Workshop II: Optimization, Search and Graph-Theoretical Algorithms for Chemical Compound Space

Monday April 11, 2011

8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*

9:00–9:50 **Jean-Loup Faulon** (Université d'Évry-Val d'Essonne)
Local Enumeration of the Chemical Space with Circular Fingerprints

10:00–10:15 *Break*

10:15–11:05 **John Irwin** (University of California, San Francisco (UCSF))
Predicting Off-targets for Approved Drugs

11:15–11:30 *Break*

11:30–12:20 **Jack Snoeyink** (University of North Carolina)
Scientific Benchmarks for Structure Prediction Code

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Klaus-Robert Müller** (Technische Universität Berlin)
Predicting Properties of Small Molecules with Kernel-Based Machine Learning Methods

3:30–4:00 *Break*

4:00–4:50 **Farhad Hormozdiari** (University of Washington)
Extended Nearest Neighbor Classification Methods for Predicting Small Molecule Activity

5:00–7:00 *Reception and Poster Session (Hosted by IPAM)*

Tuesday April 12, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **David Wales** (University of Cambridge)
Exploring Energy Landscapes: From Molecules to Nanodevices

10:00–10:15 *Break*

10:15–11:05 **Mark Tuckerman** (New York University)
Generating Free Energy Landscapes: From Solvation to Biomolecules and Crystalline Polymorphs

11:15–11:30 *Break*

(Tuesday schedule continued on next page)

(Tuesday schedule continued from previous page)

11:30–12:20 **Mauro Maggioni** (Duke University)
Geometric Analysis of Molecular Dynamics Data, Diffusion Geometry and Reaction Coordinates

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Mike McKerns** (California Institute of Technology)
A Massively-Parallel Heterogeneous Computing Framework for Optimization and Rigorous Parameter Sensitivity Analysis

3:30–4:00 *Break*

4:00–4:50 **Shawn Martin** (Sandia National Laboratories)
Topology of Cyclo-Octane Energy Landscape

Wednesday April 13, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **William Hart** (Sandia National Laboratories)
Rethinking Optimization Challenges for Molecular Docking Applications

10:00–10:15 *Break*

10:15–11:05 **Venkat Venkatasubramanian** (Purdue University)
Molecular Products Design: Challenges and Opportunities

11:15–11:30 *Break*

11:30–12:20 **Rolf Backofen** (Albert-Ludwigs-Universität Freiburg)
The Tedious Task of Finding Common RNA Sequence Structure Properties

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Danail Bonchev** (Virginia Commonwealth University)
Substructures and Patterns in 2-D Chemical Space

3:30–4:00 *Break*

4:00–4:50 **Pierre Baldi** (University of California, Irvine (UCI))
Algorithms and Data Structures for Efficiently Storing, Compressing, Retrieving, and Scoring Small Molecules in Chemical Space

Thursday April 14, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Jean-Louis Reymond** (Universität Bern)
Enumeration, Mapping and Scoring of Chemical Space for Drug Discovery

10:00–10:15 *Break*

(Thursday schedule continued on next page)

(Thursday schedule continued from previous page)

10:15–11:05 **Tamon Stephen** (Simon Fraser University)
Two pairs of boolean functions in biology

11:15–11:30 *Break*

11:30–12:20 **Berend Rinderspacher** (Army Research Laboratory)
Molecular Optimization Using Nuclear Charge Distributions

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Artem Cherkasov** (University of British Columbia)
Prediction of Highly-Connected 'Hub'-Proteins in Protein Interaction Networks Using Conventional Molecular QSAR

3:30–4:00 *Break*

4:00–4:50 **Markus Meringer** (Deutsche Forschungsanstalt für Luft- und Raumfahrt eV (DLR))
Generation of Molecular Graphs and Applications in Chemistry

Friday April 15, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Wei Wang** (University of North Carolina)
Discriminative Structural Motif Mining for Protein Classification

10:00–10:15 *Break*

10:15–11:05 **Tatsuya Akutsu** (Kyoto University)
Inference and Enumeration of Chemical Structures from Feature Vectors

11:15–11:30 *Break*

11:30–12:20 **Kyle Camarda** (University of Kansas)
An Optimization-Based Method for the Design of Novel Molecular Systems

12:30–2:30 *Lunch (on your own)*

2:30–3:20 *Panel Discussion*