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Proposing an Architecture for Drug Response Prediction by Integrating Multiomics Data and Utilizing Graph Transformers

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Abstract : Efficiently predicting drug response remains a challenge in the realm of drug discovery. To address this issue, we propose four model architectures that combine graphical representation with varying positions of multiheaded self-attention mechanisms. By leveraging two types of multi-omics data, transcriptomics and genomics, we create a comprehensive representation of target cells and enable drug response prediction in precision medicine. A majority of our architectures utilize multiple transformer models, one with a graph attention mechanism and the other with a multiheaded self-attention mechanism, to generate latent representations of both drug and omics data, respectively. Our model architectures apply an attention mechanism to both drug and multiomics data, with the goal of procuring more comprehensive latent representations. The latent representations are then concatenated and input into a fully connected network to predict the IC-50 score, a measure of cell drug response. We experiment with all four of these architectures and extract results from all of them. Our study greatly contributes to the future of drug discovery and precision medicine by looking to optimize the time and accuracy of drug response prediction.

Keywords : drug discovery, transformers, graph neural networks, multiomics
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