Spring Italian Training for AI in Drug Design

SPRINT-AIDD

Programme

Sunday 25th May

17.00-19.00	Registration	
20.00	**WELCOME BUFFET**	

Monday 26th May

Welcome address of Stefano Alcaro President of the Medicinal Chemistry Division of the Italian Chemical Society		
09.00-09.30	Smarter drugs, faster cures: new solutions for next-gen medicinal chemistry	Orazio Nicolotti *University of Bari*
09.30-10.00	Principal component analysis and clustering	Nicoletta Del Buono *University of Bari*
10.00-10.30	Molecular similarity in medicinal chemistry	Fulvio Ciriaco *University of Bari*
10.30-11.00	**COFFEE BREAK**	
11.00-11.30	Validation techniques	Massimo Baroni *Molecular Discovery*
11.30-12.00	Bioactivity Data Curation: Improving Data Quality for AI-Driven Drug Discovery	Andrea Astolfi *University of Perugia*
12.00-12.30	Optimization and machine learning algorithms	Flavia Esposito *University of Bari*
12.30-13.00	Chemical space networks, ancient tools for novel perspectives	Nicola Amoroso *University of Bari*
13.00-15.00	**SOCIAL LUNCH**	

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15.00-18.00	Training with Prometheus lab: drug discovery and predictive toxicology web platforms
18.00-20.00	**Free swimming pool/oil mill/walking**
20.00	**SOCIAL DINNER**

Tuesday 27th May

09.00-09.30	Intelligence Amplification is much better than Artificial Intelligence	Gabriele Cruciani *University of Perugia*
09.30-10.00	Molecular docking and prioritization studies	Daniela Trisciuzzi *University of Bari*
10.00-10.30	Molecular dynamics simulations in HPLC analyses	Andrea Carotti *University of Perugia*
10.30-11.00	The importance of Water	Simon Cross *Molecular Discovery*
11.00-11.30	**COFFEE BREAK**	
11.30-12.00	Hopping Around 3D Pocketomes To Aid Drug Discovery	Lydia Siragusa *Molecular Discovery*
12.00-12.30	3D-Based Prediction of Biotransformations, Metabolites, and Metabolic Pathways	Tommaso Palomba *Molecular Discovery*
12.30-13.00	MoKa, since pKa matters!	Paolo Benedetti *Molecular Discovery*
13.00-15.00	**SOCIAL LUNCH**	

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15.00-18.00	Training with Molecular Discovery Ltd.: MIF-based software for drug discovery	
18.00-20.00	**Free swimming pool/oil mill/walking**	
20.00	**SOCIAL DINNER**	

Wednesday 28th May

9.00-9.30	Chemical languages in generative chemistry	Fabrizio Mastrolorito *University of Bari*
9.30-10.00	AI-driven de novo design: a Pareto optimization approach	Nicola Gambacorta *University of Bari*
10.00-10.30	**COFFEE BREAK**	
10.30-10.40	Development of QSPR models predicting small molecule environmental fate endpoints to design greener pharmaceuticals	Matteo Bersani *Department of Drug Science and Technology, University of Turin*
10.40-10.50	Data-Driven Discovery of Natural TNKS1 Inhibitors: A Hybrid AI and Structure-Based Approach	Marina Bilotta *Dipartimento di Scienze della Salute, Università "Magna Græcia" di Catanzaro*
10.50-11.00	Mining the Conformational Ensemble of HIV-1 TAR RNA for Small-Molecule Drug Discovery	Stefano Bosio *Department of Pharmacy and Biotechnology – University of Bologna*
11.00-11.10	Towards the development of a molecular docking Meta-program to improve the docking accuracy.	Lidia Giuliani *Department of Drug Chemistry and Technology, Sapienza University of Rome*

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11.10-11.20	Unveiling the Hidden Signatures of Non-Canonical DNA: A Chemometric Journey through G-Quadruplex and i-Motif Structures	Nunzia Iaccarino *Department of Pharmacy, University of Naples Federico II*
11.20-11.30	Integrated computational and synthetic approaches to identify novel viral helicase inhibitors	Alessia Onali *Department of Life and Environmental Sciences, University of Cagliari*
11.30-11.40	Hypericum empetrifolium andH. lydium as Health Promoting Nutraceuticals: Assessing their Role Combining In Vitro In Silico and Chemical Approaches	Eleonora Procino *Department of Pharmacy, University of Chieti-Pescara*
11.40-11.50	Machine Learning-based prediction of protein-ligand binding affinity	Francesca Tanda *Dipartimento di Chimica, Università degli studi di Milano*
11.50-12.00	Closing remarks	Cosimo D. Altomare University of Bari