

Edited by S. Istrail, P. Pevzner, and M. Waterman

Editorial Board: A. Apostolico S. Brunak M. Gelfand
T. Lengauer S. Miyano G. Myers M.-F. Sagot D. Sankoff
R. Shamir T. Speed M. Vingron W. Wong

Subseries of Lecture Notes in Computer Science

João Carlos Setubal
Sergio Verjovski-Almeida (Eds.)

Advances in Bioinformatics and Computational Biology

Brazilian Symposium on Bioinformatics, BSB 2005
Sao Leopoldo, Brazil, July 27-29, 2005
Proceedings

Series Editors

Sorin Istrail, Celera Genomics, Applied Biosystems, Rockville, MD, USA

Pavel Pevzner, University of California, San Diego, CA, USA

Michael Waterman, University of Southern California, Los Angeles, CA, USA

Volume Editors

João Carlos Setubal

Virginia Bioinformatics Institute and Department of Computer Science

Virginia Polytechnic Institute and State University, Bioinformatics 1, Box 0477

Blacksburg, VA 24060-0477, USA

E-mail: setubal@vbi.vt.edu

Sergio Verjovski-Almeida

Universidade de São Paulo

Instituto de Química, Departamento de Bioquímica

Av. Prof. Lineu Prestes 748, 05508-000 São Paulo, SP, Brazil

E-mail: verjo@iq.usp.br

Library of Congress Control Number: 2005929321

CR Subject Classification (1998): H.2.8, F.2.1, I.2, G.2.2, J.2, E.1

ISSN 0302-9743

ISBN-10 3-540-28008-1 Springer Berlin Heidelberg New York

ISBN-13 978-3-540-28008-8 Springer Berlin Heidelberg New York

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, re-use of illustrations, recitation, broadcasting, reproduction on microfilms or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer. Violations are liable to prosecution under the German Copyright Law.

Springer is a part of Springer Science+Business Media

springeronline.com

© Springer-Verlag Berlin Heidelberg 2005

Printed in Germany

Typesetting: Camera-ready by author, data conversion by Scientific Publishing Services, Chennai, India
Printed on acid-free paper SPIN: 11532323 06/3142 5 4 3 2 1 0

Preface

The Brazilian Symposium on Bioinformatics (BSB 2005) was held in São Leopoldo, Brazil, July 27–29, 2005, on the campus of the Universidade Vale do Rio dos Sinos (Unisinos). BSB 2005 was the first BSB symposium, though BSB is in fact a new name for a predecessor event called the Brazilian Workshop on Bioinformatics (WOB). WOB was held in three consecutive years: 2002, 2003, and 2004. The change from workshop to symposium reflects the increased reach and quality of the meeting. BSB 2005 was held in conjunction with the Brazilian Computer Society's (SBC) annual conference.

For BSB 2005 we had 55 submissions: 45 full papers and 10 extended abstracts. These proceedings contain the 15 full papers that were accepted, plus 16 extended abstracts (a combination of the accepted abstracts and some full papers that were accepted as extended abstracts). These papers and abstracts were carefully refereed and selected by an international program committee of 40 members, with the help of some additional reviewers, all of whom are listed on the following pages. These proceedings also include papers from three of our invited speakers. We believe this volume represents a fine contribution to current research in bioinformatics and computational biology.

The editors would like to thank: the authors, for submitting their work to the symposium, and the invited speakers; the program committee members and other reviewers for their help in the review process; the Unisinos local organizers, José Mombach and Ney Lemke; Marcelo Walter from Unisinos, coordinator of the SBC conference; Ivan Sendin, from the University of Goiás, who helped with fund raising; Margaret Gabler, from VBI, who helped with the preparation of the proceedings; the symposium sponsors (see list in this volume); Guilherme Telles, Ana Bazzan, Marcelo Brígido, Sergio Lifschitz, and Georgios Pappas, members of the SBC special committee for computational biology; and Springer for agreeing to print this volume.

