

Maria Raposo
Paulo A. Ribeiro
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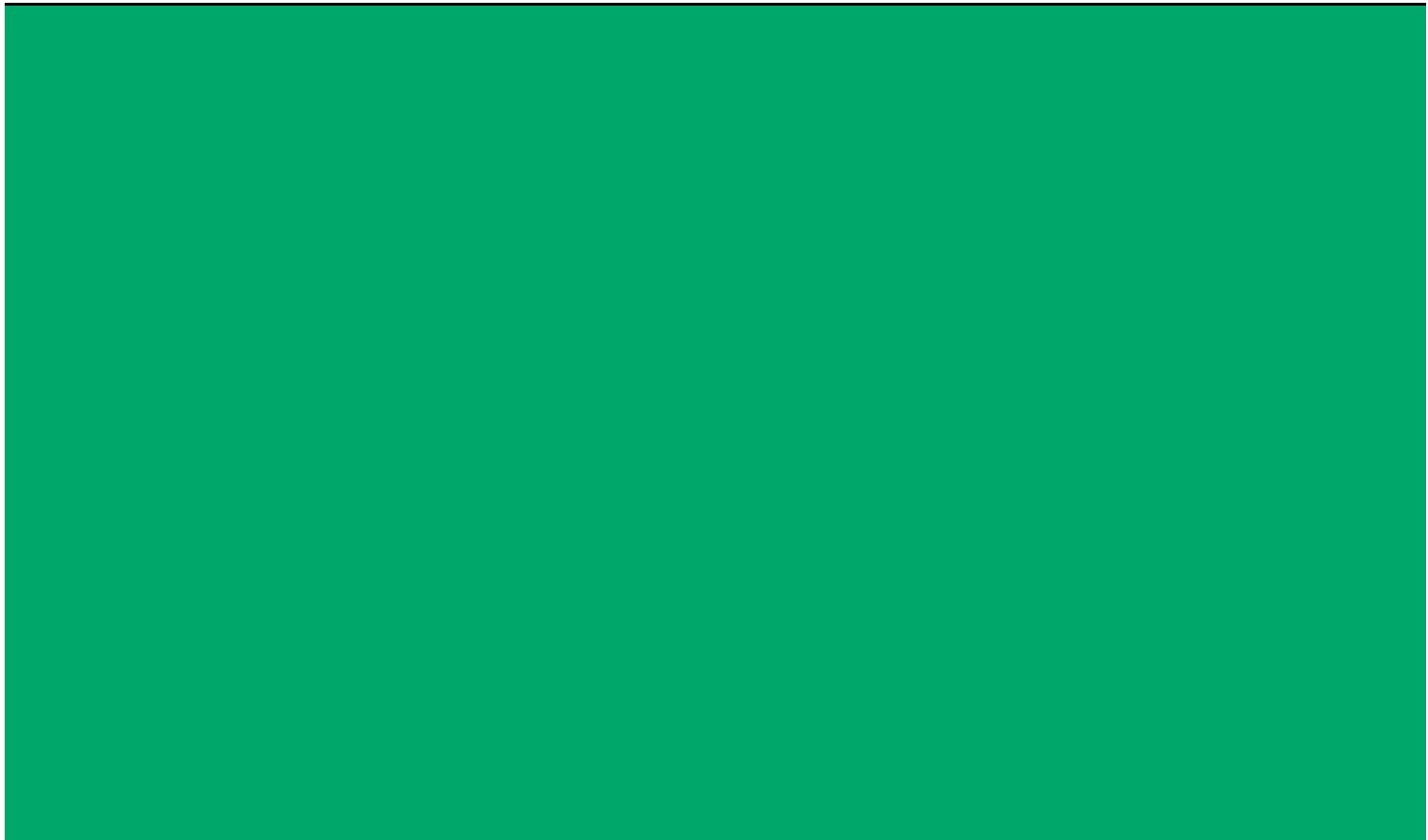
Computational Intelligence Methods for Bioinformatics and Biostatistics

15th International Meeting CIBB 2018

September 6th -8th 2018

Universidade NOVA de Lisboa, FCT, Portugal

Conference Proceedings





CIBB2018 Participants at Campus da Caparica, 7 of September 2018

This volume contains the papers presented at

CIBB 2018: Fifteenth international meeting on Computational Intelligence methods for Bioinformatics and Biostatistics

<https://eventos.fct.unl.pt/cibb2018/>

held on September 6th - 8th, 2018 at Universidade NOVA de Lisboa, Faculdade de Ciências e Tecnologia, Departamento de Física

This volume was edited by Maria Raposo, Paulo A. Ribeiro and Susana Sério.

