echeminfo

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

InterAction Meetings US & Europe

Cheminformatics & Chemical Modeling in Drug Discovery

Two meetings for the price of one...

Sessions & Chairs in Philadelphia, October 11 & 12

Virtual Screening, Docking and Scoring
Max Cummings (Johnson & Johnson Pharmaceutical Research & Development)

Simulation of Membranes & Ion Channels
Richard Pastor (FDA) and Michael Klein (Univ. Of Pennsylvania)

Drug Discovery Innovation
David Mosenkis

New Developments in Biophysical Applications of Quantum Mechanics
Ken Merz (University of Florida) & Lance Westerhoff (QuantumBio)

Protein Folding, Misfolding & Aggregation: Applications to Disease
Nikolay V. Dokholyan (University of North Carolina)

Web-Based Services in Drug Design
Marc Nicklaus (National Institutes of Health)

Come to either meeting in person, and access the other one virtually!

Sessions & Chairs in Basel, Switzerland, November 9-10

Protein Folding and Dynamics
Wilfred van Gunsteren (ETH Zürich)

Virtual Screening, Docking & Scoring
Miklos Vargyas (Chemaxon)

Applications of Machine Learning & Graph Mining in Drug Discovery
Stefan Kramer (Technische Universität München)

Computational Biochemistry
Alessandro Curioni (IBM Zürich Research Laboratory)

Biosensors and Nanofluidics
Nick Quirke (Imperial College London)

Web-based Services in Drug Design
Kim Henrick (European Bioinformatics Institute)

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Philadelphia

Virtual Screening, Docking and Scoring
Max Cummings (Johnson & Johnson Pharmaceutical R & D)

Reducing False Positives in Virtual Screens on Kinase Targets
Emanuele Perola (Vertex Pharmaceuticals)

Exploiting Protein-Specific Information in Docking
Willem Nissink (Cambridge Crystallographic Data Centre)

You Can't Find What's Not There: The Importance and Pitfalls of Multiple Representations of Molecules in Dockable Databases
John Irwin (UCSF)

Molecular Docking as a Virtual Screening Tool
Renee DesJarlais (Johnson & Johnson PRD)

New Docking Methods for Pose Prediction and Enrichment
Mark McGann (Openeye)

October 11

New Developments in Biophysical Applications of Quantum Mechanics
Ken Merz (University of Florida) & Lance Westerhoff (QuantumBio)

Use of Quantum Mechanics in the Process of Drug Discovery
Ramkumar Rajamani (Bristol-Myers Squibb)

Semi-Empirical Comparative Binding Energy Analysis (SE-COMBINE) of a Series of Trypsin Inhibitors
Martin Peters (Penn State)

Mixed Quantum Mechanics/Molecular Mechanics Modeling of Protein-Ligand Complexes
Richard Friesner (Columbia University)

A Combined QM/MM Approach for Analyzing Energy Components in Protein-Ligand Complexes
Jiali Gao (University of Minnesota)

Applications of a Database of Quantum Calculations for RNA Catalysis (QCRNA) in the Design of New Multi-Scale Quantum Models for Phosphoryl Transfer Reactions
Darrin York (University of Minnesota)

October 11

Bryn Mawr College
101 N. Merion Ave.
Bryn Mawr, PA

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Drug Discovery Innovation
David Mosenkis

An Interactive Environment for Multiparameter Optimization
James H. Wikel (Coalesix)

ABCD Chemoinformatics: Integrating Chemoinformatics Tools into Everyday Drug Discovery Practice
Victor Lobanov (Johnson & Johnson Pharmaceutical R & D)

Structure-based Design of Allosteric Protein Kinase Inhibitors
Jeff Wiseman (Locus Pharmaceuticals)

Shape Signatures: A Tool for Rapid in silico Screening and Clustering
Randy J. Zauhar (University of the Sciences in Philadelphia)

Computational Models are Needed to Make Drugs Safer and More Effective
G. Scott Lett (Bioanalytics Group)

October 11

Philadelphia

Web-based Services in Drug Design
Marc Nicklaus (National Institutes of Health)

