



ΕΘΝΙΚΟ ΙΔΡΥΜΑ ΕΡΕΥΝΩΝ
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UNIVERSITÀ
DI SIENA 1240



Green and bioinformatic approaches including

biodegradability prediction in antiparasitic drug discovery

Tuesday, 18th March 2025

This will be a mixed event on Teams platform and Cloudpharm P.C Cana Laboratories - 446 Irakliou Avenue, Iraklio 14122, Attica, Greece

18 March 2025

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

We are excited to announce an upcoming workshop titled "Green and Bioinformatic Approaches Including Biodegradability Predictions in Antiparasitic Drug Discovery". This workshop will bring together experts and researchers to explore innovative molecular modeling and experimental tools in the field of biodegradability and antiparasitic drug discovery that align with the goals of the COST CA21111 Action.

TUESDAY 18th March 2025	
9:30 - 10:30	Registration
10:30-10:35	Opening remarks: Sandra Gemma, Theodora Carogeropoulou, Marina Roussaki
10:35 - 10:45	Maria Paola Costi Action Chair – OneHealthdrugs updates
10:45 - 11:05	Presentation of Cloudpharm P.C. and CANA Laboratories
11:05 – 11:25	Marina Roussaki - Presentation of the EU-Funded Project “ENVIROMED”
11:25 – 11:45	Eleni Chontzopoulou- Biodegradability and Pharmaceutical metabolites in Environmental Toxicology
11:45 – 12:05	Vagelis Tsoukas - Machine Learning based predictive models for ecotoxicity using LC50 and bioaccumulation factors
12:05– 12:25	Coffee Break
12:25 – 12:50	to be defined
12:50 – 14:00	Visit to the facilities of CANA Laboratories
14:00 - 15:00	Lunch Break
15:00 - 15:40	Tobias Harschneck -Boehringer-Ingelheim (remote)
15:40 – 16:10	Maria Clara Vieira Martins Starling - Universidade Federal de Minas Gerais Brazil (remote)
16:10 – 16:40	Sandra Gemma - Targeting Leishmaniasis: Integrating In Silico and Experimental Approaches for Scaffold Optimization within the One Health Framework
16:40 – 17:10	Break
17:10 – 17:30	Daniele Aiello - One Health Approach to Antiparasitic Drug Discovery: Integrating Structural Analysis and Ecotoxicological Profiling for Eco-Friendly Compound Prioritization
17:30 – 17:45	Ludovica Marotta - A Design of Experiment (DoE) approach for a sustainable synthesis of chalcones as promising antimicrobial scaffold
17:45 – 18:00	Closing Remarks