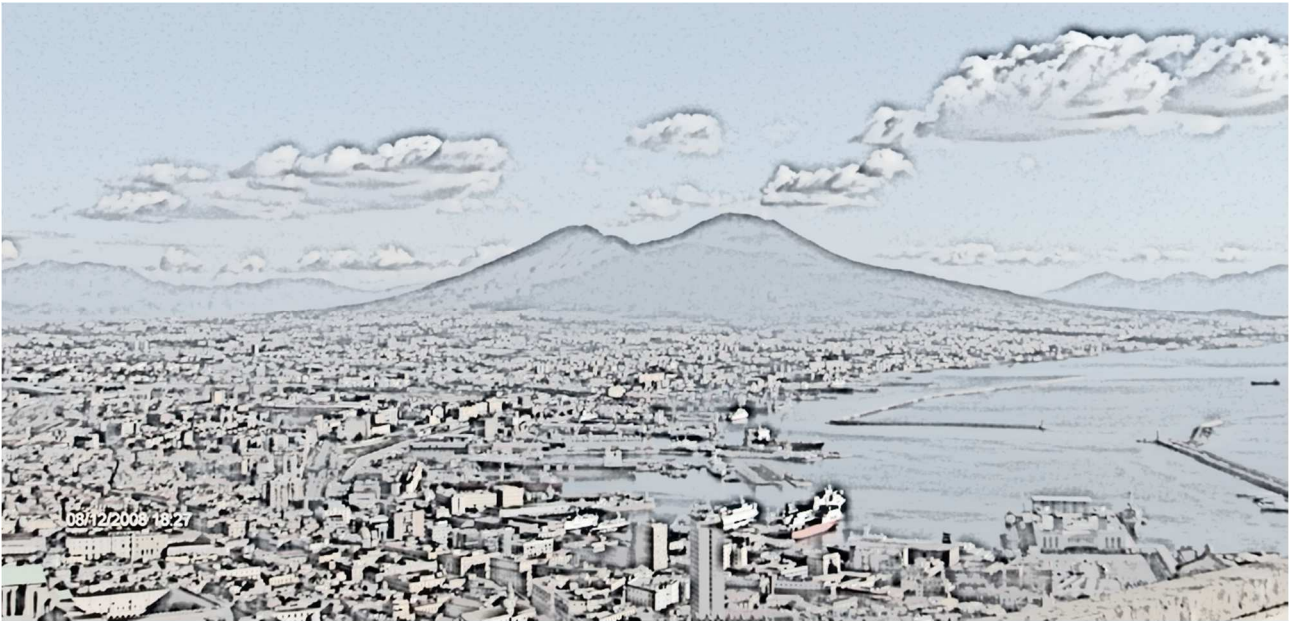


# ***BBC2017***

***International Conference on Bioinformatics and  
Computational Biology  
12<sup>th</sup> edition***



**Naples, Italy**  
**December 18-20th, 2017**

Conference Hall of CNR,  
National Research Council,  
Research Area Napoli 1

**PROGRAM**

**BBC2017**  
**December 18-20, 2017**  
**Program**

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**Monday 18**

9:30-11:00 Registration

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11:00-11:20 Conference Opening

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**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**

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**Session: Molecular simulations - Chair: Anna Marabotti**

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**

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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**

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12:50-13:50 Lunch

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**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**

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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**

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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**

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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**

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

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

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**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**

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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**

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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**

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## Tuesday 19

8:45-9:00 Registration

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**Session: Applications in Genomics – Chair: Claudia Angelini**

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**

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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**

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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**

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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**

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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**

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

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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 – Chair: Paola Festa**

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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**

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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**

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12:50 *Time for changing posters on the boards (see info at desk and poster room)*

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13:00-14:00 Lunch

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- 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 – Chair: Maria Luisa Chiusano**
- 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 Füsler, Jens Boenigk, and Dominik Heider**  
*Department of Mathematics and Computer Science, Marburg, Germany*  
**SEDE-GPS: Socio-Economic Data Enrichment based on GPS information**
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- 15:30-16:10 Poster session with coffee and tea
- 
- Session: Tools - Chair: Maria Luisa Chiusano and Paola Festa**
- 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
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## Wednesday 20

8:45-9:00 Registration

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09:00 **Session: Omics and Multi-Omics – Chair: Mario Rosario Guarracino**

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**

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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**

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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**

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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**

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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**

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

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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**

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**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 – Invited session**
- Computational methods to analyze biological big data**  
*Session proposed by National Research Council, Institute for Systems Analysis and Computer Science, Rome, Italy*
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- 14:10-14:55 *Invited lecture*  
**Emanuel Weitschek**  
**Computational methods to analyze biological big data**
- 
- 14:55-15:40 *Invited lecture*  
**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
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