







Advanced Technologies Integration into Medicinal

Chemistry Programs

June 30th,2025

Online, from 14:00 to 16:30 CET

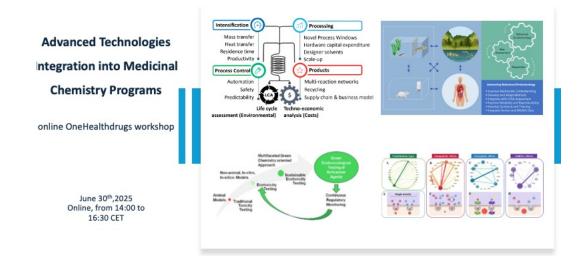
Workshop of the COST Action CA21111 One Health drugs against parasitic vector borne diseases in Europe and beyond OneHealthdrugs

The event is open to PhD, young innovators and senior scientists from both academia and pharma

<u>Description</u>. This workshop aims to showcase how advanced technologies—such as AI-driven drug design, highthroughput screening, and omics integration—can be strategically applied in medicinal chemistry pipelines. Emphasis will be placed on supporting the OneHealth*drugs* mission: coordinating the discovery of drugs that effectively combat vector-borne infections in both human and veterinary medicine, while adhering to optimal efficacy profiles across species. Participants will explore tools that enhance target specificity, accelerate development, and reduce environmental impact, fostering cross-disciplinary collaboration aligned with One Health principles.

The day program is reported below

The event registration requires two steps : 1) create an e-COST account in the <u>www.cost.eu</u> and 2) register here: <u>https://docs.google.com/forms/d/e/1FAIpQLSdcXCkvyQOfHE9xVTNjB3vVHtLs9upI-EMdNH-XGFzS23qVxA/viewform?usp=header</u>.



PROGRAM Workshop duration Discussion will be after each presentation. Each presentation lasts 18 minutes.

hrs 2pm – 4:40pm

Sustainable Medicinal Chemistry

h 2:00 Maria Laura Bolognesi

Medicinal Chemistry Meets One Health: Developing Sustainable Antiparasitic Agents from Agro-Industrial Wast Department of Pharmacy and Biotechnology, University of Bologna Via Belmeloro 6, 40126 Bologna, Italy marialaura.bolognesi@unibo.it

h 2:20 Calogeropoulou Theodora

New antiparasitic agents based on Cashew Nut Shell Liquid, a by-product of the cashew industry National Hellenic Research Foundation, Greece tcalog@eie.gr

h 2:40 GERARD Stéphane

Levulinic Acid as a valuable building block for the development of molecules of therapeutic interest University of Reims Champagne-Ardenne, UFR de Pharmacie, ICMR / UMR CNRS 7312, France. stephane.gerard@univ-reims.fr

Compounds properties predictions in drug discovery

h 3:00 Sheraz Gul

In vitro and in silico methods to annotate compounds in the drug discovery value chain Fraunhofer Institute for Translational Medicine and Pharmacology ITMP, Schnackenburgallee 114, 22525 Hamburg, Germany. sheraz.gul@itmp.fraunhofer.de

h 3:20 Lorenzo Raffellini

In vitro and in silico analysis of nature-based compounds from an ADMET and ecotoxicology perspective

PhD University of Pisa, STSM fellow Fraunhofer Hamburg University of Pisa, Department of Pharmacy, Italy; Fraunhofer Institute for Translational Medicine and Pharmacology ITMP, Hamburg, Germany Iorenzo.raffellini@phd.unipi.it

Drug delivery and One Health

h 3:40 Evgenia Mitsou

Designing Drug Delivery Carriers for Enhanced One Health Outcomes a Institute of Chemical Biology, National Hellenic Research Foundation, 48, Vassileos Constantinou Ave., Athens, 11635 Greece emitsou@eie.gr

h 4:00 José das Neves

Tackling mucus: strategies to overcome an often overlooked barrier to drug delivery. i3S – Institute for Research and Innovation in Health, University of Porto, Portugal j.dasneves@i3s.up.pt

Omics applications to accelerate drug discovery

h 4:20 Lorenzo Tagliazucchi

Leveraging a MS-based multi-omics platform to investigate Leishmaniasis drug resistance and decipher the MoA of the innovative antileishmanial agent H80 Dipartimento di Scienze degli Alimenti e del Farmaco, Università degli Studi di Parma, Parco Area delle Scienze 27/A, 43124-Parma, Italy. Iorenzo.tagliazucchi@unipr.it

To be included during the process

Podlipnik Črtomir Potential live connection with the ongoing Hackathon in Lubjana school
