MINUTES
In silico prediction method for ecotoxicity and bioaccumulation
19-21/03/2024
Prepared by Sandra Gemma (HG7 Leader), Marina Rousssaki (Local organizer) and Theodora Calogeropoulou (WG2 leader)

1. LIST OF ATTENDANTS

Number	Name	Country
1.	Aliyeva Gunel	AZ
2.	Raffellini Lorenzo	IT
3.	Kayhan Ilbeigi	BE
4.	Sebai Essia	TN
5.	Arslan Hanifi Atif	FI
6.	Aiello Daniele	IT
7.	Ebiloma Godwin	UK
8.	Dimitrov Simeon	BG
9.	Marotta Ludovica	IT
10.	Bertarini Laura	IT
11.	Valiauga Benjaminas	LT
12.	Foropoulou Theano	GR
13.	Chotzopoulou Eleni	GR
14.	Tsoukas Vaggelis	GR
15.	Panagiotopoulos Vasilis	GR
16.	Cavouras Dimitrios	GR
17.	Varsou Dimitra-Danai	GR
18.	Papadourakis Michail	GR
19.	Gul Sheraz	DE
20.	Maria Paola Costi	IT
21.	Theodora Calogeropoulou	GR

2. DESCRIPTION OF THE ACTIVITIES

The organizing committee conducted a selection process to determine the final trainees, resulting in a total of **12 participants**. The selection was primarily based on their background and expertise. E-COST invitations were sent to all of them. The training school featured **seven trainers**: **Michalis Papadourakis** (Hellenic Mediterranean University), **Vaggelis Tsoukas** (Cloudpharm P.C.), **Eleni Chontzopoulou** (Cloudpharm P.C.), **Vasilis Panagiotopoulos** (Cloudpharm P.C.), **Sheraz Gul** (Fraunhofer ITMP), **Cavouras Dionisis** (UNIWA) and **Dimitra-Danai Varsou** (NovaMechanics MIKE).

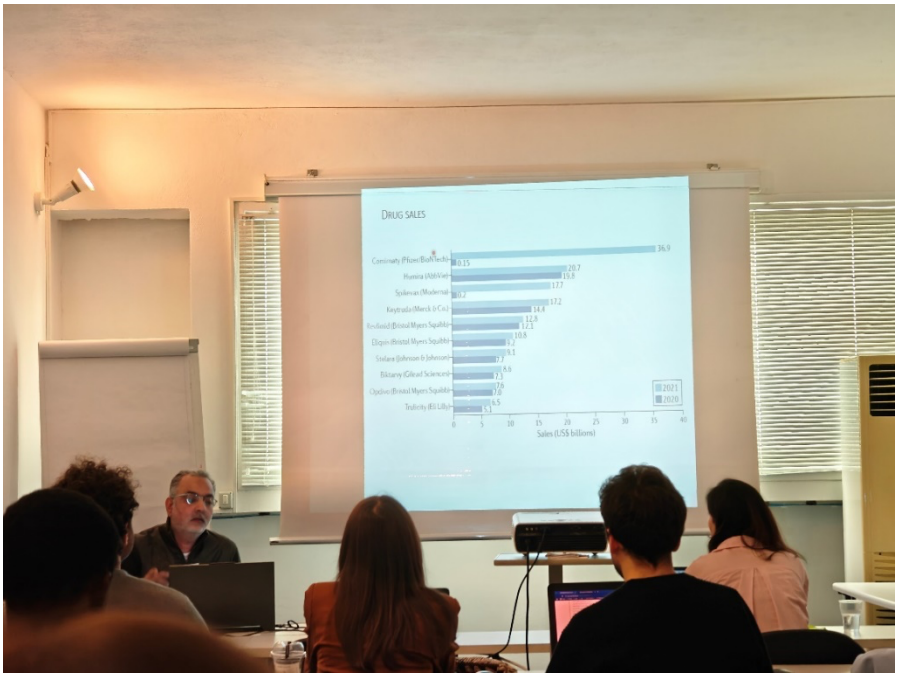
Day 1.

The 5th OHD Training School on in silico prediction methods for ecotoxicity and bioaccumulation commenced on March 19th, 2025, with opening remarks by **Maria Paola Costi**, followed by an introduction to the three-day event by **Marina Roussaki**.

