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Commentary

Mining Multi-Omics Datasets to Reveal Drug-Target Interactions in Personalized Medicine

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DESCRIPTION

The emergence of personalized medicine has redefined the landscape of biomedical research and clinical practice, emphasizing tailored healthcare solutions based on individual genetic, molecular and environmental profiles. Central to this approach is the understanding of how drugs interact with biological targets interactions that dictate therapeutic efficacy, potential side effects and resistance mechanisms. In recent years, the integration and mining of multi-omics datasets including genomics, transcriptomics, proteomics, metabolomics and epigenomics have become indispensable tools in uncovering complex drug-target interactions that are crucial for the success of personalized treatments. These diverse datasets provide a comprehensive view of biological systems and disease states, enabling a more precise mapping between molecular signatures and pharmacological responses. Traditional drug discovery methods often rely on linear models and single-omics data, which limit the depth and accuracy of predictions regarding drug action and target identification. However, diseases such as cancer, diabetes and neurological disorders are multifactorial, involving dynamic and interconnected biological networks. Single-layer omics data cannot fully capture the regulatory mechanisms and compensatory pathways that influence drug response. Multi-omics approaches offer a holistic perspective by integrating information across different biological layers for example, connecting gene mutations (genomics) to altered gene expression (transcriptomics), changes in protein abundance (proteomics), metabolite profiles (metabolomics) and chromatin states (epigenomics). Mining these integrated datasets with computational and machine learning tools enables researchers to unravel the multilayered mechanisms of drug action and resistance in a patient-specific context.

One of the key applications of multi-omics data mining in personalized medicine is the identification of drug targets and off-target effects. By analyzing genomic mutations, transcriptomic profiles and protein interaction networks, researchers can identify not only the intended protein targets of a drug but also unintended interactions that may cause adverse effects or therapeutic failure. For instance, if a patient exhibits a specific mutation that alters the binding affinity of a drug to its target, integrating structural proteomics and genomics can predict the efficacy of the treatment and suggest alternatives. Furthermore, multi-omics analysis can uncover previously unrecognized targets by revealing correlated expression or interaction patterns across different molecular layers. Another vital application is in drug repositioning identifying new uses for existing drugs. Through mining of multi-omics signatures, especially differential expression and pathway enrichment analyses, drugs can be matched to disease-specific molecular profiles even when they were initially approved for unrelated conditions. This strategy is highly valuable in cases where conventional drug development is too time-consuming or costly, such as for rare diseases or rapidly evolving conditions like certain cancers or viral infections. Integrative data mining can link the molecular fingerprint of a disease to known drug-induced expression profiles (e.g., from resources like the Connectivity Map), highlighting candidate compounds for further experimental validation.

Advanced machine learning and Artificial Intelligence (AI) techniques play a critical role in mining multi-omics data for Drug-Target Interaction (DTI) prediction. Algorithms such as deep neural networks, random forests, support vector machines and graph-based models are used to learn complex patterns from high-dimensional omics data. These models can incorporate features such as sequence similarity, structural motifs, expression dynamics and known interaction networks to predict likely DTIs. More recently, Graph Neural Networks (GNNs) and attention-based models have been applied to represent biological entities (genes, proteins, drugs) and their interactions in graph form, enhancing the interpretability and predictive accuracy of drug-target mappings. Moreover, mining multi-omics data aids in understanding drug resistance mechanisms, which is especially crucial in cancer therapy and infectious disease treatment. Resistance often arises from compensatory signaling pathways, secondary mutations, or epigenetic modifications that bypass the

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drug's effect. By comparing omics profiles of responsive and resistant samples, researchers can pinpoint molecular alterations associated with resistance. These insights not only guide combination therapy strategies but also enable early detection of resistance biomarkers, allowing clinicians to adjust treatment plans proactively.

Public repositories such as The Cancer Genome Atlas (TCGA), Genomics of Drug Sensitivity in Cancer (GDSC), LINCS L1000 and the Cancer Cell Line Encyclopedia (CCLE) have become foundational for multi-omics-based DTI research. These platforms provide access to matched omics and pharmacological data across numerous cell lines and patient samples, enabling large-scale computational mining and hypothesis generation. Integrating patient-derived data from these sources can accelerate translational research and support clinical decision-making in personalized medicine. Despite its transformative potential, mining multi-omics data for drug-target interactions presents several challenges. One significant issue is data heterogeneity, where different omics layers may have varying levels of coverage, noise and resolution. Proper data normalization, batch effect correction and feature alignment are essential to ensure compatibility and accuracy in integration. Furthermore, missing data and small sample sizes especially in rare diseases can hinder model training and generalization. Solutions such as data imputation, transfer learning and ensemble modeling are being explored to mitigate these limitations.

Interpretability and clinical validation remain key hurdles in translating computational predictions into clinical practice. Predictive models must not only perform accurately but also offer biologically meaningful explanations for their outputs. Model transparency, feature attribution techniques (e.g., SHAP values) and integration with biological pathway knowledge are crucial for building trust and ensuring regulatory compliance. Additionally, computationally identified drug-target interactions require rigorous experimental validation using techniques such as affinity assays, CRISPR screens and patient-derived organoids. In conclusion, mining multi-omics datasets represents a powerful and evolving frontier in revealing drug-target interactions critical to personalized medicine. By capturing the multidimensional complexity of biological systems, these approaches enable precise mapping between molecular profiles and therapeutic interventions, paving the way for more effective, safer and individualized treatments. As computational tools, data quality and collaborative platforms continue to advance, multi-omics data mining will become an integral part of future healthcare, transforming how we develop and deliver medical treatments tailored to the unique biology of each patient.