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ARTIFICIAL INTELLIGENCE TOOLS FOR CREATING NEW DRUGS

The pharmaceutical industry has historically relied on labor-intensive and expensive methods of the discovery new drugs, their testing and get them approved clinically. It is currently undergoing a transformational era and is at a point in its development where innovation meets the advanced capabilities of artificial intelligence (AI) and machine learning (ML) [1].

Drug discovery applications use ML algorithms such as neural networks, deep learning and natural language processing. Neural networks have an outstanding ability to analyze data, recognize patterns and make predictions. The process of drug discovery using AI involves many tools and programs (table).

Table – AI tools and programs using for the drug discovery [2 – 4]

Features	Tools and programs
1	2
Prediction of the protein space structure	AlphaFold (protein structure database)
Assessment of the affinity of protein binding to a ligand	DeltaVina, NNScore (neural-network-based scoring function for the characterization of protein-ligand complexes), PotentialNet
Prediction of molecular attributes and analysis of molecular structures	Conv_qsar_fast
Prediction chemical, physical and biological properties	QSAR (quantitative structure-activity relationship), InnerOuterRNN (inner- and outer recursive neural networks for chemoinformatics), Neural Graph Fingerprints models
Searching for or designing molecules with the most optimal specified properties	chemical_VAE (chemical variational autoencoder), JunctionTree VAE (junction tree variational autoencoder for molecular graph generation), ORGANIC
Synthesis of new compounds and molecular modeling	Chemputer, ODDT (open drug discovery toolkit), SCScore (synthetic complexity learned from a reaction corpus)

1	2
Prediction the effect of a particular substance on the human body	PPB2 (the polypharmacology browser 2)
Toxicological effect assessment	DeepTox (deep learning for toxicity prediction), Tox21 (the toxicology in the 21st century)

Thus, AI systems can process vast molecular databases to predict new drugs that will work effectively while avoiding toxic side effects. The integration of AI and ML in the pharmaceutical industry can change the approach to drug discovery, improving both the speed and efficiency of drug development.

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