Application of Deep Learning in Target Identification Through Determining the Mechanism of Action Given Cellular Signature Data

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Current techniques of target identification in drug development are costly, lengthy, and function with high degrees of uncertainty that a drug can succeed in modulating a target. To address this, the ability of computational approaches to leverage cellular signature data for in-silico target identification was explored. The NIH LINCS program has compiled and publicized data consisting of cell viability measurements and high-throughput gene-expression drug and target screens (measured by L1000 assay) of ~5000 small molecules and their respective mechanisms of action (MoA). This study involves the utilization of a neural network to convert this cellular signature data to an estimate of the mechanism of action of a compound. Validating on an isolated subset of our training data, our approach achieved 81.69% AUC (Receiver Operating Characteristic curve). After improving the performance of our model through Bayesian hyperparameter optimization, the final validation AUC increased to 91.51%. These promising results were also shown to significantly perform more efficiently than other machine learning approaches: one-dimensional convolutional neural network, and logistic regression ($p < 0.05$). Overall, the algorithm provides a reliable framework for expedited drug target identification.

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