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A New Molecular Representation for Deep Learning of Molecular Properties Prediction and De Novo Design

A deep learning approach uses lower-dimensional molecular representations to rapidly screen small molecules for drug discovery, significantly reducing time and financial costs.

Researchers at Purdue University have developed a molecular representation concept that allows deep learning models to predict molecule properties for pharmaceuticals. Through Manifold Embedding of Molecular Surface (MEMS), molecules can be represented by electronic density and pertinent attributes, rather than atomic and bonding information. This results in a molecule that can be represented in fewer dimensions, and thus computationally simpler. By applying this approach to drug discovery, small molecules can be virtually screened against selected diseases to significantly decrease the time and financial costs of drug discovery. This technology has applications in the development of pharmaceuticals and leverages promising advances in machine learning to disrupt conventional approaches to drug discovery.

Technology Validation: This technology was validated through training a model on a curated dataset of 144 molecules. When used to predict water solubility of molecules, the model resulted in a mean absolute error reduction of 70% compared to current prediction benchmarks.

Advantages:

-Lower-dimensional representations of molecules

-Prediction of molecule properties using deep learning to reduce time and cost

-De novo design of molecules for drug discovery

Applications:

-Molecule modelling

Technology ID

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Category

Artificial Intelligence & Machine Learning/Reinforcement & Federated Learning

Pharmaceuticals/Drug Discovery & Development

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-Pharmaceuticals

-Machine Learning-Assisted Drug Discovery

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Intellectual Property:

Provisional-Patent, 2022-10-17, United States | PCT-Patent, 2023-10-13, WO | NATL-Patent, 2025-04-16, United States

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