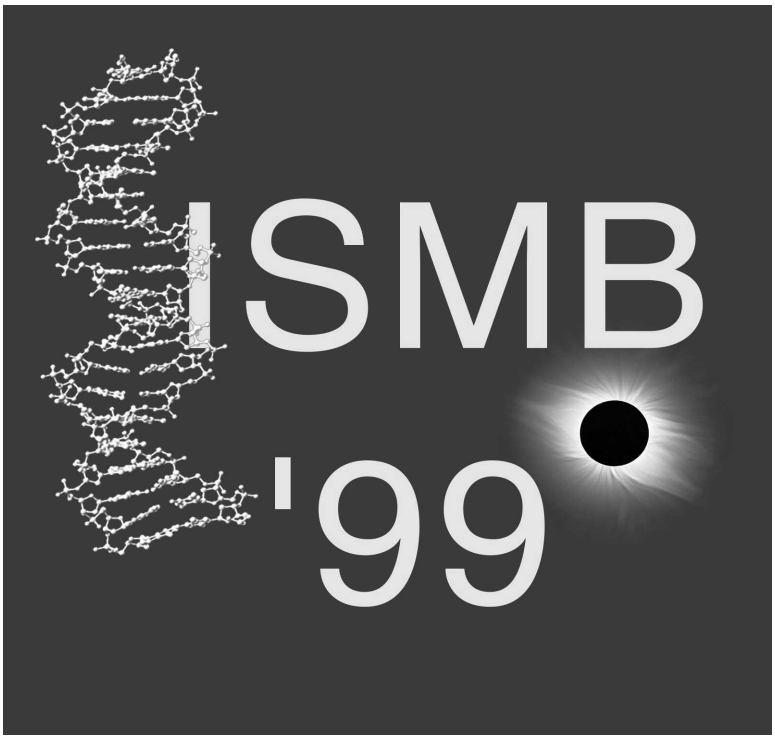
Welcome to ISMB 99
August 6 – 10, 1999
Heidelberg, Germany



The Seventh International Conference on Intelligent Systems for Molecular Biology

Final Program and Detailed Schedule

Friday, August 6, 1999

Tutorial Day

The tutorials will take place in the following rooms:

8:30 – 12:30 (Coffee break around 10:30)

Tutorial #1	Trübnersaal	Piere Baldi	Probabilistic graphical models
Tutorial #2	Robert-Schumann-Zimmer	Douglas L. Brutlag	Bioinformatics and Molecular Biology
Tutorial #3	Ballsaal	Martin Reese	The challenge of annotating a complete eukaryotic genome: A case study in *Drosophila melanogaster*
Tutorial #4	Gustav-Mahler-Zimmer	Tandy Warnow Junhyong Kim	Computational and statistical challenges involved in reconstructing evolutionary trees
Tutorial #5	Sebastian-Münster-Saal	Thomas Werner	The biology and bioinformatics of regulatory regions in genomes

Lunch (on this day served in "Grosser Saal" on the ground floor)

13:30 – 17:30 (Coffee break around 15:30)

Tutorial #6	Sebastian-Münster-Saal	Rob Miller Alan Christoffels Winston Hide	EST Clustering
Tutorial #7	Trübnersaal	Kevin Karplus Melissa Cline Christian Barrett	Getting the most out of hidden Markov models
Tutorial #8	Robert-Schumann-Zimmer	Arthur Lesk	Sequence-structure relationships and evolutionary structure changes in proteins
Tutorial #9	Gustav-Mahler-Zimmer	David States Brian Dunford Shore	PERL abstractions for databases and distributed computing
Tutorial # 10	Ballsaal	Zoltan Szallasi	Genetic network analysis - From the lab bench to computers and back

Trübnersaal is located on the second floor, please follow signs in the hallway.