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CIBB 2018 SPONSORS

Centre of Physics and Technological Research (CEFITEC), Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, <https://www.cefitec.fct.unl.pt/>

CIBB HISTORY

From 2004 to 2007, CIBB has had the format of a special session of larger conferences, namely, WIRN 2004 in Perugia, WILF 2005 in Crema, FLINS 2006 in Genoa, and WILF 2007 in Camogli. Given the great success of the special session at WILF 2007 that included 26 strongly rated papers, the Steering Committee decided to turn CIBB into an autonomous conference starting with the 2008 edition in Vietri. The following editions in Italian venues were held in Genoa (2009), Palermo (2010) and Gargnano (2011). Until 2012, CIBB meetings were held annually in Italy with an increasing number of participants. CIBB 2012 was the first edition organized outside Italy, in Houston, then in Nice, France (2013), Cambridge, UK (2014), Naples, Italy (2015), Stirling, UK (2016), Cagliari, Italy (2017) and Caparica, Portugal (2018)

A rigorous peer-review selection process is applied every time to ultimately select the papers included in the program of the conference, in the post-conference Proceedings published by LNBI-LNCS book series by Springer-Verlag, and in some cases, selected papers were published in special issues of well-qualified international journals, such as BMC Bioinformatics.

CIBB 2018, Caparica, Portugal.
CIBB 2017, Cagliari, Italy.
CIBB 2016, Stirling, UK.
CIBB 2015, Naples, Italy.
CCIB 2014, Cambridge, UK.
CCIB 2013, Nice, France.
CIBB 2012, Huston, Texas, USA.
CIBB 2011, Gargnano-Lago di Garda, Italy.
CIBB 2010, Palermo, Italy.
CIBB 2009, Genova, Italy.
CIBB 2008, Genova, Italy.
CIBB 2007, Portofino, Italy.
CIBB 2006, Genova, Italy.

CIBB 2018 OVERVIEW

This book contains the accepted papers of CIBB2018, the 15th International Conference on Computational Intelligence methods for Bioinformatics and Biostatistics, an international conference which provided a multi-disciplinary forum for researchers interested in the application of computational intelligence, in a broad sense, to open problems in bioinformatics, biostatistics, systems and synthetic biology and medical informatics. Cutting edge methodologies capable of accelerating life science discoveries were also addressed. Following its tradition and roots, this year's meeting brought together researchers from the international scientific community interested in advancements and future perspectives in bioinformatics and biostatistics. Under this compliance, current trends and future opportunities at the edge of computer and life sciences, the application of computational intelligence to a system and synthetic biology and the consequent impact on innovative medicine were of great interest for the conference. Theoretical and experimental biologists were also invited to participate to present novel challenges and foster multidisciplinary collaboration. This meeting was sponsored by Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa and Center of Physics and Technological Research (CEFITEC), Portugal. The Conference Program only included oral presentations, among which we were honored with plenary keynote lectures, given by Alberto Paccanaro (University of London, United Kingdom), Alexandra Carvalho (Universidade de Lisboa, Portugal), Benoit Lique (University of Pau and Pays de l'Adour, France), Fernando L. Ferreira (Universidade Nova de Lisboa, Portugal) and Veronica Vinciotti (Brunel University London, United Kingdom).

Revised papers following conference feed-back and discussion were considered for post-conference published by Springer, and selected ones were invited for journal publication, traditionally published by BMC Bioinformatics.

The organization has attributed four fees grants to PhD students. These grants were conferred having into account the average punctuation given by the reviewers.

The event also contributed for the strengthening of collaborative research within the fields of Computational Intelligence methods for Bioinformatics and Biostatistics. A Social Dinner on the evening of 7th September 2018 at Casa da Cerca, a beautiful monument of Almada city, contributed fruitfully to foster alliances.

Finally, we would like to express our thanks to all participants, all members of the Program Committee and to the secretariat.

