## **BBCC2021**

## Bioinformatics and Computational Biology Conference

December 1-3, 2021

Virtual Conference Program (Central Europe Time)

Day 1 <sup>st</sup> - December 1 <sup>st</sup>		
15:00-15:10	Time for Connection to the Virtual Conference Room and Registration	
15:10-15:30	Conference Opening	
	Angelo Facchiano and Margherita Mutarelli – Chairs of BBCC2021	
15:30-16:15	Invited Lecture	
	Vera Pancaldi	
	INSERM, Centre de Recherches en Cancérologie de Toulouse, France	
	Network approaches to explore the epigenomic bases of heterogeneity and plasticity in immune cells	
	Session – Transcriptomics	
	Chair: Mario Rosario Guarracino	
16:15-16:30	<u>Douglas Meyer</u> , Jacob Kames, Haim Bar, Anton Komar, Aikaterini Alexaki, Juan Ibla, Ryan Hunt, Luis Santana-Quintero, Anton Golikov, Michael DiCuccio and Chava Kimchi-Sarfaty	
	Changes in synonymous codon preferences in tumorigenesis are tumor-type specific and predictive of patient survival	
16:30-16:45	Chiara Lauritano	
	Transcriptomic approach to study marine microalgae as source of bioactive secondary metabolites	
16:45-17:00	Mattia Furlan, Stefano de Pretis and Mattia Pelizzola	
	Inference of transcriptional and post-transcriptional dynamics from sequencing experiments	
17:00-17:45	Invited lecture	
	Alice Eunjung Lee	
	Division of Genetics and Genomics at Boston Children's Hospital and Harvard Medical School, Boston, MA, USA	
	Transposon genomics: progress and challenges	
17:45-18:00	Poster Session Group A	

Day 2 <sup>nd</sup> – December 2 <sup>nd</sup>		
	Session – Metagenomics and microbiome	
	Chair: Claudia Angelini	
9:30-9:45	Marco Cappellato, <u>Francesca Longhin</u> , Claudia Del Vecchio, Giuseppina Brancaccio, Massimo Bellato, Anna Maria Cattelan, Paola Brun, Claudio Salaris, Ignazio Castagliuolo and Barbara Di Camillo  Uncover a microbiota signature of upper respiratory tract in patients with SARS-CoV-2+	
9:45-10:00	Yunxiao Ren and Dominik Heider	
7.15 10.00	Prediction of antimicrobial resistance based on whole-genome sequencing and machine learning	
10:00-10:15	Marco Cappellato, Giacomo Baruzzo and Barbara Di Camillo	
	Comprehensive assessment of microbiome differential abundance tools	
	Session – Computational methods, omics and multiomics	
	Chair: Annamaria Carissimo	
10:15-10:30	Pietro Hiram Guzzi, Giuseppe Tradigo and Pierangelo Veltri	
	A Novel Local Alignment Algorithm based on Network Embedding	
10:30-10:45	<u>Valeria Policastro</u> , Dario Righelli, Annamaria Carissimo, Luisa Cutillo and Italia De Feis	
	ROBustness In Network (robin) for Single Cell clustering	
10:45-11:00	Giacomo Baruzzo, Giulia Cesaro and Barbara Di Camillo	
	Analyze cellular communication from single cell RNA sequencing data with scSeqComm	
11:00-11:15	Break	
	Session – Computational methods, omics and multiomics continued	
	Chair: Michele Pinelli	
11:15-11:30	Eugenio Del Prete, Ana Margarida Campos, Fabio Della Rocca, Genoveffa Nuzzo and Claudia Angelini	
	A workflow for the analysis of lipidomic data	
11:30-11:45	Giulia De Riso, Daniele Vitale, Piero Pignataro, Simona Blanco, Gerarda Cappuccio, Andrea Chiariello, Lucio Nitsch, Mario Nicodemi, Rita Genesio, Nicola Brunetti-Pierri and Michele Pinelli	
	Systematic analysis of CNV positional effect implicates enhancer mediated SHH dysregulation in a patient with multiple congenital malformations	
11:45-12:00	Giulio Spinozzi, Valentina Tini, Alessio Ferrari, Ilaria Gionfriddo, Francesca Milano, Federica Mezzasoma, Brunangelo Falini and Maria Paola Martelli	
	SiCoDEA: a simple, fast and complete app for analyzing the effect of individual drugs and their combinations	
12:00-12:45	Invited lecture	
	Mario Nicodemi	
	Physics Department, University of Naples "Federico II", Naples, Italy	
	Chromatin 3D architecture: mechanisms and function	
12:45-13:00	Poster Session Group B	
13:00-14:00	Lunch break	

