictive Toxicology
Chair: Curt Breneman (Rensselaer Polytechnic Institute)

KEYNOTE: Tudor Oprea (University New Mexico)
The Physical Basis for the Rule of Five

A Roadmap for Integrating Modelling & Simulation in Pre-Clinical DMPK Research
Navita Mallalieu (Roche Pharmaceuticals)

The Statistical Significance vs. Mechanistic Interpretation of ADME/tox Models
Alex Tropsha (UNC)

Predictive ADME : How Do I Know if My Predictions will be Useful?, Curt Breneman (Rensselaer Polytechnic Institute)

An *in silico* Approach to Reduce the Burdens of Lead Discovery and Optimization
Sanji Bhal & Karim Kassam (ACD/Labs)

Integration of Early ADME Using Property Estimation and PBPK Simulation, Michael B. Bolger (Simulations Plus and USC School of Pharmacy)

Machine Intelligence in the Design of New Biologically Active Chemicals
Gilles Klopman (Multicase)

The "Structures" in Structure-Activity Relationships
Bob Clark (Tripos)

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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.

www.echeminfo.com

Do you have difficulty optimizing lead compounds for solubility or other critical molecular properties?

The latest PhysChem software from Advanced Chemistry Development (ACD/Labs) was designed to help scientists relate structural modification with critical physicochemical properties (logP, logD, solubility, and pK_a).

ACD/Structure Design Suite combines a substituent database with our industry standard molecular property prediction algorithms (deployed worldwide by GSK and Pfizer, and used by numerous chemical R&D companies, government organizations, and academic institutions).

Before committing synthetic efforts to lengthy syntheses, analogs can be optimized for physical properties that relate to select ADME parameters, to help focus on the most suitable candidates.

CHEMICAL COMPUTING GROUP

Scalable Software. Scalable Science.

Chemical Computing Group (CCG) offers MOE (Molecular Operating Environment) computational software platform for life science applications such as Structure-Based Design, Protein Modeling & Bioinformatics, Cheminformatics, High-Throughput Discovery, Molecular Modeling & Simulations, and Methodology Development & Deployment. MOE can operate under a wide range of computer platforms (Windows, Mac OS X, Linux, or Unix on laptops, workstations, or clusters), and is written in the efficient and intuitive SVL (Scientific Vector Language). SVL's high-level scripting language allows the integration of other applications or the creation of new ones for Life Sciences. Please contact us for a free trial of MOE.

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

Register now for eCheminfo's InterAction Meeting on

Latest Advances in Drug Discovery & Development

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

- ❑ Please register me for eCheminfo InterAction Meeting at Bryn Mawr College, PA, October 16-19, 2006 Registration fee $1300
- ❑ Please register me for eCheminfo InterAction Meeting at Bryn Mawr College, PA, October 16-19 at the Academic Registration fee of $650

All registration payments must be received in advance of the Meeting.

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

Name

Company/institute

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Billing Address

City Postcode

Country

Signed Date

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