Maria Raposo
Paulo A. Ribeiro
Susana Sérgio

ORGANIZING INSTITUTION

CIBB 2018 was organized by:

Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, Portugal

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KEYNOTE SPEAKERS

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Prof. Alexandra Carvalho	Universidade de Lisboa, Portugal
Prof. Benoit Lique	University of Pau, France
Prof. Fernando L. Ferreira	Universidade Nova de Lisboa, Portugal
Dr. Veronica Vinciotti	Brunel University London, UK

KEYNOTE TALKS

A Unified Regularized Group PLS Algorithm Scalable to Big Data. Application on genomics data

Benoit Liquet, University of Pau and Pays de l'Adour, France

Partial Least Squares (PLS) methods have been heavily exploited to analyse the association between two blocs of data. These powerful approaches can be applied to data sets where the number of variables is greater than the number of observations and in presence of high collinearity between variables. Different sparse versions of PLS have been developed to integrate multiple data sets while simultaneously selecting the contributing variables. Sparse modelling is a key factor in obtaining better estimators and identifying associations between multiple data sets. The cornerstone of the sparsity version of PLS methods is the link between the SVD of a matrix (constructed from deflated versions of the original matrices of data) and least squares minimisation in linear regression. We present here an accurate description of the most popular PLS methods, alongside their mathematical proofs. A unified algorithm is proposed to perform all four types of PLS including their regularised versions. Our methods enable us to identify important relationships between genomic expression and cytokine data from an HIV vaccination trial. We also proposed a new methodology by accounting for both grouping of genetic markers (e.g. genesets) and temporal effects. Finally, various approaches to decrease the computation time are offered, and we show how the whole procedure can be scalable to big data sets.

Sparse graphical models in genomics: an application to censored qPCR data

Veronica Vinciotti, Department of Mathematics, Brunel University London, Uxbridge UB8 3PH, London, UK.

Regularized inference of networks using graphical modelling approaches has seen many applications in biology, most notably in the recovery of regulatory networks from high-dimensional gene expression data. Various extensions to the standard graphical lasso approach have been proposed, such as dynamic and hierarchical graphical models. In this talk, I will focus on a latest extension to censored graphical models in order to deal with censored data such as qPCR data. We propose a computationally efficient EM-like algorithm for the estimation of the conditional independence graph and thus the recovery of the underlying regulatory network.

Answering questions in biology and medicine by making inferences on networks

Alberto Paccanaro, University of London, United Kingdom

An important idea that has emerged recently is that a cell can be viewed as a complex network of interrelating proteins, nucleic acids and other bio-molecules. At the same time, data generated by large-scale experiments often have a natural representation as networks such as protein-protein interaction networks, genetic interaction networks, co-expression networks. From a computational point of view, a central objective for systems biology and medicine is therefore the development of methods for making inferences and discovering structure in biological networks possibly using data which are also in the form of networks. In this talk, I'll

present novel computational methods for solving biological problems which can all be phrased in terms of inference and structure discovery in large scale networks. These methods are based and extend recent developments in the areas of machine learning (particularly semi-supervised learning and matrix factorization), graph theory and network science. I will show how these computational techniques can provide effective solutions for: 1) quantifying similarity between heritable diseases at molecular level using exclusively disease phenotype information; 2) disease gene prediction; 3) drug side-effect prediction.

Model selection for temporal biomedical data

Alexandra Carvalho, Universidade de Lisboa, Portugal

Human health care is changing rapidly, pressing the development of machine learning techniques for automatic diagnoses and prognosis, as well as personalized therapies for individual patients. The emerging availability of temporal data, namely via electronic medical records, is triggering this line of research. One of the main problems is to model the dynamic process underlying the data evolution. We detail how to learn efficiently Markovian data, when the dependencies can be expressed as a dynamic Bayesian network. We follow a score-based approach, and guarantee that the learned model is optimal according to several model selection criteria. Finally, we address the problem of early classification, which is essential in time-sensitive applications, such as personalized therapies.

Ethics and our moral in research, let's think about it!

Fernando Luís Ferreira, Universidade Nova de Lisboa, Portugal

As researchers, it is our will is to pursue knowledge, to contribute to society and to open new roads for the Future. Ethics is a theme always present in our minds but probably remains outside the central concerns of researchers while main subjects are developed. Sometimes we come across a formal consent or an ethics statement seen mostly as a bureaucratic task. However, lately with the so called exponential technologies, we find ourselves dueling with a variety of controversial questions resulting from the different branches of artificial intelligence as those applied to self-driving cars' decisions the exposure of privacy and Decision support systems in medicine, etc. Some are arguing that risks become clear and, one of this days, we may face a singularity and, eventually, becoming too late to stop. This short talk aims to rise some questions about present ethical issues aiming at promoting the intervention and discussion among participants at this Conference.

