

# Advances in Intelligent and Soft Computing

---

93

**Editor-in-Chief: J. Kacprzyk**

# Advances in Intelligent and Soft Computing

## Editor-in-Chief

Prof. Janusz Kacprzyk  
Systems Research Institute  
Polish Academy of Sciences  
ul. Newelska 6  
01-447 Warsaw  
Poland  
E-mail: kacprzyk@ibspan.waw.pl

---

Further volumes of this series can be found on our homepage: [springer.com](http://springer.com)

Vol. 81. J. Düh, H. Hufnagl, E. Juritsch,  
R. Pfleigl, H.-K. Schimany,  
and Hans Schönegger (Eds.)  
*Data and Mobility, 2010*  
ISBN 978-3-642-15502-4

Vol. 82. B.-Y. Cao, G.-J. Wang,  
S.-L. Chen, and S.-Z. Guo (Eds.)  
*Quantitative Logic and Soft  
Computing 2010*  
ISBN 978-3-642-15659-5

Vol. 83. J. Angeles, B. Boulet,  
J.J. Clark, J. Kovács, and K. Siddiqi (Eds.)  
*Brain, Body and Machine, 2010*  
ISBN 978-3-642-16258-9

Vol. 84. Ryszard S. Choraś (Ed.)  
*Image Processing and Communications  
Challenges 2, 2010*  
ISBN 978-3-642-16294-7

Vol. 85. Á. Herrero, E. Corchado,  
C. Redondo, and Á. Alonso (Eds.)  
*Computational Intelligence in Security  
for Information Systems 2010*  
ISBN 978-3-642-16625-9

Vol. 86. E. Mugellini, P.S. Szczepaniak,  
M.C. Pettenati, and M. Sokhn (Eds.)  
*Advances in Intelligent  
Web Mastering – 3, 2011*  
ISBN 978-3-642-18028-6

Vol. 87. E. Corchado, V. Snášel,  
J. Sedano, A.E. Hassanien, J.L. Calvo,  
and D. Ślęzak (Eds.)  
*Soft Computing Models in Industrial and  
Environmental Applications,*  
*6th International Workshop SOCO 2011*  
ISBN 978-3-642-19643-0

Vol. 88. Y. Demazeau, M. Pěchouček,  
J.M. Corchado, and J.B. Pérez (Eds.)  
*Advances on Practical Applications of Agents  
and Multiagent Systems, 2011*  
ISBN 978-3-642-19874-8

Vol. 89. J.B. Pérez, J.M. Corchado,  
M.N. Moreno, V. Julián, P. Mathieu,  
J. Canada-Bago, A. Ortega, and  
A.F. Caballero (Eds.)  
*Highlights in Practical Applications of Agents  
and Multiagent Systems, 2011*  
ISBN 978-3-642-19916-5

Vol. 90. J.M. Corchado, J.B. Pérez,  
K. Hallenborg, P. Gólińska, and  
R. Corchuelo (Eds.)  
*Trends in Practical Applications of Agents  
and Multiagent Systems, 2011*  
ISBN 978-3-642-19930-1

Vol. 91. A. Abraham, J.M. Corchado,  
S.R. González, J.F. de Paz Santana (Eds.)  
*International Symposium on Distributed  
Computing and Artificial Intelligence, 2011*  
ISBN 978-3-642-19933-2

Vol. 92. P. Novais, D. Preuveneers, and  
J.M. Corchado (Eds.)  
*Ambient Intelligence - Software and  
Applications, 2011*  
ISBN 978-3-642-19936-3

Vol. 93. M.P. Rocha, J.M.C. Rodríguez,  
F. Fdez-Riverola, and A. Valencia (Eds.)  
*5th International Conference on Practical  
Applications of Computational Biology &  
Bioinformatics (PACBB 2011), 2011*  
ISBN 978-3-642-19913-4

Miguel P. Rocha, Juan M. Corchado Rodríguez,  
Florentino Fdez-Riverola, and  
Alfonso Valencia (Eds.)

