

BBCC2023
Bioinformatics and Computational Biology Conference
December 4-7, 2023

Program

December 4

Department of Science and Technology, University "Parthenope", Naples

15:00 Round Table – for the Italian community
L'insegnamento della Bioinformatica nelle università italiane

December 5

Villa Doria d'Angri – Naples

9:00 Registration and Welcome Coffee

9:30 Opening of the Conference - Conference Chairs

9:40 Session: **Bioinformatics for Ecology**

Chair: Emanuel Di Nardo, University "Parthenope", Naples, Italy

Invited lecture

Michele Scardi – University of Rome "Tor Vergata"

Machine Learning applications in Ecology: a personal perspective

Selected oral presentations

- 10:30 An Artificial Intelligence-based Methodology for Anthozoa Images Classification
S. Cioffi, F. Ferrigno, G. Mellone, V. Scarrica, E. Di Nardo, R. Sandulli, A. Staiano, A. Ciaramella
- 10:45 Application of Coloured Petri Nets to Model Communication, Movement, Death and Duplication of Unicellular Organisms
Leila Ghanbar, David Gilbert
- 11:00 COMPARO: COMparative genomics for PARalogs and Orthologs
Luca Ambrosino, Marco Miralto, Mara Sangiovanni, Chiara Colantuono, Alessia Riccardi, Maria Luisa Chiusano
- 11:15 Characterization of microbial diversity associated with Mediterranean sponges by a metataxonomic analysis
Serena Federico, Roberta Esposito, Michele Sonnessa, Sofia Reddel, Marco Bertolino, Nadia Ruocco, Giacomo Zagami, Marco Giovine, Marina Pozzolini, Marco Guida, Valerio Zupo, Maria Costantini
- 11:30 Predicting farmed mussel bacteria contamination with HPC and AI
Ciro Giuseppe De Vita, Diana Di Luccio, Gennaro Mellone, Francesca Barchiesi, Germana Colarusso, Angelo Ciaramella, Raffaele Montella

11:45 Coffee Break – Poster session

12:15 Session: **Bioinformatics applications**
Chair: Antonino Staiano, University "Parthenope", Naples, Italy

Selected oral presentations

- 12:15 Inference and design of antibody specificity: from experiments to models and back
Jorge Fernandez-de-Cossio-Diaz, Guido Uguzzoni, Kévin Ricard, Francesca Anselmi, Clément Nizak, Andrea Pagnani, Olivier Rivoire
- 12:30 Enhancing Type 2 Diabetes Diagnosis with Machine Learning
Antonio Agliata, Deborah Giordano, Francesco Bardozzo, Salvatore Bottiglieri, Angelo Facchiano, Roberto Tagliaferri
- 12:45 Using Multilayer Networks for modelling and analysis of biological data
Ilaria Lazzaro, Marianna Milano, Mario Cannataro
- 13:00 Comparative transcriptomics between *P. oceanica* and *C. nodosa* seagrasses: an integrated approach
Alessia Riccardi, Emanuela Dattolo, Marco Miralto, Gabriele Procaccini, Maria Luisa Chiusano, Luca Ambrosino

13:15 Lunch Break

14:20 Session: **Molecular interaction**
Chair: Anna Marabotti, University of Salerno, Italy

14:30 Invited lecture

Andrea Mozzarelli – University of Parma and CNR
HINT, a code for understanding the interaction between biomolecules: a tribute to Donald J. Abraham

Selected oral presentations

- 15:15 Occurrences of Posttranscriptional Modifications in RNA Experimental 3D Structures and Effect on Base Pairing
Mohit Chawla, Utkarsh Kalra, Luigi Cavallo and Romina Oliva
- 15:30 Use of a computational strategy to identify two possible pharmacological chaperones for the GALT enzyme p.Gln188Arg
Bernardina Scafuri, Anna Verdino, Anna Marabotti
- 15:45 Methodology for an efficient in silico identification of peptides from macromolecular complex analysis
Michela Buonocore, Manuela Grimaldi, Angelo Santoro, Anna Maria D'Ursi
- 16:00 Occurrence and Stabilizing Impact of Non-Covalent Interactions in RNA Structures
Mohit Chawla, Luigi Cavallo and Romina Oliva

16:15 Coffee Break – Poster session

Session: **Molecular simulations and drugs**
Chair: Romina Oliva, University "Parthenope", Naples, Italy

Selected oral presentations

- 16:45 Peptide Dynamics in Mixed Solvents: A Molecular Dynamics Simulation Study in TFE/H₂O Environments
Simone Guerriero, Eugenio Notomista, Bruno Hay Mele
- 17:00 A Synergistic Approach to Protein Structure Prediction: AlphaFold 2 and Modeller Integration
Fabio Hernan Gil Zuluaga, Nancy D'Arminio, Francesco Bardozzo, Roberto Tagliaferri, Anna Marabotti

17:15 Identification of therapeutic targets in osteoarthritis by combining heterogeneous transcriptional datasets, drug-induced expression profiles, and known drug-target interactions

Maria Claudia Costa, Claudia Angelini, Monica Franzese, Concetta Iside, Marco Salvatore, Luigi Laezza, Francesco Napolitano and Michele Ceccarelli

17:30 Could serum metabolite concentration predict connectomes' brain parameters?
Carmen Marino, Enza Napolitano, Manuela Grimaldi, Arianna Polverino, Pierpaolo Sorrentino, Giuseppe Sorrentino and Anna Maria D'Ursi

17:45 Invited lecture

Anna Vangone – Roche, Germany

When a protein becomes a drug: computational approaches in drug development

18:30 End of the first day

20:30 *Social dinner – for reserved participants*

December 6

Villa Doria d'Angri – Naples

Session: **Open Science principles: directions and doubts for future researchers**

