BBCC2018
Bioinformatics and Computational Biology Conference

November 19-21, 2018
Centro Congressi Università di Napoli “Federico II”
Via Partenope 36, 80121 Naples, Italy

Program

Monday 19

13.30-14:30 Registration

14:30-15:00 Conference Opening

Session: Large data sets

15:00-15:30 Special Lecture
Giuseppe Longo
University of Naples "Federico II"
Cross-disciplinary applications of machine learning

15:30-16:15 Invited Lecture
Enrico Capobianco
Center for Computational Science, University of Miami, Florida, USA
Rerouting biomarkers & targets in cancer research through networks

16:15-16:45 Coffee break

16:45-17:00 Giulio Spinozzi, Valentina Tini, Laura Mincarelli, Brunangelo Falini and Maria Paola Martelli
A comprehensive RNA-Seq pipeline includes meta-analysis, interactivity and automatic reporting

17:00-17:15 Dario Righelli, Claudia Angelini and Davide Risso
Differential Enriched Scan 2 (DEScan2): a fast pipeline for broad peak analysis

17:15-17:30 Tiziana Castrignanò, Tiziano Flati, Silvia Gioiosa, Nicola Spallanzani and Giovanni Chillemi
Managing big data bioinformatics on shared high-performance computing platforms

17:30-17:45 Povilas Gibas, Mantas Sarauskas, Juozas Gordevicius, Edita Kriukiene and Saulius Klimasauskas
Estimation of DNA modification using artificial neural networks, TOP-seq data and genomic context information

17:45-18:00 Alessio Mancini, Leonardo Vito, Elisa Marcelli, Renato De Leone, Sandra Pucciarelli and Emanuela Merelli
DSaaS: Data Science as a Service - a user-friendly machine learning platform

Tuesday 20

8:45-9:00	Registration

Session: Health and Disease

9:00-9:15	Antonio Federico, Giovanni Scala, Veer Singh Marwah, Angela Serra, Valerio Costa, Alfredo Ciccodicola, Vittorio Fortino and Dario Greco *The integration of molecular networks uncovers mechanisms of drug sensitivity in cancer therapy*
9:15-9:30	Ichcha Manipur, Ilaria Granata, Lucia Maddalena, Kumar Parijat Tripathi and Mario Rosario Guarracino *Clustering analysis of tumor metabolic networks*
9:30-9:45	Maria Monticelli, Marcello Viscovo, Guglielmo Riccio, Marco Cammisa, Giuseppina Andreotti, Bruno Hay-Mele and Maria Vittoria Cubellis *Passenger mutations as a target for the personalized therapy of cancer*
9:45-10:00	Anastasia Lavrova, Eugene Postnikov, Dilyara Esmedlyaeva and Vitaly Belik *Mathematical and computational modeling of host-pathogen interaction in the lung lesion development due to Mycobacterium tuberculosis in humans*
10:00-10:10	Angelo Ciaramella, Davide Nardone and Antonino Staiano *Fuzzy similarity-based multi-view hierarchical clustering*
10:10-10:20	Esther Imperlini, Annalisa Mandola, Annamaria Mancini, Andreina Alfieri, Daniela Vitucci, Marianna Caterino, Morten Bredsgaard Randers, Jakob Friis Schmidt, Marie Hagman, Thomas Rostgaard, Peter Krustrup, Margherita Ruoppolo, Pasqualina Buono and Stefania Orrù *Molecular signatures of healthy longevity related to football training: an integrative-omics approach*
10:20-10:30	Michele Costanzo, Marianna Caterino, Armando Cevenini, Vincent Jung, Chiara Guerrera and Margherita Ruoppolo *Integration of proteomics and metabolomics data in a novel cellular knock out model of methylmalonic acidemia*

10:30-11:00	Coffee break

Session: Structural Bioinformatics

11:00-11:45	Invited Lecture **Christine Orengo** **University College of London, UK** ***CATH Functional families (FunFams) - insights into impacts of genetic variations***
11:45-12:00	Sebastian Daberdaku *Identification of protein pockets and cavities by Euclidean Distance Transform*
12:00-12:15	Luciana Esposito, Nicole Balasco, Amarinder Singh Thind, Mario Rosario Guarracino and Luigi Vitagliano *The variability of backbone geometry as a novel and powerful tool for protein structure quality evaluation*
12:15-12:30	Serena Dotolo, Sarath Dantu, Angelo Facchiano and Alessandro Pandini *Dynamics and coevolution of Sirtuin2*
12:30-12:45	Deborah Giordano, Angelo Facchiano *Microbial transglutaminases: a deep analysis of PFAM sequences*

