Dissertation Defense Announcement
To: The George Mason University Community

Candidate: Deborah Ngan

Program: PhD in Bioinformatics & Computational Biology

Date: Monday, November 13, 2023

Time: 3:00 PM EST

Join Zoom Meeting:
Deborah Ngan's dissertation defense meeting
Meeting ID: 950 5274 8344
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+12678310333,,95052748344#,,,,*184403# US (Philadelphia)

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Join by SIP
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Title: "Application of Computational Models Using Machine Learning Methods to Predict Drug Toxicity and Advance Drug Development"
Committee Chair: Dr. Iosif Vaisman
Committee Members: Dr. Donald Seto, Dr. Ancha Baranova, Dr. Ruili Huang

All are invited to attend the defense

ABSTRACT:

Drug development is a complex process that is costly, time-consuming, and has a relatively low success rate. Despite these challenges, this process is essential to better understand the specific pathways and targets involved in disease etiology and ultimately develop effective interventions essential for the improvement of human health. Toxicity testing is a critical step used to determine the adverse effect potential of the drug in development, and it is increasingly relying on the in silico modeling. For instance, in the cases of drug-induced liver injury (DILI) and cardiotoxicity (DICT) current in vivo toxicological testing is insufficient to comprehensively assess the hepatotoxic and cardiotoxic potential of compounds, thereby presenting an urgent need for alternative prediction strategies. In the adjacent areas of drug development, drug repurposing became an appealing method to address the Coronavirus 2019 (COVID-19) pandemic because of the low cost and efficiency. Compounds that exhibited anti-SARS-CoV-2 activity were found to correlate with other biological activities (e.g., human ether-a-go-go-related gene (hERG), phospholipidosis (PLD), and cytotoxicity screens), so these compounds need to be evaluated for their toxicity potential especially in terms of cardiotoxicity via hERG inhibition. Lastly, there has been considerable interest in recent years in the development of small molecule protein kinase inhibitors for the treatment of several diseases. While a number of protein kinase inhibitors have been FDA approved, there remains a need to develop effective computational models to predict protein kinase inhibition activity of small molecules. Collectively, computational approaches using machine learning algorithms can significantly improve the drug development and toxicity evaluation of small molecules that target unmet medical needs across diverse therapeutic areas.

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