Leveraging Heterogeneous Graph Neural Networks for Target Identification

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Effective target identification is a critical challenge in early-stage drug discovery, particularly when evaluating novel chemical entities with limited data. While traditional computational methods often rely on established interaction patterns, they frequently struggle to generalise to cold-start scenarios, where a candidate compound has no prior known associations within the biological network. This work employs a heterogeneous graph-based framework [1,2] to map the complex interplay between chemical structures and biological systems, facilitating the direct identification of therapeutic targets for novel compounds.

By utilising graph-based representation learning, the framework captures high-dimensional features of both ligands and proteins to predict potential interactions [3,4]. This methodology is specifically designed to handle the absence of prior binding information, facilitating the priorisation of targets for unseen compounds.

This poster will outline the overall computational strategy, including the heterogeneous graph construction and the predictive methodology, with preliminary findings to illustrate key aspects of the workflow and its potential for identifying novel therapeutic targets.

Bibliography :

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