BBCC2017
December 18-20, 2017
Program

Monday 18

9:30-11:00 Registration

11:00-11:20 Conference Opening

11:20-12:10 Invited Lecture

Amedeo Caflisch
Computational Structural Biology, University of Zurich, Switzerland
Discovery of potent and selective bromodomain inhibitors by high-throughput fragment docking

Session: Molecular simulations

12:10-12:30 **Anna Vangone, Katarina Elez, Alexandre MJJ Bonvin**
Computational Structural Biology group, Bijvoet Center for Biomolecular Research, Faculty of Science – Chemistry, Utrecht University, Utrecht, The Netherlands
A contact and energy-based approach for the classification of biological and crystallographic interfaces

12:30-12:50 **Antonella Paladino, Filippo Marchetti, Luca Ponzoni, Giorgio Colombo**
Istituto di Chimica del Riconoscimento Molecolare, CNR, Milano, Italy
The interplay between structural stability and plasticity determines mutation profiles and chaperone dependence in protein kinases

12:50-13:50 Lunch

Session continuation: Molecular simulations

13:50-14:20 **Monica Zoppè**
Scientific Visualization Unit, IFC - CNR, Pisa, Italy
A different look at molecular biology: the perceptive scale

14:20-14:40 **Mohit Chawla, Luigi Cavallo, Romina Oliva**
Department of Sciences and Technologies, University Parthenope of Naples, Napoli, Italy
Relevance of ribose-nucleobase stacking interactions in functional RNAs

14:40-15:00 **Silvia Rinaldi, Victoria Assimon, Zapporah Young, Giulia Morra, Jason Gestwicki, Giorgio Colombo**
Istituto di Chimica del Riconoscimento Molecolare, CNR, Milano, Italy
Tuning the molecular mechanism of Hsp70 via a new allosteric network

15:00-15:20 **Serena Leone, Piero Andrea Temussi, Delia Picone**
Department of Chemical Sciences, University of Naples Federico II, I-80126, Napoli, Italy
Function enhancements of sweet proteins through molecular design

15:20-15:40 **Samuele Girotto, Matteo Comin, Cinzia Pizzi**
Department of Information Engineering, University of Padova, Italy
Efficient hashing of spaced-seeds with block indexing

15:40-16:20 Poster session with coffee and tea

Session continuation: Molecular simulations

16:20-16:40 **Claudia Caudai, Monica Zoppè, Emanuele Salerno, Maria Antonietta Pascali, Anna Tonazzini**

CNR- ISTI, Pisa, Italy

New approach to Molecular Dynamics using Monte Carlo Methods and Quaternions

16:40-17:00 **Nicole Balasco, Carlo Diaferia, Giancarlo Morelli, Antonella Accardo, Luigi Vitagliano**

Institute of Biostructures and Bioimaging (IBB), CNR, Naples, Italy

The atomic-level structure of novel peptide-based nanomaterials unravelled by Molecular Dynamics

17:00-17:20 **Immacolata Castellano, Alfonsina Milito, Maria Russo, Gian Luigi Russo, Michael Lisurek**

Department of Biology and Evolution of Marine Organisms, Stazione Zoologica Anton Dohrn, Naples, Italy

Probing the Interactions of Marine Thio-histidines with an Attractive Pharmaceutical Target for Cancer Therapy

Tuesday 19

8:45-9:00 Registration

Session: Applications in Genomics

9:00-9:20 **Erik Garrison, Jouni Sirén, Adam M. Novak, Glenn Hickey, Jordan M. Eizenga, Eric T. Dawson, Will Jones, Michael F. Lin, Benedict Paten, Richard Durbin**