Web-Enabling Technology for the Design, Enumeration, Optimization and Tracking of Compound Libraries
Brad Feuston (Merck)

Pubchem
Steve Bryant
NCBI

ZINC Web Services
– Providing 3D Structures of Purchasable Compounds for Virtual Screening to Humans and Machines
John Irwin (UCSF)

A Web-based Chemoinformatics System for Drug Discovery
Brett Tounge (Johnson & Johnson Pharmaceutical R & D)

Web-based Services of the National Cancer Institute's CADD Group
Marc Nicklaus (NIH)

Search-and-Query Information System for the Study and Discovery of Novel Agents in the Treatment of Cancer
David Covell (NCI)

High Performance Applications Based on Web Services: It's Not an Oxymoron. The Use of Web Services in the ABCD Drug Discovery Platform
Dmitrii Rassokhin (Johnson & Johnson Pharmaceutical Research and Development)

October 11

Simulation of Membranes and Ion Channels
Richard Pastor (FDA) & Michael Klein (University of Pennsylvania)

Exploring Rhodopsin Activation with Large Scale Molecular Dynamics
Mike Pitman (IBM)

Response of Lipid Bilayers and Monolayers to Trehalose: Molecular Dynamics in Constant Area and Surface Tension Ensembles
Richard Pastor (FDA)

Structure of Lipid Membranes and Improving the Head Group Force Field
Jeff Klauda (NIH)

Molecular Dynamics Simulations of Oligomeric Ion Channels within Lipid Bilayers
Preston Moore (USIP)

Understanding Membrane Transport at Full Atomic Resolution – Molecular Dynamics Simulations of Lipid Bilayers and Membrane Channels
Emad Tajkhorshid (Beckman Institute, Univ. Illinois at Urbana-Champaign)

Bryn Mawr College
101 N. Merion Ave.
Bryn Mawr, PA

October 12

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Protein Folding, Misfolding & Aggregation: Applications to Disease
Nikolay V. Dokholyan (University of North Carolina)

The Assembly and Structure of Amyloid-Like Polyglutamine Aggregates Associated with Huntingdon's Disease
Ron Wetzel (University of Tennessee Medical Center)

Direct Observation of Protein Folding, Misfolding and Prion-Like Conformational Infectivity
Feng Ding (University of North Carolina)

Flexibility and Mobility in Biomolecules
Michael Thorpe
(Arizona State University)

Catalytic Origins of Protein Misfolding in End-Stage Renal Failure
Andrew Mirankar
(Yale University)

Amyloid beta-protein Oligomerization and Alzheimer's Disease
David Teplow (David Geffen School of Medicine at UCLA)

October 12

Basel

Protein Folding and Dynamics
Wilfred van Gunsteren (ETH Zürich)

Protein Dynamics Measured by Triplet-Triplet Energy Transfer
Thomas Kiefhaber (University of Basel)

Simple Yet Predictive Models
Nikolay V. Dokholyan
(University of North Carolina)

Dynamics of Protein Binding, Reaction and Structural Change
Jeremy Smith
(University of Heidelberg)

All Atom Protein Folding with Stochastic Optimization Methods
Wolfgang Wenzel (University of Karlsruhe)

Structure Determination of Native and Non-Native Protein Conformations Using NMR-Derived Restraints
Michele Vendruscolo (University of Cambridge)

Aspects of beta-Peptide Folding from Molecular-Dynamics Simulation
Xavier Daura (University of Barcelona)

November 9

Virtual Screening, Docking and Scoring
Miklos Vargyas (ChemAxon)

The Issue of Protein Flexibility in Docking-Based Virtual Screening
Xavier Barril (Vernalis)

Pattern Recognition and Grid Computing in Discovery
Graham Richards (University of Oxford)

Beyond Ligand Flexibility: Improvement and Validation of rDock for Structure-Based Drug Design
David Morley (Enspiral Discovery)

Discovery of Cell-Permeable Nonpeptide Inhibitors of beta-Secretese by High Throughput Docking and Continuum Electrostatic Calculations
Amedeo Caflisch (ETH-Zürich)

