Infectious Diseases Labs
ID LABS

Horizontal Technology Coordinating Office
EPIDEMIC PREPAREDNESS

Dr Hovakim Zakaryan

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Yerevan, Armenia

Wednesday, 6th December 2023
1pm to 2pm (SGT)

Venue: Codon A&B Matrix L5

New Computational Approaches in Antiviral Drug Discovery

In my presentation, I will focus on two novel strategies developed by my laboratory in collaboration with Denovo Sciences Inc. These methods have demonstrated a significantly higher hit discovery rate in antiviral drug development compared to conventional computational approaches. I will delve into the details of these cutting-edge techniques: Advanced Virtual Screening and AI-based molecule design. Advanced Virtual Screening combines consensus and ensemble docking methods, which enhance the accuracy and reliability of identifying potential hits. In contrast, AI-based molecule design is the construction of highly novel molecules directly within the binding pockets of proteins through the application of reinforcement learning. Both approaches have proven to be remarkably successful in designing new antiviral agents with high efficacy.

Dr Hovakim completed his PhD studies in Virology and Cell Biology. Since 2016 he has been the head of the Laboratory of Antiviral Drug Discovery in the Institute of Molecular Biology of NAS, Yerevan, Armenia, where he and his team are developing new antiviral screening technologies and applying them to find potent inhibitors against a wide range of human and animal viruses including influenza viruses and African swine fever virus. Since 2020, Hovakim is the co-founder and CEO of Denovo Sciences Inc., a techbio company focusing on AI-based drug discovery.

Hosted by : Prof Marco Vignuzzi

Questions? Contact us at **seminars@idlabs.a-star.edu.sg**