---

# 5th International Conference on Practical Applications of Computational Biology & Bioinformatics (PACBB 2011)



Springer

## **Editors**

Prof. Miguel P. Rocha  
Universidade do Minho  
Dep. Informática / CCTC  
4710 - 057 Braga  
Portugal

Prof. Juan M. Corchado Rodríguez  
University of Salamanca  
Department of Computing Science  
and Control  
Faculty of Science  
Plaza de la Merced S/N  
37008 Salamanca  
Spain  
E-mail: [corchado@usal.es](mailto:corchado@usal.es)

Prof. Florentino Fdez-Riverola  
ESEI: Escuela Superior de Ingeniería  
Informática  
Edificio Politécnico  
32004 Ourense  
Spain

Prof. Alfonso Valencia  
Spanish National Cancer  
Research Centre  
Structural Biology and BioComputing  
Programme (CNIO)  
Melchor Fdez Almagro 3  
28029 Madrid  
Spain

ISBN 978-3-642-19913-4

e-ISBN 978-3-642-19914-1

DOI 10.1007/978-3-642-19914-1

Advances in Intelligent and Soft Computing

ISSN 1867-5662

Library of Congress Control Number: 2011923223

©2011 Springer-Verlag Berlin Heidelberg

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, reuse of illustrations, recitation, broadcasting, reproduction on microfilm 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 for prosecution under the German Copyright Law.

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

*Typeset & Cover Design:* Scientific Publishing Services Pvt. Ltd., Chennai, India.

Printed on acid-free paper

5 4 3 2 1 0

[springer.com](http://springer.com)

# Preface

The growth in the Bioinformatics and Computational Biology fields over the last few years has been remarkable and the trend is to increase its pace. In fact, the need for computational techniques that can efficiently handle the huge amounts of data produced by the new experimental techniques in Biology is still increasing driven by new advances in Next Generation Sequencing, several types of the so called omics data and image acquisition, just to name a few. The analysis of the datasets that produces and its integration call for new algorithms and approaches from fields such as Databases, Statistics, Data Mining, Machine Learning, Optimization, Computer Science and Artificial Intelligence.

Within this scenario of increasing data availability, Systems Biology has also been emerging as an alternative to the reductionist view that dominated biological research in the last decades. Indeed, Biology is more and more a science of information requiring tools from the computational sciences.

In the last few years, we have seen the surge of a new generation of interdisciplinary scientists that have a strong background in the biological and computational sciences. In this context, the interaction of researchers from different scientific fields is, more than ever, of foremost importance boosting the research efforts in the field and contributing to the education of a new generation of Bioinformatics scientists. PACBB'11 hopes to contribute to this effort promoting this fruitful interaction.

PACBB'11 technical program included 50 papers from a submission pool of 78 papers spanning many different sub-fields in Bioinformatics and Computational Biology. Therefore, the conference will certainly have promoted the interaction of scientists from diverse research groups and with a distinct background (computer scientists, mathematicians, biologists). The scientific content will certainly be challenging and will promote the improvement of the work that is being developed by each of the participants.

We would like to thank all the contributing authors, as well as the members of the Program Committee and the Organizing Committee for their hard and highly valuable work. Their work has helped to contribute to the success of the PACBB'11 event. PACBB'11 wouldn't exist without your contribution.

PACBB'11 has been supported by Junta de Castilla y León (Spain).

Juan Manuel Corchado  
Miguel Rocha  
PACBB'11 Organizing Co-chairs

Florentino Fdez-Riverola  
Alfonso Valencia  
PACBB'11 Programme Co-chairs

# Organization

## General Co-chairs

Miguel P. Rocha	CCTC, Univ. Minho (Portugal)
Juan M. Corchado	University of Salamanca (Spain)
Florentino Fdez-Riverola	University of Vigo (Spain)
Alfonso Valencia	Structural Biology and BioComputing Programme (CNIO)

