PURDUE UNIVERSITY | Department of Industrial and Physical Pharmacy

Industrial & Physical Pharmacy Seminar

IPPH 69600

Monday, April 4, 2022
3:30 PM in RHPH 164

"Prediction of Drug-Drug Interactions with Deep Learning"

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Last Seminar

Drug-drug interactions (DDIs) occur when multiple drugs are used concurrently. The risk of DDIs that could seriously impact on the efficacy and safety of co-administered medications needs to be carefully evaluated. Cytochrome P450 (CYP), a superfamily of enzymes, play an important for the metabolism of most drugs currently on the market. In-silico methods can guide and prioritize efforts in drug discovery. A common goal for molecular modeling is to extract properties directly from chemical structure; however, it remains an open question as to what extent and how accurately information can be extracted and utilized. Our laboratory has studied the intermolecular interactions of organic crystals through electronic structure-based local descriptors derived from conceptual density functional theory (CDFT). We then applied manifold embedding and further posit that low-dimension manifold of molecular surface could capture most of the information of the molecular interactions and be utilized as feature vectors by deep learning algorithms. With developed manifold embedding of molecular surface descriptor, our model demonstrated enhanced prediction against different CYP targets. Using information that reside on molecule 3D surface, we can predict DDIs with improved specificity and strength.