SPECIAL SESSIONS

Machine explanation – Interpretation of Machine Learning Models for Medicine and Bioinformatics

Organizer

Ian H. Jarman	Liverpool John Moores University, UK
Alfredo Vellido	Universitat Politècnica de Catalunya, Barcelona, Spain
José D. Martín-Guerrero	University of Valencia, Spain
Davide Bacciu	Università of Pisa, Italy

Fast and Efficient Solutions for Computational Intelligence Methods in Bioinformatics, Systems and Computational Biology

Organizer

Stefano Beretta	University of Milano-Bicocca, Italy
Paolo Cazzaniga	Universidade de Lisboa, Portugal
Ivan Merelli	Institute for Biomedical Technologies, National Research Council, Italy

Engineering Bio-Interfaces and Rudimentary Cells as a Way to Develop Synthetic Biology

Organizers

Maria Raposo	Universidade Nova de Lisboa, Portugal
Quirina Ferreira	Universidade de Lisboa, Portugal
Paulo A. Ribeiro	Universidade Nova de Lisboa, Portugal
Susana Sério	Universidade Nova de Lisboa, Portugal

Soft Computing Methods for Characterizing Diseases from Omics Data

Organizers

Angelo Ciaramella	Università di Napoli Parthenope, Italy
Giosuè Lo Bosco	Università di Palermo, Italy
Riccardo Rizzo	ICAR-CNR, Italy
Antonino Staiano	Università di Napoli Parthenope, Italy

Computational Methods for Neuroimaging Analysis

Organizers

Tiago Azevedo	University of Cambridge, UK
Giovanna Maria Dimitri	University of Cambridge, UK

Pietro Liò
Angela Serra
Simeon Spasov

University of Cambridge, UK
University of Salerno, Italy
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Networking biostatistics and bioinformatics

Organizers

Clelia Di Serio
Cugnata Federica

Vita-Salute San Raffaele University, Milano, Italy
Vita-Salute San Raffaele University, Milano, Italy

Modeling and Simulation Methods for System Biology and System Medicine

Organizers

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Alex Graudenzi
Marzia Di Filippo
Dario Pescini

University of Milano-Bicocca, Italy
University of Milano-Bicocca, Italy
University of Milano-Bicocca, Italy
University of Milano-Bicocca, Italy
University of Milano-Bicocca, Italy
University of Milano-Bicocca, Italy
University of Milano-Bicocca, Italy

Machine Learning in Health Informatics and Biological Systems

Organizers

Davide Chicco
Marco Masseroli
Annalisa Barla
Anne-Christin Hauschild

Princess Margaret Cancer Centre, Toronto, Ontario, Canada
Politecnico di Milano, Milan, Italy
Università di Genova, Genoa, Italy
Krembil Research Institute, Toronto, Ontario, Canada

ACCEPTED PAPERS

CIBB Main Track

Committee-based Active Learning to Select Negative Examples for Predicting Protein Functions

Marco Frasca, Maryam Sepehri, Alessandro Petrini, Giuliano Grossi and Giorgio Valentini
CIBB2018_Paper_5 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_7

Classification of epileptic activity through temporal and spatial characterization of intracranial recordings

Vanessa D'Amario, Annalisa Barla, Gabriele Arnulfo, Lino Nobili
CIBB2018_Paper_6 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_6

Centrality speeds the subgraph isomorphism search up in target aware contexts

Vincenzo Bonnici, Simone Caligola, Antonino Aparo, Rosalba Giugno
CIBB2018_Paper_11 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_3

Computational Annotation of Genetic Biomarkers using Topologically Associating Domains

Carlos Cano, Michela Verbeni, Carmen Navarro, Maria S. Benítez-Cantos, Antonio González-Aguilar, Gema Durán-Ogalla, Manuel Benavides, Susana Pedrinaci, Mercedes López de Hierro-Ruiz, Pilar Martínez-Tirado, Francisco Ruiz-Cabello, José Luis Martín-Ruiz, Armando Blanco, Paul Lizardi
CIBB2018_Paper_21 - https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_21.pdf

Unravelling breast and prostate common gene signatures by Bayesian network learning

João Villa-Brito, Marta B. Lopes, Alexandra M. Carvalho, Susana Vinga
CIBB2018_Paper_40 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_25

Variational inference in probabilistic single-cell RNA-seq models

Pedro F. Ferreira, Alexandra M. Carvalho, Susana Vinga
CIBB2018_Paper_39 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_2