## Program Committee

Florentino Fdez-Riverola (Chairman)	University of Vigo (Spain)
Alfonso Valencia (Chairman)	Structural Biology and BioComputing Programme(CNIO)
Alicia Troncoso	Universidad de Pablo de Olavide (Spain)
Alíprio Jorge	LIAAD/INESC, Porto LA (Portugal)
Ana Rojas	IMPPC, Barcelona (Spain)
Anália Lourenço	IBB/CEB, University of Minho (Portugal)
Antonio del Sol	University of Luxembourg
Arlindo Oliveira	INESC-ID, Lisboa (Portugal)
Arlo Randall	University of California Irvine (USA)
B. Cristina Pelayo	University of Oviedo (Spain)
Christopher Henry	Argonne National Labs (USA)
Daniel Gayo	University of Oviedo (Spain)
Daniel Glez-Peña	University of Vigo (Spain)
David Posada	Univ. Vigo (Spain)
Emilio S. Corchado	University of Burgos (Spain)
Eugénio C. Ferreira	IBB/CEB, University of Minho (Portugal)
Eva Lorenzo	University of Vigo (Spain)
Fernando Diaz-Gómez	University of Valladolid (Spain)
Florencio Pazos	CNB/CSIC, Madrid (Spain)
Gonzalo Gómez-López	UBio/CNIO, Spanish National Cancer Research Centre (Spain)
Hagit Shatkay	Queens University, Ontario (Canada)
Isabel C. Rocha	IBB/CEB, University of Minho (Portugal)
Javier de las Rivas	CiC/IBMCC, University of Salamanca (Spain)

Jesús M. Hernández	University of Salamanca (Spain)
Jorge Vieira	IBMC, Porto (Portugal)
José Adserias	University of Salamanca (Spain)
José L. López	University of Salamanca (Spain)
José Luís Oliveira	Univ. Aveiro (Portugal)
José-Jesús Fernández	CNB/CSIC, Madrid (Spain)
Juan Antonio García Ranea	University of Málaga (Spain)
Juan M. Cueva	University of Oviedo (Spain)
Juanma Vacquerizas	European Bioinformatics Institute (UK)
Julio R. Banga	IIM/CSIC, Vigo (Spain)
Julio Saez-Rodríguez	European Bioinformatics Institute (UK)
Kaustubh Raosaheb Patil	Max-Planck Institute for Informatics (Germany)
Kiran R. Patil	EMBL - Heidelberg (Germany)
Lourdes Borrajo	University of Vigo (Spain)
Luis M. Rocha	Indiana University (USA)
Manuel J. Maña López	University of Huelva (Spain)
Mª Dolores Muñoz Vicente	Universidad de Salamanca
Martin Krallinger	Structural Biology and BioComputing Programme (CNIO), Madrid (Spain)
Nara Rúbia	ABO-RS (Brazil)
Nicholas Luscombe	EBI (UK)
Nuno Fonseca	CRACS/INESC, Porto (Portugal)
Oscar Sanjuan	University of Oviedo (Spain)
Paulino Gómez-Puertas	University Autónoma de Madrid (Spain)
Paulo Azevedo	University of Minho (Portugal)
Pierre Baldi	University of California Irvine (USA)
Reyes Pavón	University of Vigo (Spain)
Rita Ascenso	Polytechnic Institute of Leiria (Portugal)
Rosalía Laza	University of Vigo (Spain)
Rui Brito	University of Coimbra (Portugal)
Rui C. Mendes	CCTC, University of Minho (Portugal)
Rui Camacho	LIACC/FEUP, University of Porto (Portugal)
Rui Rijo	IP Leiria (Portugal)
Sara Madeira	IST/INESC, Lisboa (Portugal)
Sérgio Deusdado	IP Bragança (Portugal)
Vítor Costa	University of Porto (Portugal)

## Organizing Committee

Juan M. Corchado (Chairman)	University of Salamanca (Spain)
Miguel Rocha (Chairman)	CCTC, Univ. Minho (Portugal)
Juan F. De Paz	University of Salamanca (Spain)
Javier Bajo	Pontifical University of Salamanca (Spain)
Sara Rodríguez	University of Salamanca (Spain)

Dante I. Tapia	University of Salamanca (Spain)
Fernando de la Prieta Pintado	University of Salamanca (Spain)
Carolina Zato Domínguez	University of Salamanca (Spain)
Cristian I. Pinzón	University of Salamanca (Spain)
Rosa Cano	University of Salamanca (Spain)
Belén Pérez Lancho	University of Salamanca (Spain)
Angélica González Arrieta	University of Salamanca (Spain)
Vivian F. López	University of Salamanca (Spain)
Ana de Luís	University of Salamanca (Spain)
Ana B. Gil	University of Salamanca (Spain)
Jesús García Herrero	Universidad Carlos III de Madrid (Spain)
Miguel Reboiro-Jato	University of Vigo (Spain)