The first day featured insightful lectures on molecular modeling and machine learning in drug design, presented by **Michalis Papadourakis** and **Vaggelis Tsoukas**, respectively. A hands-on workshop on molecular docking, led by experts from the Hellenic Mediterranean University and Cloudpharm P.C., provided participants with practical experience. In the afternoon, **Sheraz Gul** from Fraunhofer ITMP delivered a series of lectures covering key aspects of drug discovery, lead compound properties, and drug profiling. The day concluded with a Q&A session and a preview of the upcoming sessions.

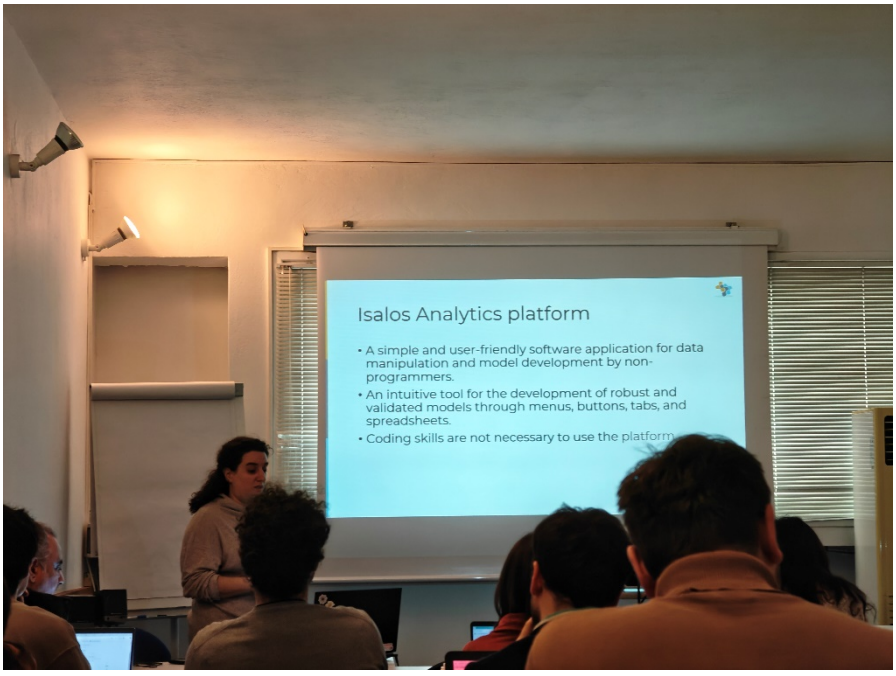
Day 2.

The second day started with a recap of the previous discussions, followed by a lecture on developing in silico tools for designing environmentally friendly pharmaceuticals by **Eleni Chontzopoulou** and **Vaggelis Tsoukas**. **Sheraz Gul** then presented an overview of assays in drug discovery. A series of hands-on workshops on machine learning for bioactivity prediction, led by experts from UNIWA and Cloudpharm P.C., occupied the rest of the day, allowing participants to apply theoretical knowledge to real-world applications.



Day 3.

On the final day, **Dimitra-Danai Varsou** introduced a hands-on workshop using the Isalos Analytics Platform for cheminformatics. This was followed by practical sessions on identifying druggable proteins, target validation, and building a drug discovery pipeline, led by **Sheraz Gul**. The event concluded with a wrap-up session and closing remarks, summarizing key takeaways and future directions in computational drug discovery.



3. CONCLUSIONS

The 5th OHD Training School provided an in-depth exploration of in silico prediction methods for ecotoxicity and bioaccumulation, equipping participants with both theoretical knowledge and hands-on experience in computational drug discovery. The event covered essential topics, including molecular modeling, machine learning applications, and drug discovery workflows, delivered by distinguished experts from academia and industry. The combination of lectures and interactive workshops ensured that attendees gained practical skills in molecular docking, bioactivity prediction, and cheminformatics tools, fostering a comprehensive understanding of modern computational approaches in pharmaceutical research.

The training school successfully highlighted the importance of integrating computational techniques in drug design to enhance efficiency, reduce environmental impact, and improve the identification of viable drug candidates. Participants benefited from engaging discussions, Q&A sessions, and networking opportunities, facilitating knowledge exchange and potential future collaborations. As the field of computational drug discovery continues to evolve, the insights gained during this training school will serve as a strong foundation for further research and innovation in developing sustainable and effective pharmaceuticals.