SCIENTIFIC PROGRAM

22 September 2021		
9.00-9.20	**Opening ceremony**	
		Chair: Gianluca Sbardella
9.20-10.20	From hits to drugs: an overview of the process	**Tiziano Bandiera** IIT, PharmaChemistry Line, Genova, Italy
10.20-10.30	Virtual coffee break	
		Chair: Federica Pellati
10.30-11.30	Ensuring data integrity and quality in drug discovery	**Barbara Vaccarini** Aptuit (Verona) Srl, an Evotec Company
11.30-12.30	Analytical techniques to support the medicinal chemistry	**Antonio Triolo** Menarini Ricerche S.p.A., Firenze, Italy
12.30-14.30	Lunch break	
	Session: Hit-to-lead: potency and selectivity	*Chair: Ersilia De Lorenzi*
14.30-15.30	NMR-based screening principles and applications in the hit-to-lead phase of drug discovery projects	**Claudio Dalvit** Scientific Consultant, Lavis (TN), Italy
15.30-16.30	The road towards the optimal lead candidate: potency and selectivity profiling by biochemical and biophysical approaches	**Edoardo Fabini** Nerviano Medical Sciences, Nerviano (MI), Italy
16.30-17.30	Design follows function in early drug discovery: in vitro assays for hit-to-lead programs	**Lia Scarabottolo** Axxam S.p.A., Bresso (MI), Italy

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	Session: Pre-ADMET studies	*Chair: Massimo Breda*
9.00-11.00	Approaches for ADMET parameters optimization during the drug discovery phase: advances and caveats	**Giulio M. Dondio** Aphad S.r.l., Buccinasco (MI), Italy
11.00-11.10	Virtual coffee break	
11.10-12.10	Mass spectrometric strategies in drug metabolism and pharmacokinetics (DMPK) studies	**Giancarlo Aldini** Università di Milano, Milan, Italy
12.10-13.10	The benefits of ion mobility mass spectrometry for metabolite identification	**Simona Scarpella** Waters S.p.A., Sesto San Giovanni (MI), Italy
13.10-14.20	Lunch break	
	Session: Bioavailability and toxicology	*Chair: Giancarlo Aldini*
14.20-15.20	In vitro and in vivo drug discovery quantitation of small molecules by LC-MS/MS: a tiered approach	**Rossella Pisano** Accelera S.r.l, Nerviano (MI), Italy
15.20 -16.20	Bioanalysis in drug discovery: challenges and approaches	**Marco Michi** Aptuit (Verona) Srl, an Evotec Company
16.20 - 16.30	Virtual coffee break	
	PhD presentations	*Chair: Francesco Epifano*
16.30-16.50	Development of advanced analytical methodologies for Alzheimer's disease drug discovery	**Lara Davani** University of Bologna, Rimini, Italy
16.50-17.10	Development of new functional ingredients from agro-food wastes	**Lucia Ferron** University of Pavia, Pavia, Italy
17.10-17.30	New strategy for in vitro drug metabolism studies	**Izadora Liranço Furlani** Federal University of São Carlos, São Carlos, Brazil
17.30-18.30	**Ceremony for the 25th anniversary**	

24 September 2021		
	PhD presentations	*Chair: Alberto Massarotti*
9.00-9.20	Optimization of polymer extraction of GPCRs from a low-yielding human cell culture	**Maciej Maj** Medical University of Lublin, Lublin, Poland
9.20-9.40	Detection and identification of biological active compounds using effect directed analysis	**Hanna Nikolaichuk** Maria Curie-Sklodowska University, Lublin, Poland
9.40-10.00	Quantitative lipidomics and proteomics in medicinal chemistry	**Silvia Radrezza** University of Milan, Milan, Italy
		Chair: Roccaldo Sardella
10.00-11.00	Analytical Supporting developability aspects of new chemical entities for early formulation screening	**Emanuela Del Vesco** Aptuit (Verona) Srl, an Evotec Company
11.00-11.10	Virtual coffee break	
	Session: Case studies	*Chair: Roccaldo Sardella*
11.10-12.10	Enabling chemical technologies to automate process optimization and medicinal chemistry	**Antimo Gioiello** University of Perugia, Perugia, Italy
12.10-13.10	“Chromatographic Isotope Effect": Retention time changes for polydeuterated laquinimod in reverse phase HPLC	**Vladimir Ioffe** Scientific expert, Kfar Saba, Israel
13.10-13.30	**Closing remarks**	