# Contents

## Applications

<b>Riskoweb: Web-Based Genetic Profiling to Complex Disease Using Genome-Wide SNP Markers .....</b>	1
<i>Sergio Torres-Sánchez, Rosana Montes-Soldado, Nuria Medina-Medina, Andrés R. Masegosa, María Mar Abad-Grau</i>	
<b>MC64: A Web Platform to Test Bioinformatics Algorithms in a Many-Core Architecture .....</b>	9
<i>Francisco José Esteban, David Díaz, Pilar Hernández, Juan Antonio Caballero, Gabriel Dorado, Sergio Gálvez</i>	
<b>Integrating Medical Patient Data with Family Trees to Improve the Quality of Information .....</b>	17
<i>Eliana Sousa, Tiago Jesus, Lina Neves, Mónica Costa, Fernando Reinaldo Ribeiro, José Carlos Metrólho, Ricardo Cruz-Correia</i>	
<b>Peptidase Detection and Classification Using Enhanced Kernel Methods with Feature Selection .....</b>	23
<i>Lionel Morgado, Carlos Pereira, Paula Veríssimo, António Dourado</i>	
<b>An Image Processing Application for Quantification of Protein Aggregates in <i>Caenorhabditis Elegans</i> .....</b>	31
<i>Andreia Teixeira-Castro, Nuno Dias, Pedro Rodrigues, João Filipe Oliveira, Nuno F. Rodrigues, Patrícia Maciel, João L. Vilaça</i>	
<b>Workflows with Model Selection: A Multilocus Approach to Phylogenetic Analysis .....</b>	39
<i>Jorge Álvarez, Roberto Blanco, Elvira Mayordomo</i>	

<b>Baiacu: A Tool for the Visual Analysis of the <i>Saccharomyces Cerevisiae</i> Regulatory Network .....</b>	49
<i>Ricardo S. Aires, João A. Carriço, Alexandre P. Francisco, Sara C. Madeira</i>	
<b>BBMS<sup>++</sup> – Basic Bioinformatics Meta-searcher .....</b>	57
<i>Márcio S. Carocho, Sérgio Deusdado</i>	
<b>Effective Parallelization of Non-bonded Interactions Kernel for Virtual Screening on GPUs .....</b>	63
<i>Ginés D. Guerrero, Horacio Pérez-Sánchez, Wolfgang Wenzel, José M. Cecilia, José M. García</i>	
<b>Tracking B Cells from Two-Photon Microscopy Images Using Sequential Monte Carlo .....</b>	71
<i>David Olivieri, Ivan Gomez Conde, Jose Faro</i>	
<b>Experiments on Computer Assisted Optimization of the <i>Escherichia Coli</i> Fermentation Process Using Optferm .....</b>	79
<i>Tânia Teixeira, Sérgio Deusdado</i>	
<b>An Intuitive Workflow to Retrieve Somatic Mutations in Next Generation Sequencing Studies .....</b>	83
<i>Daniel Glez-Peña, Miguel Reboiro-Jato, Florentino Fdez-Riverola, David G. Pisano, Gonzalo Gómez-López</i>	
<b>Building a GATK-Based Tool for Methylation Analysis in Next-Generation Bisulfite Sequencing Experiments .....</b>	87
<i>Daniel Glez-Peña, Osvaldo Graña, Florentino Fdez-Riverola, David G. Pisano</i>	
<b>EPIQuest: A Multiuser and Multiproject Web Tool to Build Online Forms for Biomedical Studies .....</b>	93
<i>M. Márquez-Cid, G. Comesaña, R. Milne, G. Andrés, N. Malats, D. Pisano</i>	
<b>Building Proteomics Applications with the AIBench Application Framework .....</b>	99
<i>Miguel Reboiro-Jato, Daniel Glez-Peña, José R. Méndez-Reboredo, Hugo M. Santos, Ricardo J. Carreira, José L. Capelo, Florentino Fdez-Riverola</i>	
<b>Neurohand Solving the Inverse Cinematic of an Anthropomorphic Arm .....</b>	109
<i>Marina Beltrán-Blanco, Javier Molina-Vilaplana, José Luis Muñoz-Lozano, Juan López-Coronado</i>	