PiXora: Simultaneous Phasing of Multiple Polyploids

Laxmi Parida, Filippo Utro
CIBB2018_Paper_8 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_5

Fusions using convolutional neural networks

Marta Lovino, Gianvito Urgese, Enrico Macii, Santa Di Cataldo, Elisa Ficarra
Paper 14 - https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_14.pdf

Benchmarking Multitask Learning for QSARS

Ivan Olier, Philippa Grace McCabe, Disha Agarwal, Sandra Ortega-Martorell
CIBB2018_Paper_38 - https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_38.pdf

Paratope identification by classification of local antibody surface patches enriched with eight physicochemical properties

Sebastian Daberdaku
CIBB2018_Paper_10 - https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_10.pdf

In Silico ADME and Toxicity prediction using N-grams for chemical fingerprinting

Leif E. Peterson, Timothy C. Thompson
CIBB2018_Paper_61 - https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_61.pdf

A Graphical Tool for the Exploration and Visual Analysis of Biomolecular Networks
Cheick Tidiane Ba, Elena Casiraghi, Marco Frasca, Jessica Gliozzo, Giuliano Grossi, Marco Mesiti, Marco Notaro, Paolo Perlasca, Alessandro Petrini, Matteo Re, Giorgio Valentini
CIBB2018_Paper_35 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_8

An innovative approach to integrate proteomics and metabolomics data in severe septic shock
Manuela Ferrario, Alice Cambiaghi, Eliandre de Olivera, Roberta Pastorelli
CIBB2018_Paper_17 – https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_17.pdf

Analysis of Extremely Obese Individuals Using Deep Learning Stacked Autoencoders and Genome-Wide Genetic Data
Casimiro A. Curbelo Montañez, Paul Fergus, Carl Chalmers and Jade Hind
CIBB2018_Paper_30 - https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_30.pdf

Smartwatch Based Fall Detection System for Elders' Surveillance
Fernando Luís-Ferreira, Daniel Rodrigues, João Sarraipa, Ricardo Goncalves
CIBB2018_Paper_41– https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_41_2.pdf

Special Track: Machine explanation – Interpretation of Machine Learning Models for Medicine and Bioinformatics

Structure finding stabilization and optimization with the PC algorithm
Raúl V. Casaña-Eslava, Ian H. Jarman, Sandra Ortega-Martorell, Paulo J. Lisboa, José D. Martín-Guerrero
CIBB2018_Paper_2- https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_2.pdf

Enabling interpretation of the outcome of a human obesity prediction machine learning analysis from genomic data
Ahsan Bilal, Alfredo Vellido, Vicent Ribas
CIBB2018_Paper_12- https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_12.pdf

Special Track: Fast and Efficient Solutions for Computational Intelligence Methods in Bioinformatics, Systems and Computational Biology

A quantitative assessment of the effect of different algorithmic schemes to the task of learning the structure of Bayesian Networks
Stefano Beretta, Mauro Castelli, Ivo Gonçalves, Daniele Ramazzotti
CIBB2018_Paper_15 - https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_15.pdf

GENHAP: Evolutionary Computation for Haplotype Assembly
Andrea Tangherloni, Simone Spolaor, Leonardo Rundo, Marco S. Nobile, Paolo Cazzaniga, Giancarlo Mauri, Pietro Liò, Daniela Besozzi, Ivan Merelli
CIBB2018_Paper_27 – https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_27.pdf

HaploVir: Inferring Viral Haplotypes from Deep Sequencing of a Mixture of Strains using a Path Decomposition Algorithm
Stefano Beretta, Paola Bonizzoni, Ivan Merelli,
CIBB2018_Paper_37– https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_37.pdf

Improved Predictor-Corrector Algorithm

Hassan Pazira

CIBB2018_Paper_19 – https://link.springer.com/chapter/10.1007/978-3-030-34585-3_9

Random Sampling Regularisation: A Proposed Methodology for Detection of Epistasis Interactions in Genomic Studies

Jade Hind, Abir Hussain, Dhiya Al-Jumeily, Casimiro A. Curbelo Montañez, Carl Chalmers, Paulo Lisboa

CIBB2018_Paper_24 – https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_24.pdf

Special Track: Engineering Bio-Interfaces and Rudimentary Cells as a Way to Develop Synthetic Biology

Drug Delivery Films for Ocular Diseases Treatment

Mónica Machado, Helena Morais, Luísa Mendonça, Jorge Morgado, Quirina Ferreira

CIBB2018_Paper_43 – https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_43r.pdf