18:00 Welcome reception in the Stadthalle Foyer

Saturday, August 7, 1999

Chair: Thomas Lengauer

9:00 **Conference Opening**

Opening address
Uwe Thomas
State Secretary
German Federal Ministry of Education and Research

9:50 **Keynote**
The Origin of Biological Information
Manfred Eigen
Max-Planck-Institut für Biophysikalische Chemie, Göttingen, Germany

10:40 **Coffee Break**

Session: Protein Structures I

Chair: Rick Lathrop

11:00 **Keynote**
Exploiting Protein Structure in the Post-genome Era
Michael J. E. Sternberg
Imperial Cancer Research Fund, London, UK

11:50 TEXTAL: A Pattern Recognition System for Interpreting Electron Density Maps
Thomas R. Ioerger, Thomas Holton, Jon A. Christopher, James C. Sacchettini
Texas A&M University, TX, USA

12:15 Crystallographic Threading
A. Ableson, J.I. Glasgow
Queen's University, Kingston, Canada

12:40 **Lunch**

14:00 Chair: Peer Bork

Keynote
Comparative Genomics: Is it Changing the Paradigm of Evolutionary Biology?
Eugene V. Koonin
National Center for Biotechnology Information, NIH, Bethesda, MD, USA

Session: Protein Structures II

Chair: Janice Glasgow

14:50 Multiple Structural Alignment and Core Detection by Geometric Hashing
Nathaniel Leibowitz, Zipora Y. Fligelman, Ruth Nussinov, Haim J. Wolfson
Tel Aviv University, Israel & Lab. of Experimental and Computational Biology, NCI, Frederick, MD, USA

15:15 Using Sequence Motifs for Enhanced Neural Network Prediction of Protein Distance Constraints
Jan Gorodkin, Ole Lund, Claus A. Andersen, Soren Brunak
The Technical University of Denmark, Lyngby, Denmark &
University of Aarhus, Denmark

15:40 Nearest Neighbor Classification in 3D Protein Databases
Mihael Ankerst, Gabi Kastenmueller, Hans-Peter Kriegel, Thomas Seidl
University of Munich, Germany & Max Planck Institute for Biochemistry, Munich, Germany

16:05 A Data Base of Minimally Frustrated Alpha-Helical Segments Extracted from Proteins According to an Entropy Criterion
Rita Casadio, Mario Compiani, Piero Fariselli, Pier Luigi Martelli
University of Bologna, Italy & University of Camerino, Italy

16:30 **Coffee Break**

16:50 **Posters and Demos**

18:30 **End of Scientific Day**

Sunday, August 8, 1999

Session: Arrays and Expression Patterns

Chair: Reinhard Schneider

9:00 **Keynote**
Genes, Chips and Genomes
David Balaban
Affymetrix, Inc., Santa Clara, CA, USA

9:50 Pharmaceutical Target Discovery using Guilt-by-Association: Schizophrenia and Parkinson's Disease Genes
Michael G. Walker, Wayne Volkmuth, Tod M. Klingler
Incyte Pharmaceuticals, Palo Alto, CA, USA

10:15 Fidelity Probes for DNA Arrays
Earl Hubbell, Pavel A. Pevzner
University of Southern California, Los Angeles, CA, USA & Affymetrix, Santa Clara, CA, USA

10:40 **Coffee Break**

Session: Remote Homologies

Chair: Ralf Zimmer

11:00 Database Search Based on Bayesian Alignment
Jun Zhu, Roland Luethy, Charles E. Lawrence
Amgen, Inc., Thousand Oaks, CA, USA & Wadsworth Center, Albany, NY, USA

11:25 Using the Fisher Kernel Method to Detect Remote Protein Homologies
Tommi Jaakkola, Mark Diekhans, David Haussler
University of California, Santa Cruz, CA, USA

11:50 Protein Fold Class Prediction: New Methods of Statistical Classification
J. Grassmann, M. Reczko, S. Suhai, L. Edler
Stanford University, Palo Alto, CA, USA & Synaptic Ltd., Acharnai, Greece & German Cancer Research Center, Heidelberg, Germany

12:15 **Lunch**

Chair: Thomas Lengauer

14:00 **Keynote**
Combinatorial Problems in Gene Expression Analysis Using DNA Microarrays
Richard M. Karp
University of Washington, Seattle, WA, USA

Session: Sequence Analysis Algorithms

Chair: Chris Rawlings

14:50 A Linear Time Algorithm for Finding All Maximal Scoring Subsequences
Walter L. Ruzzo, Martin Tompa
University of Washington, Seattle, WA, USA

