Proposal Defense

Doctor of Philosophy in Intelligent Systems

“Application of Knowledge Representation and Natural Language Processing to Identify Potential Mechanisms of Natural Product-Drug Interactions” by Sanya Bathla Taneja

Date: October 24, 2023
Time: 11:30 a.m. – 1:00 p.m.
Place: [https://pitt.co1.qualtrics.com/jfe/form/SV_0PvnOi7WInpYi2](https://pitt.co1.qualtrics.com/jfe/form/SV_0PvnOi7WInpYi2)

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Abstract:
Concomitant use of pharmaceutical drugs and botanical natural products can result in pharmacokinetic natural product-drug interactions (NPDIs) leading to adverse events or reduced efficacy. Traditionally, NPDIs are studied through experimental and clinical studies, which can be time-consuming and expensive. With increasing use of natural products across the world and growing safety concerns, there is a need for novel computational methods to identify plausible mechanisms for NPDIs that can guide scientific research. The overarching goal of this project is to develop a natural products-relevant knowledge graph (KG) that combines existing biomedical knowledge with the scientific literature to identify plausible mechanistic hypotheses for potential NPDIs and associated adverse drug reactions (ADRs) and present them to researchers. I propose to develop a large-scale, heterogeneous biomedical knowledge graph (KG) with natural products, chemical constituents, proteins, genes, diseases, and phenotypes combining information from biomedical ontologies, drug databases, and domain-specific scientific literature to identify mechanisms related to selected natural products. I will then use pharmacovigilance signals of natural product-related ADRs from spontaneous reporting systems to guide the mechanism generation in the KG through discovery patterns and embedding-based methods and provide plausible mechanistic hypotheses to researchers along with supporting evidence in a prototype tool. The tool, comprising of the KG and generated hypotheses with mechanism ranking and supporting evidence, will be evaluated with known mechanisms from natural product databases and a user study to evaluate the plausibility and accuracy of the potential mechanisms. The research presents a major step forward in computational discovery of NPDIs and has the potential to improve drug safety and clinical decision-making.