Spring Italian Training for AI in Drug Design

SPRINT-AIDD

Program

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**	

Spring Italian Training for AI in Drug Design

SPRINT-AIDD

Program

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	Insights 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**	

Spring Italian Training for AI in Drug Design

SPRINT-AIDD

Program

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**	
10.30-11.50	Selected oral presentations	
11.50-12.00	Closing remarks	Cosimo D. Altomare *University of Bari*