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Interpretation of anticancer drug action using predicted features obtained from machine learning

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Various machine learning and statistical models have successfully predicted the efficacy of anticancer drugs. However, identifying the mechanism of action (MOA) responsible for this efficacy remains a challenging problem. We conducted an exploratory data analysis to predict MOAs of anticancer drugs based on large-scale cancer cell line expression and drug response data.

Using elastic net, a simple and explainable machine learning technique, we constructed prediction models for a total of 450 drugs. We then examined the association between each drug's predictive performance and its category, target, and MOA. For the drugs that demonstrated higher prediction performance, we compared the previously known MOAs with the MOAs derived by the prediction model. We also highlighted the potential for drug repositioning by proposing new MOAs for existing drugs.