12:45-13.15 *SPOT COMMUNICATIONS*

- Carmine Nunziata, Andrea Polo, Alfredo Budillon and Susan Costantini
  Conformational analysis of SEPHS2, a selenoprotein involved in cancer
- Ahmed Roumia, Margarita C. Theodoropoulou, Konstantinos Tsirigos and Pantelis Bagos
  Computational studies on eukaryotic transmembrane β-barrel proteins
- Carolina Napoli and Anna Marabotti
  How to improve the modelling of proteins mutations? A preliminary assessment
- Bernardina Scafuri, Angelo Facchiano and Anna Marabotti
  Prediction of the stability of proteins by computational approaches: a case report
- Nicole Balasco, Giovanni Smaldone, Alessia Ruggiero and Luigi Vitagliano
  Ability of current force fields used in Molecular Dynamics to reproduce conformational preferences of residues falling in disallowed regions of the Ramachandran Plot

13:15-14:15 Lunch

Session: Systems and Synthetic Biology

14:15-15:00 Invited Lecture
David Gilbert
Brunel University London, UK
An engineering approach to whole genome bacterial metabolic design: principles, practice and challenges for Computational Synthetic Biology

15:00-15:15 Pasquale Palumbo, Marco Vanoni, Federico Papa, Stefano Busti and Lilia Alberghina
Whole yeast model: What and why

15:15-15:30 Max Conway and Pietro Liò
Understanding metabolic networks using large scale simulation and hierarchical block matrices

15:30-16:00 Coffee break

Session: Genome and Metagenome

16:00-16:15 Chiara Colantuono, Marco Miralto, Mara Sangiovanni, Luca Ambrosino and Maria Luisa Chiusano
GENOMA: a multi-genome platform for marine biology

16:15-16:30 Slobodanka Radovic, Federica Cattonaro and Fabio Marroni
Do you cov me? Effect of coverage reduction on species identification in complex biological matrices by metagenome shotgun high-throughput sequencing

16:30-16:45 Mara Sangiovanni, Roberta Piredda, Marco Miralto, Michael Tangherlini and Maria Luisa Chiusano
Data sharing and interoperability from multi-source long term observations: challenges and opportunities in marine biology

16:45-17:00 Ludovica Liguori, Valentina Citro, Bruno Hay Mele, Giuseppina Andreotti and Maria Vittoria Cubellis
E-learning for marine biotechnology: an example with a metagenomic approach

17:00-17:10 Gabriella Sferra, Marta Ponzi and Elisabetta Pizzi
Molecular interplay between organisms by phylogenetic profiling

17:30 Social tour (registered participants)
20:00 Social dinner (registered participants)

Wednesday 21

8:45-9:00 Registration

Session: Computational solutions for high-throughput data

9:00-9:15 Giles Miclotte, Pieter Audenaert and Jan Fostier
Iterative seeding for sequence to graph alignment

9:15-9:30 Filippo Geraci, Giovanni Manzini, Loredana Marialuisa Genovese, Romina D'Aurizio and Marco Pellegrini
GenTRy: A tool for genotyping polymorphic tandem repeats in high throughput sequencing data.

9:30-9:45 Md Habibur Rahman, Silong Peng, Chen Chen, Pietro Liò and Mohammad Ali Moni
Genetic effect of Type 2 diabetes to the progression of neurological diseases

9:45-10:00 Eugenio Del Prete, Angelo Facchiano and Pietro Liò
Reusing microarray clinical data from a complex disease with bioinformatics tools

10:00-10:15 Monika Krzak, Yordan Raykov, Alexis Boukouvalas, Luisa Cutillo and Claudia Angelini
Clustering scRNAseq data with ensMAP-DP

10.15-10.30 *SPOT COMMUNICATIONS*

- Amit Dubey, Pritish Varadwaj and Vijay Nema
  Interaction of CXCR4 with picroside I and picroside II of medicinal herb Picrorhiza Kurroa Royle ex benth investigated by molecular docking and molecular dynamics simulations
- Nicola Criscuolo and Claudia Angelini
  StructuRly: a novel Shiny app to produce elegant, detailed and interactive plots for STRUCTURE outputs
- Ankit Verma, Carlo Giaccari, Basilia Acurzio, Alessia Polito, Claudia Angelini and Andrea Riccio
  An approach to identify novel proteins interacting with imprinting control regions in allele-specific manner
- Alessandra Varavallo, Anita Capalbo, Rosaria Di Martino, Andrea Rosario Beccari and Alberto Luini
  SecretMaps: Signaling protein maps within the Secretory Pathway

10:30-11:00 Coffee break

11:00-11:45 Invited Lecture
Christian Blum
Artificial Intelligence Research Institute (IIIA), Spanish National Research Council (CSIC), Bellaterra – Catalonia, Spain
Useful Optimization Techniques for String Problems From Computational Biology

11:45-12:00 Nunzio D'Agostino, Pasquale Tripodi, Erik Garrison, Anders Albrechtsen, Jonas Meisner, Angelo Facchiano, Teodoro Cardi and Vincenza Colonna
Deciphering loci under selection associated with fruit size and shape in Capsicum

12:00-12:45 Invited Lecture
Roberta Bosotti
Nerviano Medical Sciences srl, Nerviano (MI), Italy
Genomics and bioinformatics in support to development of personalized medicine in oncology

12:45-13:00 **Announcements and closing remarks**