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Recent advances in drug discovery and development

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Drug discovery and development is usually a tedious process where researchers discover new drugs through insights into molecular mechanisms or by identifying novel biomolecules. This process typically takes over 14-15 years. However, due to the advancements in technology, computer-aided drug design can be utilised along with high-throughput screening to identify novel therapeutics with high accuracy and speed. Molecular docking is one such method that has been widely used for the prediction of adverse effects, polypharmacology, medication repurposing, target fishing and profiling. In contrast to traditional methods of discovering one ligand at a time, ligandomics is a new technology that can map disease-specific cellular ligands in the absence of molecular probes. Further, the attractor theory-based drug discovery methodology suggests novel approaches to target identification, drug development and drug combination design. Moreover, structure-based drug design is becoming a crucial tool for faster and cost-effective lead discovery. isoTOP-activity-based protein profiling (ABPP) is a chemical-proteomic platform that allows for cysteine reactivity profiling in complex proteomes. It is one of many approaches that help in two areas of the covalent-inhibitor development process.

Additionally, in traditional in vitro cell culture techniques, cultured cells frequently lose their natural organ functions and morphologies. Researchers can conduct large-scale in vivo screening to uncover therapeutic candidates in insects, since insects offer several advantages over experimental animals, including the minimal cost of rearing and few ethical considerations. Furthermore, spheroids, organoids, scaffolds, hydrogels, organs-on-chips and 3D bioprinting are examples of pioneering 3D cell culture technologies that have enhanced drug discovery. Recently, the “big data” concerns have arisen as a result of genomic, proteomic and structural studies. The creation of large data warehouses and bioinformatics algorithms is essential to analyse big data. These bioinformatics algorithms are also capable of identifying novel drug targets and/or biomarkers, programs to assess the tractability of targets and predict repositioning opportunities that use licensed drugs. Besides, target validation, identification of prognostic biomarkers and analysis of digital pathology data in clinical trials are all aspects of machine learning (ML) applications. Therefore, novel computational biology technologies have revolutionised drug discovery and development with the help of artificial intelligence.

Keywords: Molecular docking, Ligandomics, Nuclear magnetic resonance, Phenotypic screening, Bioinformatics, Artificial intelligence

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