

Keystone Symposia: 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^o, Genentech, Inc., USA
Unexpected SBDD Failures and Successes

Simon F. Campbell^o, 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^{*}, University of California, San Francisco, USA
A New Approach to Computing Protein-Ligand Affinity

Stephen W. Fesik^{*o}, Vanderbilt University School of Medicine, USA
Targeting Protein-Protein Interactions Using Fragment-Based Methods and Structure-Based Design

Arun K. Ghosh^o, Purdue University, USA
Structure-Based Design of Aspartic Acid Protease Inhibitors

Michael K. Gilson^{*}, University of Maryland Biotechnology Institute, USA
The Role of Configurational Entropy in Binding

Marti S. Head^{*}, GlaxoSmithKline, USA
What Works Now and What Do We Need?

Marc K. Hellerstein^o, University of California, Berkeley, USA
Systems Biology: The Full Consequences of Hitting my Target

Ismail Kola^o, 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^{*o}, AstraZeneca R&D Charnwood, UK
Overview: What Have We Learned About Attrition?

Anna K. Mapp^{*o}, University of Michigan, USA
Small Molecule Transcription-Based Therapeutics

Stephen F. Martin, University of Texas, USA
Correlating Structure and Energetics in Protein-Ligand Interactions: Paradigms and Paradoxes

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^o, 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^o, F. Hoffmann-La Roche Ltd, Switzerland
Small Molecule Conformational Preferences in Ligand Design

Andrew Stamford^o, Schering-Plough Research Institute, USA
Structure-Based Design of BACE Inhibitors

Raymond C. Stevens^o, The Scripps Research Institute, USA
Structure and Function of the Human G-Protein Coupled Receptor Family

Martin J. Stone[†], Indiana University, USA
Talk Title to be Determined

Bruce Tidor, Massachusetts Institute of Technology, USA
Electrostatic Complementarity, Affinity and Specificity

James A. Wells^o, University of California, San Francisco, USA
Protein-Protein Interactions

^{*}Keynote speaker. ^{*}Session chair. ^oJoint speaker. [†]Invited, not yet confirmed.
Program subject to change. Current as of December 3, 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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