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IIT-Madras & Ohio researchers develop new AI framework to aid discovery of next-generation drugs

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New AI framework mimics real-world chemical synthesis to generate drug candidates



Researchers from the Indian Institute of Technology (IIT) Madras' Wadhwani School of Data Science and Artificial Intelligence (WSAI) and The Ohio State University, US, have developed a breakthrough Artificial Intelligence (AI) framework that can rapidly generate drug-like molecules that are easier to synthesise in real-world laboratory settings.

The system promises to significantly cut down the early-stage timelines of drug development — currently a billion-dollar, decade-long process — and could play a crucial role in addressing drug resistance in cancer and infectious diseases.

The new framework, called 'PURE' (Policy-guided Unbiased REpresentations for Structure-Constrained Molecular Generation (SCMG), stands apart from existing molecule-generation AI tools that rely on rigid scoring mechanisms or statistical optimisation.

PURE was evaluated on widely accepted molecule-generation benchmarks, including QED (drug-likeness), DRD2 (dopamine receptor activity), and solubility tests. It delivered higher diversity and novelty in generated molecules and generated possible synthetic routes without ever being trained on those specific scoring metrics. This makes PURE a general-purpose AI engine for molecular discovery, capable of working across multiple disease and property objectives using a single trained model.

Elaborating on this Research, Prof. B. Ravindran, Head, Wadhwani School of Data Science and AI (WSAI), IIT Madras, said, "Artificial intelligence is increasingly reshaping how we think about discovery itself, and drug design offers a compelling example of that transformation. What's unique about PURE is the way it uses reinforcement learning, not just to optimize specific metrics, but to learn how molecules transform. By treating chemical design as a sequence of actions guided by real reaction rules, PURE moves us closer to AI systems that can reason through synthesis steps much like a chemist would."

This approach helps solve one of the biggest problems in AI-driven drug discovery - most AI-generated molecules look promising on a computer but are nearly impossible to synthesise in reality. PURE overcomes this by:

â®? Grounding molecular generation in real synthesis pathways

â®? Automatically learning chemical similarity instead of relying on metrics that introduce bias

â®? Suggesting viable synthetic routes along with molecular structures

â®? End Applications: faster drug pipelines and backup solutions for failing treatments