

BBCC2024

Bioinformatics and Computational Biology Conference

November 27-29, 2024

Aula Magna Facolta di Biotecnologie

Università di Napoli Federico II

Via Tommaso de Amicis 95

Naples, Italy

and

pre-conference training activities

November 27-29, 2024

Area di Ricerca del CNR, via Castellino 111

Naples, Italy

PROGRAM

BBCC2024 Conference Chairs

Dr. Angelo Facchiano – National Research Council, Institute of Food Sciences, Avellino, Italy (Chair and Coordination of the BBCC Conference Series)

Prof. Mario Guarracino – University of Cassino and Southern Lazio, Cassino, Italy.

Dr. Iaria Granata – National Research Council, Institute for High-Performance Computing and Networking, Naples, Italy

Dr. Lucia Maddalena – National Research Council, Institute for High-Performance Computing and Networking, Naples, Italy

Prof. Anna Marabotti – University of Salerno, Italy

Scientific Committee

Dr. Claudia Angelini – National Research Council, Institute for Applied Mathematics “M. Picone”, Italy

Dr. Lorraine Ayad – Brunel University London, UK

Prof. Pantelis Bagos – University of Thessaly, Greece

Prof. Maria Luisa Chiusano – University of Naples “Federico II”, Naples, Italy

Prof. Angelo Ciaramella – University of Naples “Parthenope”, Italy

Dr. Nunzio D’Agostino – University of Naples “Federico II”, Italy

Prof. Paola Festa – University of Naples “Federico II”, Italy

Prof. Vittorio Fortino – Institute of Biomedicine, School of Medicine, Faculty of Health Sciences, University of Eastern Finland, Kuopio, Finland

Prof. Christoph Friedrich – University of Applied Science and Arts Dortmund, Germany

Prof. David Gilbert – Professor (Emeritus) Computational Biology Group, Department of Computer Science, Brunel University London, UK

Dr. Giulia Guarguaglini – National Research Council, Institute of Molecular Biology and Pathology (IBPM), Rome, Italy

Dr. Bruno Hay Mele – University of Naples “Federico II”, Naples, Italy

Prof. Dominik Heider – Director of the Institute for Medical Informatics, University of Münster, Germany

Prof. Maria Klapa – Institute of Chemical Engineering Sciences, Foundation for Research & Technology – Hellas (FORTH/ICE-HT)

Dr. Margherita Mutarelli – National Research Council, Institute of Applied Sciences and Intelligent Systems, Pozzuoli (NA), Italy

Prof. Romina Oliva, University of Naples “Parthenope”, Italy

Dr. Vera Pancaldi, INSERM, Centre de Recherches en Cancérologie de Toulouse, France

Prof. Alessandro Pandini – Brunel University London, UK

Prof. Ahmed Rebai, Centre of Biotechnology of Sfax, University of Sfax, Tunisia

Dr. Mara Sangiovanni – University of Naples “Federico II”, Naples, Italy

Prof. Antonino Staiano – University of Naples “Parthenope”, Italy

Prof. Roberto Tagliaferri – University of Salerno, Italy

Prof. Ozlem Tastan Bishop – Rhodes University, South Africa

Dr. Rosa Maria Vitale – National Research Council, Institute of Biomolecular Chemistry, Pozzuoli (NA), Italy

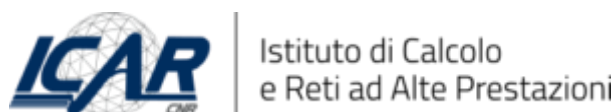
BBCC2024 edition is organized thanks to the following Partners and Sponsors:



Institute of Food Sciences of the National Research Council of Italy (ISA-CNR)



Dipartimento di Chimica e Biologia "A. Zambelli", University of Salerno, Italy



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BBCC2024 is as an Affiliated Conference of ISCB since 2017



Bioinformatics Italian Society patronizes BBCC conferences since 2006



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BBCC2024 Main Conference Program

November 27

9:30 Opening the Registration Desk

10:30 Conference Opening – Welcome and Introduction

Session: Structural Bioinformatics

10:50 Invited lecture

Marta Szachniuk

Frontiers in computational prediction of RNA structure

Francesca Ferrero

11:40 *Relevance of DNA tridimensional shape in RNA:DNA:DNA triple helix formation*

Carmen Biancaniello

Probing Structural Dynamics of Human Prion Protein and T183A Variant through NMR-Restrained MD