Wellcome Trust Sanger Institute, Wellcome Genome Campus, Hinxton, Cambridge, UK

Enabling practical pan-genomics with the variation graph toolkit

9:20-9:40 **Vincenzo Bonnici, Vincenzo Manca, Rosalba Giugno**

Department of Computer Science, University of Verona, Italy

Dictionary based method for pangenomic discovery among distal genomes

9:40-10:00 **Roberto Sirica, Marianna Buonaiuto, Valeria Petrella, Lucia Sticco, Donatella Tramontano, Dario Antonini, Caterina Missero, Ombretta Guardiola, Yali Xue, Qasim Ayub, Chris Tyler-Smith, Marco Salvemini, Giovanni D'Angelo, Vincenza Colonna**

Institute of Genetics and Biophysics, National Research Council, Naples, Italy

Natural selection at the lipid transporter ABCA12 gene

10:00-10:20 **Luca Ambrosino, Chiara Colantuono, Francesco Monticolo, Maria Luisa Chiusano**

Research Infrastructures for Marine Biological Resources, Stazione Zoologica Anton Dohrn, Napoli, Italy, and Department of Agriculture, University of Naples "Federico II," Portici (Napoli), Italy

Parallel genome annotation versions: the need for data reconciliation in genomics

10:20-10:40 **Nunzio D'Agostino, Francesca Taranto, Salvatore Camposeo, Giacomo Mangini, Valentina Fanelli, Susanna Gadaleta, Monica Marilena Miazzi, Stefano Pavan, Valentina di Rienzo, Wilma Sabetta, Samanta Zelasco, Enzo Perri, Cinzia Montemurro**

CREA Research Centre for Vegetable and Ornamental Crops, Pontecagnano Faiano, Italy

GBS-derived SNP catalogue unveiled genetic diversity of Italian olive cultivars

10:40-11:20 Poster session with coffee and tea

11:20-12:10 **Invited Lecture**

Giuseppe Lancia
Algorithms, Combinatorics & Optimization, University of Udine, Italy
Solving Bioinformatics Problems by Integer Linear Programming: An Ongoing Successful Story

Session: Applications in Medicine

12:10-12:30 **Ashar Ahmad, Holger Fröhlich**
Bonn Aachen International Center for Information Technology, University of Bonn, Germany
Patient Stratification in Cancer using Survival-based Bayesian Clustering

12:30-12:50 **Giulia Babbi, Giuseppe Profiti, Pier Luigi Martelli, Rita Casadio**
Bologna Biocomputing Group, University of Bologna, Italy
From phenotypes to molecular mechanisms and pathways

12.50 *Time for changing posters (remove odd numbers, fix even numbers)*

13:00-14:00 Lunch

14:00-14:50 **Invited Lecture**

Pier Luigi Buttigieg
HGF-MPG Group for Deep Sea Ecology and Technology, Alfred-Wegener-Institut, Helmholtz-Zentrum für Polar- und Meeresforschung, Germany
Multi-omics in the context of global biodiversity monitoring: delivering insight in a multi-stakeholder datascape

Session: Metagenomics

14:50-15:10 **Ron Hübler, Felix M Key, Christina Warinner, Kirsten Bos, Johannes Krause, Alexander Herbig**
Max Planck Institute for Science of Human History, Jena, Germany
AMPS: A pipeline for screening archaeological remains for pathogen DNA

15:10-15:30 **Theodor Sperlea, Stefan Füser, Jens Boenigk, and Dominik Heider**
Department of Mathematics and Computer Science, Marburg, Germany
SEDE-GPS: Socio-Economic Data Enrichment based on GPS information

15:30-16:10 Poster session with coffee and tea

Session: Tools

16:10-16:30 **Rohmatul Fajriyah, Kumar Parijat Tripathi, Dedi Rosadi, Mario Rosario Guarracino**
Institute for High Performance Computing and Networking, National Research Council, Naples, Italy

tscv package: a novel approach to carry out cross-variance statistical tests on micro-array datasets

16:30-16:50 **Pierrick Roger, Alexis Delabrière, Étienne A. Thévenot**
CEA, LIST, Laboratory for data analysis and systems' intelligence,
MetaboHUB4, France
The biodb R package: a unified framework to access biological and chemical databases

