YOUNG MINDS AT WORK: BLENDING BIOCHEMISTRY AND BIOINFORMATICS
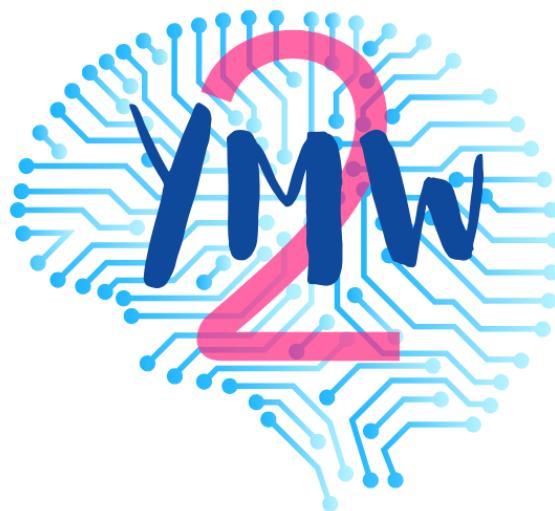
Program on-line workshop

10th**-12**th **December 2024**

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	**Manfredi Matteo**	*Alpha&ESMhFolds: a web server for comparing 42,942 AlphaFold2 and ESMFold models of the human reference proteome*
14:15-14:30	**Semente Miriam Rainha**	*Bioinformatic neoantigens prediction from Next generation sequencing data*

Time	Speaker	Title
14:30-14:45	**Baldan Matteo**	*Simulation of bacteria interaction networks: from topology to species abundances*
14:45-15:00	**Polito Maria Pia**	*Biochemical characterization of the feedforward loop between CDK1 and FOXM1 in epidermal stem cells*
15:00-15:30	**Break**	
15:30-15:45	**Giallongo Sebastiano**	*Glutamate enrichment in myelofibrosis tumor microenvironment induces mesenchymal stromal cells senescence by promoting intracellular fumarate accumulation.*
15:45-16:00	**Tussardi Gaia**	*Addressing the Biological Interpretation of High-Dimensional Cell-Cell Communication Data from Single Cell Transcriptomics Through an Interactive Web Application*
16:00-16:15	**Castro Naser Ximena Aixa**	*Role of Integrins in Maternal-Embryonic Communication: Proteomic Analysis of Early Pregnancy in Alpacas (Vicugna pacos)*
16:15-16:30	**Zarifa Osmanli**	*Large-scale analysis of structured tandem repeat proteins across the tree of life*

Special Topic Chairs: Pasqualina D'Ursi, Paola Fossa

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

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**	*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**