July 2005

João Carlos Setubal
Sergio Verjovski-Almeida

Organization

BSB 2005 Scientific Program Committee

João Carlos Setubal <i>Informatics Chair</i>	(Virginia Bioinformatics Institute, Virginia Tech, USA)
Sergio Verjovski-Almeida <i>Biology Chair</i>	(University of São Paulo, Brazil)
Nalvo Almeida Jr.	(Federal University of Mato Grosso do Sul, Brazil)
Ricardo Baeza-Yates	(ICREA-Univ. Pompeu Fabra, Spain & Univ. of Chile)
Valmir Barbosa	(Federal University of Rio de Janeiro, Brazil)
Ana Bazzan	(Federal University of Rio Grande do Sul, Brazil)
Marcelo Brígido	(University of Brasília, Brazil)
Marcelo Briones	(Federal University of São Paulo)
André Carvalho	(University of São Paulo, Brazil)
Julio Collado-Vides	(Autonomous University of Mexico)
Allan Dickerman	(Virginia Tech, USA)
Alan Durham	(University of São Paulo, Brazil)
Carlos Ferreira	(University of São Paulo, Brazil)
James Glazier	(University of Indiana, USA)
Katia Guimaraes	(Federal University of Pernambuco, Brazil)
Lenny Heath	(Virginia Tech, USA)
Victor Jongeneel	(Ludwig Institute, Lausanne, Switzerland)
João Kitajima	(Alelyx, Brazil)
Natalia Martins	(EMBRAPA, Brazil)
Wellington Martins	(Catholic University of Goiás, Brazil)
Marta Matoso	(Federal University of Rio de Janeiro, Brazil)
João Meidanis	(Scylla and University of Campinas, Brazil)
Pedro Mendes	(Virginia Tech, USA)
José Mombach	(Unisinos, Brazil)
Bernard Moret	(University of New Mexico, USA)
Eduardo Jordão Neves	(University of São Paulo)
Ney Lemke	(Unisinos, Brazil)
Sergio Lifschitz	(Catholic University, Rio de Janeiro, Brazil)
Georgios Pappas	(Catholic University of Brasilia, Brazil)
Christian Probst	(Mol.Biol.Institute, Curitiba, Brazil)
Eduardo Reis	(University of São Paulo, Brazil)
Leila Ribeiro	(Federal University of Rio Grande do Sul, Brazil)
Larry Ruzzo	(University of Washington, USA)
Marie-France Sagot	(INRIA, France)
Bruno Sobral	(Virginia Tech, USA)

VIII Organization

BSB 2005 Scientific Program Committee (continued)

Siang Song (University of São Paulo, Brazil)
Osmar Norberto de Souza (Catholic University of Rio Grande do Sul, Brazil)
Guilherme Telles (University of São Paulo, Brazil)
Fernando von Zuben (University of Campinas, Brazil)
Maria Emilia Walter (University of Brasília, Brazil)

Additional Reviewers

Edson Cáceres
Marcelo Henriques de Carvalho
Jian Chen
Vicky Choi
Lokesh Das
Luciano Digiampietri
Vladimir Espinosa
Katti Faceli
Paulo Roberto Ferreira Jr.
Julio Freyre
Abel González
Marco Gubitoso
Giampaolo Luiz Libralão
Ana Lorena
Sandro Marana
Cleber Mira
Alexey Onufriev
José Augusto Amgarten Quitzau
Cassia Trojahn dos Santos
Marcilio de Souto
Bruno de Souza
Eric Tannier

Local Organizers

José Mombach (Unisinos, Brazil)
Ney Lemke (Unisinos, Brazil)

Sponsoring Institutions

Brazilian Computer Society (SBC)

Universidade Vale do Rio dos Sinos

The Brazilian National Council for Research (CNPq)

The Rio Grande do Sul State Research Agency (FAPERGS)

Hewlett-Packard

GE Healthcare

Invitrogen

Microsoft

Table of Contents

Invited Papers

Differential Gene Expression in the Auditory System <i>Irene S. Gabashvili, Richard J. Carter, Peter Markstein, Anne B.S. Giersch</i>	1
Searching for Non-coding RNA <i>Walter L. Ruzzo</i>	9
Cyberinfrastructure for PathoSystems Biology <i>Bruno W.S. Sobral</i>	11
Analysis of Genomic Tiling Microarrays for Transcript Mapping and the Identification of Transcription Factor Binding Sites <i>Joel Rozowsky, Paul Bertone, Thomas Royce, Sherman Weissman, Michael Snyder, Mark Gerstein</i>	28

Full Papers

Perturbing Thermodynamically Unfeasible Metabolic Networks <i>R. Nigam, S. Liang</i>	30
Protein Cellular Localization with Multiclass Support Vector Machines and Decision Trees <i>Ana Carolina Lorena, André C.P.L.F. de Carvalho</i>	42
Combining One-Class Classifiers for Robust Novelty Detection in Gene Expression Data <i>Eduardo J. Spinosa, André C.P.L.F. de Carvalho</i>	54
Evaluation of the Contents of Partitions Obtained with Clustering Gene Expression Data <i>Katti Faceli, André C.P.L.F. de Carvalho, Marcílio C.P. de Souto</i>	65
Machine Learning Techniques for Predicting <i>Bacillus subtilis</i> Promoters <i>Meika I. Monteiro, Marcílio C.P. de Souto, Luiz M.G. Gonçalves, Lucymara F. Agnez-Lima</i>	77

