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A new machine learning-based approach to drug repurposing

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A new study presents a novel approach to drug repurposing that incorporates two-stage prediction and machine learning. The study is published in the peer-reviewed *OMICS: A Journal of Integrative Biology*.

Drug repurposing is a method of developing new therapeutic use(s) for

existing drugs, for which safety and pharmacokinetics have already been demonstrated in humans. This can significantly reduce the time, cost, uncertainty, and side effects associated with drug development.

Toshinori Endo, Ph.D., from Hokkaido University, and coauthors, propose a two-stage approach to drug repurposing. First, diseases are clustered by gene expression, with the thought that similar patterns of altered gene expression imply critical pathways shared in different disease conditions. Second, drug efficacy is determined based on the ability to reverse altered gene expression, and the results are clustered to identify repurposing targets. The investigators applied their approach and identified disease-specific gene expression and 20 drugs for repurposing.

"In this study, we took advantage of the large-scale identification and integration of different levels of information and biological insights that machine learning offers," stated the investigators. "The efficiency and accuracy of drug candidate calculations were superior to those of previous studies, effectively improving the likelihood of successful drug repurposing, since all drugs were derived from agents effective against other diseases that clustered together in the same group."

"Drug repurposing is of interest for therapeutics innovation in many human diseases including COVID-19. This study brings together three strands of methodological innovation: machine learning, unsupervised clustering of gene expression, and two-stage prediction. It is a timely contribution to the drug repurposing scholarship that should broadly inform life sciences discoveries, clinical trials, and translational medicine," says Vural Özdemir, MD, Ph.D., DABCP, Editor-in-Chief of *OMICS*.

More information: Yi Cong et al, A New Approach to Drug Repurposing with Two-Stage Prediction, Machine Learning, and

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Unsupervised Clustering of Gene Expression, *OMICS: A Journal of Integrative Biology* (2022). DOI: 10.1089/omi.2022.0026

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