15:15 Rapid Assessment of Extremal Statistics for Local Alignment With Gaps
Rolf Olsen, Ralf Bundschuh, Terence Hwa
University of California at San Diego, La Jolla, CA, USA

15:40 Metrics and Similarity Measures for Hidden Markov Models
Rune B. Lyngsø, Christian N. S. Pedersen, Henrik Nielsen
University of Aarhus, Denmark & Technical University of Denmark

16:05 An Exact Method for Finding Short Motifs in Sequences with Application to the Ribosome Binding Site Problem
Martin Tompa
University of Washington, Seattle, WA, USA

16:30 **Coffee Break**

16:50 **Posters and Demos**

18:30 **End of Scientific Day**

20:00 **ISCB Plenary Meeting**

Monday, August 9, 1999

Session: Databases

Chair: Peter Karp

9:00 **Keynote**
SWISS-PROT in the 21st Century !
Amos Bairoch
University of Geneva, Switzerland

9:50 Automatic extraction of biological information from Scientific text: protein-protein interactions
Christian Blaschke, Miguel A. Andrade, Christos Ouzounis, Alfonso Valencia
CNB-CSIC, Madrid, Spain & EMBL Heidelberg, Germany & EBI, Cambridge, UK

10:50 Constructing Biological Knowledge Bases by Extracting Information from Text Sources
Mark Craven, Johan Kumlien
Carnegie Mellon University, Pittsburgh, PA, USA

10:40 **Coffee Break**

Session: Systems and Networks

Chair: Peer Bork

11:00 Identify by Descent Genome Segmentation Based on Single Nucleotide Polymorphism Distributions
Thomas W. Blackwell, Eric Rouchka, David J. States
Washington University, St. Louis, MO, USA

11:25 Spatio-temporal Registration of the Expression Patterns of Drosophila Segmentation Genes
Ekaterina M. Myasnikova, David Kosman, John Reinitz, Maria G. Samsonova
Institute of High Performance Computing and Data Bases, St. Petersburg, Russia, Mount Sinai School of Medicine, New York, NY, USA

11:50 Seamless Integration of Biological Applications into a Database Framework
Thodoros Topaloglou, Anthony Kosky, Victor Markowitz
Gene Logic Inc., Berkeley, CA, USA

12:15 **Lunch**

14:00 **Solar Eclipse Lecture**
Thomas Lengauer, GMD-SCAI, Sankt Augustin, Germany

15:30 **Excursion**

Tuesday, August 10, 1999

Session: Whole Genome Analysis

Chair: Hans-Werner Mewes

9:00 **Keynote**
Computational Genomics: Biological Discovery in Complete Genomes
Anthony R. Kerlavage
Celera Genomics Corporation, Rockville, MD, USA

9:50 Building Dictionaries Of 1D and 3D Motifs By Mining The Unaligned 1D Sequences Of 17 Archeal and Bacterial Genomes
Isidore Rigoutsos, Yuan Gao, Aris Floratos, Laxmi Parida
IBM TJ Watson Research Center, Yorktown Heights, NY, USA & University of Memphis, TN, USA

10:15 Position-Specific Annotation of Protein Function Based on Multiple Homologs
Miguel A. Andrade
EMBL, Heidelberg, Germany

10:40 **Coffee Break**

Session: Molecular Interactions

Chair: Douglas Brutlag

11:00 A Motion Planning Approach to Flexible Ligand Binding
Amit P. Singh, Jean-Claude Latombe, Douglas L. Brutlag
Stanford University, CA, USA

11:25 Database Screening for HIV Protease Ligands: The Influence of Binding-Site Conformation and Representation
Volker Schnecke, Leslie A. Kuhn
Michigan State University, East Lansing, MI, USA,

11:50 INTERACT: An Object Oriented Protein-Protein Interaction Database
Karen Eilbeck, Andy Brass, Norman Paton, Charlie Hodgman
University of Manchester, UK & Glaxo Wellcome Research and Development, Stevenage, UK

12:15 Quantitative, Scalable Discrete-Event Simulation of Metabolic Pathways
Peter Meric, Michael Wise
University of Sydney, Australia

