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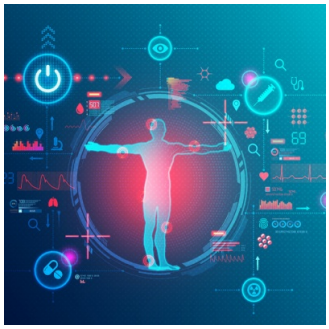
Machine Learning Identifies Promising Heart Drugs



Scientists at the University of Virginia have pioneered a novel approach to machine learning to identify drugs that could mitigate harmful scarring following a heart attack or other injuries. The team's findings have been published in Proceedings of the National Academy of Sciences (PNAS).

This innovative machine-learning tool has already pinpointed a promising candidate for minimising detrimental heart scarring, utilising a method distinct from conventional drugs. The UVA researchers believe their state-of-the-art computer model holds the potential for predicting and elucidating the effects of drugs on various diseases and explaining complex interactions within biological systems.

The research team was focused on the challenge of treating multifaceted diseases like heart disease, metabolic disorders, and cancer. Machine learning helped reduce the complexity of this process, identify crucial factors contributing to diseases, and provide deeper insights into how drugs can modify diseased cells.

According to the researchers, machine learning can assist in identifying cellular signatures induced by drugs, integrating it with human knowledge and enabling them not only to predict drugs targeting fibrosis but also to comprehend their mechanisms of action, which crucial for designing clinical trials and anticipating potential side effects.

The researchers combined decades of human knowledge with machine learning to study how drugs affect fibroblasts, cells pivotal in repairing the heart post-injury. They aimed to identify drugs capable of preventing scarring and enhancing patient outcomes.

Prior efforts to target fibroblasts and understand drug mechanisms had limitations, hindering the development of targeted treatments for heart fibrosis. To address this, the team introduced a novel approach called "logic-based mechanistic machine learning," which predicts drug effects and their impact on fibroblast behaviour.

By examining the effects of 13 promising drugs on human fibroblasts, the team trained the machine learning model to predict drug effects and cellular behaviours. For example, the model unveiled how pirfenidone, an FDA-approved drug for idiopathic pulmonary fibrosis, suppresses contractile fibres in fibroblasts, potentially easing heart stiffness. It also predicted the potential targeting of another contractile fibre by the experimental drug WH4023, validated with human cardiac fibroblasts.

While further research is necessary to confirm the drugs' efficacy in animal models and human patients, the findings suggest that mechanistic machine learning holds promise for uncovering biological cause-and-effect relationships. The researchers anticipate that this technology will advance the development of treatments for various diseases beyond heart injuries.

Source: University of Virginia
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