EKU department of mathematics & statistics

Colloquium

presenting...

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Application Of Machine Learning Algorithms In Drug Discovery And Design

The search for novel compounds for protein-aggregation associated diseases presents a huge challenge. A robust pipeline that incorporated several machine learning algorithms (MLAs) was designed, implemented, and validated in R statistical software for quantitative structure-activity relationship (QSAR) modeling. Anti-aggregative dose-response data were matched with molecular properties of the compounds to define QSAR, subsequently identifying the structural features responsible for the anti-aggregative activity of the compounds, thereby guiding further synthesis, and testing of more potent compounds. Molecular modeling, docking and simulations were used to address critical drug development questions. Our pipeline showed robust result across MLAs regardless of endpoint, suggesting that MLAs hold a great potential in addressing important research questions in drug development and other fields of study.

Wednesday, September 29th, 2021

2:30 – 3:20 p.m. Wallace Bldg. Room 149

Zoom: https://eku.zoom.us/j/91262201332