Webinar on “Revolutionizing ADMET Modelling: Exploring the Frontiers with Artificial Intelligence”

BY: ASSOCIATE PROFESSOR DR. FAZLIN MOHD FAUZI

On the 26th of April 2024, the Faculty organised a webinar on “Revolutionizing ADMET Modelling: Exploring the Frontiers with Artificial Intelligence”, where Associate Professor Dr Vasanthanathan Poongavanam from Uppsala University, Sweden was the invited speaker. In this hour-long webinar, Dr Poongavanam covered the different ways artificial intelligence is being applied in pre-clinical studies, specifically in analysing the pharmacokinetics profile of lead compounds. This is of importance as poor pharmacokinetic profile of lead compounds has been identified as one of the reasons for the high attrition rate in drug discovery and development. In his talk, Dr Poongavanam explored looking at the pharmacokinetic profile of lead compounds that go beyond the traditional Lipinski’s Rule of 5. Although this rule has guided the synthesis of orally available drugs, several classes of drugs can still be administered orally despite violating this rule, in particular antiinfective drugs. These compounds are termed ‘chameleonic compounds’ as they can shield polar functional groups when crossing lipid membranes. Through the study of the crystal structures of these chameleonic compounds, it was discovered that they contain flexible aromatic side chains and can form intramolecular hydrogen bonds. Dr Poongavanam also demonstrated several predictive models that have been developed and used by pharmaceutical companies to streamline the drug discovery process. By incorporating artificial intelligence in drug discovery, the time it takes for a drug to be approved can be reduced and/or increase the success rate. In his closing remarks, Dr Poongavanam highlighted several key points such as: i) despite the leaps and bounds that artificial intelligence has made in drug discovery, it is still a long and arduous process, and ii) a good predictive model is dependent on robust data that is being used. In summary, this webinar offered a compelling glimpse into the cutting-edge fusion of artificial intelligence and pharmacokinetic modeling, shedding light on the promising avenues for revolutionising drug discovery.

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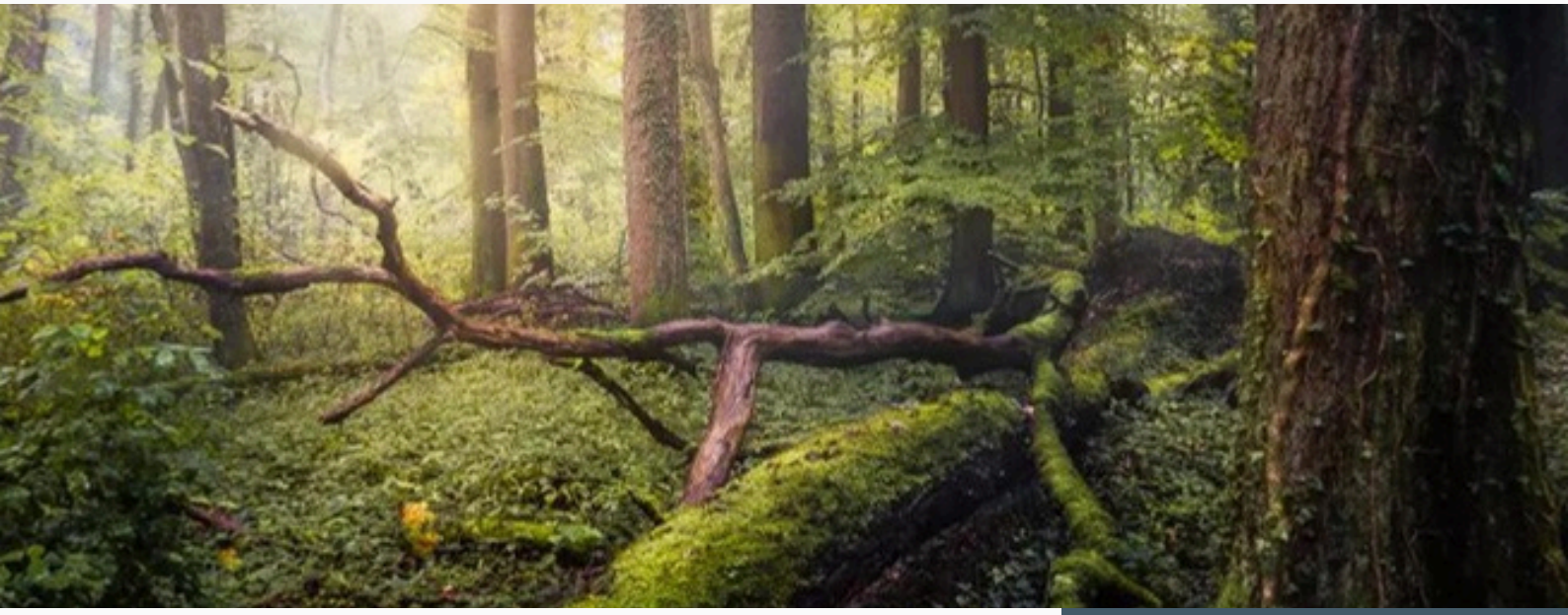

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