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ASIA EDITION

Scientists in Australia invent new AI tool for rapid and cost-effective drug discovery

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Enormous potential for AI to completely change the drug discovery landscape



Australian researchers, led by Monash University, have invented a new artificial intelligence (AI) tool which is poised to reshape virtual screening in early stage drug discovery and enhance scientists' ability to identify potential new medicines.

Although computational methods within drug discovery are well established, there is an indisputable gap when it comes to novel AI tools capable of rapidly, robustly and cost-effectively predicting the strength of interactions between molecules and proteins – a critical step in the drug discovery process.

The Australian invention 'PSICHIC' (PhySIcoCHemICal) brings together expertise at the interface of computing technology and drug discovery to offer an entirely new approach.

Published in *Nature Machine Intelligence,* the study demonstrates how PSICHIC uses only sequence data, alongside AI, to decode protein-molecule interactions with state-of-the-art accuracy, while eliminating the need for costly and less accurate processes such as 3D structures.

Dr Lauren May, co-lead author from the Monash Institute of Pharmaceutical Sciences (MIPS), said the team has already demonstrated that PSICHIC can effectively screen new drug candidates and perform selectivity profiling.