16:50-17:10 **Kumar Parijat Tripathi, Amarinder Singh Thind, Seetharaman Parashuraman, Mario Rosario Guarracino**
Institute for High-performance Computing and Networking, CNR, Via Pietro Castellino 111, Naples, Italy

RankerGUI: a web application for comparing expression profiles using a rank based statistical approach

17.30 Guided Tour - Social Dinner

Wednesday 20

8:45-9:00 Registration

09.00 **Session: Omics and Multi-Omics**

9:00-9:20 **Luca Ambrosino, Chiara Colantuono, Marco Miralto, Mara Sangiovanni, Maria Luisa Chiusano**
Research Infrastructures for Marine Biological Resources, Stazione Zoologica Anton Dohrn, Napoli, Italy, and Department of Agriculture, University of Naples "Federico II," Portici (Napoli), Italy

A multilevel comparative genomics approach to check for inter and intra species relationships and gene predictions quality

9:20-9:40 **Chiara Lauritano, Adrianna Ianora**
Integrative Marine Ecology Laboratory, Stazione Zoologica Anton Dohrn, Villa Comunale, 80121, Napoli, Italy
Gene-mining and –omics approaches to study enzymes with biotechnological potential from marine microalgae

9:40-10:00 **Alexis Boukouvalas, Luisa Cutillo, Elli Marinopoulou, Nancy Papalopulu and Magnus Rattray**

University of Manchester, Manchester, UK
OscoNet: Detecting oscillatory gene networks using an FDR calibrated non-parametric test

10:00-10:20 **Shib Sankar Bhowmick, Indrajit Saha, Debotosh Bhattacharjee, Filippo Geraci**
Institute for Informatics and telematics, National Research Council, Pisa, Italy
On using classification to compile cancer-specific panels of miRNA biomarkers

10:20-10:40 **Kevin Litchfield, Samra Turajlic, Hang Xu, Andrew Rowan, Tim Chambers, Stuart Horswell and Charles Swanton**
Translational Cancer Therapeutics Laboratory, The Francis Crick Institute, London, UK
Renal TRACERx: Deterministic evolutionary trajectories govern primary tumour growth

10:40-11:20 Poster session with coffee and tea

11:20-12:10 **Invited Lecture**

Pietro Liò
Department of Computer Science, University of Cambridge, UK
Multi omic analysis of signalling factors in inflammatory comorbidities

Session continuation: Omics and Multi-Omics
12:10-12:30 **Paolo Martini, Gabriele Sales, Monica Chiogna, Calura Enrica, Chiara Romualdi**
Department of Biology, University of Padova, Italy

	A new method for defining survival modules using multi omics data aggregation and pathways
12:30-12:50	**Antonella Iuliano, Claudia Angelini, Italia De Feis, Pietro Liò** *Istituto per le Applicazioni del Calcolo "Mauro Picone", CNR, Italy* **Integration of multi-omics data for cancer survival prediction**
12:50-13:10	**Luisa Cutillo, Mirko Signorelli** *University Parthenope of Naples, Napoli, Italy* **Community structure validation in networks**
13:10-14:10	Lunch
14:10-16:10	**Special Session** **Computational methods to analyze biological big data** *Session proposed by National Research Council, Institute for Systems Analysis and Computer Science, Rome, Italy*
14:10-14:55	**Emanuel Weitschek** **Computational methods to analyze biological big data**
14:55-15:40	**Paola Paci** **SWIM: a computational tool to unveiling crucial nodes in complex biological networks**
15:40-15:55	**Giulia Fiscon** **How does SWIM work and how to use it - Getting started and SWIM basics**
15:55-16:10	**Federica Conte** **How does SWIM work and how to use it - Usage example**
16:10-16:30	Final communications and Conference Conclusions