

## December 10th, 2024

8:45-9:00 Join the workshop

9:00-9:10 Welcome  
Prof. Anna Marabotti

9:10-13:00 ELIXIR-IT training Prof. Luana Licata Biological Network: topological analysis and visualization using Cytoscape software

13:00-14.30 Break

14:30-14:45 Welcome  
Prof. Raffaele Calogero (Presidente BITS)  
Prof. Pier Luigi Martelli (Membro del direttivo SIB)  
Dr. Anna Villa (Direttore ITB-CNR)

Opening Keynote lecture  
Chair: Mirko Treccani

14:45-15:15 Prof. Yinglong Miao Accelerated Molecular Simulations and Drug Discovery

Session 1 Chairs: Simone Pernice, Giacomo Baruzzo, Mirko Treccani

15:15-15:30 Ferrini Alessio *Angiogenesis and vascular patterning: a calibrated mathematical model using the chicken chorioallantoic membrane*

15:30-15:45 Defilippo Annamaria *Understanding Complex Systems through Differential Causal Networks*

15:45-16:00 Pietrafesa Davide *Computational Benchmarking of Aptamers for Selective Inhibition of HuR*

16:00-16:15 Ghafouri Hamidreza *Intrinsically Disorder Ensemble Tools (IDPET), A Python Package for Studying Conformational Ensembles of Disordered Proteins*

16:15-16:45 Break

16:45-17:00 Ansermino Chiara *EPS-urine derived extracellular vesicles: multi-omics profiling for prostate cancer risk stratification*

17:00-17:15 Franchina Davide G. *Integration of mass spectrometry and mass cytometry imaging for spatially resolved single cell profiling*

17:15-17:30 Lapi Francesco *Multi-omics data analysis to characterize age-specific metabolic shifts during embryo development*

December 11th, 2024

9:00-9.15      **Join the workshop**

**Opening Keynote Lecture**

**Chair:** Maria Cristina Aspromonte

9:15-9:45      **Prof. Sandra  
Macedo-Ribeiro**      Pathogen-specific structural features in *C. albicans* Ras1 activation complex

**Session 2**      Chairs: Alfonso Trezza, Giulia Babbi, Lara Console

9:45-10:00      **Lopatriello Giulia**      *Molecular determinants of response to neoadjuvant chemotherapy in esophageal adenocarcinoma at single-cell spatial resolution*

10:00-10:15      **Vono Niccolò**      *Exploring the molecular mechanisms that influence Retinoic Acid responsiveness or resistance in cancer stem cells within patient-derived cancer organoids.*

10:15-10:45      **Break**

10:45-11:00      **Bellia Fabio**      *Exploring synthetic SIL1 protein reintroduction to treat Marinesco-Sjogren Syndrome.*

11:00-11:15      **Sgambati  
Domenico**      *Two new members of Ros/MucR family: MucR2 and MucR3 from *Sinorhizobium meliloti**

11:15-11:30      **Tisi Annamaria**      *Early biochemical alterations of the endocannabinoid system in the retina of Alzheimer's disease mice*

11:30-11:45      **Barone Francesca**      *OCTN1 (SLC22A4) displays two different transport pathways for organic cations or zwitterions*

11:45-12:00      **Sabbioni Giuseppe**      *Shwachman-Diamond Syndrome: different signalling pathways driving chronic inflammation.*

12:00-13:00      **Poster session**

13:00-14.00      **Break**

**Session 3**

Chairs: Giulia Cesaro, Laura Veschetti, Beatrice Casini

14:00-14:15	<b>Manfredi Matteo</b>	<i>Alpha&amp;ESMhFolds: a web server for comparing 42,942 AlphaFold2 and ESMFold models of the human reference proteome</i>
14:15-14:30	<b>Semente Miriam Rainha</b>	<i>Bioinformatic neoantigens prediction from Next generation sequencing data</i>
14:30-14:45	<b>Baldan Matteo</b>	<i>Simulation of bacteria interaction networks: from topology to species abundances</i>
14:45-15:00	<b>Polito Maria Pia</b>	<i>Biochemical characterization of the feedforward loop between CDK1 and FOXM1 in epidermal stem cells</i>

**15:00-15:30 Break**

15:30-15:45	<b>Giallongo Sebastiano</b>	<i>Glutamate enrichment in myelofibrosis tumor microenvironment induces mesenchymal stromal cells senescence by promoting intracellular fumarate accumulation.</i>
15:45-16:00	<b>Tussardi Gaia</b>	<i>Addressing the Biological Interpretation of High-Dimensional Cell-Cell Communication Data from Single Cell Transcriptomics Through an Interactive Web Application</i>
16:00-16:15	<b>Castro Naser Ximena Aixa</b>	<i>Role of Integrins in Maternal-Embryonic Communication: Proteomic Analysis of Early Pregnancy in Alpacas (Vicugna pacos)</i>
16:15-16:30	<b>Zarifa Osmanli</b>	<i>Large-scale analysis of structured tandem repeat proteins across the tree of life</i>

**Special Topic**

Chairs: Pasqualina D'Ursi, Paola Fossa

16:30-17:00	<b>Fabio Gasparini</b>	<i>A Tool is a tool is a tool. The alignment of computational methods and clinical and laboratory practices in biomedical experimental arrangements</i>
-------------	------------------------	---

December 12th, 2024

9:00-9.15      **Join the workshop**

**Opening Keynote Lecture**

**Chair:** Lara Console

9:15-9:45      **Prof. Massimo Aureli**      Neuronal Differentiation and Degeneration: Role of the Plasma Membrane

**Session 4**      Chairs: Giulia Babbi, Beatrice Casini, Maria Cristina Aspromonte

9:45-10:00      **Scarano Naomi**      *Computational Strategies for the design of novel TAAR1 agonists*

10:00-10:15      **Mazza Tiziano**      *3D structure of the ABC transporter MRP2 by Cryo-EM. Insights Post-translational modifications*

10:15-10:45      **Break**

10:45-11:00      **Buoli Comani Valeria**      *Cryo-EM structures of hemoglobin-IsdH complexes: paving the way for novel protein-protein interaction inhibitors as antibiotics*

11:00-11:15      **Stelitano Giovanni**      *Repurposing of approved drugs to fight M. abscessus infections.*

11:15-11:30      **Anteghini Marco**      *Title: X-MAP: Explainable Mutation Analysis Platform for Predicting Genetic Variant Impacts on Protein Structure, Stability, and Human Health*

11:30-11:45      **Buttaro Veronica**      *Identifying disease biomarkers using a novel data analysis pipeline based on multi-view learning*

11:45-12:00      **Vestuto Vincenzo**      *Biochemical Characterization of a New Class of Selective Haspin kinase Inhibitors as potential anticancer drugs*

12:00-12:15      **Conclusions**

12:15-12:30      **Best Oral and Best Poster awards**