In silico **prediction method for ecotoxicity and bioaccumulation**

Wednesday 19 March – Friday 21 March 2025

Cloudpharm P.C., Cana Laboratories, Athens, Greece

Students' collaborative report

Day One Report - Opening Remarks, Molecular Modeling, and Machine Learning in Drug Design

The first day of the training school commenced with opening remarks by Maria Paola Costi. Following the opening remarks, Marina Roussaki, highlighted the importance of in silico techniques in modern drug discovery. She set the stage for the upcoming days, emphasizing the integration of computational methods in various stages of pharmaceutical development, particularly in predicting the environmental impact of new drugs.

The first technical session featured Michalis Papadourakis, who delivered an engaging lecture on molecular modeling. He discussed the various approaches to molecular modeling, explaining their applications in predicting the properties and behaviors of drug molecules. His session emphasized the role of molecular simulations in understanding interactions at the atomic level, which can help in optimizing drug efficacy and reducing side effects.

Next, Vaggelis Tsoukas presented a lecture on machine learning in drug design. His talk focused on how machine learning algorithms are being applied to accelerate drug discovery, particularly in predicting biological activity, toxicity, and other critical properties. Vaggelis Tsoukas emphasized the growing importance of data-driven approaches in improving drug design processes and making them more efficient.

In the afternoon, participants took part in a hands-on workshop on molecular docking, led by experts from the Hellenic Mediterranean University and Cloudpharm P.C. This workshop provided participants with practical experience in using docking software to simulate and predict the binding interactions between drug molecules and biological targets. The interactive session allowed participants to apply theoretical knowledge in a real-world setting, enhancing their understanding of the practical aspects of molecular modeling.

The day concluded with a Q&A session, where participants had the opportunity to engage with the speakers and ask questions. This session provided valuable insights into the current challenges and future directions in molecular modeling and drug design. A preview of the upcoming sessions was also provided, generating excitement for the second day.

Day Two Report - In Silico Tools for Designing Environmentally Friendly Pharmaceuticals and Bioactivity Prediction

Day 2 of the training school began with a recap of the previous discussions, allowing participants to reflect on what had been covered on Day 1. This was followed by a lecture by Eleni Chontzopoulou and Vaggelis Tsoukas on developing *in silico* tools for designing environmentally friendly pharmaceuticals. They discussed the importance of considering the environmental impact of pharmaceuticals during the early stages of drug development. Their lecture focused on using computational tools to predict the ecotoxicity and bioaccumulation potential of drugs, which is essential in reducing the environmental risks associated with pharmaceutical residues.

Following this, Sheraz Gul from Fraunhofer ITMP presented an insightful lecture on assays in drug discovery. Gul provided an overview of the different types of assays used to evaluate the biological activity and safety

profiles of drug candidates. He highlighted the importance of selecting appropriate assays for early-stage drug discovery to streamline the development process.

The afternoon session was dedicated to hands-on workshops on machine learning for bioactivity prediction, led by experts from UNIWA and Cloudpharm P.C. In these workshops, participants had the opportunity to apply machine learning algorithms to real-world datasets to predict the bioactivity of various chemical compounds. The session provided practical experience in training models, validating their performance, and interpreting the results to make informed decisions in drug discovery.

Day Three Report - Target Validation, Druggable Proteins, and Drug Discovery Pipelines

The final day of the training school began with Dimitra-Danai Varsou introducing a hands-on workshop using the Isalos Analytics Platform for cheminformatics. This session provided participants with an introduction to cheminformatics tools, specifically the Isalos Analytics Platform, which is widely used for drug discovery. Participants were guided through the platform's capabilities in analyzing chemical data, predicting molecular properties, and identifying potential drug candidates.

In the following session, Sheraz Gul led practical sessions on identifying druggable proteins, target validation, and building a drug discovery pipeline. Gul discussed the critical steps involved in identifying and validating biological targets for drug development. He emphasized the importance of understanding the biological context of the target, as well as the use of computational methods to predict the druggability of proteins. The session also covered strategies for developing efficient drug discovery pipelines, from target identification to clinical trials.

The training school concluded with a wrap-up session, where the key takeaways from the three days were summarized. The closing remarks highlighted the importance of computational methods in modern drug discovery and the need for continued collaboration between academia, industry, and regulatory bodies to advance the field. Future directions in computational drug discovery were also discussed, including the increasing role of artificial intelligence, machine learning, and big data analytics in shaping the future of the pharmaceutical industry.