14:00-14:15	Poster Session Group C
	Invited lecture
14:15-15:00	Tiina Salminen
	Abo Akademi University, Turku, Finland
	Siglec-9 - A gold mine of targeted therapies and diagnostics for inflammation and cancer
	Session: Molecular simulations (1)
	Chair: Anna Marabotti
15:00-15:15	<u>Domenico Loreto</u> , Giarita Ferraro and Antonello Merlino
	Protein metalation by Au-, Pt- and Ru-based complexes: a systematic analysis of metal/protein adducts in the Protein Data Bank
15:15-15:30	Tommaso Palomba, Carmine Vacca, Jenny Desantis, Massimo Baroni, Matteo Bartalucci, Gabriele Cruciani and Lydia Siragusa
	From E3 ligase Platform to scaffold-repurposing opportunities: the TRIM24-TRIM33 case study
15:30-15:45	Sohayb Bekkal Brikci, Abdelli Imane, Faiçal Hassani, Amina Belhadji and Mimouna Mostari
	In silico study the control of Citrus nematode Tylenchulus semipenetrans by natural components
15:45-16:00	Break
16:00-16:15	Magnus Kinder and Christof Seiler
	ascc: Conformalized Classifiers for Efficient Cell-Type Predictions
16:30-16:45	Sugunakar Vuree
	Phytochemicals: Remerging Tools as Epigenetic Therapeutics for Cervical Cancer Prevention
16:45-17:00	Alexandr Svidlov, Mikhail Drobotenko, Anna Elkina and Stepan Dzhimak.
	Numerical simulation of DNA dynamics under periodic force effects
17:00-17:45	Invited lecture
	Francesco Iorio
	Wellcome Sanger Institute, Hixton, UK, and Human Technopole, Milan, Italy
	Genome-editing screens and (big) data integration for Cancer Pharmacogenomics
	and therapeutic target discovery
17:45-18:00	Poster Session Group D

Day 3 – December 3rd		
	Session – System Biology and System Medicine	
	Chair: Dominik Heider	
9:30-9:45	Maurizio Giordano, Lucia Maddalena, Mario Manzo and Mario Rosario Guarracino	
	Adversarial attacks on graph embedding: applications in computational biology and bioinformatics	
9:45-10:00	Massimo Bellato, Hsih-Ho Huang, Yili Qian, Pablo Cardenas, Lorenzo Pasotti, Paolo Magni and Domitilla Del Vecchio	
	Engineering of a dCas9 feedback regulator to neutralize competition effects in CRISPRi-based genetic circuits	
10:00-10:45	Invited lecture	
	Richard Röttger	
	University of Southern Denmark (SDU), Odense, Denmark	
	Towards systems medical analysis of complex biomedical data	
10:45-11:00	Break	
	Session: Molecular simulations (2)	
	Chair: Angelo Facchiano	
11:00-11:15	Sandhya Karakkadparambil Sankaran and Achuthsankar S Nair	
	Active phytochemical compounds for inhibiting SARSCOV2 Mprotease: Molecular docking and Molecular dynamics study	
11:15-11:30	Valerio Marino, Alberto Borsatto, Gianfranco Abrusci, Gianluca Lattanzi and Daniele Dell'Orco	
	The structural and allosteric properties of Recoverin are influenced by membrane and its biological target	
11:30-11:45	Stefano Motta, Lara Callea, Laura Bonati and Alessandro Pandini	
	A Neural Network Approach for the Identification of Pathways in Molecular Dynamics Simulations of Ligand Binding	
11:45-12:00	Bernardina Scafuri, <u>Nancy D'Arminio</u> , Sara Alfieri, Mauro Petrillo, Maddalena Querci, Guy Van den Eede, Angelo Facchiano and Anna Marabotti	
	Mutations in the SARS-CoV-2 Spike protein and antibody interactions	
12:00-12:15	Olivier Sheik Amamuddy and Ozlem Tastan Bishop	
	Dynamic Residue Networks to Identify Allosteric Paths in (Homodimeric) Proteins with Mutations and Ligands	
12:15-13.00	Invited lecture	
	Franca Fraternali	
	King's College London, UK	
	Mutations and Variations in Health and Disease: Protein Interaction Networks and 3D Structure Information	
13:00-13:10	Angelo Facchiano and Margherita Mutarelli – Chairs of BBCC2021	
	Meeting announcements and closing remarks	