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Leveraging Computational Chemical-Induced Transcriptomic Cell State for Drug Response Prediction Through Transfer Learning

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Personalized medicine has drawn significant attention in recent years, with the aid from big data and deep learning models to achieve more precise drug response predictions. In this paper, we present a novel approach to drug response prediction, focusing on the utilization of a well-constructed chemical-induced transcriptomic cell state space through a transfer learning framework for translational research. Our approach is composed of three steps: LINCS pretraining, GDSC fine-tuning, and TCGA patient data validation. Initially, we pre-train our model with the comprehensive LINCS dataset, enabling it to understand the intricate cellular responses triggered by chemical perturbations. Then, GDSC fine-tuning refines the model's understanding by aligning it with drug sensitivity patterns across diverse cancer cell lines. We show that our model achieves state-of-the-art performance in IC50 prediction benchmark. Finally, to assess the clinical applicability of our approach, we validate the model's predictions using patient data from The Cancer Genome Atlas (TCGA) and examine whether it accurately identifies cancer drug responders from non-responders. Our results highlight the potential of leveraging a well-constructed chemical-induced transcriptomic cell state space for more precise drug response predictions for translational research.