



[www.onehealthdrugs.com](http://www.onehealthdrugs.com)

# *In silico* prediction method for ecotoxicity and bioaccumulation

Wednesday 19 March – Friday 21 March 2025

Cloudpharm P.C., Cana Laboratories - 446 Iraklion Avenue, Iraklio 14122, Attica, Greece

## ***Training School 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

Drug discovery is a complex process aiming to develop compounds with appropriate safety and efficacy profiles allowing to proceed to their clinical evaluation. Many of the drugs which are eventually approved are associated with ecotoxicity and bioaccumulation. *In silico* methods can be employed for predicting the ecotoxicity and bioaccumulation potential of chemicals, addressing environmental and regulatory concerns. These approaches employ mathematical models, databases, and algorithms to estimate the behaviour of compounds, without extensive laboratory testing, saving time, cost, and reducing animal testing.

This Training School aims to provide participants with a comprehensive understanding of *in silico* (computer-based) methods used to predict the ecotoxicity and bioaccumulation potential of chemicals. Through a series of lectures, hands-on workshops, and case studies, attendees will learn the principles, tools, and applications of computational techniques in environmental risk assessment. The training will cover key aspects such as predictive toxicology models, bioaccumulation forecasting, and the integration of *in silico* methods into environmental protection strategies. This event is designed for researchers and students seeking to enhance their knowledge in the field of environmental science and computational toxicology.

Applications to the Training School can be made by submitting the **Training School Application Form**, together with a **short Curriculum vitae** (no longer than one page) and an **endorsement letter from your supervisor or institutional head** to Apostolia Zarpala ([azarpala@cloudpharm.eu](mailto:azarpala@cloudpharm.eu)) with the e-mail subject **CA21111 Training School Athens**.

**Application submission deadline: 03/02/2025.**

The selection of participants will be made based on the quality of the above submitted documents with priority given to PhD Students and young researchers, alignment of research activities with the Training School Programme as well as country of affiliation, career stage and contributions to the OneHealthdrugs Cost Action.

**Successful participants will be notified by 07/02/2025**, who will need to create an e-COST account (<https://e-services.cost.eu>) after which they will receive an official invitation to the Training School.

Travel costs will be reimbursed for up to 15 participants. Reimbursement rules can be found in the ANNOTATED RULES FOR COST ACTIONS (<https://www.cost.eu/uploads/2024/11/COST-094-21-V2.0-Annotated-Rules-for-COST-Actions-Level-C.pdf>). **Please carefully read this document as the reimbursement rules have been updated recently.**

### Preliminary Programme

Day 1 – WEDNESDAY 19 <sup>th</sup> March 2025	
09:00 - 10:00	Registration
10:00 - 10:15	Opening Remarks and Welcome
10:15 - 11:00	Lecture: Molecular modelling and drug design
11:00 - 11:45	Lecture: Machine learning in drug design
11:45 - 12:00	Break
12:00 - 13:00	Hands-on workshop: Molecular docking
13:00 - 14:00	Lunch
14:00 - 14:45	Lecture: Overview of drug discovery
14:45 - 15:30	Lecture: Biological properties of drugs
15:30 - 15:45	Break
15:45 - 16:30	Lecture: Optimization of compounds in drug discovery
16:30 - 17:00	Wrap-Up, Q&A, and Preview of Day 2
Day 2 – THURSDAY 20 <sup>th</sup> March 2025	
10:00 - 10:15	Recap of Day 1
10:15 - 11:15	Lecture: Introduction to machine learning techniques for environmental risk assessment
11:15 - 12:15	Lecture: Modeling ecotoxicology with chemoinformatics and artificial intelligence
12:15 - 12:30	Break
12:30 - 13:30	Hands-on workshop: Developing deep learning models and case studies
13:30 - 14:30	Lunch
14:30 - 16:30	Hands-on workshop: To be announced
16:30 - 17:00	Wrap-Up, Q&A, and Preview of Day 3
Day 3 – FRIDAY 21 <sup>st</sup> March 2025	
10:00 - 10:15	Recap of Day 2
10:15 - 11:15	Lecture: Advanced chemoinformatics and artificial intelligence techniques for collaborative projects
11:15 - 12:15	Lecture: Future directions in chemoinformatics and artificial intelligence
12:15 - 12:30	Break
12:30 - 13:30	Team work: preparing presentations
13:30 - 14:30	Lunch
14:30 - 16:00	Team work: Team Presentations
16:00 - 16:30	Discussion
16:30 - 17:00	Wrap-Up & Closing Remarks