CANDraGAT: A Hybrid Fragment-Based Graph Attention Network To Improve Cancer Drug Response Prediction

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Cancer is a major public health problem that has caused over 10 million deaths worldwide in 2020. Precision oncology, which employs a patient's genetic profile of tumors to identify the most effective drugs, has played an important role in cancer treatment. However, this process requires advanced tools, extensive time, and considerable cost. Currently, deep learning significantly contributes to addressing these challenges. Most existing deep learning models rely on the chemical structure of drugs and multi-omics data to predict cancer drug responses. However, these models exclude the chemical functional groups of drugs that are key to drug design and development. Therefore, we herein developed CANDraGAT, a deep learning model implementing a fragment-based graph attention network to emphasize the molecular features of drugs and deep neural networks for multi-omics data. The result shows that CANDraGAT outperforms state-of-the-art and baseline methods in both regression and classification tasks. Our model effectively anticipates unknown cancer drug response values corresponding to protein-protein interaction and gene set enrichment analysis of cancer pathways. Moreover, the model is applicable to solve real-world problems, as validated by TCGA patients' data. The interpretation of CANDraGAT provides important gene mutation profiles to explore potential cancer pathways and drug targets further. Our strategy may help clinicians administer appropriate anti-cancer drugs for patients and assist pharmaceutical industries in guiding patient omics-specific drug design and development.

Awards Won:

First Award of $5,000

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