Preliminary Program CompLife '05

All sessions and talks will be held in lecture hall A703 (Konstanz, university 120k). In the breaks, coffee will be served in the foyer area in front of the lecture hall.

On Sunday evening, a reception will be held in the city hall. If the weather is good, this will take place in the picturesque courtyard. You will be able to taste the local wines.

On Monday evening, we will walk from the conference location to the Island of Mainau. You will have time to enjoy the splendid colors of the huge variety of flowers that island has to offer. In the early evening we will meet for a drink in the Rose Garden and then walk over to the Chestnut Hall where the conference dinner will be served.

The last session will close on Tuesday at 12:30 followed by lunch in the university cafeteria.

We are looking forward to seeing you at the conference and we hope that you will enjoy perusing the program.

Sunday, September 25, 2005
12:30 Bus departs from train station
12:30 - 13:00 Registration
13:00 Opening
13:00 - 14:30 Session I: "Systems Biology"
14:30 - 15:00 Coffee Break
15:00 - 16:30 Session II: "Data Analysis and Integration"
16:30 - 17:00 Coffee Break
17:00 - 18:30 Workshop Session: "Distributed Data Mining in Life Science"
18:45 Bus departs from University Main Entrance
19:00 - 21:00 Reception in City Hall

Monday, September 26, 2005
09:00 - 10:00 Plenary
  Peter Murray-Rust: "The Chemical Semantic Web"
10:00 - 10:30 Coffee Break
10:30 - 12:00 Session III: "Structural Biology"
12:00 - 13:00 Lunch
13:00 - 14:30 Session IV: "Genomics"
14:30 - 15:00 Coffee Break
15:00 - 16:30 Session V: "Computational Proteomics"
16:30 - 19:00 Free Time to explore the Island of Mainau
19:00 - 19:30 Dinner Reception
19:30 - 23:00 Conference Dinner

Tuesday, September 27, 2005
09:00 - 10:30 Session VI: "Molecular Informatics"
10:30 - 11:00 Coffee Break
11:00 - 12:30 Session VII: "Molecular Structure Determination and Simulation"
12:00 - 13:00 Lunch
12:30 Conference Closing
SESSION I: Systems Biology

- Structural Protein Interactions Predict Kinase-Inhibitor Interactions in Upregulated Pancreas Tumour Genes Expression Data
  Gihan Dawelbait, Christian Pilarsky, Yanju Zhang, Robert Grützmann, Michael Schroeder

- Biochemical Pathway Analysis via Signature Mining
  Eleftherios Panteris, Stephen Swift, Annette Payne, Xiaohui Liu

- Recurrent Neuro-Fuzzy Network Models for Reverse Engineering Gene Regulatory Interactions
  Ioannis Maraziotis, Andrei Dragomir, Anastasios Bezerianos

SESSION II: Data Analysis and Integration

- Some Applications of Dummy Point Scatterers for Phasing in Macromolecular X-Ray Crystallography
  Alexandre Urzhumtsev, Natalia Lunina, Pavel Afonine, Vladimir Y. Lunin

- BioRegistry: A Structured Metadata Repository for Bioinformatic Databases
  Malika Smaïl-Tabbone, Shazia Osman, Nizar Messai, Amedeo Napoli, Marie-Dominique Devignes

- Robust Perron Cluster Analysis for Various Applications in Computational Life Science
  Marcus Weber, Susanna Kube

SESSION III: Structural Biology

- Multiple Alignment of Protein Structures in Three Dimensions
  Evgeny Krissinel, Kim Henrick

- Protein Annotation by Secondary Structure Based Alignments (PASSTA)
  Constantin Bannert, Jens Stoye

- MAPPI: Multiple 3D Alignment of Protein-Protein Interfaces
  Alexandra Shulman-Peleg, Maxim Shatsky, Ruth Nussinov, Haim J. Wolfson

SESSION IV: Genomics

- Frequent Itemsets for Genomic Profiling
  Jeannette M. De Graaf, Renée X. De Menezes, Judith M. Boer, Walter A. Kosters

- Gene Selection Through Sensitivity Analysis of Support Vector Machines
  Defeng Wang

- The Breakpoint Graph in Ciliates
  Robert Brijder, Hendrik Jan Hoogeboom Grzegorz Rozenberg

SESSION V: Computational Proteomics

- ProSpect: An R Package for Analysing SELDI Measurements Indentifying Protein Biomarker
  Andreas Quandt, Alexander Ploner, Chuen Seng Tan, Janne Lehtiö, Yudi Pawitan

- Algorithms for the Automated Absolute Quantification of Diagnostic Markers in Complex Proteomics Samples
  Clemens Gröpl, Eva Lange, Knut Reinert, Oliver Kohlbacher, Marc Sturm

- Detection of Protein Assemblies in Crystal
  Evgeny Krissinel, Kim Henrick

SESSION VI: Molecular Informatics

- Molecular Similarity Searching Using COSMO Screening Charges (COSMO/3PP)
  Andreas Bender, Andreas Klamt, Karin Wichmann, Michael Thormann, Robert C. Glen

- Increasing Diversity in In-silico Screening with Target Flexibility
  Bernhard Fischer, Holger Merlitz, Wolfgang Wenzel

- Multiple Semi-flexible 3D Superposition of Drug-Sized Molecules
  Daniel Baum

SESSION VII: Molecular Structure Determination and Simulation

- Efficiency Considerations in Solving Smoluchowksi Equations for Rough Potentials
  Banushkina Polina, Schenk Olaf, Meuwly Markus

- Fast and Accurate Structural RNA Alignment by Progressive Lagrangian Optimization
  Markus Bauer, Gunnar W. Klau, Knut Reinert

- Visual Analysis of Molecular Conformations via a Dynamic Density Mixture Model
  Johannes Schmidt-Ehrenberg, Hans-Christian Hege

Workshop on Distributed Data Mining in Life Science

- Distributed BLAST in a Grid Computing Context
  Micha Bayer, Richard Sinnott

- Parallel Tuning of Support Vector Machine Learning Parameters for Large and Unbalanced Data Sets
  Tatjana Eidrich, Bruno Lang

- The Architecture of a Proteomic Network in the Yeast
  Emad Ramadan, Christopher Osgood, Alex Pothen