**[BIOINFO 2024]**

# Context-Aware Hierarchical Fusion for Drug Relational Learning

Yijingxiu Lu[1], Yinhua Piao[1], Sangseon Lee[2] and Sun Kim[1,3,*]

[1]*Department of Computer Science, Seoul National University*
[2]*Department of Artificial Intelligence, Inha University*
[3]*AIGENDRUG Co. Ltd*
**Corresponding author: sunkim.bioinfo@sun.ac.kr*

Drug relational learning, focused on understanding drug-pair relationships within specific contexts of interest, has emerged as a critical area of investigation for its pivotal role in enhancing the efficacy of disease treatment. The nature of drug relationships exhibits significant variations across diverse contexts, such as different types of cancer cell lines. Existing methods often encounter limitations by either neglecting the incorporation of context information or lacking explicit modeling of the intricate connections within drug-drug-context triplets, due to the difficulty in handling heterogeneous relationships between drugs and context. In this study, we present a novel context-aware hierarchical cross-fusion architecture tailored for drug relational learning. By formulating the problem as the label prediction of drug-drug-context triplets, we explicitly calculate all the relations among the triplets. Considering drugs often function as causes and contexts serve as results, our model enhances the learning of intricate drug pair relations hierarchically fusing the information from drug to context through the learned relations. Empirical results across multiple prediction tasks, including synergy, polypharmacy side effects, and drug-drug interactions, highlight the model's capability to capture essential information relevant to drug relational learning. Notably, our model demonstrates robust predictive performance even in scenarios of heightened contextual complexity, demonstrating its adaptability in learning context-aware drug relations.