



## AGENDA: 5<sup>TH</sup> OHD TRAINING SCHOOL - *In silico* prediction method for ecotoxicity and bioaccumulation

Day 1 – WEDNESDAY 19 <sup>th</sup> March 2025	
09:00-10:00	Registration
10:00-10:15	Opening Remarks and welcome Maria Paola Costi Action Chair ‘OneHealthdrugs’
10:15-10:45	<b>Lecture:</b> Molecular modelling and drug design <b>Michalis Papadourakis</b> , Hellenic Mediterranean University (HMU), Greece
10:45-11:15	<b>Lecture:</b> Machine learning in drug design <b>Vaggelis Tsoukas</b> , Cloudpharm P.C., Greece
11:15-11:30	Coffee Break
11:30-13:00	<b>Hands-on workshop:</b> Molecular docking <b>Michalis Papadourakis</b> , Hellenic Mediterranean University (HMU), Greece <b>Vaggelis Tsoukas</b> , <b>Eleni Chontzopoulou</b> , <b>Vasilis Panagiotopoulos</b> , Cloudpharm P.C., Greece
13:00-14:00	Refreshments
14:00-14:45	<b>Lecture:</b> Overview of drug discovery <b>Sheraz Gul</b> , Fraunhofer ITMP, Germany
14:45-15:30	<b>Lecture:</b> Properties of a Lead and Clinical Candidate compound <b>Sheraz Gul</b> , Fraunhofer ITMP, Germany
15:30-15:45	Coffee Break
15:45-16:30	<b>Lecture:</b> Profiles of drugs <b>Sheraz Gul</b> , Fraunhofer ITMP, Germany
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	<b>Lecture:</b> A multimodal platform for developing <i>in silico</i> tools to aid the design of pharmaceuticals with a lower environmental footprint: Key lessons learned <b>Eleni Chontzopoulou</b> , Cloudpharm P.C., Greece <b>Vaggelis Tsoukas</b> Cloudpharm P.C., Greece
11:15-12:00	<b>Lecture:</b> Assays in drug discovery <b>Sheraz Gul</b> , Fraunhofer ITMP, Germany
12:00-12:30	Coffee Break
12:30-13:30	<b>Hands-on workshop:</b> Machine learning for bioactivity prediction <b>Cavouras Dionisis</b> , UNIWA, Greece <b>Vaggelis Tsoukas</b> , Cloudpharm P.C., Greece <b>Vasilis Panagiotopoulos</b> Cloudpharm P.C., Greece
13:30-14:30	Refreshments
14:30-16:00	<b>Hands-on workshop:</b> Machine learning for bioactivity prediction <b>Cavouras Dionisis</b> UNIWA, Greece <b>Vaggelis Tsoukas</b> , Cloudpharm P.C., Greece <b>Vasilis Panagiotopoulos</b> Cloudpharm P.C., Greece
16:00-16:15	Coffee Break
16:15-16:45	<b>Hands-on workshop:</b> Machine learning for bioactivity prediction <b>Cavouras Dionisis</b> UNIWA, Greece <b>Vaggelis Tsoukas</b> , Cloudpharm P.C., Greece <b>Vasilis Panagiotopoulos</b> Cloudpharm P.C., Greece

16:45-17:00	Wrap-Up, Q&A, and Preview of Day 3
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**Day 3 – FRIDAY 21<sup>st</sup> March 2025**

10:00-10:15	Recap of Day 2
10:15-10:35	<b>Hands-on workshop:</b> Introduction <b>Dimitra-Danai Varsou</b> , NovaMechanics MIKE, Greece
10:35-12:30	<b>Hands-on workshop:</b> Point-and-Click machine learning for cheminformatics with Isalos Analytics Platform <b>Dimitra-Danai Varsou</b> , NovaMechanics MIKE, Greece
12:30-12:45	Coffee Break
12:45-13:30	<b>Hands-on workshop:</b> Identifying a druggable protein, target validation & target tractability <b>Sheraz Gul</b> , Fraunhofer ITMP, Germany
13:30-14:30	Refreshments
14:30-16:00	<b>Hands-on workshop:</b> Building a drug discovery pipeline <b>Sheraz Gul</b> , Fraunhofer ITMP, Germany
16:00-16:15	Coffee Break
16:15-17:00	Wrap-Up & Closing Remarks