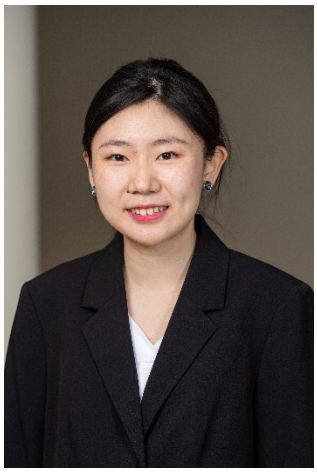
COLLEGE OF PHARMACY
PHARMACEUTICAL SCIENCES
UNIVERSITY OF MICHIGAN

Pharmaceutical Sciences Seminar Series

Wednesday, September 13, 2023
4:00pm
2548 North University Building
Zoom

"Variational Autoencoder (VAE) in Drug Discovery: Classification and Generation"

Presented by:



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Abstract: Drug discovery has experienced a paradigm shift in recent years with the integration of machine learning (ML), especially VAE. VAEs are generative models that have the capacity to enhance drug classification accuracy and facilitate the generation of innovative drug candidates. Classification tasks in drug discovery involve the identification of compounds with certain properties, such as binding affinity or potential toxicity. VAE excel in drug property classification by learning complex representations of molecular structures, encoding compounds into a lower-dimensional latent space. This enables the identification of subtle patterns and relationships among compounds that might be challenging for traditional methods to discern. In the generation task of novel drug-like molecules, VAE has shown remarkable promise to generate new molecular structures by sampling from learned latent space. Furthermore, conditional VAE allows for the targeted design of compounds with predefined characteristics such as kinase inhibition or reduced side effects. This capability streamlines the process of drug candidate generation, reducing the time and resources required for traditional experimental approaches. In conclusion, VAE has emerged as a powerful tool in drug discovery, including but not limited to virtual screening, de novo drug design and property optimization. The integration of VAEs into the drug discovery pipeline holds the potential to accelerate the development of new therapeutics, making it an indispensable technology in the pursuit of novel drug compounds.

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