Pre-conference WORKSHOP

Wednesday, 11th June 2025, 10am-12pm

School of Pharmacy, Nantes Université – France

Artificial Intelligence in Drug Discovery: A New Era of Molecular Design

Dylan Serillon [1]

1. WhiteLab Genomics; https://whitelabgx.com/, https://www.linkedin.com/in/dylan-serillon/

Artificial Intelligence (AI) is reshaping drug discovery by enhancing molecular design, optimizing ligand-target interactions, and improving predictive modeling. The integration of machine learning (ML), deep learning (DL), and computational chemistry enables faster and more accurate identification of promising drug candidates, significantly reducing development timelines.

AI-driven approaches, particularly thermodynamic and knowledge-based models, are crucial for predicting binding free energy in receptor-ligand complexes. The combination of classical and quantum mechanics with machine learning algorithms refines molecular docking predictions, leading to more precise virtual screening and structure-based drug design.

In peptide discovery and gene therapy vector engineering, AI accelerates protein-ligand interaction analysis, optimizing molecular properties for improved therapeutic efficacy. Deep learning models contribute to the design of novel peptides, while AI-guided optimization enhances viral and non-viral vectors for gene delivery.

This workshop explores key advancements in AI-powered drug design, including predictive modeling, AI-driven molecular docking, and generative design for small molecules and biologics. Emphasis will be placed on the synergy between computational simulations and experimental validation, bridging the gap between in silico predictions and real-world drug development.