12:00 *Simulations*

Nancy D'Arminio

12:20 *MDaRes: a R-driven tool for MD Data through structural alphabet approaches*

Karol Wróblewski

12:40 *Exploring Protein Flexibility and Peptide Structure Prediction with CABS-flex*

13:00 Break – Lunch buffet

Serena Rosignoli

14:40 *Developing Tools for Structural Bioinformatics: from Python to Bedside*

Maria Milanesi

15:00 *Design and Validation of Broad-Spectrum Antiviral Compounds Against SARS-CoV-2*

Simone Pirone

Exploring Phosphomannomutase Evolution Through Structural and Sequence-Based Phylogenetics:

15:20 *Implications for Brain Hypoxia Response*

Sebastian Kmiecik

15:40 *Advancing Protein-Peptide Docking: New Applications of ESMFold and CABS-dock Methods*

16:00 Coffee Break and Poster session

Session: Databases of biological information

16:30 Invited lecture

Marco Beccuti

IT Infrastructure and Computational Services in the PNRR IR SUS-MIRRI.IT Project to support the Italian Microbial Research

Elisa Mauriello

17:20 *Collating marine metagenomics resources*

Ivan Fruggiero

17:40 *An interactive genetic fingerprinting database for chestnut genotyping*

18:00 *Closing remarks of first day*

November 28

9:00 **Session: Omics and disease**

Bruno Giovanni Galuzzi

9:00 *Identification of miRNA Biomarkers for Inflammatory Bowel Disease Using Machine Learning*

Carmen Marino

9:20 *Metabolomic approach to investigating Nusinersen neurometabolic effects*

Francesco Reggiani

9:40 *Data Fusion applications for cancer genomics data analysis*

Mattia Fanelli

9:50 *Combined MERFISH and bulk-RNA seq analysis on PDAC Spheroids infected with oncolytic virus SG33*

Francesco Massaini

Spatial Profiling of the Tumor Microenvironment: A comparison of tools for the extraction of features

10:00 *predictive of therapy response*

10:10 Invited lecture

Enrico Glaab

Comprehensive blood metabolomics profiling analysis of Parkinson's disease

11:00 **Coffee Break and Poster session**

Session: Bioinformatics development and applications

Vincenzo Bonnici

11:30 *PanDelos-plus: A parallel algorithm for computing genetic sequence homology in pangenomic analysis*

Gregory Butler

11:50 *Feature Engineering for Protein Sequence Analysis*

Maurizio Giordano

12:10 *Context-specific Essential Genes Identification and Prediction by Learning Multi-Omics and Network Data*

Rodolfo Tolloi

12:30 *NaStrO: an ultra-rapid, open-source computing pipeline for Nanopore data*

Ludovica Celli

12:50 *scVAR: a tool for the integration of genomics and transcriptomics from single cell RNA-sequencing data*

13:10 **Break – Lunch buffet**

Special session: Collaborative Advancements in Bioinformatics: Integrating Infrastructure and

14:20 Industrial Solutions

Francesca De Leo

14:20 *ELIXIR Infrastructure*

Roberta Bosotti

The National Facility for Data Handling and Analysis at Human Technopole: supporting the Italian research community

14:40

Sara Riccardi

15:00 *Empowering discovery: advancing life sciences through accessible genomic innovation*

Paolo Bianco – Marco Fiorletta

15:15 *Empowering Scientific Research: Customized HPC Solutions for Optimal Performance and Efficiency*

Michelangelo Sofo – Giuseppe Labianca

15:30 *DietAdhoc - A decision support system for nutrition specialists*

Laura Casalino

OASI Biobank: Advancing Asplenia Research through Integrated Bioinformatics and Collaborative

15:45 *Infrastructure*

16:00 **Coffee Break and Poster session**

16:30 *Session: Novel and challenging methodologies and big data analysis*

16:30 **Invited lecture**

Jack Tuszyński

Investigations of metabolic changes in cancer cells resulting from pharmacological agents and low-intensity electromagnetic fields

Leili Shahriyari

Personalized Cancer Care through Digital Twin Technology: Integrating Patient-Specific Data with

17:20 *Quantitative Systems Pharmacology*

Carmine Fruggiero

17:40 *inDAGO: a user-friendly graphical interface for dual RNA-seq data analysis*

18:00 *Closing remarks of second day*

20:00 *Social dinner (upon reservation)*

November 29

9:00 *Session: Novel and challenging methodologies and big data analysis (continued)*