12:40 **Lunch**

Chair: Peer Bork

14:00 **Keynote**
Gene Function via the Mass Spectrometric Analysis of Multi-Protein Complexes
Matthias Mann
Odense University, Denmark

DNA Sequencing, Mapping, ESTs

Chair: Martin Vingron

14:50 An Algorithm Combining Discrete and Continuous Methods for Optical Mapping
R.M. Karp, I. Pe`er, R. Shamir
University of Washington, Seattle, WA, USA, Tel Aviv University, Israel

15:15 Genomics via Optical Mapping III: Contiging Genomic DNA and Variations
Thomas Anantharaman, Bud Mishra, David Schwartz
New York University, NY, USA

15:40 A Dataset Generator for Whole Genome Shotgun Sequencing
Gene Myers
Celera Genomics, Rockville, MD, USA

16:05 ESTScan: a program for detecting , evaluating, and reconstructing potential coding regions in EST sequences
Christian Iseli, C. Victor Jongeneel, Philipp Bucher
Swiss Institute of Bioinformatics, Epalinges, Switzerland

16:30 **Coffee Break**

Session: Phylogenetic Analysis and Clustering

Chair: Gary Stormo

16:50 Solving Large Scale Phylogenetic Problems using DCM2
Daniel H. Huson, Lisa Vawter, Tandy J. Warnow
Princeton University, NJ, USA & Smithkline Beecham, King of Prussia, PA, USA & University of Arizona, Tucson, AZ, USA

17:15 A Phylogentic Approach to Molecular Structure Prediction
Viatcheslav R. Akmaev, Scott T. Kelley, Gary D. Stormo
University of Colorado, Boulder, CO, USA

17:40 Reconstructing the Duplication History of a Tandem Repeat
Gary Benson, Lan Dong
Mount Sinai School of Medicine, New York, NY, USA

18:05 Analysis of ribosomal RNA sequences by combinatorial clustering
Poe Xing, Casimir Kulikowski, Ilya Muchnik, Inna Dubchak, Denise Wolf, Sylvia Spengler, Manfred Zorn
Rutgers University, Piscataway, NJ, USA, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

18:30 **Conferral of the SGI-Outstanding ISMB'99 Paper Award**

Closing Remarks

19:00 **End of Conference**

SGI-Outstanding ISMB'99 Paper Award !

SGI will donate an award for an outstanding paper presented during the ISMB'99 Conference.

Out of all the presented papers, among the top ranking papers according to the review process five will be chosen by the organizing committee as nominees. (Papers with participation from the groups of the organizing committee are excluded.)
During the conference the organizing committee will listen to the respective presentations and decide on the award winner. The final decision criteria will be a balance of: novelty of the work, significance of the work, age of the author (juniors are preferred) and presentation style.

The winner will be announced at te end of the conference. The winner will receive an SGI 320 - the new Pentium-based NT desktop machine from SGI that combines SGI's graphics technology with the standard Intel platform.

SGI-ISMB'99 Crunch Contest !

Win 120 hours of time on a 128 CPU SGI Origin 2000!

Submit your crunch idea at the SGI booth during the meeting. The organizing committee will select the winning idea and will announce the winner on the last day of the conference.
The winner will work with SGI HPC Bioinformatics specialists to perform the crunch project. Resulting data will become property of the winner.

MISCELLANEOUS

Location

All events will take place at Stadthalle Heidelberg. The rooms mentioned in this program are all located in the Stadthalle. A large floorplan of the Stadthalle pointing to the various rooms will be posted at the meeting.

Registration

The registration and conference office will open on Friday, August 6 and on Saturday, August 7 at 7:30 a.m. On the remaining conference days the office will open at 8:30 a.m. During opening hours the conference office can be reached under the telephone number +49 6221 14 22 804.

Public Transport

Transfer to the Conference Site "Stadthalle": from the Marriott Hotel, please take bus line # 35 from the Betriebshof (3 minutes walking distance from the Marriott). The bus runs every 10 minutes and stops right in front of the Stadthalle.
From the IBIS Hotel take bus line #35, 41 or 42 to the Stadthalle. The bus runs every 10 minutes.