<b>An Enhancement of the Usage of the Poincare Index for the Detection and Classification of Characteristic Points in Dactylograms .....</b>	117
<i>Angélica González, Marco A. Ameller F.</i>	

## Clinical & Diagnosis & Drugs

<b>Modelling of Tirapazamine Effects on Solid Tumour Morphology .....</b>	125
<i>N. Kazmi, M.A. Hossain, R.M. Phillips</i>	

<b>MOGA-Based Multi-drug Optimisation for Cancer Chemotherapy .....</b>	133
<i>S. Algoul, M.S. Alam, K. Sakib, M.A. Hossain, M.A.A. Majumder</i>	

<b>Multi-drug Infusion Control Using Model Reference Adaptive Algorithm .....</b>	141
<i>S. Enbiya, M.A. Hossain, F. Mahieddine</i>	

## Genomics & Phylogenetics & Sequencing

<b>Fast and Accurate Genome Anchoring Using Fuzzy Hash Maps .....</b>	149
<i>John Healy, Desmond Chambers</i>	

<b>A Parallel Niched Pareto Evolutionary Algorithm for Multiple Sequence Alignment .....</b>	157
<i>Fernando José Mateus da Silva, Juan Manuel Sánchez Pérez, Juan Antonio Gómez Pulido, Miguel A. Vega Rodríguez</i>	

<b>Phylogenetic Analysis Using an SMV Tool .....</b>	167
<i>José Ignacio Requeno, Roberto Blanco, Gregorio de Miguel Casado, José Manuel Colom</i>	

<b>An Efficient Motif Search Algorithm Based on a Minimal Forbidden Patterns Approach .....</b>	175
<i>Tarek El Falah, Thierry Lecroq, Mourad Elloumi</i>	

<b>Emerging Methodologies in Multiple Sequence Alignment Using High Throughput Data .....</b>	183
<i>Francisco M. Ortúñoz Guzman, I. Rojas, H. Pomares, J.M. Urquiza, J.P. Florido</i>	

<b>DNA Sequence Search Using Content-Based Image Search Approach .....</b>	191
<i>Heri Ramampiaro, Aleksander Grande</i>	

<b>Integrative Analysis of the Regulatory Region of the FGFR3 Oncogene.....</b>	201
<i>Josep Bau, Marta Cullell, Jordi Solé-Casals</i>	
<b>Distances between Dinucleotides in the Human Genome .....</b>	205
<i>Carlos A.C. Bastos, Vera Afreixo, Armando J. Pinho, Sara P. Garcia, João M.O.S. Rodrigues, Paulo J.S.G. Ferreira</i>	
<b>Compressing the Human Genome Using Exclusively Markov Models .....</b>	213
<i>Diogo Pratas, Armando J. Pinho</i>	

## Microarrays

<b>Highlighting Differential Gene Expression between Two Condition Microarrays through Multidimensional Scaling Comparison of <i>Lesihmania Infantum</i> Genomic Data Similarity Matrices .....</b>	221
<i>Víctor Andrés Vera-Ruiz, Liliana López-Kleine</i>	
<b>Biclustering-Based Classification of Clinical Expression Time Series: A Case Study in Patients with Multiple Sclerosis .....</b>	229
<i>André V. Carreiro, Orlando Anunciação, João A. Carriço, Sara C. Madeira</i>	
<b>A Simulation Study on the Impact of Strong Dependence in High-Dimensional Multiple-Testing I: The Case without Effects .....</b>	241
<i>Antonio Carvajal-Rodríguez, Jacobo de Uña-Álvarez</i>	
<b>Bioinformatics as a Tool to Help Characterise <i>Perkinsus Olseni</i> Up-Regulated Genes in Response to Its Host .....</b>	247
<i>Rita M.T. Ascenso</i>	

