


## Preliminary Program CompLife '05

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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.

(printable version  [120k](#))

### Sunday, September 25, 2005

|               |  |
|---------------|--|
| 12:30         | Bus departs from train station                                     |
| 12:30 - 13:00 | Registration   |
| 13:00         | Opening  |
| 13:00 - 14:30 | <u>Session I: "Systems Biology"</u>                                |
| 14:30 - 15:00 | Coffee Break   |
| 15:00 - 16:30 | <u>Session II: "Data Analysis and Integration"</u>                 |
| 16:30 - 17:00 | Coffee Break   |
| 17:00 - 18:30 | <u>Workshop Session: "Distributed Data Mining in Life Science"</u> |
| 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<br><u>Peter Murray-Rust: "The Chemical Semantic Web"</u> |
| 10:00 - 10:30 | Coffee Break   |
| 10:30 - 12:00 | <u>Session III: "Structural Biology"</u>                         |
| 12:00 - 13:00 | Lunch  |
| 13:00 - 14:30 | <u>Session IV: "Genomics"</u>                                    |
| 14:30 - 15:00 | Coffee Break   |
| 15:00 - 16:30 | <u>Session V: "Computational Proteomics"</u>                     |
| 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 | <u>Session VI: "Molecular Informatics"</u>                             |
| 10:30 - 11:00 | Coffee Break   |
| 11:00 - 12:30 | <u>Session VII: "Molecular Structure Determination and Simulation"</u> |
| 12:00 - 13:00 | Lunch  |
| 12:30         | Conference Closing   |

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### **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 Smail-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*
- MAPPIS: 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. Kusters*
- 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 Identifying 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 Smoluchowski 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 Eitrich, Bruno Lang*
- The Architecture of a Proteomic Network in the Yeast  
*Emad Ramadan, Christopher Osgood, Alex Pothen*