UNIVERSITY of GUELPH

COLLEGE of ENGINEERING AND PHYSICAL SCIENCES

SCHOOL OF COMPUTER SCIENCE

MSc Seminar

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A Machine Learning Approach for Repurposing Non-Antifungal Drugs for Antifungal Applications Using Tree Representations of Chemical Structures

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Abstract:

Antifungal drugs are essential for treating a range of fungal infections, some of which can be life-threatening. However, current antifungal treatments are limited by their narrow spectrum of activity, high toxicity, and potential for resistance, highlighting the urgent need for new antifungal agents. Creating new antifungal drugs is challenging due to the difficulty in identifying novel targets. To address this issue, this project adopts a drug repurposing strategy, aiming to identify existing marketed drugs, not originally intended as antifungals, that can be repurposed to treat fungal infections. Drug repurposing is a cost-effective and faster alternative to traditional drug discovery since the mechanism of action, cellular targets, toxicity profile and safety of these drugs are known.

For this project, we represent the chemical structures of drugs as trees, a method to address some disadvantages of graph representation. These tree representations are then standardized into uniform sizes for effective ML training and testing. The goal is to utilize ML models to identify non-antifungal drugs that exhibit structural similarities to known antifungals, as structural similarity often correlates with biological activity.