Prices: single trip: DM 3.40, 5-trip-ticket: DM 13.50, 3-day ticket: DM 20.00.

All other hotels are within walking distance (10-15 minutes), although the Marriott and the IBIS are also within walking distance (20 minutes).

Parking

Parking is available at the park garages: Kongresshaus P6 and P8.

Mail Room

There are 20 computers available for your personal use. They are located in the room behind "Trübnersaal" on the second floor.

These computers are generously sponsored by SGI.

Awards

There may be other paper and poster awards, besides SGI award, offered. Look for details on these awards at the meeting.

Poster Sessions

The number in the poster book corresponds to the number of the poster stand.

Software Demonstrations

During the Poster Session, there will also be Software Demonstrations. There is separate material in your conference bags informing you about this program item.

Industrial Exhibition

There is an industrial exhibition at ISMB'99. There is separate material in your conference bags informing you about this program item.

PLEASE WEAR YOUR BADGE AT ALL TIMES, YOU WILL NEED IT TO BE ADMITTED TO THE "GROSSER SAAL" AND TO OBTAIN MEALS.

ORGANIZATIONAL DETAILS

On Friday, August 6, lunch will be served in "Grosser Saal".

On the other conference days, lunch will be served in the Restaurant at the back of the Stadthalle and "Ballsaal" located on the first floor.
NOTE: Due to the large number of participants we ask you to please vacate your table after you finish eating and take your coffee outside the dining area (e.g. terrace, exhibition hall, foyer).

Speakers can check their slides in the slide-check-room "Tagungsbüro" located on the ground floor.

Invited speakers and tutorial speakers are asked to come to the registration desk for organizational purposes.

Messages for other participants can be placed on a board next to the registration desk.

Should you wish to take a shared limousine to Frankfurt airport on the day of your departure, please inform the personnel at the registration desk at least 48 hours in advance. The shuttle service costs DM 70,- per person (two people is DM 110,- and so on) and needs to be paid to the driver. A regular taxi costs approx. DM 150,-.

You can also take the Lufthansa shuttle service bus, which leaves from the Marriott Hotel approximately every hour. The cost is DM 36,- per person.

Trains leave from the Heidelberg train station approximately every half hour.

SOCIAL EVENTS

Friday evening, 18:00 – 20:00
Reception for all conference participants (Snacks and drinks will be served)

Sunday evening, 20:00 – 22:00
ISCB Plenary Meeting open to all the participants (Drinks will be available)

EXCURSIONS

Excursion to Neckarsteinach on Monday, August 9

Neckarsteinach is a very nice old town close to Heidelberg. It is known as the 4-castle-city.

On August 9, we will leave by boat from Heidelberg Stadthalle at **15:30** to Neckarsteinach. The trip will take 1 1/2 hours and will take you along the Neckar River. You will be able to see the 4 castles on your way up the river.

In Neckarsteinach you will have 1 1/2 hours to visit the beautiful town. You will receive a short guide to Neckarsteinach in English.

The boat will take you back to Heidelberg leaving Neckarsteinach at **18:30**. On the trip a buffet with local specialties will be offered which is included in the price. Drinks can be bought at your own expense on the boat. (Please be on time. This is the last boat).

Solar Eclipse Excursion on Wednesday, August 11

We will leave Heidelberg by bus at 9:00 on August 11. We will drive to the Castle Neipperg. From the wonderful castle grounds you will be able to follow the solar eclipse accompanied by a buffet with local specialties. After the solar eclipse there will be a wine tasting including local wines as well as wines from the regions the path of totality of the solar eclipse has touched.

We will leave the castle around 16:00.

After the eclipse tour, we will arrange for a bus to go from the Castle Neipperg via Heidelberg to Frankfurt airport (if sufficiently many people sign up). You can bring your luggage in the morning and leave it on the bus. The price depends on the number of people signing up (approx. DM 20,-). If we leave the castle at 16:00, it takes one hour to Heidelberg. From there it takes another hour to get to Frankfurt. Allowing for heavy traffic on the Autobahn, you should reach Frankfurt around 19:00 (no guarantees).