Adsorption of Triclosan on sensors based on PAH/PAZO thin-films: the effect of pH

J. Pereira-da-Silva, P. M. Zagalo, G. Magalhães-Mota, P. A. Ribeiro, M. Raposo

CIBB2018_Paper_34 – https://link.springer.com/chapter/10.1007%2F978-3-030-34585-3_29

Effect of epigallocatechin-3-gallate on DMPC oxidation revealed by infrared spectroscopy

Filipa Pires, Bárbara Rodrigues, Gonçalo Magalhães-Mota, Paulo A. Ribeiro and Maria Raposo

CIBB2018_Paper_22 – https://link.springer.com/chapter/10.1007/978-3-030-34585-3_26

Effect of EGCG on the DNA in presence of UV Radiation

Thais Pivetta, Filipa Pires, Maria Raposo

CIBB2018_Paper_29 – https://link.springer.com/chapter/10.1007/978-3-030-34585-3_27

Non-Thermal Atmospheric pressure Plasmas: Generation, Sources and Applications

Sara Pereira, Érica Pinto, Paulo António Ribeiro, Susana Sério

CIBB2018_Paper_31 – https://link.springer.com/chapter/10.1007/978-3-030-34585-3_28

Detection of Triclosan Dioxins After UV Irradiation – A Preliminar Study

Gonçalo Magalhães-Mota, Filipa Pires, Paulo A. Ribeiro and Maria Raposo

CIBB2018_Paper_53 – https://link.springer.com/chapter/10.1007/978-3-030-34585-3_30

Real-time adsorption of a Co-octaethylporphyrin monitored with scanning tunneling microscopy

Catarina L. Delfino, Jorge Morgado, Quirina Ferreira

CIBB2018_Paper_42 – https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_42r.pdf

Special Track: Soft Computing Methods for Characterizing Diseases from Omics Data

Identification of Key miRNAs in regulation of PPI Networks

Antonino Fiannaca, Massimo La Rosa, Laura La Paglia, Alfonso Urso, Riccardo Rizzo, Giosué Lo Bosco

CIBB2018_Paper_52 – https://link.springer.com/chapter/10.1007/978-3-030-34585-3_10

Recurrent Deep Neural Network for nucleosome classification

Domenico Amato, Mattia Di Gangi, Giosué Lo Bosco, Riccardo Rizzo

CIBB2018_Paper_45 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_11

Compressive Sensing and Hierarchical Clustering for Microarray Data with Missing Values

Angelo Ciaramella, Davide Nardone, Antonino Staiano

CIBB2018_Paper_49 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_1

Special Track: Computational Methods for Neuroimaging Analysis

Automatic discrimination of auditory stimuli perceived by the human brain

Angela Serra, Antonio Della Pietra, Marcus Herdener, Roberto Tagliaferri and Fabrizio Esposito

CIBB2018_Paper_1 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_18

Decoding Semantic Word Categories from Electro- and Magnetoencephalography data

Simeon Spasov, Olaf Hauk, Seyedeh-Rezvan Farahibozorg

CIBB2018_Paper_23 - https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_23.pdf

Statistical validation of State-Space Granger Causality with Time-Reverse Surrogate and its boundaries in fMRI data

Tiago Fernandes, João Pereira, Bruno Direito, Alexandre Sayal, Miguel Castelo-Branco

CIBB2018_Paper_36 - https://eventos.fct.unl.pt/cibb2018/files/cibb2018_paper_36.pdf

Neural Models for Brain Networks Connectivity Analysis

Razvan E. Kuztos, Giovanna Maria Dimitri, Pietro Liò

CIBB2018_Paper_13 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_19

Special Track: Networking biostatistics and bioinformatics

Searching for the source of difference: a graphical model approach

Vera Djordjilović, Monica Chiogna, Chiara Romualdi, Elisa Salviato

CIBB2018_Paper_4 - https://link.springer.com/chapter/10.1007/978-3-030-34585-3_12

Improving Sensitivity and Specificity Calculation from Myocardial Imaging Data

Federica Cugnata, Paola M.V. Rancoita

CIBB2018_Paper_56 -

https://eventos.fct.unl.pt/sites/default/files/cibb2018/files/cibb2018_paper_56.pdf

Longitudinal Studies and Integrative Biology with Heterogeneous data: an approach using rarefaction

Luca Del Core, Eugenio Montini, Clelia Di Serio, Andrea Calabria

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