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Exploratory data analysis for predicting anticancer drug reactivity and mechanism of action

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While various machine learning methods for predicting drug responses have been successfully developed, identifying the mechanism of drug action remains a challenge. In this study, we conducted an exploratory data analysis to gain insights into drug responsiveness and molecular mechanisms. We utilized the transcriptomes of large-scale cancer cell line panels and applied 12 distinct machine learning models to predict drug responsiveness to 387 anticancer drugs.

The results revealed that chemotherapy drugs exhibited the highest predictive performance. Furthermore, we observed a strong correlation between the distribution of drug responses and predictive power, particularly with the first percentile value.