9:00 Chair: Alice Chiodi, CNR-ITB, Segrate (MI), Italy and *young Bioinformatics Italian Society (BITS)* representative

9:10 Invited Lecture

Francesca Di Donato – CNR, Pisa

What we talk about when we talk about research quality. A discussion on open science and responsible research assessment

9:40 *Discussion with representatives of the Bioinformatics Italian Society (BITS) ISCB's RSG-Italy and Young CINI InfoLife*

10:00 Session: **Omics sciences and systems biology**

Chair: Alice Chiodi, CNR-ITB, Segrate (MI)

Selected oral presentations

10:00 Scalable Deep Learning: applications in medicine

Luca Barillaro, Giuseppe Agapito

10:15 A novel network-based integration of multiomics data in understanding TANGO2-deficiency disorder

Heather Bondi, Veronica Remori, Manuel Airoidi, Silvia Carestiato, Alfredo Brusco, Mauro Fasano

10:30 Metabolomic analysis of Greek traditional varieties of tomato (*Solanum lycopersicum*)

Georgia Tooulakou, Maria I.Klapa

10:45 Exploring hubs of gene dysregulation in rewired gene network in Alzheimer's Disease across brain regions

Sanqa Mitra, Carlos Viesi, Marcus Seldin, Manikandan Narayanan

11:00 Coffee Break – Poster session

11:30 Session: **Artificial Intelligence in biomedicine**
Chair: Angelo Ciaramella, University "Parthenope", Naples, Italy

11:30 Invited Lecture

Pietro Liò – University of Cambridge

AI, computational biology e biomedicine

Selected oral presentations

12:15 Artificial Intelligence in Medicine: Opportunities and Challenges
Mario Cannataro

12:30 Community analysis of Interactomics: a tool to identify cellular illness and design therapy
Diego Liberati

12:45 Vision Transformers for acute lymphoblastic leukemia identification by peripheral blood smear images
Salvatore Calderaro, Giosuè Lo Bosco, Riccardo Rizzo, Filippo Vella

13:00 Deep Neural Network to classify papillary thyroid cancer subtypes from methylation assay
Andrea Colacino, Ornella Affinito, Carlo Cavaliere, Michele Ceccarelli, Monica Franzese

13:15 Lunch Break – Poster session

14:20 Session: **Health and Diseases** - Introduction to the session
Chair: Angelo Facchiano, CNR-ISA, Avellino, Italy (BCC Chair)

14:30 Invited lecture

Ozlem Tastan Bishop - Rhodes University

Drug resistance from a protein structure perspective

Selected oral presentations

15:15 Exploring microbiome insights: MADAME's user-friendly (meta)data retrieval
Sara Fumagalli, Giulia Soletta, Giulia Agostinetto, Manuel Striani, Massimo Labra, Maurizio Casiraghi, Antonia Bruno

15:30 A Reinforcement Learning Algorithm for Multiple Sequence Alignment
G. Grani, U. Ferraro Petrillo, L. Di Rocco

15:45 Machine Learning Approaches for Antibiotic Resistance Prediction in Inpatient and Outpatient Settings
Marco Benedetto, Antonio Facchiano, Giuseppe Piccinni, Cristina De Leo, Luciano Sobrino, Annarita Panebianco, Francesco Facchiano, Angelo Facchiano, Stefano Tagliaferri, Michele La Rocca, Roberto Tagliaferri

16:00 Evaluating Alpha-galactosidase Interface Variants in Fabry Disease: Insights from Sequence and Structure-Based Protein Variant Effect Predictors
Bruno Hay Mele, Maria Monticelli, Federica Rossetti, Giuseppina Andreotti, Maria Vittoria Cubellis

16:15 Coffee Break – Poster session

Selected oral presentations

16:45 Data Fusion for Melanoma Classification
Francesco Reggiani, Max Pfeiffer, Ulrich Pfeiffer, Adriana Amaro

- 17:00 MiDNE: Multi-omics genes and Drugs Network Embedding for cancer-specific drug discovery
Aurora Brandi, Michele Ceccarelli, Barbara Majello, Giovanni Scala
- 17:15 Fuzzy Probability Trees: a novel Interpretable AI model
Giulia Capitoli, Emma L. Ambags, Vincenzo L'Imperio, Michele Provenzano, Marco S. Nobile, Pietro Liò
- 17:30 Feature Selection and Network driven analyses to unveil common RNA signatures in Colon and Pancreatic KRAS mutant cancers
Katia Pane, Mario Zanfardino, Anna Maria Grimaldi, Ilaria Leone, Silvia Nuzzo, Marco Salvatore, Monica Franzese
- 17:45 GenomeCruzer, a 3D interactive environment for genomic data visualisation and analysis
Claudio Isella, Jamal Elhasnaoui, Riccardo Corsi, Elena Grassi, Dalibor Stuchlík, Livio Trusolino, Aleš Křenek, Luca Vezzadini, Andrea Bertotti, Enzo Medico
- 18:00 **Communications and Closure of the Conference Sessions**
- 18:10 *Social activity: free visit to the "Naval Museum" of the Parthenope University*
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December 7

Villa Doria d'Angri – Naples

9:00 ***Parallel Tutorial activities, reservation required***

Tutorial 1: R frameworks for single cell data analysis

Tutorial 2: Demystifying New-generation Protein Structure Prediction: A Hands-On Tutorial with AlphaFold and Alphamissense

10.45 *Coffee break*

11:00 *Tutorial continuation*

13:00 *Light lunch*

14:00 *End of Tutorial activities*