Antonella Prisco

9:00 *Modeling Variations in Antibody Response Magnitude and Longevity*

Roberta Esposito

Metagenomic analyses identify biosynthetic gene clusters of Mediterranean sponges leading to bioactive products

9:20 *Aleksandra Swiercz*

9:40 *Quality of semi-automated de novo genome assembly*

10:00 *End of session and communications*

Session: Statistics and Artificial Intelligence in Data Analytics

10:10 **Invited lecture**

Audronė Jakaitienė

Predictive Analytics in Medicine and Biology

11:00 *Coffee Break and Posters*

Krzysztof Pysz

11:30 *Deep discriminative models in the detection of amyloid signaling motifs*

Marco Benedetto

11:50 *AI-Driven Antibiotic Resistance Prediction in Hospital and Clinic Settings*

Alessandro Esposito

Classification and biochemical evaluation via Raman and Surface-enhanced Raman scattering spectroscopy of breast cancer cell lines expressing different levels of HER2

12:10 *Francesca Cuturello*

Enhancing predictions of protein stability changes induced by single mutations using MSA-based language models

12:30 *End of session and communications*

13:00 *Break –Lunch buffet*

- 14:30 **Session: Systems biology**
Giovanni Scala
- 14:30 *Multi-omics data integration methods for cancer-subtyping, drug discovery and tumor-model alignment*
Debora Dallera
Integrative analysis of heterogeneous high-throughput transcriptomic data for promoter selection in bacterial
- 14:50 *genomes to support microbial synthetic biology*
Silvia Giulia Galfrè
- 15:10 *Machine learning and explainable AI for transcriptomic analysis in Multiple Sclerosis*
Chiara Cimolato
- 15:30 *Mathematical Modeling of Phage-Mediated CRISPRi System for Inhibiting Antibiotic Resistance*
Special session: Funding opportunities for young scientists
- 15:50 **Organized by youngBITS, young-infolife, and ISCB RGS-Italy groups**
Ermanno Rizzi - Italian Cystic Fibrosis Research Foundation (FFC Ricerca)
"Funding initiatives for young researchers: the experience of the Italian Cystic Fibrosis Research Foundation (FFC Ricerca)".
Daniela Guidone - Telethon Institute of Genetics and Medicine (TIGEM) and "Gianni Mastella Research Fellowship 2024"
- 16:00 *Airway surface as a battleground against bacteria*
Michele Genovese - Telethon Institute of Genetics and Medicine (TIGEM) and "Gianni Mastella Starting Grant 2024"
- 16:10 *"Alternative therapeutic target to restore the mucociliary clearance in CF"*
Round table with the session speakers and representatives of the youngBITS, young-infolife, and RGS-Italy
- 16:50 ISCB groups
- 16:50 *Announcements: best oral and poster presentation awards – Future works*
- 17:00 *Closing of the Conference*

Pre-Conference Training Activities

Two training activities are held at:

Consiglio Nazionale delle Ricerche (CNR), Via Pietro Castellino 111, Naples, Italy

Each activity is restricted to a maximum number of 15 participants, selected on the basis of demand.

November 25

One-day training activity

From raw matrices to differential expression/methylation patterns: a functional genomics approach to detect molecular insights

Instructors and Organizers:

Dr. Luca Ambrosino and Dr. Francesco Cecere

Institute of Genetics and Biophysics "Adriano Buzzati-Traverso"

Consiglio Nazionale delle Ricerche, Naples, Italy

November 26

One-day training activity

Software Environments, Containers, and Notebooks (for Bioinformatics and Computational Biology)

Instructor

Dr. Raoul Bonnal, IFOM - Research Computing & Data Science Manager

Helpers

Dr. Riccardo Lorenzo Rossi, Bioinformatics scientist, and Dr. Cristiano Petrini, Bioinformatics engineer - IFOM-ETS, Research Computing & Data Science

Organisers

Prof. Anna Marabotti, University of Salerno, ELIXIR-IT, Italy

Prof. Allegra Via, University of Rome "La Sapienza", ELIXIR-IT, Italy

Dr. Angelo Facchiano, CNR-ISA, Avellino, Italy

Dr. Ilaria Granata, CNR-ICAR, Naples, Italy

Dr. Lucia Maddalena, CNR-ICAR, Naples, Italy

This training is organized by the ELIXIR-IT Training Platform