Structure-based Identification of GPCR Ligands by High-Throughput Docking
Didier Rognan (University of Strasbourg)

November 9

Swissôtel L'Entrée Convention Center
Riehenring 118
4005 Basel

Applications of Machine Learning & Graph Mining in Drug Discovery
Stefan Kramer (Technische Universität München)

Graph-Theoretic Procedures for Searching Databases of Molecular Structures
Peter Willett (University of Sheffield)

Finding Discriminative Substructures Using Elaborate Chemical Representation
Joost N. Kok (Leiden University)

Mining of Molecular Fragments with Wildcards
Michael Berthold
(University of Konstanz)

Alignment-free Potential Pharmacophore - Point Descriptors for "Informed" Similarity Searching
Gisbert Schneider (Johann Wolfgang Goethe University)

Lazy-Structure-Activity-Relationships (Lazar) for the in-silico Prediction of Chemical Carcinogenicity
Christoph Helma (University of Freiburg)

November 10

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Basel

Computational Biochemistry
Alessandro Curioni (IBM Zürich Research Laboratory)

The Role of Quantum Mechanics in Structure-based Drug Design
Ken Merz (University of Florida)

Kinetic Isotope Effects for Enzyme-Catalysed Methyl Transfer
Ian Williams (University of Bath)

On the Art of Computing the Infra Red Spectra of Molecules in the Condensed Phase
Paul Tavan (University of Munich)

Determination of the Catalytic Reaction Pathways in Urate Oxidase Using Quantum Chemistry Tools
Gerald Monard (University Henri Poincare-Nancy)

Application of Hybrid QM/MM Methods to the Simulation of Biological Systems
Ursula Roethlisberger (Swiss Federal Institute of Technology, Lausanne)

Applications in Computational Quantum Biochemistry
Alessandro Curioni
(IBM Zürich Research Laboratory)

November 10

Biosensors and Nanofluids
Nick Quirke (Imperial College London)

Thermophoresis Between Solids: A Molecular Dynamics Study of Gold Nanoparticles Confined and Thermally Driven through Carbon Nanotubes
Jens Walther (ETH-Zürich)

Title & Speaker TBA
Philips Research Laboratories

Computational Modeling for Biosensor Devices
Richard Gilbert (e2v Technologies)

Simulating Nanoflows
Nick Quirke
(Imperial College London)

Microfluidic Systems for Controlled Production of Small Molecules & Nanoparticles
Andrew De Mello (Imperial College London)

November 10

Swissôtel L'Entrée Convention Center
Riehenring 118
4005 Basel

Web-Based Services in Drug Design
Kim Henrick (European Bioinformatics Institute)

The Representation of Chemical Structures and Its Application to Property Prediction
Johann Gasteiger (Universität Erlangen-Nürnberg)

Open Archives as a Route for the Capture, Dissemination and Access to Chemical Information
Simon Coles (University of Southampton)

Identification of Biological Units in Protein Crystals
Eugene Krissinel (European Bioinformatics Institute)

Investigating Chemical Trends in the Context of Ligand-Protein Complexes by Using Online Data Analysis Directly on the Web
Dimitris Dimitropoulos
(European Bioinformatics Institute)

SWISS-MODEL Server and Repository: Web-based Resources for Comparative Protein Structure Modeling and Their Application in Drug Discovery
Torsten Schwede (University of Basel)

November 10

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Join this international community of leading scientists...

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.

The CoP involves a diversity of subject matter expertise comprised of experienced professionals from the life science and pharmaceutical industry, vendors, research institutes, universities and government.

A blended approach is used for community interaction. Presentations (with audio) are made available through the collaborative website, periodic teleconferences are held on specific topics, and face-to-face InterAction Meetings are also held in the US and Europe. For those unable to participate directly, all materials can be accessed from the site at any time or from any location.

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We thank the following for their support...

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Register now for eCheminfo's InterAction Meetings on Drug Discovery Applications of Cheminformatics & Chemical Modeling

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

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- ❑ Conference-only registration for non-members: $1100 / SFr. 1320
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