

# Computer-Aided Drug Design

(Joint with "New Directions in Small Molecule Drug Discovery")

April 20–25, 2010 • Fairmont Chateau Whistler • Whistler, British Columbia • Canada

Scientific Organizers: Michael K. Gilson, Catherine E. Peishoff and Jeff Blaney

## PROGRAM FACULTY & TALKS

**David Baker**, University of Washington, USA

*Rosetta Ligand: From Folding to Docking*

**Jeff Blaney**<sup>\*◊</sup>, Genentech, Inc., USA

*Unexpected SBDD Failures and Successes*

**Simon F. Campbell**<sup>◊</sup>, UK

*The Future of the Pharmaceutical Industry*

**Heather A. Carlson**, University of Michigan, Ann Arbor, USA

*CSAR – An NIH-Funded Community Resource for Protein-Ligand Modeling and Validation*

**Kenneth A. Dill**<sup>\*</sup>, University of California, San Francisco, USA

*A New Approach to Computing Protein-Ligand Affinity*

**Stephen W. Fesik**<sup>\*◊</sup>, Vanderbilt University School of Medicine, USA

*Talk Title to be Determined*

**Arun K. Ghosh**<sup>◊</sup>, Purdue University, USA

*Structure-Based Design of Aspartic Acid Protease Inhibitors*

**Michael K. Gilson**<sup>\*</sup>, University of Maryland Biotechnology Institute, USA

*The Role of Configurational Entropy in Binding*

**Marti S. Head**<sup>\*</sup>, GlaxoSmithKline, USA

*What Works Now and What Do We Need?*

**Marc K. Hellerstein**<sup>\*◊</sup>, University of California, Berkeley, USA

*Systems Biology: The Full Consequences of Hitting my Target*

**Steven W. Homans**, University of Leeds, UK

*NMR Studies of Protein Dynamics and Binding Thermodynamics*

**Ismail Kola**<sup>◊</sup>, Schering-Plough Corporation, USA

*Talk Title to be Determined*

**Leslie A. Kuhn**, Michigan State University, USA

*Identifying Sites that Bind Similar Ligands in Different Proteins, to Enhance Target-Selective Design*

**Paul Leeson**<sup>\*◊</sup>, AstraZeneca R&D Charnwood, UK

*Overview: What Have We Learned About Attrition?*

**Anna K. Mapp**<sup>\*◊</sup>, University of Michigan, USA

*Small Molecule Transcription-Based Therapeutics*

**Demetri Moustakas**, AstraZeneca Pharmaceuticals LP, USA

*The Physics of Surface Water and its Role in Protein-Ligand Binding*

**Anthony Nicholls**, OpenEye Scientific Software, USA

*Validation through Blind Protein-Ligand Predictions*

**Saul H. Rosenberg**<sup>◊</sup>, Abbott Laboratories, USA

*Antagonists of BCL-2 Family Proteins*

**Benoit Roux**, University of Chicago, USA

*Electronic Polarizability and the Calculation of Binding Free Energy*

**Martin Stahl**<sup>◊</sup>, F. Hoffmann-La Roche Ltd, Switzerland

*Small Molecule Conformational Preferences in Ligand Design*

**Andrew Stamford**<sup>◊</sup>, Schering-Plough Research Institute, USA

*Structure-Based Design of BACE Inhibitors*

**Raymond C. Stevens**<sup>◊</sup>, The Scripps Research Institute, USA

*Structure and Function of the Human G-Protein Coupled Receptor Family*

**Bruce Tidor**, Massachusetts Institute of Technology, USA

*Electrostatic Complementarity, Affinity and Specificity*

**James A. Wells**<sup>◊</sup>, University of California, San Francisco, USA

*Protein-Protein Interactions*

<sup>\*</sup>Keynote speaker. <sup>\*</sup>Session chair. <sup>◊</sup>Joint speaker. <sup>◊</sup>Invited, not yet confirmed.  
Programs subject to change. Current as of November 10, 2009.



*The purpose of this meeting is to stimulate progress in the methods of computer-aided drug design. This will be accomplished by bringing theory and practice into contact at a number of levels in order to highlight interesting and important practical problems waiting to be solved, and by deepening participants' understanding of the science underlying these challenges.*

## PROGRAM PLENARY SESSIONS:

- New Opportunities in Small Molecule Drug Discovery (Joint)
- SBDD-Medchem Interface (Joint)
- Emerging Computational Methods for SBDD
- Confronting Reality
- Physics of Binding – Theory and Computation
- Physics of Binding – Experiment
- Candidate Attrition in the Pharmaceutical Industry (Joint)
- Small Molecules: Modeling and Properties (Joint)

## DEADLINES:

Abstract & Scholarship: December 21, 2009

Late-Breaking Abstract: January 20, 2010

Early Registration: February 23, 2010

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