Drug Development in this New Era

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From the ancient period of drug development, where Phyto compounds were used as drugs, the advancement in this modern era of drug development mainly focuses on Artificial Intelligence and computational techniques in drug development and design. Drug synthesis has improved since the introduction of combinational chemistry, where thousands of chemical reactions can be performed simultaneously using small reaction vessels. The best one or the lead molecules from the synthesized compounds can be further tested in animals or humans for the desired biological action. Insilico screening methods can achieve this. By selecting the target receptor of the drug, several synthesized molecules from combinational chemistry can be screened, as well as unwanted compounds with no biological activity. This eliminates the need to use colossal animal testing models, which reduces cost and time. Molecular docking is an insilico method using different algorithms. The software gives results such as binding energy, type of interactions, and RMSD or RMSF, which will help predict effective, stable binding and rank different compounds based on the desired biological activity.

Chemical databases record information about plant phytoconstituents, etc. Hence, AI has proven to predict and calculate the efficacy of synthesized compounds or plant products, accelerating drug development and formulation. Stimulated drug interaction, 3D cell culture modes, Biomarker development, Genomics, and Proteomics have been the Hallmarks of drug development in this new era. AI and computational methods have changed the pharmaceutical industry. They have helped pharmaceutical companies introduce new drugs to market quickly. The COVID-19 vaccine is a typical example of this.

Personalized medicine approaches, tailored for a particular person and giving a suitable dose for a specific disease, are now being used in practices. Drug re-profiling is a process where new therapeutic uses of existing drugs are ruled out. This helps to reduce further pre-clinical testing. An example of drug repurposing is the case of Sildenafil, which was introduced for pulmonary hypertension. Later, it was used for erectile dysfunction, and now the new therapeutic use for Sildenafil is anti-cancer therapy. Artificial Intelligence has reduced the time for processing a huge amount of data, like patients' clinical history and ADME parameter records.

Drug design has come a long way, incorporating scientific advancements to improve human health. Technologies are evolving, leading to the development of more precise and personalized medicines.