XII Table of Contents

An Improved Hidden Markov Model Methodology to Discover Prokaryotic Promoters <i>Adriana Neves dos Reis, Ney Lemke</i>	85
Modeling and Property Verification of Lactose Operon Regulation <i>Marcelo Cezar Pinto, Luciana Foss, José Carlos Merino Mombach, Leila Ribeiro</i>	95
YAMONES: A Computational Architecture for Molecular Network Simulation <i>Guilherme Balestieri Bedin, Ney Lemke</i>	107
Structure Prediction and Docking Studies of Chorismate Synthase from <i>Mycobacterium Tuberculosis</i> <i>Cláudia Lemelle Fernandes, Diógenes Santiago Santos, Luiz Augusto Basso, Osmar Norberto de Souza</i>	118
Analysis of the Effects of Multiple Sequence Alignments in Protein Secondary Structure Prediction <i>Georgios Joannis Pappas Jr., Shankar Subramaniam</i>	128
Tests of Automatic Annotation Using KOG Proteins and ESTs from 4 Eukaryotic Organisms <i>Maurício de Alfarenga Mudado, Estevam Bravo-Neto, José Miguel Ortega</i>	141
Diet as a Pressure on the Amino Acid Content of Proteomes <i>Francisco Prosdocimi, José Miguel Ortega</i>	153
A Method for Comparing Three Genomes <i>Guilherme P. Telles, Marcelo M. Brigido, Nalvo F. Almeida, Carlos J.M. Viana, Daniel A.S. Anjos, Maria Emilia M.T. Walter</i>	160
Comparison of Genomic DNA to cDNA Alignment Methods <i>Miguel Galves, Zanoni Dias</i>	170
Segmentation and Centromere Locating Methods Applied to Fish Chromosomes Images <i>Elaine Ribeiro de Faria, Denise Guliato, Jean Carlo de Sousa Santos</i>	181

Extended Abstracts

Sequence Motif Identification and Protein Family Classification Using Probabilistic Trees <i>Florencia Leonardi, Antonio Galves</i>	190
Prediction of Myotoxic and Neurotoxic Activities in Phospholipases A2 from Primary Sequence Analysis <i>Fabiano Pazzini, Fernanda Oliveira, Jorge A. Guimarães, Hermes Luís Neubauer de Amorim</i>	194
Genomics and Gene Expression Management Tools for the <i>Schistosoma Mansoni</i> cDNA Microarray Project <i>Thiago M. Venancio, Ricardo DeMarco, Katia C.P. Oliveira, Ana Carolina Quirino Simoes, Aline Maria da Silva, Sergio Verjovski-Almeida</i>	198
SAM Method as an Approach to Select Candidates for Human Prostate Cancer Markers <i>Ana C.Q. Simoes, Aline M. da Silva, Sergio Verjovski-Almeida, Eduardo M. Reis</i>	202
New EST Trimming Strategy <i>Christian Baudet, Zanoni Dias</i>	206
A Modification of the Landau-Vishkin Algorithm Computing Longest Common Extensions via Suffix Arrays <i>Rodrigo de Castro Miranda, Mauricio Ayala-Rincón</i>	210
The BioPAUÁ Project: A Portal for Molecular Dynamics Using Grid Environment <i>Alan Wilter, Carla Osthoff, Cristiane Oliveira, Diego E.B. Gomes, Eduardo Hill, Laurent E. Dardenne, Patrícia M. Barros, Pedro A.A.G.L. Loureiro, Reynaldo Novaes, Pedro G. Pascutti</i>	214
Analysis of Structure Prediction Tools in Mutated MeCP-2 <i>Dino Franklin, Ivan da Silva Sendin</i>	218
Protein Loop Classification Using Artificial Neural Networks <i>Armando Vieira, Baldomero Oliva</i>	222
VIZ - A Graphical Open-Source Architecture for Use in Structural Bioinformatics <i>Ricardo M. Czekster, Osmar Norberto de Souza</i>	226

XIV Table of Contents

Selection of Data Sets of Motifs as Attributes in the Process of Automating the Annotation of Proteins' Keywords <i>Ana L.C. Bazzan, Cassia T. dos Santos</i>	230
Bioinformatics Tools for HIV-1 Identification in Southern Brazilian States <i>Ardala Breda, Cláudia Lemelle Fernandes, Sabrina Esteves de Matos Almeida, Heitor Moreira Franco, Maria Lúcia Rosa Rossetti, Rosângela Rodrigues, Luís Fernando Brígido, Elizabeth Cortez-Herrera</i>	234
Fact and Task Oriented System for Genome Assembly and Annotation <i>Luciano A. Digiampietri, Julia M. Perdigueiro, Aloisio J. de Almeida Junior, Daniel M. Faria, Eric H. Ostroski, Gustavo G.L. Costa, Marcelo C. Perez</i>	238
A Clustering Strategy to Find Similarities in Mycoplasma Promoters <i>João Francisco Valiati, Paulo Martins Engel</i>	242
Gene Prediction by Syntenic Alignment <i>Said Sadique Adi, Carlos Eduardo Ferreira</i>	246
Real Time Immersive Visualization and Manipulation of the Visible Human Data Set <i>Ilana de Almeida Souza, Claudiney Sanches Junior, André Luiz Miranda da Rosa, Patrícia Trautenmüller, Thiago Tognoli Lopes, Marcelo Knörich Zuffo</i>	251
Author Index	257