<b>Hybridization Dynamics Compensation in Microarray Experiments .....</b>	255
<i>Raul Malutan, Pedro Gómez Vilda, Ioana Berindan Neagoe, Monica Borda</i>	

## Proteomics

<b>Identification of Peptides with Deviating Regulation Factors Using a Robust Clustering Scheme .....</b>	263
<i>Natalia Novoselova, Frank Klawonn, Thorsten Johl, Tobias Reinal, Lothar Jänsch</i>	

<b>Prediction of Protein Distance Maps by Assembling Fragments According to Physicochemical Similarities .....</b>	271
<i>Gualberto Asencio Cortés, Jesús S. Aguilar-Ruiz, Alfonso E. Márquez Chamorro</i>	
<b>Residue-Residue Contact Prediction Based on Evolutionary Computation .....</b>	279
<i>Alfonso E. Márquez Chamorro, Federico Divina, Jesús S. Aguilar-Ruiz, Gualberto Asencio Cortés</i>	
<b>NcPred for Accurate Nuclear Protein Prediction Using <i>n</i>-mer Statistics with Various Classification Algorithms .....</b>	285
<i>Md. Saiful Islam, Alaol Kabir, Kazi Sakib, Md. Alamgir Hossain</i>	

## Sytems Biology

<b>Relating Formalisms for the Qualitative Modelling of Regulatory Networks .....</b>	293
<i>Beatriz Luna, Claudine Chaouiya</i>	
<b>Interpreting the Regulatory Interplay in <i>E. coli</i> Metabolic Pathways .....</b>	303
<i>Anália Lourenço, Sónia Carneiro, José P. Pinto, Miguel Rocha, Eugénio C. Ferreira, Isabel Rocha</i>	
<b>A Systematic Modeling Approach to Elucidate the Triggering of the Stringent Response in Recombinant <i>E. coli</i> Systems .....</b>	313
<i>Sónia Carneiro, Eugénio C. Ferreira, Isabel Rocha</i>	
<b>Modeling Cellular Signaling Systems: An Abstraction-Refinement Approach .....</b>	321
<i>Diana Hermith, Carlos Olarte, Camilo Rueda, Frank D. Valencia</i>	
<b>A Study on the Robustness of Strain Optimization Algorithms .....</b>	329
<i>Paulo Vilaça, Paulo Maia, Miguel Rocha</i>	

## Text/Data Mining & AI Techniques

<b>Assessing the Suitability of MeSH Ontology for Classifying Medline Documents .....</b>	337
<i>Rosalía Laza, Reyes Pavón, Miguel Reboiro-Jato, Florentino Fdez-Riverola</i>	

<b>Assessing the Impact of Class-Imbalanced Data for Classifying Relevant/Irrelevant Medline Documents .....</b>	345
<i>Reyes Pavón, Rosalía Laza, Miguel Reboiro-Jato, Florentino Fdez-Riverola</i>	
<b>Assessing the Effect of 2D Fingerprint Filtering on ILP-Based Structure-Activity Relationships Toxicity Studies in Drug Design .....</b>	355
<i>Rui Camacho, Max Pereira, Vítor Santos Costa, Nuno A. Fonseca, Carlos J.V. Simões, Rui M.M. Brito</i>	
<b>Using Dictionaries for Biomedical Text Classification .....</b>	365
<i>R. Romero, E.L. Iglesias, L. Borrajo, C.M. Redondo Marey</i>	
<b>Using Machine Learning Techniques and Genomic/Proteomic Information from Known Databases for PPI Prediction .....</b>	373
<i>J.M. Urquiza, I. Rojas, H. Pomares, L.J. Herrera, J.P. Florido, F. Ortúño</i>	
<b>Prioritizing Literature Search Results Using a Training Set of Classified Documents .....</b>	381
<i>Sérgio Matos, José Luis Oliveira</i>	
<b>Improving Reproducibility on Tree Based Multimarker Methods: TreeDTh .....</b>	389
<i>José Javier Moreno-Ortega, Nuria Medina-Medina, Rosana Montes-Soldado, María Mar Abad-Grau</i>	
<b>Author Index .....</b>	397